Electronic Supplementary Material file

for the manuscript entitled:

New insight into environmental oxidation of phosmet insecticide initiated by HO• radical in gas and water – A theoretical study

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Computational details

Kinetics for FHT and RAF reactions between the phosmet and HO radicals were studied using the pre-reactive complexes scheme proposed by Singleton and Cvetanovic [1]. Briefly, a two-step mechanism was considered:

$$\text{phosmet} + \text{HO} \xrightarrow{k_a} \text{MCR} \quad \text{(R1)}$$

$$\text{MCR} \xrightarrow{k_b} \text{phosmet} + \text{OH} \quad \text{(R2)}$$

$$\text{MCR} \xrightarrow{k_c} \text{TS} \quad \text{(R3)}$$

This scheme involved a fast pre-equilibrium between the reactants and the pre-reactive complex (MCR), leading to the hydrogen abstraction/radical addition followed by post-reactive complexes and products. The effective rate r applied to reactions (R1-R2) for steady-state conditions was defined as follows (eq.1):

$$r = r_c = k\,[\text{OH}]\,[\text{phosmet}] \quad \text{(eq.1)}$$

where k was the total rate constant for each pathway, and it was calculated by the following equation (eq.2):

$$k = \frac{k_c k_a}{k_b + k_c} \quad \text{(eq.2)}$$

The changes in entropy in the reverse reaction (R2) were much more significant than in the reaction (R3). Thus, k_b was expected to be larger than k_c, and k can be written as (eq.3):

$$k = \frac{k_c k_a}{k_b} = k_c K_{a,b} \quad \text{(eq.3)}$$

where $K_{a,b}$ was the equilibrium constant for the separated reactants versus the pre-reactive complex (MCR). The equilibrium constant ($K_{a,b}$) of the first step was computed based on basic statistical thermodynamics principles, while k_c was calculated by conventional TST theory [2] (eq.4) (eq.5).

$$K_{a,b}(T) = \frac{Q_{MCR}(T)}{Q_{OH}(T)Q_{phosmet}(T)} exp\left(\frac{E_{phosmet} + E_{OH} - E_{MCR}}{k_B T}\right) \quad \text{(eq.4)}$$

$$k_c(T) = \kappa(T) \times \frac{k_B T}{h} \times \frac{Q_{TS}(T)}{Q_{MCR}(T)} \times exp\left(-\frac{E_{TS} - E_{MCR}}{k_B T}\right) \quad \text{(eq.5)}$$

where the terms $Q_{OH}(T)$, $Q_{PHOSMET}(T)$, $Q_{MCR}(T)$, and $Q_{TS}(T)$ were the total partition functions of the reactants (HO and phosmet), MCR, and TS at the temperature T (K), respectively. E_{OH}, $E_{PHOSMET}$, E_{MCR}, and E_{TS} were the total potential energies at 0 K (including the zero-point energy corrections) of the HO radical, phosmet, MCR, and TS, respectively. The κ (T) was the transmission coefficient used for the tunneling correction estimated by the Eckart method [3] at the temperature T, k_B and h were the Boltzmann and Planck constants.

For the SET reaction, the reaction barrier was calculated by Marcus' theory [4–6] as follows (eq.6):

$$\Delta_r G_{SET}^{\neq} = \frac{\lambda}{4}\left(1 + \frac{\Delta_r G_{SET}^{0}}{\lambda}\right)^2 \quad \text{(eq.6)}$$

where $\Delta_r G_{SET}^{0}$ was the free energy of reaction calculated by Hess' law, the energy difference between reactants and products. The λ is the nuclear reorganization energy, which is calculated by the below equation (eq.7):

$$\lambda = \Delta H_{SET} - \Delta G_{SET}^{0} \quad \text{(eq.7)}$$

where the ΔH_{SET} was the non-adiabatic energy between the reactants and vertical products.

In the aqueous phase, the apparent rate constant (k_{app}) is typically including a diffusion limit, especially for the reaction with HO radical that has the rate constant close to the diffusion limit of the solution. The k_{app} was calculated based on the Collin-Kimball as follows (eq.8) [7]:

$$k_{app} = \frac{k_D k}{k_D + k} \quad \text{(eq.8)}$$

where k was the thermal rate constant, and k_D was the steady-state Smoluchowski [8] rate constant for an irreversible bimolecular diffusion-controlled reaction (eq.9):

$$k_D = 4\pi R_{AB} D_{AB} N_A \quad \text{(eq.9)}$$

where R_{AB} was reaction distance, N_A was the Avogadro number, and D_{AB} was the mutual diffusion coefficient of reactants, and it can be estimated from D_A and D_B according to Truhlar [9]. The D_A and D_B values were calculated from the Stokes-Einstein approach [10,11] (eq.10):

$$D_{A\ or\ B} = \frac{k_B T}{6\pi\eta a_{A\ or\ B}} \quad \text{(eq.10)}$$

where k_B is the Boltzmann constant, T is the temperature, η denotes the solvent's viscosity varied as a function of temperature, and a is the radius of solute. The rate constants were calculated in a temperature range of 253 – 323 K with the GPOP program [12]. For all the reactions with HO radical, a spin-orbit correction (SOC) value being -0.833 kJ mol^{-1} was applied [13–15].

References

[1] D.L. Singleton, R.J. Cvetanovic, Temperature dependence of the reaction of oxygen atoms with olefins, J. Am. Chem. Soc. 98 (1976) 6812–6819. https://doi.org/10.1021/ja00438a006.

[2] M.G. Evans, M. Polanyi, Some applications of the transition state method to the calculation of reaction velocities, especially in solution, Trans. Faraday Soc. 31 (1935) 875–894. https://doi.org/10.1039/TF9353100875.

[3] C. Eckart, The Penetration of a Potential Barrier by Electrons, Phys. Rev. 35 (1930) 1303–1309. https://doi.org/10.1103/PhysRev.35.1303.

[4] R.A. Marcus, On the Theory of Oxidation-Reduction Reactions Involving Electron Transfer. I, J. Chem. Phys. 24 (1956) 966–978. https://doi.org/10.1063/1.1742723.

[5] R.A. Marcus, On the Theory of Oxidation-Reduction Reactions Involving Electron Transfer. II. Applications to Data on the Rates of Isotopic Exchange Reactions, J. Chem. Phys. 26 (1957) 867–871. https://doi.org/10.1063/1.1743423.

[6] R.A. Marcus, On the Theory of Oxidation-Reduction Reactions Involving Electron Transfer. III. Applications to Data on the Rates of Organic Redox Reactions, J. Chem. Phys. 26 (1957) 872–877. https://doi.org/10.1063/1.1743424.

[7] F.C. Collins, G.E. Kimball, Diffusion-controlled reaction rates, J. Colloid Sci. 4 (1949) 425–437. https://doi.org/10.1016/0095-8522(49)90023-9.

[8] M. V. Smoluchowski, Versuch einer mathematischen Theorie der Koagulationskinetik kolloider Lösungen, Zeitschrift Für Phys. Chemie. 92 (1918) 129. https://doi.org/10.1515/zpch-1918-9209.

[9] D.G. Truhlar, Nearly encounter-controlled reactions: The equivalence of the steady-state and diffusional viewpoints, J. Chem. Educ. 62 (1985) 104. https://doi.org/10.1021/ed062p104.

[10] A. Einstein, Zur Elektrodynamik bewegter Körper, Ann. Phys. 322 (1905) 891–921. https://doi.org/10.1002/andp.19053221004.

[11] G.G. Stokes, Mathematical and Physical Papers, Cambridge University Press, 1905.

[12] A. Miyoshi, GPOP software, rev. 2022.01.20m1, available from the author. See http://akrmys.com/gpop/, (2022). http://akrmys.com/gpop/.

[13] M. Šulka, K. Šulková, F. Louis, P. Neogrády, I. Černušák, A Theoretical Study of the X-Abstraction Reactions (X = H, Br, or I) from CH2IBr by OH Radicals: Implications for Atmospheric Chemistry, Zeitschrift Für Phys. Chemie. 227 (2013) 1337–1359. https://doi.org/doi:10.1524/zpch.2013.0391.

[14] K.P. Huber, G. Herzberg, Molecular Spectra and Molecular Structure. IV. Constants of Diatomic Molecules, Springer US, Boston, MA, 1979. https://doi.org/10.1007/978-1-4757-0961-2.

[15] R. Samzow, B.A. Hess, Spin—orbit effects in the Br atom in the framework of the no-pair theory, Chem. Phys. Lett. 184 (1991) 491–496. https://doi.org/10.1016/0009-2614(91)80024-R.

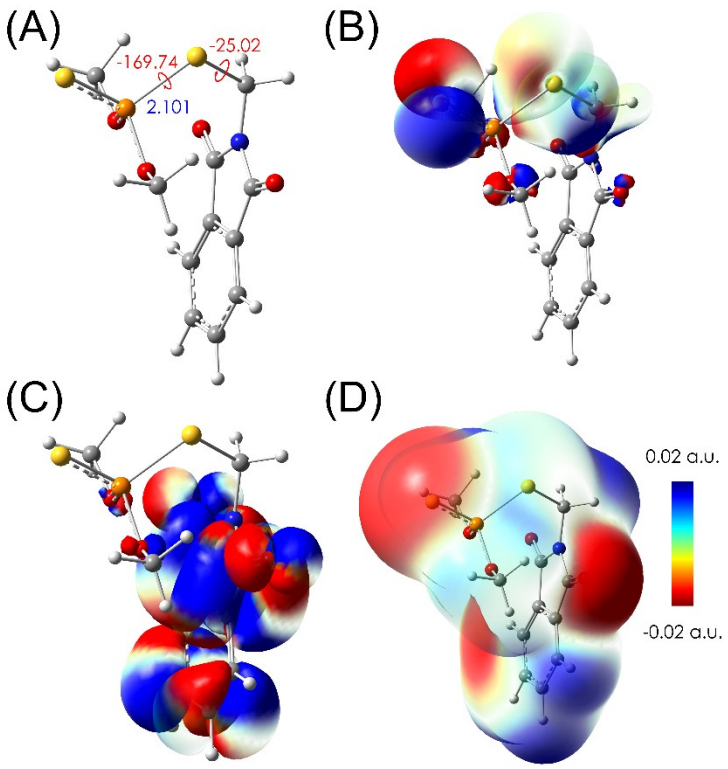


Figure S1: (A) Optimized structure, (B) HOMO, (C) LUMO distributions and (D) electrostatic potential (ESP) maps of phosmet in gas phase (Red represents regions of high negative potential and blue represents regions of high positive potential).

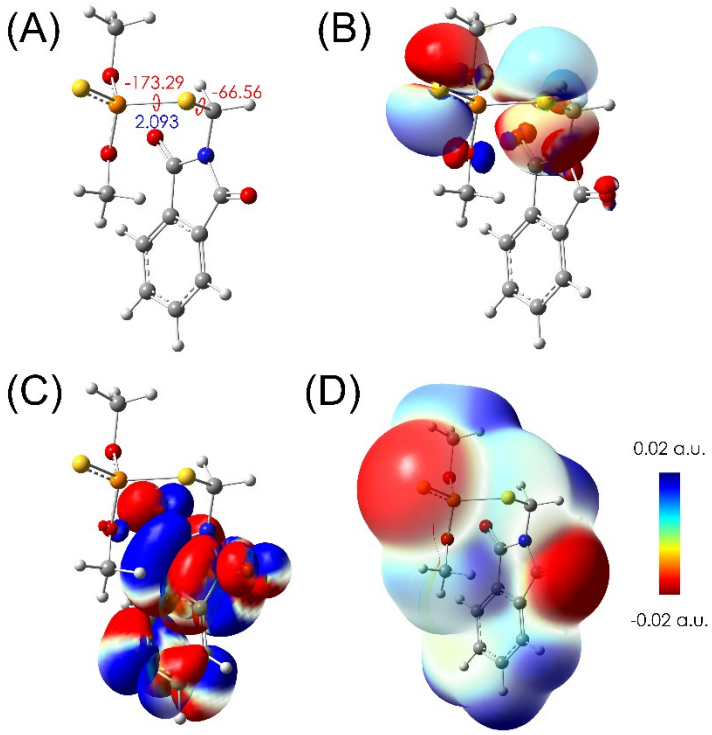


Figure S2: (A) Optimized structure, (B) HOMO, (C) LUMO distributions and (D) electrostatic potential (ESP) maps of phosmet in aqueous phase (Red represents regions of high negative potential and blue represents regions of high positive potential).

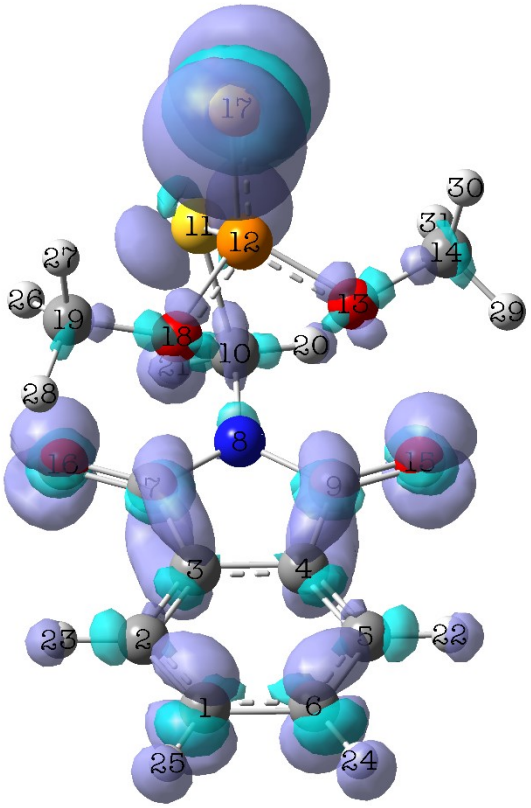


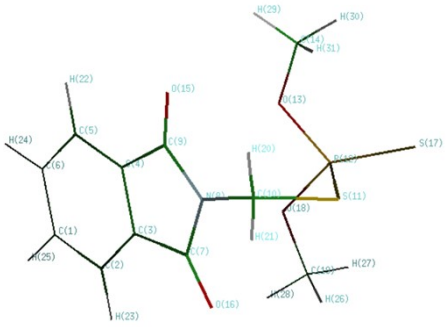
Figure S3: Plot of Fukui function for radical attack (f^0) describing the possible main reactive sites of phosmet calculating in the gas phase.

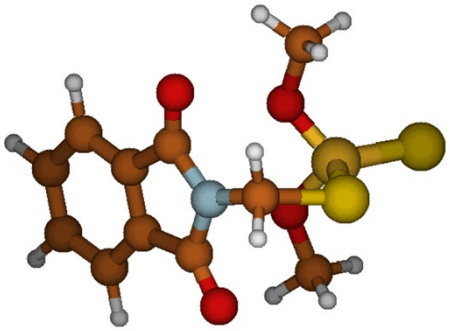
GAS PHASE DATA

Table S1. Structural data for phosmet in the gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

Phosmet

$C_1 - {}^2A$





Optimized Cartesian coordinates			
C	-4.143882	-1.013395	-1.048365
C	-3.205108	-1.485173	-0.124486
C	-2.275184	-0.576946	0.349175
C	-2.271695	0.750973	-0.066236
C	-3.197958	1.230887	-0.975241
C	-4.140158	0.321022	-1.466349
C	-1.157234	-0.767774	1.318460
N	-0.537750	0.484337	1.429650
C	-1.157982	1.459249	0.629221
C	0.649391	0.725226	2.186696
S	2.225105	0.001523	1.503952
P	1.872560	-0.180834	-0.559048
O	1.060495	1.128869	-0.997169
C	1.732697	2.395172	-1.050364
O	-0.837271	2.621741	0.579283
O	-0.819203	-1.758887	1.919563
S	3.510986	-0.615060	-1.468410
O	0.635396	-1.193298	-0.721938
C	0.852623	-2.597685	-0.515145
H	0.772090	1.805686	2.265290
H	0.555383	0.273638	3.175952
H	-3.185236	2.268901	-1.290492
H	-3.200646	-2.516997	0.211716
H	-4.882383	0.654035	-2.184470
H	-4.889692	-1.692583	-1.448431
H	1.180215	-2.778583	0.512409
H	1.589766	-2.968861	-1.230521
H	-0.114459	-3.071830	-0.678437
H	0.962245	3.127317	-1.284047
H	2.504497	2.371843	-1.823059
H	2.178207	2.629431	-0.078539

Vibrational frequencies (cm^{-1})
14, 38, 83, 89, 94, 112, 133, 144, 155, 166, 171, 186, 197, 199, 227, 239, 263, 282, 319, 356, 390, 404, 414, 432, 467, 490, 539, 548, 620, 669, 677, 683, 707, 732, 733, 793, 806, 831, 844, 868, 920, 936, 994, 1025, 1029, 1048, 1093, 1106, 1127, 1144, 1180, 1186, 1189, 1201, 1209, 1214, 1242, 1310, 1325, 1356, 1396, 1447, 1468, 1481, 1485, 1499, 1500, 1505, 1506, 1516, 1517, 1692, 1697, 1851, 1908, 3077, 3082, 3119, 3160, 3170, 3192, 3196, 3210, 3221, 3232, 3241, 3246
Rotational constants (GHz)
0.50843, 0.23933, 0.22925

Table S2. Optimized Cartesian coordinates for the stationary points involved in the H20-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

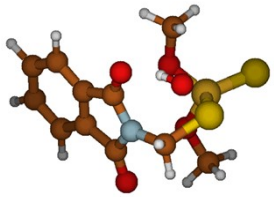
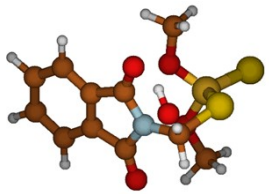
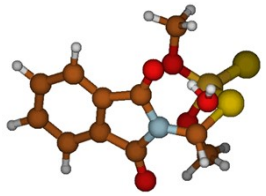
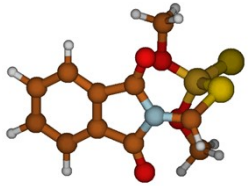
MCR(H20-abs)				TS(H20-abs)				MCP(H20-abs)				Rad(H20-abs)			
															
C	-4.375997	-1.069946	-0.725254	C	-4.218065	-1.630499	-0.016762	C	4.401702	-1.405346	0.364636	C	4.351474	0.152965	-1.330503
C	-3.445684	-1.436685	0.253390	C	-3.276953	-1.364557	0.983527	C	3.476985	-1.420495	-0.685250	C	3.434375	1.128435	-0.926068
C	-2.413969	-0.550003	0.504704	C	-2.313600	-0.411357	0.704795	C	2.435115	-0.512065	-0.620498	C	2.416347	0.724477	-0.079509
C	-2.304140	0.656344	-0.178714	C	-2.280748	0.260350	-0.513311	C	2.309084	0.380557	0.438395	C	2.304641	-0.591998	0.354083
C	-3.219688	1.033706	-1.144676	C	-3.209783	0.012046	-1.507910	C	3.220736	0.411466	1.478657	C	3.209100	-1.565042	-0.033925
C	-4.265386	0.143199	-1.411700	C	-4.185225	-0.954490	-1.240470	C	4.276280	-0.505336	1.427455	C	4.241114	-1.170503	-0.891687
C	-1.281979	-0.643707	1.469913	C	-1.191637	0.088812	1.549078	C	1.300603	-0.287821	-1.559967	C	1.297192	1.510900	0.508514
N	-0.538502	0.545368	1.297445	N	-0.524618	1.049080	0.754725	N	0.542857	0.774892	-0.998840	N	0.560402	0.596914	1.302252
C	-1.093847	1.366404	0.320293	C	-1.134971	1.211044	-0.492905	C	1.101706	1.220075	0.209220	C	1.117196	-0.703843	1.248197
C	0.714260	0.775648	1.957941	C	0.669167	1.701046	1.158246	C	-0.682637	1.176352	-1.524103	C	-0.633361	0.951279	1.915441
S	2.219946	0.778864	0.871370	S	2.215713	1.241752	0.276811	S	-2.145640	1.138498	-0.577038	S	-2.116351	0.082013	1.608484
P	1.748074	-0.644729	-0.605628	P	1.869022	-0.753312	-0.310339	P	-1.907221	-0.728816	0.425954	P	-1.979308	-0.192834	-0.507247
O	0.511156	-0.028114	-1.430506	O	0.631705	-0.711924	-1.335161	O	-0.684020	-0.508290	1.446296	O	-0.784063	-1.241274	-0.725104
C	0.767400	1.018101	-2.379744	C	0.853230	-0.238648	-2.673075	C	-0.915943	0.222864	2.659218	C	-1.018145	-2.629262	-0.437959
O	-0.655330	2.443907	-0.026786	O	-0.776697	1.997728	-1.341824	O	0.676071	2.128397	0.889014	O	0.700323	-1.666885	1.838968
O	-1.025621	-1.505146	2.272594	O	-0.882498	-0.206646	2.675108	O	1.029792	-0.851066	-2.588574	O	1.022748	2.676954	0.374651
S	3.316968	-1.148616	-1.593614	S	3.507833	-1.557098	-0.912108	S	-3.576473	-1.351926	1.148241	S	-3.695858	-0.608303	-1.266126
O	0.889201	-1.773529	0.140676	O	1.055806	-1.430903	0.891705	O	-1.087571	-1.646954	-0.598766	O	-1.165206	1.085396	-1.024772
C	1.545439	-2.698927	1.019186	C	1.731234	-1.738472	2.120528	C	-1.731629	-2.147410	-1.779627	C	-1.803111	2.370107	-1.067750
H	0.734950	1.764739	2.420910	H	0.566916	2.860940	0.951811	H	-0.302260	3.553209	-0.109660	H	-0.695300	1.976833	2.257731
H	0.818653	-0.003943	2.713285	H	0.786008	1.577680	2.236050	H	-0.750534	1.275372	-2.598409	H	3.114080	-2.587401	0.317209
H	-3.125826	1.980636	-1.666402	H	-3.177419	0.547954	-2.450929	H	3.114365	1.118725	2.294710	H	3.509262	2.158673	-1.257687
H	-3.521393	-2.374604	0.793289	H	-3.293851	-1.879881	1.938023	H	3.564503	-2.112162	-1.516429	H	4.970782	-1.902004	-1.223458
H	-5.005658	0.396824	-2.163441	H	-4.931776	-1.184321	-1.993639	H	5.012487	-0.519648	2.224489	H	5.164152	0.425246	-1.995984
H	-5.199466	-1.737355	-0.957281	H	-4.989187	-2.373573	0.158045	H	5.232557	-2.103240	0.355670	H	-2.153069	2.652930	-0.070207
H	2.124927	-2.161252	1.776712	H	2.189802	-0.836620	2.537970	H	-2.082518	-1.316779	-2.399460	H	-2.640142	2.346390	-1.769330
H	2.202903	-3.352901	0.442258	H	2.493384	-2.500273	1.942619	H	-2.567331	-2.793856	-1.501611	H	-1.034863	3.067915	-1.395155
H	0.748118	-3.263610	1.498859	H	0.959980	-2.102629	2.796360	H	-0.966721	-2.704246	-2.317340	H	-0.078106	-3.136204	-0.651155
H	-0.208020	1.310252	-2.767336	H	-0.111740	-0.309178	-3.173612	H	0.043187	0.250222	3.175016	H	-1.816284	-3.010997	-1.078533
H	1.405463	0.643007	-3.182637	H	1.592799	-0.868192	-3.172445	H	-1.664948	-0.290732	3.265947	H	-1.269720	-2.755228	0.618825
H	1.237030	1.872896	-1.883475	H	1.180821	0.804568	-2.651486	H	-1.236133	1.242882	2.427608				
O	1.783604	3.585550	1.028822	O	0.242456	4.085815	0.417677	O	-0.631512	4.069724	-0.860286				
H	0.963551	3.348538	0.543022	H	-0.027540	3.780978	-0.472473	H	-0.608607	4.991562	-0.587550				

Table S3. Optimized Cartesian coordinates for the stationary points involved in the H21-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

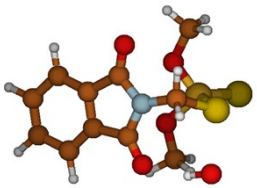
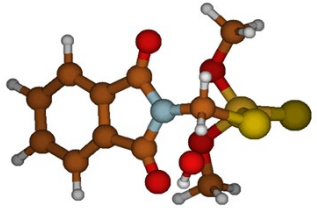
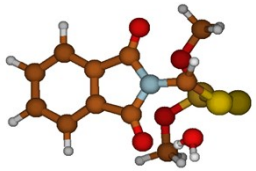
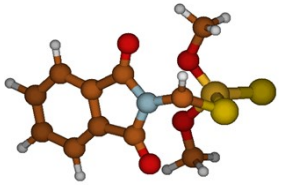
MCR(H21-abs)				TS(H21-abs)				MCP(H21-abs)				Rad(H21-abs)			
															
C	-4.265275	0.142987	1.411758	C	4.185096	-0.954349	-1.240567	C	4.276373	-0.505141	-1.427570	C	-4.241113	-1.170505	-0.891682
C	-3.219610	1.033547	1.144793	C	3.209655	0.012203	-1.507956	C	3.220778	0.411607	-1.478640	C	-3.209100	-1.565042	-0.033918
C	-2.304086	0.656303	0.178761	C	2.280674	0.260522	-0.513312	C	2.309137	0.380506	-0.438371	C	-2.304641	-0.591997	0.354087
C	-2.413910	-0.549971	-0.504779	C	2.313594	-0.411169	0.704803	C	2.435243	-0.512261	0.620387	C	-2.416345	0.724477	-0.079511
C	-3.445598	-1.436706	-0.253526	C	3.276954	-1.364374	0.983490	C	3.477166	-1.420640	0.685018	C	-3.434372	1.128432	-0.926072
C	-4.375884	-1.070089	0.725186	C	4.217997	-1.630349	-0.016857	C	4.401868	-1.405293	-0.364876	C	-4.351472	0.152961	-1.330504
C	-1.093826	1.366457	-0.320209	C	1.134872	1.211190	-0.492866	C	1.101755	1.219964	-0.209006	C	-1.117195	-0.703839	1.248201
N	-0.538461	0.545537	-1.297418	N	0.524634	1.049284	0.754831	N	0.542962	0.774583	0.999013	N	-0.560399	0.596917	1.302250
C	-1.281938	-0.643551	-1.470013	C	1.191679	0.089006	1.549147	C	1.300765	-0.288187	1.559942	C	-1.297189	1.510901	0.508511
C	0.714301	0.775835	-1.957887	C	-0.669258	1.701071	1.158324	C	-0.682472	1.175955	1.524425	C	0.633362	0.951283	1.915441
S	2.219960	0.778980	-0.871266	S	-2.215758	1.241552	0.276934	S	-2.145443	1.138659	0.577209	S	2.116355	0.082019	1.608481
P	1.748065	-0.644750	0.605574	P	-1.868850	-0.753437	-0.310310	P	-1.907360	-0.728506	-0.426001	P	1.979307	-0.192835	-0.507247
O	0.889170	-1.773457	-0.140858	O	-1.055466	-1.431009	0.891630	O	-1.087783	-1.646803	0.598659	O	1.165207	1.085393	-1.024779
C	1.545414	-2.698824	-1.019387	C	-1.730729	-1.738745	2.120497	C	-1.732285	-2.148054	1.778936	C	1.803103	2.370109	-1.067748
O	-1.025569	-1.504878	-2.272804	O	0.882582	-0.206456	2.675187	O	1.030043	-0.851580	2.588495	O	-1.022743	2.676954	0.374640
O	-0.655424	2.443988	0.026946	O	0.776486	1.997803	-1.341801	O	0.676032	2.128370	-0.888627	O	-0.700323	-1.666879	1.838977
S	3.316934	-1.148735	1.593550	S	-3.507608	-1.557369	-0.912026	S	-3.576784	-1.351303	-1.148201	S	3.695855	-0.608314	-1.266127
O	0.511108	-0.028240	1.430473	O	-0.631597	-0.711826	-1.335190	O	-0.684158	-0.508122	-1.446375	O	0.784059	-1.241273	-0.725097
C	0.767300	1.017772	2.379937	C	-0.853310	-0.238785	-2.673150	C	-0.916034	0.222892	-2.659382	C	1.018140	-2.629262	-0.437958
H	0.818707	-0.003721	-2.713265	H	-0.786068	1.577690	2.236127	H	-0.750467	1.273817	2.598832	H	0.695301	1.976839	2.257727
H	0.735026	1.764951	-2.420804	H	-0.567163	2.860937	0.951728	H	-0.301584	3.552973	0.110323	H	-3.509258	2.158669	-1.257696
H	-3.521309	-2.374565	-0.793528	H	3.293905	-1.879681	1.937996	H	3.564711	-2.112403	1.516113	H	-3.114081	-2.587400	0.317221
H	-3.125751	1.980429	1.666607	H	3.177244	0.548101	-2.450980	H	3.114368	1.118965	-2.294601	H	-5.164149	0.425240	-1.995987
H	-5.199332	-1.737539	0.957173	H	4.989113	-2.373439	0.157909	H	5.232773	-2.103129	-0.356028	H	-4.970782	-1.902006	-1.223451
H	-5.005528	0.396512	2.163552	H	4.931597	-1.184202	-1.993779	H	5.012571	-0.519297	-2.224615	H	1.269712	-2.755233	0.618827
H	1.236788	1.872734	1.883818	H	-1.181290	0.804310	-2.651676	H	-1.236219	1.242947	-2.427910	H	1.816278	-3.010995	-1.078532
H	1.405468	0.642568	3.182693	H	-1.592648	-0.868659	-3.172443	H	-1.665041	-0.290752	-3.266065	H	0.078101	-3.136203	-0.651158
H	-0.208130	1.309719	2.767659	H	0.111683	-0.309005	-3.173681	H	0.043108	0.250168	-3.175160	H	1.034866	3.067904	-1.395204
H	0.748080	-3.263319	-1.499264	H	-0.959473	-2.103545	2.795980	H	-0.966668	-2.702312	2.318310	H	2.640171	2.346387	-1.769285
H	2.202688	-3.352976	-0.442445	H	-2.493295	-2.500107	1.942498	H	-2.565768	-2.796987	1.500095	H	2.153006	2.652952	-0.070191
H	2.125105	-2.161128	-1.776745	H	-2.188721	-0.836827	2.538420	H	-2.086557	-1.317931	2.397551				
O	1.783385	3.585573	-1.028610	O	-0.243376	4.085944	0.417371	O	-0.631081	4.069663	0.860723				
H	0.963437	3.348453	-0.542672	H	0.026903	3.781092	-0.472689	H	-0.608105	4.991438	0.587782				

Table S4. Optimized Cartesian coordinates for the stationary points involved in the H22-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

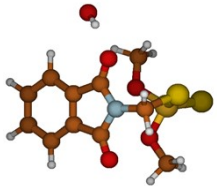
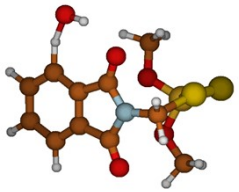
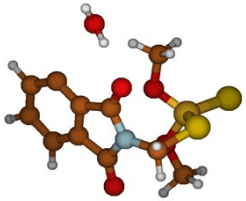
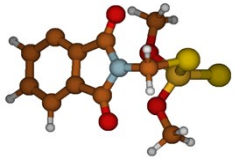
MCR(H22-abs)				TS(H22-abs)				MCP(H22-abs)				Rad(H22-abs)			
															
C	-3.908127	-1.209899	-1.469466	C	-3.793764	-1.250669	-1.520455	C	-3.846999	-1.303423	-1.498671	C	4.162498	0.194123	-1.470089
C	-2.892579	-1.940477	-0.842345	C	-2.761085	-1.975256	-0.912207	C	-2.800814	-2.002223	-0.881773	C	3.230916	1.126332	-0.997417
C	-2.053074	-1.246928	0.009867	C	-1.945803	-1.298764	-0.022637	C	-1.990562	-1.303758	-0.005449	C	2.297392	0.693382	-0.072521
C	-2.209850	0.117106	0.243938	C	-2.146968	0.048982	0.265988	C	-2.196865	0.050879	0.274601	C	2.268646	-0.624431	0.394327
C	-3.208698	0.852744	-0.371077	C	-3.160555	0.753246	-0.338266	C	-3.232768	0.699277	-0.341236	C	3.198178	-1.503213	-0.090826
C	-4.060998	0.160114	-1.239434	C	-3.996158	0.108191	-1.245264	C	-4.069257	0.055618	-1.234887	C	4.153357	-1.134246	-1.018795
C	-0.885281	-1.730112	0.799745	C	-0.758124	-1.763088	0.754239	C	-0.804879	-1.762660	0.775526	C	1.194282	1.446325	0.595833
N	-0.397505	-0.592189	1.478407	N	-0.314393	-0.633358	1.475252	N	-0.357703	-0.626804	1.480896	N	0.554359	0.514421	1.427428
C	-1.147780	0.543662	1.198069	C	-1.106915	0.485792	1.237791	C	-1.147895	0.493720	1.236273	C	1.144606	-0.756657	1.369434
C	0.818144	-0.587511	2.235160	C	0.905748	-0.610229	2.225118	C	0.865032	-0.596912	2.226746	C	-0.639693	0.802652	2.158795
S	2.244920	0.335790	1.481110	S	2.289667	0.394418	1.495697	S	2.246650	0.400025	1.484871	S	-2.211215	0.055494	1.494939
P	1.934898	0.134922	-0.589430	P	1.965844	0.267343	-0.579429	P	1.939583	0.206318	-0.588719	P	-1.846239	-0.190537	-0.559946
O	0.554885	0.892793	-0.913791	O	0.552458	0.978307	-0.858821	O	0.524569	0.894630	-0.899890	O	-0.612317	-1.212244	-0.682734
C	0.535771	2.327398	-0.983247	C	0.470638	2.414215	-0.854197	C	0.430570	2.330983	-0.958738	C	-0.836253	-2.611207	-0.443326
O	-0.928962	1.635968	1.684198	O	-0.949791	1.572479	1.752027	O	-0.969016	1.578886	1.747271	O	0.780522	-1.711959	2.007766
O	-0.428253	-2.840459	0.902953	O	-0.259317	-2.858224	0.814443	O	-0.313516	-2.860618	0.852198	O	0.899101	2.612393	0.499327
S	3.504514	0.674954	-1.557446	S	3.502305	0.912190	-1.536072	S	3.481714	0.827352	-1.553484	S	-3.479181	-0.641835	-1.469658
O	1.349494	-1.342482	-0.797284	O	1.441184	-1.224268	-0.844228	O	1.430418	-1.298442	-0.805721	O	-1.022728	1.102617	-1.026514
C	2.216170	-2.476771	-0.655599	C	2.356452	-2.325310	-0.756673	C	2.350576	-2.389169	-0.669837	C	-1.688053	2.369734	-1.125070
H	0.660896	-0.095324	3.196792	H	0.736249	-0.160323	3.205202	H	0.699013	-0.137784	3.203173	H	-0.560542	0.401788	3.170935
H	1.106108	-1.628899	2.382264	H	1.234253	-1.644477	2.332299	H	1.192027	-1.630733	2.342731	H	-0.752410	1.886830	2.181256
H	-3.313156	1.919896	-0.198291	H	-3.275178	1.980470	-0.077995	H	-2.870485	4.239012	0.609186	H	3.231348	2.154667	-1.342560
H	-2.758987	-3.002968	-1.016155	H	-2.596431	-3.024436	-1.133258	H	-2.620773	-3.052166	-1.085939	H	4.881540	-1.845652	-1.394877
H	-4.854798	0.698307	-1.747001	H	-4.796666	0.648448	-1.739414	H	-4.879587	0.584261	-1.726410	H	4.906454	0.498874	-2.199438
H	-4.587139	-1.713005	-2.150129	H	-4.450631	-1.746272	-2.228162	H	-4.497337	-1.819077	-2.198349	H	-2.439616	2.331864	-1.916835
H	2.718313	-2.453999	0.316967	H	2.860958	-2.325370	0.214906	H	2.856088	-2.344189	0.300358	H	-2.158788	2.627107	-0.171039
H	2.956803	-2.477982	-1.458281	H	3.093261	-2.258060	-1.560115	H	3.087399	-2.353642	-1.475372	H	-0.908749	3.093803	-1.354858
H	1.568775	-3.349774	-0.714165	H	1.747498	-3.222160	-0.854275	H	1.745946	-3.292489	-0.727955	H	0.135944	-3.088603	-0.560735
H	-0.492366	2.599022	-1.228840	H	-0.578747	2.652472	-1.030120	H	-0.619678	2.558728	-1.139170	H	-1.197504	-2.763409	0.577598
H	1.215341	2.672974	-1.765070	H	1.098632	2.822725	-1.648559	H	1.058831	2.707233	-1.768673	H	-1.550204	-3.001913	-1.171537
H	0.815120	2.754573	-0.015197	H	0.778296	2.802433	0.121324	H	0.736926	2.762980	-0.001105				
O	-1.908234	3.894077	0.318743	O	-3.016780	3.103552	0.314522	O	-2.363207	3.530755	0.202407				
H	-1.600358	3.251626	0.998873	H	-2.332788	2.894762	0.984674	H	-1.942821	3.037008	0.924450				

Table S5. Optimized Cartesian coordinates for the stationary points involved in the H23-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

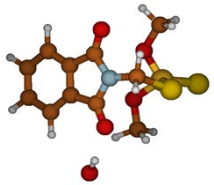
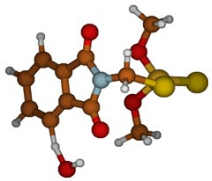
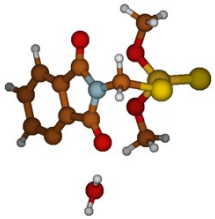
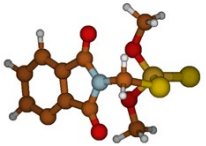
MCR(H23-abs)				TS(H23-abs)				MCP(H23-abs)				Rad(H23-abs)			
															
C	4.060823	0.160215	-1.239535	C	-3.995982	-0.108285	-1.245341	C	-4.068906	-0.055976	-1.235071	C	-4.153418	-1.134191	-1.018799
C	3.208556	0.852755	-0.371084	C	-3.160435	-0.753282	-0.338252	C	-3.232413	-0.699366	-0.341239	C	-3.198226	-1.503198	-0.090860
C	2.209822	0.117005	0.243988	C	-2.146965	-0.048956	0.266122	C	-2.196754	-0.050688	0.274711	C	-2.268670	-0.624440	0.394296
C	2.053066	-1.247018	0.009911	C	-1.945808	1.298782	-0.022558	C	-1.990607	1.303939	-0.005499	C	-2.297403	0.693385	-0.072521
C	2.892550	-1.940478	-0.842407	C	-2.761015	1.975211	-0.912244	C	-2.800868	2.002146	-0.882022	C	-3.230936	1.126371	-0.997391
C	3.907991	-1.209807	-1.469584	C	-3.793614	1.250573	-1.520562	C	-3.846862	1.303091	-1.498951	C	-4.162542	0.194188	-1.470065
C	1.147768	0.543585	1.198115	C	-1.106881	-0.485720	1.237916	C	-1.147739	-0.493309	1.236420	C	-1.144624	-0.756706	1.369382
N	0.397485	-0.592270	1.478468	N	-0.314387	0.633461	1.475350	N	-0.357637	0.627285	1.480901	N	-0.554367	0.514371	1.427414
C	0.885287	-1.730191	0.799833	C	-0.758114	1.763145	0.754267	C	-0.804885	1.763004	0.775340	C	-1.194286	1.446301	0.595857
C	-0.818159	-0.587595	2.235201	C	0.905789	0.610327	2.225157	C	0.865301	0.597531	2.226440	C	0.639673	0.802563	2.158812
S	-2.245015	0.335590	1.481073	S	2.289678	-0.394298	1.495660	S	2.246357	-0.400410	1.484878	S	2.211203	0.055417	1.494955
P	-1.934814	0.134926	-0.589405	P	1.965761	-0.267373	-0.579468	P	1.939462	-0.206502	-0.588739	P	1.846259	-0.190517	-0.559943
O	-1.349250	-1.342398	-0.797348	O	1.440928	1.224167	-0.844329	O	1.430866	1.298496	-0.805535	O	1.022780	1.102675	-1.026469
C	-2.215789	-2.476809	-0.655829	C	2.356078	2.325311	-0.756815	C	2.351437	2.388855	-0.669489	C	1.688138	2.369782	-1.124964
O	0.428272	-2.840543	0.903059	O	-0.259285	2.858280	0.814348	O	-0.313521	2.860975	0.851760	O	-0.899095	2.612369	0.499367
O	0.928981	1.635918	1.684167	O	-0.949723	-1.572388	1.752174	O	-0.968864	-1.578386	1.747614	O	-0.780549	-1.712020	2.007702
S	-3.504430	0.674871	-1.557497	S	3.502251	-0.912092	-1.536140	S	3.481314	-0.828070	-1.553602	S	3.479207	-0.641806	-1.469648
O	-0.554886	0.892996	-0.913660	O	0.552436	-0.978490	-0.858743	O	0.524201	-0.894213	-0.900021	O	0.612323	-1.212205	-0.682794
C	-0.535937	2.327582	-0.983162	C	0.470726	-2.414403	-0.853938	C	0.429524	-2.330490	-0.959196	C	0.836258	-2.611180	-0.443443
H	-1.106121	-1.628975	2.382360	H	1.234306	1.644574	2.332297	H	1.192655	1.631338	2.341543	H	0.752401	1.886739	2.181316
H	-0.660958	-0.095317	3.196791	H	0.736343	0.160463	3.205268	H	0.699478	0.139202	3.203277	H	0.560504	0.401653	3.170932
H	2.759040	-3.002966	-1.016292	H	-2.596357	3.024383	-1.133333	H	-2.620982	3.052084	-1.086350	H	-3.231358	2.154714	-1.342508
H	3.312918	1.919906	-0.198238	H	-3.275036	-1.980571	-0.078043	H	-2.870958	-4.237939	0.611766	H	-4.906507	0.498967	-2.199393
H	4.586957	-1.712859	-2.150335	H	-4.450424	1.746123	-2.228358	H	-4.497183	1.818559	-2.198784	H	-4.881620	-1.845575	-1.394886
H	4.854549	0.698443	-1.747180	H	-4.796413	-0.648593	-1.739564	H	-4.879038	-0.584827	-1.726692	H	1.197549	-2.763425	0.577461
H	-0.815630	2.754787	-0.015222	H	0.778182	-2.802445	0.121717	H	0.736165	-2.762927	-0.001856	H	1.550174	-3.001867	-1.171697
H	-1.215323	2.673045	-1.765196	H	1.098939	-2.822983	-1.648093	H	1.057189	-2.706793	-1.769568	H	-0.135950	-3.088557	-0.560830
H	0.492230	2.599348	-1.228467	H	-0.578599	-2.652764	-1.030070	H	-0.620915	-2.557737	-1.139194	H	0.908864	3.093875	-1.354776
H	-1.568196	-3.349709	-0.713772	H	1.746949	3.222098	-0.853902	H	1.747052	3.292395	-0.726799	H	2.439741	2.331909	-1.916690
H	-2.955958	-2.478372	-1.458937	H	3.092571	2.258398	-1.560573	H	3.087834	2.353551	-1.475422	H	2.158829	2.627122	-0.170902
H	-2.718518	-2.453861	0.316432	H	2.860978	2.325177	0.214563	H	2.857467	2.343164	0.300405				
O	1.908101	3.894491	0.318903	O	-3.016610	-3.103629	0.314436	O	-2.362819	-3.531133	0.203518				
H	1.600333	3.251966	0.998994	H	-2.332690	-2.894911	0.984675	H	-1.942244	-3.036281	0.924718				

Table S6. Optimized Cartesian coordinates for the stationary points involved in the H24-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

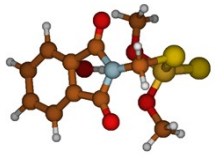
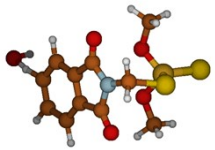
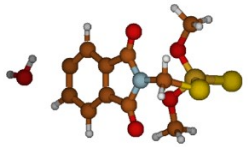
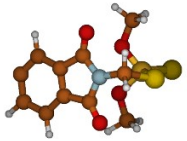
MCR(H24-abs)				TS(H24-abs)				MCP(H24-abs)				Rad(H24-abs)			
															
C	-4.103221	0.153520	-1.222538	C	-3.870674	-0.828599	-1.009526	C	-3.954344	-0.735757	0.303350	C	-4.165758	-1.023670	-1.120987
C	-3.124742	-0.843060	-1.298859	C	-2.749377	-1.633069	-0.765821	C	-2.872993	-0.770505	1.198211	C	-3.241231	-1.466635	-0.161271
C	-2.164636	-0.862231	-0.302666	C	-1.806138	-1.149784	0.124756	C	-1.825982	0.108824	0.969647	C	-2.317080	-0.544454	0.302693
C	-2.172860	0.062903	0.738899	C	-1.954365	0.076294	0.766205	C	-1.826108	1.005272	-0.096019	C	-2.292302	0.773754	-0.146515
C	-3.135826	1.053685	0.824623	C	-3.056774	0.887927	0.547598	C	-2.880567	1.071498	-0.999191	C	-3.195635	1.245775	-1.090787
C	-4.107405	1.086424	-0.182356	C	-3.994615	0.389719	-0.350812	C	-3.895719	0.173226	-0.734901	C	-4.094444	0.293036	-1.529947
C	-1.000348	-1.773399	-0.112602	C	-0.516447	-1.755893	0.569445	C	-0.557584	0.292980	1.731362	C	-1.221061	-0.717866	1.298714
N	-0.362673	-1.325539	1.058288	N	0.041507	-0.837798	1.469210	N	0.140357	1.312080	1.066318	N	-0.591963	0.531936	1.391566
C	-1.017838	-0.228465	1.635895	C	-0.771944	0.292610	1.652303	C	-0.563932	1.801596	-0.045375	C	-1.185655	1.491186	0.555893
C	0.861263	-1.870472	1.546063	C	1.338632	-0.976362	2.052867	C	1.461802	1.732773	1.410021	C	0.582694	0.781008	2.166353
S	2.403622	-0.871410	1.211941	S	2.788319	-0.732637	0.907695	S	2.834853	0.529905	1.036253	S	2.165162	0.029855	1.531630
P	1.913744	0.411018	-0.369642	P	2.045738	0.477282	-0.641678	P	2.092148	-0.641889	-0.541550	P	1.849343	-0.204505	-0.532355
O	0.684421	1.330209	0.139172	O	1.080443	1.554751	0.047802	O	1.290494	0.356378	-1.505046	O	1.054116	1.098497	-1.019067
C	0.935918	2.377756	1.097629	C	1.650295	2.619714	0.823134	C	2.015456	1.288283	-2.319787	C	1.737858	2.357495	-1.098305
O	-0.672026	0.317311	2.656014	O	-0.536487	1.205405	2.404849	O	-0.198883	2.703240	-0.759739	O	-0.857202	2.649685	0.481227
O	-0.644653	-2.719878	-0.771907	O	-0.017723	-2.811366	0.263104	O	-0.164656	-0.273327	2.722501	O	-0.904100	-1.695590	1.931818
S	3.491538	1.313866	-0.991138	S	3.494141	1.092085	-1.746965	S	3.502322	-1.723230	-1.277794	S	3.500356	-0.672858	-1.399989
O	1.028419	-0.424908	-1.411846	O	0.867779	-0.359237	-1.346460	O	0.789469	-1.393012	0.024123	O	0.607688	-1.212566	-0.690031
C	1.657896	-1.419976	-2.235767	C	1.213934	-1.459997	-2.202047	C	0.957577	-2.499911	0.923694	C	0.812330	-2.612661	-0.444436
H	0.821563	-1.947406	2.633816	H	1.411865	-0.248100	2.860812	H	1.658662	2.659955	0.871266	H	0.712463	1.862028	2.222484
H	0.993383	-2.851280	1.089227	H	1.465271	-1.991118	2.434200	H	1.531568	1.890087	2.487891	H	0.464593	0.353707	3.163730
H	-3.126914	1.775084	1.635086	H	-3.174521	1.842890	1.048942	H	-2.883948	1.769676	-1.829776	H	-3.179770	2.272171	-1.442230
H	-3.107557	-1.568350	-2.105461	H	-2.620312	-2.594473	-1.252782	H	-2.853205	-1.456313	2.039663	H	-3.246286	-2.488053	0.206689
H	-4.870590	1.857098	-0.162902	H	-5.002709	1.051690	-0.568519	H	-6.148109	-0.627518	-1.836425	H	-4.912580	-1.699320	-1.525370
H	-4.867408	0.212703	-1.990340	H	-4.642409	-1.151480	-1.700672	H	-4.812745	-1.391555	0.409531	H	1.126016	-2.769322	0.591405
H	2.406013	-0.948094	-2.876372	H	1.744012	-2.226478	-1.629868	H	1.452262	-2.165563	1.839875	H	1.555607	-3.007126	-1.140678
H	2.119345	-2.188933	-1.609530	H	1.823558	-1.104831	-3.035733	H	1.532133	-3.290726	0.436480	H	-0.155904	-3.084454	-0.607753
H	0.857688	-1.862958	-2.824912	H	0.267652	-1.862276	-2.561778	H	-0.049283	-2.844292	1.156885	H	0.978525	3.087883	-1.370705
H	-0.020410	2.881371	1.235253	H	0.806056	3.153813	1.254688	H	1.260749	1.907837	-2.800293	H	2.524682	2.303911	-1.854108
H	1.265737	1.937613	2.041502	H	2.242549	3.270901	0.176475	H	2.612666	0.747231	-3.057167	H	2.165648	2.618619	-0.125389
H	1.682498	3.067429	0.698899	H	2.275345	2.213247	1.624260	H	2.662069	1.914520	-1.697147				
O	-1.594827	2.419768	-1.248699	O	-5.852603	1.849405	-1.046125	O	-6.551352	-1.251927	-1.222730				
H	-0.823190	1.869684	-0.992295	H	-5.318781	2.313382	-1.714957	H	-7.388560	-1.516851	-1.616129				

Table S7. Optimized Cartesian coordinates for the stationary points involved in the H25-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

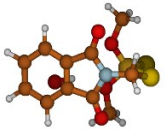
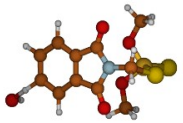
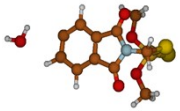
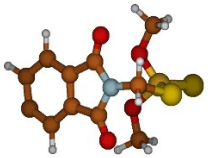
MCR(H25-abs)				TS(H25-abs)				MCP(H25-abs)				Rad(H25-abs)			
															
C	4.107267	1.086525	-0.182663	C	-3.994692	-0.373629	-0.307738	C	3.895017	0.660020	0.194176	C	-4.093748	-1.012395	-1.132183
C	3.135733	1.053916	0.824368	C	-3.058515	-0.687476	0.672478	C	2.884587	0.814293	1.123212	C	-3.200961	-1.559613	-0.230761
C	2.172843	0.063040	0.738898	C	-1.948669	0.141544	0.720127	C	1.827731	-0.071684	0.951468	C	-2.295718	-0.643512	0.290139
C	2.164629	-0.862296	-0.302493	C	-1.792407	1.211172	-0.156441	C	1.820475	-1.020278	-0.068103	C	-2.313779	0.700503	-0.074712
C	3.124679	-0.843242	-1.298738	C	-2.733581	1.511221	-1.126375	C	2.862722	-1.140492	-0.974588	C	-3.232115	1.208282	-0.979823
C	4.103095	0.153421	-1.222660	C	-3.862237	0.684156	-1.200465	C	3.945834	-0.258286	-0.836206	C	-4.157592	0.307788	-1.531105
C	1.017836	-0.228187	1.635961	C	-0.760249	0.096925	1.624017	C	0.564294	-0.212195	1.735215	C	-1.185162	-0.849748	1.268438
N	0.362679	-1.325374	1.058552	N	0.054124	1.164275	1.225046	N	-0.139689	-1.257949	1.126705	N	-0.593890	0.407995	1.435232
C	1.000363	-1.773449	-0.112252	C	-0.503393	1.893390	0.160985	C	0.557176	-1.805153	0.033602	C	-1.224139	1.400918	0.663527
C	-0.861213	-1.870241	1.546484	C	1.353327	1.423112	1.761293	C	-1.457288	-1.661561	1.502405	C	0.584504	0.642550	2.209291
S	-2.403719	-0.871583	1.211718	S	2.694642	0.218607	1.290158	S	-2.839411	-0.492853	1.056278	S	2.172375	-0.046866	1.521687
P	-1.913696	0.410901	-0.369746	P	2.045389	-0.616080	-0.525649	P	-2.092579	0.625117	-0.558332	P	1.848414	-0.138707	-0.552421
O	-1.027943	-0.424818	-1.411742	O	1.387530	0.580505	-1.364330	O	-1.274685	-0.398207	-1.480131	O	1.023489	1.179893	-0.936978
C	-1.657013	-1.419771	-2.236104	C	2.232059	1.589094	-1.938023	C	-1.984999	-1.364848	-2.267411	C	1.680692	2.455183	-0.926778
O	0.644656	-2.720048	-0.771375	O	-0.016899	2.879496	-0.335435	O	0.177935	-2.739917	-0.628764	O	-0.926124	2.570215	0.662906
O	0.672020	0.317761	2.655987	O	-0.510122	-0.663502	2.526916	O	0.187084	0.405325	2.701733	O	-0.837521	-1.858448	1.832683
S	-3.491543	1.313421	-0.991591	S	3.462669	-1.646375	-1.317808	S	-3.507509	1.665750	-1.342951	S	3.501938	-0.509458	-1.461600
O	-0.684662	1.330346	0.139347	O	0.658910	-1.366754	-0.211484	O	-0.801518	1.409587	-0.010628	O	0.625953	-1.157964	-0.776357
C	-0.936553	2.377770	1.097819	C	0.690259	-2.618052	0.493320	C	-0.989234	2.544032	0.849492	C	0.859610	-2.568015	-0.634095
H	-0.993198	-2.851281	1.090106	H	1.650505	2.417748	1.428215	H	-1.652733	-2.621668	1.024349	H	0.692390	1.722173	2.316534
H	-0.821575	-1.946627	2.634276	H	1.319553	1.374510	2.851133	H	-1.520747	-1.749841	2.588410	H	0.487856	0.165661	3.186395
H	3.107509	-1.568684	-2.105204	H	-2.595527	2.350148	-1.800583	H	2.835571	-1.888530	-1.760556	H	-3.228660	2.259490	-1.249946
H	3.126802	1.775488	1.634677	H	-3.186083	-1.517421	1.359962	H	2.895786	1.550215	1.920818	H	-3.193746	-2.606258	0.056184
H	4.867243	0.212490	-1.990510	H	-4.632679	0.866764	-1.942411	H	4.799564	-0.283487	-1.505846	H	-4.898650	0.643959	-2.249097
H	4.870400	1.857254	-0.163425	H	-5.008940	-1.056514	-0.380862	H	6.213169	1.787188	-0.424210	H	1.160899	-2.795422	0.392268
H	-1.266271	1.937488	2.041662	H	1.116677	-2.475902	1.490213	H	-1.486556	2.235152	1.773154	H	1.622234	-2.892078	-1.345592
H	-1.683349	3.067211	0.699085	H	1.265988	-3.350847	-0.076232	H	-1.569871	3.310698	0.331776	H	-0.094575	-3.047346	-0.849842
H	0.019596	2.881707	1.235504	H	-0.349150	-2.931607	0.583070	H	0.011491	2.908607	1.078097	H	0.903311	3.188181	-1.133232
H	-0.856721	-1.861709	-2.825921	H	1.558593	2.317311	-2.385599	H	-1.220489	-1.977136	-2.741503	H	2.458626	2.476334	-1.693261
H	-2.405768	-0.948031	-2.876069	H	2.885596	1.140084	-2.689199	H	-2.601120	-0.854373	-3.010972	H	2.116383	2.649863	0.058214
H	-2.117552	-2.189529	-1.610187	H	2.828671	2.072277	-1.158140	H	-2.609786	-1.992177	-1.624180				
O	1.594762	2.419788	-1.248398	O	-5.869663	-1.929635	-0.674580	O	6.569706	1.277361	-1.160371				
H	0.823089	1.869782	-0.991938	H	-5.359347	-2.500620	-1.275486	H	7.396860	1.701548	-1.408882				

Table S8. Optimized Cartesian coordinates for the stationary points involved in the H26-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

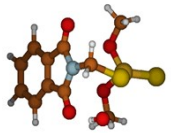
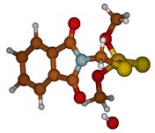
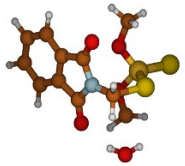
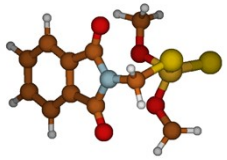
MCR(H26-abs)				TS(H26-abs)				MCP(H26-abs)				Rad(H26-abs)			
															
