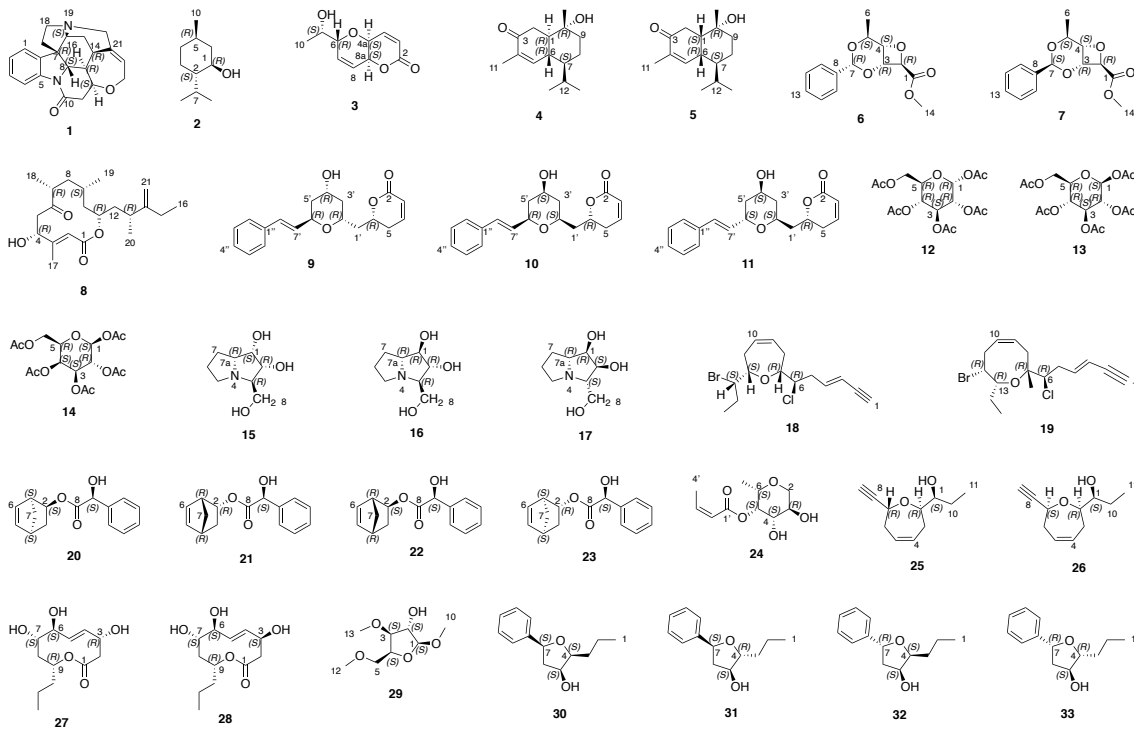


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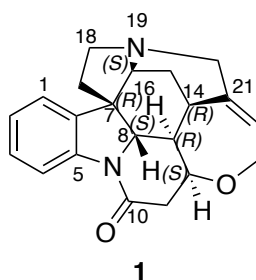
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1. Correct structures of compounds 1-33.



2. Experimental chemical shifts and isotropic magnetic shielding constants of studied isomers at MMFF 21 kJ/mol MAD 0.5 Å.

Table S1. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-13 calculated at the B3LYP/6-31G** level of theory for compound **1**¹



Isotropic shielding constants								
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7
C 1	122.26	75.41	74.46	74.46	74.61	73.65	72.94	73.64
C 2	124.20	72.70	72.09	72.10	72.63	72.71	72.38	72.71
C 3	128.56	67.27	66.67	66.68	67.08	66.38	66.3	66.39
C 4	116.23	80.77	80.07	80.08	81.79	80.88	80.95	80.89
C 5	142.23	56.07	54.16	54.15	54.98	54.66	53.71	54.66
C 6	132.72	63.80	63.35	63.35	64.32	64.04	64.83	64.04
C 7	51.96	138.10	137.51	137.50	139.63	138.98	133.11	138.98
C 8	60.10	130.19	126.20	126.20	126.48	128.09	114.09	128.10
C 10	169.28	31.97	33.43	33.44	30.50	33.96	31.34	33.96
C 11	42.48	148.80	154.32	154.32	148.37	149.84	147.00	149.84
C 12	76.85	111.36	115.47	115.47	111.68	103.13	114.45	103.12
C 13	48.22	142.06	141.92	141.91	136.45	138.33	128.22	138.33
C 14	31.60	157.84	164.66	164.66	161.17	152.06	157.83	152.06
C 15	26.84	162.26	170.39	170.39	165.67	170.62	161.27	170.62
C 16	60.28	131.18	126.62	126.64	132.41	128.73	111.86	128.74
C 17	42.85	146.49	153.18	153.18	146.04	148.79	145.24	148.78
C 18	50.35	141.84	140.25	140.25	141.99	139.97	138.77	139.97
C 20	52.68	138.82	140.76	140.76	140.15	141.48	133.28	141.48
C 21	140.45	53.43	40.46	40.44	55.10	28.64	54.07	28.65
C 22	127.34	65.62	71.64	71.64	71.70	73.50	88.43	73.51
C 23	64.60	128.72	120.77	120.79	120.10	124.25	117.04	124.25
H 1	7.17	24.59	24.51	24.51	24.60	24.52	24.48	24.52
H 2	7.10	24.76	24.70	24.70	24.78	24.75	24.76	24.75
H 3	7.26	24.49	24.44	24.44	24.50	24.44	24.44	24.44
H 4	8.09	23.52	23.47	23.48	23.72	23.63	23.69	23.63
H 8	3.86	27.80	28.04	28.03	28.32	28.01	28.21	28.01
H 11a	3.13	29.11	29.12	29.12	28.94	29.34	28.83	29.34
H 11b	2.67	28.76	29.19	29.19	29.29	29.14	29.11	29.14
H 12	4.29	27.70	27.68	27.68	28.04	27.47	28.21	27.47
H 13	1.28	30.66	28.69	28.69	30.07	28.53	29.05	28.53
H 14	3.15	28.86	28.06	28.06	28.62	28.94	27.69	28.94
H 15a	2.36	29.58	30.05	30.05	30.39	30.30	30.02	30.14

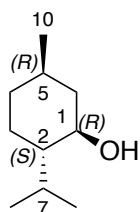
¹ Compound **1**: NMR data from Berger, S. Braun, S. 2014, 200 and More NMR Experiments, Ed. Wiley-VCH pp 802-803

H 15b	1.46	30.38	30.22	30.22	29.73	30.14	30.53	30.30
H 16	3.96	27.87	28.28	28.28	27.96	28.21	27.47	28.21
H 17a	1.89	29.83	29.19	29.20	29.87	29.33	29.65	29.33
H 17b	1.89	29.98	30.13	30.13	30.15	30.20	30.13	30.2
H 18a	3.22	28.95	28.61	28.61	29.11	28.91	28.43	28.57
H 18b	2.88	28.75	28.84	28.84	28.73	28.57	28.95	28.91
H 20a	3.72	29.21	29.02	29.02	28.06	27.95	28.55	28.71
H 20b	2.75	28.16	27.97	27.98	29.18	28.71	28.03	27.95
H 22	5.92	25.75	26.97	26.97	26.69	26.36	27.74	26.36
H 23a	4.15	27.86	27.49	27.50	27.18	27.27	27.46	27.51
H 23b	4.07	28.06	27.04	27.05	27.50	27.51	26.97	27.27
J 1,2	7.49	7.46	7.45	7.45	7.40	7.44	7.41	7.44
J 1,3	1.08	0.97	0.95	0.95	0.95	0.93	0.94	0.93
J 1,4	0.23	0.68	0.70	0.70	0.70	0.71	0.70	0.71
J 2,3	7.44	7.00	7.02	7.03	7.01	7.03	7.05	7.03
J 2,4	0.98	0.83	0.83	0.83	0.81	0.83	0.82	0.83
J 3,4	7.90	8.09	8.04	8.04	8.06	8.00	8.03	8.00
J 8,13	10.40	9.62	4.03	4.03	9.13	7.27	7.02	7.27
J 11a,12	3.34	2.60	7.21	7.20	6.08	11.82	6.72	11.82
J 11b,12	8.47	8.15	8.71	8.71	9.12	4.64	6.94	4.64
J 12,13	3.30	3.06	6.48	6.48	8.77	5.63	10.6	5.63
J 13,14	3.29	2.81	5.45	5.45	4.73	3.92	0.42	3.93
J 14,15a	4.11	4.69	2.09	2.09	2.11	4.30	6.59	2.03
J 14,15b	1.96	1.75	4.21	4.21	4.12	2.03	3.47	4.30
J 14,22	0.47	-3.35	-1.91	-1.91	-2.77	-1.54	-4.43	-1.54
J 14,20a	1.61	-0.54	-0.48	-0.48	-2.09	-1.19	-0.58	-0.60
J 15a,16	4.33	3.73	4.68	4.69	1.82	1.25	3.32	5.05
J 15b,16	2.42	2.00	1.29	1.29	4.04	5.05	1.45	1.25
J 20a,22	1.79	-0.52	-0.68	-0.68	-2.74	-3.06	-0.97	-0.80
J 22,23a	7.00	7.22	3.14	3.14	2.38	5.62	3.85	6.43
J 22,23b	6.10	6.14	2.74	2.74	4.54	6.43	2.27	5.62

Nuclei	Experimental	Isomer 8	Isomer 9	Isomer 10	Isomer 11	Isomer 12	Isomer 13
C 1	122.26	73.49	79.58	78.67	76.38	75.11	74.46
C 2	124.20	72.48	71.55	71.32	71.15	71.16	75.54
C 3	128.56	66.44	68.54	68.15	67.81	67.72	69.71
C 4	116.23	80.78	79.75	80.21	80.44	81.17	86.26
C 5	142.23	54.9	56.65	56.48	54.66	53.95	56.35
C 6	132.72	64.64	51.29	51.27	56.7	56.83	51.43
C 7	51.96	132.74	136.94	137.85	136.02	134.95	131.55
C 8	60.10	117.71	126.97	127.39	127.56	127.73	127.61
C 10	169.28	33.34	35.36	34.62	33.02	31.57	14.48
C 11	42.48	149.34	148.6	147.87	149.74	150.93	148.6
C 12	76.85	115.72	111.11	119.02	108.94	115.91	112.47
C 13	48.22	130.72	153.97	144.75	145.41	145.18	142.56
C 14	31.60	157.97	155.21	159.62	152.38	158.7	152.28
C 15	26.84	159.28	162.52	165.25	166.08	165.07	157.19
C 16	60.28	114.27	132.44	133.22	132.95	130.87	117.9
C 17	42.85	146.22	150.43	150.93	154.38	153.19	143.86

C 18	50.35	139.55	137.86	138.08	141.05	140.91	132.08
C 20	52.68	135.79	132.60	134.36	138.98	138.54	133.07
C 21	140.45	50.80	47.42	51.01	36.64	43.60	42.64
C 22	127.34	84.20	67.35	72.29	72.40	74.75	61.11
C 23	64.60	122.30	125.02	122.17	127.07	117.66	127.17
H 1	7.17	24.46	24.56	24.59	24.53	24.49	24.34
H 2	7.10	24.73	24.73	24.74	24.71	24.70	24.99
H 3	7.26	24.43	24.51	24.51	24.51	24.51	24.75
H 4	8.09	23.67	23.56	23.66	23.61	23.71	24.94
H 8	3.86	27.86	27.26	27.61	28.18	27.92	27.75
H 11a	3.13	29.13	29.28	29.41	29.15	29.31	29.67
H 11b	2.67	28.90	28.98	29.12	29.23	29.13	29.04
H 12	4.29	27.89	27.98	27.62	27.74	27.67	28.16
H 13	1.28	29.29	29.54	29.18	29.53	29.05	30.03
H 14	3.15	28.13	28.82	28.48	28.85	28.13	28.93
H 15a	2.36	29.83	30.05	30.07	30.03	30.08	30.32
H 15b	1.46	30.51	29.47	29.69	29.92	29.81	29.29
H 16	3.96	27.44	27.82	27.88	27.62	27.59	27.86
H 17a	1.89	29.67	28.40	28.93	29.43	29.45	30.11
H 17b	1.89	30.00	30.72	30.64	30.01	29.98	29.68
H 18a	3.22	28.49	29.18	29.23	29.05	29.13	28.11
H 18b	2.88	28.83	28.82	28.89	28.69	28.68	27.96
H 20a	3.72	28.59	27.93	27.82	27.99	27.93	27.57
H 20b	2.75	28.02	29.07	29.1	28.83	29.05	28.37
H 22	5.92	26.84	25.76	26.68	26.16	27.08	26.35
H 23a	4.15	27.52	28.12	27.31	27.42	26.91	28.34
H 23b	4.07	28.09	27.67	27.51	27.67	27.59	28.20
J 1,2	7.49	7.43	7.24	7.22	7.25	7.25	7.70
J 1,3	1.08	0.93	0.91	0.89	0.89	0.90	0.78
J 1,4	0.23	0.71	0.75	0.76	0.77	0.76	0.55
J 2,3	7.44	7.05	7.07	7.09	7.07	7.07	7.02
J 2,4	0.98	0.83	0.78	0.78	0.78	0.78	1.07
J 3,4	7.90	8.01	7.91	7.88	7.91	7.92	8.07
J 8,13	10.40	8.28	11.72	9.54	13.17	12.94	8.5
J 11a,12	3.34	3.93	4.42	10.33	6.24	11.62	3.83
J 11b,12	8.47	7.76	2.01	3.42	8.81	4.79	2.37
J 12,13	3.30	4.54	3.52	11.07	7.91	9.93	3.29
J 13,14	3.29	-1.62	6.02	8.88	6.05	8.43	2.88
J 14,15a	4.11	6.87	1.44	1.90	4.07	4.17	1.57
J 14,15b	1.96	2.89	4.57	3.84	1.44	1.35	4.82
J 14,22	0.47	-4.08	-3.92	-3.38	-1.90	-1.80	-2.90
J 14,20a	1.61	-0.38	-2.22	-2.37	-1.27	-1.34	-2.04
J 15a,16	4.33	3.11	2.92	2.89	1.49	1.57	6.78
J 15b,16	2.42	1.64	2.18	2.30	3.77	3.44	0.79
J 20a,22	1.79	-0.81	-1.78	-2.44	-2.74	-2.50	-2.99
J 22,23a	7.00	6.52	5.53	2.49	6.23	2.39	5.99
J 22,23b	6.10	5.41	7.82	4.69	6.55	3.78	7.38

Table S2. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-4 calculated at the B3LYP/6-31G** level of theory for compound **2**²

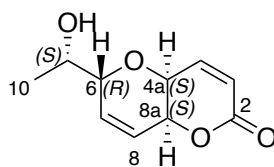


2

Isotropic shielding constants					
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4
C 1	71.6	122.89	123.38	121.66	125.06
C 2	50.2	142.56	142.99	141.98	140.48
C 3	23.2	169.11	165.42	166.09	169.38
C 4	34.6	159.39	156.13	156.56	160.16
C 5	31.7	161.94	163.19	159.07	161.75
C 6	45.1	149.53	145.34	144.57	150.54
C 7	25.9	158.36	157.92	161.16	161.6
C 8	16.1	169.63	169.6	173.61	171.93
C 9	16.1	169.73	169.85	169.95	169.85
C 10	22.2	169.1	167.63	167.82	170.15
H 1	3.43	27.55	27.58	28	27.61
H 3a	0.99	30.36	30.24	30.55	30.22
H 3b	1.64	29.78	29.92	30.13	30.09
H 2	1.13	30.71	30.73	30.37	30.56
H 4a	0.87	30.16	30.06	30.83	30.3
H 4b	1.68	30.25	30.84	30.17	30.42
H 5	1.44	29.99	29.67	30.35	29.77
H 6ax	1.98	30.06	30.62	30.34	30.49
H 6b	0.99	30.51	30.47	30.61	30.09
H 7	2.19	29.75	29.81	29.37	29.55
H 8	0.94	30.74	30.76	30.84	30.81
H 9	0.83	30.79	30.79	30.84	30.85
H 10	0.94	30.51	30.96	30.91	30.83
J 1,2	9.9	2.57	2.13	9.29	7.02
J 1ax,6ax	12	3.33	3.18	9.63	7.66
J 1ax,6eq	4	2.64	1.98	4.18	3.66
J 5ax,6ax	10.9	2.29	3.41	11.35	4.44
J 5ax,6eq	4.5	5.41	11.17	3.33	5.18

² Compound **2**: NMR data from S. Berger, D. Sicker. **2009**, Classics in Spectroscopy: Isolation and Structure Elucidation of Natural Products. 1st Edition Ed. Wiley-VCH pp 373-387.

Table S3. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-13 calculated at the B3LYP/6-31G** level of theory for compound **3**³

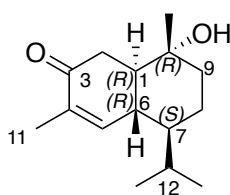


3

Isotropic shielding constants									
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 2	161.73	35.09	36.72	33.54	33.47	33.41	33.55	36.58	35.13
C 3	123.28	67.95	69.93	71.34	71.8	72.64	71.37	69.77	67.85
C 4	144.24	57.34	52.05	49.07	48.54	47.76	49.08	52.4	57.52
C 4a	64.9	124.75	124.31	119.02	123.99	122.65	119.11	124.53	124.8
C 6	74.79	111	115.11	108.53	109.43	111.98	107.04	116.34	109.74
C 7	129.57	60.51	64.87	65.14	66.44	68.65	65.17	64.61	60.36
C 8	124.68	68.52	66.25	64.04	62.85	60.52	64.06	66.6	68.51
C 8a	70	121.52	121.65	116.43	116.66	116.71	116.63	121.59	121.52
C 9	69.66	120.8	120.38	120.84	122.76	118.47	120.72	120.36	120.89
C 10	18.72	173.28	173.17	173.29	173.4	169.85	172.98	173.17	173.04
H 3	6.07	25.61	25.86	25.82	25.85	25.9	25.82	25.84	25.6
H 4	6.88	25.07	24.98	24.88	24.91	24.86	24.88	25	25.07
H 4a	4.92	27.94	26.79	27.33	27.04	26.64	27.36	26.86	27.95
H 6	4.08	27.69	27.88	27.41	27.82	27.54	27.69	27.57	27.96
H 7	6.06	25.41	25.72	25.79	25.8	25.78	25.8	25.68	25.45
H 8	6.04	25.42	25.52	25.41	25.36	25.19	25.44	25.48	25.46
H 8a	4.97	27.31	26.67	26.89	26.98	27.04	26.9	26.69	27.31
H 9	3.96	27.71	27.84	27.76	27.58	27.67	27.81	27.8	27.72
H 10a-c	1.25	30.63	30.66	30.66	30.61	30.67	30.64	30.67	30.63
J 3,4	10	10.19	10.36	10.23	10.24	10.25	10.23	10.35	10.18
J 3,4a	1.6	-0.91	-3.09	-3.33	-3.39	-3.42	-3.33	-2.93	-0.93
J 4,4a	3.1	5.9	2.97	2.34	2.37	2.39	2.35	3.18	5.9
J 4a,8a	5.6	1.6	7.22	8.93	9.01	9.06	8.94	6.8	1.61
J 4,8a	1	-0.28	0.96	-0.26	-0.26	-0.26	-0.26	0.88	-0.28
J 8,8a	2.6	5.34	2.95	2.21	2.23	2.21	2.21	3.15	5.32
J 6,8a	2.6	2.58	3.22	4.41	3.08	3.43	4.34	3.1	2.61
J 7,8	10.5	10.44	10.66	10.68	10.67	10.62	10.72	10.62	10.45
J 6,8	2.6	-3.2	-3.42	-3.36	-2.91	-3.2	-3.27	-3.48	-3.16
J 6,7	1.6	1.88	2.04	2.11	3.18	3.08	2.1	2.14	1.88
J 6,9	4.2	2.19	7.07	2.32	6.66	2.03	7.22	2.34	6.91

³ Compound **3**: NMR data from Maity, S.; Kanikarapu, S.; Murumudi, K.; Kunwar, A. C.; Yadav, J. S.; Mohapatra, D. K. *J. Org. Chem.* **2017**, *82*, 4561

Table S4. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-8 calculated at the B3LYP/6-31G** level of theory for compound **4**⁴

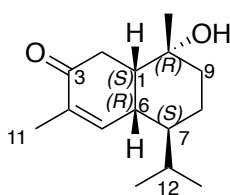


4

Isotropic shielding constants									
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 1	51.1	146.73	141.87	145.29	145.21	144.33	144.94	140.97	146.16
C 2	38.3	153.58	153.67	154.85	152.15	151.5	156.32	152.82	153.24
C 3	200.1	-2.09	-1.93	-0.17	-1.76	0.33	-1.65	-2.04	-2.29
C 4	135.4	59.24	57.39	58.88	55.81	55.03	57.84	58.32	60.48
C 5	146	48.9	53.42	47.37	54.53	56.95	50.55	51.57	46.34
C 6	40.8	146.91	149.64	153.41	151.86	151.35	152.25	150.45	148.17
C 7	45	145.16	143.71	145.76	140.71	140.37	145.45	143.83	144.7
C 8	21.5	163.98	168.04	169.17	164	166.05	167.7	169.12	164.66
C 9	41.6	151.02	147.15	153.6	146.03	147.48	153.21	148.47	152.52
C 10	71.2	120.69	121.63	121.02	120.83	120.81	121.53	122.14	121.41
C 11	15.1	172.69	172.49	172.79	172.19	172.29	172.71	172.61	172.83
C 12	26.2	161.73	161.67	160.41	159.71	159.58	160.75	161.43	162.17
C 13	15.9	167.09	175.67	168.88	168.72	169.94	175.21	169.06	168.29
C 14	21.4	168.65	169.08	175.09	169.77	168.71	168.92	175.52	167.24
C 15	26.2	166.69	167.32	160.49	164.06	160.2	161.89	161.29	161.46
H 1	1.83	29.26	29.67	29.44	29.44	29.84	29.44	30	29.59
H 2a	2.1	29.78	29.76	29.4	28.61	29.57	28.9	29.28	29.31
H 2b	2.75	28.93	28.87	29.51	29.59	28.98	29.37	29.21	29.21
H 5	6.8	25.09	24.89	24.7	24.99	25.1	24.86	24.8	25.07
H 6	2.07	29.22	29.41	28.86	28.63	28.8	29.4	28.83	28.6
H 7	1.22	30.2	30.44	30.13	30.6	30.78	30.02	30.54	30.21
H 8a	1.84	29.84	30.16	29.84	30.01	30.06	30.18	29.85	29.69
H 8b	1.44	30.29	30.41	30.38	30.6	30.21	30.4	30.34	30.02
H 9a	1.69	30.67	30.43	30.02	30.44	30.22	30.65	30.18	29.88
H 9b	1.2	29.8	30.06	30.62	30.13	30.54	29.85	30.52	30.8
H 11a-c	1.79	30.05	30.05	30.05	30.02	30.03	30.06	30.06	30.07
H 12	2.2	29.55	29.52	29.76	29.95	29.88	29.73	29.53	29.69
H 13a-c	0.83	30.78	30.86	30.82	30.76	30.79	30.83	30.81	30.8
H 14a-c	0.99	30.77	30.8	30.77	30.79	30.76	30.82	30.81	30.8
H 15a-c	1.16	30.64	30.66	30.74	30.67	30.69	30.58	30.71	30.68
J 1,6	8.4	10.48	9.62	4.02	5.03	4.3	4.07	9	9.78
J 1,2a	13.8	12.79	12.84	13.89	1.74	5.36	4	3.1	3.57
J 1,2b	3	3.61	3.18	4.1	6.08	1.88	12.74	12.9	12.86

⁴ Compound **4** and **5**: NMR data from He, K.; Zeng, L.; Shi, G.; Zhao, G. X.; Kozlowski, J. F.; McLaughlin, J. L. *J. Nat. Prod.* **1997**, *60*, 38

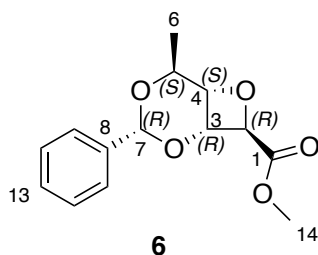
Table S5. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-8 calculated at the B3LYP/6-31G** level of theory for compound **5**



5

Isotropic shielding constants									
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 1	44.1	146.73	141.87	145.29	145.21	144.33	144.94	140.97	146.16
C 2	34.28	153.58	153.67	154.85	152.15	151.5	156.32	152.82	153.24
C 3	198.78	-2.09	-1.93	-0.17	-1.76	0.33	-1.65	-2.04	-2.29
C 4	134.4	59.24	57.39	58.88	55.81	55.03	57.84	58.32	60.48
C 5	147.94	48.9	53.42	47.37	54.53	56.95	50.55	51.57	46.34
C 6	36.75	146.91	149.64	153.41	151.86	151.35	152.25	150.45	148.17
C 7	42.24	145.16	143.71	145.76	140.71	140.37	145.45	143.83	144.7
C 8	20.6	163.98	168.04	169.17	164	166.05	167.7	169.12	164.66
C 9	33.52	151.02	147.15	153.6	146.03	147.48	153.21	148.47	152.52
C 10	70.32	120.69	121.63	121.02	120.83	120.81	121.53	122.14	121.41
C 11	26.35	172.69	172.49	172.79	172.19	172.29	172.71	172.61	172.83
C 12	20.4	161.73	161.67	160.41	159.71	159.58	160.75	161.43	162.17
C 13	14.84	167.09	175.67	168.88	168.72	169.94	175.21	169.06	168.29
C 14	18.94	168.65	169.08	175.09	169.77	168.71	168.92	175.52	167.24
C 15	26.63	166.69	167.32	160.49	164.06	160.2	161.89	161.29	161.46
H 1	2.13	29.26	29.67	29.44	29.44	29.84	29.44	30	29.59
H 2a	2.61	29.78	29.76	29.4	28.61	29.57	28.9	29.28	29.31
H 2b	2.41	28.93	28.87	29.51	29.59	28.98	29.37	29.21	29.21
H 5	6.77	25.09	24.89	24.7	24.99	25.1	24.86	24.8	25.07
H 6	2.28	29.22	29.41	28.86	28.63	28.8	29.4	28.83	28.6
H 7	1.45	30.2	30.44	30.13	30.6	30.78	30.02	30.54	30.21
H 8a	1.59	29.84	30.16	29.84	30.01	30.06	30.18	29.85	29.69
H 8b	1.13	30.29	30.41	30.38	30.6	30.21	30.4	30.34	30.02
H 9a	1.5	30.67	30.43	30.02	30.44	30.22	30.65	30.18	29.88
H 9b	1.5	29.8	30.06	30.62	30.13	30.54	29.85	30.52	30.8
H 11a-c	1.72	30.05	30.05	30.05	30.02	30.03	30.06	30.06	30.07
H 12	1.82	29.55	29.52	29.76	29.95	29.88	29.73	29.53	29.69
H 13a-c	0.86	30.78	30.86	30.82	30.76	30.79	30.83	30.81	30.8
H 14a-c	0.83	30.77	30.8	30.77	30.79	30.76	30.82	30.81	30.8
H 15a-c	1.25	30.64	30.66	30.74	30.67	30.69	30.58	30.71	30.68
J 1,6	4.2	10.48	9.62	4.02	5.03	4.3	4.07	9	9.78
J 1,2a	4.2	12.79	12.84	13.89	1.74	5.36	4	3.1	3.57
J 1,2b	13.8	3.61	3.18	4.1	6.08	1.88	12.74	12.9	12.86
J 5,6	5.9	3.04	2.63	6.07	3.13	2.96	6.02	2.68	3.06
J 6,7	10.5	3.98	10.14	10.74	4.63	4.31	10.61	10.06	3.48
J 7,12	13.8	6.43	3.28	2.73	8.68	8.59	2.89	3.25	7.14

Table S6. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-16 calculated at the B3LYP/6-31G** level of theory for compound **6**⁵

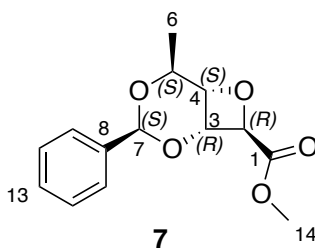


Isotropic shielding constants									
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 1	170.44	19.51	22.36	22.78	23.15	19.88	22.03	22.67	22.97
C 2	81.67	102.46	104.31	100.08	100.54	103.45	103.74	98.62	99.19
C 3	70.54	119.97	119.98	126.9	125.13	120.99	122.74	123	121.22
C 4	79.31	111.74	113.36	109.06	111.43	112.22	111.51	106.99	110.43
C 5	77.79	119.04	119.08	120.48	120.31	121.75	125.68	115.52	116.09
C 6	20.17	175.48	175.5	176.7	175.95	175.31	172.87	170.81	170.69
C 7	97.1	90.87	91.88	90.97	90.91	98.43	95.64	93.58	93.03
C 8	137.27	54.95	55.32	56.63	56.74	54.41	55.08	56.92	56.73
C 14	52.57	140.74	140.99	140.33	140.48	140.75	140.45	140.42	140.57
H 2	5.53	26.36	26.45	26.49	26.48	26.42	26.29	26.37	26.43
H 3	5.05	26.8	26.74	26.56	26.47	26.86	26.78	26.84	26.77
H 4	4.55	26.99	27.35	25.68	27.02	27.06	27.32	26.09	27.5
H 5	4.44	28.06	28.12	27.38	27.35	27.46	27.52	27.52	27.37
H 6a-c	1.42	30.5	30.41	30.59	30.49	30.46	30.62	30.55	30.57
H 7	6.16	25.85	25.89	25.67	25.7	25.46	25.53	25.45	25.55
H 14a-c	3.82	28.09	28.58	27.98	28.05	28.13	28.21	27.98	28.06
J 2,3	6.2	3.29	6.34	7.04	7.43	3.48	6.4	6.79	7.48
J 2,4	1	-0.72	-0.56	-0.87	-0.43	-0.84	-0.49	-0.83	-0.36
J 3,4	7.4	6.85	6.34	8.15	7.21	6.47	5.95	7.61	6.79
J 4,5	6.2	1.11	1.23	6.74	6.51	2.05	6.56	8.04	7.95

