Electronic Supplementary Information

Computational and experimental study on the index of antiaromaticity in 4n π-Systems (n≥2)

Tohru Nishinaga* and Hinako Hamaoka

Department of Chemistry, Graduate School of Science and Engineering, Tokyo Metropolitan University, Hachioji, Tokyo 192-0397, Japan

Contents

General

Theoretical calculations were performed with the Gaussian 09 program.[1] The structures were optimized with the π-moiety being planar structures, although the global minima for most compounds studied in this study were deviated from the planarity. TD–HF and TD–B3LYP calculations were performed with td(nstate=10) keyword. NICS calculations were conducted with GIAO method. ^{1}H and ^{13}C NMR spectra were recorded on Bruker AV500 or JEOL JNM-270 instruments. Chemical shifts are reported in ppm with reference to tetramethylsilane, using the signal of internal tetramethylsilane or the solvents. APCI mass spectra were recorded on a Bruker MicrOTOFII-SD. Only the more intense or structurally diagnostic mass spectral fragment ion peaks are reported. Electronic absorption spectra were recorded on a SHIMADZU UV-Vis-NIR scanning spectrophotometer (Model UV-3101-PC). Preparative gel-permeation chromatography (GPC) was performed with a JAI LC–08 chromatograph equipped with JAIGEL 1H and 2H columns.

Commercially available reagents were used as received. THF and diisopropylamine were distilled from relevant drying agents prior to use.

Ref. 1. Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.: Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

Table S1 Comparison of NICS (ppm) of 4n π-Systems Calculated with Various Methods

Compd[a]	GIAO-HF[b]		GIAO-B3LYP[b,c]		GIAO-M06-2X[b,d]		GIAO-PBE1PBE[b,e]		GIAO-BLYP[b,f]		GIAO-CASSCF		IGLO
	$NICS(0)_{iso}$	$NICS(1)_{zz}$	$NICS(0)_{iso}$	$NICS(1)_{zz}$	$NICS(0)_{iso}$	$NICS(1)_{zz}$	$NICS(0)_{iso}$	$NICS(1)_{zz}$	$NICS(0)_{iso}$	$NICS(1)_{zz}$	$NICS(0)_{iso}$	$NICS(1)_{zz}$	$NICS(0)_{iso}$
8A(D_{4h})	26.66	62.56	41.51	99.42	39.88	93.90	41.10	98.28	44.90	107.88	16.10[g]	37.62[g]	35.9[h]
12A(D_{2h})	13.18	27.53	24.40	57.47	22.13	51.11	23.64	55.83	28.37	67.96	–	–	24.5[h]
16A(D_{2h})	8.31	20.50	21.53	56.60	15.38	39.60	20.55	54.09	27.21	71.95	–	–	23.4[h]
20A(D_{2h})	5.17	13.94	18.32	50.52	11.08	30.35	17.11	47.27	25.29	69.81	–	–	21.5[h]
24A(C_s)	3.18	9.11	14.57	41.50	7.82	22.30	13.37	38.14	21.76	61.79	–	–	19.3[h]
2D12A(D_{2h})	12.16	36.82	28.22	78.1	22.74	63.58	27.27	75.71	33.53	91.77	–	–	
3D12A(D_{3h})	8.85	25.80	20.00	53.97	16.05	43.69	19.44	52.64	23.48	62.83	–	–	
4D16A(D_{2h})	6.08	21.76	20.08	57.61	13.88	41.85	19.01	54.82	26.08	73.03	–	–	
3D16A(C_{2v})	8.52	23.94	26.02	71.03	18.40	50.31	24.78	67.75	33.03	89.85	–	–	
3D20A(C_{2v})	5.25	15.36	20.63	58.01	12.82	36.14	19.31	54.35	28.18	78.82	–	–	
3D24A(C_{2v})	3.43	10.41	16.70	47.74	9.59	27.30	15.33	43.94	24.52	69.55	–	–	
2(D_{2h})	27.17	57.79	26.45	56.02	31.91	63.12	26.86	56.80	26.08	55.48	18.42[i]	39.27[i]	20.8[h]
3(C_{2v})	16.57	29.61	19.96	37.33	21.35	35.81	19.88	36.82	20.88	39.62	–	–	18.2[j]
4(C_{2h})	17.92	42.35	24.98	58.80	26.04	58.55	24.87	58.56	26.52	62.26	–	–	
5(C_{2h})	12.92	30.68	21.46	50.26	24.57	55.66	21.59	50.73	20.76	47.74	–	–	
6(D_{2h})	12.95	28.48	17.67	38.99	17.72	36.40	17.51	38.64	18.97	41.92	–	–	

[a] See Scheme 1 in the main text for the structural drawings. [b] With 6-311+G(d,p) basis set at the B3LYP/6-31G(d,p) optimized geometry. [c] 20% HF exchange. [d] 56% HF exchange. [e] 25% HF exchange. [f] Pure DFT (0% HF exchange). [g] CASSCF-GIAO/ 6-311+G(d)//CASSCF(8,8)/6-31G(d,p). Karadakov *J. Phys. Chem. A*, **2008**, *112*, 12709. [h] IGLO/TZ2P//B3LYP/6-31G(d). Schleyer et al. *Org. Lett.* **2003**, *5*, 2983. [i] CASSCF-GIAO/ 6-311++G(2d,2p)//CASSCF(4,4)/ 6-311++G(2d,2p). Karadakov, P. B. *J. Phys. Chem. A* **2008**, *112*, 7303. [j] PW91/IGLO-III//B3LYP/6-311+G**. Schleyer et al. *Org. Lett.* **2006**, *8*, 2983.

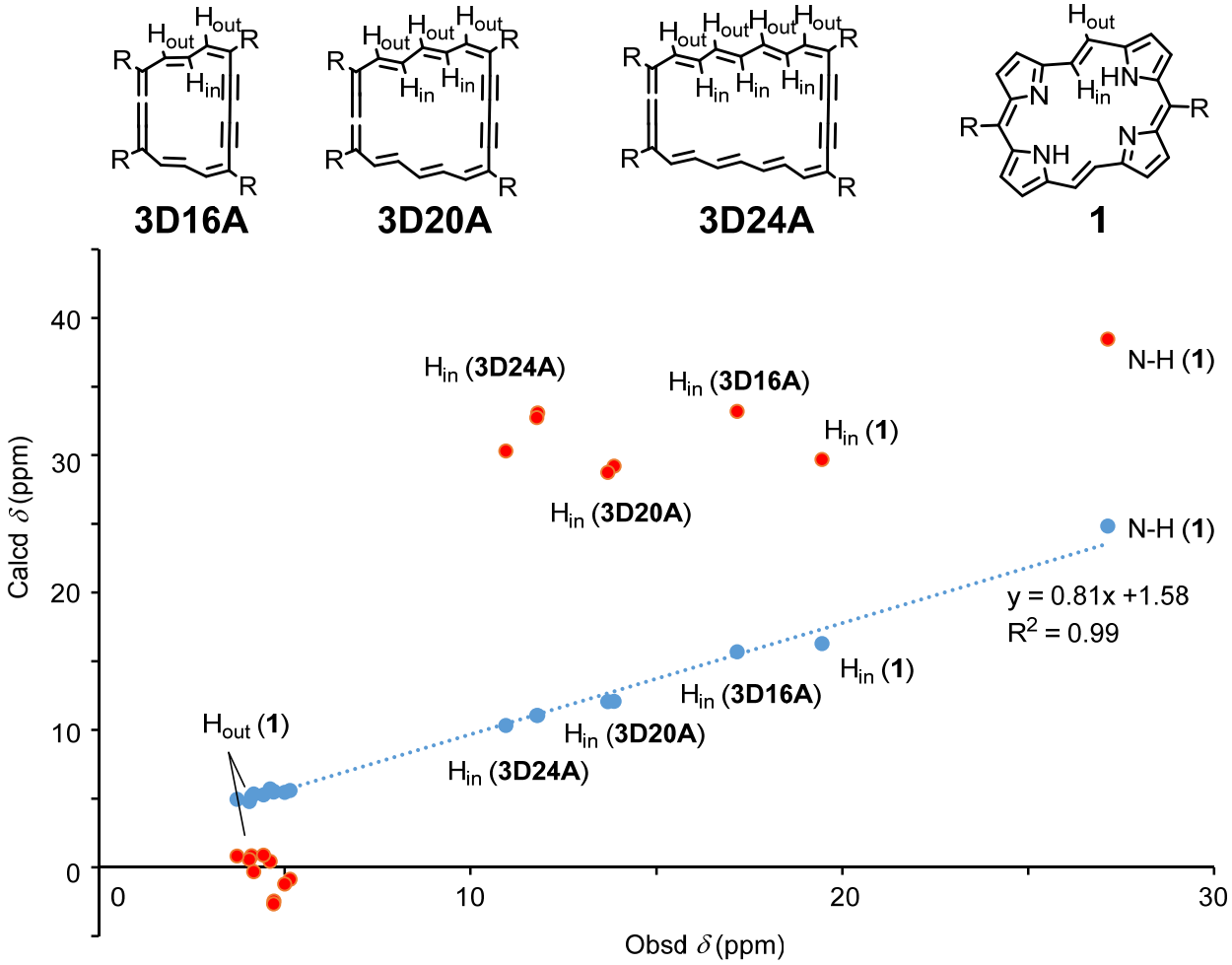


Fig. S1 Plot of observed vs calculated ^{1}H NMR chemical shifts. The blue and red circles were results calculated at the GIAO-HF/6-311G+(d,p) and GIAO-B3LYP/6–311G+(d,p) level, respectively, with the optimized structures at the B3LYP/6–31G(d,p) level. Only the results from the HF method showed a linear relation with the experimental values; **3D16A**(R = *t*-Bu): Nakatsuji et al. *Tetrahedron. Lett.* **1975**, *16*, 1233; **3D20A**(R = *t*-Bu): Nakatsuji et al. *Tetrahedron. Lett.* **1975**, *16*, 3927; **3D24A**(R = *t*-Bu): Nakatsuji et al. *Tetrahedron. Lett.* **1976**, *17*, 2623; **1** (R = Mes): Tanaka et al, *Angew. Chem. Int. Ed.* **2016**, *55*, 8095.

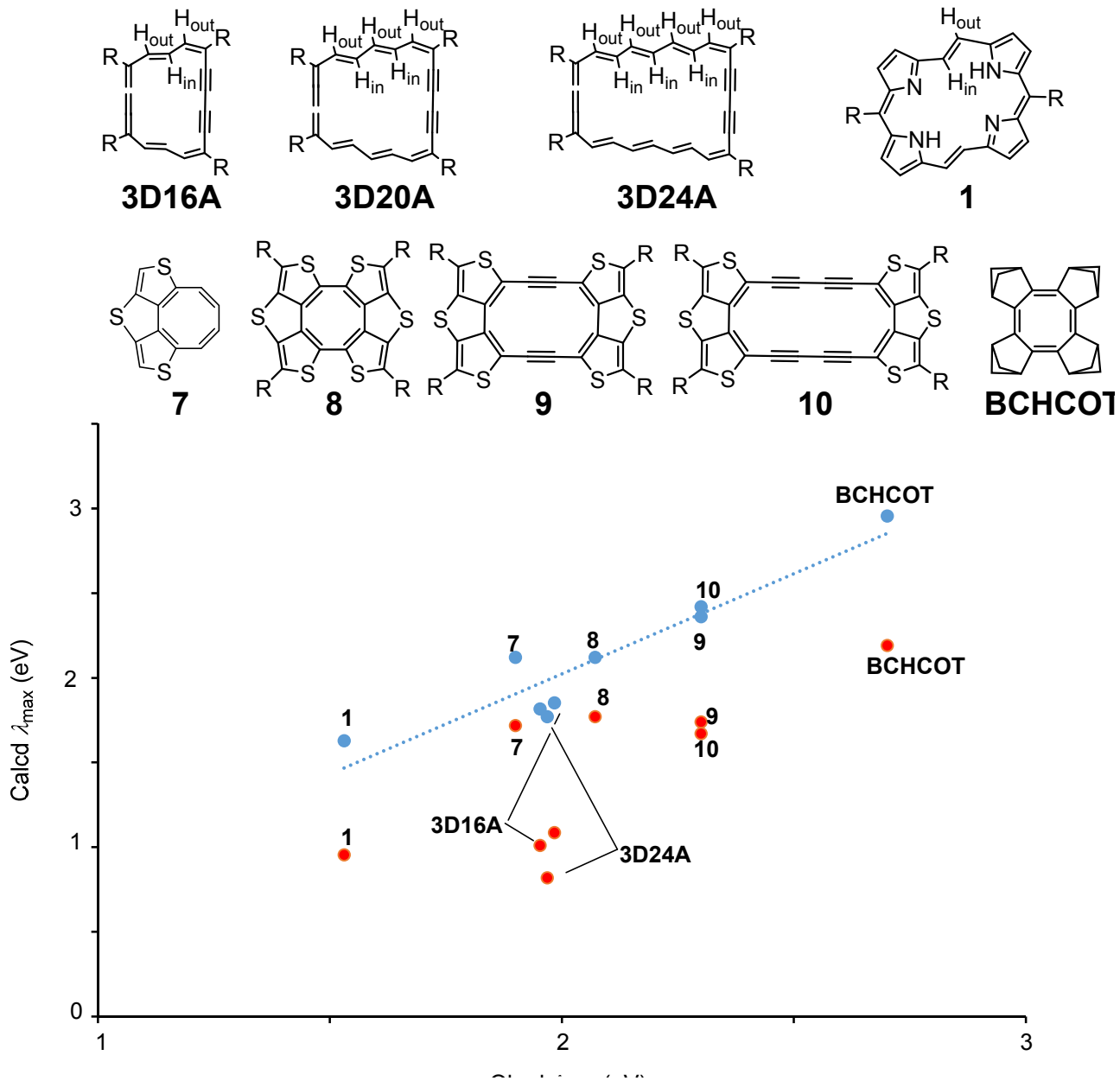


Fig. S2 Plot of observed vs calculated the longest absorption maximum. The blue and red circles were results calculated at the TD-HF/6-311G+(d,p) and TD-B3LYP/6–311G+(d,p) level, respectively, with the optimized structures at the B3LYP/6–31G(d,p) level. The results from the HF method showed a better linear relation with the experimental values; **3D16A**(R = *t*-Bu): Nakatsuji et al. *Tetrahedron. Lett.* **1975**, *16*, 1233; **3D20A**(R = *t*-Bu): Nakatsuji et al. *Tetrahedron. Lett.* **1975**, *16*, 3927; **3D24A**(R = *t*-Bu): Nakatsuji et al. *Tetrahedron. Lett.* **1976**, *17*, 2623; **1** (R = Mes): Tanaka et al, *Angew. Chem. Int. Ed.* **2016**, *55*, 8095; **7**: Aita et al. *Org. Lett.* **2013**, *15*, 3522; **8-10** (R = Mes): Nishinaga et al. *Org. Lett.* **2018**, *20*, 3426; **BCHCOT**: Matsuura et al. *J. Am. Chem. Soc.* **2001**, *123*, 1768. For **7-10**, no clear absorption maxima was observed and the energy of the absorption cut-off + 0.3 eV were used.

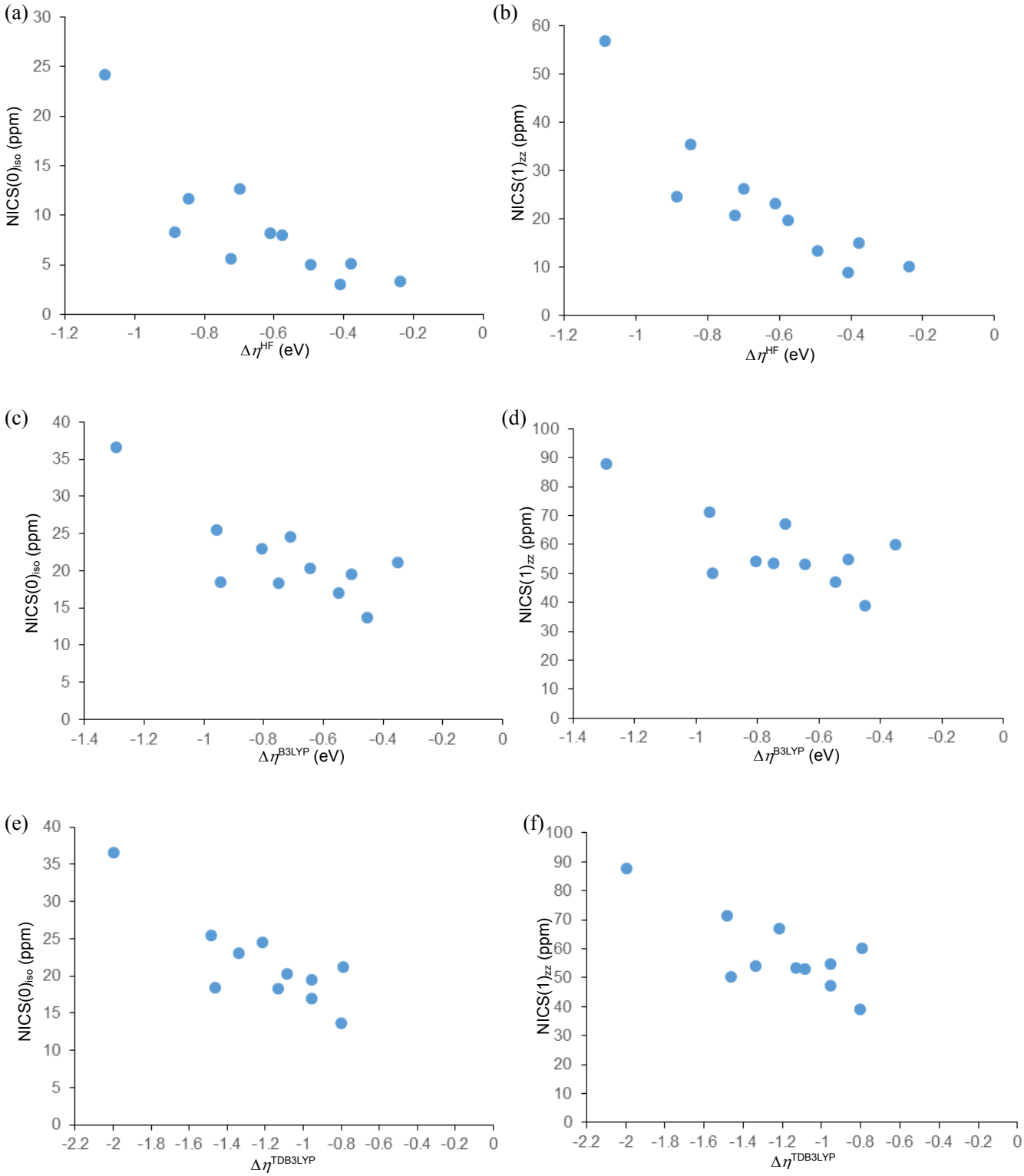


Fig. S3 Plot of (a) calculated HOMO-LUMO gap with the HF method ($\Delta\eta^{HF}$) vs. $NICS(0)_{iso}^{HF}$, (b) $\Delta\eta^{HF}$ vs. $NICS(1)_{zz}^{HF}$, (c) calculated HOMO-LUMO gap with the B3LYP method ($\Delta\eta^{B3LYP}$) vs. $NICS(0)_{iso}^{B3LYP}$, (d) $\Delta\eta^{B3LYP}$ vs. $NICS(1)_{zz}^{B3LYP}$, (e) $\Delta\eta^{TDB3LYP}$ vs. $NICS(0)_{iso}^{B3LYP}$, and (f) $\Delta\eta^{TDB3LYP}$ vs. $NICS(1)_{zz}^{B3LYP}$ of 4n (dehydro)annulenes based on the (i) type exocyclic references.

Table S2. The lowest excitation energy with the excitation weights in TD-HF calculations[a]

Compd	Excitation energy		Excitation (weight, %)	Oscillator strength
	(eV)	(nm)		
Me-**8A** (C_S)	2.056	603.1	H→L (96%)	0.0005
type (i) ref for Me-**8A** (C_S)	4.008	309.4	H→L (88%)	0.3005
8A (D_{4h})	1.986	624.2	H→L (96%)	0.0000
type (ii) ref for **8A** (C_{2h})	4.075	304.2	H→L (92%)	0.8115
Me-**12A** (C_S)	2.228	556.6	H→L (92%)	0.0004
type (i) ref for Me-**12A** (C_S)	3.183	389.6	H→L (81%)	0.2353
12A (D_{2d})	2.198	564.1	H→L (92%)	0.0000
type (ii) ref for **12A** (C_S)	3.802	326.1	H→L (88%)	2.6349
Me-**16A** (C_S)	2.151	576.5	H→L (88%)	0.0004
type (i) ref for Me-**16A** (C_S)	2.834	437.5	H→L (76%), H–1→L+1 (11%)	0.2218
16A (D_{2d})	2.116	586.0	H→L (89%)	0.0000
type (ii) ref for **16A** (C_S)	3.359	369.1	H→L (83%)	3.5324
Me-**20A** (C_S)	2.132	581.5	H→L (83%)	0.0007
type (i) ref for Me-**20A** (C_S)	2.616	473.9	H→L (73%), H–1→L+1 (15%)	0.2678
20A (D_{2h})	2.101	590.3	H→L (83%)	0.0000
type (ii) ref for **20A** (C_S)	3.069	404.0	H→L (79%), H–1→L+2 (11%)	4.4319
Me-**24A** (C_S)	2.098	591.0	H→L (76%)	0.0008
type (i) ref for Me-**24A** (C_S)	2.454	505.2	H→L (67%), H–1→L+1 (16%)	0.2745
24A (C_S)	2.072	598.3	H→L (76%)	0.0000
type (ii) ref for **24A**	2.887	429.5	H→L (74%), H–1→L+1 (15%)	5.2474
Me-**2D12A**(C_S)	2.197	564.4	H→L (93%)	0.0005
type (i) ref for Me-**2D12A** (C_S)	3.337	371.5	H→L (86%)	0.2025
2D12A (D_{2h})	2.156	575.1	H→L (93%)	0.0000
type (ii) ref for **2D12A** (C_S)	3.876	319.8	H→L (84%)	1.6756
Me-**3D12A**(C_S)	2.515	493.0	H→L (92%)	0.0005
type (i) ref for Me-**3D12A** (C_S)	3.653	339.4	H→L (82%)	0.2462
3D12A (D_{3h})	2.474	501.2	H→L (92%)	0.0000
type (ii) ref for **3D12A** (C_S)	3.800	326.3	H→L (82%)	1.2217
Me-**4D16A**(C_S)	2.279	544.1	H→L (86%)	0.0008
type (i) ref for Me-**4D16A** (C_S)	3.008	412.2	H→L (78%)	0.1595
4D16A (D_{2h})	2.233	555.2	H→L (87%)	0.0000
type (ii) ref for **4D16A** (C_{2h})	3.431	361.4	H→L (71%)	1.5524
Me-**3D16A**(R=H) (C_S)	1.963	631.5	H→L (90%)	0.0411
type (i) ref for Me-**3D16A** (C_S)	2.712	457.2	H→L (85%)	0.2356
3D16A(R=H) (C_{2v})	1.952	635.2	H→L (90%)	0.0317
type (ii) ref for **3D16A** (C_{2v})	3.115	398.0	H→L (88%)	3.0883

Me-**3D20A**(R=H) (C_S)	1.946	637.1	H→L (86%)	0.0430
type (i) ref for Me-**3D20A** (C_S)	2.379	521.1	H→L (84%)	0.2495
3D20A(R=H) (C_{2v})	1.936	640.4	H→L (86%)	0.0342
type (ii) ref for **3D20A** (C_{2v})	2.815	440.4	H→L (84%)	3.9793
Me-**3D24A**(R=H) (C_S)	1.918	646.5	H→L (81%)	0.0477
type (i) ref for Me-**3D24A** (C_S)	2.162	573.6	H→L (81%)	0.2375
3D24A(R=H) (C_{2v})	1.911	648.9	H→L (81%)	0.0389
type (ii) ref for **3D24A** (C_{2v})	2.608	475.4	H→L (89%)	4.8218
Me-**1** (C_S)	1.605	772.5	H→L (89%)	0.0003
type (i) ref for Me-**2** (C_S)	2.219	558.7	H→L (80%), H–1→L+1 (15%)	0.1100
1(R=H) (C_{2h})	1.607	771.4	H→L (89%)	0.0000
type (ii) ref for **1** (C_{2s})	2.669	464.6	H→L (80%), H–1→L+1 (14%)	2.2509
Me-**2** (C_S)	2.713	457.0	H→L+3 (87%)	0.0004
type (i) ref for Me-**2** (C_S)	5.961	208.0	H→L+3 (65%), H→L+6 (21%)	0.5882
2 (D_{2h})	2.653	467.3	H→L (89%)	0.0000
type (ii) ref for **2**(C_{2h})	5.976	207.5	H→L+2 (88%)	0.8516
Me-**3** (C_S)	2.954	419.7	H→L (90%)	0.0094
type (i) ref for Me-**3** (C_S)	5.229	237.1	H→L (80%)	0.5698
3 (C_{2v})	2.876	431.1	H→L (93%)	0.0110
type (ii) ref for **3**	5.060	245.0	H→L (87%)	0.7098
Me-**4** (C_S)	2.151	576.4	H→L (97%)	0.0005
type (i) ref for Me-**4** (C_S)	3.748	330.8	H→L (89%)	0.0184
4 (C_{2h})	2.100	590.5	H→L (97%)	0.0000
type (ii) ref for **4**	3.870	320.4	H→L (75%), H–1→L+1 (17%)	0.0176
Me-**5** (C_S)	1.716	722.6	H→L (94%)	0.0003
type (i) ref for Me-**5** (C_S)	2.736	453.2	H→L (79%), H–1→L (15%)	0.2052
5 (C_{2h})	1.554	798.0	H–1→L (98%)[b]	0.0000
type (ii) ref for **5**	2.892	428.7	H→L (71%), H–1→L (16%)	0.2555
diMe-**6** (C_S)	2.722	455.5	H→L (94%)	0.0000
type (i) ref for diMe-**6** (C_S)	4.033	307.5	H→L (82%)	0.5018
6 (D_{2h})	2.691	460.8	H→L (95%)	0.0000
type (ii) ref for **6**[c]	3.998	310.1	H→L (81%)	0.4602
Me-**5** (C_S)	2.067	599.9	H→L (95%)	0.0074
type (ii) ref for **5**	3.909	317.2	H→L (73%), H–1→L (15%)	0.3734
7 (C_{2v})	2.122	584.4	H→L (95%)	0.0079
type (ii) ref for **7**	3.908	317.3	H→L (86%)	0.7377
8 (D_{2h})	2.237	554.3	H→L (94%)	0.0000
type (ii) ref for **8** (C_{2h})	3.649	339.8	H→L (85%)	0.5052
9 (D_{2h})	2.444	507.2	H→L (89%)	0.0000

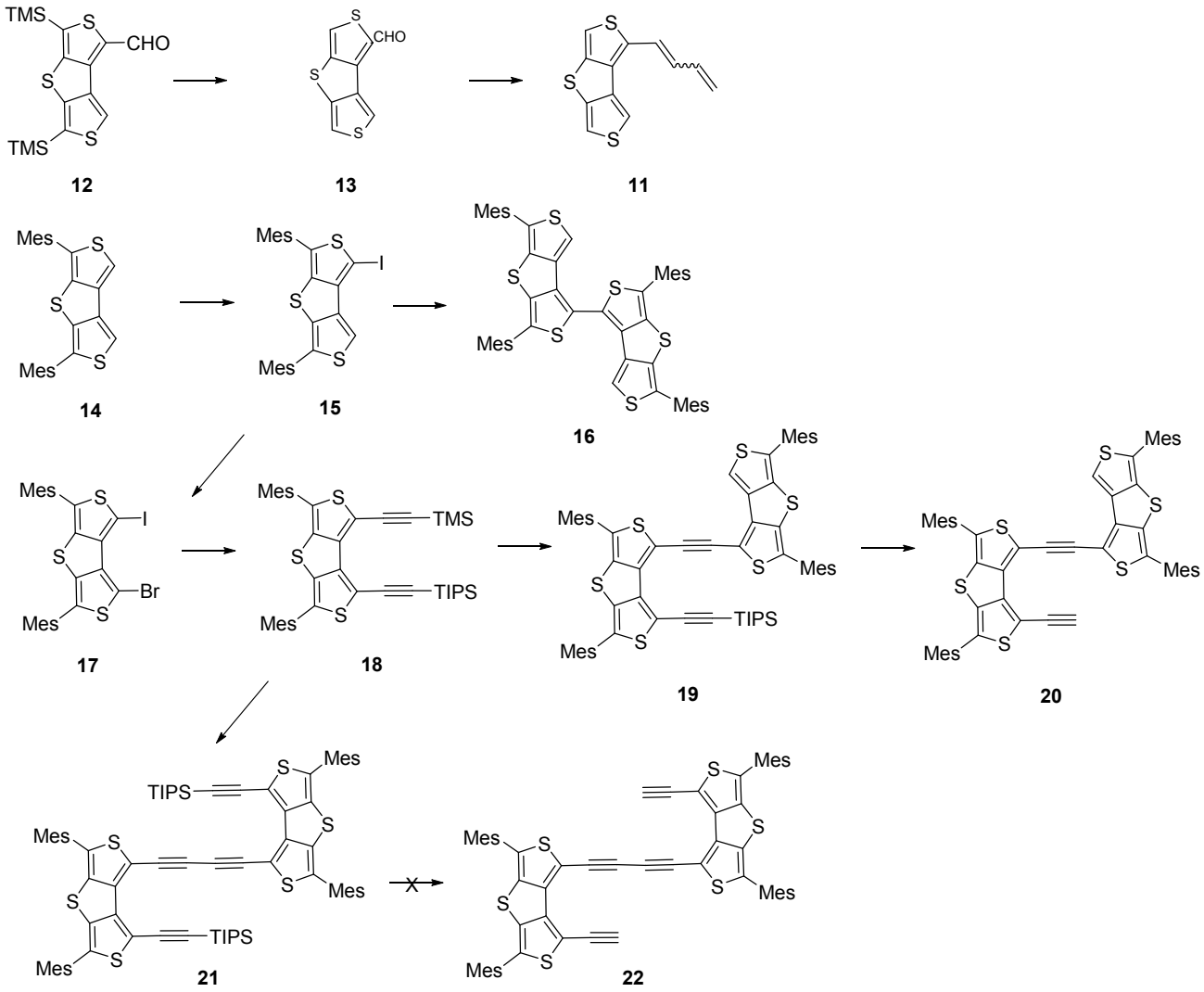
type (ii) ref for **9** (C_s)	3.320	373.5	H→L (78%)	0.5266
10 (D_{2h})	2.486	498.8	H→L (80%)	0.0000
type (ii) ref for 1**0** (C_{2h})	3.042	407.6	H→L (71%)	0.5282

[a]With 6-311+G(d,p) basis set at the B3LYP/6-31G(d,p) optimized geometry. [b] HOMO and HOMO-1 were nearly degenerate with the energy difference of 0.05 eV.

