

Supporting Information

**Taming Boroloborinines: Toward Photostable Polycyclic
Antiaromatic Hydrocarbons**

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Computational Methods

All geometries in the ground singlet and lowest-energy triplet states were optimized using the Gaussian 16 program.¹ Optimization was carried out with the M06-2X functional² and the def2-TZVPP basis set.^{3,4} M06-2X was selected because it provides a balanced description of π -systems while avoiding artificial stabilization. All optimized structures were confirmed as true minima by vibrational frequency analysis (no imaginary frequencies). To benchmark the reliability of M06-2X, all structures were also optimized at the CAM-B3LYP⁵/def2-TZVPP level. For bicyclic systems, additional geometry optimizations were performed at the CCSD/def2-SVP level, followed by CCSD(T)/def2-SVP//CCSD/def2-SVP single-point energy calculations to assess singlet–triplet (S–T) gaps. These reference energies were compared with S–T gaps obtained from M06-2X/def2-TZVPP and CAM-B3LYP/def2-TZVPP. M06-2X showed the best agreement with CCSD(T), with a mean error of 3.95 kcal/mol and a mean absolute error of 4.85 kcal/mol, whereas CAM-B3LYP exhibited significantly larger deviations (7.82 kcal/mol for both metrics). Therefore, M06-2X/def2-TZVPP was used for further property calculations and for all polycyclic systems. S–T gaps for the polycyclic species were evaluated at both M06-2X/def2-TZVPP and CAM-B3LYP/def2-TZVPP levels, and corroborating CCSD/def2-SVP and CCSD(T)/def2-SVP single-point energies were calculated using the M06-2X/def2-TZVPP geometries. Reliability of DFT results were further tested via assessing the stability of wavefunctions (stable=opt guess=mix). We found instabilities in the wavefunction of polycyclic molecules, (9 cases at M06-2X level and 13 instances at CAM-B3LYP level). Protonation energies were obtained at the M06-2X/def2-TZVPP level, which provides accurate agreement with experimental data. NMR shielding tensors were computed using the GIAO method at the same level, and corresponding WFX files were generated for wavefunction analysis in AIMAll (version 19.10.12).⁶ Magnetically induced current densities were computed with AIMAll by integrating the current flux across the interatomic surfaces under an external magnetic field perpendicular to the molecular plane. Aromaticity was further evaluated using HOMA and MCI, calculated via Multiwfn^{7,8} using FCHK files generated at the M06-2X/def2-TZVPP level. Excited-state properties, including excitation energies and oscillator strengths, were computed using TDA–TDDFT⁹ (see **Table S1**). Non-planarity was quantified using dihedral angles (**Table S2**). Multireference character was assessed using T_1 diagnostics during CCSD optimizations; values above 0.02 (singlet) or 0.04 (triplet) were taken to indicate significant multireference contributions (**Table S6**).

References

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Table S1: Computed HOMO-LUMO gaps (H-L) wavelength (λ_{max}) and oscillating strength (f) of all the studied molecules at M06-2X/def2-TZVPP level of theory.

Molecules	HL(eV)	λ_{max} (nm)	f	Molecules	HL(eV)	λ_{max} (nm)	f
1	4.65	207.75	0.31	30	4.76	234.65	0.56
2	5.03	202.18	0.23	31	4.75	201.47	0.29
3	4.8	201.9	0.31	32	3.63	250.02	0.21
4	4.76	207.85	0.29	33	4.6	242.36	0.48
5	4.86	200.83	0.20	34	3.62	256.56	0.31
6	4.84	202.18	0.23	35	3.45	245.14	1.67
7	5.35	256.43	0.04	36	3.43	268.71	0.62
8	5.26	208.04	0.12	37	3.18	266.71	0.79
9	4.84	196.84	0.15	38	4.86	236.44	1.13
10	5.58	259.96	0.07	39	3.78	240.28	1.16
11	5.11	204.89	0.18	40	4.72	252.19	1.06
12	5.06	279.06	0.05	41	4.84	244.9	1.13
13	5.41	223.93	0.14	42	5.29	223.4	0.46
14	5.17	193.92	0.27	43	5.13	217.36	0.51
15	5.26	221.04	0.13	44	5.16	237.31	0.19
16	5.02	200.47	0.23	45	3.67	266.39	0.25
17	4.99	211.07	0.07	46	4.51	261.99	0.17
18	5.59	258.02	0.06	47	5.27	226.43	0.47
19	5.36	197.49	0.21	48	3.19	300.36	1.00
20	5.24	253.43	0.03	49	3.91	251.7	0.52
21	5.38	198.23	0.15	50	3.05	271.07	0.50
22	5.26	200.61	0.16	51	5.3	242.8	0.22
23	5.56	199.58	0.09	52	4.47	245.89	0.44
24	5.58	216.42	0.07	53	4.01	239.35	0.13
25	4.83	248.65	0.14	54	2.76	298.03	0.69
26	5.32	214.68	0.69	55	5.19	228.51	0.24
27	5.5	207.05	0.08	56	3.79	432.44	0.24
28	5.57	227.82	0.05	57	4.98	218.41	0.46
29	3.43	220.8	0.87	58	5.03	235.41	0.32

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Table S2: Dihedral angles of all the studied molecules by considering both parent rings

Molecules	φ along borinine	φ along borole	Molecules	φ along borinine	φ along borole
1	-0.018	0.018	30	-0.014	0.018
2	-0.010	-0.001	31	-0.005	0.006
3	0.004	0.002	32	-0.033	0.047
4	-0.001	-0.004	33	0.037	-0.040
5	-0.002	-0.012	34	-8.262	-10.710
6	-0.002	-0.005	35	0.053	0.018
7	0.032	-3.643	36	0.009	-0.008
8	0.013	-0.012	37	-11.767	-11.821
9	-0.006	0.007	38	0.003	0.050
10	19.647	9.846	39	0.015	-0.009
11	2.988	-15.461	40	0.013	-0.005
12	-0.001	-0.053	41	-0.014	-0.030
13	-3.367	14.216	42	0.001	-0.005
14	0.003	0.000	43	-0.028	0.044
15	-2.486	-15.898	44	-0.014	0.017
16	0.005	-0.002	45	-2.396	-11.193
17	-0.296	14.793	46	10.983	23.986
18	-12.266	-16.803	47	0.053	0.023
19	-2.916	-19.939	48	-0.020	-0.065
20	-0.912	6.093	49	-0.025	-0.039
21	4.051	-19.092	50	-0.022	-0.029
22	0.666	15.886	51	-0.014	0.022
23	-4.166	16.373	52	2.345	16.060
24	-6.354	-17.741	53	1.192	2.181
25	0.002	0.017	54	-0.022	-0.010
26	0.906	22.003	55	0.008	-0.014
27	0.729	-20.260	56	11.191	12.746
28	-4.685	-21.790	57	0.013	-0.024
29	0.028	0.003	58	-0.005	-0.001

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Table S3. Singlet-triplet energy gaps in kcal/mol for bicyclic molecules at CCSD/def2-SVP, and CCSD(T)/def2SVP by using optimized geometries of Cam-b3lyp.

Molecule	CCSD	CCSD(T)	Molecule	CCSD	CCSD(T)
1	12.1	13.8	15	13.5	16.0
2	19.4	20.7	16	11.6	13.0
3	14.6	16.2	17	8.3	8.0
4	11.8	13.4	18	25.8	22.7
5	13.5	15.8	19	23.5	21.0
6	11.6	13.0	20	26.2	20.3
7	25.0	24.8	21	17.2	15.8
8	23.5	24.5	22	18.4	15.2
9	10.1	9.8	23	21.7	21.4
10	20.6	22.5	24	17.8	20.0
11	15.2	15.2	25	19.0	21.3
12	20.2	19.2	26	7.1	7.5
13	20.3	20.9	27	21.7	19.6
14	- ^a	- ^a	28	15.2	17.0

a- Triplet geometry contains spin contamination

Table S4. Singlet-triplet energy gaps in kcal/mol for polycyclic molecules at CCSD/def2-SVP, and CCSD(T)/def2-SVP by using optimized geometries of Cam-b3lyp.

Molecule	CCSD	CCSD(T)	Molecule	CCSD	CCSD(T)
29	-6.2	-2.9	44	34.9	35.9
30	25.3	27.3	45	-8.7	-0.3
31	18.5	20.1	46	7.3	10.8
32	0.2	4.2	47	25.8	27.3
33	15.6	17.2	48	-3.8	6.2
34	0.3	2.8	49	6.5	8.8
35	2.6	12.1	50	-13.5	-3.3
36	-3.1	-0.6	51	40.1	39.2
37	-7.1	0.2	52	11.6	15.3
38	32.5	34.4	53	8.8	10.9
39	10.6	14.7	54	-10.8	3.1
40	28.9	30.8	55	24.0	25.8
41	32.6	34.4	56	-5.3	4.6
42	33.9	34.7	57	20.6	22.3
43	29.4	31.0	58	23.8	25.6

Table S5. T1 diagnostic values at CCSD/def2-SVP for bicyclic molecules

Molecule	T1 diagnostic (Singlet)	T1 diagnostic (Triplet)	Molecule	T1 diagnostic (Singlet)	T1 diagnostic (Triplet)
1	0.013	0.038	15	0.016	0.039
2	0.014	0.039	16	0.018	0.039
3	0.015	0.036	17	0.019	0.032
4	0.013	0.038	18	0.022	0.033
5	0.017	0.038	19	0.022	0.058
6	0.015	0.039	20	0.019	0.052
7	0.015	0.046	21	0.024	0.059
8	0.017	0.042	22	0.028	0.059
9	0.014	0.039	23	0.024	0.047
10	0.017	0.039	24	0.018	- ^a
11	0.019	0.036	25	0.017	0.051
12	0.015	0.049	26	0.025	0.035
13	0.021	0.047	27	0.031	0.065
14	0.014	0.042	28	0.028	0.049

a. Triplet geometry failed to optimize due to large spin contamination.

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Table S6. T1 diagnostic values at CCSD/def2-SVP for Pericyclic molecules

Molecule	T1 diagnostic (Singlet)	T1 diagnostic (Triplet)	Molecule	T1 diagnostic (Singlet)	T1 diagnostic (Triplet)
29	0.018	0.039	44	0.015	0.034
30	0.012	0.040	45	0.043	0.039
31	0.012	0.041	46	0.017	0.040
32	0.017	0.038	47	0.015	0.039
33	0.012	0.039	48	0.023	0.050
34	0.013	0.042	49	0.017	0.042
35	0.016	0.038	50	0.045	0.038
36	0.012	0.041	51	0.013	0.054
37	0.016	0.035	52	0.019	0.039
38	0.012	0.044	53	0.014	0.040
39	0.014	0.041	54	0.030	0.040
40	0.012	0.042	55	0.013	0.036
41	0.012	0.037	56	0.019	0.042
42	0.015	0.045	57	0.013	0.042
43	0.016	0.042	58	0.013	0.035

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Table S7. Wavefunction stability values at M062X

Molecules	Singlet	S2	Triplet	S2
1		0		2.106
2		0		2.09
3		0		2.103
4		0		2.04
5		0		2.132
6		0		2.122
7		0		2.034
8		0		2.024
9		0		2.329
10		0		2.031
11		0		2.080
12		0		2.117
13		0		2.049
14		0		2.026
15		0		2.056
16		0		2.032
17		0		2.276
18		0		2.046
19		0		2.043
20		0		2.094
21		0		2.063
22		0		2.187
23		0		2.07
24		0		2.033
25		0		2.333
26		0		2.172
27		0		2.105
28		0		2.094
29	RHF -> UHF instability	1.027		2.163
30		0		2.106
31		0		2.291
32		0		2.252
33		0		2.142
34		0		2.425
35	RHF -> UHF instability	0.944		2.221
36	RHF -> UHF instability	1.338		2.239
37	RHF -> UHF instability	0.629		2.434
38		0		2.161
39		0		2.264
40		0		2.128
41		0		2.167
42		0		2.026
43		0		2.079
44		0		2.024
45	RHF -> UHF instability	1.436		2.068

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46		0		2.16
47		0		2.032
48	RHF -> UHF instability	1.31		2.044
49		0		2.066
50	RHF -> UHF instability	1.197		2.068
51		0		2.028
52		0		2.079
53		0		2.063
54	RHF -> UHF instability.	1.208		2.101
55		0		2.024
56	RHF -> UHF instability	1.433		2.069
57		0		2.16
58		0		2.14

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Table S8. Wavefunction stability at CAM-B3LYP

Molecules	Singlet	S2	Triplet	S2
1		0		2.176
2		0		2.117
3		0		2.139
4		0		2.06
5		0		2.194
6		0		2.2
7		0		2.056
8		0		2.101
9		0		2.53
10		0		2.097
11		0		2.12
12		0		2.077
13		0		2.069
14		0		2.184
15		0		2.084
16		0		2.112
17		0		2.419
18		0		2.062
19		0		2.067
20		0		2.187
21		0		2.11
22		0		2.305
23		0		2.092
24		0		2.114
25		0		2.499
26		0		2.332
27		0		2.083
28		0		2.093
29	RHF -> UHF instability	0.605		2.33
30		0		2.169
31		0		2.824
32	RHF -> UHF instability	1.2		2.651
33		0		2.601
34	RHF -> UHF instability	0.991		2.892
35	RHF -> UHF instability	1.667		2.697
36	RHF -> UHF instability	0.768		2.699
37	RHF -> UHF instability	0.647		3.155
38		0		2.508
39		0		2.495
40		0		2.364
41		0		2.804
42		0		2.091
43		0		2.11
44		0		2.095
45	RHF -> UHF instability	1.078		2.098

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46		0		2.2
47		0		2.094
48	RHF -> UHF instability	1.383		2.158
49	RHF -> UHF instability	1.393		2.097
50	RHF -> UHF instability	1.279		2.152
51		0		2.047
52		0		2.123
53	RHF -> UHF instability	1.61		2.101
54	RHF -> UHF instability	1.292		2.174
55		0		2.175
56	RHF -> UHF instability	1.633		2.106
57		0		2.189
58		0		2.182

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	Singlet	Triplet		Singlet	Triplet		Singlet	Triplet
1	 0.03 -1.08	 0.39 0.14	8	 -0.43 -0.27	 -0.66 -0.88	15	 0.28 -0.40	 0.38 0.12
2	 0.14 -0.93	 0.40 0.36	9	 0.12 -0.62	 0.39 0.03	16	 -0.45 -0.51	 -0.66 -1.17
3	 0.17 -1.08	 0.44 0.12	10	 -0.05 -0.59	 -0.41 -0.63	17	 0.28 -0.51	 0.53 -0.02
4	 0.00 -1.01	 0.40 0.11	11	 0.17 -0.76	 0.43 -0.11	18	 -0.34 -0.15	 -1.21 -1.46
5	 0.25 -0.61	 0.37 0.16	12	 -0.30 -0.59	 -0.23 -0.80	19	 0.04 -0.51	 -0.12 -0.46
6	 -0.42 -0.58	 0.44 0.18	13	 0.40 -0.50	 0.66 0.12	20	 -0.32 -0.30	 -0.44 -0.73
7	 -0.02 -0.99	 0.53 0.15	14	 -0.11 -1.10	 0.17 -0.20	21	 0.38 -0.31	 0.41 -0.20
	</							

Figure S1. HOMA values of bicyclic molecules. Positive and negative values, indicating aromaticity and antiaromaticity, respectively, are listed in black and red fonts.

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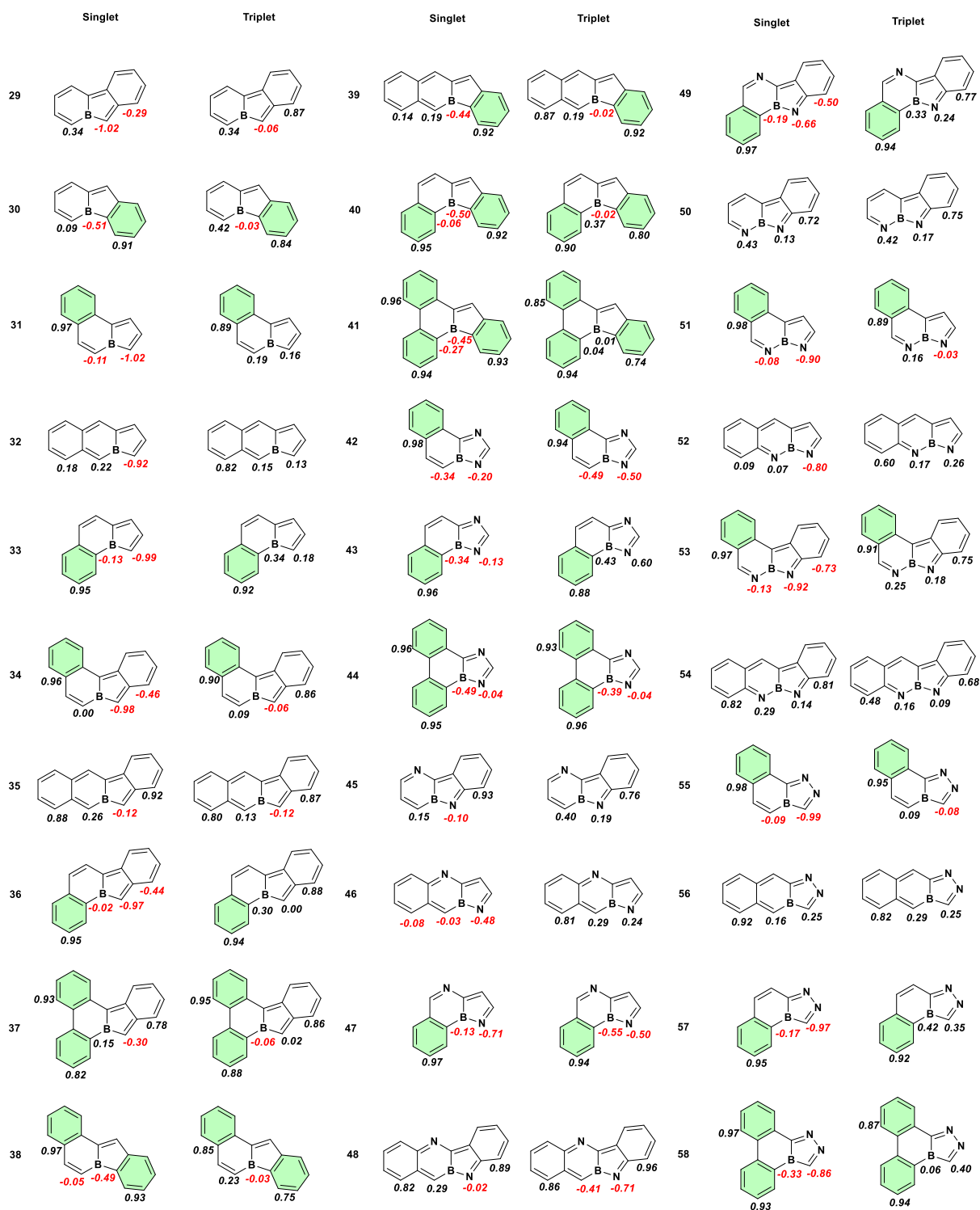
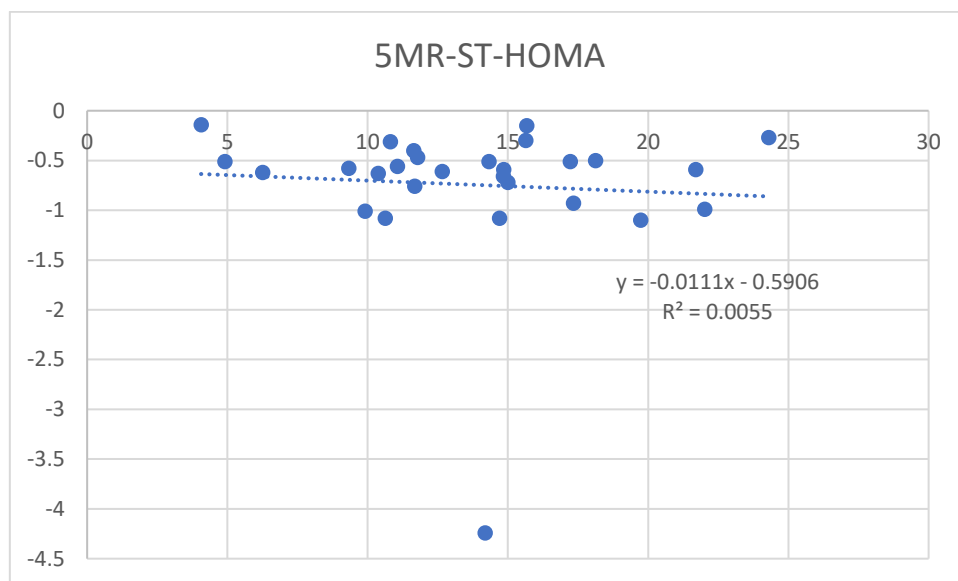


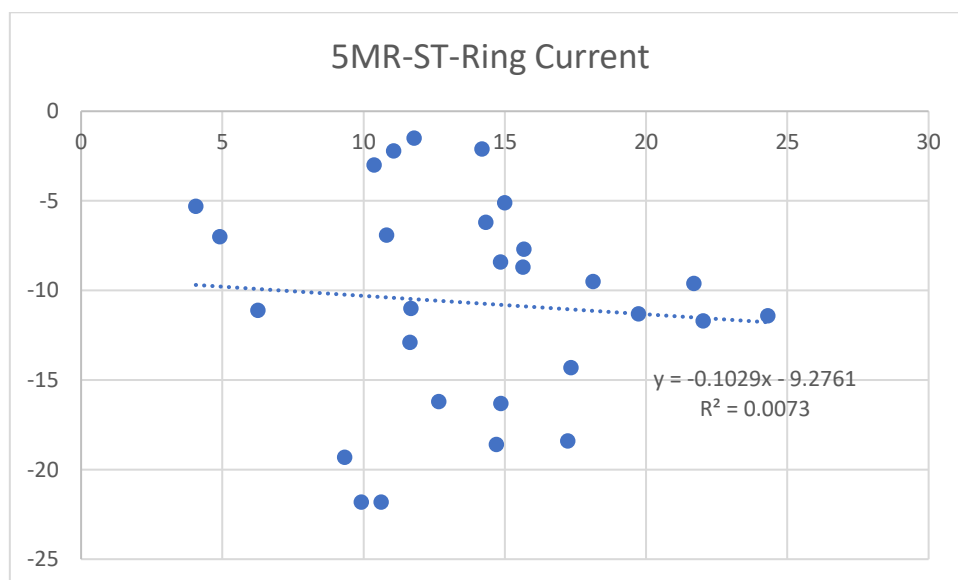
Figure S2. HOMA values of bicyclic molecules. Positive and negative values, indicating aromaticity and antiaromaticity, respectively, are listed in black and red fonts. Rings with a green filling are those that possess a Clar's sextet based on the ring current analysis.

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Figure S3. Correlation coefficients between various aromaticity indicators and the HOMO-LUMO and singlet-triplet gaps:

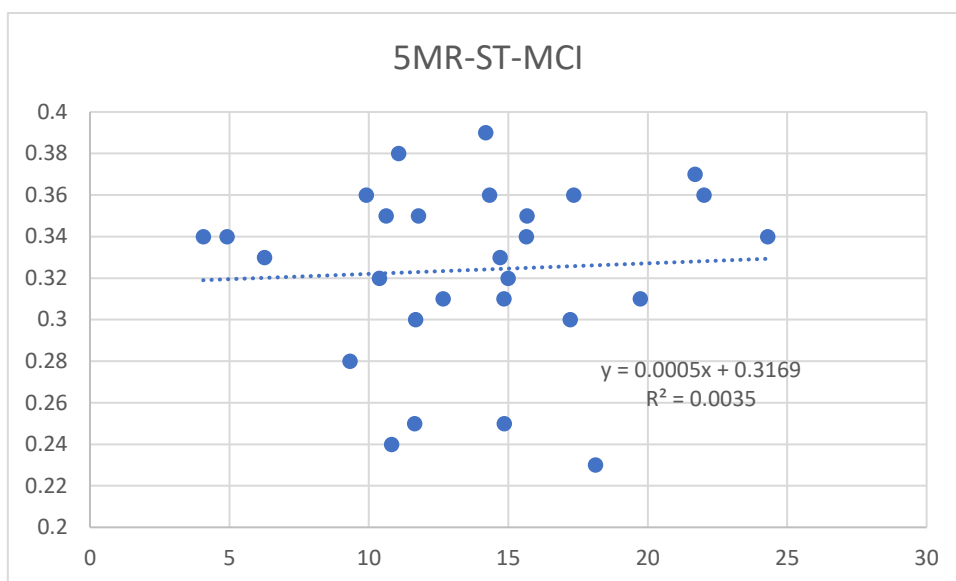


(a) Singlet-triplet gap versus HOMA values of the 5-membered rings among bicyclic species.

