

Supporting Information for:

Mechanistic study of the sPLA₂ mediated hydrolysis of a thio-ester pro anticancer ether lipid

Lars Linderoth[#], Peter Fristrup^{#,‡,*}, Martin Hansen[#], Fredrik Melander[§],

Robert Madsen[#], Thomas L. Andresen⁺ and Günther H. Peters^{§,*}

[§]Department of Chemistry, MEMPHYS-Center for Biomembrane Physics, Technical University of Denmark, DK-2800 Kgs. Lyngby Denmark; [#]Department of Chemistry, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark; [‡]Materials and Process Simulation Center (139-74), California Institute of Technology, Pasadena, California 91125, U.S.A.; [§]LiPlasome Pharma A/S, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark; ⁺DTU Nanotech, Technical University of Denmark, DK-4000 Roskilde, Denmark.

*Corresponding authors:

G.H. Peters, phone: (+45) 4525 2486, fax: (+45) 4588 3136, E-mail: ghp@kemi.dtu.dk;

P. Fristrup, phone: (+45) 4525 2123, fax: (+45) 4588 3136, E-mail: pf@kemi.dtu.dk

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Synthesis of lipids

Materials. Distearyl-*sn*-glycero-3-phosphoglycerol (DSPG) was purchased from Avanti Polar Lipids, Birmingham, AL, USA. All other chemicals were purchased from Sigma-Aldrich.

Organic synthesis. THF was distilled from sodium benzophenone, while CH₂Cl₂ was distilled from CaH₂. Thin layer chromatography was performed on aluminum plates coated with silica (Merck, Kieselgel 60 F₂₅₄). Visualization of the compounds were done by heating after dipping the plates in a solution of Ce(SO₄)₂ (2.5 g) and (NH₄)₆Mo₇O₂₄ (6.25 g) in 10% aqueous H₂SO₄ (250 mL). Flash chromatography was performed with silica gel 60. NMR spectra were recorded on a Varian Mercury 300 spectrometer with (CH₃)₄Si ($\delta_{\text{H}} = 0.0$ ppm) as an internal reference for ¹H NMR and with CDCl₃ ($\delta_{\text{C}} = 77.0$ ppm) as an internal reference for ¹³C NMR. Optical rotations were measured on a Perkin-Elmer 241 polarimeter, and the amount of hydrolysis was determined from MALDI-TOF MS data.

Synthesis of (S)-1-(Benzyloxy)-3-(octadecyloxy)propan-2-ol (2). Octadecanol (2.20 g, 8.15 mmol) was dissolved in dry THF (32 ml) under argon. The solution was cooled to 0 °C and 50 % (w/w) NaH dispersion in oil (626 mg, 13.0 mmol) was added. The reaction was heated to 80 °C for 1 h, cooled to room temperature and (S)-O-benzyl glycidol (1.07 ml, 6.52 mmol) and dry DMF (16 ml) were added. The reaction was heated to 80 °C and stirred at this temperature overnight. The reaction was cooled to room temperature, and H₂O (10 ml) was slowly added after which the reaction was stirred for 20 min. Removal of the solvent in vacuo gave a brown residue, which was dissolved in Et₂O (50 ml), washed with brine (5 x 15 ml), dried over Na₂SO₄, filtered and concentrated in vacuo. Purification by flash chromatography (5% EtOAc in heptane) gave 1.92 g (68 %) of the desired compound. ¹H-NMR (300 MHz, CDCl₃): δ 7.36-7.28 (m, 5H), 4.56 (s, 2H), 4.02-3.97 (m, 1H), 3.58-3.42 (m, 6H), 2.63 (br. s, OH), 1.58-1.49 (m, 2H), 1.25 (br. s, 30H), 0.88 (t, 3H, J=6.7 Hz). ¹³C-NMR (CDCl₃, 75 MHz): δ = 137.9, 128.4, 127.7, 73.4, 71.8, 71.7, 71.4, 69.5, 32.8, 29.7, 29.6, 29.5, 29.4, 26.0, 22.7, 14.1.

Synthesis of ((S)-1-(Benzyloxy)-3-(octadecyloxy)propan-2-yl) 4-methylbenzenesulfonate (3). Alcohol 2 (3.0 g, 6.90 mmol), TsCl (4.60 g, 24.15 mmol), Et₃N (3.36 ml, 24.15 mmol) and DMAP (253 mg, 2.07 mmol) were dissolved in DCM (20 ml), and the reaction was stirred for 96 h under argon. The reaction was diluted with Et₂O (20 ml), washed with brine (3 x 20 ml), dried over Na₂SO₄, filtered and concentrated in vacuo. Purification by flash chromatography (10 % EtOAc in heptane) gave the desired compound in quantitative yield.

(MALDI-TOF (ES⁺) Calcd. for C₃₅H₅₆O₅ (M+Na)⁺ 611.37. Found: 611.44). ¹H-NMR (300 MHz, CDCl₃): δ 7.93-7.91 (m, 1H), 7.81-7.78 (m, 1H), 7.42-7.21 (m, 7H), 4.74-4.67 (m, 1H), 4.46 (d, 1H, J=12.0Hz), 4.41 (d, 1H, J=12.2Hz), 3.65-3.58 (m, 4H), 3.32 (t, 2H, J=6.6Hz), 2.41 (s, 3H), 1.44-1.40 (m, 2H), 1.26 (br. s, 32H), 0.88 (t, 3H, J=5.9Hz). ¹³C-NMR (CDCl₃, 75 MHz): δ = 144.4, 137.6, 133.9, 129.6, 129.5, 128.3, 128.0, 127.6, 127.5, 127.0, 79.7, 73.3, 71.7, 69.2, 68.7, 31.9, 29.7, 29.6, 29.5, 29.3, 26.0, 22.7, 21.6, 14.1.

Synthesis of (R)-1-(Benzyloxy)-3-(octadecyloxy)propan-2-thiocyanate (4). Sulfonate **3** (379 mg, 0.64 mmol) was dissolved in dry DMF (5 ml), and KSCN (538 mg, 4.5 mmol) was added under N₂. The reaction was heated to 110 °C and stirred for 48 h. The reaction was poured into ice water (20 ml) and extracted with DCM (4 x 10 ml). The combined organic extracts were washed with brine (40 ml), dried over Na₂SO₄, filtered and concentrated in vacuo. Purification by flash chromatography (5 % EtOAc in heptane) gave 207 mg (68 %) of the desired compound. (MALDI-TOF (ES⁺) Calcd. for C₂₉H₄₉NO₂S (M+Na)⁺ 498.34. Found: 498.41). ¹H-NMR (300 MHz, CDCl₃): δ 7.40-7.28 (m, 5H), 4.57 (s, 2H), 3.82-3.69 (m, 4H), 3.59 (dd, 1H, J=5.8Hz, J=11.5Hz), 3.44 (t, 2H, J=6.6Hz), 1.57-1.52 (m, 2H), 1.25 (s, 30H), 0.88 (t, 3H, J=6.7Hz). ¹³C-NMR (CDCl₃, 75 MHz): δ = 137.3, 128.5, 128.0, 127.7, 111.7, 73.5, 71.8, 69.4, 68.9, 48.9, 31.9, 29.7, 29.6, 29.4, 29.3, 26.0, 22.7, 14.1.

(R)-1-(Benzyloxy)-3-(octadecyloxy)propan-2-thiol (5). LiAlH₄ (54 mg, 1.43 mmol) was added to dry Et₂O (20 ml) under N₂, and the suspension was cooled to 0 °C. A solution of thiocyanate **4** (340 mg, 0.715 mmol) in dry Et₂O (15 ml) was slowly added, and the reaction was stirred at 0 °C for 5 min. The reaction was quenched by dropwise addition of 0.5 M HCl until no more gas evolved from the solution. The reaction mixture was diluted with H₂O (10 ml) and extracted with Et₂O (3 x 15 ml). The combined organic extracts were washed with brine (15 ml), dried over Na₂SO₄, filtered and concentrated in vacuo giving 310 mg (96 %) of the desired compound. The compound was used without further purification in the next reaction. (MALDI-TOF (ES⁺) Calcd. for C₂₈H₅₀O₂S (M+Na)⁺ 473.34. Found: 473.59). ¹H-NMR (300 MHz, CDCl₃): δ 7.35-7.25 (m, 5H), 4.54 (s, 2H), 3.61 (d, 2H, J=5.8Hz), 3.56 (d, 2H, J=5.8Hz), 3.42 (t, 1H, J=6.6Hz), 3.14 (td, 1H, J=5.8Hz, J=8.1Hz), 1.91 (d, 1H, J=7.9Hz), 1.57-1.53 (m, 2H), 1.26 (s, 30H), 0.88 (t, 3H, J=6.7Hz), ¹³C-NMR (CDCl₃, 75 MHz): δ = 138.1, 128.3, 127.6, 127.5, 73.1, 72.2, 71.8, 71.3, 39.4, 31.9, 29.7, 29.6, 29.5, 29.3, 26.1, 22.7, 14.1.

Synthesis of (R)-1-(Benzyloxy)-3-(octadecyloxy)propan-2-yl octadecanethioate (6). Thiol **5** (310 mg, 0.69 mmol) was dissolved in dry DCM (10 ml), and octadecanoic acid (391 mg,

1.38 mmol) and DMAP (5 mg) were added under N₂. The solution was cooled to 0 °C and 1M DCC in DCM (1.4 ml, 1.4 mmol) was added dropwise, and the mixture was allowed to warm to room temperature and stirred overnight. The mixture was diluted with DCM (20 ml), washed with H₂O (2 x 20 ml) and brine (20 ml), dried over Na₂SO₄, filtered and concentrated in vacuo. Purification by flash chromatography (5 % Et₂O in heptane) gave 446 mg (90 %) of the desired compound. (MALDI-TOF (ES⁺) Calcd. for C₄₆H₈₄O₃S (M+Na)⁺ 739.60. Found: 739.73). ¹H-NMR (300 MHz, CDCl₃): δ 7.34-7.26 (m, 5H), 4.57 (d, 1H, J=12.2Hz), 4.53 (d, 1H, J=12.3Hz), 3.95-3.86 (m, 1H), 3.70-3.55 (m, 4H), 3.48-3.35 (m, 2H), 2.54 (t, 1H, J=7.5Hz), 1.67-1.62 (m, 2H), 1.55-1.51 (m, 2H), 1.25 (s, 58H), 0.88 (t, 6H, J=6.7Hz). ¹³C-NMR (CDCl₃, 75 MHz): δ = 199.0, 138.1, 128.3, 127.5, 73.0, 71.3, 69.4, 69.0, 44.2, 43.0, 34.9, 31.9, 29.7, 29.6, 29.5, 29.4, 29.2, 28.9, 26.1, 25.6, 22.7, 14.1.

Synthesis of (2*R*,4*S*)-2,2-Dimethyl-[1,3]dioxolan-4-ylmethyl 2-octadecanoylthio-3-octadecyloxy-propyl methyl phosphate (7). Thio-ester **6** (90 mg, 0.13 mmol) was dissolved in dry DCM (7 ml) and cooled to -30 °C under argon. 1M BCl₃ in DCM (0.34 ml, 0.34 mmol) was added dropwise, and the reaction was stirred for 30 min. Ice water (10 ml) was added, the phases were separated, and the organic phase was washed with H₂O (10 ml), dried over Na₂SO₄, filtered and concentrated in vacuo. The crude compound was dissolved in dry DCM (10 ml), and TMP (0.055 ml, 0.33 mmol) and (*i*-Pr)₂NP(OMe)Cl (0.06 ml, 0.31 mmol) were added under argon. The solution was stirred at room temperature for 40 min where after DCM (20 ml) was added, and the solution was quickly washed with sat. NaHCO₃ (2 x 20 ml), dried over Na₂SO₄, filtered and concentrated in vacuo. The crude compound was dissolved in dry DCM (7 ml) and activated molecular sieves and (*R*)-isopropylidene glycerol (0.04 ml, 0.31 mmol) were added under argon. The mixture was stirred at room temperature for 40 min. where after the solution was cooled to 0 °C and 5-phenyl-1*H*-tetrazole (48 mg, 0.33 mmol) was added. The mixture was allowed to warm to room temperature and stirred for 90 min. The solution was again cooled to 0 °C, and 5.5 M *t*-BuOOH in decane (0.06 ml, 0.33 mmol) was added. The mixture stirred at 0 °C for 90 min. and 1 M aqueous Na₂SO₃ (10 ml) and 1M sat. NaHCO₃ (10 ml) were added. The mixture was allowed to warm to room temperature and stirred for 20 min. The mixture was extracted with DCM (4 x 20 ml), and the combined organic extracts were washed with brine (15 ml), dried over Na₂SO₄, filtered and concentrated in vacuo. The crude compound was purified by flash chromatography (eluent 25 % EtOAc in Heptane) giving the desired product as a colorless oil (66 mg) in 62 % yield. ¹H-NMR (300 MHz, CDCl₃): δ 4.36-4.29 (m, 1H), 4.24-4.16 (m, 2H), 4.11-4.02 (m, 4H), 3.93-3.89 (m, 1H),

3.88-3.83 (m, 1H), 3.82-3.78 (m, 3H), 3.64 (dd, 1H, J=4.4Hz, J=9.9Hz), 3.54 (dd, 1H, J=6.2Hz, J=9.9Hz), 3.46-3.40 (m, 2H), 2.55 (t, 2H, J=7.6Hz), 1.67-1.63 (m, 2H), 1.58-1.52 (m, 2H), 1.43 (s, 3H), 1.36 (s, 3H), 1.25 (s, 58H), 0.88 (t, 6H, J=6.6Hz). ¹³C-NMR (CDCl₃, 75 MHz): δ 198.1, 109.8, 74.0, 73.9, 71.9, 68.4, 67.6, 66.3, 66.1, 54.4, 44.1, 43.0, 31.9, 29.7, 29.5, 29.4, 29.3, 29.2, 28.9, 26.7, 26.0, 25.5, 25.2, 22.7, 14.1.

Synthesis of (2R,4S)-2,3-Dihydroxypropyl 2-octadecanoylthio-3-octadecyloxy-propyl phosphate (S-ProAEL). Phosphate **7** (66 mg, 0.079 mmol) was dissolved in a solution of DCM (3 ml), CH₃CN (3 ml), isopropanol (4 ml) and 40 % aqueous Me₃N (3.75 ml), and the solution was stirred at room temperature overnight. EtOH (20 ml) and toluene (20 ml) were added, and the mixture was concentrated in vacuo. The residue was dissolved in a 7:1 DCM/MeOH (9.4 ml), and the solution was washed with 1 M HCl (10 ml). MeOH (2 ml) and 1 M HCl (0.5 ml) were added to the organic extract, which gave a 65:25:4 DCM/MeOH/1 M HCl solution. The solution stirred at room temperature overnight, NaHCO₃ (150 mg, 1.79 mmol) was added, and the mixture was stirred for an additional 24 h. The neutral (pH 7) solution was dried over Na₂SO₄, filtered and concentrated in vacuo. Purification by flash chromatography (eluent 20 % MeOH in DCM) gave 41 mg (65 %) of the desired compound as a colorless oil. (MALDI-TOF (ES⁺) Calcd. for C₄₆H₉₁O₈PS (M+Na)⁺ 803.56. Found: 803.66). ¹H-NMR (300 MHz, CDCl₃): δ 4.95-4.87 (m, 5H), 3.80-3.77 (m, 1H), 3.65-3.60 (m, 4H), 3.49-3.44 (m, 2H), 2.59-2.54 (m, 2H), 1.67-1.63 (m, 2H), 1.58-1.53 (m, 2H), 1.27 (br. s, 58H), 0.89 (t, 6H, J=6.7Hz). ¹³C-NMR (CDCl₃, 75 MHz): δ = 199.2, 71.1, 70.9, 70.1, 68.8, 65.6, 64.0, 62.1, 43.8, 43.4, 31.6, 29.3, 29.2, 29.1, 29.0, 28.9, 28.6, 25.7, 25.3, 22.3, 13.6.

Preparation of liposomes. The S-ProAEL and DSPG were hydrated in an aqueous buffer (150 mM KCl, 10 mM HEPES, 30 μM CaCl₂, 10 μM EDTA, pH = 7.5). MLVs formed spontaneously. To ensure complete hydration, the lipids were hydrated for 1 h at 60 °C. During the hydration, the lipids were vortexed every 15 min. SUVs were prepared by sonication of the MLVs for 1 h, 5 °C above the lipid main phase transition temperature regime. The total concentration of lipids in the buffer solutions was 2 mM.

Differential scanning calorimetry (DSC)

Differential scanning calorimetry of 2 mM multilamellar liposomes was performed by using a Microcal MC-2 (Northampton, MA, USA) ultrasensitive power compensating scanning calorimeter equipped with a nanovoltmeter. The scans were performed in the upscan mode at a scan rate of 10 °C/h.

Activity measurements

The conditions used to perform the sPLA₂ activity measurements were as follows: 0.40 mM phospholipid, 336 nM sPLA₂, 0.15 M KCl, 30 μM CaCl₂, 10 μM EDTA, 10 μM HEPES (pH 7.5). The catalytic reaction was initiated by addition of 20 μL of a 42 μM snake (*Agkistrodon piscivorus piscivorus*) venom sPLA₂ stock solution to a 2.5 mL liposome suspension thermostated at the main phase transition of the liposomes prior to the addition of the enzyme. The time-dependent action of sPLA₂ was monitored from the changes in the 90° static light scattering providing information about changes in the lipid morphology as non-bilayer forming lipids are generated. High-performance liquid chromatography (HPLC) quantification of the products from the enzymatic reaction was performed with a 5 μm diol column and an isocratic eluent (800:195:5 chloroform/methanol/25% ammonium hydroxide). An evaporative light scattering detector was used for detection. The turnover of the hydrolysis was followed by HPLC. Samples were collected at different time intervals by collecting 100 μL of the reaction mixture and rapidly mixing with a 1.0 mL chloroform/methanol/acetic acid (2:4:1) solution to quench the reaction. The solution was washed with 1.0 mL of water, and 50 μL of the organic phase was used for HPLC. Fluorescence measurements were performed using an SLM DMX 1100 spectrofluorometer. Purified snake venom sPLA₂ was a generous gift from Dr. R.L. Biltonen (University of Virginia, VA, USA).

Cytotoxicity assays

The sPLA₂ IIA-secreting cell line COLO205 (ECACC, Salisbury, UK) was grown in RPMI 1640 supplemented with 10 % fetal calf serum in a humidified atmosphere containing 5 % CO₂¹. The cells were plated on 96-well plates at a density of 10⁴ cells per well. The day after, cells were incubated with the drugs for 24 h, then washed and grown for an additional 48 h. Living cells were detected with a Cell Proliferation Kit I (MTT) (Roche) according to the manufacture's instructions.

