Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supplementary Information

Successful combination of computationally inexpensive GIAO ^{13}C NMR calculations and artificial neural network pattern recognition: a new strategy for simple and rapid detection of structural misassignments

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List of contents:

Instructions for using the Excel file to calculate the chemical shifts, statistical parameters and ANN output

- The Excel file contains 3 sheets, namely: ANN-MM-18, ANN-AM1-18 and ANN-HF-18 (Figure S-1)
- It must be used the corresponding sheet depending upon the level of theory employed to perform the geometry optimization step:

Sheet	Geometry optimization step at:
ANN-MM-18	MM+
ANN-AM1-18	AM1
ANN-HF-18	HF/3-21G

- Each sheet contains four main zones: A, B, C and D (Figure S-1).

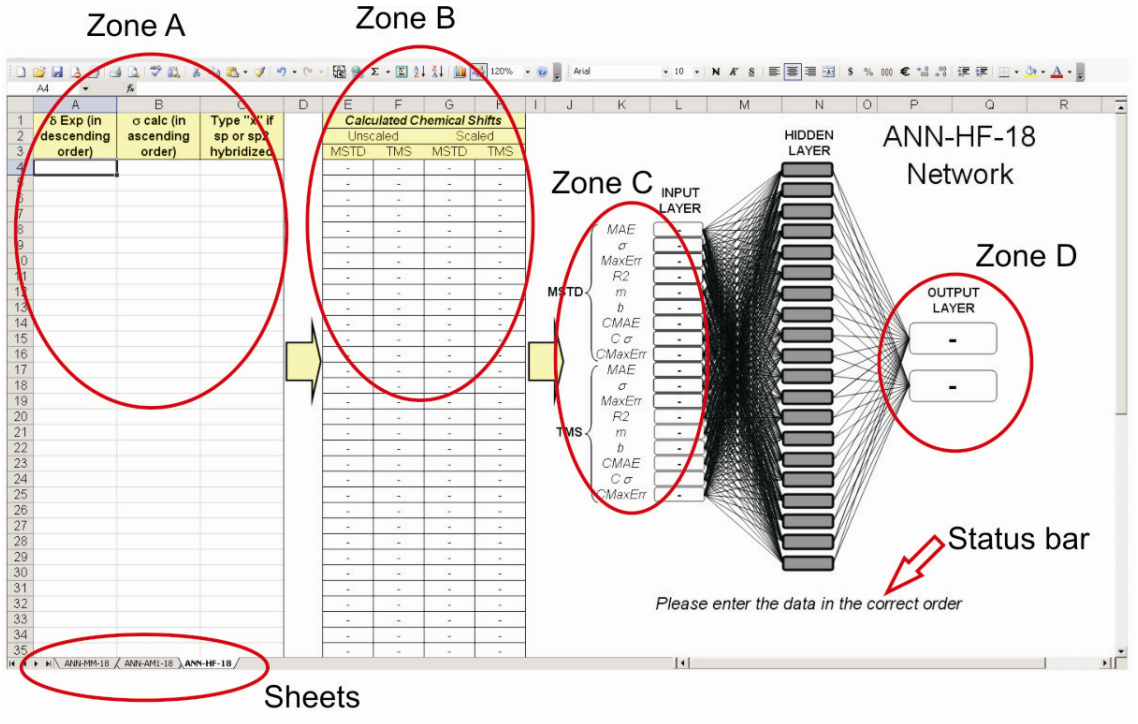


Figure S-1

Zone A: contains enabled cells to be filled by the user as follows:

- *Column A:* enter the experimental chemical shifts (in descending order)*
- *Column B:* enter the calculated GIAO shielding values (in ascending order)*
- *Column C:* type the letter "x" if the shielding value corresponds to an sp or sp^2 hybridized carbon atom (See Figure S-2).

* It is important to recall the need of inserting the data in the correct order. If not, the status bar will continue showing the message "Please enter the data in the correct order".

Once the data has been entered (Zone A), the Zones B, C and D will be automatically activated (Figure S-2).

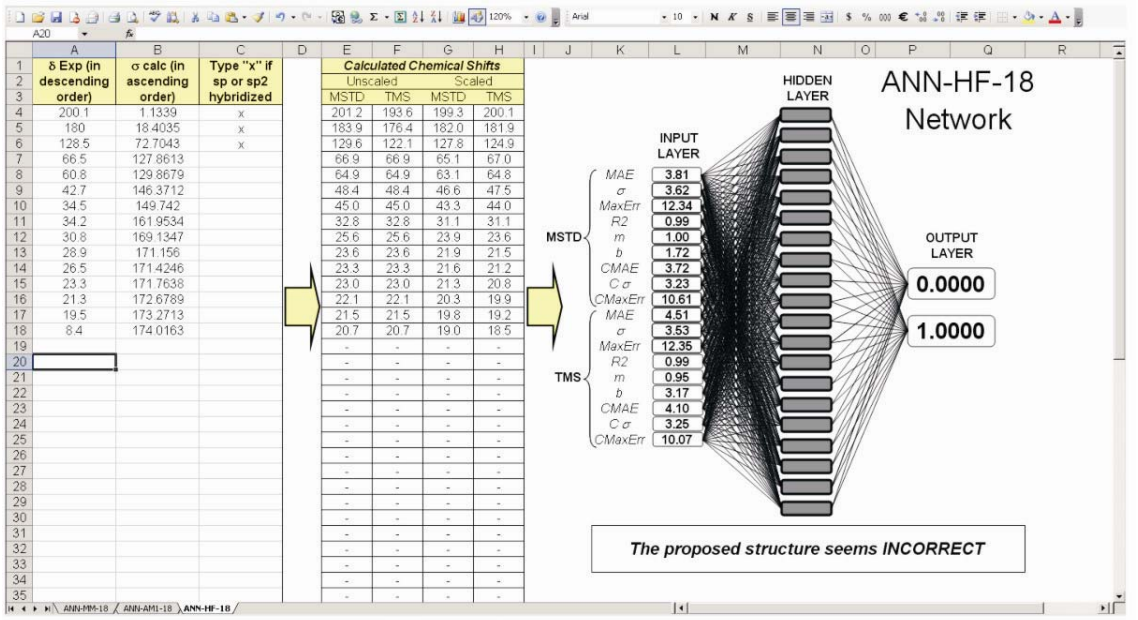


Figure S-2

Zone B shows the unscaled and scaled chemical shifts computed using TMS and MSTD as reference standards.

Zone C shows the computed 18 statistical parameters that are automatically introduced in the trained ANN.

Zone D shows the output value of the trained ANN.**

**Depending on the output value, the Status bar will display the following messages "The proposed structure seems CORRECT" or "The proposed structure seems INCORRECT".

Experimental chemical shifts and mPW1PW91/6-31G(d) Boltzmann-averaged GIAO isotropic magnetic shielding values calculated for MM+, AM1 and HF/3-21G geometries of compounds 1-200.

Compound **1**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
188.6	7.9435	9.6394	13.9991
148.1	46.4390	47.3398	57.2862
126.5	68.8269	70.6942	72.7391
101.4	90.0064	91.0434	94.5418
71.5	122.8599	121.2671	121.2435
66.3	125.1760	122.6252	127.9196

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **2**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
177.4	22.9049	24.4630	28.1272
156.4	43.4857	41.2613	46.3397
155.9	45.3968	42.9782	47.2041
133.7	66.0020	66.0628	69.6272
125.6	69.1187	69.2136	72.3851
125.2	71.6898	72.9709	75.1200
124.8	72.3461	73.3076	76.8815
118.2	77.7938	78.9526	85.0049
112.9	81.5013	81.4443	85.3765

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **3**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
160.6	44.1261	36.9208	46.5856
154.0	45.9179	40.1176	46.6024
143.5	59.0393	54.7131	59.5700
131.8	66.0395	66.4955	70.6353
128.0	67.3289	69.7172	73.4434
124.4	72.2548	75.3796	78.1257
118.8	81.2726	78.8091	82.0902
116.7	83.3092	79.4376	82.1408
116.6	85.1379	83.0156	84.7360

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **4**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
164.2	34.3502	34.7601	41.6981
150.0	49.1731	45.7258	51.8369
146.5	52.1431	48.8279	54.2927
133.4	63.6712	67.4848	70.0232
123.2	75.4226	76.1211	77.0612
107.7	87.7691	86.2403	90.3347
106.7	91.4508	88.6072	92.2698
101.3	95.2352	89.9546	94.9435
47.8	146.9867	144.5597	147.9932
34.8	161.1590	157.1545	162.3045
27.6	162.8005	161.1168	165.5911

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **5**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
139.8	56.4707	55.6004	60.8663
134.3	60.0186	59.8351	65.3053
56.6	132.7280	133.4177	136.1831
52.9	138.7237	139.7370	139.8353
52.7	141.6727	141.3644	141.6190
31.9	162.1415	158.4070	161.8985
24.8	167.4901	165.3313	167.6481
19.9	172.4470	168.5717	174.9702
19.7	173.7640	169.4778	175.2420
13.4	177.8300	174.9142	180.3795

[a] NMR data from: Barone, G.; Gomez-Paloma, L.; Duca, D.; Silvestri, A.; Riccio, R.; Bifulco, G. *Chem. Eur. J.* **2002**, *8*, 3233. Solvent: $CDCl_3$

Compound **6**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
136.0	58.3232	58.4546	63.6418
132.2	63.6260	63.5996	67.6340
132.1	63.8343	63.7405	68.2624
131.9	64.3943	65.0333	68.3908
55.1	139.8271	135.7225	137.2458
50.5	140.4646	135.9403	144.0897
46.4	147.7803	146.2989	147.2004
45.5	148.9458	147.4498	147.7450
41.5	149.9243	148.9865	151.1174
34.9	158.2992	154.8664	157.9171

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **7**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
154.4	47.7195	39.4759	48.1989
141.7	59.9389	51.1630	58.3262
133.2	65.4750	67.9850	67.9018
130	67.3671	69.3224	71.1185
128.2	67.9916	70.1691	71.1382
127.9	68.2952	70.4800	71.6032
126.6	70.0213	70.5461	72.7517
125.3	71.1666	71.8936	74.5425
116.5	76.4111	78.4847	82.2461
107.5	89.8272	88.7175	93.1415
31.1	162.2381	158.5871	163.6613
27.5	162.4678	163.1442	164.0152
19.6	172.7629	169.2526	176.2185
14.1	177.1928	173.7378	179.2000
11.4	179.2779	175.7457	181.4602

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **8**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
140.1	59.7683	59.7411	64.9777
130.7	61.4707	60.9618	65.4521
72.2	120.3111	119.9106	120.8102
48.1	143.9450	138.9962	145.7661
47.9	146.2990	143.8826	147.5223
42.7	150.4410	148.5528	149.6106
37.4	156.1678	152.6457	156.4976

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **9**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
140.1	55.2728	56.3849	59.2763
133.19	60.9725	60.6185	66.3792
72.3	120.6461	119.9370	121.1779
50	144.6543	140.2592	143.8963
45.3	145.2514	142.4688	147.4105
40.5	151.7857	150.1607	151.1568
36.9	156.0906	152.8008	155.5299

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **10**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
200.2	-6.3610	-5.2965	1.9162
135.5	59.9497	59.8838	62.3335
134.1	60.7480	61.1780	67.5071
99.3	93.1843	94.5767	97.9182
74.8	118.8495	118.6582	118.6828
70.2	123.8970	120.5621	124.0134
49.4	141.4983	136.5967	145.9710
46.9	145.1396	142.9304	146.3527
46.9	146.5057	144.5737	146.4086
46.3	148.1741	146.5304	146.8161
42.3	150.0979	148.5377	149.6788

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **11**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
201.1	-7.7516	-5.8904	1.4600
139.4	55.5945	56.4579	61.3455
136.3	57.2272	56.7650	62.6090
99.1	93.1279	94.5247	97.9016
76.8	117.1935	116.3836	116.3877
69.9	124.0048	120.8419	124.1695
48.2	145.0214	141.8263	143.9753
46.7	145.5348	142.6221	145.0795
44.9	145.7995	142.8937	148.0771
44.5	148.9613	147.3185	148.7041
41.9	150.2829	149.4130	150.9903

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **12**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
199.3	0.6546	0.7691	4.7522
146.7	45.2697	53.2989	54.1416
144.4	52.4795	54.5729	60.1736
135.5	61.1680	64.1322	64.1990
110.5	83.5061	84.0158	88.4702
43.2	149.8145	148.2023	151.0701
42.6	150.9763	149.4427	153.3734
31.3	159.3515	158.5645	162.5434
20.5	168.3856	168.6357	173.4180
15.6	173.8005	171.0654	176.0677

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **13**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
199.4	2.5098	2.1423	6.8794
160.1	39.3673	44.5806	46.4744
125.4	70.5217	71.6863	74.0225
50.8	146.7192	142.9708	147.2913
45.2	151.8513	147.3183	152.1962
33.5	154.7949	156.2369	160.3025
28.3	162.3164	162.0801	164.2319
28.3	168.0594	163.7672	169.8001
24.4	168.4224	164.3115	170.8857

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **14**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
137.7	60.2947	58.8384	59.8357
132.9	60.3507	61.8780	71.1724
101.9	85.7188	88.1422	94.4838
74.4	119.0785	118.9072	119.4047
71.2	122.9123	120.7997	121.0878
67.9	124.0238	124.6143	127.5283
50.0	141.4161	136.8137	144.4843
47.6	146.1659	144.0643	146.1757
46.4	147.3185	146.1507	146.5148
42.2	150.2679	148.7531	149.9223
39.4	152.0804	151.7363	150.9257

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **15**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
135.7	58.9745	58.3050	64.0785
135.7	60.8724	61.4912	64.4893
99.9	89.1336	92.2355	94.4098
74.4	119.0415	118.6554	119.0261
71.1	121.3074	120.2440	123.7146
69.8	122.7214	125.0858	126.6743
50.3	140.9682	136.3917	144.5478
47.8	145.8288	143.6788	145.3811
46.9	145.8547	143.7517	146.2398

46.3	146.2740	144.1488	147.6708
44.2	147.6311	146.8880	148.3094

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **16**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
173.2	32.5417	25.6578	33.6738
129.3	69.4644	68.6081	70.9594
94.2	105.9481	104.4098	108.8185
44.5	150.1474	146.9885	151.2969
31.3	164.4789	161.4322	164.0594
17.3	174.6262	173.9517	174.0157

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **17**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
146.9	50.4997	53.6853	53.2613
137.8	61.3936	60.4595	64.6906
132.9	66.5059	64.2318	66.9036
130.6	69.5352	65.5395	68.9650
125.4	76.3727	71.8960	75.1551
118.8	82.1811	79.1084	81.4440
16.7	178.4245	171.5384	177.1581

[a] NMR data from: Coskun, N.; Erden, I. *Tetrahedron* **2011**, *67*, 8607. Solvent: $CDCl_3$

Compound **18**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
205.3	-8.1844	-2.2916	1.2341
165.2	37.7965	35.3054	39.3852
158.2	42.7269	41.4361	45.8724
130.4	65.7724	66.7297	71.0180
125.3	70.6757	70.7042	74.5839
115.3	83.9058	83.8542	87.4848
109.7	86.8200	86.8666	91.3946
55.6	143.2571	135.9861	141.6239
36.4	158.0337	155.9577	159.5985
25.8	166.3244	164.5654	167.5330

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **19**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
178.0	19.8465	21.4605	25.8029
161.4	43.1968	31.9235	40.9393
152.1	50.7689	41.9994	48.7210
123.9	75.7547	74.7342	80.6183
110.1	81.8826	84.5682	90.8344
57.2	136.5283	132.0126	136.0805

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **20**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
157.2	39.4835	40.2144	45.9252
156.3	42.8516	42.2571	46.4293
144.0	58.4683	53.0443	58.9246
135.0	63.8423	63.5315	67.7833
130.1	67.7585	66.0721	70.0341
127.3	74.5111	71.4908	74.8809
122.2	76.0215	74.1961	79.3688
121.8	77.6822	75.8764	80.4055
105.3	88.1700	91.4330	95.6799
55.4	143.1990	136.1076	141.9385
25.0	169.9156	164.8729	169.9626

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **21**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
205.8	-6.5559	-9.5217	0.2571
141.3	55.7330	60.4436	60.3031
138.9	61.6994	61.1764	64.4525
132.1	66.2544	66.7898	69.6629
129.6	66.6373	67.4930	69.8931
128.5	69.2812	69.0995	72.1899
126.6	71.4219	71.7417	75.2538
40.9	154.2258	151.9377	155.0870
32.6	160.5143	157.8560	161.0237
25.3	165.9228	163.5403	168.3507
21.0	170.6011	168.1660	173.2009

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **22**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
76.3	117.1851	116.5749	119.8750
62.4	132.3353	129.3760	134.0009
48.8	143.5384	142.2574	145.0235
48.0	144.6366	143.4950	146.5390
40.2	150.8427	151.1221	153.9121
39.6	152.2677	151.6215	154.5894
38.5	152.4513	152.0999	154.9374
37.7	155.5193	154.2264	155.3487
36.3	157.2191	154.3948	156.7674
35.0	158.7412	156.0043	158.9703
30.2	163.1247	158.8064	163.3616

[a] NMR data from: Marchand, A. P.; Kumar, V. S.; Hariprakasha, H. K. *J. Org. Chem.* **2001**, *66*, 2072. Solvent: $CDCl_3$

Compound **23**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
175.2	24.9002	24.2322	32.5455
82.5	116.5241	112.5606	114.5812
49.1	143.4586	142.2855	145.3488
47.9	144.0499	142.8796	145.8519
46.6	144.9838	146.7805	149.0613
42.9	145.9050	147.1921	150.9460

42.6	146.0467	149.2389	151.6164
36.9	155.3970	154.4667	155.2248
34.9	156.7835	155.0787	157.5059
34.4	158.9708	156.0179	159.3485
28.9	163.7050	159.5918	164.3964

[a] NMR data from: Marchand, A. P.; Kumar, V. S.; Hariprakasha, H. K. *J. Org. Chem.* **2001**, *66*, 2072. Solvent: $CDCl_3$

Compound **24**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
84.0	110.6920	107.7875	111.1081
80.8	114.1411	111.0501	114.1112
69.0	123.8515	123.2110	125.9938
60.4	133.2438	131.0041	135.4931
44.5	147.4171	145.2227	147.9536
44.5	149.2799	145.2694	148.6721
43.0	150.3007	146.8245	149.8506
42.4	152.4842	147.6795	150.0972
36.1	157.1841	155.9032	157.6823
34.3	158.9894	157.3007	158.9393
32.3	159.0567	158.7712	161.9171

[a] NMR data from: Marchand, A. P.; Kumar, V. S.; Hariprakasha, H. K. *J. Org. Chem.* **2001**, *66*, 2072. Solvent: $CDCl_3$

Compound **25**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
85.2	109.5203	106.1325	109.9916
85.2	109.5212	106.1326	109.9916
48.5	143.0210	140.5361	144.9483
48.5	143.0230	140.5361	144.9484
47.5	144.4649	143.4571	146.8997
47.5	144.4803	143.4572	146.8998
42.4	154.0369	148.7264	149.7512
42.4	154.0457	148.7264	149.7512
30.4	163.3741	158.9829	163.4809
30.4	163.3766	158.9830	163.4810

[a] NMR data from: Marchand, A. P.; Kumar, V. S.; Hariprakasha, H. K. *J. Org. Chem.* **2001**, *66*, 2072. Solvent: $CDCl_3$

Compound **26**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
131.3	67.5666	67.6319	69.5957
130.8	67.8882	68.6468	70.3167
130.8	68.0013	69.0165	70.8961
128.8	68.2215	69.0638	71.0616
128.8	70.9097	69.1486	71.2211
128.5	70.9938	69.1729	71.3116
128.5	71.1025	69.6747	71.7653
128.2	71.4776	70.3949	72.6246
126.0	71.5337	72.3400	73.5276
126.0	71.7682	72.3698	75.8822
124.8	72.0063	72.4708	75.8869
124.8	72.0600	72.9542	75.9218
124.1	72.0950	73.4018	77.0858
124.1	73.1615	73.7958	77.6639
66.4	127.7955	124.6304	128.8978
58.1	137.6295	133.5516	140.7961

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **27**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
146.6	49.6050	49.3597	53.9772
139.1	59.3743	58.6548	61.4460
129.8	68.3501	69.3712	72.1727
128.6	70.3000	70.6574	73.6553
124.3	70.5126	72.4792	75.8950
120.2	78.5549	78.3396	81.0492
83.9	119.0150	120.4260	118.2907
74.6	121.7556	121.6359	119.7526
71.4	127.5417	126.9445	128.6749

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **28**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
198.1	1.1172	1.2993	5.9140
158.5	42.3721	40.5405	45.1295
137.1	61.6329	64.3289	67.0594
133.5	66.6014	67.4111	68.7613
130.0	67.8861	68.1236	72.1653
121.7	76.7808	73.9731	79.5636
109.4	85.2512	86.5530	90.6622
55.5	143.4273	135.9978	141.7996
39.0	156.2427	153.3315	157.1689
29.0	163.7531	160.6394	164.9144
23.6	167.4686	165.6483	169.7986

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **29**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
137.3	61.5879	64.3123	65.3432
137.1	62.0905	64.4759	65.6628
131.9	65.6572	64.8771	69.0998
131.6	66.8205	65.8197	69.6817
129.6	68.8344	69.6406	72.0644
128.7	69.3993	69.9489	73.1302
128.4	69.8416	70.3156	73.7603
128.3	70.3977	71.0641	73.8285
128.0	70.7734	71.0916	74.1299
127.9	71.1204	71.3559	74.1990
126.6	71.9255	71.4428	74.8642
126.4	72.4528	71.5535	75.0612
123.3	75.9373	76.8785	77.5348
122.3	76.8577	77.8473	78.4144
90.3	105.4617	105.1715	107.0031
89.6	105.9668	105.8241	107.9184

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **30**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
167.3	31.3494	29.9538	38.7069
143.9	52.3789	52.5186	56.8867
134.1	62.8708	65.0255	67.8420
132.1	65.6005	65.3524	69.1885
131.7	66.5362	65.9516	69.3780
128.6	69.7616	69.0351	72.9568
128.4	69.8492	70.1388	73.4588
128.0	70.1165	70.1890	73.6231
125.3	73.8468	74.2484	75.3840
123.0	76.5126	77.5647	78.0943
118.5	79.4942	82.6031	83.7393
91.6	104.1569	103.0011	105.4129
89.0	107.2438	106.6096	108.5519
51.8	145.2723	138.4180	143.3018

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **31**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
161.2	38.7847	35.4397	45.6344
156.1	45.0390	42.2451	47.4035
145.1	51.0183	50.3865	56.7071
144.2	56.4475	53.0257	58.4812
139.2	57.8777	55.0876	60.5061
134.0	69.7700	66.0163	68.3503
122.8	71.5349	71.7142	77.7838
121.6	74.1286	73.9721	79.4998
120.0	78.0554	74.6462	79.5788
104.2	88.3494	91.3195	95.6029
66.6	130.1907	127.4365	127.3933
60.7	140.0222	133.4095	136.4413
55.9	143.0985	135.9894	141.4393

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **32**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
183.3	11.5127	13.5292	18.0661
180.0	12.9092	15.4172	18.7968
173.5	21.7028	23.3319	32.2075
158.4	43.0019	39.9081	45.4161
141.8	55.3625	60.0333	62.0229
132.9	64.3631	64.7645	68.8857
107.5	85.7340	88.6384	94.1994
72.2	114.6246	119.1404	123.0056
68.6	127.9710	125.9608	127.9245
61.0	132.2428	131.5906	133.9661
56.4	141.9661	135.7112	140.9468
36.7	156.6283	156.0413	158.0020

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **33**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
49.1	144.6513	145.0203	147.7159
41.3	146.9787	154.2966	152.6651
40.9	147.7386	154.9408	152.9079
32.1	159.1598	159.1568	163.5311
31.3	161.4556	160.1838	164.2934
29.4	161.4631	162.3748	164.4599
28.4	162.1707	162.8881	167.5248
25.0	162.1947	167.6894	167.6127
22.1	164.1602	167.9954	171.8105
21.6	165.5975	168.4482	173.0849
20.0	172.8555	169.3432	174.8814
18.9	173.7153	170.1969	175.4931
17.4	173.8204	170.6961	177.0099
16.6	173.9385	171.7034	177.2300
15.9	175.0759	173.2537	178.5151

[a] NMR data from: Welch, S. C.; Chou, C. Y.; Gruber, J. M.; Assercq, J. M. *J. Org. Chem.* **1985**, *50*, 2668. Solvent: C_6D_6

Compound **34**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
214.6	-24.4603	-22.6469	-16.2241
203.1	-5.5319	-5.8399	-1.3525
139.4	57.2826	57.9571	62.3734
135.6	58.3718	58.2858	63.1078
135.4	58.8935	62.0174	64.4124
133.1	63.1346	65.1388	68.5832
73.7	117.3739	121.5994	121.7672
72.6	117.8194	122.0511	122.4862
53.7	139.3102	141.6473	141.0974
44.5	147.0405	147.5818	151.2033
43.4	147.4385	148.7656	151.4547
42.7	148.3190	149.3980	152.1912
31.7	161.9982	158.8424	164.3667
26.1	166.6660	161.9426	169.1432
16.3	173.9976	170.3898	176.0176
15.7	175.1770	171.8649	178.1441

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **35**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
157.0	37.8879	35.3707	43.0843
150.3	49.6995	49.0790	53.0256
143.5	57.9706	55.8048	58.2532
138.0	58.2503	56.0274	61.1580
126.5	71.3125	72.2884	75.0838
123.3	73.8401	75.6846	78.1411
123.1	75.0351	75.7982	78.5005
119.8	78.9151	78.8940	81.2823
56.6	139.7676	139.7257	140.2911
45.3	148.3484	148.4591	148.1514
43.9	149.9572	150.8808	149.6101
42.7	150.8549	152.5906	152.2196
38.5	151.3138	156.1771	154.8803
36.6	160.3582	157.1336	161.3203

28.9	165.1990	160.4046	167.0869
28.7	167.4747	162.1041	168.2905
25.4	168.5463	163.8709	170.8828
25.0	168.6257	163.9259	170.9872
15.1	176.6011	174.2270	177.6492

[a] NMR data from: Rupert, K. C.; Liu, C. C.; Nguyen, T. T.; Whitener, M. A.; Sowa Jr. J. R. *Organometallics* **2002**, *21*, 144. Solvent: $CDCl_3$

Compound **36**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
159.0	33.2778	37.4739	42.1171
105.0	87.2782	88.9731	94.0344
69.1	119.0705	117.0415	125.2360
53.3	137.2626	133.4225	139.2704
52.3	141.8649	140.0873	144.9430
47.9	142.6669	141.1900	145.4477
46.0	144.1639	143.8604	145.4772
42.3	147.4107	145.6235	151.5831
41.7	149.7380	147.1629	152.1083
40.1	151.0472	153.2299	153.1157
31.8	157.1630	153.9281	157.4972
31.5	159.2377	156.0529	159.5472
30.8	162.5800	157.0684	164.4952
29.0	163.9086	158.0795	166.8700
26.0	168.8270	160.6503	171.9620

[a] NMR data from: Singh, V.; Prathap, S.; Porinchu, M. *J. Org. Chem.* **1998**, *63*, 4011. Solvent: $CDCl_3$

Compound **37**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
198.3	2.8304	2.2913	7.0873
177.0	20.2009	17.6422	25.1819
159.9	33.6867	38.0806	41.9222
105.1	87.2454	88.0861	93.3152
98.8	96.6150	89.9801	94.0924
95.3	102.1248	100.2909	104.1587
87.6	107.9465	106.0360	107.8029
56.9	133.0946	135.9299	138.8786
53.8	140.6734	140.2737	142.6068
44.8	145.6134	142.0079	150.9822
42.8	147.1531	152.3921	151.8678
35.4	156.6245	155.5154	158.0095
31.7	157.6404	155.6783	160.0983
31.4	160.0856	156.3296	163.1200
24.4	163.6105	156.8933	171.3996

[a] NMR data from: Pettus, T. R. R.; Inoue, M.; Chen, X. T.; Danishefsky, S. J. *J. Am. Chem. Soc.* **2000**, *122*, 6160. Solvent: C_6D_6

Compound **38**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
217.7	-14.4488	-20.4331	-15.0013
212.3	-9.9890	-15.8172	-10.0577
59.3	137.4162	135.6133	137.5698
45.7	146.6083	147.0706	149.8152
44.9	148.9354	148.3549	151.4113
42.9	151.4060	148.8412	151.9812
35.7	156.9197	155.3415	159.2199
18.2	171.1948	172.0372	175.9702
12.1	173.8264	173.9999	180.2769

[a] NMR data from: Blanchard, A. N.; Burnell, D. J. *Tetrahedron Lett.* **2001**, *42*, 4779. Solvent: $CDCl_3$

Compound **39**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
187.6	8.8689	11.1489	14.5629
179.2	24.0386	17.1088	22.9942
171.6	26.7450	29.5516	33.1530
155.8	43.5916	41.7691	46.6757
134.8	59.4023	60.7534	65.6852
134.1	65.1531	64.7732	68.2136
133.9	65.2045	65.3175	68.7570
133.7	66.0481	66.1107	69.5507
133.0	68.4430	66.9254	69.8370
127.1	70.0126	67.8726	71.2579
126.7	70.2767	70.6545	72.5094
126.5	71.2217	71.8773	75.3552
123.7	72.9223	73.2348	77.2272
121.3	75.6269	76.6365	80.1972
118.6	80.4770	78.1508	84.5781
111.4	82.0372	80.7760	86.2389

[a] NMR data from: Thasana, N.; Ruchirawat, S. *Tetrahedron Lett.* **2002**, *43*, 4515. Solvent: $CDCl_3$

Compound **40**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
56.1	138.8709	137.9491	140.5317
55.5	139.4929	138.3465	141.5431
42.4	151.3611	150.1460	154.7500
39.1	153.5595	150.2294	155.8592
36.9	155.2598	153.7840	156.5440
36.8	155.9117	154.2221	158.7827
35.9	156.1173	154.7861	159.6057
35.5	157.7350	156.0644	159.9181
33.6	158.4898	160.4442	160.0171
33.3	160.6404	162.7571	162.2224
27.1	165.7870	163.3587	167.5016
26.4	166.5094	164.6920	168.3980
25.1	167.0247	164.7213	168.8792
22.0	169.4155	167.0233	172.0377
21.8	171.0022	167.0748	172.8441
19.0	172.1483	170.3542	174.9308
14.3	177.5127	172.5323	179.4879

[a] NMR data from: Barone, G.; Gomez-Paloma, L.; Duca, D.; Silvestri, A.; Riccio, R.; Bifulco, G. *Chem. Eur. J.* **2002**, *8*, 3233. Solvent: $CDCl_3$

Compound **41**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
156.0	41.2935	47.4449	47.1006
102.8	89.3171	89.9653	94.3145
56.1	137.7178	135.4867	139.7855
56.1	138.8690	138.5066	140.5743
49.2	146.0329	141.5930	146.1248
44.2	146.4168	147.2652	150.1769

44.2	149.8030	149.3305	150.2544
42.0	149.9126	150.0223	154.2352
41.3	152.6723	150.2636	154.7177
40.4	153.0609	151.5644	154.8176
39.9	153.7280	151.7425	155.5182
39.3	154.5697	154.9072	155.5470
33.7	155.6385	155.4285	159.9844
33.3	159.5769	158.9954	161.4816
33.3	160.7877	163.9629	162.3555
21.7	170.8371	167.2521	173.3165
20.3	171.3486	168.8626	173.3313
18.7	172.2432	169.1320	175.0941
18.1	173.0057	170.7192	175.3637
14.4	174.8516	171.6689	176.5545

[a] NMR data from: Barone, G.; Gomez-Paloma, L.; Duca, D.; Silvestri, A.; Riccio, R.; Bifulco, G. *Chem. Eur. J.* **2002**, *8*, 3233. Solvent: $CDCl_3$

Compound **42**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
215.3	-15.9478	-15.4584	-10.6128
56.5	137.8947	136.9745	139.1896
54.9	137.9233	139.7488	140.2383
54.6	139.9635	140.3045	141.5614
47.0	147.3722	146.8046	149.5293
38.3	151.3740	152.0529	156.0529
37.5	155.6669	155.4190	157.2802
36.9	156.0276	157.2784	158.3193
35.0	156.8821	157.2850	159.6070
31.9	158.3772	157.6299	161.5051
31.7	160.5246	159.7040	162.5238
28.8	163.3172	160.2933	165.9101
28.8	163.6685	160.6257	166.0064
26.6	166.3433	163.2675	167.7975
24.8	166.5464	164.1367	168.0108
21.9	169.9458	167.5803	172.2810
19.5	171.9127	168.3900	172.9502
17.7	175.0796	169.8397	177.2454
11.9	180.1216	175.7157	182.1286

[a] NMR data from: Barone, G.; Gomez-Paloma, L.; Duca, D.; Silvestri, A.; Riccio, R.; Bifulco, G. *Chem. Eur. J.* **2002**, *8*, 3233. Solvent: $CDCl_3$

Compound **43**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
211.0	-12.4919	-11.3309	-5.9526
54.3	139.2341	138.8527	141.7019
54.1	139.8673	138.9575	141.7276
46.7	145.2285	147.4195	148.2301
44.6	148.4554	147.7532	151.7254
40.8	150.0631	150.2057	152.5260
40.3	151.7922	150.9766	154.3267
38.8	153.1524	151.6261	155.1822
38.7	153.3334	153.5666	156.9045
38.1	154.3701	154.7461	157.2267
35.7	155.2123	157.1733	158.1350
35.7	156.8666	157.1901	158.9543
32.1	160.3692	159.6703	162.2839
29.0	162.6408	160.8442	165.4355
25.5	165.7300	163.5366	167.3341
21.5	169.3355	167.7677	171.7841
20.5	170.9012	168.8683	171.9501
17.4	175.2685	169.4344	177.5198
11.4	179.8474	175.6463	182.0397

[a] NMR data from: Barone, G.; Gomez-Paloma, L.; Duca, D.; Silvestri, A.; Riccio, R.; Bifulco, G. *Chem. Eur. J.* **2002**, *8*, 3233. Solvent: $CDCl_3$

Compound **44**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
147.7	46.0556	52.5399	52.4793
140.0	56.8791	61.7786	61.5259
121.4	72.0785	72.8436	77.2719
108.6	86.5496	85.8159	91.2689
87.9	113.1519	115.4265	114.1917
81.2	114.2514	117.7654	114.4456
74.1	125.0401	122.7070	125.1432
54.7	138.4264	138.3503	140.2386
52.5	139.5107	140.9208	143.3817
50.5	140.1053	144.0063	143.4423
42.7	149.4612	147.6218	152.7427
40.7	151.4161	149.2749	153.7761
39.9	151.9769	150.7811	154.2093
36.7	155.9090	155.9709	157.9440
35.6	157.8212	157.0585	159.0567
31.8	161.6599	159.1590	163.2180
29.2	163.5954	160.2320	164.9642
25.8	167.4509	163.6587	168.3148
22.0	168.5354	166.1025	170.5690
22.0	169.1859	166.7117	172.1184
19.9	169.6709	168.0761	172.2799
9.2	182.5606	178.4103	184.6432

[a] NMR data from: Corey, E. J.; Huang, A. X. *J. Am. Chem. Soc.* **1999**, *121*, 710. Solvent: $CDCl_3$

Compound **45**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
163.7	36.2961	36.8026	42.7387
151.3	47.3598	45.9339	51.4493
138.9	61.8500	61.5167	65.5061
116.6	74.9620	78.9962	83.3582
105.1	94.4204	92.6355	99.5325
54.1	140.0587	138.6761	142.8320
53.1	141.5171	139.1272	143.5618
49.8	146.0689	141.9554	145.2261
35.6	156.1494	154.9775	158.4602
27.8	162.0268	162.1253	165.8721
26.4	165.4833	165.0933	168.7545

[a] NMR data from: O´Neill, B. T.; Yohannes, D.; Bundesmann, M. W.; Arnold, E. P. *Org. Lett.* **2000**, *2*, 4201. Solvent: $CDCl_3$

Compound **46**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
165.3	37.9155	37.2049	44.6399
143.1	48.3323	52.5999	58.5313
142.4	56.3022	54.6278	61.8315

140.2	57.3611	59.7559	63.1981
134.1	58.6844	62.9852	65.1730
124.2	71.4670	72.8652	75.8806
122.7	74.5279	76.7173	80.3806
117.0	78.2814	78.9201	83.5146
111.3	85.3067	85.9130	87.5749
54.3	136.4968	139.2849	138.4871
49.1	146.9911	142.5255	147.8718
35.2	157.0655	155.1841	157.8719
32.8	157.9600	156.9628	159.1129
22.6	169.6730	165.9736	171.3010
12.3	180.7675	176.2657	180.8746

[a] NMR data from: Koshiba, T.; Yokoshima, S.; Fukuyama, T. *Org. Lett.* **2009**, *11*, 5354. Solvent: $CDCl_3$

Compound **47**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
155.0	41.6744	44.3463	47.4728
142.4	52.1398	47.9361	60.7343
140.6	57.0658	51.7377	61.2688
127.4	68.9550	66.7386	72.2369
122.6	75.0525	76.1556	78.5864
119.8	75.2460	76.9558	80.2728
119.2	76.0217	77.6104	80.5610
119.1	76.1183	77.6285	81.5321
118.4	76.3614	78.6242	81.6185
114.0	77.9191	78.6348	84.1506
113.5	82.8473	82.3597	88.8274
107.3	82.8599	86.7242	93.3158
76.1	122.2481	121.5837	119.0031
60.5	132.8800	137.2819	133.9243
48.7	142.4475	141.8409	146.1401
36.9	155.1921	154.7993	159.0399
36.2	157.5971	155.0120	159.6008
30.2	160.1743	156.1735	165.1610
29.3	161.6704	158.6722	165.5271
28.3	163.5944	162.5129	166.4685
23.0	169.8150	164.6166	171.3364
21.8	169.9202	167.5926	172.4846
15.3	176.9780	173.0496	176.9660

[a] NMR data from: Ueno, A.; Kitawaki, T.; Chida, N. *Org. Lett.* **2008**, *10*, 1999. Solvent: $CDCl_3$

Compound **48**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
174.1	23.3966	18.9029	28.9076
158.4	39.9990	40.2569	47.1916
152.8	44.2101	40.8637	48.3023
151.5	49.2618	48.1590	54.1169
149.0	52.7536	48.8725	54.2013
146.5	54.1609	52.4458	56.0936
132.2	61.4707	64.1808	69.8540
131.2	66.5562	66.9236	70.7263
129.5	67.0263	68.2451	71.0276
129.4	68.2069	68.3889	71.7784
128.8	68.5828	69.5491	73.1221
128.8	69.3903	70.6989	73.6033
128.5	69.4103	71.9657	74.5654
119.6	75.1650	72.0718	79.3274
99.0	95.2074	94.3723	100.1506
73.3	122.9239	122.9214	123.0938
66.4	131.8142	126.8847	124.1562
50.7	144.8534	141.7965	144.3030
31.7	154.9819	150.1976	155.7631
7.8	183.6467	179.8690	186.4906

[a] NMR data from: Blagg, B. S. J.; Boger, D. L. *Tetrahedron* **2002**, *58*, 6343. Solvent: CD_2Cl_2/CD_3OD

Compound **49**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
131.9	63.3880	63.6978	67.8474
131.6	63.6620	65.9984	67.9640
53.3	136.0807	140.7161	140.3721
52.9	137.7984	141.8823	142.0216
50.7	141.8314	143.4842	143.7979
43.3	151.5020	147.1090	153.0133
39.6	154.4534	151.3912	156.1012
37.6	156.9563	153.7568	158.4847
35.8	157.7236	154.7210	159.4566
31.1	162.0499	159.4305	163.7461
28.2	165.5411	160.8741	166.9647
25.5	165.5587	163.1467	168.0080
23.5	169.8606	165.7601	171.4282
21.8	170.0772	167.7068	172.3466
16.9	174.1674	172.0653	176.5643

[a] NMR data from: Ryckman, D. M.; Stevens, R. V. *J. Am. Chem. Soc.* **1987**, *109*, 4940. Solvent: $CDCl_3$

Compound **50**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
200.9	-4.7969	2.6857	5.5313
177.4	30.0192	23.3056	27.3534
165.1	36.8237	29.2375	38.0577
161.4	41.5348	38.1467	43.4472
154.3	42.2107	42.2724	48.7651
152.1	47.3638	42.6429	51.2038
145.8	53.2162	49.7163	55.6294
116.4	73.7114	75.4744	81.0983
113.5	84.1130	80.0273	81.7963
107.2	85.6459	85.0488	91.9560
103.5	89.7957	91.8849	94.9365
102.5	90.0008	92.1147	95.6306
91.4	105.5850	105.8544	111.2576
57.2	143.0767	135.5568	140.7682
47.1	143.5202	141.4143	140.7898
34.8	159.4846	157.1767	161.5713
28.8	163.1474	159.9720	164.1673

[a] NMR data from: Barone, G.; Gomez-Paloma, L.; Duca, D.; Silvestri, A.; Riccio, R.; Bifulco, G. *Chem. Eur. J.* **2002**, *8*, 3233. Solvent: $CDCl_3$

Compound **51**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
201.5	0.2748	0.9573	5.3304
180.4	23.9746	27.0237	30.0450
118.1	74.6156	76.0198	79.8941

79.7	114.1859	116.3640	116.2839
54.8	138.1540	139.8253	141.6785
52.7	140.9231	140.8097	144.2524
52.5	144.2101	140.9140	144.7907
50.8	145.0888	141.4766	146.8761
47.8	145.5105	142.9428	148.4718
47.2	145.6195	143.7533	148.5951
46.2	146.0319	147.0856	148.8483
40.4	152.8373	148.5768	155.4883
32.5	156.8903	158.4682	159.4178
31.4	162.3704	158.4881	162.9944
29.8	164.4343	160.1337	165.6611
26.2	164.4752	162.6563	168.0731
26.0	166.1856	162.9415	168.4703
25.2	167.3190	164.2740	168.9452
24.3	168.0172	165.4711	170.5226
23.1	169.7943	166.3852	171.9890

[a] NMR data from: Mander, L. N.; McLachlan, M. M. *J. Am. Chem. Soc.* **2003**, *125*, 2400. Solvent: $CDCl_3$

Compound **52**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
152.4	44.9011	39.1259	44.9768
152.1	48.9504	40.6182	48.9626
137.9	59.1277	63.6843	67.0638
135.7	64.7747	65.6901	69.6281
129.6	69.7463	69.7711	73.3243
125.9	70.0675	70.1076	73.4787
125.3	71.1543	70.4618	74.4478
124.9	72.7598	72.2478	75.0355
123.9	72.8964	73.3465	77.4827
120.5	73.0657	73.4797	78.2972
120.2	75.6997	75.8790	78.9337
119.2	75.9506	77.8520	80.0330
117.0	77.4023	78.1199	80.7637
116.9	79.6798	79.7968	82.2551
116.4	85.4487	83.0939	87.2570
41.7	159.5649	149.4187	154.1494

[a] NMR data from: Hayashi, K.; Choshi, T.; Chikaraishi, K.; Oda, A.; Yoshinaga, R.; Hatae, N.; Ishikura, M.; Hibino, S. *Tetrahedron* **2012**, *68*, 4274. Solvent: DMSO-d_6

Compound **53**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
158.8	35.5310	38.6463	45.4245
134.8	56.9471	58.4037	61.6806
128.9	65.7102	68.4826	71.4580
104.4	88.6556	89.7287	94.2706
71.8	119.6618	118.2652	121.0764
54.2	139.0571	134.0624	139.8503
53.6	141.8658	138.0021	143.1986
49.5	145.4491	143.1042	145.0259
42.1	150.1739	145.2636	153.3520
35.3	157.7250	155.3938	159.7748
32.3	159.3679	156.2463	160.4859
30.0	161.0218	158.8737	163.7086
24.5	171.1030	160.7684	173.5969
14.5	177.6603	174.4905	179.3315
11.2	181.1946	177.1693	183.2118

[a] NMR data from: Srikrishna, A.; Nagaraju, G. *Tetrahedron: Asymmetry* **2012**, *23*, 170. Solvent: $CDCl_3$

Compound **54**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
171.1	24.2453	23.8087	33.1645
134.2	59.7966	61.7307	65.2803
133.6	64.3770	62.4053	69.3559
131.7	64.9893	64.2513	70.1834
127.8	69.6844	68.9907	73.1822
121.7	72.3465	76.3869	78.7257
120.8	75.6302	77.4267	79.8391
119.2	77.8153	79.6932	82.6758
117.6	79.2068	81.7562	83.3156
113.0	83.7563	82.1712	87.6380
111.0	88.2846	87.3135	91.0961
59.2	132.3178	133.1340	139.1804
56.3	140.7257	135.6243	140.2543
49.6	143.7455	143.5870	144.3618
45.9	148.1903	145.9866	151.9433
42.0	149.7794	151.3682	153.1522
25.6	165.6267	163.0961	167.5331
21.6	169.2776	168.0883	172.8995
18.1	172.2755	170.6385	176.1579

[a] NMR data from: Lim, K. H.; Kam, T. S. *Org. Lett.* **2006**, *8*, 1733. Solvent: $CDCl_3$

Compound **55**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
178.6	21.0525	19.6235	24.6404
170.4	29.4069	30.1717	31.9644
153.5	47.2389	50.0610	55.0772
124.9	71.1180	68.2171	76.1728
124.5	74.7491	69.7488	77.6962
124.1	77.1928	76.2624	83.2930
116.4	80.8504	78.8352	84.7411
92.4	93.8377	95.4704	102.2695
51.2	145.0611	141.1987	143.5278
37.7	157.0967	152.8918	157.5798
19.8	170.2730	168.2218	171.5880

[a] NMR data from: Oshiyama, T.; Satoh, T.; Okano, K.; Tokuyama, H. *Tetrahedron* **2012**, *68*, 9376. Solvent: DMSO-d_6

Compound **56**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
172.0	27.2606	26.5751	34.7304
166.5	30.7903	28.3843	35.9047
147.8	47.1447	43.2301	49.3397
124.2	72.3148	76.2365	77.1787
110.3	83.3866	87.2837	88.0342
90.5	108.0123	103.0128	107.7824
68.8	125.0991	120.0587	127.5102
57.6	135.9258	132.3842	138.0908
49.1	144.9496	140.9203	147.7016

46.6	145.0031	141.8851	147.8496
27.7	162.7767	163.0872	163.3663
25.3	165.5849	165.8819	167.6233

[a] NMR data from: Medeiros, M. R.; Wood, J. L. *Tetrahedron* **2010**, *66*, 4701. Solvent: $CDCl_3$

Compound **57**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
180.8	12.2089	13.0621	16.6721
180.8	13.3760	15.2424	18.7650
151.2	46.1632	43.8977	49.8850
147.5	50.5952	45.1282	52.3926
138.4	60.6494	56.8936	65.8947
137.9	62.7576	58.6848	66.1454
132.5	64.9097	66.8542	70.4281
131.5	65.1596	67.1583	70.5305
131.4	66.4295	67.3358	70.9652
130.2	68.0760	67.7548	71.2685
129.8	68.4832	70.4066	72.1548
127.2	69.8781	70.7537	73.5633
124.8	70.5705	71.0695	75.3869
124.3	72.3746	73.1094	75.5488
123.3	73.1303	73.2821	76.4216
122.5	74.6564	75.7183	78.1713
122.3	79.3350	76.7068	78.2604
115.5	80.4143	77.5539	84.0823
113.9	87.8196	86.2201	90.0603

[a] NMR data from: Bhosale, S. M.; Gawade, R. L.; Puranik, V. G.; Kusurkar, R. S. *Tetrahedron Lett.* **2012**, *53*, 2894. Solvent: DMSO-d_6

Compound **58**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
204.6	-15.4016	-12.0582	-4.8944
80.3	101.8630	112.5566	112.3742
78.0	110.7895	112.7523	113.3652
70.2	116.0099	115.0533	123.1434
65.7	118.3702	124.7869	125.3873
59.7	123.4572	131.1933	135.1085
54.7	133.8393	132.7448	135.7169
51.5	134.6229	135.1745	141.1556
43.0	141.5871	140.5286	145.2230
42.8	145.7870	141.1880	149.0780
40.1	148.5410	149.3731	152.6049
34.9	149.8138	151.1645	154.5387
26.3	165.5616	159.3821	167.4196
20.2	168.0573	165.1044	169.8460
13.9	172.2342	169.9452	177.1634

[a] NMR data from: Mizuno, H.; Domon, K.; Masuya, K.; Tanino, K.; Kuwajima, I. *J. Org. Chem.* **1999**, *64*, 2648. Solvent: $CDCl_3$

Compound **59**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
159.9	39.3186	31.3579	42.5590
157.9	41.8477	39.5606	46.8588
155.5	48.1407	39.6525	47.4675
153.6	48.6113	41.1814	47.7635
131.9	67.5631	66.4914	70.5578
126.8	71.3810	71.2261	74.7869
125.2	71.8655	72.8006	75.6974
124.6	72.0224	72.8799	75.9304
123.5	72.7744	74.6178	77.1870
121.9	72.7780	75.0560	77.6321
121.8	72.8622	75.1315	77.7469
117.5	80.8500	78.3660	84.5107
112.6	81.1552	84.4916	87.2699
111.7	85.0329	86.1646	90.6085
105.9	87.5654	89.3019	91.2580

[a] NMR data from: Barone, G.; Gomez-Paloma, L.; Duca, D.; Silvestri, A.; Riccio, R.; Bifulco, G. *Chem. Eur. J.* **2002**, *8*, 3233. Solvent: $CDCl_3$

Compound **60**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
135.8	62.6801	58.6686	67.1485
134.7	63.9469	60.4773	67.9437
127.0	70.4127	69.4894	73.8019
120.6	76.2177	77.9952	79.7907
118.7	77.2720	78.9577	81.9897
117.6	79.0484	81.3377	82.1621
110.6	86.5914	85.3581	90.8510
107.1	88.0548	87.5687	92.0139
61.7	133.6244	130.6283	136.0759
60.1	136.0446	134.9974	139.1931
52.8	142.0418	139.8165	144.0756
41.6	151.5150	151.1634	153.7825
41.3	152.0552	151.8209	154.4570
36.3	155.4906	153.6192	156.0415
32.5	160.3905	156.7826	162.0634
30.1	162.9555	159.3954	164.7232
26.2	166.2221	163.2078	168.0343
25.8	166.6330	163.6753	168.3844
21.4	169.7993	167.5559	171.0325

[a] NMR data from: Barone, G.; Gomez-Paloma, L.; Duca, D.; Silvestri, A.; Riccio, R.; Bifulco, G. *Chem. Eur. J.* **2002**, *8*, 3233. Solvent: $CDCl_3$

Compound **61**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
166.8	32.2152	31.7703	38.4361
150.1	47.5267	43.4133	49.1820
112.3	78.3362	85.8228	88.1822
91.7	103.3654	99.5266	103.0730
88.1	103.5381	105.5525	106.0387
69.0	124.0292	124.2946	126.1943
51.4	145.4961	138.7514	143.6899
35.1	154.4450	155.0324	158.9579
32.2	160.0569	161.5283	163.6166
22.0	166.7795	168.2470	169.7945
18.7	172.4884	169.4123	176.3416

[a] NMR data from: Chang, M. Y.; Chang C. P.; Yin, W. K.; Chang, N. C. *J. Org. Chem.* **1997**, *62*, 641. Solvent: $CDCl_3$

Compound **62**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
145.6	49.7820	54.8350	56.0817
109.8	84.4785	85.2061	88.8446
57.8	136.4040	134.4739	138.1184
49.9	142.0311	135.4564	144.4354
48.1	145.4484	145.1012	147.1529
47.5	147.0531	145.5856	147.9279
45.8	147.7922	149.5143	148.3795
36.3	154.2877	154.1939	156.1640
33.3	160.8352	155.2413	162.2715
33.0	161.1199	155.5935	162.4129
26.0	165.5393	161.9075	167.6135
24.2	167.9926	163.2898	169.5798
23.5	168.2562	164.4110	171.9827
17.7	173.8710	171.3662	176.1110
14.6	178.6428	175.4129	178.6622

[a] NMR data from: Zhang, L.; Koreeda, M. *Org. Lett.* **2002**, *4*, 3755. Solvent: $CDCl_3$

Compound **63**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
141.9	59.1008	53.2067	59.9641
140.8	59.4241	54.0688	60.6235
140.4	59.4501	54.6041	60.9634
140.1	59.6919	54.9912	60.9683
137.3	60.6108	58.0435	65.0357
137.1	61.2667	58.6380	65.6591
128.9	66.4149	66.9439	70.3426
128.5	66.6264	67.7920	71.1014
128.4	67.6949	68.9821	71.7244
127.6	68.1643	69.3085	71.7398
126.9	69.5269	70.8001	73.6857
124.1	71.2256	71.1000	75.2350
123.5	72.4956	73.3309	75.5940
122.6	72.5885	73.8819	76.2989
120.6	74.6751	76.4850	79.5928
118.7	78.0107	77.9345	83.0975
114.0	78.8863	80.0717	83.7542
110.3	87.9856	87.8226	91.6353

[a] NMR data from: Shoker, T. A.; Ghattass, K. I.; Fettinger, J. C.; Kurth, M. J.; Haddadin, M. J. *Org. Lett.* **2012**, *14*, 3704. Solvent: $CDCl_3$

Compound **64**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
190.5	13.0597	13.4303	15.2870
174.7	27.1234	25.5732	33.3799
167.4	40.1792	34.6111	37.0349
144.4	57.9971	55.0812	60.3037
139.7	63.2344	62.8319	65.4174
138.8	64.6221	64.7656	66.1832
138.7	64.9822	66.6096	68.7136
134.1	66.4096	68.2908	70.4594
126.9	68.0123	70.0851	72.2300
126.7	72.7620	72.1480	74.0003
126.7	73.6899	74.3490	75.2800
122.8	76.3826	75.1079	78.5690
122.1	77.4952	75.1338	79.9041
122.0	78.2050	77.5477	81.0962
120.0	78.8308	77.7455	81.4653
118.7	79.3030	79.8407	82.6408
116.3	81.9152	82.0993	83.8281
113.2	82.1105	84.7445	87.4692
97.0	99.6668	100.4518	102.5180
34.8	156.9678	159.5489	162.6720

[a] NMR data from: Kjer, J.; Wray, V.; Edrada-Ebel, R. A.; Ebel, R., Pretsch, A.; Lin, W.; Proksch, P. *J. Nat. Prod.* **2009**, *72*, 2053. Solvent: CD_3OD

Compound **65**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
161.5	38.7140	35.3704	41.0353
153.8	41.7059	35.8182	44.4219
152.9	47.6801	43.6204	49.2897
148.4	51.5009	49.1813	54.3382
135.1	62.4771	63.6185	66.0221
116.4	79.1875	84.0863	83.5843
110.9	82.7099	87.0053	89.3783
107.9	87.9995	87.0379	91.3009
103.3	95.0360	88.2502	91.6958
102.4	95.0420	93.1518	98.9222
75.0	117.5151	118.3631	120.8989
61.7	133.6605	130.3804	135.5737
58.3	134.8832	131.2247	137.4703
54.3	140.8842	136.6165	144.6978
41.8	152.2194	145.4529	154.9087
35.1	152.8991	151.8781	158.8924
31.4	158.2947	155.0915	161.7335
29.6	164.2085	159.4185	165.3591

[a] NMR data from: Schwartz, B. D.; Banwell, M. G.; Cade, I. A. *Tetrahedron Lett.* **2011**, *52*, 4526. Solvent: $CDCl_3$

Compound **66**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
172.0	25.5543	24.8941	33.7336
105.4	86.1258	87.9065	88.0149
93.7	100.4046	97.9951	101.8380
79.5	114.6295	121.3797	114.3265
50.0	141.8049	142.1072	146.7439
45.0	146.6528	147.3343	149.3598
37.5	153.9159	154.7635	157.4610
35.9	156.6845	155.9457	160.0505
33.6	157.9084	157.1365	161.3238
32.9	158.8765	160.5971	161.7834
25.2	166.3511	163.8678	168.5308
24.8	167.1562	165.2583	171.2881
23.4	167.4918	166.0659	171.3570
19.8	172.5445	167.3933	174.3865
12.5	177.6281	174.2093	181.2422

[a] NMR data from: Yadav, J. S.; Thirupathaiah, B.; Srihari, P. *Tetrahedron* **2010**, *66*, 2005. Solvent: $CDCl_3$

Compound **67**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
194.6	-2.1320	8.8526	9.7717
160.7	40.6602	38.6116	46.8083
159.0	47.8439	41.3759	51.8167
150.8	49.3304	47.2103	54.6667
146.2	49.3426	49.1454	54.8247
143.9	52.8908	50.0045	55.1622
143.5	53.9023	50.6653	55.6878
138.8	65.1856	61.1912	62.7045
133.9	65.8868	64.5726	67.7009
133.1	66.1535	67.2057	70.9834
130.0	69.4105	71.0808	73.7288
125.3	73.5404	75.4565	78.6428
124.6	77.3473	77.4053	80.1954
122.2	80.9425	77.8053	82.0530
117.6	82.8059	78.6183	82.1730
100.4	85.7852	88.9250	96.2520
41.9	148.6876	149.9349	154.1989
35.7	158.4411	157.0567	159.8502

[a] NMR data from: Bontemps, N.; Bry, D.; López-Legentil, S.; Simon-Levert, A.; Banaigs, B. *J. Nat. Prod.* **2010**, *73*, 1044. Solvent: CD_3OD

Compound **68**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
170.2	28.5376	28.6961	39.4151
163.9	33.1784	34.4550	41.1499
160.6	40.4602	35.6717	46.8394
157.9	44.6247	43.4733	47.5998
148.0	52.3690	50.6373	56.9345
136.2	64.3724	64.4204	67.7090
133.3	66.2222	64.6923	68.1397
131.1	67.7414	66.1055	70.9085
128.8	68.1913	67.8003	71.5421
128.7	68.2089	70.6325	74.0850
128.1	70.6742	71.5972	74.4415
125.9	71.2740	71.8702	74.7704
122.6	73.4965	74.2283	78.3723
120.2	79.4812	79.7440	83.0568
116.2	80.8877	83.3455	86.3972
51.4	144.9173	141.2481	145.7891
15.4	175.5710	172.6249	178.6690

[a] NMR data from: Rahbaek, L.; Breinholt, J.; Frisvad, J. C.; Christophersen, C. *J. Org. Chem.* **1999**, *64*, 1689. Solvent: CD_3OD

Compound **69**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
144.6	55.5239	55.5336	57.7336
143.8	56.2412	55.5702	60.7971
137.4	57.9760	60.5853	62.2091
132.7	59.4739	63.9434	62.9508
127.0	69.1834	68.5284	73.2792
124.1	73.5916	74.4986	78.2734
65.4	125.0009	123.0715	128.9806
58.0	131.5503	125.7542	132.7068
50.0	143.8976	138.2018	144.7753
47.2	144.1943	140.4192	145.0264
45.4	145.0340	148.7321	146.2760
42.9	152.2730	151.2690	151.8551
36.5	154.1773	151.6330	155.3049
36.0	154.9948	151.8213	158.8812
32.8	157.8301	153.8386	160.1638
31.0	158.8442	154.9171	161.9549
28.3	160.4044	156.4532	161.9810
27.7	162.2009	159.3112	164.5386
26.0	167.2109	163.5102	169.6372
18.0	169.6300	167.0154	173.2447
17.8	173.7354	167.9203	176.7903

[a] NMR data from: Zhang, Q.; Di, Y. T.; Li, C. S.; Fang, X.; Tan, C. J.; Zhang, Z.; Zhang, Y.; He, H. P.; Li, S. L.; Hao, X. J. *Org. Lett.* **2009**, *11*, 2357. Solvent: $CDCl_3$

Compound **70**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
170.5	28.3605	29.4648	36.1763
150.0	50.0211	48.3319	51.8828
139.8	54.0514	59.7654	58.9092
136.2	57.8406	60.2732	63.7820
129.8	63.1857	62.0804	67.4494
121.1	72.8930	74.7836	77.7948
110.1	78.3885	88.5027	88.3239
97.8	103.1738	104.3001	99.2280
79.4	119.9029	120.7599	116.2227
54.4	139.6877	140.8495	138.9716
50.9	142.2389	142.0882	143.3552
48.6	142.9357	142.8360	144.4936
48.5	144.1996	146.4433	148.2760
45.2	144.2971	146.5800	150.9746
36.5	155.5476	153.4070	156.0021
27.7	158.2149	155.2721	165.6976
27.7	160.7689	158.7556	165.9899
27.2	161.6453	159.2194	166.1500
27.1	162.2903	161.3861	167.6579
26.7	163.8535	161.4895	167.7390
24.5	167.6635	164.0440	169.8102
23.5	168.2996	164.7827	171.4037
22.5	169.7189	165.9647	171.4430
15.1	170.3927	172.9030	178.3268
13.7	178.9883	175.0277	180.0052

[a] NMR data from: Acebey, L.; Sauvain, M.; Beck, S.; Moulis, C.; Gimenez, A.; Jullian, V. *Org. Lett.* **2007**, *9*, 4693. Solvent: $CDCl_3$

Compound **71**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
178.7	12.5069	17.0732	26.1102
140.0	56.0112	55.1128	62.0935
138.5	58.4023	60.2631	62.2567
131.9	64.5539	64.8068	67.1477
128.3	67.1071	68.8428	72.4832
127.9	70.0968	71.1044	74.0961
121.9	76.8682	77.7253	80.0014
112.2	82.3880	83.4794	88.5483
108.9	90.1600	89.4736	93.6086
72.1	119.9288	115.6253	124.4358

69.4	121.3044	123.5628	125.1350
66.2	131.2217	124.1002	133.0459
61.5	132.3373	130.0026	134.4477
54.1	137.1294	139.8757	139.0079
54.0	140.3885	140.7855	140.4022
50.6	141.0253	141.0101	141.8876
40.7	155.0271	152.5264	156.4432
38.2	156.5944	153.2663	160.2567
35.6	159.3026	160.5785	160.3583
22.8	168.1785	167.0262	172.0028

[a] NMR data from: Ng, F. W.; Lin, H.; Danishefsky, S. J. *J. Am. Chem. Soc.* **2002**, *124*, 9812. Solvent: $CDCl_3$

Compound **72**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
207.7	-11.9801	-10.0785	-5.4564
207.4	-11.2603	-8.4375	-5.1081
90.6	106.6811	108.6450	103.8221
80.7	116.5427	115.9121	114.2590
43.7	144.2061	151.6948	149.2714
38.6	152.1085	152.8579	154.4360
36.5	152.1667	154.5059	156.9332
36.4	154.9307	157.9751	156.9352
35.4	158.0672	160.0859	160.2948
27.2	160.2480	160.9214	163.3360
26.6	162.0830	161.7475	165.4788
25.7	165.8855	163.4857	168.5866
24.7	168.3876	163.5962	170.0841
23.0	169.2966	164.5153	170.6146

[a] NMR data from: Li, H.; Huang, H.; Shao, C.; Huang, H.; Jiang, J.; Zhu, X.; Liu, Y.; Liu, L.; Lu, Y.; Li, M.; Lin, Y.; She, Z. *J. Nat. Prod.* **2011**, *74*, 1230. Solvent: $CDCl_3$

Compound **73**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
198.6	-7.5884	-5.0302	2.8818
143.8	52.8712	54.2595	57.5087
140.9	54.9678	56.1824	60.7154
140.4	56.0169	58.1008	61.3127
140.4	57.1194	59.0863	62.9450
126.2	71.7218	71.9760	75.3760
126.1	72.3671	72.5922	75.5049
126.1	72.4861	72.6170	75.5210
125.9	72.5339	72.7468	75.7237
124.5	72.5541	73.1535	75.8766
124.5	73.5733	73.4997	76.6648
123.9	73.6326	74.2731	76.9988
122.8	74.7800	75.4204	78.7506
99.0	92.9844	94.2898	97.8423
76.7	116.5280	116.1566	116.5716
69.4	124.4459	120.6457	124.2492
49.7	143.1893	141.4060	144.2355
46.6	145.0992	144.0833	148.0278
45.1	146.4940	147.4217	148.5173
43.2	146.9090	147.4342	148.5701

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **74**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
171.0	27.4614	26.0730	33.0386
169.8	28.7704	27.5704	34.5141
144.5	58.0176	50.3529	62.3508
140.4	59.6702	55.8438	63.3554
135.4	62.6776	61.1871	67.0598
133.4	65.2375	61.3183	69.6777
126.1	70.1276	65.8001	73.6302
125.7	70.2996	70.6945	74.2618
123.8	71.1588	71.0469	75.0061
122.7	74.5420	74.4688	77.0568
121.4	74.8985	75.9514	77.8134
120.0	75.7572	76.3815	79.3589
113.0	79.6344	78.2488	83.1941
111.6	85.2140	88.0875	91.7664
109.5	88.3696	88.0925	92.6752

[a] NMR data from: Berlinck, R. G. S.; Britton, R.; Piers, E.; Lim, L.; Roberge, M.; Moreira da Rocha, R.; Andersen, R. J. *J. Org. Chem.* **1998**, *63*, 9850. Solvent: DMSO-d_6

Compound **75**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
175.9	17.9238	21.3737	30.0139
145.8	52.7175	49.5556	55.0339
143.0	54.3568	54.6462	59.9353
139.0	59.1670	57.3273	61.4160
133.7	61.8847	62.8179	64.6134
128.0	69.8196	70.7315	72.3922
127.7	72.7336	72.0814	73.4966
124.6	75.6003	72.5744	75.8076
116.6	76.9637	73.1012	76.6536
123.5	77.1728	78.6370	81.3260
105.1	92.9449	88.6089	92.4289
100.9	94.7805	92.0781	95.7561
41.2	152.2141	150.2468	154.0227
34.2	157.3504	154.7378	159.5723
29.0	164.7987	162.5597	165.9389
23.5	168.1756	166.5380	168.8494
14.7	176.7297	175.7530	178.2734

[a] NMR data from: Zhang, Z. W; Li, W. D. Z. *Org. Lett.* **2010**, *12*, 1649. Solvent: $CDCl_3$

Compound **76**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
202.4	-6.5943	-4.5562	-2.4541
161.1	41.0995	40.5415	46.4273
144.9	53.6790	50.1960	55.5959
142.3	54.4500	52.7400	57.9439
132.8	67.3324	66.2391	67.8570
124.2	72.3972	75.2332	77.8159
119.9	73.0977	76.3816	79.3397
108.7	86.6277	88.2884	92.3072
101.3	89.0501	88.6113	93.1406
99.3	94.9546	91.2803	97.0918
75.9	120.6642	120.1115	118.4483
56.4	141.9150	135.8884	139.6583
48.7	147.4523	144.6961	147.2060

35.0	156.1469	153.6054	158.3402
33.8	161.6233	156.7701	160.8990
23.6	167.3464	165.7837	169.6209
21.4	168.1779	169.1323	170.8365

[a] NMR data from: Zhang, Z. W; Li, W. D. Z. *Org. Lett.* **2010**, *12*, 1649. Solvent: $CDCl_3$

Compound **77**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
136.2	60.0087	64.7069	65.9264
122.1	70.1021	71.2085	75.6454
103.3	86.7795	92.0025	92.0457
76.7	114.3753	118.4587	118.9798
73.1	120.2931	121.5328	122.7085
71.3	121.2640	121.6339	124.4780
64.3	128.5295	128.3331	130.8019
49.0	140.8538	144.0924	145.8706
47.8	147.2372	147.3348	149.4916
43.1	147.4140	148.2604	153.2296
36.9	151.2982	158.1160	157.0471
27.8	166.0310	162.3255	166.4772
23.4	167.4481	165.6634	170.3663
22.6	169.2935	165.6871	171.3661
13.3	177.5475	174.0486	180.6177

[a] NMR data from: Kikuchi, H.; Miyagawa, Y.; Sahashi, Y.; Inatomi, S.; Haganuma, A.; Nakahata, N.; Oshima, Y. *Tetrahedron Lett.* **2004**, *45*, 6225. Solvent: $CDCl_3$

Compound **78**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
211.1	-18.2939	-14.8766	-8.7394
106.5	80.6374	85.7683	87.9166
85.1	106.0289	110.5594	109.6782
76.9	114.8396	118.1845	121.0249
73.2	120.0298	118.5208	122.1784
60.1	130.5014	135.7692	134.9667
54.9	135.0431	139.6666	139.9924
52.3	136.4702	141.4474	143.5124
43.7	148.5987	148.4277	153.5898
38.0	151.7578	152.4001	154.6895
34.3	157.4345	155.1773	159.2339
30.7	161.3630	157.6836	162.6022
14.5	176.4821	172.5616	179.9872
13.7	178.1432	173.6129	180.4483
8.3	181.2531	178.0920	183.8257

[a] NMR data from: Cook, S. P.; Polara, A.; Danishefsky, S. J. *J. Am. Chem. Soc.* **2006**, *128*, 16440. Solvent: $CDCl_3$

Compound **79**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
154.4	41.7493	46.0235	47.2413
136.8	56.8598	56.6442	62.4073
136.3	59.4142	60.6780	62.6624
133.1	63.0233	63.8537	68.3671
121.0	73.8805	76.1231	79.3386
112.0	79.7431	81.8446	84.1092
110.2	83.4949	82.6298	88.5230
99.4	90.4346	97.2024	96.9494
92.8	102.2616	102.5846	101.5377
76.8	116.4035	119.8607	117.7609
50.3	144.4895	140.6157	145.9422
43.1	148.4032	147.4963	150.5687
35.4	155.3222	154.7896	160.1454
34.4	156.9538	159.4548	160.1798
34.4	157.3947	159.8928	160.4252
26.6	163.7129	165.7066	166.6740
24.4	168.0938	165.8598	169.1395
21.6	170.2049	166.5095	172.1290
21.5	170.6151	166.8392	173.3815
20.0	171.6080	170.4256	175.5771
15.0	178.4256	174.8911	180.2634

[a] NMR data from: Winkler, J. D.; Quinn, K. J.; MacKinnon, C. H.; Hiscock, S. D.; McLaughlin, E. C. *Org. Lett.* **2003**, *5*, 1805. Solvent: $CDCl_3$

Compound **80**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
204.9	-9.0724	-6.6520	-1.3723
169.6	26.0782	25.2957	33.6996
88.2	106.1254	103.1752	108.5382
85.3	110.5094	111.8105	112.9673
70.3	129.6492	124.0005	125.3684
50.6	139.3826	144.0498	143.1477
42.8	146.0247	150.6190	150.0715
38.5	156.5207	154.2040	157.3798
30.7	159.7277	159.0473	165.6145
25.4	164.6090	163.1066	167.4617
24.8	164.6337	164.8662	168.8907
24.5	166.4960	166.0623	169.4425
23.7	168.3806	166.9591	170.3080
21.9	168.5764	167.0391	170.9635
21.4	168.7274	167.9436	172.1466
21.3	169.4736	168.4775	172.3607

[a] NMR data from: Peng, F.; Danishefsky, S. J. *Tetrahedron Lett.* **2011**, *52*, 2104. Solvent: $CDCl_3$

Compound **81**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
210.5	-14.6980	-16.4581	-10.0273
139.0	44.8370	49.8064	50.1730
129.3	71.1830	76.5698	77.3926
66.8	127.4803	125.2219	129.8901
59.5	132.5299	127.2709	133.4829
55.7	139.1322	135.0544	140.2130
48.6	144.5553	136.2184	147.9418
41.1	149.7585	149.0729	150.2406
39.8	153.6608	152.1108	155.6834
32.5	156.3156	152.9228	160.7063
27.7	163.1368	153.9264	165.3297
26.3	163.7665	163.3595	166.8041
25.5	168.5928	164.8964	167.8048
23.6	168.9866	165.8059	170.3784
18.3	171.8135	167.2175	175.1516
16.9	173.7675	168.4198	176.6459

[a] NMR data from: Xu, C.; Wang, L.; Hao, X.; Wang, D. Z. *J. Org. Chem.* **2012**, *77*, 6307. Solvent: $CDCl_3$

Compound **82**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
222.7	-31.0806	-23.9632	-18.8442
152.3	40.3348	43.8821	46.9552
116.6	77.3800	77.2864	82.1441
71.8	123.8885	121.5135	122.1667
53.4	140.4147	131.7403	141.8829
53.3	141.3000	135.4803	143.7389
48.9	141.9591	144.7377	144.2564
47.0	148.5068	147.1385	148.3701
46.2	149.0051	148.3566	148.3950
44.4	149.3935	151.4243	150.8529
33.3	153.2663	152.6330	161.0177
25.1	167.1962	160.9449	168.2619
24.8	168.1306	161.2113	171.2696
23.4	168.6743	166.1349	172.4511

[a] NMR data from: Weyermann, P.; Keese, R. *Tetrahedron* **2011**, *67*, 3874. Solvent: $CDCl_3$

Compound **83**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
169.3	35.2403	23.9446	36.2599
142.2	55.9054	51.0183	59.0859
140.6	63.7515	56.0193	59.5131
132.8	66.5149	62.8839	69.6929
128.5	67.5297	70.2963	72.9644
127.2	68.5045	70.3806	73.7229
124.2	74.6267	75.1762	78.3545
122.2	75.5335	78.0336	79.9318
116.2	84.3999	79.2604	83.9909
77.6	116.1527	114.1204	117.4465
64.6	130.1548	124.8157	130.8344
60.2	134.4713	126.6228	134.5675
60.1	135.6613	129.3579	135.4076
52.9	140.9292	133.6880	140.9488
51.9	142.7370	135.3555	143.0358
50.3	143.8579	140.5276	145.8069
48.2	145.0365	140.8104	147.8867
42.7	147.0108	143.5443	151.3398
42.5	148.2037	147.9915	152.5888
31.6	159.8790	159.6437	161.4299
26.9	163.2396	161.1912	167.2754

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **84**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
136.2	63.0710	58.4873	67.4481
135.0	63.5420	59.9216	67.7199
127.3	71.7609	70.4830	74.8591
122.3	75.1805	76.7893	78.6855
120.1	76.7457	78.3300	80.6829
119.9	77.0156	79.0214	81.4181
111.2	80.5921	79.6587	85.5159
108.8	88.0989	87.2008	91.4759
71.0	121.3088	125.8437	124.9446
60.6	133.5923	131.5605	135.1271
57.3	135.6569	133.5687	138.8861
45.6	149.2899	148.2866	152.2016
44.5	150.0894	148.6819	152.2785
40.7	153.6906	148.9399	155.8759
37.8	163.1561	162.1685	165.8367
29.6	163.6328	165.1184	165.9042
27.0	169.7031	165.3812	171.9419
22.3	170.0413	169.2344	171.9955

[a] NMR data from: Jiricek, J.; Blechert, S. *J. Am. Chem. Soc.* **2004**, *126*, 3534. Solvent: $CDCl_3$

Compound **85**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
198.6	0.6632	-2.2775	4.2598
173.0	24.8466	22.3465	31.2046
145.5	51.0369	51.5772	57.3229
131.7	61.4815	62.9598	67.5967
107.0	80.7792	85.7318	87.9031
77.4	117.3345	117.4841	121.2922
71.9	123.2855	123.7406	124.7549
66.6	128.8769	126.9360	130.5569
54.5	135.3770	141.3421	140.2375
46.0	141.3770	142.6898	143.6241
30.1	161.6188	162.9042	166.7072
27.6	164.4607	164.1227	166.9403
21.0	170.2597	167.6489	174.3906
15.2	173.8654	170.9062	176.5492
15.0	175.6544	172.8128	179.1229

[a] NMR data from: Bagno, A.; Rastrelli, F.; Saielli, G. *Chem. Eur. J.* **2006**, *12*, 5514. Solvent: DMSO-d_6

Compound **86**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
165.0	32.8701	31.6258	39.0394
152.6	48.6042	43.9952	48.7770
147.3	48.6220	47.9275	52.6438
146.4	52.7863	49.2238	54.9457
146.1	52.8181	49.3857	55.1097
138.2	53.0470	57.7897	63.3386
134.7	62.6263	65.0971	66.0699
131.0	66.1350	68.7156	69.3929
124.3	68.8563	71.1376	74.2391
117.0	79.2733	81.7253	83.5643
116.1	79.5168	82.0079	84.7655
110.4	88.7257	87.0513	91.0174
110.3	88.9718	87.1918	91.1588
101.0	95.1775	88.6481	92.2948
62.4	134.2821	130.4050	133.3755
60.3	138.6617	132.2588	134.5493
56.6	141.9544	134.7401	139.5998
42.7	149.1531	146.3607	150.3179
41.0	150.4640	149.7646	153.2823
36.0	155.1789	153.0469	157.3751

[a] NMR data from: Mirabal-Gallardo, Y.; Piérola, J.; Shankaraiah, N.; Santos, L. S. *Tetrahedron Lett.* **2012**, *53*, 3672. Solvent: $CDCl_3$

Compound **87**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
148.4	49.4879	50.0491	53.9125
146.4	53.2432	50.5612	55.6602
131.4	64.2675	60.9217	64.5773
130.9	66.0760	61.9743	65.5388
126.7	66.8359	65.6110	66.6941
126.1	68.6453	68.0923	71.4516
126.1	71.4411	71.4694	74.8632
123.9	74.5358	72.5940	78.4141
121.1	78.3700	75.1823	78.6232
119.1	79.9259	75.7959	81.8718
117.3	81.8876	76.8696	81.9736
115.7	82.6941	77.4488	83.7951
115.3	83.7645	81.8133	86.1833
113.0	85.9644	82.3758	87.9491
110.8	86.6849	86.3437	89.9484
108.0	87.6685	86.9431	90.4803
104.0	89.3720	89.0119	96.0587

[a] NMR data from: Delfourne, E.; Roubin, C.; Bastide, J. *J. Org. Chem.* **2000**, *65*, 5476. Solvent: $CDCl_3$

Compound **88**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
216.3	-26.7606	-15.0957	-9.8821
59.1	129.6443	135.6477	137.7122
45.1	148.7227	147.2654	148.8960
43.2	149.3322	149.3102	150.8031
42.9	150.1695	149.3158	151.9389
42.4	151.9473	149.7105	153.3375
39.1	152.1908	151.4490	153.7094
39.0	153.7992	153.2302	155.0398
36.7	154.8952	156.4839	157.0554
35.1	156.8612	156.7699	159.5442
33.0	159.6666	157.2158	161.8699
28.3	164.0201	163.9674	165.5414
16.3	172.2945	170.2753	178.3823
13.8	177.1519	170.9269	180.1442