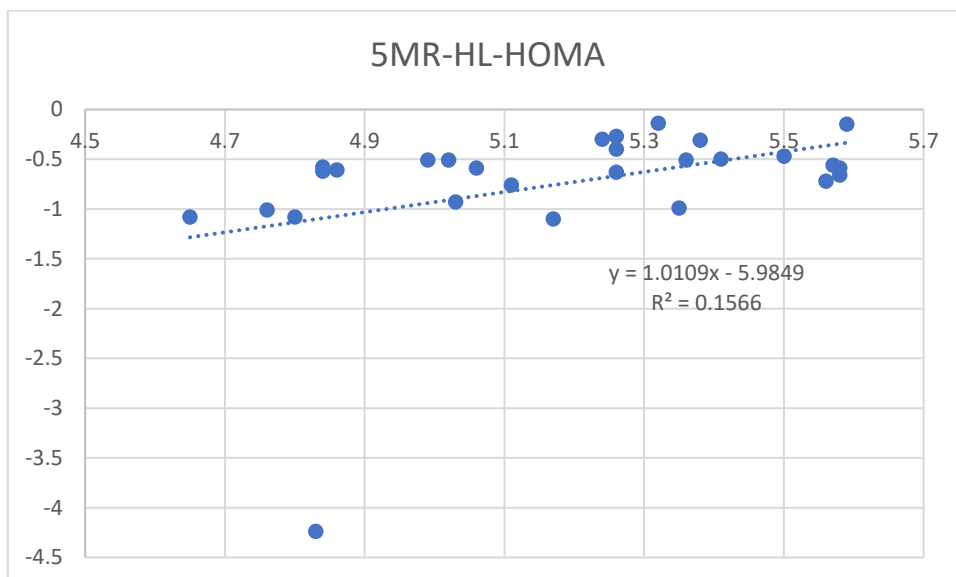


(b) Singlet-triplet gap versus ring current of the 5-membered rings among bicyclic species.

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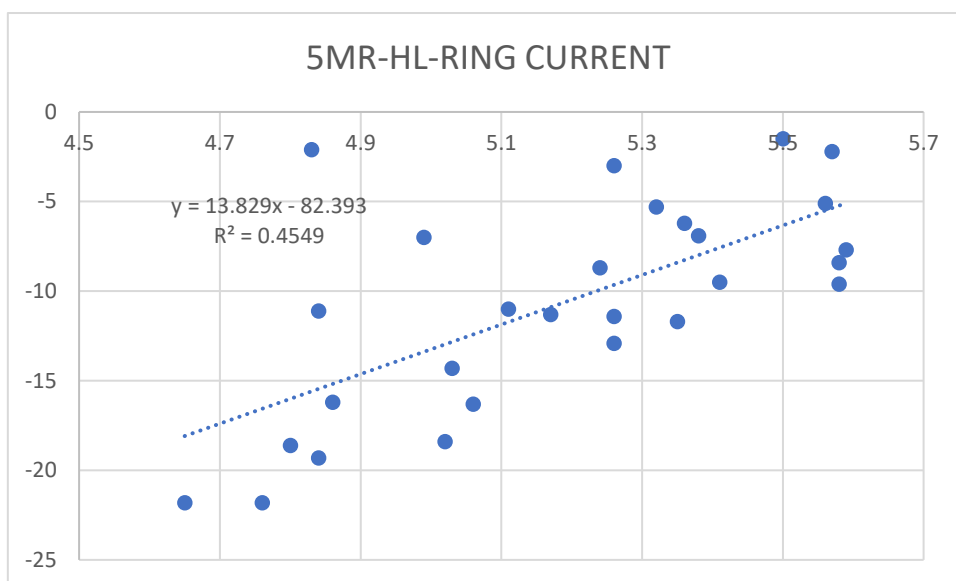


(c) Singlet-triplet gap versus MCI of the 5-membered rings among bicyclic species.

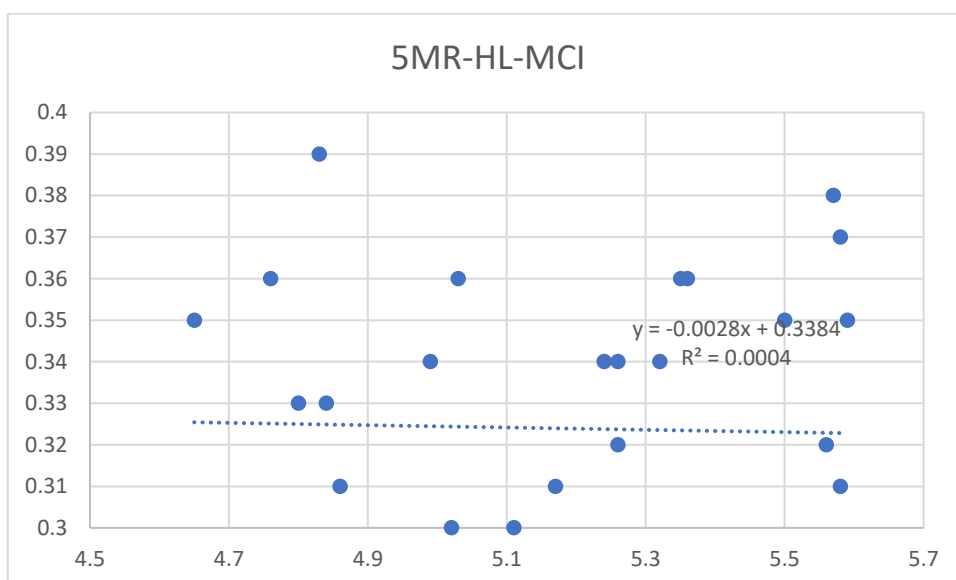


(d) HOMO-LUMO gap versus HOMA of the 5-membered rings among bicyclic species.

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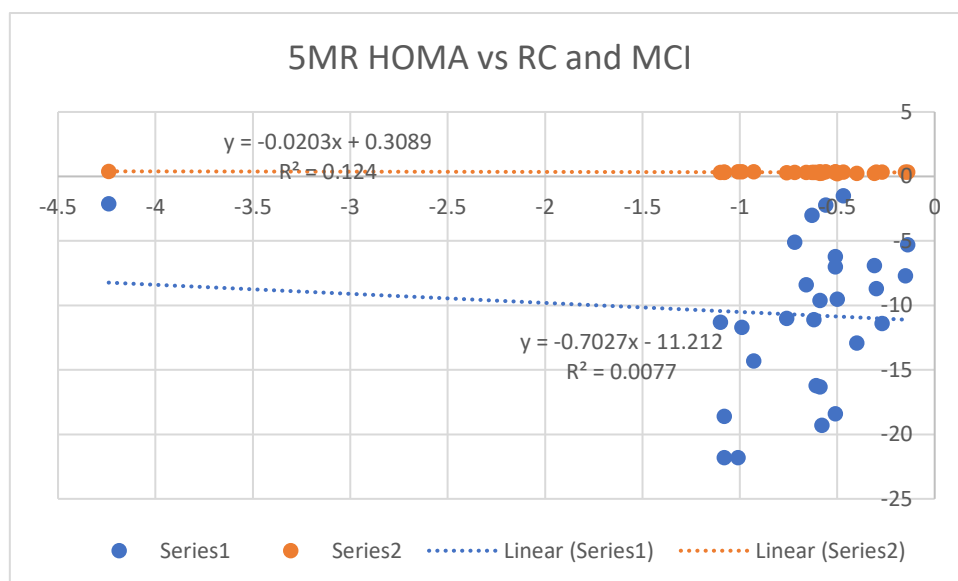


(e) HOMO-LUMO gap versus ring current of the 5-membered rings among bicyclic species.

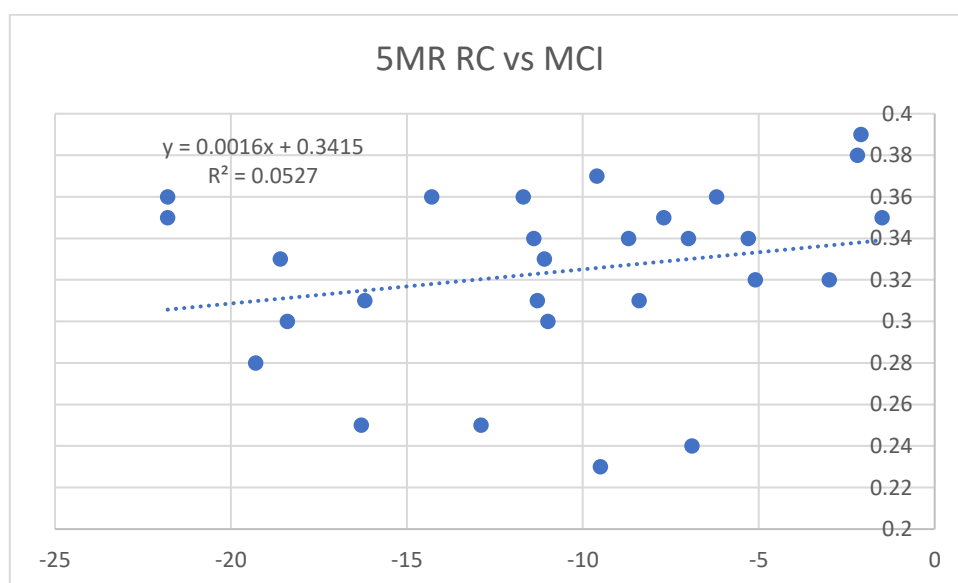


(f) HOMO-LUMO gap versus MCI of the 5-membered rings among bicyclic species.

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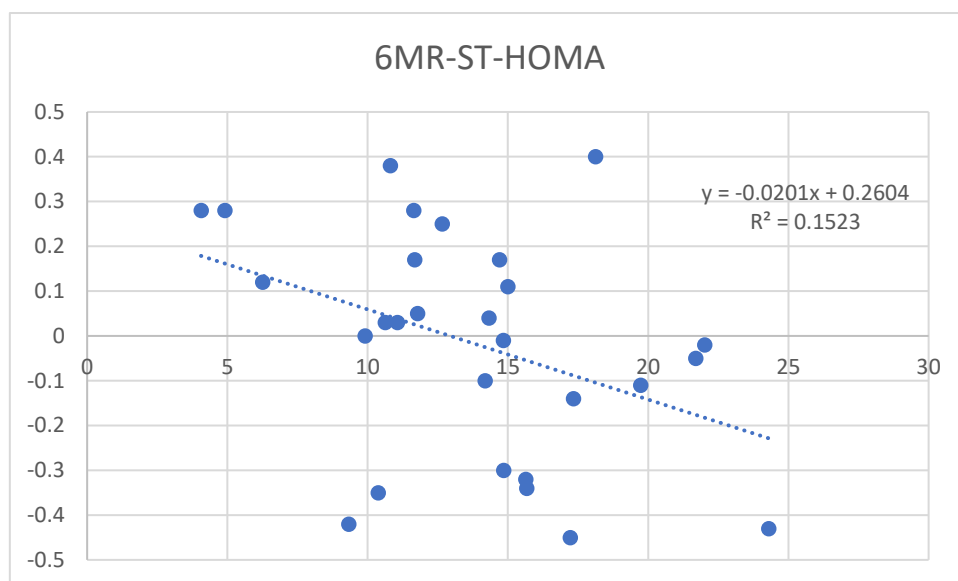


(g) HOMA vs ring current (Series 1) and MCI (Series 2) for the 5-membered rings among bicyclic species.

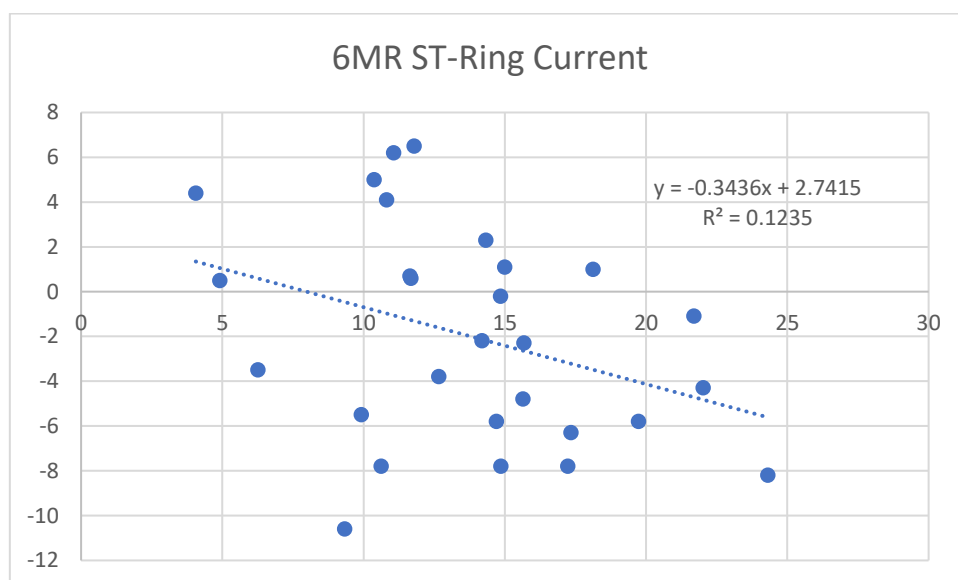


(h) Ring current versus MCI for the 5-membered rings among bicyclic species.

Supporting Information

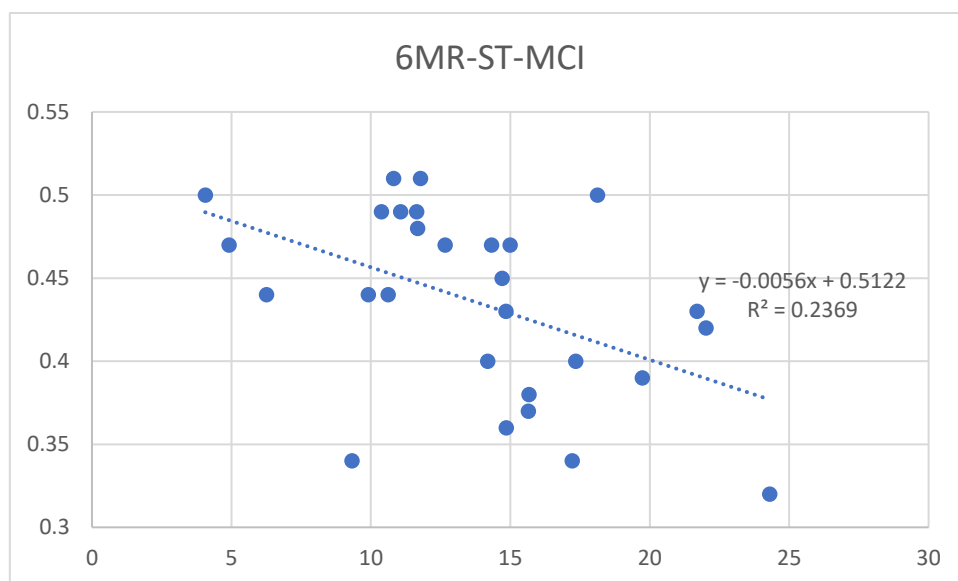


(i) Singlet-triplet gap versus HOMA values of the 6-membered rings among bicyclic species.

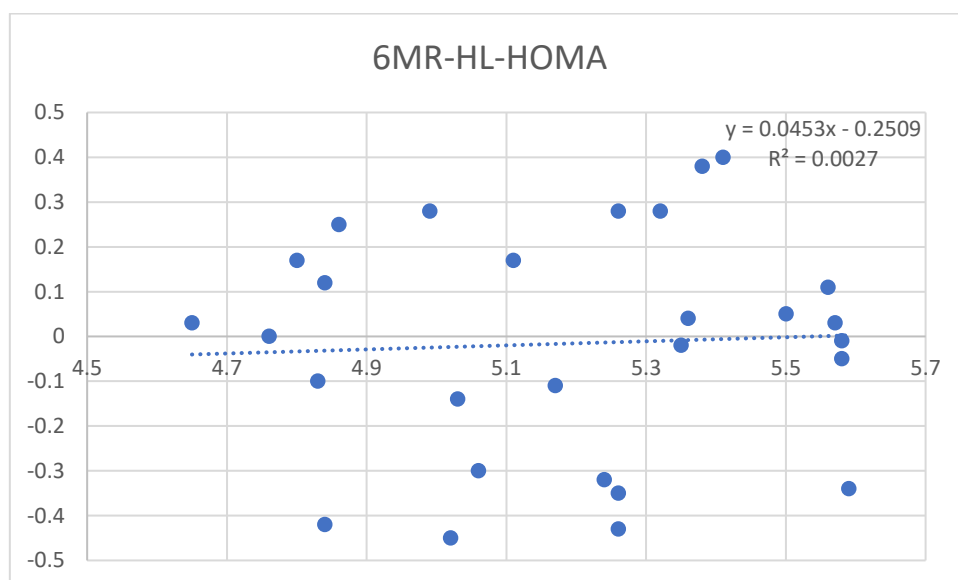


(j) Singlet-triplet gap versus ring current of the 6-membered rings among bicyclic species.

Supporting Information

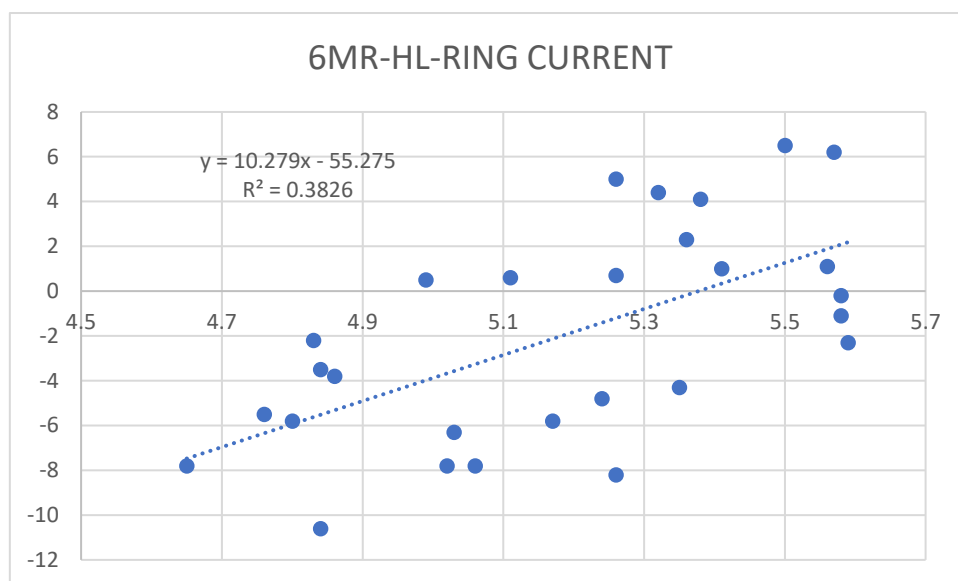


(k) Singlet-triplet gap versus MCI values of the 6-membered rings among bicyclic species.

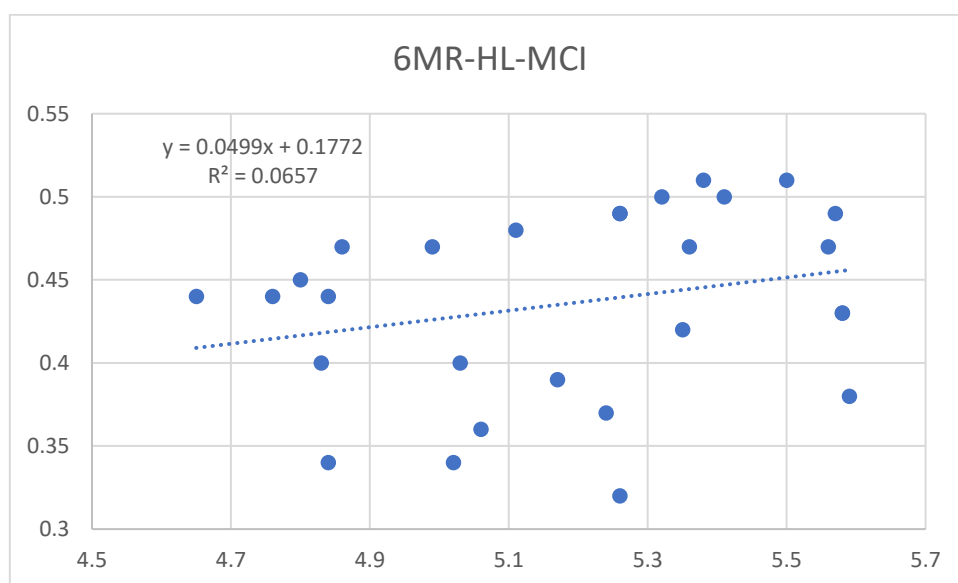


(l) HOMO-LUMO gap versus HOMA values of the 6-membered rings among bicyclic species.

Supporting Information

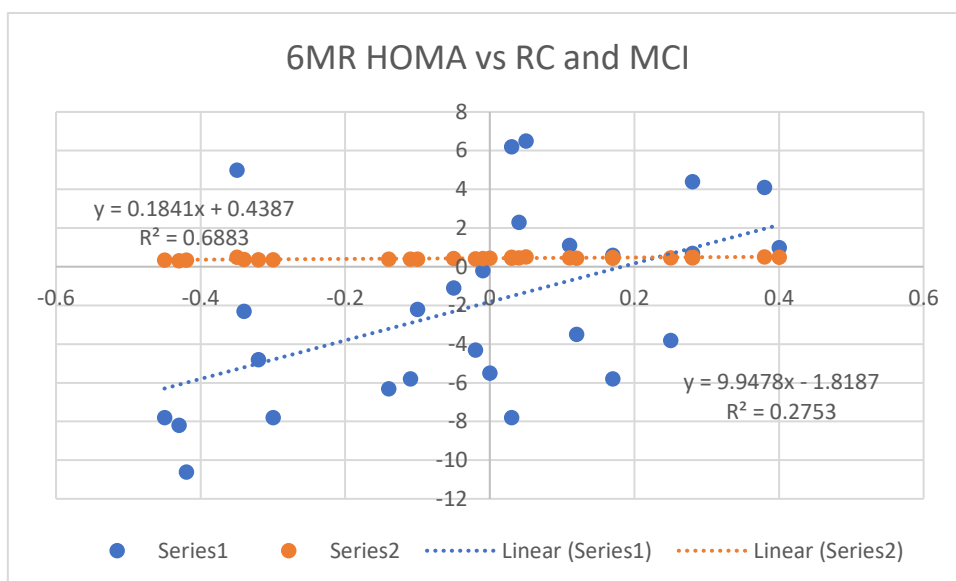


(m) HOMO-LUMO gap versus ring current values of the 6-membered rings among bicyclic species.

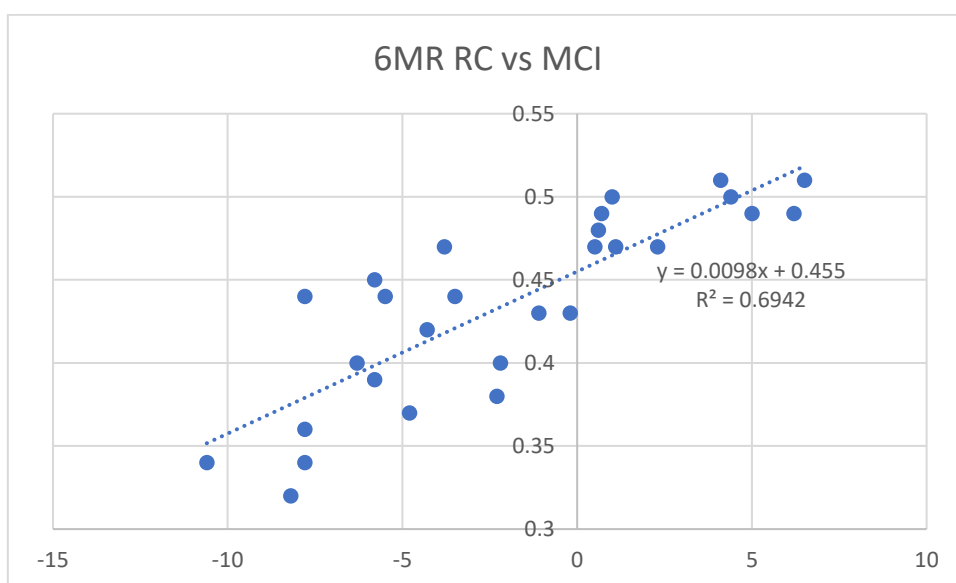


(n) HOMO-LUMO gap versus MCI values of the 6-membered rings among bicyclic species.

