

## Supplemental Information

Large-scale structural rearrangement of a serine hydrolase from *Francisella tularensis* facilitates catalysis

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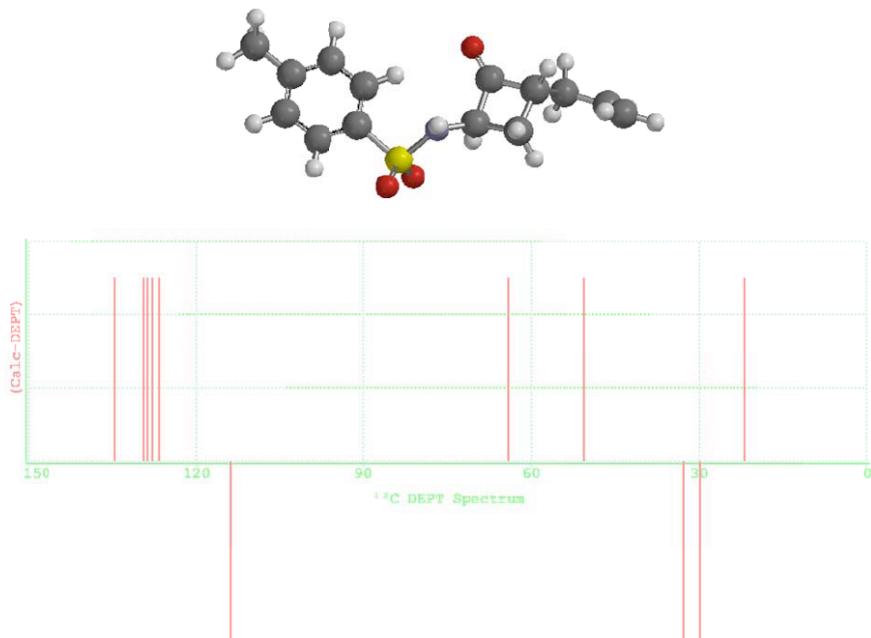
### Supplemental Tables and Figures

