BIOCHEMICALLY REALISTIC MD AND KINETIC MODELS OF THE *RHODOBACTER SPHAEROIDES* BC_1 COMPLEX

BY

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DISSERTATION

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Abstract

This work seeks to duplicate a realistic membrane for a more natural model of the *Rb. sphaeroides* bc_1 complex which in past studies has lacked several details in composition of the fatty acids and relative quantities of each lipid. Past studies have shown some distortion on MD relaxation relating to a large void volume in the protein structures. In this model we have set up the membrane with the complement of lipids reported for the chromatophore membrane, and have taken steps to ameliorate the structural distortions on relaxation of the protein by populating the void with a complement of lipids. The MD model is used to determine diffusion constants and motions of the system in preparation for calculating potentials of mean force for wild type and ISP tether mutants. The current kinetic model provides a kinetic and thermodynamic understanding of the rate-limiting reaction, and associated partial processes that lead to successive turnovers. Since both bacterial and mitochondrial complexes have essentially the same catalytic core, their mechanisms are essentially similar, and a better understanding of the bacterial system can be extrapolated to the context of mitochondrial function, and medically important roles in cellular physiology, cardiovascular disease, apoptosis, and diseases associated with aging.

Dedication

Neil M. Rose (in memory of my father) and Patricia M. Rose (mother)

Kristi Buhr (girl friend)

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Table of Contents

Chapter 1 Biochemistry of the *bc1* Complex[1]

Overall Aims

Electron transfer is central to energy conversion in all biological systems, and a fundamental aim of biophysics is to understand the physical laws that describe it. One approach to the elucidation of principles of electron transfer is by constructing models, but, for a particular system, these can represent many different levels of complexity. In this study, I have constructed realistic models of the *Rhodobacter (Rb.) sphaeroides* cytochrome bc_1 complex at structural and mechanistic levels. The structural model incudes the protein in a membrane separating aqueous phases, and is based on crystallographic data for the protein and biochemical literature on the native composition of the lipid membrane, taking care to deal with problematic features from previous studies. Under an XSEDE preliminary grant, our molecular dynamics (MD) model has been equilibrated using energy relaxation and MD simulation, and will provide a platform for atomistic studies. Although the operation of the cytochrome bc_1 complex has been extensively studied, many aspects are still controversial. Our current kinetic model is based on extensive physicochemical studies over the last 40 years. In its present form, it provides a kinetic and thermodynamic understanding of the rate-limiting reaction, and associated partial processes that lead to successive turnovers (the model is of the protein with antimycin bound, which inhibits oxidation of heme b_H via the Q_i-site). The aim is to integrate models at these two different levels of understanding so that they can be used to explore mechanism more deeply at the atomistic

[1] Some of the material presented in this chapter was previously published 5. A. R. Crofts, Lhee, S., Crofts, S.B., Cheng, J. and Rose, S., Proton pumping in the bc_1 complex: A new gating mechanism that prevents short circuits. *Biochim. Biophys. Acta* **1757**, 1019-1034 (2006).

level. An important parameter in Marcus' theory is the reorganization energy, λ, associated with dielectric response of the protein and solvent. We will determine from MD simulation the changes in electrostatic contour within the protein on change of state of redox centers involved in catalysis, and how the protein/solvent dielectric responds. We will explore changes in local structure on *in silico* mutagenesis to understand changes in function introduced. We will use umbrella sampling to follow diffusional processes. We will explore coulombic interactions that might be important in control. In the longer term, since a global model can be refined iteratively, an improved model will reflect an increasing level of understanding that can be exploited in design of experiments. Since both bacterial and mitochondrial complexes have essentially the same catalytic core, their mechanisms are essentially similar, and a better understanding of the bacterial system can be extrapolated to the context of mitochondrial bc_1 complex function, and medically important roles in cellular physiology, cardiovascular disease, apoptosis, and diseases associated with aging.

As our theoretical understanding of electron transfer pushes further into the quantum realm, it becomes clear that, at least in complex systems, there are limits to what we can *measure* in the atomistic domain with current technology. Although the Q-cycle mechanism of the bc_1 complex can be represented in kinetic models by measured rate constants and thermodynamic constraints for the main reactions, many partial processes are inaccessible to direct experimental investigation because they cannot be observed. These limits reflect both instrumentation, and the scale of computational models and calculations. The proton-pumping activity of the bc_1 complex is driven by redox free energy, and involves proton coupled electron transfer. Coupling can involve transfer of proton and electron through a common pathway, or through separate pathways, with very different coulombic consequences, playing directly into involvement of dielectric response in protein and solvent, and hence the role of reorganization energy, λ. In

addition, the Q_o-site reaction involves at least two partial processes involving substantial molecular displacements. Best characterized is the rotational displacement of the extrinsic head domain of the Rieske iron-sulfur protein (ISP) through ~30 Å to transfer an electron from QH_2 to heme c_1. It also seems likely that the $Q^{\bullet}$ intermediate formed in that reaction diffuses in the Q_o-site to bring it closer to its electron acceptor, heme b_L to facilitate rapid electron transfer. In the present model, these are both modelled as diffusional processes. Processes like diffusion can occur over an extended period of time out of range of calculation or modeling, but they can be tested in molecular dynamics simulation by constrained energy sampling techniques. These can provide important constrains to realistic models, and simulation can recover important information about energies and reaction path. The purpose of the present study is to produce an improved model of the cytochrome bc_1 complex of *Rb. sphaeroides* and then use it to calculate biophysical quantities related to the enzymatic and redox activity of the complex and its linkage to substrates, ubiquinone(Q) and ubiquinol(QH_2) and cytochrome c_2.

The kinetic model is currently under revision to extend the treatment of control and gating processes. These have been explored in recent work on longevity on mutation of the Rieske iron-sulfur protein (ISP) (strain *isp-1(qm150)*) in *C. elegans,* and suppressor strains in the same subunit. The work revealed that a spring-loaded mechanism, previously proposed on the basis of similar mutations in bacteria, could explain the data (*6, 7*). In the context of the forward chemistry, the spring-loaded control revealed subtler gating processes needed to minimize production of reactive oxygen species (ROS), but not yet incorporated in the model. In addition, we will incorporate information from the thesis work of Rodney Burton, which has shown a novel intermediate ISPH.SQ complex at the Q_o-site, generated under conditions in which the SQ can accumulate.

Biological Background

Variants of the bc_1 complex are redox driven proton pumps that operate in mitochondria, chloroplasts and many aerobic or photosynthetic bacteria as a central component of the main energy conversion processes of the biosphere. The mitochondrial bc_1 complex, more formally ubihydroquinone: cytochrome c oxidoreductase, is of interest from a human perspective because, in addition to its primary functions in energy conversion, its short-circuit reactions generate ROS. Generation of ROS is linked to cellular damage, and hence linkage to the aging process, cardiac disease, stroke, etc., and to interest in the control and gating processes associated with amelioration of these conditions. The complement of subunits increases with increased cellular complexity, but always contains a catalytic core of three subunits that carry the redox centers involved in the Q-cycle function. The bc_1 complex sits in the membrane and generates a proton gradient across the membrane coupled to the redox reaction. The resulting proton gradient provides an energy source for important energetic processes such as synthesis of ATP.

Structure of the bc_1 Complex and Modified Q-cycle Mechanism

The complex in both mitochondria and bacteria is a homodimer, with a catalytic core of three subunits in each monomer, cytochrome (cyt) *b*, cyt c_1, and ISP. In some bacterial complexes, no other subunits are structurally defined, but in *Rhodobacter sphaeroides*, the complex has an additional subunit (SU IV) of uncertain function. Mitochondrial complexes have up to 8 additional subunits. For some the function is known, for many uncertain (*8-11*), but none are directly involved in catalysis.

The bc_1 complex in both mitochondria and bacteria is a homodimer with two identical monomers. The monomers are related by two-fold symmetry having an axis extending through the membrane plane and normal to the surface. The dimeric complex has two catalytic cores,

and each core consists of three subunits cytochrome (cyt) *b*, cyt c_1, and ISP. In bacteria, each monomer has the three protein subunits of the catalytic core, and sometimes (as in *Rb. sphaeroides*) an additional subunit IV, not yet seen in crystallographic structures.

The Q-cycle function of the bc_1 complex is illustrated in Fig. 1.1, left. The schematic drawing from the PROMISE site, right, outlines the electron transfer centers. The side of the membrane on top is the matrix space of the mitochondria or the outside of the chromatophore (N-phase), and the bottom side is the intermembrane space (P phase) or inside of the chromatophore. Here, N and P refer to positive and negative values for proton potential, $\Delta p = \Delta\psi - Z\Delta\text{pH}$, where $Z = 2.303RT/F \approx 59$ mV at 25° C. The function described is for the operation of one monomer of the dimer in a modified Q-cycle.

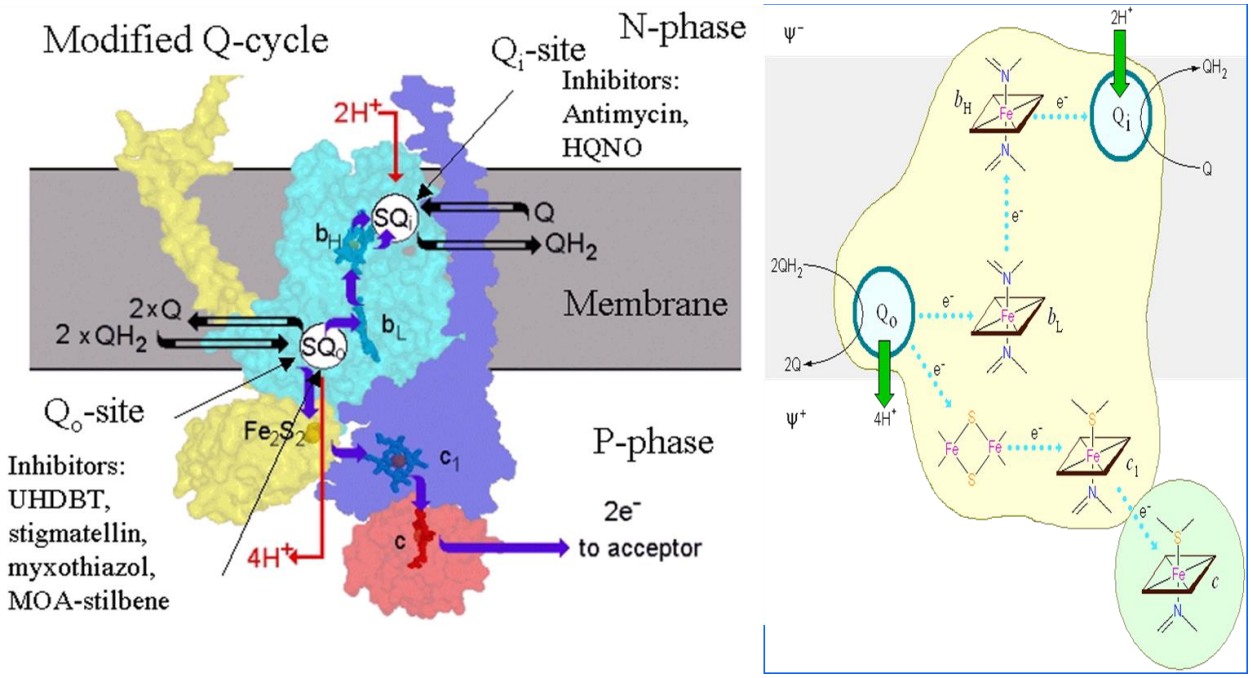

Figure 1.1 On the left is a sketch of the modified Q cycle superimposed on the structure of catalytic subunits of the bovine *bc_1 complex*. On the right is a schematic diagram of the redox centers involved.

In the Q-cycle mechanism, oxidation of quinol, QH_2, and reduction quinone, Q, occur at physically separate sites in the bc_1 complex. This absurd and apparently futile reaction is redeemed by the topology and stoichiometry, to achieve the transfer of H^+ across the membrane.

At the Q_o-site quinol is oxidized to quinone, with release of $2H^+$ to the P-phase; and at the Q_i-site (on the other side of the insulating phase), Q is reduced to QH_2, with uptake of $2H^+$ from the N-phase. At the Q_o-site, quinol is oxidized first by the Fe_2S_2 cluster in the extrinsic domain of the Rieske iron sulfur protein (ISP) which then moves away to transfer the electron to the heme of the cytochrome c_1 and release the proton. The bound heme c_1 then reduces the soluble cyt *c*. The initial product of this first electron transfer, the neutral semiquinone, $QH^{\bullet}$, at the Q_o-site, is then oxidized by heme b_L of cyt *b*, which passes the electron on to the Q_i-site via heme b_H. This bifurcation of electron transfer, with the first electron going down one path toward the cyt *c* and the second electron down the other path through cyt b_L, known as the bifurcated reaction of the Q_o-site, is the rate limiting process under conditions of substrate saturation. The key to understanding the process is that only one of the electrons from the two from a single quinol crosses the membrane. Since it takes two electrons to reduce Q to QH_2, the Q_o-site has to turnover twice in order for the Q_i-site to complete the reduction. Although 2 protons are taken in at the Q_i-site from the N-phase (outside of the chromatophore) on reduction of Q, and $4H^+$ are released to the P-phase (inside the chromatophore) on oxidation of $2QH_2$, the charges are moved on the 2 electrons crossing the membrane in the *b*-heme chain, effectively from P- to N-sides. The chemistry at the two sites is electroneutral.

Proton pumping is achieved indirectly by movement of two negative charges across the membrane, carried by the electrons passing through the cyt b-heme chain from Q_o-site to Qi-site, and by release or uptake of H^+, respectively, on oxidation or reduction of quinone, to give an overall yield of $2H^+$ pumped for each QH_2 oxidized:

$$QH_2 + 2\text{cyt } c^+ + 2H^+_N \rightleftharpoons Q + 2\text{cyt } c + 2H^+_P + 2H^+_P(\text{scalar})$$

In chromatophores, the electrogenic processes can be followed through the electrochromic carotenoid changes, which provide a "membrane voltmeter" function (*12*), and this convenience has allowed a detailed matching of electrogenic events to partial processes (*13*), (*12*), (*14*) and (*15*). By careful correction of absorbance changes in the cytochrome α-band region for contributions from carotenoid changes (*16*), this approach was extended to measurement of driving forces from electron transfer during development of the proton gradient in the coupled steady-state (*17*), (*18*), and (*19*). Under static head conditions, the poise of the electron transfer chain was close to that expected from the modified Q-cycle in equilibrium with the proton gradient, indicating a tight control. These results were in line with results from mitochondrial studies (*20*) in which the proton gradient was varied through poising of the ATPase reaction. In the chromatophore experiments, the development of both electron transfer poise and proton gradient could be resolved kinetically.

Enzyme-substrate Complex of First Turn Over at Qo site

The first electron transfer is the transfer of one electron from the Q_o site substrate, quinol (QH_2) to the ISP. Because the ISP extrinsic domain is mobile, it acts as a diffusible second substrate (albeit, a tethered one) in the reaction at the cyt *b*-interface, so that the binding of two substrates, ISP_{ox} and QH_2, is needed for formation of the enzyme substrate (*ES*-) complex. The ISP head group is docked to the Q_o site against cyt *b* and seems to be held in place in part by hydrogen bonding to the Q_o site occupant. The PDB file 1ntz has coordinates (with high B-factors) for a quinone occupant, but the experimental basis for these has not been discussed by the authors (*21*). None of the other structures currently available shows any quinone species bound at the Q_o-site. Therefore, modeling of quinone or quinol occupancy is based on occupancy of inhibitors.

Because the rate-limiting reaction involves reduction of the oxidized ISP (ISP_{ox}), requiring a relatively short electron transfer path, the most obvious choice of bound inhibitor structure has been the stigmatellin structure, which shows a direct H-bond between N_ε of His-152 of the reduced ISP (ISPH) and a carbonyl group of the Q_o-site occupant. A quinol modeled with H-bonds to the same ligands as stigmatellin can replace the inhibitor in the structure without strain, and fits within the electron density of the inhibitor (*22*) and (*2*); the quinone species modeled in 1ntz is in a similar configuration. Models of this sort have been the starting point for most discussions of the *ES*-complex (*23*), (*2*), and (*24*). The relative pK values for quinol (pK >11.5) and ISP_{ox} (pK_{ox1} ~7.6) would favor an H-bond with the quinol –OH as donor, and the N_ε of His-152 of ISP_{ox} in the dissociated form as H-bond acceptor.

From the kinetics in chromatophores of the oxidation of the bound cyt c_1 and cyt c_2 in the uninhibited complex, or with different inhibitors bound, it could be concluded that for all complexes with ISPH initially bound with Q in the Q_o-site (the ISP*b* configuration), the reaction time for oxidation of the ISPH complex is relatively rapid with a half-time in the range <30 μs (*4*); a more precise value (~10 μs) was subsequently determined in the isolated complex using flash-excitation of a ruthenium dimer bound to cyt c_1 (*25*). The Rieske ISP protein consists of three portions. One portion is an inter membrane helix anchoring the protein (resid 9-37 in the *Rba. sphaeroides* numbering). A tether region (resid 37-49) attaches the head group (resid 49-187) to the anchor portion. The ISP head group constitutes the mobile domain because its movement delivers an electron to cyt c_1 in a rapid process which is not rate limiting. The ISP head group moves from a position proximal to the cyt *b* and binding the quinol substrate to a second position proximal to the bound cyt c_1. The distance traveled by the ISP head group is thought to be in the range of 16 to 22 Å. This distance is defined around the pivot of the tether region which seems to flex in response to the release of the ISP head group from the cyt *b*

position to the position close to the cyt c_1. This motion will be further explored in Chapter 6 and defined in the context of the model generated and discussed therein.

The Q_o-site is the catalytic site where the quinol is oxidized to form quinone. The Q_o-site is located in cyt b and has a larger volume than one quinol head group. Accordingly, the regions within the Q_o-site are designated proximal and distal domains with respect to heme b_L. The occupancy of these domains has been model in terms of the reaction coordinate. The *ES*-complex with QH_2 H-boned to H152 of ISP_{ox} must be in the distal domain, and the SQ product of the first electron transfer, initially the neutral $QH^{\bullet}$, must be formed in the distal domain, but likely diffuses to the proximal domain (a distance of ~5.5 Å) to facilitate rapid electron transfer. The subject of much of this work focuses on the *ES*-complex from which for the first electron transfer on oxidation of the quinol occurs. After the first electron transfer, the SQ intermediate separates from the ISPH, a proton is released and transfer of the second electron to heme b_L occurs. However, the sequence of events is not known. Most of the evidence suggests that the proton from $QH^{\bullet}$ is released early, and the semiquinone anion ($Q^{\bullet-}$) moves, but scenarios in which the neutral semiquinone ($QH^{\bullet}$) separates from the ISPH, and then moves to donate the electron to heme b_L cannot be ruled out. In either case, all these rearrangements lead to a molecular ballet, which results in the rapid transfer of a second electron up the low potential chain of hemes in cyt *b*. The proton released on oxidation of $QH^{\bullet}$ leaves the Q_o-site through a group of residues, - Y147, E295, N279, - connected to a water chain through the protein to the P–phase water, which also connects to R94 and the heme propionates. Transfer of the electron and release of the proton leaves the quinone in the site to diffuse out and be replaced by another quinol to be oxidized in a second turnover of the Q_o-site reaction.

The different scenarios for the sequencing are discussed in (*26*), based on recent information from experiment and MD simulation. A rate constant for oxidation of SQ_o has been

determined in a mutant strain E295W, in which the bulk of the sidechain likely constrains it to the distal domain. The rate of reduction of heme b_L was so severely inhibited that the heme remained oxidized over the time in which SQ_o occupancy could be measured. The value estimated for *k* was ~10^3 s^{-1}, 1000-fold too low to account for the rate observed in wildtype at the occupancy expected in normal flux. The paradox could be resolved if the SQo could move closer to heme b_L. Movement to the proximal volume occupied by myxothiazol in known structures, a distance of ~5.5 Å, would increase the rate constant to k ~4×10^9 s^{-1}. Such a movement would require rapid diffusion in the Q_o-site volume, and our MD simulations have allowed us to estimate a value. What remains to be determined is the point in the sequence at which the H^+ is released from the initial neutral form, $QH^{\bullet}$.

The two cyt *b* hemes, cyt b_L (low E_m ~-90 mV) and cyt b_H (higher E_m ~40 mV), are arranged along the path (the low potential chain) from the Q_o-site to the Q_i-site (see Fig. 1.1 and Fig 1.2), where reduction of quinone to quinol by two electrons coming from the b_H heme occurs. The requirement for two electrons from the low potential chain means that two quinols must be oxidized in the bifurcated reaction at the Q_o-site and transferred to the Q_i-site to complete the reaction there. The kinetic model previously proposed, and further extended here, is intended to simulate experimental conditions under which kinetic parameters were determined as will be discussed in greater detail with respect to the outcomes of the studies described herein. Most of the experimental data was generated with chromatophores using inhibitors, especially antimycin, to observe the accumulation of reduced hemes under various conditions after flash activation. Antimycin is an inhibitor at the Q_i-site that blocks the transfer of electrons from the heme b_H in the low potential chain by displacing quinone. In the MD model through which we are investigating atomistic processes, we have also simulated these experimental conditions by modelling antimycin in the Q_i-site. This allows us to examine changes in configuration

associated with different binding partners in protein surrounding the Q_i-site when Q is replaced by the inhibitor, and their role in the trajectories produced herein.

Crystallographic Void in the *bc₁* Complex and Chromatophore Membrane

Previous MD simulations of the *bc₁* complex have been based on non-native membranes, and have in some cases incorporated an artificial feature of the crystallographic structures, which has led to some distortion on MD relaxation. This latter problem relates to a large void volume in the protein structures, likely resulting from disorder of the endogenous material, likely lipid, filling the void. In the *Rb. sphaeroides* model proposed here, we have set up the membrane with the complement of lipids reported for the chromatophore membrane, and have taken steps to ameliorate the structural distortions on relaxation of the protein by populating the void with a appropriate lipids. These two steps provide an improved model, and we expect that this will give us a more realistic picture of the functional operation of the protein, and of a more native environment for interaction of the protein and its reactants.

Most MD simulations start from the crystallographic structures, which are artificial in that they are frozen in a lattice constrained by contacts with neighboring components of the unit cell. For membrane proteins, the prison is even more unnatural. There is no membrane, but instead ancillary lipids, detergent molecules, and waters filling the interstices. The MD simulation is set up to liberate the native structure from this prison, an essential preliminary to mechanistic exploration. Crystallographic models of the bc_1 complex from vertebrate mitochondria or bacteria show in the dimeric structure a substantial volume in the dimer interface, to the N-side of the closely packed protein interface between the b_L hemes, which is devoid of resolved structure (Fig. 1.2). It is unlikely that this void represents a vacuum. In support of this, in higher resolution structures of the yeast mitochondrial complex, electron

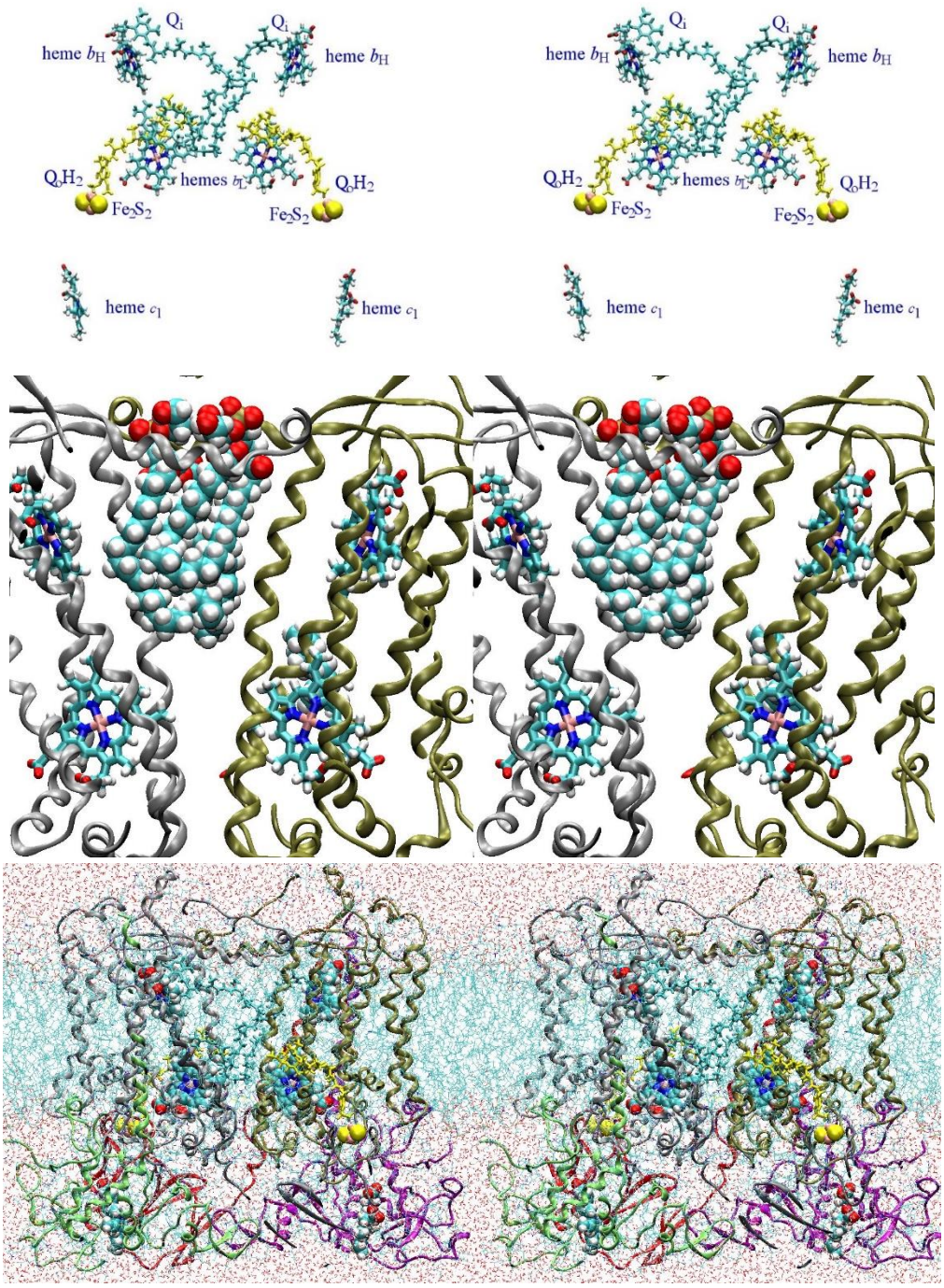

Figure 1.2 Cross-section through the MD model of the *Rb. sphaeroides* bc_1 complex after 31 ns of a production run. A (top). The initial occupants were replaced by parameterized molecules, with ubiquinone (Q_i) in the Q_i-site and ubiquinol (Q_oH_2) in the Q_o-site. A slice through the protein, shown as a cartoon, reveals the prosthetic groups colored by chain, embedded in the membrane between aqueous phases, with lipids and waters represented by lines for the bonds. The redox centers are shown by VDW spheres (for hemes and 2Fe2S-cluster), or by licorice bonds, colored as below. The "void" is the ∇-shaped space defined by a scaffold of membrane spanning and transverse amphipathic helices (center, top of protein), here occupied by lipid. (Stereo pair for crossed-eye viewing.) B (center). The protein stripped away to show the redox centers, to facilitate identity: all redox groups except Fe_2S_2 are shown by licorice bonds, the hemes are in CPK colors; QH_2 at the Q_o-site is yellow; Q at the Q_i-site is cyan; the Fe_2S_2 cluster is shown by VDW spheres. C (bottom). The same view of the protein, but zoomed to highlight two lipids (phosphatidylglycerol, shown by van der Waals spheres) occupying the void, with the *b*-type hemes (licorice bonds, CPK colors) for reference, and the scaffolding helices, showing how exchange of phospholipids would be impeded at the head group level. Structure taken from the trajectory exploring formation of the *ES*-complex, at a frame ~31 ns, when the bond to H152 had stabilized.

density in the site has been resolved, and specific phospholipids identified. One cardiolipin

molecule occupies the central cavity, and tails from other lipids contribute more peripherally (*27, 28*). The protein scaffold supporting this volume, transmembrane helices, including those binding the hemes, and transverse amphipathic helices at the level of the hydrophilic head groups, one from each monomer, restricts access at this level, but allows access from the hydrophobic lipid phase (Fig. 1.2, bottom). The former restriction might be expected to impede ready diffusion of phospholipid from the membrane into the volume. It has also been suggested that the head groups of other cardiolipins play an important mechanistic role in directing protons to the quinone reduction reactions at the Q_i-site (discussed further below).

In earlier reports, and in two more recent MD simulations accessible to the author, it was assumed that the problem of the void would be addressed by "the physics", as explored in MD simulation. In the earlier work, simulations were two short to reveal problems, but in the longer explorations possible now, the MD eliminated the void artificially. In one case, this was by partial collapse of the protein. Significantly, during 350 ns of simulation, although lipid tails explored and partly filled the volume, no phospholipid molecule diffused in. In another case, the void was filled by flooding with waters. Neither of these physical solutions is likely to be natural. In the former case, a partial unfolding of one of the transverse helices from the scaffolding seen in the crystallographic configuration disrupted the volume around one Q_i-site of the complex, precluding application to mechanistic studies involving that volume. In the latter, the waters would have introduced a high dielectric phase in a volume lined by hydrophobic residues suitable for lipid interactions. This volume is also close to the Q_i-site, which would significantly change the physical chemistry of the site. However, the focus in both the papers was the Q_o-site reaction, and since this is on the other side of the protein from the Q_i-site, it was supposed that disruption of structure at the later would have little effect on the former. The problem of eliminating the void has been averted in simulations from the Róg group by introduction of a

cardiolipin molecule to occupy the void (*29, 30*), effectively simulating the yeast configuration in a *Rhodobacter capsulatus* bc_1 complex.

A second set of problems lies in representation of the native membrane. Early MD simulations of the mitochondrial bc_1 complex had used a simple POPC membrane (*31*), still preferred in some recent efforts using a *Rhodobacter* complex (*32*). A more natural membrane model was introduced by Postila et al. (*29*), with a composition based on that of mitochondrial membranes, also adopted in the recent simulation in collaboration with our lab (*33*). In addition to a different complement of lipids, with different location of the unsaturated bond, in equilibrating the membrane model, forces unfortunately came into play that converted the *cis* fatty acid sidechains to the unnatural *trans* configuration, thereby substantially altering the membrane properties. Whether or not this was important to simulation of function is not clear. The *Rhodobacter* are versatile bacteria, and like many other bacteria, can adapt their membrane composition to cope with environmental stress. For example, under phosphate-limited growth, much of the phospholipid component of the *Rb. sphaeroides* membrane (though not cardiolipin or phosphatidylglycerol) was substituted by non-phosphorus glycolipids, strains can be engineered mutation to eliminate synthesis of cardiolipin from phosphatidylglycerol (CD^- mutant). These conditions have been used to explore the dependence of growth, expression of cytochromes, and activity of respiratory and photosynthetic chains on membrane composition. The tested parameters were not attenuated, even when the CD^- mutants were grown under phosphate limiting conditions (*34, 35*). The only phospholipid present under the latter conditions was phosphatidylglycerol. In light of this versatility, it is not obvious that modifications in lipid content would alter the protein behavior. Nevertheless, a natural membrane is obviously preferable. Of special interest is the high ubiquinone content of the native membrane. Any

natural simulation should at least include this component, even though the diffusional processes involved in substrate or product activities are not yet accessible on the MD time scale.

The idea that the void discussed above is of importance physiologically as a chamber in which quinone species can be stored, allowing easier access to the catalytic sites, has been popularized in textbooks. Since the sites are also exposed through a more favorable diffusional path to the membrane lipid, and the ubiquinone is present in >30-fold excess over the complex (*36-38*), such a special function might seem superfluous. It seems much more likely that the void

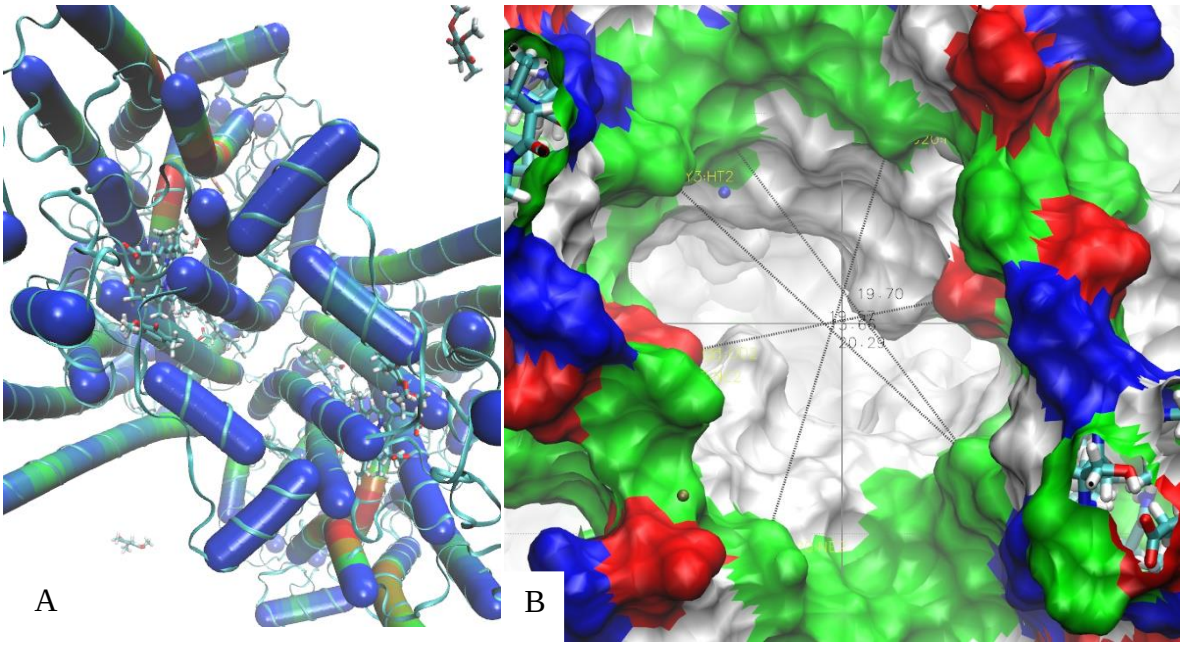

Figure 1.3 A) View of void present in coordinates from crystal structure; and B) same view as (A) except rendered with Quick Surf and measurments added

is accounted for by disorder in lipids which were naturally incorporated on assembly of the complex (perhaps including quinone species), which were not detected by X-ray diffraction. Indeed, as noted above, a more stable structure has been achieved in *Rb. capsulatus* models by populating the void by a cardiolipins (*29, 30*), as seen in the yeast complex.

Figs. 1.3 A and B show the void in the middle of the bc_1 complex crystal structure which was the starting point for the model of Fig 1.2 (accession code 2QJY) . Since nature abhors a vacuum, it has been assumed there detergent or lipids would fill this volume, which if

disordered would fail to be resolved as structured electron density in the X-ray crystallography study. As noted above, in earlier MD modeling studies of bc_1 complex in a solvated membrane system, the backbone was released early in the simulation with the void empty. In one study the site was flooded with water during the simulations and the protein collapsed inwards to reduce the void volume compared to the original crystallographic model (*32*). Another study found that reconfiguration of the protein around the void led to the collapse of the transmembrane helices inward and unfolding of one of the helices bordering the entry to the opening of the void from water layer (*39*)

Fig 1.3 A shows the view of the protein from above with helices depicted as tubes with ribbons wrapped around. Fig 1.3 B, from the same perspective, shows the central opening into the void with the protein rendered by its surface and distances between various points in a range close to where the membrane head groups line up in the membrane. The approximate dimension of the opening is 18 A by 20 A or 360 A^2. Lipid head groups occupy roughly 40 A^2 of surface area, so theoretically 9 lipids could be fit in. The space under the opening is shared by crossing alpha helices, and quinone/quinol so as a guess it would seem that there would be fewer than 9 membrane lipids. Leaving the void empty when the backbone is released has produced the artifacts mentioned in the previous paragraph. Two membrane lipids were inserted into the void in preparation for minimizing the combined protein, water, substrate, and membrane system.

Chapter 2 Methods and Materials

We have developed a new MD model using the *Rb. sphaeroides* bc_1 complex, in which the protein environment has been modeled in a native membrane, including ubiquinone. Under a startup XSEDE grant, we have validated the model running in the STAMPEDE environment, minimized energies, run equilibration protocols, and we have tested scaling parameters, and are currently using the refined model in production runs to explore mechanism at the atomistic level under additional XSEDE support.

Local computing resources were used for setting up structure files and testing whether system setups will run and begin equilibration but because of the size of the complete model (312,180 atoms) supercomputer resources are required to equilibrate and run the system and perform the associated calculations. This work uses the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation grant number ACI-1053575(*40*). We received a startup allocation of 50,000 SUs of resources on Stampede in order to perform the minimization, restrained equilibration and initial runs described below. The Stampede platform is a TACC Dell PowerEdge C8220 Cluster with Intel Xeon Phi coprocessors. In order to perform these runs Python scripting was used to generate generic configuration files that were run in batch mode. The remote job submission was managed on the XSEDE platform by the Simple Linux Utility for Resource Management (SLURM) which is an open source, highly-scalable resource management and job scheduling system for submitting, executing, monitoring, and managing batch jobs (typically, parallel jobs) on high-performance Linux clusters.

Once the system was found to run on the local system then configuration scripts were prepared for the Stampede platform and SLURM scripts were prepared for remote batch

processing through XSEDE. The NAMD molecular dynamics (MD) package has historically had efficient performance on XSEDE resources. Fig 2.1 shows scaling calculations performed on TACC Stampede using NAMD 2.11 with a 1 fs time-step on the 312,320-atom system with a range of nodes. These were the second set of scaling calculations which were performed after changing the occupants of the Q_o-site from stigmatellin to quinol which changed the number of atoms from 312,180 to 312,320. Efficiency was calculated per node, $Efficiency = (T_{1\ node} \times N)/ T_{N\ nodes}$, where $T_{1\ node}$ is the simulation time on a single node (16 cores on Stampede) and $T_{N\ nodes}$ is the simulation time of the same systems on N nodes. With the molecular system in use, Stampede demonstrated efficiency of more than 74% for calculations on 256 - 400 cores (16 to 25 nodes).

Using 320 cores 7,903 SUs will be consumed for a 10 ns simulation.The visualization package VMD(*41*) and its associated plugins are used to visualize the model and results from the plugins. NAMD 2.11 (*42*) which was used for molecular dynamics calculations is a highly parallel, publicly available MD program, with demonstrated scalability on all XSEDE platforms.

Simulations involving lipids use the latest CHARMM36 force field in which the problem with consistency of lipid density has been resolved (*43*). The simulations with proteins and prosthetic groups will use CHARMM36 force field with CMAP corrections (*44*), supplemented by custom built topologies(*45*) (Appendix A and Appendix B). Water molecules are represented explicitly by the TIP3P model (*46*). In all simulations the temperature was maintained constant at 310 K using Langevin dynamics with a damping coefficient of 1 ps^{-1} and the pressure at 1 atm using the Langevin Nose-Hoover method (*47, 48*). Long-range electrostatic forces will be calculated without truncating using the Particle Mesh Ewald (PME) method (*49*).

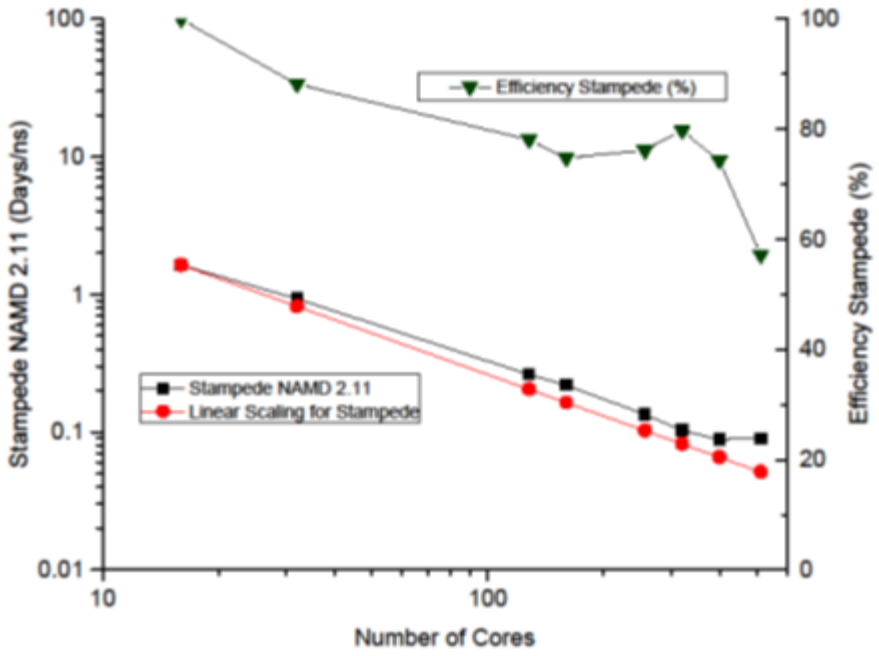

Figure 2.1 Performance of NAMD 2.11 with a 312,320-atom system on Stampede.

Topologies define the connections, relationships and charges which are then assigned by the VMD plugin called PSFGEN to create structure files (psf files) and coordinate files (pdb files). PSFGEN plugin in VMD was used to unite the protein structure fragments and ligate the hemes and iron sulfur cluster with the protein.

NAMD was used to perform molecular dynamics calculations based on a force field. Force field methods (also known as molecular mechanics) ignore the electronic motions and calculate the energy of a system as a function of the nuclear positions only.(*50*)

$$U(\vec{r}) = \sum U_{bonded}(\vec{r}) + \sum U_{nonbonded}(\vec{r})$$

After picking an appropriate set of coordinates for the bc_1 complex from the protein data base (accession code 2QJY) the structural model of the bc_1 complex was constructed.

During the equilibration phase the system is expected to evolve from the initial configuration to reach equilibrium in the new environment (*50*). Values of properties such as the

thermodynamic quantities of energy, temperature and pressure are monitored along with structural properties. Equilibration should continue until the monitored properties become stable.

Kinetic Model

A kinetic model was initially developed for Dynafit, and has now been ported to the Matlab toolbox SimBiology. The model has also been implemented using the Gillespie algorithm for stochastic kinetic modelling. The kinetic model can be used to fit data to estimated parameters determined by experiments, by fitting kinetic data while varying critical parameters (rate constants, thermodynamic parameters, etc.). Also, in order to avoid lengthy stochastic simulations with time wasted on diffusion the stochastic solver should be modified to a hybrid stochastic system where the faster processes are represented by continuous process differential equations.

Chapter 3 Membrane

In order to prepare a model of the *bc₁* complex in a state as close as possible to its natural state in chromatophores, a selection of lipid types and fatty acid tails was made that resembles the experimentally determined quantities and falls within the accepted baselines which prior studies of membrane biosynthesis and composition establish. A large amount of data has been collected for the natural *Rb sphaeroides* chromatophore system. Two of the differences between prior membrane lipid types and membrane lipids found in the natural *Rb sphaeroides* chromatophore system include: 1) the fatty acid tails of *Rb sphaeroides* chromatophores membranes have different lengths; and 2) the saturation points differ from the fatty acids found in mitochondrial membrane lipids. The degree of saturation in fatty acids is an important factor in the behavior of the membrane and changes from those found in nature would subject the output of the molecular dynamics calculation to additional unnecessary variability. Furthermore, the consistency of the membrane seems to effect its components and larger issues of overall health, i.e., remote phenotypes, as is evidenced by current research into the importance of saturated vs. unsaturated fatty acids in human health. . While it seems obvious that using an unnatural membrane would be inappropriate for modelling a natural system, this study does not attempt to quantify the differences in behavior between an unnatural and a more natural membrane.

Studies of fatty acid biosynthesis of *Rb sphaeroides* found that the typical fatty acids were palmitate, stearate and vaccinate (*51*). Further, a lack of desaturases results in no reformation or change of saturation once the fatty acid chain is formed (*51*). The double bond is

located between carbon 11 and carbon 12 as shown below in the diagrams for the different membrane lipid types.

Similar to the issue of fatty acid content of the membrane, the larger issues of human health seem to intersect with concerns with the content of the membrane where cholesterol and cardiolipin is concerned. Many different lipid types are found in bacterial membrane, some of which might have important functional roles in purple bacteria and *Rba. sphaeroides,* specifically. Ornithine and glutamine lipids have been extracted from *Rba. sphaeroides* membranes and characterized (*52*). Ornithine lipids have been reported as required for optimal steady-state amounts of *c*-type cytochromes (*53*).

Another membrane component, cardiolipin (CL) has been suggested to be important to functions relevant to the operation of membrane proteins such as cyt bc_1 complex or cytochrome *c* oxidase (*CcO).* A recent atom-scale simulation study by Róg et al. cites numerous studies pointing to the physiological involvement of CL in electron and proton transfer by membrane proteins, apoptosis, aging and oxidative stress (*54*). The charged nature of CL seems to be particularly important to its effect because when the gene for the production of CL was knocked out in *Rb. sphaeroides* non-phospholipid substitutions of the similar charge where found around functioning *CcO* in membranes from the knock out organisms (*34*). Although the selection of specific types of membrane lipids may be flexible, the overall composition is important at least in terms of charge composition.

In order to produce a realistic natural membrane a combination of lipid types and fatty acids tails were chosen that best covered the variety found in various studies of the *Rb sphaeroides* membrane. The articles mentioned above surveyed and reported on membrane content in their investigations. Additional sources were investigated to gauge the appropriate

content for the photosynthetic *Rb sphaeroides* membrane since there are differences in the acyl lipid concentration for photosynthetic bacteria grown under photosynthetic and non-photosynthetic conditions (*55*). In switching from non-photosynthetic conditions to photosynthetic conditions the membranes in *Rb sphaeroides* exhibited a shift in CL to a higher percentage (6.2 % to 11.3 %); a shift in phosphatidylcholine choline (PC) to a slightly lower percentage; and a shift in phosphatidylethanolamine (PE) to a lower percentage (35.0 % to 21.4%), inter alia (*55*). It is worth noting that the magnitude and even direction of acyl lipid concentration shifts were in some cases different for *Rb capsulatus* which is the species of bacteria for which the redox center topologies and parameters where calculated in forming the topologies used in this study (*45, 55*). Since much of the data generated for the *Rb. sphaeroides* bc_1 complex was done with chromatophores utilizing flash activation, the chromatophore membrane composition is the most natural and realistic basis for a useful model which hopes to simulate function of the complex and so uses an acyl tail composition which have been found in the *Rb. sphaeroides* membrane.

There are no CHARMM 36 force field topology files which match the specific membrane lipids with corresponding and fatty acids tails of the *Rb. sphaeroides* membrane. Given resource constraints only a limited number of lipid types were chosen. The topology files for the following six lipid types were created from the head groups of lipids from the CHARMM 36 force field and the double bond positions were shifted in the tails: DVPG di-vaccenoyl phosphatidylglycerol (2,3-divacenyl-D-glycero-1-phosphatidylglycerol); VSPG (1-vaccenoyl 2-steroeyl-D-glycero-1-phosphatidylglycerol); DVPE divaccenoyl phosphatidylethanolamine (2,3-divaccenoyl-D-glycero-1-phosphatidylethanolamine); VSPE vaccenoyl steroyl phosphatidylethanolamine (2,3-vacenoyl- steroyl D-glycero-1-phosphatidylethanolamine - steroeyl D-glycero-1-phosphatidylethanolamine); DVPC di-vaccenoyl phosphatidylcholine (2,3-

divaccenyl-D-glycero-1-phosphatidylcholine); and VSPC vaccenoyl steroyl phosphatidylcholine (3-vaccenoyl-2-steroyl-D-glycero-1-phosphatidylcholine). For each lipid type (PG, PE, PC) the dioloeyl (DO) and the palmitoyl-oleoyl (PO) corresponding respective topology files were used to generate the formatted topology sections which were then modified to reflect the correct head type, desaturation point, bonding, and interconnect files. The topology files for TVCL (tetra vaccenoyl cardio lipin) and SQDG were assembled but not formatted and tested in time for inclusion. (Appendix A)

Preparation of the membrane and solvation around the protein for running by NAMD was performed by utilizing the web-based graphical user interface for CHARMM (CHARMM-GUI) (*56*). The CHARMM-GUI resource hosts several programs to assemble and run the membrane protein complex model to produce input files for NAMD, i.e., structure files, assembled pdb, and configuration files (*57, 58*). The Membrane Builder utilized the designated Protein Data Bank accession code 2QJY to look up the protein coordinates aligned within membrane boundaries and then proceed with several steps of membrane lipid selection, solvation parameter selection and insertion of selected membrane lipids into the membrane boundaries (*59-61*). The files output from CHARMM-GUI which were used include structure files (.psf) and coordinate files (.pdb) for the solvation layers and the membrane structure. The output files from CHARMM-GUI were combined with other files using the animate command and psfgen and molefacture plugins of VMD to unite these pieces with the protein, cofactors, substrates, and quinones.

The CHARMM-GUI membrane lipid library did not include the membrane lipids for which topologies had been made. During the membrane building process in CHARM-GUI membrane lipids found in the library were used in place of the lipids whose topologies were developed to match the *Rb. sphaeroides* chromatophore. The last section of Table 1 details the lipid present in the CHARMM-GUI membrane segment output and the new lipid that replaced it.

The new membrane lipids were inserted into the membrane by replacing the lipids from membrane segment of the CHARMM-GUI output, e.g., our new lipid DVPG was substituted for DOPG as shown in Table 1. The corresponding library lipids chosen had the same connection of atoms in the head group and same fatty acid tail length as the new membrane lipids but the double bond shifted down to the C11-C12 position. Accordingly, tcl scripts were used to first rotate the dihedral of the new double bond to its cis conformation. Since this would have rotated the subject tail out of its original position into other occupied areas of the membrane segment, after setting the correct dihedral for the new double bond the other bonds starting from above the original double bond were rotated 360 degrees to find the point at which the end of the new tail was closest to the end of the original tail. This process was repeated for every carbon of every chain for every new lipid so that the resulting lipid tails would occupy roughly the same space as the original lipids they replaced.

Similar processes were used to i) fit and then renumber the Qi site UQ2 occupant and thread the additional isoprenoid units out of the active site; and ii) substitute quinones into the membrane for the cholesterol molecules inserted by CHARMM-GUI. A realistic chromatophore membrane includes quinones. Ubiquinone is the substrate for bc_1 complex in *Rb. sphaeroides*. Although substrate turnover or membrane diffusion is not within the timescale of a molecular dynamic simulation generally, the properties of the membrane are physiologically affected in important ways by constituents as can be imagined by the importance of cholesterol in human physiology. Accordingly, since there was no ubiquinone in the CHARMM-GUI Membrane Builder library, a number of cholesterols equal to the number of ubiquinones appropriate to the approximate concentration in the chromatophore were added to the membrane segment and then UQ10 substituted in with isoprenoid tail positioned toward the center of the membrane between the lipid tails.

	Zhang,X, et al (*34*)		Russell, J and Harwood, L (*55*)					Model Resname and source		
Lipid Type	Fatty Acid	(A) %	Fatty Acid	(B) %	(C) %	(D) %	(E) %	Residue name	(F)%	Charm-gui lipid library
CL	All (18:1)	**5.2%**		**11.3%**		**13.0%**		TOCL2	**11%**	TOCL2(18:1/18:1)
			16:0				6.9%		0%	PVCL2(18:1/16:0)
			16:1				0.8%			
			18:0				14.2%			
			18:1				78.0%			
			Others				2.1%			
PG	Combined	**9.1%**	combined	**44.4%**		**44.4%**		DVPG	**40%**	DOPG (18:1/18:1)
	18:1/18:1	7.4%	16:0		4.9%		9.3%	VSPG	**6%**	SOPG (18:1/18:0)
	18:0/18:1	1.4%	16:1		1%		1.4%			
	18:1/19:1	0.3%	18:0		9.7%		16.3%			
			18:1		80.8%		72.9%			
			Others		3.6%		2.1%			
PE	Combined	**35.1%**		**21.4%**		**28.3%**		DVPE	**23%**	DOPE (18:1/18:1)
	18:1/18:1	29.8%	16:0		4.2%		7.2%	VSPE	**7%**	SOPE (18:1/18:0)
	18:0/18:1	5.3%	16:1		0.9%		1.6%			
			18:0		8.4%		15.8%			
			18:1		82.0%		71.2%			
			Others		4.5%		4.2%			
PC	Combined	**14.1%**		**11.9%**		**10.0%**		DVPC	**12%**	DOPC (18:1/18:1)
	16:0/18:0	0.8%	16:0		4.8%		10.6%	VSPC	**1%**	SOPC (18:1/18:0)
	18:1/18:1	9.0%	16:1		2.2%		1.5%			
	18:0/18:1	1.0%	18:0		4.1%		13.8%			
	18:1/19:1	3.3%	18:1		84.2%		71.9%			
			Others		4.7%		2.2%			
SQDG	Combined	**5.9%**		**4.2%**		**3.7%**				
	16:0/16:0	0.5%	16:0		20.2%		21.5%			
	16:0/18:1	1.5%	16:1		0.9%		0.6%			
	16:0/18:0	0.7%	18:0		15.4%		14.5%			
	18:1/18:1	2.0%	18:1		62.4%		54.4%			
	18:0/18:1	1.0%	Others		1.1%		9.0%			
	18:0/18:0	0.2%								
OL	Total	**9.6%**		**2.3%**		na				
	20:1/18:1	2.7%								
	20:1/19:1	5.8%								
	20:0/21:1	1.2%								
QL	Combined	**0.5%**		na		na				
MMPE*	Combined	**20.6%**		na		na				
Acyl lipids**	Combined			**4.5%**						

Table 3.1 Columns: (A) percentage of total of type of lipid and fatty acid tails for *Rb sphaeroides* grown under aerobic chemoheterotrophic conditions; (B) percentage of total for each type of lipid from *Rb sphaeroides* grown under photosynthetic conditions; (C) percentage of total of fatty acid for each type of lipid from *Rb sphaeroides* grown under photosynthetic conditions; (D) percentage of total for each type of lipid from *Rb sphaeroides* chromatophores grown under photosynthetic conditions; ; (E) percentage of total of fatty acid for each type of lipid from *Rb sphaeroides* chromatophores grown under photosynthetic conditions; and (F) percentage of each type in the membrane built for the molecular dynamics model. The CHARMM-Gui lipid library column refers to the specific types found in the CHARMM-Gui library which were used to construct the topologies for the model lipids. . CL – cardiolipin; PG – phosphatidylglycerol; PC – phosphatidylcholine; PE – phosphatidylethanolamine; SQDG – sulfoquinovosyldiacylglycerol; OL – ornithine lipid; QL – glutamine lipid. * Includes MMPE, DMPE, and PE. ** Includes neutral acyl lipids and other polar acyl lipids.