Isotropic shielding constants									
Nuclei	Experimental	Isomer 9	Isomer 10	Isomer 11	Isomer 12	Isomer 13	Isomer 14	Isomer 15	Isomer 16
C 1	170.44	23.29	23.21	19.69	20.42	23.14	22.68	21.37	19.8
C 2	81.67	97.22	96.04	102.37	105.26	99.21	99.18	104.16	103.33
C 3	70.54	114.61	116.06	124.43	122.32	125.14	127.64	120.09	119.94
C 4	79.31	110.01	106.54	110.48	113.36	111.81	109.43	112.61	109.97
C 5	77.79	111.71	110.98	117.82	114.8	121.39	122.49	124.23	126.1
C 6	20.17	171.45	171.63	170.27	169.91	176.73	177.04	175.74	175.36
C 7	97.1	88.04	87.61	90.69	91.42	91.48	90.57	95.53	94.19
C 8	137.27	57.66	57.29	55.41	56.62	56.26	56.18	55.64	55.13
C 14	52.57	140.56	140.32	140.51	140.61	140.52	140.33	140.19	140.65
H 2	5.53	26.28	26.16	26.34	26.09	26.44	26.45	26.39	25.97
H 3	5.05	27.21	27.31	26.75	26.72	26.57	26.67	26.76	26.72
H 4	4.55	27.82	26.6	27.24	27.23	27.3	26.14	27.22	27.13
H 5	4.44	27.45	27.6	26.8	27.55	27.41	27.54	27.95	28.2
H 6a-c	1.42	30.62	30.65	30.51	30.49	30.43	30.58	30.51	30.63
H 7	6.16	25.65	25.78	25.33	25.69	25.39	25.35	25.1	25.07
H 14a-c	3.82	28.06	27.96	28.01	28.07	28.05	27.96	27.95	28.04
J 2,3	6.2	7.51	6.9	7.32	5.52	7.33	6.94	6.18	4.06
J 2,4	1	-0.39	-0.74	-0.18	-0.71	-0.43	-0.83	-0.5	-0.6
J 3,4	7.4	6.04	6.74	6.72	7.2	7.1	8.01	6.22	7.28
J 4,5	6.2	8.12	8.1	7.34	6.94	5.57	6.24	3.16	0.98

⁵ Compounds **6** and **7**: NMR data from S. W Johnson, D. Angus, C. Taillefumier, J. H Jones, D. J Watkin, E. Floyd, J.G Buchanan, G. W.J Fleet, *Tetrahedron: Asymmetry*, **2000**, *11*, 20

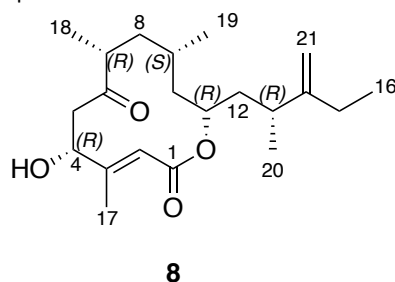
Table S7. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-16 calculated at the B3LYP/6-31G** level of theory for compound **7**



Isotropic shielding constants									
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 1	170.4	19.51	22.36	22.78	23.15	19.88	22.03	22.67	22.97
C 2	84.1	102.46	104.31	100.08	100.54	103.45	103.74	98.62	99.19
C 3	72.1	119.97	119.98	126.9	125.13	120.99	122.74	123	121.22
C 4	79.4	111.74	113.36	109.06	111.43	112.22	111.51	106.99	110.43
C 5	70.8	119.04	119.08	120.48	120.31	121.75	125.68	115.52	116.09
C 6	16.2	175.48	175.5	176.7	175.95	175.31	172.87	170.81	170.69
C 7	92.3	90.87	91.88	90.97	90.91	98.43	95.64	93.58	93.03
C 8	138.3	54.95	55.32	56.63	56.74	54.41	55.08	56.92	56.73
C 14	52.7	140.74	140.99	140.33	140.48	140.75	140.45	140.42	140.57
H 2	5.08	26.36	26.45	26.49	26.48	26.42	26.29	26.37	26.43
H 3	4.93	26.8	26.74	26.56	26.47	26.86	26.78	26.84	26.77
H 4	4.69	26.99	27.35	25.68	27.02	27.06	27.32	26.09	27.5
H 5	4.43	28.06	28.12	27.38	27.35	27.46	27.52	27.52	27.37
H 6a-c	1.38	30.5	30.41	30.59	30.49	30.46	30.62	30.55	30.57
H 7	5.72	25.85	25.89	25.67	25.7	25.46	25.53	25.45	25.55
H 14a-c	3.83	28.09	28.58	27.98	28.05	28.13	28.21	27.98	28.06
J 2,3	2.4	3.29	6.34	7.04	7.43	3.48	6.4	6.79	7.48
J 2,4	1	-0.72	-0.56	-0.87	-0.43	-0.84	-0.49	-0.83	-0.36
J 3,4	4.9	6.85	6.34	8.15	7.21	6.47	5.95	7.61	6.79
J 4,5	2.2	1.11	1.23	6.74	6.51	2.05	6.56	8.04	7.95

Isotropic shielding constants									
Nuclei	Experimental	Isomer 9	Isomer 10	Isomer 11	Isomer 12	Isomer 13	Isomer 14	Isomer 15	Isomer 16
C 1	170.4	23.29	23.21	19.69	20.42	23.14	22.68	21.37	19.8
C 2	84.1	97.22	96.04	102.37	105.26	99.21	99.18	104.16	103.33
C 3	72.1	114.61	116.06	124.43	122.32	125.14	127.64	120.09	119.94
C 4	79.4	110.01	106.54	110.48	113.36	111.81	109.43	112.61	109.97
C 5	70.8	111.71	110.98	117.82	114.8	121.39	122.49	124.23	126.1
C 6	16.2	171.45	171.63	170.27	169.91	176.73	177.04	175.74	175.36
C 7	92.3	88.04	87.61	90.69	91.42	91.48	90.57	95.53	94.19
C 8	138.3	57.66	57.29	55.41	56.62	56.26	56.18	55.64	55.13
C 14	52.7	140.56	140.32	140.51	140.61	140.52	140.33	140.19	140.65
H 2	5.08	26.28	26.16	26.34	26.09	26.44	26.45	26.39	25.97
H 3	4.93	27.21	27.31	26.75	26.72	26.57	26.67	26.76	26.72
H 4	4.69	27.82	26.6	27.24	27.23	27.3	26.14	27.22	27.13
H 5	4.43	27.45	27.6	26.8	27.55	27.41	27.54	27.95	28.2
H 6a-c	1.38	30.62	30.65	30.51	30.49	30.43	30.58	30.51	30.63
H 7	5.72	25.65	25.78	25.33	25.69	25.39	25.35	25.1	25.07
H 14a-c	3.83	28.06	27.96	28.01	28.07	28.05	27.96	27.95	28.04
J 2,3	2.4	7.51	6.9	7.32	5.52	7.33	6.94	6.18	4.06
J 2,4	1	-0.39	-0.74	-0.18	-0.71	-0.43	-0.83	-0.5	-0.6
J 3,4	4.9	6.04	6.74	6.72	7.2	7.1	8.01	6.22	7.28
J 4,5	2.2	8.12	8.1	7.34	6.94	5.57	6.24	3.16	0.98

Table S8. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-16 calculated at the B3LYP/6-31G** level of theory for compound **8**⁶



Isotropic shielding constants									
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 1	167.6	29.4	27.72	28.16	29.04	28.48	29.88	27.59	30.35
C 2	116.9	72.61	72.14	72.49	70.38	70.98	71.43	70.96	71.69
C 3	154.7	39.89	43.6	41.73	39.68	39.49	40.02	42.46	40.62
C 4	73	116.86	117.34	115.6	115.7	117.22	117.95	116.25	115.84
C 5	44.7	150.22	146.9	153.91	147.62	148.36	146.42	152.6	148.66
C 6	217	-23.01	-27.42	-25.99	-17.98	-24.28	-25.65	-25.58	-19.34
C 7	50.5	144.76	139.3	144.8	144.24	143.32	143.93	143.24	144.77
C 8	39.8	147.04	147.16	148.74	148.79	148.69	152.47	148.3	148.2
C 9	32.9	163.74	156.94	164.45	161.14	160.85	160.92	160.38	162.6
C 10	44.9	151.24	142.74	147.41	148.18	147.93	152.76	146.85	151.69
C 11	74.4	120.95	120.05	120.92	115.89	117.17	123.45	116.59	121.13
C 12	41.2	147.16	146.75	148.16	146.95	146.68	147.72	147.78	149.02
C 13	36.9	151.69	152.62	152.3	151.86	152.63	151.07	151.92	151.36
C 14	155.2	39.08	39.2	39.24	39.03	37.59	39.44	39.04	38.99
C 15	26.2	160.48	160.04	161.19	161.11	161.75	164.77	163.8	163.5
C 16	12.3	177.5	177.44	177.77	177.57	177.3	178.11	177.74	177.75
C 17	16.7	173.42	174.38	174.25	176.88	171.53	169.51	172.27	178.76
C 18	17.9	172.74	172.13	172.85	173.17	173.3	176.28	173.23	172.75
C 19	23.1	165.66	169.34	168.96	168.8	168.41	168.49	170.25	167.59
C 20	21.1	167.8	167.47	168.02	167.99	171.06	169.9	169.9	170.74
C 21	107.1	85.75	86.87	86.29	86.3	86.15	85.8	85.79	85.69
H 2	5.93	25.48	25.48	25.5	25.83	25.55	25.64	25.63	25.87
H 4	4.46	27.43	27.43	27.48	27.13	27.42	27.41	27.42	27.16
H 5a	3.07	28.75	28.84	28.88	29.33	28.81	28.75	28.94	29.31
H 5b	2.52	29.68	29.37	29.64	28.78	29.52	29.5	29.49	28.88
H 7	2.16	29.52	29.27	29.33	29.35	29.16	28.79	29.28	29.55
H 8a	0.94	31	30.87	30.6	29.8	31.02	30.29	30.06	30.17
H 8b	2.09	29.97	29.38	30.78	31.08	29.8	30.29	30.8	30.57
H 9	0.97	29.41	30.85	29.63	30.13	30.12	30	30.23	29.56
H 10a	1.44	31.08	30.22	30.61	30.05	30.63	30.24	30.39	30.11
H 10b	1.29	30.14	30.58	30.18	31.07	30.38	29.98	30.38	30.89
H 11	5.03	26.53	26.51	26.75	27.27	27.13	26.82	27.3	26.62
H 12a	1.55	29.7	30.15	29.86	29.15	30.33	30.45	30.11	30.39

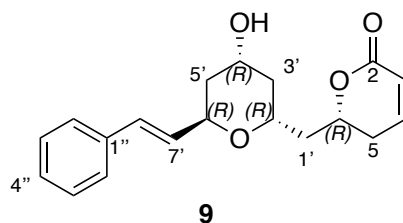
⁶ Compound **8**: NMR data from Hangyou, M.; Ishiyama, H.; Takahashi, Y.; Kobayashi, J. *Org. Lett.* **2009**, *11*, 5046

H 12b	1.62	30.25	30.14	30.27	30.34	29.48	29.75	29.6	29.63
H 13	2.23	29.42	29.46	29.29	29.22	29.31	29.39	29.39	29.47
H 15	2.01	29.62	29.6	29.58	29.6	29.63	29.42	29.69	29.69
H 16a-c	1.04	30.69	30.69	30.69	30.69	30.69	30.67	30.69	30.69
H 17a-c	2.12	29.66	29.81	29.75	29.56	29.74	29.8	29.84	29.56
H 18a-c	1.08	30.74	30.77	30.79	30.75	30.75	30.77	30.78	30.73
H 19a-c	0.92	30.78	30.91	30.82	30.89	30.85	30.76	30.86	30.82
H 20a-c	1.02	30.69	30.72	30.7	30.68	30.55	30.63	30.62	30.69
H 21a	4.78	26.61	26.61	26.64	26.65	26.77	26.8	26.78	26.78
H 21b	4.76	26.72	26.77	26.73	26.7	26.76	26.7	26.74	26.73
J 4,5a	3.1	2.84	2.82	1.97	4.43	2.95	3.22	2.42	4.25
J 4,5b	5.45	5.34	5.04	5.98	11.3	5.03	4.82	6.49	10.11
J 7,8a	7.3	1.84	3.87	11.36	9.71	1.48	9.93	10.41	6.32
J 7,8b	2.8	8.9	5.24	1.67	1.54	9.67	1.49	2.09	4.23
J 10a,11	11.4	1.02	9.52	2.69	9.7	3.62	0.93	2.41	4.76
J 10b,11	3.6	5.21	2.17	4.89	1.16	7.02	8.75	10.08	2.7
J 9,10a	7	8.37	4.14	5.4	0.87	6.26	3.31	4.48	1.61
J 9,10b	2.3	0.73	4.65	2.82	9.34	3.13	3.38	3.54	7.08
J 11,12a	8.7	10.32	9.25	9.81	10.23	3.62	5.93	6.53	4.27
J 11,12b	3.6	0.99	1.31	1.78	2.44	9.06	6.03	6.27	8.39
J 12a,13	5	3.36	3.17	3.62	3.24	9.32	6.79	6.88	7.43
J 12b,13	9	10.25	10.27	10.18	10.36	4.09	7.33	7.33	6.05

Isotropic shielding constants									
Nuclei	Experimental	Isomer 9	Isomer 10	Isomer 11	Isomer 12	Isomer 13	Isomer 14	Isomer 15	Isomer 16
C 1	167.6	29.62	27.6	26.29	28.9	28.64	29.97	27.5	30.32
C 2	116.9	72.61	71.81	72.6	70.1	71.51	73.03	72.62	71.37
C 3	154.7	40.16	45.84	45.4	39.86	38.9	40.05	41	40.31
C 4	73	116.85	117.72	116	115.76	117.19	117.6	117.11	115.16
C 5	44.7	150.15	147.11	153.37	147.63	148.39	147.23	151.51	148.95
C 6	217	-23.02	-26.99	-26.54	-17.98	-24.25	-25.7	-26.54	-17.51
C 7	50.5	144.69	138.81	146.97	144.08	143.38	143.11	143.53	145.53
C 8	39.8	147.1	147.55	152.2	148.74	148.64	152.81	147.82	147.07
C 9	32.9	163.82	156.23	163.37	161.02	161.03	160.25	161.1	163.75
C 10	44.9	151.94	143.71	149.36	148.52	148.04	151.46	144.86	150.81
C 11	74.4	121.63	118.77	119.95	116.38	116.75	120.37	116.8	120.58
C 12	41.2	148.9	147.26	149.45	146.94	146.84	147.02	146.79	147.34
C 13	36.9	151.82	152.07	149.95	152.6	152.54	152.52	152.45	151.59
C 14	155.2	38.31	38.42	41.18	37.85	38.85	39.27	38.78	39.24
C 15	26.2	162.38	163.07	167.71	161.9	160.39	161.37	160.96	160.66
C 16	12.3	177.67	177.64	178.89	177.21	177.25	177.61	177.86	177.46
C 17	16.7	173.47	175.09	174.97	176.49	172.22	173	173.31	179.76
C 18	17.9	172.73	172.43	171.52	173.28	173.18	175.34	173.33	172.82
C 19	23.1	165.76	168.75	170.14	168.55	168.69	168.73	170.77	165.67
C 20	21.1	171.28	170.85	168.78	171.13	167.73	168.08	167.69	167.98
C 21	107.1	85.97	86.01	85.49	85.99	86.48	86.1	87.35	85.61
H 2	5.93	25.49	25.47	25.52	25.82	25.57	25.6	25.71	25.85
H 4	4.46	27.43	27.43	27.51	27.09	27.41	27.38	27.39	27.13
H 5a	3.07	28.75	28.82	28.75	29.3	28.81	28.81	28.89	29.32

H 5b	2.52	29.68	29.37	29.71	28.79	29.54	29.54	29.55	28.85
H 7	2.16	29.51	29.28	29.24	29.32	29.2	29.22	29.2	29.62
H 8a	0.94	31	30.83	30.36	29.79	31.04	30.56	30.06	29.9
H 8b	2.09	29.94	29.31	30.99	31.07	29.82	29.76	30.75	31.06
H 9	0.97	29.4	30.84	29.33	30.13	30.09	30.16	30.25	29.5
H 10a	1.44	30.98	30.24	30.32	30.11	31.02	30.56	30.62	30.16
H 10b	1.29	30.13	30.48	30.27	30.94	30.05	29.71	30.23	31.08
H 11	5.03	26.47	26.77	27.33	27.23	27.15	27.09	27.2	26.57
H 12a	1.55	29.6	29.92	29.46	29.33	30.29	30.42	30.25	30.24
H 12b	1.62	30.38	30.43	30.35	30.3	29.27	29.03	29.5	29.73
H 13	2.23	29.42	29.43	29.39	29.3	29.21	29.3	29.2	29.49
H 15	2.01	29.65	29.59	29.27	29.63	29.59	29.61	29.56	29.71
H 16a-c	1.04	30.68	30.69	30.67	30.7	30.67	30.66	30.67	30.71
H 17a-c	2.12	29.66	29.87	29.83	29.59	29.7	29.74	29.79	29.5
H 18a-c	1.08	30.73	30.75	30.74	30.74	30.75	30.78	30.78	30.73
H 19a-c	0.92	30.78	30.88	30.81	30.86	30.88	30.81	30.86	30.78
H 20a-c	1.02	30.66	30.58	30.7	30.6	30.68	30.7	30.72	30.71
H 21a	4.78	26.76	26.79	26.87	26.77	26.62	26.61	26.66	26.63
H 21b	4.76	26.72	26.74	26.69	26.77	26.72	26.68	26.75	26.74
J 4,5a	3.1	2.84	2.89	2.17	4.71	2.94	3	2.47	5.46
J 4,5b	5.45	5.33	4.92	5.82	11.25	5.1	5.15	5.54	10.56
J 7,8a	7.3	1.74	4.27	11.85	9.72	1.5	8.72	11.52	9.2
J 7,8b	2.8	8.98	5.19	2.22	1.52	9.67	2.37	2.21	1.6
J 10a,11	11.4	1.06	9.57	8.02	9.66	1.13	0.82	2.48	5.25
J 10b,11	3.6	5.28	1.91	3.85	1.12	9.67	8.23	10.12	1.02
J 9,10a	7	8.34	4.48	3.93	0.74	9.17	4.28	4.99	0.66
J 9,10b	2.3	0.76	4.4	8.19	9.06	0.74	2.86	3.15	8.41
J 11,12a	8.7	9.77	8.19	3.33	8.89	2.27	2.49	1.76	1.14
J 11,12b	3.6	2.68	3.53	10.34	4.18	10.05	10.09	9.54	10.16
J 12a,13	5	4.49	4.85	11.82	4.58	10.47	10.62	10.75	9.97
J 12b,13	9	8.49	8.48	3.56	9	3.09	3.26	2.94	3.65

Table S9. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-8 calculated at the B3LYP/6-31G** level of theory for compound **9**⁷

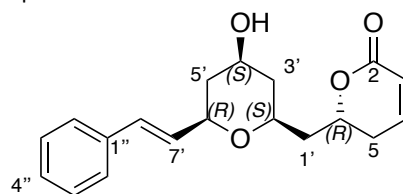


Isotropic shielding constants									
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 2	164.7	33.71	33.28	34.11	34.25	34.48	34.5	33.95	34
C 3	121.5	72.08	71.92	72.08	72.11	71.76	71.8	72.49	72.55
C 4	145.7	52.45	52.38	52.87	52.78	53.57	53.57	52.1	51.94
C 5	29.5	159.74	159.66	161.14	160.7	159.88	159.79	160.9	161.1
C 6	75.2	117.6	118.69	116.74	117.12	117.92	117.26	116.46	116.38
C 1'	40.6	147.44	145.34	148.83	149.02	146.45	146.5	149.45	151.11
C 2'	71.6	125.51	132.87	122.55	119.64	120.66	122.74	129.98	125.12
C 3'	40.8	149.4	151.72	150.74	149.14	149.62	149.25	152.29	150.8
C 4'	68.1	127.3	127.02	126.44	124.32	124.46	126.42	127.03	127.39
C 5'	41.4	153.83	154.42	153.02	149.31	148.21	153.37	153.91	152.9
C 6'	76.3	120.8	120.87	117.88	114.99	115.46	118.04	120.04	121.17
C 7'	129.5	63.63	67.05	60.91	62.29	61.5	60.63	63.26	62.81
C 8'	130.7	62.44	63.99	63.7	63.28	63.01	63.65	62.74	62.54
C 1''	136.8	58.8	61.13	58.37	58.98	58.48	58.21	59.33	58.74
C 2''-6''	126.7	69.69	69.275	70.095	70.06	70.025	70.07	69.845	70
C 3''-5''	128.8	68.465	68.25	68.39	68.29	68.36	68.425	68.22	68.345
C 4''	128	70.72	70.13	70.72	70.43	70.54	70.79	70.28	70.57
H 3	6.03	25.76	25.73	25.85	25.84	25.85	25.85	25.83	25.8
H 4	6.89	24.98	24.96	25.03	25.04	25.09	25.09	25.02	24.98
H 5a	2.4	29.75	29.89	29.72	29.85	29.85	29.76	29.8	29.86
H 5b	2.51	29.57	29.54	29.28	29.25	29.57	29.55	28.86	28.87
H 6	4.67	26.8	26.6	26.97	26.97	26.87	26.91	27.05	27.05
H 1'a	2.18	30.15	30.22	30.08	29.98	30.1	30.14	30.05	29.62
H 1'b	1.89	29.55	30.02	29.81	29.81	29.95	30.02	29.86	29.78
H 2'	3.73	27.37	27.11	27.42	28.08	27.91	27.33	27.1	27.36
H 3'a	2.04	30.25	30.4	30.43	29.93	30.71	30.3	30.22	30.15
H 3'b	1.3	30.37	30.22	30.15	30.44	29.9	30.49	30.19	30.26
H 4'	3.92	27.67	27.8	27.55	27.99	27.89	27.55	27.68	27.67
H 5'a	1.37	29.91	29.92	30.24	30.58	30.05	29.99	29.84	30.14
H 5'b	2.1	30.04	29.85	30.07	29.89	30.53	30.26	30.12	29.93
H 6'	4.01	26.95	27.01	27.21	27.89	27.83	27.17	27.22	26.94
H 7'	6.19	25.89	25.62	25.75	25.64	25.69	25.75	25.26	25.77
H 8'	6.58	24.76	24.72	24.9	25.01	24.95	24.89	24.83	24.8
H 2''-6''	7.38	24.285	24.15	24.505	24.49	24.505	24.515	24.415	24.465
H 3''-5''	7.31	24.39	24.355	24.415	24.405	24.405	24.42	24.385	24.405

⁷ Compound **9**: NMR data from Della-Felice, F.; de Assis, F. F.; Sarotti, A. M.; Pilli, R. A. *Synthesis* **2019**, 51, 154

H 4"	7.24	24.55	24.54	24.54	24.53	24.53	24.54	24.52	24.54
J 3,4	9.7	10.14	10.1	10.07	10.08	10.1	10.09	10.08	10.1
J 4,5a	2.5	3.37	2.89	2.99	2.92	3.07	3.06	2.91	2.88
J 4,5b	6	6.05	6.51	6.44	6.5	6.35	6.37	6.5	6.5
J 5a,6	4.1	3.3	2.74	2.78	2.68	2.99	3.03	2.75	2.7
J 5b,6	11.6	10	11.5	11.45	11.66	10.93	10.93	11.98	12.14
J 6,1'a	6	1.06	1.27	4.97	3.68	1.85	2.61	5.71	4.49
J 6,1'b	6	9.7	9.86	5.52	5.92	9.19	8.21	3.56	3.81
J 1'a,2'	8	8.25	9.54	3.21	3.4	9.08	8.84	2.42	4.47
J 1'b,2'	5.5	3.75	1.52	7.5	6.01	1.8	2.02	8.66	7.33
J 2',3'a	1.8	8.16	11.02	1.62	1.52	10.35	10.42	2.28	3.34
J 2',3'b	11.3	2.91	1.94	10.55	10.54	1.57	1.67	9.69	7.25
J 4',3'a	4.3	8.3	3.06	2.92	4.24	9.97	2.46	3.91	3.53
J 4',3'b	11.3	3.61	2.95	2.52	9.82	4.34	2.88	3.09	7.55
J 4',5'a	11.3	3.85	2.7	2.86	9.9	4.41	2.79	3.43	7.99
J 4',5'b	4.3	8.83	3.38	2.83	4.36	9.9	2.96	3.51	3.68
J 6',5'a	11.3	3.95	0.98	11.1	10.82	1.73	1.83	6.7	4.9
J 6',5'b	1.8	5.36	7.63	1.84	1.74	10.81	11.09	2.11	4.81
J 6',7'	5.8	3.47	2.99	5.59	6.17	6.31	5.67	5.59	4.42
J 7',8'	16	15.39	15.75	15.06	15.05	15.03	15.06	15.31	15.26

Table S10. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-8 calculated at the B3LYP/6-31G** level of theory for compound **10**⁸



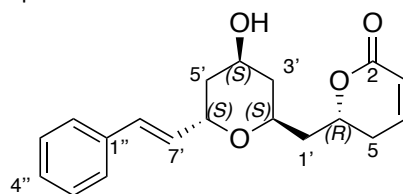
10

Isotropic shielding constants									
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 2	164.4	33.71	33.28	34.11	34.25	34.48	34.5	33.95	34
C 3	121.8	72.08	71.92	72.08	72.11	71.76	71.8	72.49	72.55
C 4	145.3	52.45	52.38	52.87	52.78	53.57	53.57	52.1	51.94
C 5	30.3	159.74	159.66	161.14	160.7	159.88	159.79	160.9	161.1
C 6	74.7	117.6	118.69	116.74	117.12	117.92	117.26	116.46	116.38
C 1'	41.9	147.44	145.34	148.83	149.02	146.45	146.5	149.45	151.11
C 2'	65.6	125.51	132.87	122.55	119.64	120.66	122.74	129.98	125.12
C 3'	41.8	149.4	151.72	150.74	149.14	149.62	149.25	152.29	150.8
C 4'	64.7	127.3	127.02	126.44	124.32	124.46	126.42	127.03	127.39
C 5'	38.7	153.83	154.42	153.02	149.31	148.21	153.37	153.91	152.9
C 6'	72.7	120.8	120.87	117.88	114.99	115.46	118.04	120.04	121.17
C 7'	129	63.63	67.05	60.91	62.29	61.5	60.63	63.26	62.81
C 8'	131.8	62.44	63.99	63.7	63.28	63.01	63.65	62.74	62.54
C 1''	136.7	58.8	61.13	58.37	58.98	58.48	58.21	59.33	58.74
2''-6''	126.8	69.69	69.275	70.095	70.06	70.025	70.07	69.845	70
3''-5''	128.9	68.465	68.25	68.39	68.29	68.36	68.425	68.22	68.345
C 4''	128	70.72	70.13	70.72	70.43	70.54	70.79	70.28	70.57
H 3	6.05	25.76	25.73	25.85	25.84	25.85	25.85	25.83	25.8
H 4	6.89	24.98	24.96	25.03	25.04	25.09	25.09	25.02	24.98
H 5a	2.39	29.75	29.89	29.72	29.85	29.85	29.76	29.8	29.86
H 5b	2.39	29.57	29.54	29.28	29.25	29.57	29.55	28.86	28.87
H 6	4.8	26.8	26.6	26.97	26.97	26.87	26.91	27.05	27.05
H 1'a	1.92	30.15	30.22	30.08	29.98	30.1	30.14	30.05	29.62
H 1'b	1.86	29.55	30.02	29.81	29.81	29.95	30.02	29.86	29.78
H 2'	4.14	27.37	27.11	27.42	28.08	27.91	27.33	27.1	27.36
H 3'a	1.95	30.25	30.4	30.43	29.93	30.71	30.3	30.22	30.15
H 3'b	1.31	30.37	30.22	30.15	30.44	29.9	30.49	30.19	30.26
H 4'	4.04	27.67	27.8	27.55	27.99	27.89	27.55	27.68	27.67
H 5'a	2.16	29.91	29.92	30.24	30.58	30.05	29.99	29.84	30.14
H 5'b	1.76	30.04	29.85	30.07	29.89	30.53	30.26	30.12	29.93
H 6'	4.8	26.95	27.01	27.21	27.89	27.83	27.17	27.22	26.94
H 7'	6.22	25.89	25.62	25.75	25.64	25.69	25.75	25.26	25.77
H 8'	6.6	24.76	24.72	24.9	25.01	24.95	24.89	24.83	24.8
H 2''-6''	7.42	24.285	24.15	24.505	24.49	24.505	24.515	24.415	24.465
H 3''-5''	7.32	24.39	24.355	24.415	24.405	24.405	24.42	24.385	24.405
H 4''	7.23	24.55	24.54	24.54	24.53	24.53	24.54	24.52	24.54
J 3,4	9.7	10.14	10.1	10.07	10.08	10.1	10.09	10.08	10.1
J 2',3'b	10.6	8.16	11.02	1.62	1.52	10.35	10.42	2.28	3.34
J 4',3'b	10.6	8.3	3.06	2.92	4.24	9.97	2.46	3.91	3.53

⁸ Compound **10** and **11**: NMR data from Della-Felice, F.; Sarotti, A. M.; Pilli, R. A. *J. Org. Chem.* **2017**, *82*, 9191

J 4',5'a	4.2	3.85	2.7	2.86	9.9	4.41	2.79	3.43	7.99
J 4',5'b	10.6	8.83	3.38	2.83	4.36	9.9	2.96	3.51	3.68
J 6',5'a	2	3.95	0.98	11.1	10.82	1.73	1.83	6.7	4.9
J 6',5'b	5.8	5.36	7.63	1.84	1.74	10.81	11.09	2.11	4.81
J 6',7'	4.2	3.47	2.99	5.59	6.17	6.31	5.67	5.59	4.42
J 7',8'	16.4	15.39	15.75	15.06	15.05	15.03	15.06	15.31	15.26

