Supplementary Information

The Contribution of Hyperconjugation and Inductive Effects to the Pseudo-Anomeric Effect in 4-Substituted Methoxycyclohexanes

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Computational Details

The axial and equatorial conformers of compounds **1**-**10** were optimized at the M06-2X/aug-cc-pVTZ theoretical level using the UltraFine integration grid, and harmonic frequency calculations were carried out at the same level in order to identify each geometry as true energy minimum, showing no imaginary frequency, using Gaussian 16 Rev C.01 program.[1] Single point energies for all optimized geometries were calculated using the Domain-Based Local Pair Natural Orbital (DLPNO)[2] approximation for CCSD(T) and with the basis set extrapolated to completeness from dunning's correlation-consistent polarized basis sets (cc-pVDZ/cc-pVTZ) as implemented in ORCA 5.0.3[3] with TightPNO and TightSCF settings. The good agreement between M06-2X/aug-cc-pVTZ and DLPNO-CCSD(T)/CBS single point energies indicate that the DFT functional and basis set chosen are suitable for the description of the molecular systems studied. Therefore, the M06-2X/aug-cc-pVTZ electronic energies were corrected with the thermal correction to Gibbs free energies obtained from the frequency calculations at the same theoretical level to afford the ring interconversion ΔG energy for compounds **1**-**10** equilibria. Molecular dipole moments and NBO analyses (using the NBO 7.0 program[4-8] implemented in Gaussian16) were also calculated at the M06-2X/aug-cc-pVTZ level of theory.

References

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Table S1. Absolute Error (AE) between M06-2X/aug-cc-pVTZ and DLPNO-CCSD(T)/CBS single point energies, in kcal mol^{-1}, obtained for compounds **1**-**10**.

Compound	$\Delta E_{(ax-eq)}$ DFT	$\Delta E_{(ax-eq)}$ DLPNO-CCSD(T)	AE
1	-1.08	-1.00	0.08
2	-0.90	-0.91	0.01
3	-0.21	-0.10	0.11
4	-1.08	-1.12	0.04
5	-0.77	-0.54	0.24
6	-1.14	-1.03	0.10
7	-0.84	-0.50	0.34
8	-0.60	-0.70	0.10
9	-1.12	-1.03	0.09
10	-5.96	-5.79	0.17
		MAE =	**0.13**

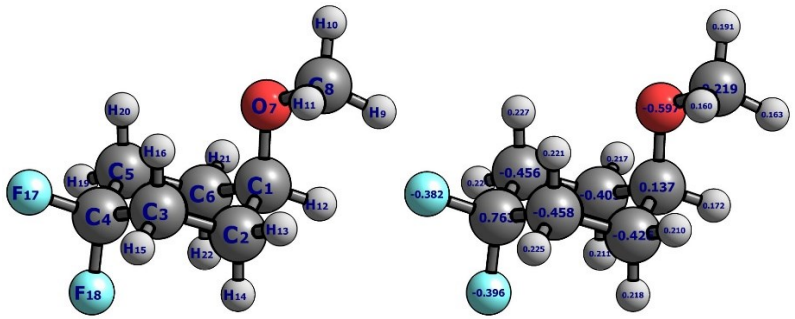

Table S2. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 1_{ax}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	F17	F18	H19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.64	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-8.24	42.43	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	11.89	-43.39	-76.77	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-8.22	21.93	27.36	-76.58	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-12.07	22.89	20.88	-41.13	40.17	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-19.08	34.50	30.63	-43.69	31.21	34.09	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-4.18	10.47	9.20	-12.27	7.84	8.05	30.86	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	2.86	-7.14	-5.83	7.99	-5.10	-5.54	-15.59	-10.81	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.65	-6.81	-6.58	9.28	-6.06	-5.91	-18.80	-12.79	5.83	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	2.61	-8.19	-7.52	9.18	-5.41	-5.21	-15.25	-10.64	4.87	5.74	-	-	-	-	-	-	-	-	-	-	-	-
H12	7.11	-11.30	-7.55	11.16	-7.52	-10.74	-16.61	-4.80	4.00	3.11	2.90	-	-	-	-	-	-	-	-	-	-	-
H13	4.39	-27.30	-14.77	15.48	-8.06	-8.17	-15.17	-5.66	4.01	3.57	4.99	4.82	-	-	-	-	-	-	-	-	-	-
H14	4.62	-28.24	-15.34	19.98	-9.94	-10.68	-12.83	-4.03	2.95	2.78	3.07	5.08	8.68	-	-	-	-	-	-	-	-	-
H15	2.93	-14.58	-31.32	26.82	-9.86	-7.70	-11.19	-3.68	2.42	2.71	3.10	2.98	6.19	6.51	-	-	-	-	-	-	-	-
H16	3.59	-14.45	-30.78	26.50	-11.95	-8.87	-16.38	-5.06	2.97	3.71	4.32	3.33	6.15	5.21	9.31	-	-	-	-	-	-	-
F17	-4.16	14.63	24.63	-70.78	24.54	13.89	17.09	5.12	-3.32	-4.06	-3.89	-4.19	-5.91	-6.86	-10.97	-10.91	-	-	-	-	-	-
F18	-5.13	19.30	25.65	-72.97	25.54	18.23	17.70	5.26	-3.62	-3.99	-3.92	-5.30	-7.11	-10.91	-11.60	-8.90	23.00	-	-	-	-	-
H19	2.92	-8.09	-9.86	26.75	-31.10	-13.82	-11.37	-3.09	2.07	2.46	2.14	2.97	3.15	3.95	3.94	4.35	-10.91	-11.56	-	-	-	-
H20	3.68	-9.56	-12.30	27.23	-31.56	-14.14	-17.25	-4.24	2.63	3.41	2.89	3.41	3.77	4.10	4.48	6.33	-11.22	-9.14	9.53	-	-	-
H21	4.60	-8.92	-8.40	16.00	-15.25	-26.85	-16.80	-4.08	2.87	3.16	2.52	5.00	3.53	4.20	3.27	3.83	-6.12	-7.30	6.35	6.63	-	-
H22	4.47	-10.82	-9.58	19.18	-14.82	-26.04	-12.68	-3.42	2.48	2.54	2.30	4.93	3.93	6.00	3.80	3.86	-6.61	-10.41	6.32	5.20	8.64	-

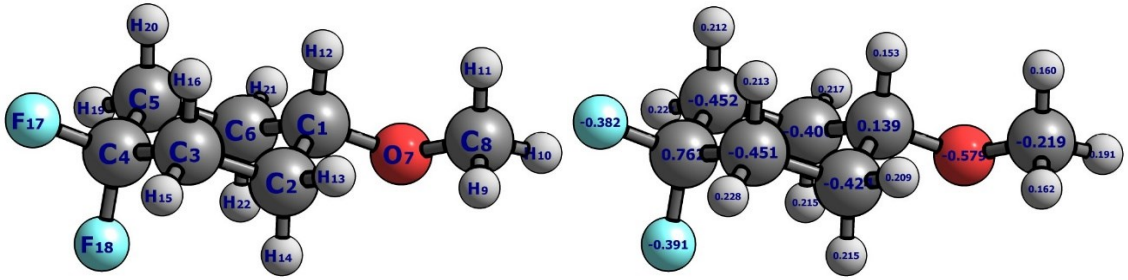

Table S3. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 1_{eq}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	F17	F18	H19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.85	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-8.29	41.60	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	12.09	-42.95	-75.50	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-8.31	21.61	26.76	-75.74	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-12.35	22.82	20.67	-41.17	39.96	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-19.00	33.36	22.95	-34.84	23.37	33.17	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-4.27	10.33	7.47	-10.69	6.74	8.07	29.93	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	2.70	-8.18	-5.72	7.83	-4.64	-5.26	-14.94	-10.75	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.70	-6.74	-5.26	7.89	-5.03	-5.92	-18.21	-12.75	5.78	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	2.87	-6.86	-5.37	7.60	-4.84	-5.49	-14.90	-10.63	4.84	5.72	-	-	-	-	-	-	-	-	-	-	-	-
H12	6.40	-9.99	-8.26	11.74	-8.26	-9.56	-14.30	-4.30	2.65	2.75	3.52	-	-	-	-	-	-	-	-	-	-	-
H13	4.47	-27.10	-14.60	15.42	-7.98	-8.16	-14.68	-5.57	5.01	3.52	3.81	4.28	-	-	-	-	-	-	-	-	-	-
H14	4.66	-27.76	-14.90	19.53	-9.68	-10.53	-15.57	-4.71	3.86	3.28	2.93	3.58	8.50	-	-	-	-	-	-	-	-	-
H15	3.03	-14.72	-31.27	27.14	-9.91	-7.84	-9.50	-3.25	2.59	2.36	2.32	3.05	6.28	6.52	-	-	-	-	-	-	-	-
H16	3.51	-13.82	-29.15	25.48	-11.40	-8.54	-9.92	-3.38	2.54	2.39	2.59	4.14	5.97	4.95	9.11	-	-	-	-	-	-	-
F17	-4.24	14.54	24.28	-70.65	24.33	13.92	13.32	4.32	-3.18	-3.27	-3.15	-4.48	-5.91	-6.74	-11.11	-10.55	-	-	-	-	-	-
F18	-5.15	18.83	24.93	-72.06	24.99	18.02	16.59	5.08	-3.79	-3.85	-3.47	-4.71	-6.96	-10.48	-11.59	-8.46	22.69	-	-	-	-	-
H19	3.04	-8.19	-9.90	27.19	-31.42	-14.12	-9.69	-2.87	1.98	2.22	2.04	3.05	3.20	3.95	4.07	4.26	-11.10	-11.62	-	-	-	-
H20	3.50	-8.88	-11.34	25.45	-29.21	-13.21	-10.03	-3.05	2.07	2.27	2.30	4.11	3.53	3.77	4.25	5.69	-10.55	-8.45	9.12	-	-	-
H21	4.69	-8.87	-8.27	15.95	-15.07	-26.89	-16.22	-4.09	2.55	3.15	2.86	4.46	3.52	4.15	3.32	3.67	-6.11	-7.20	6.47	6.14	-	-
H22	4.66	-11.00	-9.66	19.53	-14.94	-26.52	-16.08	-3.96	2.68	3.02	2.55	3.58	3.99	6.02	3.94	3.78	-6.73	-10.46	6.53	4.94	8.81	-

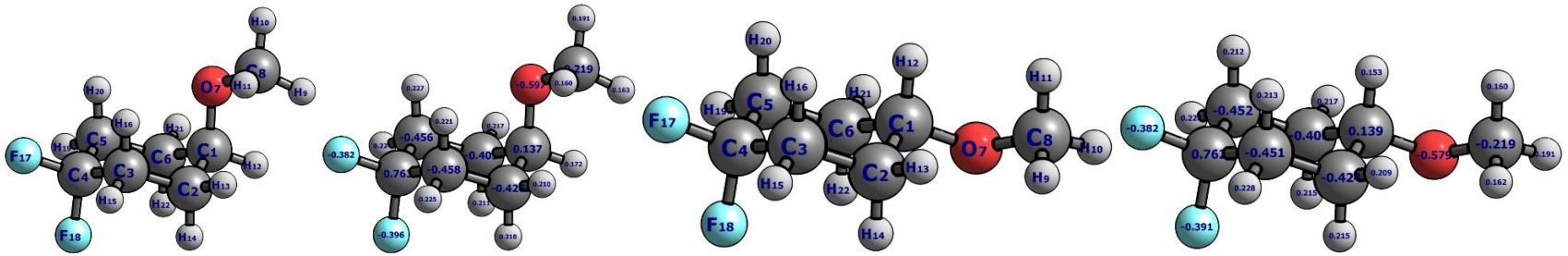

Table S4. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 1. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	F17	F18	H19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	0.21	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	0.05	0.83	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-0.20	-0.44	-1.27	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	0.09	0.32	0.60	-0.84	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	0.28	0.07	0.21	0.04	0.21	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-0.08	1.14	7.68	-8.85	7.84	0.92	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	0.09	0.14	1.73	-1.58	1.10	-0.02	0.93	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	0.16	1.04	-0.11	0.16	-0.46	-0.28	-0.65	-0.06	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	-0.05	-0.07	-1.32	1.39	-1.03	0.01	-0.59	-0.04	0.05	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	-0.26	-1.33	-2.15	1.58	-0.57	0.28	-0.35	-0.01	0.03	0.02	-	-	-	-	-	-	-	-	-	-	-	-
H12	0.71	-1.31	0.71	-0.58	0.74	-1.18	-2.31	-0.50	1.35	0.36	-0.62	-	-	-	-	-	-	-	-	-	-	-
H13	-0.08	-0.20	-0.17	0.06	-0.08	-0.01	-0.49	-0.09	-1.00	0.05	1.18	0.54	-	-	-	-	-	-	-	-	-	-
H14	-0.04	-0.48	-0.44	0.45	-0.26	-0.15	2.74	0.68	-0.91	-0.50	0.14	1.50	0.18	-	-	-	-	-	-	-	-	-
H15	-0.10	0.14	-0.05	-0.32	0.05	0.14	-1.69	-0.43	-0.17	0.35	0.78	-0.07	-0.09	-0.01	-	-	-	-	-	-	-	-
H16	0.08	-0.63	-1.63	1.02	-0.55	-0.33	-6.46	-1.68	0.43	1.32	1.73	-0.81	0.18	0.26	0.20	-	-	-	-	-	-	-
F17	0.08	0.09	0.35	-0.13	0.21	-0.03	3.77	0.80	-0.14	-0.79	-0.74	0.29	0.00	-0.12	0.14	-0.36	-	-	-	-	-	-
F18	0.02	0.47	0.72	-0.91	0.55	0.21	1.11	0.18	0.17	-0.14	-0.45	-0.59	-0.15	-0.43	-0.01	-0.44	0.31	-	-	-	-	-
H19	-0.12	0.10	0.04	-0.44	0.32	0.30	-1.68	-0.22	0.09	0.24	0.10	-0.08	-0.05	0.00	-0.13	0.09	0.19	0.06	-	-	-	-
H20	0.18	-0.68	-0.96	1.78	-2.35	-0.93	-7.22	-1.19	0.56	1.14	0.59	-0.70	0.24	0.33	0.23	0.64	-0.67	-0.69	0.41	-	-	-
H21	-0.09	-0.05	-0.13	0.05	-0.18	0.04	-0.58	0.01	0.32	0.01	-0.34	0.54	0.01	0.05	-0.05	0.16	-0.01	-0.10	-0.12	0.49	-	-
H22	-0.19	0.18	0.08	-0.35	0.12	0.48	3.40	0.54	-0.20	-0.48	-0.25	1.35	-0.06	-0.02	-0.14	0.08	0.12	0.05	-0.21	0.26	-0.17	-

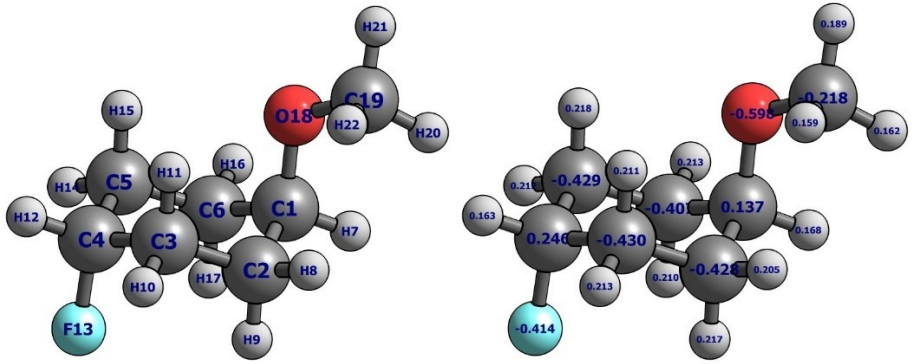

Table S5. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 2ax.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	H12	F13	H14	H15	H16	H17	O18	C19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.72	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-7.77	40.05	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	3.80	-13.92	-23.14	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-7.74	20.73	24.28	-23.08	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-12.15	23.09	19.74	-13.18	37.88	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	6.97	-11.09	-6.94	3.49	-6.91	-10.54	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	4.30	-26.77	-13.55	4.85	-7.41	-8.02	4.61	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	4.62	-28.23	-14.38	6.38	-9.35	-10.72	4.95	8.45	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.79	-13.94	-27.90	8.12	-8.77	-7.32	2.77	5.79	6.16	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	3.45	-13.91	-27.65	8.12	-10.76	-8.53	3.12	5.76	4.98	8.48	-	-	-	-	-	-	-	-	-	-	-	-
H12	1.89	-6.70	-10.80	12.22	-10.76	-6.36	1.84	2.59	3.12	4.66	4.67	-	-	-	-	-	-	-	-	-	-	-
F13	-5.35	20.18	25.01	-24.07	24.88	19.04	-5.40	-7.25	-11.40	-11.32	-8.82	-11.21	-	-	-	-	-	-	-	-	-	-
H14	2.78	-7.71	-8.78	8.10	-27.71	-13.22	2.76	2.92	3.74	3.52	3.94	4.64	-11.29	-	-	-	-	-	-	-	-	-
H15	3.54	-9.20	-11.09	8.36	-28.39	-13.64	3.20	3.53	3.93	4.06	5.79	4.82	-9.07	8.70	-	-	-	-	-	-	-	-
H16	4.51	-8.76	-7.73	5.01	-14.00	-26.33	4.78	3.38	4.11	3.03	3.59	2.68	-7.44	5.94	6.23	-	-	-	-	-	-	-
H17	4.47	-10.84	-8.98	6.11	-13.86	-25.98	4.80	3.83	5.98	3.58	3.68	3.00	-10.83	5.98	4.97	8.40	-	-	-	-	-	-
O18	-19.15	34.69	28.87	-14.01	29.38	34.26	-16.30	-14.84	-12.81	-10.66	-15.75	-7.64	18.45	-10.84	-16.59	-16.45	-12.64	-	-	-	-	-
C19	-4.18	10.49	8.64	-3.92	7.35	8.05	-4.69	-5.52	-4.01	-3.49	-4.85	-2.25	5.46	-2.92	-4.06	-3.97	-3.39	30.85	-	-	-	-
H20	2.86	-7.15	-5.46	2.55	-4.77	-5.52	3.89	3.91	2.93	2.30	2.85	1.46	-3.75	1.96	2.51	2.78	2.45	-15.55	-10.71	-	-	-
H21	2.62	-6.76	-6.11	2.94	-5.62	-5.85	3.01	3.44	2.74	2.55	3.52	1.76	-4.11	2.31	3.23	3.05	2.49	-18.61	-12.59	5.72	-	-
H22	2.60	-8.19	-7.06	2.94	-5.07	-5.20	2.83	4.85	3.04	2.95	4.15	1.71	-4.07	2.02	2.76	2.46	2.28	-15.22	-10.55	4.82	5.64	-