Molecular dynamics simulations

The crystal structures of bee-venom (*Apis Mellifera*) phospholipase A₂ complexed with the transition-state analog, L-1-*O*-octyl-2-heptylphosphonyl-*sn*-glycero-3-phosphoethanolamine (diC₈(2Ph)PE)², resolved to 2.0 Å and human phospholipase A₂ IIA complexed with 6-phenyl-4(*R*)-(7-phenyl-heptanoylamino)-hexanoic acid³ resolved to 2.1 Å were obtained from the Protein Data Bank⁴ (entry codes: 1poc and 1kqu, respectively).

The initial modeling step involved placing diC₈(2Ph)PE into the binding cleft of human phospholipase A₂ IIA, as described previously^{5,6}. The structure for the S-ProAEL was built from diC₈(2Ph)PE using SPARTAN Version 1.0.2 (Wavefunction Inc., Irvine, California, U.S.A.). Missing distance, angle and torsion parameters for the thio-ester were obtained from the Charmm27 parameter set describing similar atom types. The structure complexed with S-ProAEL was solvated using the program SOLVATE (by Grubmüller). 18 water molecules were randomly replaced with chloride ions to neutralize the systems. The final system contained 4888 water molecules, and the simulation cell dimensions were 52.7x51.7x67.3 Å³. For all simulations, NAMD⁷ was used with the Charmm27 all-atom parameter set and with the TIP3 water model.⁸ The S-ProAEL-PLA₂ complex was simulated five times starting from different initial conditions, which were obtained by varying the number of steps used in energy minimization of the systems (i.e. 250, 500, 750, 1000 and 1250 steps). This was followed by 100 ps of heating of the systems to $T = 300$ K. The simulations were carried out for 10 ns in the *NPT* ensemble; i.e. at constant number of atoms (N), pressure (P) and temperature(T). An isotropic constant ambient pressure of 1 atm was imposed using the Langevin piston method⁹ with a damping coefficient of 5 ps⁻¹, a piston period of 200 fs, and a decay of 500 fs. A time step of 1 fs was used throughout. The Particle Mesh Ewald method was used for computation of the electrostatic forces.¹⁰ The grid spacing applied was approximately 1.0 Å, and a fourth order spline was used for the interpolation. The long range part of the electrostatic forces was evaluated every fourth fs. Van der Waals interactions were cut off at 12 Å in combination with a switching function starting at 10 Å. Periodic boundary conditions were applied in x, y and z-directions. The analyses of the trajectory were performed using VMD.¹¹

Table S1

Summary of calculated distances between selected atoms that are involved in stabilization of the substrate or part of the catalytic device. Mean distances and their standard deviations are calculated from a series of simulations of a particular complex.

	Natural	S-ProAEL
distances ^a	mean \pm SD ^b (Å)	mean \pm SD (Å)
D91(OD1)- Y51(OH)	3.1 \pm 0.3	1.8 \pm 0.3
D91(OD2)- Y66(OH)	2.7 \pm 0.1	1.7 \pm 0.1
H47(HE2)- D91(OD1)	1.9 \pm 0.3	1.9 \pm 0.3
H47(ND1)- S(C21)	4.5 \pm 0.4	4.6 \pm 0.3
Ca ²⁺ - D48(OD1)	2.2 \pm 0.2	2.2 \pm 0.2
Ca ²⁺ - D48(OD2)	2.2 \pm 0.1	2.2 \pm 0.1
Ca ²⁺ - G29(O)	2.4 \pm 0.2	2.4 \pm 0.1
S(O22)- G29(HN)	2.7 \pm 0.5	2.1 \pm 0.2
S(O22)- Ca ²⁺	2.4 \pm 0.2	2.2 \pm 0.1
S(O4)- Ca ²⁺	2.1 \pm 0.1	2.1 \pm 0.1

^aAtom type refers to pdb nomenclature.

^bSD = standard deviation calculated as:

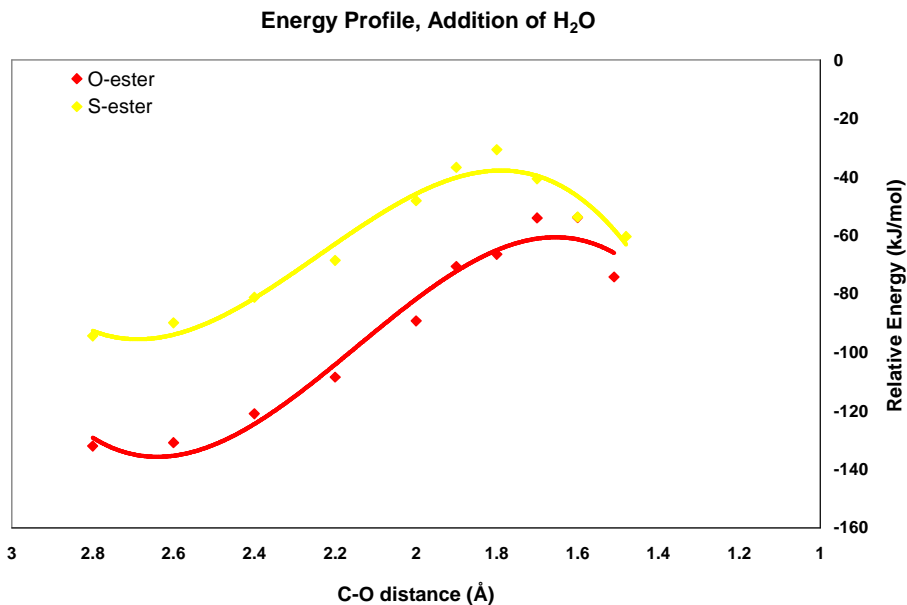
$$SD = \sqrt{\frac{\sum_{i=1}^N (x_i - \bar{x})^2}{N - 1}}$$

Density functional theory calculations

Molecular modeling was carried out using the modules Jaguar v. 7.0.207 and MacroModel v. 9.5.207 as incorporated in the Maestro suite from Schrödinger Inc. Initial conformational searches of the ester substrates were carried out using the OPLS-2005 force-field^{12;13} in combination with a GB-SA solvation water model.¹⁴ These conformational searches were carried out for 10000 steps using the MCLM algorithm^{15;16} to assure completeness, and the global minimum structure was then subjected to additional optimization using Density Functional Theory (DFT) (B3LYP¹⁷⁻¹⁹/LACVP²⁰). The initial atomic positions for the modeling of the active site were acquired from the x-ray structure of cobra-venom sPLA₂ in complex with a transition-state analog (pdb entry code: 1POB). In all subsequent energy minimizations, the two C α carbon atoms of His47 and Asp48 were constrained using a harmonic potential (force constant = 10 kcal/Å²). We found that the use of **the standard Poisson-Boltzmann solver in Jaguar (SCRF-PCM)^{21;22} with setting appropriate for water (dielectric constant: 80.370 and probe radius: 1.40Å)** improved the convergence, which can probably be ascribed to the decrease of long-range electrostatic interactions. All relative energies reported in the present study have been obtained in solution phase and are reported in kJ/mol. XYZ coordinates for the DFT-optimized structures and corresponding energies in hartrees have been included below.

XYZ coordinates and SCRF-PCM energies (in Hartrees), Addition of H₂O

Figure S1: Energy profile for the two ester substrates calculated with different, fixed distances between the oxygen atom of the water molecule and the carbon atom in the carbonyl group.



Water

E_{solv} = -76.42009975326 a.u.

O	-0.06713	-0.00783	0.00000
H	0.62087	-0.69352	0.00000
H	0.44453	0.81782	0.00000

Oester_propyl

E_{solv} = -1300.57130521695 a.u.

C	-12.13926	6.11427	-6.98915
H	-12.10280	5.71125	-8.00039
C	-11.70609	5.01227	-6.02070
H	-12.49319	4.24797	-5.97020
H	-10.79608	4.52728	-6.41598
O	-11.45884	5.59111	-4.75612
C	-11.28138	4.68094	-3.68268
H	-10.50206	3.94041	-3.92842
H	-12.21873	4.12960	-3.49818
C	-14.44688	5.90469	-7.45476
O	-13.49886	6.55890	-6.75534
O	-14.26579	4.79593	-7.93519
C	-15.69973	6.71732	-7.69059
H	-16.41450	6.05565	-8.19214

H	-15.39333	7.48205	-8.41201
C	-11.21299	7.33540	-6.86028
H	-10.29339	7.11288	-7.41898
H	-10.94364	7.47887	-5.81530
P	-12.62707	8.93073	-8.60343
O	-13.95405	9.65491	-7.97621
O	-11.85742	9.96422	-9.39115
O	-13.07616	7.67109	-9.29089
O	-11.74355	8.60056	-7.26776
C	-13.90437	11.06330	-7.69539
H	-13.15874	11.28866	-6.92498
H	-13.66842	11.63270	-8.59959
H	-14.89531	11.34548	-7.33350
C	-10.87272	5.49674	-2.45825
H	-10.75230	4.80995	-1.61084
H	-9.88418	5.93547	-2.64934
C	-11.87074	6.60910	-2.11454
H	-11.97874	7.30315	-2.95366
H	-12.86454	6.19978	-1.89372
H	-11.53873	7.18043	-1.24016
C	-16.32793	7.40059	-6.47132
H	-15.59364	8.08513	-6.03516
H	-17.15534	8.02441	-6.83311
C	-16.84090	6.41605	-5.41866
H	-17.31990	6.94308	-4.58556
H	-17.57865	5.72735	-5.85048
H	-16.02128	5.81344	-5.00805

Sester_propyl

E_solv = -1623.53919417847 a.u.

C	-12.36282	6.12239	-6.18014
H	-12.78465	5.66331	-7.07633
C	-11.45444	5.10731	-5.49635
H	-12.02554	4.20215	-5.23556
H	-10.66631	4.80944	-6.21097
O	-10.87709	5.70714	-4.34847
C	-9.88880	4.89824	-3.71170
H	-9.24758	4.42840	-4.47453
H	-10.37441	4.08463	-3.14511
C	-15.09022	6.75887	-6.41889
S	-13.81751	6.55615	-5.12722
O	-14.94144	6.27339	-7.51838
C	-16.30672	7.56899	-6.01071
H	-15.96728	8.37855	-5.35466
H	-16.95816	6.92605	-5.39955
C	-11.61350	7.40103	-6.56626
H	-10.80311	7.14024	-7.25807
H	-11.16869	7.86483	-5.68395
P	-12.57798	8.51546	-8.77638
O	-14.06198	9.20992	-8.86010
O	-11.55720	9.51860	-9.25603
O	-12.56034	7.14230	-9.39205
O	-12.48909	8.39147	-7.14012
C	-14.29421	10.07417	-9.99494
H	-13.59029	10.91092	-9.99556
H	-14.19281	9.51876	-10.93488
H	-15.31663	10.44411	-9.90270
C	-9.04133	5.77616	-2.79535
H	-8.28578	5.13311	-2.32474

H	-8.49559	6.50151	-3.41280
C	-9.84472	6.51492	-1.72043
H	-10.58951	7.17551	-2.17622
H	-10.37474	5.81092	-1.06608
H	-9.18835	7.12772	-1.09172
C	-17.06948	8.16066	-7.21116
H	-17.73598	8.94042	-6.82345
H	-16.34763	8.66602	-7.86478
C	-17.89386	7.15636	-8.02595
H	-18.64236	6.65427	-7.40120
H	-18.42517	7.66456	-8.83997
H	-17.25336	6.39078	-8.47181

ActiveSite_water_no_substrate

E_solv = -776.81419854695 a.u.

C	4.61780	11.91512	30.18577
C	3.60507	12.21095	31.29808
O	2.81390	11.34245	31.70053
C	5.97568	11.37275	30.68295
C	5.97542	10.09230	31.48466
N	7.14011	9.33900	31.56177
C	5.00360	9.49524	32.25525
C	6.86447	8.32059	32.35943
N	5.58620	8.37282	32.80166
N	3.65384	13.44894	31.82854
C	2.96628	13.84039	33.05073
C	1.97005	15.00686	32.95710
C	2.73911	16.25045	32.59514
O	3.67154	15.98961	31.79721
O	2.48794	17.40170	33.04081
Ca	5.12212	17.47902	31.25559
H	4.15326	11.18560	29.51857
H	6.59838	11.21002	29.79673
H	6.47868	12.16717	31.25233
H	3.97888	9.76532	32.43735
H	7.54811	7.52953	32.63747
H	4.13723	14.22196	31.38257
H	3.72172	14.10470	33.79790
H	1.23812	14.83348	32.15781
H	1.43201	15.12790	33.90162
H	5.14085	7.70998	33.42417
H	4.81525	12.82789	29.60922
H	2.44206	12.95707	33.41448

Oester_water

E_solv = -2153.81769877956 a.u.

C	5.42403	12.29707	29.78748
C	4.51424	12.99067	30.80227
O	3.32890	12.63625	30.92144
C	6.88025	12.02915	30.20243
C	7.04927	11.14869	31.41304
N	8.10392	11.35646	32.28866
C	6.32542	10.05489	31.83150
C	8.01354	10.41173	33.21183
N	6.95198	9.60352	32.97557
N	5.03531	14.02540	31.48848
C	4.27676	14.82598	32.44594
C	4.51112	16.32213	32.24710

C	5.95231	16.75504	32.49903
O	6.87916	15.88509	32.47247
O	6.17634	17.98308	32.72055
Ca	8.47243	17.53146	33.55683
C	9.53257	13.36068	37.11190
O	10.90675	13.57490	37.40402
C	11.21996	14.29549	38.59500
C	12.69318	14.69021	38.51129
C	13.24253	15.26380	39.82096
C	9.16846	14.11381	35.83277
O	10.15893	13.70121	34.84971
C	10.68075	14.63262	34.05688
O	9.98431	13.06110	31.08164
O	10.16249	15.73762	33.90050
C	11.96193	14.19254	33.39469
C	12.98066	13.58744	34.37932
C	14.26593	13.13850	33.67824
C	7.76798	13.82104	35.28375
O	6.76752	14.24680	36.21943
P	6.37119	15.84548	36.34581
O	6.26631	16.16362	37.80988
O	7.29317	16.64522	35.44822
O	4.89330	15.93065	35.64875
C	3.73708	15.49260	36.37782
H	4.92198	11.36051	29.52573
H	7.39061	11.57645	29.33961
H	7.41901	12.96462	30.38728
H	9.36538	12.53141	31.64181
H	5.45028	9.56127	31.43407
H	8.68338	10.27343	34.05050
H	6.01797	14.26990	31.42577
H	4.56434	14.55517	33.46757
H	4.23560	16.62712	31.22743
H	3.86748	16.88842	32.92797
H	9.36927	12.28288	36.97327
H	8.88029	13.69954	37.92437
H	10.58515	15.18933	38.68971
H	11.03711	13.66418	39.48003
H	13.27008	13.80167	38.22514
H	12.81728	15.41669	37.69761
H	14.29127	15.56090	39.70423
H	12.68032	16.14831	40.14409
H	9.27504	15.18793	35.98746
H	11.68075	13.46201	32.62448
H	12.37695	15.06529	32.87928
H	13.21800	14.32471	35.15690
H	12.51818	12.74087	34.89524
H	14.05623	12.37798	32.91528
H	14.76924	13.97843	33.18274
H	7.63068	14.31325	34.31721
H	7.62936	12.74380	35.15083
H	3.61556	14.40664	36.29213
H	3.81363	15.76917	37.43364
H	6.67164	8.80921	33.53970
H	2.86965	15.98806	35.93339
H	14.96973	12.70458	34.39839
H	13.19455	14.52447	40.62969
H	5.42560	12.91305	28.87697
H	3.22160	14.58203	32.31295

H	10.33206	12.40898	30.45107
Oester_water_tetrahed_int			
E_solv = -2153.79934165569 a.u.			
C	0.10008	-0.29063	0.35858
O	0.31574	-0.66598	1.80589
C	2.33605	-0.42855	6.24475
C	2.64947	1.06877	6.24299
O	3.32218	1.54542	7.17344
C	1.94634	-1.12519	4.93140
C	3.05949	-1.28703	3.93363
N	2.79189	-1.35281	2.57505
C	4.41321	-1.46867	4.06326
C	3.92131	-1.56249	1.89986
N	4.91835	-1.63878	2.78665
N	2.12484	1.81260	5.25534
C	2.15113	3.27407	5.22185
C	0.73479	3.85093	5.16240
C	-0.04119	3.41477	3.92149
O	0.24083	2.30217	3.37070
O	-0.95808	4.17040	3.48722
Ca	-1.11440	2.80062	1.34859
C	2.93605	0.91742	-1.66085
O	2.32496	0.45995	-2.86366
C	1.76068	1.48573	-3.67682
C	1.10149	0.83690	-4.88976
C	0.47821	1.86472	-5.84212
C	1.96834	1.10209	-0.48772
O	1.49927	-0.17869	-0.08946
O	-0.61376	0.78717	0.24546
C	-0.45251	-1.55671	-0.33687
C	-0.68009	-1.37650	-1.84113
C	-1.12747	-2.66851	-2.53464
C	2.67968	1.76382	0.70480
O	3.18306	3.07058	0.36377
P	2.28185	4.40700	0.66389
O	2.75874	5.47276	-0.28140
O	0.81420	4.03039	0.70964
O	2.68627	4.80626	2.20339
C	3.97576	5.39272	2.42841
H	3.19858	-0.92496	6.70306
H	1.56008	-2.12242	5.18342
H	1.11008	-0.61051	4.44431
H	1.83808	-1.18500	2.15627
H	5.05498	-1.49684	4.93107
H	4.01897	-1.65589	0.82905
H	1.51692	1.41829	4.54054
H	2.70660	3.60439	4.33917
H	0.16127	3.53934	6.04756
H	0.77640	4.94503	5.18014
H	3.67845	0.15557	-1.39155
H	3.47067	1.86009	-1.84151
H	1.01949	2.06790	-3.11063
H	2.55109	2.18633	-3.99576
H	1.85139	0.23697	-5.42083
H	0.33234	0.13845	-4.53671
H	-0.00029	1.36779	-6.69412
H	-0.28738	2.46756	-5.33564
H	1.12101	1.72821	-0.78169

H	0.24489	-2.38527	-0.16085
H	-1.40179	-1.82811	0.14937
H	-1.43199	-0.59353	-1.99834
H	0.25000	-1.01120	-2.29179
H	-0.37442	-3.46120	-2.42226
H	-2.06871	-3.04671	-2.11257
H	2.00086	1.81696	1.56011
H	3.55417	1.16902	0.99261
H	4.77662	4.70399	2.13684
H	4.08192	6.32685	1.86959
H	5.89401	-1.79156	2.54919
H	4.04921	5.59570	3.49964
H	-1.28421	-2.51211	-3.61004
H	1.23501	2.55348	-6.24034
H	1.50745	-0.56139	6.95439
H	2.67611	3.62100	6.11336
H	-0.44544	-1.20218	2.09097

Oester_water_fix16

E_solv = -2153.79158250806 a.u.