Table S11. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-8 calculated at the B3LYP/6-31G** level of theory for compound **11**

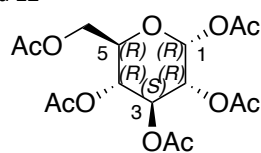


11

Isotropic shielding constants									
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 2	164.7	33.71	33.28	34.11	34.25	34.48	34.5	33.95	34
C 3	121.6	72.08	71.92	72.08	72.11	71.76	71.8	72.49	72.55
C 4	145.4	52.45	52.38	52.87	52.78	53.57	53.57	52.1	51.94
C 5	29.5	159.74	159.66	161.14	160.7	159.88	159.79	160.9	161.1
C 6	75.3	117.6	118.69	116.74	117.12	117.92	117.26	116.46	116.38
C 1'	40.6	147.44	145.34	148.83	149.02	146.45	146.5	149.45	151.11
C 2'	66.1	125.51	132.87	122.55	119.64	120.66	122.74	129.98	125.12
C 3'	41	149.4	151.72	150.74	149.14	149.62	149.25	152.29	150.8
C 4'	64.6	127.3	127.02	126.44	124.32	124.46	126.42	127.03	127.39
C 5'	38.3	153.83	154.42	153.02	149.31	148.21	153.37	153.91	152.9
C 6'	72.7	120.8	120.87	117.88	114.99	115.46	118.04	120.04	121.17
C 7'	129.1	63.63	67.05	60.91	62.29	61.5	60.63	63.26	62.81
C 8'	132.4	62.44	63.99	63.7	63.28	63.01	63.65	62.74	62.54
C 1''	136.7	58.8	61.13	58.37	58.98	58.48	58.21	59.33	58.74
C 2''-6''	126.7	69.69	69.275	70.095	70.06	70.025	70.07	69.845	70
C 3''-5''	128.9	68.465	68.25	68.39	68.29	68.36	68.425	68.22	68.345
C 4''	20	70.72	70.13	70.72	70.43	70.54	70.79	70.28	70.57
H 3	6.03	25.76	25.73	25.85	25.84	25.85	25.85	25.83	25.8
H 4	6.88	24.98	24.96	25.03	25.04	25.09	25.09	25.02	24.98
H 5a	2.39	29.75	29.89	29.72	29.85	29.85	29.76	29.8	29.86
H 5b	2.46	29.57	29.54	29.28	29.25	29.57	29.55	28.86	28.87
H 6	4.67	26.8	26.6	26.97	26.97	26.87	26.91	27.05	27.05
H 1'a	1.84	30.15	30.22	30.08	29.98	30.1	30.14	30.05	29.62
H 1'b	2.02	29.55	30.02	29.81	29.81	29.95	30.02	29.86	29.78
H 2'	3.97	27.37	27.11	27.42	28.08	27.91	27.33	27.1	27.36
H 3'a	2.01	30.25	30.4	30.43	29.93	30.71	30.3	30.22	30.15
H 3'b	1.37	30.37	30.22	30.15	30.44	29.9	30.49	30.19	30.26
H 4'	4.07	27.67	27.8	27.55	27.99	27.89	27.55	27.68	27.67
H 5'a	1.77	29.91	29.92	30.24	30.58	30.05	29.99	29.84	30.14
H 5'b	2.16	30.04	29.85	30.07	29.89	30.53	30.26	30.12	29.93
H 6'	4.76	26.95	27.01	27.21	27.89	27.83	27.17	27.22	26.94
H 7'	6.28	25.89	25.62	25.75	25.64	25.69	25.75	25.26	25.77
H 8'	6.03	24.76	24.72	24.9	25.01	24.95	24.89	24.83	24.8
H 2''-6''	6.88	24.285	24.15	24.505	24.49	24.505	24.515	24.415	24.465
H 3''-5''	2.39	24.39	24.355	24.415	24.405	24.405	24.42	24.385	24.405
H 4''	2.46	24.55	24.54	24.54	24.53	24.53	24.54	24.52	24.54
J 3,4	9.6	10.14	10.1	10.07	10.08	10.1	10.09	10.08	10.1
J 4,5a	2.7	3.37	2.89	2.99	2.92	3.07	3.06	2.91	2.88
J 4,5b	5.5	6.05	6.51	6.44	6.5	6.35	6.37	6.5	6.5

J 5a,6	5	3.3	2.74	2.78	2.68	2.99	3.03	2.75	2.7
J 5b,6	11	10	11.5	11.45	11.66	10.93	10.93	11.98	12.14
J 6,1'a	6.3	1.06	1.27	4.97	3.68	1.85	2.61	5.71	4.49
J 6,1'b	6.1	9.7	9.86	5.52	5.92	9.19	8.21	3.56	3.81
J 1'a,2'	5.3	8.25	9.54	3.21	3.4	9.08	8.84	2.42	4.47
J 1'b,2'	7.7	3.75	1.52	7.5	6.01	1.8	2.02	8.66	7.33
J 2',3'a	2.2	8.16	11.02	1.62	1.52	10.35	10.42	2.28	3.34
J 2',3'b	10.3	2.91	1.94	10.55	10.54	1.57	1.67	9.69	7.25
J 4',3'a	4.2	8.3	3.06	2.92	4.24	9.97	2.46	3.91	3.53
J 4',3'b	10.3	3.61	2.95	2.52	9.82	4.34	2.88	3.09	7.55
J 4',5'a	10.3	3.85	2.7	2.86	9.9	4.41	2.79	3.43	7.99
J 4',5'b	4.2	8.83	3.38	2.83	4.36	9.9	2.96	3.51	3.68
J 6',5'a	5.7	3.95	0.98	11.1	10.82	1.73	1.83	6.7	4.9
J 6',5'b	2	5.36	7.63	1.84	1.74	10.81	11.09	2.11	4.81
J 6',7'	5	3.47	2.99	5.59	6.17	6.31	5.67	5.59	4.42
J 7',8'	16.2	15.39	15.75	15.06	15.05	15.03	15.06	15.31	15.26

Table S12. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-16 calculated at the B3LYP/6-31G** level of theory for compound **12**⁹



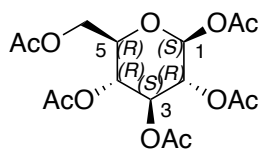
12

Isotropic shielding constants									
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 1	89.1	96.2	96.56	96.45	95.41	96.45	95.46	95.06	95.3
C 2	69.2	119.3	118.51	118.86	119.35	117.28	117.6	118.43	118.06
C 3	69.8	118.79	118.66	120.78	121.91	117.84	114.52	117.31	116.27
C 4	67.9	122.22	122.44	122.81	119.44	121.29	122.1	123.62	123.83
C 5	69.8	121.01	116.79	121.2	114.49	118.61	115.98	118.38	115.46
C 6	61.5	128.04	128.14	127.75	127.98	128.66	128.61	128.16	128.16
H 5	4.14	27.31	27.53	27.43	27.45	27.52	28.03	27.66	27.96
H 1	6.35	25.17	25.37	25.45	25.17	25.1	25.84	25.46	25.84
H 2	5.12	26.74	26.86	26.77	26.31	26.67	26.57	26.37	26.19
H 3	5.5	25.98	25.76	26.11	26.17	26.26	26.52	26.52	26.84
H 4	5.15	26.84	26.86	26.52	26.18	26.52	26.58	26.13	26.26
H 6	4.15	27.78	27.73	27.8	27.48	27.79	27.82	27.86	27.56
J 1,2	3.3	2.67	7.87	1.82	2.58	2.67	7.89	1.86	0.99
J 2,3	10.3	2.48	2.54	4.04	8.62	9.28	8.47	2.78	2.46
J 3,4	9.8	2.38	2.33	2.64	2.54	8.21	8.15	8.89	8.12
J 4,5	9.8	9.73	9.48	8.83	2.99	9.81	9.68	9.76	8.51
J 5,6a	2.2	1.51	1.52	1.79	7.13	1.37	1.35	1.44	2.24
J 5,6b	4.1	3.41	3.91	3.5	5.57	3.46	4.25	3.79	4.3

Isotropic shielding constants									
Nuclei	Experimental	Isomer 9	Isomer 10	Isomer 11	Isomer 12	Isomer 13	Isomer 14	Isomer 15	Isomer 16
C 1	89.1	96.85	96.88	97.71	97.36	95.57	95.23	95.9	94.53
C 2	69.2	119.83	119.26	117.81	117.22	119.44	119.49	119.06	119.31
C 3	69.8	120.47	120.37	117.66	121.52	119.52	115.82	119.93	118.54
C 4	67.9	120.47	120.9	119.23	118.66	120.43	121.9	122.47	123.43
C 5	69.8	120.97	116.12	119.61	119.35	119.66	116.72	120.31	116.58
C 6	61.5	128.29	128.61	128.15	127.48	129.92	130.93	129.68	130.32
H 5	4.14	26.95	27.23	27.11	27.03	27.12	27.77	27.28	27.62
H 1	6.35	25.22	25.46	25.16	25.17	25	25.73	25.2	25.81
H 2	5.12	26.37	26.57	26.61	26.75	26.29	26.24	26.8	26.37
H 3	5.5	26.39	26.06	25.97	25.93	26.42	26.81	26.57	26.82
H 4	5.15	26.67	26.89	26.77	26.63	26.13	26.34	26.34	26.49
H 6	4.15	27.5	27.21	27.65	27.49	27.22	26.93	27.21	26.88
J 1,2	3.3	2.79	7.82	7.14	2.98	2.72	7.77	1.6	1.21
J 2,3	10.3	2.72	2.66	8.2	9.16	9.76	9.23	3.04	2.49
J 3,4	9.8	4.21	4	8.24	9	2.55	2.65	2.35	2.75
J 4,5	9.8	1.68	1.32	6.34	6.77	1	0.79	1.12	2.01
J 5,6a	2.2	4.77	5.23	1.86	3.65	7.61	7.76	7.43	7.28
J 5,6b	4.1	6.8	7.1	3.76	7.33	6.14	6.04	6.25	6.49

⁹ Compound **12**, **13** and **14**: NMR data measured in our lab

Table S13. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-16 calculated at the B3LYP/6-31G** level of theory for compound **13**

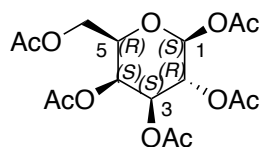


13

Isotropic shielding constants									
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 1	91.7	96.2	96.56	96.45	95.41	96.45	95.46	95.06	95.3
C 2	70.2	119.3	118.51	118.86	119.35	117.28	117.6	118.43	118.06
C 3	72.8	118.79	118.66	120.78	121.91	117.84	114.52	117.31	116.27
C 4	67.7	122.22	122.44	122.81	119.44	121.29	122.1	123.62	123.83
C 5	72.7	121.01	116.79	121.2	114.49	118.61	115.98	118.38	115.46
C 6	61.4	128.04	128.14	127.75	127.98	128.66	128.61	128.16	128.16
H 1	5.72	25.17	25.37	25.45	25.17	25.1	25.84	25.46	25.84
H 2	5.16	26.74	26.86	26.77	26.31	26.67	26.57	26.37	26.19
H 3	5.26	25.98	25.76	26.11	26.17	26.26	26.52	26.52	26.84
H 4	5.15	26.84	26.86	26.52	26.18	26.52	26.58	26.13	26.26
H 5	3.85	27.31	27.53	27.43	27.45	27.52	28.03	27.66	27.96
H 6	4.21	27.78	27.73	27.8	27.48	27.79	27.82	27.86	27.56
J 1,2	8.4	2.67	7.87	1.82	2.58	2.67	7.89	1.86	0.99
J 2,3	9.5	2.48	2.54	4.04	8.62	9.28	8.47	2.78	2.46
J 3,4	9.5	2.38	2.33	2.64	2.54	8.21	8.15	8.89	8.12
J 4,5	10	9.73	9.48	8.83	2.99	9.81	9.68	9.76	8.51
J 5,6a	2	1.51	1.52	1.79	7.13	1.37	1.35	1.44	2.24
J 5,6b	4.4	3.41	3.91	3.5	5.57	3.46	4.25	3.79	4.3

Isotropic shielding constants									
Nuclei	Experimental	Isomer 9	Isomer 10	Isomer 11	Isomer 12	Isomer 13	Isomer 14	Isomer 15	Isomer 16
C 1	91.7	96.85	96.88	97.71	97.36	95.57	95.23	95.9	94.53
C 2	70.2	119.83	119.26	117.81	117.22	119.44	119.49	119.06	119.31
C 3	72.8	120.47	120.37	117.66	121.52	119.52	115.82	119.93	118.54
C 4	67.7	120.47	120.9	119.23	118.66	120.43	121.9	122.47	123.43
C 5	72.7	120.97	116.12	119.61	119.35	119.66	116.72	120.31	116.58
C 6	61.4	128.29	128.61	128.15	127.48	129.92	130.93	129.68	130.32
H 1	5.72	25.22	25.46	25.16	25.17	25	25.73	25.2	25.81
H 2	5.16	26.37	26.57	26.61	26.75	26.29	26.24	26.8	26.37
H 3	5.26	26.39	26.06	25.97	25.93	26.42	26.81	26.57	26.82
H 4	5.15	26.67	26.89	26.77	26.63	26.13	26.34	26.34	26.49
H 5	3.85	26.95	27.23	27.11	27.03	27.12	27.77	27.28	27.62
H 6	4.21	27.5	27.21	27.65	27.49	27.22	26.93	27.21	26.88
J 1,2	8.4	2.79	7.82	7.14	2.98	2.72	7.77	1.6	1.21
J 2,3	9.5	2.72	2.66	8.2	9.16	9.76	9.23	3.04	2.49
J 3,4	9.5	4.21	4	8.24	9	2.55	2.65	2.35	2.75
J 4,5	10	1.68	1.32	6.34	6.77	1	0.79	1.12	2.01
J 5,6a	2	4.77	5.23	1.86	3.65	7.61	7.76	7.43	7.28
J 5,6b	4.4	6.8	7.1	3.76	7.33	6.14	6.04	6.25	6.49

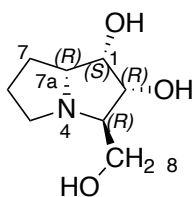
Table S14. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-16 calculated at the B3LYP/6-31G** level of theory for compound **14**



Isotropic shielding constants									
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 1	92.2	96.2	96.56	96.45	95.41	96.45	95.46	95.06	95.3
C 2	67.8	119.3	118.51	118.86	119.35	117.28	117.6	118.43	118.06
C 3	70.8	118.79	118.66	120.78	121.91	117.84	114.52	117.31	116.27
C 4	66.8	122.22	122.44	122.81	119.44	121.29	122.1	123.62	123.83
C 5	71.7	121.01	116.79	121.2	114.49	118.61	115.98	118.38	115.46
C 6	61	128.04	128.14	127.75	127.98	128.66	128.61	128.16	128.16
H 1	5.72	25.17	25.37	25.45	25.17	25.1	25.84	25.46	25.84
H 2	5.35	26.74	26.86	26.77	26.31	26.67	26.57	26.37	26.19
H 3	5.1	25.98	25.76	26.11	26.17	26.26	26.52	26.52	26.84
H 4	5.45	26.84	26.86	26.52	26.18	26.52	26.58	26.13	26.26
H 5	4.07	27.31	27.53	27.43	27.45	27.52	28.03	27.66	27.96
H 6	4.16	26.98	27.08	27.02	27.13	26.96	26.9	26.91	27.06
J 1,2	8	2.67	7.87	1.82	2.58	2.67	7.89	1.86	0.99
J 2,3	9.7	2.48	2.54	4.04	8.62	9.28	8.47	2.78	2.46
J 3,4	3.2	2.38	2.33	2.64	2.54	8.21	8.15	8.89	8.12
J 4,5	0.8	9.73	9.48	8.83	2.99	9.81	9.68	9.76	8.51
J 5,6a	6.8	1.51	1.52	1.79	7.13	1.37	1.35	1.44	2.24
J 5,6b	6.4	3.41	3.91	3.5	5.57	3.46	4.25	3.79	4.3

Isotropic shielding constants									
Nuclei	Experimental	Isomer 9	Isomer 10	Isomer 11	Isomer 12	Isomer 13	Isomer 14	Isomer 15	Isomer 16
C 1	92.2	96.85	96.88	97.71	97.36	95.57	95.23	95.9	94.53
C 2	67.8	119.83	119.26	117.81	117.22	119.44	119.49	119.06	119.31
C 3	70.8	120.47	120.37	117.66	121.52	119.52	115.82	119.93	118.54
C 4	66.8	120.47	120.9	119.23	118.66	120.43	121.9	122.47	123.43
C 5	71.7	120.97	116.12	119.61	119.35	119.66	116.72	120.31	116.58
C 6	61	128.29	128.61	128.15	127.48	129.92	130.93	129.68	130.32
H 1	5.72	25.22	25.46	25.16	25.17	25	25.73	25.2	25.81
H 2	5.35	26.37	26.57	26.61	26.75	26.29	26.24	26.8	26.37
H 3	5.1	26.39	26.06	25.97	25.93	26.42	26.81	26.57	26.82
H 4	5.45	26.67	26.89	26.77	26.63	26.13	26.34	26.34	26.49
H 5	4.07	26.95	27.23	27.11	27.03	27.12	27.77	27.28	27.62
H 6	4.16	27.45	27.75	26.8	26.93	27.8	27.95	27.77	27.7
J 1,2	8	2.79	7.82	7.14	2.98	2.72	7.77	1.6	1.21
J 2,3	9.7	2.72	2.66	8.2	9.16	9.76	9.23	3.04	2.49
J 3,4	3.2	4.21	4	8.24	9	2.55	2.65	2.35	2.75
J 4,5	0.8	1.68	1.32	6.34	6.77	1	0.79	1.12	2.01
J 5,6a	6.8	4.77	5.23	1.86	3.65	7.61	7.76	7.43	7.28
J 5,6b	6.4	6.8	7.1	3.76	7.33	6.14	6.04	6.25	6.49

Table S15. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-8 calculated at the B3LYP/6-31G** level of theory for compound **15**¹⁰

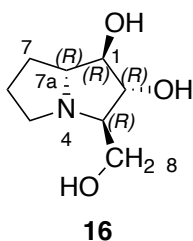


15

Isotropic shielding constants									
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 1	73.7	106.99	118.93	112.64	113.83	107.16	123.95	113.54	115.49
C 2	77.5	105.06	114.82	119.07	104.96	101.55	111.3	116.79	102.02
C 3	71.9	115.88	118.67	120.25	121.16	127.49	127.28	128.97	121.77
C 8	65.2	126.09	128.47	131.55	130.02	131.7	131.28	126.84	130.85
C 7a	67.9	116.68	125.81	120.74	123.71	123.72	120.76	122.35	119.74
C 7	26.0	159.96	166.37	159.07	166.91	163.95	168.72	159.86	168.07
C 6	28.8	165.66	163.09	164.04	162.18	162.95	163.57	162.99	162.07
C 5	57.5	136.43	137.27	136.43	138.19	145.72	146.62	143.01	145.77
H 1	3.87	28.18	27.83	28.2	27.87	28.02	28.18	27.96	28.38
H 2	3.88	27.62	27.55	27.7	27.7	27.63	27.46	27.65	27.16
H 3	2.76	28.97	28.97	29.2	29.06	29.53	29.78	28.46	29.55
H 8	3.78	28.39	28.04	28.34	27.94	28.01	27.99	27.52	28.14
H 5 α	3.05	28.95	29.32	29.31	29.43	28.96	28.98	29.4	29.01
H 5 β	2.65	29.03	28.99	28.87	28.89	30.02	30.14	29.33	29.79
H 6 α	1.74	30.33	30.12	30.17	29.98	29.83	29.88	30.09	29.77
H 6 β	1.93	29.85	29.87	30.19	29.91	29.63	29.62	30.21	29.67
H 7a	3.47	28.3	28.22	28.32	27.61	29.49	29.65	28.04	28.76
H 7 α	1.68	29.86	30.27	29.76	30.25	29.98	30.35	29.72	30.34
H 7 β	2.08	30.02	29.39	30.39	29.51	30.35	29.66	30.49	29.93
H 8'	3.58	28.22	28.34	27.79	27.91	28.04	27.97	27.73	27.94
J 2,3	9	0.85	7.92	6.38	3.08	7	6.72	8.59	3.29
J 1,7a	4	0.63	3.79	2.08	4.69	7.59	2.87	0.84	3.53
J 1,2	4	0.55	3.88	4.54	0.99	4.15	5.39	5.01	0.28
J 5 α ,6 α	8.1	3.44	6.92	7.05	7.38	1.62	1.85	10.52	3.43
J 5 α ,6 β	6.1	6.15	5.48	5.42	5.4	8.63	8.65	4.72	7.85
J 3,8	6.4	0.46	4.83	3.86	0.55	0.87	1.62	4.43	0.85
J 3,8'	3.4	3.81	1.88	0.48	2.94	1.98	3.32	9.43	2.7
J 5 β ,6 α	6.4	5.75	5.73	5.8	5.81	8.92	9.17	5.91	8.53
J 5 β ,6 β	4.9	9.34	5.5	5.35	4.99	7.17	6.89	1.43	6.09
J 7a,7 α	8.1	10.09	8.63	8.29	8.63	4.46	4.52	8.07	4.98
J 7a,7 β	6.6	5.24	5.72	6.51	6.29	9.53	10.06	8.01	10.09

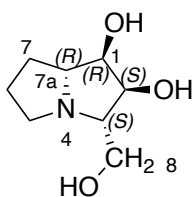
¹⁰ Compound **15** and **16**: NMR data from Asano, N. Kuroi, H. Ikeda, K. Kizu, H. Kameda, Y. Kato, A. Adachi, I. Watson, A.A. Nash, R.J. Fleet, G.W. *Tetrahedron Asymmetry*, **2000**, *11*, 1

Table S16. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-8 calculated at the B3LYP/6-31G** level of theory for compound **16**



Isotropic shielding constants									
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 1	82.9	106.99	118.93	112.64	113.83	107.16	123.95	113.54	115.49
C 2	79.8	105.06	114.82	119.07	104.96	101.55	111.3	116.79	102.02
C 3	72.1	115.88	118.67	120.25	121.16	127.49	127.28	128.97	121.77
C 8	65.3	126.09	128.47	131.55	130.02	131.7	131.28	126.84	130.85
C 7a	69.2	116.68	125.81	120.74	123.71	123.72	120.76	122.35	119.74
C 7	32.5	159.96	166.37	159.07	166.91	163.95	168.72	159.86	168.07
C 6	27.3	165.66	163.09	164.04	162.18	162.95	163.57	162.99	162.07
C 5	57.7	136.43	137.27	136.43	138.19	145.72	146.62	143.01	145.77
H 7a	3.32	28.3	28.22	28.32	27.61	29.49	29.65	28.04	28.76
H 1	3.76	28.18	27.83	28.2	27.87	28.02	28.18	27.96	28.38
H 2	3.81	27.62	27.55	27.7	27.7	27.63	27.46	27.65	27.16
H 3	2.77	28.97	28.97	29.2	29.06	29.53	29.78	28.46	29.55
H 8	3.67	28.39	28.04	28.34	27.94	28.01	27.99	27.52	28.14
H 8'	3.80	28.22	28.34	27.79	27.91	28.04	27.97	27.73	27.94
H 7 α	1.97	29.86	30.27	29.76	30.25	29.98	30.35	29.72	30.34
H 7 β	1.97	30.02	29.39	30.39	29.51	30.35	29.66	30.49	29.93
H 6 α	1.82	30.33	30.12	30.17	29.98	29.83	29.88	30.09	29.77
H 6 β	1.90	29.85	29.87	30.19	29.91	29.63	29.62	30.21	29.67
H 5 α	2.96	28.95	29.32	29.31	29.43	28.96	28.98	29.4	29.01
H 5 β	2.81	29.03	28.99	28.87	28.89	30.02	30.14	29.33	29.79
J 2,3	8.8	0.85	7.92	6.38	3.08	7	6.72	8.59	3.29
J 1,7a	7.1	0.63	3.79	2.08	4.69	7.59	2.87	0.84	3.53
J 1,2	8.8	0.55	3.88	4.54	0.99	4.15	5.39	5.01	0.28
J 5 α ,6 α	5.6	3.44	6.92	7.05	7.38	1.62	1.85	10.52	3.43
J 5 α ,6 β	5.6	6.15	5.48	5.42	5.4	8.63	8.65	4.72	7.85
J 3,8	3.9	0.46	4.83	3.86	0.55	0.87	1.62	4.43	0.85
J 3,8'	6.5	3.81	1.88	0.48	2.94	1.98	3.32	9.43	2.7
J 5 β ,6 α	5.9	5.75	5.73	5.8	5.81	8.92	9.17	5.91	8.53
J 5 β ,6 β	7.3	9.34	5.5	5.35	4.99	7.17	6.89	1.43	6.09

Table S17. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-8 calculated at the B3LYP/6-31G** level of theory for compound **17**¹¹

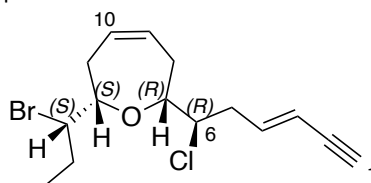


17

Isotropic shielding constants									
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 1	76.9	106.99	118.93	112.64	113.83	107.16	123.95	113.54	115.49
C 2	72.5	105.06	114.82	119.07	104.96	101.55	111.3	116.79	102.02
C 3	67.1	115.88	118.67	120.25	121.16	127.49	127.28	128.97	121.77
C 8	60.9	126.09	128.47	131.55	130.02	131.7	131.28	126.84	130.85
C 7a	72.1	116.68	125.81	120.74	123.71	123.72	120.76	122.35	119.74
C 7	30.9	159.96	166.37	159.07	166.91	163.95	168.72	159.86	168.07
C 6	27.4	165.66	163.09	164.04	162.18	162.95	163.57	162.99	162.07
C 5	49.1	136.43	137.27	136.43	138.19	145.72	146.62	143.01	145.77
H 7a	3.39	28.3	28.22	28.32	27.61	29.49	29.65	28.04	28.76
H 1	3.76	28.18	27.83	28.2	27.87	28.02	28.18	27.96	28.38
H 2	3.88	27.62	27.55	27.7	27.7	27.63	27.46	27.65	27.16
H 3	3.21	28.97	28.97	29.2	29.06	29.53	29.78	28.46	29.55
H 8	3.84	28.39	28.04	28.34	27.94	28.01	27.99	27.52	28.14
H 8'	3.81	28.22	28.34	27.79	27.91	28.04	27.97	27.73	27.94
H 7 α	2.14	29.86	30.27	29.76	30.25	29.98	30.35	29.72	30.34
H 7 β	1.50	30.02	29.39	30.39	29.51	30.35	29.66	30.49	29.93
H 6 α	1.87	30.33	30.12	30.17	29.98	29.83	29.88	30.09	29.77
H 6 β	1.69	29.85	29.87	30.19	29.91	29.63	29.62	30.21	29.67
H 5 α	2.91	28.95	29.32	29.31	29.43	28.96	28.98	29.4	29.01
H 5 β	2.79	29.03	28.99	28.87	28.89	30.02	30.14	29.33	29.79
J 2,3	9	0.85	7.92	6.38	3.08	7	6.72	8.59	3.29
J 1,7a	2.4	0.63	3.79	2.08	4.69	7.59	2.87	0.84	3.53
J 1,2	5.5	0.55	3.88	4.54	0.99	4.15	5.39	5.01	0.28
J 3,8	4.1	0.46	4.83	3.86	0.55	0.87	1.62	4.43	0.85
J 3,8'	8	3.81	1.88	0.48	2.94	1.98	3.32	9.43	2.7
J 7a,7 α	7.9	10.09	8.63	8.29	8.63	4.46	4.52	8.07	4.98
J 7a,7 β	7.9	5.24	5.72	6.51	6.29	9.53	10.06	8.01	10.09

¹¹ Compound **17**: NMR data from Izquierdo, I. Plaza, M.T. Tamayo, J.A. Franco, F. Sánchez-Cantalejo, F. *Tetrahedron*, **2010**, 66, 3788

Table S18. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-8 calculated at the B3LYP/6-31G** level of theory for compound **18**¹²

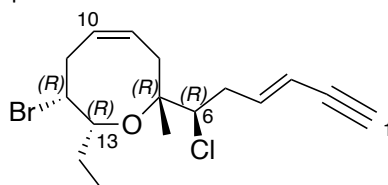


Isotropic shielding constants									
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 1	77	118.05	118.43	118.31	118.63	118.14	118.55	118.28	118.59
C 2	82	117.52	117.56	117.57	117.4	117.53	117.53	117.62	117.42
C 3	111.8	81.78	83.16	83.13	82.53	82.24	83.21	83.39	82.3
C 4	142	53	51.31	51.51	52.01	52.55	51.22	51.39	52.44
C 5	37.6	149.85	151.32	150.89	151.15	150.09	151.02	151.16	151.05
C 6	63	121.93	122.87	122.87	124.02	122.13	122.77	123.3	123.9
C 7	81.2	113.51	106.49	108.46	111.09	113.25	106.69	107.6	111
C 8	32.7	157.16	156.97	157.56	159.49	157.75	156.81	158.32	159.53
C 10	82.5	111.07	106.17	105.31	110.78	109.97	105.31	105.8	110.84
C 13	28	158.04	160.1	160.98	160.79	159.69	160.37	160.39	159.34
C 14	12.7	177.28	177.19	177.55	177.48	177.74	177.36	177.3	177.49
C 15	33.8	156.71	157.56	155.98	156.92	159.99	156.64	158.11	156.87
C 16	129.2	64.99	62.59	63.27	65.19	65.09	63.13	62.63	64.82
C 17	129	65.42	63.82	62.44	66.27	64.92	63.33	62.74	66.13
H 1	2.83	29.24	29.25	29.26	29.26	29.25	29.26	29.25	29.26
H 3	5.59	25.83	26.14	26.07	26.01	25.92	26.13	26.15	25.99
H 4	6.27	25.35	25.09	25.21	25.02	25.32	25.07	25.18	25.01
H 5a	2.56	29.37	29.29	29.43	29.24	29.4	29.26	29.46	29.21
H 5b	2.78	28.84	29.11	28.96	29.04	28.9	29.04	29.1	29.12
H 7	3.52	27.21	28.27	28.21	27.53	27.23	28.29	28.25	27.5
H 8a	2.3	29.9	29.27	29.64	29.22	29.86	29.3	29.58	29.28
H 8b	2.55	28.73	29.41	28.98	29.26	28.76	29.35	29.06	29.24
H 9	5.8	25.86	25.63	25.57	25.81	25.83	25.61	25.57	25.83
H 10	5.83	25.84	25.58	25.6	25.87	25.83	25.62	25.56	25.84
H 11a	2.55	29.84	29.47	29.11	29.04	29.59	29.61	29.11	28.92
H 11b	2.36	28.71	29.11	29.59	29.66	28.92	29.06	29.46	29.66
H 12	3.59	27.23	28.07	28.15	27.23	27.31	28.1	28.2	27.24
H 14a	1.85	29.66	29.73	29.73	29.83	29.99	29.93	30.04	29.92
H 14b	1.98	29.69	29.98	29.82	29.9	29.92	29.8	29.74	29.8
H 15	0.94	30.69	30.69	30.69	30.67	30.63	30.68	30.69	30.7
J 6,7	4	1.47	5.99	2.2	8.01	1.61	6.33	2.61	8.22
J 7,8a	2	0.39	8.42	0.44	9.34	0.39	8.62	0.43	9.35
J 7,8b	10	9.15	0.74	9.1	1.65	9.21	0.66	9.11	1.07
J 8a,9	4	7.74	4.39	8.88	3.57	7.79	4.23	8.92	3.08
J 8b,9	4	2.64	8.37	3.99	7.95	2.68	8.55	4.01	8.07
J 9,10	8	10.81	10.75	10.67	10.76	10.77	10.76	10.67	10.76

