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Supporting information for:

Predicting structural and energetic changes in Met-aromatic motifs on methionine oxidation to the sulfoxide and sulfone

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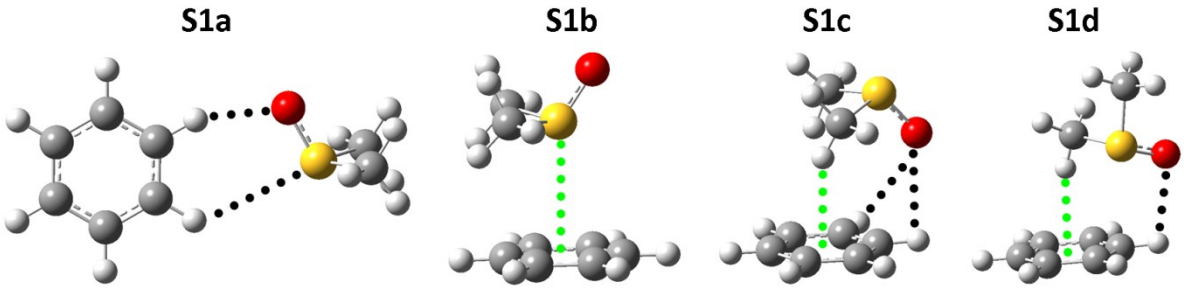

Fig. S1. Optimized geometries of the Me_2SO-benzene conformers at the MP2(full)/6-311++G(d,p) level of theory. Atom color code: hydrogen (white), carbon (gray), nitrogen (blue), oxygen (red) and sulfur (yellow). Dotted black lines show intermolecular σ-type H-bonds and dotted green lines show intermolecular π-type H-bonds or S···π interactions. The atomic coordinates are provided starting on page S26. The global minimum conformer (**1a**) is shown in Fig. 1 (but not here) and its structural and energetic properties are given in Table 2 of the main text. Note that a σ-hole···π_{ar} interaction contributes to the stability of conformer **S1b.**

Table S1. Ab initio equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of Me_2SO in the neutral complexes (e), IPV (eV), sum of Mulliken atomic spin densities for Me_2SO in the radical cation, and the MM binding energy (E^{MM}, kcal/mol) for the Me_2SO-benzene conformers in Fig. S1

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	Me_2SO charge	IPV	Me_2SO spin density
S1a	5.165	90	−4.43	−1.96	−1.82	0.011	9.15	0.0
S1b	3.338	1	−6.83	−2.23	−3.93	0.002	8.76	1.0
S1c	4.302	29	−7.43	−3.03	−3.70	−0.003	8.84	1.0
S1d	3.920	34	−7.61	−3.30	−3.26	0.000	8.91	1.0
1a[a]	4.013	31	−7.78	−3.37	−4.01	−0.002	8.83	1.0

[a] The structure of the global minimum conformer (**1a**) is shown in Fig. 1 of the main text.

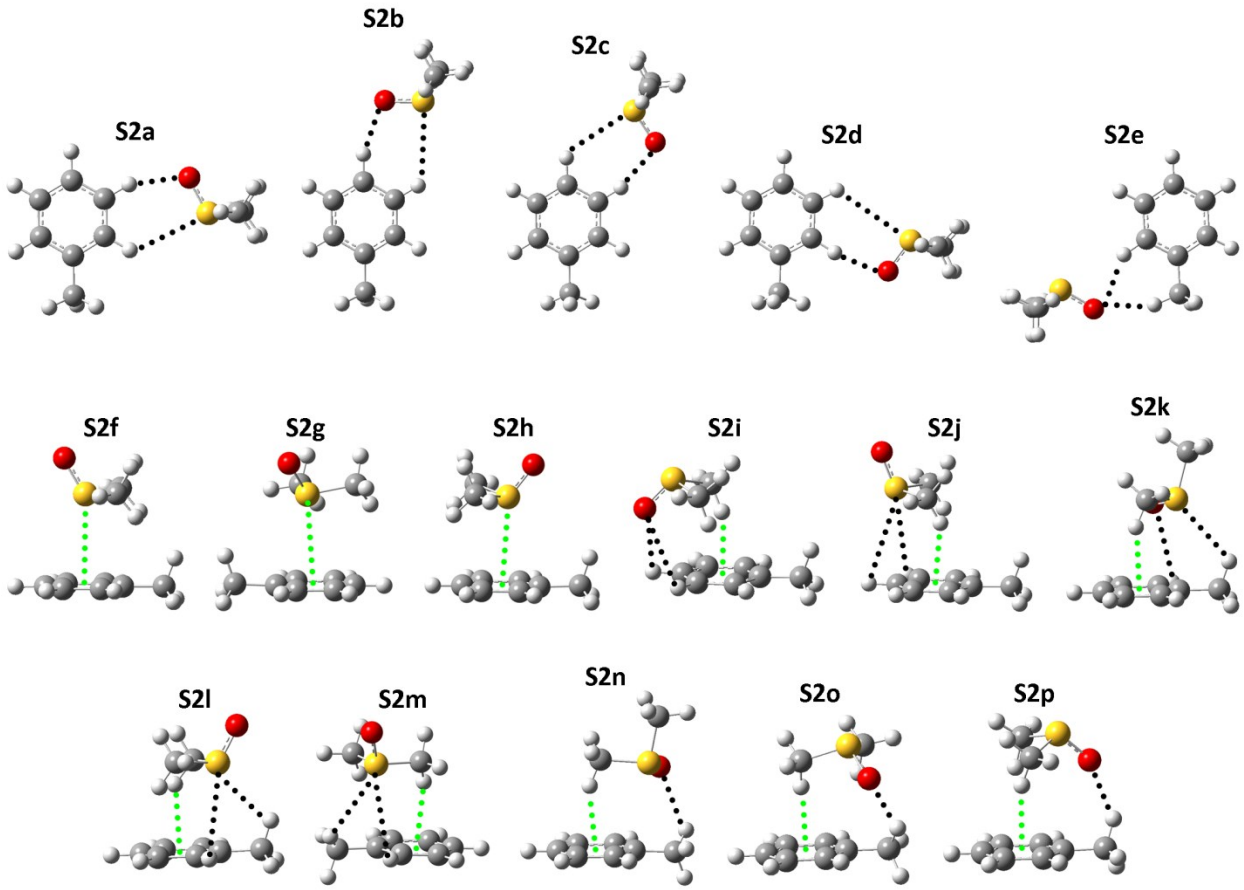

Fig. S2. Optimized geometries of the Me_2SO-toluene conformers at the MP2(full)/6-311++G(d,p) level of theory in the gas phase. See Fig. S1 for details of the structure representation and the atomic coordinates are provided starting on page S26. The global minimum conformer (**1b**) is shown in Fig. 1 (but not here) and its structural and energetic properties are given in Table 2 of the main text. Note that σ-hole$\cdots\pi_{ar}$ interactions contribute to the stability of conformers **S2f–h, S2j, S2l, S2m**.

Table S2. Ab initio equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of Me_2SO in the neutral complexes (e), IPV (eV), sum of Mulliken atomic spin densities for Me_2SO in the radical cation, and the MM binding energy (E^{MM}, kcal/mol) for the Me_2SO-toluene conformers in Fig. S2

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	Me_2SO charge	IPV	Me_2SO spin density
S2a	5.130	90	−4.26	−1.82	−1.96	0.011	8.87	0.0
S2b	5.153	90	−4.21	−1.83	−1.87	0.011	8.82	0.0
S2c	5.124	90	−4.23	−1.84	−1.84	0.011	8.88	0.0
S2d	5.192	90	−4.69	−2.07	−1.80	0.012	9.00	0.0
S2e	5.357	90	−4.85	−2.24	−1.82	0.011	9.03	0.0
S2f	3.353	1	−7.71	−2.60	−4.42	0.005	8.74	1.0
S2g	3.334	5	−7.70	−2.81	−4.31	0.005	8.75	1.0
S2h	3.324	4	−7.80	−2.97	−4.27	0.005	8.75	1.0
S2i	4.288	27	−7.53	−3.00	−3.78	−0.003	8.80	1.0
S2j	4.010	28	−8.11	−3.61	−4.16	−0.001	8.79	1.0
S2k	3.845	34	−8.34	−3.61	−3.63	0.004	8.88	1.0
S2l	3.947	32	−9.17	−4.06	−4.44	0.003	8.82	1.0
S2m	3.919	31	−9.44	−4.17	−4.67	0.005	8.80	1.0
S2n	3.827	31	−9.55	−4.50	−3.67	0.004	8.90	1.0
S2o	4.315	25	−9.71	−4.61	−4.13	0.000	8.89	1.0
S2p	4.370	25	−9.81	−4.82	−3.82	0.001	8.93	1.0
1b[a]	3.894	32	−9.88	−5.01	−4.58	0.003	8.96	1.0

[a] The structure of the global minimum conformer (**1b**) is shown in Fig. 1 of the main text.

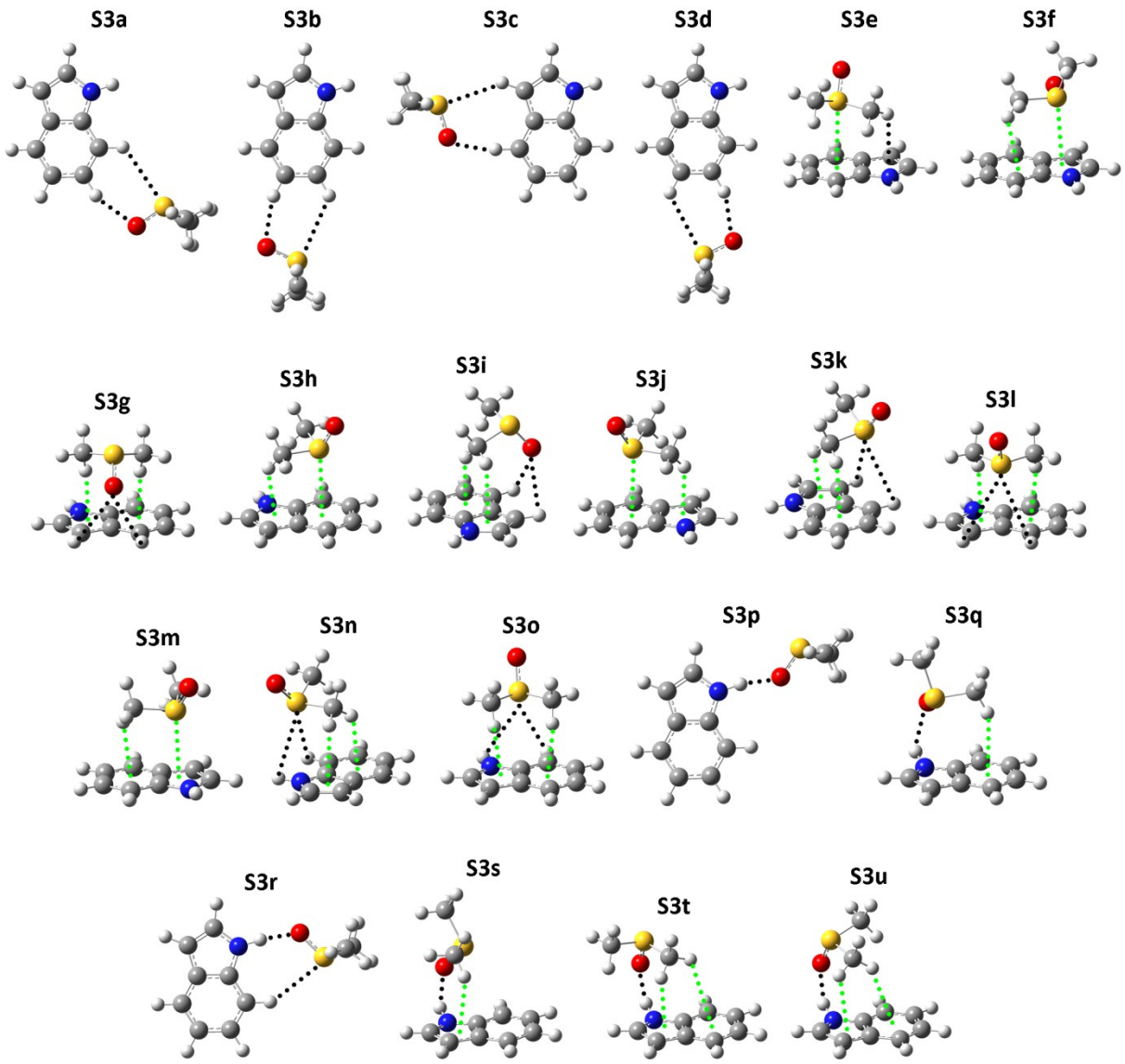

Fig. S3. Optimized geometries of the Me_2SO-indole conformers at the MP2(full)/6-311++G(d,p) level of theory in the gas phase. See Fig. S1 for details of the structure representation and the atomic coordinates are provided starting on page S26. The global minimum conformer (**1c**) is shown in Fig. 1 (but not here) and its structural and energetic properties are given in Table 2 of the main text. Note that σ-hole$\cdots\pi_{ar}$ interactions contribute to the stability of conformers **S3e, S3h, S3j–o**.

Table S3. Ab initio equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of Me_2SO in the neutral complexes (e), IPV (eV), sum of Mulliken atomic spin densities for Me_2SO in the radical cation, and the MM binding energy (E^{MM}, kcal/mol) for the Me_2SO-indole conformers in Fig. S3

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	*Me_2SO charge*	*IPV*	*Me_2SO spin density*
S3a	5.116	90	−3.82	−1.39	−1.27	0.011	8.32	0.0
S3b	5.074	90	−3.76	−1.42	−1.32	0.011	8.39	0.0
S3c	5.466	89	−4.40	−1.72	−1.71	0.015	8.30	0.0
S3d	5.046	90	−4.09	−1.73	−1.76	0.012	8.34	0.0
S3e	3.303	4	−9.43	−3.52	−5.55	0.002	8.58	1.0
S3f	3.745	32	−9.51	−3.83	−4.72	0.002	8.63	1.0
S3g	4.248	26	−9.95	−3.99	−5.17	−0.005	8.77	0.0
S3h	3.283	5	−10.12	−4.01	−5.47	0.001	8.57	1.0
S3i	4.298	31	−9.86	−4.20	−5.17	−0.001	8.68	0.0
S3j	3.283	5	−10.94	−4.65	−5.71	0.000	8.56	1.0
S3k	3.981	36	−10.40	−4.69	−4.93	0.003	8.64	1.0
S3l	3.912	31	−11.33	−5.39	−6.32	0.002	8.60	1.0
S3m	3.744	31	−12.18	−5.90	−6.61	0.006	8.64	1.0
S3n	3.920	37	−12.21	−5.95	−6.15	0.002	8.93	0.6
S3o	3.878	34	−12.30	−6.02	−6.53	0.002	8.71	1.0
S3p	6.413	90	−12.35	−8.59	−7.82	0.033	8.09	0.0
S3q	3.970	39	−14.32	−8.68	−7.20	0.010	8.64	0.0
S3r	5.333	90	−12.99	−8.78	−8.20	0.038	8.19	0.0
S3s	4.281	48	−16.30	−10.49	−9.08	0.023	8.56	0.0
S3t	4.940	48	−17.01	−10.94	−9.35	0.028	8.10	0.0
S3u	4.778	46	−17.17	−11.04	−9.41	0.021	8.65	0.0
1c[a]	4.850	48	−17.22	−11.25	−9.83	0.027	8.67	0.0

[a] The structure of the global minimum conformer (**1c**) is shown in Fig. 1 of the main text.

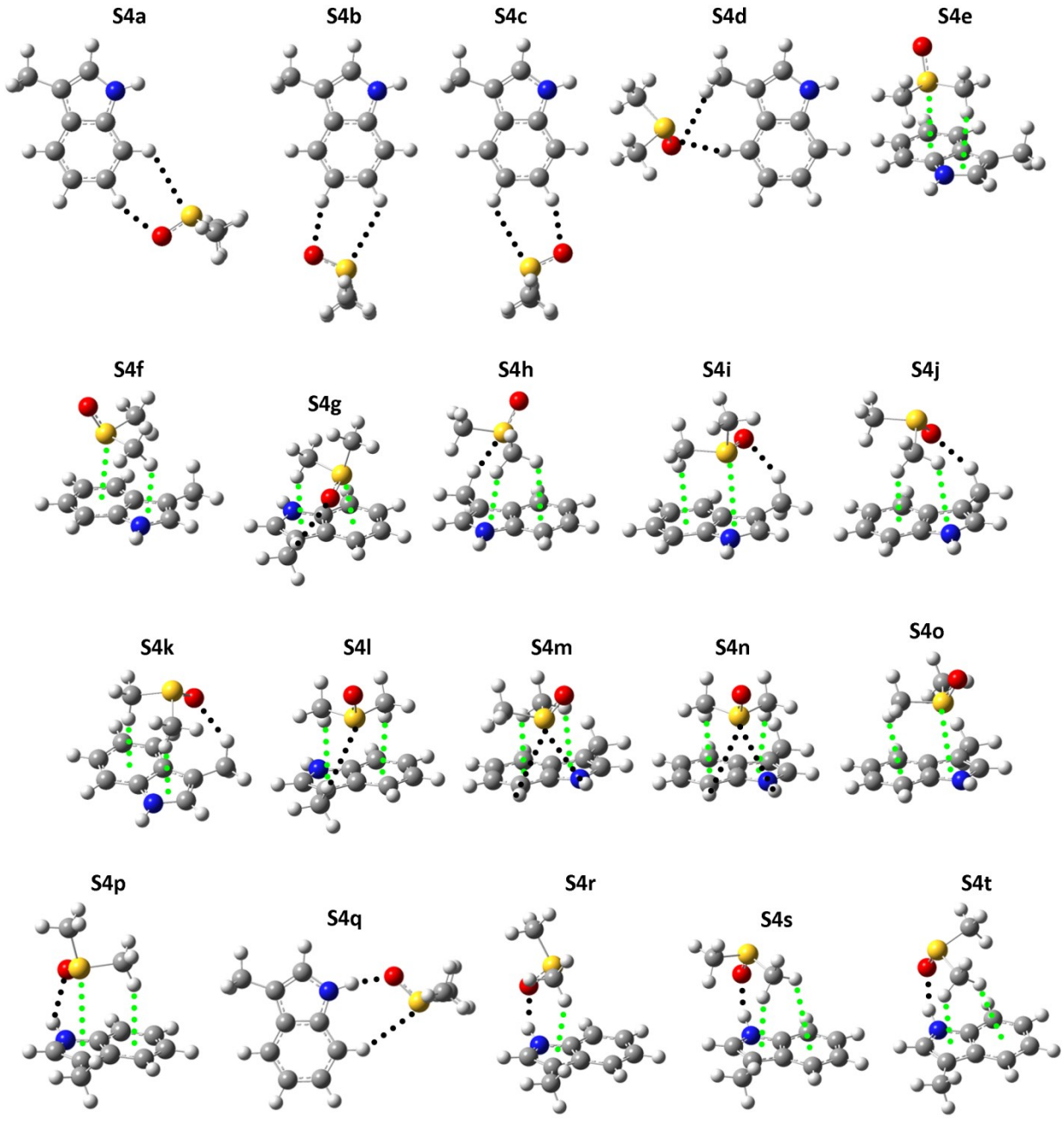

Fig. S4. Optimized geometries of the Me_2SO-3-methylindole conformers at the MP2(full)/6-311++G(d,p) level of theory in the gas phase. See Fig. S1 for details of the structure representation and the atomic coordinates are provided starting on page S26. The global minimum conformer (**1d**) is shown in Fig. 1 (but not here) and its structural and energetic properties are given in Table 2 of the main text. Note that σ-hole$\cdots\pi_{ar}$ interactions contribute to the stability of conformers **S4e, S4f, S4h, S4l–o**.

Table S4. Ab initio equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of Me_2SO in the neutral complexes (e), IPV (eV), sum of Mulliken atomic spin densities for Me_2SO in the radical cation, and the MM binding energy (E^{MM}, kcal/mol) for the Me_2SO-3-methylindole conformers in Fig. S4

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	Me_2SO charge	IPV	Me_2SO spin density
S4a	5.099	90	−3.94	−1.34	−1.30	0.011	8.20	0.0
S4b	5.054	90	−3.82	−1.39	−1.32	0.012	8.25	0.0
S4c	5.034	90	−4.20	−1.66	−1.83	0.012	8.21	0.0
S4d	5.416	74	−5.39	−2.14	−2.48	0.011	8.19	0.0
S4e	3.273	6	−11.16	−4.47	−5.68	0.002	8.54	1.0
S4f	3.275	6	−11.75	−4.90	−5.99	0.002	8.52	1.0
S4g	3.443	21	−11.44	−5.10	−4.93	0.004	8.02	0.6
S4h	3.976	35	−12.07	−5.36	−5.62	0.008	8.62	1.0
S4i	3.748	33	−12.02	−5.38	−5.11	0.005	8.03	0.7
S4j	4.313	28	−12.05	−5.60	−5.07	0.001	8.50	0.0
S4k	4.298	27	−12.50	−5.69	−5.35	−0.001	8.58	0.0
S4l	3.872	32	−12.87	−6.07	−6.69	0.005	8.59	1.0
S4m	3.903	36	−12.74	−6.17	−6.31	0.004	8.89	0.0
S4n	3.874	33	−12.97	−6.26	−6.72	0.004	8.80	0.5
S4o	3.727	32	−13.45	−6.34	−6.99	0.008	8.62	1.0
S4p	3.912	37	−14.72	−8.46	−7.22	0.009	8.48	0.0
S4q	5.317	90	−12.75	−8.51	−8.38	0.037	7.99	0.0
S4r	4.257	46	−16.60	−10.42	−9.22	0.022	8.39	0.0
S4s	4.928	48	−17.38	−10.87	−9.46	0.026	7.84	0.0
S4t	4.780	45	−17.49	−10.98	−10.66	0.021	8.47	0.0
1d[a]	4.805	46	−17.57	−11.20	−10.02	0.025	8.50	0.0

[a] The structure of the global minimum conformer (**1d**) is shown in Fig. 1 of the main text.

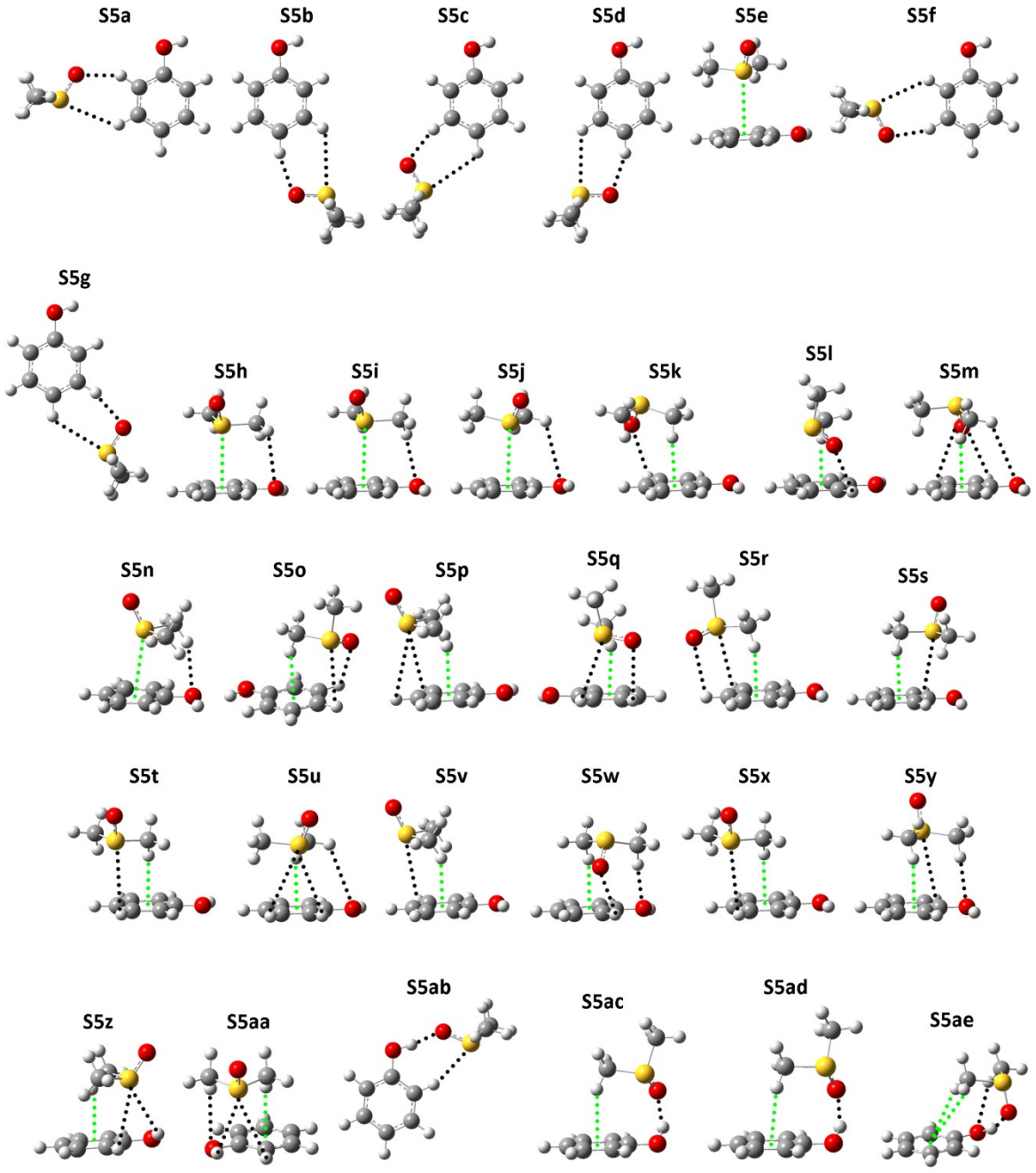

Fig. S5. Optimized geometries of the Me_2SO-phenol conformers at the MP2(full)/6-311++G(d,p) level of theory in the gas phase. See Fig. S1 for details of the structure representation and the atomic coordinates are provided starting on page S26. The global minimum conformer (**1e**) is shown in Fig. 1 (but not here) and its structural and energetic properties are given in Table 2 of the main text. Note that σ-hole$\cdots\pi_{ar}$ interactions contribute to the stability of conformers **S5e, S5i, S5g, S5n, S5p, S5s–v, S5x–z, S5aa**, and that that σ-hole$\cdots O_{ar}$ interactions contribute to the stability of conformers **S5n, S5y**.

Table S5. Ab initio equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of Me_2SO in the neutral complexes (e), IPV (eV), sum of Mulliken atomic spin densities for Me_2SO in the radical cation, and the MM binding energy (E^{MM}, kcal/mol) for the Me_2SO-phenol conformers in Fig. S5

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	Me_2SO charge	IPV	Me_2SO spin density
S5a	5.175	89	−4.28	−1.62	−0.69	0.010	8.74	0.0
S5b	5.172	89	−4.35	−1.86	−1.84	0.011	8.67	0.0
S5c	5.156	89	−4.42	−1.90	−1.63	0.011	8.76	0.0
S5d	5.112	90	−4.49	−1.97	−2.15	0.012	8.68	0.0
S5e	3.362	2	−6.86	−2.07	−3.32	0.003	8.77	1.0
S5f	5.080	89	−4.71	−2.09	−2.31	0.012	8.77	0.0
S5g	5.124	90	−4.74	−2.19	−2.30	0.012	8.73	0.0
S5h	3.311	3	−7.46	−2.28	−4.00	0.003	8.73	1.0
S5i	3.322	3	−8.02	−2.89	−4.89	0.002	8.72	1.0
S5j	3.308	4	−7.88	−2.90	−4.62	0.003	8.76	1.0
S5k	4.298	27	−7.47	−2.91	−3.57	−0.003	8.83	1.0
S5l	3.965	34	−7.50	−2.93	−2.54	−0.003	8.90	1.0
S5m	4.281	29	−7.72	−2.97	−3.09	−0.003	8.81	1.0
S5n	3.331	8	−8.32	−3.00	−4.55	0.001	8.71	1.0
S5o	3.927	34	−7.50	−3.15	−3.17	−0.002	8.90	1.0
S5p	4.032	30	−7.72	−3.21	−3.79	−0.004	8.84	1.0
S5q	3.859	35	−7.87	−3.25	−3.57	0.001	8.85	1.0
S5r	3.882	34	−7.64	−3.28	−3.67	−0.001	8.88	1.0
S5s	3.904	32	−8.50	−3.30	−4.08	0.003	8.74	1.0
S5t	3.993	29	−7.90	−3.36	−3.78	−0.002	8.81	1.0
S5u	3.991	31	−8.19	−3.38	−3.68	−0.002	8.79	1.0
S5v	4.023	30	−7.94	−3.42	−4.22	−0.003	8.81	1.0
S5w	4.295	31	−8.46	−3.48	−3.95	−0.003	8.75	1.0
S5x	3.989	29	−8.01	−3.48	−4.19	−0.002	8.83	1.0
S5y	4.017	31	−8.87	−3.90	−4.70	−0.003	8.74	1.0
S5z	3.941	38	−9.63	−4.23	−3.77	0.007	9.00	1.0
S5aa	3.907	35	−10.05	−4.45	−5.10	0.005	8.90	1.0
S5ab	5.195	90	−13.38	−8.85	−10.25	0.036	8.42	0.0
S5ac	3.991	35	−16.86	−10.78	−9.12	0.034	8.97	0.0
S5ad	4.207	38	−16.73	−10.79	−10.37	0.033	8.92	0.0
S5ae	4.792	51	−17.49	−11.71	−12.23	0.051	8.78	0.0
1e[a]	4.404	38	−18.40	−11.90	−11.67	0.041	9.01	0.0

[a] The structure of the global minimum conformer (**1e**) is shown in Fig. 1 of the main text.

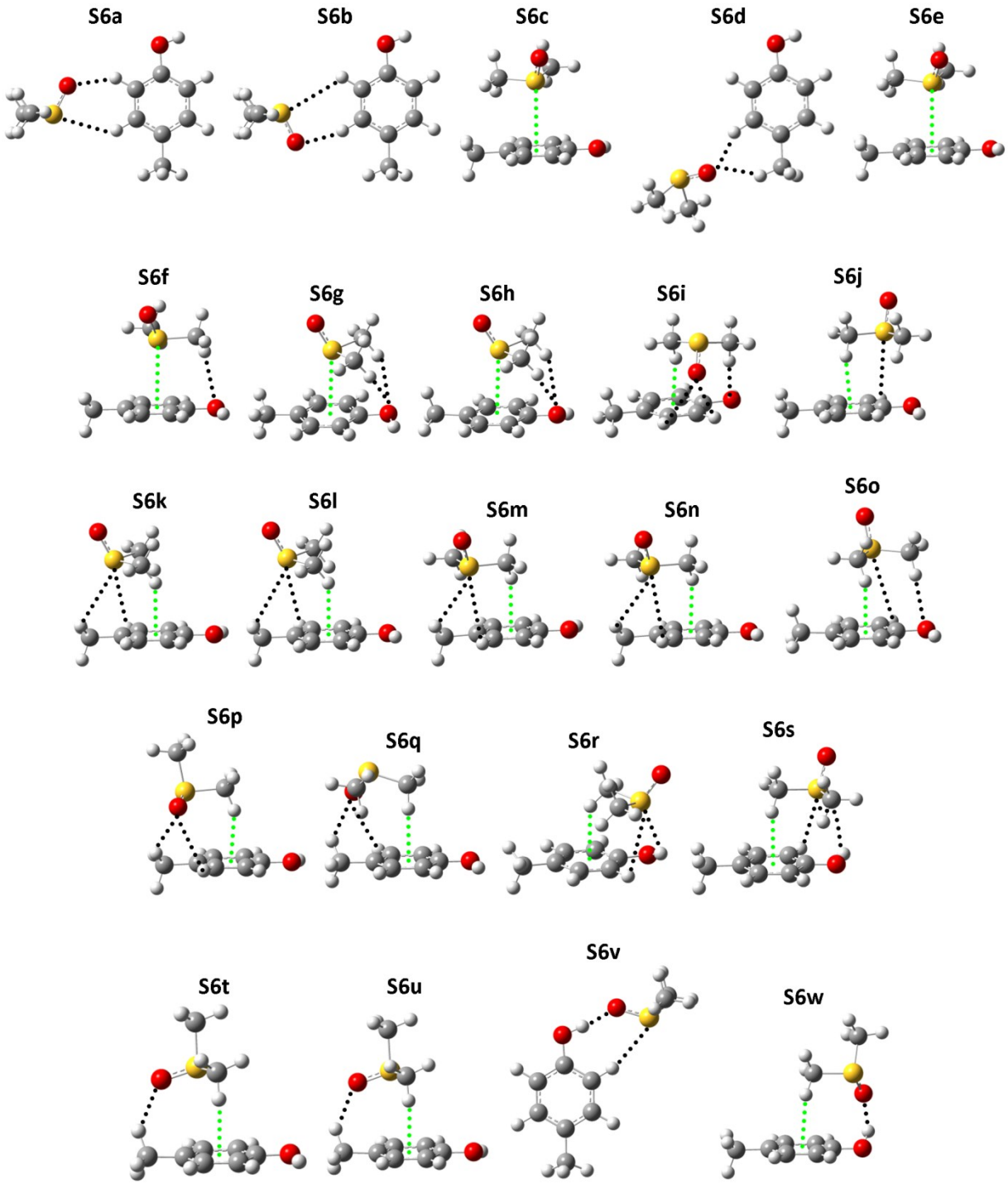

Fig. S6. Optimized geometries of the Me_2SO-4-methylphenol conformers at the MP2(full)/6-311++G(d,p) level of theory in the gas phase. See Fig. S1 for details of the structure representation and the atomic coordinates are provided starting on page S26. The global minimum conformer (**1f**) is shown in Fig. 1 (but not here) and its structural and energetic properties are given in Table 2 of the main text. Note that σ-hole$\cdots\pi_{ar}$ interactions contribute to the stability of conformers **S6c, S6e–h, S6j–o, S6r, S6s,** and that σ-hole$\cdots O_{ar}$ interactions contribute to the stability of conformers **S6f-h, S6o**.

Table S6. Ab initio equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of Me_2SO in the neutral complexes (e), IPV (eV), sum of Mulliken atomic spin densities for Me_2SO in the radical cation, and the MM binding energy (E^{MM}, kcal/mol) for the Me_2SO-4-methylphenol conformers in Fig. S6

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	Me_2SO charge	IPV	Me_2SO spin density
S6a	5.153	90	−4.17	−1.56	−0.97	0.009	8.33	0.0
S6b	5.037	90	−4.95	−2.19	−2.31	0.013	8.33	0.0
S6c	3.320	1	−7.89	−2.44	−3.75	0.006	8.73	1.0
S6d	5.823	81	−5.23	−2.60	−2.02	0.011	8.14	0.0
S6e	3.277	2	−8.78	−3.19	−4.98	0.006	8.73	1.0
S6f	3.288	2	−8.79	−3.29	−5.07	0.004	8.68	1.0
S6g	3.288	6	−8.93	−3.43	−4.64	0.003	8.68	1.0
S6h	3.270	5	−9.12	−3.55	−4.69	0.003	8.69	1.0
S6i	4.246	29	−8.96	−3.58	−4.18	−0.003	8.72	1.0
S6j	3.884	30	−8.94	−3.69	−4.26	0.003	8.70	1.0
S6k	3.947	31	−9.18	−3.87	−4.28	0.002	8.81	1.0
S6l	3.937	31	−9.38	−4.05	−4.62	0.002	8.79	1.0
S6m	3.900	30	−9.61	−4.14	−4.45	0.004	8.79	1.0
S6n	3.895	31	−9.72	−4.24	−4.81	0.004	8.80	1.0
S6o	3.969	31	−9.60	−4.25	−4.85	−0.001	8.72	1.0
S6p	3.830	31	−9.48	−4.34	−3.60	0.004	8.89	1.0
S6q	4.286	25	−9.79	−4.42	−4.09	0.000	8.36	0.5
S6r	3.919	37	−9.88	−4.46	−3.87	0.007	8.96	1.0
S6s	3.883	34	−10.39	−4.72	−5.22	0.005	8.85	1.0
S6t	3.854	32	−10.00	−4.96	−3.83	0.003	8.93	1.0
S6u	3.859	32	−10.08	−5.03	−3.81	0.002	8.47	0.5
S6v	5.188	90	−13.04	−8.61	−10.07	0.035	8.10	0.0
S6w	4.147	36	−16.76	−10.77	−9.83	0.032	8.60	0.0
1f[a]	4.358	37	−18.47	−11.88	−11.10	0.039	8.67	0.0

[a] The structure of the global minimum conformer (**1f**) is shown in Fig. 1 of the main text.