C	0.07454	-0.14839	0.12120
O	0.27744	-0.13285	1.70821
C	3.03560	-0.08303	5.86810
C	3.31713	1.40350	5.62588
O	4.36686	1.91571	6.04760
C	2.37560	-0.89192	4.73878
C	3.25092	-1.12313	3.53944
N	2.74037	-1.05991	2.25316
C	4.56920	-1.48042	3.40978
C	3.69315	-1.36600	1.37307
N	4.81181	-1.62539	2.05640
N	2.34171	2.10819	5.03041
C	2.39163	3.54658	4.77138
C	0.99360	4.16780	4.87686
C	-0.00624	3.58872	3.87228
O	0.15593	2.37996	3.49304
O	-0.95777	4.30162	3.45706
Ca	-1.14241	2.52034	1.41672
C	2.73426	1.13133	-1.99384
O	2.01700	0.54615	-3.07325
C	1.46775	1.46509	-4.01505
C	0.42092	0.73036	-4.84708
C	-0.05995	1.54293	-6.05342
C	1.87381	1.29497	-0.73943
O	1.44168	-0.00274	-0.33127
O	-0.73976	0.79763	-0.19434
C	-0.33379	-1.59631	-0.20042
C	-0.52384	-1.86055	-1.69737
C	-0.87220	-3.32485	-1.98861
C	2.66677	1.94447	0.40893
O	3.04471	3.29620	0.09547
P	2.02040	4.53314	0.45067
O	2.16024	5.55944	-0.63776
O	0.66380	3.95827	0.80183
O	2.61021	5.13094	1.85920
C	3.73270	6.02494	1.85148
H	3.98847	-0.53735	6.15611
H	2.07581	-1.86551	5.14916
H	1.44544	-0.41822	4.40672

H	1.76370	-0.73474	2.00376
H	5.34284	-1.64683	4.14403
H	3.57767	-1.39405	0.30144
H	1.53766	1.66377	4.59123
H	2.79212	3.74209	3.77187
H	0.58754	4.01851	5.88802
H	1.06163	5.24811	4.71816
H	3.57343	0.45879	-1.77054
H	3.15549	2.10444	-2.27873
H	1.01154	2.32501	-3.50269
H	2.27035	1.85919	-4.66130
H	0.85246	-0.21937	-5.18763
H	-0.42465	0.47287	-4.19781
H	-0.85331	1.01130	-6.59132
H	-0.46012	2.51863	-5.75042
H	0.99739	1.90711	-0.96346
H	0.42527	-2.27912	0.20249
H	-1.27260	-1.80698	0.33185
H	-1.31552	-1.20615	-2.08097
H	0.39119	-1.56947	-2.22276
H	-0.10081	-4.00230	-1.59882
H	-1.82388	-3.60885	-1.52038
H	2.08172	1.91202	1.33203
H	3.60366	1.40049	0.57440
H	4.66790	5.47781	1.68265
H	3.61502	6.79239	1.08115
H	5.70005	-1.88109	1.63551
H	3.76744	6.49782	2.83653
H	-0.96372	-3.51031	-3.06574
H	0.75883	1.72469	-6.76047
H	2.38482	-0.14328	6.75158
H	3.06767	4.00034	5.50066
H	-0.37582	-0.76127	2.06420

Oester_water_fix17

E_solv = -2153.79166401765 a.u.

C	0.03005	-0.02991	0.13937
O	0.02211	-0.06823	1.83892
C	1.53267	-0.10568	6.45682
C	2.84841	0.64440	6.24216
O	3.66975	0.71653	7.17294
C	0.76386	-0.63251	5.23682
C	1.42692	-1.76454	4.49910
N	1.10942	-2.02553	3.17299
C	2.32298	-2.71456	4.93074
C	1.79806	-3.10002	2.81540
N	2.54250	-3.54703	3.85028
N	3.02334	1.24994	5.05651
C	4.10452	2.18228	4.75149
C	3.55545	3.54798	4.32833
C	2.67665	3.48917	3.07784
O	2.02024	2.42744	2.82818
O	2.60611	4.51344	2.33918
Ca	1.36960	3.16383	0.56201
C	2.78943	-1.70992	-1.50305
O	2.00045	-1.83633	-2.67965
C	2.30881	-0.90621	-3.71573
C	1.36205	-1.15612	-4.88431
C	1.61763	-0.20504	-6.05995

C	2.29077	-0.63168	-0.54016
O	0.98512	-1.03424	-0.10338
O	0.30147	1.16379	-0.18491
C	-1.35563	-0.60277	-0.18201
C	-1.60164	-0.67285	-1.69566
C	-2.94859	-1.31786	-2.04228
C	3.21809	-0.48278	0.67599
O	4.52650	-0.04458	0.26932
P	4.86202	1.56242	0.18432
O	5.91937	1.73043	-0.86779
O	3.56286	2.33544	0.09469
O	5.48348	1.90408	1.66229
C	6.83576	1.51433	1.94677
H	1.75167	-0.92094	7.15580
H	-0.22605	-0.96291	5.58434
H	0.55638	0.17895	4.52935
H	0.39539	-0.94135	2.29253
H	2.81533	-2.87725	5.87919
H	1.78189	-3.57311	1.84297
H	2.31377	1.22562	4.32826
H	4.71260	1.77741	3.93786
H	2.95371	3.98071	5.14065
H	4.38296	4.24134	4.14504
H	2.74738	-2.68507	-1.00268
H	3.83846	-1.50645	-1.75838
H	2.19944	0.12765	-3.35657
H	3.35779	-1.03433	-4.03288
H	1.47197	-2.19916	-5.21075
H	0.32951	-1.04497	-4.52620
H	0.92001	-0.40669	-6.88110
H	1.48792	0.84473	-5.76141
H	2.21586	0.33457	-1.04291
H	-1.44399	-1.60281	0.25793
H	-2.11430	0.03628	0.28783
H	-1.55997	0.34107	-2.10995
H	-0.78169	-1.23507	-2.15818
H	-3.00453	-2.34790	-1.66810
H	-3.78452	-0.75974	-1.60125
H	2.78175	0.20994	1.39973
H	3.35684	-1.45232	1.16471
H	6.94604	0.42357	1.92421
H	7.53012	1.96363	1.22970
H	3.16118	-4.35041	3.83062
H	7.06202	1.87641	2.95210
H	-3.10533	-1.34871	-3.12713
H	2.63817	-0.31699	-6.45250
H	0.87890	0.58739	7.00628
H	4.72920	2.27532	5.64208
H	-0.87487	0.09879	2.18947

Oester_water_fix18

E_solv = -2153.79639051806 a.u.

C	0.20622	-0.36029	0.36126
O	0.68926	-0.68965	2.06367
C	3.04742	-0.36101	6.27938
C	3.34494	1.13717	6.20929
O	4.11812	1.64419	7.04123
C	2.55767	-1.09546	5.02399
C	3.58016	-1.25957	3.93158

N	3.17657	-1.49550	2.62586
C	4.95488	-1.27916	3.98143
C	4.28005	-1.64946	1.90897
N	5.37718	-1.52749	2.69018
N	2.68982	1.85518	5.27992
C	2.70203	3.31406	5.20720
C	1.28433	3.88608	5.25333
C	0.42582	3.44578	4.07136
O	0.66392	2.32185	3.52551
O	-0.51445	4.19888	3.68635
Ca	-0.91105	2.70041	1.65804
C	2.82591	0.83053	-1.80506
O	2.07116	0.37791	-2.92295
C	1.40737	1.40472	-3.65715
C	0.60467	0.75427	-4.77825
C	-0.13448	1.78055	-5.64399
C	1.98568	1.01785	-0.54140
O	1.47654	-0.28053	-0.19209
O	-0.50823	0.66922	0.43684
C	-0.40975	-1.71214	0.00506
C	-0.91829	-1.71621	-1.44751
C	-1.41961	-3.09584	-1.88769
C	2.81423	1.56906	0.62856
O	3.33477	2.87391	0.31548
P	2.43880	4.21778	0.61867
O	2.83729	5.24965	-0.39794
O	0.98584	3.81554	0.76740
O	2.93019	4.68490	2.10929
C	4.17788	5.38386	2.23514
H	3.95174	-0.83707	6.67297
H	2.20770	-2.08990	5.33820
H	1.67029	-0.60606	4.60490
H	1.61910	-1.10546	2.18251
H	5.65949	-1.14493	4.78903
H	4.32761	-1.84764	0.84686
H	2.04036	1.42915	4.62405
H	3.18208	3.62630	4.27487
H	0.77887	3.56872	6.17684
H	1.32425	4.97996	5.27306
H	3.58825	0.06408	-1.62023
H	3.34139	1.77210	-2.03710
H	0.73901	1.98062	-3.00161
H	2.14868	2.10939	-4.06826
H	1.28623	0.15874	-5.39808
H	-0.11234	0.05205	-4.33455
H	-0.70342	1.28400	-6.43826
H	-0.84060	2.37228	-5.04847
H	1.14699	1.69123	-0.72977
H	0.33899	-2.50044	0.14291
H	-1.24143	-1.91139	0.69239
H	-1.72568	-0.97918	-1.54701
H	-0.10524	-1.38347	-2.10466
H	-0.61806	-3.84550	-1.83752
H	-2.24156	-3.44479	-1.24855
H	2.21168	1.59698	1.54000
H	3.68260	0.92811	0.80752
H	5.01775	4.74706	1.93325
H	4.17583	6.29493	1.62958
H	6.33925	-1.59831	2.37749

H	4.28741	5.64495	3.29070
H	-1.78764	-3.06928	-2.92114
H	0.56513	2.47763	-6.12042
H	2.28805	-0.47667	7.06616
H	3.29736	3.68254	6.04432
H	0.04536	-1.26698	2.51505

Oester_water_fix19

E_solv = -2153.80121004008 a.u.

C	0.01016	-0.00471	-0.02556
O	0.00567	-0.00196	1.87444
C	1.60985	-0.01101	6.48038
C	2.89765	0.77553	6.22811
O	3.74272	0.87027	7.13488
C	0.82927	-0.57418	5.28413
C	1.49330	-1.71293	4.55586
N	1.12374	-2.02333	3.25559
C	2.43600	-2.62167	4.97859
C	1.82781	-3.08888	2.90580
N	2.63326	-3.48431	3.91825
N	3.02428	1.39449	5.04130
C	4.08758	2.34020	4.71590
C	3.51191	3.68543	4.26139
C	2.66812	3.58047	2.99215
O	2.07332	2.48543	2.73243
O	2.55997	4.59794	2.24924
Ca	1.33777	3.19313	0.48964
C	2.80783	-1.63718	-1.55592
O	2.02213	-1.78879	-2.73171
C	2.33512	-0.88333	-3.78929
C	1.37946	-1.14919	-4.94773
C	1.65026	-0.24093	-6.15263
C	2.28619	-0.54936	-0.61792
O	0.97386	-0.96885	-0.19741
O	0.25144	1.18825	-0.29862
C	-1.36954	-0.60927	-0.24368
C	-1.65285	-0.74102	-1.75325
C	-2.96711	-1.47252	-2.04782
C	3.18062	-0.36395	0.61609
O	4.49333	0.07523	0.22493
P	4.80541	1.67850	0.03384
O	5.87476	1.79520	-1.01421
O	3.49336	2.41983	-0.13007
O	5.39981	2.13510	1.48990
C	6.76398	1.81396	1.80427
H	1.87036	-0.80963	7.18297
H	-0.14896	-0.91027	5.65780
H	0.59571	0.21627	4.56078
H	0.33727	-0.85427	2.31738
H	2.97383	-2.73841	5.90804
H	1.78412	-3.59566	1.95139
H	2.31350	1.33142	4.31673
H	4.70421	1.93149	3.90855
H	2.87778	4.11264	5.05201
H	4.32122	4.40182	4.08520
H	2.77576	-2.60428	-1.03964
H	3.85437	-1.42152	-1.80937
H	2.23877	0.15972	-3.45159
H	3.38049	-1.03034	-4.10852

H	1.46775	-2.20262	-5.24241
H	0.35068	-1.00677	-4.59309
H	0.94518	-0.45005	-6.96507
H	1.54708	0.81843	-5.88697
H	2.20190	0.40507	-1.14020
H	-1.41681	-1.59274	0.23526
H	-2.12121	0.03515	0.22623
H	-1.67764	0.26060	-2.20043
H	-0.81521	-1.27318	-2.22040
H	-2.95194	-2.49473	-1.64832
H	-3.82455	-0.95282	-1.60133
H	2.72365	0.34035	1.31594
H	3.31537	-1.32030	1.13050
H	6.91125	0.72928	1.85583
H	7.44573	2.23745	1.06112
H	3.27303	-4.27054	3.89637
H	6.97186	2.25071	2.78331
H	-3.14446	-1.53972	-3.12842
H	2.66393	-0.38899	-6.54414
H	0.95075	0.67111	7.03652
H	4.71262	2.46301	5.60174
H	-0.88155	0.18308	2.23434

Oester_water_fix20

E_solv = -2153.80506873450 a.u.

C	0.25091	-0.27285	0.01222
O	0.45386	-0.36723	1.99966
C	3.10450	-0.21867	6.53744
C	3.38622	1.28437	6.49452
O	4.06431	1.80101	7.39863
C	2.48795	-0.91929	5.31804
C	3.41396	-1.12826	4.15053
N	2.92235	-1.17833	2.85462
C	4.76476	-1.39127	4.12533
C	3.95304	-1.46789	2.07264
N	5.08478	-1.60358	2.79964
N	2.83152	1.98327	5.49104
C	2.73522	3.43988	5.43527
C	1.26991	3.89059	5.45216
C	0.45347	3.32496	4.28824
O	0.74338	2.16659	3.84227
O	-0.49755	4.00737	3.81550
Ca	-0.68608	2.28075	1.86814
C	2.85939	0.82770	-2.03524
O	1.99249	0.42305	-3.08381
C	1.24099	1.47226	-3.69522
C	0.41373	0.86743	-4.82483
C	-0.40101	1.91951	-5.58594
C	2.15037	1.03664	-0.69768
O	1.57366	-0.23461	-0.31398
O	-0.45850	0.74503	-0.03845
C	-0.31082	-1.67018	-0.17234
C	-0.73322	-1.87484	-1.64251
C	-1.24566	-3.29347	-1.90917
C	3.11432	1.50359	0.40072
O	3.50613	2.86315	0.16597
P	2.57855	4.07898	0.78790
O	2.73002	5.25613	-0.13136
O	1.20840	3.51913	1.10373

O	3.28852	4.39704	2.22668
C	4.48121	5.19917	2.24313
H	4.04189	-0.70650	6.82912
H	2.11852	-1.89802	5.65639
H	1.59625	-0.38502	4.97126
H	1.37312	-0.66129	2.31909
H	5.51076	-1.45554	4.90399
H	3.92152	-1.58655	0.99901
H	2.20985	1.53935	4.81692
H	3.20982	3.79903	4.51763
H	0.79024	3.56948	6.38818
H	1.21888	4.98335	5.42705
H	3.60349	0.02960	-1.93093
H	3.39189	1.75319	-2.29730
H	0.58047	1.95746	-2.96096
H	1.92584	2.24362	-4.08487
H	1.09084	0.34421	-5.51326
H	-0.25479	0.10696	-4.40031
H	-0.99644	1.45064	-6.37720
H	-1.09195	2.45289	-4.91971
H	1.34632	1.76554	-0.78710
H	0.44034	-2.41290	0.11585
H	-1.18440	-1.79044	0.47757
H	-1.51675	-1.14697	-1.88835
H	0.11992	-1.64833	-2.29318
H	-0.47030	-4.04236	-1.70232
H	-2.11370	-3.52740	-1.27854
H	2.64547	1.39520	1.38119
H	4.03361	0.90919	0.39015
H	5.30139	4.69601	1.71736
H	4.29929	6.17630	1.78465
H	6.00564	-1.81651	2.43178
H	4.75600	5.33112	3.29275
H	-1.55193	-3.40812	-2.95692
H	0.25226	2.66589	-6.05631
H	2.42961	-0.35635	7.39401
H	3.27570	3.84798	6.29199
H	-0.15803	-1.03136	2.36911

Oester_water_fix22

E_solv = -2153.81238469342 a.u.

C	0.40573	-0.29070	-0.15380
O	0.57181	-0.25592	2.03965
C	3.06433	-0.16821	6.55930
C	3.31811	1.33196	6.39485
O	4.18676	1.88850	7.08810
C	2.46812	-0.97261	5.39195
C	3.41541	-1.25323	4.25640
N	2.98923	-1.21153	2.93825
C	4.72787	-1.66707	4.28823
C	4.01961	-1.59583	2.19788
N	5.09066	-1.87755	2.97387
N	2.51745	1.99505	5.54470
C	2.43066	3.44962	5.44336
C	0.96376	3.91010	5.55103
C	0.12602	3.33654	4.41042
O	0.12653	2.06827	4.25520
O	-0.49553	4.10616	3.62888
Ca	-0.46245	2.17076	1.85780

C	2.90848	0.78725	-2.20598
O	1.91970	0.46773	-3.16987
C	1.09711	1.55699	-3.59138
C	0.20168	1.06167	-4.72165
C	-0.71145	2.15991	-5.27308
C	2.36285	0.95627	-0.78856
O	1.73043	-0.29584	-0.41545
O	-0.27644	0.73791	-0.19665
C	-0.17375	-1.68536	-0.20734
C	-0.61771	-2.01301	-1.65126
C	-1.12902	-3.45115	-1.78585
C	3.46884	1.27975	0.22532
O	3.80969	2.67113	0.14040
P	2.96081	3.74578	1.06559
O	2.87651	5.02653	0.28573
O	1.70845	3.05695	1.56165
O	3.91517	3.94569	2.37592
C	5.10764	4.73563	2.24868
H	4.01439	-0.60961	6.87843
H	2.10956	-1.92735	5.80260
H	1.57356	-0.48550	4.98857
H	1.48060	-0.55236	2.36465
H	5.42052	-1.83441	5.10035
H	4.03036	-1.68401	1.12077
H	1.77196	1.51840	5.04237
H	2.85444	3.77745	4.48849
H	0.54558	3.57230	6.50811
H	0.91952	5.00281	5.52575
H	3.62209	-0.04539	-2.21692
H	3.45258	1.70391	-2.48100
H	0.48359	1.92371	-2.75566
H	1.73080	2.39187	-3.93246
H	0.83465	0.66100	-5.52251
H	-0.40109	0.22477	-4.34764
H	-1.34956	1.77042	-6.07436
H	-1.36651	2.56469	-4.49211
H	1.61106	1.74168	-0.74096
H	0.57548	-2.40698	0.13396
H	-1.03937	-1.73849	0.46033
H	-1.40641	-1.30958	-1.94650
H	0.22396	-1.84431	-2.33336
H	-0.34792	-4.17786	-1.52907
H	-1.98554	-3.63206	-1.12419
H	3.13210	1.01988	1.23013
H	4.38441	0.71946	0.00573
H	5.82106	4.25884	1.56704
H	4.87129	5.73934	1.88363
H	6.00018	-2.18118	2.64432
H	5.54881	4.80105	3.24584
H	-1.45138	-3.65547	-2.81391
H	-0.12784	2.99236	-5.68423
H	2.39166	-0.25844	7.42513
H	3.02586	3.88115	6.25109
H	-0.02712	-0.91796	2.42834

Oester_water_fix24

E_solv = -2153.81715192579 a.u.

