The Reaction of Sulfenic Acids with OH and HO_2 Radicals in different Environments.

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(supplementary information)

Methods.

In a first step all the reactions have been investigated with the M0-62X[1] density functional using 6-311+G(2df,2p) basis set.[2] At all stationary points we have performed harmonic frequency calculations to verify the nature of the stationary points and to obtain zero point, thermal and Gibbs free energies. In addition, for all reactions involving compounds **1**, **2**, and **3**, we have carried out IRC[3] calculations to confirm the connectivity of the transition states.

For the reactions involving sulfenic acid **4**, we have carried out, in a first step, a molecular mechanic study (MM), using the OPLS3e force field,[4] in order to search for the lowest energy conformers. As the species involved are radicals in transition states, the radical electron was saturated with a hydrogen atom. Then, the conformational search was performed fixing the position of the atoms involved in the reaction, and allowing the rest of the molecule to sample conformations. In a second step, we have taken the lowest conformers and we have employed the M0-62X[1] density functional using the 6-311+G(2df,2p) basis set in a search for the transition states. Then, starting from the transition states, we have moved along the reaction coordinate to find the corresponding reactants and products and reactants.

Finally, in order to obtain accurate relative energies, we have performed of single-point energy calculations at the optimized geometries using different theoretical approaches. First, for all stationary points, we have carried out DLPNO-CCSD(T) calculations using the aug-cc-pVTZ basis set.[5] Second, and in order to determine the accuracy of these

results, for the most representative stationary points of the reactions between CH_3SOH with OH and HO_2, we have performed single point energy calculation with the CCSD(T) method employing the aug-cc-pV(T+d)Z, aug-cc-pV(Q+d)Z and complete CBS basis sets.[2,5–8] Third, and for the most significant cases of the reactions between sulfenic acids **2** and **3** with HO_2, we have also carried out single point energy calculation with the CCSD(T) method employing the aug-cc-pV(T+d)Z. In all these calculations we have looked at the T1 diagnostic [9] with regard to the possible multireference character of the CCSD wavefunction. Our calculations show that the CCSD(T)/aug-cc-pV(T+d)Z compare very well with the results employing CCSD(T)/CBS approach, but the results obtained with the DLPNO-CCSD(T)/aug-cc-pVTZ level overestimate the reaction energies and reaction barriers by 3.8 $kcal \cdot mol^{-1}$ on average, and therefore, we have corrected the relative energies for the reactions of models **4** with OH and HO_2 with these values.

The quantum chemical calculations carried out in this work were performed by using Gaussian[10] and ORCA[11] program packages. The molecular mechanics studies were done with the Schrodinger suite.[12,13]

To account for the solvation effects, we re-optimized and characterized all stationary points employing the M06-2X functional using a polarizable implicit solvent model (PCM)[14] with water as solvent, and the solvation energies have been calculated as difference of these results with those at the gas phase calculation obtained at the same level of theory. The correction term of 1.89 $kcal \cdot mol^{-1}$ was applied to account for the conversion of the standard state between 1 atm in gas phase to 1 $mol \cdot L^{-1}$ in aqueous solution. [15] The final energies were obtained by adding the solvation energies to the CCSDS(T) or DLPNO-CCSD(T) energy values.

Our calculations shown that all reactions involving the abstraction of the acidic hydrogen of all sulfenic acids with hydroxyl radical show a free energy barrier that lies below the free energy of the separate reactants, implying that these processes are diffusion controlled and the rate constants are given by the association between the sulfenic acid and hydroxyl radical. Thus, for the gas phase reaction of CH3-SOH, CH2CHCH2-SOH and CH_3CHCH-SOH with OH, we have employed the variable-reaction-coordinate-variational transition-state theory (VRC-TST) and a multifaced dividing surface [16,17] for calculating the rate constants. In these cases, the M06-2X approach with the 6-311+G(2df,2p) basis set has been employed and the Polyrate [18]and Gaussrate [19] programs have been employed.

The high-pressure limit rate constant at the temperature T can be expressed as

$$k(T,s) = \frac{\hbar^2}{2\pi} g_e \frac{\sigma_1\sigma_2}{\sigma^{\ddagger} Q_1 Q_2}\left(\frac{2\pi}{\mu k_B T}\right)^{3/2} \int \mathrm{dE} e^{-E/kbT}\, \mathrm{dJ\ N(E,J,s)}$$

where s is the value of reaction coordinate, which is defined as the distance between two pivot points; g_e is the ratio of the electronic partition function of the transition state to the product of the electronic partition functions of reactants; μ is the reduced mass; Q_1 and Q_2 are the rotational partition functions of the reactants calculated without symmetry numbers; J is the unitless total angular momentum quantum number; N(E,J,s) is the number of accessible states of the generalized transition state, s for total energy E and angular momentum J; and σ_1 , σ_2 , and $\sigma^{\ddagger}$ are the rotational symmetry numbers for the reactants and transition state, respectively. [16,17]

For the react ions with HO_2, we have calculated the rate constants in the following manner. For the reactions of **1**, **2**, and **3**, with HO_2 we have employed conventional transition state theory considering the tunneling effect with zero-curvature approach with an unsymmetrical Eckart barrier[20,21] and for the Wigner approach as well. For all these calculations we have taken the CCSD(T)/aug-cc-pV(T+d)Z basis set energy values. The Polyrate program has been used for these calculations.[18].

The kinetic study for the reaction of **4** with HO_2 has been carried out in the framework of the multi-conformer transition state theory (MC-TST)[22] where the rate constant *k* for each elementary reaction *i*, is calculated according equation 1,

$$k_i = \kappa \frac{k_B T}{h} e^{\frac{-\Delta G}{k_B T}} \qquad (1)$$

where κ is the tunneling parameter, which has been calculated for the hydrogen transfer processes according to the Wigner formulae,[23] k_B is the Boltzmann constant, *h* is the Planck constant, T the temperature (298.15 K in the present calculations) and ΔG(298.15K) is the free energy barrier between a given transition state and their corresponding reactants. The ΔΔG values have been calculated taking into account the

DLPNO-CCSD(T) energies corrected by -3.8 kcal·mol^{-1} (see above), with the free energy corrections computed at M06-2X level of theory.

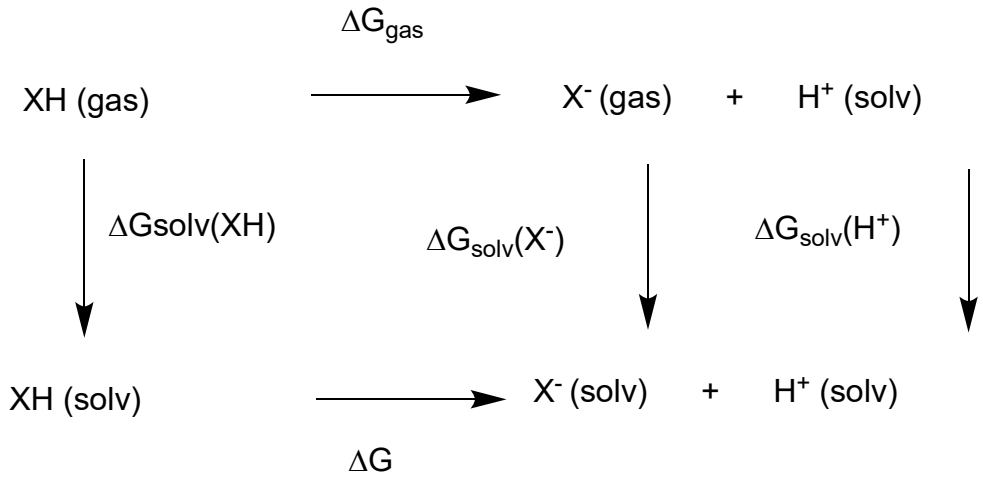
According to the MC-TST, the reaction rate constant k_R is given by equation 2,

$$k_R = \sum_i^n f_i \cdot k_i \qquad (2)$$

where the sum runs for all conformers i, and f_i is a weighted factor of the reactants corresponding to the elementary reaction i and has been computed by the Boltzmann population relative to all conformers of the reactants. These calculations has been carried out with a house made python program.[24]

The pK_a calculations have been calculated employing the thermodynamic cycle shown in Scheme S1,

Scheme S1



Where $\Delta G = \Delta G_{gas} + \Delta G_{solv}(X^-) + \Delta G_{solv}(H^+) - \Delta G_{solv}(XH)$,

and $pK_a = \Delta G/2.303RT$

We have taken $\Delta G_{gas}(H^+)$ = -6.28 kcal·mol^{-1} for the gas phase free energy of the proton,[25] and $\Delta G_{solv}(H^+)$ = -264.0 kcal·mol^{-1} as the experimental values for the Gibbs free energy of hydration of the proton.[26]

Our estimated pK_a was calculated by computing the pKa of 2-Methyl-2-propanesulfenic acid and compounds 1,2,3, and 4 and adding to the experimental value of 2-Methyl-2-propanesulfenic acid (10.47) [27] the δpKa according to the following equilibrium.

$R\text{-}SOH + (CH_3)_3CSO^-$ $R\text{-}SO^- + (CH_3)_3CSOH$

The reaction of CH_3SOH + HO_2 and OH radicals.

All stationary points have been have been optimized and characterized with the M06-2X functional and we have performed single point energies, at all stationary points, using the DLPNO-CCSD(T) approach with the aug-cc-pVTZ basis set, and using the CCSD(T) approach with the aug-cc-pV(T+d)Z, aug-cc-pV(Q+d)Z and complete CBS basis sets. These calculations have been carried out in order the look for the accuracy of our calculations and the corresponding results are displayed in Tables S1 and S2. The relative energies obtained at CCSD(T)/aug-cc-pV(T+d)Z level of theory and CCSD(T)/CBS level differ by less than 1 $kcal \cdot mol^{-1}$ and therefore we have used the CCSD(T)/aug-cc-pV(T+d)Z approach for calculating accurate results and for calculating the rate constants for the reaction of **1**, **2**, and **3** with HO_2. Since DLPNO-CCSD(T) calculations overestimated the energy barriers by -3.8 $kcal \cdot mol^{-1}$ on average, we have corrected the energy values of the reactions of **4** with OH and HO_2 by this value (Figures 3 and 6 of the main text, the calculations of the rate constants and Figures S2, S3, S5, and S6 below).

All structures of the corresponding transition states are displayed in Figures 1 and 4 of the main text, except **1BTS5** that correspond to a different con former of **1BTS1**, involving the same kind of reaction mechanism, namely *pcet*. The corresponding cartesian coordinates are given in Table S9.

Table S1. Relative energies (Δ (E+ZPE) in kcal·mol^{-1}) and free energies in gas and solvation phases (ΔGgas and ΔGsolv, in kcal·mol^{-1}) for the $CH_3SOH + HO_2$ reaction, computed at different levels of theory.[a]

	DLPNO-CCSD(T)/aug-cc-pVTZ			**CCSD(T)/aug-cc-pV(T+d)Z**			**CCSD(T)/CBS**		
	Δ (E+ZPE)	**ΔGgas**	**ΔGsolv**	**Δ (E+ZPE)**	**ΔGgas**	**ΔGsolv**	**Δ (E+ZPE)**	**ΔGgas**	**ΔGsolv**
$CH_3SOH + HO_2$	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	0.00	0.00	0.00
1ACR1	-8.10	1.45	3.17	-9.35	0.21	1.93	-9.02	0.5	2.26
1ATS1 (pcet)	3.79	14.27	14.97	0.17	10.65	11.35	0.64	11.1	11.82
1ACP1	-20.53	-12.39	-12.08	-23.61	-15.47	-15.16	-23.81	-15.7	-15.36
1ACR2	-2.67	5.66	4.59	-3.57	4.75	3.68	-3.09	5.2	4.16
1ATS2 (pcet)	11.20	21.06	21.92	4.26	14.12	14.98	4.74	14.6	15.46
1ACR3	-5.98	2.88	3.52	-6.55	2.31	2.95	-6.17	2.7	3.33
1ATS4 (addition)	8.99	19.44	18.60	5.98	16.43	15.59	6.19	16.6	15.80
$CH_3S(OH)(OOH)$	6.73	17.28	15.95	3.76	14.31	13.20	3.66	14.2	12.88
1ACR6	-5.00	3.91	3.62	-5.83	3.08	2.79			
1ATS6 (addition)	8.85	19.37	18.55	6.03	16.56	15.74			
1ACR2	-2.67	5.66	4.59	-3.57	4.75	3.68			
1ATS3 (hat)	11.04	20.68	21.55	4.36	14.00	14.88			
1ACR4	-2.90	5.37	4.51	-3.41	4.85	3.99			
1ATS5 (hat)	10.55	19.95	20.37	6.11	15.51	15.93			

a) The ZPE and free energy corrections have been calculated at M06-2X/6-311+G(2df,2p) level of theory

Table S2. Relative energies (Δ (E+ZPE) in kcal·mol-1) and free energies in gas and solvation phases (ΔGgas and ΔGsolv, in kcal·mol^{-1}) for the CH_3SOH + OH reaction, computed at different levels of theory.[a]

	DLPNO-CCSD(T)/ aug-cc-pVTZ			**CCSD(T)/ aug-cc-pV(T+d)Z**			**CCSD(T)/CBS**		
	Δ(E+ZPE)	**ΔGgas**	**ΔGsolv**	**Δ(E+ZPE)**	**ΔGgas**	**ΔGsolv**	**Δ(E+ZPE)**	**ΔGgas**	**ΔGsolv**
	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	0.00	0.00	0.00
1BCR1	-12.66	-4.02	-3.75	-14.94	-6.31	-6.04	-15.93	-7.30	-7.03
1BTS1 (*pcet*)	-11.81	-2.94	-3.04	-14.27	-5.41	-5.51	-15.27	-6.41	-6.50
1BCP1	-49.23	-42.42	-42.80	-51.77	-44.96	-45.34	-53.27	-46.46	-46.84
1BTS5 (*pcet*)	-9.02	-0.14	-1.88	-11.51	-2.64	-4.37	-12.52	-3.65	-5.38
1BTS2 (addition)	-6.59	2.25	0.80	-8.83	0.01	-1.45	-9.61	-0.77	-2.23
$CH_3S(OH)_2$	-15.97	-7.05	-7.95	-18.78	-9.85	-10.76	-20.21	-11.29	-12.19
1BCR3	-3.60	3.41	13.82	-3.96	3.05	13.47	-3.63	3.38	13.80
1BTS3 (C-H abst)	2.30	10.64	10.75	0.28	8.61	8.73	0.21	8.55	8.67
$CH_2SOH\cdot\cdot H_2O$	-28.32	-20.67	-20.64	-29.82	-22.16	-22.14	-31.59	-23.94	-23.91
1BTS4	-10.25	-1.01	-0.62	-13.47	-4.23	-3.84	-14.82	-5.57	-5.18
1BCP1	-49.23	-42.42	-42.80	-51.77	-44.96	-45.34	-53.27	-46.46	-46.84

a) The ZPE and free energy corrections have been calculated at M06-2X/6-311+G(2df,2p) level of theory

Reaction of 2 and 3 with HO_2 and OH.