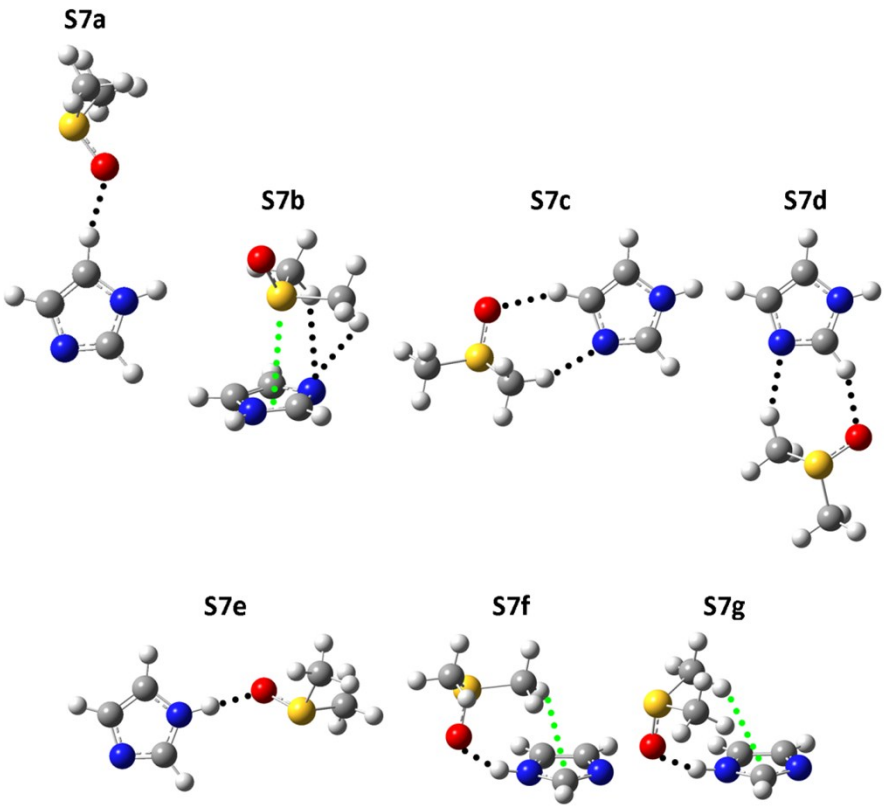

Fig. S7. Optimized geometries of the Me_2SO-imidazole conformers at the MP2(full)/6-311++G(d,p) level of theory in the gas phase. See Fig. S1 for details of the structure representation and the atomic coordinates are provided starting on page S26. The global minimum conformer (**1g**) is shown in Fig. 1 (but not here) and its structural and energetic properties are given in Table 2 of the main text. Note that σ-hole···π_{ar} and σ-hole···N_{ar} interactions contribute to the stability of conformer **S7b**.

Table S7. Ab initio equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of Me_2SO in the neutral complexes (e), IPV (eV), sum of Mulliken atomic spin densities for Me_2SO in the radical cation, and the MM binding energy (E^{MM}, kcal/mol) for the Me_2SO-imidazole conformers in Fig. S7

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	Me_2SO charge	IPV	Me_2SO spin density
S7a	5.571	90	−6.26	−3.86	−2.83	0.012	8.46	0.0
S7b	3.275	8	−8.51	−4.47	−5.59	0.002	8.76	1.0
S7c	4.806	87	−7.46	−4.86	−4.43	−0.003	8.83	1.0
S7d	4.801	87	−9.22	−6.46	−6.87	0.000	8.82	0.0
S7e	5.108	83	−12.84	−9.40	−9.17	0.035	8.30	0.0
S7f	4.280	47	−14.12	−9.79	−9.34	0.024	8.75	0.0
S7g	4.444	52	−14.26	−10.05	−9.73	0.038	8.76	0.0
1g[a]	4.358	48	−14.40	−10.05	−9.69	0.035	8.80	0.0

[a] The structure of the global minimum conformer (**1g**) is shown in Fig. 1 of the main text.

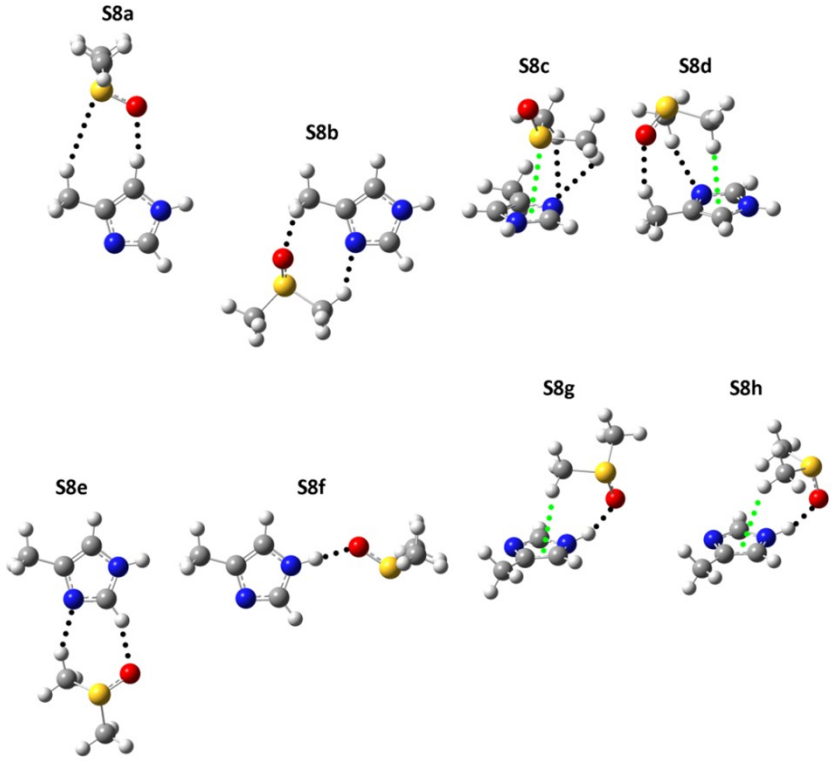

Fig. S8. Optimized geometries of the Me_2SO-4-methylimidazole conformers at the MP2(full)/6-311++G(d,p) level of theory in the gas phase. See Fig. S1 for details of the structure representation and the atomic coordinates are provided starting on page S26. The global minimum conformer (**1j**) is shown in Fig. 1 (but not here) and its structural and energetic properties are given in Table 2 of the main text. Note that σ-hole···π_{ar} and σ-hole···N_{ar} interactions contribute to the stability of conformer **S8c**.

Table S8. Ab initio equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of Me_2SO in the neutral complexes (e), IPV (eV), sum of Mulliken atomic spin densities for Me_2SO in the radical cation, and the MM binding energy (E^{MM}, kcal/mol) for the Me_2SO-4-methylimidazole conformers in Fig. S8

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	Me_2SO charge	IPV	Me_2SO spin density
S8a	5.192	90	−6.30	−3.56	−2.47	0.015	8.18	0.0
S8b	4.519	73	−6.64	−3.81	−4.21	0.003	8.66	1.0
S8c	3.262	7	−9.20	−4.61	−6.05	0.006	8.75	1.0
S8d	4.445	27	−9.00	−4.94	−5.84	−0.007	8.76	1.0
S8e	4.784	86	−9.15	−6.35	−6.74	0.003	8.47	0.0
S8f	5.102	90	−12.53	−9.04	−8.89	0.034	7.95	0.0
S8g	4.231	45	−14.10	−9.65	−8.98	0.022	8.42	0.0
S8h	4.418	51	−14.20	−9.86	−9.69	0.036	8.42	0.0
1h[a]	4.297	45	−14.51	−9.95	−9.32	0.031	8.48	0.0

[a] The structure of the global minimum conformer (**1h**) is shown in Fig. 1 of the main text.

S9a

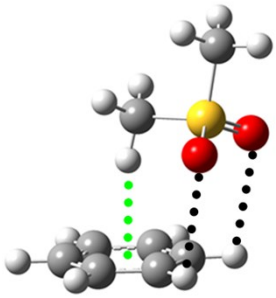

Fig. S9. Optimized geometry of the Me_2SO_2-benzene conformer at the MP2(full)/6-311++G(d,p) level of theory in the gas phase. See Fig. S1 for details of the structure representation and the atomic coordinates are provided starting on page S26. The global minimum conformer (**2a**) is shown in Fig. 1 (but not here) and its structural and energetic properties are given in Table 2 of the main text.

Table S9. Ab initio equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of Me_2SO_2 in the neutral complexes (e), IPV (eV), and the MM binding energy (E^{MM}, kcal/mol) for the Me_2SO_2-benzene conformer in Fig. S9 [a]

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	Me_2SO_2 charge	IPV
S9a	4.073	31	−8.07	−3.46	−3.87	0.000	9.52
2a[b]	4.234	28	−8.38	−3.77	−4.39	−0.003	9.86

[a] The Me_2SO_2 spin density is zero in all the $(Me_2SO_2$-aromatics$)^{\bullet+}$ so it is omitted from the table.

[b] The structure of the global minimum conformer (**2a**) is shown in Fig. 1 of the main text.

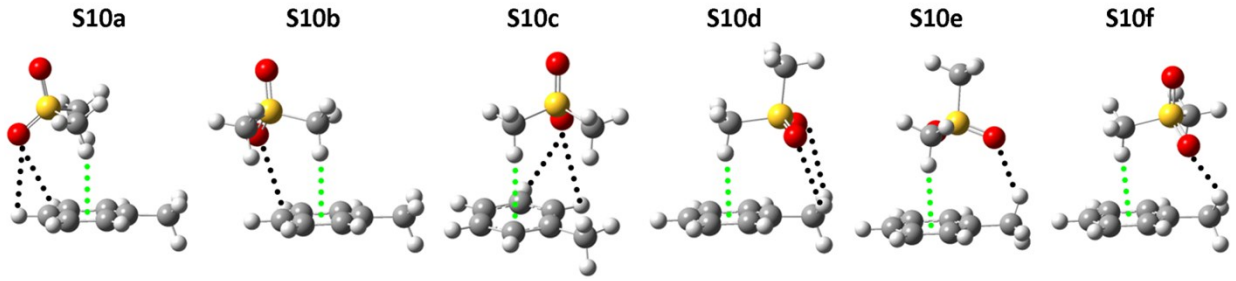

Fig. S10. Optimized geometries of the Me_2SO_2-toluene conformers at the MP2(full)/6-311++G(d,p) level of theory in the gas phase. See Fig. S1 for details of the structure representation and the atomic coordinates are provided starting on page S26. The global minimum conformer (**2b**) is shown in Fig. 1 (but not here) and its structural and energetic properties are given in Table 2 of the main text. Note that σ-hole···π_{ar} interactions contribute to the stability of conformers **S10a–c, S10f**.

Table S10. Ab initio equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of Me_2SO_2 in the neutral complexes (e), IPV (eV), and the MM binding energy (E^{MM}, kcal/mol) for the Me_2SO_2-toluene conformers in Fig. S10 [a]

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	Me_2SO_2 charge	IPV
S10a	4.230	27	−8.56	−3.92	−4.55	−0.004	9.51
S10b	4.227	27	−8.56	−3.96	−4.50	−0.004	9.52
S10c	4.223	27	−8.99	−4.09	−4.86	−0.003	9.56
S10d	4.022	29	−10.01	−4.62	−4.00	−0.001	9.43
S10e	4.055	29	−9.78	−4.64	−4.13	0.000	9.41
S10f	4.212	25	−10.49	−5.11	−4.92	−0.003	9.49
2b [b]	4.238	26	−10.35	−5.19	−5.61	−0.003	9.72

[a] The Me_2SO_2 spin density is zero in all the (Me_2SO_2-aromatics)$^{\bullet+}$ so it is omitted from the table.

[b] The structure of the global minimum conformer (**2b**) is shown in Fig. 1 of the main text.

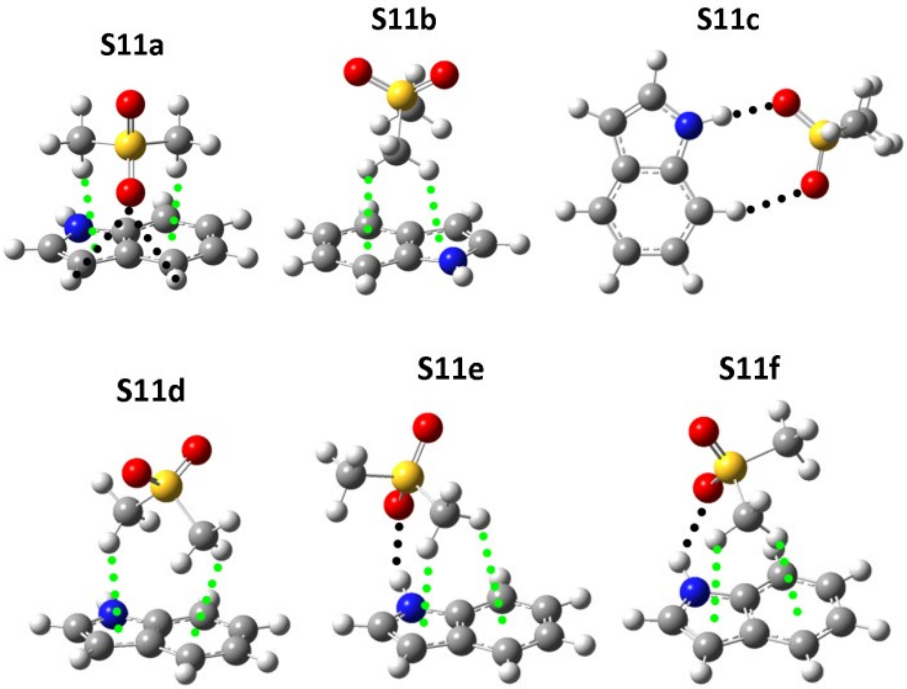

Fig. S11. Optimized geometries of the Me_2SO_2-indole conformers at the MP2(full)/6-311++G(d,p) level of theory in the gas phase. See Fig. S1 for details of the structure representation and the atomic coordinates are provided starting on page S26. The global minimum conformer (**2c**) is shown in Fig. 1 (but not here) and its structural and energetic properties are given in Table 2 of the main text. Note that σ-hole···π_{ar} interactions contribute to the stability of conformers **S11b, S11d–f**.

Table S11. Ab initio equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of Me_2SO_2 in the neutral complexes (e), IPV (eV), and the MM binding energy (E^{MM}, kcal/mol) for the Me_2SO_2-indole conformers in Fig. S11 [a]

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	Me_2SO_2 charge	IPV
S11a	4.188	26	−11.40	−5.36	−6.64	−0.007	8.39
S11b	4.586	19	−10.58	−5.58	−6.60	−0.005	8.71
S11c	5.585	90	−10.02	−6.63	−7.07	0.024	8.13
S11d	4.521	13	−10.55	−5.64	−7.25	−0.008	8.70
S11e	4.841	44	−14.28	−8.82	−7.72	0.006	8.35
S11f	4.339	38	−15.47	−9.42	−8.42	0.004	8.35
2c[b]	4.459	41	−15.34	−9.44	−8.72	0.003	8.97

[a] The Me_2SO_2 spin density is zero in all the $(Me_2SO_2\text{-aromatics})^{\bullet+}$ so it is omitted from the table.

[b] The structure of the global minimum conformer (**2c**) is shown in Fig. 1 of the main text.

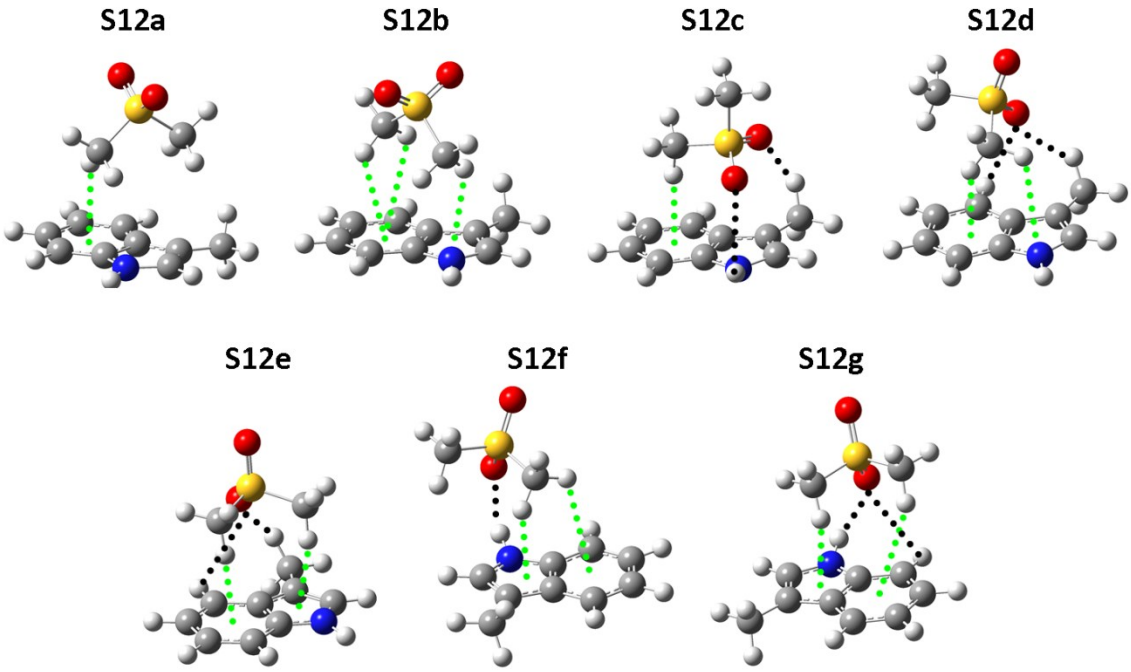

Fig. S12. Optimized geometries of the Me_2SO_2-3-methylindole conformers at the MP2(full)/6-311++G(d,p) level of theory in the gas phase. See Fig. S1 for details of the structure representation and the atomic coordinates are provided starting on page S26. The global minimum conformer (**2d**) is shown in Fig. 1 (but not here) and its structural and energetic properties are given in Table 2 of the main text. Note that σ-hole···π_{ar} interactions contribute to the stability of conformers **S12a, S12b, S12d–g**.

Table S12. Ab initio equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of Me_2SO_2 in the neutral complexes (e), IPV (eV), and the MM binding energy (E^{MM}, kcal/mol) for the Me_2SO_2-3-methylindole conformers in Fig. S12 [a]

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	Me_2SO_2 charge	IPV
S12a	4.579	17	−11.38	−5.91	−6.96	−0.005	8.40
S12b	4.522	14	−11.38	−6.02	−7.37	−0.006	8.39
S12c	4.053	28	−12.99	−6.02	−5.34	−0.001	7.71
S12d	4.199	27	−12.83	−6.35	−6.43	−0.001	8.04
S12e	4.200	26	−13.58	−6.66	−6.89	−0.004	8.13
S12f	4.872	44	−14.78	−8.90	−7.80	0.006	8.09
S12g	4.444	40	−15.79	−9.51	−8.88	0.003	8.11
2d[b]	4.333	37	−15.88	−9.55	−8.58	0.003	8.05

[a] The Me_2SO_2 spin density is zero in all the $(Me_2SO_2\text{-aromatics})^{\bullet+}$ so it is omitted from the table.

[b] The structure of the global minimum conformer (**2d**) is shown in Fig. 1 of the main text.

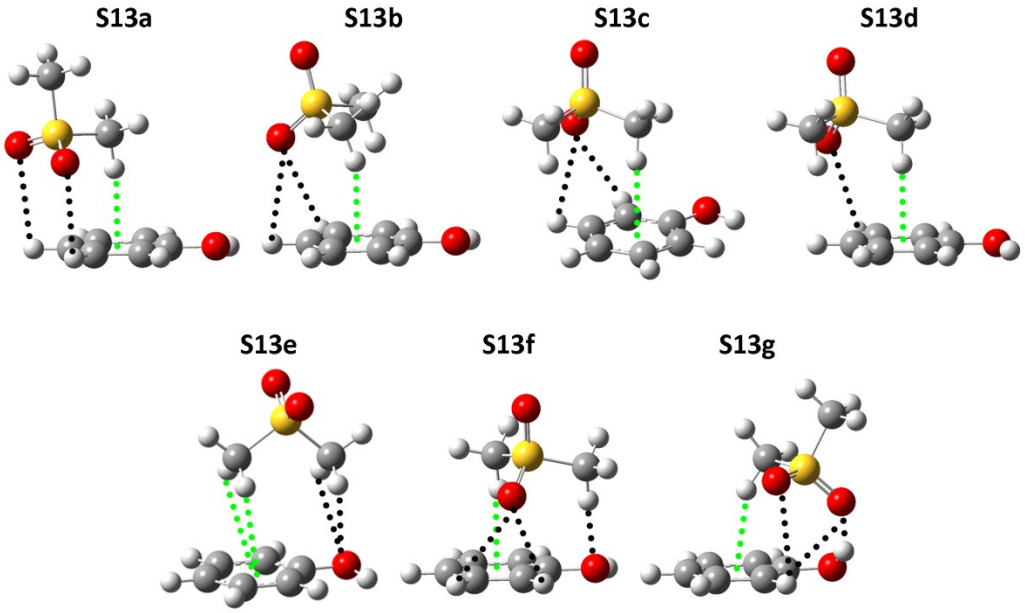

Fig. S13. Optimized geometries of the Me_2SO_2-phenol conformers at the MP2(full)/6-311++G(d,p) level of theory in the gas phase. See Fig. S1 for details of the structure representation and the atomic coordinates are provided starting on page S26. The global minimum conformer (**2e**) is shown in Fig. 1 (but not here) and its structural and energetic properties are given in Table 2 of the main text. Note that σ-hole···π_{ar} interactions contribute to the stability of conformers **S13b–f**.

Table S13. Ab initio equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of Me_2SO_2 in the neutral complexes (e), IPV (eV), and the MM binding energy (E^{MM}, kcal/mol) for the Me_2SO_2-phenol conformers in Fig. S13 [a]

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	Me_2SO_2 charge	IPV
S13a	4.083	31	−8.01	−3.34	−3.89	−0.001	9.10
S13b	4.248	27	−8.25	−3.55	−4.34	−0.004	9.32
S13c	4.216	28	−8.50	−3.64	−3.62	−0.003	9.46
S13d	4.235	27	−8.35	−3.65	−4.13	−0.003	9.42
S13e	4.576	14	−7.82	−3.86	−5.54	−0.006	9.72
S13f	4.237	30	−9.67	−4.41	−5.35	−0.006	9.50
S13g	4.174	40	−14.68	−8.89	−8.96	0.017	9.09
2e[b]	4.241	35	−15.48	−9.44	−8.83	0.010	9.39

[a] The Me_2SO_2 spin density is zero in all the $(Me_2SO_2$-aromatics$)^{\bullet+}$ so it is omitted from the table.

[b] The structure of the global minimum conformer (**2e**) is shown in Fig. 1 of the main text.

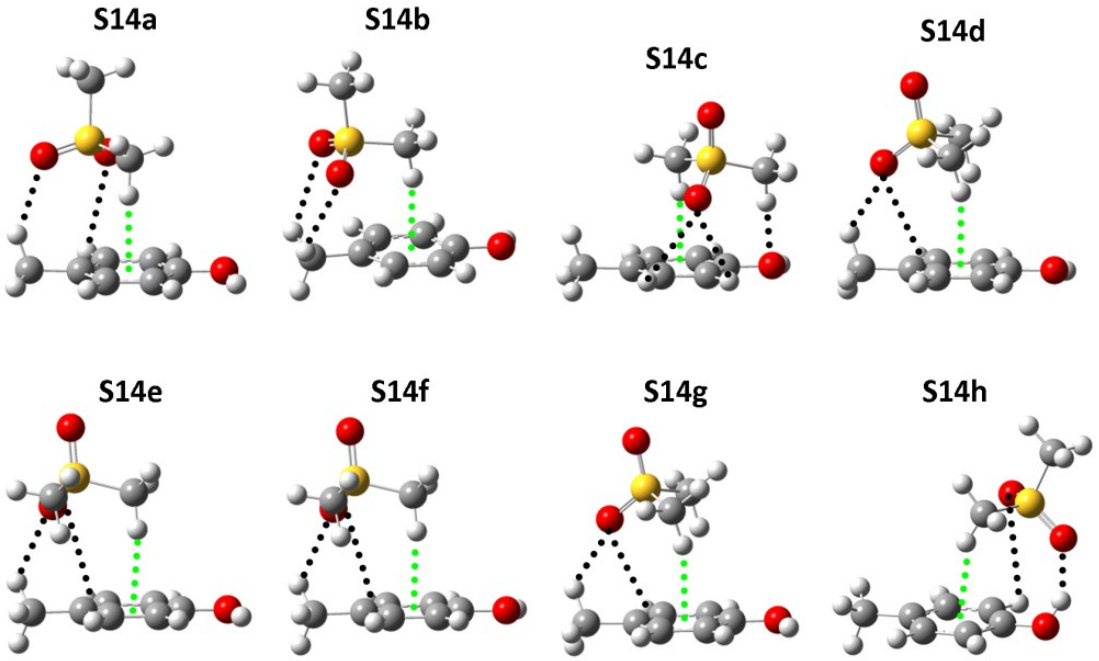

Fig. S14. Optimized geometries of the Me_2SO_2-4-methylphenol conformers at the MP2(full)/6-311++G(d,p) level of theory in the gas phase. See Fig. S1 for details of the structure representation and the atomic coordinates are provided starting on page S26. The global minimum conformer (**2f**) is shown in Fig. 1 (but not here) and its structural and energetic properties are given in Table 2 of the main text. Note that σ-hole$\cdots\pi_{ar}$ interactions contribute to the stability of conformers **S14c–g**.

Table S14. Ab initio equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of Me_2SO_2 in the neutral complexes (e), IPV (eV), and the MM binding energy (E^{MM}, kcal/mol) for the Me_2SO_2-4-methylphenol conformers in Fig. S14 [a]

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	Me_2SO_2 charge	IPV
S14a	4.062	29	−9.74	−4.47	−4.15	0.002	8.62
S14b	4.021	28	−10.09	−4.58	−4.38	−0.001	8.56
S14c	4.192	28	−10.16	−4.67	−5.43	−0.005	9.02
S14d	4.235	25	−10.30	−4.96	−4.51	−0.003	8.86
S14e	4.202	25	−10.49	−4.96	−4.81	−0.003	8.96
S14f	4.201	25	−10.71	−5.17	−5.37	−0.003	8.87
S14g	4.216	26	−10.60	−5.18	−5.05	−0.003	8.86
S14h	4.117	37	−14.81	−8.94	−8.51	0.015	8.73
2f [b]	4.216	33	−15.61	−9.55	−8.75	0.010	9.00

[a] The Me_2SO_2 spin density is zero in all the $(Me_2SO_2$-aromatics$)^{\bullet+}$ so it is omitted from the table.

[b] The structure of the global minimum conformer (**2f**) is shown in Fig. 1 of the main text.

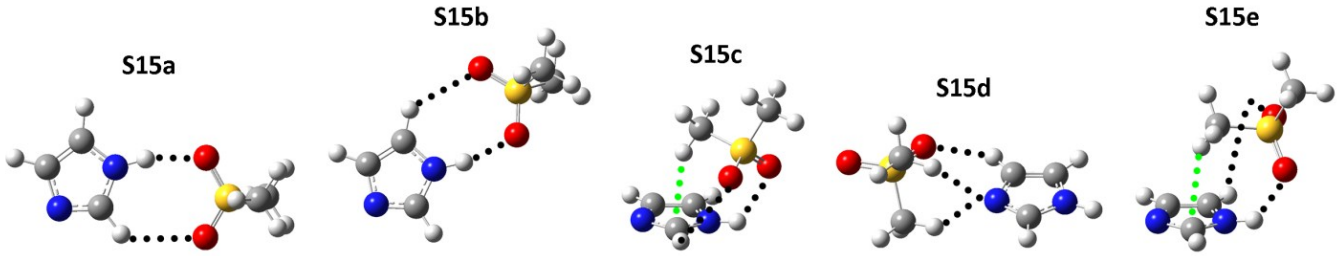

Fig. S15. Optimized geometries of the Me_2SO_2-imidazole conformers at the MP2(full)/6-311++G(d,p) level of theory in the gas phase. See Fig. S1 for details of the structure representation and the atomic coordinates are provided starting on page S26. The global minimum conformer (**2i**) is shown in Fig. 1 (but not here) and its structural and energetic properties are given in Table 2 of the main text. Note that a σ-hole···N_{ar} interaction contributes to the stability of conformer **S15d**.

Table S15. Ab initio equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of Me_2SO_2 in the neutral complexes (e), IPV (eV), and the MM binding energy (E^{MM}, kcal/mol) for the Me_2SO_2-imidazole conformers in Fig. S15 [a]

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	Me_2SO_2 charge	IPV
S15a	4.805	90	−9.77	−6.96	−9.02	0.023	8.37
S15b	4.826	90	−9.89	−7.09	−8.26	0.023	8.37
S15c	3.951	38	−11.21	−7.24	−8.92	0.003	8.96
S15d	4.743	90	−10.19	−7.27	−7.47	−0.005	9.33
S15e	4.006	39	−11.58	−7.69	−8.19	0.004	8.98
2g[b]	4.174	38	−11.64	−7.74	−7.78	0.001	9.24

[a] The Me_2SO_2 spin density is zero in all the $(Me_2SO_2\text{-aromatics})^{\bullet+}$ so it is omitted from the table.

[b] The structure of the global minimum conformer (**2g**) is shown in Fig. 1 of the main text.

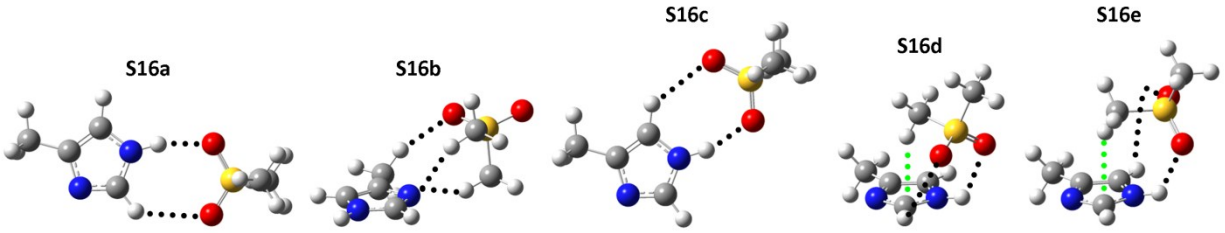

Fig. S16. Optimized geometries of the Me_2SO_2-4-methylimidazole conformers at the MP2(full)/6-311++G(d,p) level of theory in the gas phase. See Fig. S1 for details of the structure representation and the atomic coordinates are provided starting on page S26. The global minimum conformer (**2j**) is shown in Fig. 1 (but not here) and its structural and energetic properties are given in Table 2 of the main text. Note that a σ-hole···N_{ar} interaction contributes to the stability of conformer **S16b**.

Table S16. Ab initio equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of Me_2SO_2 in the neutral complexes (e), IPV (eV), and the MM binding energy (E^{MM}, kcal/mol) for the Me_2SO_2-4-methylimidazole conformers in Fig. S16 [a]

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	Me_2SO_2 charge	IPV
S16a	4.810	90	−9.54	−6.68	−8.74	0.023	8.02
S16b	4.926	80	−9.89	−6.70	−7.86	−0.008	9.02
S16c	4.823	90	−9.69	−6.82	−7.90	0.023	8.01
S16d	4.935	37	−11.30	−7.15	−8.18	0.003	8.61
S16e	3.973	37	−11.77	−7.63	−7.99	0.003	8.63
2h[b]	4.153	36	−11.83	−7.76	−7.86	0.001	8.86

[a] The Me_2SO_2 spin density is zero in all the $(Me_2SO_2\text{-aromatics})^{\bullet+}$ so it is omitted from the table.

[b] The structure of the global minimum conformer (**2h**) is shown in Fig. 1 of the main text.

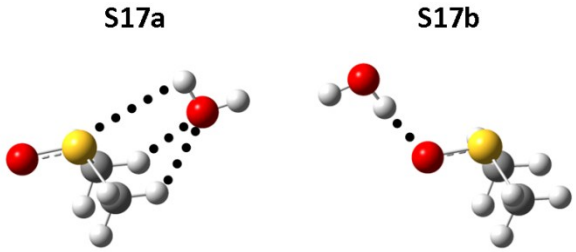

Fig. S17. Optimized geometries of the Me_2SO-H_2O conformers at the MP2(full)/6−311++G(d,p) level of theory in the gas phase. See Fig. S1 for details of the structure representation and the atomic coordinates are provided starting on page S26. The global minimum conformer (**1w**) is shown in Fig. 1 (but not here) and its structural and energetic properties are given in Table 2 of the main text. Note that a σ−hole···O interaction contributes to the stability of conformer **S17a**.

Table S17. Ab initio equilibrium distance (r_{SO}, Å), binding energy (E and E^{CP}, kcal/mol), net charge of Me_2SO in the neutral complexes (e), IPV (eV), sum of Mulliken atomic spin densities for Me_2SO in the radical cation, and the MM binding energy (E^{MM}, kcal/mol) for the Me_2SO-H_2O conformers in Fig. S17 [a]

Conformer	r_{SO}	E	E^{CP}	E^{MM}	*Me_2SO charge*	IPV	Me_2SO spin density
S17a	3.306	−5.56	−3.37	−3.49	0.000	8.90	1.0
S17b	3.789	−9.29	−6.63	−8.59	0.022	9.70	1.0
1w[a]	3.373	−11.90	−8.88	−9.31	0.028	9.49	1.0

[a] The structure of the global minimum conformer (**1w**) is shown in Fig. 1 of the main text.

S18a

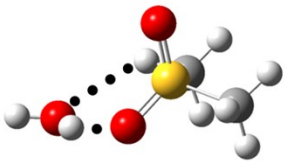

Fig. S18. Optimized geometries of the Me_2SO_2−H_2O conformer at the MP2(full)/6−311++G(d,p) level of theory in the gas phase. See Fig. S1 for details of the structure representation and the atomic coordinates are provided starting on page S26. The global minimum conformer (**2w**) is shown in Fig. 1 (but not here) and its structural and energetic properties are given in Table 2 of the main text.

Table S18. Ab initio equilibrium distance (r_{SO}, Å), binding energy (E and E^{CP}, kcal/mol), net charge of Me_2SO_2 in the neutral complexes (e), IPV (eV), sum of Mulliken atomic spin densities for Me_2SO_2 in the radical cation, and the MM binding energy (E^{MM}, kcal/mol) for the Me_2SO_2-H_2O conformer in Fig. S18

Conformer	r_{SO}	E	E^{CP}	E^{MM}	Me_2SO_2 charge	IPV	Me_2SO_2 spin density
S18a	3.515	−8.46	−6.20	−7.54	0.011	10.78	1.0
2w[a]	3.372	−9.93	−7.38	−8.16	0.009	10.67	1.0

[a] The structure of the global minimum conformer (**2w**) is shown in Fig. 1 of the main text.

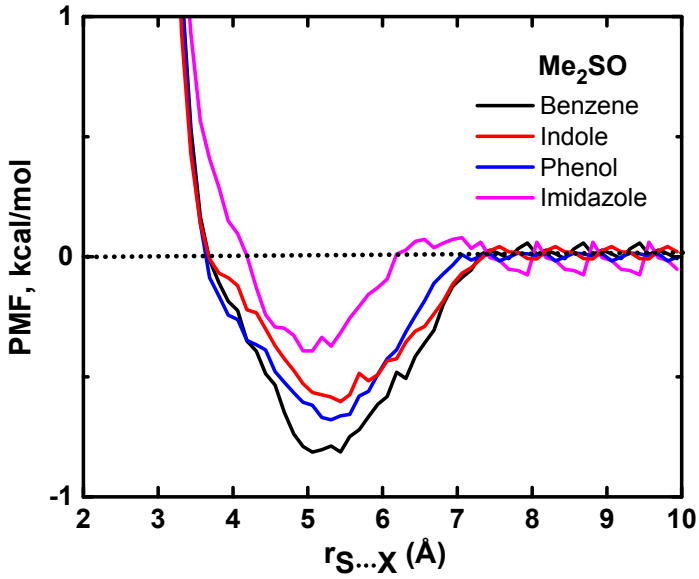

Fig. S19. Potential of mean force (PMF kcal/mol) as a function of distance between the S atom of Me_2SO and the ring centroid X (r_{SX}, Å) of benzene, indole and phenol in bulk water calculated using the parameters of Jas and Kuczera for Me_2SO (Ref. 47 of the main text).