[c] Two five membered rings were opened.

Synthesis of type (ii) reference compounds for 7-9

The synthesis of compound **12**[2] and **14**[3] was reported previously. The butadiene moiety in compound **11** was found to be a mixture of cis and trans isomers as observed in the case of the same Wittig reaction from formylthiophene.[4] The TD-HF calculations predicted that the cis isomer of **11** has a slightly longer (i.e., energetically lower) absorption maximum than that of the trans isomer. Consequently, the observed absorption edge was expected to reflect the cis isomer that is the actual reference compound for **7**. Unfortunately, treatment of **21** with TBAF resulted in complex mixtures. Thus, the attempted synthesis of **22** as type (ii) reference compound for **10** was failed. We also conducted the optimization of the structure of **21** at the B3LYP/6-31G(d,p) level and found that two dithienothiophene moieties were perpendicularly arranged due to the presence of the sterically demanding TIPS groups. Therefore, **21** was considered to be inappropriate as the reference for **10**.



Scheme S1. Synthesis of **11**, **16**, and **20** as the type (ii) reference compounds for **7-9**

Synthesis of 11. To a solution of **12** (102 mg, 0.277 mmol) in THF (1 mL) and conc HCl_{aq} (60 mg, ~0.6 mmol) was added TBAF in THF (1.0 M, 0.83 mL) and the mixture was stirred at rt for 90 min. After evaporation and dried in vacuo, the mixture was separated through SiO_2 short column eluted with hexane-dichloromethane (1:1) to give crude **13** (60 mg, 97%) as yellow solid; ^{1}H NMR ($CDCl_3$, 270 MHz) δ 10.01 (s, 1H), 8.40 (m, 1H), 7.47 (m, 1H), 7.11 (m, 1H) ; ^{13}C NMR ($CDCl_3$, 67.5 MHz) δ 180.5, 145.8, 143.5, 138.9, 135.5, 130.2, 121.33, 121.28, 111.9.

To a solution of allyltriphenylphosphonium bromide (313 mg, 0.816 mmol) in anhydrous THF (2 ml) was added a suspension of *t*-BuOK (61 mg, 0.54 mmol) in anhydrous THF (2 ml) at 0 °C and the mixture was stirred for 1 h under N_2. To this reaction mixture, **13** (60 mg, 0.27 mmol) in anhydrous THF (2 ml) was added, and the mixture was stirred overnight at room temperature. After standard workup with ether, volatiles were removed in vacuo, and the residue was purified through SiO_2 short column eluted with hexane-dichloromethane (3:2) followed by preparative GPC separation eluted with chloroform to give **11** (15 mg, 0.060 mmol, 22%) as unstable pale yellow solid (easily polymerized in the solid state) which included inseparable trans/cis isomers (5/1 judged by the assignment for 1-(2-thienyl)-1,3-butadiene;[4] the cis derivative seemed to be more labile); ^{1}H NMR ($CDCl_3$, 500 MHz) (trans isomer) δ 7.49 (d, J = 2.5 Hz, 1H), 6.88-7.02 (m, 2H), 6.83 (s, 1H), 6.70 (dd, J = 10.0, 15.3 Hz, 1H), 6.54 (ddd, J = 10.0, 10.0, 16.7 Hz, 1H), 5.39 (d, J = 16.7 Hz, 1H), 5.24 (d, J = 10.0 Hz, 1H); (cis isomer) δ 7.43 (d, J = 2.5 Hz, 1H), 6.88-7.10 (m, 3H), 6.79 (d, J = 11.5 Hz, 1H), 6.32 (dd, J = 11.5, 11.5 Hz, 1H), 5.49 (d, J = 16.5 Hz, 1H), 5.35(partially overlapped to the signal of trans isomer); ^{13}C NMR ($CDCl_3$, 125 MHz) (trans+cis) δ 143.1, 143.04, 142.97, 142.7, 136.4, 136.21, 136.15, 134.6, 133.4, 133.2, 132.2, 130.8, 130.4, 129.7, 123.5, 121.3, 120.4, 118.8, 114.9, 114.5, 111.6, 111.4, 111.3, 110.1; MS(APCI-TOF) calcd for $C_{12}H_9S_3$ [$(M+H)^+$] = 249; found 249.

Synthesis of 16. To a solution of **14** (195 mg, 0.45 mmol) in chloroform (4.5 ml) was added NIS (106 mg, 0.47 mmol). The reaction mixture was stirred at rt in the dark overnight. After evaporation, the residue was separated by silica gel column chromatography using hexane as eluent to give crude **15** (244 mg) as colorless solid (which was gradually turned pink under room light).

To a solution of crude **15** (27 mg, 0.048 mmol), $Pd(OAc)_2$ (0.54 mg, 0.0024 mmol) and tetrabutylammonium bromide (7.7 mg, 0.024 mmol) in dry toluene (1 mL) was added disopropylethylamine (6.2 mg 0.048 mmol) under N_2. The reation mixture was refluxed overnight. After evaporation, the residue was separated by silica gel column chromatography using hexane as eluent to give crude **16** (10 mg, 0.011 mmol, 48%) as pale yellow solid which was further purified by recrystallization from dichloromethane/ethanol; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.56 (s, 2H), 6.94 (s, 4H), 6.90 (s, 4H), 2.2-2.3 (m, 24H), 2.17 (s, 12H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 141.0, 140.3, 138.83, 138.79, 138.4, 135.0, 134.8, 129.9, 129.6, 128.3, 127.1, 115.9, 107.3, 104.7, 99.7, 98.2, 21.1, 20.3, 18.9, 11.7, 0.1; MS(APCI-TOF) calcd for $C_{52}H_{46}S_6$ [M^+] = 862; found 862.

Synthesis of 18. To a solution of crude **15** (244 mg, 0.437 mmol) in chloroform (4 mL) and acetic acid (4 mL) was added NBS (82 mg, 0.46 mmol) under N_2. The reaction mixture was stirred at rt for 2 h. After quenching with aqueous Na_2CO_3, the organic layer was extracted with dichloromethane. The combined organic layer was dried over $MgSO_4$. After filtration and evaporation, the residue was separated by silica gel column chromatography using hexane as eluent to give crude **17** (258 mg) as colorless solid.

To a solution of this crude **17**, Pd $(PPh_3)_4$ (24 mg, 0.020 mmol), CuI (8 mg, 0.04 mmol) in dry toluene (4 mL) and dry diisopropylamine (0.8 mL) under N_2 was added TMS-acetylene (0.061 mL, 0.44 mmol). The mixture was stirred in a seal tube at rt for 19h. Then, TIPS-acetylene (0.14 mL, 0.60 mmol) and additional Pd $(PPh_3)_4$ (24 mg, 0.020 mmol) and CuI (8 mg, 0.04 mmol) was added to this reaction mixture and stirred at 90 °C overnight. After removal of volatiles, the residue was purified by silica gel column chromatography with hexane as eluent, followed by preparative GPC separation eluted with chloroform to give **18** (82 mg, 0.12 mmol, 26% from **15**) as pale yellow solid; ^{1}H NMR ($CDCl_3$, 270 MHz) δ 6.86 (s, 4H), 2.26 (s, 6H), 2.14 (s, 12H), 1.3-1.9 (m, 21 H), 0.28 (s, 9H) ; ^{13}C NMR ($CDCl_3$, 67.5 MHz) δ 141.0, 138.9, 138.4, 135.7, 129.7, 128.3, 127.1, 115.3, 106.8, 97.8, 21.1, 20.2, 0.1; MS(APCI-TOF) calcd for $C_{42}H_{53}S_3Si_2$ [$(M+H)^+$] = 709; found 709.

Synthesis of 20 To a solution of **18** (49 mg, 0.069 mmol) in dichloromethane (1 ml) and methanol (1 mL) was added K_2CO_3 (23 mg, 0.17 mmol) under N_2 and the mixture was stirred at rt for 3 h. The volatiles was evaporated and the residue was separated by silica gel column chromatography using hexane as eluent to give crude TMS deprotected product (41 mg) as pale yellow solid. A mixture of this crude ethynyl compound, crude **15** prepared from **14** (31 mg, 0.071 mmol), Pd $(PPh_3)_4$ (8 mg, 0.007 mmol), CuI (3 mg, 0.01 mmol) was dissolved in toluene (2 mL) and diisopropylamine (0.4 mL) and stirred at 90 °C overnight. After removal of volatiles, the residue was purified by silica gel column chromatography with hexane-dichloromethane (9:1) as eluent, followed by preparative GPC separation eluted with chloroform to give **19** (53 mg, 0.049 mmol, 72% from **18**) as pale yellow solid; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.98 (s, 1H), 6.8-6.9 (m, 8H), 2.1-2.3 (m, 36H), 0.9-1.0 (m, 21 H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ141.2, 141.0, 140.9, 140.8, 139.8, 139.0, 138.9, 138.5, 138.4, 136.4, 136.1, 135.4, 130.9, 130.4, 129.7, 128.39, 128.37, 128.35, 128.25, 127.8, 127.7, 127.4, 127.1, 117.3, 116.0, 114.7, 112.3, 105.1, 99.3, 92.1, 90.3, 21.1, 20.5, 20.40, 20.37, 20.35, 18.8, 11.7.

To a solution of **19** (25 mg, 0.023 mmol) in wet THF (2 ml) was added TBAF in THF (1.0 M 0.06 mL) and the mixture was stirred at rt for 2 h. After removal of volatiles, the residue was purified by silica gel column chromatography with hexane-dichloromethane (9:1) as eluent, followed by preparative GPC separation eluted with chloroform to give **20** (20 mg, 0.049 mmol, 95%) as pale yellow solid; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.91 (s, 1H), 6.8-6.9 (m, 8H), 3,72 (s, 1H), 2.1-2.3 (m, 36H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ141.4, 141.2, 141.0, 140.9, 139.14, 139.06, 138.96, 138.6, 138.5, 138.44, 138.40, 137.08, 135.8, 130.4, 130.0, 129.7, 128.41, 128.39, 128.26, 128.0, 127.7, 127.2, 126.9, 117.0, 114.5, 113.6, 112.0, 91.7, 90.9, 87.9, 21.11, 21.09, 20.41, 20.35, 20.39; MS(APCI-TOF) calcd for $C_{56}H_{47}S_6$ $[(M+H)^+]$ = 911; found 911.

Synthesis of 21 TMS deprotected product of **18** (31 mg, 0.044 mmol) was synthesized as shown above. To a mixture of this crude product, Pd $(PPh_3)_4$ (5 mg, 0.004 mmol), CuI (0.8 mg, 0.004 mmol) in dry THF (1 mL) and dry diisopropylamine (1 mL) under N_2 was added I_2 (5.6 mg, 0.022 mmol) in THF under N_2. The reaction mixture was heated at 40 °C overnight. After removal of volatiles, the residue was purified by silica gel column chromatography with hexane-ether (50:1) as eluent, followed by preparative GPC separation eluted with chloroform to give **21** (19 mg, 0.015 mmol, 68%) as pale yellow solid; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 6.885 (s, 4H), 6.873 (s, 4H), 2.273 (s, 6H), 2.266 (s, 6H), 2.15 (s, 12H), 2.14 (s, 12H). 1.0-1.2 (m, 21H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ141.3, 140.7, 139.1, 138.8, 138.7, 138.37, 138.33, 135.0, 131.5, 129.4, 128.4, 128.3, 127.1, 127.0, 116.8, 113.6, 105.4, 98.6, 86.0, 78.5, 21.1, 20.3, 20.2, 18.9, 18.8, 11.7; MS(APCI-TOF) calcd for $C_{56}H_{47}S_6$ $[(M+H)^+]$ = 1271; found 1271.

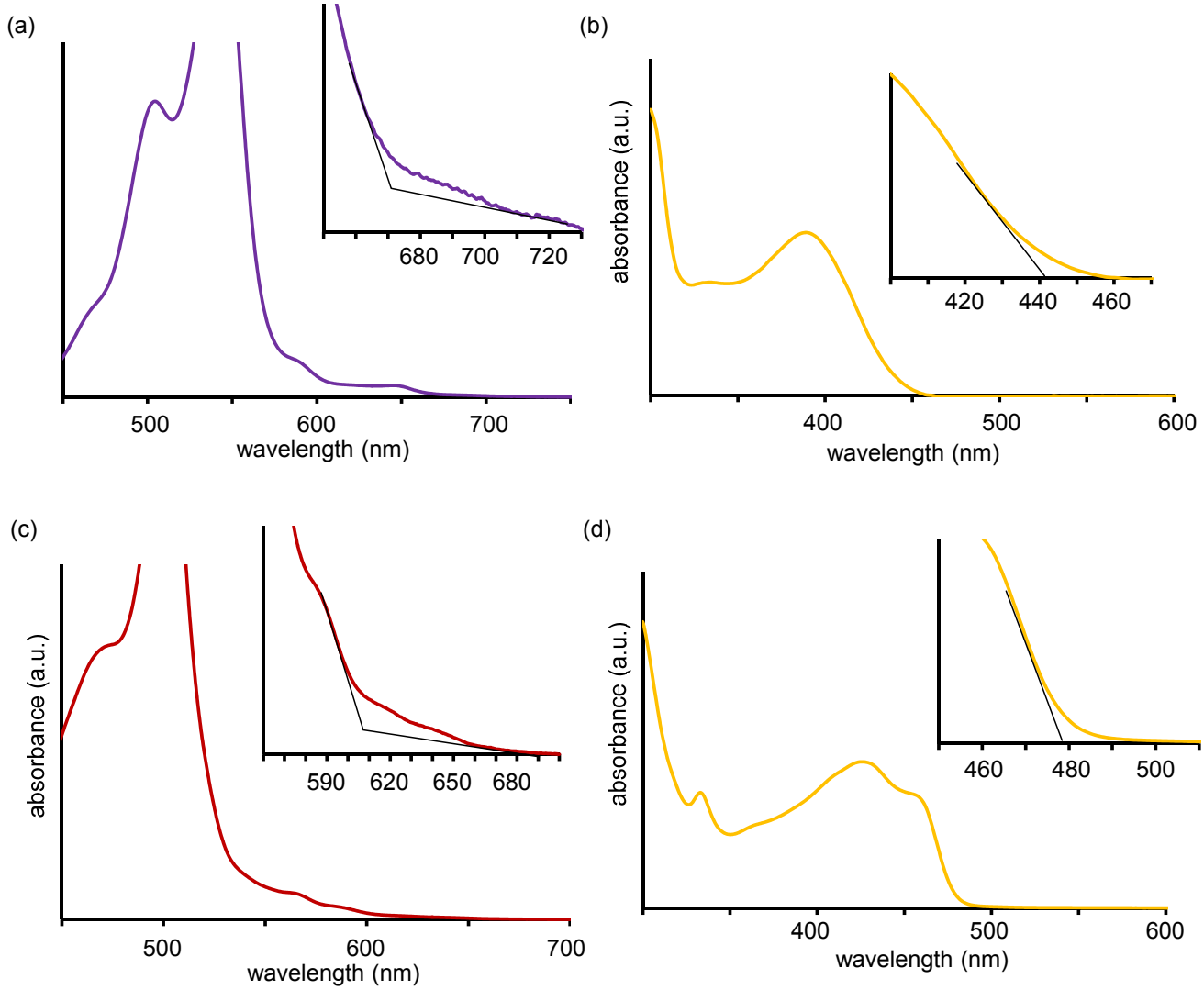
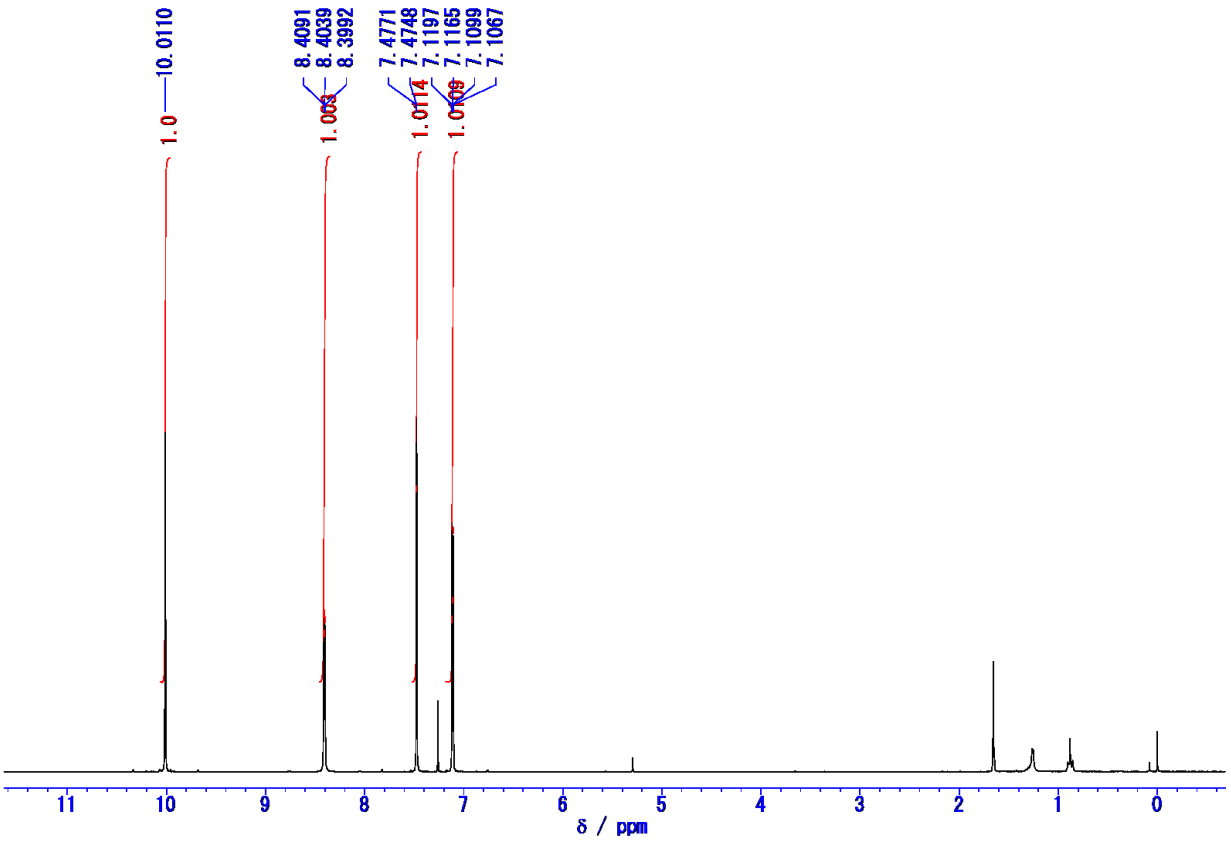
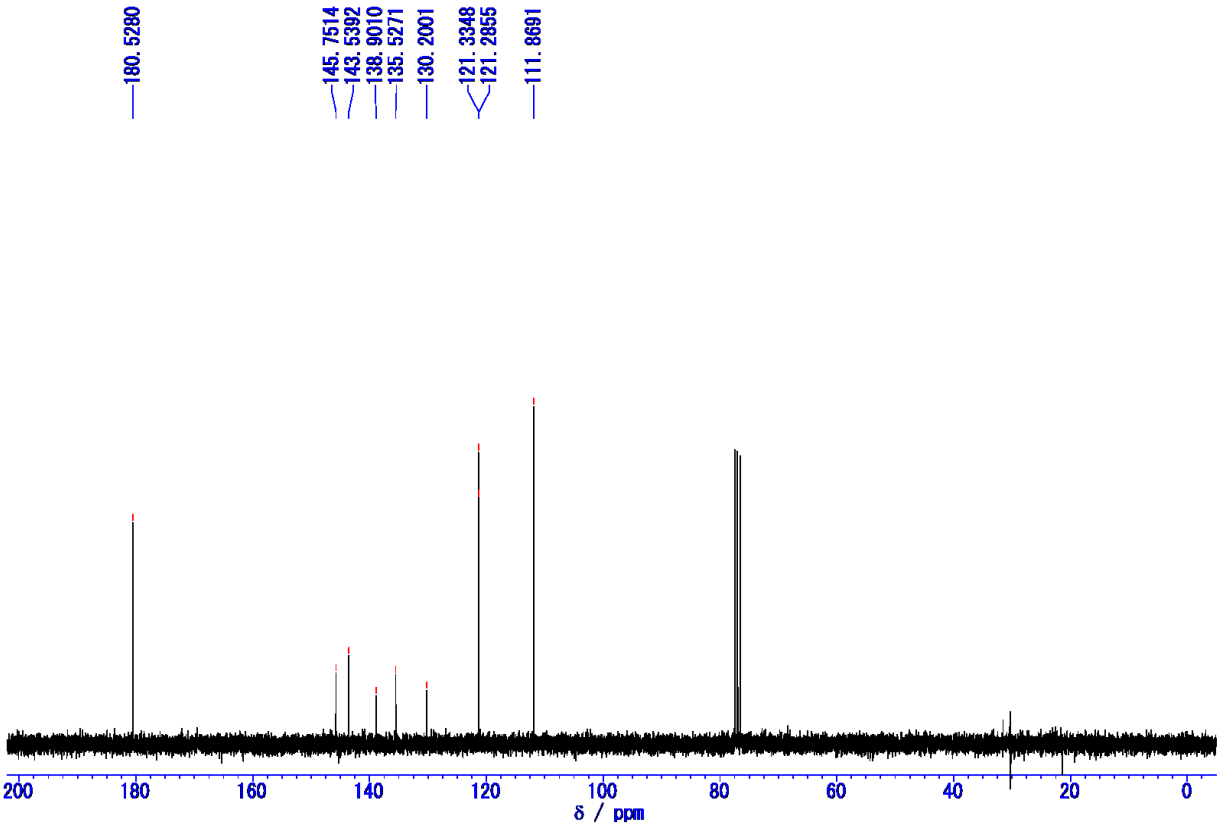


Fig. S4. Absorption spectra (inset: enlargement in the region of absorption edge) of (a) **8** and (c) **9** and (c) their acyclic reference (c) **16** and (d) **20**.