C	4.265315	0.143313	-1.411773	C	4.192465	0.972955	-1.126469	C	4.252049	0.182312	-1.466615	C	4.183180	0.080074	-1.462213
C	3.219639	1.033824	-1.144677	C	3.195771	1.488657	-0.290425	C	3.192418	1.072031	-1.260422	C	3.237966	1.061870	-1.146592
C	2.304126	0.656445	-0.178689	C	2.317982	0.580906	0.274905	C	2.284883	0.750534	-0.266814	C	2.293213	0.741981	-0.187525
C	2.413969	-0.549933	0.504675	C	2.417848	-0.785451	0.032420	C	2.417366	-0.401882	0.501205	C	2.280813	-0.497850	0.442351
C	3.445656	-1.436625	0.253283	C	3.401553	-1.307724	-0.788279	C	3.463808	-1.286757	0.311062	C	3.213831	-1.475234	0.143893
C	4.375937	-1.069861	-0.725382	C	4.293102	-0.400131	-1.370949	C	4.385382	-0.976122	-0.694759	C	4.171655	-1.166301	-0.828074
C	1.093835	1.366473	0.320377	C	1.160269	0.809529	1.185197	C	1.067937	1.482316	0.186903	C	1.170020	1.558464	0.357920
N	0.538499	0.545375	1.297474	N	0.623561	-0.451087	1.447092	N	0.520376	0.706364	1.213880	N	0.528704	0.733444	1.301076
C	1.282003	-0.643696	1.469903	C	1.332382	-1.476348	0.787168	C	1.284990	-0.446912	1.468897	C	1.142794	-0.521857	1.407238
C	-0.714187	0.775726	1.958046	C	-0.586791	-0.682740	2.178771	C	-0.694726	1.001219	1.905214	C	-0.692690	1.096762	1.955576
S	-2.220031	0.778475	0.871634	S	-2.125345	0.055779	1.453054	S	-2.235008	0.141778	1.278123	S	-2.180668	0.073559	1.529662
P	-1.748008	-0.644758	-0.605631	P	-1.831513	-0.215521	-0.606505	P	-1.708835	-0.754390	-0.533388	P	-1.931715	-0.250357	-0.521594
O	-0.888911	-1.773640	0.140293	O	-1.032463	-1.599289	-0.733534	O	-0.421212	-1.674459	-0.274037	O	-0.614765	-1.156398	-0.688293
C	-1.544963	-2.699168	1.018822	C	-1.712967	-2.839695	-0.498598	C	-0.592219	-2.932092	0.402281	C	-0.696096	-2.559437	-0.390907
O	1.025667	-1.505145	2.272576	O	1.088909	-2.653564	0.878200	O	1.030802	-1.259170	2.323829	O	0.786069	-1.406014	2.148211
O	0.655297	2.443990	-0.026635	O	0.738934	1.850151	1.638853	O	0.628748	2.538230	-0.210765	O	0.857509	2.695120	0.101941
S	-3.316937	-1.148622	-1.593588	S	-3.452752	0.040571	-1.599362	S	-3.252469	-1.553145	-1.350428	S	-3.553693	-0.863969	-1.344969
O	-0.511229	-0.027813	-1.430472	O	-0.561520	0.711518	-0.997802	O	-0.898819	0.367897	-1.388439	O	-1.232791	1.101641	-1.078844
C	-0.767694	1.018529	-2.379507	C	-0.738821	2.056006	-1.387903	C	-1.577892	1.409976	-1.972710	C	-1.934862	2.285170	-1.108508
H	-0.818457	-0.003645	2.713632	H	-0.702829	-1.764101	2.263018	H	-0.595645	0.671821	2.940009	H	-0.599630	0.979188	3.037382
H	-0.734910	1.764962	2.420705	H	-0.524664	-0.231891	3.171739	H	-0.902471	2.070112	1.839221	H	-0.896703	2.137528	1.698183
H	3.521365	-2.374568	0.793140	H	3.469611	-2.375025	-0.970373	H	3.559592	-2.179939	0.919782	H	3.197298	-2.436575	0.647390
H	3.125773	1.980775	-1.666364	H	3.108561	2.551504	-0.088758	H	3.079607	1.975497	-1.850391	H	3.236081	2.032818	-1.630604
H	5.199382	-1.737276	-0.957475	H	5.077815	-0.766172	-2.024905	H	5.220217	-1.644039	-0.880354	H	4.920674	-1.904614	-1.095521
H	5.005560	0.396959	-2.163534	H	4.901459	1.648553	-1.593828	H	4.985439	0.392861	-2.238071	H	4.939844	0.286723	-2.212026
H	-1.237127	1.873260	-1.882943	H	-1.137901	2.719450	-0.482316	H	-2.636344	2.995288	0.128892	H	-2.976722	2.235326	-1.402543
H	-1.406040	0.643592	-3.182248	H	-1.486159	2.157934	-2.178753	H	-2.558179	1.193596	-2.382781	H	-1.297412	3.138995	-1.281463
H	0.207627	1.310671	-2.767347	H	0.240204	2.444306	-1.664994	H	-0.915378	2.155576	-2.386937	H	0.302710	-2.955414	-0.572220
H	-0.747508	-3.263508	1.498677	H	-0.933412	-3.598794	-0.464410	H	0.401827	-3.372870	0.457484	H	-0.964922	-2.704540	0.659423
H	-2.202109	-3.353420	0.441852	H	-2.418725	-3.031818	-1.309668	H	-1.268258	-3.570190	-0.170701	H	-1.423762	-3.038314	-1.049785
H	-2.124750	-2.161610	1.776201	H	-2.245862	-2.809928	0.457655	H	-0.974978	-2.764850	1.412575				
O	-1.783911	3.585288	1.028692	O	-1.452872	3.487515	0.587135	O	-2.007265	3.585248	0.560253				
H	-0.963800	3.348306	0.542978	H	-0.875444	3.038411	1.236646	H	-1.167945	3.440614	0.099648				

Table S9. Optimized Cartesian coordinates for the stationary points involved in the H27-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

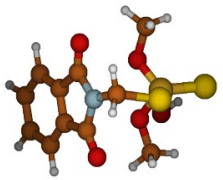
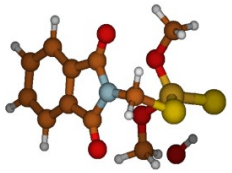
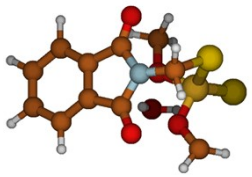
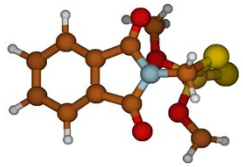
MCR(H27-abs)				TS(H27-abs)				MCP(H27-abs)				Rad(H27-abs)			
															
C	4.091672	1.546755	0.011494	C	4.032573	1.767508	-0.501822	C	4.144849	1.094152	1.020914	C	4.183455	0.081157	-1.462172
C	3.198208	1.128480	1.003258	C	3.128786	1.620404	0.555998	C	3.252341	0.152182	1.543613	C	3.238270	1.062727	-1.145755
C	2.334728	0.097336	0.679200	C	2.356392	0.472601	0.569971	C	2.357715	-0.426272	0.660157	C	2.293469	0.742077	-0.186996
C	2.352300	-0.505660	-0.575037	C	2.472012	-0.500084	-0.418915	C	2.345193	-0.093896	-0.690734	C	2.280999	-0.498278	0.441857
C	3.234823	-0.104285	-1.562269	C	3.365842	-0.368449	-1.466843	C	3.227041	0.831156	-1.221215	C	3.213993	-1.475445	0.142612
C	4.109571	0.941142	-1.248665	C	4.148947	0.790448	-1.495219	C	4.132905	1.427537	-0.337118	C	4.171864	-1.165739	-0.829067
C	1.273409	-0.554654	1.498200	C	1.309827	0.035407	1.537973	C	1.291907	-1.440217	0.905715	C	1.170225	1.558121	0.359046
N	0.699440	-1.526757	0.665668	N	0.849783	-1.200623	1.062170	N	0.679765	-1.652583	-0.345069	N	0.528848	0.732382	1.301446
C	1.307853	-1.569239	-0.601990	C	1.510288	-1.598395	-0.114798	C	1.263665	-0.876009	-1.356382	C	1.142961	-0.523015	1.406714
C	-0.427216	-2.323690	1.026564	C	-0.230433	-1.929524	1.644386	C	-0.494133	-2.453207	-0.515297	C	-0.692577	1.095338	1.956132
S	-2.075925	-1.448508	1.089851	S	-1.931446	-1.195090	1.433097	S	-2.030774	-1.545696	-1.033652	S	-2.180446	0.072160	1.530004
P	-1.827547	0.207904	-0.165879	P	-1.792311	-0.066845	-0.324742	P	-1.896205	0.215446	0.072346	P	-1.931964	-0.249931	-0.521606
O	-0.981813	-0.281903	-1.431396	O	-0.879309	-0.897039	-1.339959	O	-0.612630	1.020014	-0.474509	O	-0.615306	-1.156175	-0.689382
C	-1.594601	-1.131643	-2.413377	C	-1.401706	-2.080125	-1.964847	C	-0.708093	1.707701	-1.739454	C	-0.696769	-2.559267	-0.392146
O	1.023069	-2.348155	-1.478860	O	1.318677	-2.637635	-0.697433	O	0.919260	-0.878897	-2.513480	O	0.786124	-1.407714	2.146968
O	0.939168	-0.346885	2.639658	O	0.903918	0.580856	2.535706	O	0.995043	-2.007085	1.928131	O	0.857792	2.695010	0.103945
S	-3.534281	1.060192	-0.485758	S	-3.552854	0.484466	-0.885779	S	-3.567397	1.166648	0.132128	S	-3.554193	-0.862140	-1.345528
O	-0.673653	1.121887	0.465490	O	-0.699588	1.087552	-0.047756	O	-1.194812	-0.195401	1.473404	O	-1.232528	1.102425	-1.077484
C	-0.929425	1.868164	1.671071	C	-1.018755	2.189919	0.777396	C	-1.863687	-0.989017	2.379896	C	-1.934876	2.285754	-1.107779
H	-0.502102	-3.134955	0.302252	H	-0.228823	-2.926342	1.202776	H	-0.351359	-3.185746	-1.312630	H	-0.599509	0.977486	3.037911
H	-0.297053	-2.714051	2.037372	H	-0.102534	-1.984936	2.727018	H	-0.685848	-2.951465	0.436654	H	-0.896706	2.136175	1.699084
H	3.238357	-0.581355	-2.536613	H	3.447200	-1.133605	-2.231655	H	3.210179	1.078410	-2.277856	H	3.197434	-2.437204	0.645309
H	3.175826	1.589345	1.985394	H	3.032898	2.369731	1.335173	H	3.251125	-0.114434	2.595237	H	3.236421	2.034078	-1.628959
H	4.813877	1.291993	-1.995788	H	4.859299	0.936632	-2.302299	H	4.839054	2.162656	-0.709079	H	4.920866	-1.903852	-1.097108
H	4.782610	2.356864	0.220620	H	4.654923	2.654787	-0.554587	H	4.859036	1.577474	1.679430	H	4.940151	0.288387	-2.211793
H	-1.098068	1.178325	2.501611	H	-1.596453	1.899725	1.659118	H	-2.920192	-0.794014	2.521558	H	-2.976239	2.235789	-1.403527
H	-1.783223	2.532364	1.523775	H	-1.646859	2.982289	0.154108	H	-0.457393	2.826785	0.811486	H	-1.297379	3.139862	-1.279196
H	-0.027765	2.453095	1.844543	H	-0.084426	2.685066	1.038941	H	-1.211254	-1.378877	3.146290	H	0.301989	-2.955310	-0.573570
H	-0.803426	-1.384911	-3.115966	H	-0.568928	-2.510634	-2.517024	H	0.277441	2.140292	-1.907927	H	-0.965483	-2.704450	0.658199
H	-2.407752	-0.596291	-2.908496	H	-2.223872	-1.811770	-2.631728	H	-0.942166	0.991784	-2.531720	H	-1.424547	-3.037935	-1.051043
H	-1.972288	-2.043994	-1.941943	H	-1.745441	-2.789560	-1.205885	H	-1.459410	2.496875	-1.674018				
O	-1.128809	3.534142	-0.901480	O	-2.413783	3.740071	-0.669543	O	-0.976708	3.638014	0.861847				
H	-1.970205	3.046439	-1.031707	H	-2.992587	3.021428	-0.993328	H	-1.893189	3.333598	0.873546				

Table S10. Optimized Cartesian coordinates for the stationary points involved in the H28-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

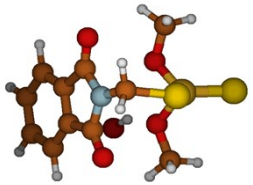
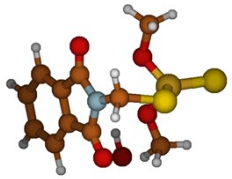
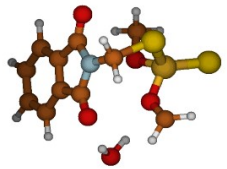
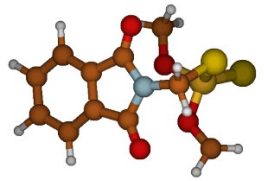
MCR(H28-abs)				TS(H28-abs)				MCP(H28-abs)				Rad(H28-abs)			
															
C	4.107170	1.086652	-0.183221	C	4.178680	0.816036	-0.549279	C	4.130889	0.570404	-1.095883	C	4.183650	0.080516	-1.462045
C	3.135789	1.054181	0.823958	C	3.237403	1.018893	0.466277	C	3.183707	1.228704	-0.303444	C	3.238637	1.062330	-1.145871
C	2.172934	0.063242	0.738766	C	2.231608	0.075906	0.587225	C	2.243739	0.438235	0.335761	C	2.293733	0.742002	-0.187090
C	2.164569	-0.862305	-0.302431	C	2.156681	-1.030363	-0.254928	C	2.231088	-0.946353	0.193524	C	2.281009	-0.498230	0.442013
C	3.124504	-0.843391	-1.298798	C	3.085309	-1.244339	-1.258579	C	3.165731	-1.607760	-0.582709	C	3.213820	-1.475619	0.142998
C	4.102878	0.153330	-1.223033	C	4.104575	-0.295424	-1.395325	C	4.125122	-0.821092	-1.230581	C	4.171779	-1.166265	-0.828715
C	1.018067	-0.227781	1.636063	C	1.088792	0.014897	1.543346	C	1.117915	0.822274	1.233643	C	1.170549	1.558265	0.358687
N	0.362783	-1.325024	1.058947	N	0.381869	-1.150095	1.211340	N	0.467941	-0.371298	1.569428	N	0.528786	0.732778	1.301032
C	1.000323	-1.773421	-0.111801	C	0.968525	-1.842425	0.137868	C	1.078656	-1.486472	0.969885	C	1.142814	-0.522574	1.406715
C	-0.860882	-1.869908	1.547382	C	-0.839815	-1.548190	1.833402	C	-0.782122	-0.412762	2.269883	C	-0.692561	1.096093	1.955763
S	-2.403954	-0.872673	1.210795	S	-2.344216	-0.519925	1.439704	S	-2.234914	-1.009713	1.284811	S	-2.180388	0.072459	1.530092
P	-1.913598	0.410780	-0.369908	P	-1.939229	0.310337	-0.440611	P	-1.963398	-0.051032	-0.552156	P	-1.932052	-0.250127	-0.521486
O	-1.026762	-0.424008	-1.411746	O	-1.185332	-0.815922	-1.292594	O	-0.592406	-0.613644	-1.175073	O	-0.615617	-1.156591	-0.689418
C	-1.654997	-1.418789	-2.237035	C	-1.923388	-1.950425	-1.773285	C	-0.594786	-1.905183	-1.807220	C	-0.697155	-2.559564	-0.391645
O	0.644542	-2.720224	-0.770588	O	0.569070	-2.888643	-0.312457	O	0.696985	-2.624663	1.088754	O	0.785853	-1.407086	2.147147
O	0.672490	0.318327	2.656090	O	0.787070	0.766760	2.438434	O	0.798166	1.918063	1.640049	O	0.858209	2.695152	0.103316
S	-3.491648	1.312455	-0.992392	S	-3.514991	1.139052	-1.162612	S	-3.546264	-0.129512	-1.631786	S	-3.554401	-0.862011	-1.345419
O	-0.685438	1.330836	0.140173	O	-0.631266	1.245063	-0.250360	O	-1.343683	1.407877	-0.185624	O	-1.232360	1.102145	-1.077298
C	-0.938471	2.377317	1.099381	C	-0.750494	2.511789	0.374206	C	-2.108809	2.326393	0.503726	C	-1.934485	2.285605	-1.108325
H	-0.992334	-2.851647	1.092362	H	-1.038928	-2.577587	1.534527	H	-0.732125	-1.113577	3.105855	H	-0.599381	0.978650	3.037565
H	-0.821268	-1.944708	2.635278	H	-0.746389	-1.471177	2.918291	H	-0.985748	0.598312	2.627280	H	-0.896909	2.136747	1.698180
H	3.107290	-1.568960	-2.105148	H	3.017133	-2.110415	-1.908411	H	3.148132	-2.688534	-0.680781	H	3.197019	-2.437304	0.645828
H	3.126872	1.775890	1.634142	H	3.272450	1.886260	1.116302	H	3.164842	2.309628	-0.214940	H	3.236968	2.033562	-1.629318
H	4.866901	0.212298	-1.991016	H	4.851426	-0.421050	-2.172561	H	4.876220	-1.297272	-1.852484	H	4.920597	-1.904605	-1.096645
H	4.870258	1.857432	-0.164250	H	4.979445	1.535433	-0.686125	H	4.881716	1.151375	-1.621143	H	4.940378	0.287445	-2.211714
H	-1.267471	1.936020	2.042992	H	-0.730101	2.417889	1.462605	H	-1.549750	3.211758	0.768688	H	-1.296873	3.139423	-1.280779
H	-1.686179	3.066095	0.701208	H	-1.593810	3.082535	-0.019892	H	-3.172402	2.337206	0.294463	H	-2.976088	2.235595	-1.403172
H	0.017076	2.882342	1.237244	H	0.241669	3.085887	0.063380	H	0.836188	3.221996	0.125447	H	0.301375	-2.955900	-0.573657
H	-0.853996	-1.860948	-2.825721	H	-1.190533	-2.595332	-2.253611	H	0.430685	-2.069767	-2.137028	H	-0.965097	-2.704319	0.658957
H	-2.402680	-0.946743	-2.878015	H	-2.686570	-1.620818	-2.481693	H	-0.880703	-2.675360	-1.084744	H	-1.425511	-3.038317	-1.049840
H	-2.116655	-2.188416	-1.611792	H	-2.386877	-2.482157	-0.936757	H	-1.276093	-1.901005	-2.660600				
O	1.594174	2.420461	-1.247790	O	1.403451	3.328368	-0.591904	O	0.808174	3.471193	-0.808897				
H	0.822949	1.870340	-0.990247	H	1.402524	2.516916	-1.134269	H	0.248613	2.798461	-1.215242				

Table S11. Optimized Cartesian coordinates for the stationary points involved in the H29-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

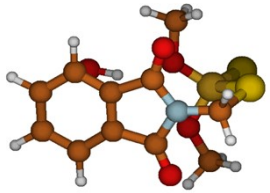
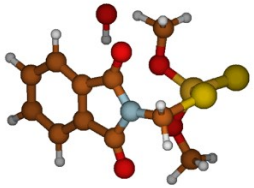
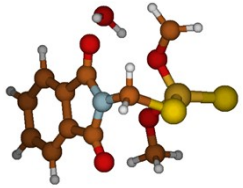
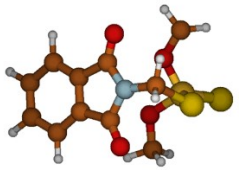
MCR(H29-abs)				TS(H29-abs)				MCP(H29-abs)				Rad(H29-abs)			
															
C	-4.102880	0.153461	-1.222922	C	-4.105079	-0.296167	-1.395100	C	-4.124463	-0.822369	-1.230550	C	-4.171771	-1.166292	-0.828701
C	-3.124467	-0.843210	-1.298861	C	-3.085697	-1.244922	-1.258112	C	-3.165117	-1.608520	-0.581984	C	-3.213802	-1.475632	0.143005
C	-2.164537	-0.862249	-0.302498	C	-2.156936	-1.030423	-0.254694	C	-2.230706	-0.946523	0.194014	C	-2.280998	-0.498233	0.442010
C	-2.172888	0.063102	0.738874	C	-2.231838	0.076201	0.586996	C	-2.243541	0.438159	0.335421	C	-2.293742	0.741997	-0.187096
C	-3.135789	1.053984	0.824224	C	-3.237729	1.019050	0.465786	C	-3.183438	1.228118	-0.304523	C	-3.238662	1.062315	-1.145866
C	-4.107182	1.086590	-0.182940	C	-4.179152	0.815655	-0.549525	C	-4.130375	0.569205	-1.096753	C	-4.183664	0.080489	-1.462032
C	-1.000273	-1.773379	-0.112090	C	-0.968675	-1.842229	0.138303	C	-1.078289	-1.486037	0.970780	C	-1.142802	-0.522557	1.406712
N	-0.362718	-1.325235	1.058747	N	-0.381967	-1.149428	1.211448	N	-0.467742	-0.370359	1.569719	N	-0.528773	0.732789	1.301007
C	-1.017991	-0.228086	1.636083	C	-1.088896	0.015686	1.543002	C	-1.117945	0.822824	1.233335	C	-1.170565	1.558276	0.358672
C	0.861040	-1.870145	1.546945	C	0.839703	-1.547363	1.833642	C	0.782400	-0.411303	2.270118	C	0.692569	1.096122	1.955740
S	2.403913	-0.872417	1.210962	S	2.344011	-0.518876	1.440267	S	2.235099	-1.008705	1.285133	S	2.180396	0.072477	1.530089
P	1.913591	0.410870	-0.369804	P	1.939591	0.310119	-0.440724	P	1.963274	-0.051110	-0.552379	P	1.932059	-0.250138	-0.521485
O	0.685101	1.330594	0.140052	O	0.631493	1.244859	-0.251357	O	1.343073	1.407707	-0.186554	O	1.232351	1.102132	-1.077280
C	0.937686	2.377376	1.099055	C	0.750546	2.511763	0.372850	C	2.107532	2.326591	0.503102	C	1.934463	2.285598	-1.108357
O	-0.672344	0.317855	2.656173	O	-0.787079	0.767997	2.437684	O	-0.798712	1.918899	1.639524	O	-0.858241	2.695164	0.103299
O	-0.644491	-2.720025	-0.771107	O	-0.569176	-2.888589	-0.311652	O	-0.696393	-2.624047	1.090388	O	-0.785846	-1.407056	2.147162
S	3.491547	1.312983	-0.991957	S	3.515437	1.138572	-1.162842	S	3.546124	-0.129516	-1.632044	S	3.554412	-0.862011	-1.345420
O	1.027160	-0.424105	-1.411830	O	1.185998	-0.816737	-1.292172	O	0.592510	-0.614590	-1.174987	O	0.615625	-1.156602	-0.689409
C	1.655705	-1.418868	-2.236855	C	1.924210	-1.951510	-1.771966	C	0.595360	-1.906613	-1.806148	C	0.697148	-2.559569	-0.391611
H	0.821451	-1.945566	2.634801	H	0.746170	-1.470437	2.918533	H	0.985903	0.599969	2.627003	H	0.896919	2.136771	1.698136
H	0.992662	-2.851605	1.091374	H	1.038946	-2.576731	1.534755	H	0.732573	-1.111725	3.106434	H	0.599390	0.978698	3.037544
H	-3.126935	1.775564	1.634524	H	-3.272716	1.886731	1.115390	H	-3.164656	2.309106	-0.216852	H	-3.237011	2.033548	-1.629310
H	-3.107209	-1.568664	-2.105314	H	-3.017535	-2.111271	-1.907582	H	-3.147367	-2.689351	-0.679387	H	-3.196984	-2.437316	0.645838
H	-4.870292	1.857345	-0.163806	H	-4.979993	1.534928	-0.686571	H	-4.881123	1.149774	-1.622571	H	-4.940401	0.287406	-2.211696
H	-4.866925	0.212542	-1.990874	H	-4.852043	-0.422201	-2.172162	H	-4.875389	-1.299017	-1.852301	H	-4.920583	-1.904642	-1.096624
H	2.117428	-2.188318	-1.611434	H	2.386826	-2.483164	-0.934907	H	0.880822	-2.676200	-1.082865	H	0.965028	-2.704301	0.659011
H	2.403414	-0.946784	-2.877781	H	2.688103	-1.622258	-2.479777	H	1.277250	-1.903075	-2.659072	H	1.425547	-3.038333	-1.049749
H	0.854897	-1.861277	-2.825616	H	1.191635	-2.596350	-2.252807	H	-0.429871	-2.071471	-2.136565	H	-0.301369	-2.955913	-0.573677
H	-0.018032	2.882150	1.236665	H	-0.242161	3.085325	0.062618	H	-0.838527	3.223858	0.125198	H	1.296841	3.139402	-1.280847
H	1.685252	3.066276	0.700831	H	1.593296	3.082840	-0.021974	H	1.547413	3.210820	0.769621	H	2.976074	2.235595	-1.403175
H	1.266685	1.936361	2.042799	H	0.730898	2.418168	1.461294	H	3.170940	2.339044	0.292978				
O	-1.594444	2.420046	-1.248029	O	-1.404046	3.327750	-0.592090	O	-0.809676	3.470693	-0.809761				
H	-0.822994	1.870190	-0.990586	H	-1.402948	2.516842	-1.135266	H	-0.247379	2.798464	-1.213149				

Table S12. Optimized Cartesian coordinates for the stationary points involved in the H30-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

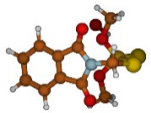
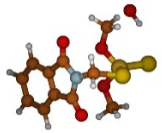
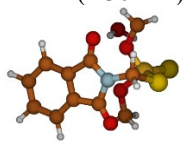
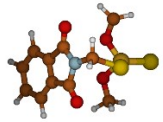
MCR(H30-abs)				TS(H30-abs)				MCP(H30-abs)				Rad(H30-abs)			
															
C	-4.126308	0.708015	-1.414371	C	-4.253233	0.348784	-1.569689	C	-4.192850	0.721552	-1.362376	C	-4.171724	-1.166177	-0.828564
C	-3.299637	-0.420647	-1.415542	C	-3.505768	-0.724489	-1.072593	C	-3.351789	-0.396301	-1.392745	C	-3.213737	-1.475556	0.143107
C	-2.400106	-0.544362	-0.371569	C	-2.554604	-0.437628	-0.109663	C	-2.438662	-0.526181	-0.361161	C	-2.280827	-0.498221	0.442060
C	-2.320900	0.406025	0.642165	C	-2.349632	0.858763	0.353078	C	-2.359931	0.406830	0.667667	C	-2.293475	0.741983	-0.187095
C	-3.135301	1.524488	0.656351	C	-3.085164	1.927808	-0.127363	C	-3.189080	1.513989	0.711814	C	-3.238353	1.062290	-1.145891
C	-4.044932	1.663806	-0.396991	C	-4.046193	1.651516	-1.105616	C	-4.112381	1.660128	-0.328935	C	-4.183476	0.080554	-1.461987
C	-1.388284	-1.605525	-0.100458	C	-1.602249	-1.343364	0.595289	C	-1.411144	-1.580005	-0.118660	C	-1.142713	-0.522574	1.406834
N	-0.748312	-1.219844	1.086311	N	-0.868971	-0.519306	1.460839	N	-0.766587	-1.214047	1.071753	N	-0.528711	0.732863	1.301131
C	-1.266211	-0.019173	1.606151	C	-1.267350	0.827599	1.378281	C	-1.287274	-0.021453	1.610904	C	-1.170326	1.558314	0.358720
C	0.357355	-1.915071	1.658031	C	0.227962	-0.968370	2.257000	C	0.379702	-1.879444	1.611073	C	0.692679	1.096119	1.955785
S	2.007435	-1.692629	0.807785	S	1.772331	-1.457914	1.333938	S	1.894156	-1.899633	0.534381	S	2.180713	0.073180	1.529815
P	1.791159	0.053649	-0.325889	P	1.708361	-0.303218	-0.410938	P	1.849754	-0.004002	-0.330287	P	1.931862	-0.250095	-0.521593
O	1.035312	1.134020	0.576137	O	1.159670	1.143648	0.025840	O	1.242863	0.980080	0.810084	O	1.232550	1.101941	-1.078241
C	1.679738	1.691259	1.736572	C	1.968108	2.026588	0.776872	C	1.969080	1.246598	1.955148	C	1.934543	2.285502	-1.108599
O	-0.912369	0.493283	2.639423	O	-0.813449	1.724899	2.045409	O	-0.922841	0.491082	2.640103	O	-0.857917	2.695115	0.103113
O	-1.133788	-2.609005	-0.722073	O	-1.451278	-2.536731	0.491165	O	-1.146493	-2.559279	-0.773430	O	-0.785630	-1.407057	2.147223
S	3.499211	0.550946	-1.086430	S	3.393344	-0.420434	-1.341805	S	3.539816	0.463904	-1.122833	H	0.896569	2.136968	1.698596
O	0.581477	-0.184902	-1.350532	O	0.387687	-0.734102	-1.211004	O	0.545806	0.073703	-1.263528	H	0.599527	0.978407	3.037575
C	0.782673	-1.036330	-2.490744	C	0.378590	-1.981525	-1.926103	C	0.562210	-0.579137	-2.544984	S	3.553877	-0.863020	-1.345347
H	0.466050	-1.576785	2.688663	H	0.480044	-0.163953	2.948501	H	0.627343	-1.383569	2.551336	O	0.615070	-1.156299	-0.688530
H	0.176665	-2.990270	1.615776	H	-0.048410	-1.873818	2.800579	H	0.170740	-2.938557	1.776172	C	0.696619	-2.559361	-0.391193
H	-3.061130	2.259794	1.450508	H	-2.914545	2.934050	0.240499	H	-3.117009	2.234731	1.519531	H	-3.236632	2.033520	-1.629337
H	-3.355569	-1.170616	-2.197895	H	-3.660462	-1.740482	-1.421358	H	-3.408105	-1.134331	-2.186509	H	-3.197071	-2.437185	0.646049
H	-4.698597	2.529287	-0.428551	H	-4.642362	2.461117	-1.513665	H	-4.778568	2.516550	-0.336878	H	-4.940244	0.287518	-2.211610
H	-4.843547	0.847011	-2.216721	H	-5.007900	0.169720	-2.328595	H	-4.921802	0.864720	-2.153347	H	-4.920688	-1.904422	-1.096351
H	1.020431	-2.051622	-2.162083	H	0.525818	-2.812060	-1.230326	H	0.694764	-1.656570	-2.412413	H	0.965798	-2.704431	0.659045
H	1.579359	-0.631987	-3.118769	H	1.153040	-1.972521	-2.695843	H	1.356262	-0.159081	-3.165967	H	1.424040	-3.038152	-1.050393
H	-0.166061	-1.038395	-3.025355	H	-0.610592	-2.052261	-2.376559	H	-0.413858	-0.379528	-2.985659	H	-0.302250	-2.955388	-0.572075
H	1.012048	2.472816	2.091768	H	1.310286	2.773897	1.217917	H	1.370502	1.720691	2.718159	H	1.296771	3.139346	-1.280335
H	2.647248	2.114355	1.458224	H	2.702364	2.602714	0.041293	H	1.209559	3.035576	-0.096481	H	2.975953	2.235745	-1.404244
H	1.793044	0.918855	2.501593	H	2.579113	1.505009	1.519745	H	3.033989	1.407168	1.834462				
O	1.718238	3.508031	-0.702776	O	3.555601	3.042092	-0.917003	O	1.890278	3.633555	-0.424915				
H	2.355041	2.872331	-1.093708	H	3.771547	2.173031	-1.310333	H	2.568252	3.049643	-0.788196				

Table S13. Optimized Cartesian coordinates for the stationary points involved in the H31-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

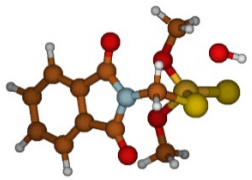
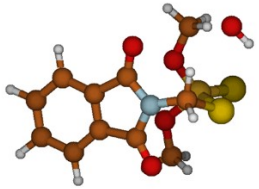
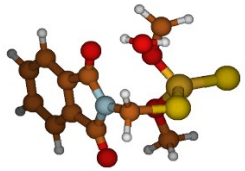
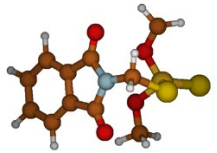
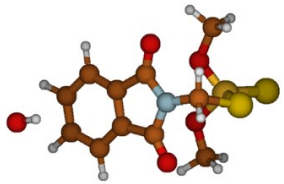
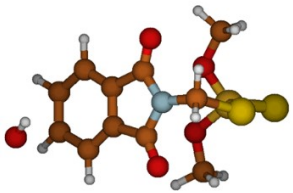
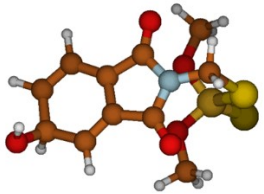
MCR(H31-abs)	TS(H31-abs)	MCP(H31-abs)	Rad(H31-abs)
			
C -4.526205 -0.940522 -0.390739	C -4.505791 -0.778169 -0.689841	C -4.385640 -0.975766 -0.694214	C -4.171689 -1.166266 -0.828079
C -3.540664 -1.126440 0.584620	C -3.576963 -1.146905 0.289295	C -3.464033 -1.286194 0.311649	C -3.213884 -1.475208 0.143904
C -2.490248 -0.225684 0.598953	C -2.506401 -0.294639 0.495443	C -2.417419 -0.401430 0.501367	C -2.280840 -0.497848 0.442357
C -2.413678 0.824073 -0.310207	C -2.356884 0.881547 -0.231763	C -2.284804 0.750712 -0.267050	C -2.293201 0.741973 -0.187537
C -3.384720 1.021892 -1.276023	C -3.270853 1.259678 -1.199584	C -3.192376 1.072007 -1.260674	C -3.237936 1.061874 -1.146616
C -4.449335 0.115082 -1.304806	C -4.355110 0.404120 -1.421450	C -4.252170 0.182384 -1.466467	C -4.183175 0.080101 -1.462235
C -1.298455 -0.158316 1.493876	C -1.360156 -0.407610 1.443597	C -1.284955 -0.446287 1.469033	C -1.142830 -0.521882 1.407249
N -0.565254 0.956022 1.065503	N -0.577322 0.734467 1.230650	N -0.520347 0.706898 1.213706	N -0.528713 0.733417 1.301094
C -1.175351 1.606212 -0.024656	C -1.113779 1.566641 0.228734	C -1.067857 1.482553 0.186473	C -1.169992 1.558445 0.357913
C 0.720785 1.321369 1.574415	C 0.685389 0.976119 1.858008	C 0.694986 1.002084 1.904477	C 0.692674 1.096713 1.955616
S 2.052572 0.054790 1.330210	S 2.027799 -0.250960 1.466020	S 2.234902 0.141635 1.278074	S 2.180693 0.073574 1.529653
P 1.625316 -0.717671 -0.587259	P 1.668160 -0.712626 -0.547006	P 1.708622 -0.754847 -0.533270	P 1.931740 -0.250343 -0.521608
O 0.984762 0.482991 -1.419292	O 1.084965 0.637558 -1.205626	O 0.899351 0.367612 -1.388789	O 1.232799 1.101625 -1.078885
C 1.818951 1.543171 -1.927497	C 1.929798 1.708158 -1.559847	C 1.578808 1.410340 -1.971331	C 1.934818 2.285195 -1.108456
O -0.760646 2.603332 -0.560572	O -0.642899 2.617142 -0.129273	O -0.628589 2.538316 -0.211470	O -0.857456 2.695089 0.101948
O -0.985326 -0.880653 2.409947	O -1.111979 -1.275206 2.246544	O -1.030777 -1.258388 2.324112	O -0.786132 -1.406037 2.148234
S 3.155630 -1.654920 -1.280966	S 3.201769 -1.545380 -1.352262	S 3.251971 -1.554754 -1.349683	S 3.553714 -0.863999 -1.344950
O 0.256758 -1.538729 -0.405230	O 0.269814 -1.500322 -0.578722	O 0.420484 -1.674115 -0.273827	O 0.614778 -1.156365 -0.688323
C 0.280032 -2.803281 0.273424	C 0.222928 -2.855780 -0.103491	C 0.590929 -2.932330 0.401509	C 0.696089 -2.559399 -0.390952
H 1.030777 2.243232 1.080942	H 1.030953 1.965549 1.550935	H 0.902896 2.070879 1.837329	H 0.896645 2.137509 1.698312
H 0.688638 1.459952 2.656901	H 0.591488 0.913899 2.944128	H 0.596127 0.673861 2.939672	H 0.599592 0.979058 3.037412
H -3.313655 1.845238 -1.978932	H -3.143073 2.180368 -1.759122	H -3.079568 1.975244 -1.850992	H -3.236023 2.032820 -1.630633
H -3.590908 -1.938246 1.303132	H -3.685435 -2.058763 0.867750	H -3.559844 -2.179130 0.920727	H -3.197376 -2.436547 0.647407
H -5.231084 0.230780 -2.048441	H -5.094168 0.660380 -2.173530	H -4.985584 0.392833 -2.237927	H -4.939828 0.286768 -2.212054
H -5.366954 -1.624871 -0.440037	H -5.359904 -1.418233 -0.885938	H -5.220596 -1.643607 -0.879534	H -4.920720 -1.904566 -1.095522
H 0.605540 -2.666667 1.308755	H 0.503809 -2.891666 0.952835	H 0.975629 -2.766210 1.411271	H 0.964943 -2.704505 0.659370
H 0.938322 -3.497830 -0.253294	H 0.882843 -3.483937 -0.706085	H 1.265172 -3.571000 -0.172928	H 1.423736 -3.038286 -1.049843
H -0.747994 -3.163501 0.257320	H -0.813995 -3.169681 -0.217363	H -0.403616 -3.371783 0.458249	H -0.302727 -2.955357 -0.572248
H 1.132152 2.252584 -2.385514	H 1.304616 2.481220 -2.003863	H 0.916680 2.157412 -2.383476	H 1.297331 3.139015 -1.281313
H 2.512636 1.135644 -2.666566	H 2.753130 1.381813 -2.199864	H 2.559138 1.194468 -2.381531	H 2.976682 2.235425 -1.402490
H 2.366465 2.018309 -1.108919	H 2.396249 2.208914 -0.601663	H 1.170131 3.441414 0.097451	
O 3.464606 2.165509 0.985270	O 3.103783 2.734712 0.492423	O 2.009030 3.585056 0.559075	
H 4.293966 1.655425 1.008001	H 3.596715 1.929678 0.744840	H 2.637749 2.993683 0.129075	

Table S14. Optimized Cartesian coordinates for the stationary points involved in the C1-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(C1-add)	TS(C1-add)	Adduct(C1-add)
		
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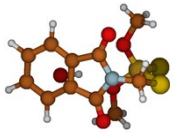
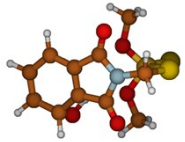
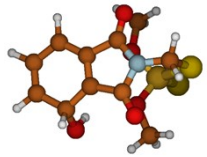
C -2.850875 -1.528833 -0.173084	C -2.942674 -1.313959 -0.196176	C -2.972861 -1.179564 0.154057
C -1.949098 -0.597030 0.308113	C -1.999481 -0.455072 0.317514	C -1.991917 -0.318308 0.492419
C -1.950250 0.722819 -0.137272	C -1.925385 0.883818 -0.078900	C -1.887119 0.992004 -0.054603
C -2.852740 1.169610 -1.085849	C -2.793780 1.421178 -1.018457	C -2.838991 1.483383 -0.970215
C -3.770008 0.236035 -1.584410	C -3.754246 0.570238 -1.557652	C -3.847388 0.650056 -1.358090
C -0.851400 -0.753105 1.306999	C -0.905633 -0.711013 1.299973	C -0.863161 -0.497823 1.456338
N -0.248388 0.508217 1.403781	N -0.233875 0.511345 1.440909	N -0.154203 0.705372 1.426585
C -0.860841 1.458707 0.568933	C -0.796158 1.527491 0.649995	C -0.722900 1.656775 0.547739
C 0.926124 0.776542 2.172656	C 0.958911 0.682806 2.209355	C 1.082170 0.917538 2.110081
S 2.514184 0.041509 1.533981	S 2.504446 -0.093157 1.515382	S 2.554466 -0.016311 1.451243
P 2.197985 -0.180771 -0.531604	P 2.150882 -0.230152 -0.551765	P 2.108052 -0.334131 -0.577003
O 1.384741 1.116104 -1.004800	O 1.397238 1.120001 -0.972642	O 1.398858 1.004428 -1.097354
C 2.051913 2.384450 -1.076067	C 2.127217 2.354883 -1.014013	C 2.178617 2.194766 -1.281440
O -0.553842 2.623822 0.501393	O -0.424968 2.675909 0.625149	O -0.305761 2.783088 0.393044
O -0.517147 -1.727102 1.936987	O -0.620137 -1.725895 1.886923	O -0.582336 -1.451932 2.141880
S 3.852573 -0.621560 -1.406327	S 3.771742 -0.721271 -1.461894	S 3.661510 -0.991820 -1.500580
O 0.968620 -1.203120 -0.695013	O 0.870449 -1.185019 -0.731821	O 0.778222 -1.237702 -0.613072
C 1.190930 -2.602903 -0.462332	C 1.027833 -2.600778 -0.545497	C 0.878164 -2.633538 -0.289066
H 1.041455 1.859526 2.222734	H 1.128120 1.754690 2.313875	H 1.299585 1.984904 2.065691
H 0.819049 0.352919 3.172897	H 0.838541 0.212775 3.187011	H 0.997034 0.581669 3.145240
H -2.844627 2.200169 -1.424750	H -2.709491 2.457864 -1.326255	H -2.764566 2.500958 -1.339867
H -2.844786 -2.552599 0.186787	H -2.999044 -2.351378 0.115494	H -3.055259 -2.166868 0.600062
H -4.501774 0.543131 -2.323754	H -4.453957 0.937087 -2.300366	H -4.612543 0.985265 -2.051868
H -4.502399 -1.783485 -1.534391	H -4.509530 -1.451738 -1.686635	H -3.908287 -1.443012 -1.737623
H 1.508471 -2.764989 0.571500	H 1.351879 -2.810067 0.477740	H 1.545596 -3.131521 -0.995666
H 1.937588 -2.981896 -1.163507	H 1.745278 -2.992663 -1.269623	H 1.234603 -2.755467 0.737506
H 0.228131 -3.084846 -0.628278	H 0.040676 -3.030894 -0.710614	H -0.134109 -3.027918 -0.371996
H 1.279128 3.109384 -1.324236	H 1.389828 3.125224 -1.231098	H 1.466355 2.974991 -1.542334
H 2.826361 2.351721 -1.845657	H 2.890711 2.306463 -1.793633	H 2.689777 2.461224 -0.351080
H 2.493581 2.636109 -0.106799	H 2.590864 2.554335 -0.042952	H 2.907299 2.038758 -2.080030
O -5.927875 0.083581 0.168692	O -5.462661 -0.558974 0.089941	O -5.322897 -1.012832 -0.400642
H -5.259994 0.348906 0.829566	H -5.108009 0.080673 0.732953	H -5.482210 -0.446389 0.365626

Table S15. Optimized Cartesian coordinates for the stationary points involved in the C2-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(C2-add)	TS(C2-add)	Adduct(C2-add)
		
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C 3.136007 1.053190 0.824980	C -3.068303 -1.194137 0.320195	C -2.933004 -1.309781 0.110923
C 2.172972 0.062502 0.738873	C -2.131749 -0.185430 0.612050	C -2.062697 -0.197881 0.584661
C 2.164799 -0.862339 -0.302948	C -2.069021 0.989851 -0.121691	C -2.018023 1.035427 -0.014218
C 3.125028 -0.842968 -1.299023	C -2.983366 1.279284 -1.123199	C -2.883704 1.415466 -1.041386
C 4.103584 0.153497 -1.222311	C -3.981608 0.324896 -1.380694	C -3.834655 0.446887 -1.484819
C 1.017813 -0.229034 1.635646	C -1.020304 -0.186254 1.602247	C -0.990609 -0.276601 1.597628
N 0.362673 -1.325952 1.057689	N -0.323374 1.013268 1.379581	N -0.289775 0.946892 1.502378
C 1.000416 -1.773470 -0.113289	C -0.907104 1.788514 0.367307	C -0.866398 1.800709 0.560775
C -0.861491 -1.870883 1.544978	C 0.902010 1.347727 2.025730	C 0.959821 1.185545 2.139620
S -2.403238 -0.870258 1.213121	S 2.454620 0.617077 1.277678	S 2.478550 0.569544 1.225560
P -1.913935 0.411214 -0.369418	P 1.878113 -0.328283 -0.506428	P 1.819155 -0.314016 -0.562602
O -1.030117 -0.425914 -1.411946	O 0.929916 0.689924 -1.306525	O 0.815995 0.721816 -1.270650
C -1.661013 -1.421338 -2.234343	C 1.511746 1.837898 -1.945475	C 1.350616 1.902170 -1.891616
O 0.644736 -2.719684 -0.772984	O -0.519090 2.876262 0.016052	O -0.479135 2.912880 0.292077
O 0.671890 0.316545 2.655828	O -0.735211 -1.000821 2.445615	O -0.717799 -1.154220 2.382242
S -3.491508 1.315110 -0.989947	S 3.441761 -1.014453 -1.388778	S 3.346187 -0.928441 -1.556501
O -0.683530 1.329630 0.138098	O 0.700804 -1.363657 -0.141886	O 0.679249 -1.388432 -0.192694
C -0.933599 2.378248 1.095779	C 1.021195 -2.574362 0.574931	C 1.052879 -2.603045 0.490213
H -0.994212 -2.850888 1.086591	H 1.019679 2.430916 1.997342	H 1.094844 2.260587 2.258251
H -0.821628 -1.949665 2.632604	H 0.873953 0.979705 3.051747	H 0.966216 0.676136 3.103234
H 3.107903 -1.568056 -2.105809	H -2.924765 2.209635 -1.678277	H -2.817424 2.400426 -1.489001
H 3.127084 1.774337 1.635668	H -3.229681 -2.010087 1.013552	H -3.497258 -1.752319 0.942020
H 4.867871 0.212819 -1.990002	H -4.720647 0.519948 -2.150417	H -4.522033 0.714742 -2.280839
H 4.870980 1.856712 -0.162120	H -4.813781 -1.590988 -0.895289	H -4.588510 -1.536270 -1.334076
H -1.263719 1.939186 2.040053	H 1.413909 -2.322743 1.563147	H 1.720753 -3.186479 -0.146972
H -1.679492 3.068451 0.696683	H 1.746259 -3.155755 0.001686	H 1.535070 -2.360199 1.440478
H 0.023334 2.880902 1.232727	H 0.076565 -3.107666 0.671187	H 0.117303 -3.128458 0.676370
H -0.861270 -1.867169 -2.821962	H 0.682671 2.368493 -2.409890	H 0.495403 2.425208 -2.316323
H -2.407677 -0.949168 -2.876429	H 2.238918 1.514949 -2.693682	H 1.829352 2.536143 -1.140433
H -2.124671 -2.188070 -1.606984	H 1.985035 2.482712 -1.199818	H 2.061811 1.620043 -2.670989
O 1.595089 2.420201 -1.248924	O -1.972884 -2.411757 -0.779032	O -2.145313 -2.390195 -0.396143
H 0.823810 1.869042 -0.993737	H -1.221041 -1.828651 -1.003400	H -1.434975 -2.013989 -0.938526

Table S16. Optimized Cartesian coordinates for the stationary points involved in the C3-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

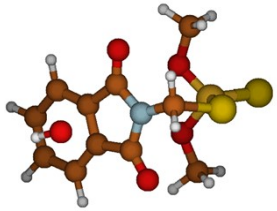
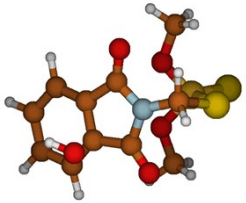
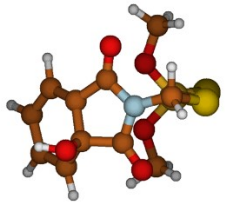
MCR(C3-add)	TS(C3-add)	Adduct(C3-add)
		
C -3.819999 -1.670595 -1.023694	C -3.627699 -1.317356 -1.400022	C -3.078840 2.074161 0.518875
C -2.948054 -1.726152 0.068299	C -2.942799 -1.510045 -0.205495	C -2.762342 1.389732 -0.616699
C -2.091682 -0.652642 0.247539	C -2.192666 -0.429134 0.296147	C -2.392845 -0.053053 -0.532321
C -2.095708 0.439420 -0.616413	C -2.022623 0.739589 -0.479566	C -1.999658 -0.480587 0.845940
C -2.956726 0.507239 -1.699064	C -2.698576 0.933137 -1.662937	C -2.310982 0.230606 1.966763
C -3.823914 -0.572555 -1.892715	C -3.520694 -0.112944 -2.113158	C -2.914841 1.499414 1.814847
C -1.064954 -0.408576 1.305100	C -1.105564 -0.440183 1.334796	C -1.194715 -0.535942 -1.370531
N -0.499665 0.833997 0.998354	N -0.467789 0.799151 1.216717	N -0.514907 -1.467473 -0.593849
C -1.078073 1.422433 -0.136433	C -0.990275 1.586430 0.179729	C -0.996332 -1.553131 0.733045
C 0.577640 1.421669 1.727162	C 0.677807 1.173647 1.984130	C 0.669560 -2.141148 -1.029449
S 2.249336 0.629925 1.496960	S 2.254082 0.266418 1.578238	S 2.184155 -1.072723 -1.213809
P 2.135011 -0.300357 -0.382572	P 2.035848 -0.303307 -0.432407	P 1.903654 0.502968 0.148467
O 1.326080 0.699736 -1.337600	O 1.319103 0.921918 -1.175593	O 1.244228 -0.138923 1.459087
C 1.947725 1.915095 -1.778269	C 2.049783 2.134140 -1.410035	C 2.033311 -0.984240 2.308532
O -0.795024 2.506996 -0.582098	O -0.640573 2.710702 -0.087722	O -0.580793 -2.330805 1.559553
O -0.752943 -1.099712 2.243756	O -0.808929 -1.304362 2.117173	O -0.914318 -0.232496 -2.501169
S 3.880453 -0.901524 -0.924937	S 3.710141 -0.961776 -1.113086	S 3.532164 1.512623 0.319941
O 0.966258 -1.399366 -0.280211	O 0.765583 -1.288488 -0.500367	O 0.582577 1.293819 -0.320914
C 1.217089 -2.613912 0.443784	C 0.910111 -2.635599 -0.021578	C 0.675987 2.162917 -1.462690
H 0.645941 2.466494 1.423641	H 0.839235 2.240826 1.830840	H 0.880767 -2.928518 -0.305791
H 0.385886 1.340972 2.798643	H 0.506478 0.955658 3.039742	H 0.515065 -2.559503 -2.025715
H -2.951258 1.365632 -2.362556	H -2.568902 1.844782 -2.236462	H -2.011568 -0.133458 2.945099
H -2.938555 -2.567562 0.753623	H -3.010861 -2.431495 0.362746	H -2.889172 1.814382 -1.607978
H -4.512502 -0.563136 -2.731432	H -4.063088 -0.001161 -3.046252	H -3.175813 2.080718 2.691524
H -4.506265 -2.491733 -1.204099	H -4.248490 -2.113713 -1.796709	H -3.450857 3.091544 0.447312
H 1.429918 -2.387538 1.492254	H 1.153905 -2.629865 1.044250	H 0.929887 1.582678 -2.353897
H 2.047613 -3.155197 -0.014788	H 1.681278 -3.152751 -0.596478	H 1.419995 2.940357 -1.276697
H 0.296700 -3.192673 0.375606	H -0.060820 -3.106863 -0.170967	H -0.314775 2.600217 -1.580144
H 1.185604 2.447030 -2.344288	H 1.327370 2.838475 -1.817960	H 1.344526 -1.376350 3.054285
H 2.813955 1.682606 -2.401972	H 2.861901 1.945099 -2.115679	H 2.831153 -0.399531 2.771929
H 2.252532 2.518660 -0.917749	H 2.451200 2.523996 -0.469425	H 2.458034 -1.811849 1.732050
O -3.450586 1.314759 1.656615	O -3.462005 0.194830 1.691452	O -3.466117 -0.860923 -1.049493
H -4.284034 1.001554 1.255378	H -4.166239 0.561407 1.127467	H -4.243243 -0.709038 -0.494551

Table S17. Optimized Cartesian coordinates for the stationary points involved in the C4-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

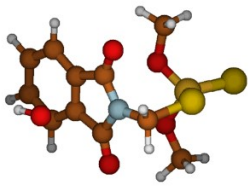
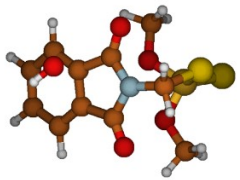
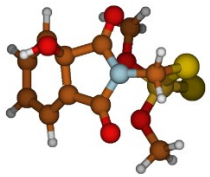
MCR(C4-add)	TS(C4-add)	Adduct(C4-add)
		
C 3.823814 -0.574434 -1.892615	C -3.520498 0.112599 -2.113199	C 2.914842 1.499415 1.814846
C 2.956693 0.505599 -1.699961	C -2.698423 -0.933379 -1.662725	C 2.310983 0.230607 1.966763
C 2.095790 0.438917 -0.617173	C -2.022425 -0.739500 -0.479415	C 1.999658 -0.480587 0.845940
C 2.091820 -0.652259 0.247898	C -2.192604 0.429246 0.296079	C 2.392845 -0.053054 -0.532321
C 2.948165 -1.725960 0.069707	C -2.942594 1.510082 -0.205886	C 2.762342 1.389732 -0.616700
C 3.819986 -1.671562 -1.022476	C -3.627414 1.317203 -1.400335	C 3.078840 2.074162 0.518874
C 1.078126 1.422388 -0.138188	C -0.990258 -1.586348 0.180178	C 0.996332 -1.553130 0.733046
N 0.499796 0.835120 0.997254	N -0.467925 -0.798980 1.217144	N 0.514907 -1.467473 -0.593847
C 1.065202 -0.407071 1.305318	C -1.105530 0.440488 1.334779	C 1.194715 -0.535943 -1.370530
C -0.577548 1.423501 1.725439	C 0.677762 -1.173287 1.984515	C -0.669560 -2.141149 -1.029447
S -2.248998 0.630903 1.496707	S 2.254092 -0.266333 1.578166	S -2.184155 -1.072724 -1.213808
P -2.135000 -0.300831 -0.382128	P 2.035715 0.303195 -0.432510	P -1.903654 0.502968 0.148467
O -0.966060 -1.399576 -0.279158	O 0.765534 1.288490 -0.500481	O -0.582577 1.293819 -0.320916
C -1.216487 -2.613578 0.445853	C 0.910230 2.635536 -0.021550	C -0.675988 2.162916 -1.462693
O 0.753325 -1.097208 2.244756	O -0.808769 1.304917 2.116826	O 0.914318 -0.232498 -2.501169
O 0.794996 2.506457 -0.584991	O -0.640652 -2.710704 -0.087056	O 0.580793 -2.330804 1.559554
S -3.880457 -0.902661 -0.923731	S 3.710008 0.961449 -1.113380	S -3.532165 1.512623 0.319942
O -1.326367 0.698686 -1.338009	O 1.318792 -0.922038 -1.175493	O -1.244227 -0.138923 1.459087
C -1.948466 1.913329 -1.779975	C 2.049380 -2.134305 -1.410004	C -2.033311 -0.984237 2.308534
H -0.385582 1.344440 2.797008	H 0.506584 -0.954946 3.040077	H -0.515064 -2.559504 -2.025714
H -0.646205 2.467874 1.420433	H 0.839115 -2.240522 1.831543	H -0.880767 -2.928519 -0.305790
H 2.938742 -2.566652 0.755915	H -3.010545 2.431688 0.362113	H 2.889171 1.814381 -1.607979
H 2.951230 1.363318 -2.364319	H -2.568681 -1.845131 -2.236062	H 2.011570 -0.133457 2.945099
H 4.506184 -2.492926 -1.202118	H -4.248133 2.113511 -1.797232	H 3.450857 3.091544 0.447310
H 4.512305 -0.565880 -2.731422	H -4.062891 0.000628 -3.046270	H 3.175815 2.080719 2.691522
H -2.254623 2.517154 -0.920106	H 2.860975 -1.945455 -2.116298	H -2.831148 -0.399524 2.771935
H -2.813912 1.679840 -2.404386	H 2.451499 -2.523796 -0.469543	H -2.458040 -1.811842 1.732054
H -1.186161 2.445501 -2.345530	H 1.326723 -2.838824 -1.817183	H -1.344525 -1.376351 3.054284
H -0.296062 -3.192297 0.377775	H -0.061098 3.106469 -0.169380	H 0.314774 2.600216 -1.580147
H -2.047119 -3.155318 -0.011988	H 1.155572 2.629681 1.043926	H -0.929887 1.582676 -2.353898
H -1.428958 -2.386432 1.494231	H 1.680384 3.153091 -0.597442	H -1.419995 2.940355 -1.276699
O 3.449323 1.317254 1.656568	O -3.461916 -0.194404 1.691295	O 3.466117 -0.860924 -1.049492
H 4.283545 0.997997 1.261778	H -4.165036 -0.563413 1.127507	H 4.243243 -0.709036 -0.494552

Table S18. Optimized Cartesian coordinates for the stationary points involved in the C5-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

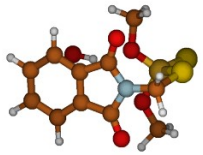
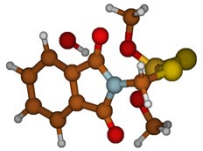
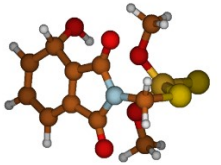
MCR(C5-add)	TS(C5-add)	Adduct(C5-add)
		