[a] NMR data from: Harmata, M.; Rashatasakhon, P. *Org. Lett.* **2001**, *3*, 2533. Solvent: $CDCl_3$

Compound **89**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
194.3	2.7919	0.9167	5.6118
191.3	5.5905	3.1298	9.8870
159.7	43.4582	39.1592	41.6093
149.3	50.2263	47.6315	52.7725
139.2	55.6136	54.0991	62.4709
134.0	61.8900	60.2220	68.7353
130.5	67.8941	67.9568	72.1330
127.1	68.1029	70.3147	74.6166
125.7	71.4132	71.3008	75.0574
124.9	71.5341	72.9744	75.1135
122.5	74.6520	74.5726	79.5250
119.9	78.1456	75.7720	80.3636
119.5	78.9583	76.9210	82.3698
109.0	84.0350	86.1454	90.9247
103.6	88.9020	87.3543	91.0966
84.6	110.8587	109.4733	110.6187
53.5	128.7027	137.9107	138.2663
53.2	128.8536	138.2431	138.6396
52.4	132.3903	138.6699	139.1708
51.7	134.3477	139.2193	139.4563

[a] NMR data from: Miyashita, K.; Sakai, T.; Imanishi, T. *Org. Lett.* **2003**, *5*, 2683. Solvent: $CDCl_3$

Compound **90**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
150.3	47.2882	49.7108	52.7985
136.7	56.6836	62.3053	62.4433
119.5	74.9137	73.9683	79.3735
109.2	85.5413	87.2341	90.7536
79.6	115.1550	115.3785	116.3473
53.0	142.1685	141.6845	142.5598
47.8	147.0667	144.8038	149.2459
43.2	149.8036	150.7852	153.0045
38.8	149.8990	153.7298	153.9502
38.6	150.4538	154.5877	154.7763
37.7	153.1108	157.1041	157.4355
35.0	156.5758	158.7256	158.5226
34.2	158.8064	158.7466	160.7520
28.3	165.6078	160.8606	167.3502
27.4	165.7852	164.1603	168.6385
25.1	166.0638	164.3217	169.2186
23.4	168.1905	164.5192	169.5609
22.2	170.8955	165.8821	172.4241
21.8	171.2390	166.3394	173.2219
15.6	174.9448	169.7587	178.0708

[a] NMR data from: Yajima, A.; Toda, K.; Okada, K.; Yamane, H.; Yamamoto, M.; Hasegawa, M.; Katsuta, R.; Nukada, T. *Tetrahedron Lett.* **2011**, *52*, 3212. Solvent: $CDCl_3$

Compound **91**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
171.1	27.7591	27.5535	34.7204
150.0	46.0367	45.5881	50.5389
149.6	47.7907	47.2310	51.3409
148.1	49.6475	51.1800	55.2312
122.4	70.7309	74.1205	75.0975
119.8	77.2419	74.9552	82.1688
106.6	82.3273	88.3730	91.2627
62.0	130.7746	128.0238	132.7869
40.1	149.6123	154.6695	152.9511
26.4	159.5284	162.5325	166.0594
22.5	164.1490	163.9156	169.3734
22.1	168.5940	166.4438	171.5156
21.4	168.9636	167.8964	171.8188
17.0	170.0109	171.8101	176.2277
8.6	183.5002	180.1752	183.7967

[a] NMR data from: Yue, G.; Yang, L.; Yuan, C.; Jiang, X.; Liu, B. *Org. Lett.* **2011**, *13*, 5406. Solvent: $CDCl_3$

Compound **92**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
195.3	5.7486	7.0685	10.4790
168.2	31.6856	29.3038	34.6988
146.8	49.7638	49.3515	54.3855
142.7	56.0444	55.9024	58.9327
128.1	70.8466	71.7223	74.2913
126.9	71.4677	72.5652	75.3389
123.5	75.2256	75.6554	78.3618
121.8	75.9881	77.0263	80.0310
113.9	78.3451	82.5917	85.0490
98.6	94.5206	92.4527	96.1757
91.8	106.1271	100.1816	103.0912
51.7	138.6788	134.3916	140.2468
50.7	146.0391	142.8657	147.6578
46.8	149.8088	146.6141	147.9339
41.3	154.5690	150.6532	156.0337
32.9	154.9900	156.2477	161.3791
29.8	162.5317	163.3949	164.2785
28.0	168.9926	163.5096	170.5553

[a] NMR data from: Cahskan, R., Ali, M. F.; Sahin, E.; Watson, W. H.; Balci, M. *J. Org. Chem.* **2007**, *72*, 3353. Solvent: $CDCl_3$

Compound **93**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
134.8	57.8639	61.4128	63.8056
133.0	65.2240	66.3527	69.2353
102.5	83.6993	84.9880	89.1375
90.0	102.4391	103.6381	104.3728
76.1	116.9105	116.4044	118.4618
66.4	123.1306	127.1211	124.4199
64.8	127.3054	127.1939	132.0094
52.8	138.8331	141.4555	141.3347
49.1	143.3895	147.8955	145.1522
43.2	149.1466	148.5401	153.0788
41.0	150.3841	149.9258	153.8184
35.4	156.1147	153.7191	160.0496
29.7	164.2601	161.9010	167.5733
21.6	166.0857	162.4945	169.2502
15.7	171.2500	167.6608	174.6850

[a] NMR data from: Dai, M.; Krauss, I. J.; Danishefsky, S. J. *J. Org. Chem.* **2008**, *73*, 9576. Solvent: $CDCl_3$

Compound **94**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
167.5	30.5993	31.4369	37.7250
154.6	47.8536	39.1413	44.4204
136.0	59.2716	59.3516	67.4224
134.5	63.0749	60.5826	67.8049
127.3	68.6812	69.8575	73.8451
121.4	77.3365	77.9092	79.7551
119.4	78.1748	79.1161	82.0412
118.0	82.2115	81.4490	82.3143
110.8	83.3815	86.1956	91.3970
107.9	87.9810	87.3304	91.6986
106.8	92.4566	92.7806	94.3016
73.8	124.1112	119.5175	120.8879
60.1	135.8221	135.0110	139.2766
56.9	138.0854	135.3404	140.2825
53.2	142.2345	139.1259	143.9629
50.9	146.4677	139.6816	143.9865
41.0	152.6603	153.0141	154.1562
33.0	160.3192	159.4518	160.5971
30.7	161.2218	162.7306	163.2403
21.9	169.5257	167.2943	170.9027
15.0	174.3971	171.7150	179.2044

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **95**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
209.9	-7.3077	-15.4452	-3.3919
158.0	44.8102	43.1636	47.7636
153.4	47.4164	44.0652	49.2355
138.5	52.0369	48.8421	54.1095
131.0	66.9396	65.9881	70.8685
117.0	80.3125	85.7252	87.0047
113.3	82.6647	86.0771	90.3357
111.9	88.5592	90.5207	93.5879
103.5	96.9333	91.6165	98.6969
79.2	118.6161	114.5099	115.9031
79.0	118.6706	117.5807	118.7503
77.7	122.0817	122.2931	120.0387
54.8	136.4422	137.6221	144.6756
50.4	138.9820	140.2398	146.3448
45.2	150.9155	151.4743	151.1354
40.9	151.5837	152.3116	152.8778
40.4	152.0971	153.2252	153.8785
37.6	155.1122	155.1543	159.2139
32.3	161.9069	159.2481	163.3957
22.5	170.3996	164.9295	173.7405

[a] NMR data from: Corey, E. J.; Wu, L. I. *J. Am. Chem. Soc.* **1993**, *115*, 9327. Solvent: acetone-d_6

Compound **96**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
203.4	-15.8972	-6.5719	-1.7822
173.8	19.9121	23.9872	30.7784
89.7	97.9826	105.2449	106.4617
87.8	106.7218	108.8323	108.5891
66.9	120.9841	128.1360	129.9455
62.6	127.2200	133.2289	130.8002
58.4	128.6140	133.6072	132.7493
57.1	132.9713	134.1275	132.8157
55.1	133.4203	139.0849	138.8615
51.7	136.1028	139.4554	142.0212
51.1	136.2368	140.9924	142.9353
50.8	138.5213	141.1709	143.7643
44.3	150.8980	147.8927	153.2216
24.3	166.1739	163.2763	170.6018
22.8	166.8778	166.1361	172.0781

[a] NMR data from: Bagno, A.; Rastrelli, F.; Saielli, G. *Chem. Eur. J.* **2006**, *12*, 5514. Solvent: C_5D_5N

Compound **97**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
206.8	-7.6393	-6.1104	-0.4847
140.2	54.7873	57.2840	61.2529
138.7	55.7859	59.2662	63.0143
129.9	58.1653	59.9753	66.1681
127.3	61.6519	68.0865	71.4500
84.3	103.2123	110.5644	110.0739
80.5	114.6824	112.1485	114.6669
75.3	116.0175	118.4818	120.0046
72.5	124.0537	123.5271	124.6851
67.0	126.0617	125.4920	126.3419
44.1	149.5237	146.1346	149.5266
39.8	152.8606	148.9468	152.6483
31.0	154.0468	158.1187	163.6436
28.6	158.8868	161.0232	167.3132
24.0	160.9699	167.7382	167.6812
23.2	165.5184	169.5646	170.5586
23.1	167.1259	169.8169	170.8620
17.4	174.9670	170.9941	177.7964
15.6	175.7671	172.9442	178.6293
15.5	177.0720	173.3871	178.7408

[a] NMR data from: Tanino, K.; Onuki, K.; Asano, K.; Miyashita, M.; Nakamura, T.; Takahashi, Y.; Kuwajima, I. *J. Am. Chem. Soc.* **2003**, *125*, 1498. Solvent: $CDCl_3$

Compound **98**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
207.9	-7.9679	-9.1362	-1.1036
179.6	32.4603	27.4158	33.4218
170.5	35.7407	32.6385	36.7293
147.8	55.9794	49.9411	54.9919
146.7	57.3507	54.8462	56.5603
130.3	64.5619	65.6281	70.6144
113.8	78.7530	84.8442	85.7126
111.4	78.8746	88.4381	88.4025
80.6	113.6082	110.1134	120.0363
76.0	116.8398	114.7208	123.6322
69.9	130.5715	127.4633	127.6331
65.0	132.3567	127.4794	133.8804
56.2	139.2637	134.5251	138.6210
54.8	140.8319	135.9530	143.2071
52.9	143.0519	145.5326	144.0629
41.3	156.1542	153.0205	156.1246
34.0	159.0246	156.5938	163.2228
30.2	162.3122	157.5836	166.2216
29.0	163.0119	160.7768	167.8732
26.1	166.2266	162.2945	169.1816
26.0	169.3874	167.9245	172.0283

[a] NMR data from: Bagno, A.; Rastrelli, F.; Saielli, G. *Chem. Eur. J.* **2006**, *12*, 5514. Solvent: CD_3OD

Compound **99**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
185.2	11.2029	14.0348	17.6301
176.4	18.5666	18.9244	26.2289
170.4	26.3288	26.0730	33.3210
146.8	53.6769	44.2300	53.7631
145.2	58.3592	48.1335	56.4907
134.3	62.3806	61.1419	66.0028
120.9	72.6649	72.3439	77.9606
75.8	122.4220	119.1278	119.8242
75.0	125.6455	122.6512	121.3334
54.9	140.4271	138.2569	140.8163
49.5	140.7670	146.0115	144.8691
44.1	146.3923	146.8825	149.6280
34.5	158.2515	157.3541	160.5922
29.5	159.9333	158.3202	164.0766
21.2	172.5593	169.4252	175.0356
18.7	172.5870	170.1552	175.3821
18.6	172.6865	170.9581	176.3025
15.7	173.2022	171.0079	177.1253
14.6	177.3097	171.4063	179.8860
9.8	180.6805	176.3474	183.7652
8.8	182.2864	177.9423	184.7719

[a] NMR data from: Sarotti, A. M.; Pellegrinet, S. C. *J. Org. Chem.* **2009**, *74*, 7254. Solvent: $CDCl_3$

Compound **100**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
167.7	27.0714	25.7278	34.6507
162.0	34.6450	36.8458	42.0094
156.5	44.7441	39.2417	44.0666
155.8	47.5440	39.3307	48.5121
151.3	48.2712	46.2021	50.0831
150.5	50.0601	47.0017	50.5708
143.4	57.7470	51.1930	57.0091
138.8	59.4701	58.2954	63.8682
130.5	68.6553	68.2631	71.4790
123.6	72.2152	72.9398	75.5891
121.5	76.1105	77.1294	80.2792
116.2	80.0438	80.7124	81.5053
113.3	83.2617	82.5833	84.4010
113.0	83.8542	83.9408	88.2033
105.6	85.7182	87.1473	89.8783
105.2	88.5134	88.5248	92.3290
104.8	89.0989	92.6429	93.5833
92.5	104.9341	101.0815	106.0523
78.0	122.0528	121.6683	117.6784
60.1	139.6405	127.2489	134.0332
45.8	149.8119	146.2086	149.5584
37.8	153.4167	156.8514	155.7833
36.6	156.2617	157.9202	156.2907
32.2	159.1136	160.3759	159.8543
28.3	163.1951	161.2415	167.1313
24.1	167.8693	161.9631	171.9552
24.0	168.0110	161.9667	172.8433

[a] NMR data from: Nakashima, K.; Oyama, M.; Ito, T.; Akao, Y.; Witono, J. R.; Darnaedi, D.; Tanaka, T.; Murata, J.; Iinuma, M. *Tetrahedron* **2012**, *68*, 2421. Solvent: $CDCl_3$

Compound **101**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
188.6	1.7290	2.7741	8.3253
148.1	47.1853	52.3386	53.7939
126.5	69.8684	71.3582	73.7452
101.4	95.0042	95.3249	97.5324

71.5	114.9283	113.6893	114.7059
66.3	130.5174	128.9941	130.9038

[a] NMR data from compound **1**

Compound **102**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
177.4	44.1261	36.9208	46.5856
156.4	45.9179	40.1176	46.6024
155.9	59.0393	54.7131	59.5700
133.7	66.0395	66.4955	70.6353
125.6	67.3289	69.7172	73.4434
125.2	72.2548	75.3796	78.1257
124.8	81.2726	78.8091	82.0902
118.2	83.3092	79.4376	82.1408
112.9	85.1379	83.0156	84.7360

[a] NMR data from compound **2**

Compound **103**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
160.6	22.9049	24.4630	28.1272
154.0	43.4857	41.2613	46.3397
143.5	45.3968	42.9782	47.2041
131.8	66.0020	66.0628	69.6272
128.0	69.1187	69.2136	72.3851
124.4	71.6898	72.9709	75.1200
118.8	72.3461	73.3076	76.8815
116.7	77.7938	78.9526	85.0049
116.6	81.5013	81.4443	85.3765

[a] NMR data from compound **3**

Compound **104**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
177.4	15.5377	16.5786	17.9544
156.4	34.0658	29.9063	36.1226
155.9	47.5682	43.4511	47.7518
133.7	63.5161	63.1147	66.0367
125.6	70.4767	71.3333	74.4379
125.2	73.2262	73.0326	78.0421
124.8	74.5879	76.2109	78.9323
118.2	86.7259	85.6796	90.0019
112.9	97.8487	94.0913	102.5714

[a] NMR data from compound **2**

Compound **105**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
139.8	55.7977	55.0648	59.9114
134.3	59.0715	59.9701	63.9952
56.6	138.4244	134.9209	138.5716
52.9	138.7566	140.5845	142.6104
52.7	150.9034	148.1001	150.7994
31.9	151.3928	149.3231	152.2406
24.8	151.6832	156.5834	152.7697
19.9	166.8812	161.9403	168.2504
19.7	167.7440	163.2240	169.8994
13.4	177.2878	174.7419	180.2670

[a] NMR data from compound **5**

Compound **106**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
136.0	53.3137	50.6749	54.5207
132.2	59.8864	57.2170	61.3922
132.1	61.6257	61.1707	65.4151
131.9	62.0611	61.8628	66.1090
55.1	152.1987	149.8204	151.0147
50.5	152.7959	150.8796	151.3941
46.4	153.7143	151.2406	152.7602
45.5	155.9043	154.6063	155.5998
41.5	157.8017	155.5343	161.6863
34.9	167.5901	165.1032	168.6301

[a] NMR data from compound **6**

Compound **107**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
154.4	40.8281	35.4436	42.2436
141.7	53.4285	58.5988	58.3477
133.2	60.1244	62.6699	63.6726
130.0	65.1462	66.4132	67.3887
128.2	68.9682	68.8091	72.9403
127.9	69.1202	72.3578	73.2107
126.6	69.1648	72.8406	75.1426
125.3	73.3336	74.6717	77.0348
116.5	79.7618	81.9394	84.6243
107.5	88.3226	86.8445	90.9798
31.1	122.0861	112.9564	116.6741
27.5	166.0275	161.5286	165.5527
19.6	170.9664	166.3786	171.8325
14.1	176.0658	171.9168	177.0743
11.4	177.1208	173.1163	178.1727

[a] NMR data from compound **7**

Compound **108**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
154.4	38.8495	37.7075	42.1933
141.7	43.1587	37.9901	45.0102
133.2	60.7227	64.0361	65.3388
130.0	61.7212	66.9268	67.1541
128.2	65.9127	69.4678	71.9752
127.9	66.9995	70.0740	72.2031
126.6	68.9986	71.9119	72.4146
125.3	69.2099	72.2147	74.4167
116.5	88.5859	86.8283	91.6246
107.5	97.9821	99.0938	104.4632
31.1	152.6708	150.1738	150.8908
27.5	166.7252	163.2880	167.2268
19.6	171.2688	166.6395	172.2012
14.1	175.2682	171.3361	176.4186
11.4	177.1532	173.1572	178.1591

[a] NMR data from compound **7**

Compound **109**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
200.2	-11.4052	-8.9555	-5.0877
135.5	59.7869	60.8400	64.7143

134.1	61.3277	60.8551	65.8131
99.3	87.7585	90.3431	91.9702
74.8	116.8096	116.6118	116.3135
70.2	126.8336	125.8457	126.7475
49.4	141.3189	136.4017	144.5586
46.9	145.3388	143.6407	145.2022
46.9	146.8257	145.2697	145.8779
46.3	148.2009	146.4984	148.6571
42.3	148.3551	149.0100	150.0202

[a] NMR data from compound **10**

Compound **110**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
201.1	-12.4381	-9.8302	-6.3639
139.4	55.5136	56.8531	60.9574
136.3	57.5687	57.1214	62.0933
99.1	86.5115	88.3258	90.3156
76.8	116.3055	116.3196	116.6382
69.9	127.0854	126.3627	127.2274
48.2	145.3712	142.5073	143.7898
46.7	146.3087	143.5628	145.8693
44.9	147.6189	145.6492	147.5484
44.5	147.8177	145.7388	149.8366
41.9	148.5055	149.8908	151.2762

[a] NMR data from compound **11**

Compound **111**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
157.2	38.5225	38.0614	43.7738
156.3	40.7247	39.2213	43.9713
144.0	51.9139	51.9722	57.8530
135.0	66.2957	62.7001	64.6383
130.1	69.9804	70.4855	73.7602
127.3	76.2059	75.6472	78.4540
122.2	80.0037	77.8469	81.8110
121.8	80.6356	78.5452	82.4975
105.3	88.8178	91.5347	95.4142
55.4	143.2172	136.0797	141.7751
25.0	171.2982	167.3464	171.9199

[a] NMR data from compound **20**

Compound **112**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
205.8	-3.4030	-3.6754	2.2705
141.3	36.7918	48.9881	52.5407
138.9	46.5850	49.7554	54.1662
132.1	48.4680	58.1068	60.4782
129.6	66.4848	72.0304	72.8112
128.5	70.7356	72.7589	73.2614
126.6	72.0087	79.0580	78.6676
40.9	140.8351	135.3167	140.1722
32.6	155.5069	151.1133	155.5446
25.3	156.9297	157.7436	159.4959
21.0	170.4591	168.8155	169.1168

[a] NMR data from compound **21**

Compound **113**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
76.3	122.2102	122.0956	125.4026
62.4	132.3620	130.1203	134.4503
48.8	154.2384	154.8371	156.5379
48.0	157.2097	156.0733	156.9091
40.2	157.2863	156.0868	158.2116
39.6	157.6519	156.2671	158.2443
38.5	158.3778	157.8345	158.9082
37.7	161.5943	157.9444	159.0745
36.3	162.9419	158.2624	162.1733
35.0	169.3198	167.0602	171.7735
30.2	173.3856	170.8667	175.7525

[a] NMR data from compound **22**

Compound **114**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
175.2	25.7406	24.7124	34.5064
82.5	130.2937	125.9926	127.7839
49.1	145.2243	142.0135	144.5401
47.9	148.2273	144.1381	146.1376
46.6	148.9670	147.5264	153.2624
42.9	152.6889	151.7074	153.6473
42.6	153.9791	151.7429	153.6727
36.9	155.0939	152.2461	155.8071
34.9	155.1008	153.5137	155.8448
34.4	155.5742	155.5646	157.4394
28.9	163.0954	156.1612	158.9709

[a] NMR data from compound **23**

Compound **115**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
161.2	30.2823	27.8670	39.2335
156.1	38.9161	32.9842	45.7263
145.1	44.0512	41.7732	46.3695
144.2	52.9245	50.7578	57.0749
139.2	55.1828	53.0015	58.7570
134.0	68.4516	64.3808	67.0596
122.8	70.8001	74.6549	77.2085
121.6	78.2999	81.3086	84.2003
120.0	89.1299	87.6368	91.3826
104.2	90.6208	91.4794	95.8936
66.6	140.1731	133.7211	136.9651
60.7	143.0607	136.0050	141.3706
55.9	162.4553	161.7594	164.3584

[a] NMR data from compound **31**

Compound **116**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
183.3	14.6821	17.4386	21.7991
180.0	18.4615	22.9579	25.9431
173.5	29.7628	27.4693	34.8498
158.4	43.4966	36.7253	43.9752
141.8	44.3539	40.9109	46.2450
132.9	73.9660	76.3907	80.9468
107.5	86.7176	89.2049	94.0287

72.2	117.9165	115.1485	114.4794
68.6	121.9051	116.5433	115.6420
61.0	141.7304	135.3211	140.6777
56.4	166.3684	165.3930	170.0589
36.7	168.0382	166.9058	170.3827

[a] NMR data from compound **32**

Compound **117**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
183.3	13.0570	14.7445	19.3414
180.0	16.4942	20.0685	24.2760
173.5	21.2373	23.6042	32.3236
158.4	44.3448	40.8040	46.6397
141.8	47.4917	43.9784	49.1069
132.9	80.4732	80.3654	87.0784
107.5	86.0577	88.9141	94.5340
72.2	130.7126	125.8444	128.2455
68.6	132.6515	127.4232	129.9541
61.0	141.6451	135.6420	140.9007
56.4	156.6986	159.1349	162.5138
36.7	162.5835	162.2609	163.2733

[a] NMR data from compound **32**

Compound **118**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
183.3	20.9645	19.3237	23.4565
180.0	21.5785	19.4656	25.4129
173.5	23.0141	23.1018	32.1901
158.4	33.8613	32.8928	38.3830
141.8	60.6180	62.1073	64.9073
132.9	60.8619	62.4823	65.8274
107.5	90.1768	92.2091	98.1845
72.2	114.9623	119.1897	123.0991
68.6	127.7356	125.5821	127.1954
61.0	131.6846	130.8959	133.0412
56.4	142.5274	135.1072	140.0354
36.7	156.4748	156.0426	158.1285

[a] NMR data from compound **32**

Compound **119**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
183.3	11.3782	12.7434	17.1307
180.0	14.1436	16.5175	20.2028
173.5	22.1250	23.1680	30.9586
158.4	42.4421	39.6515	45.2041
141.8	57.4767	60.8055	61.8445
132.9	58.7626	61.8564	65.8369
107.5	86.5133	89.4323	94.6971
72.2	93.9159	93.8065	98.4112
68.6	133.4450	131.8486	132.5734
61.0	142.4860	135.5797	140.8366
56.4	156.2492	158.1743	159.1180
36.7	160.0795	158.5126	160.3702

[a] NMR data from compound **32**

Compound **120**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
49.1	138.4958	137.0286	140.2507
41.3	140.7396	141.7647	145.4658
40.9	145.6099	145.2462	146.8069
32.1	145.7845	145.5646	147.0781
31.3	147.1131	152.1961	152.6104
29.4	152.0941	153.2661	152.8446
28.4	154.6094	154.0418	153.1265
25.0	158.3806	154.5312	158.5427
22.1	159.0178	156.2432	160.5164
21.6	162.4267	161.2194	165.4476
20.0	164.6995	163.3191	167.0503
18.9	168.1201	165.3505	170.9652
17.4	171.5002	166.5518	173.3294
16.6	174.0989	169.3234	176.1565
15.9	177.5369	174.5603	179.8024

[a] NMR data from compound **33**

Compound **121**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
157.0	42.5515	41.7793	49.7010
150.3	52.8156	54.4432	58.3972
143.5	59.7462	58.7630	61.4476
138.0	61.0437	60.0587	61.8088
126.5	72.9821	72.8238	75.6864
123.3	73.6992	73.5389	75.7714
123.1	74.0981	74.4212	76.5062
119.8	74.4432	75.1236	77.2891
56.6	134.7673	131.3708	132.6688
45.3	137.4769	136.6115	137.6327
43.9	147.3488	152.6857	150.7956
42.7	148.9614	153.6722	151.7499
38.5	151.5409	155.8462	153.2954
36.6	160.7720	157.5506	163.7877
28.9	165.1099	159.0075	163.9504
28.7	165.7384	159.8583	167.7725
25.4	167.0213	162.3190	168.4328
25.0	169.3144	162.6933	171.5076
15.1	179.8198	176.6187	181.9484

[a] NMR data from compound **35**

Compound **122**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
157.0	49.7115	47.5640	50.0837
150.3	56.7870	53.9501	58.9287
143.5	62.5703	59.6687	62.2897
138.0	65.4379	62.4332	65.4330
126.5	73.2555	73.2063	75.3836
123.3	73.9617	73.3873	76.3563
123.1	74.1164	74.1952	76.4773
119.8	75.4646	75.4999	77.4947
56.6	143.1142	140.9663	140.6469
45.3	146.5192	151.0055	153.7118
43.9	154.0611	151.2197	156.1465
42.7	157.7112	159.3104	158.2195
38.5	161.7685	159.5492	165.8717

36.6	164.2124	159.9423	166.1422
28.9	164.5424	164.9475	167.4423
28.7	166.0766	170.8736	171.9716
25.4	167.3175	172.5575	172.8188
25.0	177.1729	175.0654	179.0711
15.1	180.0453	176.5876	182.0095

[a] NMR data from compound **35**

40.1	163.8803	161.2581	165.9854
31.8	164.3112	163.8214	166.8008
31.5	165.3757	164.5722	168.2482
30.8	166.5702	166.5559	168.2669
29.0	167.2014	173.3935	174.8927
26.0	171.9487	176.9990	179.6726

[a] NMR data from compound **36**

Compound **123**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
159.0	36.8067	41.3978	45.3029
105.0	88.5977	89.9175	95.0807
69.1	139.1206	137.5358	142.2417
53.3	143.2401	140.6782	146.9006
52.3	151.8649	149.7705	150.6466
47.9	156.1032	155.5433	157.5481
46.0	158.5903	155.8099	159.7782
42.3	159.1729	156.2152	162.0274
41.7	160.6140	157.2645	162.8955
40.1	160.7346	162.1418	162.9823
31.8	161.4121	162.7301	164.6344
31.5	165.0389	162.9374	166.9159
30.8	167.7636	165.3697	169.5486
29.0	168.5425	166.4337	172.2586
26.0	174.7644	172.7364	176.4249

[a] NMR data from compound **36**

Compound **124**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
159.0	47.6532	49.3683	52.1497
105.0	84.1573	82.4927	91.5109
69.1	136.2143	126.5290	142.8087
53.3	148.6638	143.5195	148.1508
52.3	149.6167	144.4421	152.3594
47.9	151.1960	151.8338	153.1666
46.0	152.2704	152.2584	154.9632
42.3	153.0774	156.6515	155.3314
41.7	157.5833	157.6446	157.0049
40.1	160.9531	157.6765	163.1486
31.8	161.9687	159.7401	163.1511
31.5	164.2178	162.8146	167.9682
30.8	165.8495	163.6047	168.2392
29.0	169.5875	167.6640	168.9338
26.0	171.3168	170.4643	172.9055

[a] NMR data from compound **36**

Compound **125**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
159.0	48.2937	55.0333	54.0018
105.0	85.1841	84.6703	90.0177
69.1	142.7045	140.0613	142.4436
53.3	154.7553	151.3612	154.8617
52.3	156.6082	157.7983	161.9679
47.9	157.4654	158.2326	162.0724
46.0	159.7564	159.6776	164.0630
42.3	162.5116	160.3224	164.7831
41.7	162.7667	160.4898	165.7349

Compound **126**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
159.0	45.6696	52.0416	52.7167
105.0	84.1921	83.9854	89.3913
69.1	131.9056	136.6824	135.3828
53.3	141.0986	139.5598	142.6497
52.3	146.1426	139.7431	149.2747
47.9	146.6883	150.4247	149.7203
46.0	150.7956	152.7711	150.6932
42.3	156.4884	154.3169	158.3331
41.7	158.0825	156.4706	159.9245
40.1	158.2989	158.4089	159.9746
31.8	162.7738	158.4891	164.5636
31.5	162.9328	159.9119	165.2830
30.8	166.6253	160.4652	168.7250
29.0	169.2924	163.2048	172.0703
26.0	171.4583	164.9063	174.5721

[a] NMR data from compound **36**

Compound **127**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
198.3	-8.2433	-8.0038	-3.8839
177.0	41.3749	39.3417	43.4777
159.9	43.7166	45.7641	47.4478
105.1	74.2500	72.6755	78.8299
98.8	97.9084	91.9195	96.2275
95.3	109.0194	107.2488	109.7568
87.6	110.2961	109.0431	112.7038
56.9	137.1327	137.6841	139.3854
53.8	140.3741	140.2755	143.3859
44.8	152.4515	150.9061	154.1399
42.8	153.6970	152.8895	155.9369
35.4	155.6718	153.6485	157.4013
31.7	155.8304	155.2683	158.3892
31.4	161.9758	157.1768	164.9647
24.4	163.1211	158.3056	165.2601

[a] NMR data from compound **37**

Compound **128**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
198.3	1.8532	2.8071	8.9262
177.0	2.6119	4.5275	9.7408
159.9	35.4844	41.7416	42.7708
105.1	80.5115	84.4834	90.3284
98.8	84.7147	86.0090	91.0435
95.3	89.5364	90.3034	93.7919
87.6	92.0440	93.0590	97.8322
56.9	129.2000	127.9470	130.2884
53.8	131.4302	131.8029	133.3578

44.8	136.1211	132.9418	140.0602
42.8	150.2652	154.1315	152.3777
35.4	154.9903	154.2503	156.4514
31.7	160.2820	154.3301	161.9840
31.4	160.5203	156.3904	164.8134
24.4	165.6763	160.0468	167.9440

[a] NMR data from compound **37**

Compound **129**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
198.3	-6.8011	-1.6164	4.1204
177.0	24.4431	19.2996	27.7181
159.9	63.5907	65.4919	69.2090
105.1	69.0757	69.8294	73.5145
98.8	96.7727	89.9714	93.9791
95.3	99.0173	99.2690	103.1624
87.6	108.8889	107.5349	108.3260
56.9	136.5724	138.8193	139.5344
53.8	149.6416	145.7191	153.8515
44.8	152.3945	150.8317	155.0590
42.8	153.7537	152.1790	157.7639
35.4	154.1539	155.3912	158.0044
31.7	155.7508	158.9106	158.1063
31.4	164.4706	160.7427	166.8632
24.4	166.7869	162.4893	170.3219

[a] NMR data from compound **37**

Compound **130**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
217.7	-9.5812	-16.0810	-10.0098
212.3	-8.0012	-14.3699	-8.3820
59.3	147.3301	146.6849	149.7786
45.7	147.4187	147.4816	150.5695
44.9	148.4015	149.8889	151.0110
42.9	152.3881	152.1858	156.0601
35.7	162.5304	161.2845	165.6599
18.2	167.5430	166.4026	171.3589
12.1	167.5875	167.5768	173.7697

[a] NMR data from compound **38**

Compound **131**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
217.7	-17.1282	-15.4894	-9.0764
212.3	-15.0870	-14.2372	-7.6344
59.3	141.6911	143.7219	146.2553
45.7	146.5860	144.2322	149.6901
44.9	153.1263	149.3482	155.3636
42.9	154.5276	151.7979	158.2502
35.7	159.1517	156.5610	161.7795
18.2	169.7323	166.3347	173.1832
12.1	173.5989	169.4625	174.2065

[a] NMR data from compound **38**

Compound **132**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
187.6	1.7751	3.1285	6.6136
179.2	37.8605	35.4762	44.6282
171.6	46.4615	42.3117	48.5951
155.8	47.1669	45.5848	50.7740
134.8	50.2069	50.2870	53.2959
134.1	56.1914	59.2182	61.0716
133.9	66.6208	64.3402	68.6795
133.7	68.1024	66.2908	70.7547
133.0	69.3234	68.6935	72.6665
127.1	71.2273	69.0713	73.4626
126.7	73.4345	74.0828	77.2408
126.5	73.4460	74.8107	77.4304
123.7	73.9610	77.5911	77.5560
121.3	76.7162	79.0590	81.9174
118.6	80.2744	80.6144	83.4198
111.4	82.3465	83.3075	85.9376

[a] NMR data from compound **39**

Compound **133**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
187.6	6.9420	9.3681	11.5736
179.2	40.4669	36.2259	39.0724
171.6	42.4767	37.2368	43.5804
155.8	43.3358	42.5234	51.4571
134.8	55.2096	58.0899	60.2474
134.1	64.6280	63.4077	67.8685
133.9	65.4525	63.9895	68.8410
133.7	65.8261	65.4503	69.4308
133.0	68.7376	66.7743	69.4697
127.1	70.5451	70.8404	74.3182
126.7	72.2701	72.7161	76.7519
126.5	73.3118	73.1333	77.2564
123.7	73.9403	75.2531	78.1426
121.3	78.2109	77.5119	83.0658
118.6	80.1416	81.4269	83.7146
111.4	81.4811	82.9898	84.0513

[a] NMR data from compound **39**

Compound **134**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
187.6	-10.3059	1.3040	3.4505
179.2	37.7118	34.7758	44.2271
171.6	47.5375	42.8840	47.1685
155.8	49.7655	44.0418	49.7937
134.8	58.1076	50.1582	53.4534
134.1	59.5955	57.4532	61.4406
133.9	61.7712	62.8269	62.9211
133.7	65.8146	64.8050	68.3393
133.0	67.0515	65.5130	69.6090
127.1	67.9959	66.1590	70.7105
126.7	71.8664	74.3982	74.7801
126.5	72.8200	75.1997	74.9543
123.7	74.3860	75.9438	76.9764
121.3	76.3912	76.7703	79.5904
118.6	79.6110	79.5461	81.6206
111.4	81.5642	82.7873	84.7562

[a] NMR data from compound **39**

Compound **135**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
187.6	2.4284	3.4889	7.3585
179.2	22.6264	24.1414	27.1575
171.6	39.7906	37.4424	42.4518
155.8	44.2743	41.8678	46.7132
134.8	46.5689	46.3223	50.6100
134.1	50.8180	50.6122	54.1500
133.9	64.7871	63.9742	67.9767
133.7	67.7490	64.7055	68.2853
133.0	69.1627	68.0165	71.4372
127.1	70.3005	71.5358	75.4329
126.7	72.4601	71.9090	76.2441
126.5	72.7333	73.3757	77.0125
123.7	73.8132	75.3785	77.7387
121.3	74.3240	75.5472	77.8705
118.6	81.7063	78.7827	85.0794
111.4	87.3793	83.9637	89.9935

[a] NMR data from compound **39**

Compound **136**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
156.0	66.6764	68.6273	71.0290
102.8	67.2238	68.9370	72.1506
56.1	138.7157	137.4344	139.7707
56.1	138.8700	137.6617	140.8233
49.2	149.1330	142.2872	149.9779
44.2	149.1677	145.3474	151.2698
44.2	149.8244	147.8335	153.5595
42.0	153.1136	149.9694	154.0774
41.3	153.9960	153.4487	155.0262
40.4	155.7851	153.9950	160.0179
39.9	156.6118	157.7041	160.4348
39.3	158.7221	160.2163	160.7161
33.7	160.3428	163.3739	161.9484
33.3	161.3381	163.8017	162.9308
33.3	166.1055	164.8021	168.2192
21.7	170.9719	166.5887	172.8362
20.3	171.7819	168.5338	174.4663
18.7	172.0781	169.4406	174.9815
18.1	172.9890	170.5344	175.7701
14.4	174.0168	171.6593	175.8204

[a] NMR data from compound **41**

Compound **137**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
215.3	-12.4919	-11.3309	-5.9526
56.5	139.2341	138.8527	141.7019
54.9	139.8673	138.9575	141.7276
54.6	145.2285	147.4195	148.2301
47.0	148.4554	147.7532	151.7254
38.3	150.0631	150.2057	152.5260
37.5	151.7922	150.9766	154.3267
36.9	153.1524	151.6261	155.1822
35.0	153.3334	153.5666	156.9045
31.9	154.3701	154.7461	157.2267
31.7	155.2123	157.1733	158.1350
28.8	156.8666	157.1901	158.9543
28.8	160.3692	159.6703	162.2839
26.6	162.6408	160.8442	165.4355
24.8	165.7300	163.5366	167.3341
21.9	169.3355	167.7677	171.7841
19.5	170.9012	168.8683	171.9501
17.7	175.2685	169.4344	177.5198
11.9	179.8474	175.6463	182.0397

[a] NMR data from compound **42**

Compound **138**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
211.0	-15.9478	-15.4584	-10.6128
54.3	137.8947	136.9745	139.1896
54.1	137.9233	139.7488	140.2383
46.7	139.9635	140.3045	141.5614
44.6	147.3722	146.8046	149.5293
40.8	151.3740	152.0529	156.0529
40.3	155.6669	155.4190	157.2802
38.8	156.0276	157.2784	158.3193
38.7	156.8821	157.2850	159.6070
38.1	158.3772	157.6299	161.5051
35.7	160.5246	159.7040	162.5238
35.7	163.3172	160.2933	165.9101
32.1	163.6685	160.6257	166.0064
29.0	166.3433	163.2675	167.7975
25.5	166.5464	164.1367	168.0108
21.5	169.9458	167.5803	172.2810
20.5	171.9127	168.3900	172.9502
17.4	175.0796	169.8397	177.2454
11.4	180.1216	175.7157	182.1286

[a] NMR data from compound **43**

Compound **139**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
147.7	48.5905	54.7233	53.7071
140.0	58.7309	61.5814	62.6371
121.4	59.5550	64.4183	63.3985
108.6	82.0586	80.1392	86.1127
87.9	113.1680	115.4235	114.1951
81.2	114.4001	117.9494	114.6133
74.1	124.8186	122.6959	125.0525
54.7	139.0347	138.5066	142.9457
52.5	139.4406	145.4746	144.8437
50.5	151.6947	147.4973	154.4177
42.7	152.3397	150.3151	154.4281
40.7	152.8102	153.3672	154.8730
39.9	154.6234	154.1262	155.4432
36.7	158.3445	154.4316	159.0571
35.6	162.0853	158.5061	162.6915
31.8	162.6033	160.1459	164.3976
29.2	163.6710	160.2817	165.7627
25.8	164.7416	161.6873	165.8689
22.0	166.3135	163.5517	168.3280
22.0	167.8595	165.3468	169.8484
19.9	169.9829	168.6664	172.7080
9.2	182.8612	178.2777	184.7851

[a] NMR data from compound **44**

Compound **140**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
163.7	36.6125	36.8137	43.0452
151.3	47.4391	46.3712	52.0246
138.9	61.3466	61.1950	65.0525
116.6	75.1540	79.0115	83.1229
105.1	93.8230	91.5874	98.5209
54.1	143.3117	139.3566	143.8579
53.1	144.9344	145.2397	148.9519
49.8	154.3870	153.2092	156.8865
35.6	158.1523	157.2669	160.3359
27.8	160.1974	157.3423	161.4199
26.4	165.7526	162.9382	167.5225

[a] NMR data from compound **45**

Compound **141**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
163.7	38.1761	38.1860	44.2308
151.3	42.6413	38.5805	48.0603
138.9	60.4092	61.0726	64.4052
116.6	75.5977	77.2740	81.3456
105.1	99.3605	97.5174	103.9511
54.1	146.5057	137.4281	146.0343
53.1	148.4790	148.1099	151.2451
49.8	148.9148	149.3302	151.2888
35.6	154.4433	154.3487	151.5252
27.8	154.8158	159.1802	157.8455
26.4	163.3781	160.9305	164.4784

[a] NMR data from compound **45**

Compound **142**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
165.3	37.9240	37.2549	44.7083
143.1	40.0948	46.3181	48.6415
142.4	56.5484	54.7769	62.0635
140.2	58.7699	59.8945	63.2902
134.1	63.6605	68.9794	71.7467
124.2	66.2992	69.4842	71.7568
122.7	74.3461	76.5373	80.2148
117.0	79.0552	79.6252	84.3634
111.3	95.1229	93.0742	97.2253
54.3	136.3591	138.6669	139.0374
49.1	143.8184	139.0860	145.5237
35.2	144.6825	144.3920	148.4831
32.8	157.5205	154.6615	158.5872
22.6	174.0017	170.0761	175.5604
12.3	174.2517	170.8695	177.2315

[a] NMR data from compound **46**

Compound **143**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
165.3	37.9124	37.1911	44.6729
143.1	56.5550	54.6248	61.8088
142.4	57.6808	59.2773	62.7085
140.2	58.6747	63.0292	64.7416
134.1	66.2128	68.9786	70.9026
124.2	66.6069	69.7907	73.2275
122.7	72.9035	76.9393	76.8951
117.0	75.0381	77.6519	80.6498
111.3	76.4055	78.0415	82.2656
54.3	133.5957	136.4634	136.3672
49.1	151.7524	147.0208	151.4012
35.2	153.5946	153.3102	155.1492
32.8	159.1394	156.3151	159.7107
22.6	169.1853	161.9433	172.3258
12.3	170.0644	164.1198	174.4453

[a] NMR data from compound **46**

Compound **144**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
165.3	38.1505	37.4673	45.0311
143.1	47.8086	52.8553	52.6641
142.4	53.7222	53.0108	59.4198
140.2	55.7268	57.6894	61.3668
134.1	56.9953	62.1951	64.3759
124.2	64.2259	66.5324	73.3440
122.7	74.8569	77.0534	78.3298
117.0	75.4052	77.3197	81.1392
111.3	81.2044	82.6298	84.8635
54.3	134.4285	136.3445	136.1806
49.1	148.6216	145.4616	150.2186
35.2	156.5765	152.5805	157.6813
32.8	158.1729	155.5468	159.1031
22.6	166.3972	161.5357	167.6395
12.3	169.7179	166.0220	171.3439

[a] NMR data from compound **46**

Compound **145**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
155.0	47.1514	38.7177	43.9997
142.4	60.8287	52.3267	60.8004
140.6	64.0058	53.3359	65.5967
127.4	67.9552	68.4050	73.5268
122.6	73.4983	75.5737	78.0070
119.8	74.7309	75.7193	78.4916
119.2	77.3004	78.2237	80.4061
119.1	77.7710	78.3411	82.3596
118.4	80.6237	78.6699	84.1000
114.0	82.6077	84.5289	87.6375
113.5	82.6249	84.6999	90.5795
107.3	87.0465	85.3669	92.4120
76.1	87.1442	103.8274	102.0669
60.5	131.9590	135.3892	131.7870
48.7	140.5111	149.4376	151.3351
36.9	154.0690	151.1747	153.3879
36.2	156.5062	156.4381	162.4907
30.2	163.6862	157.5837	166.4003
29.3	168.8465	159.3164	166.9893
28.3	171.4417	162.0225	170.2101
23.0	172.7440	170.4342	174.5717
21.8	177.0025	173.1204	177.4363
15.3	177.7027	173.3433	177.7202

[a] NMR data from compound **47**

Compound **146**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
155.0	51.3284	50.2509	53.3705
142.4	58.4968	56.6696	62.9353
140.6	63.8136	60.6426	67.9974
127.4	72.5483	71.3268	75.0438
122.6	74.8497	75.7303	78.3212
119.8	77.3627	77.6248	80.6389
119.2	77.4490	78.5569	80.8169
119.1	78.1249	79.8007	82.5774
118.4	80.3353	80.9239	84.1768
114.0	81.1100	81.0764	85.6054
113.5	81.7148	86.5096	90.6232
107.3	86.1291	86.9106	91.6941
76.1	112.0434	111.4293	111.3562
60.5	137.4374	141.3587	139.1359
48.7	145.9759	142.2403	148.5214
36.9	149.5597	144.7387	150.3281
36.2	150.1865	146.1291	152.8428
30.2	150.2701	151.0746	153.5006
29.3	152.4504	154.0309	155.4900
28.3	163.2736	157.7430	165.3103
23.0	165.7393	160.3900	168.4088
21.8	167.7601	163.7818	170.6646
15.3	176.2830	171.2921	176.4286

[a] NMR data from compound **47**

Compound **147**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
155.0	46.8042	46.2893	50.7224
142.4	50.5188	46.5173	56.3675
140.6	52.2119	47.7932	57.1118
127.4	68.1571	66.1048	71.1048
122.6	75.2267	76.2554	78.9008
119.8	75.5246	76.4589	80.5800
119.2	75.8638	76.8935	80.9419
119.1	77.7752	77.9874	81.1758
118.4	78.0378	78.8051	81.8688
114.0	78.2486	79.0745	82.4914
113.5	79.5239	79.1108	85.9060
107.3	80.4455	82.6768	89.3881
76.1	111.6905	110.5406	109.4470
60.5	133.8868	139.2771	133.2815
48.7	146.4551	140.9851	148.3748
36.9	146.5740	143.6479	148.6981
36.2	151.4922	150.7555	153.4842
30.2	152.3636	151.8565	154.4877
29.3	153.4988	152.1939	155.9926
28.3	161.3783	154.0453	163.9601
23.0	161.9150	157.5767	166.4568
21.8	167.2889	163.6337	170.5847
15.3	176.2932	171.3137	176.9075

[a] NMR data from compound **47**

Compound **148**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
174.1	34.2546	31.8872	40.5209
158.4	36.0939	36.3941	40.8496
152.8	44.4348	40.7511	49.0597
151.5	52.5693	48.6911	53.9384
149.0	53.9780	48.8249	57.2643
146.5	58.5935	59.3077	64.2478
132.2	61.8279	64.9397	67.3991
131.2	64.3092	66.6819	70.6114
129.5	66.2934	68.0128	70.6153
129.4	67.1737	68.1588	70.8913
128.8	67.9015	68.4104	71.3913
128.8	68.7634	69.6705	73.2001
128.5	69.1379	70.3911	73.2991
119.6	75.1638	71.9587	74.5443
99.0	95.1650	92.4271	98.0099
73.3	119.1392	118.0544	119.3749
66.4	123.5777	124.1742	123.9603
50.7	144.3904	141.4574	143.4744
31.7	157.5545	154.9932	160.0382
7.8	183.7236	178.6283	185.4968

[a] NMR data from compound **48**

Compound **149**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
131.9	56.4417	55.3283	60.6599
131.6	65.1501	64.1749	68.8428
53.3	131.8356	131.0095	131.6787
52.9	137.3730	135.3640	138.0242
50.7	139.4819	142.3270	141.6194
43.3	151.8959	152.3424	155.2908
39.6	158.8823	156.4757	160.5445
37.6	163.7916	159.3942	164.4945
35.8	163.7990	160.1504	165.1627
31.1	164.5417	161.2431	165.4911
28.2	165.5695	163.1267	166.6796
25.5	166.3319	163.3992	168.5375
23.5	168.8478	166.3105	170.6559
21.8	169.5058	167.3250	171.4571
16.9	176.8850	171.5791	179.1332

[a] NMR data from compound **49**

Compound **150**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
200.9	-4.6812	2.8035	5.7667
177.4	31.4717	24.6332	29.3435
165.1	42.0960	38.9464	48.6913
161.4	49.3162	42.2311	50.9401
154.3	52.2631	47.1072	54.1307
152.1	53.0526	48.8133	54.7690
145.8	58.2862	55.7996	60.6354
116.4	72.3964	75.4906	79.0087
113.5	75.7055	76.0159	82.5609
107.2	79.7749	77.5168	82.8264
103.5	86.0881	84.3354	87.3045
102.5	89.0880	90.2295	94.7253

91.4	90.5428	92.8047	95.7822
57.2	142.9921	135.7641	139.7951
47.1	143.2212	140.6535	141.6877
34.8	159.7979	157.6976	161.4086
28.8	167.9960	165.7348	169.2222

[a] NMR data from compound **50**

Compound **151**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
201.5	-2.7240	-1.2161	3.9443
180.4	33.3047	38.4505	38.5544
118.1	66.8871	70.9851	76.0208
79.7	115.2688	117.4777	116.0171
54.8	137.4724	136.5293	140.8083
52.7	139.6585	139.2999	141.8538
52.5	140.0164	139.6959	144.2578
50.8	144.6563	142.4357	146.6477
47.8	145.3455	144.1718	147.6942
47.2	146.4507	145.9918	147.7808
46.2	154.6174	152.6282	157.2846
40.4	156.0095	155.2160	159.1223
32.5	156.3131	155.3612	159.2215
31.4	162.4495	156.7441	163.7707
29.8	164.2476	159.3911	165.6516
26.2	165.2770	162.0089	167.2772
26.0	165.3042	162.3793	168.2005
25.2	166.8010	163.5144	168.5088
24.3	168.9648	165.5180	170.9939
23.1	169.7693	167.7113	172.2337

[a] NMR data from compound **51**

Compound **152**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
201.5	0.9436	1.7150	6.8143
180.4	25.6065	28.9628	30.3027
118.1	71.7097	74.6400	78.2580
79.7	113.8907	115.8313	115.4623
54.8	128.9410	125.0996	129.9696
52.7	145.2362	141.7959	146.1135
52.5	145.4623	141.8678	148.0739
50.8	145.7553	143.7944	148.1206
47.8	145.9429	145.2913	148.2350
47.2	146.3312	147.9153	149.8390
46.2	154.3649	148.2551	155.4585
40.4	155.0815	150.8458	157.5649
32.5	156.5786	158.0880	159.2765
31.4	157.4424	158.5832	159.5356
29.8	158.7507	158.6714	161.7123
26.2	163.5118	159.2146	164.4585
26.0	163.7176	160.7329	165.0990
25.2	166.6312	165.2766	168.2691
24.3	167.5995	165.3736	169.3058
23.1	170.3477	165.4098	172.2077

[a] NMR data from compound **51**

Compound **153**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
201.5	3.6614	0.6429	4.7424
180.4	11.9735	22.1676	25.2632
118.1	80.6219	75.2363	80.2758
79.7	117.4755	117.3712	114.7946
54.8	138.3856	140.4783	143.0322
52.7	139.6962	140.9881	143.2128
52.5	139.7166	142.1929	144.1725
50.8	140.1775	142.5016	144.9969
47.8	145.8403	142.8257	145.8970
47.2	153.7708	152.1597	152.8051
46.2	157.0151	154.4508	157.2149
40.4	160.8916	158.2872	162.9120
32.5	163.6959	160.9590	166.6299
31.4	165.2506	162.8944	167.8793
29.8	166.0151	163.1782	168.2520
26.2	166.5515	163.8548	168.7210
26.0	166.8862	164.5443	168.8479
25.2	167.2681	164.9017	169.2143
24.3	169.0808	166.3452	172.3403
23.1	170.1795	167.5765	172.6711

[a] NMR data from compound **51**

Compound **154**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
152.4	44.9892	36.0391	45.3016
152.1	45.9454	39.8693	48.8508
137.9	58.5273	61.6124	65.6454
135.7	64.7769	64.3968	67.8708
129.6	68.0776	67.9604	71.5602
125.9	69.1838	69.5717	72.4173
125.3	69.4082	69.6294	72.5879
124.9	71.1559	71.8304	73.8619
123.9	73.3561	72.0501	75.8759
120.5	74.9419	76.7744	79.9675
120.2	75.5967	77.3279	80.3864
119.2	76.7462	77.3375	80.7741
117.0	77.8205	79.2394	81.1826
116.9	79.4368	80.1053	82.8819
116.4	84.3475	83.2214	87.6029
41.7	163.4649	158.1406	163.6486

[a] NMR data from compound **52**

Compound **155**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
158.8	37.0181	37.9267	46.0438
134.8	56.3014	60.3207	61.7396
128.9	67.4874	75.4798	74.5695
104.4	88.8354	89.4084	93.7597
71.8	129.8671	127.1958	128.4800
54.2	135.8605	133.9597	137.1596
53.6	143.6118	148.2249	148.3224
49.5	149.1035	149.4556	152.9564
42.1	154.5663	150.3180	155.8651
35.3	154.7076	153.0867	157.3182
32.3	159.8709	157.3885	160.0878

30.0	160.1345	160.6262	161.7689
24.5	169.2994	163.9517	174.5635
14.5	174.5209	169.9880	174.9929
11.2	174.8904	170.6446	175.9528

[a] NMR data from compound **53**

Compound **156**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
178.6	23.7427	16.3959	23.5676
170.4	39.9815	29.7793	36.2419
153.5	40.2793	41.1038	50.8754
124.9	53.2446	49.7816	54.5838
124.5	57.8203	67.3623	71.1846
124.1	68.3996	69.6738	78.4132
116.4	80.9496	76.5992	81.2743
92.4	84.4829	78.8233	83.9113
51.2	147.9820	138.5661	145.0233
37.7	158.1678	152.6873	155.5766
19.8	164.3820	163.4982	165.9702

[a] NMR data from compound **55**

Compound **157**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
172.0	34.8547	34.4608	38.1840
166.5	35.1789	37.5924	41.9624
147.8	49.0137	47.7019	49.9223
124.2	60.3646	60.1029	63.3215
110.3	85.2887	88.1530	90.1656
90.5	120.9771	115.9958	123.0647
68.8	123.2897	120.6421	123.6048
57.6	126.2958	122.8628	125.5095
49.1	144.6506	141.8511	147.6195
46.6	148.7077	145.6580	149.7760
27.7	163.1620	160.8058	163.9723
25.3	163.8023	163.6001	164.7643

[a] NMR data from compound **56**

Compound **158**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
180.8	13.1858	0.7759	15.8851
180.8	23.2492	15.2027	29.9775
151.2	39.4264	39.2373	44.5358
147.5	49.2875	50.3128	56.3387
138.4	55.4211	51.7841	60.6087
137.9	62.1363	58.9207	65.4264
132.5	62.9341	64.5050	66.3539
131.5	69.0580	64.9350	67.2743
131.4	69.1161	69.1131	72.6447
130.2	69.5057	69.5734	72.7445
129.8	69.5440	70.2622	72.9084
127.2	70.8475	70.4821	73.1598
124.8	71.6967	71.2080	74.0301
124.3	72.2545	73.4835	75.8971
123.3	72.6416	73.8706	76.7897
122.5	73.5421	73.9295	76.9561
122.3	76.2506	75.1847	82.0384
115.5	78.3499	80.0618	85.1882
113.9	87.3904	86.5056	90.1792

[a] NMR data from compound **57**

Compound **159**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
204.6	-15.4610	-12.7361	-6.0075
80.3	103.9206	102.7222	105.8953
78.0	105.1886	110.3413	112.1579
70.2	111.6059	111.5706	114.7449
65.7	112.5962	113.7972	117.3275
59.7	125.3458	123.5480	124.8407
54.7	126.6300	129.5327	131.4943
51.5	142.7200	140.5921	146.0003
43.0	142.8451	142.5867	147.9553
42.8	144.6976	143.2595	148.1453
40.1	145.9774	143.3906	148.6472
34.9	147.9023	149.9944	151.9418
26.3	165.5073	159.3995	168.6789
20.2	171.0591	165.6033	174.7721
13.9	171.9141	171.0091	177.8835

[a] NMR data from compound **58**

Compound **160**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
159.9	24.1804	25.8332	29.9641
157.9	35.6520	27.4024	37.1429
155.5	44.5430	43.3628	48.0490
153.6	54.2187	44.8790	52.2058
131.9	65.8206	66.0405	69.9011
126.8	68.7395	67.9408	71.8137
125.2	71.8021	72.2845	75.0016
124.6	71.8599	72.5147	75.3695
123.5	72.5517	72.8855	75.7014
121.9	72.5992	73.1384	76.0256
121.8	73.2274	74.1299	77.2315
117.5	73.3558	75.1271	77.4050
112.6	81.1713	78.3939	84.8415
111.7	88.3683	86.4957	91.1754
105.9	88.6333	91.8281	96.6999

[a] NMR data from compound **59**

Compound **161**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
159.9	29.2822	33.6765	36.8891
157.9	43.6710	39.7437	46.5635
155.5	48.9355	41.5146	47.9861
153.6	52.3659	46.7979	52.7978
131.9	57.5474	51.7215	60.3028
126.8	65.7267	66.1464	69.7729
125.2	68.7649	68.4854	71.6838
124.6	69.8143	69.7663	72.3752
123.5	71.6164	72.1496	73.6894
121.9	72.9782	73.5065	77.3534
121.8	73.5175	74.9698	77.9063

117.5	75.2083	76.1651	79.1963
112.6	76.7992	76.8960	80.9842
111.7	81.1129	77.9911	84.7827
105.9	85.6775	84.2103	88.7946

[a] NMR data from compound **59**

Compound **162**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
135.8	58.1424	48.2569	62.2471
134.7	67.8266	61.4474	71.2792
127.0	69.4269	67.6905	72.7547
120.6	77.1981	77.8880	81.5045
118.7	79.6102	80.3835	83.2009
117.6	81.8963	83.5533	84.9227
110.6	89.8001	87.4512	93.2796
107.1	104.9304	97.0591	108.6745
61.7	139.3864	135.0925	139.0547
60.1	143.2932	137.5677	142.2619
52.8	152.0923	149.8529	154.5823
41.6	153.0207	151.6730	155.3870
41.3	153.3297	152.3119	155.8840
36.3	160.2611	156.9356	162.1061
32.5	161.8615	158.6312	163.2077
30.1	163.4909	159.4411	164.9149
26.2	166.5236	163.3580	168.2674
25.8	166.7695	163.7348	168.5613
21.4	172.9574	169.9775	174.3318

[a] NMR data from compound **60**

Compound **163**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
166.8	30.4915	30.7262	38.1550
150.1	57.1089	58.2627	63.0449
112.3	58.4996	64.5383	64.8956
91.7	84.2470	86.1900	90.3558
88.1	93.1657	93.9690	97.9253
69.0	118.4970	118.8032	120.6210
51.4	134.4710	133.2729	133.8825
35.1	138.8896	137.7790	140.1657
32.2	145.0287	138.1557	143.0717
22.0	145.0344	140.8636	144.7644
18.7	176.1342	171.9418	178.5601

[a] NMR data from compound **61**

Compound **164**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
145.6	50.4662	56.9083	57.0735
109.8	85.2407	85.2846	89.0269
57.8	144.6243	144.7188	145.1047
49.9	148.0585	145.5554	149.0074
48.1	148.2328	149.5409	150.6200
47.5	148.6548	149.5751	150.8443
45.8	153.4425	151.4071	154.2237
36.3	154.2817	151.5476	154.8607
33.3	154.8003	153.4052	157.2046
33.0	157.6540	157.1298	159.9699
26.0	162.9052	157.7909	165.6899
24.2	164.3548	162.7936	165.7302
23.5	168.3891	163.6588	169.7623
17.7	170.9731	166.0943	174.7081
14.6	177.3122	169.9314	179.8687

[a] NMR data from compound **62**

Compound **165**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
172.0	25.7043	25.2973	31.8089
105.4	88.4318	89.9191	88.3812
93.7	110.1247	106.0717	103.9472
79.5	117.9436	118.3062	114.7525
50.0	125.4949	125.7681	127.1433
45.0	144.0942	146.2458	146.8972
37.5	151.3395	153.7205	154.8310
35.9	153.3102	155.4811	157.3092
33.6	155.9031	156.4988	158.6936
32.9	160.6934	157.5018	162.7595
25.2	160.9073	158.0530	163.5239
24.8	162.1123	160.1616	164.7785
23.4	163.3772	161.2551	166.8660
19.8	166.2687	164.2411	171.0188
12.5	172.9110	168.0539	174.6830

[a] NMR data from compound **66**

Compound **166**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
170.2	26.2506	26.2775	35.8576
163.9	33.5880	34.6221	41.3771
160.6	43.9350	40.2029	47.4259
157.9	44.2225	43.1575	49.7000
148.0	51.6679	49.7162	56.0976
136.2	60.6613	59.9237	66.6016
133.3	64.3527	64.1396	68.0292
131.1	66.2220	64.7044	69.5634
128.8	68.2770	68.0587	71.8132
128.7	70.9022	70.4593	74.2413
128.1	71.1779	72.2300	75.2162
125.9	73.7567	74.8734	77.2619
122.6	73.8634	74.8746	79.2754
120.2	85.4715	88.6777	91.4279
116.2	90.6385	88.9064	92.7016
51.4	151.7565	149.1044	152.7481
15.4	177.4473	175.5707	181.7299

[a] NMR data from compound **68**

Compound **167**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
170.2	30.9098	29.8060	36.8069
163.9	34.2921	34.4904	43.6817
160.6	45.9749	45.1270	49.3137
157.9	50.5269	48.2471	56.6034
148.0	53.3960	52.8354	63.4345
136.2	64.1859	64.5974	67.7668
133.3	65.0327	66.3541	68.6906
131.1	65.5158	66.4922	69.5821
128.8	67.7569	67.6793	71.3526

128.7	70.7391	69.8693	74.5696
128.1	70.9615	70.8859	74.9742
125.9	73.5264	74.3029	78.2424
122.6	75.1627	76.1013	78.6917
120.2	78.5208	80.7660	84.5491
116.2	83.5438	80.9507	86.0598
51.4	140.0268	139.8288	141.2510
15.4	172.7058	168.6287	175.6855

[a] NMR data from compound **68**

Compound **168**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
144.6	49.5503	50.4200	52.0513
143.8	52.9624	50.6785	58.6433
137.4	61.6066	66.5585	65.5580
132.7	63.0509	66.6736	67.1325
127.0	67.9690	67.7011	72.6109
124.1	74.3476	76.1976	78.4938
65.4	111.7727	106.0606	117.4841
58.0	133.6522	130.7435	137.8244
50.0	138.5932	136.2539	138.7219
47.2	141.9917	138.7282	143.6957
45.4	142.8289	139.5336	145.5949
42.9	145.8868	142.4345	148.5471
36.5	148.7709	146.4893	150.6690
36.0	157.9162	154.8837	157.8940
32.8	158.3772	158.9444	159.6655
31.0	162.9457	159.3457	163.6897
28.3	164.1111	160.0214	165.9039
27.7	165.9994	161.8121	169.4712
26.0	168.4681	163.2839	172.1203
18.0	170.5787	165.1850	174.0342
17.8	173.3831	170.6697	175.1612

[a] NMR data from compound **69**

Compound **169**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
170.5	27.8615	29.3955	36.1663
150.0	49.1465	47.4804	50.7286
139.8	57.7183	58.7920	62.1422
136.2	58.2004	59.4266	63.7188
129.8	60.9376	61.7837	66.0344
121.1	68.5371	68.1691	72.4716
110.1	78.7488	90.9006	91.2113
97.8	98.9295	98.6584	96.4338
79.4	119.8786	120.7364	115.4760
54.4	134.6896	131.7316	136.3874
50.9	135.0731	133.2004	137.5769
48.6	140.0543	143.2060	141.4437
48.5	141.6195	143.6740	143.0128
45.2	146.1593	144.5254	144.8452
36.5	148.4952	147.1248	149.0955
27.7	150.6000	149.0605	150.6578
27.7	160.9526	154.2499	164.5119
27.2	161.8105	158.7073	164.7881
27.1	163.0531	159.9582	166.1584
26.7	163.1301	160.9510	166.3828
24.5	169.6954	164.9738	170.2680
23.5	172.8217	166.1914	171.8507
22.5	172.9430	170.7618	175.6571
15.1	176.6897	173.5525	178.5574
13.7	180.3532	176.6492	181.6388

[a] NMR data from compound **70**

Compound **170**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
178.7	14.4012	17.8559	27.0871
140.0	52.6866	51.9124	58.3841
138.5	58.4830	55.9371	62.6732
131.9	63.0579	63.2777	66.5135
128.3	68.0038	68.8201	72.6680
127.9	69.8860	70.8454	73.9103
121.9	76.7292	77.5539	80.2341
112.2	83.5524	83.1499	90.4462
108.9	90.0833	89.5180	93.6531
72.1	118.9266	122.1619	123.4690
69.4	121.5208	122.7915	124.3281
66.2	131.5623	123.8415	133.1720
61.5	131.7233	128.8447	134.2715
54.1	142.8335	142.6885	143.2850
54.0	143.4661	146.4991	144.7084
50.6	143.8405	147.1590	146.2974
40.7	158.6968	151.8258	161.4798
38.2	159.0401	155.2120	163.1640
35.6	159.4120	156.6110	164.8515
22.8	162.7314	163.2730	167.8900

[a] NMR data from compound **71**

Compound **171**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
207.7	-9.2976	-8.3288	-2.5301
207.4	-5.0832	-4.4081	5.8414
90.6	108.0369	109.6378	104.5351
80.7	116.9455	119.0634	116.0263
43.7	137.6352	148.5407	144.6433
38.6	149.4918	149.2368	151.4953
36.5	149.6125	151.5135	152.5913
36.4	152.0581	154.3634	157.4314
35.4	155.8708	158.2296	158.4089
27.2	158.2297	161.2184	160.6902
26.6	163.8569	161.8107	167.4116
25.7	165.7665	163.9499	168.7740
24.7	168.7849	164.3439	170.5988
23.0	169.7470	165.9601	171.3721

[a] NMR data from compound **72**

Compound **172**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
171.0	26.9056	26.9161	33.9021
169.8	29.5684	28.9083	35.7824
144.5	64.7413	59.5553	68.3443
140.4	66.5773	61.9752	69.2962
135.4	69.2938	67.6615	74.3030
133.4	71.2120	67.8688	74.7334
126.1	71.9762	70.0890	75.6071

125.7	72.2004	72.0529	75.7244
123.8	73.4234	72.4351	77.0273
122.7	73.6325	73.3729	77.4631
121.4	75.2573	74.5306	78.4647
120.0	75.5242	75.6091	78.7805
113.0	78.2720	80.6210	86.2212
111.6	89.1625	87.7115	91.5866
109.5	94.7155	89.4912	98.4216

[a] NMR data from compound **74**

Compound **173**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
175.9	27.3173	29.6688	36.2271
145.8	51.9890	48.4240	53.2798
143.0	59.9076	57.8854	61.4565
139.0	60.1610	60.2676	61.9352
133.7	60.7459	62.9671	66.6180
128.0	72.9552	67.6164	74.2093
127.7	77.9772	75.6314	79.1398
124.6	78.8814	77.9954	79.4872
116.6	78.9463	78.2127	81.4360
123.5	78.9979	80.3077	83.2272
105.1	94.8547	88.9940	92.6446
100.9	98.0494	97.0001	99.5626
41.2	147.6268	144.4966	146.2504
34.2	159.8450	158.0700	161.5945
29.0	166.2019	164.0768	167.4947
23.5	172.5988	171.2396	175.4284
14.7	176.8578	173.0489	178.2045

[a] NMR data from compound **75**

Compound **174**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
175.9	21.5077	24.4651	32.0515
145.8	53.2463	49.7505	55.9265
143.0	54.6936	51.2728	56.9861
139.0	64.0213	61.8764	67.9437
133.7	67.3830	72.4204	72.0255
128.0	76.5666	77.6721	78.8905
127.7	77.3465	77.8515	80.2644
124.6	78.1734	79.2003	82.4477
116.6	84.0933	84.5679	86.7846
123.5	91.5600	88.5909	92.3500
105.1	93.8463	91.6191	94.9190
100.9	95.1535	92.0037	96.0845
41.2	149.6864	146.0975	149.8956
34.2	164.1084	161.0257	164.6537
29.0	165.4328	162.5986	166.6282
23.5	168.9788	164.9724	170.6947
14.7	171.1415	168.9864	172.0211

[a] NMR data from compound **75**

Compound **175**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
136.2	61.3997	65.6158	67.7376
122.1	68.4540	69.9721	73.5497
103.3	80.9361	87.2976	88.8281
76.7	115.6597	119.9652	121.6794
73.1	118.6049	121.3275	122.0871
71.3	125.9046	124.8911	128.2760
64.3	126.6107	125.2831	130.1413
49.0	141.2884	148.5034	148.0807
47.8	148.7233	155.6748	155.1476
43.1	158.3720	160.5655	163.9177
36.9	163.9254	163.0238	166.3902
27.8	166.4429	163.0617	167.3532
23.4	167.8360	165.5172	170.0070
22.6	169.3447	165.8184	171.5528
13.3	178.1999	175.0702	181.5388

[a] NMR data from compound **77**

Compound **176**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
136.2	50.5460	53.9032	56.5935
122.1	74.5993	76.1726	80.2990
103.3	91.6464	94.5045	98.3156
76.7	109.1326	113.9722	113.8587
73.1	117.4585	114.4771	117.1010
71.3	119.3691	118.5763	119.6854
64.3	124.1957	120.4588	125.5474
49.0	140.2135	146.7611	145.3551
47.8	142.9347	148.0750	145.7296
43.1	155.9329	153.9017	159.0853
36.9	157.6220	154.0387	159.4098
27.8	157.8244	154.0934	160.0498
23.4	169.7314	167.6218	171.5010
22.6	170.9170	167.9508	172.8019
13.3	174.8125	170.7922	178.6496

[a] NMR data from compound **77**

Compound **177**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
211.1	-21.4110	-14.2792	-8.5904
106.5	74.5718	75.9083	79.6576
85.1	113.1579	117.6342	118.0760
76.9	119.0738	120.4517	120.4998
73.2	119.7943	124.0662	120.8929
60.1	123.9778	128.7948	129.8350
54.9	131.0220	135.4888	138.5017
52.3	135.1209	137.2705	139.0502
43.7	147.5460	143.9996	149.2874
38.0	156.1720	156.7036	160.0673
34.3	159.1136	156.7171	163.5518
30.7	160.5103	159.5193	163.8345
14.5	173.2815	168.0746	176.0863
13.7	180.9448	180.8628	184.3822
8.3	182.1474	181.6241	186.3329

[a] NMR data from compound **78**

Compound **178**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
154.4	53.7731	60.3953	60.1100
136.8	57.7854	62.1461	63.6948
136.3	62.4420	62.3539	66.8039

133.1	65.5477	68.6541	70.7762
121.0	73.2462	75.4589	78.4723
112.0	85.2188	84.1862	87.6840
110.2	90.6341	95.3702	97.3515
99.4	94.6641	101.0566	101.9684
92.8	112.1869	113.7214	114.1235
76.8	112.9908	116.0966	115.1229
50.3	144.1364	141.0780	145.3016
43.1	153.9662	153.8967	158.9493
35.4	155.6389	157.0907	160.6997
34.4	156.5590	159.3302	161.1518
34.4	157.4064	160.5983	161.6051
26.6	163.7063	165.9454	166.8690
24.4	168.2602	166.0827	169.7902
21.6	170.1263	166.5472	171.9046
21.5	170.2310	166.5889	173.7810
20.0	171.6937	167.8846	174.6586
15.0	178.9014	175.5088	180.9998

[a] NMR data from compound **79**

Compound **179**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
204.9	-9.0297	-7.1359	-1.8742
169.6	25.7243	26.6347	35.1657
88.2	104.0310	104.4013	106.5092
85.3	109.0734	105.7235	111.4061
70.3	127.8690	122.7774	123.8172
50.6	135.3353	136.6322	137.1278
42.8	136.9988	141.9314	140.9291
38.5	153.5024	152.3976	155.8560
30.7	154.2445	153.3772	156.3043
25.4	155.3309	154.1982	157.4059
24.8	156.8979	155.2990	159.2829
24.5	161.0679	157.6676	163.7297
23.7	163.8907	162.4884	167.0991
21.9	165.0714	163.1221	167.1855
21.4	168.8235	167.8118	170.0249
21.3	172.8417	171.1634	175.1729

[a] NMR data from compound **80**

Compound **180**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
222.7	-24.2796	-22.1848	-15.3636
152.3	58.6648	62.9934	62.5124
116.6	76.3542	80.9698	86.2083
71.8	138.1235	133.8664	133.8555
53.4	140.6892	136.0125	142.8680
53.3	147.9498	146.0789	148.2703
48.9	149.9348	149.1522	148.8903
47.0	153.0162	149.5122	151.0899
46.2	153.9035	153.9215	157.0363
44.4	161.2902	156.6268	157.3729
33.3	162.1061	159.0007	163.0382
25.1	168.8108	165.9731	170.2435
24.8	168.8600	166.6362	173.6358
23.4	171.7501	167.9364	175.9996

[a] NMR data from compound **82**

Compound **181**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
169.3	-14.9263	-11.9080	-6.2884
142.2	53.1326	53.1747	57.6671
140.6	55.0639	55.5567	59.9683
132.8	59.6258	59.4386	61.7953
128.5	67.5643	70.6505	73.7486
127.2	69.7863	71.0326	73.9050
124.2	70.5050	71.3439	74.3528
122.2	70.7005	71.6768	74.6864
116.2	77.7354	79.1328	80.8398
77.6	110.1495	108.9876	113.3045
64.6	117.7227	116.5560	118.9484
60.2	123.6756	122.6727	124.4443
60.1	129.8498	125.9173	131.2810
52.9	131.9955	128.1179	136.3986
51.9	132.2424	130.5861	136.6340
50.3	139.4517	133.5109	143.1371
48.2	140.4827	134.5641	143.4893
42.7	145.5693	144.3877	149.3589
42.5	151.4824	145.9565	155.7916
31.6	157.5641	156.8192	159.9644
26.9	166.5315	162.6687	169.8397

[a] NMR data from compound **83**

Compound **182**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
169.3	23.6647	25.8135	28.4251
142.2	28.8617	28.9732	38.8264
140.6	55.6066	51.8177	58.9194
132.8	66.7001	64.6236	70.6341
128.5	69.3001	69.9344	72.6674
127.2	75.6192	76.5429	79.1552
124.2	76.0791	77.7358	79.5122
122.2	84.2202	80.9916	86.2635
116.2	90.9220	88.5502	88.9799
77.6	125.1729	118.7906	121.9948
64.6	126.0683	121.6165	128.7636
60.2	135.8713	133.3464	139.6053
60.1	139.4866	134.7939	142.3161
52.9	139.7752	138.3644	145.5393
51.9	143.7692	141.7381	147.3977
50.3	146.5414	144.0694	148.9836
48.2	151.1385	146.2974	152.2395
42.7	153.0581	152.1313	155.1721
42.5	156.7513	154.1056	161.1089
31.6	165.5078	163.4288	168.4382
26.9	166.3908	166.4062	168.6444

[a] NMR data from compound **83**

Compound **183**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
169.3	21.4506	25.5976	36.5566
142.2	39.5274	48.9404	53.5036
140.6	41.4633	52.0267	59.3005
132.8	54.0948	62.7483	70.3612
128.5	67.4584	69.1808	71.1000

127.2	69.5860	70.0440	72.7508
124.2	75.4045	75.1121	78.2929
122.2	75.8765	77.6621	79.6810
116.2	86.0163	79.4658	84.0942
77.6	120.6692	117.2812	116.2683
64.6	132.3512	121.9111	131.4764
60.2	134.6579	130.7831	136.9431
60.1	137.7419	133.2421	138.3865
52.9	139.7312	134.2002	140.3987
51.9	141.5419	140.1732	144.5986
50.3	143.2813	140.2458	150.6092
48.2	149.2428	140.8916	150.9247
42.7	150.4378	150.2230	151.8580
42.5	152.5981	151.3388	152.9455
31.6	153.4947	152.4712	153.8349
26.9	162.9884	161.3611	167.7219

[a] NMR data from compound **83**

Compound **184**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
169.3	11.0840	11.6122	24.8516
142.2	47.0875	47.1597	51.8772
140.6	49.6751	49.0129	54.8816
132.8	64.1147	60.3834	66.2114
128.5	70.0153	71.0643	73.5867
127.2	70.7763	74.1429	78.5914
124.2	74.5871	76.4222	78.8295
122.2	74.8484	76.7704	78.9864
116.2	81.1785	81.3461	86.4365
77.6	107.4464	109.0108	109.8195
64.6	132.1869	124.5403	129.9680
60.2	132.7544	128.2717	134.0205
60.1	137.7427	135.5803	140.4231
52.9	139.0985	136.1937	141.4010
51.9	139.9088	139.8766	142.2159
50.3	140.3199	140.6175	144.9095
48.2	148.0141	150.4232	149.0844
42.7	155.6301	152.5789	156.5135
42.5	159.5950	156.5816	161.9745
31.6	161.4895	161.2484	162.3522
26.9	172.5831	169.9800	173.2336

[a] NMR data from compound **83**

Compound **185**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
169.3	28.7499	26.8269	38.4475
142.2	55.7893	51.7201	60.0323
140.6	57.5397	65.4869	65.8071
132.8	65.7381	65.9204	69.3340
128.5	69.1299	69.8521	72.6943
127.2	69.4488	69.9245	73.0988
124.2	74.5802	75.5774	78.4087
122.2	76.1810	76.3846	78.6033
116.2	80.6621	79.0811	84.3323
77.6	114.4382	115.7931	120.3780
64.6	123.6450	121.1077	128.4210
60.2	125.5414	122.4275	130.0974
60.1	128.5833	123.7681	130.5566
52.9	134.0484	132.4527	132.3900
51.9	137.8559	134.6114	138.3997
50.3	138.6156	138.6655	142.6399
48.2	141.5949	143.2355	143.1128
42.7	152.5282	149.7479	153.9163
42.5	161.0933	157.7142	162.1469
31.6	162.5044	159.4957	162.8289
26.9	163.3324	162.0898	165.1155