Supporting Information

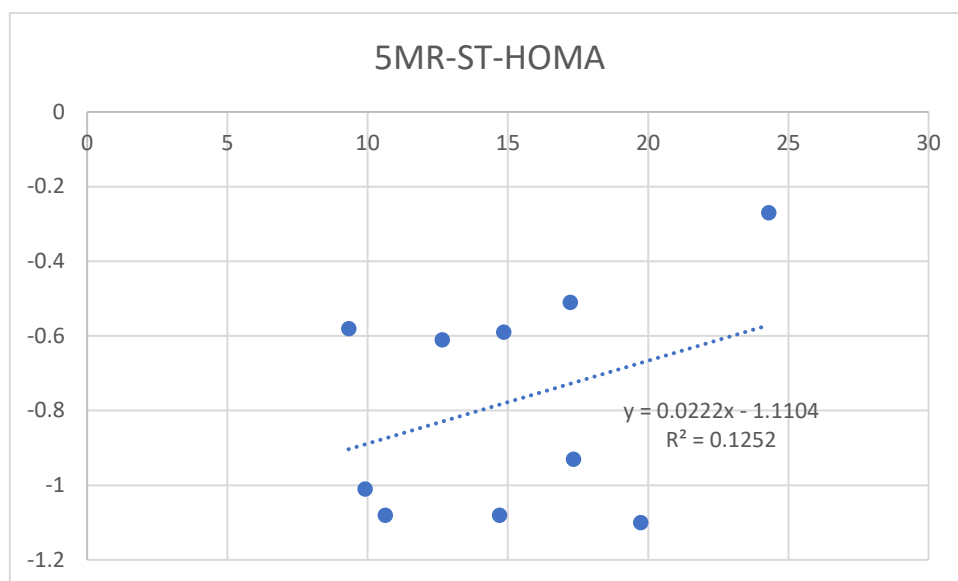


(o) HOMA vs ring current (Series 1) and MCI (Series 2) for the 6-membered rings among bicyclic species.

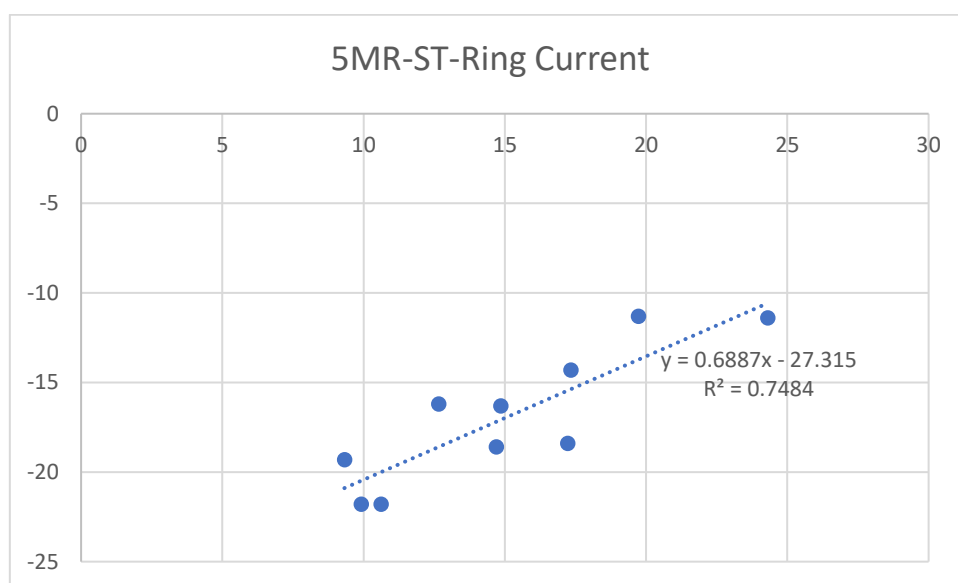


(p) Ring current versus MCI for the 6-membered rings among bicyclic species.

Supporting Information

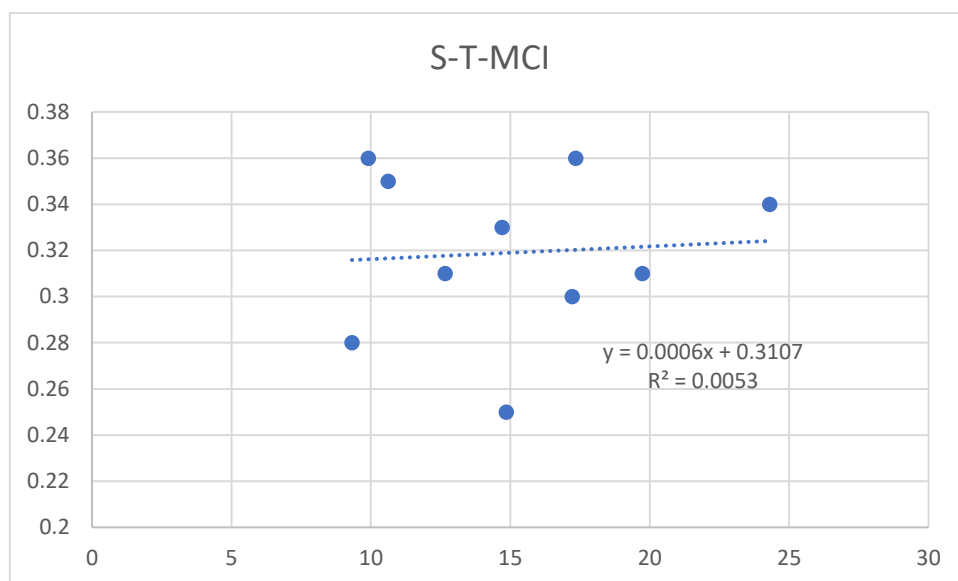


(q) Singlet-triplet gap versus HOMA values of the 5-membered rings among planar bicyclic species.

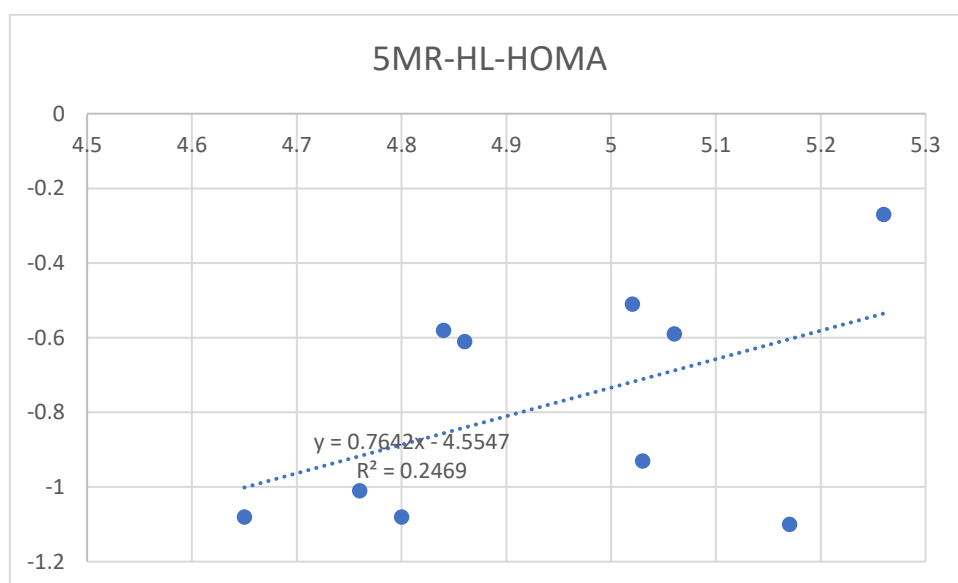


(r) Singlet-triplet gap versus ring current values of the 5-membered rings among planar bicyclic species.

Supporting Information

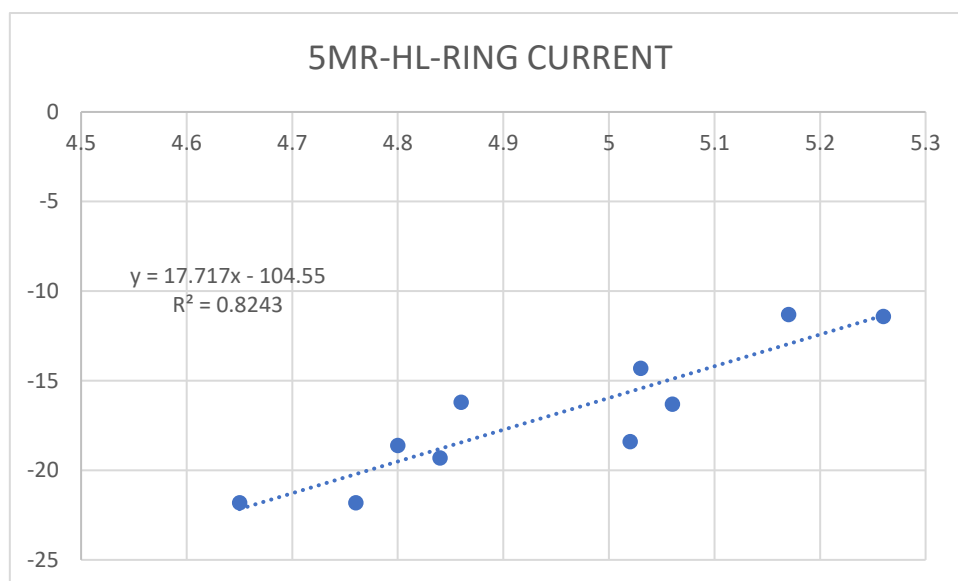


(s) Singlet-triplet gap versus MCI values of the 5-membered rings among planar bicyclic species.

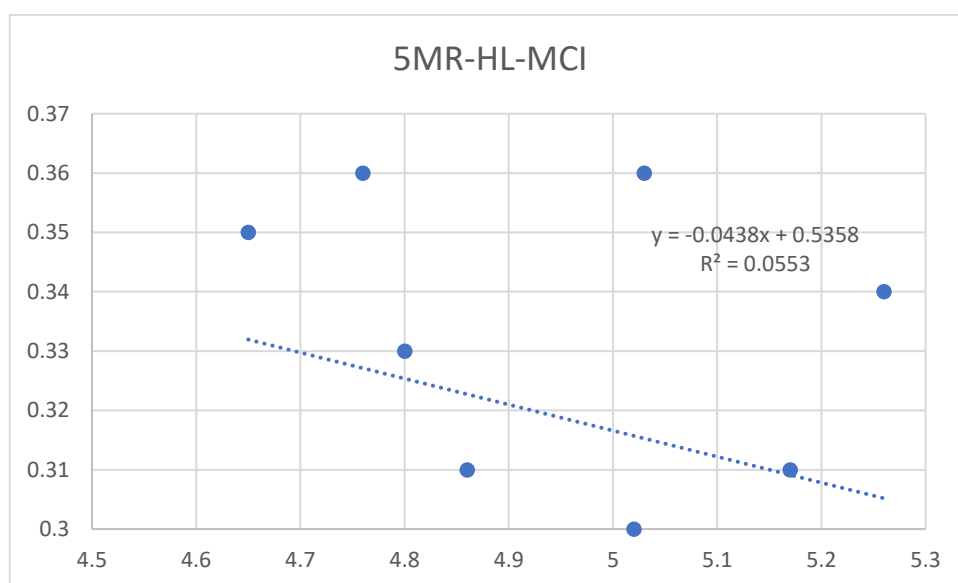


(t) HOMO-LUMO gap versus HOMA values of the 5-membered rings among planar bicyclic species.

Supporting Information

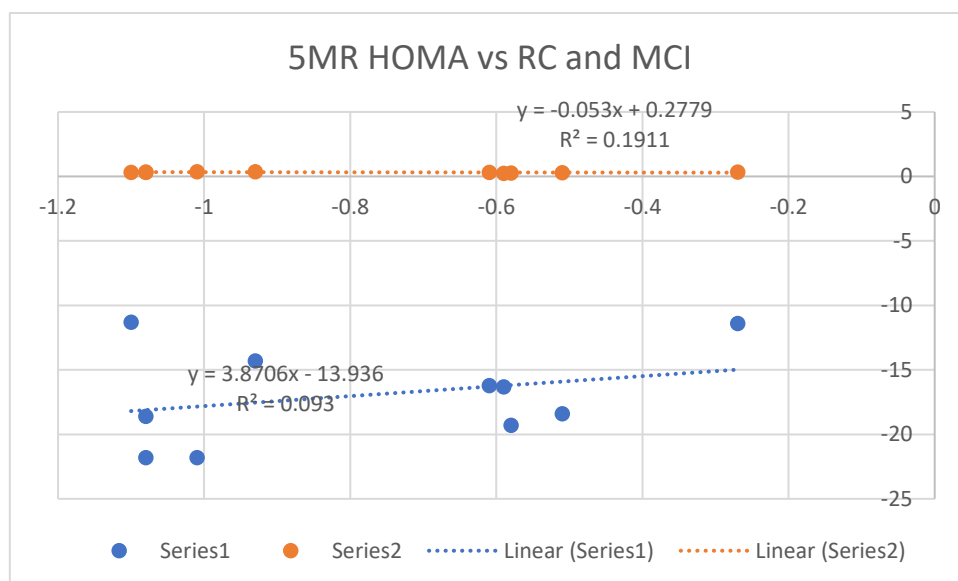


(u) HOMO-LUMO gap versus ring current values of the 5-membered rings among planar bicyclic species.

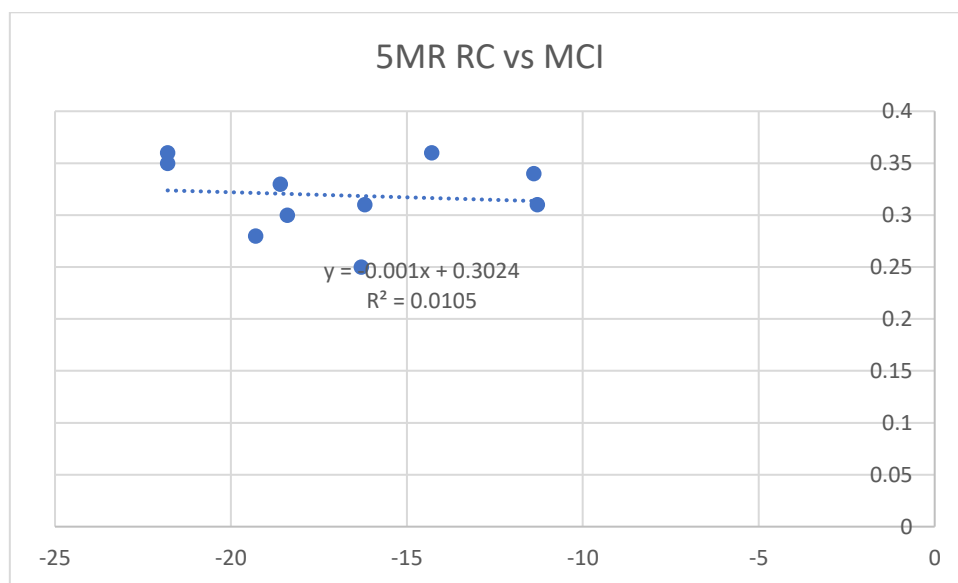


(v) HOMO-LUMO gap versus MCI values of the 5-membered rings among planar bicyclic species.

Supporting Information

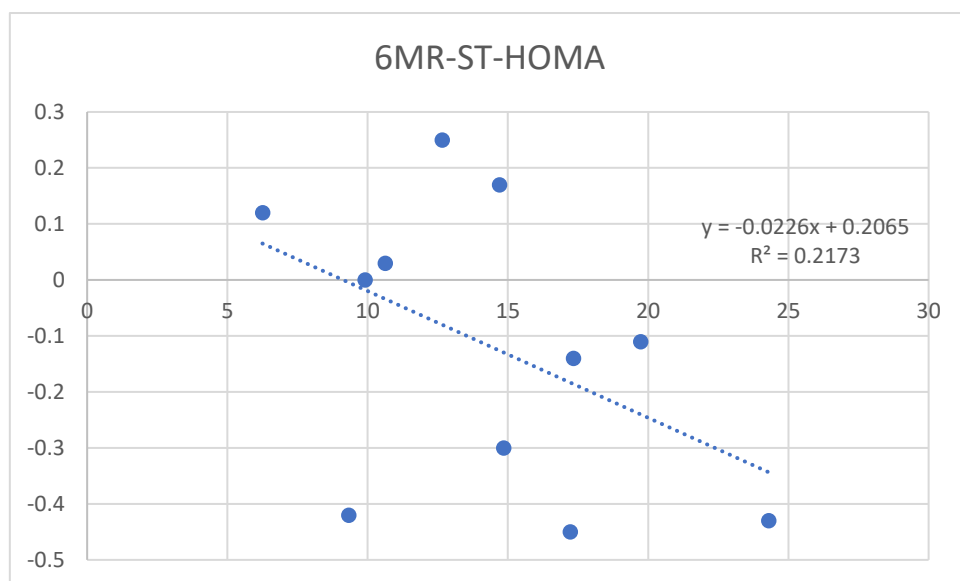


(w) HOMA vs ring current (Series 1) and MCI (Series 2) for the 5-membered rings among planar bicyclic species.

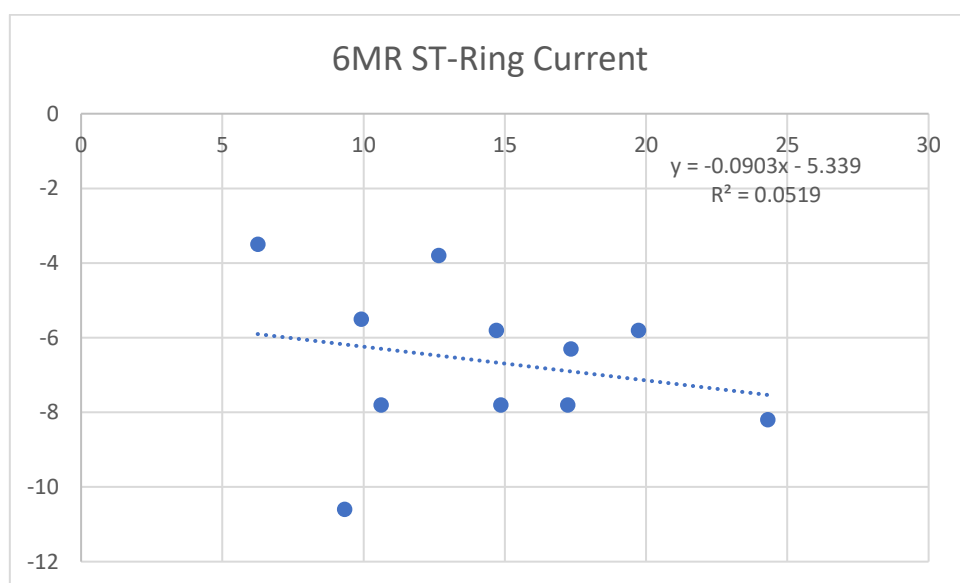


(x) Ring current versus MCI for the 5-membered rings among planar bicyclic species.

Supporting Information

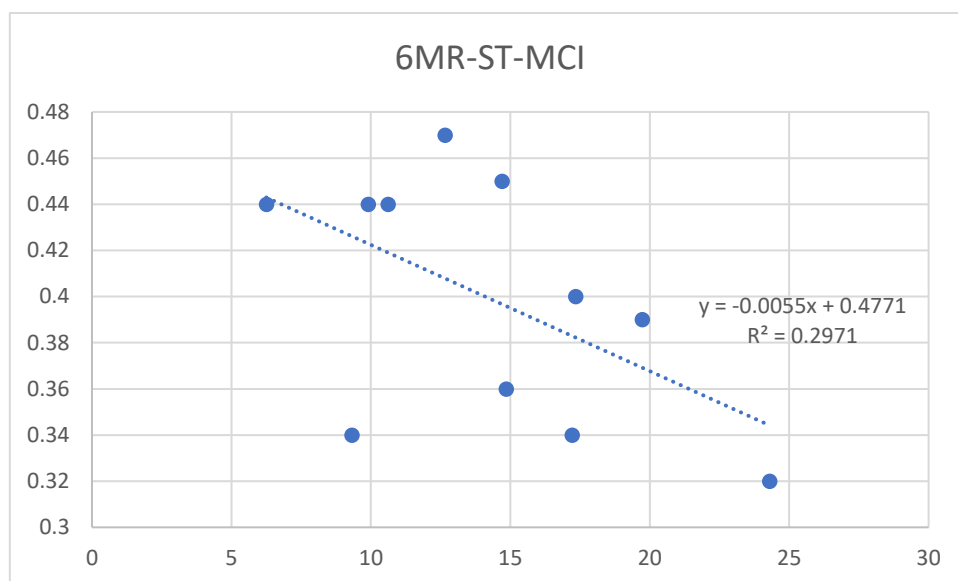


(y) Singlet-triplet gap versus HOMA values of the 6-membered rings among planar bicyclic species.

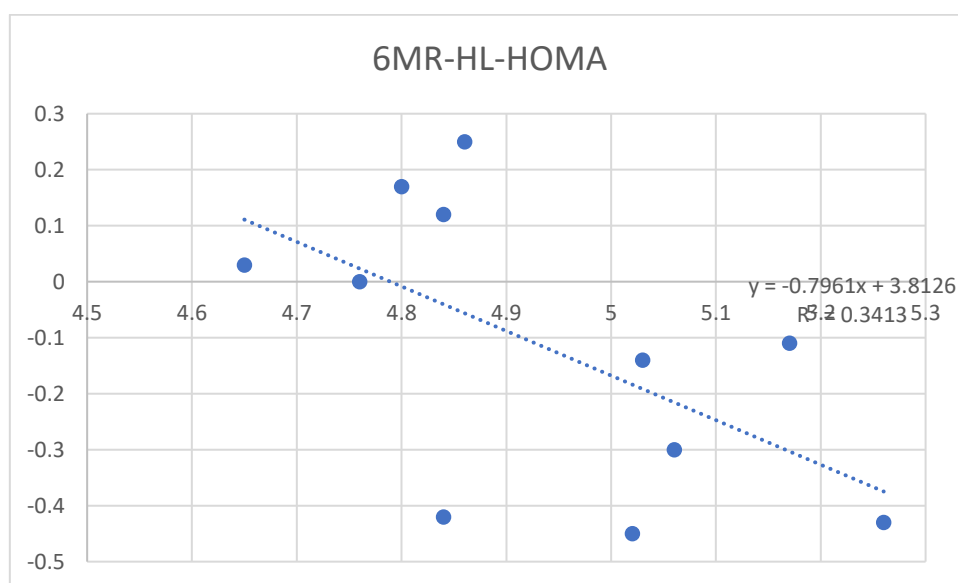


(z) Singlet-triplet gap versus ring current values of the 6-membered rings among planar bicyclic species.

Supporting Information

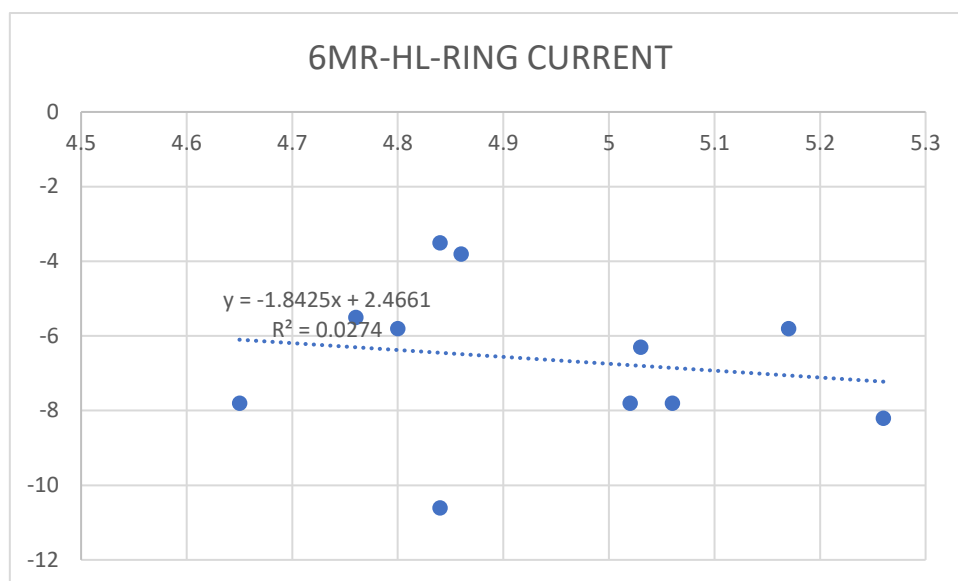


(aa) Singlet-triplet gap versus MCI values of the 6-membered rings among planar bicyclic species.

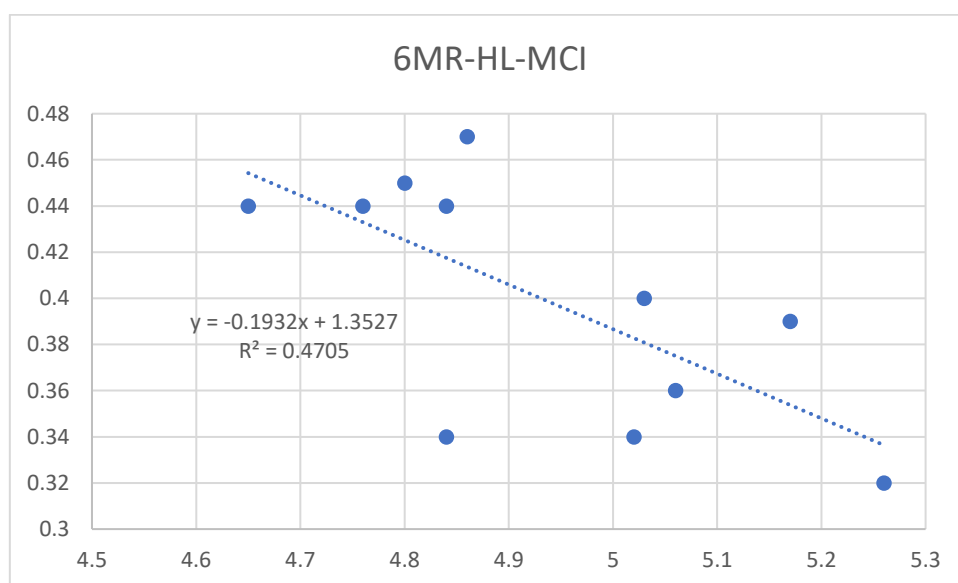


(ba) HOMO-LUMO gap versus HOMA values of the 6-membered rings among planar bicyclic species.