C -4.103198 0.153471 -1.222565	C -3.981549 -0.324754 -1.380763	C 3.834761 0.446644 -1.484829
C -3.124715 -0.843107 -1.298865	C -2.983343 -1.279183 -1.123344	C 2.883903 1.415317 -1.041454
C -2.164614 -0.862259 -0.302666	C -2.069053 -0.989878 -0.121758	C 2.018116 1.035365 -0.014325
C -2.172847 0.062889 0.738886	C -2.131786 0.185329 0.612107	C 2.062667 -0.197910 0.584621
C -3.135819 1.053669 0.824589	C -3.068346 1.194059 0.320378	C 2.932991 -1.309872 0.111033
C -4.107391 1.086390 -0.182397	C -4.041079 0.864800 -0.668744	C 3.880727 -0.806806 -0.952499
C -1.000326 -1.773422 -0.112586	C -0.907120 -1.788570 0.367156	C 0.866534 1.800775 0.560587
N -0.362661 -1.325548 1.058303	N -0.323373 -1.013403 1.379487	N 0.289820 0.947062 1.502236
C -1.017834 -0.228470 1.635897	C -1.020311 0.186086 1.602277	C 0.990570 -0.276466 1.597595
C 0.861279 -1.870466 1.546086	C 0.902027 -1.347929 2.025575	C -0.959780 1.185811 2.139411
S 2.403656 -0.871469 1.211861	S 2.454592 -0.616969 1.277750	S -2.478582 0.569988 1.225352
P 1.913727 0.411034 -0.369650	P 1.878110 0.328322 -0.506399	P -1.819236 -0.314039 -0.562580
O 0.684400 1.330191 0.139217	O 0.700727 1.363650 -0.141937	O -0.679403 -1.388436 -0.192385
C 0.935931 2.377681 1.097735	C 1.021098 2.574403 0.574816	C -1.053226 -2.602934 0.490627
O -0.672024 0.317320 2.656007	O -0.735183 1.000601 2.445682	O 0.717741 -1.153989 2.382311
O -0.644625 -2.719905 -0.771883	O -0.519098 -2.876283 0.015801	O 0.479362 2.912958 0.291819
S 3.491501 1.313911 -0.991149	S 3.441758 1.014616 -1.388655	S -3.346220 -0.928677 -1.556420
O 1.028388 -0.424851 -1.411881	O 0.930031 -0.689947 -1.306547	O -0.815962 0.721542 -1.270837
C 1.657881 -1.419895 -2.235824	C 1.511961 -1.837921 -1.945412	C -1.350499 1.902028 -1.891662
H 0.821589 -1.947335 2.633845	H 0.873938 -0.980155 3.051680	H -0.966240 0.676424 3.103038
H 0.993372 -2.851307 1.089312	H 1.019757 -2.431104 1.996936	H -1.094722 2.260864 2.258046
H -3.126916 1.775079 1.635042	H -3.229699 2.009985 1.013772	H 3.497337 -1.752179 0.942210
H -3.107524 -1.568410 -2.105456	H -2.924709 -2.209453 -1.678551	H 2.817776 2.400299 -1.489040
H -4.870577 1.857063 -0.162958	H -4.813771 1.591044 -0.895118	H 4.588383 -1.536623 -1.334015
H -4.867383 0.212639 -1.990371	H -4.720541 -0.519688 -2.150561	H 4.522205 0.714415 -2.280823
H 2.119914 -2.188522 -1.609609	H 1.984973 -2.482826 -1.199659	H -1.828752 2.536161 -1.140314
H 2.405539 -0.947881 -2.876865	H 2.239382 -1.514975 -2.693380	H -2.062065 1.620042 -2.670748
H 0.857581 -1.863329 -2.824504	H 0.682983 -2.368410 -2.410120	H -0.495298 2.424788 -2.316731
H -0.020490 2.881007 1.235756	H 0.076473 3.107726 0.671009	H -0.117775 -3.128665 0.676503
H 1.682189 3.067605 0.698839	H 1.746190 3.155756 0.001568	H -1.721499 -3.186162 -0.146330
H 1.266187 1.937513 2.041444	H 1.413769 2.322839 1.563063	H -1.535022 -2.359895 1.441041
O -1.594903 2.419936 -1.248558	O -1.973007 2.411796 -0.778883	O 2.145353 -2.390406 -0.395787
H -0.823283 1.869810 -0.992199	H -1.221147 1.828701 -1.003244	H 1.435011 -2.014388 -0.938296

Table S19. Optimized Cartesian coordinates for the stationary points involved in the C6-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

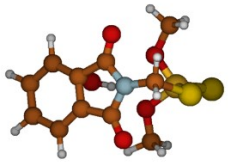
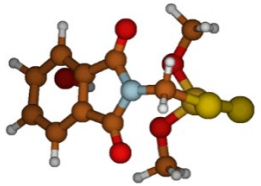
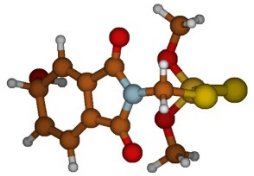
MCR(C6-add)	TS(C6-add)	Adduct(C6-add)
		
C 4.152596 1.165701 0.144902	C -3.952006 0.458947 -1.007331	C 3.923391 0.469618 -1.132316
C 3.176015 0.927583 1.117990	C -2.956024 -0.379204 -1.497173	C 2.897527 1.350333 -0.946370
C 2.206230 -0.012905 0.820377	C -1.991849 -0.811342 -0.597109	C 1.936992 1.051635 0.039889
C 2.201351 -0.702691 -0.389866	C -2.028839 -0.458903 0.755133	C 2.015943 -0.138534 0.817076
C 3.161687 -0.473919 -1.360500	C -3.012335 0.355395 1.267084	C 3.007049 -1.042265 0.678208
C 4.143674 0.480291 -1.072509	C -3.953839 0.894845 0.346833	C 4.088005 -0.808766 -0.344991
C 1.038411 -0.471868 1.625253	C -0.777239 -1.641328 -0.829694	C 0.709676 1.768636 0.414890
N 0.395974 -1.440040 0.841034	N -0.142806 -1.737428 0.416914	N 0.093923 0.979507 1.408239
C 1.042924 -1.642160 -0.392837	C -0.850611 -1.071834 1.432723	C 0.824847 -0.174088 1.719357
C -0.840248 -2.063193 1.191584	C 1.151866 -2.307346 0.606879	C -1.189198 1.268926 1.961506
S -2.333567 -0.952864 1.235393	S 2.590976 -1.284608 -0.002038	S -2.658487 0.910920 0.865965
P -1.948830 0.470248 -0.249338	P 1.869164 0.683251 -0.156313	P -1.963088 -0.446820 -0.578374
O -1.186787 -0.293042 -1.433983	O 0.952708 0.950164 1.131862	O -1.028019 -1.500776 0.185350
C -1.902818 -1.187059 -2.298617	C 1.570909 1.108564 2.418617	C -1.625171 -2.470987 1.059054
O 0.702952 -2.443953 -1.228064	O -0.533773 -1.048655 2.596565	O 0.526107 -0.982956 2.564628
O 0.671412 -0.123026 2.721829	O -0.373680 -2.147085 -1.849348	O 0.261150 2.816449 0.004480
S -3.526382 1.495138 -0.634116	S 3.331584 1.875877 -0.522744	S -3.445180 -1.099904 -1.616078
O -0.630536 1.284665 0.219911	O 0.646385 0.653195 -1.201642	O -0.764102 0.281898 -1.362666
C -0.736086 2.264373 1.268816	C 0.932614 0.510445 -2.602906	C -1.078670 1.327319 -2.296684
H -1.016189 -2.862846 0.471433	H 1.286186 -2.476988 1.675168	H -1.297800 0.680652 2.872664
H -0.787904 -2.464045 2.205897	H 1.226980 -3.242766 0.050383	H -1.263011 2.336880 2.172846
H 3.139094 -1.005886 -2.305538	H -3.035050 0.632374 2.315272	H 3.040208 -1.956959 1.262917
H 3.171071 1.455009 2.066426	H -2.924073 -0.683948 -2.537983	H 2.803786 2.251946 -1.543565
H 4.906500 0.700792 -1.811615	H -4.828138 1.407615 0.727570	H 5.059440 -0.776322 0.171233
H 4.927022 1.901970 0.333042	H -4.720476 0.840079 -1.670595	H 4.676008 0.643915 -1.895350
H -1.039154 1.775872 2.198454	H 1.444691 -0.438239 -2.785385	H -1.567564 2.156883 -1.778831
H -1.449213 3.039208 0.980083	H 1.538248 1.352481 -2.944696	H -1.714790 0.934089 -3.092698
H 0.264450 2.682184 1.378480	H -0.035591 0.503951 -3.102068	H -0.122630 1.662055 -2.697303
H -1.147624 -1.648151 -2.931907	H 0.752899 1.236452 3.124672	H -0.796588 -3.032394 1.486027
H -2.628043 -0.624630 -2.890518	H 2.224163 1.983782 2.408472	H -2.291309 -3.121568 0.487938
H -2.411647 -1.956518 -1.709689	H 2.140041 0.210563 2.676473	H -2.176857 -1.969272 1.859566
O 1.413963 1.841696 -1.828732	O -3.123629 2.685747 0.103388	O 4.211807 -1.929822 -1.217151
H 0.661014 1.521582 -1.287359	H -2.208631 2.431211 -0.119400	H 3.380743 -2.029697 -1.700568

Table S20. Optimized Cartesian coordinates for the stationary points involved in the C7-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

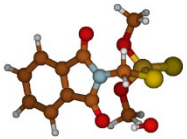
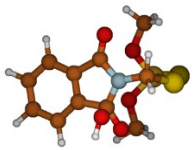
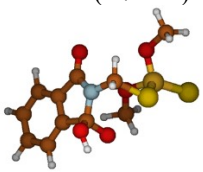
MCR(C7-add)	TS(C7-add)	Adduct(C7-add)
		
C -4.265215 0.142321 1.411660	C 3.948166 0.478995 1.719368	C -4.497060 0.931355 -0.772389
C -3.219642 1.033078 1.145002	C 3.132900 -0.588755 1.328881	C -3.638688 -0.114641 -1.123498
C -2.304109 0.656271 0.178809	C 2.236882 -0.354570 0.302206	C -2.548199 -0.342834 -0.300035
C -2.413841 -0.549725 -0.505211	C 2.139719 0.885960 -0.316425	C -2.301375 0.439231 0.821220
C -3.445443 -1.436653 -0.254270	C 2.945108 1.948059 0.057276	C -3.146941 1.478098 1.176551
C -4.375728 -1.070500 0.724615	C 3.858590 1.725485 1.091885	C -4.253571 1.718588 0.358219
C -1.093870 1.366746 -0.319792	C 1.244435 -1.271783 -0.340921	C -1.421060 -1.371097 -0.446076
N -0.538436 0.546294 -1.297385	N 0.526598 -0.472627 -1.237177	N -0.666492 -1.165337 0.773966
C -1.281798 -0.642828 -1.470406	C 1.060926 0.818293 -1.343820	C -1.072534 -0.057885 1.505150
C 0.714562 0.776540 -1.957477	C -0.580216 -0.939509 -2.007068	C 0.589325 -1.815292 0.971984
S 2.219883 0.779562 -0.870427	S -2.195234 -1.118873 -1.093532	S 1.771680 -1.583755 -0.427928
P 1.747908 -0.645061 0.605542	P -2.038987 0.236837 0.503083	P 2.193608 0.479360 -0.238824
O 0.889433 -1.773488 -0.141856	O -1.309836 1.539623 -0.076034	O 2.464064 0.668987 1.329340
C 1.546133 -2.697925 -1.021043	C -2.014644 2.404344 -0.977667	C 3.690070 0.194959 1.895410
O -1.025318 -1.503838 -2.273502	O 0.694272 1.659606 -2.128659	O -0.538249 0.363116 2.504857
O -0.655590 2.444094 0.028044	O 0.789489 -2.348976 0.132688	O -0.766401 -0.959549 -1.574027
S 3.316597 -1.149302 1.593661	S -3.747039 0.432165 1.369273	S 3.555692 1.017387 -1.487253
O 0.510604 -0.029313 1.430501	O -0.800972 -0.254320 1.402889	O 0.784551 1.235040 -0.281596
C 0.766355 1.016156 2.380699	C -0.987837 -1.371240 2.284444	C 0.310066 1.831322 -1.499182
H 0.819115 -0.003040 -2.712812	H -0.727015 -0.234841 -2.826031	H 1.019454 -1.419267 1.894756
H 0.735526 1.765645 -2.420380	H -0.365063 -1.938952 -2.390945	H 0.462283 -2.898362 1.039258
H -3.521086 -2.374316 -0.794622	H 2.857250 2.912073 -0.432708	H -2.944189 2.072893 2.061341
H -3.125841 1.979773 1.667168	H 3.194105 -1.557707 1.814815	H -3.824285 -0.722328 -2.003389
H -5.199099 -1.738124 0.956375	H 4.505112 2.532754 1.419930	H -4.938227 2.524271 0.602362
H -5.005472 0.395476 2.163574	H 4.661771 0.340217 2.525108	H -5.366504 1.138209 -1.388057
H 1.236244 1.871343 1.885349	H -1.279188 -2.257353 1.713305	H 0.395696 1.133560 -2.333439
H 1.403978 0.640417 3.183633	H -1.743978 -1.130255 3.034877	H 0.877097 2.741590 -1.702779
H -0.209280 1.308030 2.767969	H -0.019567 -1.540675 2.754165	H -0.740420 2.063170 -1.319268
H 0.749057 -3.262158 -1.501655	H -1.295586 3.163283 -1.279357	H 3.640453 0.439078 2.955264
H 2.203374 -3.352466 -0.444502	H -2.872044 2.850090 -0.468200	H 4.540575 0.695982 1.426623
H 2.125953 -2.159428 -1.777731	H -2.347114 1.845131 -1.857735	H 3.780074 -0.888290 1.761590
O 1.784066 3.585878 -1.028101	O 2.231943 -2.305461 -1.477986	O -1.796298 -2.712947 -0.511780
H 0.964301 3.349010 -0.541760	H 2.662949 -2.976038 -0.917223	H -1.820174 -2.959670 -1.445239

Table S21. Optimized Cartesian coordinates for the stationary points involved in the C9-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

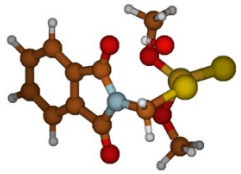
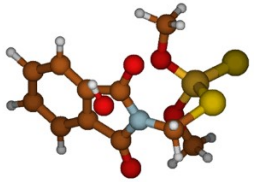
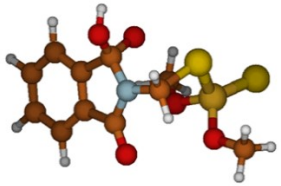
MCR(C9-add)	TS(C9-add)	Adduct(C9-add)
		
C 4.376061 -1.070067 0.725123	C -3.859057 -1.724491 -1.092835	C 4.253652 1.718574 0.358163
C 3.445696 -1.436774 -0.253487	C -2.945433 -1.947911 -0.058533	C 3.147066 1.478059 1.176552
C 2.413962 -0.550086 -0.504689	C -2.139808 -0.886193 0.315746	C 2.301483 0.439200 0.821239
C 2.304139 0.656240 0.178759	C -2.236890 0.354764 -0.302037	C 2.548264 -0.342823 -0.300059
C 3.219755 1.033572 1.144671	C -3.133080 0.589807 -1.328366	C 3.638708 -0.114611 -1.123575
C 4.265470 0.143058 1.411608	C -3.948567 -0.477556 -1.719445	C 4.497092 0.931381 -0.772481
C 1.281973 -0.643765 -1.469892	C -1.060993 -0.819304 1.343176	C 1.072679 -0.057938 1.505216
N 0.538512 0.545320 -1.297433	N -0.526609 0.471667 1.237471	N 0.666601 -1.165372 0.774015
C 1.093878 1.366345 -0.320270	C -1.244366 1.271448 0.341697	C 1.421104 -1.371069 -0.446084
C -0.714292 0.775474 -1.957893	C 0.580299 0.937886 2.007642	C -0.589238 -1.815276 0.972019
S -2.219841 0.779175 -0.871174	S 2.195142 1.118474 1.094090	S -1.771615 -1.583776 -0.427911
P -1.748139 -0.644624 0.605637	P 2.039110 -0.236477 -0.503208	P -2.193670 0.479301 -0.238803
O -0.511010 -0.028298 1.430471	O 0.801068 0.255017 -1.402786	O -0.784604 1.235002 -0.281323
C -0.767002 1.017762 2.379948	C 0.987854 1.372360 -2.283826	C -0.310017 1.831409 -1.498825
O 0.655426 2.443862 0.026821	O -0.789389 2.348969 -0.131200	O 0.766476 -0.959378 -1.573992
O 1.025612 -1.505234 -2.272546	O -0.694450 -1.661292 2.127353	O 0.538476 0.363034 2.504977
S -3.317029 -1.148280 1.593736	S 3.747162 -0.431266 -1.369512	S -3.555615 1.017407 -1.487357
O -0.889602 -1.773516 -0.140950	O 1.310060 -1.539592 0.075310	O -2.464397 0.668820 1.329350
C -1.546189 -2.698800 -1.019328	C 2.015039 -2.404769 0.976382	C -3.690731 0.195058 1.894976
H -0.734987 1.764399 -2.421218	H 0.365120 1.936844 2.392776	H -0.462239 -2.898348 1.039303
H -0.818795 -0.004376 -2.712956	H 0.727301 0.232275 2.825756	H -1.019401 -1.419205 1.894754
H 3.125945 1.980486 1.666436	H -3.194240 1.559110 -1.813607	H 3.824252 -0.722281 -2.003488
H 3.521362 -2.374668 -0.793435	H -2.857657 -2.912265 0.430796	H 2.944371 2.072826 2.061373
H 5.005785 0.396685 2.163306	H -4.662314 -0.338116 -2.524946	H 5.366503 1.138268 -1.388183
H 5.199556 -1.737466 0.957087	H -4.505767 -2.531436 -1.421309	H 4.938318 2.524254 0.602292
H -2.126540 -2.161068 -1.776159	H 2.348637 -1.845785 1.856170	H -4.540963 0.696141 1.425762
H -2.202924 -3.353270 -0.442137	H 2.871728 -2.851055 0.466197	H -3.780799 -0.888199 1.761279
H -0.749043 -3.262978 -1.499895	H 1.295730 -3.163241 1.278656	H -3.641498 0.439327 2.954812
H 0.208537 1.310109 2.767098	H 0.019545 1.542027 -2.753385	H 0.740273 2.063832 -1.318521
H -1.404596 0.642448 3.183106	H 1.743924 1.131719 -3.034441	H -0.394958 1.133483 -2.333012
H -1.237047 1.872542 1.884036	H 1.279278 2.258199 -1.712302	H -0.877450 2.741353 -1.702748
O -1.783230 3.585520 -1.029133	O -2.231719 2.304446 1.479488	O 1.796238 -2.712937 -0.511875
H -0.963130 3.348552 -0.543370	H -2.663066 2.975293 0.919307	H 1.820249 -2.959565 -1.445356

Table S22. Optimized Cartesian coordinates for the stationary points involved in the P12-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

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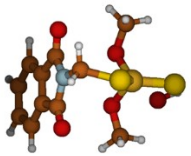
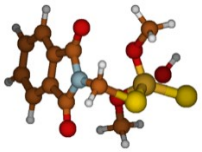
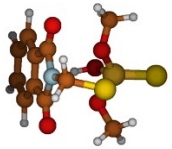
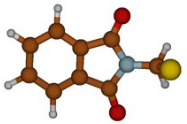
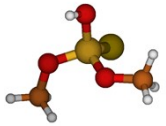
																			
C	-4.099118	1.663196	-0.085234	C	-4.188214	-1.562555	-0.191962	C	-3.081968	-1.885855	1.094985	C	3.463717	0.699620	0.351260	P	-0.022233	0.078168	0.342429
C	-3.238524	1.138300	-1.055338	C	-3.314794	-1.239066	0.852127	C	-2.444355	-0.775950	1.663516	C	2.286876	1.423845	0.132327	O	0.353342	0.006323	1.900246
C	-2.388607	0.120764	-0.660025	C	-2.425057	-0.202707	0.631842	C	-1.931957	0.172090	0.793765	C	1.129679	0.696045	-0.082747	O	-1.528435	-0.464422	0.387430
C	-2.388976	-0.368398	0.642704	C	-2.399959	0.496495	-0.570848	C	-2.042228	0.032631	-0.585719	C	1.129910	-0.696012	-0.082577	O	0.696680	-1.196542	-0.333736
C	-3.238204	0.139400	1.609824	C	-3.261133	0.189005	-1.609270	C	-2.673030	-1.057211	-1.161748	C	2.287324	-1.423413	0.132664	S	0.338478	1.776271	-0.471962
C	-4.098678	1.172565	1.224152	C	-4.161447	-0.861193	-1.401328	C	-3.194829	-2.023912	-0.294482	C	3.463943	-0.698774	0.351422	C	-2.251728	-0.613957	-0.840894
C	-1.360534	-0.626118	-1.441429	C	-1.374346	0.364919	1.526974	C	-1.156536	1.420611	1.075144	C	-0.267052	1.163407	-0.337586	C	2.063020	-1.105245	-0.753341
N	-0.795772	-1.541250	-0.540515	N	-0.772175	1.397054	0.790823	N	-0.869847	1.973533	-0.175222	N	-1.024870	-0.000409	-0.519482	H	0.001175	-0.789068	2.327590
C	-1.368833	-1.452143	0.740087	C	-1.338779	1.541439	-0.486068	C	-1.338849	1.184504	-1.229190	C	-0.266657	-1.163917	-0.337295	H	-1.776312	-1.376103	-1.463370
C	0.309871	-2.389737	-0.851185	C	0.368694	2.136259	1.233146	C	-0.019162	3.119773	-0.359128	C	-2.456015	-0.000682	-0.663016	H	2.709899	-0.888760	0.101606
S	1.959465	-1.548309	-1.062315	S	1.968903	1.195132	1.326291	S	1.744295	2.811849	-0.136538	O	-0.703462	-2.288100	-0.389658	H	-2.288656	0.340837	-1.371894
P	1.787298	0.198283	0.089091	P	1.768831	-0.303698	-0.154306	P	1.383810	-1.318429	0.044047	O	-0.704263	2.287411	-0.390264	H	-3.256812	-0.927460	-0.563784
O	1.025445	-0.208229	1.432504	O	1.112192	0.435950	-1.401966	O	0.860697	-0.416986	-1.184593	H	2.273467	-2.508300	0.132053	H	2.172779	-0.322306	-1.507288
C	1.680257	-1.023080	2.413733	C	1.821393	1.464198	-2.104125	C	0.956512	-0.947628	-2.513940	H	2.272707	2.508728	0.131473	H	2.315328	-2.077661	-1.174009
O	-1.079612	-2.154149	1.678559	O	-1.016095	2.375305	-1.298009	O	-1.197128	1.429835	-2.403487	H	4.394490	-1.229052	0.525819				
O	-1.045784	-0.520475	-2.601811	O	-1.071151	0.053350	2.652281	O	-0.835279	1.902714	2.135176	H	4.394087	1.230247	0.525540				
S	3.548396	1.004523	0.205671	S	3.591007	-1.063889	-0.224995	S	3.194117	-1.945542	-0.041201	H	-2.747501	-0.891674	-1.226640				
O	0.593655	1.047722	-0.541729	O	0.514531	-1.153198	0.328765	O	0.951961	-0.355855	1.246989	S	-3.377120	0.000519	0.889295				
C	0.827815	1.850770	-1.710750	C	0.707185	-2.289510	1.186331	C	1.887174	0.140233	2.218100	H	-2.747788	0.889408	-1.227933				
H	0.395309	-3.121791	-0.047765	H	0.492836	2.977246	0.550064	H	-0.186011	3.499371	-1.370772								
H	0.140969	-2.884397	-1.809396	H	0.209782	2.490883	2.253235	H	-0.300932	3.895166	0.360358								
H	-3.227703	-0.249681	2.622492	H	-3.229732	0.740722	-2.542863	H	-2.743554	-1.156524	-2.240107								
H	-3.231615	1.508189	-2.075578	H	-3.328204	-1.773195	1.796766	H	-2.337624	-0.663620	2.737413								
H	-4.777830	1.603733	1.952376	H	-4.851601	-1.139169	-2.191198	H	-3.688595	-2.899977	-0.701852								
H	-4.779653	2.465597	-0.350927	H	-4.899859	-2.371686	-0.063547	H	-3.490904	-2.657170	1.739414								
H	1.166237	1.218390	-2.536528	H	1.166289	-1.972936	2.127130	H	2.168066	-0.664949	2.899965								
H	1.554440	2.629576	-1.473031	H	1.319230	-3.029530	0.667361	H	2.773917	0.538289	1.722989								
H	-0.138454	2.289131	-1.957736	H	-0.292381	-2.678056	1.378494	H	1.357471	0.932361	2.747438								
H	0.916928	-1.262933	3.151383	H	1.081927	1.943369	-2.742943	H	0.412558	-1.895268	-2.581437								
H	2.504580	-0.465545	2.863891	H	2.624247	1.018143	-2.696471	H	0.498929	-0.203395	-3.164916								
H	2.053223	-1.945152	1.956883	H	2.236465	2.194464	-1.402636	H	2.006114	-1.100607	-2.776826								
O	1.941785	3.088478	0.965868	O	2.002552	-2.201698	-1.531244	O	0.302993	-2.509645	0.135960								
H	2.755990	3.350067	1.431125	H	2.447726	-2.025496	-2.374842	H	-0.582840	-2.199104	0.389831								

Table S23. Optimized Cartesian coordinates for the stationary points involved in the S17-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

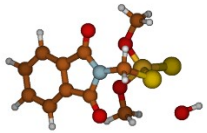
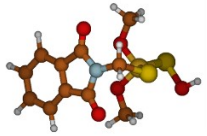
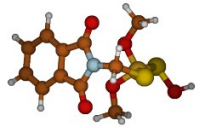
MCR(S17-add)	TS(S17-add)	Adduct(S17-add)
		
C -4.230709 -1.401405 -1.014687	C -4.176934 -1.495495 -0.953192	C -3.887133 -2.111513 0.060649
C -3.229141 -1.749766 -0.102064	C -3.265939 -1.678849 0.092660	C -3.139482 -1.443302 1.036318
C -2.412031 -0.731448 0.355983	C -2.449836 -0.608503 0.412502	C -2.421984 -0.332458 0.630105
C -2.577437 0.584318 -0.063585	C -2.529356 0.601594 -0.268762	C -2.442949 0.110024 -0.688361
C -3.567710 0.942713 -0.961265	C -3.428972 0.797104 -1.301881	C -3.181566 -0.539287 -1.661677
C -4.396890 -0.078586 -1.436875	C -4.256897 -0.278997 -1.638339	C -3.907349 -1.667496 -1.265167
C -1.267032 -0.778849 1.311971	C -1.385867 -0.492189 1.452331	C -1.529494 0.571910 1.413067
N -0.800799 0.540332 1.408041	N -0.883486 0.812113 1.333919	N -1.068060 1.529180 0.499342
C -1.548327 1.426447 0.612282	C -1.525823 1.537155 0.316406	C -1.573287 1.318166 -0.791988
C 0.382407 0.934486 2.112326	C 0.245232 1.309186 2.061049	C -0.088990 2.523845 0.814736
S 1.973703 0.180679 1.521960	S 1.866781 0.479604 1.659832	S 1.652973 1.889844 1.000287
P 1.687785 0.152323 -0.556767	P 1.687316 -0.090578 -0.388028	P 1.767632 -0.046449 -0.038378
O 0.788163 1.434699 -0.886561	O 0.852706 1.092710 -1.073608	O 0.926371 0.229795 -1.394781
C 1.369805 2.745510 -0.861885	C 1.439857 2.390417 -1.254401	C 1.442589 1.145338 -2.368712
O -1.375235 2.619564 0.550518	O -1.298043 2.689293 0.035194	O -1.345757 2.017989 -1.750047
O -0.806163 -1.720057 1.910413	O -1.004574 -1.308562 2.255528	O -1.244168 0.541951 2.585945
S 3.352142 -0.007332 -1.542921	S 3.357633 -0.448554 -1.571100	S 3.173688 -1.653662 -0.969642
O 0.548200 -0.933379 -0.842880	O 0.520571 -1.193293 -0.487709	O 0.611367 -0.932330 0.668673
C 0.847045 -2.337333 -0.703450	C 0.828636 -2.519927 -0.012908	C 0.948244 -1.558987 1.915554
H 0.441093 2.021778 2.048775	H 0.319171 2.377383 1.855092	H -0.108374 3.268650 0.018809
H 0.327778 0.619628 3.156871	H 0.111764 1.130323 3.130139	H -0.330335 2.976752 1.778167
H -3.686389 1.972836 -1.280330	H -3.481244 1.745987 -1.825271	H -3.188969 -0.184300 -2.686872
H -3.092473 -2.771509 0.237269	H -3.196660 -2.616350 0.634932	H -3.118107 -1.775680 2.069201
H -5.183638 0.157052 -2.146103	H -4.974468 -0.170654 -2.445105	H -4.496753 -2.209764 -1.997393
H -4.892092 -2.169258 -1.402791	H -4.834710 -2.309743 -1.239486	H -4.462148 -2.990111 0.334780
H 1.118197 -2.557184 0.331641	H 1.055773 -2.487850 1.055760	H 1.128042 -0.797843 2.680502
H 1.662768 -2.611403 -1.375019	H 1.673499 -2.929520 -0.572055	H 1.824097 -2.203347 1.790021
H -0.073639 -2.853402 -0.973453	H -0.071980 -3.107528 -0.186382	H 0.079825 -2.154936 2.194327
H 0.533303 3.437236 -0.942762	H 0.615613 3.050968 -1.516358	H 0.721009 1.151735 -3.183469
H 2.061616 2.857403 -1.699408	H 2.184289 2.349135 -2.052437	H 2.421563 0.808648 -2.723992
H 1.899143 2.911383 0.082309	H 1.905316 2.732386 -0.324445	H 1.517663 2.149964 -1.942697
O 3.732952 -2.084617 0.161706	O 3.961813 -1.406816 -0.114839	O 4.232461 -1.704753 0.334634
H 4.636410 -1.721453 0.155504	H 4.753289 -0.943084 0.199569	H 4.994086 -1.144865 0.136029

Table S24. Vibrational frequencies and rotational constants for the stationary points involved in the H20-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H20-abs) $C_1 - {}^2A$	TS(H20-abs) $C_1 - {}^2A$	MCP(H20-abs) $C_1 - {}^2A$	Rad(H20-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
25, 39, 52, 84, 95, 103, 108, 116, 132, 142, 151, 153, 162, 166, 187, 195, 198, 241, 246, 282, 290, 324, 366, 388, 403, 414, 432, 465, 486, 493, 529, 541, 555, 620, 670, 676, 683, 714, 733, 735, 790, 807, 831, 854, 869, 921, 940, 996, 1020, 1031, 1049, 1092, 1107, 1127, 1142, 1181, 1186, 1189, 1202, 1210, 1214, 1242, 1311, 1320, 1355, 1398, 1446, 1480, 1482!, 1485, 1499 ,1501, 1505, 1508, 1517, 1519, 1694, 1698, 1835, 1905, 3076, 3079, 3121, 3160, 3166, 3192, 3194, 3210, 3222, 3232, 3240, 3245, 3665	**1179i**, 27, 37, 63, 84, 89, 91, 110, 124, 137, 146, 156, 157, 172, 188, 195, 196, 220, 246, 263, 283, 323, 362, 390, 400, 405, 416, 431, 468, 486, 539, 545, 615, 665, 676, 684, 701, 732, 741, 757, 792, 807, 835, 867, 883, 920, 928, 992, 996, 1030, 1035, 1055, 1092, 1106, 1118, 1143, 1181, 1185, 1189, 1201, 1209, 1213, 1246, 1256, 1312, 1353, 1398, 1437, 1479, 1481, 1484, 1499, 1500, 1505, 1506, 1516, 1517, 1691, 1696, 1841, 1907, 3078, 3082, 3161, 3164, 3170, 3197, 3211, 3222, 3233, 3242, 3247, 3723	27, 36, 40, 72, 77, 84, 92, 110, 114, 121, 129, 137, 140, 155, 162, 189, 195, 197, 228, 246, 261, 286, 310, 326, 364, 384, 400, 408, 420, 430, 452, 470, 475, 537, 551, 614, 664, 674, 705, 724, 734, 787, 805, 808, 833, 866, 904, 920, 995, 1031, 1039, 1070, 1094, 1106, 1122, 1145, 1180, 1184, 1187, 1201, 1209 ,1213, 1254, 1312, 1338, 1399, 1422, 1480, 1485, 1498, 1500, 1501, 1504, 1516, 1517, 1615, 1692, 1695, 1836, 1906, 3079, 3080, 3162, 3166, 3196, 3210, 3223, 3234, 3242, 3246, 3268, 3801, 3970	34, 41, 74, 98, 105, 113, 127, 136, 143, 155, 165, 186, 196, 197, 240, 246, 278, 285, 322, 356, 388, 402, 415, 427, 464, 467, 499, 537, 548, 611, 662, 672, 704, 723, 733, 786, 805, 810, 837, 867, 906, 920, 995, 1030, 1040, 1065, 1093, 1106, 1123, 1144, 1181, 1186, 1188, 1201, 1209, 1214, 1256, 1312, 1349, 1400, 1413, 1482, 1486, 1499, 1501, 1502, 1505, 1515, 1518, 1692, 1695, 1854, 1912, 3079, 3082, 3162, 3170, 3199, 3211, 3221, 3232, 3240, 3245, 3245
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.40528, 0.22568, 0.20735	0.39329, 0.22671, 0.20866	0.39255, 0.21843, 0.20165	0.53425, 0.23200, 0.21574

Table S25. Vibrational frequencies and rotational constants for the stationary points involved in the H21-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H21-abs) $C_1 - {}^2A$	TS(H21-abs) $C_1 - {}^2A$	MCP(H21-abs) $C_1 - {}^2A$	Rad(H21-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
25, 39, 52, 84, 95, 103, 108, 116, 132, 142, 151, 153, 162, 166, 187, 195, 198, 241, 246, 282, 290, 324, 366, 388, 403, 414, 432, 465, 486, 493, 530, 541, 555, 620, 670, 676, 683, 714, 733, 735, 790, 807, 831, 854, 869, 921, 940, 996, 1020, 1031, 1049, 1092, 1107, 1127, 1142, 1181, 1186, 1189, 1202, 1210, 1214, 1242, 1311, 1320, 1355, 1398, 1447, 1480, 1482, 1485, 1499, 1501, 1505, 1508, 1517, 1519, 1694, 1698, 1835, 1905, 3076, 3079, 3121, 3160, 3166, 3192, 3194, 3210, 3222, 3232, 3240, 3245, 3665	**1179i**, 27, 37, 63, 84, 88, 91, 110, 124, 137, 146, 156, 157, 172, 188, 195, 196, 220, 246, 263, 283, 323, 362, 390, 400, 405, 416, 431, 468, 486, 539, 545, 615, 665, 676, 684, 701, 732, 741, 757, 792, 807, 835, 867, 883, 920, 928, 992, 996, 1030, 1035, 1055, 1092, 1106, 1118, 1143, 1181, 1185, 1189, 1201, 1209, 1213, 1246, 1256, 1312, 1353, 1398, 1437, 1479, 1481, 1484, 1499, 1500, 1505, 1506, 1516, 1517, 1691, 1696, 1841, 1907, 3078, 3082, 3161, 3164, 3170, 3197, 3211, 3222, 3233, 3242, 3247, 3723	27, 36, 40, 72, 77, 84, 91, 110, 114, 120, 129, 137, 140, 155, 162, 189, 195, 197, 229, 246, 261, 286, 310, 326, 364, 384, 400, 408, 420, 430, 452, 470, 475, 537, 551, 614, 664, 674, 705, 724, 734, 787, 805, 808, 833, 866, 904, 920, 995, 1031, 1039, 1070, 1094, 1106, 1122, 1145, 1180, 1184, 1187, 1201, 1209, 1213, 1254, 1312, 1338, 1399, 1422, 1480, 1485, 1498, 1500, 1500, 1504, 1516, 1517, 1615, 1692, 1695, 1836, 1906, 3079, 3080, 3162, 3166, 3196, 3210, 3223, 3234, 3242, 3246, 3268, 3801, 3970	34, 41, 74, 98, 105, 113, 127, 136, 143, 155, 165, 186, 196, 197, 240, 246, 278, 285, 322, 356, 388, 402, 415, 427, 464, 467, 499, 537, 548, 611, 662, 672, 704, 723, 733, 786, 805, 810, 837, 867, 906, 920, 995, 1030, 1040, 1065, 1093, 1106, 1123, 1144, 1181, 1186, 1188, 1201, 1209, 1214, 1256, 1312, 1349, 1400, 1413, 1482, 1486, 1499, 1501, 1502, 1505, 1515, 1518, 1692, 1695, 1854, 1912, 3079, 3082, 3162, 3170, 3199, 3211, 3221, 3232, 3240, 3245, 3245
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.40527, 0.22569, 0.20736	0.39327, 0.22672, 0.20867	0.39256, 0.21841, 0.20164	0.53425, 0.23200, 0.21574

Table S26. Vibrational frequencies and rotational constants for the stationary points involved in the H22-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H22-abs) $C_1 - {}^2A$	TS(H22-abs) $C_1 - {}^2A$	MCP(H22-abs) $C_1 - {}^2A$	Rad(H22-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
29, 43, 63, 79, 87, 91, 100, 116, 126, 141, 149, 157, 170, 189, 190, 200, 211, 230, 239, 280, 282, 322, 367, 389, 404, 413, 431, 436, 465, 488, 528, 541, 553, 623, 669, 676, 686, 713, 733, 736, 789, 808, 830, 847, 869, 925, 937, 1001, 1024, 1033, 1055, 1092, 1107, 1131, 1144, 1184, 1184, 1187, 1205, 1206, 1214, 1242, 1316, 1323, 1355, 1398, 1452, 1474, 1476, 1481, 1500, 1504, 1505, 1507, 1516, 1518, 1690, 1695, 1830, 1903, 3074, 3076, 3119, 3160, 3164, 3181, 3190, 3209, 3221, 3229, 3238, 3245, 3611	**1664i**, 26, 40, 53, 82, 95, 105, 114, 125, 142, 145, 153, 162, 172, 185, 192, 195, 236, 239, 275, 283, 322, 352, 379, 393, 404, 430, 437, 455, 473, 491, 538, 561, 622, 653, 669, 683, 709, 732, 739, 772, 786, 830, 838, 844, 866, 927, 937, 956, 1019, 1037, 1079, 1092, 1126, 1140, 1144, 1181, 1186, 1189, 1209, 1214, 1234, 1270, 1321, 1354, 1386, 1430, 1449, 1473, 1480, 1485, 1500, 1502, 1504, 1505, 1507, 1529, 1670, 1695, 1839, 1905, 3076, 3077, 3120, 3160, 3168, 3191, 3191, 3209, 3224, 3239, 3246, 3687	28, 38, 64, 76, 81, 89, 97, 114, 120, 128, 137, 143, 154, 162, 185, 189, 193, 215, 228, 240, 278, 282, 316, 334, 367, 390, 406, 431, 435, 457, 486, 515, 538, 549, 619, 657, 667, 684, 710, 730, 741, 779, 807, 833, 843, 867, 933, 939, 1014, 1026, 1069, 1090, 1107, 1132, 1144, 1174, 1186, 1190, 1205, 1213, 1225, 1264, 1320, 1355, 1382, 1443, 1468, 1479, 1483, 1486, 1493, 1500, 1505, 1508, 1510, 1609, 1641, 1695, 1837, 1903, 3074, 3078, 3119, 3158, 3167, 3190, 3203, 3208, 3221, 3235, 3246, 3771, 3969	21, 39, 84, 90, 94, 114, 133, 145, 159, 164, 180, 186, 196, 197, 229, 239, 266, 283, 320, 357, 391, 406, 432, 436, 458, 489, 537, 548, 618, 653, 670, 682, 705, 730, 740, 779, 806, 831, 841, 868, 933, 937, 1012, 1026, 1068, 1092, 1108, 1131, 1144, 1173, 1187, 1189, 1210, 1214, 1225, 1262, 1323, 1356, 1377, 1441, 1468, 1480, 1483, 1486, 1491, 1500, 1502, 1505, 1507, 1637, 1694, 1853, 1910, 3077, 3082, 3120, 3160, 3171, 3193, 3196, 3210, 3220, 3233, 3246
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.39197, 0.23585, 0.20155	0.41737, 0.22836, 0.20248	0.39852, 0.23325, 0.20176	0.51040, 0.24097, 0.23208

Table S27. Vibrational frequencies and rotational constants for the stationary points involved in the H23-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H23-abs) $C_1 - {}^2A$	TS(H23-abs) $C_1 - {}^2A$	MCP(H23-abs) $C_1 - {}^2A$	Rad(H23-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
29, 43, 63, 79, 87, 91, 100, 116, 126, 142, 149, 157, 170, 189, 190, 200, 211, 230, 239, 280, 282, 322, 367, 389, 404, 413, 431, 436, 465, 488, 528, 541, 553, 623, 669, 676, 686, 713, 733, 736, 789, 808, 830, 847, 869, 925, 937, 1001, 1024, 1033, 1055, 1092, 1107, 1131, 1144, 1184, 1184, 1187, 1205, 1206, 1214, 1242, 1316, 1323, 1355, 1398, 1452, 1474, 1476, 1481, 1500, 1504, 1505, 1507, 1516, 1518, 1690, 1695, 1830, 1903, 3074, 3076, 3119, 3160, 3164, 3181, 3190, 3209, 3221, 3229, 3238, 3245	**1664i**, 26, 40, 53, 81, 95, 105, 113, 125, 142, 145, 153, 162, 171, 185, 192, 195, 236, 239, 275, 283, 322, 352, 379, 393, 404, 430, 437, 455, 473, 491, 538, 561, 622, 653, 669, 683, 709, 732, 739, 772, 786, 830, 838, 844, 866, 927, 937, 956, 1019, 1037, 1079, 1092, 1126, 1140, 1144, 1181, 1186, 1189, 1209, 1214, 1234, 1270, 1321, 1354, 1386, 1430, 1449, 1473, 1480, 1485, 1500, 1502, 1504, 1505, 1507, 1529, 1670, 1695, 1839, 1905, 3076, 3078, 3120, 3160, 3168, 3191, 3191, 3209, 3224, 3239, 3246, 3687	28, 38, 65, 76, 81, 89, 97, 114, 120, 129, 137, 143, 154, 162, 185, 189, 193, 215, 228, 240, 278, 282, 316, 334, 367, 390, 406, 431, 435, 457, 486, 515, 538, 549, 619, 657, 667, 684, 710, 730, 741, 779, 807, 833, 843, 867, 933, 939, 1014, 1026, 1069, 1090, 1107, 1132, 1144, 1174, 1186, 1190, 1205, 1214, 1225, 1264, 1320, 1355, 1382, 1443, 1468, 1479, 1483, 1486, 1493, 1500, 1505, 1508, 1510, 1609, 1641, 1695, 1837, 1903, 3074, 3078, 3119, 3158, 3167, 3190, 3203, 3208, 3221, 3235, 3246, 3771, 3968	21, 39, 84, 90, 94, 114, 133, 145, 159, 164, 180, 186, 196, 197, 229, 239, 266, 283, 320, 357, 391, 406, 432, 436, 458, 489, 537, 548, 618, 653, 670, 682, 705, 730, 740, 779, 806, 831, 841, 868, 933, 937, 1012, 1026, 1068, 1092, 1108, 1131, 1144, 1173, 1187, 1189, 1210, 1214, 1225, 1262, 1323, 1356, 1377, 1441, 1468, 1480, 1483, 1486, 1491, 1500, 1502, 1505, 1507, 1637, 1694, 1853, 1910, 3077, 3082, 3120, 3160, 3171, 3193, 3196, 3210, 3220, 3233, 3246
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.39194, 0.23586, 0.20156	0.41735, 0.22836, 0.20249	0.39850, 0.23326, 0.20178	0.51040, 0.24096, 0.23208

Table S28. Vibrational frequencies and rotational constants for the stationary points involved in the H24-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H24-abs) $C_1 - {}^2A$	TS(H24-abs) $C_1 - {}^2A$	MCP(H24-abs) $C_1 - {}^2A$	Rad(H24-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
14, 30, 39, 78, 85, 92, 108, 112, 133, 138, 140, 153, 167, 172, 187, 194, 202, 229, 239, 266, 289, 319, 356, 390, 399, 408, 420, 438, 464, 478, 499, 539, 549, 620, 673, 675, 680, 704, 731, 732, 790, 804, 824, 842, 866, 918, 936, 993, 1026, 1028, 1050, 1080, 1105, 1126, 1137, 1181, 1185, 1190, 1201, 1210, 1216, 1242, 1311, 1328, 1356, 1399, 1448, 1467, 1482, 1486, 1497, 1498, 1503, 1505, 1515, 1515, 1690, 1693, 1851, 1907, 3081, 3087, 3122, 3166, 3181, 3195, 3200, 3212, 3225, 3235, 3243, 3248, 3679	**1407i**, 17, 28, 56, 66, 82, 93, 97, 111, 126, 141, 154, 160, 163, 182, 187, 194, 201, 230, 238, 263, 282, 317, 331, 376, 393, 403, 426, 433, 474, 493, 540, 575, 619, 652, 669, 684, 694, 730, 750, 772, 786, 832, 857, 868, 870, 933, 941, 1002, 1032, 1049, 1080, 1092, 1123, 1131, 1142, 1185, 1189, 1190, 1209, 1213, 1233, 1276, 1292, 1325, 1355, 1384, 1446, 1469, 1471, 1478, 1483, 1498, 1499, 1504, 1506, 1509, 1673, 1687, 1853, 1910, 3079, 3083, 3122, 3163, 3171, 3194, 3196, 3210, 3229, 3241, 3242, 3806	17, 21, 43, 52, 82, 89, 99, 101, 110, 122, 129, 143, 148, 153, 159, 163, 176, 188, 195, 201, 231, 239, 265, 284, 319, 358, 391, 402, 410, 432, 475, 487, 537, 547, 618, 658, 669, 681, 705, 727, 746, 785, 829, 837, 854, 867, 906, 929, 1002, 1028, 1044, 1094, 1106, 1126, 1144, 1182, 1186, 1190, 1210, 1214, 1227, 1266, 1325, 1354, 1383, 1444, 1450, 1467, 1480, 1484, 1488, 1499, 1501, 1502, 1506, 1605, 1646, 1688, 1851, 1908, 3078, 3082, 3120, 3161, 3170, 3192, 3196, 3210, 3228, 3236, 3239, 3864, 3991	13, 39, 78, 86, 95, 109, 123, 140, 154, 158, 166, 187, 194, 200, 229, 239, 264, 283, 319, 356, 390, 402, 409, 431, 472, 489, 537, 546, 618, 655, 669, 681, 704, 726, 744, 785, 829, 834, 840, 868, 907, 929, 989, 1028, 1042, 1093, 1103, 1127, 1143, 1183, 1185, 1189, 1209, 1213, 1226, 1265, 1324, 1355, 1383, 1443, 1449, 1468, 1479, 1483, 1487, 1497, 1500, 1504, 1506, 1647, 1689, 1852, 1909, 3077, 3082, 3120, 3161, 3170, 3192, 3196, 3210, 3225, 3237, 3239
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.44329, 0.23031, 0.21851	0.44432, 0.18440, 0.17977	0.45612, 0.17233, 0.16885	0.51114, 0.24346, 0.23226

Table S29. Vibrational frequencies and rotational constants for the stationary points involved in the H25-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H25-abs) $C_1 - {}^2A$	TS(H25-abs) $C_1 - {}^2A$	MCP(H25-abs) $C_1 - {}^2A$	Rad(H25-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
14, 30, 39, 77, 85, 92, 108, 112, 133, 138, 139, 153, 167, 172, 187, 194, 202, 229, 239, 266, 289, 319, 356, 390, 399, 408, 420, 438, 464, 478, 499, 539, 549, 620, 673, 675, 680, 704, 731, 732, 790, 804, 824, 842, 866, 918, 936, 993, 1026, 1028, 1050, 1080, 1105, 1126, 1137, 1181, 1185, 1190, 1201, 1210, 1216, 1242, 1311, 1328, 1356, 1399, 1448, 1467, 1482, 1486, 1497, 1498, 1503, 1504, 1515, 1515, 1690, 1693, 1851, 1907, 3081, 3087, 3122, 3166, 3181, 3195, 3200, 3212, 3225, 3235, 3243, 3248, 3679	**1400i**, 18, 28, 57, 63, 83, 90, 93, 111, 131, 139, 148, 150, 159, 164, 189, 195, 201, 227, 239, 263, 285, 317, 331, 376, 393, 402, 427, 432, 473, 494, 545, 571, 619, 651, 668, 680, 706, 730, 740 ,777, 787, 831, 856, 865, 868, 931, 940, 999, 1033, 1055, 1077, 1092, 1123, 1131, 1143, 1186, 1189, 1189, 1208, 1213, 1232, 1274, 1293, 1325, 1355, 1384, 1445, 1466, 1472, 1481, 1484, 1498, 1499, 1502, 1506, 1508, 1672, 1687, 1853, 1910, 3078, 3082, 3121, 3162, 3170, 3193, 3195, 3210, 3229, 3237, 3243, 3807	16, 23, 42, 52, 80, 88, 90, 92, 109, 119, 123, 135, 144, 148, 158, 162 ,186, 188, 195, 200, 233, 239, 265, 285, 319, 358, 391, 401, 410, 432, 476, 488, 541, 545, 619, 657, 667, 682, 704, 727, 746, 785, 829, 838, 854, 866, 905, 930, 1003, 1028, 1043, 1093, 1107, 1126, 1144, 1183, 1186, 1190, 1209, 1214, 1227, 1266, 1325, 1354, 1383, 1442, 1451, 1468, 1480, 1484, 1488, 1498, 1499, 1502, 1505, 1606, 1646, 1686, 1851, 1908, 3078, 3082, 3120, 3162, 3170, 3193, 3196, 3210, 3232, 3233, 3244, 3865, 3991	18, 38, 83, 87, 96, 112, 132, 143, 157, 158, 164, 187, 195, 200, 229, 239, 263, 282, 319, 357, 390, 401, 409, 431, 473, 488, 539, 543, 618, 655, 667, 682, 704, 726, 744, 785, 829, 837, 838, 866, 907, 929, 990, 1027, 1042, 1093, 1103, 1126, 1144, 1183, 1185, 1189, 1209, 1214, 1226, 1266, 1324, 1353, 1383, 1441, 1449, 1468, 1481, 1483, 1488, 1499, 1501, 1504, 1507, 1647, 1688, 1852, 1909, 3077, 3082, 3120, 3160, 3170, 3192, 3197, 3210, 3225, 3235, 3240
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.44328, 0.23032, 0.21852	0.44612, 0.18779, 0.17641	0.45657, 0.17237, 0.16845	0.51085, 0.24319, 0.23298

Table S30. Vibrational frequencies and rotational constants for the stationary points involved in the H26-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H26-abs) $C_1 - {}^2A$	TS(H26-abs) $C_1 - {}^2A$	MCP(H26-abs) $C_1 - {}^2A$	Rad(H26-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
25, 39, 52, 84, 95, 103, 108, 116, 132, 142, 151, 153, 162, 166, 187, 195, 198, 241, 246, 282, 290, 324, 366, 388, 403, 414, 432, 465, 486, 493, 529, 541, 555, 620, 670, 676, 683, 714, 733, 735, 790, 807, 831, 854, 869, 921, 940, 996, 1020, 1031, 1049, 1092, 1107, 1127, 1142, 1181, 1186, 1189, 1202, 1210, 1214, 1242, 1311, 1320, 1355, 1398, 1447, 1480, 1482, 1485, 1499, 1501, 1505, 1508, 1517, 1519, 1694, 1698, 1835, 1905, 3076, 3079, 3121, 3161, 3166, 3192, 3194, 3210, 3222, 3232, 3240, 3245, 3665	**1192i**, 28, 38, 56, 80, 89, 96, 109, 120, 137, 146, 153, 169, 190, 196, 201, 230, 238, 261, 278, 289, 320, 334, 358, 387, 403, 414, 434, 468, 492, 538, 545, 619, 670, 679, 685, 713, 733, 736, 772, 794, 808, 827, 849, 861, 889, 922, 936, 997, 1021, 1033, 1048, 1106, 1110, 1129, 1156, 1181, 1185, 1189, 1201, 1208, 1215, 1241, 1310, 1320, 1354, 1359, 1397, 1447, 1468, 1472, 1482, 1486, 1502, 1509, 1517, 1517, 1693, 1696, 1844, 1906, 3073, 3112, 3113, 3158, 3184, 3208, 3209, 3222, 3233, 3241, 3247, 3738	38, 39, 64, 82, 95, 108, 117, 126, 133, 143, 146, 162, 168, 187, 196, 203, 232, 239, 248, 264, 292, 298, 318, 328, 362, 391, 407, 414, 431, 468, 491, 500, 541, 550, 621, 669, 676, 677, 679, 704, 733, 734, 792, 807, 819, 846, 863, 920, 943, 996, 1024, 1031, 1049, 1105, 1107, 1129, 1181, 1188, 1189, 1202, 1210, 1238, 1243, 1312, 1332, 1357, 1397, 1449, 1472, 1484, 1486, 1497, 1503, 1517, 1518, 1615, 1693, 1697, 1843, 1906, 3085, 3126, 3173, 3178, 3200, 3203, 3222, 3233, 3242, 3246, 3334, 3818, 3940	36, 42, 81, 98, 108, 121, 130, 149, 158, 167, 187, 196, 197, 224, 231, 242, 262, 287, 320, 357, 389, 404, 415, 429, 467, 493, 537, 545, 601, 617, 672, 678, 684, 714, 732, 736, 793, 807, 823, 848, 861, 922, 937, 996, 1021, 1030, 1048, 1106, 1109, 1129, 1180, 1183, 1190, 1201, 1212, 1237, 1242, 1309, 1318, 1351, 1395, 1443, 1468, 1473, 1485, 1502, 1506, 1516, 1517, 1692, 1697, 1852, 1909, 3080, 3114, 3169, 3184, 3186, 3194, 3220, 3232, 3240, 3246, 3343
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.40528, 0.22569, 0.20735	0.41609, 0.23149, 0.20460	0.40287, 0.23133, 0.20282	0.52229, 0.23760, 0.22659

Table S31. Vibrational frequencies and rotational constants for the stationary points involved in the H27-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H27-abs) $C_1 - {}^2A$	TS(H27-abs) $C_1 - {}^2A$	MCP(H27-abs) $C_1 - {}^2A$	Rad(H27-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
18, 30, 44, 58, 72, 86, 93, 108, 117, 129, 139, 150, 163, 183, 187, 196, 201, 230, 239, 265, 283, 316, 348, 356, 374, 393, 407, 415, 431, 467, 497, 539, 549, 619, 669, 678, 679, 706, 732, 733, 793, 807, 835, 846, 862, 920, 936, 995, 1026, 1030, 1051, 1089, 1106, 1127, 1141, 1181, 1186, 1192, 1201, 1208, 1213, 1243, 1312, 1326, 1355, 1398, 1447, 1468, 1482, 1487, 1495, 1498, 1498, 1503, 1517, 1518, 1692, 1698, 1852, 1908, 3079, 3089, 3123, 3163, 3180, 3196, 3207, 3214, 3223, 3233, 3241, 3246, 3679	**1147i**, 20, 31, 42, 83, 84, 96, 100, 124, 134, 139, 152, 158, 184, 191, 195, 228, 237, 263, 266, 290, 319, 337, 357, 390, 402, 413, 429, 466, 491, 539, 548, 619, 666, 677, 679, 707, 732, 733, 785, 792, 807, 819, 844, 866, 921, 923, 937, 996, 1025, 1031, 1050, 1106, 1111, 1127, 1150, 1181, 1184, 1187, 1201, 1212, 1220, 1242, 1312, 1326, 1341, 1355, 1398, 1447, 1452, 1468, 1481, 1493, 1500, 1506, 1517, 1518, 1693, 1698, 1852, 1909, 3079, 3110, 3121, 3164, 3194, 3209, 3213, 3223, 3232, 3240, 3246, 3730	25, 30, 45, 60, 83, 94, 112, 120, 131, 139, 152, 160, 169, 186, 193, 200, 220, 229, 241, 253, 261, 291, 298, 322, 358, 372, 393, 407, 415, 431, 467, 497, 537, 545, 608, 617, 673, 678, 681, 712, 731, 734, 793, 808, 821, 846, 858, 922, 936, 997, 1021, 1032, 1049, 1091, 1106, 1127, 1180, 1182, 1192, 1201, 1211, 1233, 1242, 1309, 1318, 1348, 1396, 1442, 1469, 1470, 1486, 1497, 1499, 1516, 1517, 1632, 1692, 1696, 1852, 1909, 3087, 3113, 3182, 3184, 3186, 3200, 3223, 3233, 3241, 3247, 3347, 3845, 3950	36, 42, 81, 98, 108, 121, 130, 149, 158, 167, 187, 196, 198, 224, 231, 242, 262, 287, 320, 357, 389, 404, 415, 429, 467, 493, 537, 545, 601, 617, 672, 678, 684, 714, 732, 736, 793, 807, 823, 848, 861, 922, 937, 996, 1021, 1030, 1048, 1106, 1109, 1129, 1180, 1183, 1190, 1201, 1212, 1237, 1242, 1309, 1318, 1351, 1395, 1443, 1468, 1473, 1485, 1502, 1506, 1516, 1517, 1692, 1697, 1852, 1909, 3080, 3114, 3169, 3184, 3186, 3194, 3220, 3232, 3240, 3246, 3343
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.40835, 0.23048, 0.21111	0.39934, 0.22630, 0.19859	0.40932, 0.22896, 0.20790	0.52232, 0.23758, 0.22656