[a] NMR data from compound **83**

Compound **186**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
136.2	54.2850	53.4415	61.5860
135.0	65.4628	63.3586	69.8775
127.3	70.7467	66.7427	74.4713
122.3	73.2015	71.8939	75.9400
120.1	76.1641	77.8518	79.7210
119.9	77.0168	78.6232	81.6121
111.2	78.4538	80.4688	81.9672
108.8	88.6387	88.1463	92.2037
71.0	105.8936	108.9720	105.8753
60.6	128.9402	122.5662	130.5979
57.3	132.2227	128.5942	132.6158
45.6	138.6681	141.3839	144.9127
44.5	144.8519	143.3988	145.0088
40.7	151.5512	151.9239	155.3085
37.8	158.5328	155.2355	157.7918
29.6	161.3001	156.4049	163.6636
27.0	161.9803	156.9371	165.5716
22.3	169.6743	168.4242	172.1327

[a] NMR data from compound **84**

Compound **187**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
198.6	1.2951	1.0039	5.5620
173.0	21.6627	21.3540	30.8177
145.5	56.7898	58.9777	61.8535
131.7	58.7873	61.0807	64.6646
107.0	81.6199	87.0505	87.1630
77.4	118.8641	116.5395	120.0378
71.9	120.9442	120.8029	122.3288
66.6	128.5059	125.4045	129.4142
54.5	141.2812	146.6135	148.4846
46.0	145.8039	149.5352	149.6098
30.1	161.7253	156.0284	161.0054
27.6	162.0924	158.0449	162.4722
21.0	172.6805	166.9978	172.0108
15.2	173.9051	171.4830	175.9074
15.0	176.0167	175.0147	180.5198

[a] NMR data from compound **85**

Compound **188**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
148.4	50.7722	51.2659	53.9199
146.4	64.4663	57.0226	66.0955
131.4	69.0632	61.1459	67.9698
130.9	69.0667	63.9714	70.7682

126.7	71.7791	69.5194	72.7748
126.1	72.0358	69.9984	72.9668
126.1	73.6576	71.9625	75.4243
123.9	73.7421	72.0450	75.7073
121.1	73.8671	73.6225	76.8721
119.1	75.9899	74.3347	77.0748
117.3	80.5143	74.3493	80.3493
115.7	80.9893	79.3465	80.6967
115.3	82.0431	80.8414	82.6751
113.0	82.2809	81.0393	83.5289
110.8	82.9301	81.3503	84.3033
108.0	83.9888	82.0315	85.8126
104.0	92.6029	90.2576	95.6045

[a] NMR data from compound **87**

Compound **189**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
216.3	-31.5232	-23.2135	-15.3323
59.1	130.0872	132.5287	136.5444
45.1	136.7619	135.0911	139.1978
43.2	137.3465	140.2312	139.9688
42.9	141.7828	142.0700	142.6916
42.4	142.2406	142.5247	143.5514
39.1	145.3386	142.7558	146.6231
39.0	148.2235	147.5339	148.9511
36.7	156.0578	151.0694	153.8812
35.1	159.2605	156.0139	158.7369
33.0	161.0665	160.9181	161.1047
28.3	162.3003	162.7551	163.1766
16.3	170.7267	166.0324	174.2815
13.8	173.7860	166.8326	177.8491

[a] NMR data from compound **88**

Compound **190**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
171.1	31.6679	31.0073	38.6016
150.0	46.4155	44.7697	50.5325
149.6	49.6866	49.3485	51.5507
148.1	51.1701	51.8380	54.0398
122.4	67.2696	70.5601	69.9282
119.8	80.9304	83.3051	88.0744
106.6	82.1760	87.9129	91.0672
62.0	131.1463	130.4328	133.6109
40.1	147.4425	152.2483	150.5672
26.4	160.4929	164.3097	167.4997
22.5	164.4352	164.9779	168.8964
22.1	169.6129	165.9489	172.2769
21.4	170.9811	170.6559	174.4127
17.0	171.2003	172.1915	176.6466
8.6	180.9830	177.7462	182.5116

[a] NMR data from compound **91**

Compound **191**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
171.1	27.9613	27.9291	35.3455
150.0	45.3697	45.8227	49.7722
149.6	46.8265	46.5004	50.3026
148.1	47.3264	49.2974	54.4249
122.4	69.9885	74.9344	74.6555
119.8	76.3820	75.0740	83.6673
106.6	84.1569	90.1256	95.6562
62.0	140.9115	138.1352	142.0495
40.1	149.8081	144.8397	143.8705
26.4	155.1305	152.4056	151.3699
22.5	155.1543	152.6429	151.9797
22.1	166.3458	160.2424	163.0710
21.4	166.3613	162.1558	169.1954
17.0	167.8294	165.8728	169.4986
8.6	183.0782	180.1299	183.6803

[a] NMR data from compound **91**

Compound **192**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
171.1	25.7733	25.3799	32.0132
150.0	36.5181	37.4941	38.1251
149.6	40.3245	41.8989	48.3506
148.1	49.6740	53.0687	52.0899
122.4	71.3436	75.6091	76.7243
119.8	82.7349	85.1380	88.9764
106.6	83.4437	86.0758	89.1143
62.0	123.8846	117.1697	119.6662
40.1	148.7352	148.3845	151.3376
26.4	150.0257	153.0415	153.6195
22.5	156.8989	162.3233	164.9208
22.1	166.0029	165.0669	170.1838
21.4	168.3235	166.8448	172.0182
17.0	168.9956	171.6632	176.0346
8.6	183.3526	179.5147	183.7600

[a] NMR data from compound **91**

Compound **193**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
195.3	6.9002	8.6432	11.9736
168.2	24.1871	16.3239	26.6145
146.8	49.6587	48.8276	54.3641
142.7	56.1241	54.8354	60.6830
128.1	70.1708	71.4191	73.8679
126.9	71.4321	72.5645	75.0870
123.5	76.9653	77.6925	80.6089
121.8	77.2388	78.0709	80.8498
113.9	80.2758	82.6621	86.1632
98.6	110.5127	102.1015	105.3994
91.8	111.4689	108.2695	109.9955
51.7	113.4386	110.8512	113.1652
50.7	141.4048	139.1919	141.0627
46.8	146.1105	141.6774	146.9445
41.3	153.2946	153.5151	158.7457
32.9	157.3639	156.3914	159.9648
29.8	162.7760	161.8327	164.5296
28.0	167.9511	162.7607	169.9323

[a] NMR data from compound **92**

Compound **194**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
209.9	5.4381	4.6244	15.4236
158.0	38.8615	38.3167	38.4252
153.4	45.6087	44.4119	48.5131
138.5	61.0556	63.2260	66.1826
131.0	66.6407	66.0075	69.7114
117.0	74.4130	76.3106	77.7941
113.3	76.7334	78.9843	84.0334
111.9	83.7642	84.4660	89.0902
103.5	87.7685	86.0400	89.7973
79.2	110.5161	113.0800	114.6787
79.0	110.9142	114.0988	116.7554
77.7	115.8988	120.7671	120.0801
54.8	129.8955	123.5201	126.2834
50.4	136.1863	135.6979	139.7811
45.2	140.6944	138.5642	143.2714
40.9	147.6838	147.9910	150.6433
40.4	151.7384	149.5022	151.1089
37.6	151.7430	154.7085	154.9827
32.3	160.7537	156.4733	164.2468
22.5	169.8376	164.0289	172.7397

[a] NMR data from compound **95**

Compound **195**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
203.4	-17.0197	-15.6534	-8.0222
173.8	19.1302	22.0941	29.3324
89.7	101.8782	110.5522	112.0786
87.8	116.5610	119.4877	119.9149
66.9	120.4444	126.0177	127.1233
62.6	127.5388	131.9303	130.4113
58.4	127.8124	132.7872	131.4434
57.1	130.5351	135.8821	134.8579
55.1	133.9074	140.3499	142.0868
51.7	136.1993	141.0783	142.3770
51.1	142.1743	141.4163	145.2146
50.8	147.2840	150.3693	149.4682
44.3	151.5795	151.6036	154.3414
24.3	167.8761	163.3814	173.3965
22.8	171.2492	165.8262	174.6427

[a] NMR data from compound **96**

Compound **196**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
203.4	-6.7479	-5.8013	0.0013
173.8	20.1819	23.2397	31.0601
89.7	96.9682	104.1618	104.4568
87.8	103.5035	107.2056	108.8639
66.9	122.8607	129.4464	130.0675
62.6	126.6622	133.0448	132.1466
58.4	129.1340	134.0177	132.3370
57.1	132.0882	135.7801	134.3842
55.1	134.9329	136.4399	137.6699
51.7	135.2234	136.8514	138.7021
51.1	135.8859	138.7241	141.0215
50.8	137.1248	139.1467	141.7261
44.3	160.5972	159.7855	163.7327
24.3	169.0780	163.2357	168.5674
22.8	171.9764	168.9255	175.9410

[a] NMR data from compound **96**

Compound **197**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
206.8	-17.6228	-11.5631	-6.3750
140.2	53.7896	55.4464	55.2426
138.7	54.3664	58.2678	62.4550
129.9	60.9820	62.3099	65.2700
127.3	64.9431	69.7062	77.3052
84.3	103.8081	111.0832	107.8093
80.5	116.0953	114.1987	115.0284
75.3	116.1808	118.8680	118.6491
72.5	119.9496	124.0849	124.2972
67.0	126.5126	125.2836	129.6046
44.1	142.1765	141.0196	146.4422
39.8	143.0876	146.7269	148.0613
31.0	146.2366	147.8080	148.3943
28.6	152.9936	147.9745	155.4867
24.0	156.2656	157.9889	157.2732
23.2	160.7373	161.4954	161.1474
23.1	162.7571	161.4988	164.9171
17.4	167.9697	162.5420	169.9727
15.6	175.3941	169.1356	178.5979
15.5	177.0888	174.0160	178.6065

[a] NMR data from compound **97**

Compound **198**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
207.9	-7.0986	-9.9588	-1.0844
179.6	32.6188	26.7878	29.6633
170.5	39.0852	35.1065	41.6745
147.8	44.2735	37.0712	41.7531
146.7	61.2498	58.0345	63.1399
130.3	65.3913	62.8995	69.1790
113.8	67.9861	71.0453	71.7211
111.4	77.6951	84.0990	88.1506
80.6	126.2650	122.8876	128.5776
76.0	126.3444	122.9206	130.0137
69.9	127.0809	124.6888	130.0405
65.0	132.2125	128.0843	132.3645
56.2	140.4442	136.8818	137.3275
54.8	141.3671	137.2919	142.1762
52.9	142.5763	144.4604	144.1631
41.3	155.9398	151.6640	156.4572
34.0	161.3660	153.7695	161.5132
30.2	163.5800	156.5415	164.7122
29.0	164.0999	161.6101	168.6718
26.1	170.6652	167.0805	170.8308
26.0	171.8181	167.9847	175.5380

[a] NMR data from compound **98**

Compound **199**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
207.9	0.1576	7.0367	9.0553
179.6	29.1477	24.8400	33.4333
170.5	32.9121	26.2691	34.3524
147.8	50.8550	43.0334	45.7285
146.7	57.0581	53.1273	55.2899
130.3	68.8150	73.8761	76.2301
113.8	71.3544	75.4519	77.6422
111.4	79.2468	88.4288	88.1022
80.6	113.9098	110.4955	119.6697
76.0	116.2395	115.1229	123.3868
69.9	128.3111	124.3573	126.2434
65.0	135.1871	133.5689	137.7513
56.2	137.5366	134.8012	138.4374
54.8	139.2030	135.0995	141.9179
52.9	141.6451	144.1704	142.5713
41.3	155.8926	152.8241	155.3098
34.0	159.5999	157.9784	166.4950
30.2	164.5289	159.2225	166.5365
29.0	166.2741	162.8115	169.0598
26.1	168.5338	165.6086	170.0280
26.0	170.9760	167.0586	170.1461

[a] NMR data from compound **98**

Compound **200**

δ_{exp} [a]	mPW1PW91/6-31G(d) Shielding Values		
	MM+	AM1	RHF/3-21G
167.7	21.4694	22.2992	29.2605
162.0	32.5854	34.4889	40.1071
156.5	39.3364	36.9256	42.7704
155.8	47.5834	39.9744	45.7887
151.3	48.0276	45.9429	49.0206
150.5	49.6902	46.7122	50.2662
143.4	57.2088	48.9038	55.6865
138.8	57.5815	57.7285	63.9440
130.5	67.7111	67.6435	71.2833
123.6	71.6693	72.1367	75.2922
121.5	71.9891	74.4041	79.3954
116.2	74.1730	76.2033	79.7143
113.3	75.0880	77.3195	80.2556
113.0	76.2032	77.9811	80.7889
105.6	77.0522	79.3709	82.4193
105.2	85.0874	83.4066	88.0975
104.8	88.8584	89.5913	94.0841
92.5	94.3463	92.5926	99.6233
78.0	116.4918	116.0458	113.7012
60.1	138.1789	131.2990	133.4300
45.8	146.4404	144.7589	146.5035
37.8	150.3655	149.7673	148.3863
36.6	156.0684	156.7351	156.8036
32.2	161.2375	157.8876	162.5819
28.3	161.5324	160.7912	166.1814
24.1	163.6192	161.0498	166.2162
24.0	170.2376	161.4126	173.9674

[a] NMR data from compound **100**

Statistical parameters computed for compounds **1-200** at the mPW1PW91/6-31G(d)//MM+ level of theory

Reference Standard	Parameter	Compound														
		1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**
MSTD	MAE	2.69	2.35	2.42	1.63	2.05	2.22	2.50	1.66	2.23	1.97	2.19	3.07	2.83	1.93	1.87
	σ	1.37	1.50	1.64	1.26	1.59	1.44	1.40	2.39	1.72	1.78	2.12	2.27	1.51	2.15	1.54
	MaxErr	4.60	4.74	5.58	3.67	4.82	4.82	6.23	6.97	4.98	5.30	5.79	7.17	5.37	6.05	4.64
	R^2	0.9991	0.9950	0.9708	0.9982	0.9990	0.9992	0.9983	0.9971	0.9990	0.9994	0.9994	0.9986	0.9975	0.9973	0.9990
	m	1.02	0.90	0.92	1.01	1.02	1.03	0.99	1.03	1.03	1.03	1.03	1.00	0.99	1.03	1.03
	b	-0.17	14.94	10.39	-0.08	0.55	-1.05	2.82	-0.64	-0.59	-0.94	-0.80	3.30	0.59	-0.63	-0.40
	CMAE	1.18	1.14	2.51	1.50	1.16	1.05	1.67	1.46	1.03	0.99	1.05	1.90	2.76	1.52	0.88
	Cσ	0.65	0.93	0.99	1.29	0.83	0.72	1.44	1.70	0.79	0.61	0.76	1.47	1.61	0.93	0.58
	CMaxErr	2.08	2.42	4.53	3.32	2.44	2.02	4.77	4.08	2.08	2.10	2.19	4.55	5.11	3.18	1.94
TMS	MAE	1.62	3.12	5.06	2.66	2.17	1.41	3.17	2.33	1.69	1.52	1.77	3.12	3.56	2.55	2.34
	σ	1.45	2.40	2.94	1.57	1.60	1.26	1.91	1.43	1.42	1.19	1.11	1.88	2.17	1.84	1.46
	MaxErr	3.40	6.49	9.92	4.41	5.48	3.85	7.31	5.06	4.26	3.91	4.11	5.92	7.10	7.19	5.78
	R^2	0.9991	0.9950	0.9708	0.9990	0.9987	0.9991	0.9986	0.9969	0.9992	0.9995	0.9996	0.9991	0.9979	0.9953	0.9975
	m	0.97	0.90	0.92	0.96	0.98	0.97	0.94	0.97	0.98	0.99	0.99	0.95	0.95	0.98	0.97
	b	4.71	10.61	6.06	2.72	3.17	2.88	4.81	3.35	3.29	2.51	2.59	5.36	2.94	3.46	3.92
	CMAE	1.12	1.14	2.51	1.13	1.26	1.10	1.54	1.78	0.90	1.02	0.87	1.49	2.32	1.66	1.10
	Cσ	0.77	0.93	0.99	0.93	1.04	0.70	1.19	1.44	0.80	0.52	0.52	1.18	1.78	1.71	1.30
	CMaxErr	2.09	2.42	4.53	3.04	3.74	2.42	4.29	3.87	2.09	2.07	1.98	4.36	5.43	5.90	4.51

Reference Standard	Parameter	Compound														
		16	**17**	**18**	**19**	**20**	**21**	**22**	**23**	**24**	**25**	**26**	**27**	**28**	**29**	**30**
MSTD	MAE	2.14	1.28	2.40	3.03	2.13	1.48	1.07	2.35	0.88	1.55	1.26	1.80	1.83	0.89	1.55
	σ	2.27	0.91	1.50	2.92	1.91	0.84	0.96	1.83	0.72	0.97	0.91	1.64	1.68	1.10	1.15
	MaxErr	6.60	2.63	5.19	7.21	5.72	2.86	2.72	5.35	2.31	2.78	2.95	4.38	5.26	3.61	3.38
	R^2	0.9987	0.9991	0.9975	0.9904	0.9956	0.9994	0.9930	0.9963	0.9972	0.9903	0.9972	0.9964	0.9981	0.9981	0.9969
	m	0.97	1.01	1.01	0.97	1.02	1.00	0.97	0.97	0.97	0.99	1.03	1.06	1.00	0.93	1.02
	b	1.03	-2.20	-0.70	4.33	-2.67	1.25	2.12	2.95	1.99	0.62	-3.03	-6.31	-0.02	9.39	-1.44
	CMAE	1.81	0.97	2.34	3.40	1.96	1.13	0.96	1.70	0.75	1.54	1.06	1.31	1.83	0.46	1.13
	Cσ	1.05	0.76	1.51	2.14	1.80	0.85	0.53	1.83	0.60	1.00	0.46	1.00	1.67	0.38	1.00
	CMaxErr	3.34	2.12	4.83	6.94	6.00	2.60	1.73	5.94	1.82	2.90	2.04	3.17	5.29	1.30	2.94
TMS	MAE	4.04	4.33	3.24	4.95	3.75	2.94	2.00	3.57	1.40	1.78	3.03	3.36	3.36	3.46	2.92
	σ	3.87	2.26	2.46	3.35	2.23	1.49	1.17	1.62	1.10	1.23	1.45	2.29	1.82	1.11	1.10
	MaxErr	10.93	6.96	8.19	9.83	7.61	5.79	3.86	6.16	3.45	3.29	4.90	8.09	6.02	4.45	4.65
	R^2	0.9991	0.9984	0.9980	0.9917	0.9964	0.9994	0.9930	0.9968	0.9972	0.9903	0.9972	0.9945	0.9987	0.9981	0.9987
	m	0.93	0.97	0.97	0.92	0.97	0.96	0.97	0.93	0.97	0.99	0.95	1.03	0.96	0.93	0.98
	b	3.03	-0.49	1.06	6.40	-0.28	3.18	3.26	5.69	3.13	1.76	3.17	-6.40	2.12	5.05	-0.78
	CMAE	1.50	1.34	2.24	3.31	1.80	1.20	0.96	1.69	0.75	1.54	1.05	1.60	1.68	0.46	0.78
	Cσ	0.78	1.01	1.12	1.69	1.57	0.77	0.53	1.55	0.60	1.00	0.48	1.27	1.18	0.38	0.60
	CMaxErr	2.81	2.88	3.98	5.34	4.72	2.86	1.73	4.61	1.82	2.90	1.91	3.85	4.06	1.30	1.85

Statistical parameters computed for compounds **1-200** at the mPW1PW91/6-31G(d)//MM+ level of theory

Reference Standard	Parameter	Compound														
		31	**32**	**33**	**34**	**35**	**36**	**37**	**38**	**39**	**40**	**41**	**42**	**43**	**44**	**45**
MSTD	MAE	3.51	3.47	3.36	2.95	1.60	3.20	3.39	2.84	2.00	1.22	1.81	1.46	1.60	2.41	2.01
	σ	2.04	2.19	2.28	2.11	1.38	2.11	1.70	2.38	1.74	0.67	1.82	0.99	0.85	1.71	2.11
	MaxErr	7.08	6.81	7.41	9.00	4.25	6.86	6.80	7.74	5.71	2.52	7.03	4.00	2.83	5.66	7.58
	R^2	0.9899	0.9962	0.9494	0.9993	0.9985	0.9978	0.9970	0.9988	0.9890	0.9962	0.9957	0.9992	0.9996	0.9968	0.9970
	m	1.05	1.03	0.98	1.02	1.01	1.05	0.99	0.97	0.96	0.92	1.01	0.99	0.99	1.02	0.99
	b	-5.91	-1.58	3.91	1.33	-0.65	0.37	3.30	3.02	6.82	3.40	1.00	1.70	1.95	0.82	1.37
	CMAE	3.01	2.39	1.94	1.30	1.46	1.29	2.45	1.98	1.85	0.62	1.73	0.90	0.67	1.55	2.02
	Cσ	1.84	2.18	1.19	1.03	1.34	0.96	1.73	1.74	1.40	0.31	1.20	0.80	0.48	1.66	1.90
	CMaxErr	7.21	6.04	4.04	3.59	3.99	3.25	5.95	5.33	3.86	1.21	5.11	2.78	1.80	7.35	7.01
TMS	MAE	3.77	2.64	4.49	2.79	2.38	3.39	3.28	4.26	3.50	2.05	2.28	2.52	2.81	2.62	3.26
	σ	2.54	2.36	2.30	1.41	1.77	1.88	2.09	3.33	2.07	1.02	1.63	1.36	0.91	1.52	1.94
	MaxErr	8.94	7.95	8.55	4.67	6.66	6.64	6.80	8.88	8.43	3.66	5.56	5.14	3.97	6.24	5.94
	R^2	0.9924	0.9956	0.9494	0.9989	0.9984	0.9971	0.9984	0.9991	0.9890	0.9962	0.9974	0.9993	0.9997	0.9966	0.9975
	m	0.99	0.98	0.98	0.98	0.96	1.00	0.95	0.94	0.96	0.92	0.96	0.96	0.96	0.96	0.94
	b	-1.88	1.83	5.05	3.72	2.17	3.43	5.92	5.22	2.49	4.54	3.68	3.74	4.06	3.64	4.34
	CMAE	2.56	2.69	1.94	1.62	1.55	1.51	1.95	1.74	1.85	0.62	1.37	0.82	0.58	1.58	1.81
	Cσ	1.65	2.17	1.19	1.28	1.36	1.06	0.95	1.51	1.40	0.31	0.89	0.76	0.45	1.70	1.76
	CMaxErr	5.54	7.54	4.04	5.25	4.52	3.43	3.86	4.75	3.86	1.21	3.18	3.02	1.46	6.72	6.01
Reference Standard	Parameter	Compound														
		46	**47**	**48**	**49**	**50**	**51**	**52**	**53**	**54**	**55**	**56**	**57**	**58**	**59**	**60**
MSTD	MAE	2.90	3.01	2.64	1.77	3.86	1.82	2.97	2.66	2.40	2.75	2.32	2.32	7.28	2.68	1.64
	σ	2.01	2.10	1.70	1.46	2.77	1.79	1.80	2.07	1.38	3.54	1.88	1.46	2.68	1.89	1.00
	MaxErr	7.71	8.98	6.99	4.26	9.03	6.43	7.60	7.40	5.15	12.90	5.46	6.18	11.48	5.68	3.99
	R^2	0.9970	0.9975	0.9957	0.9983	0.9914	0.9978	0.9878	0.9985	0.9985	0.9931	0.9974	0.9911	0.9972	0.9884	0.9988
	m	1.01	1.02	1.00	1.03	0.99	0.98	1.07	1.04	1.01	0.99	1.00	1.07	1.02	0.86	1.01
	b	1.26	0.90	1.67	0.11	2.23	1.66	-6.94	-0.75	0.79	2.77	1.07	-7.14	5.81	19.18	0.22
	CMAE	1.98	1.55	2.24	1.20	3.77	1.44	2.24	1.47	1.33	2.89	2.05	1.43	1.98	1.66	1.14
	Cσ	2.03	1.76	1.88	0.83	2.80	1.86	1.40	0.95	1.22	3.18	1.62	0.98	1.20	0.90	0.96
	CMaxErr	6.65	6.96	5.95	2.61	8.46	7.39	4.82	3.24	4.83	11.68	6.22	3.14	4.58	2.98	3.36
TMS	MAE	2.81	2.21	3.13	1.98	4.01	2.69	2.95	1.89	2.36	4.10	2.33	2.96	8.06	3.15	2.00
	σ	1.90	1.39	2.14	1.65	3.04	2.25	2.27	1.22	1.24	2.56	1.54	1.85	2.67	2.54	1.08
	MaxErr	8.41	4.65	8.13	5.40	12.61	9.56	7.04	3.79	4.47	8.57	4.45	6.90	12.62	8.83	3.84
	R^2	0.9972	0.9984	0.9968	0.9979	0.9937	0.9983	0.9900	0.9990	0.9983	0.9949	0.9989	0.9911	0.9965	0.9884	0.9996
	m	0.96	0.97	0.95	0.98	0.95	0.94	1.02	0.99	0.96	0.94	0.96	1.07	1.00	0.86	0.95
	b	3.84	3.77	4.24	2.99	4.21	4.16	-4.85	2.03	3.78	4.53	4.27	-11.48	8.24	14.85	3.57
	CMAE	2.05	1.32	1.95	1.30	3.28	1.46	1.97	1.20	1.55	2.54	1.32	1.43	2.21	1.66	0.68
	Cσ	1.81	1.38	1.57	0.93	2.33	1.39	1.37	0.84	1.10	2.71	1.06	0.98	1.38	0.90	0.57
	CMaxErr	5.80	4.79	5.87	3.76	7.85	5.01	4.12	2.70	3.78	9.90	4.14	3.14	5.27	2.98	2.03

Statistical parameters computed for compounds **1-200** at the mPW1PW91/6-31G(d)//MM+ level of theory

Reference Standard	Parameter	Compound														
		61	**62**	**63**	**64**	**65**	**66**	**67**	**68**	**69**	**70**	**71**	**72**	**73**	**74**	**75**
MSTD	MAE	2.76	1.60	2.65	2.56	2.24	1.83	3.11	1.69	2.93	3.82	2.34	3.22	1.92	2.37	1.93
	σ	2.39	1.42	1.56	2.09	1.76	0.80	3.29	1.01	1.74	2.84	1.81	1.83	1.73	1.65	1.55
	MaxErr	8.51	4.86	6.26	8.44	5.67	3.54	12.96	3.38	6.97	10.65	7.94	6.22	8.13	6.51	5.58
	R^2	0.9961	0.9984	0.9639	0.9930	0.9966	0.9995	0.9856	0.9974	0.9977	0.9936	0.9980	0.9977	0.9986	0.9882	0.9982
	m	1.00	1.03	0.83	0.94	0.99	0.99	0.99	0.99	0.99	0.99	1.04	1.00	1.02	0.93	1.00
	b	2.30	0.09	23.55	6.11	1.54	2.22	2.10	1.56	3.13	3.02	-1.70	2.47	-0.16	10.71	0.73
	CMAE	2.18	1.22	1.39	1.98	2.24	0.73	3.23	1.62	1.68	3.05	1.64	2.38	1.09	1.61	1.68
	Cσ	2.20	0.69	1.16	1.68	1.40	0.61	3.20	1.04	1.41	2.49	1.09	1.81	1.06	1.20	1.30
	CMaxErr	6.80	2.12	5.19	5.78	4.80	1.92	12.45	3.75	4.99	9.87	4.26	5.73	4.47	4.58	4.25
TMS	MAE	3.27	1.78	2.38	5.42	2.64	2.85	5.19	3.80	3.66	3.88	2.16	3.58	2.73	2.82	2.87
	σ	1.64	1.30	1.96	3.13	2.12	1.05	3.06	1.84	1.88	2.43	1.51	2.20	0.99	1.91	1.67
	MaxErr	6.03	4.22	6.19	12.77	6.81	4.68	12.03	7.71	7.18	9.32	4.25	7.36	4.70	7.71	5.86
	R^2	0.9975	0.9990	0.9639	0.9946	0.9977	0.9995	0.9840	0.9979	0.9976	0.9956	0.9967	0.9982	0.9962	0.9882	0.9977
	m	0.95	0.98	0.83	0.91	0.94	0.96	0.95	0.95	0.94	0.95	0.98	0.97	0.96	0.93	0.96
	b	5.18	2.86	19.22	7.10	4.93	4.33	3.40	3.12	6.13	5.66	2.02	4.74	3.61	6.38	3.09
	CMAE	1.94	0.95	1.39	1.66	1.85	0.72	3.59	1.54	1.80	2.60	2.03	2.23	1.83	1.61	1.81
	Cσ	1.55	0.57	1.16	1.55	1.09	0.65	3.17	0.77	1.37	1.94	1.48	1.44	1.75	1.20	1.56
	CMaxErr	5.07	2.30	5.19	5.34	4.19	2.75	11.18	3.21	4.85	7.21	5.60	4.60	7.95	4.58	5.61

Reference Standard	Parameter	Compound														
		76	**77**	**78**	**79**	**80**	**81**	**82**	**83**	**84**	**85**	**86**	**87**	**88**	**89**	**90**
MSTD	MAE	3.14	2.64	3.13	2.52	3.17	2.89	2.81	1.93	1.90	3.29	2.66	1.90	2.45	3.91	2.29
	σ	2.04	1.87	1.79	1.77	1.36	3.59	2.61	1.65	2.13	2.85	2.08	1.95	2.55	3.46	1.75
	MaxErr	8.79	6.94	6.53	7.40	6.28	15.31	7.52	5.36	7.35	11.36	7.90	5.79	9.60	11.62	5.76
	R^2	0.9956	0.9971	0.9991	0.9985	0.9971	0.9954	0.9980	0.9970	0.9968	0.9966	0.9946	0.9713	0.9988	0.9940	0.9976
	m	1.01	1.02	1.02	1.02	0.99	1.02	1.04	0.98	1.03	1.00	1.02	0.97	1.04	0.94	1.02
	b	0.40	1.35	1.98	1.03	2.17	1.21	-0.65	2.12	-2.31	2.93	-1.80	5.59	0.38	10.89	0.89
	CMAE	2.96	1.59	1.19	1.35	2.28	2.60	1.97	2.05	1.61	2.50	2.55	1.72	1.29	2.60	1.73
	Cσ	1.82	1.14	0.82	1.26	1.83	2.52	1.58	1.21	1.74	2.31	1.60	1.09	1.11	1.88	0.98
	CMaxErr	7.48	3.51	2.88	4.33	8.13	10.99	6.30	4.29	6.05	8.78	6.09	4.07	3.90	7.70	3.37
TMS	MAE	2.85	3.07	3.90	2.23	3.36	3.40	2.12	3.08	2.34	3.38	3.06	2.87	3.08	4.23	2.25
	σ	1.99	1.74	1.64	1.45	1.98	2.78	2.09	2.82	1.58	2.29	1.42	1.53	1.76	4.00	1.83
	MaxErr	7.39	6.61	7.67	4.98	5.99	10.97	8.24	9.69	6.15	7.43	6.39	4.87	6.22	12.76	6.11
	R^2	0.9968	0.9971	0.9989	0.9990	0.9978	0.9957	0.9983	0.9977	0.9965	0.9980	0.9954	0.9713	0.9989	0.9919	0.9981
	m	0.96	0.98	1.00	0.97	0.96	0.98	1.00	0.92	0.97	0.96	0.97	0.97	1.01	0.89	0.97
	b	2.95	4.13	4.17	3.69	4.44	3.57	1.84	6.02	1.34	5.39	1.93	1.26	2.55	14.05	3.68
	CMAE	2.53	1.59	1.27	1.14	1.86	2.38	1.69	1.72	1.68	2.10	2.22	1.72	1.24	3.00	1.45
	Cσ	1.54	1.12	0.96	0.96	1.74	2.56	1.59	1.22	1.81	1.58	1.69	1.09	1.06	2.21	0.99
	CMaxErr	5.40	3.42	3.99	3.93	7.32	9.89	6.40	4.48	6.58	6.51	6.33	4.07	3.45	6.73	3.80

Statistical parameters computed for compounds **1-200** at the mPW1PW91/6-31G(d)//MM+ level of theory

Reference Standard	Parameter	Compound														
		91	**92**	**93**	**94**	**95**	**96**	**97**	**98**	**99**	**100**	**101**	**102**	**103**	**104**	**105**
MSTD	MAE	3.93	2.33	2.96	2.21	2.71	4.95	4.06	3.71	3.10	2.83	4.76	6.70	5.29	4.73	6.63
	σ	2.93	1.90	2.49	1.49	2.04	2.51	3.43	3.22	1.63	1.94	2.61	7.53	5.02	3.76	4.82
	MaxErr	10.21	6.90	7.47	4.94	8.61	11.64	11.06	12.87	6.98	7.82	8.81	22.38	15.64	11.61	17.19
	R^2	0.9978	0.9966	0.9955	0.9968	0.9955	0.9974	0.9949	0.9930	0.9972	0.9953	0.9932	0.8761	0.9516	0.9647	0.9761
	m	0.98	1.00	1.01	1.01	0.99	1.03	1.01	0.98	0.99	1.00	1.06	0.66	1.16	1.18	0.97
	b	5.14	-0.04	2.53	0.04	0.56	2.30	3.23	0.73	1.70	1.09	-4.06	41.66	-15.91	-25.03	5.94
	CMAE	2.26	2.27	2.12	2.12	2.61	1.88	3.14	3.52	2.58	2.51	2.81	7.04	3.06	3.41	5.15
	Cσ	1.58	1.94	1.21	1.50	2.17	1.67	2.16	3.07	2.01	2.12	2.38	3.18	1.77	2.00	4.75
	CMaxErr	6.80	6.53	4.28	4.61	9.22	5.76	7.06	10.97	8.31	7.41	6.72	12.42	6.07	6.49	14.78
TMS	MAE	4.26	3.32	3.79	2.64	3.73	5.09	4.06	4.03	3.44	3.25	3.08	9.44	3.75	5.87	6.37
	σ	2.46	1.62	2.34	1.95	2.14	2.57	3.02	4.34	2.14	2.03	2.92	8.58	3.23	4.81	5.66
	MaxErr	8.88	6.92	8.61	7.66	8.00	7.80	9.80	17.20	8.75	8.53	8.38	26.72	11.31	15.94	18.33
	R^2	0.9982	0.9971	0.9943	0.9979	0.9962	0.9972	0.9960	0.9940	0.9976	0.9967	0.9919	0.8761	0.9516	0.9647	0.9768
	m	0.94	0.96	0.97	0.95	0.94	1.00	0.97	0.93	0.95	0.95	1.00	0.66	1.16	1.18	0.92
	b	7.26	2.94	5.44	3.13	3.48	5.30	5.71	3.60	3.93	3.52	0.82	37.33	-20.24	-29.36	8.56
	CMAE	2.06	2.27	2.08	1.78	2.34	2.04	2.92	3.39	2.40	2.12	3.45	7.04	3.06	3.41	4.90
	Cσ	1.37	1.57	1.81	1.16	2.07	1.65	1.70	2.64	1.87	1.75	1.95	3.18	1.77	2.00	4.89
	CMaxErr	5.32	5.68	6.78	3.37	8.92	5.55	5.55	9.53	6.69	5.74	7.30	12.42	6.07	6.49	14.45
Reference Standard	Parameter	Compound														
		106	**107**	**108**	**109**	**110**	**111**	**112**	**113**	**114**	**115**	**116**	**117**	**118**	**119**	**120**
MSTD	MAE	7.94	5.62	5.68	3.48	3.50	3.22	8.31	6.29	3.77	7.72	7.52	7.82	3.59	7.92	9.00
	σ	2.62	9.76	3.17	2.87	3.34	1.27	7.39	3.50	5.17	6.27	7.82	5.00	2.16	7.86	4.38
	MaxErr	13.63	40.48	14.28	10.35	10.48	5.07	21.09	11.54	19.12	24.73	29.07	19.40	6.90	27.51	15.78
	R^2	0.9969	0.9679	0.9908	0.9980	0.9979	0.9947	0.9827	0.9513	0.9785	0.9844	0.9736	0.9864	0.9936	0.9649	0.8892
	m	1.17	0.95	1.01	1.05	1.06	1.04	0.99	1.08	0.95	1.23	1.08	1.10	1.00	1.06	1.15
	b	-16.34	10.70	3.14	-1.91	-2.02	-5.29	9.12	-9.88	0.89	-29.13	-12.71	-15.15	0.47	-6.10	4.92
	CMAE	1.88	5.21	3.41	1.79	1.70	2.53	6.96	2.69	3.85	3.54	6.57	4.43	3.51	6.29	2.94
	Cσ	1.58	8.23	3.82	1.35	1.62	1.44	3.63	1.22	4.69	2.63	5.58	4.28	2.24	7.88	1.88
	CMaxErr	5.79	33.30	10.35	4.95	4.99	5.96	14.14	5.09	16.86	7.58	19.46	11.38	6.44	27.49	6.10
TMS	MAE	5.52	4.83	4.37	2.95	2.95	4.16	8.46	5.16	4.05	6.52	8.21	6.81	4.08	6.69	10.14
	σ	3.55	10.33	4.25	2.41	2.66	3.05	5.10	3.48	5.00	6.86	7.00	6.11	2.96	8.52	4.38
	MaxErr	12.49	41.62	11.04	7.75	9.20	8.72	16.76	10.40	17.98	23.59	27.93	18.60	9.48	28.65	16.92
	R^2	0.9970	0.9630	0.9884	0.9966	0.9968	0.9938	0.9820	0.9513	0.9807	0.9837	0.9719	0.9862	0.9933	0.9613	0.8892
	m	1.11	0.90	0.96	1.01	1.01	0.99	0.94	1.08	0.91	1.17	1.04	1.05	0.95	1.01	1.15
	b	-12.41	12.68	5.13	1.53	1.37	-2.90	11.05	-8.74	3.64	-25.10	-9.31	-11.75	3.88	-2.69	6.06
	CMAE	1.86	5.85	3.80	2.47	2.12	2.80	7.20	2.69	3.66	3.70	6.65	4.47	3.64	6.22	2.94
	Cσ	1.54	8.70	4.35	1.48	1.96	1.39	3.46	1.22	4.43	2.56	5.93	4.31	2.24	8.61	1.88
	CMaxErr	5.56	35.83	12.04	5.22	6.40	4.70	14.40	5.09	15.95	8.32	19.94	13.22	7.54	29.95	6.10

Statistical parameters computed for compounds **1**-**200** at the mPW1PW91/6-31G(d)//MM+ level of theory

Reference Standard	Parameter	Compound														
		121	**122**	**123**	**124**	**125**	**126**	**127**	**128**	**129**	**130**	**131**	**132**	**133**	**134**	**135**
MSTD	MAE	2.48	4.21	6.72	5.61	9.14	4.14	6.16	7.73	6.51	6.23	3.90	5.72	3.98	6.06	4.46
	σ	2.51	2.87	3.82	3.24	4.98	2.63	6.19	6.11	7.78	5.09	2.64	6.31	6.04	7.25	5.63
	MaxErr	10.89	8.50	14.55	11.64	18.13	9.95	19.79	19.53	24.97	13.98	7.97	18.92	20.52	21.85	17.77
	R^2	0.9957	0.9938	0.9838	0.9810	0.9652	0.9877	0.9752	0.9891	0.9671	0.9917	0.9962	0.8536	0.9037	0.8266	0.9053
	m	0.99	1.00	1.08	1.01	1.02	1.02	0.97	1.03	0.99	0.94	0.99	0.85	0.83	0.90	0.96
	b	1.86	-2.96	-9.56	-4.74	-8.87	-4.02	2.49	5.29	1.23	3.19	0.48	20.89	23.09	14.13	6.75
	CMAE	2.47	3.71	3.57	3.39	5.46	2.70	6.30	4.92	6.58	4.99	3.88	6.23	4.69	6.22	5.05
	Cσ	2.33	1.56	2.62	3.43	3.58	2.77	6.19	3.02	7.87	5.05	2.65	6.77	5.54	8.09	5.10
	CMaxErr	9.76	7.04	9.52	13.70	15.75	11.36	21.03	11.51	25.60	13.55	7.65	21.04	17.03	29.27	16.59
TMS	MAE	3.64	4.93	5.44	4.76	8.15	3.32	6.16	7.70	6.24	7.32	4.30	7.42	6.19	6.78	6.20
	σ	3.13	3.87	3.86	3.38	5.19	2.65	6.33	4.88	8.04	5.61	2.84	6.36	6.45	7.71	4.09
	MaxErr	12.03	12.28	13.41	11.84	16.99	9.86	23.56	15.20	28.68	15.12	9.11	23.25	24.86	24.33	16.58
	R^2	0.9949	0.9944	0.9863	0.9848	0.9700	0.9901	0.9770	0.9886	0.9672	0.9921	0.9966	0.8536	0.9037	0.8266	0.9053
	m	0.94	0.95	1.03	0.96	0.97	0.97	0.93	0.99	0.95	0.91	0.96	0.85	0.83	0.90	0.96
	b	4.68	-0.14	-6.50	-1.68	-5.81	-0.97	5.12	7.91	3.85	5.39	2.68	16.56	18.76	9.80	2.42
	CMAE	2.77	3.44	3.33	3.05	5.12	2.62	5.79	5.18	6.40	4.85	3.74	6.23	4.69	6.22	5.05
	Cσ	2.43	1.73	2.33	3.04	3.22	2.25	6.25	2.80	8.00	4.93	2.40	6.77	5.54	8.09	5.10
	CMaxErr	10.99	6.39	8.53	12.09	14.26	9.66	18.96	11.00	25.24	13.22	7.16	21.04	17.03	29.27	16.59
Reference Standard	Parameter	Compound														
		136	**137**	**138**	**139**	**140**	**141**	**142**	**143**	**144**	**145**	**146**	**147**	**148**	**149**	**150**
MSTD	MAE	4.68	4.00	2.41	3.55	3.29	5.35	4.92	4.68	5.49	4.26	4.40	5.36	3.65	3.75	7.40
	σ	7.63	2.11	1.52	4.06	3.41	2.88	4.79	3.76	3.09	5.96	3.35	3.30	1.94	3.18	3.44
	MaxErr	29.12	8.00	7.01	18.19	10.52	11.05	15.95	11.44	11.65	30.47	13.25	11.40	9.21	10.76	12.17
	R^2	0.9230	0.9936	0.9959	0.9858	0.9919	0.9855	0.9859	0.9898	0.9923	0.9783	0.9921	0.9935	0.9925	0.9878	0.9743
	m	0.94	0.95	1.02	1.04	1.01	0.99	0.98	0.97	0.99	1.01	0.94	0.98	0.97	1.07	0.95
	b	2.31	4.39	-0.62	-0.98	-1.52	0.73	4.71	5.32	4.88	0.67	7.58	6.85	4.79	-2.64	6.10
	CMAE	4.36	2.78	2.17	3.53	3.37	5.34	4.46	4.18	3.56	3.84	3.47	3.06	3.23	3.29	7.64
	Cσ	8.22	2.02	1.50	3.18	3.14	2.96	4.29	3.14	2.82	5.91	2.37	2.27	2.08	2.03	2.88
	CMaxErr	35.10	8.47	6.50	13.72	9.48	10.55	14.08	11.50	8.72	28.62	8.72	7.42	8.69	7.28	11.80
TMS	MAE	4.51	4.83	2.32	3.48	4.34	5.74	5.75	5.34	4.47	4.38	5.20	4.58	3.64	3.63	7.53
	σ	7.68	2.67	1.83	3.18	2.32	3.16	4.22	2.79	3.09	6.48	4.09	3.97	3.83	2.57	4.74
	MaxErr	27.87	9.14	8.15	13.86	9.38	12.19	14.93	12.45	12.79	31.61	14.39	12.30	13.54	9.64	15.91
	R^2	0.9245	0.9937	0.9957	0.9866	0.9929	0.9854	0.9839	0.9910	0.9932	0.9729	0.9922	0.9934	0.9932	0.9861	0.9750
	m	0.89	0.93	0.99	0.99	0.96	0.94	0.93	0.92	0.94	0.96	0.88	0.92	0.92	1.02	0.91
	b	5.00	6.43	1.50	1.84	1.45	3.70	7.29	7.90	7.46	3.54	10.46	9.72	7.36	0.24	8.08
	CMAE	4.33	2.82	2.20	3.29	3.14	5.30	4.59	3.98	3.41	4.12	3.45	3.30	3.01	3.40	7.46
	Cσ	8.12	1.89	1.59	3.27	2.94	3.08	4.77	2.86	2.56	6.74	2.34	1.94	2.09	2.36	3.01
	CMaxErr	34.37	8.07	7.05	13.97	9.22	10.70	15.16	11.01	8.09	32.87	8.37	6.82	7.50	8.18	14.19

Statistical parameters computed for compounds **1-200** at the mPW1PW91/6-31G(d)//MM+ level of theory

Reference Standard	Parameter	Compound														
		151	**152**	**153**	**154**	**155**	**156**	**157**	**158**	**159**	**160**	**161**	**162**	**163**	**164**	**165**
MSTD	MAE	2.97	3.81	2.92	3.27	4.28	9.59	5.75	2.90	8.21	4.74	6.19	3.40	13.30	4.07	5.93
	σ	4.25	2.88	2.91	2.45	2.30	7.38	5.61	2.16	4.10	3.70	2.30	3.98	9.28	1.83	4.48
	MaxErr	14.56	9.93	9.55	11.50	8.04	22.26	17.81	8.52	15.33	15.06	9.96	12.89	28.34	8.75	18.17
	R^2	0.9894	0.9913	0.9939	0.9904	0.9906	0.9570	0.9760	0.9707	0.9926	0.9245	0.9257	0.9884	0.9500	0.9841	0.9811
	m	0.98	0.97	1.01	1.12	1.02	0.98	0.97	1.00	1.03	0.99	0.83	1.01	0.92	0.99	0.93
	b	1.57	2.50	-1.65	-12.70	0.63	8.18	3.39	1.77	6.25	4.46	26.25	-3.11	17.85	1.34	7.83
	CMAE	3.01	3.46	3.17	2.09	3.50	8.92	5.43	2.63	2.90	3.28	3.38	3.63	8.98	3.79	3.65
	Cσ	4.19	3.08	2.21	1.06	2.74	6.20	6.03	1.79	2.48	3.83	3.68	2.91	6.90	2.26	4.62
	CMaxErr	15.76	10.58	8.15	3.88	9.65	16.71	19.14	6.83	8.22	12.08	12.95	11.07	21.44	9.65	15.01
TMS	MAE	3.60	4.42	3.26	2.54	3.68	8.38	6.12	3.37	8.91	3.33	3.71	4.09	13.98	3.92	6.76
	σ	4.26	3.08	2.59	2.73	2.28	6.55	5.27	2.41	4.33	3.87	3.50	4.38	8.80	2.27	4.48
	MaxErr	18.89	11.20	10.35	10.35	8.72	17.93	16.67	9.19	16.47	13.01	11.16	17.22	27.78	7.61	19.32
	R^2	0.9901	0.9920	0.9938	0.9927	0.9925	0.9609	0.9785	0.9707	0.9909	0.9245	0.9257	0.9879	0.9463	0.9865	0.9825
	m	0.94	0.93	0.97	1.07	0.97	0.93	0.92	1.00	1.00	0.99	0.83	0.95	0.88	0.94	0.90
	b	4.07	5.00	0.85	-10.61	3.41	9.94	6.59	-2.56	8.68	0.13	21.92	0.23	20.73	4.11	9.93
	CMAE	3.07	3.45	3.18	1.78	3.28	8.55	5.10	2.63	3.30	3.28	3.38	3.54	9.47	3.44	3.37
	Cσ	3.93	2.82	2.24	1.00	2.22	5.80	5.73	1.79	2.63	3.83	3.68	3.18	6.94	2.16	4.56
	CMaxErr	13.71	10.35	8.12	3.77	8.18	16.10	17.67	6.83	8.30	12.08	12.95	12.97	21.05	8.84	15.75

Reference Standard	Parameter	Compound														
		166	**167**	**168**	**169**	**170**	**171**	**172**	**173**	**174**	**175**	**176**	**177**	**178**	**179**	**180**
MSTD	MAE	2.90	2.35	3.58	4.62	3.18	4.34	3.87	3.00	3.61	3.82	4.21	4.60	3.14	5.96	5.46
	σ	2.75	2.64	3.72	3.67	2.18	3.34	2.98	1.87	3.83	2.90	3.34	3.85	2.93	4.32	5.12
	MaxErr	9.49	9.28	16.50	15.37	8.14	12.33	10.10	6.54	15.92	9.43	12.40	12.60	11.32	13.87	16.25
	R^2	0.9912	0.9945	0.9933	0.9908	0.9952	0.9951	0.9319	0.9956	0.9909	0.9881	0.9885	0.9922	0.9922	0.9916	0.9891
	m	1.03	0.94	1.00	1.00	1.04	0.96	0.94	0.98	0.97	1.06	1.04	1.04	0.97	0.97	1.01
	b	-4.46	7.01	3.39	3.36	-2.99	4.96	7.51	0.80	1.53	-2.68	0.94	1.31	1.93	7.06	-4.98
	CMAE	3.00	1.97	2.66	3.67	2.19	3.58	4.42	2.75	3.40	3.36	3.12	3.52	3.09	4.10	4.85
	Cσ	1.97	2.05	2.71	2.96	2.14	2.52	2.22	1.84	3.38	2.09	2.35	2.55	2.88	2.82	3.28
	CMaxErr	6.24	7.43	13.03	11.93	9.68	9.31	8.91	6.47	13.80	7.23	7.63	8.65	11.11	9.71	11.72
TMS	MAE	4.99	5.28	4.07	4.64	2.67	5.50	5.71	4.66	6.05	3.91	4.45	4.87	3.64	6.33	5.16
	σ	3.42	3.17	4.03	3.45	2.04	3.37	4.31	3.33	4.74	2.40	3.00	3.97	3.17	5.02	5.31
	MaxErr	12.03	13.62	17.64	16.51	9.28	13.48	14.43	10.87	20.25	10.57	9.19	13.74	13.36	15.01	16.15
	R^2	0.9907	0.9947	0.9908	0.9914	0.9943	0.9953	0.9319	0.9954	0.9884	0.9863	0.9883	0.9918	0.9937	0.9920	0.9896
	m	0.99	0.90	0.95	0.96	0.99	0.93	0.94	0.93	0.92	1.02	1.00	1.01	0.93	0.94	0.97
	b	-2.90	8.57	6.38	6.00	0.73	7.22	3.18	3.16	3.90	0.10	3.73	3.49	4.59	9.33	-2.49
	CMAE	2.97	1.89	3.06	3.62	2.64	3.58	4.42	2.70	3.86	3.50	3.30	3.61	2.73	3.88	4.73
	Cσ	2.19	2.06	3.22	2.79	2.03	2.32	2.22	2.04	3.80	2.43	2.14	2.62	2.60	2.93	3.20
	CMaxErr	7.52	7.00	15.40	12.26	8.95	9.78	8.91	6.42	15.42	8.27	7.89	8.78	8.95	8.92	10.84

Statistical parameters computed for compounds **1**-**200** at the mPW1PW91/6-31G(d)//MM+ level of theory

Reference Standard	Parameter	Compound														
		181	**182**	**183**	**184**	**185**	**186**	**187**	**188**	**189**	**190**	**191**	**192**	**193**	**194**	**195**
MSTD	MAE	7.07	4.89	4.67	4.33	3.14	4.61	3.30	2.97	6.80	4.07	6.10	7.09	4.69	4.66	4.96
	σ	9.12	5.89	5.21	4.47	2.67	4.05	2.90	2.98	4.56	3.31	4.22	4.73	7.11	4.12	3.56
	MaxErr	44.81	28.08	17.41	18.80	9.88	16.78	10.52	11.76	14.37	10.37	16.02	17.24	28.53	16.20	12.76
	R^2	0.9699	0.9783	0.9864	0.9919	0.9933	0.9888	0.9955	0.9227	0.9936	0.9959	0.9915	0.9921	0.9731	0.9907	0.9910
	m	1.08	1.07	1.08	1.09	0.99	1.00	1.00	0.74	1.05	0.97	0.97	0.98	0.98	0.94	1.05
	b	0.25	-6.67	-4.02	-6.58	2.69	4.09	1.75	32.68	4.26	5.42	7.21	8.19	3.21	8.12	-1.02
	CMAE	4.95	4.04	4.06	3.45	2.32	3.15	3.08	2.34	3.22	3.08	3.67	4.25	4.87	3.65	3.50
	Cσ	5.95	5.17	3.14	1.88	2.76	3.16	2.39	2.56	2.16	2.21	4.06	3.07	7.04	3.25	3.17
	CMaxErr	28.96	23.48	9.81	8.52	12.33	12.60	8.47	9.30	6.46	7.96	15.07	9.76	27.07	13.10	13.35
TMS	MAE	6.29	5.19	4.25	4.17	4.31	4.80	3.31	3.53	7.40	5.18	5.66	6.93	5.45	5.20	4.87
	σ	8.74	5.38	3.82	3.08	2.41	3.99	2.30	3.64	4.33	2.21	4.82	4.76	6.92	4.39	3.01
	MaxErr	40.48	23.75	13.08	14.47	9.10	17.92	7.48	16.10	14.26	7.96	17.16	18.38	29.67	20.53	9.55
	R^2	0.9619	0.9744	0.9851	0.9883	0.9909	0.9847	0.9969	0.9227	0.9930	0.9964	0.9921	0.9907	0.9726	0.9922	0.9909
	m	1.02	1.01	1.02	1.04	0.93	0.94	0.96	0.74	1.02	0.93	0.93	0.94	0.93	0.90	1.01
	b	4.14	-2.78	-0.13	-2.69	6.58	7.73	4.21	28.35	6.43	7.54	9.33	10.31	6.19	11.03	1.98
	CMAE	5.68	4.51	4.27	4.08	2.91	3.82	2.56	2.34	3.29	2.99	3.54	4.56	4.83	3.54	3.64
	Cσ	6.66	5.53	3.27	2.42	3.03	3.55	2.04	2.56	2.33	1.91	3.94	3.43	7.18	2.70	3.06
	CMaxErr	32.37	25.02	10.55	10.72	13.38	15.52	6.50	9.30	6.85	6.76	13.86	11.05	29.10	10.83	12.59

Reference Standard	Parameter	Compound				
		196	**197**	**198**	**199**	**200**
MSTD	MAE	4.76	6.90	5.76	3.58	4.98
	σ	2.72	4.41	4.79	3.89	4.23
	MaxErr	11.23	16.44	17.35	13.98	16.49
	R^2	0.9923	0.9919	0.9834	0.9916	0.9888
	m	1.02	0.99	1.00	0.98	1.01
	b	1.82	7.29	-1.73	0.32	3.09
	CMAE	3.02	3.82	5.00	3.38	4.11
	Cσ	3.17	2.91	5.23	3.87	2.95
	CMaxErr	13.59	9.55	19.61	15.96	12.31
TMS	MAE	5.12	6.56	5.34	4.14	4.05
	σ	3.03	5.02	5.38	4.28	2.99
	MaxErr	10.09	17.58	17.36	13.89	12.16
	R^2	0.9907	0.9922	0.9856	0.9931	0.9907
	m	0.98	0.95	0.95	0.94	0.96
	b	4.82	9.77	1.14	3.19	5.52
	CMAE	3.46	3.76	4.67	3.30	3.70
	Cσ	3.34	2.83	4.85	3.25	2.72
	CMaxErr	14.38	9.81	18.11	14.28	11.29

Statistical parameters computed for compounds **1-200** at the mPW1PW91/6-31G(d)//AM1 level of theory

Reference Standard	Parameter	Compound														
		1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**
MSTD	MAE	2.23	2.02	1.72	2.39	2.10	2.60	2.15	2.56	2.10	2.93	2.64	1.51	2.44	2.56	2.66
	σ	1.31	1.62	1.45	1.63	1.83	1.34	1.82	2.32	1.70	1.40	1.77	1.45	1.72	1.07	1.49
	MaxErr	3.70	4.79	5.02	5.20	5.00	4.68	6.28	7.48	5.33	4.42	6.07	4.62	5.54	4.36	5.43
	R^2	0.9978	0.9939	0.9918	0.9971	0.9976	0.9985	0.9984	0.9952	0.9982	0.9974	0.9977	0.9989	0.9987	0.9967	0.9945
	m	1.03	0.92	1.05	1.03	1.04	1.05	1.01	1.04	1.04	1.04	1.04	1.00	0.99	1.05	1.04
	b	-3.77	12.16	-4.59	-1.98	-1.81	-3.40	0.31	-2.77	-2.58	-3.50	-3.23	0.21	-1.17	-4.41	-3.99
	CMAE	1.98	1.47	1.21	2.28	1.71	1.25	1.67	2.40	1.39	1.90	1.87	1.51	1.90	1.54	1.89
	Cσ	0.44	0.66	0.76	0.88	1.39	1.15	1.24	1.52	1.09	1.68	1.54	1.45	1.28	1.26	1.62
	CMaxErr	2.51	2.35	2.46	4.26	4.51	3.65	4.23	4.72	3.23	4.84	4.59	4.60	4.31	4.40	4.47
TMS	MAE	3.10	5.72	5.52	3.56	2.41	2.69	4.31	2.37	2.33	2.24	2.01	4.41	4.06	1.75	1.98
	σ	2.32	2.32	1.73	2.89	1.02	1.72	2.29	2.91	1.56	1.58	1.31	3.04	4.26	1.73	1.77
	MaxErr	6.10	9.72	7.64	8.74	3.83	5.70	9.04	7.70	4.38	6.15	4.35	7.92	12.54	5.33	5.45
	R^2	0.9986	0.9939	0.9918	0.9972	0.9991	0.9980	0.9977	0.9956	0.9991	0.9984	0.9992	0.9994	0.9990	0.9968	0.9967
	m	0.94	0.92	1.05	0.94	0.95	0.94	0.93	0.94	0.94	0.96	0.96	0.93	0.92	0.95	0.94
	b	5.55	5.17	-11.59	3.64	3.50	4.23	4.50	4.96	4.97	3.27	3.45	4.52	3.65	3.50	4.33
	CMAE	1.41	1.47	1.21	1.99	1.01	1.34	1.86	2.18	1.01	1.58	1.31	1.27	1.68	1.41	1.45
	Cσ	0.82	0.66	0.76	1.38	0.89	1.48	1.70	1.63	0.69	1.26	0.62	0.90	1.12	1.36	1.28
	CMaxErr	2.58	2.35	2.46	4.46	3.04	4.70	5.21	4.23	2.22	5.01	2.73	2.54	4.06	4.32	4.24

Reference Standard	Parameter	Compound														
		16	**17**	**18**	**19**	**20**	**21**	**22**	**23**	**24**	**25**	**26**	**27**	**28**	**29**	**30**
MSTD	MAE	1.52	1.66	1.94	2.75	1.60	1.48	1.81	1.86	1.57	1.11	1.13	2.27	1.60	1.37	1.67
	σ	1.10	0.71	1.23	2.63	0.98	1.09	0.78	1.62	0.99	0.76	0.56	2.36	1.30	1.23	1.24
	MaxErr	3.28	3.00	3.87	5.78	3.00	3.39	3.42	5.60	2.76	1.88	2.20	6.75	3.50	3.75	4.53
	R^2	0.9997	0.9990	0.9984	0.9964	0.9991	0.9992	0.9977	0.9981	0.9977	0.9980	0.9990	0.9943	0.9987	0.9904	0.9956
	m	1.02	1.00	1.00	1.02	1.02	1.01	0.95	1.00	0.98	0.97	1.04	1.08	1.01	0.91	1.00
	b	-2.78	1.68	-0.53	0.48	-1.44	-1.30	0.69	-1.59	-0.31	0.54	-4.21	-9.82	-0.86	12.18	0.86
	CMAE	0.84	0.94	1.85	2.26	1.00	1.35	0.45	1.34	0.73	0.69	0.54	1.61	1.66	0.99	1.44
	Cσ	0.34	0.93	1.31	0.84	0.60	0.92	0.46	1.15	0.46	0.48	0.47	1.34	1.11	0.93	1.06
	CMaxErr	1.21	2.59	3.58	3.69	1.84	3.08	1.47	3.88	1.39	1.30	1.60	4.36	3.45	2.87	3.53
TMS	MAE	3.51	5.48	4.95	3.72	4.61	4.88	1.10	2.20	1.13	1.78	5.45	6.34	4.70	6.53	5.55
	σ	3.09	1.54	3.50	2.53	1.85	2.67	0.79	1.95	0.97	1.01	1.94	2.51	3.11	1.82	2.05
	MaxErr	6.71	8.44	10.86	7.32	6.67	9.56	3.14	7.29	2.42	3.11	7.67	12.17	9.29	9.45	8.93
	R^2	0.9993	0.9993	0.9996	0.9955	0.9992	0.9981	0.9977	0.9992	0.9977	0.9980	0.9991	0.9934	0.9988	0.9904	0.9939
	m	0.95	0.92	0.93	0.94	0.94	0.94	0.95	0.93	0.98	0.97	0.89	1.03	0.93	0.91	0.93
	b	1.43	5.38	3.26	4.82	3.45	2.80	3.38	3.94	2.38	3.22	7.44	-9.31	3.60	5.18	2.70
	CMAE	1.16	0.82	0.80	2.42	1.01	1.97	0.45	0.93	0.73	0.69	0.54	1.66	1.57	0.99	1.65
	Cσ	1.07	0.74	0.80	1.27	0.54	1.70	0.46	0.64	0.46	0.48	0.35	1.52	1.20	0.93	1.34
	CMaxErr	2.95	1.79	2.52	4.35	1.99	6.03	1.47	2.18	1.39	1.30	1.35	4.94	3.59	2.87	4.09

Statistical parameters computed for compounds **1-200** at the mPW1PW91/6-31G(d)//AM1 level of theory

Reference Standard	Parameter	Compound														
		31	**32**	**33**	**34**	**35**	**36**	**37**	**38**	**39**	**40**	**41**	**42**	**43**	**44**	**45**
MSTD	MAE	3.27	2.69	2.20	3.17	2.51	2.40	4.24	2.79	1.98	2.13	2.85	2.12	2.17	2.44	1.96
	σ	1.45	1.10	2.04	2.00	2.67	1.37	2.69	1.38	1.78	1.91	2.04	1.88	1.41	1.98	0.96
	MaxErr	4.87	5.08	6.40	7.19	6.87	5.17	10.36	5.46	6.96	6.60	7.81	5.45	4.66	7.35	3.54
	R^2	0.9959	0.9989	0.9831	0.9976	0.9971	0.9959	0.9920	0.9989	0.9913	0.9719	0.9902	0.9969	0.9976	0.9945	0.9988
	m	1.07	1.04	0.78	1.03	1.04	1.02	1.01	1.02	0.96	0.86	0.99	0.99	0.99	1.00	1.02
	b	-6.48	-5.43	4.31	-2.73	-4.05	0.41	0.09	-2.41	6.69	2.94	-1.12	-1.00	-1.29	-1.17	-2.42
	CMAE	2.03	1.19	0.97	2.52	2.38	1.76	4.16	1.89	1.67	1.24	2.35	2.14	1.75	2.33	1.51
	Cσ	0.95	1.25	0.87	1.83	1.37	1.36	2.65	1.77	1.22	1.49	2.12	1.04	1.05	1.81	0.90
	CMaxErr	3.07	3.61	2.57	5.22	4.84	4.96	9.55	5.45	4.58	5.67	8.50	3.90	4.05	6.32	3.51
TMS	MAE	3.45	3.52	2.24	3.02	3.79	3.85	3.89	2.60	5.46	2.17	2.50	2.70	2.08	3.57	3.30
	σ	2.04	2.88	1.30	2.19	2.30	1.82	2.86	2.09	2.20	1.26	2.71	1.72	2.00	2.94	3.10
	MaxErr	7.85	9.71	4.08	6.09	7.23	6.42	10.85	6.04	9.01	5.31	11.30	7.70	7.52	11.18	8.36
	R^2	0.9980	0.9983	0.9831	0.9981	0.9972	0.9956	0.9959	0.9993	0.9913	0.9719	0.9940	0.9980	0.9985	0.9952	0.9994
	m	0.96	0.96	0.78	0.96	0.95	0.93	0.94	0.97	0.96	0.86	0.91	0.94	0.94	0.91	0.93
	b	1.33	1.26	7.00	2.18	1.61	6.49	5.40	2.16	-0.31	5.63	4.30	3.28	3.12	4.49	3.51
	CMAE	1.20	1.68	0.97	2.29	2.39	1.58	2.88	1.39	1.67	1.24	1.80	1.75	1.39	2.05	1.02
	Cσ	0.98	1.39	0.87	1.63	1.30	1.69	2.03	1.47	1.22	1.49	1.71	0.79	0.84	1.84	0.76
	CMaxErr	3.94	5.43	2.57	6.18	6.70	5.31	7.49	4.46	4.58	5.67	7.03	3.32	3.38	8.10	2.26

Reference Standard	Parameter	Compound														
		46	**47**	**48**	**49**	**50**	**51**	**52**	**53**	**54**	**55**	**56**	**57**	**58**	**59**	**60**
MSTD	MAE	1.91	3.30	2.96	1.88	3.83	2.51	3.01	2.14	2.13	3.60	2.13	2.41	3.40	2.57	2.16
	σ	1.22	2.72	2.60	1.78	2.25	2.42	1.99	1.69	1.43	3.10	2.28	2.00	1.97	1.88	1.88
	MaxErr	4.13	8.80	7.56	5.36	7.80	8.28	7.61	5.94	4.23	11.27	8.11	6.51	6.58	7.88	5.64
	R^2	0.9983	0.9946	0.9935	0.9960	0.9934	0.9969	0.9891	0.9977	0.9986	0.9925	0.9977	0.9896	0.9951	0.9925	0.9975
	m	1.01	1.04	1.01	1.02	1.01	0.98	1.05	1.02	1.04	1.00	1.03	1.06	1.00	1.05	1.04
	b	-0.75	-2.03	-0.13	-1.99	0.35	-0.50	-4.10	-0.18	-3.02	1.94	-2.42	-5.33	2.29	-4.16	-2.94
	CMAE	1.79	2.59	2.80	1.73	3.40	2.02	1.90	1.75	1.50	3.63	1.67	1.48	2.65	1.13	1.88
	Cσ	1.17	2.33	2.24	1.40	2.34	1.91	1.64	1.32	0.83	2.60	1.83	1.16	1.54	1.03	1.00
	CMaxErr	4.43	8.85	7.50	4.41	8.95	8.39	5.11	3.95	2.93	9.68	5.51	4.74	5.90	3.58	5.00
TMS	MAE	4.39	3.44	4.71	2.52	3.55	3.17	4.45	3.16	3.49	4.59	3.24	4.83	4.63	4.55	2.96
	σ	2.59	2.10	2.90	1.18	3.13	3.51	2.79	1.90	2.25	3.56	2.34	2.27	2.99	1.55	1.84
	MaxErr	10.36	7.24	10.25	5.47	11.44	15.28	9.44	6.88	7.21	11.42	8.29	8.06	8.64	6.25	6.79
	R^2	0.9991	0.9960	0.9941	0.9983	0.9978	0.9985	0.9841	0.9983	0.9982	0.9958	0.9965	0.9896	0.9968	0.9925	0.9984
	m	0.92	0.94	0.93	0.93	0.94	0.91	0.96	0.93	0.94	0.92	0.95	1.06	0.95	1.05	0.93
	b	4.48	3.72	5.09	3.77	4.52	4.59	0.27	5.41	2.93	5.71	3.91	-12.32	7.27	-11.15	3.66
	CMAE	1.20	2.34	2.55	1.10	2.11	1.44	2.33	1.60	1.60	2.63	2.47	1.48	2.08	1.13	1.44
	Cσ	0.97	1.82	2.29	0.95	1.10	1.28	1.95	0.97	1.17	2.09	1.74	1.16	1.37	1.03	0.92
	CMaxErr	3.36	6.72	8.04	2.99	4.19	4.48	6.20	3.28	4.78	6.29	6.05	4.74	4.42	3.58	3.26

Statistical parameters computed for compounds **1**-**200** at the mPW1PW91/6-31G(d)//AM1 level of theory

Reference Standard	Parameter	Compound														
		61	**62**	**63**	**64**	**65**	**66**	**67**	**68**	**69**	**70**	**71**	**72**	**73**	**74**	**75**
MSTD	MAE	2.25	2.29	3.04	2.55	2.94	2.79	2.74	1.41	2.52	3.15	2.50	3.21	1.57	3.25	2.54
	σ	1.85	1.65	1.12	2.15	2.53	2.66	2.33	0.95	1.70	3.25	1.81	2.99	1.37	2.06	2.23
	MaxErr	5.63	5.86	5.07	8.00	9.52	11.42	9.81	3.19	5.70	12.64	6.72	9.79	5.57	7.89	9.44
	R^2	0.9975	0.9935	0.9907	0.9911	0.9942	0.9935	0.9912	0.9982	0.9968	0.9916	0.9982	0.9964	0.9991	0.9865	0.9967
	m	1.03	1.00	1.06	1.00	1.02	0.99	1.01	1.01	0.99	1.00	1.05	1.00	1.04	0.99	1.03
	b	-2.62	-0.22	-4.36	-1.78	-0.88	-1.17	-0.27	-0.51	2.16	-0.12	-5.26	-2.35	-4.43	4.81	-1.61
	CMAE	2.08	2.31	0.62	2.52	2.64	2.36	2.79	1.36	1.86	3.22	1.53	3.28	0.91	1.63	2.00
	Cσ	1.33	1.61	0.66	1.43	2.24	2.47	2.17	0.90	1.86	3.17	1.05	1.83	0.79	1.41	2.05
	CMaxErr	4.35	5.63	2.70	6.34	7.36	9.46	9.48	3.02	6.51	12.18	3.51	7.72	3.31	4.54	7.78
TMS	MAE	2.62	3.36	3.95	7.63	3.81	2.45	5.83	5.97	5.18	4.45	3.39	3.84	4.17	3.97	3.81
	σ	1.95	2.17	1.12	2.79	2.23	2.53	3.37	2.07	1.90	2.67	2.23	1.85	2.53	1.87	2.64
	MaxErr	6.43	8.29	5.98	13.17	8.34	8.74	11.31	9.23	8.39	9.96	7.48	7.10	7.34	7.54	9.99
	R^2	0.9981	0.9948	0.9907	0.9956	0.9954	0.9958	0.9926	0.9974	0.9962	0.9953	0.9965	0.9976	0.9965	0.9865	0.9970
	m	0.95	0.91	1.06	0.94	0.93	0.94	0.94	0.93	0.90	0.91	0.95	0.95	0.94	0.99	0.94
	b	3.15	5.34	-11.36	0.64	5.79	3.23	2.69	2.92	8.12	5.22	2.00	2.33	2.91	-2.18	3.25
	CMAE	1.75	1.92	0.62	1.58	2.30	1.94	2.58	1.60	1.96	2.43	2.07	2.71	1.84	1.63	1.94
	Cσ	1.25	1.65	0.66	1.29	2.05	1.94	1.96	1.11	2.07	2.34	1.59	1.37	1.58	1.41	1.93
	CMaxErr	3.71	6.39	2.70	5.23	8.42	7.96	6.99	3.95	6.92	7.50	6.30	5.26	7.85	4.54	6.48

Reference Standard	Parameter	Compound														
		76	**77**	**78**	**79**	**80**	**81**	**82**	**83**	**84**	**85**	**86**	**87**	**88**	**89**	**90**
MSTD	MAE	2.60	3.47	3.20	2.97	2.29	3.60	3.45	2.10	3.50	3.60	1.98	4.01	2.85	2.65	2.92
	σ	2.44	2.04	1.95	2.23	2.28	2.89	1.88	1.70	2.93	1.91	1.32	1.99	1.20	1.54	1.88
	MaxErr	9.23	5.85	6.41	7.20	7.65	10.33	6.37	5.93	10.51	6.41	3.91	6.85	5.29	5.84	5.67
	R^2	0.9961	0.9913	0.9953	0.9950	0.9974	0.9938	0.9953	0.9979	0.9952	0.9961	0.9987	0.9734	0.9973	0.9980	0.9940
	m	1.02	1.00	0.99	1.02	1.01	1.01	1.01	1.03	1.08	1.03	1.04	0.96	0.99	1.05	1.02
	b	-1.84	-1.94	-1.24	-2.48	-2.12	1.13	-0.84	-0.81	-7.03	-2.35	-3.24	9.36	-1.14	-4.32	-2.03
	CMAE	2.46	2.74	2.91	2.75	2.27	3.47	3.46	1.74	2.16	3.05	1.26	1.70	1.94	1.33	2.74
	Cσ	2.17	1.98	1.66	1.92	1.58	2.33	1.63	0.97	1.92	1.98	0.79	0.98	1.60	1.27	1.54
	CMaxErr	8.61	8.34	5.63	6.48	6.43	9.08	5.99	3.32	6.33	5.71	2.50	3.37	6.12	4.18	5.81
TMS	MAE	3.69	2.75	2.85	2.92	2.56	4.57	3.90	3.78	3.26	3.02	3.82	2.99	2.17	3.24	2.99
	σ	2.48	2.09	1.80	1.93	1.44	3.84	2.11	2.25	2.52	1.63	2.14	1.99	2.99	1.99	2.21
	MaxErr	9.50	8.76	5.75	8.28	6.10	13.73	7.00	8.13	7.82	6.04	7.65	6.34	9.06	6.71	7.87
	R^2	0.9974	0.9963	0.9974	0.9982	0.9988	0.9921	0.9962	0.9955	0.9952	0.9983	0.9967	0.9734	0.9981	0.9974	0.9968
	m	0.94	0.93	0.95	0.94	0.96	0.94	0.95	0.92	0.97	0.96	0.94	0.96	0.94	0.96	0.93
	b	3.34	3.65	3.29	2.89	2.57	5.98	4.24	6.75	0.10	2.68	4.02	2.36	3.36	1.94	3.57
	CMAE	2.24	1.75	2.24	1.67	1.56	3.71	2.84	2.33	2.32	2.14	1.98	1.70	1.66	1.85	1.91
	Cσ	1.43	1.35	1.07	1.16	1.07	2.90	1.95	1.81	1.73	1.10	1.29	0.98	1.32	0.99	1.30
	CMaxErr	4.95	4.48	4.33	3.78	4.03	13.20	5.91	6.12	6.85	4.25	5.18	3.37	5.26	3.57	4.72

Statistical parameters computed for compounds **1**-**200** at the mPW1PW91/6-31G(d)//AM1 level of theory

Reference Standard	Parameter	Compound														
		91	**92**	**93**	**94**	**95**	**96**	**97**	**98**	**99**	**100**	**101**	**102**	**103**	**104**	**105**
MSTD	MAE	1.97	2.03	3.26	2.57	4.10	3.29	2.67	2.79	3.48	3.29	4.62	4.98	5.24	4.23	5.83
	σ	1.76	1.40	2.07	1.78	2.98	2.03	2.35	2.63	2.37	2.25	2.85	4.96	4.97	4.01	3.09
	MaxErr	5.31	4.11	7.54	5.65	11.80	7.18	9.24	8.98	8.20	10.21	7.77	15.18	14.08	12.83	11.34
	R^2	0.9986	0.9982	0.9896	0.9973	0.9936	0.9968	0.9961	0.9966	0.9961	0.9953	0.9907	0.9306	0.9632	0.9734	0.9807
	m	1.01	1.02	0.99	1.04	1.05	1.02	1.02	1.00	1.02	1.03	1.07	0.77	1.19	1.19	0.99
	b	0.04	-2.29	-0.70	-3.72	-5.70	-3.74	-1.82	-2.19	-0.85	-2.14	-8.04	29.07	-20.42	-25.20	2.91
	CMAE	1.56	1.69	3.09	2.00	2.86	2.21	2.67	2.60	3.14	2.41	3.59	4.16	2.72	2.89	5.24
	Cσ	1.52	1.37	2.11	1.34	2.88	1.69	1.98	1.93	2.22	2.20	2.32	3.91	1.40	1.83	3.37
	CMaxErr	5.84	4.74	6.92	5.67	10.48	5.11	8.89	6.88	8.78	10.41	7.04	12.58	4.59	6.78	13.85
TMS	MAE	3.90	4.11	3.22	3.51	4.30	2.42	2.88	4.71	3.34	3.89	4.91	9.49	4.59	7.32	6.07
	σ	1.50	3.11	2.93	2.49	3.27	1.94	2.06	3.72	2.03	2.14	2.71	6.74	2.09	3.97	4.26
	MaxErr	7.14	10.22	8.78	7.41	10.58	5.64	8.57	14.82	7.09	7.52	8.29	22.18	7.08	14.85	10.92
	R^2	0.9991	0.9973	0.9903	0.9973	0.9933	0.9985	0.9983	0.9964	0.9981	0.9962	0.9869	0.9306	0.9632	0.9734	0.9833
	m	0.94	0.93	0.93	0.94	0.96	0.95	0.95	0.93	0.95	0.95	0.97	0.77	1.19	1.19	0.91
	b	4.45	3.65	5.13	2.42	0.12	2.24	3.23	3.56	3.77	2.84	1.28	22.08	-27.41	-32.20	8.22
	CMAE	1.22	2.25	2.64	1.97	3.08	1.53	1.69	2.96	2.18	2.35	4.54	4.16	2.72	2.89	4.81
	Cσ	1.30	1.45	2.49	1.34	2.77	1.18	1.39	1.55	1.57	1.74	2.16	3.91	1.40	1.83	3.24
	CMaxErr	4.80	6.32	7.79	5.03	10.07	3.59	6.29	6.38	5.95	6.63	8.14	12.58	4.59	6.78	13.17