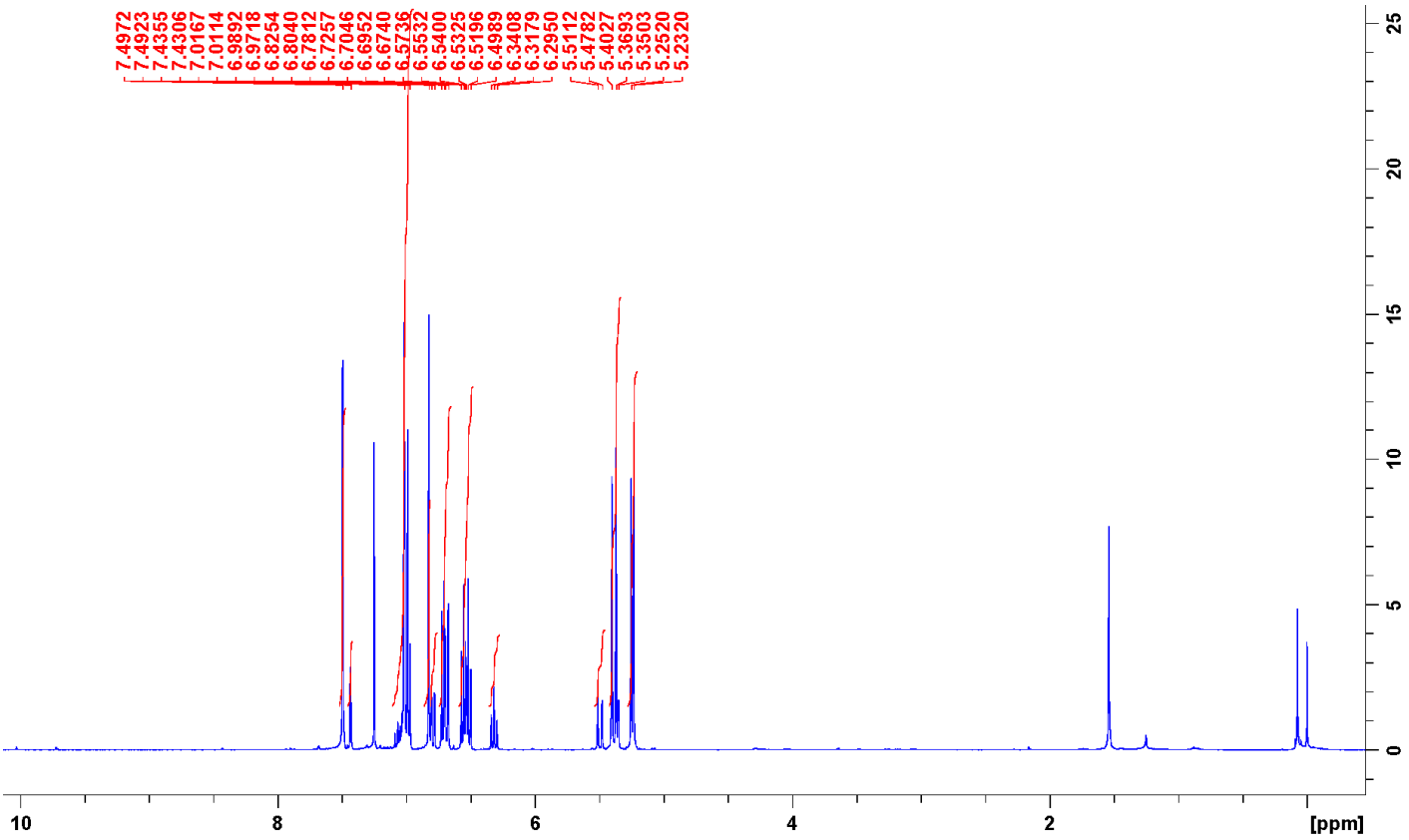
^{1}H NMR of **13**



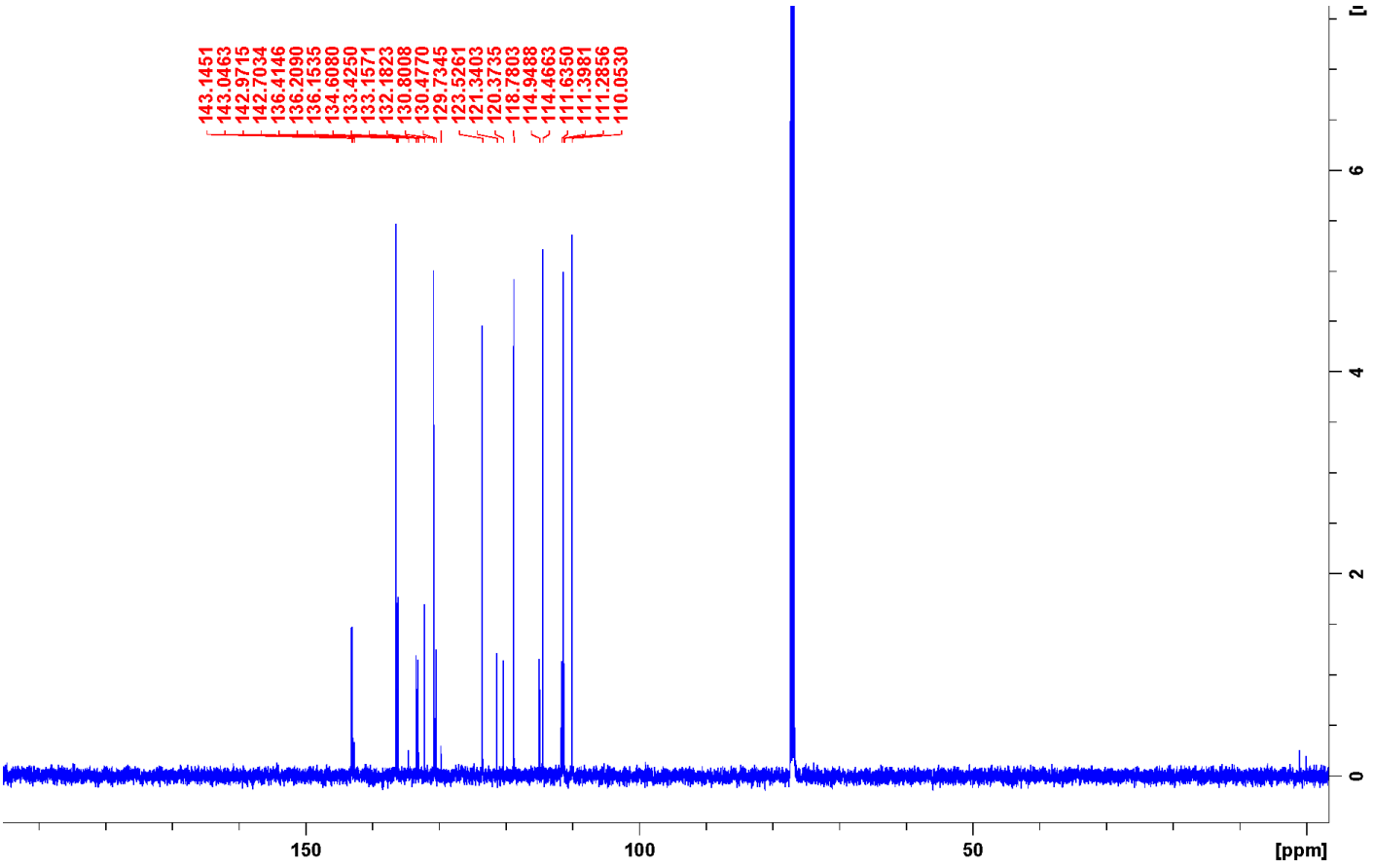
^{13}C NMR of **13**



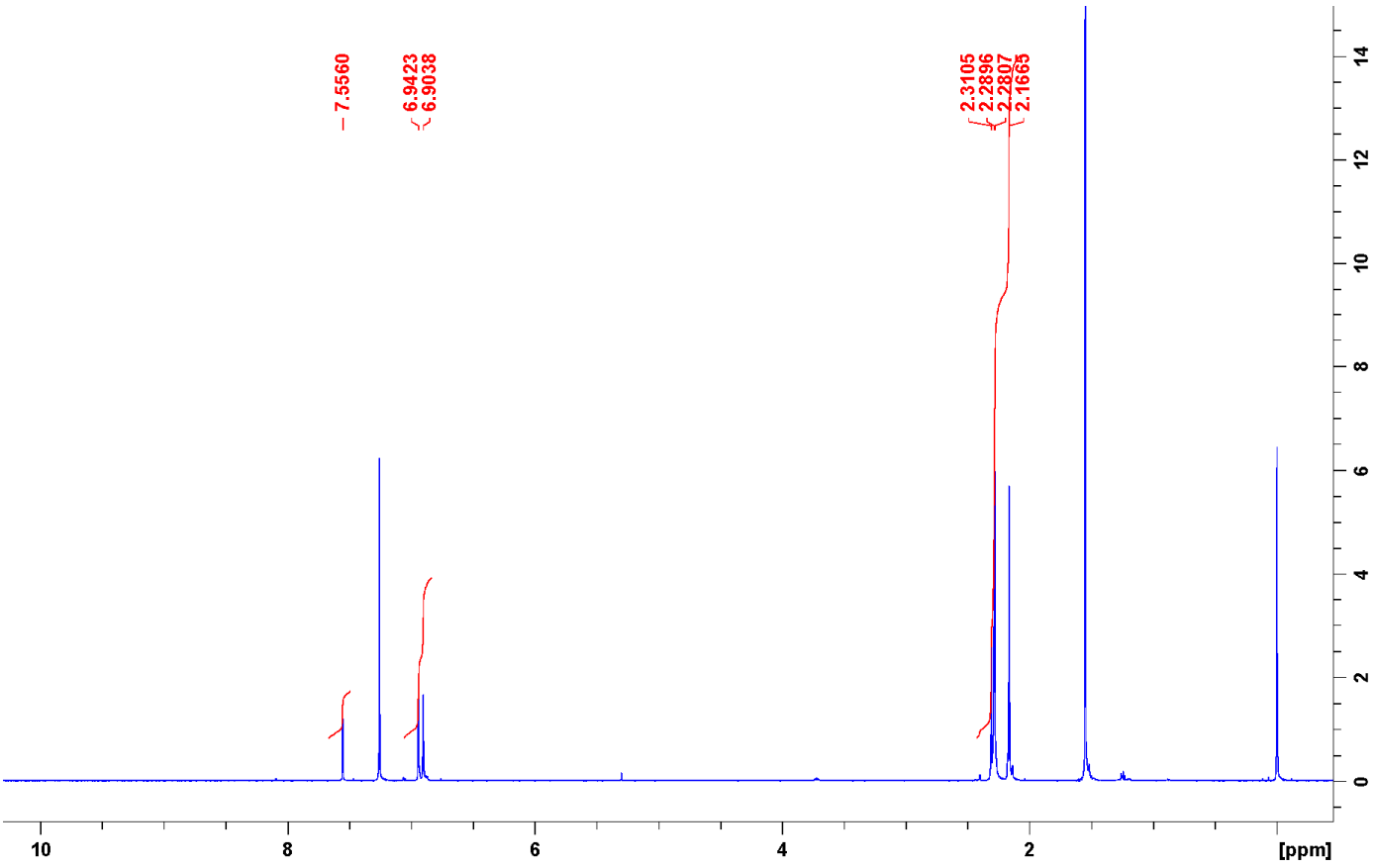
^{1}H NMR of **11**



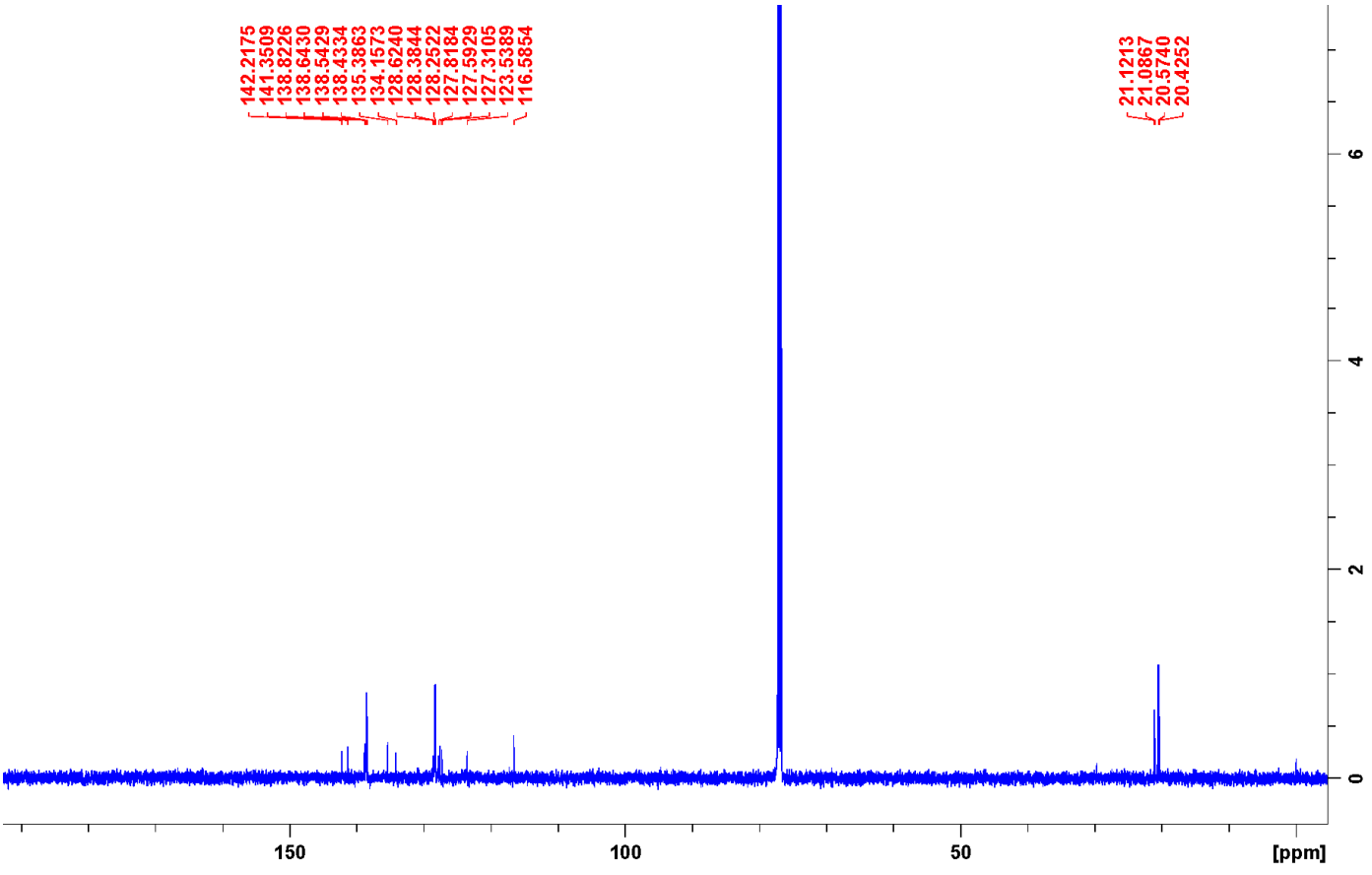
^{13}C NMR of **11**



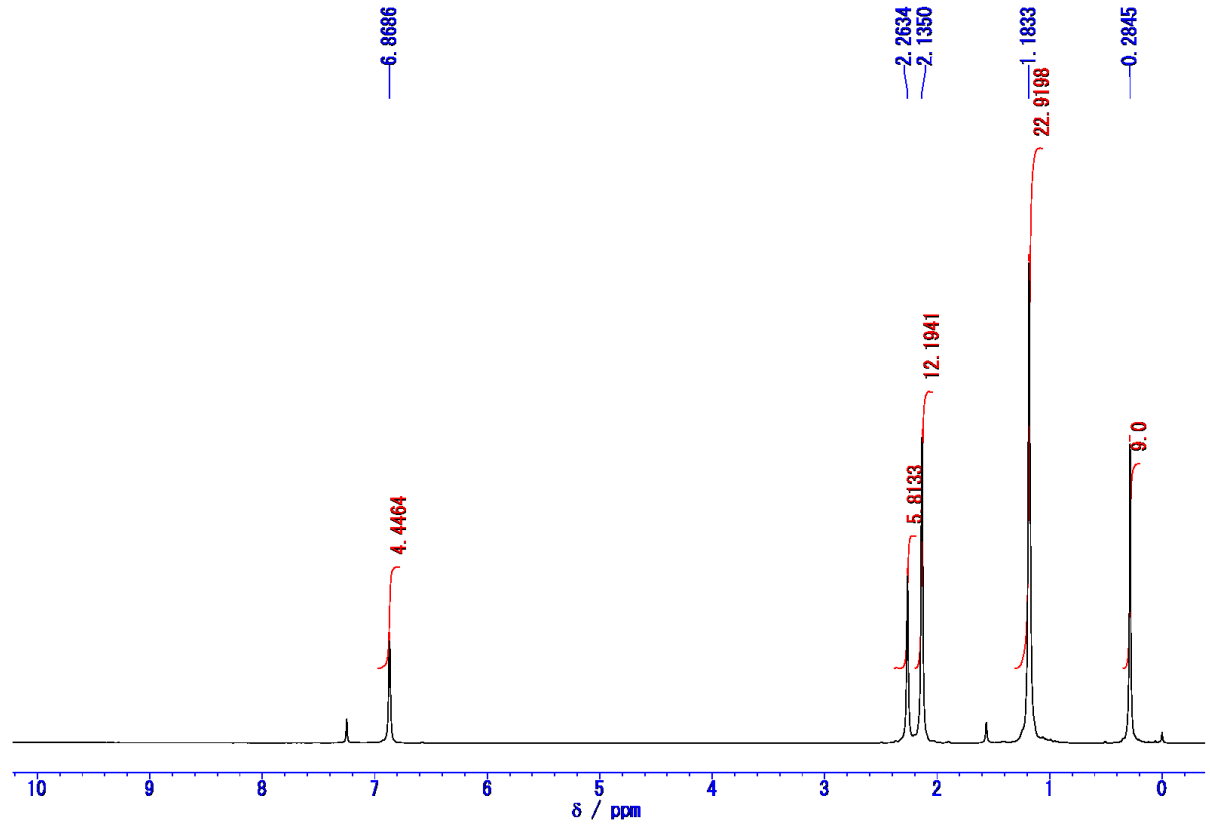
^{1}H NMR of **16**



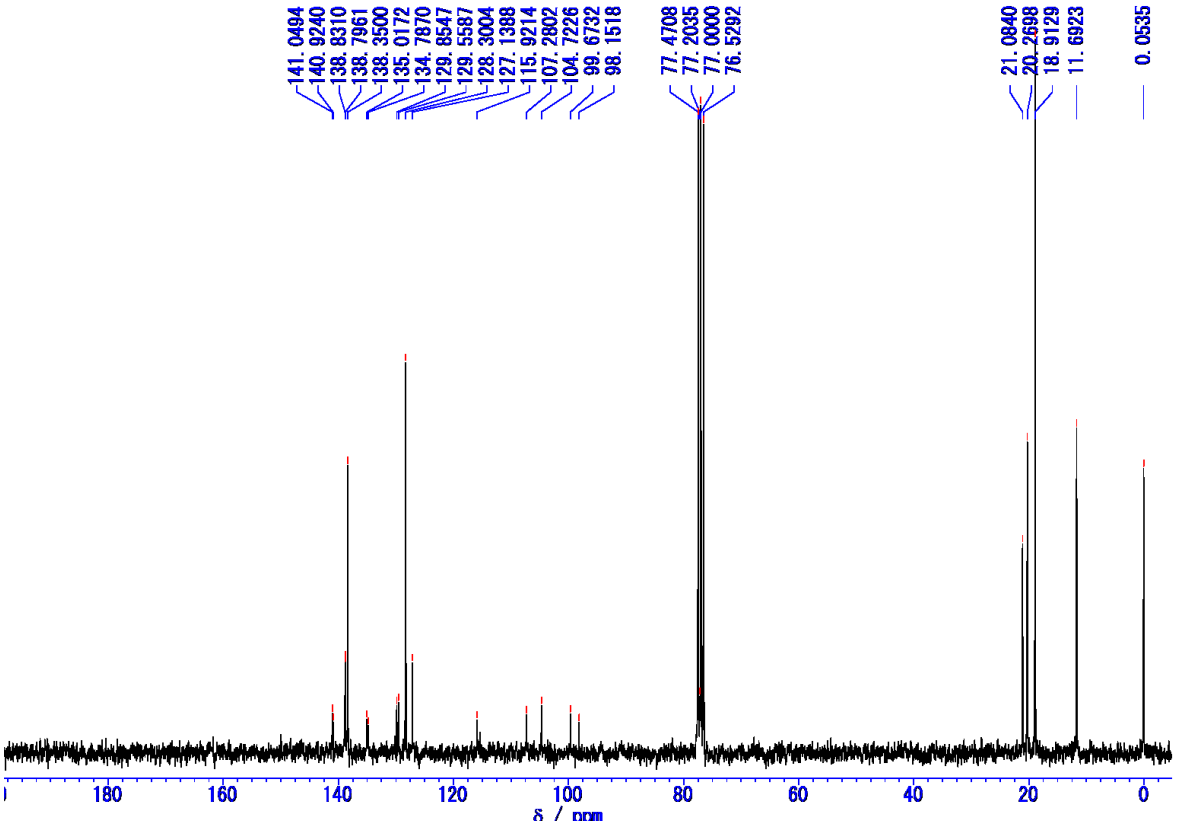
^{13}C NMR of **16**



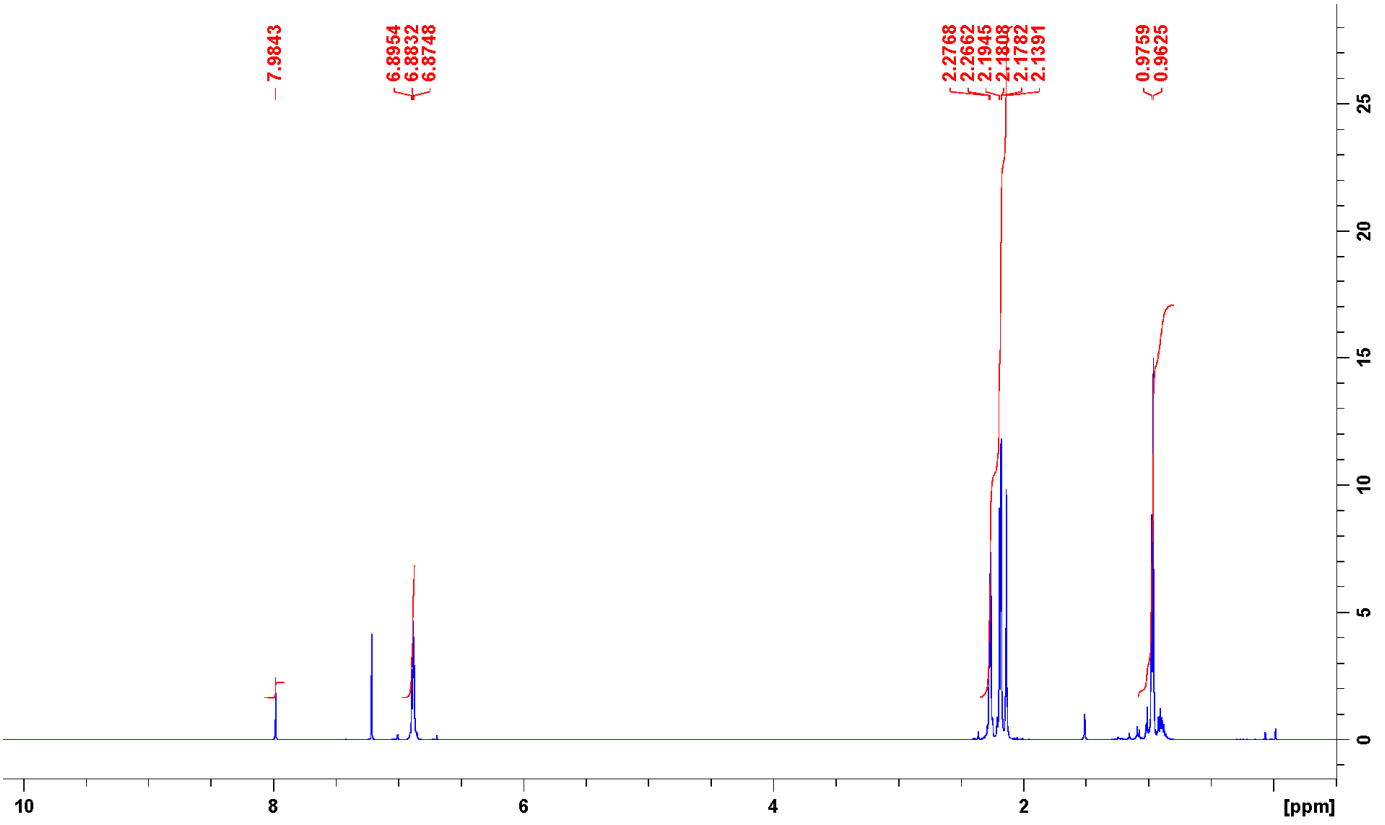
^{1}H NMR of **18**



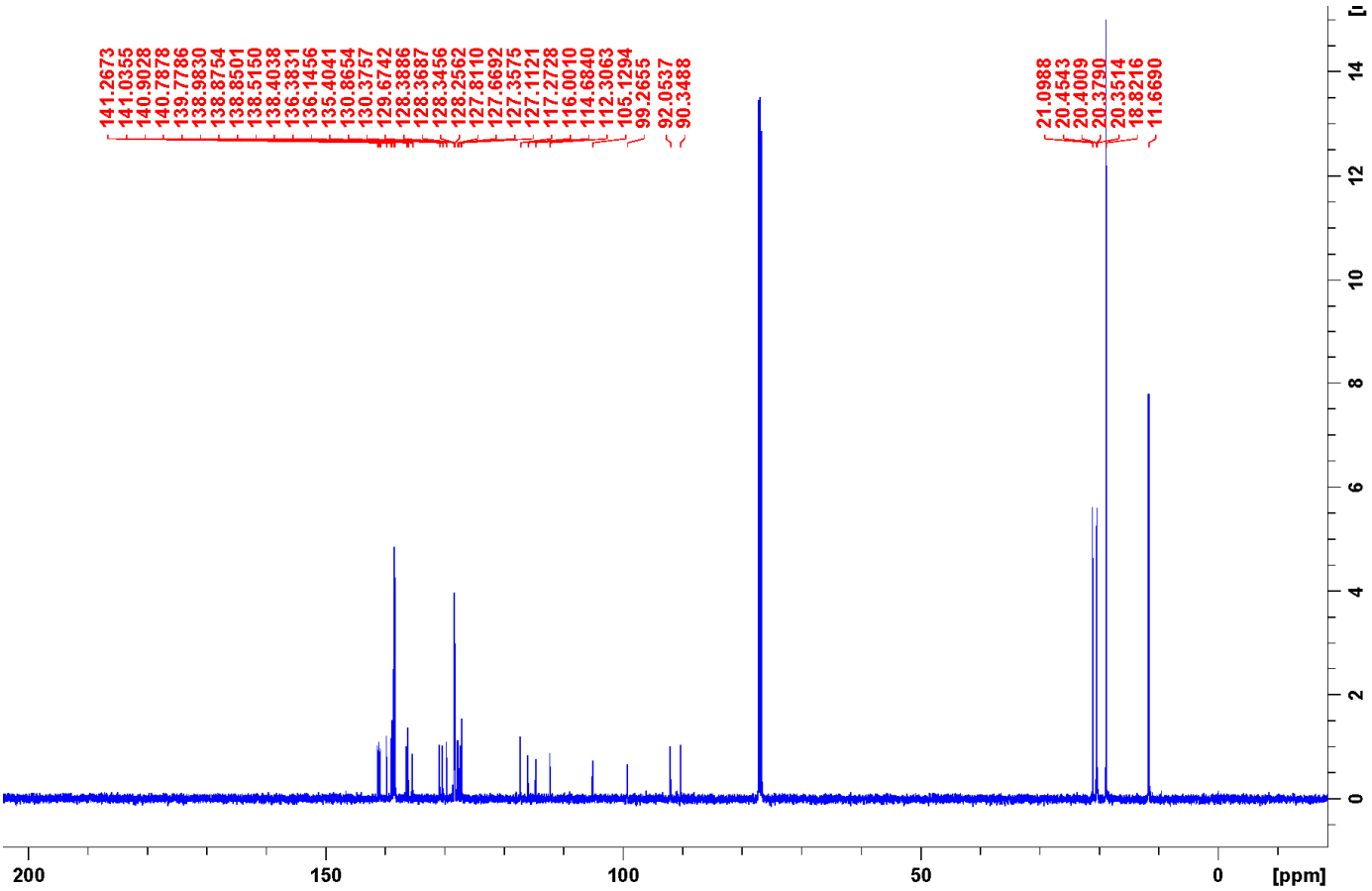
^{13}C NMR of **18**



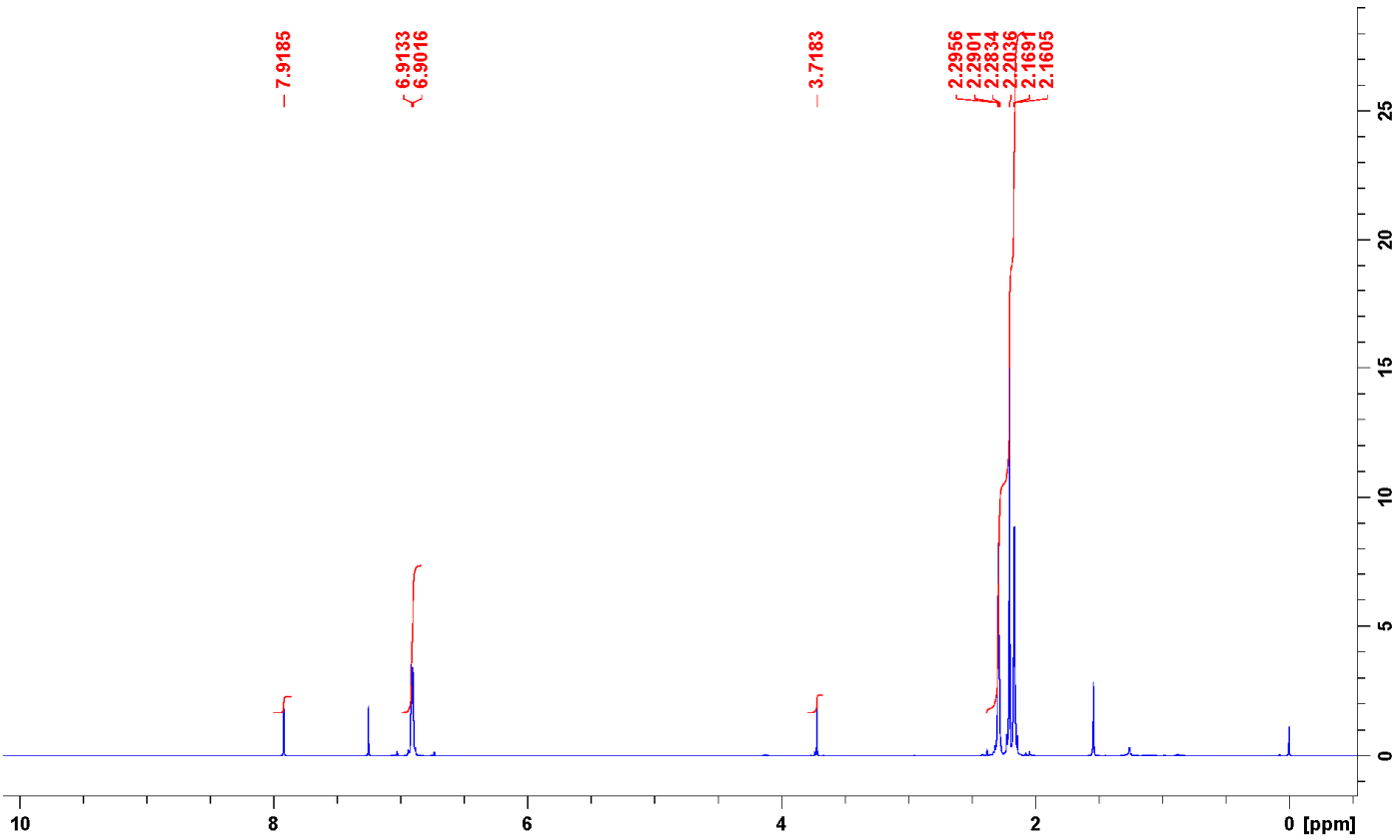
^{1}H NMR of **19**



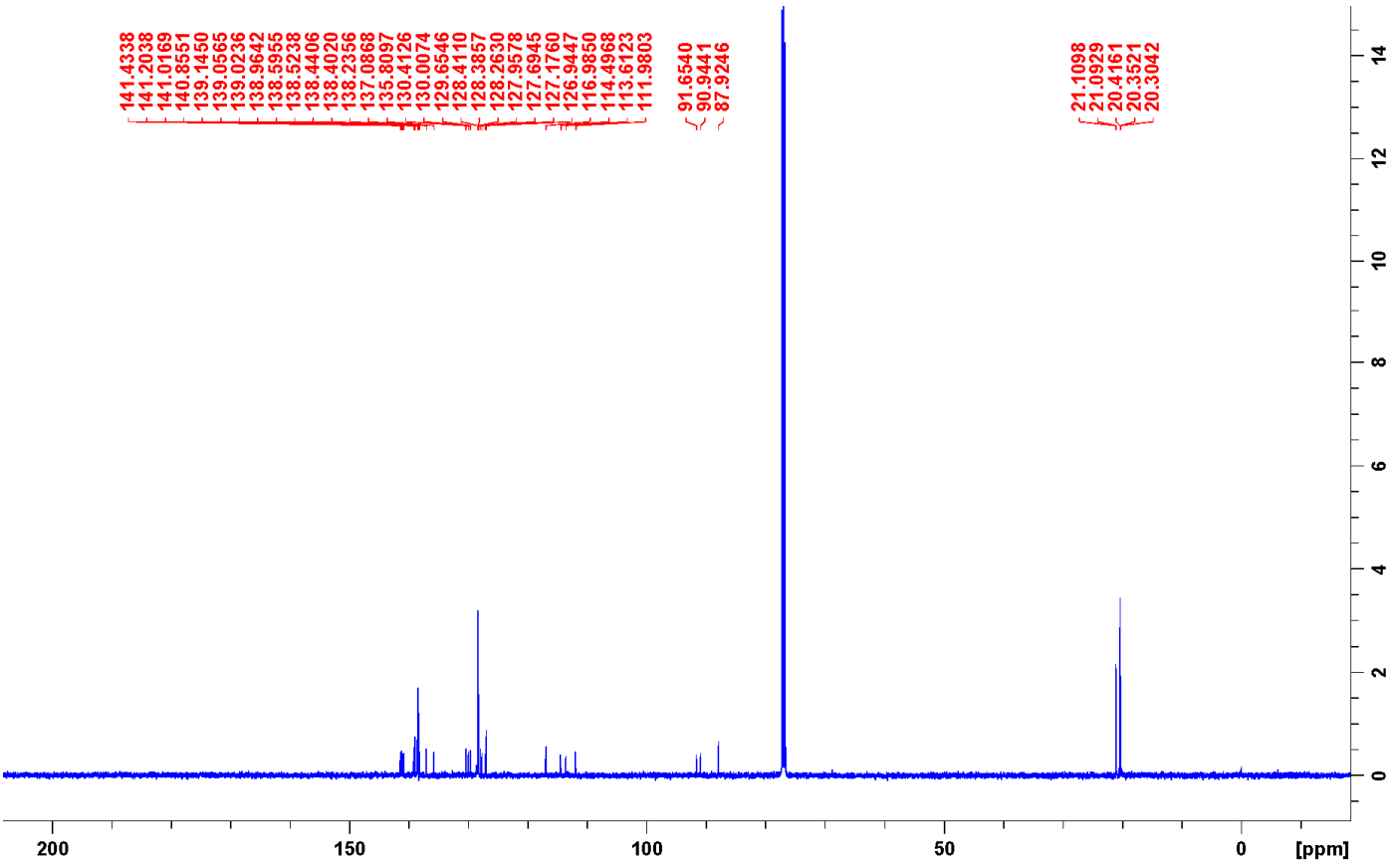
^{13}C NMR of **19**



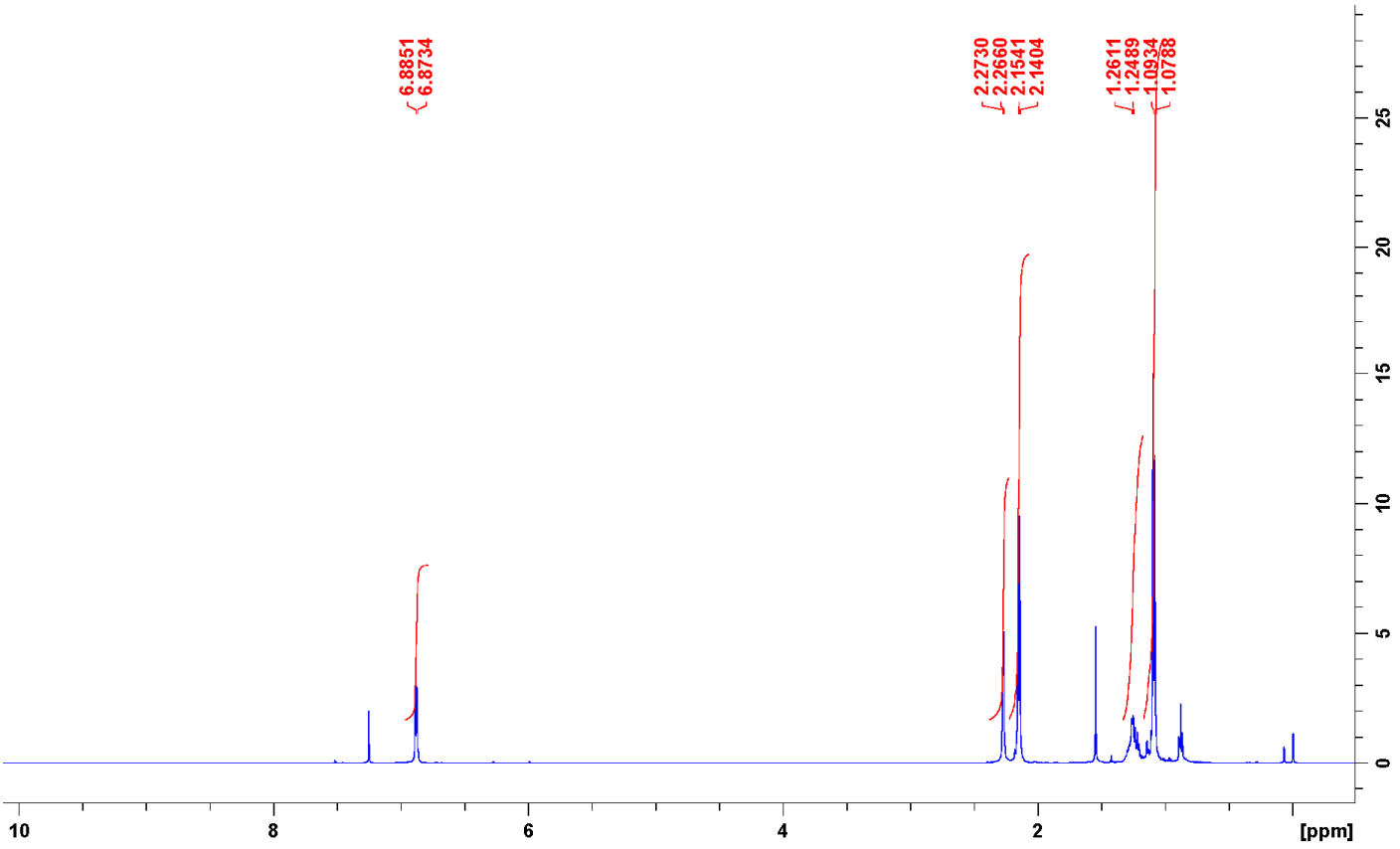
^{1}H NMR of **20**



^{13}C NMR of **20**



^{1}H NMR of **21**



^{13}C NMR of **21**

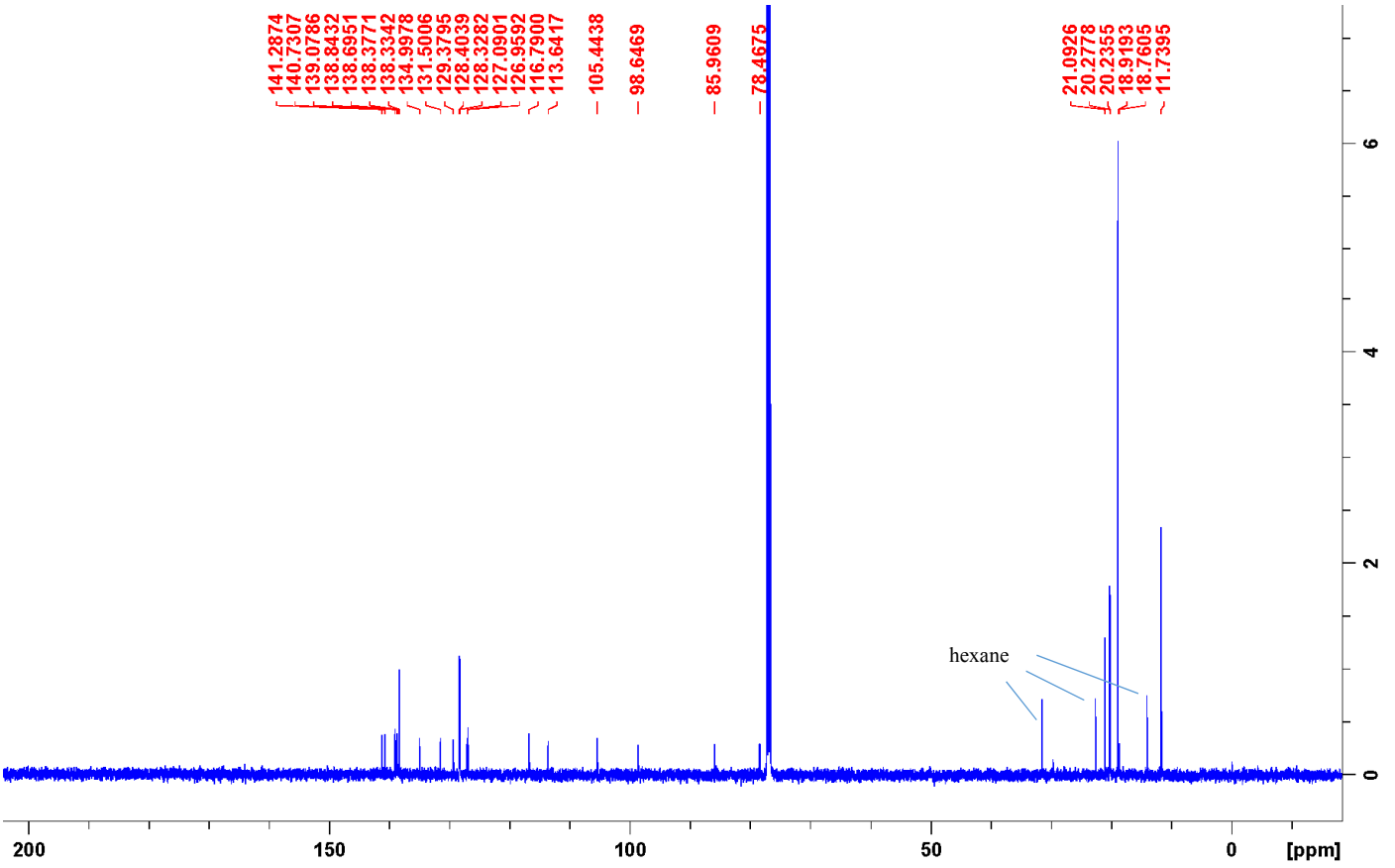


Table S3. Cartesian coordinate of optimized structure of Me-**8A** (C_S) at the B3LYP/6-31G(d,p) level

C	1.33556743	0.77777324	0.00000000
H	2.13183921	1.52075720	0.00000000
C	1.79865884	-0.48526228	0.00000000
H	2.88637962	-0.54166990	0.00000000
C	1.20366100	-1.83353876	0.00000000
H	1.97050477	-2.60609033	0.00000000
C	-0.05497101	-2.30819037	0.00000000
H	-0.11805497	-3.39524613	0.00000000
C	-1.38902411	-1.68818554	0.00000000
H	-2.17786549	-2.43832874	0.00000000
C	-1.84455115	-0.42085807	0.00000000
H	-2.93177481	-0.35614768	0.00000000
C	-1.24912197	0.92733871	0.00000000
H	-2.02942787	1.68635335	0.00000000
C	0.00000000	1.43699953	0.00000000
C	0.14450220	2.94548863	0.00000000
H	0.71058685	3.28281785	0.87865620
H	0.71058685	3.28281785	-0.87865620
H	-0.82110166	3.45534593	0.00000000

Table S4. Cartesian coordinate of optimized structure of type (i) reference compound for Me-**8A** (C_S) at the B3LYP/6-31G(d,p) level

C	-1.31898310	0.91992506	0.00000000
H	-2.08647636	1.69250111	0.00000000
C	-1.84958029	-0.33378067	0.00000000
H	-2.93875110	-0.31296647	0.00000000
C	-1.36130804	-1.68840855	0.00000000
H	-2.17738363	-2.40916541	0.00000000
C	-0.12970356	-2.26292930	0.00000000
H	-0.15632496	-3.35146847	0.00000000
C	1.22282417	-1.75816223	0.00000000
H	1.95108705	-2.56831776	0.00000000
C	1.79895687	-0.53702553	0.00000000
H	2.88924651	-0.58145013	0.00000000
C	0.00000000	1.52969968	0.00000000
C	0.01836220	2.88323206	0.00000000
H	0.94925327	3.44286686	0.00000000
C	1.39221967	0.90222228	0.00000000
H	1.91453785	1.34598631	0.86161831
H	1.91453785	1.34598631	-0.86161831
H	-0.89645395	3.46739076	0.00000000

Table S5. Cartesian coordinate of optimized structure of **8A** (D_{4h}) at the B3LYP/6-31G(d,p) level

C	0.67253864	1.71585976	-0.00000000
H	1.11155741	2.71215649	0.00000000
C	-0.67253864	1.71585976	-0.00000000
H	-1.11155741	2.71215649	-0.00000000
C	-1.71585976	0.67253864	0.00000000
H	-2.71215649	1.11155741	0.00000000
C	-1.71585976	-0.67253864	-0.00000000
H	-2.71215649	-1.11155741	-0.00000000
C	-0.67253864	-1.71585976	-0.00000000
H	-1.11155741	-2.71215649	0.00000000
C	0.67253864	-1.71585976	-0.00000000
H	1.11155741	-2.71215649	-0.00000000
C	1.71585976	-0.67253864	0.00000000
H	2.71215649	-1.11155741	0.00000000
C	1.71585976	0.67253864	-0.00000000
H	2.71215649	1.11155741	-0.00000000

Table S6. Cartesian coordinate of optimized structure of type (ii) reference compound for **8A** (C_{2h}) at the B3LYP/6-31G(d,p) level

C	0.30368100	1.87237100	0.00000000
H	-0.38299600	2.71729700	0.00000000
C	-0.30368100	0.65361200	0.00000000
H	-1.38706700	0.68353000	0.00000000
C	0.30368100	-0.65361200	0.00000000
H	1.38706700	-0.68353000	0.00000000
C	-0.30368100	-1.87237100	0.00000000
H	0.38299600	-2.71729700	0.00000000
C	-1.70361400	-2.29248900	0.00000000
H	-1.81486400	-3.37661200	0.00000000
C	1.70361400	2.29248900	0.00000000
H	1.81486400	3.37661200	0.00000000
C	-2.84761000	-1.58605500	0.00000000
H	-3.80240000	-2.10248000	0.00000000
H	-2.89556100	-0.50455000	0.00000000
C	2.84761000	1.58605500	0.00000000
H	3.80240000	2.10248000	0.00000000
H	2.89556100	0.50455000	0.00000000

Table S7. Cartesian coordinate of optimized structure of Me-**12A** (C_S) at the B3LYP/6-31G(d,p) level

C	2.24737807	1.53987301	0.00000000
C	-1.76513281	-2.14899962	-0.00000000
C	-0.45710761	-2.94014064	-0.00000000
C	0.93498577	2.32650928	0.00000000
C	-0.24327625	1.65525916	-0.00000000
C	0.72472592	-2.27307569	0.00000000
C	-1.71972612	-0.79231463	0.00000000
C	2.20669906	0.18389483	0.00000000
C	-1.71705821	1.69728913	0.00000000
C	2.18889120	-2.29158132	0.00000000
C	-2.41731339	0.49396693	-0.00000000
C	2.90693233	-1.10294024	0.00000000
H	0.47804830	-1.24553521	0.00000000
H	-0.00000000	0.62813605	0.00000000
H	1.18254925	-0.07662187	0.00000000
H	-0.69445070	-0.53726384	0.00000000
H	-0.55013767	-4.02419528	0.00000000
H	1.02538416	3.41080022	0.00000000
H	3.16225127	2.12851424	0.00000000
H	-2.68232334	-2.73384857	-0.00000000
H	2.74487306	-3.22608633	0.00000000
H	3.99271667	-1.15855299	0.00000000
H	-3.50421009	0.54453569	0.00000000
C	-2.44013161	3.01576201	0.00000000
H	-2.16407987	3.61075422	0.87955768
H	-2.16407987	3.61075422	-0.87955768
H	-3.52573928	2.88759629	0.00000000

Table S8. Cartesian coordinate of optimized structure of type (i) reference compound for Me-**12A** (C_S) at the B3LYP/6-31G(d,p) level

C	2.30939893	1.49168377	-0.00000000
C	-1.81973959	-2.07637740	0.00000000
C	-0.55159693	-2.90143858	0.00000000
C	1.05368984	2.31313861	-0.00000000
C	-0.17117166	1.70922125	-0.00000000
C	0.65466521	-2.26673277	0.00000000
C	-1.75611449	-0.72371983	0.00000000
C	2.21589926	0.12846695	-0.00000000
C	-1.62336651	1.89199664	-0.00000000
C	2.09707411	-2.33565257	0.00000000
C	2.86284698	-1.16080916	0.00000000
H	0.43088165	-1.23247287	0.00000000
H	0.00000000	0.66647547	-0.00000000
H	1.18019984	-0.08651032	-0.00000000
H	-0.73231327	-0.45931716	0.00000000
H	-0.67436044	-3.98254266	0.00000000
H	1.18570447	3.39355485	-0.00000000
H	3.25013887	2.03816807	-0.00000000

H	-2.75379498	-2.63567841	0.00000000
H	2.62418086	-3.28693818	0.00000000
H	3.94594660	-1.25844228	0.00000000
C	-2.53129042	0.57726736	-0.00000000
H	-3.19294364	0.64180755	-0.87378103
H	-3.19294364	0.64180755	0.87378103
C	-2.24835680	3.08342156	-0.00000000
H	-3.33188920	3.16229016	-0.00000000
H	-1.69043460	4.01500319	-0.00000000

Table S9. Cartesian coordinate of optimized structure of **12A** (D_{2d}) at the B3LYP/6-31G(d,p) level

C	0.00000000	2.61776520	0.76498806
C	-0.00000000	-2.61776520	-0.76498806
C	-0.00000000	-2.61776520	0.76498806
C	0.00000000	2.61776520	-0.76498806
C	0.00000000	1.43490611	-1.42892011
C	-0.00000000	-1.43490611	1.42892011
C	-0.00000000	-1.43490611	-1.42892011
C	-0.00000000	1.43490611	1.42892011
C	0.00000000	0.69399005	-2.69321621
C	-0.00000000	-0.69399005	2.69321621
C	0.00000000	-0.69399005	-2.69321621
C	-0.00000000	0.69399005	2.69321621
H	-0.00000000	-0.68317105	0.68615705
H	0.00000000	0.68317105	-0.68615705
H	0.00000000	0.68317105	0.68615705
H	-0.00000000	-0.68317105	-0.68615705
H	-0.00000000	-3.59307527	1.24671010