The lateral diffusion coefficient of membrane lipid molecules, ubiquinone, ubiquinol and the protein in the xy plane D was calculated by fitting the time-dependent mean square displacement of the center of mass of the lipid headgroups using the Einstein equation (*62*):

(eq 3.1)

$$D = \frac{1}{2d} \lim_{t \to \infty} \frac{\langle dr^2 \rangle}{t}$$

The results of the calculation by equation 2.1 of the two dimensional diffusion coefficient for the new lipids across the course of a trajectory for the completely oxidized configuration (conf1_3) is shown in Figure 3.1. The calculations were performed using the script listed in Appendix C.

The results of the calculation by equation 3.1 of the two dimensional diffusion coefficient for ubiquinone (UQ10) (UBIQ) and ubiquinol (UQ10) (UQL) across the course of a trajectory for the completely oxidized configuration is shown in Figure 3.2. The approximate value for D, the diffusion constant is 3 $\mu m^2/s$ from Figure 3.2. One group has found a value of 190 to 290 $\mu m^2/s$ in combination of phospholipid vesicles (*63*) while values of 2 orders of magnitude less are found with photobleaching measurements (*64*).

The results of the calculation by equation 3.1 of the protein center of mass diffusion constant for each conf1_2 and conf1_3 trajectory is shown in Figure 3.3. There is a difference between the movement of the protein by a factor of 2X but given the small sampling space this difference is probably statistically insignificant. The two dimensional diffusion constant can very quiet a bit for proteins depending on their size and environment but the apparent diffusion constant reached in our calculation is within the approximate values reported experimentally for similar proteins and environments.

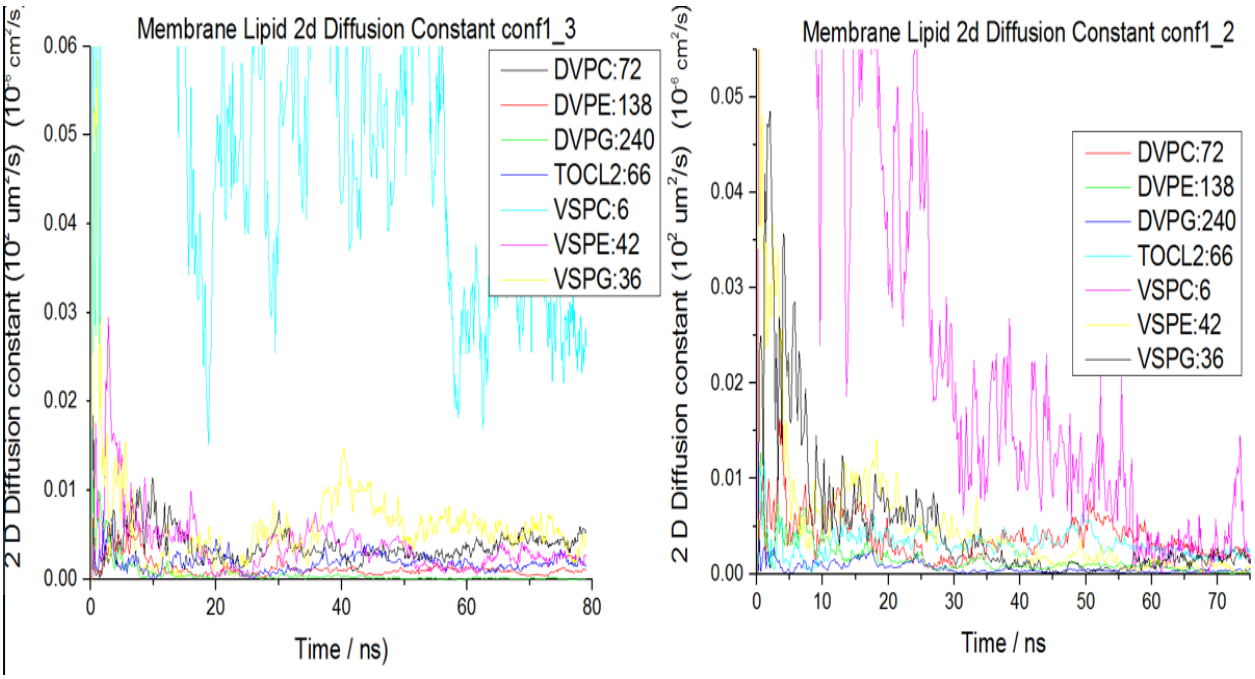

Figure 3.1 Graph of 2 dimension (q=4) diffusion constant for trajectory of conf1_3 and conf1_2 from Einsteins relationship for diffusion (eq-3.1). The legend indicates the name of the membrane lipid and the number of lipids in the membrane

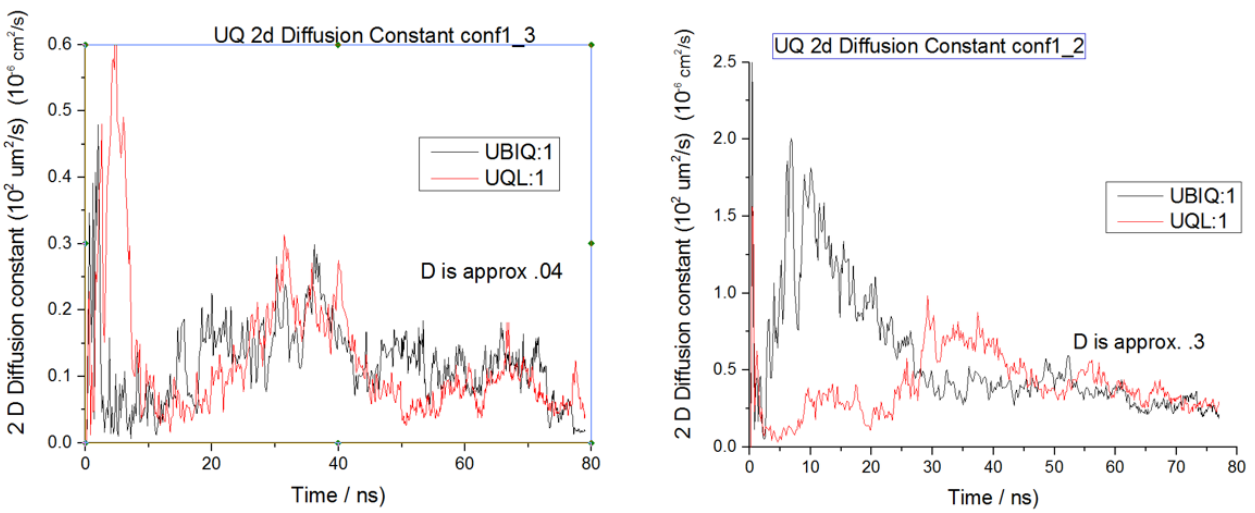

Figure 3.2 Ubiquinone (UBIQ) head group center of mass and ubiquinol (UQL) head group center of mass two dimensional (2d) diffusion constant calculated from Einstein equation (eq. 3.1).

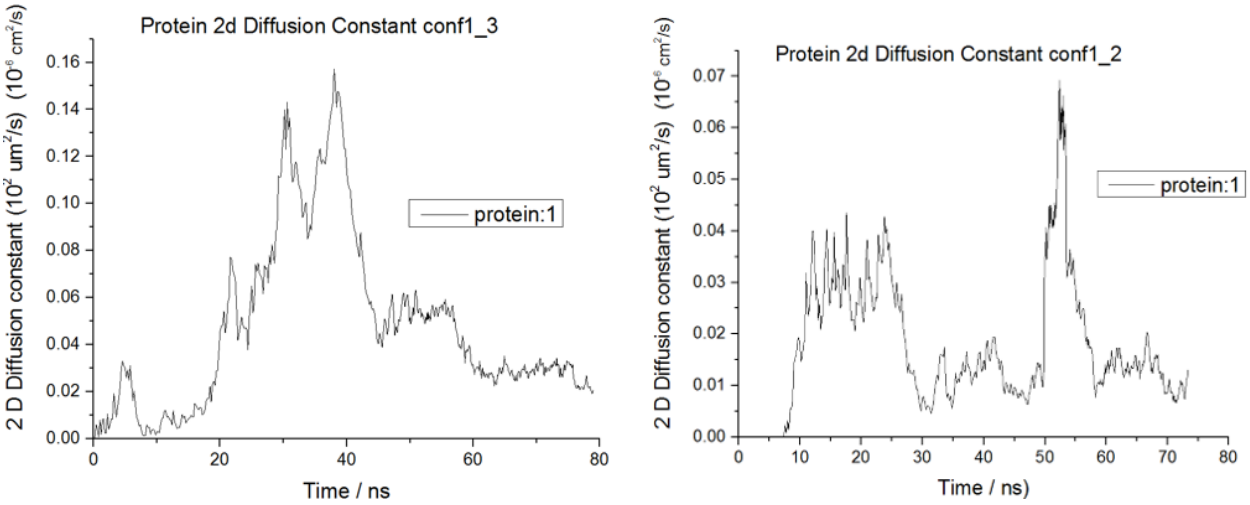

Figure 3.3 Protein diffusion constant graphed from Einstein equation (eq. 2.1) for protein center of mass in conf1_2 trajectory and conf1_3 trajectory.

Chapter 4 Simulation Set Up and Configurations

Equilibration and Preparation

The currently running model is part of a lipid stabilized simulation and includes (i) the model of the *bc_1* complex with two lipids inside of the interior space, quinol (UQ10) in the Q_o-site (the inhibitor stigmatellin was originally in the crystal structure) and UQ10 in the Qi-site; (ii.) the membrane with new lipids, cardiolipin, and UQ10; and (iii.) water box solvated with sufficient charges to counter the charge in the membrane and the protein. The Q_o-site occupant stigmatellin was replaced with the substrate UQ10 and after a 10000 steps of minimization the system was released again and continue to equilibrate while running for another 15 ns approximately to a total run time of about 50 ns. After about 50 ns the "production run" starts with the protein and bonds unconstrained at a 1 fs time step.

Table 4.1 shows these first stages of running the simulation. Initial equilibration runs (Run No. 0, conf file eq_0 and No. 1, conf file eqR_0) were at 1 fs time step with 10, 000 minimization steps. The energy stabilized and the equilibration was continued after the initial scaling. Run Nos. 1-6 were harmonically restrained equilibration cycles where the restraints were gradually released.. An extra bonds file was generated with dihedral angles and improper angles. These extra bonds were subject to additional restraining forces so that the double bonds are maintained in a natural cis- configuration so there is no isomerization even during extended minimization.

The dihedral force constant ('dihed fc') is applied to dihedral and improper angles of the components of the membrane which include membrane lipids and quinols . This harmonic force constant is in units of kcal/rad^2. The force constant was started at 500 and then stepped down to

50 in the last equilibration run before being released. The backbone, head groups of substrate stigmatellin and quinone 'head' group were restrained to their initial positions with a force constant starting at 10 kcal*mol^{-1}/A^2 and stepping down to 0.5 10 kcal*mol^{-1}/A^2.

The final equilibration runs and first production runs have been run with a 2 fs time step. All runs were conducted with the rigidBonds parameter set to 'yes' to keep the bonds between atoms from vibrating. The protein movement is shown as stabilizing at a fairly low rmsd value in Fig. 4.1.

Run No.	conf file	timestep(fs)	dihed fc*	bb*	steps	Actual Steps	Time (ps)
0	eq_0	1	500	10		258000	258
0	eqR_0	1	500	10		2758000	2758
1	eq_01	1	500	10		2769000	2769
2	eq_02	2	500	10	2500000	5269000	7769
3	eq_03	2	200	5	1250000	6519000	10269
4	eq_04	2	200	2.5	1250000	7769000	12769
5	eq_05	2	100	1	1250000	9019000	15269
6	eq_06	2	50	0.5	1250000	10269000	17769
7	run_01	2	0	0	1250000	11519000	20269
8	run_02	2	0	0	2500000	14019000	25269
Insert Q							
0	prod_eq_0	1	500	10	200000	210000	210
1	prod_eq_1	2	500	10	90000	300000	390
2	prod_eq_2	2	200	5	105000	405000	600
3	prod_eq_3	2	100	2.5	100000	505000	800
4	prod_eq_4	2	50	1	100000	605000	1000

Table 4.1 Restraining forces, steps executed, and clock time model run. The 'bb' restraints are applied to protein backbone, substrates and quinone head groups. *The dihed fc is applied to a list of dihed and improper angles so that the double bonds and impropers of the membrane lipids and quinones are maintained and the units are kcal/rad^2. **The units of 'bb' are kcal*mol^{-1}/A^2.

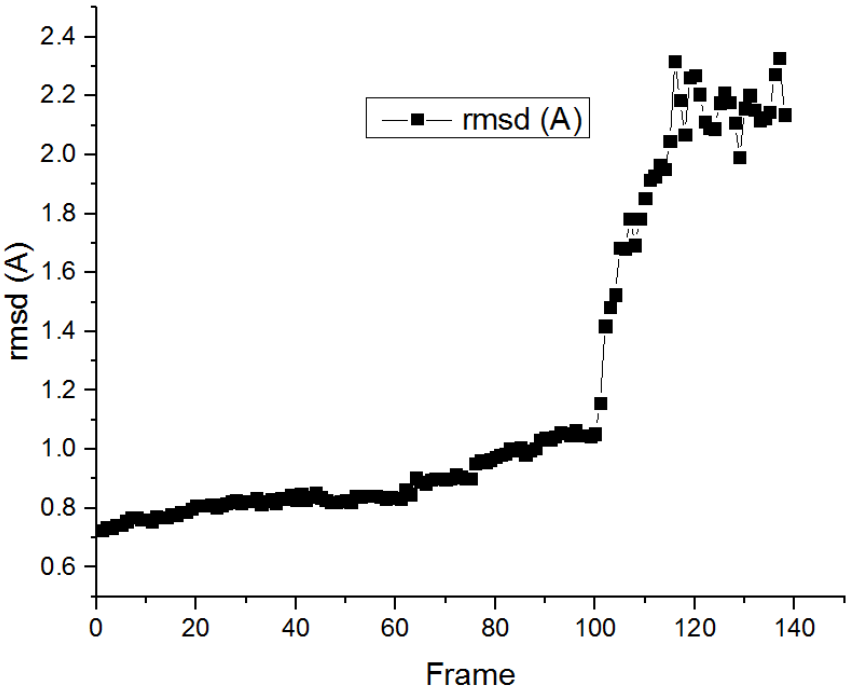

Figure 4.1 Plot of rmsd from NAMD energy for protein from the first frame to frame 140 (25269ps)

Three different configurations or simulations were run from the end of the preparation described above: conf1_1, conf1_2, conf1_3 (Table 4.2). These first three are versions of the first intended configurations which represent states of the bc_1 complex as indicated by Table 4.3. Conf1 represents the fully oxidized state of the system with a substrate in the Q_o-site as a precursor to the process of forming the enzyme substrate complex (ES complex). Conf2 models the system after the first oxidation of this substrate to a neutral semiquinone and reduced ISP head group with protonated liganding histidine (His152). The first three versions of Conf1 originate from the same starting state and each have slight errors in topologies and coordinates such as conf1_1 used a topology with only eight isoprenoid units and slight irregularities in the head group which had to be corrected by creating new topologies.

Conf1_2 represents a fortunate accident in that a mistake with inserting the inhibitor antimycin in the Q_i-site caused the quinol in the Q_o-site to withdraw from hydrogen bonding with

the ISP head group and release the ISP head group to move away. The mistake which caused this was the positioning of the antimycin such that a lipid tail of one of the two void-filling lipids intersected a ring of the antimycin structure. Although ring crossings should generate fatal errors on attempt to minimized, the Con1_2 simulation did minimized, and ran without eror messages for the times indicated. The lasso configuration generated an asymmetry in the central volume, which was likely the cause of the displacement of QH_2, but we did not attempt to analyze the mechanism. This configuration can be used to examine ISP head group movement in preparation for deriving replicas for replica exchange.

The next state of Conf2 has started running but for less than 5 ns so no relevant data has been gathered yet. The initial few nanoseconds show the neutral semiquinone moving away from the ISP head group.

config	Run #	Config file	Timestep(fs)	Dihed fc	bb	steps
conf1_1						
Reverse Quinone to quinol assignment						
	0	prod_conf1_1_eq_0	2	0	0	2010000
	1	prod_conf1_1_eq_1	2	0	0	5342000
	2	prod_conf1_1_eq_2	2	0	0	9342000
	3	prod_conf1_1_eq_3	2	0	0	13114000
	4	prod_conf1_1_eq_4	2	0	0	17114000
	5	prod_conf1_1_eq_5	2	0	0	21114000
	6	prod_conf1_1_run_6	1	0	0	26114000
	7	prod_conf1_1_run_7	1	0	0	36114000
	8	prod_conf1_1_run_8	1	0	0	46114000
	9	prod_conf1_1_run_9	1	0	0	56114000
	10	prod_con1_1_run_10	1	0	0	66114000
	11	prod_conf1_1_run_11	1	0	0	
conf1_2						
FixQH2 + inh(ANT)					bb+Q(head)	
	0	prod_conf1_2_eq_0	2	0	10	510000
	1	prod_conf1_2_eq_1	2	0	5	1510000
	2	prod_conf1_2_eq_2	2	0	2	2510000
	3	prod_conf1_2_eq_3	2	0	1	3510000
	4	prod_conf1_2_eq_4	2	0	0	8510000
	5	prod_conf1_2_eq_5	2	0	0	18510000
	6	prod_conf1_2_eq_6	2	0	0	28510000
	7	prod_conf1_2_run_7	1	0	0	38510000
	8	prod_conf1_2_run_8	1	0	0	48510000
	9	prod_conf1_2_run_9	1	0	0	
conf1_2a						
	0	prod_conf1_2a_eq_0	2	20 (+H)	0	510000
	1	prod_conf1_2a_run_1	1	0	0	
conf1_3						
	0	prod_conf1_3_eq_0	2	0	10	510000
	1	prod_conf1_3_eq_1	2	0	5	1510000
	2	prod_conf1_3_eq_2	2	0	2	2510000
	3	prod_conf1_3_eq_3	2	0	1	3510000
	4	prod_conf1_3_eq_4	2	0	0	8510000
	5	prod_conf1_3_eq_5	2	0	0	18510000
	6	prod_conf1_3_eq_6	2	0	0	28510000
	7	prod_conf1_3_run_7	1	0	0	38510000
	8	prod_conf1_3_run_8	1	0	0	48510000
	9	prod_conf1_3_run_9	1	0	0	58510000

Table 4.2 Restraining forces and steps executed. The 'bb' restraints are applied to protein backbone, substrates and quinone head groups. *The dihed fc is applied to a list of dihed and improper angles so that the double bonds and improper.

Conf1		Monomer		Conf2		Monmer	
		First	Second			First	Second
	cyt c	O	O		cyt c	O	O
	cyt b-bL	O	O		cyt b-bL	O	O
	cytb-bH	O	O		cytb-bH	O	O
	FES	O	O		FES	R	O
	Qo	QH2	QH2		Qo	UQS (neutral)	QH2
	Qi	Q /Ant	Q/Ant		Qi	Q	Q
	Glu295	O^-	O^-		Glu295	O^-	O^-

Table 4.3 Redox states /species in each monomer for the first two simulation configurations

Chapter 5 Modified Q-cycle: ES complex Formation[2]

Crofts lab has developed a kinetic model for the reaction at the Q_o-site that includes kinetic and thermodynamic parameters for 15 partial processes determined directly using conventional protocols. The model was implemented in the Dynafit software environment (*65, 66*). In this work, I have extended the model by porting it to the Matlab toolbox SimBiology, and developed an implementation using the Gillespie algorithm for stochastic kinetic modelling.

Typically, reactions are kinetically modeled using differential solvers, which essentially find the limit of the difference equation for small Δt (dt) and large population, i.e., a continuous sampling, but in modeling the reactions within a complex, the differential approximation can be considered inaccurate in a sense. Direct repeated calculation of the master equation is not possible but a stochastic algorithm was proposed by Gillespie for numerical simulation of the time evolution of a given set of kinetic equations (*67*). This method has been used by Ransac et al. (*68*), and they were able to model the main features of the Q-cycle using Moser-Dutton based rate constants, and driving forces from thermodynamic parameters. However, they failed to take into account the features of the mechanism associated with control and gating, and their model failed under conditions where these are important. In our version of a Gillespie model, these features could be included through explicit partial processes, and then reproduced the same

[2] Some of this material was previously published in 5.A. R. Crofts, Lhee, S., Crofts, S.B., Cheng, J. and Rose, S., Proton pumping in the bc_1 complex: A new gating mechanism that prevents short circuits. *Biochim. Biophys. Acta* **1757**, 1019-1034 (2006).and 26. A. R. Crofts *et al.,* The Q-cycle Mechanism of the bc1 Complex: a Biologist's Perspective on Atomistic Studies. *The Journal of Physical Chemistry B,* (2017).

kinetics as the model using differential equations. In exploring the potential for integration of this approach into MD simulation in our own models, we found that when timescales became large, steps like diffusion, where the atomistic timescales are small, would consume enormous amounts of processor time in unnecessary recalculation of reaction probabilities, and this points to at least one aspect that is challenging.

In the present study, we would like to examine kinetics in the context of a molecular dynamics model of a system consisting of the enzyme, the substrate, and a membrane representing the natural membrane in relative proportion of membrane lipid types and approximate proportion of fatty acid tails. Our aim is to use the kinetic model in iterative mode, in conjunction with differential and stochastic solvers and data from experiments, to incorporate values calculated from the molecular dynamics into the traditional physicochemical representation by means of fitting procedures.

The kinetic model for the monomeric bc_1 complex developed for this study is shown diagrammatically in Fig. 5.1 by its different states. The model for the dimeric complex including electron transfer across the interface between dimers is not shown and will used in the future for the iterative parameter fitting and simulations discussed infra. The model includes 15 partial processes and includes various other partial process which have rate constants estimated based on thermodynamic constraints. The model is based on an antimycin inhibited bc_1 complex where full reduction of all components would involve two quinols being reduced at the Qo-site to deliver two electrons to b_L and b_H hemes. The resultant model has 54 reactions including diffusion reactions and proton distribution 'reactions'. The model shows the reactions advancing from state to state in the process of two quinols being oxidized. In the current model parameters can be selected for fitting to experimental data. This model represents an improvement because

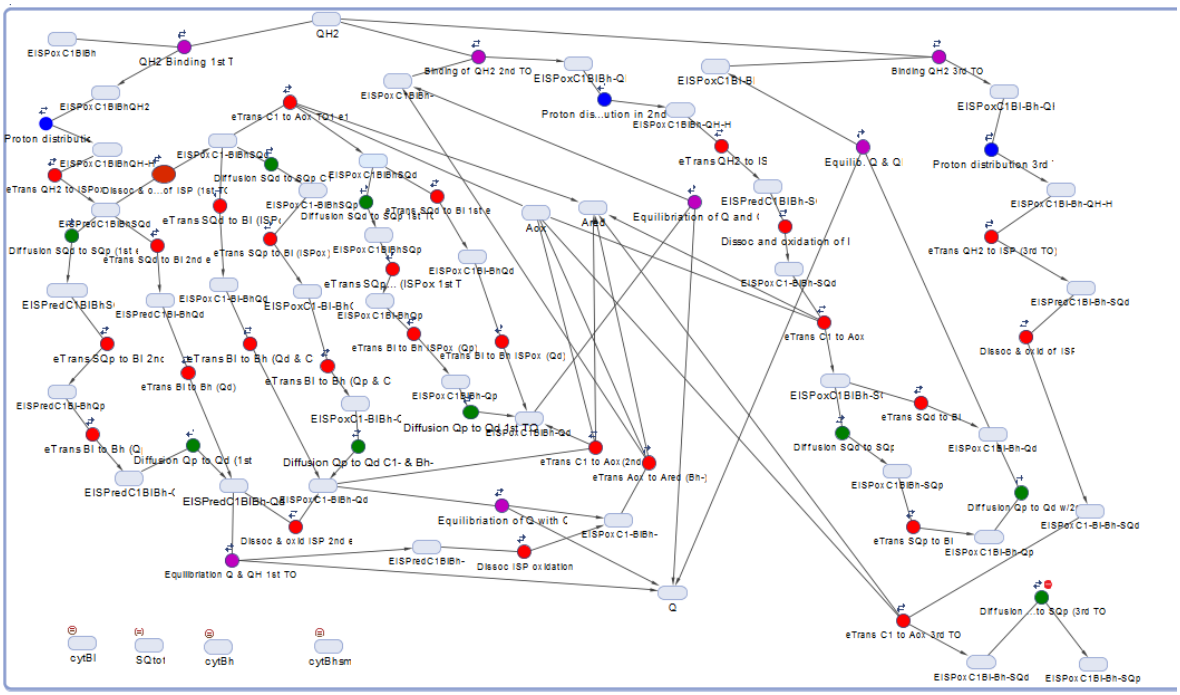

Figure 5.1 Matlab Simbiology tool kit diagram of the kinetic model of three QH_2 to Q turnovers of the complex derived from the kinetic model developed and parameterized by Prof. Crofts

each of the states of the enzyme in the overall reaction is separately represented. A model which represents the partial reactions in relation to the oxidation and reduction of a single heme without taking into account the change in state of the redox components of the overall complex fails to capture the columbic effects exerted by reduced hemes on oxidized hemes. The lack of linearly arranged states is particularly inaccurate for using stochastic methods for solving the system (Ransac (*68*))

The first step in the modified Q-cycle is the formation of the ES complex where the substrate quinol enters the Q_o-site and associates with the first catalytic interface of the bc_1 complex, i.e., the ISP head group (Fig 5.1 and Fig 5.2). The volume initially left void in the previous simulation, was now occupied by two lipids, retained for at least 75 ns (in contrast with the free diffusion of phospholipids in the bulk membrane). Water-chains previously observed crystallographically were populated by waters, but these exchanged rapidly with the bulk. No waters were found in the "void" volume. Ubiquinone, like the other native phospholipids in the

membrane, diffusing stochastically (Fig. 1.2a). The modifications to correct previous defects therefore appeared to have been effectively implemented. Both the overall structure, and configurations for both the Q_o- and Q_i-sites (occupied in the initial crystallographic model respectively by stigmatellin and ubiquinone), retained configurations close to those seen in the starting crystallographic model when occupied by UQ-10 respectively in reduced or oxidized

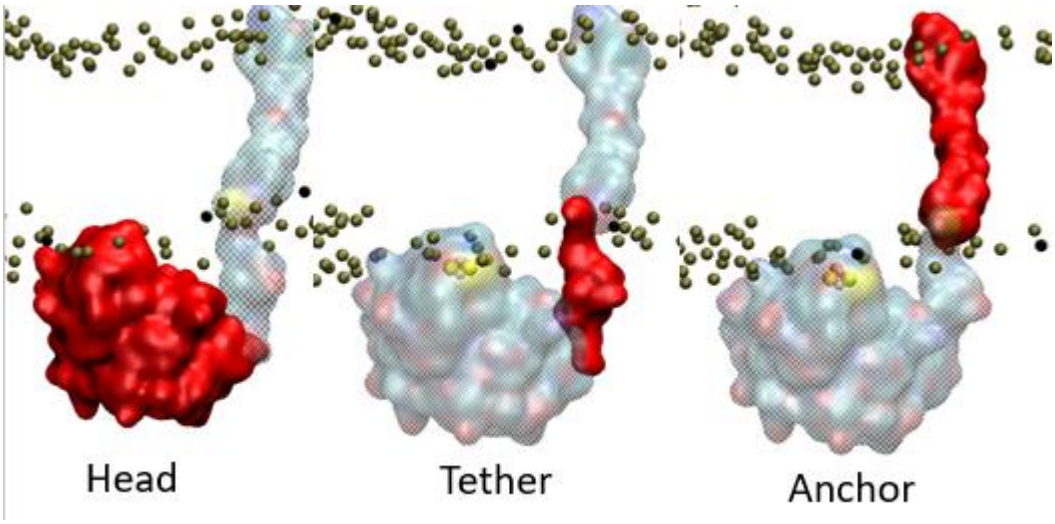

Figure 5.2 ISP head group, Tether and Anchor in red with gold potassium ions from membrane lipids to indicate membrane location.

form at Q_o- and Q_i-sites (Fig. 1.2), a state appropriate to steady-state turnover. This is in line with the recent simulations reported by Postila et al. (*29*), in which the Q_i-site mechanism was simulated in a *Rb. capsulatus* model of the bc_1 complex with cardiolipin in the void.

Conf1, the versions of our oxidized bc_1 complex shows properties which include significant differences from those previously reported. The basis of these differences obviously needs to be resolved. In the Barragan et al.(*33*) complex leading to productive forward chemistry, three H-bonds stabilized the structure: from H156 N_ε to QH_2 -OH, from Y147 -OH to QH_2 -OH (the other end), and from Y147 -OH to E295 $-COO^-$. On the positive side, the three residues involved in stabilizing the *ES*-complex were all found to participate in H-bond pairing, suggesting that drastic revision of previous work might not be necessary. However, the configuration in which all three H-bonds were engaged, which formed the basis of the QC

calculations, has not yet been reached in our simulation after 87 ns (conf1_3). Fig. 5.3, 5.4 A and show states of the Q_o-site in which important H-bonds or potential H-bonding are highlighted, and (in Fig. 5.4 B and C), the distances for the H-bonds above, read from the trajectory of conf1_3 as it evolves. In the time courses shown, ISP_{ox} and QH_2 are start separate (monomer 2) or start together (monomer 1), but over the first 130 frames (26 ns), the H-bond from QH_2 -OH to ISP_{ox} N_ε of H152 forms in monomer 2, and stabilizes the *ES*-complex. During the entire trajectory, Y147, E295, and N279 explore configurations in which Y147 visits QH_2. Mostly, E295 is busy swapping its association between the other two residues. This volume of the protein also includes several exchangeable waters which are involve in H-bonding with the polar residues, and connecting to the heme b_L propionates and Arg-94, likely providing H^+ conducting pathways, including one to the P-phase water. Over the remaining time captured in

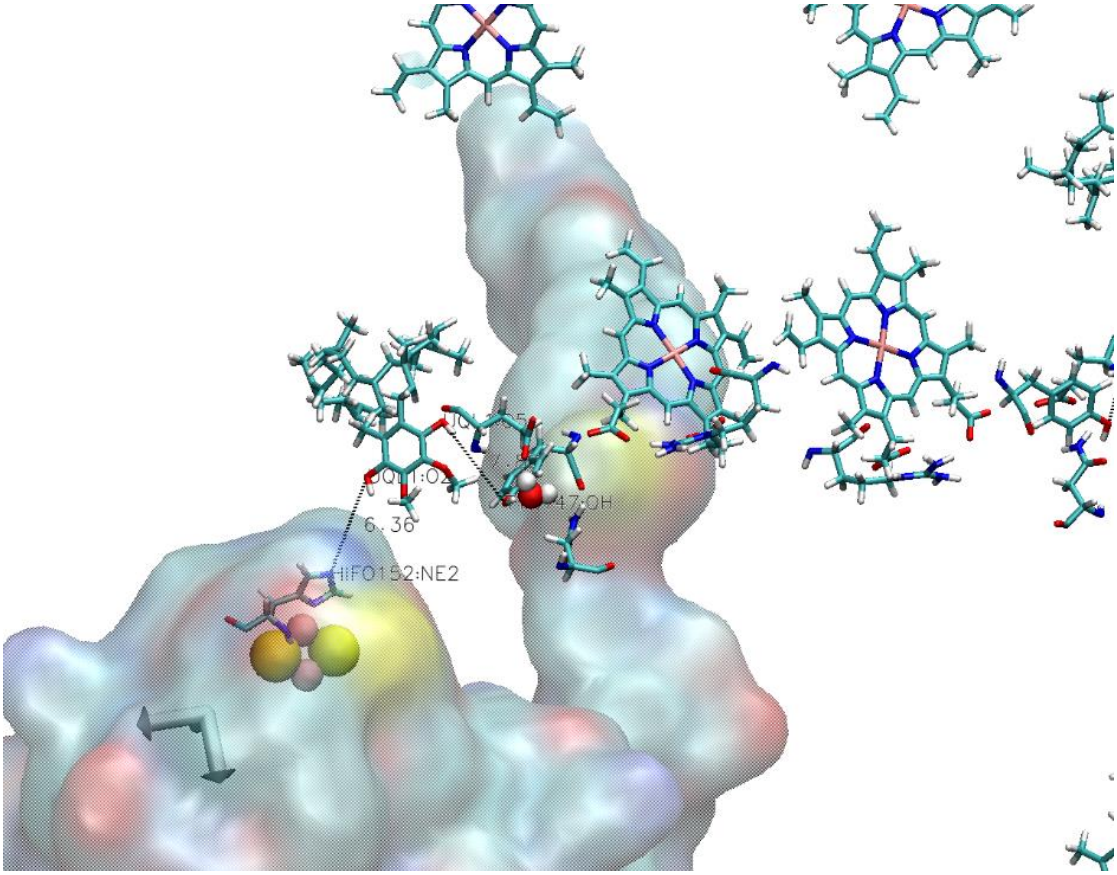

Figure 5.3 Formation of ES-complex H-bond network from conf1_1 being formed early in the trajectory

this trajectory, Y147 occasionally H-bonds with QH_2 as shown in A, about only 30% of the time (see time course in Fig. 5.4 B and C) although Y147 of monomer 1 seems to stay in the neighbor of QH_2 for most of the trajectory. In the frame captured in Fig 5.4 A, the two primary H-bonds to QH_2 stabilizing the *ES*-complex (from H152 and Y147) are both present, but E295 is distant. This pattern persists, though we should note that the *ES*-complex at the Q_o-site of monomer 2 was somewhat less stable than monomer 1, with an interesting time dependence that might suggest some interaction between sites.

Our current simulation with antimycin occupying the Qi-site (conf1_3), a commonly used experimental situation since it allows ready measurement of turnover of the Q_o-site through reduction of heme b_H. The measured rate of QH_2 oxidation (in the first turnover) when heme b_H is initially oxidized is the same in the absence or presence of antimycin(*13, 69*). In line with this, the configuration of the *ES*-complex followed essentially the same pattern (not shown). If this pattern is confirmed in additional runs, it would require at least a modest change in interpretation of the previous result; that the release of a H^+ from $QH^\bullet$ involves collisional exchange via stochastic H-bonding, rather than the direct relay previously suggested(*70*). However, more extensive revision could be justified; it is possible that the earlier modeling (*2-4, 23*) of the *ES*-complex as involving E295 as a direct ligand to QH_2 has biased thinking towards an emphasis on a direct role in H^+ release. If so, an alternative scenario would be that the product state $QH^\bullet$.ISPH dissociates to release the neutral SQ to diffuse in the site, and that E295 is involved only in transfer of the H^+ to the heme propionate after the $QH^\bullet$ is close enough to transfer the electron, thus facilitating an electrostatically linked PCET. The stochastic proton exchanges among this group of residues would enable transfers fast enough to make these last two models indistinguishable experimentally from the earlier model. One consideration in deciding between these scenarios is the need to contain the SQ in the Q_o-site. Preference might depend on a simple

physical principle; the low probability (high energy cost) of solvating a charged species, favors mechanisms involving $Q^{\bullet -}$ as the liberated form, rather than $QH^{\bullet}$, since the former would have a much lower probability of escape into the lipid phase via the hydrophobic entrance channel.

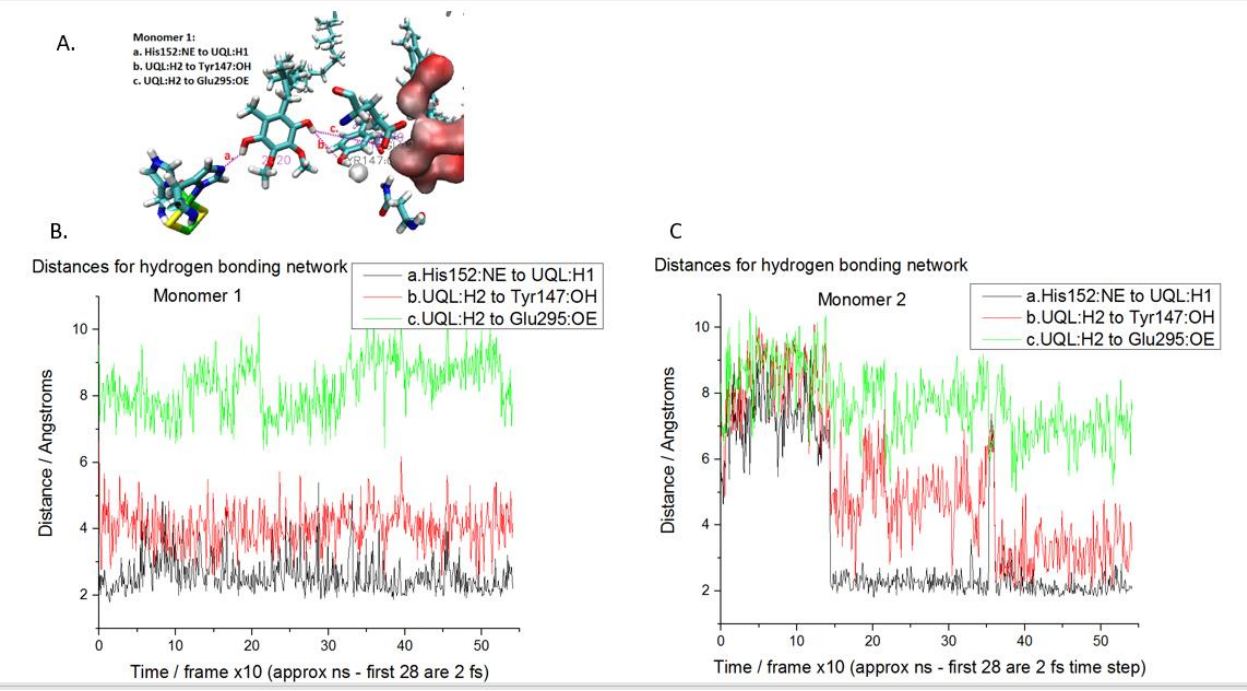

Figure 5.4 ES complex formation. A. The Hbond network around the quinol with the potential hbonds indicated including the distance to Glu295. B and C) Graph of the distances across the conf1_3 trajectory of the Hbonds for the corresponding, respective monomers, monomer 1 and monomer 2.

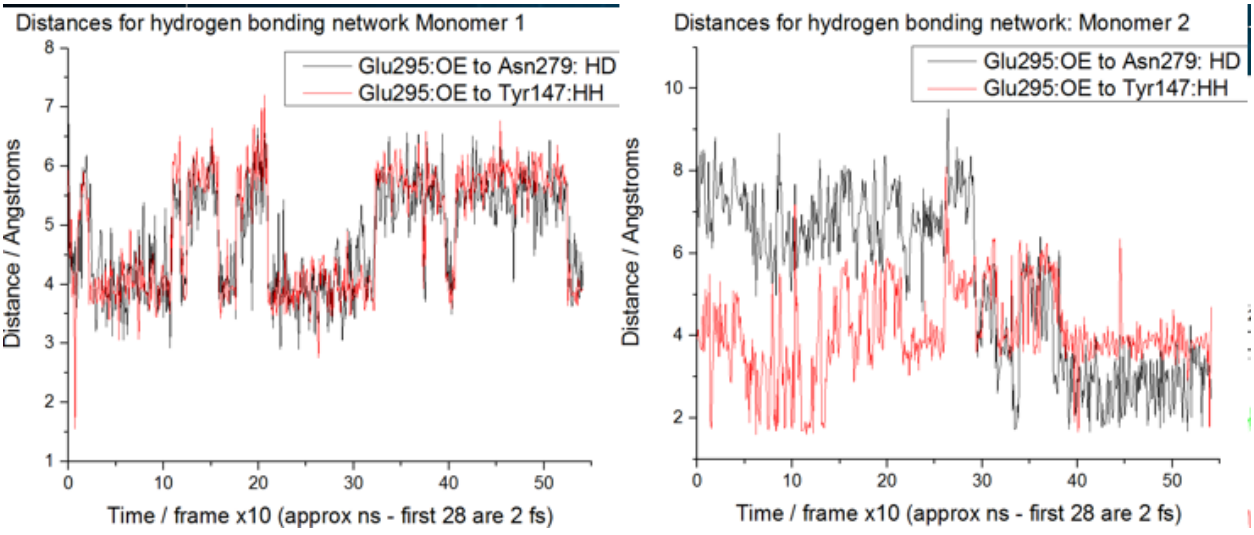

Figure 5.5 Details of the trajectory (conf1_3) showing other potential H-bonding partners for the Glu295.

Chapter 6 ISP Head Group Dynamics[3]

Molecular dynamics simulations of the bc_1 complex will be run in different redox states in order to sample a range of conformations which may be used to calculate a variety of potentials of mean force (PMF). Umbrella sampling (US) (*71*) with the weighted histogram analysis method (WHAM) (*72-74*) can be used in the study goals set forth below to calculate the energetics associated with the studied processes. However, before Umbrella sampling can be used effectively the motions of all parts of the simulation must be understood.

One goal of the calculations will be the *C. elegans* mutations which have focused attention in the role of ISP and movement of its extrinsic head-domain in control and gating of ROS production. Using molecular modeling the potential mean force of diffusion of the ISP head group and energy parameters of the 'hinge region' or tether during the constrained motion of the head group will be calculated for each redox state of the headgroup, i.e., before and after the reduction of the ISP. The physicochemical underpinnings of our spring-loaded model (*6, 7*) are based on studies of changes in binding free-energy in these complexes in ISP tether-span mutants (*75*). The Hamiltonian replica exchange (RE) method will be used to access otherwise inaccessible thermodynamic states orthogonal to the reaction path (*76*). The distance of the path is approximately 30 angstroms and will require windows of about 1 angstrom.

Additional PMF umbrella calculations will study diffusional displacements of the quinone/quinol substrates and semiquinone intermediate. Diffusion of the semiquinone within the Q_o-site is important to the proposed mechanism. The diffusional distance is 6-7 angstroms,

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[3] Some of this material was published in: 5. A. R. Crofts, Lhee, S., Crofts, S.B., Cheng, J. and Rose, S., Proton pumping in the bc_1 complex: A new gating mechanism that prevents short circuits. *Biochim. Biophys. Acta* **1757**, 1019-1034 (2006).and 26. A. R. Crofts *et al.*, The Q-cycle Mechanism of the bc1 Complex: a Biologist's Perspective on Atomistic Studies. *The Journal of Physical Chemistry B*, (2017).

and the diffusion occurs under varying conditions of coulombic steering due to the redox state of heme b_L.

Set Up of Pathway of Head Group Movement

The "spring" is physicochemical, with the forces determined by configuration of the tether region, mainly by the stretching or collapse to helical form, as the headgroup of the ISP moves between the Q_o-site and the electron-acceptor with heme c_1. Structures showing different configurations of the tether (cf. (*3*)) a crystallographic database for intermediate states in the forward reaction trajectory (see Figure 6.1). Movement of the head group is shown from differences found in crystallographic studies. Figure 6.1 shows the first and last position of the ISP head group on the left from four mitochondrial crystal structures which were assembled and aligned according to their anchor portions.

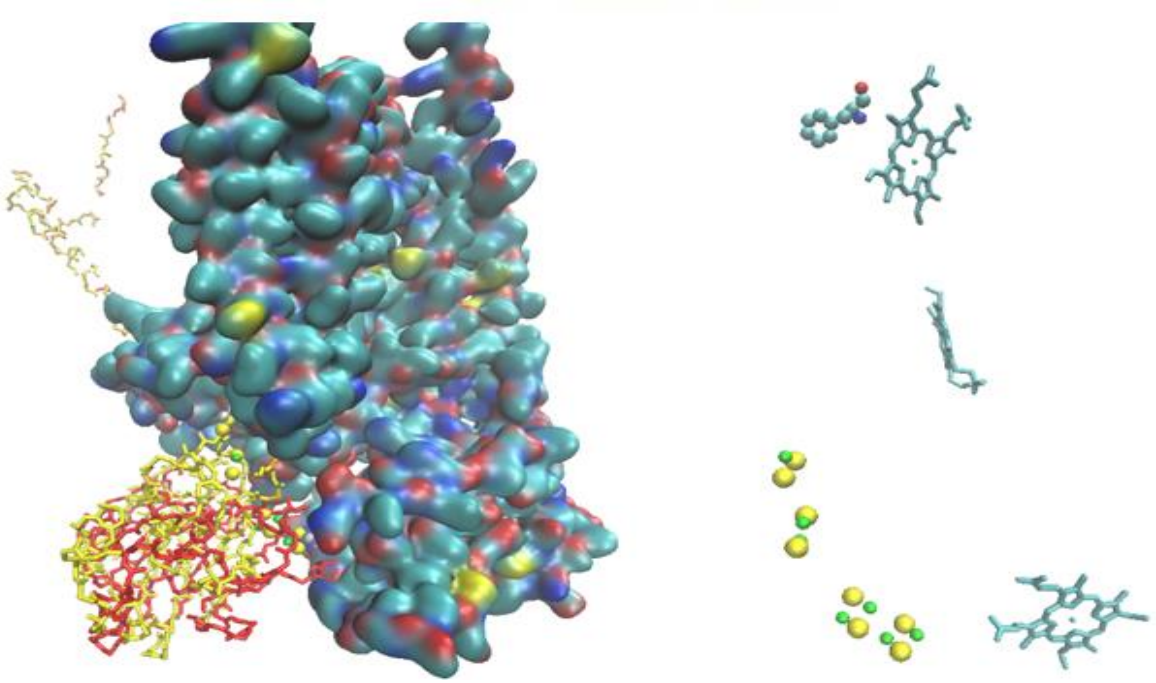

Figure 6.1 Mitochondrial bc_1 complex with ISP structures from four mitochondrial bc_1 complexes aligned to the anchor portion. The figure on the left has the first and last head group positions indicated by corresponding, respective yellow and red head group backbone representations. On the right the protein has been removed leaving the FES clusters for the four positions and the cyt c_1, and the cyt b hemes (heme b_L and heme b_H).

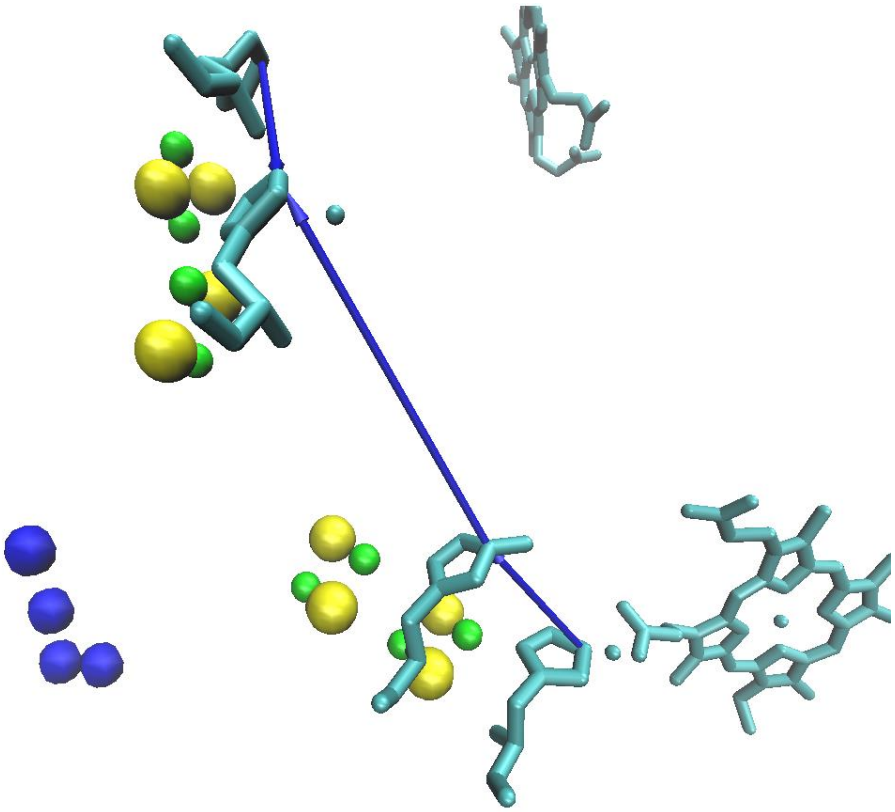

Figure 6.2 The center of mass of the ISP head group of each position of the four aligned head group position is shown as blue spheres and blue vectors are drawn connecting the liganding histidine of the FeS cluster.

The head displacement appears to be a complicated process included in the dynamic process of gating the electron transfer (Fig. 6.2). The process is more complicated than a group rotation of the ISP head group around a pivot. An example of the way the motion is complex is shown by the difference in the paths taken by the liganding His152 of the FeS cluster (blue arrows) vs the path of the center of mass of the ISP head group (blue spheres) in Figure 6.2. The blue spheres located at the calculated center of mass for the head group show a boomerang shaped trajectory where the center of mass turns sharply upward in the last frame where the head group achieves closest approach to the propionate of cytochrome c_1.

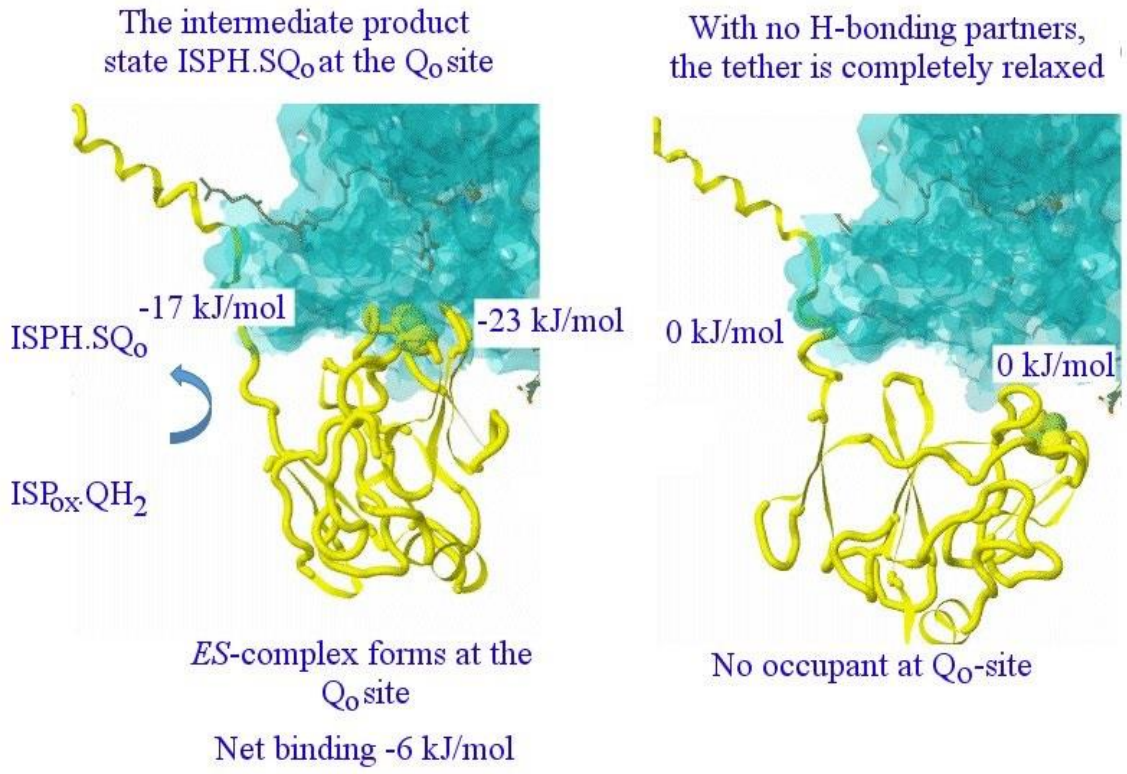

Figure 6.3 The ISP subunit from structures of mitochondrial *bc*$_1$ complexes showing conformations that change with the occupancy of the Q_o-site (adapted from (*1-4*)). The structures show ISP with the fully extended tether (left) on binding at the Q_o-site (here with stigmatellin) and with the fully relaxed tether (right) when no bond is formed with a Q_o-site occupant.

The extrinsic head of ISP moves to dock on cyt *b*, and the driving force is associated with substrate binding (predominantly, the H-bond with His-152) and the protein interfaces involved. The work involved in binding contributes one set of the counteracting forces in the spring-loaded scenario. The other set of forces is associated with a change from helical to elongated chain in the tether span where the suppressor mutations are located. The binding force pulls on the tether to extend it. In the spring-loaded mechanism (*6, 7, 77*), the experimentally determined binding free-energy (~-6 kJ/mol) is the difference between the work involved in binding (-23 kJ/mol), and the work needed to extend the tether (-17 kJ/mol), referred to the relaxed state. The values shown are estimated from work on ISP mutants in *Rb. capsulatus* and *Rb. Sphaeroides (77-80).* The curved arrow shows the first electron transfer reaction after formation of the *ES*-complex.

ES-complex Separation: A Fortunate Accident

When the antimycin was inserted to replace Q in the fully oxidized configuration (conf1) it was positioned (through carelessness) in such a way that one of the DVPG lipid tails was lassoed by the ring of the antimycin, as shown in the top portion of Fig. 6.4. During extensive minimization after setup, no error message was generated by the software to indicate that improper steric constraints were involved, and no error was indicated during the subsequent simulation, and the lassoed lipid tail in the antimycin ring was not detected until the trajectory generated by the simulation (conf1_2, run for 77 ns) was examined; the anomalous exit of QH_2 from one of the Q_o-sites required an asymmetric driving force, and the cause then became apparent. After the mistake was detected, the antimycin position was corrected so the lipid tail did not intersect the antimycin ring. The resultant configuration (conf1_3) was then run. The major difference between these two configuration trajectories was the release of the ES complex observed in conf1_2.

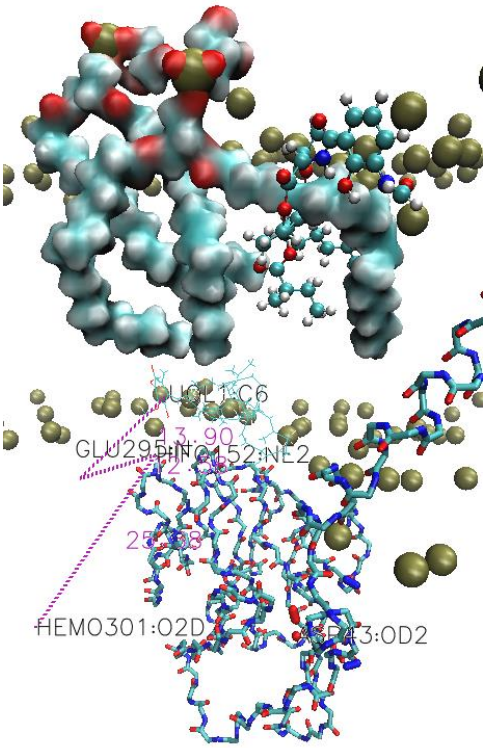

Figure 6.4 Lipid fatty acid tail of a DVPG membrane lipid penetrates one of the rings of the antimycin in the Q_i-site.