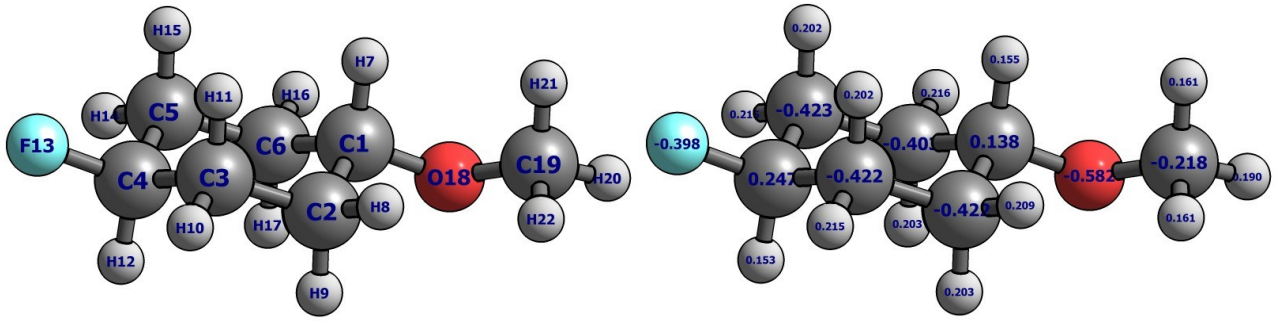

Table S6. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 2eq.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	H12	F13	H14	H15	H16	H17	O18	C19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.69	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-7.71	38.70	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	3.88	-13.84	-22.87	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-7.73	20.17	23.70	-22.93	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-12.20	22.53	19.30	-13.27	37.16	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	6.46	-10.08	-7.82	3.82	-7.83	-9.65	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	4.43	-26.83	-13.60	4.98	-7.47	-8.09	4.34	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	4.37	-25.95	-13.12	5.99	-8.54	-9.83	3.43	7.99	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.85	-13.87	-27.66	8.22	-8.77	-7.34	2.93	5.97	5.77	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	3.33	-13.09	-25.93	7.81	-10.34	-8.16	4.00	5.64	4.43	8.20	-	-	-	-	-	-	-	-	-	-	-	-
H12	2.10	-7.67	-9.95	11.45	-9.98	-7.35	1.96	2.81	3.93	4.43	3.38	-	-	-	-	-	-	-	-	-	-	-
F13	-4.36	15.00	23.57	-23.46	23.61	14.36	-4.68	-6.12	-6.61	-10.84	-10.36	-10.09	-	-	-	-	-	-	-	-	-	-
H14	2.85	-7.68	-8.76	8.24	-27.79	-13.30	2.93	3.01	3.49	3.60	3.87	4.44	-10.83	-	-	-	-	-	-	-	-	-
H15	3.32	-8.48	-10.29	7.80	-25.97	-12.50	3.98	3.38	3.40	3.86	5.33	3.37	-10.35	8.21	-	-	-	-	-	-	-	-
H16	4.64	-8.78	-7.74	5.15	-14.03	-26.60	4.52	3.50	3.89	3.12	3.51	2.90	-6.32	6.14	5.79	-	-	-	-	-	-	-
H17	4.38	-10.28	-8.53	6.00	-13.16	-24.81	3.43	3.74	5.32	3.49	3.41	3.94	-6.61	5.79	4.42	8.29	-	-	-	-	-	-
O18	-18.93	33.28	21.57	-11.34	21.95	33.06	-14.56	-14.66	-14.81	-9.02	-9.49	-6.69	13.89	-9.20	-9.58	-16.19	-15.30	-	-	-	-	-
C19	-4.23	10.22	6.96	-3.45	6.30	8.00	-4.36	-5.52	-4.45	-3.07	-3.21	-2.03	4.47	-2.71	-2.90	-4.07	-3.74	30.00	-	-	-	-
H20	2.66	-6.65	-4.89	2.54	-4.67	-5.84	2.78	3.48	3.08	2.21	2.25	1.52	-3.37	2.08	2.15	3.12	2.84	-18.16	-12.64	-	-	-
H21	2.85	-6.80	-5.01	2.45	-4.54	-5.46	3.58	3.78	2.76	2.19	2.45	1.39	-3.26	1.94	2.19	2.86	2.42	-14.98	-10.62	5.69	-	-
H22	2.68	-8.08	-5.33	2.52	-4.32	-5.20	2.68	4.95	3.64	2.44	2.40	1.50	-3.29	1.86	1.97	2.52	2.52	-14.93	-10.67	5.72	4.82	-

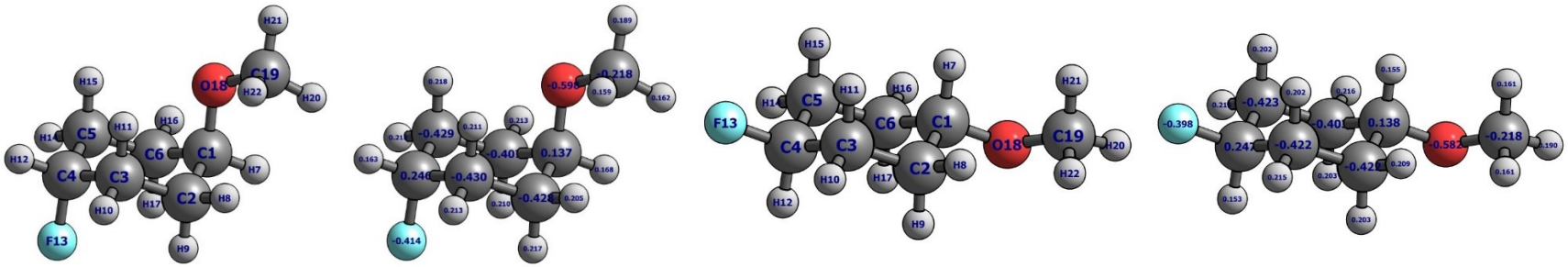

Table S7. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 2. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	H12	F13	H14	H15	H16	H17	O18	C19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-0.03	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-0.06	1.35	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-0.08	-0.08	-0.27	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-0.01	0.56	0.58	-0.15	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	0.05	0.56	0.44	0.09	0.72	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	0.51	-1.01	0.88	-0.33	0.92	-0.89	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	-0.13	0.06	0.05	-0.13	0.06	0.07	0.27	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	0.25	-2.28	-1.26	0.39	-0.81	-0.89	1.52	0.46	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	-0.06	-0.07	-0.24	-0.10	0.00	0.02	-0.16	-0.18	0.39	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	0.12	-0.82	-1.72	0.31	-0.42	-0.37	-0.88	0.12	0.55	0.28	-	-	-	-	-	-	-	-	-	-	-	-
H12	-0.21	0.97	-0.85	0.77	-0.78	0.99	-0.12	-0.22	-0.81	0.23	1.29	-	-	-	-	-	-	-	-	-	-	-
F13	-0.99	5.18	1.44	-0.61	1.27	4.68	-0.72	-1.13	-4.79	-0.48	1.54	-1.12	-	-	-	-	-	-	-	-	-	-
H14	-0.07	-0.03	-0.02	-0.14	0.08	0.08	-0.17	-0.09	0.25	-0.08	0.07	0.20	-0.46	-	-	-	-	-	-	-	-	-
H15	0.22	-0.72	-0.80	0.56	-2.42	-1.14	-0.78	0.15	0.53	0.20	0.46	1.45	1.28	0.49	-	-	-	-	-	-	-	-
H16	-0.13	0.02	0.01	-0.14	0.03	0.27	0.26	-0.12	0.22	-0.09	0.08	-0.22	-1.12	-0.20	0.44	-	-	-	-	-	-	-
H17	0.09	-0.56	-0.45	0.11	-0.70	-1.17	1.37	0.09	0.66	0.09	0.27	-0.94	-4.22	0.19	0.55	0.11	-	-	-	-	-	-
O18	-0.22	1.41	7.30	-2.67	7.43	1.20	-1.74	-0.18	2.00	-1.64	-6.26	-0.95	4.56	-1.64	-7.01	-0.26	2.66	-	-	-	-	-
C19	0.05	0.27	1.68	-0.47	1.05	0.05	-0.33	0.00	0.44	-0.42	-1.64	-0.22	0.99	-0.21	-1.16	0.10	0.35	0.85	-	-	-	-
H20	0.20	-0.50	-0.57	0.01	-0.10	0.32	1.11	0.43	-0.15	0.09	0.60	-0.06	-0.38	-0.12	0.36	-0.34	-0.39	2.61	1.93	-	-	-
H21	-0.23	0.04	-1.10	0.49	-1.08	-0.39	-0.57	-0.34	-0.02	0.36	1.07	0.37	-0.85	0.37	1.04	0.19	0.07	-3.63	-1.97	0.03	-	-
H22	-0.08	-0.11	-1.73	0.42	-0.75	0.00	0.15	-0.10	-0.60	0.51	1.75	0.21	-0.78	0.16	0.79	-0.06	-0.24	-0.29	0.12	-0.90	0.82	-

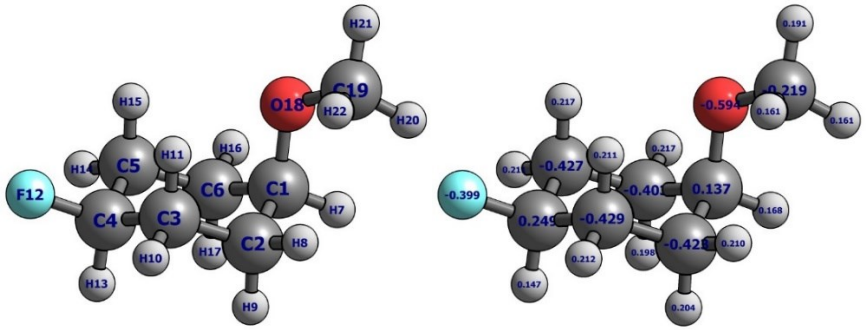

Table S8. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 3ax.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	F12	H13	H14	H15	H16	H17	O18	C19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.56	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-7.73	39.50	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	3.86	-14.07	-23.44	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-7.69	20.46	24.26	-23.33	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-12.00	22.58	19.52	-13.33	37.33	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	6.96	-10.98	-6.93	3.56	-6.88	-10.44	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	4.38	-27.03	-13.79	5.03	-7.55	-8.10	4.70	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	4.34	-26.27	-13.47	6.15	-8.74	-9.94	4.69	8.14	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.77	-13.72	-27.72	8.18	-8.71	-7.21	2.75	5.89	5.73	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	3.45	-13.73	-27.54	8.21	-10.88	-8.50	3.12	5.84	4.67	8.42	-	-	-	-	-	-	-	-	-	-	-	-
F12	-4.31	15.11	23.99	-23.70	23.86	14.34	-4.26	-6.14	-6.71	-10.71	-10.78	-	-	-	-	-	-	-	-	-	-	-
H13	2.00	-7.48	-9.77	11.13	-9.70	-7.06	1.99	2.73	3.88	4.21	3.40	-9.76	-	-	-	-	-	-	-	-	-	-
H14	2.76	-7.57	-8.72	8.15	-27.46	-13.00	2.74	2.96	3.48	3.48	3.96	-10.65	4.20	-	-	-	-	-	-	-	-	-
H15	3.52	-9.14	-11.20	8.42	-28.14	-13.42	3.19	3.62	3.69	4.08	5.96	-11.08	3.49	8.60	-	-	-	-	-	-	-	-
H16	4.60	-8.85	-7.89	5.21	-14.23	-26.63	4.88	3.52	3.94	3.08	3.69	-6.36	2.80	6.04	6.30	-	-	-	-	-	-	-
H17	4.21	-10.08	-8.45	5.90	-13.01	-24.28	4.56	3.68	5.26	3.35	3.48	-6.48	3.70	5.58	4.66	8.13	-	-	-	-	-	-
O18	-19.03	34.11	28.48	-14.00	28.94	33.73	-16.21	-15.09	-11.99	-10.53	-15.60	17.52	-6.84	-10.70	-16.36	-16.78	-11.88	-	-	-	-	-
C19	-4.18	10.40	8.59	-3.96	7.32	7.99	-4.70	-5.66	-3.79	-3.48	-4.81	5.28	-2.02	-2.91	-4.05	-4.08	-3.22	30.72	-	-	-	-
H20	2.84	-7.05	-5.41	2.57	-4.72	-5.45	3.88	3.99	2.76	2.28	2.81	-3.41	1.37	1.94	2.48	2.83	2.31	-15.39	-10.69	-	-	-
H21	2.64	-6.74	-6.12	2.98	-5.63	-5.85	3.03	3.55	2.61	2.56	3.51	-4.17	1.53	2.32	3.23	3.15	2.38	-18.66	-12.73	5.75	-	-
H22	2.62	-8.16	-7.05	2.98	-5.08	-5.19	2.85	5.01	2.89	2.95	4.11	-4.04	1.52	2.02	2.78	2.53	2.17	-15.25	-10.67	4.84	5.74	-

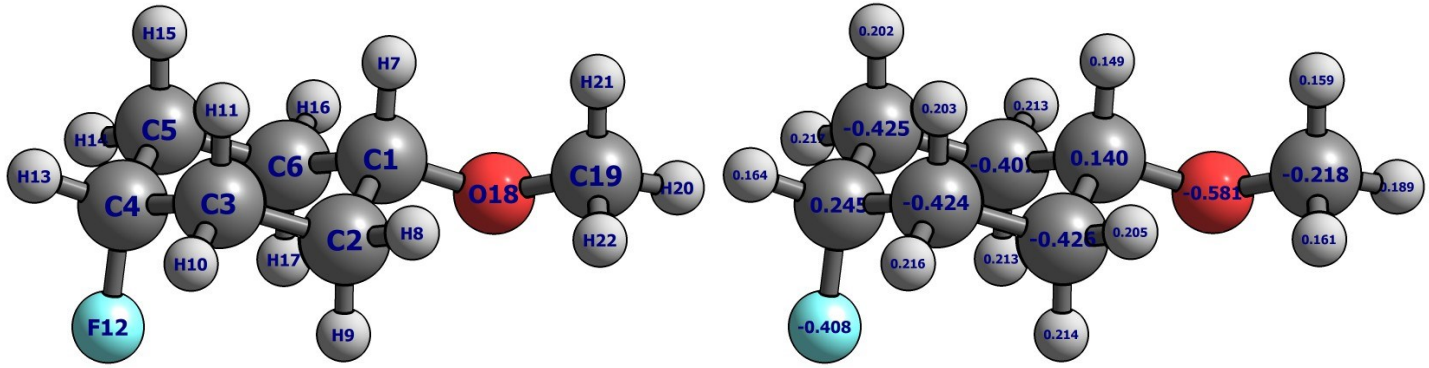

Table S9. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 3eq.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	F12	H13	H14	H15	H16	H17	O18	C19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.93	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-7.81	39.18	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	3.86	-13.73	-22.68	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-7.83	20.41	23.73	-22.74	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-12.43	23.02	19.53	-13.16	37.65	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	6.28	-9.81	-7.59	3.66	-7.60	-9.39	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	4.39	-26.59	-13.40	4.82	-7.35	-8.03	4.09	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	4.65	-27.69	-13.93	6.21	-9.07	-10.54	3.49	8.27	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.89	-14.10	-27.90	8.21	-8.83	-7.47	2.84	5.89	6.17	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	3.36	-13.24	-26.06	7.75	-10.22	-8.18	3.87	5.58	4.70	8.27	-	-	-	-	-	-	-	-	-	-	-	-
F12	-5.38	19.70	24.31	-23.71	24.36	18.85	-4.80	-7.11	-10.94	-11.34	-8.35	-	-	-	-	-	-	-	-	-	-	-
H13	1.93	-6.66	-10.65	12.17	-10.67	-6.38	1.97	2.60	3.06	4.73	4.50	-11.09	-	-	-	-	-	-	-	-	-	-
H14	2.90	-7.82	-8.83	8.23	-28.05	-13.53	2.84	2.98	3.74	3.65	3.85	-11.38	4.74	-	-	-	-	-	-	-	-	-
H15	3.35	-8.50	-10.16	7.73	-26.09	-12.65	3.84	3.29	3.58	3.84	5.17	-8.33	4.50	8.28	-	-	-	-	-	-	-	-
H16	4.60	-8.73	-7.62	4.99	-13.85	-26.41	4.27	3.38	4.05	3.08	3.43	-7.36	2.69	6.07	5.74	-	-	-	-	-	-	-
H17	4.65	-11.00	-9.05	6.20	-13.96	-26.45	3.48	3.89	5.99	3.72	3.59	-10.91	3.05	6.19	4.68	8.58	-	-	-	-	-	-
O18	-19.07	33.54	21.61	-11.14	22.00	33.35	-14.03	-14.41	-15.51	-9.07	-9.50	17.37	-5.98	-9.26	-9.59	-15.94	-16.01	-	-	-	-	-
C19	-4.27	10.33	6.99	-3.41	6.32	8.07	-4.19	-5.44	-4.67	-3.09	-3.22	5.29	-1.91	-2.72	-2.90	-4.00	-3.93	29.96	-	-	-	-
H20	2.68	-6.69	-4.90	2.50	-4.67	-5.88	2.67	3.42	3.22	2.22	2.26	-3.98	1.43	2.09	2.15	3.06	2.97	-18.09	-12.59	-	-	-
H21	2.84	-6.82	-5.00	2.41	-4.51	-5.45	3.41	3.69	2.88	2.19	2.45	-3.59	1.38	1.93	2.17	2.77	2.51	-14.81	-10.51	5.61	-	-
H22	2.70	-8.17	-5.36	2.49	-4.34	-5.26	2.58	4.89	3.82	2.46	2.42	-3.95	1.41	1.88	1.97	2.49	2.66	-14.94	-10.68	5.71	4.78	-

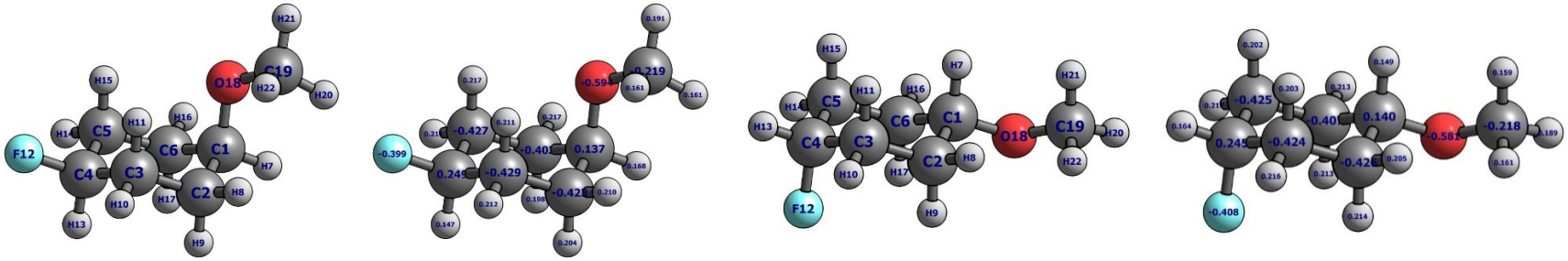

Table S10. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 3. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	F12	H13	H14	H15	H16	H17	O18	C19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	0.37	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	0.08	0.32	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	0.00	-0.34	-0.76	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	0.14	0.05	0.53	-0.59	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	0.43	-0.44	-0.01	-0.17	-0.32	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	0.68	-1.17	0.66	-0.10	0.72	-1.05	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	-0.01	-0.44	-0.39	0.21	-0.20	-0.07	0.61	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	-0.31	1.42	0.46	-0.06	0.33	0.60	1.20	-0.13	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	-0.12	0.38	0.18	-0.03	0.12	0.26	-0.09	0.00	-0.44	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	0.09	-0.49	-1.48	0.46	-0.66	-0.32	-0.75	0.26	-0.03	0.15	-	-	-	-	-	-	-	-	-	-	-	-
F12	1.07	-4.59	-0.32	0.01	-0.50	-4.51	0.54	0.97	4.23	0.63	-2.43	-	-	-	-	-	-	-	-	-	-	-
H13	0.07	-0.82	0.88	-1.04	0.97	-0.68	0.02	0.13	0.82	-0.52	-1.10	1.33	-	-	-	-	-	-	-	-	-	-
H14	-0.14	0.25	0.11	-0.08	0.59	0.53	-0.10	-0.02	-0.26	-0.17	0.11	0.73	-0.54	-	-	-	-	-	-	-	-	-
H15	0.17	-0.64	-1.04	0.69	-2.05	-0.77	-0.65	0.33	0.11	0.24	0.79	-2.75	-1.01	0.32	-	-	-	-	-	-	-	-
H16	0.00	-0.12	-0.27	0.22	-0.38	-0.22	0.61	0.14	-0.11	0.00	0.26	1.00	0.11	-0.03	0.56	-	-	-	-	-	-	-
H17	-0.44	0.92	0.60	-0.30	0.95	2.17	1.08	-0.21	-0.73	-0.37	-0.11	4.43	0.65	-0.61	-0.02	-0.45	-	-	-	-	-	-
O18	0.04	0.57	6.87	-2.86	6.94	0.38	-2.18	-0.68	3.52	-1.46	-6.10	0.15	-0.86	-1.44	-6.77	-0.84	4.13	-	-	-	-	-
C19	0.09	0.07	1.60	-0.55	1.00	-0.08	-0.51	-0.22	0.88	-0.39	-1.59	-0.01	-0.11	-0.19	-1.15	-0.08	0.71	0.76	-	-	-	-
H20	0.16	-0.36	-0.51	0.07	-0.05	0.43	1.21	0.57	-0.46	0.06	0.55	0.57	-0.06	-0.15	0.33	-0.23	-0.66	2.70	1.90	-	-	-
H21	-0.20	0.08	-1.12	0.57	-1.12	-0.40	-0.38	-0.14	-0.27	0.37	1.06	-0.58	0.15	0.39	1.06	0.38	-0.13	-3.85	-2.22	0.14	-	-
H22	-0.08	0.01	-1.69	0.49	-0.74	0.07	0.27	0.12	-0.93	0.49	1.69	-0.09	0.11	0.14	0.81	0.04	-0.49	-0.31	0.01	-0.87	0.96	-