H	0.00000000	3.59307527	-1.24671010
H	0.00000000	3.59307527	1.24671010
H	-0.00000000	-3.59307527	-1.24671010
H	-0.00000000	-1.20744709	3.65149228
H	0.00000000	1.20744709	-3.65149228
H	-0.00000000	1.20744709	3.65149228
H	0.00000000	-1.20744709	-3.65149228

Table S10. Cartesian coordinate of optimized structure of type (ii) reference compound for **12A** (C_S) at the B3LYP/6-31G(d,p) level

C	-0.01160900	-0.71731300	0.00000000
C	0.01160900	0.71731300	0.00000000
C	1.14557500	1.46941900	0.00000000
C	-3.62312600	-3.33879900	0.00000000
C	3.62312600	3.33879900	0.00000000
C	-1.14557500	-1.46941900	0.00000000
C	1.14557500	2.90820900	0.00000000
C	-2.22868100	-3.73165900	0.00000000
C	2.22868100	3.73165900	0.00000000
C	-1.14557500	-2.90820900	0.00000000
H	-3.85100000	-2.27490200	0.00000000
H	2.10295100	0.95175400	0.00000000
H	-2.10295100	-0.95175400	0.00000000
H	3.85100000	2.27490200	0.00000000
H	-0.95212200	1.22770200	0.00000000
H	0.95212200	-1.22770200	0.00000000
H	-2.04463700	-4.80482100	0.00000000
H	0.16269600	3.37766800	0.00000000
H	-0.16269600	-3.37766800	0.00000000
H	2.04463700	4.80482100	0.00000000
C	-4.64385000	-4.21313600	0.00000000
H	-5.67756600	-3.88423500	0.00000000
H	-4.47094100	-5.28634500	0.00000000
C	4.64385000	4.21313600	0.00000000
H	5.67756600	3.88423500	0.00000000
H	4.47094100	5.28634500	0.00000000

Table S11. Cartesian coordinate of optimized structure of Me-**16A** (C_S) at the B3LYP/6-31G(d,p) level

C	3.54945632	-1.25980328	0.00000000
C	-3.49262792	0.56650521	0.00000000
C	-2.02468411	2.72662393	0.00000000
C	2.08516395	-3.42576259	0.00000000
C	3.48371796	0.22564731	0.00000000
C	-3.43563581	-0.91923661	0.00000000
C	-0.72090080	3.18955498	0.00000000
C	0.77534946	-3.86207050	0.00000000
C	2.28787910	0.86709350	0.00000000
C	-2.24293045	-1.56705880	0.00000000
C	0.36889428	2.22575258	0.00000000
C	-0.32339875	-2.92212896	0.00000000
C	2.42301637	-2.01887010	0.00000000
C	-2.36213964	1.32025540	0.00000000
C	1.73604599	2.21626489	0.00000000
C	-1.69143254	-2.91521374	0.00000000
H	2.36038432	3.10621348	0.00000000
H	-2.31191593	-3.80805185	0.00000000
H	-0.00000000	1.21442744	0.00000000
H	0.03916818	-1.90712335	0.00000000
H	1.45004744	0.18264149	0.00000000
H	-1.40399531	-0.88415093	0.00000000
H	0.57881184	-4.93132695	0.00000000
H	-2.82634204	3.46362091	0.00000000
H	2.88029173	-4.16840128	0.00000000
H	-4.48149219	1.02125901	0.00000000
H	4.54093990	-1.70890488	0.00000000
H	-4.38358753	-1.45207813	0.00000000
H	4.42845301	0.76411328	0.00000000
H	1.53608663	-1.41503773	0.00000000
H	-1.47885792	0.71119685	0.00000000
C	-0.41101705	4.66299672	0.00000000
H	0.18248005	4.94023324	0.88019654
H	0.18248005	4.94023324	-0.88019654
H	-1.32149052	5.26783659	0.00000000

Table S12. Cartesian coordinate of optimized structure of type (i) reference compound for Me-**16A** (C_S) at the B3LYP/6-31G(d,p) level

C	-3.56068578	-1.30356159	0.00000000
C	3.47556764	0.61585376	0.00000000
C	-2.06962950	-3.45127424	0.00000000
C	-3.48800944	0.16485848	0.00000000
C	3.41548129	-0.86687092	0.00000000
C	0.59486838	3.30033269	0.00000000
C	-0.74065867	-3.86126466	0.00000000
C	-2.29035546	0.81922342	0.00000000
C	2.22326159	-1.51868708	0.00000000
C	-0.42315842	2.25698825	0.00000000
C	0.32874065	-2.90770424	0.00000000
C	-2.42597761	-2.06378090	0.00000000
C	2.36557438	1.38510645	0.00000000
C	-1.79149361	2.17390653	0.00000000
C	1.70168882	-2.86809587	0.00000000
H	-2.45473157	3.03618078	0.00000000
H	2.34125261	-3.74763893	0.00000000
H	0.00000000	1.26741228	0.00000000
H	-0.04962903	-1.89835162	0.00000000
H	-1.43769535	0.15255515	0.00000000
H	1.38023084	-0.83852885	0.00000000
H	-0.52480698	-4.92703447	0.00000000
H	-2.84690123	-4.21248694	0.00000000
H	4.47067609	1.05890241	0.00000000
H	-4.55157853	-1.75343233	0.00000000
H	4.36274129	-1.40144682	0.00000000
H	-4.42915802	0.71021640	0.00000000
H	-1.54817176	-1.44771720	0.00000000
H	1.46452808	0.80221992	0.00000000
C	2.09935239	2.87137132	0.00000000
H	2.57384849	3.34110765	0.87249249
H	2.57384849	3.34110765	-0.87249249

C	0.30414596	4.61554740	0.00000000
H	-0.72068035	4.97318873	0.00000000
H	1.08395124	5.37205334	0.00000000

Table S13. Cartesian coordinate of optimized structure of **16A** (D_{2d}) at the B3LYP/6-31G(d,p) level

C	1.98006074	3.05596351	0.00000000
C	-1.98006074	-3.05596351	-0.00000000
C	-3.56715207	-0.97960367	-0.00000000
C	3.56715207	0.97960367	0.00000000
C	0.55239316	3.47116948	0.00000000
C	-0.55239316	-3.47116948	-0.00000000
C	-3.56715207	0.40069511	-0.00000000
C	3.56715207	-0.40069511	0.00000000
C	-0.43686119	2.54188655	0.00000000
C	0.43686119	-2.54188655	-0.00000000
C	-2.32735322	1.14572573	0.00000000
C	2.32735322	-1.14572573	0.00000000
C	2.33970341	1.74602520	0.00000000
C	-2.33970341	-1.74602520	-0.00000000
C	-1.89026206	2.44199456	0.00000000
C	1.89026206	-2.44199456	-0.00000000
H	-2.54257386	3.31172936	0.00000000
H	2.54257386	-3.31172936	-0.00000000
H	-1.47893588	0.48061636	0.00000000
H	1.47893588	-0.48061636	0.00000000
H	-0.05143832	1.53134318	0.00000000
H	0.05143832	-1.53134318	-0.00000000
H	-4.51908475	0.92565887	0.00000000
H	4.51908475	-0.92565887	0.00000000
H	-4.52325571	-1.49893636	0.00000000
H	4.52325571	1.49893636	0.00000000
H	-2.72360178	-3.85090288	-0.00000000
H	2.72360178	3.85090288	0.00000000
H	-0.34542120	-4.53856935	-0.00000000
H	0.34542120	4.53856935	0.00000000
H	1.48585144	1.09599785	0.00000000
H	-1.48585144	-1.09599785	-0.00000000

Table S14. Cartesian coordinate of optimized structure of type (ii) reference compound for **16A** (C_S) at the B3LYP/6-31G(d,p) level

C	1.06490300	-0.51781700	0.00000000
C	-1.70909800	6.39920900	0.00000000
C	1.96993300	-2.81189500	0.00000000
C	0.00000000	0.43886100	0.00000000
C	-1.79712500	5.04080400	0.00000000
C	1.87899400	-4.17444500	0.00000000
C	0.17828400	1.79058400	0.00000000
C	-0.53363700	-7.12698600	0.00000000
C	-0.71153800	4.09826700	0.00000000
C	0.67730900	-4.96398500	0.00000000
C	0.88827000	-1.86978800	0.00000000
C	-0.49848200	7.19423300	0.00000000
C	-0.88743100	2.74755300	0.00000000
C	0.66730000	-6.32163700	0.00000000
H	-1.90497100	2.35525100	0.00000000
H	1.61815800	-6.85520700	0.00000000
H	0.30722200	4.48107800	0.00000000
H	-0.28019900	-4.44564700	0.00000000
H	1.19618400	2.18140800	0.00000000
H	-1.47988300	-6.58585500	0.00000000
H	-2.79601600	4.60637200	0.00000000
H	2.81205500	-4.73577800	0.00000000
H	-2.64035600	6.96339500	0.00000000
H	2.97013700	-2.38092700	0.00000000
H	2.08271200	-0.12632200	0.00000000
H	-1.01805200	0.04829800	0.00000000
H	-0.13127400	-2.25098300	0.00000000
H	0.45416400	6.66838400	0.00000000

C	-0.48847200	8.53836700	0.00000000
H	0.43812800	9.10240600	0.00000000
H	-1.41164900	9.11233700	0.00000000
C	-0.55021300	-8.47106800	0.00000000
H	-1.47996100	-9.02970900	0.00000000
H	0.36961800	-9.05004300	0.00000000

Table S15. Cartesian coordinate of optimized structure of Me-**20A** (C_S) at the B3LYP/6-31G(d,p) level

