BIOCHEMICALLY REALISTIC MD AND KINETIC MODELS OF THE *RHODOBACTER SPHAEROIDES* BC₁ COMPLEX

BY

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DISSERTATION

Submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Biophysics and Computational Biology in the Graduate College of the University of Illinois at Urbana-Champaign, 2017

Urbana, Illinois

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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)

Acknowledgements

- Prof. Antony Crofts and his Laboratory
- Prof. Taras Pogorelov
- Prof. Bob Gennis
- Prof. Martin Gruebele
- Dr. Josh Vermaas invaluable scripting help

This work used the Extreme Science and Engineering Discovery Environment

(XSEDE), which is supported by National Science Foundation grant number ACI-

1548562

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Chapter 1 Biochemistry of the *bc*₁ Complex₁ 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 $b_{\rm H}$ 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_0 -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 QH₂ to heme c_1 . It also seems likely that the Q^{*} intermediate formed in that reaction diffuses in the Q₀site 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(QH₂) 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_0 -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,

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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, $\Delta p = \Delta \psi - Z\Delta pH$, where Z = 2.303RT/F ≈ 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 *bc1 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_0 -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 Nphase. At the Q_0 -site, quinol is oxidized first by the Fe₂S₂ 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, at the Q_0 -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 $b_{\rm L}$, 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 QH₂, the Q₀-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 2QH₂, 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 Q₀-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 QH₂ oxidized:

 $QH_2 + 2cyt c^+ + 2H_N \rightleftharpoons Q + 2cyt c + 2H_P + 2H_P(scalar)$

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_0 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_{0x} and QH₂, is needed for formation of the enzyme substrate (*ES*-) complex. The ISP head group is docked to the Q_0 site against cyt *b* and seems to be held in place in part by hydrogen bonding to the Q_0 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_0 -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 Q₀-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 Q₀-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_0 -site is the catalytic site where the quinol is oxidized to form quinone. The Q_0 -site is located in cyt b and has a larger volume than one quinol head group. Accordingly, the regions within the Q_0 -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 QH₂ 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[•], 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 $b_{\rm L}$ occurs. However, the sequence of events is not known. Most of the evidence suggests that the proton from QH^{\cdot} is released early, and the semiguinone anion (Q^{\cdot}) moves, but scenarios in which the neutral semiguinone (QH) separates from the ISPH, and then moves to donate the electron to heme $b_{\rm L}$ 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 OH' leaves the O_0 -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_0 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 SQ₀ occupancy could be measured. The value estimated for *k* was ~10³ 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 × 10⁹ s⁻¹. Such a movement would require rapid diffusion in the Q₀-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^{*}.

The two cyt *b* hemes, cyt b_L (low $E_m \sim -90 \text{ mV}$) and cyt b_H (higher $E_m \sim 40 \text{ mV}$), are arranged along the path (the low potential chain) from the Q₀-site to the Q₁-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 Q₀-site and transferred to the Q₁-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 Q₁-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 Q₁-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 *bc*¹ Complex and Chromatophore Membrane

Previous MD simulations of the *bc*₁ 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 (Q₀H₂) in the Q₀-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 Fe₂S₂ are shown by Icorice bonds, the hemes are in CPK colors; QH₂ at the Q₀-site is yellow; Q at the Q_i-site is cyan; the Fe₂S₂ cluster is 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 Qi-site, which would significantly change the physical chemistry of the site. However, the focus in both the papers was the Q₀-site reaction, and since this is on the other side of the protein from the Qi-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 (CDmutant). 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 A². Lipid head groups occupy roughly 40 A² 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 Q₀-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 bc_1 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 2steroeyl-D-glycero-1-phosphatidylglycerol); DVPE divaccenoyl phosphatidylethanolamine (2,3divaccenoyl-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 (2,3divaccenyl-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.

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	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* grown under under photosynthetic conditions; (E) percentage of total of fatty acid for each type of lipid from *Rb sphaeroides* grown under conditions; (E) percentage of total of fatty acid 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 μ m²/s from Figure 3.2. One group has found a value of 190 to 290 μ m²/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.

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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 Q₀-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 Q₀-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/rad². 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/A² and stepping down to 0.5 10 kcal*mol⁻¹/A².

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/rad². **The units of 'bb' are kcal*mol⁻¹/A².


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 bc₁ complex as indicated by Table 4.3. Conf1 represents the fully oxidized state of the system with a substrate in the Q₀-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 QH₂, 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 Q	uinone 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 + i	nh(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	0	0		cyt c	0	0
	cyt b-				cyt b-		
	bL	0	0		bL	0	0
	cytb-bH	0	0		cytb-bH	0	0
	FES	0	0		FES	R	0
	Qo	QH2	QH2		Qo	UQS (neutral)	QH2
	Qi	Q /Ant	Q/Ant		Qi	Q	Q
	Glu295	0-	0-		Glu295	0-	0-

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

Chapter 5 Modified Q-cycle: ES complex Formation₂

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 QH₂ 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_0 -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_0 - 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 QH₂ -OH, from Y147 -OH to QH₂ -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 QH₂ are start separate (monomer 2) or start together (monomer 1), but over the first 130 frames (26 ns), the H-bond from QH₂ -OH to ISP_{ox} N_e 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 QH₂. 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_0 -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 (confl 3), a commonly used experimental situation since it allows ready measurement of turnover of the Q₀-site through reduction of heme $b_{\rm H}$. The measured rate of QH₂ oxidation (in the first turnover) when heme $b_{\rm H}$ 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[•] 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 EScomplex as involving E295 as a direct ligand to QH₂ has biased thinking towards an emphasis on a direct role in H⁺ release. If so, an alternative scenario would be that the product state OH[•].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 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_0 -site. Preference might depend on a simple

physical principle; the low probability (high energy cost) of solvating a charged species, favors mechanisms involving Q⁻ as the liberated form, rather than QH⁺, 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 Dynamics3

Molecular dynamics simulations of the bc₁ 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 Q₀-site is important to the proposed mechanism. The diffusional distance is 6-7 angstroms,

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_0 -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 Q₀-site (adapted from (*I-4*)). The structures show ISP with the fully extended tether (left) on binding at the Q₀-site (here with stigmatellin) and with the fully relaxed tether (right) when no bond is formed with a Q₀-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



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

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 QH₂ 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.

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_0 -site.



Frame 1

Frame 486

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 QH2 measured by the distance between QH2 -O and ISP H152 Nε.

Relative distances or separation distances between His152: NE (the epsilon nitrogen) and QH₂ (right) allows visualization of the diffusion of the QH₂ out of the Q₀-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 QH₂ 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 Q₀-site mechanism, where the SQ₀ 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 SQ₀ moves through ~5.5 Å, 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_0 -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_0 -site entry way shows an abrupt quick change and then gradual steps in and out of the entry way until the head group of UQH₂ is situated well outside the Q_0 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 c1 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.