Reference Standard	Parameter	Compound														
		106	**107**	**108**	**109**	**110**	**111**	**112**	**113**	**114**	**115**	**116**	**117**	**118**	**119**	**120**
MSTD	MAE	9.78	5.60	4.59	3.30	3.20	2.45	6.20	8.77	4.09	8.31	8.34	7.68	3.14	7.64	6.25
	σ	3.12	11.26	4.78	2.28	2.52	1.11	3.96	3.90	5.30	7.01	9.02	7.51	2.05	8.21	2.97
	MaxErr	15.46	45.40	19.45	7.89	7.87	3.92	13.23	14.62	19.04	28.24	32.31	26.05	7.87	25.09	11.78
	R^2	0.9961	0.9556	0.9877	0.9975	0.9980	0.9974	0.9888	0.9285	0.9793	0.9838	0.9669	0.9824	0.9962	0.9669	0.9091
	m	1.21	0.93	1.00	1.06	1.06	1.04	0.97	1.03	0.97	1.26	1.09	1.11	1.03	1.07	1.01
	b	-20.24	11.82	2.57	-5.15	-5.42	-4.70	6.97	-10.01	-1.41	-31.74	-14.25	-17.10	-4.28	-9.52	5.79
	CMAE	2.29	6.65	4.02	1.68	1.68	1.69	5.47	3.28	4.10	3.56	7.68	4.97	2.24	5.68	2.22
	Cσ	1.48	9.40	4.37	1.88	1.51	1.11	3.12	1.56	4.30	2.75	5.88	4.98	2.33	7.97	2.22
	CMaxErr	5.73	38.58	16.40	5.47	5.55	4.31	9.56	5.78	15.69	8.89	21.36	13.66	7.09	25.71	6.86
TMS	MAE	5.92	8.41	6.90	2.23	2.11	5.15	7.75	6.08	4.35	7.21	9.95	8.50	4.16	8.40	8.81
	σ	3.64	11.17	3.92	1.94	1.49	3.38	4.77	3.90	4.61	6.79	7.34	6.56	4.14	7.76	3.24
	MaxErr	12.78	48.09	14.45	6.34	4.72	10.82	15.92	11.93	16.35	25.56	29.62	23.36	11.78	26.10	14.47
	R^2	0.9962	0.9427	0.9818	0.9967	0.9975	0.9940	0.9852	0.9285	0.9830	0.9782	0.9619	0.9808	0.9952	0.9596	0.9091
	m	1.10	0.84	0.92	0.98	0.99	0.96	0.89	1.03	0.91	1.16	1.01	1.03	0.95	0.99	1.01
	b	-12.62	16.01	6.76	1.62	1.26	0.20	11.07	-7.32	4.11	-23.94	-7.56	-10.41	2.42	-2.83	8.48
	CMAE	2.28	7.74	4.90	2.25	1.98	2.61	6.21	3.28	3.84	4.26	8.05	5.17	2.74	5.54	2.22
	Cσ	1.47	10.66	5.33	1.77	1.59	1.64	3.78	1.56	3.74	3.00	6.61	5.23	2.37	9.38	2.22
	CMaxErr	5.31	43.87	18.95	5.68	4.72	5.54	12.26	5.78	13.97	8.98	22.40	14.05	7.39	30.02	6.86

Statistical parameters computed for compounds **1**-**200** at the mPW1PW91/6-31G(d)//AM1 level of theory

Reference Standard	Parameter	Compound														
		121	**122**	**123**	**124**	**125**	**126**	**127**	**128**	**129**	**130**	**131**	**132**	**133**	**134**	**135**
MSTD	MAE	3.12	5.75	8.63	7.64	13.19	6.42	7.69	6.44	7.51	6.34	4.87	4.99	2.93	5.28	4.35
	σ	2.37	3.39	4.45	2.46	4.33	4.66	5.72	5.05	7.72	4.59	3.97	5.28	4.44	5.49	5.43
	MaxErr	7.54	12.55	17.18	11.65	20.64	16.33	21.36	17.61	26.25	16.53	13.57	15.54	16.29	15.34	18.02
	R^2	0.9944	0.9957	0.9833	0.9801	0.9621	0.9693	0.9706	0.9869	0.9650	0.9911	0.9939	0.8933	0.9515	0.8836	0.9143
	m	1.01	1.05	1.07	1.04	1.03	0.98	0.99	1.02	1.00	1.00	0.99	0.89	0.87	0.88	0.95
	b	-0.94	-9.07	-11.75	-8.10	-13.46	-4.03	-0.17	3.25	-2.16	-2.77	-1.20	15.29	17.90	17.25	9.44
	CMAE	3.19	2.77	3.60	3.19	4.84	4.70	7.62	4.92	6.99	5.50	4.57	5.47	3.49	5.77	4.75
	Cσ	2.15	1.95	2.68	3.78	4.88	3.97	5.86	4.03	7.95	4.84	3.95	5.37	3.60	5.62	4.86
	CMaxErr	8.21	6.11	9.51	15.24	19.37	16.52	23.03	11.32	25.89	13.73	12.01	16.20	11.86	17.30	16.40
TMS	MAE	5.25	6.33	6.67	5.39	10.86	4.73	6.87	7.38	6.22	6.73	5.78	8.47	7.60	7.58	7.17
	σ	3.04	3.38	3.88	3.57	5.59	5.37	6.40	3.27	8.47	4.47	4.18	6.03	5.34	6.24	3.64
	MaxErr	12.60	12.42	14.49	16.22	21.89	18.90	24.20	14.40	33.25	13.84	10.88	22.53	23.28	22.34	16.90
	R^2	0.9938	0.9967	0.9879	0.9849	0.9695	0.9761	0.9756	0.9859	0.9676	0.9918	0.9947	0.8933	0.9515	0.8836	0.9143
	m	0.91	0.96	0.98	0.95	0.94	0.89	0.92	0.95	0.93	0.95	0.94	0.89	0.87	0.88	0.95
	b	4.73	-3.40	-5.66	-2.02	-7.37	2.05	5.14	8.56	3.15	1.79	3.37	8.29	10.90	10.26	2.44
	CMAE	3.31	2.46	3.15	2.92	4.47	4.34	6.70	5.12	6.24	5.19	4.35	5.47	3.49	5.77	4.75
	Cσ	2.31	1.59	2.14	3.16	4.20	3.20	5.61	4.17	8.06	4.70	3.58	5.37	3.60	5.62	4.86
	CMaxErr	10.29	5.06	7.67	12.51	17.00	13.75	19.48	11.80	27.55	13.18	11.35	16.20	11.86	17.30	16.40

Reference Standard	Parameter	Compound														
		136	**137**	**138**	**139**	**140**	**141**	**142**	**143**	**144**	**145**	**146**	**147**	**148**	**149**	**150**
MSTD	MAE	6.41	2.80	3.55	4.28	4.01	4.56	3.96	4.16	3.95	3.45	3.67	5.39	3.10	3.93	5.35
	σ	7.46	2.93	2.23	3.40	3.95	3.90	2.92	3.54	2.91	2.62	3.23	3.38	2.44	3.33	3.55
	MaxErr	27.40	12.56	6.62	13.32	13.55	11.75	9.86	13.04	11.13	9.57	12.37	10.71	7.71	11.87	14.42
	R^2	0.9153	0.9926	0.9938	0.9833	0.9909	0.9887	0.9915	0.9899	0.9934	0.9951	0.9919	0.9901	0.9927	0.9890	0.9845
	m	0.94	0.96	1.02	1.02	1.03	1.04	0.98	0.96	0.99	1.05	0.95	1.00	0.99	1.09	0.98
	b	-0.42	1.13	-3.33	-2.45	-4.54	-4.08	2.80	4.48	3.71	-3.28	5.46	4.58	2.23	-5.09	3.79
	CMAE	5.57	2.65	2.82	4.15	3.67	4.62	3.87	4.23	3.38	2.45	2.74	3.64	2.82	3.33	5.49
	Cσ	8.03	2.60	1.66	3.06	3.19	2.75	2.77	3.01	2.45	2.22	3.27	2.99	2.57	1.56	3.15
	CMaxErr	35.51	11.89	5.29	12.73	10.29	9.24	9.45	9.76	8.31	8.51	15.78	14.70	7.49	5.35	13.31
TMS	MAE	5.69	4.56	2.85	4.54	5.34	5.53	6.26	6.50	4.97	3.97	7.06	5.77	4.99	3.37	6.08
	σ	7.64	2.47	1.60	3.09	3.13	3.51	4.10	4.28	3.61	2.55	2.88	3.43	3.84	1.87	4.31
	MaxErr	32.48	11.82	5.14	11.18	10.86	10.47	12.55	15.72	13.82	12.26	13.15	11.65	13.84	7.80	11.90
	R^2	0.9166	0.9937	0.9943	0.9851	0.9927	0.9882	0.9892	0.9921	0.9953	0.9923	0.9924	0.9896	0.9944	0.9881	0.9886
	m	0.86	0.91	0.97	0.93	0.94	0.94	0.89	0.88	0.90	0.95	0.86	0.90	0.90	1.00	0.91
	b	5.00	5.42	1.08	3.21	1.39	1.85	8.04	9.72	8.95	2.47	11.22	10.33	7.44	0.67	7.97
	CMAE	5.65	2.39	2.73	3.75	2.90	4.82	4.03	3.71	2.74	3.09	2.89	3.90	2.36	3.33	4.54
	Cσ	7.87	2.47	1.55	3.13	3.29	2.64	3.56	2.68	2.25	2.76	2.95	2.83	2.35	1.86	2.98
	CMaxErr	34.23	11.35	5.53	13.10	9.90	9.31	10.98	8.67	7.10	13.99	14.25	13.12	7.84	7.24	10.58

Statistical parameters computed for compounds **1-200** at the mPW1PW91/6-31G(d)//AM1 level of theory

Reference Standard	Parameter	Compound														
		151	**152**	**153**	**154**	**155**	**156**	**157**	**158**	**159**	**160**	**161**	**162**	**163**	**164**	**165**
MSTD	MAE	3.97	3.95	4.38	3.51	4.58	8.02	5.27	3.53	5.08	4.30	5.70	3.98	11.09	5.07	5.13
	σ	4.72	2.86	3.16	3.19	3.72	9.31	5.73	4.11	2.22	4.38	3.86	4.30	8.91	3.21	3.86
	MaxErr	19.71	10.22	11.20	10.70	12.37	27.92	17.04	17.61	9.92	13.84	15.52	15.08	26.59	13.06	13.69
	R^2	0.9876	0.9917	0.9943	0.9933	0.9840	0.9680	0.9774	0.9753	0.9963	0.9594	0.9519	0.9885	0.9558	0.9715	0.9790
	m	0.96	0.97	1.01	1.15	1.00	1.01	0.99	1.15	1.02	1.09	0.89	1.07	0.90	0.95	0.94
	b	-0.05	0.35	-4.35	-16.69	-0.78	6.96	1.03	-17.65	3.55	-8.01	20.30	-6.24	16.49	1.08	4.27
	CMAE	3.67	3.43	2.80	1.39	4.74	6.71	5.24	2.19	1.80	2.80	2.80	3.36	8.62	5.11	5.17
	Cσ	4.19	2.97	2.49	1.40	3.40	6.55	5.86	1.94	2.03	2.27	2.80	3.19	6.16	3.01	3.31
	CMaxErr	15.22	11.25	8.97	4.31	11.52	20.28	16.97	6.50	7.11	6.30	11.50	11.69	18.33	12.00	13.45
TMS	MAE	4.12	4.30	3.59	4.88	5.23	6.13	6.72	5.41	6.76	4.61	3.55	4.67	13.17	5.91	5.84
	σ	5.74	4.36	3.16	2.05	3.54	7.06	5.16	2.28	3.38	2.03	2.39	3.42	8.38	2.56	4.47
	MaxErr	26.71	17.22	10.42	7.95	12.24	20.92	14.35	10.62	12.61	6.84	8.52	12.01	29.28	10.37	16.38
	R^2	0.9890	0.9927	0.9961	0.9904	0.9869	0.9735	0.9804	0.9753	0.9950	0.9594	0.9519	0.9870	0.9511	0.9783	0.9829
	m	0.90	0.90	0.94	1.06	0.91	0.93	0.90	1.15	0.97	1.09	0.89	0.96	0.83	0.87	0.89
	b	5.04	5.44	0.74	-12.32	4.81	10.73	7.36	-24.65	8.54	-15.01	13.31	0.35	22.26	6.64	8.67
	CMAE	3.34	3.08	2.34	1.69	4.37	6.23	5.40	2.19	2.40	2.80	2.80	3.48	9.32	4.48	4.38
	Cσ	4.05	2.95	2.03	1.65	2.91	5.81	4.89	1.94	2.01	2.27	2.80	3.50	6.13	2.56	3.40
	CMaxErr	14.64	13.32	7.08	5.79	10.69	17.78	14.30	6.50	7.19	6.30	11.50	14.17	21.18	10.68	14.71
Reference Standard	Parameter	Compound														
		166	**167**	**168**	**169**	**170**	**171**	**172**	**173**	**174**	**175**	**176**	**177**	**178**	**179**	**180**
MSTD	MAE	3.02	2.15	3.49	3.88	3.73	2.83	2.58	3.91	4.33	5.38	4.25	4.12	4.95	3.99	6.53
	σ	3.07	2.13	3.90	3.55	2.89	3.50	1.65	1.93	2.98	4.80	3.14	3.86	5.36	2.79	5.67
	MaxErr	11.05	7.01	18.00	12.70	11.04	10.78	5.52	8.44	12.95	14.21	9.04	13.28	17.07	9.86	16.21
	R^2	0.9916	0.9953	0.9901	0.9894	0.9943	0.9961	0.9746	0.9927	0.9907	0.9768	0.9801	0.9884	0.9840	0.9941	0.9892
	m	1.05	0.96	1.00	1.00	1.07	0.98	0.94	1.00	0.98	1.03	1.02	1.01	0.96	0.98	1.00
	b	-7.37	4.54	2.74	1.63	-6.79	-0.75	8.43	-1.14	0.36	-6.13	-1.34	-2.01	-1.29	3.62	-6.00
	CMAE	2.80	2.07	3.36	3.85	2.49	2.96	2.69	3.83	3.96	4.81	3.96	4.11	4.77	3.55	5.18
	Cσ	2.12	1.61	3.15	3.30	2.21	2.53	1.21	1.86	2.76	2.77	3.31	3.41	3.70	2.15	2.58
	CMaxErr	8.00	5.37	15.62	12.11	8.08	8.48	5.10	7.54	10.65	9.22	8.58	11.72	12.80	6.91	9.94
TMS	MAE	7.05	7.47	5.70	5.04	3.54	4.39	6.33	5.74	7.64	4.85	4.26	4.48	5.58	5.30	6.45
	σ	3.68	3.09	4.58	3.61	2.60	3.01	3.06	4.09	5.47	3.61	2.80	3.11	5.58	4.04	6.17
	MaxErr	16.73	14.00	20.68	15.38	8.35	10.85	11.91	13.42	19.95	11.52	10.25	10.59	22.65	12.55	23.15
	R^2	0.9899	0.9955	0.9842	0.9904	0.9942	0.9975	0.9746	0.9939	0.9861	0.9779	0.9822	0.9883	0.9907	0.9950	0.9888
	m	0.98	0.89	0.90	0.92	0.97	0.93	0.94	0.92	0.89	0.96	0.95	0.96	0.89	0.92	0.93
	b	-3.93	7.98	8.71	6.96	0.46	3.93	1.43	3.72	5.22	-0.53	4.25	2.52	4.08	8.30	-0.92
	CMAE	2.96	1.98	4.25	3.81	2.65	2.34	2.69	3.39	4.99	4.72	4.30	3.95	3.73	3.02	4.98
	Cσ	2.49	1.64	4.02	2.95	2.08	2.03	1.21	1.91	3.15	2.65	2.24	3.63	2.66	2.35	3.24
	CMaxErr	10.19	5.11	20.28	11.73	7.23	6.25	5.10	6.63	13.31	9.81	7.87	11.37	10.39	7.59	12.54

Statistical parameters computed for compounds **1**-**200** at the mPW1PW91/6-31G(d)//AM1 level of theory

Reference Standard	Parameter	Compound														
		181	**182**	**183**	**184**	**185**	**186**	**187**	**188**	**189**	**190**	**191**	**192**	**193**	**194**	**195**
MSTD	MAE	5.83	5.51	3.09	4.73	3.28	4.01	4.13	4.52	4.89	2.64	5.14	4.59	4.99	4.62	6.01
	σ	8.64	5.42	2.09	4.63	2.67	2.79	2.77	2.21	2.67	1.70	4.10	3.81	6.92	3.97	4.81
	MaxErr	41.79	27.97	8.00	18.27	10.72	9.50	11.66	9.10	9.26	6.18	14.31	11.65	26.90	15.39	17.83
	R^2	0.9730	0.9823	0.9953	0.9928	0.9913	0.9933	0.9930	0.9564	0.9922	0.9972	0.9923	0.9936	0.9735	0.9862	0.9868
	m	1.08	1.09	1.04	1.12	1.01	1.03	1.01	0.80	1.01	1.00	0.97	1.00	1.00	0.96	1.06
	b	-0.71	-9.28	-2.78	-10.08	-0.61	0.75	-1.21	28.14	3.00	0.03	6.34	3.38	0.43	4.18	-8.03
	CMAE	4.58	3.50	2.46	3.23	3.09	2.87	4.19	2.01	3.61	2.67	3.07	3.90	5.14	4.89	4.11
	Cσ	5.74	4.77	1.70	1.83	2.71	1.85	2.48	1.57	2.29	1.57	4.26	2.69	6.75	3.37	4.01
	CMaxErr	27.60	22.03	6.55	7.65	10.53	6.41	10.87	5.49	7.70	5.69	15.48	9.41	26.33	12.46	14.14
TMS	MAE	7.10	5.39	3.41	4.63	5.19	4.67	4.24	3.35	5.86	4.06	7.26	6.06	6.87	5.26	4.10
	σ	7.07	5.15	2.45	2.98	3.39	3.24	3.51	2.83	4.24	3.54	3.96	4.10	6.45	5.32	4.00
	MaxErr	34.79	20.97	8.07	11.27	13.92	12.17	12.33	11.32	11.95	10.96	17.00	12.97	29.59	22.38	15.14
	R^2	0.9582	0.9753	0.9942	0.9859	0.9864	0.9874	0.9945	0.9564	0.9918	0.9977	0.9921	0.9899	0.9699	0.9905	0.9890
	m	0.97	0.99	0.94	1.01	0.91	0.92	0.94	0.80	0.96	0.92	0.89	0.92	0.92	0.88	1.00
	b	6.85	-1.72	4.78	-2.52	6.95	7.88	3.82	21.14	7.51	4.45	10.76	7.80	6.37	10.00	-2.05
	CMAE	6.07	4.13	2.81	4.47	4.03	3.75	3.23	2.01	3.67	2.11	3.59	4.60	5.55	4.03	3.89
	Cσ	6.89	5.66	1.81	2.69	3.18	2.84	2.91	1.57	2.38	1.89	3.90	3.80	7.17	2.84	3.49
	CMaxErr	33.80	24.67	5.61	11.54	12.22	10.93	10.07	5.49	8.26	6.90	13.29	12.34	29.91	11.77	12.82

Reference Standard	Parameter	Compound				
		196	**197**	**198**	**199**	**200**
MSTD	MAE	3.72	5.33	5.81	4.29	4.87
	σ	3.63	3.09	4.11	3.95	3.80
	MaxErr	14.63	12.91	14.31	15.80	14.17
	R^2	0.9936	0.9894	0.9859	0.9908	0.9921
	m	1.03	0.98	1.02	1.00	1.04
	b	-4.81	4.45	-3.79	-2.07	0.42
	CMAE	3.00	4.45	4.97	3.60	3.41
	Cσ	2.62	3.24	4.41	3.98	2.53
	CMaxErr	10.72	10.01	14.94	13.17	10.01
TMS	MAE	3.29	5.89	5.12	4.61	3.38
	σ	2.94	4.26	4.50	5.52	2.18
	MaxErr	11.94	15.60	14.19	22.79	7.17
	R^2	0.9939	0.9920	0.9890	0.9923	0.9950
	m	0.96	0.91	0.95	0.92	0.95
	b	1.17	9.50	1.96	3.68	5.40
	CMAE	2.46	3.79	4.39	3.81	2.84
	Cσ	3.04	2.93	3.90	3.10	1.79
	CMaxErr	11.95	9.69	13.80	10.80	7.62

Statistical parameters computed for compounds **1-200** at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Reference Standard	Parameter	Compound														
		1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**
MSTD	MAE	1.70	1.93	1.60	2.07	1.33	1.84	1.93	2.22	2.18	1.60	1.86	1.80	2.68	2.04	1.32
	σ	1.22	1.54	1.58	1.20	0.92	0.74	1.07	1.92	0.85	1.24	0.92	0.99	1.27	1.46	0.86
	MaxErr	3.08	4.32	4.88	4.27	2.70	2.66	3.56	6.15	3.10	4.47	3.39	3.33	4.27	4.77	2.52
	R^2	0.9980	0.9923	0.9868	0.9973	0.9997	0.9998	0.9994	0.9960	0.9997	0.9988	0.9992	0.9992	0.9984	0.9962	0.9988
	m	0.98	0.92	0.91	1.00	1.01	1.01	1.01	1.00	1.01	1.00	0.99	0.99	0.99	0.99	1.01
	b	2.18	11.85	12.68	0.31	0.61	1.21	1.15	0.93	1.67	1.24	2.26	1.54	-0.27	2.28	0.20
	CMAE	1.65	1.44	1.29	2.04	0.69	0.48	1.05	1.86	0.58	1.20	0.96	1.60	2.15	1.70	0.94
	Cσ	1.08	1.13	1.31	1.20	0.39	0.39	0.73	1.87	0.47	1.26	1.12	0.89	1.37	1.25	0.67
	CMaxErr	3.10	3.21	3.78	3.94	1.38	1.43	2.44	4.66	1.15	3.54	3.56	2.80	4.95	4.37	2.62
TMS	MAE	4.45	7.03	7.27	4.75	1.97	3.04	4.15	2.62	2.72	2.69	3.02	4.09	4.56	2.54	1.85
	σ	4.04	2.50	2.30	3.26	1.97	2.02	2.22	3.45	1.54	2.33	2.15	3.45	4.22	2.54	1.81
	MaxErr	10.62	10.76	12.42	11.14	5.90	5.60	7.84	10.31	4.81	7.35	7.80	9.81	11.81	9.31	5.43
	R^2	0.9971	0.9923	0.9868	0.9984	0.9988	0.9997	0.9995	0.9953	0.9997	0.9992	0.9996	0.9995	0.9989	0.9962	0.9985
	m	0.91	0.92	0.91	0.93	0.95	0.92	0.94	0.92	0.93	0.94	0.93	0.93	0.93	0.91	0.93
	b	7.34	4.31	5.14	2.59	2.65	5.06	2.31	4.86	5.45	4.42	5.36	2.81	1.40	6.34	4.58
	CMAE	1.74	1.44	1.29	1.50	1.27	0.56	0.96	2.28	0.60	1.03	0.80	1.07	1.83	1.72	1.02
	Cσ	1.65	1.13	1.31	1.05	0.81	0.51	0.77	1.67	0.40	0.92	0.53	0.92	1.03	1.26	0.82
	CMaxErr	4.56	3.21	3.78	3.01	2.45	1.75	2.75	4.62	1.21	2.98	1.76	3.38	3.02	4.50	2.69
Reference Standard	Parameter	Compound														
		16	**17**	**18**	**19**	**20**	**21**	**22**	**23**	**24**	**25**	**26**	**27**	**28**	**29**	**30**
MSTD	MAE	2.07	1.75	1.84	1.37	0.87	1.35	1.10	1.72	1.18	1.12	1.66	1.09	1.33	1.22	1.64
	σ	1.63	0.91	1.07	0.69	0.85	1.02	0.51	1.46	0.80	0.86	1.00	0.90	0.78	1.51	1.68
	MaxErr	4.57	2.74	4.23	2.18	2.62	3.73	1.71	5.44	2.31	2.61	4.14	2.27	2.54	5.00	5.28
	R^2	0.9985	0.9995	0.9989	0.9988	0.9992	0.9993	0.9983	0.9995	0.9977	0.9980	0.9986	0.9990	0.9993	0.9988	0.9952
	m	0.97	1.01	0.99	0.98	1.01	0.99	0.93	0.95	0.96	0.97	1.06	1.00	0.99	0.89	0.96
	b	1.85	0.90	0.97	2.39	-0.93	1.30	3.83	3.04	3.09	2.72	-6.23	0.68	0.40	14.73	5.54
	CMAE	1.89	0.62	1.60	1.08	0.92	1.20	0.49	0.68	0.71	0.69	0.70	0.76	1.28	0.35	1.31
	Cσ	1.10	0.70	1.00	0.89	0.71	1.03	0.24	0.59	0.51	0.46	0.45	0.38	0.75	0.31	1.36
	CMaxErr	3.59	2.03	3.30	2.45	2.13	2.96	0.97	1.64	1.68	1.42	1.53	1.33	2.62	1.12	4.10
TMS	MAE	5.16	5.02	6.22	6.67	6.22	5.04	1.11	2.41	1.18	1.12	5.52	5.71	5.48	6.42	5.93
	σ	4.45	2.05	3.65	2.94	2.59	3.59	0.50	3.59	0.80	0.87	1.57	2.16	3.35	1.59	2.63
	MaxErr	12.11	7.73	11.77	9.72	8.32	11.26	1.71	12.98	2.31	2.61	7.12	7.50	9.41	7.99	11.20
	R^2	0.9986	0.9994	0.9996	0.9966	0.9996	0.9997	0.9983	0.9995	0.9977	0.9980	0.9976	0.9940	0.9996	0.9988	0.9987
	m	0.91	0.94	0.93	0.92	0.94	0.93	0.93	0.90	0.96	0.97	0.95	0.96	0.93	0.89	0.91
	b	3.04	1.70	1.83	3.68	0.79	2.40	3.83	5.25	3.09	2.72	0.74	-1.01	1.79	7.20	4.89
	CMAE	1.65	0.83	0.88	2.00	0.62	0.80	0.49	0.72	0.71	0.69	0.85	1.66	0.89	0.35	0.74
	Cσ	1.37	0.54	0.65	1.30	0.48	0.51	0.24	0.47	0.51	0.46	0.67	1.35	0.77	0.31	0.63
	CMaxErr	3.46	1.83	2.06	4.37	1.82	1.76	0.97	1.53	1.68	1.42	2.32	4.67	2.29	1.12	2.11

Statistical parameters computed for compounds **1-200** at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Reference Standard	Parameter	Compound														
		31	**32**	**33**	**34**	**35**	**36**	**37**	**38**	**39**	**40**	**41**	**42**	**43**	**44**	**45**
MSTD	MAE	1.80	1.42	0.85	1.19	1.48	2.11	2.11	0.90	1.36	0.93	1.18	0.84	1.02	1.46	1.63
	σ	1.27	1.19	0.61	1.24	0.82	1.43	2.47	0.89	1.45	0.70	1.25	0.78	0.77	1.67	1.18
	MaxErr	4.57	3.50	2.15	3.93	3.16	5.46	9.41	2.38	4.66	2.39	5.19	2.39	2.75	6.66	4.14
	R^2	0.9961	0.9989	0.9902	0.9996	0.9992	0.9958	0.9966	0.9997	0.9941	0.9951	0.9972	0.9996	0.9995	0.9976	0.9989
	m	1.00	1.01	0.96	1.01	1.01	1.01	1.00	1.00	0.96	0.92	1.00	0.98	0.98	1.01	0.99
	b	-0.36	-1.34	1.30	-0.47	-0.98	0.66	0.71	-0.05	6.19	2.33	0.26	0.80	1.06	0.15	0.32
	CMAE	1.79	1.41	0.82	1.08	1.20	1.74	2.21	0.88	1.44	0.56	1.23	0.65	0.79	1.25	1.34
	Cσ	1.26	0.99	0.54	0.70	0.89	1.43	2.35	0.87	0.88	0.57	1.19	0.60	0.53	1.51	1.01
	CMaxErr	4.77	3.47	1.95	2.66	2.74	4.48	9.16	2.47	3.01	1.99	4.99	1.88	1.73	5.46	3.74
TMS	MAE	5.86	4.90	0.85	2.56	3.66	2.52	3.02	2.56	6.85	0.93	1.42	1.24	1.42	2.08	4.63
	σ	2.99	3.86	0.61	2.65	2.66	1.83	3.12	3.03	1.89	0.70	1.85	2.21	2.24	2.31	4.39
	MaxErr	12.11	10.95	2.15	7.01	8.56	6.35	10.62	7.94	9.99	2.39	8.34	9.92	10.28	7.33	11.68
	R^2	0.9978	0.9979	0.9902	0.9993	0.9989	0.9948	0.9988	0.9999	0.9941	0.9951	0.9990	0.9997	0.9996	0.9987	0.9988
	m	0.92	0.94	0.96	0.96	0.94	0.94	0.94	0.96	0.96	0.92	0.94	0.94	0.94	0.94	0.91
	b	3.63	1.78	1.30	1.26	1.34	3.31	2.76	1.41	-1.35	2.33	2.39	2.05	2.41	2.46	2.85
	CMAE	1.22	2.02	0.82	1.23	1.55	1.98	1.40	0.51	1.44	0.56	0.76	0.59	0.66	1.03	1.31
	Cσ	1.08	1.23	0.54	1.11	0.76	1.52	1.33	0.56	0.88	0.57	0.67	0.48	0.51	1.02	1.12
	CMaxErr	3.18	4.96	1.95	3.71	2.69	5.28	5.28	1.57	3.01	1.99	2.51	1.43	1.61	4.51	4.11
Reference Standard	Parameter	Compound														
		46	**47**	**48**	**49**	**50**	**51**	**52**	**53**	**54**	**55**	**56**	**57**	**58**	**59**	**60**
MSTD	MAE	2.25	1.16	1.74	0.99	3.35	1.86	2.57	1.79	1.39	2.40	2.37	1.77	3.05	1.55	1.58
	σ	1.70	1.11	1.84	0.82	2.26	1.98	1.25	1.52	1.00	2.75	1.71	1.13	1.73	1.39	1.21
	MaxErr	7.64	4.20	7.30	2.72	7.90	8.14	4.92	5.82	3.62	7.63	5.16	4.88	6.56	5.14	4.53
	R^2	0.9974	0.9992	0.9976	0.9993	0.9940	0.9981	0.9901	0.9980	0.9987	0.9956	0.9968	0.9927	0.9985	0.9939	0.9980
	m	0.98	1.01	0.97	1.02	0.98	0.97	1.02	1.02	1.01	0.97	0.99	1.04	0.99	0.93	1.01
	b	2.44	-0.06	3.75	-0.79	3.07	0.74	-0.62	-0.41	-0.59	3.11	0.81	-3.86	3.48	10.13	-0.48
	CMAE	1.94	1.04	1.71	0.74	3.11	1.34	2.04	1.56	1.31	2.62	2.37	1.31	1.37	1.06	1.49
	Cσ	1.76	0.76	1.36	0.59	2.43	1.69	1.22	1.35	1.00	2.20	1.69	0.87	0.97	0.87	1.17
	CMaxErr	6.67	3.05	4.54	1.73	9.11	7.16	4.65	4.19	3.50	7.33	5.25	3.13	3.42	2.55	4.62
TMS	MAE	5.29	3.46	6.23	1.30	5.87	2.56	5.59	2.28	4.52	6.06	3.84	6.41	3.21	6.45	3.53
	σ	3.90	3.00	2.96	1.55	3.42	4.03	2.70	2.49	2.93	4.73	3.36	1.80	1.79	1.80	2.70
	MaxErr	15.18	8.37	10.85	5.02	11.67	15.68	10.57	9.46	9.50	13.81	11.97	9.53	6.56	10.00	8.19
	R^2	0.9981	0.9993	0.9971	0.9993	0.9970	0.9987	0.9894	0.9978	0.9993	0.9960	0.9983	0.9927	0.9984	0.9939	0.9992
	m	0.91	0.93	0.91	0.95	0.92	0.92	0.95	0.95	0.93	0.91	0.93	1.04	0.95	0.93	0.93
	b	4.43	2.33	5.72	1.61	4.22	2.61	0.69	1.85	1.96	3.96	3.65	-11.39	5.27	2.60	2.56
	CMAE	1.89	0.98	1.79	0.74	1.84	1.21	1.96	1.66	0.93	2.48	1.45	1.31	1.48	1.06	0.89
	Cσ	1.22	0.73	1.62	0.53	2.11	1.29	1.50	1.37	0.84	2.13	1.53	0.87	0.98	0.87	0.79
	CMaxErr	5.04	2.56	5.22	2.10	6.90	4.36	4.76	4.16	2.60	6.41	4.96	3.13	3.44	2.55	2.86

Statistical parameters computed for compounds **1-200** at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Reference Standard	Parameter	Compound														
		61	**62**	**63**	**64**	**65**	**66**	**67**	**68**	**69**	**70**	**71**	**72**	**73**	**74**	**75**
MSTD	MAE	1.29	1.11	1.87	2.34	2.27	0.96	2.65	1.99	2.00	1.74	1.54	1.17	1.10	2.33	2.39
	σ	1.18	0.85	1.32	1.55	2.10	0.88	2.02	1.88	1.79	1.37	1.27	1.19	0.64	1.61	2.12
	MaxErr	3.02	3.66	4.55	5.78	7.31	3.43	8.52	7.31	6.65	5.05	4.49	4.22	2.99	6.11	9.05
	R^2	0.9988	0.9987	0.9809	0.9933	0.9959	0.9993	0.9927	0.9965	0.9980	0.9983	0.9982	0.9996	0.9994	0.9837	0.9966
	m	1.00	1.01	0.93	0.98	1.02	0.99	0.98	0.97	1.00	1.00	1.01	0.99	0.99	0.91	1.00
	b	0.62	0.07	10.78	1.60	-1.53	0.51	1.80	2.26	1.92	0.61	-1.33	1.54	1.34	12.78	1.66
	CMAE	1.34	1.07	1.03	2.15	2.22	0.87	2.60	1.80	1.70	1.50	1.46	0.88	0.59	2.00	2.08
	Cσ	1.04	0.64	0.80	1.32	1.86	0.74	1.90	1.39	1.20	1.37	1.18	0.85	0.79	1.26	2.04
	CMaxErr	3.02	2.55	2.92	4.38	6.84	2.38	7.32	5.04	5.24	5.58	3.95	2.93	2.93	4.51	7.85
TMS	MAE	2.46	1.55	5.72	7.93	3.80	1.47	7.43	7.93	3.08	2.35	4.05	2.24	4.89	6.77	4.37
	σ	3.27	1.73	1.40	2.84	2.72	2.69	4.04	3.43	2.79	2.62	2.99	2.48	2.73	2.79	3.33
	MaxErr	10.47	6.92	8.00	13.32	7.98	10.97	16.05	14.85	9.83	11.91	10.05	7.53	8.58	12.09	11.15
	R^2	0.9981	0.9992	0.9809	0.9965	0.9983	0.9973	0.9934	0.9983	0.9974	0.9990	0.9979	0.9995	0.9980	0.9837	0.9976
	m	0.94	0.94	0.93	0.93	0.95	0.95	0.93	0.92	0.92	0.94	0.93	0.95	0.92	0.91	0.93
	b	3.02	2.31	3.24	1.40	1.57	1.84	2.02	2.85	4.47	2.67	2.23	3.09	4.97	5.24	3.36
	CMAE	1.85	0.71	1.03	1.52	1.43	1.52	2.57	1.26	1.88	1.22	1.69	1.09	1.38	2.00	1.69
	Cσ	1.11	0.68	0.80	1.00	1.18	1.57	1.64	0.96	1.44	1.01	1.13	0.83	1.20	1.26	1.79
	CMaxErr	3.40	2.26	2.92	4.31	4.07	4.92	6.83	3.53	5.07	4.73	3.65	2.59	5.19	4.51	6.68
Reference Standard	Parameter	Compound														
		76	**77**	**78**	**79**	**80**	**81**	**82**	**83**	**84**	**85**	**86**	**87**	**88**	**89**	**90**
MSTD	MAE	2.10	1.12	1.10	1.48	1.43	2.49	1.35	0.96	2.11	2.22	1.38	2.77	1.03	1.44	1.33
	σ	1.90	1.12	1.05	1.52	0.69	2.98	1.01	0.82	2.17	2.06	0.77	2.48	1.08	1.17	0.94
	MaxErr	7.86	4.56	3.16	6.19	3.51	13.13	3.56	3.22	8.88	7.40	3.76	8.91	4.12	3.60	3.43
	R^2	0.9975	0.9982	0.9991	0.9984	0.9994	0.9956	0.9992	0.9992	0.9969	0.9974	0.9991	0.9592	0.9997	0.9992	0.9987
	m	1.00	1.01	0.99	1.01	0.98	1.01	1.01	1.00	1.04	1.00	1.01	0.99	0.97	0.99	1.01
	b	1.01	-0.43	0.56	-0.35	0.97	0.38	-0.18	0.12	-3.85	0.60	0.30	3.47	1.23	2.95	-0.33
	CMAE	1.83	1.21	1.11	1.33	1.13	2.26	1.33	0.97	1.56	2.29	0.88	1.92	0.69	1.03	1.28
	Cσ	1.91	0.95	0.96	1.38	0.76	2.73	0.94	0.80	1.74	1.95	0.86	1.54	0.55	0.55	0.71
	CMaxErr	6.86	4.02	3.10	5.00	3.16	10.60	3.03	3.40	6.26	7.13	3.02	6.20	1.84	2.27	2.54
TMS	MAE	3.73	1.49	1.60	2.10	2.38	2.73	2.02	3.46	4.18	3.35	4.46	4.94	1.57	5.23	1.94
	σ	3.35	1.80	1.94	2.21	2.54	2.88	2.42	3.40	3.00	3.13	2.74	2.13	2.97	2.32	2.07
	MaxErr	12.76	7.36	7.60	6.88	8.76	11.93	9.09	10.76	8.89	9.44	9.28	7.59	11.65	7.97	8.34
	R^2	0.9978	0.9986	0.9991	0.9990	0.9996	0.9955	0.9995	0.9993	0.9967	0.9984	0.9982	0.9592	0.9996	0.9961	0.9990
	m	0.94	0.95	0.96	0.95	0.94	0.96	0.96	0.92	0.95	0.94	0.93	0.99	0.94	0.92	0.94
	b	2.95	1.84	2.00	1.74	2.53	2.06	1.68	3.92	-0.39	2.42	3.86	-4.07	2.65	5.74	1.94
	CMAE	1.76	0.97	1.20	1.21	0.90	2.06	1.03	0.98	1.67	1.83	1.20	1.92	0.81	2.24	1.07
	Cσ	1.75	0.93	0.85	0.83	0.69	2.94	0.81	0.68	1.73	1.44	1.26	1.54	0.54	1.23	0.68
	CMaxErr	6.13	3.05	2.87	3.12	2.43	9.54	2.43	2.33	7.02	5.71	5.37	6.20	1.97	5.63	2.40

Statistical parameters computed for compounds **1-200** at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Reference Standard	Parameter	Compound														
		91	**92**	**93**	**94**	**95**	**96**	**97**	**98**	**99**	**100**	**101**	**102**	**103**	**104**	**105**
MSTD	MAE	2.05	1.35	1.84	1.49	2.25	1.58	1.57	3.03	1.11	2.05	3.83	5.90	4.47	4.93	5.72
	σ	1.37	1.44	1.62	1.21	2.21	1.35	1.58	2.34	0.77	1.70	2.88	7.01	4.99	4.33	5.30
	MaxErr	4.80	3.79	4.38	4.61	9.69	4.84	6.21	10.67	3.44	6.82	8.55	21.68	13.57	13.17	17.19
	R^2	0.9990	0.9986	0.9963	0.9983	0.9966	0.9983	0.9984	0.9972	0.9996	0.9977	0.9906	0.9124	0.9612	0.9714	0.9771
	m	0.99	1.00	1.01	1.00	1.00	0.99	1.00	0.99	1.00	1.00	1.02	0.66	1.19	1.23	0.97
	b	2.38	-0.54	0.42	-0.28	-1.36	0.77	0.92	-1.47	0.46	0.86	-0.66	42.53	-20.58	-31.93	5.59
	CMAE	1.38	1.43	1.88	1.46	1.87	1.61	1.44	2.20	1.06	1.85	3.40	4.66	2.56	3.07	5.22
	Cσ	1.31	1.33	1.17	1.20	2.29	1.27	1.55	1.97	0.75	1.32	2.69	4.51	1.86	1.76	4.41
	CMaxErr	3.92	3.55	3.80	4.60	10.59	4.56	5.77	7.39	3.11	5.44	7.67	14.61	5.49	6.09	12.98
TMS	MAE	3.88	4.45	2.35	4.25	4.83	2.49	2.34	5.27	2.88	4.17	4.99	11.24	5.31	8.17	5.91
	σ	3.15	3.39	2.10	3.12	3.96	2.77	2.94	4.46	2.99	2.86	2.56	8.54	1.94	6.10	5.22
	MaxErr	11.06	11.02	7.47	10.42	11.75	9.82	11.57	18.21	8.96	9.55	8.56	29.22	7.21	20.71	17.19
	R^2	0.9994	0.9979	0.9942	0.9987	0.9960	0.9976	0.9988	0.9985	0.9997	0.9986	0.9881	0.9124	0.9612	0.9714	0.9776
	m	0.93	0.94	0.95	0.93	0.94	0.94	0.94	0.93	0.94	0.94	0.94	0.66	1.19	1.23	0.90
	b	3.73	1.99	2.87	2.42	1.08	3.34	2.76	0.92	1.96	2.64	4.51	34.99	-28.12	-39.46	7.63
	CMAE	1.31	1.85	2.25	1.24	2.12	1.85	1.66	1.59	0.78	1.56	4.29	4.66	2.56	3.07	4.99
	Cσ	0.67	1.45	1.63	1.13	2.41	1.57	0.83	1.48	0.62	0.89	2.16	4.51	1.86	1.76	4.60
	CMaxErr	2.71	4.38	5.22	4.61	10.27	5.03	3.57	7.01	2.39	3.51	8.60	14.61	5.49	6.09	13.33
Reference Standard	Parameter	Compound														
		106	**107**	**108**	**109**	**110**	**111**	**112**	**113**	**114**	**115**	**116**	**117**	**118**	**119**	**120**
MSTD	MAE	7.60	5.80	5.41	2.64	2.89	1.96	6.52	6.19	4.46	6.04	9.06	6.99	2.65	6.08	8.22
	σ	2.70	11.55	4.22	1.81	2.03	0.77	4.22	4.04	4.32	6.81	8.47	7.31	1.80	7.93	4.31
	MaxErr	11.78	46.99	15.59	7.19	7.57	3.47	13.68	12.01	15.52	25.54	31.67	24.12	5.54	24.11	15.57
	R^2	0.9972	0.9551	0.9873	0.9988	0.9987	0.9981	0.9923	0.9230	0.9833	0.9818	0.9582	0.9802	0.9967	0.9691	0.8764
	m	1.17	0.93	0.99	1.03	1.03	1.03	0.94	1.03	0.91	1.19	1.05	1.07	0.99	1.04	1.14
	b	-15.46	12.46	3.91	-0.31	-0.33	-3.57	10.68	-7.34	3.88	-24.63	-9.61	-12.58	0.33	-4.90	4.32
	CMAE	1.84	6.51	3.89	1.47	1.44	1.45	4.77	3.60	4.00	4.00	8.24	5.22	2.20	5.35	3.22
	Cσ	1.44	9.59	4.61	0.88	1.12	0.95	2.05	1.09	3.47	2.57	7.20	5.36	2.08	7.80	1.84
	CMaxErr	4.54	39.59	12.99	3.82	4.16	3.21	6.90	5.43	13.12	9.68	23.81	14.32	7.16	25.50	6.52
TMS	MAE	5.78	7.34	6.12	2.58	2.51	6.64	7.11	6.19	5.15	8.61	12.06	10.08	5.54	9.21	8.23
	σ	3.17	11.14	4.77	1.77	1.78	2.88	4.46	4.04	5.32	6.18	7.15	7.21	5.19	6.56	4.31
	MaxErr	11.35	46.99	17.20	5.45	5.59	11.01	13.68	12.01	15.52	25.54	31.67	25.26	12.02	24.11	15.57
	R^2	0.9970	0.9454	0.9826	0.9968	0.9970	0.9965	0.9912	0.9230	0.9860	0.9797	0.9520	0.9778	0.9955	0.9633	0.8764
	m	1.09	0.86	0.93	0.97	0.97	0.96	0.89	1.03	0.86	1.11	0.99	1.00	0.92	0.97	1.14
	b	-11.61	13.63	5.08	2.87	2.78	-1.85	11.78	-7.34	6.10	-20.64	-6.49	-9.45	3.45	-1.77	4.33
	CMAE	1.92	7.51	4.53	2.40	2.16	2.06	4.98	3.60	3.79	4.10	8.47	5.50	2.55	5.78	3.22
	Cσ	1.49	10.41	5.44	1.41	1.77	1.12	2.49	1.09	2.99	2.93	8.21	5.71	2.41	8.58	1.84
	CMaxErr	4.11	43.70	15.60	4.18	5.45	4.09	8.80	5.43	11.56	9.80	24.80	15.81	7.40	28.91	6.52

Statistical parameters computed for compounds **1-200** at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Reference Standard	Parameter	Compound														
		121	**122**	**123**	**124**	**125**	**126**	**127**	**128**	**129**	**130**	**131**	**132**	**133**	**134**	**135**
MSTD	MAE	3.27	4.50	7.26	6.18	11.18	5.23	6.54	5.90	6.85	5.43	5.17	5.70	3.68	6.03	4.10
	σ	2.81	2.66	4.06	3.94	4.64	2.78	5.35	4.60	8.26	4.22	3.22	6.59	4.82	6.41	5.43
	MaxErr	11.83	9.61	16.58	17.15	19.51	9.72	18.37	15.56	26.81	14.32	10.79	21.53	15.97	21.13	16.89
	R^2	0.9932	0.9956	0.9865	0.9798	0.9685	0.9855	0.9767	0.9901	0.9638	0.9932	0.9952	0.8492	0.9384	0.8453	0.9126
	m	0.99	1.04	1.04	0.99	1.03	1.00	0.98	1.01	0.98	0.98	0.98	0.83	0.85	0.82	0.95
	b	1.53	-6.11	-9.34	-4.79	-11.75	-4.28	1.25	4.40	0.24	-0.62	-0.67	22.93	19.81	25.35	7.88
	CMAE	3.33	2.86	3.04	3.33	4.84	3.11	6.56	4.64	6.89	4.60	4.23	6.26	3.79	6.43	4.84
	Cσ	2.66	1.88	2.67	3.70	3.92	2.82	5.45	2.94	8.28	4.48	3.28	6.96	4.26	7.00	4.87
	CMaxErr	10.94	6.63	9.86	11.93	15.58	11.96	19.76	10.57	26.32	12.67	9.65	21.21	14.03	23.08	16.07
TMS	MAE	4.99	6.54	7.97	6.41	11.21	5.22	6.07	5.49	7.35	7.10	6.85	9.45	8.85	7.94	8.13
	σ	4.22	3.63	3.58	4.88	5.70	4.18	6.64	3.83	8.76	4.64	4.28	7.72	5.98	7.68	3.89
	MaxErr	13.93	14.47	16.58	17.15	19.50	16.95	25.71	12.46	34.35	14.32	13.86	29.07	23.51	28.66	19.29
	R^2	0.9918	0.9962	0.9899	0.9850	0.9740	0.9885	0.9800	0.9886	0.9652	0.9937	0.9958	0.8492	0.9384	0.8453	0.9126
	m	0.92	0.96	0.98	0.92	0.96	0.93	0.92	0.95	0.92	0.94	0.93	0.83	0.85	0.82	0.95
	b	3.85	-3.78	-6.70	-2.14	-9.10	-1.64	3.29	6.44	2.28	0.84	0.80	15.39	12.27	17.81	0.34
	CMAE	3.49	2.66	2.68	2.75	4.43	3.05	5.84	5.27	6.91	4.51	4.04	6.26	3.79	6.43	4.84
	Cσ	3.10	1.74	2.24	3.28	3.48	2.13	5.33	2.61	7.98	4.17	2.96	6.96	4.26	7.00	4.87
	CMaxErr	12.76	5.73	8.45	10.34	13.50	9.56	16.83	10.65	26.37	12.19	9.05	21.21	14.03	23.08	16.07
Reference Standard	Parameter	Compound														
		136	**137**	**138**	**139**	**140**	**141**	**142**	**143**	**144**	**145**	**146**	**147**	**148**	**149**	**150**
MSTD	MAE	4.94	3.63	2.47	3.47	3.73	5.69	4.26	4.27	4.34	3.17	3.86	4.26	3.33	3.76	6.33
	σ	7.52	2.11	1.91	4.05	3.43	2.59	3.51	2.42	2.85	3.25	3.03	2.84	3.14	3.22	3.27
	MaxErr	27.35	8.07	6.85	17.50	11.93	9.58	11.08	8.74	11.12	16.63	11.11	10.12	12.32	9.75	12.28
	R^2	0.9243	0.9934	0.9951	0.9857	0.9919	0.9848	0.9895	0.9922	0.9930	0.9917	0.9930	0.9951	0.9909	0.9871	0.9818
	m	0.94	0.94	1.01	1.04	1.00	0.97	0.97	0.96	0.97	1.02	0.94	0.97	0.96	1.07	0.94
	b	1.21	3.47	-1.47	-1.77	-1.99	1.66	4.21	4.66	5.41	-1.25	6.44	5.99	5.65	-3.10	7.20
	CMAE	4.31	2.81	2.38	3.64	3.37	5.69	3.93	3.78	3.20	2.84	3.34	2.63	3.24	3.31	5.91
	Cσ	8.14	2.05	1.67	3.09	3.13	2.57	3.60	2.55	2.91	3.23	2.11	2.00	2.79	2.22	3.50
	CMaxErr	34.43	8.94	7.18	13.48	9.88	10.08	11.73	8.84	8.86	15.91	8.29	7.22	10.68	8.50	12.33
TMS	MAE	4.93	4.03	2.67	3.46	6.68	7.79	6.81	6.16	5.15	5.61	6.74	5.13	6.33	3.52	7.74
	σ	7.77	3.21	2.04	3.07	3.89	3.62	4.74	4.31	3.89	3.48	3.48	2.96	4.98	2.83	5.94
	MaxErr	32.27	14.58	6.85	10.15	11.98	14.29	15.25	15.21	15.57	16.64	13.87	11.00	19.86	9.75	19.03
	R^2	0.9259	0.9936	0.9947	0.9880	0.9930	0.9841	0.9873	0.9938	0.9943	0.9873	0.9920	0.9935	0.9912	0.9841	0.9835
	m	0.88	0.91	0.98	0.97	0.93	0.90	0.90	0.89	0.90	0.95	0.87	0.90	0.89	1.00	0.88
	b	3.34	4.72	-0.13	0.54	0.53	4.19	6.20	6.65	7.39	1.14	8.83	8.38	7.62	-0.71	8.35
	CMAE	4.40	2.77	2.40	2.98	3.01	5.63	4.11	3.47	2.97	3.37	3.41	3.10	3.17	3.55	5.68
	Cσ	7.98	2.01	1.84	3.23	3.04	3.02	4.17	2.09	2.53	4.15	2.47	2.21	2.73	2.68	3.20
	CMaxErr	33.37	8.40	7.99	13.81	9.55	9.49	13.10	7.93	7.88	20.81	10.03	9.74	9.14	10.46	11.22

Statistical parameters computed for compounds **1**-**200** at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Reference Standard	Parameter	Compound														
		151	**152**	**153**	**154**	**155**	**156**	**157**	**158**	**159**	**160**	**161**	**162**	**163**	**164**	**165**
MSTD	MAE	2.86	3.96	2.89	3.05	4.35	7.16	6.62	2.85	5.66	3.80	5.20	3.35	13.10	3.38	4.06
	σ	4.08	2.59	2.54	2.34	2.07	8.98	5.64	2.06	3.61	3.24	2.41	4.00	8.78	2.00	4.26
	MaxErr	16.65	9.99	8.65	10.59	7.70	25.99	18.80	8.43	11.69	12.44	10.10	13.47	28.00	8.14	17.62
	R^2	0.9918	0.9918	0.9963	0.9914	0.9887	0.9638	0.9716	0.9663	0.9916	0.9575	0.9639	0.9894	0.9462	0.9872	0.9886
	m	0.96	0.96	1.00	1.11	0.99	0.96	0.96	0.98	1.02	1.04	0.85	1.01	0.88	0.98	0.95
	b	0.86	1.99	-2.44	-12.57	0.74	9.86	3.79	4.12	4.31	-2.27	23.54	-3.54	19.40	0.86	5.96
	CMAE	2.74	3.48	2.42	1.92	4.27	7.37	6.32	2.73	3.45	2.81	2.45	3.34	8.95	3.41	2.72
	Cσ	3.61	2.84	1.82	1.10	2.30	6.74	6.15	2.07	2.08	2.41	2.36	2.93	7.69	1.98	3.67
	CMaxErr	12.34	10.56	6.29	3.76	8.04	20.47	20.07	8.58	7.77	7.85	7.25	11.28	22.34	8.08	14.86
TMS	MAE	3.24	4.50	3.63	5.86	5.04	7.83	7.43	6.53	5.67	5.15	3.84	5.75	13.79	3.92	4.57
	σ	5.69	4.20	3.61	2.37	2.63	5.85	5.95	3.43	3.60	3.04	3.45	5.28	7.50	2.13	4.38
	MaxErr	24.19	15.94	11.48	10.59	10.08	18.45	18.80	15.96	11.70	11.04	11.63	21.01	28.00	8.14	17.62
	R^2	0.9922	0.9923	0.9964	0.9932	0.9907	0.9681	0.9742	0.9663	0.9885	0.9575	0.9639	0.9883	0.9410	0.9903	0.9874
	m	0.91	0.91	0.95	1.04	0.92	0.90	0.90	0.98	0.98	1.04	0.85	0.93	0.82	0.91	0.92
	b	2.74	3.87	-0.57	-11.26	3.00	10.70	6.63	-3.42	6.10	-9.81	16.00	-0.50	21.80	3.10	7.29
	CMAE	2.92	3.44	2.41	1.66	3.87	6.84	6.12	2.73	4.07	2.81	2.45	3.19	9.67	3.00	2.81
	Cσ	3.31	2.70	1.74	1.06	2.09	6.40	5.72	2.07	2.40	2.41	2.36	3.43	7.71	1.66	3.89
	CMaxErr	11.94	12.13	6.33	3.45	7.45	18.48	18.05	8.58	7.86	7.85	7.25	13.98	25.52	6.82	15.87

Reference Standard	Parameter	Compound														
		166	**167**	**168**	**169**	**170**	**171**	**172**	**173**	**174**	**175**	**176**	**177**	**178**	**179**	**180**
MSTD	MAE	3.23	3.38	3.02	3.53	2.75	3.12	3.85	3.53	4.00	3.59	3.67	3.08	3.46	4.74	4.97
	σ	2.99	3.40	2.87	3.72	2.22	3.30	2.91	2.48	3.22	3.73	3.02	2.66	4.15	4.03	3.75
	MaxErr	9.39	12.20	11.88	16.40	7.42	10.94	10.54	9.83	13.55	12.26	9.51	8.60	12.79	11.95	12.51
	R^2	0.9924	0.9920	0.9944	0.9925	0.9958	0.9974	0.9452	0.9928	0.9925	0.9861	0.9857	0.9933	0.9897	0.9940	0.9959
	m	1.02	0.92	1.00	0.99	1.03	0.95	0.90	0.98	0.95	1.04	1.02	1.00	0.97	0.95	0.98
	b	-4.73	7.38	2.17	3.53	-4.17	4.11	11.26	1.38	2.74	-4.51	0.12	0.00	0.01	6.84	-3.68
	CMAE	2.93	2.67	2.59	3.11	2.07	2.86	4.03	3.62	3.19	3.68	3.37	3.07	3.63	3.50	3.05
	Cσ	1.58	2.17	2.30	2.94	2.01	1.37	1.77	2.19	2.94	2.21	2.76	2.62	3.20	2.28	1.85
	CMaxErr	6.45	8.31	9.59	13.32	7.20	4.85	8.05	7.84	11.04	9.12	9.02	8.77	9.70	7.88	6.09
TMS	MAE	9.33	9.43	4.15	4.09	5.05	4.19	9.50	6.59	8.27	3.71	3.67	3.58	4.93	5.69	6.58
	σ	3.56	4.65	3.08	3.97	2.75	5.21	4.49	4.38	5.45	3.96	2.67	2.79	5.19	4.07	5.29
	MaxErr	16.86	19.74	11.88	16.41	11.02	18.48	18.08	17.36	21.09	12.25	7.64	8.61	19.75	11.96	20.05
	R^2	0.9928	0.9930	0.9913	0.9910	0.9953	0.9968	0.9452	0.9935	0.9901	0.9851	0.9847	0.9919	0.9929	0.9938	0.9957
	m	0.96	0.87	0.93	0.93	0.96	0.91	0.90	0.91	0.89	0.99	0.97	0.97	0.91	0.91	0.93
	b	-4.15	7.97	4.73	5.59	-0.61	5.66	3.72	3.07	4.43	-2.25	2.39	1.44	2.10	8.40	-1.82
	CMAE	2.57	2.49	3.27	3.65	2.48	3.18	4.03	3.25	3.89	3.74	3.81	3.56	2.88	3.48	3.07
	Cσ	1.99	2.02	2.83	2.92	1.75	1.45	1.77	2.40	3.14	2.41	2.38	2.67	2.79	2.50	2.02
	CMaxErr	8.10	7.75	12.66	13.89	5.97	5.36	8.05	8.49	13.14	9.56	8.70	10.39	8.69	8.97	8.25

Statistical parameters computed for compounds **1**-**200** at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Reference Standard	Parameter	Compound														
		181	**182**	**183**	**184**	**185**	**186**	**187**	**188**	**189**	**190**	**191**	**192**	**193**	**194**	**195**
MSTD	MAE	5.85	4.80	2.54	3.36	3.04	3.74	3.37	4.29	5.32	3.07	6.51	5.61	4.48	4.82	3.84
	σ	8.18	4.35	2.40	3.21	2.69	4.17	2.57	2.77	3.89	2.87	6.03	4.77	6.90	5.43	3.27
	MaxErr	39.33	21.28	9.33	9.67	9.85	17.89	8.22	10.23	11.59	9.97	20.28	14.74	29.90	23.02	12.95
	R^2	0.9746	0.9880	0.9940	0.9939	0.9920	0.9884	0.9948	0.9210	0.9933	0.9954	0.9870	0.9908	0.9748	0.9826	0.9917
	m	1.08	1.08	1.01	1.07	0.97	1.00	0.99	0.74	0.98	0.98	0.93	0.99	0.98	0.94	1.03
	b	-1.62	-8.49	-0.97	-5.37	2.89	3.13	1.39	35.55	6.09	2.34	10.23	5.59	3.14	7.28	-3.42
	CMAE	4.62	2.96	2.45	2.85	2.79	3.08	3.19	2.34	3.48	2.97	5.00	4.45	4.70	5.06	3.33
	Cσ	5.39	3.84	2.35	1.90	2.80	3.33	2.75	2.62	1.82	2.69	4.56	3.54	6.83	4.40	3.06
	CMaxErr	25.28	17.43	9.75	7.20	11.96	14.66	9.05	9.53	6.41	9.72	16.23	10.75	28.68	18.29	11.57
TMS	MAE	5.75	6.49	4.20	4.07	5.65	4.73	4.09	4.57	5.67	4.55	8.66	5.96	6.97	5.29	3.92
	σ	6.57	3.69	3.25	3.58	3.39	4.16	3.88	4.01	3.72	4.41	4.97	4.69	6.68	6.87	3.40
	MaxErr	31.79	13.74	11.05	10.99	12.94	17.89	12.59	17.77	11.59	14.94	20.28	14.74	29.90	30.56	12.95
	R^2	0.9642	0.9844	0.9941	0.9895	0.9902	0.9818	0.9961	0.9210	0.9922	0.9956	0.9857	0.9876	0.9717	0.9847	0.9918
	m	1.00	1.00	0.93	0.98	0.89	0.91	0.93	0.74	0.94	0.92	0.87	0.93	0.91	0.87	0.98
	b	2.18	-4.70	2.82	-1.57	6.68	6.58	3.22	28.01	7.50	3.69	11.58	6.94	5.67	9.73	-0.85
	CMAE	5.70	3.48	2.46	3.84	2.95	4.07	2.71	2.34	3.85	2.84	5.50	4.91	5.00	4.66	3.66
	Cσ	6.27	4.31	2.31	2.33	3.23	3.97	2.45	2.62	1.76	2.73	4.50	4.45	7.24	4.21	2.62
	CMaxErr	29.78	19.10	9.29	10.36	13.43	18.98	8.32	9.53	6.99	8.89	14.53	13.11	31.66	15.47	10.39

Reference Standard	Parameter	Compound				
		196	**197**	**198**	**199**	**200**
MSTD	MAE	3.07	5.19	5.65	4.41	3.96
	σ	3.08	4.54	4.78	4.03	3.71
	MaxErr	13.27	15.38	16.77	14.65	14.28
	R^2	0.9924	0.9913	0.9843	0.9901	0.9933
	m	0.99	0.96	1.01	0.98	1.01
	b	0.27	7.02	-2.71	-0.88	3.09
	CMAE	3.01	4.24	4.87	3.74	3.13
	Cσ	3.16	2.59	5.07	4.12	2.35
	CMaxErr	13.32	9.85	18.69	13.67	10.50
TMS	MAE	4.08	5.38	6.56	5.55	3.89
	σ	3.72	4.67	5.40	5.83	2.55
	MaxErr	13.27	15.38	17.36	22.19	8.58
	R^2	0.9905	0.9913	0.9867	0.9922	0.9944
	m	0.94	0.91	0.95	0.93	0.94
	b	2.84	8.86	-0.32	1.50	4.87
	CMAE	3.35	4.06	4.46	3.55	2.89
	Cσ	3.54	2.89	4.68	3.41	2.11
	CMaxErr	14.43	10.24	16.56	11.72	8.93

Weight and bias matrices for the trained ANN-MM-18 network

w_{ji}		*i*																		b_j
		1	*2*	*3*	*4*	*5*	*6*	*7*	*8*	*9*	*10*	*11*	*12*	*13*	*14*	*15*	*16*	*17*	*18*	
j	*1*	0.0987	-0.2897	0.0320	0.9320	0.0811	0.3723	-0.7581	0.0948	-0.2180	-0.0933	0.2727	-0.7644	-0.1133	-0.1355	0.5970	-0.3694	-0.3656	-0.2103	-2.5655
	2	0.0444	-0.5954	-0.6780	-0.4387	-0.0805	-0.2048	0.3432	-0.4359	-0.0507	0.4356	0.4218	-0.2536	0.8186	0.0465	0.0169	-0.0677	-0.1934	-0.1802	-1.6000
	3	-0.6023	0.3705	-0.2642	0.5124	0.3473	-0.4000	-0.5479	0.3511	0.0665	0.4712	-0.2596	0.0779	-0.3326	0.0806	0.5537	0.3355	-0.2250	0.4126	1.4461
	4	-0.1791	-0.3082	0.3339	0.4685	0.2942	0.3991	-0.5428	0.2175	-0.0581	-0.6579	0.4665	0.5188	-0.1578	0.3794	-0.5058	-0.3928	-0.2323	-0.2750	1.1777
	5	0.5353	-0.3213	-0.3045	-0.0409	-0.2368	-0.4734	-0.2851	-0.5235	0.0915	0.0048	0.3415	0.4086	-0.5279	-0.6007	-0.6091	-0.3557	0.1748	0.4003	-1.1834
	6	0.6219	-0.1881	-0.0021	-0.9032	0.0163	-0.0862	0.0776	-0.0557	0.3443	0.0745	-0.5708	0.1321	-0.0865	-0.3461	-0.4715	0.3101	-0.0259	0.6269	-0.6558
	7	-0.3698	-0.6414	0.3463	-0.5006	0.2706	-0.1786	0.4728	-0.5997	-0.7439	-0.3180	0.4292	0.1800	0.3341	-0.1790	-0.1378	-0.3283	-0.0133	-0.0650	0.7985
	8	-0.1083	-0.5683	-0.0100	0.5595	0.0297	-0.5607	-0.1968	-0.3857	-0.4674	0.4639	-0.3207	0.5739	-0.4314	0.4131	0.2887	0.2507	-0.3689	-0.2138	0.3835
	9	0.2233	-0.5777	-0.2871	0.1105	0.3866	0.4432	-0.1620	-0.5082	-0.7602	-0.5221	0.3069	-0.4977	0.1299	0.3360	0.4122	-0.4433	0.4552	0.2843	0.1182
	10	-0.5458	0.1982	0.4623	0.4426	0.3673	-0.6814	0.5136	-0.1438	0.4720	0.6058	0.0148	-0.1250	0.2759	0.0125	0.1653	0.1717	0.4391	0.5876	0.0893
	11	-0.2466	-0.5183	-0.6074	-0.5634	-0.0928	0.5032	-0.3064	-0.0360	0.3319	0.4332	-0.5917	-0.7946	-0.1815	-0.7947	0.6098	-0.7587	0.5054	-0.5022	-0.6152
	12	-0.6670	-0.0079	0.5348	-0.0185	-0.1489	0.5479	-0.7080	0.5268	0.0599	0.4571	-0.6628	-0.5684	-0.1605	-0.1599	0.8944	-0.8103	-0.1192	-0.6164	-0.7563
	13	0.2951	0.2910	0.2033	0.3469	0.1769	-0.2370	-0.0438	0.6827	0.6474	-0.5996	-0.1294	0.2904	-0.6018	-0.5047	-0.5120	0.1089	0.2756	0.0444	0.8238
	14	-0.1146	-0.4136	-0.2282	-0.7694	0.0369	0.6817	-0.5692	0.3715	-0.6514	0.1645	0.4639	-0.0019	-0.6869	0.0763	0.2375	-0.5912	-0.0193	0.2838	-0.3580
	15	0.6010	-0.5343	-0.4931	0.5557	0.3807	0.1157	-0.1892	-0.5904	-0.3839	0.5897	-0.2856	0.4832	-0.1928	0.1364	0.0970	-0.2258	0.2856	-0.1342	0.7136
	16	0.2612	0.6697	0.7045	-0.2201	0.1823	0.5511	0.3982	0.6353	-0.0321	0.4247	-0.2946	-0.3318	-0.1867	0.2858	0.1299	-0.1689	-0.1687	0.5208	0.8829
	17	0.1191	0.2435	-0.5257	0.4857	-0.5500	0.0625	0.2161	0.0988	-0.3501	0.0280	0.6565	-0.5073	-0.5727	0.6279	0.1065	-0.0996	-0.4436	0.2114	1.1466
	18	0.4154	0.3554	0.4433	-0.0191	-0.3238	-0.3839	-0.4863	0.6158	0.2878	0.0066	0.3406	-0.2067	0.0732	-0.0023	-0.2080	-0.2498	0.6191	-0.6661	1.4377
	19	0.4431	0.0821	-0.5087	0.3273	0.0515	-0.1707	-0.7116	0.5509	-0.2903	-0.0416	-0.6627	-0.4398	0.0223	-0.2451	-0.2740	-0.0435	-0.3984	-0.6200	1.4408
	20	0.7097	0.1046	0.6405	0.0512	-0.1385	-0.4398	-0.0965	0.4528	-0.0012	0.1655	0.3067	-0.1442	-1.1297	0.2987	-0.6019	1.0548	0.6756	0.3714	1.7693

w_{kj}		*j*																			b_k
		1	*2*	*3*	*4*	*5*	*6*	*7*	*8*	*9*	*10*	*11*	*12*	*13*	*14*	*15*	*16*	*17*	*18*	*19*	*20*	
k	*1*	1.1506	0.0739	-0.0493	0.2808	-0.1309	-0.1413	0.2366	0.2577	-0.1763	-0.0659	0.8387	1.1304	-0.3332	-0.3920	-0.2579	-0.2725	-0.5328	-0.1385	-0.4529	-1.3839	-1.7600
	2	-1.5938	-0.5025	0.4747	0.5302	-0.8221	0.0592	0.6428	0.0826	0.2343	-0.4318	-0.5624	-1.3570	0.4962	0.6363	-0.0207	0.3774	0.3577	0.4868	0.0460	1.6685	-0.8367

Weight and bias matrices for the trained ANN-AM1-18 network

w_{ji}		*i*																		b_j
		1	*2*	*3*	*4*	*5*	*6*	*7*	*8*	*9*	*10*	*11*	*12*	*13*	*14*	*15*	*16*	*17*	*18*	
j	*1*	-0.2743	-0.9269	-0.1505	0.1998	-0.0136	0.2780	0.6014	0.2732	0.2381	0.4180	-0.2729	0.2733	0.4317	-0.7727	-0.4738	-0.9800	-1.2736	-0.1085	-2.2275
	2	0.1176	-0.6090	0.6308	-0.1261	-0.1769	-0.3554	-0.2063	0.1219	-0.2736	0.5000	0.3074	0.2747	-0.3813	-0.3663	-0.5850	-0.0048	0.7036	-0.3071	-1.4878
	3	0.5507	-0.2743	0.2452	0.7849	0.6783	-1.0065	0.3261	0.0328	-0.0469	-0.0250	-0.3885	-0.8241	0.1103	0.1746	-0.1619	0.6379	-0.1620	0.5516	-0.9611
	4	0.0027	-0.0867	0.6085	0.1211	-0.1793	-0.5868	-0.4691	-0.4545	0.4709	-0.7953	0.5775	-0.4107	0.0656	0.2541	-0.6093	-0.6072	-0.2921	0.4155	0.6648
	5	-0.4748	-0.3341	0.2729	0.5304	-0.0205	-0.1648	0.1619	-0.4782	-0.3080	0.6135	0.6601	-0.4279	-0.5679	0.2077	0.2796	0.0699	-0.3825	0.3149	0.8635
	6	0.6726	-0.2046	-0.4352	-0.3018	0.2424	0.2101	0.1502	0.5759	-0.0414	-0.6675	-0.3341	-0.0431	-0.5538	0.6724	0.2699	0.0598	-0.3607	-0.5993	-0.7461
	7	0.5326	0.4771	-0.7249	0.3948	0.8052	-0.1902	-0.2517	0.1876	-0.8711	0.2340	0.5249	0.4322	0.2912	0.2238	0.2722	1.3773	-0.0425	-0.1675	0.2380
	8	-0.1162	-0.1032	-0.5227	0.8406	-0.3237	-0.4829	-0.4285	0.2522	-0.5496	-0.4400	-0.3227	0.1463	0.5515	-0.4487	0.4629	0.2382	0.3907	-0.2059	-0.2646
	9	0.2489	0.4765	-0.5215	-0.3876	-0.5707	0.1741	-0.4096	-0.0795	0.0199	-0.0518	-0.8027	-0.3130	0.7660	-0.1877	0.3760	0.2146	-0.1969	0.1302	-0.4539
	10	0.6960	0.0231	-0.1541	0.4591	0.7171	-0.6665	0.1946	0.6755	-0.4575	-0.6186	0.5348	0.3519	-0.1183	0.5704	-0.2462	-0.0147	-0.1233	-0.1395	0.1046
	11	0.1550	-0.2573	0.1172	-0.7066	-0.5101	-0.6846	-0.1496	0.0215	-0.4305	0.2561	0.3245	0.0512	-0.4436	0.2351	-0.0216	0.1901	0.6769	0.6584	-0.0388
	12	0.0126	-0.0009	0.6318	0.3779	-0.4597	-0.4281	0.2340	0.2682	0.0677	-0.4292	0.2697	0.5604	-0.2527	-0.7261	-0.4209	-0.3067	0.1208	0.4009	-0.0532
	13	-0.1944	-0.2454	-0.6939	-0.5225	-0.6509	0.4116	0.1667	-0.6111	-0.0275	0.4689	-0.3814	0.6375	-0.3037	0.3603	-0.6725	-0.1605	-0.7387	0.2265	0.1631
	14	0.1324	-0.5226	-0.2550	-0.3600	-1.1004	1.2331	-0.1307	-0.3278	-0.1299	2.2475	1.3648	0.9088	-0.6992	-1.5375	1.4829	0.7206	1.2008	-0.3949	1.6139
	15	-1.4592	-0.7278	-0.0744	-0.5531	-0.5592	1.3057	0.4618	0.1539	0.6121	0.7029	0.0422	0.6005	1.0056	-0.8119	0.0336	-1.4663	-0.7901	-0.1666	-1.6808
	16	0.2887	0.2057	-0.3628	0.4001	0.5192	0.1797	-0.1185	0.5923	-0.4010	0.1372	-0.5783	0.0046	-0.2304	-0.3805	-0.1379	-0.7475	-0.6515	-0.0990	1.0713
	17	0.2086	0.2950	-0.1778	0.5910	-0.4987	0.0681	-0.4849	-0.4117	-0.6431	-0.4894	-0.3628	0.0312	-0.2243	0.4836	0.5809	0.0429	-0.0730	0.4150	1.1589
	18	-0.4080	0.4275	0.3787	-0.2830	0.3458	0.4938	-0.5187	-0.4574	0.2709	-0.3048	0.4448	-0.4691	-0.0479	0.0168	-0.5321	0.4709	0.2790	0.3839	-1.4177
	19	0.1587	-0.4839	-0.3905	-0.6398	0.1825	-0.3760	0.0750	-0.5948	-0.6295	-0.3406	-0.1934	-0.4831	0.1683	0.2423	-0.0602	0.0090	-0.4996	-0.5260	1.4951
	20	0.8266	-0.3038	0.3305	-0.1618	-0.3535	0.0814	0.5808	-0.3222	-0.4095	0.3491	0.0359	-0.3478	0.4226	0.2293	-0.2374	0.6465	0.1784	-0.0303	1.7572

w_{kj}		*j*																			b_k
		1	*2*	*3*	*4*	*5*	*6*	*7*	*8*	*9*	*10*	*11*	*12*	*13*	*14*	*15*	*16*	*17*	*18*	*19*	*20*	
k	*1*	2.0310	-0.2477	-0.6450	0.5257	0.3125	-0.4451	-1.0563	-0.1031	0.4023	-0.5386	0.1630	-0.2798	0.6078	-3.0036	2.0470	-0.5355	-0.6984	0.6305	-0.1687	-0.4163	-1.7575
	2	-2.3590	-0.6454	0.4779	-0.4068	0.1967	0.6241	1.1006	-0.6862	-0.3231	0.5452	0.2885	0.0783	-0.7910	3.2008	-2.4688	0.3506	0.3378	-0.3561	0.7222	0.7270	1.6952

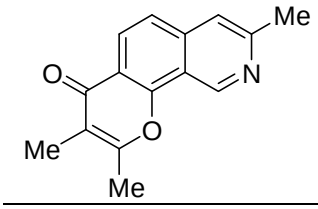
Weight and bias matrices for the trained ANN-HF-18 network

w_{ji}		*i*																		b_j
		1	*2*	*3*	*4*	*5*	*6*	*7*	*8*	*9*	*10*	*11*	*12*	*13*	*14*	*15*	*16*	*17*	*18*	
j	*1*	0.6162	-0.2072	0.3726	-0.2596	-1.0092	0.1893	0.4360	0.3838	0.2493	-0.2271	0.9893	0.6211	-0.0388	-1.3101	0.8012	1.0480	0.9463	0.7029	2.5099
	2	0.1253	0.0781	0.3079	-0.0152	0.6683	-0.9696	-0.3509	0.4060	-0.3622	0.1483	0.3391	-0.0525	-0.3609	-0.2323	-0.0130	1.0451	0.1843	0.4989	1.5469
	3	-0.6392	-0.4108	-0.5880	-0.4376	0.1572	0.3107	0.0429	-0.5574	0.4151	0.2919	0.1964	0.0337	0.2074	0.2791	-0.0350	0.6016	0.4258	-0.2687	1.4746
	4	0.0240	-0.3177	0.1843	0.3004	-0.2781	0.6159	-0.0718	0.2188	-0.0235	0.7168	0.0470	0.3607	0.4789	-0.2532	-0.1829	0.7057	0.0694	0.7220	-1.1513
	5	-0.6612	-0.5449	0.4729	0.2567	-0.5726	0.0585	-0.4425	-0.6921	-0.0356	-0.2963	0.1614	-0.2090	0.0461	0.2178	-0.4941	0.2330	0.3534	-0.4215	1.0221
	6	0.3684	0.0602	0.2373	-0.0393	0.4438	-0.1618	-0.1190	-0.1040	0.7222	-0.6812	0.5230	0.5718	-0.5254	-0.1927	-0.1137	-0.0943	0.5899	0.2465	-0.8650
	7	0.3499	0.4072	0.8273	-0.1142	0.2791	0.4305	0.2703	-0.3468	-0.4849	0.6595	-0.2681	0.5662	0.0526	-0.4616	0.6679	0.7865	0.5738	0.2707	0.5896
	8	-0.0619	0.2299	-0.0225	0.4840	0.5860	-0.3016	0.4411	0.4479	-0.1504	-0.3678	0.5082	0.0270	-0.5343	-0.3340	0.1215	0.9107	-0.0411	-0.3040	0.4600
	9	-1.4585	0.4532	-0.1672	0.0744	-0.9354	0.5740	-0.5501	-0.0232	0.9209	-0.0195	-0.1611	0.0151	-0.7378	0.6149	0.0104	-1.1241	-0.4518	-0.0847	-0.9779
	10	0.3921	0.2810	-0.6479	-0.0821	0.7448	-0.3080	0.4711	0.1500	0.2620	-0.3227	-0.7659	-0.4404	-0.3901	-0.3759	-0.1386	0.0816	0.2850	0.0522	0.0891
	11	-0.0266	-0.7565	0.5966	0.1191	0.0078	-0.0815	-0.5640	-0.4996	-0.4219	-0.7754	-0.2988	-0.0427	-0.2591	-0.0389	0.3434	0.1432	-0.1836	-0.2770	-0.0547
	12	-0.4745	0.3381	0.0643	0.2113	-0.4965	-0.1526	-0.5189	0.5191	-0.3229	0.2517	-0.3051	-0.3850	-0.5873	-0.3959	0.4982	-0.7223	0.2647	-0.1509	-0.1589
	13	1.3459	-0.4662	-0.2892	-0.1219	-0.0368	0.1949	0.3191	-0.0675	-0.7991	-0.1473	-0.3255	-0.3048	0.1855	-0.3277	-0.2838	0.7590	-0.5249	0.6267	0.8283
	14	1.0877	0.4988	-0.1846	0.2157	1.0110	-0.8091	0.2770	0.1599	0.2320	0.5916	-0.4603	-0.5847	0.1869	-0.1375	-0.6700	0.9695	0.1215	-0.0664	0.6666
	15	-1.8756	0.6245	0.1386	-0.2388	0.2191	1.0605	0.1017	0.0878	0.1741	0.0492	0.0402	0.1891	0.0256	-0.0275	-1.0914	-1.8297	-0.2831	-0.2427	-1.6142
	16	-1.3555	0.1000	0.3820	0.4626	-0.7082	0.2500	0.2485	-0.0126	0.4169	-0.6035	0.4172	0.5230	0.3585	0.5440	-0.0640	-1.0821	-0.4263	0.1417	-1.2971
	17	-0.3851	-0.0537	0.1327	0.4224	0.0893	0.1805	-0.2409	0.3265	-0.4085	0.0664	-0.4072	0.3536	-0.6850	0.4679	0.4617	-0.1644	0.4571	0.6356	-1.1656
	18	1.2105	-0.0936	0.1410	-0.4679	0.5868	-0.5575	-0.3892	0.1842	-0.5274	-0.1716	-0.6095	-0.4929	-0.4719	0.4754	-0.4185	1.1858	0.4574	0.4360	1.7302
	19	0.1659	-0.7045	-0.1752	0.6521	0.0700	-0.8487	0.2460	0.1023	-0.2193	-0.2558	0.0948	-0.0828	0.6610	0.9109	-0.8717	0.5249	0.4973	-0.1307	-1.3913
	20	0.4746	0.3938	0.0397	-0.4086	0.7452	0.0791	0.3714	-0.6307	-0.0664	0.1024	-0.2455	0.3393	0.1825	0.1892	0.3594	0.8383	-0.1569	-0.3570	1.7191

w_{kj}		*j*																		b_k
		1	*2*	*3*	*4*	*5*	*6*	*7*	*8*	*9*	*10*	*11*	*12*	*13*	*14*	*15*	*16*	*17*	*18*	*19*	*20*	
k	*1*	-2.0105	-0.7600	-0.5010	0.0492	-0.2451	0.9407	-0.6375	-0.3356	1.4622	-0.0893	-0.1292	-0.0702	-0.7303	-0.9707	2.3424	1.3417	0.2282	-1.5892	-0.7145	-1.0344	0.6622
	2	2.3777	0.8477	0.3512	-0.3460	0.5389	0.2996	0.7642	0.0479	-1.3264	0.3698	-0.2905	-0.7635	1.2932	1.0865	-1.7840	-1.6709	-0.0068	1.1961	0.8801	0.1624	1.7019

Experimental chemical shifts, mPW1PW91/6-31G(d)//MM+ Boltzmann-averaged GIAO isotropic magnetic shielding values, unscaled and scaled chemical shifts computed using TMS and MSTD, and statistical parameters computed for compounds 201-247.