C	2.26784800	-4.15374400	0.00000000
C	0.98462600	-4.65572700	0.00000000
C	-2.18236400	3.49217000	0.00000000
C	-0.91084800	4.03131600	0.00000000
C	4.27511800	0.53890800	0.00000000
C	-3.67176700	-2.56439800	0.00000000
C	-4.20092600	-1.19326400	0.00000000
C	3.73817200	1.90745500	0.00000000
C	-0.17617800	-3.80596700	0.00000000
C	2.54362500	-2.74157700	0.00000000
C	0.24633100	3.15998000	0.00000000
C	-2.45088200	2.07921400	0.00000000
C	2.40447300	2.16728500	0.00000000
C	-3.39021200	-0.10181800	0.00000000
C	-2.33824100	-2.82834300	0.00000000
C	3.47065000	-0.55654600	0.00000000
C	-1.52569100	-4.02235500	0.00000000
C	3.68206300	-1.98562100	0.00000000
C	1.59621900	3.36622500	0.00000000
C	-3.59283900	1.32803900	0.00000000
H	-3.02762800	4.17829600	0.00000000
H	3.10129300	-4.85271500	0.00000000
H	0.84715300	-5.73479400	0.00000000
H	0.00000000	2.10688800	0.00000000
H	-1.56261600	1.45994200	0.00000000
H	0.06105900	-2.74937200	0.00000000
H	1.65268200	-2.12605100	0.00000000
H	1.76540700	1.28941800	0.00000000
H	-2.32721500	-0.32317400	0.00000000
H	-1.70044900	-1.94984700	0.00000000
H	2.40650500	-0.34073000	0.00000000
H	2.05030500	4.35476100	0.00000000
H	-4.58987400	1.76406300	0.00000000
H	-1.96839500	-5.01645800	0.00000000
H	4.68160400	-2.41582500	0.00000000
H	4.45992000	2.72176900	0.00000000
H	-5.28299600	-1.07986400	0.00000000
H	-4.39729300	-3.37529300	0.00000000
H	5.35784900	0.43181900	0.00000000
C	-0.70389700	5.52386000	0.00000000
H	-0.13206700	5.84215300	0.88037200
H	-0.13206700	5.84215300	-0.88037200
H	-1.65484500	6.06230600	0.00000000

Table S16. Cartesian coordinate of optimized structure of type (i) reference compound for Me-**20A** (C_S) at the B3LYP/6-31G(d,p) level

C	-4.71255185	-0.62750528	0.00000000
C	-4.35269697	-1.96572797	0.00000000
C	3.86162882	1.79074219	0.00000000
C	-2.10637245	3.75233658	0.00000000
C	0.10281758	-4.43988232	0.00000000
C	1.51011125	-4.03844477	0.00000000
C	-0.69407644	4.11563725	0.00000000
C	-2.98817087	-2.38969987	0.00000000
C	-3.74455436	0.42303623	0.00000000
C	2.44197457	2.12300113	0.00000000
C	3.18145095	-0.72648346	0.00000000
C	0.31238589	3.19488912	0.00000000
C	1.90681104	-2.73814385	0.00000000

C	-0.91217068	-3.53099266	0.00000000
C	-2.52377867	2.45313698	0.00000000
C	-2.34708416	-3.60251461	0.00000000
C	-3.79890731	1.79452848	0.00000000
C	1.74623413	3.29920661	0.00000000
C	3.19687471	-2.08124236	0.00000000
H	-5.77037103	-0.37395403	0.00000000
H	-5.14114172	-2.71520263	0.00000000
H	1.77991062	1.26908491	0.00000000
H	2.17635119	-0.32658386	0.00000000
H	-2.28022331	-1.57040996	0.00000000
H	-2.72105540	0.06987686	0.00000000
H	0.00000000	2.15432920	0.00000000
H	1.10768280	-2.00200622	0.00000000
H	-0.59016555	-2.49401132	0.00000000
H	-1.72231316	1.72043178	0.00000000
H	2.23032381	4.27412052	0.00000000
H	4.11797325	-2.66254708	0.00000000
H	-2.87489420	-4.55416026	0.00000000
H	-4.73316003	2.35245660	0.00000000
H	-0.45633093	5.17770010	0.00000000
H	2.25130682	-4.83531416	0.00000000
H	-0.10982989	-5.50697501	0.00000000
H	-2.82975685	4.56499285	0.00000000
C	4.83416726	2.72338198	0.00000000
H	5.88502591	2.44913800	0.00000000
C	4.28599100	0.29621810	0.00000000
H	4.93492724	0.13534449	0.87195124
H	4.93492724	0.13534449	-0.87195124
H	4.61031257	3.78547961	0.00000000

Table S17. Cartesian coordinate of optimized structure of **20A** (D_{2h}) at the B3LYP/6-31G(d,p) level

C	0.68875050	4.36960602	0.00000000
C	-0.68875050	4.36960602	-0.00000000
C	-0.68875050	-4.36960602	-0.00000000
C	0.68875050	-4.36960602	0.00000000
C	4.27272820	0.73505529	0.00000000
C	-4.27272820	0.73505529	-0.00000000
C	-4.27272820	-0.73505529	-0.00000000
C	4.27272820	-0.73505529	0.00000000
C	-1.46136648	3.15538094	0.00000000
C	1.46136648	3.15538094	0.00000000
C	1.46136648	-3.15538094	0.00000000
C	-1.46136648	-3.15538094	0.00000000
C	3.12390511	-1.46160415	-0.00000000
C	-3.12390511	-1.46160415	-0.00000000
C	-3.12390511	1.46160415	-0.00000000
C	3.12390511	1.46160415	-0.00000000
C	-2.79750918	2.86894558	0.00000000
C	2.79750918	2.86894558	0.00000000
C	2.79750918	-2.86894558	0.00000000
C	-2.79750918	-2.86894558	0.00000000
H	-1.20990237	-5.32438992	0.00000000
H	1.20990237	-5.32438992	0.00000000
H	1.20990237	5.32438992	0.00000000
H	-1.20990237	5.32438992	-0.00000000
H	0.85700960	-2.25677741	0.00000000
H	-0.85700960	-2.25677741	-0.00000000
H	-0.85700960	2.25677741	-0.00000000
H	0.85700960	2.25677741	-0.00000000
H	2.21177646	-0.87291239	0.00000000
H	-2.21177646	-0.87291239	-0.00000000
H	-2.21177646	0.87291239	-0.00000000
H	2.21177646	0.87291239	-0.00000000
H	3.56975833	-3.63559034	-0.00000000
H	-3.56975833	-3.63559034	-0.00000000
H	-3.56975833	3.63559034	-0.00000000
H	3.56975833	3.63559034	-0.00000000
H	5.24160189	-1.23009261	0.00000000
H	-5.24160189	-1.23009261	-0.00000000
H	-5.24160189	1.23009261	-0.00000000

H	5.24160189	1.23009261	−0.00000000

Table S18. Cartesian coordinate of optimized structure of type (ii) reference compound for **20A**(C_S) at the B3LYP/6-31G(d,p) level

C	2.22728500	5.12330200	0.00000000
C	3.30100600	5.96791700	0.00000000
C	−3.30100600	−5.96791700	0.00000000
C	−2.22728500	−5.12330200	0.00000000
C	0.00051500	0.71464900	0.00000000
C	−0.00051500	−0.71464900	0.00000000
C	4.69159600	5.60391400	0.00000000
C	2.25051100	3.68994200	0.00000000
C	−2.25051100	−3.68994200	0.00000000
C	−4.69159600	−5.60391400	0.00000000
C	−1.12661100	−1.48639200	0.00000000
C	−7.10917000	−6.15244800	0.00000000
C	7.10917000	6.15244800	0.00000000
C	1.12661100	1.48639200	0.00000000
C	5.70711000	6.50544800	0.00000000
C	1.12661100	2.91631500	0.00000000
C	−1.12661100	−2.91631500	0.00000000
C	−5.70711000	−6.50544800	0.00000000
H	−3.09341200	−7.03681700	0.00000000
H	−1.23800500	−5.57876600	0.00000000
H	1.23800500	5.57876600	0.00000000
H	3.09341200	7.03681700	0.00000000
H	−3.21586200	−3.18697100	0.00000000
H	−4.94792000	−4.54577100	0.00000000
H	4.94792000	4.54577100	0.00000000
H	3.21586200	3.18697100	0.00000000
H	−2.09718200	−0.98951500	0.00000000
H	−7.34085300	−5.08730100	0.00000000
H	7.34085300	5.08730100	0.00000000
H	2.09718200	0.98951500	0.00000000
H	−0.15518900	−3.41188200	0.00000000
H	−5.46690600	−7.56898600	0.00000000
H	5.46690600	7.56898600	0.00000000
H	0.15518900	3.41188200	0.00000000
H	0.97002000	−1.21162500	0.00000000
H	−0.97002000	1.21162500	0.00000000
C	8.11860100	7.04024100	0.00000000
H	9.15613400	6.72394700	0.00000000
H	7.93241200	8.11102500	0.00000000
C	−8.11860100	−7.04024100	0.00000000
H	−9.15613400	−6.72394700	0.00000000
H	−7.93241200	−8.11102500	0.00000000

Table S19. Cartesian coordinate of optimized structure of Me-**24A** (C_S) at the B3LYP/6-31G(d,p) level

C	−4.09545300	0.12346400	0.00000000
C	−4.69314500	1.42733200	0.00000000
C	−4.03491000	2.63460800	0.00000000
C	−2.59212000	2.71193300	0.00000000
C	−1.80645100	3.82653800	0.00000000
C	−0.37478200	3.71698900	0.00000000
C	0.52871300	4.73579100	0.00000000
C	1.97011500	4.58271400	0.00000000
C	2.64282300	3.39808200	0.00000000
C	4.06893200	3.24020000	0.00000000
C	4.73421000	2.04174000	0.00000000
C	4.10578700	0.75296100	0.00000000
C	4.71581900	−0.46758100	0.00000000
C	3.93766700	−1.67141300	0.00000000
C	4.38582800	−2.95786800	0.00000000
C	3.53880400	−4.13426400	0.00000000
C	2.17632000	−4.12264400	0.00000000
C	1.31474200	−5.26913100	0.00000000
C	−0.05567100	−5.22443200	0.00000000
C	−0.83929000	−4.02326900	0.00000000

C	-2.19979500	-3.92120100	0.00000000
C	-2.83970800	-2.63807600	0.00000000
C	-4.17674900	-2.37768500	0.00000000
C	-4.77507400	-1.05804100	0.00000000
H	-5.78242800	1.45256000	0.00000000
H	-3.01118900	0.07650500	0.00000000
H	-5.86371900	-1.02321300	0.00000000
H	-4.86609000	-3.22054800	0.00000000
H	-2.15187500	-1.79342200	0.00000000
H	-2.81926900	-4.81770800	0.00000000
H	-0.29573200	-3.08123100	0.00000000
H	-0.59840200	-6.16792900	0.00000000
H	1.79457600	-6.24640400	0.00000000
H	1.68625100	-3.15413900	0.00000000
H	4.04731800	-5.09740800	0.00000000
H	5.46043600	-3.13261400	0.00000000
H	2.86138700	-1.50507100	0.00000000
H	5.80293600	-0.54093500	0.00000000
H	3.01818400	0.73689000	0.00000000
H	2.05370200	2.48616400	0.00000000
H	-2.05733400	1.76609500	0.00000000
H	0.00000000	2.69427100	0.00000000
H	-2.24638800	4.82189900	0.00000000
H	0.15222800	5.75752900	0.00000000
H	2.55210600	5.50345400	0.00000000
H	5.82249200	2.06089400	0.00000000
H	4.66235900	4.15304600	0.00000000
C	-4.82579400	3.92032800	0.00000000
H	-4.59271400	4.53141200	0.88071300
H	-4.59271400	4.53141200	-0.88071300
H	-5.90103200	3.72604400	0.00000000

Table S20. Cartesian coordinate of optimized structure of type (i) reference compound for Me-**24A**(C_S) at the B3LYP/6-31G(d,p) level

C	4.18037066	0.23430330	0.00000000
C	4.08672284	2.86753933	0.00000000
C	2.62583292	2.82623461	0.00000000
C	1.75265054	3.87113893	0.00000000
C	0.33320778	3.68068217	0.00000000
C	-0.60204613	4.67507777	0.00000000
C	-2.03428672	4.50286936	0.00000000
C	-2.69702915	3.30853450	0.00000000
C	-4.11634842	3.14551188	0.00000000
C	-4.78227181	1.94190069	0.00000000
C	-4.15473499	0.66126486	0.00000000
C	-4.75985297	-0.56681312	0.00000000
C	-3.97210781	-1.75587637	0.00000000
C	-4.39827583	-3.05433351	0.00000000
C	-3.52891271	-4.20589821	0.00000000
C	-2.16327058	-4.15590212	0.00000000
C	-1.26624774	-5.26649360	0.00000000
C	0.10485195	-5.16865888	0.00000000
C	0.84668186	-3.94538622	0.00000000
C	2.20503601	-3.81108910	0.00000000
C	2.83220555	-2.52202203	0.00000000
C	4.16859758	-2.27415210	0.00000000
C	4.80260104	-0.96255277	0.00000000
H	3.09584342	0.23994446	0.00000000
H	5.89292377	-0.97420539	0.00000000
H	4.84501490	-3.12778365	0.00000000
H	2.14525326	-1.67594397	0.00000000
H	2.84032516	-4.69676969	0.00000000
H	0.27808458	-3.01810721	0.00000000
H	0.68105443	-6.09230654	0.00000000
H	-1.70732271	-6.26187922	0.00000000
H	-1.70407098	-3.17258774	0.00000000
H	-4.01084615	-5.18247477	0.00000000
H	-5.46948455	-3.24882135	0.00000000
H	-2.89850962	-1.57485154	0.00000000
H	-5.84650577	-0.64636718	0.00000000

H	-3.06698449	0.64740257	0.00000000
H	-2.09825463	2.40243782	0.00000000
H	2.16724137	1.84296483	0.00000000
H	0.00000000	2.64364395	0.00000000
H	2.11570095	4.89765388	0.00000000
H	-0.24419628	5.70375185	0.00000000
H	-2.62841041	5.41575110	0.00000000
H	-5.87061080	1.96214828	0.00000000
H	-4.71304952	4.05621341	0.00000000
C	4.90048925	1.56113591	0.00000000
H	5.56968543	1.59468435	0.87057273
H	5.56968543	1.59468435	-0.87057273
C	4.78357833	4.02192254	0.00000000
H	5.86950858	4.02277480	0.00000000
H	4.30327587	4.99441564	0.00000000

Table S21. Cartesian coordinate of optimized structure of **24A**(D_{4h}) at the B3LYP/6-31G(d,p) level

C	4.31792936	0.57978500	0.00000000
C	4.80001421	1.93085747	0.00000000
C	4.01127352	3.05198210	0.00000000
C	2.57722147	3.04784118	0.00000000
C	1.74414369	4.12834873	0.00000000
C	0.32099538	3.95336484	0.00000000
C	-0.63920646	4.91944900	0.00000000
C	-2.06825894	4.67605742	0.00000000
C	-2.66091508	3.44927256	0.00000000
C	-4.07189750	3.19101713	0.00000000
C	-4.64844531	1.94739230	0.00000000
C	-3.92783678	0.70751236	0.00000000
C	-4.44761601	-0.55398100	0.00000000
C	-3.58496716	-1.69922585	0.00000000
C	-3.94145537	-3.01379947	0.00000000
C	-3.01575622	-4.12932563	0.00000000
C	-1.65701423	-4.02872965	0.00000000
C	-0.72782307	-5.12156053	0.00000000
C	0.63740660	-4.99911331	0.00000000
C	1.35103434	-3.75516435	0.00000000
C	2.70332312	-3.57437261	0.00000000
C	3.26351956	-2.25450500	0.00000000
C	4.58030506	-1.90622340	0.00000000
C	5.08392767	-0.54693976	0.00000000
H	5.88025765	2.06673345	0.00000000
H	3.23993350	0.45197276	0.00000000
H	6.16713019	-0.43331732	0.00000000
H	5.32605000	-2.69943897	0.00000000
H	2.52290746	-1.45587504	0.00000000
H	3.37458168	-4.43259389	0.00000000
H	0.75389161	-2.84605609	0.00000000
H	1.23269598	-5.91033825	0.00000000
H	-1.15021912	-6.12506510	0.00000000
H	-1.22938583	-3.03100819	0.00000000
H	-3.45839496	-5.12445302	0.00000000
H	-5.00119671	-3.26338437	0.00000000
H	-2.52309223	-1.45694350	0.00000000
H	-5.52654896	-0.70574511	0.00000000
H	-2.84190603	0.77050317	0.00000000
H	-2.01086715	2.57989573	0.00000000
H	2.08901536	2.07584632	0.00000000
H	0.00000000	2.91252157	0.00000000
H	4.50272011	4.02314424	0.00000000
H	2.15155055	5.13888632	0.00000000
H	-0.32517837	5.96190097	0.00000000
H	-2.70832823	5.55730062	0.00000000
H	-5.73521244	1.88734870	0.00000000
H	-4.72981522	4.05852791	0.00000000

Table S22. Cartesian coordinate of optimized structure of type (ii) reference compound for **24A**(C_S) at the B3LYP/6-31G(d,p) level

C	-11.64382400	-0.12751600	0.00000000
C	-10.82434400	-1.32147900	0.00000000
C	-9.46411800	-1.38160800	0.00000000
C	-8.54437900	-0.27731500	0.00000000
C	-7.18968700	-0.42497600	0.00000000
C	-6.25639800	0.66025600	0.00000000
C	-4.89996100	0.51175700	0.00000000
C	-3.96879900	1.59665500	0.00000000
C	-2.61108000	1.45150300	0.00000000
C	-1.69680100	2.55216300	0.00000000
C	-0.32821200	2.49408500	0.00000000
C	0.48919000	1.32001800	0.00000000
C	1.85471300	1.34924000	0.00000000
C	2.69004000	0.19001500	0.00000000
C	4.05513800	0.22183100	0.00000000
C	4.89041500	-0.93839100	0.00000000
C	6.25467700	-0.91027800	0.00000000
C	7.07175100	-2.08802500	0.00000000
C	8.43659600	-2.14832400	0.00000000
C	9.35459600	-1.04228800	0.00000000
C	10.70518700	-1.18378500	0.00000000
C	11.63910500	-0.08003900	0.00000000
H	-11.36917600	-2.26417500	0.00000000
H	-11.13737300	0.83560100	0.00000000
H	11.20670900	0.92059700	0.00000000
H	11.12929900	-2.18823900	0.00000000
H	8.94666600	-0.03290100	0.00000000
H	8.89091400	-3.13791300	0.00000000
H	6.53363000	-3.03489100	0.00000000
H	6.74550100	0.06142900	0.00000000
H	4.39122600	-1.90796400	0.00000000
H	4.55247500	1.19216800	0.00000000
H	2.19302900	-0.78052400	0.00000000
H	2.35286400	2.31931100	0.00000000
H	0.00000000	0.34737500	0.00000000
H	-2.20680500	0.44075800	0.00000000
H	-8.94796300	0.73340500	0.00000000
H	-6.66889400	1.66956000	0.00000000
H	-9.00945500	-2.37145300	0.00000000
H	-6.77615700	-1.43407800	0.00000000
H	-4.48729900	-0.49753900	0.00000000
H	-4.38293500	2.60544100	0.00000000
H	0.20711600	3.44245400	0.00000000
H	-2.15001500	3.54241200	0.00000000
C	12.97675100	-0.21350500	0.00000000
H	13.63571700	0.64805300	0.00000000
H	13.44918400	-1.19228800	0.00000000
C	-12.98796600	-0.14464500	0.00000000
H	-13.57050600	0.77044000	0.00000000
H	-13.54330200	-1.07914200	0.00000000

Table S23. Cartesian coordinate of optimized structure of Me-**2D12A** (C_S) at the B3LYP/6-31G(d,p) level

C	1.15723066	0.93958697	0.00000000
C	-0.00000000	1.31392245	0.00000000
C	0.23750032	-2.06882861	0.00000000
C	-0.91640352	-1.68310376	0.00000000
C	-1.29714185	1.90544271	0.00000000
C	-2.49365217	1.26093412	0.00000000
C	-2.91555330	-0.13914326	0.00000000
H	-4.00081509	-0.22294824	0.00000000
C	-2.29065140	-1.34391275	0.00000000
H	-2.95415445	-2.20880886	0.00000000
C	1.54839232	-2.60060935	0.00000000
H	1.58541342	-3.69012598	0.00000000
C	2.75334086	-1.97741774	0.00000000
H	3.60008427	-2.66076963	0.00000000
C	3.17919300	-0.57851078	0.00000000
H	4.26359765	-0.48649633	0.00000000
C	2.53744740	0.61659696	0.00000000
H	3.18796363	1.49143546	0.00000000
H	-3.34974611	1.93291799	0.00000000

C	-1.26601002	3.42277397	0.00000000
H	-0.73015996	3.79703813	0.87965284
H	-0.73015996	3.79703813	-0.87965284
H	-2.27417712	3.84433381	0.00000000

Table S24. Cartesian coordinate of optimized structure of type (i) reference compound for Me-**2D12A** (C_S) at the B3LYP/6-31G(d,p) level

C	-1.14450500	0.96123100	0.00000000
C	0.00000000	1.38449500	0.00000000
C	-0.32709400	-2.04084900	0.00000000
C	0.83043100	-1.65636100	0.00000000
C	1.27434600	2.00270400	0.00000000
C	2.89823300	-0.19937900	0.00000000
H	3.97800600	-0.35221800	0.00000000
C	2.20691200	-1.36098800	0.00000000
H	2.83307800	-2.25458000	0.00000000
C	-1.63074600	-2.55678600	0.00000000
H	-1.68483700	-3.64568900	0.00000000
C	-2.83149900	-1.90764800	0.00000000
H	-3.69212200	-2.57357600	0.00000000
C	-3.20743400	-0.51453200	0.00000000
H	-4.28726800	-0.37890600	0.00000000
C	-2.51816500	0.66460900	0.00000000
H	-3.14383200	1.55802700	0.00000000
C	2.62598200	1.27959300	0.00000000
H	3.18164400	1.67532000	0.86348100
H	3.18164400	1.67532000	-0.86348100
C	1.31702400	3.35396500	0.00000000
H	0.40986800	3.94657200	0.00000000
H	2.26290800	3.88940300	0.00000000

Table S25. Cartesian coordinate of optimized structure of **2D12A** (D_{2h}) at the B3LYP/6-31G(d,p) level

C	1.57552052	0.60826477	0.00000000
C	1.57552052	-0.60826477	0.00000000
C	-1.57552052	0.60826477	-0.00000000
C	-1.57552052	-0.60826477	-0.00000000
C	1.68455789	-2.02032531	0.00000000
H	2.71312636	-2.38144485	0.00000000
C	0.73156550	-2.98544469	0.00000000
H	1.13600426	-3.99565531	0.00000000
C	-0.73156550	-2.98544469	-0.00000000
H	-1.13600426	-3.99565531	-0.00000000
C	-1.68455789	-2.02032531	-0.00000000
H	-2.71312636	-2.38144485	-0.00000000
C	-1.68455789	2.02032531	-0.00000000
H	-2.71312636	2.38144485	-0.00000000
C	-0.73156550	2.98544469	-0.00000000
H	-1.13600426	3.99565531	-0.00000000
C	0.73156550	2.98544469	-0.00000000
H	1.13600426	3.99565531	-0.00000000
C	1.68455789	2.02032531	-0.00000000
H	2.71312636	2.38144485	-0.00000000

Table S26. Cartesian coordinate of optimized structure of type (ii) reference compound for **2D12A** (C_S) at the B3LYP/6-31G(d,p) level

C	0.00000000	0.53293000	0.00000000
C	-1.13972600	0.97360000	0.00000000
C	2.57011900	-4.10583700	0.00000000
C	-2.47475700	1.42991000	0.00000000
H	-3.24609400	0.66190300	0.00000000
C	-2.86095900	2.73331300	0.00000000
H	-3.92855900	2.94404200	0.00000000
C	-1.96934700	3.87346500	0.00000000
H	-0.90288700	3.65737400	0.00000000
C	1.22541800	-3.65603900	0.00000000
H	0.46103400	-4.43022700	0.00000000

C	0.83504200	-2.35433100	0.00000000
H	-0.23064800	-2.14077600	0.00000000
C	1.72779900	-1.22616900	0.00000000
H	2.79347800	-1.43839800	0.00000000
C	1.33398400	0.07804200	0.00000000
H	2.10399200	0.84751600	0.00000000
C	3.70786300	-4.52575600	0.00000000
H	4.70935700	-4.88884900	0.00000000
C	-2.39141400	5.14861800	0.00000000
H	-3.44966600	5.39727800	0.00000000
H	-1.69413800	5.97967000	0.00000000

Table S27. Cartesian coordinate of optimized structure of Me-**3D12A** (C_S) at the B3LYP/6-31G(d,p) level

C	-1.40479319	1.97864683	0.00000000
C	-2.29128911	0.94599169	0.00000000
H	-3.35543552	1.17251027	0.00000000
C	-1.90588441	-0.41858604	0.00000000
C	0.00000000	1.72479690	0.00000000
C	1.19227076	1.48217253	0.00000000
C	-1.52835867	-1.57611114	0.00000000
C	-1.01886461	-2.89896211	0.00000000
H	-1.73233336	-3.71990018	0.00000000
C	0.30873727	-3.18715169	0.00000000
H	0.62125573	-4.22852985	0.00000000
C	1.31324618	-2.18617479	0.00000000
C	2.12091537	-1.27538189	0.00000000
C	2.99894466	-0.16226857	0.00000000
H	4.06931150	-0.35473311	0.00000000
C	2.56588498	1.12475947	0.00000000
H	3.30154907	1.92553152	0.00000000
C	-1.85453481	3.41854453	0.00000000
H	-1.46852887	3.94554827	0.88016627
H	-1.46852887	3.94554827	-0.88016627
H	-2.94493612	3.49237049	0.00000000

Table S28. Cartesian coordinate of optimized structure of type (i) reference compound for Me-**3D12A** (C_S) at the B3LYP/6-31G(d,p) level

C	1.37886900	2.10861100	0.00000000
C	1.90188000	-0.38248900	0.00000000
C	0.00000000	1.77846800	0.00000000
C	-1.18349300	1.48119400	0.00000000
C	1.48749900	-1.52481700	0.00000000
C	0.98464400	-2.84393900	0.00000000
H	1.70813800	-3.65658200	0.00000000
C	-0.34329800	-3.15721600	0.00000000
H	-0.63189700	-4.20574900	0.00000000
C	-1.35561800	-2.18381000	0.00000000
C	-2.16617400	-1.27015600	0.00000000
C	-3.01103700	-0.15036200	0.00000000
H	-4.08643200	-0.31329400	0.00000000
C	-2.54633000	1.13545300	0.00000000
H	-3.27085900	1.94710000	0.00000000
C	2.42518000	0.97720700	0.00000000
H	3.07466500	1.11395400	0.87533300
H	3.07466500	1.11395400	-0.87533300
C	1.79342900	3.39014800	0.00000000
H	1.08733300	4.21217100	0.00000000
H	2.85108400	3.63869800	0.00000000

Table S29. Cartesian coordinate of optimized structure of **3D12A** (D_{3h}) at the B3LYP/6-31G(d,p) level

C	2.70420707	0.77731966	0.00000000
H	3.79129649	0.79909811	0.00000000
C	2.02528211	1.95325219	0.00000000
H	2.58768751	2.88381002	0.00000000
C	0.60846727	2.03031309	0.00000000
C	2.06253635	-0.48820843	-0.00000000

C	1.45406908	-1.54210466	0.00000000
C	-0.60846727	2.03031309	-0.00000000
C	-2.02528211	1.95325219	0.00000000
H	-2.58768751	2.88381002	0.00000000
C	-2.70420707	0.77731966	-0.00000000
H	-3.79129649	0.79909811	-0.00000000
C	-2.06253635	-0.48820843	-0.00000000
C	-1.45406908	-1.54210466	0.00000000
C	-0.67892496	-2.73057185	0.00000000
H	-1.20360898	-3.68290813	0.00000000
C	0.67892496	-2.73057185	0.00000000
H	1.20360898	-3.68290813	0.00000000

Table S30. Cartesian coordinate of optimized structure of type (ii) reference compound for **3D12A** (C_S) at the B3LYP/6-31G(d,p) level

C	-2.20907200	-3.52710300	0.00000000
H	-1.20169600	-3.94228300	0.00000000
C	-2.30078100	-2.11348400	0.00000000
C	3.50832500	2.64151200	0.00000000
C	-2.32070900	-0.89402300	0.00000000
C	-2.41204100	0.51080700	0.00000000
H	-3.41372300	0.93639200	0.00000000
C	-1.35657300	1.37329800	0.00000000
H	-1.57175500	2.44001900	0.00000000
C	0.00000000	1.00226600	0.00000000
C	1.19236900	0.74097400	0.00000000
C	2.55018000	0.37031200	0.00000000
H	2.76549400	-0.69655500	0.00000000
C	3.60377400	1.22960500	0.00000000
H	4.60694700	0.80887800	0.00000000
C	-3.26376100	-4.36046400	0.00000000
H	-4.28302700	-3.98884100	0.00000000
H	-3.12241700	-5.43590200	0.00000000
C	3.47431000	3.85313900	0.00000000
H	3.42405200	4.91725600	0.00000000