Table S32. Vibrational frequencies and rotational constants for the stationary points involved in the H28-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H28-abs) $C_1 - {}^2A$	TS(H28-abs) $C_1 - {}^2A$	MCP(H28-abs) $C_1 - {}^2A$	Rad(H28-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
14, 30, 39, 78, 85, 92, 108, 112, 133, 138, 139, 153, 167, 172, 187, 194, 202, 229, 239, 266, 289, 319, 356, 390, 399, 408, 420, 438, 464, 477, 499, 539, 549, 620, 673, 675, 680, 704, 731, 732, 790, 804, 824, 842, 866, 918, 936, 993, 1026, 1028, 1050, 1080, 1105, 1126, 1136, 1181, 1185, 1190, 1201, 1210, 1216, 1242, 1311, 1328, 1356, 1399, 1448, 1467, 1482, 1486, 1497, 1498, 1503, 1504, 1515, 1515, 1690, 1693, 1851, 1907, 3081, 3087, 3122, 3166, 3181, 3195, 3200, 3212, 3225, 3235, 3243, 3248, 3680	**1158i**, 18, 33, 57, 72, 88, 100, 103, 111, 127, 144, 161, 163, 178, 191, 198, 226, 236, 249, 262, 279, 313, 323, 356, 382, 403, 417, 420, 467, 491, 539, 547, 619, 662, 677, 680, 708, 730, 732, 737, 793, 809, 840, 844, 880, 918, 928, 936, 997, 1025, 1032, 1050, 1104, 1107, 1128, 1153, 1170, 1181, 1186, 1202, 1211, 1242, 1296, 1312, 1315, 1326, 1355, 1396, 1447, 1466, 1478, 1482, 1499, 1505, 1515, 1516, 1574, 1689, 1695, 1851, 1908, 3080, 3103, 3119, 3164, 3192, 3199, 3215, 3222, 3235, 3244, 3251, 3772	37, 42, 60, 74, 84, 92, 105, 114, 120, 135, 140, 146, 159, 172, 195, 203, 207, 229, 240, 259, 269, 284, 325, 338, 365, 390, 406, 413, 435, 465, 493, 521, 536, 547, 621, 651, 676, 679, 685, 713, 732, 737, 791, 807, 817, 847, 862, 917, 937, 994, 1020, 1031, 1052, 1105, 1108, 1131, 1182, 1188, 1190, 1204, 1210, 1228, 1241, 1312, 1319, 1350, 1397, 1446, 1470, 1476, 1484, 1502, 1504, 1515, 1518, 1639, 1691, 1694, 1839, 1903, 3081, 3114, 3171, 3181, 3184, 3195, 3223, 3233, 3242, 3250, 3336, 3828, 3937	36, 42, 81, 98, 108, 120, 130, 149, 158, 166, 187, 196, 197, 224, 231, 242, 262, 287, 320, 357, 389, 404, 415, 429, 467, 492, 537, 545, 600, 617, 672, 678, 684, 714, 732, 736, 792, 807, 823, 848, 861, 922, 937, 996, 1021, 1030, 1048, 1106, 1109, 1129, 1180, 1183, 1190, 1201, 1212, 1237, 1242, 1309, 1318, 1351, 1395, 1443, 1467, 1473, 1485, 1502, 1506, 1516, 1517, 1692, 1697, 1851, 1909, 3080, 3114, 3169, 3184, 3186, 3194, 3220, 3232, 3240, 3246, 3343
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.44324, 0.23031, 0.21853	0.42052, 0.23272, 0.20672	0.41815, 0.23128, 0.20891	0.52231, 0.23757, 0.22655

Table S33. Vibrational frequencies and rotational constants for the stationary points involved in the H29-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H29-abs) $C_1 - {}^2A$	TS(H29-abs) $C_1 - {}^2A$	MCP(H29-abs) $C_1 - {}^2A$	Rad(H29-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
14, 30, 39, 78, 85, 92, 108, 112, 133, 138, 139, 153, 167, 172, 187, 194, 202, 229, 239, 266, 289, 319, 356, 390, 399, 408, 420, 438, 464, 478, 499, 539, 549, 620, 673, 675, 680, 704, 731, 732, 790, 804, 824, 842, 866, 918, 936, 993, 1026, 1028, 1050, 1080, 1105, 1126, 1137, 1181, 1185, 1190, 1201, 1210, 1216, 1242, 1311, 1328, 1356, 1399, 1448, 1467, 1482, 1486, 1497, 1498, 1503, 1504, 1515, 1515, 1690, 1693, 1851, 1907, 3081, 3087, 3122, 3166, 3181, 3195, 3200, 3212, 3225, 3235, 3243, 3248, 3680	**1158i**, 18, 33, 57, 72, 89, 100, 103, 111, 127, 144, 161, 163, 178, 191, 198, 226, 236, 249, 262, 279, 314, 323, 356, 382, 403, 417, 420, 467, 491, 539, 547, 619, 662, 677, 680, 708, 730, 733, 737, 793, 809, 840, 844, 880, 918, 928, 936, 998, 1025, 1032, 1050, 1104, 1107, 1128, 1153, 1170, 1181, 1187, 1202, 1211, 1242, 1296, 1312, 1315, 1326, 1355, 1396, 1447, 1466, 1478, 1483, 1499, 1505, 1515, 1516, 1574, 1689, 1695, 1851, 1908, 3080, 3103, 3119, 3164, 3191, 3199, 3215, 3222, 3235, 3244, 3251, 3772	38, 42, 60, 74, 84, 92, 105, 114, 120, 135, 140, 146, 159, 172, 195, 203, 207, 230, 240, 259, 269, 285, 325, 340, 365, 390, 406, 413, 435, 465, 493, 522, 536, 547, 621, 651, 676, 679, 685, 713, 732, 737, 791, 807, 817, 847, 862, 917, 937, 994, 1020, 1031, 1052, 1105, 1108, 1131, 1182, 1188, 1189, 1204, 1210, 1228, 1241, 1312, 1319, 1350, 1397, 1446, 1470, 1476, 1484, 1502, 1504, 1515, 1518, 1639, 1691, 1694, 1839, 1903, 3081, 3114, 3171, 3181, 3185, 3195, 3223, 3233, 3242, 3250, 3336, 3828, 3937	36, 42, 81, 98 ,108, 120, 130, 149, 158, 166, 187, 196, 197, 224, 231, 242, 262, 287, 320, 357, 389, 404, 415, 429, 467, 492, 537, 545, 600, 617, 672, 678, 684, 714, 732, 736, 792, 807, 823, 848, 861, 922, 937, 996, 1021, 1030, 1048, 1106, 1109, 1129, 1180, 1183, 1190, 1201, 1212, 1237, 1242, 1309, 1318, 1351, 1395, 1443, 1467, 1473, 1485, 1502, 1506, 1516, 1517, 1692, 1697, 1851, 1909, 3080, 3114, 3169, 3184, 3186, 3194, 3220, 3232, 3240, 3246, 3343
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.44326, 0.23032, 0.21853	0.42059, 0.23269, 0.20669	0.41811, 0.23131, 0.20894	0.52232, 0.23757, 0.22655

Table S34. Vibrational frequencies and rotational constants for the stationary points involved in the H30-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H30-abs) $C_1 - {}^2A$	TS(H30-abs) $C_1 - {}^2A$	MCP(H30-abs) $C_1 - {}^2A$	Rad(H30-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
18, 32, 42 ,57, 84, 89 ,108, 121, 129, 141, 152, 153, 161, 171, 186, 197, 200, 232, 238, 269, 283, 316, 336, 356, 379, 394, 409, 416, 431, 467, 495, 539, 549, 620, 668, 677 ,678, 704, 732, 733, 793, 807, 835, 845, 860, 920, 937, 995, 1026, 1030, 1051, 1088, 1106, 1126, 1139, 1181, 1186, 1189, 1201, 1208, 1212, 1243, 1312, 1328, 1356, 1398, 1447, 1469, 1483, 1487, 1492, 1497, 1500, 1502, 1517, 1518, 1692, 1698, 1853, 1909, 3084, 3088, 3124, 3172, 3174, 3197, 3201, 3219, 3222, 3232, 3241, 3246, 3682	**1163i**, 20, 38, 42, 77, 83, 110, 117, 128, 145, 151, 159, 159, 187, 192, 198, 227, 238, 262, 276, 293, 319, 341, 357, 391, 402, 414, 431, 468, 493, 539, 547, 619, 668, 677, 678, 707, 732, 733, 792, 795, 808, 821, 843, 860, 921, 922, 937, 997, 1025, 1031, 1050, 1104, 1106, 1127, 1152, 1181, 1187, 1190, 1201, 1210, 1228, 1242, 1311, 1325, 1352, 1358, 1397, 1446, 1458, 1469, 1483, 1498, 1500, 1502, 1516, 1517, 1692, 1697, 1851, 1908, 3082, 3101, 3121, 3172, 3193, 3198, 3214, 3222, 3232, 3241, 3246, 3730	17, 34, 38, 56, 83, 95, 115, 119, 126, 143, 154, 159, 168, 184, 188, 196, 205, 228, 240, 258, 262, 274, 290, 322, 338, 358, 391, 406, 415, 431, 466, 496, 538, 545, 617, 634, 674, 678, 681, 712, 732, 734, 792, 807, 820, 846, 859, 921, 936, 997, 1022, 1031, 1049, 1104, 1107, 1127, 1181, 1182, 1190, 1201, 1212, 1223, 1242, 1310, 1319, 1351, 1397, 1442, 1466, 1471, 1485, 1504, 1505, 1517, 1518, 1630, 1693, 1697, 1852, 1909, 3082, 3113, 3172, 3185, 3186, 3197, 3222, 3232, 3241, 3246, 3346, 3849, 3959	36, 42, 81, 98, 108, 121, 130, 149, 158, 167, 187, 196, 198, 224, 231, 242, 262, 287, 320, 357, 389, 404, 415, 429, 467, 492, 537, 545, 601, 617, 672, 678, 685, 714, 732, 736, 793, 807, 823, 848, 861, 922, 937, 996, 1021, 1030, 1048, 1106, 1109, 1129, 1180, 1183, 1190, 1201, 1212, 1237, 1242, 1309, 1318, 1351, 1395, 1443, 1468, 1473, 1485, 1502, 1506, 1516, 1517, 1692, 1697, 1852, 1909, 3080, 3114, 3169, 3184, 3186, 3194, 3220, 3232, 3240, 3246, 3343
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.40853, 0.22736, 0.21161	0.41960, 0.21385, 0.19725	0.41081, 0.22172, 0.20672	0.52231, 0.23759, 0.22657

Table S35. Vibrational frequencies and rotational constants for the stationary points involved in the H31-abstraction pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H31-abs) $C_1 - {}^2A$	TS(H31-abs) $C_1 - {}^2A$	MCP(H31-abs) $C_1 - {}^2A$	Rad(H31-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
30 ,36, 48, 77, 82, 93, 113, 120, 127, 137, 144, 156, 160, 163, 187, 195, 197, 220, 231, 240, 262, 281, 319, 356, 386, 402, 414, 428, 466, 482, 537, 540, 545, 618, 659, 677, 684, 713, 732, 736, 792, 806, 835, 853, 871, 920, 940, 995, 1023, 1030, 1049, 1091, 1106, 1127, 1141, 1180, 1190, 1194, 1201, 1210, 1218, 1242, 1308, 1316, 1339, 1396, 1445, 1472, 1483, 1487, 1501, 1505, 1509, 1517, 1518, 1520, 1693, 1698, 1852, 1910, 3080, 3083, 3122, 3168, 3172, 3195, 3198, 3210, 3221, 3232, 3241, 3246, 3802	**950i**, 33, 37, 49, 80, 100, 109, 125, 136, 139, 154, 160, 175, 185, 195, 198, 234, 241, 267, 282, 295, 302, 320, 357, 390, 404, 414, 428, 467, 493, 538, 545, 618, 669, 677, 680, 712, 732, 734, 791, 803, 807, 812, 847, 859, 920, 941, 953, 996, 1023, 1030, 1049, 1105, 1107, 1148, 1180, 1190, 1197, 1202, 1211, 1217, 1242, 1310, 1319, 1349, 1396, 1410, 1444, 1454, 1480, 1484, 1498, 1502, 1506, 1517, 1518, 1693, 1697, 1852, 1910, 3082, 3112, 3114, 3171, 3186, 3195, 3217, 3220, 3231, 3239, 3244, 3753	38, 39, 65, 82, 95, 108, 117, 126, 135, 143, 146, 162, 168, 187, 196, 203, 232, 239, 248, 265, 292, 298, 318, 329, 362, 391, 407, 414, 431, 468, 490, 500, 541, 550, 621, 668, 676, 677, 679, 704, 733, 734, 792, 807, 819, 846, 863, 920, 943, 996, 1024, 1031, 1049, 1105, 1107, 1129, 1181, 1188, 1189, 1202, 1210, 1238, 1243, 1312, 1332, 1357, 1397, 1449, 1472, 1484, 1486, 1497, 1503, 1517, 1518, 1615, 1693, 1697, 1843, 1906, 3085, 3126, 3173, 3178, 3200, 3203, 3222, 3233, 3242, 3246, 3334, 3818, 3939	36, 42, 81, 98 ,108, 121, 130, 149, 158, 167, 187, 196, 198, 224, 231, 242, 262, 287, 320, 357, 389, 404, 415, 429, 467, 493, 537, 545, 601, 617, 672, 678, 684, 714, 732, 736, 793, 807, 823, 848, 861, 922, 937, 996, 1021, 1030, 1048, 1106, 1109, 1129, 1180, 1183, 1190, 1201, 1212, 1237, 1242, 1309, 1318, 1351, 1395, 1443, 1468, 1473, 1485, 1502, 1506, 1516, 1517, 1692, 1697, 1852, 1909, 3080, 3114, 3169, 3184, 3186, 3194, 3221, 3232, 3240, 3246, 3343
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.45604, 0.21412 ,0.20015	0.44182, 0.22019, 0.19917	0.40288, 0.23134, 0.20280	0.52229, 0.23760, 0.22659

Table S36. Vibrational frequencies and rotational constants for the stationary points involved in the C1-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(C1-add) $C_1 - {}^2A$	TS(C1-add) $C_1 - {}^2A$	Adduct(C1-add) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
16, 25, 26, 37, 84, 90, 95, 112, 127, 136, 145, 149, 157, 165, 169, 187, 196, 202, 228, 239, 264, 283, 320, 356, 371, 390, 405, 416, 432, 470, 489, 539, 548, 619, 669, 677, 683, 708, 732, 735, 796, 809, 831, 845, 868, 921, 936, 994, 1023, 1024, 1046, 1092, 1106, 1127, 1143, 1182, 1186, 1189, 1200, 1209, 1214, 1240, 1310, 1324, 1356, 1396, 1446, 1469, 1481, 1485, 1499, 1500, 1504, 1506, 1513, 1513, 1686, 1695, 1852, 1908, 3077, 3082, 3119, 3161, 3170, 3192, 3196, 3210, 3230, 3237, 3244, 3251, 3772	**558i**, 14, 35, 63, 84, 86, 95, 108, 114, 139, 149, 160, 164, 170, 186, 188, 196, 211, 230, 241, 265, 283, 321, 355, 387, 399, 411, 431, 449, 489, 539, 544, 617, 644, 670, 681, 705, 727, 743, 786, 794, 831, 839, 846, 869, 917, 936, 978, 997, 1028, 1040, 1092, 1099, 1127, 1143, 1171, 1186, 1189, 1197, 1208, 1213, 1231, 1306, 1324, 1356, 1384, 1444, 1469, 1480, 1483, 1486, 1498, 1500, 1504, 1506, 1506, 1637, 1668, 1851, 1907, 3078, 3082, 3121, 3162, 3171, 3193, 3196, 3209, 3235, 3243, 3247, 3257, 3796	23, 34, 59, 83, 93, 96, 110, 132, 144, 149, 157, 187, 190, 193, 201, 210, 239, 260, 284, 311, 332, 340, 371, 383, 401, 427, 434, 462, 490, 525, 538, 608, 619, 663, 670, 699, 710, 736, 758, 789, 826, 835, 865, 868, 908, 930, 998, 1017, 1063, 1092, 1093, 1125, 1143, 1150, 1178, 1186, 1191, 1210, 1214, 1219, 1231, 1292, 1323, 1345, 1353, 1385, 1414, 1440, 1461, 1472, 1480, 1485, 1498, 1499, 1506, 1510, 1565, 1691, 1830, 1890, 3017, 3078, 3083, 3120, 3161, 3172, 3193, 3195, 3211, 3223, 3227, 3240, 3859
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.50575, 0.18506, 0.17921	0.44276, 0.23058, 0.21869	0.48621, 0.19392, 0.18580

Table S37. Vibrational frequencies and rotational constants for the stationary points involved in the C2-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(C2-add) $C_1 - {}^2A$	TS(C2-add) $C_1 - {}^2A$	Adduct(C2-add) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
14, 30, 39, 79, 86, 92, 108, 112, 134, 139, 140, 154, 168, 172, 187, 194, 202, 229, 239, 266, 289, 319, 356, 390, 399, 408, 420, 438, 464, 478, 499, 539, 549, 620, 673, 675, 680, 704, 731, 732, 790, 804, 824, 842, 866, 918, 936, 994, 1026, 1028, 1050, 1080, 1105, 1126, 1137, 1181, 1185, 1191, 1201, 1210, 1216, 1242, 1311, 1328, 1356, 1399, 1448, 1468, 1482, 1486, 1497, 1498, 1503, 1505, 1515, 1515, 1690, 1693, 1851, 1907, 3081, 3087, 3122, 3166, 3181, 3195, 3201, 3212, 3225, 3235, 3243, 3248, 3679	**604i**, 24, 61, 72, 88, 110, 118, 130, 135, 145, 157, 168, 169, 184, 191, 196, 207, 234, 240, 269, 287, 317, 355, 385, 402, 404, 417, 436, 465, 488, 537, 547, 618, 645, 668, 679, 699, 726, 741, 787, 807, 827, 839, 865, 899, 933, 940, 989, 1012, 1027, 1044, 1078, 1095, 1124, 1134, 1181, 1187, 1189, 1192, 1210, 1217, 1230, 1304, 1329, 1357, 1392, 1448, 1468, 1482, 1482, 1486, 1497, 1502, 1504, 1505, 1506, 1639, 1662, 1851, 1906, 3083, 3086, 3129, 3169, 3177, 3201, 3208, 3209, 3228, 3240, 3247, 3257, 3740	29, 62, 75, 91, 107, 115, 137, 142, 153, 165, 170, 182, 185, 194, 198, 206, 237, 262, 288, 309, 322, 358, 395, 404, 417, 426, 437, 477, 489, 531, 537, 595, 621, 668, 671, 687, 703, 743, 763, 797, 823, 836, 864, 874, 918, 939, 1003, 1029, 1033, 1064, 1079, 1116, 1128, 1134, 1184, 1188, 1192, 1211, 1218, 1223, 1250, 1286, 1325, 1351, 1372, 1408, 1423, 1443, 1457, 1469, 1483, 1486, 1497, 1504, 1505, 1506, 1577, 1628, 1841, 1896, 3062, 3084, 3086, 3131, 3171, 3175, 3203, 3203, 3209, 3219, 3234, 3249, 3812
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.44331, 0.23031, 0.21847	0.44117, 0.23535, 0.22069	0.43099, 0.24215, 0.22736

Table S38. Vibrational frequencies and rotational constants for the stationary points involved in the C3-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(C3-add) $C_1 - {}^2A$	TS(C3-add) $C_1 - {}^2A$	Adduct(C3-add) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
21, 33, 36, 52, 60, 83, 88, 93, 110, 121, 137, 145, 154, 166, 176, 192, 196, 207, 229, 243, 264, 284, 311, 322, 356, 390, 404, 419, 432, 470, 490, 539, 549, 621, 669, 678, 682, 707, 732, 734, 794, 809, 832, 844, 867, 921, 937, 997, 1026, 1031, 1049, 1094, 1107, 1130, 1144, 1179, 1187, 1191, 1201, 1209, 1214, 1243, 1310, 1324, 1357, 1393, 1452, 1469, 1482, 1485, 1498, 1500, 1505, 1508, 1514, 1517, 1687, 1695, 1854, 1913, 3077, 3083, 3121, 3160, 3171, 3194, 3196, 3211, 3221, 3231, 3240, 3244, 3767	**541i**, 26, 37, 70, 86, 96, 105, 114, 135, 142, 145, 162, 167, 178, 184, 191, 198, 201, 229, 243, 267, 286, 326, 355, 389, 393, 408, 433, 454, 488, 536, 546, 618, 652, 671, 680, 701, 718, 742, 770, 796, 813, 830, 844, 867, 906, 936, 986, 1017, 1022, 1043, 1091, 1107, 1131, 1143, 1171, 1187, 1190, 1193, 1210, 1214, 1228, 1309, 1322, 1357, 1375, 1446, 1469, 1479, 1482, 1485, 1500, 1501, 1505, 1507, 1510, 1636, 1669, 1855, 1919, 3078, 3083, 3122, 3161, 3172, 3194, 3195, 3210, 3224, 3235, 3244, 3248, 3795	32, 44, 69, 77, 91, 108, 115, 134, 143, 161, 178, 182, 188, 202, 207, 233, 253, 259, 278, 286, 298, 340, 356, 392, 403, 419, 435, 482, 499, 519, 544, 602, 620, 670, 677, 686, 699, 745, 767, 788, 830, 841, 854, 868, 928, 950, 976, 1001, 1004, 1064, 1078, 1089, 1109, 1134, 1141, 1154, 1180, 1185, 1191, 1208, 1213, 1272, 1319, 1329, 1344, 1357, 1404, 1434, 1439, 1469, 1479, 1483, 1499, 1500, 1505, 1506, 1576, 1644, 1847, 1910, 3077, 3083, 3121, 3160, 3172, 3195, 3197, 3210, 3218, 3226, 3234, 3247, 3853
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.47058, 0.20986, 0.20514	0.46504, 0.21943, 0.21814	0.44751, 0.24109, 0.23484

Table S36. Vibrational frequencies and rotational constants for the stationary points involved in the C4-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(C4-add) $C_1 - {}^2A$	TS(C4-add) $C_1 - {}^2A$	Adduct(C4-add) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
21, 36, 41, 59, 65, 83, 88, 93, 110, 121, 137, 145, 154, 166, 176, 192, 196, 207, 229, 243, 264, 283, 308, 322, 356, 390, 404, 419, 432, 470, 490, 539, 549, 621, 669, 678, 682, 707, 733, 734, 794, 809, 832, 844, 867, 921, 937, 997, 1026, 1031, 1049, 1094, 1107, 1130, 1144, 1179, 1187, 1191, 1201, 1209, 1214, 1243, 1310, 1324, 1357, 1393, 1452, 1469, 1482, 1485, 1498, 1500, 1505, 1508, 1514, 1517, 1687, 1695, 1854, 1913, 3077, 3083, 3121, 3160, 3171, 3194, 3196, 3211, 3221, 3231, 3240, 3244, 3768	**541i**, 26, 37, 70, 86, 96, 104, 114, 135, 142, 145, 162, 166, 176, 183, 191, 198, 201, 229, 243, 267, 286, 326, 355, 389, 393, 408, 433, 454, 488, 536, 546, 618, 652, 671, 680, 701, 718, 742, 770, 796, 813, 830, 844, 867, 906, 936, 986, 1017, 1022, 1043, 1091, 1107, 1131, 1143, 1171, 1187, 1190, 1193, 1210, 1214, 1228, 1309, 1322, 1357, 1375, 1446, 1469, 1479, 1482, 1485, 1500, 1501, 1505, 1507, 1510, 1636, 1669, 1855, 1919, 3078, 3083, 3122, 3161, 3172, 3194, 3195, 3210, 3224, 3235, 3244, 3248, 3795	32, 44, 69, 77, 91, 108, 115, 134, 143, 161, 178, 182, 188, 202, 207, 233, 253, 259, 278, 286, 298, 340, 356, 392, 403, 419, 435, 482, 499, 519, 544, 602, 620, 670, 677, 686, 699, 745, 767, 788, 830, 841, 854, 868, 928, 950, 976, 1001, 1004, 1064, 1078, 1089, 1109, 1134, 1141, 1154, 1180, 1185 ,1191, 1208, 1213, 1272, 1319, 1329, 1344, 1357, 1404, 1434, 1439, 1469, 1479, 1483, 1499, 1500, 1505, 1506, 1576, 1644, 1847, 1910, 3077, 3083, 3121, 3160, 3172, 3195, 3197, 3210, 3218, 3226, 3234, 3247, 3853
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.47052, 0.20987, 0.20515	0.46504, 0.21945, 0.21816	0.44751, 0.24109, 0.23484

Table S37. Vibrational frequencies and rotational constants for the stationary points involved in the C5-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(C5-add) $C_1 - {}^2A$	TS(C5-add) $C_1 - {}^2A$	Adduct(C5-add) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
14, 30, 39, 78, 85, 92, 108, 112, 133, 138, 140, 153, 167, 172, 187, 194, 202, 229, 239, 266, 289, 319, 356, 390, 399, 408, 420, 438, 464, 478, 499, 539, 549, 620, 673, 675, 680, 704, 731, 732, 790, 804, 824, 842, 866, 918, 936, 994, 1026, 1028, 1050, 1080, 1105, 1126, 1137, 1181, 1185, 1190, 1201, 1210, 1216, 1242, 1311, 1328, 1356, 1399, 1448, 1467, 1482, 1486, 1497, 1498, 1503, 1505, 1515, 1515, 1690, 1693, 1851, 1907, 3081, 3087, 3122, 3166, 3181, 3195, 3200, 3212, 3225, 3235, 3243, 3248, 3679	**604i**, 24, 61, 72, 88, 110, 118, 130, 135, 145, 157, 168, 169, 184, 191, 196, 207, 234, 240, 269, 287, 317, 355, 385, 402, 404, 417, 436, 465, 488, 537, 547, 618, 645, 668, 679, 699, 726, 741, 787, 807, 827, 839, 865, 899, 933, 940, 989, 1012, 1027, 1044, 1078, 1095, 1124, 1134, 1181, 1187, 1189, 1192, 1210, 1217, 1230, 1304, 1329, 1357, 1392, 1448, 1468, 1482, 1482, 1486, 1497, 1502, 1504, 1505, 1506, 1639, 1662, 1851, 1906, 3083, 3086, 3129, 3169, 3177, 3201, 3208, 3209, 3228, 3240, 3247, 3257, 3740	29, 62, 75, 91, 107, 115, 137, 142, 153, 165, 170, 182, 186, 194, 199, 206, 237, 262, 288, 309, 322, 358, 395, 404, 417, 426, 437, 477, 489, 531, 537, 595, 621, 668, 671, 687, 703, 743, 763, 797, 823, 836, 864, 874, 918, 939, 1003, 1029, 1033, 1065, 1079, 1116, 1128, 1134, 1184, 1188, 1192, 1211, 1218, 1223, 1250, 1286, 1325, 1351, 1371, 1408, 1423, 1443, 1457, 1469, 1483, 1486, 1497, 1504, 1505, 1506, 1577, 1628, 1841, 1896, 3062, 3084, 3086, 3131, 3171, 3175, 3203, 3203, 3209, 3219, 3234, 3249, 3812
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.44328, 0.23031 ,0.21851	0.44117, 0.23535, 0.22068	0.43098, 0.24215, 0.22735

Table S38. Vibrational frequencies and rotational constants for the stationary points involved in the C6-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(C6-add) $C_1 - {}^2A$	TS(C6-add) $C_1 - {}^2A$	Adduct(C6-add) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
27, 37, 40, 80, 83, 93, 109, 113, 127, 131, 139, 155, 165, 171, 187, 192, 197, 227, 239, 263, 280, 319, 357, 382, 392, 406, 415, 429, 436, 464, 501, 538, 546, 618, 674, 675, 680, 708, 731, 732, 790, 804, 819, 845, 866, 917, 935, 993, 1024, 1027, 1049, 1088, 1105, 1127, 1146, 1181, 1187, 1191, 1201, 1210, 1215, 1241, 1310, 1323, 1353, 1399, 1445, 1468, 1481, 1484, 1499, 1500, 1505, 1506, 1514, 1515, 1689, 1693, 1850, 1906, 3078, 3085, 3118, 3163, 3178, 3190, 3195, 3214, 3224, 3235, 3242, 3249, 3704	**578i**, 12, 30, 66, 86, 92, 95, 109, 116, 138, 145, 158, 164, 176, 188, 195, 212, 230, 240, 257, 267, 286, 323, 357, 393, 399, 409, 432, 446, 488, 536, 546, 617, 644, 671, 677, 703, 726, 744, 784, 818, 829, 840, 851, 868, 915, 938, 982, 995, 1027, 1039, 1090, 1099, 1125, 1142, 1171, 1186, 1189, 1197, 1209, 1214, 1232, 1306, 1326, 1355, 1382, 1445, 1469, 1482, 1485, 1488, 1497, 1499, 1504, 1505, 1505, 1636, 1666, 1851, 1907, 3081, 3083, 3125, 3166, 3171, 3197, 3198, 3212, 3234, 3245, 3249, 3258, 3770	5, 27, 64, 78, 88, 98, 112, 126, 143, 148, 161, 164, 185, 193, 196, 211, 238, 264, 286, 311, 330, 343, 384, 386, 401, 431, 435, 467, 488, 520, 534, 610, 624, 666, 670, 693, 711, 739, 757, 793, 824, 833, 864, 872, 907, 931, 998, 1018, 1061, 1089, 1092, 1125, 1142, 1151, 1181, 1185, 1190, 1209, 1213, 1221, 1231, 1292, 1325, 1350, 1355, 1387, 1415, 1441, 1462, 1471, 1481, 1485, 1498, 1499, 1502, 1504, 1564, 1691, 1831, 1890, 3028, 3080, 3083, 3124, 3164, 3172, 3196, 3197, 3210, 3221, 3231, 3237, 3853
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.45433, 0.22486, 0.22099	0.42736, 0.22446, 0.21559	0.44261, 0.20634, 0.20249

Table S39. Vibrational frequencies and rotational constants for the stationary points involved in the C7-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(C7-add) $C_1 - {}^2A$	TS(C7-add) $C_1 - {}^2A$	Adduct(C7-add) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
25, 39, 53, 84, 95, 103, 108, 116, 132, 142, 151, 153, 162, 166, 187, 195, 198, 241, 246, 282, 290, 324, 366, 388, 403, 414, 432, 465, 486, 493, 529, 541, 555, 620, 670, 676, 683, 714, 733, 735, 790, 807, 831, 854, 869, 921, 940, 996, 1020, 1031, 1049, 1092, 1107, 1127, 1142, 1181, 1186, 1189, 1202, 1210, 1214, 1242, 1311, 1319, 1355, 1398, 1446, 1480, 1482, 1485, 1499, 1501, 1505, 1508, 1517, 1519, 1694, 1698, 1835, 1905, 3076, 3079, 3121, 3160, 3166, 3192, 3194, 3210, 3222, 3232, 3240, 3245, 3665	**629i**, 25, 35, 81, 85, 94, 108, 118, 130, 135, 149, 157, 164, 173, 195, 200, 228, 250, 270, 281, 291, 315, 343, 371, 391, 404, 422, 432, 474, 491, 544, 548, 607, 620, 668, 677, 699, 719, 731, 780, 805, 831, 844, 865, 881, 917, 944, 993, 1028, 1030, 1052, 1095, 1104, 1128, 1145, 1180, 1185, 1188, 1200, 1209, 1214, 1243, 1310, 1323, 1354, 1393, 1450, 1467, 1479, 1483, 1498, 1500, 1502, 1506, 1508, 1518, 1568, 1693, 1701, 1880, 3078, 3080, 3118, 3160, 3167, 3191, 3195, 3211, 3220, 3229, 3238, 3245, 3794	29, 29, 62, 77, 93 ,103, 119, 124, 140, 146, 160, 166, 183, 195, 198, 228, 256, 271, 279, 292, 320, 345, 366, 399, 422, 425, 428, 488, 499, 522, 567, 598, 654, 658, 680, 698, 718, 731, 780, 804, 837, 851, 865, 910, 945, 987, 993, 1026, 1048, 1053, 1097, 1103, 1139, 1147, 1169, 1183, 1184, 1189, 1209, 1213, 1228, 1256, 1293, 1303, 1314, 1364, 1383, 1417, 1458, 1484, 1489, 1500, 1503, 1504, 1511, 1512, 1518, 1683, 1689, 1869, 3071, 3090, 3109, 3154, 3179, 3184, 3191, 3201, 3220, 3230, 3237, 3244, 3880
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.40525, 0.22569 ,0.20737	0.44567, 0.22034, 0.21429	0.50916, 0.20117, 0.19575

Table S40. Vibrational frequencies and rotational constants for the stationary points involved in the C9-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(C9-add) $C_1 - {}^2A$	TS(C9-add) $C_1 - {}^2A$	Adduct(C9-add) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
25, 39, 52, 84, 95, 103, 108, 116, 132, 142, 151, 153, 162, 166, 187, 195, 198, 241, 246, 282, 290, 324, 366, 388, 403, 414, 432, 465, 486, 493, 530, 541, 555, 620, 670, 676, 683, 714, 733, 735, 790, 807, 831, 854, 869, 921, 940, 996, 1020, 1031, 1049, 1092, 1107, 1127, 1142, 1181, 1186, 1189, 1202, 1210, 1214, 1242, 1311, 1320, 1355, 1398, 1446, 1480, 1482 ,1485, 1499, 1501, 1505, 1508, 1517, 1519, 1694, 1698, 1835, 1905, 3076, 3079, 3121, 3160, 3166, 3192, 3194, 3210, 3222, 3232, 3240, 3245, 3665	**629i**, 25, 35, 81, 84, 93, 108, 118, 130, 135, 149, 157, 164, 173, 195, 200, 228, 250, 270, 281, 291, 315, 343, 371, 391, 404, 422, 432, 474, 491, 544, 548, 607, 620, 668, 677, 699, 719, 731, 780, 805, 831, 844, 865, 881, 917, 944, 993, 1028, 1030, 1052, 1095, 1104, 1128, 1145, 1180, 1185, 1188, 1200, 1209, 1214, 1243, 1310, 1323, 1354, 1393, 1450, 1467, 1479, 1483, 1498, 1500, 1502, 1506, 1508, 1518, 1568, 1693, 1701, 1880, 3078, 3080, 3118, 3160, 3167, 3191, 3195, 3211, 3220, 3229, 3238, 3245, 3794	29, 29, 62, 77, 93, 103, 119, 124, 140, 146, 160, 166, 183, 195, 198, 228, 257, 271, 279, 292, 320, 345, 366, 399, 422, 425, 428, 488, 499, 522, 567, 598, 654, 658, 680, 698, 718, 731, 780, 804, 837, 851, 865, 910, 945, 987, 993, 1026, 1048, 1053, 1097, 1103, 1139, 1147, 1169, 1183, 1184, 1189, 1209, 1213, 1228, 1256, 1293, 1303, 1314, 1364, 1383, 1417, 1458, 1484, 1489, 1500, 1503, 1504, 1511, 1512, 1518, 1683, 1689, 1869, 3071, 3090, 3109, 3154, 3179, 3184, 3191, 3201, 3220, 3230, 3237, 3244, 3880
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.40528, 0.22568, 0.20735	0.44570, 0.22033, 0.21428	0.50917, 0.20116, 0.19574

Table S41. Vibrational frequencies and rotational constants for the stationary points involved in the P12-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(P12-add) $C_1 - {}^2A$	TS(P12-add) $C_1 - {}^2A$	MCP(P12-add) $C_1 - {}^2A$	Product1(P12-add) $C_1 - {}^2A$	Product2(P12-add) $C_1 - {}^1A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
19, 34, 41, 69, 81, 85, 90, 120, 123, 133, 140, 146, 155, 161, 183, 190, 193, 199, 227, 239, 264, 287, 320, 357, 388, 403, 415, 428, 467, 477, 491, 539, 548, 619, 654, 678, 680, 707, 732, 733, 794, 807, 840, 849 ,860, 920, 936, 995, 1025, 1030, 1050, 1100, 1106, 1127, 1148, 1180, 1185, 1190, 1201, 1211, 1215, 1243, 1311, 1325, 1355, 1396, 1446, 1468, 1478, 1481, 1498, 1499, 1504, 1505, 1516, 1517, 1692, 1698, 1852, 1909, 3076, 3083, 3120, 3159, 3176, 3193, 3199, 3210, 3222, 3232, 3241, 3246, 3805	**190i**, 25, 39, 66, 73, 82, 89, 107, 125, 134, 140, 157, 162, 185, 193, 198, 228, 237, 261, 265, 291, 334, 359, 366, 385, 397, 415, 436, 468, 469, 538, 545, 604, 621, 679, 684, 705, 709, 732, 734, 795, 807, 842, 854, 862, 920, 937, 995, 1024, 1031, 1049, 1105, 1109, 1128, 1147, 1180, 1185, 1187, 1201, 1213, 1217, 1242, 1310, 1324, 1355, 1396, 1445, 1470, 1478, 1484, 1500, 1500, 1507, 1508, 1516, 1517, 1691, 1698, 1850, 1908, 3075, 3081, 3119, 3155, 3175, 3189, 3199, 3210, 3222, 3232, 3240, 3246, 3846	30, 41, 44, 64, 66, 78, 92, 103, 110, 124, 145, 152, 155, 160, 194, 206, 209, 229, 242, 266, 323, 340, 358, 368, 383, 414, 430, 470, 479, 527, 540, 620, 631, 671, 676, 715, 732, 733, 745, 793, 811, 829, 842, 893, 915, 921, 994, 1013, 1027, 1036, 1046, 1089, 1102, 1110, 1147, 1178, 1187, 1190, 1201, 1214, 1219, 1236, 1306, 1314, 1347, 1388, 1416, 1455, 1482, 1487, 1502, 1506, 1509, 1512, 1514, 1514, 1686, 1696, 1846, 1906, 3072, 3090, 3093, 3146, 3156, 3181, 3198, 3200, 3225, 3234, 3242, 3247 ,3793	19, 54, 127, 140, 185, 229, 266, 338, 367, 417, 467, 527, 539, 619, 674, 680, 713, 733, 741, 742, 793, 808, 895, 922, 998, 1012, 1031, 1048, 1095, 1107, 1180, 1201, 1236, 1310, 1317, 1342, 1395, 1411, 1449, 1516, 1516, 1691, 1697, 1852, 1907, 3097, 3150, 3222, 3234, 3242, 3246	64, 87, 124, 140, 171, 220, 248, 295, 340, 411, 435, 466, 629, 830, 847, 938, 1050, 1116, 1142, 1188, 1189, 1211, 1215, 1484, 1485, 1505, 1506, 1512, 1513, 3079, 3080, 3163, 3164, 3196, 3200, 3844
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.42376, 0.22542, 0.21102	0.45269, 0.22135, 0.21363	0.32941, 0.29421, 0.22867	1.49425, 0.49220, 0.39886	1.97226, 1.67961, 1.42457

Table S42. Vibrational frequencies and rotational constants for the stationary points involved in the S17-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(S17-add) $C_1 - {}^2A$	TS(S17-add) $C_1 - {}^2A$	Adduct(S17-add) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
29, 33, 50, 75, 87, 97, 104, 112, 128, 135, 141, 158, 165, 190, 191, 198, 199, 214, 229, 240, 262, 281, 320, 358, 389, 400, 415, 426, 467, 481, 496, 538, 545, 618, 661, 678, 684, 713, 732, 735, 793, 807, 836, 848, 857, 921, 935, 996, 1022, 1030, 1049, 1088, 1106, 1128, 1141, 1179, 1186, 1189, 1201, 1212, 1215, 1242, 1309, 1319, 1354, 1395, 1444, 1471, 1481, 1488, 1497, 1501, 1502, 1509, 1516, 1517, 1692, 1698, 1851, 1908, 3073, 3090, 3113, 3158, 3184, 3185, 3199, 3210, 3222, 3232, 3240, 3245, 3804	**427i**, 14, 34, 45, 75, 82, 91, 96, 122, 129, 147, 148, 152, 164, 187, 189, 201, 228, 255, 258, 264, 277, 308, 352, 381, 387, 413, 422, 423, 467, 534, 538, 541, 618, 665, 678, 706, 730, 731, 792, 806, 826, 834, 844, 921, 931, 996, 1020, 1026, 1030, 1048, 1080, 1106, 1120, 1136, 1180, 1183, 1188, 1201, 1211, 1215, 1242, 1302, 1312, 1348, 1395, 1443, 1468, 1480, 1487, 1498, 1501, 1502, 1507, 1516, 1517, 1692, 1698, 1849, 1907, 3075, 3082, 3114, 3159, 3171, 3190, 3198, 3210, 3221, 3232, 3240, 3245, 3824	18, 30, 43, 56, 77, 84, 114, 116, 123, 124, 150, 153, 161, 170, 185, 199, 206, 230, 259, 268, 288, 298, 342, 359, 370, 380, 402, 415, 432, 468, 534, 541, 618, 673, 679, 703, 730, 732, 784, 792, 803, 811, 818, 837, 919, 930, 994, 1022, 1029, 1048, 1088, 1105, 1119, 1136, 1176, 1179, 1185, 1187, 1200, 1209, 1214, 1241, 1306, 1312, 1352, 1396, 1446, 1466, 1481, 1485, 1498, 1500, 1505, 1506, 1516, 1517, 1693, 1699, 1847, 1906, 3068, 3071, 3118, 3150, 3152, 3190, 3191, 3206, 3221, 3232, 3240, 3245, 3866
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.46754, 0.21315, 0.19767	0.46773, 0.20941, 0.20195	0.41194, 0.21380, 0.20165

Table S43. Rate constant and branching ratio (Γ, %) values in gas phase calculated at the M06-2X/6-311++G(3df,3pd)//M06-2X/6-31+G(d,p) level of theory.

(A) Abstraction pathways

T (K)	k (cm^3 $molecule^{-1}$ s^{-1})												
	H20-abs	H21-abs	H22-abs	H23-abs	H24-abs	H25-abs	H26-abs	H27-abs	H28-abs	H29-abs	H30-abs	H31-abs	FHT
253	3.40×10^{-11}	3.43×10^{-11}	1.15×10^{-13}	8.43×10^{-14}	1.13×10^{-15}	1.60×10^{-15}	1.05×10^{-12}	1.25×10^{-12}	4.90×10^{-14}	4.83×10^{-14}	7.13×10^{-13}	1.98×10^{-13}	7.18E-11
258	2.88×10^{-11}	2.90×10^{-11}	1.01×10^{-13}	7.58×10^{-14}	1.14×10^{-15}	1.62×10^{-15}	9.30×10^{-13}	1.14×10^{-12}	4.69×10^{-14}	4.62×10^{-14}	6.54×10^{-13}	1.84×10^{-13}	6.10E-11
263	2.46×10^{-11}	2.48×10^{-11}	8.99×10^{-14}	6.84×10^{-14}	1.17×10^{-15}	1.65×10^{-15}	8.32×10^{-13}	1.06×10^{-12}	4.51×10^{-14}	4.45×10^{-14}	6.03×10^{-13}	1.72×10^{-13}	5.22E-11
268	2.11×10^{-11}	2.13×10^{-11}	8.07×10^{-14}	6.29×10^{-14}	1.20×10^{-15}	1.69×10^{-15}	7.49×10^{-13}	9.83×10^{-13}	4.37×10^{-14}	4.30×10^{-14}	5.58×10^{-13}	1.61×10^{-13}	4.51E-11
273	1.83×10^{-11}	1.85×10^{-11}	7.30×10^{-14}	5.79×10^{-14}	1.24×10^{-15}	1.75×10^{-15}	6.79×10^{-13}	9.17×10^{-13}	4.25×10^{-14}	4.18×10^{-14}	5.20×10^{-13}	1.52×10^{-13}	3.93E-11
278	1.60×10^{-11}	1.61×10^{-11}	6.66×10^{-14}	5.37×10^{-14}	1.28×10^{-15}	1.81×10^{-15}	6.20×10^{-13}	8.59×10^{-13}	4.15×10^{-14}	4.08×10^{-14}	4.86×10^{-13}	1.43×10^{-13}	3.45E-11
283	1.41×10^{-11}	1.42×10^{-11}	6.12×10^{-14}	5.01×10^{-14}	1.34×10^{-15}	1.88×10^{-15}	5.69×10^{-13}	8.09×10^{-13}	4.06×10^{-14}	4.00×10^{-14}	4.56×10^{-13}	1.36×10^{-13}	3.04E-11
288	1.25×10^{-11}	1.25×10^{-11}	5.66×10^{-14}	4.70×10^{-14}	1.40×10^{-15}	1.96×10^{-15}	5.25×10^{-13}	7.64×10^{-13}	3.99×10^{-14}	3.93×10^{-14}	4.30×10^{-13}	1.29×10^{-13}	2.70E-11
293	1.11×10^{-11}	1.12×10^{-11}	5.28×10^{-14}	4.44×10^{-14}	1.46×10^{-15}	2.06×10^{-15}	4.87×10^{-13}	7.25×10^{-13}	3.94×10^{-14}	3.88×10^{-14}	4.07×10^{-13}	1.23×10^{-13}	2.42E-11
298	9.92×10^{-12}	9.99×10^{-12}	4.94×10^{-14}	4.21×10^{-14}	1.54×10^{-15}	2.16×10^{-15}	4.54×10^{-13}	6.89×10^{-13}	3.90×10^{-14}	3.84×10^{-14}	3.86×10^{-13}	1.18×10^{-13}	2.17E-11
303	8.92×10^{-12}	8.98×10^{-12}	4.66×10^{-14}	4.01×10^{-14}	1.62×10^{-15}	2.27×10^{-15}	4.24×10^{-13}	6.58×10^{-13}	3.86×10^{-14}	3.80×10^{-14}	3.68×10^{-13}	1.13×10^{-13}	1.96E-11
308	8.06×10^{-12}	8.12×10^{-12}	4.42×10^{-14}	3.84×10^{-14}	1.71×10^{-15}	2.39×10^{-15}	3.99×10^{-13}	6.30×10^{-13}	3.84×10^{-14}	3.78×10^{-14}	3.51×10^{-13}	1.09×10^{-13}	1.78E-11
313	7.31×10^{-12}	7.37×10^{-12}	4.20×10^{-14}	3.69×10^{-14}	1.80×10^{-15}	2.52×10^{-15}	3.76×10^{-13}	6.04×10^{-13}	3.82×10^{-14}	3.76×10^{-14}	3.37×10^{-13}	1.05×10^{-13}	1.63E-11
318	6.67×10^{-12}	6.72×10^{-12}	4.02×10^{-14}	3.56×10^{-14}	1.91×10^{-15}	2.66×10^{-15}	3.56×10^{-13}	5.81×10^{-13}	3.81×10^{-14}	3.75×10^{-14}	3.23×10^{-13}	1.01×10^{-13}	1.49E-11
323	6.10×10^{-12}	6.15×10^{-12}	3.86×10^{-14}	3.45×10^{-14}	2.02×10^{-15}	2.82×10^{-15}	3.37×10^{-13}	5.61×10^{-13}	3.81×10^{-14}	3.75×10^{-14}	3.11×10^{-13}	9.80×10^{-14}	1.37E-11

T (K)	k (M^{-1} s^{-1})												
	H20-abs	H21-abs	H22-abs	H23-abs	H24-abs	H25-abs	H26-abs	H27-abs	H28-abs	H29-abs	H30-abs	H31-abs	FHT
253	2.05E+10	2.06E+10	6.93E+07	5.07E+07	6.80E+05	9.63E+05	6.31E+08	7.50E+08	2.95E+07	2.91E+07	4.29E+08	1.19E+08	4.32E+10
258	1.73E+10	1.75E+10	6.10E+07	4.57E+07	6.89E+05	9.75E+05	5.60E+08	6.89E+08	2.82E+07	2.78E+07	3.94E+08	1.11E+08	3.67E+10
263	1.48E+10	1.49E+10	5.42E+07	4.14E+07	7.03E+05	9.95E+05	5.01E+08	6.37E+08	2.72E+07	2.68E+07	3.63E+08	1.03E+08	3.15E+10
268	1.27E+10	1.28E+10	4.86E+07	3.79E+07	7.22E+05	1.02E+06	4.51E+08	5.92E+08	2.63E+07	2.59E+07	3.36E+08	9.70E+07	2.72E+10
273	1.10E+10	1.11E+10	4.39E+07	3.49E+07	7.45E+05	1.05E+06	4.09E+08	5.52E+08	2.56E+07	2.52E+07	3.13E+08	9.12E+07	2.37E+10
278	9.65E+09	9.72E+09	4.01E+07	3.23E+07	7.73E+05	1.09E+06	3.73E+08	5.18E+08	2.50E+07	2.46E+07	2.93E+08	8.62E+07	2.08E+10
283	8.48E+09	8.54E+09	3.68E+07	3.02E+07	8.05E+05	1.13E+06	3.43E+08	4.87E+08	2.45E+07	2.41E+07	2.75E+08	8.17E+07	1.83E+10
288	7.50E+09	7.56E+09	3.41E+07	2.83E+07	8.41E+05	1.18E+06	3.16E+08	4.60E+08	2.41E+07	2.37E+07	2.59E+08	7.77E+07	1.63E+10
293	6.67E+09	6.72E+09	3.18E+07	2.67E+07	8.81E+05	1.24E+06	2.93E+08	4.36E+08	2.37E+07	2.34E+07	2.45E+08	7.42E+07	1.46E+10
298	5.97E+09	6.02E+09	2.98E+07	2.54E+07	9.25E+05	1.30E+06	2.73E+08	4.15E+08	2.35E+07	2.31E+07	2.33E+08	7.10E+07	1.31E+10
303	5.37E+09	5.41E+09	2.81E+07	2.42E+07	9.74E+05	1.37E+06	2.56E+08	3.96E+08	2.33E+07	2.29E+07	2.22E+08	6.81E+07	1.18E+10
308	4.85E+09	4.89E+09	2.66E+07	2.31E+07	1.03E+06	1.44E+06	2.40E+08	3.79E+08	2.31E+07	2.28E+07	2.12E+08	6.55E+07	1.07E+10
313	4.40E+09	4.44E+09	2.53E+07	2.22E+07	1.09E+06	1.52E+06	2.26E+08	3.64E+08	2.30E+07	2.27E+07	2.03E+08	6.31E+07	9.79E+09
318	4.02E+09	4.05E+09	2.42E+07	2.14E+07	1.15E+06	1.60E+06	2.14E+08	3.50E+08	2.30E+07	2.26E+07	1.95E+08	6.10E+07	8.98E+09
323	3.68E+09	3.70E+09	2.33E+07	2.07E+07	1.22E+06	1.70E+06	2.03E+08	3.38E+08	2.29E+07	2.26E+07	1.87E+08	5.90E+07	8.26E+09

T (K)	Branching ratio (□, %)												
	H20-abs	H21-abs	H22-abs	H23-abs	H24-abs	H25-abs	H26-abs	H27-abs	H28-abs	H29-abs	H30-abs	H31-abs	FHT
253	32.57%	32.81%	0.11%	0.08%	0.00%	0.00%	1.00%	1.19%	0.05%	0.05%	0.68%	0.19%	68.73%
258	32.08%	32.32%	0.11%	0.08%	0.00%	0.00%	1.04%	1.28%	0.05%	0.05%	0.73%	0.21%	67.95%
263	31.63%	31.86%	0.12%	0.09%	0.00%	0.00%	1.07%	1.36%	0.06%	0.06%	0.78%	0.22%	67.24%
268	31.20%	31.43%	0.12%	0.09%	0.00%	0.00%	1.11%	1.45%	0.06%	0.06%	0.82%	0.24%	66.59%
273	30.80%	31.02%	0.12%	0.10%	0.00%	0.00%	1.14%	1.54%	0.07%	0.07%	0.87%	0.25%	65.99%
278	30.42%	30.64%	0.13%	0.10%	0.00%	0.00%	1.18%	1.63%	0.08%	0.08%	0.92%	0.27%	65.46%
283	30.06%	30.29%	0.13%	0.11%	0.00%	0.00%	1.21%	1.73%	0.09%	0.09%	0.97%	0.29%	64.97%
288	29.73%	29.95%	0.14%	0.11%	0.00%	0.00%	1.25%	1.82%	0.10%	0.09%	1.03%	0.31%	64.53%
293	29.41%	29.63%	0.14%	0.12%	0.00%	0.01%	1.29%	1.92%	0.10%	0.10%	1.08%	0.33%	64.14%
298	29.12%	29.33%	0.15%	0.12%	0.00%	0.01%	1.33%	2.02%	0.11%	0.11%	1.13%	0.35%	63.79%
303	28.83%	29.05%	0.15%	0.13%	0.01%	0.01%	1.37%	2.13%	0.12%	0.12%	1.19%	0.37%	63.48%
308	28.57%	28.78%	0.16%	0.14%	0.01%	0.01%	1.41%	2.23%	0.14%	0.13%	1.25%	0.39%	63.21%
313	28.32%	28.53%	0.16%	0.14%	0.01%	0.01%	1.45%	2.34%	0.15%	0.15%	1.30%	0.41%	62.97%
318	28.08%	28.29%	0.17%	0.15%	0.01%	0.01%	1.50%	2.45%	0.16%	0.16%	1.36%	0.43%	62.76%
323	27.85%	28.06%	0.18%	0.16%	0.01%	0.01%	1.54%	2.56%	0.17%	0.17%	1.42%	0.45%	62.58%

(a) addition pathways

T (K)	k (cm^3 $molecule^{-1}$ s^{-1})											
	C1-add	C2-add	C3-add	C4-add	C5-add	C6-add	C7-add	C9-add	P-12add	S17-add	RAF	Overall
253	7.30×10^{-16}	1.39×10^{-15}	8.68×10^{-17}	8.97×10^{-17}	1.39×10^{-15}	1.51×10^{-15}	1.25×10^{-23}	1.26×10^{-23}	3.26×10^{-11}	3.96×10^{-21}	3.27E-11	1.04E-10
258	8.07×10^{-16}	1.42×10^{-15}	9.73×10^{-17}	1.00×10^{-16}	1.43×10^{-15}	1.64×10^{-15}	1.85×10^{-23}	1.87×10^{-23}	2.87×10^{-11}	5.64×10^{-21}	2.88E-11	8.97E-11
263	8.89×10^{-16}	1.45×10^{-15}	1.09×10^{-16}	1.12×10^{-16}	1.46×10^{-15}	1.77×10^{-15}	2.72×10^{-23}	2.75×10^{-23}	2.54×10^{-11}	7.93×10^{-21}	2.55E-11	7.77E-11
268	9.77×10^{-16}	1.49×10^{-15}	1.21×10^{-16}	1.25×10^{-16}	1.50×10^{-15}	1.91×10^{-15}	3.94×10^{-23}	3.98×10^{-23}	2.26×10^{-11}	1.10×10^{-20}	2.26E-11	6.78E-11
273	1.07×10^{-15}	1.53×10^{-15}	1.34×10^{-16}	1.39×10^{-16}	1.53×10^{-15}	2.05×10^{-15}	5.63×10^{-23}	5.69×10^{-23}	2.02×10^{-11}	1.51×10^{-20}	2.03E-11	5.96E-11
278	1.17×10^{-15}	1.56×10^{-15}	1.49×10^{-16}	1.53×10^{-16}	1.57×10^{-15}	2.21×10^{-15}	7.96×10^{-23}	8.04×10^{-23}	1.82×10^{-11}	2.06×10^{-20}	1.82E-11	5.27E-11
283	1.28×10^{-15}	1.60×10^{-15}	1.64×10^{-16}	1.69×10^{-16}	1.61×10^{-15}	2.37×10^{-15}	1.11×10^{-22}	1.12×10^{-22}	1.64×10^{-11}	2.77×10^{-20}	1.64E-11	4.68E-11
288	1.39×10^{-15}	1.64×10^{-15}	1.81×10^{-16}	1.73×10^{-16}	1.65×10^{-15}	2.53×10^{-15}	1.54×10^{-22}	1.55×10^{-22}	1.49×10^{-11}	3.69×10^{-20}	1.49E-11	4.19E-11
293	1.51×10^{-15}	1.68×10^{-15}	1.98×10^{-16}	1.77×10^{-16}	1.69×10^{-15}	2.71×10^{-15}	2.10×10^{-22}	2.12×10^{-22}	1.35×10^{-11}	4.88×10^{-20}	1.35E-11	3.77E-11
298	1.64×10^{-15}	1.72×10^{-15}	2.17×10^{-16}	1.81×10^{-16}	1.73×10^{-15}	2.89×10^{-15}	2.85×10^{-22}	2.88×10^{-22}	1.23×10^{-11}	6.39×10^{-20}	1.23E-11	3.41E-11
303	1.77×10^{-15}	1.76×10^{-15}	2.37×10^{-16}	1.86×10^{-16}	1.77×10^{-15}	3.08×10^{-15}	3.83×10^{-22}	3.86×10^{-22}	1.13×10^{-11}	8.30×10^{-20}	1.13E-11	3.09E-11
308	1.91×10^{-15}	1.81×10^{-15}	2.59×10^{-16}	1.90×10^{-16}	1.81×10^{-15}	3.28×10^{-15}	5.09×10^{-22}	5.14×10^{-22}	1.04×10^{-11}	1.07×10^{-19}	1.04E-11	2.82E-11
313	2.06×10^{-15}	1.85×10^{-15}	2.82×10^{-16}	1.94×10^{-16}	1.86×10^{-15}	3.49×10^{-15}	6.72×10^{-22}	6.78×10^{-22}	9.56×10^{-12}	1.37×10^{-19}	9.56E-12	2.58E-11
318	2.22×10^{-15}	1.89×10^{-15}	3.06×10^{-16}	1.91×10^{-16}	1.90×10^{-15}	3.71×10^{-15}	8.79×10^{-22}	8.88×10^{-22}	8.83×10^{-12}	1.74×10^{-19}	8.84E-12	2.37E-11
323	2.38×10^{-15}	1.94×10^{-15}	3.32×10^{-16}	2.02×10^{-16}	1.94×10^{-15}	3.93×10^{-15}	1.14×10^{-21}	1.15×10^{-21}	8.19×10^{-12}	2.19×10^{-19}	8.20E-12	2.19E-11