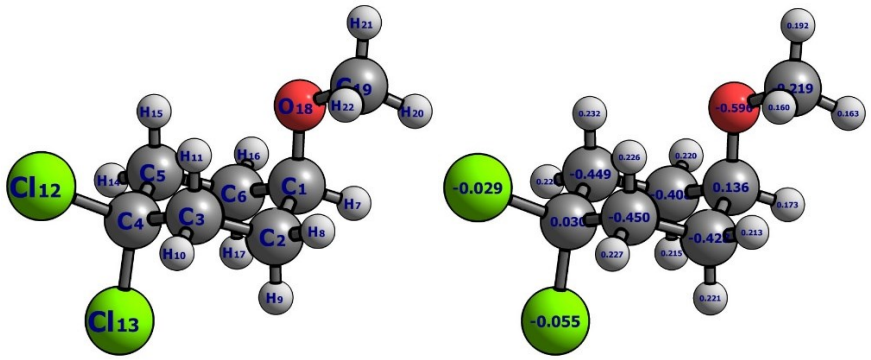

Table S11. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 4ax.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	Cl12	Cl13	H14	H15	H16	H17	O18	C19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.67	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-8.09	41.95	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	0.46	-1.69	-2.94	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-8.07	21.71	26.60	-2.93	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-12.12	23.14	20.71	-1.60	39.76	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	7.13	-11.41	-7.47	0.44	-7.44	-10.86	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	4.44	-27.77	-14.79	0.61	-8.06	-8.33	4.90	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	4.67	-28.81	-15.30	0.78	-9.90	-10.87	5.20	8.93	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.96	-14.83	-31.20	1.05	-9.79	-7.82	3.03	6.41	6.65	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	3.69	-14.91	-30.96	1.06	-12.16	-9.20	3.44	6.43	5.42	9.65	-	-	-	-	-	-	-	-	-	-	-	-
Cl12	-0.29	1.02	1.62	-0.16	1.61	0.97	-0.30	-0.43	-0.48	-0.76	-0.79	-	-	-	-	-	-	-	-	-	-	-
Cl13	-0.65	2.44	3.03	-0.30	3.02	2.31	-0.70	-0.93	-1.44	-1.46	-1.13	0.18	-	-	-	-	-	-	-	-	-	-
H14	2.95	-8.20	-9.79	1.05	-30.99	-14.08	3.02	3.22	4.02	4.00	4.52	-0.76	-1.45	-	-	-	-	-	-	-	-	-
H15	3.78	-9.90	-12.50	1.09	-31.71	-14.60	3.52	3.94	4.27	4.66	6.76	-0.81	-1.16	9.88	-	-	-	-	-	-	-	-
H16	4.65	-9.09	-8.40	0.63	-15.28	-27.36	5.08	3.63	4.32	3.35	4.01	-0.44	-0.96	6.58	6.91	-	-	-	-	-	-	-
H17	4.54	-11.03	-9.58	0.76	-14.81	-26.66	5.05	4.04	6.14	3.89	4.03	-0.47	-1.38	6.47	5.42	8.91	-	-	-	-	-	-
O18	-19.03	34.64	30.09	-1.70	30.69	34.27	-16.69	-15.42	-13.01	-11.33	-16.86	1.22	2.26	-11.54	-17.78	-17.09	-12.89	-	-	-	-	-
C19	-4.17	10.49	9.01	-0.48	7.71	8.09	-4.83	-5.74	-4.10	-3.72	-5.17	0.37	0.68	-3.13	-4.36	-4.15	-3.48	30.82	-	-	-	-
H20	2.86	-7.17	-5.73	0.31	-5.02	-5.58	4.03	4.06	3.00	2.45	3.05	-0.24	-0.48	2.10	2.70	2.92	2.53	-15.61	-10.82	-	-	-
H21	2.65	-6.85	-6.46	0.36	-5.97	-5.96	3.14	3.63	2.83	2.75	3.80	-0.30	-0.52	2.51	3.51	3.22	2.59	-18.83	-12.81	5.85	-	-
H22	2.60	-8.19	-7.35	0.36	-5.31	-5.23	2.92	5.07	3.11	3.14	4.39	-0.28	-0.51	2.16	2.97	2.56	2.33	-15.24	-10.64	4.88	5.76	-

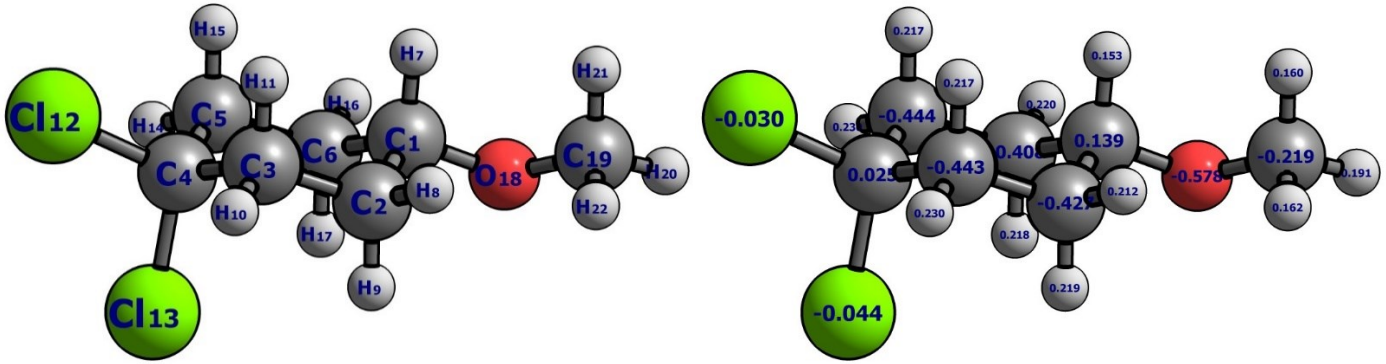

Table S12. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 4eq.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	Cl12	Cl13	H14	H15	H16	H17	O18	C19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.92	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-8.14	41.08	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	0.39	-1.38	-2.38	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-8.15	21.34	25.88	-2.38	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-12.43	23.08	20.45	-1.32	39.45	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	6.42	-10.08	-8.12	0.38	-8.12	-9.65	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	4.53	-27.57	-14.58	0.50	-7.95	-8.32	4.36	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	4.72	-28.37	-14.84	0.63	-9.62	-10.71	3.65	8.74	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	3.06	-14.96	-31.04	0.88	-9.80	-7.94	3.09	6.49	6.66	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	3.61	-14.24	-29.19	0.84	-11.53	-8.84	4.27	6.21	5.14	9.41	-	-	-	-	-	-	-	-	-	-	-	-
Cl12	-0.30	1.03	1.62	-0.14	1.63	0.99	-0.33	-0.43	-0.48	-0.79	-0.77	-	-	-	-	-	-	-	-	-	-	-
Cl13	-0.53	1.93	2.37	-0.20	2.38	1.85	-0.49	-0.74	-1.12	-1.17	-0.86	0.15	-	-	-	-	-	-	-	-	-	-
H14	3.07	-8.30	-9.79	0.88	-31.15	-14.36	3.09	3.27	4.02	4.12	4.42	-0.79	-1.18	-	-	-	-	-	-	-	-	-
H15	3.59	-9.19	-11.48	0.84	-29.22	-13.61	4.24	3.68	3.92	4.40	6.06	-0.77	-0.86	9.41	-	-	-	-	-	-	-	-
H16	4.74	-9.03	-8.24	0.52	-15.02	-27.34	4.54	3.61	4.25	3.38	3.83	-0.45	-0.76	6.67	6.38	-	-	-	-	-	-	-
H17	4.74	-11.19	-9.62	0.63	-14.88	-27.14	3.65	4.09	6.15	4.01	3.93	-0.48	-1.12	6.68	5.13	9.06	-	-	-	-	-	-
O18	-18.97	33.48	22.50	-1.12	22.89	33.32	-14.31	-14.78	-15.82	-9.58	-10.15	0.97	1.77	-9.77	-10.26	-16.32	-16.35	-	-	-	-	-
C19	-4.27	10.38	7.33	-0.34	6.62	8.12	-4.31	-5.62	-4.81	-3.29	-3.46	0.32	0.55	-2.90	-3.13	-4.13	-4.03	29.89	-	-	-	-
H20	2.70	-6.79	-5.18	0.25	-4.94	-5.96	2.76	3.56	3.34	2.38	2.45	-0.24	-0.42	2.24	2.33	3.19	3.08	-18.20	-12.77	-	-	-
H21	2.87	-6.90	-5.27	0.24	-4.75	-5.53	3.53	3.85	2.98	2.35	2.64	-0.23	-0.37	2.07	2.36	2.89	2.60	-14.88	-10.64	5.73	-	-
H22	2.71	-8.23	-5.63	0.25	-4.56	-5.29	2.66	5.05	3.95	2.62	2.60	-0.23	-0.41	2.00	2.13	2.57	2.73	-14.93	-10.76	5.80	4.84	-

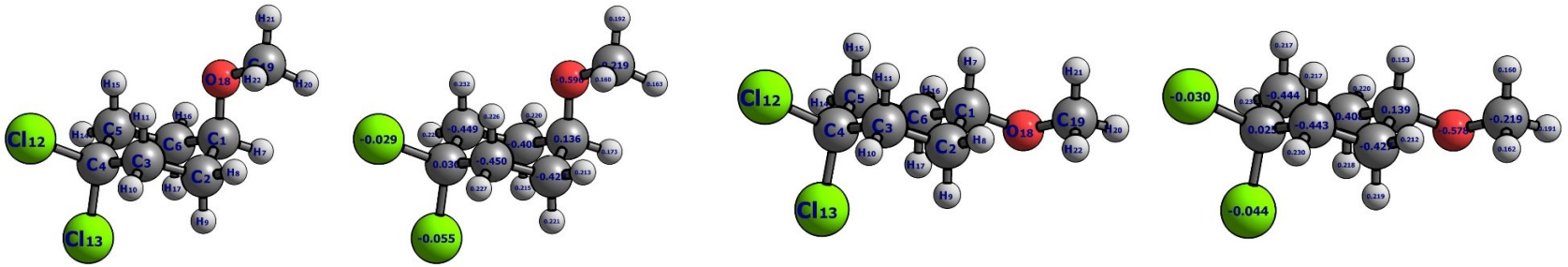

Table S13. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 4. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	Cl12	Cl13	H14	H15	H16	H17	O18	C19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	0.25	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	0.05	0.87	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	0.07	-0.31	-0.56	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	0.08	0.37	0.72	-0.55	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	0.31	0.06	0.26	-0.28	0.31	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	0.71	-1.33	0.65	0.06	0.68	-1.21	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	-0.09	-0.20	-0.21	0.11	-0.11	-0.01	0.54	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	-0.05	-0.44	-0.46	0.15	-0.28	-0.16	1.55	0.19	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	-0.10	0.13	-0.16	0.17	0.01	0.12	-0.06	-0.08	-0.01	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	0.08	-0.67	-1.77	0.22	-0.63	-0.36	-0.83	0.22	0.28	0.24	-	-	-	-	-	-	-	-	-	-	-	-
Cl12	0.01	-0.01	0.00	-0.02	-0.02	-0.02	0.03	0.00	0.00	0.03	-0.02	-	-	-	-	-	-	-	-	-	-	-
Cl13	-0.12	0.51	0.66	-0.10	0.64	0.46	-0.21	-0.19	-0.32	-0.29	-0.27	0.03	-	-	-	-	-	-	-	-	-	-
H14	-0.12	0.10	0.00	0.17	0.16	0.28	-0.07	-0.05	0.00	-0.12	0.10	0.03	-0.27	-	-	-	-	-	-	-	-	-
H15	0.19	-0.71	-1.02	0.25	-2.49	-0.99	-0.72	0.26	0.35	0.26	0.70	-0.04	-0.30	0.47	-	-	-	-	-	-	-	-
H16	-0.09	-0.06	-0.16	0.11	-0.26	-0.02	0.54	0.02	0.07	-0.03	0.18	0.01	-0.20	-0.09	0.53	-	-	-	-	-	-	-
H17	-0.20	0.16	0.04	0.13	0.07	0.48	1.40	-0.05	-0.01	-0.12	0.10	0.01	-0.26	-0.21	0.29	-0.15	-	-	-	-	-	-
O18	-0.06	1.16	7.59	-0.58	7.80	0.95	-2.38	-0.64	2.81	-1.75	-6.71	0.25	0.49	-1.77	-7.52	-0.77	3.46	-	-	-	-	-
C19	0.10	0.11	1.68	-0.14	1.09	-0.03	-0.52	-0.12	0.71	-0.43	-1.71	0.05	0.13	-0.23	-1.23	-0.02	0.55	0.93	-	-	-	-
H20	0.16	-0.38	-0.55	0.06	-0.08	0.38	1.27	0.50	-0.34	0.07	0.60	0.00	-0.06	-0.14	0.37	-0.27	-0.55	2.59	1.95	-	-	-
H21	-0.22	0.05	-1.19	0.12	-1.22	-0.43	-0.39	-0.22	-0.15	0.40	1.16	-0.07	-0.15	0.44	1.15	0.33	-0.01	-3.95	-2.17	0.12	-	-
H22	-0.11	0.04	-1.72	0.11	-0.75	0.06	0.26	0.02	-0.84	0.52	1.79	-0.05	-0.10	0.16	0.84	-0.01	-0.40	-0.31	0.12	-0.92	0.92	-

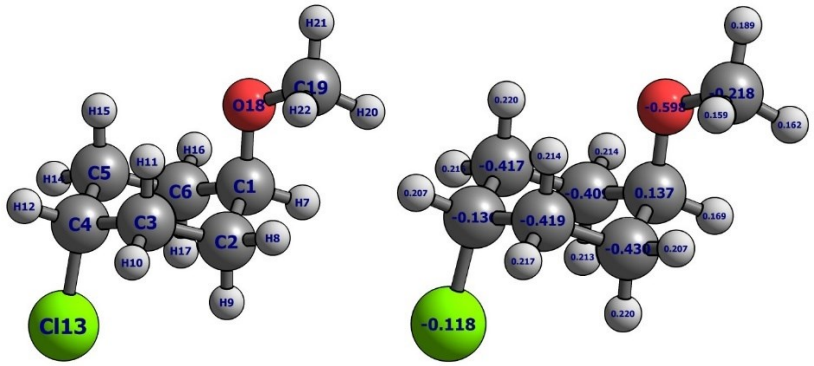

Table S14. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 5ax.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	H12	Cl13	H14	H15	H16	H17	O18	C19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.78	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-7.56	39.20	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-2.09	7.68	12.41	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-7.53	20.27	23.00	12.37	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-12.22	23.33	19.35	7.29	37.13	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	7.01	-11.21	-6.80	-1.93	-6.77	-10.67	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	4.34	-27.12	-13.33	-2.69	-7.28	-8.14	4.67	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	4.67	-28.71	-14.16	-3.53	-9.17	-10.87	5.05	8.62	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.84	-14.27	-27.68	-4.54	-8.67	-7.49	2.83	5.96	6.33	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	3.51	-14.20	-27.20	-4.56	-10.66	-8.73	3.19	5.91	5.10	8.74	-	-	-	-	-	-	-	-	-	-	-	-
H12	2.40	-8.53	-13.35	-8.60	-13.30	-8.11	2.34	3.32	3.97	5.98	6.06	-	-	-	-	-	-	-	-	-	-	-
Cl13	-1.38	5.17	5.98	2.91	5.95	4.90	-1.44	-1.92	-3.01	-2.96	-2.27	-3.47	-	-	-	-	-	-	-	-	-	-
H14	2.83	-7.87	-8.68	-4.53	-27.48	-13.55	2.83	2.99	3.82	3.63	4.07	5.96	-2.95	-	-	-	-	-	-	-	-	-
H15	3.60	-9.40	-10.98	-4.69	-27.89	-13.93	3.27	3.62	4.02	4.20	6.02	6.24	-2.33	8.96	-	-	-	-	-	-	-	-
H16	4.54	-8.88	-7.59	-2.78	-13.76	-26.73	4.85	3.44	4.18	3.11	3.68	3.44	-1.98	6.12	6.37	-	-	-	-	-	-	-
H17	4.52	-11.01	-8.86	-3.39	-13.68	-26.53	4.90	3.90	6.08	3.69	3.78	3.83	-2.88	6.15	5.10	8.60	-	-	-	-	-	-
O18	-19.14	34.88	28.05	7.71	28.56	34.49	-16.40	-15.02	-12.96	-10.86	-16.00	-9.72	4.80	-11.05	-16.87	-16.64	-12.82	-	-	-	-	-
C19	-4.17	10.52	8.37	2.16	7.14	8.10	-4.72	-5.57	-4.06	-3.55	-4.89	-2.86	1.44	-2.98	-4.12	-4.02	-3.44	30.86	-	-	-	-
H20	2.86	-7.17	-5.31	-1.41	-4.65	-5.58	3.94	3.93	2.97	2.34	2.88	1.86	-1.01	2.00	2.55	2.82	2.49	-15.58	-10.74	-	-	-
H21	2.63	-6.79	-5.93	-1.62	-5.47	-5.91	3.03	3.48	2.78	2.60	3.55	2.24	-1.10	2.36	3.28	3.09	2.54	-18.65	-12.62	5.75	-	-
H22	2.60	-8.21	-6.82	-1.61	-4.91	-5.23	2.85	4.91	3.08	2.99	4.16	2.17	-1.07	2.05	2.79	2.48	2.31	-15.22	-10.56	4.83	5.66	-

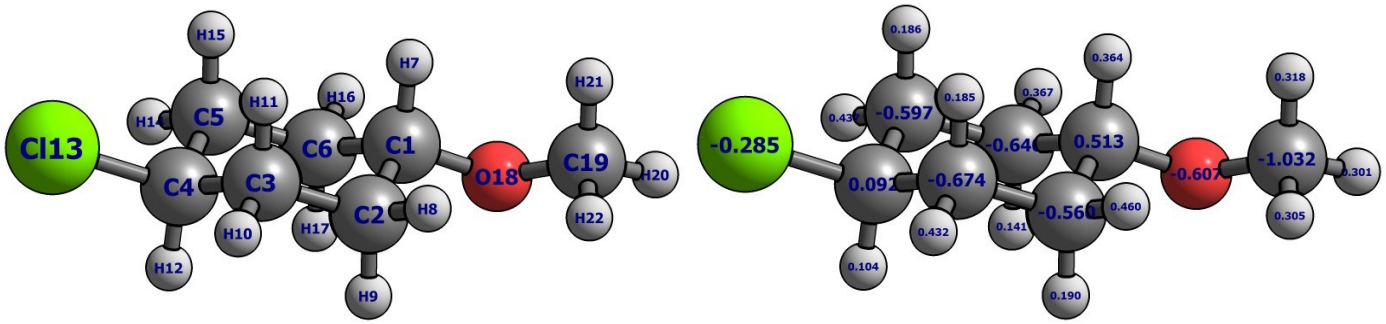

Table S15. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 5eq.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	H12	Cl13	H14	H15	H16	H17	O18	C19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.62	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-7.47	37.54	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-2.33	8.32	13.38	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-7.48	19.56	22.39	13.41	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-12.12	22.43	18.72	7.97	36.02	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	6.45	-10.08	-7.62	-2.30	-7.63	-9.65	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	4.43	-26.90	-13.32	-3.02	-7.31	-8.11	4.37	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	4.36	-25.93	-12.79	-3.62	-8.31	-9.82	3.44	8.05	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.88	-14.05	-27.35	-5.02	-8.64	-7.43	2.98	6.11	5.88	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	3.36	-13.20	-25.52	-4.74	-10.14	-8.22	4.06	5.75	4.49	8.44	-	-	-	-	-	-	-	-	-	-	-	-
H12	2.72	-9.98	-12.62	-9.03	-12.65	-9.57	2.56	3.68	5.13	5.84	4.45	-	-	-	-	-	-	-	-	-	-	-
Cl13	-0.88	3.00	4.43	2.42	4.43	2.87	-0.96	-1.26	-1.34	-2.21	-2.09	-2.50	-	-	-	-	-	-	-	-	-	-
H14	2.89	-7.77	-8.64	-5.03	-27.46	-13.48	2.98	3.07	3.55	3.70	3.96	5.86	-2.21	-	-	-	-	-	-	-	-	-
H15	3.34	-8.55	-10.09	-4.73	-25.54	-12.61	4.03	3.43	3.44	3.95	5.42	4.44	-2.08	8.44	-	-	-	-	-	-	-	-
H16	4.65	-8.81	-7.57	-3.12	-13.73	-26.67	4.55	3.54	3.92	3.18	3.57	3.81	-1.30	6.29	5.90	-	-	-	-	-	-	-
H17	4.37	-10.27	-8.31	-3.62	-12.82	-24.79	3.44	3.77	5.34	3.55	3.45	5.14	-1.34	5.89	4.48	8.34	-	-	-	-	-	-
O18	-18.85	33.17	20.96	6.83	21.33	32.95	-14.58	-14.72	-14.81	-9.16	-9.58	-8.72	2.87	-9.34	-9.68	-16.26	-15.30	-	-	-	-	-
C19	-4.22	10.20	6.78	2.08	6.13	7.99	-4.37	-5.55	-4.46	-3.12	-3.24	-2.64	0.93	-2.75	-2.93	-4.09	-3.75	29.99	-	-	-	-
H20	2.66	-6.64	-4.77	-1.53	-4.55	-5.83	2.78	3.50	3.09	2.25	2.28	1.99	-0.71	2.12	2.18	3.14	2.84	-18.18	-12.67	-	-	-
H21	2.84	-6.79	-4.88	-1.48	-4.42	-5.46	3.59	3.80	2.77	2.23	2.48	1.82	-0.68	1.97	2.22	2.87	2.42	-14.98	-10.64	5.70	-	-
H22	2.67	-8.06	-5.19	-1.52	-4.21	-5.19	2.69	4.98	3.65	2.48	2.43	1.96	-0.69	1.89	1.99	2.54	2.52	-14.93	-10.69	5.73	4.83	-