Distances for ISP hinge region extension



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 <<<<<<
* 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
1
      2. RESI CDL
                    -2.00 ! (Not finished)
1
      3. RESI DVPG -1.00 ! 2,3-divacenyl-D-glycero-1-phosphatidylglycerol
L
     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
1
             ! Vaccenyl - CH
                   (-)
1
             (+)
             CH2 - PO4 - CH2 - CH2 - N-(CH3)3!
1
!!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
!!
                  0.00 ! 3-palmitoyl-2-oleoyl-D-glycero-1-Phosphatidylcholine
!!RESI POPC
!!
  Palmitoyl - CH2
!!
!!
     Oleyol - CH
!!
11
              (-)
                                   (+)
11
              CH2 - PO4 - CH2 - CH2 - N-(CH3)3
!!
!! Polar Head and glycerol backbone
!!
GROUP
                    !
                                   H15B
ATOM N NTL -0.60 !
                                    H15A-C15-H15C
ATOM C12 CTL2 -0.10 !
ATOM H12A HL 0.25 !
                                    |
ATOM H12B HL
               0.25 ! H13B
                                         H14A
               -0.35 !
ATOM C13 CTL5
                              0.25 ! H13A-C13----N----C14-H14B
0.25 ! | | |
0.25 ! H13C | H14C
ATOM H13A HL
                                                      (+)
ATOM H13B HL
ATOM H13C HL
ATOM C14 CTL5 -0.35 !
ATOM H14A HL 0.25 !
ATOM H14B HL 0.25 !
                                      | alpha6
```

АТОМ	H14C	HL	0.25 !	
АТОМ	C15	CTL5	-0.35 !	
АТОМ	H15A	HL	0.25 !	H12AC12H12B
АТОМ	Н15В	HL	0.25 !	
АТОМ	H15C	HL	0.25 !	
GROUI	2		!	alpha5
АТОМ	C11	CTL2	-0.08 !	
АТОМ	H11A	HAL2	0.09 !	H11AC11H11B
АТОМ	Н11В	HAL2	0.09 !	alpha4
АТОМ	Р	PL	1.50 !	(-) 013 012
АТОМ	013	02L	-0.78 !	\/ alpha3
АТОМ	014	02L	-0.78 !	P (+)
АТОМ	012	OSLP	-0.57 !	/ \ alpha2
ATOM	011	OSLP	-0.57 !	(-) 014 011
ATOM	C1	CTL2	-0.08 !	alpha1
ATOM	HA	HAL2	0.09 !	нас1нв
ATOM	HB	HAL2	0.09 !	theta1
GROUI	2		!	
ATOM	C2	CTL1	0.17 !	HSC2
ATOM	HS	HAL1	0.09 !	beta1
ATOM	021	OSL	-0.49 !	022 021 theta3
ATOM	C21	CL	0.90 !	\\/ beta2
ATOM	022	OBL	-0.63 !	C21
ATOM	C22	CTL2	-0.22 !	beta3
ATOM	H2R	HAL2	0.09 !	H2RC22H2S
ATOM	H2S	HAL2	0.09 !	
GROUI	2		!	beta4
ATOM	C3	CTL2	0.08 !	
ATOM	ΗX	HAL2	0.09 !	НХСЗНҮ
ATOM	ΗY	HAL2	0.09 !	gamma1
ATOM	031	OSL	-0.49 !	032 031
ATOM	C31	CL	0.90 !	\\ / gamma2
ATOM	032	OBL	-0.63 !	C31
ATOM	C32	CTL2	-0.22 !	gamma3
ATOM	H2X	HAL2	0.09 !	Н2ХС32Н2Ү
АТОМ	H2Y	HAL2	0.09 !	
GROUI	2		!	gamma4
ATOM	C23	CTL2	-0.18 !	
ATOM	H3R	HAL2	0.09 !	H3RC23H3S
ATOM	H3S	HAL2	0.09 !	
GROUI	2		!	
АТОМ	C24	CTL2	-0.18 !	
ATOM	H4R	HAL2	0.09 !	H4RC24H4S
ATOM	H4S	HAL2	0.09 !	
GROUI		0.000	!	
ATOM	C25	CTLZ	-0.18 !	
ATOM	H5R UF Q	HALZ	0.09 !	H5RC25H5S
ATOM	нэр	HALZ	0.09 !	
GROUI			0 10 1	
ATOM	CZ6	CTLZ	-0.18 !	
	HOR	TALZ	0.09 !	HORC20HOS
CROTH	поз	TALZ	0.09 :	
ALOON MULTE	- C27	CTT 2	-0 1 2 1	
ATOM	U7D		-0.10 :	и7РU7S
	н7с	HAL2	0.09 !	
GROTI		ے لید عد ہ	0.09 !	
	- C28	CTT.2	-0 1 2 1	
ATOM	H8R	HAT.2	0 09 1	наяс2яная I
ATOM	H8S	HAL2	0.09 1	
GROUI	2			
ATOM	C29	CTL2	-0.18 '	
ATOM	H9R	HAL2	0.09 !	н9RС29Н9S I
ATOM	H9S	HAL2	0.09 !	

GROUE	>		!	
ATOM	C210	CTL2	-0.18 !	
ATOM	H10R	HAL2	0.09 !	H10RC210H10S
ATOM	H10S	HAL2	0.09 !	
GROUE	2011	007.1	0 1 5 1	
ATOM	CZII	CELI	-0.15 !	
ATOM CDOUL	HIIK	HELI	0.15 !	HIIR = -CZII
GROUE		OPT 1	0 15 1	
ATOM	ULL 2D	UET 1	-0.15 !	
GROUE	DIZK	пстт	0.13 :	
ATOM	C213	CTL2	-0.18	
ATOM	H13R	HAL2	0.09 !	H13RC213H13S
ATOM	H13S	HAL2	0.09 !	
GROUE	>		!	
ATOM	C214	CTL2	-0.18 !	i i
ATOM	H14R	HAL2	0.09 !	H14RC214H14S
ATOM	H14S	HAL2	0.09 !	
GROUE	2		!	
ATOM	C215	CTL2	-0.18 !	
ATOM	H15R	HAL2	0.09 !	H15RC215H15S
ATOM	H15S	HAL2	0.09 !	
GROUE	þ		!	
ATOM	C216	CTL2	-0.18 !	
ATOM	H16R	HAL2	0.09 !	H16RC216H16S
ATOM	H16S	HAL2	0.09 !	
GROUE	2		!	
ATOM	C217	CTL2	-0.18 !	
ATOM	H17R	HAL2	0.09 !	H17RC217H17S
ATOM	H17S	HAL2	0.09 !	
GROUE	2		!	
ATOM	C218	CTL3	-0.27 !	
ATOM	H18R	HAL3	0.09 !	H18RC218H18S
ATOM	H18S	HAL3	0.09 !	
ATOM	H18T	HAL3	0.09 !	H18T
GROUE	2		!	
ATOM	C33	CTL2	-0.18 !	
A'I'OM	HJX	HAL2	0.09 !	НЗХСЗЗНЗҮ
ATOM CDOUL	НЗХ	HALZ	0.09 !	
GROUE	C24	C TT 2	0 10 1	
ATOM	U/V	UNT 2	-0.10 !	члуСЗЛЧЛУ
ATOM	п4л u/v	UNI 2	0.09 :	п4хс54п41
CROTIE	1141	IIALLZ	0.09 :	
ATOM	C35	CTT.2	-0 18 1	
ATOM	СЭЭ Н5Х	НДТ.2	0.10 1	
ATOM	H5Y	HAT.2	0.09 !	
GROUE	,		!	
ATOM	C36	CTL2	-0.18 !	
ATOM	H6X	HAL2	0.09 !	нбхс36нбу
ATOM	НбҮ	HAL2	0.09 !	
GROUE	2		!	
ATOM	C37	CTL2	-0.18 !	
ATOM	H7X	HAL2	0.09 !	Н7ХС37Н7Ү
ATOM	H7Y	HAL2	0.09 !	
GROUE	þ		!	l I
ATOM	C38	CTL2	-0.18 !	
ATOM	H8X	HAL2	0.09 !	Н8ХС38Н8Ү
ATOM	H8Y	HAL2	0.09 !	
GROUE	2		!	l I
ATOM	C39	CTL2	-0.18 !	l I
ATOM	Н9Х	HAL2	0.09 !	Н9ХСЗ9Н9Ү
ATOM	Н9Ү	HAL2	0.09 !	
GROUE	2		!	

ATOM	C310	CTL2	-0.2	18 !					
ATOM	H10X	HAL2	0.0	09!				H10X	-С310Н10Ү
ATOM	H10Y	HAL2	0.0	09!					
GROUF	>			!					
ATOM	C311	CEL1	-0.1	15 !					
ATOM	H11X	HEL1	0.	15 !				H11X	-C311
GROUE	>			1					
АТОМ	C312	CEL1	-0.	15 !					
ATOM	H12X	HEL1	0	 15 I				н12х	-0312
GROUE	>		•••	±0 . I				11 ± 2 /1	1
ATOM	C313	CTTT 2	_0	10. I					
ATOM	U12V		0.					u12v	-0212-u12V
ATOM		TALZ	0.0					птэх	-сэтэ-нтэт
ATOM	нтэт	HALZ	0.0	09 !					
GROUP	~ ~ 1 4	0.000	0	!					
ATOM	C314	CTL2	-0.	18 !					
ATOM	H14X	HAL2	0.0	09!				H14X	-C314H14Y
ATOM	H14Y	HAL2	0.0	09!					
GROUF	2			!					
ATOM	C315	CTL2	-0.1	18 !					
ATOM	H15X	HAL2	0.0	09!				H15X	-С315Н15Ү
ATOM	H15Y	HAL2	0.0	09!					
GROUE	>			!					
АТОМ	C316	CTL2	-0.	18 1					
ATOM	H16X	HAT.2	0 1	19 I				н16Х	-С316Н16У
ATOM	u16V	UNT 2	0.1	09. Ng 1				111 073	1
CROTT		IIAUZ	0.0	1					
GROUP	0217		0	101					
ATOM	C317	CTLZ	-0.	18 !					
ATOM	HI/X	HALZ	0.0	09!				HI/X	-C31/H1/Y
ATOM	H17Y	HAL2	0.0	09!					
GROUF	2			!					
ATOM	C318	CTL3	-0.2	27 !					
ATOM	H18X	hal3	0.0	09 !				H18X	-C318H18Y
ATOM	H18Y	HAL3	0.0	09!					
АТОМ АТОМ	H18Y H18Z	HAL3 HAL3	0.0	09 ! 09 !					 H18Z
ATOM ATOM	H18Y H18Z	HAL3 HAL3	0.0	09 ! 09 !					 H18Z
ATOM ATOM ! Pol	H18Y H18Z ar He	HAL3 HAL3 ad	0.0	09 ! 09 !					 H18Z
ATOM ATOM ! Pol BOND	H18Y H18Z .ar He N	HAL3 HAL3 ead C13	0.0	09 ! 09 ! N	C14	N	C15		 H18Z
ATOM ATOM ! Pol BOND BOND	H18Y H18Z ar He N C13	HAL3 HAL3 ead C13 H13A	0.0	09! 09! N C13	C14 H13B	N C13	C15 H13C		 H18Z
ATOM ATOM ! Pol BOND BOND BOND	H18Y H18Z .ar He N C13 C14	HAL3 HAL3 ead C13 H13A H14A	0.0	09 ! 09 ! N C13 C14	C14 H13B H14B	N C13 C14	C15 H13C H14C		 H18Z
ATOM ATOM ! Pol BOND BOND BOND	H18Y H18Z .ar He N C13 C14 C15	HAL3 HAL3 ead C13 H13A H14A H15A	0.0	09 ! 09 ! N C13 C14 C15	C14 H13B H14B H15B	N C13 C14 C15	C15 H13C H14C H15C		 H18Z
ATOM ATOM ! Pol BOND BOND BOND BOND	H18Y H18Z ar He N C13 C14 C15 N	HAL3 HAL3 ead C13 H13A H14A H15A C12	0.0	09 ! 09 ! C13 C14 C15	C14 H13B H14B H15B	N C13 C14 C15	C15 H13C H14C H15C		 H18Z
ATOM ATOM ! Pol BOND BOND BOND BOND BOND	H18Y H18Z .ar He N C13 C14 C15 N C12	HAL3 HAL3 ead C13 H13A H14A H15A C12 H127	0.0	09 ! 09 ! N C13 C14 C15	C14 H13B H14B H15B	N C13 C14 C15	C15 H13C H14C H15C		 H18Z
ATOM ATOM ! Pol BOND BOND BOND BOND BOND	H18Y H18Z .ar He N C13 C14 C15 N C12	HAL3 HAL3 c13 H13A H14A H15A C12 H12A	0.0	09 ! 09 ! N C13 C14 C15 C12	C14 H13B H14B H15B H12B	N C13 C14 C15 C12	C15 H13C H14C H15C C11	01	 H18Z
ATOM ATOM ! Pol BOND BOND BOND BOND BOND BOND	H18Y H18Z ar He N C13 C14 C15 N C12 C11	HAL3 HAL3 c13 H13A H14A H15A C12 H12A H11A	0.0	N C13 C14 C15 C12 C11	C14 H13B H14B H15B H12B H11B	N C13 C14 C15 C12 C11	C15 H13C H14C H15C C11 012	01	 H18Z
ATOM ATOM ! Pol BOND BOND BOND BOND BOND BOND BOND	H18Y H18Z ar He C13 C14 C15 N C12 C11 O12	HAL3 HAL3 c13 H13A H14A H15A C12 H12A H11A P	0.0	N C13 C14 C15 C12 C11 P	C14 H13B H14B H15B H12B H11B O11	N C13 C14 C15 C12 C11 P	C15 H13C H14C H15C C11 O12 O13	O1 P	 H18Z 1 C1 014
ATOM ATOM ! Pol BOND BOND BOND BOND BOND BOND BOND BOND	H18Y H18Z ar He N C13 C14 C15 N C12 C11 O12 Vcerol	HAL3 HAL3 C13 H13A H14A H15A C12 H12A H11A P Backb	0.0 0.0	N C13 C14 C15 C12 C11 P	C14 H13B H14B H15B H12B H11B O11	N C13 C14 C15 C12 C11 P	C15 H13C H14C H15C C11 O12 O13	01 P	 H18Z 1 C1 014
ATOM ATOM ! Pol BOND BOND BOND BOND BOND BOND BOND ! Gly BOND	H18Y H18Z .ar He N C13 C14 C15 N C12 C11 012 Vcerol C1	HAL3 HAL3 C13 H13A H14A H15A C12 H12A H11A P Backb HA	0.0 0.0	N C13 C14 C15 C12 C11 P C1	C14 H13B H14B H15B H12B H11B O11 HB	N C13 C14 C15 C12 C11 P C1	C15 H13C H14C H15C C11 012 013 C2	O1 P	 H18Z 1 C1 014
ATOM ATOM ! Pol BOND BOND BOND BOND BOND BOND BOND ! Gly BOND BOND	H18Y H18Z .ar He N C13 C14 C15 N C12 C11 O12 Vcerol C1 C2	HAL3 HAL3 ead C13 H13A H14A H15A C12 H12A H11A P Backb HA HS	0.0 0.0	09 ! 09 ! N C13 C14 C15 C12 C11 P C1 C2	C14 H13B H14B H15B H12B H11B O11 HB C3	N C13 C14 C15 C12 C11 P C1 C2	C15 H13C H14C H15C C11 012 013 C2 021	O1 P	 H18Z 1 C1 014
ATOM ATOM ! Pol BOND BOND BOND BOND BOND BOND BOND BOND	H18Y H18Z .ar He N C13 C14 C15 N C12 C11 O12 Vcerol C1 C2 C3	HAL3 HAL3 ead C13 H13A H14A H15A C12 H12A H11A P Backb HA HS HX	0.0 0.0	N C13 C14 C15 C12 C11 P C1 C2 C3	C14 H13B H14B H15B H12B H11B O11 HB C3 HY	N C13 C14 C15 C12 C11 P C1 C2 C3	C15 H13C H14C H15C C11 012 013 C2 021 031	O1 P	 H18Z 1 C1 014
ATOM ATOM ! Pol BOND BOND BOND BOND BOND BOND BOND BOND	H18Y H18Z ar He N C13 C14 C15 N C12 C11 O12 Vcerol C1 C2 C3 ain fr	HAL3 HAL3 ead C13 H13A H14A H15A C12 H12A H11A P Backb HA HS HX rom C2	0.0 0.0	N C13 C14 C15 C12 C11 P C1 C2 C3	C14 H13B H14B H15B H12B H11B O11 HB C3 HY	N C13 C14 C15 C12 C11 P C1 C2 C3	C15 H13C H14C H15C C11 012 013 C2 021 031	01 P	 H18Z 1 C1 014
ATOM ATOM ! Pol BOND BOND BOND BOND BOND BOND BOND BOND	H18Y H18Z .ar He N C13 C14 C15 N C12 C11 O12 Vcerol C1 C2 C3 ain fr O21	HAL3 HAL3 ead C13 H13A H14A H15A C12 H12A H11A P Backb HA HS HX rom C2 C21	0.0 0.0	N C13 C14 C15 C12 C11 P C1 C2 C3	C14 H13B H14B H15B H12B H11B O11 HB C3 HY	N C13 C14 C15 C12 C11 P C1 C2 C3	C15 H13C H14C H15C C11 O12 O13 C2 O21 O31	01 P	 H18Z 1 C1 014
ATOM ATOM ! Pol BOND BOND BOND BOND BOND BOND BOND BOND	H18Y H18Z .ar He N C13 C14 C15 N C12 C11 O12 VCerol C1 C2 C3 ain fr O21 C21	HAL3 HAL3 ead C13 H13A H14A H15A C12 H12A H11A P Backb HA HS HX com C2 C21 C22	0.0 0.0	N C13 C14 C15 C12 C11 P C1 C2 C3	C14 H13B H14B H15B H12B H11B O11 HB C3 HY	N C13 C14 C15 C12 C11 P C1 C2 C3	C15 H13C H14C H15C C11 012 013 C2 021 031	01 P	 H18Z 1 C1 014
ATOM ATOM ! Pol BOND BOND BOND BOND BOND BOND BOND BOND	H18Y H18Z Ar He N C13 C14 C15 N C12 C11 O12 Vcerol C1 C2 C3 Ain fr O21 C21 LE C2	HAL3 HAL3 ead C13 H13A H14A H15A C12 H12A H11A P Backb HA HS HX com C2 C21 C22 1 022	0.0 0.0	N C13 C14 C15 C12 C11 P C1 C2 C3	C14 H13B H14B H15B H12B H11B O11 HB C3 HY	N C13 C14 C15 C12 C11 P C1 C2 C3	C15 H13C H14C H15C C11 012 013 C2 021 031	01 P	 H18Z 1 C1 014
ATOM ATOM ! Pol BOND BOND BOND BOND BOND BOND BOND BOND	H18Y H18Z ar He N C13 C14 C15 N C12 C11 O12 VCerol C1 C2 C3 ain fr O21 C21 LE C2 C22	HAL3 HAL3 ead C13 H13A H14A H15A C12 H12A H11A P Backb HA HS HX COM C2 C21 C22 1 022 H2R	0.0 0.0	09 ! 09 ! N C13 C14 C15 C12 C11 P C1 C2 C3	C14 H13B H14B H15B H12B H11B O11 HB C3 HY H2S	N C13 C14 C15 C12 C11 P C1 C2 C3	C15 H13C H14C H15C C11 012 013 C2 021 031	01 P	 H18Z 1 C1 014
ATOM ATOM ! Pol BOND BOND BOND BOND BOND BOND BOND BOND	H18Y H18Z .ar He N C13 C14 C15 N C12 C11 O12 VCerol C1 C2 C3 ain fr O21 C21 LE C22 C23	HAL3 HAL3 ead C13 H13A H14A H15A C12 H12A H11A P Backb HA HS HX COM C2 C21 C22 C21 C22 C21 C22 H2R H3R	0.0 0.0	09 ! 09 ! N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C23	C14 H13B H14B H15B H12B H11B O11 HB C3 HY H2S H3S	N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C23	C15 H13C H14C H15C C11 012 013 C2 021 031 C23 C23 C24	01 P	 H18Z 1 C1 014
ATOM ATOM ! Pol BOND BOND BOND BOND BOND BOND BOND BOND	H18Y H18Z .ar He N C13 C14 C15 N C12 C11 O12 VCerol C1 C2 C3 ain fr O21 C21 LE C22 C23 C24	HAL3 HAL3 ead C13 H13A H14A H15A C12 H12A H11A P Backb HA HS HX COM C2 C21 C22 C21 C22 C21 C22 C21 C22 H2R H3R H4R	0.0 0.0	09 ! 09 ! N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C23 C24	C14 H13B H14B H15B H12B H11B O11 HB C3 HY H2S H3S H4S	N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C23 C24	C15 H13C H14C H15C C11 012 013 C2 021 031 C23 C24 C25	O1 P	 H18Z 1 C1 014
ATOM ATOM ! Pol BOND BOND BOND BOND BOND BOND BOND BOND	H18Y H18Z ar He N C13 C14 C15 N C12 C11 O12 VCerol C1 C2 C3 ain fr O21 C21 C21 C22 C23 C24 C25	HAL3 HAL3 ead C13 H13A H14A H15A C12 H12A H11A P Backb HA HS HX COM C2 C21 C22 C21 C22 C21 C22 C21 C22 C21 C22 H3R H4R H5R	0.0 0.0	09 ! 09 ! N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C23 C24 C25	C14 H13B H14B H15B H12B H11B O11 HB C3 HY H2S H3S H4S H5S	N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C23 C24 C25	C15 H13C H14C H15C C11 012 013 C2 021 031 C2 021 031 C23 C24 C25 C26	O1 P	 H18Z 1 C1 014
ATOM ATOM ! Pol BOND BOND BOND BOND BOND BOND BOND BOND	H18Y H18Z Ar He N C13 C14 C15 N C12 C11 O12 Vcerol C1 C2 C3 C1 C2 C3 C1 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2	HAL3 HAL3 ead C13 H13A H14A H15A C12 H12A H11A P Backb HA HS HX C21 C22 C21 C22 C21 C22 C21 C22 H2R H3R H4R H5R H6R	0.0 0.0	09 ! 09 ! N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C23 C24 C25 C26	C14 H13B H14B H15B H12B H11B O11 HB C3 HY H2S H3S H4S H5S H6S	N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C23 C24 C25 C26	C15 H13C H14C H15C C11 012 013 C2 021 031 C23 C24 C25 C26 C27	01 P	 H18Z 1 C1 014
ATOM ATOM I Pol BOND BOND BOND BOND BOND BOND BOND BOND	H18Y H18Z N C13 C14 C15 N C12 C11 O12 Vcerol C1 C2 C3 C1 C2 C3 C21 C2 C22 C23 C24 C25 C25 C27	HAL3 HAL3 ead C13 H13A H14A H15A C12 H12A H11A P Backb HA HS HX C21 C22 C21 C22 C21 C22 C21 C22 C21 C22 C21 C22 C21 C22 H2R H3R H4R H5R H5R H5R H5R H5R H5R H5R H5R H5R H5	0.0 0.0	09 ! 09 ! N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C23 C24 C25 C26 C27	C14 H13B H14B H15B H12B H11B O11 HB C3 HY H2S H3S H4S H5S H6S H7S	N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C23 C24 C25 C26 C27	C15 H13C H14C H15C C11 012 013 C2 021 031 C2 021 031 C23 C24 C25 C26 C27 C28	01 P	 H18Z 1 C1 014
ATOM ATOM ATOM Poll BOND BOND BOND BOND BOND BOND BOND BOND	H18Y H18Z Ar He N C13 C14 C15 N C12 C11 O12 C2 C3 C1 C2 C3 C21 C2 C22 C23 C24 C25 C26 C26 C27 C20	HAL3 HAL3 HAL3 ead C13 H13A H14A H15A C12 H12A H11A P Backb HA HS HX C21 C22 C21 C22 C21 C22 C21 C22 C21 C22 C21 C22 C21 C22 H2R H3R H4R H5R H6R H7R H5R H6R H7R	one	09 ! 09 ! N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C23 C24 C25 C26 C27 C22	C14 H13B H14B H15B H12B H11B O11 HB C3 HY H2S H3S H4S H5S H6S H7S	N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C23 C24 C25 C26 C27 C22	C15 H13C H14C H15C C11 012 013 C2 021 031 C2 021 031 C23 C24 C25 C26 C27 C28 C29	01 P	 H18Z 1 C1 014
ATOM ATOM ATOM Poll BOND BOND BOND BOND BOND BOND BOND BOND	H18Y H18Z Ar He N C13 C14 C15 N C12 C11 O12 VCCCOI C1 C2 C3 Fin fr O21 C21 C2 C23 C24 C25 C26 C27 C26 C27 C26 C27 C26 C27	HAL3 HAL3 HAL3 ead C13 H13A H14A H15A C12 H12A H11A P Backb HA HS HX C22 C21 C22 C21 C22 C21 C22 C21 C22 C21 C22 C21 C22 H2R H3R H4R H5R H6R H7R H8R H7R H8R	one	09 ! 09 ! N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C23 C24 C25 C26 C27 C28	C14 H13B H14B H15B H12B H11B O11 HB C3 HY H2S H3S H4S H4S H5S H6S H7S H8S	N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C3 C24 C25 C26 C27 C28 C22	C15 H13C H14C H15C C11 012 013 C2 021 031 C2 021 031 C23 C24 C25 C26 C27 C28 C29 C210	O1 P	 H18Z 1 C1 014
ATOM ATOM ATOM SOND BOND BOND BOND BOND BOND BOND BOND B	H18Y H18Z Ar He N C13 C14 C15 N C12 C11 O12 C2 C3 Fin fr O21 C2 C2 C23 C24 C25 C26 C27 C28 C29 C29 C20 C27	HAL3 HAL3 HAL3 ead C13 H13A H14A H15A C12 H12A H11A P Backb HA HS HX C0m C2 C21 C22 C21 C22 C21 C22 C21 C22 C21 C22 C21 C22 C21 C22 C21 C22 H2R H3R H4R H5R H6R H7R H8R H9R H9R	one	09 ! 09 ! N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C23 C24 C25 C26 C27 C28 C29 C21 C29 C21 C29 C21 C29 C21 C29 C21 C29 C21 C29 C29 C29 C29 C29 C29 C29 C29 C29 C29	C14 H13B H14B H15B H12B H11B O11 HB C3 HY H2S H3S H4S H5S H6S H7S H8S H9S	N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C23 C24 C25 C26 C27 C28 C29 C21C	C15 H13C H14C H15C C11 012 013 C2 021 031 C2 021 031 C23 C24 C25 C26 C27 C28 C29 C210	O1 P	 H18Z 1 C1 014
ATOM ATOM ATOM SOND BOND BOND BOND BOND BOND BOND BOND B	H18Y H18Z Ar He N C13 C14 C15 N C12 C11 O12 C2 C3 C11 C2 C3 C11 C2 C2 C3 C11 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2	HAL3 HAL3 HAL3 ead C13 H13A H14A H15A C12 H12A H11A P Backb HA HS HX COM C2 C21 C22 C21 C22 C21 C22 C21 C22 C21 C22 C21 C22 C21 C22 H2R H3R H4R H5R H6R H7R H9R H9R	one	09 ! 09 ! N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C23 C24 C25 C26 C27 C28 C29 C210	C14 H13B H14B H15B H12B H11B O11 HB C3 HY H2S H3S H4S H4S H5S H6S H7S H8S H9S H10S	N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C3 C24 C25 C26 C27 C28 C29 C210	C15 H13C H14C H15C C11 012 013 C2 021 031 C2 021 031 C2 021 031 C2 C23 C24 C25 C26 C27 C28 C29 C210 C211	O1 P	 H18Z 1 C1 014
ATOM ATOM ATOM Poll BOND BOND BOND BOND BOND BOND BOND BOND	H18Y H18Z ar He N C13 C14 C15 N C12 C11 O12 C2 C3 C11 C2 C3 C11 C2 C2 C3 C11 C2 C2 C3 C12 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2	HAL3 HAL3 HAL3 ead C13 H13A H14A H15A C12 H12A H11A P Backb HA HS HX C0m C2 C21 C22 C21 C22 C21 C22 C21 C22 H2R H3R H4R H5R H6R H7R H9R H10R H11R	0.0 0.0	09 ! 09 ! N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C23 C24 C25 C26 C27 C28 C29 C210	C14 H13B H14B H15B H12B H11B O11 HB C3 HY H2S H3S H4S H5S H4S H5S H6S H7S H8S H9S H10S	N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C3 C24 C25 C26 C27 C28 C29 C210	C15 H13C H14C H15C C11 012 013 C2 021 031 C2 021 031 C2 021 031 C2 C23 C24 C25 C26 C27 C28 C29 C210 C211	O1 P	 H18Z 1 C1 014
ATOM ATOM ATOM SOND BOND BOND BOND BOND BOND BOND BOND B	H18Y H18Z Ar He N C13 C14 C15 N C12 C11 O12 C2 C3 C11 C2 C3 C1 C2 C3 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2	HAL3 HAL3 HAL3 ead C13 H13A H14A H15A C12 H12A H11A P Backb HA HS HX COM C2 C21 C22 C21 C22 C21 C22 C21 C22 C21 C22 C21 C22 C21 C22 H2R H3R H4R H5R H6R H7R H9R H10R H11R C12 H12A H11A C12 H12A H11A H14A H15A C12 H12A H11A H15A C12 H12A H11A H15A C12 H12A H11A H15A C12 H12A H11A H15A C12 H12A H11A H15A C12 H12A H11A P C2C C21 C22 C21 C22 C21 C22 C21 C22 H2C H2C H2C H2C H2C H2C H2C H2C H2C	0.0 0.0	09 ! 09 ! N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C23 C24 C25 C26 C27 C28 C29 C210	C14 H13B H14B H15B H12B H11B O11 HB C3 HY H2S H3S H4S H5S H4S H5S H6S H7S H8S H9S H10S	N C13 C14 C15 C12 C11 P C1 C2 C3 C22 C3 C24 C25 C26 C27 C28 C29 C210	C15 H13C H14C H15C C11 012 013 C2 021 031 C2 021 031 C2 021 031 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2	O1 P	 H18Z 1 C1 014

BOND C31 C32 BONN C32 E3X C32 C32 C33 BONN C32 E3X C33 E3Y C33 C34 BONN C34 H4X C34 H4Y C34 C35 BONN C34 H4X C34 H4Y C34 C35 BONN C34 H4X C34 H4Y C34 C35 BONN C30 H5Y C35 C35 B35 C36 BONN C30 H5Y C37 C38 B35 B35 BONN C31 H1X C31 H14Y C31 C31 B37 BOND C313 H13X C313 C315 C31 B37 C31	BOND C212 BOND C214 BOND C215 BOND C216 BOND C217 BOND C217 ! Chain Fr BOND C311 BOND C311	3 H13R 4 H14R 5 H15R 6 H16R 7 H17R 8 H18R rom C3 C31	C2 C2 C2 C2 C2 C2 C2 C2	13 H13S 14 H14S 15 H15S 16 H16S 17 H17S 18 H18S	C213 C214 C215 C216 C217 C218	C214 C215 C216 C217 C218 H18T					
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 C314 H14X C314 H14Y C314 C315 BOND C316 H16X C316 H16Y C316 C317 BOND C317 H17X C317 H17Y C317 C318 BOND C318 H18X C318 H18Y C318 H18Z IMFR 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 C14 1.4955 110.60 122.73 109.67 1.4976 IC C13 C12 *N C14 1.4955 110.60 57.52 116.83 1.5412 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 H13A 1.4976 110.99 179.50 109.35 1.0869 IC H13A N *C13 H13A 1.4976 110.99 179.50 109.35 1.0869 IC H13A N *C13 H13A 1.4976 110.99 179.50 109.35 1.0869 IC H13A N *C13 H13A 1.4976 110.99 179.50 109.35 1.0869 IC H13A N *C13 H13A 1.4976 110.99 179.50 109.35 1.0869 IC H14A N *C14 H14A 1.4955 110.99 -179.22 109.65 1.0877 IC H14A N *C14 H14B 1.0877 109.65 118.91 H11.32 1.0813 IC H13A N *C15 H15A 1.4955 109.44 -64.69 111.04 1.0951 IC H14A N *C14 H14C 1.0877 109.65 118.74 110.91 1.0420 IC H14A N *C15 H15C 1.0951 111.04 122.93 113.87 1.0740 IC H14A N *C15 H15C 1.0951 111.04 122.93 113.87 1.0740 IC H15A N *C15 H15C 1.0951 111.04 123.93 113.25 1.0388 IC N11A C12 *C11 H11A 1.4232 108.22 -67.94 118.41 1.5875 IC C12 C12 *C11 H11A 1.4232 108.22 -67.94 118.41 1.5875 IC C12 C12 *C11 H11A 1.4232 118.41 -166.85 104.55 1.4795 IC C12 C12 *C11 H11A 1.4232 118.41 -166.85 104.55 1.4795 IC C11 O12 *P O13 1.5781 104.05 1.17.80 100.05 1.4795 IC C12 C12 *C11 H11A 1.4232 118.41 -166.85 104.55 1.5783 IC C11 O12 *P O13 1.5781 104.05 1.17.80 100.05 1.4795 IC C11 O12 *P O13 1.5781 104.05 1.17.80 100.05 1.4795 IC C11 C1 C2 C3 C1 *C2 C3 1.4316 110.80 -117.71 1.05753 IC C11 C12 C2 O21 C21 1.5573 110.71 1.18.37 106.71 1.1170 'defines chirality IC C3 C1 *C2 O21 C21 C21 1.5573 110.	BOND C31 DOUBLE C3 BOND C32 BOND C33 BOND C34 BOND C35 BOND C36 BOND C37 BOND C38 BOND C39 BOND C31	C32 31 032 H2X H3X H4X H5X H6X H7X H8X H9X 0 H10X	C3 C3 C3 C3 C3 C3 C3 C3 C3 C3	2 H2Y 3 H3Y 4 H4Y 5 H5Y 6 H6Y 7 H7Y 8 H8Y 9 H9Y 10 H10Y	C32 C33 C34 C35 C36 C37 C38 C39 C310	C33 C34 C35 C36 C37 C38 C39 C310 C311					
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	BOND C31 DOUBLE C3 BOND C312 BOND C312 BOND C314 BOND C314 BOND C316 BOND C317 BOND C318	HIIX 11 C312 2 H12X 3 H13X 4 H14X 5 H15X 6 H16X 7 H17X 8 H18X	C3 C3 C3 C3 C3 C3 C3 C3	12 C313 13 H13Y 14 H14Y 15 H15Y 16 H16Y 17 H17Y 18 H18Y	C313 C314 C315 C316 C317 C318	C314 C315 C316 C317 C318 H18Z					
Chirality IC C3 C1 *C2 HS 1.5573 110.71 -118.37 106.71 1.1170 !defines chirality IC C1 C2 021 C21 1.5508 108.02 147.52 115.15 1.3177 IC C2 021 C22 1.4410 115.15 179.16 108.63 1.5289	IMPR C21 C IC C15 IC C13 IC C13 IC C13 IC C14 IC H12A IC C14 IC H13A IC C13 IC H14A IC H14A IC H14A IC H15A IC H15A IC H15A IC H15A IC H11A IC C12 IC H11A IC C12 IC C11 IC 011 IC 012 IC P IC C2 IC HA IC 011 IC 02 IC HA IC 011 IC 011 IC 011 IC 02 IC HA IC 011 IC 02 IC HA IC 011	N C12 C12 C12 N N N N N N N N N N N N N N N N N N N	C12 *N *N C12 *C12 *C12 C13 *C13 *C13 *C13 *C13 *C13 *C13 *C14 *C14 *C14 *C14 *C14 *C15 *C15 *C15 C11 *C11 O12 P *P *P O11 C1 *C1 *C12 *C12 *C12 *C12 *C12 *C12	C31 031 C11 C14 C15 C11 H12A H12B H13A H13B H13C H14A H14B H14C H15A H15B H15C O12 H11A H11B P O11 O13 O14 C1 C2 HA HB C3 O21	1.5031 1.4955 1.4955 1.4955 1.4955 1.5412 1.078 1.4976 1.0869 1.0869 1.4955 1.0877 1.0877 1.0951 1.0951 1.5223 1.4232 1.1138 1.5781 1.5781 1.5781 1.5578	L 108.03 110.60 110.60 110.60 110.60 116.83 111.94 109.35 109.35 109.35 109.65 109.65 109.44 111.04 116.83 108.22 113.25 108.22 118.41 104.05 104.05 104.05 110.80 111.41 10.80 110.80 110.71	-62.19 122.73 -119.76 57.52 -126.40 -116.29 179.50 118.93 -119.04 -179.22 118.74 -119.76 -64.69 123.93 -112.38 127.52 -123.07 -118.71 -67.94 -166.85 117.80 -117.37 167.61 168.12 -119.17 -120.80 176.77 120.62	116.82 109.67 108.04 116.83 111.94 108.17 109.35 111.32 111.19 109.65 110.91 111.49 111.04 113.87 110.25 108.22 113.25 109.20 118.41 104.05 108.05 106.82 118.26 110.80 111.41 110.01 110.71 108.02	1.5409 1.4976 1.5032 1.5412 1.0787 1.0974 1.0869 1.0813 1.0811 1.0877 1.0820 1.0812 1.0951 1.0740 1.0938 1.4232 1.1138 1.1129 1.5875 1.5781 1.4795 1.4822 1.4316 1.5508 1.1170 1.1146 1.5573 1.4410	!defines	5 S
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	chirality IC C3 chirality	C1	*C2	HS	1.5573	3 110.71	-118.37	106.71	1.1170	!defines	; S
	IC C1 IC C2	C2 021	021 C21	C21 C22	1.5508 1.4410	3 108.02) 115.15	147.52 179.16	115.15 108.63	1.3177 1.5289		

IC	C22	021	*C21	022	1.5289	108.63	-178.85	126.55	1.2187	
IC	021	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	031	1.5508	110.71	176.05	112.62	1.4438	
IC	031	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	С3	031	C31	1.5573	112.62	87.12	115.04	1.3313	
IC	C3	031	C31	C32	1.4438	115.04	-172.98	108.55	1.5288	
IC	C32	031	*C31	032	1.5288	108.55	-178.89	125.60	1.2170	
IC	031	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	1.539	9 113.	57 -173.	39 113.	79 1.53	375
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
!ci	ls db									
IC	C213	C210	*C212	H12R		1.5099	126.94	-177.42	118.69	1.1018
IC	C211	C212	C213	C214	1.350	2 126.	69 180.	00 111.	86 1.54	117
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	1.509	7 125.	28 121.	00 119.	65 1.10	004
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
⊥C T ≃	CJI	C32	633	C34	1.5405	110.8	5 180.0	U 126.13	5 ⊥.595	1
1C	C34	032	*033	нзх	1.5410	113.3	ь -119.9 г 101 г	6 111.74	± 1.114	8
TC	C34	032	*(:33	нзт	1.5192	121.3	5 121.0	U 106.97	1.112	8 0
ТC	C32	633	C34	C35	⊥.6060	126.1	з т80.0	U 113.36	o ⊥.541	U

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	Н6Х	1.5396	113.52	-123.43	110.53	1.1101	
IC C37	C35	*C36	Н6Ү	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	Н9Х	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	H1OX	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 VSP(! Vacce) !	C 0. nyl - Ci	00 ! 3 H2 I	-vacce	noyl-2-steroyl	-D-glyce	ero-1-ph	osphatidy	vlcholine	