Compound **201**

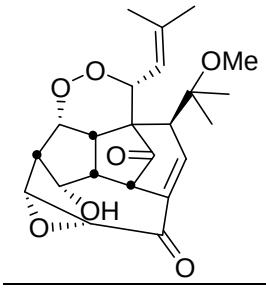


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
182.1	25.0562	174.1	169.8	173.2	174.5	MAE	4.3	4.0
164.0	39.0953	160.0	155.7	159.3	160.0	σ	2.7	4.2
156.7	39.4165	159.7	155.4	159.0	159.7	MaxErr	8.6	12.9
146.2	45.1033	154.0	149.7	153.4	153.8	R^2	0.9907	0.9913
145.6	48.3370	150.8	146.5	150.2	150.5	*m*	1.0	1.0
141.3	66.4199	132.7	128.4	132.4	131.9	*b*	-1.4	0.0
133.7	67.1303	132.0	127.7	131.7	131.2	CMAE	4.0	3.9
124.1	71.5344	127.6	123.3	127.3	126.7	Cσ	2.9	2.7
120.5	72.8354	126.3	122.0	126.0	125.3	CMaxErr	8.9	9.4
119.5	74.3810	124.8	120.4	124.5	123.8			
119.3	77.1098	122.0	117.7	121.8	121.0			
114.6	84.5325	114.6	110.3	114.5	113.3			
24.7	170.4122	23.3	24.4	24.3	25.1			
20.4	174.7182	19.0	20.1	20.1	20.6			
17.5	182.3903	11.3	12.4	12.5	12.7			

[a] NMR data from: Kohno, J.; Hiramatsu, H.; Nishio, M.; Sakurai, M.; Okuda, T.; Komatsubara, S. *Tetrahedron* **1999**, *55*, 11247. Solvent: $CDCl_3$

[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

Compound **202**

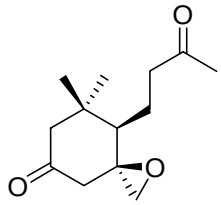


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
202.9	-6.7532	205.9	201.6	196.7	197.7	MAE	5.4	5.6
192.8	-6.3405	205.5	201.2	196.3	197.3	σ	4.2	3.6
142.2	44.2943	154.8	150.5	147.3	146.2	MaxErr	12.8	13.9
139.6	56.9207	142.2	137.9	135.1	133.4	R^2	0.9946	0.9925
132.5	66.4145	132.7	128.4	125.9	123.9	*m*	1.0	1.0
120.7	69.0197	130.1	125.8	123.4	121.2	*b*	2.6	5.6
77.3	103.5703	90.1	91.2	84.6	86.4	CMAE	3.2	3.6
75.8	106.6600	87.0	88.2	81.6	83.2	Cσ	2.1	2.7
72.7	112.0288	81.6	82.8	76.4	77.8	CMaxErr	7.3	9.1
71.5	116.9014	76.8	77.9	71.7	72.9			
61.0	129.2163	64.5	65.6	59.8	60.5			
60.5	129.8411	63.8	65.0	59.2	59.9			
54.5	130.7055	63.0	64.1	58.4	59.0			

53.2	136.4969	57.2	58.3	52.8	53.1
53.1	136.6260	57.0	58.2	52.6	53.0
49.1	137.0669	56.6	57.7	52.2	52.6
47.8	144.0898	49.6	50.7	45.4	45.5
40.9	147.6462	46.0	47.2	42.0	41.9
40.4	150.5376	43.1	44.3	39.2	39.0
26.6	166.3290	27.3	28.5	23.9	23.0
26.1	167.0875	26.6	27.7	23.2	22.3
24.7	167.1670	26.5	27.6	23.1	22.2
18.6	176.6602	17.0	18.2	13.9	12.6

[a] NMR data from: Rychnovsky, S. D. *Org. Lett.* **2006**, *8*, 2895. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

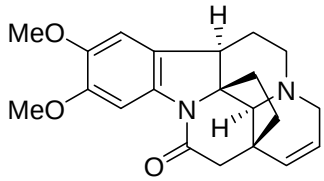
Compound **203**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
208.7	-10.1753	209.3	205.0	213.0	212.7	MAE	4.6	4.8
207.2	-8.8858	208.0	203.7	211.7	211.4	σ	4.9	4.5
83.4	122.7122	71.0	72.1	72.6	73.5	MaxErr	16.1	15.0
78.3	131.5121	62.2	63.3	63.6	64.3	R^2	0.9893	0.9906
53.1	143.5858	50.1	51.2	51.4	51.7	*m*	1.0	1.0
49.4	144.7283	48.9	50.1	50.2	50.5	*b*	-0.6	1.9
48.6	148.1181	45.6	46.7	46.8	46.9	CMAE	4.8	4.5
43.4	152.4008	41.3	42.4	42.4	42.5	Cσ	4.4	4.1
42.6	153.7788	39.9	41.0	41.1	41.0	CMaxErr	14.7	14.0
30.0	164.0351	29.6	30.8	30.6	30.3			
24.9	164.1562	29.5	30.7	30.5	30.1			
20.8	165.3016	28.4	29.5	29.4	28.9			
18.7	168.8553	24.8	26.0	25.8	25.2			

[a] NMR data from: Macías, F. A.; Varela, R. M.; Torres, A.; Oliva, R. M.; Molinillo, J. M. G. *Phytochemistry* **1997**, *48*, 631. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

Compound **204**

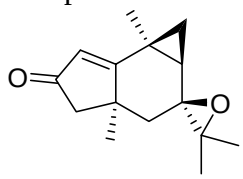


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
173.8	32.7253	166.4	162.1	167.4	169.0	MAE	5.3	5.8
147.7	53.0928	146.0	141.7	146.1	146.5	σ	3.2	3.3
145.3	55.4655	143.7	139.3	143.6	143.9	MaxErr	11.9	13.0
131.5	61.6286	137.5	133.2	137.2	137.0	R^2	0.9861	0.9870
131.0	62.3514	136.8	132.5	136.4	136.3	*m*	1.0	0.9
120.0	72.5948	126.5	122.2	125.8	124.9	*b*	6.0	9.3
117.4	72.7889	126.4	122.0	125.6	124.7	CMAE	4.2	4.3
111.3	90.0472	109.1	104.8	107.5	105.6	Cσ	3.6	3.2
102.6	94.9075	104.2	99.9	102.5	100.2	CMaxErr	14.7	12.9
84.4	120.8393	72.8	74.0	69.7	71.6			
56.1	125.6620	68.0	69.1	64.7	66.2			

56.0	141.8600	51.8	53.0	47.8	48.3
47.9	142.8520	50.8	52.0	46.7	47.2
46.0	143.0033	50.7	51.8	46.6	47.1
44.5	143.5041	50.2	51.3	46.1	46.5
44.3	145.4014	48.3	49.4	44.1	44.4
37.7	148.7892	44.9	46.0	40.5	40.7
36.6	149.2573	44.4	45.6	40.0	40.1
35.0	157.0731	36.6	37.7	31.9	31.5
26.8	159.8255	33.8	35.0	29.0	28.4
24.8	167.2798	26.4	27.5	21.2	20.2

[a] NMR data from: Hubbs, J. L.; Heathcock, C. H. *Org. Lett.* **1999**, *1*, 1315. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

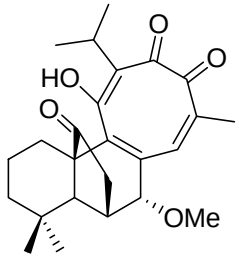
Compound **205**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
200.1	0.8635	198.3	193.9	193.8	194.2	MAE	6.2	7.4
180.0	4.3859	194.8	190.4	190.2	190.5	σ	5.3	4.6
128.5	73.2147	125.9	121.6	120.8	118.5	MaxErr	15.4	16.6
66.5	116.1405	77.5	78.7	72.0	73.6	R^2	0.9901	0.9883
60.8	120.5597	73.1	74.3	67.6	69.0	*m*	1.0	1.0
42.7	146.3374	47.3	48.5	41.6	42.0	*b*	6.1	8.3
34.5	147.2750	46.4	47.5	40.6	41.0	CMAE	5.1	5.5
34.2	154.5794	39.1	40.2	33.3	33.4	Cσ	2.9	3.2
30.8	162.7617	30.9	32.0	25.0	24.8	CMaxErr	10.2	10.5
28.9	163.4861	30.2	31.3	24.3	24.1			
26.5	163.7882	29.9	31.0	24.0	23.8			
23.3	169.2359	24.4	25.6	18.5	18.1			
21.3	169.2895	24.4	25.5	18.4	18.0			
19.5	169.6991	24.0	25.1	18.0	17.6			
8.4	169.8494	23.8	25.0	17.9	17.4			

[a] NMR data from: Tori, M.; Nakashima, K.; Toyota, M.; Asakawa, Y. *Tetrahedron Lett.* **1993**, *34*, 3751. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

Compound **206**

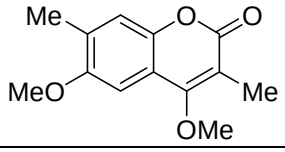


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
203.1	5.9549	193.2	188.9	198.2	199.4	MAE	4.2	4.5
189.1	6.0851	193.1	188.7	198.0	199.3	σ	5.5	6.8
175.7	19.4047	179.7	175.4	184.2	184.9	MaxErr	27.1	31.4
175.4	50.8212	148.3	144.0	151.6	150.9	R^2	0.9886	0.9883
149.1	52.8066	146.3	142.0	149.6	148.7	*m*	1.0	0.9
146.6	59.5067	139.6	135.3	142.6	141.5	*b*	2.1	4.5
132.1	60.3891	138.8	134.4	141.7	140.5	CMAE	4.3	4.3
132.0	67.7395	131.4	127.1	134.1	132.6	Cσ	5.1	5.3
119.8	71.5669	127.6	123.2	130.1	128.4	CMaxErr	23.8	24.5

79.5	115.6489	78.0	79.2	78.7	80.7
73.0	124.5630	69.1	70.2	69.5	71.1
59.2	135.7370	57.9	59.1	57.9	59.0
50.2	139.2263	54.4	55.6	54.3	55.2
45.8	147.6694	46.0	47.1	45.5	46.1
38.1	154.9507	38.7	39.9	38.0	38.2
31.3	157.7107	36.0	37.1	35.1	35.2
31.3	158.0831	35.6	36.7	34.7	34.8
30.2	161.6534	32.0	33.2	31.0	31.0
28.1	165.3501	28.3	29.5	27.2	27.0
26.4	170.4172	23.3	24.4	21.9	21.5
22.8	171.9394	21.7	22.9	20.3	19.8
22.3	172.8521	20.8	22.0	19.4	18.8
21.9	172.8896	20.8	21.9	19.4	18.8
18.6	173.5611	20.1	21.2	18.7	18.1

[a] NMR data from: Yang, J.; Huang, S. X.; Zhao, Q. S. *J. Phys. Chem. A* **2008**, *112*, 12132. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

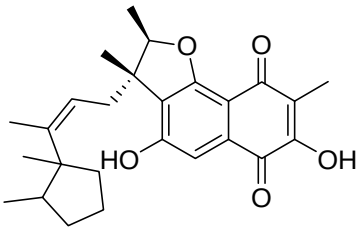
Compound **207**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
177.6	36.3314	162.8	158.5	169.6	170.6	MAE	10.0	10.3
162.6	37.0961	162.0	157.7	168.8	169.8	σ	7.4	8.2
160.7	47.1958	151.9	147.6	157.6	158.1	MaxErr	25.6	29.9
158.5	52.8520	146.3	142.0	151.3	151.5	R^2	0.9529	0.9573
156.5	68.2005	130.9	126.6	134.3	133.7	*m*	0.9	0.9
110.9	76.8550	122.3	118.0	124.7	123.7	*b*	9.8	11.3
108.0	77.6917	121.5	117.1	123.8	122.7	CMAE	10.8	10.2
105.3	79.0768	120.1	115.7	122.3	121.1	Cσ	5.9	5.8
91.1	91.3167	107.8	103.5	108.7	106.9	CMaxErr	22.2	22.8
56.0	139.2188	54.5	55.6	49.5	51.4			
55.4	142.9297	50.7	51.9	45.4	47.1			
19.4	174.5183	19.2	20.3	10.4	10.4			
7.3	181.4494	12.2	13.4	2.7	2.4			

[a] NMR data from: Kalinin, A. V.; Snieckus, V. *Tetrahedron Lett.* **1998**, *39*, 4999. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

Compound **208**

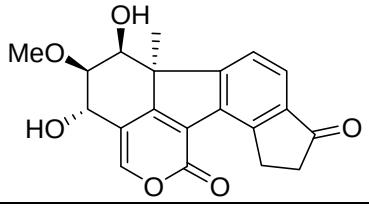


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
182.9	16.3461	182.8	178.5	182.0	183.5	MAE	4.8	5.3
180.4	16.4115	182.7	178.4	182.0	183.4	σ	3.9	4.0
159.9	39.5758	159.6	155.2	158.1	158.4	MaxErr	14.2	15.3
157.7	45.1249	154.0	149.7	152.3	152.4	R^2	0.9942	0.9939
153.6	47.5384	151.6	147.3	149.8	149.8	*m*	1.0	0.9
138.9	47.7530	151.4	147.1	149.6	149.6	*b*	6.3	8.4
131.6	66.0709	133.1	128.7	130.7	129.8	CMAE	3.4	3.6

127.3	68.0526	131.1	126.8	128.7	127.7	Cσ	3.0	3.0
123.9	72.7725	126.4	122.0	123.8	122.6	CMaxErr	10.7	10.7
120.3	74.9098	124.2	119.9	121.6	120.3			
107.9	86.3960	112.7	108.4	109.8	107.9			
107.9	87.8182	111.3	107.0	108.3	106.4			
86.3	113.7859	79.9	81.0	75.9	78.4			
46.0	141.9987	51.7	52.8	46.8	47.9			
39.7	143.9139	49.8	50.9	44.8	45.9			
32.8	146.6874	47.0	48.1	41.9	42.9			
31.0	150.2462	43.4	44.6	38.3	39.0			
30.5	156.1706	37.5	38.6	32.2	32.6			
26.6	158.0812	35.6	36.7	30.2	30.6			
25.1	166.5004	27.2	28.3	21.5	21.5			
20.9	168.1483	25.5	26.7	19.8	19.7			
19.7	169.5779	24.1	25.2	18.3	18.2			
18.8	172.4822	21.2	22.3	15.3	15.0			
15.7	175.7235	17.9	19.1	12.0	11.5			
15.1	176.7602	16.9	18.1	10.9	10.4			
8.6	183.1926	10.5	11.6	4.3	3.5			

[a] NMR data from: Kalaitzis, J. A.; Hamano, Y.; Nilsen, G.; Moore, B. S. *Org. Lett.* **2003**, *5*, 4449. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

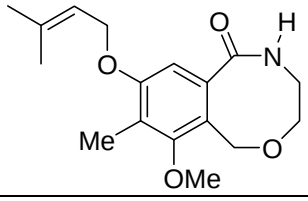
Compound **209**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
206.7	-11.9837	211.1	206.8	211.6	214.4	MAE	3.4	4.6
173.4	33.5158	165.6	161.3	165.5	165.9	σ	3.0	3.6
158.6	39.2833	159.9	155.5	159.6	159.8	MaxErr	11.5	12.7
158.0	43.9849	155.2	150.8	154.8	154.8	R^2	0.9928	0.9908
145.7	46.7539	152.4	148.1	152.0	151.8	*m*	1.0	0.9
145.6	50.0286	149.1	144.8	148.7	148.4	*b*	2.4	5.4
142.4	59.3556	139.8	135.5	139.3	138.4	CMAE	3.6	4.3
136.9	62.9161	136.2	131.9	135.7	134.6	Cσ	2.6	2.6
129.8	68.9519	130.2	125.9	129.5	128.2	CMaxErr	9.9	10.5
127.3	73.4058	125.7	121.4	125.0	123.5			
127.3	73.6431	125.5	121.2	124.8	123.2			
122.1	74.1579	125.0	120.7	124.3	122.7			
81.7	107.6967	86.0	87.1	84.7	87.0			
71.7	120.9813	72.7	73.8	71.3	72.8			
62.6	123.8001	69.9	71.0	68.4	69.8			
60.7	137.9508	55.7	56.9	54.1	54.8			
42.3	139.8343	53.8	55.0	52.2	52.8			
36.5	157.0677	36.6	37.7	34.7	34.4			
30.5	163.3316	30.3	31.5	28.3	27.8			
28.4	167.8367	25.8	27.0	23.8	23.0			

[a] NMR data from: Wipf, P.; Kerekes, A. D. *J. Nat. Prod.* **2003**, *66*, 716. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

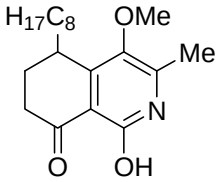
Compound **210**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
167.5	34.1646	165.0	160.6	164.2	164.9	MAE	4.1	4.8
158.7	42.5000	156.6	152.3	155.6	155.8	σ	2.8	3.6
152.4	42.8773	156.3	151.9	155.2	155.4	MaxErr	11.3	12.4
138.0	57.5435	141.6	137.3	140.0	139.5	R^2	0.9952	0.9928
132.2	70.3095	128.8	124.5	126.8	125.6	*m*	1.0	0.9
125.1	70.5141	128.6	124.3	126.6	125.3	*b*	6.2	9.2
121.8	74.0800	125.1	120.7	122.9	121.5	CMAE	2.9	3.3
120.5	76.5692	122.6	118.2	120.4	118.7	Cσ	2.1	2.8
99.7	84.2415	109.4	110.6	106.8	110.4	CMaxErr	7.1	10.7
68.7	123.0752	70.6	71.7	66.6	68.1			
59.7	129.8596	63.8	65.0	59.6	60.7			
56.4	130.1240	63.5	64.7	59.3	60.4			
49.2	133.1604	60.5	61.6	56.2	57.1			
45.1	148.3739	45.3	46.4	40.4	40.6			
26.0	164.3888	29.3	30.4	23.9	23.1			
18.5	172.1056	21.6	22.7	15.9	14.7			
10.2	178.4594	15.2	16.4	9.3	7.8			

[a] NMR data from: Cornella, I.; Kelly, T. R. *J. Org. Chem.* **2004**, *69*, 2191. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

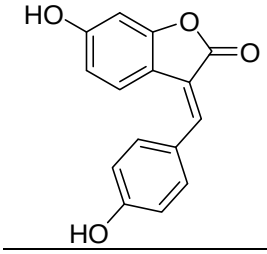
Compound **211**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
194.6	-0.4701	199.6	195.3	199.0	200.7	MAE	6.6	6.8
172.8	36.6508	162.5	158.2	161.2	161.2	σ	4.0	4.6
147.5	39.0701	160.1	155.7	158.7	158.6	MaxErr	17.1	21.4
139.0	46.3442	152.8	148.5	151.3	150.9	R^2	0.9865	0.9855
138.9	53.7351	145.4	141.1	143.7	143.0	*m*	1.0	0.9
132.2	84.0088	115.1	110.8	112.9	110.8	*b*	4.5	6.7
59.4	139.9036	53.8	54.9	50.2	51.3	CMAE	4.4	4.6
32.2	154.9375	38.7	39.9	34.9	35.3	Cσ	5.6	5.8
31.8	157.4519	36.2	37.4	32.3	32.6	CMaxErr	19.3	21.4
30.5	159.0710	34.6	35.7	30.7	30.9			
30.3	159.5438	34.1	35.3	30.2	30.4			
29.6	159.9721	33.7	34.8	29.8	29.9			
29.5	160.0632	33.6	34.7	29.7	29.8			
29.2	160.2327	33.4	34.6	29.5	29.6			
28.4	161.0989	32.6	33.7	28.6	28.7			
24.3	161.7840	31.9	33.0	27.9	28.0			
22.6	167.0817	26.6	27.7	22.5	22.3			
14.5	173.5130	20.2	21.3	15.9	15.5			
14.0	177.1451	16.5	17.7	12.2	11.6			

[a] NMR data from: Bringmann, J.; Schlauer, H.; Rischer, H.; Wohlfarth, J.; Mühlbacher, J.; Buske, A.; Porzel, A.; Schmidt, J.; Adam, G. *Tetrahedron* **2000**, *56*, 3691. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

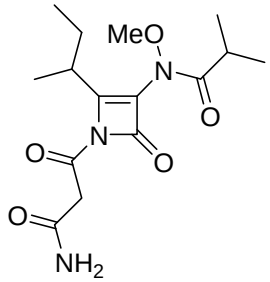
Compound **212**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
174.8	29.6252	169.5	165.2	177.0	177.0	MAE	3.8	6.5
162.8	43.8806	155.3	150.9	160.6	160.6	σ	3.8	4.9
157.6	44.1884	155.0	150.6	160.2	160.2	MaxErr	14.4	18.7
157.2	44.5192	154.6	150.3	159.9	159.9	R^2	0.9594	0.9594
152.9	60.6368	138.5	134.2	141.4	141.4	*m*	0.9	0.9
130.1	68.5988	130.5	126.2	132.2	132.2	*b*	15.3	11.0
127.3	70.2721	128.9	124.5	130.3	130.3	CMAE	3.6	3.6
123.6	73.0221	126.1	121.8	127.2	127.2	Cσ	2.8	2.8
122.6	75.4687	123.7	119.3	124.4	124.4	CMaxErr	11.5	11.5
116.6	77.4168	121.7	117.4	122.1	122.1			
115.3	83.2999	115.8	111.5	115.4	115.4			
115.0	87.6840	111.5	107.1	110.3	110.3			
102.2	99.2318	99.9	95.6	97.1	97.1			

[a] NMR data from: Suzuki, K.; Yahara, S.; Kazutomo, M.; Uyeda, M. *J. Nat. Prod.* **2001**, *64*, 204. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

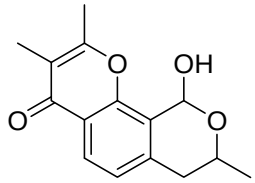
Compound **213**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
168.0	21.9493	177.2	172.9	165.5	165.9	MAE	8.4	7.7
166.0	22.2339	176.9	172.6	165.3	165.6	σ	8.6	7.1
161.5	23.9683	175.2	170.8	163.6	163.9	MaxErr	32.3	27.9
152.0	30.3566	168.8	164.5	157.7	157.7	R^2	0.9801	0.9794
135.0	31.8889	167.3	162.9	156.3	156.3	*m*	1.1	1.0
134.9	77.0461	122.1	117.8	114.4	112.6	*b*	-1.0	1.3
64.1	141.7589	51.9	53.1	49.2	50.1	CMAE	5.3	5.3
41.1	151.6719	42.0	43.1	40.0	40.5	Cσ	7.3	7.5
33.7	157.7408	35.9	37.1	34.3	34.6	CMaxErr	21.3	22.3
30.7	161.2945	32.4	33.5	31.0	31.2			
27.5	161.4282	32.2	33.4	30.9	31.1			
19.9	171.5787	22.1	23.2	21.5	21.2			
19.9	173.3111	20.4	21.5	19.9	19.6			
18.2	173.4524	20.2	21.4	19.7	19.4			
12.6	177.5994	16.1	17.2	15.9	15.4			

[a] NMR data from: Kita, M.; Miwa, R.; Widianti, T.; Ozaki, Y.; Aoyama, S.; Yamada, K.; Uemura, D. *Tetrahedron Lett.* **2007**, *48*, 8628. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

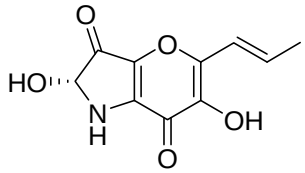
Compound **214**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
182.5	24.4320	174.7	170.4	173.0	174.2	MAE	3.4	3.5
162.5	38.7490	160.4	156.1	158.8	159.3	σ	2.8	3.1
144.5	45.3159	153.8	149.5	152.3	152.5	MaxErr	9.3	12.1
142.0	56.4845	142.7	138.3	141.2	140.9	R^2	0.9940	0.9938
131.1	67.8517	131.3	127.0	129.9	129.1	*m*	1.0	1.0
122.7	72.2772	126.9	122.5	125.6	124.5	*b*	0.2	2.5
122.5	73.5232	125.6	121.3	124.3	123.2	CMAE	3.1	3.2
122.0	74.2159	124.9	120.6	123.6	122.5	Cσ	2.8	2.9
119.1	74.6459	124.5	120.2	123.2	122.1	CMaxErr	9.5	8.3
87.5	101.5591	92.1	93.3	91.1	94.1			
62.2	130.1524	63.5	64.7	62.8	64.5			
36.5	156.9683	36.7	37.8	36.2	36.6			
21.0	171.2930	22.4	23.5	22.0	21.8			
20.1	174.8136	18.9	20.0	18.5	18.1			
17.0	182.7473	10.9	12.1	10.7	9.9			

[a] NMR data from: Lin, W. H.; Brauers, G.; Ebel, R.; Wray, V.; Berg, A.; Surdasono; Proksch, P. *J. Nat. Prod.* **2003**, *66*, 57. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

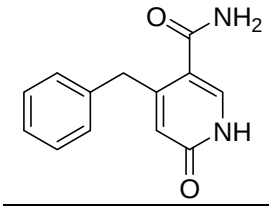
Compound **215**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
174.2	-4.5526	203.7	199.4	197.6	199.6	MAE	9.1	9.3
169.1	31.2726	167.9	163.5	162.1	162.5	σ	10.0	8.1
165.0	50.8256	148.3	144.0	142.6	142.2	MaxErr	29.5	25.2
146.0	53.1406	146.0	141.7	140.3	139.8	R^2	0.9368	0.9338
142.2	56.4511	142.7	138.4	137.0	136.4	*m*	1.0	1.0
131.7	59.3413	139.8	135.5	134.2	133.4	*b*	4.7	6.7
118.9	61.2394	137.9	133.6	132.3	131.5	CMAE	9.1	8.9
111.7	75.5436	123.6	119.3	118.1	116.6	Cσ	7.9	8.7
75.2	116.2921	77.4	78.5	72.2	74.4	CMaxErr	23.4	25.4
18.7	172.5695	21.1	22.2	16.3	16.1			

[a] NMR data from: Hiort, J.; Maksimenka, K.; Reichert, M.; Perovi-Ottstadt, S.; Lin, W. H.; Wray, V.; Steube, K.; Schaumann, K.; Weber, H.; Proksch, P.; Ebel, R.; Müller, W. E. G.; Bringmann, G. *J. Nat. Prod.* **2004**, *67*, 1532. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

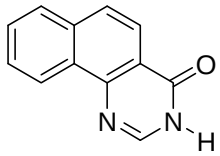
Compound **216**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
178.1	29.2618	169.9	165.5	173.3	174.7	MAE	2.9	5.5
165.9	38.6876	160.5	156.1	163.3	164.2	σ	2.7	3.3
151.2	45.3344	153.8	149.5	156.2	156.8	MaxErr	8.2	12.6
142.2	60.6246	138.5	134.2	139.9	139.8	R^2	0.9876	0.9894
137.4	66.1165	133.0	128.7	134.0	133.7	*m*	0.9	0.9
129.3	67.1650	132.0	127.6	132.9	132.5	*b*	7.5	8.7
129.3	69.7126	129.4	125.1	130.2	129.7	CMAE	2.8	2.6
129.2	70.0021	129.1	124.8	129.8	129.4	Cσ	2.2	2.1
129.2	70.2121	128.9	124.6	129.6	129.1	CMaxErr	7.8	7.2
127.5	72.2516	126.9	122.6	127.4	126.8			
118.9	72.9239	126.2	121.9	126.7	126.1			
118.0	82.3607	116.8	112.4	116.7	115.6			
38.2	153.8927	39.8	40.9	34.4	35.9			

[a] NMR data from: Hiort, J.; Maksimenka, K.; Reichert, M.; Perovi-Ottstadt, S.; Lin, W. H.; Wray, V.; Steube, K.; Schaumann, K.; Weber, H.; Proksch, P.; Ebel, R.; Müller, W. E. G.; Bringmann, G. *J. Nat. Prod.* **2004**, *67*, 1532. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

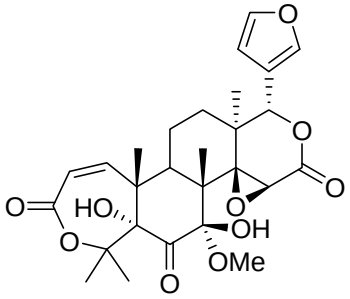
Compound **217**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
164.0	37.5062	161.6	157.3	181.4	181.4	MAE	5.8	7.5
150.5	52.1486	147.0	142.7	156.2	156.2	σ	6.4	5.9
148.5	56.4529	142.7	138.4	148.7	148.7	MaxErr	22.8	18.5
144.3	68.2468	130.9	126.6	128.4	128.4	R^2	0.7594	0.7594
136.0	68.3434	130.8	126.5	128.2	128.2	*m*	0.6	0.6
132.8	68.4860	130.7	126.3	128.0	128.0	*b*	56.5	52.2
130.4	69.4184	129.7	125.4	126.4	126.4	CMAE	6.5	6.5
128.7	70.5054	128.6	124.3	124.5	124.5	Cσ	6.4	6.4
125.0	70.7253	128.4	124.1	124.1	124.1	CMaxErr	17.4	17.4
123.6	71.4610	127.7	123.3	122.8	122.8			
118.7	74.1003	125.0	120.7	118.3	118.3			
101.6	74.7249	124.4	120.1	117.2	117.2			

[a] NMR data from: Morita, H.; Sato, Y.; Chan, K. L.; Choo, C. Y.; Itokawa, H.; Takeya, K.; Kobayashi, J. *J. Nat. Prod.* **2000**, *63*, 1707. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

Compound **218**

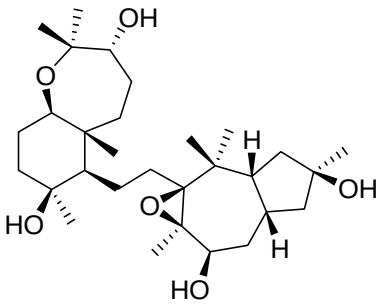


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
216.9	-22.4985	221.6	217.3	226.3	228.7	MAE	5.0	6.0
167.8	31.0674	168.1	163.7	169.5	169.3	σ	3.3	4.0
166.7	34.2885	164.9	160.5	166.1	165.7	MaxErr	11.5	12.6
153.9	52.5337	146.6	142.3	146.7	145.5	R^2	0.9956	0.9949
143.0	60.1448	139.0	134.7	138.6	137.1	*m*	0.9	0.9
141.1	60.3594	138.8	134.5	138.4	136.9	*b*	8.4	11.0
123.1	71.6548	127.5	123.2	126.4	124.3	CMAE	3.0	3.0
121.0	76.8173	122.3	118.0	120.9	118.6	Cσ	2.1	2.6
109.9	84.2003	114.9	110.6	113.1	110.4	CMaxErr	9.4	11.8
108.2	87.4535	106.2	107.4	103.8	106.8			
88.6	105.7830	87.9	89.0	84.4	86.5			
80.9	112.0487	81.6	82.8	77.7	79.6			
78.4	115.0867	78.6	79.7	74.5	76.2			
68.5	119.2643	74.4	75.5	70.1	71.6			
57.3	131.6181	62.1	63.2	57.0	57.9			
52.0	133.0402	60.6	61.8	55.4	56.3			
49.9	134.4263	59.2	60.4	54.0	54.8			
49.7	135.8978	57.8	58.9	52.4	53.1			
46.8	142.5209	51.1	52.3	45.4	45.8			
39.5	148.5173	45.2	46.3	39.0	39.2			
27.4	159.8132	33.9	35.0	27.0	26.6			
26.3	162.7438	30.9	32.1	23.9	23.4			
24.1	163.4114	30.3	31.4	23.2	22.7			
18.3	164.6552	29.0	30.2	21.9	21.3			
17.3	164.8867	28.8	29.9	21.7	21.0			
15.2	167.4260	26.2	27.4	19.0	18.2			
14.7	175.7748	17.9	19.0	10.1	8.9			

[a] NMR data from: Kubo, I.; Tanis, S. P.; Lee, Y. W.; Miura, I.; Nakanishi, K.; Chapya, A. *Heterocycles* **1976**, *5*, 485. Solvent: $CDCl_3$

[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

Compound **219**



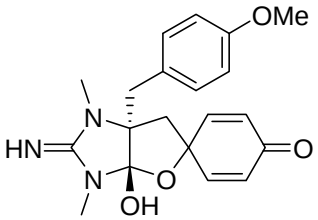
δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
77.8	106.2501	87.4	88.6	81.4	81.4	MAE	4.3	5.5
77.2	109.7675	83.9	85.0	78.0	78.0	σ	2.5	2.5
76.8	114.9496	78.7	79.9	73.1	73.1	MaxErr	9.8	11.0

72.7	116.0272	77.6	78.8	72.0	72.0	R^2	0.9872	0.9872
72.2	116.0750	77.6	78.7	72.0	72.0	*m*	1.0	1.0
70.0	119.2726	74.4	75.5	68.9	68.9	*b*	2.3	3.5
69.5	119.8524	73.8	75.0	68.4	68.4	CMAE	1.8	1.8
65.7	122.4058	71.3	72.4	65.9	65.9	Cσ	1.3	1.3
55.7	135.6303	58.0	59.2	53.3	53.3	CMaxErr	5.4	5.4
42.9	143.0699	50.6	51.7	46.2	46.2			
40.2	143.6442	50.0	51.2	45.6	45.6			
39.3	145.8357	47.8	49.0	43.5	43.5			
39.2	148.6119	45.1	46.2	40.9	40.9			
38.0	151.6522	42.0	43.2	38.0	38.0			
36.7	152.8793	40.8	41.9	36.8	36.8			
35.6	152.9978	40.7	41.8	36.7	36.7			
34.5	155.5382	38.1	39.3	34.2	34.2			
31.8	156.2108	37.5	38.6	33.6	33.6			
31.3	159.0038	34.7	35.8	30.9	30.9			
30.4	161.0474	32.6	33.8	29.0	29.0			
30.2	163.0178	30.7	31.8	27.1	27.1			
29.5	163.1661	30.5	31.6	26.9	26.9			
29.2	163.6572	30.0	31.2	26.5	26.5			
26.8	165.1903	28.5	29.6	25.0	25.0			
25.4	166.7654	26.9	28.0	23.5	23.5			
25.3	166.8174	26.9	28.0	23.5	23.5			
21.4	166.8752	26.8	27.9	23.4	23.4			
21.0	170.8334	22.8	24.0	19.6	19.6			
16.8	171.0815	22.6	23.7	19.4	19.4			
13.4	175.2703	18.4	19.5	15.4	15.4			

[a] NMR data from: Jain, S.; Laphookhieo, S.; Shi, Z.; Fu, L. W.; Akiyama, S.; Chen, Z. S.; Youssef, D. T. A.; von Soest, R. W. M.; El Sayed, K. A. *J. Nat. Prod.* **2007**, *70*, 928. Solvent: $CDCl_3$

[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

Compound **220**

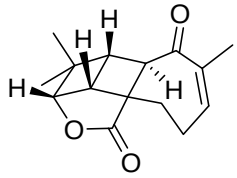


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
185.4	15.1379	184.0	179.7	182.8	184.5	MAE	3.5	4.2
159.5	41.9761	157.2	152.8	156.0	156.3	σ	3.4	2.8
158.9	42.6454	156.5	152.2	155.3	155.6	MaxErr	15.8	11.5
151.0	46.1803	153.0	148.6	151.8	151.9	R^2	0.9903	0.9907
150.1	49.9114	149.2	144.9	148.1	148.0	*m*	1.0	1.0
132.8	65.0594	134.1	129.8	133.0	132.1	*b*	0.8	4.0
132.8	67.6307	131.5	127.2	130.4	129.4	CMAE	3.5	3.2
127.5	69.4594	129.7	125.4	128.6	127.4	Cσ	3.2	3.4
126.9	69.5746	129.6	125.2	128.5	127.3	CMaxErr	14.7	13.5
125.9	69.9895	129.2	124.8	128.1	126.9			
112.7	70.6167	128.5	124.2	127.4	126.2			
112.7	83.2472	115.9	111.6	114.8	113.0			
102.5	84.6956	109.0	110.1	107.9	111.5			
82.5	111.1896	82.5	83.6	81.5	83.6			
77.1	120.8453	72.8	74.0	71.8	73.5			
54.2	143.5433	50.1	51.3	49.2	49.7			
46.9	150.4391	43.2	44.4	42.3	42.4			
37.1	160.5217	33.1	34.3	32.2	31.8			

24.7	162.2403	31.4	32.6	30.5	30.0			
24.5	167.4373	26.2	27.4	25.3	24.6			

[a] NMR data from: Ralifo, P.; Crews, P. *J. Org. Chem.* **2004**, *69*, 9025. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

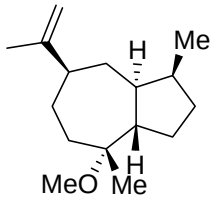
Compound **221**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
211.9	-7.1784	206.3	202.0	204.6	205.4	MAE	7.9	7.1
177.5	12.6830	186.5	182.1	185.4	185.5	σ	4.8	4.4
135.1	56.2387	142.9	138.6	143.2	141.7	MaxErr	15.9	14.7
131.1	57.4413	141.7	137.4	142.0	140.5	R^2	0.9801	0.9825
84.2	122.2704	71.4	72.5	73.9	75.3	*m*	1.0	1.0
62.8	135.3343	58.3	59.5	61.2	62.1	*b*	-4.8	-2.3
62.6	146.3812	47.3	48.4	50.5	51.0	CMAE	7.7	7.1
54.5	151.7540	41.9	43.1	45.3	45.6	Cσ	3.4	3.4
54.5	155.0849	38.6	39.7	42.1	42.3	CMaxErr	12.4	12.2
41.9	159.9522	33.7	34.9	37.4	37.4			
28.6	162.0355	31.6	32.8	35.3	35.3			
22.8	164.0079	29.7	30.8	33.4	33.3			
22.6	167.7711	25.9	27.0	29.8	29.5			
22.2	170.9491	22.7	23.9	26.7	26.3			
22.2	173.8984	19.8	20.9	23.8	23.4			

[a] NMR data from: Lodewyk, M. W.; Soldi, C.; Jones, P. B.; Olmstead, M. M.; Rita, J.; Shaw, J. T.; Dean J. Tantillo, D. J. *J. Am. Chem. Soc.* **2012**, *134*, 18550. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

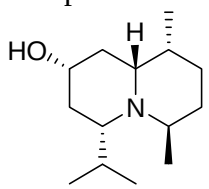
Compound **222**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
153.0	43.8315	155.3	151.0	151.8	151.7	MAE	3.5	4.1
107.8	85.2082	113.9	109.6	110.5	108.4	σ	3.0	3.2
78.9	113.3843	80.3	81.4	76.9	79.0	MaxErr	10.0	11.1
52.7	136.4730	57.2	58.3	53.9	54.9	R^2	0.9919	0.9914
49.0	141.0986	52.6	53.7	49.3	50.0	*m*	1.0	1.0
45.9	144.1408	49.5	50.7	46.3	46.9	*b*	3.2	5.8
45.3	150.2874	43.4	44.5	40.1	40.4	CMAE	2.6	2.7
39.0	152.8644	40.8	41.9	37.6	37.8	Cσ	1.9	2.0
30.5	153.1847	40.5	41.6	37.2	37.4	CMaxErr	6.7	6.9
30.4	154.5771	39.1	40.2	35.9	36.0			
28.4	158.0246	35.6	36.8	32.4	32.4			
27.7	164.1662	29.5	30.6	26.3	26.0			
26.1	165.5192	28.2	29.3	24.9	24.5			
25.1	168.1161	25.6	26.7	22.3	21.8			
20.2	173.3670	20.3	21.4	17.1	16.3			
16.5	176.5802	17.1	18.2	13.9	13.0			

[a] NMR data from: Fleischer, T. C.; Waigh, R. D.; Waterman, P. G. *J. Nat. Prod.* **1997**, *60*, 1054. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

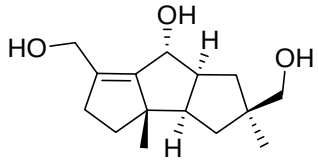
Compound **223**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
73.0	124.2294	69.4	70.6	82.3	82.3	MAE	9.2	8.0
72.8	132.6901	61.0	62.1	72.9	72.9	σ	4.1	4.1
68.6	139.1266	54.5	55.7	65.8	65.8	MaxErr	16.1	15.0
67.1	142.6832	51.0	52.1	61.8	61.8	R^2	0.9591	0.9591
49.6	151.4942	42.2	43.3	52.1	52.1	*m*	0.9	0.9
49.5	157.2421	36.4	37.6	45.7	45.7	*b*	-4.7	-3.6
41.3	159.0138	34.7	35.8	43.7	43.7	CMAE	3.1	3.1
41.1	162.6021	31.1	32.2	39.7	39.7	Cσ	2.5	2.5
41.0	164.3570	29.3	30.5	37.8	37.8	CMaxErr	9.4	9.4
40.0	164.8828	28.8	29.9	37.2	37.2			
22.0	173.0061	20.7	21.8	28.2	28.2			
22.0	177.8843	15.8	16.9	22.8	22.8			
21.9	178.4884	15.2	16.3	22.1	22.1			
18.3	183.9838	9.7	10.8	16.0	16.0			

[a] NMR data from: Kazmi, S. N.; Ahmed, Z.; Ahmed, W.; Malik, A. *Heterocycles* **1989**, *29*, 1901. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

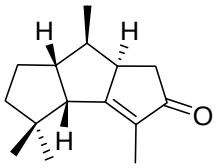
Compound **224**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
145.8	34.1278	165.0	160.7	154.4	154.3	MAE	5.8	5.9
129.1	65.3767	133.8	129.4	124.7	123.2	σ	5.0	4.7
74.3	118.9033	74.8	75.9	68.6	69.9	MaxErr	19.2	14.9
72.1	122.7913	70.9	72.0	64.9	66.1	R^2	0.9836	0.9841
59.0	135.4984	58.2	59.3	52.9	53.4	*m*	1.1	1.0
50.5	135.8814	57.8	58.9	52.5	53.0	*b*	2.6	5.6
45.9	136.7555	56.9	58.1	51.7	52.2	CMAE	3.8	3.9
45.5	140.5268	53.1	54.3	48.1	48.4	Cσ	2.6	2.3
45.1	142.4769	51.2	52.3	46.2	46.5	CMaxErr	8.6	8.5
40.8	148.8973	44.8	45.9	40.1	40.1			
36.1	151.2198	42.4	43.6	37.9	37.8			
36.0	155.4587	38.2	39.4	33.9	33.5			
25.1	157.9283	35.7	36.9	31.5	31.1			
22.7	168.4973	25.2	26.3	21.5	20.6			
20.3	170.7754	22.9	24.0	19.3	18.3			

[a] NMR data from: Huang, Z.; Dan, Y.; Huang, Y.; Lin, L.; Li, T.; Ye, W.; Wei, X. *J. Nat. Prod.* **2004**, *67*, 2121. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

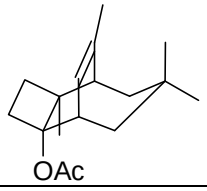
Compound **225**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
208.2	-9.3278	208.5	204.1	207.5	208.4	MAE	8.7	9.8
176.3	17.0531	182.1	177.8	179.7	179.6	σ	4.8	4.8
140.3	61.0423	138.1	133.8	133.5	131.6	MaxErr	15.8	17.0
42.5	139.8379	53.8	55.0	44.9	45.6	R^2	0.9947	0.9933
40.2	141.7997	51.9	53.0	42.8	43.5	*m*	1.0	0.9
32.5	145.3433	48.3	49.5	39.1	39.6	*b*	11.1	13.2
32.3	146.4110	47.3	48.4	38.0	38.5	CMAE	3.6	4.0
31.7	149.1608	44.5	45.6	35.1	35.4	Cσ	2.8	3.2
29.5	151.9156	41.8	42.9	32.2	32.4	CMaxErr	9.3	10.0
28.5	156.0592	37.6	38.8	27.8	27.9			
25.9	157.9361	35.7	36.9	25.9	25.9			
21.1	164.6150	29.1	30.2	18.8	18.6			
17.4	166.5022	27.2	28.3	16.8	16.5			
16.5	175.6871	18.0	19.1	7.2	6.5			
8.2	180.7321	12.9	14.1	1.9	1.0			

[a] NMR data from: Romo de Vivar, A.; Nieto, D. A.; Gaviño, R.; Pérez, A. L. C. *Phytochemistry* **1995**, *40*, 167. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

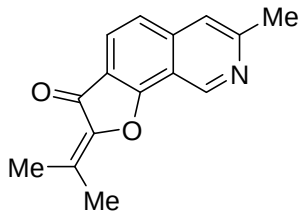
Compound **226**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
169.6	26.8698	172.3	167.9	167.3	167.8	MAE	3.5	3.8
130.7	52.9876	146.2	141.8	142.0	141.4	σ	3.4	2.3
130.3	70.1606	129.0	124.6	125.4	124.0	MaxErr	15.5	11.1
80.1	113.0702	80.6	81.7	78.6	80.6	R^2	0.9907	0.9910
47.7	145.0390	48.6	49.8	47.6	48.2	*m*	1.0	1.0
44.7	145.5216	48.1	49.3	47.1	47.7	*b*	-0.5	2.1
44.5	154.1237	39.5	40.7	38.8	39.0	CMAE	3.3	3.2
41.8	157.9214	35.7	36.9	35.1	35.2	Cσ	2.7	2.7
38.1	158.6698	35.0	36.1	34.4	34.4	CMaxErr	11.3	10.7
37.8	158.9370	34.7	35.9	34.2	34.2			
31.6	159.5823	34.1	35.2	33.5	33.5			
31.1	159.7813	33.9	35.0	33.3	33.3			
30.5	162.0377	31.6	32.8	31.1	31.0			
26.5	164.4663	29.2	30.3	28.8	28.6			
21.5	168.8013	24.9	26.0	24.6	24.2			
21.5	169.6222	24.0	25.2	23.8	23.3			
18.1	173.2550	20.4	21.6	20.3	19.7			

[a] NMR data from: Rodríguez Brasco, M. F.; Seldes, A. M.; Palermo, J. A. *Org. Lett.* **2001**, *3*, 1415. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

Compound **227**

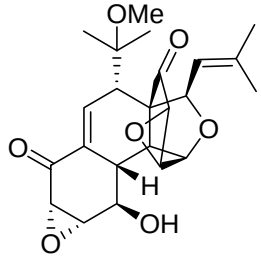


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
182.1	18.3599	180.8	176.5	180.7	182.3	MAE	3.2	3.6
164.0	35.6469	163.5	159.2	163.1	164.0	σ	1.8	3.3
156.7	38.7416	160.4	156.1	159.9	160.7	MaxErr	6.1	10.5
146.2	48.2201	150.9	146.6	150.3	150.6	R^2	0.9956	0.9954
145.6	56.4229	142.7	138.4	141.9	141.9	*m*	1.0	0.9
141.3	63.9768	135.2	130.8	134.3	133.9	*b*	3.2	4.6
133.7	65.4108	133.7	129.4	132.8	132.4	CMAE	2.9	2.8
124.1	69.8258	129.3	125.0	128.3	127.7	Cσ	1.7	2.1
120.5	74.8244	124.3	120.0	123.2	122.4	CMaxErr	7.0	7.4
119.5	75.7816	123.4	119.0	122.3	121.4			
119.3	76.6490	122.5	118.2	121.4	120.5			
114.6	86.9271	112.2	107.9	110.9	109.6			
24.7	170.2287	23.4	24.6	20.6	21.2			
20.4	170.5677	23.1	24.2	20.3	20.8			
17.5	170.5710	23.1	24.2	20.3	20.8			

[a] NMR data from: Kohno, J.; Hiramatsu, H.; Nishio, M.; Sakurai, M.; Okuda, T.; Komatsubara, S. *Tetrahedron* **1999**, *55*, 11247. Solvent: $CDCl_3$

[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

Compound **228**

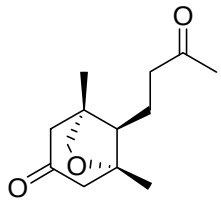


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
202.9	-11.9998	211.1	206.8	205.2	206.6	MAE	3.0	3.3
192.8	6.8555	192.3	188.0	186.8	187.4	σ	2.6	1.9
142.2	51.1642	148.0	143.6	143.5	142.2	MaxErr	8.2	8.2
139.6	51.7290	147.4	143.1	143.0	141.7	R^2	0.9979	0.9974
132.5	65.1624	134.0	129.6	129.8	128.0	*m*	1.0	1.0
120.7	72.1958	126.9	122.6	123.0	120.8	*b*	1.0	4.0
77.3	112.0547	81.6	82.8	78.7	80.2	CMAE	1.8	2.1
75.8	117.7119	76.0	77.1	73.2	74.4	Cσ	1.5	1.6
72.7	118.0442	75.6	76.8	72.9	74.1	CMaxErr	6.0	5.4
71.5	119.0500	74.6	75.8	71.9	73.1			
61.0	125.6084	68.1	69.2	65.5	66.4			
60.5	130.3692	63.3	64.4	60.8	61.5			
54.5	133.4058	60.3	61.4	57.8	58.5			
53.2	138.6772	55.0	56.1	52.7	53.1			
53.1	139.6197	54.1	55.2	51.8	52.1			
49.1	143.6487	50.0	51.2	47.8	48.0			
47.8	145.1444	48.5	49.7	46.4	46.5			
40.9	148.9246	44.7	45.9	42.7	42.6			
40.4	153.8150	39.9	41.0	37.9	37.7			

26.6	165.3278	28.3	29.5	26.7	25.9
26.1	166.6482	27.0	28.2	25.4	24.6
24.7	167.7328	25.9	27.1	24.3	23.5
18.6	175.4691	18.2	19.3	16.8	15.6

[a] NMR data from: Rychnovsky, S. D. *Org. Lett.* **2006**, *8*, 2895. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

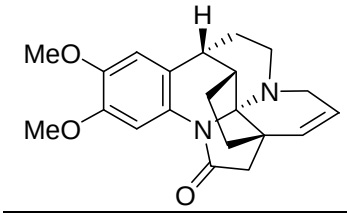
Compound **229**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
208.7	-11.3235	210.5	206.1	209.2	208.8	MAE	2.2	2.6
207.2	-9.6954	208.8	204.5	207.5	207.1	σ	1.3	1.9
83.4	106.3888	87.3	88.4	86.1	87.4	MaxErr	4.4	5.6
78.3	117.3312	76.3	77.5	75.1	76.2	R^2	0.9987	0.9987
53.1	139.2235	54.4	55.6	53.2	53.6	*m*	1.0	1.0
49.4	144.9506	48.7	49.9	47.5	47.7	*b*	1.2	3.6
48.6	145.5490	48.1	49.3	46.9	47.1	CMAE	1.9	1.8
43.4	146.5600	47.1	48.3	45.9	46.0	Cσ	1.1	1.3
42.6	153.1885	40.5	41.6	39.3	39.2	CMaxErr	3.3	4.0
30.0	164.8677	28.8	29.9	27.6	27.2			
24.9	166.7202	26.9	28.1	25.8	25.2			
20.8	169.5125	24.2	25.3	23.0	22.4			
18.7	170.5387	23.1	24.3	21.9	21.3			

[a] NMR data from: Macías, F. A.; Varela, R. M.; Torres, A.; Oliva, R. M.; Molinillo, J. M. G. *Phytochemistry* **1997**, *48*, 631. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

Compound **230**

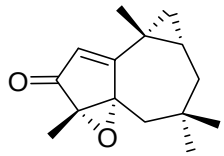


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
173.8	20.2341	178.9	174.6	178.6	180.8	MAE	2.7	3.4
147.7	53.5975	145.5	141.2	145.1	145.5	σ	1.5	2.1
145.3	57.0951	142.0	137.7	141.6	141.8	MaxErr	5.4	8.3
131.5	62.5261	136.6	132.3	136.2	136.0	R^2	0.9958	0.9954
131.0	72.0964	127.0	122.7	126.6	125.8	*m*	1.0	0.9
120.0	76.0177	123.1	118.8	122.7	121.7	*b*	0.8	4.0
117.4	83.5351	115.6	111.3	115.1	113.7	CMAE	2.4	2.5
111.3	85.7413	113.4	109.1	112.9	111.4	Cσ	1.8	2.0
102.6	94.5356	104.6	100.3	104.1	102.1	CMaxErr	6.1	7.1
84.4	109.5266	84.1	85.3	83.6	86.2			
56.1	142.7231	50.9	52.1	50.3	51.0			
56.0	143.0991	50.6	51.7	49.9	50.6			
47.9	144.6513	49.0	50.2	48.4	48.9			
46.0	145.8631	47.8	48.9	47.1	47.6			
44.5	146.6815	47.0	48.1	46.3	46.8			
44.3	148.0059	45.7	46.8	45.0	45.4			

37.7	154.2381	39.4	40.6	38.7	38.7
36.6	155.5773	38.1	39.2	37.4	37.3
35.0	156.9698	36.7	37.8	36.0	35.8
26.8	164.3040	29.4	30.5	28.6	28.1
24.8	166.8880	26.8	27.9	26.1	25.3

[a] NMR data from: Hubbs, J. L.; Heathcock, C. H. *Org. Lett.* **1999**, *1*, 1315. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

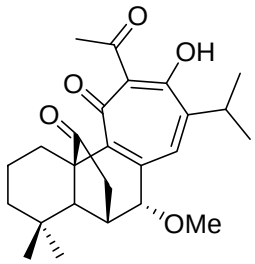
Compound **231**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
200.1	-2.7657	201.9	197.6	202.4	203.1	MAE	4.5	5.5
180.0	25.3511	173.8	169.5	173.4	173.0	σ	2.6	2.9
128.5	63.2519	135.9	131.6	134.4	132.5	MaxErr	7.9	10.5
66.5	119.3054	74.4	75.5	71.0	72.5	R^2	0.9969	0.9968
60.8	130.2507	63.4	64.6	59.7	60.8	*m*	1.0	0.9
42.7	150.5863	43.1	44.2	38.7	39.1	*b*	5.5	7.7
34.5	153.4900	40.2	41.3	35.7	36.0	CMAE	2.7	2.6
34.2	155.7590	37.9	39.1	33.4	33.5	Cσ	1.9	2.1
30.8	162.2686	31.4	32.5	26.7	26.6	CMaxErr	6.6	7.0
28.9	162.8293	30.8	32.0	26.1	26.0			
26.5	163.2030	30.5	31.6	25.7	25.6			
23.3	164.3380	29.3	30.5	24.5	24.4			
21.3	164.8213	28.8	30.0	24.0	23.8			
19.5	168.2252	25.4	26.6	20.5	20.2			
8.4	178.7322	14.9	16.1	9.7	9.0			

[a] NMR data from: Tori, M.; Nakashima, K.; Toyota, M.; Asakawa, Y. *Tetrahedron Lett.* **1993**, *34*, 3751. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

Compound **232**

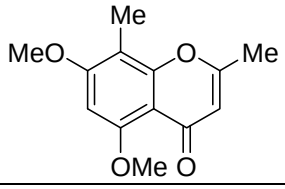


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
203.1	-3.9409	203.1	198.8	204.0	205.5	MAE	3.3	3.9
189.1	7.5841	191.6	187.2	192.3	193.3	σ	4.3	4.6
175.7	16.9138	182.2	177.9	182.8	183.4	MaxErr	19.9	24.2
175.4	43.6558	155.5	151.2	155.7	155.1	R^2	0.9928	0.9930
149.1	49.5551	149.6	145.3	149.7	148.9	*m*	1.0	0.9
146.6	52.5273	146.6	142.3	146.7	145.7	*b*	2.1	4.5
132.1	61.2263	137.9	133.6	137.9	136.5	CMAE	3.1	3.0
132.0	66.6586	132.5	128.2	132.3	130.8	Cσ	4.4	4.3
119.8	68.9300	130.2	125.9	130.0	128.4	CMaxErr	19.7	20.3
79.5	115.7269	77.9	79.1	77.0	78.9			
73.0	125.4147	68.3	69.4	67.2	68.6			
59.2	136.7291	56.9	58.1	55.7	56.7			
50.2	139.8660	53.8	54.9	52.5	53.3			
45.8	146.9192	46.8	47.9	45.3	45.9			

38.1	155.7430	37.9	39.1	36.4	36.6
31.3	157.5236	36.1	37.3	34.6	34.7
31.3	161.9224	31.7	32.9	30.1	30.0
30.2	162.1277	31.5	32.7	29.9	29.8
28.1	163.7312	29.9	31.1	28.3	28.1
26.4	165.8482	27.8	29.0	26.1	25.9
22.8	168.2962	25.4	26.5	23.6	23.3
22.3	170.0549	23.6	24.8	21.8	21.4
21.9	170.5780	23.1	24.2	21.3	20.9
18.6	171.4510	22.2	23.4	20.4	19.9

[a] NMR data from: Yang, J.; Huang, S. X.; Zhao, Q. S. *J. Phys. Chem. A* **2008**, *112*, 12132. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

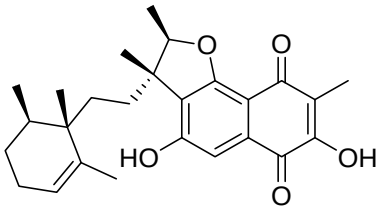
Compound **233**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
177.6	23.3492	175.8	171.5	175.9	177.0	MAE	3.2	3.9
162.6	37.5569	161.6	157.3	161.5	162.1	σ	2.3	2.1
160.7	41.2655	157.9	153.5	157.8	158.2	MaxErr	8.6	7.2
158.5	41.4446	157.7	153.4	157.6	158.0	R^2	0.9950	0.9972
156.5	43.6440	155.5	151.2	155.4	155.7	*m*	1.0	1.0
110.9	79.6829	119.5	115.1	119.1	117.9	*b*	1.3	2.9
108.0	86.1596	113.0	108.7	112.5	111.1	CMAE	3.1	2.1
105.3	91.4208	107.7	103.4	107.2	105.5	Cσ	2.5	2.1
91.1	103.7808	95.4	91.0	94.8	92.6	CMaxErr	8.2	7.0
56.0	143.0114	50.7	51.8	49.7	51.4			
55.4	143.2290	50.4	51.6	49.5	51.1			
19.4	172.9697	20.7	21.8	19.5	19.9			
7.3	183.5844	10.1	11.2	8.8	8.8			

[a] NMR data from: Kalinin, A. V.; Snieckus, V. *Tetrahedron Lett.* **1998**, *39*, 4999. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

Compound **234**

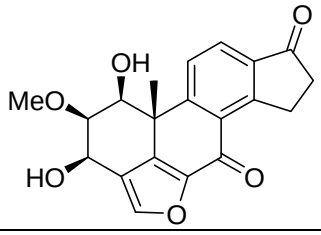


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
182.9	16.3255	182.8	178.5	181.9	183.3	MAE	2.9	3.3
180.4	16.4697	182.7	178.3	181.8	183.2	σ	1.6	2.0
159.9	39.6765	159.5	155.1	158.3	158.7	MaxErr	6.3	7.9
157.7	45.0601	154.1	149.8	152.9	153.0	R^2	0.9981	0.9986
153.6	47.7441	151.4	147.1	150.2	150.2	*m*	1.0	0.9
138.9	55.3138	143.8	139.5	142.5	142.2	*b*	2.7	4.8
131.6	66.0784	133.1	128.7	131.6	130.8	CMAE	1.9	1.7
127.3	68.4790	130.7	126.3	129.2	128.3	Cσ	1.9	1.6
123.9	69.8395	129.3	125.0	127.8	126.8	CMaxErr	8.2	5.7
120.3	74.9127	124.2	119.9	122.7	121.5			
107.9	86.4126	112.7	108.4	111.1	109.3			
107.9	88.0104	111.1	106.8	109.5	107.7			

86.3	113.6240	80.0	81.2	78.1	80.6
46.0	142.3833	51.3	52.4	49.0	50.3
39.7	149.4984	44.2	45.3	41.9	42.8
32.8	158.1027	35.6	36.7	33.2	33.7
31.0	160.7113	33.0	34.1	30.5	30.9
30.5	161.0675	32.6	33.7	30.2	30.5
26.6	165.3871	28.3	29.4	25.8	26.0
25.1	166.9230	26.7	27.9	24.3	24.4
20.9	170.7271	22.9	24.1	20.4	20.3
19.7	171.7705	21.9	23.0	19.4	19.2
18.8	171.9205	21.7	22.9	19.2	19.1
15.7	175.9037	17.8	18.9	15.2	14.9
15.1	176.5198	17.1	18.3	14.6	14.2
8.6	183.1756	10.5	11.6	7.8	7.2

[a] NMR data from: Kalaitzis, J. A.; Hamano, Y.; Nilsen, G.; Moore, B. S. *Org. Lett.* **2003**, *5*, 4449. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

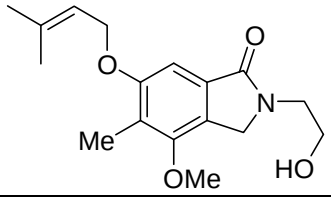
Compound **235**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
206.7	-11.7998	210.9	206.6	209.1	211.8	MAE	2.3	3.3
173.4	21.0207	178.1	173.8	176.3	177.3	σ	2.1	2.0
158.6	40.5592	158.6	154.3	156.7	156.8	MaxErr	6.8	6.3
158.0	41.1605	158.0	153.6	156.1	156.1	R^2	0.9979	0.9965
145.7	53.6210	145.5	141.2	143.6	143.0	*m*	1.0	1.0
145.6	55.4932	143.6	139.3	141.8	141.1	*b*	2.1	5.1
142.4	57.8702	141.3	136.9	139.4	138.6	CMAE	2.0	2.6
136.9	61.0305	138.1	133.8	136.2	135.2	Cσ	1.2	1.6
129.8	68.6170	130.5	126.2	128.6	127.3	CMaxErr	4.9	5.4
127.3	69.0691	130.1	125.7	128.2	126.8			
127.3	69.5024	129.6	125.3	127.7	126.3			
122.1	70.2380	128.9	124.6	127.0	125.6			
81.7	106.8127	86.9	88.0	84.9	87.1			
71.7	116.8039	76.9	78.0	74.9	76.6			
62.6	127.1836	66.5	67.6	64.5	65.7			
60.7	132.9941	60.7	61.8	58.7	59.6			
42.3	149.0679	44.6	45.7	42.6	42.7			
36.5	156.9876	36.7	37.8	34.7	34.4			
30.5	162.9500	30.7	31.9	28.7	28.1			
28.4	162.9574	30.7	31.9	28.7	28.1			

[a] NMR data from: Wipf, P.; Kerekes, A. D. *J. Nat. Prod.* **2003**, *66*, 716. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

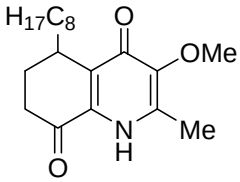
Compound **236**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
167.5	29.2562	169.9	165.6	166.7	167.5	MAE	2.4	2.0
158.7	42.3378	156.8	152.5	153.9	154.1	σ	2.4	1.7
152.4	47.5500	151.6	147.3	148.9	148.8	MaxErr	8.4	6.2
138.0	52.7920	146.4	142.0	143.8	143.4	R^2	0.9971	0.9977
132.2	64.8944	134.2	129.9	132.0	131.0	*m*	1.0	1.0
125.1	66.9980	132.1	127.8	129.9	128.9	*b*	-1.2	1.8
121.8	73.2858	125.9	121.5	123.8	122.4	CMAE	2.0	1.8
120.5	74.2242	124.9	120.6	122.9	121.5	Cσ	1.9	1.7
99.7	92.5603	101.1	102.3	99.7	102.7	CMaxErr	5.8	5.4
68.7	128.0558	65.6	66.8	65.1	66.4			
59.7	135.1105	58.6	59.7	58.2	59.2			
56.4	139.7199	53.9	55.1	53.7	54.5			
49.2	144.4835	49.2	50.3	49.1	49.6			
45.1	148.5133	45.2	46.3	45.1	45.5			
26.0	167.7728	25.9	27.0	26.4	25.8			
18.5	175.5732	18.1	19.2	18.8	17.8			
10.2	182.6316	11.0	12.2	11.9	10.6			

[a] NMR data from: Cornella, I.; Kelly, T. R. *J. Org. Chem.* **2004**, *69*, 2191. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

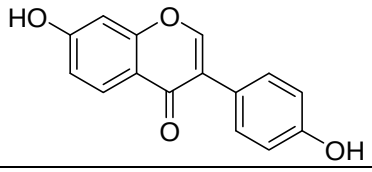
Compound **237**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
194.6	1.2103	197.9	193.6	198.5	200.1	MAE	2.3	3.6
172.8	25.7598	173.4	169.1	173.6	174.2	σ	1.0	1.6
147.5	55.0953	144.0	139.7	143.9	143.2	MaxErr	4.5	7.8
139.0	58.1969	140.9	136.6	140.7	139.9	R^2	0.9988	0.9985
138.9	63.4025	135.7	131.4	135.5	134.4	*m*	1.0	0.9
132.2	65.9807	133.2	128.8	132.8	131.7	*b*	2.0	4.3
59.4	138.8007	54.9	56.0	53.5	54.7	CMAE	1.4	1.5
32.2	159.6891	34.0	35.1	32.4	32.6	Cσ	1.6	1.8
31.8	160.5508	33.1	34.3	31.5	31.7	CMaxErr	5.9	5.5
30.5	160.8082	32.9	34.0	31.2	31.4			
30.3	160.9040	32.8	33.9	31.1	31.3			
29.6	161.8743	31.8	32.9	30.1	30.3			
29.5	162.0576	31.6	32.8	30.0	30.1			
29.2	162.8324	30.8	32.0	29.2	29.3			
28.4	163.4600	30.2	31.4	28.5	28.6			
24.3	167.0670	26.6	27.7	24.9	24.8			
22.6	167.2662	26.4	27.5	24.7	24.6			
14.5	177.1419	16.5	17.7	14.7	14.2			
14.0	177.2401	16.4	17.6	14.6	14.1			

[a] NMR data from: Bringmann, J.; Schlauer, H.; Rischer, H.; Wohlfarth, J.; Mühlbacher, J.; Buske, A.; Porzel, A.; Schmidt, J.; Adam, G. *Tetrahedron* **2000**, *56*, 3691. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

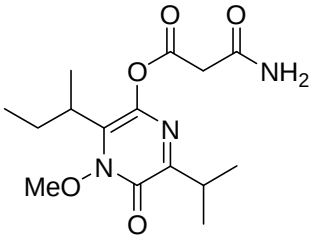
Compound **238**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
174.8	23.4659	175.7	171.3	178.5	178.5	MAE	3.4	4.1
162.8	41.7412	157.4	153.1	158.3	158.3	σ	2.6	2.9
157.6	41.7850	157.4	153.0	158.2	158.2	MaxErr	8.9	9.7
157.2	44.7947	154.3	150.0	154.9	154.9	R^2	0.9714	0.9714
152.9	49.7644	149.4	145.0	149.4	149.4	*m*	0.9	0.9
130.1	65.1859	134.0	129.6	132.3	132.3	*b*	14.7	10.4
127.3	66.2574	132.9	128.6	131.1	131.1	CMAE	3.4	3.4
123.6	66.6791	132.5	128.1	130.6	130.6	Cσ	1.6	1.6
122.6	72.5728	126.6	122.2	124.1	124.1	CMaxErr	7.0	7.0
116.6	76.1882	123.0	118.6	120.1	120.1			
115.3	83.7701	115.4	111.0	111.7	111.7			
115.0	85.2556	113.9	109.6	110.0	110.0			
102.2	95.2198	103.9	99.6	98.9	98.9			

[a] NMR data from: Suzuki, K.; Yahara, S.; Kazutomo, M.; Uyeda, M. *J. Nat. Prod.* **2001**, *64*, 204. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

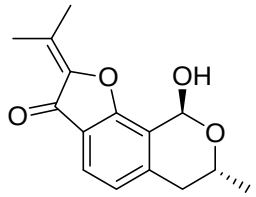
Compound **239**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
168.0	30.9897	168.2	163.8	167.0	167.4	MAE	2.2	3.2
166.0	31.0289	168.1	163.8	167.0	167.4	σ	2.1	1.9
161.5	37.0302	162.1	157.8	160.9	161.1	MaxErr	6.7	6.9
152.0	43.7645	155.4	151.0	154.2	154.1	R^2	0.9981	0.9981
135.0	61.7042	137.4	133.1	136.3	135.3	*m*	1.0	1.0
134.9	64.2641	134.9	130.5	133.7	132.7	*b*	1.3	3.5
64.1	136.2732	57.4	58.5	56.2	57.5	CMAE	1.9	2.0
41.1	148.6665	45.0	46.1	43.8	44.5	Cσ	2.0	1.9
33.7	154.1786	39.5	40.6	38.3	38.8	CMaxErr	7.9	6.6
30.7	159.4617	34.2	35.3	33.0	33.2			
27.5	165.1606	28.5	29.6	27.3	27.3			
19.9	173.5791	20.1	21.2	18.8	18.5			
19.9	174.3914	19.3	20.4	18.0	17.6			
18.2	174.8986	18.8	19.9	17.5	17.1			
12.6	179.2603	14.4	15.6	13.2	12.6			

[a] NMR data from: Kita, M.; Miwa, R.; Widianti, T.; Ozaki, Y.; Aoyama, S.; Yamada, K.; Uemura, D. *Tetrahedron Lett.* **2007**, *48*, 8628. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

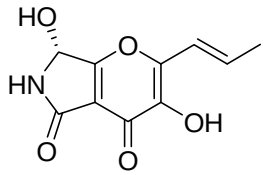
Compound **240**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
182.5	9.5712	189.6	185.2	186.1	187.9	MAE	2.6	2.8
162.5	39.9365	159.2	154.9	156.2	156.6	σ	2.3	1.8
144.5	53.7089	145.4	141.1	142.6	142.4	MaxErr	7.1	7.6
142.0	55.0005	144.1	139.8	141.4	141.1	R^2	0.9978	0.9969
131.1	66.9288	132.2	127.9	129.6	128.8	*m*	1.0	1.0
122.7	69.9969	129.1	124.8	126.6	125.6	*b*	0.5	2.9
122.5	70.8546	128.3	124.0	125.8	124.7	CMAE	1.8	2.4
122.0	74.7077	124.4	120.1	122.0	120.8	Cσ	1.8	1.8
119.1	78.7251	120.4	116.1	118.0	116.6	CMaxErr	6.3	5.9
87.5	101.7509	91.9	93.1	90.0	92.9			
62.2	130.0265	63.6	64.8	62.1	63.8			
36.5	156.9154	36.8	37.9	35.7	36.1			
21.0	171.2189	22.5	23.6	21.6	21.3			
20.1	173.0072	20.7	21.8	19.8	19.5			
17.0	177.3038	16.4	17.5	15.6	15.1			

[a] NMR data from: Lin, W. H.; Brauers, G.; Ebel, R.; Wray, V.; Berg, A.; Surdasono; Proksch, P. *J. Nat. Prod.* **2003**, *66*, 57. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

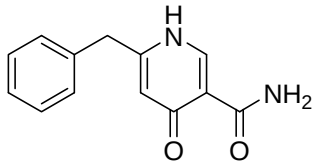
Compound **241**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
174.2	28.8864	170.3	165.9	169.8	170.6	MAE	2.6	3.7
169.1	29.9763	169.2	164.8	168.7	169.5	σ	2.7	2.2
165.0	34.3936	164.7	160.4	164.1	164.7	MaxErr	8.2	8.3
146.0	52.9206	146.2	141.9	145.0	144.7	R^2	0.9958	0.9973
142.2	56.5596	142.6	138.3	141.3	140.8	*m*	1.0	0.9
131.7	63.4482	135.7	131.4	134.2	133.4	*b*	5.7	7.6
118.9	75.1587	124.0	119.7	122.1	120.8	CMAE	2.4	2.0
111.7	79.2606	119.9	115.5	117.8	116.3	Cσ	1.9	1.4
75.2	116.2634	77.4	78.5	74.0	76.4	CMaxErr	6.1	4.6
18.7	172.8337	20.8	22.0	15.6	15.5			

[a] NMR data from: Hiort, J.; Maksimenka, K.; Reichert, M.; Perovi-Ottstadt, S.; Lin, W. H.; Wray, V.; Steube, K.; Schaumann, K.; Weber, H.; Proksch, P.; Ebel, R.; Müller, W. E. G.; Bringmann, G. *J. Nat. Prod.* **2004**, *67*, 1532. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

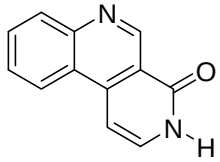
Compound **242**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
178.1	23.6281	175.5	171.2	176.2	177.7	MAE	1.8	3.9
165.9	31.8956	167.2	162.9	167.6	168.7	σ	1.7	1.6
151.2	48.5186	150.6	146.3	150.4	150.8	MaxErr	6.5	6.9
142.2	57.7009	141.4	137.1	140.9	140.9	R^2	0.9956	0.9959
137.4	60.0530	139.1	134.8	138.5	138.4	*m*	1.0	0.9
129.3	68.3547	130.8	126.5	129.9	129.4	*b*	5.3	6.5
129.3	69.6280	129.5	125.2	128.6	128.0	CMAE	1.7	1.6
129.2	70.3418	128.8	124.5	127.8	127.3	Cσ	1.2	1.3
129.2	71.1081	128.0	123.7	127.0	126.4	CMaxErr	5.4	4.7
127.5	72.0815	127.1	122.7	126.0	125.4			
118.9	73.7077	125.4	121.1	124.3	123.6			
118.0	77.5758	121.6	117.2	120.3	119.5			
38.2	152.8681	40.8	41.9	36.7	38.2			

[a] NMR data from: Hiort, J.; Maksimenka, K.; Reichert, M.; Perovi-Ottstadt, S.; Lin, W. H.; Wray, V.; Steube, K.; Schaumann, K.; Weber, H.; Proksch, P.; Ebel, R.; Müller, W. E. G.; Bringmann, G. *J. Nat. Prod.* **2004**, *67*, 1532. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

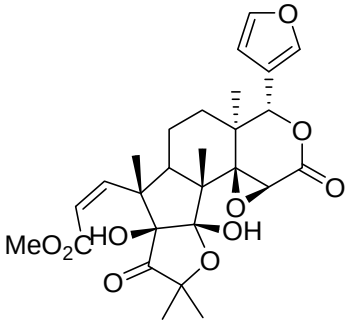
Compound **243**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
164.0	37.2219	161.9	157.6	163.7	163.7	MAE	1.8	4.3
150.5	44.8619	154.3	149.9	155.6	155.6	σ	1.2	2.2
148.5	54.1141	145.0	140.7	145.7	145.7	MaxErr	3.8	7.8
144.3	56.1572	143.0	138.7	143.5	143.5	R^2	0.9845	0.9845
136.0	65.0260	134.1	129.8	134.1	134.1	*m*	0.9	0.9
132.8	66.1582	133.0	128.7	132.9	132.9	*b*	8.4	4.1
130.4	67.6640	131.5	127.1	131.3	131.3	CMAE	1.4	1.4
128.7	70.6873	128.5	124.1	128.0	128.0	Cσ	1.4	1.4
125.0	72.1983	126.9	122.6	126.4	126.4	CMaxErr	5.1	5.1
123.6	76.9713	122.2	117.8	121.3	121.3			
118.7	79.3189	119.8	115.5	118.8	118.8			
101.6	94.5252	104.6	100.3	102.6	102.6			