The first and last frames of the conf1_2 trajectory are shown in Figure 6.5. With regard to the separation of the ES complex the conf1_2 trajectory shows a small amount of movement of the FeS cluster toward the electron accepter of the cyt c_1 propianate located at the second catalytic interface for the ISP head group. The distance from the cluster liganding His152: NE to

the cyt c_2 heme propionate changes 2.24 Å from the time zero through to 77 ns. The quinol pulls away from the ISP head group and then leaves the channel leading out of Q_o-site.

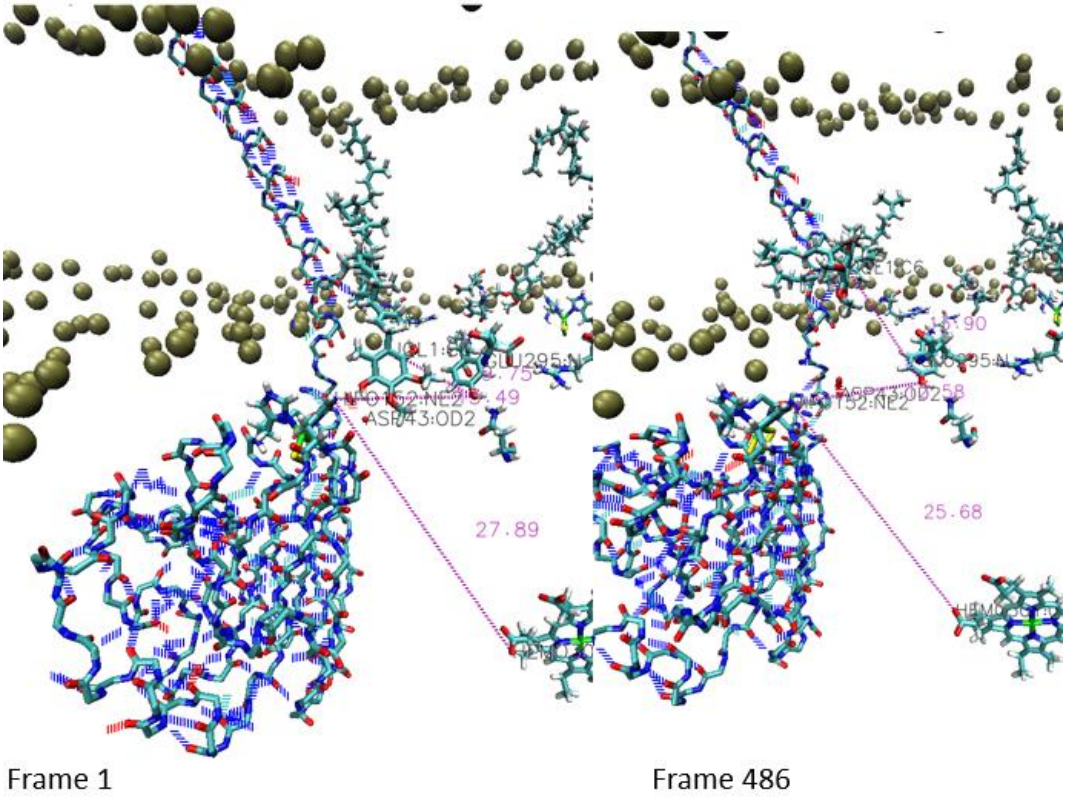

Figure 6.5 Representations from the first and last frames of the conf1_2 configuration trajectory

The absolute motion of the quinol head group relative to its position in the first frame fails to show the relative motions of the head group and the quinol. Figure 6.6 shows the absolute motion of the ISP center of mass (ISP_CofM), ISP FeS cluster (FES2_vo), and the quinol head group (UqH2head_movement). All of these motions appear substantial and relatively fast compared to the time frame in which they are required to occur in. However, the distance the center of mass of the protein moves from its initial position explains much of the large scale absolute movement of the ISP head group.

During the 77 ns trajectory of conf1_2 the net motion is consistent with ranges defined by experiments observing effects of different experimental conditions on rate limiting processes which occur after ES complex separation. So a better way to observe the motions is by looking

at the separation distance between the participants in the ES complex, i.e., ISP head group, ubiquinol, and cyt b (Fig. 6.6). The destination of the ISP head group for passing an electron, as indicated by the bond shown to the propionate in Fig 6.5, is cyt c_1 and constitutes a second catalytic interface for the ISP head group.

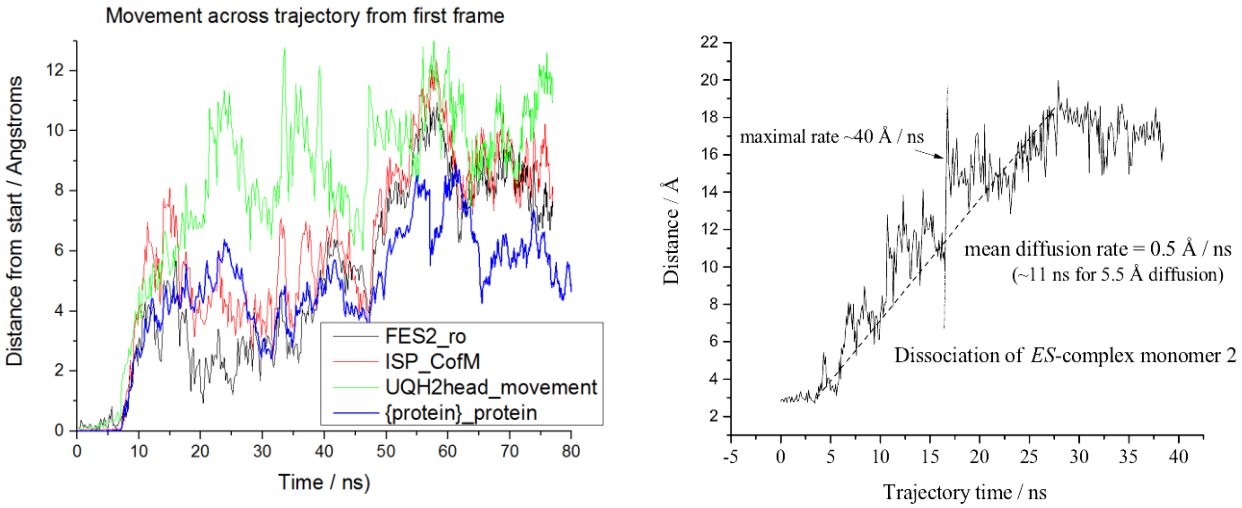

Figure 6.6 Left: Movement of the FES cluster center of mass (FES2_ro), the ISP head group center of mass (ISP_CofM), ubiquinol head center of mass movement (UQH2head_movement) and protein center of mass movement (protein_protein) where the movement in Angstroms is the magnitude of the displacement vector measured from the initial position at time 0 ns. Right. Exit of QH_2 measured by the distance between QH_2 -O and ISP H152 Nε.

Relative distances or separation distances between His152: NE (the epsilon nitrogen) and QH_2 (right) allows visualization of the diffusion of the QH_2 out of the Q_o-site. The pathway followed is through the access channel from the lipid phase, so this diffusion is essentially 1-D. The kinetic parameters from measurements of turnover of partial processes show that entry and exit of Q or QH_2 is rapid compared to the rate limiting step (10^3 s^{-1}), so the diffusional rate shown here would certainly allow rapid passage. However, this needs to be applied in determination of collisional frequency to relate it to kinetics. The diffusional rates are also relevant in the Q_o-site mechanism, where the SQ_o must move closer to heme b_L to transfer the electron rapidly. In the kinetic model, this process has a rate ~10^7 s^{-1} and the SQ_o moves through ~5.5 Å̊, so the mean rate seen here is quite sufficient (see Fig.6.6, right). Also shown are

distances to the heme propionate of cyt c_1 (Hem:O) and a relatively fixed point near the opening of the Q_o-site, Tyr147, are shown in Fig. 6.7. The distance between the quinol and the point picked to represent a fixed position relative to the protein, Tyr147, is also shown in Fig. 6.7. The ISP head group moves about 5 Å closer to the heme propionate of cyt c_1 within 13 frames and then oscillates within 2 to 5 Å for the rest of the trajectory (Fig. 6.7). The His152: NE of the ISP head group moves at much as 3 Å from the Tyr147 in 8 frames and then oscillates between that distance and 1 Å separation. The distance of separation of the quinol head group from proximate to the Tyr147 to outside the Q_o-site entry way shows an abrupt quick change and then gradual steps in and out of the entry way until the head group of UQH_2 is situated well outside the Q_o-site after 20 frames which is about 40 ns of simulation time since the trajectory starts at a 2 fs time step (Fig. 6.7)

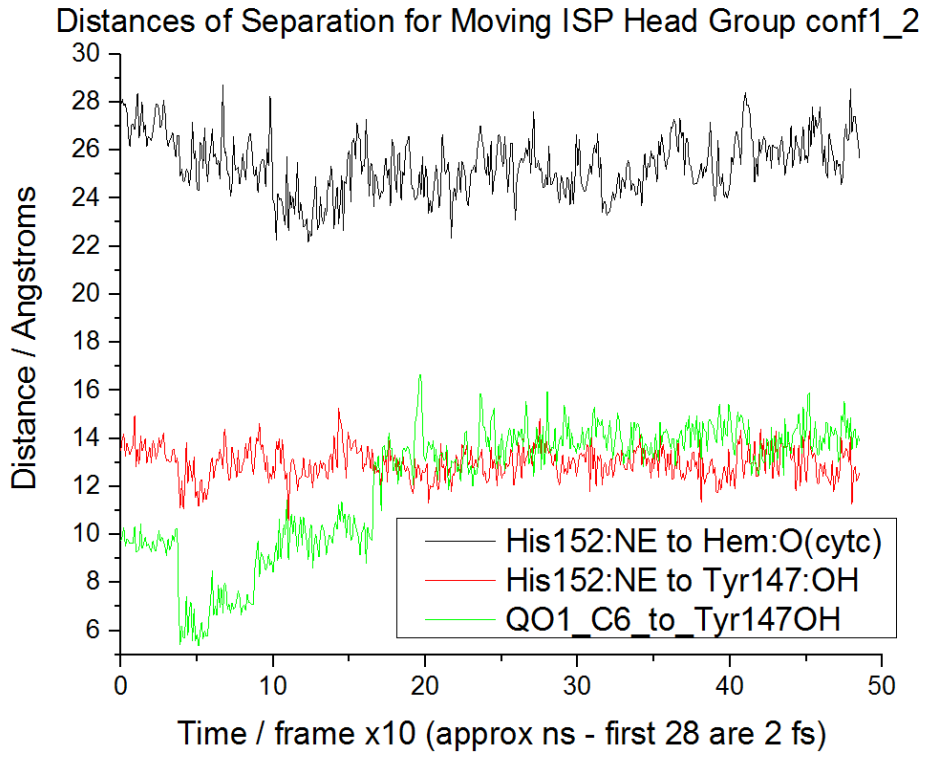

Figure 6.7 distances of separation between the indicated protein residue Tyr147, liganding His152 and cyt c_1 propianate.

Changes in the tether region are shown in Figure 6.8 which shows the formation of various hydrogen bond from before ES complex separation (frame 0) to after ES – complex formation. The ISP tether region is represented with only the backbone atoms. The hydrogen bonds can be seen more easily but since some hydrogen bonds are forming with side chains and surrounding residues, they seem to float proximate to the ISP tether region representation. The indicated bonds between arbitrarily picked pairs of points along the tether region have their separation distances graphed in Fig 6.10. As seen in Fig. 6.10 this portion of the tether region seems to be relaxing toward a more structured configuration with more interlinking hydrogen

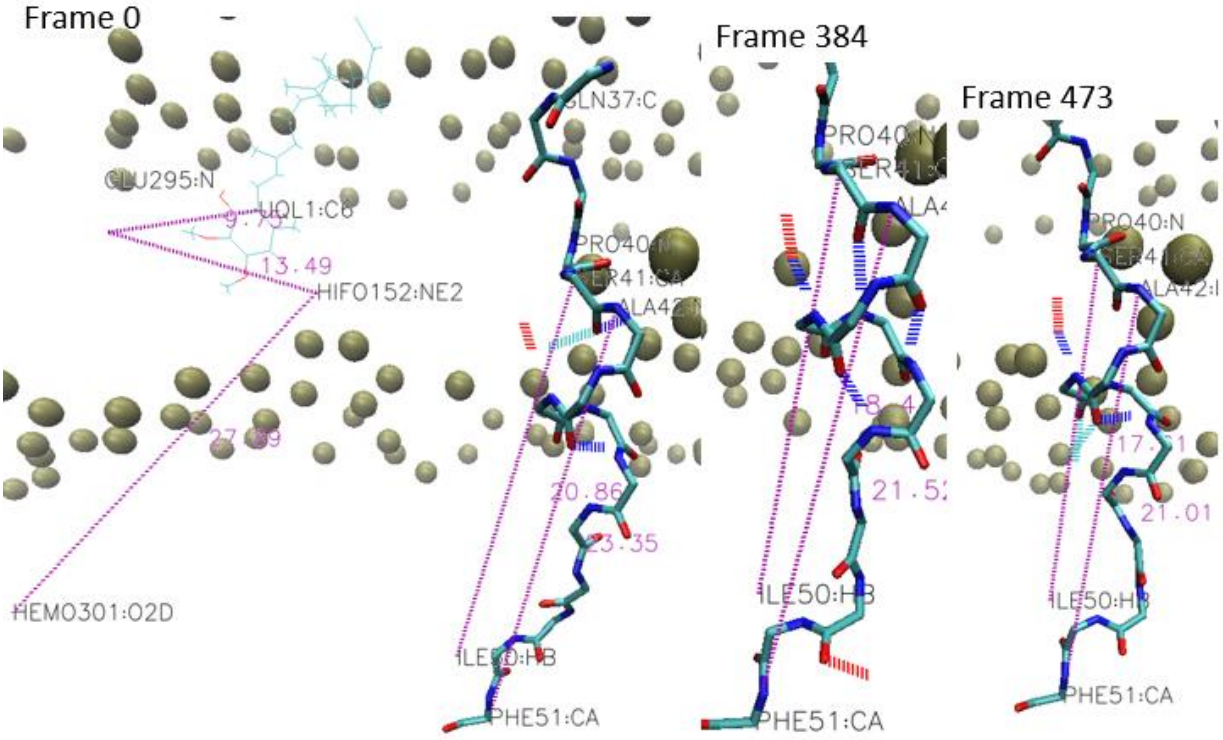

Figure 6.8 Changes in the ISP tether region for conf1_2 with bond indications from Fig. 6.5 left in to give context to the ISP tether region represented with only the back bone and hydrogen bonds indicated with thick broken red and blue lines.

bonds. These additional hydrogen bonds are part of the gating force for the ES complex as discussed above with reference to the calculation of these relative forces shown in Fig. 6.3. The number and frequency of hydrogen bonds can be tracked with the VMD timeline plugin shown in Fig. 6.10.

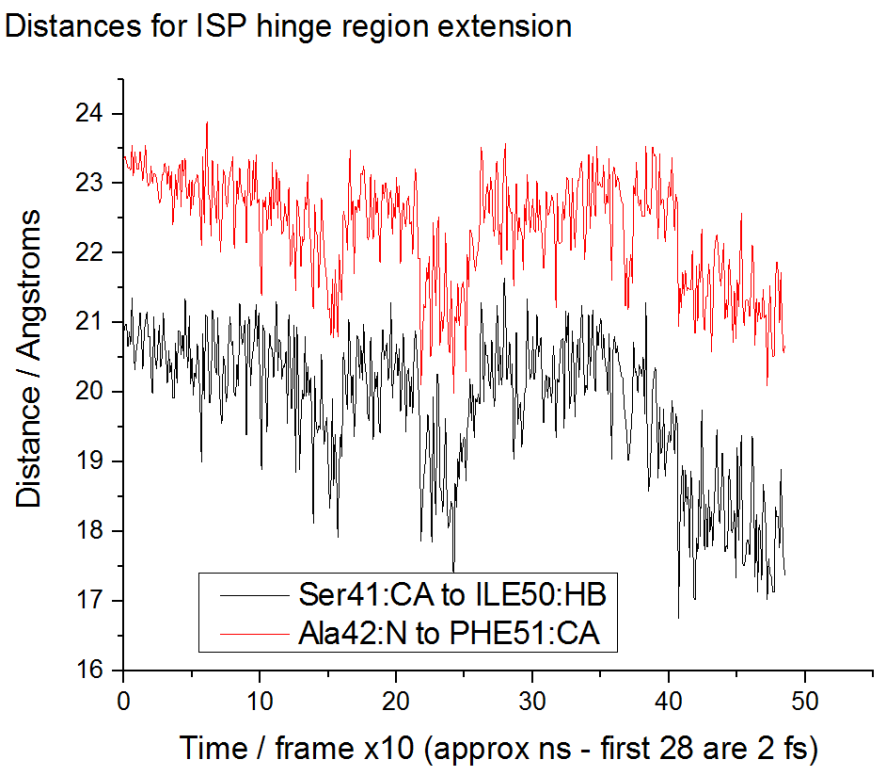

Figure 6.9 Distances between the two pairs of arbitrarily selected points along the ISP tether region as indicated in Figure 6.8.

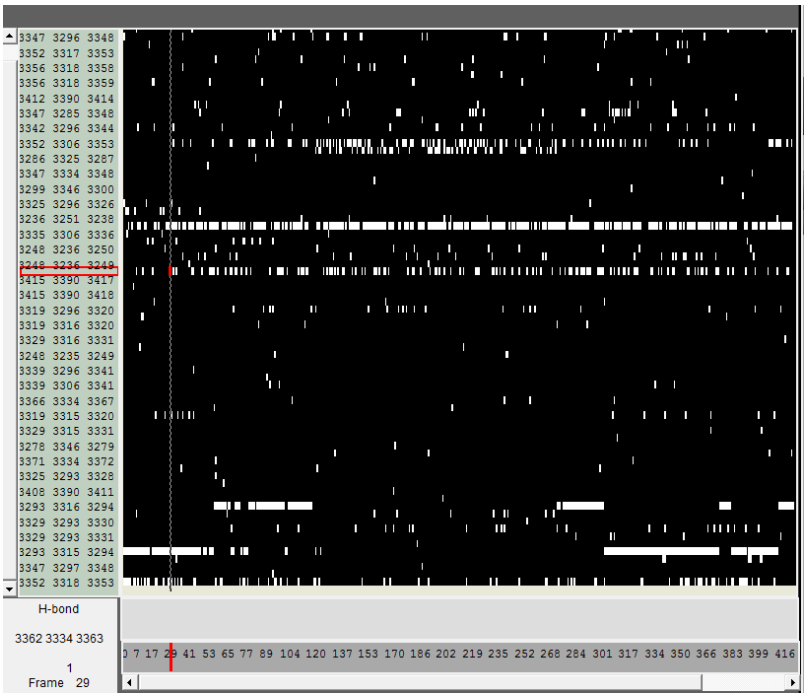

Figure 6.10 Timeline representation of H-bonding across conf1_2 trajectory where the color scheme is a binary representation of the presence or absence of an H-bond according to the H-bond definition so that white portions show frames in which an H-bond exists and black portions show when there is no H-bond.

The energy parameters can be entered into the kinetic model to (i.) compare to earlier guesses based on different assumptions; and (ii.) adjust other parameters by using these energy terms change the other terms by changing the partitioning of energy between partial processes in the kinetic model. These experiments will help characterize a mechanism which is predicted to be ‘spring-loaded’ with respect to the ISP headgroup involvement.

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Appendixes

Appendix A. Membrane Lipid Topologies

File: < RbSph_C36_lipid.inp>

```
*>>>>>>>>CHARMM36 All-Hydrogen Topology File for Proteins <<<<<<
*>>>>> Includes phi, psi cross term map (CMAP) correction <<<<<<<
*>>>>>>>>>>>>>>>>>>>>>>>>>> May 2015 <<<<<<<<<<<<<<<<<<<<<<<<<<
* All comments to the CHARMM web site: www.charmm.org
*             parameter set discussion forum
*

!List of membrane lipids:
!      1.  RESI DVPC       0.00 !  2,3-divaccenyl-D-glycero-1-phosphatidylcholine
!      1a. RESI VSPC
!      2.  RESI CDL     -2.00 !  (Not finished)
!      3.  RESI DVPG    -1.00 ! 2,3-divacenyl-D-glycero-1-phosphatidylglycerol
!      3a. RESI VSPG
!      4.  RESI DVPE       0.00 ! 2,3-divacenyl-D-glycero-1-phosphatidylethanolamine
!      4a.    RESI VSPE
!      5.  RESI SQDG              !sulfoquinovosyldiacylglycerol


! PCs


RESI DVPC    0.00  !  2,3-divaccenyl-D-glycero-1-phosphatidylcholine
!  Vaccenyl - CH2
!              |
!  Vaccenyl -  CH
!              |     (-)              (+)
!              CH2 - PO4 - CH2 - CH2 - N-(CH3)3!
!
!!Derived form the following files
!!     By Stuart Rose 9/10/2013 - Use of IC files was different between these two:
!!
!!RESI DOPC         0.00 ! 2,3-dioleoyl-D-glycero-1-phosphatidylcholine
!!
!!RESI POPC         0.00 ! 3-palmitoyl-2-oleoyl-D-glycero-1-Phosphatidylcholine
!!
!!  Palmitoyl - CH2
!!              |
!!     Oleyol - CH
!!              |     (-)              (+)
!!              CH2 - PO4 - CH2 - CH2 - N-(CH3)3
!!
!! Polar Head and glycerol backbone
!!
GROUP                   !               H15B
ATOM N    NTL    -0.60 !                 |
ATOM C12  CTL2   -0.10 !           H15A-C15-H15C
ATOM H12A HL      0.25 !                 |
ATOM H12B HL      0.25 !         H13B    |    H14A
ATOM C13  CTL5   -0.35 !           |     |     |
ATOM H13A HL      0.25 !     H13A-C13----N----C14-H14B     (+)
ATOM H13B HL      0.25 !           |     |     |
ATOM H13C HL      0.25 !         H13C    |    H14C
ATOM C14  CTL5   -0.35 !                 |
ATOM H14A HL      0.25 !                 |
ATOM H14B HL      0.25 !                 |    alpha6
```

```
ATOM H14C HL      0.25 !                 |
ATOM C15  CTL5   -0.35 !                 |
ATOM H15A HL      0.25 !          H12A--C12---H12B
ATOM H15B HL      0.25 !                 |
ATOM H15C HL      0.25 !                 |
GROUP                  !                 |     alpha5
ATOM C11  CTL2   -0.08 !                 |
ATOM H11A HAL2    0.09 !          H11A--C11---H11B
ATOM H11B HAL2    0.09 !                 |     alpha4
ATOM P    PL      1.50 !        (-) O13  O12
ATOM O13  O2L    -0.78 !              \ /      alpha3
ATOM O14  O2L    -0.78 !               P (+)
ATOM O12  OSLP   -0.57 !              / \      alpha2
ATOM O11  OSLP   -0.57 !        (-) O14  O11
ATOM C1   CTL2   -0.08 !                 |     alpha1
ATOM HA   HAL2    0.09 !             HA---C1---HB
ATOM HB   HAL2    0.09 !                 |     theta1
GROUP                  !                 |
ATOM C2   CTL1    0.17 !             HS---C2--------------
ATOM HS   HAL1    0.09 !                  | beta1        |
ATOM O21  OSL    -0.49 !             O22  O21          theta3
ATOM C21  CL      0.90 !              \\ /  beta2        |
ATOM O22  OBL    -0.63 !                C21             |
ATOM C22  CTL2   -0.22 !                |   beta3        |
ATOM H2R  HAL2    0.09 !        H2R---C22---H2S         |
ATOM H2S  HAL2    0.09 !                |                 |
GROUP                  !                |    beta4        |
ATOM C3   CTL2    0.08 !                |                 |
ATOM HX   HAL2    0.09 !                |           HX---C3---HY
ATOM HY   HAL2    0.09 !                |                 |   gamma1
ATOM O31  OSL    -0.49 !                |           O32  O31
ATOM C31  CL      0.90 !                |            \\ /    gamma2
ATOM O32  OBL    -0.63 !                |              C31
ATOM C32  CTL2   -0.22 !                |              |     gamma3
ATOM H2X  HAL2    0.09 !                |        H2X---C32---H2Y
ATOM H2Y  HAL2    0.09 !                |               |
GROUP                  !                |               |      gamma4
ATOM C23  CTL2   -0.18 !                |               |
ATOM H3R  HAL2    0.09 !        H3R ---C23---H3S        |
ATOM H3S  HAL2    0.09 !                |               |
GROUP                  !                |               |
ATOM C24  CTL2   -0.18 !                |               |
ATOM H4R  HAL2    0.09 !        H4R ---C24---H4S        |
ATOM H4S  HAL2    0.09 !                |               |
GROUP                  !                |               |
ATOM C25  CTL2   -0.18 !                |               |
ATOM H5R  HAL2    0.09 !        H5R ---C25---H5S        |
ATOM H5S  HAL2    0.09 !                |               |
GROUP                  !                |               |
ATOM C26  CTL2   -0.18 !                |               |
ATOM H6R  HAL2    0.09 !        H6R ---C26---H6S        |
ATOM H6S  HAL2    0.09 !                |               |
GROUP                  !                |               |
ATOM C27  CTL2   -0.18 !                |               |
ATOM H7R  HAL2    0.09 !        H7R ---C27---H7S        |
ATOM H7S  HAL2    0.09 !                |               |
GROUP                  !                |               |
ATOM C28  CTL2   -0.18 !                |               |
ATOM H8R  HAL2    0.09 !        H8R ---C28---H8S        |
ATOM H8S  HAL2    0.09 !                |               |
GROUP                  !                |               |
ATOM C29  CTL2   -0.18 !                |               |
ATOM H9R  HAL2    0.09 !        H9R ---C29---H9S        |
ATOM H9S  HAL2    0.09 !                |               |
```

```
GROUP                  !               |              |
ATOM C210 CTL2   -0.18 !               |              |
ATOM H10R HAL2    0.09 !        H10R---C210--H10S     |
ATOM H10S HAL2    0.09 !               |              |
GROUP                  !               |              |
ATOM C211 CEL1   -0.15 !               |              |
ATOM H11R HEL1    0.15 !        H11R --C211           |
GROUP                  !               ||  (CIS)      |
ATOM C212 CEL1   -0.15 !               ||             |
ATOM H12R HEL1    0.15 !        H12R---C212           |
GROUP                  !               |              |
ATOM C213 CTL2   -0.18 !               |              |
ATOM H13R HAL2    0.09 !        H13R---C213--H13S     |
ATOM H13S HAL2    0.09 !               |              |
GROUP                  !               |              |
ATOM C214 CTL2   -0.18 !               |              |
ATOM H14R HAL2    0.09 !        H14R---C214--H14S     |
ATOM H14S HAL2    0.09 !               |              |
GROUP                  !               |              |
ATOM C215 CTL2   -0.18 !               |              |
ATOM H15R HAL2    0.09 !        H15R---C215--H15S     |
ATOM H15S HAL2    0.09 !               |              |
GROUP                  !               |              |
ATOM C216 CTL2   -0.18 !               |              |
ATOM H16R HAL2    0.09 !        H16R---C216--H16S     |
ATOM H16S HAL2    0.09 !               |              |
GROUP                  !               |              |
ATOM C217 CTL2   -0.18 !               |              |
ATOM H17R HAL2    0.09 !        H17R---C217--H17S     |
ATOM H17S HAL2    0.09 !               |              |
GROUP                  !               |              |
ATOM C218 CTL3   -0.27 !               |              |
ATOM H18R HAL3    0.09 !        H18R---C218--H18S     |
ATOM H18S HAL3    0.09 !               |              |
ATOM H18T HAL3    0.09 !             H18T             |
GROUP                  !                              |
ATOM C33  CTL2   -0.18 !                              |
ATOM H3X  HAL2    0.09 !                      H3X ---C33---H3Y
ATOM H3Y  HAL2    0.09 !                             |
GROUP                  !                             |
ATOM C34  CTL2   -0.18 !                             |
ATOM H4X  HAL2    0.09 !                      H4X ---C34---H4Y
ATOM H4Y  HAL2    0.09 !                             |
GROUP                  !                             |
ATOM C35  CTL2   -0.18 !                             |
ATOM H5X  HAL2    0.09 !                      H5X ---C35---H5Y
ATOM H5Y  HAL2    0.09 !                             |
GROUP                  !                             |
ATOM C36  CTL2   -0.18 !                             |
ATOM H6X  HAL2    0.09 !                      H6X ---C36---H6Y
ATOM H6Y  HAL2    0.09 !                             |
GROUP                  !                             |
ATOM C37  CTL2   -0.18 !                             |
ATOM H7X  HAL2    0.09 !                      H7X ---C37---H7Y
ATOM H7Y  HAL2    0.09 !                             |
GROUP                  !                             |
ATOM C38  CTL2   -0.18 !                             |
ATOM H8X  HAL2    0.09 !                      H8X ---C38---H8Y
ATOM H8Y  HAL2    0.09 !                             |
GROUP                  !                             |
ATOM C39  CTL2   -0.18 !                             |
ATOM H9X  HAL2    0.09 !                      H9X ---C39---H9Y
ATOM H9Y  HAL2    0.09 !                             |
GROUP                  !                             |
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ATOM C310 CTL2   -0.18 !                          |
ATOM H10X HAL2    0.09 !                    H10X---C310--H10Y
ATOM H10Y HAL2    0.09 !                          |
GROUP                  !                          |
ATOM C311 CEL1   -0.15 !                          |
ATOM H11X HEL1    0.15 !                    H11X---C311
GROUP                  !                          ||
ATOM C312 CEL1   -0.15 !                          ||
ATOM H12X HEL1    0.15 !                    H12X---C312
GROUP                  !                          |
ATOM C313 CTL2   -0.18 !                          |
ATOM H13X HAL2    0.09 !                    H13X---C313--H13Y
ATOM H13Y HAL2    0.09 !                          |
GROUP                  !                          |
ATOM C314 CTL2   -0.18 !                          |
ATOM H14X HAL2    0.09 !                    H14X---C314--H14Y
ATOM H14Y HAL2    0.09 !                          |
GROUP                  !                          |
ATOM C315 CTL2   -0.18 !                          |
ATOM H15X HAL2    0.09 !                    H15X---C315--H15Y
ATOM H15Y HAL2    0.09 !                          |
GROUP                  !                          |
ATOM C316 CTL2   -0.18 !                          |
ATOM H16X HAL2    0.09 !                    H16X---C316--H16Y
ATOM H16Y HAL2    0.09 !                          |
GROUP                  !                          |
ATOM C317 CTL2   -0.18 !                          |
ATOM H17X HAL2    0.09 !                    H17X---C317--H17Y
ATOM H17Y HAL2    0.09 !                          |
GROUP                  !                          |
ATOM C318 CTL3   -0.27 !                          |
ATOM H18X HAL3    0.09 !                    H18X---C318--H18Y
ATOM H18Y HAL3    0.09 !                          |
ATOM H18Z HAL3    0.09 !                         H18Z

! Polar Head
BOND  N    C13       N    C14       N    C15
BOND  C13  H13A      C13  H13B      C13  H13C
BOND  C14  H14A      C14  H14B      C14  H14C
BOND  C15  H15A      C15  H15B      C15  H15C
BOND  N    C12
BOND  C12  H12A      C12  H12B      C12  C11
BOND  C11  H11A      C11  H11B      C11  O12       O11  C1
BOND  O12  P         P    O11       P    O13       P    O14
! Glycerol Backbone
BOND  C1   HA        C1    HB       C1   C2
BOND  C2   HS        C2    C3       C2   O21
BOND  C3   HX        C3    HY       C3   O31
! Chain from C2
BOND  O21  C21
BOND  C21  C22
DOUBLE  C21  O22
BOND  C22  H2R       C22  H2S       C22  C23
BOND  C23  H3R       C23  H3S       C23  C24
BOND  C24  H4R       C24  H4S       C24  C25
BOND  C25  H5R       C25  H5S       C25  C26
BOND  C26  H6R       C26  H6S       C26  C27
BOND  C27  H7R       C27  H7S       C27  C28
BOND  C28  H8R       C28  H8S       C28  C29
BOND  C29  H9R       C29  H9S       C29  C210
BOND  C210 H10R      C210 H10S      C210 C211
BOND  C211 H11R
DOUBLE  C211 C212
BOND  C212 H12R      C212 C213
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BOND  C213 H13R      C213 H13S      C213 C214
BOND  C214 H14R      C214 H14S      C214 C215
BOND  C215 H15R      C215 H15S      C215 C216
BOND  C216 H16R      C216 H16S      C216 C217
BOND  C217 H17R      C217 H17S      C217 C218
BOND  C218 H18R      C218 H18S      C218 H18T
! Chain From C3
BOND  O31  C31
BOND  C31  C32
DOUBLE  C31  O32
BOND  C32  H2X       C32  H2Y       C32  C33
BOND  C33  H3X       C33  H3Y       C33  C34
BOND  C34  H4X       C34  H4Y       C34  C35
BOND  C35  H5X       C35  H5Y       C35  C36
BOND  C36  H6X       C36  H6Y       C36  C37
BOND  C37  H7X       C37  H7Y       C37  C38
BOND  C38  H8X       C38  H8Y       C38  C39
BOND  C39  H9X       C39  H9Y       C39  C310
BOND  C310 H10X      C310 H10Y      C310 C311
BOND  C311 H11X
DOUBLE C311 C312
BOND  C312 H12X      C312 C313
BOND  C313 H13X      C313 H13Y      C313 C314
BOND  C314 H14X      C314 H14Y      C314 C315
BOND  C315 H15X      C315 H15Y      C315 C316
BOND  C316 H16X      C316 H16Y      C316 C317
BOND  C317 H17X      C317 H17Y      C317 C318
BOND  C318 H18X      C318 H18Y      C318 H18Z

IMPR C21 O21 C22 O22    C31 O31 C32 O32

IC C15    N      C12    C11        1.5031  108.03  -62.19  116.82   1.5409
IC C13    C12    *N     C14        1.4955  110.60  122.73  109.67   1.4976
IC C13    C12    *N     C15        1.4955  110.60 -119.76  108.04   1.5032
IC C13    N      C12    C11        1.4955  110.60   57.52  116.83   1.5412
IC C11    N      *C12   H12A       1.5412  116.83 -126.40  111.94   1.0787
IC H12A   N      *C12   H12B       1.0787  111.94 -116.29  108.17   1.0974
IC C14    N      C13    H13A       1.4976  110.99  179.50  109.35   1.0869
IC H13A   N      *C13   H13B       1.0869  109.35  118.93  111.32   1.0813
IC H13A   N      *C13   H13C       1.0869  109.35 -119.04  111.19   1.0811
IC C13    N      C14    H14A       1.4955  110.99 -179.22  109.65   1.0877
IC H14A   N      *C14   H14B       1.0877  109.65  118.74  110.91   1.0820
IC H14A   N      *C14   H14C       1.0877  109.65 -119.76  111.49   1.0812
IC C13    N      C15    H15A       1.4955  109.44  -64.69  111.04   1.0951
IC H15A   N      *C15   H15B       1.0951  111.04  123.93  113.87   1.0740
IC H15A   N      *C15   H15C       1.0951  111.04 -112.38  110.25   1.0938
IC N      C12    C11    O12        1.5223  116.83  127.52  108.22   1.4232
IC O12    C12    *C11   H11A       1.4232  108.22 -123.07  113.25   1.1138
IC H11A   C12    *C11   H11B       1.1138  113.25 -118.71  109.20   1.1129
IC C12    C11    O12    P          1.5412  108.22  -67.94  118.41   1.5875
IC C11    O12    P      O11        1.4232  118.41 -166.85  104.05   1.5781
IC O11    O12    *P     O13        1.5781  104.05  117.80  108.05   1.4795
IC O11    O12    *P     O14        1.5781  104.05 -117.37  106.82   1.4822
IC O12    P      O11    C1         1.5875  104.05  167.61  118.26   1.4316
IC P      O11    C1     C2         1.5781  118.26  168.12  110.80   1.5508
IC C2     O11    *C1    HA         1.5508  110.80 -119.17  111.41   1.1170
IC HA     O11    *C1    HB         1.1170  111.41 -120.80  110.01   1.1146
IC O11    C1     C2     C3         1.4316  110.80  176.77  110.71   1.5573
IC C3     C1     *C2    O21        1.5573  110.71  120.62  108.02   1.4410 !defines S
chirality
IC C3     C1     *C2    HS         1.5573  110.71 -118.37  106.71   1.1170 !defines S
chirality
IC C1     C2     O21    C21        1.5508  108.02  147.52  115.15   1.3177
IC C2     O21    C21    C22        1.4410  115.15  179.16  108.63   1.5289
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IC C22    O21    *C21   O22        1.5289  108.63 -178.85  126.55   1.2187
IC O21    C21    C22    C23        1.3177  108.63 -177.70  112.21   1.5449
IC C23    C21    *C22   H2R        1.5449  112.21 -121.72  107.88   1.1092
IC H2R    C21    *C22   H2S        1.1092  107.88 -117.16  107.60   1.1093
IC C1     C2     C3     O31        1.5508  110.71  176.05  112.62   1.4438
IC O31    C2     *C3    HX         1.4438  112.62 -118.51  106.65   1.1128
IC HX     C2     *C3    HY         1.1128  106.65 -115.12  109.46   1.1145
IC C2     C3     O31    C31        1.5573  112.62   87.12  115.04   1.3313
IC C3     O31    C31    C32        1.4438  115.04 -172.98  108.55   1.5288
IC C32    O31    *C31   O32        1.5288  108.55 -178.89  125.60   1.2170
IC O31    C31    C32    C33        1.3313  108.55 -166.73  113.05   1.5447
IC C33    C31    *C32   H2X        1.5447  113.05 -121.10  107.23   1.1103
IC H2X    C31    *C32   H2Y        1.1103  107.23 -117.00  108.11   1.1090
IC C21    C22    C23    C24        1.5289  112.21  175.76  112.39   1.5338
IC C24    C22    *C23      H3R             1.5360  113.21 -119.83  108.42   1.1148
IC C24    C22    *C23      H3S             1.5396  113.52 -123.43  110.53   1.1101
IC C22    C23    C24       C25             1.5450  113.21 -172.34  113.68   1.5399
IC C25    C23    *C24      H4R             1.5399  113.68  120.91  108.91   1.1136
IC C25    C23    *C24      H4S             1.5396  113.52 -123.43  110.53   1.1101
IC C23    C24    C25       C26             1.5360  113.68  -56.95  113.57   1.5353
IC C26    C24    *C25      H5R             1.5353  113.57  121.41  108.70   1.1129
IC C26    C24    *C25      H5S             1.5396  113.52 -123.43  110.53   1.1101
IC C24    C25    C26       C27             1.5399  113.57 -173.39  113.79   1.5375
IC C27    C25    *C26      H6R             1.5375  113.79  122.09  109.21   1.1127
IC C27    C25    *C26      H6S             1.5396  113.52 -123.43  110.53   1.1101
IC C25    C26    C27       C28             1.5353  113.79  177.45  113.35   1.5458
IC C28    C26    *C27      H7R             1.5458  113.35  119.87  108.07   1.1139
IC C28    C26    *C27      H7S             1.5396  113.52 -123.43  110.53   1.1101
IC C26    C27    C28       C29        1.5399  113.57 -173.39  113.79   1.5375
IC C29    C27    *C28      H8R             1.5375  113.79  122.09  109.21   1.1127
IC C29    C27    *C28      H8S             1.5396  113.52 -123.43  110.53   1.1101
IC C27    C28    C29       C210            1.5353  113.79  177.45  113.35   1.5458
IC C210   C28    *C29      H9R             1.5458  113.35  119.87  108.07   1.1139
IC C210   C28    *C29      H9S             1.5396  113.52 -123.43  110.53   1.1101
IC C28    C29    C210      C211            1.5375  113.35   67.78  114.46   1.5115
IC C211   C29    *C210     H10R            1.5115  114.46  121.34  107.89   1.1131
IC C211   C29    *C210     H10S            1.5396  113.52 -123.43  110.53   1.1101
IC C29    C210   C211      C212            1.5458  114.46  180.00  126.91   1.3502
IC C212   C210   *C211     H11R            1.3502  126.91 -178.81  114.69   1.1010
IC C210   C211   C212      C213            1.5115  126.91    0.00  126.69   1.5092
!cis db
IC C213   C210   *C212     H12R            1.5099  126.94 -177.42  118.69   1.1018
IC C211   C212   C213      C214       1.3502  126.69  180.00  111.86   1.5417
IC C214   C212   *C213     H13R            1.5396  113.52 -123.43  110.53   1.1101
IC C214   C212   *C213     H13S            1.5097  125.28  121.00  119.65   1.1004
IC C212   C213   C214      C215            1.5092  111.86  180.00  113.99   1.5334
IC C215   C213   *C214     H14R            1.5396  113.52 -123.43  110.53   1.1101
IC C215   C213   *C214     H14S            1.5097  125.28  121.00  119.65   1.1004
IC C213   C214   C215      C216            1.5417  113.99  180.00  111.46   1.5365
IC C216   C214   *C215     H15R            1.5396  113.52 -123.43  110.53   1.1101
IC C216   C214   *C215     H15S       1.5097  125.28  121.00  119.65   1.1004
IC C214   C215   C216      C217            1.5376  114.97  180.00  113.95   1.5347
IC C217   C215   *C216     H16R            1.5396  113.52 -123.43  110.53   1.1101
IC C217   C215   *C216     H16S            1.5097  125.28  121.00  119.65   1.1004
IC C215   C216   C217      C218            1.5385  113.95  180.00  113.05   1.5311
IC C218   C216   *C217     H17R            1.5396  113.52 -123.43  110.53   1.1101
IC C218   C216   *C217     H17S            1.5097  125.28  121.00  119.65   1.1004
IC C216   C217   C218      H18R            1.5347  113.05  180.00  110.58   1.1110
IC H18R   C217   *C218     H18S            1.5396  113.52 -123.43  110.53   1.1101
IC H18R   C217   *C218     H18T            1.5097  125.28  121.00  119.65   1.1004
IC C31    C32    C33    C34          1.5405  116.85  180.00  126.13   1.5951
IC C34    C32    *C33   H3X          1.5410  113.36 -119.96  111.74   1.1148
IC C34    C32    *C33   H3Y          1.5192  121.35  121.00  106.97   1.1128
IC C32    C33    C34    C35          1.6060  126.13  180.00  113.36   1.5410
```

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IC C35    C33    *C34   H4X         1.5396  113.52 -123.43  110.53   1.1101
IC C35    C33    *C34   H4Y         1.5192  121.35  121.00  106.97   1.1128
IC C33    C34    C35    C36         1.5951  113.36  180.00  113.52   1.5396
IC C36    C34    *C35   H5X         1.5396  113.52 -123.43  110.53   1.1101
IC C36    C34    *C35   H5Y         1.5192  121.35  123.34  106.97   1.1128
IC C34    C35    C36    C37         1.5410  113.52  180.00  114.47   1.5397
IC C37    C35    *C36   H6X         1.5396  113.52 -123.43  110.53   1.1101
IC C37    C35    *C36   H6Y         1.5192  121.35  123.34  106.97   1.1128
IC C35    C36    C37    C38         1.5396  114.47  180.00  113.41   1.5386
IC C38    C36    *C37   H7X         1.5396  113.52 -123.43  110.53   1.1101
IC C38    C36    *C37   H7Y         1.5192  121.35  123.34  106.97   1.1128
IC C36    C37    C38    C39         1.5397  113.41  180.00  113.71   1.5382
IC C39    C37    *C38   H8X         1.5396  113.52 -123.43  110.53   1.1101
IC C39    C37    *C38   H8Y         1.5192  121.35  123.34  106.97   1.1128
IC C37    C38    C39    C310        1.5353  113.79  177.45  113.35   1.5458
IC C310   C38    *C39   H9X         1.5458  113.35  119.87  108.07   1.1139
IC C310   C38    *C39   H9Y         1.5396  113.52 -123.43  110.53   1.1101
IC C38    C39    C310   C311        1.5375  113.35   67.78  114.46   1.5115
IC C311   C39    *C310  H10X        1.5115  114.46  121.34  107.89   1.1131
IC C311   C39    *C310  H10Y        1.5396  113.52 -123.43  110.53   1.1101
IC C39    C310   C311   C312        1.5458  114.46  180.00  126.91   1.3502
IC C312   C310   *C311  H11X        1.3502  126.91 -178.81  114.69   1.1010
IC C310   C311   C312   C313        1.5115  126.91    0.00  126.69   1.5092 !cis db
IC C313   C310   *C312  H12X        1.5099  126.94 -177.42  118.69   1.1018
IC C311   C312   C313   C314        1.3502  126.69  180.00  111.86   1.5417
IC C314   C312   *C313  H13X        1.5396  113.52 -123.43  110.53   1.1101
IC C314   C312   *C313  H13Y        1.5097  125.28  121.00  119.65   1.1004
IC C312   C313   C314   C315        1.5092  111.86  180.00  113.99   1.5334
IC C315   C313   *C314  H14X        1.5396  113.52 -123.43  110.53   1.1101
IC C315   C313   *C314  H14Y        1.5097  125.28  121.00  119.65   1.1004
IC C313   C314   C315   C316        1.5377  113.85  180.00  111.81   1.5374
IC C316   C314   *C315  H15X        1.5396  113.52 -123.43  110.53   1.1101
IC C316   C314   *C315  H15Y        1.5192  121.35  123.34  106.97   1.1128
IC C314   C315   C316   C317        1.5357  111.81  180.00  114.29   1.5985
IC C317   C315   *C316  H16X        1.5396  113.52 -123.43  110.53   1.1101
IC C317   C315   *C316  H16Y        1.5192  121.35  123.34  106.97   1.1128
IC C315   C316   C317   C318        1.5374  114.29  180.00  130.92   1.5745
IC C318   C316   *C317  H17X        1.5396  113.52 -123.43  110.53   1.1101
IC C318   C316   *C317  H17Y        1.5192  121.35  123.34  106.97   1.1128
IC C316   C317   C318   H18X        1.5985  130.92  180.00  110.90   1.1113
IC H18X   C317   *C318  H18Y       1.5396  113.52 -123.43  110.53   1.1101
IC H18X   C317   *C318  H18Z        1.5192  121.35  123.34  106.97   1.1128


RESI VSPC    0.00  !  3-vaccenoyl-2-steroyl-D-glycero-1-phosphatidylcholine
!  Vaccenyl - CH2
!              |
!  Vaccenyl -  CH
!              |     (-)              (+)
!              CH2 - PO4 - CH2 - CH2 - N-(CH3)3!
!
!!Derived form the following files
!!     By Stuart Rose 9/10/2013 - Use of IC files was different between these two:
!!
!!RESI DOPC         0.00 ! 2,3-dioleoyl-D-glycero-1-phosphatidylcholine
!!
!!RESI POPC         0.00 ! 3-palmitoyl-2-oleoyl-D-glycero-1-Phosphatidylcholine
!!
!!  Palmitoyl - CH2
!!              |
!!     Oleyol - CH
!!              |     (-)              (+)
!!              CH2 - PO4 - CH2 - CH2 - N-(CH3)3
!!
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```
!! Polar Head and glycerol backbone
!!
GROUP                  !               H15B
ATOM N    NTL    -0.60 !                 |
ATOM C12  CTL2   -0.10 !           H15A-C15-H15C
ATOM H12A HL      0.25 !                 |
ATOM H12B HL      0.25 !         H13B    |    H14A
ATOM C13  CTL5   -0.35 !           |     |     |
ATOM H13A HL      0.25 !     H13A-C13----N----C14-H14B     (+)
ATOM H13B HL      0.25 !           |     |     |
ATOM H13C HL      0.25 !         H13C    |    H14C
ATOM C14  CTL5   -0.35 !                 |
ATOM H14A HL      0.25 !                 |
ATOM H14B HL      0.25 !                 |    alpha6
ATOM H14C HL      0.25 !                 |
ATOM C15  CTL5   -0.35 !                 |
ATOM H15A HL      0.25 !          H12A--C12---H12B
ATOM H15B HL      0.25 !                 |
ATOM H15C HL      0.25 !                 |
GROUP                  !                 |     alpha5
ATOM C11  CTL2   -0.08 !                 |
ATOM H11A HAL2    0.09 !          H11A--C11---H11B
ATOM H11B HAL2    0.09 !                 |     alpha4
ATOM P    PL      1.50 !        (-) O13  O12
ATOM O13  O2L    -0.78 !              \ /      alpha3
ATOM O14  O2L    -0.78 !               P (+)
ATOM O12  OSLP   -0.57 !              / \      alpha2
ATOM O11  OSLP   -0.57 !        (-) O14  O11
ATOM C1   CTL2   -0.08 !                 |     alpha1
ATOM HA   HAL2    0.09 !            HA---C1---HB
ATOM HB   HAL2    0.09 !                 |     theta1
GROUP                  !                 |
ATOM C2   CTL1    0.17 !            HS---C2--------------
ATOM HS   HAL1    0.09 !                 | beta1        |
ATOM O21  OSL    -0.49 !            O22  O21          theta3
ATOM C21  CL      0.90 !             \\ /  beta2        |
ATOM O22  OBL    -0.63 !               C21              |
ATOM C22  CTL2   -0.22 !                |   beta3        |
ATOM H2R  HAL2    0.09 !        H2R---C22---H2S         |
ATOM H2S  HAL2    0.09 !                |                |
GROUP                  !                |    beta4       |
ATOM C3   CTL2    0.08 !                |                |
ATOM HX   HAL2    0.09 !                |           HX---C3---HY
ATOM HY   HAL2    0.09 !                |                |   gamma1
ATOM O31  OSL    -0.49 !                |           O32  O31
ATOM C31  CL      0.90 !                |            \\ /    gamma2
ATOM O32  OBL    -0.63 !                |              C31
ATOM C32  CTL2   -0.22 !                |              |     gamma3
ATOM H2X  HAL2    0.09 !                |        H2X---C32---H2Y
ATOM H2Y  HAL2    0.09 !                |              |
GROUP                  !                |              |      gamma4
ATOM C23  CTL2   -0.18 !                |              |
ATOM H3R  HAL2    0.09 !        H3R ---C23---H3S       |
ATOM H3S  HAL2    0.09 !                |              |
GROUP                  !                |              |
ATOM C24  CTL2   -0.18 !                |              |
ATOM H4R  HAL2    0.09 !        H4R ---C24---H4S       |
ATOM H4S  HAL2    0.09 !                |              |
GROUP                  !                |              |
ATOM C25  CTL2   -0.18 !                |              |
ATOM H5R  HAL2    0.09 !        H5R ---C25---H5S       |
ATOM H5S  HAL2    0.09 !                |              |
GROUP                  !                |              |
ATOM C26  CTL2   -0.18 !                |              |
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ATOM H6R  HAL2    0.09 !        H6R ---C26---H6S      |
ATOM H6S  HAL2    0.09 !               |              |
GROUP                  !               |              |
ATOM C27  CTL2   -0.18 !               |              |
ATOM H7R  HAL2    0.09 !        H7R ---C27---H7S      |
ATOM H7S  HAL2    0.09 !               |              |
GROUP                  !               |              |
ATOM C28  CTL2   -0.18 !               |              |
ATOM H8R  HAL2    0.09 !        H8R ---C28---H8S      |
ATOM H8S  HAL2    0.09 !               |              |
GROUP                  !               |              |
ATOM C29  CTL2   -0.18 !               |              |
ATOM H9R  HAL2    0.09 !        H9R ---C29---H9S      |
ATOM H9S  HAL2    0.09 !               |              |
GROUP                  !               |              |
ATOM C210 CTL2   -0.18 !               |              |
ATOM H10R HAL2    0.09 !        H10R---C210--H10S     |
ATOM H10S HAL2    0.09 !               |              |
GROUP                  !               |              |
ATOM C211 CEL1   -0.15 !               |              |
ATOM H11R HEL1    0.15 !        H11R --C211           |
GROUP                  !               ||  (CIS)      |
ATOM C212 CEL1   -0.15 !               ||             |
ATOM H12R HEL1    0.15 !        H12R---C212           |
GROUP                  !               |              |
ATOM C213 CTL2   -0.18 !               |              |
ATOM H13R HAL2    0.09 !        H13R---C213--H13S     |
ATOM H13S HAL2    0.09 !               |              |
GROUP                  !               |              |
ATOM C214 CTL2   -0.18 !               |              |
ATOM H14R HAL2    0.09 !        H14R---C214--H14S     |
ATOM H14S HAL2    0.09 !               |              |
GROUP                  !               |              |
ATOM C215 CTL2   -0.18 !               |              |
ATOM H15R HAL2    0.09 !        H15R---C215--H15S     |
ATOM H15S HAL2    0.09 !               |              |
GROUP                  !               |              |
ATOM C216 CTL2   -0.18 !               |              |
ATOM H16R HAL2    0.09 !        H16R---C216--H16S     |
ATOM H16S HAL2    0.09 !               |              |
GROUP                  !               |              |
ATOM C217 CTL2   -0.18 !               |              |
ATOM H17R HAL2    0.09 !        H17R---C217--H17S     |
ATOM H17S HAL2    0.09 !               |              |
GROUP                  !               |              |
ATOM C218 CTL3   -0.27 !               |              |
ATOM H18R HAL3    0.09 !        H18R---C218--H18S     |
ATOM H18S HAL3    0.09 !               |              |
ATOM H18T HAL3    0.09 !             H18T             |
GROUP                  !                              |
ATOM C33  CTL2   -0.18 !                              |
ATOM H3X  HAL2    0.09 !                     H3X ---C33---H3Y
ATOM H3Y  HAL2    0.09 !                             |
GROUP                  !                             |
ATOM C34  CTL2   -0.18 !                             |
ATOM H4X  HAL2    0.09 !                     H4X ---C34---H4Y
ATOM H4Y  HAL2    0.09 !                             |
GROUP                  !                             |
ATOM C35  CTL2   -0.18 !                             |
ATOM H5X  HAL2    0.09 !                     H5X ---C35---H5Y
ATOM H5Y  HAL2    0.09 !                             |
GROUP                  !                             |
ATOM C36  CTL2   -0.18 !                             |
ATOM H6X  HAL2    0.09 !                     H6X ---C36---H6Y
```