*Supplemental Spectrum:*

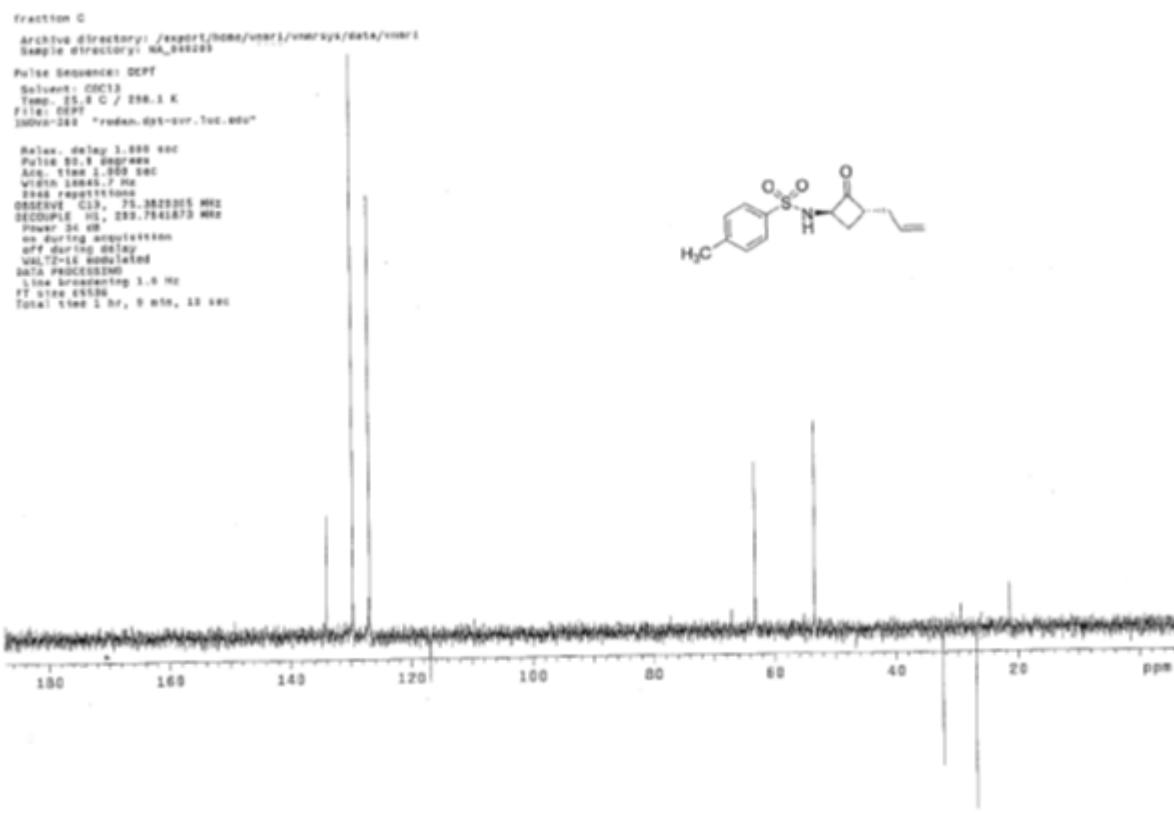
S2-S5

## Supplemental DEPT Spectrum

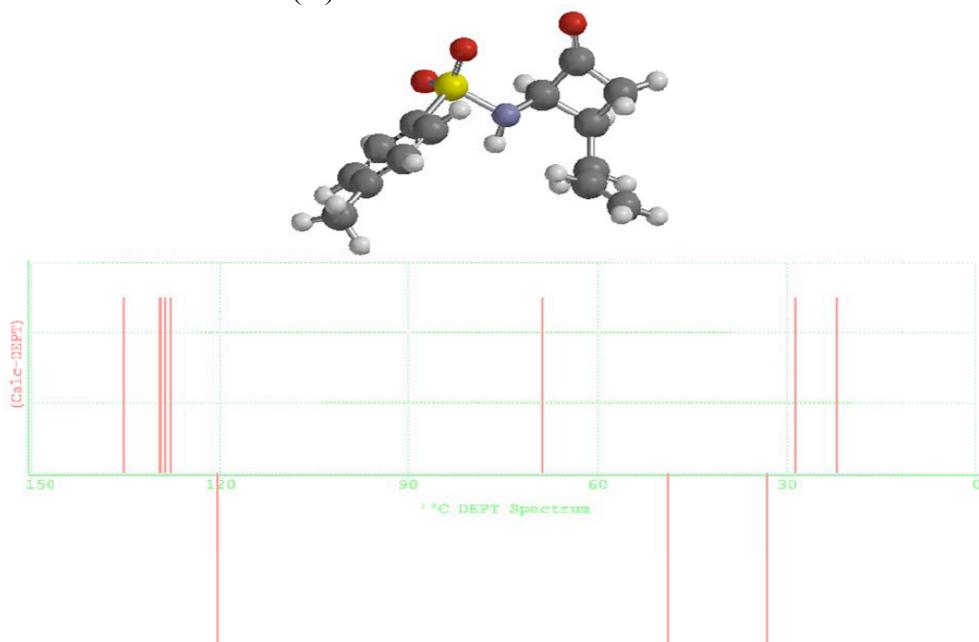
( $\pm$ )-N-trans-(3-allyl-2-oxocyclobutyl)-4-methylbenzenesulfonamide (iii) calculated DEPT spectra generated by SpartanPro'10 (Wavefunction) from ab initio density functional level of theory using the RB3LYP functional and the 6-31-G(D) basis sets



DEPT spectrum of ( $\pm$ )-N-trans-(3-allyl-2-oxocyclobutyl)-4-methylbenzenesulfonamide (iii)