Table S19. Minima in the PMF (kcal/mol) vs. r_{SX} (Å) plots in Fig. S19

Aromatic	$r_{SX}1$	PMF1	$r_{SX}2$	PMF2
Benzene	3.7	−0.1	4.9–5.4	−0.8
Indole	3.7	−0.1	5.1–5.6	−0.6
Phenol	3.7	−0.1	5.2–5.6	−0.7
Imidazole	3.7	+0.3	4.9–5.1	−0.4

Atomic coordinates of the global minimum complexes in Fig. 1 of the main text

Me_2SO complexes (Fig. 1)

Conformer 1a, benzene

C	−2.130558	−1.339123	0.430834
C	−2.685367	−0.779145	−0.725731
C	−2.584493	0.598211	−0.954332
C	−1.932679	1.415942	−0.023178
C	−1.376696	0.854491	1.132024
C	−1.473074	−0.523290	1.357878
H	−2.212277	−2.407560	0.610115
H	−3.198427	−1.412276	−1.444131
H	−3.019639	1.033861	−1.849428
H	−1.867668	2.487382	−0.193389
H	−0.875068	1.487857	1.858754
H	−1.038009	−0.957220	2.253493
C	2.007566	1.532492	−0.265682
H	2.495537	1.584203	−1.242149
H	0.989227	1.924170	−0.307600
H	2.595235	2.087538	0.466946
S	1.975130	−0.192083	0.268874
C	1.009839	−0.791462	−1.131005
H	1.565955	−0.583335	−2.048665
H	0.896139	−1.869351	−1.006916
H	0.027638	−0.315580	−1.134717
O	3.379006	−0.724382	0.101358

Conformer 1b, toluene

C	1.239787	0.340092	1.175591
C	1.631867	1.007344	0.003207
C	2.304586	0.272152	−0.983464
C	2.573981	−1.092067	−0.812841
C	2.173589	−1.743894	0.358024
C	1.502150	−1.021766	1.352816
H	0.712162	0.896301	1.946787
H	1.191904	−1.516330	2.269758
H	2.385530	−2.800517	0.496288
H	3.102310	−1.640358	−1.588481
H	2.621223	0.772583	−1.896193
C	1.302415	2.463321	−0.184798
H	1.766728	2.859013	−1.092110
H	0.216457	2.581060	−0.252593
H	1.654968	3.054267	0.666184
C	−3.683210	−0.449981	−0.208806
H	−3.824937	0.005371	−1.191653
H	−3.889925	−1.522709	−0.233756
H	−4.332269	0.037748	0.519521
S	−1.981564	−0.171303	0.326970
C	−1.200100	−0.967104	−1.086849
H	−1.502209	−0.437705	−1.994242

H	−0.122125	−0.890728	−0.947459
H	−1.494850	−2.019080	−1.124022
O	−1.731292	1.314167	0.189147

Conformer 1c, indole

C	−1.730486	0.610684	−1.443761
H	−0.682213	0.400669	−1.218692
H	−1.997567	0.244359	−2.438550
H	−1.915733	1.684214	−1.387418
S	−2.814218	−0.185829	−0.238495
C	−2.141522	−1.844545	−0.438744
H	−1.065818	−1.821510	−0.250931
H	−2.639822	−2.482434	0.292639
H	−2.358234	−2.200010	−1.449047
O	−2.388734	0.289550	1.143600
C	1.048974	0.175304	0.675901
C	1.956315	0.711008	−0.285433
C	2.919954	−0.142624	−0.863223
C	2.948189	−1.479647	−0.480821
C	2.042927	−1.989175	0.481460
C	1.093380	−1.167662	1.083087
C	0.556179	2.339536	0.411912
C	1.622218	2.096139	−0.433645
H	3.631805	0.239341	−1.591073
H	3.684442	−2.147533	−0.919701
H	2.107244	−3.034173	0.772895
H	0.416546	−1.544109	1.845989
H	0.003994	3.254493	0.583045
H	2.114248	2.826200	−1.062218
N	0.235309	1.196399	1.111157
H	−0.705464	1.008460	1.471669

Conformer 1d, 4−methylindole

C	−1.606189	−1.040383	1.322858
H	−0.661615	−0.549335	1.076890
H	−1.856772	−0.900730	2.377932
H	−1.542587	−2.106066	1.098571
S	−2.952894	−0.361279	0.329063
C	−2.671705	1.361060	0.776391
H	−1.640065	1.631544	0.540381
H	−3.365041	1.962089	0.186243
H	−2.880468	1.493129	1.840888
O	−2.558361	−0.500209	−1.134242
C	0.768681	0.388729	−0.816938
C	1.827420	−0.046831	0.032286
C	2.586599	0.915365	0.730647
C	2.272312	2.261867	0.570749
C	1.219861	2.674231	−0.281558
C	0.466156	1.746965	−0.998030
C	0.831803	−1.842097	−0.887482
C	1.853147	−1.480345	−0.027181

H	3.407862	0.612728	1.376543
H	2.847631	3.014709	1.102925
H	1.013770	3.734921	−0.398718
H	−0.323627	2.059400	−1.676787
H	0.514774	−2.832370	−1.192005
N	0.205187	−0.723375	−1.400515
H	−0.780839	−0.724405	−1.678760
C	2.831097	−2.385114	0.654370
H	3.848457	−2.223841	0.281584
H	2.845511	−2.211900	1.735860
H	2.574812	−3.434791	0.484311

Conformer 1e, phenol

C	1.323502	−0.031801	−1.265526
C	2.262680	−1.008243	−0.923355
C	2.926270	−0.956168	0.308187
C	2.638176	0.083307	1.200157
C	1.692461	1.058674	0.868001
C	1.018992	0.994823	−0.358748
H	0.802070	−0.065780	−2.217692
H	2.491105	−1.800732	−1.631213
H	3.659189	−1.713882	0.568629
H	3.155290	0.141301	2.154194
H	1.457775	1.872412	1.548805
O	0.083859	1.944421	−0.640327
H	−0.658896	1.466586	−1.074267
C	−1.108331	−1.671802	0.489300
H	−0.190373	−1.135307	0.736317
H	−1.487332	−2.228693	1.350376
H	−0.925240	−2.356190	−0.340247
S	−2.392911	−0.526346	−0.050450
C	−2.269907	0.596387	1.354427
H	−1.257788	1.002059	1.406265
H	−2.987205	1.401442	1.189758
H	−2.527929	0.049593	2.264610
O	−1.852252	0.230286	−1.257547

Conformer 1f, 4−methylphenol

C	0.878653	0.622926	−1.287209
C	1.984283	−0.222389	−1.166425
C	2.685769	−0.342164	0.043146
C	2.240357	0.415794	1.136472
C	1.129019	1.258652	1.031937
C	0.430320	1.353904	−0.177576
H	0.336128	0.700941	−2.225156
H	2.315972	−0.789104	−2.034576
H	2.769865	0.348616	2.084961
H	0.783692	1.841467	1.881852
O	−0.670131	2.156813	−0.242338
H	−1.339777	1.642687	−0.746809
C	3.906815	−1.220094	0.150391

H	4.812007	−0.671122	−0.131014
H	4.042341	−1.581866	1.173423
H	3.826777	−2.088155	−0.509910
C	−1.068453	−1.783612	0.123974
H	−0.261126	−1.135161	0.469203
H	−1.279887	−2.575037	0.848181
H	−0.803510	−2.224746	−0.837946
S	−2.584029	−0.838468	−0.131641
C	−2.590904	−0.027082	1.478056
H	−1.673998	0.553998	1.593360
H	−3.458288	0.633828	1.504042
H	−2.681048	−0.788945	2.256189
O	−2.282349	0.244747	−1.159679

Conformer 1g, imidazole

C	−1.117720	−0.790527	1.346920
H	−0.185514	−0.222202	1.318860
H	−1.655289	−0.617027	2.282542
H	−0.909407	−1.855880	1.239129
S	−2.196437	−0.318124	−0.022039
C	−2.174035	1.452668	0.306568
H	−1.139933	1.803186	0.293181
H	−2.747134	1.933687	−0.486809
H	−2.642316	1.648717	1.273903
O	−1.413203	−0.518816	−1.311405
C	1.708243	1.117590	−0.439787
C	2.749098	0.862173	0.437234
C	2.036285	−1.045259	−0.223007
N	1.278952	−0.114295	−0.867262
H	0.383249	−0.299260	−1.335269
H	1.283604	2.036540	−0.815524
H	3.367692	1.578044	0.959853
H	1.889952	−2.106503	−0.367165
N	2.948545	−0.491227	0.569205

Conformer 1h, 4−methylimidazole

C	−1.369388	−0.108734	1.538157
H	−0.383256	0.230303	1.213040
H	−1.751480	0.515679	2.349823
H	−1.317367	−1.146181	1.871096
S	−2.551952	−0.044754	0.174259
C	−2.245446	1.672945	−0.273685
H	−1.185680	1.794553	−0.507245
H	−2.853862	1.889211	−1.152552
H	−2.542463	2.322974	0.552627
O	−1.990532	−0.885011	−0.963391
C	1.397084	0.357938	−0.940283
C	2.450297	0.316008	−0.039285
C	1.424289	−1.567878	0.114018
N	0.769428	−0.861259	−0.847489
H	−0.183375	−1.056745	−1.175438

H	1.087922	1.110628	−1.651068
H	1.118468	−2.562442	0.407990
N	2.455380	−0.895583	0.615576
C	3.492876	1.352923	0.225456
H	3.531615	1.596469	1.290798
H	4.482430	0.992100	−0.069282
H	3.280610	2.268297	−0.333686

Conformer 1w, H_2O

C	0.636840	1.345026	0.757295
H	−0.369224	1.248198	1.170356
H	1.400137	1.312739	1.538319
H	0.725222	2.275397	0.194913
C	0.636557	−1.345049	0.757328
H	−0.369473	−1.248069	1.170428
H	0.724604	−2.275420	0.194859
H	1.400054	−1.313031	1.538143
S	0.926289	−0.000057	−0.407038
O	−0.255727	0.000014	−1.364793
O	−2.356565	0.000095	0.365377
H	−1.810168	0.000201	−0.443911
H	−3.263824	0.000160	0.057082

Me_2SO_2 complexes (Fig. 1)

Conformer 2a, benzene

C	1.736129	−0.725835	1.209851
C	2.435717	−1.338596	0.164938
C	2.930002	−0.569413	−0.896102
C	2.732585	0.816192	−0.906767
C	2.043924	1.431800	0.146590
C	1.543497	0.660268	1.201787
H	1.326078	−1.320583	2.019723
H	2.590897	−2.413958	0.173664
H	3.472998	−1.046441	−1.707331
H	3.122973	1.414868	−1.725141
H	1.908589	2.510541	0.147781
H	1.000844	1.130110	2.017019
C	−1.875125	1.628157	−0.065605
H	−0.849338	1.922192	0.156802
H	−2.193793	1.985199	−1.045379
H	−2.554360	1.993620	0.706191
C	−0.818700	−0.656946	−1.259815
H	0.167641	−0.270983	−1.003780
H	−0.812110	−1.748003	−1.241346
H	−1.156759	−0.299821	−2.233305
O	−1.494649	−0.590964	1.282747
S	−1.989413	−0.149549	−0.019734
O	−3.325502	−0.526252	−0.472548

Conformer 2b, Toluene

C	−1.849846	1.000376	0.181094
C	−2.450810	0.449879	−0.960362
C	−2.696325	−0.925596	−1.058152
C	−2.347237	−1.776205	−0.004169
C	−1.753397	−1.238977	1.145481
C	−1.506438	0.135005	1.232884
H	−2.732801	1.105841	−1.781227
H	−3.168644	−1.329118	−1.949876
H	−2.546915	−2.842034	−0.070686
H	−1.501465	−1.889095	1.980122
H	−1.042696	0.548588	2.125864
C	−1.556686	2.473267	0.281178
H	−2.052973	3.028536	−0.519114
H	−1.901299	2.873194	1.239450
H	−0.477903	2.642875	0.214913
C	2.080667	−1.193952	1.131535
H	1.060363	−1.304094	1.498601
H	2.463483	−2.127032	0.716913
H	2.738881	−0.837718	1.925587
C	0.985843	−0.569028	−1.354790
H	0.009243	−0.730157	−0.899202
H	0.919500	0.197298	−2.129046
H	1.397862	−1.489028	−1.771332
O	1.513577	1.273482	0.443319
S	2.106766	0.064633	−0.128603
O	3.447983	0.100170	−0.704757

Conformer 2c, Indole

C	−1.407981	0.823596	−1.278355
H	−0.344103	0.627636	−1.134957
H	−1.740380	0.534882	−2.276391
H	−1.625141	1.878793	−1.104466
C	−1.903008	−1.775999	−0.413419
H	−0.824505	−1.887837	−0.292606
H	−2.435755	−2.382923	0.320720
H	−2.228721	−2.034636	−1.421526
O	−1.853532	0.253155	1.256700
S	−2.355096	−0.088628	−0.079994
O	−3.771295	0.080857	−0.387410
C	1.341512	0.228012	0.702801
C	2.194915	0.528660	−0.399738
C	2.906224	−0.523589	−1.015032
C	2.742017	−1.817301	−0.531306
C	1.897411	−2.089000	0.572639
C	1.189615	−1.072330	1.208123
C	1.218962	2.434806	0.322510
C	2.100136	1.941001	−0.620793
H	3.570888	−0.326031	−1.852464
H	3.285595	−2.635901	−0.995011
H	1.809469	−3.108907	0.937850

H	0.546891	−1.269527	2.061747
H	0.874870	3.447188	0.487885
H	2.625156	2.525756	−1.363875
N	0.790876	1.410309	1.138508
H	−0.049078	1.438169	1.704524

Conformer 2d, 3–Methylindole

C	1.062791	−0.428305	−1.277118
H	0.471698	0.474870	−1.119562
H	1.428097	−0.498356	−2.302543
H	0.466943	−1.307867	−1.020882
C	3.117036	1.234125	−0.401280
H	2.359833	1.952195	−0.084109
H	4.000858	1.298898	0.235176
H	3.394011	1.376808	−1.446428
O	1.997875	−0.508685	1.198486
S	2.471029	−0.410760	−0.186845
O	3.456173	−1.366254	−0.683624
C	−1.061122	0.328492	0.937250
C	−2.053919	0.138848	−0.066925
C	−2.439687	1.237443	−0.862374
C	−1.834976	2.471767	−0.640194
C	−0.856592	2.638408	0.370283
C	−0.466138	1.574275	1.181195
C	−1.593340	−1.845678	0.889218
C	−2.381405	−1.257682	−0.084254
H	−3.194155	1.123843	−1.637560
H	−2.120122	3.327048	−1.246907
H	−0.419738	3.620779	0.531117
H	0.280339	1.695328	1.961309
H	−1.537216	−2.884614	1.189877
N	−0.834211	−0.888069	1.534124
H	0.031218	−1.086762	2.021528
C	−3.404240	−1.925360	−0.948928
H	−4.412688	−1.563486	−0.721851
H	−3.214522	−1.729995	−2.009851
H	−3.394387	−3.008535	−0.798789

Conformer 2e, Phenol

C	2.986498	1.221273	0.276927
C	2.402251	1.079776	−0.987494
C	1.619144	−0.038382	−1.286439
C	1.403736	−1.018475	−0.307891
C	2.001417	−0.892971	0.951655
C	2.788987	0.226114	1.241132
H	3.598858	2.088812	0.503279
H	2.563056	1.837348	−1.749708
H	1.842316	−1.677189	1.686760
H	3.250951	0.316831	2.220356
H	1.158789	−0.152109	−2.263624
O	0.631320	−2.121092	−0.546850

H	−0.106301	−1.822627	−1.103078
C	−1.889654	−0.873802	1.341294
H	−0.854511	−1.206077	1.422101
H	−2.229992	−0.367714	2.245330
H	−2.541587	−1.719535	1.116042
C	−0.946538	1.578177	0.400253
H	0.057999	1.190449	0.573351
H	−0.945367	2.259500	−0.452165
H	−1.347955	2.078883	1.282128
O	−1.481959	−0.434431	−1.215288
S	−2.038501	0.242994	−0.035231
O	−3.402522	0.754931	−0.074572

Conformer 2f, 4−Methylphenol

C	−1.486948	1.249741	1.021943
C	−2.472223	0.263880	1.140294
C	−2.833623	−0.540905	0.049353
C	−2.185498	−0.314814	−1.175015
C	−1.205769	0.671954	−1.310515
C	−0.840582	1.447945	−0.202834
H	−1.209943	1.872370	1.868604
H	−2.965434	0.118175	2.099240
H	−2.454243	−0.916022	−2.041416
H	−0.704264	0.830247	−2.261159
O	0.129209	2.410777	−0.277692
H	0.822640	2.053271	−0.855139
C	−3.921684	−1.577221	0.172558
H	−3.987803	−1.958203	1.195283
H	−4.897215	−1.153355	−0.088905
H	−3.737133	−2.422758	−0.495755
C	0.916306	−1.617088	0.174012
H	1.173278	−2.304722	0.980778
H	0.003195	−1.060268	0.387734
H	0.814378	−2.160564	−0.766788
C	2.283783	0.445241	1.463543
H	2.474838	−0.234892	2.294332
H	3.100694	1.162828	1.369846
H	1.332717	0.967174	1.570828
O	3.505947	−1.253367	−0.138735
S	2.270044	−0.485156	−0.052459
O	1.913723	0.442192	−1.135845

Conformer 2g, Imidazole

C	2.487741	−1.102039	−0.218166
C	3.096186	−0.287347	0.721305
C	1.894472	1.002773	−0.496999
N	1.739595	−0.255915	−0.996226
H	1.018001	−0.522315	−1.656433
H	2.532367	−2.165063	−0.399887
H	3.784049	−0.576624	1.502760
H	1.414748	1.862029	−0.943488

N	2.721856	1.023653	0.542711
C	−1.906061	1.613214	0.264949
H	−2.371840	1.772972	1.237677
H	−0.912311	2.058944	0.219910
H	−2.541943	2.012122	−0.526854
C	−0.687255	−0.694748	1.249022
H	−1.181905	−0.549646	2.210038
H	−0.523648	−1.758790	1.071316
H	0.258148	−0.152541	1.196632
O	−3.091145	−0.736707	0.174932
S	−1.780483	−0.135900	−0.039444
O	−1.099928	−0.309790	−1.328261

Conformer 2h, 4−Methylimidazole

C	−2.094424	0.095394	−1.138609
C	−2.776969	0.207056	0.062879
C	−1.381166	−1.416379	0.294876
N	−1.226420	−0.956153	−0.977631
H	−0.439132	−1.182497	−1.574452
H	−2.165693	0.647314	−2.064177
H	−0.817422	−2.255611	0.677547
N	−2.320777	−0.742794	0.950701
C	−3.864654	1.163202	0.429581
H	−4.788796	0.625973	0.659750
H	−3.587349	1.743482	1.313987
H	−4.064193	1.856054	−0.392026
C	2.301376	−0.740965	1.421605
H	2.625571	−0.069845	2.217361
H	1.352360	−1.219197	1.664252
H	3.069729	−1.490326	1.225153
C	0.822565	1.339715	0.297419
H	1.178999	2.018007	1.073527
H	0.624525	1.894545	−0.620998
H	−0.071439	0.799635	0.613204
O	3.352763	0.939179	−0.311855
S	2.123719	0.187898	−0.086407
O	1.633904	−0.735357	−1.116721

Conformer 2w, H_2O

C	−0.194695	−1.394862	−0.857099
H	0.872139	−1.348011	−1.077739
H	−0.803679	−1.381759	−1.761325
H	−0.425374	−2.280470	−0.263003
C	−0.195508	1.395206	−0.856585
H	−0.803854	1.381583	−1.761239
H	−0.427580	2.280455	−0.262524
H	0.871490	1.349742	−1.076745
S	−0.632046	−0.000145	0.156213
O	0.267068	−0.000005	1.317993
O	−2.075917	−0.000580	0.355592
O	2.733698	0.001180	−0.053800
H	3.621313	−0.008265	0.308598
H	2.150717	0.002211	0.718410

Atomic coordinates of the local minima complexes presented in Fig. S1–S18 of the Supporting Information

Me_2SO–benzene (Fig. S1)

Conformer S1a

C	1.528157	0.563502	−0.018566
C	2.689720	1.344030	−0.013684
C	3.949868	0.735686	−0.023726
C	4.053456	−0.658844	0.025060
C	2.895649	−1.444321	0.018954
C	1.637676	−0.831585	0.029348
H	0.544593	1.025372	−0.018185
H	2.610452	2.427200	−0.045201
H	4.848710	1.346244	−0.024719
H	5.031635	−1.131841	0.022532
H	2.974616	−2.527649	0.051507
H	0.738544	−1.442223	0.028861
C	−3.600376	−0.160942	1.331816
H	−4.228908	0.720997	1.189589
H	−4.193344	−1.078558	1.325270
H	−3.055801	−0.077593	2.273024
S	−2.370364	−0.214281	0.015340
C	−3.543638	−0.254322	−1.352383
H	−4.177709	0.633378	−1.297159
H	−2.959405	−0.233245	−2.273060
H	−4.136388	−1.171066	−1.309008
O	−1.716780	1.147281	−0.018726

Conformer S1b

C	1.758422	1.210103	−0.694823
C	1.924185	1.214100	0.694471
C	2.015858	0.004980	1.391527
C	1.927283	−1.208711	0.702050
C	1.761465	−1.213841	−0.687232
C	1.676625	−0.004146	−1.386277
H	1.699883	2.149899	−1.237839
H	1.993366	2.156550	1.230553
H	2.143834	0.008519	2.470098
H	1.999052	−2.147605	1.243995
H	1.705419	−2.157154	−1.224376
H	1.563403	−0.007669	−2.467708
C	−1.805861	−1.337678	−0.828569
H	−2.842093	−1.261099	−1.168040
H	−1.103210	−1.280997	−1.661950
H	−1.665509	−2.276629	−0.290783
S	−1.476529	−0.000061	0.339707
C	−1.807017	1.335910	−0.830131
H	−2.843254	1.258103	−1.169315
H	−1.667367	2.275612	−0.293471

H	−1.104488	1.278776	−1.663577
O	−2.620041	0.000046	1.328876

Conformer S1c

C	2.117309	1.311263	0.101954
C	2.682151	0.309713	0.901409
C	2.487331	−1.037553	0.576011
C	1.735333	−1.380858	−0.555013
C	1.164776	−0.378288	−1.347012
C	1.351750	0.968455	−1.016984
H	2.269052	2.357080	0.355324
H	3.272888	0.577256	1.773347
H	2.929413	−1.815572	1.192538
H	1.596715	−2.426993	−0.816465
H	0.562306	−0.637143	−2.212494
H	0.876407	1.737185	−1.616800
C	−2.261417	−1.472982	−0.068228
H	−1.251157	−1.726768	−0.395636
H	−2.533133	−2.022255	0.836642
H	−2.978127	−1.689220	−0.861644
S	−2.339785	0.303006	0.249413
C	−1.024591	0.324447	1.487766
H	−0.120438	−0.133714	1.084380
H	−0.831002	1.371244	1.726711
H	−1.371375	−0.201059	2.381629
O	−1.812607	0.987084	−0.989695

Conformer S1d

C	1.980021	0.967037	−0.921724
C	2.673003	−0.243174	−1.041433
C	2.735429	−1.125008	0.044551
C	2.107217	−0.793096	1.250604
C	1.418642	0.420239	1.369627
C	1.351629	1.300169	0.283327
H	1.921758	1.647863	−1.765935
H	3.163781	−0.498577	−1.976647
H	3.275236	−2.063506	−0.047320
H	2.162785	−1.472345	2.097066
H	0.931857	0.678920	2.305862
H	0.791603	2.225638	0.364482
C	−3.529494	−0.574786	0.014654
H	−3.738589	−0.583145	−1.057564
H	−3.616864	−1.575411	0.444865
H	−4.216747	0.107641	0.516247
S	−1.861215	0.061030	0.284121
C	−1.020905	−1.172520	−0.725475
H	−1.391091	−1.092856	−1.750819
H	0.045046	−0.949560	−0.693579
H	−1.203120	−2.168158	−0.312775
O	−1.780823	1.374304	−0.458552

Me_2SO–toluene (Fig. S2)

Conformer S2a

C	1.177416	−0.992870	−0.006676
C	2.267039	−1.870081	−0.017885
C	3.570690	−1.363014	−0.024652
C	3.785407	0.018578	0.014019
C	2.705744	0.913358	0.018466
C	1.405627	0.387498	0.027951
H	0.156905	−1.366360	0.002130
H	2.098917	−2.943094	−0.042598
H	4.419856	−2.041229	−0.027347
H	4.801690	0.407483	0.015645
H	0.557313	1.069280	0.041970
C	2.936511	2.403477	0.018198
H	3.868081	2.657529	0.531576
H	3.003042	2.792423	−1.003853
H	2.117933	2.926637	0.520350
C	−3.736377	0.387360	−1.364606
H	−4.477297	−0.414237	−1.323890
H	−4.210600	1.370879	−1.325919
H	−3.144379	0.296085	−2.276027
S	−2.599163	0.196824	0.020984
C	−3.847564	0.293070	1.317795
H	−4.577789	−0.504155	1.161710
H	−3.332640	0.140576	2.267016
H	−4.322576	1.276897	1.306037
O	−2.119850	−1.235269	−0.009776

Conformer S2b

C	−0.985413	0.757341	0.001801
C	−2.098657	1.604580	−0.012931
C	−3.392875	1.074114	−0.006306
C	−3.604070	−0.312317	0.011498
C	−2.483659	−1.155396	0.030975
C	−1.188318	−0.627357	0.024658
H	0.024907	1.157074	−0.000129
H	−1.957031	2.681985	−0.024892
H	−4.250969	1.743279	−0.013929
H	−0.333223	−1.298433	0.041918
H	−2.628589	−2.233814	0.052993
C	−4.999824	−0.881987	−0.015053
H	−5.342314	−1.037702	−1.043837
H	−5.039868	−1.846531	0.498556
H	−5.708393	−0.206923	0.472649
C	4.010775	−0.385112	−1.355596
H	4.716840	0.445212	−1.283622
H	4.524202	−1.349002	−1.324100
H	3.435428	−0.300887	−2.278272
S	2.837012	−0.267690	0.007512
C	4.060058	−0.338606	1.329905

H	4.761335	0.489374	1.204230
H	3.518881	−0.223945	2.269804
H	4.573842	−1.302646	1.311729
O	2.300581	1.144305	−0.007123

Conformer S2c

C	1.074460	−0.324068	0.014900
C	2.293446	−1.010039	0.021462
C	3.516441	−0.323479	0.003450
C	3.494209	1.078680	0.008333
C	2.282214	1.776661	0.000422
C	1.071856	1.075687	0.012413
H	0.132980	−0.866928	0.028863
H	2.293903	−2.098185	0.027993
H	0.129266	1.616421	0.010071
H	2.284700	2.863548	0.004928
H	4.433655	1.627677	0.003645
C	4.823191	−1.075138	−0.024423
H	5.132455	−1.289376	−1.053241
H	5.620417	−0.495470	0.448974
H	4.737120	−2.029572	0.502091
C	−3.997851	0.067424	−1.366481
H	−4.596126	−0.842408	−1.280244
H	−4.626980	0.960619	−1.358663
H	−3.409242	0.035879	−2.284086
S	−2.829361	0.125113	0.004918
C	−4.062264	0.071255	1.318875
H	−4.654755	−0.839616	1.207439
H	−3.518663	0.044052	2.263959
H	−4.691182	0.963657	1.277050
O	−2.121498	−1.209249	0.023603

Conformer S2d

C	−1.312660	0.088132	0.012789
C	−2.462712	0.891098	0.012593
C	−3.720361	0.269688	0.007099
C	−3.832162	−1.124213	−0.010187
C	−2.680699	−1.918717	−0.015870
C	−1.422995	−1.307035	−0.003651
H	−0.329961	0.554602	0.026579
H	−0.523036	−1.917219	−0.002427
H	−2.764552	−3.001973	−0.026081
H	−4.814776	−1.588409	−0.013555
H	−4.619757	0.882375	0.015490
C	−2.341546	2.393840	0.002095
H	−2.426722	2.786550	−1.017011
H	−3.129281	2.856471	0.603832
H	−1.372525	2.707433	0.398413
C	3.783435	−0.133618	−1.365034
H	4.348774	0.793864	−1.249931

H	4.443731	−1.003916	−1.381146
H	3.196240	−0.096137	−2.283302
S	2.614287	−0.272788	−0.000246
C	3.839852	−0.210122	1.319986
H	4.398839	0.724514	1.236050
H	3.292505	−0.229116	2.263096
H	4.501103	−1.077513	1.256237
O	1.858739	1.034846	0.052346

Conformer S2e

C	2.098117	0.868584	0.005695
C	3.499522	0.792746	−0.001530
C	4.152860	−0.443032	0.010984
C	3.410175	−1.629218	−0.009523
C	2.013569	−1.566426	−0.001591
C	1.364943	−0.326424	−0.012098
H	1.428275	−2.482407	−0.015941
H	3.916009	−2.590666	−0.001077
H	5.238929	−0.481090	0.005323
H	0.281164	−0.262915	−0.009784
H	4.083249	1.711302	0.010860
C	1.388952	2.199343	0.000383
H	0.306019	2.056367	−0.005084
H	1.659116	2.786804	0.884110
H	1.668468	2.783939	−0.882237
C	−3.783005	−0.278508	1.353623
H	−4.361803	0.643465	1.263801
H	−4.429730	−1.158898	1.334983
H	−3.204324	−0.262568	2.277914
S	−2.599981	−0.358063	−0.003932
C	−3.813899	−0.271914	−1.333569
H	−4.389352	0.650320	−1.226595
H	−3.256851	−0.252922	−2.270988
H	−4.461013	−1.151703	−1.303330
O	−1.858232	0.958635	−0.009161

Conformer S2f

C	1.676786	0.088359	1.204983
C	1.576226	−1.306737	1.208319
C	1.534737	−2.009057	0.000162
C	1.576876	−1.306685	−1.208017
C	1.677616	0.088333	−1.204618
C	1.726864	0.805944	0.000232
H	1.728614	0.627114	2.149498
H	1.548519	−1.844428	2.152232
H	1.549739	−1.844372	−2.151951
H	1.730071	0.627112	−2.149105
H	1.458949	−3.092397	0.000125
C	1.833844	2.310093	−0.000036
H	0.844696	2.784613	−0.011849

H	2.357840	2.666475	0.890965
H	2.377677	2.664635	−0.879856
C	−1.736790	0.916944	−1.337850
H	−2.651290	1.510295	−1.256418
H	−0.843566	1.542312	−1.289652
H	−1.744123	0.359656	−2.275974
S	−1.710065	−0.296478	0.000124
C	−1.736685	0.918692	1.336534
H	−2.650820	1.512443	1.254026
H	−1.744700	0.362551	2.275337
H	−0.843050	1.543465	1.287952
O	−3.066796	−0.963895	0.000553

Conformer S2g

C	−1.343919	1.982149	0.072371
C	−1.593621	1.357120	−1.154650
C	−1.855612	−0.014854	−1.201334
C	−1.851319	−0.791006	−0.033153
C	−1.613921	−0.151320	1.191423
C	−1.358010	1.223577	1.247663
H	−1.154910	3.051617	0.113263
H	−1.601651	1.940745	−2.071378
H	−1.629605	−0.734837	2.110225
H	−2.045972	−0.494810	−2.158893
H	−1.190066	1.704328	2.208647
C	−2.063267	−2.280633	−0.100302
H	−2.784430	−2.540804	−0.879851
H	−1.123253	−2.793362	−0.334345
H	−2.432310	−2.670665	0.852052
C	1.844006	−0.633561	1.480826
H	2.912886	−0.580524	1.703929
H	1.269122	0.067690	2.088193
H	1.485152	−1.649872	1.652056
S	1.602423	−0.268541	−0.271428
C	2.263146	1.410068	−0.193752
H	3.298810	1.367476	0.153463
H	2.231452	1.814325	−1.206611
H	1.639403	2.016160	0.466284
O	2.615214	−1.101254	−1.026092

Conformer S2h

C	−1.393615	−1.300770	1.209479
C	−1.750760	0.051407	1.204523
C	−1.930585	0.746120	−0.000055
C	−1.752455	0.050096	−1.204136
C	−1.395434	−1.302109	−1.208143
C	−1.210784	−1.982163	0.000907
H	−1.268375	−1.823950	2.154301
H	−1.894056	0.574452	2.147855
H	−1.897076	0.572122	−2.147829

H	−1.271583	−1.826324	−2.152570
H	−0.947626	−3.036934	0.001279
C	−2.245837	2.218404	−0.000622
H	−1.321821	2.807309	−0.001610
H	−2.822409	2.497784	−0.886501
H	−2.821149	2.498729	0.885781
C	2.127636	−0.661286	−1.333049
H	3.209520	−0.796758	−1.254428
H	1.594860	−1.611864	−1.268274
H	1.887458	−0.166385	−2.275315
S	1.581000	0.429019	−0.001317
C	2.128131	−0.650378	1.339094
H	3.209855	−0.787250	1.260712
H	1.889170	−0.147268	2.277318
H	1.594691	−1.601150	1.282976
O	2.513094	1.620907	−0.006324

Conformer S2i

C	−1.547681	1.731711	−0.596790
C	−2.342611	0.605575	−0.841989
C	−2.339736	−0.485211	0.040047
C	−1.530222	−0.412135	1.185205
C	−0.726945	0.706530	1.429317
C	−0.730266	1.782648	0.535964
H	−1.531621	−1.241357	1.890931
H	−0.089209	0.741220	2.307681
H	−0.081508	2.633457	0.714453
H	−1.566850	2.567210	−1.291757
H	−2.974864	0.573224	−1.727162
C	−3.172182	−1.711108	−0.239741
H	−4.053650	−1.459407	−0.835532
H	−2.596598	−2.459443	−0.796035
H	−3.510459	−2.175831	0.690483
C	2.243170	−1.558453	0.696019
H	1.256558	−1.402450	1.137084
H	2.281277	−2.494084	0.132444
H	3.005369	−1.565225	1.476451
S	2.614167	−0.170127	−0.398182
C	1.174621	−0.394548	−1.467032
H	0.262456	−0.416929	−0.868901
H	1.147297	0.458338	−2.146887
H	1.299602	−1.319045	−2.037498
O	2.394579	1.086538	0.409894

Conformer S2j

C	1.638949	1.794357	−0.423336
C	2.358909	0.677033	−0.859871
C	2.383693	−0.506524	−0.106043
C	1.680078	−0.536633	1.108088
C	0.955291	0.576237	1.548494

C	0.931138	1.746212	0.782021
H	1.637643	2.702981	−1.019399
H	2.911123	0.723912	−1.796158
H	0.368652	2.610351	1.123003
H	0.422168	0.536298	2.494890
H	1.706260	−1.438982	1.716264
C	3.133105	−1.719549	−0.595461
H	3.484243	−2.328112	0.242091
H	2.491179	−2.349851	−1.220784
H	4.000010	−1.429194	−1.194790
C	−2.086861	−1.428982	0.825671
H	−2.389681	−2.214502	0.128765
H	−1.044158	−1.543085	1.128469
H	−2.737781	−1.445815	1.701059
S	−2.313838	0.171627	0.020954
C	−1.189220	−0.159949	−1.348592
H	−1.559394	−1.030287	−1.896712
H	−1.203458	0.716687	−1.997820
H	−0.179088	−0.318879	−0.966680
O	−3.714600	0.176153	−0.545412

Conformer S2k

C	2.285714	−1.647654	−0.003550
C	2.633364	−0.753293	1.016096
C	2.267376	0.593626	0.920607
C	1.546814	1.068967	−0.186370
C	1.208959	0.162355	−1.202304
C	1.566750	−1.186790	−1.111224
H	2.572117	−2.693335	0.066067
H	3.198466	−1.100740	1.876965
H	2.549008	1.285812	1.711778
H	1.276146	−1.871696	−1.902196
H	0.645673	0.506557	−2.066046
C	1.139414	2.517272	−0.275106
H	1.082012	2.843663	−1.316945
H	0.153061	2.675134	0.175014
H	1.855607	3.158301	0.246518
C	−3.567261	0.221523	0.595253
H	−3.924043	−0.795451	0.774381
H	−3.554435	0.806606	1.518145
H	−4.202740	0.707873	−0.145908
S	−1.901744	0.145797	−0.099397
C	−1.158271	−0.746538	1.277943
H	−1.689002	−1.692915	1.411062
H	−0.117214	−0.934967	1.016742
H	−1.207368	−0.133813	2.181964
O	−1.968317	−0.808825	−1.268156

Conformer S2l

C	−2.178827	0.725447	0.831001
C	−2.591808	−0.584549	1.095778

C	−2.333040	−1.601999	0.170217
C	−1.662791	−1.296600	−1.019791
C	−1.248653	0.015375	−1.275114
C	−1.494418	1.043217	−0.351642
H	−2.391393	1.512939	1.551189
H	−3.125077	−0.808366	2.015718
H	−2.661917	−2.618311	0.367887
H	−1.478601	−2.075025	−1.755987
H	−0.737525	0.248984	−2.206730
C	−1.018348	2.447649	−0.613243
H	−1.672969	3.179470	−0.132375
H	−0.003863	2.594037	−0.226010
H	−0.993607	2.660103	−1.685237
C	2.202793	−1.468554	−0.733390
H	2.749365	−2.079072	−0.010315
H	1.222530	−1.895250	−0.955896
H	2.789247	−1.371820	−1.648210
S	1.999664	0.190637	−0.051240
C	1.093463	−0.331563	1.417286
H	1.740606	−0.987538	2.005583
H	0.860881	0.565375	1.993557
H	0.167660	−0.830277	1.124388
O	3.366227	0.645503	0.406959