! Vaccer	nyl – (СН (-)	(+)					
!	(СН2 - РО	4 - CH	2 - CH2 - N-(C	НЗ)З!				
!	1 6			C 1					
!!Derive	a torm	tne toil	owing :	tiles	<u></u>				
!! B3	/ Stuart	: Rose 9,	/10/201	.3 - Use of IC	files w	as diffe	rent bet	ween thes	e two:
!!		_			_				
!!RESI DO	DPC	0.0	0 ! 2,	3-dioleoyl-D-g	⊥ycero-1	-phospha	atidylcho	line	
!!		_							
!!RESI PO	OPC	0.0	0 ! 3-]	palmitoyl-2-ol	eoyl-D-g	glycero-1	l-Phospha	tidylchol	ine
!! Palm	itoyl -	CH2							

!! Palmitoy1 - CH2
!! |
!! Oleyo1 - CH
!! | (-) (+)
!! CH2 - PO4 - CH2 - CH2 - N-(CH3)3
!!

!! Polar	Head ar	nd glycerol	backbone		
GROUP		1	H1 5	B	
ATOM N	NTT.	-0 60 !	111.0		
ATOM C12	CTL2	-0 10 !	H15A-C1	5-H15C	
лтом µ12л	UT	0.25 1	1110/1 01	10 11100	
ATOM H12A		0.25 1	ן ערנים	<u>ц</u> 1 / л	
ATOM HIZD	пц Стт 5	-0.35 1		n14A	
ATOM CIS		-0.35 :	ן א 10 גנוז		(1)
ATOM HIJA	пц	0.25 :	HISA-CISK	иСІ4-пІ4Б	(+)
ATOM HISB	пц	0.25 !	I I	111.40	
ATOM HISC	HL OTT F	0.25 !	HISC	HI4C	
ATOM CI4	CTL5	-0.35 !			
ATOM HI4A	HL	0.25 !			
ATOM HI4B	HL	0.25 !		alpha6	
ATOM H14C	HL -	0.25 !			
ATOM C15	CTL5	-0.35 !			
ATOM H15A	HL	0.25 !	H12AC1	12H12B	
ATOM H15B	HL	0.25 !			
ATOM H15C	HL	0.25 !			
GROUP		!		alpha5	
ATOM C11	CTL2	-0.08 !			
ATOM H11A	HAL2	0.09 !	H11AC1	1H11B	
ATOM H11B	HAL2	0.09 !		alpha4	
ATOM P	PL	1.50 !	(-) 013 0	012	
ATOM 013	02L	-0.78 !	\setminus /	alpha3	
ATOM 014	02L	-0.78 !	P	(+)	
ATOM 012	OSLP	-0.57 !	/ \	alpha2	
ATOM 011	OSLP	-0.57 !	(-) 014 0	011	
ATOM C1	CTL2	-0.08 !		alpha1	
АТОМ НА	HAL2	0.09 !	НАС	21НВ	
ATOM HB	HAL2	0.09 !		theta1	
GROUP		!			
ATOM C2	CTL1	0.17 !	HSC	2	
ATOM HS	HAT.1	0 09 1	110	betal	I
ATOM 021	OSL	-0 49 1	022 ()21 t	-heta3
ATOM C21	CT.	0 90 1		heta?	
ATOM 022	OBL	-0 63 1	C21	Decaz	
ATOM C22	CTL2	-0 22 1	120	hota3	
ATOM H2R	HAL2	0.22 .	н2вС22-	H2S	
ATOM H29	UNT 2	0.09 1	1121(022	112.5	
CPOUR	IIALLZ	0.05		hot al	
JTOM C2	CTT 2			Deta4	
ATOM UV	UNT 2	0.00 :		UV_	
ATOM IIX		0.09 :		11/4	
ATOM HI	NALZ	0.09 !		022	
ATOM USI	CI	-0.49 !		032	031
ATOM CSI	ODI	0.90 !		\ \	/ yallillaz
ATOM 032	OBL CEL 2	-0.03 !		C	
ATOM C32	UTLZ	-0.22 !			ganimas
ATOM HZX	HALZ	0.09 !		HZX(C3ZHZY
ATOM HZY	HALZ	0.09 !			
GROUP	~ ~ ~ ^	!			gamma4
ATOM C23	CTL2	-0.18 !			
ATOM H3R	HAL2	0.09 !	H3RC23	3H3S	
ATOM H3S	HAL2	0.09 !			
GROUP		!			
ATOM C24	CTL2	-0.18 !			
ATOM H4R	HAL2	0.09 !	H4RC24	1H4S	
ATOM H4S	HAL2	0.09 !			
GROUP		!			
ATOM C25	CTL2	-0.18 !			
ATOM H5R	HAL2	0.09 !	H5RC25	5Н5S	
ATOM H5S	HAL2	0.09 !			
GROUP		!			
ATOM C26	CTL2	-0.18 !			

ATOM ATOM	H6R H6S	HAL2 HAL2	0.09	H6RC26H6S					
GROUE	2								
ATOM	C27	CTL2	-0.18						
ATOM	H7R	HAL2	0.09	H7RC27H7S					
ATOM GROUE	H7S	HAL2	0.09						
ATOM	C28	CTL2	-0.18	!					
ATOM	H8R	HAL2	0.09	H8RC28H8S					
ATOM	H8S	HAL2	0.09						
GROUE	2		!						
ATOM	C29	CTL2	-0.18						
ATOM	H9R	HAL2	0.09	H9RC29H9S					
ATOM	H9S	HAL2	0.09						
ATOM	C210	CTT.2	-0 18						
ATOM	U10D		0.10	ч10рC210ч10с I					
ATOM			0.09						
CDOUL	TIUS	ПАЦА	0.09						
GROUE A TOM	C011	CET 1	0 15						
ATOM	UZII	CELI	-0.15						
GROUE	HIIK >	нггт	0.15	(CIS)					
ATOM	C212	CEL1	-0 15						
ATOM	H12R	HEL1	0.15	H12RC212					
CROUE)		0.10						
ATOM	C213	CTT.2	-0 18						
ATOM	U215 Н13Р	HAL2	0.10	н13вС213н13с Г					
ATOM	u130		0.09						
GROUE	2	IIAUZ	0.05						
ATOM	C214	CTL2	-0.18						
ATOM	H14R	HAL2	0.09	H14RC214H14S					
ATOM	H14S	HAL2	0.09						
GROUE	2								
ATOM	C215	CTL2	-0.18						
ATOM	H15R	HAL2	0.09	H15RC215H15S					
ATOM	H15S	HAL2	0.09						
GROUE	>								
ATOM	C216	CTL2	-0.18						
ATOM	H16R	HAL2	0.09	H16RС216Н16S					
ATOM	H16S	HAL2	0.09						
GROUE	2								
ATOM	C217	CTL2	-0.18						
ATOM	H17R	HAL2	0.09	H17RC217H17S					
ATOM	H17S	HAL2	0.09						
GROUE	2								
ATOM	C218	CTL3	-0.27						
ATOM	H18R	HAL3	0.09	H18RC218H18S					
ATOM	H18S	HAL3	0.09						
ATOM	н18т	HAT.3	0.09	н18т і					
GROUE	>								
ATOM	C33	CTL2	-0.18						
ATOM	нзх	HAL2	0.09	НЗХСЗЗНЗҮ					
ATOM	НЗҮ	HAL2	0.09						
GROUF	2			· ·					
ATOM	C34	CTL2	-0.18						
ATOM	H4X	HAL2	0.09	Н4ХСЗ4Н4Ү					
ATOM	H4Y	HAL2	0.09						
GROUF	-								
ATOM	C35	CTL2	-0.18						
ATOM	H5X	HAL2	0.09	Н5ХС35Н5Ү					
ATOM	H5Y	HAL2	0.09						
GROUF	2								
ATOM	C36	CTL2	-0.18						
ATOM	H6X	HAL2	0.09	н6хс36н6х					
ATOM	Н6Ү	HAL2	0.09	!				I	
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GROUI	2		!	!				1	
ATOM	C37	CTL2	-0.18	!				1	
ATOM	H7X	HAL2	0.09					Н7ХС	37Н7Ү
ATOM	H7Y	HAL2	0.09					1	
GROUE	>							i	
ATOM	C38	CTT.2	-0 18					i i	
ATOM	48Y	HAL2	0 09					H8XC	38H8V
ATOM	UQV		0.00					1107 0.	101
ATOM CDOUU	пот	HALZ	0.09					1	
GROUE								l I	
ATOM	C39	CTL2	-0.18					I	
ATOM	н9х	HAL2	0.09	!				H9XC	39Н9Ү
ATOM	H9Y	HAL2	0.09	!					
GROUE	2		!	!					
ATOM	C310	CTL2	-0.18	!				1	
ATOM	H10X	HAL2	0.09					H10XC	310H10Y
АТОМ	H10Y	HAL2	0.09					1	
CROUI	>		0.05					1	
ATTOM	C211	CTT 2	_0 10					1	
ATOM	UIIV		-0.18						011 TT11T
ATOM	HIIX	HALZ	0.09					HIIXC.	SIIHIII
A'I'OM	HI2Y	HAL2	0.	.09 !					
GROUI	5								
ATOM	C312	CTL2	-0.18	!					
ATOM	H12X	HAL2	0.09	!				H12XC	312H12Y
ATOM	H12Y	HAL2	0.	.09 !					
GROUE	2							1	
АТОМ	C313	CTL2	-0.18					i	
ATOM	H13Y	HAL2	0 09					H13XC	313H13V
ATOM	111 J X		0.00						JIJ 111JI
CDOU	птэт	TALZ	0.09					1	
GROUP	~ ~ 1 1	~~~ ^	0 1 0					I	
ATOM	C314	CTLZ	-0.18						
ATOM	H14X	HAL2	0.09	!				H14XC	314H14Y
ATOM	H14Y	HAL2	0.09	!					
GROUI	2		!	!				1	
ATOM	C315	CTL2	-0.18	!				1	
ATOM	H15X	HAL2	0.09					H15XC	315н15ү
АТОМ	H15Y	HAT.2	0.09					1	
GROUF	>							i	
ATOM	C316	CTT.2	-0 18					1	
ATOM	U16V		0.10					u16VC	216U16V
ATOM	HI CV		0.09					HIUXC.	310HI01
ATOM	HIQI	HALZ	0.09					I I	
GROUE	-							I.	
ATOM	C317	CTL2	-0.18					I	
ATOM	H17X	HAL2	0.09	!				H17XC	317H17Y
ATOM	H17Y	HAL2	0.09	!					
GROUE	2		!	!				1	
ATOM	C318	CTL3	-0.27					1	
ATOM	H18X	HAL3	0.09					H18XC	318H18Y
ΔТОМ	H18Y	НАТ.З	0 09					-	
ATOM	u1 9 7	цут 3	0.09					ц. Ц.	1.9.7
AIOM	11102	пацэ	0.09					11.	102
I Dol	lar Uc	and							
: FOI	Lai IIe	au .		014			01 F		
BOND	IN COLO	C13	IN C 1 C	C14	IN		C15		
BOND	CI3	HIJA	CL	S HI3B	С	213	HI3C		
BOND	C14	H14A	C14	H14B	С	14	H14C		
BOND	C15	H15A	C15	5 H15B	С	:15	H15C		
BOND	Ν	C12							
BOND	C12	H12A	C12	2 H12B	С	:12	C11		
BOND	C11	H11A	C11	H11B	С	:11	012	011	C1
BOND	012	Р	P	011	P)	013	P	014
! Glv	vcerol	Backbo	one		_		-		
BOND	C1	HA	- C1	HB	C	:1	C2		
BOND	C2	HS	C2	с 3	C C	2	021		
BOND	C 3	HY	C2	цv	C C	· 2	031		
	5	117	60	пı	C	<i>.</i> .	JJT		

! Chai	ln fi	com C2								
BOND	021	C21								
BOND	C21	C22								
DOUBLE	E C2	21 022								
BOND	C22	H2R	C2	2 H2S		C22	C23			
BOND	C23	H3R	C2	3 H3S		C23	C24			
BOND	C24	H4R	C2	4 H4S		C24	C25			
BOND	C25	H5R	C2	5 H5S		C25	C26			
BOND	C26	H6R	C2	6 H6S		C26	C27			
BOND	C27	H7R	C2	7 H7S		C27	C28			
BOND	C28	H8R	C2	8 H8S		C28	C29			
BOND	C29	HOR	C2	9 H9S		C29	C210			
BOND	C210	11JI() 1110D	C2	10 H109		C210	C211			
BOND	C210		C2	IO HIUS		CZIU	0211			
DOUDT		11 001	n							
DOUDLE		LL CZL. 0 11100	2 00	10 0010						
BOND	0212	HIZR	C2	12 (213		0010	0014			
BOND	CZI	S HIJK	02	13 H13S		C213	C214			
BOND	C214	I HI4R	C2	14 H14S		C214	C215			
BOND	C215	9 H15R	C2	15 H15S		C215	C216			
BOND	C216	5 H16R	C2	16 H16S		C216	C217			
BOND	C217	7 H17R	C2	17 H17S		C217	C218			
BOND	C218	8 H18R	C2	18 H18S		C218	H18T			
! Chai	in Fi	com C3								
BOND	031	C31								
BOND	C31	C32								
DOUBLE	E C3	31 032								
BOND	C32	H2X	C3	2 Н2Ү		C32	C33			
BOND	C33	нзх	C3	З НЗҮ		C33	C34			
BOND	C34	H4X	C3	4 H4Y		C34	C35			
BOND	C35	н5х	C3	5 H5Y		C35	C36			
BOND	C36	н6х	C3	6 Н6Ү		C36	C37			
BOND	C37	H7X	C3	7 H7Y		C37	C38			
BOND	C38	H8X	C 3	8 H8Y		C 3 8	C 3 9			
BOND	C39	цох	C3	о нот 9 нот		C39	C310			
BOND	C310	119A	C3	10 H10V		C310	C311			
DOND	C311		C3	10 III0I		COID	CJII 2011 0010			
BOND	0210		0				2010 0012			
BOND	C312	2 HIZX	03	12 H12Y		a 2 1 2				
BOND	C313	S HIJX	03	13 HI3Y		C313	0314			
BOND	C314	HI4X	03	14 H14Y		C314	0315			
BOND	C315	D HI5X	03	15 H15Y		C315	0316			
BOND	C316	b H16X	C3	16 H16Y		C316	C317			
BOND	C31	/ H1/X	C3	17 H17Y		C317	C318			
BOND	C318	8 H18X	C3	18 H18Y		C318	H18Z			
IMPR C	C21 (D21 C22	022	C31 O31	C32	032				
IC C15	5	N	C12	C11		1.5031	L 108.03	-62.19	116.82	1.5409
IC C13	3	C12	*N	C14		1.4955	5 110.60	122.73	109.67	1.4976
IC C13	3	C12	*N	C15		1.4955	5 110.60	-119.76	108.04	1.5032
IC C13	3	Ν	C12	C11		1.4955	5 110.60	57.52	116.83	1.5412
IC C11	L	Ν	*C12	H12A		1.5412	2 116.83	-126.40	111.94	1.0787
IC H12	2A	N	*C12	H12B		1.078	7 111.94	-116.29	108.17	1.0974
IC C14	1	Ν	C13	H13A		1.4976	5 110.99	179.50	109.35	1.0869
IC H13	3A	Ν	*C13	H13B		1.0869	9 109.35	118.93	111.32	1.0813
TC H13	3A	N	*C13	H13C		1.0869	9 109.35	-119.04	111.19	1.0811
TC C13	3	N	C14	H14A		1 495	5 110 99	-179 22	109 65	1 0877
TC H14	1 Z	N	*014	H14B		1 087	7 109 65	118 74	110 91	1 0820
TC U1/	17\	N	*014	u14C		1 007	7 100.65	_110.76	111 /0	1 0012
	2	M	C15	1114C 1114		1 /05'	5 100 44	-61 60	111 01	1 0051
TO TIT	י ה ד	TN VI	ULU *015			1 0051	$J \pm 0 $	-04.09	112 07	1 0740
TO HIS	DA T	IN	*C15	HIJE C		1 0051	1 111 04	110 20	110 05	1.0/40
IC HIS	A	IN Q1 Q	^C15	HIDC 010		1.095.	116.02	-112.38	110.25	1.0938
IC N		C12	CII	012		1.5223	5 116.83	127.52	108.22	1.4232
IC 012	2	C12	*C11	HIIA		1.4232	2 108.22	-123.07	113.25	1.1138
IC H11	LA	C12	*C11	H11B		1.1138	3 113.25	-118.71	109.20	1.1129

IC C12	C11	012	P	1.5412 108.22 -67.94 118.41 1.5875
IC C11	012	Р	011	1.4232 118.41 -166.85 104.05 1.5781
IC 011	012	*P	013	1.5781 104.05 117.80 108.05 1.4795
IC 011	012	*P	014	1.5781 104.05 -117.37 106.82 1.4822
IC 012	P	011	C1	1.5875 104.05 167.61 118.26 1.4316
TC P	011	C1	C2	1 5781 118 26 168 12 110 80 1 5508
	011	*01	на	1.5508 110.80 -119.17 111.41 1.1170
	011	*C1	UD	1,3300 110.00 119.17 111.41 1.1170 1 1170 111 41 -120 90 110 01 1 1146
IC HA	011 C1	C2		1,1170 111.41 - 120.00 110.01 1.1140 $1,4216 110.00 176 77 110 71 1 5572$
		LZ	001	1.4316 110.80 176.77 110.71 1.5573
10 03	CI	×CZ	021	1.55/3 110./1 120.62 108.02 1.4410 defines S
chirality				
IC C3	C1	*C2	HS	1.5573 110.71 -118.37 106.71 1.1170 !defines S
chirality				
IC Cl	C2	021	C21	1.5508 108.02 147.52 115.15 1.3177
IC C2	021	C21	C22	1.4410 115.15 179.16 108.63 1.5289
IC C22	021	*C21	022	1.5289 108.63 -178.85 126.55 1.2187
IC 021	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
TC C1	C2	C3	031	1.5508 110.71 176.05 112.62 1.4438
TC 031	C2	*C3	нх	1 4438 112 62 -118 51 106 65 1 1128
IC HX	C2	*03	HV	1 1128 106 65 -115 12 109 46 1 1145
	C2	021	0.21	1.5572 110.00 110.12 100.40 1.1140
	021	031	C31 G30	1.3373 112.02 07.12 113.04 1.3313
	031	C31	032	1.4438 115.04 -172.98 108.55 1.5288
IC C32	031	*C31	032	1.5288 108.55 -178.89 125.60 1.2170
IC 031	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	НЗR	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
TC C25	C23	*C24	H4R	1.5399 113.68 120.91 108.91 1.1136
TC C25	C23	*024	ндс	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 C25	C24	*025	U5D	1.53500 113.00 30.93 113.07 1.3333
10 020	024	+025	IIJK	1.5555 115.57 121.41 100.70 1.1129
IC C26	024	~CZ5	пре	1.5390 113.52 -123.45 110.55 1.1101
10 024	C25	020	C27	1.5399 113.57 -173.39 113.79 1.5375
	C25	*C26	H6R	1.5375 113.79 122.09 109.21 1.1127
1C C2/	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
TC C28	C29	C210	C211	1.5375 113.35 67.78 114.46 1.5115
TC 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
	C210	0210	0212	1 5450 114 46 100 00 126 01 1 2502
10 029	0210	+0011		1.3436 114.46 160.00 126.91 1.3302
	CZIU	^CZII	HIIR	1.3502 126.91 -178.81 114.69 1.1010
10 0210	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	1.509	7 125.2	8 121.0	0 119.6	5 1.100	4
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
TC	C218	C216	*C217	H17S		1 5097	125 28	121 00	119 65	1 1004
TC	C216	C217	C218	H18R		1 5347	113 05	180 00	110 58	1 1110
TC	U1 9 D	C217	*C218	u199		1 5396	113 52 .	-123 /3	110.53	1 1101
TC		0217	*0210	11105		1 5007	125.02	123.43	110.55	1 1004
TC	HIØK GO1	CZ17	^CZ18	HIOT	1 5405	110 05	125.28	121.00	1 5051	1.1004
IC	C31	032	033	034	1.5405	110.85	180.00	126.13	1.5951	
IC	C34	C32	*033	HJX	1.5410	113.36	-119.96	111./4	1.1148	
IC	C34	C32	*C33	НЗҮ	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	нбх	1.5396	113.52	-123.43	110.53	1.1101	
IC	C37	C35	*C36	НбҮ	1,5192	121.35	123.34	106.97	1,1128	
TC	C35	C36	C37	C 3 8	1 5396	114 47	180 00	113 41	1 5386	
TC	C38	C36	*C37	630 Н7Х	1 5396	113 52	-123 43	110 53	1 1101	
TC	C38	C36	*037	117X 117V	1 5192	121 35	123.43	106 97	1 1128	
TC	C36	C30	C30	C 2 0	1 5207	112 /1	120.04	112 71	1 5202	
TC	C30	027	+020	U0V	1 5200	112 50	100.00	110 52	1 1101	
TC	C39 C39	C37	*C30	HOX	1.5396	101 05	-123.43	10.53	1.1101	
TC	C39 C37	C37	^C38	HOI	1.5192	112 70	123.34	112 25	1.1128	
IC	C37	C38	039	0310	1.5353	113.79	1//.45	113.35	1.5458	
IC	C310	038	*039	НЭХ	1.5458	113.35	119.8/	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	H1OX	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	
TC	C315	C313	*C314	H14X	1.5396	113.52	-123.43	110.53	1.1101	
TC	C315	C313	*0314	H14Y	1 5097	125 28	121 00	119 65	1 1004	
TC	C313	C314	C315	C316	1 5377	113 85	180 00	111 81	1 5374	
TC	C316	C314	*0315	u15v	1 5396	113 52	-123 /3	110 53	1 1101	
TC	C316	C314	*0215	III JA III EV	1 5102	101 25	100 04	106.07	1 1120	
TC	0214	0215	0210	п131 0217	1 5257	111 01	123.34	114 20	1 5005	
IC	0314	0315	0316	0317	1.5357	111.81	180.00	114.29	1.5985	
тс	C317	C315	*C316	ні бх	1.5396	113.52	-123.43	10.53	1.1101	
ТС	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. ! Cardiolipins IN PROGRESS

RESI TVCL2

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

GROUE	>			!	
ATOM HG31	С3	CTL2	-0.08	!	
ATOM ATOM	HG31 HG32	HAL2 HAL2	0.09 0.09	! !	١
ATOM	РЗ	PL	1.50	!	
ATOM	OP33	02L	-0.78	!	
ATOM OP31	OP34	O2L	-0.78	!	
ATOM	OP31	OSLP	-0.57	!	
АТОМ РЗ (+)	OP32 OP3	OSLP 34(-)	-0.57	!	OP13(-)
ATOM	C31	CTL2	-0.08	!	
ATOM OP32	H31J	HAL2	0.09	!	
ATOM 	Н31К	HAL2	0.09	!	
GROUE	, -−H31⊮	ζ		!	H11J
ATOM ATOM ATOM	C2 HG22 OG12	CTL1 HAL1 OHL	0.14 0.09 -0.65	! ! !	H12J
ATOM	H012	HOL	0.42	!	
GROUE	>		I	!	
ATOM H33K	C1	CTL2	-0.08	!	Н
ATOM 	HG11	HAL2	0.09	!	
ATOM I	HG12	HAL2	0.09	!	
АТОМ 033	P1	PL	1.50	!	
ATOM 	OP13	O2L	-0.78	!	I
ATOM CD1=C	OP14 DD1	02L	-0.78 CC	! 1=0C1	
ATOM 	OP11	OSLP	-0.57	!	
atom -cd2-	OP12 -H2Y	OSLP	-0.57 H2RC	! С2Н2S	<u>:</u>
ATOM 	C11	CTL2	-0.08 	!	
atom -cd3-	H11J -H3Y	HAL2	0.09 H3RC	! С3НЗЅ	
ATOM 	H11K	HAL2	0.09	!	
GROUE	>			!	i
-CD4-	-H4Y	0 1	H4RC	C4H4S	
atom 	CT2	CTLI	0.1/	!	
ATOM	H12J	HAL1	0.09	!	H5D
-CD5-	-н5Ү 012	OST.	H5KC	USH5S	
		USL CI	-0.49	:	
-CD6-	-H6Y	СГ	0.90 H6RC	: СбН6S	

HG11	OG12H012	
\setminus	1	/
C1	C2	
/ \		/
/ HG12	HG22	HG32
OP11		
L3(-)P1(+)OP14(-)		OP33(-)
I		
OP12		
I		
H11JC11H11K		H31J-
l		
H12JC12012	2	H32J-
Ι	I	
I	I	1
Н13ЈС13Н13К	I	H33JC33
I	I	
I	I	
013	I	
I	I	I
CB1=OB1	CA1=OA1	
I	I	I
H2DCB2H2E	Н2АСА2Н2В	H2X-
I	Ι	
H3DCB3H3E	НЗАСАЗНЗВ	НЗХ-
I	I	I
H4DCB4H4E	Н4АСА4Н4В	H4X-
I	I	I
H5DCB5H5E	Н5АСА5Н5В	н5х-
I	Í.	I
H6DCB6H6E	Н6АСА6Н6В	н6х-

ATOM OA1 OBL -0.63 ! 1 ATOM CA2 CTL2 -0.22 ! 1 1 _____ ATOM H2A HAL2 0.09 ! Н7D--СВ7--Н7Е Н7А--СА7--Н7В H7X--CD7--H7Y H7R--CC7--H7S ATOM H2B HAL2 0.09 ! H8D--CB8--H8E GROUP ! Н8А--СА8--Н8В H8X--CD8--H8Y H8R--CC8--H8S ATOM C13 CTL2 0.08 ! Н9А--СА9 ATOM H13J HAL2 0.09 ! H9D--CB9 H9X--CD9 H9R--CC9 0.09 ! ATOM H13K HAL2 ATOM 013 OSL -0.49 ! ATOM CB1 CL 0.90 ! H10D--CB10 H10A--CA10 H10X--CD10 H10R--CC10 ATOM OB1 OBL -0.63 ! 1 _____ ATOM CB2 CTL2 -0.22 ! H11D--CB11--H11E H11A--CA11--H11B H11X--CD11--H11Y H11R--CC11--H11S ATOM H2D HAL2 0.09 ! - I _____ 1 ATOM H2E HAL2 0.09 ! H12D--CB12--H12E H12A--CA12--H12B H12X--CD12--H12Y H12R--CC12--H12S GROUP ! 1 ATOM C32 CTL1 0.17 ! Н13D--СВ13--Н13Е Н13А--СА13--Н13В ATOM H32J HAL1 0.09 ! H13X--CD13--H13Y H13R--CC13--H13S ATOM 032 OSL -0.49 ! - I ATOM CC1 CL 0.90 ! H14D--CB14--H14E H14A--CA14--H14B H14X--CD14--H14Y H14R--CC14--H14S ATOM OC1 OBL -0.63 ! 1 1 1 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 ! Н17D--СВ17--Н17Е Н17А--СА17--Н17В H17X--CD17--H17Y H17R--CC17--H17S ATOM H33J HAL2 0.09 ! 1 ATOM H33K HAL2 0.09 ! H18D--CB18--H18E H18A--CA18--H18B H18X--CD18--H18Y H18R--CC18--H18S ATOM 033 OSL -0.49 ! 1 0.90 ! ATOM CD1 CL 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 1 ATOM CA3 CTL2 -0.18 !

ATOM	НЗА	HAL2	0.09 !	
ATOM	НЗВ	HAL2	0.09 !	
GROUE	>		!	
ATOM	CA4	CTT.2	-0 18 1	
	U/7		0.10 .	
ATOM	1146		0.09 :	
ATOM	H4B	HALZ	0.09 !	
GROUE	2		!	
ATOM	CA5	CTL2	-0.18 !	
ATOM	H5A	HAL2	0.09 !	
ATOM	H5B	HAL2	0.09 !	
GROUF	>		1	
	CAG	CTT.2	-0 18 1	
	UGA		0.10 1	
ATOM	HOA	HALZ	0.09 !	
ATOM	нов	HALZ	0.09 !	
GROUE	2		!	
ATOM	CA7	CTL2	-0.18 !	
ATOM	H7A	HAL2	0.09 !	
ATOM	Н7В	HAL2	0.09 !	
GROUE	>		!	
ATOM	CAS	CTT.2	-0 18 1	
	U07		0.10 .	
ATOM	HOR	TALZ	0.09 !	
ATOM	HSR	HALZ	0.09 !	
GROUE	2		!	
ATOM	CA9	CEL1	-0.15 !	
ATOM	H9A	HEL1	0.15 !	
GROUE	2		!	
АТОМ	CA10	CEL1	-0.15 !	
ATOM	U107	UET 1	0 15 1	
CDOUL	IIIUA		0.13 :	
GROUP		0777 0	. 10 !	
ATOM	CAII	CTLZ	-0.18 !	
ATOM	H11A	HAL2	0.09 !	
ATOM	H11B	HAL2	0.09 !	
GROUE	2		!	
ATOM	CA12	CTL2	-0.18 !	
АТОМ	H12A	HAT.2	0.09 1	
ATOM	u12p	UNT 2	0.09.	
CDOUL		IIALLZ	0.09 :	
GROUE	~	~~~ ^	:	
A'I'OM	CA13	CTL2	-0.18 !	
ATOM	H13A	HAL2	0.09 !	
ATOM	H13B	HAL2	0.09 !	
GROUE	2		!	
ATOM	CA14	CTL2	-0.18 !	
АТОМ	H14A	HAL2	0.09 !	
ATOM	u1/D	UNT 2	0 09 1	
CDOUL	IITAD	IIALLZ	0.09 :	
GROUE	~	~~~ ^	:	
A'I'OM	CA15	CTL2	-0.18 !	
ATOM	H15A	HAL2	0.09 !	
ATOM	H15B	HAL2	0.09 !	
GROUE	2		!	
АТОМ	CA16	CTL2	-0.18 !	
ATOM	H16D	нат.2	0 09 1	
			0.00 !	
AIOM	птор	HALZ	0.09 !	
GROUE	2		!	
ATOM	CA17	CTL2	-0.18 !	
ATOM	H17A	HAL2	0.09 !	
ATOM	Н17В	HAL2	0.09 !	
GROUF	>		i	
	CAIR	CTT 3	-0 27 1	
	U107	0 T T O	0.00	
ALOM	III OF	HALJ	0.09 !	
A'I'OM	HT8B	HAL3	0.09 !	
ATOM	H18C	HAL3	0.09 !	
GROUE	2		!	
ATOM	CB3	CTL2	-0.18 !	
ATOM	HЗD	HAL2	0.09 !	
		-		

ATOM	H3E	HAL2	0.09 !
GROUI	2		!
ATOM	CB4	CTL2	-0.18 !
ATOM	H4D	HAL2	0.09 !
ATOM	H4E	HAL2	0.09 !
GROUE	2		!
ATOM	CB5	CTL2	-0.18 !
ATOM	H5D	HAL2	0.09 !
ATOM	H5E	HAL2	0.09 !
GROUE	>		!
ATOM	CB6	CTT.2	-0 18 1
	H6D	HAL2	0.10 .
ATOM	IIGE		0.09 :
CDOUU	пов	HALZ	0.09 !
GROUP	- 		
ATOM	CB/	CTL2	-0.18 !
A'I'OM	H/D	HAL2	0.09 !
ATOM	H'/E	HAL2	0.09 !
GROUI	2		!
ATOM	CB8	CTL2	-0.18 !
ATOM	H8D	HAL2	0.09 !
ATOM	H8E	HAL2	0.09 !
GROUE	2		!
ATOM	CB9	CEL1	-0.15 !
ATOM	H9D	HEL1	0.15 !
GROUF	>		1
ATOM	CB10	CEL1	-0 15 I
	н10р	HEL1	0 15 1
			0.10
A TOM	CD11	CTTT 2	-0 10 1
ATOM			-0.10 !
ATOM	HIID	HALZ	0.09 !
A'I'OM	HIIE	HALZ	0.09 !
GROUI	2		!
ATOM	CB12	CTL2	-0.18 !
ATOM	H12D	HAL2	0.09 !
ATOM	H12E	HAL2	0.09 !
GROUI	2		!
ATOM	CB13	CTL2	-0.18 !
ATOM	H13D	HAL2	0.09 !
ATOM	H13E	HAL2	0.09 !
GROUE	2		!
АТОМ	CB14	CTL2	-0.18
ATOM	н14р	HAT.2	0 09 1
	H14F	HAL2	0.09 1
CROTT	, , , , , , , , , , , , , , , , , , ,	1111112	0.05 :
ATTOM		C TT 2	0 10 1
ATOM	CBID	CTLZ	-0.18 !
ATOM	HI5D	HALZ	0.09 !
ATOM	H15E	HAL2	0.09 !
GROUI	2		!
ATOM	CB16	CTL2	-0.18 !
ATOM	H16D	HAL2	0.09 !
ATOM	H16E	HAL2	0.09 !
GROUE	2		!
АТОМ	CB17	CTL2	-0.18 !
ATOM	H17D	HAT.2	0.09 1
ATOM	H17E	HAT.2	0 09 1
GRUIT	···· / ⊔		
	010	د تسې	-0 27 1
		CTTO CTTO	-0.27 !
ATOM	HTSD	нацз	0.09 !
ATOM	H18E	HAL3	0.09 !
ATOM	H18F	HAL3	0.09 !
GROUI	2		!
ATOM	CC3	CTL2	-0.18 !
ATOM	H3R	HAL2	0.09 !
ATOM	НЗS	HAL2	0.09 !

GROUE	2		!
ATOM	CC4	CTL2	-0.18 !
ATOM	H4R	HAL2	0.09 !
ATOM	H4S	HAL2	0.09 !
GROUE	~~-	~ ~ ~ ^	!
A'I'OM	CC5	CTL2	-0.18 !
A'I'OM	H5R	HAL2	0.09 !
ATOM CDOUL	HSS	HALZ	0.09 !
GROUE			0 10 1
	UCO		-0.18 !
ATOM	HOR	HALZ	0.09 !
	пор	ΠΑLΖ	0.09 !
GROUP ATTOM	CC7	CTT 2	-0 19 1
ATOM	U7D		-0.18 !
ATOM	117 К Н7 S	HAL2	0.09 !
GROUE	5	IIAUZ	0.05 !
ATOM	CC8	CTT.2	-0 18 1
ATOM	H8R	HAT.2	0 09 1
ATOM	H8S	HAT.2	0 09 1
GROUF	5	111102	
ATOM	CC9	CEL1	-0.15 !
ATOM	H9R	HEL1	0.15 !
GROUE	>		!
ATOM	CC10	CEL1	-0.15 !
ATOM	H10R	HEL1	0.15 !
GROUE	>		!
ATOM	CC11	CTL2	-0.18 !
ATOM	H11R	HAL2	0.09 !
ATOM	H11S	HAL2	0.09 !
GROUE	2		!
ATOM	CC12	CTL2	-0.18 !
ATOM	H12R	HAL2	0.09 !
ATOM	H12S	HAL2	0.09 !
GROUE	2		!
ATOM	CC13	CTL2	-0.18 !
ATOM	H13R	HAL2	0.09 !
ATOM	H13S	HAL2	0.09 !
GROUE	2		!
ATOM	CC14	CTL2	-0.18 !
ATOM	H14R	HAL2	0.09 !
ATOM	H14S	HAL2	0.09 !
GROUE	2	_	!
ATOM	CC15	CTL2	-0.18 !
ATOM	H15R	HAL2	0.09 !
ATOM	H15S	HAL2	0.09 !
GROUE	~~1.6	~ ~ ~ ^	!
A'I'OM	CC16	CTL2	-0.18 !
ATOM	H16R	HAL2	0.09 !
A'I'OM	HI6S	HAL2	0.09 !
GROUE	20017	0007.0	!
ATOM	CCI/	CTL2	-0.18 !
ATOM	HI/R	HALZ	0.09 !
ATOM CDOUL	HI/S	HALZ	0.09 !
GRUUE	CC10	C TT 2	-0 27 1
	ULO Ulor	СТТЭ С т Ч П	-0.2/!
ALOM	U100	UNT O	0.09 !
ATOM	UI OM	пацэ цат э	0.09 !
AIUM CROTT	что.т,	пацэ	0.09 !
GROUP ATOM	202	CTT 2	-0 18 !
	U L L L L L L	ULLZ HAT.2	0.10 1
	HJV	HAT.2	0.09 !
GRUIT	, 11 J T	كىددىيد	1
JICOF			-

ATOM	CD4	CTL2	-0.	18	!				
ATOM	H4X	HAL2	Ο.	09	!				
АТОМ	H4Y	HAL2	0.	09	!				
GROUF	>				1				
ATOM	CD5	CTT.2	-0	18					
ATOM	UEV		0.	10					
ATOM	пол	HALZ	0.	09	-				
ATOM	HSY	HAL2	0.	09	!				
GROUE	2				!				
ATOM	CD6	CTL2	-0.	18	!				
ATOM	H6X	HAL2	Ο.	09	!				
ATOM	H6Y	HAL2	Ο.	09	!				
GROUE	2				!				
ATOM	CD7	CTL2	-0.	18	!				
ATOM	H7X	HAT.2	0.	09	i.				
ATOM	H7V	HAT.2	0	ΛĢ					
CDOIII	, TT / T	11111112	0.	00	·				
JECOUL			0	10	-				
ATOM	CD8	CTLZ	-0.	18	:				
A'I'OM	H8X	HAL2	0.	09	!				
ATOM	H8Y	HAL2	0.	09	!				
GROUE	2				!				
ATOM	CD9	CEL1	-0.	15	!				
ATOM	н9х	HEL1	Ο.	15	!				
GROUE	>				!				
ATOM	CD10	CEL1	-0	15					
ATOM	u10v		0.	15					
CDOUI		111111	0.	тJ	-				
GROUP	GD11		0	1 0	-				
ATOM	CDII	CTLZ	-0.	18	!				
ATOM	H11X	HAL2	0.	09	!				
ATOM	H11Y	HAL2	0.	09	!				
GROUE	2				!				
ATOM	CD12	CTL2	-0.	18	!				
ATOM	H12X	HAL2	Ο.	09	!				
ATOM	H12Y	HAL2	Ο.	09	!				
GROUE	>				1				
ATOM	CD13	CTT.2	-0	18					
ATOM	U12V		0.	10					
ATOM		TALZ	0.	09	-				
A'I'OM	HIJY	HAL2	0.	09	!				
GROUI	2				!				
ATOM	CD14	CTL2	-0.	18	!				
ATOM	H14X	HAL2	Ο.	09	!				
ATOM	H14Y	HAL2	Ο.	09	!				
GROUE	2				!				
ATOM	CD15	CTL2	-0.	18	!				
ATOM	H15X	HAT.2	0	09	i.				
ATOM	u15v	UNT 2	0	00					
CDOUI	TITOT	IIALLZ	0.	09	-				
GROUP			0	1 0	-				
ATOM	CDI6	CTL2	-0.	18	:				
A'I'OM	H16X	HAL2	0.	09	!				
ATOM	H16Y	HAL2	0.	09	!				
GROUE	2				!				
ATOM	CD17	CTL2	-0.	18	!				
ATOM	H17X	HAL2	Ο.	09	!				
атом	н17ү	НАТ.2	0	09	1				
CROUE))	1111112	•••	0.5					
ATTOM	0010	C TT 2	0	27	-				
ATOM	ULL OV	CIT2	-0.	27	-				
ATOM	HISX	HAL3	0.	09	!				
A'I'OM	HI8X	HAL3	0.	09	!				
ATOM	H18Z	hal3	0.	09	!!				
! Gly	cerol	head	d						
BOND	C1	C2	C1	HO	511	C1	HG12		
BOND	C2	OG12	C2	HC	522	OG12	H012	C2	C3
BOND	C3	HG31	C3	HC	32				
! Pho	sphat	ces							
	- <u>-</u>								

BOND C1 OP11 C3 OP31 BOND P1 OP11 P1 OP12 P1 OP13 P1 OP14 OP31 P3 OP32 P3 OP33 P3 OP34 BOND P3 ! Glycerol Backbones BOND OP12 C11 C11 H11J C11 H11K BOND C11 C12 BOND C12 H12J C12 012 BOND C12 C13 BOND C13 H13J C13 H13K C13 O13 BOND OP32 C31 C31 H31J C31 H31K BOND C31 C32 BOND C32 H32J C32 032 BOND C32 C33 BOND C33 H33J C33 H33K C33 O33 ! Acyl chain 1 CB1 032 CC1 033 CD1 BOND 012 CA1 013 BOND CA1 OA1 CA1 CA2 H2A CA2 BOND 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 H3R CC3 BOND CC3 H3S CC3 CC4 BOND CC4 CC4 H4R 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

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 НЗҮ CD3 CD4 BOND CD4 H4X CD4 H4Y CD4 CD5 BOND CD5 H5X CD5 H5Y CD5 CD6 BOND CD6 нбх CD6 Н6Ү CD6 CD7 H7X CD7 BOND 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 013 CB2 OB1 IMPR CA1 012 CA2 OA1 IMPR CD1 033 CD2 OD1 IMPR CC1 032 CC2 OC1 *C3 1.4633 109.99 126.99 106.69 IC OP31 C2 HG31 1.1112 IC HG31 C2 *C3 HG32 1.1112 106.69 120.70 112.94 1.1110 IC C2 C3 OP31 PЗ 1.5211 109.99 154.06 117.47 1.5924 IC C3 OP31 PЗ OP32 1.4633 117.47 66.74 101.68 1.6525 OP33 1.6525 101.68 -113.70 109.39 1.4926 IC OP32 OP31 *P3 IC OP32 *P3 OP34 1.6525 101.68 112.29 106.74 OP31 1.4836 IC OP31 PЗ OP32 C31 1.5924 101.68 55.76 110.28 1.4698 110.28 -172.41 IC P3 OP32 C31 C32 1.6525 110.74 1.5958 IC C32 OP32 *C31 H31J 1.5958 110.74 116.75 110.82 1.1115 110.82 111.29 110.26 IC H31J OP32 *C31 H31K 1.1115 1.1103 -61.74 114.49 IC HG31 CЗ C2 C1 1.1112 106.69 1.5241 IC C1 *C2 OG12 1.5241 114.49 -122.33 108.64 C3 1.4665 1.5241 114.49 124.23 104.11 IC C1 *C2 CB HG22 1.1108 IC C3 C2 OG12 HO12 1.5211 108.64 -38.03 96.97 0.9599 1.5211 114.49 175.92 108.99 IC C3 C2 C1 OP11 1.3945 1.3945 108.99 -131.04 104.78 IC OP11 C2 *C1 HG11 1.1106 IC HG11 C2 *C1 HG12 1.1106 104.78 -113.14 109.09 1.1119 IC C2 C1OP11 Р1 1.5241 108.99 -84.99 120.20 1.5652 OP12 1.3945 120.20 -27.24 102.68 IC C1 OP11 Р1 1.5816 1.4705 IC OP12 OP11 *P1 OP13 1.5816 102.68 118.64 109.06 108.43 OP11 *P1 OP14 1.5816 102.68 -114.38 IC OP12 1.4438 129.51 IC OP11 Ρ1 OP12 C11 1.5652 102.68 -105.08 1.3844 IC P1 C12 129.51 79.30 OP12 C11 1.5816 113.33 1.5572 IC C12 *C11 H11J 1.5572 113.33 -123.60 109.70 OP12 1.1106 111.37 IC H11J OP12 *C11 H11K 1.1106 109.70 -125.75 1.1111 113.33 172.10 111.92 IC OP12 C11 C12 C13 1.3844 1.5430 IC C13 1.5430 111.92 120.38 106.67 1.4690 C11 *C12 012 IC 012 *C12 1.4690 106.67 123.36 105.85 1.1110 C11 H12J 1.5572 106.67 139.57 111.75 IC C11 C12 012 CA1 1.3546 1.4690 111.75 -177.04 105.16 IC C12 012 CA1 CA2 1.4819

TC	CA2	012	*CA1	OA1	1 4819	105 16 175 26	126 65	1 2359
10	012	012	0711	0111	1 2540	105.10 1/5.20	100.05	1 5144
IC	012	CAL	CAZ	CAS	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	013	1.5572	111.92 -172.11	107.78	1.5003
ТC	013	C12	*C13	н1 3.т	1 5003	107 78 -115 91	112 20	1 1109
TC	U12T	C12	* 01 2	111.00	1 1100	112 20 121 54	112.20	1 1122