Table S31. Cartesian coordinate of optimized structure of Me-**4D16A** (C_S) at the B3LYP/6-31G(d,p) level

C	-2.52790065	1.07158120	0.00000000
C	-2.01280031	-2.11161891	0.00000000
C	-0.79900552	-1.96264438	0.00000000
C	-1.33665251	1.35051456	0.00000000
C	0.53436119	-1.70864967	0.00000000
C	1.71665262	-1.39617688	0.00000000
C	1.21518924	1.72800025	0.00000000
C	0.00000000	1.58639332	0.00000000
C	2.57632725	2.08616877	0.00000000
H	2.73096048	3.16569031	0.00000000
C	3.71410227	1.33358262	0.00000000
C	3.90808441	-0.12067920	0.00000000
H	4.96652506	-0.37546916	0.00000000
C	3.11455499	-1.22529690	0.00000000
H	3.65762002	-2.17163313	0.00000000
C	-3.92710881	0.91989939	0.00000000
H	-4.46595045	1.86831837	0.00000000
C	-4.71693342	-0.18970358	0.00000000
H	-5.77952056	0.04420716	0.00000000
C	-4.48465314	-1.62546553	0.00000000
H	-5.41910783	-2.18301452	0.00000000
C	-3.38427100	-2.42752061	0.00000000
H	-3.58959789	-3.49853008	0.00000000
C	5.03378290	2.08285701	0.00000000
H	5.63314304	1.81890882	0.88016674
H	5.63314304	1.81890882	-0.88016674
H	4.89040798	3.16516460	0.00000000

Table S32. Cartesian coordinate of optimized structure of type (i) reference compound for Me-**4D16A** (C_S) at the B3LYP/6-

31G(d,p) level

C	2.50936853	0.96776959	0.00000000
C	1.95960826	-2.18921606	0.00000000
C	0.75062758	-1.98571770	0.00000000
C	1.32591505	1.28118441	0.00000000
C	-0.56340324	-1.67320769	0.00000000
C	-1.73493955	-1.31218807	0.00000000
C	-1.19740610	1.80205200	0.00000000
C	0.00000000	1.57706523	0.00000000
C	-3.81262717	1.42346541	0.00000000
C	-3.93806799	-0.03220249	0.00000000
H	-4.98981043	-0.31200712	0.00000000
C	-3.12390179	-1.12529680	0.00000000
H	-3.66660300	-2.07239705	0.00000000
C	3.90051906	0.78938386	0.00000000
H	4.45306402	1.73012686	0.00000000
C	4.68084980	-0.33280932	0.00000000
H	5.74533216	-0.10724856	0.00000000
C	4.43372495	-1.75571287	0.00000000
H	5.35821202	-2.32971167	0.00000000
C	3.31352037	-2.54011844	0.00000000
H	3.49760055	-3.61510611	0.00000000
C	-2.55599638	2.31630871	0.00000000
H	-2.64871722	2.97891794	0.87168080
H	-2.64871722	2.97891794	-0.87168080
C	-4.97563323	2.11256418	0.00000000
H	-4.99635287	3.19832974	0.00000000
H	-5.93695698	1.61023429	0.00000000

Table S33. Cartesian coordinate of optimized structure of **4D16A** (D_{2h}) at the B3LYP/6-31G(d,p) level

C	1.61307301	1.89964381	-0.00000000
C	-1.61307301	1.89964381	0.00000000
C	-1.68520512	0.67875927	0.00000000
C	1.68520512	0.67875927	-0.00000000
C	-1.68520512	-0.67875927	0.00000000
C	-1.61307301	-1.89964381	0.00000000
C	1.61307301	-1.89964381	-0.00000000
C	1.68520512	-0.67875927	-0.00000000
C	1.69563430	-3.30517700	-0.00000000
H	2.71908467	-3.68196698	-0.00000000
C	0.72750588	-4.26214128	0.00000000
H	1.12811016	-5.27374309	0.00000000
C	-0.72750588	-4.26214128	0.00000000
H	-1.12811016	-5.27374309	0.00000000
C	-1.69563430	-3.30517700	0.00000000
H	-2.71908467	-3.68196698	0.00000000
C	1.69563430	3.30517700	-0.00000000
H	2.71908467	3.68196698	-0.00000000
C	0.72750588	4.26214128	-0.00000000
H	1.12811016	5.27374309	-0.00000000
C	-0.72750588	4.26214128	-0.00000000
H	-1.12811016	5.27374309	-0.00000000
C	-1.69563430	3.30517700	-0.00000000
H	-2.71908467	3.68196698	0.00000000

Table S34. Cartesian coordinate of optimized structure of type (ii) reference compound for Me-**4D16A** (C_{2h}) at the B3LYP/6-31G(d,p) level

C	0.00931300	1.90263200	0.00000000
C	3.43954500	5.93965000	0.00000000
C	0.00000000	0.67683800	0.00000000
C	-3.43975500	-5.93946600	0.00000000
C	-0.00913500	-1.90281900	0.00000000
C	0.00030900	-0.67702400	0.00000000
C	0.03638100	-3.30821100	0.00000000
H	1.02854900	-3.75672200	0.00000000
C	-1.04766700	-4.13471600	0.00000000
H	-0.87094000	-5.20685900	0.00000000

C	-2.41727600	-3.69586300	0.00000000
H	-2.59491200	-2.62368800	0.00000000
C	-3.49580500	-4.52298200	0.00000000
H	-4.49059800	-4.08251900	0.00000000
C	-0.03628700	3.30802200	0.00000000
H	-1.02849300	3.75644900	0.00000000
C	1.04768200	4.13462600	0.00000000
H	0.87084200	5.20675200	0.00000000
C	2.41733800	3.69592400	0.00000000
H	2.59510200	2.62377000	0.00000000
C	3.49576800	4.52317300	0.00000000
H	4.49061500	4.08283100	0.00000000
C	3.42872900	7.15229000	0.00000000
H	3.41373800	8.21757600	0.00000000
C	-3.42908500	-7.15210700	0.00000000
H	-3.41423400	-8.21739500	0.00000000

Table S35. Cartesian coordinate of optimized structure of Me-**3D16A**(R=H) (C_S) at the B3LYP/6-31G(d,p) level

C	-2.52538976	-1.04145238	0.00000000
C	-2.44440102	0.17825515	0.00000000
C	-2.13943029	1.50501204	0.00000000
C	-1.69007937	2.64228370	0.00000000
C	-2.44359269	-2.46178178	0.00000000
C	-0.97240242	3.86140591	0.00000000
H	-1.52921701	4.79471976	0.00000000
C	-1.21374605	-3.05611964	0.00000000
H	-1.17685474	-4.14439340	0.00000000
C	0.39092709	3.88437654	0.00000000
H	0.88714936	4.85295052	0.00000000
C	0.04341647	-2.34873240	0.00000000
H	0.00000000	-1.26280404	0.00000000
C	1.22105870	2.70482164	0.00000000
H	0.71119933	1.74512650	0.00000000
C	1.25985430	-2.95173714	0.00000000
H	1.30703976	-4.03938740	0.00000000
C	2.57814401	2.72261658	0.00000000
H	3.09135635	3.68296205	0.00000000
C	2.54337609	-2.27673067	0.00000000
H	3.42048869	-2.92421238	0.00000000
C	3.44202308	1.55729683	0.00000000
H	4.51362270	1.75592658	0.00000000
C	2.77551966	-0.95659301	0.00000000
C	3.06678276	0.27034424	0.00000000
C	-3.72924413	-3.25182231	0.00000000
H	-4.33655293	-3.01172189	0.88037025
H	-4.33655293	-3.01172189	-0.88037025
H	-3.52857711	-4.32610423	0.00000000

Table S36. Cartesian coordinate of optimized structure of type (i) reference compound for Me-**3D16A**(R=H) (C_S) at the B3LYP/6-31G(d,p) level

C	2.47185087	-1.28513783	0.00000000
C	2.41344877	-0.06155854	0.00000000
C	2.22068701	1.27712654	0.00000000
C	1.89502114	2.46021286	0.00000000
C	2.37277810	-2.69792678	0.00000000
C	1.31726639	3.73707249	0.00000000
H	1.96850884	4.60734438	0.00000000
C	-0.04606861	3.90777148	0.00000000
H	-0.43247750	4.92527992	0.00000000
C	-0.20547720	-2.38514972	0.00000000
H	0.00000000	-1.31852628	0.00000000
C	-0.98383283	2.83283605	0.00000000
H	-0.57840974	1.82443234	0.00000000
C	-1.48673615	-2.81119404	0.00000000
H	-1.67642821	-3.88450919	0.00000000
C	-2.34101076	2.97882617	0.00000000
H	-2.76313211	3.98240558	0.00000000
C	-2.68466299	-1.99632998	0.00000000

H	-3.62402957	-2.55040402	0.00000000
C	-3.28838031	1.89834071	0.00000000
H	-4.34232918	2.17527227	0.00000000
C	-2.79561134	-0.65799374	0.00000000
C	-3.00702217	0.58128820	0.00000000
C	0.97126478	-3.32837206	0.00000000
H	0.90849848	-3.99147882	0.87367502
H	0.90849848	-3.99147882	-0.87367502
C	3.47197973	-3.47745512	0.00000000
H	4.46863597	-3.05184588	0.00000000
H	3.38969797	-4.56063165	0.00000000

Table S37. Cartesian coordinate of optimized structure of **3D16A**(R=H) (C_{2v}) at the B3LYP/6-31G(d,p) level

C	0.00000000	1.88758700	-2.47600500
C	0.00000000	0.68050000	-2.67238800
C	0.00000000	-0.68050000	-2.67238800
C	0.00000000	-1.88758700	-2.47600500
C	0.00000000	3.23470400	-2.04455500
H	0.00000000	4.02180700	-2.79410600
C	0.00000000	-3.23470400	-2.04455500
H	0.00000000	-4.02180700	-2.79410600
C	0.00000000	3.56026900	-0.72095300
H	0.00000000	4.61465200	-0.45186400
C	0.00000000	-3.56026900	-0.72095300
H	0.00000000	-4.61465200	-0.45186400
C	0.00000000	2.59362000	0.35066900
H	0.00000000	1.54466600	0.06611700
C	0.00000000	-2.59362000	0.35066900
H	0.00000000	-1.54466600	0.06611700
C	0.00000000	2.91250600	1.66946200
H	0.00000000	3.96263700	1.95688600
C	0.00000000	-2.91250600	1.66946200
H	0.00000000	-3.96263700	1.95688600
C	0.00000000	1.96849300	2.77169200
H	0.00000000	2.40299200	3.77131100
C	0.00000000	-1.96849300	2.77169200
H	0.00000000	-2.40299200	3.77131100
C	0.00000000	0.63065800	2.69735600
C	0.00000000	-0.63065800	2.69735600

Table S38. Cartesian coordinate of optimized structure of type (ii) reference compound for **3D16A**(R=H) (C_{2v}) at the B3LYP/6-31G(d,p) level

C	0.00000000	7.15637400	0.13246100
C	0.00000000	-7.15637400	0.13246100
C	0.00000000	6.32363700	1.27815700
H	0.00000000	6.82926000	2.24124300
C	0.00000000	-6.32363700	1.27815700
H	0.00000000	-6.82926000	2.24124300
C	0.00000000	4.96219200	1.25442600
H	0.00000000	4.44363800	2.21122000
C	0.00000000	-4.96219200	1.25442600
H	0.00000000	-4.44363800	2.21122000
C	0.00000000	4.14997700	0.07248200
H	0.00000000	4.66566000	-0.88610600
C	0.00000000	-4.14997700	0.07248200
H	0.00000000	-4.66566000	-0.88610600
C	0.00000000	2.78701100	0.09594100
H	0.00000000	2.27147100	1.05478800
C	0.00000000	-2.78701100	0.09594100
H	0.00000000	-2.27147100	1.05478800
C	0.00000000	1.97122900	-1.08188500
H	0.00000000	2.48185000	-2.04542200
C	0.00000000	-1.97122900	-1.08188500
H	0.00000000	-2.48185000	-2.04542200
C	0.00000000	0.62809500	-1.07344900
C	0.00000000	-0.62809500	-1.07344900
C	0.00000000	7.89716700	-0.82827600
H	0.00000000	8.54373700	-1.67487100

C	0.00000000	-7.89716700	-0.82827600
H	0.00000000	-8.54373700	-1.67487100

Table S39. Cartesian coordinate of optimized structure of **3D16A**(R=*t*-Bu) (C_{2v}at the B3LYP/6-31G(d,p) level

C	0.00000000	1.88701220	-2.80100973
C	0.00000000	0.68049905	-2.99590255
C	-0.00000000	-0.68049905	-2.99590255
C	-0.00000000	-1.88701220	-2.80100973
C	0.00000000	3.24900972	-2.38496981
C	-0.00000000	-3.24900972	-2.38496981
C	0.00000000	3.49963051	-1.04216816
H	0.00000000	4.53496310	-0.71246803
C	-0.00000000	-3.49963051	-1.04216816
H	-0.00000000	-4.53496310	-0.71246803
C	0.00000000	2.50484899	0.00681232
H	0.00000000	1.45725582	-0.27952757
C	-0.00000000	-2.50484899	0.00681232
H	-0.00000000	-1.45725582	-0.27952757
C	0.00000000	2.85235069	1.32083861
H	0.00000000	3.91589088	1.53410847
C	-0.00000000	-2.85235069	1.32083861
H	-0.00000000	-3.91589088	1.53410847
C	0.00000000	1.97941163	2.48464761
C	-0.00000000	-1.97941163	2.48464761
C	0.00000000	0.63108345	2.38775929
C	-0.00000000	-0.63108345	2.38775929
C	0.00000000	2.60592208	3.91305213
C	-0.00000000	-2.60592208	3.91305213
C	-0.00000000	-4.32735996	-3.47928529
C	0.00000000	4.32735996	-3.47928529
C	1.26056260	-4.14352570	-4.35673409
H	1.26440166	-4.87272653	-5.17438997
H	1.29495483	-3.14141879	-4.79410067
H	2.17229125	-4.28606089	-3.76753013
C	-1.26056260	-4.14352570	-4.35673409
H	-1.29495483	-3.14141879	-4.79410067
H	-1.26440166	-4.87272653	-5.17438997
H	-2.17229125	-4.28606089	-3.76753013
C	-0.00000000	-5.74948102	-2.89601543
H	0.88780618	-5.93776985	-2.28355331
H	-0.88780618	-5.93776985	-2.28355331
H	-0.00000000	-6.48019812	-3.71107057
C	1.26056260	4.14352570	-4.35673409
H	1.29495483	3.14141879	-4.79410067
H	1.26440166	4.87272653	-5.17438997
H	2.17229125	4.28606089	-3.76753013
C	0.00000000	5.74948102	-2.89601543
H	-0.88780618	5.93776985	-2.28355331
H	0.88780618	5.93776985	-2.28355331
H	0.00000000	6.48019812	-3.71107057
C	-1.26056260	4.14352570	-4.35673409
H	-2.17229125	4.28606089	-3.76753013
H	-1.26440166	4.87272653	-5.17438997
H	-1.29495483	3.14141879	-4.79410067
C	1.26267058	2.14113457	4.67191426
H	1.27354821	2.55636932	5.68602568
H	1.29882791	1.05258345	4.75043865
H	2.17223940	2.47100553	4.15942859
C	0.00000000	4.14773118	3.89976570
H	0.88849616	4.55910553	3.41019178
H	-0.88849616	4.55910553	3.41019178
H	0.00000000	4.51067493	4.93262618
C	-1.26267058	2.14113457	4.67191426
H	-1.29882791	1.05258345	4.75043865
H	-1.27354821	2.55636932	5.68602568
H	-2.17223940	2.47100553	4.15942859
C	1.26267058	-2.14113457	4.67191426
H	1.29882791	-1.05258345	4.75043865
H	1.27354821	-2.55636932	5.68602568
H	2.17223940	-2.47100553	4.15942859
C	-0.00000000	-4.14773118	3.89976570

H	−0.88849616	−4.55910553	3.41019178
H	0.88849616	−4.55910553	3.41019178
H	−0.00000000	−4.51067493	4.93262618
C	−1.26267058	−2.14113457	4.67191426
H	−1.29882791	−1.05258345	4.75043865
H	−2.17223940	−2.47100553	4.15942859
H	−1.27354821	−2.55636932	5.68602568

Table S40. Cartesian coordinate of optimized structure of Me-**3D20A**(R=H) (C_S) at the B3LYP/6-31G(d,p) level

C	4.59196036	0.28724837	0.00000000
C	3.98944491	1.48829391	0.00000000
C	3.45645631	2.62735917	0.00000000
C	2.91059192	3.85529952	0.00000000
C	3.94515916	−1.00290329	0.00000000
C	1.50045082	4.16433835	0.00000000
C	2.60047763	−1.21967784	0.00000000
C	0.48844390	3.25331203	0.00000000
C	−0.91008066	3.57217999	0.00000000
C	1.97327193	−2.50995972	0.00000000
C	−1.87844323	2.61549337	0.00000000
C	0.62126920	−2.66945549	0.00000000
C	−0.07005588	−3.92997339	0.00000000
C	−3.29504203	2.85792239	0.00000000
C	−4.23919891	1.87079598	0.00000000
C	−1.43100610	−4.07092804	0.00000000
C	−2.26031173	−2.91951989	0.00000000
C	−3.90098733	0.50094009	0.00000000
C	−2.90435126	−1.87868332	0.00000000
C	−3.48888265	−0.65202729	0.00000000
H	5.68167643	0.28109058	0.00000000
H	3.59383198	4.70389949	0.00000000
H	4.61120139	−1.86379912	0.00000000
H	1.24887913	5.22344540	0.00000000
H	1.93884515	−0.35421215	0.00000000
H	0.74835803	2.19552930	0.00000000
H	−1.19209929	4.62537815	0.00000000
H	2.61925344	−3.38819610	0.00000000
H	−1.56891730	1.57261609	0.00000000
H	0.00000000	−1.77645790	0.00000000
H	0.53271746	−4.83663519	0.00000000
H	−3.63578835	3.89133632	0.00000000
H	−5.29321577	2.13753782	0.00000000
C	−2.10395703	−5.42337289	0.00000000
H	−2.74579300	−5.54175905	0.88047585
H	−2.74579300	−5.54175905	−0.88047585
H	−1.36441240	−6.22810681	0.00000000

Table S41. Cartesian coordinate of optimized structure of type (i) reference compound for Me-**3D20A**(R=H) (C_S) at the B3LYP/6-31G(d,p) level

C	−1.17662930	−4.36366889	0.00000000
C	−2.25165155	−3.55181287	0.00000000
C	−3.28424131	−2.83993402	0.00000000
C	−4.40076044	−2.08289030	0.00000000
C	0.20827496	−3.97769216	0.00000000
C	−4.44267755	−0.64972182	0.00000000
C	0.70035798	−2.70645006	0.00000000
C	−3.34743837	0.16949007	0.00000000
C	−3.37653376	1.59300581	0.00000000
C	2.10325325	−2.38745215	0.00000000
C	−2.23212292	2.34205390	0.00000000
C	2.59071474	−1.12786187	0.00000000
C	−2.16247656	3.76618546	0.00000000
C	−0.98686133	4.47565818	0.00000000
C	4.42080558	0.70407773	0.00000000
C	3.37571799	1.66230332	0.00000000
C	0.27038290	3.85442407	0.00000000
C	2.41748830	2.42548848	0.00000000
C	1.31747428	3.21463360	0.00000000

H	-1.37510344	-5.43539792	0.00000000
H	-5.35748292	-2.60366320	0.00000000
H	0.92046214	-4.80119311	0.00000000
H	-5.43332269	-0.19862365	0.00000000
H	0.00000000	-1.87213190	0.00000000
H	-2.36396980	-0.29861445	0.00000000
H	-4.34696682	2.08984558	0.00000000
H	2.79635072	-3.23057051	0.00000000
H	-1.28136068	1.81301015	0.00000000
H	1.88971552	-0.29690168	0.00000000
H	-3.09516664	4.32676312	0.00000000
H	-1.01993550	5.56254243	0.00000000
C	4.05850504	-0.78896913	0.00000000
H	4.54157262	-1.24725411	0.87378676
H	4.54157262	-1.24725411	-0.87378676
C	5.71162780	1.09222659	0.00000000
H	5.98913714	2.13979676	0.00000000
H	6.51523950	0.36108304	0.00000000

Table S42. Cartesian coordinate of optimized structure of **3D20A**(R=H) (D_{4h}) at the B3LYP/6-31G(d,p) level

C	0.00000000	1.97193100	4.01769500
C	0.00000000	0.62888400	3.98491400
C	0.00000000	-0.62888400	3.98491400
C	0.00000000	-1.97193100	4.01769500
C	0.00000000	2.85908000	2.87857700
C	0.00000000	-2.85908000	2.87857700
C	0.00000000	2.47457800	1.57248800
C	0.00000000	-2.47457800	1.57248800
C	0.00000000	-3.36753500	0.44925900
C	0.00000000	3.36753500	0.44925900
C	0.00000000	-2.92458600	-0.83768300
C	0.00000000	2.92458600	-0.83768300
C	0.00000000	3.75781900	-2.00940800
C	0.00000000	-3.75781900	-2.00940800
C	0.00000000	-3.27752000	-3.28791900
C	0.00000000	3.27752000	-3.28791900
C	0.00000000	1.89687400	-3.57845400
C	0.00000000	-1.89687400	-3.57845400
C	0.00000000	0.67908900	-3.70744800
C	0.00000000	-0.67908900	-3.70744800
H	0.00000000	2.44422300	4.99959000
H	0.00000000	-2.44422300	4.99959000
H	0.00000000	3.92289600	3.10902200
H	0.00000000	-3.92289600	3.10902200
H	0.00000000	1.40848100	1.34911400
H	0.00000000	-1.40848100	1.34911400
H	0.00000000	-4.43890300	0.65113900
H	0.00000000	4.43890300	0.65113900
H	0.00000000	-1.85064100	-1.01120200
H	0.00000000	1.85064100	-1.01120200
H	0.00000000	4.83666000	-1.86809300
H	0.00000000	-4.83666000	-1.86809300
H	0.00000000	-3.97542300	-4.12169300
H	0.00000000	3.97542300	-4.12169300

Table S43. Cartesian coordinate of optimized structure of type (ii) reference compound for **3D20A**(R=H) (C_S) at the B3LYP/6-31G(d,p) level

C	0.00000000	1.97284900	-1.79250900
C	0.00000000	0.62740700	-1.78363900
C	0.00000000	-0.62740700	-1.78363900
C	0.00000000	-1.97284900	-1.79250900
C	0.00000000	2.78890700	-0.61910800
C	0.00000000	-2.78890700	-0.61910800
C	0.00000000	4.15514100	-0.64312200
C	0.00000000	-4.15514100	-0.64312200
C	0.00000000	-4.97752900	0.52595600
C	0.00000000	4.97752900	0.52595600
C	0.00000000	-6.34066000	0.50831000

C	0.00000000	6.34066000	0.50831000
C	0.00000000	7.14976900	1.69260100
C	0.00000000	-7.14976900	1.69260100
C	0.00000000	-8.51113200	1.72191300
C	0.00000000	8.51113200	1.72191300
C	0.00000000	9.34845400	0.57947100
C	0.00000000	-9.34845400	0.57947100
H	0.00000000	2.48093400	-2.75756200
H	0.00000000	-2.48093400	-2.75756200
H	0.00000000	2.27704800	0.34154800
H	0.00000000	-2.27704800	0.34154800
H	0.00000000	4.66049500	-1.60877800
H	0.00000000	-4.66049500	-1.60877800
H	0.00000000	-4.46747400	1.48978200
H	0.00000000	4.46747400	1.48978200
H	0.00000000	-6.86045300	-0.44811200
H	0.00000000	6.86045300	-0.44811200
H	0.00000000	6.62816000	2.64788300
H	0.00000000	-6.62816000	2.64788300
H	0.00000000	-9.01306400	2.68692600
H	0.00000000	9.01306400	2.68692600
C	0.00000000	10.09336200	-0.37814800
H	0.00000000	10.74339600	-1.22203100
C	0.00000000	-10.09336200	-0.37814800
H	0.00000000	-10.74339600	-1.22203100

Table S44. Cartesian coordinate of optimized structure of **3D20A**(R=*t*-Bu) (C_{2v}at the B3LYP/6-31G(d,p) level

C	0.00000000	1.98205163	3.81372985
C	0.00000000	0.62861517	3.76124879
C	0.00000000	-0.62861517	3.76124879
C	0.00000000	-1.98205163	3.81372985
C	0.00000000	2.78753418	2.61166434
C	-0.00000000	-2.78753418	2.61166434
C	0.00000000	2.34955969	1.31993123
C	-0.00000000	-2.34955969	1.31993123
C	-0.00000000	-3.23470707	0.19121451
C	0.00000000	3.23470707	0.19121451
C	-0.00000000	-2.81729065	-1.10475571
C	0.00000000	2.81729065	-1.10475571
C	0.00000000	3.69866631	-2.24296350
C	-0.00000000	-3.69866631	-2.24296350
C	-0.00000000	-3.29255413	-3.55018167
C	0.00000000	3.29255413	-3.55018167
C	-0.00000000	1.89670042	-3.82042879
C	-0.00000000	-1.89670042	-3.82042879
C	-0.00000000	0.67970768	-3.95052712
C	-0.00000000	-0.67970768	-3.95052712
H	0.00000000	3.86307143	2.75456344
H	-0.00000000	-3.86307143	2.75456344
H	0.00000000	1.27970926	1.11806749
H	-0.00000000	-1.27970926	1.11806749
H	-0.00000000	-4.30518664	0.40102929
H	0.00000000	4.30518664	0.40102929
H	-0.00000000	-1.74875303	-1.30534849
H	0.00000000	1.74875303	-1.30534849
H	0.00000000	4.76389223	-2.03091193
H	-0.00000000	-4.76389223	-2.03091193
C	0.00000000	-2.65667343	5.21560883
C	0.00000000	2.65667343	5.21560883
C	-0.00000000	-4.24093592	-4.76150919
C	0.00000000	4.24093592	-4.76150919
C	1.26159419	-2.21418890	5.99042124
H	1.29432402	-1.12785729	6.10368994
H	1.27221709	-2.66178676	6.99065080
H	2.17246003	-2.52527144	5.46858553
C	0.00000000	-4.19559607	5.14083764
H	-0.88822282	-4.58483759	4.63284754
H	0.88822282	-4.58483759	4.63284754
H	0.00000000	-4.60342460	6.15679520
C	-1.26159419	-2.21418890	5.99042124
H	-1.27221709	-2.66178676	6.99065080

H	-1.29432402	-1.12785729	6.10368994
H	-2.17246003	-2.52527144	5.46858553
C	1.26159419	2.21418890	5.99042124
H	1.27221709	2.66178676	6.99065080
H	1.29432402	1.12785729	6.10368994
H	2.17246003	2.52527144	5.46858553
C	0.00000000	4.19559607	5.14083764
H	0.88822282	4.58483759	4.63284754
H	-0.88822282	4.58483759	4.63284754
H	0.00000000	4.60342460	6.15679520
C	-1.26159419	2.21418890	5.99042124
H	-2.17246003	2.52527144	5.46858553
H	-1.29432402	1.12785729	6.10368994
H	-1.27221709	2.66178676	6.99065080
C	0.00000000	5.72001399	-4.34229923
H	-0.88781446	5.97685218	-3.75515883
H	0.88781446	5.97685218	-3.75515883
H	0.00000000	6.35388113	-5.23477527
C	-1.26070093	3.95994414	-5.61230092
H	-1.26589338	4.59401868	-6.50575680
H	-1.29420448	2.91568183	-5.93593525
H	-2.17231651	4.16596331	-5.04206438
C	1.26070093	3.95994414	-5.61230092
H	1.29420448	2.91568183	-5.93593525
H	1.26589338	4.59401868	-6.50575680
H	2.17231651	4.16596331	-5.04206438
C	1.26070093	-3.95994414	-5.61230092
H	1.26589338	-4.59401868	-6.50575680
H	1.29420448	-2.91568183	-5.93593525
H	2.17231651	-4.16596331	-5.04206438
C	-0.00000000	-5.72001399	-4.34229923
H	0.88781446	-5.97685218	-3.75515883
H	-0.88781446	-5.97685218	-3.75515883
H	-0.00000000	-6.35388113	-5.23477527
C	-1.26070093	-3.95994414	-5.61230092
H	-2.17231651	-4.16596331	-5.04206438
H	-1.29420448	-2.91568183	-5.93593525
H	-1.26589338	-4.59401868	-6.50575680

Table S45. Cartesian coordinate of optimized structure of Me-**3D24A**(R=H) (C_S) at the B3LYP/6-31G(d,p) level