T (K)	k (M^{-1} s^{-1})											
	C1-add	C2-add	C3-add	C4-add	C5-add	C6-add	C7-add	C9-add	P-12add	S17-add	RAF	Overall
253	4.40E+05	8.34E+05	5.23E+04	5.40E+04	8.38E+05	9.11E+05	7.50E-03	7.58E-03	1.97E+10	2.38E+00	1.97E+10	6.29E+10
258	4.86E+05	8.55E+05	5.86E+04	6.05E+04	8.58E+05	9.86E+05	1.12E-02	1.13E-02	1.73E+10	3.40E+00	1.73E+10	5.40E+10
263	5.35E+05	8.76E+05	6.55E+04	6.76E+04	8.80E+05	1.07E+06	1.64E-02	1.65E-02	1.53E+10	4.78E+00	1.53E+10	4.68E+10
268	5.88E+05	8.97E+05	7.29E+04	7.52E+04	9.01E+05	1.15E+06	2.37E-02	2.40E-02	1.36E+10	6.64E+00	1.36E+10	4.08E+10
273	6.45E+05	9.19E+05	8.09E+04	8.35E+04	9.23E+05	1.24E+06	3.39E-02	3.43E-02	1.22E+10	9.12E+00	1.22E+10	3.59E+10
278	7.05E+05	9.42E+05	8.95E+04	9.24E+04	9.46E+05	1.33E+06	4.79E-02	4.84E-02	1.09E+10	1.24E+01	1.10E+10	3.17E+10
283	7.70E+05	9.65E+05	9.88E+04	1.02E+05	9.69E+05	1.42E+06	6.70E-02	6.76E-02	9.88E+09	1.67E+01	9.88E+09	2.82E+10
288	8.38E+05	9.88E+05	1.09E+05	1.12E+05	9.93E+05	1.53E+06	9.26E-02	9.35E-02	8.94E+09	2.22E+01	8.95E+09	2.52E+10
293	9.10E+05	1.01E+06	1.19E+05	1.23E+05	1.02E+06	1.63E+06	1.27E-01	1.28E-01	8.13E+09	2.94E+01	8.14E+09	2.27E+10
298	9.86E+05	1.04E+06	1.31E+05	1.35E+05	1.04E+06	1.74E+06	1.72E-01	1.73E-01	7.42E+09	3.85E+01	7.43E+09	2.05E+10
303	1.07E+06	1.06E+06	1.43E+05	1.48E+05	1.07E+06	1.86E+06	2.30E-01	2.33E-01	6.80E+09	5.00E+01	6.80E+09	1.86E+10
308	1.15E+06	1.09E+06	1.56E+05	1.61E+05	1.09E+06	1.98E+06	3.07E-01	3.10E-01	6.24E+09	6.44E+01	6.25E+09	1.70E+10
313	1.24E+06	1.11E+06	1.70E+05	1.75E+05	1.12E+06	2.10E+06	4.04E-01	4.08E-01	5.75E+09	8.23E+01	5.76E+09	1.56E+10
318	1.34E+06	1.14E+06	1.84E+05	1.90E+05	1.14E+06	2.23E+06	5.29E-01	5.34E-01	5.32E+09	1.05E+02	5.33E+09	1.43E+10
323	1.44E+06	1.17E+06	2.00E+05	2.06E+05	1.17E+06	2.37E+06	6.87E-01	6.94E-01	4.93E+09	1.32E+02	4.94E+09	1.32E+10

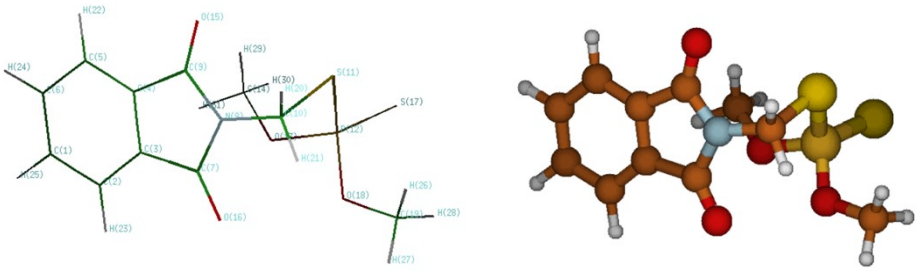
T (K)	Branching ratio (Γ, %)											
	C1-add	C2-add	C3-add	C4-add	C5-add	C6-add	C7-add	C9-add	P-12add	S17-add	RAF	Overall
253	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	31.26%	0.00%	31.27%	100.00%
258	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	32.04%	0.00%	32.05%	100.00%
263	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	32.75%	0.00%	32.76%	100.00%
268	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	33.40%	0.00%	33.41%	100.00%
273	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	33.99%	0.00%	34.01%	100.00%
278	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	34.53%	0.00%	34.54%	100.00%
283	0.00%	0.00%	0.00%	0.00%	0.00%	0.01%	0.00%	0.00%	35.01%	0.00%	35.03%	100.00%
288	0.00%	0.00%	0.00%	0.00%	0.00%	0.01%	0.00%	0.00%	35.45%	0.00%	35.47%	100.00%
293	0.00%	0.00%	0.00%	0.00%	0.00%	0.01%	0.00%	0.00%	35.84%	0.00%	35.86%	100.00%
298	0.00%	0.01%	0.00%	0.00%	0.01%	0.01%	0.00%	0.00%	36.18%	0.00%	36.21%	100.00%
303	0.01%	0.01%	0.00%	0.00%	0.01%	0.01%	0.00%	0.00%	36.49%	0.00%	36.52%	100.00%
308	0.01%	0.01%	0.00%	0.00%	0.01%	0.01%	0.00%	0.00%	36.76%	0.00%	36.79%	100.00%
313	0.01%	0.01%	0.00%	0.00%	0.01%	0.01%	0.00%	0.00%	36.99%	0.00%	37.03%	100.00%
318	0.01%	0.01%	0.00%	0.00%	0.01%	0.02%	0.00%	0.00%	37.19%	0.00%	37.24%	100.00%
323	0.01%	0.01%	0.00%	0.00%	0.01%	0.02%	0.00%	0.00%	37.37%	0.00%	37.42%	100.00%

AQUEOUS PHASE DATA

Table S44. Structural data for phosmet in the aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

Phosmet

$C_1 - {}^2A$



Optimized Cartesian coordinates			
C	-4.244960	-1.594462	0.402722
C	-3.125049	-1.308540	1.193617
C	-2.331295	-0.247735	0.795208
C	-2.628429	0.507313	-0.337595
C	-3.733135	0.236676	-1.125303
C	-4.543116	-0.836718	-0.733975
C	-1.076936	0.284105	1.389995
N	-0.685781	1.358664	0.575834
C	-1.564729	1.533989	-0.496973
C	0.596808	1.999403	0.659479
S	1.768634	1.512404	-0.682468
P	2.104221	-0.504389	-0.235010
O	0.674073	-1.232801	-0.252246
C	0.032367	-1.535016	-1.509781
O	-1.425329	2.373214	-1.364423
O	-0.483718	-0.080562	2.382942
S	3.483207	-1.226968	-1.385053
O	2.312491	-0.591597	1.349115
C	3.500005	-0.035164	1.951155
H	0.490314	3.079565	0.545417
H	1.033746	1.775552	1.633472
H	-3.958353	0.825697	-2.008365
H	-2.886720	-1.895144	2.074885
H	-5.418135	-1.087646	-1.324453
H	-4.892953	-2.421171	0.674453
H	3.578132	1.030842	1.721205
H	3.380141	-0.178093	3.023320
H	4.383696	-0.567944	1.594032
H	-0.164493	-0.611811	-2.064455
H	0.659727	-2.207369	-2.098082
H	-0.906733	-2.023447	-1.251255

Vibrational frequencies (cm^{-1})
26, 43, 65, 75, 91, 113, 124, 134, 149, 169, 181, 192, 212, 212, 233, 243, 270, 292, 331, 358, 387, 397, 412, 426, 469, 492, 524, 539, 615, 648, 679, 687, 707, 729, 735, 797, 811, 817, 830, 845, 924, 932, 1004, 1010, 1041, 1046, 1056, 1103, 1120, 1124, 1168, 1180, 1186, 1191, 1202, 1206, 1236, 1312, 1326, 1352, 1396, 1431, 1455, 1479, 1481, 1485, 1487, 1490, 1497, 1510, 1511, 1689, 1689, 1766, 1855, 3080, 3090, 3134, 3173, 3178, 3203, 3205, 3216, 3233, 3241, 3247, 3252
Rotational constants (GHz)
0.55877, 0.21047, 0.20568

Table S45. Optimized Cartesian coordinates for the stationary points involved in the H20-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

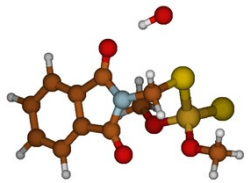
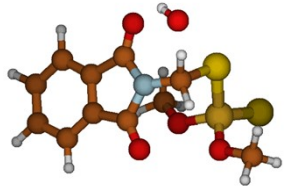
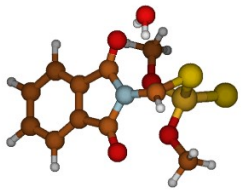
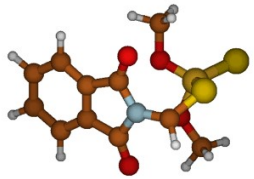
MCR(H20-abs)				TS(H20-abs)				MCP(H20-abs)				Rad(H20-abs)			
															
C	-4.396560	-1.604629	-0.328758	C	-4.313455	-1.751388	0.413554	C	-4.329706	-1.486326	-0.335341	C	4.316566	0.063232	-1.352306
C	-3.283116	-1.763638	0.506028	C	-3.192248	-1.480186	1.207324	C	-3.424457	-1.444202	0.732381	C	3.409048	1.073571	-1.011002
C	-2.419701	-0.687915	0.608654	C	-2.367748	-0.448464	0.794714	C	-2.403773	-0.513128	0.652308	C	2.401286	0.737746	-0.123864
C	-2.642414	0.501262	-0.082204	C	-2.636802	0.292083	-0.355443	C	-2.279959	0.346658	-0.437463	C	2.291627	-0.544709	0.409941
C	-3.738098	0.671225	-0.909465	C	-3.743321	0.035814	-1.145653	C	-3.170024	0.318205	-1.496219	C	3.183188	-1.550851	0.082476
C	-4.619770	-0.411180	-1.022070	C	-4.583496	-1.008234	-0.739805	C	-4.204787	-0.623024	-1.428086	C	4.205255	-1.223892	-0.817304
C	-1.156101	-0.544293	1.376774	C	-1.108382	0.060338	1.394768	C	-1.289753	-0.237505	1.592506	C	1.288066	1.561335	0.409235
N	-0.685503	0.757009	1.114301	N	-0.676449	1.107682	0.552869	N	-0.538711	0.815932	1.012339	N	0.555552	0.718192	1.276665
C	-1.518714	1.423361	0.220836	C	-1.551274	1.290150	-0.526697	C	-1.098640	1.213283	-0.216504	C	1.120174	-0.576521	1.319395
C	0.611751	1.226393	1.518651	C	0.603257	1.715853	0.643613	C	0.692524	1.228010	1.511718	C	-0.655026	1.094048	1.844665
S	1.841706	1.345152	0.145429	S	1.784584	1.272471	-0.684036	S	2.139550	1.155980	0.531334	S	-2.105710	0.153003	1.595718
P	2.031635	-0.664665	-0.429283	P	2.108421	-0.754180	-0.228309	P	1.892847	-0.739055	-0.410562	P	-1.960887	-0.241628	-0.493488
O	0.562641	-1.189665	-0.800377	O	0.671565	-1.464170	-0.251264	O	0.636611	-0.587684	-1.392436	O	-0.696531	-1.206365	-0.682394
C	-0.033412	-0.841051	-2.069027	C	0.038088	-1.780967	-1.510143	C	0.791217	0.077472	-2.664922	C	-0.817509	-2.617962	-0.403594
O	-1.316083	2.544405	-0.213519	O	-1.391928	2.126059	-1.393999	O	-0.673307	2.121170	-0.902144	O	0.704845	-1.482519	2.007238
O	-0.606778	-1.336460	2.109949	O	-0.528704	-0.296449	2.395442	O	-1.013791	-0.765546	2.645640	O	1.002126	2.716514	0.182899
S	3.412847	-0.846195	-1.771022	S	3.490285	-1.478622	-1.369566	S	3.560945	-1.341528	-1.176088	S	-3.657094	-0.844589	-1.195830
O	2.168916	-1.503364	0.925896	O	2.303153	-0.827150	1.356766	O	1.142569	-1.648339	0.668520	O	-1.263216	1.056562	-1.112942
C	3.353108	-1.370979	1.740199	C	3.487457	-0.270080	1.966218	C	1.820792	-2.068249	1.872310	C	-1.959991	2.320649	-1.140840
H	0.543902	2.243801	1.908815	H	0.499119	2.881222	0.518590	H	0.391549	4.147126	1.452051	H	-0.748423	2.122669	2.169643
H	0.988980	0.560229	2.295983	H	1.024869	1.550360	1.636828	H	0.795395	1.286130	2.588125	H	3.090824	-2.547787	0.501077
H	-3.904448	1.598353	-1.448084	H	-3.946745	0.613609	-2.041204	H	-3.067438	0.991696	-2.340883	H	3.490425	2.073895	-1.423234
H	-3.102901	-2.688797	1.043618	H	-2.976086	-2.054540	2.102175	H	-3.516786	-2.111884	1.582614	H	4.924792	-1.982854	-1.105970
H	-5.491976	-0.324197	-1.661458	H	-5.460595	-1.247719	-1.331838	H	-4.923594	-0.684859	-2.238473	H	5.121659	0.281876	-2.045911
H	-5.099275	-2.423504	-0.441978	H	-4.985331	-2.554818	0.696629	H	-5.144278	-2.202801	-0.315449	H	-2.119451	2.684409	-0.122383
H	4.232052	-1.689103	1.175823	H	4.373127	-0.803235	1.614880	H	2.033401	-1.202135	2.504646	H	-2.912578	2.211981	-1.663641
H	3.467804	-0.336938	2.075657	H	3.566323	0.795731	1.735901	H	2.743058	-2.595101	1.618296	H	-1.308288	3.002844	-1.683291
H	3.195824	-2.025725	2.595042	H	3.360133	-0.412612	3.037468	H	1.130383	-2.740148	2.378379	H	0.195507	-3.014651	-0.458434
H	-1.026744	-1.288750	-2.059300	H	-0.911198	-2.248675	-1.251129	H	-0.216295	0.177862	-3.066641	H	-1.452232	-3.087024	-1.157197
H	-0.111789	0.246707	-2.164928	H	-0.137750	-0.865825	-2.084660	H	1.238959	1.065240	-2.527307	H	-1.226817	-2.776288	0.597589
H	0.560468	-1.254033	-2.886385	H	0.660730	-2.475018	-2.077637	H	1.406480	-0.535059	-3.326005				
O	1.052783	4.087894	-0.147233	O	0.229417	4.184502	0.094512	O	0.473907	4.409776	0.525567				
H	0.165590	3.655787	-0.139695	H	-0.416162	3.967010	-0.610190	H	0.150992	3.644852	0.021437				

Table S46. Optimized Cartesian coordinates for the stationary points involved in the H21-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

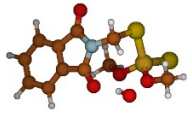
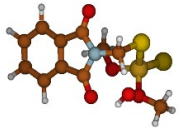
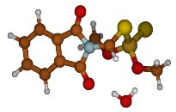
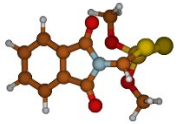
MCR(H21-abs)				TS(H21-abs)				MCP(H21-abs)				Rad(H21-abs)			
															
C	4.434236	0.339802	-1.580995	C	4.313958	-0.617329	-1.549990	C	4.748595	0.321478	-1.320137	C	4.316404	0.063014	-1.352405
C	3.234682	1.046400	-1.427072	C	3.142035	0.109711	-1.792140	C	3.594450	1.104160	-1.193544	C	3.408969	1.073436	-1.011138
C	2.436958	0.697014	-0.352335	C	2.360152	0.419503	-0.693555	C	2.654461	0.687784	-0.267308	C	2.401213	0.737735	-0.123927
C	2.804010	-0.307692	0.540598	C	2.717028	0.031276	0.595216	C	2.841034	-0.456055	0.506505	C	2.291479	-0.544654	0.409984
C	3.986357	-1.011570	0.400160	C	3.872713	-0.686425	0.848009	C	3.977629	-1.236374	0.391482	C	3.182968	-1.550871	0.082581
C	4.802441	-0.668748	-0.685537	C	4.672365	-1.007303	-0.255724	C	4.936346	-0.825716	-0.543165	C	4.205008	-1.224059	-0.817286
C	1.116951	1.231938	0.070168	C	1.061637	1.136699	-0.624447	C	1.339717	1.276243	0.080869	C	1.288128	1.561484	0.409121
N	0.759302	0.529150	1.222645	N	0.702215	1.161898	0.735100	N	0.791691	0.455253	1.088878	N	0.555535	0.718399	1.276739
C	1.723146	-0.434921	1.552766	C	1.650447	0.484048	1.523035	C	1.656556	-0.626403	1.383815	C	1.120071	-0.576285	1.319538
C	-0.520801	0.606835	1.871251	C	-0.565191	1.553592	1.265381	C	-0.490322	0.623603	1.596463	C	-0.655154	1.094375	1.844412
S	-1.607493	-0.851444	1.563928	S	-1.747040	0.219240	1.634603	S	-1.628144	-0.708620	1.591408	S	-2.105572	0.152897	1.595770
P	-2.056945	-0.610874	-0.465115	P	-1.972002	-0.787370	-0.202658	P	-2.200558	-0.603592	-0.453684	P	-1.960787	-0.241700	-0.493447
O	-0.657982	-0.543097	-1.245723	O	-0.501220	-1.173933	-0.703769	O	-0.823467	-0.486231	-1.262124	O	-0.696426	-1.206454	-0.682383
C	0.111724	-1.747382	-1.449440	C	0.191915	-2.306724	-0.132078	C	-0.023002	-1.662952	-1.505580	C	-0.817409	-2.618058	-0.403487
O	1.626758	-1.195065	2.493646	O	1.543378	0.320627	2.719861	O	1.424875	-1.477326	2.212660	O	0.704830	-1.482219	2.007547
O	0.461241	2.116396	-0.446778	O	0.422257	1.634468	-1.527050	O	0.786844	2.250391	-0.385248	O	1.002193	2.716621	0.182744
S	-3.327665	-1.955933	-1.033909	S	-3.259929	-2.212500	0.007411	S	-3.419798	-2.033478	-0.909018	S	-3.657022	-0.844595	-1.195899
O	-2.443442	0.930223	-0.675427	O	-2.249937	0.337938	-1.300720	O	-2.668364	0.904928	-0.709892	O	-1.263089	1.056533	-1.112805
C	-3.684696	1.430336	-0.129673	C	-3.554528	0.953275	-1.384853	C	-3.888228	1.389316	-0.109311	C	-1.960008	2.320527	-1.140983
H	-0.388219	0.623225	2.954513	H	-0.437024	2.096465	2.204604	H	-0.837855	1.641879	1.722518	H	-0.748668	2.123097	2.169031
H	-1.024823	1.520922	1.556611	H	-1.078517	2.328409	0.537931	H	-2.150055	3.420667	0.790547	H	3.090553	-2.547776	0.501246
H	4.266928	-1.794546	1.096864	H	4.143535	-0.989466	1.854053	H	4.117034	-2.127113	0.995065	H	3.490385	2.073735	-1.423420
H	2.942354	1.828669	-2.119809	H	2.856352	0.410981	-2.794618	H	3.442322	1.995129	-1.793672	H	4.924459	-1.983113	-1.105931
H	5.738511	-1.196260	-0.836240	H	5.586843	-1.571509	-0.105482	H	5.842323	-1.409252	-0.668744	H	5.121494	0.281534	-2.046052
H	5.090417	0.577830	-2.411569	H	4.955878	-0.886330	-2.382272	H	5.512538	0.609709	-2.034467	H	-2.121100	2.683681	-0.122562
H	-4.505964	0.751753	-0.371348	H	-4.286375	0.216411	-1.720464	H	-3.753954	1.494118	0.970675	H	-2.911781	2.211985	-1.665286
H	-3.591956	1.549920	0.952714	H	-3.843962	1.368703	-0.416351	H	-4.714189	0.708947	-0.327984	H	-1.307595	3.003157	-1.682038
H	-3.851720	2.395372	-0.605393	H	-3.455482	1.751079	-2.118327	H	-4.075615	2.361147	-0.561940	H	0.195557	-3.014821	-0.458707
H	1.012768	-1.435477	-1.976361	H	1.156144	-2.344603	-0.638020	H	0.919229	-1.297698	-1.912399	H	-1.452474	-3.087073	-1.156828
H	0.375486	-2.195946	-0.486294	H	0.335170	-2.159614	0.943151	H	0.156090	-2.208441	-0.573367	H	-1.226339	-2.776296	0.597864
H	-0.455272	-2.455724	-2.056465	H	-0.371516	-3.221950	-0.321364	H	-0.525211	-2.308213	-2.228379				
O	-1.819256	3.701491	0.062643	O	-1.566931	3.285368	-0.324414	O	-1.584961	3.821136	0.117264				
H	-1.115529	3.035739	-0.125561	H	-1.140599	2.913230	-1.125294	H	-0.861896	3.186095	-0.014791				

Table S47. Optimized Cartesian coordinates for the stationary points involved in the H22-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

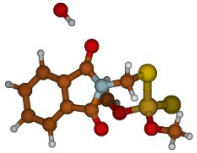
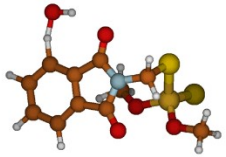
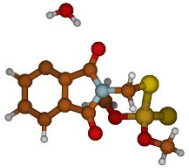
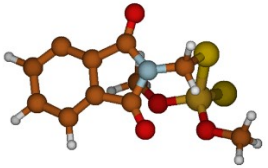
MCR(H22-abs)				TS(H22-abs)				MCP(H22-abs)				Rad(H22-abs)			
															
C	3.799869	-2.210205	0.838986	C	-3.826549	1.996755	0.914990	C	3.765870	-2.254687	0.815911	C	-4.294299	-1.552165	0.423906
C	2.625188	-2.422241	0.106383	C	-2.654735	2.292217	0.205986	C	2.588426	-2.433647	0.075843	C	-3.175585	-1.223610	1.202270
C	1.990510	-1.301467	-0.397266	C	-1.978585	1.233541	-0.373755	C	1.961770	-1.303273	-0.416048	C	-2.369852	-0.188751	0.763281
C	2.491155	-0.016563	-0.192181	C	-2.440572	-0.077089	-0.264180	C	2.469696	-0.017611	-0.197360	C	-2.643772	0.521486	-0.411373
C	3.652386	0.204677	0.527366	C	-3.592692	-0.351545	0.432835	C	3.622491	0.111902	0.527013	C	-3.746637	0.169039	-1.139224
C	4.303541	-0.922511	1.044136	C	-4.301388	0.683568	1.034246	C	4.295574	-0.976682	1.048804	C	-4.590994	-0.856116	-0.757642
C	0.731155	-1.188999	-1.178218	C	-0.705890	1.200353	-1.145678	C	0.701278	-1.164769	-1.195676	C	-1.115527	0.363666	1.344380
N	0.543141	0.184713	-1.415117	N	-0.481617	-0.149921	-1.472932	N	0.525307	0.213276	-1.410946	N	-0.707053	1.393568	0.483879
C	1.551424	0.942989	-0.827939	C	-1.475541	-0.973542	-0.950915	C	1.538728	0.960968	-0.817577	C	-1.567664	1.529520	-0.608447
C	-0.674116	0.746309	-1.933400	C	0.760981	-0.646044	-1.999419	C	-0.689135	0.791768	-1.919163	C	0.578292	2.032218	0.559485
S	-1.713977	1.581200	-0.657192	S	1.791384	-1.541561	-0.757453	S	-1.719911	1.613428	-0.627795	S	1.768498	1.479293	-0.739200
P	-2.288696	-0.041031	0.535756	P	2.292291	0.006696	0.561128	P	-2.307803	-0.024964	0.537374	P	2.081533	-0.519640	-0.200212
O	-0.939070	-0.732648	1.061481	O	0.912099	0.626680	1.097067	O	-0.963261	-0.735235	1.051218	O	0.644749	-1.235058	-0.207813
C	-0.188328	-0.127370	2.136237	C	0.156898	-0.061640	2.117702	C	-0.207777	-0.153290	2.135635	C	0.021581	-1.589150	-1.461249
O	1.585456	2.161182	-0.857724	O	-1.498510	-2.185560	-1.051847	O	1.588583	2.176571	-0.828447	O	-1.409559	2.323661	-1.512283
O	-0.008629	-2.062089	-1.575707	O	0.016082	2.116086	-1.471077	O	-0.044352	-2.026504	-1.604532	O	-0.538190	0.041138	2.359767
S	-3.575797	0.524319	1.865769	S	3.559877	-0.617651	1.883439	S	-3.591014	0.527316	1.876224	S	3.470056	-1.300239	-1.299419
O	-2.697961	-1.220495	-0.465158	O	2.693982	1.262282	-0.345535	O	-2.725172	-1.183482	-0.484332	O	2.266341	-0.541683	1.388808
C	-3.901376	-1.110466	-1.254063	C	3.910037	1.230766	-1.121825	C	-3.928757	-1.051912	-1.269808	C	3.455314	0.019568	1.983487
H	-0.452769	1.530375	-2.659324	H	0.574951	-1.383052	-2.782305	H	-0.462173	1.584970	-2.633303	H	0.478104	3.106613	0.396012
H	-1.242527	-0.049783	-2.416528	H	1.319810	0.194204	-2.413780	H	-1.263381	0.007032	-2.413804	H	0.996713	1.849914	1.550201
H	4.043531	1.204161	0.689987	H	-3.963019	-1.520343	0.519796	H	4.633939	2.754246	0.225627	H	-2.946080	-1.766401	2.113245
H	2.227189	-3.418907	-0.053955	H	-2.288829	3.310214	0.122539	H	2.179903	-3.423478	-0.098548	H	-5.461415	-1.125878	-1.347449
H	5.215649	-0.793959	1.617381	H	-5.209545	0.483172	1.592665	H	5.207538	-0.859099	1.625476	H	-4.946077	-2.361974	0.735497
H	4.328585	-3.060099	1.257617	H	-4.381938	2.799375	1.388986	H	4.280748	-3.119557	1.221550	H	4.333793	-0.544424	1.663502
H	-4.775319	-1.098844	-0.599748	H	4.774857	1.175029	-0.457726	H	-4.801989	-1.049335	-0.614495	H	3.556406	1.072796	1.708311
H	-3.871995	-0.206351	-1.868055	H	3.900075	0.379871	-1.808232	H	-3.895649	-0.135826	-1.865581	H	3.317419	-0.073794	3.058925
H	-3.917026	-1.993204	-1.890358	H	3.924162	2.162828	-1.683280	H	-3.949015	-1.921620	-1.923688	H	-0.932253	-2.045144	-1.197503
H	0.675860	-0.772640	2.291366	H	-0.730539	0.547318	2.288340	H	0.652410	-0.806677	2.278701	H	-0.145282	-0.692415	-2.066832
H	0.139499	0.877395	1.850922	H	-0.132538	-1.058070	1.768518	H	0.126058	0.854087	1.866915	H	0.646335	-2.303241	-2.001033
H	-0.797732	-0.086531	3.040948	H	0.747323	-0.135305	3.032792	H	-0.816067	-0.124172	3.041533				
O	3.611012	3.701343	0.351773	O	-4.010434	-2.782042	0.432627	O	3.916668	3.372644	0.417907				
H	2.897008	3.159359	-0.065573	H	-3.185529	-2.922461	-0.080276	H	3.133668	2.984492	-0.009177				

Table S48. Optimized Cartesian coordinates for the stationary points involved in the H23-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

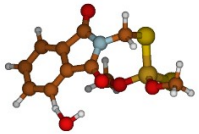
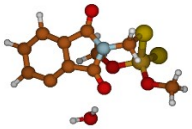
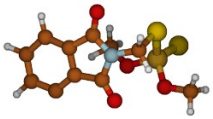
MCR(H23-abs)				TS(H23-abs)				MCP(H23-abs)				Rad(H23-abs)			
															
C	-4.154969	1.332251	0.555632	C	-4.168340	0.780438	0.998615	C	-4.208147	1.334850	0.527134	C	-4.292113	-1.535000	0.721780
C	-3.062297	1.501222	-0.304024	C	-3.109339	1.225940	0.214224	C	-3.102024	1.435787	-0.294876	C	-3.166051	-1.088220	1.386462
C	-2.275717	0.387786	-0.542185	C	-2.235275	0.318756	-0.334812	C	-2.283338	0.371893	-0.555227	C	-2.341073	-0.127768	0.869462
C	-2.556555	-0.849021	0.035249	C	-2.404691	-1.047008	-0.112683	C	-2.585321	-0.862177	0.031161	C	-2.660112	0.419854	-0.378424
C	-3.635789	-1.029507	0.881508	C	-3.447098	-1.532420	0.657095	C	-3.680661	-1.031710	0.858541	C	-3.773831	0.019128	-1.094082
C	-4.435907	0.091697	1.136127	C	-4.328812	-0.595432	1.211711	C	-4.492100	0.086011	1.100473	C	-4.589721	-0.970163	-0.527598
C	-1.034532	0.248981	-1.344029	C	-1.012673	0.517440	-1.154120	C	-1.031975	0.225394	-1.340977	C	-1.080379	0.497328	1.350000
N	-0.636177	-1.085106	-1.231781	N	-0.503303	-0.760538	-1.402927	N	-0.639306	-1.108112	-1.198356	N	-0.704365	1.411706	0.355093
C	-1.496055	-1.801936	-0.386523	C	-1.278582	-1.752100	-0.785633	C	-1.512941	-1.817435	-0.363412	C	-1.595148	1.402666	-0.721941
C	0.666342	-1.559146	-1.614302	C	0.815064	-1.004826	-1.922812	C	0.662135	-1.595747	-1.568778	C	0.573452	2.068092	0.317231
S	1.819336	-1.800961	-0.191796	S	2.030687	-1.537999	-0.639853	S	1.807040	-1.817801	-0.137842	S	1.738162	1.370526	-0.933746
P	2.070998	0.158966	0.503353	P	2.175551	0.183605	0.544971	P	2.088650	0.159316	0.495729	P	2.099429	-0.535954	-0.147558
O	0.612926	0.725406	0.858864	O	0.695567	0.518400	1.069340	O	0.638714	0.756501	0.833821	O	0.674909	-1.263350	-0.016019
C	-0.037735	0.355600	2.093590	C	0.124184	-0.236486	2.160002	C	-0.021465	0.420352	2.072831	C	0.019804	-1.790111	-1.189801
O	-1.336968	-2.966479	-0.085459	O	-1.020391	-2.936590	-0.817283	O	-1.360413	-2.978017	-0.046760	O	-1.468085	2.079537	-1.721492
O	-0.444870	1.091539	-1.995343	O	-0.532602	1.555391	-1.562089	O	-0.441160	1.056325	-2.001244	O	-0.476809	0.309485	2.383403
S	3.407662	0.203316	1.902291	S	3.562729	-0.033210	1.876388	S	3.427237	0.229027	1.891457	S	3.469780	-1.440301	-1.172108
O	2.292098	1.077718	-0.788623	O	2.275332	1.421258	-0.464104	O	2.320184	1.032686	-0.825123	O	2.329237	-0.343807	1.424598
C	3.504668	0.950076	-1.560402	C	3.465130	1.607115	-1.259537	C	3.531111	0.866786	-1.592289	C	3.513810	0.328914	1.900147
H	0.591494	-2.546331	-2.072629	H	0.794172	-1.828091	-2.638766	H	0.581280	-2.590075	-2.010351	H	0.453904	3.112394	0.023739
H	1.096099	-0.855426	-2.328126	H	1.165599	-0.097940	-2.417134	H	1.097767	-0.907187	-2.293737	H	1.019128	2.016214	1.311453
H	-3.847589	-1.992789	1.333919	H	-3.572899	-2.595755	0.832446	H	-3.899732	-1.992511	1.312298	H	-4.005556	0.451454	-2.061809
H	-2.839569	2.462442	-0.758487	H	-2.920074	2.423135	0.008261	H	-1.433639	3.795880	-0.388116	H	-5.470036	-1.311143	-1.062918
H	-5.289533	-0.002060	1.799251	H	-5.155551	-0.937160	1.825896	H	-5.356689	-0.009650	1.749361	H	-4.935121	-2.301533	1.142721
H	-4.794914	2.179754	0.777657	H	-4.862916	1.483775	1.445326	H	-4.844547	2.189484	0.733785	H	4.404164	-0.232334	1.609389
H	4.367087	1.222384	-0.948563	H	4.317634	1.817578	-0.610728	H	4.396356	1.152332	-0.990596	H	3.557000	1.346233	1.502163
H	3.609928	-0.071481	-1.935019	H	3.658053	0.719011	-1.867275	H	3.626756	-0.168220	-1.930914	H	3.421293	0.355684	2.984083
H	3.397965	1.643721	-2.392126	H	3.258415	2.461160	-1.901512	H	3.430328	1.531743	-2.447804	H	-0.922949	-2.208074	-0.838176
H	-0.997479	0.872572	2.085712	H	-0.875084	0.172026	2.309430	H	-0.966572	0.963280	2.058255	H	-0.169912	-0.987889	-1.909971
H	-0.193390	-0.727384	2.129437	H	0.061434	-1.296633	1.894273	H	-0.206728	-0.657471	2.121558	H	0.634351	-2.570479	-1.642546
H	0.561990	0.683585	2.944561	H	0.725764	-0.104313	3.061181	H	0.586605	0.742283	2.920263				
O	-0.427975	3.498807	-0.438804	O	-2.425165	3.521185	-0.379940	O	-0.502722	3.551627	-0.475726				
H	-0.356231	2.720554	-1.040197	H	-1.658667	3.166614	-0.879730	H	-0.502696	2.780595	-1.066522				

Table S49. Optimized Cartesian coordinates for the stationary points involved in the H24-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

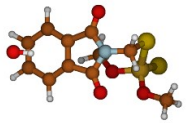
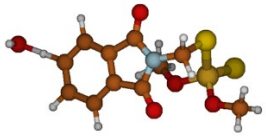
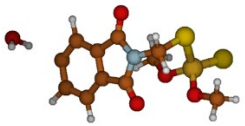
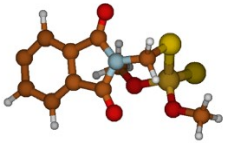
MCR(H24-abs)				TS(H24-abs)				MCP(H24-abs)				Rad(H24-abs)			
															
C	3.891559	1.614540	0.656737	C	3.933767	0.658608	1.417472	C	3.896756	0.226976	1.574187	C	-4.286264	-1.662309	0.236444
C	2.836199	1.023723	1.365402	C	2.723404	0.123863	1.881990	C	2.661111	-0.349757	1.913299	C	-3.172001	-1.415712	1.056450
C	2.054744	0.112769	0.678768	C	1.908274	-0.490570	0.947488	C	1.845334	-0.752059	0.868080	C	-2.382040	-0.323339	0.735628
C	2.297408	-0.207089	-0.656821	C	2.258722	-0.584074	-0.397788	C	2.213482	-0.602479	-0.468895	C	-2.663244	0.509822	-0.346688
C	3.332932	0.370129	-1.368393	C	3.448765	-0.065923	-0.883021	C	3.427320	-0.038763	-0.839649	C	-3.756581	0.296512	-1.176317
C	4.135619	1.293231	-0.683647	C	4.252710	0.554780	0.068844	C	4.206281	0.347295	0.234994	C	-4.512894	-0.804173	-0.819921
C	0.858253	-0.647230	1.126943	C	0.572550	-1.122546	1.121135	C	0.489324	-1.359751	0.906668	C	-1.137420	0.167584	1.382907
N	0.445610	-1.408995	0.022823	N	0.191160	-1.581471	-0.148959	N	0.112173	-1.559395	-0.431078	N	-0.738561	1.300202	0.654555
C	1.253145	-1.171787	-1.093454	C	1.149107	-1.268855	-1.116613	C	1.093040	-1.103501	-1.313688	C	-1.599350	1.550086	-0.416161
C	-0.810648	-2.101741	-0.046112	C	-1.129188	-2.051318	-0.465871	C	-1.216548	-1.918972	-0.842169	C	0.540163	1.937799	0.805034
S	-2.077188	-1.255247	-1.090542	S	-2.147144	-0.838491	-1.415156	S	-2.183847	-0.519009	-1.559350	S	1.726976	1.565224	-0.559395
P	-2.422525	0.494945	0.005119	P	-2.404706	0.684895	-0.001615	P	-2.409020	0.726649	0.108428	P	2.078613	-0.476076	-0.256023
O	-1.010033	1.242026	0.156144	O	-0.939431	1.165880	0.442234	O	-0.933081	1.079422	0.630466	O	0.654241	-1.212584	-0.323890
C	-0.455163	1.974858	-0.957261	C	-0.164114	2.019367	-0.426628	C	-0.129524	2.052154	-0.071119	C	0.021760	-1.450468	-1.599647
O	1.076672	-1.677666	-2.183805	O	1.038555	-1.522132	-2.298766	O	0.993498	-1.126848	-2.523488	O	-1.453207	2.447844	-1.220305
O	0.321519	-0.659565	2.214313	O	-0.082641	-1.259445	2.131396	O	-0.187063	-1.662689	1.865939	O	-0.555333	-0.268049	2.352977
S	-3.879528	1.500470	-0.777989	S	-3.613847	2.035595	-0.679823	S	-3.581788	2.208266	-0.310572	S	3.462855	-1.107193	-1.452475
O	-2.539445	0.056177	1.539761	O	-2.766516	-0.034842	1.381469	O	-2.793426	-0.221851	1.338356	O	2.287439	-0.671724	1.318796
C	-3.679079	-0.708611	1.985186	C	-4.034995	-0.705945	1.531965	C	-4.080192	-0.873839	1.371186	C	3.471029	-0.148659	1.957347
H	-0.680895	-3.077817	-0.516590	H	-1.075352	-2.926932	-1.114916	H	-1.177737	-2.660032	-1.642499	H	0.428589	3.022982	0.779844
H	-1.191181	-2.233058	0.967522	H	-1.634319	-2.316221	0.464002	H	-1.744176	-2.336030	0.016846	H	0.967086	1.636078	1.762430
H	3.514887	0.121998	-2.408909	H	3.728041	-0.133761	-1.929349	H	3.724036	0.085833	-1.876397	H	-3.981913	0.936197	-2.023875
H	2.639908	1.271745	2.403356	H	2.440045	0.193057	2.927190	H	2.358828	-0.469007	2.948936	H	-2.939382	-2.057245	1.900530
H	4.960342	1.771417	-1.201675	H	5.287722	1.047349	-0.301141	H	6.335441	2.149482	-0.170656	H	-4.940993	-2.505200	0.433992
H	4.531555	2.335966	1.153952	H	4.613234	1.152997	2.103798	H	4.579237	0.566553	2.346927	H	4.359141	-0.644378	1.560145
H	-4.592526	-0.123461	1.861139	H	-4.851878	0.011286	1.428736	H	-4.875642	-0.127650	1.423398	H	3.537324	0.932031	1.805958
H	-3.747802	-1.646588	1.427796	H	-4.131418	-1.503727	0.790755	H	-4.207336	-1.506467	0.488651	H	3.356050	-0.370984	3.016435
H	-3.501750	-0.913144	3.039220	H	-4.027139	-1.127233	2.535280	H	-4.076616	-1.485585	2.271185	H	-0.917240	-1.954795	-1.373212
H	0.500223	2.364253	-0.606405	H	0.777828	2.191015	0.093515	H	0.813236	2.102196	0.472785	H	-0.174487	-0.500603	-2.107338
H	-0.298088	1.306998	-1.810310	H	0.020341	1.518650	-1.382539	H	0.047723	1.725399	-1.100824	H	0.655199	-2.089598	-2.217630
H	-1.120087	2.795464	-1.232849	H	-0.686470	2.964479	-0.585787	H	-0.625016	3.024790	-0.060166				
O	5.699363	-0.666849	0.741545	O	6.500388	1.359585	-0.657449	O	7.061615	1.611328	-0.513477				
H	4.837054	-1.128270	0.795970	H	6.930840	0.495555	-0.507885	H	6.877600	0.719745	-0.188087				

Table S50. Optimized Cartesian coordinates for the stationary points involved in the H25-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

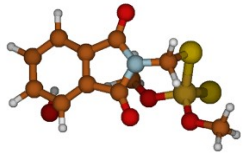
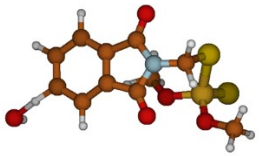
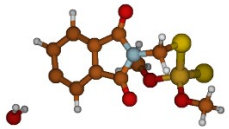
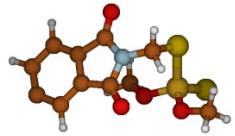
MCR(H25-abs)				TS(H25-abs)				MCP(H25-abs)				Rad(H25-abs)			
															
C	-4.352785	-0.800457	0.648770	C	-4.117822	-0.681078	0.093619	C	-4.125380	-0.466347	-0.148715	C	-4.204017	-1.559981	0.624596
C	-3.163499	-0.616436	1.369099	C	-3.018120	-0.753571	0.943953	C	-3.075468	-0.744279	0.706385	C	-3.119593	-1.203616	1.404092
C	-2.224125	0.238644	0.820025	C	-2.043094	0.206188	0.724880	C	-2.048733	0.188749	0.642831	C	-2.349743	-0.188305	0.851357
C	-2.443575	0.889452	-0.392075	C	-2.163342	1.164627	-0.279206	C	-2.102357	1.290108	-0.211005	C	-2.667036	0.398026	-0.373389
C	-3.608530	0.709125	-1.117513	C	-3.262613	1.219857	-1.118230	C	-3.177907	1.527303	-1.051897	C	-3.767632	0.008499	-1.119793
C	-4.568123	-0.152973	-0.573424	C	-4.264148	0.258557	-0.919759	C	-4.234635	0.601906	-1.014875	C	-4.567967	-1.018483	-0.591079
C	-0.891060	0.652581	1.333425	C	-0.735662	0.407493	1.406857	C	-0.754511	0.233831	1.378979	C	-1.099702	0.441980	1.358905
N	-0.383689	1.568384	0.399921	N	-0.132656	1.502665	0.770704	N	-0.094726	1.385866	0.930012	N	-0.733262	1.399480	0.402524
C	-1.255008	1.738105	-0.678732	C	-0.926761	1.992712	-0.270097	C	-0.838473	2.056003	-0.046530	C	-1.620534	1.408815	-0.679298
C	0.948454	2.103752	0.439180	C	1.241286	1.878718	0.958104	C	1.279421	1.687187	1.221802	C	0.539263	2.066135	0.388126
S	2.083043	1.404355	-0.836362	S	2.346156	1.391832	-0.438943	S	2.428199	1.385101	-0.190990	S	1.710893	1.420174	-0.885177
P	2.279123	-0.567392	-0.163109	P	2.296199	-0.696754	-0.301063	P	2.338814	-0.700054	-0.356078	P	2.076972	-0.514678	-0.174461
O	0.796707	-1.176283	-0.090091	O	0.757949	-1.137138	-0.429103	O	0.798833	-1.083572	-0.594219	O	0.654939	-1.252113	-0.073033
C	0.106965	-1.537552	-1.305053	C	0.110918	-1.139110	-1.719750	C	0.195640	-0.879148	-1.889755	C	0.007877	-1.744428	-1.266006
O	-1.029934	2.454643	-1.633644	O	-0.608865	2.909864	-0.999283	O	-0.465643	3.060167	-0.618440	O	-1.499379	2.121198	-1.655196
O	-0.325409	0.320614	2.353598	O	-0.255908	-0.204830	2.336016	O	-0.326216	-0.529577	2.217194	O	-0.497811	0.223266	2.387873
S	3.582639	-1.522250	-1.228604	S	3.551085	-1.485822	-1.545408	S	3.624112	-1.326592	-1.660638	S	3.450032	-1.372956	-1.234778
O	2.500893	-0.489255	1.420060	O	2.439318	-1.053478	1.252332	O	2.422298	-1.279477	1.133195	O	2.305070	-0.385374	1.404312
C	3.744250	0.017225	1.949044	C	3.686161	-0.808064	1.936072	C	3.655652	-1.180210	1.875661	C	3.485395	0.273631	1.908721
H	0.931667	3.174515	0.228607	H	1.333875	2.964708	1.011151	H	1.395519	2.749210	1.444363	H	0.413683	3.119163	0.130770
H	1.359991	1.933532	1.435046	H	1.599054	1.435705	1.888371	H	1.588023	1.096802	2.085635	H	0.984517	1.982846	1.380406
H	-3.772664	1.217642	-2.061925	H	-3.344528	1.966075	-1.901874	H	-3.203470	2.387198	-1.713769	H	-4.000924	0.471209	-2.073563
H	-2.989943	-1.119313	2.314983	H	-2.925952	-1.508455	1.718045	H	-3.045171	-1.606953	1.364766	H	-2.878198	-1.669991	2.354183
H	-5.498183	-0.321989	-1.106033	H	-5.145125	0.247356	-1.552963	H	-5.104640	0.730270	-1.651102	H	-5.441857	-1.370126	-1.130475
H	-5.122202	-1.453630	1.047061	H	-5.001621	-1.486133	0.243682	H	-6.253306	-1.906118	0.611685	H	4.378837	-0.273373	1.600739
H	4.569282	-0.632270	1.649713	H	4.481327	-1.408930	1.490096	H	4.438836	-1.754411	1.376568	H	3.526399	1.305144	1.549075
H	3.916462	1.038917	1.600312	H	3.939854	0.254414	1.891228	H	3.954723	-0.133487	1.975574	H	3.388888	0.259801	2.992561
H	3.628638	0.006836	3.031052	H	3.519203	-1.108837	2.968491	H	3.443314	-1.603159	2.855629	H	-0.936716	-2.173689	-0.933096
H	-0.881890	-1.869854	-0.992660	H	-0.914334	-1.458680	-1.534777	H	-0.840155	-1.201078	-1.786723	H	-0.177930	-0.921617	-1.963697
H	0.020346	-0.669356	-1.966227	H	0.118505	-0.131829	-2.148335	H	0.234541	0.180472	-2.162078	H	0.626318	-2.510493	-1.737422
H	0.637482	-2.347751	-1.809113	H	0.611627	-1.841915	-2.388290	H	0.707235	-1.484961	-2.640075				
O	-3.148103	-3.150269	-0.132756	O	-5.810575	-2.503857	0.226626	O	-6.359317	-2.762598	0.175921				
H	-3.061952	-2.663240	-0.978002	H	-5.358295	-3.049453	-0.445564	H	-5.770677	-2.720332	-0.589763				

Table S51. Optimized Cartesian coordinates for the stationary points involved in the H26-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

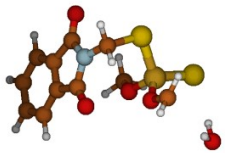
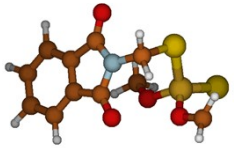
MCR(H26-abs)				TS(H26-abs)				MCP(H26-abs)				Rad(H26-abs)			
															
C	-4.201053	-1.967044	-0.167025	C	-4.351515	-1.952059	-0.147216	C	-4.192766	-2.111225	-0.101701	C	-4.229248	-1.560109	0.430254
C	-3.082058	-1.847336	0.666499	C	-3.214831	-1.873241	0.667065	C	-3.090269	-1.920687	0.740448	C	-3.115936	-1.250462	1.221411
C	-2.429509	-0.627436	0.667457	C	-2.534035	-0.668920	0.677201	C	-2.476480	-0.681543	0.697923	C	-2.310328	-0.211876	0.789778
C	-2.861607	0.437790	-0.120126	C	-2.955718	0.420049	-0.083180	C	-2.930653	0.335607	-0.139323	C	-2.589356	0.499261	-0.375731
C	-3.966922	0.332764	-0.945737	C	-4.077702	0.355116	-0.890205	C	-4.019867	0.160101	-0.974425	C	-3.687028	0.204225	-1.164561
C	-4.634875	-0.898070	-0.957256	C	-4.774364	-0.859584	-0.910766	C	-4.648449	-1.090909	-0.942268	C	-4.509327	-0.846657	-0.739216
C	-1.211564	-0.196388	1.402317	C	-1.295885	-0.277559	1.400202	C	-1.281474	-0.183266	1.426990	C	-1.059705	0.334873	1.378053
N	-0.981636	1.136623	1.025534	N	-1.046641	1.058975	1.048618	N	-1.088043	1.139931	0.997553	N	-0.653739	1.376191	0.528287
C	-1.924855	1.573266	0.090069	C	-1.993501	1.532419	0.134549	C	-2.032103	1.507555	0.032639	C	-1.517101	1.512119	-0.563507
C	0.229927	1.849349	1.316246	C	0.178338	1.744921	1.343927	C	0.096555	1.899993	1.272526	C	0.624950	2.021239	0.611994
S	1.367025	2.016294	-0.131808	S	1.311360	1.920766	-0.106933	S	1.249934	2.040789	-0.166777	S	1.827091	1.487455	-0.687529
P	1.927100	0.028148	-0.444706	P	1.821216	-0.066903	-0.485850	P	1.834494	0.057977	-0.434854	P	2.124679	-0.521369	-0.201073
O	0.587829	-0.820292	-0.682533	O	0.465824	-0.882375	-0.724909	O	0.518794	-0.823228	-0.656887	O	0.693017	-1.239024	-0.209183
C	-0.092401	-0.761218	-1.955855	C	-0.226969	-0.789304	-1.990854	C	-0.145806	-0.829152	-1.941711	C	0.068818	-1.593635	-1.463638
O	-1.917194	2.674114	-0.423615	O	-1.970829	2.642659	-0.357732	O	-2.049258	2.584797	-0.528220	O	-1.359952	2.313901	-1.462440
O	-0.530549	-0.816962	2.190673	O	-0.613228	-0.927980	2.162580	O	-0.588747	-0.748969	2.245692	O	-0.477770	0.004986	2.389467
S	3.295995	-0.088773	-1.814564	S	3.175064	-0.161858	-1.870118	S	3.235631	-0.063641	-1.766990	S	3.530207	-1.289294	-1.279000
O	2.264365	-0.596215	0.990622	O	2.154517	-0.736123	0.940810	O	2.152664	-0.528771	1.039194	O	2.297108	-0.572125	1.408496
C	3.395527	-0.112779	1.747591	C	3.309827	-0.362014	1.668994	C	3.196279	-0.040253	1.803389	C	3.379235	0.029953	2.025887
H	0.009189	2.878819	1.602869	H	-0.022502	2.773126	1.649236	H	-0.156598	2.934934	1.508590	H	0.521889	3.095833	0.450702
H	0.742701	1.342688	2.134769	H	0.689261	1.215985	2.149405	H	0.614902	1.447560	2.119324	H	1.044324	1.838742	1.602698
H	-4.297593	1.164336	-1.559456	H	-4.400136	1.205142	-1.482626	H	-4.367464	0.953844	-1.627561	H	-3.898336	0.758876	-2.072973
H	-2.738183	-2.674480	1.278942	H	-2.880002	-2.718573	1.259328	H	-2.729184	-2.710021	1.391614	H	-2.891373	-1.802866	2.128040
H	-5.504850	-1.026701	-1.592698	H	-5.658737	-0.956634	-1.531768	H	-5.504370	-1.274343	-1.583337	H	-5.379932	-1.114651	-1.328705
H	-4.741438	-2.907138	-0.203133	H	-4.914869	-2.878348	-0.188676	H	-4.702522	-3.068937	-0.104897	H	-4.886515	-2.370399	0.727898
H	4.313889	-0.225224	1.166513	H	4.230148	-0.939349	1.247903	H	4.770715	-1.912110	1.127123	H	3.846461	0.872994	1.530256
H	3.242715	0.933921	2.022243	H	3.526113	0.707599	1.603621	H	3.614606	0.926502	1.548592	H	3.372032	-0.102959	3.097461
H	3.436450	-0.733994	2.640100	H	3.178576	-0.704461	2.694495	H	3.202279	-0.446632	2.804310	H	-0.879444	-2.059145	-1.197228
H	-0.964123	-1.406774	-1.853177	H	-1.109632	-1.419392	-1.887429	H	-1.000555	-1.494348	-1.824316	H	-0.107747	-0.695197	-2.063388
H	-0.407307	0.265277	-2.168939	H	-0.522994	0.246583	-2.183395	H	-0.484722	0.180060	-2.195083	H	0.698795	-2.300090	-2.007266
H	0.562746	-1.132171	-2.746179	H	0.412935	-1.161323	-2.792929	H	0.530670	-1.211608	-2.708019				
O	3.418110	-2.942087	0.395231	O	5.253422	-1.628583	0.504294	O	4.870756	-2.393009	0.292960				
H	3.798293	-2.383326	-0.316169	H	4.997758	-1.281891	-0.375575	H	4.458630	-1.812347	-0.364941				

Table S52. Optimized Cartesian coordinates for the stationary points involved in the H27-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

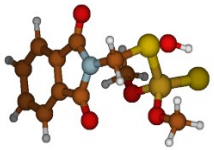
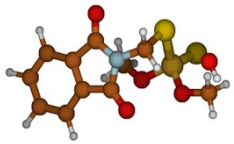
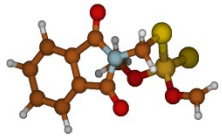
MCR(H27-abs)				TS(H27-abs)				MCP(H27-abs)				Rad(H27-abs)			
															
C	-4.547486	-1.156889	0.646872	C	-4.537871	0.678710	-1.285357	C	-4.567462	-0.665894	1.164662	C	-4.223882	-1.543319	0.486770
C	-3.396231	-0.869897	1.390606	C	-3.335092	0.131387	-1.749007	C	-3.359190	-0.195070	1.693477	C	-3.113740	-1.199899	1.268346
C	-2.498957	0.024763	0.835176	C	-2.477587	-0.392429	-0.798011	C	-2.463870	0.370209	0.803059	C	-2.308259	-0.178431	0.797570
C	-2.724647	0.618601	-0.404935	C	-2.790910	-0.381183	0.559781	C	-2.745425	0.471819	-0.558000	C	-2.584294	0.484343	-0.396738
C	-3.859417	0.345047	-1.147940	C	-3.976826	0.154370	1.029870	C	-3.936561	0.012995	-1.091778	C	-3.679041	0.155860	-1.176392
C	-4.774602	-0.560887	-0.597564	C	-4.852603	0.689497	0.076967	C	-4.850687	-0.563094	-0.200718	C	-4.501184	-0.878267	-0.711519
C	-1.185585	0.498793	1.343927	C	-1.132924	-1.005445	-0.957837	C	-1.104954	0.924535	1.037717	C	-1.059775	0.392597	1.366967
N	-0.687609	1.382603	0.372815	N	-0.707729	-1.353007	0.333925	N	-0.637846	1.351708	-0.215473	N	-0.651707	1.398999	0.477151
C	-1.554824	1.480218	-0.720424	C	-1.647620	-0.979372	1.299277	C	-1.567120	1.085797	-1.226102	C	-1.512209	1.489780	-0.621788
C	0.665708	1.861209	0.350503	C	0.632316	-1.763534	0.645584	C	0.721249	1.737432	-0.466491	C	0.628189	2.045215	0.536884
S	1.727188	1.020467	-0.906093	S	1.642066	-0.459120	1.476664	S	1.709185	0.463929	-1.370750	S	1.828385	1.461508	-0.741929
P	1.798750	-0.946562	-0.169643	P	1.826691	0.958881	-0.043617	P	1.787574	-1.082811	0.027671	P	2.119306	-0.528332	-0.180308
O	0.281110	-1.457043	-0.080152	O	0.347111	1.367063	-0.504369	O	0.283140	-1.471917	0.412151	O	0.687673	-1.246375	-0.160439
C	-0.417542	-1.881707	-1.271056	C	-0.435637	2.272863	0.304971	C	-0.507120	-2.284107	-0.485405	C	0.063827	-1.650933	-1.399524
O	-1.330005	2.145240	-1.711851	O	-1.496300	-1.132209	2.495050	O	-1.382108	1.323414	-2.402957	O	-1.353741	2.255352	-1.551526
O	-0.621877	0.227333	2.382630	O	-0.496806	-1.207267	-1.970535	O	-0.486913	1.030073	2.075727	O	-0.481129	0.104072	2.392902
S	3.039503	-1.998570	-1.215559	S	3.025277	2.380758	0.483158	S	2.965453	-2.492640	-0.564579	S	3.521604	-1.340773	-1.229977
O	2.029141	-0.835589	1.408051	O	2.178173	0.135306	-1.387019	O	2.115486	-0.377225	1.452157	O	2.292107	-0.516746	1.430204
C	3.302415	-0.392136	1.924332	C	3.431487	-0.508626	-1.523790	C	3.311256	0.284872	1.652657	C	3.330254	0.184632	2.019530
H	0.697063	2.914048	0.065791	H	0.625024	-2.591161	1.357274	H	0.758847	2.613514	-1.116808	H	0.526656	3.113488	0.337516
H	1.098856	1.734160	1.343409	H	1.123232	-2.079210	-0.275387	H	1.195337	1.968815	0.489155	H	1.048541	1.898128	1.533218
H	-4.028967	0.806684	-2.115242	H	-4.214590	0.164033	2.088545	H	-4.150183	0.091392	-2.152767	H	-3.888082	0.672987	-2.107215
H	-3.211943	-1.333082	2.354495	H	-3.083700	0.123801	-2.804547	H	-3.131985	-0.275357	2.751498	H	-2.891329	-1.715001	2.197194
H	-5.676492	-0.808389	-1.147706	H	-5.792645	1.123639	0.401096	H	-5.796230	-0.939899	-0.576415	H	-5.369399	-1.171224	-1.292600
H	-5.276560	-1.857097	1.041061	H	-5.238671	1.105337	-1.995352	H	-5.297546	-1.121412	1.825489	H	-4.880883	-2.342007	0.814859
H	4.081476	-1.109712	1.659569	H	4.262376	0.121061	-1.194740	H	4.183079	-0.075446	1.116686	H	4.275462	0.224178	1.490297
H	3.544911	0.599252	1.533062	H	3.449734	-1.467678	-0.859663	H	3.552442	2.438695	0.666381	H	3.256406	0.201153	3.097169
H	3.180519	-0.347718	3.004827	H	3.526678	-0.824666	-2.560532	H	3.374650	0.726688	2.637204	H	-0.888391	-2.097860	-1.115850
H	-1.415701	-2.166942	-0.939567	H	-1.391283	2.373739	-0.208320	H	-1.477706	-2.393123	-0.002872	H	-0.105109	-0.778815	-2.039000
H	-0.481111	-1.056409	-1.987286	H	-0.586923	1.852039	1.304093	H	-0.619845	-1.779224	-1.449940	H	0.690075	-2.384691	-1.910282
H	0.092671	-2.736926	-1.717761	H	0.063948	3.241124	0.369916	H	-0.036536	-3.260172	-0.616787				
O	3.476648	2.855968	0.092144	O	3.592381	-2.780650	-0.280587	O	3.706246	3.301653	0.252738				
H	4.227105	2.241955	-0.036736	H	3.876190	-3.235816	-1.097780	H	2.835279	3.720158	0.230686				