IC	HIJJ		^CI3	HIJK	1.1109	112.20 -121.54	112.00	1.1122
IC	C12	C13	013	CB1	1.5430	107.78 77.67	115.10	1.2970
IC	C13	013	CB1	CB2	1.5003	115.10 -179.81	109.11	1.4434
IC	CB2	013	*CB1	OB1	1.4434	109.11 -173.82	130.35	1.2113
ТC	013	CB1	CB2	CB3	1 2970	109 11 173 87	116 83	1 5195
TC	CD 2	CD1	* CD 2	1120	1 5105	116 92 121 02	100.00	1 1110
IC	CBS	CBI	~CBZ	HZD	1.5195	110.03 -121.03	109.00	1.1112
TC	HZD	CBI	*CB2	HZE	1.1112	109.80 -114.30	107.94	1.110/
IC	OP32	C31	C32	C33	1.4698	110.74 -72.15	111.19	1.5682
IC	C33	C31	*C32	032	1.5682	111.19 124.56	112.11	1.3898
IC	032	C31	*C32	Н32Ј	1.3898	112.11 122.90	114.56	1.1112
TC	C31	C32	032	CC1	1 5958	112 11 62 25	119 56	1 3075
TC	C31	002	002	001	1 2000	110 56 174 00	104 05	1 4000
IC	032	032	CCI	CCZ	1.3898	119.56 -1/4.92	104.05	1.4829
IC	CC2	032	*CC1	OC1	1.4829	104.05 -166.47	126.62	1.2264
IC	032	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
TC	H2R	CC1	*002	н29	1 1110	107 06 -105 63	111 30	1 1109
TC	021	CC1	CC2	022	1	107.00 103.05	110.00	1 4270
IC	031	032	033	033	1.5958	111.19 -1/3./9	110.26	1.4370
IC	033	C32	*C33	H33J	1.4370	110.26 118.41	109.85	1.1107
IC	H33J	C32	*C33	НЗЗК	1.1107	109.85 116.35	110.86	1.1105
IC	C32	C33	033	CD1	1.5682	110.26 -82.05	116.23	1.3711
ТC	C33	033	CD1	CD2	1 4370	116 23 156 92	111 58	1 5654
TC	CD2	022	*CD1	001	1 5654	111 50 176 12	124 00	1 1050
IC	CDZ	033	~CDI	ODI	1.3034	111.30 -170.12	124.00	1.1050
TC	033	CDI	CD2	CD3	1.3/11	111.58 /9.99	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
TC	CDA	C 7 2	* 073	U 3 N	1 5645	117 75 _127 81	100 37	1 1111
TC		CA2	t CAD	IIJA	1 1111	100 27 117 62	101 55	1 1105
IC	HJA	CAZ	^CA3	нзв		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
TC	CA3	CA4	CA5	CA6	1 5645	111 41 74 25	110 88	1 5499
TC	CAG	C7.4	* C 7 5		1 5400	110 00 125 00	110.00	1 1111
IC	CAO	CA4	~CAJ	HJA	1.5499	110.00 -125.09	112.10	1.1114
TC	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	нба	CA5	*CA6	H6B	1.1107	112.61 -124.17	99.78	1.1108
TC	C 7 5	CN6	C 7 7	C78	1 5/99	112 07 74 00	120 92	1 5501
TC	CAJ	CAU	+ 377	UZD	1.5499	122.07 74.00	104 20	1.1105
IC	CA8	CA6	^CA/	H/A	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
тс	над	C A 7	*CA8	HSB	1 1111	114 99 -115 64	104 49	1 1114
TC	CN 7	CA /	CAO	010D	1 5501	110 70 00 64	122 44	1 2410
IC	CA/	CA8	CA9	CAIU	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
TC	CA9	CA10	CA11	CA12	1.3410	129.79 -125 54	110.53	1.5132
TC	CA12	CA10	* 07.11	u117	1 5120	110 53 -10/ 00	111 01	1 1100
тС		CALU	CAII	1111D	1 1100	111 04 116 05	110 75	1 1107
тC	нттч	CALU	^ CALL	нттв	T.TT03	111.84 -116.05	110./5	T.TTO/
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
TC	CA11	CA12	CA13	CD14	1 5132	113 10 66 70	118 /3	1 5736
тС тС		CA12	+0110	UT 1 2 7	1 5700	110 /2 110 /2	104 (2)	1 111 /
TC	CAL4	CAIZ	CAL3	ni ja	1.5/30	110.43 -112.65	104.03	1.1114
ТС	н⊥ЗА	CA12	*CA13	нізв	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

тa		0710	+ ~ 1 1	111 A D	1 1100	107 00 110 00	100 04	1 1110
IC	HI4A	CAI3	*CAI4	HI4B	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
TC	CA16	CA14	*CA15	н15д	1 5814	102 80 -121 30	114 89	1 1112
±0		0711 1	01110	111 571	1 1110	102.00 121.00	100.00	1 1110
ТC	HISA	CA14	*CAI5	HISB	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
тс	C717	C715	*0716	U167	1 4020	109 65 -121 70	105 06	1 1117
IC	CAI /	CAIS	~CAI0	HIOA	1.4920	100.05 -121.79	103.90	1.11/
IC	H16A	CA15	*CA16	H16B	1.1117	105.96 -110.08	103.15	1.1108
TC	CA15	CA16	CA17	CA18	1 5814	108 65 -168 13	114 64	1 5103
±0	07110	07110			1 51021	100.05 100.15	105 50	1 1117
ТC	CA18	CAI 6	*CAL/	HI/A	1.5103	114.64 -123.69	105.58	$\bot \bullet \bot \bot \bot \bot /$
IC	H17A	CA16	*CA17	H17B	1.1117	105.58 -117.14	106.96	1.1108
тс	C716	C 7 1 7	C710	U107	1 4020	111 61 _07 30	116 70	1 1116
ΤC	CAIO	CALI	CAIO	NIOA	1.4920	114.04 -97.30	110.70	1.1110
IC	H18A	CA17	*CA18	H18B	1.1116	116.78 -112.38	110.91	1.1109
TC	H18A	CA17	*CA18	H18C	1 1116	116 78 124 13	107 97	1 1105
- C	0D1	0112 / 0D0	0000	0D 4	1 4424	110 00 155 75	114 05	1 5000
IC	CBI	CBZ	CB3	CB4	1.4434	116.83 -155.75	114.25	1.3868
IC	CB4	CB2	*CB3	H3D	1.5868	114.25 -122.78	114.66	1.1117
TC	нзр	CB2	*CB3	нзе	1 1117	114 66 -129 44	120 87	1 1109
10	1150		CDJ	115E	1. 51.05	114.00 129.44	120.07	1.1105
ТC	CB2	CB3	CB4	CB5	1.5195	114.25 -52.65	114.56	1.513/
IC	CB5	CB3	*CB4	H4D	1,5137	114.56 - 115.68	101.27	1.1103
TC		CD 2	* CD /		1 1102	101 27 110 02	105 41	1 1106
IC	H4D	CBS	°CB4	П4 <u>С</u>	1.1103	101.27 -119.02	103.41	1.1100
IC	CB3	CB4	CB5	CB6	1.5868	114.56 -179.99	120.50	1.5634
TC	CB6	CB4	*CB5	H5D	1.5634	120.50 - 122.72	117.24	1.1113
±0	UED	CD 1	+ 000	1100	1 1110	117 04 100 04	100 45	1 1107
IC	нэр	CB4	VCB2	HDE	1.1113	11/.24 -123.34	103.45	1.110/
IC	CB4	CB5	CB6	CB7	1.5137	120.50 39.76	116.61	1.5133
тс	CB7	CB5	*CB6	46D	1 5133	116 61 -120 56	106 07	1 1110
TC		CBJ	CDO	1100	1.0100	110.01 120.00	100.07	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
τo	CD 0	CDC	+007	1170	1 5170	110 40 100 72	100 74	1 1100
ΤC	CB8	CB0	×CB/	H/D	1.51/3	110.49 -120.73	106.74	1.1100
IC	H7D	CB6	*CB7	H7E	1.1106	106.74 -117.79	112.10	1.1106
TC	CB6	CB7	CB8	CB9	1 5133	110 49 -82 21	120 66	1 5172
±0	CD 0	CD7	000	000	1 5130	100.10 02.21	100.00	1 1105
ТC	CB 9	CB /	*CB8	HSD	1.51/2	120.66 -115.86	108.05	1.1105
IC	H8D	CB7	*CB8	H8E	1.1105	108.05 -111.89	111.52	1.1117
тс	CB7	CBS	CBQ	CB10	1 5173	120 66 -107 87	126 23	1 3089
ΤC		CDO	CDJ	CDIU	1.51/5	120.00 107.07	120.25	1.5005
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
±0	CD11	CD 0	*CD10	U1 0D	1 5400	120.20 177.07	114 04	1 1001
ΤC	CBII	CBA	*CBI0	HIUD	1.5488	129.20 -1//.8/	114.84	1.1001
IC	CB9	CB10	CB11	CB12	1.3089	129.20 89.60	118.95	1.5198
тс	CB12	CB10	*CB11	н11р	1 5198	118 95 -127 92	113 12	1 1108
10	CDIZ	CDIO	CDII		1.0100	110.00 110.00	100.12	1.1100
ТC	HIID	CBIO	*CBII	HIIE	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
тс	CB13	CB11	*CB12	ם 2 ש	1 / 805	108 85 -124 66	111 86	1 1106
тC	CDIJ	CDII	CDIZ	11120	1.4005	100.05 124.00	111.00	1.1100
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
тC	CP1/	CD12	*CD12	u12D	1 5460	11/ 00 _122 70	110 67	1 1111
ΤC	CD14	CDIZ	CBIJ	птэр	1.5400	114.90 -122.78	110.07	1.1114
IC	H13D	CB12	*CB13	H13E	1.1114	110.67 -118.72	111.28	1.1107
TC	CB12	CB13	CB14	CB15	1.4805	114.90 68.37	114.96	1.5755
±0	OD 1 E	CD12	+ CD1 /	U1 4 D	1 5755	114 06 107 02	107.00	1 1104
тС	CDIC	CDIC	CD14	п140	1.0/00	114.90 -12/.83	T01.90	1.104
IC	H14D	CB13	*CB14	H14E	1.1104	107 96 -116 62	100 21	
TC	CD12					10/.00 110.02	100.21	$\bot \bullet \bot \bot \bot \bot \bot$
±0		CB14	CB15	CB16	1 5460	114 96 166 45	100.21	1.1111
ТC	CBIS	CB14	CB15	CB16	1.5460	114.96 166.45	117.74	1.5429
	CB15 CB16	CB14 CB14	CB15 *CB15	CB16 H15D	1.5460 1.5429	114.96 166.45 117.74 -122.27	117.74 110.71	1.1111 1.5429 1.1109
IC	CB15 CB16 H15D	CB14 CB14 CB14	CB15 *CB15 *CB15	CB16 H15D H15E	1.5460 1.5429 1.1109	114.96 166.45 117.74 -122.27 110.71 -117.71	108.21 117.74 110.71 99.91	1.1111 1.5429 1.1109 1.1101
IC	CB15 CB16 H15D CB14	CB14 CB14 CB14 CB15	CB15 *CB15 *CB15 CB16	CB16 H15D H15E CB17	1.5460 1.5429 1.1109	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	108.21 117.74 110.71 99.91	1.1111 1.5429 1.1109 1.1101
IC IC	CB15 CB16 H15D CB14	CB14 CB14 CB14 CB15	CB15 *CB15 *CB15 CB16	CB16 H15D H15E CB17	1.5460 1.5429 1.1109 1.5755	114.96 166.45 117.74 -122.27 110.71 -117.71 117.74 174.50	108.21 117.74 110.71 99.91 116.45	1.1111 1.5429 1.1109 1.1101 1.5273
IC IC IC	CB13 CB16 H15D CB14 CB17	CB14 CB14 CB15 CB15 CB15	CB15 *CB15 *CB15 CB16 *CB16	CB16 H15D H15E CB17 H16D	1.5460 1.5429 1.1109 1.5755 1.5273	114.96 166.45 117.74 -122.27 110.71 -117.71 117.74 174.50 116.45 -126.26	108.21 117.74 110.71 99.91 116.45 106.79	1.1111 1.5429 1.1109 1.1101 1.5273 1.1119
IC IC IC IC	CB13 CB16 H15D CB14 CB17 H16D	CB14 CB14 CB14 CB15 CB15 CB15	CB15 *CB15 *CB15 CB16 *CB16 *CB16	CB16 H15D H15E CB17 H16D H16E	1.5460 1.5429 1.1109 1.5755 1.5273 1.1119	114.96 166.45 117.74 -122.27 110.71 -117.71 117.74 174.50 116.45 -126.26 106.79 -120.93	108.21 117.74 110.71 99.91 116.45 106.79 108.80	1.1111 1.5429 1.1109 1.1101 1.5273 1.1119 1.1106
IC IC IC IC	CB13 CB16 H15D CB14 CB17 H16D CP15	CB14 CB14 CB14 CB15 CB15 CB15 CB15	CB15 *CB15 *CB15 CB16 *CB16 *CB16 CB17	CB16 H15D H15E CB17 H16D H16E CB18	1.5460 1.5429 1.1109 1.5755 1.5273 1.1119	114.96 166.45 117.74 -122.27 110.71 -117.71 117.74 174.50 116.45 -126.26 106.79 -120.93	108.21 117.74 110.71 99.91 116.45 106.79 108.80	1.1111 1.5429 1.1109 1.1101 1.5273 1.1119 1.1106
IC IC IC IC IC	CB13 CB16 H15D CB14 CB17 H16D CB15	CB14 CB14 CB15 CB15 CB15 CB15 CB16	CB15 *CB15 *CB15 CB16 *CB16 *CB16 CB17	CB16 H15D CB17 H16D H16E CB18	1.5460 1.5429 1.1109 1.5755 1.5273 1.1119 1.5429	114.96 166.45 117.74 -122.27 110.71 -117.71 117.74 174.50 116.45 -126.26 106.79 -120.93 116.45 176.52	108.21 117.74 110.71 99.91 116.45 106.79 108.80 110.28	1.1111 1.5429 1.1109 1.1101 1.5273 1.1119 1.1106 1.5697
IC IC IC IC IC IC	CB13 CB16 H15D CB14 CB17 H16D CB15 CB18	CB14 CB14 CB15 CB15 CB15 CB15 CB16 CB16	CB15 *CB15 *CB15 CB16 *CB16 *CB16 CB17 *CB17	CB16 H15D H15E CB17 H16D H16E CB18 H17D	1.5460 1.5429 1.1109 1.5755 1.5273 1.1119 1.5429 1.5697	114.96 166.45 117.74 -122.27 110.71 -117.71 117.74 174.50 116.45 -126.26 106.79 -120.93 116.45 176.52 110.28 -130.06	108.21 117.74 110.71 99.91 116.45 106.79 108.80 110.28 105.87	1.1111 1.5429 1.1109 1.1101 1.5273 1.1119 1.1106 1.5697 1.1105
IC IC IC IC IC IC IC	CB13 CB16 H15D CB14 CB17 H16D CB15 CB18 H17D	CB14 CB14 CB15 CB15 CB15 CB15 CB16 CB16 CB16	CB15 *CB15 *CB15 CB16 *CB16 *CB16 CB17 *CB17 *CB17	CB16 H15D H15E CB17 H16D H16E CB18 H17D H17E	1.5460 1.5429 1.1109 1.5755 1.5273 1.1119 1.5429 1.5697 1.1105	114.96 166.45 117.74 -122.27 110.71 -117.71 117.74 174.50 116.45 -126.26 106.79 -120.93 116.45 176.52 110.28 -130.06 105.87 -115.72	108.21 117.74 110.71 99.91 116.45 106.79 108.80 110.28 105.87 106.22	1.1111 1.5429 1.1109 1.1101 1.5273 1.1119 1.1106 1.5697 1.1105 1.1106
IC IC IC IC IC IC	CB13 CB16 H15D CB14 CB17 H16D CB15 CB18 H17D CB16	CB14 CB14 CB15 CB15 CB15 CB15 CB16 CB16 CB16 CB17	CB15 *CB15 *CB15 CB16 *CB16 *CB16 CB17 *CB17 *CB17 CB17	CB16 H15D H15E CB17 H16D H16E CB18 H17D H17E	1.5460 1.5429 1.1109 1.5755 1.5273 1.1119 1.5429 1.5697 1.1105	114.96 166.45 117.74 -122.27 110.71 -117.71 117.74 174.50 116.45 -126.26 106.79 -120.93 116.45 176.52 110.28 -130.06 105.87 -115.72	108.21 117.74 110.71 99.91 116.45 106.79 108.80 110.28 105.87 106.22	1.1111 1.5429 1.1109 1.1101 1.5273 1.1119 1.1106 1.5697 1.1105 1.1106
IC IC IC IC IC IC IC	CB13 CB16 H15D CB14 CB17 H16D CB15 CB18 H17D CB16	CB14 CB14 CB15 CB15 CB15 CB15 CB16 CB16 CB16 CB17	CB15 *CB15 *CB15 CB16 *CB16 *CB16 CB17 *CB17 *CB17 CB18	CB16 H15D H15E CB17 H16D H16E CB18 H17D H17E H18D	1.5460 1.5429 1.1109 1.5755 1.5273 1.1119 1.5429 1.5697 1.1105 1.5273	114.96 166.45 117.74 -122.27 110.71 -117.71 117.74 174.50 116.45 -126.26 106.79 -120.93 116.45 176.52 110.28 -130.06 105.87 -115.72 110.28 -159.07	108.21 117.74 110.71 99.91 116.45 106.79 108.80 110.28 105.87 106.22 103.32	1.1111 1.5429 1.1109 1.1101 1.5273 1.1119 1.1106 1.5697 1.1105 1.1106 1.1112
IC IC IC IC IC IC IC IC IC	CB13 CB16 H15D CB14 CB17 H16D CB15 CB18 H17D CB16 H18D	CB14 CB14 CB15 CB15 CB15 CB16 CB16 CB16 CB17 CB17	CB15 *CB15 *CB15 CB16 *CB16 *CB16 CB17 *CB17 *CB17 CB18 *CB18	CB16 H15D H15E CB17 H16D H16E CB18 H17D H17E H18D H18E	1.5460 1.5429 1.1109 1.5755 1.5273 1.1119 1.5429 1.5697 1.1105 1.5273 1.1112	114.96 166.45 117.74 -122.27 110.71 -117.71 117.74 174.50 116.45 -126.26 106.79 -120.93 116.45 176.52 110.28 -130.06 105.87 -115.72 110.28 -159.07 103.32 -120.33	108.21 117.74 110.71 99.91 116.45 106.79 108.80 110.28 105.87 106.22 103.32 105.93	1.1111 1.5429 1.1109 1.1101 1.5273 1.1119 1.1106 1.5697 1.1105 1.1106 1.1112 1.1103
IC IC IC IC IC IC IC IC IC	CB13 CB16 H15D CB14 CB17 H16D CB15 CB18 H17D CB16 H18D H18D	CB14 CB14 CB15 CB15 CB15 CB16 CB16 CB16 CB17 CB17 CB17	CB15 *CB15 *CB15 CB16 *CB16 *CB16 CB17 *CB17 *CB17 CB18 *CB18 *CB18	CB16 H15D H15E CB17 H16D H16E CB18 H17D H17E H18D H18E H18F	1.5460 1.5429 1.1109 1.5755 1.5273 1.1119 1.5429 1.5697 1.1105 1.5273 1.1112 1.1112	114.96 166.45 117.74 -122.27 110.71 -117.71 117.74 174.50 116.45 -126.26 106.79 -120.93 116.45 176.52 110.28 -130.06 105.87 -115.72 110.28 -159.07 103.32 -120.33 103.32 118.79	108.21 117.74 110.71 99.91 116.45 106.79 108.80 110.28 105.87 106.22 103.32 105.93 110.62	1.1111 1.5429 1.1109 1.1101 1.5273 1.1119 1.1106 1.5697 1.1105 1.1105 1.1106 1.1112 1.1103 1.1116
IC IC IC IC IC IC IC IC IC	CB13 CB16 H15D CB14 CB17 H16D CB15 CB18 H17D CB16 H18D H18D CC1	CB14 CB14 CB15 CB15 CB15 CB16 CB16 CB16 CB16 CB17 CB17 CB17 CB17	CB15 *CB15 *CB15 CB16 *CB16 *CB16 CB17 *CB17 *CB17 *CB17 CB18 *CB18 *CB18 *CB18	CB16 H15D H15E CB17 H16D H16E CB18 H17D H17E H18D H18E H18F CC4	1.5460 1.5429 1.1109 1.5755 1.5273 1.1119 1.5429 1.5697 1.1105 1.5273 1.1112 1.1112	114.96 166.45 117.74 -122.27 110.71 -117.71 117.74 174.50 116.45 -126.26 106.79 -120.93 116.45 176.52 110.28 -130.06 105.87 -115.72 110.28 -159.07 103.32 -120.33 103.32 118.79	108.21 117.74 110.71 99.91 116.45 106.79 108.80 110.28 105.87 106.22 103.32 105.93 110.62	1.1111 1.5429 1.1109 1.1101 1.5273 1.1119 1.1106 1.5697 1.1105 1.1106 1.1112 1.1103 1.1116
IC IC IC IC IC IC IC IC IC IC	CB13 CB16 H15D CB14 CB17 H16D CB15 CB18 H17D CB16 H18D H18D CC1	CB14 CB14 CB15 CB15 CB15 CB16 CB16 CB16 CB17 CB17 CB17 CC2	CB15 *CB15 *CB15 CB16 *CB16 *CB16 CB17 *CB17 *CB17 *CB17 CB18 *CB18 *CB18 *CB18 CC3	CB16 H15D H15E CB17 H16D H16E CB18 H17D H17E H18D H18E H18F CC4	1.5460 1.5429 1.1109 1.5755 1.5273 1.1119 1.5429 1.5697 1.1105 1.5273 1.1112 1.1112 1.1112 1.4829	114.96 166.45 117.74 -122.27 110.71 -117.71 117.74 174.50 116.45 -126.26 106.79 -120.93 116.45 176.52 110.28 -130.06 105.87 -115.72 110.28 -159.07 103.32 -120.33 103.32 118.79 115.59 49.93	108.21 117.74 110.71 99.91 116.45 106.79 108.80 110.28 105.87 106.22 103.32 105.93 110.62 117.90	1.1111 1.5429 1.1109 1.1101 1.5273 1.1119 1.1106 1.5697 1.1105 1.1106 1.1112 1.1103 1.1116 1.5366
IC IC IC IC IC IC IC IC IC IC IC IC	CB13 CB16 H15D CB14 CB17 H16D CB15 CB18 H17D CB16 H18D H18D CC1 CC4	CB14 CB14 CB15 CB15 CB15 CB16 CB16 CB16 CB17 CB17 CB17 CC2 CC2	CB15 *CB15 *CB15 CB16 *CB16 *CB16 CB17 *CB17 *CB17 *CB17 CB18 *CB18 *CB18 *CB18 *CB18 CC3 *CC3	CB16 H15D H15E CB17 H16D H16E CB18 H17D H17E H18D H18E H18F CC4 H3R	1.5460 1.5429 1.1109 1.5755 1.5273 1.1119 1.5429 1.5697 1.1105 1.5273 1.1112 1.1112 1.1112 1.4829 1.5366	114.96 166.45 117.74 -122.27 110.71 -117.71 117.74 174.50 116.45 -126.26 106.79 -120.93 116.45 176.52 110.28 -130.06 105.87 -115.72 110.28 -159.07 103.32 -120.33 103.32 118.79 115.59 49.93 117.90 -115.05	108.21 117.74 110.71 99.91 116.45 106.79 108.80 110.28 105.87 106.22 103.32 105.93 110.62 117.90 111.28	1.1111 1.5429 1.1109 1.1101 1.5273 1.1119 1.1106 1.5697 1.1105 1.1106 1.1105 1.1106 1.1112 1.1103 1.1116 1.5366 1.1107
IC IC IC IC IC IC IC IC IC IC IC IC	CB13 CB16 H15D CB14 CB17 H16D CB15 CB18 H17D CB16 H18D H18D CC1 CC4 H3R	CB14 CB14 CB15 CB15 CB15 CB16 CB16 CB16 CB17 CB17 CB17 CC2 CC2 CC2 CC2	CB15 *CB15 *CB15 CB16 *CB16 *CB16 *CB16 CB17 *CB17 *CB17 *CB17 CB18 *CB18 *CB18 *CB18 CC3 *CC3 *CC3	CB16 H15D H15E CB17 H16D H16E CB18 H17D H17E H18D H18E H18F CC4 H3R H3S	1.5460 1.5429 1.1109 1.5755 1.5273 1.1119 1.5429 1.5697 1.1105 1.5273 1.1112 1.1112 1.4829 1.5366 1.1107	114.96 166.45 117.74 -122.27 110.71 -117.71 117.74 174.50 116.45 -126.26 106.79 -120.93 116.45 176.52 110.28 -130.06 105.87 -115.72 110.28 -159.07 103.32 118.79 115.59 49.93 117.90 -115.05 11.28 -122.62	108.21 117.74 110.71 99.91 116.45 106.79 108.80 110.28 105.87 106.22 103.32 105.93 110.62 117.90 111.28 109.57	1.1111 1.5429 1.1109 1.1101 1.5273 1.1119 1.1106 1.5697 1.1105 1.1106 1.1102 1.1103 1.1116 1.5366 1.1107 1.1107
IC IC IC IC IC IC IC IC IC IC IC IC IC I	CB13 CB16 H15D CB14 CB17 H16D CB15 CB18 H17D CB16 H18D H18D CC1 CC4 H3R CC2	CB14 CB14 CB15 CB15 CB15 CB16 CB16 CB16 CB17 CB17 CB17 CC2 CC2 CC2 CC2	CB15 *CB15 *CB15 CB16 *CB16 *CB16 CB17 *CB17 *CB17 CB18 *CB18 *CB18 *CB18 *CC3 *CC3 *CC3	CB16 H15D H15E CB17 H16D H16E CB18 H17D H17E H18D H18E H18F CC4 H3R H3S CC5	1.5460 1.5429 1.1109 1.5755 1.5273 1.1119 1.5429 1.5697 1.1105 1.5273 1.1112 1.1112 1.4829 1.5366 1.1107	114.96 166.45 117.74 -122.27 110.71 -117.71 117.74 174.50 116.45 -126.26 106.79 -120.93 116.45 176.52 110.28 -130.06 105.87 -115.72 110.28 -159.07 103.32 -120.33 103.32 118.79 115.59 49.93 117.90 -115.05 11.28 -122.62	108.21 117.74 110.71 99.91 116.45 106.79 108.80 110.28 105.87 106.22 103.32 105.93 110.62 117.90 111.28 109.57	1.1111 1.5429 1.1109 1.1101 1.5273 1.1119 1.1106 1.5697 1.1105 1.1106 1.1112 1.1103 1.1116 1.5366 1.1107 1.1107
IC IC IC IC IC IC IC IC IC IC IC IC IC I	CB13 CB16 H15D CB14 CB17 H16D CB15 CB18 H17D CB16 H18D H18D CC1 CC4 H3R CC2	CB14 CB14 CB15 CB15 CB15 CB16 CB16 CB16 CB17 CB17 CB17 CC2 CC2 CC2 CC2 CC3	CB15 *CB15 *CB15 CB16 *CB16 *CB16 CB17 *CB17 *CB17 *CB17 CB18 *CB18 *CB18 *CB18 *CB18 CC3 *CC3 *CC3 *CC3 CC4	CB16 H15D H15E CB17 H16D H16E CB18 H17D H17E H18D H18E H18F CC4 H3R H3S CC5	$\begin{array}{c} 1.5460\\ 1.5429\\ 1.1109\\ 1.5755\\ 1.5273\\ 1.1119\\ 1.5429\\ 1.5697\\ 1.1105\\ 1.5273\\ 1.1112\\ 1.1112\\ 1.4829\\ 1.5366\\ 1.1107\\ 1.5435 \end{array}$	114.96 166.45 117.74 -122.27 110.71 -117.71 117.74 174.50 116.45 -126.26 106.79 -120.93 116.45 176.52 110.28 -130.06 105.87 -115.72 110.28 -159.07 103.32 -120.33 103.32 118.79 115.59 49.93 117.90 -115.05 11.28 -122.62 117.90 41.42	108.21 117.74 110.71 99.91 116.45 106.79 108.80 110.28 105.87 106.22 103.32 105.93 110.62 117.90 111.28 109.57 122.16	1.1111 1.5429 1.1109 1.1101 1.5273 1.1119 1.1106 1.5697 1.1105 1.1106 1.1105 1.1106 1.1112 1.1103 1.1116 1.5366 1.1107 1.1107 1.4856

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
TC	H6R	CC5	*006	H6S	1 1104	99 65 -115 34	114 89	1 1110
TC	CC5	CC6	CC7	CC8	1 5779	114 14 86 04	111 08	1 5443
TC	CC8	CC6	*CC7	660 Н7В	1 5443	111 08 -126 84	118 56	1 1115
TC	UC0 Н7В	CC6	*CC7	H7S	1 1115	118 56 -116 67	107 70	1 1111
TC	CC6	CC7	CC8	CC 9	1 5103	111 08 -167 74	113 25	1 5055
TC	CC0	CC7	*~~~	LOD	1 5055	112 25 _126 00	111 16	1 1112
TC	LOD	CC7	*	101	1 1112	111 16 -112 40	107 06	1 1105
TC	CC7			по5	1 5442	112 25 100 97	126 20	1 2527
TC			+		1 2527	126.20 170.02	110 50	1 0000
TC			^CC9	HYR CC11	1 5055/	126.39 -170.92	120.30	1 4 6 2 0
IC	008	009	+ 2 2 1 0		1.5955	120.39 15.86	128.70	1.4629
IC		009	^CCIU	HIUR	1.4629	128.70 175.07	123.34	1.1002
IC	CC9	CCIO	CCII	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	HIIR	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
TC	CC16	CC17	CC18	H18R	1.5605	113.48 -167.53	105.19	1.1114
TC	H18R	CC17	*CC18	H18S	1.1114	105.19 123.30	114.77	1.1107
TC	H18R	CC17	*CC18	н18т	1 1114	105 19 -120 49	105 29	1 1117
TC	CD1	CD2	CD3	CD4	1.5654	113.19 -162.40	114.80	1.5512
TC	CD4	CD2	*CD3	нзх	1 5512	114 80 -117 81	118 26	1 1102
TC	нзх	CD2	*CD3	нзу	1 1102	118 26 -125 60	110 95	1 1112
TC	CD2	CD2	CD4	CD5	1 5154	114 80 63 81	109 67	1 6095
TC	CD5	CD3	*CD4	HAX	1 6095	109 67 -112 22	109.07	1 1107
TC	HAY	CD3	*CD4	HAV	1 1107	109.67 112.22	110 95	1 1100
TC	CD3	CD4	CD5	CD6	1 5512	109.67 -171 66	110.00	1 5117
TC	CDS	CD4 CD4	*CD5	USV	1 5117	110 10 _112 00	105 22	1 1100
TC	CDO	CD4 CD4	*CD5	ПЈА	1 1100	105 22 120 00	110.25	1 1100
TC	CD4	CD4 CD5	~CDJ		1.1100	103.23 -120.00	111 04	1 5055
TC	CD4 CD7	CDS			1 5055	110.10 170.09	105 25	1.3033
TC		CD5	*CD6	НОХ	1.5055	111.04 -114.76	105.35	1 1100
TC TC	ных	CDC	^ CD6	гон	1 5117	111 04 170 00	115 71	1.1108
IC	CD5	CD6	CD7	CD8	1.511/	111.04 -1/2.02	115./1	1.5289
тс	CD8	CD6	^ CD /	п/Х	1.5289	110./1 -123.94	107.05	1 1100
TC TC	н/Х	CD6		п/1	1.1110	114.08 -126./8	LU/.85	1.1109
тC	CD6	CD7	CDS	CD9	1.5055	115./1 -61.83	11/.36	1.5186
1C	CD9	CD/	*CD8	нвх	1.5186	11/.36 -129.63	101.79	1.1109
ТС	ных	CD/	×CD8	нах	1.1109	101./9 -111.91	105.86	1.1107
IC	CD'/	CD8	CD9	CD10	1.5289	11/.36 179.97	120.32	1.3356
IC	CD10	CD8	*CD9	н9х	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	HlOX	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

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 | (-) | (-) | ! ! 1 CH2 - PO4 - CH2 - CH - CH2 - PO4 - CH2 1 ! Derived from CDL ! by Stuart Rose 9/29/2013 ! ! GROUP ATOM C1 CTL1 0.14 ! ATOM H1 HAL1 0.09 ! ATOM H1 HAL1 _____ 1 ATOM 01 OHL -0.66 ! ATOM HO1 HOL 0.43 ! Н1---С1-О1-НО1 GROUP -0.08 ! 0.09 ! 0.09 ! ATOM CA2 CTL2 НА22---СА2---НА21 ATOM HA21 HAL2 ATOM HA22 HAL2 \ / · · P (-)OA3 OA2 ATOM PA2 PL 1.50 ! / \ ATOM 0A3 02L -0.78 ! PA2(+) -0.78 ! ATOM OA4 O2L (-)OA4 OA5 ATOM OA2 OSLP -0.57 ! 1 ATOM OA5 OSLP -0.57 ! -0.08 ! 0.09 ! ATOM CA3 CTL2 HA31---CA3---HA32 ATOM HA31 HAL2 0.09 ! ATOM HA32 HAL2 GROUP ! | ATOM CB2 CTL2 -0.08 ! HB22---CB2---HB21 | 0.09 ! | 0.09 ! | 0.09 ! (-) OB3 OB2 .50 ! \/ -0.78 ! PB2 (+) -0.78 ! / \ ATOM HB21 HAL2 ATOM HB22 HAL2 ATOM PB2 PL 1.50 ! ATOM OB3 O2L -0.78 ! PB2(+) ATOM OB4 O2L -0.57 ! (-)OB4 OB5 -0.57 ! | ATOM OB2 OSLP ATOM OB5 OSLP ATOM CB3 CTL2 -0.08 ! HB31---CB3---HB32 |

ATOM HB31 ATOM HB32 GROUP	HAL2 HAL2	0.09 ! 0.09 ! !	I	
ATOM CA4	CTL1	0.17 !	I	HA4CA4
ATOM HA4	HAL1	0.09 !		
ATOM OA6	OSL	-0.49 !		OA6 OA7
ATOM CA5	CL 0	.90 !	I	$\langle //$
ATOM OA7	OBL	-0.63 !		CA5 I
ATOM CIZ	CTLZ	-0.22 !		
ATOM H2K	HALZ	0.09 !		
GROUP	TALZ	0.09 :	1	
GIGODI			1	1 1
ATOM CA6	CTL2	0.08 !		HA61CA6HA62
АТОМ НА61	HAL2	0.09 !		
ATOM HA62	HAL2	0.09 !		OA8 OA9
ATOM OA8	OSL	-0.49 !		\ //
ATOM CA7	CL 0	.90 !	I	CA7
ATOM OA9	OBL	-0.63 !		
ATOM C22	CTL2	-0.22 !		H2LC22H2R
ATOM H2R	HAL2	0.09 !		
ATOM H2L	HAL2	0.09 !	I	
GROUP		! tail 1		
ATOM C13	CTL2	-0.18 !		
ATOM H3K	HAL2	0.09 !		H3KC13H3L
ATOM H3L	HALZ	0.09 !		
ATOM C14	CTT.2	: -0 18 I		
ATOM H4K	HAL2	0.10 :		нак ———С14———Н4т. I
ATOM H4L	HAL2	0.09 !		
GROUP		!		
ATOM C15	CTL2	-0.18 !	I	
АТОМ Н5К	HAL2	0.09 !		H5KC15H5L
ATOM H5L	HAL2	0.09 !		
GROUP		!		
ATOM C16	CTL2	-0.18 !	I	
ATOM H6K	HALZ	0.09 !		НокСтоног
CROUP	NALZ	0.09 :		
ATOM C17	CTL2	-0.18 !		
ATOM H7K	HAL2	0.09 !		Н7КС17Н7L
ATOM H7L	HAL2	0.09 !		
GROUP		!		
ATOM C18	CTL2	-0.18 !		
ATOM H8K	HAL2	0.09 !		H8KC18H8SL
ATOM H8L	HAL2	0.09 !		
ATOM C10	CTT 2	! _0 10 I		
ATOM H9K	HAL2	0.09.1		і і няк ———С19———няст. І
ATOM H9L	HAL2	0.09 !		
GROUP		!		
ATOM C110	CTL2	-0.18 !		
ATOM H10K	HAL2	0.09 !		H10KC110H10L
ATOM H10L	HAL2	0.09 !		
GROUP		!		
ATOM C111	CEL1	-0.15 !		
ATOM HIIK	ныгт	U.15 !		
ATOM C112	CFT.1	-0 15 I	1	
	TTTT	···· ·	1	

Ι

' ATOM H12K HEL1 0.15 ! GROUP 1 ATOM C113 CTL2 -0.18 ! ATOM H13K HAL2 0.09 ! ATOM H13L HAL2 0.09 ! GROUP 1 ATOM C114 CTL2 -0.18 ! ATOM H14K HAL2 0.09 ! ATOM H14L HAL2 0.09 ! GROUP 1 ATOM C115 CTL2 -0.18 ! ATOM H15K HAL2 0.09 ! 0.09 ! ATOM H15L HAL2 GROUP ATOM C116 CTL2 -0.18 ! ATOM H16K HAL2 0.09 ! ATOM H16L HAL2 0.09 ! GROUP 1 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 1 ATOM C24 CTL2 -0.18 ! ATOM H4R HAL2 0.09 ! ATOM H4S HAL2 0.09 ! GROUP 1 ATOM C25 CTL2 -0.18 ! ATOM H5R HAL2 0.09 ! ATOM H5S HAL2 0.09 ! GROUP 1 ATOM C26 CTL2 -0.18 ! ATOM H6X HAL2 0.09 ! ATOM H6Y HAL2 0.09 ! GROUP 1 ATOM C27 CTL2 -0.18 ! ATOM H7R HAL2 0.09 ! ATOM H7S HAL2 0.09 ! GROUP 1 ATOM C28 CTL2 -0.18 ! ATOM H8R HAL2 0.09 ! ATOM H8S HAL2 0.09 ! GROUP 1 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 1

H12K---C112 | 1 H13K---C113--H13L | H14K---C114--H14L H15K---C115--H15L 1 H16K---C116--H16L H17K---C117--H17L H18K---C118--H18L 1 H18M H3R ---C23---H3S H4R ---C24---H4S H5R ---C25---H5S H6R ---C26---H6S H7R ---C27---H7S H8R ---C28---H8S H9R ---C29---H9S 1 H10R---C210---H10S H11R---C211 || (CIS)

ATOM C212 CTL2 -0.18 ! ATOM H12R HAL2 0.09 ! H12R---C212 GROUP 1 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 ! 1 GROUP 1 ATOM C215 CTL2 -0.18 ! ATOM H15R HAL2 0.09 ! ATOM H15S HAL2 0.09 ! H15R---C215--H15S GROUP ATOM C216 CTL2 -0.18 ! ATOM H16R HAL2 0.09 ! H16R---C216--H16S ATOM H16S HAL2 0.09 ! GROUP 1 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 ! Н18Т GROUP 1 ATOM CB4 CTL1 0.17 ! НВ4---СВ4-----ATOM HB4 HAL1 0.09 ! ATOM OB6 OSL -0.49 ! OB6 OB7 1 //ATOM CB5 CL 0.90 ! ATOM OB7 OBL -0.63 ! CB5 ATOM C32 CTL2 -0.22 ! ATOM H2X HAL2 0.09 ! Н2Х ---С32---Н2Ү | ATOM H2Y HAL2 | 0.09 ! GROUP ! ATOM CB6 CTL2 0.08 ! НВ61---СВ6---НВ62 ATOM HB61 HAL2 0.09 ! OB8 OB9 ATOM HB62 HAL2 0.09 ! ATOM OB8 OSL \ // -0.49 ! ATOM CB7 CL 0.90 ! CB7 ATOM OB9 OBL -0.63 ! 1 H2Q---C42---H2W ATOM C42 CTL2 -0.22 ! ATOM H3Q HAL2 0.09 ! ATOM H3W HAL2 0.09 ! 1 GROUP ! tail 3 ATOM C33 CTL2 -0.18 ! НЗХ ---СЗЗ---НЗҮ | ATOM H3X HAL2 0.09 !

ATOM H3	3Y	HAL2	0.09	!		
GROUP	~ 4	0.577.0	!	1.0		
ATOM C:	34	CTLZ	-0	.18	!	
A'I'OM H4	4X	HAL2	0.09	!		H4YC34H4X
ATOM H4 GROUP	4Y	HAL2	0.09	!		
ATOM C3	35	CTL2	-0.18	!		
ATOM HS	5X	HAL2	0.09	1		H5XC35H5Y
ATOM H	5Y	HAT.2	0 09			
GROUP		111112	!	•		
ATOM C3	36	CTL2	-0.18	!		
ATOM HE	5X	HAL2	0.09	!		Н6ХСЗ6Н6Ү
ATOM HE GROUP	6Y	HAL2	0.09 !	!		
ATOM C3	37	CTL2	-0.18	!		
ATOM HT	7X	HAL2	0.09	!		H7XC37H7Y
ATOM H	7Y	HAL2	0.09	1		I I
GROUP	-		!	·		i i
ATOM C3	38	CTL2	-0	.18	!	
ATOM H8	ЗX	hal2	0.09	!		H8XC38H8Y
ATOM H8	ΒY	HAL2	0.09	!		