Conformer S2m

C	2.467442	−0.509992	1.187435
C	2.518458	−1.458876	0.160882
C	1.976218	−1.149663	−1.091815
C	1.383985	0.097413	−1.311116
C	1.342441	1.066200	−0.295774
C	1.884441	0.742131	0.956625
H	2.886673	−0.739656	2.163355
H	2.978367	−2.427566	0.334282
H	2.010383	−1.880253	−1.895593
H	1.865007	1.482116	1.754537
H	0.960355	0.330256	−2.285648
C	0.771096	2.433315	−0.569197
H	−0.133326	2.362458	−1.180530
H	0.521517	2.952166	0.360515
H	1.493256	3.052319	−1.111886
C	−1.931318	0.868587	1.228179
H	−2.502679	0.351110	2.003061
H	−0.893368	1.016576	1.532655
H	−2.401579	1.827680	1.005849
S	−1.983142	−0.123386	−0.280486
C	−1.171325	−1.564425	0.436756
H	−1.789563	−1.934587	1.258788
H	−1.106578	−2.322996	−0.344736
H	−0.167948	−1.294690	0.772046
O	−3.429860	−0.493612	−0.511347

Conformer S2n

C	−2.182863	−0.651687	1.300366
C	−2.617457	−1.394610	0.195462
C	−2.388571	−0.906378	−1.095412
C	−1.737594	0.320295	−1.275732
C	−1.306590	1.078524	−0.177041
C	−1.526825	0.568527	1.112440
H	−2.349780	−1.025200	2.307212
H	−3.129802	−2.341825	0.339630
H	−2.721228	−1.474956	−1.959944
H	−1.572224	0.700077	−2.282032
H	−1.166567	1.129244	1.971029
C	−0.656818	2.425381	−0.357905
H	0.188130	2.532016	0.327685
H	−0.295976	2.552689	−1.382309
H	−1.372852	3.228120	−0.151291
C	3.564488	−0.505652	−0.400203
H	3.862513	−1.090822	0.472943
H	3.650883	−1.090853	−1.318935
H	4.182375	0.390504	−0.469285
S	1.856934	0.040189	−0.187130
C	1.143557	−1.604034	−0.016566
H	1.607240	−2.102251	0.838766
H	0.075822	−1.473468	0.157972
H	1.302138	−2.167557	−0.939600
O	1.785053	0.701133	1.171224

Conformer S2o

C	−2.098963	−0.849680	−1.175001
C	−2.546777	−1.356032	0.051817
C	−2.327583	−0.620719	1.220892
C	−1.676826	0.618764	1.156943
C	−1.224492	1.137468	−0.065038
C	−1.439092	0.380670	−1.228660
H	−1.068039	0.757492	−2.178421
H	−2.263690	−1.413969	−2.089222
H	−3.059583	−2.312903	0.095572
H	−2.673627	−1.001926	2.178173
H	−1.528255	1.195131	2.068406
C	−0.529476	2.470170	−0.150778
H	0.440739	2.344536	−0.640518
H	−1.124775	3.179007	−0.735312
H	−0.375326	2.900228	0.843403
C	2.163916	0.298793	1.438278
H	1.118467	0.601702	1.526559
H	2.433764	−0.412945	2.222597
H	2.816053	1.171904	1.489151
S	2.412163	−0.460150	−0.181805
C	1.148196	−1.731548	0.021112
H	0.195399	−1.266034	0.276845
H	1.061166	−2.248828	−0.935576

H	1.468092	−2.434047	0.795404
O	1.893949	0.526966	−1.203195

Conformer S2p

C	2.183986	0.492328	0.894987
C	2.507366	−0.868690	0.962999
C	2.170426	−1.722561	−0.092187
C	1.512950	−1.202471	−1.214413
C	1.190158	0.156934	−1.272371
C	1.519122	1.025197	−0.218511
H	2.454902	1.151145	1.717440
H	3.026364	−1.258989	1.834577
H	2.426903	−2.777403	−0.047221
H	1.261361	−1.854672	−2.047415
H	0.667845	0.555432	−2.139277
C	1.125736	2.475799	−0.282255
H	1.448847	2.925281	−1.226212
H	0.035609	2.554742	−0.222581
H	1.574382	3.042927	0.537863
C	−2.400822	−1.258252	−0.850971
H	−1.390399	−1.295189	−1.263259
H	−2.673704	−2.209903	−0.388074
H	−3.118054	−1.007734	−1.633740
S	−2.470314	0.060647	0.378378
C	−1.167603	−0.602441	1.436303
H	−0.268483	−0.780995	0.845253
H	−0.965227	0.151616	2.198601
H	−1.521630	−1.522249	1.909624
O	−1.910202	1.297573	−0.288890

Me_2SO−indole (Fig. S3)

Conformer S3a

C	−4.389497	−0.590492	1.307285
H	−5.206224	0.125739	1.192469
H	−4.751637	−1.619907	1.253083
H	−3.884523	−0.423530	2.259451
S	−3.173949	−0.295898	0.008807
C	−4.298798	−0.549655	−1.377032
H	−5.123288	0.162195	−1.295052
H	−3.730977	−0.352147	−2.287038
H	−4.661283	−1.580353	−1.380348
O	−2.855800	1.179503	0.041659
C	3.191441	0.427347	0.013960
C	2.153921	−0.547291	−0.002126
C	0.795966	−0.199213	0.034374
C	0.473789	1.155225	0.010034
C	1.491875	2.138083	0.008408
C	2.838167	1.792169	−0.025479

C	4.435093	−0.284498	−0.007159
C	4.129221	−1.629621	−0.000157
H	0.016760	−0.957832	0.030249
H	−0.571675	1.450545	0.033048
H	1.207208	3.186370	−0.013268
H	3.608094	2.559783	−0.027258
H	5.431565	0.135250	−0.010147
H	4.780786	−2.492780	−0.008905
N	2.758884	−1.785480	−0.004724
H	2.275528	−2.668949	0.039956

Conformer S3b

C	−4.608682	−0.273763	1.337998
H	−5.302306	0.566072	1.255430
H	−5.134892	−1.230523	1.299987
H	−4.045487	−0.196207	2.268751
S	−3.413606	−0.173767	−0.008307
C	−4.619833	−0.230993	−1.347130
H	−5.312165	0.606126	−1.232392
H	−4.064514	−0.124550	−2.279746
H	−5.146286	−1.188290	−1.334531
O	−2.857760	1.230011	0.011982
C	2.832512	0.721257	0.023095
C	2.887703	−0.701224	−0.016537
C	1.734082	−1.497664	0.013882
C	0.506564	−0.841188	0.005080
C	0.420951	0.572058	0.022184
C	1.571517	1.352470	−0.000085
C	4.185978	1.191809	0.004785
C	4.999982	0.078425	−0.008836
H	1.792928	−2.583344	−0.004045
H	−0.408183	−1.427482	0.024148
H	−0.559611	1.040268	0.012973
H	1.499151	2.437100	0.015509
H	4.522904	2.219149	0.016826
H	6.078736	0.003117	−0.023347
N	4.218110	−1.057887	−0.025232
H	4.568083	−2.003169	−0.012502

Conformer S3c

C	4.127473	0.122585	1.350087
H	4.745483	−0.773258	1.256561
H	4.735133	1.030396	1.328861
H	3.554436	0.080132	2.277096
S	2.935626	0.147288	−0.002072
C	4.145616	0.122690	−1.338012
H	4.761665	−0.773617	−1.236500
H	3.585192	0.081155	−2.272734
H	4.753607	1.030018	−1.308055
O	2.264584	−1.205849	−0.006804
C	−1.488436	0.187217	0.016403

C	−2.886818	0.453074	−0.015603
C	−3.844862	−0.570063	0.018527
C	−3.376853	−1.880680	−0.006809
C	−1.990455	−2.163793	0.005658
C	−1.039177	−1.149926	−0.015914
C	−0.822626	1.457000	0.000541
C	−1.803689	2.426995	−0.002556
H	−4.910172	−0.353154	0.008682
H	−4.090137	−2.700214	0.011892
H	−1.663759	−3.199821	−0.014094
H	0.026042	−1.367692	−0.008850
H	0.243444	1.635150	0.011281
H	−1.719513	3.505354	−0.008675
N	−3.043356	1.822383	0.001072
H	−3.925650	2.308464	−0.039314

Conformer S3d

C	−4.606763	0.256595	−1.328002
H	−5.306811	−0.576186	−1.229685
H	−5.123767	1.218360	−1.290686
H	−4.056552	0.166939	−2.265400
S	−3.395220	0.157003	0.003263
C	−4.582790	0.235626	1.357322
H	−5.284269	−0.595925	1.258721
H	−4.016026	0.131967	2.283337
H	−5.100521	1.197631	1.343742
O	−2.852009	−1.252400	−0.012787
C	2.906277	0.782887	0.018934
C	2.799876	−0.636673	−0.015935
C	1.564408	−1.299743	−0.000250
C	0.412323	−0.519904	−0.026649
C	0.498217	0.893451	−0.014536
C	1.723872	1.550255	−0.024332
C	4.304137	1.097965	0.017687
C	4.986718	−0.100984	0.018968
H	1.502474	−2.385165	−0.014129
H	−0.564608	−0.995846	−0.019930
H	−0.419504	1.474793	−0.040453
H	1.771941	2.636482	−0.013204
H	4.755594	2.080378	0.031845
H	6.050190	−0.297538	0.019270
N	4.081809	−1.140835	−0.007786
H	4.321133	−2.119753	0.021925

Conformer S3e

C	−1.243101	−1.598734	−0.713440
H	−2.075169	−2.270689	−0.941415
H	−0.789139	−1.197985	−1.621554
H	−0.486320	−2.122089	−0.126001
S	−1.872791	−0.244106	0.300674
C	−2.921762	0.466095	−0.988549

H	−3.615210	−0.296335	−1.352824
H	−3.482052	1.280982	−0.527578
H	−2.293172	0.856435	−1.792413
O	−2.801340	−0.867315	1.319791
C	1.546692	0.087996	0.764266
C	1.541346	0.132007	−0.659911
C	1.026243	1.223222	−1.374600
C	0.593200	2.322369	−0.636350
C	0.639932	2.321111	0.777386
C	1.126768	1.226608	1.481759
C	2.102979	−1.177162	1.140691
C	2.395356	−1.851993	−0.027005
H	1.011388	1.236278	−2.462387
H	0.209297	3.195552	−1.157292
H	0.303453	3.201286	1.318009
H	1.145411	1.229963	2.568487
H	2.265859	−1.549541	2.142706
H	2.829305	−2.831460	−0.176298
N	2.039983	−1.070852	−1.107703
H	2.225943	−1.301329	−2.072116

Conformer S3f

C	3.555694	−0.210791	−0.727375
H	4.035171	−1.093195	−0.296830
H	3.494795	−0.283955	−1.816195
H	4.112305	0.683731	−0.444555
S	1.894096	−0.045670	−0.034406
C	1.296471	−1.651720	−0.591889
H	1.951720	−2.432590	−0.196461
H	0.289239	−1.770117	−0.191958
H	1.263117	−1.674520	−1.684347
O	2.052032	−0.131141	1.465936
C	−1.227344	0.531536	0.746581
C	−1.478832	0.552264	−0.656325
C	−2.077647	−0.523082	−1.329101
C	−2.403840	−1.647396	−0.574635
C	−2.141599	−1.698517	0.815929
C	−1.544815	−0.630681	1.478376
C	−0.667117	1.801886	1.092710
C	−0.599866	2.538620	−0.070125
H	−2.280609	−0.484840	−2.396864
H	−2.876090	−2.496774	−1.060618
H	−2.404920	−2.595000	1.370605
H	−1.335599	−0.681112	2.543319
H	−0.321850	2.117533	2.066823
H	−0.232245	3.541870	−0.238383
N	−1.064611	1.778439	−1.125564
H	−1.231169	2.127031	−2.057464

Conformer S3g

C	−1.641569	1.436898	−0.933770
H	−0.582144	1.193688	−0.841940

H	−1.943835	1.504724	−1.982488
H	−1.846280	2.381598	−0.427415
S	−2.636406	0.172059	−0.114663
C	−1.929834	−1.218135	−1.027269
H	−0.844506	−1.207534	−0.916664
H	−2.337840	−2.129921	−0.588399
H	−2.224408	−1.146086	−2.077780
O	−2.149442	0.065480	1.310818
C	1.700510	−0.368803	−0.455240
C	1.101419	−0.289237	0.834729
C	0.947722	0.973657	1.441275
C	1.401537	2.099802	0.764305
C	1.989462	2.000096	−0.519681
C	2.140080	0.767481	−1.151436
C	1.235036	−2.462126	0.235526
C	0.815678	−1.628678	1.250437
H	0.467206	1.056780	2.411215
H	1.297639	3.079548	1.222599
H	2.331171	2.900467	−1.023083
H	2.595324	0.692330	−2.136132
H	1.196689	−3.540347	0.156618
H	0.335064	−1.933845	2.168951
N	1.737684	−1.702629	−0.805095
H	2.209928	−2.075514	−1.615000

Conformer S3h

C	1.473146	−1.595995	−0.863069
H	2.293716	−2.290835	−0.664166
H	0.534753	−1.938305	−0.421448
H	1.344800	−1.476053	−1.940088
S	1.914063	0.021227	−0.194548
C	2.036233	−0.539120	1.520088
H	2.831006	−1.287152	1.584636
H	2.297460	0.328555	2.127855
H	1.076134	−0.947208	1.841861
O	3.327246	0.310527	−0.650569
C	−1.574162	0.052253	−0.715968
C	−1.407524	0.027885	0.697974
C	−0.990636	1.150871	1.427248
C	−0.733745	2.316278	0.711327
C	−0.877593	2.359642	−0.694768
C	−1.294393	1.245303	−1.413564
C	−2.059664	−1.239761	−1.102326
C	−2.157229	−1.994798	0.047528
H	−0.882889	1.119175	2.509018
H	−0.412926	3.208089	1.242397
H	−0.660026	3.285615	−1.219230
H	−1.410929	1.293388	−2.493335
H	−2.300333	−1.578075	−2.100999
H	−2.487556	−3.015534	0.185962
N	−1.725413	−1.245293	1.126685
H	−1.874884	−1.503800	2.091257

Conformer S3i

C	−3.118569	1.053130	−0.284055
H	−2.319846	1.665584	0.141497
H	−3.373041	1.381892	−1.294838
H	−4.002700	1.093428	0.353696
S	−2.556622	−0.662387	−0.323356
C	−1.149499	−0.356360	−1.418870
H	−0.587060	0.517146	−1.085237
H	−0.514826	−1.244116	−1.373886
H	−1.527810	−0.218193	−2.435888
O	−2.019547	−0.968792	1.054865
C	2.002068	0.072436	−0.331414
C	1.187523	−0.210585	0.801984
C	0.502885	0.845971	1.434552
C	0.636931	2.131133	0.919410
C	1.441606	2.389775	−0.217015
C	2.125141	1.363328	−0.865062
C	2.051188	−2.148720	0.034329
C	1.236100	−1.624242	1.015360
H	−0.142129	0.642942	2.283498
H	0.120765	2.958792	1.399240
H	1.522445	3.405340	−0.595238
H	2.738860	1.562520	−1.740377
H	2.346600	−3.172242	−0.153896
H	0.703139	−2.182750	1.771342
N	2.488237	−1.131620	−0.793912
H	3.188031	−1.235678	−1.513055

Conformer S3j

C	−2.111171	−0.473856	1.533451
H	−2.852614	−1.275203	1.591034
H	−1.145433	−0.788931	1.933548
H	−2.473251	0.400967	2.075790
S	−1.921821	0.013771	−0.195841
C	−1.365927	−1.607534	−0.763730
H	−2.174566	−2.325709	−0.601694
H	−1.160784	−1.523931	−1.832543
H	−0.458778	−1.896545	−0.228435
O	−3.318676	0.208819	−0.744790
C	1.404853	0.035754	0.777966
C	1.550486	0.053714	−0.639367
C	1.275530	1.191681	−1.411781
C	0.862321	2.335010	−0.736217
C	0.716773	2.344657	0.670800
C	0.990139	1.214810	1.432911
C	1.795382	−1.268792	1.222537
C	2.156382	−1.985963	0.097869
H	1.393090	1.188539	−2.492597
H	0.637325	3.234802	−1.301427
H	0.397954	3.259483	1.162568

H	0.887696	1.237258	2.515407
H	1.829452	−1.634057	2.240136
H	2.516217	−3.001816	0.004836
N	2.006638	−1.189795	−1.016789
H	2.207153	−1.474061	−1.963950

Conformer S3k

C	−1.139123	−0.277808	−1.319649
H	−1.792309	−0.370301	−2.191866
H	−0.588006	0.664902	−1.327560
H	−0.438213	−1.113741	−1.283338
S	−2.177158	−0.364134	0.153741
C	−3.035470	1.197508	−0.148991
H	−3.512774	1.157551	−1.131413
H	−3.798503	1.298503	0.624332
H	−2.321860	2.022146	−0.082953
O	−3.185548	−1.465497	−0.084356
C	1.158824	0.278224	0.858782
C	1.900376	0.479007	−0.339682
C	2.519073	−0.573610	−1.028665
C	2.396852	−1.848856	−0.484833
C	1.661597	−2.073024	0.703900
C	1.048581	−1.026062	1.382465
C	0.624752	1.550760	1.240115
C	1.043492	2.463642	0.292450
H	3.076025	−0.404349	−1.946818
H	2.864715	−2.689847	−0.988732
H	1.582452	−3.083858	1.093752
H	0.482393	−1.209019	2.291626
H	0.026670	1.774708	2.112908
H	0.870038	3.529323	0.224769
N	1.787555	1.812512	−0.670269
H	2.281672	2.267841	−1.423191

Conformer S3l

C	−1.778122	−1.212671	−0.953789
H	−2.359376	−1.039590	−1.863572
H	−0.704790	−1.191440	−1.150657
H	−2.056999	−2.171314	−0.514314
S	−2.205821	0.072602	0.240184
C	−1.629360	1.444042	−0.781063
H	−2.207303	1.447237	−1.709145
H	−1.820093	2.363732	−0.225996
H	−0.558645	1.343953	−0.969743
O	−3.716093	0.150503	0.270309
C	1.184880	−0.270455	0.858424
C	1.757774	−0.364942	−0.442987
C	2.191803	0.761927	−1.157444
C	2.051476	2.002313	−0.539919
C	1.492413	2.118854	0.755133
C	1.051977	1.000989	1.454357

C	0.902862	−1.605677	1.291305
C	1.302362	−2.450036	0.276499
H	2.629443	0.674044	−2.148825
H	2.386094	2.895794	−1.059569
H	1.405531	3.103328	1.206450
H	0.622714	1.099225	2.448042
H	0.464770	−1.909317	2.232057
H	1.263224	−3.528992	0.210834
N	1.794952	−1.702133	−0.774272
H	2.224259	−2.083445	−1.604179

Conformer S3m

C	−1.274418	−1.861126	0.268249
H	−2.008561	−2.528525	−0.191058
H	−0.311153	−1.898975	−0.245997
H	−1.140788	−2.128451	1.317622
S	−1.912864	−0.175410	0.220250
C	−2.084912	−0.112672	−1.575951
H	−2.800793	−0.880450	−1.881442
H	−2.467741	0.875765	−1.833192
H	−1.107261	−0.267142	−2.036552
O	−3.313372	−0.211909	0.794399
C	1.289366	0.646986	−0.692365
C	1.274910	0.546710	0.730175
C	1.801556	−0.560853	1.410673
C	2.323737	−1.596470	0.641295
C	2.343733	−1.522157	−0.772316
C	1.830238	−0.417123	−1.444392
C	0.708512	1.911527	−1.026756
C	0.377290	2.527134	0.163258
H	1.799782	−0.612738	2.496706
H	2.739346	−2.470330	1.135145
H	2.772578	−2.343872	−1.339376
H	1.868670	−0.362506	−2.529942
H	0.568913	2.329386	−2.014611
H	−0.085524	3.487702	0.344794
N	0.752996	1.722408	1.216143
H	0.474283	1.873366	2.174501

Conformer S3n

C	2.760338	−1.503566	−0.0157521
H	3.269625	−1.646116	0.9406451
H	1.922841	−2.195753	−0.1295391
H	3.471781	−1.634009	−0.8325871
S	2.150898	0.193530	−0.1054091
C	1.144187	0.101117	1.3871991
H	1.820477	−0.015318	2.2385881
H	0.592619	1.039136	1.4740541
H	0.440577	−0.731154	1.3139741
O	3.324010	1.099027	0.1989411
C	−1.997408	0.324266	0.3755342

C	−1.175812	0.239892	−0.7867362
C	−0.786793	−0.984685	−1.3486632
C	−1.226027	−2.145318	−0.7169092
C	−2.030628	−2.087194	0.4465052
C	−2.424948	−0.869328	0.9920212
C	−2.141820	1.714166	0.6848432
C	−1.423229	2.412760	−0.2649052
H	−0.176993	−1.027714	−2.2473992
H	−0.952275	−3.113104	−1.1285912
H	−2.354350	−3.013860	0.9123612
H	−3.048730	−0.837623	1.8818782
H	−2.703697	2.151071	1.4988152
H	−1.275633	3.477549	−0.3839602
N	−0.853278	1.524351	−1.1514072
H	−0.226922	1.775061	−1.9021852

Conformer S3o

C	−1.562188	1.442510	0.848408
H	−2.176752	1.462171	1.752408
H	−0.506100	1.288389	1.080373
H	−1.685885	2.376235	0.298066
S	−2.163115	0.109523	−0.207994
C	−1.817485	−1.208840	0.973683
H	−2.391928	−1.017070	1.883852
H	−2.149967	−2.145838	0.523753
H	−0.745172	−1.253088	1.177285
O	−3.666841	0.248848	−0.289675
C	1.813736	−0.412684	0.473177
C	1.155987	−0.278470	−0.784432
C	0.980769	0.961026	−1.417874
C	1.485194	2.084184	−0.770374
C	2.127768	1.980006	0.486712
C	2.299275	0.748919	1.111212
C	1.842173	−1.811145	0.782382
C	1.216234	−2.465728	−0.260208
H	0.482527	1.040457	−2.380468
H	1.375686	3.060550	−1.234199
H	2.506247	2.879942	0.963457
H	2.807319	0.679881	2.069889
H	2.276842	−2.282414	1.653247
H	1.032798	−3.521087	−0.410355
N	0.792917	−1.541562	−1.190433
H	0.319757	−1.759012	−2.055101

Conformer S3p

C	4.185069	−0.678707	1.327820
H	4.016220	−1.731266	1.091294
H	5.251007	−0.446967	1.386415
H	3.698352	−0.429069	2.271087
S	3.412742	0.327474	0.052982
C	4.316160	−0.356109	−1.343751

H	4.134297	−1.432070	−1.382766
H	3.922689	0.118567	−2.243058
H	5.380523	−0.132905	−1.240488
O	1.995094	−0.201633	−0.081150
C	−2.882685	0.735590	0.029949
C	−1.689753	−0.046211	−0.020998
C	−1.712116	−1.449449	−0.023049
C	−2.956748	−2.069983	−0.064327
C	−4.153694	−1.314363	−0.026560
C	−4.128875	0.075837	−0.014242
C	−2.472663	2.105837	0.059339
C	−1.089177	2.105468	0.051430
H	−0.788855	−2.022367	−0.051234
H	−3.012504	−3.155239	−0.074793
H	−5.107907	−1.833377	−0.057434
H	−5.055467	0.644339	0.013425
H	−3.106263	2.981734	0.090675
H	−0.397816	2.937853	0.068188
N	−0.621617	0.814040	0.013704
H	0.359318	0.528504	−0.019423

Conformer S3q

C	1.464139	−1.682239	0.660747
H	2.041839	−2.406349	0.080509
H	1.606637	−1.828093	1.734526
H	0.404207	−1.758240	0.414571
S	1.993931	−0.019136	0.221557
C	3.718050	−0.212243	0.709554
H	4.156099	−1.039950	0.147260
H	4.228001	0.717372	0.454198
H	3.776839	−0.386859	1.786414
O	2.003891	0.071024	−1.296118
C	−1.782135	0.659443	0.567279
C	−1.135511	0.397919	−0.675524
C	−1.282442	−0.815750	−1.362943
C	−2.063070	−1.799079	−0.761539
C	−2.702588	−1.569428	0.481062
C	−2.572228	−0.355005	1.147930
C	−1.417391	1.991657	0.947557
C	−0.583646	2.474129	−0.042108
H	−0.783032	−0.984985	−2.312823
H	−2.196696	−2.754791	−1.261367
H	−3.311574	−2.357399	0.916070
H	−3.081289	−0.186438	2.093933
H	−1.734291	2.532938	1.828685
H	−0.083342	3.430111	−0.121009
N	−0.451961	1.534431	−1.043066
H	0.347241	1.483219	−1.667572

Conformer S3r

C	−4.018545	−0.254480	1.348514
H	−4.604191	0.658515	1.222472

H	−4.655781	−1.141769	1.351043
H	−3.447582	−0.204630	2.276232
S	−2.827308	−0.364998	0.006464
C	−4.008769	−0.324932	−1.348075
H	−4.594047	0.594030	−1.274789
H	−3.431360	−0.325041	−2.273125
H	−4.647169	−1.210467	−1.307793
O	−2.119738	0.979670	−0.026284
C	2.839944	0.516047	0.007690
C	1.475105	0.097614	−0.012951
C	1.109360	−1.257182	0.031743
C	2.131332	−2.201443	0.005397
C	3.491049	−1.807935	0.013401
C	3.852459	−0.465592	−0.019865
C	2.829043	1.946137	−0.003498
C	1.500864	2.332627	−0.004385
H	0.065416	−1.560086	0.026678
H	1.882200	−3.258948	0.032346
H	4.263073	−2.572332	−0.004688
H	4.900673	−0.176305	−0.014229
H	3.682590	2.610143	−0.003033
H	1.067722	3.323972	−0.009785
N	0.690698	1.223209	−0.001325
H	−0.332672	1.217906	−0.013034

Conformer S3s

C	−3.984869	0.390220	0.579690
H	−4.200102	−0.676090	0.676571
H	−4.134161	0.914802	1.526346
H	−4.618162	0.826831	−0.193224
S	−2.278569	0.595657	0.042008
C	−1.525512	−0.308413	1.407594
H	−1.897649	−1.336096	1.400770
H	−0.443979	−0.299852	1.262279
H	−1.773939	0.195840	2.345040
O	−2.141542	−0.275134	−1.199365
C	2.114274	−0.583848	0.319684
C	1.151175	−0.166410	−0.646141
C	1.013211	1.173376	−1.042904
C	1.871216	2.102322	−0.460326
C	2.847541	1.707763	0.486053
C	2.986338	0.378321	0.871195
C	1.930527	−1.993489	0.496772
C	0.887745	−2.365908	−0.331193
H	0.274996	1.464634	−1.785336
H	1.796059	3.148748	−0.743505
H	3.508516	2.459844	0.908283
H	3.744738	0.088021	1.594364
H	2.498183	−2.654021	1.138281
H	0.436979	−3.338037	−0.481734
N	0.447871	−1.277019	−1.050840
H	−0.487013	−1.188527	−1.452019

Conformer S3t

C	3.432684	0.686564	0.730696
H	2.742686	1.510353	0.534494
H	3.682986	0.629224	1.792651
H	4.341793	0.807697	0.140501
S	2.659077	−0.855793	0.211929
C	1.211312	−0.717329	1.283273
H	0.733080	0.258363	1.166489
H	0.514383	−1.508366	1.001456
H	1.543031	−0.869644	2.314202
O	2.205277	−0.632681	−1.223830
C	−1.173499	0.105028	−0.711465
C	−1.860079	0.929051	0.227264
C	−2.985806	0.406837	0.898643
C	−3.346447	−0.916646	0.669997
C	−2.630540	−1.727098	−0.244278
C	−1.532352	−1.231636	−0.941283
C	−0.114271	2.072041	−0.638218
C	−1.171947	2.185374	0.246781
H	−3.543297	1.018411	1.603995
H	−4.206368	−1.335000	1.185877
H	−2.943043	−2.755926	−0.401607
H	−0.987651	−1.843873	−1.655552
H	0.638487	2.799956	−0.912567
H	−1.432804	3.068457	0.814909
N	−0.136292	0.834653	−1.244316
H	0.708991	0.378787	−1.603329

Conformer S3u

C	1.280781	−0.005568	−1.415071
H	0.601048	0.752020	−1.019760
H	1.632465	0.264962	−2.414554
H	0.772001	−0.971648	−1.453555
S	2.727412	−0.189473	−0.347868
C	3.071857	1.569782	−0.186077
H	2.203929	2.051486	0.270117
H	3.942543	1.673455	0.462225
H	3.285718	1.992643	−1.170542
O	2.249022	−0.638769	1.025244
C	−1.107609	−0.204898	0.690596
C	−2.081367	−0.540280	−0.294383
C	−2.894117	0.483109	−0.825404
C	−2.732814	1.781580	−0.353030
C	−1.757879	2.091990	0.626079
C	−0.951567	1.100741	1.179796
C	−0.881008	−2.380507	0.230689
C	−1.914155	−1.935363	−0.573720
H	−3.648259	0.257806	−1.575671
H	−3.352065	2.579365	−0.754071
H	−1.666953	3.115284	0.980840
H	−0.213136	1.326656	1.944867

H	−0.443908	−3.367060	0.313231
H	−2.494486	−2.543134	−1.255044
N	−0.424857	−1.350526	1.025165
H	0.531609	−1.299951	1.382849

Me_2SO–4–methylindole (Fig. S4)

Conformer S4a

C	4.857742	−0.555872	−1.277469
H	5.670485	0.160459	−1.137641
H	5.218149	−1.585198	−1.211387
H	4.382781	−0.389440	−2.245042
S	3.602328	−0.260666	−0.017570
C	4.683444	−0.515077	1.402554
H	5.510905	0.195835	1.346109
H	4.087738	−0.316525	2.294336
H	5.044507	−1.546170	1.417580
O	3.285979	1.214875	−0.060194
C	−2.762163	0.352075	−0.013127
C	−1.719349	−0.616121	−0.007698
C	−0.364981	−0.257165	−0.049963
C	−0.052474	1.100537	−0.024537
C	−1.076655	2.076284	−0.011089
C	−2.420904	1.719357	0.029916
C	−4.010914	−0.355741	0.003335
C	−3.691730	−1.699108	−0.010764
H	0.420441	−1.009486	−0.055143
H	0.990124	1.405551	−0.053674
H	−0.798836	3.126445	0.012436
H	−3.196446	2.481747	0.040783
H	−4.345356	−2.562084	−0.004794
N	−2.318902	−1.856312	0.001223
H	−1.836007	−2.735585	−0.097713
C	−5.379192	0.249448	0.020804
H	−5.522128	0.879372	0.905318
H	−5.546545	0.876198	−0.861555
H	−6.149515	−0.526984	0.032719

Conformer S4b

C	4.952710	−0.105850	−1.334097
H	5.596469	0.772632	−1.249683
H	5.533151	−1.030615	−1.293727
H	4.389258	−0.061301	−2.266861
S	3.749041	−0.074704	0.007977
C	4.952146	−0.061180	1.350839
H	5.595072	0.814726	1.238080
H	4.388510	0.012937	2.281595
H	5.533403	−0.986256	1.340344
O	3.112464	1.294323	−0.015252

C	−2.524011	0.318148	−0.018295
C	−2.473875	−1.104117	0.017105
C	−1.263709	−1.810134	−0.019133
C	−0.088241	−1.062580	−0.014955
C	−0.108601	0.352793	−0.024318
C	−1.315812	1.044199	0.003920
C	−3.906970	0.702049	−0.001473
C	−4.632806	−0.472438	0.011428
H	−1.239505	−2.897296	−0.005138
H	0.867740	−1.578815	−0.039149
H	0.833376	0.894596	−0.017467
H	−1.324796	2.131637	−0.005924
H	−5.705219	−0.619512	0.027519
N	−3.774469	−1.555319	0.038681
H	−4.056957	−2.520570	−0.029144
C	−4.444114	2.098494	−0.008709
H	−4.083878	2.664332	0.856991
H	−4.132571	2.638531	−0.909007
H	−5.537457	2.096583	0.021314

Conformer S4c

C	4.909611	0.431325	1.357334
H	5.684363	−0.332291	1.257609
H	5.336970	1.436759	1.344522
H	4.355241	0.275185	2.283501
S	3.733565	0.245414	0.003600
C	4.930679	0.457394	−1.327679
H	5.704300	−0.307684	−1.230459
H	4.390851	0.318627	−2.265146
H	5.357252	1.462503	−1.289291
O	3.321748	−1.207760	−0.014025
C	−2.586185	0.390425	0.010008
C	−2.370018	−1.016318	−0.015255
C	−1.085987	−1.577943	0.007572
C	0.001399	−0.708857	−0.024368
C	−0.194924	0.692987	−0.016934
C	−1.469872	1.250375	−0.030918
C	−4.004195	0.610969	0.000130
C	−4.587903	−0.640735	0.006007
H	−0.936718	−2.654998	0.002435
H	1.012302	−1.107591	−0.015616
H	0.674260	1.344830	−0.042519
H	−1.603648	2.329803	−0.024108
H	−5.636033	−0.911686	0.005015
N	−3.609446	−1.615473	0.013115
H	−3.778048	−2.607478	−0.047679
C	−4.701326	1.934718	0.019430
H	−4.463109	2.496044	0.929283
H	−4.403891	2.550472	−0.836115
H	−5.786672	1.805221	−0.020595

Conformer S4d

C	3.981179	1.278885	0.168904
H	4.610342	1.001050	1.017613
H	4.580960	1.637488	−0.671083
H	3.270730	2.048433	0.472818
S	3.016603	−0.159735	−0.332007
C	4.425046	−1.235815	−0.662535
H	5.017103	−1.332207	0.250332
H	4.023339	−2.209625	−0.944995
H	5.019930	−0.826188	−1.482349
O	2.355360	−0.685529	0.921219
C	−1.638092	0.134649	0.109655
C	−3.030893	0.046453	−0.169000
C	−3.698110	−1.182471	−0.260281
C	−2.958638	−2.331497	0.009596
C	−1.576151	−2.261061	0.301064
C	−0.909365	−1.042200	0.380741
C	−1.288136	1.527286	0.116459
C	−2.446268	2.218444	−0.179714
H	−4.760699	−1.238204	−0.484143
H	−3.445476	−3.301625	−0.042528
H	−1.033525	−3.179272	0.509303
H	0.151509	−0.997469	0.617788
H	−2.608657	3.284906	−0.271847
N	−3.485782	1.329821	−0.381670
H	−4.454728	1.590894	−0.479506
C	0.076217	2.099791	0.340586
H	0.551330	1.636670	1.210996
H	0.724273	1.920919	−0.525730
H	0.024779	3.180684	0.504535

Conformer S4e

C	1.118466	−1.966644	−0.289173
H	1.815044	−2.753883	0.012484
H	0.260889	−1.903903	0.384342
H	0.772070	−2.152737	−1.307436
S	2.009144	−0.396261	−0.306299
C	2.368271	−0.393207	1.465630
H	2.974207	−1.272430	1.700673
H	2.937046	0.513448	1.678012
H	1.432040	−0.390129	2.027554
O	3.324094	−0.653563	−1.009636
C	−1.395210	0.332142	−0.366781
C	−0.971883	0.782331	0.914798
C	−0.222721	1.954113	1.088828
C	0.087685	2.689037	−0.052772
C	−0.311107	2.252833	−1.336950
C	−1.054667	1.089398	−1.505605
C	−2.172690	−0.859314	−0.171865
C	−2.178847	−1.097649	1.187569
H	0.084179	2.292791	2.075840

H	0.661148	3.606684	0.044274
H	−0.040037	2.847800	−2.204455
H	−1.363793	0.767998	−2.497433
H	−2.655070	−1.894439	1.745142
N	−1.413573	−0.142968	1.839754
H	−1.458357	0.026907	2.834425
C	−2.817538	−1.685469	−1.238880
H	−3.503043	−1.080987	−1.841728
H	−2.070621	−2.112646	−1.917309
H	−3.388304	−2.510426	−0.803588