C	4.72721591	-3.37237206	0.00000000
C	5.13005289	-2.08773849	0.00000000
C	5.52382365	-0.89560828	0.00000000
C	5.95661449	0.37930977	0.00000000
C	3.36645740	-3.83942080	0.00000000
C	5.12704986	1.55515152	0.00000000
C	2.25272172	-3.04986709	0.00000000
C	3.76222711	1.56430034	0.00000000
C	2.94620696	2.73798787	0.00000000
C	0.90601654	-3.52951366	0.00000000
C	1.58250507	2.69203873	0.00000000
C	-0.17914001	-2.70208198	0.00000000
C	-1.55131866	-3.11502080	0.00000000
C	0.70046156	3.82092690	0.00000000
C	-0.65571993	3.68861514	0.00000000
C	-2.58506333	-2.22727078	0.00000000
C	-1.59888209	4.76919076	0.00000000
C	-2.95615833	4.60425685	0.00000000
C	-4.73723094	-0.27806953	0.00000000
C	-3.57655043	3.33989134	0.00000000
C	-4.04085923	2.20592042	0.00000000
C	-4.45830867	0.91469248	0.00000000
H	7.03384310	0.54135225	0.00000000
H	3.23667425	-4.92010508	0.00000000
H	5.65387123	2.50772238	0.00000000
H	2.38987094	-1.96906876	0.00000000
H	3.24376345	0.60621749	0.00000000
H	3.44647904	3.70653094	0.00000000
H	0.75125087	-4.60856369	0.00000000
H	1.10676454	1.71112816	0.00000000
H	0.00000000	-1.62656462	0.00000000

H	-1.76061216	-4.18483445	0.00000000
H	1.14471728	4.81642671	0.00000000
H	-1.07369805	2.68384425	0.00000000
H	-2.34904866	-1.16492691	0.00000000
H	-1.20936300	5.78522070	0.00000000
H	-3.59824674	5.48208378	0.00000000
H	5.50373391	-4.13666402	0.00000000
C	-5.00664696	-1.66856263	0.00000000
C	-3.97753951	-2.57236377	0.00000000
H	-4.23510553	-3.63018710	0.00000000
C	-6.45555979	-2.09920476	0.00000000
H	-6.97992740	-1.71089433	0.88045545
H	-6.97992740	-1.71089433	-0.88045545
H	-6.53929134	-3.18894828	0.00000000

Table S46. Cartesian coordinate of optimized structure of type (i) reference compound for Me-**3D24A**(R=H) (C_S) at the B3LYP/6-31G(d,p) level

C	4.88246500	2.98903000	0.00000000
C	5.23449100	1.68613600	0.00000000
C	5.58983900	0.48494900	0.00000000
C	5.96539900	-0.81246200	0.00000000
C	3.54971900	3.51649100	0.00000000
C	5.07767000	-1.93576500	0.00000000
C	2.39054800	2.79032300	0.00000000
C	3.71019000	-1.85949300	0.00000000
C	2.81950000	-2.96742600	0.00000000
C	1.08187600	3.36267000	0.00000000
C	1.45822000	-2.81626700	0.00000000
C	-0.07114400	2.63540500	0.00000000
C	-1.39705000	3.19691700	0.00000000
C	0.49281600	-3.86375800	0.00000000
C	-0.85194600	-3.61587500	0.00000000
C	-2.52603800	2.45729700	0.00000000
C	-1.88048900	-4.60386900	0.00000000
C	-3.22268800	-4.31981900	0.00000000
C	-5.07930000	2.02959400	0.00000000
C	-4.79296200	0.64029400	0.00000000
C	-3.73427400	-3.01369100	0.00000000
C	-4.12512400	-1.85071400	0.00000000
C	-4.49302800	-0.54731100	0.00000000
H	7.03333900	-1.02620600	0.00000000
H	3.47370100	4.60245000	0.00000000
H	5.54556800	-2.91853200	0.00000000
H	2.46030300	1.70314800	0.00000000
H	3.25876400	-0.86816400	0.00000000
H	3.24465000	-3.97117100	0.00000000
H	1.01314000	4.45095000	0.00000000
H	1.06472500	-1.79953200	0.00000000
H	0.00000000	1.54749900	0.00000000
H	-1.46803500	4.28592900	0.00000000
H	0.85013700	-4.89365600	0.00000000
H	-1.17879000	-2.57766300	0.00000000
H	-2.44041100	1.37319300	0.00000000
H	-1.58406500	-5.65089400	0.00000000
H	-3.93729200	-5.13983800	0.00000000
H	5.69205500	3.71838200	0.00000000
C	-3.91745800	3.03445500	0.00000000
H	-4.04413200	3.68820400	0.87371200
H	-4.04413200	3.68820400	-0.87371200
C	-6.35544400	2.46427900	0.00000000
H	-7.19024400	1.77326200	0.00000000
H	-6.58401100	3.52609000	0.00000000

Table S47. Cartesian coordinate of optimized structure of **3D24A**(R=H) (C_{2v}) at the B3LYP/6-31G(d,p) level

C	-0.00000000	1.97381105	5.26580185
C	-0.00000000	0.62780148	5.24892776
C	-0.00000000	-0.62780148	5.24892776
C	-0.00000000	-1.97381105	5.26580185

C	-0.00000000	2.83804253	4.11496229
C	-0.00000000	-2.83804253	4.11496229
C	-0.00000000	2.42825884	2.81315720
C	-0.00000000	-2.42825884	2.81315720
C	-0.00000000	-3.29717717	1.67765125
C	-0.00000000	3.29717717	1.67765125
C	0.00000000	-2.83860857	0.39267157
C	-0.00000000	2.83860857	0.39267157
C	0.00000000	3.64775673	-0.79006320
C	0.00000000	-3.64775673	-0.79006320
C	0.00000000	-3.11261225	-2.04290295
C	0.00000000	3.11261225	-2.04290295
C	0.00000000	-3.85875740	-3.26825740
C	0.00000000	-3.29199156	-4.51247418
C	0.00000000	1.89978517	-4.72326383
C	0.00000000	-1.89978517	-4.72326383
C	0.00000000	-0.67806741	-4.82211962
C	0.00000000	0.67806741	-4.82211962
H	-0.00000000	-2.46008384	6.24075732
H	-0.00000000	3.90626876	4.32383698
H	-0.00000000	-3.90626876	4.32383698
H	-0.00000000	1.35747122	2.61280683
H	-0.00000000	-1.35747122	2.61280683
H	-0.00000000	-4.37202065	1.85927247
H	-0.00000000	4.37202065	1.85927247
H	0.00000000	-1.75954450	0.23715775
H	-0.00000000	1.75954450	0.23715775
H	-0.00000000	4.73087803	-0.66688963
H	0.00000000	-4.73087803	-0.66688963
H	0.00000000	-2.02857575	-2.13898924
H	0.00000000	2.02857575	-2.13898924
H	0.00000000	-4.94488896	-3.20325148
H	0.00000000	-3.93559163	-5.38924540
H	-0.00000000	2.46008384	6.24075732
C	0.00000000	3.29199156	-4.51247418
H	0.00000000	3.93559163	-5.38924540
C	0.00000000	3.85875740	-3.26825740
H	0.00000000	4.94488896	-3.20325148

Table S48. Cartesian coordinate of optimized structure of type (ii) reference compound for **3D24A**(R=H) (C_{2v}) at the B3LYP/6-31G(d,p) level

C	0.00000000	1.97393700	2.45864200
C	0.00000000	0.62695700	2.44990900
C	0.00000000	-0.62695700	2.44990900
C	0.00000000	-1.97393700	2.45864200
C	0.00000000	2.78931100	1.28741100
C	0.00000000	-2.78931100	1.28741100
C	0.00000000	4.15749300	1.31145700
C	0.00000000	-4.15749300	1.31145700
C	0.00000000	-4.97993700	0.14602600
C	0.00000000	4.97993700	0.14602600
C	0.00000000	-6.34603900	0.16410900
C	0.00000000	6.34603900	0.16410900
C	0.00000000	7.16555200	-1.00757300
C	0.00000000	-7.16555200	-1.00757300
C	0.00000000	-8.52858400	-0.99493400
C	0.00000000	8.52858400	-0.99493400
C	0.00000000	9.33335400	-2.18229400
C	0.00000000	-9.33335400	-2.18229400
C	0.00000000	-10.69451700	-2.21749300
C	0.00000000	10.69451700	-2.21749300
C	0.00000000	11.53669300	-1.07853800
C	0.00000000	-11.53669300	-1.07853800
H	0.00000000	2.48115200	3.42420500
H	0.00000000	-2.48115200	3.42420500
H	0.00000000	2.27858000	0.32616400
H	0.00000000	-2.27858000	0.32616400
H	0.00000000	4.66064000	2.27849000
H	0.00000000	-4.66064000	2.27849000
H	0.00000000	-4.47311200	-0.81930900

H	0.00000000	4.47311200	−0.81930900
H	0.00000000	−6.85577700	1.12753700
H	0.00000000	6.85577700	1.12753700
H	0.00000000	6.65251400	−1.96993700
H	0.00000000	−6.65251400	−1.96993700
H	0.00000000	−9.05191800	−0.04043500
H	0.00000000	9.05191800	−0.04043500
H	0.00000000	8.80786700	−3.13550400
H	0.00000000	−8.80786700	−3.13550400
H	0.00000000	−11.19234600	−3.18462200
H	0.00000000	11.19234600	−3.18462200
C	0.00000000	12.28559600	−0.12401800
H	0.00000000	12.93905400	0.71718700
C	0.00000000	−12.28559600	−0.12401800
H	0.00000000	−12.93905400	0.71718700

Table S49. Cartesian coordinate of optimized structure of **3D24**(R=*t*-Bu) (D_{4h}) at the B3LYP/6-31G(d,p) level

C	−0.00000000	1.98406874	5.10592477
C	−0.00000000	0.62731548	5.07423402
C	−0.00000000	−0.62731548	5.07423402
C	−0.00000000	−1.98406874	5.10592477
C	−0.00000000	2.75920939	3.88984216
C	−0.00000000	−2.75920939	3.88984216
C	−0.00000000	2.28233972	2.60826478
C	−0.00000000	−2.28233972	2.60826478
C	−0.00000000	−3.12439797	1.45419574
C	−0.00000000	3.12439797	1.45419574
C	−0.00000000	−2.66674246	0.16802410
C	0.00000000	2.66674246	0.16802410
C	0.00000000	3.49612618	−1.00008063
C	−0.00000000	−3.49612618	−1.00008063
C	0.00000000	−3.00088728	−2.26969704
C	0.00000000	3.00088728	−2.26969704
C	0.00000000	−3.80246230	−3.46174594
C	0.00000000	−3.30739797	−4.73943130
C	0.00000000	1.90008692	−4.92495827
C	0.00000000	−1.90008692	−4.92495827
C	0.00000000	−0.67904631	−5.02227655
C	0.00000000	0.67904631	−5.02227655
H	−0.00000000	3.83837688	4.00332997
H	−0.00000000	−3.83837688	4.00332997
H	−0.00000000	1.20620069	2.44377371
H	−0.00000000	−1.20620069	2.44377371
H	−0.00000000	−4.20179753	1.62355158
H	0.00000000	4.20179753	1.62355158
H	−0.00000000	−1.58915288	0.00280212
H	0.00000000	1.58915288	0.00280212
H	0.00000000	4.57613296	−0.84907159
H	−0.00000000	−4.57613296	−0.84907159
H	0.00000000	−1.92119157	−2.40145419
H	0.00000000	1.92119157	−2.40145419
H	0.00000000	−4.87957636	−3.32337075
C	0.00000000	3.30739797	−4.73943130
C	0.00000000	3.80246230	−3.46174594
H	0.00000000	4.87957636	−3.32337075
C	−0.00000000	−2.68032293	6.49522453
C	−0.00000000	2.68032293	6.49522453
C	0.00000000	4.17687144	−6.01007234
C	0.00000000	−4.17687144	−6.01007234
C	−1.26125503	2.24863832	7.27723140
H	−1.29310294	1.16378694	7.40631165
H	−1.27155289	2.71077983	8.27081423
H	−2.17252890	2.55158662	6.75136119
C	1.26125503	2.24863832	7.27723140
H	1.27155289	2.71077983	8.27081423
H	1.29310294	1.16378694	7.40631165
H	2.17252890	2.55158662	6.75136119
C	−0.00000000	4.21723763	6.39305628
H	0.88811119	4.59638819	5.87725182
H	−0.88811119	4.59638819	5.87725182
H	−0.00000000	4.64476700	7.40086906

C	-1.26125503	-2.24863832	7.27723140
H	-1.27155289	-2.71077983	8.27081423
H	-1.29310294	-1.16378694	7.40631165
H	-2.17252890	-2.55158662	6.75136119
C	1.26125503	-2.24863832	7.27723140
H	1.29310294	-1.16378694	7.40631165
H	1.27155289	-2.71077983	8.27081423
H	2.17252890	-2.55158662	6.75136119
C	-0.00000000	-4.21723763	6.39305628
H	-0.88811119	-4.59638819	5.87725182
H	0.88811119	-4.59638819	5.87725182
H	-0.00000000	-4.64476700	7.40086906
C	-1.26070437	-3.84393904	-6.84196644
H	-1.29525765	-2.78170506	-7.09999470
H	-1.26427714	-4.42143974	-7.77295692
H	-2.17228262	-4.08659731	-6.28628546
C	1.26070437	-3.84393904	-6.84196644
H	1.26427714	-4.42143974	-7.77295692
H	1.29525765	-2.78170506	-7.09999470
H	2.17228262	-4.08659731	-6.28628546
C	0.00000000	-5.68029432	-5.68714674
H	0.88792498	-5.97553660	-5.11854216
H	-0.88792498	-5.97553660	-5.11854216
H	0.00000000	-6.25356230	-6.61967416
C	0.00000000	5.68029432	-5.68714674
H	-0.88792498	5.97553660	-5.11854216
H	0.88792498	5.97553660	-5.11854216
H	0.00000000	6.25356230	-6.61967416
C	-1.26070437	3.84393904	-6.84196644
H	-1.26427714	4.42143974	-7.77295692
H	-1.29525765	2.78170506	-7.09999470
H	-2.17228262	4.08659731	-6.28628546
C	1.26070437	3.84393904	-6.84196644
H	2.17228262	4.08659731	-6.28628546
H	1.29525765	2.78170506	-7.09999470
H	1.26427714	4.42143974	-7.77295692

Table S50. Cartesian coordinate of optimized structure of Me-**1**(R=H) (C_s) at the B3LYP/6-31G(d,p) level

C	-3.64811067	1.53674433	0.00000000
C	-4.09273228	2.87881685	0.00000000
C	-2.95662661	3.69976097	0.00000000
C	-1.81225688	2.86443429	0.00000000
N	-2.27443977	1.59006409	0.00000000
H	-1.77619191	0.68952929	0.00000000
H	-5.12460517	3.20247537	0.00000000
H	-2.95159090	4.78004726	0.00000000
C	-0.36836849	3.14314959	0.00000000
C	-4.31496654	0.27892225	0.00000000
H	-5.40140606	0.29319826	0.00000000
C	0.46531520	2.06916914	0.00000000
H	0.00000000	1.09138247	0.00000000
C	-3.66378705	-0.94995126	0.00000000
C	-4.18620537	-2.30345313	0.00000000
N	-2.27864471	-1.01240543	0.00000000
C	-3.10272862	-3.14540101	0.00000000
H	-5.23261177	-2.58190700	0.00000000
C	-1.92423160	-2.29522345	0.00000000
H	-3.11271278	-4.22729638	0.00000000
C	1.90004258	1.85802759	0.00000000
C	3.08172093	2.70715552	0.00000000
N	2.25720309	0.57449108	0.00000000
C	4.16500591	1.86496918	0.00000000
H	3.09503145	3.78851073	0.00000000
C	3.64263872	0.51231916	0.00000000
H	5.21149778	2.14319132	0.00000000
C	-0.48833423	-2.49937220	0.00000000
H	-0.03112129	-1.51600975	0.00000000
C	0.36461150	-3.55142309	0.00000000
H	0.03345583	-4.58578444	0.00000000
C	1.80149741	-3.29309229	0.00000000
C	2.93886481	-4.13561807	0.00000000
N	2.26615108	-2.02116708	0.00000000

C	4.07892514	-3.31924261	0.00000000
H	2.91694834	-5.21646942	0.00000000
C	3.63942078	-1.97387062	0.00000000
H	1.77016836	-1.11748857	0.00000000
H	5.10960498	-3.64665655	0.00000000
C	4.30132637	-0.71361704	0.00000000
H	5.38777778	-0.72042826	0.00000000
C	0.10963940	4.57561503	0.00000000
H	0.72451020	4.78413790	0.88228366
H	0.72451020	4.78413790	-0.88228366
H	-0.71911553	5.28563659	0.00000000

Table S51. Cartesian coordinate of optimized structure of type (i) reference compound for Me-**1**(R=H) (C_s) at the B3LYP/6-31G(d,p) level

C	-3.65831402	-1.60043724	0.00000000
C	-4.12571031	-2.93683574	0.00000000
C	-3.00920754	-3.77806158	0.00000000
C	-1.85054040	-2.96461727	0.00000000
N	-2.28318363	-1.67886162	0.00000000
H	-1.76638396	-0.78723213	0.00000000
H	-5.16383018	-3.24001403	0.00000000
H	-3.01925360	-4.85853340	0.00000000
C	-0.40354978	-3.25380350	0.00000000
C	-4.30546736	-0.33755381	0.00000000
H	-5.39189881	-0.33665508	0.00000000
C	-3.63768235	0.88405502	0.00000000
C	-4.16070325	2.23856459	0.00000000
N	-2.25682666	0.93893281	0.00000000
C	-3.07799410	3.07864774	0.00000000
H	-5.20747676	2.51584820	0.00000000
C	-1.90017319	2.22755548	0.00000000
H	-3.08579079	4.16060907	0.00000000
C	1.92546609	-1.81064119	0.00000000
C	3.09683780	-2.66340464	0.00000000
N	2.28062909	-0.53948691	0.00000000
C	4.18810473	-1.82413410	0.00000000
H	3.11608088	-3.74425365	0.00000000
C	3.67190519	-0.47293990	0.00000000
H	5.23246180	-2.10942040	0.00000000
C	-0.47676859	2.44944872	0.00000000
H	0.00000000	1.47539352	0.00000000
C	0.35668866	3.52391636	0.00000000
H	-0.00017209	4.54968253	0.00000000
C	1.79076855	3.29778740	0.00000000
C	2.91812267	4.15975160	0.00000000
N	2.27913973	2.03458427	0.00000000
C	4.06875837	3.36289779	0.00000000
H	2.87959908	5.24023143	0.00000000
C	3.65029476	2.00806251	0.00000000
H	1.79996137	1.11897871	0.00000000
H	5.09400047	3.70715236	0.00000000
C	4.32500434	0.75440118	0.00000000
H	5.41128929	0.76786590	0.00000000
C	0.41844419	-1.98041918	0.00000000
H	0.08532619	-1.39157749	0.86481269
H	0.08532619	-1.39157749	-0.86481269
C	0.07117805	-4.50868453	0.00000000
H	1.13317415	-4.71739469	0.00000000
H	-0.59349803	-5.36661742	0.00000000

Table S52. Cartesian coordinate of optimized structure of **1**(R=H) (C_{2h}) at the B3LYP/6-31G(d,p) level

C	3.68546313	1.67401518	0.00000000
C	4.15215731	3.01044789	0.00000000
C	3.02951008	3.84999467	0.00000000
C	1.87458242	3.03122209	0.00000000
N	2.31288717	1.75009420	0.00000000
H	1.79762122	0.85819750	0.00000000
H	5.18932602	3.31664423	0.00000000
H	3.03011018	4.93104302	0.00000000
C	0.44364967	3.32146892	0.00000000

H	0.13639575	4.36324922	0.00000000
C	4.32440090	0.40224571	0.00000000
H	5.41084266	0.39059601	0.00000000
C	-0.43376500	2.28980980	0.00000000
H	0.00081820	1.29592042	0.00000000
C	3.64444880	-0.81243479	0.00000000
C	4.13558477	-2.17727295	0.00000000
N	2.25840037	-0.84471301	0.00000000
C	3.03342878	-2.99527169	0.00000000
H	5.17538477	-2.47934758	0.00000000
C	1.87458242	-2.11941032	0.00000000
H	3.01969507	-4.07711740	0.00000000
C	-1.87458242	2.11941032	0.00000000
C	-3.03342878	2.99527169	0.00000000
N	-2.25840037	0.84471301	0.00000000
C	-4.13558477	2.17727295	0.00000000
H	-3.01969507	4.07711740	0.00000000
C	-3.64444880	0.81243479	0.00000000
H	-5.17538477	2.47934758	0.00000000
C	0.43376500	-2.28980980	0.00000000
H	-0.00081820	-1.29592042	0.00000000
C	-0.44364967	-3.32146892	0.00000000
H	-0.13639575	-4.36324922	0.00000000
C	-1.87458242	-3.03122209	0.00000000
C	-3.02951008	-3.84999467	0.00000000
N	-2.31288717	-1.75009420	0.00000000
C	-4.15215731	-3.01044789	0.00000000
H	-3.03011018	-4.93104302	0.00000000
C	-3.68546313	-1.67401518	0.00000000
H	-1.79762122	-0.85819750	0.00000000
H	-5.18932602	-3.31664423	0.00000000
C	-4.32440090	-0.40224571	0.00000000
H	-5.41084266	-0.39059601	0.00000000

Table S53. Cartesian coordinate of optimized structure of type (ii) reference compound for **1** (C_{2s}) at the B3LYP/6-31G(d,p) level

C	-1.79871400	-3.38076100	0.00000000
C	-0.48240500	-3.89295800	0.00000000
C	0.39466400	-2.81177600	0.00000000
C	-0.37912700	-1.62707400	0.00000000
N	-1.69065800	-2.00849700	0.00000000
H	-2.53992400	-1.43830100	0.00000000
H	-0.22453200	-4.94315200	0.00000000
H	1.47420700	-2.85165800	0.00000000
C	0.00000000	-0.24242400	0.00000000
H	-0.82111600	0.47151900	0.00000000
C	-3.04439000	-4.05195000	0.00000000
H	-3.00536600	-5.13773500	0.00000000
C	1.27699800	0.22040300	0.00000000
H	2.10695200	-0.48187300	0.00000000
C	-4.28459000	-3.44910900	0.00000000
C	-5.57739700	-4.10583500	0.00000000
N	-4.45631300	-2.06453800	0.00000000
C	-6.51047300	-3.11274500	0.00000000
H	-5.74233700	-5.17584800	0.00000000
C	-5.76838800	-1.85771700	0.00000000
H	-7.58687200	-3.21873200	0.00000000
C	1.66016000	1.60792300	0.00000000
C	0.78803900	2.77861000	0.00000000
N	2.94639800	1.95811000	0.00000000
C	1.60982200	3.86401800	0.00000000
H	-0.29367500	2.77290000	0.00000000
C	2.96686000	3.34915900	0.00000000
H	1.33118700	4.91024600	0.00000000
C	-6.30766000	-0.50789400	0.00000000
H	-5.55526000	0.27788000	0.00000000
C	7.69052700	3.21982900	0.00000000
N	5.70373200	2.20156200	0.00000000
C	6.69525800	4.21035600	0.00000000
H	8.76067600	3.36837900	0.00000000

C	5.44802300	3.56093600	0.00000000
H	4.92240000	1.54290500	0.00000000
H	6.83923100	5.28200300	0.00000000
C	4.13237300	4.08671200	0.00000000
H	4.04777800	5.16998400	0.00000000
C	-7.60954200	-0.18481200	0.00000000
H	-7.93232800	0.85083100	0.00000000
H	-8.39220200	-0.93754600	0.00000000
C	7.04013400	1.98498000	0.00000000
H	7.44803200	0.98451600	0.00000000

Table S54. Cartesian coordinate of optimized structure of **1**(R=Mes) (C_{2h}) at the B3LYP/6-31G(d,p) level

C	1.68364214	-3.68614368	0.00000000
C	3.02529035	-4.14043318	0.00000000
C	3.85419817	-3.00998626	0.00000000
C	3.02471822	-1.86314253	0.00000000
N	1.74755425	-2.31269475	0.00000000
H	0.84796484	-1.80728191	0.00000000
H	3.33658973	-5.17535837	0.00000000
H	4.93527926	-3.00057784	0.00000000
C	3.30407157	-0.43044132	0.00000000
H	4.34384874	-0.11649742	0.00000000
C	0.41760624	-4.35886471	0.00000000
C	2.26821347	0.44245492	0.00000000
H	1.27605687	0.00388799	0.00000000
C	-0.79654510	-3.65774917	0.00000000
C	-2.16364520	-4.14329848	0.00000000
N	-0.82519327	-2.27228489	0.00000000
C	-2.97766125	-3.03690101	0.00000000
H	-2.46688208	-5.18187220	0.00000000
C	-2.09921370	-1.88277561	0.00000000
H	-4.05953572	-3.01999394	0.00000000
C	2.09921370	1.88277561	0.00000000
C	2.97766125	3.03690101	0.00000000
N	0.82519327	2.27228489	0.00000000
C	2.16364520	4.14329848	0.00000000
H	4.05953572	3.01999394	0.00000000
C	0.79654510	3.65774917	0.00000000
H	2.46688208	5.18187220	0.00000000
C	-2.26821347	-0.44245492	0.00000000
H	-1.27605687	-0.00388799	0.00000000
C	-3.30407157	0.43044132	0.00000000
H	-4.34384874	0.11649742	0.00000000
C	-3.02471822	1.86314253	0.00000000
C	-3.85419817	3.00998626	0.00000000
N	-1.74755425	2.31269475	0.00000000
C	-3.02529035	4.14043318	0.00000000
H	-4.93527926	3.00057784	0.00000000
C	-1.68364214	3.68614368	0.00000000
H	-0.84796484	1.80728191	0.00000000
H	-3.33658973	5.17535837	0.00000000
C	-0.41760624	4.35886471	0.00000000
C	-0.41741489	5.85711974	0.00000000
C	-0.41744509	6.55955725	1.22319199
C	-0.41744509	6.55955725	-1.22319199
C	-0.41744509	7.95774636	1.19808220
C	-0.41744509	7.95774636	-1.19808220
C	-0.42064981	8.67676637	0.00000000
H	-0.41333723	8.49764966	2.14241389
H	-0.41333723	8.49764966	-2.14241389
C	0.41741489	-5.85711974	0.00000000
C	0.41744509	-6.55955725	-1.22319199
C	0.41744509	-6.55955725	1.22319199
C	0.41744509	-7.95774636	-1.19808220
C	0.41744509	-7.95774636	1.19808220
C	0.42064981	-8.67676637	0.00000000
H	0.41333723	-8.49764966	-2.14241389
H	0.41333723	-8.49764966	2.14241389
C	-0.41016381	5.82825974	2.54642743

H	-1.27778950	5.16703479	2.64330289
H	0.48034380	5.19972430	2.65190580
H	-0.42763411	6.53362597	3.38110232
C	-0.41016381	5.82825974	-2.54642743
H	0.48034380	5.19972430	-2.65190580
H	-1.27778950	5.16703479	-2.64330289
H	-0.42763411	6.53362597	-3.38110232
C	-0.45418730	10.18690208	0.00000000
H	0.03916791	10.59841010	-0.88560007
H	-1.48596166	10.56026584	0.00000000
H	0.03916791	10.59841010	0.88560007
C	0.41016381	-5.82825974	2.54642743
H	1.27778950	-5.16703479	2.64330289
H	-0.48034380	-5.19972430	2.65190580
H	0.42763411	-6.53362597	3.38110232
C	0.41016381	-5.82825974	-2.54642743
H	-0.48034380	-5.19972430	-2.65190580
H	1.27778950	-5.16703479	-2.64330289
H	0.42763411	-6.53362597	-3.38110232
C	0.45418730	-10.18690208	0.00000000
H	-0.03916791	-10.59841010	-0.88560007
H	1.48596166	-10.56026584	0.00000000
H	-0.03916791	-10.59841010	0.88560007

Table S55. Cartesian coordinate of optimized structure of Me-**2** (C_S) at the B3LYP/6-31G(d,p) level

C	0.00000000	0.43894883	0.00000000
C	-1.10370988	-0.31754412	0.00000000
H	-2.16848529	-0.11802919	0.00000000
C	-0.22131503	-1.61568596	0.00000000
H	-0.43650930	-2.67761783	0.00000000
C	0.89002434	-0.87691320	0.00000000
H	1.95390832	-1.08115685	0.00000000
C	0.32968955	1.88317407	0.00000000
H	0.92969474	2.15419007	0.87972946
H	0.92969474	2.15419007	-0.87972946
H	-0.57643706	2.49654600	0.00000000