```
ATOM H6Y  HAL2    0.09 !                          |
GROUP                  !                          |
ATOM C37  CTL2   -0.18 !                          |
ATOM H7X  HAL2    0.09 !                      H7X ---C37---H7Y
ATOM H7Y  HAL2    0.09 !                          |
GROUP                  !                          |
ATOM C38  CTL2   -0.18 !                          |
ATOM H8X  HAL2    0.09 !                      H8X ---C38---H8Y
ATOM H8Y  HAL2    0.09 !                          |
GROUP                  !                          |
ATOM C39  CTL2   -0.18 !                          |
ATOM H9X  HAL2    0.09 !                      H9X ---C39---H9Y
ATOM H9Y  HAL2    0.09 !                          |
GROUP                  !                          |
ATOM C310 CTL2   -0.18 !                          |
ATOM H10X HAL2    0.09 !                     H10X---C310--H10Y
ATOM H10Y HAL2    0.09 !                          |
GROUP                  !                          |
ATOM C311 CTL2   -0.18 !                          |
ATOM H11X HAL2    0.09 !                     H11X---C311--H11Y
ATOM H12Y HAL2        0.09 !                                    |
GROUP                  !                          |
ATOM C312 CTL2   -0.18 !                          |
ATOM H12X HAL2    0.09 !                     H12X---C312--H12Y
ATOM H12Y HAL2        0.09 !                                    |
GROUP                  !                          |
ATOM C313 CTL2   -0.18 !                          |
ATOM H13X HAL2    0.09 !                     H13X---C313--H13Y
ATOM H13Y HAL2    0.09 !                          |
GROUP                  !                          |
ATOM C314 CTL2   -0.18 !                          |
ATOM H14X HAL2    0.09 !                     H14X---C314--H14Y
ATOM H14Y HAL2    0.09 !                          |
GROUP                  !                          |
ATOM C315 CTL2   -0.18 !                          |
ATOM H15X HAL2    0.09 !                     H15X---C315--H15Y
ATOM H15Y HAL2    0.09 !                          |
GROUP                  !                          |
ATOM C316 CTL2   -0.18 !                          |
ATOM H16X HAL2    0.09 !                     H16X---C316--H16Y
ATOM H16Y HAL2    0.09 !                          |
GROUP                  !                          |
ATOM C317 CTL2   -0.18 !                          |
ATOM H17X HAL2    0.09 !                     H17X---C317--H17Y
ATOM H17Y HAL2    0.09 !                          |
GROUP                  !                          |
ATOM C318 CTL3   -0.27 !                          |
ATOM H18X HAL3    0.09 !                     H18X---C318--H18Y
ATOM H18Y HAL3    0.09 !                          |
ATOM H18Z HAL3    0.09 !                         H18Z

! Polar Head
BOND  N    C13       N    C14       N    C15
BOND  C13  H13A      C13  H13B      C13  H13C
BOND  C14  H14A      C14  H14B      C14  H14C
BOND  C15  H15A      C15  H15B      C15  H15C
BOND  N    C12
BOND  C12  H12A      C12  H12B      C12  C11
BOND  C11  H11A      C11  H11B      C11  O12       O11  C1
BOND  O12  P         P    O11       P    O13       P    O14
! Glycerol Backbone
BOND  C1   HA        C1    HB       C1   C2
BOND  C2   HS        C2    C3       C2   O21
BOND  C3   HX        C3    HY       C3   O31
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```
! Chain from C2
BOND  O21  C21
BOND  C21  C22
DOUBLE  C21  O22
BOND  C22  H2R       C22  H2S       C22  C23
BOND  C23  H3R       C23  H3S       C23  C24
BOND  C24  H4R       C24  H4S       C24  C25
BOND  C25  H5R       C25  H5S       C25  C26
BOND  C26  H6R       C26  H6S       C26  C27
BOND  C27  H7R       C27  H7S       C27  C28
BOND  C28  H8R       C28  H8S       C28  C29
BOND  C29  H9R       C29  H9S       C29  C210
BOND  C210 H10R      C210 H10S      C210 C211
BOND  C211 H11R
DOUBLE  C211 C212
BOND  C212 H12R      C212 C213
BOND  C213 H13R      C213 H13S      C213 C214
BOND  C214 H14R      C214 H14S      C214 C215
BOND  C215 H15R      C215 H15S      C215 C216
BOND  C216 H16R      C216 H16S      C216 C217
BOND  C217 H17R      C217 H17S      C217 C218
BOND  C218 H18R      C218 H18S      C218 H18T
! Chain From C3
BOND  O31  C31
BOND  C31  C32
DOUBLE  C31  O32
BOND  C32  H2X       C32  H2Y       C32  C33
BOND  C33  H3X       C33  H3Y       C33  C34
BOND  C34  H4X       C34  H4Y       C34  C35
BOND  C35  H5X       C35  H5Y       C35  C36
BOND  C36  H6X       C36  H6Y       C36  C37
BOND  C37  H7X       C37  H7Y       C37  C38
BOND  C38  H8X       C38  H8Y       C38  C39
BOND  C39  H9X       C39  H9Y       C39  C310
BOND  C310 H10X      C310 H10Y      C310 C311
BOND  C311 H11X      C311 H11Y          C311 C312
BOND  C312 H12X      C312 H12Y          C312 C313
BOND  C313 H13X      C313 H13Y      C313 C314
BOND  C314 H14X      C314 H14Y      C314 C315
BOND  C315 H15X      C315 H15Y      C315 C316
BOND  C316 H16X      C316 H16Y      C316 C317
BOND  C317 H17X      C317 H17Y      C317 C318
BOND  C318 H18X      C318 H18Y      C318 H18Z

IMPR C21 O21 C22 O22    C31 O31 C32 O32

IC C15    N      C12    C11        1.5031  108.03  -62.19  116.82   1.5409
IC C13    C12    *N     C14        1.4955  110.60  122.73  109.67   1.4976
IC C13    C12    *N     C15        1.4955  110.60 -119.76  108.04   1.5032
IC C13    N      C12    C11        1.4955  110.60   57.52  116.83   1.5412
IC C11    N      *C12   H12A       1.5412  116.83 -126.40  111.94   1.0787
IC H12A   N      *C12   H12B       1.0787  111.94 -116.29  108.17   1.0974
IC C14    N      C13    H13A       1.4976  110.99  179.50  109.35   1.0869
IC H13A   N      *C13   H13B       1.0869  109.35  118.93  111.32   1.0813
IC H13A   N      *C13   H13C       1.0869  109.35 -119.04  111.19   1.0811
IC C13    N      C14    H14A       1.4955  110.99 -179.22  109.65   1.0877
IC H14A   N      *C14   H14B       1.0877  109.65  118.74  110.91   1.0820
IC H14A   N      *C14   H14C       1.0877  109.65 -119.76  111.49   1.0812
IC C13    N      C15    H15A       1.4955  109.44  -64.69  111.04   1.0951
IC H15A   N      *C15   H15B       1.0951  111.04  123.93  113.87   1.0740
IC H15A   N      *C15   H15C       1.0951  111.04 -112.38  110.25   1.0938
IC N      C12    C11    O12        1.5223  116.83  127.52  108.22   1.4232
IC O12    C12    *C11   H11A       1.4232  108.22 -123.07  113.25   1.1138
IC H11A   C12    *C11   H11B       1.1138  113.25 -118.71  109.20   1.1129
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IC C12    C11    O12    P          1.5412  108.22  -67.94  118.41   1.5875
IC C11    O12    P      O11        1.4232  118.41 -166.85  104.05   1.5781
IC O11    O12    *P     O13        1.5781  104.05  117.80  108.05   1.4795
IC O11    O12    *P     O14        1.5781  104.05 -117.37  106.82   1.4822
IC O12    P      O11    C1         1.5875  104.05  167.61  118.26   1.4316
IC P      O11    C1     C2         1.5781  118.26  168.12  110.80   1.5508
IC C2     O11    *C1    HA         1.5508  110.80 -119.17  111.41   1.1170
IC HA     O11    *C1    HB         1.1170  111.41 -120.80  110.01   1.1146
IC O11    C1     C2     C3         1.4316  110.80  176.77  110.71   1.5573
IC C3     C1     *C2    O21        1.5573  110.71  120.62  108.02   1.4410 !defines S
chirality
IC C3     C1     *C2    HS         1.5573  110.71 -118.37  106.71   1.1170 !defines S
chirality
IC C1     C2     O21    C21        1.5508  108.02  147.52  115.15   1.3177
IC C2     O21    C21    C22        1.4410  115.15  179.16  108.63   1.5289
IC C22    O21    *C21   O22        1.5289  108.63 -178.85  126.55   1.2187
IC O21    C21    C22    C23        1.3177  108.63 -177.70  112.21   1.5449
IC C23    C21    *C22   H2R        1.5449  112.21 -121.72  107.88   1.1092
IC H2R    C21    *C22   H2S        1.1092  107.88 -117.16  107.60   1.1093
IC C1     C2     C3     O31        1.5508  110.71  176.05  112.62   1.4438
IC O31    C2     *C3    HX         1.4438  112.62 -118.51  106.65   1.1128
IC HX     C2     *C3    HY         1.1128  106.65 -115.12  109.46   1.1145
IC C2     C3     O31    C31        1.5573  112.62   87.12  115.04   1.3313
IC C3     O31    C31    C32        1.4438  115.04 -172.98  108.55   1.5288
IC C32    O31    *C31   O32        1.5288  108.55 -178.89  125.60   1.2170
IC O31    C31    C32    C33        1.3313  108.55 -166.73  113.05   1.5447
IC C33    C31    *C32   H2X        1.5447  113.05 -121.10  107.23   1.1103
IC H2X    C31    *C32   H2Y        1.1103  107.23 -117.00  108.11   1.1090
IC C21    C22    C23    C24        1.5289  112.21  175.76  112.39   1.5338
IC C24    C22    *C23      H3R             1.5360  113.21 -119.83  108.42   1.1148
IC C24    C22    *C23      H3S             1.5396  113.52 -123.43  110.53   1.1101
IC C22    C23    C24       C25             1.5450  113.21 -172.34  113.68   1.5399
IC C25    C23    *C24      H4R             1.5399  113.68  120.91  108.91   1.1136
IC C25    C23    *C24      H4S             1.5396  113.52 -123.43  110.53   1.1101
IC C23    C24    C25       C26             1.5360  113.68  -56.95  113.57   1.5353
IC C26    C24    *C25      H5R             1.5353  113.57  121.41  108.70   1.1129
IC C26    C24    *C25      H5S             1.5396  113.52 -123.43  110.53   1.1101
IC C24    C25    C26       C27             1.5399  113.57 -173.39  113.79   1.5375
IC C27    C25    *C26      H6R             1.5375  113.79  122.09  109.21   1.1127
IC C27    C25    *C26      H6S             1.5396  113.52 -123.43  110.53   1.1101
IC C25    C26    C27       C28             1.5353  113.79  177.45  113.35   1.5458
IC C28    C26    *C27      H7R             1.5458  113.35  119.87  108.07   1.1139
IC C28    C26    *C27      H7S             1.5396  113.52 -123.43  110.53   1.1101
IC C26    C27    C28       C29          1.5399  113.57 -173.39  113.79   1.5375
IC C29    C27    *C28      H8R             1.5375  113.79  122.09  109.21   1.1127
IC C29    C27    *C28      H8S             1.5396  113.52 -123.43  110.53   1.1101
IC C27    C28    C29       C210            1.5353  113.79  177.45  113.35   1.5458
IC C210   C28    *C29      H9R             1.5458  113.35  119.87  108.07   1.1139
IC C210   C28    *C29      H9S             1.5396  113.52 -123.43  110.53   1.1101
IC C28    C29    C210      C211            1.5375  113.35   67.78  114.46   1.5115
IC C211   C29    *C210     H10R            1.5115  114.46  121.34  107.89   1.1131
IC C211   C29    *C210     H10S            1.5396  113.52 -123.43  110.53   1.1101
IC C29    C210   C211      C212            1.5458  114.46  180.00  126.91   1.3502
IC C212   C210   *C211     H11R            1.3502  126.91 -178.81  114.69   1.1010
IC C210   C211   C212      C213            1.5115  126.91    0.00  126.69   1.5092
!cis db
IC C213   C210   *C212     H12R            1.5099  126.94 -177.42  118.69   1.1018
IC C211   C212   C213      C214         1.3502  126.69  180.00  111.86   1.5417
IC C214   C212   *C213     H13R            1.5396  113.52 -123.43  110.53   1.1101
IC C214   C212   *C213     H13S            1.5097  125.28  121.00  119.65   1.1004
IC C212   C213   C214      C215            1.5092  111.86  180.00  113.99   1.5334
IC C215   C213   *C214     H14R            1.5396  113.52 -123.43  110.53   1.1101
IC C215   C213   *C214     H14S            1.5097  125.28  121.00  119.65   1.1004
IC C213   C214   C215      C216            1.5417  113.99  180.00  111.46   1.5365
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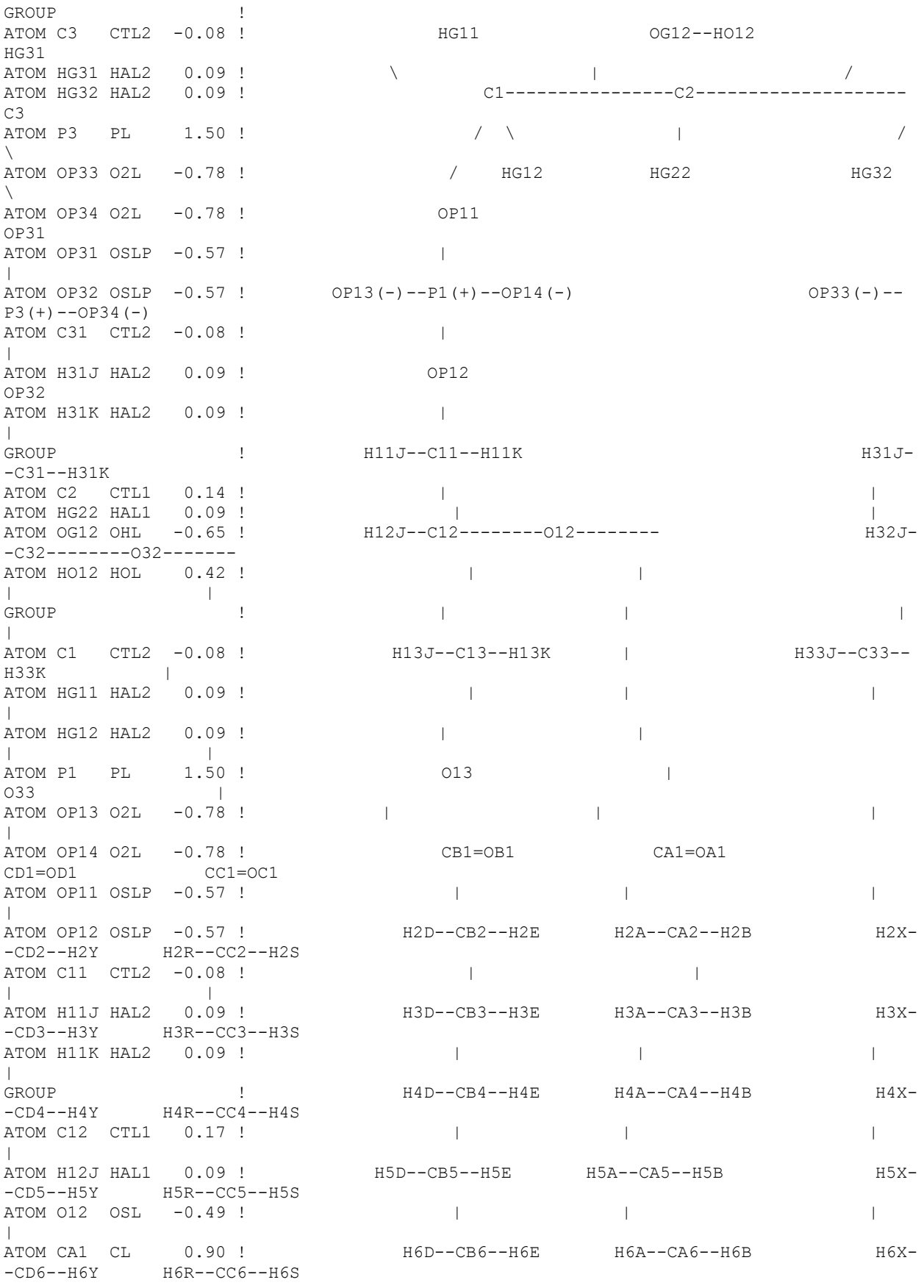
IC C216   C214   *C215    H15R           1.5396  113.52 -123.43  110.53   1.1101
IC C216   C214   *C215    H15S        1.5097  125.28  121.00  119.65   1.1004
IC C214   C215   C216     C217           1.5376  114.97  180.00  113.95   1.5347
IC C217   C215   *C216    H16R           1.5396  113.52 -123.43  110.53   1.1101
IC C217   C215   *C216    H16S           1.5097  125.28  121.00  119.65   1.1004
IC C215   C216   C217     C218           1.5385  113.95  180.00  113.05   1.5311
IC C218   C216   *C217    H17R           1.5396  113.52 -123.43  110.53   1.1101
IC C218   C216   *C217    H17S           1.5097  125.28  121.00  119.65   1.1004
IC C216   C217   C218     H18R           1.5347  113.05  180.00  110.58   1.1110
IC H18R   C217   *C218    H18S           1.5396  113.52 -123.43  110.53   1.1101
IC H18R   C217   *C218    H18T           1.5097  125.28  121.00  119.65   1.1004
IC C31    C32    C33     C34         1.5405  116.85  180.00  126.13   1.5951
IC C34    C32    *C33    H3X         1.5410  113.36 -119.96  111.74   1.1148
IC C34    C32    *C33    H3Y         1.5192  121.35  121.00  106.97   1.1128
IC C32    C33    C34     C35         1.6060  126.13  180.00  113.36   1.5410
IC C35    C33    *C34    H4X         1.5396  113.52 -123.43  110.53   1.1101
IC C35    C33    *C34    H4Y         1.5192  121.35  121.00  106.97   1.1128
IC C33    C34    C35     C36         1.5951  113.36  180.00  113.52   1.5396
IC C36    C34    *C35    H5X         1.5396  113.52 -123.43  110.53   1.1101
IC C36    C34    *C35    H5Y         1.5192  121.35  123.34  106.97   1.1128
IC C34    C35    C36     C37         1.5410  113.52  180.00  114.47   1.5397
IC C37    C35    *C36    H6X         1.5396  113.52 -123.43  110.53   1.1101
IC C37    C35    *C36    H6Y         1.5192  121.35  123.34  106.97   1.1128
IC C35    C36    C37     C38         1.5396  114.47  180.00  113.41   1.5386
IC C38    C36    *C37    H7X         1.5396  113.52 -123.43  110.53   1.1101
IC C38    C36    *C37    H7Y         1.5192  121.35  123.34  106.97   1.1128
IC C36    C37    C38     C39         1.5397  113.41  180.00  113.71   1.5382
IC C39    C37    *C38    H8X         1.5396  113.52 -123.43  110.53   1.1101
IC C39    C37    *C38    H8Y         1.5192  121.35  123.34  106.97   1.1128
IC C37    C38    C39     C310        1.5353  113.79  177.45  113.35   1.5458
IC C310   C38    *C39    H9X         1.5458  113.35  119.87  108.07   1.1139
IC C310   C38    *C39    H9Y         1.5396  113.52 -123.43  110.53   1.1101
IC C38    C39    C310    C311        1.5375  113.35   67.78  114.46   1.5115
IC C311   C39    *C310   H10X        1.5115  114.46  121.34  107.89   1.1131
IC C311   C39    *C310   H10Y        1.5396  113.52 -123.43  110.53   1.1101
IC C39    C310   C311    C312        1.5458  114.46  180.00  126.91   1.3502
IC C312   C310   *C311   H11X        1.3502  126.91 -178.81  114.69   1.1010
IC C310   C311   C312    C313        1.5115  126.91    0.00  126.69   1.5092 !cis db
IC C313   C310   *C312   H12X        1.5099  126.94 -177.42  118.69   1.1018
IC C311   C312   C313    C314        1.3502  126.69  180.00  111.86   1.5417
IC C314   C312   *C313   H13X        1.5396  113.52 -123.43  110.53   1.1101
IC C314   C312   *C313   H13Y        1.5097  125.28  121.00  119.65   1.1004
IC C312   C313   C314    C315        1.5092  111.86  180.00  113.99   1.5334
IC C315   C313   *C314   H14X        1.5396  113.52 -123.43  110.53   1.1101
IC C315   C313   *C314   H14Y        1.5097  125.28  121.00  119.65   1.1004
IC C313   C314   C315    C316        1.5377  113.85  180.00  111.81   1.5374
IC C316   C314   *C315   H15X        1.5396  113.52 -123.43  110.53   1.1101
IC C316   C314   *C315   H15Y        1.5192  121.35  123.34  106.97   1.1128
IC C314   C315   C316    C317        1.5357  111.81  180.00  114.29   1.5985
IC C317   C315   *C316   H16X        1.5396  113.52 -123.43  110.53   1.1101
IC C317   C315   *C316   H16Y        1.5192  121.35  123.34  106.97   1.1128
IC C315   C316   C317    C318        1.5374  114.29  180.00  130.92   1.5745
IC C318   C316   *C317   H17X        1.5396  113.52 -123.43  110.53   1.1101
IC C318   C316   *C317   H17Y        1.5192  121.35  123.34  106.97   1.1128
IC C316   C317   C318    H18X        1.5985  130.92  180.00  110.90   1.1113
IC H18X   C317   *C318   H18Y      1.5396  113.52 -123.43  110.53   1.1101
IC H18X   C317   *C318   H18Z        1.5192  121.35  123.34  106.97   1.1128


! These are not done.   IN PROGRESS
! Cardiolipins

RESI TVCL2      -2.00 ! Tetravaccinyl Cardiolipin with head group charge = -2
                      ! Cardiolipin headgroup + 4 oleoly chains
```


GROUP !
ATOM C3 CTL2 -0.08 ! HG11 OG12--HO12
HG31
ATOM HG31 HAL2 0.09 ! \ | /
ATOM HG32 HAL2 0.09 ! C1----------C2----------
C3
ATOM P3 PL 1.50 ! / \ | /
\
ATOM OP33 O2L -0.78 ! / HG12 HG22 HG32
\
ATOM OP34 O2L -0.78 ! OP11
OP31
ATOM OP31 OSLP -0.57 ! |
|
ATOM OP32 OSLP -0.57 ! OP13(-)--P1(+)--OP14(-) OP33(-)--
P3(+)--OP34(-)
ATOM C31 CTL2 -0.08 ! |
|
ATOM H31J HAL2 0.09 ! OP12
OP32
ATOM H31K HAL2 0.09 ! |
|
GROUP ! H11J--C11--H11K H31J-
-C31--H31K
ATOM C2 CTL1 0.14 ! | |
ATOM HG22 HAL1 0.09 ! | |
ATOM OG12 OHL -0.65 ! H12J--C12--------O12-------- H32J-
-C32--------O32-------
ATOM HO12 HOL 0.42 ! | |
| |
GROUP ! | | |
|
ATOM C1 CTL2 -0.08 ! H13J--C13--H13K | H33J--C33--
H33K |
ATOM HG11 HAL2 0.09 ! | | |
|
ATOM HG12 HAL2 0.09 ! | |
| |
ATOM P1 PL 1.50 ! O13 |
O33 |
ATOM OP13 O2L -0.78 ! | | |
|
ATOM OP14 O2L -0.78 ! CB1=OB1 CA1=OA1
CD1=OD1 CC1=OC1
ATOM OP11 OSLP -0.57 ! | | |
|
ATOM OP12 OSLP -0.57 ! H2D--CB2--H2E H2A--CA2--H2B H2X-
-CD2--H2Y H2R--CC2--H2S
ATOM C11 CTL2 -0.08 ! | |
| |
ATOM H11J HAL2 0.09 ! H3D--CB3--H3E H3A--CA3--H3B H3X-
-CD3--H3Y H3R--CC3--H3S
ATOM H11K HAL2 0.09 ! | | |
|
GROUP ! H4D--CB4--H4E H4A--CA4--H4B H4X-
-CD4--H4Y H4R--CC4--H4S
ATOM C12 CTL1 0.17 ! | | |
|
ATOM H12J HAL1 0.09 ! H5D--CB5--H5E H5A--CA5--H5B H5X-
-CD5--H5Y H5R--CC5--H5S
ATOM O12 OSL -0.49 ! | | |
|
ATOM CA1 CL 0.90 ! H6D--CB6--H6E H6A--CA6--H6B H6X-
-CD6--H6Y H6R--CC6--H6S

```
ATOM OA1  OBL   -0.63 !                   |               |                        |
|
ATOM CA2  CTL2  -0.22 !                  |                  |
|                  |
ATOM H2A  HAL2   0.09 !              H7D--CB7--H7E       H7A--CA7--H7B
H7X--CD7--H7Y      H7R--CC7--H7S
ATOM H2B  HAL2   0.09 !                   |               |                         |
|
GROUP                 !              H8D--CB8--H8E       H8A--CA8--H8B           H8X-
-CD8--H8Y      H8R--CC8--H8S
ATOM C13  CTL2   0.08 !                   |               |                        |
|
ATOM H13J HAL2   0.09 !              H9D--CB9        H9A--CA9
H9X--CD9           H9R--CC9
ATOM H13K HAL2   0.09 !                   ||            ||                        ||
||
ATOM O13  OSL   -0.49 !                ||                 ||
||                 ||
ATOM CB1  CL     0.90 !             H10D--CB10             H10A--CA10            H10X-
-CD10         H10R--CC10
ATOM OB1  OBL   -0.63 !                   |               |                        |
|
ATOM CB2  CTL2  -0.22 !           H11D--CB11--H11E    H11A--CA11--H11B           H11X-
-CD11--H11Y   H11R--CC11--H11S
ATOM H2D  HAL2   0.09 !                    |              |                        |
|
ATOM H2E  HAL2   0.09 !             H12D--CB12--H12E    H12A--CA12--H12B         H12X-
-CD12--H12Y   H12R--CC12--H12S
GROUP                 !                  |                 |
|                  |
ATOM C32  CTL1   0.17 !                   |               |                        |
|
ATOM H32J HAL1   0.09 !             H13D--CB13--H13E    H13A--CA13--H13B         H13X-
-CD13--H13Y   H13R--CC13--H13S
ATOM O32  OSL   -0.49 !                   |               |                        |
|
ATOM CC1  CL     0.90 !             H14D--CB14--H14E    H14A--CA14--H14B         H14X-
-CD14--H14Y   H14R--CC14--H14S
ATOM OC1  OBL   -0.63 !                   |               |                        |
|
ATOM CC2  CTL2  -0.22 !           H15D--CB15--H15E    H15A--CA15--H15B           H15X-
-CD15--H15Y   H15R--CC15--H15S
ATOM H2R  HAL2   0.09 !                   |               |                        |
|
ATOM H2S  HAL2   0.09 !           H16D--CB16--H16E    H16A--CA16--H16B           H16X-
-CD16--H16Y   H16R--CC16--H16S
GROUP                 !                   |               |                        |
|
ATOM C33  CTL2   0.08 !           H17D--CB17--H17E    H17A--CA17--H17B           H17X-
-CD17--H17Y   H17R--CC17--H17S
ATOM H33J HAL2   0.09 !                   |               |                        |
|
ATOM H33K HAL2   0.09 !             H18D--CB18--H18E    H18A--CA18--H18B
H18X--CD18--H18Y   H18R--CC18--H18S
ATOM O33  OSL   -0.49 !                   |               |                        |
|
ATOM CD1  CL     0.90 !                   H18F                H18C
H18Z               H18T
ATOM OD1  OBL   -0.63 !
ATOM CD2  CTL2  -0.22 !
ATOM H2X  HAL2   0.09 !
ATOM H2Y  HAL2   0.09 !
GROUP                 !
ATOM CA3  CTL2  -0.18 !
```

```
ATOM H3A  HAL2   0.09 !
ATOM H3B  HAL2   0.09 !
GROUP                 !
ATOM CA4  CTL2  -0.18 !
ATOM H4A  HAL2   0.09 !
ATOM H4B  HAL2   0.09 !
GROUP                 !
ATOM CA5  CTL2  -0.18 !
ATOM H5A  HAL2   0.09 !
ATOM H5B  HAL2   0.09 !
GROUP                 !
ATOM CA6  CTL2  -0.18 !
ATOM H6A  HAL2   0.09 !
ATOM H6B  HAL2   0.09 !
GROUP                 !
ATOM CA7  CTL2  -0.18 !
ATOM H7A  HAL2   0.09 !
ATOM H7B  HAL2   0.09 !
GROUP                 !
ATOM CA8  CTL2  -0.18 !
ATOM H8A  HAL2   0.09 !
ATOM H8B  HAL2   0.09 !
GROUP                 !
ATOM CA9  CEL1  -0.15 !
ATOM H9A  HEL1   0.15 !
GROUP                 !
ATOM CA10 CEL1  -0.15 !
ATOM H10A HEL1   0.15 !
GROUP                 !
ATOM CA11 CTL2  -0.18 !
ATOM H11A HAL2   0.09 !
ATOM H11B HAL2   0.09 !
GROUP                 !
ATOM CA12 CTL2  -0.18 !
ATOM H12A HAL2   0.09 !
ATOM H12B HAL2   0.09 !
GROUP                 !
ATOM CA13 CTL2  -0.18 !
ATOM H13A HAL2   0.09 !
ATOM H13B HAL2   0.09 !
GROUP                 !
ATOM CA14 CTL2  -0.18 !
ATOM H14A HAL2   0.09 !
ATOM H14B HAL2   0.09 !
GROUP                 !
ATOM CA15 CTL2  -0.18 !
ATOM H15A HAL2   0.09 !
ATOM H15B HAL2   0.09 !
GROUP                 !
ATOM CA16 CTL2  -0.18 !
ATOM H16A HAL2   0.09 !
ATOM H16B HAL2   0.09 !
GROUP                 !
ATOM CA17 CTL2  -0.18 !
ATOM H17A HAL2   0.09 !
ATOM H17B HAL2   0.09 !
GROUP                 !
ATOM CA18 CTL3  -0.27 !
ATOM H18A HAL3   0.09 !
ATOM H18B HAL3   0.09 !
ATOM H18C HAL3   0.09 !
GROUP                 !
ATOM CB3  CTL2  -0.18 !
ATOM H3D  HAL2   0.09 !
```

```
ATOM H3E  HAL2   0.09 !
GROUP                 !
ATOM CB4  CTL2  -0.18 !
ATOM H4D  HAL2   0.09 !
ATOM H4E  HAL2   0.09 !
GROUP                 !
ATOM CB5  CTL2  -0.18 !
ATOM H5D  HAL2   0.09 !
ATOM H5E  HAL2   0.09 !
GROUP                 !
ATOM CB6  CTL2  -0.18 !
ATOM H6D  HAL2   0.09 !
ATOM H6E  HAL2   0.09 !
GROUP                 !
ATOM CB7  CTL2  -0.18 !
ATOM H7D  HAL2   0.09 !
ATOM H7E  HAL2   0.09 !
GROUP                 !
ATOM CB8  CTL2  -0.18 !
ATOM H8D  HAL2   0.09 !
ATOM H8E  HAL2   0.09 !
GROUP                 !
ATOM CB9  CEL1  -0.15 !
ATOM H9D  HEL1   0.15 !
GROUP                 !
ATOM CB10 CEL1  -0.15 !
ATOM H10D HEL1   0.15 !
GROUP                 !
ATOM CB11 CTL2  -0.18 !
ATOM H11D HAL2   0.09 !
ATOM H11E HAL2   0.09 !
GROUP                 !
ATOM CB12 CTL2  -0.18 !
ATOM H12D HAL2   0.09 !
ATOM H12E HAL2   0.09 !
GROUP                 !
ATOM CB13 CTL2  -0.18 !
ATOM H13D HAL2   0.09 !
ATOM H13E HAL2   0.09 !
GROUP                 !
ATOM CB14 CTL2  -0.18 !
ATOM H14D HAL2   0.09 !
ATOM H14E HAL2   0.09 !
GROUP                 !
ATOM CB15 CTL2  -0.18 !
ATOM H15D HAL2   0.09 !
ATOM H15E HAL2   0.09 !
GROUP                 !
ATOM CB16 CTL2  -0.18 !
ATOM H16D HAL2   0.09 !
ATOM H16E HAL2   0.09 !
GROUP                 !
ATOM CB17 CTL2  -0.18 !
ATOM H17D HAL2   0.09 !
ATOM H17E HAL2   0.09 !
GROUP                 !
ATOM CB18 CTL3  -0.27 !
ATOM H18D HAL3   0.09 !
ATOM H18E HAL3   0.09 !
ATOM H18F HAL3   0.09 !
GROUP                 !
ATOM CC3  CTL2  -0.18 !
ATOM H3R  HAL2   0.09 !
ATOM H3S  HAL2   0.09 !
```

```
GROUP                   !
ATOM CC4  CTL2  -0.18 !
ATOM H4R  HAL2   0.09 !
ATOM H4S  HAL2   0.09 !
GROUP                   !
ATOM CC5  CTL2  -0.18 !
ATOM H5R  HAL2   0.09 !
ATOM H5S  HAL2   0.09 !
GROUP                   !
ATOM CC6  CTL2  -0.18 !
ATOM H6R  HAL2   0.09 !
ATOM H6S  HAL2   0.09 !
GROUP                   !
ATOM CC7  CTL2  -0.18 !
ATOM H7R  HAL2   0.09 !
ATOM H7S  HAL2   0.09 !
GROUP                   !
ATOM CC8  CTL2  -0.18 !
ATOM H8R  HAL2   0.09 !
ATOM H8S  HAL2   0.09 !
GROUP                   !
ATOM CC9  CEL1  -0.15 !
ATOM H9R  HEL1   0.15 !
GROUP                   !
ATOM CC10 CEL1  -0.15 !
ATOM H10R HEL1   0.15 !
GROUP                   !
ATOM CC11 CTL2  -0.18 !
ATOM H11R HAL2   0.09 !
ATOM H11S HAL2   0.09 !
GROUP                   !
ATOM CC12 CTL2  -0.18 !
ATOM H12R HAL2   0.09 !
ATOM H12S HAL2   0.09 !
GROUP                   !
ATOM CC13 CTL2  -0.18 !
ATOM H13R HAL2   0.09 !
ATOM H13S HAL2   0.09 !
GROUP                   !
ATOM CC14 CTL2  -0.18 !
ATOM H14R HAL2   0.09 !
ATOM H14S HAL2   0.09 !
GROUP                   !
ATOM CC15 CTL2  -0.18 !
ATOM H15R HAL2   0.09 !
ATOM H15S HAL2   0.09 !
GROUP                   !
ATOM CC16 CTL2  -0.18 !
ATOM H16R HAL2   0.09 !
ATOM H16S HAL2   0.09 !
GROUP                   !
ATOM CC17 CTL2  -0.18 !
ATOM H17R HAL2   0.09 !
ATOM H17S HAL2   0.09 !
GROUP                   !
ATOM CC18 CTL3  -0.27 !
ATOM H18R HAL3   0.09 !
ATOM H18S HAL3   0.09 !
ATOM H18T HAL3   0.09 !
GROUP                   !
ATOM CD3  CTL2  -0.18 !
ATOM H3X  HAL2   0.09 !
ATOM H3Y  HAL2   0.09 !
GROUP                   !
```

```
ATOM CD4  CTL2  -0.18 !
ATOM H4X  HAL2   0.09 !
ATOM H4Y  HAL2   0.09 !
GROUP                 !
ATOM CD5  CTL2  -0.18 !
ATOM H5X  HAL2   0.09 !
ATOM H5Y  HAL2   0.09 !
GROUP                 !
ATOM CD6  CTL2  -0.18 !
ATOM H6X  HAL2   0.09 !
ATOM H6Y  HAL2   0.09 !
GROUP                 !
ATOM CD7  CTL2  -0.18 !
ATOM H7X  HAL2   0.09 !
ATOM H7Y  HAL2   0.09 !
GROUP                 !
ATOM CD8  CTL2  -0.18 !
ATOM H8X  HAL2   0.09 !
ATOM H8Y  HAL2   0.09 !
GROUP                 !
ATOM CD9  CEL1  -0.15 !
ATOM H9X  HEL1   0.15 !
GROUP                 !
ATOM CD10 CEL1  -0.15 !
ATOM H10X HEL1   0.15 !
GROUP                 !
ATOM CD11 CTL2  -0.18 !
ATOM H11X HAL2   0.09 !
ATOM H11Y HAL2   0.09 !
GROUP                 !
ATOM CD12 CTL2  -0.18 !
ATOM H12X HAL2   0.09 !
ATOM H12Y HAL2   0.09 !
GROUP                 !
ATOM CD13 CTL2  -0.18 !
ATOM H13X HAL2   0.09 !
ATOM H13Y HAL2   0.09 !
GROUP                 !
ATOM CD14 CTL2  -0.18 !
ATOM H14X HAL2   0.09 !
ATOM H14Y HAL2   0.09 !
GROUP                 !
ATOM CD15 CTL2  -0.18 !
ATOM H15X HAL2   0.09 !
ATOM H15Y HAL2   0.09 !
GROUP                 !
ATOM CD16 CTL2  -0.18 !
ATOM H16X HAL2   0.09 !
ATOM H16Y HAL2   0.09 !
GROUP                 !
ATOM CD17 CTL2  -0.18 !
ATOM H17X HAL2   0.09 !
ATOM H17Y HAL2   0.09 !
GROUP                 !
ATOM CD18 CTL3  -0.27 !
ATOM H18X HAL3   0.09 !
ATOM H18Y HAL3   0.09 !
ATOM H18Z HAL3   0.09 !!

! Glycerol head
BOND C1   C2   C1   HG11  C1   HG12
BOND C2   OG12 C2   HG22  OG12 HO12 C2 C3
BOND C3   HG31 C3   HG32
! Phosphates
```