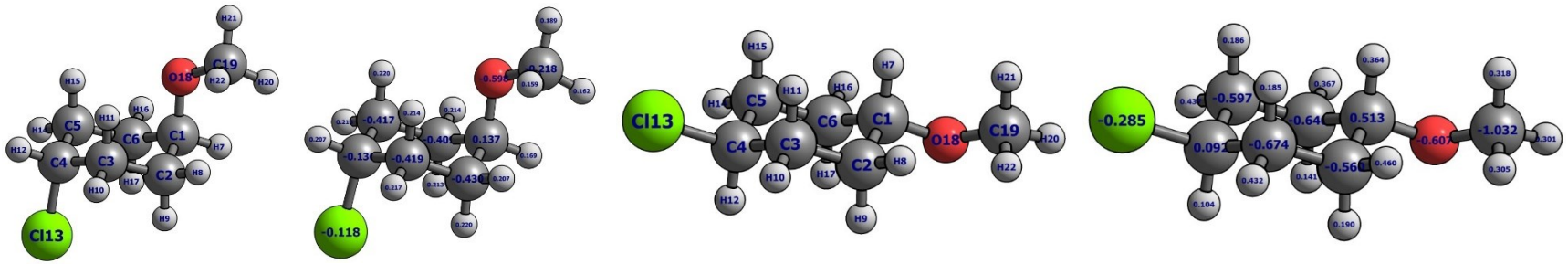

Table S16. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 5. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	H12	Cl13	H14	H15	H16	H17	O18	C19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-0.16	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-0.09	1.66	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	0.24	-0.64	-0.97	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-0.05	0.71	0.61	-1.04	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-0.10	0.90	0.63	-0.68	1.11	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	0.56	-1.13	0.82	0.37	0.86	-1.02	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	-0.09	-0.22	-0.01	0.33	0.03	-0.03	0.30	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	0.31	-2.78	-1.37	0.09	-0.86	-1.05	1.61	0.57	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	-0.04	-0.22	-0.33	0.48	-0.03	-0.06	-0.15	-0.15	0.45	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	0.15	-1.00	-1.68	0.18	-0.52	-0.51	-0.87	0.16	0.61	0.30	-	-	-	-	-	-	-	-	-	-	-	-
H12	-0.32	1.45	-0.73	0.43	-0.65	1.46	-0.22	-0.36	-1.16	0.14	1.61	-	-	-	-	-	-	-	-	-	-	-
Cl13	-0.50	2.17	1.55	0.49	1.52	2.03	-0.48	-0.66	-1.67	-0.75	-0.18	-0.97	-	-	-	-	-	-	-	-	-	-
H14	-0.06	-0.10	-0.04	0.50	-0.02	-0.07	-0.15	-0.08	0.27	-0.07	0.11	0.10	-0.74	-	-	-	-	-	-	-	-	-
H15	0.26	-0.85	-0.89	0.04	-2.35	-1.32	-0.76	0.19	0.58	0.25	0.60	1.80	-0.25	0.52	-	-	-	-	-	-	-	-
H16	-0.11	-0.07	-0.02	0.34	-0.03	-0.06	0.30	-0.10	0.26	-0.07	0.11	-0.37	-0.68	-0.17	0.47	-	-	-	-	-	-	-
H17	0.15	-0.74	-0.55	0.23	-0.86	-1.74	1.46	0.13	0.74	0.14	0.33	-1.31	-1.54	0.26	0.62	0.26	-	-	-	-	-	-
O18	-0.29	1.71	7.09	0.88	7.23	1.54	-1.82	-0.30	1.85	-1.70	-6.42	-1.00	1.93	-1.71	-7.19	-0.38	2.48	-	-	-	-	-
C19	0.05	0.32	1.59	0.08	1.01	0.11	-0.35	-0.02	0.40	-0.43	-1.65	-0.22	0.51	-0.23	-1.19	0.07	0.31	0.87	-	-	-	-
H20	0.20	-0.53	-0.54	0.12	-0.10	0.25	1.16	0.43	-0.12	0.09	0.60	-0.13	-0.30	-0.12	0.37	-0.32	-0.35	2.60	1.93	-	-	-
H21	-0.21	0.00	-1.05	-0.14	-1.05	-0.45	-0.56	-0.32	0.01	0.37	1.07	0.42	-0.42	0.39	1.06	0.22	0.12	-3.67	-1.98	0.05	-	-
H22	-0.07	-0.15	-1.63	-0.09	-0.70	-0.04	0.16	-0.07	-0.57	0.51	1.73	0.21	-0.38	0.16	0.80	-0.06	-0.21	-0.29	0.13	-0.90	0.83	-

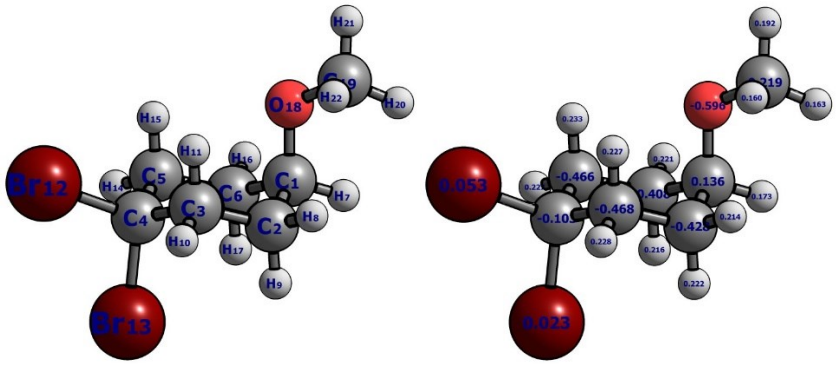

Table S17. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 6ax.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	Br12	Br13	H14	H15	H16	H17	O18	C19	H20	H21	H22
C1		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.62	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-8.36	43.55	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-1.57	5.79	10.47	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-8.34	22.55	28.67	10.45	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-12.08	23.19	21.53	5.51	41.33	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	7.12	-11.45	-7.77	-1.50	-7.74	-10.91	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	4.44	-27.89	-15.43	-2.10	-8.40	-8.38	4.92	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	4.66	-28.90	-15.91	-2.69	-10.29	-10.89	5.23	8.98	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.95	-14.89	-32.50	-3.61	-10.18	-7.85	3.05	6.47	6.68	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	3.69	-15.03	-32.29	-3.67	-12.70	-9.27	3.47	6.51	5.47	9.74	-	-	-	-	-	-	-	-	-	-	-	-
Br12	0.51	-1.78	-2.90	-0.92	-2.89	-1.69	0.53	0.76	0.84	1.33	1.39	-	-	-	-	-	-	-	-	-	-	-
Br13	0.27	-1.00	-1.27	-0.40	-1.26	-0.95	0.29	0.39	0.59	0.59	0.46	0.13	-	-	-	-	-	-	-	-	-	-
H14	2.95	-8.23	-10.18	-3.60	-32.29	-14.15	3.04	3.25	4.03	4.01	4.56	1.33	0.59	-	-	-	-	-	-	-	-	-
H15	3.79	-9.97	-13.05	-3.77	-33.08	-14.72	3.56	3.99	4.30	4.69	6.84	1.42	0.47	9.97	-	-	-	-	-	-	-	-
H16	4.65	-9.13	-8.76	-2.18	-15.94	-27.51	5.11	3.66	4.34	3.38	4.05	0.78	0.40	6.64	6.99	-	-	-	-	-	-	-
H17	4.53	-11.06	-9.98	-2.60	-15.42	-26.79	5.08	4.06	6.16	3.91	4.06	0.82	0.57	6.51	5.46	8.98	-	-	-	-	-	-
O18	-18.94	34.67	31.20	5.81	31.84	34.32	-16.73	-15.50	-13.04	-11.36	-16.96	-2.17	-0.93	-11.58	-17.90	-17.18	-12.94	-	-	-	-	-
C19	-4.15	10.48	9.33	1.63	8.00	8.10	-4.85	-5.76	-4.10	-3.73	-5.18	-0.66	-0.28	-3.14	-4.38	-4.17	-3.49	30.81	-	-	-	-
H20	2.85	-7.16	-5.93	-1.07	-5.22	-5.60	4.05	4.06	3.01	2.46	3.06	0.43	0.20	2.11	2.72	2.94	2.54	-15.61	-10.82	-	-	-
H21	2.64	-6.85	-6.70	-1.24	-6.20	-5.98	3.15	3.64	2.84	2.76	3.82	0.54	0.22	2.52	3.53	3.24	2.60	-18.84	-12.82	5.85	-	-
H22	2.59	-8.19	-7.60	-1.22	-5.51	-5.24	2.94	5.10	3.12	3.14	4.39	0.51	0.21	2.16	2.98	2.58	2.34	-15.24	-10.64	4.88	5.76	-

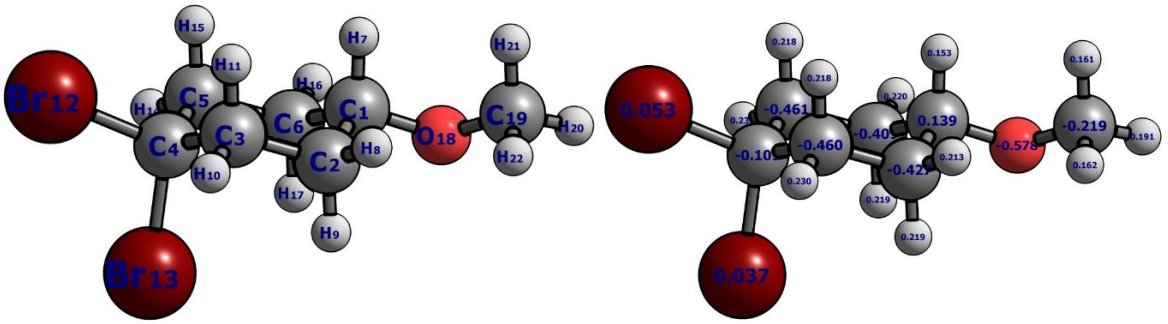

Table S18. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 6eq.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	Br12	Br13	H14	H15	H16	H17	O18	C19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.89	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-8.42	42.70	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-1.71	6.13	10.98	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-8.43	22.19	27.90	10.99	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-12.41	23.16	21.27	5.89	41.00	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	6.40	-10.11	-8.45	-1.68	-8.44	-9.68	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	4.53	-27.71	-15.21	-2.24	-8.29	-8.36	4.39	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	4.72	-28.49	-15.44	-2.81	-10.00	-10.75	3.66	8.80	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	3.06	-15.03	-32.33	-3.89	-10.18	-7.97	3.11	6.55	6.68	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	3.61	-14.33	-30.41	-3.75	-12.02	-8.90	4.30	6.28	5.17	9.47	-	-	-	-	-	-	-	-	-	-	-	-
Br12	0.52	-1.77	-2.85	-0.98	-2.85	-1.69	0.56	0.75	0.83	1.34	1.33	-	-	-	-	-	-	-	-	-	-	-
Br13	0.43	-1.56	-1.96	-0.68	-1.96	-1.49	0.40	0.60	0.91	0.95	0.70	0.20	-	-	-	-	-	-	-	-	-	-
H14	3.06	-8.32	-10.18	-3.90	-32.43	-14.42	3.11	3.29	4.03	4.12	4.44	1.34	0.95	-	-	-	-	-	-	-	-	-
H15	3.60	-9.25	-11.98	-3.74	-30.44	-13.71	4.27	3.72	3.95	4.43	6.11	1.33	0.70	9.48	-	-	-	-	-	-	-	-
H16	4.74	-9.07	-8.59	-2.31	-15.66	-27.48	4.56	3.64	4.27	3.40	3.86	0.78	0.62	6.73	6.45	-	-	-	-	-	-	-
H17	4.73	-11.23	-10.01	-2.82	-15.47	-27.27	3.66	4.11	6.17	4.03	3.96	0.83	0.91	6.70	5.17	9.12	-	-	-	-	-	-
O18	-18.89	33.52	23.35	4.95	23.75	33.36	-14.33	-14.82	-15.86	-9.60	-10.19	-1.67	-1.45	-9.80	-10.31	-16.37	-16.40	-	-	-	-	-
C19	-4.26	10.41	7.61	1.53	6.87	8.14	-4.32	-5.64	-4.83	-3.30	-3.48	-0.55	-0.45	-2.90	-3.14	-4.15	-4.05	29.88	-	-	-	-
H20	2.69	-6.80	-5.38	-1.13	-5.13	-5.97	2.77	3.58	3.36	2.39	2.46	0.42	0.35	2.25	2.34	3.20	3.09	-18.20	-12.78	-	-	-
H21	2.86	-6.91	-5.48	-1.08	-4.93	-5.54	3.53	3.87	2.99	2.35	2.66	0.41	0.30	2.07	2.37	2.90	2.61	-14.88	-10.65	5.74	-	-
H22	2.70	-8.25	-5.85	-1.12	-4.73	-5.31	2.66	5.07	3.97	2.63	2.61	0.41	0.34	2.01	2.14	2.58	2.74	-14.93	-10.76	5.80	4.85	-

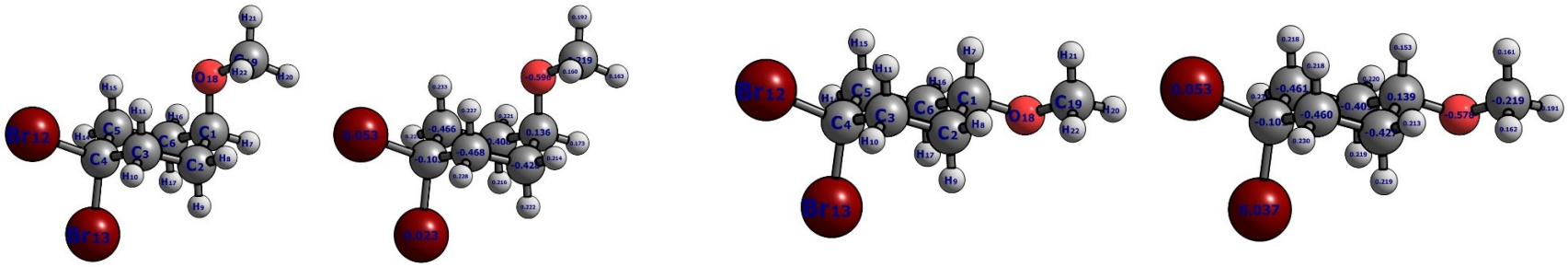

Table S19. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 6. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	Br12	Br13	H14	H15	H16	H17	O18	C19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	0.27	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	0.06	0.85	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	0.14	-0.34	-0.51	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	0.09	0.36	0.77	-0.54	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	0.33	0.03	0.26	-0.38	0.33	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	0.72	-1.34	0.68	0.18	0.70	-1.23	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	-0.09	-0.18	-0.22	0.14	-0.11	-0.02	0.53	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	-0.06	-0.41	-0.47	0.12	-0.29	-0.14	1.57	0.18	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	-0.11	0.14	-0.17	0.28	0.00	0.12	-0.06	-0.08	0.00	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	0.08	-0.70	-1.88	0.08	-0.68	-0.37	-0.83	0.23	0.30	0.27	-	-	-	-	-	-	-	-	-	-	-	-
Br12	-0.01	-0.01	-0.05	0.06	-0.04	0.00	-0.03	0.01	0.01	-0.01	0.06	-	-	-	-	-	-	-	-	-	-	-
Br13	-0.16	0.56	0.69	0.28	0.70	0.54	-0.11	-0.21	-0.32	-0.36	-0.24	-0.07	-	-	-	-	-	-	-	-	-	-
H14	-0.11	0.09	0.00	0.30	0.14	0.27	-0.07	-0.04	0.00	-0.11	0.12	-0.01	-0.36	-	-	-	-	-	-	-	-	-
H15	0.19	-0.72	-1.07	-0.03	-2.64	-1.01	-0.71	0.27	0.35	0.26	0.73	0.09	-0.23	0.49	-	-	-	-	-	-	-	-
H16	-0.09	-0.06	-0.17	0.13	-0.28	-0.03	0.55	0.02	0.07	-0.02	0.19	0.00	-0.22	-0.09	0.54	-	-	-	-	-	-	-
H17	-0.20	0.17	0.03	0.22	0.05	0.48	1.42	-0.05	-0.01	-0.12	0.10	-0.01	-0.34	-0.19	0.29	-0.14	-	-	-	-	-	-
O18	-0.05	1.15	7.85	0.86	8.09	0.96	-2.40	-0.68	2.82	-1.76	-6.77	-0.50	0.52	-1.78	-7.59	-0.81	3.46	-	-	-	-	-
C19	0.11	0.07	1.72	0.10	1.13	-0.04	-0.53	-0.12	0.73	-0.43	-1.70	-0.11	0.17	-0.24	-1.24	-0.02	0.56	0.93	-	-	-	-
H20	0.16	-0.36	-0.55	0.06	-0.09	0.37	1.28	0.48	-0.35	0.07	0.60	0.01	-0.15	-0.14	0.38	-0.26	-0.55	2.59	1.96	-	-	-
H21	-0.22	0.06	-1.22	-0.16	-1.27	-0.44	-0.38	-0.23	-0.15	0.41	1.16	0.13	-0.08	0.45	1.16	0.34	-0.01	-3.96	-2.17	0.11	-	-
H22	-0.11	0.06	-1.75	-0.10	-0.78	0.07	0.28	0.03	-0.85	0.51	1.78	0.10	-0.13	0.15	0.84	0.00	-0.40	-0.31	0.12	-0.92	0.91	-

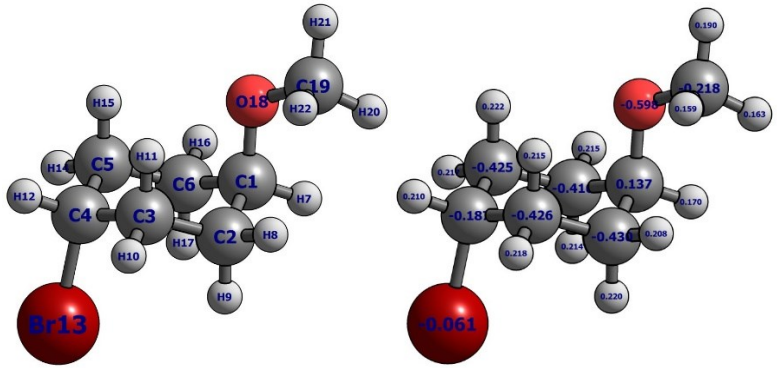

Table S20. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 7ax.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	H12	Br13	H14	H15	H16	H17	O18	C19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.79	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-7.70	39.97	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-2.88	10.60	17.45	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-7.67	20.66	23.85	17.39	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-12.23	23.37	19.72	10.06	37.87	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	7.02	-11.25	-6.94	-2.67	-6.91	-10.71	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	4.35	-27.22	-13.61	-3.72	-7.43	-8.17	4.69	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	4.68	-28.81	-14.45	-4.87	-9.36	-10.89	5.08	8.67	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.85	-14.37	-28.36	-6.29	-8.88	-7.54	2.86	6.02	6.37	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	3.53	-14.33	-27.87	-6.35	-10.93	-8.81	3.22	5.98	5.15	8.85	-	-	-	-	-	-	-	-	-	-	-	-
H12	2.43	-8.66	-13.79	-12.07	-13.74	-8.24	2.39	3.38	4.04	6.10	6.20	-	-	-	-	-	-	-	-	-	-	-
Br13	-0.69	2.60	3.02	1.93	3.00	2.46	-0.74	-0.98	-1.52	-1.49	-1.15	-1.74	-	-	-	-	-	-	-	-	-	-
H14	2.85	-7.92	-8.89	-6.28	-28.16	-13.65	2.85	3.02	3.85	3.67	4.12	6.08	-1.49	-	-	-	-	-	-	-	-	-
H15	3.63	-9.49	-11.27	-6.53	-28.59	-14.06	3.31	3.66	4.06	4.25	6.11	6.38	-1.18	9.08	-	-	-	-	-	-	-	-
H16	4.56	-8.91	-7.75	-3.85	-14.06	-26.83	4.87	3.46	4.20	3.14	3.72	3.50	-1.00	6.18	6.45	-	-	-	-	-	-	-
H17	4.53	-11.03	-9.04	-4.69	-13.96	-26.63	4.92	3.92	6.10	3.71	3.82	3.90	-1.46	6.20	5.15	8.64	-	-	-	-	-	-
O18	-19.13	34.92	28.56	10.65	29.09	34.53	-16.44	-15.07	-12.99	-10.92	-16.14	-9.87	2.43	-11.12	-17.02	-16.70	-12.86	-	-	-	-	-
C19	-4.17	10.53	8.52	2.98	7.28	8.12	-4.74	-5.59	-4.07	-3.58	-4.93	-2.91	0.74	-3.00	-4.15	-4.04	-3.46	30.88	-	-	-	-
H20	2.86	-7.20	-5.41	-1.94	-4.74	-5.59	3.95	3.96	2.98	2.36	2.90	1.89	-0.51	2.01	2.57	2.84	2.51	-15.60	-10.76	-	-	-
H21	2.63	-6.81	-6.05	-2.24	-5.58	-5.92	3.04	3.49	2.79	2.62	3.58	2.27	-0.56	2.38	3.31	3.10	2.55	-18.67	-12.64	5.76	-	-
H22	2.60	-8.21	-6.94	-2.23	-5.01	-5.24	2.86	4.92	3.08	3.01	4.19	2.20	-0.55	2.07	2.82	2.49	2.31	-15.23	-10.57	4.84	5.66	-