Table S56. Cartesian coordinate of optimized structure of type (i) reference compound for Me-**2** (C_S) at the B3LYP/6-31G(d,p) level

C	0.00000000	0.55289851	0.00000000
C	-0.21876279	-1.48870014	0.00000000
H	-0.34512991	-2.56573454	0.00000000
C	-1.07940924	-0.44836554	0.00000000
H	-2.16158280	-0.36677398	0.00000000
C	1.02490147	-0.60361455	0.00000000
H	1.65981478	-0.66463806	0.89191337
H	1.65981478	-0.66463806	-0.89191337
C	0.09343906	1.88232891	0.00000000
H	1.05733409	2.38202578	0.00000000
H	-0.79126185	2.51247572	0.00000000

Table S57. Cartesian coordinate of optimized structure of **2** (D_{2h}) at the B3LYP/6-31G(d,p) level

C	0.00000000	0.67640822	0.77300144
H	-0.00004315	1.43872444	1.52607105
C	-0.00000000	-0.67640822	0.77300144
H	0.00004315	-1.43872444	1.52607105
C	-0.00000000	-0.67640822	-0.77300144
H	0.00004315	-1.43872444	-1.52607105
C	0.00000000	0.67640822	-0.77300144
H	-0.00004315	1.43872444	-1.52607105

Table S58. Cartesian coordinate of optimized structure of type (ii) reference compound for **2** at the B3LYP/6-31G(d,p) level

C	0.60177412	1.75079207	0.00000000
H	-0.32541928	2.31841040	0.00000000
H	1.52392194	2.32236909	0.00000000

C	0.60177412	0.41081168	0.00000000
H	1.55117110	-0.12457459	0.00000000
C	-0.60177412	-0.41081168	0.00000000
H	-1.55117110	0.12457459	0.00000000
C	-0.60177412	-1.75079207	0.00000000
H	0.32541928	-2.31841040	0.00000000
H	-1.52392194	-2.32236909	0.00000000

Table S59. Cartesian coordinate of optimized structure of Me-**3** (C_S) at the B3LYP/6-31G(d,p) level

C	-0.52474820	1.67618646	0.00000000
C	-1.06695050	0.44848557	0.00000000
C	0.00000000	-0.64541412	0.00000000
C	1.23674289	-0.10271213	0.00000000
H	-1.10823662	2.59056487	0.00000000
H	-2.12728366	0.20031821	0.00000000
H	2.14124006	-0.70213453	0.00000000
B	1.04766635	1.45246581	0.00000000
H	1.89489391	2.29233716	0.00000000
C	-0.39379039	-2.08588776	0.00000000
H	-1.01112874	-2.32015378	0.87788673
H	-1.01112874	-2.32015378	-0.87788673
H	0.47578927	-2.74705535	0.00000000

Table S60. Cartesian coordinate of optimized structure of type (i) reference compound for Me-**3** (C_S) at the B3LYP/6-31G(d,p) level

C	0.81960020	1.46919205	0.00000000
C	1.15083746	0.14634331	0.00000000
C	-0.00000000	-0.75562988	0.00000000
H	1.57605366	2.24867400	0.00000000
H	2.16639709	-0.24921235	0.00000000
B	-0.71827036	1.57632995	0.00000000
H	-1.38089183	2.56915174	0.00000000
C	-1.26666844	0.08956942	0.00000000
H	-1.89886678	-0.12641771	0.87284015
H	-1.89886678	-0.12641771	-0.87284015
C	0.09046690	-2.09476232	0.00000000
H	1.05385956	-2.59771878	0.00000000
H	-0.79174983	-2.72798440	0.00000000

Table S61. Cartesian coordinate of optimized structure of **3** (C_{2v}) at the B3LYP/6-31G(d,p) level

C	0.00000000	1.25523704	0.35073130
C	0.00000000	0.75936984	-0.89915234
C	-0.00000000	-0.75936984	-0.89915234
C	-0.00000000	-1.25523704	0.35073130
H	0.00000000	2.31584326	0.57587029
H	0.00000000	1.32883456	-1.82632862
H	-0.00000000	-1.32883456	-1.82632862
H	-0.00000000	-2.31584326	0.57587029
B	-0.00000000	0.00000000	1.31492732
H	0.00000000	0.00000000	2.50733250

Table S62. Cartesian coordinate of optimized structure of type (ii) reference compound for **3** (C_s) at the B3LYP/6-31G(d,p) level

C	2.27449165	-0.20909302	0.00000000
H	2.70183423	0.79065181	0.00000000
H	2.97391198	-1.03869137	0.00000000
C	0.94565958	-0.40264500	0.00000000
H	0.54581198	-1.41237126	0.00000000
C	0.00000000	0.69868704	0.00000000
H	0.46582638	1.68713008	0.00000000
C	-1.36084537	0.61324246	0.00000000
H	-1.88315774	1.57052755	0.00000000
B	-2.18331520	-0.68117796	0.00000000

H	-3.37805895	-0.63335765	0.00000000
H	-1.66542709	-1.75914825	0.00000000

Table S63. Cartesian coordinate of optimized structure of Me-**4** (C_S) at the B3LYP/6-31G(d,p) level

C	0.00000000	0.88268950	0.00000000
C	-1.29603154	0.49819207	0.00000000
C	-1.34530050	-1.00937593	0.00000000
C	-0.07386804	-1.48358913	0.00000000
H	-2.18126778	1.12664002	0.00000000
H	0.21876459	-2.52618534	0.00000000
C	0.83185210	-0.32292122	0.00000000
C	2.12956375	0.06150228	0.00000000
H	3.01341431	-0.56717980	0.00000000
C	2.16744350	1.56041674	0.00000000
H	3.08175986	2.14159751	0.00000000
C	0.90389553	2.04794947	0.00000000
H	0.60912571	3.08926299	0.00000000
C	-2.62329364	-1.78530556	0.00000000
H	-3.23648424	-1.54969124	0.87989295
H	-3.23648424	-1.54969124	-0.87989295
H	-2.43439520	-2.86210222	0.00000000

Table S64. Cartesian coordinate of optimized structure of type (i) reference compound for Me-**4** (C_S) at the B3LYP/6-31G(d,p) level

C	0.00000000	-0.85705535	0.00000000
C	-1.32469852	-0.55558311	0.00000000
C	-1.51845827	0.89489499	0.00000000
H	-2.15511743	-1.25503480	0.00000000
C	0.79330201	0.38483157	0.00000000
C	2.10441912	0.04543897	0.00000000
H	2.96801927	0.69955335	0.00000000
C	2.17394408	-1.43017803	0.00000000
H	3.10355956	-1.98944849	0.00000000
C	0.92122223	-1.97589906	0.00000000
H	0.66572597	-3.02667191	0.00000000
C	-2.70401823	1.52352209	0.00000000
H	-2.77758301	2.60659644	0.00000000
C	-0.13548798	1.56621090	0.00000000
H	-0.01418056	2.20993292	0.88021865
H	-0.01418056	2.20993292	-0.88021865
H	-3.63758983	0.96804179	0.00000000

Table S65. Cartesian coordinate of optimized structure of **4** (C_{2h}) at the B3LYP/6-31G(d,p) level

C	-0.03711848	0.72905015	0.00000000
C	-1.34456843	1.08613248	0.00000000
C	-2.16579128	-0.16531305	0.00000000
C	-1.34456843	-1.24362850	0.00000000
H	-1.76339422	2.08679176	0.00000000
H	-3.24880475	-0.17869783	0.00000000
H	-1.64154996	-2.28441970	0.00000000
C	0.03711848	-0.72905015	0.00000000
C	1.34456843	-1.08613248	0.00000000
H	1.76339422	-2.08679176	0.00000000
C	2.16579128	0.16531305	0.00000000
H	3.24880475	0.17869783	0.00000000
C	1.34456843	1.24362850	0.00000000
H	1.64154996	2.28441970	0.00000000

Table S66. Cartesian coordinate of optimized structure of type (ii) reference compound for **4** at the B3LYP/6-31G(d,p) level

C	0.00000000	0.33893926	0.00000000
C	1.11491268	-0.43949033	0.00000000
C	1.14397211	-1.88557761	0.00000000
H	2.08426317	0.05896862	0.00000000
H	0.18942296	-2.40665159	-0.00000000
C	-2.17230929	1.04581083	0.00000000

H	-3.25534376	1.08587220	0.00000000
C	-1.29349113	2.22546210	-0.00000000
H	-1.64039752	3.25193206	-0.00000000
C	-0.00337227	1.80772414	0.00000000
H	0.88986458	2.41960379	-0.00000000
C	-1.41050624	-0.07694967	0.00000000
H	-1.76353714	-1.09933901	0.00000000
C	2.28184462	-2.60062582	0.00000000
H	2.27434062	-3.68537875	0.00000000
H	3.25508421	-2.11676469	-0.00000000

Table S67. Cartesian coordinate of optimized structure of Me-**5** (C_S) at the B3LYP/6-31G(d,p) level

C	-1.04886551	0.01426328	0.00000000
C	-0.73569981	-1.32240389	0.00000000
C	0.64208527	-1.69613935	0.00000000
C	1.68975738	-0.68584118	0.00000000
C	1.37669279	0.65187392	0.00000000
C	0.00000000	1.02417626	0.00000000
H	-1.50976377	-2.08727190	0.00000000
H	2.15083184	1.41675360	0.00000000
C	-2.31302621	0.72655262	0.00000000
H	-3.29288760	0.26266838	0.00000000
C	-2.06281388	2.08132413	0.00000000
C	-0.62572084	2.26413556	0.00000000
H	-0.12688860	3.22820868	0.00000000
C	2.95849563	-1.39284112	0.00000000
H	3.93526758	-0.92420266	0.00000000
C	2.69703441	-2.74280050	0.00000000
H	3.43154542	-3.53810006	0.00000000
C	1.26762357	-2.93740229	0.00000000
H	0.76913615	-3.90064828	0.00000000
C	-3.06983707	3.19281371	0.00000000
H	-2.96052671	3.83782329	0.88066291
H	-2.96052671	3.83782329	-0.88066291
H	-4.09054190	2.80067881	0.00000000

Table S68. Cartesian coordinate of optimized structure of type (i) reference compound for Me-**5** (C_S) at the B3LYP/6-31G(d,p) level

C	1.08163750	0.05183348	0.00000000
C	0.81746588	-1.27929779	0.00000000
C	-0.55364809	-1.71219182	0.00000000
C	-1.64830793	-0.71370010	0.00000000
C	-1.38037180	0.62042294	0.00000000
C	0.00000000	1.03540263	0.00000000
H	1.61563969	-2.01809539	0.00000000
H	-2.17023696	1.36769080	0.00000000
C	1.97265158	2.27167971	0.00000000
C	0.52317659	2.30299377	0.00000000
H	-0.05403254	3.22220967	0.00000000
C	-2.90376927	-1.45454479	0.00000000
H	-3.89135499	-1.01208828	0.00000000
C	-2.59095283	-2.78248123	0.00000000
H	-3.30056749	-3.60203343	0.00000000
C	-1.14018967	-2.95246201	0.00000000
H	-0.62712948	-3.90689145	0.00000000
C	2.39737628	0.80300817	0.00000000
H	3.00917085	0.57008819	0.88018397
H	3.00917085	0.57008819	-0.88018397
C	2.78489313	3.34443103	0.00000000
H	3.86572744	3.24499598	0.00000000
H	2.38384442	4.35347182	0.00000000

Table S69. Cartesian coordinate of optimized structure of **5** (C_{2h}) at the B3LYP/6-31G(d,p) level

C	-1.24823202	0.65525685	0.00000000
C	-1.24823202	-0.72462082	0.00000000
C	0.00091890	-1.39841753	0.00000000

C	1.24823202	-0.65525685	0.00000000
C	1.24823202	0.72462082	0.00000000
C	-0.00091890	1.39841753	0.00000000
H	-2.17807406	-1.29028146	0.00000000
H	2.17807406	1.29028146	0.00000000
C	-2.31714992	1.62787358	0.00000000
H	-3.37550704	1.39526327	0.00000000
C	-1.75560205	2.89125916	0.00000000
H	-2.29444310	3.83001467	0.00000000
C	-0.32974598	2.75810687	0.00000000
H	0.37637114	3.58126007	0.00000000
C	2.31714992	-1.62787358	0.00000000
H	3.37550704	-1.39526327	0.00000000
C	1.75560205	-2.89125916	0.00000000
H	2.29444310	-3.83001467	0.00000000
C	0.32974598	-2.75810687	0.00000000
H	-0.37637114	-3.58126007	0.00000000

Table S70. Cartesian coordinate of optimized structure of type (ii) reference compound for **5** at the B3LYP/6-31G(d,p) level

C	-1.62938558	-0.83338163	-0.00000000
C	-0.55854441	-1.78335894	-0.00000000
C	0.82833708	-1.29528962	-0.00000000
C	1.08731925	0.03796666	0.00000000
C	0.00000000	1.00565749	0.00000000
H	-2.65784011	-1.18573837	-0.00000000
H	2.10770506	0.41547526	0.00000000
C	-0.57053975	3.46730560	0.00000000
H	-1.63965579	3.27129599	0.00000000
C	0.32891906	2.34316482	0.00000000
H	1.38960376	2.59239017	0.00000000
C	1.69575300	-2.46595979	0.00000000
H	2.77787133	-2.44547618	0.00000000
C	0.88872733	-3.56851477	-0.00000000
H	1.22166525	-4.59995185	0.00000000
C	-0.50951860	-3.15703166	-0.00000000
H	-1.35654780	-3.83296272	-0.00000000
C	-1.36533437	0.50256592	-0.00000000
H	-2.18491021	1.21194326	-0.00000000
C	-0.14901798	4.74704398	0.00000000
H	0.90912108	4.99509376	0.00000000
H	-0.84730275	5.57692224	0.00000000

Table S71. Cartesian coordinate of optimized structure of diMe-**6** (C_S) at the B3LYP/6-31G(d,p) level

C	-2.37042717	0.72697051	0.00000000
C	-1.18033200	1.44351326	0.00000000
C	0.00038886	0.67690252	0.00000000
C	-0.00038886	-0.67690252	0.00000000
C	-1.18033200	-1.43990435	0.00000000
C	-2.36974226	-0.72352687	0.00000000
H	-3.33468284	1.22857348	0.00000000
C	1.18033200	1.43990435	0.00000000
C	1.18033200	-1.44351326	0.00000000
H	-3.33477407	-1.22426177	0.00000000
C	2.37042717	-0.72697051	0.00000000
C	2.36974226	0.72352687	0.00000000
H	3.33468284	-1.22857348	0.00000000
H	3.33477407	1.22426177	0.00000000
C	0.68037296	-2.84471885	0.00000000
H	1.30067372	-3.73373235	0.00000000
C	-0.68962654	-2.85781547	0.00000000
C	0.68962654	2.85781547	0.00000000
C	-0.68037296	2.84471885	0.00000000
H	-1.30067372	3.73373235	0.00000000
C	-1.57528732	-4.06295784	0.00000000
H	-2.23078588	-4.07429140	0.88005014
H	-2.23078588	-4.07429140	-0.88005014
H	-0.99294388	-4.98806445	0.00000000
C	1.57528732	4.06295784	0.00000000

H	2.23078588	4.07429140	0.88005014
H	2.23078588	4.07429140	-0.88005014
H	0.99294388	4.98806445	0.00000000

Table S72. Cartesian coordinate of optimized structure of type (i) reference compound for diMe-**6** (C_S) at the B3LYP/6-31G(d,p) level

C	2.38266827	0.71500421	0.00000000
C	1.19175260	1.42893396	0.00000000
C	0.00104227	0.68958943	0.00000000
C	-0.00104227	-0.68958943	0.00000000
C	1.19178866	-1.43624984	0.00000000
C	2.38482379	-0.71915867	0.00000000
H	3.34181754	1.22641149	0.00000000
C	-1.19178866	1.43624984	0.00000000
C	-1.19175260	-1.42893396	0.00000000
H	3.34409324	-1.22983240	0.00000000
C	-2.38266827	-0.71500421	0.00000000
C	-2.38482379	0.71915867	0.00000000
H	-3.34181754	-1.22641149	0.00000000
H	-3.34409324	1.22983240	0.00000000
C	0.77805892	-2.85923661	0.00000000
C	-0.77805892	2.85923661	0.00000000
C	0.77805892	2.89585724	0.00000000
H	1.15426120	3.43328459	0.87919198
H	1.15426120	3.43328459	-0.87919198
C	-0.77805892	-2.89585724	0.00000000
H	-1.15426120	-3.43328459	0.87919198
H	-1.15426120	-3.43328459	-0.87919198
C	1.56621226	-3.94077567	0.00000000
H	1.15724074	-4.94659076	0.00000000
C	-1.56621226	3.94077567	0.00000000
H	-1.15724074	4.94659076	0.00000000
H	2.64840264	-3.85387880	0.00000000
H	-2.64840264	3.85387880	0.00000000

Table S73. Cartesian coordinate of optimized structure of **6** (D_{2h}) at the B3LYP/6-31G(d,p) level

C	-0.00000000	2.37147125	0.72509226
C	-0.00000000	1.18104204	1.44133722
C	-0.00000000	0.00000000	0.67717341
C	0.00000000	0.00000000	-0.67717341
C	0.00000000	1.18104204	-1.44133722
C	0.00000000	2.37147125	-0.72509226
H	-0.00000000	3.33554435	1.22701107
C	-0.00000000	-1.18104204	1.44133722
C	-0.00000000	-1.18104204	-1.44133722
H	0.00000000	3.33554435	-1.22701107
C	-0.00000000	-2.37147125	-0.72509226
C	-0.00000000	-2.37147125	0.72509226
H	-0.00000000	-3.33554435	-1.22701107
H	-0.00000000	-3.33554435	1.22701107
C	0.00000000	-0.68317421	-2.84705436
H	0.00000000	-1.30612299	-3.73349884
C	0.00000000	0.68317421	-2.84705436
H	0.00000000	1.30612299	-3.73349884
C	-0.00000000	-0.68317421	2.84705436
H	-0.00000000	-1.30612299	3.73349884
C	0.00000000	0.68317421	2.84705436
H	0.00000000	1.30612299	3.73349884

Table S74. Cartesian coordinate of optimized structure of type (ii) reference compound for **6** at the B3LYP/6-31G(d,p) level

C	-1.46345776	2.07357176	-0.00000000
C	-0.08672195	1.90775399	0.00000000
C	0.44954201	0.56551056	0.00000000
C	-0.44954201	-0.56551056	0.00000000
C	-2.33735386	0.97537192	-0.00000000

H	-1.88394862	3.07338476	0.00000000
C	0.08672195	-1.90775399	-0.00000000
H	-3.41005031	1.14488733	-0.00000000
C	1.46345776	-2.07357176	0.00000000
C	2.33735386	-0.97537192	0.00000000
H	1.88394862	-3.07338476	-0.00000000
H	3.41005031	-1.14488733	0.00000000
C	-0.80513599	-3.08339486	0.00000000
H	-1.87064421	-2.88216986	0.00000000
C	0.80513599	3.08339486	0.00000000
H	1.87064421	2.88216986	0.00000000
C	1.84669982	0.31045630	0.00000000
H	2.55250710	1.13073449	0.00000000
C	0.44954201	4.37513732	0.00000000
H	-0.58179160	4.71393856	0.00000000
H	1.20590528	5.15283436	0.00000000
C	-1.84669982	-0.31045630	-0.00000000
H	-2.55250710	-1.13073449	-0.00000000
C	-0.44954201	-4.37513732	-0.00000000
H	-1.20590528	-5.15283436	0.00000000
H	0.58179160	-4.71393856	-0.00000000

Table S75. Cartesian coordinate of optimized structure of Me-**7** (C_S) at the B3LYP/6-31G(d,p) level

C	-0.76758208	-2.00224245	0.00000000
C	0.00000000	-0.79135982	0.00000000
C	1.36076781	-1.01137298	0.00000000
S	1.66143423	-2.74309272	0.00000000
C	-0.86173294	0.38054327	0.00000000
C	-2.24704251	0.01652490	0.00000000
C	-0.66138324	1.74263454	0.00000000
S	-2.21607699	2.55903257	0.00000000
S	-2.52533132	-1.73781446	0.00000000
C	-0.01931381	-3.14888804	0.00000000
H	-0.34098572	-4.17969751	0.00000000
C	-3.11075226	1.08010071	0.00000000
H	-4.19067961	1.08667817	0.00000000
C	0.52369204	2.58360173	0.00000000
H	0.27758659	3.64410557	0.00000000
C	1.85786601	2.34164583	0.00000000
H	2.42713566	3.26794160	0.00000000
C	2.76399153	1.17820548	0.00000000
C	2.54200446	-0.16295766	0.00000000
H	3.45739074	-0.75427113	0.00000000
C	4.24388702	1.57243790	0.00000000
H	4.76048362	1.17817990	0.88195479
H	4.76048362	1.17817990	-0.88195479
H	4.38175805	2.65563683	0.00000000

Table S76. Cartesian coordinate of optimized structure of type (i) reference compound for Me-**7** (C_S) at the B3LYP/6-31G(d,p) level

C	0.83061482	1.97432646	0.00000000
C	-0.00000000	0.78071080	0.00000000
C	-1.34260486	1.07447344	0.00000000
S	-1.56385596	2.82350647	0.00000000
C	0.81627192	-0.41196852	0.00000000
C	2.22305657	-0.10248001	0.00000000
C	0.57550190	-1.77430067	0.00000000
S	2.10982662	-2.64783917	0.00000000
S	2.57441512	1.63707601	0.00000000
C	0.14564221	3.14502078	0.00000000
H	0.51500471	4.15982311	0.00000000
C	3.04652646	-1.18871987	0.00000000
H	4.12593141	-1.22708668	0.00000000
C	-0.61248252	-2.58011777	0.00000000
H	-0.38405609	-3.64483427	0.00000000
C	-1.95022284	-2.33648861	0.00000000
H	-2.52189789	-3.26230190	0.00000000
C	-2.86867933	-1.20352831	0.00000000
C	-4.18175759	-1.53437708	0.00000000
H	-4.96307526	-0.78027522	0.00000000

C	-2.64396304	0.31667103	0.00000000
H	-3.20766044	0.68193015	0.86764253
H	-3.20766044	0.68193015	-0.86764253
H	-4.51018072	-2.56840827	0.00000000

Table S77. Cartesian coordinate of optimized structure of type (ii) reference compound for **7** at the B3LYP/6-31G(d,p) level

C	0.35097652	1.73963171	0.00000000
C	-0.00000000	0.34446484	0.00000000
C	1.10910425	-0.49417507	0.00000000
S	2.57437759	0.48159154	0.00000000
C	-1.44227915	0.16116543	0.00000000
C	-2.13711123	1.42984042	0.00000000
S	-3.96829026	-0.34918900	0.00000000
S	-1.04933916	2.83564502	0.00000000
C	1.69182934	1.97994712	0.00000000
H	2.22094246	2.92162408	0.00000000
C	-3.49565835	1.32593815	0.00000000
H	-4.24391830	2.10459529	0.00000000
C	3.48668357	-2.71882758	0.00000000
H	3.90048179	-1.71453510	0.00000000
C	2.04667735	-2.88077697	-0.00000000
H	1.70705104	-3.91521879	-0.00000000
C	1.06899526	-1.93783261	-0.00000000
H	0.05271074	-2.32109319	-0.00000000
C	-2.32221913	-0.89330924	0.00000000
H	-2.11938648	-1.95379270	-0.00000000
C	4.33925436	-3.75806669	-0.00000000
H	3.98242816	-4.78499321	-0.00000000
H	5.41420336	-3.61334428	-0.00000000

Table S78. Cartesian coordinate of optimized structure of type (ii) reference compound for **8** at the B3LYP/6-31G(d,p) level

C	0.42327546	3.04334715	-0.00000000
C	0.99198252	1.71141986	0.00000000
C	-0.01440066	0.72708797	0.00000000
S	-1.59054758	1.51280623	0.00000000
C	2.45928878	1.80661610	0.00000000
C	2.90280083	3.18981846	0.00000000
S	5.05083006	1.82686971	0.00000000
S	1.59054758	4.37252168	0.00000000
C	0.01440066	-0.72708797	-0.00000000
C	-0.99198252	-1.71141986	-0.00000000
S	1.59054758	-1.51280623	-0.00000000
C	-0.42327546	-3.04334715	0.00000000
C	-2.45928878	-1.80661610	0.00000000
S	-1.59054758	-4.37252168	0.00000000
C	-2.90280083	-3.18981846	-0.00000000
S	-5.05083006	-1.82686971	0.00000000
C	-0.93412772	3.10405836	0.00000000
H	-1.58242082	3.96763042	0.00000000
C	4.25227307	3.36730690	-0.00000000
H	4.81971580	4.28595120	-0.00000000
C	-4.25227307	-3.36730690	0.00000000
H	-4.81971580	-4.28595120	0.00000000
C	0.93412772	-3.10405836	-0.00000000
H	1.58242082	-3.96763042	-0.00000000
C	3.55119063	0.96578648	0.00000000
H	3.58984016	-0.10777814	0.00000000
C	-3.55119063	-0.96578648	0.00000000
H	-3.58984016	0.10777814	0.00000000

Table S79. Cartesian coordinate of optimized structure of type (ii) reference compound for **9** at the B3LYP/6-31G(d,p) level

C	-1.67258960	-3.91002894	0.00000000
C	-0.32635534	-4.12066236	0.00000000
C	0.48136265	-2.92434191	0.00000000
C	-0.30582068	-1.77514519	0.00000000
S	-2.01749419	-2.21088779	0.00000000
H	-2.47548992	-4.63274693	0.00000000

C	1.89670331	-3.24725293	0.00000000
C	3.10069389	-2.55428714	0.00000000
C	2.10827349	-4.67553642	0.00000000
S	4.45618497	-3.67683062	0.00000000
C	3.41491366	-5.06226443	0.00000000
H	3.82953554	-6.05988713	0.00000000
S	0.61093584	-5.62642566	0.00000000
C	3.39431287	-1.17795190	0.00000000
C	0.00000000	-0.40969412	0.00000000
C	0.12209398	0.80611549	-0.00000000
C	-2.21167590	3.11031849	-0.00000000
S	-4.76528150	2.83809715	0.00000000
C	-2.77580992	4.44016612	0.00000000
C	-0.76586904	3.14775664	-0.00000000
C	-4.13821803	4.46435479	-0.00000000
S	-1.54548392	5.72720837	-0.00000000
C	0.24648058	2.19815720	-0.00000000
C	-0.26319827	4.49292204	-0.00000000
H	-4.81220805	5.30813925	-0.00000000
S	1.81816427	3.00007588	-0.00000000
C	1.09836929	4.58303263	-0.00000000
H	1.72628814	5.46216259	-0.00000000
C	3.74942906	-0.01925364	0.00000000
H	4.04034347	1.00512480	-0.00000000
C	-3.18025853	2.13886057	0.00000000
H	-3.05790147	1.06581952	0.00000000

Table S80. Cartesian coordinate of optimized structure of type (ii) reference compound for **10** at the B3LYP/6-31G(d,p) level

C	-1.01495652	1.60699826	0.00000000
C	1.82231828	3.49897035	0.00000000
C	-1.82226364	2.74421793	0.00000000
C	-1.50619271	4.10151764	0.00000000
S	-3.57572795	2.52766497	0.00000000
C	-2.68963594	4.92399322	0.00000000
C	-0.30128664	4.90919922	0.00000000
S	-2.35571965	6.66654556	0.00000000
C	-0.61536933	6.31766138	0.00000000
C	1.07069602	4.68921922	0.00000000
S	1.93497227	6.22100975	0.00000000
C	-0.36832975	0.56582169	0.00000000
C	-1.82226364	-3.49885137	0.00000000
C	-1.07071389	-4.68914673	0.00000000
C	0.30126117	-4.90918543	0.00000000
S	-1.93505359	-6.22089656	0.00000000
C	1.50619782	-4.10155244	0.00000000
C	0.61528435	-6.31765789	0.00000000
C	1.82231867	-2.74426842	0.00000000
C	2.68961040	-4.92407611	0.00000000
S	2.35562064	-6.66661806	0.00000000
C	1.01506224	-1.60701283	0.00000000
S	3.57579523	-2.52778104	0.00000000
C	0.36844546	-0.56583023	0.00000000
C	0.46770486	7.14507700	0.00000000
H	0.50019423	8.22491694	0.00000000
C	-3.86765670	4.23659783	0.00000000
H	-4.87830597	4.61852566	0.00000000
C	-0.46782283	-7.14502885	0.00000000
H	-0.50035485	-8.22486715	0.00000000
C	3.86765742	-4.23672679	0.00000000
H	4.87829271	-4.61869217	0.00000000
C	2.52758827	2.51403116	0.00000000
H	3.10878862	1.62117905	0.00000000
C	-2.52737900	-2.51379968	0.00000000
H	-3.10845243	-1.62086514	0.00000000