Table S53. Optimized Cartesian coordinates for the stationary points involved in the H28-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

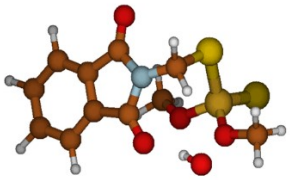
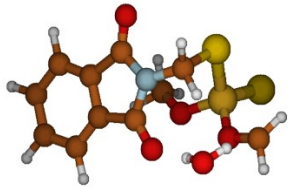
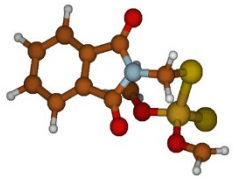
MCR(H28-abs)	TS(H28-abs)	MCP(H28-abs)	Rad(H28-abs)
			
C 4.435601 0.341388 -1.580375	C 4.236430 0.194964 -1.665928	C 4.251108 -0.137011 -1.620514	C -4.223352 -1.541636 0.490978
C 3.235711 1.047402 -1.426352	C 3.062771 0.949327 -1.544434	C 3.084377 0.637384 -1.633903	C -3.113400 -1.195840 1.271761
C 2.437662 0.696794 -0.352258	C 2.306431 0.749777 -0.403457	C 2.303701 0.611645 -0.491983	C -2.307859 -0.175748 0.798113
C 2.804732 -0.308538 0.539972	C 2.687053 -0.158562 0.581968	C 2.657489 -0.143490 0.624090	C -2.583647 0.483430 -0.398228
C 3.987384 -1.011866 0.399416	C 3.844800 -0.908461 0.474087	C 3.808952 -0.909797 0.650654	C -3.678223 0.152577 -1.177135
C 4.803800 -0.667802 -0.685643	C 4.620016 -0.715085 -0.676064	C 4.606551 -0.894834 -0.500417	C -4.500426 -0.880175 -0.709356
C 1.117354 1.230973 0.070280	C 1.009093 1.350766 -0.002725	C 1.004121 1.272352 -0.210251	C -1.059471 0.396900 1.366041
N 0.759644 0.527196 1.222128	N 0.672008 0.773812 1.227465	N 0.641529 0.889884 1.087349	N -0.651378 1.400907 0.473513
C 1.723671 -0.436813 1.551800	C 1.631563 -0.166730 1.627870	C 1.584296 0.011196 1.639942	C -1.511567 1.488233 -0.626015
C -0.520111 0.605015 1.871365	C -0.622291 0.878690 1.839913	C -0.665167 1.083262 1.650345	C 0.628707 2.046853 0.531305
S -1.607792 -0.852370 1.563366	S -1.674772 -0.629797 1.649563	S -1.712967 -0.439535 1.663414	S 1.828677 1.459206 -0.746006
P -2.057867 -0.610160 -0.465286	P -1.888961 -0.771242 -0.425512	P -1.943708 -0.834096 -0.373472	P 2.118880 -0.529121 -0.178867
O -0.659191 -0.542735 -1.246409	O -0.417932 -0.860181 -1.056682	O -0.482740 -0.980672 -1.012771	O 0.686766 -1.246144 -0.156302
C 0.110388 -1.747103 -1.450091	C 0.314350 -2.105147 -1.025704	C 0.257990 -2.211890 -0.852873	C 0.062961 -1.655598 -1.393756
O 1.627309 -1.197619 2.492150	O 1.546947 -0.835146 2.637437	O 1.475485 -0.499879 2.735437	O -1.352862 2.250996 -1.558010
O 0.461423 2.115530 -0.446226	O 0.349252 2.190332 -0.583222	O 0.358769 2.015194 -0.923128	O -0.480849 0.111134 2.392764
S -3.329726 -1.953998 -1.034473	S -3.146647 -2.167594 -0.876942	S -3.200131 -2.272993 -0.651746	S 3.520066 -1.345501 -1.226930
O -2.443397 0.931375 -0.674550	O -2.184799 0.713002 -0.968931	O -2.263409 0.588328 -1.081470	O 2.292422 -0.513155 1.431555
C -3.684923 1.431567 -0.129440	C -3.338694 1.440314 -0.585129	C -3.361297 1.345516 -0.714974	C 3.329381 0.191592 2.018894
H -0.386968 0.620374 2.954576	H -0.521993 0.996025 2.920386	H -0.588725 1.361470 2.702994	H 0.527592 3.114619 0.329107
H -1.023789 1.519640 1.557794	H -1.139300 1.745717 1.428906	H -1.177618 1.874494 1.102897	H 1.049138 1.902314 1.527979
H 4.267971 -1.795322 1.095575	H 4.134318 -1.618432 1.241810	H 4.077062 -1.500667 1.520341	H -3.887059 0.666931 -2.109540
H 2.943390 1.830176 -2.118522	H 2.756869 1.652743 -2.311852	H 2.800271 1.222676 -2.502319	H -2.891169 -1.708180 2.202177
H 5.740137 -1.194828 -0.836391	H 5.534359 -1.284804 -0.804819	H 5.516136 -1.485696 -0.526492	H -5.368510 -1.174897 -1.289739
H 5.092060 0.580410 -2.410442	H 4.858783 0.315007 -2.546476	H 4.890645 -0.153001 -2.496855	H -4.880405 -2.339352 0.821325
H -4.506538 0.754488 -0.374093	H -4.037437 1.507737 -1.419541	H -4.115421 0.885052 -0.086983	H 4.273863 0.233233 1.488545
H -3.593748 1.548409 0.953379	H -3.798031 1.071016 0.334995	H -3.597162 2.109012 -1.442197	H 3.256694 0.209115 3.096591
H -3.850063 2.397973 -0.603033	H -2.964270 2.529833 -0.365769	H -2.353089 3.670329 0.029249	H -0.890299 -2.099323 -1.108539
H 1.011473 -1.435296 -1.976990	H 1.273444 -1.892669 -1.497630	H 1.204918 -2.052231 -1.367894	H -0.103876 -0.786403 -2.037738
H 0.374055 -2.195728 -0.486953	H 0.466126 -2.429763 0.008491	H 0.434931 -2.409564 0.208982	H 0.688155 -2.393065 -1.900440
H -0.456685 -2.455389 -2.057117	H -0.225147 -2.868206 -1.589877	H -0.289164 -3.037616 -1.311054	
O -1.817905 3.701731 0.066903	O -2.142036 3.659531 -0.202602	O -1.559166 4.106329 -0.310676	
H -1.114029 3.036525 -0.122622	H -1.285255 3.186569 -0.300504	H -0.952553 3.378039 -0.526479	

Table S54. Optimized Cartesian coordinates for the stationary points involved in the H29-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

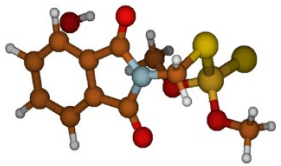
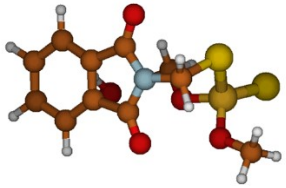
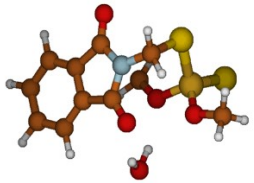
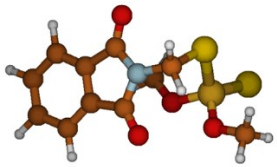
MCR(H29-abs)				TS(H29-abs)				MCP(H29-abs)				Rad(H29-abs)			
															
C	4.218368	0.149401	1.513730	C	4.342401	0.854673	0.928844	C	4.288886	1.316856	-0.530469	C	4.311670	-1.522963	0.534309
C	2.994156	-0.449196	1.833358	C	3.169642	0.448282	1.578275	C	3.172130	1.526263	0.288716	C	3.187661	-1.739630	-0.272884
C	2.155012	-0.764866	0.778605	C	2.274174	-0.305266	0.840460	C	2.348260	0.437758	0.513428	C	2.363737	-0.652799	-0.504662
C	2.506756	-0.502754	-0.543470	C	2.527545	-0.661662	-0.482776	C	2.611945	-0.812196	-0.043950	C	2.634008	0.602520	0.036956
C	3.718304	0.079699	-0.874689	C	3.681262	-0.265371	-1.136315	C	3.712456	-1.032238	-0.852049	C	3.741464	0.829952	0.833704
C	4.575295	0.407753	0.185862	C	4.591219	0.508289	-0.403470	C	4.553595	0.062783	-1.088908	C	4.583389	-0.263109	1.075999
C	0.807392	-1.395520	0.783730	C	0.959466	-0.879154	1.230327	C	1.091826	0.338403	1.298136	C	1.099132	-0.561181	-1.279933
N	0.416172	-1.482074	-0.560352	N	0.501502	-1.594293	0.113614	N	0.665397	-0.990451	1.186844	N	0.678326	0.773626	-1.178204
C	1.381881	-0.940375	-1.412749	C	1.386046	-1.486690	-0.962605	C	1.520240	-1.735547	0.365036	C	1.540928	1.523861	-0.372954
C	-0.895615	-1.870837	-0.996482	C	-0.799271	-2.193855	0.020006	C	-0.606541	-1.466409	1.652586	C	-0.590350	1.253506	-1.647465
S	-1.935591	-0.465168	-1.585676	S	-1.973218	-1.299396	-1.088509	S	-1.824199	-1.811738	0.308522	S	-1.804619	1.621325	-0.306258
P	-2.300886	0.546655	0.209329	P	-2.234313	0.498899	-0.056809	P	-2.140210	0.090480	-0.483252	P	-2.143932	-0.278274	0.485532
O	-0.870519	0.910938	0.836247	O	-0.767425	1.164307	0.069657	O	-0.678461	0.639311	-0.949099	O	-0.693129	-0.850657	0.945195
C	-0.073135	1.967964	0.264545	C	-0.175216	1.792306	-1.056690	C	0.049971	0.007390	-1.940436	C	0.045076	-0.215503	1.929272
O	1.263861	-0.865713	-2.619514	O	1.201922	-1.991924	-2.051972	O	1.345809	-2.903323	0.082636	O	1.373784	2.696006	-0.101232
O	0.151642	-1.795893	1.722010	O	0.372158	-0.799297	2.288320	O	0.515746	1.197619	1.936221	O	0.516052	-1.423355	-1.903164
S	-3.545075	2.001692	-0.075354	S	-3.615739	1.567264	-0.885991	S	-3.514130	0.053398	-1.837431	S	-3.516531	-0.224240	1.842377
O	-2.672300	-0.570434	1.294276	O	-2.375476	0.135913	1.492110	O	-2.276979	1.109033	0.738007	O	-2.306777	-1.287265	-0.741044
C	-3.928346	-1.274373	1.199448	C	-3.567485	-0.525055	1.969942	C	-3.478066	1.104253	1.542060	C	-3.504082	-1.244625	-1.548712
H	-0.824553	-2.537175	-1.857852	H	-0.726076	-3.191083	-0.417910	H	-0.491923	-2.426768	2.158469	H	-0.469150	2.207361	-2.164049
H	-1.396655	-2.386901	-0.176163	H	-1.219641	-2.266603	1.023951	H	-1.018530	-0.733031	2.346715	H	-1.008530	0.515981	-2.333575
H	3.990937	0.276228	-1.906688	H	3.872775	-0.542038	-2.167894	H	3.911794	-2.006261	-1.286799	H	3.945272	1.808539	1.256003
H	2.713421	-0.653854	2.861337	H	2.968490	0.718719	2.609702	H	2.960014	2.497302	0.724650	H	2.969997	-2.715811	-0.693871
H	5.533466	0.870381	-0.027157	H	5.508006	0.843871	-0.876849	H	5.427438	-0.063134	-1.719614	H	5.462611	-0.131327	1.697991
H	4.905052	0.418375	2.309405	H	5.070801	1.452615	1.466516	H	4.961119	2.142931	-0.737291	H	4.983813	-2.348078	0.745406
H	-4.758272	-0.572833	1.305871	H	-4.428671	0.136048	1.856420	H	-4.334975	1.392529	0.930400	H	-4.371446	-1.510601	-0.941564
H	-3.995419	-1.803304	0.245053	H	-3.727628	-1.459438	1.425358	H	-3.634480	0.115313	1.980579	H	-3.630634	-0.249825	-1.983585
H	-3.928522	-1.986859	2.022053	H	-3.384861	-0.732836	3.022382	H	-3.307005	1.839117	2.325912	H	-3.352083	-1.980680	-2.335396
H	0.829069	2.014096	0.873146	H	0.729507	2.400295	-0.628521	H	-0.261516	2.605541	-0.553145	H	0.893506	-0.803153	2.251375
H	0.181934	1.729629	-0.773965	H	0.221786	1.064980	-1.770305	H	0.902649	0.591346	-2.259084	H	-0.469490	0.474933	2.587991
H	-0.612624	2.916041	0.314748	H	-0.839619	2.528435	-1.514628	H	-0.475168	-0.670599	-2.603592				
O	3.295447	2.865686	-0.396055	O	1.883618	3.031605	-0.171826	O	0.123830	3.335986	-0.046757				
H	2.547464	2.508438	-0.917859	H	2.525561	2.393920	-0.545686	H	0.391458	2.912119	0.783215				

Table S55. Optimized Cartesian coordinates for the stationary points involved in the H30-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

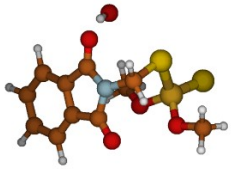
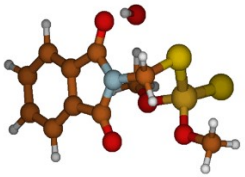
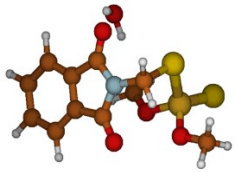
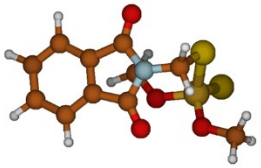
MCR(H30-abs)				TS(H30-abs)				MCP(H30-abs)				Rad(H30-abs)			
															
C	-4.076326	-1.083736	-1.466132	C	-4.105645	-0.532712	-1.619163	C	-4.123926	-1.180809	-1.444401	C	-4.310639	-1.524412	-0.531659
C	-2.982128	-1.782125	-0.939224	C	-3.031305	-1.380839	-1.321184	C	-2.972740	-1.828071	-0.977776	C	-3.186862	-1.739175	0.276363
C	-2.220066	-1.125993	0.010565	C	-2.241684	-1.033370	-0.239717	C	-2.212926	-1.153815	-0.038932	C	-2.363322	-0.651664	0.506291
C	-2.526022	0.167017	0.430626	C	-2.500366	0.104128	0.521554	C	-2.571851	0.109782	0.426710	C	-2.633662	0.602523	-0.037904
C	-3.602918	0.867915	-0.082005	C	-3.556487	0.951356	0.236693	C	-3.707206	0.758849	-0.024705	C	-3.740856	0.828034	-0.835557
C	-4.380144	0.215251	-1.047005	C	-4.363038	0.610616	-0.856112	C	-4.483883	0.086940	-0.977248	C	-4.582441	-0.265704	-1.075967
C	-0.975996	-1.552895	0.703208	C	-1.009429	-1.671569	0.291905	C	-0.935617	-1.542936	0.613888	C	-1.098938	-0.558324	1.281665
N	-0.613126	-0.485071	1.546655	N	-0.608777	-0.892798	1.394626	N	-0.595789	-0.478267	1.466378	N	-0.678319	0.776453	1.177405
C	-1.486972	0.589476	1.401620	C	-1.440905	0.213971	1.554576	C	-1.530663	0.554746	1.388404	C	-1.540737	1.524851	0.370300
C	0.688996	-0.353350	2.143641	C	0.695055	-0.984409	1.994127	C	0.686893	-0.329566	2.094392	C	0.590471	1.257060	1.645477
S	1.766127	0.884749	1.296224	S	1.826756	0.407674	1.545772	S	1.760477	0.943222	1.293783	S	1.804811	1.621763	0.303497
P	2.068317	-0.015250	-0.569064	P	2.026428	0.146427	-0.517619	P	2.188171	0.033293	-0.535542	P	2.143482	-0.279329	-0.485118
O	0.621743	-0.266843	-1.219882	O	0.527443	0.179201	-1.125625	O	0.752800	-0.231112	-1.258000	O	0.692171	-0.851977	-0.942986
C	-0.079130	0.815319	-1.868475	C	-0.078687	1.383250	-1.555533	C	0.047312	0.805290	-1.836877	C	-0.045503	-0.219253	-1.928922
O	-1.351585	1.659280	1.970100	O	-1.259161	1.093861	2.377000	O	-1.445253	1.599184	2.006893	O	-1.373604	2.696370	0.095900
O	-0.359601	-2.591486	0.609268	O	-0.426424	-2.659483	-0.097687	O	-0.285560	-2.558122	0.487185	O	-0.515668	-1.419108	1.906563
S	3.335316	1.015604	-1.606938	S	3.299702	1.397319	-1.255706	S	3.486515	1.051298	-1.536244	S	3.515234	-0.227832	-1.842792
O	2.386930	-1.557432	-0.282427	O	2.250882	-1.418209	-0.760353	O	2.474116	-1.508777	-0.238140	O	2.306621	-1.286310	0.743101
C	3.622731	-1.927218	0.364701	C	3.463702	-2.051399	-0.298858	C	3.689018	-1.895104	0.442396	C	3.504050	-1.242077	1.550515
H	0.605943	0.014750	3.167431	H	0.623256	-0.928252	3.081510	H	0.572262	0.023537	3.120661	H	0.469577	2.212192	2.159783
H	1.170012	-1.332390	2.144819	H	1.141331	-1.936835	1.705106	H	1.190995	-1.296772	2.093602	H	1.008464	0.521002	2.333273
H	-3.828794	1.878370	0.243238	H	-3.745495	1.841162	0.828526	H	-3.979528	1.744573	0.338710	H	-3.944781	1.805705	-1.259920
H	-2.736735	-2.786505	-1.268536	H	-2.822012	-2.263819	-1.916147	H	-2.686223	-2.810041	-1.339828	H	-2.969108	-2.714447	0.699407
H	-5.232465	0.727170	-1.481300	H	-5.201465	1.246705	-1.119825	H	-5.381105	0.559458	-1.363030	H	-5.461448	-0.135376	-1.698567
H	-4.698023	-1.557084	-2.218876	H	-4.748569	-0.763593	-2.462109	H	-4.747880	-1.670259	-2.184878	H	-4.982494	-2.350120	-0.741348
H	4.472089	-1.624163	-0.251065	H	4.328221	-1.611127	-0.799991	H	4.554575	-1.645554	-0.174188	H	4.371410	-1.508708	0.943645
H	3.684774	-1.466454	1.354117	H	3.556269	-1.947154	0.785227	H	3.754069	-1.396694	1.413118	H	3.630316	-0.246588	1.983878
H	3.592271	-3.010970	0.458339	H	3.366061	-3.101501	-0.566764	H	3.617378	-2.972169	0.578459	H	3.352419	-1.977005	2.338323
H	-1.027005	0.395464	-2.205250	H	-1.085374	1.140139	-1.895974	H	-0.900992	0.480431	-2.244233	H	-0.893879	-0.807506	-2.250078
H	-0.261113	1.627774	-1.156184	H	-0.182939	2.145617	-0.673153	H	-0.815613	2.699898	-0.663867	H	0.469280	0.469758	-2.588965
H	0.499535	1.179978	-2.719045	H	0.518001	1.893456	-2.315213	H	0.620968	1.616114	-2.274259				
O	-0.729547	3.644153	-0.074394	O	-0.367332	3.199413	0.285980	O	-1.267170	3.465968	-0.278534				
H	-1.032112	3.093332	0.682680	H	-0.696129	2.646083	1.025438	H	-1.540748	3.154663	0.597230				

Table S56. Optimized Cartesian coordinates for the stationary points involved in the H31-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

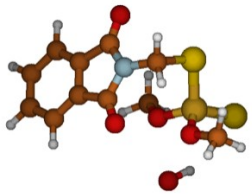
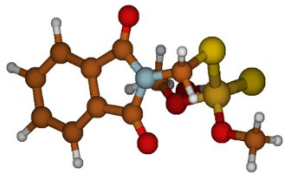
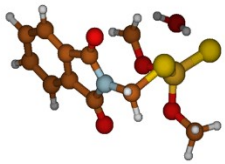
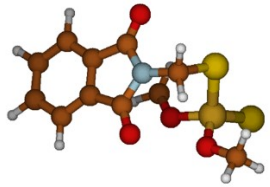
MCR(H31-abs)	TS(H31-abs)	MCP(H31-abs)	Rad(H31-abs)
			
C 4.233760 1.709950 0.323766	C 4.275235 1.234205 1.167297	C 4.282822 1.443930 1.001072	C 4.304170 -1.562923 0.418911
C 3.128173 1.393335 1.123049	C 3.207982 0.498733 1.697912	C 3.221660 0.768379 1.617168	C 3.177494 -1.717843 -0.398723
C 2.407672 0.264304 0.776482	C 2.454870 -0.244124 0.806401	C 2.478912 -0.087219 0.823604	C 2.356926 -0.614669 -0.550146
C 2.761721 -0.527376 -0.314224	C 2.740644 -0.265775 -0.557513	C 2.768010 -0.273414 -0.527083	C 2.633338 0.598598 0.077612
C 3.852732 -0.226416 -1.109964	C 3.793051 0.455009 -1.093329	C 3.814185 0.386102 -1.146477	C 3.743834 0.765000 0.885272
C 4.588926 0.915736 -0.770865	C 4.562303 1.212212 -0.200939	C 4.573704 1.255705 -0.353340	C 4.581963 -0.345574 1.047620
C 1.186835 -0.316892 1.394268	C 1.257797 -1.092873 1.043025	C 1.292401 -0.915244 1.162743	C 1.092294 -0.463476 -1.316162
N 0.873002 -1.456291 0.636660	N 0.891114 -1.605190 -0.211656	N 0.932615 -1.579034 -0.020783	N 0.674811 0.861744 -1.116677
C 1.767804 -1.628041 -0.423847	C 1.725656 -1.122586 -1.225251	C 1.765347 -1.218960 -1.085170	C 1.543957 1.551192 -0.265518
C -0.361535 -2.179305 0.754351	C -0.339295 -2.298612 -0.464366	C -0.265308 -2.353811 -0.173813	H -0.475660 2.366736 -1.987099
S -1.555271 -1.852069 -0.618284	S -1.603454 -1.283725 -1.351999	S -1.565814 -1.533873 -1.198987	S -1.802443 1.642569 -0.171126
P -2.048762 0.144773 -0.256457	P -2.068325 0.155321 0.085222	P -2.065701 0.091870 0.002940	P -2.143092 -0.314961 0.466317
O -0.681791 0.986270 -0.295560	O -0.697311 0.927791 0.449999	O -0.698357 0.933462 0.246579	O -0.688285 -0.922478 0.864121
C -0.044112 1.289080 -1.555976	C -0.127014 1.878545 -0.433122	C -0.056436 1.583392 -0.791543	C 0.010589 -0.431364 1.951374
O 1.688231 -2.517833 -1.247218	O 1.587603 -1.382916 -2.403631	O 1.636863 -1.629946 -2.220812	O 1.381353 2.701438 0.089486
O 0.563045 0.059904 2.363518	O 0.684883 -1.339857 2.082856	O 0.721291 -1.041921 2.225052	O 0.507634 -1.275470 -2.001667
S -3.462932 0.729627 -1.448263	S -3.556732 1.244158 -0.513731	S -3.554717 1.069894 -0.759095	S -3.506596 -0.374783 1.831162
O -2.282918 0.290660 1.318459	O -2.193122 -0.599111 1.485852	O -2.175473 -0.430333 1.505169	O -2.312384 -1.216107 -0.840843
C -3.431972 -0.326704 1.937100	C -3.304412 -1.489566 1.731562	C -3.273289 -1.286276 1.894459	C -3.508035 -1.097643 -1.642945
H -0.180839 -3.254227 0.702949	H -0.169497 -3.149442 -1.126376	H -0.054518 -3.282888 -0.706679	C -0.595411 1.376608 -1.543610
H -0.820907 -1.930220 1.711884	H -0.744417 -2.648414 0.485887	H -0.662003 -2.580437 0.816820	H -1.018184 0.692913 -2.280977
H 4.122055 -0.843999 -1.960548	H 4.009209 0.437891 -2.156524	H 4.033026 0.239856 -2.199156	H 3.953018 1.710681 1.374569
H 2.845949 2.007492 1.971966	H 2.978062 0.514946 2.758232	H 2.989219 0.912671 2.667201	H 2.955242 -2.660804 -0.887578
H 5.450857 1.191687 -1.369358	H 5.395787 1.795792 -0.577780	H 5.402646 1.796071 -0.798323	H 5.463072 -0.261487 1.675154
H 4.825423 2.589331 0.555830	H 4.890396 1.834840 1.829116	H 4.890099 2.128035 1.584452	H 4.974001 -2.403127 0.569080
H -4.349898 0.101953 1.529841	H -4.242517 -0.932449 1.693829	H -4.220095 -0.757921 1.767601	H -4.379119 -1.401958 -1.059529
H -3.411489 -1.408145 1.778786	H -3.308946 -2.299594 0.997625	H -3.262543 -2.204632 1.302100	H -3.624337 -0.070540 -1.998193
H -3.348807 -0.102564 2.998669	H -3.141501 -1.889818 2.730093	H -3.105077 -1.515239 2.944630	H -3.362523 -1.770869 -2.485207
H 0.849701 1.858494 -1.302989	H 0.875939 2.103024 -0.069099	H 0.781917 2.180681 -0.464842	H 0.851051 -1.046122 2.235645
H 0.230478 0.362749 -2.070811	H -0.134981 1.547078 -1.475620	H -0.197481 1.222571 -1.803425	H -0.122489 0.605710 2.234646
H -0.710961 1.888216 -2.179807	H -0.719160 2.877944 -0.369659	H -1.115545 3.988465 -0.501453	
O -1.641767 3.450567 0.094195	O -1.558933 4.043017 -0.253691	O -2.013251 4.149573 -0.178709	
H -2.288321 3.158164 -0.583422	H -2.404204 3.565391 -0.385934	H -2.474578 3.309418 -0.326186	

Table S57. Optimized Cartesian coordinates for the stationary points involved in the C1-addition pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

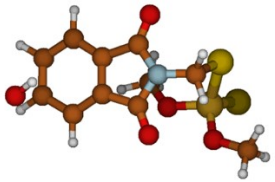
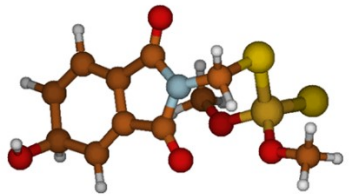
MCR(C1-add)	TS(C1-add)	Adduct(C1-add)
		
C -3.853577 -1.595109 0.109140	C -4.005806 -1.403563 -0.353043	C 4.209319 -1.143392 0.500494
C -2.836902 -1.176193 0.979500	C -2.908494 -1.397387 0.552955	C 3.006843 -1.350521 -0.380022
C -2.044912 -0.124645 0.555933	C -2.079349 -0.301557 0.520777	C 2.108324 -0.355496 -0.511225
C -2.242554 0.495822 -0.676316	C -2.267228 0.743117 -0.391564	C 2.246665 0.908934 0.136963
C -3.249483 0.100548 -1.539335	C -3.292598 0.734266 -1.324808	C 3.347600 1.195349 0.966350
C -4.057810 -0.964879 -1.124493	C -4.146672 -0.366479 -1.313586	C 4.284937 0.218303 1.143076
C -0.859326 0.495336 1.202326	C -0.861481 -0.004900 1.319398	C 0.853174 -0.315155 -1.310319
N -0.395292 1.474396 0.308443	N -0.383048 1.229370 0.852436	N 0.333951 0.969747 -1.138268
C -1.172879 1.513915 -0.853372	C -1.169012 1.725797 -0.190993	C 1.117633 1.745325 -0.261557
C 0.896744 2.094304 0.411272	C 0.911642 1.757855 1.183636	C -0.967668 1.371634 -1.591163
S 2.144130 1.416562 -0.772784	S 2.150859 1.597624 -0.175883	S -2.208425 1.556627 -0.236493
P 2.374349 -0.543111 -0.070580	P 2.374925 -0.481236 -0.295349	P -2.387126 -0.416587 0.435764
O 0.924259 -1.231140 -0.108263	O 0.920599 -1.095055 -0.586395	O -0.919165 -0.898677 0.869718
C 0.375574 -1.696142 -1.360603	C 0.359848 -1.033526 -1.915634	C -0.353015 -0.454141 2.121007
O -0.952783 2.244794 -1.798237	O -0.941690 2.757259 -0.790567	O 0.839873 2.892398 0.053758
O -0.361810 0.256556 2.281945	O -0.354851 -0.649916 2.211643	O 0.353934 -1.182958 -1.998895
S 3.802417 -1.437277 -1.023294	S 3.793397 -0.933218 -1.531903	S -3.793610 -0.547302 1.759346
O 2.469059 -0.445327 1.523652	O 2.478048 -1.013437 1.210024	O -2.480239 -1.338015 -0.869322
C 3.624536 0.159546 2.140874	C 3.641362 -0.704748 2.005829	C -3.645643 -1.271269 -1.717187
H 0.834187 3.154309 0.159484	H 0.848891 2.831480 1.368677	H -0.923277 2.360405 -2.051300
H 1.255756 1.981618 1.435117	H 1.273086 1.252301 2.080095	H -1.320716 0.642581 -2.321760
H -3.396621 0.584742 -2.499134	H -3.411030 1.538029 -2.043534	H 3.447198 2.167915 1.437564
H -2.673083 -1.661880 1.935973	H -2.755161 -2.216403 1.247564	H 2.902638 -2.302410 -0.893361
H -4.855783 -1.314069 -1.771507	H -4.956582 -0.432456 -2.031968	H 5.157639 0.395437 1.764295
H -4.489128 -2.428043 0.391798	H -4.572443 -2.317315 -0.485502	H 4.179154 -1.897918 1.300525
H 4.522022 -0.412237 1.894855	H 4.531360 -1.146845 1.553296	H -4.534929 -1.563695 -1.154928
H 3.730626 1.197109 1.812014	H 3.759258 0.377948 2.101232	H -3.763295 -0.261759 -2.120030
H 3.436758 0.124828 3.212469	H 3.454845 -1.147454 2.982341	H -3.461638 -1.976601 -2.525259
H -0.604660 -2.106657 -1.118483	H -0.624143 -1.496022 -1.841317	H 0.651053 -0.875819 2.155562
H 0.270536 -0.861736 -2.061390	H 0.261693 0.008007 -2.238158	H -0.301763 0.638932 2.149261
H 1.016619 -2.471510 -1.784212	H 0.988636 -1.590701 -2.612553	H -0.950098 -0.828424 2.954732
O -5.741055 -0.090925 1.340662	O -5.458188 -0.782630 0.954179	O 5.414591 -1.434102 -0.214117
H -5.218008 0.684173 1.042233	H -5.093686 0.098861 1.158714	H 5.498880 -0.793856 -0.937213

Table S58. Optimized Cartesian coordinates for the stationary points involved in the C2-addition pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

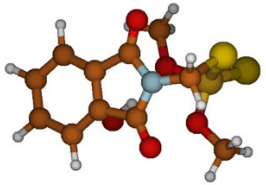
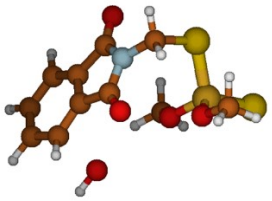
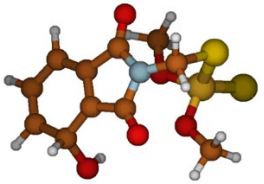
MCR(C2-add)	TS(C2-add)	Adduct(C2-add)
		
C -4.160838 -0.506174 1.045123	C -4.297471 -1.136701 0.140429	C 4.024526 0.312329 -1.112769
C -3.179461 0.440899 1.367485	C -3.132031 -1.129980 0.955974	C 3.131040 1.222662 -0.309413
C -2.214820 0.695915 0.407134	C -2.239785 -0.063235 0.740718	C 2.115397 0.424012 0.430785
C -2.214071 0.042304 -0.823487	C -2.431102 0.857351 -0.270424	C 2.026610 -0.947683 0.360479
C -3.175553 -0.896346 -1.151833	C -3.541761 0.811717 -1.108007	C 2.891484 -1.727088 -0.400243
C -4.158437 -1.161617 -0.189253	C -4.476235 -0.207490 -0.880943	C 3.903335 -1.042844 -1.145825
C -1.050515 1.620573 0.442755	C -0.962212 0.249947 1.427147	C 1.036530 0.922426 1.288282
N -0.406079 1.478587 -0.795870	N -0.462196 1.405645 0.807001	N 0.299508 -0.213317 1.697834
C -1.048070 0.533980 -1.603159	C -1.284954 1.811171 -0.245650	C 0.845472 -1.376574 1.166813
C 0.855168 2.083272 -1.110681	C 0.853054 1.934541 1.042789	C -0.971831 -0.139484 2.349047
S 2.278941 0.904919 -1.299832	S 2.051491 1.635719 -0.330074	S -2.443239 -0.584195 1.293806
P 1.941921 -0.484638 0.222744	P 2.180996 -0.453944 -0.322167	P -1.919272 0.066384 -0.625039
O 0.562663 -1.238994 -0.137667	O 0.691408 -1.003589 -0.559713	O -0.647927 -0.793713 -1.093773
C 0.545910 -2.292525 -1.126783	C 0.115150 -0.934786 -1.883197	C -0.819011 -2.156266 -1.536181
O -0.677257 0.221480 -2.716292	O -1.059931 2.759632 -0.968882	O 0.407753 -2.495513 1.348419
O -0.701950 2.379519 1.322262	O -0.430437 -0.330681 2.348986	O 0.788716 2.060209 1.642613
S 3.499379 -1.599822 0.484037	S 3.555572 -1.048828 -1.548159	S -3.473605 0.031490 -1.778780
O 1.340855 0.320208 1.465796	O 2.284681 -0.901867 1.209660	O -1.117360 1.440848 -0.458626
C 2.156873 1.264188 2.190986	C 3.475771 -0.604632 1.968246	C -1.789275 2.619148 0.032632
H 0.810245 2.593825 -2.074363	H 0.814860 3.021386 1.135036	H -1.023176 -0.845806 3.179600
H 1.087852 2.799770 -0.323057	H 1.235158 1.502216 1.968570	H -1.102426 0.877452 2.717976
H -3.167173 -1.404436 -2.110731	H -3.680925 1.542115 -1.898186	H 2.790526 -2.805776 -0.441963
H -3.173459 0.949794 2.325930	H -3.087181 -1.715087 1.867372	H 3.745629 1.800636 0.395167
H -4.931879 -1.891565 -0.403868	H -5.363639 -0.264858 -1.501741	H 4.579669 -1.626211 -1.761812
H -4.934944 -0.738615 1.768882	H -5.046199 -1.903966 0.307676	H 4.790864 0.807315 -1.702277
H 3.044772 0.764558 2.584097	H 4.332533 -1.126688 1.537490	H -2.642809 2.856205 -0.606426
H 2.441385 2.096193 1.541624	H 3.655314 0.473690 1.985521	H -2.114668 2.465101 1.064839
H 1.534313 1.624192 3.007765	H 3.280177 -0.966578 2.975746	H -1.052335 3.418832 -0.011425
H -0.507435 -2.516313 -1.296180	H -0.905939 -1.297267 -1.778039	H 0.188542 -2.555584 -1.651639
H 1.009726 -1.947035 -2.054080	H 0.115119 0.098388 -2.245138	H -1.366384 -2.735295 -0.787608
H 1.065358 -3.169304 -0.737416	H 0.676985 -1.574604 -2.566510	H -1.345016 -2.170268 -2.492246
O -1.333957 -1.753592 1.953493	O -2.099625 -2.581188 -0.023241	O 2.519673 2.216287 -1.140886
H -0.678111 -1.498959 1.263590	H -2.778310 -3.275363 0.070483	H 1.941165 1.765365 -1.775507

Table S59. Optimized Cartesian coordinates for the stationary points involved in the C3-addition pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

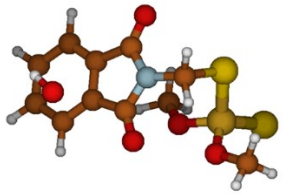
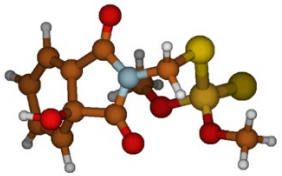
MCR(C3-add)	TS(C3-add)	Adduct(C3-add)
		
C -4.021128 1.211517 -1.377519	C -3.788341 1.452239 -1.245791	C -3.423703 1.721408 -1.133311
C -2.968969 0.337985 -1.681049	C -2.873415 0.481323 -1.642388	C -2.703695 0.666400 -1.609126
C -2.175004 -0.077074 -0.625003	C -2.230941 -0.254314 -0.628115	C -2.406651 -0.479203 -0.696955
C -2.408228 0.347974 0.682689	C -2.389290 0.110243 0.729481	C -2.464783 -0.102032 0.749564
C -3.446053 1.206561 0.994432	C -3.288860 1.071451 1.124585	C -3.176190 0.972125 1.204378
C -4.255303 1.635833 -0.066372	C -4.007394 1.732368 0.109990	C -3.734384 1.856033 0.253852
C -1.005302 -0.995364 -0.612442	C -0.997716 -1.098471 -0.722384	C -1.028508 -1.145729 -0.807590
N -0.593490 -1.079717 0.726005	N -0.574528 -1.311296 0.594269	N -0.595944 -1.416284 0.481642
C -1.379661 -0.276499 1.556791	C -1.364744 -0.618306 1.517299	C -1.429580 -0.847468 1.465623
C 0.636593 -1.687962 1.149250	C 0.693900 -1.899480 0.931903	C 0.688104 -1.991091 0.783894
S 1.955007 -0.474662 1.596148	S 1.942117 -0.673193 1.519130	S 1.904362 -0.785491 1.469559
P 2.360394 0.406140 -0.259127	P 2.237842 0.489135 -0.198611	P 2.178538 0.510998 -0.151537
O 0.979755 1.018295 -0.801799	O 0.806745 1.078967 -0.623976	O 0.735115 1.110645 -0.518083
C 0.466744 2.249929 -0.250342	C 0.249915 2.213165 0.076027	C 0.159856 2.143485 0.312258
O -1.201663 -0.149567 2.751919	O -1.173547 -0.620359 2.716744	O -1.210160 -0.947270 2.660308
O -0.490718 -1.592814 -1.533550	O -0.462623 -1.547009 -1.709981	O -0.459352 -1.468895 -1.826219
S 3.869249 1.610353 -0.115873	S 3.669710 1.758073 0.093094	S 3.593744 1.772425 0.238433
O 2.438872 -0.787471 -1.322426	O 2.364060 -0.532608 -1.423385	O 2.316921 -0.404897 -1.455210
C 3.536234 -1.723079 -1.271948	C 3.518383 -1.392229 -1.527686	C 3.485977 -1.232366 -1.631283
H 0.479735 -2.266120 2.061546	H 0.582812 -2.596307 1.764307	H 0.587198 -2.748930 1.562825
H 0.989799 -2.346855 0.355014	H 1.072796 -2.429114 0.056959	H 1.084963 -2.446791 -0.123987
H -3.625459 1.533114 2.013534	H -3.412219 1.338507 2.168927	H -3.228119 1.197907 2.265661
H -2.784172 -0.000375 -2.695469	H -2.682668 0.262267 -2.687628	H -2.456827 0.559234 -2.661071
H -5.080396 2.311600 0.133051	H -4.723095 2.500662 0.382432	H -4.318286 2.705433 0.588518
H -4.667568 1.564996 -2.173899	H -4.332244 2.013151 -1.997957	H -3.754588 2.498673 -1.814671
H 4.478724 -1.203437 -1.456595	H 4.421897 -0.791046 -1.647918	H 4.377307 -0.606706 -1.710956
H 3.561414 -2.225861 -0.301564	H 3.598107 -2.028818 -0.642561	H 3.583905 -1.932403 -0.797301
H 3.342650 -2.445839 -2.062057	H 3.350401 -2.002788 -2.412681	H 3.322697 -1.777361 -2.558976
H -0.461071 2.448433 -0.785840	H -0.726900 2.386007 -0.376994	H -0.810279 2.369200 -0.128850
H 0.265195 2.130297 0.819071	H 0.135845 1.984577 1.140612	H 0.032331 1.780239 1.336942
H 1.179758 3.059901 -0.415370	H 0.890425 3.086436 -0.060071	H 0.796729 3.030179 0.298937
O -3.676221 -2.345456 -0.496983	O -3.342373 -1.936384 -0.780169	O -3.293615 -1.574697 -1.004809
H -4.397918 -1.787814 -0.139158	H -4.177399 -1.568363 -0.435077	H -4.203126 -1.259075 -0.879127

Table S60. Optimized Cartesian coordinates for the stationary points involved in the C4-addition pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

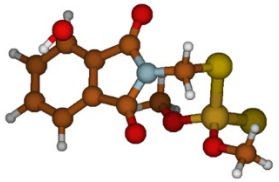
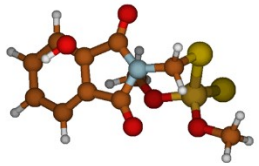
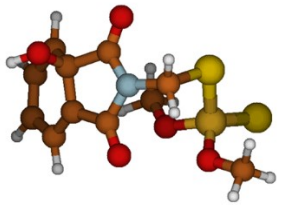
MCR(C4-add)	TS(C4-add)	Adduct(C4-add)
		
C -3.952561 -1.953971 0.640651	C -3.720647 -1.988704 0.724760	C 3.426643 2.094139 0.754897
C -2.862776 -1.447839 1.362324	C -2.718394 -1.332888 1.465347	C 2.567398 1.277563 1.524569
C -2.122992 -0.447109 0.760046	C -2.107000 -0.254668 0.872265	C 2.158552 0.087415 0.993540
C -2.445010 0.043791 -0.505007	C -2.501662 0.226544 -0.398363	C 2.716914 -0.469362 -0.278359
C -3.520192 -0.446662 -1.226990	C -3.427374 -0.496610 -1.175474	C 3.315943 0.581433 -1.155780
C -4.274294 -1.464335 -0.628296	C -4.052943 -1.585777 -0.575808	C 3.722784 1.757825 -0.600849
C -0.931623 0.293258 1.253380	C -0.921112 0.521834 1.308162	C 0.953414 -0.662552 1.345483
N -0.606071 1.217751 0.249844	N -0.586537 1.360907 0.233645	N 0.617269 -1.423901 0.201973
C -1.464935 1.109622 -0.847257	C -1.453656 1.199809 -0.845486	C 1.529443 -1.275709 -0.825445
C 0.600168 1.997132 0.236900	C 0.652729 2.085926 0.150186	C -0.644808 -2.098396 0.044255
S 1.865954 1.397294 -0.965524	S 1.866195 1.349893 -1.029300	S -1.787892 -1.270210 -1.140431
P 2.413448 -0.431541 -0.107656	P 2.290881 -0.485682 -0.114041	P -2.249814 0.491346 -0.106576
O 1.075080 -1.308057 0.014809	O 0.894994 -1.260530 0.052910	O -0.860344 1.236608 0.188664
C 0.503798 -1.920317 -1.160839	C 0.282880 -1.904563 -1.085686	C -0.167073 1.923233 -0.875179
O -1.375330 1.780848 -1.855579	O -1.340145 1.759115 -1.914310	O 1.419813 -1.762652 -1.930767
O -0.340713 0.179644 2.306459	O -0.319315 0.474080 2.359738	O 0.287896 -0.649605 2.363693
S 3.900828 -1.210386 -1.070836	S 3.705050 -1.398665 -1.068570	S -3.611098 1.486998 -1.055633
O 2.579489 -0.166042 1.461970	O 2.495388 -0.182406 1.443642	O -2.534587 0.067886 1.409810
C 3.688458 0.622122 1.943142	C 3.651753 0.558660 1.886340	C -3.724654 -0.680532 1.735971
H 0.387189 3.019321 -0.080156	H 0.479510 3.093847 -0.230858	H -0.489423 -3.094207 -0.375134
H 1.018484 2.006391 1.244334	H 1.087477 2.141042 1.149083	H -1.116320 -2.180905 1.024320
H -3.767391 -0.057281 -2.209310	H -3.664186 -0.181562 -2.186154	H 3.533338 0.321965 -2.187474
H -2.610513 -1.824677 2.348137	H -2.416386 -1.688608 2.444843	H 2.163426 1.634401 2.467727
H -5.125290 -1.879577 -1.157864	H -4.801787 -2.142653 -1.128349	H 4.269991 2.475801 -1.203367
H -4.558934 -2.742065 1.074741	H -4.223666 -2.846673 1.157872	H 3.779974 3.035007 1.160032
H 4.629936 0.116882 1.718271	H 4.561918 0.000611 1.657334	H -4.612530 -0.087477 1.507508
H 3.671529 1.617194 1.490565	H 3.676805 1.542351 1.410098	H -3.742812 -1.623481 1.183058
H 3.548480 0.699560 3.019562	H 3.536055 0.667908 2.962901	H -3.665120 -0.875649 2.804871
H -0.388496 -2.442256 -0.817012	H -0.661171 -2.310839 -0.721962	H 0.707340 2.379428 -0.412634
H 0.231278 -1.152609 -1.892040	H 0.096675 -1.174829 -1.880353	H 0.143044 1.211157 -1.647029
H 1.211882 -2.627741 -1.596769	H 0.925524 -2.708186 -1.449768	H -0.810226 2.693005 -1.306789
O -4.095615 2.073765 0.257429	O -3.700399 1.791857 0.045598	O 3.693492 -1.502988 -0.036085
H -4.527429 1.429754 0.856202	H -4.345769 1.312511 0.598247	H 4.472022 -1.084886 0.365540

Table S61. Optimized Cartesian coordinates for the stationary points involved in the C5-addition pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

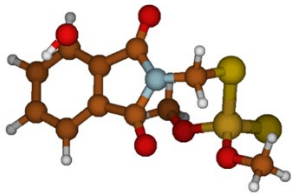
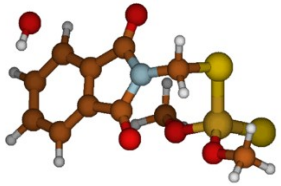
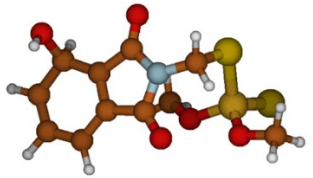
MCR(C5-add)	TS(C5-add)	Adduct(C5-add)
		
C -3.955117 -1.955920 0.633943	C -3.847161 -1.995374 0.360708	C -3.868580 -2.045100 0.107388
C -2.863979 -1.454484 1.356885	C -2.751686 -1.646680 1.166941	C -2.698067 -1.864738 0.909324
C -2.123742 -0.451604 0.758738	C -2.034205 -0.512066 0.811363	C -2.018185 -0.657704 0.780511
C -2.446613 0.045717 -0.503580	C -2.378988 0.256195 -0.287551	C -2.419312 0.343324 -0.074311
C -3.523223 -0.439895 -1.226707	C -3.510615 -0.029502 -1.069198	C -3.657755 0.272449 -0.899105
C -4.277754 -1.459736 -0.632201	C -4.205339 -1.227219 -0.741530	C -4.314132 -1.075285 -0.737662
C -0.931259 0.285383 1.254479	C -0.814838 0.080945 1.425298	C -0.764223 -0.216026 1.460388
N -0.606032 1.214511 0.255017	N -0.507799 1.215316 0.658518	N -0.484272 1.055111 0.957343
C -1.466137 1.112480 -0.841624	C -1.400959 1.368101 -0.405350	C -1.439253 1.433617 -0.005286
C 0.599918 1.994355 0.244924	C 0.729466 1.938372 0.762748	C 0.760773 1.740055 1.151831
S 1.865326 1.400359 -0.960763	S 1.912287 1.599420 -0.613969	S 1.893378 1.684281 -0.308286
P 2.415280 -0.430805 -0.109502	P 2.389117 -0.409850 -0.268239	P 2.378356 -0.350149 -0.383424
O 1.077877 -1.308998 0.010910	O 1.010069 -1.230657 -0.301548	O 0.997246 -1.153316 -0.540289
C 0.504995 -1.916039 -1.166629	C 0.381571 -1.536595 -1.565096	C 0.310739 -1.169191 -1.810054
O -1.377258 1.788722 -1.846672	O -1.338299 2.250541 -1.237252	O -1.391263 2.478856 -0.631539
O -0.339482 0.166421 2.306454	O -0.190951 -0.287946 2.396363	O -0.109945 -0.799471 2.299377
S 3.902836 -1.205018 -1.076145	S 3.793843 -0.983969 -1.469421	S 3.748288 -0.672361 -1.712874
O 2.581924 -0.170186 1.460877	O 2.627832 -0.555744 1.307432	O 2.664090 -0.808058 1.123249
C 3.690045 0.618033 1.943919	C 3.779978 0.059289 1.921285	C 3.838980 -0.330031 1.811137
H 0.386210 3.017764 -0.067653	H 0.547759 3.012870 0.706292	H 0.587852 2.804965 1.315528
H 1.018771 1.999519 1.252161	H 1.192319 1.695494 1.720171	H 1.260120 1.312848 2.022542
H -3.771118 -0.045333 -2.206790	H -3.668749 0.462578 -2.021633	H -3.415570 0.438127 -1.957270
H -2.611150 -1.836378 2.340607	H -2.468414 -2.245849 2.026091	H -2.353850 -2.636394 1.588557
H -5.129813 -1.871421 -1.162839	H -5.050027 -1.523378 -1.354149	H -5.213924 -1.233682 -1.325290
H -4.561812 -2.745494 1.064888	H -4.417870 -2.887248 0.595413	H -4.413581 -2.980158 0.185001
H 4.632173 0.115309 1.716159	H 4.695671 -0.377173 1.517190	H 4.738520 -0.689720 1.307441
H 3.670872 1.614795 1.495153	H 3.766380 1.139741 1.755081	H 3.836061 0.762459 1.852790
H 3.551042 0.691112 3.020765	H 3.696108 -0.156124 2.984684	H 3.778592 -0.742198 2.816513
H -0.386105 -2.440585 -0.823693	H -0.530832 -2.078012 -1.316592	H -0.585478 -1.768645 -1.653069
H 0.230328 -1.145014 -1.893509	H 0.137115 -0.612642 -2.099336	H 0.035216 -0.150894 -2.103274
H 1.212948 -2.620606 -1.607403	H 1.040951 -2.163159 -2.168620	H 0.943934 -1.627550 -2.572300
O -4.097184 2.074331 0.259727	O -4.785219 1.327020 -0.233460	O -4.573145 1.327976 -0.576650
H -4.529722 1.429325 0.856852	H -4.791430 0.967724 0.673646	H -4.831750 1.230447 0.353190

Table S62. Optimized Cartesian coordinates for the stationary points involved in the C6-addition pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

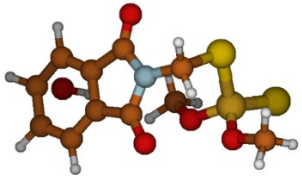
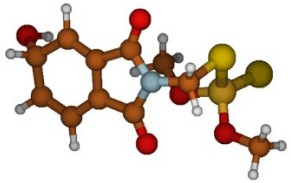
MCR(C6-add)	TS(C6-add)	Adduct(C6-add)
		
C 4.280759 0.341789 1.359774	C 4.173948 0.522787 1.306511	C 4.033262 0.714762 1.338446
C 3.042295 -0.133573 1.807535	C 2.962734 0.039115 1.796182	C 2.859528 0.215243 1.825706
C 2.171353 -0.616385 0.846591	C 2.102274 -0.544131 0.878589	C 2.024423 -0.489042 0.937667
C 2.503562 -0.629287 -0.506954	C 2.425835 -0.661761 -0.478164	C 2.366376 -0.650000 -0.439164
C 3.726263 -0.169377 -0.962575	C 3.617439 -0.199388 -0.984528	C 3.506280 -0.170913 -0.973789
C 4.618796 0.321546 0.001593	C 4.491623 0.461198 -0.076788	C 4.498043 0.526827 -0.082925
C 0.809773 -1.199291 0.995009	C 0.758282 -1.148145 1.085625	C 0.709581 -1.086087 1.153544
N 0.390645 -1.535877 -0.299737	N 0.341274 -1.603821 -0.172859	N 0.297314 -1.599729 -0.097847
C 1.351380 -1.197397 -1.256300	C 1.286446 -1.326452 -1.164185	C 1.231779 -1.352590 -1.099177
C -0.928693 -1.995392 -0.631557	C -0.986058 -2.072889 -0.459293	C -1.028330 -2.085022 -0.358868
S -1.972561 -0.728842 -1.472235	S -2.015898 -0.859565 -1.392708	S -2.069285 -0.922984 -1.347490
P -2.349877 0.588434 0.109222	P -2.298156 0.630825 0.050200	P -2.328412 0.655953 0.002430
O -0.924526 1.060304 0.671359	O -0.843394 1.116578 0.518887	O -0.864825 1.162992 0.418863
C -0.114443 1.995148 -0.069096	C -0.051971 1.986782 -0.316559	C -0.084328 1.960019 -0.496622
O 1.211791 -1.361535 -2.451914	O 1.142786 -1.593223 -2.339923	O 1.089622 -1.664129 -2.266935
O 0.165330 -1.395279 2.003625	O 0.125559 -1.270067 2.112661	O 0.051844 -1.177625 2.176296
S -3.595107 1.965586 -0.437842	S -3.517479 1.983033 -0.606504	S -3.549720 1.969260 -0.726644
O -2.725598 -0.316903 1.375253	O -2.661044 -0.123036 1.415340	O -2.679090 -0.005570 1.417319
C -3.975202 -1.037904 1.399571	C -3.923079 -0.810445 1.544150	C -3.953591 -0.653350 1.611662
H -0.871645 -2.819698 -1.344720	H -0.945268 -2.951126 -1.105863	H -0.988455 -2.992586 -0.963607
H -1.418548 -2.336240 0.281895	H -1.473486 -2.333945 0.481043	H -1.514859 -2.300116 0.593377
H 3.982053 -0.183941 -2.017021	H 3.876096 -0.299364 -2.033293	H 3.745017 -0.272393 -2.028844
H 2.777033 -0.124180 2.859598	H 2.706875 0.107538 2.848081	H 2.563321 0.370265 2.858205
H 5.591258 0.688882 -0.309693	H 5.504314 0.684186 -0.390048	H 5.413866 -0.084423 -0.059807
H 4.994199 0.733292 2.077340	H 4.887266 0.982819 1.981674	H 4.702439 1.281078 1.979109
H -4.812150 -0.337450 1.366821	H -4.747565 -0.102762 1.435724	H -4.760775 0.075924 1.517252
H -4.026603 -1.734506 0.558469	H -3.999906 -1.603752 0.795893	H -4.082499 -1.461709 0.887079
H -3.979292 -1.586994 2.339037	H -3.923129 -1.239339 2.544263	H -3.926585 -1.057909 2.621519
H 0.739145 2.209834 0.572715	H 0.821737 2.244370 0.280758	H 0.863199 2.145818 0.008865
H 0.219595 1.544489 -1.009341	H 0.249522 1.462038 -1.228712	H 0.088262 1.409172 -1.426985
H -0.676657 2.910761 -0.264710	H -0.616291 2.888139 -0.564069	H -0.595390 2.902592 -0.701659
O 3.693082 2.845209 -0.530894	O 3.998200 2.388111 -0.576770	O 4.916464 1.767098 -0.654447
H 2.802223 2.438779 -0.530241	H 3.035616 2.323184 -0.431872	H 4.151279 2.361494 -0.677575