[a] NMR data from: Morita, H.; Sato, Y.; Chan, K. L.; Choo, C. Y.; Itokawa, H.; Takeya, K.; Kobayashi, J. *J. Nat. Prod.* **2000**, *63*, 1707. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

Compound **244**

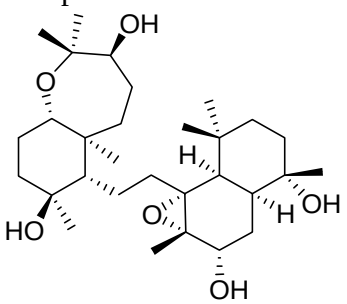


δ_{exp} [a]	Shielding Values [b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
216.9	-35.9203	235.1	230.7	230.8	233.2	MAE	5.2	5.7
167.8	26.0581	173.1	168.8	168.6	168.4	σ	3.9	3.3
166.7	30.7862	168.4	164.0	163.9	163.5	MaxErr	18.2	13.8
153.9	46.0594	153.1	148.8	148.6	147.5	R^2	0.9936	0.9924
143.0	59.9330	139.2	134.9	134.7	133.1	*m*	1.0	1.0
141.1	60.6659	138.5	134.1	133.9	132.3	*b*	4.9	7.5
123.1	71.5348	127.6	123.3	123.0	120.9	CMAE	3.1	3.4
121.0	73.7244	125.4	121.1	120.8	118.7	Cσ	3.2	3.6
109.9	75.6688	123.5	119.1	118.9	116.6	CMaxErr	13.9	16.3
108.2	84.4497	109.2	110.4	104.6	107.4			
88.6	102.8908	90.8	91.9	86.1	88.2			
80.9	108.1073	85.6	86.7	80.9	82.7			
78.4	113.5678	80.1	81.2	75.4	77.0			
68.5	119.1038	74.6	75.7	69.8	71.3			
57.3	133.8587	59.8	61.0	55.1	55.8			
52.0	135.1923	58.5	59.6	53.7	54.5			
49.9	135.4354	58.2	59.4	53.5	54.2			
49.7	137.9486	55.7	56.9	51.0	51.6			
46.8	145.2380	48.4	49.6	43.6	44.0			
39.5	149.6559	44.0	45.2	39.2	39.3			
27.4	161.3587	32.3	33.5	27.5	27.1			
26.3	162.5926	31.1	32.2	26.2	25.8			
24.1	166.6262	27.0	28.2	22.2	21.6			
18.3	167.5568	26.1	27.3	21.3	20.7			
17.3	168.3277	25.3	26.5	20.5	19.8			
15.2	169.1435	24.5	25.7	19.7	19.0			
14.7	175.6629	18.0	19.1	13.1	12.2			

[a] NMR data from: Kubo, I.; Tanis, S. P.; Lee, Y. W.; Miura, I.; Nakanishi, K.; Chapya, A. *Heterocycles* **1976**, *5*, 485. Solvent: $CDCl_3$

[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

Compound **245**



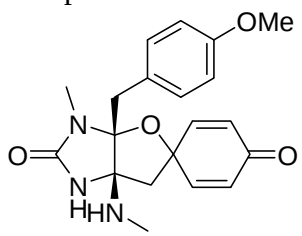
δ_{exp} [a]	Shielding Values [b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
77.8	108.4519	85.2	86.4	81.6	81.6	MAE	2.8	3.9
77.2	115.3211	78.3	79.5	74.9	74.9	σ	1.8	1.8
76.8	115.5473	78.1	79.3	74.7	74.7	MaxErr	7.4	8.6

72.7	118.8078	74.9	76.0	71.5	71.5	R^2	0.9924	0.9924
72.2	118.8739	74.8	75.9	71.5	71.5	*m*	1.0	1.0
70.0	119.2316	74.4	75.6	71.1	71.1	*b*	1.5	2.7
69.5	119.3234	74.3	75.5	71.0	71.0	CMAE	1.4	1.4
65.7	121.4471	72.2	73.4	69.0	69.0	Cσ	1.1	1.1
55.7	138.7885	54.9	56.0	52.0	52.0	CMaxErr	3.8	3.8
42.9	146.4896	47.2	48.3	44.5	44.5			
40.2	150.3070	43.4	44.5	40.8	40.8			
39.3	151.1565	42.5	43.7	40.0	40.0			
39.2	151.9788	41.7	42.8	39.2	39.2			
38.0	154.3899	39.3	40.4	36.8	36.8			
36.7	155.7747	37.9	39.0	35.5	35.5			
35.6	156.5368	37.1	38.3	34.7	34.7			
34.5	157.1604	36.5	37.6	34.1	34.1			
31.8	159.0558	34.6	35.8	32.3	32.3			
31.3	159.7886	33.9	35.0	31.6	31.6			
30.4	161.4395	32.2	33.4	30.0	30.0			
30.2	161.9728	31.7	32.8	29.4	29.4			
29.5	162.5226	31.1	32.3	28.9	28.9			
29.2	162.5841	31.1	32.2	28.8	28.8			
26.8	163.8827	29.8	30.9	27.6	27.6			
25.4	166.6868	27.0	28.1	24.8	24.8			
25.3	167.7944	25.9	27.0	23.8	23.8			
21.4	168.5018	25.2	26.3	23.1	23.1			
21.0	171.7446	21.9	23.1	19.9	19.9			
16.8	171.8629	21.8	22.9	19.8	19.8			
13.4	174.7754	18.9	20.0	17.0	17.0			

[a] NMR data from: Jain, S.; Laphookhieo, S.; Shi, Z.; Fu, L. W.; Akiyama, S.; Chen, Z. S.; Youssef, D. T. A.; von Soest, R. W. M.; El Sayed, K. A. *J. Nat. Prod.* **2007**, *70*, 928. Solvent: $CDCl_3$

[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

Compound **246**

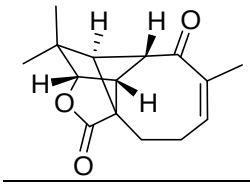


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
185.4	15.2967	183.8	179.5	185.2	187.1	MAE	2.3	3.8
159.5	43.0129	156.1	151.8	156.7	157.0	σ	1.6	2.2
158.9	43.4430	155.7	151.4	156.2	156.5	MaxErr	6.2	7.7
151.0	48.4051	150.7	146.4	151.1	151.1	R^2	0.9976	0.9980
150.1	48.5790	150.6	146.2	150.9	151.0	*m*	1.0	0.9
132.8	64.2141	134.9	130.6	134.8	134.0	*b*	4.0	7.1
132.8	64.4836	134.7	130.3	134.6	133.7	CMAE	1.8	1.6
127.5	68.9860	130.2	125.8	129.9	128.8	Cσ	1.5	1.4
126.9	69.9626	129.2	124.8	128.9	127.8	CMaxErr	6.6	6.2
125.9	71.3704	127.8	123.4	127.5	126.2			
112.7	84.8656	114.3	109.9	113.6	111.6			
112.7	85.9214	113.2	108.9	112.5	110.4			
102.5	90.0490	103.6	104.8	102.6	106.0			
82.5	112.1093	81.6	82.7	79.9	82.0			
77.1	117.1452	76.5	77.7	74.7	76.6			
54.2	143.5058	50.2	51.3	47.6	48.0			
46.9	143.5148	50.2	51.3	47.6	48.0			
37.1	151.5659	42.1	43.2	39.3	39.2			
24.7	162.8044	30.9	32.0	27.7	27.0			

24.5	165.8844	27.8	28.9	24.5	23.7

[a] NMR data from: Ralifo, P.; Crews, P. *J. Org. Chem.* **2004**, *69*, 9025. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

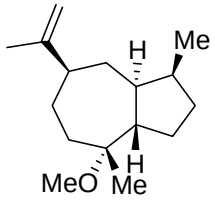
Compound **247**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
211.9	-17.3624	216.5	212.2	212.2	213.3	MAE	2.9	2.3
177.5	18.3055	180.8	176.5	177.4	177.2	σ	2.4	1.9
135.1	59.6197	139.5	135.2	137.0	135.3	MaxErr	7.5	6.3
131.1	61.7072	137.4	133.1	135.0	133.2	R^2	0.9969	0.9977
84.2	116.9370	76.7	77.9	75.8	77.2	*m*	1.0	1.0
62.8	130.5030	63.2	64.3	62.5	63.5	*b*	-0.9	1.6
62.6	132.0143	61.7	62.8	61.1	62.0	CMAE	2.2	1.9
54.5	136.2283	57.4	58.6	56.9	57.7	Cσ	2.4	2.1
54.5	145.3817	48.3	49.4	48.0	48.4	CMaxErr	8.4	7.0
41.9	148.8814	44.8	45.9	44.6	44.9			
28.6	164.4112	29.3	30.4	29.4	29.2			
22.8	168.0423	25.6	26.8	25.9	25.5			
22.6	170.7591	22.9	24.1	23.2	22.7			
22.2	170.8066	22.9	24.0	23.2	22.7			
22.2	171.6685	22.0	23.1	22.4	21.8			

[a] NMR data from: Lodewyk, M. W.; Soldi, C.; Jones, P. B.; Olmstead, M. M.; Rita, J.; Shaw, J. T.; Dean J. Tantillo, D. J. *J. Am. Chem. Soc.* **2012**, *134*, 18550. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

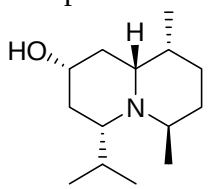
Compound **222**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
152.4	43.8315	155.3	151.0	150.9	150.8	MAE	2.3	2.8
108.4	85.2082	113.9	109.6	110.4	108.4	σ	1.2	1.2
77.1	113.3843	80.3	81.4	77.5	79.5	MaxErr	5.5	4.3
54.7	136.4730	57.2	58.3	54.9	55.9	R^2	0.9990	0.9986
49.4	141.0986	52.6	53.7	50.4	51.2	*m*	1.0	1.0
49.4	144.1408	49.5	50.7	47.4	48.0	*b*	1.0	3.8
41.1	150.2874	43.4	44.5	41.4	41.7	CMAE	0.8	1.0
39.2	152.8644	40.8	41.9	38.9	39.1	Cσ	0.7	0.9
37.7	153.1847	40.5	41.6	38.6	38.8	CMaxErr	2.3	3.1
37.4	154.5771	39.1	40.2	37.2	37.3			
34.2	158.0246	35.6	36.8	33.9	33.8			
27.6	164.1662	29.5	30.6	27.9	27.5			
25.4	165.5192	28.2	29.3	26.5	26.1			
24.1	168.1161	25.6	26.7	24.0	23.5			
21.2	173.3670	20.3	21.4	18.9	18.1			
15.3	176.5802	17.1	18.2	15.7	14.8			

[a] NMR data from: Booker-Milburn, K. I.; Jankins, H.; Charmant, J. P. H.; Mohr, P. *Org. Lett.* **2003**, *5*, 3309. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

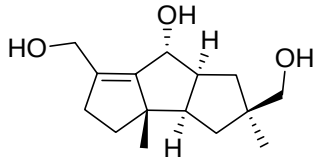
Compound **223**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
69.8	124.2294	69.4	70.6	69.5	69.5	MAE	1.2	2.1
61.8	132.6901	61.0	62.1	60.8	60.8	σ	1.0	1.3
55.4	139.1266	54.5	55.7	54.2	54.2	MaxErr	3.2	4.3
47.9	142.6832	51.0	52.1	50.5	50.5	R^2	0.9961	0.9961
41.7	151.4942	42.2	43.3	41.4	41.4	*m*	1.0	1.0
35.0	157.2421	36.4	37.6	35.5	35.5	*b*	2.0	3.1
34.4	159.0138	34.7	35.8	33.7	33.7	CMAE	0.9	0.9
27.9	162.6021	31.1	32.2	30.0	30.0	Cσ	0.7	0.7
27.8	164.3570	29.3	30.5	28.2	28.2	CMaxErr	2.6	2.6
27.1	164.8828	28.8	29.9	27.6	27.6			
20.6	173.0061	20.7	21.8	19.3	19.3			
15.0	177.8843	15.8	16.9	14.3	14.3			
14.1	178.4884	15.2	16.3	13.6	13.6			
8.2	183.9838	9.7	10.8	8.0	8.0			

[a] NMR data from: Comins, D. L.; Zheng, X.; Goehring, R. R. *Org. Lett.* **2002**, *4*, 1611. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

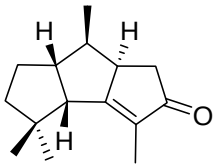
Compound **224**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
153.3	34.1278	165.0	160.7	157.9	157.8	MAE	2.5	2.6
130.0	65.3767	133.8	129.4	128.2	126.7	σ	2.8	1.9
75.8	118.9033	74.8	75.9	72.3	73.6	MaxErr	11.7	7.4
71.7	122.7913	70.9	72.0	68.6	69.7	R^2	0.9953	0.9961
61.6	135.4984	58.2	59.3	56.5	57.1	*m*	1.1	1.0
55.8	135.8814	57.8	58.9	56.2	56.7	*b*	-1.4	1.8
55.6	136.7555	56.9	58.1	55.3	55.8	CMAE	1.9	1.8
50.4	140.5268	53.1	54.3	51.8	52.1	Cσ	1.6	1.4
48.5	142.4769	51.2	52.3	49.9	50.1	CMaxErr	5.1	4.5
41.8	148.8973	44.8	45.9	43.8	43.8			
41.6	151.2198	42.4	43.6	41.6	41.5			
36.3	155.4587	38.2	39.4	37.6	37.3			
35.7	157.9283	35.7	36.9	35.2	34.8			
22.7	168.4973	25.2	26.3	25.2	24.3			
22.4	170.7754	22.9	24.0	23.1	22.0			

[a] NMR data from: Mehta, G.; Pallavi, K. *Tetrahedron Lett.* **2006**, *47*, 8355. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

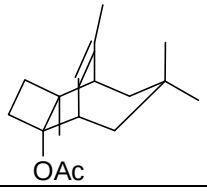
Compound **225**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
211.8	-9.3278	208.5	204.1	210.4	211.2	MAE	2.2	3.2
183.9	17.0531	182.1	177.8	183.5	183.3	σ	1.1	2.2
134.4	61.0423	138.1	133.8	138.5	136.7	MaxErr	3.8	7.7
54.4	139.8379	53.8	55.0	52.4	53.2	R^2	0.9991	0.9994
53.4	141.7997	51.9	53.0	50.4	51.1	*m*	1.0	0.9
46.2	145.3433	48.3	49.5	46.8	47.3	*b*	2.5	4.8
44.9	146.4110	47.3	48.4	45.7	46.2	CMAE	1.5	1.3
41.9	149.1608	44.5	45.6	42.9	43.3	Cσ	1.1	0.8
39.2	151.9156	41.8	42.9	40.1	40.4	CMaxErr	4.1	3.2
36.9	156.0592	37.6	38.8	35.9	36.0			
32.4	157.9361	35.7	36.9	34.0	34.0			
30.1	164.6150	29.1	30.2	27.1	26.9			
25.8	166.5022	27.2	28.3	25.2	24.9			
15.1	175.6871	18.0	19.1	15.8	15.2			
9.1	180.7321	12.9	14.1	10.7	9.9			

[a] NMR data from: Mehta, G.; Murthy, S. K.; Umarye, J. D. *Tetrahedron Lett.* **2002**, *43*, 8301. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

Compound **226**

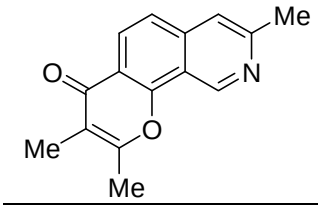


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
169.6	26.8698	172.3	167.9	168.5	168.9	MAE	2.1	1.8
141.5	52.9876	146.2	141.8	143.0	142.3	σ	1.8	1.4
122.2	70.1606	129.0	124.6	126.2	124.8	MaxErr	6.8	4.0
85.3	113.0702	80.6	81.7	79.0	81.1	R^2	0.9975	0.9985
49.3	145.0390	48.6	49.8	47.8	48.5	*m*	1.0	1.0
45.3	145.5216	48.1	49.3	47.4	48.0	*b*	-0.4	2.2
38.7	154.1237	39.5	40.7	39.0	39.2	CMAE	1.7	1.4
36.7	157.9214	35.7	36.9	35.3	35.3	Cσ	1.5	1.0
35.7	158.6698	35.0	36.1	34.6	34.6	CMaxErr	6.3	4.2
35.6	158.9370	34.7	35.9	34.3	34.3			
34.2	159.5823	34.1	35.2	33.7	33.6			
31.8	159.7813	33.9	35.0	33.5	33.4			
29.4	162.0377	31.6	32.8	31.3	31.1			
28.6	164.4663	29.2	30.3	28.9	28.7			
23.9	168.8013	24.9	26.0	24.7	24.3			
21.8	169.6222	24.0	25.2	23.9	23.4			
21.6	173.2550	20.4	21.6	20.3	19.7			

[a] NMR data from: Inanaga, K.; Takasu, K.; Ihara, M. *J. Am. Chem. Soc.* **2004**, *126*, 1352. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//MM+ level of theory

Experimental chemical shifts, mPW1PW91/6-31G(d)//AM1 Boltzmann-averaged GIAO isotropic magnetic shielding values, unscaled and scaled chemical shifts computed using TMS and MSTD, and statistical parameters computed for compounds 201-247.

Compound **201**

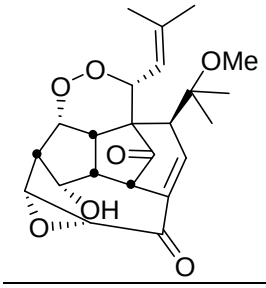


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
182.1	26.5294	172.6	165.6	171.3	173.5	MAE	4.1	5.6
164.0	37.4997	161.6	154.6	160.5	161.9	σ	2.9	4.2
156.7	39.4185	159.7	152.7	158.6	159.8	MaxErr	9.8	16.5
146.2	43.1276	156.0	149.0	155.0	155.9	R^2	0.9912	0.9920
145.6	47.5882	151.6	144.6	150.6	151.2	*m*	1.0	0.9
141.3	61.1768	138.0	131.0	137.2	136.8	*b*	-1.4	1.8
133.7	68.4084	130.7	123.7	130.1	129.1	CMAE	3.8	3.6
124.1	74.3025	124.8	117.8	124.3	122.9	Cσ	2.9	2.9
120.5	75.1632	124.0	117.0	123.4	122.0	CMaxErr	10.8	9.7
119.5	76.4249	122.7	115.7	122.2	120.7			
119.3	77.2671	121.9	114.9	121.4	119.8			
114.6	80.2736	118.9	111.9	118.4	116.6			
24.7	164.2664	25.2	27.9	26.2	27.6			
20.4	170.5258	18.9	21.6	20.0	21.0			
17.5	179.5936	9.9	12.6	11.1	11.4			

[a] NMR data from: Kohno, J.; Hiramatsu, H.; Nishio, M.; Sakurai, M.; Okuda, T.; Komatsubara, S. *Tetrahedron* **1999**, *55*, 11247. Solvent: $CDCl_3$

[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

Compound **202**

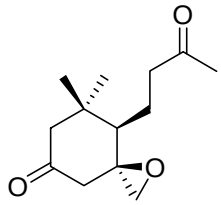


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
202.9	-5.5842	204.7	197.7	199.8	201.9	MAE	3.3	4.0
192.8	-1.6139	200.8	193.8	196.0	197.8	σ	3.6	3.7
142.2	44.9792	154.2	147.2	151.0	149.2	MaxErr	12.0	13.1
139.6	65.6470	133.5	126.5	131.0	127.7	R^2	0.9930	0.9899
132.5	66.6358	132.5	125.5	130.0	126.7	*m*	1.0	1.0
120.7	75.8088	123.3	116.3	121.2	117.1	*b*	-2.0	4.0
77.3	102.2928	87.2	89.9	86.2	89.5	CMAE	3.1	3.5
75.8	104.3152	85.1	87.8	84.2	87.4	Cσ	3.0	3.9
72.7	117.0807	72.4	75.1	71.9	74.1	CMaxErr	8.9	12.2
71.5	120.4904	69.0	71.7	68.6	70.5			
61.0	133.5779	55.9	58.6	55.9	56.9			
60.5	134.5191	54.9	57.6	55.0	55.9			
54.5	135.4110	54.0	56.7	54.2	55.0			

53.2	137.6699	51.8	54.5	52.0	52.6
53.1	140.3897	49.1	51.8	49.4	49.8
49.1	140.7143	48.7	51.4	49.0	49.5
47.8	140.7377	48.7	51.4	49.0	49.4
40.9	148.7159	40.7	43.4	41.3	41.1
40.4	152.1940	37.3	40.0	38.0	37.5
26.6	161.7874	27.7	30.4	28.7	27.5
26.1	163.1395	26.3	29.0	27.4	26.1
24.7	164.4576	25.0	27.7	26.1	24.7
18.6	172.1668	17.3	20.0	18.6	16.7

[a] NMR data from: Rychnovsky, S. D. *Org. Lett.* **2006**, *8*, 2895. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

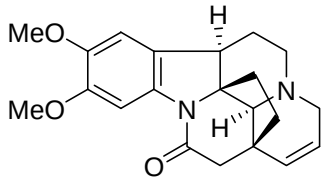
Compound **203**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
208.7	-11.8238	211.0	204.0	216.5	216.2	MAE	8.8	8.6
207.2	-9.5970	208.7	201.7	214.3	213.9	σ	9.2	7.9
83.4	136.6614	52.8	55.5	58.8	59.8	MaxErr	30.6	27.9
78.3	136.6802	52.8	55.5	58.8	59.7	R^2	0.9699	0.9723
53.1	143.4180	46.0	48.7	52.1	52.6	*m*	1.0	0.9
49.4	144.9812	44.5	47.2	50.5	51.0	*b*	-6.2	-1.2
48.6	148.9588	40.5	43.2	46.6	46.8	CMAE	8.3	8.0
43.4	152.9464	36.5	39.2	42.6	42.6	Cσ	7.3	7.0
42.6	159.1545	30.3	33.0	36.4	36.1	CMaxErr	24.6	23.6
30.0	160.0560	29.4	32.1	35.5	35.1			
24.9	160.4930	29.0	31.7	35.1	34.6			
20.8	160.9572	28.5	31.2	34.6	34.2			
18.7	168.1615	21.3	24.0	27.4	26.6			

[a] NMR data from: Macías, F. A.; Varela, R. M.; Torres, A.; Oliva, R. M.; Molinillo, J. M. G. *Phytochemistry* **1997**, *48*, 631. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

Compound **204**

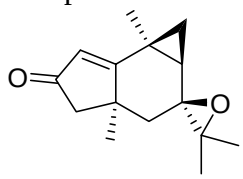


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
173.8	33.0131	166.1	159.1	164.6	167.3	MAE	4.5	5.7
147.7	48.2218	150.9	143.9	149.2	150.3	σ	3.7	3.8
145.3	53.1544	146.0	139.0	144.2	144.7	MaxErr	12.6	14.7
131.5	57.3373	141.8	134.8	140.0	140.0	R^2	0.9872	0.9883
131.0	65.8256	133.3	126.3	131.4	130.5	*m*	1.0	0.9
120.0	71.9611	127.2	120.2	125.2	123.7	*b*	3.4	9.8
117.4	74.0864	125.1	118.1	123.1	121.3	CMAE	3.6	3.9
111.3	86.0703	113.1	106.1	110.9	107.9	Cσ	3.9	3.3
102.6	93.9896	105.1	98.2	102.9	99.0	CMaxErr	15.2	11.9
84.4	117.5678	71.9	74.6	69.3	72.6			
56.1	122.1340	67.3	70.0	64.7	67.5			

56.0	134.1486	55.3	58.0	52.5	54.0
47.9	135.9562	53.5	56.2	50.7	52.0
46.0	139.6607	49.8	52.5	46.9	47.8
44.5	140.9055	48.6	51.2	45.7	46.4
44.3	144.5706	44.9	47.6	42.0	42.3
37.7	146.3506	43.1	45.8	40.2	40.3
36.6	149.5842	39.9	42.6	36.9	36.7
35.0	154.0549	35.4	38.1	32.4	31.7
26.8	159.6012	29.9	32.5	26.8	25.5
24.8	165.6035	23.9	26.5	20.7	18.8

[a] NMR data from: Hubbs, J. L.; Heathcock, C. H. *Org. Lett.* **1999**, *1*, 1315. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

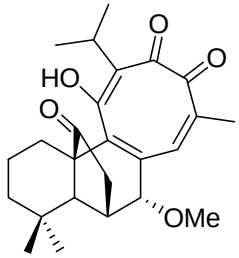
Compound **205**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
200.1	-3.5956	202.7	195.7	200.5	201.6	MAE	4.2	4.4
180.0	15.0939	184.0	177.1	182.1	182.0	σ	3.2	2.9
128.5	65.8848	133.3	126.3	132.1	128.7	MaxErr	11.9	9.8
66.5	134.9056	54.6	57.2	54.7	56.3	R^2	0.9926	0.9936
60.8	136.0794	53.4	56.1	53.5	55.1	*m*	1.0	1.0
42.7	141.6677	47.8	50.5	48.0	49.2	*b*	-1.0	3.6
34.5	149.7372	39.7	42.4	40.1	40.7	CMAE	3.9	3.6
34.2	154.3033	35.2	37.8	35.6	36.0	Cσ	3.3	3.0
30.8	164.2974	25.2	27.8	25.7	25.5	CMaxErr	11.8	10.2
28.9	164.5446	24.9	27.6	25.5	25.2			
26.5	165.1113	24.3	27.0	24.9	24.6			
23.3	165.1991	24.3	26.9	24.8	24.5			
21.3	167.7149	21.7	24.4	22.4	21.9			
19.5	170.1357	19.3	22.0	20.0	19.3			
8.4	173.9691	15.5	18.2	16.2	15.3			

[a] NMR data from: Tori, M.; Nakashima, K.; Toyota, M.; Asakawa, Y. *Tetrahedron Lett.* **1993**, *34*, 3751. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

Compound **206**

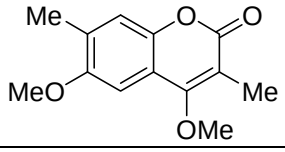


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
203.1	-2.1718	201.3	194.3	205.6	208.4	MAE	4.6	5.5
189.1	1.1126	198.0	191.0	202.3	204.9	σ	5.8	7.6
175.7	22.5832	176.6	169.6	180.5	181.3	MaxErr	27.6	34.6
175.4	51.3583	147.8	140.8	151.2	149.8	R^2	0.9875	0.9858
149.1	61.2930	137.8	130.9	141.1	139.0	*m*	1.0	0.9
146.6	61.8605	137.3	130.3	140.6	138.3	*b*	-1.1	3.9
132.1	62.3300	136.8	129.8	140.1	137.8	CMAE	4.9	5.1
132.0	64.1962	134.9	127.9	138.2	135.8	Cσ	5.1	5.5
119.8	74.3192	124.8	117.8	127.9	124.7	CMaxErr	24.2	25.6

79.5	112.9146	76.5	79.2	78.8	82.5
73.0	122.3786	67.1	69.8	69.2	72.1
59.2	131.9719	57.5	60.2	59.5	61.6
50.2	137.5354	51.9	54.6	53.8	55.5
45.8	150.3936	39.1	41.8	40.8	41.4
38.1	151.0661	38.4	41.1	40.1	40.7
31.3	156.4524	33.0	35.7	34.6	34.8
31.3	163.4397	26.0	28.7	27.5	27.2
30.2	164.1428	25.3	28.0	26.8	26.4
28.1	164.8686	24.6	27.3	26.0	25.6
26.4	165.8410	23.6	26.3	25.1	24.5
22.8	166.4885	23.0	25.7	24.4	23.8
22.3	166.7136	22.7	25.4	24.2	23.6
21.9	167.9851	21.5	24.2	22.9	22.2
18.6	170.2858	19.2	21.9	20.5	19.7

[a] NMR data from: Yang, J.; Huang, S. X.; Zhao, Q. S. *J. Phys. Chem. A* **2008**, *112*, 12132. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

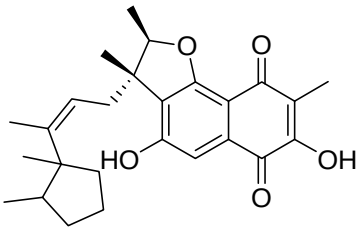
Compound **207**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
177.6	34.3320	164.8	157.8	170.2	172.0	MAE	7.8	8.6
162.6	34.9490	164.2	157.2	169.5	171.3	σ	6.6	8.6
160.7	45.7735	153.4	146.4	157.7	158.5	MaxErr	22.9	29.9
158.5	46.8259	152.3	145.3	156.6	157.3	R^2	0.9692	0.9749
156.5	65.5076	133.6	126.6	136.2	135.3	*m*	0.9	0.8
110.9	76.3741	122.8	115.8	124.4	122.5	*b*	8.5	11.8
108.0	82.0052	117.1	110.1	118.3	115.8	CMAE	8.4	7.0
105.3	85.3161	113.8	106.8	114.7	111.9	Cσ	5.2	5.5
91.1	93.6625	105.5	98.5	105.6	102.1	CMaxErr	20.3	21.2
56.0	133.6009	55.9	58.5	51.6	55.0			
55.4	135.6667	53.8	56.5	49.3	52.6			
19.4	170.5230	18.9	21.6	11.4	11.5			
7.3	177.4828	12.0	14.7	3.8	3.3			

[a] NMR data from: Kalinin, A. V.; Snieckus, V. *Tetrahedron Lett.* **1998**, *39*, 4999. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

Compound **208**

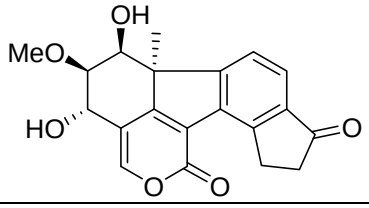


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
182.9	16.3284	182.8	175.8	181.2	183.8	MAE	3.7	5.7
180.4	16.8142	182.3	175.3	180.7	183.2	σ	2.9	3.2
159.9	32.8326	166.3	159.3	164.4	165.6	MaxErr	10.9	11.7
157.7	44.8568	154.3	147.3	152.2	152.4	R^2	0.9966	0.9959
153.6	46.1758	153.0	146.0	150.9	151.0	*m*	1.0	0.9
138.9	49.3605	149.8	142.8	147.7	147.5	*b*	4.2	8.5
131.6	67.6875	131.5	124.5	129.1	127.3	CMAE	2.7	3.1

127.3	68.0555	131.1	124.1	128.7	126.9	Cσ	2.2	2.2
123.9	74.1582	125.0	118.0	122.5	120.2	CMaxErr	8.8	8.6
120.3	76.2917	122.8	115.9	120.4	117.9			
107.9	86.9295	112.2	105.2	109.6	106.2			
107.9	87.6754	111.5	104.5	108.8	105.4			
86.3	104.6584	84.8	87.5	81.8	86.7			
46.0	145.8899	43.6	46.3	40.0	41.4			
39.7	148.2732	41.2	43.9	37.5	38.8			
32.8	149.5812	39.9	42.6	36.2	37.4			
31.0	149.8261	39.6	42.3	36.0	37.1			
30.5	149.9422	39.5	42.2	35.8	37.0			
26.6	154.8685	34.6	37.3	30.8	31.6			
25.1	163.3564	26.1	28.8	22.2	22.3			
20.9	165.0772	24.4	27.1	20.5	20.4			
19.7	166.8070	22.6	25.3	18.7	18.5			
18.8	168.6019	20.9	23.5	16.9	16.5			
15.7	169.8363	19.6	22.3	15.7	15.1			
15.1	170.9895	18.5	21.2	14.5	13.9			
8.6	179.2080	10.2	12.9	6.2	4.8			

[a] NMR data from: Kalaitzis, J. A.; Hamano, Y.; Nilsen, G.; Moore, B. S. *Org. Lett.* **2003**, *5*, 4449. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

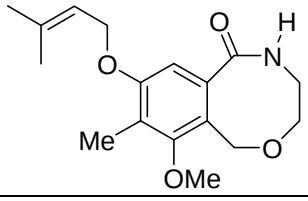
Compound **209**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
206.7	-5.9558	205.1	198.1	205.1	209.6	MAE	4.0	6.3
173.4	29.6681	169.5	162.5	169.8	171.1	σ	2.2	4.3
158.6	39.1268	160.0	153.0	160.4	160.8	MaxErr	9.5	12.9
158.0	39.1725	160.0	153.0	160.4	160.8	R^2	0.9929	0.9886
145.7	43.9321	155.2	148.2	155.6	155.6	*m*	1.0	0.9
145.6	47.5305	151.6	144.6	152.1	151.7	*b*	-1.7	4.3
142.4	60.4238	138.7	131.7	139.3	137.8	CMAE	3.7	4.8
136.9	62.2873	136.9	129.9	137.4	135.8	Cσ	2.3	2.9
129.8	74.1507	125.0	118.0	125.7	123.0	CMaxErr	9.9	9.9
127.3	74.8169	124.3	117.3	125.0	122.2			
127.3	77.7276	121.4	114.4	122.1	119.1			
122.1	82.1375	117.0	110.0	117.7	114.3			
81.7	105.8427	83.6	86.3	84.6	88.7			
71.7	121.3565	68.1	70.8	69.2	71.9			
62.6	122.3197	67.1	69.8	68.3	70.8			
60.7	134.3284	55.1	57.8	56.4	57.9			
42.3	140.9162	48.5	51.2	49.8	50.7			
36.5	155.4289	34.0	36.7	35.4	35.0			
30.5	162.8066	26.6	29.3	28.1	27.1			
28.4	165.3709	24.1	26.8	25.6	24.3			

[a] NMR data from: Wipf, P.; Kerekes, A. D. *J. Nat. Prod.* **2003**, *66*, 716. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

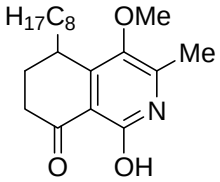
Compound **210**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
167.5	24.3636	174.8	167.8	171.7	173.6	MAE	2.9	4.9
158.7	40.8235	158.3	151.3	155.3	155.8	σ	3.1	3.4
152.4	41.3734	157.8	150.8	154.8	155.2	MaxErr	11.0	13.7
138.0	60.9950	138.1	131.1	135.3	133.9	R^2	0.9959	0.9917
132.2	66.5430	132.6	125.6	129.8	127.9	*m*	1.0	0.9
125.1	73.1962	125.9	118.9	123.2	120.6	*b*	1.8	7.7
121.8	74.6950	124.4	117.4	121.7	119.0	CMAE	2.6	4.2
120.5	74.7287	124.4	117.4	121.7	119.0	Cσ	2.1	2.1
99.7	88.6479	100.8	103.5	98.3	103.9	CMaxErr	8.8	10.7
68.7	119.0121	70.4	73.1	68.1	70.9			
59.7	126.4187	63.0	65.7	60.8	62.9			
56.4	126.5401	62.9	65.6	60.7	62.8			
49.2	129.2334	60.2	62.9	58.0	59.9			
45.1	146.8511	42.6	45.3	40.5	40.7			
26.0	163.4783	26.0	28.7	24.0	22.7			
18.5	171.3114	18.1	20.8	16.2	14.2			
10.2	178.1156	11.3	14.0	9.5	6.8			

[a] NMR data from: Cornella, I.; Kelly, T. R. *J. Org. Chem.* **2004**, *69*, 2191. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

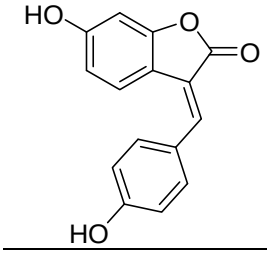
Compound **211**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
194.6	-0.7540	199.9	192.9	196.5	199.3	MAE	5.5	6.6
172.8	30.4797	168.7	161.7	165.4	165.8	σ	5.7	5.9
147.5	32.4049	166.7	159.7	163.5	163.8	MaxErr	20.8	27.8
139.0	47.8559	151.3	144.3	148.2	147.2	R^2	0.9856	0.9830
138.9	52.7794	146.4	139.4	143.3	142.0	*m*	1.0	0.9
132.2	87.7662	111.4	104.4	108.5	104.5	*b*	2.3	6.8
59.4	132.1267	57.3	60.0	54.7	57.0	CMAE	3.9	4.0
32.2	154.6605	34.8	37.5	32.3	32.8	Cσ	6.3	7.0
31.8	154.6928	34.8	37.5	32.3	32.8	CMaxErr	23.7	27.7
30.5	155.9391	33.5	36.2	31.1	31.5			
30.3	156.9163	32.5	35.2	30.1	30.4			
29.6	157.3877	32.1	34.8	29.6	29.9			
29.5	157.9255	31.5	34.2	29.1	29.3			
29.2	157.9364	31.5	34.2	29.1	29.3			
28.4	158.7535	30.7	33.4	28.3	28.4			
24.3	162.2497	27.2	29.9	24.8	24.7			
22.6	163.5458	25.9	28.6	23.5	23.3			
14.5	170.6910	18.8	21.5	16.4	15.6			
14.0	172.5274	16.9	19.6	14.6	13.7			

[a] NMR data from: Bringmann, J.; Schlauer, H.; Rischer, H.; Wohlfarth, J.; Mühlbacher, J.; Buske, A.; Porzel, A.; Schmidt, J.; Adam, G. *Tetrahedron* **2000**, *56*, 3691. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

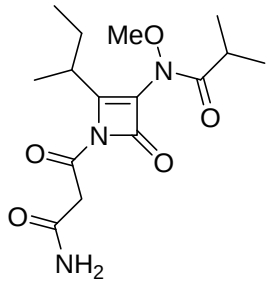
Compound **212**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
174.8	28.5420	170.6	163.6	174.9	174.9	MAE	3.1	9.1
162.8	40.8350	158.3	151.3	161.9	161.9	σ	3.6	4.3
157.6	41.0235	158.1	151.1	161.7	161.7	MaxErr	13.6	20.6
157.2	42.0430	157.1	150.1	160.6	160.6	R^2	0.9649	0.9649
152.9	59.8225	139.3	132.3	141.8	141.8	*m*	0.9	0.9
130.1	63.7274	135.4	128.4	137.7	137.7	*b*	5.3	-1.7
127.3	74.3057	124.8	117.8	126.5	126.5	CMAE	2.8	2.8
123.6	77.1047	122.0	115.0	123.5	123.5	Cσ	3.2	3.2
122.6	77.1875	122.0	115.0	123.4	123.4	CMaxErr	11.1	11.1
116.6	82.8218	116.3	109.3	117.5	117.5			
115.3	83.5053	115.6	108.6	116.7	116.7			
115.0	87.6679	111.5	104.5	112.3	112.3			
102.2	99.7167	99.4	92.4	99.6	99.6			

[a] NMR data from: Suzuki, K.; Yahara, S.; Kazutomo, M.; Uyeda, M. *J. Nat. Prod.* **2001**, *64*, 204. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

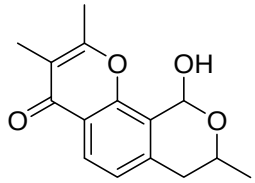
Compound **213**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
168.0	11.7374	187.4	180.4	172.7	173.8	MAE	6.9	6.2
166.0	18.0134	181.1	174.1	167.0	167.7	σ	9.0	6.1
161.5	31.7139	167.4	160.4	154.5	154.3	MaxErr	30.2	23.2
152.0	31.8000	167.3	160.3	154.4	154.2	R^2	0.9881	0.9870
135.0	33.9647	165.2	158.2	152.5	152.1	*m*	1.1	1.0
134.9	70.5398	128.6	121.6	119.2	116.5	*b*	-2.5	2.2
64.1	128.7068	60.7	63.4	57.5	59.7	CMAE	4.2	4.3
41.1	149.5953	39.9	42.5	38.5	39.4	Cσ	5.5	5.9
33.7	154.6300	34.8	37.5	33.9	34.4	CMaxErr	17.5	18.4
30.7	157.3393	32.1	34.8	31.5	31.8			
27.5	161.5245	27.9	30.6	27.7	27.7			
19.9	169.5407	19.9	22.6	20.4	19.9			
19.9	169.7464	19.7	22.4	20.2	19.7			
18.2	171.0609	18.4	21.1	19.0	18.4			
12.6	174.1545	15.3	18.0	16.2	15.4			

[a] NMR data from: Kita, M.; Miwa, R.; Widianti, T.; Ozaki, Y.; Aoyama, S.; Yamada, K.; Uemura, D. *Tetrahedron Lett.* **2007**, *48*, 8628. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

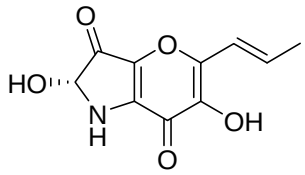
Compound **214**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
182.5	25.8356	173.3	166.3	172.5	174.7	MAE	3.3	5.2
162.5	37.1231	162.0	155.0	161.4	162.6	σ	3.5	3.9
144.5	42.9586	156.2	149.2	155.7	156.4	MaxErr	11.7	16.2
142.0	59.3251	139.8	132.8	139.6	138.9	R^2	0.9929	0.9932
131.1	68.0495	131.1	124.1	131.0	129.6	*m*	1.0	0.9
122.7	72.4287	126.7	119.7	126.7	124.9	*b*	-1.9	3.0
122.5	75.2362	123.9	116.9	123.9	121.9	CMAE	3.1	2.9
122.0	75.7315	123.4	116.4	123.4	121.3	Cσ	3.4	3.4
119.1	78.2523	120.9	113.9	120.9	118.6	CMaxErr	11.2	11.9
87.5	103.8254	85.6	88.3	86.2	91.3			
62.2	131.3687	58.1	60.8	59.1	61.8			
36.5	154.1249	35.3	38.0	36.7	37.5			
21.0	167.1748	22.3	25.0	23.8	23.5			
20.1	170.4287	19.0	21.7	20.6	20.1			
17.0	179.6929	9.8	12.5	11.5	10.1			

[a] NMR data from: Lin, W. H.; Brauers, G.; Ebel, R.; Wray, V.; Berg, A.; Surdasono; Proksch, P. *J. Nat. Prod.* **2003**, *66*, 57. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

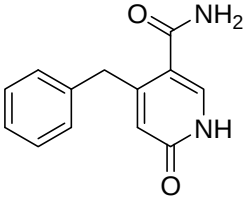
Compound **215**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
174.2	7.2045	191.9	184.9	185.8	188.5	MAE	8.7	7.3
169.1	32.8886	166.3	159.3	160.0	160.7	σ	5.9	4.6
165.0	43.1135	156.0	149.0	149.8	149.6	MaxErr	17.9	16.0
146.0	48.7355	150.4	143.4	144.2	143.6	R^2	0.9686	0.9679
142.2	51.6949	147.4	140.4	141.2	140.3	*m*	1.0	0.9
131.7	53.7488	145.4	138.4	139.1	138.1	*b*	6.7	10.8
118.9	62.3206	136.8	129.8	130.5	128.8	CMAE	6.7	6.6
111.7	78.4151	120.7	113.7	114.4	111.4	Cσ	5.0	5.3
75.2	109.7614	79.7	82.4	73.2	77.5	CMaxErr	15.2	15.4
18.7	168.4043	21.1	23.7	14.4	14.1			

[a] NMR data from: Hiort, J.; Maksimenka, K.; Reichert, M.; Perovi-Ottstadt, S.; Lin, W. H.; Wray, V.; Steube, K.; Schaumann, K.; Weber, H.; Proksch, P.; Ebel, R.; Müller, W. E. G.; Bringmann, G. *J. Nat. Prod.* **2004**, *67*, 1532. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

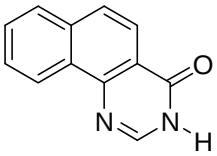
Compound **216**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
178.1	28.6768	170.5	163.5	173.0	175.4	MAE	2.6	7.6
165.9	37.9676	161.2	154.2	163.4	165.1	σ	2.5	4.1
151.2	47.1642	152.0	145.0	154.0	154.9	MaxErr	7.6	14.6
142.2	62.3248	136.8	129.8	138.4	138.2	R^2	0.9894	0.9926
137.4	62.7962	136.3	129.3	137.9	137.6	*m*	1.0	0.9
129.3	68.1863	131.0	124.0	132.3	131.7	*b*	2.3	5.1
129.3	70.0287	129.1	122.1	130.4	129.6	CMAE	2.7	2.0
129.2	70.0391	129.1	122.1	130.4	129.6	Cσ	2.0	1.9
129.2	70.2884	128.9	121.9	130.2	129.3	CMaxErr	7.1	6.0
127.5	72.3024	126.8	119.8	128.1	127.1			
118.9	74.3302	124.8	117.8	126.0	124.9			
118.0	83.8924	115.2	108.3	116.2	114.3			
38.2	154.0400	35.4	38.1	34.0	36.6			

[a] NMR data from: Hiort, J.; Maksimenka, K.; Reichert, M.; Perovi-Ottstadt, S.; Lin, W. H.; Wray, V.; Steube, K.; Schaumann, K.; Weber, H.; Proksch, P.; Ebel, R.; Müller, W. E. G.; Bringmann, G. *J. Nat. Prod.* **2004**, *67*, 1532. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

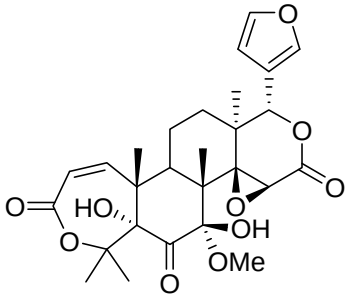
Compound **217**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
164.0	36.2418	162.9	155.9	176.9	176.9	MAE	5.0	8.5
150.5	49.5342	149.6	142.6	156.4	156.4	σ	6.2	4.9
148.5	50.9253	148.2	141.2	154.3	154.3	MaxErr	22.1	16.7
144.3	64.5729	134.6	127.6	133.3	133.3	R^2	0.7905	0.7905
136.0	69.4361	129.7	122.7	125.8	125.8	*m*	0.7	0.7
132.8	69.8181	129.3	122.3	125.3	125.3	*b*	47.8	40.8
130.4	69.9320	129.2	122.2	125.1	125.1	CMAE	6.9	6.9
128.7	70.4270	128.7	121.7	124.3	124.3	Cσ	4.6	4.6
125.0	71.2150	127.9	120.9	123.1	123.1	CMaxErr	15.1	15.1
123.6	71.4897	127.6	120.7	122.7	122.7			
118.7	73.0665	126.1	119.1	120.3	120.3			
101.6	75.3975	123.7	116.7	116.7	116.7			

[a] NMR data from: Morita, H.; Sato, Y.; Chan, K. L.; Choo, C. Y.; Itokawa, H.; Takeya, K.; Kobayashi, J. *J. Nat. Prod.* **2000**, *63*, 1707. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

Compound **218**

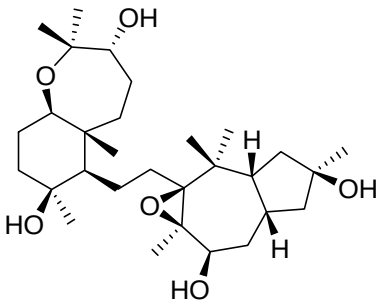


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
216.9	-21.1278	220.3	213.3	221.5	225.2	MAE	5.7	5.4
167.8	27.6269	171.5	164.5	172.0	171.9	σ	3.1	4.4
166.7	29.0102	170.1	163.1	170.6	170.4	MaxErr	12.1	14.1
153.9	46.1893	152.9	146.0	153.1	151.6	R^2	0.9869	0.9905
143.0	50.7355	148.4	141.4	148.5	146.6	*m*	1.0	0.9
141.1	51.0896	148.0	141.1	148.1	146.2	*b*	2.2	7.4
123.1	72.2985	126.8	119.8	126.6	123.0	CMAE	5.8	4.8
121.0	82.3521	116.8	109.8	116.4	112.0	Cσ	2.8	2.6
109.9	83.0349	116.1	109.1	115.7	111.3	CMaxErr	12.8	9.0
108.2	93.3877	96.1	98.8	95.4	99.9			
88.6	111.6465	77.8	80.5	76.8	80.0			
80.9	114.2409	75.2	77.9	74.2	77.1			
78.4	117.1376	72.3	75.0	71.2	74.0			
68.5	127.5696	61.9	64.6	60.6	62.5			
57.3	133.8292	55.6	58.3	54.3	55.7			
52.0	140.4883	49.0	51.7	47.5	48.4			
49.9	140.6372	48.8	51.5	47.4	48.3			
49.7	142.9463	46.5	49.2	45.0	45.7			
46.8	145.4544	44.0	46.7	42.5	43.0			
39.5	155.8913	33.6	36.3	31.9	31.6			
27.4	156.0367	33.4	36.1	31.7	31.4			
26.3	156.9901	32.5	35.2	30.8	30.4			
24.1	159.7527	29.7	32.4	28.0	27.3			
18.3	161.3152	28.1	30.8	26.4	25.6			
17.3	161.5971	27.9	30.5	26.1	25.3			
15.2	162.8869	26.6	29.3	24.8	23.9			
14.7	168.0695	21.4	24.1	19.5	18.2			

[a] NMR data from: Kubo, I.; Tanis, S. P.; Lee, Y. W.; Miura, I.; Nakanishi, K.; Chapya, A. *Heterocycles* **1976**, *5*, 485. Solvent: $CDCl_3$

[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

Compound **219**



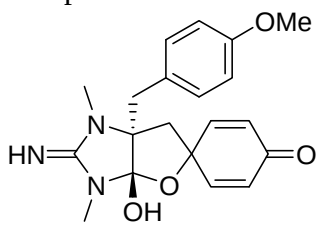
δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
77.8	112.6100	76.8	79.5	82.7	82.7	MAE	2.8	3.8
77.2	115.4461	74.0	76.7	79.4	79.4	σ	2.1	2.0
76.8	118.6636	70.8	73.5	75.6	75.6	MaxErr	6.8	7.7

72.7	119.7798	69.7	72.4	74.3	74.3	R^2	0.9876	0.9876
72.2	121.6489	67.8	70.5	72.1	72.1	*m*	0.9	0.9
70.0	125.9578	63.5	66.2	67.1	67.1	*b*	6.0	8.6
69.5	126.7112	62.7	65.4	66.2	66.2	CMAE	1.7	1.7
65.7	128.7147	60.7	63.4	63.9	63.9	Cσ	1.4	1.4
55.7	139.0990	50.4	53.0	51.8	51.8	CMaxErr	4.9	4.9
42.9	142.4838	47.0	49.7	47.8	47.8			
40.2	145.3334	44.1	46.8	44.5	44.5			
39.3	149.1565	40.3	43.0	40.1	40.1			
39.2	149.2023	40.3	42.9	40.0	40.0			
38.0	150.4961	39.0	41.6	38.5	38.5			
36.7	152.2241	37.2	39.9	36.5	36.5			
35.6	154.6927	34.8	37.5	33.6	33.6			
34.5	155.0368	34.4	37.1	33.2	33.2			
31.8	156.4784	33.0	35.7	31.5	31.5			
31.3	156.8734	32.6	35.3	31.1	31.1			
30.4	158.1810	31.3	34.0	29.5	29.5			
30.2	159.6209	29.8	32.5	27.8	27.8			
29.5	159.6842	29.8	32.5	27.8	27.8			
29.2	160.6156	28.8	31.5	26.7	26.7			
26.8	160.9919	28.5	31.2	26.3	26.3			
25.4	161.6837	27.8	30.5	25.4	25.4			
25.3	162.2130	27.2	29.9	24.8	24.8			
21.4	163.1982	26.3	28.9	23.7	23.7			
21.0	163.4779	26.0	28.7	23.4	23.4			
16.8	168.2996	21.2	23.8	17.7	17.7			
13.4	171.1008	18.4	21.0	14.5	14.5			

[a] NMR data from: Jain, S.; Laphookhieo, S.; Shi, Z.; Fu, L. W.; Akiyama, S.; Chen, Z. S.; Youssef, D. T. A.; von Soest, R. W. M.; El Sayed, K. A. *J. Nat. Prod.* **2007**, *70*, 928. Solvent: $CDCl_3$

[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

Compound **220**

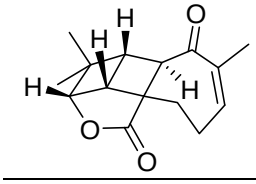


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
185.4	15.2459	183.9	176.9	180.5	183.3	MAE	4.4	5.2
159.5	22.9461	176.2	169.2	172.9	175.1	σ	4.7	3.3
158.9	41.3119	157.8	150.8	154.9	155.3	MaxErr	16.7	11.3
151.0	46.9001	152.2	145.2	149.4	149.3	R^2	0.9851	0.9867
150.1	50.4868	148.7	141.7	145.9	145.4	*m*	1.0	0.9
132.8	65.1219	134.0	127.0	131.5	129.7	*b*	0.2	6.4
132.8	66.5677	132.6	125.6	130.1	128.1	CMAE	4.6	4.1
127.5	68.2523	130.9	123.9	128.4	126.3	Cσ	3.7	3.7
126.9	69.1926	129.9	123.0	127.5	125.3	CMaxErr	13.4	15.6
125.9	71.3492	127.8	120.8	125.4	123.0			
112.7	71.3825	127.8	120.8	125.3	123.0			
112.7	77.7640	121.4	114.4	119.1	116.1			
102.5	88.2912	101.2	103.9	99.2	104.8			
82.5	109.7526	79.7	82.4	78.1	81.7			
77.1	116.6220	72.8	75.5	71.4	74.3			
54.2	136.2646	53.2	55.9	52.0	53.2			
46.9	149.8987	39.6	42.2	38.6	38.5			
37.1	154.0131	35.4	38.1	34.6	34.1			
24.7	156.1529	33.3	36.0	32.5	31.8			

24.5	160.3322	29.1	31.8	28.4	27.3

[a] NMR data from: Ralifo, P.; Crews, P. *J. Org. Chem.* **2004**, *69*, 9025. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

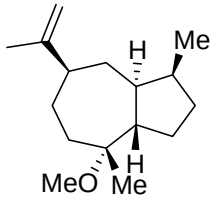
Compound **221**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
211.9	-7.4514	206.6	199.6	207.9	209.7	MAE	8.0	7.5
177.5	15.6405	183.5	176.5	185.4	185.6	σ	6.7	5.7
135.1	61.4771	137.7	130.7	140.9	138.0	MaxErr	22.3	19.6
131.1	62.6829	136.5	129.5	139.7	136.7	R^2	0.9790	0.9825
84.2	115.8628	73.6	76.3	78.5	81.4	*m*	1.0	1.0
62.8	140.9441	48.5	51.2	54.1	55.3	*b*	-7.1	-2.0
62.6	149.1446	40.3	43.0	46.2	46.8	CMAE	7.9	6.9
54.5	149.1617	40.3	43.0	46.1	46.8	Cσ	3.5	3.9
54.5	153.7576	35.7	38.4	41.7	42.0	CMaxErr	16.4	15.8
41.9	156.7976	32.7	35.3	38.7	38.9			
28.6	159.4723	30.0	32.7	36.1	36.1			
22.8	163.1506	26.3	29.0	32.5	32.2			
22.6	163.6444	25.8	28.5	32.1	31.7			
22.2	166.9751	22.5	25.2	28.8	28.3			
22.2	170.0710	19.4	22.1	25.8	25.0			

[a] NMR data from: Lodewyk, M. W.; Soldi, C.; Jones, P. B.; Olmstead, M. M.; Rita, J.; Shaw, J. T.; Dean J. Tantillo, D. J. *J. Am. Chem. Soc.* **2012**, *134*, 18550. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

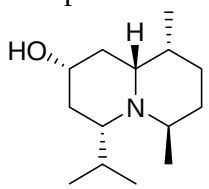
Compound **222**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
153.0	49.1005	150.0	143.0	153.4	153.3	MAE	3.3	4.6
107.8	86.2849	112.9	105.9	114.9	111.4	σ	3.0	3.0
78.9	121.2018	68.3	70.9	68.8	72.0	MaxErr	10.6	10.0
52.7	135.8801	53.6	56.3	53.6	55.5	R^2	0.9850	0.9886
49.0	140.6213	48.8	51.5	48.7	50.1	*m*	1.0	0.9
45.9	142.1960	47.3	49.9	47.1	48.4	*b*	1.7	7.0
45.3	151.2701	38.2	40.9	37.7	38.1	CMAE	3.3	3.2
39.0	152.0442	37.4	40.1	36.9	37.3	Cσ	3.0	2.1
30.5	152.6446	36.8	39.5	36.3	36.6	CMaxErr	10.1	7.2
30.4	154.0160	35.4	38.1	34.9	35.0			
28.4	156.6090	32.8	35.5	32.2	32.1			
27.7	163.5487	25.9	28.6	25.0	24.3			
26.1	163.6653	25.8	28.5	24.9	24.2			
25.1	165.0836	24.4	27.1	23.5	22.6			
20.2	169.0369	20.4	23.1	19.4	18.1			
16.5	169.4280	20.0	22.7	19.0	17.7			

[a] NMR data from: Fleischer, T. C.; Waigh, R. D.; Waterman, P. G. *J. Nat. Prod.* **1997**, *60*, 1054. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

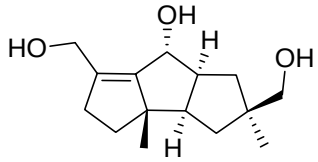
Compound **223**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
73.0	124.2149	65.2	67.9	84.5	84.5	MAE	11.6	9.3
72.8	131.5576	57.9	60.6	75.4	75.4	σ	5.9	5.3
68.6	139.2543	50.2	52.9	65.8	65.8	MaxErr	22.7	20.0
67.1	145.0486	44.4	47.1	58.6	58.6	R^2	0.9170	0.9170
49.6	147.8504	41.6	44.3	55.1	55.1	*m*	0.8	0.8
49.5	157.1887	32.3	35.0	43.5	43.5	*b*	-2.7	0.0
41.3	157.5706	31.9	34.6	43.0	43.0	CMAE	4.7	4.7
41.1	161.5301	27.9	30.6	38.1	38.1	Cσ	3.3	3.3
41.0	161.7266	27.7	30.4	37.8	37.8	CMaxErr	11.5	11.5
40.0	165.0874	24.4	27.1	33.6	33.6			
22.0	166.6681	22.8	25.5	31.7	31.7			
22.0	173.6621	15.8	18.5	23.0	23.0			
21.9	173.6737	15.8	18.5	23.0	23.0			
18.3	179.8835	9.6	12.3	15.2	15.2			

[a] NMR data from: Kazmi, S. N.; Ahmed, Z.; Ahmed, W.; Malik, A. *Heterocycles* **1989**, *29*, 1901. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

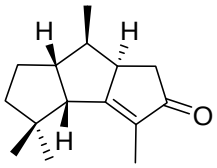
Compound **224**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
145.8	37.6816	161.5	154.5	157.2	157.2	MAE	4.8	6.3
129.1	72.8348	126.3	119.3	122.3	119.2	σ	3.9	3.7
74.3	116.1745	73.3	76.0	69.7	72.3	MaxErr	15.7	11.7
72.1	121.2280	68.2	70.9	64.7	66.9	R^2	0.9799	0.9797
59.0	130.2098	59.2	61.9	55.8	57.2	*m*	1.0	0.9
50.5	133.5801	55.9	58.6	52.5	53.5	*b*	2.9	9.1
45.9	134.5657	54.9	57.6	51.5	52.5	CMAE	4.3	4.0
45.5	139.1677	50.3	53.0	46.9	47.5	Cσ	2.8	3.2
45.1	147.2344	42.2	44.9	39.0	38.8	CMaxErr	11.4	11.4
40.8	147.3018	42.2	44.8	38.9	38.7			
36.1	148.8439	40.6	43.3	37.4	37.0			
36.0	152.4084	37.0	39.7	33.8	33.2			
25.1	156.5457	32.9	35.6	29.7	28.7			
22.7	160.7927	28.7	31.4	25.5	24.1			
20.3	162.9840	26.5	29.2	23.3	21.7			

[a] NMR data from: Huang, Z.; Dan, Y.; Huang, Y.; Lin, L.; Li, T.; Ye, W.; Wei, X. *J. Nat. Prod.* **2004**, *67*, 2121. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

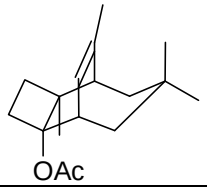
Compound **225**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
208.2	-7.2710	206.4	199.4	205.8	207.4	MAE	8.2	10.9
176.3	14.7153	184.4	177.4	182.8	182.8	σ	3.9	4.2
140.3	62.4046	136.7	129.7	132.8	129.3	MaxErr	14.0	16.7
42.5	134.4194	55.0	57.7	47.1	48.6	R^2	0.9949	0.9924
40.2	138.1450	51.3	54.0	43.2	44.4	*m*	1.0	0.9
32.5	142.9284	46.5	49.2	38.1	39.0	*b*	10.2	14.4
32.3	147.4376	42.0	44.7	33.4	34.0	CMAE	3.6	4.1
31.7	148.8054	40.7	43.3	32.0	32.4	Cσ	2.7	3.5
29.5	151.6713	37.8	40.5	29.0	29.2	CMaxErr	8.4	11.0
28.5	154.3348	35.1	37.8	26.2	26.2			
25.9	154.3920	35.1	37.8	26.1	26.2			
21.1	156.1683	33.3	36.0	24.3	24.2			
17.4	160.5288	28.9	31.6	19.7	19.3			
16.5	168.8003	20.7	23.3	11.0	10.0			
8.2	179.4788	10.0	12.7	-0.2	-2.0			

[a] NMR data from: Romo de Vivar, A.; Nieto, D. A.; Gaviño, R.; Pérez, A. L. C. *Phytochemistry* **1995**, *40*, 167. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

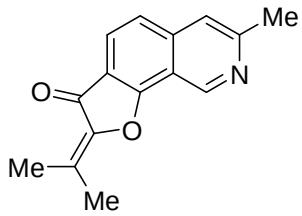
Compound **226**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
169.6	27.2198	171.9	164.9	168.6	169.6	MAE	3.5	3.3
130.7	56.4911	142.6	135.7	140.4	139.1	σ	3.0	2.3
130.3	71.0239	128.1	121.1	126.5	124.0	MaxErr	11.9	9.2
80.1	111.2964	78.2	80.8	78.4	82.0	R^2	0.9918	0.9927
47.7	143.9366	45.5	48.2	46.9	48.0	*m*	1.0	1.0
44.7	150.7934	38.7	41.4	40.3	40.9	*b*	-3.2	2.1
44.5	152.0286	37.4	40.1	39.1	39.6	CMAE	3.2	2.9
41.8	153.9932	35.5	38.2	37.3	37.5	Cσ	2.4	2.4
38.1	155.2928	34.2	36.9	36.0	36.2	CMaxErr	9.7	8.4
37.8	157.1019	32.4	35.0	34.3	34.3			
31.6	157.4375	32.0	34.7	33.9	33.9			
31.1	159.9376	29.5	32.2	31.5	31.3			
30.5	160.2296	29.2	31.9	31.3	31.0			
26.5	164.2766	25.2	27.9	27.4	26.8			
21.5	164.7495	24.7	27.4	26.9	26.3			
21.5	165.5508	23.9	26.6	26.1	25.5			
18.1	170.7497	18.7	21.4	21.1	20.1			

[a] NMR data from: Rodríguez Brasco, M. F.; Seldes, A. M.; Palermo, J. A. *Org. Lett.* **2001**, *3*, 1415. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

Compound **227**

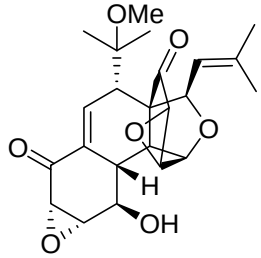


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
182.1	19.7966	179.3	172.3	177.7	180.5	MAE	2.9	5.0
164.0	30.7633	168.4	161.4	166.7	168.6	σ	1.3	2.5
156.7	39.1781	160.0	153.0	158.2	159.4	MaxErr	5.5	9.8
146.2	48.3214	150.8	143.8	149.0	149.5	R^2	0.9977	0.9972
145.6	50.8029	148.3	141.3	146.5	146.8	*m*	1.0	0.9
141.3	60.4098	138.7	131.7	136.8	136.4	*b*	2.9	6.1
133.7	64.3879	134.8	127.8	132.8	132.1	CMAE	2.0	2.3
124.1	72.0563	127.1	120.1	125.1	123.7	Cσ	1.4	1.5
120.5	75.4733	123.7	116.7	121.6	120.0	CMaxErr	4.5	4.9
119.5	75.6751	123.5	116.5	121.4	119.8			
119.3	77.3605	121.8	114.8	119.7	118.0			
114.6	83.7840	115.4	108.4	113.3	111.0			
24.7	166.0626	23.4	26.1	20.7	21.7			
20.4	166.3757	23.1	25.8	20.4	21.4			
17.5	166.4565	23.0	25.7	20.3	21.3			

[a] NMR data from: Kohno, J.; Hiramatsu, H.; Nishio, M.; Sakurai, M.; Okuda, T.; Komatsubara, S. *Tetrahedron* **1999**, *55*, 11247. Solvent: $CDCl_3$

[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

Compound **228**

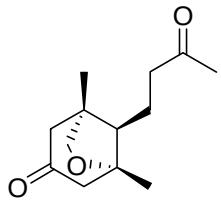


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
202.9	-12.4439	211.6	204.6	207.0	209.6	MAE	3.3	2.5
192.8	4.9965	194.1	187.1	190.3	191.6	σ	2.1	1.9
142.2	50.7290	148.4	141.4	146.4	144.4	MaxErr	8.7	6.2
139.6	58.3000	140.8	133.8	139.2	136.5	R^2	0.9968	0.9974
132.5	65.8876	133.3	126.3	131.9	128.7	*m*	1.0	1.0
120.7	75.0208	124.1	117.1	123.1	119.3	*b*	-4.3	1.7
77.3	117.1502	72.3	75.0	73.4	75.7	CMAE	2.4	2.2
75.8	118.1131	71.3	74.0	72.5	74.7	Cσ	1.6	1.5
72.7	118.4034	71.1	73.7	72.2	74.4	CMaxErr	6.2	6.7
71.5	119.7723	69.7	72.4	70.9	73.0			
61.0	132.9859	56.5	59.2	58.2	59.4			
60.5	134.7267	54.7	57.4	56.6	57.6			
54.5	137.7626	51.7	54.4	53.7	54.4			
53.2	141.0502	48.4	51.1	50.5	51.0			
53.1	141.3480	48.1	50.8	50.2	50.7			
49.1	143.5822	45.9	48.6	48.1	48.4			
47.8	143.6961	45.8	48.4	48.0	48.3			
40.9	151.7359	37.7	40.4	40.3	40.0			
40.4	153.1224	36.3	39.0	38.9	38.6			

26.6	162.1921	27.3	30.0	30.2	29.2
26.1	163.3776	26.1	28.8	29.1	28.0
24.7	163.6352	25.8	28.5	28.9	27.7
18.6	167.8682	21.6	24.3	24.8	23.3

[a] NMR data from: Rychnovsky, S. D. *Org. Lett.* **2006**, *8*, 2895. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

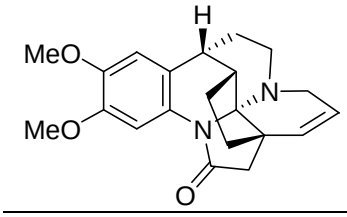
Compound **229**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
208.7	-13.3460	212.5	205.5	211.5	211.0	MAE	2.7	2.3
207.2	-8.9574	208.1	201.1	207.2	206.4	σ	1.6	2.0
83.4	111.8529	77.6	80.3	78.8	80.9	MaxErr	5.8	6.1
78.3	113.6405	75.8	78.5	77.1	79.0	R^2	0.9982	0.9990
53.1	138.3954	51.1	53.7	52.7	53.3	*m*	1.0	1.0
49.4	143.3681	46.1	48.8	47.8	48.1	*b*	-2.5	2.4
48.6	143.7952	45.7	48.3	47.4	47.7	CMAE	2.1	1.6
43.4	148.9175	40.5	43.2	42.4	42.4	Cσ	1.6	1.2
42.6	152.1640	37.3	40.0	39.2	39.0	CMaxErr	5.0	4.1
30.0	161.3724	28.1	30.8	30.1	29.4			
24.9	164.0139	25.4	28.1	27.5	26.7			
20.8	165.7437	23.7	26.4	25.8	24.9			
18.7	170.1434	19.3	22.0	21.5	20.3			

[a] NMR data from: Macías, F. A.; Varela, R. M.; Torres, A.; Oliva, R. M.; Molinillo, J. M. G. *Phytochemistry* **1997**, *48*, 631. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

Compound **230**

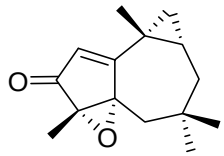


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
173.8	22.6820	176.5	169.5	173.9	177.4	MAE	1.7	3.4
147.7	48.4741	150.7	143.7	148.7	149.6	σ	1.0	2.1
145.3	52.4488	146.7	139.7	144.8	145.3	MaxErr	3.6	8.9
131.5	65.7319	133.4	126.4	131.8	131.0	R^2	0.9988	0.9981
131.0	66.4475	132.7	125.7	131.1	130.2	*m*	1.0	0.9
120.0	77.6279	121.5	114.5	120.1	118.1	*b*	-1.3	5.1
117.4	83.6744	115.5	108.5	114.2	111.6	CMAE	1.3	1.5
111.3	84.2513	114.9	107.9	113.7	111.0	Cσ	1.0	1.4
102.6	92.9199	106.2	99.2	105.2	101.6	CMaxErr	3.2	5.8
84.4	105.7743	83.7	86.4	83.1	87.7			
56.1	135.5796	53.9	56.6	54.0	55.6			
56.0	135.8804	53.6	56.3	53.7	55.3			
47.9	142.2289	47.2	49.9	47.5	48.4			
46.0	142.3605	47.1	49.8	47.4	48.3			
44.5	146.8661	42.6	45.3	42.9	43.4			
44.3	147.7354	41.7	44.4	42.1	42.5			

37.7	151.4444	38.0	40.7	38.5	38.5
36.6	152.9456	36.5	39.2	37.0	36.8
35.0	153.4584	36.0	38.7	36.5	36.3
26.8	160.9754	28.5	31.2	29.1	28.2
24.8	165.0126	24.4	27.1	25.2	23.8

[a] NMR data from: Hubbs, J. L.; Heathcock, C. H. *Org. Lett.* **1999**, *1*, 1315. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

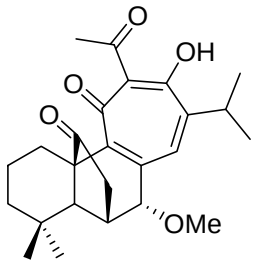
Compound **231**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
200.1	-0.5288	199.7	192.7	199.2	200.3	MAE	2.8	2.9
180.0	19.9784	179.2	172.2	179.0	178.7	σ	2.2	2.5
128.5	63.5220	135.6	128.6	135.9	132.8	MaxErr	7.1	7.8
66.5	129.5468	59.9	62.6	61.1	63.2	R^2	0.9969	0.9983
60.8	134.0939	55.4	58.1	56.6	58.4	*m*	1.0	0.9
42.7	149.2104	40.2	42.9	41.6	42.4	*b*	-1.9	2.7
34.5	157.3505	32.1	34.8	33.6	33.8	CMAE	2.5	1.9
34.2	158.2138	31.2	33.9	32.7	32.9	Cσ	2.1	1.5
30.8	159.8324	29.6	32.3	31.1	31.2	CMaxErr	7.4	4.4
28.9	161.2043	28.3	30.9	29.8	29.8			
26.5	162.2242	27.2	29.9	28.8	28.7			
23.3	163.9658	25.5	28.2	27.0	26.9			
21.3	169.7028	19.8	22.4	21.4	20.8			
19.5	175.1280	14.3	17.0	16.0	15.1			
8.4	178.9922	10.5	13.2	12.2	11.0			

[a] NMR data from: Tori, M.; Nakashima, K.; Toyota, M.; Asakawa, Y. *Tetrahedron Lett.* **1993**, *34*, 3751. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

Compound **232**

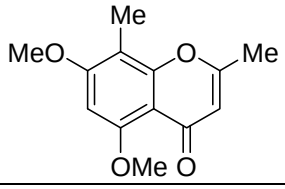


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
203.1	-0.7879	199.9	192.9	200.6	203.0	MAE	3.0	4.6
189.1	0.2654	198.9	191.9	199.5	201.9	σ	2.8	4.0
175.7	19.2856	179.9	172.9	180.5	181.4	MaxErr	11.3	18.2
175.4	34.9920	164.1	157.2	164.8	164.5	R^2	0.9959	0.9955
149.1	52.7227	146.4	139.4	147.1	145.5	*m*	1.0	0.9
146.6	54.3604	144.8	137.8	145.5	143.7	*b*	-0.8	4.1
132.1	66.2201	132.9	125.9	133.6	131.0	CMAE	2.9	2.8
132.0	67.2985	131.8	124.8	132.6	129.8	Cσ	2.7	3.2
119.8	77.0668	122.1	115.1	122.8	119.3	CMaxErr	10.6	12.8
79.5	114.1231	75.3	78.0	76.1	79.4			
73.0	121.8715	67.6	70.3	68.4	71.1			
59.2	132.0319	57.4	60.1	58.2	60.2			
50.2	137.5976	51.9	54.5	52.6	54.2			
45.8	150.4391	39.0	41.7	39.8	40.4			

38.1	151.8695	37.6	40.3	38.4	38.9
31.3	156.8165	32.6	35.3	33.4	33.5
31.3	160.5744	28.9	31.6	29.7	29.5
30.2	160.5897	28.9	31.6	29.7	29.5
28.1	163.1405	26.3	29.0	27.1	26.7
26.4	164.5066	24.9	27.6	25.8	25.3
22.8	164.5640	24.9	27.6	25.7	25.2
22.3	165.1157	24.3	27.0	25.1	24.6
21.9	165.6897	23.8	26.5	24.6	24.0
18.6	170.3984	19.1	21.7	19.9	18.9

[a] NMR data from: Yang, J.; Huang, S. X.; Zhao, Q. S. *J. Phys. Chem. A* **2008**, *112*, 12132. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

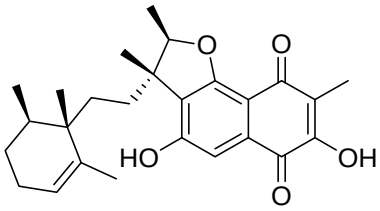
Compound **233**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
177.6	25.6039	173.5	166.5	173.0	174.9	MAE	2.3	4.5
162.6	36.7749	162.4	155.4	161.7	162.8	σ	1.8	3.1
160.7	38.7182	160.4	153.4	159.8	160.7	MaxErr	6.1	11.1
158.5	39.6919	159.4	152.5	158.8	159.6	R^2	0.9975	0.9990
156.5	40.9406	158.2	151.2	157.6	158.3	*m*	1.0	0.9
110.9	82.1070	117.0	110.0	116.2	113.8	*b*	1.4	4.7
108.0	87.2814	111.9	104.9	111.0	108.2	CMAE	2.1	1.1
105.3	89.5518	109.6	102.6	108.7	105.8	Cσ	1.8	1.3
91.1	106.8658	92.3	85.3	91.3	87.0	CMaxErr	5.3	4.1
56.0	135.9881	53.5	56.2	52.3	55.6			
55.4	136.2539	53.2	55.9	52.1	55.3			
19.4	169.2023	20.3	22.9	19.0	19.7			
7.3	180.3051	9.2	11.8	7.8	7.7			

[a] NMR data from: Kalinin, A. V.; Snieckus, V. *Tetrahedron Lett.* **1998**, *39*, 4999. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

Compound **234**

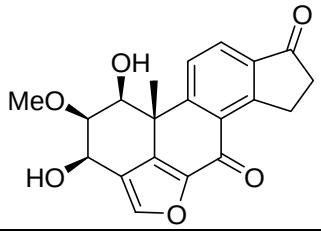


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
182.9	16.5155	182.6	175.6	181.1	183.6	MAE	2.4	4.2
180.4	17.2874	181.9	174.9	180.3	182.8	σ	1.9	2.4
159.9	32.7884	166.4	159.4	164.9	166.2	MaxErr	6.9	10.5
157.7	44.9667	154.2	147.2	152.9	153.1	R^2	0.9976	0.9981
153.6	45.9182	153.2	146.2	151.9	152.1	*m*	1.0	0.9
138.9	61.2512	137.9	130.9	136.7	135.6	*b*	0.1	4.5
131.6	67.6858	131.5	124.5	130.3	128.7	CMAE	2.3	2.0
127.3	67.7928	131.3	124.4	130.2	128.6	Cσ	1.7	1.7
123.9	70.5103	128.6	121.6	127.5	125.7	CMaxErr	7.2	6.4
120.3	74.4999	124.6	117.6	123.6	121.4			
107.9	87.5961	111.5	104.5	110.6	107.4			
107.9	88.0913	111.0	104.1	110.1	106.8			

86.3	105.4960	84.0	86.6	83.2	88.2
46.0	148.1525	41.3	44.0	40.9	42.4
39.7	156.6240	32.8	35.5	32.5	33.3
32.8	156.9085	32.5	35.2	32.2	33.0
31.0	159.2370	30.2	32.9	29.9	30.5
30.5	159.9171	29.5	32.2	29.2	29.8
26.6	162.3662	27.1	29.8	26.8	27.1
25.1	163.8920	25.6	28.3	25.2	25.5
20.9	166.3383	23.1	25.8	22.8	22.9
19.7	167.3780	22.1	24.8	21.8	21.8
18.8	168.5076	20.9	23.6	20.7	20.6
15.7	171.3246	18.1	20.8	17.9	17.5
15.1	172.3639	17.1	19.8	16.8	16.4
8.6	179.9748	9.5	12.2	9.3	8.3

[a] NMR data from: Kalaitzis, J. A.; Hamano, Y.; Nilsen, G.; Moore, B. S. *Org. Lett.* **2003**, *5*, 4449. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