GROUP			!			
ATOM C	39	CTL2	-0	.18	1	i i
ATOM H	AX	HAT.2	0 0 9	1	•	нохСзоносу
111011 111	//1	111112	0.05	•		
ATOM HS	9Y	HAL2	0.09	!		
GROUP			!			
ATOM C?	310	CTT.2	-0	18	1	
ATOM UI	10v	UNT 2	0 0 0		•	u10yC310u10y
AIOM III	LUX	IIALLZ	0.09	•		
ATOM H1	10Y	HAL2	0.09	!		
GROUP			!			
ATOM C?	311	CEL1	-0 15	1		
ATOM UI	11v		0.15			u11yC311
CDOUD	LIA		0.13	-		
GROUP		o = = 1	0 1 5	:		
ATOM C:	312	CELI	-0.15	1		
ATOM H1	12X	HEL1	0.15	!		H12XC312
GROUP				!		
ATOM C3	313	CTL2	-0.18	!		
ATOM H1	L3X	HAL2	0.09	!		H13XC313H13Y
3 TOM 111	1 2 37		0 00			
ATOM HI	131	HALZ	0.09	:		
GROUP				!		
ATOM C:	314	CTL2	-0.18	!		
ATOM H1	14X	HAL2	0.09	!		H14XC314H14Y
ATOM H1	14Y	hal2	0.09	!		
GROUP				!		
ATOM C3	315	CTL2	-0.18	!		
ATOM H1	15X	HAL2	0.09	!		H15XC315H15Y
ATOM H1	1.5Y	HAL2	0.09	1		
GROUP			0.00	1		
ATTOM CO	216	CTTT 2	_0 10			
ATOM UI	1 GV		0.10	-		
ATOM HI		HALZ	0.09	-		HI0XC310HI01
ATOM HI	LGI	HALZ	0.09	!		
GROUP				!		
ATOM C3	317	CTL2	-0.18	!		
ATOM H1	17X	HAL2	0.09	!		Н17ХС317Н17Ү
ATOM H1	17Y	HAL2	0.09	!		
GROUP				!		
ATOM C	318	CTL3	-0.27	!		
ATOM H1	18X	HAT.3	0 09	1		Н18ХС318Н18У
ΔTOM U1	1 8 V	ндт.З	0.00			
	107	C TATI	0.09	-		
ATOM H	LÖΖ	пАЦЗ	0.09	1		HIQ7

GROUE	þ		!	tail4
ATOM	C43	CTL2	-0.18	!
ATOM	НЗQ	HAL2	0.09 !	!
ATOM	нзพ	HAL2	0.09 !	!
GROUE	2		!	!
ATOM	C44	CTL2	-0.18 !	!
ATOM	Н4О	HAL2	0.09	1
ATOM	H4W	HAL2	0.09	1
GROUE	>			
ATOM	C45	CTL2	-0.18	
АТОМ	H50	HAT.2	0.09	1
ATOM	н5W	HAT.2	0 09	
GROUF	>	111112	0.05	•
ATOM	C46	CTT-2	-0 18	•
	н60	HAL2	0 09 1	•
	н6у н6у	HAL2	0.09	
CROUE		IIAUZ	0.05	
ATTOM	C17	CTT 2	_0 18 1	I
ATOM	U70		0.10	:
ATOM	п/Q 117м		0.09	1
CDOUL	п/М	ПАЦА	0.09	1
GROUE A TOM	C10	C TT 2	0 1 0	1
ATOM	C40		-0.10	
ATOM	HSQ	HALZ	0.09	
ATOM GROUIT	HSM	HALZ	0.09	
GROUE	~	~~~ ^	0 1 0	
ATOM	C49	CTL2	-0.18	
ATOM	H9Q	HAL2	0.09	
ATOM	H9W	HAL2	0.	.09 !
GROUE	2		!	
ATOM	C410	CTL2	-0.18 !	
ATOM	H10Q	HAL2	0.09 !	
ATOM	H10W	HAL2	0.	.09 !
GROUE	2		!	
ATOM	C411	CEL1	-0.15 !	
ATOM	H11Q	HEL1	0.15 !	
GROUE	2		!	
ATOM	C412	CEL1	-0.18 !	!
ATOM	H12Q	HEL1	0.09 !	!
GROUE	2		!	!
ATOM	C413	CTL2	-0.18 !	!
ATOM	H13Q	HAL2	0.09 !	!
ATOM	H13W	HAL2	0.09 !	!
GROUE	2		!	!
ATOM	C414	CTL2	-0.18 !	!
ATOM	H14Q	HAL2	0.09 !	!
ATOM	H14W	HAL2	0.09 !	!
GROUE	>		!	!
ATOM	C415	CTL2	-0.18 !	!
ATOM	Н150	HAL2	0.09	1
ATOM	H15W	HAL2	0.09	1
GROUE	þ			1
ATOM	C416	CTL2	-0.18	1
АТОМ	H160	HAL2	0.09	1
АТОМ	H16W	HAT.2	0.09	1
GROUF	>			1
ATOM	C417	CTL2	-0.18	
ATOM	H170	НДТ.2	0 09 1	•
	нт / У н1 7 м		0.00	I
CRUIT) 117 \ M	שעתוי	0.09	I
	CAIR	ר ער א	-0 27	I
	U120	СТТЭ	0.2/	I
	нтоу Н1 Ям	CTENT CTENT	0.09	I
	H18C	HDT 3	0.09	I
111011	TTOG	כתעוו	0.09	

H3QC43H3W
H4QC44H4W
H5QC45H5W
н6QС46н6W
H7QC47H7W
н8QС48н8W
н90с49н9W
н10QС410н10W
 H11QC411 (CIS)
H12QC412
H13QC413H13W
 H14QC414H14W
 H15QC415H15W
 H16QC416H16W
 H17QC417H17W
 H18QC418H18W
HI8G

Ι

BOND C1 H1 C1 01 01 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 CA6 HA61 BOND CA4 CA6 CA6 HA62 CA4 OA6 BOND CA6 OA8 OB5 CB3 CB3 HB31 CB3 HB32 CB4 CB6 BOND CB3 CB4 CB4 HB4 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 C15 C14 H4L 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 C115 H15L BOND C115 H15K 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 C25 C24 H4S BOND C25 C25 H5S C25 C26 H5R BOND C26 H6R C26 H6S C26 C27 C27 BOND C27 H7R 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 нзх C33 НЗҮ C33 C34 C34 C34 C35 BOND C34 H4X H4Y C35 H5Y C35 C36 BOND C35 H5X СЗ6 Н6Ү C36 C37 BOND C36 H6X СЗ7 Н7Ү BOND C37 H7X C37 C38 C38 H8Y BOND C38 H8X C38 C39

BOND C39 H9X СЗ9 Н9Ү СЗ9 СЗ10 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 C317 H17Y C317 C318 BOND C317 H17X 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 C45 H5W C45 C46 BOND C45 H5Q C46 C47 BOND C46 H60 C46 H6W BOND C47 H70 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 C413 H13W BOND C413 H130 C413 C414 C414 H14W BOND C414 H140 C414 C415 BOND C415 H150 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 1 1 CH2 - PO4 - CH2 - CH(OH) - CH2OH 1 ! 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 ! Н13В--С13--ОС3--НОЗ ATOM HO3 HOL 0.42 !

GROUP		!	
ATOM C12	CTL1	0.14 !	
ATOM H12A	HAL1	0.09 !	
ATOM OC2	OHL	-0.65 !	Н12АС12ОС2НО2
АТОМ НО2	HOL	0.42 !	
GROUP		!	alpha5
ATOM C11	CTL2	-0.08 !	
ATOM H11A	HAL2	0.09 !	Н11АС11Н11В
ATOM H11B	HAL2	0.09 !	alpha4
ATOM P	PL	1.50 !	(-) 013 012
ATOM 013	02L	-0.78 !	\/ alpha3
ATOM 014	02L	-0.78 !	P (+)
ATOM 012	OSLP	-0.57 !	/ \ alpha2
ATOM 011	OSLP	-0.57 !	(-) 014 011
ATOM C1	CTL2	-0.08 !	alpha1
АТОМ НА	HAL2	0.09 !	НАС1НВ
ATOM HB	HAL2	0.09 !	theta1
GROUP		!	
ATOM C2	CTL1	0.17 !	HSC2
ATOM HS	HAL1	0.09 !	beta1
ATOM 021	OSL	-0.49 !	022 021 theta3
ATOM C21	CL	0.90 !	\\/ beta2
ATOM 022	OBL	-0.63 !	C21
ATOM C22	CTL2	-0.22 !	beta3
ATOM H2R	HAL2	0.09 !	H2RC22H2S
ATOM H2S	HAL2	0.09 !	
GROUP		!	beta4
АТОМ СЗ	CTL2	0.08 !	
АТОМ НХ	HAL2	0.09 !	НХСЗНҮ
ATOM HY	HAL2	0.09 !	gamma1
ATOM 031	OSL	-0.49 !	032 031
ATOM C31	CL	0.90 !	\\ / gamma2
ATOM 032	OBL	-0.63 !	C31
ATOM C32	CTL2	-0.22 !	gamma3
ATOM H2X	HAT.2		
	IIAUZ	0.09 !	H2XC32H2Y
ATOM H2Y	HAL2	0.09 ! 0.09 !	H2XC32H2Y
ATOM H2Y GROUP	HAL2	0.09 ! 0.09 ! !	H2XC32H2Y gamma4
ATOM H2Y GROUP ATOM C23	HAL2 CTL2	0.09 ! 0.09 ! ! -0.18 !	H2XC32H2Y gamma4
ATOM H2Y GROUP ATOM C23 ATOM H3R	HAL2 CTL2 HAL2	0.09 ! 0.09 ! ! -0.18 ! 0.09 !	H2XC32H2Y gamma4 H3RC23H3S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3S	HAL2 CTL2 HAL2 HAL2	0.09 ! 0.09 ! ! -0.18 ! 0.09 ! 0.09 !	H2XC32H2Y gamma4 H3RC23H3S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3S GROUP	HAL2 CTL2 HAL2 HAL2	0.09 ! 0.09 ! ! -0.18 ! 0.09 ! 0.09 !	H2XC32H2Y H3RC23H3S H3RC23H3S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3S GROUP ATOM C24	HAL2 CTL2 HAL2 HAL2 CTL2	0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 !	H2XC32H2Y H3RC23H3S H3RC23H3S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3S GROUP ATOM C24 ATOM H4R	HAL2 HAL2 HAL2 HAL2 CTL2 HAL2 CTL2 HAL2	0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 ! 0.09 ! 1 -0.18 ! 0.09 !	H2XC32H2Y H3RC23H3S H3RC23H3S H4RC24H4S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3S GROUP ATOM C24 ATOM H4R ATOM H4S	HAL2 HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 HAL2	0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 ! 0.09 ! -0.18 ! 0.09 ! 0.09 !	H2XC32H2Y H3RC23H3S H4RC24H4S H4RC24H4S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3S GROUP ATOM C24 ATOM H4R ATOM H4S GROUP	HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 HAL2 HAL2	0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 ! 0.09 ! -0.18 ! 0.09 !	H2XC32H2Y H3RC23H3S H4RC24H4S H4RC24H4S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3S GROUP ATOM C24 ATOM H4R ATOM H4S GROUP ATOM C25	HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 HAL2 HAL2 CTL2 CTL2	0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 ! 0.09 ! -0.18 !	H2XC32H2Y H3RC23H3S H4RC24H4S H4RC24H4S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3S GROUP ATOM C24 ATOM H4R ATOM H4S GROUP ATOM C25 ATOM H5R	HAL2 HAL2 CTL2 HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 CTL2 HAL2	0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 ! 0.09 !	H2XC32H2Y H2XC32H2Y H3RC23H3S H4RC24H4S H4RC24H4S H5RC25H5S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3S GROUP ATOM C24 ATOM H4R ATOM H4S GROUP ATOM C25 ATOM H5R ATOM H5S	HAL2 HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 HAL2	0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 ! 0.09 !	H2XC32H2Y H2XC32H2Y Gamma4 H3RC23H3S H4RC24H4S H5RC25H5S H5RC25H5S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3S GROUP ATOM C24 ATOM H4R ATOM H4S GROUP ATOM C25 ATOM H5R ATOM H5S GROUP	HAL2 HAL2 CTL2 HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 CTL2 HAL2 HAL2	0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! 1 -0.18 ! 0.09 ! 0.09 !	H2XC32H2Y H2XC32H2Y H3RC23H3S H4RC24H4S H5RC25H5S H5RC25H5S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3S GROUP ATOM C24 ATOM H4R ATOM H4S GROUP ATOM C25 ATOM H5R ATOM H5S GROUP ATOM C26	HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 CTL2	0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! 1 -0.18 ! 0.09 ! 0.09 ! -0.18 ! 0.09 ! -0.18 !	H2XC32H2Y H3RC23H3S H4RC24H4S H4RC24H4S H5RC25H5S H5RC25H5S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3S GROUP ATOM C24 ATOM H4R ATOM H4S GROUP ATOM C25 ATOM H5R ATOM H5S GROUP ATOM C26 ATOM H6R	HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2	0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 ! 0.09 ! -0.18 ! 0.09 ! -0.18 ! 0.09 ! -0.18 ! 0.09 ! -0.18 ! 0.09 !	H2XC32H2Y H3RC23H3S H3RC23H3S H4RC24H4S H5RC25H5S H5RC25H5S H6RC26H6S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3S GROUP ATOM C24 ATOM H4R ATOM H4S GROUP ATOM C25 ATOM H5R ATOM H5S GROUP ATOM C26 ATOM H6R ATOM H6S	HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 HAL2	0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 ! 0.09 ! -0.18 ! 0.09 ! -0.18 ! 0.09 ! -0.18 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! 0.09 ! 0.09 ! 0.09 !	H2XC32H2Y H2XC32H2Y Gamma4 H3RC23H3S H4RC24H4S H5RC25H5S H6RC26H6S H6RC26H6S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3R ATOM H3S GROUP ATOM C24 ATOM H4R ATOM H4S GROUP ATOM C25 ATOM H5R ATOM H5S GROUP ATOM C26 ATOM H6R ATOM H6S GROUP	HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 HAL2	0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 !	H2XC32H2Y H2XC32H2Y gamma4 H3RC23H3S H4RC24H4S H5RC25H5S H6RC26H6S H6RC26H6S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3S GROUP ATOM C24 ATOM H4R ATOM H4S GROUP ATOM C25 ATOM H5S GROUP ATOM C26 ATOM H6R ATOM H6S GROUP ATOM C27	HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 CTL2 HAL2 CTL2	0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 !	H2XC32H2Y H3RC23H3S H4RC24H4S H4RC24H4S H5RC25H5S H6RC26H6S H6RC26H6S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3R ATOM H3S GROUP ATOM C24 ATOM H4R ATOM H4S GROUP ATOM C25 ATOM H5R ATOM H5S GROUP ATOM C26 ATOM H6R ATOM H6S GROUP ATOM C27 ATOM H7R	HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2	0.09 ! 0.09 ! 1 -0.18 ! 0.09 ! 0.09 ! -0.18 ! 0.09 ! -0.09 ! -0.18 ! 0.09 ! -0.09 !	H2XC32H2Y H3RC23H3S H4RC24H4S H4RC24H4S H5RC25H5S H6RC25H5S H6RC26H6S H6RC26H6S H7RC27H7S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3R ATOM H3S GROUP ATOM C24 ATOM H4R ATOM H48 GROUP ATOM C25 ATOM H58 GROUP ATOM C26 ATOM H68 GROUP ATOM C27 ATOM H78 ATOM H78	HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 HAL2	0.09 ! 0.09 ! 1. -0.18 ! 0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 ! 0.09 ! 1. -0.18 ! 0.09 ! -0.18 ! 0.09 ! -0.18 ! 0.09 ! -0.18 ! 0.09 ! -0.18 ! 0.09 ! -0.18 ! 0.09 !	H2XC32H2Y H3RC23H3S H4RC24H4S H4RC24H4S H5RC25H5S H6RC25H5S H6RC26H6S H7RC27H7S H7RC27H7S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3R ATOM H3S GROUP ATOM C24 ATOM H4R ATOM H4S GROUP ATOM C25 ATOM H5R ATOM H5S GROUP ATOM C26 ATOM H6R ATOM H6S GROUP ATOM C27 ATOM H7R ATOM H7S GROUP	HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 HAL2	0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 ! 0.09 !	H2XC32H2Y H3RC23H3S H4RC24H4S H4RC24H4S H5RC25H5S H6RC25H5S H6RC26H6S H7RC27H7S H7RC27H7S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3R ATOM H3S GROUP ATOM C24 ATOM H4R ATOM H48 GROUP ATOM C25 ATOM H58 GROUP ATOM C26 ATOM H68 GROUP ATOM C27 ATOM H78 ATOM H78 GROUP ATOM C28	HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 CTL2 CTL2 CTL2 CTL2 CTL2 CTL2 CT	0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 !	H2XC32H2Y H3RC23H3S H4RC24H4S H4RC24H4S H5RC25H5S H6RC26H6S H7RC27H7S H7RC27H7S H7RC27H7S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3R ATOM H3S GROUP ATOM C24 ATOM H4R ATOM H4S GROUP ATOM C25 ATOM H5R ATOM H5S GROUP ATOM C26 ATOM H6R ATOM H6S GROUP ATOM C27 ATOM H7R ATOM H7S GROUP ATOM C28 ATOM K38	HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 HAL2 HAL2 HAL2 HAL2 HAL2 HAL2 HA	0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 ! 0.09 ! -0.09 ! -0.18 ! 0.09 ! -0.09 !	H2XC32H2Y H3RC23H3S H4RC24H4S H4RC24H4S H5RC25H5S H6RC25H5S H6RC26H6S H7RC27H7S H7RC27H7S H8RC28H8S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3R ATOM H3S GROUP ATOM C24 ATOM H4R ATOM H4R ATOM H4S GROUP ATOM C25 ATOM H5R ATOM H5S GROUP ATOM C26 ATOM H6R ATOM H6S GROUP ATOM C27 ATOM H7R ATOM H7S GROUP ATOM C28 ATOM H8R ATOM H8S	HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 HAL2 CTL2 HAL2 HAL2 HAL2 CTL2 HAL2 HAL2 HAL2 HAL2 CTL2 HAL2 HAL2 HAL2 HAL2 HAL2 HAL2 HAL2 HA	0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 ! 0.09 ! -0.09 ! -0.18 ! 0.09 ! -0.09 !	H2XC32H2Y H3RC23H3S H4RC24H4S H4RC24H4S H5RC25H5S H6RC25H5S H6RC26H6S H7RC27H7S H8RC28H8S H8RC28H8S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3R ATOM H3S GROUP ATOM C24 ATOM H4R ATOM H48 GROUP ATOM C25 ATOM H58 ATOM H58 GROUP ATOM C26 ATOM H68 GROUP ATOM C27 ATOM H68 GROUP ATOM C27 ATOM H78 GROUP ATOM C28 ATOM H88 ATOM H88 GROUP	HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 HAL2	0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 ! 0.09 !	H2XC32H2Y H3RC23H3S H4RC24H4S H4RC24H4S H5RC25H5S H6RC25H5S H6RC26H6S H7RC27H7S H8RC28H8S H8RC28H8S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3R ATOM H3S GROUP ATOM C24 ATOM H4R ATOM H4R ATOM H4S GROUP ATOM C25 ATOM H5R ATOM H5S GROUP ATOM C26 ATOM H6R ATOM H68 GROUP ATOM C27 ATOM H78 ATOM H78 GROUP ATOM C28 ATOM H88 ATOM H88 GROUP ATOM C29	HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 CTL2 CTL2 HAL2 CTL2 CTL2 CTL2 CTL2 CTL2 CTL2 CTL2 CT	0.09 ! 0.09 ! -0.18 ! 0.09 ! 0.09 ! -0.18 !	H2XC32H2Y H3RC23H3S H4RC24H4S H4RC24H4S H5RC25H5S H6RC25H5S H6RC26H6S H7RC27H7S H8RC28H8S H8RC28H8S H8RC28H8S
ATOM H2Y GROUP ATOM C23 ATOM H3R ATOM H3R ATOM H3S GROUP ATOM C24 ATOM H4R ATOM H48 GROUP ATOM C25 ATOM H58 GROUP ATOM C26 ATOM H68 GROUP ATOM C27 ATOM H68 GROUP ATOM C27 ATOM H78 GROUP ATOM C28 ATOM H88 ATOM H88 GROUP ATOM C29 ATOM C29 ATOM C29 ATOM H98	HAL2 CTL2 HAL2 HAL2 CTL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 HAL2 CTL2 CTL2 HAL2 CTL2 CTL2 CTL2 CTL2 CTL2 CTL2 CTL2 CT	0.09 ! 0.09 ! -0.18 ! 0.09 ! -0.09 ! -0.00 ! -0	H2XC32H2Y H3RC23H3S H4RC24H4S H4RC24H4S H5RC25H5S H6RC25H5S H6RC26H6S H7RC27H7S H7RC28H8S H7RC28H8S H7RC29H9S

GROUE	2		!		I		
ATOM	C210	CTL2	-0.18 !				
ATOM	H10R	HAL2	0.09 !		H10RC210H10S	1	
ATOM	H10S	HAL2	0.	09 !			
GROUE	2		!				
ATOM	C211	CTL2	-0.15 !			1	
ATOM	H11R	HEL1	0.15 !		H11RC211		
GROUE	þ		!		(CIS)		
ATOM	C212	CTL2	-0.15 !		11		
ATOM	H12R	HEL1	0.15 !		H12RC212	1	
GROUE	>		!			1	
ATOM	C213	CTL2	-0.18 !		1	1	
ATOM	H13R	HAL2	0.09 !		H13RC213H13S	1	
ATOM	H13S	HAL2	0.09 !			1	
GROUE	>		!			1	
ATOM	C214	CTL2	-0.18 !			1	
ATOM	H14R	HAL2	0.09 !		H14RC214H14S	Í	
ATOM	H14S	HAL2	0.09 !			Ì	
GROUE	þ		!			İ	
ATOM	C215	CTL2	-0.18 !			İ	
ATOM	H15R	HAL2	0.09 !		H15RC215H15S	i	
ATOM	H15S	HAL2	0.09 !			İ	
GROUE	b		!			i	
ATOM	C216	CTL2	-0.18 !			Ì	
АТОМ	H16R	HAL2	0.09 !		H16RC216H16S	Ì	
ATOM	H16S	HAL2	0.09 !			1	
GROUF))					1	
ATOM	C217	CTT.2	-0 18 !			1	
ATOM	H17R	HAL2	0 09 1		н17вС217н17s	1	
ATOM	H17S	HAL2	0 09 1			1	
GROUF))	111112	0.05 .			1	
ATOM	C218	CTT.3	-0 27 !			1	
	H18R	нат.3	0.27		н18вС218н18s	1	
	H189	натз	0.09 1			1	
	н19т	натз	0.09 1		н 1 8 т	1	
CROUE)))	IIAIJ	0.05 :		11101	1	
ATOM	C33	CTT 2	-0 18 1			1	
ATOM	U3V		0.10 :		пзх		u3v
ATOM	UJV UJV	UNT 2	0.09 :		НЭХ	035	пэт
CROTIE	11.J I	IIALLZ	0.09 :			1	
ATOM	C34	CTT 2	-0 18 1			1	
ATOM	U/V		0.10 :		ЧЛУ		U/V
ATOM	U/V	UNT 2	0.09 :		1147	1	1141
CROTIE	1141	IIALLZ	0.09 :			1	
3 TOM	C 2 5	Cmt 2	-0 19 1			1	
ATOM	U5V		-0.10 :		ЧБУ	C35	U5V
ATOM	115X 115V	UNT 2	0.09 :		115X	1	11.5 1
CROTIE	11.5 1	IIALLZ	0.09 :			1	
ATTOM	C36	CTT 2	-0 18 1			1	
ATOM	USU USV		-0.10 :		чех		U6V
ATOM	HOA UGV	UNT 2	0.09 :		НОХ	030	пот
CDOUL	пот	TALZ	0.09 !			1	
3 TOM	727	CILIT O	0 1 0 1			1	
ATOM	U37	UTLZ	-0.18 !		1173	1	11737
ATOM		HALZ	0.09 !		H/X		n/i
CDOUL	H/I	HALZ	0.09 !			1	
GROUE		C TT O	0 10 1				
ATOM	U30		-0.18 ;				
ATOM	нөх	HALZ	0.09 !		нях	038	н8Ү
AT'UM	нат	HALZ	0.09 !				
GROUE	~ ~ ~ ^ ^ ^		. 10 !				
ATOM	U39	UTLZ	-0.18 ;		** ^ **		11037
ATOM ATOM	н УХ ЦОУ	HALZ	0.09 !	001	н9х	039	н9Ү
ATOM CDOUT	пэт	ПАЦИ	υ.	09 !		1	
GKUUE			!			I	

ATOM	C310	CTL2	-0.18 !								
ATOM	H10X	HAL2	0.09 !				H10	ХС	310H10Y		
ATOM	H10Y	HAL2	0.09 !								
GROUI	2		!								
ATOM	C311	CTL2	-0.15 !								
ATOM	H11X	HEL1	0.15 !				H11	ХС	311		
GROUI	2		!					I			
ATOM	C312	CTL2	-0.15 !								
ATOM	H12X	HEL1	0.15 !				H12	ХС	312		
GROUI	2		!								
ATOM	C313	CTL2	-0.18 !								
ATOM	H13X	HAL2	0.09 !				H13	ХС	313H13Y		
ATOM	H13Y	HAL2	0.09 !								
GROUI	2		!								
ATOM	C314	CTL2	-0.18 !								
ATOM	H14X	HAL2	0.09 !				H14	хС	314H14Y		
ATOM	H14Y	HAL2	0.09 !								
GROUI	2		!								
ATOM	C315	CTL2	-0.18 !								
ATOM	H15X	HAL2	0.09 !				H15	хС	315H15Y		
ATOM	H15Y	HAL2	0.09 !								
GROUI	-		!								
ATOM	C316	CTL2	-0.18 !								
ATOM	H16X	HAL2	0.09 !				H16	хС	316H16Y		
ATOM	H16Y	HAL2	0.09 !								
GROUI	-		!								
ATOM	C317	CTL2	-0.18 !								
ATOM	H17X	HAL2	0.09 !				H17	XC	317Н17Ү		
ATOM	H17Y	HAL2	0.09 !								
GROUI	2		!								
ATOM	C318	CTL3	-0.27 !								
ATOM	H18X	HAL3	0.09 !				H18	хС	318H18Y		
ATOM	H18Y	HAL3	0.09 !								
ATOM	H18Z	HAL3	0.09 !					H	18Z		
! Pol	lar He	ad									
BOND	ноз	OC3	OC3	C13	C13	H13A		C13	H13B	C13	C12
BOND	HO2	OC2	OC2	C12	C12	H12A		C12	C11		
BOND	C11	H11A	C11	H11B	C11	012		011	C1		
BOND	012	P	P	011	P	013		Ρ	014		
! Gl3	ycerol	Backbo	ne								
BOND	C1	HA	C1	HB	C1	C2					
BOND	C2	HS	C2	C3	C2	021					
BOND	C3	HX	C3	ΗY	C3	031					
! Cha	ain fr	om C2									
BOND	021	C21									
BOND											
	C21	C22									
DOUBI	C21 LE C2	C22									
BOND	C21 LE C2 C22	C22 1 O22 H2R	C22	H2S	C22	C23					
BOND BOND	C21 C22 C22 C23	C22 1 O22 H2R H3R	C22 C23	H2S H3S	C22 C23	C23 C24					
BOND BOND BOND	C21 C22 C22 C23 C24	C22 1 O22 H2R H3R H4R	C22 C23 C24	H2S H3S H4S	C22 C23 C24	C23 C24 C25					
BOND BOND BOND BOND	C21 C22 C22 C23 C24 C25	C22 1 022 H2R H3R H4R H5R	C22 C23 C24 C25	H2S H3S H4S H5S	C22 C23 C24 C25	C23 C24 C25 C26					
BOND BOND BOND BOND BOND	C21 C22 C23 C23 C24 C25 C26	C22 H2R H3R H4R H5R H6R	C22 C23 C24 C25 C26	H2S H3S H4S H5S H6S	C22 C23 C24 C25 C26	C23 C24 C25 C26 C27					
BOND BOND BOND BOND BOND BOND	C21 C22 C23 C24 C25 C26 C27	C22 H2R H3R H4R H5R H6R H7R	C22 C23 C24 C25 C26 C27	H2S H3S H4S H5S H6S H7S	C22 C23 C24 C25 C26 C27	C23 C24 C25 C26 C27 C28					
BOND BOND BOND BOND BOND BOND BOND	C21 C22 C23 C24 C25 C26 C27 C28	C22 H2R H3R H4R H5R H6R H7R H8R	C22 C23 C24 C25 C26 C27 C28	H2S H3S H4S H5S H6S H7S H8S	C22 C23 C24 C25 C26 C27 C28	C23 C24 C25 C26 C27 C28 C29					
BOND BOND BOND BOND BOND BOND BOND BOND	C21 C22 C23 C24 C25 C26 C27 C28 C29	C22 H2R H3R H4R H5R H6R H7R H8R H9R	C22 C23 C24 C25 C26 C27 C28	H2S H3S H4S H5S H6S H7S H8S C29 H9S	C22 C23 C24 C25 C26 C27 C28	C23 C24 C25 C26 C27 C28 C29 C29	210				
BOND BOND BOND BOND BOND BOND BOND BOND	C21 C22 C23 C24 C25 C26 C27 C28 C29 C210	C22 H2R H3R H4R H5R H6R H7R H8R H9R H10R	C22 C23 C24 C25 C26 C27 C28 C21	H2S H3S H4S H5S H6S H7S H8S C29 H9S O H10S	C22 C23 C24 C25 C26 C27 C28 C21	C23 C24 C25 C26 C27 C28 C29 C29 C29 C29 C21	2210 1				
BOND BOND BOND BOND BOND BOND BOND BOND	C21 C22 C23 C24 C25 C26 C27 C28 C29 C210 C211	C22 H2R H3R H4R H5R H6R H7R H8R H9R H10R H11R	C22 C23 C24 C25 C26 C27 C28 C21	H2S H3S H4S H5S H6S H7S H8S C29 H9S O H10S	C22 C23 C24 C25 C26 C27 C28 C21	C23 C24 C25 C26 C27 C28 C29 C29 C29 C29 C21	210 L				
BOND BOND BOND BOND BOND BOND BOND BOND	C21 C22 C22 C23 C24 C25 C26 C27 C28 C29 C210 C211 LE C2	C22 H2R H3R H4R H5R H6R H7R H8R H9R H10R H11R H11 C212	C22 C23 C24 C25 C26 C27 C28 C21	H2S H3S H4S H5S H6S H7S H8S C29 H9S O H10S	C22 C23 C24 C25 C26 C27 C28 C21	C23 C24 C25 C26 C27 C28 C29 C29 C29 C29 C21	2210 L				
BOND BOND BOND BOND BOND BOND BOND BOND	C21 C22 C22 C23 C24 C25 C26 C27 C28 C29 C210 C211 LE C2 C212	C22 H2R H3R H4R H5R H6R H7R H8R H9R H10R H11R H11 C212 H12R	C22 C23 C24 C25 C26 C27 C28 C21	H2S H3S H4S H5S H6S H7S H8S C29 H9S 0 H10S 2 C213	C22 C23 C24 C25 C26 C27 C28 C21	C23 C24 C25 C26 C27 C28 C29 C29 C29 C29 C29 C21	210				
BOUBI BOND BOND BOND BOND BOND BOND BOND BOND	C21 C22 C22 C23 C24 C25 C26 C27 C28 C29 C210 C211 LE C2 C212 C213	C22 H2R H3R H4R H5R H6R H7R H8R H9R H10R H11R H11 C212 H12R H13R	C22 C23 C24 C25 C26 C27 C28 C21 C21 C21	H2S H3S H4S H5S H6S H7S H8S C29 H9S 0 H10S 2 C213 3 H13S	C22 C23 C24 C25 C26 C27 C28 C213	C23 C24 C25 C26 C27 C28 C29 C29 C29 C29 C214	:210 1				
BOUBI BOND BOND BOND BOND BOND BOND BOND BOND	C21 C22 C23 C24 C25 C26 C27 C28 C29 C210 C211 LE C2 C212 C213 C214	C22 H2R H3R H4R H5R H6R H7R H8R H9R H10R H11R H11 C212 H12R H13R H14R	C22 C23 C24 C25 C26 C27 C28 C21 C21 C21 C21	H2S H3S H4S H5S H6S H7S H8S C29 H9S 0 H10S 2 C213 3 H13S 4 H14S	C22 C23 C24 C25 C26 C27 C28 C213 C213 C214	C23 C24 C25 C26 C27 C28 C29 C29 C29 C29 C212 C214 C214	:210 L				
BOUBI BOND BOND BOND BOND BOND BOND BOND BOND	C21 C22 C23 C24 C25 C26 C27 C28 C29 C210 C211 LE C2 C212 C213 C214 C215	C22 H2R H3R H4R H5R H6R H7R H8R H9R H10R H11R H11C C212 H12R H13R H14R H15R	C22 C23 C24 C25 C26 C27 C28 C21 C21 C21 C21 C21 C21	H2S H3S H4S H5S H6S H7S H8S C29 H9S 0 H10S 2 C213 3 H13S 4 H14S 5 H15S	C22 C23 C24 C25 C26 C27 C28 C21 C213 C213 C214 C215	C23 C24 C25 C26 C27 C28 C29 C29 C29 C212 C214 C214 C215 C216	:210 L				

BONI	D C217 D C218 bain Fr	7 H17R 3 H18R	C2: C2:	17 H17S 18 H18S	С217 С. С218 Н	218 18T			
BONI	D 031 D C31 BLE C3	C31 C32 C32							
BON	D C32	H2X	C32	2 H2Y	C32 C	33			
BON	D C33	H3X H4Y	C3:	3 H3Y	C33 C	34 35			
BON	D C34	H5X	C3	5 H5Y	C35 C	36			
BONI	D C36	Н6Х	C3	б НбҮ	C36 C	37			
BONI	D C37	H7X Н8Х	C3	7 Н7Ү 8 н8ү	C37 C	38 39			
BON	D C39	н9х	001	СЗ9 Н9Ү	C3	9 C310			
BON	D C310) H10X	C3:	10 H11Y	C310 C	311			
DOUI	D C311 BLE C31	1 HIIX 1 C312							
BON	D C312	2 H12X	C3	12 C313					
BON	D C313	B H13X	C31	13 H13Y	C313 C	314			
BON	D C314 D C315	5 H15X	C3:	14 H141 15 H15Y	C314 C	315 316			
BON	D C316	5 H16X	C3	16 H16Y	C316 C	317			
BON	D C317	7 H17X 8 H18X	C3:	17 H17Y 18 H18Y	С317 С	318 187			
IMPI	R C21 C	021 C22	022	C31 O31 C3	2 032	102			
тс	C13	C12	C11	012	1 5583	113 89	93 01	113 50	1 /205
IC (0C3	C12	C12	C11	1.4375	112.31	69.20	113.89	1.5573
IC (0C3	C12	*C13	H13A	1.4375	112.31	119.90	108.06	1.1118
IC	OC3 C12	C12	*C13	H13B H03	1.4375	112.31	-123.06	109.89	1.1097
IC (C12	C13	*C12	0C2	1.5573	113.89	-121.65	100.90	1.4259
IC (OC2	C13	*C12	H12A	1.4259	107.64	-117.84	109.30	1.1131
IC (C13	C12	OC2 *C11	HO2	1.5583	107.64	38.09	100.52	0.9671
ICI	H11A	C12 C12	*C11	H11B	1.1125	109.70	-115.65	109.70	1.1123
IC (C12	C11	012	P	1.5573	113.50	-72.69	124.80	1.5783
IC (C11	012	P *P	011	1.4295	124.80	-30.02	102.66	1.5825
IC (011	012	*P	014	1.5825	102.00	-115.27	109.00	1.4781
IC (012	P	011	C1	1.5783	102.66	-80.21	120.83	1.4246
ICI	P C2	011	C1 *C1	C2	1.5825	120.83	177.68	108.67	1.5488
ICI	HA	011	*C1	HB	1.1145	111.25	-120.91	110.06	1.1143
IC (011	C1	C2	С3	1.4246	108.67	45.70	110.42	1.5580
IC (C3	C1	*C2	021	1.5580	110.42	120.25	110.13	1.4420
IC (C1	C1 C2	021	C21	1.5488	110.42	74.82	114.08	1.3218
IC (C2	021	C21	C22	1.4420	114.08	-171.58	108.87	1.5297
IC (C22	021	*C21	022	1.5297	108.87	-179.18	126.27	1.2166
IC	C23	C21	*C22	H2R	1.5460	112.03	-121.40	108.25	1.1088
ICI	H2R	C21	*C22	H2S	1.1088	108.25	-117.05	107.34	1.1068
IC (C1	C2	C3	031	1.5488	110.42	-172.10	112.95	1.4472
IC (031 HX	C2 C2	*C3 *C3	HX HY	1.4472	112.95	-119.90	106.80 109.95	1.1123
IC (C2	C3	031	C31	1.5580	112.95	84.38	114.39	1.3267
IC (С3	031	C31	C32	1.4472	114.39	176.82	109.50	1.5275
IC (C32 031	031 C31	*C31 C32	032	1.5275	109.50	-179.44	126.11 112 63	1.2173
IC (C33	C31	*C32	H2X	1.5535	112.63	121.43	107.50	1.1085
IC I	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

ТC	C24	C22	*023	H3R	1 5338	112 39	-120 69	109 57	1 1147
TC	U3D	C22	*023	U30	1 1147	109 57	-117 65	109.61	1 11/2
TC	п <u>э</u> к	C22	~CZ5	п.).5 С.).Е	1 5440	112 20	170.20	110 25	1 5246
IC	C22	C23	CZ4	C25	1.5449	112.39	-1/9.39	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
ТC	C24	C25	C26	C27	1.5346	112.80	-179.44	112.48	1.5356
TC	C27	C25	*C26	H6R	1 5356	112 48	-121 49	109 32	1 1129
TC	UCD	C25	*026	UEC	1 1120	100 22	117 17	100.01	1 1120
TC	ROK	C25	~CZ0	п05 с00	1.1129	109.32	-11/.4/	100.94	1.1132
IC	C25	C26	C27	C28	1.5344	112.48	1/6.92	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
TC	C27	C28	C29	C210	1 5344	112 48	176 92	112 46	1 5398
TC	C210	C20	* C 2 0	UQD	1 5200	112.10	_121 20	100 10	1 1120
TC	CZIU HOD	C20	* 229	пэк	1 1120	100 4	-121.30	100.40	1 1120
IC	H9R	028	^CZ9	H9S	1.1139	108.4	0 -116.93	108.//	1.1139
IC	C28	C29	C210	C211	1.5356	112.46	-178.53	111.43	1.5097
IC	C211	C29	*C210	H1OR	1.5097	111.43	-123.58	107.80	1.1132
IC	H10R	C29	*C210	H9S	1.1132	107.8	0 -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
TC	C210	C211	C212	C213	1 5097	126 62	-1 69	126 32	1 5088
TC	C213	C211	*0212	U1 2D	1 5000	126.02	-170 55	110 70	1 1012
TC	0213	C211 2010	~CZIZ	ПІ2К 2014	1.5000	120.52	-179.33	110.79	1.1012