C	0.19029	-0.10223	-0.12859
O	0.24437	-0.09341	2.27078

C	2.99261	-0.03740	6.67636
C	3.25969	1.45852	6.48978
O	4.20027	2.00153	7.09278
C	2.36120	-0.82054	5.51339
C	3.25122	-0.99603	4.31225
N	2.73521	-0.94229	3.02841
C	4.59313	-1.29562	4.24068
C	3.73880	-1.21022	2.20617
N	4.88068	-1.42815	2.89739
N	2.39826	2.12985	5.70962
C	2.36243	3.58064	5.55362
C	0.91966	4.10592	5.67173
C	-0.00709	3.50620	4.61384
O	0.02373	2.23869	4.45010
O	-0.75215	4.25288	3.92775
Ca	-0.80553	2.20211	2.14175
C	2.79375	0.98927	-2.10166
O	1.91336	0.51242	-3.10567
C	1.31732	1.51303	-3.93218
C	0.34806	0.81876	-4.88326
C	-0.23346	1.76580	-5.93675
C	2.10009	1.22778	-0.75959
O	1.51293	-0.04182	-0.36477
O	-0.53108	0.89222	-0.10874
C	-0.31170	-1.52539	-0.14618
C	-0.58897	-1.97909	-1.59845
C	-0.99983	-3.45314	-1.66356
C	3.09031	1.66826	0.32863
O	3.34535	3.07482	0.22360
P	2.37710	4.11125	1.07509
O	2.14115	5.31642	0.21197
O	1.21731	3.30632	1.62385
O	3.29680	4.51394	2.36503
C	4.25677	5.57712	2.25995
H	3.94680	-0.48844	6.96703
H	2.07003	-1.80831	5.89913
H	1.42398	-0.35621	5.18623
H	1.16621	-0.36035	2.57400
H	5.35161	-1.43263	4.99762
H	3.67872	-1.25829	1.12840
H	1.60788	1.66894	5.26233
H	2.77328	3.86144	4.57792
H	0.51839	3.85889	6.66510
H	0.91781	5.19558	5.57544
H	3.56367	0.21854	-1.96661
H	3.29832	1.91590	-2.40991
H	0.78950	2.26205	-3.32246
H	2.10264	2.04273	-4.49585
H	0.88002	-0.00449	-5.37632
H	-0.45811	0.36373	-4.29473
H	-0.94800	1.24012	-6.57999
H	-0.75904	2.60954	-5.47377
H	1.29845	1.96217	-0.84041
H	0.43759	-2.17976	0.31141
H	-1.23175	-1.57896	0.44424
H	-1.38146	-1.35134	-2.02528
H	0.30682	-1.80625	-2.20620
H	-0.21509	-4.10245	-1.25477
H	-1.91640	-3.63506	-1.08882

H	2.69071	1.41812	1.31148
H	4.05651	1.16769	0.20201
H	5.12006	5.26877	1.65897
H	3.80324	6.46651	1.81532
H	5.78676	-1.64379	2.49626
H	4.58794	5.80091	3.27648
H	-1.18566	-3.76224	-2.69851
H	0.55501	2.17550	-6.57925
H	2.33749	-0.12683	7.55572
H	2.99111	4.02319	6.32990
H	-0.32533	-0.82052	2.57592

Oester_water_fix26

E_solv = -2153.82092085183 a.u.

C	0.49664	-0.39678	-0.03595
O	0.71371	-0.39498	2.55497
C	3.01948	-0.14031	7.06420
C	3.34925	1.34245	6.87241
O	4.28264	1.86670	7.50342
C	2.51636	-0.94398	5.85185
C	3.54953	-1.21324	4.79085
N	3.20580	-1.22532	3.44809
C	4.87572	-1.56056	4.91703
C	4.29975	-1.57268	2.78538
N	5.33224	-1.78347	3.63402
N	2.52887	2.02632	6.06001
C	2.52895	3.47425	5.87682
C	1.08270	4.00685	5.88641
C	0.26362	3.37590	4.76143
O	0.15461	2.09893	4.75278
O	-0.22956	4.09518	3.85549
Ca	-0.24129	1.91966	2.33055
C	2.92130	0.83854	-2.09724
O	1.88929	0.58676	-3.03536
C	1.07212	1.70830	-3.37700
C	0.13206	1.27483	-4.49731
C	-0.78527	2.40634	-4.97303
C	2.43893	0.88260	-0.64769
O	1.79248	-0.39017	-0.36953
O	-0.16637	0.62627	0.12805
C	-0.08055	-1.78920	-0.05976
C	-0.69393	-2.08111	-1.44981
C	-1.24511	-3.50666	-1.54659
C	3.58749	1.06229	0.35383
O	3.97786	2.43804	0.41148
P	3.17396	3.44913	1.45173
O	3.03719	4.77496	0.75933
O	1.95944	2.71260	1.97496
O	4.21586	3.57648	2.70613
C	5.36516	4.42680	2.55523
H	3.91722	-0.60650	7.48285
H	2.12761	-1.90086	6.22964
H	1.65806	-0.45482	5.37797
H	1.63624	-0.65555	2.85290
H	5.52197	-1.67689	5.77510
H	4.38856	-1.68458	1.71383
H	1.74438	1.56627	5.60192
H	3.01408	3.72789	4.92669
H	0.61370	3.76871	6.84955

H	1.09345	5.09378	5.76670
H	3.63964	0.01790	-2.21045
H	3.44521	1.78080	-2.31833
H	0.49397	2.04898	-2.50438
H	1.70717	2.54752	-3.70406
H	0.73528	0.90235	-5.33533
H	-0.46765	0.42728	-4.14045
H	-1.45014	2.05789	-5.77168
H	-1.41378	2.78432	-4.15667
H	1.70847	1.67368	-0.49019
H	0.70777	-2.51463	0.16557
H	-0.85513	-1.86319	0.70895
H	-1.49583	-1.35728	-1.64292
H	0.06980	-1.91845	-2.22025
H	-0.45435	-4.25067	-1.38833
H	-2.02635	-3.68203	-0.79625
H	3.26760	0.70559	1.33450
H	4.47094	0.49463	0.03934
H	6.04895	4.03016	1.79505
H	5.06650	5.44220	2.27755
H	6.27478	-2.04867	3.36992
H	5.87358	4.44526	3.52209
H	-1.68312	-3.68734	-2.53514
H	-0.20551	3.25052	-5.36638
H	2.25634	-0.18777	7.85492
H	3.10864	3.92543	6.68591
H	0.15134	-1.12548	2.86324

Oester_water_fix28

E_solv = -2153.82136570774 a.u.

C	0.16799	-0.11893	0.00330
O	-0.00255	-0.09422	2.79799
C	2.96688	-0.03138	6.89061
C	3.27652	1.45428	6.69273
O	4.30010	1.95359	7.19226
C	2.30199	-0.78197	5.72525
C	3.15996	-0.95023	4.50072
N	2.58695	-0.96906	3.23943
C	4.51091	-1.18264	4.38124
C	3.56963	-1.21133	2.38495
N	4.74999	-1.34651	3.03155
N	2.35990	2.17674	6.03175
C	2.42274	3.62161	5.83024
C	1.01826	4.24184	5.88762
C	0.07010	3.67976	4.82507
O	0.04562	2.41102	4.66493
O	-0.65512	4.45739	4.15881
Ca	-0.88458	2.22717	2.39480
C	2.63994	1.20791	-1.95772
O	1.66727	0.73287	-2.87700
C	1.39577	1.57065	-4.00038
C	0.30139	0.89675	-4.82094
C	-0.04894	1.67090	-6.09518
C	2.02422	1.29892	-0.56629
O	1.47896	-0.01675	-0.26338
O	-0.56334	0.85131	0.16935
C	-0.29463	-1.55321	-0.01946
C	-0.40818	-2.06942	-1.47163
C	-0.86400	-3.52930	-1.53068

C	3.03021	1.65526	0.53295
O	3.33203	3.05581	0.51411
P	2.28952	4.10205	1.26893
O	2.04304	5.24650	0.32692
O	1.15018	3.27209	1.80959
O	3.15788	4.61244	2.55350
C	3.95909	5.80367	2.47178
H	3.91109	-0.51108	7.16782
H	1.99793	-1.77175	6.09530
H	1.37044	-0.29202	5.42180
H	0.94179	-0.38943	2.95502
H	5.30621	-1.25099	5.10833
H	3.46831	-1.29423	1.31251
H	1.54286	1.75078	5.59757
H	2.87612	3.85038	4.85847
H	0.57328	4.05362	6.87495
H	1.09512	5.32603	5.76207
H	3.49141	0.51201	-1.94365
H	3.02159	2.19772	-2.23725
H	1.07089	2.56784	-3.66493
H	2.30681	1.70466	-4.60546
H	0.63457	-0.11670	-5.07893
H	-0.58846	0.78205	-4.18881
H	-0.84404	1.16274	-6.65263
H	-0.39843	2.68502	-5.86561
H	1.20150	2.01220	-0.55644
H	0.42111	-2.16807	0.53740
H	-1.26318	-1.60888	0.48402
H	-1.11312	-1.43618	-2.02527
H	0.56263	-1.95556	-1.96460
H	-0.16959	-4.18464	-0.99012
H	-1.85868	-3.65480	-1.08591
H	2.62406	1.36413	1.50262
H	3.97960	1.13237	0.37540
H	4.94716	5.57548	2.05776
H	3.47146	6.56048	1.85362
H	5.64868	-1.52980	2.59858
H	4.07237	6.18061	3.49061
H	-0.91425	-3.87742	-2.56885
H	0.81974	1.75912	-6.75930
H	2.31451	-0.10514	7.77256
H	3.05984	4.05145	6.60728
H	-0.54745	-0.82660	3.13221

Oester_Hshift_water_min

E_solv = -2153.83289722426 a.u.

C	5.60807	12.16763	29.74200
C	4.48286	12.82182	30.54741
O	3.30324	12.51707	30.31001
C	7.01291	12.06406	30.35776
C	7.13259	11.12287	31.52387
N	8.13066	11.28915	32.47309
C	6.44957	9.99128	31.88836
C	8.06727	10.31173	33.37689
N	7.05188	9.51136	33.03830
N	4.84167	13.75087	31.44885
C	3.91491	14.65509	32.12844
C	4.24736	16.12268	31.82750
C	5.65199	16.50528	32.29340

O	6.59453	15.66303	32.11908
O	5.84737	17.63251	32.82552
Ca	8.22665	16.81706	33.50016
C	9.45516	13.45626	37.48114
O	10.84075	13.78001	37.39897
C	11.39774	14.28421	38.61053
C	12.84930	14.67556	38.35464
C	13.50974	15.30756	39.58464
C	8.99169	13.22183	36.04603
O	9.73438	12.14842	35.44839
C	10.38552	14.15370	32.82125
O	9.63111	13.44384	32.09155
O	10.04080	15.24580	33.36136
C	11.83323	13.66880	32.97786
C	12.71780	14.46563	33.93982
C	14.17428	13.98561	33.92941
C	7.51689	12.82118	35.93008
O	6.66050	13.62481	36.75186
P	6.13483	15.10601	36.25874
O	5.79281	15.86454	37.51073
O	7.11970	15.67747	35.26400
O	4.77147	14.76354	35.41493
C	3.56479	14.48122	36.14277
H	5.24515	11.17718	29.44680
H	7.70124	11.73160	29.56820
H	7.39148	13.04427	30.66788
H	8.81967	12.08512	32.45843
H	5.60422	9.48871	31.44347
H	8.71056	10.20501	34.23710
H	5.80883	14.05561	31.54299
H	3.98066	14.48813	33.20795
H	4.18109	16.30560	30.74504
H	3.51576	16.77591	32.31416
H	9.30256	12.55723	38.10214
H	8.89138	14.28487	37.93126
H	10.81802	15.16009	38.94619
H	11.33250	13.52429	39.40661
H	13.40875	13.78524	38.04104
H	12.87739	15.38021	37.51322
H	14.55376	15.56688	39.37540
H	12.99178	16.22673	39.88647
H	9.16496	14.14313	35.48229
H	11.79296	12.61109	33.27373
H	12.27439	13.67206	31.96810
H	12.67670	15.52914	33.67216
H	12.30811	14.39101	34.95585
H	14.24845	12.92472	34.20655
H	14.61848	14.09824	32.93088
H	7.20629	12.87109	34.88032
H	7.39551	11.79030	36.28317
H	3.65640	13.54436	36.70630
H	3.32700	15.29853	36.83091
H	6.76272	8.69078	33.56199
H	2.76503	14.38068	35.40269
H	14.78900	14.55770	34.63609
H	13.50150	14.62261	40.44174
H	5.69047	12.74388	28.80955
H	2.90284	14.41128	31.79902
H	10.67179	12.32593	35.64520

Sester_water_tetrahed_int

E_solv = -2476.76198401560 a.u.

C	14.97904	3.93669	6.11155
C	13.47155	3.69122	6.22446
O	12.82228	4.27359	7.10844
C	15.66982	3.62291	4.77542
C	15.18151	4.43957	3.61271
N	15.28735	3.97594	2.30972
C	14.61340	5.68386	3.52555
C	14.81196	4.88858	1.46177
N	14.39720	5.93337	2.18268
N	12.92835	2.81716	5.36081
C	11.54364	2.35981	5.39413
C	11.46557	0.84828	5.62383
C	12.26539	0.01294	4.62134
O	13.11552	0.57279	3.86058
O	12.07314	-1.23906	4.61724
Ca	13.56788	-1.55212	2.59917
C	13.02230	0.99508	-2.06923
O	13.90701	0.51941	-3.07261
C	14.17234	-0.88055	-3.04472
C	15.02424	-1.22500	-4.26365
C	15.42567	-2.70323	-4.31003
C	13.54481	0.95693	-0.61855
S	15.23405	1.64120	-0.44838
C	16.00974	0.39647	0.95209
O	16.15242	1.36535	2.06238
O	15.23142	-0.59236	1.21124
C	17.43824	0.06457	0.46911
C	17.52133	-0.93724	-0.68387
C	18.96671	-1.23439	-1.10216
C	12.60249	1.73180	0.31636
O	11.21904	1.35242	0.13686
P	10.56902	0.13213	1.01468
O	9.36962	-0.35527	0.25086
O	11.65967	-0.84567	1.40399
O	10.09335	0.85625	2.40571
C	8.92568	1.68922	2.36686
H	15.14384	4.98166	6.39593
H	16.74834	3.78933	4.90140
H	15.56840	2.56075	4.52318
H	15.65346	3.03638	2.04795
H	14.34249	6.40260	4.28413
H	14.76960	4.79769	0.38733
H	13.49029	2.28988	4.69741
H	11.06694	2.60256	4.43817
H	11.83334	0.59582	6.62834
H	10.42098	0.51898	5.58543
H	12.79425	2.02986	-2.35276
H	12.07980	0.42883	-2.10384
H	14.70515	-1.14825	-2.12165
H	13.22450	-1.44508	-3.06258
H	14.46903	-0.95636	-5.17174
H	15.92420	-0.59659	-4.24908
H	16.03387	-2.91473	-5.19692
H	16.01561	-2.98407	-3.42844
H	13.62454	-0.07412	-0.26313
H	17.95777	0.99502	0.20438

H	17.96868	-0.35354	1.34224
H	17.02087	-1.86701	-0.38725
H	16.96401	-0.53993	-1.54084
H	19.47978	-0.32238	-1.43476
H	19.54673	-1.65493	-0.27002
H	12.90511	1.59253	1.35797
H	12.64403	2.79997	0.07850
H	9.07996	2.55423	1.71069
H	8.05434	1.12490	2.01944
H	13.98078	6.77487	1.79509
H	8.75100	2.03992	3.38665
H	19.00075	-1.95485	-1.92862
H	14.54592	-3.35768	-4.34541
H	15.45753	3.33363	6.89541
H	11.02391	2.90167	6.18608
H	16.92473	1.09155	2.59248

Sester_water_fix16

E_solv = -2476.75940701126 a.u.