```
BOND C1   OP11 C3   OP31
BOND P1   OP11 P1   OP12  P1  OP13 P1  OP14
BOND P3   OP31 P3   OP32  P3  OP33 P3  OP34
! Glycerol Backbones
BOND OP12 C11  C11  H11J C11 H11K
BOND C11  C12
BOND C12  H12J C12  O12
BOND C12  C13
BOND C13  H13J C13  H13K C13 O13
BOND OP32 C31  C31  H31J C31 H31K
BOND C31  C32
BOND C32  H32J C32  O32
BOND C32  C33
BOND C33  H33J C33  H33K C33 O33
! Acyl chain 1
BOND O12  CA1  O13  CB1  O32  CC1  O33  CD1
BOND CA1  OA1  CA1  CA2
BOND CA2  H2A  CA2  H2B  CA2  CA3
BOND CA3  H3A  CA3  H3B  CA3  CA4
BOND CA4  H4A  CA4  H4B  CA4  CA5
BOND CA5  H5A  CA5  H5B  CA5  CA6
BOND CA6  H6A  CA6  H6B  CA6  CA7
BOND CA7  H7A  CA7  H7B  CA7  CA8
BOND CA8  H8A  CA8  H8B  CA8  CA9
BOND CA9  H9A  CA9  CA10
BOND CA10 H10A CA10 CA11
BOND CA11 H11A CA11 H11B CA11 CA12
BOND CA12 H12A CA12 H12B CA12 CA13
BOND CA13 H13A CA13 H13B CA13 CA14
BOND CA14 H14A CA14 H14B CA14 CA15
BOND CA15 H15A CA15 H15B CA15 CA16
BOND CA16 H16A CA16 H16B CA16 CA17
BOND CA17 H17A CA17 H17B CA17 CA18
BOND CA18 H18A CA18 H18B CA18 H18C
! Acyl chain 2
BOND CB1  OB1  CB1  CB2
BOND CB2  H2D  CB2  H2E  CB2  CB3
BOND CB3  H3D  CB3  H3E  CB3  CB4
BOND CB4  H4D  CB4  H4E  CB4  CB5
BOND CB5  H5D  CB5  H5E  CB5  CB6
BOND CB6  H6D  CB6  H6E  CB6  CB7
BOND CB7  H7D  CB7  H7E  CB7  CB8
BOND CB8  H8D  CB8  H8E  CB8  CB9
BOND CB9  H9D  CB9  CB10
BOND CB10 H10D CB10 CB11
BOND CB11 H11D CB11 H11E CB11 CB12
BOND CB12 H12D CB12 H12E CB12 CB13
BOND CB13 H13D CB13 H13E CB13 CB14
BOND CB14 H14D CB14 H14E CB14 CB15
BOND CB15 H15D CB15 H15E CB15 CB16
BOND CB16 H16D CB16 H16E CB16 CB17
BOND CB17 H17D CB17 H17E CB17 CB18
BOND CB18 H18D CB18 H18E CB18 H18F
! Acyl chain 3
BOND CC1  OC1  CC1  CC2
BOND CC2  H2R  CC2  H2S  CC2  CC3
BOND CC3  H3R  CC3  H3S  CC3  CC4
BOND CC4  H4R  CC4  H4S  CC4  CC5
BOND CC5  H5R  CC5  H5S  CC5  CC6
BOND CC6  H6R  CC6  H6S  CC6  CC7
BOND CC7  H7R  CC7  H7S  CC7  CC8
BOND CC8  H8R  CC8  H8S  CC8  CC9
BOND CC9  H9R  CC9  CC10
BOND CC10 H10R CC10 CC11
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BOND CC11 H11R CC11 H11S CC11 CC12
BOND CC12 H12R CC12 H12S CC12 CC13
BOND CC13 H13R CC13 H13S CC13 CC14
BOND CC14 H14R CC14 H14S CC14 CC15
BOND CC15 H15R CC15 H15S CC15 CC16
BOND CC16 H16R CC16 H16S CC16 CC17
BOND CC17 H17R CC17 H17S CC17 CC18
BOND CC18 H18R CC18 H18S CC18 H18T
! Acyl chain 4
BOND CD1  OD1  CD1  CD2
BOND CD2  H2X  CD2  H2Y  CD2  CD3
BOND CD3  H3X  CD3  H3Y  CD3  CD4
BOND CD4  H4X  CD4  H4Y  CD4  CD5
BOND CD5  H5X  CD5  H5Y  CD5  CD6
BOND CD6  H6X  CD6  H6Y  CD6  CD7
BOND CD7  H7X  CD7  H7Y  CD7  CD8
BOND CD8  H8X  CD8  H8Y  CD8  CD9
BOND CD9  H9X  CD9  CD10
BOND CD10 H10X CD10 CD11
BOND CD11 H11X CD11 H11Y CD11 CD12
BOND CD12 H12X CD12 H12Y CD12 CD13
BOND CD13 H13X CD13 H13Y CD13 CD14
BOND CD14 H14X CD14 H14Y CD14 CD15
BOND CD15 H15X CD15 H15Y CD15 CD16
BOND CD16 H16X CD16 H16Y CD16 CD17
BOND CD17 H17X CD17 H17Y CD17 CD18
BOND CD18 H18X CD18 H18Y CD18 H18Z
!
! IC TABLE
!
IMPR CB1  O13  CB2  OB1
IMPR CA1  O12  CA2  OA1
IMPR CD1  O33  CD2  OD1
IMPR CC1  O32  CC2  OC1
IC OP31    C2      *C3      HG31      1.4633  109.99  126.99  106.69   1.1112
IC HG31    C2      *C3      HG32      1.1112  106.69  120.70  112.94   1.1110
IC C2      C3      OP31     P3        1.5211  109.99  154.06  117.47   1.5924
IC C3      OP31    P3       OP32      1.4633  117.47   66.74  101.68   1.6525
IC OP32    OP31    *P3      OP33      1.6525  101.68 -113.70  109.39   1.4926
IC OP32    OP31    *P3      OP34      1.6525  101.68  112.29  106.74   1.4836
IC OP31    P3      OP32     C31       1.5924  101.68   55.76  110.28   1.4698
IC P3      OP32    C31      C32       1.6525  110.28 -172.41  110.74   1.5958
IC C32     OP32    *C31     H31J      1.5958  110.74  116.75  110.82   1.1115
IC H31J    OP32    *C31     H31K      1.1115  110.82  111.29  110.26   1.1103
IC HG31    C3      C2       C1        1.1112  106.69  -61.74  114.49   1.5241
IC C1      C3      *C2      OG12      1.5241  114.49 -122.33  108.64   1.4665
IC C1      C3      *C2      HG22      1.5241  114.49  124.23  104.11   1.1108
IC C3      C2      OG12     HO12      1.5211  108.64  -38.03   96.97   0.9599
IC C3      C2      C1       OP11      1.5211  114.49  175.92  108.99   1.3945
IC OP11    C2      *C1      HG11      1.3945  108.99 -131.04  104.78   1.1106
IC HG11    C2      *C1      HG12      1.1106  104.78 -113.14  109.09   1.1119
IC C2      C1      OP11     P1        1.5241  108.99  -84.99  120.20   1.5652
IC C1      OP11    P1       OP12      1.3945  120.20  -27.24  102.68   1.5816
IC OP12    OP11    *P1      OP13      1.5816  102.68  118.64  109.06   1.4705
IC OP12    OP11    *P1      OP14      1.5816  102.68 -114.38  108.43   1.4438
IC OP11    P1      OP12     C11       1.5652  102.68 -105.08  129.51   1.3844
IC P1      OP12    C11      C12       1.5816  129.51   79.30  113.33   1.5572
IC C12     OP12    *C11     H11J      1.5572  113.33 -123.60  109.70   1.1106
IC H11J    OP12    *C11     H11K      1.1106  109.70 -125.75  111.37   1.1111
IC OP12    C11     C12      C13       1.3844  113.33  172.10  111.92   1.5430
IC C13     C11     *C12     O12       1.5430  111.92  120.38  106.67   1.4690
IC O12     C11     *C12     H12J      1.4690  106.67  123.36  105.85   1.1110
IC C11     C12     O12      CA1       1.5572  106.67  139.57  111.75   1.3546
IC C12     O12     CA1      CA2       1.4690  111.75 -177.04  105.16   1.4819
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IC CA2     O12     *CA1     OA1       1.4819  105.16  175.26  126.65   1.2359
IC O12     CA1     CA2      CA3       1.3546  105.16 -166.84  109.95   1.5144
IC CA3     CA1     *CA2     H2A       1.5144  109.95 -122.50  115.81   1.1105
IC H2A     CA1     *CA2     H2B       1.1105  115.81 -121.44  107.35   1.1109
IC C11     C12     C13      O13       1.5572  111.92 -172.11  107.78   1.5003
IC O13     C12     *C13     H13J      1.5003  107.78 -115.91  112.20   1.1109
IC H13J    C12     *C13     H13K      1.1109  112.20 -121.54  112.00   1.1122
IC C12     C13     O13      CB1       1.5430  107.78   77.67  115.10   1.2970
IC C13     O13     CB1      CB2       1.5003  115.10 -179.81  109.11   1.4434
IC CB2     O13     *CB1     OB1       1.4434  109.11 -173.82  130.35   1.2113
IC O13     CB1     CB2      CB3       1.2970  109.11  173.87  116.83   1.5195
IC CB3     CB1     *CB2     H2D       1.5195  116.83 -121.03  109.80   1.1112
IC H2D     CB1     *CB2     H2E       1.1112  109.80 -114.30  107.94   1.1107
IC OP32    C31     C32      C33       1.4698  110.74  -72.15  111.19   1.5682
IC C33     C31     *C32     O32       1.5682  111.19  124.56  112.11   1.3898
IC O32     C31     *C32     H32J      1.3898  112.11  122.90  114.56   1.1112
IC C31     C32     O32      CC1       1.5958  112.11   62.25  119.56   1.3075
IC C32     O32     CC1      CC2       1.3898  119.56 -174.92  104.05   1.4829
IC CC2     O32     *CC1     OC1       1.4829  104.05 -166.47  126.62   1.2264
IC O32     CC1     CC2      CC3       1.3075  104.05  170.64  115.59   1.5435
IC CC3     CC1     *CC2     H2R       1.5435  115.59 -124.86  107.06   1.1110
IC H2R     CC1     *CC2     H2S       1.1110  107.06 -105.63  111.30   1.1109
IC C31     C32     C33      O33       1.5958  111.19 -173.79  110.26   1.4370
IC O33     C32     *C33     H33J      1.4370  110.26  118.41  109.85   1.1107
IC H33J    C32     *C33     H33K      1.1107  109.85  116.35  110.86   1.1105
IC C32     C33     O33      CD1       1.5682  110.26  -82.05  116.23   1.3711
IC C33     O33     CD1      CD2       1.4370  116.23  156.92  111.58   1.5654
IC CD2     O33     *CD1     OD1       1.5654  111.58 -176.12  124.80   1.1850
IC O33     CD1     CD2      CD3       1.3711  111.58   79.99  113.19   1.5154
IC CD3     CD1     *CD2     H2X       1.5154  113.19 -122.11  106.99   1.1106
IC H2X     CD1     *CD2     H2Y       1.1106  106.99 -114.65  110.19   1.1109
IC CA1     CA2     CA3      CA4       1.4819  109.95  160.84  117.75   1.5645
IC CA4     CA2     *CA3     H3A       1.5645  117.75 -127.81  109.37   1.1111
IC H3A     CA2     *CA3     H3B       1.1111  109.37 -117.63  101.55   1.1105
IC CA2     CA3     CA4      CA5       1.5144  117.75  157.03  111.41   1.5424
IC CA5     CA3     *CA4     H4A       1.5424  111.41 -119.03  108.09   1.1114
IC H4A     CA3     *CA4     H4B       1.1114  108.09 -126.38  120.58   1.1101
IC CA3     CA4     CA5      CA6       1.5645  111.41   74.25  110.88   1.5499
IC CA6     CA4     *CA5     H5A       1.5499  110.88 -125.89  112.16   1.1114
IC H5A     CA4     *CA5     H5B       1.1114  112.16 -116.89  114.30   1.1106
IC CA4     CA5     CA6      CA7       1.5424  110.88  177.26  112.07   1.5702
IC CA7     CA5     *CA6     H6A       1.5702  112.07 -121.41  112.61   1.1107
IC H6A     CA5     *CA6     H6B       1.1107  112.61 -124.17   99.78   1.1108
IC CA5     CA6     CA7      CA8       1.5499  112.07   74.00  120.92   1.5501
IC CA8     CA6     *CA7     H7A       1.5501  120.92 -128.07  104.29   1.1105
IC H7A     CA6     *CA7     H7B       1.1105  104.29 -118.23  103.40   1.1112
IC CA6     CA7     CA8      CA9       1.5702  120.92  170.69  112.79   1.5329
IC CA9     CA7     *CA8     H8A       1.5329  112.79 -117.60  114.99   1.1111
IC H8A     CA7     *CA8     H8B       1.1111  114.99 -115.64  104.49   1.1114
IC CA7     CA8     CA9      CA10      1.5501  112.79   82.54  132.44   1.3410
IC CA10    CA8     *CA9     H9A       1.3410  132.44 -165.92  110.30   1.0996
IC CA8     CA9     CA10     CA11      1.5329  132.44   11.31  129.79   1.4668
IC CA11    CA9     *CA10    H10A      1.4668  129.79  173.10  113.82   1.1006
IC CA9     CA10    CA11     CA12      1.3410  129.79 -125.54  110.53   1.5132
IC CA12    CA10    *CA11    H11A      1.5132  110.53 -124.22  111.84   1.1109
IC H11A    CA10    *CA11    H11B      1.1109  111.84 -116.05  116.75   1.1107
IC CA10    CA11    CA12     CA13      1.4668  110.53  161.55  113.19   1.4862
IC CA13    CA11    *CA12    H12A      1.4862  113.19 -115.99  104.44   1.1104
IC H12A    CA11    *CA12    H12B      1.1104  104.44 -109.05  111.86   1.1114
IC CA11    CA12    CA13     CA14      1.5132  113.19   66.72  118.43   1.5736
IC CA14    CA12    *CA13    H13A      1.5736  118.43 -112.65  104.63   1.1114
IC H13A    CA12    *CA13    H13B      1.1114  104.63 -117.70  113.84   1.1109
IC CA12    CA13    CA14     CA15      1.4862  118.43   62.79  110.33   1.5584
IC CA15    CA13    *CA14    H14A      1.5584  110.33 -118.07  107.82   1.1108
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IC H14A    CA13    *CA14    H14B       1.1108  107.82 -113.03  108.64   1.1112
IC CA13    CA14    CA15     CA16       1.5736  110.33 -175.93  102.80   1.5814
IC CA16    CA14    *CA15    H15A       1.5814  102.80 -121.30  114.89   1.1112
IC H15A    CA14    *CA15    H15B       1.1112  114.89 -125.40  120.38   1.1112
IC CA14    CA15    CA16     CA17       1.5584  102.80 -177.33  108.65   1.4920
IC CA17    CA15    *CA16    H16A       1.4920  108.65 -121.79  105.96   1.1117
IC H16A    CA15    *CA16    H16B       1.1117  105.96 -110.08  103.15   1.1108
IC CA15    CA16    CA17     CA18       1.5814  108.65 -168.13  114.64   1.5103
IC CA18    CA16    *CA17    H17A       1.5103  114.64 -123.69  105.58   1.1117
IC H17A    CA16    *CA17    H17B       1.1117  105.58 -117.14  106.96   1.1108
IC CA16    CA17    CA18     H18A       1.4920  114.64  -97.38  116.78   1.1116
IC H18A    CA17    *CA18    H18B       1.1116  116.78 -112.38  110.91   1.1109
IC H18A    CA17    *CA18    H18C       1.1116  116.78  124.13  107.97   1.1105
IC CB1     CB2     CB3      CB4        1.4434  116.83 -155.75  114.25   1.5868
IC CB4     CB2     *CB3     H3D        1.5868  114.25 -122.78  114.66   1.1117
IC H3D     CB2     *CB3     H3E        1.1117  114.66 -129.44  120.87   1.1109
IC CB2     CB3     CB4      CB5        1.5195  114.25  -52.65  114.56   1.5137
IC CB5     CB3     *CB4     H4D        1.5137  114.56 -115.68  101.27   1.1103
IC H4D     CB3     *CB4     H4E        1.1103  101.27 -119.02  105.41   1.1106
IC CB3     CB4     CB5      CB6        1.5868  114.56 -179.99  120.50   1.5634
IC CB6     CB4     *CB5     H5D        1.5634  120.50 -122.72  117.24   1.1113
IC H5D     CB4     *CB5     H5E        1.1113  117.24 -123.34  103.45   1.1107
IC CB4     CB5     CB6      CB7        1.5137  120.50   39.76  116.61   1.5133
IC CB7     CB5     *CB6     H6D        1.5133  116.61 -120.56  106.07   1.1110
IC H6D     CB5     *CB6     H6E        1.1110  106.07 -117.54  106.11   1.1114
IC CB5     CB6     CB7      CB8        1.5634  116.61  176.57  110.49   1.5173
IC CB8     CB6     *CB7     H7D        1.5173  110.49 -120.73  106.74   1.1106
IC H7D     CB6     *CB7     H7E        1.1106  106.74 -117.79  112.10   1.1106
IC CB6     CB7     CB8      CB9        1.5133  110.49  -82.21  120.66   1.5172
IC CB9     CB7     *CB8     H8D        1.5172  120.66 -115.86  108.05   1.1105
IC H8D     CB7     *CB8     H8E        1.1105  108.05 -111.89  111.52   1.1117
IC CB7     CB8     CB9      CB10       1.5173  120.66 -107.87  126.23   1.3089
IC CB10    CB8     *CB9     H9D        1.3089  126.23  177.32  108.46   1.0998
IC CB8     CB9     CB10     CB11       1.5172  126.23   -9.03  129.20   1.5488
IC CB11    CB9     *CB10    H10D       1.5488  129.20 -177.87  114.84   1.1001
IC CB9     CB10    CB11     CB12       1.3089  129.20   89.60  118.95   1.5198
IC CB12    CB10    *CB11    H11D       1.5198  118.95 -127.92  113.12   1.1108
IC H11D    CB10    *CB11    H11E       1.1108  113.12 -116.33  107.89   1.1110
IC CB10    CB11    CB12     CB13       1.5488  118.95   47.44  108.85   1.4805
IC CB13    CB11    *CB12    H12D       1.4805  108.85 -124.66  111.86   1.1106
IC H12D    CB11    *CB12    H12E       1.1106  111.86 -115.71  106.95   1.1117
IC CB11    CB12    CB13     CB14       1.5198  108.85  158.33  114.90   1.5460
IC CB14    CB12    *CB13    H13D       1.5460  114.90 -122.78  110.67   1.1114
IC H13D    CB12    *CB13    H13E       1.1114  110.67 -118.72  111.28   1.1107
IC CB12    CB13    CB14     CB15       1.4805  114.90   68.37  114.96   1.5755
IC CB15    CB13    *CB14    H14D       1.5755  114.96 -127.83  107.96   1.1104
IC H14D    CB13    *CB14    H14E       1.1104  107.96 -116.62  108.21   1.1111
IC CB13    CB14    CB15     CB16       1.5460  114.96  166.45  117.74   1.5429
IC CB16    CB14    *CB15    H15D       1.5429  117.74 -122.27  110.71   1.1109
IC H15D    CB14    *CB15    H15E       1.1109  110.71 -117.71   99.91   1.1101
IC CB14    CB15    CB16     CB17       1.5755  117.74  174.50  116.45   1.5273
IC CB17    CB15    *CB16    H16D       1.5273  116.45 -126.26  106.79   1.1119
IC H16D    CB15    *CB16    H16E       1.1119  106.79 -120.93  108.80   1.1106
IC CB15    CB16    CB17     CB18       1.5429  116.45  176.52  110.28   1.5697
IC CB18    CB16    *CB17    H17D       1.5697  110.28 -130.06  105.87   1.1105
IC H17D    CB16    *CB17    H17E       1.1105  105.87 -115.72  106.22   1.1106
IC CB16    CB17    CB18     H18D       1.5273  110.28 -159.07  103.32   1.1112
IC H18D    CB17    *CB18    H18E       1.1112  103.32 -120.33  105.93   1.1103
IC H18D    CB17    *CB18    H18F       1.1112  103.32  118.79  110.62   1.1116
IC CC1     CC2     CC3      CC4        1.4829  115.59   49.93  117.90   1.5366
IC CC4     CC2     *CC3     H3R        1.5366  117.90 -115.05  111.28   1.1107
IC H3R     CC2     *CC3     H3S        1.1107  111.28 -122.62  109.57   1.1107
IC CC2     CC3     CC4      CC5        1.5435  117.90   41.42  122.16   1.4856
IC CC5     CC3     *CC4     H4R        1.4856  122.16 -129.12  107.74   1.1116
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IC H4R     CC3     *CC4     H4S       1.1116  107.74 -110.63  106.93   1.1114
IC CC3     CC4     CC5      CC6       1.5366  122.16   79.03  118.09   1.5779
IC CC6     CC4     *CC5     H5R       1.5779  118.09 -121.27  111.33   1.1111
IC H5R     CC4     *CC5     H5S       1.1111  111.33 -121.85  103.83   1.1116
IC CC4     CC5     CC6      CC7       1.4856  118.09 -175.62  114.14   1.5193
IC CC7     CC5     *CC6     H6R       1.5193  114.14 -112.92   99.65   1.1104
IC H6R     CC5     *CC6     H6S       1.1104   99.65 -115.34  114.89   1.1110
IC CC5     CC6     CC7      CC8       1.5779  114.14   86.04  111.08   1.5443
IC CC8     CC6     *CC7     H7R       1.5443  111.08 -126.84  118.56   1.1115
IC H7R     CC6     *CC7     H7S       1.1115  118.56 -116.67  107.70   1.1111
IC CC6     CC7     CC8      CC9       1.5193  111.08 -167.74  113.25   1.5955
IC CC9     CC7     *CC8     H8R       1.5955  113.25 -126.88  111.16   1.1113
IC H8R     CC7     *CC8     H8S       1.1113  111.16 -113.40  107.96   1.1105
IC CC7     CC8     CC9      CC10      1.5443  113.25 -109.87  126.39   1.3527
IC CC10    CC8     *CC9     H9R       1.3527  126.39 -170.92  110.56   1.0998
IC CC8     CC9     CC10     CC11      1.5955  126.39   15.86  128.70   1.4629
IC CC11    CC9     *CC10    H10R      1.4629  128.70  175.07  123.34   1.1002
IC CC9     CC10    CC11     CC12      1.3527  128.70  101.47  118.70   1.5861
IC CC12    CC10    *CC11    H11R      1.5861  118.70 -125.10  109.20   1.1112
IC H11R    CC10    *CC11    H11S      1.1112  109.20 -110.25  111.88   1.1101
IC CC10    CC11    CC12     CC13      1.4629  118.70   67.74  108.82   1.5353
IC CC13    CC11    *CC12    H12R      1.5353  108.82 -126.41  105.67   1.1103
IC H12R    CC11    *CC12    H12S      1.1103  105.67 -116.13  112.54   1.1110
IC CC11    CC12    CC13     CC14      1.5861  108.82 -177.19  124.76   1.5291
IC CC14    CC12    *CC13    H13R      1.5291  124.76 -126.31  102.56   1.1109
IC H13R    CC12    *CC13    H13S      1.1109  102.56 -101.72  109.52   1.1110
IC CC12    CC13    CC14     CC15      1.5353  124.76 -147.35  108.06   1.5835
IC CC15    CC13    *CC14    H14R      1.5835  108.06 -127.34  119.98   1.1117
IC H14R    CC13    *CC14    H14S      1.1117  119.98 -118.05  109.10   1.1109
IC CC13    CC14    CC15     CC16      1.5291  108.06   78.94  118.04   1.5648
IC CC16    CC14    *CC15    H15R      1.5648  118.04 -130.95  115.54   1.1114
IC H15R    CC14    *CC15    H15S      1.1114  115.54 -107.98  103.32   1.1109
IC CC14    CC15    CC16     CC17      1.5835  118.04  170.34  112.62   1.5605
IC CC17    CC15    *CC16    H16R      1.5605  112.62  116.67  109.09   1.1110
IC H16R    CC15    *CC16    H16S      1.1110  109.09  118.07  101.73   1.1110
IC CC15    CC16    CC17     CC18      1.5648  112.62 -160.59  113.48   1.5455
IC CC18    CC16    *CC17    H17R      1.5455  113.48 -119.35  112.75   1.1111
IC H17R    CC16    *CC17    H17S      1.1111  112.75 -118.74  109.01   1.1114
IC CC16    CC17    CC18     H18R      1.5605  113.48 -167.53  105.19   1.1114
IC H18R    CC17    *CC18    H18S      1.1114  105.19  123.30  114.77   1.1107
IC H18R    CC17    *CC18    H18T      1.1114  105.19 -120.49  105.29   1.1117
IC CD1     CD2     CD3      CD4       1.5654  113.19 -162.40  114.80   1.5512
IC CD4     CD2     *CD3     H3X       1.5512  114.80 -117.81  118.26   1.1102
IC H3X     CD2     *CD3     H3Y       1.1102  118.26 -125.60  110.95   1.1112
IC CD2     CD3     CD4      CD5       1.5154  114.80   63.81  109.67   1.6095
IC CD5     CD3     *CD4     H4X       1.6095  109.67 -112.22  109.63   1.1107
IC H4X     CD3     *CD4     H4Y       1.1107  109.63 -120.86  110.95   1.1109
IC CD3     CD4     CD5      CD6       1.5512  109.67 -171.66  110.10   1.5117
IC CD6     CD4     *CD5     H5X       1.5117  110.10 -113.98  105.23   1.1108
IC H5X     CD4     *CD5     H5Y       1.1108  105.23 -128.80  116.89   1.1106
IC CD4     CD5     CD6      CD7       1.6095  110.10  170.09  111.04   1.5055
IC CD7     CD5     *CD6     H6X       1.5055  111.04 -114.76  105.35   1.1116
IC H6X     CD5     *CD6     H6Y       1.1116  105.35 -122.63  110.38   1.1108
IC CD5     CD6     CD7      CD8       1.5117  111.04 -172.02  115.71   1.5289
IC CD8     CD6     *CD7     H7X       1.5289  115.71 -123.94  114.68   1.1110
IC H7X     CD6     *CD7     H7Y       1.1110  114.68 -126.78  107.85   1.1109
IC CD6     CD7     CD8      CD9       1.5055  115.71  -61.83  117.36   1.5186
IC CD9     CD7     *CD8     H8X       1.5186  117.36 -129.63  101.79   1.1109
IC H8X     CD7     *CD8     H8Y       1.1109  101.79 -111.91  105.86   1.1107
IC CD7     CD8     CD9      CD10      1.5289  117.36  179.97  120.32   1.3356
IC CD10    CD8     *CD9     H9X       1.3356  120.32 -177.34  116.78   1.1009
IC CD8     CD9     CD10     CD11      1.5186  120.32   -9.60  131.58   1.4710
IC CD11    CD9     *CD10    H10X      1.4710  131.58 -172.61  113.16   1.1005
IC CD9     CD10    CD11     CD12      1.3356  131.58 -124.79  115.05   1.5361
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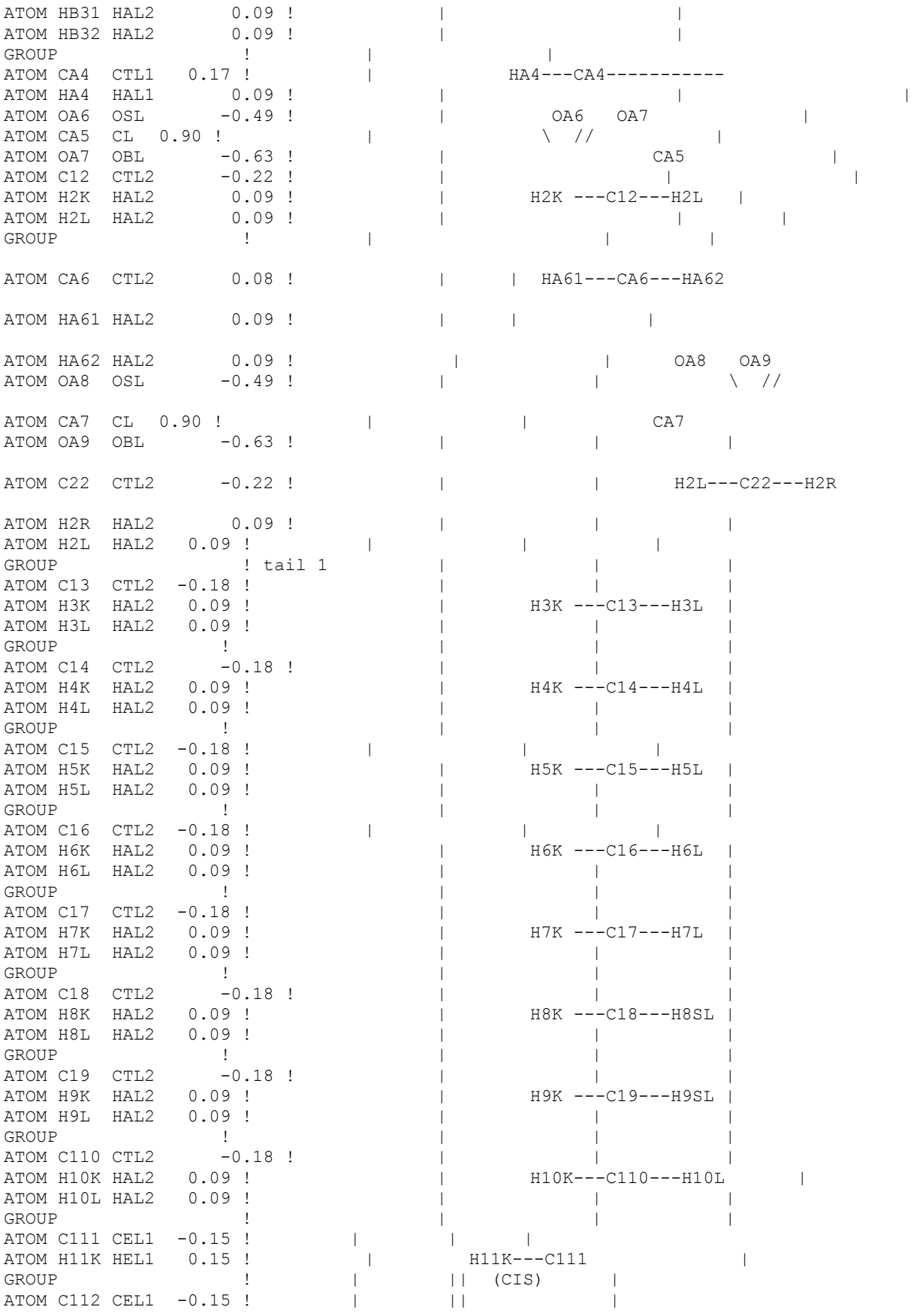
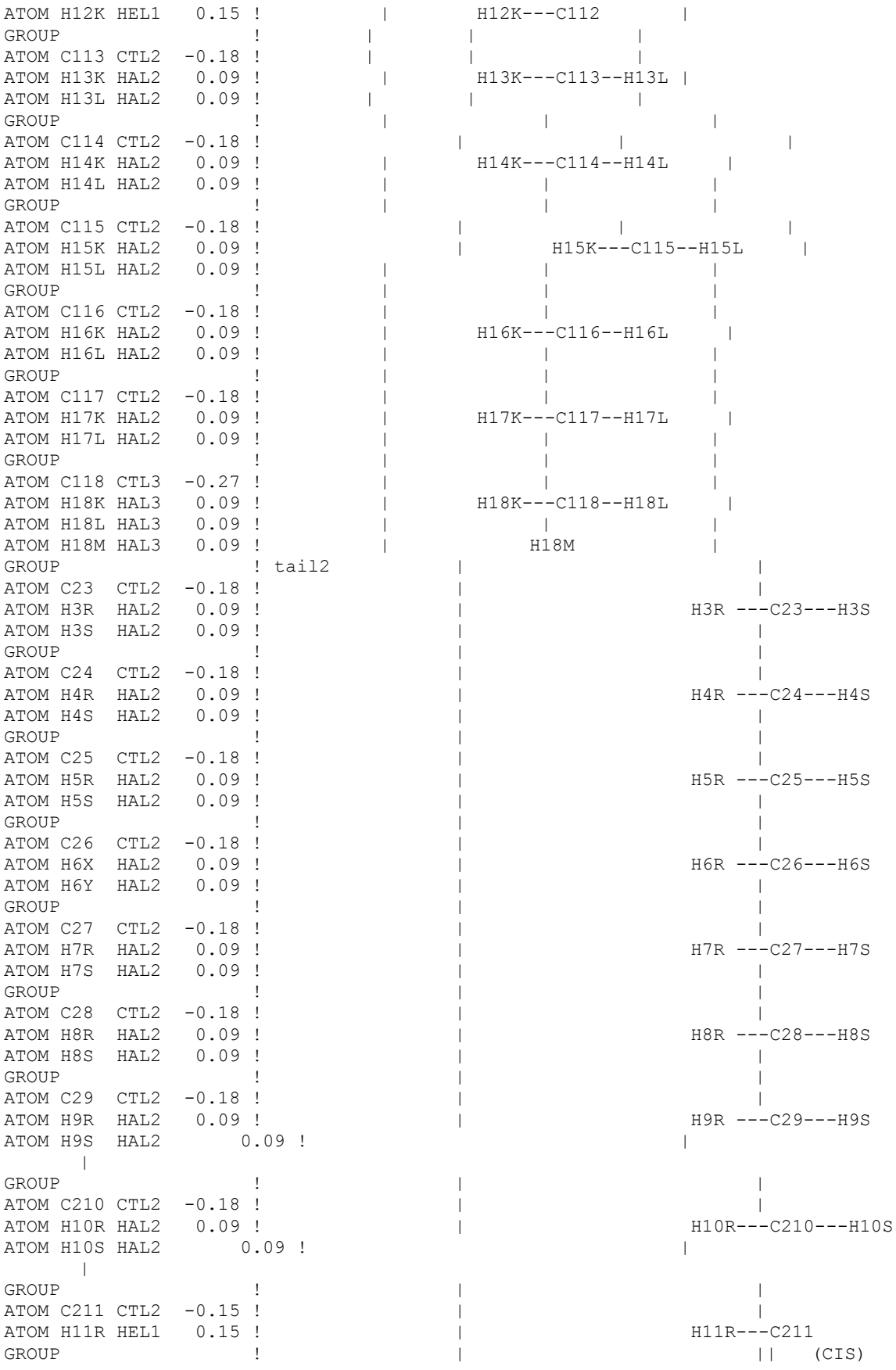
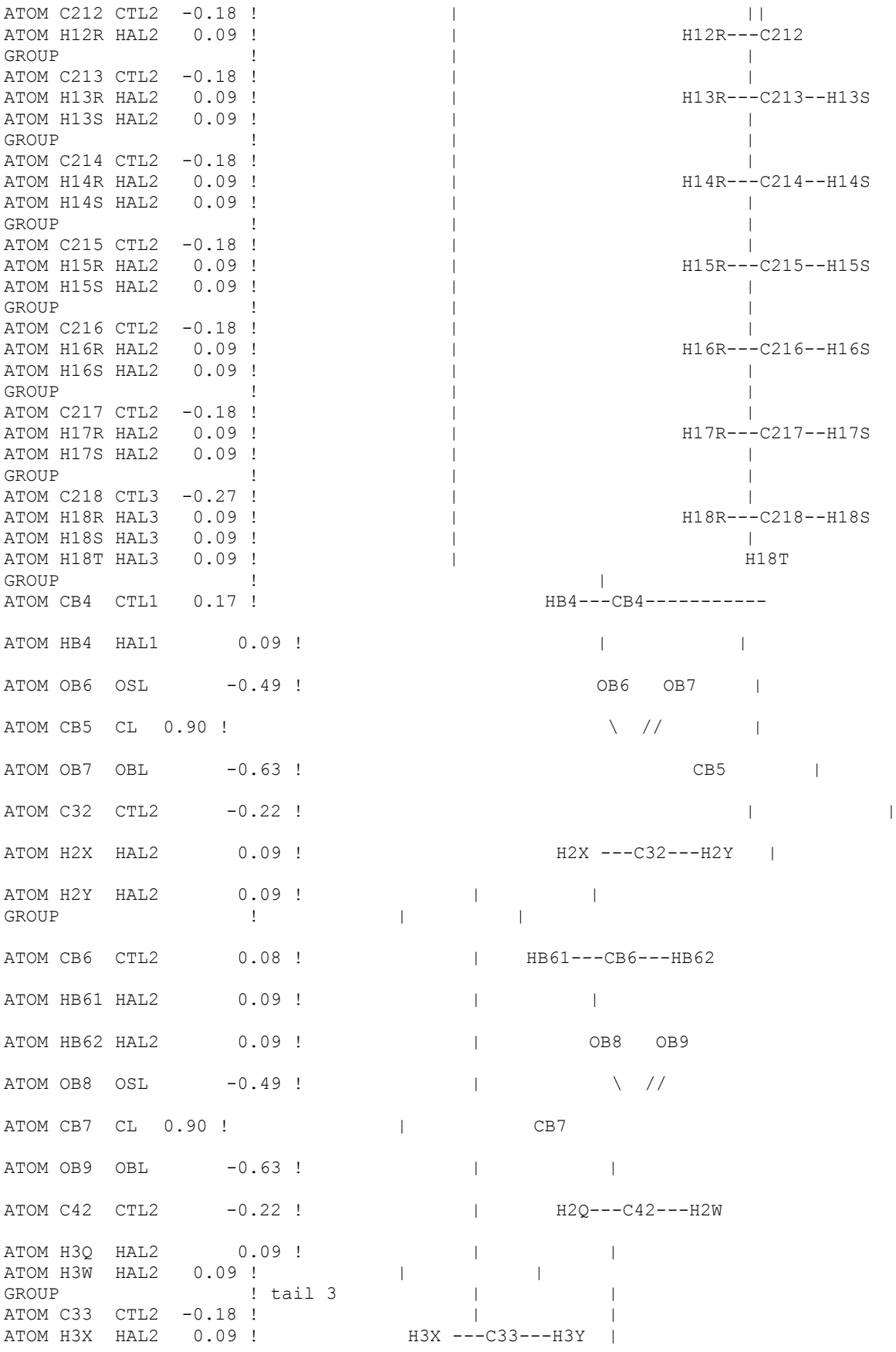
IC CD12    CD10    *CD11    H11X       1.5361  115.05 -128.95  111.59   1.1111
IC H11X    CD10    *CD11    H11Y       1.1111  111.59 -111.21  111.18   1.1111
IC CD10    CD11    CD12     CD13       1.4710  115.05  -77.11  105.04   1.4788
IC CD13    CD11    *CD12    H12X       1.4788  105.04 -112.96  106.48   1.1110
IC H12X    CD11    *CD12    H12Y       1.1110  106.48 -120.99  113.58   1.1114
IC CD11    CD12    CD13     CD14       1.5361  105.04  168.60  110.84   1.5429
IC CD14    CD12    *CD13    H13X       1.5429  110.84 -122.83  114.36   1.1104
IC H13X    CD12    *CD13    H13Y       1.1104  114.36 -113.84  114.06   1.1110
IC CD12    CD13    CD14     CD15       1.4788  110.84  -80.22  114.95   1.5099
IC CD15    CD13    *CD14    H14X       1.5099  114.95 -125.08  104.06   1.1112
IC H14X    CD13    *CD14    H14Y       1.1112  104.06 -114.53  108.61   1.1117
IC CD13    CD14    CD15     CD16       1.5429  114.95  173.02  110.69   1.5313
IC CD16    CD14    *CD15    H15X       1.5313  110.69 -123.13  108.31   1.1109
IC H15X    CD14    *CD15    H15Y       1.1109  108.31 -110.71  116.76   1.1116
IC CD14    CD15    CD16     CD17       1.5099  110.69 -176.63  112.38   1.5367
IC CD17    CD15    *CD16    H16X       1.5367  112.38 -134.03  107.87   1.1113
IC H16X    CD15    *CD16    H16Y       1.1113  107.87 -110.75  102.38   1.1114
IC CD15    CD16    CD17     CD18       1.5313  112.38 -173.09  106.45   1.5289
IC CD18    CD16    *CD17    H17X       1.5289  106.45 -115.92  116.45   1.1117
IC H17X    CD16    *CD17    H17Y       1.1117  116.45 -114.48  108.29   1.1110
IC CD16    CD17    CD18     H18X       1.5367  106.45  178.60  109.03   1.1112
IC H18X    CD17    *CD18    H18Y       1.1112  109.03 -120.60  108.05   1.1107
IC H18X    CD17    *CD18    H18Z       1.1112  109.03  119.06  114.08   1.1116


RESI CDL     -2.00!
!
!    Vaccenyl - CH2                              CH2 - Vaccenyl
!             |                           |
!    Vaccenyl - CH           OH            CH  - Vaccenyl
!             |     (-)       |         (-)   |
!             CH2 - PO4 - CH2 - CH - CH2 - PO4 - CH2
!
! Derived from CDL
!    by Stuart Rose 9/29/2013
!
!
GROUP
ATOM C1   CTL1       0.14 !
ATOM H1   HAL1       0.09 !                ---------------
ATOM O1   OHL   -0.66 !           |              |
ATOM HO1  HOL        0.43 !         H1---C1-O1-HO1     |
GROUP                                            |                 |
ATOM CA2  CTL2      -0.08 !                     |        HA22---CA2---HA21
ATOM HA21 HAL2       0.09 !                     |               |
ATOM HA22 HAL2       0.09 !                     |        (-)OA3 OA2
ATOM PA2  PL  1.50 !                    |           \ /
ATOM OA3  O2L       -0.78 !                     |             PA2(+)
ATOM OA4  O2L       -0.78 !                     |            / \
ATOM OA2  OSLP      -0.57 !                     |        (-)OA4 OA5
ATOM OA5  OSLP      -0.57 !              |            |
ATOM CA3  CTL2      -0.08 !                     |   HA31---CA3---HA32
ATOM HA31 HAL2       0.09 !                     |               |
ATOM HA32 HAL2   0.09 !                  |            |
GROUP                 !                  |            |
ATOM CB2  CTL2  -0.08 !    HB22---CB2---HB21 |
ATOM HB21 HAL2       0.09 !              |            |
ATOM HB22 HAL2       0.09 !       (-)OB3 OB2          |
ATOM PB2  PL  1.50 !           \ /             |
ATOM OB3  O2L       -0.78 !            PB2(+)     |
ATOM OB4  O2L       -0.78 !           / \             |
ATOM OB2  OSLP      -0.57 !       (-)OB4 OB5          |
ATOM OB5  OSLP      -0.57 !             |                      |
ATOM CB3  CTL2      -0.08 !  HB31---CB3---HB32    |
```


ATOM HB31 HAL2 0.09 !
ATOM HB32 HAL2 0.09 !
GROUP !
ATOM CA4 CTL1 0.17 !
ATOM HA4 HAL1 0.09 !
ATOM OA6 OSL -0.49 !
ATOM CA5 CL 0.90 !
ATOM OA7 OBL -0.63 !
ATOM C12 CTL2 -0.22 !
ATOM H2K HAL2 0.09 !
ATOM H2L HAL2 0.09 !
GROUP !
ATOM CA6 CTL2 0.08 !
ATOM HA61 HAL2 0.09 !
ATOM HA62 HAL2 0.09 !
ATOM OA8 OSL -0.49 !
ATOM CA7 CL 0.90 !
ATOM OA9 OBL -0.63 !
ATOM C22 CTL2 -0.22 !
ATOM H2R HAL2 0.09 !
ATOM H2L HAL2 0.09 !
GROUP ! tail 1
ATOM C13 CTL2 -0.18 !
ATOM H3K HAL2 0.09 !
ATOM H3L HAL2 0.09 !
GROUP !
ATOM C14 CTL2 -0.18 !
ATOM H4K HAL2 0.09 !
ATOM H4L HAL2 0.09 !
GROUP !
ATOM C15 CTL2 -0.18 !
ATOM H5K HAL2 0.09 !
ATOM H5L HAL2 0.09 !
GROUP !
ATOM C16 CTL2 -0.18 !
ATOM H6K HAL2 0.09 !
ATOM H6L HAL2 0.09 !
GROUP !
ATOM C17 CTL2 -0.18 !
ATOM H7K HAL2 0.09 !
ATOM H7L HAL2 0.09 !
GROUP !
ATOM C18 CTL2 -0.18 !
ATOM H8K HAL2 0.09 !
ATOM H8L HAL2 0.09 !
GROUP !
ATOM C19 CTL2 -0.18 !
ATOM H9K HAL2 0.09 !
ATOM H9L HAL2 0.09 !
GROUP !
ATOM C110 CTL2 -0.18 !
ATOM H10K HAL2 0.09 !
ATOM H10L HAL2 0.09 !
GROUP !
ATOM C111 CEL1 -0.15 !
ATOM H11K HEL1 0.15 !
GROUP !
ATOM C112 CEL1 -0.15 !
HA4---CA4
OA6 OA7
CA5
H2K ---C12---H2L
HA61---CA6---HA62
OA8 OA9
CA7
H2L---C22---H2R
H3K ---C13---H3L
H4K ---C14---H4L
H5K ---C15---H5L
H6K ---C16---H6L
H7K ---C17---H7L
H8K ---C18---H8SL
H9K ---C19---H9SL
H10K---C110---H10L
H11K---C111
(CIS)


ATOM H12K HEL1 0.15 !
GROUP !
ATOM C113 CTL2 -0.18 !
ATOM H13K HAL2 0.09 !
ATOM H13L HAL2 0.09 !
GROUP !
ATOM C114 CTL2 -0.18 !
ATOM H14K HAL2 0.09 !
ATOM H14L HAL2 0.09 !
GROUP !
ATOM C115 CTL2 -0.18 !
ATOM H15K HAL2 0.09 !
ATOM H15L HAL2 0.09 !
GROUP !
ATOM C116 CTL2 -0.18 !
ATOM H16K HAL2 0.09 !
ATOM H16L HAL2 0.09 !
GROUP !
ATOM C117 CTL2 -0.18 !
ATOM H17K HAL2 0.09 !
ATOM H17L HAL2 0.09 !
GROUP !
ATOM C118 CTL3 -0.27 !
ATOM H18K HAL3 0.09 !
ATOM H18L HAL3 0.09 !
ATOM H18M HAL3 0.09 !
GROUP ! tail2
ATOM C23 CTL2 -0.18 !
ATOM H3R HAL2 0.09 !
ATOM H3S HAL2 0.09 !
GROUP !
ATOM C24 CTL2 -0.18 !
ATOM H4R HAL2 0.09 !
ATOM H4S HAL2 0.09 !
GROUP !
ATOM C25 CTL2 -0.18 !
ATOM H5R HAL2 0.09 !
ATOM H5S HAL2 0.09 !
GROUP !
ATOM C26 CTL2 -0.18 !
ATOM H6X HAL2 0.09 !
ATOM H6Y HAL2 0.09 !
GROUP !
ATOM C27 CTL2 -0.18 !
ATOM H7R HAL2 0.09 !
ATOM H7S HAL2 0.09 !
GROUP !
ATOM C28 CTL2 -0.18 !
ATOM H8R HAL2 0.09 !
ATOM H8S HAL2 0.09 !
GROUP !
ATOM C29 CTL2 -0.18 !
ATOM H9R HAL2 0.09 !
ATOM H9S HAL2 0.09 !
GROUP !
ATOM C210 CTL2 -0.18 !
ATOM H10R HAL2 0.09 !
ATOM H10S HAL2 0.09 !
GROUP !
ATOM C211 CTL2 -0.15 !
ATOM H11R HEL1 0.15 !
GROUP !
H12K---C112
H13K---C113--H13L
H14K---C114--H14L
H15K---C115--H15L
H16K---C116--H16L
H17K---C117--H17L
H18K---C118--H18L
H18M
H3R ---C23---H3S
H4R ---C24---H4S
H5R ---C25---H5S
H6R ---C26---H6S
H7R ---C27---H7S
H8R ---C28---H8S
H9R ---C29---H9S
H10R---C210---H10S
H11R---C211
(CIS)


ATOM C212 CTL2 -0.18 !
ATOM H12R HAL2 0.09 !
GROUP !
ATOM C213 CTL2 -0.18 !
ATOM H13R HAL2 0.09 !
ATOM H13S HAL2 0.09 !
GROUP !
ATOM C214 CTL2 -0.18 !
ATOM H14R HAL2 0.09 !
ATOM H14S HAL2 0.09 !
GROUP !
ATOM C215 CTL2 -0.18 !
ATOM H15R HAL2 0.09 !
ATOM H15S HAL2 0.09 !
GROUP !
ATOM C216 CTL2 -0.18 !
ATOM H16R HAL2 0.09 !
ATOM H16S HAL2 0.09 !
GROUP !
ATOM C217 CTL2 -0.18 !
ATOM H17R HAL2 0.09 !
ATOM H17S HAL2 0.09 !
GROUP !
ATOM C218 CTL3 -0.27 !
ATOM H18R HAL3 0.09 !
ATOM H18S HAL3 0.09 !
ATOM H18T HAL3 0.09 !
GROUP !
ATOM CB4 CTL1 0.17 !
H12R---C212
H13R---C213--H13S
H14R---C214--H14S
H15R---C215--H15S
H16R---C216--H16S
H17R---C217--H17S
H18R---C218--H18S
H18T
HB4---CB4----------
ATOM HB4 HAL1 0.09 !
ATOM OB6 OSL -0.49 !
ATOM CB5 CL 0.90 !
ATOM OB7 OBL -0.63 !
ATOM C32 CTL2 -0.22 !
ATOM H2X HAL2 0.09 !
ATOM H2Y HAL2 0.09 !
GROUP !
OB6 OB7
CB5
H2X ---C32---H2Y
ATOM CB6 CTL2 0.08 !
ATOM HB61 HAL2 0.09 !
ATOM HB62 HAL2 0.09 !
ATOM OB8 OSL -0.49 !
ATOM CB7 CL 0.90 !
ATOM OB9 OBL -0.63 !
ATOM C42 CTL2 -0.22 !
ATOM H3Q HAL2 0.09 !
ATOM H3W HAL2 0.09 !
GROUP ! tail 3
ATOM C33 CTL2 -0.18 !
ATOM H3X HAL2 0.09 !
HB61---CB6---HB62
OB8 OB9
CB7
H2Q---C42---H2W
H3X ---C33---H3Y

```
ATOM H3Y  HAL2   0.09 !                   |           |
GROUP              !                     |           |
ATOM C34  CTL2      -0.18 !              |           |
ATOM H4X  HAL2   0.09 !              H4Y ---C34---H4X  |
ATOM H4Y  HAL2   0.09 !                   |           |
GROUP              !                     |           |
ATOM C35  CTL2  -0.18 !             |           |
ATOM H5X  HAL2   0.09 !              H5X ---C35---H5Y  |
ATOM H5Y  HAL2   0.09 !                   |           |
GROUP              !                     |           |
ATOM C36  CTL2  -0.18 !             |           |
ATOM H6X  HAL2   0.09 !              H6X ---C36---H6Y         |

ATOM H6Y  HAL2   0.09 !                   |           |
GROUP              !                     |           |
ATOM C37  CTL2  -0.18 !                   |           |
ATOM H7X  HAL2   0.09 !              H7X ---C37---H7Y  |
ATOM H7Y  HAL2   0.09 !                   |           |
GROUP              !                     |           |
ATOM C38  CTL2      -0.18 !              |           |
ATOM H8X  HAL2   0.09 !              H8X ---C38---H8Y  |
ATOM H8Y  HAL2   0.09 !                   |           |
GROUP              !                     |           |
ATOM C39  CTL2      -0.18 !              |           |
ATOM H9X  HAL2   0.09 !              H9X ---C39---H9SY        |

ATOM H9Y  HAL2   0.09 !                   |           |
GROUP              !                     |           |
ATOM C310 CTL2      -0.18 !              |           |
ATOM H10X HAL2   0.09 !              H10X---C310---H10Y       |

ATOM H10Y HAL2   0.09 !                   |           |
GROUP              !                     |           |
ATOM C311 CEL1  -0.15 !             |             |
ATOM H11X HEL1   0.15 !       H11X---C311               |
GROUP                !            ||  (CIS)      |
ATOM C312 CEL1  -0.15 !            ||             |
ATOM H12X HEL1   0.15 !       H12X---C312             |
GROUP                !            |              |
ATOM C313 CTL2  -0.18 !            |              |
ATOM H13X HAL2   0.09 !             H13X---C313--H13Y        |

ATOM H13Y HAL2   0.09 !            |              |
GROUP                !            |              |
ATOM C314 CTL2  -0.18 !            |              |
ATOM H14X HAL2   0.09 !       H14X---C314--H14Y     |
ATOM H14Y HAL2   0.09 !            |              |
GROUP                !            |              |
ATOM C315 CTL2  -0.18 !            |              |
ATOM H15X HAL2   0.09 !             H15X---C315--H15Y     |
ATOM H15Y HAL2   0.09 !            |              |
GROUP                !            |              |
ATOM C316 CTL2  -0.18 !            |              |
ATOM H16X HAL2   0.09 !       H16X---C316--H16Y     |
ATOM H16Y HAL2   0.09 !            |              |
GROUP                !            |              |
ATOM C317 CTL2  -0.18 !            |              |
ATOM H17X HAL2   0.09 !       H17X---C317--H17Y     |
ATOM H17Y HAL2   0.09 !            |              |
GROUP                !            |              |
ATOM C318 CTL3  -0.27 !            |              |
ATOM H18X HAL3   0.09 !       H18X---C318--H18Y     |
ATOM H18Y HAL3   0.09 !            |              |
ATOM H18Z HAL3   0.09 !           H18Z            |
```

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GROUP                ! tail4                        |
ATOM C43  CTL2  -0.18 !                         |
ATOM H3Q  HAL2   0.09 !                      H3Q ---C43---H3W
ATOM H3W  HAL2   0.09 !                         |
GROUP                !                          |
ATOM C44  CTL2  -0.18 !                         |
ATOM H4Q  HAL2   0.09 !                      H4Q ---C44---H4W
ATOM H4W  HAL2   0.09 !                         |
GROUP                !                          |
ATOM C45  CTL2  -0.18 !                         |
ATOM H5Q  HAL2   0.09 !                      H5Q ---C45---H5W
ATOM H5W  HAL2   0.09 !                         |
GROUP                !                          |
ATOM C46  CTL2  -0.18 !                         |
ATOM H6Q  HAL2   0.09 !                      H6Q ---C46---H6W
ATOM H6Y  HAL2   0.09 !                         |
GROUP                !                          |
ATOM C47  CTL2  -0.18 !                         |
ATOM H7Q  HAL2   0.09 !                      H7Q ---C47---H7W
ATOM H7W  HAL2   0.09 !                         |
GROUP                !                          |
ATOM C48  CTL2  -0.18 !                         |
ATOM H8Q  HAL2   0.09 !                      H8Q ---C48---H8W
ATOM H8W  HAL2   0.09 !                         |
GROUP                !                          |
ATOM C49  CTL2  -0.18 !                         |
ATOM H9Q  HAL2   0.09 !                      H9Q ---C49---H9W
ATOM H9W  HAL2      0.09 !                                  |
GROUP                !                          |
ATOM C410 CTL2  -0.18 !                         |
ATOM H10Q HAL2   0.09 !                      H10Q---C410---H10W
ATOM H10W HAL2      0.09 !                                  |
GROUP                !                          |
ATOM C411 CEL1  -0.15 !                         |
ATOM H11Q HEL1   0.15 !                      H11Q---C411
GROUP                !                          ||   (CIS)
ATOM C412 CEL1  -0.18 !                         ||
ATOM H12Q HEL1   0.09 !                      H12Q---C412
GROUP                !                          |
ATOM C413 CTL2  -0.18 !                         |
ATOM H13Q HAL2   0.09 !                      H13Q---C413--H13W
ATOM H13W HAL2   0.09 !                         |
GROUP                !                          |
ATOM C414 CTL2  -0.18 !                         |
ATOM H14Q HAL2   0.09 !                      H14Q---C414--H14W
ATOM H14W HAL2   0.09 !                         |
GROUP                !                          |
ATOM C415 CTL2  -0.18 !                         |
ATOM H15Q HAL2   0.09 !                      H15Q---C415--H15W
ATOM H15W HAL2   0.09 !                         |
GROUP                !                          |
ATOM C416 CTL2  -0.18 !                         |
ATOM H16Q HAL2   0.09 !                      H16Q---C416--H16W
ATOM H16W HAL2   0.09 !                         |
GROUP                !                          |
ATOM C417 CTL2  -0.18 !                         |
ATOM H17Q HAL2   0.09 !                      H17Q---C417--H17W
ATOM H17W HAL2   0.09 !                         |
GROUP                !                          |
ATOM C418 CTL3  -0.27 !                         |
ATOM H18Q HAL3   0.09 !                      H18Q---C418--H18W
ATOM H18W HAL3   0.09 !                         |
ATOM H18G HAL3   0.09 !                       H18G
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```
BOND  C1  H1          C1  O1      O1  HO1    C1  CA2
BOND  C1  CB2    CA2 HA21   CA2 HA22   CA2 OA2
BOND  CB2 HB21   CB2 HB22   CB2 OB2    OA2 PA2
BOND  PA2 OA3    PA2 OA4    PA2 OA5    OB2 PB2
BOND  PB2 OB3    PB2 OB4    PB2 OB5    OA5 CA3
BOND  CA3 HA31   CA3 HA32   CA3 CA4    CA4 HA4
BOND  CA4 CA6    CA6 HA61   CA6 HA62   CA4 OA6
BOND  CA6 OA8    OB5 CB3    CB3 HB31   CB3 HB32
BOND  CB3 CB4    CB4 HB4    CB4 CB6    CB6 HB61
BOND  CB6 HB62   CB4 OB6    CB6 OB8
! Chain Starting CA4
BOND  OA6 CA5  CA5 C12
DOUBLE CA5 OA7
BOND  C12  H2K    C12  H2L    C12  C13
BOND  C13  H3K    C13  H3L    C13  C14
BOND  C14  H4K    C14  H4L    C14  C15
BOND  C15  H5K    C15  H5L    C15  C16
BOND  C16  H6K    C16  H6L    C16  C17
BOND  C17  H7K    C17  H7L    C17  C18
BOND  C18  H8K    C18  H8L    C18  C19
BOND  C19  H9K    C19  H9L    C19  C110
BOND  C110 H10K   C110 H110L  C110 C111
BOND  C111 H11K
DOUBLE  C111 C112
BOND  C112 H12K   C112 C113
BOND  C113 H13K   C113 H13L   C113 C114
BOND  C114 H14K   C114 H14L   C114 C115
BOND  C115 H15K   C115 H15L   C115 C116
BOND  C116 H16K   C116 H16L   C116 C117
BOND  C117 H17K   C117 H17L   C117 C118
BOND  C118 H18K   C118 H18L   C118 H18M
! Chain Starting CA6
BOND  OA8 CA7  CA7 C22
DOUBLE CA7 OA9
BOND  C22  H2R    C22  H2S    C22  C23
BOND  C23  H3R    C23  H3S    C23  C24
BOND  C24  H4R    C24  H4S    C24  C25
BOND  C25  H5R    C25  H5S    C25  C26
BOND  C26  H6R    C26  H6S    C26  C27
BOND  C27  H7R    C27  H7S    C27  C28
BOND  C28  H8R    C28  H8S    C28  C29
BOND  C29  H9R    C29  H9S    C29  C210
BOND  C210 H10R   C210 H10S   C210 C211
BOND  C211 H11R
DOUBLE  C211 C212
BOND  C212 H12R   C212 C213
BOND  C213 H13R   C213 H13S   C213 C214
BOND  C214 H14R   C214 H14S   C214 C215
BOND  C215 H15R   C215 H15S   C215 C216
BOND  C216 H16R   C216 H16S   C216 C217
BOND  C217 H17R   C217 H17S   C217 C218
BOND  C218 H18R   C218 H18S   C218 H18T
! Chain Starting CB4
BOND  OB6 CB5  CB5 C32
DOUBLE CB5 OB7
BOND  C32  H2X    C32  H2Y    C32  C33
BOND  C33  H3X    C33  H3Y    C33  C34
BOND  C34  H4X    C34  H4Y    C34  C35
BOND  C35  H5X    C35  H5Y    C35  C36
BOND  C36  H6X    C36  H6Y    C36  C37
BOND  C37  H7X    C37  H7Y    C37  C38
BOND  C38  H8X    C38  H8Y    C38  C39
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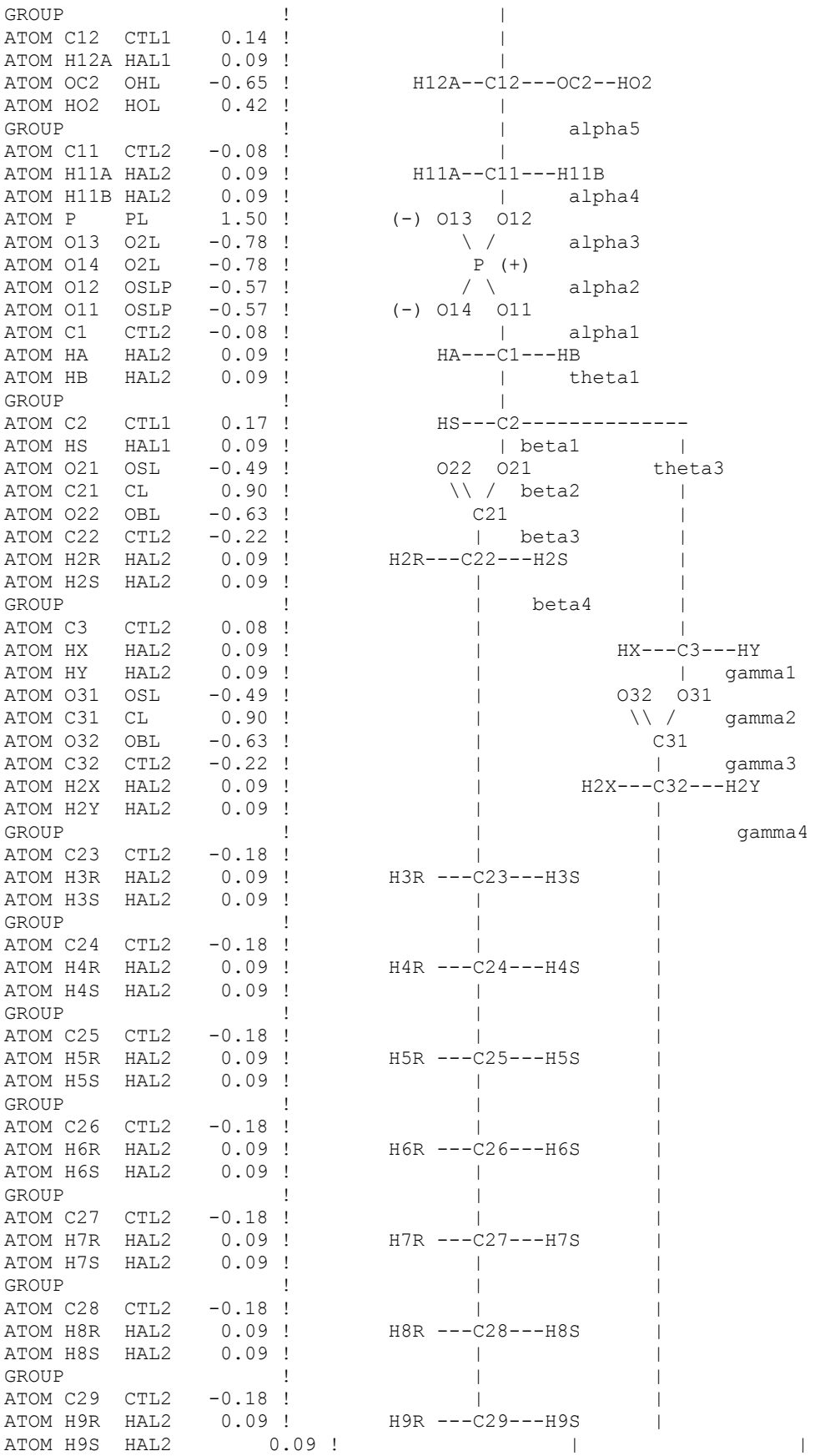
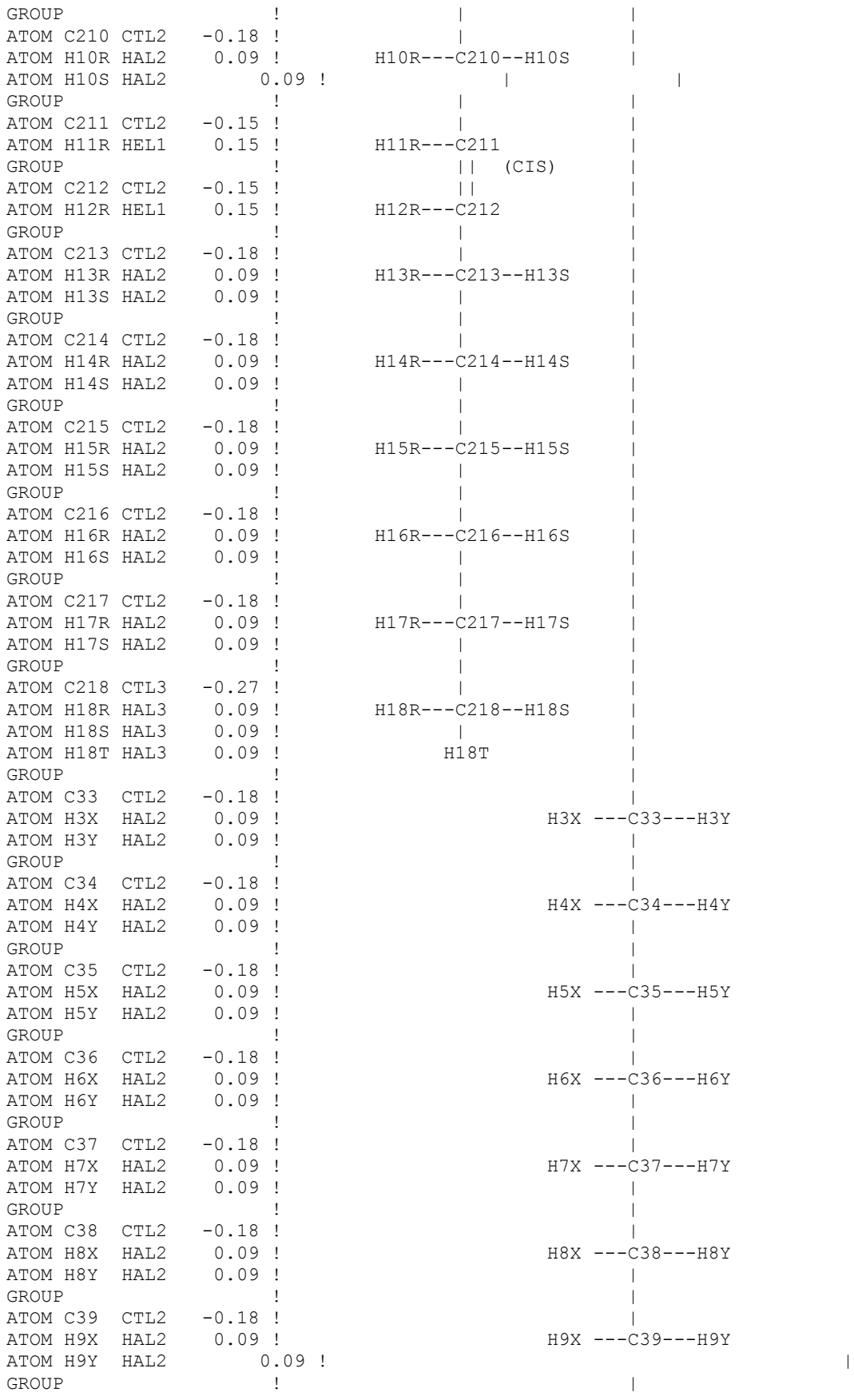
BOND  C39  H9X    C39  H9Y    C39  C310
BOND  C310 H10X   C310 H110Y  C310 C311
BOND  C311 H11X
DOUBLE  C311 C312
BOND  C312 H12X   C312 C313
BOND  C313 H13X   C313 H13Y   C313 C314
BOND  C314 H14X   C314 H14Y   C314 C315
BOND  C315 H15X   C315 H15Y   C315 C316
BOND  C316 H16X   C316 H16Y   C316 C317
BOND  C317 H17X   C317 H17Y   C317 C318
BOND  C318 H18X   C318 H18Y   C318 H18Z
! Chain Starting CB6
BOND  OB8 CB7  CB7 C42
DOUBLE CB7 OB9
BOND  C42  H2Q    C42  H2W    C42  C43
BOND  C43  H3Q    C43  H3W    C43  C44
BOND  C44  H4Q    C44  H4W    C44  C45
BOND  C45  H5Q    C45  H5W    C45  C46
BOND  C46  H6Q    C46  H6W    C46  C47
BOND  C47  H7Q    C47  H7W    C47  C48
BOND  C48  H8Q    C48  H8W    C48  C49
BOND  C49  H9Q    C49  H9W    C49  C410
BOND  C410 H10Q   C410 H10W   C410 C411
BOND  C411 H11Q
DOUBLE  C411 C412
BOND  C412 H12Q   C412 C413
BOND  C413 H13Q   C413 H13W   C413 C414
BOND  C414 H14Q   C414 H14W   C414 C415
BOND  C415 H15Q   C415 H15W   C415 C416
BOND  C416 H16Q   C416 H16W   C416 C417
BOND  C417 H17Q   C417 H17W   C417 C418
BOND  C418 H18Q   C418 H18W   C418 H18G

IMPR CA5 OA6 C12 OA7 CA7 OA8 C32 OA9
IMPR CB5 OB6 C52 OB7 CB7 OB8 C72 OB9


!PGs

RESI DVPG      -1.00 ! 2,3-divacenyl-D-glycero-1-phosphatidylglycerol
!  R1 - CH2
!       |
!  R2 - CH
!       |
!       CH2 - PO4 - CH2 - CH(OH) - CH2OH
!
! Polar Head and glycerol backbone
!!Derived from Mackerell top_all36_lipid.rf
!!   by Stuart Rose 9/10/2013
!!RESI DOPG        -1.00 ! 2,3-dioleoyl-D-glycero-1-phosphatidylglycerol
!!
!!  R1 - CH2
!!       |
!!  R2 - CH
!!       |
!!       CH2 - PO4 - CH2 - CH(OH) - CH2OH
!!
!! Polar Head and glycerol backbone
GROUP                   !
ATOM C13  CTL2    0.05 !
ATOM H13A HAL2    0.09 !                H13A
ATOM H13B HAL2    0.09 !                 |
ATOM OC3  OHL    -0.65 !                 |
ATOM HO3  HOL     0.42 !          H13B--C13---OC3--HO3
```


GROUP
ATOM C12 CTL1 0.14
ATOM H12A HAL1 0.09
ATOM OC2 OHL -0.65
ATOM HO2 HOL 0.42
GROUP
ATOM C11 CTL2 -0.08
ATOM H11A HAL2 0.09
ATOM H11B HAL2 0.09
ATOM P PL 1.50
ATOM O13 O2L -0.78
ATOM O14 O2L -0.78
ATOM O12 OSLP -0.57
ATOM O11 OSLP -0.57
ATOM C1 CTL2 -0.08
ATOM HA HAL2 0.09
ATOM HB HAL2 0.09
GROUP
ATOM C2 CTL1 0.17
ATOM HS HAL1 0.09
ATOM O21 OSL -0.49
ATOM C21 CL 0.90
ATOM O22 OBL -0.63
ATOM C22 CTL2 -0.22
ATOM H2R HAL2 0.09
ATOM H2S HAL2 0.09
GROUP
ATOM C3 CTL2 0.08
ATOM HX HAL2 0.09
ATOM HY HAL2 0.09
ATOM O31 OSL -0.49
ATOM C31 CL 0.90
ATOM O32 OBL -0.63
ATOM C32 CTL2 -0.22
ATOM H2X HAL2 0.09
ATOM H2Y HAL2 0.09
GROUP
ATOM C23 CTL2 -0.18
ATOM H3R HAL2 0.09
ATOM H3S HAL2 0.09
GROUP
ATOM C24 CTL2 -0.18
ATOM H4R HAL2 0.09
ATOM H4S HAL2 0.09
GROUP
ATOM C25 CTL2 -0.18
ATOM H5R HAL2 0.09
ATOM H5S HAL2 0.09
GROUP
ATOM C26 CTL2 -0.18
ATOM H6R HAL2 0.09
ATOM H6S HAL2 0.09
GROUP
ATOM C27 CTL2 -0.18
ATOM H7R HAL2 0.09
ATOM H7S HAL2 0.09
GROUP
ATOM C28 CTL2 -0.18
ATOM H8R HAL2 0.09
ATOM H8S HAL2 0.09
GROUP
ATOM C29 CTL2 -0.18
ATOM H9R HAL2 0.09
ATOM H9S HAL2 0.09
H12A--C12---OC2--HO2
alpha5
H11A--C11---H11B
alpha4
(-) O13 O12
alpha3
P (+)
alpha2
(-) O14 O11
alpha1
HA---C1---HB
theta1
HS---C2--------------
beta1
O22 O21
theta3
beta2
C21
beta3
H2R---C22---H2S
beta4
HX---C3---HY
gamma1
O32 O31
gamma2
C31
gamma3
H2X---C32---H2Y
gamma4
H3R ---C23---H3S
H4R ---C24---H4S
H5R ---C25---H5S
H6R ---C26---H6S
H7R ---C27---H7S
H8R ---C28---H8S
H9R ---C29---H9S