TC	0211	C212	C213	C214	1.5392	112.29	1/9.81	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
ТC	H14R	C213	*C214	H14S	1.1132	109.09	-117.37	109.11	1.1133
TC	C213	C214	C215	C216	1 5345	112 59	-179 58	112 63	1 5347
TC	C216	C211	*0215	U15D	1 5247	112.55	-121 36	100.00	1 1122
TC	CZIU U1ED	0214	+ C215	HIJK H1FQ	1 1120	100.00	-121.30	109.09	1 1122
TC	HISK	C214	^CZ15	HISS	1.1132	109.09	-11/.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
ТC	H17R	C216	*C217	H17S	1.1140	108.75	-116.65	108.73	1.1141
TC	C216	C217	C218	H1 8R	1 5339	113 30	-59 98	110 46	1 1113
TC	U10D	C217	+0010	11101	1 1112	110 40	110 04	110.40	1 1114
TC	HI8R	C217	^CZ18	HI8S	1.1113	110.46	119.84	110.45	1.1114
TC	HI8K	C217	*C218	HI8I	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	НЗХ	1.5343	111.73	-120.85	109.62	1.1140
IC	нзх	C32	*C33	НЗҮ	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
TC	C35	C33	*C34	H4X	1 5345	112 91	-121 67	109 15	1 1134
TC	H4 Y	C33	*C34	HAV	1 1134	109 15	-117 32	108 98	1 1134
TC	022	C34	C25	0.36	1 5242	112 01	170 62	112 42	1 5240
IC	C33	C34 ~?.1	635	0.50	1.5545	112.91	1/0.03	112.42	1.5549
TC	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	нбх	1.5356	112.80	-121.69	109.16	1.1130
IC	нбх	C35	*C36	НбҮ	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
TC	C 3 8	C36	*037	H7X	1 5402	112 27	-121 37	108 23	1 1129
TC	U7V	C36	*037	u7v	1 1120	100 22	_117 01	100.25	1 1127
тС	11/A	027	- CS /	11/1	1 E 2 E C	110.23	174 00	111 00	1 5000
тC	C36	037	U38	C39	1.5356	112.2/	-1/4.92	111.69	1.2099
ТС	C39	C37	*C38	нвх	1.5099	111.69	-124.14	10/.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	н9х	1.5402	112.27	-121.37	108.23	1.1139
IC	н9х	C38	*СЗ9 Н9	Ϋ́	1.1139 108.	.23 -117.	01 109.	.05 1.13	137
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	H1OX	C39	*C310 H1	0Y	1.1124 107.	.77 -115.	13 108.	.30 1.13	128
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 1 ! R1 - CH2 1 R2 - CH 1 1 ! 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 11 !! Polar Head and glycerol backbone GROUP ! ATOM C13 CTL2 0.05 ! 0.09 ! ATOM H13A HAL2 H13A 0.09 ! ATOM H13B HAL2 -0.65 ! ATOM OC3 OHL ATOM HO3 HOL 0.42 ! Н13В--С13---ОС3--НОЗ 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 H11A--C11---H11B 0.09 ! ATOM H11B HAL2 0.09 ! | alpha4

ATOM P	PL	1.50 !	(-) 013 012
ATOM 013	02L	-0.78 !	\/ alpha3
ATOM 014	021	-0 78 !	P (+)
ATOM 012	OSTR	-0 57 1	$\langle \cdot \rangle$ $alpha?$
ATOM OIZ	OSLF	-0.57 !	
ATOM OII	OSLP	-0.57 !	(-) 014 011
ATOM C1	CTL2	-0.08 !	alpha1
АТОМ НА	HAL2	0.09 !	НАС1НВ
ATOM HB	HAL2	0.09 1	l thetal
CROUD			
GROOP	OET 1		
ATOM CZ	CILI	0.1/ !	HSC2
ATOM HS	HAL1	0.09 !	betal
ATOM 021	OSL	-0.49 !	022 021 theta3
ATOM C21	CL	0.90 !	\\/ beta2
ATOM 022	OBL	-0 63 1	C21
ATOM C22		0.00	
ATOM CZZ	CTLZ	-0.22 !	Deta3
ATOM H2R	HAL2	0.09 !	H2RC22H2S
ATOM H2S	HAL2	0.09 !	
GROUP		!	beta4
ATOM C3	CTT.2	0 08 1	
ATOM UV	UAT 2		
	IIALZ	0.09 :	
ATOM HY	HALZ	0.09 !	gammal
ATOM 031	OSL	-0.49 !	032 031
ATOM C31	CL	0.90 !	\\ / gamma2
ATOM 032	OBL	-0.63 !	L C31
ATOM C32	CTL2	-0 22 1	
ATOM UOV		0.22 :	
ATOM HZX	HALZ	0.09 !	H2XC3ZH2Y
ATOM H2Y	HAL2	0.09 !	
GROUP		!	gamma4
ATOM C23	CTL2	-0.18 !	
ATOM H3R	HAT.2	0 0 9 1	H3BC23H3S
ATOM USC	UNT 2	0.09.1	
ATOM 1155	IIALLZ	0.09 :	
GROUP		1	
ATOM C24	CTL2	-0.18 !	
ATOM H4R	HAL2	0.09 !	H4RC24H4S
ATOM H4S	HAL2	0.09 !	
CROUP		1	
	0007.0		
ATOM C25	CTLZ	-0.18 !	
ATOM H5R	HAL2	0.09 !	H5RC25H5S
ATOM H5S	HAL2	0.09 !	
GROUP		!	
ATOM C26	CTL2	-0.18 !	
ATOM USP	UNT 2	0 09 1	46P026469
		0.00	
ATOM H65	HALZ	0.09	
GROUP		!	
ATOM C27	CTL2	-0.18 !	
ATOM H7R	HAL2	0.09 !	H7RC27H7S
ATOM H7S	HAL2	0.09 1	
GROUP		1	
	0007.0		
ATOM C28	CTLZ	-0.18 !	
ATOM H8R	HAL2	0.09 !	H8RC28H8S
ATOM H8S	HAL2	0.09 !	
GROUP		!	
ATOM C29	CTT.2	-0 18 1	
ATOM UOD		0.10 :	
ATOM H9R	HALZ	0.09 !	H9RC29H95
ATOM H9S	HAL2	0.09 !	
GROUP		!	
ATOM C210	CTL2	-0.18 !	
ATOM H10R	HAL2	0.09 !	H10RС210Н10S
ATOM U100	HAL?	0 00 1	
CDOUD	IIAUZ	0.09 :	
GKUUP		!	
ATOM C211	CEL1	-0.15 !	
ATOM H11R	HEL1	0.15 !	H11RC211
GROUP		!	(CIS)
ATOM C212	CEL1	-0.15 !	
		·· ·	

ATOM H12R	HEL1	0.15 !	H12RC212
GROUP		0 10 1	
ATOM ULI 2D	UTLZ	-0.18 !	
ATOM HISR	HALZ	0.09 !	HISRC213HISS
ATOM HI3S	HALZ	0.09 !	
GROUP	077.0	. 10 .	
ATOM C214	CTL2	-0.18 !	
ATOM HI4R	HALZ	0.09 !	H14R = -C214 = -H14S
ATOM HI4S	HAL2	0.09 !	
GROUP		!	
ATOM C215	CTL2	-0.18 !	
ATOM H15R	HAL2	0.09 !	H15RC215H15S
ATOM H15S	HAL2	0.09 !	
GROUP		!	
ATOM C216	CTL2	-0.18 !	
ATOM H16R	HAL2	0.09 !	H16RC216H16S
ATOM H16S	HAL2	0.09 !	
GROUP		!	
ATOM C217	CTL2	-0.18 !	
ATOM H17R	HAL2	0.09 !	H17RC217H17S
ATOM H17S	HAL2	0.09 !	
GROUP		!	
ATOM C218	CTL3	-0.27 !	
ATOM H18R	HAL3	0.09 !	H18RC218H18S
ATOM H18S	hal3	0.09 !	
ATOM H18T	HAL3	0.09 !	H18T
GROUP		!	
ATOM C33	CTL2	-0.18 !	
АТОМ НЗХ	HAL2	0.09 !	НЗХСЗЗНЗҮ
АТОМ НЗҮ	HAL2	0.09 !	
GROUP		!	
ATOM C34	CTL2	-0.18 !	
ATOM H4X	HAL2	0.09 !	Н4ХС34Н4Ү
ATOM H4Y	HAL2	0.09 !	
GROUP		!	
ATOM C35	CTL2	-0.18 !	
ATOM H5X	HAL2	0.09 !	н5хС35Н5Ү
ATOM H5Y	HAL2	0.09 !	
GROUP		1	
ATOM C36	CTL2	-0.18 !	
ATOM H6X	HAL2	0 09 1	нбхСзбнбү
ATOM H6Y	HAL2	0 09 1	
GROUP	1111112	0.05	
ATOM C37	CTT.2	-0 18 I	
ATOM H7X	HAL2	0.10 .	Н7ХСЗ7Н7Х
ATOM H7Y	HAL2	0.09 !	
CROUP	1111112	0.05 1	
ATOM C38	CTT.2	-0 18 I	
ATOM USV	UNI 2	0.10 :	H8Y038U8Y
ATOM HOA	UNI 2	0.09 !	нохсзонот
CROUP	IIALLZ	0.09 :	
GROUP	CTT 2	-0 19 1	
ATOM UOV		-0.10 !	
ATOM H9X	HALZ	0.09 !	пэхсзэпэт
CROUP	паци	0.09	שי ב ו
GRUUP		· · · ·	
ATOM USIU		-0.10 ;	
ATOM HIUX	HALZ	0.09 !	HIUXC3IUHIUY
ATOM HIUY	HALZ	0.09 !	
GKUUP	087.0	!	
ATOM C311	CTL2	-0.18 !	,
ATOM H11X	HAL2	0.09 !	H11XC311H11Y
ATOM HIIY	HAL2	0.09	9 !
GROUP		!	
ATOM C312	CTL2	-0.18 !	

Ι

ATOM H12X HAL2	0.09	!				H12X	KC	312H12Y			
ATOM H12Y HAL2		0.09	!								
GROUP		!					1				
ATOM C313 CTL2	-0.18	!					1				
ATOM H13X HAL2	0.09	!				H13X	(C	313Н1ЗҮ			
ATOM H13Y HAL2	0.09	!					1				
GROUP		!					1				
ATOM C314 CTL2	-0.18	!					Í				
ATOM H14X HAL2	0.09	1				н14х	C	314н14ү			
ATOM H14Y HAL2	0 09	1									
CDUID	0.05										
	_0 10										
ATOM ULEY UNIO	-0.10	-				TT1 E V		215 U15V			
ATOM HIJA HALZ	0.09	-				нтэх	<u> </u>	313HI31			
ATOM HISY HALZ	0.09										
GROUP	0 1 0	1									
ATOM C316 CTL2	-0.18	!									
ATOM HI6X HAL2	0.09	!				HI6X	(C	316H16Y			
ATOM H16Y HAL2	0.09	!									
GROUP		!									
ATOM C317 CTL2	-0.18	!									
ATOM H17X HAL2	0.09	!				H17X	(C	317н17Ү			
ATOM H17Y HAL2	0.09	!					1				
GROUP		!					1				
ATOM C318 CTL3	-0.27	!					Í				
ATOM H18X HAL3	0.09	1				H18X		318н18ү			
ATOM H18Y HAL3	0.09	1					-				
ATOM H187 HAL3	0.09						, H	187			
	0.05	•						100			
! Polar Head											
BOND HO3 OC3	0		13	C13	н 13д		C13	н13в	C13	C12	
BOND HO2 OC2	0		12	C12	ш1 2 л		C12	C11	010	012	
DOND C11 U117		исд С 11 и	110	C12 C11	012		011	C1			
DOND CII HIIA			11	CII	012		DII	014			
BOND OIZ P	P	. 0	ΤT	P	013		Р	014			
! GIYCEROI BACH	anoa	- 1		a 1	~ ^ ^						
BOND CI HA	C	1	нв	CI	CZ						
BOND C2 HS	C	2	C3	C2	021						
BOND C3 HX	C	3	HY	C3	031						
! Chain from C2	2										
BOND 021 C21											
BOND C21 C22											
DOUBLE C21 02	22										
BOND C22 H2R	С	22 н	2S	C22	C23						
BOND C23 H3R	С	23 н	3S	C23	C24						
BOND C24 H4R	С	24 н	4S	C24	C25						
BOND C25 H5R	С	25 н	5S	C25	C26						
BOND C26 H6R	С	26 н	6S	C26	C27						
BOND C27 H7R	С	27 н	7S	C27	C28						
BOND C28 H8R	С	28 н	8S	C28	C29						
BOND C29 H9R		C2	9 H9S		29 C2	210					
BOND C210 H10E		210 H	109	C21	0 0211	110					
BOND C211 H111		.210 11	100	021	0 0211						
DOUBLE C211 C	, 12										
BOND C212 U12) C	212 0	213								
		יז 212 U	210 130	C010	C21/						
		-213 H	1/0	C213	C214 C21F						
DOND CZ14 H14H		.214 H	150	0214	0213						
DOND C215 H15H		.213 H	100	0215	0215						
BUND C216 H16H	K C	216 H	TPR	C216	CZI/						
BOND C217 H17	K C	217 H	⊥/S	C217	C218						
BOND C218 H181	K C	218 H	182	C218	H18T						
! Chain From C	3										
BOND 031 C31											
BOND C31 C32											
DOUBLE C31 03	32										

BOND C33	нзх	C3:	3 НЗҮ	C33 C	34			
BOND C34	H4X	C34	4 H4Y	C34 C	35			
BOND C35	H5X	C3	5 Н5Ү	C35 C	36			
BOND C36	нбх	C3	б НбҮ	C36 C	37			
BOND C37	H7X	C3	7 Н7Ү	C37 C	38			
BOND C38	H8X	C3	8 H8Y	C38 C	39			
BOND C39	Н9Х		СЗ9 Н9	у СЗ	9 C310			
BOND C310) H10X	C3:	10 H10Y	C310 C	311			
BOND C311	l H11X	C3:	11 H11Y	C311 C312				
BOND C312	2 H12X	C31	12 H12Y	С3	12 C313			
BOND C313	3 H13X	C3:	13 H13Y	C313 C	314			
BOND C314	4 H14X	C31	14 H14Y	C314 C	315			
BOND C315	5 H15X	C31	15 H15Y	C315 C	316			
BOND C316	5 H16X	C3:	16 H16Y	C316 C	317			
BOND C31	7 H17X	C3:	17 H17Y	C317 C	318			
BOND C318	8 H18X	C3:	18 H18Y	С318 Н	18Z			
THER 001 (0.1 000	000	aa1 aa1	~~~~~				
IMPR CZI (JZI CZZ	022	031 031	032 032				
IC C13	C12	C11	012	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	ноз	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 012	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	012	P	1.5573	113.50	-72.69	124.80	1.5783
IC C11	012	Р	011	1.4295	124.80	-30.02	102.66	1.5825
IC 011	012	*P	013	1.5825	102.66	113.88	109.00	1.4783
IC 011	012	*P	014	1.5825	102.66	-115.27	109.77	1.4781
IC 012	P	011	C1	1.5783	102.66	-80.21	120.83	1.4246
IC P	011	C1	C2	1.5825	120.83	177.68	108.67	1.5488
IC C2	011	*C1	HA	1.5488	108.67	-120.91	111.25	1.1145
IC HA	011	*C1	HB	1.1145	111.25	-120.47	110.06	1.1152
IC 011	C1	C2	C3	1.4246	108.67	45.70	110.42	1.5580
IC C3	C1	*C2	021	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 Cl	C2	021	C21	1.5488	110.13	74.82	114.08	1.3218
IC C2	021	C21	C22	1.4420	114.08	-171.58	108.87	1.5297
IC C22	021	*C21	022	1.5297	108.87	-179.18	126.27	1.2166
IC 021	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	-11/.05	107.34	1.1068
	C2	03	031	1.5488	110.42	-1/2.10	112.95	1.44/2
	CZ	^C3	HX	1.44/2	112.95	-119.90	106.80	1.1123
IC HX	C2	*03	HY	1.1123	106.80	-114.66	109.95	1.114/
	C3	031	C31	1.5580	112.95	84.38	114.39	1.3267
	031	C31 + 221	032	1.44/2	114.39	176.82	109.50	1.52/5
10 032	031	*C31	032	1.52/5	109.50	-1/9.44	126.11	1.21/3
10 031	C31	C32	033	1.3267	109.50	-66./6	112.63	1.5535
10 033	C31	*C32	HZX	1.5535	112.63	121.43	107.50	1.1085
IC HZX	C31	*032	HZY	1.1085	107.50	116.64	107.32	1.1097
	C22	CZ3	C24	1.5289	112.21	1/5./6	112.39	1.5338
10 024	022	*023	нзк	1.5338	100 55	-120.69	109.5/	1.1147
IC H3R	022	*CZ3	HJS	1.114/	1109.5/	-11/.65	110.64	1.1142
IC CZZ	023	CZ4	CZ5	1.5449	110 05	-1/9.39	100 41	1.5346
IC C25	023	^CZ4	н4К	1 1 1 2 1	100 41	-121.52	100.41	1.1131
IC H4R	023	^CZ4	H45 G2C	1.5220	112 25	-176.21	112 00	1.1134
	C24	UZD *C25		1 5338	112.00	10101	100 OF	1 1125
IC UED	C24	*025	HURC	1 110F	100 05	-121.UI	100.95	1 1120
тс цэк	UZ4	·· UZ 3	про	T.TT22	TA0.23	-11/.24	TU2.TQ	1.1132

та	004	00F	000	007	1 5 2 4 6	110 00	170 44	110 40	1 5 2 5 6	
ΤC	CZ4	C25	C26	CZ/	1.5346	112.80	-1/9.44	112.48	1.0000	
IC	C27	C25	*C26	H6R	1.5356	112.48	-121.49	109.32	1.1129	
тС	UGD	C25	*026	чбс	1 1129	109 32	_117 /7	108 9/	1 1132	
TC	TIOK	020	020	1105	1.1129	109.52	11/.4/	100.94	1.1152	
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	
тс	U7D	C26	* ~ 2 7	U70	1 1120	100 /0	-116 02	100 77	1 1120	
ΤC	п/К	C20	nCZ /	п/Б	1.1139	100.40	-110.93	100.//	1.1139	
IC	C26	C27	C28	C29	1.5356	112.46	-178.53	111.43	1.5097	
TC	C29	C27	*028	H8R	1 5097	111 43	-123 58	107 80	1 1132	
- O	U0D	g07	+ 3 0 0	11010	1 1100	107.00	115 40	100.07	1 1100	
ΤC	HOK	CZI	^CZ8	HØS	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	
ТC	C210	C28	*029	нар	1 5398	112 46	-121 38	108 40	1 1139	
±0	0210	220	020	11910	1.0000	1 1120	100 40	116 00	100 77	1 1100
ТC	H9R	C28	*C29	H9S		1.1139	108.40	-116.93	108.//	1.1139
IC	C28	C29	C210	C211	1.5356	112.46	-178.53	111.43	1.5097	
тС	C211	C29	*0210	u10D	1 5097	111 /3	-123 58	107 80	1 1132	
TC	0211	029	0210	111.01	1.3037	111.45	123.30	107.00	1.11.52	
IC	HIOR	C29	*C210	H9S	1	.1132 1	07.80 -1	15.43 10)8.37 1	.1128
IC	C29	C210	C211	C212	1.5398	111.43	-126.96	126.62	1.3465	
TC	C212	C210	* 0 2 1 1	0	1 2465	126 62	170 /1	114 65	1 1012	
ΤC	CZIZ	CZIU	~CZII	HIIK	1.3403	120.02	1/0.41	114.00	1.1012	
IC	C210	C211	C212	C213	1.5097	126.62	-1.69	126.32	1.5088	
TC	C213	C211	*C212	H12R	1 5088	126 32	-179 55	118 79	1 1012	
±0	0210	0211	0212	a014	1.5000	110.02	170.00	110.70	1 5045	
ТC	CZII	CZIZ	C213	C214	1.5392	112.29	1/9.81	112.68	1.5345	
IC	C214	C212	*C213	H13R	1.5345	112.68	-121.26	109.04	1.1132	
ТС	H13P	C212	*0213	H139	1 1120	109 04	-117 30	109 10	1 1121	
ΤC		~~1~	C2IJ		1.1132	109.04	100 00	100.10	1 5 2 2 5	
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	
тс		0212	* 0211	11140	1 1122	100 00	117 27	100 11	1 1122	
ΤC	UTAK	CZIJ	··CZ14	п145	1.1132	109.09	-11/.3/	109.11	1.1155	
IC	C213	C214	C215	C216	1.5345	112.59	-179.58	112.63	1.5347	
ТC	C216	C214	*C215	H1.5R	1.5347	112.63	-121.36	109.09	1.1132	
- 0 - 0	U1 E D	0011	+ 0015	111 5 0	1 1120	100.00	117 20	100.07	1 1120	
TC	HICK	CZ14	^CZ15	HIDS	1.1132	109.09	-11/.38	109.07	1.1132	
IC	C214	C215	C216	C217	1.5347	112.63	179.65	112.69	1.5339	
TC	C217	C215	*C216	H16R	1 5339	112 69	-121 27	109 11	1 1132	
±0	0217 1110	0210	0210	111 010	1 1 1 2 0	100 11	117 20	100.14	1 1100	
ТC	HI6R	C215	*C216	HI6S	1.1132	109.11	-11/.36	109.14	1.1132	
IC	C215	C216	C217	C218	1.5347	112.69	-179.93	113.30	1.5309	
тс	C218	C216	*0217	H17P	1 5309	113 30	-121 70	108 75	1 1140	
TC	0210	C210	0217		1.5505	113.50	121.70	100.75	1.1140	
ТC	HI/R	C216	*C217	HI/S	1.1140	108./5	-116.65	108./3	1.1141	
IC	C216	C217	C218	H18R	1.5339	113.30	-59.98	110.46	1.1113	
тС	U10D	C217	*0210	U100	1 1112	110 46	110 01	110 /5	1 111/	
ΤC	HIOK	CZI/	CZI0	птор	1.1113	110.40	119.04	110.45	1.114	
IC	H18R	C217	*C218	H18T	1.1113	110.46	-120.09	110.62	1.1112	
ТC	C31	C32	C33	C.34	1.5288	113.05	179.24	111.73	1.5343	
±0	001 001	d 2 2	* 4 3 3	11211	1 5240	111 70	100 05	100 00	1 1140	
TC	034	032	^C33	HJX	1.5343	111./3	-120.85	109.62	1.1140	
IC	нзх	C32	*C33	НЗҮ	1.1140	109.62	-117.95	109.78	1.1144	
TC	C32	C 3 3	C34	C35	1 5447	111 73	-176 74	112 91	1 5345	
- O	00E	d000	+ 0 2 1	11 4 37	1 5045	110 01	101 07	100 15	1 1124	
TC	035	033	^C34	H4X	1.5345	112.91	-121.6/	109.15	1.1134	
IC	H4X	C33	*C34	H4Y	1.1134	109.15	-117.32	108.98	1.1134	
тс	C 3 3	C34	C35	C36	1 5343	112 91	178 63	112 42	1 5349	
±0	000	CO 1	000		1.5515	110 10	100.00	100 04	1 1100	
ТC	036	C34	*C35	HSX	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	
TC	C34	C35	C36	C37	1 5345	112 42	-176 73	112 80	1 5356	
±0	201	205	000		1.5515	110 00	101 00	100 10	1 1120	
ТC	C37	C35	*036	нөх	1.5356	112.80	-121.69	109.16	1.1130	
IC	нбх	C35	*C36	HGY	1.1130	109.16	-117.32	108.94	1.1133	
тС	C35	C36	C 3 7	C 3 8	1 53/9	112 80	178 92	112 27	1 5/02	
т С	200	000			1.0049	110 00	101 07	100 00	1 1 1 0 2	
тC	C38	C36	×C3/	н/Х	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	
тС	C36	C37	C 3 8	C30	1 5356	110 07	-17/ 02	111 60	1 5000	
ΤC	0.50	0.57	0.00	53	1.0000	112.21	-114.92	111.09	1.0099	
ſC	C39	C37	*C38	нях	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	
тс	C37	030	C30	0210	1 5240	112 00	170 00	110 07	1 5/00	
ΤC	0.57	0.50	59	CSIU	1.5549	112.00	10.92	112.2/	1.0402	
IC	C310	C38	*C39	H9X	1.5402	112.27	-121.37	108.23	1.1139	
IC	н9х	C38 *C	39 н9	Y	1.1139 108	23 -117	01 109	05 1.1	137	
TC	C30	030	0210	0011	1 5050	110 07	_17/ 00	111 00	1 5000	
ΤC	0.50	0.59	COIU		1.0000	112.21	-114.92	111.09	1.0099	
IC	C311	C39	*C310	HlOX	1.5099	111.69	-124.14	107.77	1.1124	
IC	H10X	C39 *C	310 н1	ΟY	1.1124 107.	77 -115	13 108	30 1.1	128	
тс	C30	0310	C311	C210	1 5/00	111 60	_101 00	107 25	1 2/70	
ΤC	53	COIU	COTT	CJIZ	1.5402	111.09	-121.39	121.33	1.34/0	
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

!PEs

RESI DVPE 0.00 ! 2,3-divacenoyl-D-glycero-1-phosphatidylethanolamine ! R1 - CH2 ! ! (angles and atom names from Sundaralingam) R2 - CH ! 1 CH2 - PO4 - CH2 - CH2 - NH3 1 1 ! 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 11 !! R1 - CH2 11 (angles and atom names from Sundaralingam) !! R2 - CH !! CH2 - PO4 - CH2 - CH2 - NH3 !! !! !! Polar Head and glycerol backbone GROUP 1 ΑΤΟΜ Ν 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 1 ATOM C11 CTL2 -0.08 ! ATOM H11A HAL2 0.09 ! H11A--C11---H11B ATOM H11B HAL2 0.09 ! 1 alpha4 (-) 013 012 ATOM P PL 1.50 ! ATOM 013 02L \setminus / -0.78 ! alpha3 P (+) ATOM 014 02L -0.78 ! ATOM 011 OSLP -0.57 ! alpha2 ATOM 012 OSLP -0.57 ! (-) 014 011 1 ATOM C1 CTL2 -0.08 ! alpha1

ATOM HA	HAL2	0.09	! НАС1НВ
АТОМ НВ	HAL2	0.09	! theta1
GROUP			<u> </u>
ATOM C2	CTL1	0.17	HSC2
ATOM HS	HAL1	0.09	! beta1
ATOM 021	OSL	-0.49	! 022 021 theta3
ATOM C21	CL	0.90	// beta2 /
ATOM 022	OBL	-0.63	
ATOM C22	CTL2	-0.22	l beta3
ATOM H2R	HAL2	0.22	$H^{2}R^{}C^{2}C^{}H^{2}S$
ATOM U29	UNT 2	0.09	
CPOUD	IIALLZ	0.09	botal
ATTOM C2	CILL O	0 0 0	
ATOM US		0.08	
ATOM HA	HALZ	0.09	
ATOM HI	HALZ	0.09	
ATOM 031	OSL	-0.49	
ATOM C31	CL	0.90	! \\/ gamma2
ATOM 032	OBL	-0.63	. C31
ATOM C32	CTL2	-0.22	! gamma3
ATOM H2X	HAL2	0.09	Н2ХС32Н2Ү
ATOM H2Y	HAL2	0.09	!
GROUP			! gamma4
ATOM C23	CTL2	-0.18	!
ATOM H3R	HAL2	0.09	! H3RC23H3S
ATOM H3S	HAL2	0.09	!
GROUP			!
ATOM C24	CTL2	-0.18	!
ATOM H4R	HAL2	0.09	! H4RC24H4S
ATOM H4S	HAL2	0.09	· · ·
GROUP			
ATOM C25	CTT.2	-0 18	
ATOM H5R	HAT.2	0 09	. нъвС25нъс I
ATOM H5S	HAT.2	0.09	
CPOUD	IIAUZ	0.05	
ATTOM C26	CTT 2	_0 10	
ATOM USD	UNT 2	-0.18	
ATOM HOR	TALZ	0.09	. nokC20nos
ATOM H65	HALZ	0.09	
GROUP	0000	0 1 0	
ATOM CZ7	CTLZ	-0.18	
ATOM H/R	HALZ	0.09	H/R = -CZ/H/S
ATOM H/S	HAL2	0.09	
GROUP			
ATOM C28	CTL2	-0.18	!
ATOM H8R	HAL2	0.09	! H8RC28H8S
ATOM H8S	HAL2	0.09	!
GROUP			!
ATOM C29	CTL2	-0.18	!
ATOM H9R	HAL2	0.09	! H9RC29H9S
ATOM H9S	HAL2	0.09	!
GROUP			!
ATOM C210	CTL2	-0.18	!
ATOM H10R	HAL2	0.09	! H10RC210H10S
ATOM H10S	HAL2	0.09	
GROUP			
ATOM C211	CEL1	-0.15	
ATOM H11R	HEL1	0.15	! H11RC211
GROUP		3.10	! (CTS)
ATOM C212	CEL1	-0 15	
ΔTOM H12D	HET.1	0 15	· · · · · · · · · · · · · · · · · · ·
CROUP	لل تل تنبي	0.10	
ATOM CO12	ር ሞፕ ን	<u> </u>	
ATOM U13D	стыс цато	0.10	· I II3RC213H13C I
ATOM UISC	идц <i>а</i>	0.09	
CDOLLD	папс	0.09	
GRUUP			

Ι
ATOM	C214	CTL2	-0.18	!
ATOM	H14R	HAL2	0.09	! H14RC214H14S
ATOM	H14S	HAL2	0.09	!
GROUE	>			! ! !
ATOM	C215	CTL2	-0.18	!
ATOM	H15R	HAT.2	0 0 9	H15BC215H15S
ATOM	H159	HAT.2	0.09	
CROTT	111.2.2	IIAUZ	0.09	
JECOUL			0 1 0	
ATOM	C210	CTLZ	-0.18	
ATOM	HI6R	HALZ	0.09	! HI6RC216HI6S
ATOM	H16S	HAL2	0.09	!
GROUI	2			!
ATOM	C217	CTL2	-0.18	!
ATOM	H17R	HAL2	0.09	! H17RC217H17S
ATOM	H17S	HAL2	0.09	!
GROUE	2			!
ATOM	C218	CTL3	-0.27	!
АТОМ	H18R	HAL3	0.09	! H18RC218H18S
ATOM	H18S	HAT.3	0.09	
ATOM	н18т	HAT.3	0 09	
CPOIII		IIAUJ	0.05	
ATTOM		Cmt 2	0 1 0	
ATOM	033		-0.10	
ATOM	HJX	HALZ	0.09	НЗХСЗЗНЗҮ
ATOM	НЗҮ	HAL2	0.09	!
GROUI	2			!
ATOM	C34	CTL2	-0.18	!
ATOM	H4X	HAL2	0.09	! н4хсз4н4у
ATOM	H4Y	HAL2	0.09	!
GROUE	2			!
ATOM	C35	CTL2	-0.18	1
ATOM	H5X	HAT.2	0.09	Н5ХС35Н5Ү
ATOM	HSY	HAT.2	0 09	
CROTI	5	111112	0.05	• 1
JECOUL	- 		0 1 0	
ATOM	0.50		-0.10	
ATOM	НбХ	HALZ	0.09	Н6ХС36Н6Ү
A'I'OM	Н6Ү	HAL2	0.09	!
GROUI	2			!
ATOM	C37	CTL2	-0.18	!
ATOM	H7X	HAL2	0.09	! H7XС37Н7Ү
ATOM	H7Y	HAL2	0.09	!
GROUE	2			!
ATOM	C38	CTL2	-0.18	!
ATOM	H8X	HAL2	0.09	! Н8ХС38Н8Ү
АТОМ	H8Y	HAL2	0.09	!
GROUF	>			1
ATOM	C39	CTT.2	-0 18	1
ATOM	нду	HAT.2	0 09	нохсзонох
ATOM	цох		0.05	
CDOU	1191	IIALLZ	0	.05 :
GROUP	- 		0 1 0	
ATOM	0310	CTLZ	-0.18	
A'I'OM	HIOX	HAL2	0.09	! HI0XC310HI0Y
ATOM	HIOY	HAL2	0	.09 !
GROUI	2			!
ATOM	C311	CEL1	-0.15	!
ATOM	H11X	HEL1	0.15	! H11XC311
GROUE	2			! (CIS)
ATOM	C312	CEL1	-0.15	!
АТОМ	H12X	HEL1	0.15	! H12XC312
GROUT	>			
	C313	CTT.?	-0.18	• 1
7 T OM	U1 2V	СТПС НДТ О	0.10	· U12V0212U12V
	птэм птэм		0.09	: птэхсэтэнтэт
CDOTT	UT 21	ΠΑLΖ	0.09	
GROUP		0.007.0	0 1 0	
A'T'OM	C314	CTL2	-0.18	:

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ATOM H ATOM H GROUP	H14X H H14Y H	HAL2 0.09 HAL2 0.09	9 ! 9 ! !			H14X	-C314H 	14Y
ATOM (C315 (CTL2 -0.18	3!					
ATOM H	H15X H	HAL2 0.09	9!			H15X	-С315Н	15Y
ATOM H	415Y B	HAL2 0.09	9!					
GROUP			!					
ATOM (2316 (CTL2 -0.18	3 !					
ATOM H	416X H	HAL2 0.09	9!			H16X	-С316Н	16Y
ATOM H	416Y H	HAL2 0.09	9!					
GROUP			!					
ATOM (C317 (CTL2 -0.18	3 !					
ATOM H	117X I	HAL2 0.09	9!			H17X	-С317Н	17Y
ATOM H	417Y B	HAL2 0.09	9!					
GROUP			!					
ATOM (2318 (CTL3 -0.27	7!					
ATOM H	418X I	HAL3 0.09	9!			H18X	-С318Н	18Y
ATOM H	418Y H	HAL3 0.09	9!					
ATOM H	418Z B	HAL3 0.09	9!				H18Z	
! Pola	ar Hea	ad		_		_		
BOND	Ν	HN1	Ν	HN2	Ν	HN3	N	C12
BOND	C12	H12A	C12	H12B	C12	C11		
BOND	C11	H11A	C11	H11B	C11	012		
BOND	012	P	Р	011	Р	013	P	014
! Glyd	cerol	Backbone						
BOND	C1	HA	C1	HB	C1	C2	C1	011
BOND	C2	HS	C2	C3	C2	021		
BOND	C3	HX	C3	HY	C3	031		
! Chai	in fro	om C2						
BOND	021	C21						
BOND	C21	C22						
DOUBLE	E C21	1 022						
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	H'/R	C27	H/S	C27	C28		
BOND	C28	H8R	C28	H8S	C28	C29		
BOND	C29	H9R	~ 0 1 0	C29 H9S	C29	C210		
BOND	C210	HIUR	C210	HIUS	C210	CZII		
BOND	CZII	HIIR						
DOURTH	4 CZ.	LI CZIZ	0010	0010				
BOND	CZ12	HIZR	CZ12	U213	0010	0014		
BOND	C213	HIJR	C213	HIJS HIJAC	C213	C214 C215		
BOND	C214	HI4R U1ED	C214	HI4S	C214	C215		
BOND	C215	HIJR	C215	HIJS	C215	C210 C217		
BOND	C210	HIOR	C210	H105	C210	C217		
BOND	C217	HI/K U19D	C217	П1/5 U190	C217	CZI0 1110m		
L Cha-	CZIO in Fra	DIOK Dm C3	C210	птор	C210	птот		
ROND	031	C31						
BOND	C31	C32						
ם עונים די די די די	C31	032						
BUND	- C37	H2X	C 3 2	н2ү	C32	C33		
BOND	C32	нзх	C32	H3Y	C32	C34		
BOND	C31	HAY	C31	HAV	C31	C35		
BOND	C 3 5	H5X	C 3 5	нтт Н5Ү	C 3 5	C36		
BOND	C36	нбх	C36	HEY	C36	C37		
BOND	C37	н7х	C37	н7ү	C37	C38		
BOND	C38	H8X	C38	H8Y	C38	C39		
BOND	C39	H9X		239 ноч	C39	C310		
BOND	C310	H10X	C310	H10Y	C31	0 C311		
					201			

BONDC31DOUBLEC3BONDC31BONDC31BONDC31BONDC31BONDC31BONDC31BONDC31	1 H11X 11 C312 2 H12X 3 H13X 4 H14X 5 H15X 6 H16X 7 H17X 8 H18X	С С С С С С С С С С	312 C313 313 H13Y 314 H14Y 315 H15Y 316 H16Y 317 H17Y 318 H18Y		C313 C C314 C C315 C C316 C C317 C C318 H	314 315 316 317 318 182		
IMPR C21	021 C22	022	C31 O31	C32	032			
IC N IC HN1 IC HN1 IC HN1 IC C11 IC H12A IC 012 IC H11A IC C12 IC C11 IC 011 IC 011 IC 011 IC 011 IC 012 IC P IC C2 IC AA IC 011 IC C3 IC C3 IC C3 IC C3 IC C2 IC C2 IC C2 IC C2 IC C2 IC C3 IC C1 IC C2 IC C3 IC C1 IC C2 IC C3 IC C3 IC C3 IC C3 IC C1 IC C2 IC C2 IC C2 IC C2 IC C3 IC C3 IC C3 IC C3 IC C3 IC C3 IC C3 IC C4 IC C3 IC C4 IC C3 IC C4 IC	C12 C12 C12 C12 N N C12 C12 C12 C12 C12 C12 C12 C12 C12 C12	C11 *N C12 *C12 *C12 *C12 *C11 O12 P *P O11 C1 *C1 *C1 *C2 *C2 C21 *C22 *C22 *C22	012 HN2 HN3 C11 H12A H12B H11A H11B P 011 013 014 C1 C2 HA HB C3 021 HS C21 C22 022 C23 H2R H2S 031 HX HY C31 C32 032 C33 H2X H2Y C31 C32 032 C33 H2X H2Y C31 HX HY C31 C32 C33 H2X H2S C31 HX HY C31 C32 C33 H2X H2S C33 H2X H2S C33 H2X H2S C33 H2X H2S C33 H2X H3R C32 C33 H2X H3S C25 H4R H3S C25 H3R H3S C25 H3R H3S C25 H3R H3S C25 H3R H3S C25 H3R H3S C25 H3R H3S C25 H3R H3S C25 H3R H3S C25 H4R H7S C27 H6R H7S H7S H7S H7S H7S H7S H7S H7S H7S H7S		1.5110 1.0342 1.0342 1.0342 1.5465 1.1086 1.4308 1.1167 1.5465 1.4308 1.5751 1.5751 1.5751 1.5536 1.4308 1.5553 1.5553 1.5553 1.5553 1.5553 1.4410 1.5533 1.5553 1.4410 1.5553 1.4410 1.5553 1.4432 1.5553 1.5553 1.4432 1.5553 1.5553 1.4432 1.5553 1.5553 1.4432 1.5553 1.5553 1.4432 1.5553 1.5553 1.4432 1.5553 1.5553 1.4432 1.5553 1.5553 1.4432 1.5553 1.5553 1.4432 1.5553 1.5553 1.5553 1.5553 1.5553 1.4432 1.5553 1.5536 1.1294 1.5346 1.133 1.5346 1.1324 1.5356 1.1294 1.5346 1.1339 1.5346 1.1294 1.5346 1.1339 1.5346 1.1324 1.5356 1.1294 1.5356 1.5356 1.1294 1.5356 1.1294 1.5356 1.5356 1.1294 1.5356 1.1294 1.5356 1.5356 1.1294 1.5356	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	112.46 105.60 110.56 111.97 107.97 107.67 111.01 107.63 120.62 104.60 103.31 107.16 120.34 111.72 108.93 112.18 110.59 108.20 107.37 115.07 109.17 126.38 111.62 107.66 107.26 113.52 109.19 125.26 112.50 107.84 108.28 111.62 107.66 107.26 113.52 109.19 125.26 112.50 107.84 108.28 112.35 109.57 109.64 112.35 109.41 108.97 112.80 109.57 109.64 112.35 109.41 108.97 112.80 109.32 108.94 112.48	1.4308 1.0654 1.0397 1.5465 1.104 1.1104 1.1167 1.1146 1.5839 1.5751 1.4823 1.4736 1.4318 1.5536 1.1133 1.1155 1.5553 1.4410 1.1169 1.3229 1.5330 1.2173 1.5472 1.1095 1.1081 1.4432 1.1152 1.3270 1.5276 1.2176 1.2176 1.5449 1.1092 1.1081 1.5338 1.1147 1.1142 1.5346 1.1131 1.5346 1.1131 1.1132 1.5356 1.1132 1.5356 1.1132 1.5356 1.1132 1.5356 1.1132 1.5356 1.1132 1.5356 1.1132 1.5356 1.1132 1.5356 1.1132 1.5356 1.1132 1.5356 1.1132 1.5356 1.1132 1.5356 1.1132 1.5356 1.1132 1.5356 1.1132 1.5356 1.1132
	~_ /	220						

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	*С29 Н9	S	1.1139	108.4	0 -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	107.8	0 -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	нзх	1.5343	111.73	-120.85	109.62	1.1140
IC	НЗХ	C32	*C33	НЗҮ	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	нбх	1.5356	112.80	-121.69	109.16	1.1130
IC	нбх	C35	*C36	НбҮ	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	н9х	1.5402	112.27	-121.37	108.23	1.1139
IC	н9х	C38	*СЗ9 Н9Ү		1.1139	108.2	3 -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	H1OX	1.5099	111.69	-124.14	107.77	1.1124
IC	H1OX		C39 *C3	310 H10Y	1.1124	107.7	7 -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