C	0.03624	0.00324	-0.00096
C	0.03666	0.01999	1.53125
O	1.11681	0.04172	2.14330
C	-1.22923	0.47508	-0.73197
C	-1.59878	1.90755	-0.47326
N	-2.89651	2.35889	-0.65891
C	-0.87141	2.99651	-0.07110
C	-2.96624	3.66051	-0.38212
N	-1.74497	4.06702	-0.02451
N	-1.16035	-0.02556	2.13974
C	-1.36904	-0.16023	3.57766
C	-2.12772	-1.44868	3.91044
C	-3.46220	-1.60642	3.18026
O	-3.70545	-0.90795	2.14477
O	-4.27454	-2.47381	3.61676
Ca	-6.05220	-1.73121	1.98767
C	-8.08768	3.23353	1.76214
O	-9.21955	3.32908	0.91167
C	-10.09456	2.20390	0.92048
C	-11.31106	2.54536	0.06356
C	-12.30121	1.38164	-0.05423
C	-7.01628	2.19833	1.36071
S	-6.58138	2.29175	-0.41634
C	-6.30922	0.38725	-0.85265
O	-4.73987	0.44202	-1.15951
O	-6.59442	-0.41430	0.09741
C	-6.94623	0.14278	-2.23348
C	-8.47497	0.04914	-2.22012
C	-9.06079	-0.17539	-3.61959
C	-5.73420	2.38878	2.18774
O	-5.99646	2.47205	3.60664
P	-6.05250	1.11271	4.52111
O	-6.91942	1.42038	5.70986
O	-6.38419	-0.06444	3.62800
O	-4.49932	0.90054	4.99865
C	-4.00149	1.71394	6.07146
H	0.90586	0.58865	-0.31853
H	-1.07448	0.33412	-1.81030
H	-2.08846	-0.15771	-0.47945
H	0.16975	3.10671	0.18945

H	-3.85050	4.27727	-0.43507
H	-2.02701	-0.13146	1.61725
H	-1.94821	0.69860	3.93425
H	-1.51322	-2.32494	3.65877
H	-2.31996	-1.50151	4.98717
H	-7.64768	4.23804	1.77058
H	-8.40849	3.00581	2.78947
H	-9.58273	1.31926	0.51573
H	-10.40151	1.97293	1.95453
H	-11.81091	3.42436	0.49076
H	-10.96263	2.83793	-0.93547
H	-13.15999	1.66137	-0.67511
H	-11.83117	0.50347	-0.51460
H	-7.38427	1.18055	1.50988
H	-6.61894	0.92685	-2.92823
H	-6.53332	-0.80762	-2.60937
H	-8.77847	-0.76770	-1.55369
H	-8.88503	0.97268	-1.79312
H	-8.79944	0.64927	-4.29567
H	-8.68265	-1.10345	-4.06830
H	-5.02898	1.57994	1.97650
H	-5.26441	3.34258	1.92581
H	-3.98188	2.77299	5.78702
H	-4.61439	1.59341	6.96973
H	-1.50870	5.01492	0.25227
H	-2.98162	1.37943	6.27537
H	-10.15496	-0.24363	-3.58545
H	-12.68465	1.07874	0.92788
H	0.24387	-1.03203	-0.30469
H	-0.39421	-0.14580	4.06811
H	-4.56626	-0.24356	-1.83104
H	-3.69871	1.73586	-0.92633

Sester_water_dist_17

E_solv = -2476.75445344818 a.u.

C	0.13359	0.11082	-0.04722
C	0.13004	0.11918	1.48417
O	1.20813	0.16075	2.09927
C	-1.13258	0.57294	-0.78381
C	-1.53575	1.99420	-0.50875
N	-2.84629	2.41616	-0.68205
C	-0.82719	3.09916	-0.11436
C	-2.93813	3.71754	-0.40974
N	-1.72305	4.15115	-0.06199
N	-1.06885	0.05608	2.08783
C	-1.27579	-0.11724	3.52260
C	-2.00687	-1.42884	3.82352
C	-3.34965	-1.58855	3.10569
O	-3.57320	-0.93288	2.03693
O	-4.18047	-2.41848	3.57496
Ca	-5.93525	-1.71462	1.86215
C	-7.98037	3.31113	1.66454
O	-9.16986	3.36611	0.89204
C	-10.01057	2.21981	0.98847
C	-11.30668	2.50704	0.23708
C	-12.26711	1.31307	0.24960
C	-6.93948	2.26181	1.22901
S	-6.59776	2.34968	-0.57072
C	-6.24696	0.47900	-0.99512

O	-4.61777	0.57205	-1.47163
O	-6.36417	-0.31878	-0.01935
C	-6.94429	0.14677	-2.32468
C	-8.45849	-0.05927	-2.20448
C	-9.10495	-0.42962	-3.54525
C	-5.61836	2.44692	1.98932
O	-5.81462	2.54409	3.41545
P	-5.86711	1.19626	4.35041
O	-6.73410	1.52315	5.53426
O	-6.18971	-0.00132	3.48334
O	-4.31170	1.01042	4.83365
C	-3.80659	1.89198	5.84779
H	0.99695	0.71103	-0.35574
H	-0.95785	0.45517	-1.86192
H	-1.98337	-0.08015	-0.55881
H	0.21556	3.23345	0.13155
H	-3.83376	4.31751	-0.45852
H	-1.92690	-0.09527	1.56028
H	-1.87241	0.71961	3.89933
H	-1.37685	-2.28228	3.53357
H	-2.17804	-1.51892	4.90118
H	-7.54585	4.31592	1.60069
H	-8.22612	3.12398	2.71981
H	-9.51069	1.34563	0.54838
H	-10.21868	1.99301	2.04773
H	-11.79001	3.38593	0.68294
H	-11.05949	2.77510	-0.79837
H	-13.18567	1.54446	-0.30116
H	-11.81256	0.43086	-0.21834
H	-7.30699	1.25040	1.41043
H	-6.73560	0.93524	-3.06032
H	-6.47624	-0.77650	-2.69562
H	-8.65692	-0.84711	-1.46821
H	-8.91639	0.85781	-1.81428
H	-8.94866	0.35744	-4.29422
H	-8.68376	-1.35905	-3.94958
H	-4.93474	1.62710	1.75263
H	-5.15352	3.39416	1.69654
H	-3.81269	2.93390	5.50512
H	-4.39739	1.81039	6.76537
H	-1.50505	5.10326	0.21528
H	-2.77613	1.58849	6.04815
H	-10.18617	-0.57446	-3.43649
H	-12.55180	1.03787	1.27281
H	0.35818	-0.91843	-0.35855
H	-0.30108	-0.09526	4.01337
H	-4.62704	0.68153	-2.44043
H	-3.64678	1.77041	-0.97022

Sester_water_fix18

E_solv = -2476.75064379958 a.u.

C	0.13614	0.02692	0.05463
C	0.08165	0.01480	1.58474
O	1.13705	0.02374	2.24096
C	-1.11502	0.49913	-0.69975
C	-1.53782	1.90982	-0.38920
N	-2.86736	2.29263	-0.47096
C	-0.78496	3.00353	-0.03049
C	-2.91251	3.58420	-0.17290

N	-1.67438	4.05081	0.10021
N	-1.13756	-0.03714	2.14659
C	-1.40132	-0.17731	3.57279
C	-2.16419	-1.47061	3.87493
C	-3.47820	-1.64191	3.10790
O	-3.69081	-0.97532	2.04415
O	-4.30456	-2.49800	3.54432
Ca	-6.04899	-1.79653	1.87335
C	-8.07802	3.29270	1.74094
O	-9.24171	3.38889	0.93622
C	-10.11281	2.26039	0.97375
C	-11.34669	2.58577	0.13667
C	-12.32766	1.41135	0.04881
C	-7.04234	2.23475	1.30411
S	-6.73025	2.33700	-0.50632
C	-6.41131	0.52857	-0.92677
O	-4.70319	0.68621	-1.47217
O	-6.45548	-0.31499	-0.00773
C	-6.97816	0.20101	-2.31169
C	-8.49651	-0.03718	-2.28031
C	-9.06609	-0.31922	-3.67550
C	-5.72010	2.40442	2.06630
O	-5.93254	2.46712	3.48941
P	-6.02184	1.09726	4.39050
O	-6.91944	1.40318	5.55661
O	-6.33495	-0.07356	3.48193
O	-4.48295	0.88072	4.90761
C	-4.00140	1.70799	5.97879
H	1.00454	0.63774	-0.21639
H	-0.92102	0.39583	-1.77649
H	-1.95491	-0.17660	-0.49451
H	0.27283	3.13399	0.14508
H	-3.80004	4.20036	-0.15562
H	-1.98070	-0.12078	1.58631
H	-1.99729	0.67698	3.90964
H	-1.53505	-2.34075	3.63779
H	-2.38491	-1.52914	4.94603
H	-7.62370	4.29021	1.71759
H	-8.35330	3.07794	2.78368
H	-9.60660	1.37446	0.56391
H	-10.39533	2.03618	2.01595
H	-11.84615	3.46452	0.56467
H	-11.01710	2.87096	-0.87096
H	-13.19784	1.67530	-0.56291
H	-11.85672	0.53125	-0.40743
H	-7.42257	1.22807	1.48525
H	-6.73656	1.01203	-3.00830
H	-6.46885	-0.70359	-2.67000
H	-8.71862	-0.87794	-1.61129
H	-8.99095	0.84562	-1.85599
H	-8.88414	0.52318	-4.35524
H	-8.61066	-1.21247	-4.12182
H	-5.03064	1.59397	1.81495
H	-5.25607	3.35839	1.79699
H	-3.97226	2.76287	5.68010
H	-4.63110	1.60172	6.86735
H	-1.44491	5.00211	0.36724
H	-2.98669	1.37310	6.20595
H	-10.14941	-0.48331	-3.62995

H	-12.69363	1.11760	1.04040
H	0.38055	-0.99658	-0.26280
H	-0.44553	-0.15973	4.09969
H	-4.31934	-0.20838	-1.41081
H	-4.05639	1.33156	-0.96504

Sester_water_fix19

E_solv = -2476.75294835522 a.u.

C	0.27827	0.17340	-0.10017
C	0.25756	0.14334	1.42992
O	1.32708	0.16913	2.06274
C	-0.98991	0.63987	-0.83229
C	-1.40860	2.05305	-0.52586
N	-2.72127	2.46240	-0.70494
C	-0.66466	3.12362	-0.08728
C	-2.76299	3.74755	-0.38191
N	-1.54159	4.18646	-0.00296
N	-0.94756	0.05325	2.01567
C	-1.17897	-0.14273	3.44126
C	-1.91261	-1.45965	3.70986
C	-3.23524	-1.62441	2.95859
O	-3.45386	-0.95646	1.89814
O	-4.06103	-2.47658	3.40141
Ca	-5.80271	-1.77427	1.72178
C	-7.91585	3.36238	1.56570
O	-9.13543	3.41247	0.84304
C	-10.00071	2.29321	1.02485
C	-11.32256	2.59164	0.32473
C	-12.30687	1.41988	0.40596
C	-6.91833	2.27453	1.11877
S	-6.70468	2.32055	-0.70908
C	-6.32764	0.53458	-1.08481
O	-4.52887	0.68210	-1.67867
O	-6.28424	-0.27006	-0.14315
C	-6.87324	0.12420	-2.45446
C	-8.37449	-0.20832	-2.39578
C	-8.92245	-0.64945	-3.75778
C	-5.55473	2.45231	1.80327
O	-5.68368	2.54720	3.23233
P	-5.77942	1.19354	4.16401
O	-6.67594	1.51806	5.32353
O	-6.08020	0.00760	3.27075
O	-4.23922	0.99593	4.69151
C	-3.77833	1.83928	5.75835
H	1.13569	0.79447	-0.38342
H	-0.81231	0.53287	-1.91202
H	-1.83173	-0.02947	-0.61732
H	0.37814	3.22890	0.17360
H	-3.63677	4.38365	-0.41284
H	-1.79742	-0.05012	1.46760
H	-1.78285	0.68740	3.82145
H	-1.27315	-2.30879	3.42853
H	-2.11172	-1.56074	4.78167
H	-7.46390	4.35403	1.44767
H	-8.11338	3.21127	2.63646
H	-9.54650	1.38761	0.59559
H	-10.16140	2.11217	2.10050
H	-11.76636	3.49039	0.77196
H	-11.11496	2.83234	-0.72596

H	-13.24398	1.66073	-0.10812
H	-11.89366	0.51762	-0.06283
H	-7.30182	1.28079	1.35602
H	-6.69992	0.92249	-3.18682
H	-6.31038	-0.76013	-2.77952
H	-8.53873	-1.00201	-1.65739
H	-8.92628	0.67176	-2.04261
H	-8.79562	0.13776	-4.51198
H	-8.40899	-1.54819	-4.12270
H	-4.88546	1.63223	1.53091
H	-5.10186	3.39685	1.48559
H	-3.73684	2.88867	5.44153
H	-4.42872	1.75333	6.63396
H	-1.31643	5.12599	0.30451
H	-2.77050	1.50446	6.01480
H	-9.99263	-0.87935	-3.69107
H	-12.55068	1.17295	1.44654
H	0.52670	-0.84499	-0.43113
H	-0.21247	-0.12849	3.94872
H	-4.47879	0.89622	-2.62993
H	-3.95443	1.39574	-1.22969

Sester_water_fix20

E_solv = -2476.75729531437 a.u.

C	0.23058	0.18533	-0.08697
C	0.20062	0.17484	1.44258
O	1.26425	0.21172	2.08471
C	-1.01201	0.69970	-0.83120
C	-1.39100	2.12475	-0.52691
N	-2.69433	2.56364	-0.70605
C	-0.61913	3.17776	-0.09253
C	-2.70260	3.85030	-0.38801
N	-1.46993	4.26169	-0.01001
N	-1.00946	0.08741	2.01905
C	-1.24925	-0.11870	3.44290
C	-1.95896	-1.45177	3.69655
C	-3.27832	-1.62736	2.93947
O	-3.49898	-0.95569	1.88117
O	-4.10069	-2.48687	3.37513
Ca	-5.84728	-1.81598	1.69261
C	-7.87783	3.35140	1.58538
O	-9.12372	3.40923	0.91040
C	-9.98491	2.29201	1.12395
C	-11.33491	2.59665	0.48263
C	-12.31371	1.42286	0.59562
C	-6.91555	2.24661	1.10618
S	-6.78071	2.27956	-0.72842
C	-6.38452	0.52082	-1.10282
O	-4.49074	0.71995	-1.71434
O	-6.29767	-0.29285	-0.17825
C	-6.86159	0.11260	-2.49252
C	-8.35459	-0.26441	-2.48097
C	-8.85144	-0.68894	-3.86679
C	-5.52295	2.40482	1.73231
O	-5.59503	2.51786	3.16476
P	-5.78934	1.18442	4.10788
O	-6.71410	1.56912	5.22913
O	-6.12533	-0.00070	3.22563
O	-4.28142	0.92633	4.69406

C	-3.79421	1.78821	5.73540
H	1.11489	0.76618	-0.37238
H	-0.82439	0.58922	-1.90930
H	-1.87952	0.05953	-0.63041
H	0.42659	3.25857	0.16610
H	-3.55997	4.50911	-0.41761
H	-1.85313	-0.03374	1.46417
H	-1.87159	0.69798	3.82089
H	-1.30197	-2.28430	3.40512
H	-2.15730	-1.57037	4.76704
H	-7.42001	4.33732	1.44478
H	-8.03506	3.20698	2.66356
H	-9.55267	1.38673	0.67222
H	-10.10024	2.10735	2.20471
H	-11.76107	3.49079	0.95550
H	-11.17109	2.84618	-0.57386
H	-13.27219	1.66701	0.12373
H	-11.91953	0.52539	0.10182
H	-7.30479	1.26106	1.36520
H	-6.69050	0.92653	-3.20716
H	-6.26249	-0.74951	-2.80948
H	-8.51503	-1.07811	-1.76407
H	-8.94180	0.59055	-2.12445
H	-8.73859	0.12309	-4.59563
H	-8.29352	-1.55550	-4.24280
H	-4.87990	1.56910	1.44576
H	-5.06365	3.33637	1.38868
H	-3.71381	2.82441	5.38528
H	-4.44926	1.75243	6.61121
H	-1.22114	5.19741	0.29111
H	-2.79992	1.42582	6.00694
H	-9.91225	-0.96254	-3.83118
H	-12.51295	1.16621	1.64358
H	0.43409	-0.84616	-0.40779
H	-0.28707	-0.08741	3.95779
H	-4.42123	0.92470	-2.66540
H	-3.94149	1.43819	-1.26859

Sester_water_fix22

E_solv = -2476.76507870383 a.u.

C	0.22021	0.13975	-0.04205
C	0.15475	0.13712	1.48593
O	1.19907	0.23275	2.15304
C	-0.99620	0.67975	-0.81020
C	-1.36044	2.10659	-0.49626
N	-2.65501	2.56444	-0.68985
C	-0.58058	3.14242	-0.03562
C	-2.65048	3.84505	-0.35275
N	-1.41777	4.23626	0.04858
N	-1.06089	-0.01630	2.03698
C	-1.31944	-0.16592	3.46381
C	-2.02611	-1.48947	3.76786
C	-3.35256	-1.68400	3.03043
O	-3.58726	-1.03124	1.96370
O	-4.16845	-2.53545	3.49476
Ca	-5.94506	-1.85853	1.85611
C	-7.96508	3.29551	1.74067
O	-9.16810	3.39417	0.99635
C	-10.04381	2.27166	1.08899

C	-11.29631	2.57742	0.27620
C	-12.27428	1.39856	0.24268
C	-6.98143	2.20370	1.26678
S	-6.84488	2.23378	-0.56716
C	-6.56428	0.48003	-0.93778
O	-4.47259	0.62594	-1.60377
O	-6.44847	-0.34413	-0.03459
C	-6.97711	0.10436	-2.35083
C	-8.49091	-0.19432	-2.41685
C	-8.94405	-0.54920	-3.83678
C	-5.59157	2.38008	1.89502
O	-5.67713	2.49062	3.32612
P	-5.82557	1.14793	4.26434
O	-6.72590	1.51125	5.41163
O	-6.16688	-0.03458	3.38261
O	-4.30009	0.90301	4.80509
C	-3.79450	1.76075	5.84085
H	1.12103	0.70403	-0.30666
H	-0.78362	0.57862	-1.88460
H	-1.88013	0.05465	-0.63855
H	0.46223	3.20575	0.23861
H	-3.49782	4.51653	-0.38639
H	-1.89223	-0.14834	1.46788
H	-1.95090	0.66185	3.80251
H	-1.37459	-2.33398	3.49944
H	-2.21478	-1.57052	4.84334
H	-7.49422	4.28194	1.66598
H	-8.18404	3.10904	2.80175
H	-9.55371	1.37291	0.68849
H	-10.29636	2.07543	2.14352
H	-11.78585	3.46631	0.69307
H	-10.98987	2.83651	-0.74514
H	-13.15803	1.64267	-0.35601
H	-11.81038	0.50782	-0.19907
H	-7.35690	1.21222	1.52552
H	-6.72901	0.91669	-3.04390
H	-6.40569	-0.78395	-2.64378
H	-8.72800	-1.01790	-1.73109
H	-9.04794	0.68328	-2.06444
H	-8.74160	0.27446	-4.53315
H	-8.42588	-1.44100	-4.21130
H	-4.93736	1.55150	1.60942
H	-5.14225	3.31789	1.55299
H	-3.73625	2.80094	5.49770
H	-4.42580	1.70856	6.73325
H	-1.16104	5.16385	0.36706
H	-2.78925	1.40716	6.08121
H	-10.02180	-0.75156	-3.86112
H	-12.61590	1.13050	1.24934
H	0.40944	-0.89617	-0.35750
H	-0.36319	-0.10887	3.98719
H	-4.33677	0.71953	-2.56209
H	-3.92706	1.36377	-1.21185

Sester_water_fix24

E_solv = -2476.76987643271 a.u.