In Tables S3 to S6 we have collected the computed relative energies and free energies of the reactions of **2** and **3** with HO_2 and OH, respectively. All Cartesian coordinates are given in Table S9. For the reaction of **2** with HO_2 (Table S3) we have found two elementary reaction involving the abstraction of the acidic hydrogen by the radical, which follow a *pcet* mechanism (**2ATS1** and **2ATS1a**), and differ in the relative orientation of the OOH moiety and they have almost the same energy barrier. In addition, we have found a reaction path also involving the abstraction of the acidic hydrogen by the radical, but following the *hat* mechanism (**2ATS2**) which requires a higher free energy barrier of about 5 kcal·mnol^{-1}, and three elementary reactions where the HO_2 radical adds to the S atom (**2ATS3, 2ATS3a, and 2ATS3b**), which have a free energy barrier greater than **2ATS1** by about 5 kcal·mol^{-1}.

Table S3. Calculated relative energies (Δ (E+ZPE)), gas phase and solvation free energies (ΔG_{gas} and ΔG_{solv}) at 298 K (in kcal·mol^{-1}) for the reaction of CH_2=$CHCH_2SOH$ (**2**) with HO_2 at different levels of theory. [a]

	DLPNO-CCSD(T)/aug-cc-pVTZ			**CCSD(T)/aug-cc-pV(T+d)Z**		
	Δ(E+ZPE)	**ΔG_{gas}**	**ΔG_{sol}**	**Δ(E+ZPE)**	**ΔG_{gas}**	**ΔG_{sol}**
	CH_2=$CHCH_2SOH$ + HO_2. → CH_2=$CHCH_2SO\cdots H_2O_2$					
2	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00
2ACR1	-8.19	1.63	3.35	-9.30	0.52	2.24
2ATS1 (*pcet*)	3.78	14.42	15.14	0.23	10.86	11.59
2ACP1	-19.73	-10.27	-9.77	-22.52	-13.07	-12.56
2	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00
2ACR1a	-8.69	1.12	3.16	-9.60	0.21	2.25
2ATS1a (*pcet*)	3.12	13.68	14.75	-0.45	10.11	11.19
2ACP1a	-20.45	-10.37	-9.36	-23.70	-13.63	-12.61
2	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00
2ACR2	-2.46	6.56	5.46	-3.61	5.41	4.31
2ATS2 (*hat*)	10.76	21.23	22.37	4.89	15.35	16.50
2ACP2	-20.48	-10.82	-9.92	-23.54	-13.87	-12.98
	CH_2=$CHCH_2SOH$ + HO_2. → CH_2=$CHCH_2S(OH)(OOH)$					
2	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00

2ACR3	-6.00	3.82	4.60	-6.77	3.05	3.83
2ATS3 (addition)	7.95	18.87	18.60	4.96	15.88	15.61
2ACP3	6.39	17.42	16.72	3.17	14.20	13.51
2A2	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00
2ACR3a	-6.23	3.50	8.74	-7.01	2.71	7.96
2ATS3a(addition)	9.93	20.60	20.45	6.87	17.55	17.40
2ACP3a	7.69	18.32	17.82	4.89	15.52	15.01
2A2	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00
2ACR3b	-6.29	3.29	4.32	-7.30	2.28	3.31
2ATS3b(addition)	9.48	19.86	19.10	6.44	16.82	16.06
2ACP3b	7.19	18.03	17.60	3.80	14.65	14.21

a) The ZPE and free energy corrections have been calculated at M06-2X/6-311+G(2df,2p) level of theory

The reaction of **3** with HO_2 (Table S4) have the same features than the reaction of **2** with HO_2, and we have found one elementary reaction for the abstraction of the acidic hydrogen by the HO_2 radical, showing a *pcet* mechanism, and one elementary reaction for the addition of the radical to the S atom of the sulfenic acid, for which we have calculated a higher energy barrier.

Table S4. Relative energies (Δ(E+ZPE) in kcal·mol-1) and free energies in gas and solvation phases (ΔGgas and ΔGsolv, in kcal·mol^{-1}) for the reactions between CH_3CH=CHSOH (**3**) with HO_2 reaction, computed at different levels of theory.[a]

	DLPNO-CCSD(T)/aug-cc-pVTZ			**CCSD(T)/aug-cc-pV(T+d)Z**		
	Δ(E+ZPE)	**ΔG_{gas}**	**ΔG_{sol}**	**Δ(E+ZPE)**	**ΔG_{gas}**	**ΔG_{sol}**
	CH_3CH=CHSOH + HO_2. → CH_2CH=$CH_2SO\cdots H_2O_2$					
3AR1	0.00	0.00	0.00	0.00	0.00	0.00
3ACR1	-8.31	1.11	2.96	-9.32	0.10	1.96
3ATS1 (*pcet*)	4.16	14.76	15.41	0.37	10.98	11.62
3ACP1	-21.92	-12.62	-12.51	-24.45	-15.15	-15.05
	CH_3CH=CHSOH + HO_2. → CH_2CH=CH_2S(OH)(OOH)					
3AR1	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00
3ACR2	-6.31	2.33	2.84	-6.95	1.69	2.20

3ATS2 (addition)	8.92	19.88	19.35	5.96	16.93	16.40
3ACP2	7.11	18.00	17.27	4.37	15.26	14.52

a) The ZPE and free energy corrections have been calculated at M06-2X/6-311+G(2df,2p) level of theory

Tables S5 and S6 contains the relative energies for the elementary reaction of **2** and **3** with OH, and the corresponding results show the same trends as discussed for the reaction of CH_3SOH + OH.

Regarding the reaction of **3** + OH, we have found, in general, three conformers for each process. **2BTS1**, **2BTS1a**, and **2BTS1b** correspond to the acidic hydrogen abstraction by the OH radical, following a pcet mechanism with the same electronic features than **1BTS1**discussed in the main text. The free energy of the transition states lie below the free energy of the separate reactants so that the corresponding reaction are diffusion controlled. **2BTS2, 2BTS2a**, and **2BTS2b** correspond to the addition of the radical to the S atom, producing CH_2=$CHCH_2$-$S(OH)_2$. Further work has shown that this adduct easily hydrolyses leading to the formation of CH_2=$CHCH_2$-SO + $2H_2O$, in a similar manner as described for the addition of the OH radical to CH_3SOH. Therefore, this process constitutes an indirect path for the abstraction of the acidic hydrogen by the OH radical.

The process via **2BTS3** involves the abstraction of the hydrogen of the CH_2 group producing CH2=CHCHSOH··H_2O, which can decompose into CH_2=CHCHSOH + H_2O or follow a intermolecular water assisted hydrogen transfer (via **2BTS4**) between of the acidic hydrogen leading to the formation of CH_2=$CHCH_2$SO··H_2O, that is, the same product than the direct acidic hydrogen abstraction by OH. Finally, the elementary reaction through **2BTS5** involve the addition of the OH radical to the π bond of CH_2=$CHCH_2$-SOH.

Table S5. Calculated relative energies (Δ(E+ZPE)), gras phase ang solvation free energies (ΔG_{gas} and ΔG_{solv}) at 298 K for the reaction between CH_2=$CHCH_2$-SOH and OH, computed at DLPNO-CCSD(T)/aug-cc-p)Z level, with zero point energy and free energy corrections obtained at M06-2X level. Values in kcal·mol^{-1}.

	Δ(E+ZPE)	**ΔG_{gas}**	**ΔG_{solv}**
CH_2=$CHCH_2$-SOH + OH → CH_2=$CHCH_2$-SO + H_2O			
CH_2=$CHCH_2$-SOH + OH	0.00	0.00	0.00
2BCR1	-13.77	-4.75	-3.64

2BTS1 (*pcet*)	-12.95	-3.91	-3.07
2BCP1	-49.48	-41.79	-41.56
CH_2CHCH_2-SOH + OH	0.00	0.00	0.00
2BCR1a	-12.75	-3.98	-3.30
2BTS1a (*pcet*)	-12.03	-2.85	-2.31
2BCP1	-49.48	-41.79	-41.56
CH_2CHCH_2-SOH + OH	-0.00	-0.00	-0.00
2BCR1b	-10.16	-1.36	-1.43
2BTS1b (*pcet*)	-9.29	-0.36	-1.07
2BCP1b	-45.80	-39.29	-41.50
CH_2=$CHCH_2$-SOH + OH → CH_2=$CHCH_2$-S(OH)$_2$			
CH_2=$CHCH_2$-SOH + OH	-0.00	-0.00	-0.00
2BCR2	-13.47	-4.41	-3.26
2BTS2	-6.92	2.43	1.74
2BCP2	-15.18	-5.81	-6.33
CH_2=$CHCH_2$-SOH + OH	-0.00	-0.00	-0.00
2BCR2a	-12.96	-4.29	-3.64
2BTS2a	-6.91	1.99	0.80
2BCP2a	-15.57	-6.65	-7.34
CH_2=$CHCH_2$-SOH + OH	-0.00	-0.00	-0.00
2BR2b	-10.57	-1.91	-1.99
2BTS2b	-6.54	2.59	1.65
2BCP2b	-16.44	-7.16	-7.44
CH_2=$CHCH_2$-SOH + OH → CH_2=CHCH-SOH·H_2O → CH_2=$CHCH_2$-SO + H_2O			
CH_2=$CHCH_2$-SOH + OH	-0.00	-0.00	-0.00
2BCR3	-3.60	3.21	3.02
2BTS3	5.84	14.26	14.47
CH2=CHCHSOH··H2O	-39.78	-32.17	-32.68
2BTS4	-12.36	-3.13	-3.35
2BCP1	-49.48	-41.79	-41.56
CH_2=$CHCH_2$-SOH + OH → $CH_2CH(OH)CH$-SOH···H_2O			
CH_2=$CHCH_2$-SOH + OH	-0.00	-0.00	-0.00
2BCR5	-26.22	-17.00	-16.73

2BTS5	-0.88	7.20	5.74
$CH_2CH(OH)CH\text{-}SOH\cdots H_2O$	-1.45	5.42	4.77

Finally, Table S6 contains the relative energies for the reaction of **3** + OH. In a similar way as described for **1** + OH and for **2** + OH, the abstraction of the acidic hydrogen by the radical takes place via **3BTS1**, with a free energy at the transition state lying below the free energy of the reactants, whereas the processes via **3BTS2** and **3BTS3** correspond to the addition of the radical to the S atom and to the addition of the OH to the π bond.

Table S6. Calculated relative energies (Δ(E+ZPE)), gras phase ang solvation free energies (ΔG_{gas} and ΔG_{solv}) at 298 K for the reaction between $CH_3CHCH\text{-}SOH$ and OH, computed at DLPNO-CCSD(T)/aug-cc-p)Z level, with zero point energy and free energy corrections obtained at M06-2X level. Values in kcal·mol^{-1}. [a]

	Δ(E+ZPE)	**ΔG_{gas}**	**ΔG_{solv}**
$CH_3CH{=}CH\text{-}SOH + OH \rightarrow CH_3CH{=}CH\text{-}SO + H_2O$			
$CH_3CH{=}CH\text{-}SOH + OH$	0.00	0.00	0.00
3BCR1	-12.50	-3.89	-3.78
3BTS1 (*pcet*)	-11.91	-3.12	-3.81
3BCP1	-51.05	-43.97	-44.27
$CH_3CH{=}CH\text{-}SOH + OH \rightarrow CH_3CH{=}CH\text{-}S(OH)_2$			
$CH_3CH{=}CH\text{-}SOH + OH$	0.00	0.00	0.00
3BCR2	-10.89	-2.13	-1.95
3BTS2	-5.22	3.79	2.53
3BCP2	-15.44	-6.21	-6.87
$CH_3CH{=}CH\text{-}SOH + OH \rightarrow CH_3CH(OH)CH\text{-}SOH$			
$CH_3CH{=}CH\text{-}SOH + OH$	0.00	0.00	0.00
3BCR3	-4.39	3.22	3.25
3BTS3	-2.83	5.59	4.88
3BCP3	-33.70	-25.05	-25.22

a) Energies at DLPNO-CCSD(T)/aug-cc-pVTZ level with ZPE and free energy corrections at M06-2X/6-311+G(2df,2p) level.

In summary, our results indicate that only the abstraction of the acidic hydrogen by the radical will occur for both, the reactions of **2** and **3** with HO_2 and OH. For the reactions with HO_2, this is the reaction path with the lowest free energy barrier and the remaining processes have much greater free energy barriers (by more than 5 kcal·mol^{-1}). The reactions of **2** and **3** with OH are diffusion controlled regarding the process involving the acidic hydrogen abstraction by the radical and therefore it is expected that this is the only reaction to occur. It is also worth pointing out that the lowest reaction paths *pcet* mechanism for the reaction of the sulfenic acids with both radicals.

Reaction of 4 with HO_2 and OH.

In the main text we have reported the results of the acidic hydrogen abstraction by HO_2 and OH radicals, involving a *pcet* mechanism, and pointing out the importance of side interactions that stabilize some of the conformers which results in a greater rate constant for the reaction with HO_2 compared with the reactions of **1**, **2**, and **3** with this radical. However, we have also considered additional processes, as the addition of the radical to the S atom of the sulfenic acid. In previous sections of this supplementary[28,29] information we have discussed these processes for reactions of **1**, **2**, and **3** with HO_2 and OH radicals, and in Figures S2 and S3 we have plotted the relative free energy barriers of the different reaction paths involving all conformers found, for the reactions of **4** with HO_2 and OH radicals.

The addition of the HO_2 radical to **4** will form the **4**-S(OH)(OOH) adduct, and Figure S1 shows that our results follow the same trends as discussed above for the addition of the HO_2 radical to the S atom in compounds **1**, **2**, and **3**. They have a much higher free energy barrier than the abstraction of the acidic hydrogen and therefore we can conclude that the reaction is not feasible.

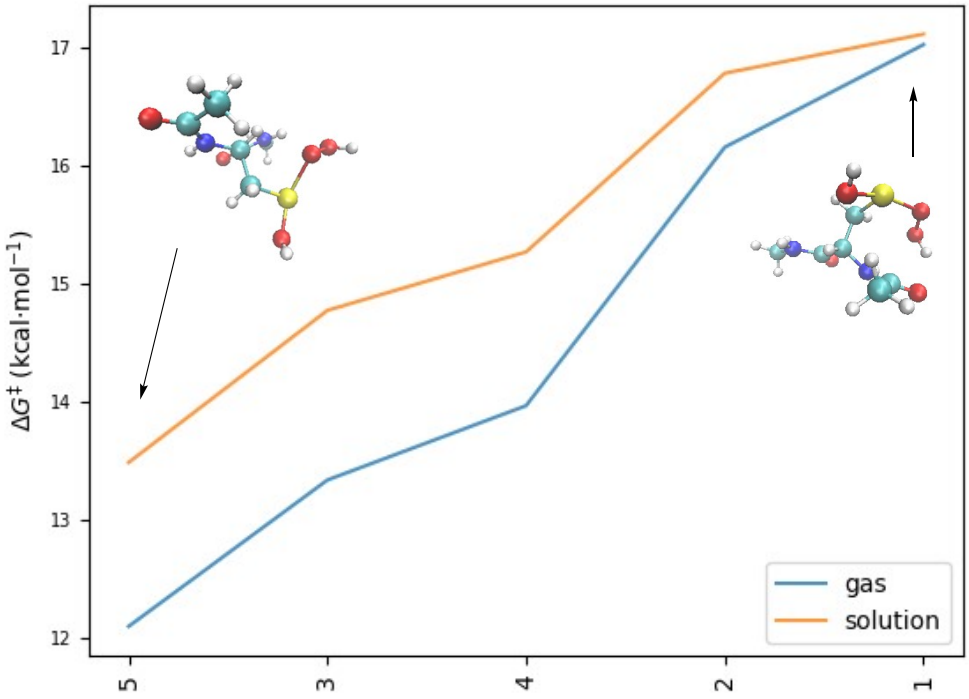


Figure S1. Free energy barriers at 298K of the different conformers of the transition states relative to their reactants for the addition of HO_2 radical to compound **4**. The free energies are computed at DLPNO-CCSD(T)/aug-cc-pVTZ level of theory, with free energy corrections obtained at M06-2X level. The values are corrected by -3.8 kcal·mol^{-1}.