Conformer S4f

C	−1.783695	−1.429788	1.250728
H	−2.350072	−2.337184	1.024426
H	−0.714498	−1.632038	1.336142
H	−2.154471	−0.985145	2.175658
S	−2.066498	−0.229300	−0.070426
C	−1.388307	−1.268374	−1.382277
H	−2.007575	−2.165953	−1.465411
H	−1.446909	−0.696786	−2.310360
H	−0.347599	−1.515592	−1.160148
O	−3.562869	−0.177350	−0.291910
C	1.291482	0.226519	0.443158
C	1.160738	0.865530	−0.823025
C	0.541283	2.114096	−0.973709
C	0.087416	2.744638	0.180989
C	0.224921	2.139311	1.451758
C	0.832063	0.896455	1.596337
C	1.985556	−1.011719	0.234214
C	2.234604	−1.088128	−1.124540
H	0.440299	2.586236	−1.947948
H	−0.396068	3.714130	0.102228
H	−0.136970	2.666601	2.330117
H	0.941261	0.443622	2.579507
H	2.745125	−1.858658	−1.688543
N	1.729978	0.030320	−1.757332
H	1.820435	0.231137	−2.741879
C	2.401168	−1.992555	1.285801
H	3.057258	−1.518855	2.023781
H	1.539573	−2.399812	1.826551
H	2.943924	−2.832249	0.842707

Conformer S4g

C	−1.572549	−0.557399	−1.586842
H	−2.263836	−1.382534	−1.778908
H	−1.622515	0.197560	−2.376042
H	−0.554740	−0.938828	−1.500959
S	−1.978773	0.196588	−0.000799
C	−3.713939	0.523646	−0.386846
H	−4.210968	−0.420244	−0.623524
H	−4.163914	0.963359	0.504278

H	−3.776215	1.226714	−1.221352
O	−1.976365	−0.919751	1.021474
C	1.226669	−0.116897	0.508786
C	1.670001	0.483462	−0.703165
C	1.664101	1.872387	−0.894035
C	1.295003	2.664379	0.191152
C	0.887391	2.087366	1.417044
C	0.868912	0.708619	1.593759
C	1.342249	−1.539301	0.360329
C	1.825059	−1.752187	−0.916124
H	1.985906	2.320306	−1.831444
H	1.293626	3.745706	0.083354
H	0.607073	2.738941	2.240213
H	0.529016	0.268495	2.527289
H	2.053973	−2.683064	−1.419818
N	1.987966	−0.540852	−1.569627
H	2.460567	−0.424358	−2.453449
C	0.952015	−2.564252	1.376120
H	1.507780	−2.422455	2.309334
H	−0.116524	−2.474962	1.597207
H	1.156826	−3.574989	1.011119

Conformer S4h

C	−1.066630	−0.976412	−1.323106
H	−1.720401	−1.344992	−2.118750
H	−0.532117	−0.074506	−1.627924
H	−0.351452	−1.748732	−1.033835
S	−2.106964	−0.617778	0.106820
C	−2.934261	0.806854	−0.637552
H	−3.404149	0.497428	−1.574796
H	−3.701679	1.135819	0.065101
H	−2.204014	1.603365	−0.799892
O	−3.134562	−1.724587	0.189464
C	1.135676	0.398460	0.591379
C	1.879073	0.265071	−0.614923
C	2.578887	−0.904581	−0.940961
C	2.573372	−1.933215	−0.002588
C	1.851609	−1.817296	1.209521
C	1.153312	−0.656808	1.525685
C	0.502566	1.685951	0.571459
C	0.852380	2.267096	−0.633638
H	3.126720	−0.999057	−1.875344
H	3.111722	−2.852264	−0.216464
H	1.866021	−2.643824	1.914403
H	0.596327	−0.580643	2.456023
H	0.596542	3.242500	−1.028498
N	1.649923	1.401844	−1.359503
H	2.123043	1.638319	−2.218914
C	−0.310095	2.300096	1.667707
H	−1.138442	1.646856	1.961037
H	0.303051	2.475459	2.558085

H	−0.728051	3.261220	1.353568

Conformer S4i

C	−3.548826	−0.763242	0.642281
H	−4.043678	−1.309114	−0.164609
H	−3.473507	−1.373116	1.546119
H	−4.098492	0.154482	0.856015
S	−1.895551	−0.277956	0.095476
C	−1.309500	−1.948191	−0.239699
H	−1.980742	−2.421338	−0.961536
H	−0.308589	−1.854179	−0.662233
H	−1.262548	−2.515478	0.693552
O	−2.081142	0.399519	−1.245264
C	1.210114	0.555854	−0.314535
C	1.456260	−0.029227	0.961480
C	2.018688	−1.305602	1.103683
C	2.408070	−1.967665	−0.059249
C	2.192141	−1.395635	−1.336007
C	1.613390	−0.137205	−1.473659
C	0.651981	1.858893	−0.096188
C	0.546546	2.002102	1.272558
H	2.195080	−1.743967	2.083395
H	2.867032	−2.949828	0.015054
H	2.506374	−1.943045	−2.220625
H	1.442113	0.292087	−2.457499
H	0.162824	2.834658	1.848708
N	0.991364	0.855252	1.907592
H	1.161463	0.778609	2.899156
C	0.199302	2.817795	−1.149748
H	1.002709	3.023967	−1.864996
H	−0.653037	2.394827	−1.690678
H	−0.107591	3.768561	−0.703959

Conformer S4j

C	−3.246016	1.029547	0.037239
H	−2.468182	1.513947	0.632616
H	−3.543574	1.654956	−0.808300
H	−4.113605	0.807202	0.659936
S	−2.593254	−0.540964	−0.567018
C	−1.237219	0.187366	−1.514437
H	−0.727219	0.948988	−0.922979
H	−0.544669	−0.624068	−1.750103
H	−1.646191	0.611256	−2.436268
O	−1.991970	−1.241835	0.631259
C	1.887286	0.578832	−0.464414
C	1.217071	−0.122991	0.577729
C	0.503203	0.607226	1.548038
C	0.459332	1.994412	1.441736
C	1.123001	2.673119	0.391038
C	1.831998	1.974148	−0.584644
C	2.183973	−1.627547	−0.784279

C	1.425032	−1.526124	0.365076
H	−0.035191	0.087836	2.335452
H	−0.083653	2.573898	2.184250
H	1.070383	3.757301	0.337355
H	2.334830	2.497039	−1.394925
H	2.560300	−2.510973	−1.284736
N	2.428756	−0.367697	−1.306391
H	3.086837	−0.172528	−2.045862
C	0.895651	−2.637853	1.213757
H	1.272899	−2.558966	2.239123
H	−0.196820	−2.592036	1.243723
H	1.200515	−3.610686	0.816647

Conformer S4k

C	1.593594	−1.928316	−0.410693
H	0.543767	−1.632110	−0.393964
H	1.857316	−2.404517	−1.359123
H	1.796083	−2.611950	0.415405
S	2.644527	−0.481438	−0.167627
C	1.938546	0.479119	−1.523535
H	0.858979	0.552436	−1.384202
H	2.386887	1.472960	−1.478441
H	2.186700	0.000231	−2.474643
O	2.203837	0.186782	1.115938
C	−1.701270	0.025679	−0.704279
C	−1.097283	0.387919	0.533598
C	−1.017603	−0.569534	1.564587
C	−1.522903	−1.844743	1.333708
C	−2.103350	−2.190590	0.089935
C	−2.189515	−1.266065	−0.949908
C	−1.120868	2.198295	−0.801017
C	−0.738099	1.774977	0.455979
H	−0.544585	−0.317316	2.509414
H	−1.472371	−2.593727	2.119422
H	−2.486408	−3.196393	−0.060289
H	−2.641688	−1.533327	−1.902239
H	−1.026834	3.175989	−1.256847
N	−1.662571	1.140477	−1.514581
H	−2.147161	1.230266	−2.395103
C	−0.044347	2.565253	1.518157
H	−0.622743	2.562387	2.448338
H	0.935805	2.122689	1.721867
H	0.089712	3.605824	1.207816

Conformer S4l

C	1.780230	0.589375	−1.448443
H	2.400109	0.131706	−2.224477
H	0.716171	0.483422	−1.667475
H	2.035460	1.645402	−1.348111
S	2.167682	−0.211678	0.122425
C	1.613455	−1.852346	−0.385650

H 2.210093 −2.163762 −1.247320
H 1.794773 −2.528429 0.451219
H 0.546384 −1.830020 −0.617027
O 3.676784 −0.265854 0.219980
C −1.137244 0.341462 0.563658
C −1.740838 0.020632 −0.686116
C −2.206650 −1.268114 −0.985207
C −2.104157 −2.233219 0.014949
C −1.528675 −1.929781 1.271870
C −1.052577 −0.654702 1.558081
C −0.805735 1.737303 0.540636
C −1.196505 2.203462 −0.699228
H −2.656811 −1.502542 −1.946864
H −2.469080 −3.238473 −0.176715
H −1.472912 −2.707129 2.029050
H −0.607303 −0.431436 2.524555
H −1.124907 3.201228 −1.113558
N −1.726790 1.168211 −1.448127
H −2.190697 1.278740 −2.337491
C −0.158237 2.518081 1.639646
H −0.741773 2.450689 2.563775
H 0.846911 2.139010 1.852671
H −0.074461 3.574881 1.370837

Conformer S4m

C 3.240727 0.926157 −0.416209
H 3.648251 0.780680 −1.419805
H 2.591558 1.803718 −0.371565
H 4.057509 1.023528 0.300605
S 2.295866 −0.540927 0.047781
C 1.160689 −0.470509 −1.351191
H 1.740585 −0.664853 −2.257803
H 0.412483 −1.252964 −1.210096
H 0.668243 0.503915 −1.387132
O 3.201006 −1.733866 −0.170073
C −1.768346 0.226232 −0.047225
C −0.827419 0.328062 1.018052
C −0.131144 1.512792 1.294771
C −0.382530 2.609947 0.473159
C −1.307075 2.529483 −0.595593
C −2.004676 1.353633 −0.858891
C −2.233968 −1.129085 −0.084825
C −1.577006 −1.787486 0.937792
H 0.572015 1.577377 2.121333
H 0.133244 3.547553 0.663058
H −1.479167 3.406778 −1.213216
H −2.715351 1.304720 −1.680675
H −1.646666 −2.822650 1.247001
N −0.751024 −0.908243 1.610379
H −0.080940 −1.171104 2.317878
C −3.244809 −1.700014 −1.028867
H −4.211477 −1.196563 −0.923405

H −2.923875 −1.586101 −2.069956
H −3.397798 −2.765839 −0.838630

Conformer S4n

C 1.970331 0.927396 −1.182085
H 2.430855 0.596033 −2.116672
H 0.887513 1.032442 −1.279440
H 2.406398 1.878435 −0.873057
S 2.361224 −0.285453 0.094945
C 1.526460 −1.660912 −0.721528
H 1.991905 −1.815876 −1.698576
H 1.673982 −2.546861 −0.101642
H 0.459464 −1.444079 −0.812003
O 3.846810 −0.557110 0.010071
C −1.650973 0.148242 −0.119530
C −0.825532 0.369470 1.021011
C −0.294309 1.629128 1.333526
C −0.596327 2.680837 0.472956
C −1.395942 2.481929 −0.677823
C −1.925436 1.230942 −0.981733
C −2.056711 −1.227889 −0.099291
C −1.475381 −1.782192 1.026190
H 0.324083 1.781490 2.214386
H −0.206800 3.672337 0.686770
H −1.608355 3.326874 −1.327111
H −2.550952 1.093392 −1.860691
H −1.534484 −2.795510 1.402982
N −0.724707 −0.829697 1.685096
H −0.218770 −0.976725 2.545809
C −2.943355 −1.912578 −1.091469
H −3.918366 −1.418204 −1.154379
H −2.502150 −1.902633 −2.094155
H −3.112378 −2.955339 −0.808910

Conformer S4o

C −1.595800 −1.832428 −0.586228
H −2.350059 −2.066800 −1.342226
H −0.590735 −1.789174 −1.013360
H −1.625954 −2.579752 0.208258
S −1.997005 −0.240342 0.161422
C −1.970880 0.682479 −1.390404
H −2.762462 0.291701 −2.035599
H −2.166113 1.729443 −1.153843
H −0.987265 0.579055 −1.852699
O −3.443369 −0.308200 0.605102
C 1.331593 0.453300 −0.210297
C 1.172682 −0.245955 1.021450
C 1.507816 −1.599842 1.162243
C 1.980824 −2.264714 0.033456
C 2.144850 −1.590784 −1.200387

C	1.821901	−0.242901	−1.334576
C	0.922800	1.810205	0.008772
C	0.549647	1.887066	1.337154
H	1.397614	−2.116166	2.112874
H	2.248370	−3.315173	0.106593
H	2.532476	−2.138472	−2.055182
H	1.969747	0.269409	−2.282889
H	0.180817	2.735716	1.899329
N	0.744749	0.668218	1.955388
H	0.349600	0.421956	2.851227
C	0.982779	2.931550	−0.979766
H	2.019226	3.176997	−1.235364
H	0.467172	2.673498	−1.911086
H	0.514083	3.833449	−0.575826

Conformer S4p

C	1.706299	1.200835	−1.208870
H	2.438001	1.982106	−0.986774
H	1.734692	0.917979	−2.264352
H	0.703099	1.535667	−0.942683
S	2.072894	−0.249522	−0.206582
C	3.739195	−0.520858	−0.840435
H	4.337596	0.375211	−0.660673
H	4.158928	−1.361225	−0.286223
H	3.692218	−0.761375	−1.905204
O	2.251375	0.216614	1.228734
C	−1.662837	−0.228993	−0.153847
C	−0.936408	0.297446	0.952380
C	−0.826528	1.673557	1.193881
C	−1.462238	2.532543	0.300168
C	−2.193880	2.032445	−0.804059
C	−2.309448	0.663656	−1.033717
C	−1.555932	−1.658768	−0.091084
C	−0.773044	−1.933753	1.013890
H	−0.256254	2.051144	2.038022
H	−1.398671	3.606325	0.455141
H	−2.685859	2.733024	−1.473642
H	−2.884426	0.291770	−1.878963
H	−0.444212	−2.891607	1.397672
N	−0.439979	−0.764757	1.673392
H	0.404538	−0.662751	2.226957
C	−2.193736	−2.641750	−1.021115
H	−3.286564	−2.581484	−0.975653
H	−1.896017	−2.455300	−2.058784
H	−1.903175	−3.664920	−0.766297

Conformer S4q

C	−4.339547	−0.007642	−1.347987
H	−4.819400	−0.984542	−1.259303
H	−5.071892	0.802368	−1.317789

H	−3.767912	0.042767	−2.275255
S	−3.166240	0.182799	0.001044
C	−4.335284	−0.038440	1.349095
H	−4.816745	−1.012368	1.238958
H	−3.760269	−0.010874	2.275252
H	−5.066686	0.772948	1.340924
O	−2.313542	−1.074868	−0.014624
C	2.550824	0.011407	0.011236
C	1.144094	0.254456	−0.013876
C	0.613608	1.553023	0.029160
C	1.510480	2.618043	0.003114
C	2.908573	2.398073	0.004873
C	3.434332	1.110032	−0.023205
C	2.734492	−1.408674	−0.001139
C	1.462307	−1.955802	0.001486
H	−0.459888	1.724569	0.027575
H	1.131009	3.636169	0.028751
H	3.578842	3.253178	−0.015394
H	4.510892	0.954098	−0.019528
H	1.165403	−2.997264	−0.005378
N	0.511134	−0.961701	−0.001100
H	−0.503710	−1.090328	−0.007627
C	4.037306	−2.145123	0.002191
H	4.653877	−1.864743	−0.858852
H	4.616751	−1.930233	0.906789
H	3.872861	−3.225794	−0.040824

Conformer S4r

C	4.154135	−0.307115	−0.766040
H	4.163336	−1.394556	−0.664999
H	4.311292	−0.001614	−1.803153
H	4.922109	0.130153	−0.127176
S	2.567494	0.319963	−0.188515
C	1.545719	−0.657146	−1.307233
H	1.718252	−1.717998	−1.108041
H	0.501013	−0.404262	−1.118237
H	1.805036	−0.400387	−2.337696
O	2.389437	−0.264563	1.205824
C	−1.933554	−0.033557	−0.062821
C	−0.865694	0.375818	0.788346
C	−0.472716	1.717875	0.906121
C	−1.183900	2.659649	0.165439
C	−2.263978	2.277505	−0.665759
C	−2.654302	0.945963	−0.777261
C	−2.016672	−1.463590	0.021989
C	−1.010602	−1.852200	0.889139
H	0.345296	2.007386	1.560625
H	−0.909440	3.708949	0.233451
H	−2.804551	3.043387	−1.215497
H	−3.489068	0.666031	−1.416038
H	−0.737025	−2.848477	1.214683
N	−0.349666	−0.748444	1.389827

H 0.616960 −0.763940 1.718850
C −3.020582 −2.341542 −0.656821
H −4.036324 −2.126147 −0.307700
H −3.007618 −2.195453 −1.742324
H −2.814120 −3.396833 −0.456460

Conformer S4s

C −3.406709 1.023775 −0.605053
H −2.624862 1.689960 −0.233140
H −3.605290 1.204353 −1.664166
H −4.321991 1.157679 −0.027173
S −2.872874 −0.682146 −0.375402
C −1.367362 −0.546863 −1.364566
H −0.772547 0.313247 −1.046506
H −0.795495 −1.465983 −1.225861
H −1.663587 −0.452523 −2.413174
O −2.466454 −0.797676 1.086731
C 1.003600 −0.440729 0.781892
C 1.801086 0.448613 0.006203
C 2.866837 −0.072008 −0.756766
C 3.072964 −1.448243 −0.763900
C 2.250361 −2.317865 −0.008183
C 1.208665 −1.827753 0.775937
C 0.187426 1.619883 1.049400
C 1.268344 1.767415 0.196200
H 3.505134 0.585888 −1.342387
H 3.885353 −1.866904 −1.351739
H 2.442028 −3.387282 −0.033069
H 0.583387 −2.490258 1.369235
H −0.477088 2.378886 1.445280
N 0.052415 0.302547 1.442248
H −0.858162 −0.100822 1.685714
C 1.810065 3.040849 −0.373643
H 2.814705 3.251294 0.009063
H 1.878555 2.989433 −1.465697
H 1.168903 3.888504 −0.114660

Conformer S4t

C −1.358622 −0.351082 1.375557
H −0.891202 0.593537 1.090120
H −1.655414 −0.341045 2.428040
H −0.662006 −1.173823 1.196221
S −2.836632 −0.660010 0.382682
C −3.537417 0.988096 0.564328
H −2.831203 1.711299 0.149835
H −4.471003 1.010134 0.001186
H −3.732392 1.188192 1.620613
O −2.412918 −0.764826 −1.075141
C 1.902625 0.050848 0.015591
C 0.810509 0.340902 −0.851222
C 0.361357 1.649862 −1.077596

C	1.000201	2.676218	−0.384330
C	2.091862	2.410520	0.477093
C	2.542738	1.110840	0.690368
C	2.045662	−1.376583	0.050135
C	1.057968	−1.876812	−0.780923
H	−0.464989	1.848635	−1.755541
H	0.680189	3.703742	−0.536490
H	2.573910	3.238003	0.990778
H	3.383419	0.920085	1.353751
H	0.824418	−2.907188	−1.020757
N	0.344861	−0.847084	−1.363846
H	−0.635755	−0.940701	−1.638859
C	3.091908	−2.151979	0.787628
H	4.091790	−1.950526	0.388038
H	3.103519	−1.889523	1.851038
H	2.909404	−3.227427	0.707385

Me_2SO−phenol (Fig. S5)

Conformer S5a

C	1.344254	0.277275	−0.016575
C	2.600999	0.890149	0.002716
C	3.766755	0.116291	−0.013624
C	3.676303	−1.279412	0.020917
C	2.426399	−1.903826	0.005492
C	1.268426	−1.116660	0.019056
H	0.438582	0.876443	−0.015333
H	4.741462	0.600855	−0.004377
H	4.586209	−1.872959	0.014369
H	2.356245	−2.986991	0.030308
H	0.289926	−1.589185	0.009634
O	2.629831	2.260346	−0.005375
H	3.548706	2.542694	−0.043369
C	−3.854618	−0.048792	1.339102
H	−4.349438	0.916711	1.212469
H	−4.574462	−0.870664	1.328856
H	−3.295520	−0.056491	2.275462
S	−2.655916	−0.263627	0.009752
C	−3.834004	−0.116289	−1.346946
H	−4.330228	0.854224	−1.276432
H	−3.260476	−0.170642	−2.272977
H	−4.554497	−0.936675	−1.306821
O	−1.813448	0.989441	−0.015706

Conformer S5b

C	−1.018621	0.736444	0.012283
C	−2.135138	1.581413	0.006657
C	−3.430431	1.059793	0.022864

C	−3.617598	−0.325137	−0.011402
C	−2.512974	−1.182399	0.003016
C	−1.220265	−0.646902	−0.020307
H	−0.009095	1.136302	0.002325
H	−2.662126	−2.260588	−0.015602
H	−0.367040	−1.319966	−0.016196
H	−1.996229	2.658733	0.026535
H	−4.302098	1.706956	0.020452
O	−4.910820	−0.784876	−0.009289
H	−4.888487	−1.744217	−0.075920
C	4.061027	−0.305935	−1.328402
H	4.739596	0.540009	−1.197939
H	4.599668	−1.256254	−1.306988
H	3.523410	−0.205012	−2.271897
S	2.828316	−0.267830	−0.013839
C	3.995695	−0.355398	1.356771
H	4.680317	0.493049	1.289414
H	3.412539	−0.286258	2.275782
H	4.534310	−1.305538	1.328542
O	2.254821	1.129475	−0.001456

Conformer S5c

C	1.104846	−0.352174	0.007869
C	2.308265	−1.059736	−0.002253
C	3.524279	−0.369793	0.012015
C	3.539793	1.027841	−0.031045
C	2.332504	1.734816	−0.014140
C	1.115510	1.048415	−0.027974
H	0.156835	−0.883219	0.005122
H	4.488191	1.561893	−0.027686
H	2.351192	2.820878	−0.040173
H	0.179617	1.599034	−0.018810
H	2.321043	−2.145055	0.021620
O	4.672840	−1.120605	0.018816
H	5.424318	−0.521083	0.054033
C	−4.060342	0.026577	−1.326110
H	−4.626141	−0.897270	−1.186559
H	−4.715038	0.901144	−1.312419
H	−3.514922	−0.014205	−2.269637
S	−2.831791	0.157297	−0.013711
C	−3.999662	0.109304	1.358368
H	−4.571239	−0.819707	1.300476
H	−3.411692	0.123586	2.276799
H	−4.654352	0.983225	1.322209
O	−2.086629	−1.156579	0.010435

Conformer S5d

C	−1.000711	0.738441	0.016396
C	−2.121396	1.573657	0.006129
C	−3.412912	1.035702	0.026706

C	−3.588112	−0.351133	−0.013127
C	−2.476342	−1.198227	−0.001501
C	−1.192429	−0.648899	−0.015548
H	0.004612	1.149065	0.008088
H	−2.634799	−2.272087	−0.023836
H	−0.332250	−1.312928	−0.011430
H	−1.994098	2.652304	0.028558
H	−4.280925	1.692554	0.025616
O	−4.827357	−0.940804	−0.014937
H	−5.490827	−0.245405	−0.055416
C	4.023124	−0.329175	−1.330769
H	4.735647	0.488238	−1.199295
H	4.522804	−1.300594	−1.312523
H	3.488673	−0.204277	−2.273191
S	2.794842	−0.245061	−0.014329
C	3.959627	−0.383765	1.354157
H	4.678169	0.436319	1.288506
H	3.381029	−0.294038	2.274273
H	4.459105	−1.354918	1.322136
O	2.277396	1.174196	0.002825

Conformer S5e

C	1.654824	−0.190784	1.176896
C	1.892438	−0.792517	−0.063662
C	1.856504	−0.028533	−1.234156
C	1.559498	1.332617	−1.161309
C	1.312481	1.943698	0.073999
C	1.367330	1.177294	1.241724
H	1.701792	−0.785123	2.088066
H	1.529347	1.919967	−2.074616
H	1.093408	3.006035	0.126602
H	1.198333	1.641240	2.210258
H	2.047738	−0.516324	−2.184840
O	2.161634	−2.127821	−0.197344
H	2.258324	−2.510296	0.680471
C	−2.236117	1.365943	0.362781
H	−3.253379	1.226309	0.737778
H	−1.557481	1.704201	1.147857
H	−2.242431	2.088582	−0.454621
S	−1.648087	−0.199857	−0.318744
C	−1.793386	−1.128380	1.224210
H	−2.839296	−1.122467	1.542074
H	−1.482624	−2.152946	1.012762
H	−1.140347	−0.689259	1.980911
O	−2.739812	−0.708208	−1.232117

Conformer S5f

C	−1.172349	−0.954930	−0.015061
C	−2.272009	−1.821625	−0.001691
C	−3.567436	−1.298008	−0.015411

C	−3.770852	0.085954	0.015757
C	−2.669743	0.947253	−0.001015
C	−1.372405	0.427367	0.017608
H	−0.156347	−1.340475	−0.010029
H	−0.532963	1.116018	0.013660
H	−2.117411	−2.895883	−0.023189
H	−4.427478	−1.961838	−0.007883
H	−4.780579	0.492229	0.005794
O	−2.799257	2.314222	0.003907
H	−3.735551	2.527680	0.060851
C	3.783363	0.316467	1.337165
H	4.531171	−0.469560	1.210227
H	4.241300	1.308330	1.325321
H	3.246387	0.166724	2.274528
S	2.571393	0.183493	0.009799
C	3.741184	0.373045	−1.348120
H	4.492331	−0.416851	−1.277255
H	3.174836	0.261363	−2.273424
H	4.199532	1.364033	−1.309995
O	2.114752	−1.256822	−0.014004

Conformer S5g

C	1.086189	−0.315495	0.018587
C	2.285153	−1.035376	−0.002121
C	3.509952	−0.360421	0.009204
C	3.542689	1.036565	−0.029126
C	2.344307	1.753089	−0.013551
C	1.115629	1.082414	−0.018333
H	0.134690	−0.840576	0.020259
H	4.504174	1.540535	−0.028602
H	2.373974	2.839013	−0.037535
H	0.186872	1.644846	−0.005509
H	2.265036	−2.123535	0.019275
O	4.715263	−1.016007	0.009366
H	4.542001	−1.960544	0.067751
C	−4.020494	0.035774	−1.338432
H	−4.610912	−0.873214	−1.203344
H	−4.653249	0.926417	−1.335139
H	−3.464780	−0.021253	−2.275085
S	−2.805321	0.140518	−0.011623
C	−3.990143	0.124501	1.346315
H	−4.583893	−0.790194	1.283830
H	−3.413067	0.126983	2.271732
H	−4.622483	1.014242	1.300115
O	−2.091878	−1.191158	0.024754

Conformer S5h

C	−1.750893	0.825576	0.027190
C	−1.789416	0.167878	−1.205845
C	−1.660335	−1.220910	−1.251311

C	−1.487698	−1.959175	−0.075006
C	−1.452032	−1.295428	1.154098
C	−1.575978	0.097800	1.209266
H	−1.392476	−3.039803	−0.115495
H	−1.331918	−1.857163	2.076633
H	−1.555704	0.613138	2.168505
H	−1.690832	−1.726754	−2.211892
H	−1.932070	0.753441	−2.108972
O	−1.866502	2.192328	0.011886
H	−2.035208	2.493802	0.910094
C	2.252963	−0.697109	1.309197
H	3.173553	−0.164881	1.562087
H	1.481138	−0.549350	2.067662
H	2.464786	−1.761762	1.199150
S	1.650069	−0.111982	−0.290492
C	1.522576	1.622831	0.196725
H	2.528734	1.996491	0.404736
H	1.086350	2.171061	−0.639320
H	0.872809	1.715617	1.068696
O	2.813327	−0.204940	−1.251872

Conformer S5i

C	−1.724406	0.846092	0.081379
C	−1.818510	0.233421	−1.172373
C	−1.737126	−1.158651	−1.271261
C	−1.537595	−1.938680	−0.129161
C	−1.441521	−1.316590	1.120467
C	−1.533661	0.073038	1.230799
H	−1.470366	−3.019066	−0.210065
H	−1.301987	−1.914008	2.017510
H	−1.482810	0.570039	2.195654
H	−1.812062	−1.628189	−2.247646
H	−1.968283	0.838295	−2.064805
O	−1.789650	2.205623	0.249238
H	−2.023733	2.606349	−0.594173
C	2.119098	−0.639998	1.371565
H	3.080626	−0.183286	1.619747
H	1.339434	−0.344997	2.076291
H	2.220458	−1.726348	1.364285
S	1.653078	−0.138079	−0.299690
C	1.603349	1.631539	0.055918
H	2.591664	1.949719	0.397841
H	1.363379	2.138117	−0.880546
H	0.829108	1.847254	0.794354
O	2.865596	−0.368828	−1.173913

Conformer S5j

C	1.594817	−0.180786	1.206568
C	1.797808	−0.840511	−0.009566
C	1.851376	−0.114294	−1.203466

C	1.640096	1.267111	−1.184761
C	1.411677	1.932252	0.023440
C	1.395392	1.201434	1.217748
H	1.585280	−0.762582	2.123771
H	1.670268	1.822962	−2.117564
H	1.259341	3.007372	0.036036
H	1.242623	1.710289	2.166248
H	2.020982	−0.629669	−2.146617
O	1.956031	−2.199222	0.039403
H	1.989136	−2.535076	−0.862251
C	−2.282596	1.423492	0.200479
H	−3.298686	1.274006	0.574732
H	−1.636019	1.874751	0.955865
H	−2.308145	2.055418	−0.688521
S	−1.599397	−0.169906	−0.303691
C	−1.774313	−0.958361	1.310961
H	−2.837235	−1.007756	1.561743
H	−1.368261	−1.967672	1.226031
H	−1.210051	−0.396797	2.057544
O	−2.621586	−0.814373	−1.213950

Conformer S5k

C	1.722638	−0.425109	1.154634
C	2.411364	−0.409190	−0.062967
C	2.233890	0.651078	−0.958156
C	1.366982	1.700401	−0.626626
C	0.670223	1.684177	0.584658
C	0.846074	0.613368	1.469384
H	2.772873	0.662808	−1.903816
H	1.243830	2.527827	−1.320602
H	−0.011255	2.489781	0.839274
H	0.278553	0.577289	2.392535
H	1.874058	−1.259720	1.832527
O	3.240130	−1.469393	−0.326904
H	3.715783	−1.286802	−1.143203
C	−2.706948	0.842653	−1.046091
H	−1.797801	1.437798	−0.936466
H	−2.871165	0.558494	−2.088529
H	−3.567335	1.401256	−0.675076
S	−2.552531	−0.639551	−0.026004
C	−1.056315	−1.254838	−0.830465
H	−0.290182	−0.478357	−0.833464
H	−0.710985	−2.111739	−0.250066
H	−1.305731	−1.571615	−1.846873
O	−2.167329	−0.171787	1.357353

Conformer S5l

C	−2.115922	0.817794	−0.039102
C	−2.585434	−0.127702	0.881186
C	−2.250697	−1.477542	0.723501

C	−1.449759	−1.885151	−0.348404
C	−0.981307	−0.929420	−1.258107
C	−1.309099	0.419184	−1.108872
H	−0.916960	1.165735	−1.790739
H	−0.344534	−1.223900	−2.086663
H	−1.193534	−2.932968	−0.472485
H	−2.623081	−2.205929	1.438489
H	−3.210590	0.187156	1.714930
O	−2.399006	2.153797	0.069047
H	−3.005812	2.276748	0.805727
C	3.769068	0.209560	0.564204
H	3.715168	1.264041	0.844712
H	4.023413	−0.418148	1.421605
H	4.508903	0.078701	−0.226445
S	2.175135	−0.298048	−0.115593
C	1.200210	0.154554	1.333180
H	1.270260	1.236520	1.473351
H	0.167297	−0.131414	1.137582
H	1.575520	−0.385248	2.206496
O	1.845185	0.692429	−1.206869

Conformer S5m

C	2.079250	−0.690329	0.088067
C	2.474792	0.296806	−0.822245
C	2.018568	1.610270	−0.663382
C	1.169328	1.937772	0.399156
C	0.773702	0.939362	1.297573
C	1.227072	−0.371934	1.148614
H	3.132065	0.042065	−1.651777
H	2.334385	2.373695	−1.369088
H	0.822323	2.959311	0.525211
H	0.092788	1.166528	2.111486
H	0.894646	−1.154799	1.821628
O	2.466981	−2.000232	−0.033032
H	3.135240	−2.056334	−0.723247
C	−2.748764	1.197850	−0.361624
H	−1.838298	1.728263	−0.073640
H	−3.026163	1.421456	−1.394793
H	−3.566685	1.466885	0.308140
S	−2.465170	−0.575886	−0.175369
C	−1.083104	−0.657598	−1.338377
H	−0.338907	0.102710	−1.096604
H	−0.643364	−1.651464	−1.237372
H	−1.469768	−0.524604	−2.352577
O	−1.910807	−0.778859	1.214512

Conformer S5n

C	−1.641232	0.303665	−1.192445
C	−1.832624	−1.081565	−1.219931
C	−1.889187	−1.810386	−0.029146

C	−1.763740	−1.143435	1.194382
C	−1.581745	0.240387	1.231995
C	−1.514860	0.959799	0.035746
H	−1.815511	−1.699911	2.125833
H	−1.497842	0.776059	2.173024
H	−2.028382	−2.886441	−0.053900
H	−1.932940	−1.587270	−2.176000
H	−1.589435	0.869526	−2.121031
O	−1.276397	2.311279	0.129802
H	−1.493589	2.718422	−0.715213
C	1.799414	0.761712	1.335312
H	2.796108	1.207401	1.279369
H	1.016971	1.520181	1.266846
H	1.700118	0.204787	2.268388
S	1.626690	−0.423582	−0.016947
C	1.820057	0.802598	−1.330844
H	2.822889	1.231698	−1.257715
H	1.712618	0.281254	−2.283285
H	1.052281	1.572164	−1.232470
O	2.883044	−1.264679	−0.023941

Conformer S5o

C	−1.912375	−0.256927	−1.201004
C	−2.558470	0.435640	−0.170571
C	−2.311234	0.099599	1.164829
C	−1.413775	−0.932642	1.466185
C	−0.763344	−1.624591	0.441254
C	−1.013746	−1.279059	−0.892318
H	−2.118290	0.022150	−2.229881
H	−0.484180	−1.790953	−1.688694
H	−0.058918	−2.417172	0.671859
H	−1.231921	−1.193975	2.505102
H	−2.817563	0.637018	1.964681
O	−3.424848	1.433633	−0.535191
H	−3.818499	1.799713	0.262924
C	3.791285	0.821116	0.204660
H	3.845126	1.396661	−0.722330
H	3.862797	1.470107	1.080833
H	4.591914	0.080681	0.222980
S	2.230527	−0.085995	0.242842
C	1.165884	1.361126	0.092995
H	1.390140	1.865096	−0.850718
H	0.134853	1.008807	0.091263
H	1.332100	2.023519	0.946521
O	2.147180	−0.842546	−1.061831

Conformer S5p

C	1.652515	1.781846	−0.209628
C	2.385973	0.752711	−0.803267
C	2.415955	−0.511927	−0.204556

C	1.720736	−0.739790	0.989160
C	0.987975	0.298316	1.575947
C	0.947958	1.561689	0.979901
H	1.636623	2.762059	−0.677704
H	2.939722	0.909848	−1.723791
H	0.375557	2.362614	1.436667
H	0.455098	0.117125	2.505406
H	1.759431	−1.719548	1.462385
O	3.149525	−1.481482	−0.831858
H	3.111559	−2.285330	−0.303854
C	−2.115984	−1.520024	0.624278
H	−2.439368	−2.192315	−0.174347
H	−1.072850	−1.694722	0.895347
H	−2.759161	−1.650732	1.495762
S	−2.319077	0.183386	0.058961
C	−1.210879	0.030276	−1.354736
H	−1.602097	−0.744563	−2.019013
H	−1.209560	0.991329	−1.870912
H	−0.202177	−0.202674	−1.009528
O	−3.723655	0.293251	−0.485942

Conformer S5q

C	1.647059	−1.860607	0.080381
C	2.395902	−1.111406	0.992741
C	2.553591	0.268446	0.815430
C	1.962923	0.897254	−0.285867
C	1.223338	0.150963	−1.209047
C	1.061963	−1.223097	−1.020083
H	1.514188	−2.927841	0.225742
H	2.859847	−1.594630	1.848060
H	3.132097	0.850587	1.530469
H	0.459240	−1.790981	−1.721151
H	0.778769	0.659030	−2.059116
O	2.062388	2.246734	−0.509723
H	2.682107	2.614972	0.127916
C	−3.587374	0.794852	0.312232
H	−3.976208	0.152530	1.105789
H	−3.462603	1.823955	0.657982
H	−4.262562	0.769299	−0.543976
S	−1.997368	0.146280	−0.246457
C	−1.177734	0.238847	1.355694
H	−1.749445	−0.348894	2.078501
H	−0.182648	−0.187956	1.232703
H	−1.097045	1.283914	1.666263
O	−2.214371	−1.318732	−0.547122