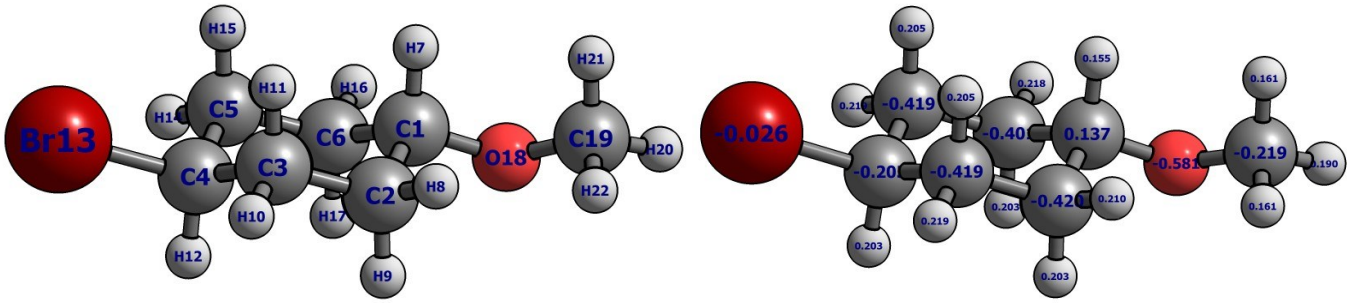

Table S21. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 7eq.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	H12	Br13	H14	H15	H16	H17	O18	C19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.53	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-7.57	38.11	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-3.19	11.44	18.80	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-7.59	19.86	23.21	18.83	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-12.04	22.32	19.02	10.97	36.57	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	6.42	-10.06	-7.77	-3.18	-7.78	-9.63	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	4.42	-26.87	-13.59	-4.17	-7.45	-8.11	4.38	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	4.34	-25.89	-13.03	-4.99	-8.47	-9.81	3.45	8.07	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.88	-14.08	-27.98	-6.94	-8.83	-7.44	3.00	6.15	5.91	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	3.35	-13.20	-26.07	-6.54	-10.34	-8.21	4.07	5.78	4.51	8.49	-	-	-	-	-	-	-	-	-	-	-	-
H12	2.76	-10.13	-13.09	-12.70	-13.11	-9.70	2.60	3.75	5.22	5.97	4.54	-	-	-	-	-	-	-	-	-	-	-
Br13	-0.25	0.86	1.28	0.91	1.28	0.82	-0.28	-0.37	-0.39	-0.64	-0.60	-0.72	-	-	-	-	-	-	-	-	-	-
H14	2.89	-7.78	-8.83	-6.95	-28.08	-13.50	3.00	3.09	3.56	3.73	3.98	5.99	-0.64	-	-	-	-	-	-	-	-	-
H15	3.34	-8.54	-10.29	-6.53	-26.08	-12.61	4.05	3.45	3.45	3.97	5.43	4.53	-0.60	8.49	-	-	-	-	-	-	-	-
H16	4.64	-8.81	-7.72	-4.31	-14.01	-26.65	4.56	3.55	3.93	3.20	3.58	3.88	-0.38	6.33	5.93	-	-	-	-	-	-	-
H17	4.35	-10.26	-8.47	-5.00	-13.06	-24.74	3.44	3.78	5.35	3.56	3.46	5.23	-0.39	5.92	4.50	8.36	-	-	-	-	-	-
O18	-18.75	33.07	21.34	9.41	21.71	32.86	-14.58	-14.74	-14.82	-9.19	-9.60	-8.86	0.83	-9.37	-9.70	-16.28	-15.30	-	-	-	-	-
C19	-4.20	10.17	6.90	2.87	6.24	7.97	-4.37	-5.55	-4.46	-3.13	-3.25	-2.69	0.27	-2.76	-2.94	-4.10	-3.75	29.99	-	-	-	-
H20	2.65	-6.63	-4.86	-2.11	-4.64	-5.82	2.79	3.51	3.09	2.26	2.29	2.02	-0.21	2.13	2.18	3.15	2.85	-18.18	-12.69	-	-	-
H21	2.83	-6.77	-4.97	-2.04	-4.50	-5.45	3.59	3.80	2.77	2.24	2.49	1.85	-0.20	1.98	2.23	2.88	2.43	-14.99	-10.65	5.71	-	-
H22	2.66	-8.04	-5.28	-2.10	-4.28	-5.17	2.69	4.99	3.64	2.49	2.44	2.00	-0.20	1.90	2.00	2.54	2.52	-14.93	-10.69	5.74	4.83	-

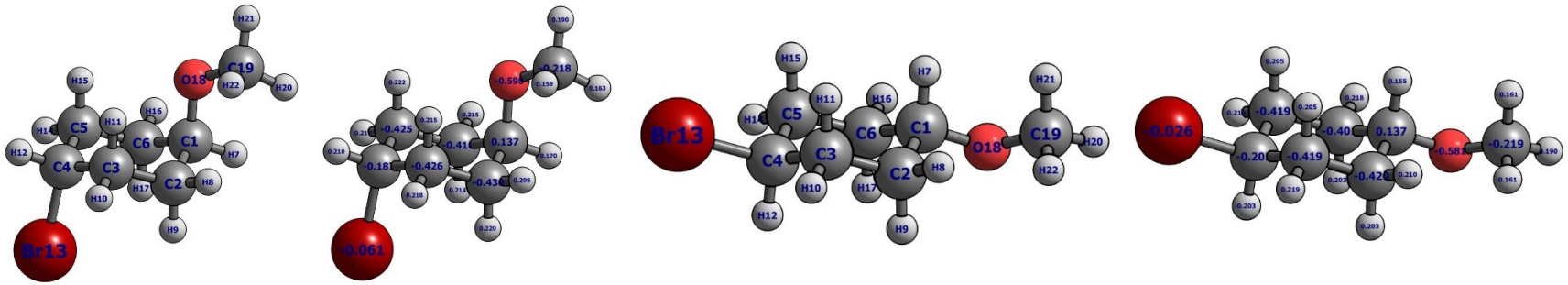

Table S22. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 7. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	H12	Br13	H14	H15	H16	H17	O18	C19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-0.26	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-0.13	1.86	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	0.31	-0.84	-1.35	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-0.08	0.80	0.64	-1.44	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-0.19	1.05	0.70	-0.91	1.30	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	0.60	-1.19	0.83	0.51	0.87	-1.08	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	-0.07	-0.35	-0.02	0.45	0.02	-0.06	0.31	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	0.34	-2.92	-1.42	0.12	-0.89	-1.08	1.63	0.60	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	-0.03	-0.29	-0.38	0.65	-0.05	-0.10	-0.14	-0.13	0.46	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	0.18	-1.13	-1.80	0.19	-0.59	-0.60	-0.85	0.20	0.64	0.36	-	-	-	-	-	-	-	-	-	-	-	-
H12	-0.33	1.47	-0.70	0.63	-0.63	1.46	-0.21	-0.37	-1.18	0.13	1.66	-	-	-	-	-	-	-	-	-	-	-
Br13	-0.44	1.74	1.74	1.02	1.72	1.64	-0.46	-0.61	-1.13	-0.85	-0.55	-1.02	-	-	-	-	-	-	-	-	-	-
H14	-0.04	-0.14	-0.06	0.67	-0.08	-0.15	-0.15	-0.07	0.29	-0.06	0.14	0.09	-0.85	-	-	-	-	-	-	-	-	-
H15	0.29	-0.95	-0.98	0.00	-2.51	-1.45	-0.74	0.21	0.61	0.28	0.68	1.85	-0.58	0.59	-	-	-	-	-	-	-	-
H16	-0.08	-0.10	-0.03	0.46	-0.05	-0.18	0.31	-0.09	0.27	-0.06	0.14	-0.38	-0.62	-0.15	0.52	-	-	-	-	-	-	-
H17	0.18	-0.77	-0.57	0.31	-0.90	-1.89	1.48	0.14	0.75	0.15	0.36	-1.33	-1.07	0.28	0.65	0.28	-	-	-	-	-	-
O18	-0.38	1.85	7.22	1.24	7.38	1.67	-1.86	-0.33	1.83	-1.73	-6.54	-1.01	1.60	-1.75	-7.32	-0.42	2.44	-	-	-	-	-
C19	0.03	0.36	1.62	0.11	1.04	0.15	-0.37	-0.04	0.39	-0.45	-1.68	-0.22	0.47	-0.24	-1.21	0.06	0.29	0.89	-	-	-	-
H20	0.21	-0.57	-0.55	0.17	-0.10	0.23	1.16	0.45	-0.11	0.10	0.61	-0.13	-0.30	-0.12	0.39	-0.31	-0.34	2.58	1.93	-	-	-
H21	-0.20	-0.04	-1.08	-0.20	-1.08	-0.47	-0.55	-0.31	0.02	0.38	1.09	0.42	-0.36	0.40	1.08	0.22	0.12	-3.68	-1.99	0.05	-	-
H22	-0.06	-0.17	-1.66	-0.13	-0.73	-0.07	0.17	-0.07	-0.56	0.52	1.75	0.20	-0.35	0.17	0.82	-0.05	-0.21	-0.30	0.12	-0.90	0.83	-

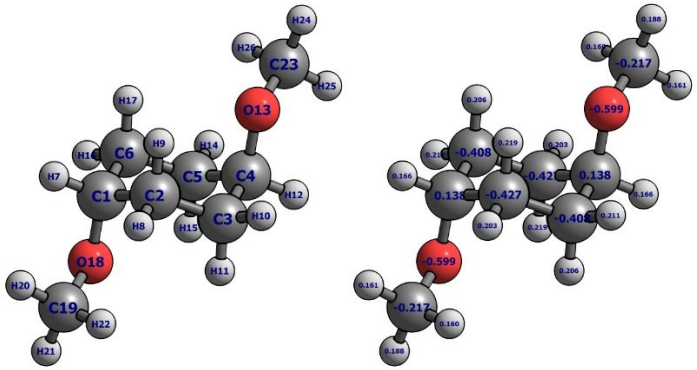

Table S23. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 8ax.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	H12	O13	H14	H15	H16	H17	O18	C19	H20	H21	H22	C23	H24	H25
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.80	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-7.42	37.82	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	2.15	-7.79	-12.28	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-7.79	20.63	23.04	-12.80	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-12.28	23.04	18.77	-7.42	37.82	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	6.94	-10.91	-6.49	1.93	-6.79	-10.42	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	4.29	-26.34	-12.67	2.68	-7.31	-7.93	4.49	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	4.70	-28.38	-13.75	3.62	-9.35	-10.77	4.94	8.40	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.79	-13.80	-26.19	4.51	-8.67	-7.27	2.71	5.67	6.16	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	3.39	-13.51	-25.51	4.42	-10.56	-8.36	3.00	5.54	4.89	8.17	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H12	1.93	-6.79	-10.42	6.94	-10.91	-6.49	1.84	2.60	3.19	4.68	4.64	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O13	-7.78	29.25	34.38	-19.31	34.58	27.18	-7.72	-10.42	-16.83	-16.40	-12.40	-16.10	-	-	-	-	-	-	-	-	-	-	-	-	-
H14	2.68	-7.31	-7.93	4.29	-26.34	-12.67	2.60	2.75	3.56	3.31	3.70	4.49	-14.72	-	-	-	-	-	-	-	-	-	-	-	-
H15	3.62	-9.35	-10.77	4.70	-28.38	-13.75	3.19	3.56	4.00	4.10	5.86	4.94	-12.91	8.40	-	-	-	-	-	-	-	-	-	-	-
H16	4.51	-8.67	-7.27	2.79	-13.80	-26.19	4.68	3.31	4.10	2.98	3.48	2.71	-10.52	5.67	6.16	-	-	-	-	-	-	-	-	-	-
H17	4.42	-10.56	-8.36	3.39	-13.51	-25.51	4.64	3.70	5.86	3.48	3.52	3.00	-15.22	5.54	4.89	8.17	-	-	-	-	-	-	-	-	-
O18	-19.31	34.59	27.18	-7.78	29.25	34.38	-16.10	-14.72	-12.91	-10.52	-15.22	-7.72	26.44	-10.42	-16.83	-16.40	-12.40	-	-	-	-	-	-	-	-
C19	-4.20	10.42	8.11	-2.18	7.30	8.04	-4.61	-5.46	-4.03	-3.44	-4.66	-2.27	7.84	-2.80	-4.10	-3.94	-3.32	30.78	-	-	-	-	-	-	-
H20	2.86	-7.09	-5.13	1.42	-4.71	-5.50	3.82	3.86	2.94	2.26	2.73	1.47	-5.39	1.86	2.52	2.74	2.39	-15.45	-10.60	-	-	-	-	-	-
H21	2.62	-6.68	-5.71	1.62	-5.55	-5.83	2.95	3.38	2.74	2.50	3.36	1.76	-5.86	2.20	3.24	3.01	2.43	-18.49	-12.45	5.64	-	-	-	-	-
H22	2.63	-8.18	-6.66	1.64	-5.06	-5.23	2.79	4.82	3.07	2.92	4.00	1.74	-5.88	1.94	2.81	2.45	2.23	-15.27	-10.54	4.80	5.62	-	-	-	-
C23	-2.18	7.30	8.04	-4.20	10.42	8.10	-2.27	-2.80	-4.10	-3.94	-3.32	-4.61	30.78	-5.46	-4.03	-3.44	-4.66	7.84	2.35	-1.63	-1.82	-1.73	-	-	-
H24	1.62	-5.55	-5.83	2.62	-6.68	-5.71	1.76	2.20	3.24	3.01	2.43	2.95	-18.49	3.38	2.74	2.50	3.36	-5.86	-1.82	1.29	1.41	1.35	-12.45	-	-
H25	1.42	-4.71	-5.50	2.86	-7.09	-5.13	1.47	1.86	2.52	2.74	2.39	3.82	-15.45	3.86	2.94	2.26	2.73	-5.39	-1.63	1.12	1.29	1.21	-10.60	5.64	-
H26	1.64	-5.06	-5.23	2.63	-8.18	-6.66	1.74	1.94	2.81	2.45	2.23	2.79	-15.27	4.82	3.07	2.92	4.00	-5.88	-1.73	1.21	1.35	1.24	-10.54	5.62	4.80

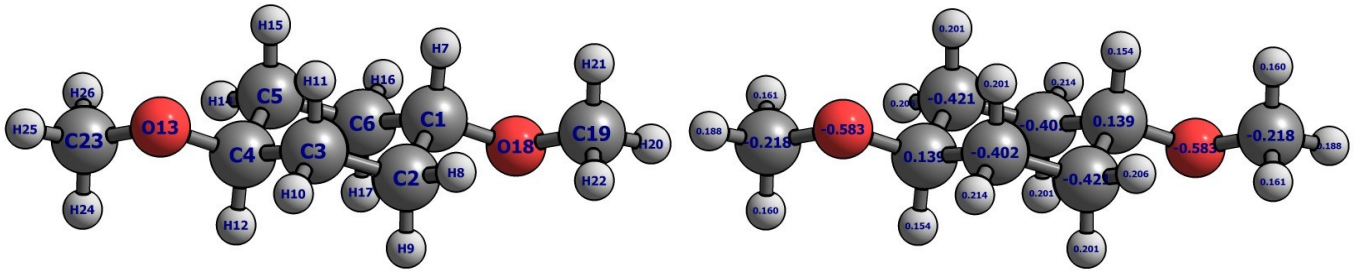

Table S24. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 8eq.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	H12	O13	H14	H15	H16	H17	O18	C19	H20	H21	H22	C23	H24	H25
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.71	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-7.36	36.77	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	2.16	-7.69	-12.18	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-7.69	20.00	22.42	-12.70	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-12.18	22.42	18.32	-7.36	36.77	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	6.43	-10.00	-7.40	2.12	-7.73	-9.55	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	4.39	-26.46	-12.79	2.75	-7.34	-7.97	4.26	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	4.34	-25.66	-12.37	3.31	-8.41	-9.71	3.38	7.83	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.84	-13.76	-26.12	4.59	-8.66	-7.27	2.89	5.87	5.68	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	3.32	-12.99	-24.49	4.36	-10.21	-8.08	3.96	5.55	4.37	8.11	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H12	2.12	-7.73	-9.55	6.43	-10.00	-7.40	1.96	2.80	3.93	4.43	3.38	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O13	-6.34	21.84	32.96	-18.99	33.24	20.55	-6.76	-8.86	-9.54	-16.03	-15.19	-14.49	-	-	-	-	-	-	-	-	-	-	-	-	-
H14	2.75	-7.34	-7.97	4.39	-26.46	-12.79	2.80	2.85	3.32	3.42	3.67	4.26	-14.50	-	-	-	-	-	-	-	-	-	-	-	-
H15	3.31	-8.41	-9.71	4.34	-25.66	-12.37	3.93	3.32	3.34	3.81	5.25	3.38	-14.69	7.83	-	-	-	-	-	-	-	-	-	-	-
H16	4.59	-8.66	-7.27	2.84	-13.76	-26.12	4.43	3.42	3.81	3.06	3.45	2.89	-8.98	5.87	5.68	-	-	-	-	-	-	-	-	-	-
H17	4.36	-10.21	-8.08	3.32	-12.99	-24.49	3.38	3.67	5.25	3.45	3.37	3.96	-9.44	5.55	4.37	8.11	-	-	-	-	-	-	-	-	-
O18	-18.99	33.24	20.55	-6.34	21.84	32.96	-14.49	-14.50	-14.69	-8.98	-9.44	-6.76	20.20	-8.86	-9.54	-16.03	-15.19	-	-	-	-	-	-	-	-
C19	-4.24	10.19	6.61	-1.93	6.24	7.95	-4.32	-5.44	-4.40	-3.04	-3.18	-2.04	6.51	-2.59	-2.88	-4.01	-3.70	30.01	-	-	-	-	-	-	-
H20	2.65	-6.59	-4.62	1.41	-4.61	-5.77	2.74	3.41	3.03	2.18	2.22	1.52	-4.88	1.98	2.12	3.05	2.79	-18.06	-12.52	-	-	-	-	-	-
H21	2.84	-6.77	-4.75	1.37	-4.49	-5.41	3.54	3.73	2.73	2.17	2.43	1.40	-4.74	1.85	2.17	2.80	2.39	-14.94	-10.56	5.62	-	-	-	-	-
H22	2.68	-8.06	-5.06	1.41	-4.29	-5.17	2.66	4.89	3.61	2.42	2.38	1.52	-4.80	1.79	1.96	2.49	2.50	-14.95	-10.64	5.67	4.80	-	-	-	-
C23	-1.93	6.24	7.95	-4.24	10.18	6.61	-2.04	-2.59	-2.88	-4.01	-3.70	-4.32	30.01	-5.44	-4.40	-3.04	-3.18	6.51	2.09	-1.61	-1.51	-1.53	-	-	-
H24	1.37	-4.49	-5.41	2.84	-6.77	-4.75	1.40	1.85	2.17	2.80	2.39	3.54	-14.94	3.73	2.73	2.17	2.43	-4.74	-1.51	1.17	1.07	1.11	-10.56	-	-
H25	1.41	-4.61	-5.77	2.65	-6.59	-4.62	1.52	1.98	2.12	3.05	2.79	2.74	-18.06	3.41	3.03	2.18	2.22	-4.88	-1.61	1.25	1.17	1.18	-12.52	5.62	-
H26	1.41	-4.29	-5.17	2.68	-8.06	-5.06	1.52	1.79	1.96	2.49	2.50	2.66	-14.95	4.89	3.61	2.42	2.38	-4.80	-1.53	1.18	1.11	1.09	-10.64	4.80	5.67