The addition of OH to the sulfenic acid produces the adduct **4**-S(OH)$_2$, and the results displayed in Figure S2 indicate that the free energy barrier of most of the conformers lies below the free energy of the reactants, so that these processes would be diffusion controlled. According to our findings regarding the same process in the addition of the hydroxyl radical to compounds **1** and **2**, we would expect an easy hydrolysis of **4**-S(OH)$_2$ producing the corresponding sulfoxide radical (**4**-SO) and H_2O.

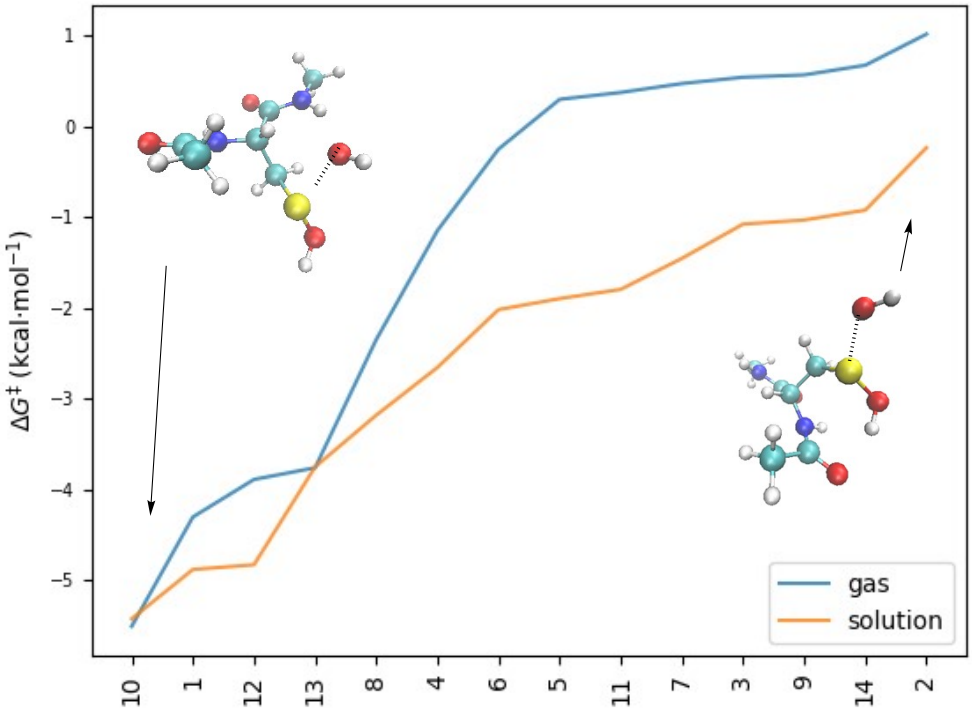


Figure S2. Free energy barriers at 298K of the different conformers of the transition states relative to their reactants for the addition of OH radical to compound **4**. The free energies are computed at DLPNO-CCSD(T)/aug-cc-pVTZ level of theory, with free energy corrections obtained at M06-2X level. The and values are corrected by -3.8 kcal·mol^{-1}.

In Table S9 we have reported the Cartesian coordinates of the transition state having the smaller free energy barrier.

Water as a co-reactant in the hydrogen abstraction by HO_2 and OH radicals

In the main text we have wondered if the inclusion of one explicit solvent water molecule could have any impact on the free energy barrier of the acidic hydrogen abstraction by the HO_2 radical. This has been done for the reaction of **2**+HO_2 using a similar quantum level as the one used in reference [30]. The authors used a discrete-continuum solvation model in which one explicit water molecule was included in the calculations, and the PCM model was used to account for the interactions with the dielectric continuum and they reported an increase of the free energy barrier of bout 1.5 kcal·mol^{-1}, with respect to the free energy barrier calculated with a pure PCM approach. In this work we have carried out a similar study for a reaction path for the reaction of **4** + HO_2, and our results are collected in Figure S3, which shows the structure of the reactants and transition state

optimized using a pure PCM method (**4**, and **4ATS1**) and those considering one explicit water molecule (**4**···$\mathbf{H_2O}$, and **4ATS1**···$\mathbf{H_2O}$), and our calculations also predict an increase of the free energy barrier of 1.5 kcal·mol^{-1} compared with the free energy barrier of the model considering a pure PCM approach, that is, the same results obtained for **2**+ HO_2.[30]

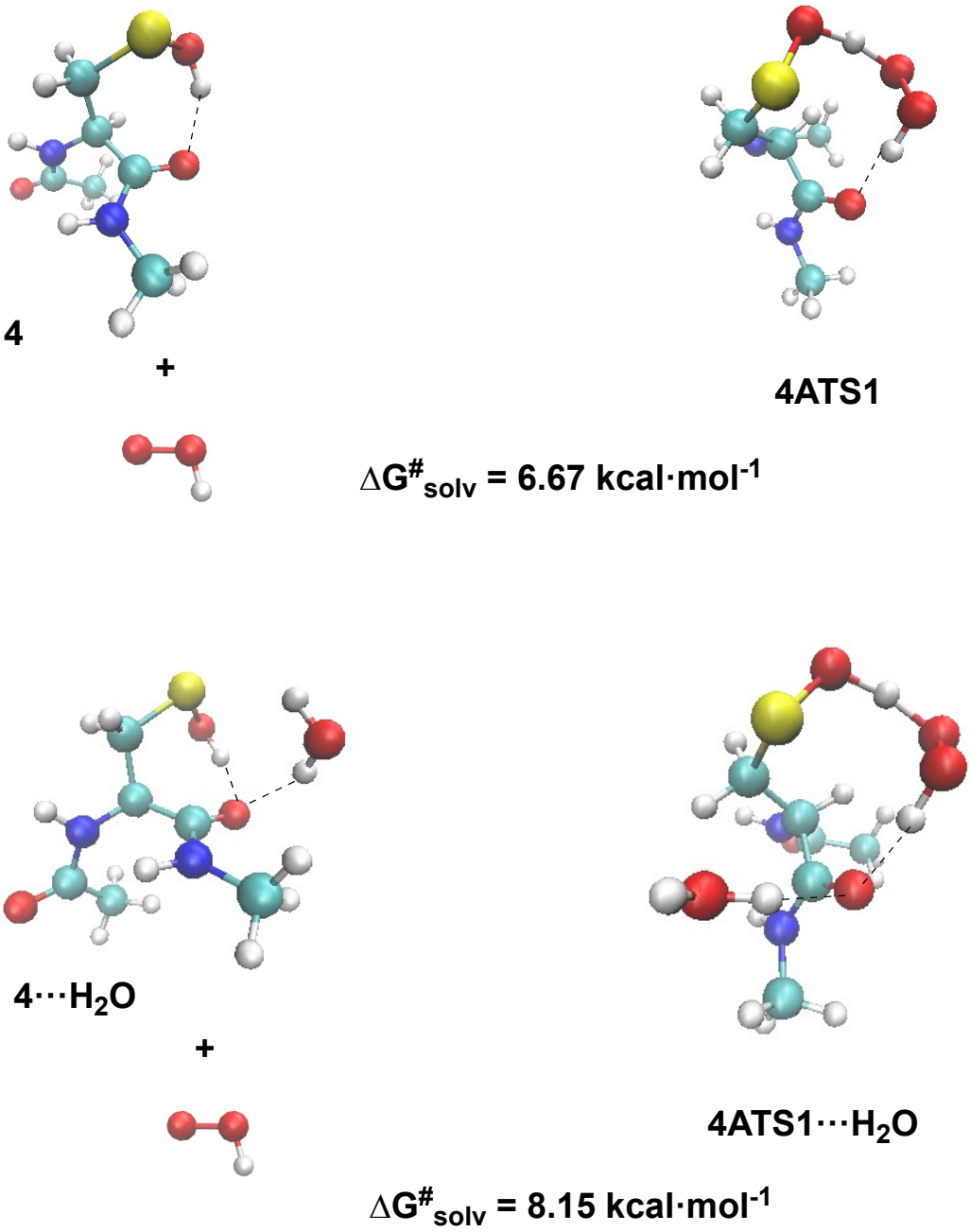


Figure S3. Structure of the reactants and transition state without and with and explicit solvation water molecule for the reaction of **4** + HO_2, and their effect on the free energy barrier.

Beyond the effect of an explicit water molecule on the energetics of the reaction, we have also considered whether a water molecule can actively assist the processes by participating as a proton relay. We have considered this possibility for the acidic hydrogen abstraction in all reactions investigated, namely for the reactions of **1**, **2**, **3**, and **4** with HO_2 and OH. In Figure S4 we have plotted the more relevant electronic features for the reaction of **4** with HO_2 (Figure S4a) and OH (Figure S4b) assisted by a water molecule, whereas Tables S7, S8, and Figures S5 and S6 we have collected the corresponding energetics. Figure S4 shows that, in both cases, the reaction follow a *pcet* mechanism, but here, there is a double proton transfer. This is a system of three electrons in two orbitals where one electron is transferred from the S atom to the terminal O atom of OH or HO_2, whereas the acidic proton of the sulfenic acid is transferred to the water molecule and simultaneously, one proton from water is transferred to the OH or HO_2 moiety.

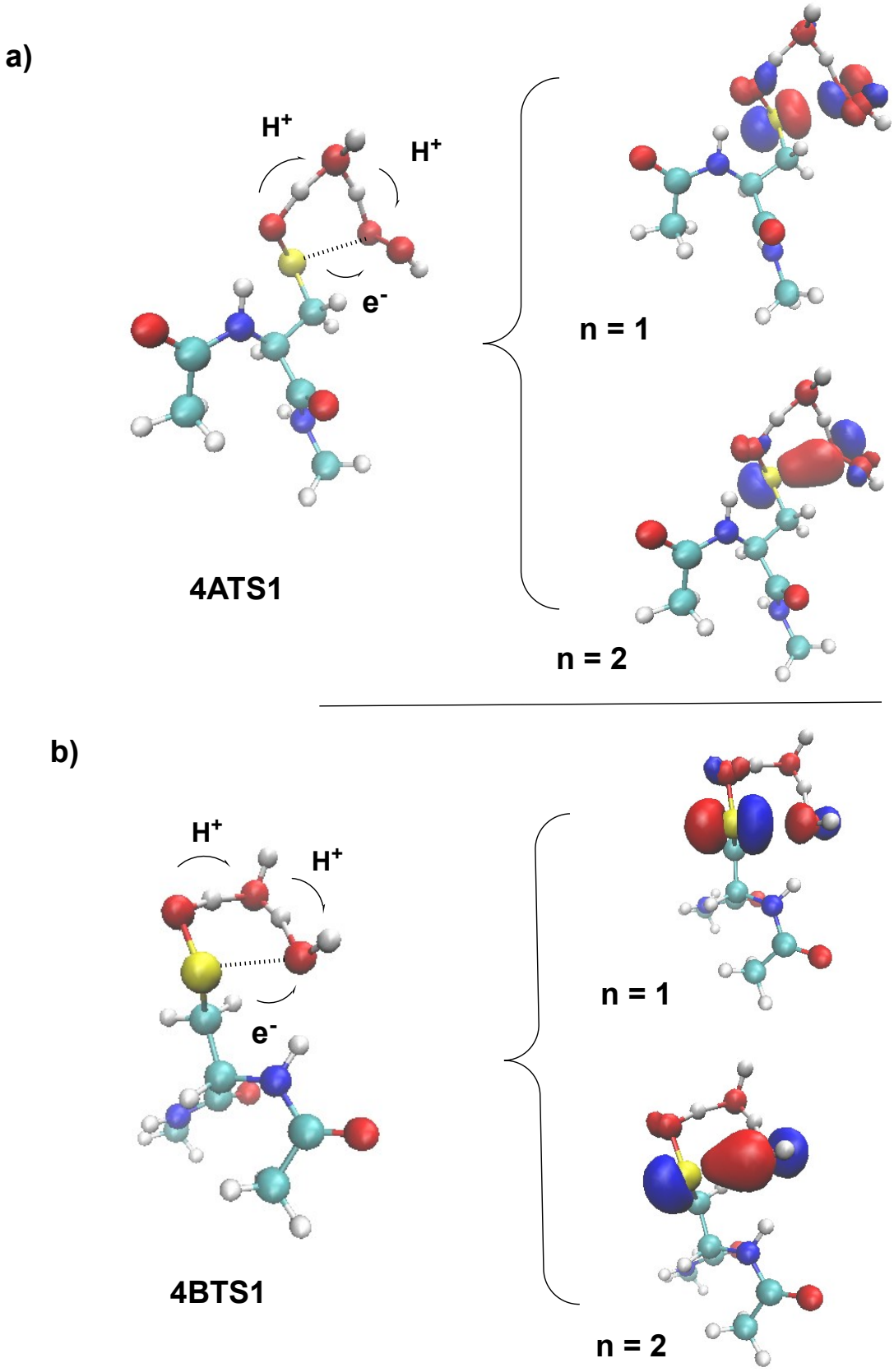


Figure S4. Electronic features of the the reaction of **4** with HO_2 and OH assisted by a water molecule. n stands for the occupation number.

For the reaction of **1, 2**, **3** and **4** with HO_2 assisted by a water molecule, the results displayed in Table S7 and in Figure S5 show that the free energy barrier is about 4 kcal·mol^{-1} greater than the corresponding results of the naked reaction (see Table 2 and Figure 3 of the main text), these results implying that the contribution of these process should be minor.

For the reaction of **1**, **2**, **3** and **4** with OH assisted by a water molecule, the results displayed in Table S8 and in Figure S6 show that the free energy barrier still lies below the free energy of the reactants and, consequently, the reaction is diffusion controlled and therefore contributing to the whole process.