C	0.18680	0.05759	0.01335
C	0.09524	0.06324	1.54071
O	1.12553	0.16776	2.22812

C	-0.99972	0.64701	-0.76440
C	-1.34207	2.06805	-0.40396
N	-2.63078	2.54667	-0.58002
C	-0.54779	3.07852	0.09025
C	-2.60893	3.81494	-0.20226
N	-1.37123	4.17921	0.21175
N	-1.12801	-0.09042	2.07239
C	-1.41642	-0.16324	3.49943
C	-2.16296	-1.45082	3.85428
C	-3.47063	-1.66151	3.08959
O	-3.69555	-1.01647	2.01902
O	-4.28161	-2.52240	3.54518
Ca	-6.07262	-1.89501	1.92247
C	-8.04612	3.29995	1.79664
O	-9.23354	3.40420	1.02764
C	-10.11665	2.28470	1.09744
C	-11.32978	2.58169	0.22145
C	-12.30694	1.40225	0.15219
C	-7.06067	2.20278	1.33979
S	-6.91296	2.21903	-0.49485
C	-6.69340	0.46968	-0.85151
O	-4.41066	0.58593	-1.58333
O	-6.53242	-0.35127	0.04446
C	-7.05405	0.09349	-2.27468
C	-8.57219	-0.17417	-2.40193
C	-8.97077	-0.54288	-3.83593
C	-5.67268	2.36942	1.97616
O	-5.76740	2.47079	3.40820
P	-5.93201	1.12020	4.33646
O	-6.84698	1.47977	5.47411
O	-6.26357	-0.05466	3.44150
O	-4.41307	0.86980	4.89373
C	-3.91965	1.71327	5.94635
H	1.11107	0.58954	-0.23544
H	-0.76616	0.57756	-1.83679
H	-1.90121	0.03799	-0.63231
H	0.49602	3.12030	0.36591
H	-3.45084	4.49432	-0.20144
H	-1.95387	-0.21006	1.49218
H	-2.03299	0.69561	3.78574
H	-1.52462	-2.32483	3.66068
H	-2.39137	-1.46206	4.92547
H	-7.56813	4.28386	1.72956
H	-8.28534	3.11445	2.85390
H	-9.61241	1.37700	0.73488
H	-10.41737	2.10686	2.14300
H	-11.83954	3.47440	0.60547
H	-10.97417	2.83118	-0.78681
H	-13.16343	1.64154	-0.48802
H	-11.82317	0.50865	-0.26248
H	-7.44261	1.21541	1.60016
H	-6.76072	0.89479	-2.96121
H	-6.48872	-0.80720	-2.53653
H	-8.85599	-0.98122	-1.71380
H	-9.12472	0.72068	-2.08800
H	-8.71739	0.26343	-4.53547
H	-8.45862	-1.45283	-4.17185
H	-5.02170	1.53828	1.69152
H	-5.21548	3.30640	1.64091

H	-3.85052	2.75750	5.61853
H	-4.56537	1.65391	6.82827
H	-1.10495	5.09168	0.56460
H	-2.92030	1.35127	6.19920
H	-10.05076	-0.72018	-3.90684
H	-12.69470	1.14133	1.14460
H	0.34145	-0.98415	-0.30273
H	-0.46933	-0.10316	4.03911
H	-4.22678	0.67322	-2.53496
H	-3.88660	1.32041	-1.16873

Sester_water_fix26

E_solv = -2476.77320107770 a.u.

C	0.21166	0.05406	0.03784
C	0.08986	0.06181	1.56247
O	1.10649	0.18513	2.26753
C	-0.95697	0.64685	-0.76490
C	-1.30495	2.06725	-0.40650
N	-2.58780	2.55043	-0.60910
C	-0.52118	3.06937	0.11944
C	-2.57523	3.81276	-0.21015
N	-1.34685	4.16943	0.23666
N	-1.14104	-0.10782	2.07489
C	-1.44368	-0.16804	3.49969
C	-2.19243	-1.45190	3.86049
C	-3.51099	-1.65000	3.11042
O	-3.76730	-0.95611	2.07915
O	-4.30155	-2.54436	3.54217
Ca	-6.13515	-1.88421	1.99111
C	-8.04860	3.31725	1.80380
O	-9.22936	3.40569	1.02250
C	-10.10701	2.28192	1.09489
C	-11.31471	2.56196	0.20599
C	-12.28565	1.37734	0.14642
C	-7.05993	2.21422	1.37025
S	-6.87584	2.22064	-0.46158
C	-6.76097	0.46974	-0.80239
O	-4.30860	0.54837	-1.66245
O	-6.62665	-0.34849	0.10031
C	-7.07303	0.09008	-2.23225
C	-8.58776	-0.16084	-2.41225
C	-8.93337	-0.54009	-3.85569
C	-5.68223	2.36749	2.02948
O	-5.80289	2.47067	3.45751
P	-5.99218	1.12339	4.38560
O	-6.88198	1.51037	5.53340
O	-6.37548	-0.04147	3.49431
O	-4.47662	0.82751	4.92521
C	-3.94162	1.67460	5.95498
H	1.14305	0.58286	-0.19136
H	-0.69675	0.58183	-1.83158
H	-1.86113	0.03645	-0.65906
H	0.51516	3.10470	0.42291
H	-3.41418	4.49598	-0.22783
H	-1.95725	-0.22111	1.48179
H	-2.06020	0.69520	3.77322
H	-1.56060	-2.32900	3.66174
H	-2.41065	-1.46219	4.93423
H	-7.57291	4.30148	1.72877

H	-8.29671	3.14502	2.86072
H	-9.59511	1.37462	0.74325
H	-10.41541	2.11114	2.13932
H	-11.83172	3.45779	0.57308
H	-10.95289	2.79749	-0.80344
H	-13.13974	1.60503	-0.50107
H	-11.79626	0.48057	-0.25468
H	-7.45426	1.22952	1.62349
H	-6.74466	0.88485	-2.91080
H	-6.50847	-0.81739	-2.46784
H	-8.90609	-0.95808	-1.72819
H	-9.14101	0.74337	-2.12858
H	-8.63832	0.25357	-4.55352
H	-8.42254	-1.46212	-4.15928
H	-5.03478	1.52987	1.75560
H	-5.21038	3.30020	1.70329
H	-3.85289	2.71038	5.60574
H	-4.57000	1.64705	6.85053
H	-1.08767	5.07762	0.60515
H	-2.94675	1.29156	6.19311
H	-10.01206	-0.70061	-3.96652
H	-12.67711	1.12736	1.14015
H	0.36951	-0.98817	-0.27383
H	-0.50065	-0.10527	4.04536
H	-4.13415	0.66676	-2.61161
H	-3.81524	1.29395	-1.23730

Sester_water_fix28

E_solv = -2476.77491289769 a.u.

C	0.22457	0.05829	0.08250
C	0.08863	0.04346	1.60573
O	1.10975	0.08528	2.31401
C	-0.95065	0.59688	-0.74275
C	-1.35375	2.01439	-0.42822
N	-2.66225	2.42334	-0.62426
C	-0.61399	3.07584	0.04185
C	-2.70944	3.69935	-0.28039
N	-1.49382	4.13633	0.12993
N	-1.15189	-0.05502	2.11562
C	-1.45027	-0.14251	3.54093
C	-2.17861	-1.44207	3.89039
C	-3.50057	-1.63815	3.14919
O	-3.78175	-0.91646	2.14534
O	-4.26914	-2.56460	3.56159
Ca	-6.12917	-1.89462	2.08585
C	-8.04274	3.27377	1.78690
O	-9.17957	3.33960	0.94190
C	-10.07732	2.23252	1.00870
C	-11.27816	2.54364	0.11980
C	-12.26982	1.37767	0.03194
C	-7.00973	2.18440	1.42430
S	-6.70376	2.17540	-0.39262
C	-6.77458	0.42861	-0.75417
O	-4.16712	0.32788	-1.76956
O	-6.71102	-0.42100	0.12745
C	-7.08700	0.09851	-2.19514
C	-8.61725	-0.02925	-2.39124
C	-8.98369	-0.33141	-3.84787
C	-5.67935	2.37077	2.17105

O	-5.90501	2.46461	3.58843
P	-6.03541	1.10158	4.50050
O	-6.92037	1.44832	5.66429
O	-6.38977	-0.06121	3.59423
O	-4.50584	0.84001	5.01723
C	-3.98165	1.69493	6.04648
H	1.13662	0.62744	-0.12964
H	-0.67708	0.51306	-1.80510
H	-1.83758	-0.03829	-0.63422
H	0.42482	3.17725	0.32188
H	-3.58314	4.33625	-0.31352
H	-1.97153	-0.12204	1.52077
H	-2.08016	0.70783	3.82402
H	-1.54149	-2.30983	3.66952
H	-2.38572	-1.47699	4.96670
H	-7.57965	4.26503	1.73011
H	-8.34710	3.10771	2.82969
H	-9.58127	1.31760	0.65330
H	-10.39175	2.06138	2.05151
H	-11.78113	3.44128	0.50163
H	-10.90956	2.79254	-0.88408
H	-13.11921	1.63782	-0.60970
H	-11.79674	0.48285	-0.39199
H	-7.40430	1.19457	1.66174
H	-6.68636	0.87472	-2.85446
H	-6.59302	-0.84764	-2.43632
H	-8.99862	-0.82341	-1.73688
H	-9.10145	0.90482	-2.07855
H	-8.63676	0.46716	-4.51492
H	-8.53402	-1.27278	-4.18581
H	-4.99367	1.55101	1.93986
H	-5.21034	3.31600	1.87837
H	-3.93172	2.73633	5.70758
H	-4.59611	1.63723	6.95041
H	-1.27540	5.07174	0.45404
H	-2.97236	1.34012	6.26645
H	-10.07060	-0.41731	-3.96430
H	-12.66778	1.10964	1.01854
H	0.43680	-0.97482	-0.22829
H	-0.50603	-0.07073	4.08312
H	-3.79677	0.38477	-2.66782
H	-3.76742	1.10637	-1.30416

Sester_Hshift_water_min

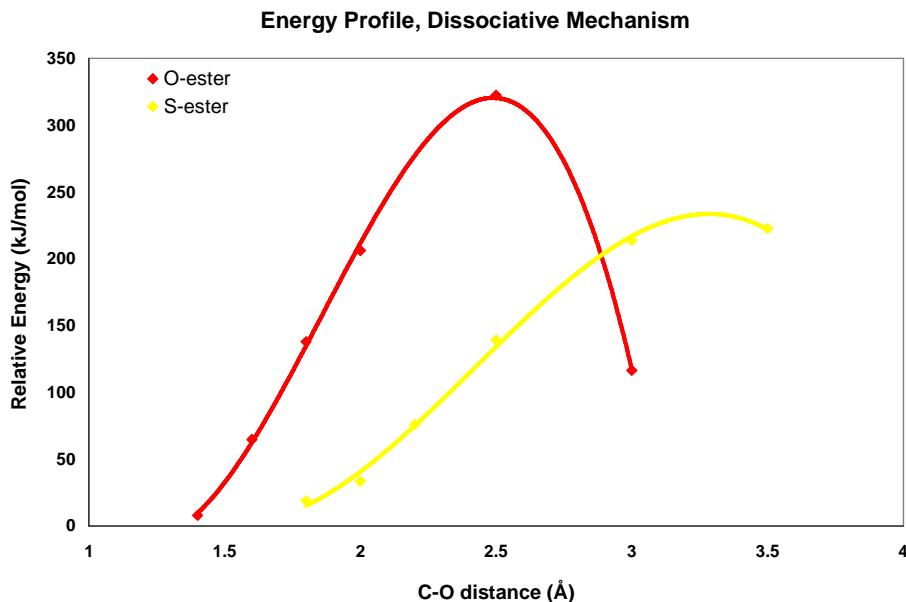
E_solv = -2476.79743344357 a.u.

C	15.09129	4.15552	6.10641
C	13.57926	3.97026	6.26623
O	12.95837	4.65778	7.09341
C	15.73702	3.74776	4.77115
C	15.22562	4.51187	3.58257
N	15.16271	3.94571	2.31803
C	14.78569	5.80359	3.44512
C	14.71121	4.84733	1.44459
N	14.47308	5.98060	2.11020
N	13.00719	3.02636	5.49853
C	11.65343	2.50950	5.67894
C	11.68326	1.02415	6.07298
C	12.39836	0.14939	5.04048
O	13.49747	0.56639	4.54307

O	11.90005	-0.96702	4.72276
Ca	13.60894	-1.21691	2.83502
C	12.47505	0.78588	-2.45171
O	13.34764	0.23906	-3.42596
C	14.00671	-0.97119	-3.05947
C	14.80923	-1.45902	-4.26268
C	15.49471	-2.80484	-4.00716
C	13.15731	1.50543	-1.27139
S	14.49172	2.65937	-1.82176
C	16.37173	0.43286	1.34307
O	16.36075	1.66838	1.59424
O	15.41082	-0.37369	1.53158
C	17.69681	-0.14024	0.80934
C	17.55114	-1.14200	-0.34483
C	18.90105	-1.67432	-0.84059
C	12.14518	2.31511	-0.44324
O	10.95106	1.57393	-0.16008
P	10.80285	0.75246	1.26134
O	9.59452	-0.12488	1.09695
O	12.14913	0.17107	1.61828
O	10.50778	1.94115	2.34935
C	9.22838	2.59445	2.29848
H	15.30131	5.20827	6.32760
H	16.82167	3.89844	4.85791
H	15.61028	2.67565	4.58449
H	15.47172	2.96880	2.06663
H	14.66505	6.60027	4.16396
H	14.57601	4.68822	0.38421
H	13.58349	2.38368	4.95589
H	11.09709	2.62025	4.74307
H	12.20826	0.91141	7.03252
H	10.66143	0.65774	6.21304
H	11.84278	1.50307	-2.99195
H	11.81980	0.00200	-2.04463
H	14.67297	-0.80774	-2.19763
H	13.25951	-1.72637	-2.76309
H	14.13461	-1.54085	-5.12438
H	15.55900	-0.70096	-4.52081
H	16.07613	-3.11809	-4.88139
H	16.18152	-2.75022	-3.15352
H	13.66801	0.79075	-0.61755
H	18.33789	0.69540	0.50901
H	18.20293	-0.63412	1.65387
H	16.91967	-1.97407	-0.01644
H	17.02070	-0.66025	-1.17787
H	19.53643	-0.85876	-1.21063
H	19.44969	-2.18194	-0.03540
H	12.61941	2.65800	0.48046
H	11.82354	3.19300	-1.01403
H	9.12379	3.17337	1.37375
H	8.41652	1.86387	2.36323
H	14.11439	6.83409	1.69181
H	9.18116	3.27058	3.15586
H	18.77122	-2.39326	-1.65978
H	14.76102	-3.59196	-3.79481
H	15.56925	3.57996	6.91143
H	11.15854	3.10419	6.44982
H	13.74952	3.37704	-2.69746

XYZ coordinates and SCRF-PCM energies (in Hartrees), Dissociative mechanism

Figure S2: Energy profile for the two ester substrates calculated with different, fixed distances between the oxygen atom in the ester and the carbon atom in the carbonyl group. At 3.0Å the H₂O molecule in the O-ester calculation has recombined with the carbonyl group to give the acid. For the S-ester this does not take place and at 3.5Å the ester is clearly separated in an alcohol and a carbonyl part.



DFT_smallmodel_Ctetr_OH2_water_DissociativeMechanism

E_solv = -2153.81466422573 a.u.

C	-0.24702	-0.39201	0.01804
C	-0.12567	-0.52905	1.53804
O	0.97077	-0.79679	2.06404
C	-1.06146	0.81253	-0.48144
C	-0.57260	2.14778	0.01636
N	-1.26238	3.30724	-0.30274
C	0.51083	2.46809	0.80277
C	-0.61235	4.29821	0.28547
N	0.46697	3.83761	0.96571
N	-1.25921	-0.37047	2.24488
C	-1.34136	-0.40437	3.69975
C	-2.46792	-1.31728	4.18497
C	-3.85514	-0.94293	3.66117
O	-3.96459	-0.17475	2.65472
O	-4.86256	-1.44695	4.24343
Ca	-6.45866	0.02924	3.00444
C	-6.12083	5.68779	2.63369
O	-7.48545	6.05607	2.46957

C	-8.18321	6.35312	3.67832
C	-9.65444	6.57631	3.34010
C	-10.47658	7.01044	4.55894
C	-5.91587	4.21128	2.31845
O	-6.24522	4.03738	0.91459
C	-6.72629	2.77577	0.54456
O	-3.20301	2.76707	-2.28907
O	-6.75543	1.83871	1.32620
C	-7.19338	2.73309	-0.88218
C	-8.26876	3.79212	-1.20272
C	-8.85430	3.60345	-2.60518
C	-4.47933	3.72286	2.55622
O	-4.13104	3.85092	3.93844
P	-4.66617	2.76213	5.05721
O	-5.14692	3.54106	6.24993
O	-5.59585	1.77114	4.38444
O	-3.31040	1.92864	5.43859
C	-2.36725	2.51460	6.34839
H	0.77689	-0.34409	-0.36509
H	-1.05366	0.80804	-1.58062
H	-2.11918	0.69739	-0.21056
H	-2.60022	3.03921	-1.55503
H	1.27791	1.86380	1.26236
H	-0.87514	5.34706	0.24896
H	-2.14005	-0.13619	1.79555
H	-1.52438	0.60874	4.07224
H	-2.27033	-2.35834	3.89313
H	-2.50667	-1.30497	5.28026
H	-5.51361	6.30526	1.95720
H	-5.77360	5.87536	3.65641
H	-8.07612	5.52634	4.39814
H	-7.75569	7.25362	4.14993
H	-9.71988	7.33641	2.54890
H	-10.06485	5.64863	2.92043
H	-11.53183	7.14421	4.29258
H	-10.42794	6.26377	5.36211
H	-6.60024	3.60518	2.91463
H	-6.31480	2.87175	-1.52529
H	-7.57498	1.72280	-1.05846
H	-9.07217	3.72797	-0.45745
H	-7.83215	4.79062	-1.10716
H	-8.07517	3.66636	-3.37503
H	-9.34392	2.62600	-2.70090
H	-4.37570	2.68386	2.23101
H	-3.77499	4.33921	1.98971
H	-1.84336	3.35557	5.88444
H	-2.86696	2.85993	7.25899
H	1.11388	4.39745	1.50971
H	-1.64187	1.73533	6.59550
H	-9.60261	4.37485	-2.82164
H	-10.11363	7.96247	4.96623
H	-0.69289	-1.31639	-0.37341
H	-0.37626	-0.74392	4.08180
H	-2.61607	2.74733	-3.06550

DFT_smallmodel_Ctetr_OH2_water_DissociativeMechanism

E_solv = -2153.79303785464 a.u.