**( $\pm$ )-N-cis-(2-allyl-4-oxocyclobutyl)-4-methylbenzenesulfonamide (iv)** calculated DEPT spectra generated by SpartanPro'10 (Wavefunction) from ab initio density functional level of theory using the RB3LYP functional and the 6-31-G(D) basis sets



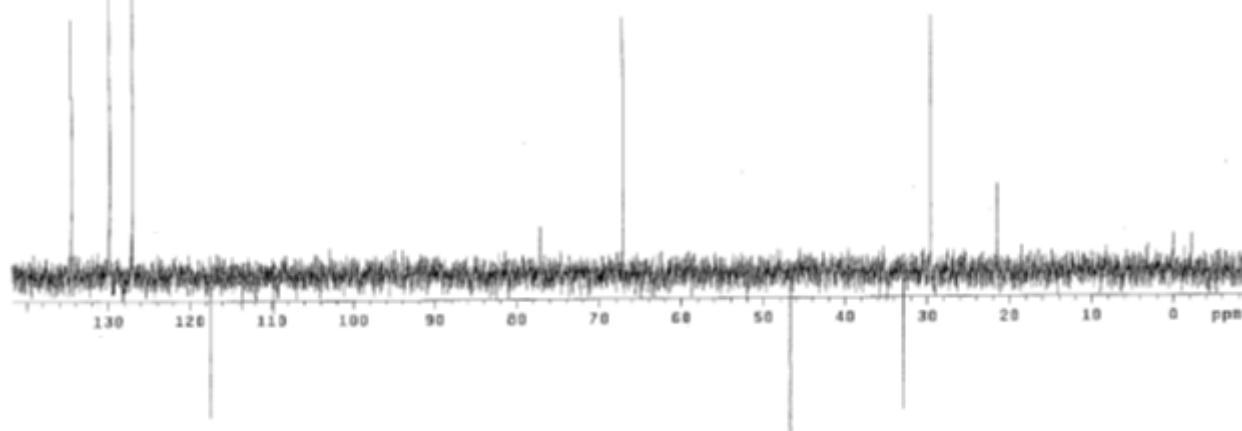
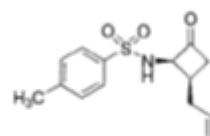
DEPT spectrum of ( $\pm$ )-N-cis-(2-allyl-4-oxocyclobutyl)-4-methylbenzenesulfonamide (iv)

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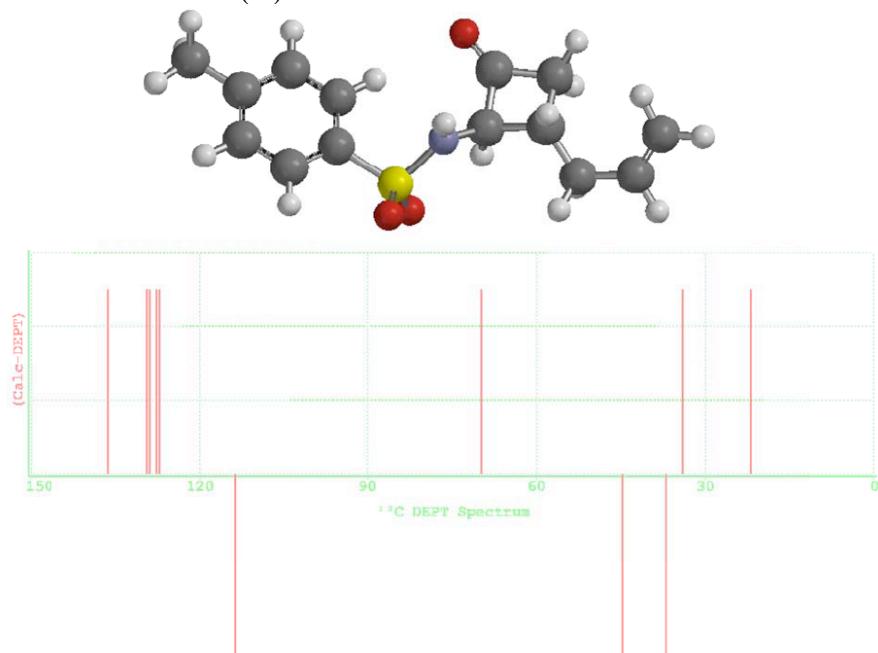
NA_348289
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Solvent: CDCl3
Temp: 29.0 C / 298.1 K
File: DEPT135_Proban,opt-evr,1sC,40u"
INCDIM=353 Program,opt-evr,1sC,40u"