¹² Compound **18** and **19**: NMR data from A. Fukuzawa and T. Masamune, *Tetrahedron Lett.*, **1981**, 22, 4081

J 10,11a	4	7.71	8.7	4.1	3.42	7.74	8.66	4.04	3.09
J 10,11b	4	2.65	3.82	8.87	6.86	2.82	3.95	8.9	7.08
J 11a,12	10	0.39	0.49	8.97	9.69	0.4	0.59	9.04	9.47
J 11b,12	2	9	9.09	0.48	0.85	8.74	8.86	0.48	0.64
J 12,13	4	1.47	2.56	4.02	3.12	3.98	3.57	2.94	2.89

Table S19. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-8 calculated at the B3LYP/6-31G** level of theory for compound **19**

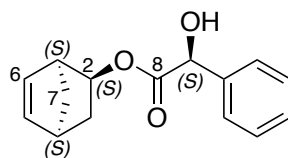


19

Isotropic shielding constants									
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 1	76.8	118.33	118.34	117.84	118.03	118.24	118.13	117.92	118.35
C 2	81.9	117.59	117.51	117.8	117.78	117.7	117.71	117.57	117.59
C 3	111.8	83.32	82.06	82.67	83.14	83.45	82.95	81.82	83.08
C 4	141.9	51.19	52.9	52.27	51.61	51.3	51.8	52.8	51.16
C 5	36.6	152.33	150.32	149.79	150.56	152.04	149.64	149.26	150.91
C 6	63	123.9	123.47	122.39	122.19	124.2	124.75	120.92	122.51
C 7	82.1	106	113.52	114.35	103.61	104.08	113.37	116.81	105.14
C 8	29.4	161.12	158.12	158.22	158.68	161.41	161.15	154.88	157.22
C 9	130.3	61.46	61.49	64.14	64.14	63.69	66.68	61.06	61.95
C 10	129.9	64.36	68.32	66.45	63.42	63.81	63.97	69.81	64.05
C 11	35.5	153.51	153.64	153.33	155.99	156.19	151.12	153.14	153.56
C 13	81.5	107.14	114.84	113.22	106.16	105.01	111.7	114.95	107.66
C 14	28.9	160.93	160.33	160.87	163.05	162.15	162.31	160.5	161.47
C 15	10.3	179.54	178.95	180.47	181.25	180.15	180.49	178.66	180.11
H 1	2.86	29.25	29.24	29.22	29.23	29.25	29.24	29.23	29.25
H 3	5.61	26.15	26.07	26.12	26.18	26.19	26.15	25.96	26.13
H 4	6.29	25.12	24.95	25.21	25.17	25.17	25.12	25.19	25.12
H 5a	2.5	29.08	29.26	29.08	29.21	29.2	29.03	28.82	28.97
H 5b	2.8	29.53	29.13	29.34	29.36	29.52	29.49	29.33	29.39
H 6	3.97	27.83	28.04	28.04	27.97	27.81	27.9	28.13	28.08
H 7	3.51	28.29	27.32	27.52	28.38	28.3	27.95	26.89	28.39
H 8a	2.56	29.44	29.5	29.74	29.29	29.45	29.28	29.75	29.26
H 8b	2.32	29.23	29.12	28.98	29.62	29.37	29.42	28.86	29.47
H 9	5.9	25.58	25.69	25.79	25.57	25.53	25.81	25.71	25.59
H 10	5.7	25.76	25.77	25.65	25.31	25.3	25.73	25.86	25.76
H 11a	3.12	28.72	28.78	29.09	29.33	28.84	28.95	29.13	29.22
H 11b	2.65	29.22	29.17	28.92	28.83	29.35	28.97	28.74	28.71
H 12	4.1	27.6	27.56	27.64	27.55	27.66	27.42	27.58	27.56
H 13	3.49	27.94	27.52	27.6	28.17	28.22	27.71	27.41	27.97
H 14a	1.54	30.03	30.07	29.95	30.04	29.86	29.93	29.74	29.98
H 14b	1.74	30.01	29.97	29.73	29.87	30.21	29.9	30.15	29.85
H 15a-c	0.89	30.93	30.89	30.71	30.79	30.78	30.75	30.82	30.97
J 6,7	4	2.96	7.44	2.78	4.12	2.88	7.46	1.43	5.61
J 7,8a	1	0.52	9.88	1.62	8.98	0.48	6.84	0.85	8.96
J 7,8b	10	9.44	1.3	9.19	0.66	9.44	2.99	9.77	0.72
J 8a,9	8	8.26	6.06	6.53	6.68	8.34	7.72	5.64	6.84
J 8b,9	1.5	6.81	6.03	5.93	8.37	6.65	6.74	5.2	8.34
J 9,10	10	10.45	11.17	11.23	10.63	10.64	11.05	11.4	10.45
J 10,11a	2	9.05	7.13	7.75	6.73	8.41	7.11	8.63	7.15

J 10,11b	6	7.19	7.95	7.1	8.41	6.72	6.14	6.71	9.02
J 11a,12	10	11.21	8.64	6.69	2.5	3.81	2.62	6.36	5.41
J 11b,12	5	5.54	5.55	3.01	3.81	2.3	9.45	9.67	10.98
J 12,13	2	1.78	0.76	9.39	9.52	9.32	9.28	0.73	1.77

Table S20. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-4 calculated at the B3LYP/6-31G** level of theory for compound **20**¹³

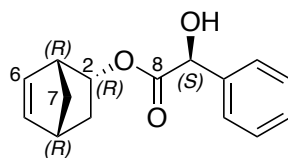


20

Isotropic shielding constants					
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4
C 1	45.5	145.29	143.53	143.87	145.37
C 2	76.8	115.08	115.56	115.56	115.24
C 3	34.1	155.53	155.48	155.08	155.81
C 4	42	148.88	150.17	150.29	148.72
C 5	138.2	54.28	51.52	51.18	54.62
C 6	130.9	60.9	59.41	59.65	60.41
C 7	47.4	141.9	141.37	141.4	142.03
C 8	173.7	18.29	18.32	18.4	18.19
C 9	72.6	116.43	116.34	116.17	116.41
C 10,11,12,13,14,15	138.3	66.93	66.83	66.805	66.905
H 1	3	28.77	29.21	29.05	28.93
H 2	5.34	26.51	27	27.03	26.48
H 3x	2.13	30.85	29.9	30.48	29.52
H 3n	0.99	29.6	30.17	29.98	30.59
H 4	2.82	29.27	29.24	29.31	29.24
H 5	6.22	25.32	25.22	25.22	25.3
H 6	5.4	25.59	25.48	25.46	25.89
H 7anti	1.28	30.54	30.45	30.11	30.28
H 7syn	1.4	30.21	30.2	30.4	30.58
H 9	5.06	26.58	26.56	26.56	26.59
H 10,11,12,13,14,15	7.35	24.362	24.318	24.326	24.332
J 5,6	5.6	6.61	6.63	6.63	6.61
J 1,6	2.8	3.24	3.58	3.57	3.25
J 2,3n	3.6	2.4	6.54	1.88	7.44
J 3n,4	3.1	7.38	1.89	6.42	2.39
J 2,3x	3.9	0.55	0.59	3.78	3.9
J 3x,4	8.3	3.92	3.8	0.6	0.55
J 1,7syn	1.9	1.97	1.62	2.09	1.79

¹³ Compounds **20-23**: NMR data from Pisano, P. L.; Sarotti, A. M.; Pellegrinet, S. C. *Tetrahedron Lett.* **2009**, 50, 6121

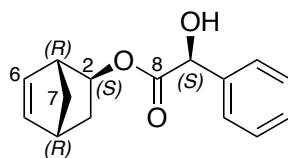
Table S21. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-4 calculated at the B3LYP/6-31G** level of theory for compound **21**



21

Isotropic shielding constants					
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4
C 1	45.6	145.29	143.53	143.87	145.37
C 2	77	115.08	115.56	115.56	115.24
C 3	34.2	155.53	155.48	155.08	155.81
C 4	42	148.88	150.17	150.29	148.72
C 5	138.5	54.28	51.52	51.18	54.62
C 6	131	60.9	59.41	59.65	60.41
C 7	47.4	141.9	141.37	141.4	142.03
C 8	173.5	18.29	18.32	18.4	18.19
C 9	72.5	116.43	116.34	116.17	116.41
C 10,11,12,13,14,15	138.1	66.93	66.84	66.81	66.91
H 1	3.19	28.77	29.21	29.05	28.93
H 2	5.34	26.51	27	27.03	26.48
H 3x	0.68	30.85	29.9	30.48	29.52
H 3n	2.04	29.6	30.17	29.98	30.59
H 4	2.78	29.27	29.24	29.31	29.24
H 5	6.22	25.32	25.22	25.22	25.3
H 6	5.92	25.59	25.48	25.46	25.89
H 7anti	1.28	30.54	30.45	30.11	30.28
H 7syn	1.47	30.21	30.2	30.4	30.58
H 9	5.08	26.58	26.56	26.56	26.59
H 10,11,12,13,14,15	7.35	24.36	24.32	24.33	24.33
J 5,6	5.6	6.61	6.63	6.63	6.61
J 1,6	2.8	3.24	3.58	3.57	3.25
J 2,3n	3.2	2.4	6.54	1.88	7.44
J 3n,4	3.6	7.38	1.89	6.42	2.39
J 2,3x	8.1	0.55	0.59	3.78	3.9
J 3x,4	3.9	3.92	3.8	0.6	0.55
J 1,7syn	1.9	1.97	1.62	2.09	1.79

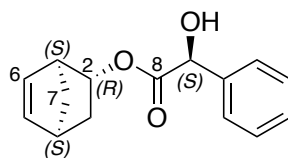
Table S22. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-4 calculated at the B3LYP/6-31G** level of theory for compound **22**



22

Isotropic shielding constants					
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4
C 1	47	145.29	143.53	143.87	145.37
C 2	77.1	115.08	115.56	115.56	115.24
C 3	34.3	155.53	155.48	155.08	155.81
C 4	40.4	148.88	150.17	150.29	148.72
C 5	141.3	54.28	51.52	51.18	54.62
C 6	132.1	60.9	59.41	59.65	60.41
C 7	46	141.9	141.37	141.4	142.03
C 8	173.7	18.29	18.32	18.4	18.19
C 9	72.8	116.43	116.34	116.17	116.41
H 1	2.68	28.77	29.21	29.05	28.93
H 2	4.74	26.51	27	27.03	26.48
H 3x	1.72	30.85	29.9	30.48	29.52
H 3n	1.44	29.6	30.17	29.98	30.59
H 4	2.82	29.27	29.24	29.31	29.24
H 5	6.22	25.32	25.22	25.22	25.3
H 6	5.9	25.59	25.48	25.46	25.89
H 7anti	1.44	30.54	30.45	30.11	30.28
H 7syn	1.44	30.21	30.2	30.4	30.58
H 9	5.14	26.58	26.56	26.56	26.59
J 5,6	5.5	6.61	6.63	6.63	6.61
J 1,6	3.3	3.24	3.58	3.57	3.25
J 3n,4	2.5	0.55	0.59	3.78	3.9

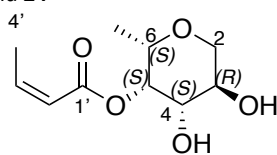
Table S23. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-4 calculated at the B3LYP/6-31G** level of theory for compound **23**



23

Isotropic shielding constants					
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4
C 1	47.1	145.29	143.53	143.87	145.37
C 2	77.1	115.08	115.56	115.56	115.24
C 3	34.4	155.53	155.48	155.08	155.81
C 4	40.4	148.88	150.17	150.29	148.72
C 5	141.4	54.28	51.52	51.18	54.62
C 6	132	60.9	59.41	59.65	60.41
C 7	46.1	141.9	141.37	141.4	142.03
C 8	173.5	18.29	18.32	18.4	18.19
C 9	72.8	116.43	116.34	116.17	116.41
H 1	2.94	28.77	29.21	29.05	28.93
H 2	4.74	26.51	27	27.03	26.48
H 3x	1.11	30.85	29.9	30.48	29.52
H 3n	1.62	29.6	30.17	29.98	30.59
H 4	2.77	29.27	29.24	29.31	29.24
H 5	6.22	25.32	25.22	25.22	25.3
H 6	5.95	25.59	25.48	25.46	25.89
H 7anti	1.56	30.54	30.45	30.11	30.28
H 7syn	1.56	30.21	30.2	30.4	30.58
H 9	5.15	26.58	26.56	26.56	26.59
J 5,6	5.7	6.61	6.63	6.63	6.61
J 1,6	3.3	3.24	3.58	3.57	3.25
J 2,3n	2.3	2.4	6.54	1.88	7.44
J 3n,4	2.5	7.38	1.89	6.42	2.39
J 2,3x	3.4	0.55	0.59	3.78	3.9

Table S24. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-8 calculated at the B3LYP/6-31G** level of theory for compound **24**¹⁴

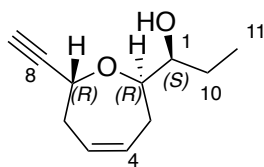


24

Isotropic shielding constants									
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 2	69.7	125.22	123.44	124.43	123.1	127.54	123.92	123.79	120.43
C 3	67.7	122.85	121.76	118.09	120.47	121.29	121.81	122.67	120.54
C 4	74.7	119.85	119.9	111.42	115.49	118.75	120.72	113.06	121.23
C 5	72.9	114.83	117.74	111.97	112.93	115.3	116.68	116.19	116.68
C 6	73.8	121.89	120.27	118.06	119.02	121.53	119.91	116.8	116.28
C 7	16.7	172.91	171.95	171.81	171.77	176.62	173.87	172.83	172.62
C 1'	167	33.38	33.58	28.76	28.94	29.62	32.06	29	32.79
C 2'	119.9	74.78	74.69	75.19	74.81	74.46	74.27	74.61	74.32
C 3'	147	46.09	46.51	44.46	45.3	45.9	46.94	45.93	46.82
C 4'	15.7	175.35	175.36	175.28	175.21	175.33	175.55	175.54	175.5
H 2ax	3.18	28.24	27.8	28.61	28.45	27.88	27.93	28.58	28.36
H 2eq	3.99	28.05	28.2	27.87	27.63	28.06	28.04	27.73	27.7
H 3	3.83	28.12	28.01	27.85	27.98	27.9	28.29	27.65	28.24
H 4	3.67	27.5	27.6	28.07	28.13	27.84	27.58	27.98	28.37
H 5	5.18	27.33	26.79	27.36	26.95	26.66	27.29	26.9	26.6
H 6	3.67	27.83	27.92	28.31	28.47	27.54	27.72	28.15	28.39
H 7a-c	1.14	30.7	30.68	30.62	30.6	30.62	30.6	30.6	30.63
H 2'	5.89	25.95	25.97	25.82	25.83	25.81	25.89	25.73	25.91
H 3'	6.41	25.16	25.17	25.06	25.09	25.13	25.19	25.12	25.17
H 4'a-c	2.14	29.6	29.61	29.57	29.58	29.59	29.61	29.6	29.6
J 2ax,3	10	8.79	1.37	10.46	1.23	2.2	2.14	10.25	1.17
J 2eq,3	5.4	4.93	2.28	5.31	1.61	2.89	3.53	5.4	1.78
J 3,4	9.6	2.91	3.97	8.17	3.27	3.02	4.04	8.64	2.63
J 4,5	3.5	2.43	2.75	8.16	7.72	6.7	3.77	2.81	3.41
J 5,6	1.1	8.16	8.79	8.95	9.01	4.81	2.21	0.84	0.72

¹⁴ Compounds **24**: NMR data from Reátegui, R. F.; Gloer, J. B.; Campbell, J.; Shearer, C. A. *J. Nat. Prod.* **2005**, *68*, 701.

Table S25. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-4 calculated at the B3LYP/6-31G** level of theory for compound **25**¹⁵

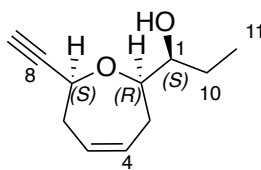


25

Isotropic shielding constants					
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4
C 1	75.3	114.02	115.3	114.66	114.65
C 2	76	115.19	105.21	106.24	114.6
C 3	30.8	158.24	156.73	157.45	156.49
C 4	130.9	60.85	62.38	61.54	61.56
C 5	127.1	66.23	64.09	64.27	66.48
C 6	35.7	154.97	152.29	152.49	154.98
C 7	66.4	125.65	120.72	120.87	125.51
C 8	82.3	118.11	115.82	115.76	117.86
C 9	74.4	123.48	125.03	125.17	123.42
C 10	25.3	164.3	163.04	164.48	162.57
C 11	10.4	178.26	178.94	178.3	179.03
H 1	3.55	28.24	28.29	28.32	28.34
H 2	4.03	27.64	28.73	28.45	27.8
H 3a	2.24	29.78	29.29	29.87	29.23
H 3b	2.38	29.17	29.71	29.15	29.66
H 4	5.88	25.53	25.64	25.58	25.58
H 5	5.73	25.72	25.7	25.69	25.74
H 6a	2.51	29.46	28.9	29.48	29.07
H 6b	2.63	29.01	29.49	28.9	29.37
H 7	4.82	27.05	27.71	27.73	27.01
H 9	2.45	29.94	29.93	29.95	29.91
H 10a	1.49	30.25	30.32	30.24	30.3
H 10b	1.49	30.48	30.34	30.46	30.33
H 11a-c	0.98	30.74	30.72	30.73	30.74
J 2,3b	10.6	9.33	0.6	9.51	0.58
J 2,3a	1.8	0.38	9.54	0.49	9.4
J 6b,7	3.8	3.82	0.76	9.95	4.56
J 4,5	11	10.64	11	10.87	10.7
J 3a,4	7.5	8.44	3.55	8.71	4.11
J 3b,4	0	4.09	8.75	3.7	8.2
J 1,2	3.85	2.15	6.06	2.31	5.25
J 1,10b	8.3	9.19	8.95	9.18	8.6
J 1,10a	4.1	2.08	2.14	1.98	2.4

¹⁵ Compounds **25** and **26**: NMR data measured in our lab

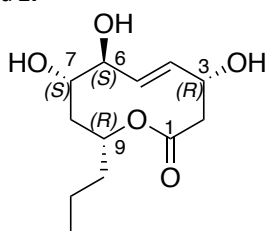
Table S26. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-4 calculated at the B3LYP/6-31G** level of theory for compound **26**



26

Isotropic shielding constants					
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4
C 1	75.7	114.02	115.3	114.66	114.65
C 2	83.4	115.19	105.21	106.24	114.6
C 3	31.5	158.24	156.73	157.45	156.49
C 4	130.6	60.85	62.38	61.54	61.56
C 5	128.3	66.23	64.09	64.27	66.48
C 6	38.5	154.97	152.29	152.49	154.98
C 7	70.4	125.65	120.72	120.87	125.51
C 8	83.7	118.11	115.82	115.76	117.86
C 9	72.3	123.48	125.03	125.17	123.42
C 10	25.4	164.3	163.04	164.48	162.57
C 11	10.4	178.26	178.94	178.3	179.03
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H 1	3.56	28.24	28.29	28.32	28.34
H 2	3.35	27.64	28.73	28.45	27.8
H 3a	2.23	29.78	29.29	29.87	29.23
H 3b	2.37	29.17	29.71	29.15	29.66
H 4	5.85	25.53	25.64	25.58	25.58
H 5	5.73	25.72	25.7	25.69	25.74
H 6a	2.47	29.46	28.9	29.48	29.07
H 6b	2.66	29.01	29.49	28.9	29.37
H 7	4.19	27.05	27.71	27.73	27.01
H 9	2.45	29.94	29.93	29.95	29.91
H 10a	1.5	30.25	30.32	30.24	30.3
H 10b	1.5	30.48	30.34	30.46	30.33
H 11a-c	0.97	30.74	30.72	30.73	30.74
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J 2,3b	10.5	9.33	0.6	9.51	0.58
J 2,3a	1.5	0.38	9.54	0.49	9.4
J 6b,7	10.55	3.82	0.76	9.95	4.56
J 6a,7	1.95	3.79	10.04	0.72	3.78
J 4,5	11.15	10.64	11	10.87	10.7
J 3a,4	7.9	8.44	3.55	8.71	4.11
J 3b,4	3.1	4.09	8.75	3.7	8.2
J 1,2	4	2.15	6.06	2.31	5.25
J 1,10b	8.5	9.19	8.95	9.18	8.6
J 1,10a	4	2.08	2.14	1.98	2.4

Table S27. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-8 calculated at the B3LYP/6-31G** level of theory for compound **27**¹⁶

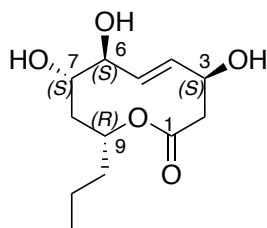


27

Isotropic shielding constants									
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 1	169.4	23.2	24.14	22.75	24.78	22.42	24.98	23	25.32
C 2	45.2	149.69	150.07	148.93	149.22	148.16	149.32	149.18	150.61
C 3	71.6	123.46	120.38	123.99	119.03	123.27	119.34	124.17	119.21
C 4	136.4	55.95	54.97	61.54	55.45	58.2	59.24	57.06	55.53
C 5	128.1	62.95	61.98	63.68	61.31	62.89	59.74	63.83	60.36
C 6	78.1	115.71	113.42	116.48	115.24	116.71	120.3	112.22	116.66
C 7	76	115.76	113.49	114.82	118.38	119.11	118.32	113.69	115.48
C 8	41.1	156.47	151.17	149.26	152.93	152.49	158.02	148.69	156.36
C 9	72.5	119.09	117.25	121.5	123.07	123.17	120.39	121.79	120.87
C 10	39	155.28	150.82	150.35	151	150.81	151.19	150.17	154.71
C 11	18.1	169.65	169.72	170.51	170.11	169.54	169.28	170.77	169.79
C 12	13.2	176.07	176.08	177.48	176.12	176.07	176.42	177.55	176.29
H 2a	2.51	29.28	29.23	29.22	29.2	29.24	29.12	29.29	29.19
H 2b	2.21	29.43	29.47	29.31	29.47	29.29	29.51	29.32	29.38
H 3	4.22	27.21	27.24	27.22	27.19	27.23	26.99	27.34	27.1
H 4	5.61	25.36	25.64	25.61	25.82	25.68	25.51	25.71	25.25
H 5	5.06	25.64	25.99	25.79	25.66	25.64	25.91	25.76	25.81
H 6	3.57	27.66	27.83	27.09	27.74	27.59	27.69	27.76	27.7
H 7	3.23	27.56	27.92	27.98	27.45	27.6	27.72	27.88	27.55
H 8a	1.71	30.22	29.97	29.27	29.67	30.09	30.03	29.88	29.71
H 8b	1.71	29.54	29.74	30.06	30.06	29.64	29.85	29.93	30.18
H 9	4.68	26.88	27.15	26.68	26.41	26.3	26.69	26.59	26.82
H 10a	1.39	30.11	29.94	30.41	30.23	30.39	29.66	30.46	29.98
H 10b	1.39	30.01	30.42	29.96	30.33	30.18	30.23	30.02	30.2
H 11a	1.19	30.33	30.41	30.42	30.34	30.39	30.46	30.45	30.32
H 11b	1.19	30.28	30.4	30.57	30.42	30.38	30.38	30.59	30.33
H 12a-c	0.79	30.8	30.86	30.77	30.85	30.84	30.85	30.76	30.8
J 2a,3	5.8	4.42	4.93	4.55	4.77	4.48	5.12	4.52	5.87
J 2b,3	10.4	2.83	10.09	2.71	12.3	2.73	11.68	2.81	11.4
J 3,4	8.6	3.27	6.92	3.72	7.77	3.28	7.47	3.73	8.09
J 6,7	9.1	7.69	8	2.35	2.54	3.22	3.99	8.01	7.36

¹⁶ Compounds **27** and **28**: NMR data from J. McNulty, D. McLeod, H. A. Jenkins, *Eur. J. Org. Chem.* **2016**

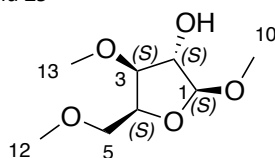
Table S28. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-8 calculated at the B3LYP/6-31G** level of theory for compound **28**



28

Isotropic shielding constants									
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 1	170.3	23.2	24.14	22.75	24.78	22.42	24.98	23	25.32
C 2	44.5	149.69	150.07	148.93	149.22	148.16	149.32	149.18	150.61
C 3	67.6	123.46	120.38	123.99	119.03	123.27	119.34	124.17	119.21
C 4	136.3	55.95	54.97	61.54	55.45	58.2	59.24	57.06	55.53
C 5	127.2	62.95	61.98	63.68	61.31	62.89	59.74	63.83	60.36
C 6	79.7	115.71	113.42	116.48	115.24	116.71	120.3	112.22	116.66
C 7	76.9	115.76	113.49	114.82	118.38	119.11	118.32	113.69	115.48
C 8	42	156.47	151.17	149.26	152.93	152.49	158.02	148.69	156.36
C 9	73	119.09	117.25	121.5	123.07	123.17	120.39	121.79	120.87
C 10	39	155.28	150.82	150.35	151	150.81	151.19	150.17	154.71
C 11	19	169.65	169.72	170.51	170.11	169.54	169.28	170.77	169.79
C 12	14.2	176.07	176.08	177.48	176.12	176.07	176.42	177.55	176.29
H 2a	2.44	29.28	29.23	29.22	29.2	29.24	29.12	29.29	29.19
H 2b	2.55	29.43	29.47	29.31	29.47	29.29	29.51	29.32	29.38
H 3	4.67	27.21	27.24	27.22	27.19	27.23	26.99	27.34	27.1
H 4	5.88	25.36	25.64	25.61	25.82	25.68	25.51	25.71	25.25
H 5	5.58	25.64	25.99	25.79	25.66	25.64	25.91	25.76	25.81
H 6	3.74	27.66	27.83	27.09	27.74	27.59	27.69	27.76	27.7
H 7	3.35	27.56	27.92	27.98	27.45	27.6	27.72	27.88	27.55
H 9	4.74	26.88	27.15	26.68	26.41	26.3	26.69	26.59	26.82
H 10a	1.49	30.11	29.94	30.41	30.23	30.39	29.66	30.46	29.98
H 10b	1.49	30.01	30.42	29.96	30.33	30.18	30.23	30.02	30.2
H 11a	1.3	30.33	30.41	30.42	30.34	30.39	30.46	30.45	30.32
H 11b	1.3	30.28	30.4	30.57	30.42	30.38	30.38	30.59	30.33
H 12a-c	0.89	30.8	30.86	30.77	30.85	30.84	30.85	30.76	30.8
H 8a	1.83	30.22	29.97	29.27	29.67	30.09	30.03	29.88	29.71
H 8b	1.83	29.54	29.74	30.06	30.06	29.64	29.85	29.93	30.18
J 2a,3	3.3	4.42	4.93	4.55	4.77	4.48	5.12	4.52	5.87
J 2b,3	3.9	2.83	10.09	2.71	12.3	2.73	11.68	2.81	11.4
J 3,4	3.1	3.27	6.92	3.72	7.77	3.28	7.47	3.73	8.09

Table S29. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-8 calculated at the B3LYP/6-31G** level of theory for compound **29**¹⁷