GROUP ! | |
ATOM C210 CTL2 -0.18 ! | |
ATOM H10R HAL2 0.09 ! H10R---C210--H10S |
ATOM H10S HAL2 0.09 ! | |
GROUP ! | |
ATOM C211 CTL2 -0.15 ! | |
ATOM H11R HEL1 0.15 ! H11R---C211 |
GROUP ! || (CIS) |
ATOM C212 CTL2 -0.15 ! || |
ATOM H12R HEL1 0.15 ! H12R---C212 |
GROUP ! | |
ATOM C213 CTL2 -0.18 ! | |
ATOM H13R HAL2 0.09 ! H13R---C213--H13S |
ATOM H13S HAL2 0.09 ! | |
GROUP ! | |
ATOM C214 CTL2 -0.18 ! | |
ATOM H14R HAL2 0.09 ! H14R---C214--H14S |
ATOM H14S HAL2 0.09 ! | |
GROUP ! | |
ATOM C215 CTL2 -0.18 ! | |
ATOM H15R HAL2 0.09 ! H15R---C215--H15S |
ATOM H15S HAL2 0.09 ! | |
GROUP ! | |
ATOM C216 CTL2 -0.18 ! | |
ATOM H16R HAL2 0.09 ! H16R---C216--H16S |
ATOM H16S HAL2 0.09 ! | |
GROUP ! | |
ATOM C217 CTL2 -0.18 ! | |
ATOM H17R HAL2 0.09 ! H17R---C217--H17S |
ATOM H17S HAL2 0.09 ! | |
GROUP ! | |
ATOM C218 CTL3 -0.27 ! | |
ATOM H18R HAL3 0.09 ! H18R---C218--H18S |
ATOM H18S HAL3 0.09 ! | |
ATOM H18T HAL3 0.09 ! H18T |
GROUP ! |
ATOM C33 CTL2 -0.18 ! |
ATOM H3X HAL2 0.09 ! H3X ---C33---H3Y
ATOM H3Y HAL2 0.09 ! |
GROUP ! |
ATOM C34 CTL2 -0.18 ! |
ATOM H4X HAL2 0.09 ! H4X ---C34---H4Y
ATOM H4Y HAL2 0.09 ! |
GROUP ! |
ATOM C35 CTL2 -0.18 ! |
ATOM H5X HAL2 0.09 ! H5X ---C35---H5Y
ATOM H5Y HAL2 0.09 ! |
GROUP ! |
ATOM C36 CTL2 -0.18 ! |
ATOM H6X HAL2 0.09 ! H6X ---C36---H6Y
ATOM H6Y HAL2 0.09 ! |
GROUP ! |
ATOM C37 CTL2 -0.18 ! |
ATOM H7X HAL2 0.09 ! H7X ---C37---H7Y
ATOM H7Y HAL2 0.09 ! |
GROUP ! |
ATOM C38 CTL2 -0.18 ! |
ATOM H8X HAL2 0.09 ! H8X ---C38---H8Y
ATOM H8Y HAL2 0.09 ! |
GROUP ! |
ATOM C39 CTL2 -0.18 ! |
ATOM H9X HAL2 0.09 ! H9X ---C39---H9Y
ATOM H9Y HAL2 0.09 ! |
GROUP ! |

```
ATOM C310 CTL2   -0.18 !                          |
ATOM H10X HAL2    0.09 !                      H10X---C310--H10Y
ATOM H10Y HAL2    0.09 !                                       |
GROUP                  !                          |
ATOM C311 CTL2   -0.15 !                          |
ATOM H11X HEL1    0.15 !                      H11X---C311
GROUP                  !                          ||
ATOM C312 CTL2   -0.15 !                          ||
ATOM H12X HEL1    0.15 !                      H12X---C312
GROUP                  !                          |
ATOM C313 CTL2   -0.18 !                          |
ATOM H13X HAL2    0.09 !                      H13X---C313--H13Y
ATOM H13Y HAL2    0.09 !                          |
GROUP                  !                          |
ATOM C314 CTL2   -0.18 !                          |
ATOM H14X HAL2    0.09 !                      H14X---C314--H14Y
ATOM H14Y HAL2    0.09 !                          |
GROUP                  !                          |
ATOM C315 CTL2   -0.18 !                          |
ATOM H15X HAL2    0.09 !                      H15X---C315--H15Y
ATOM H15Y HAL2    0.09 !                          |
GROUP                  !                          |
ATOM C316 CTL2   -0.18 !                          |
ATOM H16X HAL2    0.09 !                      H16X---C316--H16Y
ATOM H16Y HAL2    0.09 !                          |
GROUP                  !                          |
ATOM C317 CTL2   -0.18 !                          |
ATOM H17X HAL2    0.09 !                      H17X---C317--H17Y
ATOM H17Y HAL2    0.09 !                          |
GROUP                  !                          |
ATOM C318 CTL3   -0.27 !                          |
ATOM H18X HAL3    0.09 !                      H18X---C318--H18Y
ATOM H18Y HAL3    0.09 !                          |
ATOM H18Z HAL3    0.09 !                         H18Z

! Polar Head
BOND  HO3  OC3       OC3  C13       C13  H13A      C13  H13B      C13  C12
BOND  HO2  OC2       OC2  C12       C12  H12A      C12  C11
BOND  C11  H11A      C11  H11B      C11  O12       O11  C1
BOND  O12  P         P    O11       P    O13       P    O14
! Glycerol Backbone
BOND  C1   HA        C1    HB       C1   C2
BOND  C2   HS        C2    C3       C2   O21
BOND  C3   HX        C3    HY       C3   O31
! Chain from C2
BOND  O21  C21
BOND  C21  C22
DOUBLE  C21  O22
BOND  C22  H2R       C22  H2S       C22  C23
BOND  C23  H3R       C23  H3S       C23  C24
BOND  C24  H4R       C24  H4S       C24  C25
BOND  C25  H5R       C25  H5S       C25  C26
BOND  C26  H6R       C26  H6S       C26  C27
BOND  C27  H7R       C27  H7S       C27  C28
BOND  C28  H8R       C28  H8S       C28  C29
BOND  C29  H9R           C29  H9S       C29  C210
BOND  C210 H10R      C210 H10S       C210 C211
BOND  C211 H11R
DOUBLE  C211 C212
BOND  C212 H12R      C212 C213
BOND  C213 H13R      C213 H13S      C213 C214
BOND  C214 H14R      C214 H14S      C214 C215
BOND  C215 H15R      C215 H15S      C215 C216
BOND  C216 H16R      C216 H16S      C216 C217
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BOND  C217 H17R      C217 H17S      C217 C218
BOND  C218 H18R      C218 H18S      C218 H18T
! Chain From C3
BOND  O31  C31
BOND  C31  C32
DOUBLE  C31  O32
BOND  C32  H2X       C32  H2Y       C32  C33
BOND  C33  H3X       C33  H3Y       C33  C34
BOND  C34  H4X       C34  H4Y       C34  C35
BOND  C35  H5X       C35  H5Y       C35  C36
BOND  C36  H6X       C36  H6Y       C36  C37
BOND  C37  H7X       C37  H7Y       C37  C38
BOND  C38  H8X       C38  H8Y       C38  C39
BOND  C39  H9X           C39  H9Y       C39  C310
BOND  C310 H10X      C310 H11Y      C310 C311
BOND  C311 H11X
DOUBLE C311 C312
BOND  C312 H12X      C312 C313
BOND  C313 H13X      C313 H13Y      C313 C314
BOND  C314 H14X      C314 H14Y      C314 C315
BOND  C315 H15X      C315 H15Y      C315 C316
BOND  C316 H16X      C316 H16Y      C316 C317
BOND  C317 H17X      C317 H17Y      C317 C318
BOND  C318 H18X      C318 H18Y      C318 H18Z

IMPR C21 O21 C22 O22    C31 O31 C32 O32

IC C13    C12    C11    O12        1.5583  113.89   93.01  113.50   1.4295
IC OC3    C13    C12    C11        1.4375  112.31   69.20  113.89   1.5573
IC OC3    C12    *C13   H13A       1.4375  112.31  119.90  108.06   1.1118
IC OC3    C12    *C13   H13B       1.4375  112.31 -123.06  109.89   1.1097
IC C12    C13    OC3    HO3        1.5583  112.31 -141.84  106.96   0.9777
IC C11    C13    *C12   OC2        1.5573  113.89 -121.65  107.64   1.4259
IC OC2    C13    *C12   H12A       1.4259  107.64 -117.84  109.30   1.1131
IC C13    C12    OC2    HO2        1.5583  107.64   38.09  100.52   0.9671
IC O12    C12    *C11   H11A       1.4295  113.50 -126.35  109.70   1.1125
IC H11A   C12    *C11   H11B       1.1125  109.70 -115.65  107.71   1.1131
IC C12    C11    O12    P          1.5573  113.50  -72.69  124.80   1.5783
IC C11    O12    P      O11        1.4295  124.80  -30.02  102.66   1.5825
IC O11    O12    *P     O13        1.5825  102.66  113.88  109.00   1.4783
IC O11    O12    *P     O14        1.5825  102.66 -115.27  109.77   1.4781
IC O12    P      O11    C1         1.5783  102.66  -80.21  120.83   1.4246
IC P      O11    C1     C2         1.5825  120.83  177.68  108.67   1.5488
IC C2     O11    *C1    HA         1.5488  108.67 -120.91  111.25   1.1145
IC HA     O11    *C1    HB         1.1145  111.25 -120.47  110.06   1.1152
IC O11    C1     C2     C3         1.4246  108.67   45.70  110.42   1.5580
IC C3     C1     *C2    O21        1.5580  110.42  120.25  110.13   1.4420
IC C3     C1     *C2    HS         1.5580  110.42 -116.94  108.10   1.1164
IC C1     C2     O21    C21        1.5488  110.13   74.82  114.08   1.3218
IC C2     O21    C21    C22        1.4420  114.08 -171.58  108.87   1.5297
IC C22    O21    *C21   O22        1.5297  108.87 -179.18  126.27   1.2166
IC O21    C21    C22    C23        1.3218  108.87  167.60  112.03   1.5460
IC C23    C21    *C22   H2R        1.5460  112.03 -121.40  108.25   1.1088
IC H2R    C21    *C22   H2S        1.1088  108.25 -117.05  107.34   1.1068
IC C1     C2     C3     O31        1.5488  110.42 -172.10  112.95   1.4472
IC O31    C2     *C3    HX         1.4472  112.95 -119.90  106.80   1.1123
IC HX     C2     *C3    HY         1.1123  106.80 -114.66  109.95   1.1147
IC C2     C3     O31    C31        1.5580  112.95   84.38  114.39   1.3267
IC C3     O31    C31    C32        1.4472  114.39  176.82  109.50   1.5275
IC C32    O31    *C31   O32        1.5275  109.50 -179.44  126.11   1.2173
IC O31    C31    C32    C33        1.3267  109.50  -66.76  112.63   1.5535
IC C33    C31    *C32   H2X        1.5535  112.63  121.43  107.50   1.1085
IC H2X    C31    *C32   H2Y        1.1085  107.50  116.64  107.32   1.1097
IC C21    C22    C23    C24        1.5289  112.21  175.76  112.39   1.5338
```

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IC C24    C22    *C23   H3R       1.5338  112.39 -120.69  109.57   1.1147
IC H3R    C22    *C23   H3S       1.1147  109.57 -117.65  109.64   1.1142
IC C22    C23    C24    C25       1.5449  112.39 -179.39  112.35   1.5346
IC C25    C23    *C24   H4R       1.5346  112.35 -121.52  109.41   1.1131
IC H4R    C23    *C24   H4S       1.1131  109.41 -117.57  108.97   1.1134
IC C23    C24    C25    C26       1.5338  112.35  176.31  112.80   1.5344
IC C26    C24    *C25   H5R       1.5344  112.80 -121.01  108.95   1.1135
IC H5R    C24    *C25   H5S       1.1135  108.95 -117.24  109.16   1.1132
IC C24    C25    C26    C27       1.5346  112.80 -179.44  112.48   1.5356
IC C27    C25    *C26   H6R       1.5356  112.48 -121.49  109.32   1.1129
IC H6R    C25    *C26   H6S       1.1129  109.32 -117.47  108.94   1.1132
IC C25    C26    C27    C28       1.5344  112.48  176.92  112.46   1.5398
IC C28    C26    *C27   H7R       1.5398  112.46 -121.38  108.40   1.1139
IC H7R    C26    *C27   H7S       1.1139  108.40 -116.93  108.77   1.1139
IC C26    C27    C28    C29       1.5356  112.46 -178.53  111.43   1.5097
IC C29    C27    *C28   H8R       1.5097  111.43 -123.58  107.80   1.1132
IC H8R    C27    *C28   H8S       1.1132  107.80 -115.43  108.37   1.1128
IC C27    C28    C29    C210      1.5344  112.48  176.92  112.46   1.5398
IC C210   C28    *C29   H9R       1.5398  112.46 -121.38  108.40   1.1139
IC H9R    C28    *C29   H9S        1.1139  108.40 -116.93  108.77   1.1139
IC C28    C29    C210   C211      1.5356  112.46 -178.53  111.43   1.5097
IC C211   C29    *C210  H10R      1.5097  111.43 -123.58  107.80   1.1132
IC H10R   C29    *C210  H9S        1.1132  107.80 -115.43  108.37   1.1128
IC C29    C210   C211   C212      1.5398  111.43 -126.96  126.62   1.3465
IC C212   C210   *C211  H11R      1.3465  126.62  178.41  114.65   1.1012
IC C210   C211   C212   C213      1.5097  126.62   -1.69  126.32   1.5088
IC C213   C211   *C212  H12R      1.5088  126.32 -179.55  118.79   1.1012
IC C211   C212   C213   C214      1.5392  112.29  179.81  112.68   1.5345
IC C214   C212   *C213  H13R      1.5345  112.68 -121.26  109.04   1.1132
IC H13R   C212   *C213  H13S      1.1132  109.04 -117.39  109.10   1.1131
IC C212   C213   C214   C215      1.5354  112.68  179.80  112.59   1.5347
IC C215   C213   *C214  H14R      1.5347  112.59 -121.29  109.09   1.1132
IC H14R   C213   *C214  H14S      1.1132  109.09 -117.37  109.11   1.1133
IC C213   C214   C215   C216      1.5345  112.59 -179.58  112.63   1.5347
IC C216   C214   *C215  H15R      1.5347  112.63 -121.36  109.09   1.1132
IC H15R   C214   *C215  H15S      1.1132  109.09 -117.38  109.07   1.1132
IC C214   C215   C216   C217      1.5347  112.63  179.65  112.69   1.5339
IC C217   C215   *C216  H16R      1.5339  112.69 -121.27  109.11   1.1132
IC H16R   C215   *C216  H16S      1.1132  109.11 -117.36  109.14   1.1132
IC C215   C216   C217   C218      1.5347  112.69 -179.93  113.30   1.5309
IC C218   C216   *C217  H17R      1.5309  113.30 -121.70  108.75   1.1140
IC H17R   C216   *C217  H17S      1.1140  108.75 -116.65  108.73   1.1141
IC C216   C217   C218   H18R      1.5339  113.30  -59.98  110.46   1.1113
IC H18R   C217   *C218  H18S      1.1113  110.46  119.84  110.45   1.1114
IC H18R   C217   *C218  H18T      1.1113  110.46 -120.09  110.62   1.1112
IC C31    C32    C33    C34       1.5288  113.05  179.24  111.73   1.5343
IC C34    C32    *C33   H3X       1.5343  111.73 -120.85  109.62   1.1140
IC H3X    C32    *C33   H3Y       1.1140  109.62 -117.95  109.78   1.1144
IC C32    C33    C34    C35       1.5447  111.73 -176.74  112.91   1.5345
IC C35    C33    *C34   H4X       1.5345  112.91 -121.67  109.15   1.1134
IC H4X    C33    *C34   H4Y       1.1134  109.15 -117.32  108.98   1.1134
IC C33    C34    C35    C36       1.5343  112.91  178.63  112.42   1.5349
IC C36    C34    *C35   H5X       1.5349  112.42 -120.99  108.94   1.1133
IC H5X    C34    *C35   H5Y       1.1133  108.94 -117.41  109.31   1.1131
IC C34    C35    C36    C37       1.5345  112.42 -176.73  112.80   1.5356
IC C37    C35    *C36   H6X       1.5356  112.80 -121.69  109.16   1.1130
IC H6X    C35    *C36   H6Y       1.1130  109.16 -117.32  108.94   1.1133
IC C35    C36    C37    C38       1.5349  112.80  178.92  112.27   1.5402
IC C38    C36    *C37   H7X       1.5402  112.27 -121.37  108.23   1.1139
IC H7X    C36    *C37   H7Y       1.1139  108.23 -117.01  109.05   1.1137
IC C36    C37    C38    C39       1.5356  112.27 -174.92  111.69   1.5099
IC C39    C37    *C38   H8X       1.5099  111.69 -124.14  107.77   1.1124
IC H8X    C37    *C38   H8Y       1.1124  107.77 -115.13  108.30   1.1128
IC C37    C38    C39    C310      1.5349  112.80  178.92  112.27   1.5402
```

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IC C310   C38    *C39   H9X        1.5402  112.27 -121.37  108.23   1.1139
IC H9X    C38  *C39   H9Y     1.1139  108.23 -117.01  109.05   1.1137
IC C38    C39    C310   C311       1.5356  112.27 -174.92  111.69   1.5099
IC C311   C39    *C310  H10X       1.5099  111.69 -124.14  107.77   1.1124
IC H10X   C39  *C310  H10Y    1.1124  107.77 -115.13  108.30   1.1128
IC C39    C310   C311   C312       1.5402  111.69 -121.39  127.35   1.3470
IC C312   C310   *C311  H11X       1.3470  127.35  179.11  114.24   1.1012
IC C310   C311   C312   C313       1.5099  127.35   -0.69  127.25   1.5096
IC C313   C311   *C312  H12X       1.5096  127.25  179.82  118.43   1.1012
IC C311   C312   C313   C314       1.3470  127.25  106.03  111.65   1.5393
IC C314   C312   *C313  H13X       1.5393  111.65 -121.49  112.10   1.1123
IC H13X   C312   *C313  H13Y       1.1123  112.10 -117.95  109.83   1.1127
IC C312   C313   C314   C315       1.5096  111.65  179.63  112.41   1.5355
IC C315   C313   *C314  H14X       1.5355  112.41 -121.09  109.75   1.1135
IC H14X   C313   *C314  H14Y       1.1135  109.75 -118.07  109.46   1.1143
IC C313   C314   C315   C316       1.5347  112.66 -179.12  112.61   1.5348
IC C316   C314   *C315  H15X       1.5348  112.61 -121.34  109.09   1.1132
IC H15X   C314   *C315  H15Y       1.1132  109.09 -117.41  109.09   1.1132
IC C314   C315   C316   C317       1.5347  112.61  179.83  112.71   1.5340
IC C317   C315   *C316  H16X       1.5340  112.71 -121.28  109.10   1.1132
IC H16X   C315   *C316  H16Y       1.1132  109.10 -117.35  109.13   1.1133
IC C315   C316   C317   C318       1.5348  112.71 -179.67  113.30   1.5309
IC C318   C316   *C317  H17X       1.5309  113.30 -121.68  108.77   1.1141
IC H17X   C316   *C317  H17Y       1.1141  108.77 -116.68  108.76   1.1141
IC C316   C317   C318   H18X       1.5340  113.30  -59.94  110.46   1.1113
IC H18X   C317   *C318  H18Y       1.1113  110.46  119.86  110.45   1.1113
IC H18X   C317   *C318  H18Z       1.1113  110.46 -120.06  110.61   1.1112


RESI VSPG      -1.00 ! 1-Vaccinyl 2-stereoyl-D-glycero-1-phosphatidylglycerol
!
!  R1 - CH2
!       |
!  R2 - CH
!       |
!       CH2 - PO4 - CH2 - CH(OH) - CH2OH
!
! Polar Head and glycerol backbone
!!Derived from Mackerell top_all36_lipid.rf
!!   by Stuart Rose 9/10/2013
!!RESI DOPG        -1.00 ! 2,3-dioleoyl-D-glycero-1-phosphatidylglycerol
!!
!!  R1 - CH2
!!       |
!!  R2 - CH
!!       |
!!       CH2 - PO4 - CH2 - CH(OH) - CH2OH
!!
!! Polar Head and glycerol backbone
GROUP                  !
ATOM C13  CTL2    0.05 !
ATOM H13A HAL2    0.09 !                H13A
ATOM H13B HAL2    0.09 !                 |
ATOM OC3  OHL    -0.65 !                 |
ATOM HO3  HOL     0.42 !          H13B--C13---OC3--HO3
GROUP                  !                 |
ATOM C12  CTL1    0.14 !                 |
ATOM H12A HAL1    0.09 !                 |
ATOM OC2  OHL    -0.65 !          H12A--C12---OC2--HO2
ATOM HO2  HOL     0.42 !                 |
GROUP                  !                 |     alpha5
ATOM C11  CTL2   -0.08 !                 |
ATOM H11A HAL2    0.09 !          H11A--C11---H11B
ATOM H11B HAL2    0.09 !                 |     alpha4
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ATOM P    PL      1.50 !        (-) O13  O12
ATOM O13  O2L    -0.78 !              \ /      alpha3
ATOM O14  O2L    -0.78 !               P (+)
ATOM O12  OSLP   -0.57 !              / \      alpha2
ATOM O11  OSLP   -0.57 !        (-) O14  O11
ATOM C1   CTL2   -0.08 !                  |     alpha1
ATOM HA   HAL2    0.09 !              HA---C1---HB
ATOM HB   HAL2    0.09 !                  |     theta1
GROUP                  !                  |
ATOM C2   CTL1    0.17 !              HS---C2--------------
ATOM HS   HAL1    0.09 !                   | beta1        |
ATOM O21  OSL    -0.49 !              O22  O21          theta3
ATOM C21  CL      0.90 !               \\ /  beta2        |
ATOM O22  OBL    -0.63 !                 C21              |
ATOM C22  CTL2   -0.22 !                  |   beta3        |
ATOM H2R  HAL2    0.09 !         H2R---C22---H2S         |
ATOM H2S  HAL2    0.09 !                  |               |
GROUP                  !                  |    beta4      |
ATOM C3   CTL2    0.08 !                  |               |
ATOM HX   HAL2    0.09 !                  |           HX---C3---HY
ATOM HY   HAL2    0.09 !                  |                |   gamma1
ATOM O31  OSL    -0.49 !                  |           O32  O31
ATOM C31  CL      0.90 !                  |            \\ /    gamma2
ATOM O32  OBL    -0.63 !                  |              C31
ATOM C32  CTL2   -0.22 !                  |              |     gamma3
ATOM H2X  HAL2    0.09 !                  |        H2X---C32---H2Y
ATOM H2Y  HAL2    0.09 !                  |              |
GROUP                  !                  |              |      gamma4
ATOM C23  CTL2   -0.18 !                  |              |
ATOM H3R  HAL2    0.09 !         H3R ---C23---H3S       |
ATOM H3S  HAL2    0.09 !                  |              |
GROUP                  !                  |              |
ATOM C24  CTL2   -0.18 !                  |              |
ATOM H4R  HAL2    0.09 !         H4R ---C24---H4S       |
ATOM H4S  HAL2    0.09 !                  |              |
GROUP                  !                  |              |
ATOM C25  CTL2   -0.18 !                  |              |
ATOM H5R  HAL2    0.09 !         H5R ---C25---H5S       |
ATOM H5S  HAL2    0.09 !                  |              |
GROUP                  !                  |              |
ATOM C26  CTL2   -0.18 !                  |              |
ATOM H6R  HAL2    0.09 !         H6R ---C26---H6S       |
ATOM H6S  HAL2    0.09 !                  |              |
GROUP                  !                  |              |
ATOM C27  CTL2   -0.18 !                  |              |
ATOM H7R  HAL2    0.09 !         H7R ---C27---H7S       |
ATOM H7S  HAL2    0.09 !                  |              |
GROUP                  !                  |              |
ATOM C28  CTL2   -0.18 !                  |              |
ATOM H8R  HAL2    0.09 !         H8R ---C28---H8S       |
ATOM H8S  HAL2    0.09 !                  |              |
GROUP                  !                  |              |
ATOM C29  CTL2   -0.18 !                  |              |
ATOM H9R  HAL2    0.09 !         H9R ---C29---H9S       |
ATOM H9S  HAL2        0.09 !                  |              |
GROUP                  !                  |              |
ATOM C210 CTL2   -0.18 !                  |              |
ATOM H10R HAL2    0.09 !         H10R---C210--H10S      |
ATOM H10S HAL2        0.09 !              |             |
GROUP                  !                  |              |
ATOM C211 CEL1   -0.15 !                  |              |
ATOM H11R HEL1    0.15 !         H11R---C211            |
GROUP                  !                  ||  (CIS)      |
ATOM C212 CEL1   -0.15 !                  ||             |
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ATOM H12R HEL1    0.15 !        H12R---C212           |
GROUP                  !               |              |
ATOM C213 CTL2   -0.18 !               |              |
ATOM H13R HAL2    0.09 !        H13R---C213--H13S     |
ATOM H13S HAL2    0.09 !               |              |
GROUP                  !               |              |
ATOM C214 CTL2   -0.18 !               |              |
ATOM H14R HAL2    0.09 !        H14R---C214--H14S     |
ATOM H14S HAL2    0.09 !               |              |
GROUP                  !               |              |
ATOM C215 CTL2   -0.18 !               |              |
ATOM H15R HAL2    0.09 !        H15R---C215--H15S     |
ATOM H15S HAL2    0.09 !               |              |
GROUP                  !               |              |
ATOM C216 CTL2   -0.18 !               |              |
ATOM H16R HAL2    0.09 !        H16R---C216--H16S     |
ATOM H16S HAL2    0.09 !               |              |
GROUP                  !               |              |
ATOM C217 CTL2   -0.18 !               |              |
ATOM H17R HAL2    0.09 !        H17R---C217--H17S     |
ATOM H17S HAL2    0.09 !               |              |
GROUP                  !               |              |
ATOM C218 CTL3   -0.27 !               |              |
ATOM H18R HAL3    0.09 !        H18R---C218--H18S     |
ATOM H18S HAL3    0.09 !               |              |
ATOM H18T HAL3    0.09 !             H18T             |
GROUP                  !                              |
ATOM C33  CTL2   -0.18 !                              |
ATOM H3X  HAL2    0.09 !                    H3X ---C33---H3Y
ATOM H3Y  HAL2    0.09 !                           |
GROUP                  !                           |
ATOM C34  CTL2   -0.18 !                           |
ATOM H4X  HAL2    0.09 !                    H4X ---C34---H4Y
ATOM H4Y  HAL2    0.09 !                           |
GROUP                  !                           |
ATOM C35  CTL2   -0.18 !                           |
ATOM H5X  HAL2    0.09 !                    H5X ---C35---H5Y
ATOM H5Y  HAL2    0.09 !                           |
GROUP                  !                           |
ATOM C36  CTL2   -0.18 !                           |
ATOM H6X  HAL2    0.09 !                    H6X ---C36---H6Y
ATOM H6Y  HAL2    0.09 !                           |
GROUP                  !                           |
ATOM C37  CTL2   -0.18 !                           |
ATOM H7X  HAL2    0.09 !                    H7X ---C37---H7Y
ATOM H7Y  HAL2    0.09 !                           |
GROUP                  !                           |
ATOM C38  CTL2   -0.18 !                           |
ATOM H8X  HAL2    0.09 !                    H8X ---C38---H8Y
ATOM H8Y  HAL2    0.09 !                           |
GROUP                  !                           |
ATOM C39  CTL2   -0.18 !                           |
ATOM H9X  HAL2    0.09 !                    H9X ---C39---H9Y
ATOM H9Y  HAL2       0.09 !                                    |
GROUP                  !                           |
ATOM C310 CTL2   -0.18 !                           |
ATOM H10X HAL2    0.09 !                    H10X---C310--H10Y
ATOM H10Y HAL2    0.09 !                                  |
GROUP                  !                           |
ATOM C311 CTL2   -0.18 !                           |
ATOM H11X HAL2    0.09 !                    H11X---C311--H11Y
ATOM H11Y HAL2       0.09 !                                       |
GROUP                  !                           |
ATOM C312 CTL2   -0.18 !                           |
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ATOM H12X HAL2    0.09 !                      H12X---C312--H12Y
ATOM H12Y HAL2        0.09 !                                    |
GROUP                   !                       |
ATOM C313 CTL2   -0.18 !                        |
ATOM H13X HAL2    0.09 !                      H13X---C313--H13Y
ATOM H13Y HAL2    0.09 !                        |
GROUP                   !                       |
ATOM C314 CTL2   -0.18 !                        |
ATOM H14X HAL2    0.09 !                      H14X---C314--H14Y
ATOM H14Y HAL2    0.09 !                        |
GROUP                   !                       |
ATOM C315 CTL2   -0.18 !                        |
ATOM H15X HAL2    0.09 !                      H15X---C315--H15Y
ATOM H15Y HAL2    0.09 !                        |
GROUP                   !                       |
ATOM C316 CTL2   -0.18 !                        |
ATOM H16X HAL2    0.09 !                      H16X---C316--H16Y
ATOM H16Y HAL2    0.09 !                        |
GROUP                   !                       |
ATOM C317 CTL2   -0.18 !                        |
ATOM H17X HAL2    0.09 !                      H17X---C317--H17Y
ATOM H17Y HAL2    0.09 !                        |
GROUP                   !                       |
ATOM C318 CTL3   -0.27 !                        |
ATOM H18X HAL3    0.09 !                      H18X---C318--H18Y
ATOM H18Y HAL3    0.09 !                        |
ATOM H18Z HAL3    0.09 !                       H18Z

! Polar Head
BOND  HO3  OC3       OC3  C13       C13  H13A      C13  H13B      C13  C12
BOND  HO2  OC2       OC2  C12       C12  H12A      C12  C11
BOND  C11  H11A      C11  H11B      C11  O12       O11  C1
BOND  O12  P         P    O11       P    O13       P    O14
! Glycerol Backbone
BOND  C1   HA        C1    HB       C1   C2
BOND  C2   HS        C2    C3       C2   O21
BOND  C3   HX        C3    HY       C3   O31
! Chain from C2
BOND  O21  C21
BOND  C21  C22
DOUBLE  C21  O22
BOND  C22  H2R       C22  H2S       C22  C23
BOND  C23  H3R       C23  H3S       C23  C24
BOND  C24  H4R       C24  H4S       C24  C25
BOND  C25  H5R       C25  H5S       C25  C26
BOND  C26  H6R       C26  H6S       C26  C27
BOND  C27  H7R       C27  H7S       C27  C28
BOND  C28  H8R       C28  H8S       C28  C29
BOND  C29  H9R           C29  H9S       C29  C210
BOND  C210 H10R      C210 H10S       C210 C211
BOND  C211 H11R
DOUBLE  C211 C212
BOND  C212 H12R      C212 C213
BOND  C213 H13R      C213 H13S      C213 C214
BOND  C214 H14R      C214 H14S      C214 C215
BOND  C215 H15R      C215 H15S      C215 C216
BOND  C216 H16R      C216 H16S      C216 C217
BOND  C217 H17R      C217 H17S      C217 C218
BOND  C218 H18R      C218 H18S      C218 H18T
! Chain From C3
BOND  O31  C31
BOND  C31  C32
DOUBLE  C31  O32
BOND  C32  H2X       C32  H2Y       C32  C33
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BOND  C33  H3X       C33  H3Y       C33  C34
BOND  C34  H4X       C34  H4Y       C34  C35
BOND  C35  H5X       C35  H5Y       C35  C36
BOND  C36  H6X       C36  H6Y       C36  C37
BOND  C37  H7X       C37  H7Y       C37  C38
BOND  C38  H8X       C38  H8Y       C38  C39
BOND  C39  H9X           C39  H9Y       C39  C310
BOND  C310 H10X      C310 H10Y      C310 C311
BOND  C311 H11X      C311 H11Y   C311 C312
BOND  C312 H12X      C312 H12Y          C312 C313
BOND  C313 H13X      C313 H13Y      C313 C314
BOND  C314 H14X      C314 H14Y      C314 C315
BOND  C315 H15X      C315 H15Y      C315 C316
BOND  C316 H16X      C316 H16Y      C316 C317
BOND  C317 H17X      C317 H17Y      C317 C318
BOND  C318 H18X      C318 H18Y      C318 H18Z

IMPR C21 O21 C22 O22    C31 O31 C32 O32

IC C13    C12    C11    O12        1.5583  113.89   93.01  113.50   1.4295
IC OC3    C13    C12    C11        1.4375  112.31   69.20  113.89   1.5573
IC OC3    C12    *C13   H13A       1.4375  112.31  119.90  108.06   1.1118
IC OC3    C12    *C13   H13B       1.4375  112.31 -123.06  109.89   1.1097
IC C12    C13    OC3    HO3        1.5583  112.31 -141.84  106.96   0.9777
IC C11    C13    *C12   OC2        1.5573  113.89 -121.65  107.64   1.4259
IC OC2    C13    *C12   H12A       1.4259  107.64 -117.84  109.30   1.1131
IC C13    C12    OC2    HO2        1.5583  107.64   38.09  100.52   0.9671
IC O12    C12    *C11   H11A       1.4295  113.50 -126.35  109.70   1.1125
IC H11A   C12    *C11   H11B       1.1125  109.70 -115.65  107.71   1.1131
IC C12    C11    O12    P          1.5573  113.50  -72.69  124.80   1.5783
IC C11    O12    P      O11        1.4295  124.80  -30.02  102.66   1.5825
IC O11    O12    *P     O13        1.5825  102.66  113.88  109.00   1.4783
IC O11    O12    *P     O14        1.5825  102.66 -115.27  109.77   1.4781
IC O12    P      O11    C1         1.5783  102.66  -80.21  120.83   1.4246
IC P      O11    C1     C2         1.5825  120.83  177.68  108.67   1.5488
IC C2     O11    *C1    HA         1.5488  108.67 -120.91  111.25   1.1145
IC HA     O11    *C1    HB         1.1145  111.25 -120.47  110.06   1.1152
IC O11    C1     C2     C3         1.4246  108.67   45.70  110.42   1.5580
IC C3     C1     *C2    O21        1.5580  110.42  120.25  110.13   1.4420
IC C3     C1     *C2    HS         1.5580  110.42 -116.94  108.10   1.1164
IC C1     C2     O21    C21        1.5488  110.13   74.82  114.08   1.3218
IC C2     O21    C21    C22        1.4420  114.08 -171.58  108.87   1.5297
IC C22    O21    *C21   O22        1.5297  108.87 -179.18  126.27   1.2166
IC O21    C21    C22    C23        1.3218  108.87  167.60  112.03   1.5460
IC C23    C21    *C22   H2R        1.5460  112.03 -121.40  108.25   1.1088
IC H2R    C21    *C22   H2S        1.1088  108.25 -117.05  107.34   1.1068
IC C1     C2     C3     O31        1.5488  110.42 -172.10  112.95   1.4472
IC O31    C2     *C3    HX         1.4472  112.95 -119.90  106.80   1.1123
IC HX     C2     *C3    HY         1.1123  106.80 -114.66  109.95   1.1147
IC C2     C3     O31    C31        1.5580  112.95   84.38  114.39   1.3267
IC C3     O31    C31    C32        1.4472  114.39  176.82  109.50   1.5275
IC C32    O31    *C31   O32        1.5275  109.50 -179.44  126.11   1.2173
IC O31    C31    C32    C33        1.3267  109.50  -66.76  112.63   1.5535
IC C33    C31    *C32   H2X        1.5535  112.63  121.43  107.50   1.1085
IC H2X    C31    *C32   H2Y        1.1085  107.50  116.64  107.32   1.1097
IC C21    C22    C23    C24        1.5289  112.21  175.76  112.39   1.5338
IC C24    C22    *C23   H3R        1.5338  112.39 -120.69  109.57   1.1147
IC H3R    C22    *C23   H3S        1.1147  109.57 -117.65  109.64   1.1142
IC C22    C23    C24    C25        1.5449  112.39 -179.39  112.35   1.5346
IC C25    C23    *C24   H4R        1.5346  112.35 -121.52  109.41   1.1131
IC H4R    C23    *C24   H4S        1.1131  109.41 -117.57  108.97   1.1134
IC C23    C24    C25    C26        1.5338  112.35  176.31  112.80   1.5344
IC C26    C24    *C25   H5R        1.5344  112.80 -121.01  108.95   1.1135
IC H5R    C24    *C25   H5S        1.1135  108.95 -117.24  109.16   1.1132
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IC C24    C25    C26    C27        1.5346  112.80 -179.44  112.48   1.5356
IC C27    C25    *C26   H6R        1.5356  112.48 -121.49  109.32   1.1129
IC H6R    C25    *C26   H6S        1.1129  109.32 -117.47  108.94   1.1132
IC C25    C26    C27    C28        1.5344  112.48  176.92  112.46   1.5398
IC C28    C26    *C27   H7R        1.5398  112.46 -121.38  108.40   1.1139
IC H7R    C26    *C27   H7S        1.1139  108.40 -116.93  108.77   1.1139
IC C26    C27    C28    C29        1.5356  112.46 -178.53  111.43   1.5097
IC C29    C27    *C28   H8R        1.5097  111.43 -123.58  107.80   1.1132
IC H8R    C27    *C28   H8S        1.1132  107.80 -115.43  108.37   1.1128
IC C27    C28    C29    C210       1.5344  112.48  176.92  112.46   1.5398
IC C210   C28    *C29   H9R        1.5398  112.46 -121.38  108.40   1.1139
IC H9R    C28    *C29   H9S               1.1139  108.40 -116.93  108.77   1.1139
IC C28    C29    C210   C211       1.5356  112.46 -178.53  111.43   1.5097
IC C211   C29    *C210  H10R       1.5097  111.43 -123.58  107.80   1.1132
IC H10R   C29    *C210  H9S             1.1132  107.80 -115.43  108.37   1.1128
IC C29    C210   C211   C212       1.5398  111.43 -126.96  126.62   1.3465
IC C212   C210   *C211  H11R       1.3465  126.62  178.41  114.65   1.1012
IC C210   C211   C212   C213       1.5097  126.62   -1.69  126.32   1.5088
IC C213   C211   *C212  H12R       1.5088  126.32 -179.55  118.79   1.1012
IC C211   C212   C213   C214       1.5392  112.29  179.81  112.68   1.5345
IC C214   C212   *C213  H13R       1.5345  112.68 -121.26  109.04   1.1132
IC H13R   C212   *C213  H13S       1.1132  109.04 -117.39  109.10   1.1131
IC C212   C213   C214   C215       1.5354  112.68  179.80  112.59   1.5347
IC C215   C213   *C214  H14R       1.5347  112.59 -121.29  109.09   1.1132
IC H14R   C213   *C214  H14S       1.1132  109.09 -117.37  109.11   1.1133
IC C213   C214   C215   C216       1.5345  112.59 -179.58  112.63   1.5347
IC C216   C214   *C215  H15R       1.5347  112.63 -121.36  109.09   1.1132
IC H15R   C214   *C215  H15S       1.1132  109.09 -117.38  109.07   1.1132
IC C214   C215   C216   C217       1.5347  112.63  179.65  112.69   1.5339
IC C217   C215   *C216  H16R       1.5339  112.69 -121.27  109.11   1.1132
IC H16R   C215   *C216  H16S       1.1132  109.11 -117.36  109.14   1.1132
IC C215   C216   C217   C218       1.5347  112.69 -179.93  113.30   1.5309
IC C218   C216   *C217  H17R       1.5309  113.30 -121.70  108.75   1.1140
IC H17R   C216   *C217  H17S       1.1140  108.75 -116.65  108.73   1.1141
IC C216   C217   C218   H18R       1.5339  113.30  -59.98  110.46   1.1113
IC H18R   C217   *C218  H18S       1.1113  110.46  119.84  110.45   1.1114
IC H18R   C217   *C218  H18T       1.1113  110.46 -120.09  110.62   1.1112
IC C31    C32    C33    C34        1.5288  113.05  179.24  111.73   1.5343
IC C34    C32    *C33   H3X        1.5343  111.73 -120.85  109.62   1.1140
IC H3X    C32    *C33   H3Y        1.1140  109.62 -117.95  109.78   1.1144
IC C32    C33    C34    C35        1.5447  111.73 -176.74  112.91   1.5345
IC C35    C33    *C34   H4X        1.5345  112.91 -121.67  109.15   1.1134
IC H4X    C33    *C34   H4Y        1.1134  109.15 -117.32  108.98   1.1134
IC C33    C34    C35    C36        1.5343  112.91  178.63  112.42   1.5349
IC C36    C34    *C35   H5X        1.5349  112.42 -120.99  108.94   1.1133
IC H5X    C34    *C35   H5Y        1.1133  108.94 -117.41  109.31   1.1131
IC C34    C35    C36    C37        1.5345  112.42 -176.73  112.80   1.5356
IC C37    C35    *C36   H6X        1.5356  112.80 -121.69  109.16   1.1130
IC H6X    C35    *C36   H6Y        1.1130  109.16 -117.32  108.94   1.1133
IC C35    C36    C37    C38        1.5349  112.80  178.92  112.27   1.5402
IC C38    C36    *C37   H7X        1.5402  112.27 -121.37  108.23   1.1139
IC H7X    C36    *C37   H7Y        1.1139  108.23 -117.01  109.05   1.1137
IC C36    C37    C38    C39        1.5356  112.27 -174.92  111.69   1.5099
IC C39    C37    *C38   H8X        1.5099  111.69 -124.14  107.77   1.1124
IC H8X    C37    *C38   H8Y        1.1124  107.77 -115.13  108.30   1.1128
IC C37    C38    C39    C310       1.5349  112.80  178.92  112.27   1.5402
IC C310   C38    *C39   H9X        1.5402  112.27 -121.37  108.23   1.1139
IC H9X    C38  *C39   H9Y     1.1139  108.23 -117.01  109.05   1.1137
IC C38    C39    C310   C311       1.5356  112.27 -174.92  111.69   1.5099
IC C311   C39    *C310  H10X       1.5099  111.69 -124.14  107.77   1.1124
IC H10X   C39  *C310  H10Y    1.1124  107.77 -115.13  108.30   1.1128
IC C39    C310   C311   C312       1.5402  111.69 -121.39  127.35   1.3470
IC C312   C310   *C311  H11X       1.3470  127.35  179.11  114.24   1.1012
IC C310   C311   C312   C313       1.5099  127.35   -0.69  127.25   1.5096
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IC C313   C311   *C312  H12X       1.5096  127.25  179.82  118.43   1.1012
IC C311   C312   C313   C314       1.3470  127.25  106.03  111.65   1.5393
IC C314   C312   *C313  H13X       1.5393  111.65 -121.49  112.10   1.1123
IC H13X   C312   *C313  H13Y       1.1123  112.10 -117.95  109.83   1.1127
IC C312   C313   C314   C315       1.5096  111.65  179.63  112.41   1.5355
IC C315   C313   *C314  H14X       1.5355  112.41 -121.09  109.75   1.1135
IC H14X   C313   *C314  H14Y       1.1135  109.75 -118.07  109.46   1.1143
IC C313   C314   C315   C316       1.5347  112.66 -179.12  112.61   1.5348
IC C316   C314   *C315  H15X       1.5348  112.61 -121.34  109.09   1.1132
IC H15X   C314   *C315  H15Y       1.1132  109.09 -117.41  109.09   1.1132
IC C314   C315   C316   C317       1.5347  112.61  179.83  112.71   1.5340
IC C317   C315   *C316  H16X       1.5340  112.71 -121.28  109.10   1.1132
IC H16X   C315   *C316  H16Y       1.1132  109.10 -117.35  109.13   1.1133
IC C315   C316   C317   C318       1.5348  112.71 -179.67  113.30   1.5309
IC C318   C316   *C317  H17X       1.5309  113.30 -121.68  108.77   1.1141
IC H17X   C316   *C317  H17Y       1.1141  108.77 -116.68  108.76   1.1141
IC C316   C317   C318   H18X       1.5340  113.30  -59.94  110.46   1.1113
IC H18X   C317   *C318  H18Y       1.1113  110.46  119.86  110.45   1.1113
IC H18X   C317   *C318  H18Z       1.1113  110.46 -120.06  110.61   1.1112



!PEs

RESI DVPE         0.00 ! 2,3-divacenoyl-D-glycero-1-phosphatidylethanolamine
!
!  R1 - CH2
!       |          (angles and atom names from Sundaralingam)
!  R2 - CH
!       |
!       CH2 - PO4 - CH2 - CH2 - NH3
!
! Polar Head and glycerol backbone

!!Derived from Mackerell top_all36_lipid.rf
!!   by Stuart Rose 9/10/2013
!!RESI DOPE         0.00 ! 2,3-dioleoyl-D-glycero-1-phosphatidylethanolamine
!!
!!  R1 - CH2
!!       |          (angles and atom names from Sundaralingam)
!!  R2 - CH
!!       |
!!       CH2 - PO4 - CH2 - CH2 - NH3
!!
!! Polar Head and glycerol backbone
GROUP                  !
ATOM N    NH3L  -0.30 !           HN2
ATOM HN1  HCL    0.33 !            |
ATOM HN2  HCL    0.33 !  (+) HN1---N---HN3
ATOM HN3  HCL    0.33 !            |
ATOM C12  CTL2   0.13 !            |
ATOM H12A HAL2   0.09 !     H12A--C12---H12B
ATOM H12B HAL2   0.09 !            |
GROUP                  !            |     alpha5
ATOM C11  CTL2  -0.08 !            |
ATOM H11A HAL2   0.09 !     H11A--C11---H11B
ATOM H11B HAL2   0.09 !            |     alpha4
ATOM P    PL     1.50 !   (-) O13  O12
ATOM O13  O2L   -0.78 !         \ /      alpha3
ATOM O14  O2L   -0.78 !          P (+)
ATOM O11  OSLP  -0.57 !         / \      alpha2
ATOM O12  OSLP  -0.57 !   (-) O14  O11
ATOM C1   CTL2  -0.08 !            |     alpha1
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ATOM HA   HAL2   0.09 !       HA---C1---HB
ATOM HB   HAL2   0.09 !            |     theta1
GROUP                 !            |
ATOM C2   CTL1   0.17 !       HS---C2- - - - - - -
ATOM HS   HAL1   0.09 !            | beta1        |
ATOM O21  OSL   -0.49 !       O22  O21          theta3
ATOM C21  CL     0.90 !        \\ /  beta2        |
ATOM O22  OBL   -0.63 !          C21
ATOM C22  CTL2  -0.22 !           |   beta3        |
ATOM H2R  HAL2   0.09 !   H2R---C22---H2S
ATOM H2S  HAL2   0.09 !           |                |
GROUP                 !              beta4
ATOM C3   CTL2   0.08 !           |                |
ATOM HX   HAL2   0.09 !                       HX---C3---HY
ATOM HY   HAL2   0.09 !           |                |   gamma1
ATOM O31  OSL   -0.49 !                       O32  O31
ATOM C31  CL     0.90 !           |             \\ /    gamma2
ATOM O32  OBL   -0.63 !                          C31
ATOM C32  CTL2  -0.22 !           |                |     gamma3
ATOM H2X  HAL2   0.09 !                    H2X---C32---H2Y
ATOM H2Y  HAL2   0.09 !           |                |
GROUP                 !                                gamma4
ATOM C23  CTL2  -0.18 !           |                |
ATOM H3R  HAL2   0.09 !   H3R ---C23---H3S        |
ATOM H3S  HAL2   0.09 !           |                |
GROUP                 !           |                |
ATOM C24  CTL2  -0.18 !           |                |
ATOM H4R  HAL2   0.09 !   H4R ---C24---H4S        |
ATOM H4S  HAL2   0.09 !           |                |
GROUP                 !           |                |
ATOM C25  CTL2  -0.18 !           |                |
ATOM H5R  HAL2   0.09 !   H5R ---C25---H5S        |
ATOM H5S  HAL2   0.09 !           |                |
GROUP                 !           |                |
ATOM C26  CTL2  -0.18 !           |                |
ATOM H6R  HAL2   0.09 !   H6R ---C26---H6S        |
ATOM H6S  HAL2   0.09 !           |                |
GROUP                 !           |                |
ATOM C27  CTL2  -0.18 !           |                |
ATOM H7R  HAL2   0.09 !   H7R ---C27---H7S        |
ATOM H7S  HAL2   0.09 !           |                |
GROUP                 !           |                |
ATOM C28  CTL2  -0.18 !           |                |
ATOM H8R  HAL2   0.09 !   H8R ---C28---H8S        |
ATOM H8S  HAL2   0.09 !           |                |
GROUP                 !           |                |
ATOM C29  CTL2  -0.18 !           |                |
ATOM H9R  HAL2   0.09 !   H9R ---C29---H9S        |
ATOM H9S  HAL2   0.09 !                 |                          |
GROUP                 !           |                |
ATOM C210 CTL2  -0.18 !           |                |
ATOM H10R HAL2   0.09 !   H10R---C210--H10S       |
ATOM H10S HAL2   0.09 !           |                          |
GROUP                 !           |                |
ATOM C211 CEL1  -0.15 !           |                |
ATOM H11R HEL1   0.15 !   H11R---C211              |
GROUP                 !           ||  (CIS)        |
ATOM C212 CEL1  -0.15 !           ||               |
ATOM H12R HEL1   0.15 !   H12R---C212           |
GROUP                 !           |                |
ATOM C213 CTL2  -0.18 !           |                |
ATOM H13R HAL2   0.09 !   H13R---C213--H13S       |
ATOM H13S HAL2   0.09 !           |                |
GROUP                 !           |                |
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ATOM C214 CTL2  -0.18 !          |              |
ATOM H14R HAL2   0.09 !   H14R---C214--H14S     |
ATOM H14S HAL2   0.09 !          |              |
GROUP                 !          |              |
ATOM C215 CTL2  -0.18 !          |              |
ATOM H15R HAL2   0.09 !   H15R---C215--H15S     |
ATOM H15S HAL2   0.09 !          |              |
GROUP                 !          |              |
ATOM C216 CTL2  -0.18 !          |              |
ATOM H16R HAL2   0.09 !   H16R---C216--H16S     |
ATOM H16S HAL2   0.09 !          |              |
GROUP                 !          |              |
ATOM C217 CTL2  -0.18 !          |              |
ATOM H17R HAL2   0.09 !   H17R---C217--H17S     |
ATOM H17S HAL2   0.09 !          |              |
GROUP                 !          |              |
ATOM C218 CTL3  -0.27 !          |              |
ATOM H18R HAL3   0.09 !   H18R---C218--H18S     |
ATOM H18S HAL3   0.09 !          |              |
ATOM H18T HAL3   0.09 !        H18T             |
GROUP                 !                         |
ATOM C33  CTL2  -0.18 !                         |
ATOM H3X  HAL2   0.09 !                 H3X ---C33---H3Y
ATOM H3Y  HAL2   0.09 !                         |
GROUP                 !                         |
ATOM C34  CTL2  -0.18 !                         |
ATOM H4X  HAL2   0.09 !                 H4X ---C34---H4Y
ATOM H4Y  HAL2   0.09 !                         |
GROUP                 !                         |
ATOM C35  CTL2  -0.18 !                         |
ATOM H5X  HAL2   0.09 !                 H5X ---C35---H5Y
ATOM H5Y  HAL2   0.09 !                         |
GROUP                 !                         |
ATOM C36  CTL2  -0.18 !                         |
ATOM H6X  HAL2   0.09 !                 H6X ---C36---H6Y
ATOM H6Y  HAL2   0.09 !                         |
GROUP                 !                         |
ATOM C37  CTL2  -0.18 !                         |
ATOM H7X  HAL2   0.09 !                 H7X ---C37---H7Y
ATOM H7Y  HAL2   0.09 !                         |
GROUP                 !                         |
ATOM C38  CTL2  -0.18 !                         |
ATOM H8X  HAL2   0.09 !                 H8X ---C38---H8Y
ATOM H8Y  HAL2   0.09 !                         |
GROUP                 !                         |
ATOM C39  CTL2  -0.18 !                         |
ATOM H9X  HAL2   0.09 !                 H9X ---C39---H9Y
ATOM H9Y  HAL2       0.09 !                                          |
GROUP                 !                         |
ATOM C310 CTL2  -0.18 !                         |
ATOM H10X HAL2   0.09 !                 H10X---C310---H10Y
ATOM H10Y HAL2       0.09 !                                          |
GROUP                 !                         |
ATOM C311 CEL1  -0.15 !                         |
ATOM H11X HEL1   0.15 !                 H11X---C311
GROUP                 !                         ||   (CIS)
ATOM C312 CEL1  -0.15 !                         ||
ATOM H12X HEL1   0.15 !                 H12X---C312
GROUP                 !                         |
ATOM C313 CTL2  -0.18 !                         |
ATOM H13X HAL2   0.09 !                 H13X---C313--H13Y
ATOM H13Y HAL2   0.09 !                         |
GROUP                 !                         |
ATOM C314 CTL2  -0.18 !                         |
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ATOM H14X HAL2   0.09 !                  H14X---C314--H14Y
ATOM H14Y HAL2   0.09 !                         |
GROUP                 !                         |
ATOM C315 CTL2  -0.18 !                         |
ATOM H15X HAL2   0.09 !                  H15X---C315--H15Y
ATOM H15Y HAL2   0.09 !                         |
GROUP                 !                         |
ATOM C316 CTL2  -0.18 !                         |
ATOM H16X HAL2   0.09 !                  H16X---C316--H16Y
ATOM H16Y HAL2   0.09 !                         |
GROUP                 !                         |
ATOM C317 CTL2  -0.18 !                         |
ATOM H17X HAL2   0.09 !                  H17X---C317--H17Y
ATOM H17Y HAL2   0.09 !                         |
GROUP                 !                         |
ATOM C318 CTL3  -0.27 !                         |
ATOM H18X HAL3   0.09 !                  H18X---C318--H18Y
ATOM H18Y HAL3   0.09 !                         |
ATOM H18Z HAL3   0.09 !                        H18Z

! Polar Head
BOND  N    HN1       N    HN2       N    HN3       N    C12
BOND  C12  H12A      C12  H12B      C12  C11
BOND  C11  H11A      C11  H11B      C11  O12
BOND  O12  P         P    O11       P    O13       P    O14
! Glycerol Backbone
BOND  C1   HA        C1    HB       C1   C2        C1   O11
BOND  C2   HS        C2    C3       C2   O21
BOND  C3   HX        C3    HY       C3   O31
! Chain from C2
BOND  O21  C21
BOND  C21  C22
DOUBLE  C21  O22
BOND  C22  H2R       C22  H2S       C22  C23
BOND  C23  H3R       C23  H3S       C23  C24
BOND  C24  H4R       C24  H4S       C24  C25
BOND  C25  H5R       C25  H5S       C25  C26
BOND  C26  H6R       C26  H6S       C26  C27
BOND  C27  H7R       C27  H7S       C27  C28
BOND  C28  H8R       C28  H8S       C28  C29
BOND  C29  H9R           C29  H9S    C29 C210
BOND  C210 H10R      C210 H10S      C210 C211
BOND  C211 H11R
DOUBLE  C211 C212
BOND  C212 H12R      C212 C213
BOND  C213 H13R      C213 H13S      C213 C214
BOND  C214 H14R      C214 H14S      C214 C215
BOND  C215 H15R      C215 H15S      C215 C216
BOND  C216 H16R      C216 H16S      C216 C217
BOND  C217 H17R      C217 H17S      C217 C218
BOND  C218 H18R      C218 H18S      C218 H18T
! Chain From C3
BOND  O31  C31
BOND  C31  C32
DOUBLE C31  O32
BOND  C32  H2X       C32  H2Y       C32  C33
BOND  C33  H3X       C33  H3Y       C33  C34
BOND  C34  H4X       C34  H4Y       C34  C35
BOND  C35  H5X       C35  H5Y       C35  C36
BOND  C36  H6X       C36  H6Y       C36  C37
BOND  C37  H7X       C37  H7Y       C37  C38
BOND  C38  H8X       C38  H8Y       C38  C39
BOND  C39  H9X           C39  H9Y    C39  C310
BOND  C310 H10X      C310 H10Y       C310 C311
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BOND  C311 H11X
DOUBLE C311 C312
BOND  C312 H12X      C312 C313
BOND  C313 H13X      C313 H13Y      C313 C314
BOND  C314 H14X      C314 H14Y      C314 C315
BOND  C315 H15X      C315 H15Y      C315 C316
BOND  C316 H16X      C316 H16Y      C316 C317
BOND  C317 H17X      C317 H17Y      C317 C318
BOND  C318 H18X      C318 H18Y      C318 H18Z

IMPR C21 O21 C22 O22   C31 O31 C32 O32

IC N      C12    C11    O12        1.5110  111.97   65.84  112.46   1.4308
IC HN1    C12    *N     HN2        1.0342  114.60  119.70  105.60   1.0654
IC HN1    C12    *N     HN3        1.0342  114.60 -127.78  110.56   1.0397
IC HN1    N      C12    C11        1.0342  114.60 -177.91  111.97   1.5465
IC C11    N      *C12   H12A       1.5465  111.97 -121.58  107.97   1.1086
IC H12A   N      *C12   H12B       1.1086  107.97 -118.25  107.67   1.1104
IC O12    C12    *C11   H11A       1.4308  112.46 -126.31  111.01   1.1167
IC H11A   C12    *C11   H11B       1.1167  111.01 -115.41  107.63   1.1146
IC C12    C11    O12    P          1.5465  112.46  -80.62  120.62   1.5839
IC C11    O12    P      O11        1.4308  120.62 -156.78  104.60   1.5751
IC O11    O12    *P     O13        1.5751  104.60 -117.47  103.31   1.4823
IC O11    O12    *P     O14        1.5751  104.60  120.67  107.16   1.4736
IC O12    P      O11    C1         1.5839  104.60  -58.82  120.34   1.4318
IC P      O11    C1     C2         1.5751  120.34  -92.48  111.72   1.5536
IC C2     O11    *C1    HA         1.5536  111.72 -119.08  108.93   1.1133
IC HA     O11    *C1    HB         1.1133  108.93 -117.83  112.18   1.1155
IC O11    C1     C2     C3         1.4318  111.72  162.49  110.59   1.5553
IC C3     C1     *C2    O21        1.5553  110.59  120.51  108.20   1.4410
IC C3     C1     *C2    HS         1.5553  110.59 -117.47  107.37   1.1169
IC C1     C2     O21    C21        1.5536  108.20  145.45  115.07   1.3229
IC C2     O21    C21    C22        1.4410  115.07  175.60  109.17   1.5330
IC C22    O21    *C21   O22        1.5330  109.17  179.92  126.38   1.2173
IC O21    C21    C22    C23        1.3229  109.17 -134.07  111.55   1.5472
IC C23    C21    *C22   H2R        1.5472  111.55 -119.81  106.70   1.1095
IC H2R    C21    *C22   H2S        1.1095  106.70 -117.59  109.58   1.1081
IC C1     C2     C3     O31        1.5536  110.59  178.88  111.62   1.4432
IC O31    C2     *C3    HX         1.4432  111.62 -121.40  107.66   1.1142
IC HX     C2     *C3    HY         1.1142  107.66 -116.77  107.26   1.1152
IC C2     C3     O31    C31        1.5553  111.62  174.54  113.52   1.3270
IC C3     O31    C31    C32        1.4432  113.52  178.76  109.19   1.5276
IC C32    O31    *C31   O32        1.5276  109.19 -179.68  125.26   1.2176
IC O31    C31    C32    C33        1.3270  109.19 -153.26  112.50   1.5449
IC C33    C31    *C32   H2X        1.5449  112.50  120.40  107.84   1.1092
IC H2X    C31    *C32   H2Y        1.1092  107.84  117.16  108.28   1.1081
IC C21    C22    C23    C24        1.5289  112.21  175.76  112.39   1.5338
IC C24    C22    *C23   H3R        1.5338  112.39 -120.69  109.57   1.1147
IC H3R    C22    *C23   H3S        1.1147  109.57 -117.65  109.64   1.1142
IC C22    C23    C24    C25        1.5449  112.39 -179.39  112.35   1.5346
IC C25    C23    *C24   H4R        1.5346  112.35 -121.52  109.41   1.1131
IC H4R    C23    *C24   H4S        1.1131  109.41 -117.57  108.97   1.1134
IC C23    C24    C25    C26        1.5338  112.35  176.31  112.80   1.5344
IC C26    C24    *C25   H5R        1.5344  112.80 -121.01  108.95   1.1135
IC H5R    C24    *C25   H5S        1.1135  108.95 -117.24  109.16   1.1132
IC C24    C25    C26    C27        1.5346  112.80 -179.44  112.48   1.5356
IC C27    C25    *C26   H6R        1.5356  112.48 -121.49  109.32   1.1129
IC H6R    C25    *C26   H6S        1.1129  109.32 -117.47  108.94   1.1132
IC C25    C26    C27    C28        1.5344  112.48  176.92  112.46   1.5398
IC C28    C26    *C27   H7R        1.5398  112.46 -121.38  108.40   1.1139
IC H7R    C26    *C27   H7S        1.1139  108.40 -116.93  108.77   1.1139
IC C26    C27    C28    C29        1.5346  112.80 -179.44  112.48   1.5356
IC C29    C27    *C28   H8R        1.5356  112.48 -121.49  109.32   1.1129
IC H8R    C27    *C28   H8S        1.1129  109.32 -117.47  108.94   1.1132
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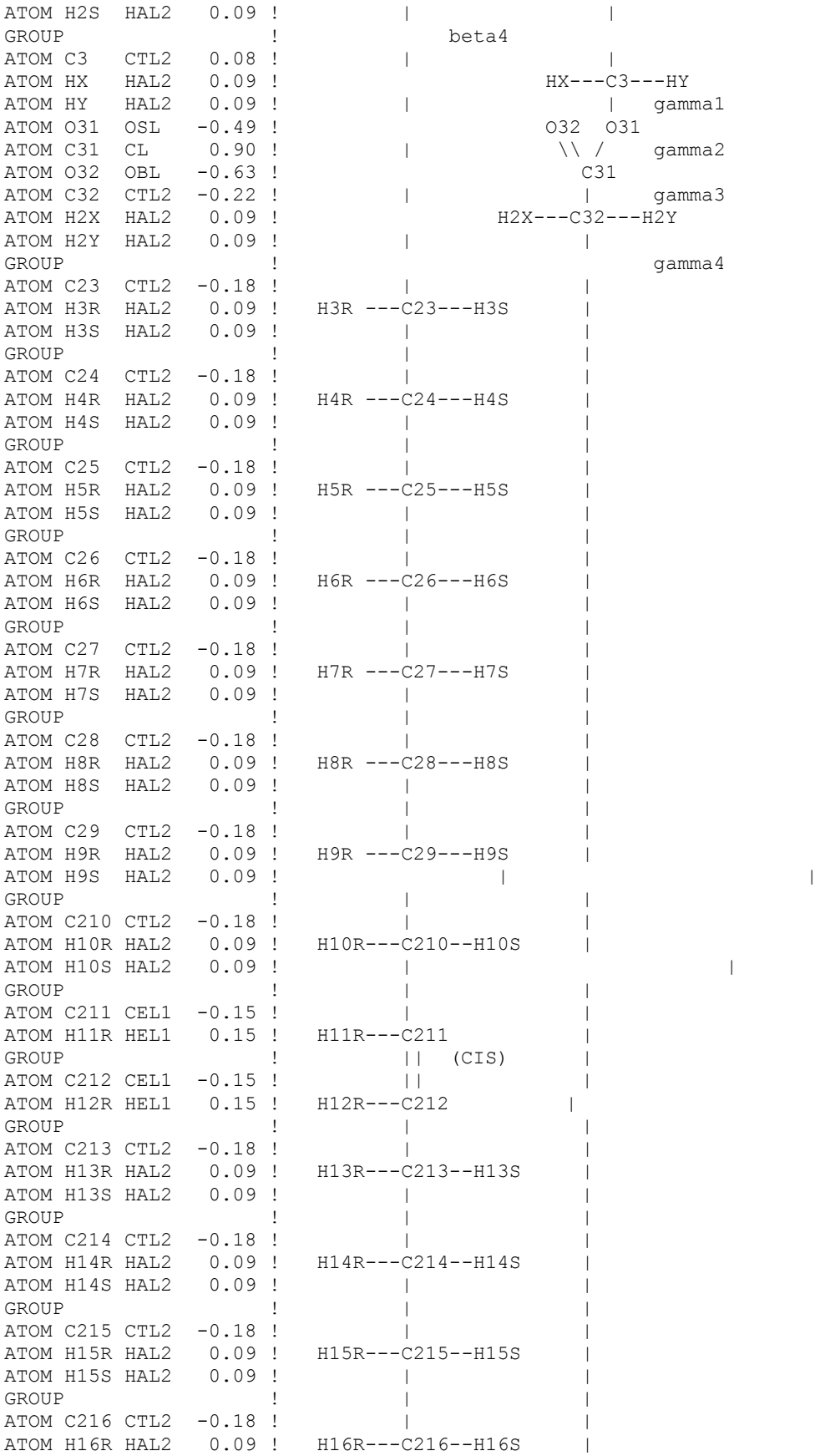
IC C27    C28    C29    C210       1.5344  112.48  176.92  112.46   1.5398
IC C210   C28    *C29   H9R        1.5398  112.46 -121.38  108.40   1.1139
IC H9R   C28   *C29   H9S          1.1139  108.40 -116.93  108.77   1.1139
IC C28    C29    C210   C211       1.5356  112.46 -178.53  111.43   1.5097
IC C211   C29    *C210  H10R       1.5097  111.43 -123.58  107.80   1.1132
IC H10R   C29    *C210  H10S       1.1132  107.80 -115.43  108.37   1.1128
IC C29    C210   C211   C212       1.5398  111.43 -126.96  126.62   1.3465
IC C212   C210   *C211  H11R       1.3465  126.62  178.41  114.65   1.1012
IC C210   C211   C212   C213       1.5097  126.62   -1.69  126.32   1.5088
IC C213   C211   *C212  H12R       1.5088  126.32 -179.55  118.79   1.1012
IC C211   C212   C213   C214       1.3465  126.32   93.02  112.15   1.5392
IC C214   C212   *C213  H13R       1.5392  112.15 -121.30  111.28   1.1133
IC H13R   C212   *C213  H13S       1.1133  111.28 -117.50  110.00   1.1126
IC C212   C213   C214   C215       1.5088  112.15 -178.81  112.29   1.5354
IC C215   C213   *C214  H14R       1.5354  112.29 -121.34  109.78   1.1133
IC H14R   C213   *C214  H14S       1.1133  109.78 -118.01  109.42   1.1144
IC C213   C214   C215   C216       1.5345  112.59 -179.58  112.63   1.5347
IC C216   C214   *C215  H15R       1.5347  112.63 -121.36  109.09   1.1132
IC H15R   C214   *C215  H15S       1.1132  109.09 -117.38  109.07   1.1132
IC C214   C215   C216   C217       1.5347  112.63  179.65  112.69   1.5339
IC C217   C215   *C216  H16R       1.5339  112.69 -121.27  109.11   1.1132
IC H16R   C215   *C216  H16S       1.1132  109.11 -117.36  109.14   1.1132
IC C215   C216   C217   C218       1.5347  112.69 -179.93  113.30   1.5309
IC C218   C216   *C217  H17R       1.5309  113.30 -121.70  108.75   1.1140
IC H17R   C216   *C217  H17S       1.1140  108.75 -116.65  108.73   1.1141
IC C216   C217   C218   H18R       1.5339  113.30  -59.98  110.46   1.1113
IC H18R   C217   *C218  H18S       1.1113  110.46  119.84  110.45   1.1114
IC H18R   C217   *C218  H18T       1.1113  110.46 -120.09  110.62   1.1112
IC C31    C32    C33    C34        1.5288  113.05  179.24  111.73   1.5343
IC C34    C32    *C33   H3X        1.5343  111.73 -120.85  109.62   1.1140
IC H3X    C32    *C33   H3Y        1.1140  109.62 -117.95  109.78   1.1144
IC C32    C33    C34    C35        1.5447  111.73 -176.74  112.91   1.5345
IC C35    C33    *C34   H4X        1.5345  112.91 -121.67  109.15   1.1134
IC H4X    C33    *C34   H4Y        1.1134  109.15 -117.32  108.98   1.1134
IC C33    C34    C35    C36        1.5343  112.91  178.63  112.42   1.5349
IC C36    C34    *C35   H5X        1.5349  112.42 -120.99  108.94   1.1133
IC H5X    C34    *C35   H5Y        1.1133  108.94 -117.41  109.31   1.1131
IC C34    C35    C36    C37        1.5345  112.42 -176.73  112.80   1.5356
IC C37    C35    *C36   H6X        1.5356  112.80 -121.69  109.16   1.1130
IC H6X    C35    *C36   H6Y        1.1130  109.16 -117.32  108.94   1.1133
IC C35    C36    C37    C38        1.5343  112.91  178.63  112.42   1.5349
IC C38    C36    *C37   H7X        1.5349  112.42 -120.99  108.94   1.1133
IC H7X    C36    *C37   H7Y        1.1133  108.94 -117.41  109.31   1.1131
IC C36    C37    C38    C39        1.5345  112.42 -176.73  112.80   1.5356
IC C39    C37    *C38   H8X        1.5356  112.80 -121.69  109.16   1.1130
IC H8X    C37    *C38   H8Y        1.1130  109.16 -117.32  108.94   1.1133
IC C37    C38    C39    C310       1.5349  112.80  178.92  112.27   1.5402
IC C310   C38    *C39   H9X        1.5402  112.27 -121.37  108.23   1.1139
IC H9X    C38  *C39  H9Y           1.1139  108.23 -117.01  109.05   1.1137
IC C38    C39    C310   C311       1.5356  112.27 -174.92  111.69   1.5099
IC C311   C39    *C310  H10X       1.5099  111.69 -124.14  107.77   1.1124
IC H10X        C39   *C310 H10Y     1.1124  107.77 -115.13  108.30   1.1128
IC C39    C310   C311   C312       1.5402  111.69 -121.39  127.35   1.3470
IC C312   C310   *C311  H11X       1.3470  127.35  179.11  114.24   1.1012
IC C310   C311   C312   C313       1.5099  127.35    0.00  127.25   1.5096
IC C313   C311   *C312  H12X       1.5096  127.25  179.82  118.43   1.1012
IC C311   C312   C313   C314       1.3470  127.25  106.03  111.65   1.5393
IC C314   C312   *C313  H13X       1.5393  111.65 -121.49  112.10   1.1123
IC H13X   C312   *C313  H13Y       1.1123  112.10 -117.95  109.83   1.1127
IC C312   C313   C314   C315       1.5096  111.65  179.63  112.41   1.5355
IC C315   C313   *C314  H14X       1.5355  112.41 -121.09  109.75   1.1135
IC H14X   C313   *C314  H14Y       1.1135  109.75 -118.07  109.46   1.1143
IC C313   C314   C315   C316       1.5347  112.66 -179.12  112.61   1.5348
IC C316   C314   *C315  H15X       1.5348  112.61 -121.34  109.09   1.1132
```