Table S7. Relative energies (Δ (E+ZPE) in kcal·mol^{-1}) and free energies in gas and solvation phases (ΔGgas and ΔGsolv, in kcal·mol^{-1}) for the $CH_3SOH\cdots H_2O + HO_2$, $CH_2{=}CHCH_2SOH\cdots H_2O + HO_2$, and $CH_3CH{=}CHSOH\cdots H_2O + HO_2$ reactions, computed at different levels of theory.[a]

	DLPNO-CCSD(T)/auv-cc-pVTZ			**CCSD(T)/aug-cc-pV(T+d)Z**		
	Δ (E+ZPE)	**ΔGgas**	**ΔGsolv**	**Δ (E+ZPE)**	**ΔGgas**	**ΔGsolv**
$CH_3SOH\cdot\cdot H_2O + OH \rightarrow CH_3SO + H_2O\cdot + H_2O_2$						
$CH_3SOH\cdot\cdot H_2O + HO_2$	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00
1ACR7	-1.52	7.80	6.13	-2.93	6.38	4.71
1ATS7 (*pcet*)	6.13	17.92	18.63	2.17	13.95	14.66
1ACP7	-20.59	-11.24	-10.41	-23.91	-14.56	-13.73
$CH_2{=}CHCH_2SOH\cdots H_2O + HO_2. \rightarrow CH_2{=}CHCH_2SO + H_2O\cdot + H_2O_2$						
$CH_2{=}CHCH_2SOH\cdot H_2O$	0.00	0.00	0.00	0.00	0.00	0.00
2ACR4	-2.24	8.64	8.31	-3.63	7.25	6.92
2ATS4 (*pcet*)	5.70	18.22	20.25	1.34	13.86	15.89
2ACP4	-22.19	-12.15	-10.09	-25.05	-15.01	-12.95
$CH_3CH{=}CHSOH\cdots H_2O + HO_2 \rightarrow CH_3CH{=}CHSO + H_2O\cdot + H_2O_2$						
$CH_3CH{=}CHSOH\cdot\cdot H_2O$	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00
3ACR3	-2.60	5.99	5.32	-3.52	5.07	4.40
3ATS3 (*pcet*)	6.66	17.95	18.82	2.60	13.89	14.76
3ACP3	-23.24	-14.48	-13.74	-25.80	-17.05	-16.30

a) The ZPE and free energy corrections have been calculated at M06-2X/6-311+G(2df,2p) level of theory

Table S8. Relative energies (Δ (E+ZPE) in kcal·mol^{-1}) and free energies in gas and solvation phases (ΔGgas and ΔGsolv, in kcal·mol^{-1}) for the $CH_3SOH\cdots H_2O$ + OH , and $CH_3CH{=}CHSOH\cdots H_2O$ + OH reactions, computed at different levels of theory.[a]

	DLPNO-CCSD(T)/auv-cc-pVTZ			**CCSD(T)/aug-cc-pV(T+d)Z**			**CCSD(T)/CBS**		
	Δ (E+ZPE)	**ΔGgas**	**ΔGsolv**	**Δ (E+ZPE)**	**ΔGgas**	**ΔGsolv**	**Δ (E+ZPE)**	**ΔGgas**	**ΔGsolv**
	$CH_3SOH\cdots H_2O + OH \rightarrow CH_3SO + 2H_2O$								
Reactants	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1BCR6	-16.44	-6.97	-6.23	-19.21	-9.74	-9.00	-19.79	-10.32	-9.59
1BTS6 (*pcet*)	-16.46	-6.60	-6.13	-19.52	-9.67	-9.20	-20.00	-10.15	-9.68
1BCP6	-49.13	-42.62	-40.15	-51.84	-45.33	-42.85	-53.10	-46.59	-44.11
	$CH_3CHCH\text{-}SOH\cdots H_2O + OH \rightarrow CH_3CHCH\text{-}SO + 2H_2O$								
Reactants	0.00	0.00	0.00						
3BCR4	-15.16	-5.54	-4.47						
3BTS4(*pcet*)	-14.54	-4.03	-3.38						
3BCP4	-51.37	-44.38	-43.68						

a) The ZPE and free energy corrections have been calculated at M06-2X/6-311+G(2df,2p) level of theory

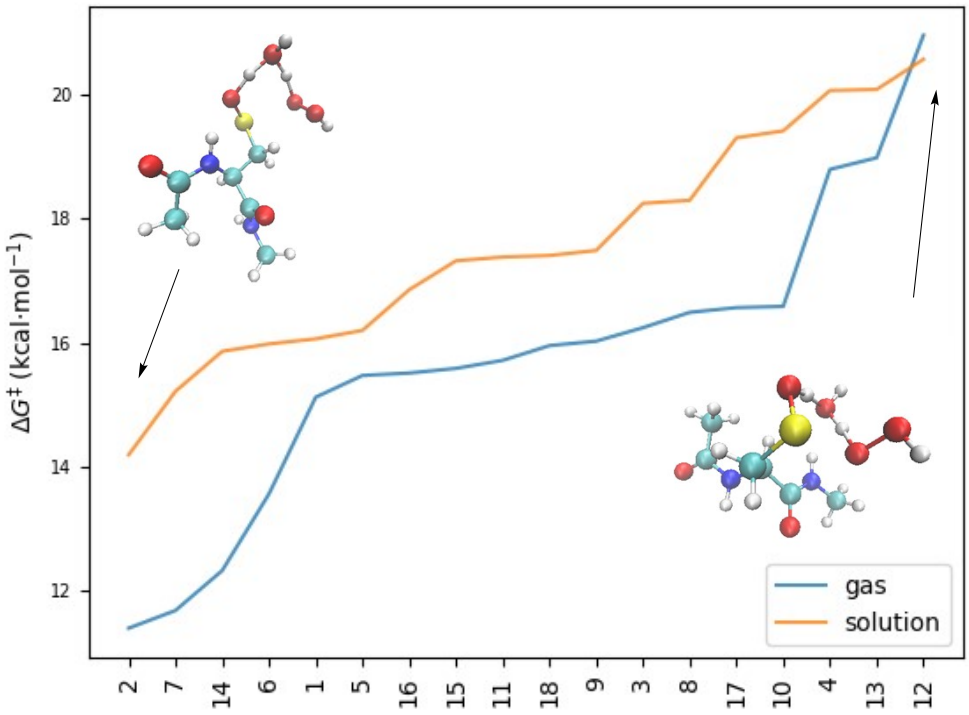


Figure S5. Free energy barriers at 298K of the different conformers of the transition states relative to their reactants for the abstraction in compound **4** of the acidic hydrogen by the HO_2 radical assisted by a H_2O molecule. The free energies are computed at DLPNO-CCSD(T)/aug-cc-pVTZ level of theory, with free energy corrections obtained at M06-2X level. The and values are corrected by -3.8 kcal·mol^{-1}[11].

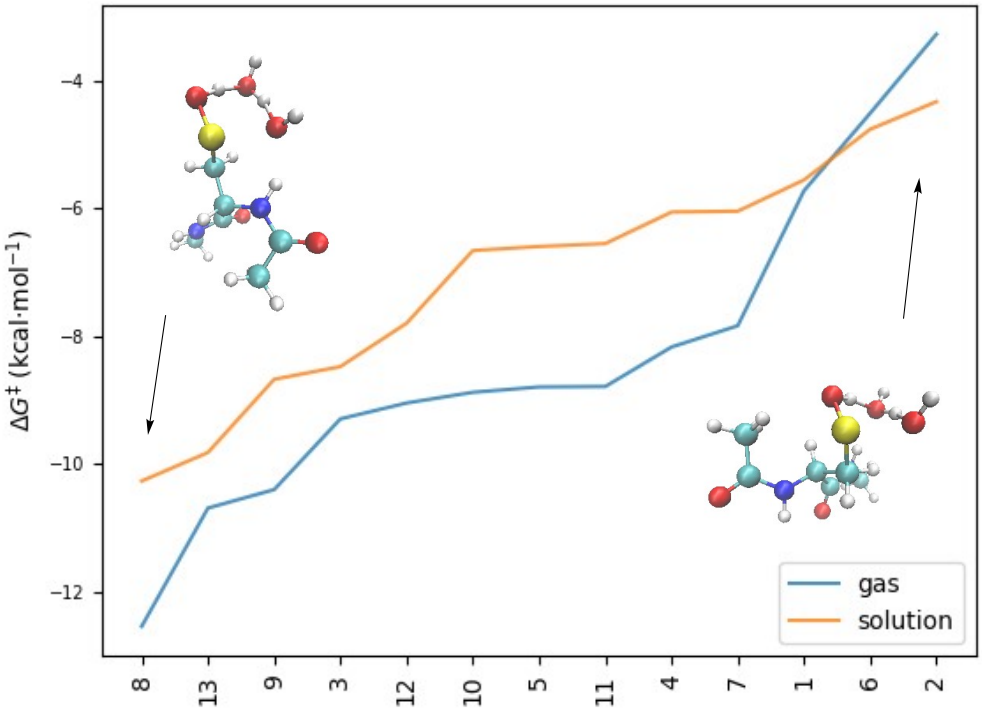


Figure S6. Free energy barriers at 298K of the different conformers of the transition states relative to their reactants for the abstraction in compound **4** of the acidic hydrogen by the OH radical assisted by a H_2O molecule. The free energies are computed at DLPNO-CCSD(T)/aug-cc-pVTZ level of theory, with free energy corrections obtained at M06-2X level. The and values are corrected by -3.8 kcal·mol^{-1}.

Cartesian coordinates

Table S9. Cartesian coordinates of the stationary points.

1ACR1

S	-1.097154	-0.380500	-0.251546
C	-1.184763	-0.254946	1.538579
H	-0.229267	0.061135	1.952293
H	-1.431954	-1.250252	1.907167
H	-1.971773	0.441206	1.816779
O	-0.783966	1.185649	-0.652127
H	0.168817	1.322395	-0.542879
O	1.974733	0.522011	-0.060436
O	1.977591	-0.776094	-0.162090
H	1.022485	-1.017545	-0.288050

1ATS1

S	0.089320	-0.005089	-0.046302
C	0.058837	-0.010626	1.746740
H	1.075053	0.067984	2.126441
H	-0.379704	-0.958358	2.056128
H	-0.552516	0.814992	2.102878

O	0.724210	1.423884	-0.354422
H	1.767284	1.371402	-0.266055
O	3.089308	0.923192	-0.113842
O	2.880866	-0.359714	0.219153
H	2.936342	-0.853682	-0.613322

1ACP1

S	-1.415109	-0.264888	-0.238447
C	-0.903873	-0.358942	1.480080
H	0.155426	-0.604354	1.521189
H	-1.498348	-1.137495	1.954948
H	-1.093025	0.603460	1.951507
O	-0.659111	0.887558	-0.831297
H	1.121739	0.961943	-0.241538
O	1.940504	0.597032	0.137509
O	1.778895	-0.785750	-0.142666
H	2.357989	-0.908973	-0.901983

1ACR2

C	-1.248945	0.419013	-1.291871
S	-1.016321	0.679259	0.468110
H	-0.340367	0.037348	-1.754206
H	-2.077936	-0.263805	-1.462905
H	-1.490103	1.393725	-1.716197
O	-0.783594	-0.880318	0.964573
H	0.161610	-1.062884	0.881388
O	1.957981	-0.307024	0.302040
O	2.101288	-0.382745	-0.994688
H	2.858009	0.188289	-1.210123

1ATS2

C	0.000000	0.000000	0.000000
S	0.000000	0.000000	1.792307
H	1.026324	0.000000	-0.364250
H	-0.531415	-0.876906	-0.364101
H	-0.510191	0.906939	-0.320713
O	0.721367	-1.375075	2.119829
H	1.763638	-1.182276	1.947563
O	2.940637	-0.642893	1.621930
O	3.204398	-1.103091	0.375510
H	4.109597	-1.437195	0.432975

1ACR4

S	0.226484	-0.813001	0.810900
O	-0.315771	0.221942	1.987272
C	1.583918	0.146045	0.133092
H	2.374258	0.268157	0.869394
H	1.950845	-0.426728	-0.717349
H	1.223902	1.112228	-0.212437
O	-0.117528	-0.966092	-2.336982

O	-1.190889	-0.358635	-1.917836
H	0.108184	-0.010110	2.818708
H	-1.110869	-0.376498	-0.932344

1ATS4

S	0.002974	-0.000081	0.008733
O	0.008212	0.004724	1.691919
C	1.787260	0.001336	-0.205207
H	2.198792	-0.977978	0.034053
H	2.002990	0.247367	-1.239522
H	2.194368	0.757132	0.459901
O	-0.010421	-0.949411	-1.829311
O	-1.286530	-0.916136	-2.324856
H	0.278252	-0.856852	2.026000
H	-1.539460	-1.846155	-2.364884

CH3S(OH)(OOH)

S	-0.100677	0.266865	0.350946
O	-0.118278	0.279630	2.069986
C	1.694383	0.303154	0.238812
H	2.103880	-0.667994	0.514071
H	1.973059	0.542194	-0.781487
H	2.043685	1.069004	0.923897
O	-0.035632	-0.542020	-1.318700
O	-1.340582	-0.535758	-1.824833
H	0.467963	-0.388836	2.441246
H	-1.556442	-1.473879	-1.860981

1ACR6

S	-0.163121	0.777027	0.452434
O	-0.119926	0.536871	2.090191
C	1.550610	0.466671	0.021194
H	1.816751	-0.576975	0.173265
H	1.633522	0.702674	-1.038446
H	2.193089	1.121760	0.603847
O	-0.142572	-0.967819	-2.264205
O	-0.930014	-1.598617	-1.438604
H	-0.242887	-0.397263	2.282062
H	-0.968663	-1.010507	-0.645292

1ATS6

S	-0.018871	-0.187120	0.153907
O	0.010695	0.108774	1.809721
C	1.752882	-0.058311	-0.115880
H	2.260347	-0.942749	0.265983
H	1.925384	0.031340	-1.183157
H	2.097691	0.831883	0.401797
O	0.035868	-1.454276	-1.483630
O	-1.245235	-1.639187	-1.931215
H	0.368468	-0.653300	2.276617

H	-1.405463	-2.578479	-1.781802

1ACR3

C	-1.178165	-0.395086	-1.375279
S	-1.232500	-0.127987	0.398451
H	-0.207243	-0.118393	-1.782762
H	-1.947626	0.246454	-1.804995
H	-1.404755	-1.433791	-1.604751
O	1.688824	0.970806	0.443908
O	1.933122	1.069709	-0.836231
H	2.175774	1.998771	-0.987614
O	-0.102597	-1.229796	0.891202
H	0.752284	-0.779734	0.874119

1ATS3

C	-0.337766	-0.084762	-0.042123
S	-0.439138	-0.161104	1.744438
H	0.491292	0.559103	-0.333159
H	-1.278242	0.331251	-0.400291
H	-0.196823	-1.087358	-0.440711
O	2.213321	1.146539	1.760961
O	2.772571	1.025066	0.530831
H	3.648017	1.422325	0.630316
O	0.942590	-0.838753	2.125359
H	1.655907	-0.039505	2.014714

1ACR5

C	0.698516	0.689758	-1.853398
S	0.963358	0.803570	-0.081325
H	1.575591	0.265029	-2.335941
H	-0.186098	0.096895	-2.078603
H	0.547919	1.708933	-2.209189
O	1.279785	-0.783014	0.264545
H	0.427416	-1.221244	0.386923
O	-1.592290	-1.029081	0.216014
O	-2.013512	-0.812915	1.430987
H	-2.899539	-0.422849	1.341134

1ATS5

C	0.357706	0.083334	-0.271381
S	0.509046	0.314160	1.500594
H	1.085263	-0.649247	-0.613147
H	-0.652215	-0.242383	-0.512910
H	0.553684	1.047955	-0.737311
O	0.231799	-1.151776	2.041451
H	-0.829380	-1.229661	2.242202
O	-2.130643	-1.139021	2.270619
O	-2.606766	-1.795641	3.348933
H	-3.118736	-2.526359	2.976229

CH3SOH··H2O

C	-0.126494	-0.061637	0.080709
S	-0.383027	-0.363285	1.833799
H	0.856999	0.372586	-0.081510
H	-0.893426	0.648123	-0.228813
H	-0.235107	-0.983968	-0.486443
O	0.850070	-1.418689	2.130490
H	0.535441	-2.301794	1.882149
O	-0.955247	-3.350660	1.167057
H	-1.350071	-4.135559	1.550503
H	-1.530587	-2.611922	1.400274