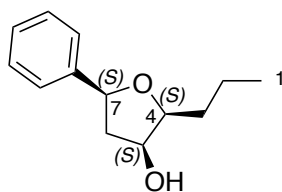


29

Isotropic shielding constants									
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 1	109.6	84.89	85.41	84.72	85.94	78.53	81.07	76.85	80.18
C 2	78.8	116.58	113.58	116.89	116.14	119.04	117.4	117.21	113.79
C 3	86	107.21	106.77	109	110.46	112.24	109.06	103.1	107.09
C 4	80.1	112.07	110.7	106.75	111.58	112.1	112.25	105.96	111.03
C 5	72.2	119.35	117.53	116.34	119.32	120.53	117.54	115.44	117.48
C 10	59.2	137.9	138.26	138.6	138.7	137.88	137.78	138.32	138.2
C 12	58.6	135.43	135.63	134.62	133.97	136.77	135.64	136.38	135.66
C 13	55.8	134.29	134.39	133.92	134.11	134.18	134.22	134.59	134.08
H 1	4.83	26.87	27.03	27.02	27.09	26.99	26.91	26.89	27.01
H 2	4.21	27.46	27.66	27.48	27.77	27.72	27.54	27.66	27.38
H 3	3.77	28.07	27.97	28.27	28.4	27.75	27.92	28.23	28.09
H 4	4.48	27.26	27.62	27.47	27.61	27.56	27.45	27.36	27.32
H 5a	3.66	28.34	28.51	28.6	28.43	28.56	28.38	28.34	28.38
H 5b	3.57	28.48	28.4	28.57	28.16	28.25	28.52	28.62	28.26
H 10a-c	3.43	28.36	28.4	28.45	28.48	28.52	28.5	28.52	28.47
H 12a-c	3.44	28.36	28.37	28.37	28.32	28.41	28.42	28.55	28.46
H 13a-c	3.44	28.54	28.51	28.55	28.51	28.41	28.49	28.48	28.52
J 1,2	1.3	3.89	3.79	4.67	4.74	0.17	0.89	0.19	2.62
J 2,3	2.3	4.84	5.31	5	4.19	4.81	4.35	0.27	4.69
J 3,4	5.9	5.47	5.31	0.43	3.6	8.33	6.01	0.93	5.91
J 4,5a	4.2	4.53	3.83	3.15	5.25	2.57	3.87	1.9	5.58
J 4,5b	7.7	3.99	5.81	2.03	6.49	0.65	5.93	1.18	3.82

¹⁷ Compounds **29**: NMR data measured in our lab (Francisco, C. G.; Martin, C. G.; Suárez, E. J. *Org. Chem.* **1998**, 63, 2099)

Table S30. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-4 calculated at the B3LYP/6-31G** level of theory for compound **30**¹⁸

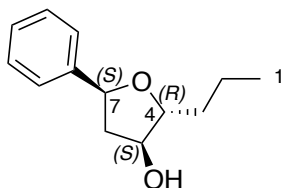


30

Isotropic shielding constants					
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4
C 1	14.3	175.53	175.79	175.76	175.54
C 2	19.6	168.96	168.85	168.78	168.48
C 3	30.9	156.16	152.28	151.38	157.09
C 4	83.6	109.06	105.91	105.78	109.33
C 5	73.1	117.98	115.47	115.94	117.59
C 6	44.3	148.14	148.16	147.87	147.56
C 7	78.7	113.26	113.4	112.38	112.3
C 8	143	49.06	50.22	51.14	51.13
C 9	125.9	71.79	72.5	72.02	72.59
C 10	128.4	68.46	68.48	69.16	69.02
C 11	127.3	70.91	71.05	71.35	71.44
C 12	128.4	68.3	68.69	69.02	68.9
C 13	125.9	72.58	72.24	72.1	72.61
H 1a-c	0.92	30.76	30.77	30.77	30.75
H 2a	1.47	30.21	30.09	30.07	30.26
H 2b	1.4	30.18	30.26	30.27	30.04
H 3a	1.71	29.99	30.38	30.38	30
H 3b	1.63	30.15	30.31	30.27	30.39
H 4	3.68	27.66	27.63	27.79	27.59
H 5	4.19	27.81	27.72	27.66	27.69
H 6a	2.62	29.31	29.29	29.92	30.07
H 6b	1.83	29.54	29.74	29.56	29.37
H 7	4.78	26.5	26.43	26.2	26.12
H 9	7.25	24.31	24.2	24.32	24.34
H 10	7.24	24.34	24.34	24.4	24.4
H 11	7.17	24.53	24.54	24.56	24.56
H 12	7.24	24.34	24.36	24.39	24.39
H 13	7.25	24.16	24.33	24.28	24.3
J 4,5	3.5	2.74	3.21	2.58	2.33
J 5,6a	6.2	4.52	4.99	4.68	3.92
J 5,6b	1.9	0.89	4.57	3.9	1.19
J 6a,7	8.8	10.2	7.74	7.67	10.48
J 6b,7	6.2	1.33	5.7	6.7	6.23

¹⁸ Compounds **30-33**: NMR data from Grimblat, N. Gavín, J.A. Daranas, A.H., Sarotti, A, *Org. Lett.* **2019**, *21*, 11, 4003-4007

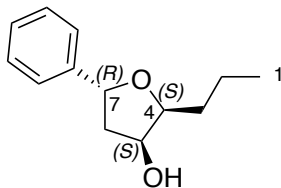
Table S31. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-4 calculated at the B3LYP/6-31G** level of theory for compound **31**



31

Isotropic shielding constants					
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4
C 1	14.1	175.53	175.79	175.76	175.54
C 2	19.1	168.96	168.85	168.78	168.48
C 3	35.3	156.16	152.28	151.38	157.09
C 4	85.6	109.06	105.91	105.78	109.33
C 5	76.8	117.98	115.47	115.94	117.59
C 6	43.4	148.14	148.16	147.87	147.56
C 7	79.7	113.26	113.4	112.38	112.3
C 8	143.3	49.06	50.22	51.14	51.13
C 9	125.6	71.79	72.5	72.02	72.59
C 10	128.5	68.46	68.48	69.16	69.02
C 11	127.3	70.91	71.05	71.35	71.44
C 12	128.5	68.3	68.69	69.02	68.9
C 13	125.6	72.58	72.24	72.1	72.61
H 1a-c	0.89	30.76	30.77	30.77	30.75
H 2a	1.46	30.21	30.09	30.07	30.26
H 2b	1.37	30.18	30.26	30.27	30.04
H 3a	1.46	29.99	30.38	30.38	30
H 3b	1.46	30.15	30.31	30.27	30.39
H 4	3.9	27.66	27.63	27.79	27.59
H 5	4.05	27.81	27.72	27.66	27.69
H 6a	2.57	29.31	29.29	29.92	30.07
H 6b	1.87	29.54	29.74	29.56	29.37
H 7	4.96	26.5	26.43	26.2	26.12
H 9	7.26	24.31	24.2	24.32	24.34
H 10	7.25	24.34	24.34	24.4	24.4
H 11	7.18	24.53	24.54	24.56	24.56
H 12	7.25	24.34	24.36	24.39	24.39
H 13	7.26	24.16	24.33	24.28	24.3
J 4,5	4.5	2.74	3.21	2.58	2.33
J 5,6a	6.5	4.52	4.99	4.68	3.92
J 5,6b	5.5	0.89	4.57	3.9	1.19
J 6a,7	7.3	10.2	7.74	7.67	10.48
J 6b,7	7.3	1.33	5.7	6.7	6.23

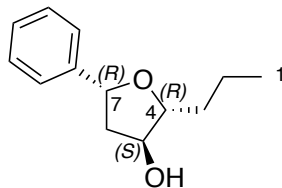
Table S32. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-4 calculated at the B3LYP/6-31G** level of theory for compound **32**



32

Isotropic shielding constants					
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4
C 1	14.1	175.53	175.79	175.76	175.54
C 2	19.1	168.96	168.85	168.78	168.48
C 3	35.6	156.16	152.28	151.38	157.09
C 4	87.1	109.06	105.91	105.78	109.33
C 5	76.7	117.98	115.47	115.94	117.59
C 6	44	148.14	148.16	147.87	147.56
C 7	79.5	113.26	113.4	112.38	112.3
C 8	142.1	49.06	50.22	51.14	51.13
C 9	125.8	71.79	72.5	72.02	72.59
C 10	128.3	68.46	68.48	69.16	69.02
C 11	127.4	70.91	71.05	71.35	71.44
C 12	128.3	68.3	68.69	69.02	68.9
C 13	125.8	72.58	72.24	72.1	72.61
H 1a-c	0.91	30.76	30.77	30.77	30.75
H 2a	1.46	30.21	30.09	30.07	30.26
H 2b	1.41	30.18	30.26	30.27	30.04
H 3a	1.54	29.99	30.38	30.38	30
H 3b	1.5	30.15	30.31	30.27	30.39
H 4	3.83	27.66	27.63	27.79	27.59
H 5	4.09	27.81	27.72	27.66	27.69
H 6a	1.89	29.31	29.29	29.92	30.07
H 6b	2.13	29.54	29.74	29.56	29.37
H 7	5.04	26.5	26.43	26.2	26.12
H 9	7.27	24.31	24.2	24.32	24.34
H 10	7.26	24.34	24.34	24.4	24.4
H 11	7.19	24.53	24.54	24.56	24.56
H 12	7.26	24.34	24.36	24.39	24.39
H 13	7.27	24.16	24.33	24.28	24.3
J 4,5	2.7	2.74	3.21	2.58	2.33
J 5,6a	5.9	4.52	4.99	4.68	3.92
J 5,6b	1.9	0.89	4.57	3.9	1.19
J 6a,7	10.3	10.2	7.74	7.67	10.48
J 6b,7	5.7	1.33	5.7	6.7	6.23

Table S33. Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) of isomers 1-4 calculated at the B3LYP/6-31G** level of theory for compound **33**



33

Isotropic shielding constants					
Nuclei	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4
C 1	14.3	175.53	175.79	175.76	175.54
C 2	19.7	168.96	168.85	168.78	168.48
C 3	31.3	156.16	152.28	151.38	157.09
C 4	83.1	109.06	105.91	105.78	109.33
C 5	73.8	117.98	115.47	115.94	117.59
C 6	44.7	148.14	148.16	147.87	147.56
C 7	78.2	113.26	113.4	112.38	112.3
C 8	143.8	49.06	50.22	51.14	51.13
C 9	125.3	71.79	72.5	72.02	72.59
C 10	128.3	68.46	68.48	69.16	69.02
C 11	127.1	70.91	71.05	71.35	71.44
C 12	128.3	68.3	68.69	69.02	68.9
C 13	125.3	72.58	72.24	72.1	72.61
H 1a-c	0.94	30.76	30.77	30.77	30.75
H 2a	1.48	30.21	30.09	30.07	30.26
H 2b	1.4	30.18	30.26	30.27	30.04
H 3a	1.66	29.99	30.38	30.38	30
H 3b	1.58	30.15	30.31	30.27	30.39
H 4	3.99	27.66	27.63	27.79	27.59
H 5	4.3	27.81	27.72	27.66	27.69
H 6a	2.02	29.31	29.29	29.92	30.07
H 6b	2.39	29.54	29.74	29.56	29.37
H 7	5.19	26.5	26.43	26.2	26.12
H 9	7.26	24.31	24.2	24.32	24.34
H 10	7.25	24.34	24.34	24.4	24.4
H 11	7.18	24.53	24.54	24.56	24.56
H 12	7.25	24.34	24.36	24.39	24.39
H 13	7.26	24.16	24.33	24.28	24.3
J 4,5	2.9	2.74	3.21	2.58	2.33
J 5,6a	4.5	4.52	4.99	4.68	3.92
J 5,6b	1	0.89	4.57	3.9	1.19
J 6a,7	9.7	10.2	7.74	7.67	10.48
J 6b,7	6.5	1.33	5.7	6.7	6.23

3. Comparison of isotropic magnetic shielding constants (σ) for the correct isomer in all FF for strychnine

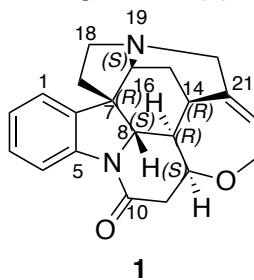


Table S34. Boltzmann averaged ^{13}C and ^1H GIAO isotropic magnetic shielding constants (σ) of isomers 1 calculated at the B3LYP/6-31G** level of theory for compound **1** for each FF and maximum $\Delta\sigma$

Nuclei	AMBER	MM3	MMFF	OPLS2005	OPLS4	Max $\Delta\sigma$
C 1	73.65	75.79	75.41	72.46	75.06	3.33
C 2	70.50	71.93	72.70	69.83	73.49	3.66
C 3	65.53	66.95	67.27	65.18	68.20	3.02
C 4	76.71	77.49	80.75	77.80	80.03	4.03
C 5	55.24	61.05	56.06	53.52	55.47	7.53
C 6	62.50	71.93	63.80	61.34	62.47	10.58
C 7	138.73	136.02	138.09	137.58	138.66	2.71
C 8	132.59	130.07	130.23	132.25	131.30	2.53
C 10	32.32	35.64	31.98	30.92	32.63	4.72
C 11	149.02	145.73	148.61	148.88	148.11	3.29
C 12	113.73	110.58	111.18	111.66	113.77	3.19
C 13	142.32	140.68	142.13	143.44	142.11	2.76
C 14	158.13	155.70	157.80	155.97	156.11	2.42
C 15	163.16	159.96	162.27	162.57	163.43	3.47
C 16	130.65	130.35	131.17	129.64	127.70	3.47
C 17	147.69	144.26	146.47	147.50	147.29	3.43
C 18	141.06	139.32	141.82	141.81	143.28	3.96
C 20	138.26	137.70	138.85	137.42	137.35	1.50
C 21	51.99	54.91	53.34	52.19	48.30	6.62
C 22	64.00	64.76	65.54	66.96	67.13	3.13
C 23	128.68	126.21	128.71	127.80	130.30	4.09

Nuclei	AMBER	MM3	MMFF	OPLS2005	OPLS4	Max $\Delta\sigma$
H 1	24.57	24.49	24.59	24.48	24.73	0.25
H 2	24.67	24.53	24.75	24.69	24.82	0.29
H 3	24.39	24.26	24.48	24.41	24.53	0.27
H 4	23.45	23.36	23.51	23.79	23.81	0.46
H 8	28.05	27.71	27.79	27.74	28.02	0.34
H 11a	27.87	27.35	27.71	28.01	27.62	0.66
H 11b	31.03	30.37	30.67	30.67	30.76	0.66
H 12	29.00	28.39	28.86	29.16	28.92	0.77
H 13	28.03	27.57	27.86	27.96	27.91	0.46
H 14	25.79	25.46	25.72	25.94	25.90	0.47
H 15a	29.35	28.72	29.11	29.27	29.33	0.63
H 15b	28.93	28.43	28.74	29.14	28.93	0.71
H 16	29.80	29.13	29.57	29.72	29.73	0.66
H 17a	30.62	29.97	30.37	30.51	30.49	0.65
H 17b	30.02	29.40	29.82	30.07	30.00	0.67
H 18a	30.11	29.55	29.97	30.09	30.12	0.58
H 18b	29.05	28.55	28.94	29.12	28.99	0.57
H 20a	28.80	28.34	28.75	28.91	28.63	0.56
H 20b	29.33	28.88	29.20	29.47	29.37	0.59
H 22	28.27	27.78	28.16	28.37	28.26	0.59
H 23a	27.95	27.51	27.86	27.89	28.01	0.50
H 23b	28.11	27.69	28.07	28.18	28.06	0.49

4. Summary of errors

Table S35. CMAE for ^1H and ^{13}C for compounds **1-33**

CMAE ^1H	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	0.08	0.09	0.09	0.14	0.08
2	0.08	0.10	0.08	0.08	0.11
3	0.11	0.10	0.11	0.09	0.14
4	0.10	0.10	0.09	0.09	0.12
5	0.09	0.13	0.09	0.11	0.12
6	0.18	0.24	0.08	0.09	0.19
7	0.14	0.11	0.17	0.07	0.12
8	0.12	0.16	0.10	0.13	0.12
9	0.12	0.13	0.14	0.12	0.15
10	0.09	0.16	0.11	0.10	0.09
11	0.12	0.18	0.17	0.11	0.14
12	0.26	0.03	0.10	0.12	0.18
13	0.30	0.15	0.09	0.08	0.12
14	0.24	0.13	0.13	0.14	0.11
15	0.13	0.16	0.14	0.26	0.11
16	0.13	0.15	0.13	0.17	0.12
17	0.12	0.16	0.14	0.53	0.14
18	0.15	0.16	0.13	0.12	0.09
19	0.16	0.15	0.12	0.12	0.12
20	0.26	0.42	0.32	0.30	0.35
21	0.18	0.17	0.15	0.14	0.22
22	0.19	0.21	0.18	0.14	0.23
23	0.32	0.38	0.34	0.33	0.33
24	0.17	0.14	0.11	0.14	0.10
25	0.19	0.15	0.17	0.13	0.13
26	0.23	0.20	0.18	0.17	0.13
27	0.12	0.09	0.10	0.09	0.11
28	0.15	0.10	0.11	0.10	0.12
29	0.11	0.09	0.08	0.09	0.12
30	0.17	0.13	0.14	0.15	0.13
31	0.11	0.12	0.10	0.13	0.09
32	0.11	0.11	0.10	0.10	0.09
33	0.14	0.13	0.14	0.16	0.12

CMAE ¹³ C	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	1.23	2.22	1.39	1.22	1.86
2	0.93	1.21	1.28	1.37	1.59
3	2.82	1.77	1.55	1.29	1.89
4	1.83	1.97	1.77	1.91	2.23
5	2.51	2.50	2.37	2.26	2.55
6	2.71	2.58	1.97	1.68	1.87
7	3.18	3.02	1.27	1.68	2.04
8	1.69	1.38	2.09	1.25	1.23
9	1.70	1.53	1.12	0.93	1.51
10	1.47	1.30	1.32	0.70	1.41
11	1.59	1.41	1.07	0.78	1.54
12	0.43	0.89	0.64	1.44	0.81
13	1.49	0.59	0.62	1.03	0.89
14	0.48	0.72	1.06	1.33	1.69
15	1.99	2.11	2.07	2.53	1.37
16	1.02	1.62	1.14	1.26	1.31
17	1.25	2.11	1.81	2.53	1.31
18	2.47	2.94	2.55	1.51	1.48
19	2.21	2.73	2.35	1.49	1.41
20	2.40	3.45	3.66	2.83	4.42
21	1.40	1.06	1.07	1.29	1.18
22	1.40	1.27	1.08	1.35	1.12
23	2.45	3.52	0.71	2.86	4.43
24	2.05	1.72	1.63	1.90	2.02
25	2.07	2.39	2.46	1.69	1.72
26	2.90	2.57	2.37	1.72	1.55
27	1.88	2.13	0.99	0.83	1.12
28	2.36	1.83	0.92	1.05	1.06
29	2.49	2.09	2.27	2.60	2.08
30	1.22	1.31	1.77	1.22	1.81
31	0.91	1.22	1.54	1.08	0.43
32	1.00	1.39	1.61	1.42	1.50
33	0.87	1.18	1.52	0.99	1.53

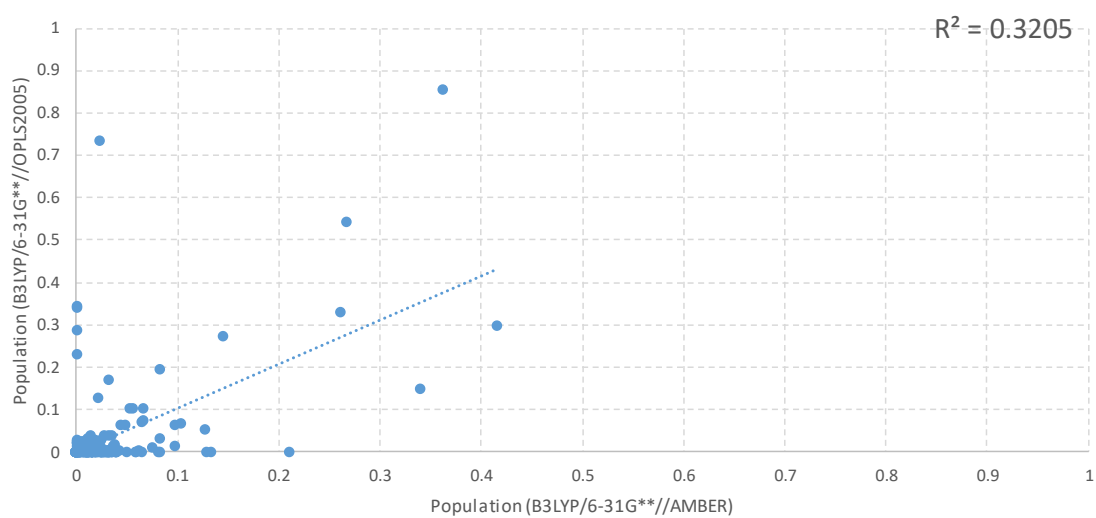
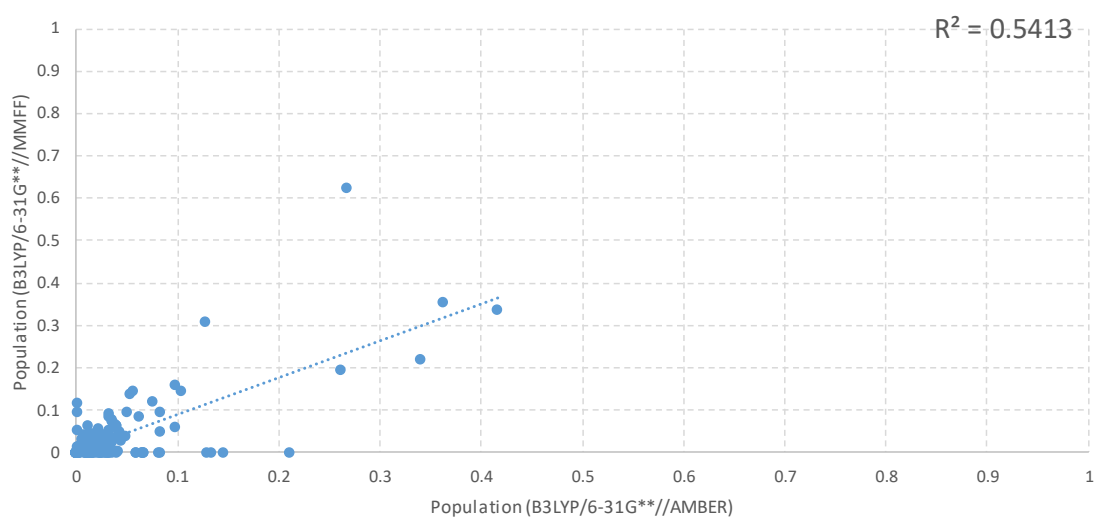
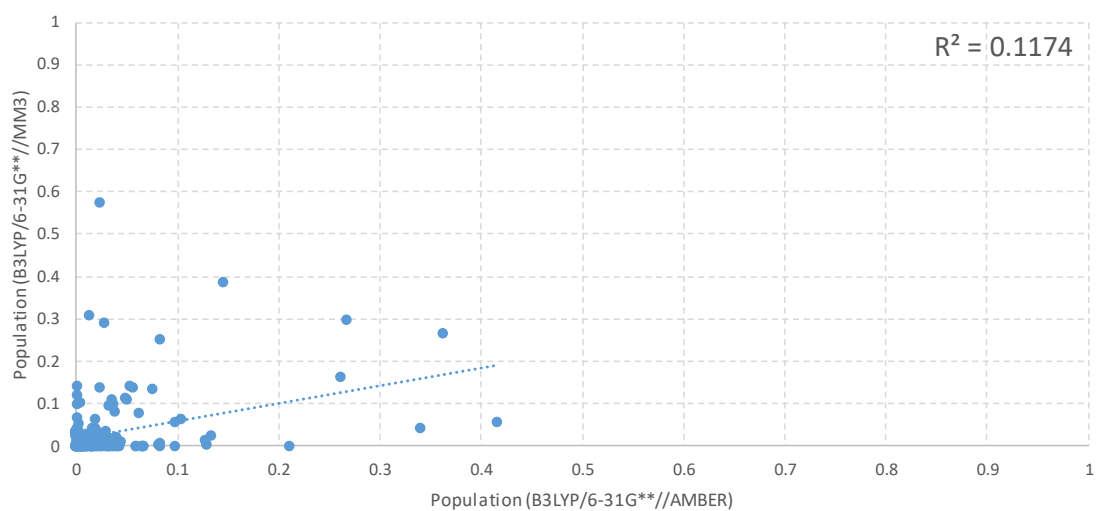
Table S36. Maximum Error for ^1H and ^{13}C for compounds **1-33**

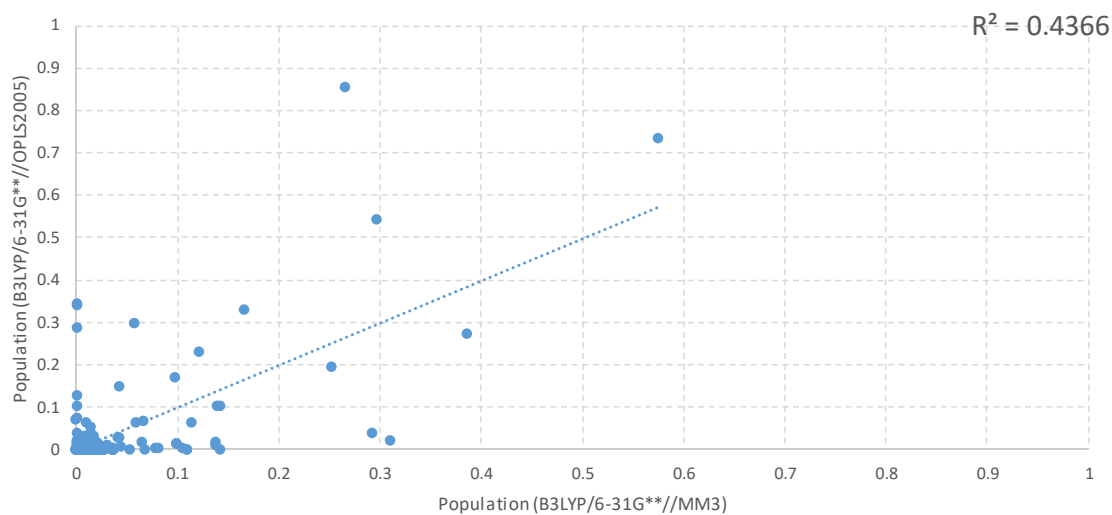
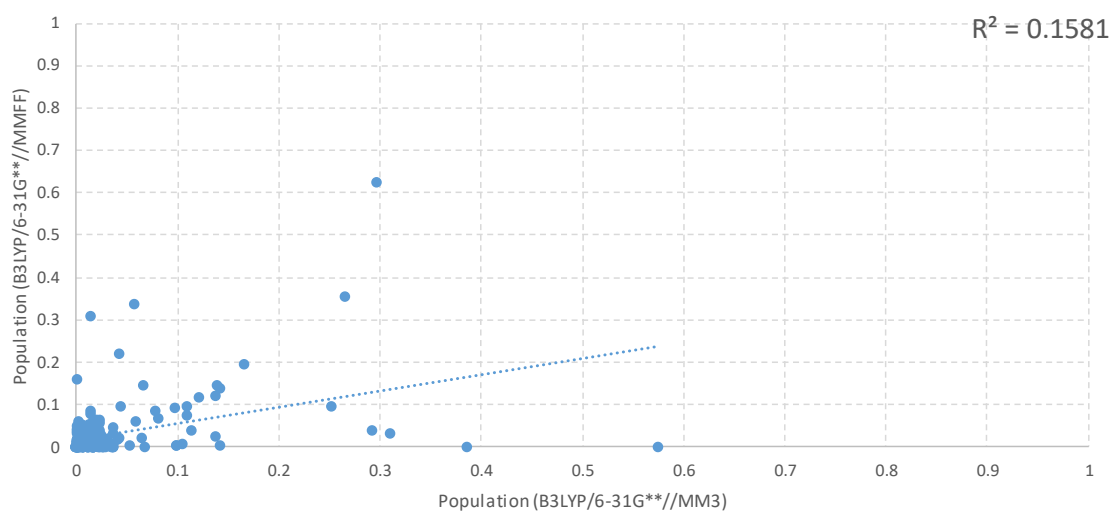
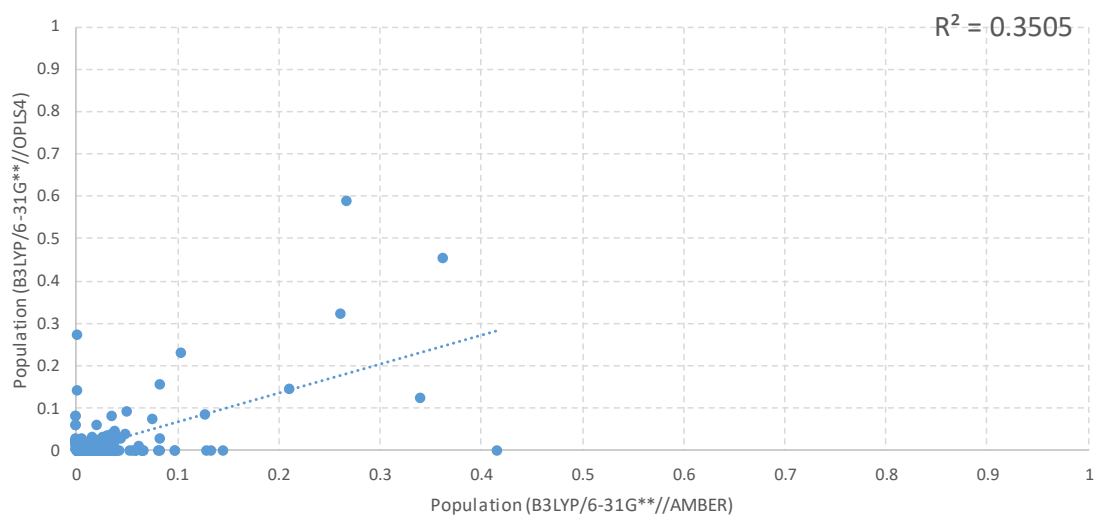
MaxErr ^1H	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	0.20	0.23	0.27	0.36	0.19
2	0.17	0.28	0.22	0.19	0.27
3	0.28	0.29	0.27	0.16	0.29
4	0.23	0.23	0.27	0.26	0.34
5	0.20	0.30	0.21	0.21	0.31
6	0.36	0.77	0.16	0.15	0.33
7	0.21	0.31	0.32	0.19	0.22
8	0.28	0.41	0.29	0.27	0.33
9	0.30	0.28	0.43	0.41	0.44
10	0.22	0.51	0.30	0.25	0.24
11	0.38	0.59	0.51	0.34	0.42
12	0.55	0.06	0.16	0.25	0.26
13	0.50	0.22	0.17	0.13	0.25
14	0.51	0.24	0.21	0.20	0.24
15	0.38	0.37	0.36	0.45	0.31
16	0.27	0.47	0.34	0.47	0.23
17	0.31	0.39	0.31	1.15	0.28
18	0.33	0.37	0.29	0.28	0.27
19	0.39	0.52	0.32	0.28	0.33
20	0.29	0.36	0.31	0.29	0.49
21	0.28	0.32	0.32	0.28	0.52
22	0.28	0.36	0.32	0.25	0.51
23	0.34	0.34	0.33	0.30	0.36
24	0.48	0.35	0.38	0.42	0.36
25	0.46	0.46	0.51	0.23	0.26
26	0.49	0.49	0.52	0.26	0.33
27	0.32	0.18	0.29	0.25	0.34
28	0.39	0.38	0.39	0.31	0.24
29	0.23	0.18	0.18	0.27	0.45
30	0.38	0.29	0.38	0.40	0.39
31	0.30	0.23	0.23	0.44	0.25
32	0.26	0.31	0.40	0.32	0.25
33	0.31	0.38	0.35	0.41	0.39