Table S63. Optimized Cartesian coordinates for the stationary points involved in the C7-addition pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

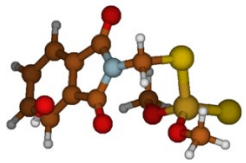
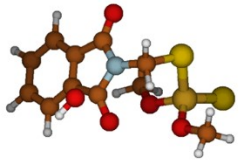
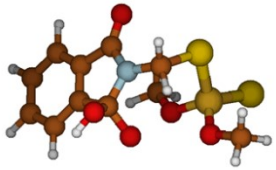
MCR(C7-add)	TS(C7-add)	Adduct(C7-add)
		
C 4.085285 -0.822083 -1.584132	C 4.153895 -0.860083 -1.501423	C 4.289187 -0.586326 -1.488961
C 3.051344 0.121971 -1.612078	C 3.130096 0.083973 -1.645995	C 3.308983 0.412522 -1.516913
C 2.243199 0.197584 -0.491841	C 2.323626 0.304651 -0.544644	C 2.431943 0.466513 -0.446885
C 2.446440 -0.616864 0.619959	C 2.518237 -0.368137 0.657370	C 2.519484 -0.428548 0.611616
C 3.466565 -1.551001 0.660677	C 3.530542 -1.300964 0.813101	C 3.488007 -1.419826 0.652957
C 4.288491 -1.642069 -0.469624	C 4.352184 -1.538379 -0.293985	C 4.379200 -1.486679 -0.421616
C 1.072412 1.071391 -0.218547	C 1.151945 1.217944 -0.380832	C 1.290439 1.426230 -0.192649
N 0.631097 0.739863 1.069692	N 0.660613 0.970492 0.918005	N 0.694335 0.899528 1.023964
C 1.399898 -0.288660 1.624827	C 1.453499 0.057352 1.603080	C 1.408799 -0.144686 1.556990
C -0.607410 1.198397 1.633697	C -0.601582 1.454788 1.400920	C -0.574198 1.346671 1.526389
S -1.941434 -0.078765 1.657195	S -1.866491 0.130421 1.647058	S -1.866239 0.026545 1.635797
P -2.292346 -0.351015 -0.388193	P -2.242427 -0.468929 -0.320993	P -2.246452 -0.423878 -0.367520
O -0.897537 -0.790393 -1.048726	O -0.833468 -0.888277 -0.962243	O -0.834494 -0.762183 -1.050751
C -0.406307 -2.137274 -0.879322	C -0.234118 -2.157305 -0.626135	C -0.197137 -2.030779 -0.795127
O 1.195862 -0.779041 2.717247	O 1.249543 -0.306235 2.747460	O 1.136927 -0.716493 2.605008
O 0.576001 1.927731 -0.921502	O 0.441252 1.708578 -1.297748	O 0.392372 1.567325 -1.241769
S -3.811977 -1.518485 -0.661578	S -3.664167 -1.783488 -0.361390	S -3.632730 -1.772368 -0.491773
O -2.329610 1.108454 -1.044108	O -2.428659 0.867474 -1.182296	O -2.487043 0.961791 -1.132238
C -3.413719 2.009019 -0.736016	C -3.582634 1.705678 -0.966178	C -3.675206 1.732372 -0.856976
H -0.470853 1.466083 2.682748	H -0.489709 1.901744 2.390746	H -0.488561 1.698006 2.557452
H -0.939693 2.073647 1.073751	H -0.978685 2.203097 0.702216	H -0.935600 2.162505 0.897922
H 3.621105 -2.184932 1.527652	H 3.673198 -1.829174 1.750304	H 3.543814 -2.117814 1.482367
H 2.887541 0.762352 -2.473089	H 2.971965 0.613322 -2.580332	H 3.236589 1.109100 -2.346749
H 5.099658 -2.362637 -0.482136	H 5.154983 -2.264357 -0.218233	H 5.149811 -2.250532 -0.433226
H 4.741887 -0.920377 -2.442291	H 4.805995 -1.071694 -2.342515	H 4.990822 -0.667002 -2.312955
H -4.362672 1.576590 -1.059926	H -4.496417 1.147764 -1.181439	H -4.564501 1.158773 -1.126313
H -3.436432 2.220601 0.336276	H -3.593704 2.075210 0.062532	H -3.707095 2.013259 0.198955
H -3.205196 2.920956 -1.292052	H -3.476478 2.536978 -1.660396	H -3.598829 2.622662 -1.478094
H 0.548971 -2.169808 -1.402262	H 0.721086 -2.180459 -1.150077	H 0.776166 -1.976504 -1.282079
H -0.260746 -2.357308 0.183170	H -0.071895 -2.228719 0.454231	H -0.072741 -2.189633 0.280854
H -1.105374 -2.848681 -1.323125	H -0.873035 -2.973771 -0.968181	H -0.791410 -2.838209 -1.227415
O 2.714508 3.422817 -0.108616	O 1.895199 2.888962 -0.237313	O 1.670567 2.759941 0.038297
H 3.072908 3.106670 -0.963516	H 2.390269 2.998488 -1.075237	H 2.237838 3.062180 -0.691430

Table S64. Optimized Cartesian coordinates for the stationary points involved in the C9-addition pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

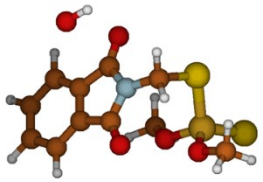
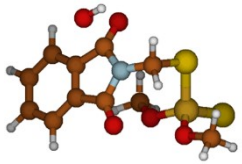
MCR(C9-add)	TS(C9-add)	Adduct(C9-add)
		
C -3.897268 -2.239592 0.459481	C -3.942648 -2.114236 0.364425	C -4.164358 -1.816122 0.377997
C -2.811151 -1.808325 1.231454	C -2.856627 -1.741105 1.162783	C -3.034334 -1.562334 1.160477
C -2.128155 -0.691802 0.783175	C -2.174319 -0.591382 0.799401	C -2.251212 -0.472275 0.812033
C -2.500699 -0.021825 -0.380421	C -2.548535 0.162781 -0.307753	C -2.582853 0.340390 -0.265666
C -3.574623 -0.434255 -1.148719	C -3.621848 -0.191532 -1.104100	C -3.696386 0.102324 -1.053821
C -4.272151 -1.565543 -0.706841	C -4.316790 -1.354125 -0.749048	C -4.491040 -0.995801 -0.708102
C -0.943154 -0.000462 1.356401	C -0.965328 0.027390 1.400595	C -1.014509 0.048744 1.443837
N -0.666060 1.071961 0.494074	N -0.662346 1.137684 0.611811	N -0.675170 1.195349 0.758241
C -1.553092 1.105737 -0.583031	C -1.594522 1.308380 -0.429583	C -1.517069 1.411681 -0.426006
C 0.512305 1.887680 0.574208	C 0.560907 1.879474 0.704301	C 0.588990 1.854872 0.903086
S 1.767021 1.522968 -0.730738	S 1.779774 1.518522 -0.639377	S 1.775384 1.562079 -0.486239
P 2.354001 -0.417265 -0.207887	P 2.277384 -0.472304 -0.239550	P 2.206387 -0.480050 -0.239326
O 1.028717 -1.322155 -0.216174	O 0.911324 -1.314344 -0.269464	O 0.814336 -1.266178 -0.278656
C 0.446474 -1.739247 -1.469592	C 0.268227 -1.601302 -1.529354	C 0.297748 -1.809354 -1.513985
O -1.500910 1.917917 -1.487177	O -1.314501 1.952883 -1.477668	O -0.836700 1.061414 -1.569134
O -0.322027 -0.250756 2.367355	O -0.334424 -0.320525 2.379906	O -0.409516 -0.404254 2.405836
S 3.833571 -0.997277 -1.312607	S 3.704065 -1.056517 -1.411429	S 3.589297 -1.031675 -1.475237
O 2.545205 -0.425190 1.380999	O 2.502478 -0.585341 1.341192	O 2.470605 -0.667089 1.329512
C 3.632742 0.310648 1.978802	C 3.643262 0.051409 1.952993	C 3.630956 -0.070667 1.945307
H 0.256383 2.937797 0.419373	H 0.366031 2.950093 0.609329	H 0.460201 2.940063 0.910361
H 0.955630 1.760680 1.562775	H 1.015637 1.677341 1.675235	H 1.040662 1.536721 1.844254
H -3.860204 0.092802 -2.053384	H -3.908124 0.400226 -1.967630	H -3.942168 0.737799 -1.898209
H -2.516113 -2.328094 2.137164	H -2.554726 -2.328841 2.023685	H -2.777854 -2.188676 2.009038
H -5.119415 -1.927482 -1.279898	H -5.162153 -1.673611 -1.349700	H -5.376546 -1.218050 -1.294618
H -4.459096 -3.114031 0.770805	H -4.503124 -3.010667 0.608354	H -4.801923 -2.661028 0.616428
H 4.588400 -0.076957 1.619825	H 4.566728 -0.379238 1.560370	H 4.541081 -0.489450 1.510821
H 3.541432 1.375183 1.747642	H 3.617616 1.129213 1.772064	H 3.612639 1.015045 1.818457
H 3.540019 0.152051 3.051421	H 3.555990 -0.150495 3.018795	H 3.565828 -0.323998 3.001675
H -0.444176 -2.308436 -1.205291	H -0.633923 -2.159319 -1.280064	H -0.755123 -2.019162 -1.323689
H 0.169937 -0.865797 -2.068970	H 0.004749 -0.669448 -2.040531	H 0.391630 -1.088773 -2.327530
H 1.150004 -2.369079 -2.017409	H 0.926241 -2.206557 -2.156092	H 0.832797 -2.730064 -1.751767
O -3.359355 3.129233 0.095247	O -2.668162 2.725137 0.019593	O -2.063580 2.691880 -0.476617
H -2.660287 3.805076 -0.022273	H -2.041099 3.472960 0.113227	H -1.392494 3.321454 -0.787892

Table S65. Optimized Cartesian coordinates for the stationary points involved in the P12-addition pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

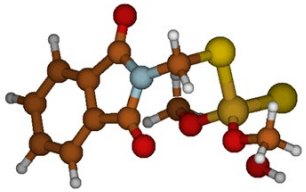
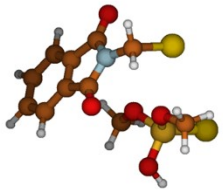
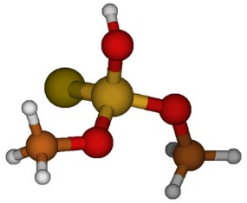
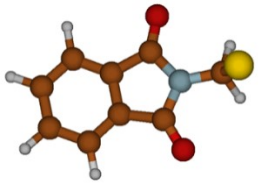
MCR(P12-add)				TS(P12-add)				MCP(P12-add)				Product1(P12-add)				Product2(P12-add)			
																			
C	-4.225282	-1.849103	0.444628	C	-4.298160	-1.758857	0.388925	C	-3.736812	-1.945862	0.489443	P	0.005266	0.044001	0.325265	C	-0.608413	3.430079	-0.698840
C	-3.150581	-1.422614	1.234605	C	-3.209181	-1.392851	1.189796	C	-2.730009	-1.368817	1.274832	O	-0.561955	-0.048762	1.816878	C	-0.305053	2.271723	-1.425733
C	-2.464879	-0.300181	0.805742	C	-2.482432	-0.285697	0.790293	C	-2.173950	-0.190190	0.812630	O	1.440397	-0.634176	0.486790	C	-0.005467	1.134876	-0.696981
C	-2.822871	0.381130	-0.356068	C	-2.813720	0.438590	-0.352978	C	-2.589625	0.401006	-0.377467	O	-0.797886	-1.125967	-0.409760	C	-0.005467	1.134876	0.696981
C	-3.884195	-0.029116	-1.143445	C	-3.888581	0.088509	-1.150766	C	-3.587149	-0.154830	-1.159005	S	-0.048173	1.790942	-0.513519	C	-0.305053	2.271723	1.425733
C	-4.585086	-1.165550	-0.720980	C	-4.631265	-1.032218	-0.758323	C	-4.158613	-1.349760	-0.702736	C	2.282913	-0.805361	-0.673620	C	-0.608413	3.430079	0.698840
C	-1.278041	0.374280	1.392415	C	-1.273644	0.332600	1.395151	C	-1.073570	0.637967	1.379081	C	-2.179105	-0.925361	-0.775701	C	0.347762	-0.236109	-1.154792
N	-0.990510	1.458712	0.547237	N	-0.947705	1.428208	0.582442	N	-0.886291	1.698546	0.487763	H	-0.528476	0.782797	2.318201	N	0.602990	-0.978820	-0.000000
C	-1.866661	1.504073	-0.542958	C	-1.817106	1.531843	-0.506985	C	-1.760420	1.616813	-0.594497	H	3.180635	-1.307048	-0.317635	C	0.347762	-0.236109	1.154792
C	0.217716	2.226928	0.621766	C	0.294729	2.145749	0.676170	C	0.180693	2.668795	0.572888	H	-2.759438	-0.619232	0.097937	C	0.862361	-2.396113	-0.000000
S	1.450017	1.817773	-0.698041	S	1.510427	1.719311	-0.641692	S	1.397186	2.573156	-0.756307	H	2.538525	0.169046	-1.095028	S	-0.608413	-3.438430	-0.000001
P	1.933705	-0.144005	-0.187073	P	1.968427	-0.292184	-0.168567	P	1.947076	-1.099624	-0.066241	H	1.775327	-1.424107	-1.416661	O	0.411704	-0.680825	2.284004
O	0.592500	-1.002166	-0.209045	O	0.556939	-1.029383	-0.231615	O	0.407853	-0.987410	-0.473056	H	-2.533607	-1.887567	-1.140618	O	0.411704	-0.680825	-2.284004
C	0.019592	-1.438641	-1.463348	C	-0.000818	-1.419028	-1.506041	C	-0.222988	-2.124952	-1.101392	H	-2.248486	-0.173413	-1.564205	H	1.457097	-2.646265	0.883426
O	-1.797582	2.320583	-1.439443	O	-1.722042	2.369922	-1.381845	O	-1.796829	2.418445	-1.508955					H	1.457097	-2.646265	-0.883426
O	-0.656187	0.101295	2.396819	O	-0.665337	0.009092	2.393733	O	-0.460669	0.479009	2.415600					H	-0.304894	2.266131	2.510860
S	3.395084	-0.709280	-1.382281	S	3.418207	-0.672757	-1.482311	S	3.247888	-1.253634	-1.494947					H	-0.304894	2.266131	-2.510860
O	2.186781	-0.195570	1.380768	O	2.200765	-0.265766	1.404729	O	2.007426	0.211431	0.838161					H	-0.849134	4.345087	1.229965
C	3.375386	0.399664	1.949797	C	3.390986	0.339080	1.955660	C	3.262581	0.628025	1.413554					H	-0.849134	4.345087	-1.229965
H	0.009352	3.286744	0.466767	H	0.122137	3.216163	0.554296	H	-0.232471	3.682908	0.544337								
H	0.667293	2.079939	1.604482	H	0.729180	1.955888	1.658407	H	0.679684	2.534898	1.535680								
H	-4.156998	0.502552	-2.049228	H	-4.141293	0.653472	-2.042116	H	-3.905959	0.309153	-2.086760								
H	-2.864412	-1.951071	2.138126	H	-2.943795	-1.954408	2.079624	H	-2.395536	-1.830330	2.198415								
H	-5.422364	-1.525210	-1.309942	H	-5.480939	-1.344806	-1.356333	H	-4.940722	-1.824488	-1.286004								
H	-4.788844	-2.728012	0.739803	H	-4.894147	-2.623690	0.661126	H	-4.197919	-2.874055	0.810864								
H	4.254215	-0.169691	1.640688	H	4.261627	-0.272251	1.708000	H	3.957662	0.921080	0.623451								
H	3.463473	1.444084	1.640473	H	3.512944	1.356690	1.575952	H	3.028088	1.483283	2.046460								
H	3.242319	0.338092	3.027790	H	3.235779	0.357144	3.032477	H	3.686071	-0.178985	2.016195								
H	-0.896177	-1.964962	-1.196533	H	-0.959839	-1.881876	-1.275293	H	-0.270722	-2.957656	-0.396418								
H	-0.211645	-0.574813	-2.093958	H	-0.149550	-0.537908	-2.137805	H	-1.227233	-1.802165	-1.374219								
H	0.712709	-2.112670	-1.970026	H	0.658562	-2.139004	-1.994927	H	0.329429	-2.412476	-1.999517								
O	2.996710	-2.711754	-0.140665	O	2.768038	-2.415731	-0.087498	O	1.975608	-2.306304	0.993414								
H	3.809097	-2.596006	0.381749	H	3.566940	-2.416374	0.466625	H	2.638408	-2.989542	0.801544								

Table S66. Optimized Cartesian coordinates for the stationary points involved in the S17-addition pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

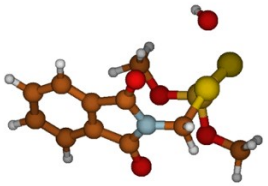
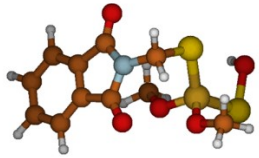
MCR(S17-add)	TS(S17-add)	Adduct(S17-add)
		
C 4.415279 -0.045836 -1.623912	C -4.298951 -1.331446 1.206059	C -3.999152 -1.930606 0.994384
C 3.357535 0.860991 -1.481738	C -3.281364 -0.500693 1.691465	C -3.035786 -1.127214 1.617044
C 2.539680 0.700815 -0.377396	C -2.540942 0.196206 0.753237	C -2.465055 -0.126352 0.851147
C 2.754531 -0.311782 0.555448	C -2.792448 0.083969 -0.612368	C -2.830200 0.081759 -0.476742
C 3.797377 -1.211920 0.427639	C -3.796498 -0.731193 -1.104193	C -3.783343 -0.702636 -1.102192
C 4.630951 -1.061820 -0.687665	C -4.551671 -1.444020 -0.164610	C -4.365753 -1.722066 -0.338976
C 1.335152 1.466647 0.038073	C -1.385305 1.112715 0.937091	C -1.394784 0.846659 1.192971
N 0.888535 0.871951 1.228821	N -1.005549 1.525439 -0.349572	N -1.181514 1.616632 0.040246
C 1.685814 -0.221077 1.584929	C -1.796070 0.920792 -1.331776	C -1.995213 1.190167 -1.012162
C -0.377014 1.157425 1.843921	C 0.229939 2.198938 -0.638922	C -0.026797 2.456096 -0.145644
S -1.634171 -0.175891 1.599433	S 1.516348 1.077205 -1.364531	S 1.260721 1.701749 -1.231922
P -1.977301 0.019510 -0.446536	P 1.907202 -0.288206 0.228561	P 1.930613 -0.065405 -0.117267
O -0.604132 -0.241495 -1.213778	O 0.508305 -0.986083 0.606405	O 0.546124 -0.865488 0.182367
C -0.025203 -1.561981 -1.330410	C -0.008116 -2.022863 -0.257791	C 0.056144 -1.757499 -0.837402
O 1.484500 -0.924471 2.554404	O -1.641534 1.079370 -2.526601	O -1.974879 1.664482 -2.131275
O 0.815040 2.425531 -0.491739	O -0.852837 1.477576 1.964008	O -0.807617 0.999397 2.243780
S -3.545832 -1.022098 -1.023368	S 3.507242 -1.625454 0.285176	S 3.599015 -1.730176 0.186434
O -2.072892 1.577589 -0.765683	O 2.000486 0.617347 1.545154	O 2.071619 0.516020 1.390897
C -3.194014 2.361438 -0.297041	C 3.063921 1.582279 1.693899	C 3.072763 1.513385 1.669956
H -0.269223 1.220000 2.928209	H 0.075023 2.972158 -1.393732	H -0.311006 3.386766 -0.640518
H -0.747138 2.107734 1.457423	H 0.602890 2.651419 0.280431	H 0.391141 2.679485 0.836680
H 3.957935 -2.000781 1.155175	H -3.985775 -0.818594 -2.169104	H -4.060329 -0.540585 -2.138816
H 3.183697 1.649603 -2.206453	H -3.077379 -0.412784 2.753649	H -2.743137 -1.287625 2.649625
H 5.459074 -1.748119 -0.830491	H -5.346871 -2.098717 -0.505644	H -5.113648 -2.365564 -0.790504
H 5.079702 0.038754 -2.477456	H -4.901634 -1.901255 1.905581	H -4.468545 -2.732535 1.554560
H -4.099240 2.064134 -0.829311	H 4.032656 1.077926 1.687289	H 4.043832 1.213959 1.265367
H -3.322451 2.234965 0.780983	H 3.015037 2.324710 0.893449	H 2.772309 2.475712 1.247828
H -2.941134 3.394736 -0.525506	H 2.893983 2.058865 2.657399	H 3.130846 1.583416 2.754929
H 0.906788 -1.419436 -1.876115	H -0.958874 -2.326551 0.179922	H -0.830878 -2.235919 -0.421117
H 0.174317 -1.973612 -0.337207	H -0.167018 -1.630035 -1.266963	H -0.211255 -1.196390 -1.738851
H -0.697566 -2.214067 -1.891091	H 0.682440 -2.869734 -0.280826	H 0.806947 -2.517663 -1.074480
O -2.557402 -2.842145 0.197438	O 3.616217 -1.528659 -1.540666	O 3.857919 -2.059254 -1.440240
H -2.406385 -3.339865 -0.625076	H 3.088812 -2.274921 -1.872127	H 3.207089 -2.714990 -1.738164

Table S67. Vibrational frequencies and rotational constants for the stationary points involved in the H20-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H20-abs) $C_1 - {}^2A$	TS(H20-abs) $C_1 - {}^2A$	MCP(H20-abs) $C_1 - {}^2A$	Rad(H20-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
26, 33, 44, 59, 70, 91, 101, 111, 116, 134, 145, 149, 166, 184, 190, 195, 212, 234, 253, 272, 292, 331, 363, 386, 396, 409, 425, 463, 477, 487, 525, 540, 559, 617, 648, 676, 687, 709, 730, 733, 792, 810, 818, 832, 847, 922, 933, 1003, 1010, 1040, 1045, 1056, 1102, 1119, 1122, 1168, 1181, 1183, 1191, 1201, 1205, 1236, 1311, 1324, 1346, 1397, 1430, 1455, 1478, 1480, 1485, 1486, 1490, 1497, 1510, 1510, 1687, 1690, 1757, 1855, 3081 3090, 3134, 3174, 3179, 3202, 3206, 3217, 3234, 3241, 3247, 3252, 3557	**1291i**, 22, 41, 58, 60, 78, 85, 99, 113, 121, 131, 146, 165, 178, 185, 188, 207, 230, 238, 263, 268, 295, 331, 360, 386, 396, 411, 423, 466, 489, 522, 539, 611, 644, 677, 686, 706, 730, 736, 772, 791, 810, 819, 837, 862, 908, 922, 994, 1003, 1029, 1041, 1051, 1055, 1101, 1106, 1121, 1169, 1180, 1183, 1191, 1200, 1205, 1235, 1241, 1313, 1349, 1399, 1406, 1443, 1479, 1480, 1484, 1485, 1490, 1492, 1510, 1511, 1686, 1688, 1773, 1859, 3081, 3090, 3173, 3174, 3179, 3207, 3218, 3235, 3242, 3248, 3253, 3698	31, 37, 44, 69, 72, 109, 112, 118, 124, 129, 139, 151, 162, 183, 186, 191, 199, 210, 243, 249, 279, 287, 318, 336, 364, 386, 395, 407, 412, 424, 463, 463, 467, 535, 547, 611, 642, 675, 702, 726, 732, 787, 802, 809, 820, 838, 900, 922, 1003, 1036, 1042, 1056, 1061, 1098, 1111, 1121, 1168, 1178, 1181, 1191, 1203, 1207, 1251, 1311, 1341, 1399, 1411, 1478, 1481, 1484, 1485, 1489, 1490, 1509, 1509, 1625, 1685, 1688, 1771, 1859, 3090, 3091, 3180, 3183, 3209, 3218, 3234, 3241, 3247, 3252, 3261, 3749, 3891	32, 43, 70, 102, 110, 115, 122, 140, 157, 159, 179, 187, 190, 196, 237, 245, 277, 281, 317, 356, 383, 393, 409, 422, 459, 461, 463, 534, 546, 610, 642, 674, 702, 721, 731, 785, 803, 805, 820, 838, 899, 920, 1001, 1036, 1039, 1057, 1058, 1101, 1113, 1122, 1169, 1179, 1182, 1191, 1203, 1207, 1251, 1311, 1345, 1400, 1408, 1480, 1482, 1484, 1484, 1489, 1492, 1509, 1510, 1685, 1689, 1774, 1861, 3091, 3092, 3180, 3184, 3209, 3217, 3233, 3241, 3247, 3252, 3259
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.42058, 0.20803, 0.18298	0.41750, 0.20792, 0.18165	0.37883, 0.22112, 0.20147	0.52946, 0.23389, 0.21740

Table S68. Vibrational frequencies and rotational constants for the stationary points involved in the H21-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H21-abs) $C_1 - {}^2A$	TS(H21-abs) $C_1 - {}^2A$	MCP(H21-abs) $C_1 - {}^2A$	Rad(H21-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
24, 40, 53, 60, 70, 101, 106, 117, 125, 135, 149, 156, 171, 191, 199, 208, 216, 236, 254, 271, 304, 333, 359, 379, 387, 397, 410, 427, 467, 495, 524, 541, 580, 619, 650, 677, 690, 709, 731, 734, 791, 810, 817, 828, 845, 920, 931, 1001, 1009, 1040, 1045, 1051, 1103, 1115, 1124, 1168, 1178, 1183, 1190, 1201, 1205, 1235, 1311, 1327, 1344, 1398, 1439, 1460, 1479, 1481, 1482, 1486, 1491, 1498, 1510, 1511, 1688, 1691, 1761, 1853, 3083, 3088, 3139, 3174, 3177, 3206, 3208, 3209, 3234, 3242, 3248, 3252, 3559	**1324i**, 29, 52, 64, 66, 93, 116, 123, 126, 139, 147, 154, 169, 174, 193, 197, 205, 234, 253, 267, 286, 305, 332, 361, 387, 401, 413, 425, 465, 474, 522, 540, 606, 640, 672, 679, 698, 724, 731, 760, 781, 793, 811, 824, 839, 884, 923, 958, 1004, 1034, 1041, 1053, 1053, 1100, 1107, 1118, 1169, 1175, 1184, 1191, 1200, 1205, 1238, 1261, 1312, 1331, 1395, 1404, 1427, 1478, 1481, 1484, 1485, 1486, 1499, 1511, 1512, 1687, 1691, 1772, 1859, 3082, 3092, 3165, 3177, 3183, 3206, 3219, 3233, 3241, 3248, 3252, 3683	19, 33, 39, 59, 68, 81, 95, 103, 119, 136, 141, 148, 156, 177, 189, 195, 204, 232, 259, 262, 269, 324, 344, 354, 364, 387, 395, 411, 418, 457, 462, 470, 524, 540, 573, 613, 639, 674, 705, 722, 731, 785, 806, 808, 819, 834, 900, 919, 1001, 1036, 1039, 1057, 1057, 1101, 1115, 1121, 1169, 1178, 1183, 1191, 1202, 1207, 1251, 1312, 1349, 1397, 1410, 1479, 1481, 1486, 1486, 1489, 1501, 1510, 1511, 1630, 1684, 1691, 1769, 1859, 3082, 3088, 3175, 3176, 3208, 3216, 3235, 3243, 3249, 3253, 3272, 3756, 3906	32, 43, 70, 102, 111, 115, 122, 140, 157, 160, 179, 188, 190, 196, 237, 245, 277, 281, 317, 357, 383, 393, 409, 422, 459, 461, 463, 534, 546, 610, 642, 674, 702, 721, 731, 784, 803, 805, 820, 838, 899, 920, 1001, 1036, 1039, 1057, 1058, 1101, 1113, 1122, 1169, 1179, 1182, 1191, 1203, 1207, 1251, 1311, 1345, 1400, 1408, 1480, 1482, 1484, 1484, 1489, 1492, 1509, 1510, 1685, 1689, 1774, 1861, 3091, 3092, 3180, 3184, 3209, 3217, 3233, 3241, 3247, 3252, 3259
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.44676, 0.19445, 0.18127	0.45443, 0.20342, 0.19180	0.45313, 0.18690, 0.16688	0.52944, 0.23391, 0.21741

Table S69. Vibrational frequencies and rotational constants for the stationary points involved in the H22-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H22-abs) $C_1 - {}^2A$	TS(H22-abs) $C_1 - {}^2A$	MCP(H22-abs) $C_1 - {}^2A$	Rad(H22-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
9, 28, 48, 69, 81, 98, 110, 117, 125, 134, 150, 156, 171, 182, 193, 199, 205, 235, 255, 272, 303, 334, 370, 389, 398, 411, 426, 467, 469, 493, 522 ,539, 570, 620, 652, 677, 692, 711, 731, 735, 793, 808, 817, 831, 847, 920, 936, 1001, 1012, 1038, 1055, 1057, 1111, 1120, 1128, 1170, 1182, 1184, 1198, 1201, 1207, 1236, 1316, 1326, 1354, 1398, 1435, 1458, 1479, 1483, 1484, 1487, 1494, 1499, 1510, 1513, 1688, 1690, 1758, 1855, 3081, 3090, 3136, 3174, 3180, 3204, 3205, 3219, 3234, 3241, 3248, 3253, 3506	**1574i**, 19, 41, 49, 78, 85, 95, 117, 121, 124, 143, 156, 168, 181, 188, 193, 205, 235, 257, 270, 302, 334, 340, 358, 383, 395, 405, 425, 432, 461, 494, 533, 549, 621, 645, 650, 688, 706, 730, 737, 776, 791, 815, 830, 844, 849, 899, 934, 964, 1025, 1028, 1055, 1074, 1120, 1124, 1132, 1170, 1179, 1183, 1201, 1206, 1231, 1268, 1324, 1351, 1383, 1406, 1433, 1458, 1479, 1482, 1483, 1486, 1492, 1496, 1497, 1521, 1666, 1690, 1767, 1859, 3079, 3091, 3139, 3173, 3180, 3204, 3207, 3217, 3237, 3246, 3253, 3663	24, 29, 50, 71, 78, 92, 107, 118, 125, 135, 148, 152, 171, 183, 191, 195, 207, 227, 234, 251, 272, 304, 334, 358, 372, 390, 401, 426, 433, 459, 493, 519, 532, 539, 617, 650, 652, 689, 708, 732, 743, 785, 808, 817, 831, 843, 933, 948, 1013, 1023, 1055, 1065, 1107, 1120, 1128, 1162, 1182, 1184, 1200, 1207, 1222, 1260, 1326, 1353, 1379, 1431, 1452, 1479, 1480, 1482, 1484, 1488, 1488, 1494, 1498, 1611, 1638, 1689, 1766, 1859, 3081, 3090, 3137, 3174, 3180, 3203, 3206, 3219, 3232, 3241, 3250, 3728, 3897	29, 41, 64, 82, 99, 112, 123, 136, 147, 166, 179, 184, 191, 208, 231, 244, 268, 299, 332, 358, 388, 399, 425, 433, 457, 493, 527, 537, 613, 649, 652, 686, 705, 729, 740, 784, 808, 817, 831, 842, 931, 946, 1012, 1022, 1055, 1066, 1105, 1120, 1126, 1162, 1179, 1182, 1201, 1206, 1221, 1260, 1326, 1351, 1376, 1428, 1453, 1478, 1479, 1480, 1482, 1486, 1487, 1491, 1493, 1635, 1688, 1769, 1858, 3080, 3090, 3137, 3173, 3179, 3205, 3207, 3217, 3231, 3240, 3249
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.42636, 0.19319, 0.17420	0.46720, 0.18912, 0.17854	0.43628, 0.18995, 0.17324	0.56199, 0.21172, 0.20648

Table S70. Vibrational frequencies and rotational constants for the stationary points involved in the H23-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H23-abs) $C_1 - {}^2A$	TS(H23-abs) $C_1 - {}^2A$	MCP(H23-abs) $C_1 - {}^2A$	Rad(H23-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
10, 39, 48, 56, 74, 83, 106, 112, 127, 138, 145, 153, 170, 177, 186, 198, 203, 232, 250, 271, 300, 335, 340, 367, 389, 400, 417, 428, 466, 490, 505, 525, 541, 619, 649, 679, 689, 708, 730, 737, 798, 811, 818, 831, 846, 926, 936, 1004, 1010, 1040, 1050, 1056, 1105, 1121, 1124, 1169, 1177, 1182, 1192, 1200, 1206, 1236, 1313, 1323, 1351, 1398, 1434, 1456, 1477, 1480, 1482, 1486, 1490, 1492, 1510, 1512, 1687, 1690, 1759, 1851, 3079, 3089, 3139, 3173, 3178, 3200, 3208, 3217, 3231, 3237, 3244, 3251, 3574	**1579i**, 30, 38, 49, 74, 81, 98, 115, 122, 132, 139, 158, 174, 182, 196, 208, 230, 237, 256, 272, 301, 336, 349, 363, 382, 396, 407, 424, 429, 461, 493, 538, 540, 620, 650, 652, 684, 701, 724, 731, 783, 789, 815, 830, 843, 849, 885, 934, 963, 1024, 1029, 1055, 1073, 1119, 1122, 1131, 1170, 1180, 1186, 1203, 1208, 1231, 1265, 1324, 1346, 1383, 1399, 1433, 1456, 1480, 1483, 1485, 1488, 1492, 1496, 1501, 1519, 1664, 1688, 1769, 1858, 3084, 3090, 3138, 3176, 3179, 3204, 3205, 3217, 3234, 3245, 3250, 3659	15, 30, 44, 52, 65, 72, 95, 108, 119, 125, 138, 150, 155, 174, 184, 190, 192, 198, 230, 248, 270, 293, 303, 337, 365, 389, 401, 427, 435, 457, 491, 501, 525, 541, 617, 649, 652, 687, 705, 731, 746, 780, 810, 817, 830, 842, 931, 945, 1012, 1022, 1057, 1066, 1106, 1121, 1126, 1163, 1177, 1180, 1200, 1205, 1224, 1260, 1324, 1352, 1378, 1429, 1451, 1477, 1478, 1480, 1481, 1484, 1488, 1490, 1490, 1601, 1637, 1688, 1766, 1856, 3078, 3089, 3141, 3171, 3177, 3200, 3209, 3216, 3232, 3242, 3251, 3752, 3894	30, 50, 62, 70, 98, 115, 123, 141, 150, 164, 169, 181, 193, 199, 230, 246, 271, 300, 331, 359, 388, 398, 426, 434, 457, 490, 524, 541, 614, 649, 651, 685, 705, 729, 744, 778, 810, 817, 829, 841, 928, 942, 1012, 1022, 1056, 1066, 1107, 1119, 1122, 1164, 1180, 1184, 1201, 1206, 1223, 1259, 1325, 1343, 1378, 1430, 1450, 1478, 1480, 1480, 1481, 1487, 1488, 1489, 1497, 1637, 1690, 1769, 1858, 3081, 3090, 3136, 3173, 3179, 3204, 3205, 3217, 3231, 3241, 3251
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.44263, 0.21426, 0.19411	0.43802, 0.20367, 0.18616	0.43931, 0.21224, 0.19083	0.56690, 0.20999, 0.20535

Table S71. Vibrational frequencies and rotational constants for the stationary points involved in the H24-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H24-abs) $C_1 - {}^2A$	TS(H24-abs) $C_1 - {}^2A$	MCP(H24-abs) $C_1 - {}^2A$	Rad(H24-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
22, 28, 34 ,47, 56, 65, 91, 113, 118, 131, 136, 148, 167, 176, 185, 196, 198, 203, 233, 245, 268, 290, 333, 358, 387, 396, 412, 425, 467, 492, 525, 540, 612, 616, 648, 676, 688, 708, 730, 735, 794, 811, 817, 830, 846, 920, 934, 999, 1011, 1035, 1043, 1056, 1103, 1120, 1125, 1169, 1180, 1183, 1190, 1200, 1205, 1233, 1310, 1327, 1352, 1397, 1433, 1455, 1478, 1481, 1482, 1487, 1487, 1497, 1508, 1508, 1686, 1689, 1766, 1855, 3081, 3089, 3138, 3173, 3178, 3202, 3208, 3217, 3235, 3242, 3248, 3253, 3730	**1349i**, 27, 44, 62, 64, 73, 77, 101, 122, 130, 143, 150, 170, 182, 195, 197, 205, 220, 235, 248, 271, 295, 332, 336, 377, 395, 409, 426, 430, 481, 495, 534, 577, 616, 649, 658, 694, 705, 729, 754, 787, 795, 816, 832, 858, 875, 933, 937, 1008, 1017, 1057, 1058, 1074, 1120, 1121, 1125, 1180, 1182, 1186, 1203, 1208, 1211, 1241, 1282, 1322, 1351, 1387, 1432, 1454, 1470, 1479, 1481, 1485, 1486, 1491, 1500, 1504, 1670, 1686, 1769, 1859, 3080, 3091, 3138, 3174, 3179, 3205, 3206, 3217, 3239, 3245, 3249, 3758	19, 27, 35, 43, 64, 73, 96, 105, 115, 121, 135, 148, 164, 167, 182, 189, 191, 204, 213, 234, 249, 269, 276, 293, 330, 359, 387, 396, 405, 425, 479, 492, 523, 541, 615, 651, 662, 688, 706, 724, 749, 791, 815, 829, 839, 844, 910, 929, 998, 1012, 1044, 1056, 1099, 1121, 1127, 1173, 1181, 1184, 1201, 1206, 1219, 1264, 1326, 1356, 1386, 1432, 1446, 1453, 1478, 1482, 1483, 1483, 1484, 1491, 1501, 1598, 1644, 1688, 1768, 1859, 3080, 3088, 3136, 3173, 3177, 3204, 3206, 3218, 3233, 3238, 3245, 3830, 3926	22, 43, 59, 63, 94, 113, 121, 135, 148, 165, 183, 192, 202, 215, 232, 247, 269, 290, 332, 357, 387, 396, 405, 426, 472, 491, 522, 540, 614, 648, 656, 685, 705, 724, 749, 791, 816, 827, 836, 842, 906, 926, 996, 1012, 1044, 1057, 1100, 1120, 1122, 1174, 1181, 1185, 1202, 1207, 1220, 1264, 1325, 1344, 1386, 1430, 1445, 1451, 1479, 1481, 1483, 1483, 1487, 1490, 1501, 1643, 1687, 1768, 1858, 3081, 3089, 3137, 3174, 3177, 3204, 3205, 3217, 3232, 3238, 3244
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.54391, 0.16956, 0.16747	0.52174, 0.15875, 0.15621	0.50496, 0.15269, 0.14959	0.56146, 0.21345, 0.20821

Table S72. Vibrational frequencies and rotational constants for the stationary points involved in the H25-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H25-abs) $C_1 - {}^2A$	TS(H25-abs) $C_1 - {}^2A$	MCP(H25-abs) $C_1 - {}^2A$	Rad(H25-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
25, 29, 44, 56, 63, 70, 97, 107, 119, 122, 135, 147, 154, 159, 179, 189, 197, 231, 246, 267, 295, 327, 357, 373, 387, 402, 410, 424, 436, 468, 493, 525, 539, 615, 650, 678, 689, 709, 729, 733, 792, 812, 819, 831, 847, 922, 934, 1002, 1008, 1037, 1044, 1056, 1101, 1120, 1127, 1167, 1177, 1181, 1189, 1203, 1209, 1235, 1310, 1327, 1354, 1395, 1436, 1456, 1476, 1479, 1482, 1485, 1490, 1492, 1507, 1509, 1684, 1686, 1764, 1854, 3081, 3090, 3136, 3172, 3179, 3205, 3217, 3221, 3234, 3241, 3247, 3252, 3733	**1349i**, 27, 46, 60, 68, 71, 87, 98, 115, 120, 125, 137, 159, 169, 186, 196, 201, 218, 236, 248, 270, 286, 329, 342, 381, 394, 398, 426, 431, 478, 496, 528, 583, 615, 652, 661, 692, 703, 729, 753, 786, 790, 817, 833, 858, 873, 928, 935, 1006, 1017, 1057, 1058, 1069, 1119, 1121, 1125, 1179, 1179, 1185, 1202, 1207, 1209, 1244, 1281, 1326, 1347, 1388, 1431, 1452, 1469, 1480, 1482, 1484, 1486, 1491, 1499, 1504, 1670, 1686, 1770, 1859, 3082, 3089, 3138, 3175, 3178, 3204, 3206, 3218, 3239, 3244, 3249, 3763	19, 25, 30, 45, 64, 74, 94, 102, 110, 124, 136, 150, 166, 172, 179, 181, 183, 192, 204, 230, 247, 267, 268, 293, 330, 358, 386, 396, 405, 425, 474, 492, 521, 542, 614, 649, 661, 685, 706, 723, 749, 789, 816, 829, 838, 844, 912, 929, 998, 1011, 1045, 1056, 1100, 1120, 1124, 1174, 1179, 1182, 1200, 1205, 1220, 1265, 1323, 1351, 1386, 1432, 1446, 1453, 1478, 1481, 1483, 1483, 1485, 1490, 1492, 1590, 1643, 1688, 1769, 1859, 3080, 3089, 3136, 3172, 3178, 3203, 3204, 3217, 3233, 3239, 3246, 3833, 3930	30, 47, 64, 75, 98, 113, 118, 135, 150, 165, 181, 183, 194, 202, 231, 250, 272, 300, 332, 359, 387, 396, 404, 426, 472, 491, 521, 541, 614, 648, 657, 685, 705, 724, 746, 788, 816, 828, 837, 843, 907, 927, 995, 1012, 1044, 1057, 1101, 1120, 1122, 1174, 1181, 1183, 1201, 1206, 1220, 1264, 1323, 1346, 1387, 1431, 1447, 1453, 1478, 1480, 1481, 1483, 1487, 1489, 1497, 1643, 1688, 1769, 1858, 3080, 3090, 3136, 3173, 3179, 3203, 3204, 3217, 3233, 3240, 3247
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.46833, 0.18981, 0.17493	0.46778, 0.17198, 0.15955	0.45294, 0.16392, 0.15074	0.56316, 0.21320, 0.20915

Table S73. Vibrational frequencies and rotational constants for the stationary points involved in the H26-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H26-abs) $C_1 - {}^2A$	TS(H26-abs) $C_1 - {}^2A$	MCP(H26-abs) $C_1 - {}^2A$	Rad(H26-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
18, 27, 48, 53, 69, 96, 104, 117, 124, 129, 138, 147, 161, 167, 182, 185, 192, 197, 232, 246, 273, 294, 333, 357, 388, 393, 412, 426, 428, 465, 497, 526, 540, 616, 655, 678, 687, 707, 729, 734, 794, 810, 818, 827, 847, 921, 934, 1001, 1011, 1037, 1045, 1053, 1102, 1119, 1125, 1167, 1180, 1182, 1190, 1200, 1205, 1235, 1310, 1329, 1351, 1397, 1433, 1454, 1478, 1482, 1483, 1487, 1489, 1499, 1509, 1510, 1688, 1690, 1766, 1856, 3081, 3089, 3139, 3174, 3177, 3204, 3208, 3219, 3232, 3239, 3245, 3251, 3688	**1096i**, 22, 30, 41, 55, 64, 83, 110, 125, 133, 148, 166, 174, 185, 192, 198, 199, 233, 246, 271, 292, 299, 334, 357, 387, 397, 411, 425, 465, 495, 526, 540, 616, 651, 678, 687, 707, 729, 734, 774, 795, 797, 810, 828, 846, 920, 934, 952, 1001, 1012, 1037, 1044, 1081, 1102, 1124, 1156, 1167, 1182, 1189, 1202, 1218, 1235, 1272, 1309, 1329, 1352, 1396, 1397, 1432, 1437, 1453, 1479, 1484, 1495, 1497, 1508, 1510, 1688, 1690, 1767, 1856, 3083, 3118, 3139, 3178, 3207, 3208, 3221, 3233, 3240, 3246, 3251, 3694	21, 28, 45, 56, 73, 100, 108, 121, 134, 140, 149, 162, 170, 178, 187, 190, 195, 198, 234, 244, 246, 272, 302, 329, 357, 372, 390, 400, 412, 426, 467, 496, 527, 540, 551, 615, 653, 678, 685, 707, 729, 734, 795, 803, 812, 830, 848, 921, 936, 1001, 1012, 1038, 1047, 1074, 1103, 1123, 1168, 1172, 1183, 1191, 1202, 1219, 1237, 1312, 1329, 1349, 1398, 1435, 1456, 1475, 1481, 1484, 1496, 1510, 1511, 1605, 1689, 1690, 1768, 1857, 3083, 3137, 3178, 3188, 3205, 3207, 3233, 3240, 3246, 3251, 3346, 3787, 3879	27, 42, 64, 94, 106, 118, 131, 147, 150, 165, 173, 186, 193, 207, 232, 246, 271, 306, 330, 358, 389, 399, 411, 426, 466, 494, 526, 535, 539, 615, 654, 678, 685, 707, 729, 734, 794, 803, 811, 829, 847, 921, 935, 1002, 1012, 1040, 1046, 1075, 1102, 1125, 1167, 1174, 1180, 1191, 1201, 1216, 1237, 1312, 1329, 1354, 1396, 1435, 1457, 1474, 1479, 1482, 1491, 1509, 1510, 1688, 1688, 1768, 1856, 3082, 3135, 3176, 3192, 3203, 3207, 3233, 3240, 3246, 3251, 3350
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.46615, 0.19536, 0.18017	0.51854, 0.17560, 0.16952	0.48150, 0.18266, 0.17146	0.56060, 0.21312, 0.20822

Table S74. Vibrational frequencies and rotational constants for the stationary points involved in the H27-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H27-abs) $C_1 - {}^2A$	TS(H27-abs) $C_1 - {}^2A$	MCP(H27-abs) $C_1 - {}^2A$	Rad(H27-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
24, 41, 46, 57, 63, 72, 97, 105, 122, 126, 141, 150, 165, 171, 181, 195, 199, 230, 244, 264, 273, 289, 333, 358, 387, 398, 410, 425, 467, 476, 491, 525, 540, 615, 643, 679, 688, 709, 730, 734, 794, 810, 818, 832, 848, 919, 934, 1000, 1011, 1040, 1046, 1056, 1103, 1117, 1120, 1168, 1182, 1185, 1191, 1201, 1206, 1236, 1310, 1319, 1341, 1397, 1430, 1451, 1480, 1481, 1482, 1486, 1491, 1496, 1510, 1511, 1689, 1689, 1767, 1856, 3082, 3098, 3138, 3175, 3188, 3204, 3209, 3218, 3232, 3240, 3246, 3251, 3741	**1101i**, 23, 36, 48, 65, 78, 105, 112, 121, 132, 144, 147, 168, 174, 180, 195, 203, 232, 246, 265, 288, 298, 332, 358, 385, 397, 411, 425, 466, 495, 526, 540, 616, 652, 679, 688, 707, 730, 733, 736, 792, 794, 811, 826, 845, 907, 920, 935, 1001, 1011, 1039, 1047, 1080, 1103, 1125, 1160, 1169, 1184, 1191, 1201, 1204, 1235, 1240, 1312, 1329, 1347, 1369, 1398, 1433, 1451, 1477, 1482, 1483, 1495, 1511, 1511, 1556, 1689, 1690, 1765, 1855, 3081, 3120, 3142, 3175, 3207, 3214, 3228, 3233, 3241, 3247, 3252, 3750	21, 28, 45, 52, 67, 97, 106, 120, 123, 135, 146, 149, 167, 183, 189, 200, 207, 222, 233, 246, 274, 298, 305, 331, 358, 388, 400, 411, 413, 425, 467, 496, 532, 540, 618, 654, 679, 685, 692, 707, 730, 735, 795, 798, 811, 829, 850, 923, 936, 1003, 1013, 1040, 1047, 1075, 1103, 1126, 1169, 1174, 1183, 1191, 1202, 1213, 1237, 1312, 1329, 1359, 1398, 1434, 1458, 1470, 1480, 1486, 1495, 1510, 1511, 1612, 1689, 1690, 1766, 1855, 3084, 3134, 3178, 3180, 3203, 3208, 3233, 3241, 3247, 3252, 3335, 3790, 3906	27, 38, 60, 73, 102, 118, 123, 147, 164, 179, 182, 186, 191, 201, 231, 246, 274, 305, 330, 358, 388, 398, 411, 425, 466, 494, 526, 540, 615, 618, 653, 678, 686, 707, 729, 733, 793, 804, 811, 828, 847, 921, 935, 1002, 1011, 1040, 1046, 1075, 1102, 1120, 1167, 1171, 1178, 1191, 1200, 1211, 1237, 1312, 1326, 1345, 1397, 1435, 1458, 1469, 1477, 1482, 1492, 1510, 1511, 1688, 1689, 1767, 1856, 3082, 3134, 3175, 3185, 3201, 3207, 3233, 3240, 3246, 3251, 3343
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.46485, 0.19717, 0.18160	0.46817, 0.19185, 0.17994	0.43638, 0.19452, 0.17624	0.55997, 0.21367, 0.20891

Table S75. Vibrational frequencies and rotational constants for the stationary points involved in the H28-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H28-abs) $C_1 - {}^2A$	TS(H28-abs) $C_1 - {}^2A$	MCP(H28-abs) $C_1 - {}^2A$	Rad(H28-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
24, 40, 53, 59, 70, 100, 106, 117, 125, 135, 149, 155, 171, 190, 199, 208, 217, 235, 254, 271, 303, 333, 358, 376, 387, 397, 410, 427, 467, 495, 524, 541, 580, 619, 650, 677, 690, 709, 731, 734, 791, 810, 817, 828, 845, 920, 931, 1001, 1009, 1040, 1045, 1051, 1103, 1115, 1124, 1168, 1178, 1183, 1190, 1201, 1205, 1235, 1311, 1327, 1344, 1398, 1439, 1460, 1479, 1481, 1482, 1487, 1490, 1498, 1510, 1511, 1688, 1691, 1761, 1853, 3083, 3088, 3140, 3174, 3177, 3206, 3208, 3209, 3234, 3242, 3248, 3252, 3560	**1228i**, 32, 40, 51, 74, 88, 100, 117, 129, 133, 149, 165, 169, 190, 194, 215, 231, 250, 268, 271, 300, 329, 361, 389, 393, 411, 421, 466, 490, 493, 527, 541, 617, 650, 677, 686, 707, 731, 735, 775, 793, 810, 818, 842, 850, 918, 921, 933, 1001, 1012, 1039, 1047, 1079, 1103, 1123, 1157, 1167, 1184, 1188, 1191, 1205, 1237, 1311, 1320, 1332, 1347, 1348, 1399, 1437, 1453, 1458, 1482, 1486, 1498, 1511, 1511, 1521, 1689, 1691, 1763, 1853, 3082, 3113, 3139, 3175, 3205, 3209, 3210, 3234, 3241, 3247, 3252, 3622	28, 38, 54, 58, 74, 92, 101, 114, 126, 131, 151, 161, 173, 190, 197, 207, 216, 232, 242, 256, 277, 294, 307, 334, 364, 390, 401, 411, 428, 462, 469, 493, 526, 541, 618, 641, 655, 678, 684, 707, 730, 736, 794, 798, 813, 826, 847, 922, 934, 1004, 1011, 1043, 1046, 1073, 1104, 1120, 1170, 1175, 1186, 1192, 1206, 1218, 1237, 1313, 1325, 1346, 1399, 1435, 1465, 1476, 1484, 1488, 1497, 1512, 1512, 1609, 1689, 1691, 1764, 1854, 3082, 3145, 3177, 3186, 3206, 3218, 3234, 3241, 3247, 3253, 3340, 3745, 3873	27, 38, 59, 73, 102, 117, 123, 147, 164, 180, 180, 186, 191, 200, 231, 246, 274, 305, 330, 358, 388, 398, 411, 425, 466, 494, 526, 540, 615, 617, 653, 678, 686, 707, 729, 733, 793, 804, 811, 828, 847, 922, 935, 1002, 1011, 1040, 1046, 1075, 1102, 1120, 1167, 1171, 1178, 1191, 1200, 1211, 1237, 1312, 1326, 1345, 1397, 1435, 1458, 1470, 1477, 1482, 1492, 1510, 1511, 1689, 1689, 1767, 1856, 3081, 3134, 3175, 3185, 3201, 3207, 3233, 3240, 3246, 3251, 3343
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.44689, 0.19438, 0.18120	0.42493, 0.20861, 0.19135	0.40475, 0.21052, 0.18822	0.55986, 0.21373, 0.20897

Table S76. Vibrational frequencies and rotational constants for the stationary points involved in the H29-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H29-abs) $C_1 - {}^2A$	TS(H29-abs) $C_1 - {}^2A$	MCP(H29-abs) $C_1 - {}^2A$	Rad(H29-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
21, 27, 35, 54, 57, 64, 93, 106, 112, 131, 137, 149, 164, 171, 182, 190, 200, 228, 247, 265, 291, 297, 328, 356, 386, 397, 407, 423, 465, 493, 497, 525, 540, 616, 649, 679, 688, 706, 729, 734, 794, 810, 817, 830, 846, 919, 934, 1000, 1009, 1037, 1046, 1058, 1102, 1123, 1127, 1168, 1179, 1181, 1190, 1200, 1207, 1236, 1311, 1327, 1353, 1397, 1435, 1456, 1473, 1477, 1481, 1485, 1491, 1494, 1508, 1511, 1686, 1687, 1765, 1855, 3073, 3089, 3137, 3165, 3178, 3204, 3205, 3218, 3234, 3241, 3247, 3253, 3728	**1144i**, 25, 47, 51, 73, 82, 92, 101, 110, 120, 131, 152, 160, 170, 177, 193, 228, 245, 262, 293, 304, 324, 357, 373, 391, 410, 417, 425, 470, 493, 526, 539, 616, 650, 679, 688, 708, 730, 732, 758, 795, 810, 833, 843, 848, 920, 932, 935, 1000, 1011, 1036, 1045, 1082, 1103, 1125, 1138, 1168, 1175, 1180, 1189, 1190, 1203, 1235, 1310, 1327, 1350, 1372, 1396, 1421, 1436, 1454, 1480, 1484, 1489, 1490, 1509, 1510, 1687, 1688, 1765, 1855, 3089, 3100, 3133, 3179, 3193, 3202, 3218, 3233, 3241, 3247, 3252, 3739	33, 44, 56, 61, 73, 88, 95, 106, 121, 131, 145, 148, 168, 180, 187, 195, 200, 232, 246, 256, 277, 294, 305, 329, 362, 387, 395, 409, 410, 428, 464, 496, 526, 540, 617, 648, 655, 675, 688, 709, 730, 730, 785, 789, 807, 836, 849, 920, 936, 1000, 1012, 1037, 1045, 1078, 1102, 1123, 1168, 1169, 1181, 1190, 1204, 1212, 1235, 1310, 1325, 1348, 1398, 1437, 1457, 1467, 1481, 1486, 1490, 1509, 1511, 1609, 1688, 1690, 1764, 1852, 3091, 3138, 3182, 3182, 3207, 3220, 3233, 3239, 3245, 3251, 3333, 3792, 3869	31, 45, 61, 74, 97, 108, 115, 134, 148, 150, 176, 184, 195, 199, 232, 246, 273, 293, 328, 357, 387, 397, 409, 423, 464, 493, 526, 539, 615, 648, 654, 674, 687, 708, 729, 730, 788, 791, 807, 835, 848, 919, 935, 999, 1012, 1037, 1045, 1078, 1102, 1121, 1167, 1168, 1183, 1190, 1205, 1212, 1235, 1310, 1326, 1347, 1397, 1435, 1456, 1470, 1483, 1487, 1492, 1510, 1511, 1688, 1690, 1765, 1854, 3091, 3138, 3182, 3183, 3206, 3221, 3233, 3239, 3245, 3251, 3335
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.48121, 0.18611, 0.17791	0.47644, 0.19747, 0.18506	0.46290, 0.20953, 0.18946	0.57592, 0.20837, 0.20408