Supporting Information

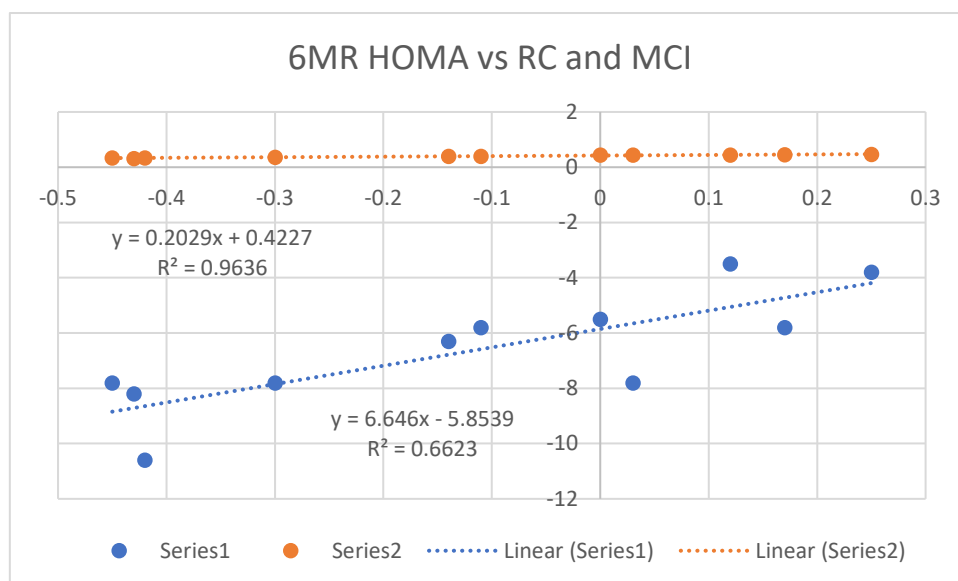


(ca) HOMO-LUMO gap versus ring current values of the 6-membered rings among planar bicyclic species.

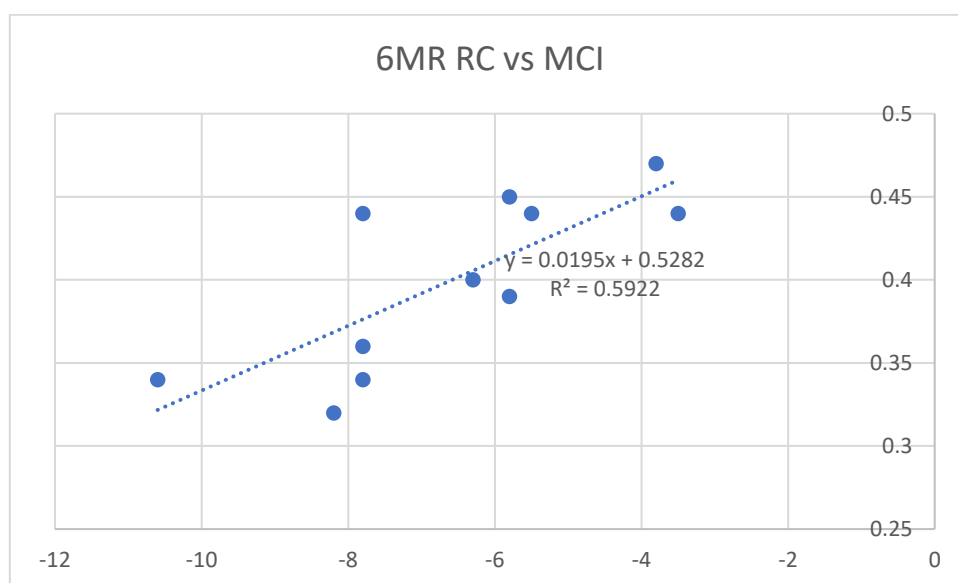


(da) HOMO-LUMO gap versus MCI values of the 6-membered rings among planar bicyclic species.

Supporting Information

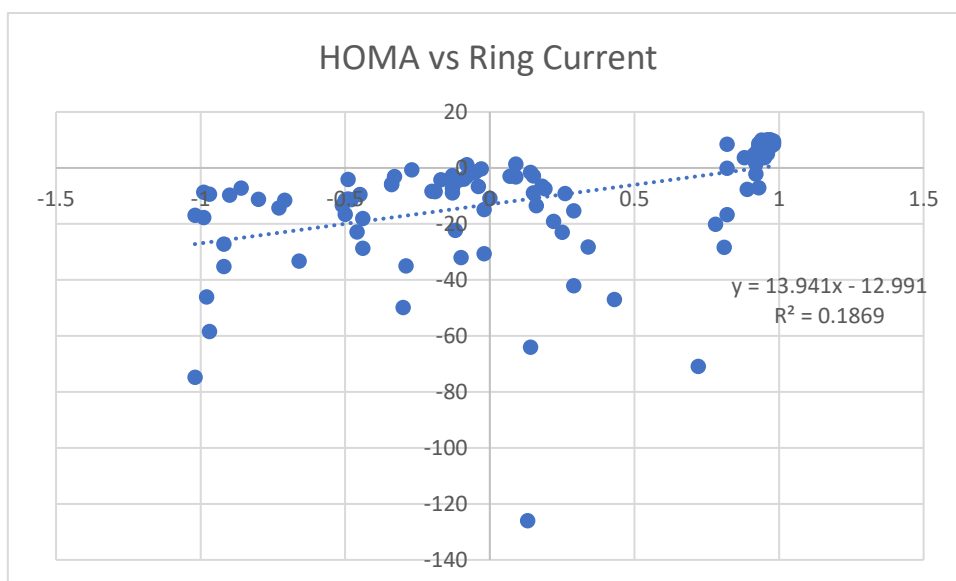


(ea) HOMA vs ring current (Series 1) and MCI (Series 2) for the 6-membered rings among planar bicyclic species.

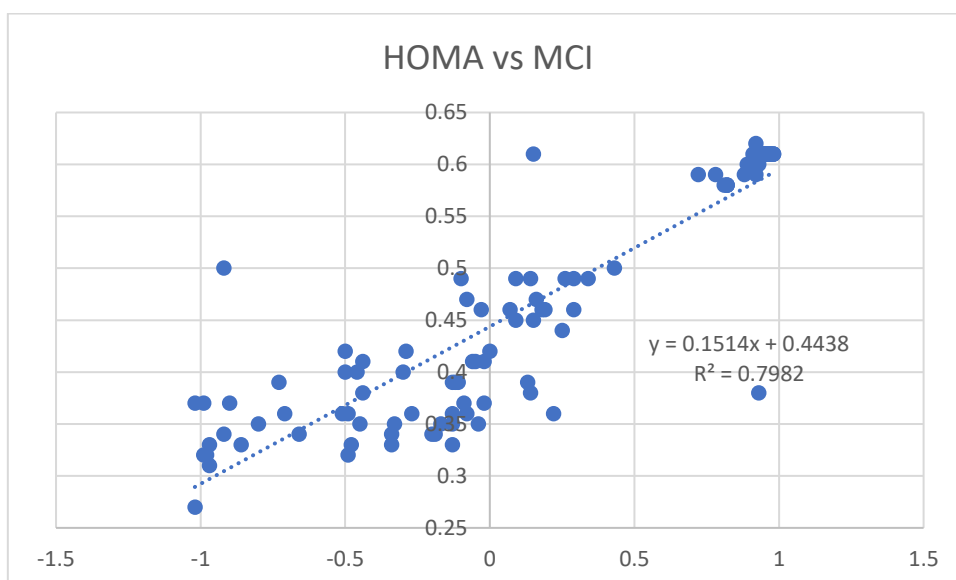


(fa) Ring current versus MCI for the 6-membered rings among planar bicyclic species.

Supporting Information

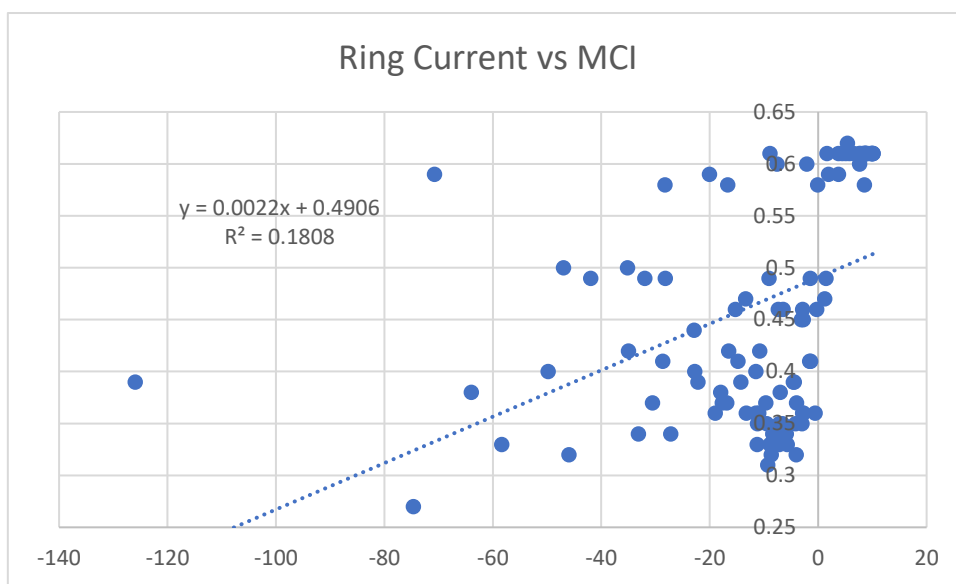


(ga) HOMA versus ring current for all rings among polycyclic species.

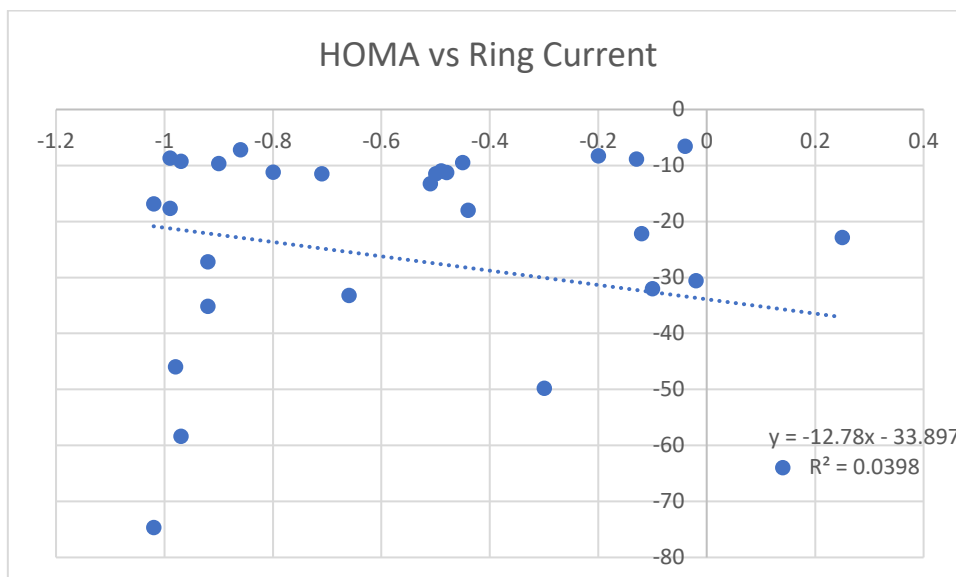


(ha) HOMA versus MCI for all rings among polycyclic species.

Supporting Information

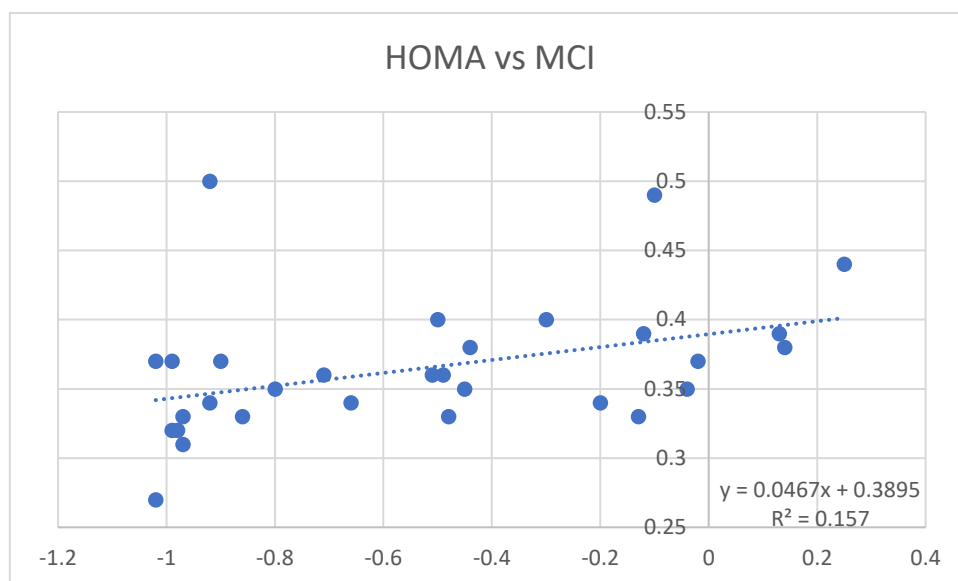


(ia) Ring current versus MCI for all rings among polycyclic species.

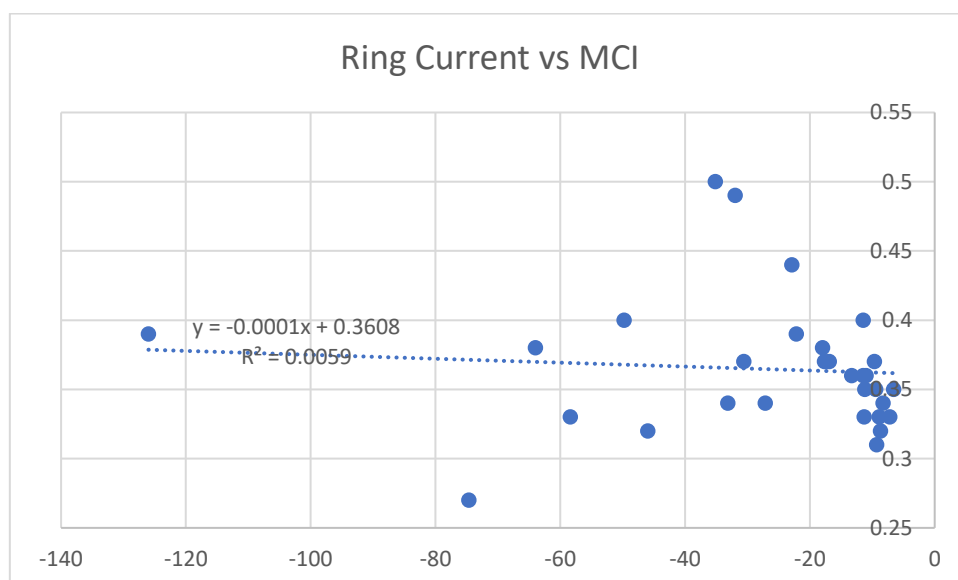


(ja) HOMA versus ring current for 5-membered rings among polycyclic species.

Supporting Information

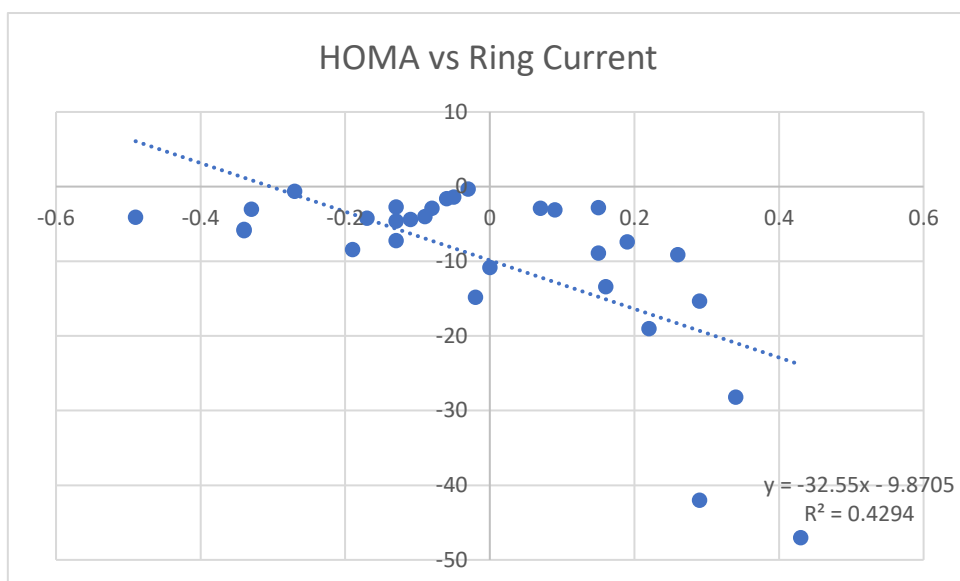


(ka) HOMA versus MCI for 5-membered rings among polycyclic species.

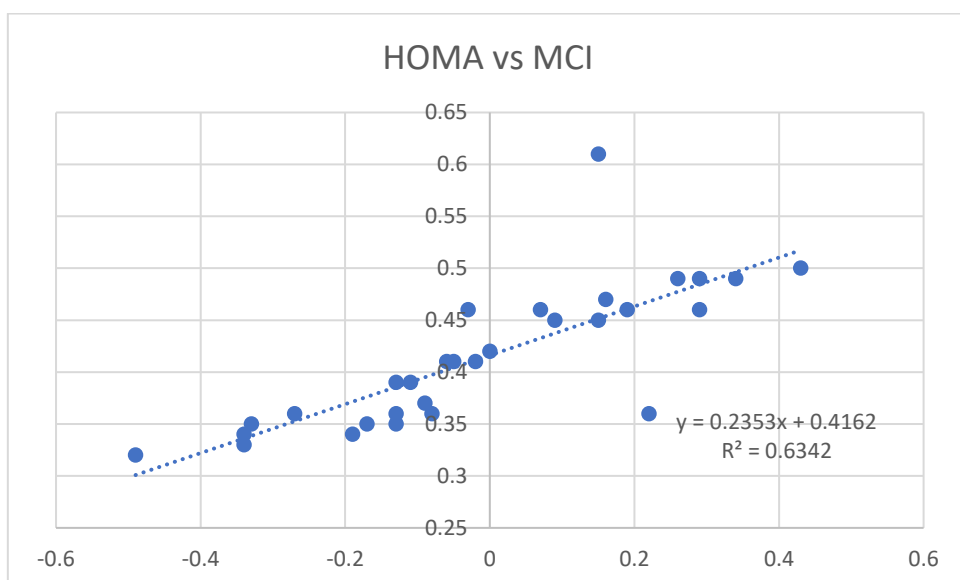


(la) Ring current versus MCI for 5-membered rings among polycyclic species.

Supporting Information

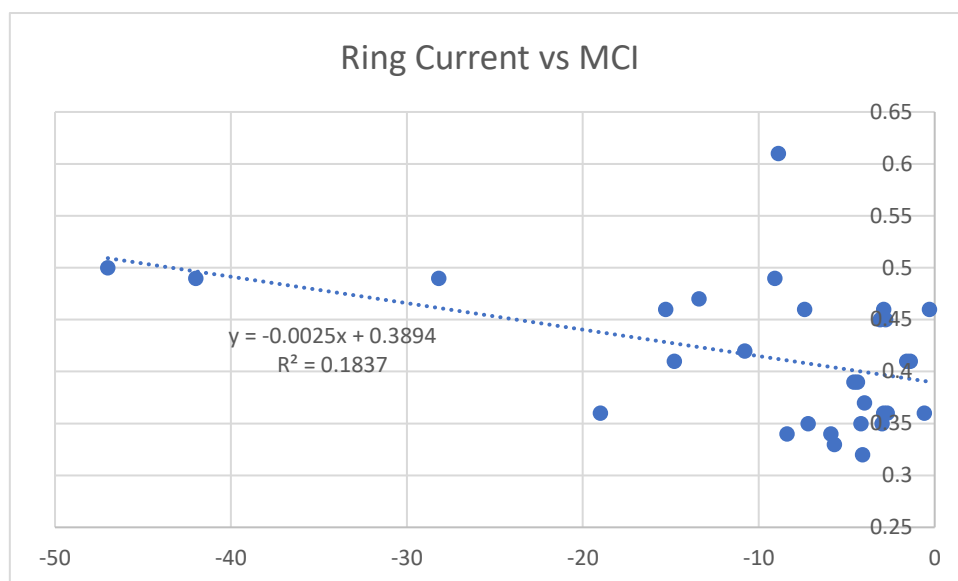


(ma) HOMA versus ring current for 6-membered rings among polycyclic species.

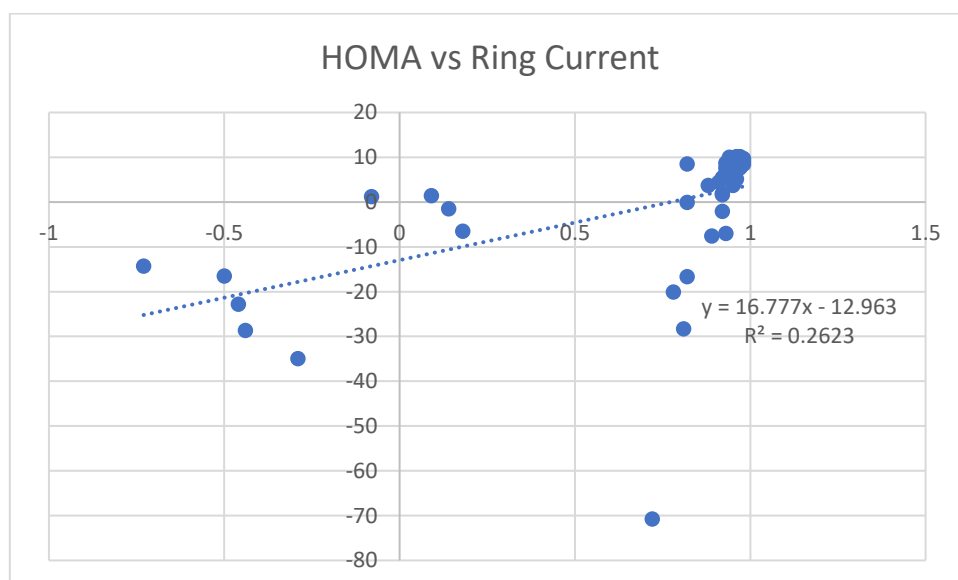


(na) HOMA versus MCI for 6-membered rings among polycyclic species.

Supporting Information

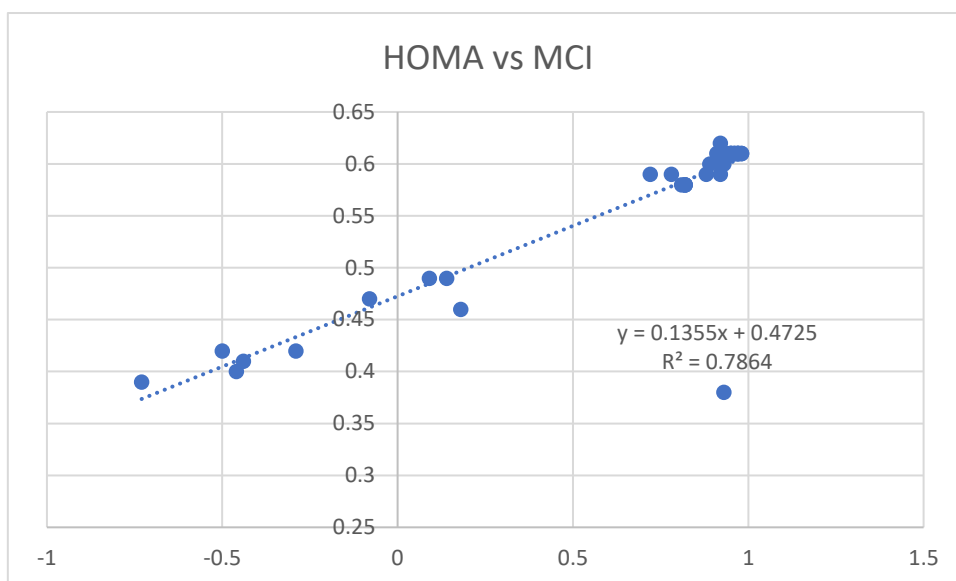


(oa) Ring current versus MCI for 6-membered rings among polycyclic species.