1ACR7

C	-1.035996	-0.189630	-1.544602
S	-1.388993	0.324688	0.137328
H	-0.051820	-0.652009	-1.614541
H	-1.059525	0.713694	-2.155932
H	-1.801949	-0.877841	-1.894573
O	-1.413375	-1.134650	0.892616
H	-0.502814	-1.315822	1.189122
O	1.282324	-1.066262	1.467996
H	1.975578	-1.621208	1.108095
H	1.423461	-0.182835	1.098588
O	1.491449	1.375698	-0.060750
O	1.989767	0.818279	-1.142620
H	1.861272	1.466178	-1.854666

1ATS7

C	0.174946	-0.089307	0.009993
S	0.031835	0.230737	1.756069
H	1.208292	-0.349937	-0.216038
H	-0.109739	0.823251	-0.511196
H	-0.503250	-0.900106	-0.247508
O	0.326339	-1.165193	2.398238
H	1.388272	-1.181170	2.852490
O	2.547762	-0.934506	3.247643
H	3.187476	-1.577407	2.933688
H	2.624059	-0.034749	2.634606
O	2.408049	0.962797	1.765158
O	3.092908	0.431331	0.653951
H	3.322157	1.224385	0.158761

1ACP7

C	-1.279041	0.035866	-1.687117
S	-1.745480	0.046965	0.042002
H	-0.194194	0.095230	-1.753934
H	-1.737695	0.906031	-2.153790
H	-1.650678	-0.879816	-2.142875
O	-1.126370	-1.183301	0.635744
H	0.560885	-1.204386	1.517810

O	1.454074	-0.891030	1.724283
H	2.042041	-1.476090	1.241599
H	1.378584	0.574839	0.715433
O	1.291054	1.163631	-0.063549
O	1.947781	0.376346	-1.050317
H	2.738873	0.896686	-1.224441

1BCR1

C	0.295348	0.549147	-1.504805
S	0.238797	0.557144	0.276658
H	1.326981	0.443322	-1.831412
H	-0.331260	-0.263802	-1.861761
H	-0.105949	1.505438	-1.837086
O	0.916412	-0.866097	0.642740
H	0.156320	-1.479128	0.635405
O	-1.536776	-0.658407	0.189594
H	-2.124242	-0.289046	0.857544

1BTS1

C	0.024639	0.032939	-0.014363
S	0.022978	0.055193	1.770895
H	1.038965	-0.151239	-0.361792
H	-0.656036	-0.749871	-0.339320
H	-0.320999	1.007339	-0.354774
O	0.482432	-1.412358	2.152590
H	-0.522849	-1.801402	2.091031
O	-1.803700	-1.328362	1.738557
H	-2.406861	-1.172515	2.471544

1BCP1

C	0.191853	0.648847	-1.391668
S	1.248485	0.722106	0.058792
H	0.155219	-0.374979	-1.758167
H	-0.813099	0.964788	-1.119797
H	0.622365	1.315450	-2.136911
O	0.632419	-0.199223	1.070478
H	-1.014921	-1.054074	0.498147
O	-1.743804	-1.255597	-0.103632
H	-2.310698	-1.869482	0.364240

1BTS5

C	0.003511	-0.163566	-0.183190
S	0.430992	-1.077585	1.293893
H	-1.065498	0.039202	-0.174322
H	0.563991	0.767657	-0.196990
H	0.262232	-0.779472	-1.042581
O	0.118336	-0.039922	2.448461
H	1.100253	0.387480	2.429019
O	2.339748	0.091304	1.808406

H	2.748933	0.604921	1.105954

1BTS2

S	0.020182	0.178175	-0.040716
O	0.052201	-0.081343	1.586525
C	1.762079	0.048300	-0.394573
H	2.080976	-0.981854	-0.254595
H	1.881951	0.318441	-1.440839
H	2.303803	0.738030	0.246862
O	-0.101728	-1.528892	-1.330791
H	-1.055866	-1.612027	-1.447088
H	0.107161	-1.032524	1.740767

CH3S(OH)2

S	-0.373806	0.120271	-0.011626
O	-0.229645	0.403240	1.713551
C	1.395605	0.255791	-0.277975
H	1.878804	-0.668838	0.035119
H	1.565193	0.408775	-1.338015
H	1.755341	1.097228	0.304277
O	-0.416757	-0.915469	-1.456166
H	-1.341300	-1.143483	-1.597356
H	0.480350	-0.116260	2.106277

1BTS3

C	-0.270216	0.526152	-0.267761
S	-0.958427	0.776333	1.334778
H	0.791513	0.149946	-0.092929
H	-0.808145	-0.234492	-0.829290
H	-0.227670	1.472259	-0.803622
O	-0.840638	-0.768424	1.886504
H	0.106863	-0.984814	1.896730
O	1.821084	-0.757802	0.736864
H	1.928900	-1.492633	0.113578

CH2SOH··H2O

C	-0.410242	0.622125	-1.348987
S	-0.682277	0.714441	0.310104
H	1.755145	-0.346867	-0.823372
H	-0.752439	-0.245519	-1.897073
H	-0.272963	1.566087	-1.856463
O	-0.545687	-0.844788	0.790401
H	0.388393	-1.101692	0.678286
O	2.072827	-0.932505	-0.124398
H	2.538152	-1.648071	-0.561592

1BTS4

C	0.001980	-0.042272	-0.022454
S	0.352884	-0.196137	1.644379
H	0.890511	-0.013781	-0.654252

H	-0.732634	-0.775362	-0.335575
H	-0.287384	1.421931	0.011637
O	1.028991	1.157771	2.022323
H	0.538381	2.011440	1.268324
O	-0.122759	2.494004	0.425314
H	0.416323	2.990550	-0.196556

1BCR6

C	0.087179	0.970256	-1.468848
S	0.204229	1.031230	0.308734
H	1.038254	1.271218	-1.901407
H	-0.188488	-0.039208	-1.765066
H	-0.703599	1.662344	-1.751037
O	1.272293	-0.110291	0.630946
H	0.895095	-1.017137	0.365107
O	-0.021843	-2.157328	-0.142716
H	-0.106433	-2.973167	0.351708
H	-0.828893	-1.570720	0.050159
O	-1.637691	-0.274854	0.246423
H	-2.021145	-0.129318	1.117019

1BTS6

C	0.003355	-0.049371	0.071233
S	0.166237	-0.042149	1.847911
H	0.943247	0.270728	-0.372818
H	-0.268462	-1.052824	-0.247212
H	-0.799201	0.643003	-0.173829
O	1.187761	-1.206841	2.126769
H	0.740201	-2.158787	1.849764
O	-0.101364	-3.146587	1.453665
H	-0.142759	-3.914976	2.024563
H	-0.959268	-2.499820	1.620355
O	-1.729120	-1.390944	1.742362
H	-2.134963	-1.298571	2.608891

1BCP6

C	0.068718	0.915101	-1.409615
S	0.576954	1.221094	0.284384
H	0.913479	1.085600	-2.074518
H	-0.286728	-0.109449	-1.486279
H	-0.742803	1.604700	-1.632968
O	1.401006	0.032587	0.691467
H	0.697657	-1.618218	0.174444
O	0.026439	-2.227264	-0.172644
H	0.299220	-3.112417	0.070880
H	-1.553982	-1.234990	0.156720
O	-2.130639	-0.458088	0.202265
H	-2.633161	-0.552930	1.011956

2

S	-0.621460	-0.157997	-0.710161
C	-0.774464	-0.400563	1.064189
H	0.213835	-0.605953	1.482382
H	-1.339749	-1.334610	1.146428
C	-1.451035	0.692619	1.841261
O	0.386143	1.162065	-0.758455
H	1.293828	0.848346	-0.802449
C	-1.913469	1.830147	1.351644
H	-1.534296	0.496718	2.906391
H	-2.384718	2.557973	1.997249
H	-1.831121	2.070088	0.299846

2ACR1

S	-0.644288	-0.140671	-0.724365
C	-0.769617	-0.395446	1.054711
H	0.232770	-0.582837	1.448306
H	-1.322126	-1.335835	1.148451
C	-1.445347	0.694633	1.835485
O	0.375132	1.150019	-0.800940
H	1.275719	0.809663	-0.693031
O	2.488123	-0.805246	-0.455983
O	1.910962	-1.906052	-0.844564
H	0.960516	-1.654265	-0.979215
C	-1.915230	1.830554	1.349911
H	-1.518374	0.496502	2.900512
H	-2.383307	2.555806	2.000457
H	-1.841836	2.076446	0.298828

2ATS1 (pcet)

S	0.210844	0.446864	-0.130647
C	0.025325	0.152754	1.633618
H	1.002755	-0.151780	2.014251
H	-0.624455	-0.725162	1.694343
C	-0.538379	1.287040	2.440593
O	1.351752	1.554477	-0.181974
H	2.298543	1.092961	-0.087049
O	3.327977	0.176560	-0.004176
O	2.637969	-0.968603	0.133902
H	2.561122	-1.331124	-0.761871
C	-0.830992	2.499859	2.003134
H	-0.691094	1.048285	3.488760
H	-1.228417	3.245087	2.677806
H	-0.675333	2.793621	0.973552

2ACP1

S	-1.349440	-0.357943	-0.955331
C	-1.066248	-0.690785	0.796008
H	-0.156694	-1.291352	0.862916
H	-1.907654	-1.324681	1.090204

C	-0.970528	0.521293	1.677905
O	-0.202458	0.491007	-1.421864
H	1.317712	0.392088	-0.310004
O	1.985428	-0.060266	0.235096
O	1.845910	-1.400315	-0.213955
H	2.588210	-1.493000	-0.820243
C	-1.158810	1.782512	1.326459
H	-0.706440	0.290732	2.704877
H	-1.062679	2.572277	2.058035
H	-1.394695	2.077566	0.312791

2ACR1a

S	-0.598604	0.349446	-0.830246
C	-0.877209	0.318758	0.967035
H	0.050763	0.640691	1.439963
C	-1.227472	-1.087669	1.335212
H	-1.676427	1.014283	1.214029
O	0.162843	1.796857	-1.021581
H	1.095779	1.659033	-0.801262
O	2.518613	0.318103	-0.139523
O	2.182100	-0.918069	-0.373652
H	1.235213	-0.863542	-0.670699
C	-2.467538	-1.500132	1.550313
H	-0.404182	-1.792338	1.390949
H	-2.685763	-2.530334	1.795010
H	-3.304228	-0.814251	1.494483

2ATS1a (pcet)

S	0.112462	0.204507	-0.233663
C	-0.143108	0.060561	1.558903
H	0.825549	0.282165	2.007246
C	-0.587643	-1.333441	1.857713
H	-0.875888	0.799842	1.878123
O	1.113592	1.440324	-0.338436
H	2.087890	1.114226	-0.137788
O	3.216556	0.319551	0.149432
O	2.639076	-0.867313	0.390119
H	2.658164	-1.339111	-0.456924
C	-1.828294	-1.653998	2.192805
H	0.169734	-2.103507	1.758448
H	-2.112760	-2.678203	2.389810
H	-2.597579	-0.897499	2.290415

2ACP1a

S	-0.813531	0.628145	-0.887702
C	-0.713630	0.256128	0.896037
H	0.327315	0.426581	1.168732
C	-1.142529	-1.156646	1.115109
H	-1.358301	0.964323	1.417000
O	0.334188	1.539987	-1.206414

H	1.940680	0.941937	-0.429621
O	2.503896	0.312588	0.055681
O	1.850122	-0.917094	-0.221956
H	2.419324	-1.301690	-0.897169
C	-2.314365	-1.497111	1.630966
H	-0.434806	-1.913080	0.795989
H	-2.593462	-2.533438	1.759516
H	-3.028200	-0.748525	1.953639

2ACR2

C	-1.060222	-0.191235	-0.657055
S	-0.521628	0.104174	1.052442
H	-0.249971	-0.722869	-1.155703
H	-1.957930	-0.806803	-0.661065
C	-1.303420	1.141563	-1.286625
O	0.116323	-1.373798	1.431227
H	1.057143	-1.339502	1.212824
O	2.644407	-0.426626	0.378712
O	2.361831	-0.413500	-0.894696
H	3.026521	0.163130	-1.309003
C	-2.508568	1.643516	-1.511596
H	-0.421032	1.725991	-1.525657
H	-2.640900	2.622949	-1.950287
H	-3.402861	1.084548	-1.263996

2ATS2 (hat)

C	-0.175319	-0.099739	0.244538
S	0.138045	-0.058833	2.031174
H	0.782727	-0.322348	-0.227625
H	-0.882287	-0.901882	0.035336
C	-0.706428	1.235288	-0.167301
O	0.974243	-1.387544	2.261145
H	1.966182	-1.149974	1.923287
O	3.053293	-0.559566	1.426870
O	3.224295	-1.075294	0.186729
H	4.146694	-1.364433	0.174816
C	-1.982018	1.463537	-0.440228
H	0.012261	2.046227	-0.207731
H	-2.331980	2.446850	-0.721448
H	-2.716947	0.668752	-0.395615

2ACP2

C	-0.336828	0.843991	-0.360182
S	-0.669771	-0.291020	1.025629
H	0.413155	1.544123	0.008460
H	0.087781	0.249882	-1.168745
C	-1.618308	1.508136	-0.744913
O	0.653525	-0.582215	1.668715
H	2.026195	-0.725354	0.412649
O	2.406135	-0.874115	-0.471270

O	1.403051	-1.681041	-1.070160
H	1.785885	-2.562601	-1.008639
C	-2.327052	1.163485	-1.809524
H	-1.979975	2.288268	-0.083971
H	-3.260896	1.653460	-2.047070
H	-1.987346	0.385360	-2.482299

2ACR3

S	-0.579361	0.910449	0.545781
O	-0.185077	0.483585	2.090305
C	1.065734	0.815504	-0.216607
C	1.558649	-0.592152	-0.183610
H	0.921034	1.181313	-1.232563
H	1.717029	1.493524	0.333446
O	-0.956207	-0.457750	-2.320422
O	-1.607179	-1.230738	-1.497776
H	0.055766	-0.451285	2.102885
H	-1.497249	-0.793358	-0.617542
C	2.398319	-1.048854	0.737050
H	1.150096	-1.260749	-0.934111
H	2.709101	-2.084494	0.753450
H	2.817461	-0.390452	1.489056

2ATS3 (addition)

S	0.118476	-0.052376	0.029773
O	0.516875	-0.190714	1.646834
C	1.827624	0.011398	-0.586836
C	2.498435	-1.297247	-0.333376
H	1.755621	0.246114	-1.645069
H	2.315522	0.826828	-0.055985
O	-0.295905	-0.856913	-1.843283
O	-1.655626	-0.876109	-2.011422
H	1.094358	-0.955771	1.774286
H	-1.865454	-1.815702	-2.069137
C	3.387595	-1.488973	0.633180
H	2.179693	-2.122551	-0.960593
H	3.832643	-2.458928	0.807901
H	3.715002	-0.670220	1.263744

2ACP3

S	-0.638340	0.489025	0.257446
O	-0.256821	0.348318	1.906904
C	1.100766	0.571753	-0.276534
C	1.788511	-0.726117	-0.010543
H	1.079623	0.819109	-1.334074
H	1.547336	1.386946	0.289112
O	-0.957200	-0.202430	-1.472730
O	-2.342847	-0.240453	-1.647046
H	0.442123	-0.306647	2.041616
H	-2.525491	-1.184709	-1.700552