Table S77. Vibrational frequencies and rotational constants for the stationary points involved in the H30-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H30-abs) $C_1 - {}^2A$	TS(H30-abs) $C_1 - {}^2A$	MCP(H30-abs) $C_1 - {}^2A$	Rad(H30-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
31, 35, 40, 53, 58, 73, 96, 109, 128, 129, 139, 158, 182, 187, 193, 200, 217, 235, 245, 272, 299, 336, 353, 375, 387, 399, 412, 427, 462, 482, 494, 524, 540, 617, 648, 676, 687, 711, 730, 737, 795, 811, 818, 830, 850, 920, 937, 1001, 1010, 1039, 1045, 1056, 1103, 1120, 1124, 1170, 1179, 1183, 1191, 1197, 1204, 1235, 1311, 1328, 1349, 1397, 1434, 1460, 1471, 1479, 1483, 1485, 1490, 1491, 1510, 1511, 1687, 1690, 1758, 1854, 3074, 3089, 3141, 3169, 3177, 3203, 3208, 3217, 3233, 3240, 3246, 3251, 3633	**1168i**, 35, 40, 50, 66, 78, 96, 105, 118, 135, 145, 153, 162, 184, 189, 203, 232, 240, 250, 274, 291, 317, 337, 359, 386, 398, 412, 431, 467, 494, 523, 540, 616, 652, 676, 684, 710, 730, 737, 742, 794, 811, 825, 830, 846, 869, 921, 935, 1002, 1010, 1040, 1045, 1080, 1104, 1120, 1156, 1168, 1182, 1185, 1192, 1205, 1211, 1237, 1311, 1322, 1345, 1349, 1397, 1431, 1456, 1474, 1484, 1485, 1493, 1511, 1512, 1550, 1688, 1691, 1763, 1856, 3090, 3121, 3135, 3179, 3203, 3213, 3219, 3233, 3241, 3247, 3252, 3702	26, 32, 44, 61, 73, 79, 98, 112, 128, 135, 143, 158, 168, 176, 188, 195, 207, 232, 246, 255, 281, 296, 305, 321, 337, 362, 390, 398, 410, 427, 462, 495, 524, 539, 616, 654, 674, 687, 708, 727, 729, 734, 787, 791, 811, 836, 847, 919, 935, 1000, 1010, 1039, 1045, 1078, 1103, 1124, 1169, 1176, 1181, 1191, 1204, 1210, 1236, 1311, 1326, 1349, 1397, 1434, 1457, 1467, 1480, 1486, 1491, 1510, 1510, 1610, 1688, 1689, 1766, 1855, 3092, 3140, 3172, 3182, 3209, 3221, 3233, 3240, 3246, 3252, 3324, 3788, 3870	31, 45, 61, 74, 96, 108, 115, 134, 148, 150, 176, 183, 195, 199, 232, 246, 273, 292, 328, 357, 387, 397, 409, 423, 464, 493, 526, 539, 615, 647, 654, 674, 687, 708, 729, 730, 788, 791, 807, 835, 848, 919, 935, 999, 1012, 1037, 1045, 1078, 1102, 1121, 1167, 1168, 1183, 1190, 1205, 1212, 1235, 1310, 1326, 1347, 1397, 1435, 1456, 1470, 1483, 1487, 1492, 1510, 1511, 1688, 1690, 1765, 1854, 3091, 3138, 3182, 3183, 3206, 3221, 3233, 3239, 3245, 3251, 3335
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.43373, 0.21273, 0.19766	0.45020, 0.21677, 0.20481	0.44796, 0.20433, 0.19024	0.57576, 0.20842, 0.20414

Table S78. Vibrational frequencies and rotational constants for the stationary points involved in the H31-abstraction pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(H31-abs) $C_1 - {}^2A$	TS(H31-abs) $C_1 - {}^2A$	MCP(H31-abs) $C_1 - {}^2A$	Rad(H31-abs) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
21, 32, 44, 52, 67, 75, 100, 108, 119, 130, 141, 149, 169, 181, 193, 205, 224, 231, 243, 254, 270, 291, 330, 354, 365, 388, 400, 411, 428, 467, 497, 526, 539, 615, 652, 678, 685, 707, 729, 734, 795, 811, 816, 830, 846, 921, 933, 1002, 1010, 1041, 1045, 1053, 1103, 1119, 1125, 1168, 1180, 1185, 1190, 1202, 1207, 1236, 1312, 1332, 1350, 1396, 1433, 1455, 1479, 1481, 1483, 1487, 1491, 1501, 1510, 1510, 1688, 1688, 1766, 1856, 3080, 3091, 3138, 3172, 3179, 3204, 3206, 3219, 3233, 3240, 3246, 3251, 3697	**1071i**, 17, 28, 37, 45, 66, 95, 101, 115, 133, 142, 144, 153, 173, 183, 194, 198, 228, 246, 265, 291, 306, 332, 358, 387, 395, 410, 424, 466, 495, 525, 540, 616, 648, 678, 685, 707, 729, 734, 764, 783, 794, 811, 835, 845, 920, 932, 973, 1001, 1011, 1040, 1047, 1089, 1103, 1122, 1146, 1169, 1178, 1191, 1202, 1206, 1232, 1236, 1312, 1325, 1347, 1365, 1398, 1433, 1452, 1452, 1479, 1484, 1490, 1493, 1511, 1511, 1689, 1690, 1767, 1856, 3091, 3109, 3137, 3181, 3206, 3208, 3221, 3232, 3240, 3246, 3251, 3700	23, 28, 47, 61, 65, 74, 101, 103, 115, 133, 140, 148, 179, 182, 195, 204, 214, 234, 241, 247, 251, 277, 299, 328, 357, 366, 389, 395, 403, 409, 424, 463, 497, 528, 540, 615, 651, 675, 687, 708, 730, 730, 788, 792, 808, 835, 849, 921, 936, 1001, 1011, 1038, 1045, 1079, 1102, 1129, 1167, 1168, 1182, 1190, 1204, 1213, 1235, 1310, 1332, 1356, 1398, 1436, 1457, 1476, 1483, 1487, 1489, 1509, 1510, 1611, 1688, 1690, 1767, 1855, 3092, 3136, 3183, 3194, 3207, 3222, 3233, 3240, 3246, 3252, 3354, 3782, 3888	27, 45, 55, 62, 93, 106, 122, 137, 144, 153, 178, 188, 192, 219, 233, 245, 270, 293, 304, 328, 357, 388, 398, 409, 423, 464, 495, 526, 539, 615, 656, 675, 687, 708, 729, 730, 788, 791, 808, 835, 846, 923, 932, 1002, 1010, 1037, 1046, 1080, 1102, 1122, 1163, 1168, 1181, 1190, 1204, 1209, 1235, 1311, 1325, 1346, 1397, 1433, 1454, 1472, 1482, 1485, 1489, 1510, 1510, 1688, 1689, 1767, 1855, 3092, 3135, 3183, 3195, 3204, 3220, 3233, 3241, 3247, 3252, 3358
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.45168, 0.20557, 0.18487	0.42298, 0.20277, 0.18124	0.41724, 0.20034, 0.17795	0.57451, 0.20866, 0.20428

Table S79. Vibrational frequencies and rotational constants for the stationary points involved in the C1-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(C1-add) $C_1 - {}^2A$	TS(C1-add) $C_1 - {}^2A$	Adduct(C1-add) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
12, 19, 31, 46, 66, 72, 98, 112, 119, 127, 138, 154, 167, 181, 191, 199, 205, 210, 231, 244, 272, 292, 334, 359, 388, 398, 410, 427, 433, 467, 491, 524, 540, 614, 648, 677, 686, 706, 728, 734, 794, 811, 817, 831, 846, 919, 933, 999, 1009, 1035, 1043, 1055, 1102, 1118, 1121, 1166, 1181, 1183, 1190, 1201, 1207, 1234, 1310, 1326, 1344, 1393, 1431, 1453, 1478, 1482, 1484, 1485, 1490, 1498, 1507, 1509, 1684, 1687, 1767, 1856, 3080, 3087, 3137, 3173, 3176, 3202, 3206, 3214, 3233, 3241, 3247, 3251, 3702	**488i**, 17, 43, 55, 69, 85, 87, 108, 118, 129, 139, 163, 168, 182, 188, 199, 208, 219, 238, 249, 271, 297, 334, 358, 383, 394, 406, 426, 443, 491, 520, 541, 614, 646, 648, 684, 705, 724, 743, 789, 813, 816, 831, 839, 851, 917, 934, 974, 1000, 1017, 1035, 1056, 1098, 1120, 1125, 1161, 1180, 1182, 1187, 1201, 1205, 1224, 1307, 1326, 1354, 1386, 1432, 1455, 1479, 1481, 1482, 1483, 1483, 1490, 1496, 1500, 1635, 1664, 1768, 1856, 3080, 3089, 3137, 3173, 3177, 3202, 3206, 3217, 3244, 3249, 3254, 3260, 3762	30, 35, 49, 75, 84, 98, 108, 115, 140, 151, 161, 178, 183, 193, 206, 217, 237, 271, 295, 318, 335, 343, 369, 380, 394, 425, 435, 460, 491, 513, 532, 607, 629, 650, 672, 690, 712, 750, 758, 788, 816, 827, 834, 871, 915, 929, 994, 1007, 1054, 1057, 1080, 1120, 1123, 1143, 1172, 1179, 1183, 1200, 1207, 1223, 1235, 1295, 1324, 1348, 1354, 1384, 1417, 1432, 1448, 1472, 1477, 1481, 1484, 1487, 1492, 1494, 1562, 1697, 1737, 1823, 3044, 3082, 3089, 3136, 3173, 3178, 3204, 3205, 3217, 3230, 3233, 3244, 3815
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.52451, 0.17135, 0.16922	0.53338, 0.17292, 0.17024	0.53094, 0.17081, 0.16652

Table S80. Vibrational frequencies and rotational constants for the stationary points involved in the C2-addition pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(C2-add) $C_1 - {}^2A$	TS(C2-add) $C_1 - {}^2A$	Adduct(C2-add) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
28, 43, 57, 78, 83, 109, 111, 116, 126, 138, 151, 154, 158, 168, 186, 189, 199, 237, 240, 274, 285, 319, 356, 390, 395, 408, 433, 464, 486, 511, 518, 535, 542, 616, 654, 676, 679, 711, 729, 730, 792, 803, 810, 836, 853, 918, 934, 997, 1015, 1036, 1045, 1054, 1102, 1120, 1122, 1168, 1178, 1183, 1190, 1204, 1208, 1236, 1309, 1323, 1351, 1397, 1440, 1463, 1478, 1481, 1484, 1484, 1486, 1499, 1508, 1509, 1685, 1688, 1769, 1857, 3089, 3090, 3135, 3178, 3186, 3204, 3207, 3217, 3232, 3240, 3246, 3251, 3608	**519i,** 25, 54, 63, 72, 82, 90, 111, 114, 118, 134, 155, 162, 179, 188, 196, 204, 211, 233, 249, 273, 290, 328, 357, 384, 393, 412, 427, 462, 491, 523, 536, 614, 644, 649, 687, 708, 725, 746, 790, 810, 816, 819, 830, 844, 928, 937, 976, 1007, 1031, 1040, 1052, 1094, 1117, 1125, 1167, 1176, 1180, 1182, 1199, 1205, 1234, 1304, 1327, 1352, 1391, 1433, 1455, 1470, 1478, 1479, 1485, 1487, 1491, 1497, 1506, 1643, 1652, 1769, 1857, 3081, 3088, 3135, 3172, 3177, 3204, 3214, 3217, 3238, 3246, 3252, 3255, 3772	35, 42, 65, 93, 96, 103, 115, 134, 143, 158, 161, 173, 174, 186, 187, 208, 232, 270, 279, 304, 323, 352, 372, 390, 399, 419, 426, 469, 488, 523, 538, 579, 620, 650, 669, 687, 704, 743, 757, 800, 816, 834, 840, 890, 917, 932, 1010, 1025, 1035, 1059, 1067, 1113, 1123, 1124, 1172, 1178, 1181, 1200, 1204, 1217, 1243, 1282, 1324, 1348, 1380, 1403, 1410, 1435, 1456, 1472, 1475, 1480, 1481, 1483, 1487, 1490, 1570, 1635, 1748, 1833, 3050, 3088, 3090, 3137, 3177, 3181, 3203, 3210, 3216, 3225, 3240, 3253, 3812
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.45497, 0.22464, 0.22034	0.48688, 0.20302, 0.19065	

Table S81. Vibrational frequencies and rotational constants for the stationary points involved in the C3-addition pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(C3-add) $C_1 - {}^2A$	TS(C3-add) $C_1 - {}^2A$	Adduct(C3-add) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
20, 26, 34, 47, 64, 80, 98, 104, 120, 125, 139, 148, 169, 180, 183, 190, 200, 207, 232, 246, 271, 298, 332, 358, 387, 397, 412, 426, 448, 469, 491, 525, 539, 615, 648, 679, 688, 706, 729, 734, 792, 810, 817, 828, 846, 919, 934, 1000, 1010, 1039, 1045, 1056, 1103, 1120, 1126, 1170, 1182, 1186, 1190, 1201, 1205, 1234, 1312, 1331, 1352, 1398, 1434, 1454, 1480, 1481, 1485, 1486, 1491, 1498, 1507, 1510, 1685, 1688, 1766, 1856, 3080, 3089, 3138, 3173, 3177, 3205, 3206, 3216, 3233, 3241, 3247, 3252, 3726	**482i**, 28, 43, 50, 60, 89, 99, 112, 121, 125, 135, 138, 161, 179, 183, 187, 198, 226, 236, 247, 273, 295, 336, 357, 381, 389, 401, 427, 452, 492, 524, 536, 614, 646, 649, 684, 710, 715, 734, 767, 793, 799, 814, 830, 845, 911, 933, 994, 1002, 1034, 1042, 1055, 1104, 1120, 1125, 1163, 1179, 1182, 1185, 1201, 1205, 1225, 1310, 1326, 1349, 1384, 1431, 1455, 1474, 1478, 1480, 1485, 1489, 1489, 1497, 1502, 1627, 1664, 1771, 1864, 3080, 3089, 3137, 3174, 3178, 3199, 3205, 3218, 3238, 3245, 3250, 3255, 3767	38, 57, 65, 73, 89, 105, 120, 126, 138, 160, 172, 184, 197, 203, 219, 231, 263, 274, 286, 303, 330, 343, 355, 387, 398, 413, 428, 481, 497, 522, 526, 602, 613, 649, 669, 696, 715, 736, 765, 787, 816, 830, 839, 859, 926, 957, 967, 1003, 1007, 1047, 1054, 1086, 1107, 1118, 1132, 1159, 1172, 1182, 1187, 1201, 1206, 1274, 1323, 1338, 1344, 1356, 1400, 1426, 1434, 1452, 1477, 1480, 1487, 1488, 1491, 1502, 1569, 1642, 1747, 1848, 3082, 3089, 3138, 3174, 3177, 3207, 3211, 3217, 3229, 3231, 3242, 3255, 3804
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.50257, 0.18607, 0.18159	0.49390, 0.20015, 0.19420	0.48499, 0.20914, 0.20192

Table S82. Vibrational frequencies and rotational constants for the stationary points involved in the C4-addition pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(C4-add) $C_1 - {}^2A$	TS(C4-add) $C_1 - {}^2A$	Adduct(C4-add) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
22, 34, 44, 47, 65, 91, 103, 111, 121, 124, 143, 149, 167, 181, 192, 201, 202, 214, 233, 245, 268, 298, 329, 358, 386, 396, 410, 425, 466, 493, 495, 524, 539, 615, 649, 676, 688, 707, 728, 732, 791, 807, 817, 830, 845, 918, 933, 998, 1010, 1037, 1045, 1056, 1101, 1120, 1125, 1168, 1181, 1184, 1190, 1200, 1205, 1233, 1310, 1327, 1352, 1398, 1434, 1456, 1478, 1481, 1484, 1485, 1492, 1496, 1507, 1508, 1685, 1687, 1765, 1855, 3082, 3090, 3138, 3174, 3179, 3205, 3207, 3217, 3233, 3240, 3246, 3251, 3727	**482i**, 30, 45, 59, 84, 92, 96, 115, 119, 128, 143, 144, 167, 171, 183, 187, 200, 210, 233, 248, 271, 295, 334, 356, 381, 389, 399, 426, 453, 492, 524, 538, 614, 646, 650, 687, 702, 715, 742, 777, 797, 815, 817, 831, 846, 912, 932, 994, 1002, 1034, 1042, 1055, 1103, 1120, 1126, 1163, 1181, 1183, 1185, 1200, 1205, 1223, 1309, 1326, 1349, 1384, 1432, 1456, 1473, 1477, 1481, 1483, 1484, 1492, 1502, 1502, 1626, 1665, 1771, 1861, 3080, 3090, 3139, 3174, 3179, 3200, 3207, 3217, 3238, 3244, 3250, 3255, 3765	44, 52, 54, 88, 91, 106, 113, 123, 140, 160, 167, 178, 195, 204, 212, 230, 251, 270, 275, 290, 301, 340, 355, 388, 396, 412, 426, 481, 495, 519, 528, 599, 613, 651, 674, 691, 705, 742, 764, 795, 817, 830, 842, 858, 925, 955, 964, 1003, 1007, 1051, 1055, 1085, 1108, 1120, 1131, 1155, 1173, 1181, 1183, 1199, 1206, 1271, 1324, 1337, 1344, 1354, 1401, 1427, 1430, 1452, 1474, 1481, 1484, 1488, 1492, 1502, 1571, 1643, 1752, 1844, 3080, 3089, 3136, 3170, 3178, 3205, 3207, 3218, 3228, 3230, 3241, 3255, 3799
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.51921, 0.18288, 0.17540	0.50895, 0.19672, 0.18792	0.50364, 0.20401, 0.19329

Table S83. Vibrational frequencies and rotational constants for the stationary points involved in the C5-addition pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(C5-add) $C_1 - {}^2A$	TS(C5-add) $C_1 - {}^2A$	Adduct(C5-add) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
22, 33, 45, 47, 65, 90, 102, 111, 121, 124, 142, 149, 166, 180, 191, 197, 200, 214, 233, 245, 268, 298, 329, 358, 386, 396, 410, 424, 466, 488, 493, 525, 539, 615, 649, 676, 688, 707, 728, 732, 791, 807, 817, 830, 845, 918, 934, 998, 1010, 1037, 1045, 1056, 1101, 1120, 1126, 1168, 1181, 1184, 1190, 1200, 1205, 1233, 1310, 1328, 1352, 1398, 1434, 1456, 1478, 1481, 1483, 1485, 1492, 1496, 1507, 1508, 1685, 1687, 1765, 1855, 3082, 3090, 3138, 3174, 3179, 3205, 3207, 3217, 3233, 3240, 3246, 3251, 3727	**500i**, 21, 46, 58, 71, 80, 92, 111, 120, 128, 142, 157, 170, 182, 196, 203, 221, 232, 240, 248, 269, 289, 333, 356, 384, 394, 412, 426, 461, 492, 522, 537, 613, 647, 648, 686, 707, 726, 739, 795, 808, 815, 820, 830, 845, 930, 939, 980, 1006, 1030, 1040, 1055, 1093, 1119, 1124, 1167, 1177, 1180, 1186, 1203, 1207, 1228, 1303, 1332, 1350, 1386, 1432, 1456, 1478, 1480, 1482, 1487, 1487, 1491, 1499, 1503, 1642, 1654, 1768, 1857, 3080, 3089, 3139, 3173, 3178, 3204, 3207, 3218, 3239, 3246, 3253, 3257, 3769	22, 42, 49, 76, 79, 96, 109, 117, 136, 154, 165, 170, 173, 184, 199, 216, 226, 270, 296, 309, 330, 355, 379, 385, 396, 425, 427, 465, 488, 508, 539, 581, 624, 648, 680, 693, 702, 743, 763, 804, 817, 825, 836, 892, 913, 932, 1011, 1021, 1031, 1057, 1063, 1117, 1122, 1123, 1173, 1179, 1183, 1198, 1206, 1215, 1236, 1285, 1324, 1345, 1378, 1404, 1412, 1432, 1447, 1464, 1476, 1482, 1482, 1485, 1491, 1493, 1571, 1635, 1740, 1833, 3065, 3078, 3089, 3136, 3170, 3177, 3204, 3205, 3216, 3226, 3240, 3255, 3809
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.51955, 0.18274, 0.17524	0.53479, 0.18005, 0.17447	0.53115, 0.18070, 0.17486

Table S84. Vibrational frequencies and rotational constants for the stationary points involved in the C6-addition pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(C6-add) $C_1 - {}^2A$	TS(C6-add) $C_1 - {}^2A$	Adduct(C6-add) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
26, 27, 37, 60, 83, 86, 95, 110, 112, 131, 134, 142, 155, 170, 183, 192, 208, 227, 245, 255, 271, 293, 329, 358, 385, 397, 410, 424, 467, 485, 496, 525, 539, 615, 650, 677, 691, 707, 730, 734, 792, 810, 817, 830, 843, 919, 932, 999, 1009, 1036, 1044, 1059, 1102, 1123, 1126, 1168, 1181, 1184, 1190, 1204, 1218, 1234, 1311, 1328, 1346, 1395, 1433, 1452, 1474, 1482, 1487, 1491, 1495, 1503, 1508, 1509, 1685, 1687, 1765, 1854, 3080, 3090, 3137, 3170, 3179, 3205, 3205, 3217, 3234, 3242, 3248, 3253, 3760	**486i**, 36, 43, 57, 64, 90, 98, 106, 125, 130, 131, 139, 171, 172, 184, 194, 225, 230, 241, 247, 270, 300, 332, 358, 388, 398, 401, 424, 450, 492, 523, 539, 613, 645, 650, 689, 706, 725, 747, 790, 817, 829, 837, 841, 862, 918, 936, 974, 1000, 1018, 1035, 1058, 1097, 1122, 1127, 1161, 1181, 1186, 1188, 1205, 1219, 1224, 1307, 1325, 1353, 1386, 1433, 1456, 1476, 1481, 1482, 1485, 1491, 1493, 1500, 1507, 1635, 1664, 1767, 1854, 3083, 3090, 3139, 3174, 3178, 3208, 3209, 3217, 3243, 3249, 3253, 3260, 3789	24, 42, 65, 73, 78, 109, 120, 127, 143, 146, 162, 175, 184, 194, 208, 218, 234, 269, 300, 324, 337, 345, 380, 392, 396, 425, 428, 471, 489, 506, 532, 603, 626, 648, 668, 692, 712, 743, 764, 789, 816, 822, 833, 868, 916, 929, 994, 1005, 1058, 1061, 1086, 1120, 1123, 1143, 1169, 1181, 1184, 1201, 1207, 1221, 1234, 1297, 1320, 1347, 1349, 1382, 1417, 1430, 1452, 1471, 1478, 1481, 1481, 1487, 1492, 1498, 1559, 1699, 1740, 1819, 3029, 3078, 3091, 3137, 3171, 3179, 3202, 3206, 3218, 3230, 3234, 3244, 3823
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.48511, 0.18051, 0.17189	0.49333, 0.18393, 0.17591	0.50883, 0.17590, 0.17119

Table S85. Vibrational frequencies and rotational constants for the stationary points involved in the C7-addition pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(C7-add) $C_1 - {}^2A$	TS(C7-add) $C_1 - {}^2A$	Adduct(C7-add) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
26, 30, 44, 49, 66, 71, 93, 102, 119, 125, 136, 151, 178, 180, 182, 195, 200, 212, 233, 246, 271, 302, 333, 358, 388, 398, 412, 418, 426, 471, 492, 526, 540, 616, 650, 680, 688, 708, 730, 733, 796, 808, 817, 830, 847, 916, 934, 997, 1010, 1036, 1045, 1057, 1102, 1121, 1124, 1167, 1178, 1182, 1190, 1201, 1206, 1236, 1311, 1326, 1351, 1397, 1436, 1457, 1479, 1481, 1484, 1486, 1489, 1496, 1510, 1511, 1688, 1690, 1763, 1853, 3080, 3088, 3137, 3173, 3176, 3205, 3205, 3216, 3232, 3238, 3245, 3251, 3731	**638i**, 16, 42, 63, 72, 98, 104, 114, 118, 135, 147, 155, 172, 186, 193, 201, 237, 254, 271, 292, 309, 342, 352, 383, 396, 397, 421, 426, 473, 495, 526, 546, 610, 614, 649, 682, 700, 721, 728, 777, 808, 817, 828, 843, 900, 919, 943, 1000, 1018, 1038, 1048, 1057, 1103, 1121, 1125, 1167, 1180, 1184, 1187, 1201, 1206, 1238, 1310, 1321, 1347, 1391, 1432, 1457, 1479, 1481, 1484, 1485, 1490, 1495, 1501, 1513, 1541, 1690, 1692, 1799, 3079, 3088, 3131, 3171, 3176, 3200, 3201, 3217, 3231, 3238, 3243, 3250, 3728	28, 42, 65, 68, 89, 101, 108, 123, 134, 142, 158, 172, 186, 201, 209, 232, 261, 267, 277, 301, 325, 352, 375, 385, 396, 426, 427, 473, 496, 530, 550, 599, 621, 650, 678, 703, 719, 727, 785, 811, 815, 827, 848, 919, 929, 997, 1000, 1036, 1046, 1058, 1088, 1120, 1135, 1153, 1164, 1178, 1180, 1199, 1202, 1205, 1236, 1283, 1314, 1321, 1348, 1368, 1385, 1439, 1466, 1476, 1479, 1484, 1485, 1490, 1497, 1510, 1519, 1686, 1692, 1765, 3080, 3090, 3121, 3171, 3178, 3188, 3203, 3217, 3228, 3234, 3241, 3247, 3795
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.45126, 0.19486, 0.18310	0.48093, 0.19946, 0.19114	0.49801, 0.19860, 0.19055

Table S86. Vibrational frequencies and rotational constants for the stationary points involved in the C9-addition pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(C9-add) $C_1 - {}^2A$	TS(C9-add) $C_1 - {}^2A$	Adduct(C9-add) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
18, 27, 40, 47, 66, 73, 92, 100, 106, 120, 121, 137, 157, 172, 181, 183, 193, 204, 234, 249, 272, 295, 330, 358, 384, 389, 397, 411, 425, 467, 491, 527, 540, 616, 650, 678, 689, 708, 730, 735, 794, 810, 818, 831, 846, 922, 934, 1002, 1012, 1039, 1047, 1057, 1103, 1121, 1124, 1169, 1180, 1184, 1191, 1202, 1207, 1236, 1312, 1329, 1349, 1399, 1435, 1454, 1479, 1480, 1484, 1486, 1491, 1496, 1511, 1512, 1690, 1691, 1760, 1853, 3080, 3090, 3134, 3172, 3178, 3203, 3205, 3217, 3232, 3239, 3244, 3251, 3732	**647i**, 16, 46, 57, 71, 96, 104, 115, 120, 133, 146, 163, 184, 197, 201, 216, 229, 260, 269, 288, 305, 333, 347, 359, 387, 396, 419, 426, 472, 493, 524, 545, 609, 620, 649, 681, 702, 710, 728, 776, 804, 815, 827, 838, 898, 917, 945, 999, 1018, 1037, 1047, 1056, 1102, 1120, 1123, 1167, 1180, 1185, 1186, 1203, 1207, 1238, 1311, 1326, 1350, 1391, 1427, 1452, 1480, 1482, 1486, 1487, 1491, 1491, 1501, 1511, 1536, 1689, 1692, 1807, 3080, 3089, 3128, 3172, 3177, 3198, 3203, 3217, 3231, 3238, 3245, 3250, 3698	25, 43, 62, 64, 92, 103, 114, 127, 140, 143, 162, 166, 176, 195, 202, 229, 263, 268, 274, 313, 336, 356, 369, 393, 421, 425, 437, 481, 489, 521, 560, 601, 639, 658, 675, 698, 713, 733, 778, 807, 815, 828, 844, 913, 923, 977, 998, 1037, 1044, 1055, 1058, 1100, 1119, 1132, 1160, 1170, 1178, 1181, 1204, 1208, 1232, 1247, 1294, 1311, 1337, 1355, 1384, 1424, 1446, 1479, 1481, 1483, 1485, 1491, 1493, 1509, 1514, 1680, 1682, 1761, 3089, 3098, 3122, 3177, 3194, 3196, 3203, 3217, 3231, 3238, 3244, 3250, 3796
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.46306, 0.19296, 0.17676	0.48450, 0.20028, 0.18679	0.50786, 0.20188, 0.19396

Table S87. Vibrational frequencies and rotational constants for the stationary points involved in the P12-addition pathway in gas phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(P12-add) $C_1 - {}^2A$	TS(P12-add) $C_1 - {}^2A$	MCP(P12-add) $C_1 - {}^2A$	Product1(P12-add) $C_1 - {}^2A$	Product2(P12-add) $C_1 - {}^1A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
19, 36, 52, 60, 69, 90, 99, 114, 125, 129, 145, 160, 169, 172, 184, 194, 212, 222, 243, 255, 276, 287, 330, 357, 383, 392, 411, 419, 465, 490, 524, 540, 613, 622, 677, 681, 697, 706, 729, 734, 794, 811, 822, 837, 845, 923, 933, 1003, 1011, 1040, 1047, 1057, 1104, 1118, 1118, 1169, 1178, 1181, 1191, 1203, 1207, 1237, 1312, 1324, 1344, 1399, 1432, 1452, 1480, 1483, 1484, 1486, 1487, 1490, 1512, 1512, 1689, 1691, 1767, 1856, 3084, 3092, 3139, 3179, 3183, 3208, 3209, 3222, 3232, 3239, 3245, 3251, 3805	**215i**, 21, 43, 44, 57, 91, 103, 112, 127, 145, 151, 157, 175, 187, 195, 206, 236, 247, 294, 309, 319, 347, 366, 378, 399, 409, 415, 459, 466, 483, 523, 539, 576, 616, 677, 690, 709, 730, 735, 791, 792, 811, 825, 845, 848, 923, 933, 1003, 1009, 1039, 1046, 1063, 1103, 1113, 1119, 1168, 1176, 1180, 1191, 1202, 1207, 1236, 1312, 1324, 1345, 1397, 1432, 1457, 1478, 1482, 1484, 1485, 1488, 1491, 1510, 1511, 1689, 1690, 1763, 1853, 3081, 3089, 3138, 3176, 3178, 3206, 3206, 3218, 3232, 3240, 3246, 3251, 3813	28, 34, 43, 61, 66, 73, 78, 86, 107, 113, 148, 156, 162, 170, 174, 192, 202, 228, 238, 269, 297, 330, 339, 367, 395, 410, 415, 467, 482, 520, 539, 615, 623, 679, 691, 716, 729, 741, 779, 792, 808, 832, 839, 888, 902, 919, 999, 1004, 1037, 1037, 1044, 1059, 1102, 1105, 1126, 1167, 1182, 1185, 1189, 1207, 1211, 1233, 1300, 1311, 1340, 1395, 1413, 1454, 1479, 1482, 1486, 1491, 1494, 1495, 1509, 1510, 1689, 1690, 1754, 1848, 3089, 3091, 3097, 3164, 3179, 3180, 3204, 3210, 3231, 3238, 3244, 3250, 3813	61, 77, 124, 133, 164, 213, 239, 288, 329, 396, 420, 470, 616, 814, 834, 911, 1051, 1076, 1107, 1179, 1182, 1209, 1210, 1478, 1481, 1487, 1488, 1492, 1493, 3092, 3093, 3182, 3183, 3214, 3216, 3805	39, 50, 127, 138, 184, 237, 281, 343, 367, 413, 466, 524, 538, 619, 675, 680, 714, 733, 737, 741, 793, 811, 889, 921, 1002, 1006, 1040, 1046, 1076, 1103, 1170, 1189, 1232, 1310, 1321, 1337, 1398, 1403, 1449, 1510, 1511, 1689, 1690, 1756, 1848, 3110, 3154, 3232, 3240, 3247, 3251
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.48136, 0.19813, 0.18448	0.50061, 0.19708, 0.18722	0.39418, 0.23316, 0.19162	2.00720, 1.66892, 1.38915	1.50573, 0.49208, 0.39851

Table S88. Vibrational frequencies and rotational constants for the stationary points involved in the S17-addition pathway in aqueous phase calculated at the M06-2X/6-31+G(d,p) level of theory.

MCR(S17-add) $C_1 - {}^2A$	TS(S17-add) $C_1 - {}^2A$	Adduct(S17-add) $C_1 - {}^2A$
Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})	Vibrational frequencies (cm^{-1})
28, 44, 60, 87, 96, 97, 105, 116, 118, 136, 149, 163, 165, 177, 194, 209, 214, 236, 248, 263, 288, 303, 331, 358, 385, 391, 412, 418, 468, 488, 524, 540, 613, 625, 679, 680, 684, 707, 729, 735, 798, 810, 814, 827, 844, 924, 933, 1004, 1010, 1039, 1045, 1059, 1103, 1121, 1125, 1169, 1180, 1183, 1191, 1200, 1206, 1236, 1311, 1327, 1352, 1397, 1433, 1454, 1476, 1481, 1484, 1486, 1491, 1495, 1510, 1510, 1688, 1689, 1767, 1855, 3087, 3093, 3136, 3183, 3184, 3207, 3208, 3221, 3233, 3241, 3247, 3252, 3797	**462i**, 24, 45, 56, 63, 72, 86, 98 ,118, 138, 150, 154, 170, 176, 178, 183, 206, 245, 249, 275, 284, 305, 323, 355, 379, 380, 409, 411, 418, 466, 492, 520, 540, 615, 670, 679, 703, 728, 735, 796, 806, 812, 819, 839, 921, 928, 1002, 1009, 1040, 1046, 1052, 1068, 1103, 1113, 1117, 1168, 1177, 1179, 1191, 1199, 1205, 1236, 1304, 1313, 1347, 1397, 1432, 1456, 1475, 1481, 1482, 1482, 1489, 1491, 1511, 1511, 1689, 1690, 1764, 1854, 3078, 3090, 3132, 3168, 3178, 3200, 3204, 3217, 3233, 3240, 3247, 3251, 3790	27, 33, 53, 56, 71, 81, 85, 101, 113, 131, 145, 151, 161, 169, 185, 186, 212, 240, 263, 272, 288, 316, 341, 356, 366, 376, 393, 408, 422, 467, 518, 539, 615, 679, 684, 705, 729, 732, 761, 788, 793, 796, 811, 838, 920, 929, 1001, 1008, 1039, 1045, 1053, 1103, 1112, 1116, 1168, 1177, 1180, 1191, 1191, 1203, 1208, 1235, 1306, 1314, 1349, 1395, 1430, 1456, 1479, 1481, 1486, 1488, 1489, 1493, 1510, 1511, 1689, 1690, 1760, 1852, 3068, 3080, 3133, 3151, 3163, 3190, 3203, 3207, 3233, 3240, 3246, 3251, 3800
Rotational constants (GHz)	Rotational constants (GHz)	Rotational constants (GHz)
0.48193, 0.19436, 0.18803	0.48595, 0.18982, 0.18610	0.44286, 0.19425, 0.17693

Table S89. Rate constants in aqueous phase calculated at the M06-2X/6-311++G(3df,3pd)//M06-2X/6-31+G(d,p) level of theory.

(a) abstraction pathways

T (K)	k (L mol^{-1} s^{-1})												
	H20-abs	H21-abs	H22-abs	H23-abs	H24-abs	H25-abs	H26-abs	H27-abs	H28-abs	H29-abs	H30-abs	H31-abs	FHT
253	4.33×10^{7}	1.13×10^{7}	1.16×10^{5}	7.90×10^{4}	2.04×10^{4}	3.73×10^{4}	2.13×10^{7}	5.61×10^{6}	8.10×10^{6}	5.17×10^{6}	1.87×10^{7}	5.47×10^{7}	1.69E+08
258	4.32×10^{7}	1.09×10^{7}	1.20×10^{5}	8.01×10^{4}	2.24×10^{4}	4.09×10^{4}	2.17×10^{7}	5.77×10^{6}	7.84×10^{6}	5.22×10^{6}	1.86×10^{7}	5.67×10^{7}	1.70E+08
263	4.29×10^{7}	1.06×10^{7}	1.24×10^{5}	8.17×10^{4}	2.46×10^{4}	4.49×10^{4}	2.22×10^{7}	5.94×10^{6}	7.62×10^{6}	5.29×10^{6}	1.84×10^{7}	5.85×10^{7}	1.72E+08
268	4.27×10^{7}	1.03×10^{7}	1.29×10^{5}	8.37×10^{4}	2.70×10^{4}	4.93×10^{4}	2.26×10^{7}	6.11×10^{6}	7.42×10^{6}	5.36×10^{6}	1.83×10^{7}	6.03×10^{7}	1.73E+08
273	4.25×10^{7}	1.00×10^{7}	1.35×10^{5}	8.60×10^{4}	2.98×10^{4}	5.42×10^{4}	2.30×10^{7}	6.30×10^{6}	7.25×10^{6}	5.45×10^{6}	1.82×10^{7}	6.20×10^{7}	1.75E+08
278	4.23×10^{7}	9.80×10^{6}	1.41×10^{5}	8.88×10^{4}	3.28×10^{4}	5.96×10^{4}	2.35×10^{7}	6.49×10^{6}	7.11×10^{6}	5.54×10^{6}	1.81×10^{7}	6.37×10^{7}	1.77E+08
283	4.22×10^{7}	9.60×10^{6}	1.49×10^{5}	9.20×10^{4}	3.61×10^{4}	6.56×10^{4}	2.40×10^{7}	6.69×10^{6}	6.99×10^{6}	5.64×10^{6}	1.80×10^{7}	6.55×10^{7}	1.79E+08
288	4.21×10^{7}	9.44×10^{6}	1.56×10^{5}	9.55×10^{4}	3.97×10^{4}	7.21×10^{4}	2.45×10^{7}	6.90×10^{6}	6.88×10^{6}	5.74×10^{6}	1.80×10^{7}	6.72×10^{7}	1.81E+08
293	4.22×10^{7}	9.30×10^{6}	1.65×10^{5}	9.95×10^{4}	4.38×10^{4}	7.94×10^{4}	2.50×10^{7}	7.12×10^{6}	6.80×10^{6}	5.86×10^{6}	1.79×10^{7}	6.90×10^{7}	1.84E+08
298	4.22×10^{7}	9.19×10^{6}	1.74×10^{5}	1.04×10^{5}	4.82×10^{4}	8.73×10^{4}	2.55×10^{7}	7.35×10^{6}	6.72×10^{6}	5.98×10^{6}	1.79×10^{7}	7.09×10^{7}	1.86E+08
303	4.23×10^{7}	9.10×10^{6}	1.84×10^{5}	1.09×10^{5}	5.31×10^{4}	9.60×10^{4}	2.61×10^{7}	7.59×10^{6}	6.67×10^{6}	6.11×10^{6}	1.80×10^{7}	7.28×10^{7}	1.89E+08
308	4.25×10^{7}	9.03×10^{6}	1.94×10^{5}	1.14×10^{5}	5.84×10^{4}	1.06×10^{5}	2.67×10^{7}	7.84×10^{6}	6.62×10^{6}	6.24×10^{6}	1.80×10^{7}	7.47×10^{7}	1.92E+08
313	4.28×10^{7}	8.98×10^{6}	2.06×10^{5}	1.20×10^{5}	6.42×10^{4}	1.16×10^{5}	2.73×10^{7}	8.10×10^{6}	6.59×10^{6}	6.38×10^{6}	1.80×10^{7}	7.67×10^{7}	1.95E+08
318	4.30×10^{7}	8.94×10^{6}	2.18×10^{5}	1.26×10^{5}	7.06×10^{4}	1.27×10^{5}	2.79×10^{7}	8.36×10^{6}	6.56×10^{6}	6.53×10^{6}	1.81×10^{7}	7.88×10^{7}	1.99E+08
323	4.34×10^{7}	8.92×10^{6}	2.31×10^{5}	1.33×10^{5}	7.75×10^{4}	1.40×10^{5}	2.86×10^{7}	8.64×10^{6}	6.55×10^{6}	6.69×10^{6}	1.82×10^{7}	8.09×10^{7}	2.02E+08

(b) addition pathways

T (K)	k (L mol^{-1} s^{-1})												
	C1-add	C2-add	C3-add	C4-add	C5-add	C6-add	C7-add	C9-add	P-12add	S17-add	RAF	SET	Overall
253	5.84×10^{5}	3.32×10^{5}	2.26×10^{5}	1.21×10^{5}	1.87×10^{5}	5.81×10^{5}	1.04×10^{-4}	2.26×10^{-4}	4.44×10^{8}	9.06×10^{-3}	4.46E+08	5.30E-19	6.15E+08
258	6.45×10^{5}	3.66×10^{5}	2.53×10^{5}	1.36×10^{5}	2.09×10^{5}	6.32×10^{5}	1.69×10^{-4}	3.65×10^{-4}	5.42×10^{8}	1.42×10^{-2}	5.44E+08	2.33E-18	7.14E+08
263	7.10×10^{5}	4.02×10^{5}	2.83×10^{5}	1.52×10^{5}	2.32×10^{5}	6.86×10^{5}	2.70×10^{-4}	5.80×10^{-4}	6.43×10^{8}	2.18×10^{-2}	6.46E+08	9.69E-18	8.17E+08
268	7.80×10^{5}	4.40×10^{5}	3.15×10^{5}	1.69×10^{5}	2.57×10^{5}	7.44×10^{5}	4.26×10^{-4}	9.08×10^{-4}	7.45×10^{8}	3.31×10^{-2}	7.48E+08	3.83E-17	9.21E+08
273	8.54×10^{5}	4.81×10^{5}	3.50×10^{5}	1.88×10^{5}	2.85×10^{5}	8.04×10^{5}	6.61×10^{-4}	1.40×10^{-3}	8.43×10^{8}	4.94×10^{-2}	8.46E+08	1.44E-16	1.02E+09
278	9.33×10^{5}	5.25×10^{5}	3.87×10^{5}	2.08×10^{5}	3.14×10^{5}	8.67×10^{5}	1.01×10^{-3}	2.12×10^{-3}	9.33×10^{8}	7.28×10^{-2}	9.37E+08	5.15E-16	1.11E+09
283	1.02×10^{6}	5.71×10^{5}	4.28×10^{5}	2.30×10^{5}	3.45×10^{5}	9.33×10^{5}	1.52×10^{-3}	3.18×10^{-3}	1.01×10^{9}	1.06×10^{-1}	1.02E+09	1.77E-15	1.20E+09
288	1.11×10^{6}	6.20×10^{5}	4.71×10^{5}	2.53×10^{5}	3.79×10^{5}	1.00×10^{6}	2.26×10^{-3}	4.70×10^{-3}	1.08×10^{9}	1.52×10^{-1}	1.08E+09	5.80E-15	1.26E+09
293	1.20×10^{6}	6.72×10^{5}	5.17×10^{5}	2.78×10^{5}	4.14×10^{5}	1.08×10^{6}	3.32×10^{-3}	6.86×10^{-3}	1.13×10^{9}	2.16×10^{-1}	1.14E+09	1.83E-14	1.32E+09
298	1.30×10^{6}	7.27×10^{5}	5.66×10^{5}	3.04×10^{5}	4.52×10^{5}	1.15×10^{6}	4.82×10^{-3}	9.89×10^{-3}	1.17×10^{9}	3.04×10^{-1}	1.17E+09	5.57E-14	1.36E+09
303	1.40×10^{6}	7.84×10^{5}	6.19×10^{5}	3.32×10^{5}	4.93×10^{5}	1.23×10^{6}	6.91×10^{-3}	1.41×10^{-2}	1.20×10^{9}	4.23×10^{-1}	1.20E+09	1.63E-13	1.39E+09
308	1.51×10^{6}	8.45×10^{5}	6.75×10^{5}	3.62×10^{5}	5.35×10^{5}	1.31×10^{6}	9.80×10^{-3}	1.99×10^{-2}	1.21×10^{9}	5.81×10^{-1}	1.21E+09	4.63E-13	1.41E+09
313	1.63×10^{6}	9.09×10^{5}	7.35×10^{5}	3.94×10^{5}	5.81×10^{5}	1.40×10^{6}	1.37×10^{-2}	2.78×10^{-2}	1.21×10^{9}	7.92×10^{-1}	1.22E+09	1.27E-12	1.41E+09
318	1.75×10^{6}	9.75×10^{5}	7.98×10^{5}	4.28×10^{5}	6.28×10^{5}	1.49×10^{6}	1.91×10^{-2}	3.84×10^{-2}	1.20×10^{9}	1.07×10^{0}	1.21E+09	3.37E-12	1.41E+09
323	1.88×10^{6}	1.05×10^{6}	8.65×10^{5}	4.64×10^{5}	6.79×10^{5}	1.58×10^{6}	2.63×10^{-2}	5.26×10^{-2}	1.19×10^{9}	1.43×10^{0}	1.20E+09	8.70E-12	1.40E+09

Table S90. Branching ratio (Γ, %) in aqueous phase calculated at the M06-2X/6-311++G(3df,3pd)//M06-2X/6-31+G(d,p) level of theory.

(a) abstraction pathways

T (K)	Branching ratio (Γ, %)												
	H20-abs	H21-abs	H22-abs	H23-abs	H24-abs	H25-abs	H26-abs	H27-abs	H28-abs	H29-abs	H30-abs	H31-abs	FHT
253	7.05%	1.84%	0.02%	0.01%	0.00%	0.01%	3.47%	0.91%	1.32%	0.84%	3.05%	8.90%	27.41%
258	6.04%	1.53%	0.02%	0.01%	0.00%	0.01%	3.05%	0.81%	1.10%	0.73%	2.60%	7.94%	23.83%
263	5.25%	1.30%	0.02%	0.01%	0.00%	0.01%	2.71%	0.73%	0.93%	0.65%	2.25%	7.16%	21.01%
268	4.63%	1.12%	0.01%	0.01%	0.00%	0.01%	2.45%	0.66%	0.81%	0.58%	1.99%	6.55%	18.82%
273	4.16%	0.98%	0.01%	0.01%	0.00%	0.01%	2.25%	0.62%	0.71%	0.53%	1.78%	6.07%	17.14%
278	3.80%	0.88%	0.01%	0.01%	0.00%	0.01%	2.11%	0.58%	0.64%	0.50%	1.62%	5.72%	15.88%
283	3.53%	0.80%	0.01%	0.01%	0.00%	0.01%	2.00%	0.56%	0.58%	0.47%	1.51%	5.48%	14.96%
288	3.33%	0.75%	0.01%	0.01%	0.00%	0.01%	1.93%	0.55%	0.54%	0.45%	1.42%	5.32%	14.32%
293	3.19%	0.70%	0.01%	0.01%	0.00%	0.01%	1.89%	0.54%	0.51%	0.44%	1.36%	5.23%	13.91%
298	3.10%	0.68%	0.01%	0.01%	0.00%	0.01%	1.88%	0.54%	0.49%	0.44%	1.32%	5.21%	13.68%
303	3.05%	0.66%	0.01%	0.01%	0.00%	0.01%	1.88%	0.55%	0.48%	0.44%	1.29%	5.24%	13.61%
308	3.03%	0.64%	0.01%	0.01%	0.00%	0.01%	1.90%	0.56%	0.47%	0.44%	1.28%	5.32%	13.67%
313	3.03%	0.64%	0.01%	0.01%	0.00%	0.01%	1.94%	0.57%	0.47%	0.45%	1.28%	5.44%	13.85%
318	3.06%	0.64%	0.02%	0.01%	0.01%	0.01%	1.99%	0.59%	0.47%	0.46%	1.29%	5.60%	14.12%
323	3.10%	0.64%	0.02%	0.01%	0.01%	0.01%	2.05%	0.62%	0.47%	0.48%	1.30%	5.79%	14.49%

(b) addition pathways

T (K)	Branching ratio (Γ, %)												
	C1-add	C2-add	C3-add	C4-add	C5-add	C6-add	C7-add	C9-add	P-12add	S17-add	RAF	SET	Overall
253	0.09%	0.05%	0.04%	0.02%	0.03%	0.09%	0.00%	0.00%	72.26%	0.00%	72.59%	0.00%	100.00%
258	0.09%	0.05%	0.04%	0.02%	0.03%	0.09%	0.00%	0.00%	75.85%	0.00%	76.17%	0.00%	100.00%
263	0.09%	0.05%	0.03%	0.02%	0.03%	0.08%	0.00%	0.00%	78.69%	0.00%	78.99%	0.00%	100.00%
268	0.08%	0.05%	0.03%	0.02%	0.03%	0.08%	0.00%	0.00%	80.89%	0.00%	81.18%	0.00%	100.00%
273	0.08%	0.05%	0.03%	0.02%	0.03%	0.08%	0.00%	0.00%	82.57%	0.00%	82.86%	0.00%	100.00%
278	0.08%	0.05%	0.03%	0.02%	0.03%	0.08%	0.00%	0.00%	83.83%	0.00%	84.12%	0.00%	100.00%
283	0.09%	0.05%	0.04%	0.02%	0.03%	0.08%	0.00%	0.00%	84.74%	0.00%	85.04%	0.00%	100.00%
288	0.09%	0.05%	0.04%	0.02%	0.03%	0.08%	0.00%	0.00%	85.38%	0.00%	85.68%	0.00%	100.00%
293	0.09%	0.05%	0.04%	0.02%	0.03%	0.08%	0.00%	0.00%	85.78%	0.00%	86.09%	0.00%	100.00%
298	0.10%	0.05%	0.04%	0.02%	0.03%	0.08%	0.00%	0.00%	85.99%	0.00%	86.32%	0.00%	100.00%
303	0.10%	0.06%	0.04%	0.02%	0.04%	0.09%	0.00%	0.00%	86.04%	0.00%	86.39%	0.00%	100.00%
308	0.11%	0.06%	0.05%	0.03%	0.04%	0.09%	0.00%	0.00%	85.95%	0.00%	86.33%	0.00%	100.00%
313	0.12%	0.06%	0.05%	0.03%	0.04%	0.10%	0.00%	0.00%	85.75%	0.00%	86.15%	0.00%	100.00%
318	0.12%	0.07%	0.06%	0.03%	0.04%	0.11%	0.00%	0.00%	85.44%	0.00%	85.88%	0.00%	100.00%
323	0.13%	0.07%	0.06%	0.03%	0.05%	0.11%	0.00%	0.00%	85.05%	0.00%	85.51%	0.00%	100.00%

Table S91: Calculated standard enthalpies of reaction ($\Delta_r H_{298K}$) and standard Gibbs energies of reaction ($\Delta_r G_{298K}$), enthalpy of activation ($\Delta H^{\neq}_{298K}$) and Gibbs energy of activation ($\Delta G^{\neq}_{298K}$) at 298 K for FHT reactions in the gas phase using the M06-2X/6-311++G(3df,3pd)// M06-2X/6-31+G(d,p) level of theory.

Position	$\Delta_r H_{298K}$, (kJ/mol)	$\Delta_r G_{298K}$, (kJ/mol)	$\Delta H^{\neq}_{298K}$, (kJ/mol)	$\Delta G^{\neq}_{298K}$, (kJ/mol)
H20	-100.40	-102.16	-13.87	28.60
H21	-100.40	-102.16	-13.87	28.58
H22	-16.20	-17.88	4.21	46.30
H23	-16.20	-17.89	4.21	46.29
H24	-23.79	-27.71	17.49	52.95
H25	-23.88	-26.63	17.01	52.02
H26	-78.33	-78.07	-6.56	36.65
H27	-78.32	-78.05	-5.29	37.92
H28	-78.33	-78.58	2.24	42.64
H29	-78.33	-78.08	2.24	42.68
H30	-78.32	-78.05	-5.50	36.55
H31	-78.32	-78.57	-6.35	38.48

Table S92: Relative standard reaction enthalpies at 0K for reactant complex (RC), transition states (TS), product complex (PC) and product (P) of FHT reactions in the gas phase using the M06-2X/6-311++G(3df,3pd)// M06-2X/6-31+G(d,p) level of theory.

Position	**RC**	**TS**	**PC**	**P**
H20	-30.35	-9.80	-121.25	-101.36
H21	-30.35	-9.80	-121.27	-101.36
H22	-29.25	7.87	-42.52	-16.60
H23	-24.32	7.86	-42.52	-16.60
H24	-27.34	19.63	-33.36	-24.55
H25	-27.35	18.98	-33.33	-24.51
H26	-30.35	-2.29	-102.26	-78.82
H27	-21.84	-1.40	-95.70	-78.81
H28	-27.35	5.95	-102.27	-78.82
H29	-27.35	5.96	-102.24	-78.83
H30	-21.20	-1.22	-93.22	-78.81
H31	-24.32	-1.73	-102.26	-78.81

Table S93: Calculated standard enthalpies of reaction ($\Delta_r H_{298K}$) and standard Gibbs energies of reaction ($\Delta_r G_{298K}$), enthalpy of activation ($\Delta H^{\neq}_{298K}$) and Gibbs energy of activation ($\Delta G^{\neq}_{298K}$) at 298 K for FHT reactions in the aqueous phase using the M06-2X/6-311++G(3df,3pd)// M06-2X/6-31+G(d,p) level of theory.

Positions	$\Delta_r H_{298K}$, **(kJ/mol)**	$\Delta_r G_{298K}$, **(kJ/mol)**	$\Delta H^{\neq}_{298K}$, **(kJ/mol)**	$\Delta G^{\neq}_{298K}$, **(kJ/mol)**
H20	-98.21	-100.78	3.74	41.52
H21	-98.21	-100.74	2.85	45.66
H22	-24.08	-27.07	18.87	58.03
H23	-24.10	-27.12	18.82	59.65
H24	-31.03	-35.46	21.29	59.42
H25	-30.99	-33.81	21.00	57.92
H26	-79.95	-82.78	4.13	41.59
H27	-81.39	-84.96	5.64	43.11
H28	-81.40	-85.04	1.93	45.87
H29	-85.57	-89.85	4.97	45.55
H30	-85.57	-89.91	1.15	42.66
H31	-84.03	-90.43	4.15	38.85

Table S94: Relative standard reaction enthalpies (in kJ/mol) at 0K for reactant complex (RC), transition states (TS), product complex (PC) and product (P) of FHT reactions in the aqueous phase using the M06-2X/6-311++G(3df,3pd)// M06-2X/6-31+G(d,p) level of theory.

Positions	**RC**	**TS**	**PC**	**P**
H20	-15.29	6.83	-110.58	-99.31
H21	-17.17	6.78	-104.75	-99.30
H22	-11.21	22.11	-34.79	-24.45
H23	-15.03	22.35	-37.42	-24.77
H24	-10.03	24.09	-34.69	-31.80
H25	-9.93	23.39	-35.34	-31.65
H26	-11.07	7.60	-92.42	-80.93
H27	-8.92	9.08	-91.67	-82.33
H28	-17.21	6.79	-95.18	-82.35
H29	-12.32	8.88	-100.33	-86.86
H30	-11.08	5.05	-98.94	-86.88
H31	-10.58	7.10	-95.81	-86.09

Table S95: Relative standard reaction enthalpies at 0K for reactant complex (RC), transition states (TS), and product (P) of RAF reactions in the gas phase using the M06-2X/6-311++G(3df,3pd)// M06-2X/6-31+G(d,p) level of theory.

Position	**RC**	**TS**	**P**
C1	-12.39	11.79	-82.11
C2	-27.31	5.59	-79.06
C3	-15.78	13.60	-63.35
C4	-15.67	13.57	-63.35
C5	-27.33	5.59	-79.06
C6	-27.73	10.10	-82.44
C7	-30.34	46.17	-20.67
C9	-30.35	46.16	-20.67
S17	-21.50	38.08	12.42
P12	-21.69	-13.84	-198.15

Table S96: Calculated standard enthalpies of reaction ($\Delta_r H_{298K}$) and standard Gibbs energies of reaction ($\Delta_r G_{298K}$), enthalpy of activation ($\Delta H^{\neq}_{298K}$) and Gibbs energy of activation ($\Delta G^{\neq}_{298K}$) at 298 K for RAF reactions in the gas phase using the M06-2X/6-311++G(3df,3pd)// M06-2X/6-31+G(d,p) level of theory.

Position	$\Delta_r H_{298K}$, (kJ/mol)	$\Delta_r G_{298K}$, (kJ/mol)	$\Delta H^{\neq}_{298K}$, (kJ/mol)	$\Delta G^{\neq}_{298K}$, (kJ/mol)
C1	-86.66	-43.16	8.43	47.56
C2	-84.56	-35.51	0.52	47.59
C3	-68.12	-21.77	9.86	49.93
C4	-68.12	-21.77	9.85	52.45
C5	-84.56	-35.51	0.52	47.58
C6	-86.77	-47.81	6.39	46.22
C7	-25.47	18.76	41.40	86.37
C9	-25.47	18.75	41.40	86.35
S17	10.76	44.81	35.17	72.39
P12	-200.58	-163.99	-18.04	24.73

Table S97: Calculated standard enthalpies of reaction ($\Delta_r H_{298K}$) and standard Gibbs energies of reaction ($\Delta_r G_{298K}$), enthalpy of activation ($\Delta H^{\neq}_{298K}$) and Gibbs energy of activation ($\Delta G^{\neq}_{298K}$) at 298 K for RAF reactions in the aqueous phase using the M06-2X/6-311++G(3df,3pd)// M06-2X/6-31+G(d,p) level of theory.

Positions	$\Delta_r H_{298K}$, **(kJ/mol)**	$\Delta_r G_{298K}$, **(kJ/mol)**	$\Delta H^{\neq}_{298K}$, **(kJ/mol)**	$\Delta G^{\neq}_{298K}$, **(kJ/mol)**
C1	-86.16	-44.16	7.83	46.68
C2	-76.41	-31.60	7.91	48.24
C3	-65.60	-19.22	9.54	48.73
C4	-66.50	-20.89	9.51	50.27
C5	-78.53	-37.31	9.10	49.33
C6	-86.65	-43.36	6.21	46.98
C7	-3.80	39.87	51.44	94.13
C9	-19.33	24.31	50.61	93.51
S17	25.72	58.92	45.53	84.46
P12	-182.58	-149.59	-15.13	27.70

Table S98: Relative standard reaction enthalpies (in kJ/mol) at 0 K for reactant complex (RC), transition states (TS), product complex (PC) and product (P) of RAF reactions in the aqueous phase using the M06-2X/6-311++G(3df,3pd)// M06-2X/6-31+G(d,p) level of theory.

Positions	**RC**	**TS**	**P**
C1	-9.45	11.26	-81.80
C2	-16.59	11.54	-71.89
C3	-11.51	12.71	-60.65
C4	-11.10	12.88	-61.87
C5	-11.19	12.79	-74.36
C6	-11.88	9.82	-82.00
C7	-8.01	56.22	0.91
C9	-8.24	55.39	-14.56
S17	-11.31	48.75	27.13
P12	-18.57	-10.17	-180.69