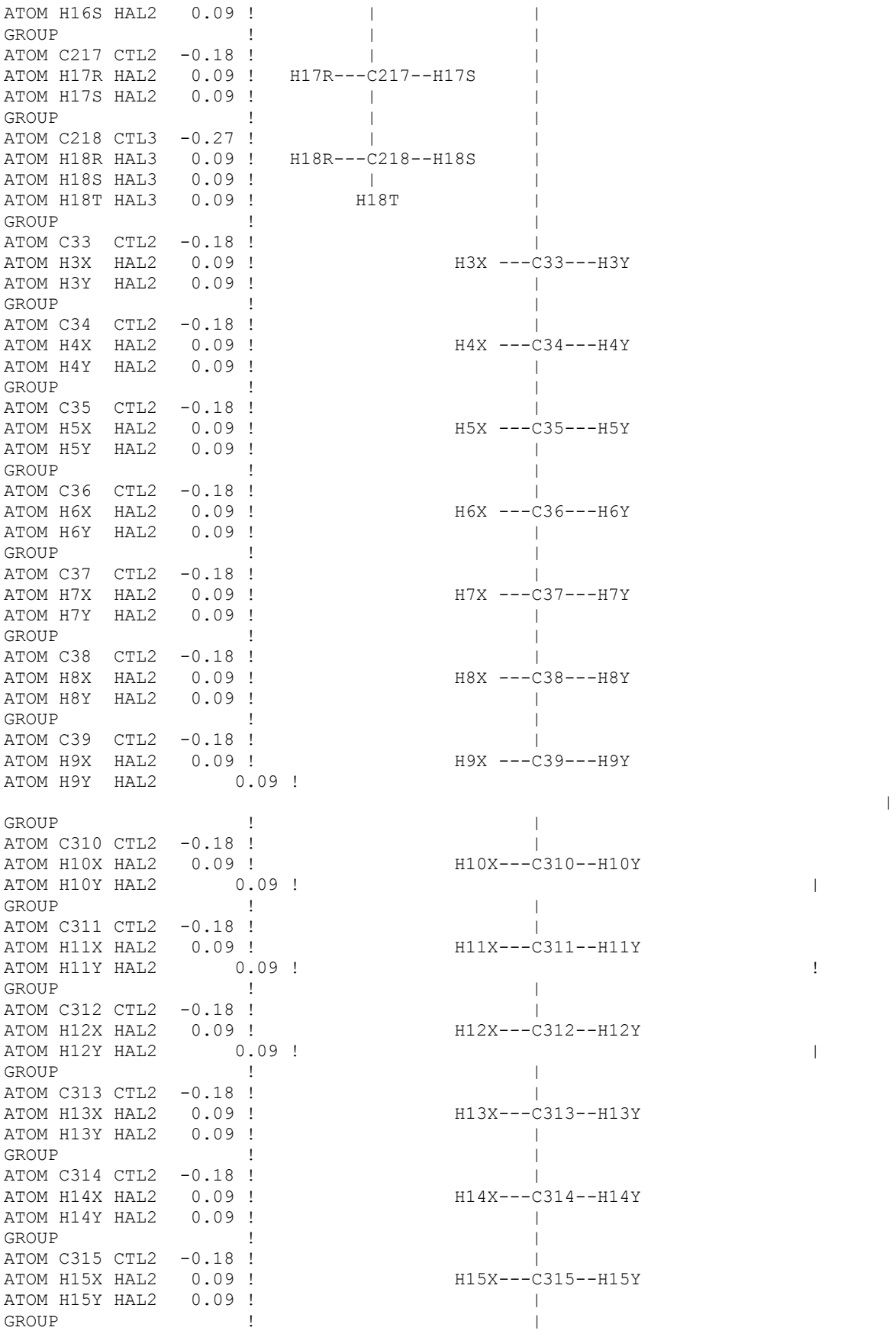
```
IC H15X   C314   *C315  H15Y       1.1132  109.09 -117.41  109.09   1.1132
IC C314   C315   C316   C317       1.5347  112.61  179.83  112.71   1.5340
IC C317   C315   *C316  H16X       1.5340  112.71 -121.28  109.10   1.1132
IC H16X   C315   *C316  H16Y       1.1132  109.10 -117.35  109.13   1.1133
IC C315   C316   C317   C318       1.5348  112.71 -179.67  113.30   1.5309
IC C318   C316   *C317  H17X       1.5309  113.30 -121.68  108.77   1.1141
IC H17X   C316   *C317  H17Y       1.1141  108.77 -116.68  108.76   1.1141
IC C316   C317   C318   H18X       1.5340  113.30  -59.94  110.46   1.1113
IC H18X   C317   *C318  H18Y       1.1113  110.46  119.86  110.45   1.1113
IC H18X   C317   *C318  H18Z       1.1113  110.46 -120.06  110.61   1.1112


!PEs

RESI VSPE         0.00 ! ? 2,3-vacenyl- steroeyl D-glycero-1-phosphatidylethanolamine
!  VSPE stands for 18:0/18:1 configuration
!:: removed C311 - C312 double bond but did not do detailed rearrangement of IC
!  R1 - CH2
!       |          (angles and atom names from Sundaralingam)
!  R2 - CH
!       |
!       CH2 - PO4 - CH2 - CH2 - NH3
!
! Polar Head and glycerol backbone

!!Derived from Mackerell top_all36_lipid.rf
!!   by Stuart Rose 9/10/2013
!!RESI DOPE         0.00 ! 2,3-dioleoyl-D-glycero-1-phosphatidylethanolamine
!!
!!  R1 - CH2
!!       |          (angles and atom names from Sundaralingam)
!!  R2 - CH
!!       |
!!       CH2 - PO4 - CH2 - CH2 - NH3
!!
!! Polar Head and glycerol backbone
GROUP                  !
ATOM N    NH3L  -0.30 !           HN2
ATOM HN1  HCL    0.33 !            |
ATOM HN2  HCL    0.33 !  (+) HN1---N---HN3
ATOM HN3  HCL    0.33 !            |
ATOM C12  CTL2   0.13 !            |
ATOM H12A HAL2   0.09 !     H12A--C12---H12B
ATOM H12B HAL2   0.09 !            |
GROUP                  !            |     alpha5
ATOM C11  CTL2  -0.08 !            |
ATOM H11A HAL2   0.09 !     H11A--C11---H11B
ATOM H11B HAL2   0.09 !            |     alpha4
ATOM P    PL     1.50 !   (-) O13  O12
ATOM O13  O2L   -0.78 !         \ /      alpha3
ATOM O14  O2L   -0.78 !          P (+)
ATOM O11  OSLP  -0.57 !         / \      alpha2
ATOM O12  OSLP  -0.57 !   (-) O14  O11
ATOM C1   CTL2  -0.08 !            |     alpha1
ATOM HA   HAL2   0.09 !       HA---C1---HB
ATOM HB   HAL2   0.09 !            |     theta1
GROUP                  !            |
ATOM C2   CTL1   0.17 !       HS---C2- - - - - - -
ATOM HS   HAL1   0.09 !            | beta1        |
ATOM O21  OSL   -0.49 !       O22  O21          theta3
ATOM C21  CL     0.90 !        \\ /  beta2        |
ATOM O22  OBL   -0.63 !          C21
ATOM C22  CTL2  -0.22 !           |   beta3        |
ATOM H2R  HAL2   0.09 !   H2R---C22---H2S
```


ATOM H2S HAL2 0.09 !
GROUP !
ATOM C3 CTL2 0.08 !
ATOM HX HAL2 0.09 !
ATOM HY HAL2 0.09 !
ATOM O31 OSL -0.49 !
ATOM C31 CL 0.90 !
ATOM O32 OBL -0.63 !
ATOM C32 CTL2 -0.22 !
ATOM H2X HAL2 0.09 !
ATOM H2Y HAL2 0.09 !
GROUP !
ATOM C23 CTL2 -0.18 !
ATOM H3R HAL2 0.09 !
ATOM H3S HAL2 0.09 !
GROUP !
ATOM C24 CTL2 -0.18 !
ATOM H4R HAL2 0.09 !
ATOM H4S HAL2 0.09 !
GROUP !
ATOM C25 CTL2 -0.18 !
ATOM H5R HAL2 0.09 !
ATOM H5S HAL2 0.09 !
GROUP !
ATOM C26 CTL2 -0.18 !
ATOM H6R HAL2 0.09 !
ATOM H6S HAL2 0.09 !
GROUP !
ATOM C27 CTL2 -0.18 !
ATOM H7R HAL2 0.09 !
ATOM H7S HAL2 0.09 !
GROUP !
ATOM C28 CTL2 -0.18 !
ATOM H8R HAL2 0.09 !
ATOM H8S HAL2 0.09 !
GROUP !
ATOM C29 CTL2 -0.18 !
ATOM H9R HAL2 0.09 !
ATOM H9S HAL2 0.09 !
GROUP !
ATOM C210 CTL2 -0.18 !
ATOM H10R HAL2 0.09 !
ATOM H10S HAL2 0.09 !
GROUP !
ATOM C211 CEL1 -0.15 !
ATOM H11R HEL1 0.15 !
GROUP !
ATOM C212 CEL1 -0.15 !
ATOM H12R HEL1 0.15 !
GROUP !
ATOM C213 CTL2 -0.18 !
ATOM H13R HAL2 0.09 !
ATOM H13S HAL2 0.09 !
GROUP !
ATOM C214 CTL2 -0.18 !
ATOM H14R HAL2 0.09 !
ATOM H14S HAL2 0.09 !
GROUP !
ATOM C215 CTL2 -0.18 !
ATOM H15R HAL2 0.09 !
ATOM H15S HAL2 0.09 !
GROUP !
ATOM C216 CTL2 -0.18 !
ATOM H16R HAL2 0.09 !
beta4
HX---C3---HY
O32 O31
\\ /
C31
H2X---C32---H2Y
gamma1
gamma2
gamma3
gamma4
H3R ---C23---H3S
H4R ---C24---H4S
H5R ---C25---H5S
H6R ---C26---H6S
H7R ---C27---H7S
H8R ---C28---H8S
H9R ---C29---H9S
H10R---C210--H10S
H11R---C211
(CIS)
H12R---C212
H13R---C213--H13S
H14R---C214--H14S
H15R---C215--H15S
H16R---C216--H16S


ATOM H16S HAL2 0.09 !
GROUP !
ATOM C217 CTL2 -0.18 !
ATOM H17R HAL2 0.09 !
ATOM H17S HAL2 0.09 !
GROUP !
ATOM C218 CTL3 -0.27 !
ATOM H18R HAL3 0.09 !
ATOM H18S HAL3 0.09 !
ATOM H18T HAL3 0.09 !
GROUP !
ATOM C33 CTL2 -0.18 !
ATOM H3X HAL2 0.09 !
ATOM H3Y HAL2 0.09 !
GROUP !
ATOM C34 CTL2 -0.18 !
ATOM H4X HAL2 0.09 !
ATOM H4Y HAL2 0.09 !
GROUP !
ATOM C35 CTL2 -0.18 !
ATOM H5X HAL2 0.09 !
ATOM H5Y HAL2 0.09 !
GROUP !
ATOM C36 CTL2 -0.18 !
ATOM H6X HAL2 0.09 !
ATOM H6Y HAL2 0.09 !
GROUP !
ATOM C37 CTL2 -0.18 !
ATOM H7X HAL2 0.09 !
ATOM H7Y HAL2 0.09 !
GROUP !
ATOM C38 CTL2 -0.18 !
ATOM H8X HAL2 0.09 !
ATOM H8Y HAL2 0.09 !
GROUP !
ATOM C39 CTL2 -0.18 !
ATOM H9X HAL2 0.09 !
ATOM H9Y HAL2 0.09 !
GROUP !
ATOM C310 CTL2 -0.18 !
ATOM H10X HAL2 0.09 !
ATOM H10Y HAL2 0.09 !
GROUP !
ATOM C311 CTL2 -0.18 !
ATOM H11X HAL2 0.09 !
ATOM H11Y HAL2 0.09 !
GROUP !
ATOM C312 CTL2 -0.18 !
ATOM H12X HAL2 0.09 !
ATOM H12Y HAL2 0.09 !
GROUP !
ATOM C313 CTL2 -0.18 !
ATOM H13X HAL2 0.09 !
ATOM H13Y HAL2 0.09 !
GROUP !
ATOM C314 CTL2 -0.18 !
ATOM H14X HAL2 0.09 !
ATOM H14Y HAL2 0.09 !
GROUP !
ATOM C315 CTL2 -0.18 !
ATOM H15X HAL2 0.09 !
ATOM H15Y HAL2 0.09 !
GROUP !
H17R---C217--H17S
H18R---C218--H18S
H18T
H3X ---C33---H3Y
H4X ---C34---H4Y
H5X ---C35---H5Y
H6X ---C36---H6Y
H7X ---C37---H7Y
H8X ---C38---H8Y
H9X ---C39---H9Y
H10X---C310--H10Y
H11X---C311--H11Y
H12X---C312--H12Y
H13X---C313--H13Y
H14X---C314--H14Y
H15X---C315--H15Y

```
ATOM C316 CTL2  -0.18 !                       |
ATOM H16X HAL2   0.09 !                  H16X---C316--H16Y
ATOM H16Y HAL2   0.09 !                       |
GROUP                 !                       |
ATOM C317 CTL2  -0.18 !                       |
ATOM H17X HAL2   0.09 !                  H17X---C317--H17Y
ATOM H17Y HAL2   0.09 !                       |
GROUP                 !                       |
ATOM C318 CTL3  -0.27 !                       |
ATOM H18X HAL3   0.09 !                  H18X---C318--H18Y
ATOM H18Y HAL3   0.09 !                       |
ATOM H18Z HAL3   0.09 !                      H18Z

! Polar Head
BOND  N    HN1       N    HN2       N    HN3       N    C12
BOND  C12  H12A      C12  H12B      C12  C11
BOND  C11  H11A      C11  H11B      C11  O12
BOND  O12  P         P    O11       P    O13       P    O14
! Glycerol Backbone
BOND  C1   HA        C1    HB       C1   C2        C1   O11
BOND  C2   HS        C2    C3       C2   O21
BOND  C3   HX        C3    HY       C3   O31
! Chain from C2
BOND  O21  C21
BOND  C21  C22
DOUBLE  C21  O22
BOND  C22  H2R       C22  H2S       C22  C23
BOND  C23  H3R       C23  H3S       C23  C24
BOND  C24  H4R       C24  H4S       C24  C25
BOND  C25  H5R       C25  H5S       C25  C26
BOND  C26  H6R       C26  H6S       C26  C27
BOND  C27  H7R       C27  H7S       C27  C28
BOND  C28  H8R       C28  H8S       C28  C29
BOND  C29  H9R           C29  H9S    C29 C210
BOND  C210 H10R      C210 H10S      C210 C211
BOND  C211 H11R
DOUBLE  C211 C212
BOND  C212 H12R      C212 C213
BOND  C213 H13R      C213 H13S      C213 C214
BOND  C214 H14R      C214 H14S      C214 C215
BOND  C215 H15R      C215 H15S      C215 C216
BOND  C216 H16R      C216 H16S      C216 C217
BOND  C217 H17R      C217 H17S      C217 C218
BOND  C218 H18R      C218 H18S      C218 H18T
! Chain From C3
BOND  O31  C31
BOND  C31  C32
DOUBLE C31  O32
BOND  C32  H2X       C32  H2Y       C32  C33
BOND  C33  H3X       C33  H3Y       C33  C34
BOND  C34  H4X       C34  H4Y       C34  C35
BOND  C35  H5X       C35  H5Y       C35  C36
BOND  C36  H6X       C36  H6Y       C36  C37
BOND  C37  H7X       C37  H7Y       C37  C38
BOND  C38  H8X       C38  H8Y       C38  C39
BOND  C39  H9X           C39  H9Y    C39  C310
BOND  C310 H10X      C310 H10Y       C310 C311
BOND  C311 H11X      C311 H11Y          C311 C312
BOND  C312 H12X      C312 H12Y          C312 C313
BOND  C313 H13X      C313 H13Y      C313 C314
BOND  C314 H14X      C314 H14Y      C314 C315
BOND  C315 H15X      C315 H15Y      C315 C316
BOND  C316 H16X      C316 H16Y      C316 C317
BOND  C317 H17X      C317 H17Y      C317 C318
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BOND  C318 H18X      C318 H18Y      C318 H18Z

IMPR C21 O21 C22 O22   C31 O31 C32 O32

IC N      C12    C11    O12        1.5110  111.97   65.84  112.46   1.4308
IC HN1    C12    *N     HN2        1.0342  114.60  119.70  105.60   1.0654
IC HN1    C12    *N     HN3        1.0342  114.60 -127.78  110.56   1.0397
IC HN1    N      C12    C11        1.0342  114.60 -177.91  111.97   1.5465
IC C11    N      *C12   H12A       1.5465  111.97 -121.58  107.97   1.1086
IC H12A   N      *C12   H12B       1.1086  107.97 -118.25  107.67   1.1104
IC O12    C12    *C11   H11A       1.4308  112.46 -126.31  111.01   1.1167
IC H11A   C12    *C11   H11B       1.1167  111.01 -115.41  107.63   1.1146
IC C12    C11    O12    P          1.5465  112.46  -80.62  120.62   1.5839
IC C11    O12    P      O11        1.4308  120.62 -156.78  104.60   1.5751
IC O11    O12    *P     O13        1.5751  104.60 -117.47  103.31   1.4823
IC O11    O12    *P     O14        1.5751  104.60  120.67  107.16   1.4736
IC O12    P      O11    C1         1.5839  104.60  -58.82  120.34   1.4318
IC P      O11    C1     C2         1.5751  120.34  -92.48  111.72   1.5536
IC C2     O11    *C1    HA         1.5536  111.72 -119.08  108.93   1.1133
IC HA     O11    *C1    HB         1.1133  108.93 -117.83  112.18   1.1155
IC O11    C1     C2     C3         1.4318  111.72  162.49  110.59   1.5553
IC C3     C1     *C2    O21        1.5553  110.59  120.51  108.20   1.4410
IC C3     C1     *C2    HS         1.5553  110.59 -117.47  107.37   1.1169
IC C1     C2     O21    C21        1.5536  108.20  145.45  115.07   1.3229
IC C2     O21    C21    C22        1.4410  115.07  175.60  109.17   1.5330
IC C22    O21    *C21   O22        1.5330  109.17  179.92  126.38   1.2173
IC O21    C21    C22    C23        1.3229  109.17 -134.07  111.55   1.5472
IC C23    C21    *C22   H2R        1.5472  111.55 -119.81  106.70   1.1095
IC H2R    C21    *C22   H2S        1.1095  106.70 -117.59  109.58   1.1081
IC C1     C2     C3     O31        1.5536  110.59  178.88  111.62   1.4432
IC O31    C2     *C3    HX         1.4432  111.62 -121.40  107.66   1.1142
IC HX     C2     *C3    HY         1.1142  107.66 -116.77  107.26   1.1152
IC C2     C3     O31    C31        1.5553  111.62  174.54  113.52   1.3270
IC C3     O31    C31    C32        1.4432  113.52  178.76  109.19   1.5276
IC C32    O31    *C31   O32        1.5276  109.19 -179.68  125.26   1.2176
IC O31    C31    C32    C33        1.3270  109.19 -153.26  112.50   1.5449
IC C33    C31    *C32   H2X        1.5449  112.50  120.40  107.84   1.1092
IC H2X    C31    *C32   H2Y        1.1092  107.84  117.16  108.28   1.1081
IC C21    C22    C23    C24        1.5289  112.21  175.76  112.39   1.5338
IC C24    C22    *C23   H3R        1.5338  112.39 -120.69  109.57   1.1147
IC H3R    C22    *C23   H3S        1.1147  109.57 -117.65  109.64   1.1142
IC C22    C23    C24    C25        1.5449  112.39 -179.39  112.35   1.5346
IC C25    C23    *C24   H4R        1.5346  112.35 -121.52  109.41   1.1131
IC H4R    C23    *C24   H4S        1.1131  109.41 -117.57  108.97   1.1134
IC C23    C24    C25    C26        1.5338  112.35  176.31  112.80   1.5344
IC C26    C24    *C25   H5R        1.5344  112.80 -121.01  108.95   1.1135
IC H5R    C24    *C25   H5S        1.1135  108.95 -117.24  109.16   1.1132
IC C24    C25    C26    C27        1.5346  112.80 -179.44  112.48   1.5356
IC C27    C25    *C26   H6R        1.5356  112.48 -121.49  109.32   1.1129
IC H6R    C25    *C26   H6S        1.1129  109.32 -117.47  108.94   1.1132
IC C25    C26    C27    C28        1.5344  112.48  176.92  112.46   1.5398
IC C28    C26    *C27   H7R        1.5398  112.46 -121.38  108.40   1.1139
IC H7R    C26    *C27   H7S        1.1139  108.40 -116.93  108.77   1.1139
IC C26    C27    C28    C29        1.5346  112.80 -179.44  112.48   1.5356
IC C29    C27    *C28   H8R        1.5356  112.48 -121.49  109.32   1.1129
IC H8R    C27    *C28   H8S        1.1129  109.32 -117.47  108.94   1.1132
IC C27    C28    C29    C210       1.5344  112.48  176.92  112.46   1.5398
IC C210   C28    *C29   H9R        1.5398  112.46 -121.38  108.40   1.1139
IC H9R   C28   *C29   H9S          1.1139  108.40 -116.93  108.77   1.1139
IC C28    C29    C210   C211       1.5356  112.46 -178.53  111.43   1.5097
IC C211   C29    *C210  H10R       1.5097  111.43 -123.58  107.80   1.1132
IC H10R   C29    *C210  H10S       1.1132  107.80 -115.43  108.37   1.1128
IC C29    C210   C211   C212       1.5398  111.43 -126.96  126.62   1.3465
IC C212   C210   *C211  H11R       1.3465  126.62  178.41  114.65   1.1012
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IC C210   C211   C212   C213       1.5097  126.62   -1.69  126.32   1.5088
IC C213   C211   *C212  H12R       1.5088  126.32 -179.55  118.79   1.1012
IC C211   C212   C213   C214       1.3465  126.32   93.02  112.15   1.5392
IC C214   C212   *C213  H13R       1.5392  112.15 -121.30  111.28   1.1133
IC H13R   C212   *C213  H13S       1.1133  111.28 -117.50  110.00   1.1126
IC C212   C213   C214   C215       1.5088  112.15 -178.81  112.29   1.5354
IC C215   C213   *C214  H14R       1.5354  112.29 -121.34  109.78   1.1133
IC H14R   C213   *C214  H14S       1.1133  109.78 -118.01  109.42   1.1144
IC C213   C214   C215   C216       1.5345  112.59 -179.58  112.63   1.5347
IC C216   C214   *C215  H15R       1.5347  112.63 -121.36  109.09   1.1132
IC H15R   C214   *C215  H15S       1.1132  109.09 -117.38  109.07   1.1132
IC C214   C215   C216   C217       1.5347  112.63  179.65  112.69   1.5339
IC C217   C215   *C216  H16R       1.5339  112.69 -121.27  109.11   1.1132
IC H16R   C215   *C216  H16S       1.1132  109.11 -117.36  109.14   1.1132
IC C215   C216   C217   C218       1.5347  112.69 -179.93  113.30   1.5309
IC C218   C216   *C217  H17R       1.5309  113.30 -121.70  108.75   1.1140
IC H17R   C216   *C217  H17S       1.1140  108.75 -116.65  108.73   1.1141
IC C216   C217   C218   H18R       1.5339  113.30  -59.98  110.46   1.1113
IC H18R   C217   *C218  H18S       1.1113  110.46  119.84  110.45   1.1114
IC H18R   C217   *C218  H18T       1.1113  110.46 -120.09  110.62   1.1112
IC C31    C32    C33    C34        1.5288  113.05  179.24  111.73   1.5343
IC C34    C32    *C33   H3X        1.5343  111.73 -120.85  109.62   1.1140
IC H3X    C32    *C33   H3Y        1.1140  109.62 -117.95  109.78   1.1144
IC C32    C33    C34    C35        1.5447  111.73 -176.74  112.91   1.5345
IC C35    C33    *C34   H4X        1.5345  112.91 -121.67  109.15   1.1134
IC H4X    C33    *C34   H4Y        1.1134  109.15 -117.32  108.98   1.1134
IC C33    C34    C35    C36        1.5343  112.91  178.63  112.42   1.5349
IC C36    C34    *C35   H5X        1.5349  112.42 -120.99  108.94   1.1133
IC H5X    C34    *C35   H5Y        1.1133  108.94 -117.41  109.31   1.1131
IC C34    C35    C36    C37        1.5345  112.42 -176.73  112.80   1.5356
IC C37    C35    *C36   H6X        1.5356  112.80 -121.69  109.16   1.1130
IC H6X    C35    *C36   H6Y        1.1130  109.16 -117.32  108.94   1.1133
IC C35    C36    C37    C38        1.5343  112.91  178.63  112.42   1.5349
IC C38    C36    *C37   H7X        1.5349  112.42 -120.99  108.94   1.1133
IC H7X    C36    *C37   H7Y        1.1133  108.94 -117.41  109.31   1.1131
IC C36    C37    C38    C39        1.5345  112.42 -176.73  112.80   1.5356
IC C39    C37    *C38   H8X        1.5356  112.80 -121.69  109.16   1.1130
IC H8X    C37    *C38   H8Y        1.1130  109.16 -117.32  108.94   1.1133
IC C37    C38    C39    C310       1.5349  112.80  178.92  112.27   1.5402
IC C310   C38    *C39   H9X        1.5402  112.27 -121.37  108.23   1.1139
IC H9X    C38  *C39  H9Y            1.1139  108.23 -117.01  109.05   1.1137
IC C38    C39    C310   C311       1.5356  112.27 -174.92  111.69   1.5099
IC C311   C39    *C310  H10X       1.5099  111.69 -124.14  107.77   1.1124
IC H10X        C39   *C310 H10Y      1.1124  107.77 -115.13  108.30   1.1128
IC C39    C310   C311   C312       1.5402  111.69 -121.39  127.35   1.3470
IC C312   C310   *C311  H11X       1.3470  127.35  179.11  114.24   1.1012
IC H11X   C310       *C311 H9Y            1.1139  108.23 -117.01  109.05   1.1137  !
5/17/2015 need to check around C311 C312
IC C310   C311   C312   C313       1.5099  127.35    0.00  127.25   1.5096
IC C313   C311   *C312  H12X       1.5096  127.25  179.82  118.43   1.1012
IC H12X        C311  *C312 H10Y      1.1124  107.77 -115.13  108.30   1.1128
IC C311   C312   C313   C314       1.3470  127.25  106.03  111.65   1.5393
IC C314   C312   *C313  H13X       1.5393  111.65 -121.49  112.10   1.1123
IC H13X   C312   *C313  H13Y       1.1123  112.10 -117.95  109.83   1.1127
IC C312   C313   C314   C315       1.5096  111.65  179.63  112.41   1.5355
IC C315   C313   *C314  H14X       1.5355  112.41 -121.09  109.75   1.1135
IC H14X   C313   *C314  H14Y       1.1135  109.75 -118.07  109.46   1.1143
IC C313   C314   C315   C316       1.5347  112.66 -179.12  112.61   1.5348
IC C316   C314   *C315  H15X       1.5348  112.61 -121.34  109.09   1.1132
IC H15X   C314   *C315  H15Y       1.1132  109.09 -117.41  109.09   1.1132
IC C314   C315   C316   C317       1.5347  112.61  179.83  112.71   1.5340
IC C317   C315   *C316  H16X       1.5340  112.71 -121.28  109.10   1.1132
IC H16X   C315   *C316  H16Y       1.1132  109.10 -117.35  109.13   1.1133
IC C315   C316   C317   C318       1.5348  112.71 -179.67  113.30   1.5309
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IC C318   C316   *C317  H17X       1.5309  113.30 -121.68  108.77   1.1141
IC H17X   C316   *C317  H17Y       1.1141  108.77 -116.68  108.76   1.1141
IC C316   C317   C318   H18X       1.5340  113.30  -59.94  110.46   1.1113
IC H18X   C317   *C318  H18Y       1.1113  110.46  119.86  110.45   1.1113
IC H18X   C317   *C318  H18Z       1.1113  110.46 -120.06  110.61   1.1112



RESI SQDG    -1.00  !
!
!
!
!
!

! Adaped from:
!      RESI SAPI          -1.00 ! Phosphatidylinositol
!
!     Stearoyl - CH2                    Uses RESI INI1 - cyclic myi-inositol,
!                |
!  Arachidonyl - CH                         RESI SAPC
!                |     (-)
!                CH2 - PO4 - inositol
!
GROUP
ATOM S    SG3O1     1.35  !              O7
ATOM O7   OG2P1    -0.716 !              |
ATOM O8   OG2P1    -0.716 !           O8---S---O9
ATOM O9   OG2P1    -0.716 !              |
GROU                      !              |
ATOM C1   CC3162    0.340 !              |
ATOM H1   HCA1      0.090 !         H61---C6--H62
ATOM O1   OC311    -0.650 !              |
ATOM C5   CC3163    0.075 !            H5-C5---O5
ATOM H5   HCA1      0.074 !         H4   /       \    H1
ATOM O5   OC3C61   -0.457 !           \ / HO3     \  /
GROU                      !            C4 |        C1
ATOM C2   CC3161   -0.008 !           / \ O3   H2 /  \
ATOM H2   HCA1      0.075 !    HO4-O4   \|    | /    O6
ATOM O2   OC311    -0.681 !              C3---C2     |
ATOM HO2  HCP1      0.439 !              |    |      |
GROU                      !              H3   O2-HO2 |
ATOM C3   CC3161    0.357 !                        |
ATOM H3   HCA1      0.012 !
ATOM O3   OC311    -0.712 !                        |
ATOM HO3  HCP1      0.413 !
GROU                      !                     |
ATOM C4   CC3161    0.340 !
ATOM H4   HCA1      0.000 !                       |
ATOM O4   OC311    -0.718 !                    --------
ATOM HO4  HCP1      0.440 !                  |
GROU                      !
ATOM C6   CC321    -0.288 !                  |
ATOM H61  HCA2      0.064 !
ATOM H62  HCA2      0.064 !                  |
GROU                      !              |
ATOM C44   CTL2     0.305 !                  |     alpha1
ATOM HA   HAL2      0.005 !           H44A---C44---H44B
ATOM HB   HAL2      0.005 !                  |     theta1
GROUP                     !                  |
ATOM C45  CTL1      0.214 !            H45---C45-------------
ATOM H45  HAL1      0.036 !                  | beta1        |
ATOM O47  OSL      -0.531 !             O49  O47          theta3
ATOM C7   CL        0.927 !              \\ /  beta2        |
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ATOM O49  OBL      -0.625 !              C7               |
ATOM C8   CTL2     -0.376 !              |   beta3        |
ATOM H8R  HAL2      0.131 !        H8R---C8---H8S        |
ATOM H8S  HAL2      0.131 !              |               |
GROUP                     !              |    beta4      |
ATOM C46  CTL2      0.146 !              |               |
ATOM H46X HAL2      0.056 !              |          H46X--C46--H46Y
ATOM H46Y HAL2      0.056 !              |                |   gamma1
ATOM O48  OSL      -0.406 !              |           O32  O31
ATOM C23  CL        0.913 !              |            \\ /    gamma2
ATOM O10  OBL      -0.644 !              |              C23
ATOM C24  CTL2     -0.409 !              |              |     gamma3
ATOM H24X HAL2      0.145 !              |       1H24X---C24---H24Y
ATOM H24Y HAL2      0.145 !              |              |
GROUP                     !              |              |      gamma4
ATOM C23  CTL2     -0.18  !              |              |
ATOM H3R  HAL2      0.09  !       H9R ---C9---H9S       |
ATOM H3S  HAL2      0.09  !              |              |
GROUP                     !              |              |
ATOM C24  CTL2     -0.18  !              |              |
ATOM H4R  HAL2      0.09  !       HR ---C24---H4S       |
ATOM H4S  HAL2      0.09  !              |              |
GROUP                     !              |              |
ATOM C25  CEL1     -0.15  !              |              |
ATOM H5R  HEL1      0.15  !       H5R ---C25            |
GROUP                     !              |!  (CIS)      |
ATOM C26  CEL1     -0.15  !              |!             |
ATOM H6R  HEL1      0.15  !       H6R ---C26            |
GROUP                     !              |              |
ATOM C27  CTL2     -0.18  !              |              |
ATOM H7R  HAL2      0.09  !       H7R ---C27---H7S      |
ATOM H7S  HAL2      0.09  !              |              |
GROUP                     !              |              |
ATOM C28  CEL1     -0.15  !              |              |
ATOM H8R  HEL1      0.15  !       H8R ---C28            |
GROUP                     !              |!  (CIS)      |
ATOM C29  CEL1     -0.15  !              |!             |
ATOM H9R  HEL1      0.15  !       H9R ---C29            |
GROUP                     !              |              |
ATOM C210 CTL2     -0.18  !              |              |
ATOM H10R HAL2      0.09  !       H10R---C210--H10S     |
ATOM H10S HAL2      0.09  !              |              |
GROUP                     !              |              |
ATOM C211 CEL1     -0.15  !              |              |
ATOM H11R HEL1      0.15  !       H11R---C211           |
GROUP                     !              |!  (CIS)      |
ATOM C212 CEL1     -0.15  !              |!             |
ATOM H12R HEL1      0.15  !       H12R---C212           |
GROUP                     !              |              |
ATOM C213 CTL2     -0.18  !              |              |
ATOM H13R HAL2      0.09  !       H13R---C213--H13S     |
ATOM H13S HAL2      0.09  !              |              |
GROUP                     !              |              |
ATOM C214 CEL1     -0.15  !              |              |
ATOM H14R HEL1      0.15  !       H14R---C214           |
GROUP                     !              |!  (CIS)      |
ATOM C215 CEL1     -0.15  !              |!             |
ATOM H15R HEL1      0.15  !       H15R---C215           |
GROUP                     !              |              |
ATOM C216 CTL2     -0.18  !              |              |
ATOM H16R HAL2      0.09  !       H16R---C216--H16S     |
ATOM H16S HAL2      0.09  !              |              |
GROUP                     !              |              |
ATOM C217 CTL2     -0.18  !              |              |
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ATOM H17R HAL2      0.09  !        H17R---C217--H17S     |
ATOM H17S HAL2      0.09  !               |              |
GROUP                     !               |              |
ATOM C218 CTL2     -0.27  !               |              |
ATOM H18R HAL2      0.09  !        H18R---C218--H18S     |
ATOM H18S HAL2      0.09  !               |              |
GROUP                     !               |              |
ATOM C219 CTL2     -0.18  !               |              |
ATOM H19R HAL2      0.09  !        H19R---C219--H19S     |
ATOM H19S HAL2      0.09  !               |              |
GROUP                     !               |              |
ATOM C220 CTL3     -0.18  !               |              |
ATOM H20R HAL3      0.09  !        H20R---C220--H20S     |
ATOM H20S HAL3      0.09  !               |              |
ATOM H20T HAL3      0.09  !             H20T             |
GROUP                     !                              |
ATOM C33  CTL2     -0.18  !                              |
ATOM H3X  HAL2      0.09  !                     H3X ---C33---H3Y
ATOM H3Y  HAL2      0.09  !                              |
GROUP                     !                              |
ATOM C34  CTL2     -0.18  !                              |
ATOM H4X  HAL2      0.09  !                     H4X ---C34---H4Y
ATOM H4Y  HAL2      0.09  !                              |
GROUP                     !                              |
ATOM C35  CTL2     -0.18  !                              |
ATOM H5X  HAL2      0.09  !                     H5X ---C35---H5Y
ATOM H5Y  HAL2      0.09  !                              |
GROUP                     !                              |
ATOM C36  CTL2     -0.18  !                              |
ATOM H6X  HAL2      0.09  !                     H6X ---C36---H6Y
ATOM H6Y  HAL2      0.09  !                              |
GROUP                     !                              |
ATOM C37  CTL2     -0.18  !                              |
ATOM H7X  HAL2      0.09  !                     H7X ---C37---H7Y
ATOM H7Y  HAL2      0.09  !                              |
GROUP                     !                              |
ATOM C38  CTL2     -0.18  !                              |
ATOM H8X  HAL2      0.09  !                     H8X ---C38---H8Y
ATOM H8Y  HAL2      0.09  !                              |
GROUP                     !                              |
ATOM C39  CTL2     -0.18  !                              |
ATOM H9X  HAL2      0.09  !                     H9X ---C39---H9Y
ATOM H9Y  HAL2      0.09  !                              |
GROUP                     !                              |
ATOM C310 CTL2     -0.18  !                              |
ATOM H10X HAL2      0.09  !                     H10X---C310--H10Y
ATOM H10Y HAL2      0.09  !                              |
GROUP                     !                              |
ATOM C311 CTL2     -0.18  !                              |
ATOM H11X HAL2      0.09  !                     H11X---C311--H11Y
ATOM H11Y HAL2      0.09  !                              |
GROUP                     !                              |
ATOM C312 CTL2     -0.18  !                              |
ATOM H12X HAL2      0.09  !                     H12X---C312--H12Y
ATOM H12Y HAL2      0.09  !                              |
GROUP                     !                              |
ATOM C313 CTL2     -0.18  !                              |
ATOM H13X HAL2      0.09  !                     H13X---C313--H13Y
ATOM H13Y HAL2      0.09  !                              |
GROUP                     !                              |
ATOM C314 CTL2     -0.18  !                              |
ATOM H14X HAL2      0.09  !                     H14X---C314--H14Y
ATOM H14Y HAL2      0.09  !                              |
GROUP                     !                              |
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ATOM C315 CTL2     -0.18  !                          |
ATOM H15X HAL2      0.09  !                       H15X---C315--H15Y
ATOM H15Y HAL2      0.09  !                          |
GROUP                     !                          |
ATOM C316 CTL2     -0.18  !                          |
ATOM H16X HAL2      0.09  !                       H16X---C316--H16Y
ATOM H16Y HAL2      0.09  !                          |
GROUP                     !                          |
ATOM C317 CTL2     -0.18  !                          |
ATOM H17X HAL2      0.09  !                       H17X---C317--H17Y
ATOM H17Y HAL2      0.09  !                          |
GROUP                     !                          |
ATOM C318 CTL3     -0.27  !                          |
ATOM H18X HAL3      0.09  !                       H18X---C318--H18Y
ATOM H18Y HAL3      0.09  !                          |
ATOM H18Z HAL3      0.09  !                         H18Z


! Sulfonate Head Group
BOND  S   O7            S    O8            S         O9
BOND  S   C6

! Sugar
BOND C1   O1        C1   H1        O1   HO1       C1   O5        C1   C2
BOND C2   H2        C2   O2        O2   HO2       C2   C3        C3   H3
BOND C3   O3        O3   HO3       C3   C4        C4   H4        C4   O4
BOND O4   HO4       C4   C5        C5   H5        C5   C6        C6   H61
BOND C6   H62       C5   O5


! Inositol Head Group
BOND  C11  H1        C11  C16       C11  C12       C11  O12
BOND  C12  H2        C12  O2        O2   HO2       C12  C13       C13  H3
BOND  C13  O3        O3   HO3       C13  C14       C14  H4        C14  O4
BOND  O4   HO4       C14  C15       C15  H5        C15  C16       C16  H6
BOND  C16  O6        O6   HO6       C15  O5        O5   HO5
BOND  O12  P         P    O11       P    O13       P    O14       O11  C1
! Glycerol Backbone
BOND  C1   HA        C1    HB       C1   C2
BOND  C2   HS        C2    C3       C2   O21
BOND  C3   HX        C3    HY       C3   O31
! Chain from C2
BOND  O21  C21
BOND  C21  C22
DOUBLE  C21  O22
BOND  C22  H2R       C22  H2S       C22  C23
BOND  C23  H3R       C23  H3S       C23  C24
BOND  C24  H4R       C24  H4S       C24  C25
BOND  C25  H5R
DOUBLE  C25 C26
BOND  C26  H6R       C26  C27
BOND  C27  H7R       C27  H7S       C27  C28
BOND  C28  H8R
DOUBLE  C28 C29
BOND  C29  H9R       C29  C210
BOND  C210 H10R      C210 H10S      C210 C211
BOND  C211 H11R
DOUBLE  C211 C212
BOND  C212 H12R      C212 C213
BOND  C213 H13R      C213 H13S      C213 C214
BOND  C214 H14R
DOUBLE  C214 C215
BOND  C215 H15R      C215 C216
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BOND  C216 H16R      C216 H16S      C216 C217
BOND  C217 H17R      C217 H17S      C217 C218
BOND  C218 H18R      C218 H18S      C218 C219
BOND  C219 H19R      C219 H19S      C219 C220
BOND  C220 H20R      C220 H20S      C220 H20T
! Chain From C3
BOND  O31  C31
BOND  C31  C32
DOUBLE  C31  O32
BOND  C32  H2X       C32  H2Y       C32  C33
BOND  C33  H3X       C33  H3Y       C33  C34
BOND  C34  H4X       C34  H4Y       C34  C35
BOND  C35  H5X       C35  H5Y       C35  C36
BOND  C36  H6X       C36  H6Y       C36  C37
BOND  C37  H7X       C37  H7Y       C37  C38
BOND  C38  H8X       C38  H8Y       C38  C39
BOND  C39  H9X       C39  H9Y       C39  C310
BOND  C310 H10X      C310 H10Y      C310 C311
BOND  C311 H11X      C311 H11Y      C311 C312
BOND  C312 H12X      C312 H12Y      C312 C313
BOND  C313 H13X      C313 H13Y      C313 C314
BOND  C314 H14X      C314 H14Y      C314 C315
BOND  C315 H15X      C315 H15Y      C315 C316
BOND  C316 H16X      C316 H16Y      C316 C317
BOND  C317 H17X      C317 H17Y      C317 C318
BOND  C318 H18X      C318 H18Y      C318 H18Z

IMPR C21 O21 C22 O22    C31 O31 C32 O32

ACCEPTOR O1 S
ACCEPTOR O2 S
ACCEPTOR O3 S


!    I    J    K    L      R(IK)   T(IKJ)    PHI   T(JKL)   R(KL)
! Sulfonate
ACCEPTOR O1 S
ACCEPTOR O2 S
ACCEPTOR O3 S
IC C2   C1   S    O1   0.0        0.00    180.00       0.0     0.0
IC C1   O1   *S   O2   0.0        0.00    120.00       0.0     0.0
IC C1   O1   *S   O3   0.0        0.00   -120.00       0.0     0.0
IC S    C2   *C1  H11  0.0        0.00    120.00       0.0     0.0
IC S    C2   *C1  H12  0.0        0.00   -120.00       0.0     0.0
IC S    C1   C2   C3   0.0        0.00    180.00       0.0     0.0

! Inositol Head Group
IC C11   C12   C13   C14    1.5530  107.31  -59.93  109.11   1.5612
IC C12   C13   C14   C15    1.4341  109.11   59.27  114.44   1.4654
IC C13   C12   C11   O12    1.4341  107.31 -175.79  117.69   1.4086
IC C13   C14   C15   C16    1.5612  114.44  -55.48  109.80   1.5350
IC C14   C15   C16   C11    1.4654  109.80   55.05  107.18   1.5598
IC C12   C13   C14   O4     1.4341  109.11 -177.27  106.06   1.4595
IC C13   C14   C15   O5     1.5612  114.44  171.27  114.28   1.4386
IC C12   C13   C14   H4     1.4341  109.11  -64.25  106.39   1.1684
IC O12   C12   *C11  H1     1.4086  117.69 -121.05  110.98   1.1834
IC O12   C11   C12   O2     1.4086  117.69   51.01  111.79   1.4490
IC O12   C11   C12   H2     1.4086  117.69  -61.28   98.22   1.1105
IC C13   C14   C15   H5     1.5612  114.44   52.34  110.34   1.0922
IC O2    C11   *C12  C13    1.4490  111.79  133.20  107.31   1.4341
IC O3    C14   *C13  H3     1.4537  110.99  114.31  113.73   1.1394
IC O3    C12   *C13  C14    1.4537  105.59  119.36  109.11   1.5612
IC O4    C13   *C14  C15    1.4595  106.06 -123.46  114.44   1.4654
IC C16   C14   *C15  O5     1.5350  109.80 -133.25  114.28   1.4386
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IC C14   C15   O5    HO5    1.4654  114.28  -73.20  108.55   0.9726
IC C14   C15   C16   O6     1.4654  109.80 -179.24  110.87   1.4043
IC C16   C11   O12   P      1.5530  117.69  300.00  114.27   0.9451 ! gauche
IC C11   C12   O2    HO2    1.5530  111.79  -31.80  115.65   0.9404
IC C12   C13   O3    HO3    1.4341  105.59   37.19  107.10   0.9920
IC C13   C14   O4    HO4    1.5612  106.06   35.00  105.15   0.9686
IC C15   C16   O6    HO6    1.5350  110.87   51.35  112.65   0.9879
IC C14   C15   C16   H6     1.4654  109.80  -58.40  111.34   1.0796
! Phosphate Linker
IC C11   O12   P     O11    1.3655  121.23  153.36  102.74   1.5058
IC O11   O12   *P    O13    1.5867  101.18 -114.47  107.73   1.4832
IC O11   O12   *P    O14    1.5867  101.18  116.82  109.30   1.4741
IC O12   P     O11   C1     1.5958  101.18  180.00  122.31   1.4271 ! trans
IC P     O11   C1    C2     1.5867  122.31  180.00  111.45   1.5517 ! trans
IC C2    O11   *C1   HA     1.5517  111.45  117.99  107.86   1.1119
IC HA    O11   *C1   HB     1.1119  107.86  116.85  112.59   1.1137
IC O11   C1    C2    O21    1.4271  111.45 -175.58  109.40   1.4420
! Backbone
IC O21   C1    *C2   C3     1.4420  109.40 -121.10  110.56   1.5561
IC C3    C1    *C2   HS     1.5561  110.56 -116.88  109.10   1.1148
IC C1    C2    O21   C21    1.5517  109.40   75.31  115.18   1.3240
IC C2    O21   C21   C22    1.4420  115.18 -167.64  109.38   1.5349
IC C22   O21   *C21  O22    1.5349  109.38  177.97  125.87   1.2208
IC O21   C21   C22   C23    1.3240  109.38 -106.88  114.46   1.5510
IC C23   C21   *C22  H2R    1.5510  114.46  120.85  107.59   1.1114
IC H2R   C21   *C22  H2S    1.1114  107.59  115.88  108.08   1.1076
IC C1    C2    C3    O31    1.5517  110.56 -174.46  111.33   1.4462
IC O31   C2    *C3   HX     1.4462  111.33 -122.32  107.11   1.1154
IC HX    C2    *C3   HY     1.1154  107.11 -116.45  107.97   1.1151
IC C2    C3    O31   C31    1.5561  111.33 -170.38  113.09   1.3331
IC C3    O31   C31   C32    1.4462  113.09 -178.75  108.33   1.5405
IC C32   O31   *C31  O32    1.5405  108.33 -179.57  125.60   1.2151
IC O31   C31   C32   C33    1.3331  108.33 -179.15  116.85   1.6060
IC C33   C31   *C32  H2X    1.6060  116.85 -121.70  105.08   1.1113
IC H2X   C31   *C32  H2Y    1.1113  105.08 -115.26  107.43   1.1071
! Acyl Chain 1
IC C21   C22   C23   C24    1.5329  113.78  180.00  112.27   1.5435
IC C24   C22   *C23  H3R    1.5435  112.27 -122.24  109.63   1.1133
IC C24   C22   *C23  H3S    1.5435  112.27  120.06  108.89   1.1154
IC C22   C23   C24   C25    1.5483  112.27  180.00  115.67   1.5107
IC C25   C23   *C24  H4R    1.5107  115.67 -121.06  107.11   1.1144
IC C25   C23   *C24  H4S    1.5107  115.67  124.06  108.43   1.1128
IC C23   C24   C25   C26    1.5435  115.67  180.00  125.97   1.3453
IC C26   C24   *C25  H5R    1.3453  125.97 -176.85  115.39   1.1011
IC C24   C25   C26   C27    1.5107  125.97    0.00  125.28   1.5097 !cis db
IC C27   C25   *C26  H6R    1.5097  125.28  178.19  119.65   1.1004
IC C25   C26   C27   C28    1.3453  125.28  120.00  121.35   1.5192
IC C28   C26   *C27  H7R    1.5192  121.35 -124.15  108.68   1.1135
IC C28   C26   *C27  H7S    1.5192  121.35  123.34  106.97   1.1121
IC C26   C27   C28   C29    1.5097  121.35  120.00  132.80   1.3549
IC C29   C27   *C28  H8R    1.3549  132.80 -178.43  111.35   1.1010
IC C27   C28   C29   C210   1.5192  132.80    0.00  130.38   1.5115 !cis db
IC C210  C28   *C29  H9R    1.5115  130.38  178.53  117.07   1.1014
IC C28   C29   C210  C211   1.3549  130.38  120.00  111.80   1.5083
IC C211  C29   *C210 H10R   1.5192  121.35 -124.15  108.68   1.1135
IC C211  C29   *C210 H10S   1.5192  121.35  123.34  106.97   1.1128
IC C29   C210  C211  C212   1.5115  111.80  120.00  124.32   1.3436
IC C212  C210  *C211 H11R   1.3453  125.97 -176.85  115.39   1.1011
IC C210  C211  C212  C213   1.5083  124.32    0.00  125.45   1.5067 !cis db
IC C213  C211  *C212 H12R   1.5097  125.28  178.19  119.65   1.1004
IC C211  C212  C213  C214   1.3436  125.45  120.00  111.57   1.5090
IC C214  C212  *C213 H13R   1.5192  121.35 -124.15  108.68   1.1135
IC C214  C212  *C213 H13S   1.5192  121.35  123.34  106.97   1.1128
IC C212  C213  C214  C215   1.5067  111.57  120.00  126.10   1.3471
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IC C215  C213  *C214 H14R   1.3453  125.97 -176.85  115.39   1.1011
IC C213  C214  C215  C216   1.5090  126.10    0.00  125.86   1.5091 !cis db
IC C216  C214  *C215 H15R   1.5097  125.28  178.19  119.65   1.1004
IC C214  C215  C216  C217   1.3471  125.86  180.00  113.25   1.5428
IC C217  C215  *C216 H16R   1.5192  121.35 -124.15  108.68   1.1135
IC C217  C215  *C216 H16S   1.5192  121.35  123.34  106.97   1.1128
IC C215  C216  C217  C218   1.5091  113.25  180.00  115.19   1.5395
IC C218  C216  *C217 H17R   1.5192  121.35 -124.15  108.68   1.1135
IC C218  C216  *C217 H17S   1.5192  121.35  123.34  106.97   1.1128
IC C216  C217  C218  C219   1.5428  115.19  180.00  113.95   1.5345
IC C219  C217  *C218 H18R   1.5192  121.35 -124.15  108.68   1.1135
IC C219  C217  *C218 H18S   1.5192  121.35  123.34  106.97   1.1128
IC C217  C218  C219  C220   1.5395  113.95  180.00  112.95   1.5309
IC C220  C218  *C219 H19R   1.5192  121.35 -124.15  108.68   1.1135
IC C220  C218  *C219 H19S   1.5192  121.35  123.34  106.97   1.1128
IC C218  C219  C220  H20T   1.5345  112.95  180.00  110.39   1.1115
IC H20T  C219  *C220 H20R   1.5192  121.35 -124.15  108.68   1.1135
IC H20T  C219  *C220 H20S   1.5192  121.35  123.34  106.97   1.1128
! Acyl Chain 2
IC C31   C32   C33   C34    1.5405  116.85  180.00  126.13   1.5951
IC C34   C32   *C33  H3X    1.5410  113.36 -119.96  111.74   1.1148
IC C34   C32   *C33  H3Y    1.5192  121.35  123.34  106.97   1.1128
IC C32   C33   C34   C35    1.6060  126.13  180.00  113.36   1.5410
IC C35   C33   *C34  H4X    1.5396  113.52 -123.43  110.53   1.1101
IC C35   C33   *C34  H4Y    1.5192  121.35  123.34  106.97   1.1128
IC C33   C34   C35   C36    1.5951  113.36  180.00  113.52   1.5396
IC C36   C34   *C35  H5X    1.5396  113.52 -123.43  110.53   1.1101
IC C36   C34   *C35  H5Y    1.5192  121.35  123.34  106.97   1.1128
IC C34   C35   C36   C37    1.5410  113.52  180.00  114.47   1.5397
IC C37   C35   *C36  H6X    1.5396  113.52 -123.43  110.53   1.1101
IC C37   C35   *C36  H6Y    1.5192  121.35  123.34  106.97   1.1128
IC C35   C36   C37   C38    1.5396  114.47  180.00  113.41   1.5386
IC C38   C36   *C37  H7X    1.5396  113.52 -123.43  110.53   1.1101
IC C38   C36   *C37  H7Y    1.5192  121.35  123.34  106.97   1.1128
IC C36   C37   C38   C39    1.5397  113.41  180.00  113.71   1.5382
IC C39   C37   *C38  H8X    1.5396  113.52 -123.43  110.53   1.1101
IC C39   C37   *C38  H8Y    1.5192  121.35  123.34  106.97   1.1128
IC C37   C38   C39   C310   1.5386  113.71  180.00  113.75   1.5392
IC C310  C38   *C39  H9X    1.5396  113.52 -123.43  110.53   1.1101
IC C310  C38   *C39  H9Y    1.5192  121.35  123.34  106.97   1.1128
IC C38   C39   C310  C311   1.5382  113.75  180.00  114.19   1.5353
IC C311  C39   *C310 H10X   1.5396  113.52 -123.43  110.53   1.1101
IC C311  C39   *C310 H10Y   1.5192  121.35  123.34  106.97   1.1128
IC C39   C310  C311  C312   1.5392  114.19  180.00  112.28   1.5347
IC C312  C310  *C311 H11X   1.5396  113.52 -123.43  110.53   1.1101
IC C312  C310  *C311 H11Y   1.5192  121.35  123.34  106.97   1.1128
IC C310  C311  C312  C313   1.5353  112.28  180.00  113.98   1.5367
IC C313  C311  *C312 H12X   1.5396  113.52 -123.43  110.53   1.1101
IC C313  C311  *C312 H12Y   1.5192  121.35  123.34  106.97   1.1128
IC C311  C312  C313  C314   1.5347  113.98  180.00  113.72   1.5377
IC C314  C312  *C313 H13X   1.5396  113.52 -123.43  110.53   1.1101
IC C314  C312  *C313 H13Y   1.5192  121.35  123.34  106.97   1.1128
IC C312  C313  C314  C315   1.5367  113.72  180.00  113.85   1.5357
IC C315  C313  *C314 H14X   1.5396  113.52 -123.43  110.53   1.1101
IC C315  C313  *C314 H14Y   1.5192  121.35  123.34  106.97   1.1128
IC C313  C314  C315  C316   1.5377  113.85  180.00  111.81   1.5374
IC C316  C314  *C315 H15X   1.5396  113.52 -123.43  110.53   1.1101
IC C316  C314  *C315 H15Y   1.5192  121.35  123.34  106.97   1.1128
IC C314  C315  C316  C317   1.5357  111.81  180.00  114.29   1.5985
IC C317  C315  *C316 H16X   1.5396  113.52 -123.43  110.53   1.1101
IC C317  C315  *C316 H16Y   1.5192  121.35  123.34  106.97   1.1128
IC C315  C316  C317  C318   1.5374  114.29  180.00  130.92   1.5745
IC C318  C316  *C317 H17X   1.5396  113.52 -123.43  110.53   1.1101
IC C318  C316  *C317 H17Y   1.5192  121.35  123.34  106.97   1.1128
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IC C316  C317  C318  H18X   1.5985  130.92  180.00  110.90   1.1113
IC H18X  C317  *C318 H18Y   1.5396  113.52 -123.43  110.53   1.1101
IC H18X  C317  *C318 H18Z   1.5192  121.35  123.34  106.97   1.1128
```