C	2.694123	-0.892882	0.944813
H	1.479215	-1.562330	-0.627848
H	3.157411	-1.853567	1.122650
H	3.017013	-0.063145	1.563457

2ACR3a

S	-0.442003	-0.431630	1.149502
O	-0.201211	1.117860	1.677474
C	1.155413	-0.768927	0.357336
H	1.069604	-1.816476	0.063826
C	1.406018	0.119485	-0.813455
H	1.935423	-0.675558	1.112767
O	-1.164903	-1.890892	-1.493996
O	-1.854341	-0.792066	-1.606148
H	0.139462	1.083866	2.576387
H	-1.651667	-0.292598	-0.778251
C	2.280366	1.113387	-0.800627
H	0.806943	-0.074726	-1.696687
H	2.424425	1.750821	-1.661643
H	2.882244	1.321496	0.075783

2ATS3a (addition)

S	0.103068	0.067202	-0.134337
O	0.282597	0.473312	1.486436
C	1.810263	-0.488339	-0.457545
H	1.794248	-1.578443	-0.498208
C	2.351127	0.087319	-1.727651
H	2.386934	-0.154423	0.401943
O	-0.324934	-1.280126	-1.655869
O	-1.520931	-0.939563	-2.226132
H	0.296342	-0.323193	2.026841
H	-2.087495	-1.697218	-2.036775
C	3.401052	0.892001	-1.773426
H	1.829707	-0.196083	-2.634040
H	3.768929	1.282046	-2.712350
H	3.928451	1.186959	-0.874295

2ACP3a

S	-0.609642	0.167309	0.556659
O	-0.458528	0.593768	2.211466
C	1.127462	-0.344191	0.326952
H	1.139608	-1.435108	0.325666
C	1.701115	0.204219	-0.941563
H	1.664245	0.036530	1.191346
O	-0.939119	-1.020452	-0.846155
O	-2.173663	-0.673436	-1.404631
H	-0.118696	-0.137643	2.738094
H	-2.716306	-1.445323	-1.209603
C	2.696204	1.076591	-0.966003
H	1.251770	-0.153536	-1.859547

H	3.092423	1.449799	-1.900144
H	3.146805	1.448323	-0.053597

2ACR3b

S	-0.206051	-1.278321	0.538305
O	-0.310395	-0.624026	2.054298
C	1.396511	-0.629327	-0.008740
H	2.170098	-1.022043	0.650913
H	1.513742	-1.077241	-0.997722
C	1.420937	0.860289	-0.068337
O	-0.733124	-0.173462	-2.372907
O	-1.647416	0.409915	-1.651775
H	0.055935	-1.252032	2.684376
H	-1.486980	0.071918	-0.736438
C	2.106767	1.611048	0.779261
H	0.820359	1.317326	-0.847369
H	2.092942	2.690037	0.716821
H	2.708447	1.167531	1.563431

2ATS3b (addition)

S	0.006920	-0.097681	0.053283
O	0.256455	-0.208349	1.703704
C	1.718757	0.258958	-0.455241
H	2.272001	-0.680434	-0.502766
H	1.617889	0.649792	-1.465620
C	2.379580	1.237710	0.453948
O	-0.122365	-0.929234	-1.859226
O	-1.446551	-1.103356	-2.159636
H	0.953875	-0.840820	1.908686
H	-1.543029	-2.061274	-2.219648
C	3.490509	0.975684	1.124886
H	1.898155	2.204577	0.553602
H	3.950058	1.714447	1.766258
H	3.984175	0.014298	1.043184

2ACP3b

S	-0.703985	-0.101599	0.119232
O	-0.420506	-0.220115	1.796469
C	1.014791	0.325411	-0.335349
H	1.573896	-0.607176	-0.421469
H	0.928982	0.768818	-1.324410
C	1.653577	1.258322	0.635112
O	-0.770561	-0.758634	-1.628635
O	-2.114802	-1.054510	-1.887007
H	0.508425	-0.355008	2.021264
H	-2.105852	-2.013813	-1.972883
C	2.745320	0.957022	1.323493
H	1.177602	2.224141	0.766061
H	3.192476	1.662831	2.009480
H	3.237078	-0.002060	1.207532

2BCR1

C	0.467479	0.186015	-0.914603
S	0.345031	-0.176373	0.849533
H	1.503566	0.419970	-1.153306
H	0.153433	-0.730865	-1.411266
C	-0.455734	1.322753	-1.211176
O	0.901728	-1.691641	0.956019
H	0.106379	-2.230044	0.778479
O	-1.485596	-1.203970	0.376702
H	-2.102997	-0.939287	1.066842
C	-0.039043	2.546731	-1.498992
H	-1.511732	1.087631	-1.151497
H	-0.738504	3.346079	-1.700204
H	1.016223	2.786197	-1.551566

CH2CHCH2SOH···H2O

C	0.094675	-0.124358	-0.149420
S	0.072942	-0.044496	1.666439
H	1.131394	-0.268936	-0.454175
C	-0.455723	1.166434	-0.664036
H	-0.501503	-0.974019	-0.476716
O	0.995527	-1.358571	2.044074
H	1.917629	-1.062438	2.092596
O	3.145332	0.441283	2.101428
H	3.881183	0.804682	1.607367
H	2.402542	1.044593	1.983686
C	-1.686008	1.304910	-1.134553
H	0.198383	2.029831	-0.602624
H	-2.056020	2.260884	-1.478297
H	-2.361889	0.460314	-1.193019

2ACR4

C	-0.786115	-0.601321	-0.830629
S	-0.951301	-0.690863	0.971949
H	0.284790	-0.624479	-1.045481
C	-1.412027	0.672489	-1.308638
H	-1.254448	-1.468034	-1.294403
O	-0.007961	-1.999583	1.288766
H	0.896024	-1.665711	1.431882
O	2.315708	-0.514762	1.536025
H	3.128540	-0.615563	1.038338
H	1.970297	0.358864	1.310999
O	1.096427	1.789721	0.227926
O	1.570968	1.478240	-0.950851
H	0.891971	1.754749	-1.595117
C	-2.286206	0.749864	-2.301826
H	-1.140394	1.574048	-0.763043
H	-2.711175	1.696609	-2.606028
H	-2.609085	-0.133733	-2.838623

2ATS4

C	-0.003959	-0.000159	-0.002323
S	0.007363	-0.009707	1.800025
H	1.045302	-0.002930	-0.299094
C	-0.712276	1.234316	-0.455872
H	-0.497977	-0.911016	-0.339431
O	1.027270	-1.137381	2.163918
H	2.005287	-0.667033	2.548114
O	2.938486	0.096771	2.897820
H	3.767882	-0.121120	2.466757
H	2.503099	0.952544	2.389884
O	1.739653	1.765181	1.623994
O	2.459665	1.611619	0.418719
H	2.297785	2.449351	-0.027076
C	-1.891946	1.228374	-1.057576
H	-0.213542	2.171264	-0.233934
H	-2.373542	2.147001	-1.362242
H	-2.411544	0.302089	-1.270798

2ACP4

C	-0.706600	-0.554557	-0.895382
S	-1.206596	-0.770368	0.840016
H	0.379230	-0.464904	-0.884791
C	-1.369206	0.670903	-1.433399
H	-1.005062	-1.456469	-1.430471
O	-0.212897	-1.715359	1.450217
H	1.590630	-1.161939	1.543076
O	2.334795	-0.546037	1.459193
H	2.905764	-0.909391	0.779904
H	1.545138	0.944473	0.938759
O	1.054984	1.636722	0.446911
O	1.657561	1.522154	-0.836739
H	2.185631	2.326112	-0.882856
C	-2.432999	0.636190	-2.222204
H	-0.940523	1.612398	-1.112003
H	-2.898490	1.544125	-2.579503
H	-2.866483	-0.302521	-2.546786

2BTS1

C	0.276647	0.081783	0.210640
S	0.219926	-0.284777	1.981806
H	1.303769	0.327079	-0.057674
H	-0.031828	-0.846760	-0.268085
C	-0.668442	1.203600	-0.068639
O	0.517862	-1.837348	2.072446
H	-0.505033	-2.098759	1.844506
O	-1.699894	-1.431501	1.494920
H	-2.353742	-1.372740	2.198224
C	-0.279066	2.425308	-0.400183

H	-1.718412	0.958577	0.042794
H	-0.995935	3.212789	-0.586121
H	0.769905	2.674766	-0.505486

2BCP1

C	0.545606	0.203069	-1.145996
S	1.540982	-0.446058	0.231209
H	1.272743	0.568394	-1.872980
H	-0.003316	-0.646503	-1.555086
C	-0.376816	1.285197	-0.683633
O	0.579884	-1.127073	1.159497
H	-1.159511	-1.534268	0.447769
O	-1.867831	-1.513704	-0.209904
H	-2.495172	-2.188166	0.052237
C	-0.226549	2.560528	-1.006829
H	-1.196943	0.962166	-0.053501
H	-0.913503	3.314255	-0.648242
H	0.581881	2.892278	-1.647433

2BCR1a

C	-0.161357	-0.002755	-0.959327
S	-0.252445	0.528445	0.759556
C	1.252278	-0.149654	-1.417550
H	-0.730402	-0.931697	-0.997380
H	-0.699068	0.759288	-1.525709
O	0.372166	-0.749833	1.532788
H	-0.410895	-1.312935	1.687853
O	-2.054452	-0.618690	0.969086
H	-2.660345	-0.050261	1.455984
C	1.775229	0.534071	-2.423383
H	1.853559	-0.866119	-0.869045
H	2.803513	0.393254	-2.725208
H	1.189815	1.254252	-2.982114

2BTS1a

C	-0.191478	-0.182261	-0.204247
S	-0.235962	0.356192	1.518459
C	1.215427	-0.425369	-0.644668
H	-0.812524	-1.077770	-0.232393
H	-0.671839	0.610069	-0.779621
O	0.263099	-0.930731	2.299943
H	-0.727360	-1.355291	2.339939
O	-2.015345	-1.044238	1.850346
H	-2.642430	-0.707904	2.497941
C	1.809997	0.248288	-1.617013
H	1.747125	-1.203054	-0.108074
H	2.830546	0.036435	-1.903608
H	1.294269	1.029589	-2.162323

2BCP1a

C	-0.226225	0.822973	-0.805455
S	0.251500	1.436648	0.839046
C	0.708399	-0.243937	-1.278095
H	-1.246340	0.449096	-0.707013
H	-0.206194	1.701268	-1.452537
O	-0.008710	0.313311	1.798684
H	-1.075677	-1.153914	1.149237
O	-1.559836	-1.659634	0.482467
H	-2.076013	-2.308636	0.961602
C	1.562929	-0.077315	-2.275833
H	0.646060	-1.186720	-0.747490
H	2.224612	-0.873563	-2.586539
H	1.622501	0.856676	-2.821890

2BCR1b

C	0.419853	0.754888	-0.972306
S	0.220371	0.874245	0.824454
H	1.492664	0.767193	-1.163282
C	-0.223706	-0.451871	-1.569251
H	-0.015304	1.686030	-1.341347
O	0.785576	-0.553531	1.324094
H	0.001941	-1.134154	1.294481
O	-1.661460	-0.183785	0.808717
H	-2.169848	0.309803	1.461957
C	0.481242	-1.487020	-1.999636
H	-1.304259	-0.460434	-1.597091
H	-0.000208	-2.357500	-2.423110
H	1.563182	-1.496657	-1.943673

2BTS1b

C	0.005558	0.015324	-0.042225
S	-0.226753	0.176561	1.750810
H	1.083334	-0.051995	-0.196595
C	-0.701822	-1.158758	-0.630128
H	-0.350212	0.967332	-0.440945
O	0.165410	-1.249603	2.310126
H	-0.849720	-1.617362	2.246224
O	-2.110360	-1.153772	1.821978
H	-2.673039	-0.839058	2.537290
C	-0.061234	-2.247578	-1.024380
H	-1.780749	-1.099210	-0.676937
H	-0.593690	-3.093749	-1.435489
H	1.015835	-2.330269	-0.943264

2BCP1b

C	0.787214	0.913107	-1.178289
S	0.578477	1.431725	0.562825
H	1.811146	0.553280	-1.282748
C	-0.207537	-0.138425	-1.531730
H	0.668613	1.833422	-1.753110

O	0.516537	0.166967	1.360563
H	-1.078267	-1.063315	0.888348
O	-1.990397	-1.338035	0.738653
H	-2.384999	-1.376077	1.611187
C	0.114640	-1.413332	-1.682878
H	-1.245920	0.168664	-1.586554
H	-0.642116	-2.160122	-1.876993
H	1.141468	-1.748761	-1.601183

2BCR2

S	-0.608084	0.568023	0.520356
O	-0.942316	0.007955	2.000405
C	1.055498	-0.060193	0.207418
H	1.050513	-1.073530	0.606095
C	1.278910	-0.046023	-1.269836
H	1.771293	0.562252	0.741302
O	-1.307359	-1.385832	-0.051227
H	-2.069485	-1.220266	-0.616361
H	-1.299261	-0.883464	1.822974
C	2.091891	0.804847	-1.877783
H	0.705904	-0.775225	-1.830043
H	2.223493	0.788482	-2.950669
H	2.659912	1.539740	-1.320257

2BTS2

S	0.183680	0.140117	-0.004682
O	0.212925	0.164994	1.645070
C	1.882306	-0.395765	-0.304998
H	1.945762	-1.425872	0.046274
C	2.202869	-0.298008	-1.763025
H	2.514573	0.257113	0.294611
O	-0.298194	-1.675922	-1.010564
H	-1.251436	-1.583509	-1.124435
H	0.060237	-0.732328	1.965514
C	3.043612	0.596304	-2.259414
H	1.693086	-1.007862	-2.401388
H	3.258469	0.636694	-3.318212
H	3.548596	1.314192	-1.624283

2BCP2

S	-0.960829	-0.037695	0.397485
O	-0.730910	0.586823	2.022237
C	0.814624	-0.336351	0.130684
H	1.002151	-1.362641	0.451857
C	1.219395	-0.135856	-1.295204
H	1.329112	0.363636	0.782242
O	-1.256767	-1.352390	-0.764553
H	-2.206618	-1.365274	-0.919427
H	-0.200210	-0.009387	2.562223
C	2.035961	0.833260	-1.678232

H	0.806937	-0.832893	-2.012649
H	2.321066	0.950690	-2.714403
H	2.447540	1.541422	-0.968935

2BCR2a

S	-0.846846	0.193181	-0.422266
O	-1.369108	-0.018264	1.096055
C	0.909412	-0.174347	-0.260850
H	0.950956	-1.192503	0.126158
H	1.299241	-0.171218	-1.280019
C	1.603103	0.823193	0.607384
O	-1.238320	-1.914900	-0.520826
H	-1.869488	-2.019761	-1.240580
H	-1.595720	-0.968048	1.118810
C	2.600681	1.590393	0.196478
H	1.238445	0.895429	1.625971
H	3.076424	2.297732	0.861133
H	2.977708	1.533037	-0.817490

2BTS2a

S	0.119700	0.085183	-0.124086
O	-0.296863	0.147453	1.472395
C	1.884742	-0.236797	0.052039
H	1.967008	-1.212247	0.533888
H	2.245386	-0.337554	-0.970399
C	2.581887	0.852647	0.797459
O	0.144742	-1.818098	-1.098219
H	-0.753525	-1.858670	-1.447615
H	-0.438105	-0.756311	1.780385
C	3.566048	1.573239	0.282961
H	2.241912	1.036582	1.810365
H	4.053587	2.351127	0.853899
H	3.919840	1.405784	-0.727149