```
0.00 ! ? 2,3-vacenyl- steroeyl D-glycero-1-phosphatidylethanolamine
RESI VSPE
! 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
1
1
! 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
    1
11
                  (angles and atom names from Sundaralingam)
  R2 - CH
!!
       1
1.1
11
        CH2 - PO4 - CH2 - CH2 - NH3
!!
!! Polar Head and glycerol backbone
GROUP
                   1
ΑΤΟΜ Ν
         NH3L -0.30 !
                               HN2
ATOM HN1 HCL 0.33 !
                               ATOM HN2 HCL
              0.33 ! (+) HN1---N---HN3
ATOM HN3 HCL
               0.33 !
                                0.13 !
ATOM C12 CTL2
ATOM H12A HAL2
               0.09 !
                         H12A--C12---H12B
              0.09 !
ATOM H12B HAL2
                                GROUP
                                     alpha5
                    1
                                ATOM C11 CTL2 -0.08 !
                                ATOM H11A HAL2
              0.09 !
                        H11A--C11---H11B
ATOM H11B HAL2
              0.09 !
                               alpha4
                        (-) 013 012
              1.50 !
ATOM P
        PL
             -0.78 !
                             \setminus /
ATOM 013 02L
                                      alpha3
ATOM 014 02L -0.78 !
                              P (+)
                            / \
ATOM 011 OSLP -0.57 !
                                      alpha2
ATOM 012 OSLP -0.57 !
                        (-) 014 011
ATOM C1 CTL2 -0.08 !
                            |
                                      alpha1
        HAL2 0.09 !
ΑΤΟΜ ΗΑ
                            НА---С1---НВ
                            |
              0.09 !
ATOM HB
         HAL2
                                    theta1
GROUP
                  !
                                ATOM C2
         CTL1
               0.17 !
                           HS---C2- - - - - -
ATOM HS
         HAL1
               0.09 !
                            | betal
                                        1
                           022 021
               -0.49 !
ATOM 021
        OSL
                                            theta3
               0.90 !
                            \ \ / beta2
ATOM C21
        CL
                                           -0.63 !
ATOM 022 OBL
                             C21
                           | beta3
ATOM C22 CTL2 -0.22 !
                                             ATOM H2R HAL2 0.09 ! H2R---C22---H2S
```

ATOM H2S	HAL2	0.09	!
GROUP			! beta4
ATOM C3	CTL2	0.08	!
ΑΤΟΜ ΗΧ	HAL2	0.09	! НХСЗНҮ
ATOM HY	HAL2	0.09	! gamma1
ATOM 031	OSL	-0.49	. 032 031
ATOM C31	CL	0.90	! \\/ gamma2
ATOM 032	OBL	-0.63	. C31
ATOM C32	CTL2	-0.22	! gamma3
ATOM H2X	HAL2	0.09	! H2XC32H2Y
ATOM H2Y	HAL2	0.09	!
GROUP			! gamma4
ATOM C23	CTL2	-0.18	!
ATOM H3R	HAL2	0.09	! H3RC23H3S
ATOM H3S	HAL2	0.09	!
GROUP			!
ATOM C24	CTL2	-0.18	!
ATOM H4R	HAL2	0.09	! H4RC24H4S
ATOM H4S	HAL2	0.09	!
GROUP			!
ATOM C25	CTL2	-0.18	!
ATOM H5R	HAL2	0.09	! H5RC25H5S
ATOM H5S	HAL2	0.09	!
GROUP			!
ATOM C26	CTL2	-0.18	!
ATOM H6R	HAL2	0.09	! H6RC26H6S
ATOM H6S	HAL2	0.09	!
GROUP			!
ATOM C27	CTL2	-0.18	!
ATOM H7R	HAL2	0.09	! H7RC27H7S
ATOM H7S	HAL2	0.09	!
GROUP			!
ATOM C28	CTL2	-0.18	!
ATOM H8R	HAL2	0.09	! H8RC28H8S
ATOM H8S	HAL2	0.09	!
GROUP			!
ATOM C29	CTL2	-0.18	!
ATOM H9R	HAL2	0.09	! H9RC29H9S
ATOM H9S	HAL2	0.09	!
GROUP			!
ATOM C210	CTL2	-0.18	!
ATOM H10R	HAL2	0.09	! H10RC210H10S
ATOM H10S	HAL2	0.09	!
GROUP			!
ATOM C211	CEL1	-0.15	!
ATOM H11R	HEL1	0.15	! H11RC211
GROUP			! (CIS)
ATOM C212	CEL1	-0.15	!
ATOM H12R	HEL1	0.15	! H12RC212
GROUP			
ATOM C213	CTL2	-0.18	
ATOM H13R	HAL2	0.09	! H13RC213H13S
ATOM H13S	HAL2	0.09	!
GROUP			
ATOM C214	CTL2	-0.18	
ATOM H14R	HAL2	0.09	H14RC214H14S
ATOM H14S	HAL2	0.09	
GROUP		<u> </u>	
ATOM C215	CTL2	-0.18	
ATOM H15R	HAL2	0.09	H15RC215H15S
ATOM H15S	HAL2	0.09	
GROUP	am= 0	0 1 0	
ATOM C216	C'TL2	-0.18	
ATOM H16R	HAL2	0.09	нтекС2теН1ес

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ATOM H16S	HAL2	0.09	!
GROUP			!
ATOM C217	CTL2	-0.18	!
ATOM H17R	HAL2	0.09	! H17RC217H17S
ATOM H17S	HAL2	0.09	!
GROUP			!
ATOM C218	CTL3	-0.27	!
ATOM H18R	HAL3	0.09	! H18RC218H18S
ATOM H18S	HAL3	0.09	
ATOM H18T	HAT.3	0.09	н 18т Г
GROUP		0.05	· · · · · · · · · · · · · · · · · · ·
ATOM C33	CTT.2	-0 18	• 1
ATOM USV		0.10	
ATOM H3X		0.09	: IISA 655 IISI
CDOUD	NALZ	0.09	
ATTOM C24	CET 2	0 1 0	
ATOM C34	CTLZ	-0.18	
ATOM H4X	HALZ	0.09	Н4ХСЗ4Н4Ү
ATOM H4Y	HAL2	0.09	!
GROUP			!
ATOM C35	CTL2	-0.18	!
АТОМ Н5Х	HAL2	0.09	Н5ХС35Н5Ү
АТОМ Н5Ү	HAL2	0.09	!
GROUP			!
ATOM C36	CTL2	-0.18	!
АТОМ Н6Х	HAL2	0.09	! нбхСЗбНбҮ
АТОМ Н6Ү	HAL2	0.09	!
GROUP			!
ATOM C37	CTL2	-0.18	!
АТОМ Н7Х	HAL2	0.09	! H7XС37Н7Y
АТОМ Н7Ү	HAL2	0.09	!
GROUP			· · · · · · · · · · · · · · · · · · ·
ATOM C38	CTL2	-0.18	· · · · · · · · · · · · · · · · · · ·
ATOM H8X	HAT.2	0 0 9	НахСзанау
ATOM H8Y	нат.2	0.09	
CROUD	IIAUZ	0.05	· I
ATOM C39	CTT 2	_0 18	· I
ATOM CS9		-0.18	
ATOM H9X	HALZ	0.09	нэхсээнэт
ATOM H91	HALZ	0.	.09 !
000110			
GROUP	~ ~ ~ ^	0 1 0	
ATOM C310	CTL2	-0.18	!
ATOM H10X	HAL2	0.09	! H10XC310H10Y
ATOM H10Y	HAL2	0.	.09 !
GROUP			!
ATOM C311	CTL2	-0.18	!
ATOM H11X	HAL2	0.09	! Н11ХС311Н11Ү
ATOM H11Y	HAL2	Ο.	.09 !
GROUP			!
ATOM C312	CTL2	-0.18	!
ATOM H12X	HAL2	0.09	! H12XС312Н12Y
ATOM H12Y	HAL2	0.	.09 !
GROUP			!
ATOM C313	CTT.2	-0 18	1
ATOM H13X	HAT.2	0 0 9	Н1 ЗХСЗ1 ЗН1 ЗҮ
ATOM H13V	нат.2	0.09	
GROUP	كللدغدة	0.05	• 1
ATOM C314	ር ሞ፣ ጋ	_0 1 8	•
ATOM CS14		-0.10	
ATOM HI4X	HALZ	0.09	н14ХС314Н14Ү
ATOM H14Y	HAL2	0.09	
GROUP			!
ATOM C315	CTL2	-0.18	!
ATOM H15X	HAL2	0.09	! H15XC315H15Y
ATOM H15Y	HAL2	0.09	!
GROUP			!

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ATOM (C316 (CTL2 -0.18	3!			1		
ATOM H	H16X 1	HAL2 0.09	9!			H16XC3	316Н	16Y
ATOM H	H16Y 1	HAL2 0.09	9!			1		
GROUP			!			I		
ATOM (C317 (CTL2 -0.18	3!			I		
ATOM I	H17X I	HAL2 0.09	9!			H17XC3	317H	17Y
ATOM I	H17Y I	HAL2 0.09	9!			I		
GROUP			!			1		
ATOM (C318 (CTL3 -0.2	7 !					
ATOM H	H18X	HAL3 0.09	9!			H18XC3	318H	18Y
ATOM H	H18Y 1	HAL3 0.09	9!				o –	
A'I'OM I	HI8Z I	HAL3 0.09	9!			HI	.82	
I Pola	ar He	ad						
BOND	N	HN1	N	HN2	N	HN3	N	C12
BOND	C12	H12A	C12	H12B	C12	C11		
BOND	C11	H11A	C11	H11B	C11	012		
BOND	012	Р	Р	011	P	013	P	014
! Glvo	cerol	Backbone						
BOND	C1	HA	C1	HB	C1	C2	C1	011
BOND	C2	HS	C2	C3	C2	021		
BOND	C3	HX	C3	ΗY	C3	031		
! Cha:	in fr	om C2						
BOND	021	C21						
BOND	C21	C22						
DOUBLE	E C2	1 022						
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						
DOUBLI	E C2	11 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		
! Cha:	in Fr	om C3						
BOND	031	C31						
BOND		032						
DOURTI	E C31	032	a20		a 2 2	G 2 2 2		
BOND	C32	HZX	C32	HZY	C32	C33		
BOND	033	HJX	033	HJY	033	C34		
BOND	C34 C35	H4X	C34 C25	H41 UEV	C34 C35	C35		
DOND	C35	HJA	C35	HJI	C35 C36	C30		
DOND	C30	10A 117V	030 C27	ПО1 1177	C30	C3 /		
BOND	C30	11/A H8Y	(2) (2)	л/1 Н8V	C30	C30		
BOND	C 3 0	HOX	000	030 HOV	C20	C310		
BOND	C310	HIOY	C210	н10v	C21	0 0310		
DOND	C311	1110A 1111V	C311	11101 1110	(J)	~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~		
BOND	C312	нтту н12х	C310	нттт н12v		COTT COTC		
BOND	C312	H13X	C312	H13Y	C 2 1 2	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	H182
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IMPR C21 021 C22 022 C31 031 C32 032

IC	Ν	C12	C11	012	1.5110	111.97	65.84	112.46	1,4308
TC	HN1	C12	*N	HN2	1 0342	114 60	119 70	105 60	1 0654
TC	UN1	C12	*N	un3	1 0342	11/ 60	-127 78	110 56	1 0397
TC		N	C1 2	C11	1 0242	114.00	177 01	111 07	1 5465
TC		IN	CIZ		1.0342	111.07	-1//.91	107 07	1.0400
IC	CII	IN	^C12	HIZA	1.5465	111.97	-121.58	107.97	1.1086
IC	HIZA	Ν	*C12	HIZB	1.1086	10/.9/	-118.25	10/.6/	1.1104
IC	012	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	012	P	1.5465	112.46	-80.62	120.62	1.5839
IC	C11	012	P	011	1.4308	120.62	-156.78	104.60	1.5751
IC	011	012	*P	013	1.5751	104.60	-117.47	103.31	1.4823
TC	011	012	*P	014	1 5751	104 60	120 67	107 16	1 4736
TC	012	P	011	C1	1 5839	104 60	-58 82	120 34	1 4318
TC	DIZ		011	C1	1 5751	120 24	00.02	111 70	1 5520
TC	r ao	011		C2	1.5751	120.34	-92.40	111.72	1.1100
IC	C2	011	*CI	HA	1.5536	111.72	-119.08	108.93	1.1133
IC	HA	011	*C1	HB	1.1133	108.93	-117.83	112.18	1.1155
IC	011	C1	C2	C3	1.4318	111.72	162.49	110.59	1.5553
IC	C3	C1	*C2	021	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	021	C21	1.5536	108.20	145.45	115.07	1.3229
IC	C2	021	C21	C22	1.4410	115.07	175.60	109.17	1.5330
ТĊ	C22	021	*C21	022	1.5330	109.17	179.92	126.38	1.2173
TC	021	C21	C22	C23	1 3229	109.17	-134 07	111 55	1 5472
TC	021	C21	*022	1120	1 5470	111 55	110 01	106 70	1 1005
TC	UZS UDD	C21 001	* C22	HZR HOQ	1.005	106 70	-119.01	100.70	1.1095
IC	HZR	C21	*C22	HZS	1.1095	106.70	-11/.59	109.58	1.1081
IC	C1	C2	C3	031	1.5536	110.59	178.88	111.62	1.4432
IC	031	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	031	C31	1.5553	111.62	174.54	113.52	1.3270
IC	C3	031	C31	C32	1.4432	113.52	178.76	109.19	1.5276
IC	C32	031	*C31	032	1.5276	109.19	-179.68	125.26	1.2176
IC	031	C31	C32	C33	1.3270	109.19	-153.26	112.50	1.5449
TC	C 3 3	C31	*C32	H2X	1 5449	112 50	120 40	107 84	1 1092
TC	H2X	C31	*C32	H2V	1 1092	107 84	117 16	108 28	1 1081
TC	C21	C31	C22	C24	1 5200	112 21	175 76	112 20	1 5220
TC	C21	022	+ 2 2 2	U2D	1 5209	112.21	120 00	100 57	1 1147
IC	CZ4	C22	^CZ3	HJR	1.5338	112.39	-120.69	109.57	1.114/
IC	H3R	C22	*C23	HJS	1.114/	109.57	-11/.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
TC	C27	C25	*026	H6R	1 5356	112 48	-121 49	109 32	1 1129
TC	UGD	C25	*026	u69	1 1129	109 32	_117 /7	109.92	1 1132
TC	COE	C25	C20	0.00	1 5244	112 10	176 02	110.94	1 5200
TC	C25	026	+ 2 2 7	UZ0	1.5544	112.40	101 20	112.40	1 1120
IC	C28	026	^CZ7	H/R	1.5398	112.46	-121.38	108.40	1.1139
IC	H/R	C26	*C27	H'/S	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 *C	:29 н9	S	1.1139	108.4	0 -116.93	108.77	1.1139
IC	C28	C29	C210	C211	1.5356	112.46	-178.53	111.43	1.5097
TC	C211	C29	*0210	HIOR	1 5097	111 43	-123 58	107 80	1 1132
TC		C20	*0210	1110IX	1 1120	107 0	12J.JU	100 27	1 1100
тС	UT OK	C210	C211	C212	1 5200	111 / 2	-126 0C	126 62	1 2/65
тС	023		LZII + 0011		1 2465	106 60	-120.90	114 65	1 1010
тC	CZ12	C210	*CZII	HIIK	1.3465	126.62	⊥/8.4⊥	114.65	1.1012

тс	C210	C211	C212	C213	1 5007	126 62	-1 69	126 32	1 5088	
TC	0210	0211	+ 2010	U1 0D	1 5000	120.02	170 55	110.70	1 1010	
IC	C213	CZII	*C212	HIZK	1.5088	126.32	-1/9.55	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	
TC	C215	C213	*C214	H14R	1.5354	112.29	-121.34	109.78	1.1133	
TC	H14R	C213	*C214	н149	1 1133	109 78	-118 01	109 42	1 1144	
TC	C212	C210	C215	C216	1 52/5	112 50	_170 50	112 63	1 5247	
TC	C215 C216	0214	CZIJ *0215	U1ED	1.5345	112.09	-179.30	100 00	1 1122	
IC	C216	CZI4	^CZ15	HIJK	1.5347	112.03	-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	
TC	C218	C216	*C217	H17R	1 5309	113 30	-121 70	108 75	1 1140	
TC	U17D	C216	*C217	u179	1 1140	108 75	-116 65	108 73	1 11/1	
TC	001C	0210	0217	III / 5 III / 5	1.5220	112 20	110.00	110.75	1 1110	
IC	0216	CZI/	0218	HI8K	1.5339	113.30	-59.98	110.46	1.1113	
TC	HI8K	C217	*C218	HI8S	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	НЗХ	1.5343	111.73	-120.85	109.62	1.1140	
IC	нзх	C32	*C33	НЗҮ	1.1140	109.62	-117.95	109.78	1.1144	
TC	C32	C 3 3	C34	C 3 5	1 5447	111 73	-176 74	112 91	1 5345	
TC	C35	C33	*C34	U/V	1 53/5	112 01	-121 67	100 15	1 113/	
TC		C33	+024	1147	1 1124	100 15	117 22	109.13	1 1124	
IC	H4X	C33	^C34	H41	1.1134	109.15	-117.32	108.98	1.1134	
IC	033	C34	035	036	1.5343	112.91	1/8.63	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	нбх	1.5356	112.80	-121.69	109.16	1.1130	
TC	н6х	C35	*C36	HGY	1.1130	109.16	-117.32	108.94	1.1133	
TC	C35	C36	C 3 7	C 3 8	1 53/3	112 01	178 63	112 /2	1 53/9	
TC	C33	020	+027	U7V	1.5343	112.91	120.00	100 04	1 1122	
TC	0.50	030	~C37	П/А	1.3349	112.42	-120.99	100.94	1.1100	
IC	H/X	036	*C37	H/Y	1.1133	108.94	-11/.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	
TC	C310	C38	*C39	нөх	1.5402	112.27	-121.37	108.23	1.1139	
TC	49X	C38 -	*СЗО НОV		1 1139	108 2	3 -117 01	109 05	1 1137	
TC	030	C30	C210	C 2 1 1	1 5256	112 27	_17/ 02	111 60	1 5000	
TC	C30 C311	C39	+0210	ULOV	1.5550	112.27	104 14	107 77	1 1104	
IC	0311	639	^C310	HIUX	1.5099	111.69	-124.14	107.77	1.1124	
IC	HIOX		C39 *C3	310 H10Y	1.1124	107.7	7 -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	*C3	311 Н9Ү		1.1139	108.23 -	-117.01 1	L09.05 1.113	7!
5/3	17/2015	need	to check	around C31	1 C312					
IC	C310	C311	C312	C313	1,5099	127.35	0.00	127.25	1,5096	
TC	C313	C311	*C312	H12X	1 5096	127 25	179 82	118 43	1 1012	
TC	U1 2V	0011	C311 *C1	212 U10V	1 1124	107 7	7 _115 13	100.10	1 1120	
TC	RIZA 2211	0010	C311 °C.		1 2470	107.7	100.00	111 65	1 5202	
IC	0311	C312	0313	0314	1.34/0	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	
TC	C316	C 3 1 /	*^215	H15X	1 53/9	112 61	-121 34	109 09	1 1132	
TC	U15V	C214	*~?15	u15v	1 1100	100 00	_117 /1	100.00	1 1122	
TC	111JA	0215		0217	1 5247	110 01	170 02	110 71	1 5240	
TC	0314	C315	C316	C31/	1.534/	112.61	1/9.83	112./1	1.3340	
ТС	C317	C315	*C316	н⊥6Х	1.5340	112.71	-121.28	T03.10	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 C318C316*C317H17X1.5309113.30-121.68108.771.1141IC H17XC316*C317H17Y1.1141108.77-116.68108.761.1141IC C316C317C318H18X1.5340113.30-59.94110.461.1113IC H18XC317*C318H18Y1.1113110.46119.86110.451.1113IC H18XC317*C318H18Z1.1113110.46-120.06110.611.1112 RESI SQDG -1.00 ! 1 1 ! ! 1 ! Adaped from: ! RESI SAPI -1.00 ! Phosphatidylinositol 1 Stearoyl - CH2 1 Uses RESI INI1 - cyclic myi-inositol, ! ! Arachidonyl - CH RESI SAPC ! | (-) CH2 - PO4 - inositol ! 1 GROUP

 ATOM S
 SG301
 1.35
 !

 ATOM 07
 OG2P1
 -0.716
 !

 ATOM 08
 OG2P1
 -0.716
 !

 ATOM 09
 OG2P1
 -0.716
 !

 07 08---S---09 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 H2
 HCA1
 0.075 !
 H04-04
 \| |
 \/

 ATOM O2
 OC311
 -0.681 !
 C3---C2 |
 I

 ATOM H02
 HCP1
 0.439 !
 |
 |
 I

 ATOM C1 CC3162 0.340 ! GROU 02-H02 | ! ΗЗ CC3161 0.357 ! HCA1 0.012 ! ATOM C3 | ATOM H3 HCA1 ATOM H3 HCA1 0.012 ! ATOM O3 OC311 -0.712 ! ATOM HO3 HCP1 0.413 ! GROU 1 ATOM C4 CC3161 0.340 ! ATOM H4 HCA1 0.000 ! ATOM 04 0C311 -0.718 ! ATOM HO4 HCP1 0.440 ! 1 GROU ! ATOM C6 CC321 -0.288 ! T 0.064 ! ATOM H61 HCA2 0.064 ! ATOM H62 HCA2 | | alpha1 -¤44B GROU !
 ATOM C44
 CTL2
 0.305
 !

 ATOM HA
 HAL2
 0.005
 !

 ATOM HB
 HAL2
 0.005
 !
 H44A---C44---H44B | theta1 GROUP 1 ATOM C45 CTL1 0.214 ! ATOM H45 HAL1 0.036 ! H45---C45-----049 047 thet \\/ beta2 | ATOM 047 OSL -0.531 ! theta3 0.927 ! ATOM C7 CL

ATOM 049	OBL	-0.625 !	С7		
ATOM C8	CTL2	-0.376 !	beta3	1	
ATOM H8R	HAL2	0.131 !	H8RC8H8S	i	
ATOM H8S	HAL2	0.131 !		i	
GROUP		!	l beta4		
ATOM C46	CTL2	0.146 !			
ATOM H46X	HAL2	0.056 !		H46XC46	н4бү
ATOM H46Y	нат.2	0.056 !		111011 010	camma1
ATOM 048	OST.	-0 406 !		032 031	gannar
ATOM C23	CL	0.100 .	1	\\ /	anma?
ATOM 010	OBI	-0 644 1	l I	C23	gannaz
ATOM C24		-0.409.1		625	~~~~~ ?
ATOM U24		-0.409 !		248 024	yannia J
ATOM H24X	HALZ	0.145 !		242	n241
ATOM HZ41	HALZ	0.145 !		I	
GROUP		! 0 10 I			gamma4
ATOM C23		-0.18 !		I	
ATOM H3R	HALZ	0.09 !	нэк ===Сэ===нэз	I I	
ATOM H3S	HAL2	0.09 !		I	
GROUP		!		I	
ATOM C24	CTL2	-0.18 !		l	
ATOM H4R	HAL2	0.09 !	HRC24H4S		
ATOM H4S	HAL2	0.09 !		I	
GROUP		!	I	I	
ATOM C25	CEL1	-0.15 !	I	I	
ATOM H5R	HEL1	0.15 !	H5RC25	I	
GROUP		!	! (CIS)		
ATOM C26	CEL1	-0.15 !	!		
ATOM H6R	HEL1	0.15 !	H6RC26	1	
GROUP		!	I		
ATOM C27	CTL2	-0.18 !		1	
ATOM H7R	HAL2	0.09 !	H7RC27H7S	1	
ATOM H7S	HAL2	0.09 !	I	ĺ	
GROUP		!		Í	
ATOM C28	CEL1	-0.15 !		i	
ATOM H8R	HEL1	0.15 !	H8RC28	i	
GROUP		!	! (CIS)	ĺ	
ATOM C29	CEL1	-0 15 !		i	
ATOM H9R	HEL1	0 15 1	H9BC29	1	
GROUP		1		1	
ATOM C210	CTT.2	-0 18 1		1	
ATOM H10R	HAL2	0 09 1	H10BC210H10S	1	
ATOM H10S	нат.2	0.09 1		1	
GROUP	111112	1		I	
ATOM C211	CET 1	-0 15 1	1	1	
ATOM U11D		0.15	u11pC211	I	
CPOUD	111111	0.13		I	
ATTOM C212	CET 1	-0 15 1	: (CIS)	1	
ATOM U12D	UET 1	-0.15	: u12pC212	I	
CDOUD	перт	0.13 !	HIZKCZIZ	1	
GROUP		! 0 10 I			
ATOM CZIS		-0.18 !		I	
ATOM HISR	HALZ	0.09 !	HI3RC2I3HI3S	I	
ATOM HI3S	HAL2	0.09 !	l	I	
GROUP	0.007.1	!		I	
ATOM C214	CEL1	-0.15 !		l	
ATOM H14R	HEL1	0.15 !	H14RC214	I	
GROUP		!	! (CIS)		
ATOM C215	CEL1	-0.15 !	!	I	
ATOM H15R	HEL1	0.15 !	H15RC215	I	
GROUP		!		I	
ATOM C216	CTL2	-0.18 !	I	I	
ATOM H16R	HAL2	0.09 !	H16RC216H16S	I	
ATOM H16S	HAL2	0.09 !		I	
GROUP		!		I	
ATOM C217	CTL2	-0.18 !		I	

ATOM H17R	HAL2	0.09	! H17RC217H17S
ATOM H17S	HAL2	0.09	!
GROUP			1
ATOM C218	CTT-2	-0 27	• • • •
ATOM H18R	НДТ.2	0 09	н18вС218н18с I
ATOM H189	HAT.2	0.09	
CROUD	IIAUZ	0.05	•
ATOM C219	CTT 2	_0 18	
ATOM U10D		0.10	· u10pC210u10g
ATOM HIGK	HALZ	0.09	: HI9RC219H193
CDOUD	TALZ	0.09	
ATTOM C220	C TT 2	0 1 0	
ATOM U20D		-0.10	
ATOM HZUR	HALS	0.09	HZURCZZUHZUS
ATOM H2US	HAL3	0.09	
ATOM HZUT	HAL3	0.09	HZUT
GROUP	~~~ ^	0 1 0	!
ATOM C33	CTL2	-0.18	!
ATOM H3X	HAL2	0.09	НЗХСЗЗНЗҮ
АТОМ НЗҮ	HAL2	0.09	!
GROUP			!
ATOM C34	CTL2	-0.18	!
ATOM H4X	HAL2	0.09	! Н4ХСЗ4Н4Ү
ATOM H4Y	HAL2	0.09	!
GROUP			!
ATOM C35	CTL2	-0.18	!
ATOM H5X	HAL2	0.09	! н5хс35н5ү
ATOM H5Y	HAL2	0.09	!
GROUP			!
ATOM C36	CTL2	-0.18	· · · · · · · · · · · · · · · · · · ·
АТОМ Н6Х	HAL2	0.09	Н6ХС36Н6Ү
АТОМ Н6Ү	HAT.2	0.09	1
GROUP			1
ATOM C37	CTT-2	-0 18	•
ATOM H7X	НДТ.2	0.10	н7хН7х
ATOM U7X	UAT 2	0.09	
CPOUD	IIALIZ	0.09	· · · ·
JTOM C29	CTT 2	_0 10	
ATOM USS		-0.10	
ATOM HOX	HALZ	0.09	
CDOUD	HALZ	0.09	
GROUP		0 1 0	
ATOM C39	UTL2	-0.18	
ATOM H9X	HALZ	0.09	Н9ХСЗ9Н9Ү
ATOM H9Y	HAL2	0.09	!
GROUP			!
ATOM C310	CTL2	-0.18	!
ATOM H10X	HAL2	0.09	Н10ХС310Н10Ү
ATOM H10Y	HAL2	0.09	!
GROUP			!
ATOM C311	CTL2	-0.18	!
ATOM H11X	HAL2	0.09	! Н11ХС311Н11Ү
ATOM H11Y	HAL2	0.09	!
GROUP			!
ATOM C312	CTL2	-0.18	!
ATOM H12X	HAL2	0.09	! H12XC312H12Y
ATOM H12Y	HAL2	0.09	!
GROUP			!
ATOM C313	CTL2	-0.18	!
ATOM H13X	HAL2	0.09	! H13XС313Н13Y
ATOM H13Y	HAL2	0.09	!
GROUP			!
ATOM C314	CTL2	-0.18	!
ATOM H14X	HAL2	0.09	! H14XC314H14Y
ATOM H14Y	HAL2	0.09	!
GROUP			!
			•

ATOM C315	CTL2	-0.18	!	
ATOM H15X	HAL2	0.09	!	Н15ХС315Н15Ү
ATOM H15Y	HAL2	0.09	!	
GROUP			!	
ATOM C316	CTL2	-0.18	!	
ATOM H16X	HAL2	0.09	!	H16XC316H16Y
ATOM H16Y	HAL2	0.09	!	
GROUP			!	
ATOM C317	CTL2	-0.18	!	
ATOM H17X	HAL2	0.09	!	Н17ХС317Н17Ү
ATOM H17Y	HAL2	0.09	!	
GROUP			!	
ATOM C318	CTL3	-0.27	!	
ATOM H18X	hal3	0.09	!	H18XC318H18Y
ATOM H18Y	HAL3	0.09	!	
ATOM H18Z	HAL3	0.09	!	H18Z

! Sul	fonat	te Head (Group							
BOND	S	07	S	08		S	C)9		
BOND	S	C6								
! Suc	Jar									
BOND	C1	01	C1 I	41	01	HO1	C1	0.5	C1	C.2
BOND	C2	H2	C2 (12 12	02	HO2	C2	C 3	C3	н3
BOND	C3	03	03 1	103	C3	C1	C4	U /	C1	04
DOND	01	0.5	C1 (105	C5	115	C4 C5	06	C4 C6	1161
DOND	04	HU4	C4 (0	пр	05	0	Co	нот
BOND	60	HOZ	C5 (5						
I Tra										
! Inc	SILO.	L Head GI	roup	01.0	011	a 1 0	01.1	010		
BOND	CII	HL	CII	CI6	CII	C12	CII	012	- 1 0	0
BOND	C12	H2	C12	02	02	HO2	C12	C13	C13	H3
BOND	C13	03	03	ноз	C13	C14	C14	H4	C14	04
BOND	04	HO4	C14	C15	C15	H5	C15	C16	C16	НG
BOND	C16	06	06	HO6	C15	05	05	HO5		
BOND	012	P	P	011	P	013	P	014	011	C1
! Gly	cero	l Backbor	ne							
BOND	C1	HA	C1	HB	C1	C2				
BOND	C2	HS	C2	C3	C2	021				
BOND	C3	HX	C3	ΗY	C3	031				
! Cha	ain fi	rom C2								
BOND	021	C21								
BOND	C21	C22								
DOUBT	E C	21 022								
BOND	C22	H2R	C22	H2S	C22	C23				
BOND	C23	H3B	C23	H3S	C23	C24				
BOND	C24	u/D	C24	1135 U/C	C24	C25				
BOND	C24		024	1145	024	620				
DOUD										
DOUDI			C 2 6	C 2 7						
BOND	020	HOR	C20	UZ /	007	a 0 0				
BOND	C27	H/R	C27	H/S	C27	C28				
BOND	C28	H8R								
DOUBI	LE C2	28 C29								
BOND	C29	H9R	C29	C210						
BOND	C21() H10R	C210	H10S	C210	C211				
BOND	C211	l H11R								
DOUBI	LE C2	211 C212								
BOND	C212	2 H12R	C212	C213						
BOND	C213	3 H13R	C213	H13S	C213	C214				
BOND	C214	4 H14R								
DOUBI	LE C2	214 C215								
BOND	C215	5 H15R	C215	C216						

BOND BOND	C216 C217	H16R H17R	C216 C217	5 H16S 7 H17S	C216 C217	C217 C218		
BOND	C218	H18R	C218	8 H18S	C218	C219		
BOND	C219	H19R	C219	H19S	C219	C220		
BOND	C220	H2OR	C220) H20S	C220	Н20Т		
! Cha	in Fro	m C3						
BOND	031	C31						
BOND	C31	032						
DOORT	C33	U3Z U2V	C 30	цоv	C 30	C 2 2		
BOND	C32	127 137	C32	П2 I U 2 V	C32	C31		
BOND	C34	пјл нду	C34	HAV	C34	C35		
BOND	C35	H5X	C35	H5Y	C35	C36		
BOND	C36	нбх	C36	нбү	C36	C37		
BOND	C37	H7X	C37	H7Y	C37	C38		
BOND	C38	H8X	C38	H8Y	C38	C39		
BOND	C39	н9х	C39	Н9Ү	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	8 H13Y	C313	C314		
BOND	C314	H14X	C314	H14Y	C314	C315		
BOND	C315	H15X	C315	6 H15Y	C315	C316		