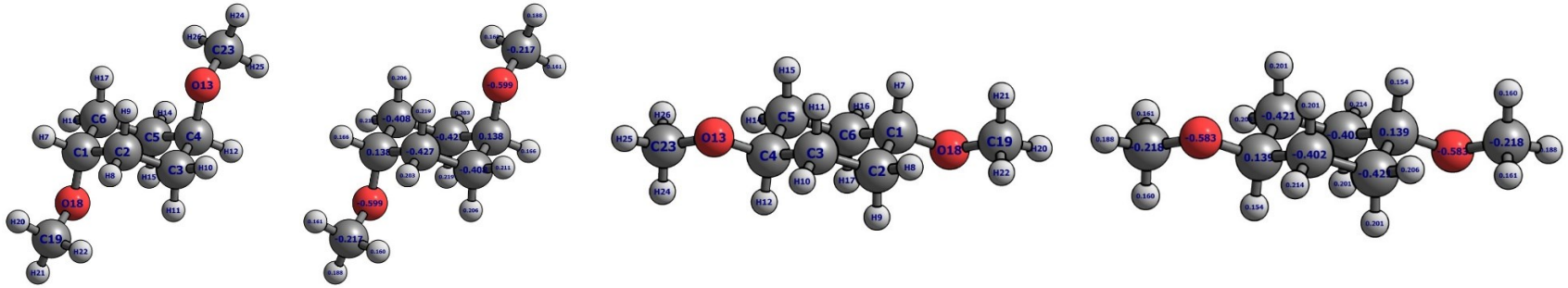

Table S25. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 8. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	H12	O13	H14	H15	H16	H17	O18	C19	H20	H21	H22	C23	H24	H25
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-0.09	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-0.06	1.05	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-0.01	-0.10	-0.10	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-0.10	0.63	0.62	-0.10	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-0.10	0.62	0.45	-0.06	1.05	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	0.51	-0.91	0.91	-0.19	0.94	-0.87	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	-0.10	0.12	0.12	-0.07	0.03	0.04	0.23	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	0.36	-2.72	-1.38	0.31	-0.94	-1.06	1.56	0.57	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	-0.05	-0.04	-0.07	-0.08	-0.01	0.00	-0.18	-0.20	0.48	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	0.07	-0.52	-1.02	0.06	-0.35	-0.28	-0.96	-0.01	0.52	0.06	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H12	-0.19	0.94	-0.87	0.51	-0.91	0.91	-0.12	-0.20	-0.74	0.25	1.26	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O13	-1.44	7.41	1.42	-0.32	1.34	6.63	-0.96	-1.56	-7.29	-0.37	2.79	-1.61	-	-	-	-	-	-	-	-	-	-	-	-	-
H14	-0.07	0.03	0.04	-0.10	0.12	0.12	-0.20	-0.10	0.24	-0.11	0.03	0.23	-0.22	-	-	-	-	-	-	-	-	-	-	-	-
H15	0.31	-0.94	-1.06	0.36	-2.72	-1.38	-0.74	0.24	0.66	0.29	0.61	1.56	1.78	0.57	-	-	-	-	-	-	-	-	-	-	-
H16	-0.08	-0.01	0.00	-0.05	-0.04	-0.07	0.25	-0.11	0.29	-0.08	0.03	-0.18	-1.54	-0.20	0.48	-	-	-	-	-	-	-	-	-	-
H17	0.06	-0.35	-0.28	0.07	-0.52	-1.02	1.26	0.03	0.61	0.03	0.15	-0.96	-5.78	-0.01	0.52	0.06	-	-	-	-	-	-	-	-	-
O18	-0.32	1.35	6.63	-1.44	7.41	1.42	-1.61	-0.22	1.78	-1.54	-5.78	-0.96	6.24	-1.56	-7.29	-0.37	2.79	-	-	-	-	-	-	-	-
C19	0.04	0.23	1.50	-0.25	1.06	0.09	-0.29	-0.02	0.37	-0.40	-1.48	-0.23	1.33	-0.21	-1.22	0.07	0.38	0.77	-	-	-	-	-	-	-
H20	0.21	-0.50	-0.51	0.01	-0.10	0.27	1.08	0.45	-0.09	0.08	0.51	-0.05	-0.51	-0.12	0.40	-0.31	-0.40	2.61	1.92	-	-	-	-	-	-
H21	-0.22	0.09	-0.96	0.25	-1.06	-0.42	-0.59	-0.35	0.01	0.33	0.93	0.36	-1.12	0.35	1.07	0.21	0.04	-3.55	-1.89	0.02	-	-	-	-	-
H22	-0.05	-0.12	-1.60	0.23	-0.77	-0.06	0.13	-0.07	-0.54	0.50	1.62	0.22	-1.08	0.15	0.85	-0.04	-0.27	-0.32	0.10	-0.87	0.82	-	-	-	-
C23	-0.25	1.06	0.09	0.04	0.24	1.49	-0.23	-0.21	-1.22	0.07	0.38	-0.29	0.77	-0.02	0.37	-0.40	-1.48	1.33	0.26	-0.02	-0.31	-0.20	-	-	-
H24	0.25	-1.06	-0.42	-0.22	0.09	-0.96	0.36	0.35	1.07	0.21	0.04	-0.59	-3.55	-0.35	0.01	0.33	0.93	-1.12	-0.31	0.12	0.34	0.24	-1.89	-	-
H25	0.01	-0.10	0.27	0.21	-0.50	-0.51	-0.05	-0.12	0.40	-0.31	-0.40	1.08	2.61	0.45	-0.09	0.08	0.51	-0.51	-0.02	-0.13	0.12	0.03	1.92	0.02	-
H26	0.23	-0.77	-0.06	-0.05	-0.12	-1.60	0.22	0.15	0.85	-0.04	-0.27	0.13	-0.32	-0.07	-0.54	0.50	1.62	-1.08	-0.20	0.03	0.24	0.15	0.10	0.82	-0.87

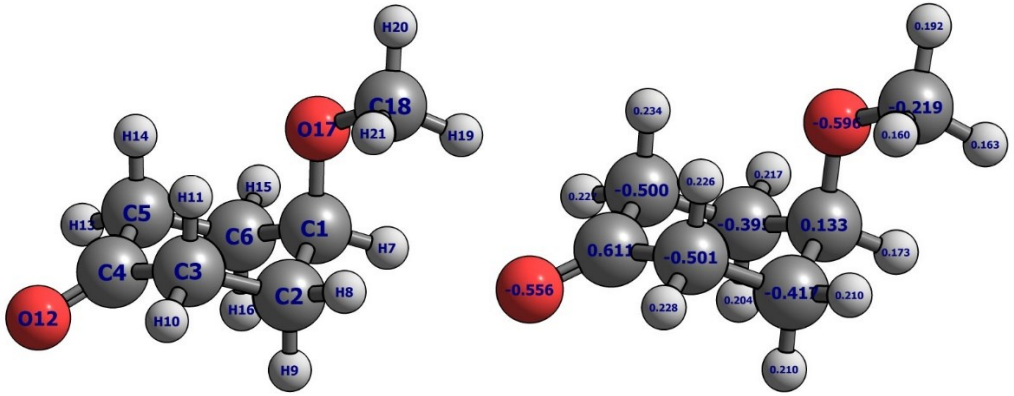

Table S26. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 9ax.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	O12	H13	H14	H15	H16	O17	C18	H19	H20	H21
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.06	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-8.78	45.27	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	9.24	-33.74	-67.12	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-8.76	23.45	32.62	-67.08	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-11.49	21.85	22.23	-31.84	42.81	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	6.95	-11.08	-8.28	8.91	-8.25	-10.51	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	4.27	-26.63	-16.11	12.31	-8.80	-7.96	4.84	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	4.34	-26.56	-16.12	15.24	-10.51	-10.07	4.90	8.35	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.89	-14.39	-34.83	21.66	-10.91	-7.59	3.02	6.25	6.31	-	-	-	-	-	-	-	-	-	-	-	-
H11	3.60	-14.55	-34.39	21.64	-13.24	-8.83	3.44	6.33	5.14	9.63	-	-	-	-	-	-	-	-	-	-	-
O12	-6.04	22.04	38.77	-93.49	38.67	20.79	-6.35	-8.82	-10.95	-16.73	-13.81	-	-	-	-	-	-	-	-	-	-
H13	2.88	-8.02	-10.89	21.62	-34.66	-13.62	3.01	3.18	3.86	4.04	4.46	-16.66	-	-	-	-	-	-	-	-	-
H14	3.70	-9.58	-13.68	22.41	-35.52	-14.29	3.53	3.85	4.06	4.63	6.52	-14.30	9.94	-	-	-	-	-	-	-	-
H15	4.47	-8.70	-9.14	12.71	-16.63	-26.10	5.00	3.52	4.05	3.30	3.90	-9.06	6.39	6.87	-	-	-	-	-	-	-
H16	4.21	-10.23	-10.08	14.58	-15.62	-24.48	4.77	3.79	5.60	3.70	3.79	-10.48	6.16	5.17	8.31	-	-	-	-	-	-
O17	-18.58	33.70	33.56	-35.07	34.13	33.21	-16.64	-15.08	-12.33	-11.34	-16.92	23.67	-11.50	-17.80	-16.69	-12.21	-	-	-	-	-
C18	-4.08	10.27	10.14	-9.88	8.61	7.87	-4.83	-5.65	-3.89	-3.75	-5.27	7.13	-3.13	-4.38	-4.07	-3.31	30.87	-	-	-	-
H19	2.80	-7.00	-6.42	6.42	-5.60	-5.41	4.02	4.01	2.84	2.46	3.09	-4.76	2.10	2.72	2.86	2.40	-15.61	-10.85	-	-	-
H20	2.59	-6.68	-7.24	7.48	-6.65	-5.78	3.12	3.56	2.69	2.76	3.85	-5.56	2.50	3.53	3.15	2.45	-18.81	-12.84	5.85	-	-
H21	2.55	-8.04	-8.32	7.41	-5.94	-5.09	2.92	4.98	2.96	3.16	4.53	-5.40	2.17	2.97	2.52	2.22	-15.26	-10.68	4.89	5.76	-

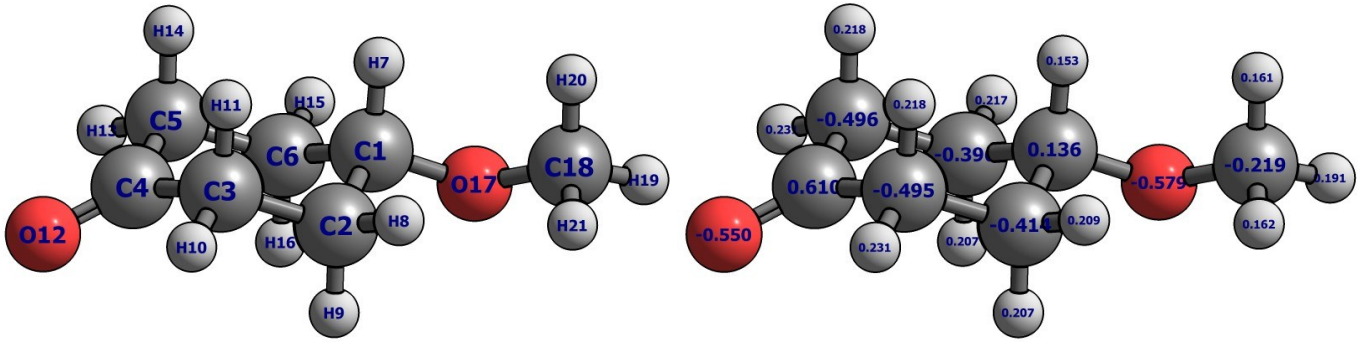

Table S27. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 9eq.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	O12	H13	H14	H15	H16	O17	C18	H19	H20	H21
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.26	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-8.86	44.45	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	9.42	-33.35	-66.18	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-8.88	23.07	31.97	-66.38	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-11.78	21.78	22.07	-31.94	42.65	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	6.28	-9.79	-9.08	9.46	-9.08	-9.37	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	4.35	-26.38	-15.94	12.25	-8.71	-7.95	4.27	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	4.39	-26.09	-15.71	14.89	-10.22	-9.93	3.46	8.17	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	3.00	-14.53	-34.89	21.94	-10.98	-7.74	3.10	6.33	6.34	-	-	-	-	-	-	-	-	-	-	-	-
H11	3.52	-13.90	-32.68	20.85	-12.64	-8.51	4.28	6.14	4.89	9.45	-	-	-	-	-	-	-	-	-	-	-
O12	-6.09	21.56	37.82	-92.34	37.89	20.63	-6.23	-8.67	-10.59	-16.76	-13.19	-	-	-	-	-	-	-	-	-	-
H13	3.00	-8.10	-10.97	21.98	-35.03	-13.92	3.10	3.23	3.86	4.18	4.38	-16.77	-	-	-	-	-	-	-	-	-
H14	3.51	-8.86	-12.60	20.86	-32.78	-13.30	4.25	3.59	3.72	4.38	5.85	-13.20	9.47	-	-	-	-	-	-	-	-
H15	4.57	-8.65	-9.03	12.69	-16.47	-26.19	4.45	3.51	4.00	3.35	3.74	-8.96	6.52	6.33	-	-	-	-	-	-	-
H16	4.39	-10.38	-10.19	14.89	-15.74	-24.91	3.46	3.84	5.63	3.85	3.72	-10.57	6.35	4.89	8.48	-	-	-	-	-	-
O17	-18.56	32.61	25.15	-27.76	25.60	32.40	-14.34	-14.68	-15.01	-9.63	-10.20	19.92	-9.81	-10.32	-16.23	-15.49	-	-	-	-	-
C18	-4.17	10.05	8.18	-8.53	7.39	7.88	-4.32	-5.54	-4.52	-3.29	-3.48	6.33	-2.90	-3.14	-4.10	-3.81	29.93	-	-	-	-
H19	2.64	-6.59	-5.78	6.30	-5.52	-5.79	2.77	3.52	3.15	2.39	2.46	-4.82	2.25	2.34	3.16	2.91	-18.24	-12.77	-	-	-
H20	2.80	-6.67	-5.88	6.08	-5.32	-5.37	3.54	3.77	2.80	2.34	2.66	-4.50	2.08	2.37	2.87	2.46	-14.93	-10.65	5.74	-	-
H21	2.64	-7.96	-6.28	6.24	-5.08	-5.13	2.67	5.01	3.69	2.62	2.62	-4.70	2.00	2.13	2.54	2.58	-14.94	-10.74	5.79	4.85	-

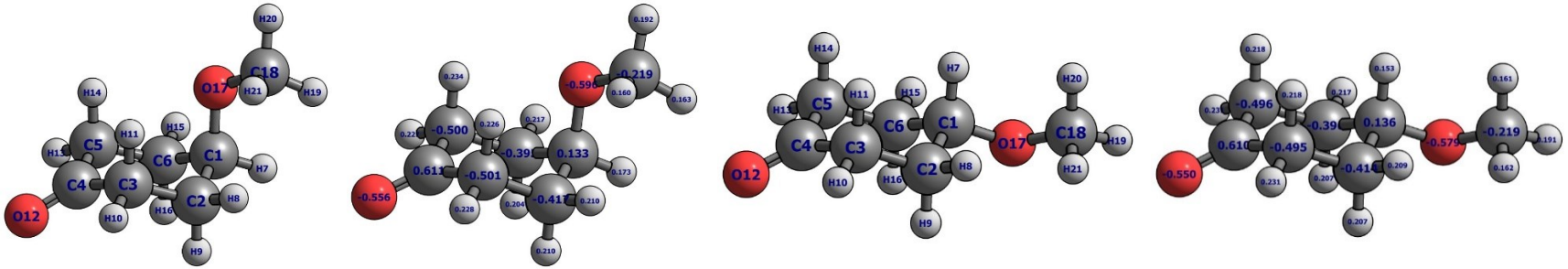

Table S28. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 9. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	O12	H13	H14	H15	H16	O17	C18	H19	H20	H21
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	0.20	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	0.08	0.82	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-0.18	-0.39	-0.94	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	0.12	0.38	0.65	-0.70	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	0.29	0.07	0.16	0.10	0.16	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	0.67	-1.29	0.80	-0.55	0.83	-1.14	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	-0.08	-0.25	-0.17	0.06	-0.09	-0.01	0.57	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	-0.05	-0.47	-0.41	0.35	-0.29	-0.14	1.44	0.18	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	-0.11	0.14	0.06	-0.28	0.07	0.15	-0.08	-0.08	-0.03	-	-	-	-	-	-	-	-	-	-	-	-
H11	0.08	-0.65	-1.71	0.79	-0.60	-0.32	-0.84	0.19	0.25	0.18	-	-	-	-	-	-	-	-	-	-	-
O12	0.05	0.48	0.95	-1.15	0.78	0.16	-0.12	-0.15	-0.36	0.03	-0.62	-	-	-	-	-	-	-	-	-	-
H13	-0.12	0.08	0.08	-0.36	0.37	0.30	-0.09	-0.05	0.00	-0.14	0.08	0.11	-	-	-	-	-	-	-	-	-
H14	0.19	-0.72	-1.08	1.55	-2.74	-0.99	-0.72	0.26	0.34	0.25	0.67	-1.10	0.47	-	-	-	-	-	-	-	-
H15	-0.10	-0.05	-0.11	0.02	-0.16	0.09	0.55	0.01	0.05	-0.05	0.16	-0.10	-0.13	0.54	-	-	-	-	-	-	-
H16	-0.18	0.15	0.11	-0.31	0.12	0.43	1.31	-0.05	-0.03	-0.15	0.07	0.09	-0.19	0.28	-0.17	-	-	-	-	-	-
O17	-0.02	1.09	8.41	-7.31	8.53	0.81	-2.30	-0.40	2.68	-1.71	-6.72	3.75	-1.69	-7.48	-0.46	3.28	-	-	-	-	-
C18	0.09	0.22	1.96	-1.35	1.22	-0.01	-0.51	-0.11	0.63	-0.46	-1.79	0.80	-0.23	-1.24	0.03	0.50	0.94	-	-	-	-
H19	0.16	-0.41	-0.64	0.12	-0.08	0.38	1.25	0.49	-0.31	0.07	0.63	0.06	-0.15	0.38	-0.30	-0.51	2.63	1.92	-	-	-
H20	-0.21	-0.01	-1.36	1.40	-1.33	-0.41	-0.42	-0.21	-0.11	0.42	1.19	-1.06	0.42	1.16	0.28	-0.01	-3.88	-2.19	0.11	-	-
H21	-0.09	-0.08	-2.04	1.17	-0.86	0.04	0.25	-0.03	-0.73	0.54	1.91	-0.70	0.17	0.84	-0.02	-0.36	-0.32	0.06	-0.90	0.91	-

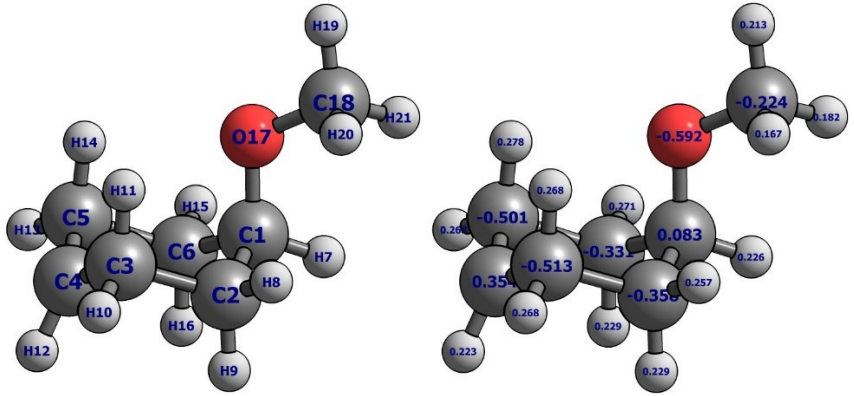

Table S29. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 10ax.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	H12	H13	H14	H15	H16	O17	C18	H19	H20	H21
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-6.49	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-5.56	37.95	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	3.61	-18.02	-41.98	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-5.39	19.87	34.22	-41.43	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-6.03	15.85	19.21	-17.09	33.82	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	5.68	-12.55	-11.00	7.23	-10.69	-11.68	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	3.23	-28.06	-20.24	9.25	-10.81	-8.17	7.54	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	2.92	-25.03	-17.48	10.28	-11.12	-9.16	7.02	11.10	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.13	-14.47	-42.11	14.85	-13.06	-7.59	4.68	9.24	8.14	-	-	-	-	-	-	-	-	-	-	-	-
H11	2.70	-14.63	-41.99	14.92	-16.46	-8.94	5.37	9.41	6.62	13.18	-	-	-	-	-	-	-	-	-	-	-
H12	1.78	-9.09	-17.43	24.05	-17.15	-8.63	3.92	4.93	6.08	8.16	6.50	-	-	-	-	-	-	-	-	-	-
H13	2.12	-8.05	-13.30	14.82	-41.17	-13.30	4.67	4.61	4.85	5.64	6.42	8.15	-	-	-	-	-	-	-	-	-
H14	2.82	-9.96	-17.36	15.38	-42.52	-13.97	5.61	5.80	5.27	6.64	9.94	6.70	13.55	-	-	-	-	-	-	-	-
H15	3.44	-9.35	-11.84	9.97	-21.00	-27.41	8.07	5.35	5.48	4.93	5.92	5.33	9.90	10.34	-	-	-	-	-	-	-
H16	2.92	-9.91	-11.69	10.59	-16.86	-23.12	6.98	5.18	6.79	4.98	5.14	6.32	8.02	6.82	11.64	-	-	-	-	-	-
O17	-11.66	28.99	34.38	-21.25	34.43	27.70	-21.54	-18.54	-13.41	-13.41	-20.51	-10.30	-13.76	-22.35	-20.55	-13.60	-	-	-	-	-
C18	-2.60	8.59	9.95	-5.83	8.73	6.76	-6.62	-6.63	-4.23	-4.28	-5.96	-3.03	-3.80	-5.44	-5.28	-3.79	30.94	-	-	-	-
H19	1.80	-6.32	-8.15	4.91	-7.52	-5.41	4.53	4.79	3.24	3.59	5.06	2.57	3.36	4.89	4.40	3.07	-20.74	-14.62	-	-	-
H20	1.71	-6.95	-7.91	4.29	-5.96	-4.45	4.35	6.25	3.37	3.53	4.75	2.26	2.60	3.60	3.31	2.61	-15.75	-11.38	6.69	-	-
H21	1.90	-6.10	-6.76	4.16	-6.28	-5.18	5.87	4.63	3.23	3.00	3.80	2.24	2.83	3.75	4.21	3.02	-17.29	-12.42	7.27	5.69	-