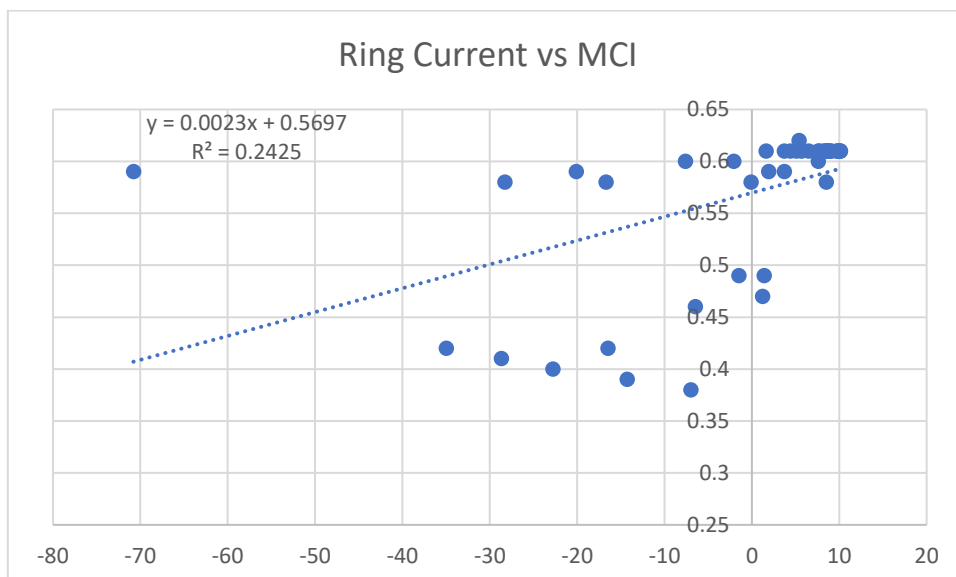


(pa) HOMA versus ring current for benzene rings among polycyclic species.

Supporting Information

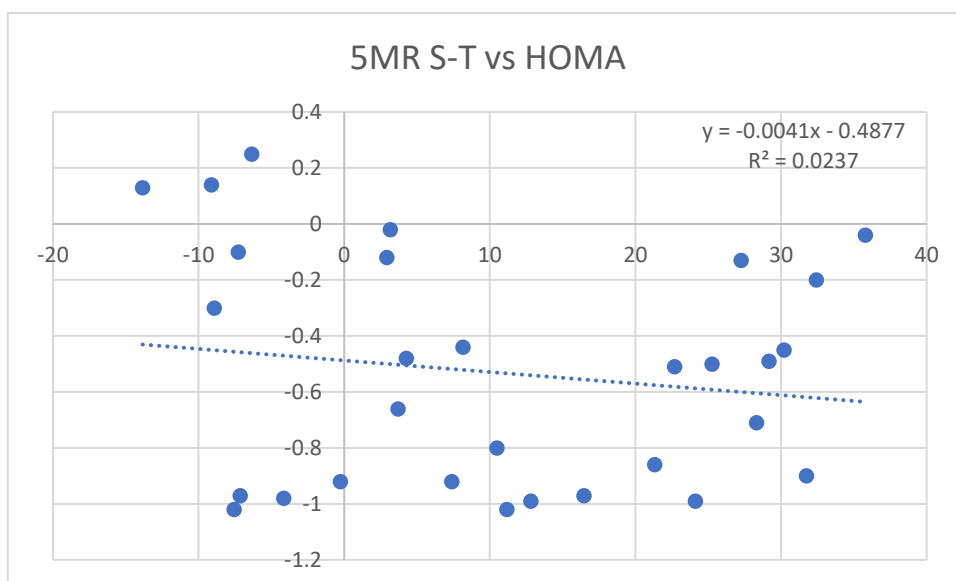


(qa) HOMA versus MCI for benzene rings among polycyclic species.

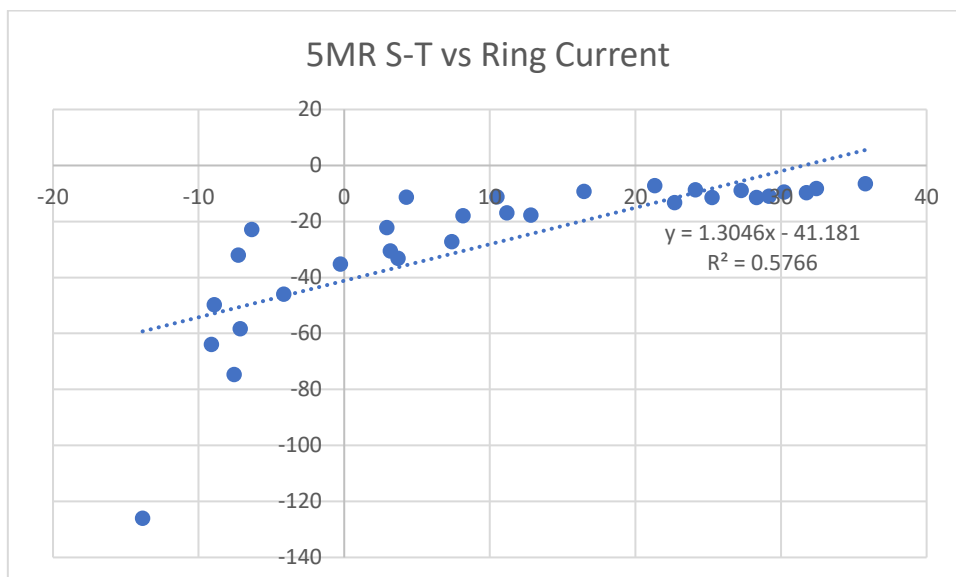


(ra) Ring current versus MCI for benzene rings among polycyclic species.

Supporting Information

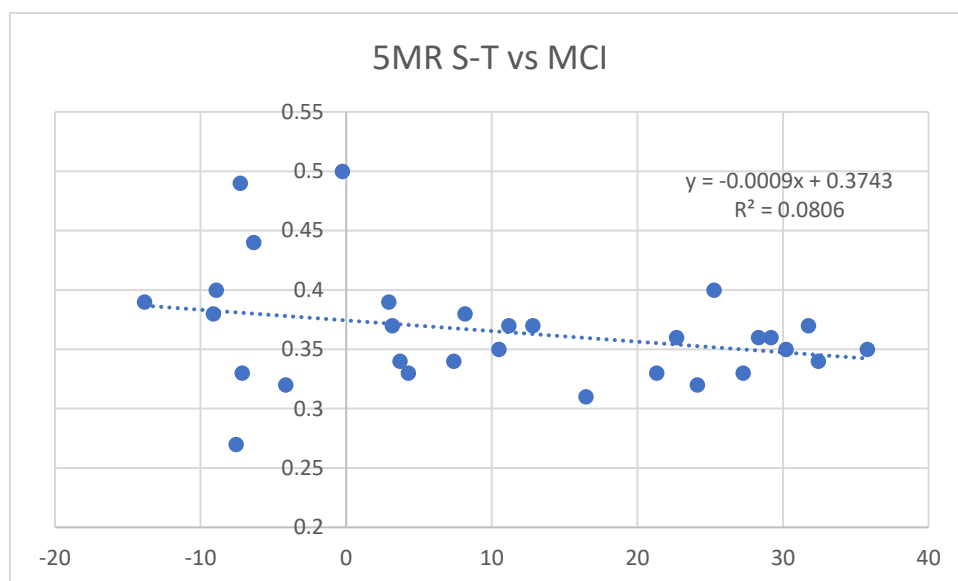


(sa) Singlet-triplet gap versus HOMA for 5-membered rings among polycyclic species.

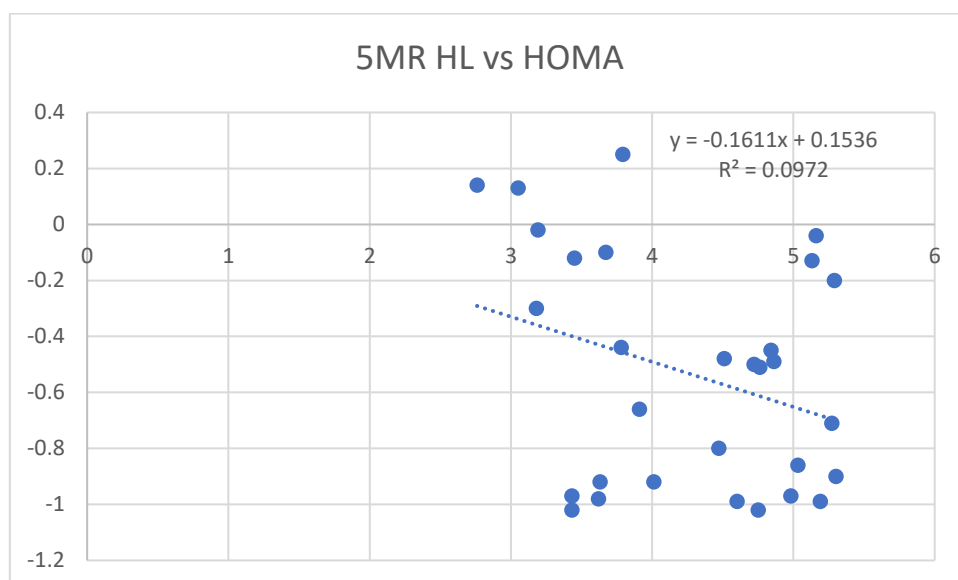


(ta) Singlet-triplet gap versus ring current for 5-membered rings among polycyclic species.

Supporting Information

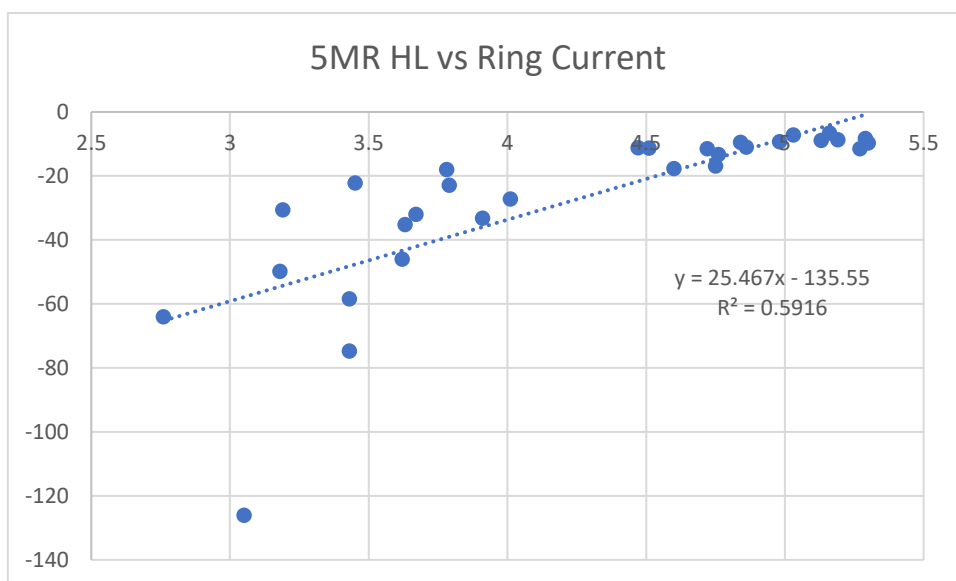


(ua) Singlet-triplet gap versus ring current for 5-membered rings among polycyclic species.

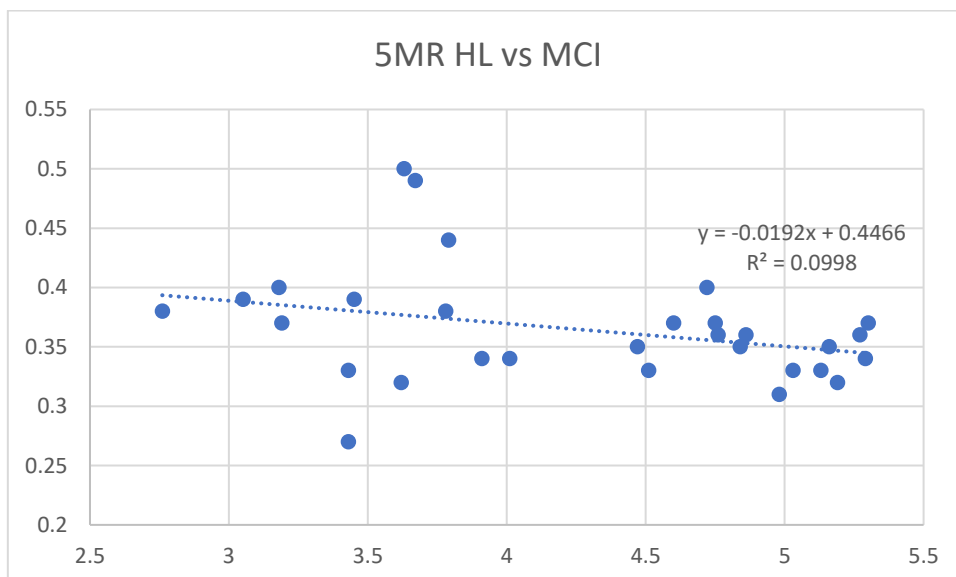


(va) HOMO-LUMO gap versus HOMA for 5-membered rings among polycyclic species.

Supporting Information

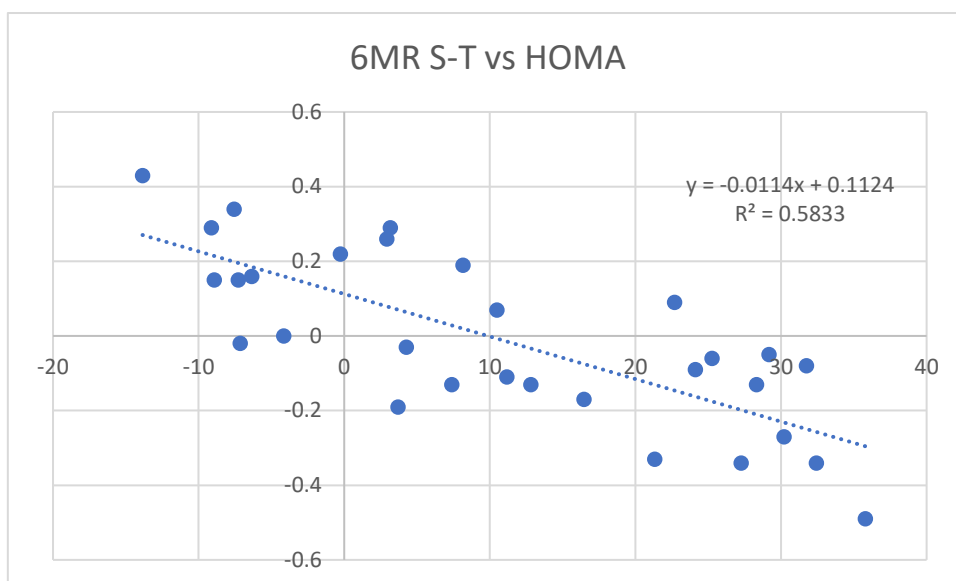


(wa) HOMO-LUMO gap versus ring current for 5-membered rings among polycyclic species.

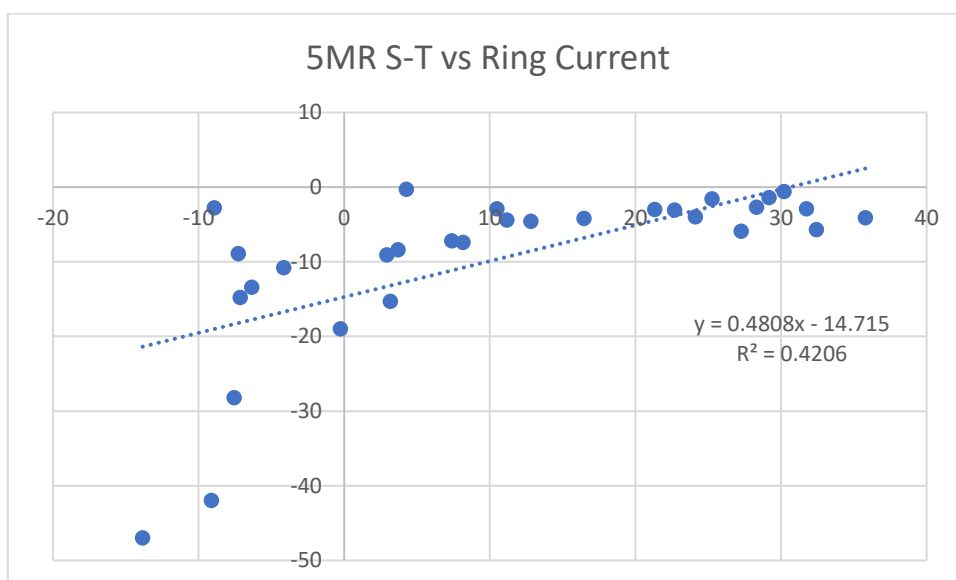


(xa) HOMO-LUMO gap versus MCI for 5-membered rings among polycyclic species.

Supporting Information

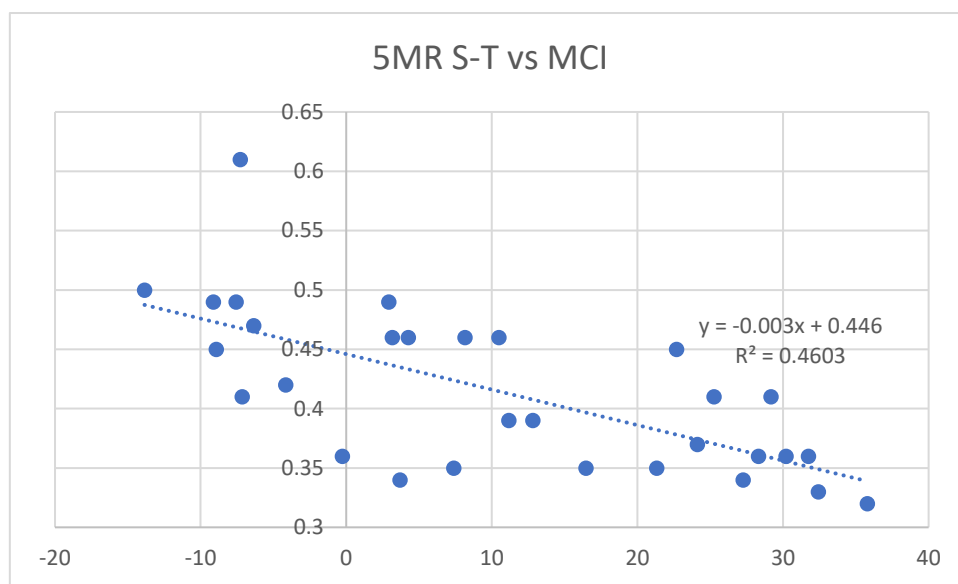


(ya) Singlet-triplet gap versus HOMA for 6-membered rings among polycyclic species.

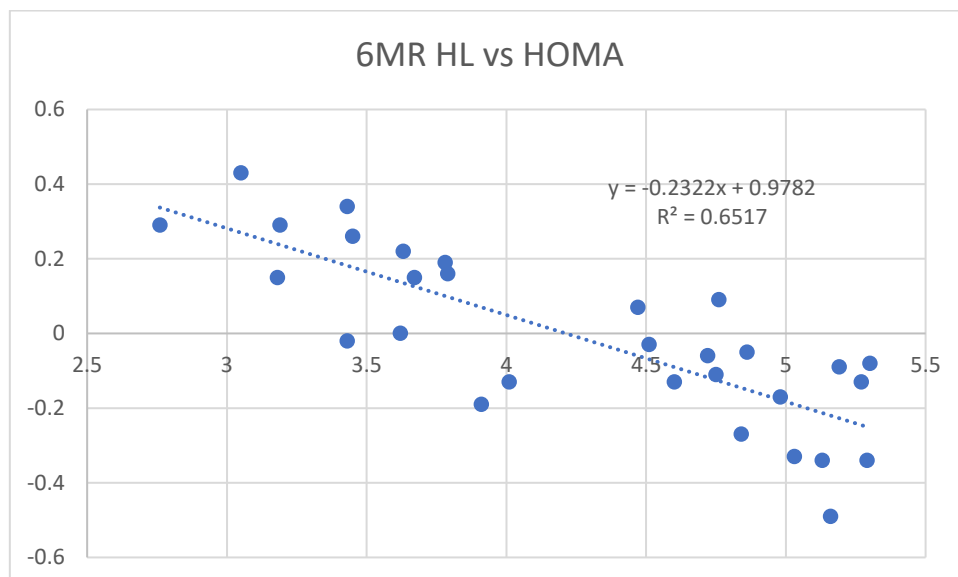


(za) Singlet-triplet gap versus ring current for 6-membered rings among polycyclic species.

Supporting Information

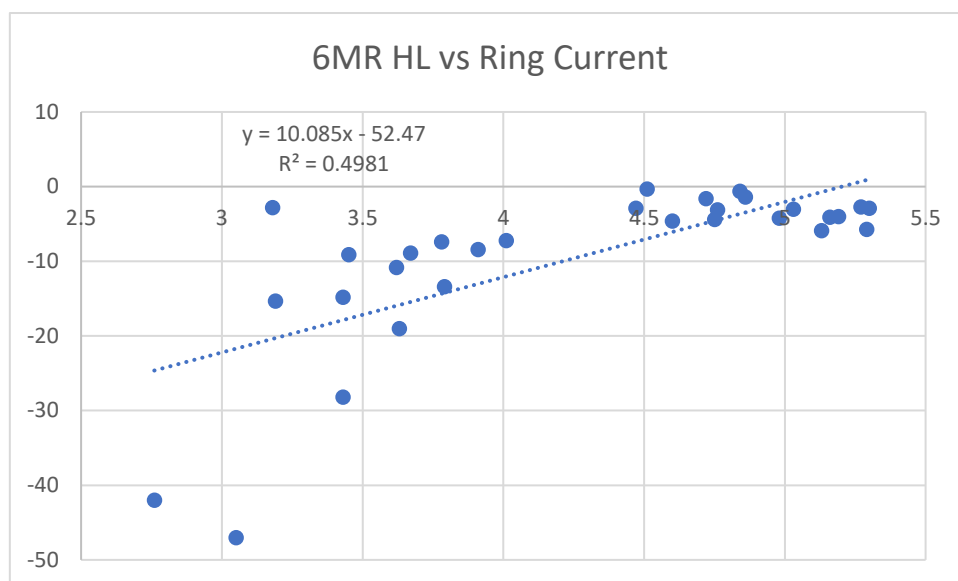


(ab) Singlet-triplet gap versus MCI for 6-membered rings among polycyclic species.

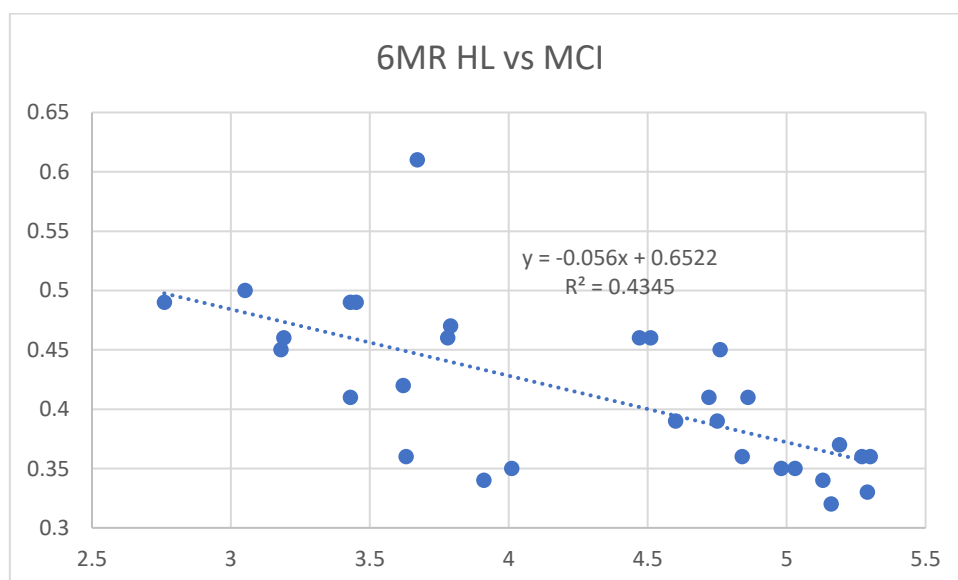


(bb) HOMO-LUMO gap versus HOMA for 6-membered rings among polycyclic species.