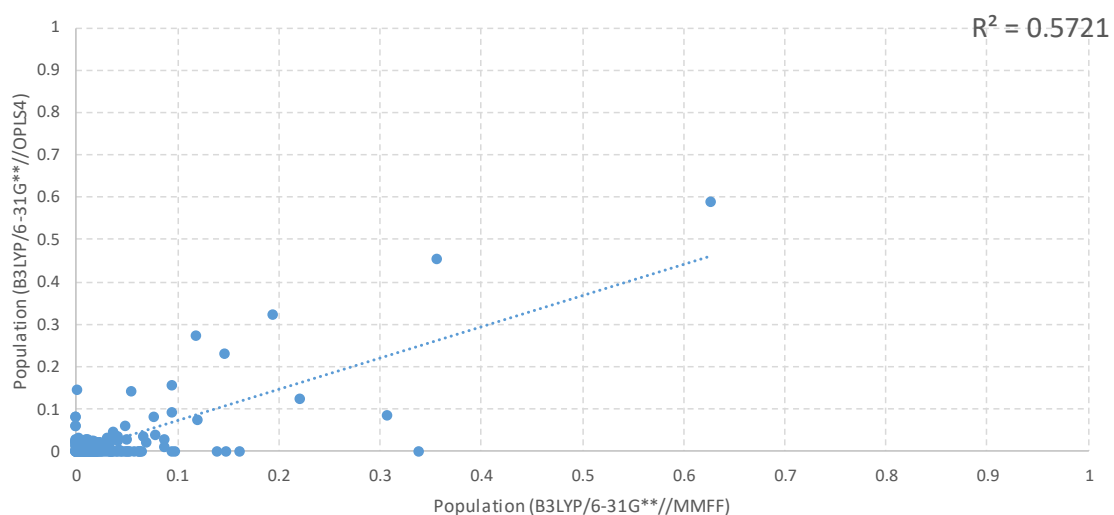
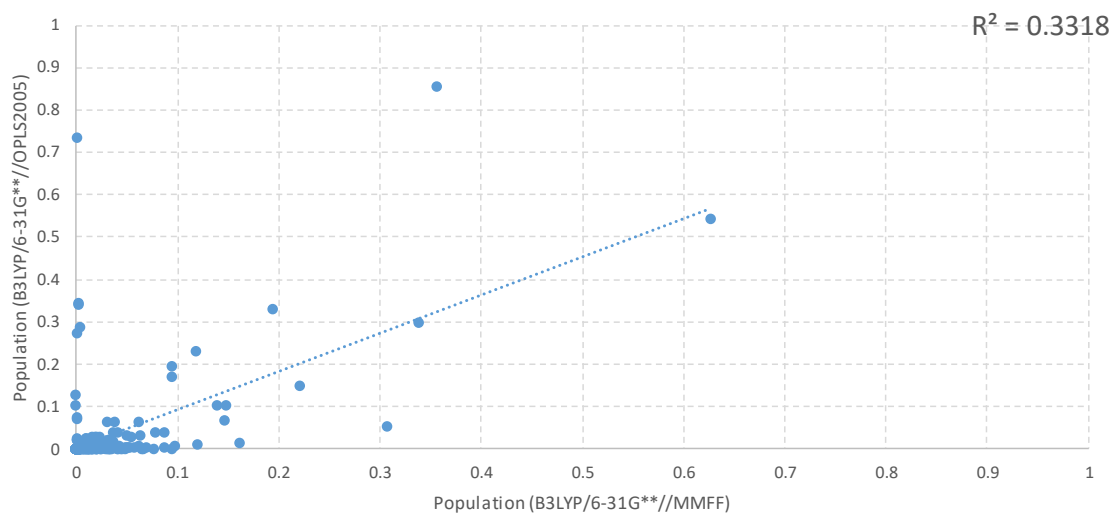
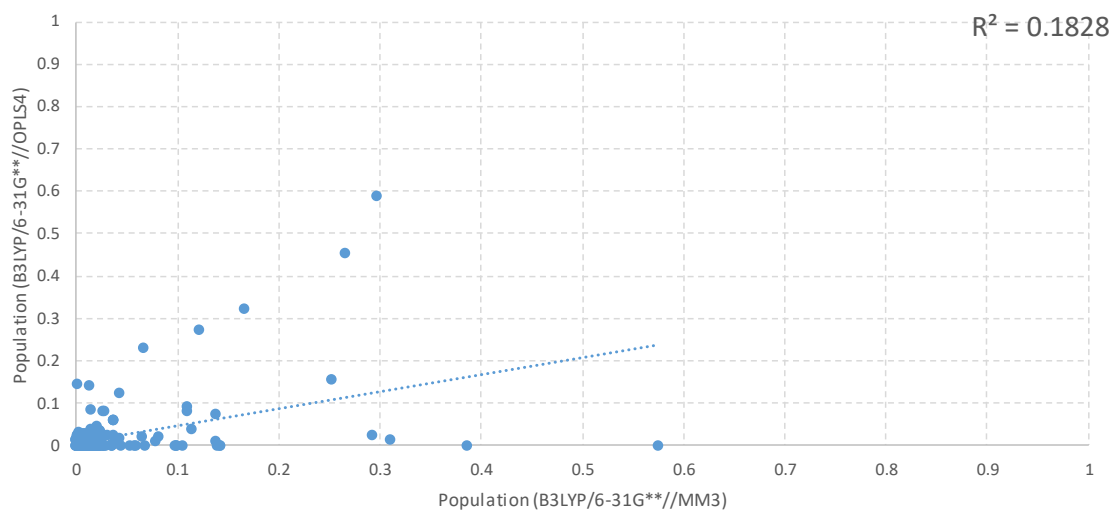
MaxErr ¹³ C	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	4.65	7.33	4.62	3.58	8.43
2	1.98	2.05	2.50	2.41	2.90
3	9.09	4.08	3.32	3.64	5.22
4	5.99	6.49	5.98	6.99	7.97
5	3.75	4.24	4.73	4.17	3.70
6	4.21	10.26	4.36	3.82	5.02
7	4.87	8.95	3.94	3.16	3.94
8	6.44	4.11	5.38	3.79	3.81
9	7.81	5.10	2.87	2.89	4.95
10	8.78	4.34	4.69	1.88	4.05
11	8.50	4.38	3.89	2.08	4.61
12	0.94	1.33	1.50	2.96	2.36
13	2.36	1.24	1.03	1.62	1.72
14	1.01	1.54	2.32	2.67	3.70
15	1.81	3.36	2.22	2.68	2.15
16	3.43	4.56	3.43	4.16	2.83
17	3.53	6.10	3.43	6.02	2.42
18	8.47	11.86	8.18	6.07	6.63
19	8.36	11.54	8.03	6.03	6.62
20	2.24	2.67	1.81	2.53	3.19
21	3.71	2.91	2.53	3.77	3.76
22	3.75	3.35	2.45	3.78	3.91
23	2.28	2.67	1.71	2.66	2.99
24	5.20	4.74	3.64	3.33	4.11
25	7.48	7.91	7.90	5.20	5.88
26	6.00	7.45	7.23	5.46	6.01
27	5.43	4.95	3.12	2.10	3.50
28	6.30	5.45	2.73	2.39	2.69
29	4.35	4.74	3.59	4.75	4.79
30	2.68	3.93	5.52	3.01	5.14
31	2.56	2.63	4.42	2.01	4.26
32	2.37	3.46	4.83	4.27	4.60
33	2.58	2.57	3.19	2.52	2.94

5. Scatter plots of the Boltzmann's amplitudes (w_i)

Figure 2. Scatter plots of the Boltzmann's amplitudes (w_i) calculated for the case study 9 at the B3LYP/6-31G** level using the geometries optimized at the different FFs under study as inputs.







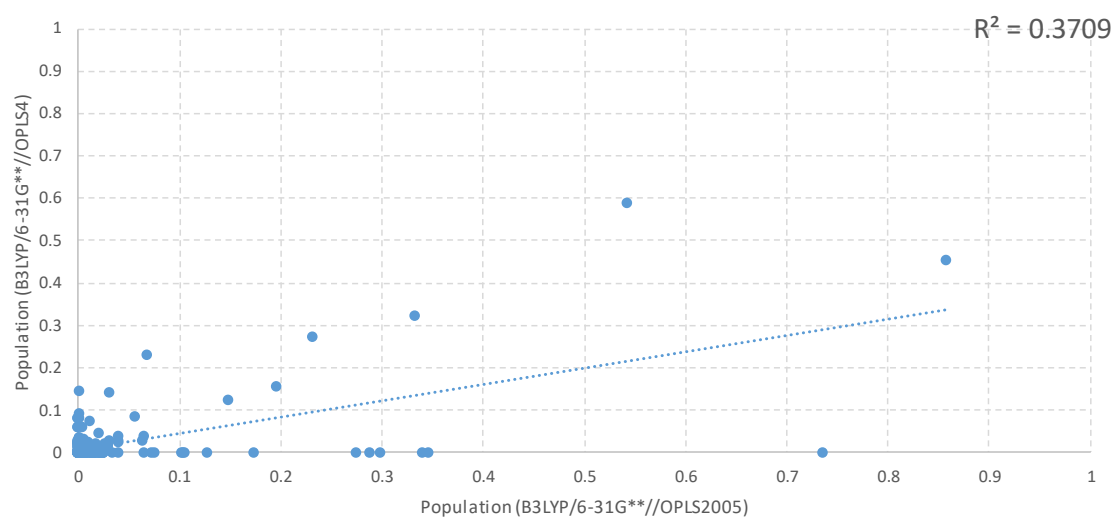
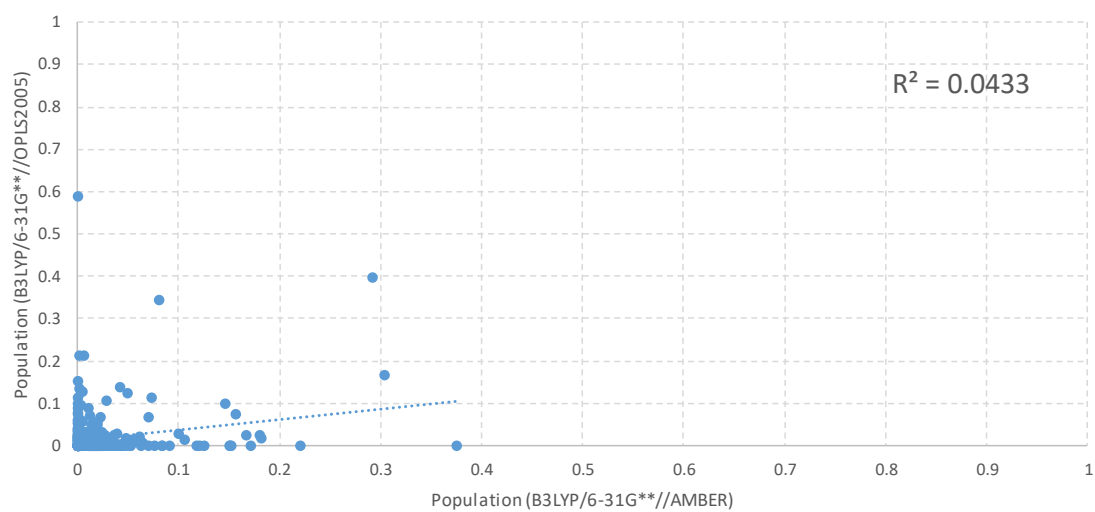
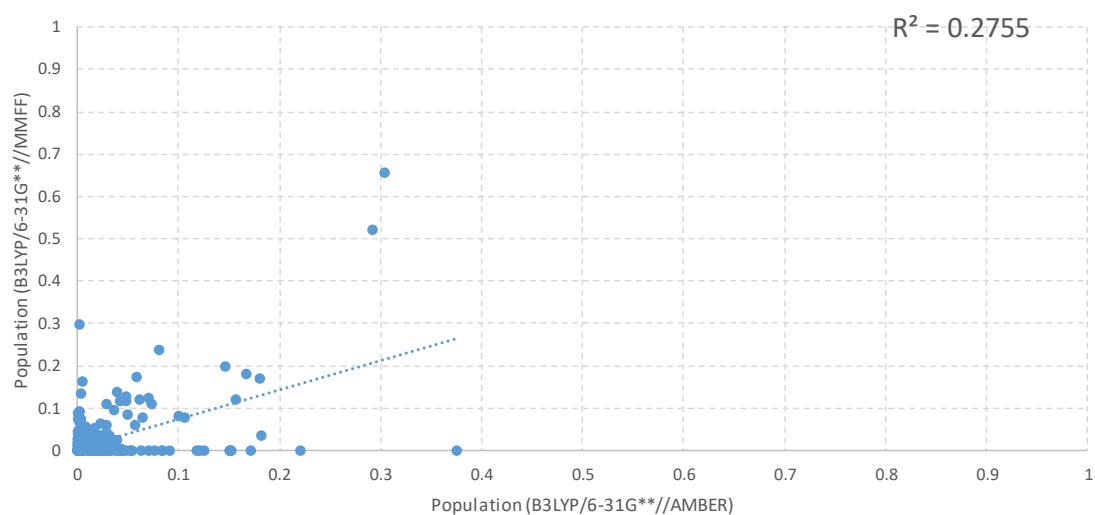
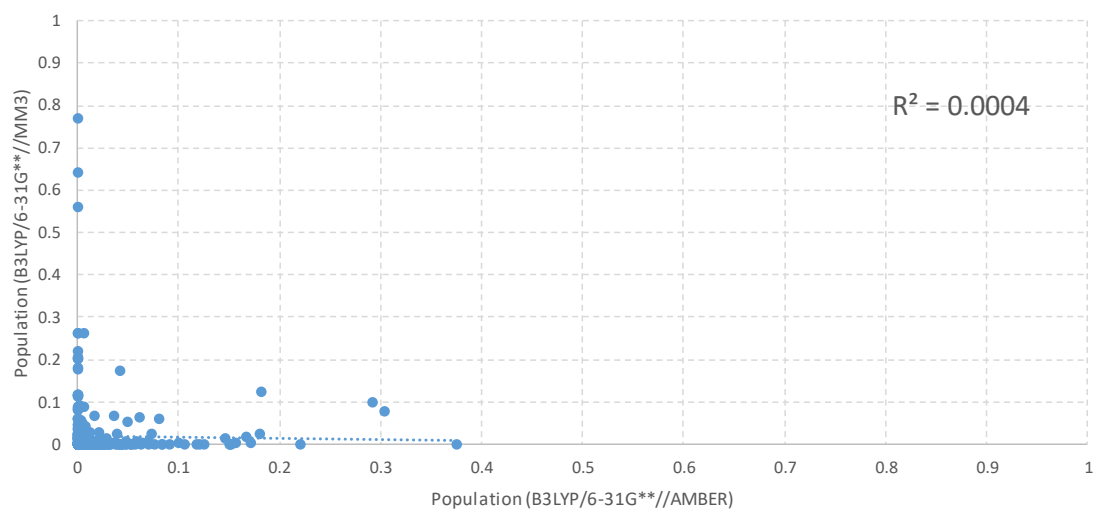
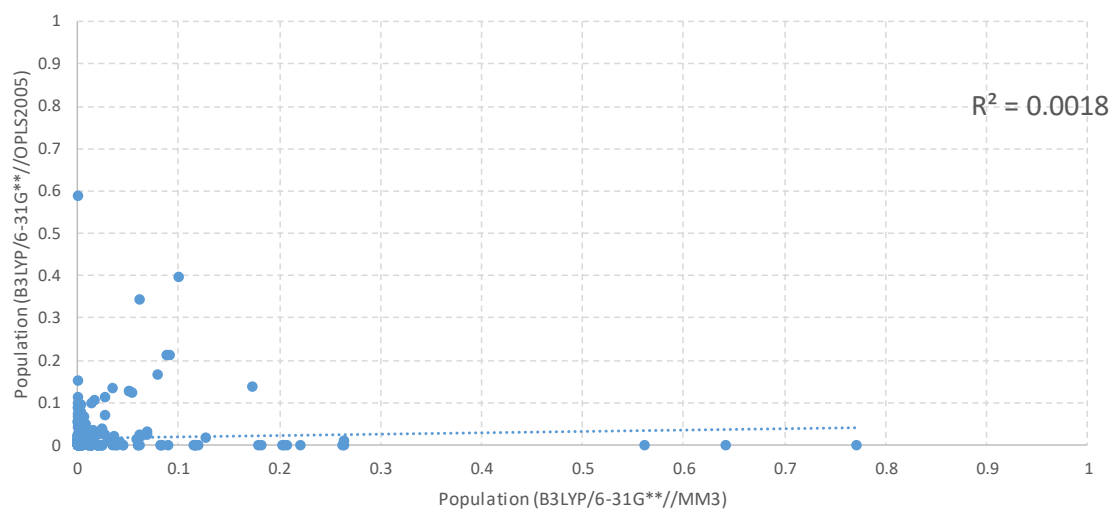
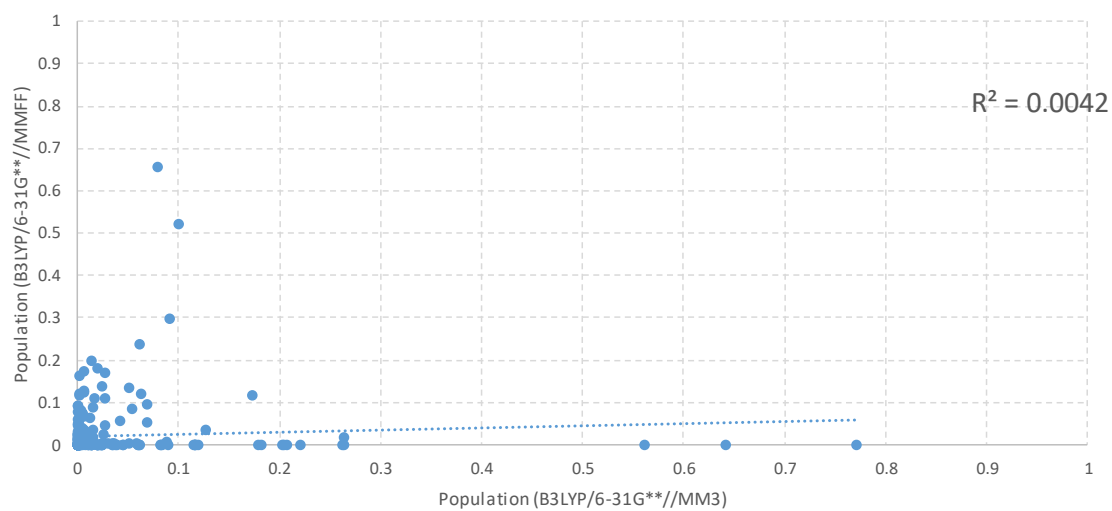
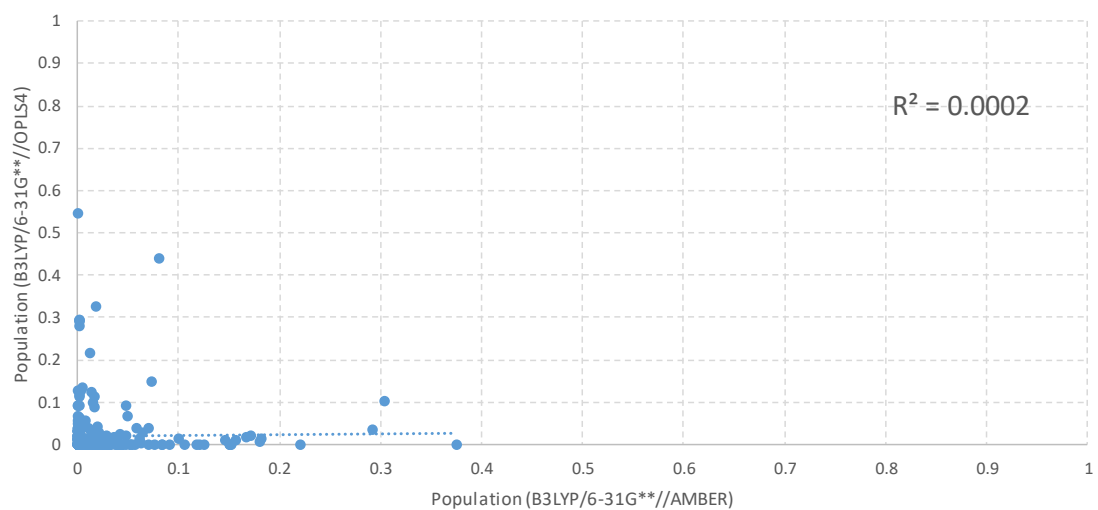
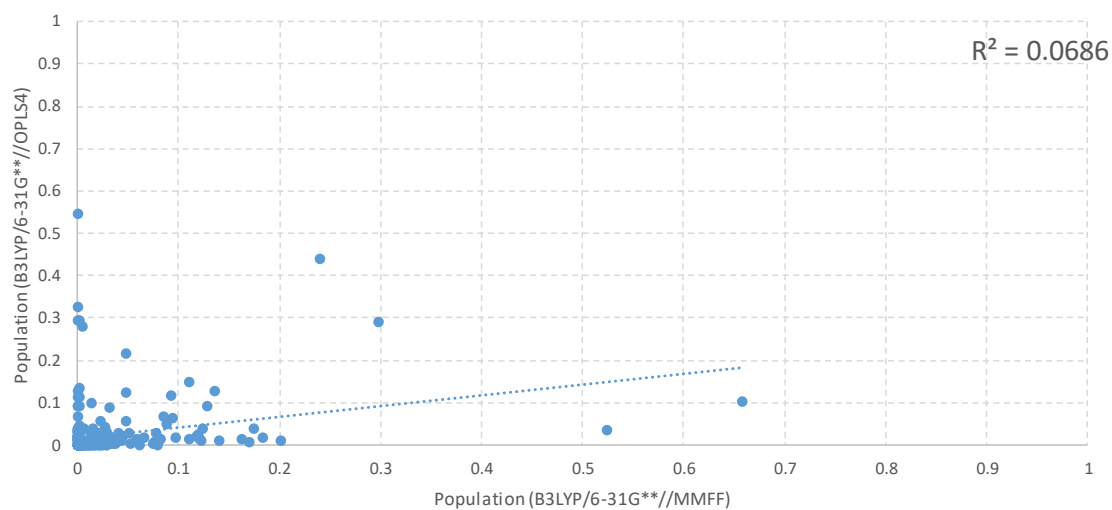
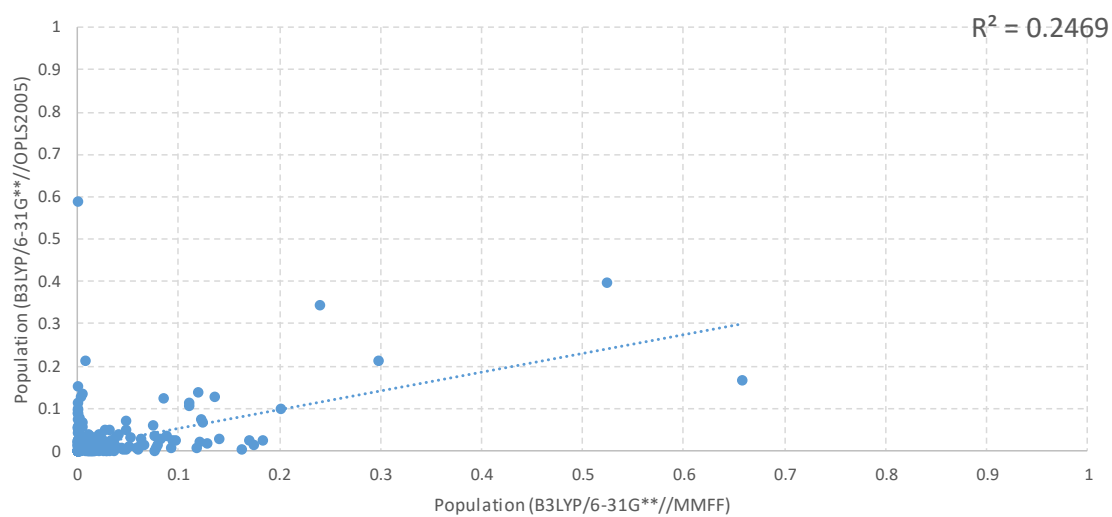
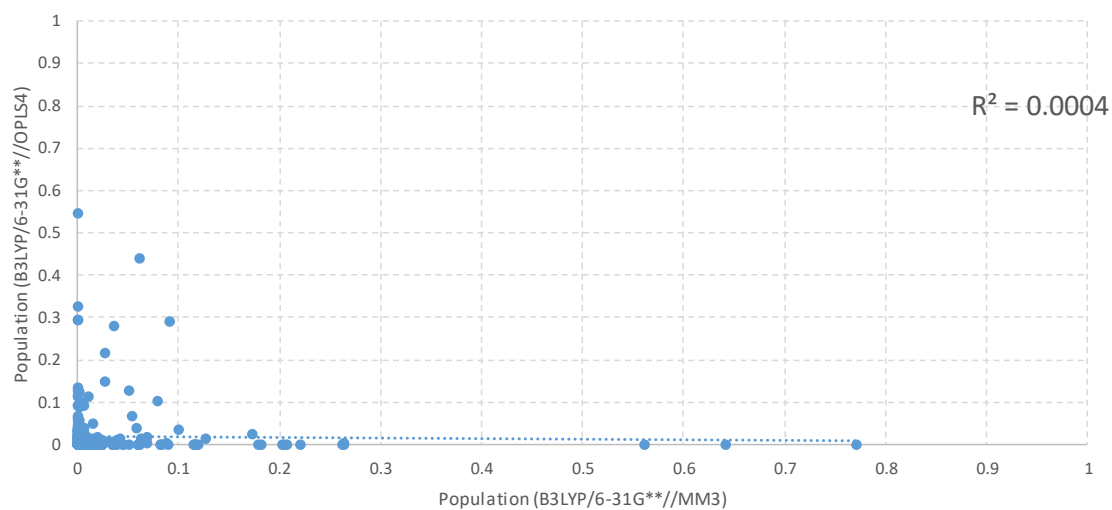
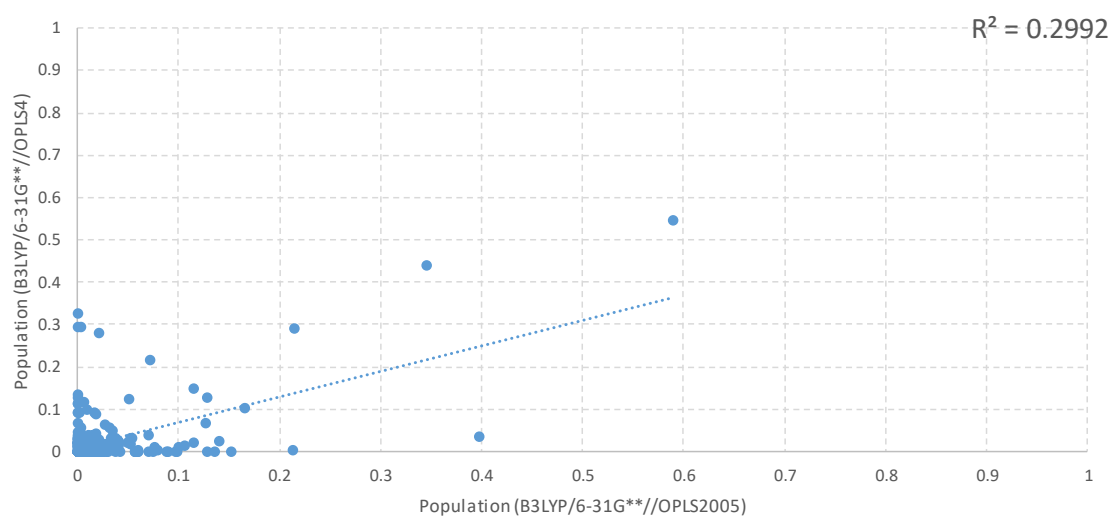


Figure 3. Scatter plots of the Boltzmann's amplitudes (w_i) calculated for the case study **27** at the B3LYP/6-31G** level using the geometries optimized at the different FFs under study as inputs.