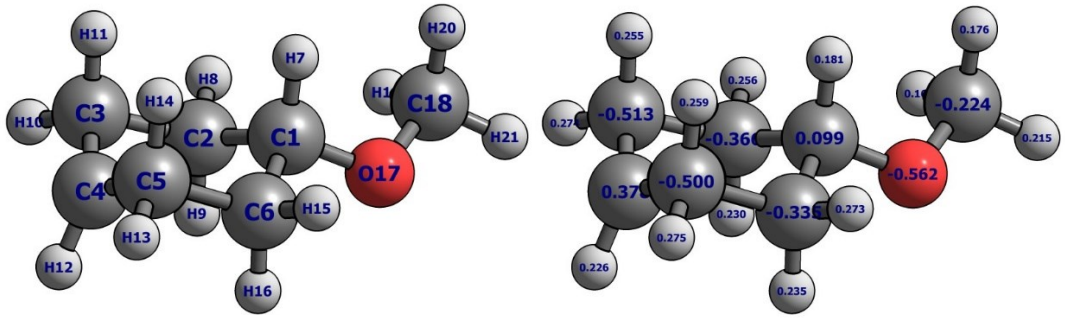

Table S30. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 10eq.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	H12	H13	H14	H15	H16	O17	C18	H19	H20	H21
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-7.87	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-6.60	39.24	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	4.61	-19.81	-44.68	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-6.32	20.15	34.03	-44.10	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-7.24	16.30	19.52	-18.80	34.36	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	5.42	-10.19	-10.91	7.21	-10.60	-9.34	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	3.83	-28.62	-20.28	9.87	-10.72	-8.21	6.18	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	3.52	-25.64	-17.62	11.05	-11.02	-9.20	4.53	11.07	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.58	-15.14	-42.91	16.15	-13.27	-7.85	4.30	9.36	8.36	-	-	-	-	-	-	-	-	-	-	-	-
H11	2.99	-14.15	-39.92	15.13	-15.58	-8.58	5.82	8.88	6.29	12.83	-	-	-	-	-	-	-	-	-	-	-
H12	2.19	-9.59	-17.69	26.09	-17.39	-9.09	3.35	5.02	6.30	8.43	6.27	-	-	-	-	-	-	-	-	-	-
H13	2.58	-8.40	-13.61	16.20	-42.06	-13.85	4.34	4.69	4.94	5.90	6.26	8.47	-	-	-	-	-	-	-	-	-
H14	3.05	-9.43	-16.17	15.32	-39.58	-13.07	6.02	5.38	4.88	6.33	8.81	6.36	13.02	-	-	-	-	-	-	-	-
H15	4.12	-9.59	-11.95	10.81	-21.10	-27.94	6.60	5.36	5.50	5.07	5.65	5.54	10.22	9.57	-	-	-	-	-	-	-
H16	3.59	-10.30	-12.01	11.76	-17.26	-23.96	4.62	5.25	6.87	5.21	4.99	6.80	8.44	6.49	12.10	-	-	-	-	-	-
O17	-13.27	28.19	25.17	-18.01	24.66	26.96	-16.43	-16.92	-16.46	-11.12	-11.52	-9.58	-11.34	-11.92	-19.34	-17.32	-	-	-	-	-
C18	-3.11	8.99	8.49	-5.66	7.52	6.86	-5.25	-6.57	-5.15	-3.93	-4.08	-3.04	-3.53	-3.83	-5.22	-4.45	29.48	-	-	-	-
H19	2.03	-7.32	-6.67	4.21	-5.28	-4.54	3.37	6.08	4.27	3.20	3.16	2.29	2.48	2.68	3.31	3.03	-15.07	-11.48	-	-	-
H20	2.21	-6.22	-6.38	4.21	-5.77	-4.99	4.52	4.66	3.35	2.93	3.24	2.21	2.70	3.08	3.96	3.07	-15.80	-11.98	5.50	-	-
H21	2.17	-6.56	-6.66	4.60	-6.18	-5.54	3.66	4.69	4.01	3.17	3.19	2.55	3.01	3.13	4.41	3.76	-19.87	-14.76	6.78	7.06	-

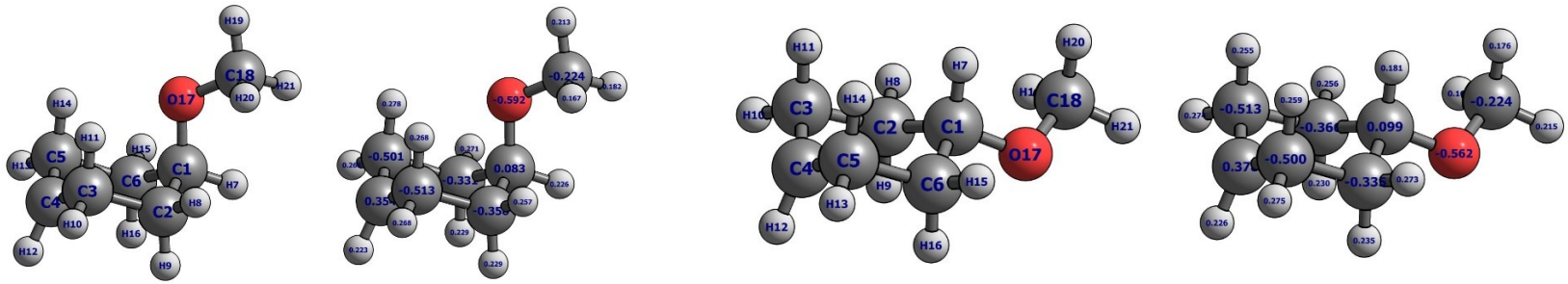

Table S31. Atom-atom electrostatic interactions (kcal mol-1) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 10. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	C4	C5	C6	H7	H8	H9	H10	H11	H12	H13	H14	H15	H16	O17	C18	H19	H20	H21
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	1.38	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	1.04	-1.29	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-1.00	1.79	2.70	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	0.93	-0.28	0.19	2.67	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	1.21	-0.45	-0.31	1.71	-0.54	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H7	0.26	-2.36	-0.09	0.02	-0.09	-2.34	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H8	-0.60	0.56	0.04	-0.62	-0.09	0.04	1.36	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	-0.60	0.61	0.14	-0.77	-0.10	0.04	2.49	0.03	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	-0.45	0.67	0.80	-1.30	0.21	0.26	0.38	-0.12	-0.22	-	-	-	-	-	-	-	-	-	-	-	-
H11	-0.29	-0.48	-2.07	-0.21	-0.88	-0.36	-0.45	0.53	0.33	0.35	-	-	-	-	-	-	-	-	-	-	-
H12	-0.41	0.50	0.26	-2.04	0.24	0.46	0.57	-0.09	-0.22	-0.27	0.23	-	-	-	-	-	-	-	-	-	-
H13	-0.46	0.35	0.31	-1.38	0.89	0.55	0.33	-0.08	-0.09	-0.26	0.16	-0.32	-	-	-	-	-	-	-	-	-
H14	-0.23	-0.53	-1.19	0.06	-2.94	-0.90	-0.41	0.42	0.39	0.31	1.13	0.34	0.53	-	-	-	-	-	-	-	-
H15	-0.68	0.24	0.11	-0.84	0.10	0.53	1.47	-0.01	-0.02	-0.14	0.27	-0.21	-0.32	0.77	-	-	-	-	-	-	-
H16	-0.67	0.39	0.32	-1.17	0.40	0.84	2.36	-0.07	-0.08	-0.23	0.15	-0.48	-0.42	0.33	-0.46	-	-	-	-	-	-
O17	1.61	0.80	9.21	-3.24	9.77	0.74	-5.11	-1.62	3.05	-2.29	-8.99	-0.72	-2.42	-10.43	-1.21	3.72	-	-	-	-	-
C18	0.51	-0.40	1.46	-0.17	1.21	-0.10	-1.37	-0.06	0.92	-0.35	-1.88	0.01	-0.27	-1.61	-0.06	0.66	1.46	-	-	-	-
H19	-0.23	1.00	-1.48	0.70	-2.24	-0.87	1.16	-1.29	-1.03	0.39	1.90	0.28	0.88	2.21	1.09	0.04	-5.67	-3.14	-	-	-
H20	-0.50	-0.73	-1.53	0.08	-0.19	0.54	-0.17	1.59	0.02	0.60	1.51	0.05	-0.10	0.52	-0.65	-0.46	0.05	0.60	1.19	-	-
H21	-0.27	0.46	-0.10	-0.44	-0.10	0.36	2.21	-0.06	-0.78	-0.17	0.61	-0.31	-0.18	0.62	-0.20	-0.74	2.58	2.34	0.49	-1.37	-

Table S32. Gas-phase calculated total relative electronic energy (Δ*E*), total relative enthalpy energy (Δ*H*) and total relative Gibbs free energy (Δ*G*) obtained at the M06-2X/aug-cc-pVTZ theoretical level for compounds 1-10, in kcal mol^{-1}. Positive values represent axial preference, and the positive ones equatorial preference.

Compound	Δ*E*	Δ*H*	Δ*G*
1	1.08	1.00	0.74
2	0.90	0.77	0.46
3	0.21	0.16	-0.06
4	1.08	0.98	0.69
5	0.77	0.60	0.10
6	1.14	1.05	0.93
7	0.84	0.74	0.25
8	0.60	0.45	0.09
9	1.12	1.01	0.70
10	5.96	4.60	5.57

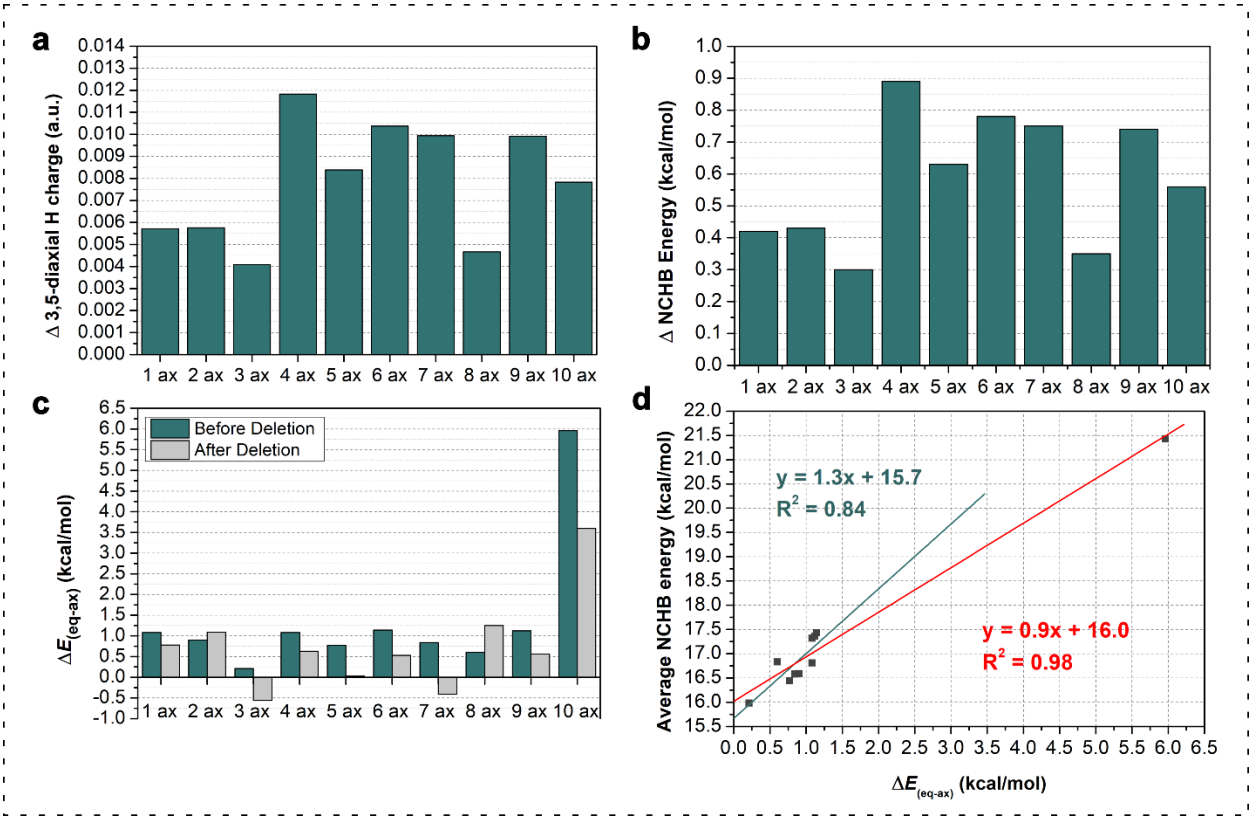

Figure S1. a) Delta average NPA atomic charge over 3,5-diaxial hydrogens in compounds **1-10** ($\Delta_{after\ -\ before}$ deletion of acceptor orbitals in position 4 of the ring). **b)** Delta average NCHB stabilizing energy, in kcal mol^{-1}, in compounds **1-10** ($\Delta E_{after\ -\ before}$ deletion of acceptor orbitals in position 4 of the ring). **c)** $\Delta E_{(eq\text{-}ax)}$, in kcal mol^{-1}, in compounds **1-10** before and after the deletion of acceptor orbitals in position 4 of the ring. **d)** Linear regression showing a positive correlation between NCHB stabilizing energy and axial isomer preference (without orbital deletion). In red, the linear regression considering all compounds, and in green the linear regression considering only compounds **1-9**. Energies and atomic charges were calculated at the M06-2X/aug-cc-pVTZ theoretical level.

Table S33. Cartesian coordinates, electronic energy and lowest harmonic vibrational frequency for compounds **1-10** calculated at the M06-2X/aug-cc-pVTZ.

1_{ax} **Energy (hartree) = -548.890031** **Lowest harmonic vibrational frequency (cm^{-1}) = 66.32**				**1_{eq}** **Energy (hartree) = -548.888314** **Lowest harmonic vibrational frequency (cm^{-1}) = 65.15**			
C	-1.26523000	0.53962000	0.57865000	C	-1.21754000	0.22801000	-0.27729000
C	-0.58093000	-0.69928000	1.15887000	C	-0.60783000	-1.08645000	0.20866000
C	0.45755000	-1.25358000	0.18654000	C	0.79784000	-1.27627000	-0.35681000
C	1.45240000	-0.17788000	-0.18083000	C	1.67064000	-0.08658000	-0.03340000
C	0.82182000	1.08346000	-0.71901000	C	1.08135000	1.23506000	-0.46587000
C	-0.23554000	1.61197000	0.24960000	C	-0.32683000	1.40303000	0.09641000
O	-1.95255000	0.25857000	-0.62926000	O	-2.48506000	0.48117000	0.28774000
C	-3.03702000	-0.62518000	-0.49190000	C	-3.49670000	-0.40437000	-0.12491000
H	-3.68393000	-0.32986000	0.34150000	H	-3.37483000	-1.40000000	0.30952000
H	-3.60840000	-0.58179000	-1.41598000	H	-4.44355000	0.00892000	0.21379000
H	-2.70897000	-1.65647000	-0.33185000	H	-3.51873000	-0.49624000	-1.21658000
H	-1.98399000	0.92975000	1.31017000	H	-1.31758000	0.18552000	-1.37415000
H	-1.31387000	-1.46627000	1.40714000	H	-1.22916000	-1.93196000	-0.08455000
H	-0.09588000	-0.41334000	2.09376000	H	-0.57350000	-1.06357000	1.30019000
H	1.00400000	-2.09349000	0.61414000	H	1.27557000	-2.16980000	0.04346000
H	-0.02218000	-1.58609000	-0.73476000	H	0.76587000	-1.37103000	-1.44401000
F	2.34876000	-0.66996000	-1.08653000	F	2.90098000	-0.25189000	-0.60422000
F	2.19348000	0.13544000	0.93480000	F	1.89279000	-0.05403000	1.31997000
H	1.61205000	1.81436000	-0.88740000	H	1.74529000	2.03145000	-0.13180000
H	0.36380000	0.84121000	-1.67738000	H	1.06688000	1.24436000	-1.55742000
H	-0.74115000	2.47207000	-0.18703000	H	-0.77656000	2.32520000	-0.26850000
H	0.24056000	1.93720000	1.17588000	H	-0.28865000	1.46653000	1.18559000
2_{ax} **Energy (hartree) = -449.621103** **Lowest harmonic vibrational frequency (cm^{-1}) = 72.69**				**2_{eq}** **Energy (hartree) = -449.619668** **Lowest harmonic vibrational frequency (cm^{-1}) = 68.44**			
C	-0.88423700	0.36367900	0.72015500	C	0.99965700	0.22189000	0.21797700
C	-0.24536600	-1.02187200	0.81056800	C	0.42729300	-1.08973000	-0.31629600
C	0.59012600	-1.31893900	-0.43210100	C	-1.02234000	-1.27497600	0.12937200
C	1.64054100	-0.24570200	-0.65013600	C	-1.86492200	-0.09247500	-0.30098700
C	1.04717700	1.14902000	-0.68843900	C	-1.31590500	1.21025900	0.24154500
C	0.18853100	1.42833900	0.54431000	C	0.13242300	1.39797100	-0.20190100
H	-1.45780900	0.55988100	1.63506900	H	1.02659800	0.17066300	1.31791700
H	-1.00455700	-1.79082500	0.95496600	H	1.02358200	-1.93691000	0.02178400
H	0.39363800	-1.04122000	1.69510600	H	0.48968700	-1.06328000	-1.40837400
H	1.08034500	-2.28879800	-0.34743900	H	-1.44131300	-2.19419600	-0.27921700
H	-0.05240700	-1.34610200	-1.31511800	H	-1.07542700	-1.34797700	1.21924600
H	2.22015700	-0.44648600	-1.55235400	H	-1.92393400	-0.05020800	-1.39314100
F	2.54907000	-0.30720600	0.41611200	F	-3.16606200	-0.26898800	0.16129600
H	1.85404300	1.87765300	-0.76798400	H	-1.93665100	2.04031800	-0.09456300
H	0.43397800	1.23107500	-1.58724500	H	-1.37806500	1.17512300	1.33266900
H	-0.28628400	2.40532100	0.45822000	H	0.54866500	2.31631100	0.21025400
H	0.81722800	1.43902500	1.43607600	H	0.18724900	1.48159200	-1.29093100
O	-1.75826800	0.48336900	-0.39273700	O	2.30304200	0.48183300	-0.25988800
C	-2.88485400	-0.35371500	-0.33914500	C	3.28737600	-0.39901500	0.22182500
H	-3.37752900	-0.29191700	0.63771600	H	4.25385300	0.01536100	-0.05484900
H	-3.57769500	-0.01496600	-1.10603100	H	3.23744000	-0.48719900	1.31286200
H	-2.63010600	-1.39959500	-0.53536600	H	3.19704600	-1.39691900	-0.21542200
3_{ax} **Energy (hartree) = -449.620108** **Lowest harmonic vibrational frequency (cm^{-1}) = 71.19**				**3_{eq}** **Energy (hartree) = -449.619781** **Lowest harmonic vibrational frequency (cm^{-1}) = 69.89**			
C	-1.10574300	0.49420400	0.59635200	C	0.90919100	0.24632700	0.26820800
C	-0.45946100	-0.77423500	1.15622100	C	0.31012500	-1.10745700	-0.10298000
C	0.69581200	-1.23748900	0.27078600	C	-1.04189600	-1.30947000	0.57979800
C	1.71750400	-0.12695200	0.13754500	C	-2.00052000	-0.17635400	0.26859500
C	1.10487700	1.13742000	-0.42732400	C	-1.40425000	1.18220000	0.58379500
C	-0.06640700	1.59618000	0.44211700	C	-0.04932900	1.36815100	-0.09354200
H	-1.89978900	0.82562700	1.27815200	H	1.09428500	0.26466000	1.35504300
H	-1.19856600	-1.56694100	1.27089300	H	0.98223900	-1.91835500	0.17792700
H	-0.09338100	-0.54715500	2.16116800	H	0.18790800	-1.13903400	-1.18801100
H	1.17113200	-2.12809300	0.68145200	H	-1.49083600	-2.25426100	0.27350800
H	0.32625300	-1.48321500	-0.72732600	H	-0.91198000	-1.34934500	1.66495800
F	2.74623700	-0.55060800	-0.69971300	F	-2.29823400	-0.21890500	-1.09705900
H	2.17547500	0.07710900	1.11149400	H	-2.94822400	-0.31568800	0.79146900
H	1.86552000	1.91515800	-0.49385200	H	-2.10085100	1.96038300	0.27232400
H	0.75153000	0.92500000	-1.43749800	H	-1.29799400	1.25742900	1.66956200
H	-0.53944800	2.47435000	0.00415700	H	0.39362600	2.32392900	0.18474200