Supporting Information

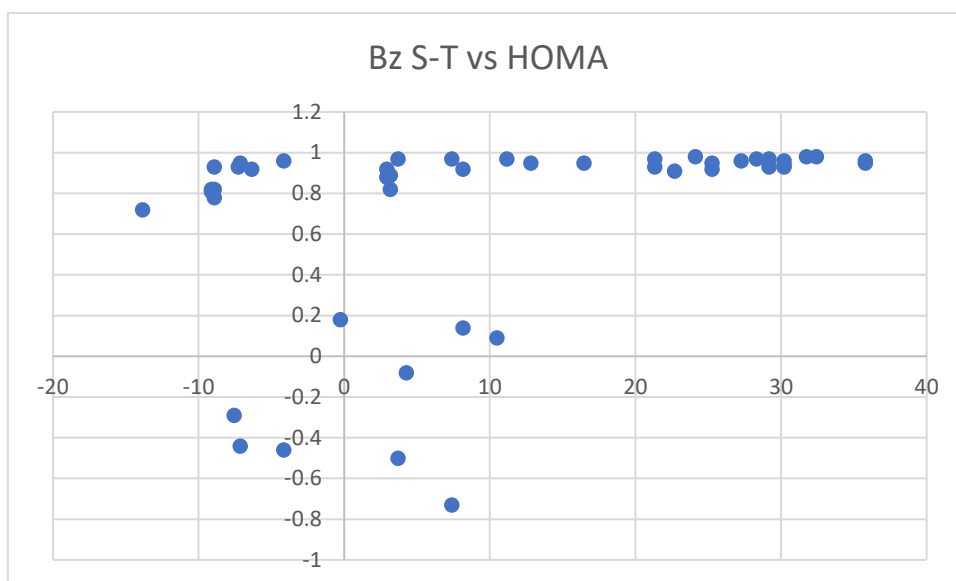


(cb) HOMO-LUMO gap versus ring current for 6-membered rings among polycyclic species.

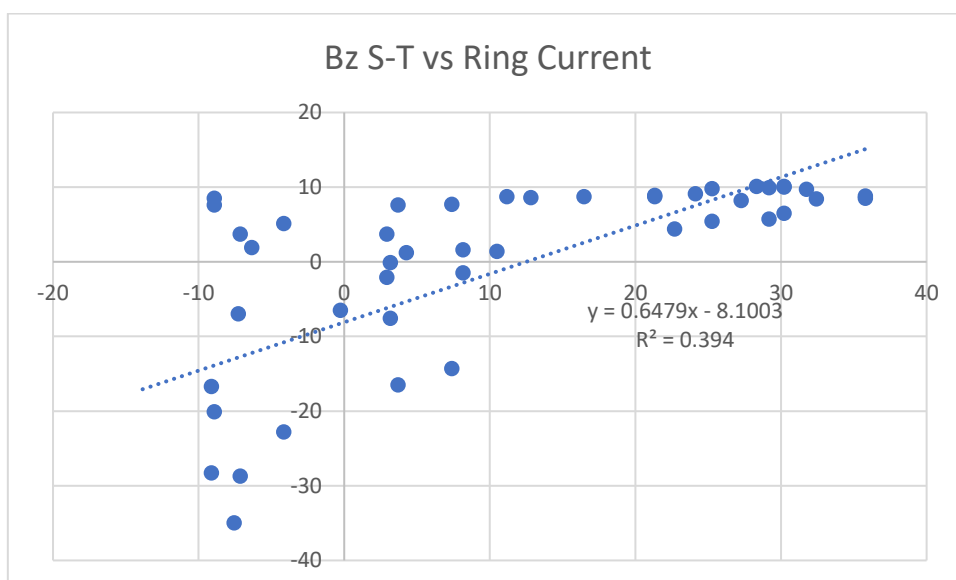


(db) HOMO-LUMO gap versus MCI for 6-membered rings among polycyclic species.

Supporting Information

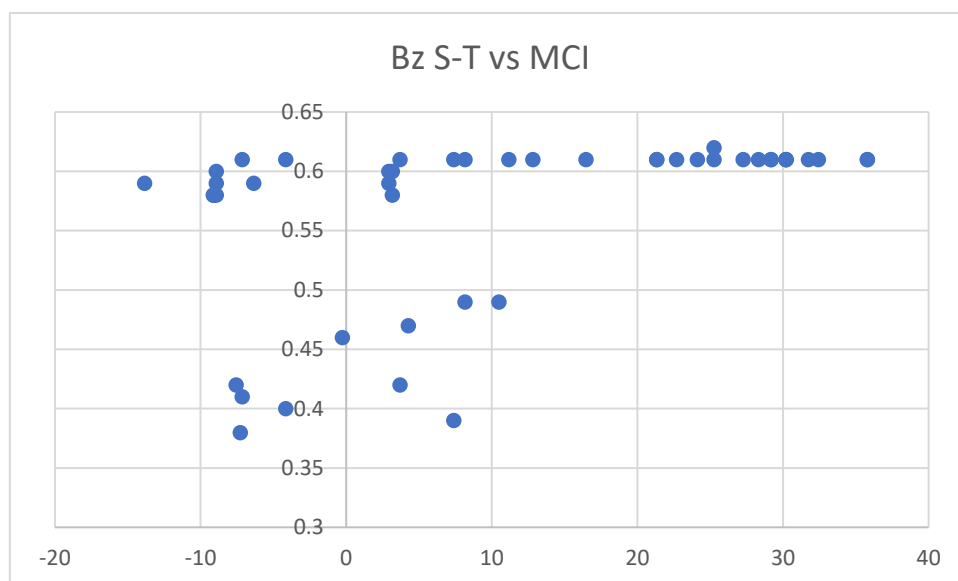


(eb) Singlet-triplet gap versus HOMA for benzene rings among polycyclic species.

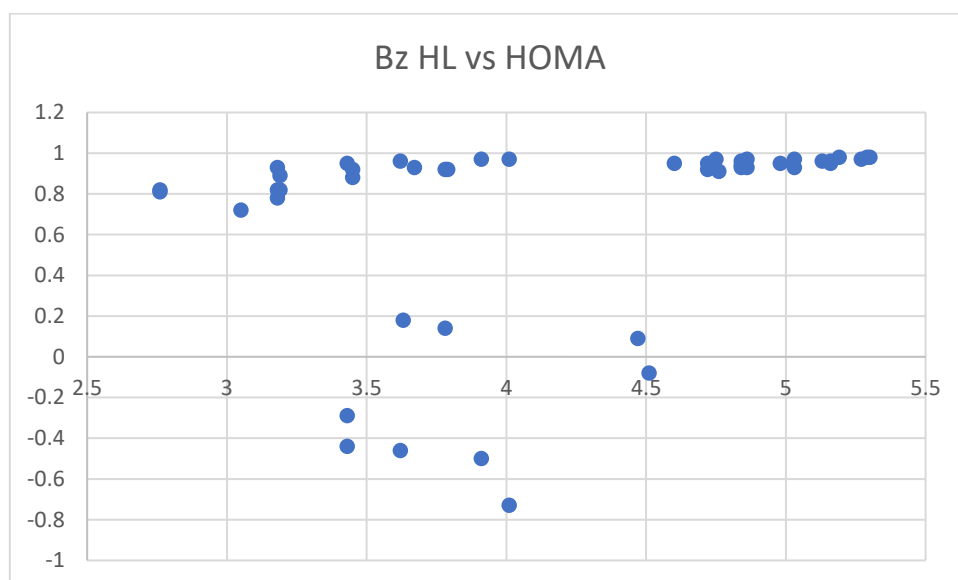


(fb) Singlet-triplet gap versus ring current for benzene rings among polycyclic species.

Supporting Information

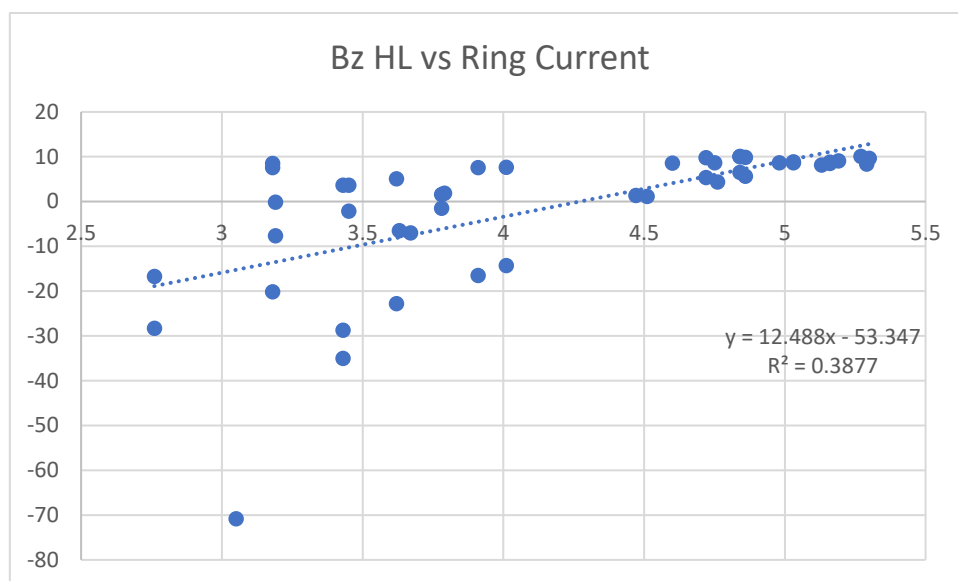


(gb) Singlet-triplet gap versus MCI for benzene rings among polycyclic species.

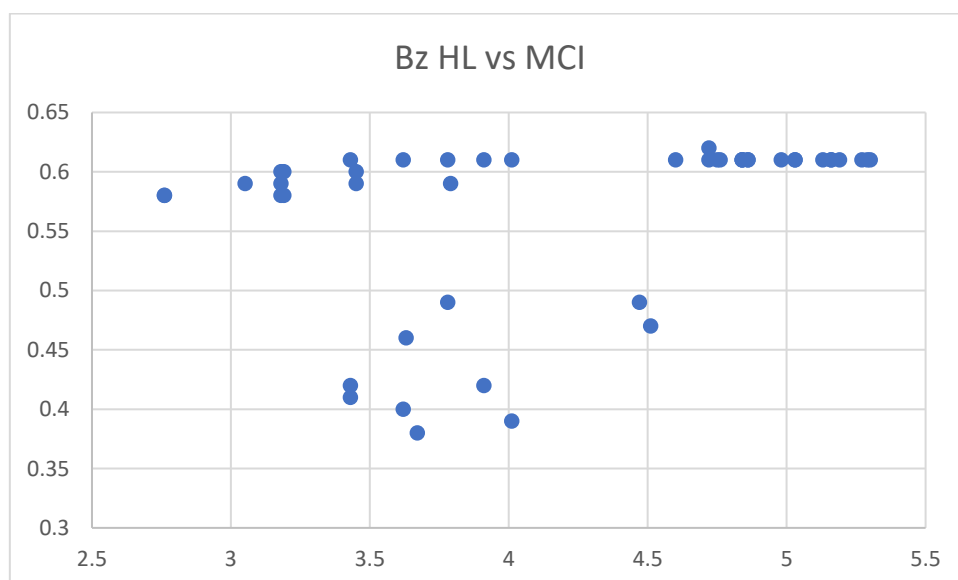


(hb) HOMO-LUMO gap versus HOMA for benzene rings among polycyclic species.

Supporting Information



(ib) HOMO-LUMO gap versus ring current for benzene rings among polycyclic species.



(jb) HOMO-LUMO gap versus MCI for benzene rings among polycyclic species.

Supporting Information

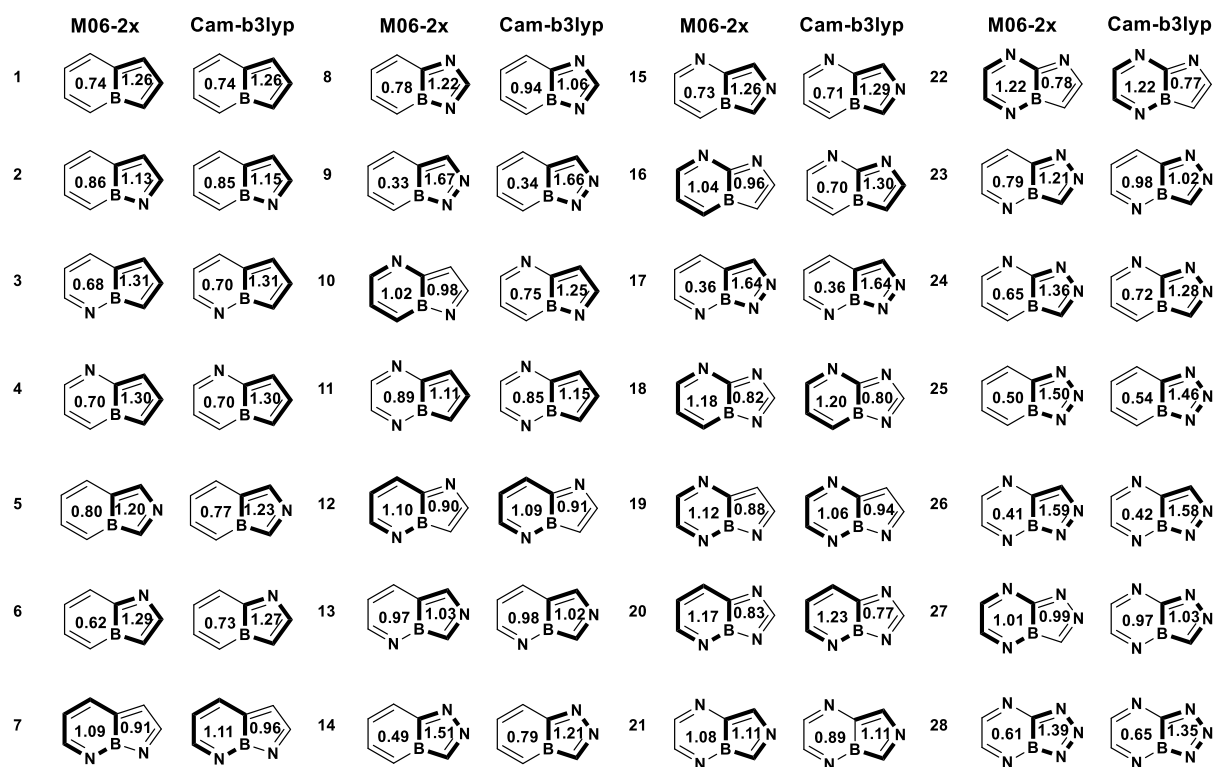


Figure S4. Ring spin densities of the studied bicyclic molecules

Supporting Information

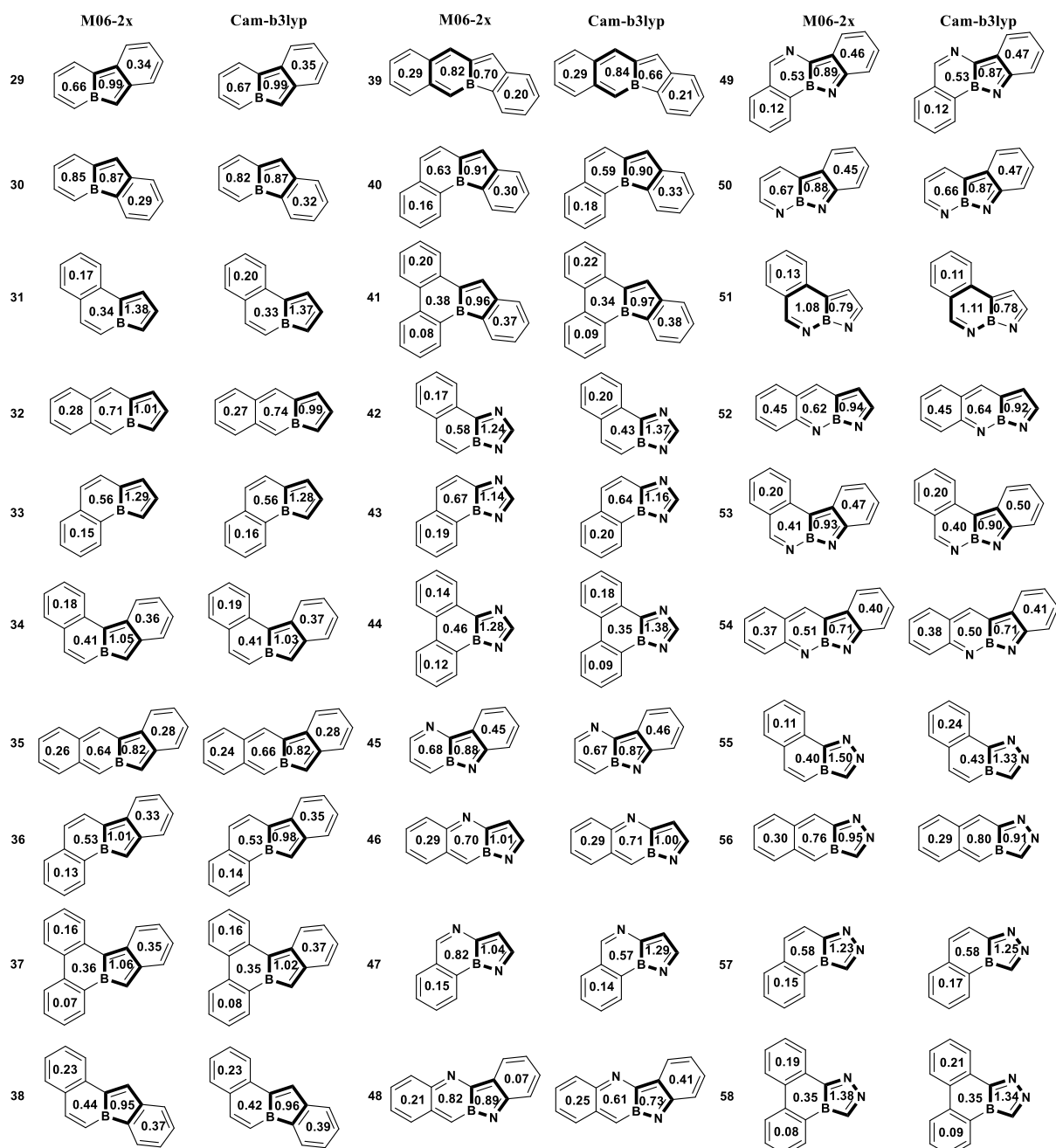


Figure S5. Ring spin density of the studied pericyclic molecules

Supporting Information

Optimized Cartesian Coordinates of the studied molecules

1

6	2.149738000	-0.733868000	0.000532000
6	1.054499000	-1.538826000	0.000597000
5	-0.291455000	-0.829027000	0.000541000
6	-1.853300000	-1.176264000	-0.000119000
6	-2.486887000	-0.000166000	-0.000347000
6	-1.522857000	1.162821000	-0.000267000
6	-0.248261000	0.735430000	0.000078000
6	1.002601000	1.449391000	0.000115000
6	2.141394000	0.728104000	0.000361000
1	3.138002000	-1.185789000	0.000690000
1	1.215105000	-2.610328000	0.000749000
1	-2.374763000	-2.122793000	-0.000246000
1	-3.559023000	0.152619000	-0.000707000
1	-1.861095000	2.194330000	-0.000623000
1	1.033054000	2.533358000	-0.000047000
1	3.101647000	1.226608000	0.000391000

2

6	2.086446000	-0.783308000	0.000672000
6	0.965877000	-1.544248000	0.000526000
5	-0.345710000	-0.767438000	0.000370000
7	-1.801651000	-1.148192000	-0.000107000
6	-2.403364000	-0.031052000	-0.000295000
6	-1.516248000	1.219831000	-0.000463000
6	-0.245561000	0.803769000	0.000110000
6	1.037845000	1.466353000	0.000243000
6	2.134150000	0.687256000	0.000507000
1	3.058588000	-1.267911000	0.000937000
1	1.071507000	-2.621902000	0.000594000
1	-3.490860000	0.048488000	-0.000807000
1	-1.907427000	2.230838000	-0.000919000
1	1.122635000	2.546599000	0.000138000
1	3.117373000	1.139817000	0.000595000

3

6	2.041530000	-0.775426000	0.000794000
7	0.988464000	-1.523273000	0.000992000
5	-0.245446000	-0.787407000	0.001148000
6	-1.797990000	-1.178339000	0.000001000
6	-2.457601000	-0.016172000	-0.000395000
6	-1.524458000	1.172652000	-0.000165000
6	-0.240574000	0.775285000	0.000873000
6	1.018228000	1.465110000	0.000368000
6	2.124797000	0.692797000	0.000132000
1	3.011922000	-1.279303000	0.000984000
1	-2.292302000	-2.138903000	-0.000141000
1	-3.532397000	0.113323000	-0.001040000
1	-1.891908000	2.194013000	-0.001390000
1	1.086852000	2.547773000	0.000290000
1	3.115783000	1.125870000	-0.000251000

4

6	2.115187000	-0.700886000	0.000569000
6	1.067802000	-1.556416000	0.000432000
5	-0.297187000	-0.867494000	0.000266000
6	-1.857252000	-1.197876000	-0.000074000
6	-2.473142000	-0.011189000	-0.000290000

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6	-1.500944000	1.145287000	-0.000186000
6	-0.236684000	0.690089000	0.000218000
7	0.923431000	1.458949000	0.000336000
6	2.006563000	0.771802000	0.000490000
1	3.134068000	-1.077242000	0.000809000
1	1.268732000	-2.621313000	0.000477000
1	-2.391897000	-2.136734000	-0.000120000
1	-3.543651000	0.151751000	-0.000537000
1	-1.807239000	2.184897000	-0.000412000
1	2.942810000	1.323576000	0.000722000

5

6	2.164260000	-0.722905000	0.000561000
6	1.070736000	-1.540006000	0.000493000
5	-0.260644000	-0.828637000	0.000312000
6	-1.866463000	-1.097417000	-0.000036000
7	-2.503063000	0.011235000	-0.000422000
6	-1.527341000	1.094986000	-0.000348000
6	-0.237143000	0.713290000	0.000231000
6	0.998949000	1.445407000	0.000371000
6	2.146337000	0.732317000	0.000528000
1	3.154600000	-1.169909000	0.000664000
1	1.238723000	-2.609895000	0.000553000
1	-2.447960000	-2.014961000	-0.000165000
1	-1.933957000	2.100048000	-0.000815000
1	1.018451000	2.529138000	0.000346000
1	3.102017000	1.239009000	0.000627000

6

6	2.137945000	-0.745508000	0.000607000
6	1.072598000	-1.577274000	0.000452000
5	-0.294711000	-0.891575000	0.000056000
6	-1.832649000	-1.172019000	-0.000178000
6	-2.384838000	0.046028000	-0.000535000
7	-1.464249000	1.195286000	-0.000484000
6	-0.282355000	0.705030000	-0.000118000
6	0.963602000	1.451674000	0.000125000
6	2.096824000	0.734336000	0.000467000
1	3.139921000	-1.165151000	0.000941000
1	1.257669000	-2.644385000	0.000660000
1	-2.417467000	-2.078409000	-0.000106000
1	-3.438340000	0.293460000	-0.000783000
1	0.962621000	2.534395000	-0.000030000
1	3.055129000	1.237712000	0.000628000

7

6	1.984707000	-0.808669000	-0.027936000
7	0.910842000	-1.515452000	-0.000417000
5	-0.292898000	-0.732639000	0.042711000
7	-1.736263000	-1.151096000	0.015880000
6	-2.364455000	-0.051023000	-0.032569000
6	-1.507759000	1.225882000	-0.036546000
6	-0.233237000	0.839352000	0.060948000
6	1.055486000	1.485101000	0.032828000
6	2.120696000	0.666828000	-0.032669000
1	2.938917000	-1.342236000	-0.032005000
1	-3.452319000	0.003808000	-0.067194000
1	-1.920398000	2.223721000	-0.130117000
1	1.170167000	2.562833000	0.056281000
1	3.128603000	1.058298000	-0.067336000

Supporting Information

8

6	2.072693000	-0.809843000	0.000663000
6	0.972587000	-1.592857000	0.000591000
5	-0.348037000	-0.823279000	0.000102000
7	-1.797143000	-1.112545000	-0.000006000
6	-2.309950000	0.048902000	-0.000585000
7	-1.445264000	1.259221000	-0.000375000
6	-0.262953000	0.769596000	0.000016000
6	1.013309000	1.459750000	0.000104000
6	2.101536000	0.674991000	0.000456000
1	3.055299000	-1.272114000	0.000915000
1	1.097614000	-2.668030000	0.000826000
1	-3.378969000	0.245490000	-0.000595000
1	1.076867000	2.540158000	-0.000045000
1	3.086210000	1.125460000	0.000634000

9

6	2.112011000	-0.759985000	0.000644000
6	0.993274000	-1.533678000	0.000566000
5	-0.298887000	-0.754001000	0.000081000
7	-1.809308000	-1.096828000	-0.000036000
7	-2.444590000	-0.041442000	-0.000446000
6	-1.510701000	1.161938000	-0.000306000
6	-0.232683000	0.790969000	-0.000029000
6	1.040223000	1.470647000	0.000178000
6	2.147847000	0.704441000	0.000518000
1	3.086686000	-1.239255000	0.000896000
1	1.104729000	-2.610010000	0.000787000
1	-1.986514000	2.133952000	-0.000536000
1	1.109589000	2.551302000	0.000066000
1	3.125625000	1.167650000	0.000717000