2BCP2a

S	-0.972013	-0.292674	-0.242738
O	-1.323550	0.019966	1.449630
C	0.812029	-0.445837	0.069524
H	0.936574	-1.274238	0.771167
H	1.262946	-0.720806	-0.878449
C	1.390114	0.824682	0.607124
O	-0.751116	-1.355498	-1.653703
H	-1.612623	-1.412951	-2.080265
H	-0.924943	-0.641608	2.026108
C	2.372620	1.476089	0.005135
H	0.965337	1.203229	1.528966
H	2.779096	2.387874	0.420298
H	2.803534	1.118517	-0.922158

2BCR2b

S	-0.882730	0.832800	-0.179228
O	-0.716062	0.477946	1.387342
C	0.816695	0.666681	-0.782880
C	1.419737	-0.674221	-0.529895
H	0.734153	0.893083	-1.847985
H	1.389194	1.457553	-0.298264
O	-1.300148	-1.279999	-0.327102
H	-2.199908	-1.279910	-0.672325
H	-0.840656	-0.489323	1.419360
C	2.345575	-0.870012	0.396295
H	1.036236	-1.496146	-1.118033
H	2.767695	-1.850469	0.568608
H	2.711629	-0.056372	1.010810

2BTS2b

S	0.134024	0.082875	0.164242
O	0.557957	-0.145803	1.725887
C	1.755909	-0.077605	-0.622072
C	2.398633	-1.382796	-0.283203
H	1.540084	0.012752	-1.685945
H	2.354424	0.769436	-0.289314
O	-0.337401	-1.778779	-0.884153
H	-1.290481	-1.798575	-0.737455
H	0.921030	-1.039919	1.814103
C	3.358806	-1.488373	0.626268
H	1.999921	-2.254276	-0.784348
H	3.799638	-2.445556	0.869205
H	3.747166	-0.617539	1.141680

2BCP2b

S	-1.022576	0.399628	0.050424
O	-0.401661	0.681266	1.647377
C	0.631961	0.422901	-0.698100
C	1.399199	-0.794971	-0.303112
H	0.463890	0.470482	-1.770220
H	1.110400	1.333463	-0.345224
O	-1.505600	-0.672262	-1.307877
H	-2.435065	-0.881010	-1.169332
H	0.357048	0.108998	1.823843
C	2.460521	-0.763294	0.492007
H	1.017290	-1.736025	-0.682649
H	2.983510	-1.667061	0.772532
H	2.852681	0.174260	0.869795

2BCR3

C	0.209130	0.539857	-0.649867
S	-0.400339	-0.397490	0.779503
H	0.984485	1.240387	-0.344468
H	0.614589	-0.182059	-1.360595
C	-0.976654	1.250791	-1.221704

O	0.823349	-1.520358	0.970202
H	1.499102	-1.155569	1.549052
O	1.297752	-2.345385	-1.704469
H	1.166403	-2.421823	-0.740093
C	-1.212150	2.541810	-1.043516
H	-1.676347	0.637618	-1.778116
H	-2.089144	3.017327	-1.459849
H	-0.529371	3.165456	-0.479103

2BTS3

C	-0.010560	-0.006253	0.001476
S	-0.073496	-0.176436	1.778561
H	1.094412	0.026980	-0.240537
H	-0.423466	-0.898205	-0.466085
C	-0.689723	1.259142	-0.407995
O	0.706804	-1.620132	1.924732
H	1.623570	-1.468754	1.647403
O	2.649698	-0.439275	0.067045
H	2.814332	-0.972447	-0.726297
C	-0.134023	2.452777	-0.254819
H	-1.691500	1.168627	-0.811320
H	-0.657342	3.357975	-0.528840
H	0.867571	2.553563	0.146753

CH2CHCHSOH··H2O

C	-0.918688	-0.085734	-0.509179
S	-0.292447	-0.136064	1.085392
H	1.685054	0.077495	-0.994333
H	-1.243554	-1.038362	-0.907148
C	-1.058448	1.097720	-1.246775
O	0.391813	-1.630055	1.109594
H	1.201560	-1.564794	0.574030
O	2.263532	-0.648676	-0.738125
H	2.563903	-1.047585	-1.556850
C	-0.604265	2.334153	-0.888399
H	-1.578897	1.001213	-2.193522
H	-0.771235	3.188738	-1.525719
H	-0.061699	2.495765	0.033436

2BTS4

S	0.000573	-0.393449	0.014845
C	0.223611	-0.128428	1.698691
H	1.061524	-0.723256	2.046671
C	-0.927116	-0.048202	2.622611
H	-0.669107	-0.239945	3.659240
C	-2.182693	0.276227	2.323579
H	-2.935514	0.316750	3.097075
H	-2.493009	0.507523	1.312608
O	-0.740064	0.866868	-0.512430
H	-0.360252	1.865758	0.272354

O	0.139904	2.389072	1.117449
H	0.924694	2.840863	0.791632
H	0.431187	1.351688	1.561611

2BCP4

S	0.000573	-0.393449	0.014845
C	0.223611	-0.128428	1.698691
H	1.061524	-0.723256	2.046671
C	-0.927116	-0.048202	2.622611
H	-0.669107	-0.239945	3.659240
C	-2.182693	0.276227	2.323579
H	-2.935514	0.316750	3.097075
H	-2.493009	0.507523	1.312608
O	-0.740064	0.866868	-0.512430
H	-0.360252	1.865758	0.272354
O	0.139904	2.389072	1.117449
H	0.924694	2.840863	0.791632
H	0.431187	1.351688	1.561611

2BCR5

C	-0.359002	-0.228181	0.070889
S	0.459131	0.187907	1.668370
H	0.419320	-0.568043	-0.610311
H	-0.993682	-1.076607	0.329043
C	-1.128842	0.900139	-0.477245
H	-2.138174	1.063281	-0.123208
C	-0.447015	2.045891	-1.145316
H	-0.250568	2.839224	-0.417547
H	-1.096181	2.474266	-1.917172
O	1.214177	1.602393	1.253442
H	1.921203	1.412483	0.626558
O	0.821828	1.709254	-1.682698
H	0.695177	1.132685	-2.439347

2BTS5

C	0.026678	0.010280	0.069655
S	0.045872	0.009809	1.883324
H	1.045422	0.042872	-0.314123
H	-0.403528	-0.961503	-0.183535
C	-0.791235	1.131010	-0.461574
H	-1.864127	1.067192	-0.315819
C	-0.255355	2.193750	-1.086211
H	0.815768	2.315792	-1.156496
H	-0.866573	3.022935	-1.410960
O	0.775645	1.471297	2.165254
H	1.723856	1.326664	2.234821
O	-0.131393	1.094160	-2.943357
H	-1.078657	0.950431	-3.080523

2BCP5

C	0.047608	0.099233	0.013313
S	0.078369	-0.077368	1.814034
H	1.063292	0.193001	-0.369794
H	-0.359471	-0.851051	-0.338603
C	-0.804798	1.245712	-0.411767
H	-1.869576	1.142814	-0.231308
C	-0.318968	2.371444	-0.924142
H	0.743585	2.495505	-1.091778
H	-0.963884	3.201345	-1.180288
O	0.768947	1.368557	2.242475
H	1.721887	1.247014	2.281631
O	-0.287223	0.368384	-2.871662
H	-0.852394	1.050099	-3.266655

3

C	-0.003618	-0.018599	-0.011994
S	0.010522	-0.003087	1.736150
H	0.961872	-0.021621	-0.507471
C	-1.137317	0.083951	-0.697533
H	-2.075780	0.059808	-0.152546
C	-1.212427	0.253220	-2.180736
H	-0.223858	0.212452	-2.634516
H	-1.833804	-0.525955	-2.624298
H	-1.668822	1.210310	-2.439295
O	1.017041	-1.288742	2.061775
H	1.899589	-0.943034	2.220964

3ACR1

C	-0.056275	-0.257312	0.046939
S	0.014595	-0.043809	1.786592
H	0.836858	-0.650123	-0.428685
C	-1.115156	0.132775	-0.653355
H	-1.985291	0.498174	-0.116803
C	-1.189078	0.119434	-2.145264
H	-0.287538	-0.303466	-2.584000
H	-2.048917	-0.463166	-2.478274
H	-1.320152	1.130933	-2.533151
O	0.505978	-1.532818	2.298781
H	1.473034	-1.545140	2.246238
O	3.192305	-0.585963	1.748557
O	3.040426	0.705558	1.686181
H	2.061611	0.845396	1.758575

3ATS1

C	-0.099306	-0.278138	0.044454
S	-0.052400	-0.118176	1.786047
H	0.812874	-0.659786	-0.401926
C	-1.147435	0.113328	-0.670660
H	-2.032469	0.470452	-0.151760
C	-1.191920	0.107656	-2.164473

H	-0.274380	-0.299760	-2.584596
H	-2.034628	-0.486821	-2.520306
H	-1.328817	1.118908	-2.551445
O	0.756232	-1.413933	2.241495
H	1.786828	-1.233522	2.164275
O	3.042902	-0.649775	1.951859
O	2.678357	0.505586	1.374746
H	2.646563	1.154454	2.094620

3ACP1

C	-0.254862	-0.416477	0.260748
S	-0.638908	-0.515836	1.952386
H	0.750513	-0.714985	-0.014744
C	-1.163656	0.031537	-0.607556
H	-2.145524	0.318205	-0.239050
C	-0.923417	0.178697	-2.072368
H	0.083567	-0.132844	-2.340326
H	-1.639923	-0.416652	-2.640749
H	-1.060081	1.217342	-2.378318
O	0.522412	-1.159831	2.650230
H	2.179424	-1.011750	1.847278
O	2.857821	-0.638056	1.256052
O	2.416330	0.709157	1.159595
H	3.018707	1.161965	1.759151

3ACR2

C	0.131680	-0.382284	-0.105255
S	0.413764	-1.140529	1.448675
H	1.007838	0.004056	-0.614412
C	-1.069301	-0.393561	-0.673556
H	-1.909320	-0.795824	-0.115038
C	-1.339017	0.087361	-2.061553
H	-1.699024	-0.732053	-2.685774
H	-2.121589	0.846933	-2.053245
H	-0.446080	0.505979	-2.521842
O	1.202157	0.069933	2.272015
H	2.147124	-0.104740	2.235120
O	-3.127791	-1.418197	1.827152
O	-2.515085	-0.668015	2.698725
H	-1.560865	-0.714272	2.450161

3ATS2

C	-0.158266	0.019379	0.025345
S	-0.094326	-0.037320	1.779762
H	0.823389	0.189322	-0.401029
C	-1.240932	-0.065573	-0.742136
H	-2.213154	-0.189262	-0.284133
C	-1.186264	0.008600	-2.234530
H	-1.589564	-0.903897	-2.677128
H	-1.797839	0.835337	-2.599778

H	-0.167987	0.145220	-2.594350
O	1.564241	0.225279	1.908549
H	2.038622	-0.584391	1.693857
O	-1.759139	-1.245655	1.705717
O	-2.443553	-1.081096	2.883379
H	-2.410736	-1.956158	3.287649

3ACP2

C	-0.189242	0.022550	0.031843
S	-0.147706	-0.105825	1.784391
H	0.771376	0.324072	-0.365563
C	-1.241168	-0.135020	-0.768006
H	-2.203479	-0.388210	-0.345247
C	-1.160359	0.034264	-2.250506
H	-1.458122	-0.886074	-2.755721
H	-1.848106	0.813625	-2.582672
H	-0.154865	0.297167	-2.573709
O	1.550837	0.119174	1.887173
H	2.022826	-0.548710	1.378104
O	-1.711697	-1.130630	1.702177
O	-2.338567	-0.986933	2.944785
H	-2.277235	-1.874663	3.314126

CH3CHCHSOH···H2O

C	0.057925	-0.021992	0.086251
S	0.088252	0.026707	1.835917
H	1.028910	0.051266	-0.394571
C	-1.070955	-0.064657	-0.619249
H	-2.014051	-0.152694	-0.086289
C	-1.137640	0.061429	-2.108829
H	-0.141285	0.080079	-2.546818
H	-1.697010	-0.766256	-2.546806
H	-1.652615	0.980092	-2.395469
O	1.366118	-0.971093	2.140716
H	1.060555	-1.878246	1.972496
O	-0.077081	-3.115079	1.023711
H	-0.823880	-3.443008	1.529053
H	-0.442079	-2.458008	0.419793

3ACR3

C	0.171256	0.384446	-0.046412
S	0.375227	0.457710	1.689689
H	0.970668	0.853941	-0.611288
C	-0.906670	-0.122027	-0.636623
H	-1.666301	-0.596962	-0.023609
C	-1.163753	-0.051141	-2.109186
H	-0.317828	0.388491	-2.634950
H	-1.349657	-1.044898	-2.519189
H	-2.047826	0.552612	-2.322638
O	2.004086	0.256854	1.819940

H	2.188197	-0.686295	1.652673
O	1.947697	-2.412058	1.111987
H	2.078095	-3.085589	1.782698
H	0.997369	-2.414873	0.934751
O	-0.930960	-2.443548	1.537160
O	-0.697801	-2.949211	2.721237
H	-1.471960	-2.723553	3.263490

3ATS3

C	0.122153	0.267977	-0.026571
S	0.241440	0.226729	1.713686
H	1.014882	0.625435	-0.528348
C	-0.983854	-0.101290	-0.666195
H	-1.810515	-0.498382	-0.085605
C	-1.159121	-0.024355	-2.146443
H	-0.266154	0.361383	-2.634071
H	-1.381438	-1.012505	-2.551918
H	-2.001551	0.621198	-2.400645
O	1.742402	-0.119655	1.970523
H	1.947748	-1.193051	1.552802
O	1.853217	-2.328635	1.073582
H	2.235944	-2.984450	1.661563
H	0.754769	-2.354885	1.196234
O	-0.501310	-2.095569	1.520995
O	-0.469458	-2.648367	2.817191
H	-1.399317	-2.652679	3.062949

3ACP3

C	0.158588	0.241426	0.107005
S	0.887961	1.429258	1.133378
H	0.614385	-0.741534	0.123103
C	-0.911358	0.520678	-0.641332
H	-1.335301	1.521192	-0.609787
C	-1.575441	-0.482391	-1.521894
H	-1.074523	-1.445643	-1.457826
H	-2.617126	-0.612544	-1.222932
H	-1.579946	-0.139080	-2.558154
O	1.973828	0.733475	1.904817
H	2.131286	-1.089716	1.973636
O	2.112668	-2.062090	1.944889
H	2.201805	-2.356701	2.852235
H	0.891592	-2.793088	0.897417
O	0.172246	-3.040104	0.280124
O	-0.968728	-2.531198	0.960392
H	-1.382100	-3.338040	1.284659

3BCR1

C	-0.445320	-0.437872	0.009624
S	-0.684285	-0.559144	1.727722
H	0.468131	-0.890265	-0.357651

C	-1.383278	0.086539	-0.772209
H	-2.267515	0.516656	-0.311486
C	-1.311982	0.112723	-2.263328
H	-0.375883	-0.309160	-2.622706
H	-2.137023	-0.455668	-2.695853
H	-1.402083	1.135517	-2.631659
O	0.699637	0.005517	2.352765
H	1.243196	-0.798414	2.454576
O	0.443283	-2.381232	1.754145
H	-0.141707	-3.033422	2.153154