Appendix B. Ubiquinones (UQ10 – UQ, UQH2, and neutral semiquinone)

File: <ubiquinone.inp>

```
        !This is a reduced topology file, suitable for building Ubiquinone and derivatives.
        !Uses lipid nomenclature to build isoprene tails, which can get built up from isoprenoid
units.
        MASS   1   H      1.00800 H ! polar H
        MASS 136  HL    1.008000 H ! polar H (equivalent to protein H)
        MASS 137  HCL   1.008000 H ! charged H for PE (equivalent to protein HC)
        MASS 138  HOL   1.008000 H ! Nucleic acid phosphate hydroxyl proton
        MASS 139  HAL1  1.008000 H ! alphatic proton
        MASS 140  HAL2  1.008000 H ! alphatic proton
        MASS 141  HAL3  1.008000 H ! alphatic proton
        MASS 142  HEL1  1.008000 H ! for alkene; RHC=CR
        MASS 143  HEL2  1.008000 H ! for alkene; H2C=CR. Currently unused.
        MASS 144  HBL   1.008000 H ! POPS SER backbone H
        MASS 145  CL   12.011000 C ! carbonyl C (acetic acid/methyl acetate)
        MASS 146  CTL1 12.011000 C ! sp3 carbon with 1 H  (-CH1-)
        MASS 147  CTL2 12.011000 C ! carbon of methylene group (-CH2-)
        MASS 148  CTL3 12.011000 C ! carbon of methyl group (-CH3)
        MASS 149  CTL5 12.011000 C ! carbon of methyl group (-CH3) for tetramethylammonium
        MASS 150  CEL1 12.011000 C ! for alkene; RHC=CR
        MASS 151  CEL2 12.011000 C ! for alkene; H2C=CR. Currently unused.
        MASS 201   HAN    1.00800 H ! nonpolar H
        MASS 202   CN    12.01100 C ! polar C
        MASS 203   CTN   12.01100 C ! tetrahedral C
        MASS 225   CUQ1  12.01100 C ! for quinones
        MASS 226   CUQ2  12.01100 C ! for quinones
        MASS 227   CUQ3  12.01100 C ! for quinones
        MASS 228   CUQ4  12.01100 C ! for quinones
        MASS 229   OUQ1  15.99900 O ! for quinones
        MASS 230   OUQ2  15.99900 O ! for quinones
        !When QA and QB are populated by different quinones, they need distinct types to keep the
parameters consistent.
        MASS 201   HAN2   1.00800 H ! nonpolar H
        MASS 202   CN2   12.01100 C ! polar C
        MASS 203   CTN2  12.01100 C ! tetrahedral C
        MASS 225   CUQ5  12.01100 C ! for quinones
        MASS 226   CUQ6  12.01100 C ! for quinones
        MASS 227   CUQ7  12.01100 C ! for quinones
        MASS 228   CUQ8  12.01100 C ! for quinones
        MASS 229   OUQ3  15.99900 O ! for quinones
        MASS 230   OUQ4  15.99900 O ! for quinones
        MASS 240   CNQ1  12.01100 C ! for naphthoquinone
        MASS 241   CNQ2  12.01100 C ! for naphthoquinone
        MASS 242   HP     1.00800 H ! aromatic hydrogen

        RESI NAPQ      0.00000 !Naphthoquinone (vitamin K)

        GROUP  ! ubiquinone ring

        ATOM C1   CUQ3   -0.317    !
        ATOM C2   CUQ1    0.586    !           H7\        /H4
        ATOM O2   OUQ1   -0.456    !              C10--C11
        ATOM C3   CUQ2    0.055    !             //      \\
        ATOM C12  CNQ1   -0.336    !          H6-C9      C12-H5
        ATOM C4   CUQ2    0.055    !              \ ____ /
        ATOM C9   CNQ1   -0.336    !              C4----C3
        ATOM C5   CUQ1    0.586    !              /      \
        ATOM O5   OUQ1   -0.456    !            __/        \__
        ATOM C6   CUQ4    0.014    !         05--C5      C2--O2
        ATOM C1M  CTN    -0.120    !             \        /
        ATOM C11  CNQ2   -0.045    !              \ ____ /
        ATOM C10  CNQ2   -0.045    !              C6----C1
        ATOM H1   HAN     0.09     !               |     |  /H1
        ATOM H2   HAN     0.09     !           H10-C7-H11 C1M-H2
        ATOM H3   HAN     0.09     !                |        \H3
        ATOM H4   HAN     0.14     !            H14-C8-H12
```

```
ATOM H5   HAN     0.14     !               |
ATOM H6   HAN     0.14     !               H13
ATOM H7   HAN     0.14     !
!ATOM H8   HAN     0.09     !
!ATOM H9   HAN     0.09     !
                           !
!     isoprenic tail stub  !
                           !
ATOM C7   CTN   -0.175     !
ATOM C8   CN    -0.27      !
ATOM H10  HAN    0.09      !
ATOM H11  HAN    0.09      !
ATOM H12  HAN    0.09      !
ATOM H13  HAN    0.09      !
ATOM H14  HAN    0.09      !

!      bonds for ubiquinone  ring
BOND C1 C2    C2 C3    C3 C4    C4 C5
BOND C5 C6    C6 C1
BOND C2 O2    C3 O3    C4 O4    C5 O5
BOND O4 C4M   C4M H7   C4M H8   C4M H9
BOND O3 C3M   C3M H4   C3M H5   C3M H6
BOND C1 C1M   C1M H1   C1M H2   C1M H3
!Isoprene tail stub
BOND C6 C7    C7 H10   C7 H11   C7 C8    C8 H12   C8 H13 C8 H14
AUTOGENERATE ANGLES DIHEDRALS

RESI UBIQ      0.00000 !UBIQUINONE 6 FOR SPHAER FEHER, M SIDE

GROUP  ! ubiquinone ring

ATOM C1   CUQ3   -0.317    !
ATOM C2   CUQ1    0.586    !           H7\        /H4
ATOM O2   OUQ1   -0.456    !           H8-C4M  C3M-H5
ATOM C3   CUQ2    0.055    !           H9/ |    | \H6
ATOM O3   OUQ2   -0.336    !               O4   O3
ATOM C4   CUQ2    0.055    !                |____|
ATOM O4   OUQ2   -0.336    !              C4----C3
ATOM C5   CUQ1    0.586    !              /      \
ATOM O5   OUQ1   -0.456    !           __/        \__
ATOM C6   CUQ4    0.014    !         05--C5      C2--O2
ATOM C1M  CTN    -0.120    !             \         /
ATOM C3M  CTN    -0.045    !              \ ____ /
ATOM C4M  CTN    -0.045    !              C6----C1
ATOM H1   HAN     0.09     !               |     |  /H1
ATOM H2   HAN     0.09     !          H10-C7-H11 C1M-H2
ATOM H3   HAN     0.09     !               |        \H3
ATOM H4   HAN     0.09     !           H14-C8-H12
ATOM H5   HAN     0.09     !               |
ATOM H6   HAN     0.09     !               H13
ATOM H7   HAN     0.09     !
ATOM H8   HAN     0.09     !
ATOM H9   HAN     0.09     !
                           !
!     isoprenic tail stub  !
                           !
ATOM C7   CTN   -0.175     !
ATOM C8   CN    -0.27      !
ATOM H10  HAN    0.09      !
ATOM H11  HAN    0.09      !
ATOM H12  HAN    0.09      !
ATOM H13  HAN    0.09      !
ATOM H14  HAN    0.09      !

!      bonds for ubiquinone  ring
BOND C1 C2    C2 C3    C3 C4    C4 C5
BOND C5 C6    C6 C1
BOND C2 O2    C3 O3    C4 O4    C5 O5
BOND O4 C4M   C4M H7   C4M H8   C4M H9
BOND O3 C3M   C3M H4   C3M H5   C3M H6
BOND C1 C1M   C1M H1   C1M H2   C1M H3
!Isoprene tail stub
```

```
BOND C6 C7    C7 H10   C7 H11   C7 C8    C8 H12   C8 H13 C8 H14
AUTOGENERATE ANGLES DIHEDRALS

RESI 3MEO      0.00000 !3-methoxy Ubiquinone

GROUP  ! ubiquinone ring

ATOM C1   CUQ3   -0.059    !
ATOM C2   CUQ1    0.462    !           H7\        /H4
ATOM O2   OUQ1   -0.439    !           H8-C4M  C3M-H5
ATOM C3   CUQ2    0.037    !           H9/ |    | \H6
ATOM O3   OUQ2   -0.247    !               |    O3
ATOM C4   CUQ2   -0.012    !               |____|
!ATOM O4   OUQ2   -0.20    !              C4----C3
ATOM C5   CUQ1    0.395    !              /      \
ATOM O5   OUQ1   -0.447    !           __/        \__
ATOM C6   CUQ4    0.034    !         05--C5      C2--O2
ATOM C1M  CTN    -0.231    !             \        /
ATOM C3M  CTN    -0.060    !              \ ____ /
ATOM C4M  CTN    -0.266    !              C6----C1
ATOM H1   HAN     0.09     !               |     |  /H1
ATOM H2   HAN     0.09     !          H10-C7-H11 C1M-H2
ATOM H3   HAN     0.09     !               |        \H3
ATOM H4   HAN     0.09     !          H14-C8-H12
ATOM H5   HAN     0.09     !               |
ATOM H6   HAN     0.09     !               H13
ATOM H7   HAN     0.09     !
ATOM H8   HAN     0.09     !
ATOM H9   HAN     0.09     !
                           !
!     isoprenic tail stub  !
                           !
ATOM C7   CTN   -0.157     !
ATOM C8   CN    -0.27      !
ATOM H10  HAN    0.09      !
ATOM H11  HAN    0.09      !
ATOM H12  HAN    0.09      !
ATOM H13  HAN    0.09      !
ATOM H14  HAN    0.09      !

!       bonds for ubiquinone  ring
BOND C1 C2    C2 C3    C3 C4    C4 C5
BOND C5 C6    C6 C1
BOND C2 O2    C3 O3    C4 C4M    C5 O5
BOND C4M H7   C4M H8   C4M H9
BOND O3 C3M   C3M H4   C3M H5   C3M H6
BOND C1 C1M   C1M H1   C1M H2   C1M H3
!Isoprene tail stub
BOND C6 C7    C7 H10   C7 H11   C7 C8    C8 H12   C8 H13 C8 H14
AUTOGENERATE ANGLES DIHEDRALS


RESI 2MEO      0.00000 !2-methoxy Ubiquinone

GROUP  ! ubiquinone ring

ATOM C1   CUQ3    0.029    !
ATOM C2   CUQ1    0.480    !           H7\        /H4
ATOM O2   OUQ1   -0.459    !           H8-C4M  C3M-H5
ATOM C3   CUQ2   -0.056    !           H9/ |    | \H6
!ATOM O3   OUQ2   -0.20    !               O4   |
ATOM C4   CUQ2   -0.001    !               |____|
ATOM O4   OUQ2   -0.286    !              C4----C3
ATOM C5   CUQ1    0.486    !              /      \
ATOM O5   OUQ1   -0.368    !           __/        \__
ATOM C6   CUQ4   -0.148    !         05--C5      C2--O2
ATOM C1M  CTN    -0.226    !             \        /
ATOM C3M  CTN    -0.256    !              \ ____ /
ATOM C4M  CTN    -0.014    !              C6----C1
ATOM H1   HAN     0.09     !               |     |  /H1
ATOM H2   HAN     0.09     !          H10-C7-H11 C1M-H2
ATOM H3   HAN     0.09     !               |        \H3
```

```
ATOM H4   HAN     0.09     !           H14-C8-H12
ATOM H5   HAN     0.09     !               |
ATOM H6   HAN     0.09     !               H13
ATOM H7   HAN     0.09     !
ATOM H8   HAN     0.09     !
ATOM H9   HAN     0.09     !
                           !
!     isoprenic tail stub  !
                           !
ATOM C7   CTN   -0.171     !
ATOM C8   CN    -0.27      !
ATOM H10  HAN    0.09      !
ATOM H11  HAN    0.09      !
ATOM H12  HAN    0.09      !
ATOM H13  HAN    0.09      !
ATOM H14  HAN    0.09      !


!       bonds for ubiquinone  ring
BOND C1 C2    C2 C3    C3 C4    C4 C5
BOND C5 C6    C6 C1
BOND C2 O2    C3 C3M   C4 O4    C5 O5
BOND O4 C4M   C4M H7   C4M H8   C4M H9
BOND C3M H4   C3M H5   C3M H6
BOND C1 C1M   C1M H1   C1M H2   C1M H3
!Isoprene tail stub
BOND C6 C7    C7 H10   C7 H11   C7 C8    C8 H12   C8 H13 C8 H14
AUTOGENERATE ANGLES DIHEDRALS

RESI 3MOM      0.00000 !3-methoxy Ubiquinone with mixed-appropriate naming.

GROUP  ! ubiquinone ring

ATOM C1   CUQ7   -0.059    !
ATOM C2   CUQ5    0.462    !           H7\        /H4
ATOM O2   OUQ3   -0.439    !           H8-C4M  C3M-H5
ATOM C3   CUQ6    0.037    !           H9/ |    | \H6
ATOM O3   OUQ4   -0.247    !               |    O3
ATOM C4   CUQ6   -0.012    !               |____|
!ATOM O4   OUQ4   -0.20    !              C4----C3
ATOM C5   CUQ5    0.395    !              /      \
ATOM O5   OUQ3   -0.447    !           __/        \__
ATOM C6   CUQ8    0.034    !         05--C5      C2--O2
ATOM C1M  CTN2   -0.231    !             \        /
ATOM C3M  CTN2   -0.060    !              \ ____ /
ATOM C4M  CTN2   -0.266    !              C6----C1
ATOM H1   HAN2    0.09     !                |     |  /H1
ATOM H2   HAN2    0.09     !          H10-C7-H11 C1M-H2
ATOM H3   HAN2    0.09     !                |        \H3
ATOM H4   HAN2    0.09     !          H14-C8-H12
ATOM H5   HAN2    0.09     !                |
ATOM H6   HAN2    0.09     !                H13
ATOM H7   HAN2    0.09     !
ATOM H8   HAN2    0.09     !
ATOM H9   HAN2    0.09     !
                           !
!     isoprenic tail stub  !
                           !
ATOM C7   CTN2  -0.157     !
ATOM C8   CN2   -0.27      !
ATOM H10  HAN2   0.09      !
ATOM H11  HAN2   0.09      !
ATOM H12  HAN2   0.09      !
ATOM H13  HAN2   0.09      !
ATOM H14  HAN2   0.09      !

!       bonds for ubiquinone  ring
BOND C1 C2    C2 C3    C3 C4    C4 C5
BOND C5 C6    C6 C1
BOND C2 O2    C3 O3    C4 C4M    C5 O5
BOND C4M H7   C4M H8   C4M H9
BOND O3 C3M   C3M H4   C3M H5   C3M H6
```

```
BOND C1 C1M   C1M H1   C1M H2   C1M H3
!Isoprene tail stub
BOND C6 C7    C7 H10   C7 H11   C7 C8    C8 H12   C8 H13 C8 H14
AUTOGENERATE ANGLES DIHEDRALS


RESI 2MOM      0.00000 !2-methoxy Ubiquinone with mixed-appropriate naming.

GROUP  ! ubiquinone ring

ATOM C1   CUQ7    0.029    !
ATOM C2   CUQ5    0.480    !           H7\        /H4
ATOM O2   OUQ3   -0.459    !           H8-C4M  C3M-H5
ATOM C3   CUQ6   -0.056    !           H9/ |    | \H6
!ATOM O3   OUQ4   -0.20    !               O4   |
ATOM C4   CUQ6   -0.001    !               |____|
ATOM O4   OUQ4   -0.286    !              C4----C3
ATOM C5   CUQ5    0.486    !              /      \
ATOM O5   OUQ3   -0.368    !           __/        \__
ATOM C6   CUQ8   -0.148    !         05--C5      C2--O2
ATOM C1M  CTN2   -0.226    !            \         /
ATOM C3M  CTN2   -0.256    !             \ ____ /
ATOM C4M  CTN2   -0.014    !              C6----C1
ATOM H1   HAN2    0.09     !               |     |  /H1
ATOM H2   HAN2    0.09     !          H10-C7-H11 C1M-H2
ATOM H3   HAN2    0.09     !               |        \H3
ATOM H4   HAN2    0.09     !            H14-C8-H12
ATOM H5   HAN2    0.09     !               |
ATOM H6   HAN2    0.09     !               H13
ATOM H7   HAN2    0.09     !
ATOM H8   HAN2    0.09     !
ATOM H9   HAN2    0.09     !
                           !
!     isoprenic tail stub  !
                           !
ATOM C7   CTN2  -0.171     !
ATOM C8   CN2   -0.27      !
ATOM H10  HAN2   0.09      !
ATOM H11  HAN2   0.09      !
ATOM H12  HAN2   0.09      !
ATOM H13  HAN2   0.09      !
ATOM H14  HAN2   0.09      !


!      bonds for ubiquinone  ring
BOND C1 C2    C2 C3    C3 C4    C4 C5
BOND C5 C6    C6 C1
BOND C2 O2    C3 C3M   C4 O4    C5 O5
BOND O4 C4M   C4M H7   C4M H8   C4M H9
BOND C3M H4   C3M H5   C3M H6
BOND C1 C1M   C1M H1   C1M H2   C1M H3
!Isoprene tail stub
BOND C6 C7    C7 H10   C7 H11   C7 C8    C8 H12   C8 H13 C8 H14
AUTOGENERATE ANGLES DIHEDRALS

RESI Q0      0.00000 !2,3-Dimethoxy-5-dimethyl-1,4-benzoquinone

GROUP  ! ubiquinone ring

ATOM C1   CUQ3   -0.317    !
ATOM C2   CUQ1    0.586    !           H7\        /H4
ATOM O2   OUQ1   -0.456    !           H8-C4M  C3M-H5
ATOM C3   CUQ2    0.055    !           H9/ |    | \H6
ATOM O3   OUQ2   -0.336    !               O4   O3
ATOM C4   CUQ2    0.055    !               |____|
ATOM O4   OUQ2   -0.336    !              C4----C3
ATOM C5   CUQ1    0.586    !              /      \
ATOM O5   OUQ1   -0.456    !           __/        \__
ATOM C6   CUQ4    0.014    !         05--C5      C2--O2
ATOM C1M  CTN    -0.120    !            \         /
ATOM C3M  CTN    -0.045    !             \ ____ /
ATOM C4M  CTN    -0.045    !              C6----C1
```

```
ATOM H1   HAN     0.09     !               |     |  /H1
ATOM H2   HAN     0.09     !              H10   C1M-H2
ATOM H3   HAN     0.09     !                        \H3
ATOM H4   HAN     0.09     !
ATOM H5   HAN     0.09     !
ATOM H6   HAN     0.09     !
ATOM H7   HAN     0.09     !
ATOM H8   HAN     0.09     !
ATOM H9   HAN     0.09     !
!isoprene tail stub stub.
ATOM H10  HAN     0.085    !

!  bonds for ubiquinone  ring
BOND C1 C2    C2 C3    C3 C4    C4 C5
BOND C5 C6    C6 C1
BOND C2 O2    C3 O3    C4 O4    C5 O5
BOND O4 C4M   C4M H7   C4M H8   C4M H9
BOND O3 C3M   C3M H4   C3M H5   C3M H6
BOND C1 C1M   C1M H1   C1M H2   C1M H3
!Isoprene tail stub
BOND C6 H10
AUTOGENERATE ANGLES DIHEDRALS

RESI Q0M      0.00000 !2,3-Dimethoxy-5,6-dimethyl-1,4-benzoquinone

GROUP  ! ubiquinone ring

ATOM C1   CUQ3   -0.317    !
ATOM C2   CUQ1    0.586    !           H7\         /H4
ATOM O2   OUQ1   -0.456    !           H8-C4M  C3M-H5
ATOM C3   CUQ2    0.055    !           H9/ |    | \H6
ATOM O3   OUQ2   -0.336    !               O4   O3
ATOM C4   CUQ2    0.055    !               |____|
ATOM O4   OUQ2   -0.336    !              C4----C3
ATOM C5   CUQ1    0.586    !              /      \
ATOM O5   OUQ1   -0.456    !           __/        \__
ATOM C6   CUQ4    0.014    !         05--C5      C2--O2
ATOM C1M  CTN    -0.120    !             \         /
ATOM C3M  CTN    -0.045    !              \ ____ /
ATOM C4M  CTN    -0.045    !              C6----C1
ATOM H1   HAN     0.09     !               |     |  /H1
ATOM H2   HAN     0.09     !          H10-C7-H11 C1M-H2
ATOM H3   HAN     0.09     !               |        \H3
ATOM H4   HAN     0.09     !              H12
ATOM H5   HAN     0.09     !
ATOM H6   HAN     0.09     !
ATOM H7   HAN     0.09     !
ATOM H8   HAN     0.09     !
ATOM H9   HAN     0.09     !
                           !
!     isoprenic tail stub  !
                           !
ATOM C7   CTN   -0.265     ! -0.175 - 0.09
ATOM H10  HAN    0.09      !
ATOM H11  HAN    0.09      !
ATOM H12  HAN    0.09      !

!       bonds for ubiquinone  ring
BOND C1 C2    C2 C3    C3 C4    C4 C5
BOND C5 C6    C6 C1
BOND C2 O2    C3 O3    C4 O4    C5 O5
BOND O4 C4M   C4M H7   C4M H8   C4M H9
BOND O3 C3M   C3M H4   C3M H5   C3M H6
BOND C1 C1M   C1M H1   C1M H2   C1M H3
!Isoprene tail stub
BOND C6 C7    C7 H10   C7 H11   C7 H12
AUTOGENERATE ANGLES DIHEDRALS

RESI ISOP 0.0000 !Isoprene unit.
GROUP                !             H8
ATOM C1   CTL2 -0.18  !              \
ATOM H1   HAL2  0.09  !      H3       C5---H9
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```
ATOM H2   HAL2  0.09  !       \      /  \
GROUP                 !        C2==C3   H7
ATOM C2   CEL1 -0.15  !       /      \
ATOM H3   HEL1  0.15  !   H1-C1-H2    C4-H(4-6)
GROUP                 !
ATOM C3   CEL1  0.00 !Also try CG2D1 from cgenff. Basically the same.
GROUP
ATOM C4   CTL3 -0.27
ATOM H4   HAL3  0.09
ATOM H5   HAL3  0.09
ATOM H6   HAL3  0.09
GROUP
ATOM C5   CTL3 -0.27
ATOM H7   HAL3  0.09
ATOM H8   HAL3  0.09
ATOM H9   HAL3  0.09
BOND C1 C2 C2 C3 C3 C4 C3 C5
BOND C1 H1 C1 H2 C2 H3
BOND C4 H4 C4 H5 C4 H6
BOND C5 H7 C5 H8 C5 H9

!I don't like these impropers. However the parameters you guys have used for these rings
contains them. Odds are we can just supply zeros for the parameters we use, or comment these out.
!IMPR C2 H3 C1 C3
!IMPR C3 C2 C4 C5
AUTOGENERATE ANGLES DIHEDRALS

RESI  SMA     0.11   ! Stigmatellin

GROUP  !

! methoxy groups           !   H4\               /H9
ATOM  C5M  CG331  -0.0740  !   H6-C5M         C7M-H10
ATOM   H4  HGA3    0.0820  !   H5/  |          |  \H8
ATOM   H5  HGA3    0.0820  !        O5   H7    O7
ATOM   H6  HGA3    0.0820  !        |     |    |
ATOM  C7M  CG331  -0.0360  !        |     C6---C7
ATOM   H8  HGA3    0.0830  !        |    //      \\
ATOM   H9  HGA3    0.0830  !        -----C5      C8-O8-H44
ATOM  H10  HGA3    0.0830  !              \ ____ /
ATOM   O5  OG301  -0.1590  !              C4A----C8A
ATOM   O7  OG301  -0.2820  !              /       \
! top ring                 !        _____/         \
ATOM   C5  CG2R61  0.0940  !        04--C4          O1
ATOM   C6  CG2R61 -0.2580  !             \         /
ATOM   H7  HGR61   0.1740  !              \_____ /
ATOM   C7  CG2R61  0.0940  !              C3----C2
ATOM   C8  CG2R61  0.2220  !         H1\ /      |
ATOM   O8  OG311  -0.6230  !         H3-C3M H12-C9-H11
ATOM   H44 HGP1    0.4470  !         H2/        |
ATOM  C4A  CG2R61 -0.1090  !                 H14-C10-H13
ATOM  C8A  CG2R61  0.0420  !             H30\    |
! bottom ring              !             H31-C22-C11-H15
ATOM   O1  OG3R60 -0.08000 !             H29/    |         /H32
ATOM   C2  CG2D1O -0.0170  !                 H16-C12-O12-C23-H34
ATOM   C3  CG2R62  -0.0430 !                     |         \H33
!  methyl group            !                     |      /H36
ATOM  C3M  CG331  -0.1860  !                 H17-C13-C24-H37
ATOM  H1   HGA3    0.0750  !                     |      \H35
ATOM  H2   HGA3    0.0750  !          H38\       |
ATOM  H3   HGA3    0.0750  !         H40-C25-O14-C14-H18
                           !          H39/       |
ATOM   C4  CG2R63  0.4880  !                 H19-C15
ATOM   O4  OG2D4  -0.5420  !                      \\
!tail                  !                     C16-H21
ATOM   C9  CG321  -0.0860  !                     /
ATOM  H11  HGA2    0.0800  !                 H22-C17
ATOM  H12  HGA2    0.0800  !                     \\
ATOM  C10  CG321  -0.1030  !                     C18-H23
ATOM  H13   HGA2   0.0860  !                      |
ATOM  H14   HGA2   0.0860  !                     C19
ATOM  C11  CG311   0.0650  !                    //  \   /H41
```

```
ATOM  C12  CG311  -0.0390  !               H25-C20   C26-H43
ATOM  C13  CG311   0.0230  !                    |       \H42
ATOM  C14  CG311  -0.0200  !                   C21
ATOM  C15  CG2DC1 -0.2420  !                H26/|\H27
ATOM  C16  CG2DC1 -0.0960  !                   H28
ATOM  C17  CG2DC2 -0.0440
ATOM  C18  CG2DC2 -0.3240
ATOM  C19  CG2DC1  0.0820
ATOM  C20  CG2DC1 -0.0114
ATOM  C21  CG331  -0.2660
ATOM  C22  CG331  -0.5000
ATOM  C23  CG331   0.0540
ATOM  C24  CG331  -0.2330
ATOM  C25  CG331   0.0020
ATOM  C26  CG331  -0.0760
ATOM  O12  OG301  -0.3970
ATOM  O14  OG301  -0.3010
ATOM  H15   HGA1   0.0790
ATOM  H16   HGA1   0.1600
ATOM  H17   HGA1   0.0840
ATOM  H18   HGA1   0.1750
ATOM  H19   HGA4   0.1370
ATOM  H29   HGA3   0.1330
ATOM  H30   HGA3   0.1330
ATOM  H31   HGA3   0.1330
ATOM  H32   HGA3   0.0440
ATOM  H33   HGA3   0.0440
ATOM  H34   HGA3   0.0440
ATOM  H35   HGA3   0.0640
ATOM  H36   HGA3   0.0640
ATOM  H37   HGA3   0.0640
ATOM  H38   HGA3   0.0490
ATOM  H39   HGA3   0.0490
ATOM  H40   HGA3   0.0490
ATOM  H21   HGA4   0.1500
ATOM  H22   HGA4   0.1240
ATOM  H23   HGA4   0.1420
ATOM  H41   HGA3   0.0380
ATOM  H42   HGA3   0.0380
ATOM  H43   HGA3   0.0380
ATOM  H25   HGA4   0.1070
ATOM  H26   HGA3   0.0910
ATOM  H27   HGA3   0.0910
ATOM  H28   HGA3   0.0910

BOND C2  C3   C2  O1   C2 C9    C3  C4
BOND C3 C3M   C3M H1   C3M H2   C3M H3
BOND C4  C4A  C4 O4    C4A C8A  C4A C5
BOND C5  C6   C5 O5    C5M O5
BOND C5M H4   C5M H5   C5M H6   C6 C7
BOND C6  H7   C7  C8   C7 O7    C7M O7
BOND C7M H8   C7M H9   C7M H10  C8 O8
BOND C8 C8A   O8  H44  C8A O1
BOND C9 H11   C9  H12  C9 C10   C10 H13
BOND C10 H14  C10 C11
BOND C11 C22  C11 C12  C11 H15  C12 O12
BOND C12 C13  C12 H16  C13 C24  C13 C14
BOND C13 H17  C14 O14  C14 C15  C14 H18
BOND C15 C16  C15 H19  C16 C17  C16 H21
BOND C17 C18  C17 H22  C18 C19  C18 H23
BOND C19 C20  C19 C26  C20 C21  C20 H25
BOND C21 H26  C21 H27  C21 H28  C22 H29
BOND C22 H30  C22 H31  C23 O12  C23 H32
BOND C23 H33  C23 H34  C24 H35  C24 H36
BOND C24 H37  C25 O14  C25 H38  C25 H40
BOND C25 H39  C26 H41  C26 H43  C26 H42

AUTOGENERATE ANGLES DIHEDRALS
```

```
PRES UILK 0.0000 !Ubiquinone-isoprene link Ubiquinone(1), Isoprene (2)
DELETE ATOM 1C8
DELETE ATOM 1H12
DELETE ATOM 1H13
DELETE ATOM 1H14
DELETE ATOM 2C1
DELETE ATOM 2H1
DELETE ATOM 2H2
BOND 1C7 2C2
AUTO ANGL DIHE

PRES IILK 0.0000 !Isoprene-isoprene link
DELETE ATOM 1H9
ATOM 1C5 CTL2 -0.18
ATOM 1H7 HAL2  0.09
ATOM 1H8 HAL2  0.09
BOND 1C5 2C1
AUTO ANGL DIHE
```

Appendix C. Script for calculation of Diffusion for Membrane Lipids

```
# Membrance diffusion
# Author: Stuart Rose
# Date: 4/7/2017
#
#  Notes:  needs to be run in run file for configuration.  Need to load last
xscfile
#          in
#           Run proc MSDcalc after changing restart extened configuration
files *.xsc
#                 in Doft
#
#
# lipidnames: DVPC DVPE DVPG TOCL2 VSPC VSPE VSPG

proc ::MSDcalc {} {

      set A [atomselect top "segname MEMB"]
      set lipidnames [lsort -unique [$A get resname]]
      # set lipidnames "VSPG"
      foreach k $lipidnames {
            # Exclude interior lipids
            if {$k == "VSPG"} {
                  set seltext "resname VSPG and not resid 610 611"
                  set headtext "C1 C11 C12 C13 OC2 OC3 O11 O12 O13 O14 P"
            } else {
                  set seltext "resname $k"
            }
            if {$k == "DVPC"} {
                  set headtext "C1 C11 C12 C13 C14 N O11 O12 O13 O14 P"
            }
            if {$k == "DVPE"} {
                  set headtext "C1 C11 C12 N O11 O12 O13 O14 P"
            }
            if {$k == "DVPG"} {
                  set headtext "C1 C11 C12 C13 OC2 OC3 O11 O12 O13 O14 P1"
            }
            if {$k == "TOCL2"} {
                  set headtext "C1 C2 C3 C11 C31 OG12 OP11 OP12 OP13 OP31
OP32 OP34 P1 P3 "
            }
            if {$k == "VSPC" } {
                  set headtext "C1 C11 C12 C13 C14 N O11 O12 O13 O14 P"
            }
            if {$k == "VSPE" } {
                  set headtext "C1 C11 C12 N O11 O12 O13 O14 P"
            }
            set sel [atomselect top $seltext]
            set lipids [lsort -unique [$sel get residue]]

            Doft $k $headtext $headtext "prod_conf1_2_run_8" $lipids
            $sel delete
      # close bracket for "foreach k $lipidnames"
      }
```

```
#close bracket for proc ::MSDcalc
}


proc ::get_xy { xscfile } {
      set fd [open $xscfile r]
      gets $fd
      gets $fd
      gets $fd line
      puts "$line"
      set x_coord [lindex $line 1]
      set y_coord [lindex $line 5]
      close $fd
      return "$x_coord $y_coord"
}


proc ::Doft { name headtext1 headtext2 f_xsc_in lipids } {

      set nf [molinfo top get numframes]

      set N [llength $lipids]
      puts "there are $N lipids and lipids are: $lipids"

      set xy [get_xy ./$f_xsc_in.restart.xsc]

      set outfile1 [open ./output/Doft_$name w]
      set outfile2 [open ./output/Sum_$name w]
      puts $outfile1 "t $name:$N"
      puts $outfile2 "t $name:$N"

      foreach j $lipids {
            for {set k 1} {$k <= $nf} {incr k} {
                  set simdata1($k.r) "0"
            }
            set seltext1 "residue $j and name $headtext1"
            set seltext2 "residue $j and name $headtext2"

            # atom selection sel0 is the reference
            set sel0 [atomselect top "$seltext1"]
            $sel0 frame 0

            set lipidname [lsort -unique [$sel0 get resname]]
            set outfile [open ./output/${lipidname}_$j w]
            puts $outfile "t ${lipidname}_$j"

            set sel1 [atomselect top "$seltext1"]
            $sel1 frame 0

            set sel2 [atomselect top "$seltext2"]
            $sel2 frame 0

            set com0 [measure center $sel0 weight mass]
            set com1 $com0
            set com2 $com0

            set sum 0
            set adjx 0
```

```
            set adjy 0

            for {set i 1} {$i < 286} {incr i} {
                  $sel2 frame $i
                  set com2 [measure center $sel2 weight mass]

                  set jump [expr {[lindex $com2 0] - [lindex $com1 0]}]

                  if {[expr {$jump < -50}]} {set adjx [expr {$adjx == 0 ? 1 :
0}]}
                  if {[expr {$jump > 50}]} {set adjx [expr {$adjx == 0 ? -1 :
0}]}

                  set jump [expr [lindex $com2 1] - [lindex $com1 1]]

                  if { $jump < -100 }     {set adjy [expr {$adjy == 0 ? 1 :
0}]}
                  if { $jump > 100 } {
                        set adjy [expr {$adjy == 0 ? -1 : 0} ]
                  }

                  set com1 $com2
                  set com2 "[expr {[lindex $com2 0]+[expr {$adjx * [lindex
$xy 0]}] }] [expr {[lindex $com2 1]+[expr {$adjy * [lindex $xy 1]}] }]
[lindex $com2 2]"

                  if {$adjy == 1 } {puts "${lipidname}_$j: com1: $com1, com2:
$com2"}

                  # measure distance from start and accumulate for total dist
from start (dr)
                  set simdata($i.r) [expr { $i > 1 ? [expr {[veclength
[vecsub $com0 $com2]]}] : 0}]

                  set simdata1($i.r) [expr {$simdata1($i.r) + [expr
$simdata($i.r) * $simdata($i.r)]}]

                  set j [expr 2*$i]
            }

            # this is 1 fs timestep frames
            for {set i 286} {$i < $nf} {incr i} {
                  set j [expr 1 + $j]

                  $sel2 frame $i

                  set com2 [measure center $sel2 weight mass]

                  set jump [expr {[lindex $com2 0] - [lindex $com1 0]}]

                  if {[expr {$jump < -100}]}  {puts "second jump"}
                  if {[expr {$jump < -100}]}  {set adjx [expr {$adjx == 0 ? 1
: 0}]}
                  if { $jump > 100 } { set adjx [expr {$adjx == 0 ? -1 : 0}]}

                  set jump [expr {[lindex $com2 1] - [lindex $com1 1]}]
                  if { $jump < -100 } {set adjy [expr {$adjy == 0 ?  1 : 0}]}
                  if { $jump > 100 } {set adjy [expr {$adjy == 0 ? -1 : 0}]}
```

```
                  set com1 $com2
                  set com2 "[expr {[lindex $com2 0]+[expr {$adjx * [lindex
$xy 0]}] }] [expr {[lindex $com2 1]+[expr {$adjy * [lindex $xy 1]}] }]
[lindex $com2 2]"

                  # measure distance from start and accumulate for total dist
from start (dr)
                  set simdata($i.r) [expr { $i > 1 ? [expr {[veclength
[vecsub $com0 $com2]]}] : 0}]
                  puts $outfile "[expr $j] $simdata($i.r)"

                  set simdata1($i.r) [expr {$simdata1($i.r) + [expr
$simdata($i.r) * $simdata($i.r)]}]

            }
            close $outfile
      # close bracket for each of j $lipids
      }

      for {set i 1} {$i < 286} {incr i} {
            set j [expr 2*$i]
            set bottom [expr {$j * $N * 4}]
            puts $outfile2 "$i  $simdata1($i.r)"

            set simdata2($j.r) [expr {$simdata1($i.r)/($bottom)}]
            puts $outfile1 "$j  $simdata2($j.r)"
      }

      for {set i 286} {$i < $nf} {incr i} {

            set j  [expr 1 + $j]
            set bottom [expr {$j * $N * 4}]
            puts $outfile2 "$i  $simdata1($i.r)"
            set simdata2($j.r) [expr {$simdata1($i.r)/($bottom)}]
            puts $outfile1 "$j  $simdata2($j.r)"
      }

      close $outfile1
      close $outfile2

      $sel0 delete
      $sel1 delete
      $sel2 delete
}
```