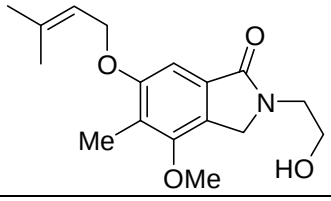
Compound **235**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
206.7	-5.5205	204.7	197.7	201.7	205.7	MAE	2.7	3.8
173.4	25.7360	173.4	166.4	171.3	172.7	σ	2.5	3.1
158.6	37.5177	161.6	154.6	159.9	160.2	MaxErr	8.3	10.6
158.0	44.7732	154.4	147.4	152.8	152.6	R^2	0.9962	0.9969
145.7	45.1212	154.0	147.0	152.5	152.2	*m*	1.0	0.9
145.6	45.9698	153.2	146.2	151.7	151.3	*b*	-3.0	3.0
142.4	53.8029	145.3	138.3	144.1	143.0	CMAE	2.4	2.2
136.9	61.3321	137.8	130.8	136.7	135.1	Cσ	2.1	1.9
129.8	68.9558	130.2	123.2	129.3	127.0	CMaxErr	6.8	6.5
127.3	70.1875	129.0	122.0	128.2	125.7			
127.3	71.0061	128.1	121.1	127.4	124.8			
122.1	72.8143	126.3	119.3	125.6	122.9			
81.7	111.4327	78.0	80.7	78.7	82.1			
71.7	120.0742	69.4	72.1	70.3	73.0			
62.6	129.2537	60.2	62.9	61.4	63.3			
60.7	130.4459	59.0	61.7	60.2	62.0			
42.3	154.1631	35.3	38.0	37.2	37.0			
36.5	155.2428	34.2	36.9	36.2	35.8			
30.5	158.9898	30.5	33.2	32.5	31.9			
28.4	161.0187	28.4	31.1	30.6	29.7			

[a] NMR data from: Wipf, P.; Kerekes, A. D. *J. Nat. Prod.* **2003**, *66*, 716. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

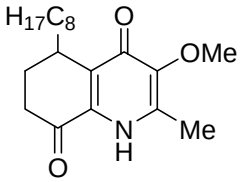
Compound **236**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
167.5	26.5182	172.6	165.6	169.8	171.5	MAE	2.3	3.4
158.7	41.2215	157.9	150.9	155.4	155.8	σ	2.0	2.2
152.4	46.5156	152.6	145.6	150.2	150.2	MaxErr	6.6	7.8
138.0	60.4562	138.7	131.7	136.6	135.3	R^2	0.9976	0.9978
132.2	64.5533	134.6	127.6	132.6	130.9	*m*	1.0	0.9
125.1	67.4333	131.7	124.7	129.8	127.8	*b*	-0.9	5.1
121.8	72.7845	126.4	119.4	124.5	122.1	CMAE	2.0	2.0
120.5	74.9228	124.2	117.2	122.4	119.8	Cσ	1.5	1.3
99.7	91.8441	97.6	100.3	96.4	101.7	CMaxErr	4.9	5.3
68.7	125.1371	64.3	67.0	63.8	66.2			
59.7	126.1896	63.3	66.0	62.8	65.0			
56.4	132.1283	57.3	60.0	57.0	58.7			
49.2	140.6306	48.8	51.5	48.6	49.6			
45.1	145.9828	43.5	46.2	43.4	43.9			
26.0	163.3825	26.1	28.8	26.4	25.3			
18.5	171.4693	18.0	20.7	18.4	16.7			
10.2	178.3974	11.1	13.7	11.7	9.2			

[a] NMR data from: Cornella, I.; Kelly, T. R. *J. Org. Chem.* **2004**, *69*, 2191. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

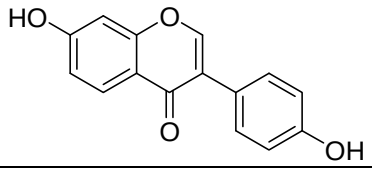
Compound **237**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
194.6	0.9161	198.2	191.2	196.3	199.1	MAE	1.8	4.2
172.8	26.8118	172.3	165.3	170.5	171.3	σ	1.2	1.4
147.5	48.5972	150.5	143.5	148.9	148.0	MaxErr	4.5	7.5
139.0	57.3942	141.7	134.8	140.1	138.6	R^2	0.9991	0.9990
138.9	59.8500	139.3	132.3	137.7	136.0	*m*	1.0	0.9
132.2	64.7642	134.4	127.4	132.8	130.7	*b*	0.8	5.4
59.4	134.5978	54.9	57.5	53.8	55.9	CMAE	1.4	1.5
32.2	154.6269	34.8	37.5	33.9	34.4	Cσ	1.1	1.2
31.8	155.6962	33.8	36.4	32.8	33.3	CMaxErr	5.6	4.5
30.5	157.0822	32.4	35.1	31.4	31.8			
30.3	157.7327	31.7	34.4	30.8	31.1			
29.6	157.9797	31.5	34.2	30.5	30.9			
29.5	158.5234	30.9	33.6	30.0	30.3			
29.2	160.3639	29.1	31.8	28.2	28.3			
28.4	161.2661	28.2	30.9	27.3	27.3			
24.3	163.4841	26.0	28.7	25.1	25.0			
22.6	165.5481	23.9	26.6	23.0	22.8			
14.5	172.4632	17.0	19.7	16.1	15.3			
14.0	176.3063	13.1	15.8	12.3	11.2			

[a] NMR data from: Bringmann, J.; Schlauer, H.; Rischer, H.; Wohlfarth, J.; Mühlbacher, J.; Buske, A.; Porzel, A.; Schmidt, J.; Adam, G. *Tetrahedron* **2000**, *56*, 3691. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

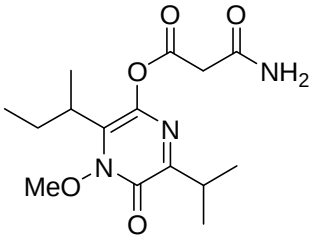
Compound **238**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
174.8	25.7417	173.4	166.4	174.8	174.8	MAE	2.1	5.8
162.8	39.6018	159.5	152.5	160.0	160.0	σ	1.6	2.4
157.6	40.2062	158.9	151.9	159.3	159.3	MaxErr	4.7	10.3
157.2	43.0884	156.1	149.1	156.2	156.2	R^2	0.9926	0.9926
152.9	46.0667	153.1	146.1	153.0	153.0	*m*	0.9	0.9
130.1	65.4376	133.7	126.7	132.3	132.3	*b*	10.2	3.2
127.3	67.1849	132.0	125.0	130.4	130.4	CMAE	1.7	1.7
123.6	72.0552	127.1	120.1	125.2	125.2	Cσ	0.9	0.9
122.6	76.1089	123.0	116.0	120.9	120.9	CMaxErr	3.1	3.1
116.6	78.0711	121.1	114.1	118.8	118.8			
115.3	82.9450	116.2	109.2	113.5	113.5			
115.0	83.4948	115.6	108.6	113.0	113.0			
102.2	95.0694	104.1	97.1	100.6	100.6			

[a] NMR data from: Suzuki, K.; Yahara, S.; Kazutomo, M.; Uyeda, M. *J. Nat. Prod.* **2001**, *64*, 204. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

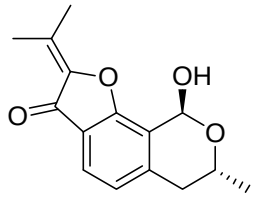
Compound **239**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
168.0	25.0783	174.1	167.1	168.3	169.2	MAE	3.6	2.3
166.0	31.7496	167.4	160.4	161.9	162.3	σ	2.5	2.0
161.5	32.8791	166.3	159.3	160.8	161.1	MaxErr	8.0	5.6
152.0	40.3801	158.8	151.8	153.6	153.4	R^2	0.9981	0.9990
135.0	56.1336	143.0	136.0	138.5	137.0	*m*	1.0	1.0
134.9	56.3424	142.8	135.8	138.3	136.8	*b*	-1.0	3.7
64.1	129.0719	60.4	63.1	59.0	61.5	CMAE	2.4	1.8
41.1	151.2629	38.2	40.9	37.7	38.5	Cσ	1.4	0.9
33.7	155.9728	33.5	36.2	33.2	33.6	CMaxErr	5.1	3.7
30.7	161.4954	28.0	30.6	27.9	27.9			
27.5	163.1440	26.3	29.0	26.3	26.2			
19.9	167.5021	22.0	24.6	22.1	21.7			
19.9	167.5471	21.9	24.6	22.0	21.7			
18.2	169.5538	19.9	22.6	20.1	19.6			
12.6	174.4884	15.0	17.7	15.4	14.5			

[a] NMR data from: Kita, M.; Miwa, R.; Widianti, T.; Ozaki, Y.; Aoyama, S.; Yamada, K.; Uemura, D. *Tetrahedron Lett.* **2007**, *48*, 8628. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

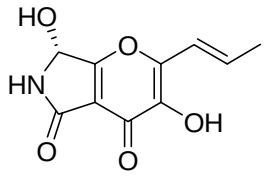
Compound **240**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
182.5	18.1414	181.0	174.0	178.5	181.2	MAE	2.2	3.7
162.5	33.2843	165.9	158.9	163.7	165.1	σ	1.6	2.3
144.5	50.6568	148.5	141.5	146.6	146.6	MaxErr	4.8	8.5
142.0	56.7327	142.4	135.4	140.7	140.1	R^2	0.9982	0.9988
131.1	64.4178	134.7	127.7	133.1	131.9	*m*	1.0	0.9
122.7	71.6096	127.5	120.5	126.1	124.2	*b*	-1.1	3.8
122.5	72.6118	126.5	119.5	125.1	123.2	CMAE	1.9	1.6
122.0	75.2988	123.8	116.8	122.5	120.3	Cσ	1.3	1.0
119.1	80.3865	118.8	111.8	117.5	114.9	CMaxErr	4.2	4.2
87.5	103.9587	85.5	88.2	84.9	89.8			
62.2	131.3981	58.1	60.7	58.0	60.6			
36.5	153.7510	35.7	38.4	36.1	36.8			
21.0	167.1626	22.3	25.0	22.9	22.5			
20.1	169.5363	19.9	22.6	20.6	20.0			
17.0	173.2509	16.2	18.9	16.9	16.0			

[a] NMR data from: Lin, W. H.; Brauers, G.; Ebel, R.; Wray, V.; Berg, A.; Surdasono; Proksch, P. *J. Nat. Prod.* **2003**, *66*, 57. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

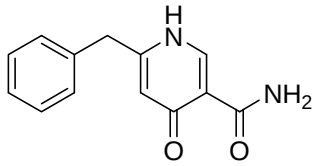
Compound **241**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
174.2	20.7541	178.4	171.4	176.3	178.3	MAE	3.1	4.5
169.1	33.1118	166.0	159.0	163.9	164.8	σ	1.8	2.6
165.0	33.6542	165.5	158.5	163.3	164.3	MaxErr	7.0	10.1
146.0	49.5015	149.6	142.6	147.3	147.0	R^2	0.9970	0.9967
142.2	52.6523	146.5	139.5	144.2	143.6	*m*	1.0	0.9
131.7	65.1121	134.0	127.0	131.6	130.0	*b*	3.6	7.7
118.9	78.2844	120.9	113.9	118.3	115.6	CMAE	2.0	2.3
111.7	80.4002	118.7	111.7	116.2	113.3	Cσ	1.6	1.3
75.2	112.3566	77.1	79.8	74.2	78.5	CMaxErr	5.2	4.3
18.7	168.5687	20.9	23.6	17.4	17.3			

[a] NMR data from: Hiort, J.; Maksimenka, K.; Reichert, M.; Perovi-Ottstadt, S.; Lin, W. H.; Wray, V.; Steube, K.; Schaumann, K.; Weber, H.; Proksch, P.; Ebel, R.; Müller, W. E. G.; Bringmann, G. *J. Nat. Prod.* **2004**, *67*, 1532. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

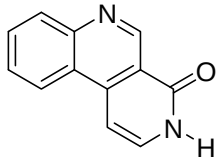
Compound **242**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
178.1	25.0855	174.1	167.1	175.4	178.0	MAE	2.7	6.5
165.9	33.2516	165.9	158.9	166.9	168.9	σ	2.4	3.5
151.2	53.9450	145.2	138.2	145.4	145.7	MaxErr	8.0	13.0
142.2	54.0273	145.1	138.1	145.3	145.6	R^2	0.9882	0.9903
137.4	66.1994	132.9	125.9	132.6	132.0	*m*	1.0	0.9
129.3	67.6587	131.5	124.5	131.1	130.3	*b*	5.4	8.1
129.3	68.0516	131.1	124.1	130.7	129.9	CMAE	2.8	2.3
129.2	69.0669	130.1	123.1	129.6	128.7	Cσ	2.2	2.2
129.2	70.4173	128.7	121.7	128.2	127.2	CMaxErr	7.4	6.2
127.5	70.6736	128.5	121.5	128.0	126.9			
118.9	72.2743	126.9	119.9	126.3	125.1			
118.0	77.8970	121.2	114.2	120.4	118.9			
38.2	150.7853	38.7	41.4	34.6	37.2			

[a] NMR data from: Hiort, J.; Maksimenka, K.; Reichert, M.; Perovi-Ottstadt, S.; Lin, W. H.; Wray, V.; Steube, K.; Schaumann, K.; Weber, H.; Proksch, P.; Ebel, R.; Müller, W. E. G.; Bringmann, G. *J. Nat. Prod.* **2004**, *67*, 1532. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

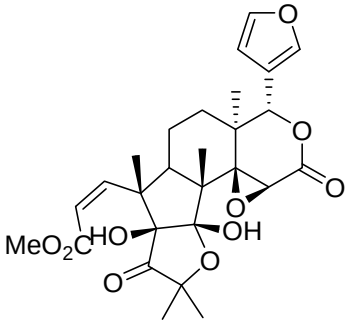
Compound **243**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
164.0	36.4291	162.7	155.7	162.5	162.5	MAE	1.5	6.8
150.5	44.5443	154.6	147.6	154.4	154.4	σ	1.2	2.0
148.5	48.0733	151.1	144.1	150.9	150.9	MaxErr	4.1	10.4
144.3	58.2235	140.9	133.9	140.8	140.8	R^2	0.9855	0.9855
136.0	62.6031	136.5	129.5	136.4	136.4	*m*	1.0	1.0
132.8	66.5640	132.6	125.6	132.4	132.4	*b*	-0.2	-7.2
130.4	67.7252	131.4	124.4	131.3	131.3	CMAE	1.5	1.5
128.7	72.4681	126.7	119.7	126.5	126.5	Cσ	1.2	1.2
125.0	74.5136	124.6	117.6	124.5	124.5	CMaxErr	3.9	3.9
123.6	76.5084	122.6	115.6	122.5	122.5			
118.7	79.6848	119.5	112.5	119.3	119.3			
101.6	96.4604	102.7	95.7	102.6	102.6			

[a] NMR data from: Morita, H.; Sato, Y.; Chan, K. L.; Choo, C. Y.; Itokawa, H.; Takeya, K.; Kobayashi, J. *J. Nat. Prod.* **2000**, *63*, 1707. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

Compound **244**

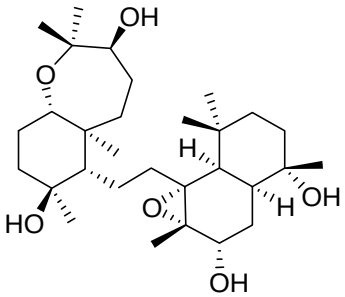


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
216.9	-23.6854	222.8	215.8	219.6	223.1	MAE	5.0	4.1
167.8	26.7889	172.4	165.4	169.9	169.6	σ	2.8	3.6
166.7	27.6947	171.4	164.4	169.0	168.7	MaxErr	10.7	13.4
153.9	45.7127	153.4	146.4	151.3	149.6	R^2	0.9904	0.9931
143.0	49.7931	149.3	142.4	147.2	145.3	*m*	1.0	0.9
141.1	51.1285	148.0	141.0	145.9	143.9	*b*	-0.1	5.1
123.1	72.3524	126.8	119.8	125.0	121.4	CMAE	4.7	3.8
121.0	75.8626	123.3	116.3	121.6	117.7	Cσ	2.9	2.6
109.9	80.0565	119.1	112.1	117.4	113.3	CMaxErr	10.5	9.7
108.2	83.3537	106.1	108.8	104.6	109.8			
88.6	108.7893	80.7	83.4	79.6	82.8			
80.9	110.8695	78.6	81.3	77.5	80.6			
78.4	117.0323	72.4	75.1	71.5	74.1			
68.5	129.9823	59.5	62.2	58.7	60.4			
57.3	135.2381	54.2	56.9	53.5	54.9			
52.0	138.0834	51.4	54.1	50.7	51.8			
49.9	142.3298	47.1	49.8	46.6	47.3			
49.7	146.0497	43.4	46.1	42.9	43.4			
46.8	147.7115	41.7	44.4	41.3	41.6			
39.5	156.7938	32.7	35.4	32.3	32.0			
27.4	159.4286	30.0	32.7	29.7	29.2			
26.3	161.9539	27.5	30.2	27.2	26.6			
24.1	161.9576	27.5	30.2	27.2	26.6			
18.3	162.7954	26.7	29.3	26.4	25.7			
17.3	163.4454	26.0	28.7	25.8	25.0			
15.2	163.5532	25.9	28.6	25.7	24.9			
14.7	170.9710	18.5	21.2	18.3	17.0			

[a] NMR data from: Kubo, I.; Tanis, S. P.; Lee, Y. W.; Miura, I.; Nakanishi, K.; Chapya, A. *Heterocycles* **1976**, *5*, 485. Solvent: $CDCl_3$

[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

Compound **245**



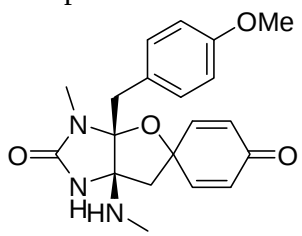
δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
77.8	113.8014	75.7	78.3	84.7	84.7	MAE	3.0	3.2
77.2	120.0926	69.4	72.1	77.2	77.2	σ	3.0	1.9
76.8	121.4575	68.0	70.7	75.5	75.5	MaxErr	8.8	6.2

72.7	124.3560	65.1	67.8	72.1	72.1	R^2	0.9907	0.9907
72.2	125.1739	64.3	67.0	71.1	71.1	*m*	0.8	0.8
70.0	125.4935	64.0	66.7	70.7	70.7	*b*	4.8	7.5
69.5	128.0323	61.4	64.1	67.7	67.7	CMAE	1.3	1.3
65.7	131.0548	58.4	61.1	64.1	64.1	Cσ	1.4	1.4
55.7	141.5757	47.9	50.6	51.5	51.5	CMaxErr	6.9	6.9
42.9	147.1602	42.3	45.0	44.8	44.8			
40.2	147.9870	41.5	44.2	43.8	43.8			
39.3	151.2396	38.2	40.9	39.9	39.9			
39.2	152.7726	36.7	39.4	38.1	38.1			
38.0	153.8866	35.6	38.3	36.7	36.7			
36.7	155.2480	34.2	36.9	35.1	35.1			
35.6	155.3929	34.1	36.8	34.9	34.9			
34.5	156.0923	33.4	36.1	34.1	34.1			
31.8	158.0131	31.4	34.1	31.8	31.8			
31.3	158.0937	31.4	34.1	31.7	31.7			
30.4	158.0954	31.4	34.0	31.7	31.7			
30.2	158.5186	30.9	33.6	31.2	31.2			
29.5	159.9953	29.5	32.1	29.4	29.4			
29.2	160.1599	29.3	32.0	29.2	29.2			
26.8	162.6295	26.8	29.5	26.3	26.3			
25.4	163.8419	25.6	28.3	24.8	24.8			
25.3	165.4178	24.0	26.7	23.0	23.0			
21.4	165.5080	23.9	26.6	22.8	22.8			
21.0	167.1199	22.3	25.0	20.9	20.9			
16.8	169.4106	20.0	22.7	18.2	18.2			
13.4	172.5346	16.9	19.6	14.4	14.4			

[a] NMR data from: Jain, S.; Laphookhieo, S.; Shi, Z.; Fu, L. W.; Akiyama, S.; Chen, Z. S.; Youssef, D. T. A.; von Soest, R. W. M.; El Sayed, K. A. *J. Nat. Prod.* **2007**, *70*, 928. Solvent: $CDCl_3$

[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

Compound **246**

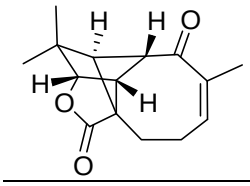


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
185.4	15.2753	183.9	176.9	183.0	186.1	MAE	2.0	5.0
159.5	32.4448	166.7	159.7	165.7	167.2	σ	1.6	2.2
158.9	40.9177	158.2	151.2	157.2	157.8	MaxErr	7.2	8.5
151.0	47.6147	151.5	144.5	150.4	150.4	R^2	0.9980	0.9959
150.1	47.6731	151.5	144.5	150.4	150.3	*m*	1.0	0.9
132.8	63.2170	135.9	128.9	134.7	133.2	*b*	2.1	8.3
132.8	64.3868	134.8	127.8	133.5	131.9	CMAE	1.5	2.2
127.5	70.7679	128.4	121.4	127.1	124.8	Cσ	1.6	2.1
126.9	72.1240	127.0	120.0	125.7	123.3	CMaxErr	6.2	7.7
125.9	72.5861	126.6	119.6	125.3	122.8			
112.7	84.5161	114.6	107.6	113.3	109.7			
112.7	85.2381	113.9	106.9	112.5	108.9			
102.5	85.2989	104.2	106.8	102.7	108.8			
82.5	105.0214	84.4	87.1	82.9	87.0			
77.1	115.2160	74.2	76.9	72.6	75.8			
54.2	136.2650	53.2	55.9	51.4	52.5			
46.9	140.2588	49.2	51.9	47.4	48.1			
37.1	150.6281	38.8	41.5	37.0	36.7			
24.7	160.2566	29.2	31.9	27.3	26.0			

24.5	161.8142	27.6	30.3	25.7	24.3

[a] NMR data from: Ralifo, P.; Crews, P. *J. Org. Chem.* **2004**, *69*, 9025. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

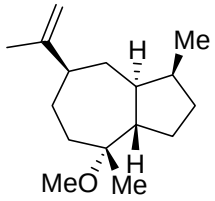
Compound **247**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
211.9	-18.4057	217.5	210.6	214.9	217.2	MAE	2.4	3.0
177.5	19.5059	179.6	172.6	177.9	177.6	σ	2.0	1.9
135.1	62.3801	136.8	129.8	136.0	132.8	MaxErr	5.9	7.7
131.1	68.7319	130.4	123.4	129.8	126.2	R^2	0.9981	0.9981
84.2	111.1420	78.3	81.0	79.0	81.9	*m*	1.0	1.0
62.8	128.7795	60.7	63.4	61.7	63.5	*b*	-2.6	2.6
62.6	131.8021	57.7	60.3	58.8	60.3	CMAE	2.2	2.2
54.5	134.7558	54.7	57.4	55.9	57.2	Cσ	1.3	1.4
54.5	139.2528	50.2	52.9	51.5	52.5	CMaxErr	5.2	5.2
41.9	151.5836	37.9	40.6	39.5	39.7			
28.6	160.6648	28.8	31.5	30.6	30.2			
22.8	165.8857	23.6	26.3	25.5	24.7			
22.6	165.9103	23.5	26.2	25.5	24.7			
22.2	166.2247	23.2	25.9	25.2	24.4			
22.2	168.8941	20.6	23.3	22.6	21.6			

[a] NMR data from: Lodewyk, M. W.; Soldi, C.; Jones, P. B.; Olmstead, M. M.; Rita, J.; Shaw, J. T.; Dean J. Tantillo, D. J. *J. Am. Chem. Soc.* **2012**, *134*, 18550. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

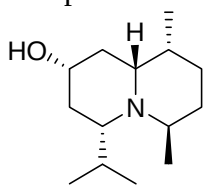
Compound **222**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
152.4	49.1005	150.0	143.0	152.4	152.3	MAE	2.3	2.7
108.4	86.2849	112.9	105.9	114.7	111.2	σ	2.2	2.6
77.1	121.2018	68.3	70.9	69.5	72.7	MaxErr	8.8	9.4
54.7	135.8801	53.6	56.3	54.7	56.5	R^2	0.9929	0.9969
49.4	140.6213	48.8	51.5	49.9	51.2	*m*	1.0	0.9
49.4	142.1960	47.3	49.9	48.3	49.5	*b*	-0.4	5.1
41.1	151.2701	38.2	40.9	39.1	39.5	CMAE	1.8	1.4
39.2	152.0442	37.4	40.1	38.3	38.6	Cσ	2.4	1.4
37.7	152.6446	36.8	39.5	37.7	38.0	CMaxErr	7.6	4.4
37.4	154.0160	35.4	38.1	36.3	36.4			
34.2	156.6090	32.8	35.5	33.7	33.6			
27.6	163.5487	25.9	28.6	26.6	25.9			
25.4	163.6653	25.8	28.5	26.5	25.8			
24.1	165.0836	24.4	27.1	25.1	24.2			
21.2	169.0369	20.4	23.1	21.1	19.9			
15.3	169.4280	20.0	22.7	20.7	19.4			

[a] NMR data from: Booker-Milburn, K. I.; Jankins, H.; Charmant, J. P. H.; Mohr, P. *Org. Lett.* **2003**, *5*, 3309. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

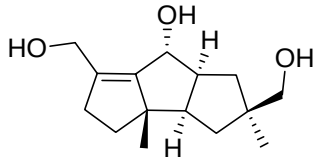
Compound **223**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
69.8	124.2149	65.2	67.9	70.8	70.8	MAE	2.2	2.2
61.8	131.5576	57.9	60.6	62.5	62.5	σ	1.7	1.6
55.4	139.2543	50.2	52.9	53.8	53.8	MaxErr	5.2	4.9
47.9	145.0486	44.4	47.1	47.2	47.2	R^2	0.9941	0.9941
41.7	147.8504	41.6	44.3	44.0	44.0	*m*	0.9	0.9
35.0	157.1887	32.3	35.0	33.5	33.5	*b*	2.6	5.3
34.4	157.5706	31.9	34.6	33.1	33.1	CMAE	1.2	1.2
27.9	161.5301	27.9	30.6	28.6	28.6	Cσ	0.8	0.8
27.8	161.7266	27.7	30.4	28.4	28.4	CMaxErr	2.5	2.5
27.1	165.0874	24.4	27.1	24.6	24.6			
20.6	166.6681	22.8	25.5	22.8	22.8			
15.0	173.6621	15.8	18.5	14.9	14.9			
14.1	173.6737	15.8	18.5	14.9	14.9			
8.2	179.8835	9.6	12.3	7.9	7.9			

[a] NMR data from: Comins, D. L.; Zheng, X.; Goehring, R. R. *Org. Lett.* **2002**, *4*, 1611. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

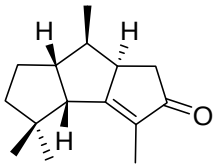
Compound **224**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
153.3	37.6816	161.5	154.5	160.7	160.7	MAE	2.8	3.2
130.0	72.8348	126.3	119.3	125.9	122.8	σ	2.5	3.2
75.8	116.1745	73.3	76.0	73.4	76.0	MaxErr	8.2	10.7
71.7	121.2280	68.2	70.9	68.4	70.5	R^2	0.9896	0.9897
61.6	130.2098	59.2	61.9	59.5	60.8	*m*	1.0	0.9
55.8	133.5801	55.9	58.6	56.2	57.2	*b*	-0.8	5.6
55.6	134.5657	54.9	57.6	55.2	56.1	CMAE	2.8	2.6
50.4	139.1677	50.3	53.0	50.6	51.1	Cσ	2.4	2.6
48.5	147.2344	42.2	44.9	42.6	42.4	CMaxErr	7.4	7.4
41.8	147.3018	42.2	44.8	42.6	42.4			
41.6	148.8439	40.6	43.3	41.0	40.7			
36.3	152.4084	37.0	39.7	37.5	36.8			
35.7	156.5457	32.9	35.6	33.4	32.4			
22.7	160.7927	28.7	31.4	29.2	27.8			
22.4	162.9840	26.5	29.2	27.0	25.4			

[a] NMR data from: Mehta, G.; Pallavi, K. *Tetrahedron Lett.* **2006**, *47*, 8355. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

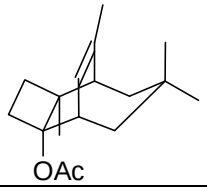
Compound **225**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
211.8	-7.2710	206.4	199.4	208.9	210.2	MAE	2.3	4.2
183.9	14.7153	184.4	177.4	186.5	186.3	σ	1.6	3.3
134.4	62.4046	136.7	129.7	137.9	134.4	MaxErr	5.5	12.4
54.4	134.4194	55.0	57.7	54.6	56.0	R^2	0.9982	0.9988
53.4	138.1450	51.3	54.0	50.8	52.0	*m*	1.0	0.9
46.2	142.9284	46.5	49.2	45.9	46.8	*b*	1.5	6.2
44.9	147.4376	42.0	44.7	41.3	41.9	CMAE	2.2	1.9
41.9	148.8054	40.7	43.3	39.9	40.4	Cσ	1.2	0.9
39.2	151.6713	37.8	40.5	37.0	37.3	CMaxErr	4.4	3.5
36.9	154.3348	35.1	37.8	34.3	34.4			
32.4	154.3920	35.1	37.8	34.2	34.3			
30.1	156.1683	33.3	36.0	32.4	32.4			
25.8	160.5288	28.9	31.6	27.9	27.6			
15.1	168.8003	20.7	23.3	19.5	18.6			
9.1	179.4788	10.0	12.7	8.6	7.0			

[a] NMR data from: Mehta, G.; Murthy, S. K.; Umarye, J. D. *Tetrahedron Lett.* **2002**, *43*, 8301. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

Compound **226**

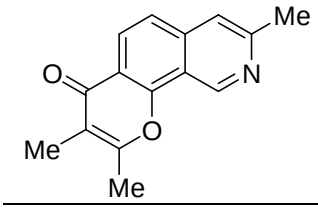


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
169.6	27.2198	171.9	164.9	169.9	170.8	MAE	2.8	2.3
141.5	56.4911	142.6	135.7	141.5	140.1	σ	2.0	1.9
122.2	71.0239	128.1	121.1	127.4	124.8	MaxErr	7.1	5.8
85.3	111.2964	78.2	80.8	78.9	82.5	R^2	0.9960	0.9979
49.3	143.9366	45.5	48.2	47.2	48.2	*m*	1.0	1.0
45.3	150.7934	38.7	41.4	40.5	41.0	*b*	-3.1	2.3
38.7	152.0286	37.4	40.1	39.3	39.7	CMAE	2.0	1.7
36.7	153.9932	35.5	38.2	37.4	37.7	Cσ	2.1	1.1
35.7	155.2928	34.2	36.9	36.1	36.3	CMaxErr	6.4	4.3
35.6	157.1019	32.4	35.0	34.4	34.4			
34.2	157.4375	32.0	34.7	34.1	34.1			
31.8	159.9376	29.5	32.2	31.6	31.4			
29.4	160.2296	29.2	31.9	31.3	31.1			
28.6	164.2766	25.2	27.9	27.4	26.9			
23.9	164.7495	24.7	27.4	27.0	26.4			
21.8	165.5508	23.9	26.6	26.2	25.5			
21.6	170.7497	18.7	21.4	21.1	20.1			

[a] NMR data from: Inanaga, K.; Takasu, K.; Ihara, M. *J. Am. Chem. Soc.* **2004**, *126*, 1352. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//AM1 level of theory

Experimental chemical shifts, mPW1PW91/6-31G(d)//HF/3-21G Boltzmann-averaged GIAO isotropic magnetic shielding values, unscaled and scaled chemical shifts computed using TMS and MSTD, and statistical parameters computed for compounds 201-247.

Compound **201**

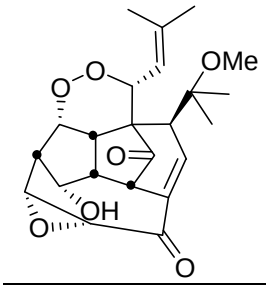


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
182.1	28.2857	174.0	166.5	173.4	175.2	MAE	3.2	6.5
164.0	40.7669	161.5	154.0	161.1	162.2	σ	2.7	4.1
156.7	44.6156	157.7	150.1	157.3	158.2	MaxErr	8.2	15.6
146.2	48.1506	154.2	146.6	153.9	154.5	R^2	0.9938	0.9945
145.6	53.3915	148.9	141.4	148.7	149.1	*m*	1.0	1.0
141.3	63.2476	139.1	131.5	139.0	138.8	*b*	-2.4	-2.0
133.7	71.8966	130.4	122.9	130.5	129.8	CMAE	3.2	3.0
124.1	78.3125	124.0	116.5	124.2	123.2	Cσ	2.5	2.4
120.5	78.5906	123.7	116.2	123.9	122.9	CMaxErr	8.7	8.3
119.5	80.7719	121.5	114.0	121.8	120.6			
119.3	82.3809	119.9	112.4	120.2	118.9			
114.6	84.5228	117.8	110.2	118.1	116.7			
24.7	169.9426	24.8	24.8	26.7	27.9			
20.4	176.9028	17.9	17.9	19.9	20.6			
17.5	185.4950	9.3	9.3	11.4	11.7			

[a] NMR data from: Kohno, J.; Hiramatsu, H.; Nishio, M.; Sakurai, M.; Okuda, T.; Komatsubara, S. *Tetrahedron* **1999**, *55*, 11247. Solvent: $CDCl_3$

[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Compound **202**

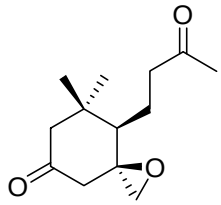


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
202.9	-6.2980	208.6	201.1	201.4	203.1	MAE	4.7	4.2
192.8	6.1311	196.2	188.6	189.2	190.2	σ	4.6	4.6
142.2	51.5645	150.7	143.2	144.8	143.1	MaxErr	19.8	19.8
139.6	61.2664	141.0	133.5	135.3	133.1	R^2	0.9920	0.9883
132.5	66.9580	135.3	127.8	129.8	127.2	*m*	1.0	1.0
120.7	73.8939	128.4	120.9	123.0	120.0	*b*	2.5	5.1
77.3	97.6868	97.1	97.1	92.4	95.3	CMAE	3.5	4.2
75.8	106.7687	88.0	88.0	83.5	85.9	Cσ	3.0	3.8
72.7	115.8075	79.0	79.0	74.7	76.6	CMaxErr	15.1	18.0
71.5	117.0460	77.7	77.7	73.5	75.3			
61.0	134.5064	60.3	60.3	56.4	57.2			
60.5	135.8001	59.0	59.0	55.2	55.8			
54.5	136.5907	58.2	58.2	54.4	55.0			

53.2	136.7023	58.1	58.1	54.3	54.9
53.1	136.8934	57.9	57.9	54.1	54.7
49.1	137.3500	57.4	57.4	53.6	54.2
47.8	146.5418	48.2	48.2	44.7	44.7
40.9	148.2381	46.5	46.5	43.0	43.0
40.4	152.9394	41.8	41.8	38.4	38.1
26.6	168.4498	26.3	26.3	23.3	22.0
26.1	169.4508	25.3	25.3	22.3	21.0
24.7	169.7418	25.0	25.0	22.0	20.7
18.6	176.7000	18.1	18.1	15.2	13.5

[a] NMR data from: Rychnovsky, S. D. *Org. Lett.* **2006**, *8*, 2895. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

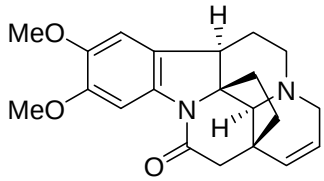
Compound **203**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
208.7	-5.6170	207.9	200.4	209.4	208.9	MAE	5.0	6.2
207.2	-3.9081	206.2	198.7	207.7	207.1	σ	4.8	4.6
83.4	96.0086	98.8	98.8	98.2	100.7	MaxErr	15.4	15.4
78.3	130.8089	64.0	64.0	62.7	63.7	R^2	0.9882	0.9874
53.1	138.1248	56.6	56.6	55.3	55.9	*m*	1.0	0.9
49.4	147.7919	47.0	47.0	45.4	45.6	*b*	2.4	4.2
48.6	149.2224	45.5	45.5	44.0	44.1	CMAE	4.7	4.6
43.4	150.7425	44.0	44.0	42.4	42.4	Cσ	5.0	5.5
42.6	156.0416	38.7	38.7	37.0	36.8	CMaxErr	15.6	17.3
30.0	157.5393	37.2	37.2	35.5	35.2			
24.9	167.2264	27.5	27.5	25.6	24.9			
20.8	167.2949	27.5	27.5	25.6	24.8			
18.7	172.6118	22.1	22.2	20.1	19.2			

[a] NMR data from: Macías, F. A.; Varela, R. M.; Torres, A.; Oliva, R. M.; Molinillo, J. M. G. *Phytochemistry* **1997**, *48*, 631. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Compound **204**

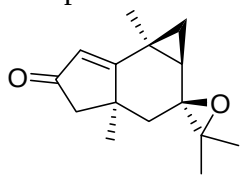


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
173.8	39.5762	162.7	155.2	164.1	166.2	MAE	4.7	5.6
147.7	53.5634	148.7	141.2	149.5	150.3	σ	3.5	4.5
145.3	57.6880	144.6	137.1	145.2	145.7	MaxErr	12.4	18.6
131.5	64.1643	138.1	130.6	138.4	138.3	R^2	0.9867	0.9880
131.0	68.5363	133.8	126.2	133.9	133.4	*m*	1.0	0.9
120.0	76.5288	125.8	118.2	125.5	124.4	*b*	5.4	8.3
117.4	77.7627	124.5	117.0	124.3	123.0	CMAE	4.2	4.3
111.3	92.8641	109.4	101.9	108.5	105.9	Cσ	3.5	2.8
102.6	98.0664	104.2	96.7	103.1	100.0	CMaxErr	14.9	12.3
84.4	122.6743	72.1	72.1	69.5	72.1			
56.1	129.7734	65.0	65.0	62.1	64.1			

56.0	141.0825	53.7	53.7	50.3	51.3
47.9	141.4891	53.3	53.3	49.9	50.9
46.0	143.5744	51.2	51.2	47.7	48.5
44.5	145.4373	49.3	49.3	45.8	46.4
44.3	150.0826	44.7	44.7	40.9	41.1
37.7	150.1656	44.6	44.6	40.8	41.0
36.6	150.6387	44.1	44.1	40.4	40.5
35.0	158.7047	36.1	36.1	31.9	31.4
26.8	162.6378	32.1	32.1	27.8	26.9
24.8	169.6033	25.2	25.2	20.6	19.0

[a] NMR data from: Hubbs, J. L.; Heathcock, C. H. *Org. Lett.* **1999**, *1*, 1315. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

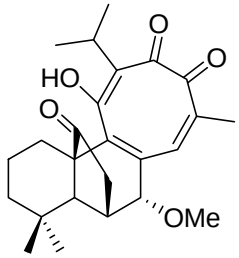
Compound **205**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
200.1	1.1339	201.2	193.6	199.3	200.1	MAE	3.8	4.5
180.0	18.4035	183.9	176.4	182.0	181.9	σ	3.6	3.5
128.5	72.7043	129.6	122.1	127.8	124.9	MaxErr	12.3	12.3
66.5	127.8613	66.9	66.9	65.1	67.0	R^2	0.9930	0.9921
60.8	129.8679	64.9	64.9	63.1	64.8	*m*	1.0	1.0
42.7	146.3712	48.4	48.4	46.6	47.5	*b*	1.7	3.2
34.5	149.7420	45.0	45.0	43.3	44.0	CMAE	3.7	4.1
34.2	161.9534	32.8	32.8	31.1	31.1	Cσ	3.2	3.2
30.8	169.1347	25.6	25.6	23.9	23.6	CMaxErr	10.6	10.1
28.9	171.1560	23.6	23.6	21.9	21.5			
26.5	171.4246	23.3	23.3	21.6	21.2			
23.3	171.7638	23.0	23.0	21.3	20.8			
21.3	172.6789	22.1	22.1	20.3	19.9			
19.5	173.2713	21.5	21.5	19.8	19.2			
8.4	174.0163	20.7	20.7	19.0	18.5			

[a] NMR data from: Tori, M.; Nakashima, K.; Toyota, M.; Asakawa, Y. *Tetrahedron Lett.* **1993**, *34*, 3751. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Compound **206**

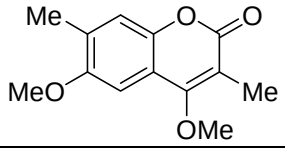


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
203.1	-2.1718	204.5	196.9	206.2	208.4	MAE	5.5	5.5
189.1	1.1126	201.2	193.7	202.8	204.9	σ	5.0	6.9
175.7	22.5832	179.7	172.2	180.6	181.3	MaxErr	24.5	32.0
175.4	51.3583	150.9	143.4	150.9	149.8	R^2	0.9873	0.9858
149.1	61.2930	141.0	133.5	140.7	139.0	*m*	1.0	0.9
146.6	61.8605	140.4	132.9	140.1	138.3	*b*	4.8	6.5
132.1	62.3300	140.0	132.4	139.6	137.8	CMAE	4.9	5.1
132.0	64.1962	138.1	130.6	137.7	135.8	Cσ	5.2	5.5
119.8	74.3192	128.0	120.4	127.2	124.7	CMaxErr	24.5	25.6

79.5	112.9146	81.8	81.8	79.6	82.5
73.0	122.3786	72.4	72.4	69.8	72.1
59.2	131.9719	62.8	62.8	59.9	61.6
50.2	137.5354	57.2	57.2	54.2	55.5
45.8	150.3936	44.4	44.4	40.9	41.4
38.1	151.0661	43.7	43.7	40.2	40.7
31.3	156.4524	38.3	38.3	34.6	34.8
31.3	163.4397	31.3	31.3	27.4	27.2
30.2	164.1428	30.6	30.6	26.7	26.4
28.1	164.8686	29.9	29.9	26.0	25.6
26.4	165.8410	28.9	28.9	24.9	24.5
22.8	166.4885	28.3	28.3	24.3	23.8
22.3	166.7136	28.0	28.0	24.0	23.6
21.9	167.9851	26.8	26.8	22.7	22.2
18.6	170.2858	24.5	24.5	20.4	19.7

[a] NMR data from: Yang, J.; Huang, S. X.; Zhao, Q. S. *J. Phys. Chem. A* **2008**, *112*, 12132. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

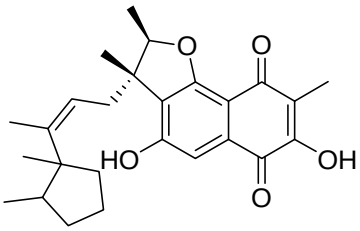
Compound **207**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
177.6	40.2945	162.0	154.5	169.7	171.2	MAE	9.1	9.7
162.6	43.1335	159.2	151.6	166.6	167.8	σ	6.6	9.7
160.7	49.4635	152.8	145.3	159.5	160.2	MaxErr	24.4	32.0
158.5	54.5099	147.8	140.3	153.8	154.2	R^2	0.9647	0.9695
156.5	70.2281	132.1	124.5	136.2	135.4	*m*	0.9	0.8
110.9	83.0937	119.2	111.7	121.8	120.1	*b*	10.5	11.0
108.0	83.1415	119.2	111.6	121.7	120.0	CMAE	8.9	8.2
105.3	84.4670	117.8	110.3	120.3	118.5	Cσ	5.8	5.5
91.1	97.7823	104.5	97.0	105.3	102.6	CMaxErr	20.3	21.1
56.0	134.9621	59.8	59.8	55.2	58.2			
55.4	141.5299	53.2	53.2	47.9	50.4			
19.4	175.9244	18.8	18.8	9.4	9.3			
7.3	182.5712	12.2	12.2	1.9	1.4			

[a] NMR data from: Kalinin, A. V.; Snieckus, V. *Tetrahedron Lett.* **1998**, *39*, 4999. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Compound **208**

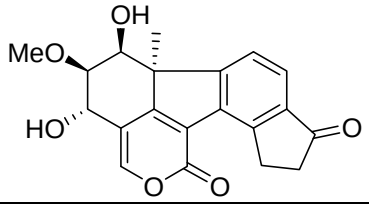


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
182.9	19.2430	183.1	175.5	181.2	183.2	MAE	3.9	5.4
180.4	20.7714	181.5	174.0	179.6	181.5	σ	3.9	3.2
159.9	41.3597	160.9	153.4	158.7	159.2	MaxErr	13.4	13.4
157.7	43.4704	158.8	151.3	156.5	156.9	R^2	0.9956	0.9941
153.6	47.0408	155.3	147.7	152.9	153.1	*m*	1.0	0.9
138.9	51.6444	150.7	143.1	148.2	148.1	*b*	5.1	6.4
131.6	70.2158	132.1	124.5	129.3	128.0	CMAE	3.0	3.6

127.3	73.3771	128.9	121.4	126.1	124.5	Cσ	2.7	2.9
123.9	79.1495	123.2	115.6	120.2	118.3	CMaxErr	9.3	10.3
120.3	79.3141	123.0	115.4	120.0	118.1			
107.9	88.5393	113.8	106.2	110.6	108.1			
107.9	91.5204	110.8	103.2	107.6	104.9			
86.3	106.4611	88.3	88.3	84.7	88.7			
46.0	144.3922	50.4	50.4	46.1	47.6			
39.7	145.2727	49.5	49.5	45.2	46.6			
32.8	148.5198	46.2	46.2	41.9	43.1			
31.0	152.5140	42.2	42.2	37.8	38.8			
30.5	157.8909	36.9	36.9	32.3	33.0			
26.6	160.2553	34.5	34.5	29.9	30.4			
25.1	167.3526	27.4	27.4	22.7	22.7			
20.9	169.3020	25.5	25.5	20.7	20.6			
19.7	171.8556	22.9	22.9	18.1	17.8			
18.8	176.4015	18.4	18.4	13.5	12.9			
15.7	179.5646	15.2	15.2	10.2	9.5			
15.1	181.1644	13.6	13.6	8.6	7.8			
8.6	183.1967	11.6	11.6	6.5	5.6			

[a] NMR data from: Kalaitzis, J. A.; Hamano, Y.; Nilsen, G.; Moore, B. S. *Org. Lett.* **2003**, *5*, 4449. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

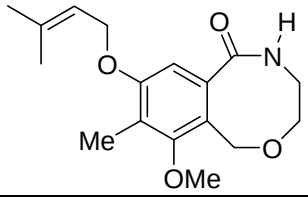
Compound **209**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
206.7	-2.3304	204.6	197.1	207.0	210.7	MAE	4.0	7.1
173.4	37.1158	165.2	157.6	166.8	167.6	σ	3.1	4.7
158.6	45.7989	156.5	149.0	158.0	158.2	MaxErr	12.9	15.8
158.0	46.5401	155.8	148.2	157.2	157.3	R^2	0.9909	0.9880
145.7	50.1071	152.2	144.7	153.6	153.5	*m*	1.0	0.9
145.6	50.8545	151.4	143.9	152.8	152.6	*b*	1.4	4.0
142.4	63.7409	138.6	131.0	139.7	138.6	CMAE	3.8	4.7
136.9	63.9815	138.3	130.8	139.5	138.3	Cσ	3.3	3.3
129.8	74.1365	128.2	120.6	129.1	127.2	CMaxErr	12.5	13.5
127.3	76.9505	125.4	117.8	126.3	124.2			
127.3	80.3037	122.0	114.5	122.8	120.5			
122.1	83.7342	118.6	111.0	119.3	116.8			
81.7	112.2122	82.5	82.6	82.6	85.7			
71.7	124.1532	70.6	70.6	70.5	72.7			
62.6	125.7222	69.0	69.0	68.9	70.9			
60.7	139.0437	55.7	55.7	55.3	56.4			
42.3	139.5811	55.2	55.2	54.8	55.8			
36.5	159.5825	35.2	35.2	34.4	34.0			
30.5	165.4162	29.3	29.3	28.4	27.6			
28.4	172.7261	22.0	22.0	21.0	19.6			

[a] NMR data from: Wipf, P.; Kerekes, A. D. *J. Nat. Prod.* **2003**, *66*, 716. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

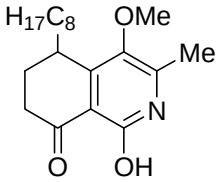
Compound **210**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
167.5	33.1901	169.1	161.6	167.0	168.1	MAE	2.8	4.7
158.7	44.0421	158.3	150.7	156.1	156.4	σ	3.5	3.6
152.4	45.6447	156.7	149.1	154.4	154.7	MaxErr	13.5	13.5
138.0	61.7121	140.6	133.1	138.3	137.3	R^2	0.9952	0.9915
132.2	69.7824	132.5	125.0	130.1	128.6	*m*	1.0	0.9
125.1	76.3840	125.9	118.4	123.5	121.5	*b*	3.4	5.9
121.8	77.3077	125.0	117.5	122.5	120.5	CMAE	2.7	3.8
120.5	79.8812	122.4	114.9	119.9	117.7	Cσ	2.3	2.8
99.7	89.9543	104.8	104.8	102.2	106.8	CMaxErr	10.6	12.2
68.7	126.3989	68.4	68.4	65.5	67.5			
59.7	129.6991	65.1	65.1	62.2	63.9			
56.4	131.0780	63.7	63.7	60.8	62.4			
49.2	132.0611	62.7	62.7	59.8	61.4			
45.1	150.0967	44.7	44.7	41.6	41.9			
26.0	168.7822	26.0	26.0	22.8	21.7			
18.5	176.3460	18.4	18.4	15.2	13.5			
10.2	183.5412	11.2	11.2	7.9	5.8			

[a] NMR data from: Cornella, I.; Kelly, T. R. *J. Org. Chem.* **2004**, *69*, 2191. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

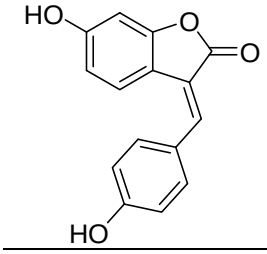
Compound **211**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
194.6	0.6201	201.7	194.1	200.3	202.7	MAE	4.9	4.4
172.8	40.0391	162.3	154.7	160.8	160.9	σ	5.6	7.0
147.5	40.3894	161.9	154.4	160.5	160.5	MaxErr	20.3	27.9
139.0	50.9825	151.3	143.8	149.9	149.3	R^2	0.9860	0.9839
138.9	58.1067	144.2	136.7	142.7	141.7	*m*	1.0	0.9
132.2	90.4400	111.9	104.3	110.4	107.4	*b*	1.7	3.1
59.4	135.8588	58.9	58.9	57.3	59.2	CMAE	4.2	4.3
32.2	161.5483	33.2	33.2	31.6	31.9	Cσ	6.0	6.6
31.8	161.6916	33.1	33.1	31.5	31.8	CMaxErr	21.8	24.8
30.5	161.8031	33.0	33.0	31.3	31.6			
30.3	162.6856	32.1	32.1	30.5	30.7			
29.6	162.7373	32.0	32.0	30.4	30.7			
29.5	163.8010	31.0	31.0	29.3	29.5			
29.2	164.4360	30.3	30.3	28.7	28.9			
28.4	166.2700	28.5	28.5	26.9	26.9			
24.3	169.1616	25.6	25.6	24.0	23.8			
22.6	169.8030	25.0	25.0	23.3	23.2			
14.5	174.8538	19.9	19.9	18.3	17.8			
14.0	179.3826	15.4	15.4	13.7	13.0			

[a] NMR data from: Bringmann, J.; Schlauer, H.; Rischer, H.; Wohlfarth, J.; Mühlbacher, J.; Buske, A.; Porzel, A.; Schmidt, J.; Adam, G. *Tetrahedron* **2000**, *56*, 3691. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

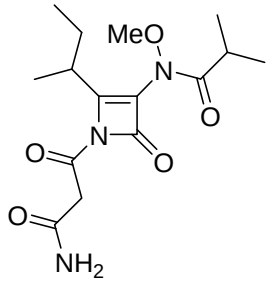
Compound **212**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
174.8	36.0974	166.2	158.7	172.6	172.6	MAE	4.3	9.8
162.8	44.6329	157.7	150.1	162.9	162.9	σ	3.5	5.1
157.6	46.5691	155.7	148.2	160.8	160.8	MaxErr	12.6	20.2
157.2	47.9906	154.3	146.8	159.2	159.2	R^2	0.9518	0.9518
152.9	62.0471	140.3	132.7	143.3	143.3	*m*	0.9	0.9
130.1	64.3621	137.9	130.4	140.7	140.7	*b*	13.0	5.5
127.3	73.9519	128.3	120.8	129.9	129.9	CMAE	3.7	3.7
123.6	80.6504	121.7	114.1	122.4	122.4	Cσ	3.4	3.4
122.6	80.8497	121.5	113.9	122.2	122.2	CMaxErr	10.6	10.6
116.6	81.4687	120.8	113.3	121.5	121.5			
115.3	86.2317	116.1	108.5	116.1	116.1			
115.0	90.8749	111.4	103.9	110.9	110.9			
102.2	104.4127	97.9	90.4	95.6	95.6			

[a] NMR data from: Suzuki, K.; Yahara, S.; Kazutomo, M.; Uyeda, M. *J. Nat. Prod.* **2001**, *64*, 204. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

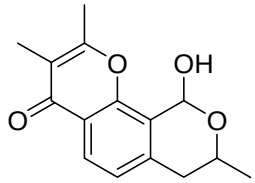
Compound **213**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
168.0	19.2698	183.0	175.5	173.3	174.3	MAE	6.1	4.5
166.0	27.4992	174.8	167.3	165.6	166.1	σ	7.2	6.4
161.5	35.9729	166.3	158.8	157.7	157.7	MaxErr	25.1	21.5
152.0	39.5091	162.8	155.3	154.3	154.2	R^2	0.9869	0.9853
135.0	42.2134	160.1	152.5	151.8	151.5	*m*	1.1	1.0
134.9	81.3707	120.9	113.4	115.1	112.7	*b*	-1.8	-0.2
64.1	132.0718	62.7	62.7	60.5	62.4	CMAE	4.2	4.3
41.1	155.1488	39.6	39.6	38.8	39.5	Cσ	5.9	6.4
33.7	156.4906	38.3	38.3	37.6	38.2	CMaxErr	19.8	22.2
30.7	162.0422	32.7	32.7	32.3	32.7			
27.5	168.1388	26.6	26.6	26.6	26.6			
19.9	175.5903	19.2	19.2	19.6	19.2			
19.9	176.0375	18.7	18.7	19.2	18.8			
18.2	176.9702	17.8	17.8	18.3	17.8			
12.6	181.3221	13.4	13.4	14.3	13.5			

[a] NMR data from: Kita, M.; Miwa, R.; Widianti, T.; Ozaki, Y.; Aoyama, S.; Yamada, K.; Uemura, D. *Tetrahedron Lett.* **2007**, *48*, 8628. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

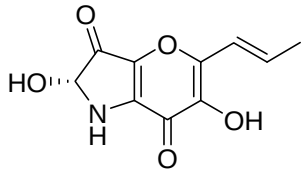
Compound **214**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
182.5	27.6423	174.7	167.1	173.6	175.3	MAE	2.7	5.2
162.5	40.4956	161.8	154.3	161.0	161.9	σ	3.0	4.1
144.5	48.6136	153.7	146.1	153.0	153.3	MaxErr	9.2	15.4
142.0	61.2254	141.1	133.5	140.6	140.1	R^2	0.9949	0.9941
131.1	72.1769	130.1	122.6	129.8	128.6	*m*	1.0	1.0
122.7	77.0584	125.2	117.7	125.0	123.5	*b*	-1.7	0.1
122.5	78.2969	124.0	116.5	123.7	122.2	CMAE	2.7	2.9
122.0	79.0170	123.3	115.7	123.0	121.4	Cσ	2.8	3.0
119.1	80.6235	121.7	114.1	121.5	119.7	CMaxErr	8.9	8.8
87.5	105.4119	89.3	89.4	89.6	93.7			
62.2	131.8757	62.9	62.9	63.6	65.9			
36.5	159.0441	35.7	35.7	36.8	37.4			
21.0	174.0701	20.7	20.7	22.0	21.7			
20.1	176.7127	18.0	18.1	19.4	18.9			
17.0	185.5898	9.2	9.2	10.7	9.6			

[a] NMR data from: Lin, W. H.; Brauers, G.; Ebel, R.; Wray, V.; Berg, A.; Surdasono; Proksch, P. *J. Nat. Prod.* **2003**, *66*, 57. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

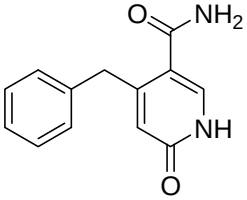
Compound **215**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
174.2	10.9218	191.4	183.8	188.5	190.8	MAE	7.7	7.5
169.1	36.5959	165.7	158.2	162.3	163.0	σ	6.9	6.4
165.0	51.9267	150.4	142.8	146.7	146.4	MaxErr	18.9	22.2
146.0	55.4803	146.8	139.3	143.1	142.5	R^2	0.9591	0.9578
142.2	58.9032	143.4	135.9	139.6	138.8	*m*	1.0	0.9
131.7	64.2704	138.0	130.5	134.1	133.0	*b*	6.5	7.6
118.9	64.5389	137.8	130.2	133.8	132.7	CMAE	7.4	7.3
111.7	80.8714	121.4	113.9	117.2	115.0	Cσ	6.1	6.5
75.2	116.1833	78.6	78.6	73.5	76.8	CMaxErr	18.3	18.6
18.7	174.4813	20.3	20.3	14.0	13.7			

[a] NMR data from: Hiort, J.; Maksimenka, K.; Reichert, M.; Perovi-Ottstadt, S.; Lin, W. H.; Wray, V.; Steube, K.; Schaumann, K.; Weber, H.; Proksch, P.; Ebel, R.; Müller, W. E. G.; Bringmann, G. *J. Nat. Prod.* **2004**, *67*, 1532. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

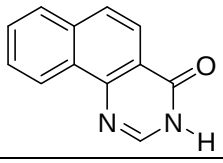
Compound **216**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
178.1	37.5410	164.8	157.2	169.6	171.4	MAE	3.6	8.9
165.9	45.5350	156.8	149.2	161.0	162.2	σ	3.8	5.4
151.2	46.8513	155.5	147.9	159.5	160.7	MaxErr	13.3	20.9
142.2	63.1745	139.1	131.6	141.8	141.8	R^2	0.9807	0.9834
137.4	67.5952	134.7	127.2	137.0	136.7	*m*	0.9	0.9
129.3	70.7058	131.6	124.1	133.6	133.1	*b*	8.6	8.7
129.3	72.8599	129.4	121.9	131.3	130.7	CMAE	3.5	3.0
129.2	73.8204	128.5	120.9	130.2	129.5	Cσ	2.8	2.9
129.2	73.8365	128.5	120.9	130.2	129.5	CMaxErr	8.5	9.5
127.5	75.6982	126.6	119.1	128.2	127.4			
118.9	79.3520	122.9	115.4	124.2	123.2			
118.0	88.3979	113.9	106.4	114.4	112.7			
38.2	155.3796	39.4	39.4	33.4	35.4			

[a] NMR data from: Hiort, J.; Maksimenka, K.; Reichert, M.; Perovi-Ottstadt, S.; Lin, W. H.; Wray, V.; Steube, K.; Schaumann, K.; Weber, H.; Proksch, P.; Ebel, R.; Müller, W. E. G.; Bringmann, G. *J. Nat. Prod.* **2004**, *67*, 1532. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

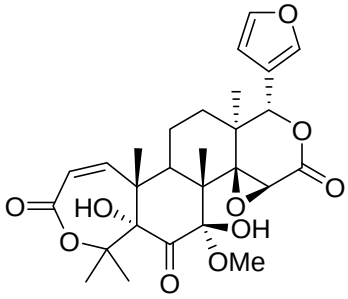
Compound **217**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
164.0	44.0850	158.2	150.7	176.1	176.1	MAE	5.8	9.8
150.5	55.3239	147.0	139.4	156.7	156.7	σ	5.3	4.7
148.5	60.6462	141.7	134.1	147.5	147.5	MaxErr	21.0	15.7
144.3	66.1724	136.1	128.6	137.9	137.9	R^2	0.8486	0.8486
136.0	71.8706	130.4	122.9	128.1	128.1	*m*	0.6	0.6
132.8	72.7709	129.5	122.0	126.5	126.5	*b*	56.3	48.8
130.4	73.2989	129.0	121.5	125.6	125.6	CMAE	5.3	5.3
128.7	73.7160	128.6	121.0	124.9	124.9	Cσ	4.2	4.2
125.0	74.0013	128.3	120.8	124.4	124.4	CMaxErr	13.0	13.0
123.6	75.1436	127.2	119.6	122.4	122.4			
118.7	76.9278	125.4	117.8	119.3	119.3			
101.6	79.6746	122.6	115.1	114.6	114.6			

[a] NMR data from: Morita, H.; Sato, Y.; Chan, K. L.; Choo, C. Y.; Itokawa, H.; Takeya, K.; Kobayashi, J. *J. Nat. Prod.* **2000**, *63*, 1707. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Compound **218**

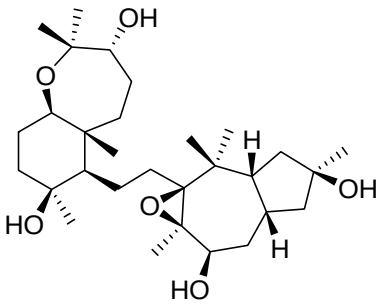


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
216.9	-16.8147	219.1	211.6	222.9	225.9	MAE	3.7	5.4
167.8	37.1095	165.2	157.7	166.6	166.2	σ	2.5	2.9
166.7	38.6697	163.6	156.1	164.9	164.4	MaxErr	9.8	10.6
153.9	50.2684	152.0	144.5	152.8	151.6	R^2	0.9968	0.9968
143.0	57.9533	144.3	136.8	144.8	143.1	*m*	1.0	0.9
141.1	59.2259	143.1	135.5	143.5	141.7	*b*	5.7	7.7
123.1	77.0499	125.3	117.7	124.9	121.9	CMAE	2.3	2.4
121.0	82.2885	120.0	112.5	119.4	116.1	Cσ	2.2	2.1
109.9	89.6084	112.7	105.2	111.7	108.0	CMaxErr	10.7	9.0
108.2	95.6995	99.1	99.1	97.5	101.3			
88.6	108.0082	86.8	86.8	84.7	87.6			
80.9	110.8417	83.9	83.9	81.7	84.5			
78.4	115.8754	78.9	78.9	76.4	78.9			
68.5	123.1583	71.6	71.6	68.8	70.8			
57.3	136.1041	58.7	58.7	55.3	56.5			
52.0	138.1909	56.6	56.6	53.1	54.2			
49.9	139.3438	55.4	55.4	51.9	52.9			
49.7	140.6635	54.1	54.1	50.6	51.4			
46.8	144.3240	50.4	50.4	46.7	47.4			
39.5	153.5820	41.2	41.2	37.1	37.1			
27.4	162.3513	32.4	32.4	27.9	27.4			
26.3	163.8088	31.0	31.0	26.4	25.8			
24.1	167.9418	26.8	26.8	22.1	21.2			
18.3	168.3854	26.4	26.4	21.6	20.7			
17.3	169.3419	25.4	25.4	20.6	19.7			
15.2	169.7237	25.0	25.0	20.2	19.2			
14.7	177.3222	17.4	17.4	12.3	10.8			

[a] NMR data from: Kubo, I.; Tanis, S. P.; Lee, Y. W.; Miura, I.; Nakanishi, K.; Chapya, A. *Heterocycles* **1976**, *5*, 485. Solvent: $CDCl_3$

[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Compound **219**



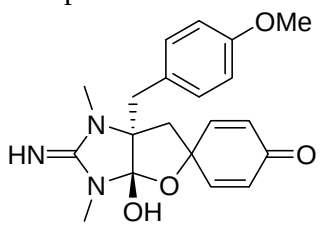
δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
77.8	112.1165	82.6	82.6	78.5	78.5	MAE	2.9	2.9
77.2	114.2365	80.5	80.5	76.5	76.5	σ	2.0	2.0
76.8	114.9707	79.8	79.8	75.8	75.8	MaxErr	8.3	8.3

72.7	117.3030	77.5	77.5	73.6	73.6	R^2	0.9850	0.9850
72.2	119.0175	75.7	75.7	72.0	72.0	*m*	1.1	1.1
70.0	120.3333	74.4	74.4	70.7	70.7	*b*	-0.6	-0.6
69.5	121.6863	73.1	73.1	69.5	69.5	CMAE	1.8	1.8
65.7	125.8951	68.9	68.9	65.5	65.5	Cσ	1.7	1.7
55.7	143.4144	51.3	51.3	49.0	49.0	CMaxErr	6.7	6.7
42.9	143.5165	51.2	51.2	48.9	48.9			
40.2	147.9708	46.8	46.8	44.7	44.7			
39.3	150.7072	44.1	44.1	42.1	42.1			
39.2	150.9396	43.8	43.8	41.9	41.9			
38.0	152.2566	42.5	42.5	40.7	40.7			
36.7	156.0016	38.8	38.8	37.1	37.1			
35.6	156.6107	38.2	38.2	36.6	36.6			
34.5	159.5399	35.2	35.2	33.8	33.8			
31.8	163.8959	30.9	30.9	29.7	29.7			
31.3	163.9861	30.8	30.8	29.6	29.6			
30.4	164.3270	30.4	30.4	29.3	29.3			
30.2	166.1263	28.6	28.6	27.6	27.6			
29.5	166.3188	28.4	28.4	27.4	27.4			
29.2	168.2109	26.5	26.6	25.6	25.6			
26.8	168.3887	26.4	26.4	25.5	25.5			
25.4	168.4826	26.3	26.3	25.4	25.4			
25.3	169.6209	25.1	25.1	24.3	24.3			
21.4	170.8586	23.9	23.9	23.1	23.1			
21.0	173.2909	21.5	21.5	20.8	20.8			
16.8	176.0880	18.7	18.7	18.2	18.2			
13.4	177.6757	17.1	17.1	16.7	16.7			

[a] NMR data from: Jain, S.; Laphookhieo, S.; Shi, Z.; Fu, L. W.; Akiyama, S.; Chen, Z. S.; Youssef, D. T. A.; von Soest, R. W. M.; El Sayed, K. A. *J. Nat. Prod.* **2007**, *70*, 928. Solvent: $CDCl_3$

[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Compound **220**

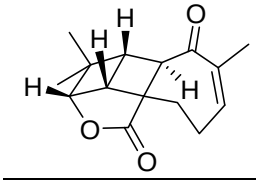


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
185.4	20.0432	182.3	174.7	182.8	185.2	MAE	3.0	5.4
159.5	45.8539	156.4	148.9	156.6	157.0	σ	2.1	3.4
158.9	47.8102	154.5	147.0	154.6	154.9	MaxErr	9.6	11.9
151.0	48.3882	153.9	146.4	154.0	154.3	R^2	0.9945	0.9950
150.1	54.9269	147.4	139.8	147.4	147.1	*m*	1.0	0.9
132.8	68.1917	134.1	126.6	133.9	132.6	*b*	2.5	5.2
132.8	70.1438	132.2	124.6	131.9	130.5	CMAE	2.8	2.5
127.5	71.8677	130.4	122.9	130.1	128.6	Cσ	2.2	2.2
126.9	72.9021	129.4	121.9	129.1	127.5	CMaxErr	9.2	8.1
125.9	75.4664	126.8	119.3	126.5	124.7			
112.7	79.9568	122.3	114.8	121.9	119.8			
112.7	86.0171	116.3	108.7	115.7	113.1			
102.5	92.1057	102.7	102.7	101.9	106.5			
82.5	106.6526	88.1	88.1	87.1	90.6			
77.1	122.1393	72.6	72.6	71.3	73.7			
54.2	142.2496	52.5	52.5	50.9	51.7			
46.9	150.5502	44.2	44.2	42.4	42.6			
37.1	155.6710	39.1	39.1	37.2	37.0			
24.7	166.2689	28.5	28.5	26.4	25.4			

24.5	168.4368	26.3	26.3	24.2	23.0			

[a] NMR data from: Ralifo, P.; Crews, P. *J. Org. Chem.* **2004**, *69*, 9025. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

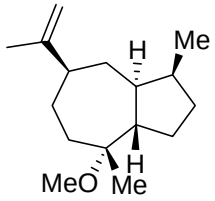
Compound **221**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
211.9	-1.9392	204.2	196.7	206.3	207.6	MAE	6.3	6.5
177.5	23.6347	178.7	171.1	180.9	180.8	σ	4.6	5.3
135.1	61.8968	140.4	132.9	143.0	140.8	MaxErr	16.0	16.0
131.1	64.0943	138.2	130.7	140.8	138.5	R^2	0.9858	0.9885
84.2	114.8687	79.9	79.9	82.9	85.4	*m*	1.0	1.0
62.8	141.6462	53.1	53.1	56.4	57.5	*b*	-3.7	-1.8
62.6	148.1985	46.6	46.6	49.9	50.6	CMAE	6.1	5.5
54.5	152.7808	42.0	42.0	45.3	45.8	Cσ	3.6	3.2
54.5	153.3135	41.4	41.4	44.8	45.3	CMaxErr	12.7	12.0
41.9	156.0387	38.7	38.7	42.1	42.4			
28.6	163.4388	31.3	31.3	34.8	34.7			
22.8	167.4476	27.3	27.3	30.8	30.5			
22.6	169.4428	25.3	25.3	28.8	28.4			
22.2	171.7630	23.0	23.0	26.5	26.0			
22.2	177.1534	17.6	17.6	21.2	20.3			

[a] NMR data from: Lodewyk, M. W.; Soldi, C.; Jones, P. B.; Olmstead, M. M.; Rita, J.; Shaw, J. T.; Dean J. Tantillo, D. J. *J. Am. Chem. Soc.* **2012**, *134*, 18550. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

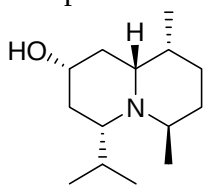
Compound **222**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
153.0	50.5694	151.7	144.2	151.5	151.3	MAE	2.7	3.1
107.8	89.7769	112.5	105.0	111.8	108.9	σ	2.5	2.8
78.9	117.3927	77.4	77.4	76.2	79.1	MaxErr	7.8	8.8
52.7	141.1216	53.6	53.6	52.2	53.4	R^2	0.9914	0.9910
49.0	143.8317	50.9	50.9	49.4	50.5	*m*	1.0	0.9
45.9	146.1449	48.6	48.6	47.1	48.0	*b*	2.1	4.2
45.3	153.2741	41.5	41.5	39.9	40.3	CMAE	2.7	2.7
39.0	154.5777	40.2	40.2	38.5	38.9	Cσ	2.0	2.0
30.5	156.4869	38.3	38.3	36.6	36.8	CMaxErr	6.1	6.3
30.4	157.4371	37.3	37.3	35.6	35.8			
28.4	160.0662	34.7	34.7	33.0	33.0			
27.7	166.9664	27.8	27.8	26.0	25.5			
26.1	167.3834	27.4	27.4	25.6	25.0			
25.1	171.6299	23.1	23.1	21.3	20.5			
20.2	174.4508	20.3	20.3	18.4	17.4			
16.5	179.2945	15.5	15.5	13.5	12.2			

[a] NMR data from: Fleischer, T. C.; Waigh, R. D.; Waterman, P. G. *J. Nat. Prod.* **1997**, *60*, 1054. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

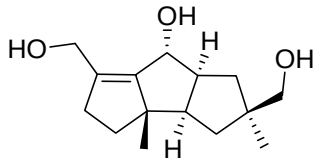
Compound **223**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
73.0	126.8242	67.9	67.9	83.6	83.6	MAE	11.1	11.1
72.8	136.5772	58.2	58.2	72.5	72.5	σ	4.6	4.6
68.6	142.0165	52.7	52.7	66.4	66.4	MaxErr	19.0	19.0
67.1	146.6811	48.1	48.1	61.1	61.1	R^2	0.9499	0.9499
49.6	155.4109	39.3	39.4	51.2	51.2	*m*	0.9	0.9
49.5	160.5561	34.2	34.2	45.4	45.4	*b*	-5.9	-5.9
41.3	161.4069	33.4	33.4	44.4	44.4	CMAE	3.4	3.4
41.1	166.3422	28.4	28.4	38.8	38.8	Cσ	2.8	2.8
41.0	167.2947	27.5	27.5	37.7	37.7	CMaxErr	10.6	10.6
40.0	167.8075	27.0	27.0	37.2	37.2			
22.0	174.9906	19.8	19.8	29.0	29.0			
22.0	180.5796	14.2	14.2	22.7	22.7			
21.9	180.7766	14.0	14.0	22.5	22.5			
18.3	186.8441	7.9	7.9	15.6	15.6			

[a] NMR data from: Kazmi, S. N.; Ahmed, Z.; Ahmed, W.; Malik, A. *Heterocycles* **1989**, *29*, 1901. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

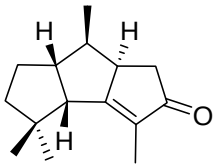
Compound **224**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
145.8	50.4210	151.9	144.3	145.6	144.8	MAE	4.9	4.1
129.1	63.5163	138.8	131.2	132.8	131.1	σ	3.8	3.6
74.3	118.7371	76.0	76.0	71.3	73.4	MaxErr	12.8	12.8
72.1	126.2293	68.5	68.5	64.0	65.5	R^2	0.9870	0.9871
59.0	134.2051	60.6	60.6	56.1	57.2	*m*	1.0	1.0
50.5	135.6311	59.1	59.1	54.7	55.7	*b*	3.2	5.9
45.9	136.0680	58.7	58.7	54.3	55.2	CMAE	3.2	3.2
45.5	143.1958	51.6	51.6	47.3	47.8	Cσ	2.5	2.6
45.1	145.9405	48.8	48.8	44.6	44.9	CMaxErr	8.4	9.3
40.8	153.1194	41.6	41.6	37.6	37.4			
36.1	154.2071	40.6	40.6	36.6	36.2			
36.0	156.1251	38.6	38.6	34.7	34.2			
25.1	160.1867	34.6	34.6	30.7	30.0			
22.7	171.8643	22.9	22.9	19.3	17.8			
20.3	172.4682	22.3	22.3	18.7	17.1			

[a] NMR data from: Huang, Z.; Dan, Y.; Huang, Y.; Lin, L.; Li, T.; Ye, W.; Wei, X. *J. Nat. Prod.* **2004**, *67*, 2121. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

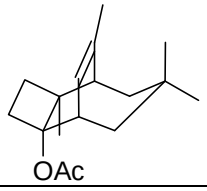
Compound **225**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
208.2	-4.4404	206.7	199.2	207.2	208.5	MAE	7.9	9.0
176.3	22.9467	179.4	171.8	178.3	178.1	σ	4.8	4.0
140.3	63.9673	138.3	130.8	135.1	132.6	MaxErr	16.1	16.1
42.5	141.0818	53.7	53.7	45.9	47.0	R^2	0.9935	0.9913
40.2	141.5404	53.2	53.2	45.4	46.5	*m*	0.9	0.9
32.5	146.1256	48.6	48.6	40.6	41.4	*b*	10.1	11.3
32.3	147.7869	47.0	47.0	38.9	39.6	CMAE	4.0	4.6
31.7	152.5668	42.2	42.2	33.8	34.3	Cσ	3.0	3.6
29.5	154.5525	40.2	40.2	31.7	32.1	CMaxErr	11.2	12.3
28.5	158.6938	36.1	36.1	27.4	27.5			
25.9	161.3607	33.4	33.4	24.6	24.5			
21.1	166.6240	28.1	28.1	19.0	18.7			
17.4	169.4494	25.3	25.3	16.0	15.6			
16.5	179.6744	15.1	15.1	5.3	4.2			
8.2	182.9250	11.8	11.8	1.9	0.6			

[a] NMR data from: Romo de Vivar, A.; Nieto, D. A.; Gaviño, R.; Pérez, A. L. C. *Phytochemistry* **1995**, *40*, 167. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

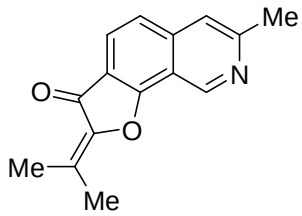
Compound **226**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
169.6	34.4395	167.9	160.3	165.8	166.4	MAE	3.4	3.9
130.7	58.8498	143.5	135.9	141.8	140.9	σ	3.2	3.3
130.3	76.1087	126.2	118.7	124.9	122.8	MaxErr	12.8	11.6
80.1	109.3460	85.4	85.4	84.7	88.0	R^2	0.9897	0.9887
47.7	147.3374	47.4	47.4	47.4	48.2	*m*	1.0	1.0
44.7	148.6484	46.1	46.1	46.1	46.9	*b*	-0.8	1.3
44.5	156.1153	38.6	38.6	38.7	39.1	CMAE	3.6	3.7
41.8	159.9136	34.8	34.8	35.0	35.1	Cσ	2.7	2.9
38.1	161.0280	33.7	33.7	33.9	33.9	CMaxErr	11.1	10.2
37.8	161.1697	33.6	33.6	33.8	33.8			
31.6	161.9901	32.8	32.8	33.0	32.9			
31.1	162.0928	32.7	32.7	32.9	32.8			
30.5	163.8572	30.9	30.9	31.1	30.9			
26.5	165.4466	29.3	29.3	29.6	29.3			
21.5	170.2364	24.5	24.5	24.9	24.3			
21.5	173.1491	21.6	21.6	22.0	21.2			
18.1	174.6482	20.1	20.1	20.5	19.7			

[a] NMR data from: Rodríguez Brasco, M. F.; Seldes, A. M.; Palermo, J. A. *Org. Lett.* **2001**, *3*, 1415. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Compound **227**