10

6	2.017899000	-0.725092000	0.150401000
6	0.935348000	-1.523519000	0.030439000
5	-0.371380000	-0.798865000	-0.306410000
7	-1.810736000	-1.153688000	-0.275314000
6	-2.350388000	-0.041212000	0.030321000
6	-1.422068000	1.157119000	0.098959000
6	-0.218001000	0.766074000	-0.351725000
7	0.976155000	1.454415000	-0.310644000
6	2.005574000	0.735003000	-0.055073000
1	2.994336000	-1.146972000	0.366469000
1	1.056041000	-2.594372000	0.143809000
1	-3.420569000	0.060401000	0.208480000
1	-1.689404000	2.119459000	0.517911000
1	2.966690000	1.240447000	-0.022874000

11

6	1.996480000	-0.717940000	-0.142955000
7	0.980341000	-1.491700000	-0.031154000
5	-0.274775000	-0.844651000	0.208257000
6	-1.805100000	-1.201969000	0.043100000
6	-2.415693000	-0.013762000	-0.047372000
6	-1.447126000	1.122991000	0.029481000
6	-0.222547000	0.711334000	0.421922000
7	0.944810000	1.427314000	0.323943000
6	1.983444000	0.752490000	-0.016713000
1	2.990264000	-1.164109000	-0.226973000

Supporting Information

1	-2.327064000	-2.147535000	0.055039000
1	-3.476827000	0.155859000	-0.176327000
1	-1.671596000	2.114360000	-0.348002000
1	2.934788000	1.270518000	-0.088846000

12

6	2.034343000	-0.796259000	0.000481000
7	1.010086000	-1.569335000	0.001394000
5	-0.244594000	-0.850787000	0.001649000
6	-1.776312000	-1.169439000	-0.000149000
6	-2.351506000	0.037132000	-0.000635000
7	-1.451704000	1.210149000	-0.001183000
6	-0.264051000	0.740626000	0.001403000
6	0.991444000	1.467250000	0.000937000
6	2.089505000	0.696885000	-0.000278000
1	3.021062000	-1.267305000	0.001750000
1	-2.338572000	-2.089619000	-0.000404000
1	-3.408369000	0.267067000	-0.001608000
1	1.030423000	2.549929000	0.000903000
1	3.081144000	1.130307000	-0.001260000

13

6	2.060349000	-0.731951000	0.096094000
7	1.001510000	-1.477102000	0.015702000
5	-0.221577000	-0.788637000	-0.150589000
6	-1.804452000	-1.109396000	-0.025579000
7	-2.451393000	-0.007950000	0.062186000
6	-1.491922000	1.068839000	0.091663000
6	-0.233582000	0.757018000	-0.284144000
6	1.006041000	1.457197000	-0.160997000
6	2.118817000	0.718056000	0.073873000
1	3.027085000	-1.237932000	0.138219000
1	-2.368217000	-2.034906000	-0.094696000
1	-1.843570000	2.009001000	0.502349000
1	1.070381000	2.534322000	-0.269955000
1	3.089432000	1.184341000	0.169289000

14

6	2.155473000	-0.739487000	0.000642000
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5	-0.259118000	-0.880276000	0.000009000
6	-1.837847000	-1.087722000	-0.000390000
7	-2.430067000	0.039174000	-0.000634000
7	-1.440413000	1.166344000	-0.000447000
6	-0.258613000	0.685108000	-0.000142000
6	0.978749000	1.444568000	0.000144000
6	2.117219000	0.732812000	0.000544000
1	3.155541000	-1.163656000	0.000895000
1	1.270065000	-2.642790000	0.000596000
1	-2.465857000	-1.970933000	-0.000009000
1	0.969054000	2.526696000	0.000084000
1	3.073463000	1.239077000	0.000829000

15

6	2.122615000	-0.667780000	-0.094395000
6	1.071143000	-1.525822000	-0.042542000
5	-0.273424000	-0.863327000	0.190590000
6	-1.865904000	-1.109896000	0.075737000
7	-2.457750000	0.013961000	-0.075204000
6	-1.449933000	1.049001000	-0.089209000

Supporting Information

6	-0.216046000	0.670137000	0.317350000
7	0.928527000	1.435088000	0.284386000
6	2.017667000	0.778390000	0.086453000
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1	1.261447000	-2.584956000	-0.169747000
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1	-1.731859000	2.013950000	-0.493118000
1	2.941795000	1.348107000	0.068798000

16

6	2.106147000	-0.733861000	0.000683000
6	1.077386000	-1.600309000	0.000495000
5	-0.297710000	-0.916922000	0.000019000
6	-1.829223000	-1.178092000	-0.000225000
6	-2.356694000	0.053360000	-0.000520000
7	-1.425819000	1.190118000	-0.000419000
6	-0.257902000	0.679348000	-0.000231000
7	0.910488000	1.454869000	-0.000013000
6	1.979248000	0.756660000	0.000433000
1	3.132485000	-1.088342000	0.001065000
1	1.285052000	-2.663477000	0.000709000
1	-2.430415000	-2.073463000	-0.000118000
1	-3.406343000	0.316806000	-0.000634000
1	2.921200000	1.300805000	0.000555000

17

6	2.003181000	-0.764958000	0.098739000
7	0.925634000	-1.472682000	-0.003198000
5	-0.260041000	-0.728154000	-0.180842000
7	-1.752094000	-1.104527000	-0.092380000
7	-2.391276000	-0.059714000	0.049766000
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6	-0.226531000	0.823121000	-0.272434000
6	1.046639000	1.479138000	-0.164520000
6	2.117385000	0.692594000	0.080939000
1	2.952878000	-1.301086000	0.152605000
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1	1.153850000	2.551777000	-0.274855000
1	3.106629000	1.114914000	0.190372000

18

6	2.058660000	-0.662054000	-0.146691000
6	1.043298000	-1.522865000	0.061610000
5	-0.312938000	-0.860185000	0.329936000
7	-1.723400000	-1.206697000	0.209057000
6	-2.231245000	-0.081940000	-0.108687000
7	-1.388795000	1.107201000	-0.225021000
6	-0.260208000	0.740952000	0.260341000
7	0.896961000	1.489574000	0.229776000
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1	3.057447000	-1.024875000	-0.365826000
1	1.236093000	-2.588108000	0.021477000
1	-3.286081000	0.072265000	-0.317257000
1	2.898004000	1.357500000	-0.004675000

19

6	1.923422000	-0.735936000	-0.184524000
7	0.886574000	-1.469412000	-0.034467000
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7	-1.755622000	-1.171570000	0.160617000

Supporting Information

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6	-1.409888000	1.159142000	-0.010211000
6	-0.213140000	0.770891000	0.471040000
7	0.979573000	1.430263000	0.393673000
6	1.977172000	0.733594000	-0.011185000
1	2.895596000	-1.217167000	-0.311986000
1	-3.388040000	0.056143000	-0.198968000
1	-1.649774000	2.121399000	-0.445134000
1	2.950279000	1.210611000	-0.073954000

20

6	2.004452000	-0.761116000	0.040139000
7	0.976629000	-1.523359000	-0.026137000
5	-0.263078000	-0.799212000	-0.094109000
7	-1.687097000	-1.178225000	-0.006116000
6	-2.266508000	-0.052684000	0.051555000
7	-1.467179000	1.208832000	0.064083000
6	-0.273913000	0.793503000	-0.123934000
6	0.982885000	1.515123000	-0.061715000
6	2.064933000	0.733595000	0.072944000
1	2.988908000	-1.235736000	0.034219000
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1	1.038815000	2.596186000	-0.094344000
1	3.055309000	1.161688000	0.159421000

21

6	2.030492000	-0.687087000	-0.152802000
7	1.007263000	-1.466663000	-0.077224000
5	-0.237283000	-0.842069000	0.175328000
6	-1.809708000	-1.122075000	0.009136000
7	-2.414365000	0.006258000	-0.052301000
6	-1.433433000	1.041096000	-0.023345000
6	-0.209841000	0.688881000	0.449795000
7	0.940412000	1.414056000	0.368950000
6	2.000152000	0.764507000	0.024048000
1	3.021756000	-1.130976000	-0.258564000
1	-2.400478000	-2.030613000	0.074024000
1	-1.678327000	1.979787000	-0.505559000
1	2.939060000	1.305299000	-0.028286000

22

6	2.006953000	-0.741852000	0.161392000
7	0.984500000	-1.465726000	-0.069531000
5	-0.289947000	-0.920639000	-0.286364000
6	-1.779423000	-1.194175000	-0.029551000
6	-2.292731000	0.040695000	0.111988000
7	-1.354013000	1.105796000	0.128783000
6	-0.237895000	0.727032000	-0.379301000
7	0.939693000	1.381081000	-0.263253000
6	1.979315000	0.734319000	0.108092000
1	3.001320000	-1.190235000	0.156102000
1	-2.362667000	-2.100935000	-0.041236000
1	-3.326597000	0.312705000	0.274271000
1	2.933193000	1.252334000	0.132209000

23

6	2.070223000	-0.759953000	0.043196000
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6	-1.775441000	-1.104152000	0.050932000

Supporting Information

7	-2.361186000	0.026949000	0.132038000
7	-1.376285000	1.089404000	0.238381000
6	-0.247959000	0.723345000	-0.249664000
6	0.998820000	1.439021000	-0.109758000
6	2.106429000	0.701631000	0.111708000
1	3.044885000	-1.249315000	-0.000033000
1	-2.393366000	-1.991508000	-0.011636000
1	1.037971000	2.518457000	-0.187965000
1	3.073503000	1.171352000	0.227198000

24

6	2.117651000	-0.703817000	-0.134422000
6	1.085403000	-1.562771000	0.023216000
5	-0.266327000	-0.894974000	0.214639000
6	-1.823950000	-1.093894000	0.032165000
7	-2.357019000	0.047618000	-0.165570000
7	-1.332930000	1.078628000	-0.290151000
6	-0.225706000	0.674786000	0.216929000
7	0.932291000	1.429001000	0.186858000
6	2.007618000	0.761567000	0.003315000
1	3.120483000	-1.073011000	-0.322936000
1	1.277649000	-2.627333000	-0.030116000
1	-2.482268000	-1.948156000	0.134603000
1	2.940203000	1.318957000	-0.006361000

25

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6	0.966264000	-1.580875000	0.000648000
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7	-1.801071000	-1.035082000	-0.000221000
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7	-1.376533000	1.332454000	-0.000353000
6	-0.236660000	0.791018000	-0.000273000
6	1.069819000	1.442130000	-0.000130000
6	2.152825000	0.648910000	0.000414000
1	3.059682000	-1.312748000	0.000828000
1	1.059558000	-2.658196000	0.000746000
1	1.145084000	2.521204000	-0.000310000
1	3.141746000	1.088195000	0.000696000

26

6	1.961748000	-0.713733000	0.176951000
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7	-1.766401000	-1.105486000	-0.108173000
7	-2.343977000	-0.021145000	0.065643000
6	-1.393026000	1.092442000	0.076805000
6	-0.204497000	0.758354000	-0.462448000
7	0.974952000	1.427710000	-0.387588000
6	1.994280000	0.744961000	0.000809000
1	2.932962000	-1.193847000	0.305084000
1	-1.677598000	2.006573000	0.579055000
1	2.955537000	1.243674000	0.062274000

27

6	2.052837000	-0.729036000	-0.114810000
7	1.021236000	-1.470037000	0.053245000
5	-0.240824000	-0.897182000	0.217392000
6	-1.772960000	-1.116450000	-0.045820000
7	-2.306681000	0.042047000	-0.170505000

Supporting Information

7	-1.313896000	1.030066000	-0.278110000
6	-0.219190000	0.704903000	0.322868000
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6	2.009592000	0.738566000	-0.062546000
1	3.045399000	-1.179502000	-0.111205000
1	-2.417309000	-1.981884000	0.040664000
1	2.952624000	1.274804000	-0.085818000

28

6	2.012351000	-0.698535000	-0.121106000
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5	-0.257504000	-0.836003000	0.273376000
7	-1.693303000	-1.126753000	0.028536000
7	-2.245678000	-0.049566000	-0.194699000
7	-1.302492000	1.060213000	-0.327491000
6	-0.231258000	0.762459000	0.316104000
7	0.938024000	1.438078000	0.256396000
6	1.988862000	0.776763000	-0.060819000
1	3.002285000	-1.154265000	-0.147410000
1	2.940739000	1.296818000	-0.088356000

29

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6	0.182650000	-1.889582000	0.000108000
6	1.177217000	-0.985519000	0.000194000
6	2.613802000	-1.191611000	0.000330000
6	3.439292000	-0.134217000	0.000370000
6	2.914953000	1.227563000	0.000294000
6	1.595717000	1.506009000	0.000168000
6	0.644923000	0.426548000	0.000021000
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6	-1.656167000	1.518635000	0.000081000
6	-2.980782000	1.223945000	-0.000227000
1	-4.547006000	-0.247650000	-0.000966000
1	-3.194157000	-2.224687000	-0.001071000
1	0.371160000	-2.955567000	0.000106000
1	2.995680000	-2.204609000	0.000407000
1	4.512064000	-0.268849000	0.000483000
1	3.630445000	2.040564000	0.000351000
1	1.244757000	2.529211000	0.000136000
1	-1.329248000	2.553171000	0.000225000
1	-3.715706000	2.017452000	-0.000340000

30

6	3.130334000	-1.153335000	0.000728000
6	1.865379000	-1.650871000	0.000648000
5	0.744891000	-0.620971000	0.000581000
6	-0.838680000	-0.564923000	0.000114000
6	-1.853426000	-1.491077000	-0.000079000
6	-3.195472000	-1.064377000	-0.000326000
6	-3.500608000	0.279125000	-0.000446000
6	-2.476502000	1.241257000	-0.000285000
6	-1.170068000	0.812341000	0.000020000
6	0.061556000	1.639760000	0.000145000
6	1.178394000	0.876882000	0.000282000
6	2.568246000	1.248875000	0.000393000
6	3.487798000	0.261012000	0.000623000
1	3.971638000	-1.840825000	0.000775000

Supporting Information

1	1.746741000	-2.728052000	0.000656000
1	-1.633381000	-2.551728000	0.000022000
1	-3.992117000	-1.796372000	-0.000447000
1	-4.534452000	0.597696000	-0.000686000
1	-2.718887000	2.296765000	-0.000397000
1	0.022731000	2.725371000	0.000026000
1	2.873841000	2.289314000	0.000327000
1	4.542543000	0.503133000	0.000726000

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6	-3.312853000	0.140745000	-0.000275000
6	-2.486107000	-0.971475000	-0.000228000
6	-1.098149000	-0.836123000	-0.000103000
6	-0.269090000	-2.048102000	-0.000039000
6	1.083068000	-2.102441000	0.000090000
5	1.812976000	-0.764664000	0.000133000
6	3.305641000	-0.226642000	0.000392000
6	3.203090000	1.106729000	0.000337000
6	1.767623000	1.573773000	0.000202000
6	0.924165000	0.530803000	0.000129000
6	-0.529406000	0.456946000	-0.000022000
6	-1.373480000	1.564321000	-0.000078000
6	-2.751571000	1.411608000	-0.000202000
1	-4.387311000	0.019210000	-0.000363000
1	-2.918031000	-1.964970000	-0.000274000
1	-0.842329000	-2.972661000	-0.000105000
1	1.548880000	-3.080784000	0.000128000
1	4.253900000	-0.744233000	0.000540000
1	4.025951000	1.811654000	0.000438000
1	1.510682000	2.627767000	0.000172000
1	-0.943179000	2.557736000	-0.000028000
1	-3.390069000	2.285003000	-0.000244000

32

6	-0.252797000	-1.412119000	0.000521000
6	-1.485394000	-0.702408000	0.000515000
6	-2.762777000	-1.152115000	0.000364000
6	-3.743212000	-0.020261000	0.000177000
6	-3.121974000	1.165359000	0.000333000
5	-1.539246000	0.851869000	-0.000310000
6	-0.222056000	1.552307000	-0.000318000
6	0.925564000	0.769846000	-0.000051000
6	2.227009000	1.392816000	-0.000213000
6	3.372623000	0.676729000	-0.000050000
6	3.359752000	-0.760134000	0.000281000
6	2.179770000	-1.410075000	0.000445000
6	0.920865000	-0.705988000	0.000271000
1	-0.221373000	-2.497864000	0.000865000
1	-3.077537000	-2.192033000	0.000334000
1	-4.811598000	-0.192230000	0.000262000
1	-3.662653000	2.101963000	0.000530000
1	-0.065500000	2.625740000	-0.000550000
1	2.260869000	2.474744000	-0.000460000
1	4.325156000	1.191351000	-0.000160000
1	4.294117000	-1.303426000	0.000405000
1	2.145293000	-2.492872000	0.000707000

33

6	-1.089753000	2.001843000	-0.000411000
6	-1.767163000	0.727922000	-0.000379000

Supporting Information

6	-3.065056000	0.386139000	-0.000249000
6	-3.219206000	-1.116321000	0.000112000
6	-2.043068000	-1.755736000	0.000334000
5	-0.948100000	-0.609208000	-0.000703000
6	0.578862000	-0.491961000	-0.000176000
6	1.456477000	-1.578167000	0.000109000
6	2.831513000	-1.398339000	0.000379000
6	3.344170000	-0.107198000	0.000396000
6	2.494640000	0.990545000	0.000136000
6	1.110230000	0.825086000	-0.000138000
6	0.254676000	2.023535000	-0.000326000
1	-1.648168000	2.931257000	-0.000482000
1	-3.918293000	1.055786000	-0.000086000
1	-4.196704000	-1.584169000	0.000482000
1	-1.961169000	-2.833003000	0.000857000
1	1.046047000	-2.581039000	0.000082000
1	3.498384000	-2.249643000	0.000576000
1	4.415481000	0.047148000	0.000617000
1	2.911301000	1.990335000	0.000163000
1	0.775695000	2.973786000	-0.000292000

34

6	1.247299000	-0.346764000	-0.155385000
6	1.533274000	-1.698102000	-0.363716000
6	2.829658000	-2.181643000	-0.272739000
6	3.881240000	-1.322611000	0.018892000
6	3.623835000	0.027799000	0.190213000
6	2.328773000	0.535268000	0.093871000
6	2.132204000	1.979552000	0.217939000
6	0.961159000	2.644370000	0.073675000
5	-0.268878000	1.797336000	-0.212467000
6	-1.839801000	2.028865000	-0.300615000
6	-2.378238000	0.804397000	-0.169369000
6	-3.777523000	0.420448000	-0.101708000
6	-4.109729000	-0.858338000	0.121759000
6	-3.086075000	-1.880872000	0.328892000
6	-1.769891000	-1.616737000	0.250126000
6	-1.319888000	-0.276569000	-0.064667000
6	-0.073784000	0.246043000	-0.227154000
1	0.735662000	-2.374649000	-0.634995000
1	3.020688000	-3.233846000	-0.437721000
1	4.891736000	-1.699566000	0.094520000
1	4.439461000	0.711187000	0.394069000
1	3.043957000	2.535533000	0.424671000
1	0.975474000	3.723122000	0.176064000
1	-2.436651000	2.925595000	-0.395072000
1	-4.532694000	1.186299000	-0.224620000
1	-5.148047000	-1.156214000	0.177974000
1	-3.416544000	-2.884273000	0.565459000
1	-1.047478000	-2.396832000	0.440002000

35

6	0.601110000	-1.135352000	-0.000045000
6	-0.413843000	-0.255081000	-0.000867000
6	-1.880916000	-0.455758000	-0.000168000
6	-2.649064000	-1.596525000	-0.000896000
6	-4.045943000	-1.480249000	-0.000697000
6	-4.666903000	-0.239216000	0.000182000
6	-3.901296000	0.923441000	0.000893000
6	-2.513210000	0.822789000	0.000674000

Supporting Information

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6	1.247942000	1.733034000	-0.000610000
6	2.281486000	0.748545000	-0.000147000
6	3.638186000	1.135288000	-0.000515000
6	4.657144000	0.209996000	-0.000209000
6	4.347864000	-1.151870000	0.000469000
6	3.028396000	-1.565876000	0.000796000
6	1.973524000	-0.650480000	0.000320000
1	0.465423000	-2.214238000	0.000434000
1	-2.187340000	-2.575520000	-0.001552000
1	-4.652826000	-2.376369000	-0.001145000
1	-5.746373000	-0.178428000	0.000272000
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1	-1.868108000	2.916803000	0.001640000
1	1.581415000	2.767099000	-0.001035000
1	3.865927000	2.194312000	-0.000977000
1	5.689033000	0.533333000	-0.000475000
1	5.142240000	-1.886375000	0.000827000
1	2.797383000	-2.624112000	0.001421000

36

6	0.147869000	2.034540000	-0.000621000
6	-0.559329000	0.785191000	-0.000375000
6	-1.880900000	0.476670000	-0.000247000
6	-3.052421000	1.321027000	-0.000314000
6	-4.274967000	0.762479000	-0.000109000
6	-4.469947000	-0.688461000	0.000200000
6	-3.434652000	-1.540025000	0.000298000
6	-2.074675000	-1.026196000	0.000084000
6	-0.906233000	-1.695814000	0.000180000
5	0.219093000	-0.569506000	-0.000249000
6	1.746476000	-0.496279000	-0.000194000
6	2.592687000	-1.608031000	0.000023000
6	3.972098000	-1.469089000	0.000013000
6	4.522131000	-0.192860000	-0.000216000
6	3.705579000	0.929206000	-0.000430000
6	2.316131000	0.805743000	-0.000420000
6	1.496226000	2.024600000	-0.000640000
1	-0.380153000	2.981869000	-0.000776000
1	-2.932506000	2.396511000	-0.000531000
1	-5.156519000	1.390387000	-0.000159000
1	-5.484978000	-1.063039000	0.000361000
1	-3.588507000	-2.611490000	0.000539000
1	-0.854348000	-2.775915000	0.000447000
1	2.152940000	-2.598483000	0.000194000
1	4.613806000	-2.339507000	0.000182000
1	5.597538000	-0.069847000	-0.000229000
1	4.151683000	1.916256000	-0.000606000
1	2.039978000	2.961763000	-0.000805000

37

6	0.164187000	-1.268805000	-0.034737000
6	-0.359852000	-2.576408000	-0.196331000
6	0.453286000	-3.673388000	-0.284276000
6	1.839359000	-3.492378000	-0.220822000
6	2.382683000	-2.232763000	-0.094939000
6	1.589274000	-1.078053000	-0.005140000
6	2.216080000	0.253708000	0.079205000
6	3.609407000	0.386505000	0.229254000

Supporting Information

6	4.211016000	1.625395000	0.258103000
6	3.440945000	2.782996000	0.137117000
6	2.072766000	2.674048000	0.011160000
6	1.431869000	1.428215000	-0.012345000
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6	-1.283430000	2.090293000	-0.382959000
6	-2.508417000	1.291146000	-0.221222000
6	-3.814729000	1.692203000	-0.268189000
6	-4.836186000	0.763952000	0.062453000
6	-4.510836000	-0.509393000	0.431319000
6	-3.149918000	-0.931113000	0.458078000
6	-2.168911000	-0.053878000	0.100262000
6	-0.673733000	-0.136487000	0.056610000
1	-1.428020000	-2.693167000	-0.289040000
1	0.035420000	-4.661560000	-0.417228000
1	2.497894000	-4.347938000	-0.294389000
1	3.457592000	-2.149163000	-0.093898000
1	4.241609000	-0.481282000	0.340333000
1	5.283744000	1.696771000	0.378332000
1	3.915837000	3.755173000	0.155269000
1	1.467422000	3.569860000	-0.058790000
1	-1.371736000	3.114432000	-0.733316000
1	-4.070350000	2.709008000	-0.538080000
1	-5.871835000	1.074002000	0.030997000
1	-5.285841000	-1.214203000	0.699560000
1	-2.928109000	-1.936557000	0.785478000

38

6	1.680397000	-0.439672000	0.000248000
6	2.425748000	-1.617357000	0.000634000
6	3.810422000	-1.585655000	0.000500000
6	4.480153000	-0.366989000	0.000071000
6	3.754776000	0.812112000	-0.000216000
6	2.358921000	0.799748000	-0.000134000
6	1.640640000	2.078172000	-0.000274000
6	0.298111000	2.244392000	0.000006000
5	-0.539763000	0.971147000	0.000114000
6	-2.063854000	0.566356000	0.000281000
6	-3.259499000	1.246326000	0.000729000
6	-4.471619000	0.533677000	0.000439000
6	-4.467437000	-0.845299000	-0.000238000
6	-3.256674000	-1.556403000	-0.000731000
6	-2.077165000	-0.848862000	-0.000489000
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6	0.225957000	-0.389665000	0.000206000
1	1.911453000	-2.569977000	0.001045000
1	4.370634000	-2.511164000	0.000779000
1	5.561169000	-0.339560000	-0.000006000
1	4.271815000	1.764025000	-0.000472000
1	2.290687000	2.950214000	-0.000577000
1	-0.085592000	3.257942000	-0.000037000
1	-3.278565000	2.329532000	0.001194000
1	-5.411716000	1.068883000	0.000772000
1	-5.404501000	-1.386214000	-0.000383000
1	-3.259953000	-2.639352000	-0.001272000
1	-0.495763000	-2.448381000	-0.001555000