 Relax. delay 2.000 sec
 Pulse 90.0 degrees
 ACG time 1.000 sec
 VNA 10000.0 Hz
 32768 repetitions
 DSCREVE CDCl3, 75.3823318 MHz
 DECUPLE H1, 288.7941873 MHz
 Power 27 dB
 on during acquisition
 off during processing
 mult=16 accumulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 4096
 Total time 1 hr, 43 min, 11 sec

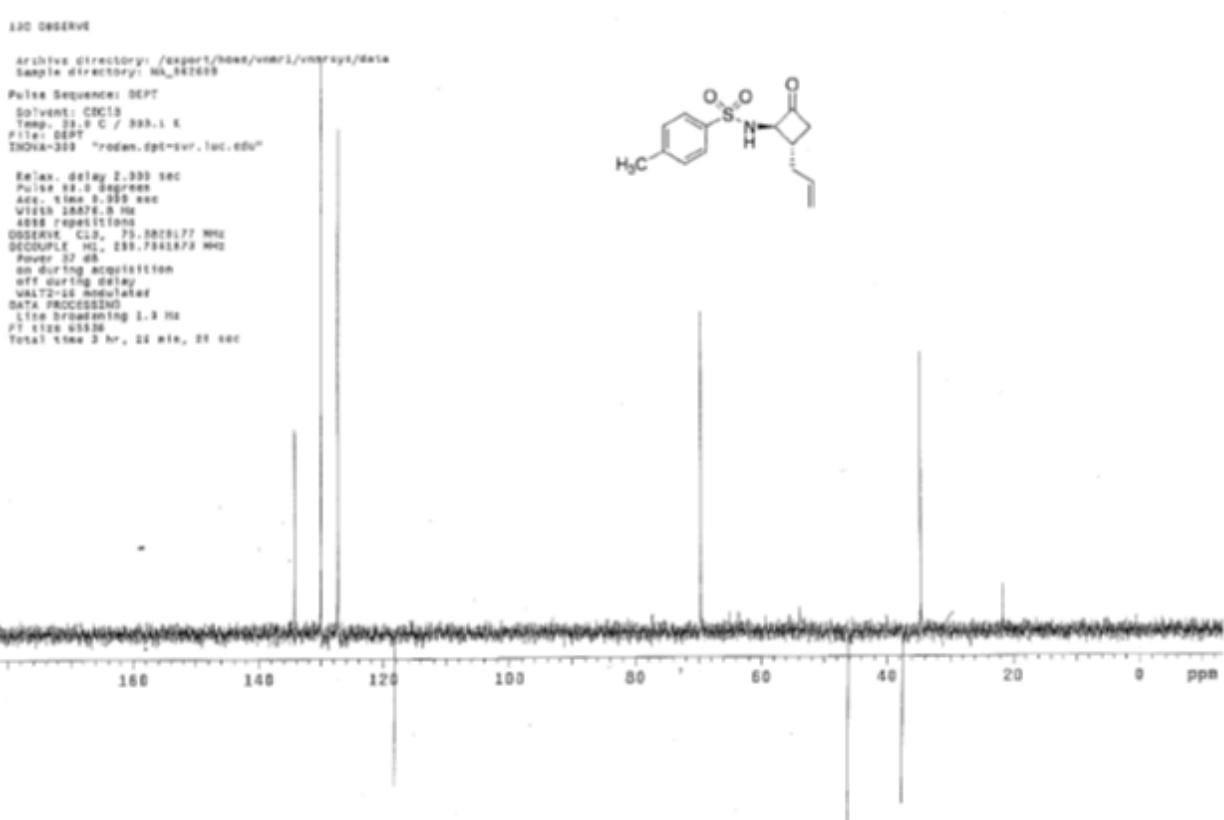
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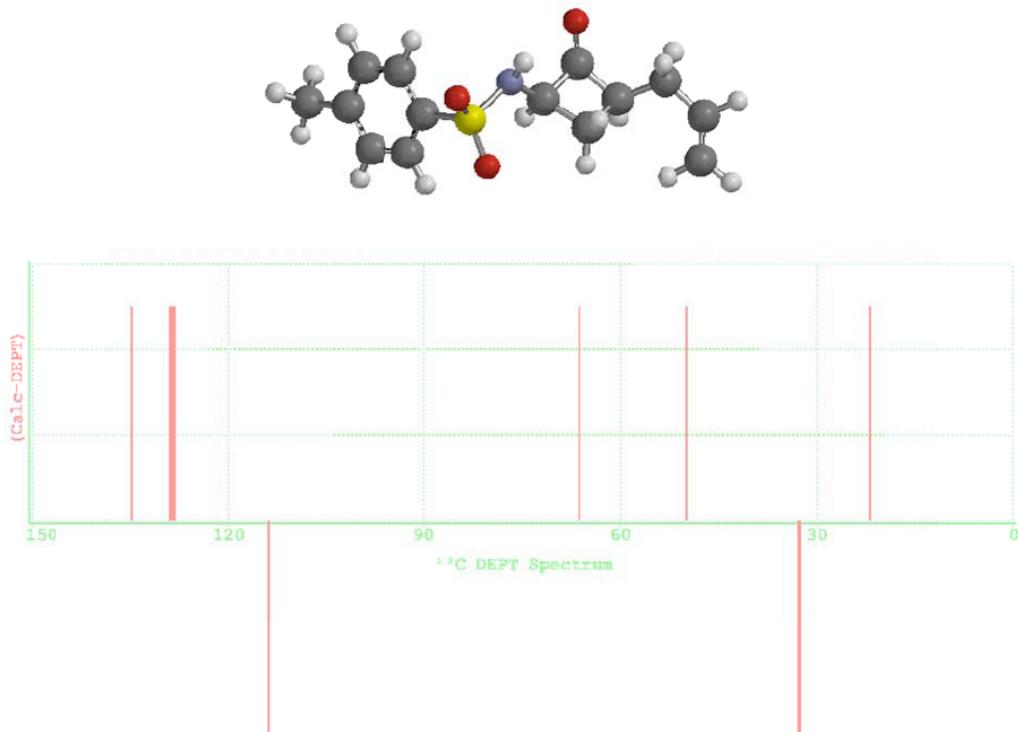
( $\pm$ )-N-trans-(2-allyl-4-oxocyclobutyl)-4-methylbenzenesulfonamide (**14**) calculated DEPT spectra generated by SpartanPro'10 (Wavefunction) from ab initio density functional level of theory using the RB3LYP functional and the 6-31-G(D) basis sets



DEPT spectrum of ( $\pm$ )-N-(trans-2-allyl-4-oxocyclobutyl)-4-methylbenzenesulfonamide (**14**)



**( $\pm$ )-N-trans-(2-allyl-4-oxocyclobutyl)-4-methylbenzenesulfonamide** calculated DEPT spectra generated by SpartanPro'10 from ab initio density functional level of theory using the RB3LYP functional and the 6-31-G(D) basis sets



**( $\pm$ )-N-cis-(3-allyl-2-oxocyclobutyl)-4-methylbenzenesulfonamide** was not detected or isolated.