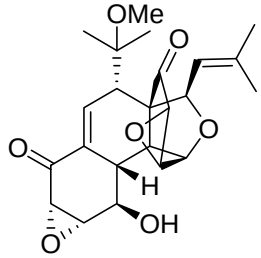


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
182.1	20.8062	181.5	174.0	180.8	183.1	MAE	1.6	5.6
164.0	37.4907	164.8	157.3	164.0	165.3	σ	0.9	2.3
156.7	44.1234	158.2	150.6	157.3	158.2	MaxErr	3.8	8.5
146.2	53.8462	148.5	140.9	147.5	147.8	R^2	0.9993	0.9991
145.6	54.9572	147.3	139.8	146.4	146.6	*m*	1.0	0.9
141.3	61.7531	140.5	133.0	139.6	139.4	*b*	2.0	2.4
133.7	69.5855	132.7	125.2	131.7	131.0	CMAE	1.1	1.4
124.1	75.2931	127.0	119.5	125.9	124.9	Cσ	0.8	0.7
120.5	80.3397	122.0	114.4	120.8	119.6	CMaxErr	2.4	2.7
119.5	80.7825	121.5	114.0	120.4	119.1			
119.3	81.3609	120.9	113.4	119.8	118.5			
114.6	86.9166	115.4	107.8	114.2	112.5			
24.7	170.6843	24.1	24.1	22.3	23.2			
20.4	172.8858	21.9	21.9	20.0	20.8			
17.5	173.4265	21.3	21.3	19.5	20.2			

[a] NMR data from: Kohno, J.; Hiramatsu, H.; Nishio, M.; Sakurai, M.; Okuda, T.; Komatsubara, S. *Tetrahedron* **1999**, *55*, 11247. Solvent: $CDCl_3$

[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Compound **228**

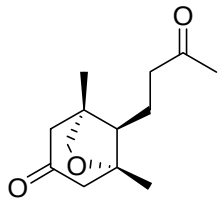


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
202.9	-3.7009	206.0	198.5	203.7	205.5	MAE	1.8	2.6
192.8	11.1239	191.2	183.6	189.0	190.0	σ	1.1	2.4
142.2	56.9577	145.3	137.8	143.7	141.9	MaxErr	4.0	9.2
139.6	63.8515	138.5	130.9	136.9	134.7	R^2	0.9987	0.9977
132.5	67.0470	135.3	127.7	133.8	131.4	*m*	1.0	1.0
120.7	77.5965	124.7	117.2	123.4	120.3	*b*	-0.2	2.4
77.3	115.9230	78.8	78.8	78.1	80.2	CMAE	1.5	2.1
75.8	116.4427	78.3	78.3	77.5	79.6	Cσ	1.0	1.3
72.7	119.5049	75.3	75.3	74.5	76.4	CMaxErr	3.8	4.9
71.5	122.1657	72.6	72.6	71.9	73.6			
61.0	131.7655	63.0	63.0	62.4	63.5			
60.5	134.3950	60.4	60.4	59.8	60.8			
54.5	136.6728	58.1	58.1	57.6	58.4			
53.2	140.6738	54.1	54.1	53.6	54.2			
53.1	142.3562	52.4	52.4	52.0	52.4			
49.1	146.3005	48.5	48.5	48.1	48.3			
47.8	148.7064	46.1	46.1	45.7	45.8			
40.9	152.1683	42.6	42.6	42.3	42.2			
40.4	157.2553	37.5	37.5	37.2	36.8			

26.6	167.7079	27.1	27.1	26.9	25.9
26.1	169.8633	24.9	24.9	24.8	23.6
24.7	171.6751	23.1	23.1	23.0	21.7
18.6	176.0648	18.7	18.7	18.7	17.1

[a] NMR data from: Rychnovsky, S. D. *Org. Lett.* **2006**, *8*, 2895. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

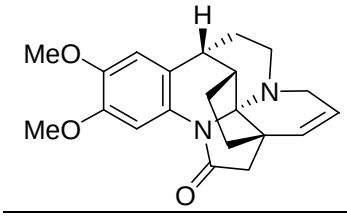
Compound **229**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
208.7	-3.7701	206.1	198.5	208.3	207.7	MAE	1.4	2.5
207.2	-3.3124	205.6	198.1	207.9	207.3	σ	0.9	3.3
83.4	111.2695	83.5	83.5	84.5	86.4	MaxErr	2.6	10.2
78.3	118.5477	76.2	76.2	77.1	78.7	R^2	0.9996	0.9994
53.1	141.7815	53.0	53.0	53.7	54.2	*m*	1.0	0.9
49.4	147.7749	47.0	47.0	47.6	47.8	*b*	-0.1	1.6
48.6	148.4833	46.3	46.3	46.9	47.1	CMAE	1.1	1.2
43.4	149.4956	45.3	45.3	45.9	46.0	Cσ	0.6	0.9
42.6	153.8775	40.9	40.9	41.4	41.4	CMaxErr	2.5	3.0
30.0	166.4368	28.3	28.3	28.8	28.2			
24.9	169.6695	25.1	25.1	25.5	24.7			
20.8	173.8491	20.9	20.9	21.3	20.3			
18.7	174.8466	19.9	19.9	20.3	19.3			

[a] NMR data from: Macías, F. A.; Varela, R. M.; Torres, A.; Oliva, R. M.; Molinillo, J. M. G. *Phytochemistry* **1997**, *48*, 631. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Compound **230**

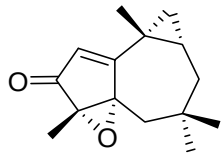


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
173.8	30.1763	172.1	164.6	171.6	174.1	MAE	1.5	3.6
147.7	53.8793	148.4	140.9	148.0	148.6	σ	0.8	3.1
145.3	57.9387	144.4	136.8	143.9	144.3	MaxErr	3.0	9.2
131.5	68.7824	133.5	126.0	133.1	132.6	R^2	0.9987	0.9991
131.0	68.8487	133.5	125.9	133.1	132.6	*m*	1.0	0.9
120.0	79.3761	122.9	115.4	122.6	121.2	*b*	-0.3	2.6
117.4	86.4110	115.9	108.4	115.6	113.7	CMAE	1.4	1.1
111.3	89.0073	113.3	105.8	113.0	110.9	Cσ	0.8	0.8
102.6	98.0712	104.2	96.7	104.0	101.1	CMaxErr	2.7	3.7
84.4	112.4753	82.3	82.3	82.2	85.6			
56.1	141.3245	53.4	53.4	53.4	54.6			
56.0	141.4011	53.4	53.4	53.4	54.5			
47.9	147.5019	47.3	47.3	47.3	48.0			
46.0	147.7231	47.0	47.0	47.1	47.7			
44.5	149.5726	45.2	45.2	45.2	45.8			
44.3	151.2204	43.5	43.5	43.6	44.0			

37.7	155.7480	39.0	39.0	39.1	39.1
36.6	159.1570	35.6	35.6	35.7	35.5
35.0	159.6566	35.1	35.1	35.2	34.9
26.8	168.0084	26.8	26.8	26.9	25.9
24.8	168.4256	26.3	26.3	26.5	25.5

[a] NMR data from: Hubbs, J. L.; Heathcock, C. H. *Org. Lett.* **1999**, *1*, 1315. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

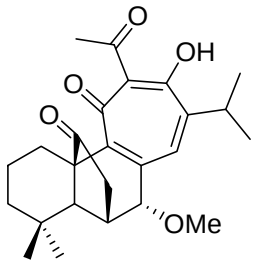
Compound **231**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
200.1	3.7982	198.5	191.0	198.1	198.8	MAE	1.8	2.9
180.0	22.3551	179.9	172.4	179.5	179.3	σ	1.2	2.5
128.5	70.5927	131.7	124.2	131.3	128.6	MaxErr	3.9	9.1
66.5	124.3685	70.4	70.4	69.9	72.0	R^2	0.9987	0.9983
60.8	130.7678	64.0	64.0	63.5	65.3	*m*	1.0	1.0
42.7	154.7498	40.0	40.0	39.5	40.0	*b*	0.5	1.9
34.5	157.5278	37.2	37.2	36.8	37.1	CMAE	1.8	1.8
34.2	162.6176	32.1	32.1	31.7	31.8	Cσ	1.0	1.6
30.8	165.7016	29.1	29.1	28.6	28.5	CMaxErr	3.4	5.5
28.9	167.2013	27.6	27.6	27.1	26.9			
26.5	168.8649	25.9	25.9	25.4	25.2			
23.3	171.3188	23.4	23.4	23.0	22.6			
21.3	172.7775	22.0	22.0	21.5	21.1			
19.5	173.5089	21.3	21.3	20.8	20.3			
8.4	184.8514	9.9	9.9	9.4	8.4			

[a] NMR data from: Tori, M.; Nakashima, K.; Toyota, M.; Asakawa, Y. *Tetrahedron Lett.* **1993**, *34*, 3751. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Compound **232**

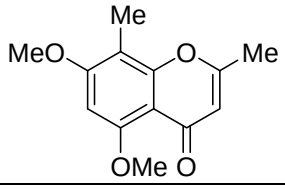


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
203.1	-1.6075	203.9	196.4	203.7	205.8	MAE	1.6	3.4
189.1	13.0602	189.2	181.7	189.0	190.2	σ	1.1	3.0
175.7	29.2826	173.0	165.5	172.8	173.0	MaxErr	4.0	10.2
175.4	29.5264	172.8	165.2	172.6	172.8	R^2	0.9991	0.9994
149.1	51.7629	150.5	143.0	150.3	149.2	*m*	1.0	0.9
146.6	53.6040	148.7	141.2	148.5	147.3	*b*	0.3	2.1
132.1	66.5595	135.7	128.2	135.5	133.6	CMAE	1.6	1.2
132.0	68.6464	133.7	126.1	133.4	131.4	Cσ	1.1	1.0
119.8	79.9005	122.4	114.9	122.2	119.4	CMaxErr	3.7	3.9
79.5	117.3684	77.4	77.4	77.1	79.8			
73.0	124.0912	70.7	70.7	70.4	72.6			
59.2	138.4441	56.3	56.3	56.0	57.4			
50.2	145.6272	49.1	49.1	48.8	49.8			
45.8	147.7844	47.0	47.0	46.7	47.5			

38.1	157.9442	36.8	36.8	36.5	36.8
31.3	159.4268	35.3	35.3	35.0	35.2
31.3	162.2297	32.5	32.5	32.2	32.2
30.2	164.2799	30.5	30.5	30.2	30.1
28.1	165.1228	29.6	29.6	29.3	29.2
26.4	168.0698	26.7	26.7	26.4	26.1
22.8	171.1878	23.6	23.6	23.3	22.8
22.3	172.8999	21.9	21.9	21.6	20.9
21.9	173.7299	21.0	21.0	20.7	20.1
18.6	175.2689	19.5	19.5	19.2	18.4

[a] NMR data from: Yang, J.; Huang, S. X.; Zhao, Q. S. *J. Phys. Chem. A* **2008**, *112*, 12132. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

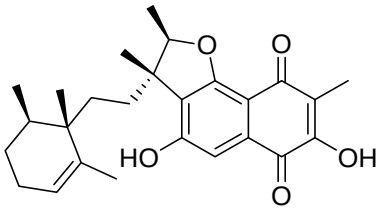
Compound **233**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
177.6	29.4907	172.8	165.3	173.9	175.4	MAE	2.2	5.7
162.6	41.5660	160.7	153.2	161.7	162.5	σ	1.7	3.8
160.7	43.9604	158.3	150.8	159.2	159.9	MaxErr	5.9	12.3
158.5	44.9216	157.4	149.8	158.3	158.9	R^2	0.9976	0.9988
156.5	45.0006	157.3	149.8	158.2	158.8	*m*	1.0	0.9
110.9	85.5083	116.8	109.3	117.2	115.4	*b*	1.1	1.7
108.0	90.8354	111.5	103.9	111.8	109.6	CMAE	2.1	1.5
105.3	97.1046	105.2	97.7	105.4	102.9	Cσ	1.8	1.3
91.1	110.4072	91.9	84.4	91.9	88.7	CMaxErr	6.3	4.5
56.0	141.6843	53.1	53.1	52.6	55.1			
55.4	141.8337	52.9	52.9	52.5	55.0			
19.4	175.2267	19.5	19.5	18.6	19.2			
7.3	185.6094	9.2	9.2	8.1	8.0			

[a] NMR data from: Kalinin, A. V.; Snieckus, V. *Tetrahedron Lett.* **1998**, *39*, 4999. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Compound **234**

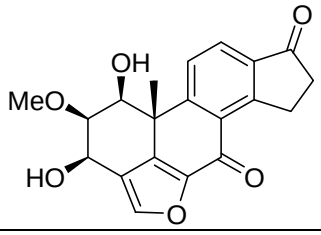


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
182.9	19.3184	183.0	175.4	182.3	184.3	MAE	1.8	3.6
180.4	20.5930	181.7	174.2	181.0	183.0	σ	1.4	3.3
159.9	41.1029	161.2	153.7	160.4	161.0	MaxErr	4.4	11.9
157.7	48.9832	153.3	145.8	152.5	152.6	R^2	0.9989	0.9988
153.6	51.8373	150.5	142.9	149.6	149.6	*m*	1.0	0.9
138.9	60.9977	141.3	133.8	140.4	139.8	*b*	1.6	2.9
131.6	70.3598	131.9	124.4	131.0	129.8	CMAE	1.5	1.6
127.3	71.2209	131.1	123.5	130.1	128.9	Cσ	1.3	1.3
123.9	74.3791	127.9	120.4	126.9	125.5	CMaxErr	5.2	5.1
120.3	79.1291	123.2	115.6	122.2	120.4			
107.9	90.3443	112.0	104.4	110.9	108.4			
107.9	93.1502	109.2	101.6	108.1	105.4			

86.3	108.0774	86.7	86.7	85.5	89.5
46.0	144.7347	50.0	50.0	48.6	50.3
39.7	152.7974	42.0	42.0	40.5	41.7
32.8	160.7716	34.0	34.0	32.5	33.2
31.0	163.3838	31.4	31.4	29.9	30.4
30.5	164.2705	30.5	30.5	29.0	29.4
26.6	167.7424	27.0	27.0	25.5	25.7
25.1	168.0664	26.7	26.7	25.2	25.4
20.9	172.8848	21.9	21.9	20.3	20.2
19.7	173.6719	21.1	21.1	19.5	19.4
18.8	173.8413	20.9	20.9	19.4	19.2
15.7	178.8594	15.9	15.9	14.3	13.8
15.1	179.7841	15.0	15.0	13.4	12.9
8.6	183.1350	11.6	11.6	10.0	9.3

[a] NMR data from: Kalaitzis, J. A.; Hamano, Y.; Nilsen, G.; Moore, B. S. *Org. Lett.* **2003**, *5*, 4449. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

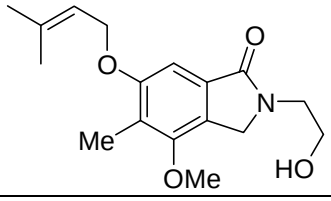
Compound **235**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
206.7	-1.9904	204.3	196.8	204.0	207.4	MAE	1.2	4.5
173.4	28.9655	173.3	165.8	173.0	174.2	σ	0.8	3.1
158.6	42.5775	159.7	152.2	159.3	159.6	MaxErr	2.4	9.9
158.0	44.7768	157.5	150.0	157.1	157.2	R^2	0.9993	0.9993
145.7	54.2655	148.0	140.5	147.6	147.0	*m*	1.0	0.9
145.6	54.6878	147.6	140.1	147.2	146.6	*b*	0.9	3.5
142.4	60.6212	141.7	134.1	141.2	140.2	CMAE	1.1	1.1
136.9	65.0273	137.3	129.7	136.8	135.5	Cσ	0.7	0.7
129.8	70.6802	131.6	124.1	131.1	129.4	CMaxErr	2.7	2.6
127.3	73.0029	129.3	121.8	128.8	126.9			
127.3	74.0714	128.2	120.7	127.7	125.8			
122.1	78.6625	123.6	116.1	123.1	120.9			
81.7	114.2815	80.5	80.5	79.8	82.6			
71.7	122.2653	72.5	72.5	71.8	74.1			
62.6	130.9958	63.8	63.8	63.1	64.7			
60.7	134.4131	60.3	60.3	59.6	61.0			
42.3	152.6353	42.1	42.1	41.4	41.5			
36.5	159.7015	35.1	35.1	34.3	33.9			
30.5	162.9483	31.8	31.8	31.0	30.4			
28.4	163.9387	30.8	30.8	30.0	29.3			

[a] NMR data from: Wipf, P.; Kerekes, A. D. *J. Nat. Prod.* **2003**, *66*, 716. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

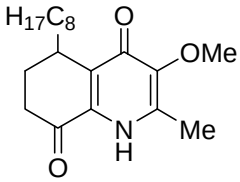
Compound **236**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
167.5	37.7269	164.6	157.0	164.1	165.1	MAE	2.2	4.2
158.7	44.9130	157.4	149.8	156.9	157.4	σ	1.6	3.0
152.4	49.7488	152.6	145.0	152.1	152.2	MaxErr	5.5	10.5
138.0	64.5555	137.7	130.2	137.2	136.2	R^2	0.9975	0.9975
132.2	68.8002	133.5	126.0	133.0	131.7	*m*	1.0	0.9
125.1	73.7094	128.6	121.1	128.0	126.4	*b*	0.9	3.5
121.8	77.2034	125.1	117.6	124.5	122.6	CMAE	2.1	2.1
120.5	77.2556	125.0	117.5	124.5	122.6	Cσ	1.5	1.5
99.7	97.0482	97.7	97.7	97.1	101.3	CMaxErr	4.8	6.7
68.7	128.8899	65.9	65.9	65.1	67.1			
59.7	129.5389	65.2	65.2	64.5	66.4			
56.4	135.4217	59.3	59.3	58.6	60.1			
49.2	144.1763	50.6	50.6	49.8	50.6			
45.1	152.5521	42.2	42.2	41.4	41.6			
26.0	169.2711	25.5	25.5	24.6	23.7			
18.5	175.9085	18.9	18.9	18.0	16.5			
10.2	183.6119	11.1	11.2	10.2	8.3			

[a] NMR data from: Cornella, I.; Kelly, T. R. *J. Org. Chem.* **2004**, *69*, 2191. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

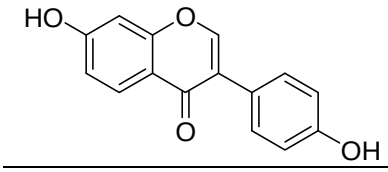
Compound **237**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
194.6	5.5042	196.8	189.3	197.1	199.3	MAE	1.2	3.2
172.8	28.5562	173.7	166.2	173.9	174.8	σ	1.0	3.4
147.5	54.5629	147.7	140.2	147.8	147.1	MaxErr	3.7	11.2
139.0	64.1688	138.1	130.6	138.2	136.9	R^2	0.9994	0.9989
138.9	67.1013	135.2	127.7	135.2	133.7	*m*	1.0	0.9
132.2	70.4040	131.9	124.4	131.9	130.2	*b*	0.5	2.0
59.4	138.0943	56.7	56.7	56.4	58.2	CMAE	1.1	1.5
32.2	161.9352	32.8	32.8	32.5	32.8	Cσ	1.0	1.4
31.8	162.9636	31.8	31.8	31.4	31.7	CMaxErr	3.7	5.2
30.5	162.9740	31.8	31.8	31.4	31.7			
30.3	163.4778	31.3	31.3	30.9	31.2			
29.6	164.0477	30.7	30.7	30.3	30.6			
29.5	164.2636	30.5	30.5	30.1	30.4			
29.2	165.5369	29.2	29.2	28.8	29.0			
28.4	165.8400	28.9	28.9	28.5	28.7			
24.3	169.3594	25.4	25.4	25.0	24.9			
22.6	169.8406	24.9	24.9	24.5	24.4			
14.5	179.3198	15.4	15.4	15.0	14.3			
14.0	182.1176	12.6	12.6	12.2	11.4			

[a] NMR data from: Bringmann, J.; Schlauer, H.; Rischer, H.; Wohlfarth, J.; Mühlbacher, J.; Buske, A.; Porzel, A.; Schmidt, J.; Adam, G. *Tetrahedron* **2000**, *56*, 3691. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

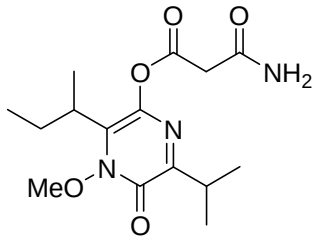
Compound **238**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
174.8	28.3442	174.0	166.4	176.1	176.1	MAE	2.5	6.9
162.8	43.8996	158.4	150.9	159.4	159.4	σ	1.8	3.1
157.6	45.6645	156.6	149.1	157.5	157.5	MaxErr	6.1	11.9
157.2	47.1886	155.1	147.6	155.9	155.9	R^2	0.9847	0.9847
152.9	50.8224	151.5	143.9	152.0	152.0	*m*	0.9	0.9
130.1	69.8424	132.5	124.9	131.6	131.6	*b*	9.8	2.3
127.3	70.9600	131.3	123.8	130.4	130.4	CMAE	2.4	2.4
123.6	72.6032	129.7	122.2	128.6	128.6	Cσ	1.4	1.4
122.6	76.4599	125.8	118.3	124.5	124.5	CMaxErr	5.0	5.0
116.6	81.2736	121.0	113.5	119.3	119.3			
115.3	87.5129	114.8	107.3	112.6	112.6			
115.0	87.8910	114.4	106.9	112.2	112.2			
102.2	101.2896	101.0	93.5	97.8	97.8			

[a] NMR data from: Suzuki, K.; Yahara, S.; Kazutomo, M.; Uyeda, M. *J. Nat. Prod.* **2001**, *64*, 204. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

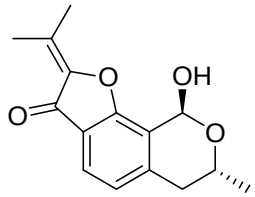
Compound **239**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
168.0	30.9124	171.4	163.9	171.3	172.1	MAE	1.4	3.8
166.0	37.6254	164.7	157.1	164.6	165.0	σ	1.2	3.3
161.5	42.5826	159.7	152.2	159.6	159.8	MaxErr	4.4	9.3
152.0	50.8724	151.4	143.9	151.4	151.0	R^2	0.9991	0.9991
135.0	66.2177	136.1	128.5	136.1	134.8	*m*	1.0	0.9
134.9	66.6795	135.6	128.1	135.6	134.3	*b*	-0.4	1.2
64.1	132.7004	62.1	62.1	62.3	64.4	CMAE	1.4	1.3
41.1	158.1009	36.7	36.7	36.9	37.6	Cσ	1.2	1.3
33.7	160.3541	34.4	34.4	34.7	35.2	CMaxErr	4.2	4.1
30.7	161.4326	33.3	33.3	33.6	34.0			
27.5	167.5668	27.2	27.2	27.5	27.5			
19.9	175.5367	19.2	19.2	19.6	19.1			
19.9	175.7725	19.0	19.0	19.3	18.9			
18.2	175.8554	18.9	18.9	19.2	18.8			
12.6	181.7229	13.0	13.0	13.4	12.6			

[a] NMR data from: Kita, M.; Miwa, R.; Widianti, T.; Ozaki, Y.; Aoyama, S.; Yamada, K.; Uemura, D. *Tetrahedron Lett.* **2007**, *48*, 8628. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

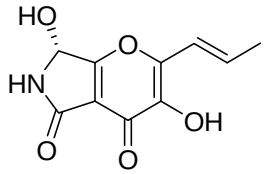
Compound **240**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
182.5	18.8789	183.4	175.9	181.0	183.2	MAE	1.5	3.8
162.5	40.2912	162.0	154.5	160.0	160.8	σ	1.1	2.7
144.5	55.1196	147.2	139.6	145.4	145.2	MaxErr	4.3	8.0
142.0	57.9624	144.3	136.8	142.6	142.3	R^2	0.9995	0.9988
131.1	69.8599	132.4	124.9	130.9	129.8	*m*	1.0	1.0
122.7	75.3075	127.0	119.5	125.5	124.1	*b*	-0.6	1.1
122.5	77.3963	124.9	117.4	123.5	121.9	CMAE	0.9	1.4
122.0	79.0578	123.2	115.7	121.8	120.1	Cσ	0.9	1.2
119.1	81.8804	120.4	112.9	119.1	117.2	CMaxErr	2.8	4.9
87.5	105.5416	89.2	89.2	88.4	92.4			
62.2	131.8708	62.9	62.9	62.5	64.8			
36.5	158.6533	36.1	36.1	36.1	36.7			
21.0	174.0808	20.7	20.7	20.9	20.5			
20.1	175.0954	19.7	19.7	19.9	19.4			
17.0	179.4505	15.3	15.3	15.6	14.9			

[a] NMR data from: Lin, W. H.; Brauers, G.; Ebel, R.; Wray, V.; Berg, A.; Surdasono; Proksch, P. *J. Nat. Prod.* **2003**, *66*, 57. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

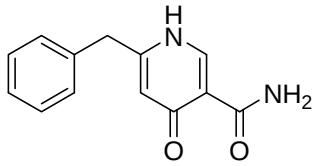
Compound **241**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
174.2	29.3946	172.9	165.4	173.9	175.3	MAE	2.2	6.1
169.1	35.1557	167.1	159.6	168.0	169.0	σ	1.6	3.8
165.0	43.1445	159.2	151.6	159.7	160.2	MaxErr	5.8	13.4
146.0	56.4226	145.9	138.3	146.1	145.7	R^2	0.9973	0.9979
142.2	57.3294	145.0	137.4	145.2	144.7	*m*	1.0	0.9
131.7	68.0859	134.2	126.7	134.1	133.0	*b*	3.8	4.9
118.9	81.2191	121.1	113.5	120.6	118.7	CMAE	1.9	1.5
111.7	87.5582	114.7	107.2	114.1	111.7	Cσ	1.5	1.5
75.2	118.6337	76.1	76.1	74.4	77.8	CMaxErr	5.3	4.8
18.7	174.6933	20.1	20.1	16.7	16.6			

[a] NMR data from: Hiort, J.; Maksimenka, K.; Reichert, M.; Perovi-Ottstadt, S.; Lin, W. H.; Wray, V.; Steube, K.; Schaumann, K.; Weber, H.; Proksch, P.; Ebel, R.; Müller, W. E. G.; Bringmann, G. *J. Nat. Prod.* **2004**, *67*, 1532. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

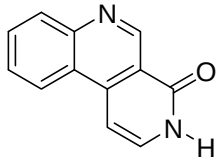
Compound **242**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
178.1	27.3977	174.9	167.4	178.3	180.5	MAE	2.4	7.7
165.9	41.5343	160.8	153.2	163.2	164.5	σ	1.9	3.4
151.2	57.5926	144.7	137.2	146.1	146.4	MaxErr	6.5	14.0
142.2	61.4252	140.9	133.3	142.0	142.0	R^2	0.9942	0.9964
137.4	66.8599	135.4	127.9	136.2	135.9	*m*	0.9	0.9
129.3	71.4612	130.8	123.3	131.3	130.7	*b*	7.8	7.9
129.3	72.2056	130.1	122.6	130.5	129.8	CMAE	1.9	1.5
129.2	72.7891	129.5	122.0	129.9	129.2	Cσ	1.5	1.3
129.2	73.1432	129.2	121.6	129.5	128.8	CMaxErr	5.1	4.8
127.5	73.5759	128.7	121.2	129.0	128.3			
118.9	79.8826	122.4	114.9	122.3	121.1			
118.0	80.8047	121.5	114.0	121.3	120.1			
38.2	154.1227	40.6	40.6	35.0	37.1			

[a] NMR data from: Hiort, J.; Maksimenka, K.; Reichert, M.; Perovi-Ottstadt, S.; Lin, W. H.; Wray, V.; Steube, K.; Schaumann, K.; Weber, H.; Proksch, P.; Ebel, R.; Müller, W. E. G.; Bringmann, G. *J. Nat. Prod.* **2004**, *67*, 1532. Solvent: DMSO-d_6
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

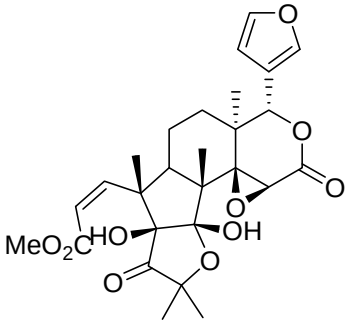
Compound **243**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
164.0	43.7550	158.5	151.0	161.1	161.1	MAE	1.5	8.3
150.5	50.2905	152.0	144.5	154.1	154.1	σ	1.6	2.1
148.5	53.3551	148.9	141.4	150.8	150.8	MaxErr	5.5	13.0
144.3	60.3914	141.9	134.4	143.3	143.3	R^2	0.9865	0.9865
136.0	69.6855	132.6	125.1	133.4	133.4	*m*	0.9	0.9
132.8	69.9239	132.4	124.8	133.1	133.1	*b*	8.0	0.4
130.4	71.7472	130.6	123.0	131.1	131.1	CMAE	1.5	1.5
128.7	75.0568	127.2	119.7	127.6	127.6	Cσ	1.2	1.2
125.0	77.5099	124.8	117.3	125.0	125.0	CMaxErr	3.6	3.6
123.6	78.8246	123.5	115.9	123.6	123.6			
118.7	81.6849	120.6	113.1	120.5	120.5			
101.6	100.3570	101.9	94.4	100.5	100.5			

[a] NMR data from: Morita, H.; Sato, Y.; Chan, K. L.; Choo, C. Y.; Itokawa, H.; Takeya, K.; Kobayashi, J. *J. Nat. Prod.* **2000**, *63*, 1707. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Compound **244**

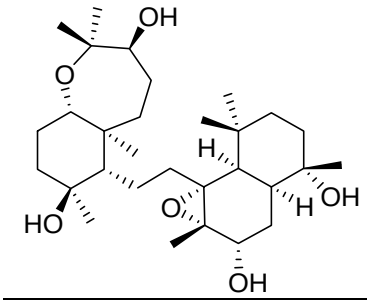


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
216.9	-18.9922	221.3	213.8	221.1	223.9	MAE	2.6	3.6
167.8	34.0606	168.2	160.7	167.2	166.9	σ	2.3	2.8
166.7	37.4170	164.9	157.3	163.8	163.3	MaxErr	7.9	9.4
153.9	48.0290	154.3	146.7	153.1	151.9	R^2	0.9979	0.9980
143.0	58.1226	144.2	136.6	142.8	141.0	*m*	1.0	0.9
141.1	59.8136	142.5	134.9	141.1	139.2	*b*	3.4	5.4
123.1	76.9686	125.3	117.8	123.7	120.8	CMAE	2.0	2.0
121.0	78.0141	124.3	116.7	122.6	119.6	Cσ	1.7	1.4
109.9	84.5492	117.8	110.2	116.0	112.6	CMaxErr	6.1	7.0
108.2	89.5550	105.2	105.2	103.3	107.2			
88.6	105.7589	89.0	89.0	86.8	89.8			
80.9	112.2503	82.5	82.5	80.2	82.9			
78.4	116.2291	78.5	78.5	76.2	78.6			
68.5	125.4609	69.3	69.3	66.8	68.7			
57.3	136.9628	57.8	57.8	55.2	56.3			
52.0	140.2896	54.5	54.5	51.8	52.7			
49.9	141.9575	52.8	52.8	50.1	50.9			
49.7	142.1548	52.6	52.6	49.9	50.7			
46.8	144.3988	50.4	50.4	47.6	48.3			
39.5	155.4098	39.4	39.4	36.4	36.5			
27.4	163.0675	31.7	31.7	28.7	28.2			
26.3	167.9232	26.8	26.8	23.7	23.0			
24.1	168.2460	26.5	26.5	23.4	22.7			
18.3	169.9359	24.8	24.8	21.7	20.9			
17.3	170.5084	24.3	24.3	21.1	20.2			
15.2	171.9747	22.8	22.8	19.6	18.7			
14.7	179.0993	15.7	15.7	12.4	11.0			

[a] NMR data from: Kubo, I.; Tanis, S. P.; Lee, Y. W.; Miura, I.; Nakanishi, K.; Chapya, A. *Heterocycles* **1976**, *5*, 485. Solvent: $CDCl_3$

[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

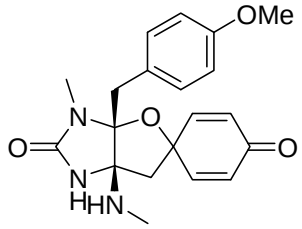
Compound **245**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
77.8	117.1785	77.6	77.6	76.8	76.8	MAE	1.4	1.4
77.2	118.1173	76.6	76.6	75.8	75.8	σ	1.0	1.0
76.8	118.7940	76.0	76.0	75.2	75.2	MaxErr	5.0	5.0
72.7	120.1449	74.6	74.6	73.9	73.9	R^2	0.9929	0.9929
72.2	120.3522	74.4	74.4	73.7	73.7	*m*	1.0	1.0
70.0	121.2606	73.5	73.5	72.8	72.8	*b*	-1.0	-1.0
69.5	122.6429	72.1	72.1	71.4	71.4	CMAE	1.3	1.3
65.7	126.3783	68.4	68.4	67.8	67.8	Cσ	1.0	1.0
55.7	144.0972	50.7	50.7	50.5	50.5	CMaxErr	5.2	5.2
42.9	150.6464	44.1	44.1	44.1	44.1			
40.2	155.3702	39.4	39.4	39.4	39.4			
39.3	156.9697	37.8	37.8	37.9	37.9			
39.2	157.0884	37.7	37.7	37.8	37.8			
38.0	157.7135	37.0	37.0	37.2	37.2			
36.7	158.5453	36.2	36.2	36.3	36.3			
35.6	160.7201	34.0	34.0	34.2	34.2			
34.5	160.8679	33.9	33.9	34.1	34.1			
31.8	162.2498	32.5	32.5	32.7	32.7			
31.3	162.3189	32.4	32.4	32.7	32.7			
30.4	163.3598	31.4	31.4	31.6	31.6			
30.2	163.9602	30.8	30.8	31.0	31.0			
29.5	165.5543	29.2	29.2	29.5	29.5			
29.2	166.3276	28.4	28.4	28.7	28.7			
26.8	166.5176	28.2	28.2	28.5	28.5			
25.4	170.2214	24.5	24.5	24.9	24.9			
25.3	171.5411	23.2	23.2	23.6	23.6			
21.4	171.6582	23.1	23.1	23.5	23.5			
21.0	174.4587	20.3	20.3	20.8	20.8			
16.8	178.5481	16.2	16.2	16.8	16.8			
13.4	179.1510	15.6	15.6	16.2	16.2			

[a] NMR data from: Jain, S.; Laphookhieo, S.; Shi, Z.; Fu, L. W.; Akiyama, S.; Chen, Z. S.; Youssef, D. T. A.; von Soest, R. W. M.; El Sayed, K. A. *J. Nat. Prod.* **2007**, *70*, 928. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Compound **246**

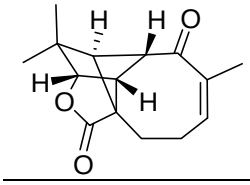


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
185.4	20.1853	182.1	174.6	183.5	186.0	MAE	1.9	5.3
159.5	45.1476	157.2	149.6	158.1	158.6	σ	1.5	3.7
158.9	49.8735	152.4	144.9	153.3	153.5	MaxErr	6.5	14.0

151.0	51.6576	150.6	143.1	151.4	151.5	R^2	0.9977	0.9979
150.1	51.6770	150.6	143.1	151.4	151.5	*m*	1.0	0.9
132.8	66.3650	135.9	128.4	136.4	135.4	*b*	2.2	4.9
132.8	68.9319	133.4	125.8	133.8	132.6	CMAE	1.8	1.7
127.5	73.5379	128.8	121.2	129.1	127.5	Cσ	1.3	1.4
126.9	73.6097	128.7	121.2	129.0	127.4	CMaxErr	5.6	5.4
125.9	74.0224	128.3	120.7	128.6	127.0			
112.7	88.5492	113.8	106.2	113.8	111.1			
112.7	88.9302	113.4	105.8	113.4	110.6			
102.5	92.6650	102.1	102.1	101.9	106.6			
82.5	115.4443	79.3	79.3	78.7	81.6			
77.1	115.9706	78.8	78.8	78.2	81.0			
54.2	142.1042	52.7	52.7	51.5	52.4			
46.9	145.8669	48.9	48.9	47.7	48.2			
37.1	157.9291	36.8	36.8	35.4	35.0			
24.7	166.6599	28.1	28.1	26.5	25.5			
24.5	169.0885	25.7	25.7	24.0	22.8			

[a] NMR data from: Ralifo, P.; Crews, P. *J. Org. Chem.* **2004**, *69*, 9025. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

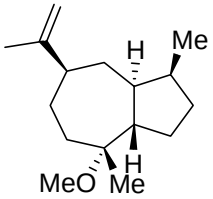
Compound **247**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
211.9	-11.6054	213.9	206.4	213.4	215.0	MAE	1.2	2.3
177.5	27.3875	174.9	167.4	174.5	174.0	σ	1.1	3.1
135.1	63.0727	139.2	131.7	138.9	136.5	MaxErr	4.1	10.1
131.1	71.3693	130.9	123.4	130.7	127.8	R^2	0.9993	0.9992
84.2	112.7061	82.1	82.1	81.9	84.4	*m*	1.0	1.0
62.8	132.7481	62.0	62.0	62.0	63.3	*b*	-0.2	1.7
62.6	133.0980	61.7	61.7	61.6	63.0	CMAE	1.2	1.3
54.5	139.8695	54.9	54.9	54.9	55.8	Cσ	1.1	1.1
54.5	140.4665	54.3	54.3	54.3	55.2	CMaxErr	3.8	3.5
41.9	152.0027	42.8	42.8	42.8	43.1			
28.6	165.3450	29.4	29.4	29.5	29.1			
22.8	170.6742	24.1	24.1	24.2	23.5			
22.6	172.2767	22.5	22.5	22.6	21.8			
22.2	172.7570	22.0	22.0	22.1	21.3			
22.2	173.3873	21.4	21.4	21.5	20.6			

[a] NMR data from: Lodewyk, M. W.; Soldi, C.; Jones, P. B.; Olmstead, M. M.; Rita, J.; Shaw, J. T.; Dean J. Tantillo, D. J. *J. Am. Chem. Soc.* **2012**, *134*, 18550. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Compound **222**

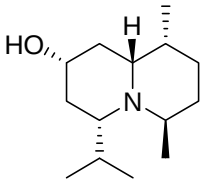


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
152.4	50.5694	151.7	144.2	150.6	150.4	MAE	0.9	1.4
108.4	89.7769	112.5	105.0	111.7	108.9	σ	1.0	2.0
77.1	117.3927	77.4	77.4	76.8	79.6	MaxErr	4.1	8.2

54.7	141.1216	53.6	53.6	53.2	54.5	R^2	0.9987	0.9985
49.4	143.8317	50.9	50.9	50.5	51.6	*m*	1.0	0.9
49.4	146.1449	48.6	48.6	48.2	49.1	*b*	0.0	2.2
41.1	153.2741	41.5	41.5	41.2	41.6	CMAE	0.9	1.1
39.2	154.5777	40.2	40.2	39.9	40.2	Cσ	0.9	0.8
37.7	156.4869	38.3	38.3	38.0	38.2	CMaxErr	3.3	2.5
37.4	157.4371	37.3	37.3	37.0	37.2			
34.2	160.0662	34.7	34.7	34.4	34.4			
27.6	166.9664	27.8	27.8	27.6	27.1			
25.4	167.3834	27.4	27.4	27.2	26.6			
24.1	171.6299	23.1	23.1	22.9	22.1			
21.2	174.4508	20.3	20.3	20.1	19.2			
15.3	179.2945	15.5	15.5	15.3	14.0			

[a] NMR data from: Booker-Milburn, K. I.; Jankins, H.; Charmant, J. P. H.; Mohr, P. *Org. Lett.* **2003**, *5*, 3309. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

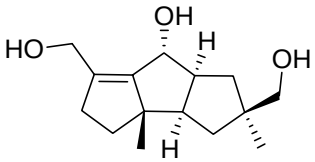
Compound **223**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
69.8	126.8242	67.9	67.9	70.5	70.5	MAE	1.1	1.1
61.8	136.5772	58.2	58.2	60.3	60.3	σ	1.1	1.1
55.4	142.0165	52.7	52.7	54.6	54.6	MaxErr	3.6	3.6
47.9	146.6811	48.1	48.1	49.7	49.7	R^2	0.9976	0.9976
41.7	155.4109	39.3	39.4	40.6	40.6	*m*	1.0	1.0
35.0	160.5561	34.2	34.2	35.2	35.2	*b*	0.5	0.5
34.4	161.4069	33.4	33.4	34.3	34.3	CMAE	0.7	0.7
27.9	166.3422	28.4	28.4	29.2	29.2	Cσ	0.5	0.5
27.8	167.2947	27.5	27.5	28.2	28.2	CMaxErr	1.8	1.8
27.1	167.8075	27.0	27.0	27.7	27.7			
20.6	174.9906	19.8	19.8	20.1	20.1			
15.0	180.5796	14.2	14.2	14.3	14.3			
14.1	180.7766	14.0	14.0	14.1	14.1			
8.2	186.8441	7.9	7.9	7.8	7.8			

[a] NMR data from: Comins, D. L.; Zheng, X.; Goehring, R. R. *Org. Lett.* **2002**, *4*, 1611. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Compound **224**

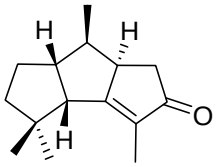


δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
153.3	50.4210	151.9	144.3	149.3	148.5	MAE	1.8	1.8
130.0	63.5163	138.8	131.2	136.4	134.8	σ	2.2	2.3
75.8	118.7371	76.0	76.0	75.0	77.0	MaxErr	8.8	9.0
71.7	126.2293	68.5	68.5	67.6	69.2	R^2	0.9948	0.9951
61.6	134.2051	60.6	60.6	59.8	60.8	*m*	1.0	1.0
55.8	135.6311	59.1	59.1	58.4	59.3	*b*	-0.5	2.4
55.6	136.0680	58.7	58.7	58.0	58.9	CMAE	1.9	2.1
50.4	143.1958	51.6	51.6	51.0	51.4	Cσ	1.8	1.4
48.5	145.9405	48.8	48.8	48.3	48.6	CMaxErr	6.4	4.8

41.8	153.1194	41.6	41.6	41.3	41.0
41.6	154.2071	40.6	40.6	40.2	39.9
36.3	156.1251	38.6	38.6	38.3	37.9
35.7	160.1867	34.6	34.6	34.4	33.6
22.7	171.8643	22.9	22.9	22.9	21.4
22.4	172.4682	22.3	22.3	22.3	20.8

[a] NMR data from: Mehta, G.; Pallavi, K. *Tetrahedron Lett.* **2006**, *47*, 8355. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

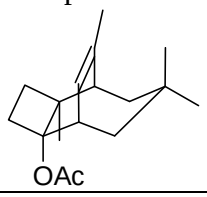
Compound **225**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
211.8	-4.4404	206.7	199.2	210.0	211.1	MAE	1.8	2.8
183.9	22.9467	179.4	171.8	182.0	181.7	σ	1.6	4.0
134.4	63.9673	138.3	130.8	140.1	137.5	MaxErr	5.0	12.6
54.4	141.0818	53.7	53.7	53.5	54.5	R^2	0.9988	0.9991
53.4	141.5404	53.2	53.2	53.0	54.1	*m*	1.0	0.9
46.2	146.1256	48.6	48.6	48.3	49.1	*b*	1.4	3.0
44.9	147.7869	47.0	47.0	46.6	47.3	CMAE	1.6	1.5
41.9	152.5668	42.2	42.2	41.7	42.2	Cσ	1.3	1.1
39.2	154.5525	40.2	40.2	39.7	40.1	CMaxErr	5.6	3.1
36.9	158.6938	36.1	36.1	35.5	35.6			
32.4	161.3607	33.4	33.4	32.7	32.7			
30.1	166.6240	28.1	28.1	27.3	27.1			
25.8	169.4494	25.3	25.3	24.5	24.0			
15.1	179.6744	15.1	15.1	14.0	13.0			
9.1	182.9250	11.8	11.8	10.7	9.5			

[a] NMR data from: Mehta, G.; Murthy, S. K.; Umarye, J. D. *Tetrahedron Lett.* **2002**, *43*, 8301. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Compound **226**



δ_{exp} [a]	Shielding Values[b]	$\delta_{calc,MSTD}$	$\delta_{calc,TMS}$	$\delta_{scaled,MSTD}$	$\delta_{scaled,TMS}$		MSTD	TMS
169.6	34.4395	167.9	160.3	166.8	167.4	MAE	1.4	2.0
141.5	58.8498	143.5	135.9	142.7	141.7	σ	1.0	2.3
122.2	76.1087	126.2	118.7	125.6	123.5	MaxErr	4.0	9.3
85.3	109.3460	85.4	85.4	85.2	88.5	R^2	0.9987	0.9988
49.3	147.3374	47.4	47.4	47.6	48.5	*m*	1.0	0.9
45.3	148.6484	46.1	46.1	46.3	47.1	*b*	-0.7	1.4
38.7	156.1153	38.6	38.6	38.9	39.3	CMAE	1.3	1.3
36.7	159.9136	34.8	34.8	35.2	35.3	Cσ	0.8	0.8
35.7	161.0280	33.7	33.7	34.1	34.1	CMaxErr	3.4	3.2
35.6	161.1697	33.6	33.6	33.9	33.9			
34.2	161.9901	32.8	32.8	33.1	33.1			
31.8	162.0928	32.7	32.7	33.0	33.0			
29.4	163.8572	30.9	30.9	31.3	31.1			
28.6	165.4466	29.3	29.3	29.7	29.4			
23.9	170.2364	24.5	24.5	25.0	24.4			

21.8	173.1491	21.6	21.6	22.1	21.3
21.6	174.6482	20.1	20.1	20.6	19.7

[a] NMR data from: Inanaga, K.; Takasu, K.; Ihara, M. *J. Am. Chem. Soc.* **2004**, *126*, 1352. Solvent: $CDCl_3$
[b] Computed at the mPW1PW91/6-31G(d)//HF/3-21G level of theory

Case study: structural revision of aquatolide

In Figure S-3 are shown the originally proposed structure of aquatolide (**221**), the revised structure (**247**) and 45 of the many alternative (incorrect) structures for aquatolide that were randomly selected (compounds **248**-**292**).

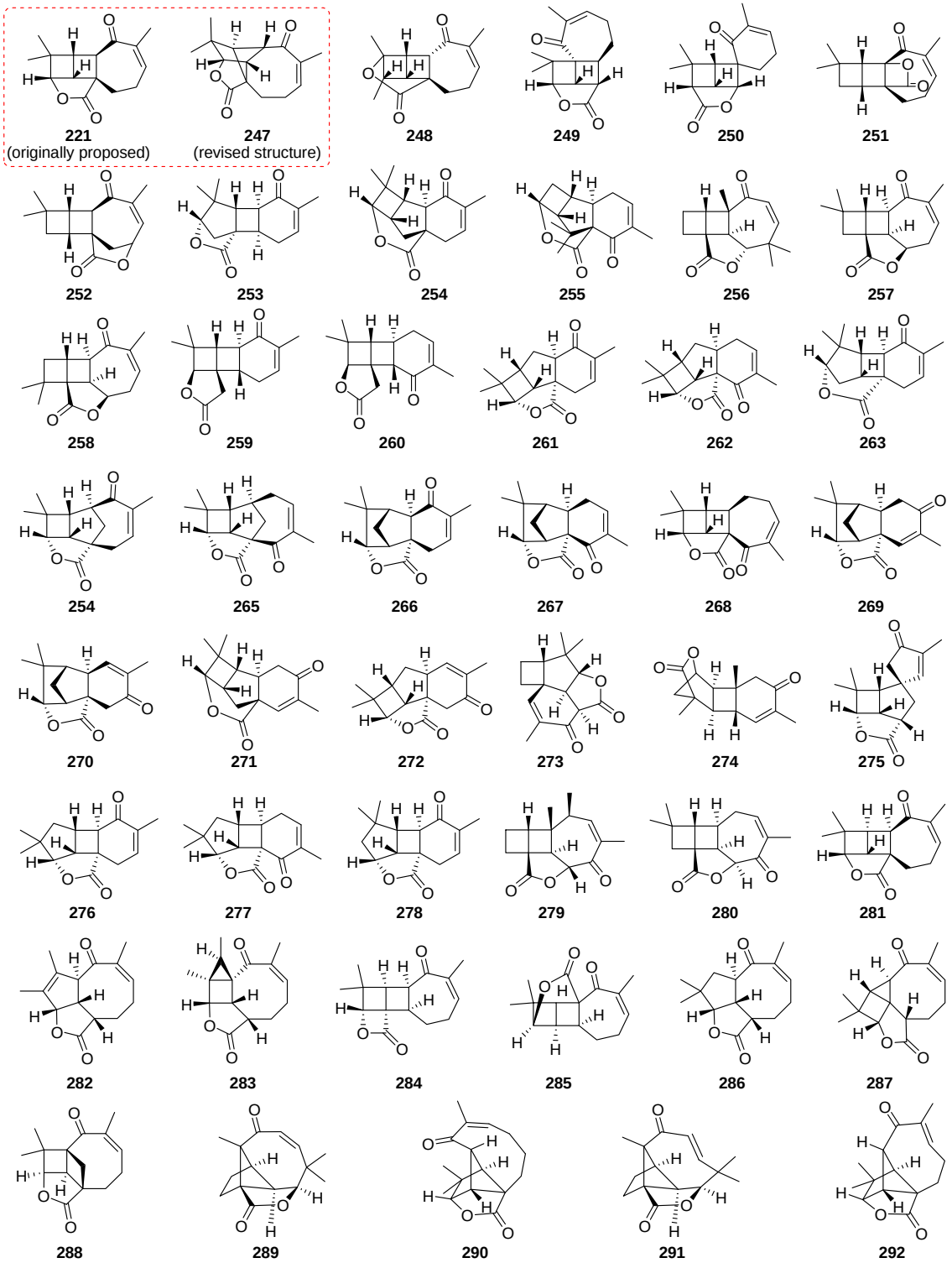


Figure S-3

mPW1PW91/6-31G(d)//MM+ Boltzmann-averaged GIAO NMR isotropic magnetic shielding values calculated for compounds **221** and **247**-**292**

221	**247**	**248**	**249**	**250**	**251**	**252**	**253**	**254**
-7.1784	-17.3624	-0.8958	-9.3657	-7.7209	-8.3057	-6.9303	-0.0407	-0.0853
12.6830	18.3055	22.6594	15.3178	19.4097	17.9987	14.8111	15.6561	22.1203
56.2387	59.6197	52.6675	56.8734	59.2437	58.2523	53.0209	54.0659	53.9375
57.4413	61.7072	54.9274	61.1590	60.5770	58.9036	58.7265	59.0703	61.3271
122.2704	116.9370	114.2278	121.9449	120.0391	104.5379	126.2828	110.0203	118.4706
135.3343	130.5030	142.8594	138.3221	139.0765	118.2592	135.0143	135.4882	138.2231
146.3812	132.0143	144.0721	141.9204	149.6574	153.8694	147.8164	138.2166	140.7537
151.7540	136.2283	148.0652	145.8153	151.8249	155.3817	149.1878	143.4685	141.6787
155.0849	145.3817	150.1210	154.1549	154.2263	156.5947	155.6055	149.8725	149.3161
159.9522	148.8814	155.9691	160.2686	157.3720	161.7386	156.6696	152.0500	155.8922
162.0355	164.4112	161.2890	160.7330	161.5485	162.0153	162.7235	156.3397	161.8493
164.0079	168.0423	166.5103	160.9593	162.8442	162.6682	163.8496	165.4183	163.2955
167.7711	170.7591	170.2560	169.9337	169.1457	165.8807	169.1297	169.3947	167.3082
170.9491	170.8066	172.6493	170.1921	169.9982	168.3704	171.7471	173.5500	173.9965
173.8984	171.6685	181.1384	172.9612	176.9930	170.3709	171.8061	174.6452	175.4456

255	**256**	**257**	**258**	**259**	**260**	**261**	**262**	**263**
3.7011	-5.0818	-9.9888	-9.7196	-0.9977	-2.1003	-1.1310	2.6427	1.8087
25.2931	13.5044	15.1706	15.7666	18.7924	19.0617	14.9032	17.8888	23.3204
55.8257	47.4442	56.2733	56.1147	53.4357	53.5656	55.8293	53.3705	54.6293
57.7710	68.2595	64.8138	65.0720	56.9693	56.4664	59.7182	58.6853	61.2053
124.4484	120.2524	123.2266	123.4569	118.5480	117.8949	121.3700	119.0443	112.1716
129.8435	139.1370	137.8223	137.1573	142.5384	141.6907	136.0515	132.0072	143.4881
141.4314	145.5522	143.8014	140.6047	147.6559	143.5099	140.0489	142.3683	144.5452
142.1187	150.3605	147.0668	149.2575	147.9767	147.6248	144.3117	143.0264	145.7811
143.9619	151.8385	148.2505	151.0453	148.7575	148.2429	148.0738	147.9869	149.0827
152.8735	157.0440	156.8688	156.0565	149.6288	154.3466	148.8247	148.9168	152.6831
156.0322	161.4515	156.9318	156.5430	155.5216	154.4220	157.8364	159.3218	158.2873
161.4919	165.2620	159.0242	159.1759	160.0576	155.9054	163.5818	162.3362	164.5687
170.4346	168.8587	164.5973	166.1500	170.2923	170.2717	165.7440	165.7391	166.0395
170.6365	173.6114	169.0177	168.4630	170.9798	170.8312	173.5928	173.6740	173.0287
173.8989	174.1573	170.5016	170.4994	177.7197	174.2802	174.6246	174.3938	174.4698

264	**265**	**266**	**267**	**268**	**269**	**270**	**271**	**272**
-3.9394	0.2513	1.6177	3.5327	-3.6374	-0.0533	2.1506	0.7505	1.1546
11.4418	16.9918	14.1372	17.7682	18.6163	15.3876	13.7142	22.3924	12.0960
58.9020	59.1108	54.9943	54.9158	54.6586	55.4167	54.8703	53.0628	56.1366
60.4557	59.6614	58.2550	58.4395	58.6430	57.4976	56.5913	62.0202	61.3431
123.4547	122.8199	117.2167	116.2733	122.1725	116.3648	117.4446	118.3452	122.4466
136.9092	133.5793	133.0593	133.5724	136.5432	134.8480	134.4798	138.4971	139.9247
140.2022	140.7629	137.0021	134.2044	145.0944	138.2869	138.9282	142.2886	143.0960
143.1660	141.8843	141.8840	136.6690	146.6894	144.1852	147.5674	148.1022	143.4196
145.1418	147.2711	147.4343	147.2608	153.7732	148.3264	148.7420	148.6455	147.8847
147.0458	148.0050	147.6674	152.4537	159.5254	150.4753	149.2990	153.5686	148.7821
149.3104	148.3781	160.9825	161.8965	160.2472	153.8730	153.9890	154.4928	153.6884
156.5862	156.7635	164.3460	164.0864	160.4401	162.5965	162.1066	160.7013	156.3411
163.8648	163.6576	167.2172	167.3706	167.7031	167.0283	167.3933	167.2005	164.6166
169.4772	170.7275	172.8369	172.6616	169.7021	172.9626	173.0784	174.6606	174.4815
175.4834	176.4441	173.2292	173.1697	173.5465	173.6101	177.0909	175.1145	175.5718

273	274	275	276	277	278	279	280	281
8.1166	-0.6879	-9.4711	2.7423	2.4779	2.2148	0.7023	-7.7823	-6.4757
19.5343	14.5371	14.4387	15.8442	19.2872	18.2447	14.1711	15.8628	13.8716
47.4271	54.6612	38.7626	55.7035	54.6988	55.6569	51.4540	57.3959	56.2804
62.7733	60.2652	53.4019	60.9950	56.4438	60.8600	59.7536	58.8145	63.7118
109.8056	121.4344	121.6941	111.7446	110.9003	117.9037	123.5342	117.4695	125.5912
133.2730	136.8248	133.7103	139.2748	140.0615	139.9925	131.4578	141.1064	128.9296
139.6686	139.7507	135.3258	142.0188	142.4435	143.5794	144.8173	147.0504	140.2032
143.0486	141.8543	139.7565	142.2252	143.0065	143.6731	150.5844	151.0255	142.7516
148.1976	143.1552	145.3933	147.6399	144.0608	145.4780	152.2375	152.5913	158.9611
153.0718	147.6872	147.4110	151.4608	147.7426	151.9291	154.5184	154.5186	162.8892
163.9494	152.8055	147.7558	153.5464	150.5274	156.7304	160.7326	156.2692	163.3626
164.6719	154.8097	151.7937	164.5562	162.8298	161.8044	171.0304	157.5862	165.8576
173.6986	169.1052	163.8803	167.7190	167.6919	164.5247	171.7380	163.2738	169.4016
174.2642	174.0797	172.1103	169.6871	169.4893	168.5153	174.6287	166.9368	170.4031
176.4687	175.3401	181.4233	174.7905	174.3196	174.1645	175.4504	170.7919	199.8055

282	283	284	285	286	287	288	289	290
-9.6246	-17.9537	-11.4890	-4.4804	-10.3491	8.3054	-14.3860	-14.3694	-0.8236
18.5057	17.7729	7.7363	25.8797	18.7010	20.7789	10.6679	21.6808	23.7209
24.3658	55.7396	55.3157	56.2011	53.0566	49.4351	54.4578	57.9921	30.4158
32.6213	67.0128	55.5641	57.2256	56.9726	58.2408	63.6222	69.4040	34.9120
51.8000	126.9795	114.8852	117.9675	110.7089	98.6012	124.6444	116.6523	108.8697
57.2662	141.2537	127.9540	133.7932	140.2215	120.2573	138.2263	127.9397	116.9883
116.1173	148.0817	137.1532	144.1003	146.1059	129.2882	150.3371	135.3653	122.8428
136.5870	149.6285	142.1706	144.9341	146.2641	131.6395	151.8741	139.7487	125.1201
139.8099	150.1418	147.1074	152.8103	149.2602	153.4443	152.1220	145.7550	140.4763
149.8439	156.9462	157.5029	160.7798	149.4667	160.2956	164.4035	149.7236	147.0482
165.9023	164.8070	160.5533	168.7252	164.2917	160.2957	165.3209	159.5910	151.1937
167.7614	167.5077	161.9549	169.4296	165.5005	165.9418	166.4827	165.1768	158.8056
172.8994	167.8622	166.4343	171.5866	167.1315	167.6329	168.5950	166.0555	166.9301
176.7960	174.8339	167.3388	172.5857	168.8285	174.2137	170.1541	167.4480	171.0368
177.2157	181.1768	169.2323	173.1975	172.6681	175.6719	172.9757	173.6527	171.4732

291	292
4.0433	-16.4129
23.5845	17.8187
27.5875	45.7781
45.6459	51.9597
105.8216	114.2205
127.4380	128.1510
133.4213	135.7762
137.2258	136.0699
140.8346	138.4679
149.9048	148.3009
158.4249	153.8112
164.7670	156.7095
166.4147	169.4349
173.7218	169.5829
174.6211	171.8564

mPW1PW91/6-31G(d)//AM1 Boltzmann-averaged GIAO NMR isotropic magnetic shielding values calculated for compounds **221** and **247**-**292**

221	**247**	**248**	**249**	**250**	**251**	**252**	**253**	**254**
-7.4514	-18.4057	-0.0989	-11.6532	-4.5328	-1.5509	-7.5547	-0.6440	2.1250
15.6405	19.5059	19.6136	17.7635	18.4544	24.2701	19.7344	18.3391	18.7393
61.4771	62.3801	57.1066	60.9836	60.2412	62.9284	55.6555	56.7549	54.7681
62.6829	68.7319	58.8781	65.4629	62.4438	63.2029	65.8862	61.1310	66.0538
115.8628	111.1420	113.4704	115.6949	114.7874	113.0307	122.5677	103.4384	115.2037
140.9441	128.7795	142.2138	133.9644	139.2314	113.1217	140.9015	133.8983	140.6853
149.1446	131.8021	145.6438	149.0743	141.8794	151.1978	147.6153	139.3863	142.0874
149.1617	134.7558	145.6770	149.4858	148.6984	151.8478	153.6920	146.1636	145.0195
153.7576	139.2528	146.8093	149.9435	154.3038	157.9964	154.5826	149.3887	153.7870
156.7976	151.5836	147.1307	155.3753	156.2893	159.7654	159.3463	155.9401	156.8049
159.4723	160.6648	162.2415	157.4892	156.7440	160.3363	160.0024	156.9374	158.8840
163.1506	165.8857	162.2663	158.9987	157.8833	162.4733	161.8167	160.9832	161.6622
163.6444	165.9103	168.6766	165.6677	160.9289	162.9500	163.9875	166.7946	162.0582
166.9751	166.2247	168.7321	166.9571	166.8738	165.3952	164.8331	168.8145	170.1370
170.0710	168.8941	178.1609	169.6740	171.9502	166.8757	167.1837	171.5334	171.7103

255	**256**	**257**	**258**	**259**	**260**	**261**	**262**	**263**
2.4341	-0.4950	-15.8291	-15.2174	1.8596	2.8907	0.3525	2.7724	1.4987
22.8150	20.9202	22.4023	23.4418	19.9474	20.1170	12.7724	16.8876	22.0778
57.3706	50.4061	52.4516	52.6558	58.9073	58.2615	58.4999	58.0006	55.5521
59.0384	72.5578	74.0568	73.7987	61.8508	61.6722	61.9020	59.1558	66.1564
121.4913	116.2279	123.9937	124.1887	112.2449	112.0087	116.2920	115.2400	108.1377
129.6766	136.3257	143.6234	141.9904	142.3518	138.8559	138.3465	128.9936	141.9577
140.2653	137.7214	144.4410	149.4241	143.1956	142.3054	138.4703	141.7660	146.8090
142.9994	149.8167	149.0480	149.4652	144.6052	145.4262	141.5217	145.7160	150.3214
147.1176	150.5179	151.0570	149.9205	146.1749	149.6123	147.4630	147.6169	151.5955
151.7463	157.5877	157.9430	155.8189	154.6845	154.2729	154.2451	154.0945	152.3507
152.9295	161.0173	158.3031	157.8968	156.8447	155.2549	155.9412	154.6109	157.0539
158.2680	162.3908	161.0347	161.3073	159.7745	155.5516	160.5490	158.2451	160.9565
165.5989	164.4624	163.5774	162.0888	165.5419	165.3770	160.8889	160.9850	161.5925
167.0576	170.1164	163.7506	164.1908	166.3834	166.0487	169.8012	169.4308	168.7769
171.1540	172.6616	168.9325	168.9936	171.9142	172.1076	171.2278	171.5006	169.8586

264	**265**	**266**	**267**	**268**	**269**	**270**	**271**	**272**
-10.3453	3.8798	1.9653	6.2894	-5.0531	0.2824	2.6345	1.1007	3.0104
15.8516	22.4072	16.5874	21.2324	20.5330	18.4747	16.5233	19.6474	13.2201
62.9091	63.4889	56.3340	56.2816	59.3818	57.9763	56.9098	56.1778	56.2241
66.6367	66.0082	62.0680	62.4128	67.4797	61.5994	60.8012	63.5234	64.2491
117.1301	116.7807	113.0589	112.4644	115.6500	112.2361	113.3394	115.4650	117.2552
136.8251	136.7235	130.9894	132.0189	134.0003	133.4000	132.0724	140.3038	133.7978
136.9193	137.5605	137.1674	134.2797	146.4716	137.3765	137.8162	140.9735	145.7639
140.8617	138.9245	144.6247	138.9584	149.8056	145.6453	149.4932	149.6097	147.3093
145.1765	149.9430	148.7813	153.8605	150.8391	150.4592	151.9238	149.8174	147.8915
152.7770	151.0034	154.0309	156.3299	153.2521	154.4824	153.8843	153.2508	148.8453
153.4217	152.2962	157.8038	159.0273	157.5581	154.9821	154.4334	154.2167	154.1204
153.7057	154.2469	162.1646	160.7781	159.5849	159.9274	159.5390	159.2597	154.5712
159.0965	159.2877	162.7075	162.4763	163.1614	161.8979	162.4201	161.9056	160.9868
163.9340	164.7328	167.8079	168.1221	166.7782	167.9706	168.0196	171.3970	170.1726
172.6490	173.6310	171.3588	171.1534	169.6352	171.5678	171.3583	171.5744	171.7819

273	274	275	276	277	278	279	280	281
10.7612	0.0153	-5.0396	4.2986	5.6411	3.2719	4.1626	-6.4855	-7.4671
23.7577	18.8512	15.6873	17.5915	21.9328	17.7449	21.7151	22.6124	15.6364
50.0731	57.6451	36.4520	57.6727	58.2761	57.2421	55.8949	61.1383	61.4736
65.5540	63.3749	54.3881	64.8455	62.4689	64.7943	65.6230	66.8034	62.7105
102.2206	117.3442	116.4080	105.6618	105.6758	112.4526	117.3718	111.8082	115.8520
135.1618	138.0715	132.6197	139.1380	137.4304	138.1028	134.1964	140.0836	140.9417
135.8409	139.2832	133.3115	141.3334	142.1858	138.7438	136.8254	145.7672	149.1461
144.9400	139.6298	139.0525	142.3776	145.1656	141.0614	148.2788	149.9075	149.1565
155.3714	142.3326	144.0598	148.1574	147.0384	150.4713	153.8536	152.0403	153.7497
155.3940	149.5007	145.6264	151.7009	147.4132	153.8360	154.8531	157.1669	156.7937
158.8559	149.7879	151.3841	153.2372	148.4196	155.1634	161.7926	157.5812	159.4802
159.8245	159.0992	151.9126	158.8852	158.7195	156.0903	161.8166	159.3543	163.1493
169.2909	163.8829	159.8834	161.9246	161.2836	159.4902	166.0646	161.1846	163.6397
169.8629	171.8709	165.2770	162.2060	161.9970	161.7779	171.2810	162.2860	166.9782
174.4642	174.2990	177.1549	170.6869	170.7599	170.5934	173.1020	164.8209	170.0664

282	283	284	285	286	287	288	289	290
-12.5433	-17.6503	-7.1982	-3.4940	-12.9053	-9.5230	-7.3724	-17.0375	5.2344
21.4201	16.2964	29.1710	23.3002	21.1916	18.2699	18.5058	28.6376	25.8878
55.3998	63.8901	61.1232	59.2825	56.9315	65.8070	57.7813	59.8621	46.3260
57.8258	70.9706	64.8986	62.0280	59.1671	70.5546	68.4088	67.3470	60.7290
60.1768	121.2742	118.2016	114.5551	105.3314	110.4488	117.4139	112.7134	100.2431
63.2236	147.0086	132.9606	134.7799	139.4944	140.7821	145.6808	129.4045	112.2229
107.1904	149.5540	140.3255	140.1732	144.0173	144.8751	147.9462	132.8618	116.6819
134.0057	150.9784	148.1681	148.3380	144.1775	145.8367	148.4414	136.5976	119.5337
142.1125	152.6725	152.0401	148.3914	150.0659	150.9051	151.2764	143.6668	133.0498
150.3155	154.6547	153.8313	152.4178	154.4339	154.0232	162.6004	155.6875	148.8501
163.6436	157.2044	157.8473	164.6320	158.8105	158.8357	163.0597	157.1086	160.0988
165.1706	164.8209	158.7981	166.0726	163.7267	161.8009	164.6637	157.2755	167.2196
167.7789	166.3049	161.8248	166.7153	164.0142	163.5372	165.2838	160.2302	167.3056
176.2561	180.6262	164.8063	166.9553	164.1108	164.9551	165.4046	165.2775	167.3183
177.2399	181.0597	165.5441	169.3049	167.7420	173.2783	168.9811	172.0360	170.5539

291	292
0.2750	-10.1938
27.3083	16.1566
55.2210	52.1346
59.7547	57.0198
97.8333	107.5619
127.5679	125.2259
132.3120	128.0707
133.8381	131.3021
145.2877	135.6480
149.2879	151.7714
153.4807	155.6987
161.8881	164.1361
164.1584	164.3316
169.8808	164.8706
171.0647	169.7102

mPW1PW91/6-31G(d)//HF/3-21G Boltzmann-averaged GIAO NMR isotropic magnetic shielding values calculated for compounds **221** and **247**-**292**

221	**247**	**248**	**249**	**250**	**251**	**252**	**253**	**254**
-1.9392	-11.6054	4.4271	-3.5439	3.7798	1.1959	-3.1687	6.4553	5.4428
23.6347	27.3875	28.1935	26.4724	27.6482	30.8655	27.4261	27.1058	27.8764
61.8968	63.0727	59.6350	61.3787	62.7605	63.1557	55.7076	60.9718	59.5072
64.0943	71.3693	60.0193	65.6643	64.1083	68.3197	71.3889	64.3480	67.1024
114.8687	112.7061	110.1099	114.7913	115.5431	115.1187	122.3653	105.7955	114.5060
141.6462	132.7481	144.7944	133.6294	142.8204	121.0694	141.8476	139.0435	141.5693
148.1985	133.0980	146.4225	146.9989	143.3610	153.1758	152.1117	141.2103	144.5795
152.7808	139.8695	148.6523	150.7950	148.5106	156.2569	153.1632	151.1987	145.1615
153.3135	140.4665	148.6694	155.1358	151.1226	157.3005	154.9455	152.1222	152.7204
156.0387	152.0027	149.9017	156.9172	157.0254	164.0890	157.4068	153.6520	157.4414
163.4388	165.3450	166.3219	161.6150	161.9252	164.2855	162.0062	156.3381	164.3308
167.4476	170.6742	166.3292	163.0027	162.3112	164.2982	165.0258	168.3934	166.1511
169.4428	172.2767	173.4110	171.8232	171.3133	169.5508	166.1895	171.6243	168.6325
171.7630	172.7570	174.3329	172.0922	172.2018	170.8224	172.2841	175.5208	175.5580
177.1534	173.3873	184.9190	176.8771	175.6920	174.2452	172.6175	175.8577	178.1073

255	**256**	**257**	**258**	**259**	**260**	**261**	**262**	**263**
6.3333	4.3260	-1.1309	-0.7093	5.7381	5.9780	4.7606	7.4510	4.4564
32.4778	28.0627	29.8791	30.8629	28.7787	28.9757	22.7342	25.8827	31.0228
60.9476	53.6467	60.4452	60.4852	62.0128	61.5561	61.0318	59.6309	60.2915
62.9594	70.1808	75.0816	74.9719	62.7430	62.1284	65.1094	65.2671	66.1142
118.9988	117.8263	119.4163	119.4667	114.7886	114.1972	113.1723	113.2990	107.4419
130.4249	137.7462	144.4682	140.4942	143.5339	142.1728	138.7185	130.9027	144.2560
144.4272	147.8292	146.3133	141.4334	144.2979	144.5792	139.4851	145.6005	146.3763
145.7638	147.9784	149.0425	152.9362	148.4674	145.7059	147.1570	146.5621	150.5434
146.8966	148.8566	151.0821	155.6071	148.9630	150.3336	150.0527	147.5319	151.1267
152.5964	151.9327	158.0696	157.0296	151.5136	152.9196	153.0679	151.7932	153.6475
158.0535	163.1041	159.6582	158.2491	160.3691	159.2538	165.2737	162.3205	161.9334
163.5547	168.3954	161.5873	161.6733	164.8227	160.3876	166.0834	165.6773	166.8397
171.9033	171.9920	165.3759	171.1685	173.2051	172.7610	168.3095	168.0296	168.4590
173.9871	174.0829	170.9115	171.6050	174.3806	174.5171	175.6487	175.9662	175.2480
175.6950	175.2389	171.7430	171.6263	175.7502	175.9981	177.5028	177.2669	175.5726

264	**265**	**266**	**267**	**268**	**269**	**270**	**271**	**272**
0.4872	8.3757	5.6590	6.6640	-1.1762	5.9149	5.3260	6.0290	7.8788
24.2909	30.7926	24.5755	27.8600	28.6497	26.8956	25.1441	29.0279	24.0675
64.9225	65.3689	59.1724	60.6130	58.7712	60.9503	61.6065	58.6524	64.2119
65.8199	66.6581	65.0506	63.2545	72.1341	63.4695	62.9927	65.5173	65.1656
117.1127	117.8532	112.5441	111.9328	113.9481	111.9281	112.2937	114.2615	117.4808
139.0692	134.5755	138.5083	135.7690	132.8946	140.8028	141.3017	141.6520	142.7364
139.6690	137.3327	140.6938	141.9285	149.0910	142.1220	143.5266	142.4741	146.0859
142.8639	144.6368	146.0021	143.0398	149.4357	145.3811	146.9435	150.5992	146.1597
149.2446	152.3486	147.6076	152.3955	152.3851	153.0609	152.1252	152.1939	146.6959
152.2148	153.4487	152.7986	153.7397	155.6798	155.0944	153.3648	154.8942	153.9076
155.0870	154.1659	161.9002	162.6416	162.1863	155.9392	155.5646	155.1284	157.3361
157.2418	156.1455	165.8979	168.1212	163.7195	163.0742	163.8069	162.9725	159.7140
165.8937	165.9475	169.7197	169.2963	169.4876	169.1429	168.8306	168.5703	166.2940
169.0708	170.0515	174.6959	174.8362	171.0029	175.0414	174.9899	176.1386	175.6678
177.9109	178.4451	175.6369	175.7796	176.9159	175.5760	175.8160	177.9254	178.4183

273	274	275	276	277	278	279	280	281
13.6506	4.5634	-1.1630	6.2680	7.4885	8.0316	9.9594	-0.2158	-1.9384
32.0945	26.0619	25.5400	25.4068	28.6154	26.2328	29.0657	30.0498	23.6395
55.5773	62.5201	44.3969	61.2031	61.3983	61.7609	58.6521	60.6266	61.8975
65.5058	64.4671	57.1039	65.4215	61.4486	65.5161	62.8296	69.0204	64.0896
107.6220	117.7388	116.5633	106.6638	106.6448	112.9459	120.2867	112.7096	114.8604
136.1392	143.4722	133.8134	145.7557	141.3133	142.6802	137.0130	141.3809	141.6452
144.4425	144.3238	137.4154	146.8086	144.8429	145.3086	144.2549	152.7145	148.2020
145.0369	146.3280	143.6431	147.5508	146.4445	148.6168	149.1427	153.5121	152.7664
152.5106	147.1228	149.3841	148.5819	151.2727	150.0032	149.9143	155.1737	153.3100
152.6270	150.9590	150.1299	152.1354	151.8075	150.5016	152.4616	157.1802	156.0360
166.2541	151.2942	151.6642	153.0816	152.8823	154.2915	162.8297	157.4266	163.4362
166.5487	155.8599	151.7971	166.6343	165.5367	166.9723	167.7652	161.9800	167.4409
174.5335	174.6565	165.7703	171.9087	172.0409	168.0596	174.0382	164.6613	169.4390
174.9341	176.0784	175.0286	173.0266	172.8444	172.5983	175.4615	169.5554	171.7595
175.8348	179.9535	181.7038	175.2450	175.9708	175.1337	178.3599	170.2529	177.1545

282	283	284	285	286	287	288	289	290
3.1295	-8.9649	1.2143	2.1446	-3.2614	-3.9173	-0.0205	-7.1699	9.0316
29.5037	26.3530	34.9127	31.8009	28.9259	27.0692	25.5063	35.6290	33.2593
56.2200	63.7477	62.2545	60.7668	58.9625	66.3715	58.6759	63.5347	46.7265
58.6421	73.2329	62.3031	62.8494	61.6425	74.1090	69.0947	74.3385	71.1583
63.6792	120.2069	118.3444	113.6250	104.9220	113.0668	116.0338	114.4964	113.0677
67.2369	148.0379	135.6717	134.8126	144.4357	144.2922	144.5492	130.1223	116.7803
105.9520	150.9650	143.8496	143.7390	147.6774	144.3685	147.5464	131.6403	122.8823
136.4949	154.0676	148.5318	147.7869	148.4963	146.2168	152.1859	143.3442	127.7220
150.7885	154.4768	150.7918	153.2231	150.9568	149.7281	154.2426	149.0995	133.2492
152.8934	154.9721	156.2508	154.7223	153.2422	155.4646	165.7189	154.5928	150.3827
169.6212	163.5071	162.1574	168.8779	166.8196	163.9674	166.3161	158.9868	157.9146
170.0502	168.4291	164.6945	171.3160	168.2399	167.5269	167.5727	167.9796	165.8151
171.4029	169.4539	170.3988	171.8187	169.3739	169.2105	168.5933	168.8765	172.6268
180.6542	185.7325	170.8244	173.0121	170.6257	169.8437	172.7388	171.1472	173.6785
181.0462	186.3043	171.2148	176.8092	171.9300	177.9650	177.2574	175.3414	177.0009

291	292
7.4205	-4.5998
34.6590	23.6452
55.0394	64.1842
64.9565	67.9088
96.3201	112.5514
123.4965	130.6474
132.2698	131.8431
137.1174	132.5744
146.1731	136.3014
149.2950	149.8577
157.9031	153.1248
166.3456	165.9975
171.2499	170.9366
176.6032	171.2847
178.0056	177.3432

Output patterns obtained after testing the optimal trained ANNs with compounds **221** and **247-292**.

Structure	**ANN-MM-18**	**ANN-AM1-18**	**ANN-HF-18**
221	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
247	**0.7839; 0.2679**	**0.9788; 0.0171**	**0.9999; 0.0001**
248	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
249	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
250	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
251	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
252	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
253	0.0001; 1.0000	0.0000; 1.0000	0.0000; 1.0000
254	0.0001; 0.9999	0.0000; 1.0000	0.0000; 1.0000
255	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
256	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
257	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
258	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
259	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
260	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
261	0.0001; 0.9999	0.0000; 1.0000	0.0000; 1.0000
262	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
263	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
264	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
265	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
266	0.0001; 1.0000	0.0000; 1.0000	0.0000; 1.0000
267	0.0001; 1.0000	0.0000; 1.0000	0.0000; 1.0000
268	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
269	0.0001; 1.0000	0.0000; 1.0000	0.0000; 1.0000
270	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
271	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
272	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
273	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
274	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
275	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
276	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
277	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
278	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
279	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
280	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
281	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
282	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
283	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
284	0.0012; 0.9990	0.0000; 1.0000	0.0000; 1.0000
285	0.0001; 1.0000	0.0000; 1.0000	0.0000; 1.0000
286	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
287	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
288	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
289	0.4557; 0.5488	0.0000; 1.0000	0.0000; 1.0000
290	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
291	0.0000; 1.0000	0.0000; 1.0000	0.0000; 1.0000
292	0.0001; 1.0000	0.4110; 0.6801	0.0005; 0.9992