Conformer S5r

C	1.510782	1.502304	−0.845136
C	2.361915	0.403226	−1.009190
C	2.513151	−0.520885	0.031052

C	1.820991	−0.343371	1.233354
C	0.975832	0.758350	1.387508
C	0.812288	1.685545	0.351267
H	1.389144	2.210178	−1.659737
H	2.903012	0.264030	−1.943483
H	0.130658	2.521211	0.463351
H	0.440262	0.891217	2.323144
H	1.961740	−1.065597	2.031934
O	3.323081	−1.622480	−0.068285
H	3.784625	−1.584025	−0.911788
C	−3.678555	−1.021834	0.045465
H	−3.934375	−1.035470	−1.016543
H	−3.541525	−2.033655	0.434761
H	−4.463363	−0.510897	0.604646
S	−2.159913	−0.071813	0.273760
C	−1.136268	−1.083664	−0.810177
H	−1.574979	−1.076016	−1.811308
H	−0.145605	−0.630871	−0.832408
H	−1.069800	−2.099186	−0.411340
O	−2.373331	1.249987	−0.426246

Conformer S5s

C	1.919623	−1.191099	−1.052376
C	2.522111	−1.424158	0.190044
C	2.522059	−0.412151	1.154509
C	1.920270	0.822719	0.884137
C	1.331703	1.049087	−0.365296
C	1.319243	0.037806	−1.332090
H	1.919550	−1.967724	−1.811993
H	2.992017	−2.379658	0.401011
H	2.988518	−0.577574	2.121512
H	1.927423	1.611746	1.634130
H	0.852954	0.236687	−2.291713
O	0.718845	2.230451	−0.689570
H	0.965539	2.892784	−0.035914
C	−1.929976	1.048778	1.063857
H	−2.540191	0.668354	1.887060
H	−0.896692	1.208934	1.376098
H	−2.356576	1.977668	0.683693
S	−1.976856	−0.158754	−0.279010
C	−1.182434	−1.482263	0.656010
H	−1.793861	−1.703339	1.534747
H	−1.145889	−2.357736	0.005753
H	−0.167895	−1.187557	0.932303
O	−3.425195	−0.552305	−0.456093

Conformer S5t

C	−1.771043	−0.520481	1.164293
C	−2.430330	−0.528779	−0.069813
C	−2.324894	0.570234	−0.930188

C	−1.556585	1.677888	−0.552183
C	−0.893338	1.690871	0.678184
C	−1.004537	0.586194	1.531796
H	−1.870873	−1.381280	1.818497
H	−0.491331	0.584900	2.488795
H	−0.305099	2.553883	0.975187
H	−1.488447	2.531473	−1.221140
H	−2.841923	0.564158	−1.887889
O	−3.159935	−1.643805	−0.377572
H	−3.579141	−1.510783	−1.233711
C	2.488982	1.173996	−0.811629
H	2.872513	0.808925	−1.767628
H	1.545338	1.708921	−0.937690
H	3.230413	1.823001	−0.343346
S	2.244983	−0.238014	0.287906
C	1.074094	−1.092433	−0.784467
H	1.578361	−1.325948	−1.725821
H	0.784590	−2.016623	−0.282271
H	0.194349	−0.465651	−0.940381
O	3.529615	−1.032656	0.264440

Conformer S5u

C	2.003240	−0.855079	−0.212411
C	2.500477	−0.102245	0.857422
C	2.277201	1.278474	0.898565
C	1.560891	1.910075	−0.123197
C	1.073307	1.147788	−1.191998
C	1.289649	−0.230492	−1.240432
H	0.911905	−0.833232	−2.060394
H	0.523685	1.626254	−1.998103
H	1.397959	2.983203	−0.094105
H	2.668885	1.856852	1.730496
H	3.057272	−0.590328	1.655025
O	2.162206	−2.210600	−0.301361
H	2.719376	−2.504288	0.426613
C	−2.430646	1.462147	0.088348
H	−2.912812	1.553963	1.064766
H	−1.489044	2.014385	0.054848
H	−3.106547	1.821916	−0.688827
S	−2.122384	−0.286813	−0.242114
C	−1.100233	−0.560361	1.218931
H	−1.720280	−0.392532	2.103504
H	−0.767413	−1.599297	1.193108
H	−0.236846	0.106997	1.198228
O	−3.428619	−1.008990	−0.008977

Conformer S5v

C	1.736403	1.761145	−0.301398
C	2.417926	0.655266	−0.821774
C	2.366912	−0.572075	−0.150683

C	1.648408	−0.688363	1.044769
C	0.969489	0.420326	1.554602
C	1.007810	1.649580	0.885732
H	1.782555	2.710382	−0.827626
H	2.986289	0.747173	−1.745333
H	0.475892	2.506717	1.286065
H	0.414990	0.325657	2.484161
H	1.638569	−1.645038	1.558895
O	3.007188	−1.693500	−0.602836
H	3.457806	−1.478866	−1.425888
C	−2.081028	−1.541075	0.585042
H	−2.425079	−2.189661	−0.224426
H	−1.030091	−1.720799	0.820133
H	−2.698749	−1.701098	1.469917
S	−2.305354	0.177101	0.078028
C	−1.223260	0.077112	−1.360761
H	−1.617050	−0.685174	−2.037951
H	−1.246409	1.051914	−1.850097
H	−0.205065	−0.151101	−1.041251
O	−3.720183	0.296598	−0.438191

Conformer S5w

C	−1.281306	−1.198140	−1.112169
C	−2.087989	−1.696190	−0.083092
C	−2.600100	−0.817851	0.877289
C	−2.313165	0.550295	0.806183
C	−1.523056	1.038422	−0.240163
C	−0.997151	0.165967	−1.196372
H	−0.356263	0.551516	−1.981187
H	−0.848703	−1.868317	−1.848264
H	−2.310039	−2.757426	−0.025220
H	−3.224419	−1.190049	1.684684
H	−2.708582	1.233081	1.556228
O	−1.191129	2.368407	−0.352915
H	−1.742012	2.871127	0.255842
C	2.128871	1.411646	0.450139
H	1.086675	1.622393	0.205055
H	2.345504	1.641397	1.496658
H	2.785275	1.995050	−0.197279
S	2.484445	−0.329414	0.132888
C	1.295503	−0.995212	1.320653
H	0.300458	−0.569109	1.178778
H	1.257730	−2.072604	1.150574
H	1.665049	−0.797518	2.330773
O	1.974701	−0.636226	−1.255543

Conformer S5x

C	−1.773204	−0.530838	1.142404
C	−2.435775	−0.519313	−0.090220
C	−2.328028	0.590856	−0.935402

C	−1.557743	1.687703	−0.541503
C	−0.891065	1.683749	0.689945
C	−1.002995	0.570713	1.528267
H	−1.861007	−1.393315	1.800488
H	−0.487888	0.552619	2.484020
H	−0.301319	2.541548	0.998818
H	−1.487899	2.551392	−1.197234
H	−2.855000	0.580802	−1.884615
O	−3.199550	−1.564734	−0.530854
H	−3.219317	−2.240831	0.153995
C	2.507385	1.192879	−0.763123
H	2.909425	0.855541	−1.721648
H	1.567979	1.734420	−0.892564
H	3.240593	1.825009	−0.260119
S	2.236470	−0.251037	0.287093
C	1.080048	−1.065124	−0.831280
H	1.594081	−1.262061	−1.775599
H	0.791031	−2.009524	−0.367794
H	0.199174	−0.436604	−0.973443
O	3.516412	−1.053536	0.261814

Conformer S5y

C	−1.983724	−1.811247	0.288029
C	−2.511369	−1.126143	−0.810716
C	−2.391801	0.265144	−0.901383
C	−1.745553	0.973145	0.118007
C	−1.215361	0.294893	1.220014
C	−1.331986	−1.094600	1.297959
H	−2.076669	−2.890654	0.354825
H	−3.021630	−1.669052	−1.601115
H	−2.800033	0.795619	−1.759555
H	−0.915871	−1.614441	2.156005
H	−0.726064	0.863903	2.004798
O	−1.574502	2.333323	0.082920
H	−2.074468	2.687765	−0.659838
C	1.926981	1.509930	−0.164786
H	2.357576	1.681807	−1.154656
H	0.869426	1.778848	−0.134456
H	2.478811	2.090294	0.576383
S	2.148528	−0.229428	0.261450
C	1.250955	−0.887264	−1.157712
H	1.740261	−0.535537	−2.069665
H	1.318265	−1.974811	−1.1020532
H	0.204504	−0.580591	−1.115113
O	3.609576	−0.546504	0.040177

Conformer S5z

C	−2.130317	0.972483	0.671159
C	−2.747453	−0.222837	1.044235
C	−2.565641	−1.385532	0.284259

C	−1.778146	−1.334918	−0.870083
C	−1.162613	−0.138772	−1.255338
C	−1.323157	1.009595	−0.470674
H	−2.250960	1.879727	1.255524
H	−3.369570	−0.246824	1.934396
H	−3.045286	−2.313661	0.579281
H	−1.652389	−2.222037	−1.485089
H	−0.567116	−0.093317	−2.164264
O	−0.726224	2.200787	−0.775394
H	0.017664	2.025064	−1.362579
C	2.117319	−1.632332	−0.465874
H	2.657814	−2.132409	0.341565
H	1.121719	−2.059218	−0.602753
H	2.691771	−1.707911	−1.390357
S	1.977419	0.121498	−0.065018
C	1.078466	−0.116178	1.479723
H	1.734174	−0.647503	2.174548
H	0.844036	0.872647	1.876571
H	0.154041	−0.666958	1.293944
O	3.363055	0.606634	0.286026

Conformer S5aa

C	2.089746	−1.156791	−0.972072
C	1.352861	−0.023958	−1.330672
C	1.214597	1.031224	−0.421323
C	1.816520	0.956980	0.839489
C	2.549142	−0.180151	1.189943
C	2.687208	−1.243177	0.289133
H	2.197371	−1.969331	−1.685065
H	0.889564	0.042625	−2.312586
H	1.710836	1.794745	1.522700
H	3.017701	−0.231077	2.168664
H	3.260209	−2.123064	0.564239
O	0.504398	2.164657	−0.708380
H	0.016976	2.017562	−1.526515
C	−1.980291	0.918848	1.200575
H	−2.513514	0.410258	2.007605
H	−0.957816	1.170247	1.487648
H	−2.517896	1.824382	0.916490
S	−1.951244	−0.162780	−0.242527
C	−1.090191	−1.523516	0.569160
H	−1.713748	−1.879043	1.393567
H	−0.968975	−2.317844	−0.168780
H	−0.109853	−1.191866	0.917643
O	−3.370460	−0.617141	−0.490442

Conformer S5ab

C	1.750900	0.756684	−0.008998
C	3.115392	1.080705	0.015215
C	4.078373	0.070996	−0.007688

C	3.699440	−1.276803	0.010384
C	2.340060	−1.599956	−0.010939
C	1.368895	−0.593865	0.015841
H	3.398315	2.129003	0.005860
H	5.131271	0.339738	0.002957
H	4.450967	−2.060001	−0.006330
H	2.026751	−2.640710	0.000405
H	0.314897	−0.851171	0.001340
O	0.861318	1.777181	−0.012744
H	−0.048461	1.419514	−0.013525
C	−3.646990	−0.257280	1.353710
H	−4.202865	0.676591	1.248353
H	−4.312370	−1.123638	1.343734
H	−3.068369	−0.243643	2.277882
S	−2.468340	−0.380389	0.001943
C	−3.652904	−0.276243	−1.346254
H	−4.206237	0.660449	−1.253322
H	−3.078681	−0.278653	−2.273262
H	−4.320128	−1.140819	−1.319177
O	−1.725149	0.944585	−0.008960

Conformer S5ac

C	1.437604	0.372187	−1.194361
C	2.211462	−0.791778	−1.220461
C	2.819474	−1.266412	−0.052098
C	2.654795	−0.556681	1.144053
C	1.875910	0.604417	1.177805
C	1.254648	1.066337	0.010870
H	0.962046	0.746891	−2.095978
H	2.348217	−1.321973	−2.159417
H	3.422403	−2.169389	−0.075224
H	3.135520	−0.906108	2.053842
H	1.735653	1.164340	2.097930
O	0.496198	2.198480	0.075024
H	−0.319242	1.997329	−0.429682
C	−3.660743	−0.487407	0.231320
H	−3.842336	−0.868021	−0.775954
H	−3.901566	−1.234995	0.990518
H	−4.247974	0.416225	0.397114
S	−1.928428	−0.024405	0.369985
C	−1.234504	−1.636580	−0.023208
H	−1.587788	−1.941416	−1.011299
H	−0.148029	−1.537304	−0.031108
H	−1.538803	−2.351212	0.745524
O	−1.660592	0.872973	−0.833718

Conformer S5ad

C	−2.811262	−0.523332	−1.031523
C	−2.040281	0.642042	−1.086691
C	−1.296351	1.044614	0.029662

C	−1.352282	0.289280	1.210785
C	−2.117587	−0.879172	1.255957
C	−2.850332	−1.293101	0.137255
H	−3.383467	−0.828369	−1.903607
H	−1.990119	1.245143	−1.988685
H	−3.449398	−2.197935	0.177825
H	−2.152971	−1.459220	2.174508
H	−0.776330	0.614269	2.072136
O	−0.543633	2.177065	−0.062350
H	0.298258	1.976649	0.396750
C	3.679615	−0.660431	0.023009
H	3.579826	−1.141960	0.997959
H	3.996065	−1.371770	−0.743162
H	4.392287	0.162362	0.085707
S	2.092623	0.049889	−0.436270
C	1.137547	−1.473267	−0.349432
H	1.194455	−1.868317	0.667632
H	0.101588	−1.233383	−0.592900
H	1.538971	−2.183454	−1.076930
O	1.677940	0.898931	0.759719

Conformer S5ae

C	2.457739	−1.303344	0.451204
C	3.298795	−0.700991	−0.490703
C	3.051514	0.619436	−0.883715
C	1.954387	1.317219	−0.372070
C	1.111700	0.708697	0.567576
C	1.366035	−0.608418	0.980329
H	2.648024	−2.322590	0.777194
H	0.710710	−1.070230	1.713492
H	4.149513	−1.242861	−0.892533
H	3.702352	1.103349	−1.606960
H	1.747328	2.340914	−0.671116
O	0.053446	1.422150	1.038090
H	−0.632737	0.777631	1.330839
C	−2.858163	1.087149	−0.703032
H	−1.938189	1.669918	−0.618762
H	−3.207642	1.033359	−1.736724
H	−3.635132	1.520614	−0.072168
S	−2.547137	−0.579291	−0.094171
C	−1.272266	−1.008562	−1.293986
H	−0.491572	−0.245793	−1.305640
H	−0.847441	−1.963578	−0.982130
H	−1.740904	−1.114070	−2.275811
O	−1.849517	−0.407790	1.251092

Me_2SO−4−methylphenol (Fig. S6)

Conformer S6a

C	−1.146357	−0.741417	−0.009971

C	−2.387691	−1.383300	0.003336
C	−3.565087	−0.628812	0.022254
C	−3.499071	0.768551	−0.009949
C	−2.267635	1.434904	−0.014578
C	−1.102020	0.653425	−0.033393
H	−0.224333	−1.313798	−0.028948
H	−4.532705	−1.127855	0.028407
H	−4.422968	1.342978	−0.002873
H	−0.130247	1.142260	−0.048786
O	−2.390565	−2.755099	0.021795
H	−3.302678	−3.053892	−0.041840
C	−2.193439	2.940806	−0.006909
H	−3.089059	3.381367	−0.453847
H	−2.104554	3.330221	1.013353
H	−1.325701	3.291873	−0.572655
C	3.954894	0.139197	1.380837
H	4.513432	−0.797893	1.325688
H	4.623385	1.003384	1.371157
H	3.344274	0.151933	2.284427
S	2.821258	0.220957	−0.018898
C	4.080287	0.088322	−1.302923
H	4.627519	−0.846399	−1.161698
H	3.557334	0.068715	−2.259776
H	4.748237	0.951991	−1.261420
O	2.057398	−1.081182	−0.029426

Conformer S6b

C	−1.024897	0.530566	−0.003188
C	−2.137979	1.385476	−0.012751
C	−3.415034	0.810226	−0.012689
C	−3.584644	−0.578716	−0.012294
C	−2.464787	−1.414555	0.008246
C	−1.183791	−0.857067	0.003595
H	−0.021138	0.950166	−0.009770
H	−0.323253	−1.519560	0.011959
H	−4.294789	1.450148	−0.029353
H	−4.585618	−1.006770	−0.018870
O	−2.559672	−2.785361	0.007733
H	−3.489934	−3.021513	0.071774
C	−1.954248	2.881628	0.012385
H	−2.760690	3.386993	−0.526796
H	−1.949788	3.261747	1.039758
H	−1.003155	3.162172	−0.447333
C	3.941330	−0.387430	−1.329058
H	4.664827	0.425850	−1.237939
H	4.429805	−1.363408	−1.278993
H	3.396298	−0.292947	−2.268979
S	2.730462	−0.238141	−0.002403
C	3.910300	−0.335884	1.356661
H	4.637581	0.472096	1.249779
H	3.343634	−0.202788	2.278958

H	4.397665	−1.313690	1.357586
O	2.228880	1.187397	−0.035080

Conformer S6c

C	1.471902	−0.744040	1.173964
C	1.628023	−1.405984	−0.047653
C	1.697099	−0.667991	−1.232702
C	1.595809	0.722250	−1.188885
C	1.441182	1.409624	0.025327
C	1.388972	0.652991	1.202975
H	1.428489	−1.312971	2.101556
H	1.643897	1.284607	−2.119034
H	1.284795	1.157228	2.162306
H	1.814348	−1.195160	−2.174599
O	1.703458	−2.769742	−0.149737
H	1.771888	−3.138569	0.736389
C	1.396131	2.915651	0.062559
H	0.896644	3.274513	0.967070
H	2.405953	3.339625	0.051407
H	0.860323	3.314248	−0.803840
C	−2.000275	1.493158	0.305446
H	−3.042091	1.607813	0.616460
H	−1.308921	1.687587	1.127267
H	−1.787891	2.171833	−0.522222
S	−1.764665	−0.189517	−0.309041
C	−2.165585	−1.002031	1.254558
H	−3.180702	−0.723654	1.549521
H	−2.119166	−2.077589	1.075813
H	−1.433584	−0.718444	2.013705
O	−2.918320	−0.465329	−1.246597

Conformer S6d

C	−1.588235	1.200951	0.188049
C	−2.945933	1.491158	−0.002116
C	−3.895600	0.470644	−0.116025
C	−3.484097	−0.865676	−0.101998
C	−2.134343	−1.172955	0.082504
C	−1.194867	−0.146225	0.203571
H	−1.830057	−2.215482	0.093673
H	−0.141103	−0.377976	0.335022
H	−3.278009	2.527383	−0.021716
H	−4.946709	0.715652	−0.259617
O	−4.363901	−1.914319	−0.225332
H	−5.242214	−1.551431	−0.373337
C	−0.566878	2.300128	0.343904
H	0.443533	1.886872	0.303265
H	−0.674603	3.050394	−0.446302
H	−0.686073	2.812402	1.304885
C	4.009880	0.555148	−1.296369
H	4.207016	1.458025	−0.714114
H	4.930452	0.141384	−1.714810

H	3.306615	0.780047	−2.099001
S	3.217792	−0.660781	−0.227295
C	4.541967	−0.745131	0.993552
H	4.696093	0.252579	1.410292
H	4.211212	−1.426288	1.778230
H	5.452856	−1.128405	0.527495
O	2.065771	0.054205	0.443122

Conformer S6e

C	1.382288	−0.815600	1.201560
C	1.467294	−1.507587	−0.009666
C	1.629171	−0.798977	−1.203775
C	1.656526	0.598021	−1.184888
C	1.560460	1.313148	0.016471
C	1.429876	0.580290	1.206029
H	1.276316	−1.379928	2.123810
H	1.766776	1.137048	−2.123502
H	1.370661	1.108640	2.156247
H	1.698944	−1.332695	−2.149642
O	1.396577	−2.874317	0.042756
H	1.349705	−3.210739	−0.857893
C	1.651348	2.817552	0.033469
H	1.140513	3.234549	0.906191
H	2.694811	3.148313	0.071799
H	1.199066	3.248991	−0.864167
C	−1.905205	1.643387	0.177143
H	−2.941697	1.831980	0.469327
H	−1.209378	1.870602	0.986893
H	−1.656553	2.241685	−0.700953
S	−1.742362	−0.092529	−0.294951
C	−2.201007	−0.758179	1.319983
H	−3.213046	−0.425625	1.565295
H	−2.181630	−1.845955	1.236006
H	−1.476602	−0.433399	2.069436
O	−2.892151	−0.393850	−1.231203

Conformer S6f

C	−1.176039	1.608653	0.059606
C	−1.469621	0.995478	−1.162558
C	−1.809868	−0.359309	−1.194988
C	−1.830488	−1.134495	−0.027573
C	−1.535893	−0.497915	1.186384
C	−1.207622	0.859472	1.238258
H	−1.559228	−1.071650	2.110913
H	−0.994299	1.353380	2.182534
H	−2.031623	−0.825172	−2.152557
H	−1.445528	1.574510	−2.084189
O	−0.820152	2.930326	0.163740
H	−0.960216	3.350905	−0.690645
C	−2.210139	−2.592071	−0.073849
H	−3.297202	−2.715318	−0.123508

H	−1.777203	−3.080830	−0.951048
H	−1.855274	−3.117306	0.816880
C	2.030856	−0.916366	1.427685
H	3.095642	−0.773401	1.629408
H	1.410109	−0.326083	2.104242
H	1.779994	−1.974200	1.521659
S	1.696384	−0.441081	−0.282300
C	2.228001	1.274593	−0.096300
H	3.275767	1.287068	0.215299
H	2.134453	1.745008	−1.076693
H	1.585522	1.792129	0.618677
O	2.742879	−1.129074	−1.131760

Conformer S6g

C	−1.170534	1.074394	−1.189340
C	−1.809285	−0.170116	−1.196059
C	−2.101023	−0.844885	−0.004053
C	−1.753142	−0.223453	1.204918
C	−1.127051	1.023638	1.229294
C	−0.827821	1.669989	0.027341
H	−1.974960	−0.722530	2.145861
H	−0.866490	1.506926	2.166657
H	−2.068108	−0.626748	−2.148781
H	−0.936916	1.574802	−2.127778
O	−0.147714	2.864414	0.104526
H	−0.240798	3.321625	−0.737514
C	−2.793917	−2.182746	−0.014538
H	−3.871844	−2.070143	0.143481
H	−2.645763	−2.692335	−0.969991
H	−2.404793	−2.828873	0.776879
C	2.202234	0.277225	1.323717
H	3.292558	0.324755	1.258615
H	1.752455	1.269165	1.245713
H	1.912175	−0.191802	2.265255
S	1.596789	−0.778164	−0.011809
C	2.214364	0.279232	−1.341242
H	3.305033	0.315974	−1.275263
H	1.918979	−0.177305	−2.287197
H	1.777393	1.275346	−1.250129
O	2.460152	−2.020401	−0.011664

Conformer S6h

C	0.882774	1.666543	0.025156
C	1.163940	1.014235	1.227996
C	1.739843	−0.257238	1.205583
C	2.057045	−0.896042	−0.002351
C	1.791978	−0.212122	−1.195667
C	1.204041	1.056945	−1.190754
H	2.038377	−0.677498	−2.147545
H	0.995750	1.567346	−2.129825
H	1.951919	−0.758817	2.147390

H	0.931560	1.513039	2.164658
O	0.253440	2.888537	0.100744
H	0.365147	3.340094	−0.742025
C	2.621184	−2.292648	−0.016085
H	3.234387	−2.460768	−0.905414
H	3.242153	−2.474145	0.865279
H	1.815647	−3.034812	−0.017838
C	−2.196850	0.333340	−1.334793
H	−3.286584	0.387650	−1.265590
H	−1.742765	1.321533	−1.240426
H	−1.911423	−0.123334	−2.283751
S	−1.593088	−0.740730	−0.012549
C	−2.179026	0.316698	1.329880
H	−3.268735	0.380489	1.268441
H	−1.892687	−0.160894	2.268244
H	−1.714685	1.302226	1.255534
O	−2.475718	−1.969624	−0.017010

Conformer S6i

C	−1.253258	−0.540659	−1.141601
C	−2.140389	−0.876206	−0.108309
C	−2.414642	0.094788	0.864720
C	−1.818442	1.360456	0.815074
C	−0.943028	1.672912	−0.230099
C	−0.659270	0.719882	−1.211011
H	0.038160	0.959147	−2.006839
H	−0.994918	−1.278729	−1.896193
H	−3.100634	−0.134847	1.677367
H	−2.040643	2.099823	1.582878
O	−0.302408	2.886571	−0.325716
H	−0.694153	3.487540	0.316164
C	−2.741327	−2.255810	−0.022164
H	−2.072164	−2.945179	0.504949
H	−3.693471	−2.238131	0.515195
H	−2.919897	−2.666995	−1.019238
C	2.699036	0.957134	0.333736
H	1.763943	1.452667	0.066585
H	2.995600	1.200320	1.357430
H	3.488397	1.256337	−0.357575
S	2.509032	−0.831608	0.174187
C	1.150583	−0.986223	1.357124
H	0.339922	−0.305137	1.095444
H	0.799799	−2.018094	1.296624
H	1.530136	−0.783527	2.362356
O	1.944888	−1.093709	−1.202654

Conformer S6j

C	1.756393	−0.430088	−1.193499
C	2.443867	−0.654316	0.010246
C	2.257095	0.264390	1.051392

C	1.401574	1.363873	0.906982
C	0.736903	1.571815	−0.305675
C	0.905547	0.663760	−1.355996
H	1.884991	−1.125541	−2.020332
H	2.775089	0.118400	1.996766
H	1.269313	2.064296	1.730056
H	0.375164	0.833995	−2.287696
O	−0.125256	2.618116	−0.510983
H	0.014164	3.269162	0.184178
C	3.383732	−1.823148	0.158165
H	4.360228	−1.600397	−0.284808
H	3.542378	−2.068877	1.211422
H	2.986617	−2.710580	−0.342546
C	−2.421886	0.652028	1.117571
H	−2.866230	0.083811	1.938818
H	−1.462609	1.085688	1.404855
H	−3.106833	1.437363	0.795756
S	−2.185244	−0.463813	−0.283078
C	−1.042428	−1.568172	0.572564
H	−1.561684	−2.003094	1.430713
H	−0.768276	−2.357573	−0.129135
H	−0.149230	−1.017781	0.875320
O	−3.481487	−1.221705	−0.457096

Conformer S6k

C	1.588966	1.315830	−0.892459
C	2.368100	0.169821	−1.054889
C	2.422994	−0.783242	−0.031722
C	1.708426	−0.569939	1.151645
C	0.937336	0.589438	1.301033
C	0.863471	1.551946	0.286440
H	1.553419	2.048231	−1.696436
H	2.931406	−0.005029	−1.966673
H	0.392747	0.747218	2.229631
H	1.756376	−1.301210	1.957150
O	3.193295	−1.894449	−0.248881
H	3.193914	−2.427297	0.552547
C	0.061640	2.815011	0.459844
H	−0.660697	2.712751	1.273145
H	0.714288	3.664024	0.689572
H	−0.490687	3.055427	−0.453327
C	−2.096171	−1.547634	1.030979
H	−2.448750	−2.422973	0.479733
H	−1.052510	−1.659322	1.332315
H	−2.727558	−1.386923	1.906093
S	−2.267540	−0.094264	−0.028587
C	−1.191101	−0.707996	−1.337872
H	−1.622488	−1.630286	−1.735872
H	−1.163366	0.051685	−2.120537
H	−0.184826	−0.865870	−0.945531
O	−3.679870	−0.114503	−0.566420

Conformer S6l

C	1.608990	1.305746	−0.890261
C	2.373885	0.143511	−1.031784
C	2.400550	−0.803180	−0.001263
C	1.679125	−0.567313	1.173130
C	0.925218	0.601900	1.300602
C	0.875414	1.559856	0.276688
H	1.594373	2.030404	−1.701785
H	2.937682	−0.030392	−1.946629
H	0.372291	0.777070	2.221153
H	1.719416	−1.302684	1.971718
O	3.120213	−1.965933	−0.073689
H	3.550885	−2.005479	−0.933477
C	0.087436	2.833751	0.434570
H	−0.677678	2.726925	1.207130
H	0.740911	3.666087	0.717109
H	−0.412610	3.103044	−0.500309
C	−2.086346	−1.566407	1.008734
H	−2.451213	−2.428911	0.445424
H	−1.040053	−1.691007	1.295385
H	−2.706483	−1.418438	1.894070
S	−2.261956	−0.093170	−0.021335
C	−1.195561	−0.683711	−1.349923
H	−1.630623	−1.598836	−1.760379
H	−1.175008	0.090078	−2.118979
H	−0.186511	−0.848812	−0.967875
O	−3.677258	−0.099472	−0.551830

Conformer S6m

C	1.836488	−0.443199	−1.213834
C	2.471179	−0.699791	0.006279
C	2.255339	0.154147	1.092477
C	1.406508	1.259646	0.951832
C	0.761183	1.532584	−0.260802
C	0.982117	0.652514	−1.333380
H	2.013381	−1.113412	−2.049901
H	0.488540	0.837514	−2.284837
H	1.261228	1.924942	1.800673
H	2.746366	−0.038141	2.044837
O	3.284181	−1.799172	0.070503
H	3.698591	−1.823474	0.938788
C	−0.106257	2.752099	−0.434761
H	0.429657	3.537912	−0.977323
H	−1.008541	2.509957	−1.004394
H	−0.409117	3.163523	0.532219
C	−2.349492	0.505606	1.273626
H	−2.752881	−0.166448	2.035443
H	−1.373555	0.897908	1.566254
H	−3.050108	1.323731	1.099562
S	−2.191564	−0.410509	−0.275484
C	−1.040751	−1.637941	0.372846

H	−1.543253	−2.189550	1.171833
H	−0.791239	−2.317293	−0.443498
H	−0.136142	−1.141191	0.728837
O	−3.509905	−1.112306	−0.505059

Conformer S6n

C	1.842641	−0.452635	−1.192168
C	2.474580	−0.691945	0.032966
C	2.251785	0.174080	1.107558
C	1.400402	1.270773	0.948900
C	0.756637	1.529181	−0.270667
C	0.984631	0.641553	−1.331448
H	2.011036	−1.122850	−2.033407
H	0.493444	0.811203	−2.286873
H	1.248336	1.946439	1.788323
H	2.750798	−0.019994	2.052359
O	3.317057	−1.750383	0.242945
H	3.398187	−2.244541	−0.579161
C	−0.110639	2.746537	−0.459867
H	0.443718	3.546633	−0.961478
H	−0.985266	2.510946	−1.073393
H	−0.459089	3.136840	0.500378
C	−2.359189	0.518513	1.259590
H	−2.774779	−0.143629	2.023455
H	−1.385269	0.909619	1.560981
H	−3.053917	1.337463	1.066961
S	−2.184504	−0.416007	−0.276340
C	−1.040503	−1.635252	0.399632
H	−1.551303	−2.175778	1.200893
H	−0.786465	−2.326032	−0.405702
H	−0.138315	−1.135860	0.758854
O	−3.499697	−1.122013	−0.512660

Conformer S6o

C	2.045437	−1.130846	−0.167559
C	2.416370	−0.289541	0.890326
C	2.041644	1.058668	0.913702
C	1.290368	1.588580	−0.140356
C	0.920971	0.769450	−1.210910
C	1.295915	−0.575422	−1.215400
H	3.005994	−0.687893	1.713088
H	2.336727	1.692884	1.747803
H	0.997556	−1.202055	−2.052898
H	0.352773	1.196344	−2.032202
O	0.865738	2.892963	−0.173804
H	1.276288	3.368540	0.555781
C	2.406470	−2.593765	−0.162410
H	3.336545	−2.767189	0.385331
H	1.621683	−3.191360	0.314557
H	2.535985	−2.968538	−1.181114
C	−2.416982	1.292954	0.123700

H	−2.863385	1.391050	1.116590
H	−1.449072	1.795086	0.066825
H	−3.095728	1.709211	−0.622471
S	−2.237146	−0.462634	−0.255779
C	−1.226007	−0.859403	1.184613
H	−1.811420	−0.640987	2.081668
H	−1.008645	−1.928017	1.141318
H	−0.295324	−0.290439	1.159958
O	−3.589584	−1.097779	−0.025697

Conformer S6p

C	−2.546400	−0.667914	0.077763
C	−2.205298	−0.164729	−1.181132
C	−1.311376	0.909179	−1.282756
C	−0.744095	1.495775	−0.144225
C	−1.088538	0.962253	1.108714
C	−1.986622	−0.098980	1.226907
H	−2.254745	−0.503533	2.198442
H	−0.635466	1.378727	2.004436
H	−1.063068	1.299289	−2.267637
H	−2.633886	−0.605519	−2.079762
O	−3.413585	−1.717195	0.252025
H	−3.786451	−1.945844	−0.605022
C	0.174731	2.685503	−0.241125
H	1.011724	2.573487	0.453303
H	0.573113	2.791027	−1.254159
H	−0.359472	3.608874	0.007439
C	3.690879	−1.077670	−0.391659
H	3.828423	−1.757695	0.452315
H	3.679601	−1.619423	−1.340561
H	4.488268	−0.333472	−0.396472
S	2.134070	−0.187740	−0.181609
C	1.081082	−1.646894	−0.115609
H	1.395374	−2.271072	0.724862
H	0.060030	−1.298549	0.037693
H	1.150878	−2.189091	−1.062169
O	2.165382	0.404382	1.209446

Conformer S6q

C	−1.891650	−0.158309	−1.215877
C	−2.486586	−0.536743	−0.007187
C	−2.132696	0.119178	1.174879
C	−1.195008	1.161039	1.137982
C	−0.585522	1.552145	−0.060503
C	−0.946961	0.866846	−1.232919
H	−2.591391	−0.169811	2.119123
H	−0.942808	1.676502	2.062840
H	−0.464738	1.132423	−2.169936
H	−2.175195	−0.677560	−2.126712
O	−3.394426	−1.565186	−0.046695
H	−3.798951	−1.644288	0.822741

C	0.418278	2.672937	−0.115934
H	1.329085	2.325056	−0.611950
H	0.019741	3.523878	−0.677889
H	0.672106	3.024838	0.888644
C	2.482697	−0.097265	1.431436
H	1.551778	0.466255	1.524075
H	2.571735	−0.842480	2.225989
H	3.338114	0.579264	1.459893
S	2.501959	−0.918036	−0.177651
C	0.956713	−1.818270	0.066994
H	0.165487	−1.120658	0.344594
H	0.711382	−2.296721	−0.882333
H	1.105967	−2.578204	0.838909
O	2.239519	0.155277	−1.209403

Conformer S6r

C	−1.564344	1.513003	0.722198
C	−2.439387	0.444401	0.922370
C	−2.493732	−0.637741	0.028271
C	−1.652926	−0.601766	−1.092450
C	−0.776235	0.466974	−1.311346
C	−0.718213	1.519047	−0.391003
H	−1.512967	2.340249	1.424074
H	−3.087196	0.447450	1.796449
H	−1.688050	−1.414319	−1.815668
H	−0.144278	0.486099	−2.196543
O	0.136215	2.578670	−0.527896
H	0.863716	2.306495	−1.098429
C	−3.465865	−1.770413	0.239479
H	−3.590959	−1.986639	1.304000
H	−4.451655	−1.521212	−0.167549
H	−3.121493	−2.682199	−0.255751
C	2.018365	−1.817070	−0.689123
H	2.375083	−2.545041	0.043710
H	0.962526	−1.969563	−0.921500
H	2.619894	−1.888464	−1.596623
S	2.259548	−0.159326	−0.017542
C	1.233158	−0.404807	1.444377
H	1.703325	−1.174758	2.061873
H	1.208316	0.540554	1.988337
H	0.220306	−0.685387	1.147574
O	3.694503	−0.075396	0.444156

Conformer S6s

C	1.890899	−0.383152	−1.184008
C	0.920926	0.605192	−1.375386
C	0.605427	1.481700	−0.331586
C	1.267240	1.367523	0.894897
C	2.233792	0.373725	1.070215
C	2.560602	−0.521596	0.039594
H	2.125941	−1.058059	−2.004308

H	0.408643	0.691899	−2.331313
H	1.021789	2.061939	1.693565
H	2.742006	0.294437	2.028907
O	−0.341199	2.464069	−0.447852
H	−0.825542	2.320283	−1.268261
C	3.631201	−1.565884	0.226976
H	4.615826	−1.171409	−0.045920
H	3.681096	−1.894327	1.268577
H	3.438438	−2.442211	−0.397661
C	−2.400836	0.453848	1.325354
H	−2.758141	−0.256220	2.075390
H	−1.451996	0.907039	1.617641
H	−3.149503	1.231317	1.167772
S	−2.195762	−0.416648	−0.241144
C	−1.005316	−1.621505	0.378316
H	−1.493070	−2.210575	1.159450
H	−0.732962	−2.269791	−0.455795
H	−0.116660	−1.108900	0.752828
O	−3.483461	−1.160089	−0.510748