C	-0.19848	-0.28206	-0.01296
C	-0.08403	-0.29486	1.51235

O	1.02218	-0.44587	2.05925
C	-1.13191	0.77908	-0.61503
C	-0.79757	2.19108	-0.21793
N	-1.64714	3.23505	-0.54702
C	0.27590	2.68500	0.48321
C	-1.09634	4.33058	-0.04878
N	0.06763	4.04502	0.58192
N	-1.23259	-0.17967	2.20299
C	-1.32484	-0.16717	3.65780
C	-2.37400	-1.15707	4.16280
C	-3.79569	-0.87584	3.67787
O	-3.99077	-0.09341	2.69426
O	-4.74653	-1.47235	4.27100
Ca	-6.48547	-0.05981	3.18005
C	-5.97933	5.51740	2.78404
O	-7.29111	5.95540	2.44548
C	-8.12447	6.29638	3.55108
C	-9.54365	6.52229	3.03803
C	-10.47618	7.06736	4.12554
C	-5.77964	4.05374	2.38389
O	-6.00020	3.95540	0.97094
C	-6.71635	2.58784	0.55036
O	-3.65662	2.41751	-2.36188
O	-6.79454	1.69118	1.34436
C	-7.18746	2.66231	-0.86149
C	-8.07551	3.88872	-1.15823
C	-8.62321	3.84528	-2.58785
C	-4.37093	3.52776	2.69732
O	-4.05921	3.67427	4.08953
P	-4.67151	2.64821	5.21885
O	-5.11315	3.48299	6.38749
O	-5.65007	1.68644	4.56912
O	-3.37153	1.74378	5.63891
C	-2.39188	2.29799	6.53056
H	0.81974	-0.15725	-0.39399
H	-1.10800	0.68256	-1.70842
H	-2.17513	0.57352	-0.34144
H	-3.03133	2.78451	-1.68924
H	1.14005	2.20865	0.92118
H	-1.49107	5.33521	-0.13128
H	-2.11670	-0.01850	1.72984
H	-1.58725	0.83946	3.99898
H	-2.11499	-2.17798	3.85004
H	-2.38544	-1.15914	5.25871
H	-5.25279	6.15426	2.25792
H	-5.78880	5.61759	3.85841
H	-8.11288	5.49524	4.30613
H	-7.74736	7.20832	4.04439
H	-9.50300	7.22317	2.19436
H	-9.93481	5.57643	2.64300
H	-11.49705	7.19111	3.74396
H	-10.52181	6.39126	4.98874
H	-6.50918	3.44114	2.92058
H	-6.29176	2.67300	-1.50197
H	-7.72149	1.72606	-1.06019
H	-8.90684	3.91776	-0.44395
H	-7.49019	4.79826	-0.99681
H	-7.81179	3.81500	-3.32532
H	-9.25358	2.96122	-2.74766

H	-4.27756	2.48239	2.39260
H	-3.62684	4.11615	2.15124
H	-1.77220	3.04238	6.01485
H	-2.87107	2.75920	7.39752
H	0.66935	4.70945	1.05304
H	-1.75727	1.47233	6.86115
H	-9.23284	4.73246	-2.79416
H	-10.13383	8.04532	4.48579
H	-0.53592	-1.27945	-0.32646
H	-0.33907	-0.41752	4.05478
H	-3.13031	2.40261	-3.17861

DFT_smallmodel_Ctetr_OH2_water_DissociativeMechanism

E_solv = -2153.76517783312 a.u.

C	-0.27344	-0.34250	-0.00499
C	-0.13220	-0.38630	1.51701
O	0.98046	-0.55462	2.04446
C	-1.16330	0.78284	-0.55768
C	-0.75477	2.16543	-0.12636
N	-1.55629	3.25780	-0.42282
C	0.34782	2.59093	0.57843
C	-0.94775	4.31334	0.09731
N	0.20744	3.95828	0.71014
N	-1.26951	-0.25919	2.22221
C	-1.34427	-0.23689	3.67699
C	-2.39512	-1.21495	4.20192
C	-3.81523	-0.93038	3.71225
O	-4.00615	-0.18164	2.70301
O	-4.77279	-1.48077	4.33753
Ca	-6.48738	-0.05946	3.23034
C	-6.02087	5.51235	2.68669
O	-7.36040	5.91240	2.41574
C	-8.13897	6.23315	3.56571
C	-9.57343	6.48261	3.11458
C	-10.48479	6.94383	4.25629
C	-5.79009	4.06613	2.23394
O	-5.97637	4.00720	0.82941
C	-6.72355	2.43098	0.38528
O	-3.71001	2.46949	-2.10126
O	-6.74715	1.59685	1.22426
C	-7.21273	2.52972	-1.00891
C	-8.23604	3.67288	-1.18715
C	-8.83783	3.67262	-2.59510
C	-4.38091	3.54947	2.56802
O	-4.05208	3.71241	3.95926
P	-4.67360	2.73822	5.12164
O	-5.12936	3.61742	6.25246
O	-5.64185	1.74206	4.50799
O	-3.38058	1.84688	5.59458
C	-2.39444	2.44348	6.44910
H	0.74207	-0.26147	-0.40496
H	-1.16318	0.71837	-1.65417
H	-2.20997	0.62317	-0.26997
H	-3.04446	2.83176	-1.46473
H	1.18780	2.06111	1.00199
H	-1.29730	5.33720	0.04984
H	-2.16335	-0.10511	1.76623
H	-1.60477	0.77345	4.01179
H	-2.13940	-2.24623	3.91884

H	-2.41078	-1.18935	5.29603
H	-5.33989	6.18040	2.13989
H	-5.78989	5.59690	3.75397
H	-8.10597	5.41447	4.30096
H	-7.73273	7.12983	4.06345
H	-9.56125	7.23517	2.31497
H	-9.96701	5.56219	2.66638
H	-11.51164	7.08641	3.90317
H	-10.51434	6.20800	5.07014
H	-6.51800	3.43473	2.75593
H	-6.33190	2.68901	-1.64715
H	-7.64669	1.55307	-1.25665
H	-9.03260	3.56244	-0.44138
H	-7.73390	4.61942	-0.97757
H	-8.06198	3.77443	-3.36364
H	-9.38693	2.74408	-2.79326
H	-4.28711	2.49891	2.27660
H	-3.63508	4.12742	2.01286
H	-1.78648	3.16958	5.89720
H	-2.86594	2.93873	7.30366
H	0.84167	4.58116	1.19708
H	-1.75005	1.63436	6.80374
H	-9.53742	4.50732	-2.71120
H	-10.14305	7.89494	4.68140
H	-0.67194	-1.30888	-0.34249
H	-0.35452	-0.48426	4.06541
H	-3.20663	2.38673	-2.92946

DFT_smallmodel_Ctetr_OH2_water_DissociativeMechanism

E_solv = -2153.73914900447 a.u.

C	-0.34005	-0.46168	-0.01769
C	-0.15589	-0.47617	1.50147
O	0.96680	-0.66383	2.00266
C	-1.26086	0.63700	-0.57230
C	-0.88014	2.03516	-0.16680
N	-1.74163	3.09535	-0.40559
C	0.24271	2.49847	0.47832
C	-1.14586	4.17030	0.08664
N	0.05563	3.85745	0.63064
N	-1.27070	-0.31270	2.23401
C	-1.31355	-0.25536	3.68988
C	-2.37262	-1.20334	4.25095
C	-3.79082	-0.90524	3.76445
O	-3.97071	-0.17090	2.74368
O	-4.75558	-1.43443	4.39589
Ca	-6.44279	-0.00993	3.25394
C	-6.04118	5.54594	2.73427
O	-7.37850	5.91718	2.40600
C	-8.24655	6.12401	3.51443
C	-9.67397	6.22953	2.98695
C	-10.68706	6.59472	4.07570
C	-5.73380	4.13670	2.20342
O	-5.85764	4.13032	0.80475
C	-6.75086	2.41302	0.30171
O	-3.98219	2.23328	-1.92486
O	-6.73511	1.59968	1.14338
C	-7.25293	2.61022	-1.06790
C	-8.21406	3.81671	-1.17039
C	-8.77116	3.95977	-2.58871

C	-4.31826	3.66038	2.57200
O	-4.02095	3.81333	3.97247
P	-4.61098	2.80136	5.11391
O	-5.07251	3.64376	6.27171
O	-5.56743	1.80313	4.49003
O	-3.29783	1.92452	5.55860
C	-2.32152	2.51598	6.43013
H	0.66204	-0.37568	-0.44755
H	-1.27486	0.55526	-1.66800
H	-2.29891	0.46122	-0.26699
H	-3.28311	2.63907	-1.35426
H	1.12393	1.99939	0.85450
H	-1.53397	5.17994	0.06560
H	-2.16955	-0.13466	1.79789
H	-1.55008	0.76787	4.00375
H	-2.14092	-2.24384	3.98104
H	-2.37310	-1.15647	5.34488
H	-5.35687	6.27437	2.27526
H	-5.87870	5.57204	3.81736
H	-8.16377	5.29350	4.23299
H	-7.96791	7.04709	4.05142
H	-9.69531	6.98543	2.19178
H	-9.94516	5.27564	2.51719
H	-11.70406	6.62133	3.66886
H	-10.67857	5.86845	4.89822
H	-6.45251	3.45135	2.67450
H	-6.36163	2.75264	-1.69430
H	-7.74052	1.66993	-1.36028
H	-9.03684	3.68595	-0.45719
H	-7.66802	4.71092	-0.86393
H	-7.96787	4.09366	-3.32428
H	-9.35175	3.07694	-2.88157
H	-4.18547	2.61702	2.26689
H	-3.58107	4.26828	2.03990
H	-1.70175	3.23907	5.89002
H	-2.80322	3.01370	7.27663
H	0.69180	4.50098	1.08728
H	-1.68608	1.70499	6.79563
H	-9.43187	4.83094	-2.65025
H	-10.47388	7.58181	4.50321
H	-0.73289	-1.44227	-0.31827
H	-0.32202	-0.51316	4.06627
H	-3.55931	2.18443	-2.79909

DFT_smallmodel_Ctetr_OH2_water_DissociativeMechanism
E_solv = -2153.69489541634 a.u.

C	-0.20961	-0.26759	-0.05451
C	-0.03580	-0.21400	1.46428
O	1.09704	-0.26853	1.96859
C	-1.28064	0.65710	-0.65247
C	-1.11712	2.10802	-0.28672
N	-2.15257	3.00325	-0.49405
C	-0.05913	2.76535	0.29394
C	-1.72788	4.17082	-0.03988
N	-0.46585	4.07650	0.44348
N	-1.16039	-0.15955	2.19715
C	-1.19735	-0.10289	3.65406
C	-2.14051	-1.16286	4.22187
C	-3.59209	-1.00629	3.76882

O	-3.87047	-0.24708	2.79119
O	-4.47986	-1.67604	4.38013
Ca	-6.32284	-0.34827	3.38143
C	-5.99876	5.42134	2.73842
O	-7.26770	5.88074	2.26443
C	-8.20263	6.22816	3.27508
C	-9.56590	6.45209	2.62539
C	-10.60391	6.99224	3.61484
C	-5.68723	4.02518	2.16349
O	-5.67153	4.05498	0.78290
C	-6.88409	1.95406	0.17808
O	-4.32590	1.87838	-1.91991
O	-6.77187	1.25337	1.08862
C	-7.43135	2.34018	-1.11192
C	-8.32256	3.60665	-0.98137
C	-8.84814	4.03789	-2.35145
C	-4.32753	3.49765	2.66641
O	-4.13553	3.64429	4.09383
P	-4.71789	2.61362	5.20911
O	-5.29297	3.43602	6.33348
O	-5.57908	1.53208	4.58087
O	-3.36589	1.83344	5.72778
C	-2.45805	2.53862	6.58415
H	0.77439	-0.04306	-0.47905
H	-1.26792	0.53587	-1.74469
H	-2.28593	0.33851	-0.35047
H	-3.69260	2.36253	-1.32779
H	0.91142	2.42775	0.62853
H	-2.28498	5.09698	-0.04344
H	-2.07226	-0.07280	1.76495
H	-1.53228	0.88681	3.97625
H	-1.80889	-2.16669	3.92019
H	-2.11549	-1.14141	5.31801
H	-5.22243	6.12684	2.40453
H	-5.98320	5.39954	3.83549
H	-8.26619	5.43013	4.03116
H	-7.87917	7.14340	3.80341
H	-9.44639	7.15493	1.79191
H	-9.91102	5.50441	2.18963
H	-11.58993	7.08852	3.14181
H	-10.71275	6.32523	4.48022
H	-6.46658	3.34717	2.56709
H	-6.55874	2.51026	-1.76126
H	-7.99048	1.46392	-1.48011
H	-9.15845	3.38631	-0.30603
H	-7.71187	4.37769	-0.50484
H	-8.02825	4.20264	-3.06486
H	-9.51937	3.28188	-2.77809
H	-4.19794	2.45259	2.37597
H	-3.52830	4.08318	2.20250
H	-1.89573	3.29408	6.02376
H	-2.99577	3.02581	7.40497
H	0.07366	4.82686	0.85678
H	-1.75926	1.80121	6.98684
H	-9.41416	4.97259	-2.25841
H	-10.31676	7.98153	3.99211
H	-0.43981	-1.30681	-0.32701
H	-0.17904	-0.25451	4.01899
H	-3.87085	1.86802	-2.77730

DFT_smallmodel_Ctetr_OH2_water_DissociativeMechanism

E_solv = -2153.77336324550 a.u.

C	0.41234	-0.09669	0.14265
C	0.42501	-0.05509	1.67521
O	1.50902	-0.11444	2.28079
C	-0.85276	0.39242	-0.58692
C	-1.24107	1.80768	-0.25957
N	-2.56602	2.19744	-0.12603
C	-0.50702	2.93419	-0.00195
C	-2.66307	3.49103	0.20671
N	-1.40733	3.94803	0.28256
N	-0.76547	0.00135	2.29370
C	-0.97441	0.00599	3.73727
C	-2.01145	-1.04511	4.13634
C	-3.35460	-0.91969	3.41297
O	-3.47297	-0.14649	2.40987
O	-4.31466	-1.62458	3.84295
Ca	-6.00662	-0.32880	2.54472
C	-6.11944	5.47348	2.88278
O	-7.24633	5.91638	2.12334
C	-8.26683	6.55227	2.87812
C	-9.33742	7.05350	1.91201
C	-10.54227	7.67921	2.62399
C	-5.55895	4.16948	2.27442
O	-5.23052	4.28380	0.94922
C	-6.34760	1.82824	-0.36316
O	-5.25125	1.67407	-1.12992
O	-6.36472	1.28603	0.73272
C	-7.51788	2.52999	-1.01232
C	-8.53682	3.12020	-0.03329
C	-9.72790	3.74710	-0.76682
C	-4.32225	3.71729	3.08223
O	-4.52517	3.64663	4.51802
P	-4.94853	2.24977	5.24167
O	-5.75683	2.60741	6.46106
O	-5.51756	1.27760	4.22852
O	-3.50742	1.60507	5.70455
C	-2.78052	2.26737	6.74913
H	1.29005	0.46840	-0.18904
H	-0.69044	0.29033	-1.66803
H	-1.69885	-0.26624	-0.35707
H	-3.39267	1.62268	-0.28104
H	0.55854	3.10177	0.01468
H	-3.64344	3.98975	0.47878
H	-1.64031	0.05983	1.78357
H	-1.33247	0.99453	4.04906
H	-1.62370	-2.05716	3.94977
H	-2.21112	-0.97762	5.21103
H	-5.33905	6.25465	2.86035
H	-6.40871	5.31659	3.93168
H	-8.70106	5.84604	3.60722
H	-7.85723	7.39676	3.46024
H	-8.88024	7.78437	1.23126
H	-9.66768	6.21199	1.28996
H	-11.28030	8.04118	1.89972
H	-11.04312	6.94863	3.27171
H	-6.34019	3.39886	2.45247
H	-7.13990	3.30150	-1.69277

H	-7.99609	1.76747	-1.65008
H	-8.89496	2.32882	0.63566
H	-8.03150	3.87046	0.58479
H	-9.40625	4.56172	-1.42779
H	-10.25557	3.00606	-1.38332
H	-3.98518	2.74597	2.70869
H	-3.51685	4.44826	2.94120
H	-2.43954	3.25680	6.42258
H	-3.39938	2.37915	7.64604
H	-1.15673	4.90086	0.52819
H	-1.91143	1.64594	6.98039
H	-10.45104	4.16343	-0.05356
H	-10.24405	8.52858	3.25011
H	0.60032	-1.13930	-0.14700
H	-0.01618	-0.18328	4.22403
H	-5.34731	2.12738	-1.98943

DFT_smallmodel_Stetr_OH2_water_ DissociativeMechanism

E_solv = -2476.77978349187 a.u.