6. DP4, dJ-DP4 and iJ/dJ-DP4 results for compounds 1-33

Table S37. DP4 results for compounds **1-33**

Comp. N°	DP4 – 12 kJ/mol – MAD 05 Å				
	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	>99.9	>99.9	>99.9	>99.9	>99.9
2	>99.9	>99.9	>99.9	>99.9	>99.9
3	94.0	>99.9	>99.9	99.5	99.9
4	99.8	99.7	99.5	92.8	61.9
5	>99.9	>99.9	>99.9	>99.9	>99.9
6	92.7	52.7	98.6	92.5	1.4
7	92.1	98.9	99.9	2.9	62.6
8	<0.1	<0.1	95.5	<0.1	48.6
9	53.2	99.7	97.4	20.5	9.7
10	99.3	73.3	99.9	99.9	99.8
11	1.8	53.1	59.1	99.8	47.2
12	43.7	67.6	52.2	26.2	1.1
13	2.7	13.5	87.2	62.7	52.6
14	62.3	50.9	1.7	23.8	33.0
15	99.5	>99.9	>99.9	>99.9	99.9
16	11.5	51.3	59.2	<0.1	55.7
17	>99.9	99.6	98.5	<0.1	99.9
18	8.6	0.7	8.2	40.8	31.1
19	96.4	99.5	99.5	99.5	98.2
20	>99.9	>99.9	>99.9	>99.9	>99.9
21	99.4	97.8	97.5	99.7	98.2
22	95.2	69.7	98.1	99.8	95.9
23	>99.9	>99.9	>99.9	>99.9	>99.9
24	99.5	13.9	98.9	99.3	99.1
25	59.8	55.6	35.7	96.3	>99.9
26	79.1	80.9	32.1	81.3	99.2
27	99.6	93.6	99.8	95.5	74.2
28	7.6	98.6	60.2	93.0	66.7
29	3.5	14.3	4.6	44.1	0.9
30	0.6	99.7	99.3	98.6	99.1
31	95.0	99.4	34.0	74.8	0.1
32	84.7	27.0	23.1	71.3	7.3
33	90.9	99.5	0.7	75.6	37.0
Average	68.9	73.0	73.9	72.4	66.1

Comp. Nº	DP4 – 21 kJ/mol – MAD 05 Å				
	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	>99.9	>99.9	>99.9	>99.9	>99.9
2	>99.9	>99.9	>99.9	>99.9	>99.9
3	92.3	>99.9	>99.9	99.5	99.4
4	99.8	99.6	99.5	92.2	60.4
5	>99.9	>99.9	>99.9	>99.9	>99.9
6	92.7	50.7	96.1	96.4	12.1
7	89.1	98.2	99.9	90.1	61.2
8	26.2	77.4	96.6	25.5	41.9
9	51.8	>99.9	99.5	21.2	28.6
10	99.2	63.1	99.8	99.9	99.8
11	82.3	1.1	54.3	99.9	35.7
12	9.5	66.4	50.1	0.7	3.8
13	1.6	12.8	88.4	81.7	65.8
14	73.0	53.8	31.5	35.7	56.9
15	99.9	>99.9	>99.9	>99.9	>99.9
16	99.9	8.3	55.7	0.2	84.9
17	99.8	60.1	98.4	<0.1	>99.9
18	1.0	0.5	7.0	1.9	22.6
19	97.0	99.3	99.5	98.4	98.6
20	>99.9	>99.9	>99.9	>99.9	>99.9
21	99.4	97.8	98.4	99.7	98.3
22	95.2	58.2	97.9	99.8	95.8
23	>99.9	>99.9	>99.9	>99.9	>99.9
24	99.0	13.9	99.0	99.5	99.8
25	51.5	55.5	22.8	58.7	46.7
26	80.1	82.9	46.7	81.2	78.2
27	99.6	93.6	99.8	96.3	80.2
28	7.4	98.6	60.2	84.3	53.9
29	0.7	4.9	0.9	30.1	1.2
30	57.9	99.7	99.2	96.1	99.2
31	99.5	99.4	27.0	78.5	76.9
32	47.7	46.0	25.6	67.7	22.5
33	92.9	99.4	1.2	76.2	31.3
Average	74.1	70.9	74.4	73.1	68.4

Comp. N ^o	DP4 – 21 kJ/mol – MAD 1 Å				
	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	>99.9	>99.9	>99.9	>99.9	>99.9
2	>99.9	>99.9	>99.9	>99.9	>99.9
3	92.3	>99.9	>99.9	99.5	99.4
4	99.8	99.6	99.5	92.2	60.4
5	>99.9	>99.9	>99.9	>99.9	>99.9
6	92.7	50.2	94.8	95.1	12.1
7	89.1	98.2	99.9	90.1	61.2
8	26.2	78.8	96.5	17.4	41.7
9	55.4	6.3	99.8	39.6	5.3
10	99.5	13.7	99.7	99.9	99.9
11	65.6	99.0	25.4	99.8	8.9
12	9.5	64.6	50.1	1.9	3.9
13	1.6	12.9	85.8	78.6	59.4
14	73.0	54.3	50.9	37.2	60.4
15	99.1	95.6	>99.9	>99.9	99.9
16	28.0	41.5	60.2	<0.1	97.3
17	99.9	73.4	99.0	<0.1	>99.9
18	0.8	0.4	7.2	2.4	26.2
19	97.0	99.3	99.4	98.1	98.4
20	>99.9	>99.9	>99.9	>99.9	>99.9
21	99.4	97.8	98.4	99.7	98.3
22	95.2	58.2	97.9	99.8	95.8
23	>99.9	>99.9	>99.9	>99.9	>99.9
24	98.9	4.8	98.5	99.6	99.7
25	57.7	61.7	36.3	66.6	46.7
26	80.9	39.9	33.3	55.0	78.1
27	98.1	94.0	99.9	98.9	94.1
28	56.2	98.8	29.1	72.3	40.2
29	1.1	3.8	1.1	54.1	2.1
30	27.3	98.5	99.2	98.7	90.5
31	99.6	99.6	18.8	84.1	67.4
32	44.7	4.0	27.1	57.2	23.1
33	93.5	99.1	1.1	80.9	73.2
Average	72.2	68.1	73.0	73.3	68.0

Comp. Nº	DP4 – 12 kJ/mol – RMSD 0.5 Å				
	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	>99.9	>99.9	>99.9	>99.9	>99.9
2	>99.9	>99.9	>99.9	>99.9	>99.9
3	93.5	>99.9	73.5	99.5	99.9
4	99.9	>99.9	97.6	<0.1	84.2
5	>99.9	>99.9	99.4	0.4	2.9
6	5.2	53.0	97.6	92.5	1.4
7	83.3	98.9	99.9	2.9	62.6
8	<0.1	<0.1	33.8	<0.1	62.8
9	<0.1	18.7	<0.1	<0.1	0.2
10	98.7	99.2	>99.9	>99.9	>99.9
11	<0.1	95.2	99.6	99.9	2.6
12	57.9	21.8	27.0	3.1	1.4
13	3.0	11.0	8.1	85.9	36.5
14	54.2	42.0	5.6	5.0	37.8
15	98.0	8<0.1	>99.9	>99.9	>99.9
16	0.1	>99.9	46.1	99.9	<0.1
17	93.7	3.4	94.2	<0.1	99.9
18	22.0	2.7	5.1	9.6	50.6
19	95.7	71.4	>99.9	88.2	22.6
20	>99.9	>99.9	>99.9	>99.9	>99.9
21	99.4	97.8	97.5	99.7	98.2
22	95.2	69.7	98.1	99.8	95.9
23	>99.9	>99.9	>99.9	>99.9	>99.9
24	>99.9	6.1	99.4	99.5	98.9
25	59.8	50.9	80.7	96.3	>99.9
26	79.0	74.8	31.4	77.4	99.1
27	99.8	94.5	>99.9	95.2	61.6
28	<0.1	96.8	3.1	92.2	93.6
29	23.7	15.6	15.5	51.4	5.0
30	1.9	97.3	52.4	99.6	78.4
31	99.2	99.6	<0.1	86.9	<0.1
32	33.9	1.3	0.5	0.3	29.7
33	86.0	99.1	26.9	90.4	86.5
Average	63.1	66.7	63.4	65.9	61.0

Comp. Nº	DP4 – 21 kJ/mol – RMSD 0.5 Å				
	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	>99.9	>99.9	>99.9	>99.9	>99.9
2	>99.9	>99.9	>99.9	>99.9	>99.9
3	93.1	>99.9	72.6	99.5	99.3
4	99.9	99.9	97.4	<0.1	82.8
5	>99.9	>99.9	99.4	0.4	7.7
6	5.2	50.2	93.9	95.1	12.1
7	45.0	98.2	99.9	90.1	61.2
8	96.0	41.4	56.6	71.7	65.3
9	<0.1	48.4	<0.1	<0.1	0.6
10	98.4	93.0	>99.9	>99.9	>99.9
11	1.8	61.1	15.8	>99.9	1.5
12	11.9	21.1	11.2	1.8	6.1
13	1.8	10.7	75.8	94.9	54.6
14	71.8	45.6	29.7	4.4	73.7
15	98.0	81.6	>99.9	>99.9	>99.9
16	0.1	>99.9	39.5	28.2	77.5
17	82.4	3.7	92.7	<0.1	>99.9
18	2.8	2.3	5.0	1.4	49.7
19	95.7	72.6	>99.9	86.5	21.8
20	>99.9	>99.9	>99.9	>99.9	>99.9
21	99.4	97.8	98.4	99.7	98.3
22	95.2	58.1	97.9	99.8	95.8
23	>99.9	>99.9	>99.9	>99.9	>99.9
24	99.9	6.2	99.5	99.7	99.7
25	51.6	50.8	58.1	58.4	46.6
26	79.8	76.1	36.7	77.9	70.5
27	99.8	94.8	0.9	87.8	53.0
28	<0.1	96.3	>99.9	95.7	94.6
29	2.4	2.3	3.1	27.5	0.5
30	2.8	97.7	52.4	99.6	82.5
31	99.8	99.7	<0.1	93.2	0.1
32	12.1	1.1	1.3	0.4	24.1
33	36.8	98.6	28.8	89.1	83.9
Average	60.1	66.9	62.6	66.7	62.5

Comp. Nº	DP4 – 21 kJ/mol – RMSD 1 Å				
	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	>99.9	>99.9	>99.9	>99.9	>99.9
2	>99.9	>99.9	>99.9	>99.9	>99.9
3	6.7	87.5	35.0	>99.9	>99.9
4	99.9	>99.9	97.6	<0.1	84.2
5	>99.9	>99.9	99.4	0.5	8.1
6	2.7	22.3	95.4	84.1	1.2
7	80.2	49.9	98.1	0.9	48.9
8	<0.1	90.5	99.9	0.9	<0.1
9	<0.1	0.2	59.2	0.1	<0.1
10	99.9	97.9	>99.9	>99.9	>99.9
11	<0.1	99.8	<0.1	2.7	<0.1
12	1.0	36.7	6.7	0.2	0.2
13	19.5	43.2	96.4	94.0	0.1
14	64.0	0.4	2.2	61.7	12.9
15	3.1	0.1	92.8	99.9	90.1
16	21.1	>99.9	1.2	0.3	0.3
17	96.8	3.2	>99.9	<0.1	98.0
18	28.4	0.8	4.6	<0.1	97.5
19	84.3	93.0	99.9	0.2	99.2
20	>99.9	>99.9	>99.9	>99.9	>99.9
21	99.4	>99.9	99.9	>99.9	98.3
22	95.2	0.2	77.6	>99.9	95.9
23	>99.9	>99.9	>99.9	>99.9	>99.9
24	>99.9	7.0	99.5	99.7	45.1
25	78.0	54.4	56.2	46.6	15.2
26	99.8	17.5	61.0	55.7	1.4
27	99.3	12.2	>99.9	96.8	49.5
28	0.5	>99.9	3.4	96.8	97.7
29	6.6	72.7	15.9	0.2	51.0
30	0.2	>99.9	28.6	0.2	83.2
31	99.9	3<0.1	<0.1	99.8	<0.1
32	2.7	<0.1	<0.1	0.2	99.3
33	<0.1	<0.1	43.9	2.6	44.7
Average	54.2	55.1	62.9	49.8	55.2

Table S38. dJ-DP4 results for compounds **1-33**

Comp. Nº	dJ-DP4 – 12 kJ/mol – MAD 05 Å				
	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	>99.9	>99.9	>99.9	>99.9	>99.9
2	>99.9	>99.9	>99.9	>99.9	>99.9
3	97.9	>99.9	>99.9	99.9	>99.9
4	>99.9	>99.9	>99.9	>99.9	>99.9
5	>99.9	>99.9	>99.9	>99.9	>99.9
6	13.1	1.7	99.8	97.4	0.2
7	79.9	96.2	99.9	0.1	43.3
8	>99.9	<0.1	0.8	<0.1	78.6
9	>99.9	>99.9	>99.9	>99.9	87.1
10	>99.9	>99.9	>99.9	>99.9	>99.9
11	99.6	>99.9	99.9	>99.9	30.1
12	>99.9	>99.9	>99.9	99.2	96.0
13	63.6	99.5	>99.9	99.9	>99.9
14	>99.9	>99.9	99.6	>99.9	>99.9
15	>99.9	>99.9	>99.9	>99.9	>99.9
16	0.1	99.9	0.1	0.1	0.1
17	>99.9	>99.9	90.7	<0.1	99.9
18	>99.9	74.1	41.2	>99.9	>99.9
19	>99.9	>99.9	>99.9	>99.9	>99.9
20	>99.9	>99.9	>99.9	>99.9	>99.9
21	99.2	97.0	97.2	99.7	97.6
22	98.9	95.3	99.8	>99.9	99.7
23	>99.9	>99.9	>99.9	>99.9	>99.9
24	>99.9	>99.9	>99.9	>99.9	>99.9
25	>99.9	>99.9	>99.9	>99.9	>99.9
26	>99.9	>99.9	>99.9	>99.9	>99.9
27	>99.9	>99.9	>99.9	>99.9	>99.9
28	99.1	>99.9	>99.9	>99.9	>99.9
29	91.8	99.8	88.3	93.2	19.3
30	0.3	>99.9	94.0	1.1	72.1
31	>99.9	>99.9	99.5	1.9	9.1
32	82.4	89.3	18.2	68.5	71.1
33	97.4	>99.9	13.9	>99.9	97.7
Average	88.6	92.5	86.1	80.6	81.9

Comp. Nº	dJ-DP4 – 21 kJ/mol – MAD 05 Å				
	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	>99.9	>99.9	>99.9	>99.9	>99.9
2	>99.9	>99.9	>99.9	>99.9	>99.9
3	98.9	>99.9	>99.9	99.9	>99.9
4	>99.9	>99.9	>99.9	>99.9	>99.9
5	>99.9	>99.9	>99.9	>99.9	>99.9
6	13.1	0.9	98.1	99.0	3.1
7	79.8	96.2	>99.9	99.2	39.8
8	99.9	99.8	3.8	<0.1	21.9
9	>99.9	>99.9	>99.9	>99.9	87.8
10	>99.9	>99.9	>99.9	>99.9	>99.9
11	>99.9	98.0	99.9	>99.9	7.4
12	99.9	>99.9	>99.9	97.4	98.5
13	<0.1	99.5	>99.9	>99.9	>99.9
14	>99.9	>99.9	>99.9	>99.9	>99.9
15	>99.9	>99.9	>99.9	>99.9	>99.9
16	99.0	0.1	<0.1	85.2	2.4
17	99.4	6.7	95.5	<0.1	>99.9
18	>99.9	61.0	33.0	>99.9	>99.9
19	>99.9	>99.9	>99.9	>99.9	>99.9
20	>99.9	>99.9	>99.9	>99.9	>99.9
21	99.2	96.9	98.2	99.7	97.6
22	98.9	92.5	99.8	>99.9	99.7
23	>99.9	>99.9	>99.9	>99.9	>99.9
24	>99.9	>99.9	>99.9	>99.9	>99.9
25	>99.9	>99.9	>99.9	>99.9	>99.9
26	>99.9	>99.9	>99.9	>99.9	>99.9
27	>99.9	>99.9	>99.9	>99.9	>99.9
28	99.1	>99.9	>99.9	>99.9	>99.9
29	5.2	82.9	16.7	96.1	0.7
30	6.3	>99.9	90.4	0.3	77.8
31	>99.9	>99.9	98.7	4.2	92.3
32	73.1	98.4	15.7	56.2	12.6
33	99.9	>99.9	26.4	>99.9	96.4
Average	87.0	88.9	84.1	86.0	79.9

Comp. Nº	dJ-DP4 – 21 kJ/mol – MAD 1 Å				
	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	>99.9	>99.9	>99.9	>99.9	>99.9
2	>99.9	>99.9	>99.9	>99.9	>99.9
3	98.9	>99.9	>99.9	99.9	>99.9
4	>99.9	>99.9	>99.9	>99.9	>99.9
5	>99.9	>99.9	>99.9	>99.9	>99.9
6	13.1	0.9	97.4	98.6	3.1
7	79.8	96.2	>99.9	99.2	39.8
8	99.9	99.9	3.2	<0.1	21.5
9	>99.9	93.4	>99.9	>99.9	91.1
10	>99.9	>99.9	>99.9	>99.9	>99.9
11	>99.9	>99.9	99.8	>99.9	1.6
12	99.9	>99.9	>99.9	99.0	98.7
13	<0.1	99.5	>99.9	>99.9	>99.9
14	>99.9	>99.9	>99.9	>99.9	>99.9
15	7<0.1	7.1	>99.9	>99.9	>99.9
16	2.7	0.7	<0.1	<0.1	99.9
17	99.8	0.7	88.0	<0.1	>99.9
18	>99.9	65.2	33.8	>99.9	>99.9
19	>99.9	>99.9	>99.9	>99.9	>99.9
20	>99.9	>99.9	>99.9	>99.9	>99.9
21	99.2	96.9	98.2	99.7	97.6
22	98.9	92.5	99.8	>99.9	99.7
23	>99.9	>99.9	>99.9	>99.9	>99.9
24	>99.9	>99.9	>99.9	>99.9	>99.9
25	>99.9	>99.9	>99.9	>99.9	>99.9
26	>99.9	>99.9	>99.9	>99.9	>99.9
27	>99.9	>99.9	>99.9	>99.9	>99.9
28	>99.9	>99.9	>99.9	>99.9	>99.9
29	14.9	68.5	20.1	99.7	4.5
30	2.3	99.9	90.9	0.3	21.9
31	>99.9	>99.9	97.4	7.4	89.9
32	74.5	93.5	16.0	81.5	10.1
33	99.9	>99.9	26.0	>99.9	99.4
Average	83.5	85.3	84.0	84.4	81.2

Comp. Nº	dJ-DP4 – 12 kJ/mol – RMSD 0.5 Å				
	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	>99.9	>99.9	>99.9	>99.9	>99.9
2	>99.9	>99.9	>99.9	>99.9	>99.9
3	97.0	>99.9	94.8	99.8	>99.9
4	>99.9	>99.9	>99.9	59.3	>99.9
5	>99.9	>99.9	>99.9	99.7	99.9
6	0.7	1.8	99.6	97.4	0.2
7	90.9	96.2	>99.9	0.1	43.3
8	>99.9	<0.1	<0.1	<0.1	96.8
9	97.6	>99.9	<0.1	>99.9	3.7
10	>99.9	>99.9	>99.9	>99.9	>99.9
11	34.4	>99.9	>99.9	>99.9	<0.1
12	>99.9	>99.9	>99.9	99.9	96.5
13	65.1	99.6	99.9	>99.9	>99.9
14	>99.9	>99.9	99.9	>99.9	>99.9
15	>99.9	>99.9	80.2	>99.9	>99.9
16	<0.1	99.6	<0.1	99.1	<0.1
17	>99.9	99.5	99.2	<0.1	>99.9
18	>99.9	23.3	12.8	>99.9	>99.9
19	>99.9	>99.9	>99.9	>99.9	>99.9
20	>99.9	>99.9	>99.9	>99.9	>99.9
21	99.2	97.0	97.2	99.7	97.6
22	98.9	95.3	99.8	>99.9	99.7
23	>99.9	>99.9	>99.9	>99.9	>99.9
24	>99.9	>99.9	>99.9	>99.9	>99.9
25	>99.9	>99.9	>99.9	>99.9	>99.9
26	>99.9	>99.9	>99.9	>99.9	>99.9
27	>99.9	>99.9	>99.9	>99.9	>99.9
28	<0.1	>99.9	99.5	>99.9	>99.9
29	98.0	98.3	99.7	79.6	35.3
30	0.5	99.7	16.6	2.9	8.8
31	>99.9	>99.9	<0.1	0.3	<0.1
32	88.3	9.1	0.3	<0.1	3.1
33	98.5	>99.9	86.3	>99.9	99.8
Average	83.9	88.5	78.4	79.9	75.3

Comp. Nº	dJ-DP4 – 21 kJ/mol – RMSD 0.5 Å				
	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	>99.9	>99.9	>99.9	>99.9	>99.9
2	>99.9	>99.9	>99.9	>99.9	>99.9
3	97.8	>99.9	94.5	99.8	>99.9
4	>99.9	>99.9	>99.9	61.1	>99.9
5	>99.9	>99.9	>99.9	99.7	>99.9
6	0.7	0.9	96.7	98.6	3.1
7	84.1	96.2	>99.9	99.2	39.8
8	>99.9	87.7	0.1	5.9	88.9
9	99.1	99.8	<0.1	>99.9	3.6
10	>99.9	>99.9	>99.9	>99.9	>99.9
11	99.9	87.2	5.4	>99.9	<0.1
12	99.9	>99.9	99.9	99.5	99.1
13	<0.1	99.6	>99.9	>99.9	>99.9
14	>99.9	>99.9	>99.9	>99.9	>99.9
15	99.8	>99.9	70.9	>99.9	>99.9
16	<0.1	99.9	<0.1	<0.1	99.8
17	>99.9	30.1	99.0	<0.1	>99.9
18	>99.9	19.3	17.3	>99.9	>99.9
19	>99.9	>99.9	>99.9	>99.9	>99.9
20	>99.9	>99.9	>99.9	>99.9	>99.9
21	99.2	96.9	98.2	99.7	97.6
22	98.9	92.5	99.8	>99.9	99.7
23	>99.9	>99.9	>99.9	>99.9	>99.9
24	>99.9	>99.9	>99.9	>99.9	>99.9
25	>99.9	>99.9	>99.9	>99.9	>99.9
26	>99.9	>99.9	>99.9	>99.9	>99.9
27	>99.9	>99.9	97.0	>99.9	>99.9
28	<0.1	>99.9	>99.9	>99.9	>99.9
29	1.5	1.2	63.7	97.3	<0.1
30	1.1	99.8	16.6	2.0	13.0
31	>99.9	>99.9	<0.1	0.8	<0.1
32	93.6	5.7	0.8	<0.1	2.8
33	93.2	>99.9	87.5	>99.9	99.7
Average	80.9	85.4	74.2	80.7	77.2

Comp. Nº	dJ-DP4 – 21 kJ/mol – RMSD 1 Å				
	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	>99.9	>99.9	>99.9	>99.9	>99.9
2	>99.9	>99.9	>99.9	>99.9	>99.9
3	0.1	99.7	73.4	>99.9	>99.9
4	>99.9	>99.9	>99.9	80.6	>99.9
5	>99.9	>99.9	>99.9	99.8	>99.9
6	0.1	0.6	99.6	75.5	0.1
7	96.4	6.4	99.2	<0.1	14.6
8	>99.9	>99.9	91.5	>99.9	<0.1
9	>99.9	>99.9	99.6	>99.9	99.6
10	>99.9	>99.9	>99.9	>99.9	>99.9
11	20.5	>99.9	<0.1	>99.9	<0.1
12	99.3	>99.9	>99.9	88.5	96.7
13	29.8	99.9	>99.9	99.8	99.4
14	>99.9	>99.9	99.7	>99.9	99.9
15	1.1	59.0	1.7	98.8	99.8
16	<0.1	>99.9	<0.1	<0.1	<0.1
17	99.9	99.9	>99.9	<0.1	>99.9
18	>99.9	>99.9	99.5	>99.9	>99.9
19	>99.9	>99.9	>99.9	>99.9	>99.9
20	>99.9	>99.9	>99.9	>99.9	>99.9
21	99.2	>99.9	99.8	>99.9	97.6
22	98.9	2.6	98.0	>99.9	99.7
23	>99.9	>99.9	>99.9	>99.9	>99.9
24	>99.9	>99.9	>99.9	>99.9	>99.9
25	>99.9	>99.9	>99.9	>99.9	>99.9
26	>99.9	99.9	>99.9	>99.9	>99.9
27	>99.9	99.5	>99.9	>99.9	>99.9
28	97.7	>99.9	99.5	>99.9	>99.9
29	64.7	94.8	5.6	0.1	98.4
30	0.2	>99.9	8.1	<0.1	12.9
31	>99.9	0.1	<0.1	>99.9	<0.1
32	95.3	0.2	<0.1	0.4	99.9
33	7.7	<0.1	93.3	98.3	97.2
Average	76.1	80.7	77.8	80.1	79.3

Table S39. iJ/dJ-DP4 results for compounds **1-33**

Comp. N°	iJ/dJ-DP4 – 12 kJ/mol – MAD 05 Å				
	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	>99.9	>99.9	>99.9	>99.9	>99.9
2	>99.9	>99.9	>99.9	>99.9	>99.9
3	>99.9	>99.9	99.9	80.8	>99.9
4	>99.9	>99.9	>99.9	>99.9	>99.9
5	>99.9	>99.9	>99.9	>99.9	>99.9
6	83.2	11.9	99.5	99.8	<0.1
7	79.9	96.2	98.7	0.3	9.5
8	>99.9	<0.1	>99.9	3.7	76.6
9	>99.9	>99.9	>99.9	>99.9	37.6
10	>99.9	>99.9	>99.9	>99.9	>99.9
11	98.7	>99.9	65.7	>99.9	>99.9
12	>99.9	>99.9	>99.9	>99.9	99.1
13	99.8	99.5	>99.9	>99.9	>99.9
14	>99.9	>99.9	99.9	>99.9	>99.9
15	>99.9	>99.9	>99.9	>99.9	>99.9
16	99.4	57.9	99.0	0.2	<0.1
17	>99.9	95.4	98.9	4.2	99.8
18	>99.9	99.9	99.9	>99.9	>99.9
19	>99.9	>99.9	>99.9	>99.9	>99.9
20	>99.9	>99.9	>99.9	>99.9	>99.9
21	99.2	97.0	97.2	99.7	97.6
22	99.0	95.4	99.8	>99.9	99.7
23	>99.9	>99.9	>99.9	>99.9	>99.9
24	>99.9	>99.9	>99.9	>99.9	>99.9
25	>99.9	>99.9	>99.9	>99.9	>99.9
26	>99.9	>99.9	>99.9	>99.9	>99.9
27	>99.9	>99.9	>99.9	>99.9	>99.9
28	>99.9	>99.9	>99.9	>99.9	>99.9
29	97.8	99.7	90.4	95.8	94.2
30	0.3	99.9	95.0	20.6	72.9
31	>99.9	>99.9	>99.9	>99.9	>99.9
32	>99.9	98.3	87.1	>99.9	>99.9
33	97.7	>99.9	13.4	>99.9	97.6
Average	95.6	92.5	95.3	85.0	87.4

Comp. Nº	iJ/dJ-DP4 – 21 kJ/mol – MAD 05 Å				
	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	>99.9	>99.9	>99.9	>99.9	>99.9
2	>99.9	>99.9	>99.9	>99.9	>99.9
3	>99.9	>99.9	>99.9	81.1	>99.9
4	>99.9	>99.9	>99.9	>99.9	>99.9
5	>99.9	>99.9	>99.9	>99.9	>99.9
6	83.2	10.2	96.6	99.9	<0.1
7	79.8	96.2	97.8	99.3	9.8
8	99.9	99.5	>99.9	73.4	83.3
9	>99.9	>99.9	>99.9	>99.9	45.3
10	>99.9	>99.9	>99.9	>99.9	>99.9
11	>99.9	>99.9	99.3	>99.9	>99.9
12	>99.9	>99.9	>99.9	63.8	99.8
13	>99.9	99.6	>99.9	>99.9	>99.9
14	>99.9	>99.9	99.9	>99.9	>99.9
15	>99.9	>99.9	>99.9	>99.9	>99.9
16	97.3	97.3	99.6	0.1	94.8
17	99.5	1.0	98.6	<0.1	99.8
18	>99.9	99.9	99.9	99.9	99.9
19	>99.9	>99.9	>99.9	>99.9	>99.9
20	>99.9	>99.9	>99.9	>99.9	>99.9
21	99.2	96.9	98.2	99.7	97.6
22	99.0	92.6	99.8	>99.9	99.7
23	>99.9	>99.9	>99.9	>99.9	>99.9
24	>99.9	>99.9	>99.9	>99.9	>99.9
25	>99.9	>99.9	>99.9	>99.9	>99.9
26	>99.9	>99.9	>99.9	>99.9	>99.9
27	>99.9	>99.9	>99.9	>99.9	>99.9
28	>99.9	>99.9	>99.9	>99.9	>99.9
29	2.2	71.1	22.7	93.8	0.4
30	76.7	99.9	95.7	42.2	73.7
31	>99.9	>99.9	>99.9	>99.9	>99.9
32	>99.9	97.4	<0.1	>99.9	91.0
33	99.7	>99.9	16.6	>99.9	96.9
Average	95.0	92.8	91.7	89.5	87.6

Comp. Nº	iJ/dJ-DP4 – 21 kJ/mol – MAD 1 Å				
	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	>99.9	>99.9	>99.9	>99.9	>99.9
2	>99.9	>99.9	>99.9	>99.9	>99.9
3	>99.9	99.9	>99.9	81.1	>99.9
4	>99.9	>99.9	>99.9	>99.9	>99.9
5	>99.9	>99.9	>99.9	>99.9	>99.9
6	83.2	10.2	95.5	99.9	<0.1
7	79.8	96.2	99.2	99.3	9.8
8	99.9	99.6	>99.9	2.5	83.0
9	>99.9	91.4	>99.9	>99.9	33.6
10	>99.9	>99.9	>99.9	>99.9	>99.9
11	>99.9	>99.9	83.4	>99.9	80.5
12	>99.9	>99.9	>99.9	>99.9	99.9
13	>99.9	99.6	>99.9	>99.9	>99.9
14	>99.9	>99.9	>99.9	>99.9	>99.9
15	69.0	6.6	>99.9	>99.9	>99.9
16	19.8	6.6	89.1	0.1	26.5
17	99.8	5.1	>99.9	<0.1	>99.9
18	>99.9	99.9	99.9	>99.9	>99.9
19	>99.9	>99.9	>99.9	>99.9	>99.9
20	>99.9	>99.9	>99.9	>99.9	>99.9
21	99.2	96.9	98.2	99.7	97.6
22	99.0	92.6	99.8	>99.9	99.7
23	>99.9	>99.9	>99.9	>99.9	>99.9
24	>99.9	>99.9	>99.9	>99.9	>99.9
25	>99.9	>99.9	>99.9	>99.9	>99.9
26	>99.9	>99.9	>99.9	>99.9	>99.9
27	>99.9	>99.9	>99.9	>99.9	>99.9
28	>99.9	>99.9	>99.9	>99.9	>99.9
29	6.9	66.0	26.2	98.8	22.4
30	47.8	99.6	96.0	38.8	18.2
31	>99.9	>99.9	>99.9	>99.9	>99.9
32	>99.9	77.3	<0.1	>99.9	91.0
33	99.8	>99.9	16.4	>99.9	99.5
Average	91.0	86.3	91.0	88.5	83.7