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6	1.182135000	-1.562951000	0.000515000
6	-0.144173000	-1.048465000	0.000505000

Supporting Information

6	-1.335214000	-1.704066000	0.000493000
6	-2.475826000	-0.768150000	0.000324000
6	-3.817612000	-1.079301000	0.000211000
6	-4.749760000	-0.030606000	-0.000017000
6	-4.318865000	1.278997000	-0.000142000
6	-2.943836000	1.584235000	-0.000062000
6	-2.014955000	0.572362000	0.000178000
5	-0.425144000	0.482010000	0.000454000
6	0.779894000	1.373064000	0.000058000
6	2.026912000	0.772884000	0.000012000
6	3.223475000	1.584068000	-0.000234000
6	4.461042000	1.046937000	-0.000230000
6	4.656526000	-0.378411000	0.000033000
6	3.587407000	-1.196932000	0.000264000
6	2.236155000	-0.688774000	0.000286000
1	1.377406000	-2.631263000	0.000677000
1	-1.475923000	-2.781771000	0.000475000
1	-4.152004000	-2.109460000	0.000302000
1	-5.808476000	-0.251789000	-0.000100000
1	-5.045239000	2.081084000	-0.000311000
1	-2.631030000	2.621119000	-0.000164000
1	0.772036000	2.458118000	-0.000175000
1	3.094441000	2.658881000	-0.000427000
1	5.328376000	1.694628000	-0.000436000
1	5.660737000	-0.778751000	0.000047000
1	3.715314000	-2.272595000	0.000463000

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6	0.917880000	-2.540770000	0.000432000
6	-0.232680000	-1.670484000	0.000327000
6	-1.554802000	-1.942461000	0.000291000
6	-2.368388000	-0.699950000	0.000178000
6	-3.739525000	-0.588358000	0.000078000
6	-4.312165000	0.693425000	-0.000115000
6	-3.513686000	1.817022000	-0.000181000
6	-2.113161000	1.691717000	-0.000109000
6	-1.531762000	0.444439000	0.000068000
5	-0.056637000	-0.122121000	0.000282000
6	1.377520000	0.419168000	0.000056000
6	1.720349000	1.774119000	-0.000189000
6	3.042198000	2.188367000	-0.000327000
6	4.052806000	1.233315000	-0.000218000
6	3.743420000	-0.117582000	0.000024000
6	2.415931000	-0.549996000	0.000139000
6	2.146743000	-1.994000000	0.000351000
1	0.801874000	-3.618808000	0.000577000
1	-2.012597000	-2.926948000	0.000325000
1	-4.370906000	-1.468139000	0.000121000
1	-5.389062000	0.798055000	-0.000205000
1	-3.966128000	2.799559000	-0.000282000
1	-1.505538000	2.588109000	-0.000140000
1	0.930054000	2.514654000	-0.000262000
1	3.288112000	3.241495000	-0.000504000
1	5.089341000	1.544665000	-0.000309000
1	4.540846000	-0.850604000	0.000102000
1	3.019264000	-2.636887000	0.000388000

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6	1.214943000	-1.445185000	0.000019000
6	1.661800000	-2.769129000	-0.000324000

Supporting Information

6	3.006167000	-3.078335000	-0.000177000
6	3.935994000	-2.045842000	0.000292000
6	3.510195000	-0.730361000	0.000475000
6	2.153078000	-0.386386000	0.000282000
6	1.736244000	1.052837000	0.000258000
6	2.699471000	2.067716000	0.000348000
6	2.345607000	3.406713000	0.000322000
6	1.011139000	3.792651000	0.000212000
6	0.042695000	2.808213000	0.000077000
6	0.372930000	1.447686000	0.000060000
5	-0.691095000	0.351088000	-0.000165000
6	-2.267169000	0.261087000	-0.000122000
6	-3.317059000	1.152441000	-0.000533000
6	-4.641056000	0.682023000	-0.000183000
6	-4.897374000	-0.673101000	0.000634000
6	-3.842707000	-1.598443000	0.001066000
6	-2.550247000	-1.126889000	0.000613000
6	-1.293350000	-1.917258000	0.000765000
6	-0.204358000	-1.121676000	-0.000015000
1	0.928387000	-3.565145000	-0.000776000
1	3.330779000	-4.110070000	-0.000434000
1	4.995185000	-2.264681000	0.000437000
1	4.268549000	0.036504000	0.000777000
1	3.752264000	1.834000000	0.000428000
1	3.125226000	4.157505000	0.000400000
1	0.740871000	4.839635000	0.000228000
1	-1.003654000	3.086128000	0.000028000
1	-3.141453000	2.220949000	-0.001173000
1	-5.462520000	1.385746000	-0.000546000
1	-5.919771000	-1.027304000	0.000936000
1	-4.048977000	-2.661478000	0.001704000
1	-1.313533000	-3.002440000	0.001687000

42

6	0.539645000	-0.478098000	0.000260000
6	1.378321000	-1.581929000	0.000378000
6	2.757766000	-1.409534000	0.000347000
6	3.292102000	-0.130381000	0.000222000
6	2.453970000	0.980355000	0.000111000
6	1.072504000	0.828321000	0.000111000
6	0.221742000	2.040832000	-0.000062000
6	-1.128656000	2.097723000	-0.000098000
5	-1.830948000	0.746469000	0.000123000
7	-3.208522000	0.223197000	0.000406000
6	-3.024646000	-1.035973000	0.000249000
7	-1.659481000	-1.600393000	0.000709000
6	-0.914714000	-0.558905000	0.000291000
1	0.935756000	-2.569408000	0.000496000
1	3.412077000	-2.270536000	0.000426000
1	4.364820000	0.007913000	0.000218000
1	2.880305000	1.975792000	0.000012000
1	0.793200000	2.965972000	-0.000105000
1	-1.603587000	3.070558000	-0.000250000
1	-3.828653000	-1.767574000	0.001156000

43

6	-1.116587000	2.012972000	-0.000624000
6	-1.779796000	0.730094000	-0.000358000
7	-3.033377000	0.452687000	-0.000338000
6	-3.047238000	-1.019985000	-0.000356000

Supporting Information

7	-1.960387000	-1.688510000	-0.000159000
5	-0.946083000	-0.626065000	0.000468000
6	0.580817000	-0.528536000	0.000301000
6	1.461140000	-1.605742000	0.000536000
6	2.837896000	-1.405816000	0.000468000
6	3.335604000	-0.113245000	0.000139000
6	2.471214000	0.979103000	-0.000122000
6	1.094454000	0.794224000	-0.000066000
6	0.228106000	1.998308000	-0.000440000
1	-1.674675000	2.940403000	-0.000963000
1	-4.034600000	-1.475316000	-0.000401000
1	1.056257000	-2.610120000	0.000829000
1	3.513995000	-2.249681000	0.000679000
1	4.404685000	0.053817000	0.000071000
1	2.877894000	1.982808000	-0.000404000
1	0.763481000	2.941501000	-0.000659000

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6	-1.515895000	-0.035716000	-0.000460000
6	-2.896352000	0.149651000	-0.000467000
6	-3.436128000	1.421704000	-0.000173000
6	-2.576980000	2.511605000	0.000187000
6	-1.200956000	2.333141000	0.000202000
6	-0.622786000	1.062655000	-0.000173000
6	0.879743000	0.905121000	-0.000199000
6	1.699917000	2.032915000	-0.000453000
6	3.085095000	1.924620000	-0.000424000
6	3.708564000	0.686000000	-0.000160000
6	2.917906000	-0.449626000	0.000014000
6	1.523929000	-0.361829000	-0.000012000
5	0.626422000	-1.588927000	-0.000126000
7	0.801783000	-3.047907000	-0.000510000
6	-0.406910000	-3.457513000	-0.000982000
7	-1.527919000	-2.506348000	-0.000672000
6	-0.937992000	-1.366115000	-0.000521000
1	-3.524655000	-0.731493000	-0.000678000
1	-4.507563000	1.566536000	-0.000174000
1	-2.977541000	3.516621000	0.000488000
1	-0.586347000	3.219184000	0.000570000
1	1.281690000	3.026983000	-0.000743000
1	3.680787000	2.828235000	-0.000632000
1	4.787241000	0.612979000	-0.000133000
1	3.368942000	-1.434215000	0.000155000
1	-0.687894000	-4.507860000	-0.000925000

45

6	-3.394158000	-0.202073000	-0.167079000
6	-2.630710000	-1.298371000	0.129975000
5	-1.118449000	-1.085667000	0.281966000
7	0.019208000	-1.748966000	-0.110179000
6	1.124475000	-0.877306000	-0.044906000
6	2.458578000	-1.213235000	-0.086793000
6	3.408158000	-0.176811000	-0.043260000
6	3.036610000	1.152669000	0.023324000
6	1.676815000	1.500404000	0.064359000
6	0.753471000	0.483544000	0.041092000
6	-0.698211000	0.458835000	0.216621000
7	-1.559627000	1.415313000	0.005713000
6	-2.842276000	1.107736000	-0.108954000
1	-4.466441000	-0.270156000	-0.299902000

Supporting Information

1	-3.144548000	-2.238977000	0.299935000
1	2.762170000	-2.248278000	-0.159723000
1	4.459819000	-0.429531000	-0.081976000
1	3.791867000	1.925814000	0.025724000
1	1.364144000	2.535629000	0.107264000
1	-3.527397000	1.949827000	-0.097219000

46

6	-0.838005000	-0.752256000	0.037794000
6	-2.131009000	-1.373753000	-0.167787000
6	-3.267709000	-0.656587000	-0.206921000
6	-3.252605000	0.778436000	-0.035404000
6	-2.095291000	1.430983000	0.158107000
6	-0.825590000	0.729404000	0.184204000
7	0.247681000	1.440875000	0.354943000
6	1.429201000	0.773664000	0.377201000
6	2.582797000	1.101567000	-0.247296000
6	3.540539000	-0.060724000	-0.130901000
7	3.043476000	-1.139462000	0.326133000
5	1.603902000	-0.791018000	0.406719000
6	0.296985000	-1.510987000	0.140192000
1	-2.151124000	-2.449443000	-0.286643000
1	-4.216378000	-1.153738000	-0.360010000
1	-4.188748000	1.319328000	-0.061653000
1	-2.050635000	2.503326000	0.288345000
1	2.765112000	1.993738000	-0.834966000
1	4.592717000	0.040490000	-0.394231000
1	0.184986000	-2.589144000	0.086490000

47

6	-1.065073000	-0.774928000	-0.000366000
6	-2.439609000	-0.984958000	0.000055000
6	-3.313083000	0.095888000	0.000313000
6	-2.825520000	1.396348000	0.000194000
6	-1.454602000	1.617137000	-0.000220000
6	-0.561971000	0.547251000	-0.000479000
5	0.966025000	0.617364000	-0.001124000
7	1.975280000	1.710763000	-0.000891000
6	3.082351000	1.074808000	0.000423000
6	3.014315000	-0.447401000	0.000293000
6	1.715518000	-0.763252000	-0.000669000
7	1.099186000	-2.016113000	-0.000800000
6	-0.180006000	-1.969544000	-0.000993000
1	-2.830227000	-1.995326000	0.000134000
1	-4.380852000	-0.079054000	0.000623000
1	-3.513246000	2.231073000	0.000423000
1	-1.062679000	2.626461000	-0.000300000
1	4.042087000	1.592904000	0.000584000
1	3.878145000	-1.098926000	0.001153000
1	-0.704238000	-2.924396000	-0.000151000

48

6	-2.205497000	-0.770155000	0.000379000
6	-3.575962000	-1.131488000	0.000457000
6	-4.573341000	-0.188846000	0.000084000
6	-4.225725000	1.165763000	-0.000410000
6	-2.899307000	1.562554000	-0.000552000
6	-1.864835000	0.631853000	-0.000179000
7	-0.562364000	1.158151000	-0.000576000
6	0.367405000	0.273762000	0.000198000

Supporting Information

6	1.839530000	0.478412000	0.000143000
6	2.632912000	1.589828000	0.000538000
6	4.033378000	1.416348000	0.000192000
6	4.589625000	0.151572000	-0.000481000
6	3.778675000	-0.990751000	-0.000851000
6	2.401627000	-0.831613000	-0.000447000
7	1.479838000	-1.878264000	-0.000400000
5	0.211617000	-1.277192000	0.000836000
6	-1.210836000	-1.771431000	0.000975000
1	-3.819145000	-2.186969000	0.000847000
1	-5.612380000	-0.485868000	0.000156000
1	-5.004288000	1.917508000	-0.000698000
1	-2.628830000	2.609126000	-0.000987000
1	2.196525000	2.580306000	0.000939000
1	4.678164000	2.284906000	0.000385000
1	5.665721000	0.042035000	-0.000742000
1	4.201732000	-1.986068000	-0.001366000
1	-1.549536000	-2.803580000	0.001559000

49

6	-2.230649000	-0.741067000	0.000224000
6	-3.609204000	-0.920600000	-0.000480000
6	-4.459639000	0.179578000	-0.000870000
6	-3.942351000	1.467164000	-0.000530000
6	-2.565046000	1.656676000	0.000178000
6	-1.696799000	0.568971000	0.000552000
5	-0.162361000	0.613096000	0.001450000
7	0.860485000	1.666373000	0.001418000
6	1.967072000	0.997094000	0.000761000
6	3.306543000	1.559298000	0.000101000
6	4.365340000	0.730668000	-0.000716000
6	4.251057000	-0.728615000	-0.000978000
6	3.053606000	-1.336826000	-0.000374000
6	1.864550000	-0.522397000	0.000632000
6	0.547220000	-0.804200000	0.001513000
7	-0.095018000	-2.033853000	0.001323000
6	-1.376208000	-1.956088000	0.000708000
1	-4.021842000	-1.922280000	-0.000731000
1	-5.531002000	0.028614000	-0.001430000
1	-4.610431000	2.317784000	-0.000840000
1	-2.150342000	2.656854000	0.000444000
1	3.413353000	2.635029000	0.000248000
1	5.364644000	1.148672000	-0.001221000
1	5.164240000	-1.307889000	-0.001658000
1	2.954206000	-2.413996000	-0.000553000
1	-1.922225000	-2.898460000	0.000629000

50

5	1.124104000	-0.951733000	-0.000366000
7	-0.036177000	-1.731927000	0.000517000
6	-1.122156000	-0.832811000	0.000127000
6	-2.444639000	-1.173804000	0.000248000
6	-3.425149000	-0.136910000	-0.000369000
6	-3.065778000	1.179687000	-0.000947000
6	-1.684111000	1.537577000	-0.000939000
6	-0.749984000	0.547711000	-0.000467000
6	0.715596000	0.549136000	-0.000573000
6	1.690647000	1.534107000	-0.000210000
6	2.990920000	1.061197000	0.000170000
6	3.355435000	-0.347806000	-0.000033000

Supporting Information

7	2.530948000	-1.336797000	-0.000272000
1	-2.736702000	-2.214883000	0.000775000
1	-4.472782000	-0.406927000	-0.000280000
1	-3.819505000	1.954140000	-0.001309000
1	-1.396633000	2.582082000	-0.001338000
1	1.492642000	2.600235000	-0.000091000
1	3.811288000	1.771328000	0.000542000
1	4.427235000	-0.549202000	0.000216000

51

5	-1.739845000	-0.698761000	-0.000732000
7	-3.187496000	-0.328858000	-0.000075000
6	-3.166248000	0.941601000	-0.000075000
6	-1.788041000	1.608376000	0.000309000
6	-0.883142000	0.627608000	-0.000762000
6	0.565312000	0.533646000	-0.000510000
6	1.456975000	1.600591000	-0.000238000
6	2.825807000	1.370306000	0.000190000
6	3.321443000	0.072250000	0.000291000
6	2.440897000	-1.000026000	-0.000083000
6	1.067587000	-0.783058000	-0.000549000
6	0.163191000	-1.960507000	-0.001385000
7	-1.117777000	-1.996994000	-0.000764000
1	-4.077499000	1.540175000	0.000976000
1	-1.649370000	2.683091000	0.001444000
1	1.075747000	2.613603000	-0.000339000
1	3.510929000	2.207500000	0.000462000
1	4.388611000	-0.101129000	0.000632000
1	2.818537000	-2.015600000	-0.000126000
1	0.702585000	-2.914013000	-0.000764000

52

5	-1.504231000	-0.754820000	-0.211126000
7	-2.934153000	-1.200747000	-0.070577000
6	-3.560841000	-0.126601000	0.172426000
6	-2.713464000	1.137346000	0.186544000
6	-1.488679000	0.828426000	-0.272854000
6	-0.241686000	1.509237000	-0.225345000
6	0.892931000	0.769067000	-0.035744000
6	2.182022000	1.411039000	0.040621000
6	3.320516000	0.694690000	0.097585000
6	3.258608000	-0.741681000	0.065480000
6	2.084178000	-1.405012000	-0.005912000
6	0.815811000	-0.713641000	-0.020026000
7	-0.285048000	-1.424797000	-0.061285000
1	-4.634147000	-0.091308000	0.353638000
1	-3.045775000	2.077613000	0.614249000
1	-0.164381000	2.584537000	-0.358023000
1	2.204684000	2.494043000	0.050325000
1	4.282087000	1.184598000	0.155901000
1	4.185177000	-1.300928000	0.097609000
1	2.038389000	-2.484663000	-0.027386000

53

5	-0.250968000	-1.669515000	-0.034749000
7	-1.694728000	-2.002204000	-0.044520000
6	-2.262400000	-0.853848000	-0.024673000
6	-3.701425000	-0.619310000	-0.014776000
6	-4.162780000	0.638227000	0.025258000
6	-3.278953000	1.805831000	0.062028000

Supporting Information

6	-1.941237000	1.691495000	0.047482000
6	-1.342890000	0.375754000	-0.009555000
6	-0.078429000	-0.089827000	-0.045107000
6	1.256736000	0.471333000	-0.028642000
6	1.593695000	1.822788000	-0.070237000
6	2.923138000	2.222540000	-0.044404000
6	3.940889000	1.281226000	0.021063000
6	3.621539000	-0.069656000	0.054379000
6	2.296375000	-0.483451000	0.028053000
6	2.017726000	-1.941977000	0.043708000
7	0.891298000	-2.547935000	0.016223000
1	-4.355783000	-1.479615000	-0.036074000
1	-5.229871000	0.820730000	0.035579000
1	-3.739072000	2.784028000	0.103924000
1	-1.318926000	2.574376000	0.081285000
1	0.815130000	2.569318000	-0.130030000
1	3.165295000	3.276391000	-0.076676000
1	4.974623000	1.597113000	0.042268000
1	4.407858000	-0.813771000	0.099298000
1	2.928363000	-2.550344000	0.075354000

54

5	-0.145075000	-1.057623000	-0.000186000
7	-1.424981000	-1.751447000	0.000253000
6	-2.370159000	-0.787744000	0.000096000
6	-3.752491000	-1.039164000	0.000319000
6	-4.629987000	0.034080000	0.000004000
6	-4.138869000	1.336355000	-0.000494000
6	-2.759879000	1.616918000	-0.000682000
6	-1.875070000	0.571602000	-0.000314000
6	-0.408226000	0.459545000	-0.000403000
6	0.628037000	1.307875000	-0.000136000
6	1.967649000	0.725618000	-0.000073000
6	3.087616000	1.544216000	0.000031000
6	4.374585000	1.015589000	0.000097000
6	4.569166000	-0.363835000	0.000065000
6	3.476802000	-1.204658000	-0.000026000
6	2.151572000	-0.707342000	-0.000105000
7	1.145218000	-1.610333000	-0.000168000
1	-4.097330000	-2.064294000	0.000713000
1	-5.697698000	-0.133732000	0.000145000
1	-4.840554000	2.160768000	-0.000729000
1	-2.418230000	2.643591000	-0.001084000
1	0.553049000	2.392717000	0.000083000
1	2.950824000	2.618990000	0.000048000
1	5.226609000	1.682302000	0.000171000
1	5.571089000	-0.770437000	0.000123000
1	3.587932000	-2.280558000	-0.000047000

55

6	0.293387000	-2.075196000	0.000428000
6	-1.061222000	-2.157707000	0.000390000
5	-1.786510000	-0.830355000	0.000083000
6	-3.214433000	-0.141049000	0.000254000
7	-3.087182000	1.127510000	-0.000207000
7	-1.649209000	1.526764000	-0.000164000
6	-0.923963000	0.478643000	0.000022000
6	0.536994000	0.435935000	0.000075000
6	1.347044000	1.561145000	-0.000141000
6	2.729770000	1.424007000	-0.000050000

Supporting Information

6	3.305078000	0.161008000	0.000225000
6	2.498711000	-0.969232000	0.000400000
6	1.110845000	-0.851877000	0.000307000
1	0.879784000	-2.991204000	0.000592000
1	-1.510791000	-3.142471000	0.000591000
1	-4.224932000	-0.532143000	0.000162000
1	0.881381000	2.537644000	-0.000355000
1	3.358611000	2.304023000	-0.000196000
1	4.381247000	0.055071000	0.000293000
1	2.948891000	-1.954214000	0.000592000

56

6	-0.996650000	-0.782813000	-0.085046000
6	-2.258100000	-1.396485000	-0.042158000
6	-3.421296000	-0.654736000	0.054321000
6	-3.345014000	0.731738000	0.104698000
6	-2.109978000	1.367863000	0.057663000
6	-0.929101000	0.644044000	-0.045576000
6	0.351853000	1.349637000	-0.100953000
6	1.474435000	0.645549000	-0.277325000
7	2.813260000	1.134476000	-0.255320000
7	3.597851000	0.199805000	0.053790000
6	2.933354000	-1.045552000	0.183777000
5	1.501654000	-0.897568000	-0.199604000
6	0.192610000	-1.582456000	-0.174382000
1	-2.305957000	-2.477795000	-0.077338000
1	-4.381510000	-1.149895000	0.092882000
1	-4.248852000	1.321429000	0.177932000
1	-2.060839000	2.448821000	0.093747000
1	0.352877000	2.422258000	0.065338000
1	3.525182000	-1.823883000	0.648131000
1	0.027820000	-2.650935000	-0.281877000

57

6	-1.131030000	-0.803062000	-0.000178000
6	-2.509460000	-0.990018000	-0.000219000
6	-3.375925000	0.097233000	-0.000149000
6	-2.885492000	1.395651000	-0.000040000
6	-1.513578000	1.599079000	0.000000000
6	-0.621727000	0.524220000	-0.000081000
5	0.894785000	0.635812000	0.000007000
6	2.102403000	1.661290000	0.000685000
7	3.207249000	1.024089000	0.000493000
7	2.988804000	-0.453122000	0.000238000
6	1.733212000	-0.685365000	0.000166000
6	1.082296000	-1.980581000	-0.000047000
6	-0.259314000	-1.998096000	-0.000206000
1	-2.912227000	-1.995102000	-0.000283000
1	-4.444446000	-0.074112000	-0.000169000
1	-3.566069000	2.235637000	-0.000001000
1	-1.119673000	2.608099000	0.000073000
1	2.159787000	2.743339000	0.001051000
1	1.664949000	-2.892497000	-0.000081000
1	-0.779444000	-2.948895000	-0.000359000

58

6	0.870085000	-0.958834000	-0.000025000
6	1.659267000	-2.109946000	-0.000177000
6	3.045341000	-2.042432000	-0.000085000
6	3.707574000	-0.822160000	0.000158000

Supporting Information

6	2.950992000	0.333374000	0.000299000
6	1.550928000	0.291559000	0.000201000
5	0.695170000	1.539596000	0.000129000
6	0.758534000	3.119989000	0.000130000
7	-0.427010000	3.592320000	0.000051000
7	-1.447549000	2.508011000	0.000024000
6	-0.853027000	1.378873000	0.000033000
6	-1.478151000	0.061724000	-0.000097000
6	-2.863592000	-0.076919000	-0.000131000
6	-3.446195000	-1.330062000	-0.000128000
6	-2.629964000	-2.452844000	-0.000068000
6	-1.250472000	-2.320996000	-0.000021000
6	-0.630660000	-1.068594000	-0.000048000
1	1.210764000	-3.090578000	-0.000392000
1	3.614316000	-2.963138000	-0.000221000
1	4.787765000	-0.781463000	0.000221000
1	3.439610000	1.300072000	0.000464000
1	1.571963000	3.835745000	0.000437000
1	-3.464089000	0.823080000	-0.000139000
1	-4.522467000	-1.434501000	-0.000152000
1	-3.067133000	-3.442267000	-0.000030000
1	-0.664603000	-3.226511000	0.000069000