3BTS1

C	-0.451462	-0.341773	0.009652
S	-0.684201	-0.426041	1.727858
H	0.502694	-0.721234	-0.337012
C	-1.417345	0.096296	-0.793150
H	-2.341464	0.460209	-0.352607
C	-1.324083	0.114769	-2.282566
H	-0.354888	-0.242775	-2.623441
H	-2.099987	-0.515271	-2.720924
H	-1.480900	1.124943	-2.663576
O	0.763263	-0.197654	2.338124
H	1.019833	-1.233829	2.285335
O	0.436108	-2.427818	1.764511
H	0.057604	-3.048047	2.394889

3BCP1

C	-0.803505	-0.166567	0.212349
S	-1.003726	0.528969	1.794163
H	-0.208816	-1.073921	0.167514
C	-1.363927	0.414067	-0.850817
H	-1.944103	1.322830	-0.709970
C	-1.250081	-0.102880	-2.245758
H	-0.652792	-1.011110	-2.282004
H	-2.238312	-0.316056	-2.656873
H	-0.791228	0.644906	-2.894854
O	-0.270365	-0.340842	2.770656
H	0.656116	-1.896563	2.096511
O	0.960444	-2.515894	1.418853
H	1.455467	-3.195165	1.877324

3BCR2

C	0.127131	0.192987	-0.090486
S	0.285059	0.164451	1.652851
H	1.012668	0.515338	-0.626212
C	-1.020537	-0.092977	-0.692910
H	-1.842954	-0.445424	-0.080782
C	-1.238892	0.016891	-2.165078
H	-2.035673	0.731261	-2.378410
H	-1.559076	-0.944460	-2.568881

H	-0.337427	0.335325	-2.684574
O	1.483283	-0.906724	1.887152
H	1.011627	-1.760039	1.917650
O	-0.957990	-1.594093	1.851199
H	-1.428757	-1.425464	2.675753

3BTS2

C	0.061742	0.072352	-0.027375
S	0.226838	-0.016112	1.708895
H	0.972636	0.409245	-0.510753
C	-1.065830	-0.155807	-0.691838
H	-1.932791	-0.494087	-0.138355
C	-1.199379	0.033974	-2.167382
H	-1.954140	0.791383	-2.386562
H	-1.534581	-0.891337	-2.638329
H	-0.259818	0.340194	-2.623883
O	1.755582	-0.627030	1.797701
H	1.717134	-1.563674	1.567025
O	-1.416098	-1.402417	1.832187
H	-1.562830	-1.379614	2.785940

3BCP2

C	-0.023209	-0.094936	0.077595
S	0.129563	-0.398073	1.799358
H	0.890058	0.321975	-0.324774
C	-1.100585	-0.275973	-0.679185
H	-2.002673	-0.672878	-0.234730
C	-1.129144	0.052382	-2.136997
H	-1.904931	0.791036	-2.345460
H	-1.373052	-0.835144	-2.723181
H	-0.174877	0.445208	-2.482755
O	1.880721	-0.539672	1.695658
H	2.141715	-1.150588	0.997666
O	-1.515287	-1.047374	1.867472
H	-1.699835	-1.148892	2.806604

3BCR3

C	-0.032598	-0.543809	-0.107231
S	0.044944	-0.201925	1.611611
H	0.829889	-1.011991	-0.569033
C	-1.126884	-0.263333	-0.813580
H	-1.953927	0.224146	-0.308042
C	-1.291261	-0.558483	-2.265019
H	-0.405038	-1.033944	-2.679718
H	-2.152289	-1.207237	-2.432627
H	-1.474991	0.372319	-2.803434
O	1.151792	1.062053	1.616286
H	2.030145	0.699350	1.763942
O	0.222531	2.076986	-1.016282
H	0.608627	2.026711	-0.121877

3NTS3

C	0.003059	-0.291599	-0.059072
S	-0.000400	0.032433	1.644544
H	0.894513	-0.747984	-0.475100
C	-1.071866	-0.025321	-0.828704
H	-1.933769	0.443025	-0.366892
C	-1.227113	-0.516444	-2.229250
H	-0.271235	-0.841904	-2.635421
H	-1.923345	-1.356691	-2.260031
H	-1.625018	0.276317	-2.859464
O	1.508487	0.701172	1.846429
H	2.109106	0.015009	2.151863
O	-0.192187	1.910441	-1.404428
H	0.185708	2.197389	-0.559478

3BCP3

C	0.155119	-0.116620	-0.099216
S	0.013050	-0.004179	1.570486
H	1.076859	-0.499652	-0.520913
C	-0.883654	0.461263	-1.008351
H	-1.792169	0.667048	-0.431744
C	-1.214836	-0.468516	-2.160757
H	-0.310094	-0.689628	-2.726771
H	-1.637199	-1.401044	-1.790811
H	-1.930121	0.010212	-2.827234
O	1.552538	0.416341	2.065640
H	1.956978	-0.354777	2.474779
O	-0.412329	1.673069	-1.595814
H	-0.113203	2.257326	-0.894298

CH3CHCH-SOH···H

C	0.212524	0.262404	0.097022
S	0.382521	0.322605	1.838255
O	2.009153	0.092800	1.988597
H	2.178135	-0.846270	1.803930
O	1.721774	-2.484685	0.892984
H	1.291108	-3.146120	1.438561
H	1.022145	-2.099286	0.352889
H	0.970535	0.805459	-0.459703
C	-0.811194	-0.333403	-0.511967
C	-1.074740	-0.258755	-1.983048
H	-1.532569	-0.875133	0.094098
H	-1.193851	-1.255321	-2.410197
H	-2.000055	0.284899	-2.181904
H	-0.264345	0.249407	-2.502572

3BCR4

C	0.150820	0.311920	-0.000615
S	0.327916	0.267992	1.735523

O	1.868662	-0.123517	1.919743
H	2.012193	-1.069429	1.577021
O	1.802374	-2.518166	1.048549
H	2.219486	-3.238935	1.522406
H	0.839350	-2.468099	1.341951
O	-0.535185	-1.824624	1.787193
H	-0.765777	-1.903736	2.719087
H	0.948461	0.841185	-0.510165
C	-0.900507	-0.207219	-0.624033
C	-1.129271	-0.095164	-2.094721
H	-1.624354	-0.759779	-0.036236
H	-1.216881	-1.088285	-2.537175
H	-2.066387	0.426356	-2.296456
H	-0.320720	0.439742	-2.588845

3BTS4

C	0.164547	0.288071	-0.023007
S	0.358768	0.238599	1.711322
O	1.866204	-0.178531	1.897079
H	1.988388	-1.213362	1.561172
O	1.786327	-2.479354	1.154646
H	2.215979	-3.144134	1.694913
H	0.733386	-2.415921	1.411928
O	-0.509320	-1.939783	1.698307
H	-0.762250	-2.086763	2.614752
H	0.991538	0.758468	-0.543773
C	-0.924574	-0.171065	-0.629141
C	-1.166360	-0.062132	-2.097596
H	-1.670956	-0.679105	-0.028739
H	-1.305269	-1.054584	-2.528781
H	-2.081229	0.499833	-2.293221
H	-0.340000	0.430003	-2.606633

3BCP4

C	-0.003431	0.257709	0.195871
S	0.867824	1.447977	1.104911
O	1.650602	0.717225	2.157970
H	1.890806	-1.125630	2.185323
O	1.962079	-2.084620	2.050137
H	2.893075	-2.262974	1.911033
H	0.648236	-2.840917	0.985745
O	-0.112827	-3.016233	0.409169
H	-0.634728	-3.676820	0.866082
H	0.080039	-0.768687	0.537394
C	-0.740220	0.598369	-0.865138
C	-1.507295	-0.391270	-1.676018
H	-0.792026	1.642131	-1.165055
H	-2.573626	-0.158041	-1.653099
H	-1.197222	-0.347821	-2.721587
H	-1.351107	-1.400159	-1.299510

4ATS1 acidic hydrogen abstraction by HO2 (pcet)

C	1.611517	-0.864980	0.821215
H	1.851447	-1.692127	0.150297
C	1.087439	0.306109	-0.030068
H	0.031419	0.134129	-0.240750
H	1.192512	1.260856	0.489005
C	2.923560	-0.467338	1.499418
O	3.977188	-0.429440	0.872607
N	2.863078	-0.133128	2.792566
H	1.987875	-0.249156	3.275087
C	4.056522	0.274573	3.511416
H	4.796114	-0.524718	3.505211
H	4.498589	1.149624	3.039205
H	3.785253	0.511481	4.535351
N	0.589547	-1.264398	1.763467
H	-0.210763	-0.665753	1.906714
C	0.491546	-2.497742	2.369833
O	-0.427734	-2.743772	3.114994
C	1.586128	-3.486288	2.050679
H	2.575273	-3.062356	2.227539
H	1.443663	-4.360968	2.675471
H	1.538772	-3.778606	1.000925
S	1.894343	0.483858	-1.636826
O	1.480439	-0.872901	-2.315676
H	2.313139	-1.638516	-2.137214
O	3.322799	-2.213573	-1.728276
O	4.197342	-1.188140	-1.653670
H	4.178990	-0.909832	-0.701119

4BTS1 acidic hydrogen abstraction by OH(pcet)

C	-0.501361	-0.011541	-0.611835
H	-0.663386	0.165486	0.452897
C	1.010548	0.070714	-0.832086
H	1.370801	1.036869	-0.481052
H	1.542009	-0.734796	-0.328840
C	-1.162606	1.181361	-1.324541
O	-0.810603	2.312881	-1.051809
N	-2.111007	0.894811	-2.232748
H	-2.291638	-0.068886	-2.457251
C	-2.746364	1.956844	-2.988144
H	-3.152954	2.701294	-2.306690
H	-2.027804	2.451995	-3.640955
H	-3.548686	1.534393	-3.585310
N	-1.021737	-1.308410	-0.971196
H	-0.548666	-1.835160	-1.695477
C	-2.142069	-1.900940	-0.445178
O	-2.537161	-2.964985	-0.865223
C	-2.842740	-1.159620	0.670651
H	-3.752236	-1.699452	0.909951

H	-3.085819	-0.136802	0.381585
H	-2.208010	-1.117112	1.556414
S	1.481424	-0.001865	-2.566603
O	1.171371	-1.513757	-2.967681
H	2.144733	-1.851261	-2.627525
O	3.253276	-1.302857	-1.975654
H	4.032087	-1.136302	-2.516299

4ATS2 (addition of HO2 to the S atom

C	0.125613	3.049018	-1.078664
H	0.858769	3.620166	-0.518674
C	0.426109	1.541060	-0.950940
H	0.464400	1.265542	0.103905
H	-0.373357	0.985277	-1.439551
C	0.167465	3.445357	-2.556915
O	-0.793742	3.240488	-3.272337
N	1.320295	3.986792	-2.988113
H	2.111601	4.010883	-2.364882
C	1.524716	4.236214	-4.401939
H	2.461814	4.769144	-4.531739
H	1.556739	3.301204	-4.962403
H	0.706440	4.838906	-4.789025
N	-1.198532	3.321531	-0.583368
H	-1.952790	3.223499	-1.251409
C	-1.548530	3.657485	0.692617
O	-2.707816	3.812266	1.007518
C	-0.417457	3.853735	1.680152
H	0.269414	3.008021	1.696074
H	-0.854198	3.989091	2.663534
H	0.156863	4.743350	1.419069
S	1.940466	0.977306	-1.772685
O	1.527876	-0.629307	-1.902896
H	1.554524	-1.056839	-1.039837
O	2.938097	2.562175	-0.730198
O	3.950304	2.985888	-1.555638
H	4.756813	2.750549	-1.080558

4BTS2 acidic addition of OH to S

C	0.499126	-2.086288	0.085240
H	0.267024	-2.697542	-0.785692
C	0.854044	-0.650988	-0.380788
H	0.425146	0.081822	0.298237
H	1.928261	-0.501206	-0.474216
C	1.751930	-2.694824	0.742760
O	1.830303	-2.820896	1.948727
N	2.723624	-3.028597	-0.120059
H	2.587086	-2.821484	-1.103541
C	3.992190	-3.533297	0.365663
H	4.608375	-3.807607	-0.485347
H	4.511640	-2.781824	0.960567

H	3.832284	-4.408061	0.993420
N	-0.582154	-2.118495	1.028997
H	-0.300744	-2.103760	2.002458
C	-1.878669	-2.491052	0.803452
O	-2.665807	-2.596279	1.717469
C	-2.283820	-2.753918	-0.630948
H	-1.760301	-3.624793	-1.026730
H	-3.351308	-2.945413	-0.642914
H	-2.059513	-1.903318	-1.274084
S	0.197756	-0.352102	-2.020457
O	0.789096	1.163094	-2.240262
H	0.057286	1.764022	-2.420004
O	1.696217	-1.848158	-2.584523
H	1.550927	-1.931837	-3.533325

4ATS3 acidic hydrogen abstraction by HO2 assisteb by one H2O moplecule

C	1.907665	-1.246361	0.688769
H	1.531555	-0.997101	1.688397
C	1.582082	-0.090210	-0.260900
H	1.915272	-0.316442	-1.274546
H	0.506534	0.093321	-0.280524
C	1.130431	-2.458607	0.145427
O	1.515467	-3.089663	-0.811934
N	-0.041047	-2.714030	0.774809
H	-0.247541	-2.245044	1.638922
C	-0.874078	-3.822430	0.348383
H	-0.389031	-4.778246	0.548506
H	-1.821584	-3.779078	0.877544
H	-1.053173	-3.752652	-0.722086
N	3.327497	-1.469457	0.717286
H	3.927464	-0.828022	0.216295
C	3.980641	-2.475811	1.376102
O	5.186219	-2.569007	1.335618
C	3.124575	-3.457952	2.143867
H	2.357091	-2.960499	2.737226
H	2.632767	-4.135486	1.444603
H	3.775932	-4.030761	2.795139
S	2.322832	1.472954	0.212034
O	3.816013	1.322494	-0.239933
H	4.002267	1.967630	-1.211903
O	3.911122	2.687959	-2.191547
H	4.246802	2.260572	-2.983639
H	2.829640	2.653827	-2.206964
O	1.525829	2.350083	-1.964729
O	1.410234	1.294890	-2.884498
H	0.460319	1.250627	-3.036625

4BTS3 acidic hydrogen abstraction by OH assisteb by one H2O moplecule

C	-0.255456	1.640377	-3.248487
H	-0.432891	2.145094	-2.291551

C	1.213497	1.225681	-3.315093
H	1.426315	0.717679	-4.256163
H	1.870027	2.087517	-3.201339
C	-0.481376	2.652048	-4.388523
O	-0.727565	2.297847	-5.517559
N	-0.333816	3.951065	-4.036511
H	-0.238896	4.193933	-3.066427
C	-0.492967	5.000834	-5.025169
H	-0.213463	5.951798	-4.581180
H	0.147294	4.798258	-5.880959
H	-1.523005	5.053087	-5.378020
N	-1.083853	0.472174	-3.360171
H	-0.634466	-0.393534	-3.650590
C	-2.452704	0.463522	-3.340853
O	-3.076291	-0.557866	-3.519179
C	-3.136302	1.787133	-3.077456
H	-4.188254	1.593296	-2.897945
H	-2.708237	2.305794	-2.219357
H	-3.036355	2.431090	-3.952524
S	1.610037	0.097361	-1.966818
O	3.158023	-0.104233	-2.127657
H	3.378175	-0.655413	-3.050237
O	3.318471	-1.346848	-4.193594
H	3.869533	-2.129431	-4.244997
H	2.299188	-1.615549	-4.010745
O	1.004336	-1.555438	-3.512659
H	0.741702	-2.318575	-2.989034

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