Conformer S6t

C	−1.135582	1.555505	−0.047508
C	−1.928417	1.045988	0.988394
C	−2.468008	−0.246212	0.928878
C	−2.222465	−1.050643	−0.187318
C	−1.439899	−0.558942	−1.237495
C	−0.908346	0.729202	−1.161147
H	−2.127867	1.661173	1.863118
H	−3.079891	−0.620372	1.748095
H	−0.293901	1.100399	−1.977889
H	−1.264928	−1.189812	−2.104221
O	−2.708388	−2.328982	−0.307708
H	−3.319189	−2.488440	0.418472
C	−0.510690	2.922366	0.028072
H	0.577163	2.820876	0.090879
H	−0.746852	3.508831	−0.865237
H	−0.871842	3.471980	0.901584
C	3.719017	−1.056442	0.181705
H	4.009444	−0.614204	1.137497
H	3.661037	−2.145677	0.248214
H	4.434163	−0.768225	−0.589769
S	2.112608	−0.392677	−0.307972
C	1.221090	−0.941770	1.157317
H	1.700090	−0.511247	2.040562
H	0.199710	−0.572748	1.067617
H	1.218339	−2.034187	1.198107
O	2.226214	1.112753	−0.211650

Conformer S6u

C	−1.143798	1.551411	−0.045695
C	−1.925920	1.039725	1.000308
C	−2.466472	−0.249654	0.950356

C	−2.224107	−1.057938	−0.162705
C	−1.445148	−0.569745	−1.218239
C	−0.924726	0.726479	−1.159073
H	−1.254010	−1.194394	−2.089507
H	−0.313659	1.093574	−1.979958
H	−2.119912	1.659120	1.873367
H	−3.079682	−0.636093	1.759136
O	−2.756022	−2.323960	−0.156318
H	−2.653672	−2.696275	−1.037592
C	−0.523238	2.920955	0.019832
H	−0.802383	3.518658	−0.853522
H	−0.847694	3.456783	0.915950
H	0.566864	2.825029	0.032820
C	3.728730	−1.022334	0.212077
H	4.018486	−0.511652	1.133311
H	3.689554	−2.105270	0.353248
H	4.433732	−0.775429	−0.582718
S	2.108530	−0.418584	−0.308059
C	1.237278	−0.873876	1.200423
H	1.706824	−0.360867	2.043768
H	0.204847	−0.543710	1.089221
H	1.267283	−1.959113	1.328860
O	2.202441	1.091065	−0.323824

Conformer S6v

C	−1.237213	1.113206	0.001222
C	−2.558296	1.582426	0.010392
C	−3.625569	0.684031	−0.009952
C	−3.417039	−0.703853	−0.007765
C	−2.093390	−1.160232	−0.020252
C	−1.013294	−0.271568	−0.000776
H	−2.727900	2.655157	0.006749
H	−4.642687	1.071173	−0.008900
H	−1.895865	−2.230641	−0.026957
H	0.003505	−0.650685	−0.014427
O	−0.238827	2.029198	0.008346
H	0.624648	1.571652	0.007414
C	−4.577276	−1.666430	0.009405
H	−4.297849	−2.625231	−0.436392
H	−4.919203	−1.861811	1.031845
H	−5.426127	−1.267431	−0.553246
C	4.008002	−0.518539	−1.349189
H	4.673612	0.339862	−1.238015
H	4.562138	−1.459947	−1.338778
H	3.440310	−0.431483	−2.276157
S	2.815696	−0.500070	−0.003626
C	3.997502	−0.547837	1.350421
H	4.663748	0.312821	1.263071
H	3.422688	−0.481116	2.274676
H	4.551881	−1.488780	1.323704
O	2.240752	0.905846	0.009454

Conformer S6w

C	−0.960335	0.721102	1.202777
C	−1.922359	−0.292150	1.208020
C	−2.678389	−0.589362	0.063747
C	−2.436709	0.164922	−1.094658
C	−1.468811	1.174257	−1.116763
C	−0.714858	1.449474	0.030034
H	−0.371936	0.935490	2.090301
H	−2.096564	−0.853712	2.124141
H	−3.011223	−0.040787	−1.995894
H	−1.271728	1.746315	−2.019123
O	0.235503	2.427401	−0.024249
H	1.019159	2.057094	0.431401
C	−3.750011	−1.649721	0.092978
H	−4.712655	−1.227700	0.401645
H	−3.886058	−2.098981	−0.894794
H	−3.496201	−2.446498	0.797824
C	3.787912	−1.220202	0.020450
H	3.598535	−1.681289	0.992023
H	3.951806	−1.973193	−0.753718
H	4.651374	−0.557576	0.085602
S	2.373235	−0.201157	−0.422141
C	1.132276	−1.502562	−0.338433
H	1.109264	−1.904239	0.677412
H	0.165633	−1.059402	−0.581646
H	1.384762	−2.275879	−1.068691
O	2.147220	0.705641	0.781607

Me_2SO−imidazole (Fig. S7)

Conformer S7a

C	3.470422	0.102443	−1.347773
H	3.604260	1.184682	−1.287575
H	4.427921	−0.421626	−1.302389
H	2.951234	−0.154288	−2.271722
S	2.417195	−0.426154	0.014860
C	3.470067	0.196082	1.337644
H	3.603909	1.271505	1.202259
H	2.950649	0.004301	2.277098
H	4.427583	−0.329849	1.329107
O	1.201839	0.475183	−0.016735
C	−1.944469	−0.073823	0.002174
C	−2.819643	−1.142450	0.038069
C	−4.054882	0.606490	−0.020081
N	−2.758246	1.034380	−0.034603
H	−2.442672	1.992176	−0.066823
H	−0.865984	0.013154	−0.000913
H	−2.574177	−2.194038	0.073107
H	−4.893272	1.287908	−0.042643
N	−4.128648	−0.715720	0.024091

Conformer S7b

C	1.510917	1.430394	−0.707433
H	2.538603	1.452773	−1.079110
H	0.788049	1.381614	−1.523548
H	1.322793	2.310956	−0.091647
S	1.317873	−0.020723	0.347386
C	1.666212	−1.221255	−0.954650
H	2.666619	−1.028709	−1.350368
H	1.641820	−2.211804	−0.497388
H	0.900745	−1.143452	−1.729147
O	2.497725	−0.040319	1.294331
C	−2.192211	0.776493	0.796893
C	−1.911159	0.999464	−0.537513
C	−1.786356	−1.122354	−0.256471
N	−2.118267	−0.584662	0.951336
H	−2.225601	−1.091962	1.817764
H	−2.436733	1.439123	1.612585
H	−1.893710	1.946320	−1.058033
H	−1.665545	−2.185971	−0.404930
N	−1.657337	−0.185513	−1.187616

Conformer S7c

C	1.542390	1.301573	0.530843
H	1.657558	1.036923	1.585143
H	2.086713	2.219016	0.292062
H	0.483977	1.410311	0.282559
S	2.176427	−0.047793	−0.476514
C	3.840605	−0.059108	0.220685
H	3.771847	−0.219945	1.298980
H	4.378292	−0.887492	−0.242014
H	4.340670	0.884988	−0.008855
O	1.503762	−1.312596	0.013618
C	−2.942269	−1.108924	0.264804
C	−1.660035	−0.630063	0.089354
C	−2.974566	1.044118	−0.238761
N	−3.767065	−0.028745	0.051119
H	−4.775038	−0.029079	0.096879
H	−3.326047	−2.087007	0.509891
H	−0.720418	−1.161988	0.165209
H	−3.378145	2.023514	−0.451945
N	−1.691374	0.713121	−0.224572

Conformer S7d

C	1.547608	−1.339364	−0.473616
H	1.636397	−1.102815	−1.537050
H	2.119476	−2.235574	−0.219626
H	0.496064	−1.469106	−0.205120
S	2.166794	0.052051	0.483072

C	3.805849	0.108676	−0.265281
H	3.697667	0.247601	−1.343290
H	4.329134	0.962279	0.166905
H	4.344120	−0.814122	−0.035897
O	1.434580	1.283434	−0.015241
C	−3.793305	0.088045	−0.072001
C	−3.068314	−1.055149	0.199909
C	−1.618793	0.516231	−0.050926
N	−2.849982	1.074892	−0.232061
H	−3.029225	2.047994	−0.429906
H	−4.851577	0.276635	−0.164762
H	−3.447459	−2.048925	0.389117
H	−0.691099	1.071839	−0.120513
N	−1.719606	−0.781568	0.212692

Conformer S7e

C	−3.355885	0.994939	−0.786672
H	−3.524502	0.313316	−1.622765
H	−4.285639	1.219712	−0.259165
H	−2.900588	1.917982	−1.146468
S	−2.185276	0.233969	0.346083
C	−3.138845	−1.252349	0.683188
H	−3.325973	−1.769257	−0.260249
H	−2.532306	−1.880866	1.335906
H	−4.071303	−0.986017	1.185966
O	−1.018484	−0.215859	−0.518215
C	2.692178	−0.936690	−0.627561
C	3.912365	−0.453259	−0.189659
C	2.432382	0.915195	0.526593
N	1.758010	−0.048228	−0.160052
H	0.743388	−0.099106	−0.293452
H	2.418662	−1.801824	−1.211869
H	4.892281	−0.876939	−0.357329
H	1.929345	1.745777	1.001431
N	3.744240	0.704454	0.531631

Conformer S7f

C	−3.363866	0.454731	0.382621
H	−3.029088	0.858195	1.340545
H	−3.818717	1.228984	−0.239369
H	−4.074766	−0.354948	0.549574
S	−1.949173	−0.252327	−0.474111
C	−0.953129	1.250722	−0.503170
H	−0.805872	1.607473	0.518622
H	0.012890	1.009141	−0.950430
H	−1.464709	2.000733	−1.111482
O	−1.301037	−1.197369	0.528433
C	2.064601	−0.849088	−0.737005
C	3.009132	0.163177	−0.744547
C	1.976307	0.319904	1.123811
N	1.430297	−0.746386	0.475907

H	0.532706	−1.181522	0.707225
H	1.815483	−1.619422	−1.4512802
H	3.730056	0.392420	−1.516456
H	1.641880	0.631875	2.103226
N	2.949266	0.890183	0.420931

Conformer S7g

C	2.073994	1.451985	0.462738
H	1.013100	1.692822	0.555720
H	2.589635	1.577734	1.417627
H	2.540610	2.082328	−0.295102
S	2.247598	−0.254087	−0.089064
C	1.295813	−0.999537	1.250561
H	0.302158	−0.549857	1.306677
H	1.212032	−2.064455	1.029061
H	1.843787	−0.862131	2.186010
O	1.410900	−0.381084	−1.354162
C	−2.065138	−1.072000	−0.277667
C	−3.007555	−0.422742	0.501523
C	−1.751382	1.103305	−0.318807
N	−1.280592	−0.078999	−0.807114
H	−0.374021	−0.209411	−1.274718
H	−1.901553	−2.114815	−0.504108
H	−3.817859	−0.861658	1.066153
H	−1.315074	2.054532	−0.590442
N	−2.807404	0.936557	0.471594

Me_2SO−4−methylimidazole (Fig. S8)

Conformer S8a

C	−3.521371	0.011973	−1.344308
H	−4.028284	−0.950358	−1.244826
H	−4.231831	0.841570	−1.321160
H	−2.954043	0.035640	−2.275362
S	−2.334523	0.183616	−0.000289
C	−3.521842	0.015239	1.343732
H	−4.028823	−0.947273	1.246353
H	−2.954805	0.041029	2.274908
H	−4.232203	0.844858	1.318412
O	−1.505954	−1.082611	0.001412
C	1.663533	−0.510121	0.000510
C	2.302076	0.717296	−0.000211
C	3.863639	−0.762018	−0.000022
N	2.678855	−1.439257	0.000734
H	2.561845	−2.441406	0.001208
H	0.617735	−0.790319	0.000982
H	4.821476	−1.262829	−0.000049
N	3.670775	0.549117	−0.000541
C	1.682446	2.076898	−0.000701

H	1.990128	2.644488	0.882305
H	1.988928	2.643337	−0.884868
H	0.591584	1.999670	0.000069

Conformer S8b

C	−1.758985	−1.602557	0.240865
H	−2.273803	−1.812769	1.181417
H	−2.107503	−2.258913	−0.560449
H	−0.679666	−1.693705	0.355244
S	−2.056387	0.114723	−0.206516
C	−3.857194	−0.009128	−0.272053
H	−4.226272	−0.343561	0.700218
H	−4.240168	0.989653	−0.485264
H	−4.151889	−0.698327	−1.067246
O	−1.738013	0.942874	1.018853
C	3.206166	0.546653	0.266849
C	1.907286	0.712427	−0.177997
C	2.301064	−1.409982	−0.208668
N	3.438756	−0.809523	0.243255
H	4.294787	−1.274622	0.506113
H	3.954019	1.254297	0.591072
H	2.218285	−2.481393	−0.326982
N	1.354475	−0.518716	−0.470291
C	1.140513	1.982575	−0.345463
H	0.842011	2.115167	−1.389795
H	0.236976	1.964180	0.269918
H	1.753797	2.839185	−0.052766

Conformer S8c

C	−1.299073	1.665200	0.207327
H	−2.260612	2.079438	0.521649
H	−0.568345	1.681084	1.017817
H	−0.920278	2.221106	−0.651623
S	−1.557851	−0.041181	−0.316513
C	−2.103797	−0.626594	1.302635
H	−2.991303	−0.061496	1.598649
H	−2.363651	−1.681158	1.196659
H	−1.290957	−0.506453	2.021744
O	−2.771375	−0.051291	−1.220186
C	1.948667	−0.394593	−1.089930
C	1.918370	0.441272	0.013002
C	1.250957	−1.491604	0.692552
N	1.535355	−1.621566	−0.633095
H	1.388071	−2.447787	−1.194529
H	2.231165	−0.225650	−2.118118
H	0.901402	−2.317512	1.296101
N	1.477549	−0.254797	1.118455
C	2.359590	1.865778	0.101282
H	1.579546	2.497064	0.534158
H	3.246821	1.953746	0.734711
H	2.606158	2.254635	−0.890268

Conformer S8d

C	−1.183552	−1.262809	−1.007550
H	−0.188867	−0.913179	−0.726091
H	−1.355103	−2.289881	−0.675488
H	−1.312445	−1.197509	−2.089074
S	−2.413563	−0.170336	−0.263828
C	−1.938974	−0.466993	1.450857
H	−0.881507	−0.226473	1.587752
H	−2.560605	0.188266	2.063237
H	−2.145415	−1.509962	1.706143
O	−1.988888	1.242762	−0.597303
C	2.334343	0.246215	−0.913242
C	1.634902	0.831975	0.127694
C	2.051603	−1.200852	0.732958
N	2.586098	−1.046504	−0.513137
H	3.110002	−1.739912	−1.027124
H	2.662489	0.629011	−1.867875
H	2.123930	−2.125988	1.287378
N	1.463985	−0.085044	1.145403
C	1.083614	2.217000	0.212002
H	−0.000094	2.201711	0.060212
H	1.301421	2.646414	1.193212
H	1.532106	2.854407	−0.554773

Conformer S8e

C	1.741632	1.287366	0.597130
H	1.904900	0.985732	1.634996
H	2.180545	2.268417	0.397672
H	0.672025	1.294242	0.371497
S	2.497248	0.066997	−0.486400
C	4.161596	0.180623	0.197470
H	4.121729	−0.049698	1.264471
H	4.773906	−0.560083	−0.318013
H	4.561170	1.182397	0.022170
O	1.960093	−1.286115	−0.061518
C	−3.378370	−0.780778	0.108322
C	−2.805914	0.466743	−0.057151
C	−1.170893	−0.942687	0.067769
N	−2.323102	−1.660147	0.188867
H	−2.383210	−2.661294	0.299319
H	−4.406830	−1.101965	0.175692
H	−0.181627	−1.384307	0.091820
N	−1.432128	0.351086	−0.081234
C	−3.484401	1.789736	−0.198758
H	−3.183869	2.467594	0.605243
H	−3.219928	2.259620	−1.150192
H	−4.570813	1.673721	−0.162240

Conformer S8f

C	−3.762534	0.178361	1.350274
H	−3.898754	1.259342	1.278408
H	−4.718152	−0.349414	1.312091
H	−3.238963	−0.068513	2.274302
S	−2.716565	−0.360079	−0.009515
C	−3.758910	0.247509	−1.342679
H	−3.896243	1.323242	−1.215497
H	−3.232361	0.049062	−2.276638
H	−4.714203	−0.282173	−1.334764
O	−1.508191	0.560999	0.015827
C	2.279692	0.905313	0.020097
C	3.445405	0.156791	0.003194
C	1.812033	−1.238932	−0.025464
N	1.248808	−0.000631	0.001467
H	0.246174	0.207993	0.006867
H	2.106147	1.970835	0.043322
H	1.220666	−2.143985	−0.044426
N	3.139933	−1.185143	−0.025352
C	4.859815	0.638344	0.012201
H	5.393752	0.257743	0.887644
H	5.392444	0.294240	−0.878995
H	4.895874	1.731010	0.034762

Conformer S8g

C	−3.749112	0.267323	0.496202
H	−3.547238	−0.360343	1.366735
H	−4.065631	1.270054	0.792225
H	−4.514567	−0.197246	−0.125991
S	−2.253750	0.376140	−0.498192
C	−1.196500	1.056571	0.794759
H	−1.188059	0.377505	1.650226
H	−0.186698	1.152701	0.390850
H	−1.577161	2.041041	1.078269
O	−1.814359	−1.063536	−0.725192
C	1.676469	−0.245537	−0.989925
C	2.641753	0.219176	−0.109953
C	1.419415	−1.169532	0.986686
N	0.923697	−1.150378	−0.280657
H	−0.007819	−1.474384	−0.552949
H	1.489546	−0.037138	−2.033337
H	0.992434	−1.787560	1.764360
N	2.469309	−0.366664	1.124943
C	3.756296	1.179299	−0.371221
H	3.726035	2.007646	0.342026
H	4.726458	0.685240	−0.266217
H	3.686607	1.588034	−1.382890

Conformer S8h

C	−2.526165	1.004258	−1.070078
H	−1.488007	1.331622	−1.155113

H	−2.921329	0.697010	−2.041177
H	−3.142412	1.803190	−0.656095
S	−2.616753	−0.382036	0.077069
C	−1.441114	−1.440908	−0.791116
H	−0.493851	−0.917654	−0.937835
H	−1.286686	−2.323589	−0.168790
H	−1.880081	−1.738584	−1.746653
O	−1.939573	0.079357	1.359589
C	1.678093	−0.535499	0.854805
C	2.635550	−0.126670	−0.060736
C	1.176427	1.448068	0.057721
N	0.765885	0.487993	0.932319
H	−0.168729	0.432380	1.356001
H	1.585730	−1.432611	1.449435
H	0.638736	2.376959	−0.075338
N	2.310864	1.117848	−0.552342
C	3.877625	−0.838036	−0.489015
H	3.900061	−0.956124	−1.575936
H	4.767830	−0.273841	−0.196791
H	3.933632	−1.829204	−0.030862

Me_2SO_2−benzene (Fig. S9)

Conformer S9a

C	1.588362	0.699708	−1.174511
C	2.244181	1.399345	−0.154832
C	2.899656	0.700276	0.865826
C	2.899640	−0.700256	0.865856
C	2.244142	−1.399360	−0.154764
C	1.588342	−0.699761	−1.174478
H	1.060168	1.241082	−1.952771
H	2.242235	2.485806	−0.155923
H	3.412163	1.243505	1.655161
H	3.412127	−1.243466	1.655217
H	2.242170	−2.485821	−0.155790
H	1.060121	−1.241149	−1.952708
C	−3.476503	0.000074	0.627083
H	−3.623663	−0.902490	1.220638
H	−3.623670	0.902793	1.220398
H	−4.151622	−0.000045	−0.229940
C	−0.792151	0.000132	1.395011
H	−0.990038	−0.902836	1.973901
H	0.238175	0.000110	1.039654
H	−0.990064	0.903194	1.973744
O	−1.638469	−1.268742	−0.751567
S	−1.827928	−0.000014	−0.052223
O	−1.638440	1.268566	−0.751828

Me_2SO_2−toluene (Fig. S10)

Conformer S10a

C	1.193047	1.823928	0.503119
C	1.944016	1.691846	−0.669181
C	2.623906	0.498058	−0.938898
C	2.574529	−0.579692	−0.041748
C	1.824997	−0.429793	1.136365
C	1.136002	0.757641	1.406787
H	0.638166	2.734569	0.704452
H	1.994268	2.513769	−1.378395
H	3.202112	0.401966	−1.855721
H	1.786989	−1.251604	1.849737
H	0.549629	0.854821	2.316192
C	3.346863	−1.846260	−0.310464
H	3.441655	−2.029122	−1.384239
H	4.357362	−1.780590	0.106987
H	2.855576	−2.711366	0.143363
C	−1.928771	−1.390674	1.014174
H	−2.048398	−2.350445	0.510589
H	−0.919466	−1.262705	1.405262
H	−2.665150	−1.291697	1.813347
C	−1.001203	−0.273778	−1.364572
H	−1.135164	−1.236420	−1.859692
H	−1.141336	0.538909	−2.079315
H	−0.024390	−0.191531	−0.888731
O	−3.561490	−0.349870	−0.763930
S	−2.272246	−0.073547	−0.135975
O	−2.040540	1.191188	0.558712

Conformer S10b

C	1.247633	0.796622	1.443121
C	2.090124	−0.288096	1.182631
C	2.696733	−0.450812	−0.073292
C	2.441978	0.508262	−1.065053
C	1.608167	1.604060	−0.808720
C	1.009737	1.750507	0.447572
H	2.271340	−1.026218	1.961382
H	0.760009	0.889703	2.408230
H	0.358618	2.595315	0.653796
H	1.435035	2.343601	−1.586850
H	2.902800	0.398933	−2.044686
C	3.627240	−1.607559	−0.335222
H	3.661108	−1.852841	−1.400077
H	4.646567	−1.366191	−0.015283
H	3.309715	−2.498784	0.213026
C	−2.344751	1.051390	−1.101632
H	−1.401690	1.597147	−1.069573
H	−2.554185	0.664978	−2.099535
H	−3.166266	1.685426	−0.764374
C	−0.876137	−1.247239	−0.538455

H	0.009659	−0.612815	−0.547951
H	−0.743972	−2.067678	0.168900
H	−1.109458	−1.638598	−1.529477
O	−1.921739	0.245598	1.360703
S	−2.265395	−0.305084	0.051316
O	−3.470423	−1.112279	−0.119991

Conformer S10c

C	−1.478142	−1.157829	1.231822
C	−2.072549	−1.889443	0.200081
C	−2.621502	−1.216309	−0.899135
C	−2.585251	0.180350	−0.954340
C	−2.011549	0.929216	0.087256
C	−1.452054	0.240598	1.173064
H	−1.019850	−1.666111	2.074560
H	−2.099898	−2.974534	0.245112
H	−0.986517	0.797267	1.983176
H	−3.080985	−1.777166	−1.708685
H	−3.020513	0.697808	−1.807210
C	−2.033796	2.437090	0.044456
H	−3.055524	2.812118	0.163020
H	−1.428966	2.864765	0.848871
H	−1.654830	2.814043	−0.911177
C	1.097794	−0.873684	−1.201261
H	0.060427	−0.645144	−0.958181
H	1.369786	−0.527043	−2.199001
H	1.276470	−1.946788	−1.114916
C	1.750115	1.627522	−0.168013
H	0.688727	1.753350	0.043614
H	2.353554	2.153964	0.573269
H	2.005140	1.969404	−1.171660
O	1.751691	−0.531412	1.324307
S	2.165486	−0.097903	−0.008690
O	3.546659	−0.271657	−0.449974

Conformer S10d

C	−1.515338	1.071501	0.000058
C	−1.833973	0.425311	−1.204579
C	−2.468083	−0.822173	−1.208970
C	−2.790567	−1.450188	0.000055
C	−2.467624	−0.822400	1.209068
C	−1.833505	0.425081	1.204684
H	−3.287965	−2.416210	0.000051
H	−2.710322	−1.302174	2.153699
H	−1.574107	0.903125	2.146346
H	−2.711133	−1.301785	−2.153594
H	−1.574970	0.903559	−2.146249
C	−0.883562	2.438147	0.000098
H	−0.255536	2.571405	−0.883760
H	−1.655104	3.216241	0.000458
H	−0.255072	2.571083	0.883681

C	3.555844	−0.655875	−0.000277
H	3.738403	−1.239596	0.902298
H	3.738153	−1.239594	−0.902904
H	4.178284	0.240268	−0.000368
C	0.920581	−1.582748	−0.000339
H	1.150938	−2.149416	0.902678
H	−0.128022	−1.284924	−0.000259
H	1.150940	−2.148857	−0.903707
O	1.637142	0.610444	1.268156
S	1.868813	−0.078411	0.000000
O	1.636841	0.610994	−1.267802

Conformer S10e

C	1.681107	1.173889	1.189945
C	1.440353	−0.203306	1.188434
C	1.851702	−1.010241	0.114967
C	2.508831	−0.396905	−0.962201
C	2.755708	0.981928	−0.968072
C	2.343983	1.771635	0.111204
H	1.344046	1.776653	2.028390
H	0.914502	−0.657186	2.024912
H	2.838006	−1.005912	−1.801642
H	3.275305	1.434913	−1.808480
H	2.538163	2.840647	0.112428
C	1.567234	−2.488990	0.121740
H	2.075087	−2.991145	−0.706172
H	1.906712	−2.944283	1.057051
H	0.490574	−2.662275	0.034144
C	−3.612929	0.162698	−0.560220
H	−3.879115	1.215889	−0.652729
H	−3.696223	−0.360474	−1.513088
H	−4.241384	−0.319320	0.190103
C	−0.979645	0.822261	−1.221755
H	−1.299168	1.861275	−1.312161
H	0.059528	0.776562	−0.895321
H	−1.105351	0.277696	−2.158371
O	−1.846192	0.823347	1.266049
S	−1.941369	0.027178	0.045373
O	−1.590913	−1.392809	0.057790

Conformer S10f

C	−1.740266	0.240432	−1.250633
C	−2.285252	−1.041573	−1.139656
C	−2.683710	−1.531928	0.110720
C	−2.534685	−0.727570	1.244920
C	−1.999653	0.562046	1.123785
C	−1.600538	1.066175	−0.122924
H	−2.395994	−1.659278	−2.026928
H	−3.109728	−2.527465	0.198317
H	−2.845237	−1.095474	2.219270
H	−1.910906	1.191672	2.007460

H	−1.413814	0.609437	−2.219770
C	−1.057719	2.463374	−0.272437
H	−1.750647	3.084265	−0.849374
H	−0.916286	2.940046	0.702017
H	−0.099912	2.442108	−0.800011
C	1.817278	0.764447	1.388193
H	0.755265	0.991994	1.482730
H	2.184618	0.198215	2.244729
H	2.397376	1.680527	1.265773
C	1.021259	−1.599788	0.154206
H	−0.007202	−1.265313	0.287045
H	1.106680	−2.204876	−0.749978
H	1.382847	−2.160527	1.017032
O	1.527885	0.587727	−1.214010
S	2.069946	−0.186301	−0.097475
O	3.457554	−0.640003	−0.115461

Me_2SO_2−indole (Fig. S11)

Conformer S11a

C	1.469867	−1.424810	−0.788252
H	0.392098	−1.284057	−0.711429
H	1.800121	−1.489452	−1.825785
H	1.770802	−2.319403	−0.240490
C	1.666968	1.344423	−0.898156
H	0.583084	1.376955	−0.791031
H	2.117254	2.224905	−0.436876
H	1.974189	1.267439	−1.941936
O	1.823015	0.032018	1.375454
S	2.298344	−0.059877	−0.003542
O	3.727819	−0.169137	−0.287164
C	−1.957933	0.317326	−0.513980
C	−1.432175	0.266088	0.809580
C	−1.274988	−0.987572	1.435408
C	−1.653019	−2.132381	0.743036
C	−2.168671	−2.060000	−0.573878
C	−2.323277	−0.837294	−1.223160
C	−1.618574	2.430314	0.190531
C	−1.223084	1.617781	1.232418
H	−0.860271	−1.049701	2.437198
H	−1.547422	−3.104884	1.215932
H	−2.454596	−2.974192	−1.086821
H	−2.727394	−0.783458	−2.231146
H	−1.623841	3.509093	0.110119
H	−0.817243	1.947862	2.178264
N	−2.033675	1.647452	−0.870419
H	−2.461903	1.998454	−1.714000

Conformer S11b

C	1.023202	−0.129402	−1.117294
H	0.416605	−0.963990	−0.763842
H	0.498366	0.820735	−1.012173
H	1.323257	−0.288825	−2.154942
C	1.972795	0.140331	1.492204
H	1.392160	−0.736654	1.777922
H	2.875824	0.217201	2.100280
H	1.382038	1.053630	1.564957
O	3.195159	−1.356675	−0.286875
S	2.535594	−0.056789	−0.185937
O	3.242997	1.164409	−0.566406
C	−2.128829	0.298377	−0.530027
C	−1.670950	0.278074	0.819533
C	−1.513733	−0.966264	1.464340
C	−1.789604	−2.130664	0.755075
C	−2.241050	−2.084278	−0.585805
C	−2.413890	−0.872020	−1.247481
C	−1.738491	2.421971	0.106941
C	−1.435937	1.637549	1.202137
H	−1.183342	−1.013692	2.499224
H	−1.670575	−3.095701	1.239553
H	−2.451489	−3.012297	−1.109596
H	−2.757391	−0.838194	−2.278381
H	−1.700357	3.496186	−0.013011
H	−1.103696	2.002459	2.164551
N	−2.144877	1.614153	−0.934023
H	−2.463089	1.944768	−1.832881

Conformer S11c

C	−3.926270	0.009626	−1.389655
H	−4.591450	−0.853990	−1.402657
H	−4.477992	0.947697	−1.326963
H	−3.288810	0.005997	−2.275232
C	−3.901885	−0.096841	1.412901
H	−4.567130	−0.959542	1.371845
H	−3.249165	−0.167062	2.284476
H	−4.454199	0.842789	1.431077
O	−2.165544	−1.420952	−0.056166
S	−2.823948	−0.120520	−0.000775
O	−2.020802	1.106968	0.039058
C	1.710893	0.126418	0.011349
C	3.073527	0.547850	−0.011699
C	4.086920	−0.432631	0.022568
C	3.724250	−1.774632	−0.009151
C	2.364344	−2.167387	−0.003949
C	1.339068	−1.226720	−0.026546
C	1.737449	2.368111	0.002646
C	3.063574	1.978993	0.003903
H	5.134990	−0.143005	0.017289
H	4.496189	−2.539191	0.011030
H	2.115062	−3.224829	−0.028862
H	0.294264	−1.523870	−0.024456

H	1.304896	3.359649	0.008218
H	3.917558	2.642477	0.001211
N	0.927885	1.256262	−0.000448
H	−0.086686	1.262517	0.011227

Conformer S11d

C	−1.447703	−1.222718	−0.720991
H	−0.902757	−0.773186	−1.550395
H	−0.762917	−1.592422	0.043062
H	−2.093598	−2.027380	−1.077113
C	−1.401616	1.198767	0.652662
H	−0.740881	1.554107	−0.139657
H	−2.023482	2.013406	1.028407
H	−0.837407	0.739265	1.463459
O	−3.280470	0.625433	−1.094226
S	−2.531484	−0.006218	−0.009842
O	−3.235221	−0.623363	1.112952
C	1.864301	0.291326	0.667403
C	1.878433	0.215628	−0.756190
C	1.962343	−1.052895	−1.367454
C	1.943090	−2.187935	−0.564668
C	1.880047	−2.088943	0.845765
C	1.815305	−0.851000	1.480340
C	1.884732	2.391034	−0.142479
C	1.899917	1.561629	−1.245922
H	2.012309	−1.140502	−2.450108
H	2.006081	−3.170991	−1.022867
H	1.865411	−2.995149	1.444794
H	1.783260	−0.778208	2.564781
H	1.901019	3.470903	−0.082452
H	1.931231	1.885111	−2.277339
N	1.846533	1.625514	1.004032
H	1.892182	1.990010	1.944079

Conformer S11e

C	1.004910	−0.544988	1.129847
H	1.354800	−0.771401	2.138040
H	0.436477	0.386761	1.099002
H	0.394429	−1.365825	0.748266
C	3.266317	1.024372	0.687549
H	3.557839	0.849927	1.723602
H	4.152155	1.149104	0.062869
H	2.609127	1.889757	0.595255
O	3.277158	−1.578427	0.284512
S	2.423660	−0.416637	0.065488
O	1.964273	−0.096044	−1.291821
C	−1.493038	0.193236	−0.737692
C	−2.172568	0.778618	0.369638
C	−3.134125	0.011559	1.060737

C	−3.343976	−1.306596	0.670707
C	−2.639145	−1.873990	−0.418590
C	−1.700951	−1.135984	−1.134171
C	−0.685937	2.265995	−0.459417
C	−1.649033	2.103605	0.520413
H	−3.681784	0.435113	1.899037
H	−4.075998	−1.911613	1.198422
H	−2.830367	−2.906575	−0.697174
H	−1.160434	−1.565195	−1.973925
H	−0.065920	3.123035	−0.687971
H	−1.951908	2.851320	1.241177
N	−0.621864	1.131780	−1.239555
H	0.189896	0.880143	−1.793194

Conformer S11f

C	−1.006153	0.123612	−1.352095
H	−0.236238	−0.602936	−1.088985
H	−1.449838	−0.092465	−2.324829
H	−0.582990	1.130869	−1.340078
C	−2.629089	−1.660212	0.038156
H	−1.725329	−2.154221	0.396930
H	−3.433429	−1.748639	0.770005
H	−2.950393	−2.058940	−0.924728
O	−1.755427	0.540338	1.152609
S	−2.300799	0.081230	−0.129802
O	−3.485825	0.727420	−0.684632
C	1.376923	0.233461	0.728529
C	2.260366	0.390193	−0.379337
C	2.801211	−0.763127	−0.985325
C	2.455317	−2.012579	−0.480261
C	1.586190	−2.141754	0.631041
C	1.044992	−1.022241	1.258175
C	1.483783	2.418712	0.241213
C	2.312937	1.791424	−0.669521
H	3.475536	−0.677342	−1.833935
H	2.863557	−2.908747	−0.939553
H	1.355648	−3.132592	1.014062
H	0.381545	−1.111065	2.113763
H	1.244440	3.467698	0.354252
H	2.895937	2.282217	−1.436972
N	0.953205	1.484905	1.105245
H	0.113046	1.625140	1.652913

Me_2SO_2−3−methylindole (Fig. S12)

Conformer S12a

C	1.283490	−0.950690	−0.874203
H	0.664249	−1.418611	−0.108123
H	0.711517	−0.238609	−1.470040
H	1.735252	−1.709743	−1.515970

C	1.821216	1.083706	0.948344
H	1.210399	0.548784	1.675988
H	2.616668	1.639592	1.448001
H	1.214833	1.747267	0.331533
O	3.346061	−1.048009	0.754332
S	2.638642	−0.098745	−0.102173
O	3.357992	0.643183	−1.136188
C	−1.933941	−0.384257	−0.819787
C	−1.682197	0.242396	0.434642
C	−1.554527	−0.562107	1.585529
C	−1.655644	−1.944347	1.453117
C	−1.909128	−2.543815	0.196486
C	−2.037230	−1.775114	−0.957840
C	−1.779297	1.834288	−1.154254
C	−1.606902	1.656934	0.205588
H	−1.374653	−0.112071	2.559426
H	−1.556945	−2.577164	2.330634
H	−1.990004	−3.624987	0.128613
H	−2.223527	−2.239038	−1.923438
H	−1.796713	2.749268	−1.732789
N	−1.947418	0.609285	−1.772020
H	−2.191717	0.482238	−2.742936
C	−1.447833	2.724460	1.242521
H	−2.316924	2.755370	1.908086
H	−0.564371	2.553526	1.866392
H	−1.344873	3.708984	0.777522

Conformer S12b

C	1.632644	0.895118	−1.069290
H	0.936856	0.273535	−1.631236
H	1.097498	1.608838	−0.441714
H	2.315178	1.415221	−1.743978
C	1.491681	−0.841758	1.103557
H	0.692836	−1.348468	0.559849
H	2.060456	−1.555485	1.702568
H	1.098520	−0.041356	1.729623
O	3.162741	−1.234075	−0.886621
S	2.652131	−0.147473	−0.052495
O	3.574320	0.705360	0.695305
C	−1.651134	0.424435	0.957104
C	−1.772216	−0.071575	−0.373187
C	−1.808047	0.846722	−1.442668
C	−1.634696	2.200269	−1.171176
C	−1.464358	2.665586	0.154232
C	−1.443518	1.783545	1.232991
C	−1.916855	−1.805950	1.055325
C	−1.950648	−1.493197	−0.290458
H	−1.939345	0.499610	−2.465100
H	−1.659103	2.919823	−1.984911
H	−1.329452	3.728606	0.333834
H	−1.328046	2.147617	2.251180
H	−2.022139	−2.767878	1.540979