H	0.29106300	1.87635600	1.43627400	H	-0.17440600	1.36888300	-1.17811500
O	-1.66933900	0.29146900	-0.68805400	O	2.12397000	0.51039700	-0.40281500
C	-2.73936900	-0.61866200	-0.71898600	C	3.19183300	-0.32210600	-0.02637700
H	-3.46658700	-0.40077200	0.07127700	H	4.09708100	0.10089900	-0.45549600
H	-3.22573700	-0.51304400	-1.68583000	H	3.29878000	-0.35805800	1.06384000
H	-2.40216400	-1.65345900	-0.60876900	H	3.07180000	-1.34221000	-0.40067600
4_{ax}				**4_{eq}**			
Energy (hartree) = -1269.590533				**Energy (hartree) = -1269.588807**			
Lowest harmonic vibrational frequency (cm^{-1}) = 63.80				**Lowest harmonic vibrational frequency (cm^{-1}) = 57.67**			
C	-1.78080300	-0.74243300	0.14716200	C	1.71672300	-0.29379200	0.30246500
C	-1.04650400	-0.63036300	-1.18864600	C	1.07116700	-0.15589800	-1.07485600
C	0.04628700	0.43359100	-1.12541700	C	-0.34012300	-0.73909300	-1.07723000
C	1.01754100	0.16282500	0.01367300	C	-1.21027100	-0.12221300	0.00715400
C	0.30601600	-0.00645100	1.34631600	C	-0.55727500	-0.21183800	1.37811400
C	-0.79939100	-1.05823500	1.26643800	C	0.85491700	0.36482100	1.36721900
H	-2.53396900	-1.53727500	0.07962500	H	1.81987500	-1.36601700	0.53580700
H	-1.74167300	-0.39253300	-1.99364900	H	1.66069400	-0.67524800	-1.83028100
H	-0.61140600	-1.60235400	-1.42542000	H	1.04811800	0.90245200	-1.34230400
H	0.59754000	0.49830000	-2.06172300	H	-0.82319500	-0.60936200	-2.04389200
H	-0.40228000	1.40924300	-0.92777700	H	-0.29885500	-1.81155200	-0.87088900
Cl	2.18037400	1.52520100	0.13283700	Cl	-2.78900000	-0.97731600	0.04895000
Cl	1.97145900	-1.32625100	-0.35399400	Cl	-1.53935500	1.60226100	-0.39362400
H	1.03604000	-0.25519900	2.11433800	H	-1.18675200	0.29013100	2.11046000
H	-0.13298200	0.96060700	1.59432100	H	-0.52660600	-1.27225300	1.64036700
H	-1.33582100	-1.08727100	2.21419000	H	1.31881400	0.22341300	2.34273200
H	-0.36814900	-2.04505800	1.09374800	H	0.82613300	1.43788600	1.17134000
O	-2.42663400	0.46673100	0.50950900	O	2.98787600	0.31322600	0.37216100
C	-3.47479200	0.84968500	-0.34561000	C	3.97777400	-0.31335600	-0.40611100
H	-4.15164800	0.01064700	-0.54056700	H	4.93318900	0.11948500	-0.12010400
H	-4.02722000	1.64109000	0.15513200	H	4.00442100	-1.39207700	-0.21560000
H	-3.10665400	1.23209900	-1.30211000	H	3.82569600	-0.14850900	-1.47598500
5_{ax}				**5_{eq}**			
Energy (hartree) = -809.980708				**Energy (hartree) = -809.979478**			
Lowest harmonic vibrational frequency (cm^{-1}) = 71.36				**Lowest harmonic vibrational frequency (cm^{-1}) = 63.16**			
C	1.18173100	0.30655200	-0.74347300	C	-1.40506400	0.21391600	-0.21885900
C	0.47873200	-1.05024000	-0.70559000	C	-0.80458300	-1.07217300	0.34352600
C	-0.27958800	-1.23637200	0.60481200	C	0.66059700	-1.22060800	-0.06789900
C	-1.26391900	-0.10395200	0.85804500	C	1.45756600	-0.00530700	0.37144600
C	-0.60012400	1.26033200	0.75479000	C	0.87967200	1.27633600	-0.20169800
C	0.17571600	1.43171900	-0.54885600	C	-0.58467300	1.41957000	0.20830900
H	1.68957900	0.42498200	-1.70901400	H	-1.40383200	0.15033500	-1.31850100
H	1.19440600	-1.86032400	-0.84657000	H	-1.36415400	-1.94224000	-0.00002300
H	-0.21674100	-1.09614300	-1.54553800	H	-0.89228500	-1.03739000	1.43352000
H	-0.80052600	-2.19258700	0.62069500	H	1.09206900	-2.12480900	0.35922000
H	0.43036900	-1.23057100	1.43692200	H	0.73752200	-1.30796900	-1.15493400
H	-1.74617300	-0.22389700	1.82398900	H	1.48713700	0.05039400	1.45931500
Cl	-2.63632500	-0.21233700	-0.33060100	Cl	3.17862100	-0.18593500	-0.13517600
H	-1.34754400	2.04473300	0.86490400	H	1.46094800	2.13257500	0.13743100
H	0.09400700	1.34132200	1.59462900	H	0.96523900	1.23690700	-1.29073900
H	0.70312100	2.38516500	-0.54416300	H	-1.01759400	2.32084200	-0.22467400
H	-0.51484600	1.43488200	-1.39380400	H	-0.66609300	1.51340300	1.29473800
O	2.14467700	0.44331600	0.29117700	O	-2.72676800	0.43823600	0.22510600
C	3.23494600	-0.43706200	0.19160900	C	-3.67185300	-0.47847100	-0.26880000
H	3.65015300	-0.43882500	-0.82240700	H	-4.65687800	-0.09130100	-0.01966500
H	3.99726500	-0.08892800	0.88477000	H	-3.59340000	-0.57732300	-1.35720800
H	2.96207200	-1.46246900	0.45835100	H	-3.56106300	-1.46798800	0.18252500
6_{ax}				**6_{eq}**			
Energy (hartree) = -5497.656912				**Energy (hartree) = -5497.655099**			
Lowest harmonic vibrational frequency (cm^{-1}) = 56.45				**Lowest harmonic vibrational frequency (cm^{-1}) = 54.52**			
C	2.43318600	0.64654800	0.22913600	C	2.34497300	-0.52875300	0.24974300
C	1.67692600	0.73122400	-1.09622000	C	1.69342900	-0.13708100	-1.07456900
C	0.53695600	-0.28450400	-1.14419400	C	0.25995700	-0.66038000	-1.15495500
C	-0.40587700	-0.12267800	0.03883100	C	-0.58002600	-0.21075100	0.03146500
C	0.33220400	-0.14579600	1.36789300	C	0.08447900	-0.55003000	1.35767700
C	1.48229900	0.86080300	1.39744200	C	1.51797200	-0.03020600	1.42305200
H	3.21868700	1.41222100	0.24623500	H	2.40991600	-1.62795000	0.29680200
H	2.34939600	0.56016300	-1.93681700	H	2.25432600	-0.54541100	-1.91530100
H	1.28558500	1.74347500	-1.20710800	H	1.71045400	0.95107400	-1.16194100
H	-0.02175800	-0.21331100	-2.07527100	H	-0.22075500	-0.35938000	-2.08367900
H	0.94957200	-1.29383500	-1.07567600	H	0.26872200	-1.75371700	-1.13108300
Br	-1.72038100	-1.57539500	0.01130700	Br	-2.32535000	-1.09845300	-0.05316400
Br	-1.40042900	1.57139300	-0.13797700	Br	-0.89511700	1.72702000	-0.07655600

H	-0.36812500	0.02994400	2.18202000	H	-0.51475600	-0.16502000	2.18021800
H	0.73806100	-1.15233200	1.48283900	H	0.08420400	-1.64080500	1.43473300
H	2.03212700	0.74524500	2.33093800	H	1.98273300	-0.35409300	2.35374100
H	1.09405900	1.87929900	1.35951100	H	1.52953300	1.06080700	1.41426500
O	3.03163000	-0.62366900	0.42652300	O	3.63850100	0.01223700	0.40228300
C	4.05787800	-0.93475900	-0.48275200	C	4.59706100	-0.50653400	-0.48676600
H	4.76762700	-0.10547600	-0.57528000	H	5.57053900	-0.16254200	-0.14622000
H	4.57997600	-1.80589800	-0.09455900	H	4.58540700	-1.60219500	-0.48312600
H	3.66864000	-1.17509300	-1.47636800	H	4.44094500	-0.15609900	-1.51035600
7_{ax}				**7_{eq}**			
Energy (hartree) = -2924.015229				**Energy (hartree) = -2924.013885**			
Lowest harmonic vibrational frequency (cm^{-1}) = 68.85				**Lowest harmonic vibrational frequency (cm^{-1}) = 60.29**			
C	1.68987800	0.27080000	-0.75935200	C	-2.04540900	0.20796100	-0.21879600
C	0.94993800	-1.06065100	-0.63247700	C	-1.42743600	-1.06035300	0.36413100
C	0.25555700	-1.17345100	0.72074700	C	0.04823900	-1.18208000	-0.02221100
C	-0.67510000	-0.00067700	0.98849300	C	0.80791300	0.05485300	0.42170300
C	0.01881700	1.33702100	0.78991600	C	0.21608200	1.32005100	-0.17258600
C	0.73073400	1.43493300	-0.55677600	C	-1.25857000	1.43386300	0.21287800
H	2.14880700	0.33666500	-1.75391600	H	-2.02377900	0.13611900	-1.31770700
H	1.63363300	-1.89735200	-0.77649200	H	-1.96203200	-1.94520500	0.01823100
H	0.21146800	-1.11732800	-1.43433900	H	-1.53362600	-1.01904600	1.45217800
H	-0.28763600	-2.11335600	0.80360600	H	0.48832600	-2.07479100	0.41949500
H	1.01120900	-1.15673800	1.51261400	H	0.14274100	-1.27833400	-1.10700000
H	-1.11102700	-0.06885000	1.98007500	H	0.82870600	0.11864100	1.50831500
Br	-2.26408000	-0.12266200	-0.19120500	Br	2.69890500	-0.10491800	-0.08336300
H	-0.69300600	2.15189200	0.91129100	H	0.77045000	2.19281400	0.16870500
H	0.76185800	1.42429000	1.58731100	H	0.31813400	1.27609700	-1.25989300
H	1.28811900	2.36944600	-0.61373700	H	-1.70254900	2.32276700	-0.23449500
H	-0.00175800	1.43181500	-1.36584100	H	-1.35952300	1.53398500	1.29704300
O	2.71010700	0.41505700	0.21781300	O	-3.37894300	0.40734200	0.20075800
C	3.76683300	-0.50296200	0.09666100	C	-4.29640100	-0.53073100	-0.30508100
H	4.12536300	-0.55859200	-0.93721500	H	-5.29323900	-0.16314300	-0.07394900
H	4.57603000	-0.15163200	0.73270900	H	-4.19766600	-0.63189100	-1.39160100
H	3.47894700	-1.50763000	0.42033200	H	-4.17257300	-1.51600600	0.15210800
8_{ax}				**8_{eq}**			
Energy (hartree) = -464.886898				**Energy (hartree) = -464.885943**			
Lowest harmonic vibrational frequency (cm^{-1}) = 59.87				**Lowest harmonic vibrational frequency (cm^{-1}) = 57.20**			
C	-1.22682200	0.39056900	0.71963100	C	1.44106600	0.22924900	0.22128800
C	-0.66974000	-1.03001600	0.79840200	C	0.92186500	-1.09841700	-0.32294500
C	0.10598500	-1.38946300	-0.46714800	C	-0.50299000	-1.36284400	0.15549200
C	1.22682900	-0.39054200	-0.71965300	C	-1.44105900	-0.22922400	-0.22124100
C	0.66974000	1.03004000	-0.79841900	C	-0.92185500	1.09844100	0.32299600
C	-0.10599100	1.38949700	0.46712400	C	0.50299500	1.36287400	-0.15543900
H	-1.73755000	0.63323500	1.66063900	H	1.49922500	0.16046600	1.31912900
H	-1.47122600	-1.74801400	0.97530300	H	1.56885700	-1.92011600	-0.01524700
H	-0.00235000	-1.08228400	1.65982500	H	0.95507400	-1.04939000	-1.41561600
H	0.53169100	-2.38923900	-0.38224200	H	-0.88503400	-2.29658300	-0.25640600
H	-0.56563400	-1.38103600	-1.32819800	H	-0.52151900	-1.46235100	1.24465400
H	1.73755600	-0.63321100	-1.66066400	H	-1.49921600	-0.16044800	-1.31908200
O	2.15377500	-0.55208900	0.34537800	O	-2.71787700	-0.56732400	0.28272400
H	1.47120100	1.74806100	-0.97533500	H	-1.56885700	1.92013800	0.01531500
H	0.00235000	1.08228000	-1.65984200	H	-0.95506300	1.04939600	1.41566600
H	-0.53171800	2.38926200	0.38219700	H	0.88504600	2.29660800	0.25646500
H	0.56562800	1.38110000	1.32817500	H	0.52153100	1.46238400	-1.24460000
O	-2.15378900	0.55206900	-0.34539700	O	2.71788200	0.56737500	-0.28266700
C	-3.32192200	-0.21679600	-0.22083900	C	3.75671100	-0.27313700	0.15261400
H	-3.75202000	-0.12393500	0.78298700	H	4.69415300	0.19529900	-0.13802900
H	-4.03796600	0.16041900	-0.94763100	H	3.74014200	-0.38880200	1.24226800
H	-3.14144100	-1.27632700	-0.42537900	H	3.70465700	-1.26446700	-0.30549900
C	3.32193700	0.21674300	0.22090400	C	-3.75673300	0.27304000	-0.15277800
H	4.03786300	-0.16037400	0.94786600	H	-3.74017600	0.38840500	-1.24246300
H	3.75220000	0.12374500	-0.78284100	H	-4.69415900	-0.19534000	0.13800400
H	3.14143400	1.27629500	0.42527800	H	-3.70470300	1.26449800	0.30506100
9_{ax}				**9_{eq}**			
Energy (hartree) = -424.388401				**Energy (hartree) = -424.386622**			
Lowest harmonic vibrational frequency (cm^{-1}) = 65.41				**Lowest harmonic vibrational frequency (cm^{-1}) = 61.98**			
C	-0.96380400	0.41839800	0.68103100	C	0.91611400	0.22876600	0.21512500
C	-0.31646900	-0.92871100	0.99961700	C	0.32494700	-1.10397700	-0.23891400
C	0.69331100	-1.32254400	-0.08346500	C	-1.07577400	-1.31442900	0.34522600
C	1.71739700	-0.22572700	-0.28202900	C	-1.98076600	-0.13859200	0.04574600
C	1.14192700	1.15543900	-0.49946800	C	-1.40066100	1.21433500	0.39572700
C	0.09665200	1.50283100	0.56835700	C	0.00668100	1.37938400	-0.18368200

H	-1.67128600	0.67574800	1.47966200	H	1.02083800	0.21393700	1.31213000
H	-1.07178500	-1.70641400	1.11317100	H	0.96683500	-1.93314000	0.05766200
H	0.18715300	-0.84180600	1.96475300	H	0.28082900	-1.09879900	-1.33103700
H	1.21180400	-2.24797800	0.15566400	H	-1.54320900	-2.22127300	-0.03078800
H	0.16228400	-1.45215600	-1.03096600	H	-1.00143400	-1.39696900	1.43467500
O	2.90389300	-0.43935000	-0.25756400	O	-3.07609900	-0.27125300	-0.43821700
H	1.95705500	1.87492000	-0.51981100	H	-2.07932900	1.98821100	0.04554100
H	0.65127500	1.15410900	-1.47608100	H	-1.35139300	1.27343500	1.48804500
H	-0.38224500	2.45036200	0.32385400	H	0.44887600	2.31867500	0.14594400
H	0.58136100	1.61782600	1.53978100	H	-0.03891000	1.40884700	-1.27485700
O	-1.65906300	0.40351800	-0.55395300	O	2.17727300	0.48735600	-0.36208200
C	-2.76576500	-0.46288200	-0.58865300	C	3.20911900	-0.35917200	0.08197600
H	-3.40559600	-0.32110600	0.28919100	H	4.14524200	0.05747500	-0.28141800
H	-3.33493400	-0.22444000	-1.48383700	H	3.23965000	-0.40181300	1.17635000
H	-2.46322200	-1.51323300	-0.63558000	H	3.10464400	-1.37529800	-0.30707600
10_{ax} **Energy (hartree) = -349.443589** **Lowest harmonic vibrational frequency (cm^{-1}) = 57.32**				**10_{eq}** **Energy (hartree) = -349.433784** **Lowest harmonic vibrational frequency (cm^{-1}) = 68.14**			
C	0.53062300	-0.26666400	0.71032300	C	0.54183500	-0.19769600	0.23269900
C	-0.02623900	1.14650200	0.81000000	C	0.04585700	1.16459100	-0.25975700
C	-0.96864500	1.41866600	-0.46082000	C	-1.44715500	1.41232600	0.22747300
C	-1.89132800	0.32716600	-0.33006800	C	-2.07105800	0.21842300	-0.28258300
C	-1.51626700	-1.00599800	-0.65069200	C	-1.91499400	-1.04107300	0.35767200
C	-0.60920400	-1.26162500	0.67784800	C	-0.42137300	-1.29011100	-0.21255100
H	1.13515200	-0.46913000	1.60456800	H	0.60759100	-0.18780700	1.33017900
H	0.74002900	1.91793900	0.76480000	H	0.62014800	1.99931600	0.13693000
H	-0.58503000	1.27910600	1.73565700	H	0.10531400	1.19397100	-1.34860300
H	-1.42089600	2.39924600	-0.35151800	H	-1.81709800	2.32788100	-0.22422600
H	-0.33284400	1.33416900	-1.33901700	H	-1.45032700	1.45789500	1.31476000
H	-2.80461600	0.48476400	0.24155000	H	-2.46483200	0.23343000	-1.29748500
H	-2.32274300	-1.73092500	-0.64923400	H	-2.55182600	-1.83805100	-0.01054400
H	-0.83159600	-1.09850600	-1.48913600	H	-1.85086000	-0.99879600	1.44141300
H	-0.26503300	-2.28549400	0.54252600	H	-0.15575800	-2.26637700	0.18990000
H	-1.21501700	-1.20628600	1.58068200	H	-0.41686300	-1.36277300	-1.30052400
O	1.28426200	-0.45635700	-0.45433800	O	1.77006000	-0.53829900	-0.33162700
C	2.60903000	0.05624000	-0.39428600	C	2.88052400	0.18105100	0.18562200
H	3.08912100	-0.20676000	-1.33121500	H	2.83659200	1.23647800	-0.09163300
H	2.61523200	1.14296700	-0.28389300	H	2.92679700	0.08859300	1.27336500
H	3.15631800	-0.39594700	0.43510500	H	3.76882800	-0.26243700	-0.25196500