BOND	C316	H16X	C316	5 H16Y	C316	C317		
BOND	C317	H17X	C317	H17Y	C317	C318		
BOND	C318	H18X	C318	8 H18Y	C318	H18Z		
IMPR (C21 O2 TOR O1	1 C22 (S	022 0	31 031 C3	32 032			
ACCEP' ACCEP'	TOR 02 TOR 03	S S						
! ! Sul ACCEP' ACCEP'	I J fonate TOR O1 TOR O2 TOR O3	K S S	L	R(IK)	T(IKJ) PHI	T(JKL)	R(KL)
TC C2	C1	S	01 0.	0	0.00	180.00	0.0	0.0
IC C1	01	~ *S	02 0.	0	0.00	120.00	0.0	0.0
IC C1	01	*S	03 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	Н12 О.	0	0.00	-120.00	0.0	0.0
IC S	C1	C2	C3 0.	0	0.00	180.00	0.0	0.0
! Ino	SITOL	Head Gi	roup	1 6600	107	21 50 02	100 11	1 5 6 1 0
		2 CI.	3 CI4	1.5530	J 107.	31 -59.93	109.11	1.5612
		3 CI4	4 CI5	1 4341	107	LL 59.27	114.44	1.4654
	3 CI 3 C1		L 012	1 5611	L 107.	JI -17J.79 AA _55 A8	109 80	1 5350
	4 C1	5 C1(5 C10	1 4654	1 109	44 55.40 80 55.05	107.18	1 5598
	2 C1	3 C14	1 04	1 4341	109.	11 - 177 27	106.06	1 4595
TC C1	3 C1	4 C15	5 05	1.5612	2 114	44 171.27	114.28	1.4386
IC C1	2 C1	3 C14	4 H4	1.4341	109.	11 -64.25	106.39	1.1684
IC 01:	2 C1	2 *C	11 H1	1.4086	5 117.	69 -121.05	110.98	1.1834
IC 01	2 C1	1 C12	2 02	1.4086	5 117.	69 51.01	111.79	1.4490
IC 01	2 C1	1 C12	2 Н2	1.4086	5 117.	69 -61.28	98.22	1.1105
IC C1	3 C1	4 C15	5 Н5	1.5612	2 114.	44 52.34	110.34	1.0922
IC 02	C1	1 *C1	12 C13	1.4490) 111.	79 133.20	107.31	1.4341
IC O3	C1	4 *C	13 H3	1.4537	110.	99 114.31	113.73	1.1394
IC O3	C1	2 *C2	13 C14	1.4537	105.	59 119.36	109.11	1.5612
IC 04	C1	3 *C2	14 C15	1.4595	106.	06 -123.46	114.44	1.4654
IC C1	6 C1	4 *C	15 05	1.5350) 109.	80 -133.25	114.28	1.4386

IC C14	C15	05	HO5	1.4654	114.28	-73.20	108.55	0.9726	
IC C14	C15	C16	06	1.4654	109.80	-179.24	110.87	1.4043	
IC C16	C11	012	P	1.5530	117.69	300.00	114.27	0.9451	! gauche
IC C11	C12	02	HO2	1.5530	111.79	-31.80	115.65	0.9404	
IC C12	C13	03	ноз	1.4341	105.59	37.19	107.10	0.9920	
IC C13	C14	04	HO4	1.5612	106.06	35.00	105.15	0.9686	
IC C15	C16	06	HO6	1.5350	110.87	51.35	112.65	0.9879	
IC C14	C15	C16	НG	1.4654	109.80	-58.40	111.34	1.0796	
! Phosph	ate Lin	nker							
IC C11	012	Р	011	1.3655	121.23	153.36	102.74	1.5058	
IC 011	012	*P	013	1.5867	101.18	-114.47	107.73	1.4832	
IC 011	012	*P	014	1.5867	101.18	116.82	109.30	1.4741	
TC 012	P	011	C1	1.5958	101.18	180.00	122.31	1.4271	! trans
TC P	011	C1	C2	1 5867	122 31	180 00	111 45	1 5517	! trans
TC C2	011	*C1	НА	1 5517	111 45	117 99	107 86	1 1119	. 010110
IC HA	011	*C1	HR	1 1119	107 86	116 85	112 59	1 1137	
		C2	021	1 1271	111 /5	_175 58	109 10	1 4420	
L Packha	70 20	02	021	1.12/1	111.40	1/5.50	107.40	1.1120	
: Backbo	c1	* ~ 2	C 2	1 4420	100 10	101 10	110 56	1 5561	
IC 021		^CZ	03	1.4420	109.40	-121.10	110.56	1.3361	
		^CZ	HS CO1	1.5561	10.56	-110.00	109.10	1,1148	
	CZ	021	CZI	1.551/	109.40	/5.31	115.18	1.3240	
IC CZ	021	CZI	CZZ	1.4420	115.18	-167.64	109.38	1.5349	
1C C22	021	*C21	022	1.5349	109.38	1//.9/	125.87	1.2208	
IC 021	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 Cl	C2	C3	031	1.5517	110.56	-174.46	111.33	1.4462	
IC 031	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	CЗ	031	C31	1.5561	111.33	-170.38	113.09	1.3331	
IC C3	031	C31	C32	1.4462	113.09	-178.75	108.33	1.5405	
IC C32	031	*C31	032	1.5405	108.33	-179.57	125.60	1.2151	
IC 031	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 C	hain 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	
TC C25	C23	*C24	H4R	1.5107	115.67	-121.06	107.11	1.1144	
TC C25	C23	*C24	H4S	1 5107	115 67	124 06	108 43	1 1128	
TC 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	1,0.00	125 28	1 5097	lais dh
IC C27	C25	*C26	H6R	1 5097	125.28	178 19	119 65	1 1004	.015 00
IC C25	C26	C27	C28	1 3453	125.28	120 00	121 35	1 5192	
IC C28	C26	*027	UZ0 U7R	1 5192	121 35	-124 15	108 68	1 1135	
IC C20	C26	*027	1171C	1 5102	121.35	122.21	106.00	1 1121	
IC C26	C20 C27	C20	п/3 С20	1 5007	121.33	120.00	132 90	1 25/0	
IC C20	C27	+C20		1 2540	122.00	170.00	111 25	1 1010	
IC C29	C27	~CZ0	пок со10	1 5102	132.00	-1/0.43	120.20	1 5115	المراجع والم
IC C27	C28	LZ9 + 220	CZIU NOD	1.5192	120.20	170 50	130.38	1.5115	!CIS db
	C28	^CZ9	H9K	1.5115	130.38	1/8.53	11/.0/	1.1014	
IC C28	C29	C210	CZII	1.3549	130.38	120.00	111.80	1.5083	
IC C211	C29	*C210	HIUR	1.5192	121.35	-124.15	108.68	1.1135	
IC C211	029	*C210	HIUS	1.5192	121.35	123.34	106.97	1.1128	
1C 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	

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	
TC	C220	C218	*C219	H19S	1.5192	121.35	123.34	106.97	1.1128	
TC	C218	C219	C220	н20т	1.5345	112.95	180.00	110.39	1.1115	
TC	н20т	C219	*C220	H20R	1 5192	121 35	-124 15	108 68	1 1135	
TC	H20T	C219	*C220	H205	1 5192	121 35	123 34	106.00	1 1128	
1 2	ACVI CH	ozin 2	0220	112.00	1.0192	121.00	123.34	100.57	1.1120	
TC	C31	C32	C 3 3	C34	1 5405	116 85	180 00	126 13	1 5951	
TC	C31	C32	*033	U3V	1 5410	112 26	_110.00	111 74	1 11/0	
TC	C34	C32	*033	113A 113V	1 5102	121 25	122 24	106 07	1 1120	
TC	022	C32	~C33	п) I с) E	1.0192	121.33	123.34	112 20	1 5410	
IC	C3Z	C33	+024		1.6060	112 52	100.00	110 50	1.5410	
TC	035	033	^C34	H4X	1.5396	101 05	-123.43	110.53	1.1101	
IC	035	033	^C34	H41	1.5192	121.35	123.34	106.97	1.1128	
IC	033	C34	035	C36	1.5951	113.30	180.00	113.52	1.5396	
IC	036	C34	*035	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	н9х	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	
TC	C316	C314	*0315	H15Y	1.5192	121 35	123 34	106 97	1 1128	
TC	C314	C315	C316	C317	1 5357	111 81	180 00	114 29	1 5985	
TC	C317	C315	*C316	H16X	1 5396	113 52	-123 43	110 53	1 1101	
TC	C317	C 3 1 5	*C316	H16Y	1 5192	121 35	123.13	106 97	1 1128	
TC	C315	C316	C317	C318	1 5374	114 29	180 00	130 92	1 5745	
TC	C318	C316	*C317	H17Y	1 5396	113 50	-123 43	110 53	1 1101	
TC	C310	C316	×C217	111 / A 11 7 V	1 5100	101 0F	103 34	106 07	1 1100	
тC	COTQ	COID	COT /	III / I	エ・フエラム	тст.3Э	123 . 34	T00.21	⊥•TT <q< td=""><td></td></q<>	

IC C3	16 C317	C318	H18X	1.5985	130.92	180.00	110.90	1.1113
IC H1	8X C317	*C318	H18Y	1.5396	113.52	-123.43	110.53	1.1101
IC H1	8X 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 redu	aced topolog	ry f:	ile, suitable for building Ubiquinone and derivatives.
	!Uses li	.pid nor	nenclature t	o bi	uild isoprene tails, which can get built up from isoprenoid
units.					
	MASS 1	. Н	1.00800	Н!	polar H
	MASS 136	5 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	[] a	alphatic proton
	MASS 140	HAL2	1.008000 H	[] a	alphatic proton
	MASS 141	. HAL3	1.008000 H	[] a	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 0	210	carbonyl C (acetic acid/methyl acetate)
	MASS 146	стт.1	12 011000 0		sp_3 carbon with 1 H (-CH1-)
	MASS 147		12 011000 0		sarbon of methylene group $(-CH^2-)$
	MAGG 140		12.011000 0	· · ·	carbon of methyl group (-CH3)
	MASS 140		12.011000 C		carbon of methyl group (-CH3)
	MASS 143		12.011000 0		Sarbon of methyl group (-CHS) for tetramethylammonium
	MASS 150	CELI	12.011000 0		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	С!	polar C
	MASS 203	CTN	12.01100	С!	tetrahedral C
	MASS 225	CUQ1	L 12.01100	С!	for quinones
	MASS 226	CUQ2	2 12.01100	С!	for quinones
	MASS 227	CUQS	3 12.01100	С!	for quinones
	MASS 228	CUO4	12.01100	С!	for quinones
	MASS 229) OUÕI	L 15.99900	0!	for quinones
	MASS 230		2 15,99900	0 !	for guinones
	When OF	and OF	are popula	ted.	by different quinones, they need distinct types to keep the
naramet	ers cons	istent	are popure		
purumee	MASS 201	илм	2 1 0.0800	чI	nonnolar H
	MAGE 201		12 01100		
	MASS 202		12.01100		potat C
	MASS 203	OTIN2	12.01100		
	MASS 225		12.01100	0 !	for quinones
	MASS 226		5 12.01100	C!	for quinones
	MASS 22	CUQ	/ 12.01100	C !	for quinones
	MASS 228	CUQ8	3 12.01100	с!	for quinones
	MASS 229	OUQ3	3 15.99900	0 !	for quinones
	MASS 230) OUQ4	1 15.99900	0 !	for quinones
	MASS 240) CNQ1	L 12.01100	С!	for naphthoquinone
	MASS 241	. CNQ2	2 12.01100	С!	for naphthoquinone
	MASS 242	HP.	1.00800	Н!	aromatic hydrogen
	RESI NAB	Q	0.00000 !Na	phtl	noquinone (vitamin K)
	GROUP !	ubiqui	inone ring		
	ATOM C1	CUQ3	-0.317	!	
	ATOM C2	CUÕ1	0.586	!	H7\ /H4
	ATOM 02	OU01	-0.456	!	C10C11
	ATOM C3	CUO2	0.055	i	
	ATOM C12	CNO1	-0.336	i	н6-С9 С12-н5
			0.055	÷	
	ATOM CO	CNQ2	0.000		
	ATOM C9	CNQ1	-0.330	-	(4C5
	ATOM CS		0.380	1	
	ATOM 05		-0.456	1	
	ATOM C6	CUQ4	0.014	1	$U_{0} = -C_{0}$ $C_{2} = -C_{2}$
	ATOM C1M	1 CTN	-0.120	!	
	ATOM C11	CNQ2	-0.045	!	
	ATOM C10	CNQ2	-0.045	!	C6C1
	ATOM H1	HAN	0.09	!	/H1
	ATOM H2	HAN	0.09	!	Н10-С7-Н11 С1М-Н2
	ATOM H3	HAN	0.09	!	\H3
	ATOM H4	HAN	0.14	!	H14-C8-H12

ATOM H5 0.14 HAN ! АТОМ Н6 0.14 H13 HAN ! АТОМ Н7 HAN 0.14 1 !ATOM H8 HAN 0.09 ! !ATOM H9 0.09 HAN 1 ! ! isoprenic tail stub 1 ATOM C7 CTN -0.175 ATOM C8 CN -0.27 1 ATOM H10 HAN 0.09 ! ATOM H11 0.09 HAN 1 ATOM H12 HAN 0.09 ! ATOM H13 HAN 0.09 1 ATOM H14 HAN 0.09 1 ! bonds for ubiquinone ring BOND C1 C2 C2 C3 C3 C4 C4 C5 BOND C5 C6 C6 C1 C4 O4 C5 O5 BOND C2 O2 C3 O3 BOND 04 C4M С4М Н7 C4M H8 С4М Н9 СЗМ Н4 СЗМ Н5 BOND O3 C3M СЗМ Н6 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 UBIO 0.00000 !UBIQUINONE 6 FOR SPHAER FEHER, M SIDE GROUP ! ubiquinone ring CUQ3 -0.317 ATOM C1 ! /H4 ATOM C2 0.586 Н7∖ CUO1 1 ATOM 02 OUQ1 -0.456 1 Н8-С4М СЗМ-Н5 H9/ | | \H6 04 03 ATOM C3 CUQ2 0.055 1 ATOM 03 OUQ2 -0.336 1 ATOM C4 0.055 CUQ2 1 ATOM 04 OUQ2 -0.336 C4----C3 1 ATOM C5 CUQ1 0.586 ! / \backslash ATOM 05 OU01 -0.456 1 ATOM C6 CUQ4 0.014 ! 05--C5 $c_{2}^{-}-o_{2}^{-}$ ATOM C1M CTN -0.120 1 ATOM C3M CTN -0.045 ! \ ATOM C4M CTN -0.045 1 C6----C1 0.09 ATOM H1 /H1 HAN 1 1 ATOM H2 HAN 0.09 ! Н10-С7-Н11 С1М-Н2 0.09 ATOM H3 HAN \H3 1 1 ATOM H4 HAN 0.09 H14-C8-H12 ! АТОМ Н5 HAN 0.09 1 1 АТОМ Н6 HAN 0.09 H13 1 ATOM H7 HAN 0.09 1 ATOM H8 HAN 0.09 1 АТОМ Н9 HAN 0.09 1 ! isoprenic tail stub - ! Т ATOM C7 CTN -0.175 ! ATOM C8 CN -0.27 1 ATOM H10 HAN 0.09 1 ATOM H11 HAN 0.09 1 ATOM H12 HAN 0.09 1 ATOM H13 HAN 0.09 1 ATOM H14 HAN 0.09 1 ! bonds for ubiquinone ring BOND C1 C2 C2 C3 C3 C4 C4 C5 C6 C1 BOND C5 C6 BOND C2 O2 C3 O3 C4 04 C5 05 BOND O4 C4M C4M H7 C4M H8 С4М Н9 СЗМ Н4 С1М Н1 СЗМ Н5 BOND 03 C3M СЗМ Н6 BOND C1 C1M C1M H2 C1M H3 !Isoprene tail stub

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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

GROUI	?!ı	ubiqui	none ri	ng	
атом	C1	CIIO3	-0 05	9 I	
ATOM	C2	CUO1	0.46	2 1	Н7\ /Н4
ATOM	02	OUO1	-0.43	9 !	H8-C4M C3M-H5
ATOM	C3	CUO2	0.03	7!	H9/ I I \H6
ATOM	03	OUO2	-0.24	7 !	0.3
ATOM	C4	CUO2	-0.01	2 !	
!ATON	1 04	0Ū02	-0.2	0 !	c4c3
ATOM	C5	CUO1	0.39	5 !	
ATOM	05	OUÕ1	-0.44	7!	
ATOM	C6	CUQ4	0.03	4 !	05C5 C2O2
ATOM	C1M	CTN	-0.23	1 !	\backslash /
ATOM	СЗМ	CTN	-0.06	0!	\setminus /
ATOM	C4M	CTN	-0.26	6!	C6C1
ATOM	Н1	HAN	0.09	!	/H1
ATOM	H2	HAN	0.09	!	H10-C7-H11 C1M-H2
ATOM	HЗ	HAN	0.09	!	\H3
ATOM	H4	HAN	0.09	!	H14-C8-H12
ATOM	Н5	HAN	0.09	!	
ATOM	НG	HAN	0.09	!	H13
ATOM	H7	HAN	0.09	!	
ATOM	Н8	HAN	0.09	!	
ATOM	Н9	HAN	0.09	!	
				!	
!	isop	prenic	tail s	tub !	
				!	
ATOM	C'/	CTN	-0.157	!	
A'I'OM	C8	CN	-0.27	!	
ATOM	HIU	HAN	0.09	1	
ATOM	HII	HAN	0.09	:	
ATOM	HIZ	HAN	0.09	:	
ATOM	H13	HAN	0.09	:	
ATOM	HI4	HAN	0.09	!	
!	bo	nds fo	r ubia	inone	ring
BOND	C1 C2	2 C.	2 C3	C3 C4	C4 C5
BOND	C5 C6	6 C	6 C1		
BOND	C2 02	2 C	3 03	C4 C4M	C5 05
BOND	C4M H	H7 C	4M H8	С4М Н9	
BOND	03 C	3M C	3M H4	СЗМ Н5	СЗМ Н6
BOND	C1 C1	1M C	1M H1	C1M H2	С1М НЗ
!Isop	orene	tail	stub		
BOND	C6 C	7 C	7 H10	C7 H11	C7 C8 C8 H12 C8 H13 C8 H14
AUTO	GENERA	ATE AN	GLES DI	HEDRALS	

RESI 2MEO 0.00000 !2-methoxy Ubiquinone

GROUP	!	ubiquinone	ring

C1	CUQ3	0.029	!		
C2	CUQ1	0.480	!	H7\	/H4
02	OUQ1	-0.459	!	H8-C4M	СЗМ-Н5
C3	CUQ2	-0.056	!	H9/	\H6
4 03	OUQ2	-0.20	!	04	
C4	CUQ2	-0.001	!		
04	OUQ2	-0.286	!	C4	C3
C5	CUQ1	0.486	!	/	\
05	OUQ1	-0.368	!	/	\
C6	CUQ4	-0.148	!	05C5	C202
C1M	CTN	-0.226	!	\	/
СЗМ	CTN	-0.256	!	\	/
C4M	CTN	-0.014	!	C6	C1
Н1	HAN	0.09	!		/H1
H2	HAN	0.09	!	H10-C7-H1	11 C1M-H2
нЗ	HAN	0.09	!		\H3
	C1 C2 C3 4 O3 C4 O4 C5 C6 C1M C3M C4M H1 H2 H3	C1 CUQ3 C2 CUQ1 O2 OUQ1 C3 CUQ2 4 O3 OUQ2 C4 CUQ2 O4 O4 OUQ2 C5 CUQ1 C5 CUQ1 C6 CUQ4 C1M CTN C3M CTN C4M CTN HAN H2 HAN HAN HAN	C1 CUQ3 0.029 C2 CUQ1 0.480 02 OUQ1 -0.459 C3 CUQ2 -0.056 4 O3 OUQ2 -0.20 C4 CUQ2 -0.001 04 0UQ2 -0.286 C5 CUQ1 0.486 05 0UQ1 -0.368 C6 CUQ4 -0.148 C1M CTN -0.226 C3M CTN -0.226 C3M CTN -0.226 C4M CTN -0.014 H1 HAN 0.09 H3 HAN 0.09 H3 HAN 0.09	C1 CUQ3 0.029 ! C2 CUQ1 0.480 ! O2 OUQ1 -0.459 ! C3 CUQ2 -0.056 ! 4 O3 OUQ2 -0.20 ! C4 CUQ2 -0.286 ! C5 CUQ1 0.486 ! O5 OUQ1 -0.368 ! C6 CUQ4 -0.148 ! C1M CTN -0.226 ! C3M CTN -0.256 ! C4M CTN -0.014 ! H1 HAN 0.09 !	C1 CUQ3 0.029 ! C2 CUQ1 0.480 ! H7\ O2 OUQ1 -0.459 ! H8-C4M C3 CUQ2 -0.056 ! H9/ 4 O3 OUQ2 -0.20 ! O4 C4 CUQ2 -0.001 ! I

0.09 ! H14-C8-H12 ATOM H4 HAN 0.09 ! АТОМ Н5 HAN АТОМ Н6 HAN 0.09 1 H13 ATOM H7 HAN 0.09 ! ATOM H8 0.09 HAN 1 АТОМ Н9 HAN 0.09 1 ! isoprenic tail stub -0.171 ATOM C7 CTN 1 ATOM C8 CN -0.27 ! ATOM H10 HAN 0.09 1 ATOM H11 HAN 0.09 ! ATOM H12 HAN 0.09 1 ATOM H13 HAN 0.09 1 ATOM H14 HAN 0.09 1 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 05 BOND 04 C4M C4M H7 C4M H8 С4М Н9 BOND C3M H4 СЗМ Н5 СЗМ Н6 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 0.00000 !3-methoxy Ubiquinone with mixed-appropriate naming. RESI 3MOM GROUP ! ubiquinone ring ATOM C1 CUQ7 -0.059 1 0.462 ATOM C2 CUQ5 H7\ /H4 1 н8-С4М СЗМ-Н5 ATOM 02 OUQ3 -0.439 1 ATOM C3 0.037 CUQ6 1 H9/ | | \H6 ATOM 03 OUQ4 -0.247 1 03 ATOM C4 CUQ6 -0.012 ! T -0.20 !ATOM 04 OUO4 1 C4----C3 ATOM C5 CUQ5 0.395 ! ATOM 05 OUQ3 -0.447 1 0.034 ATOM C6 CUQ8 ! 05--C5 C2--O2 ATOM C1M CTN2 -0.231 / 1 \ ATOM C3M CTN2 -0.060 - L \ C6----C1 ATOM C4M CTN2 -0.266 1 0.09 /н1 ATOM H1 HAN2 1 ATOM H2 HAN2 0.09 Н10-С7-Н11 С1М-Н2 1 АТОМ НЗ HAN2 0.09 1 1 \H3 ATOM H4 HAN2 0.09 H14-C8-H12 ! ATOM H5 HAN2 0.09 1 ATOM H6 HAN2 0.09 Т H13 ATOM H7 HAN2 0.09 1 0.09 ATOM H8 HAN2 1 АТОМ Н9 HAN2 0.09 1 ! isoprenic tail stub ATOM C7 CTN2 -0.157 1 ATOM C8 CN2 -0.27 1 0.09 ATOM H10 HAN2 1 ATOM H11 HAN2 0.09 1 ATOM H12 HAN2 0.09 1 ATOM H13 HAN2 0.09 ! ATOM H14 HAN2 0.09 1 bonds for ubiquinone ring 1 BOND C1 C2 C2 C3 C3 C4 C4 C5 BOND C5 C6 C6 C1 СЗ ОЗ С4М Н8 C4 C4M C5 O5 BOND C2 02 C4 C1 C4M H9 BOND C4M H7 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 ! CUQ5 ATOM C2 0.480 H7\ 1 /н4 ATOM 02 OUQ3 -0.459 Н8-С4М СЗМ-Н5 ! CUQ6 -0.056 ATOM C3 H9/ I | \H6 1 -0.20 !ATOM 03 OUQ4 ! 04 ATOM C4 -0.001 CUQ6 ! ATOM 04 OUQ4 -0.286 1 c4----c3 ATOM C5 CUQ5 0.486 ! ATOM 05 -0.368OUO3 ATOM C6 CUQ8 -0.148 ! 05 - - C5C2 - - 02ATOM C1M CTN2 -0.226 Т ATOM C3M CTN2 -0.256 1 ATOM C4M -0.014 CTN2 C6----C11 ATOM H1 /H1 HAN2 0.09 Т 1 АТОМ Н2 0.09 Н10-С7-Н11 С1М-Н2 HAN2 ! 0.09 ATOM H3 HAN2 ! \H3 ATOM H4 HAN2 0.09 H14-C8-H12 1 АТОМ Н5 HAN2 0.09 ATOM H6 HAN2 0.09 Н13 1 ATOM H7 HAN2 0.09 1 ATOM H8 HAN2 0.09 Т ATOM H9 HAN2 0.09 ! ! isoprenic tail stub ATOM C7 CTN2 -0.171 Т ATOM C8 -0.27 CN2 ! ATOM H10 HAN2 0.09 Т ATOM H11 HAN2 0.09 1 0.09 ATOM H12 HAN2 1 ATOM H13 HAN2 0.09 ! ATOM H14 HAN2 0.09 1 bonds for ubiquinone ring 1 BOND C1 C2 C2 C3 C3 C4 C4 C5 BOND C5 C6 C6 C1 BOND C2 O2 C3 C3M C4 04 C5 O5 С4М Н8 BOND 04 C4M С4М Н7 C4M H9 BOND C3M H4 C3M H5 СЗМ Н6 BOND C1 C1M C1M H1 C1M H2 C1M H3 !Isoprene tail stub BOND C6 C7 C7 H11 C7 C8 C8 H12 C8 H13 C8 H14 C7 H10 AUTOGENERATE ANGLES DIHEDRALS RESI QO 0.00000 !2,3-Dimethoxy-5-dimethyl-1,4-benzoquinone GROUP ! ubiquinone ring CUQ3 -0.317 ATOM C1 1 H7\ ATOM C2 /H4 CUQ1 0.586 ! ATOM 02 -0.456 H8-C4M СЗМ-Н5 OUQ1 1 ATOM C3 CUQ2 0.055 H9/ | | \H6 1 ATOM O3 OUQ2 -0.336 04 03 ! ATOM C4 CUQ2 0.055 1 ATOM 04 OUQ2 -0.336 C4----C3 1 ATOM C5 CUQ1 0.586 Т \backslash ATOM 05 OUQ1 -0.456 T. ATOM C6 05--C5 CUQ4 0.014 ! C2--O2 ATOM C1M CTN -0.1201 ATOM C3M CTN -0.045 1 ATOM C4M CTN -0.045 C6----C1 1

ATOM H1 0.09 | /H1 HAN ! АТОМ Н2 0.09 H10 C1M-H2 HAN ! АТОМ НЗ HAN 0.09 1 \H3 ATOM H4 HAN 0.09 ! ATOM H5 0.09 HAN 1 ATOM H6 HAN 0.09 ! ATOM H7 HAN 0.09 1 ATOM H8 HAN 0.09 Т ATOM H9 HAN 0.09 1 !isoprene tail stub stub. ATOM H10 HAN 0.085 ! ! bonds for ubiquinone ring C4 C5 BOND C1 C2 C2 C3 C3 C4 BOND C5 C6 C6 C1 BOND C2 O2 C3 O3 C4 04 C5 O5 BOND 04 C4M С4М Н7 С4М Н8 С4М Н9 BOND O3 C3M СЗМ Н4 C3M H5 СЗМ Н6 BOND C1 C1M C1M H1 C1M H2 C1M H3 !Isoprene tail stub BOND C6 H10 AUTOGENERATE ANGLES DIHEDRALS RESI OOM 0.00000 !2,3-Dimethoxy-5,6-dimethyl-1,4-benzoquinone GROUP ! ubiquinone ring ATOM C1 CUQ3 -0.317 1 ATOM C2 CUQ1 0.586 ! H7\ /H4 Н8-С4М СЗМ-Н5 ATOM 02 OUQ1 -0.456 1 ATOM C3 CUQ2 0.055 H9/ | | \H6 1 ATOM 03 -0.336 04 03 OUQ2 1 ATOM C4 CUQ2 0.055 1 ATOM 04 OUQ2 -0.336 Т C4 - - - C3ATOM C5 0.586 CUQ1 1 / \backslash ATOM 05 OUQ1 -0.456 1 c2--02 ATOM C6 CUQ4 0.014 1 05--C5 -0.120 ATOM C1M CTN 1 \backslash / ATOM C3M CTN -0.045 \ ! ATOM C4M CTN -0.045 1 C6----C1 ATOM H1 HAN 0.09 1 /H1 АТОМ Н2 HAN 0.09 Н10-С7-Н11 С1М-Н2 1 АТОМ НЗ HAN 0.09 ! \H3 ATOM H4 0.09 H12 HAN Т ATOM H5 HAN 0.09 1 АТОМ Н6 HAN 0.09 ! ATOM H7 0.09 HAN 1 ATOM H8 HAN 0.09 ! ATOM H9 HAN 0.09 1 ! isoprenic tail stub 1 CTN -0.265 ! -0.175 - 0.09 ATOM C7 ATOM H10 HAN 0.09 1 ATOM H11 HAN 0.09 1 0.09 ATOM H12 HAN 1 1 bonds for ubiquinone ring BOND C1 C2 C2 C3 C3 C4 C4 C5 BOND C5 C6 C6 C1 C5 O5 BOND C2 O2 C3 O3 C4 O4 BOND O4 C4M C4M H7 C4M H8 С4М Н9 BOND 03 C3M C3M H5 C3M H4 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 н8 1 ATOM C1 CTL2 -0.18 ! HAL2 0.09 ! ATOM H1 HЗ С5---Н9

ATOM H2 HAL2 0.09 ! / \ GROUP C2==C3 H7 ! CEL1 -0.15 HEL1 0.15 ATOM C2 1 / \ АТОМ НЗ H1-C1-H2 C4-H(4-6) ! GROUP 1 CEL1 0.00 !Also try CG2D1 from cgenff. Basically the same. ATOM C3 GROUP ATOM C4 CTL3 -0.27 ATOM H4 HAL3 0.09 HAL3 0.09 HAL3 0.09 ATOM H5 АТОМ Н6 GROUP ATOM C5 CTL3 -0.27 HAL3 0.09 HAL3 0.09 ATOM H7 ATOM H8 АТОМ Н9 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 ! H4\ /Н9 ! methoxy groups 1 ATOM C5M CG331 -0.0740 ! н6-с5м C7M-H10 0.0820 ! ATOM H4 HGA3 H5/ | | \H8 H5 HGA3 0.0820 H7 07 ATOM ! 05 ATOM H6 HGA3 0.0820 ! ATOM C7M CG331 -0.0360 ! C6---C7 ATOM 11 H8 HGA3 0.0830 ! 11 А Α А A ! А А А Α

111011	110	110/15	0.0050	•	
ATOM	Н9	HGA3	0.0830	!	С5 С8-О8-Н44
ATOM	H10	HGA3	0.0830	!	\setminus /
ATOM	05	OG301	-0.1590	!	C4AC8A
ATOM	07	OG301	-0.2820	!	/ \
! top	ring			!	/ \
ATOM	C5	CG2R61	0.0940	!	04C4 O1
ATOM	C6	CG2R61	-0.2580	!	\setminus /
ATOM	H7	HGR61	0.1740	!	\setminus /
ATOM	С7	CG2R61	0.0940	!	C3C2
ATOM	C8	CG2R61	0.2220	!	H1\ /
ATOM	08	OG311	-0.6230	!	НЗ-СЗМ Н12-С9-Н11
ATOM	H44	HGP1	0.4470	!	H2/
ATOM	C4A	CG2R61	-0.1090	!	H14-C10-H13
ATOM	C8A	CG2R61	0.0420	!	H30\
! bot	tom r	ing		!	Н31-С22-С11-Н15
ATOM	01	OG3R60	-0.08000	!	H29/ /H32
ATOM	C2	CG2D10	-0.0170	!	Н16-С12-О12-С23-Н34
ATOM	C3	CG2R62	-0.0430	!	\H33
! me	thyl (group		!	/НЗб
ATOM	СЗМ	CG331	-0.1860	!	Н17-С13-С24-Н37
ATOM	Н1	HGA3	0.0750	!	\H35
ATOM	H2	HGA3	0.0750	!	H38\
ATOM	ΗЗ	HGA3	0.0750	!	H40-C25-O14-C14-H18
				!	НЗ9/
ATOM	C4	CG2R63	0.4880	!	H19-C15
ATOM	04	OG2D4	-0.5420	!	\ \
!tail			!		C16-H21
ATOM	С9	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 ATOM	C12 C13 C14 C15 C16 C17 C18 C20 C21 C22 C23 C24 C25 C26 O14 H15 H16 H17 H18 H19 H29 H30 H31 H32 H33 H34 H35 H36 H37 H38 H39 H40 H21 H22 H23 H41 H42 H42 H42 H42 H42 H42 H42 H42 H27	CG311 CG311 CG2DC1 CG2DC2 CG2DC2 CG2DC2 CG2DC1 CG331 CG331 CG331 CG331 CG331 CG331 CG331 CG331 OG301 HGA1 HGA1 HGA1 HGA3 HGA3 HGA3 HGA3 HGA3 HGA3 HGA3 HGA3	-0.0 0.0 -0.0 -0.2 -0.0 -0.0 -0.0 -0.0 -0.2 -0.0 -0.2 -0.0 -0.2 -0.0 -0.2 -0.0 -	390 ! 230 ! 200 ! 420 ! 960 ! 440 ! 820 ! 114 660 000 540 330 020 760 970 010 790 600 840 750 370 330 330 440 440 640 640 640 640 640 490 500 240 420 380 380 380 910 910	
ATOM	H28	HGA3	0.0	910	
BOND	C2 C	3 C.2	01	C2 C9	C3 C4
BOND	C3 C31	M C3M	H1	C3M H2	СЗМ НЗ
BOND	C4 C C5 C	4A C4 (6 C5 (04 05	C4A C8A C5M O5	C4A C5
BOND	С5М Н	4 C5M	Н5	С5М Н6	C6 C7
BOND	С6 Н С7м н	7 С7 8 с7м	С8 Н9	C7 O7 C7M H10	C7M 07 C8 08
BOND	C8 C82	A 08	H44	C8A 01	00 00
BOND	C9 H1	1 C9	H12	C9 C10	C10 H13
BOND	C10 H	14 CIU 22 C11	C11 C12	С11 Н15	C12 012
BOND	C12 C	13 C12	H16	C13 C24	C13 C14
BOND	CI3 H C15 C	16 C14	014 H19	C14 C15 C16 C17	C14 H18 C16 H21
BOND	C17 C	18 C17	H22	C18 C19	C18 H23
BOND	C19 C C21 H	20 C19 26 C21	С26 H27	C20 C21	C20 H25 C22 H29
BOND	C22 H	30 C22	H31	C23 012	C23 H32
BOND	С23 Н	33 C23	H34	C24 H35	C24 H36
BOND	С24 Н. С25 Н.	37 C25 39 C26	014 H41	C25 H38 C26 H43	C25 H40 C26 H42
			-		
AU'I'OG	ENERA'	TE ANGLI	s DI	HEDRALS	

Н25-С20 С26-Н43 \H42 C21 H26/|\H27 H28

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"
            ļ
            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] ļ # 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"}</pre> 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} {</pre>
            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
      $sell delete
      $sel2 delete
}
```