N	−1.709348	−0.660637	1.800670
H	−1.756388	−0.612040	2.807636
C	−2.141559	−2.436776	−1.436380
H	−3.006097	−2.145700	−2.042118
H	−1.264977	−2.450849	−2.092946
H	−2.308707	−3.456238	−1.078220

Conformer S12c

C	3.799181	−0.614647	0.048420
H	4.102944	−0.864606	1.065245
H	3.977955	−1.440387	−0.640817
H	4.323887	0.279740	−0.291023
C	1.284731	−1.694396	0.598257
H	1.654300	−1.929928	1.597282
H	0.212922	−1.496373	0.631651
H	1.498860	−2.494896	−0.111001
O	1.855808	0.837769	1.046473
S	2.064217	−0.198025	0.036995
O	1.676082	0.029713	−1.355358
C	−1.543790	−0.155513	−0.966680
C	−1.540585	0.446963	0.326253
C	−1.961625	−0.312483	1.436708
C	−2.317659	−1.645697	1.243852
C	−2.287332	−2.232056	−0.044334
C	−1.905451	−1.494753	−1.164826
C	−0.859247	1.967885	−1.178302
C	−1.106345	1.804028	0.168084
H	−1.988997	0.130367	2.429726
H	−2.639974	−2.245415	2.091049
H	−2.577256	−3.272570	−0.163956
H	−1.901817	−1.941969	−2.156098
H	−0.484438	2.835787	−1.705355
N	−1.177833	0.813425	−1.870545
H	−0.793485	0.600610	−2.779704
C	−0.886618	2.798374	1.261303
H	−1.779996	2.909856	1.885231
H	−0.056074	2.477389	1.898638
H	−0.638154	3.780743	0.849692

Conformer S12d

C	2.903926	−1.344508	0.435695
H	2.058195	−1.813479	0.940066
H	3.289006	−1.968067	−0.372069
H	3.699370	−1.116814	1.147011
C	1.107026	−0.256513	−1.387017
H	0.429358	−0.957721	−0.900058
H	0.567646	0.654897	−1.654783
H	1.583827	−0.696967	−2.263650
O	1.743048	0.969459	0.856112
S	2.373131	0.220427	−0.230954
O	3.487443	0.801228	−0.976503

C	−2.112931	−0.442145	−0.589274
C	−1.488526	0.150816	0.546192
C	−0.896624	−0.683120	1.515759
C	−0.922186	−2.061166	1.318951
C	−1.539825	−2.630021	0.178310
C	−2.134672	−1.828654	−0.794834
C	−2.255988	1.793425	−0.782733
C	−1.599076	1.574519	0.412432
H	−0.405033	−0.250627	2.382804
H	−0.478679	−2.719308	2.062095
H	−1.548032	−3.709921	0.057433
H	−2.602489	−2.267458	−1.673026
H	−2.539075	2.727878	−1.250712
N	−2.531758	0.586396	−1.402993
H	−3.133549	0.478907	−2.205886
C	−1.086012	2.601527	1.371356
H	−1.536711	2.470400	2.360946
H	−0.001023	2.515394	1.476080
H	−1.325200	3.610826	1.024078

Conformer S12e

C	1.576684	−1.736714	−0.256464
H	0.493473	−1.619715	−0.248263
H	1.933662	−2.174489	−1.189608
H	1.894665	−2.345994	0.591304
C	1.706006	0.788367	−1.412389
H	0.618277	0.816593	−1.351604
H	2.115539	1.794809	−1.309479
H	2.053045	0.334223	−2.341464
O	1.816537	0.448807	1.191113
S	2.342187	−0.146497	−0.037555
O	3.783252	−0.302508	−0.223293
C	−1.882723	−0.166297	−0.776902
C	−1.417604	0.276858	0.494729
C	−1.288504	−0.657577	1.542300
C	−1.615518	−1.987320	1.296592
C	−2.062210	−2.410346	0.021387
C	−2.192296	−1.510100	−1.034860
C	−1.596101	2.064913	−0.859361
C	−1.241792	1.699369	0.424462
H	−0.925690	−0.341933	2.516651
H	−1.528474	−2.718915	2.095290
H	−2.309552	−3.456310	−0.138324
H	−2.544523	−1.837160	−2.010338
H	−1.609666	3.046204	−1.317012
N	−1.944496	0.942668	−1.593552
H	−2.365494	0.962905	−2.510424
C	−0.753284	2.585280	1.525570
H	−1.398622	2.504275	2.406778
H	0.261031	2.299237	1.819619
H	−0.745439	3.632549	1.209676

Conformer S12f

C	−1.164465	−0.422543	−1.182870
H	−1.468167	−0.354010	−2.228483
H	−0.459212	0.366542	−0.913908
H	−0.723408	−1.400348	−0.979342
C	−3.142171	1.393493	−0.440651
H	−3.374275	1.531678	−1.497056
H	−4.040244	1.531891	0.163449
H	−2.351175	2.068254	−0.111307
O	−3.644916	−1.178792	−0.703762
S	−2.620295	−0.288345	−0.170858
O	−2.222430	−0.396688	1.238396
C	1.308603	−0.419278	0.862792
C	2.066869	0.349580	−0.065635
C	2.984523	−0.307642	−0.911121
C	3.076127	−1.694680	−0.846655
C	2.293824	−2.441518	0.066669
C	1.396612	−1.816756	0.929388
C	0.684499	1.721543	1.064484
C	1.662098	1.718401	0.083737
H	3.590911	0.254857	−1.617380
H	3.772878	−2.217607	−1.495972
H	2.392085	−3.523289	0.092059
H	0.799437	−2.386772	1.636720
H	0.135306	2.557280	1.481304
N	0.504852	0.447285	1.566779
H	−0.358837	0.147571	2.006750
C	2.218937	2.899404	−0.647838
H	3.281460	3.039402	−0.421981
H	2.126973	2.774342	−1.732177
H	1.693060	3.816539	−0.367277

Conformer S12g

C	1.313130	−1.141297	−1.088031
H	0.329951	−0.698396	−0.919970
H	1.593326	−1.114670	−2.142027
H	1.332834	−2.169295	−0.722379
C	2.391186	1.406631	−0.778936
H	1.374228	1.763340	−0.608844
H	3.107409	2.007049	−0.215293
H	2.651359	1.407952	−1.838003
O	2.122758	−0.238998	1.253456
S	2.538869	−0.252071	−0.154174
O	3.855688	−0.767094	−0.515223
C	−1.051277	0.355034	0.889580
C	−2.025475	0.029692	−0.099144
C	−2.570072	1.064848	−0.888023
C	−2.129361	2.368630	−0.679945
C	−1.167223	2.669148	0.314468
C	−0.620826	1.670302	1.117621

C	−1.381877	−1.860015	0.941490
C	−2.225376	−1.390579	−0.049494
H	−3.321566	0.849420	−1.644203
H	−2.541000	3.176555	−1.278784
H	−0.860680	3.701129	0.464478
H	0.110571	1.894579	1.889539
H	−1.230800	−2.874967	1.288123
N	−0.707789	−0.810172	1.533786
H	0.166689	−0.906133	2.036746
C	−3.182831	−2.187668	−0.878603
H	−4.218553	−1.888810	−0.685025
H	−2.993783	−2.047968	−1.948363
H	−3.094919	−3.255064	−0.657481

Me_2SO_2−phenol (Fig. S13)

Conformer S13a

C	−1.165238	0.750768	1.344669
C	−1.129615	1.735003	0.349465
C	−1.873582	1.555431	−0.820389
C	−2.643131	0.399511	−1.000289
C	−2.675013	−0.576545	0.002535
C	−1.936519	−0.401298	1.177255
H	−0.574372	0.868888	2.246895
H	−0.513392	2.618483	0.477116
H	−1.853712	2.309875	−1.601812
H	−3.217966	0.260306	−1.914203
H	−1.972055	−1.171323	1.941770
O	−3.402020	−1.733781	−0.115326
H	−3.953719	−1.665475	−0.900725
C	3.654205	−0.856909	−0.449092
H	3.589691	−1.923068	−0.230293
H	3.852646	−0.671954	−1.504991
H	4.427756	−0.393990	0.165403
C	0.919549	−0.875757	−1.013474
H	0.876526	−1.933236	−0.750066
H	−0.036188	−0.396219	−0.803354
H	1.190793	−0.728988	−2.059811
O	1.853995	−0.413987	1.407290
S	2.125253	−0.065228	0.014718
O	2.207527	1.333908	−0.397650

Conformer S13b

C	−1.333102	−1.788262	0.544048
C	−2.092927	−1.640440	−0.622134
C	−2.688939	−0.415541	−0.934609
C	−2.527883	0.672212	−0.070198
C	−1.775933	0.531017	1.102835
C	−1.178962	−0.698330	1.404894

H	−0.852423	−2.732843	0.775272
H	−2.225935	−2.482881	−1.295160
H	−3.284539	−0.287489	−1.833343
H	−1.670064	1.374607	1.783546
H	−0.582922	−0.801224	2.306396
O	−3.127358	1.851365	−0.427745
H	−3.047753	2.468742	0.306229
C	1.922957	1.520140	0.790882
H	2.069233	2.379500	0.135801
H	0.904611	1.474324	1.176757
H	2.642529	1.545703	1.610756
C	1.025215	0.042103	−1.393252
H	1.195730	0.904166	−2.039251
H	1.157957	−0.882660	−1.957107
H	0.036133	0.063801	−0.936994
O	3.571831	0.161950	−0.741225
S	2.260825	0.022048	−0.113826
O	1.978239	−1.102554	0.775660

Conformer S13c

C	1.570522	−0.306061	1.177593
C	2.345199	−0.769978	0.109889
C	2.725943	0.102935	−0.916846
C	2.334999	1.445724	−0.868347
C	1.565109	1.918489	0.200027
C	1.184151	1.034564	1.217502
H	1.257371	−1.001358	1.949228
H	0.577216	1.380083	2.049095
H	1.276781	2.964839	0.243513
H	2.641276	2.119140	−1.663954
H	3.325814	−0.262269	−1.748416
O	2.677680	−2.097808	0.110365
H	3.277182	−2.264061	−0.624076
C	−2.342934	1.512973	−0.138447
H	−1.382990	1.974389	0.094346
H	−2.684915	1.776617	−1.139781
H	−3.093959	1.795505	0.600972
C	−0.924174	−0.620319	−1.231313
H	−0.034525	−0.028460	−1.017121
H	−0.701306	−1.684034	−1.130025
H	−1.323316	−0.409985	−2.224255
O	−1.632431	−0.561219	1.303325
S	−2.175782	−0.257433	−0.018692
O	−3.429625	−0.859904	−0.462539

Conformer S13d

C	1.259566	0.689189	1.453632
C	2.080316	−0.403614	1.172804
C	2.696697	−0.507678	−0.079682
C	2.502203	0.488177	−1.043299
C	1.688337	1.589679	−0.748732
C	1.064360	1.693898	0.497827

H	2.245377	−1.188106	1.905155
H	0.757744	0.751802	2.413446
H	0.433230	2.546310	0.729467
H	1.556092	2.367557	−1.496287
H	2.986180	0.408834	−2.014965
O	3.476824	−1.610975	−0.300869
H	3.897115	−1.520913	−1.161981
C	−2.332451	1.139344	−1.035263
H	−1.381087	1.669172	−0.984825
H	−2.559716	0.811907	−2.050234
H	−3.140250	1.765470	−0.653143
C	−0.893975	−1.209484	−0.621959
H	−0.001501	−0.584586	−0.619291
H	−0.756003	−2.064122	0.042402
H	−1.151562	−1.550144	−1.625532
O	−1.887987	0.192494	1.371873
S	−2.259379	−0.280124	0.039832
O	−3.479571	−1.057552	−0.157692

Conformer S13e

C	2.069275	0.292103	−1.231093
C	2.310390	−1.083242	−1.197061
C	2.459104	−1.750322	0.024775
C	2.380052	−1.025561	1.217418
C	2.129237	0.351068	1.194042
C	2.000985	1.011494	−0.033143
H	1.974075	0.827112	−2.171394
H	2.380992	−1.634206	−2.130776
H	2.655900	−2.817619	0.045892
H	2.499390	−1.528836	2.172741
H	2.072489	0.913329	2.124361
O	1.770717	2.358282	−0.127001
H	1.926814	2.757558	0.734959
C	−1.107697	−1.381696	−0.021024
H	−0.536749	−1.309035	−0.946079
H	−0.459031	−1.282989	0.849295
H	−1.654996	−2.325216	0.016796
C	−1.382785	1.395513	−0.013729
H	−0.771739	1.427488	−0.915107
H	−2.106555	2.212195	−0.014842
H	−0.764180	1.436209	0.882054
O	−3.101233	−0.173385	−1.234797
S	−2.343593	−0.102685	0.012141
O	−3.028271	−0.171043	1.301390

Conformer S13f

C	1.384885	0.212283	1.192967
C	1.615959	−1.164673	1.171355
C	2.328056	−1.749474	0.118086
C	2.799876	−0.946272	−0.925515
C	2.563596	0.433004	−0.917736
C	1.862568	1.008505	0.148202

H	1.225681	−1.776418	1.978666
H	2.509794	−2.819695	0.107726
H	3.353304	−1.387306	−1.749661
H	2.927591	1.056720	−1.732083
H	0.830690	0.671641	2.004938
O	1.579411	2.352510	0.205732
H	2.090578	2.802747	−0.474857
C	−1.826056	1.576181	−0.148062
H	−0.776175	1.784317	0.057751
H	−2.116535	1.914271	−1.143469
H	−2.460572	2.047974	0.604266
C	−1.042144	−0.879330	−1.227184
H	−0.011889	−0.629783	−0.975506
H	−1.191982	−1.958897	−1.171670
H	−1.321338	−0.513620	−2.216095
O	−1.691169	−0.607768	1.306640
S	−2.137858	−0.171955	−0.015403
O	−3.509973	−0.417495	−0.451903

Conformer S13g

C	−1.364930	−0.004795	−1.176302
C	−1.971039	−1.250161	−0.983662
C	−2.833628	−1.458821	0.098233
C	−3.093655	−0.405366	0.983730
C	−2.477264	0.836626	0.807370
C	−1.596729	1.033367	−0.262832
H	−0.700709	0.161761	−2.019289
H	−1.769305	−2.053622	−1.686440
H	−3.307512	−2.425126	0.242271
H	−3.772872	−0.551702	1.819181
H	−2.652590	1.658941	1.494863
O	−0.986320	2.249475	−0.382962
H	−0.082471	2.070172	−0.688566
C	3.567650	0.033436	0.677011
H	3.537662	0.851809	1.396740
H	3.881783	−0.901964	1.140353
H	4.228450	0.285230	−0.153652
C	0.916277	−0.535582	1.368924
H	0.849675	0.351547	1.999860
H	−0.067501	−0.795614	0.974854
H	1.342444	−1.383449	1.907433
O	1.559482	1.123636	−0.586778
S	1.950965	−0.180889	−0.035291
O	1.979015	−1.356358	−0.897484

Me_2SO_2−4−methylphenol (Fig. S14)

Conformer S14a

C	−2.086662	1.116975	0.972654
C	−1.329711	1.560984	−0.120118
C	−1.148290	0.671685	−1.192690
C	−1.704224	−0.608528	−1.184124

C	−2.455407	−1.031307	−0.083374
C	−2.643706	−0.168303	1.000853
H	−2.248616	1.781407	1.818715
H	−0.552335	0.979275	−2.048063
H	−1.555700	−1.288241	−2.017620
H	−3.227563	−0.491282	1.861292
O	−2.964975	−2.306046	−0.116052
H	−3.590694	−2.398283	0.609018
C	−0.705597	2.931816	−0.140399
H	0.371350	2.859643	0.039687
H	−0.854971	3.411324	−1.112257
H	−1.146751	3.573572	0.627204
C	3.709108	−0.910859	0.453431
H	3.932937	−0.627479	1.482054
H	3.674615	−1.993715	0.330607
H	4.446197	−0.479453	−0.225457
C	0.993440	−0.966684	1.107980
H	1.300828	−0.733000	2.128288
H	0.019573	−0.523824	0.898879
H	0.964728	−2.042188	0.928952
O	2.183489	1.218889	0.265314
S	2.139325	−0.214023	−0.025218
O	1.839424	−0.685103	−1.374649

Conformer S14b

C	1.420730	0.930198	−1.201636
C	0.983147	1.501748	0.003948
C	1.430275	0.922876	1.199623
C	2.292271	−0.179991	1.198132
C	2.725988	−0.723482	−0.015753
C	2.287389	−0.165365	−1.220452
H	1.074546	1.348593	−2.143658
H	1.090734	1.329587	2.149097
H	2.622079	−0.615739	2.139926
H	2.629132	−0.597673	−2.156374
O	3.565479	−1.807801	−0.088938
H	3.895874	−1.991800	0.795823
C	0.094938	2.717617	0.012427
H	−0.536287	2.725741	0.904162
H	0.694803	3.634450	0.001293
H	−0.560353	2.719879	−0.861602
C	−3.642069	−1.203135	−0.008873
H	−3.703790	−1.796288	−0.921627
H	−3.701189	−1.827024	0.883290
H	−4.433159	−0.451801	0.004978
C	−0.874114	−1.577150	−0.024165
H	−0.978274	−2.153638	−0.944112
H	0.091832	−1.072657	−0.004234
H	−0.991022	−2.202933	0.861533
O	−2.024262	0.450126	−1.250202
S	−2.107015	−0.295947	0.003826
O	−2.015469	0.400995	1.285488

Conformer S14c

C	1.082749	0.740428	1.189578
C	1.547230	−0.575315	1.158338
C	2.334174	−1.049217	0.097672
C	2.644128	−0.158252	−0.939646
C	2.176808	1.161202	−0.928475
C	1.397410	1.610545	0.142562
H	1.274729	−1.244467	1.970444
H	3.257113	−0.494508	−1.773084
H	2.425637	1.835991	−1.745750
H	0.473036	1.094336	2.014993
O	0.884504	2.884934	0.207575
H	1.296318	3.415760	−0.482076
C	2.796646	−2.483253	0.057617
H	2.029436	−3.132083	−0.379164
H	3.704382	−2.587049	−0.542756
H	3.008752	−2.853396	1.064094
C	−2.312428	1.371812	−0.102116
H	−1.324176	1.779171	0.110705
H	−2.666762	1.671362	−1.089117
H	−3.026174	1.687480	0.660854
C	−1.051657	−0.845236	−1.241280
H	−0.095523	−0.391814	−0.982122
H	−0.975249	−1.933691	−1.209229
H	−1.403520	−0.524221	−2.222558
O	−1.744616	−0.781395	1.295413
S	−2.267883	−0.406531	−0.017197
O	−3.562668	−0.910371	−0.468686

Conformer S14d

C	−1.364028	1.562881	−0.181475
C	−2.067396	1.131831	0.953493
C	−2.595684	−0.159594	1.044204
C	−2.422162	−1.054450	−0.014742
C	−1.726672	−0.645758	−1.159429
C	−1.209059	0.651731	−1.236577
H	−2.213944	1.820381	1.782831
H	−3.148467	−0.482989	1.921276
H	−1.609179	−1.331996	−1.997335
H	−0.668191	0.958309	−2.129056
O	−2.947451	−2.313679	0.126752
H	−2.908808	−2.756421	−0.726733
C	−0.770254	2.943710	−0.267618
H	0.320926	2.886717	−0.212902
H	−1.035213	3.423502	−1.214545
H	−1.132408	3.577033	0.546588
C	2.018510	−1.434125	−1.110007
H	2.189706	−2.419711	−0.675858
H	0.999751	−1.328042	−1.482529
H	2.740727	−1.243099	−1.905382

C	1.074826	−0.543801	1.355910
H	1.275821	−1.524592	1.788783
H	1.171619	0.231074	2.118353
H	0.088540	−0.496466	0.895490
O	3.625936	−0.427451	0.711591
S	2.309547	−0.186180	0.127849
O	1.990000	1.109959	−0.470482

Conformer S14e

C	−2.134539	−0.344695	−1.211914
C	−2.656858	−0.780094	0.011804
C	−2.380320	−0.060636	1.177839
C	−1.587833	1.094148	1.111554
C	−1.054465	1.544763	−0.102702
C	−1.333805	0.795862	−1.258671
H	−2.356359	−0.913406	−2.110204
H	−0.913396	1.112377	−2.209794
H	−1.401375	1.658092	2.023695
H	−2.785150	−0.390579	2.133079
O	−3.423257	−1.916297	−0.001426
H	−3.791117	−2.045549	0.878426
C	−0.231662	2.803481	−0.191409
H	−0.773451	3.581278	−0.739266
H	−0.002961	3.197185	0.803464
H	0.706562	2.606840	−0.718032
C	2.205431	0.487500	1.413714
H	1.219168	0.943022	1.506138
H	2.427694	−0.165902	2.258096
H	2.975659	1.254585	1.318651
C	0.924842	−1.616419	0.119929
H	−0.002924	−1.066023	0.272780
H	0.870809	−2.194943	−0.803807
H	1.154918	−2.271345	0.961251
O	1.910694	0.438439	−1.193321
S	2.259394	−0.461013	−0.094002
O	3.514672	−1.206252	−0.116667

Conformer S14f

C	−1.343215	0.788681	−1.257434
C	−2.143001	−0.354895	−1.189870
C	−2.658968	−0.776341	0.041924
C	−2.373881	−0.045231	1.197952
C	−1.578307	1.102481	1.112437
C	−1.053681	1.544461	−0.111569
H	−2.356061	−0.923534	−2.093579
H	−0.928936	1.092820	−2.215237
H	−1.382938	1.675820	2.016895
H	−2.784881	−0.377436	2.146716
O	−3.439559	−1.894653	0.178553
H	−3.627108	−2.243048	−0.698725
C	−0.228978	2.800869	−0.217383

H	0.701459	2.600226	−0.756262
H	−0.776623	3.578379	−0.759749
H	0.014825	3.197688	0.772567
C	2.210146	0.518603	1.390199
H	1.220208	0.966016	1.481987
H	2.446875	−0.113157	2.246956
H	2.971510	1.290920	1.269611
C	0.928478	−1.618550	0.154138
H	−0.003193	−1.068820	0.284158
H	0.884907	−2.229711	−0.748943
H	1.157409	−2.242361	1.019053
O	1.898349	0.407982	−1.213608
S	2.257600	−0.463906	−0.095321
O	3.514882	−1.206051	−0.110281

Conformer S14g

C	1.374239	1.563388	0.174983
C	2.098273	1.120347	−0.939002
C	2.603836	−0.184594	−1.011978
C	2.390661	−1.072242	0.046472
C	1.683097	−0.644685	1.176119
C	1.179629	0.656086	1.230010
H	2.274851	1.801153	−1.768823
H	3.163378	−0.504870	−1.889237
H	1.552507	−1.335975	2.004411
H	0.621933	0.976394	2.107012
O	2.849721	−2.364361	0.046123
H	3.373582	−2.500589	−0.749693
C	0.797701	2.952185	0.245373
H	−0.295157	2.904077	0.232795
H	1.102652	3.454025	1.168734
H	1.134570	3.560491	−0.598304
C	−2.007307	−1.456284	1.078353
H	−2.204001	−2.428827	0.626141
H	−0.979754	−1.377955	1.433016
H	−2.710800	−1.270278	1.891503
C	−1.081653	−0.516625	−1.376807
H	−1.291201	−1.489454	−1.823484
H	−1.188129	0.271535	−2.124251
H	−0.089222	−0.479197	−0.928650
O	−3.623834	−0.393533	−0.703935
S	−2.300087	−0.177817	−0.126427
O	−1.962721	1.102780	0.495377

Conformer S14h

C	−2.772712	−0.286022	0.940624
C	−2.717779	0.742105	−0.013953
C	−1.825076	0.593602	−1.085812
C	−1.007141	−0.534370	−1.200589
C	−1.046917	−1.530434	−0.215908
C	−1.947497	−1.410441	0.847908

H −3.462615 −0.201062 1.778006
H −1.763210 1.369212 −1.846188
H −0.321916 −0.634035 −2.037569
H −1.973526 −2.193020 1.600885
O −0.225667 −2.623231 −0.257799
H 0.638650 −2.296813 −0.554449
C −3.629920 1.939166 0.077552
H −3.165138 2.821844 −0.370177
H −4.572136 1.755103 −0.449924
H −3.871823 2.170848 1.118592
C 3.760388 0.585030 0.697663
H 3.858484 1.602641 1.076134
H 3.884628 −0.154864 1.488735
H 4.480839 0.407425 −0.102044
C 1.032430 0.641691 1.317094
H 1.254710 1.607763 1.773117
H 0.026131 0.646766 0.895077
H 1.140499 −0.176398 2.030178
O 1.957184 1.462928 −1.008555
S 2.153316 0.388563 −0.042051
O 2.058322 −1.012745 −0.473024

Me_2SO_2–imidazole (Fig. S15)

Conformer S15a

C 3.048303 −1.146969 −0.000021
C 4.032756 −0.175707 0.001562
C 2.164350 0.873294 −0.001973
N 1.862295 −0.456838 −0.002247
H 0.924115 −0.846051 −0.003501
H 3.088090 −2.225400 0.000231
H 5.103773 −0.319232 0.003457
H 1.395239 1.632307 −0.003483
N 3.475628 1.081164 0.000304
C −2.964971 −0.112960 1.406122
H −3.682503 0.707652 1.394132
H −3.457936 −1.084951 1.385874
H −2.320798 −0.035579 2.283349
C −2.978698 −0.114980 −1.396299
H −3.696118 0.705624 −1.378413
H −2.343187 −0.038823 −2.279923
H −3.471385 −1.086963 −1.369847
O −1.306030 1.368140 −0.004274
S −1.887854 0.030875 −0.000512
O −1.007661 −1.144256 −0.004031

Conformer S15b

C 2.146768 0.893507 −0.000829
C 3.527365 0.969252 0.000130
C 3.050606 −1.118096 0.000160
N 1.862766 −0.450054 −0.001085
H 0.930051 −0.852023 −0.000249

H	1.364498	1.637261	−0.001543
H	4.141257	1.858501	0.000318
H	3.108099	−2.197173	0.000163
N	4.086035	−0.287502	0.000789
C	−2.976835	−0.115931	−1.399665
H	−3.462937	−1.091314	−1.376379
H	−3.700078	0.699583	−1.382768
H	−2.339192	−0.034112	−2.281250
C	−2.973013	−0.114204	1.402565
H	−3.462530	−1.087901	1.379395
H	−2.332343	−0.036049	2.282286
H	−3.693506	0.703782	1.389067
O	−1.005979	−1.135988	−0.000578
S	−1.891374	0.034845	−0.000129
O	−1.316807	1.375693	−0.001807

Conformer S15c

C	2.333648	−1.140962	−0.257728
C	3.037481	−0.422552	0.692309
C	1.946194	1.024584	−0.456339
N	1.658770	−0.197467	−0.990673
H	0.933409	−0.394108	−1.669369
H	2.265653	−2.195412	−0.476775
H	3.710281	−0.804063	1.446995
H	1.510618	1.937298	−0.835867
N	2.789431	0.924634	0.565122
C	−3.297043	−0.273127	0.353903
H	−3.400935	−1.307851	0.680701
H	−3.611735	0.429360	1.125801
H	−3.867218	−0.107047	−0.561232
C	−0.726886	−0.244521	1.456280
H	−0.859204	−1.286425	1.749673
H	0.327597	−0.035839	1.267320
H	−1.110190	0.439918	2.214029
O	−1.184938	−0.975776	−1.037565
S	−1.597425	0.044823	−0.067976
O	−1.469719	1.457813	−0.413105

Conformer S15d

C	−3.186517	−1.082822	−0.000615
C	−1.838862	−0.787083	0.000378
C	−2.866173	1.105634	0.000429
N	−3.824570	0.135229	−0.000459
H	−4.822577	0.285875	−0.000842
H	−3.726362	−2.016909	−0.000750
H	−0.997050	−1.464916	0.000129
H	−3.105287	2.159323	0.000918
N	−1.648553	0.579329	0.000897
C	1.483705	0.796183	−1.391498
H	0.401366	0.901456	−1.302864
H	1.988280	1.762934	−1.402294

H	1.753619	0.221084	−2.278575
C	1.484656	0.792350	1.393801
H	0.402518	0.899899	1.305275
H	1.753193	0.213733	2.279008
H	1.990950	1.758161	1.408143
O	1.361149	−1.428071	−0.001854
S	2.068198	−0.145439	−0.000348
O	3.529001	−0.114565	−0.000723

Conformer S15e

C	1.985944	1.052590	0.464036
C	2.852254	0.785139	−0.581508
C	2.330605	−1.117558	0.256298
N	1.681502	−0.174946	0.997609
H	0.936563	−0.362656	1.659024
H	1.572256	1.968881	0.856342
H	3.336327	1.494579	−1.237270
H	2.246361	−2.174778	0.463438
N	3.062321	−0.568771	−0.706547
C	−0.695037	−0.409404	−1.379173
H	−0.708937	−1.496636	−1.459869
H	−1.134828	0.064986	−2.257468
H	0.326575	−0.051327	−1.237341
C	−3.281249	−0.441418	−0.310902
H	−3.294388	−1.523112	−0.445184
H	−3.882090	−0.160979	0.555368
H	−3.635351	0.081293	−1.199553
O	−1.160359	−0.701071	1.205347
S	−1.622090	0.087383	0.056459
O	−1.611005	1.545015	0.128306

Me_2SO_2−4−methylimidazole (Fig. S16)

Conformer S16a

C	−2.593806	−1.057179	−0.001694
C	−3.560024	−0.065354	0.000127
C	−1.654347	0.935343	−0.002275
N	−1.387133	−0.401012	−0.002721
H	−0.460306	−0.815537	−0.004244
H	−2.664245	−2.134642	−0.002034
H	−0.866469	1.675160	−0.003286
N	−2.960474	1.174435	−0.000317
C	−5.046330	−0.216306	0.002499
H	−5.482200	0.254808	0.888111
H	−5.485333	0.259944	−0.878780
H	−5.328235	−1.272837	−0.000041
C	3.466673	−0.150997	−1.395924
H	4.197914	0.657311	−1.377641
H	3.942809	−1.131220	−1.369752
H	2.832747	−0.063820	−2.279685

C	3.452746	−0.150239	1.406157
H	4.184220	0.657984	1.394643
H	2.810074	−0.062429	2.283522
H	3.929027	−1.130521	1.385327
O	1.820835	1.360750	−0.003380
S	2.377858	0.012924	−0.000316
O	1.477670	−1.146570	−0.004515

Conformer S16b

C	3.442067	0.441485	−0.377655
C	2.150122	0.720027	0.029025
C	2.448933	−1.399312	0.330991
N	3.613166	−0.909072	−0.179229
H	4.446143	−1.442349	−0.380666
H	4.223687	1.069269	−0.777725
H	2.315512	−2.443012	0.578427
N	1.541665	−0.440208	0.467085
C	1.447762	2.037907	0.057043
H	0.475065	1.966404	−0.434975
H	1.283447	2.365429	1.088580
H	2.045608	2.800508	−0.448732
C	−1.525083	−1.490628	−0.735199
H	−0.443818	−1.393785	−0.632128
H	−1.915508	−2.339222	−0.172337
H	−1.817489	−1.567757	−1.783552
C	−1.677712	0.099942	1.546485
H	−0.587458	0.049048	1.525872
H	−2.023210	1.059565	1.934456
H	−2.111546	−0.716915	2.124443
O	−1.694265	1.124564	−0.870153
S	−2.272778	0.004359	−0.126432
O	−3.721526	−0.185627	−0.094582

Conformer S16c

C	1.829681	−0.464495	−0.000285
C	3.212224	−0.391568	−0.000081
C	2.494476	1.635929	0.000131
N	1.390960	0.838182	−0.000122
H	0.418530	1.130064	−0.000258
H	1.138481	−1.294208	−0.000582
H	2.430485	2.714917	0.000276
N	3.616118	0.925608	0.000168
C	4.200908	−1.511671	0.000067
H	4.844452	−1.460756	−0.882843
H	4.843010	−1.461879	0.884094
H	3.689129	−2.477884	−0.000958
C	−3.369159	−0.099173	1.401029
H	−3.978186	0.804574	1.377615
H	−3.979971	−1.001985	1.385702
H	−2.725145	−0.096253	2.281797
C	−3.368849	−0.098532	−1.401198

H	−3.977860	0.805220	−1.377525
H	−2.724636	−0.095247	−2.281819
H	−3.979689	−1.001335	−1.386405
O	−1.546850	1.165843	0.000425
S	−2.274694	−0.108588	0.000037
O	−1.534242	−1.365504	−0.000173

Conformer S16d

C	1.967326	−0.059787	1.133966
C	2.729609	0.249172	0.019270
C	1.431702	−1.373317	−0.555872
N	1.163482	−1.106746	0.753762
H	0.377714	−1.462246	1.284150
H	1.940109	0.352033	2.131669
H	0.905483	−2.136674	−1.110716
N	2.382930	−0.575663	−1.029183
C	3.801724	1.280561	−0.118862
H	4.763993	0.809181	−0.337539
H	3.574436	1.967798	−0.938702
H	3.903295	1.859711	0.802824
C	−3.539515	0.832194	0.010848
H	−3.502746	1.681561	0.693153
H	−3.799422	1.137659	−1.002822
H	−4.249560	0.087418	0.373175
C	−0.849152	1.285084	−0.602022
H	−0.839965	2.112338	0.108447
H	0.142813	0.834847	−0.671237
H	−1.180679	1.605157	−1.590659
O	−1.600934	−0.289774	1.378467
S	−1.954225	0.022589	−0.010330
O	−2.004431	−1.049825	−1.000028

Conformer S16e

C	1.677087	−0.077337	−1.033513
C	2.590785	−0.367285	−0.032887
C	1.811569	1.593865	0.398314
N	1.209495	1.184046	−0.753394
H	0.394551	1.615039	−1.174154
H	1.330604	−0.642785	−1.885586
H	1.605320	2.553683	0.850623
N	2.664468	0.684174	0.855773
C	3.429873	−1.592303	0.132144
H	4.492541	−1.345830	0.054302
H	3.264114	−2.044123	1.114213
H	3.189076	−2.331682	−0.636059
C	−0.893666	−0.372728	1.350585
H	−1.040900	0.463235	2.034893
H	−1.159083	−1.323942	1.814038
H	0.141809	−0.404695	1.005509
C	−3.569974	−0.204608	0.552844
H	−3.707548	0.599327	1.276087

H	−4.228303	−0.057806	−0.304573
H	−3.745045	−1.184041	0.998285
O	−1.696541	1.216416	−0.602275
S	−1.911437	−0.142252	−0.090856
O	−1.721700	−1.288355	−0.974657

$Me_2SO{-}H_2O$ (Fig. S17)

Conformer S17a

C	0.152177	−1.338620	0.740128
H	0.768339	−1.244640	1.637298
H	−0.913900	−1.291629	0.967129
H	0.388462	−2.273935	0.230969
C	0.158399	1.341062	0.738065
H	0.769680	1.242636	1.638158
H	0.405335	2.273912	0.229380
H	−0.908971	1.304123	0.960880
S	0.570175	−0.000584	−0.392037
O	2.071398	−0.003781	−0.554726
O	−2.734263	0.003179	−0.288433
H	−3.693998	−0.020360	−0.295255
H	−2.498270	0.009394	−1.219856

Conformer S17b

C	1.587078	1.344407	0.089534
H	1.822083	1.244906	1.151255
H	2.490478	1.321285	−0.524158
H	1.045072	2.274581	−0.083410
C	1.584938	−1.345745	0.089850
H	1.820108	−1.246329	1.151543
H	1.041373	−2.275061	−0.082817
H	2.488359	−1.324285	−0.523865
S	0.491098	0.000158	−0.388556
O	−0.630469	0.001184	0.632824
O	−3.294060	−0.000009	−0.214176
H	−3.819852	0.000528	0.586511
H	−2.381061	0.000478	0.116345

$Me_2SO_2{-}H_2O$ (Fig. S18)

Conformer S18a

C	2.026682	−0.104472	−0.830050
H	2.693680	0.669750	−0.450381
H	1.784297	0.049563	−1.881453
H	2.473707	−1.088885	−0.685539

C	−0.160478	1.511826	−0.141745
H	−0.310236	1.660360	−1.211579
H	−1.127847	1.515985	0.363333
H	0.509971	2.258894	0.283230
S	0.527614	−0.105238	0.128918
O	0.888186	−0.231128	1.535754
O	−0.377561	−1.081417	−0.490026
O	−2.977305	−0.016692	−0.124986
H	−2.258313	−0.643683	−0.284504
H	−3.670864	−0.548402	0.269046