C	0.19315	0.22304	0.34578
C	-0.07389	0.11537	1.84722
O	0.85221	0.13434	2.67205
C	-0.70919	1.20552	-0.42151
C	-0.63289	2.63161	0.05413
N	-1.67386	3.51402	-0.19398
C	0.37897	3.30253	0.70216
C	-1.29213	4.68774	0.28887
N	-0.05947	4.60442	0.84142
N	-1.36080	-0.04807	2.21684
C	-1.78279	-0.07107	3.61423
C	-3.28556	-0.39156	3.71439
C	-4.13360	0.58522	2.89800
O	-4.05123	0.54100	1.62760
O	-4.85890	1.43243	3.49572
Ca	-5.68788	2.47751	1.29582
C	-8.92925	7.08929	2.90255
O	-9.97183	6.61917	3.73606
C	-9.56893	5.76051	4.80604
C	-10.75894	5.57854	5.74318
C	-10.43858	4.66089	6.92810
C	-8.37591	6.06233	1.89770
S	-9.74778	5.39717	0.86520
C	-9.02375	3.86109	0.26834
O	-4.25925	2.60765	-0.68398
O	-7.89384	3.50739	0.58126
C	-9.95233	3.04386	-0.60065
C	-10.90352	2.16553	0.24884
C	-11.82075	1.31229	-0.63200
C	-7.31122	6.68776	0.98670
O	-6.16086	7.01669	1.77567
P	-4.73697	6.22416	1.53036
O	-3.84983	6.62652	2.67092
O	-4.99837	4.75845	1.23973
O	-4.21213	6.86377	0.11704
C	-3.90262	8.26960	0.08462
H	1.24442	0.50677	0.23701
H	-0.43225	1.16048	-1.48481
H	-1.75683	0.88275	-0.38149
H	-3.34575	2.98684	-0.52145

H	1.34510	2.98816	1.06886
H	-1.87549	5.59770	0.27015
H	-2.11386	0.06151	1.54075
H	-1.57318	0.89652	4.09164
H	-3.46511	-1.40752	3.34134
H	-3.58547	-0.35244	4.76487
H	-9.34200	7.94709	2.35840
H	-8.08208	7.45062	3.50288
H	-9.23871	4.78521	4.41729
H	-8.71813	6.21022	5.34290
H	-11.07483	6.56541	6.10519
H	-11.60100	5.17017	5.16961
H	-11.31165	4.55041	7.58124
H	-10.14592	3.65851	6.59077
H	-7.93313	5.20835	2.41453
H	-10.54321	3.71161	-1.23940
H	-9.32840	2.41321	-1.24403
H	-10.30834	1.52094	0.90693
H	-11.50629	2.81009	0.89964
H	-12.44481	1.94191	-1.27808
H	-11.24107	0.63850	-1.27485
H	-7.04708	5.99408	0.18690
H	-7.69229	7.61256	0.53695
H	-4.80548	8.86962	0.24471
H	-3.16053	8.52358	0.84765
H	0.44553	5.36195	1.28811
H	-3.49703	8.48228	-0.90715
H	-12.48646	0.69931	-0.01349
H	-9.61716	5.06254	7.53457
H	0.08576	-0.77684	-0.09561
H	-1.20748	-0.82596	4.16056
H	-4.10960	1.83169	-1.24947

DFT_smallmodel_Stetr_OH2_water_ DissociativeMechanism
E_solv = -2476.77423290052 a.u.

C	0.75070	0.60061	1.56708
C	-0.22282	0.08267	2.62340
O	0.13413	-0.09845	3.79656
C	0.27702	1.84562	0.78827
C	0.02544	3.06707	1.63547
N	-1.13321	3.81440	1.48618
C	0.82945	3.67394	2.57446
C	-1.02569	4.84569	2.31096
N	0.14449	4.79764	2.99021
N	-1.48259	-0.20006	2.21993
C	-2.48983	-0.71475	3.14768
C	-3.74773	-1.17577	2.39604
C	-4.39183	-0.02468	1.61949
O	-4.00966	0.19422	0.42649
O	-5.25435	0.68913	2.20617
Ca	-5.61991	2.42403	0.38741
C	-8.73802	7.04264	2.91205
O	-9.36707	6.47975	4.04716
C	-8.50995	5.73983	4.91806
C	-9.27635	5.45053	6.20464
C	-8.44440	4.65411	7.21520
C	-8.47825	6.07219	1.74484
S	-10.07077	5.36500	1.15150
C	-9.38655	3.73570	0.21490

O	-3.21993	2.76321	-0.02827
O	-8.21466	3.47390	0.25460
C	-10.48793	2.93436	-0.42290
C	-11.21279	2.04950	0.62146
C	-12.32167	1.21212	-0.02292
C	-7.75903	6.79960	0.60225
O	-6.42954	7.14363	1.02816
P	-5.16275	6.27915	0.42347
O	-3.95995	6.65367	1.24040
O	-5.58312	4.83160	0.27042
O	-5.05094	6.85658	-1.10847
C	-4.67740	8.23325	-1.29720
H	1.68787	0.81283	2.08928
H	1.03455	2.06770	0.02406
H	-0.63737	1.62199	0.22859
H	-2.53876	3.22321	0.53987
H	1.80151	3.42274	2.97395
H	-1.76444	5.62494	2.44030
H	-1.76088	-0.06249	1.25531
H	-2.75659	0.06036	3.87847
H	-3.48862	-1.98512	1.70461
H	-4.46040	-1.56232	3.13100
H	-9.39600	7.85150	2.57156
H	-7.77406	7.49340	3.18806
H	-8.18966	4.79963	4.44331
H	-7.60267	6.32717	5.13375
H	-9.59322	6.40426	6.64598
H	-10.19262	4.90003	5.95559
H	-9.01976	4.46260	8.12803
H	-8.13756	3.68407	6.80434
H	-7.84920	5.23488	2.05734
H	-11.20164	3.61527	-0.90038
H	-10.02776	2.30867	-1.19696
H	-10.47819	1.39299	1.10381
H	-11.63401	2.68634	1.40778
H	-13.07934	1.85217	-0.49125
H	-11.91902	0.54434	-0.79419
H	-7.73570	6.17284	-0.29082
H	-8.27868	7.73367	0.35699
H	-5.43054	8.90357	-0.86813
H	-3.70520	8.43946	-0.83836
H	0.45687	5.46632	3.68575
H	-4.61642	8.40155	-2.37518
H	-12.82133	0.59378	0.73175
H	-7.53576	5.19878	7.50091
H	0.95259	-0.20925	0.85282
H	-2.06465	-1.55258	3.71070
H	-2.95823	1.82513	-0.04179

DFT_smallmodel_Stetr_OH2_water_DissociativeMechanism

E_solv = -2476.75799779257 a.u.

C	0.65329	0.94224	2.42441
C	-0.50236	0.28846	3.17824
O	-0.45836	0.11120	4.40371
C	0.27068	2.15264	1.54965
C	-0.28047	3.33938	2.29674
N	-1.39249	4.01866	1.82204
C	0.19493	3.98755	3.41430
C	-1.57774	5.05248	2.63129

N	-0.64157	5.06827	3.60901
N	-1.55984	-0.12918	2.44457
C	-2.68501	-0.83854	3.05384
C	-3.65792	-1.35368	1.98358
C	-4.27485	-0.19973	1.18656
O	-3.73805	0.15543	0.09346
O	-5.27073	0.39831	1.68923
Ca	-5.43646	2.29107	0.00019
C	-8.43035	6.88943	2.89289
O	-8.83473	6.34486	4.13564
C	-7.79850	5.72278	4.89682
C	-8.32840	5.47286	6.30533
C	-7.28294	4.82845	7.22158
C	-8.26927	5.87811	1.73946
S	-9.87323	5.01451	1.48285
C	-9.31836	3.53751	-0.05031
O	-3.03903	2.82967	-0.07366
O	-8.16526	3.38810	-0.29024
C	-10.54898	2.85364	-0.56148
C	-11.23360	1.99692	0.53086
C	-12.49173	1.30778	-0.00635
C	-7.79521	6.61173	0.47869
O	-6.44836	7.06589	0.69950
P	-5.19197	6.16416	0.13218
O	-3.96511	6.65646	0.84559
O	-5.57148	4.69634	0.15334
O	-5.15873	6.57419	-1.45823
C	-4.85970	7.93720	-1.80780
H	1.39051	1.23090	3.17897
H	1.16508	2.44897	0.98419
H	-0.46415	1.85836	0.79277
H	-2.49769	3.32455	0.60590
H	1.03257	3.79467	4.06884
H	-2.37058	5.78234	2.53404
H	-1.57804	0.01134	1.44157
H	-3.21444	-0.17211	3.74679
H	-3.13866	-2.04262	1.30852
H	-4.45496	-1.90485	2.49254
H	-9.19854	7.62430	2.62246
H	-7.47670	7.42542	3.00032
H	-7.48519	4.77600	4.42938
H	-6.91599	6.38243	4.92933
H	-8.65834	6.43114	6.72692
H	-9.21887	4.83433	6.24326
H	-7.69355	4.66434	8.22439
H	-6.95313	3.85683	6.83280
H	-7.51193	5.13241	1.98491
H	-11.23780	3.62648	-0.92248
H	-10.24091	2.23136	-1.41094
H	-10.52186	1.24761	0.89841
H	-11.49469	2.63180	1.38425
H	-13.22794	2.04293	-0.35299
H	-12.25640	0.64184	-0.84491
H	-7.84806	5.96389	-0.39778
H	-8.41160	7.49874	0.29213
H	-5.63488	8.61382	-1.43143
H	-3.88810	8.23890	-1.40367
H	-0.57326	5.75118	4.35562
H	-4.83406	7.98844	-2.89913

H	-12.96025	0.70663	0.78119
H	-6.39602	5.46637	7.32420
H	1.12241	0.17983	1.78789
H	-2.30358	-1.67778	3.64655
H	-2.63907	1.94542	-0.13401

DFT_smallmodel_Stetr_OH2_water_DissociativeMechanism
E_solv = -2476.73390882721 a.u.

C	0.32761	0.25691	0.58369
C	0.14090	0.23023	2.10243
O	1.10239	0.35863	2.87564
C	-0.67062	1.11713	-0.21260
C	-0.59500	2.59653	0.05879
N	-1.65121	3.42989	-0.28283
C	0.43017	3.36029	0.56723
C	-1.26350	4.66422	0.00703
N	-0.01446	4.66715	0.52719
N	-1.11195	-0.00331	2.54170
C	-1.48468	0.00279	3.95413
C	-2.97272	-0.37141	4.10646
C	-3.86668	0.56135	3.28999
O	-3.77588	0.50958	2.01901
O	-4.62306	1.38983	3.87276
Ca	-5.38101	2.43169	1.64711
C	-8.83139	6.95184	3.09659
O	-9.82786	6.54184	4.01622
C	-9.41686	5.59942	5.00450
C	-10.56925	5.41460	5.98768
C	-10.25553	4.38711	7.08060
C	-8.40954	5.90428	2.04035
S	-9.89369	5.14412	1.27509
C	-8.71636	3.39721	-0.07109
O	-4.21641	2.37062	-0.49060
O	-7.61959	3.16084	0.27325
C	-9.67271	2.90817	-1.09816
C	-10.82649	2.09471	-0.46231
C	-11.80990	1.61976	-1.53634
C	-7.53688	6.56339	0.96697
O	-6.31021	7.02334	1.56308
P	-4.90664	6.25415	1.18960
O	-3.85537	6.84990	2.07908
O	-5.13730	4.75409	1.17441
O	-4.66889	6.67791	-0.37452
C	-4.52789	8.07602	-0.68446
H	1.35168	0.59614	0.40064
H	-0.48716	0.94154	-1.28257
H	-1.70075	0.78395	-0.03750
H	-3.31219	2.80395	-0.46468
H	1.40977	3.10766	0.94471
H	-1.85274	5.56118	-0.12462
H	-1.89895	0.02770	1.89621
H	-1.29609	0.99124	4.39582
H	-3.12548	-1.39977	3.75649
H	-3.24665	-0.32161	5.16353
H	-9.25262	7.82495	2.58414
H	-7.92631	7.27758	3.62996
H	-9.16437	4.63699	4.53570
H	-8.51491	5.96631	5.52170
H	-10.80696	6.38625	6.43961

H	-11.46015	5.10260	5.42744
H	-11.10405	4.27603	7.76529
H	-10.04354	3.39940	6.65165
H	-7.82408	5.11066	2.51232
H	-10.06558	3.78432	-1.62456
H	-9.08971	2.29474	-1.79874
H	-10.40714	1.23648	0.07542
H	-11.34487	2.71603	0.27553
H	-12.25839	2.46917	-2.06503
H	-11.31602	0.98037	-2.27735
H	-7.32662	5.86123	0.15823
H	-8.04872	7.43604	0.54366
H	-5.46328	8.61383	-0.49391
H	-3.72485	8.52827	-0.09373
H	0.49869	5.48436	0.83935
H	-4.28105	8.14327	-1.74677
H	-12.61877	1.04195	-1.07562
H	-9.38376	4.68729	7.67518
H	0.26593	-0.77780	0.22059
H	-0.86592	-0.71424	4.50463
H	-4.07250	1.53249	-0.96171

DFT_smallmodel_Stetr_OH2_water_ DissociativeMechanism

E_solv = -2476.70552982452 a.u.

C	0.94480	0.62515	1.83714
C	0.21334	0.39150	3.15839
O	0.79984	0.45801	4.24894
C	0.27246	1.64690	0.90085
C	0.14704	3.03809	1.46352
N	-0.90834	3.85947	1.09333
C	0.98073	3.73428	2.30826
C	-0.70738	5.02184	1.69827
N	0.42052	4.98854	2.44487
N	-1.09356	0.06798	3.06568
C	-1.94751	-0.09819	4.23739
C	-3.32296	-0.64494	3.82202
C	-4.03618	0.25031	2.80398
O	-3.54143	0.36441	1.63747
O	-5.09838	0.84775	3.14692
Ca	-5.21424	2.19139	0.93614
C	-8.63690	6.73478	2.99600
O	-9.22388	6.22002	4.18052
C	-8.38022	5.40386	4.98766
C	-9.09456	5.14002	6.31052
C	-8.28200	4.24625	7.25350
C	-8.48573	5.74575	1.82477
S	-10.08952	4.95205	1.38781
C	-9.36646	3.32404	-1.02605
O	-3.08330	2.69582	-0.20784
O	-8.24923	3.05184	-1.01009
C	-10.71864	3.06377	-1.54157
C	-11.40873	1.98877	-0.65277
C	-12.80339	1.65824	-1.19128
C	-7.92243	6.47423	0.60160
O	-6.53503	6.81556	0.80635
P	-5.40001	5.86626	0.10110
O	-4.06624	6.40633	0.52989
O	-5.75035	4.40679	0.34029
O	-5.67041	6.10088	-1.49948

C	-5.50090	7.42195	-2.04266
H	1.96169	0.93974	2.08957
H	0.84255	1.67346	-0.03890
H	-0.72888	1.29974	0.62175
H	-2.35185	3.19840	0.25776
H	1.89813	3.46624	2.81116
H	-1.36303	5.88029	1.64209
H	-1.58709	0.13286	2.17838
H	-2.06506	0.85895	4.76544
H	-3.19636	-1.64095	3.37885
H	-3.94396	-0.74771	4.71585
H	-9.28707	7.56067	2.68302
H	-7.64392	7.15641	3.22066
H	-8.16284	4.45110	4.48213
H	-7.41798	5.91303	5.16270
H	-9.30720	6.10300	6.79238
H	-10.06588	4.67474	6.09907
H	-8.81857	4.08462	8.19539
H	-8.09101	3.26216	6.80702
H	-7.77048	4.96300	2.09072
H	-11.27945	4.00071	-1.56903
H	-10.56641	2.69988	-2.57006
H	-10.78648	1.08723	-0.64172
H	-11.46964	2.36093	0.37384
H	-13.45013	2.54236	-1.20006
H	-12.75422	1.25594	-2.20943
H	-8.03607	5.85704	-0.29115
H	-8.46198	7.41367	0.43036
H	-6.24635	8.11094	-1.63071
H	-4.49692	7.80456	-1.83241
H	0.77977	5.74610	3.01539
H	-5.64170	7.34121	-3.12334
H	-13.26894	0.90121	-0.55030
H	-7.31142	4.69719	7.49557
H	1.02638	-0.33519	1.31076
H	-1.47179	-0.79117	4.93928
H	-2.62293	1.94498	-0.61764

DFT_smallmodel_Stetr_OH2_water_ DissociativeMechanism
E_solv = -2476.70214190437 a.u.

C	0.54587	-0.28511	0.94523
C	0.54520	-0.00720	2.45056
O	1.59928	0.10330	3.09646
C	-0.38301	0.61132	0.10447
C	0.01655	2.06241	0.06308
N	-0.87882	3.03542	-0.36294
C	1.22710	2.65544	0.33755
C	-0.21157	4.18125	-0.35651
N	1.06137	3.99895	0.06523
N	-0.67140	0.04782	3.02132
C	-0.91861	0.38704	4.41857
C	-2.40691	0.16145	4.74308
C	-3.34244	0.94537	3.81680
O	-3.24147	0.75604	2.55943
O	-4.19250	1.73924	4.30451
Ca	-4.81214	2.65068	1.92718
C	-9.42563	6.52212	3.04787
O	-10.30459	5.97820	4.02580
C	-9.69314	5.28188	5.10613

C	-10.77026	5.00622	6.15404
C	-10.24237	4.24154	7.37219
C	-8.87183	5.52937	2.01306
S	-10.18841	4.62310	1.08302
C	-9.05518	3.14046	-1.87799
O	-3.62212	2.34990	-0.18767
O	-7.93608	3.27641	-1.77856
C	-10.42272	2.80859	-2.17628
C	-10.93183	1.62341	-1.29399
C	-12.35101	1.23415	-1.71364
C	-8.03148	6.26138	0.96890
O	-6.86674	6.89656	1.54256
P	-5.38917	6.33346	1.11183
O	-4.39607	7.16328	1.87513
O	-5.35898	4.81974	1.21146
O	-5.33950	6.66691	-0.49298
C	-5.46615	8.03852	-0.90011
H	1.58147	-0.19823	0.60420
H	-0.40510	0.20999	-0.91930
H	-1.41841	0.54435	0.45937
H	-2.69321	2.69306	-0.30436
H	2.16728	2.26132	0.69308
H	-0.60854	5.15073	-0.62690
H	-1.50862	0.09817	2.44067
H	-0.64193	1.43214	4.61957
H	-2.64423	-0.90503	4.63304
H	-2.59934	0.44457	5.78123
H	-10.00921	7.29327	2.52943
H	-8.58090	7.02143	3.54914
H	-9.24588	4.33539	4.76390
H	-8.88158	5.89067	5.53857
H	-11.20336	5.96433	6.46954
H	-11.58218	4.43826	5.68181
H	-11.04487	4.06233	8.09718
H	-9.83024	3.26616	7.08454
H	-8.22411	4.80644	2.51933
H	-11.01753	3.72064	-2.03930
H	-10.41899	2.54835	-3.24894
H	-10.25081	0.77553	-1.41266
H	-10.89904	1.93866	-0.24807
H	-13.04970	2.07056	-1.60249
H	-12.38177	0.89338	-2.75431
H	-7.73147	5.55774	0.19058
H	-8.62837	7.05392	0.50067
H	-6.46645	8.42361	-0.67112
H	-4.71657	8.66580	-0.40628
H	1.76163	4.72466	0.17230
H	-5.30858	8.06658	-1.98121
H	-12.69945	0.41411	-1.07626
H	-9.44976	4.80110	7.88433
H	0.24912	-1.33261	0.79919
H	-0.29663	-0.23797	5.06821
H	-3.61555	1.48871	-0.63723

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