Comp. №	iJ/dJ-DP4 – 12 kJ/mol – RMSD 0.5 Å				
	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	>99.9	>99.9	>99.9	>99.9	>99.9
2	>99.9	>99.9	>99.9	>99.9	>99.9
3	>99.9	99.9	>99.9	87.4	>99.9
4	>99.9	>99.9	>99.9	59.3	>99.9
5	>99.9	>99.9	>99.9	>99.9	>99.9
6	15.5	12.0	99.2	99.8	<0.1
7	90.9	96.2	99.6	0.3	9.5
8	>99.9	<0.1	98.5	9.0	97.4
9	99.3	>99.9	90.3	>99.9	1.9
10	>99.9	>99.9	>99.9	>99.9	>99.9
11	77.7	>99.9	>99.9	>99.9	>99.9
12	>99.9	>99.9	>99.9	>99.9	99.9
13	99.7	99.7	>99.9	>99.9	>99.9
14	>99.9	>99.9	>99.9	>99.9	>99.9
15	>99.9	>99.9	99.4	0.1	>99.9
16	>99.9	0.1	8.5	>99.9	<0.1
17	>99.9	>99.9	>99.9	77.8	>99.9
18	98.9	99.8	99.9	99.3	99.9
19	>99.9	>99.9	>99.9	>99.9	>99.9
20	>99.9	>99.9	>99.9	>99.9	>99.9
21	99.2	97.0	97.2	99.7	97.6
22	99.0	95.4	99.8	>99.9	99.7
23	>99.9	>99.9	>99.9	>99.9	>99.9
24	>99.9	>99.9	>99.9	>99.9	>99.9
25	>99.9	>99.9	>99.9	>99.9	>99.9
26	>99.9	>99.9	>99.9	>99.9	>99.9
27	>99.9	>99.9	>99.9	>99.9	>99.9
28	>99.9	>99.9	>99.9	>99.9	>99.9
29	89.2	97.2	98.4	84.7	99.2
30	0.5	99.2	19.8	0.1	9.2
31	>99.9	>99.9	>99.9	>99.9	>99.9
32	>99.9	99.8	0.7	>99.9	>99.9
33	98.2	>99.9	85.0	>99.9	99.7
Average	93.0	90.8	90.8	85.4	85.3

Comp. №	iJ/dJ-DP4 – 21 kJ/mol – RMSD 0.5 Å				
	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	>99.9	>99.9	>99.9	>99.9	>99.9
2	>99.9	>99.9	>99.9	>99.9	>99.9
3	>99.9	99.9	>99.9	87.7	>99.9
4	>99.9	>99.9	>99.9	61.1	>99.9
5	>99.9	>99.9	>99.9	>99.9	>99.9
6	15.5	10.2	94.9	99.9	<0.1
7	84.1	96.2	99.2	99.3	9.8
8	>99.9	68.6	95.1	99.8	99.5
9	99.4	>99.9	99.7	>99.9	2.2
10	>99.9	>99.9	>99.9	>99.9	>99.9
11	>99.9	>99.9	>99.9	>99.9	>99.9
12	>99.9	>99.9	>99.9	>99.9	>99.9
13	>99.9	99.7	>99.9	>99.9	>99.9
14	>99.9	99.9	99.9	>99.9	>99.9
15	>99.9	>99.9	99.0	0.1	>99.9
16	>99.9	7.5	7.9	97.8	26.6
17	>99.9	98.4	>99.9	<0.1	>99.9
18	99.4	99.8	>99.9	99.1	98.0
19	>99.9	>99.9	>99.9	>99.9	>99.9
20	>99.9	>99.9	>99.9	>99.9	>99.9
21	99.2	96.9	98.2	99.7	97.6
22	99.0	92.6	99.8	>99.9	99.7
23	>99.9	>99.9	>99.9	>99.9	>99.9
24	>99.9	>99.9	>99.9	>99.9	>99.9
25	>99.9	>99.9	>99.9	>99.9	>99.9
26	>99.9	>99.9	>99.9	>99.9	>99.9
27	>99.9	>99.9	>99.9	>99.9	>99.9
28	0.8	>99.9	>99.9	>99.9	>99.9
29	1.4	0.9	61.2	95.4	0.1
30	0.4	99.4	19.9	0.1	10.1
31	>99.9	>99.9	52.5	>99.9	>99.9
32	>99.9	99.7	<0.1	98.5	99.9
33	98.3	>99.9	86.3	>99.9	99.7
Average	87.8	90.0	88.3	89.0	83.1

Comp. N°	iJ/dJ-DP4 – 21 kJ/mol – RMSD 1 Å				
	AMBER	MM3	MMFF	OPLS2005	OPLS4
1	>99.9	>99.9	>99.9	>99.9	>99.9
2	>99.9	>99.9	>99.9	>99.9	>99.9
3	<0.1	>99.9	>99.9	92.9	>99.9
4	>99.9	>99.9	>99.9	80.7	>99.9
5	>99.9	>99.9	>99.9	>99.9	>99.9
6	1.6	5.1	99.0	97.3	0.2
7	96.4	6.4	99.2	1.4	98.2
8	>99.9	>99.9	87.5	>99.9	5.0
9	>99.9	92.3	98.6	>99.9	93.3
10	>99.9	>99.9	>99.9	>99.9	>99.9
11	23.4	99.9	>99.9	>99.9	89.6
12	75.7	>99.9	>99.9	<0.1	>99.9
13	93.0	99.9	>99.9	>99.9	99.7
14	>99.9	>99.9	99.4	>99.9	99.9
15	0.5	60.1	1.8	<0.1	99.9
16	96.0	<0.1	>99.9	<0.1	12.5
17	80.3	98.1	>99.9	<0.1	>99.9
18	>99.9	>99.9	>99.9	>99.9	>99.9
19	>99.9	>99.9	>99.9	>99.9	>99.9
20	>99.9	>99.9	>99.9	>99.9	>99.9
21	99.2	>99.9	99.8	>99.9	97.6
22	99.0	3.2	98.3	>99.9	99.7
23	>99.9	>99.9	>99.9	>99.9	>99.9
24	>99.9	>99.9	>99.9	>99.9	>99.9
25	>99.9	>99.9	>99.9	>99.9	>99.9
26	>99.9	<0.1	>99.9	>99.9	>99.9
27	>99.9	>99.9	>99.9	>99.9	>99.9
28	99.6	>99.9	99.9	>99.9	>99.9
29	75.8	90.6	77.4	0.2	99.8
30	<0.1	99.9	9.3	<0.1	<0.1
31	>99.9	>99.9	<0.1	>99.9	>99.9
32	>99.9	>99.9	83.2	>99.9	>99.9
33	<0.1	0.1	92.6	99.8	15.3
Average	80.0	80.5	89.3	77.9	85.2

Table S40. Dependence of DP4 and J-DP4 on the energy cutoff used during the conformational search for selected examples.

Nº	C.Search	E. Cutoff	DP4	dJ-DP4	ij/dJ-DP4
7	OPLS2005	12	2.9	0.1	0.3
	MAD 05	21	90.1	99.2	99.3
8	AMBER	12	<0.1	>99.9	>99.9
	RMS 05	21	96.0	>99.9	>99.9
11	MMFF	12	99.6	>99.9	>99.9
	RMS 05	21	15.8	5.4	>99.9
16	AMBER	12	11.5	0.1	99.4
	MAD 05	21	99.9	99.0	97.3
27	MMFF	12	>99.9	>99.9	>99.9
	RMS 05	21	0.9	97.0	>99.9
28	MMFF	12	3.1	99.4	>99.9
	RMS 05	21	>99.9	>99.9	>99.9

Table S41. Results for Mix-J-DP4.

Comp. Nº	iJ/dJ-DP4 – 12 kJ/mol – MAD 05 Å (Mix-J-DP4)			
	AMBER	MM3	MMFF	Mix-J-DP4
1	>99.9	>99.9	>99.9	>99.9
2	>99.9	>99.9	>99.9	>99.9
3	>99.9	>99.9	99.9	>99.9
4	>99.9	>99.9	>99.9	>99.9
5	>99.9	>99.9	>99.9	>99.9
6	83.2	11.9	99.5	64.9
7	79.9	96.2	98.7	91.6
8	>99.9	<0.1	>99.9	66.7
9	>99.9	>99.9	>99.9	>99.9
10	>99.9	>99.9	>99.9	>99.9
11	98.7	>99.9	65.7	88.1
12	>99.9	>99.9	>99.9	>99.9
13	99.8	99.5	>99.9	99.8
14	>99.9	>99.9	99.9	99.9
15	>99.9	>99.9	>99.9	>99.9
16	99.4	57.9	99.0	85.4
17	>99.9	95.4	98.9	98.1
18	>99.9	99.9	99.9	99.9
19	>99.9	>99.9	>99.9	>99.9
20	>99.9	>99.9	>99.9	>99.9
21	99.2	97.0	97.2	97.8
22	99.0	95.4	99.8	98.1
23	>99.9	>99.9	>99.9	>99.9
24	>99.9	>99.9	>99.9	>99.9
25	>99.9	>99.9	>99.9	>99.9
26	>99.9	>99.9	>99.9	>99.9
27	>99.9	>99.9	>99.9	>99.9
28	>99.9	>99.9	>99.9	>99.9
29	97.8	99.7	90.4	96.0
30	0.3	99.9	95.0	65.1
31	>99.9	>99.9	>99.9	>99.9
32	>99.9	98.3	87.1	95.1
33	97.7	>99.9	13.4	70.4
Average	95.6	92.5	95.3	94.4
Nº fails	1	2	1	0

7. Summary of general results

Table S42. Average number of conformers found for DP4 and dJ-DP4 approaches.

	21kJ				12kJ	
	MAD-05	RMS-05	MAD-1	RMS-1	MAD-05	RMS-05
AMBER	100.9	32.0	76.6	7.5	42.2	12.7
MM3	63.0	25.4	45.3	6.7	29.4	11.5
MMFF	83.1	26.6	62.0	6.5	36.1	11.2
OPLS2005	68.2	25.9	56.3	7.1	30.7	11.1
OPLS4	81.2	28.7	56.6	7.3	35.9	11.1

Table S43. Average number of conformers found for iJ/dJ-DP4 approach.

	21kJ				12kJ	
	MAD-05	RMS-05	MAD-1	RMS-1	MAD-05	RMS-05
AMBER	24.3	6.6	16.4	1.8	13.5	3.4
MM3	16.2	5.7	10.8	1.6	9.3	2.9
MMFF	21.0	6.3	15.1	1.7	10.9	3.0
OPLS2005	14.3	4.3	9.9	1.3	7.9	2.1
OPLS4	19.8	6.1	12.6	1.8	11.2	2.6

Table S44. Relative number of conformers found for DP4 and dJ-DP4 approaches.

	21kJ				12kJ	
	MAD-05	RMS-05	MAD-1	RMS-1	MAD-05	RMS-05
AMBER	100.0	33.4	79.4	8.0	38.4	13.1
MM3	100.0	43.4	76.3	11.9	43.4	19.2
MMFF	100.0	33.7	76.9	8.4	40.6	14.2
OPLS2005	100.0	41.1	87.0	11.5	42.2	17.5
OPLS4	100.0	37.2	72.5	9.8	40.5	14.3

Table S45. Relative number of conformers found for iJ/dJ-DP4 approach.

	21kJ				12kJ	
	MAD-05	RMS-05	MAD-1	RMS-1	MAD-05	RMS-05
AMBER	100.0	29.3	71.1	8.2	52.1	14.8
MM3	100.0	39.4	73.6	11.8	52.9	19.7
MMFF	100.0	33.2	75.3	9.6	47.2	16.0
OPLS2005	100.0	34.9	76.2	10.8	51.1	17.0
OPLS4	100.0	34.4	70.6	10.9	49.7	14.5

Table S46. Overall probability for each Force Field

	DP4	dJ-DP4	ij/dJ-DP4
AMBER	65.4	83.3	90.4
MM3	66.8	86.9	88.8
MMFF	68.4	80.8	91.1
OPLS2005	66.9	82.0	85.4
OPLS4	63.5	79.1	85.3

Table S47. Overall probability for each geometric criterion

	DP4	dJ-DP4	ij/dJ-DP4
MAD-05 Å	71.5	85.6	91.2
RMS-05 Å	63.9	80.4	88.3
MAD-1 Å	70.9	83.7	88.1
RMS-1 Å	55.4	78.8	82.0

Table S48. Overall probability for each energy cutoff

	DP4	dJ-DP4	ij/dJ-DP4
12 kJ/mol	67.45	83.57	90.10
21 kJ/mol	65.58	81.82	87.25

Table S49. Overall probability for each Force Field at 21 kJ/mol and MAD 0.5 Å

	DP4	dJ-DP4	ij/dJ-DP4
AMBER	74.4	87.1	94.6
MM3	70.8	88.2	92.1
MMFF	78.3	88.2	96.9
OPLS2005	72.2	92.3	88.4
OPLS4	69.9	81.3	86.8

Table S50. Overall probability for each Force Field at 21 kJ/mol and RMSD 0.5 Å

	DP4	dJ-DP4	ij/dJ-DP4
AMBER	62.4	80.1	89.9
MM3	68.1	87.4	88.7
MMFF	68.4	80.8	90.9
OPLS2005	66.2	88.3	88.0
OPLS4	64.6	83.8	81.5

Table S51. Overall probability for each Force Field at 21 kJ/mol and MAD 1 Å

	DP4	dJ-DP4	ij/dJ-DP4
AMBER	72.4	83.2	90.1
MM3	69.2	84.6	85.7
MMFF	78.0	87.6	96.2
OPLS2005	72.3	89.5	87.3
OPLS4	68.6	84.7	82.4

Table S52. Overall probability for each Force Field at 21 kJ/mol and RMSD 1 Å

	DP4	dJ-DP4	ij/dJ-DP4
AMBER	57.6	77.7	81.4
MM3	58.7	85.9	82.3
MMFF	69.0	85.1	89.0
OPLS2005	53.1	84.2	75.7
OPLS4	55.0	83.0	86.1

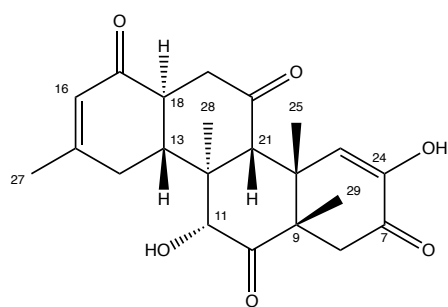
Table S53. Overall probability for each Force Field at 12 kJ/mol and MAD 0.5 Å

	DP4	dJ-DP4	ij/dJ-DP4
AMBER	67.6	88.5	95.2
MM3	73.7	92.4	91.8
MMFF	78.0	90.7	98.1
OPLS2005	71.4	85.8	83.5
OPLS4	70.2	84.5	86.2

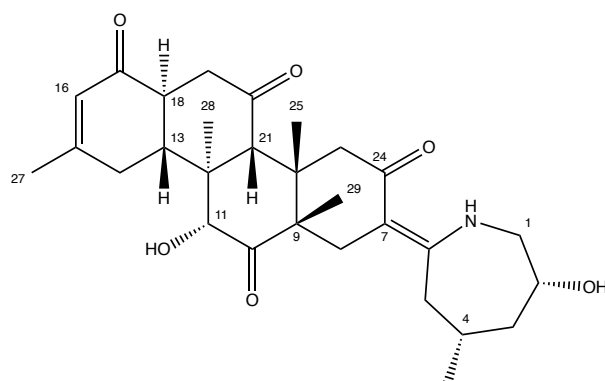
Table S54. Overall probability for each Force Field at 12 kJ/mol and RMSD 0.5 Å

	DP4	dJ-DP4	ij/dJ-DP4
AMBER	63.3	83.3	92.3
MM3	67.8	90.7	89.9
MMFF	66.6	80.6	93.7
OPLS2005	65.5	87.4	83.9
OPLS4	62.7	81.8	83.8

8. Zoarenone and Zoaramine as examples



Zoarenone (34)



Zoaramine (35)

Table S55. ^1H and ^{13}C NMR data

Zoarenone (34)				Zoaramine (35)		
N ^o	δ_{C}	δ_{H}	J (Hz)	δ_{C}	δ_{H}	J (Hz)
1a				49.9	3.42	
1b					3.42	
2				69.6	3.68	10.7, 2.0
3a				48.1	1.41	12.0, 10.7
3b					2.15	2.0, 2.0
4					1.70	12.0, 10.1, 2.0, 1.5
5a				29.1	2.29	10.1
5b				35.1	2.60	1.5
6				167.3		
7	191.5			95.3		
8a		2.88			3.03	
8b	40.6	2.51		32.1	2.09	
9	52.9			50.8		
10	211.7			212.2		
11	77.7	4.52		76.8	4.53	
12	52.1			51.6		
13	52.0	2.47	12.3, 11.0, 3.5	53.9	2.47	11.8, 11.0, 5.3
14a		2.39	3.5		2.45	11.0
14b	33.4	2.90	11.0	33.3	2.70	5.3
15	162.5			162.2		
16	124.7	5.93		125	5.92	
17	197.8			198.5		
18	45.6	2.55	12.5, 12.3, 5.1	45.3	2.55	12.4, 11.8, 5.4
19a		2.92	5.1		2.81	5.4
19b	43.2	2.46	12.5	42.9	2.46	12.4
20	207.6			207.6		
21	58.8	3.09		60.6	3.00	
22	43.8			41.7		
23a					2.24	
23b	120.7	6.74		43.7	3.09	
24	144.5			191.4		
25	21.7	1.40		21.0	1.17	
27	24.6	2.01		24.7	2.02	
28	10.7	0.81		13.0	0.87	
29	21.0	1.32		23.4	1.32	
30				24.7	1.13	

Table S56. Studied isomers for Zoarenone

Isomer	Configuration
Isomer 1	9R, 11R, 12R, 13R, 18S, 21R, 22R
Isomer 2	9S, 11R, 12R, 13R, 18S, 21R, 22R
Isomer 3	9R, 11S, 12R, 13R, 18S, 21R, 22R
Isomer 4	9S, 11S, 12R, 13R, 18S, 21R, 22R
Isomer 5	9R, 11R, 12S, 13R, 18S, 21R, 22R
Isomer 6	9S, 11R, 12S, 13R, 18S, 21R, 22R
Isomer 7	9R, 11S, 12S, 13R, 18S, 21R, 22R
Isomer 8	9S, 11S, 12S, 13R, 18S, 21R, 22R
Isomer 9	9R, 11R, 12R, 13R, 18S, 21S, 22R
Isomer 10	9S, 11R, 12R, 13R, 18S, 21S, 22R
Isomer 11	9R, 11S, 12R, 13R, 18S, 21S, 22R
Isomer 12	9S, 11S, 12R, 13R, 18S, 21S, 22R
Isomer 13	9R, 11R, 12S, 13R, 18S, 21S, 22R
Isomer 14	9S, 11R, 12S, 13R, 18S, 21S, 22R
Isomer 15	9R, 11S, 12S, 13R, 18S, 21S, 22R
Isomer 16	9S, 11S, 12S, 13R, 18S, 21S, 22R
Isomer 17	9R, 11R, 12R, 13R, 18S, 21R, 22S
Isomer 18	9S, 11R, 12R, 13R, 18S, 21R, 22S
Isomer 19	9R, 11S, 12R, 13R, 18S, 21R, 22S
Isomer 20	9S, 11S, 12R, 13R, 18S, 21R, 22S
Isomer 21	9R, 11R, 12S, 13R, 18S, 21R, 22S
Isomer 22	9S, 11R, 12S, 13R, 18S, 21R, 22S
Isomer 23	9R, 11S, 12S, 13R, 18S, 21R, 22S
Isomer 24	9S, 11S, 12S, 13R, 18S, 21R, 22S
Isomer 25	9R, 11R, 12R, 13R, 18S, 21S, 22S
Isomer 26	9S, 11R, 12R, 13R, 18S, 21S, 22S
Isomer 27	9R, 11S, 12R, 13R, 18S, 21S, 22S
Isomer 28	9S, 11S, 12R, 13R, 18S, 21S, 22S
Isomer 29	9R, 11R, 12S, 13R, 18S, 21S, 22S
Isomer 30	9S, 11R, 12S, 13R, 18S, 21S, 22S
Isomer 31	9R, 11S, 12S, 13R, 18S, 21S, 22S
Isomer 32	9S, 11S, 12S, 13R, 18S, 21S, 22S
Isomer 33	9R, 11R, 12R, 13S, 18S, 21R, 22R
Isomer 34	9S, 11R, 12R, 13S, 18S, 21R, 22R
Isomer 35	9R, 11S, 12R, 13S, 18S, 21R, 22R
Isomer 36	9S, 11S, 12R, 13S, 18S, 21R, 22R
Isomer 37	9R, 11R, 12S, 13S, 18S, 21R, 22R
Isomer 38	9S, 11R, 12S, 13S, 18S, 21R, 22R
Isomer 39	9R, 11S, 12S, 13S, 18S, 21R, 22R
Isomer 40	9S, 11S, 12S, 13S, 18S, 21R, 22R
Isomer 41	9R, 11R, 12R, 13S, 18S, 21S, 22R
Isomer 42	9S, 11R, 12R, 13S, 18S, 21S, 22R
Isomer 43	9R, 11S, 12R, 13S, 18S, 21S, 22R
Isomer 44	9S, 11S, 12R, 13S, 18S, 21S, 22R
Isomer 45	9R, 11R, 12S, 13S, 18S, 21S, 22R
Isomer 46	9S, 11R, 12S, 13S, 18S, 21S, 22R
Isomer 47	9R, 11S, 12S, 13S, 18S, 21S, 22R
Isomer 48	9S, 11S, 12S, 13S, 18S, 21S, 22R
Isomer 49	9R, 11R, 12R, 13S, 18S, 21R, 22S
Isomer 50	9S, 11R, 12R, 13S, 18S, 21R, 22S
Isomer 51	9R, 11S, 12R, 13S, 18S, 21R, 22S
Isomer 52	9S, 11S, 12R, 13S, 18S, 21R, 22S
Isomer 53	9R, 11R, 12S, 13S, 18S, 21R, 22S
Isomer 54	9S, 11R, 12S, 13S, 18S, 21R, 22S
Isomer 55	9R, 11S, 12S, 13S, 18S, 21R, 22S
Isomer 56	9S, 11S, 12S, 13S, 18S, 21R, 22S
Isomer 57	9R, 11R, 12R, 13S, 18S, 21S, 22S
Isomer 58	9S, 11R, 12R, 13S, 18S, 21S, 22S
Isomer 59	9R, 11S, 12R, 13S, 18S, 21S, 22S

Isomer 60	9S, 11S, 12R, 13S, 18S, 21S, 22S
Isomer 61	9R, 11R, 12S, 13S, 18S, 21S, 22S
Isomer 62	9S, 11R, 12S, 13S, 18S, 21S, 22S
Isomer 63	9R, 11S, 12S, 13S, 18S, 21S, 22S
Isomer 64	9S, 11S, 12S, 13S, 18S, 21S, 22S

Table S57. Studied isomers for Zoaramine

Isomer	Configuration
Isomer 1	2R, 4R, 9S, 11R, 12S, 13R, 18S, 21R, 22S
Isomer 2	2R, 4R, 9S, 11S, 12S, 13R, 18S, 21R, 22S
Isomer 3	2S, 4R, 9S, 11R, 12S, 13R, 18S, 21R, 22S
Isomer 4	2S, 4R, 9S, 11S, 12S, 13R, 18S, 21R, 22S
Isomer 5	2R, 4S, 9S, 11R, 12S, 13R, 18S, 21R, 22S
Isomer 6	2R, 4S, 9S, 11S, 12S, 13R, 18S, 21R, 22S
Isomer 7	2S, 4S, 9S, 11R, 12S, 13R, 18S, 21R, 22S
Isomer 8	2S, 4S, 9S, 11S, 12S, 13R, 18S, 21R, 22S

Table S58. Studied Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) and coupling constants of isomers calculated at the PCM/B3LYP/6-31G**//AMBER level of theory after elimination of conformations incompatible with experimental $^3J_{\text{HH}}$ of Zoarenone according to iJ/dJ-DP4.

Isotropic shielding constants								
Nuclei	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 7	7.17	6.87	7.41	7.80	10.17	6.96	8.74	6.32
C 8	145.52	148.01	145.89	146.55	147.79	147.39	145.92	146.96
C 9	136.93	134.64	136.95	136.10	135.30	132.69	135.75	132.78
C 10	-17.21	-22.06	-20.93	-23.13	-19.44	-20.51	-16.01	-17.52
C 11	113.32	113.80	121.11	119.67	116.00	116.64	114.76	114.64
C 12	141.90	145.95	137.12	148.29	140.14	139.24	143.09	142.81
C 13	142.78	148.88	141.20	142.45	138.46	138.14	145.01	144.47
C 14	158.73	156.94	154.68	158.35	158.41	158.14	160.49	160.08
C 15	34.37	33.47	30.07	32.36	33.15	33.15	33.80	33.22
C 16	67.90	68.71	69.14	68.84	68.69	68.62	68.02	68.16
C 17	2.59	2.86	4.05	3.11	3.81	3.67	3.73	3.60
C 18	142.14	148.59	143.64	149.38	148.27	147.81	147.56	147.02
C 19	148.90	152.71	147.89	147.11	147.57	147.95	147.42	147.91
C 20	-13.36	-14.65	-15.15	-15.03	-12.06	-12.11	-13.39	-13.37
C 21	128.85	135.62	127.32	133.45	133.13	136.74	136.16	139.04
C 22	144.14	142.05	144.09	148.28	144.75	144.61	145.17	145.40
C 23	56.86	60.22	57.93	61.04	61.09	58.83	62.29	58.32
C 24	49.60	46.47	49.42	46.32	47.24	47.03	47.55	47.01
C 25	167.81	160.53	167.86	162.69	169.69	164.55	168.70	162.93
C 27	165.92	166.12	165.82	165.55	165.64	165.71	165.65	165.76
C 28	163.98	152.41	165.18	163.14	176.87	176.53	174.89	173.96
C 29	163.32	167.37	164.27	169.10	171.46	169.58	171.21	168.73
H 8a	29.65	28.78	29.54	29.26	29.94	28.81	29.93	28.96
H 8b	28.93	29.58	29.04	29.06	29.15	29.61	28.24	29.53
H 11	28.03	27.35	27.55	27.50	27.61	27.49	28.11	28.08
H 13	30.10	29.74	30.13	30.41	29.83	29.78	29.08	29.10
H 14a	29.32	29.73	29.14	29.38	29.43	29.42	29.81	29.82
H 14b	29.75	28.60	29.34	29.36	29.28	29.34	29.59	29.48
H 16	25.86	25.92	25.89	25.90	25.88	25.88	25.87	25.84
H 18	28.67	29.34	29.47	29.37	29.55	29.51	29.53	29.50
H 19a	28.87	29.03	28.80	28.69	28.79	28.80	28.77	28.79
H 19b	29.74	29.62	29.79	29.67	29.85	29.81	29.81	29.77
H 21	29.78	29.09	29.60	29.14	28.93	29.16	28.53	28.83
H 23	25.85	24.42	25.88	25.10	25.05	24.98	25.12	24.98
H 25a-c	30.21	30.44	30.35	30.36	30.59	30.20	30.56	30.15
H 27a-c	29.95	30.01	29.94	29.92	29.92	29.91	29.95	29.94
H 28a-c	30.85	30.47	30.80	30.81	31.05	31.02	31.06	31.05
H 29a-c	30.30	30.58	30.53	30.53	30.59	30.59	30.66	30.38

Isotropic shielding constants								
Nuclei	Isomer 9	Isomer 10	Isomer 11	Isomer 12	Isomer 13	Isomer 14	Isomer 15	Isomer 16
C 7	7.81	7.82	8.25	8.02	7.27	7.15	7.41	7.91
C 8	147.55	145.39	148.13	146.36	144.93	145.54	147.77	144.07
C 9	136.77	137.79	136.44	138.08	138.03	134.87	137.60	137.73
C 10	-15.88	-20.94	-20.35	-24.31	-23.18	-21.09	-20.00	-21.44
C 11	111.92	115.14	117.30	116.46	114.12	114.87	112.22	111.82
C 12	146.30	151.55	143.81	150.46	143.60	140.05	142.15	146.89
C 13	142.03	138.76	142.22	140.92	144.50	138.52	153.07	149.54
C 14	161.83	152.81	156.63	156.23	157.81	159.92	155.91	152.52
C 15	34.15	31.73	32.38	33.10	32.41	31.98	33.23	31.30
C 16	67.94	67.99	68.36	67.39	68.49	68.63	68.69	68.72
C 17	2.85	3.21	3.49	3.07	3.80	3.36	3.54	3.81
C 18	147.67	144.96	148.03	144.85	148.19	150.34	147.42	144.74
C 19	146.48	152.39	149.85	152.92	148.61	146.85	150.06	152.14
C 20	-16.05	-13.85	-13.55	-12.53	-13.26	-14.61	-12.76	-16.21
C 21	140.47	137.00	138.20	135.51	129.55	128.44	130.81	129.63
C 22	144.67	146.77	143.49	147.80	146.19	145.46	143.45	148.35
C 23	61.94	57.91	64.66	59.98	62.44	57.63	67.04	61.70
C 24	46.66	49.01	46.86	48.27	46.11	49.38	47.17	46.74
C 25	170.52	155.17	169.15	154.67	169.09	156.80	167.65	152.82
C 27	165.71	165.89	165.73	165.92	165.70	165.51	165.94	165.89
C 28	167.21	159.68	166.19	162.81	170.47	170.86	167.28	161.64
C 29	165.83	163.17	168.50	162.96	168.65	165.86	167.14	167.63
H 8a	29.79	29.42	29.66	29.53	29.33	28.91	29.73	29.28
H 8b	28.95	29.04	29.10	29.05	29.40	29.59	29.11	29.12
H 11	28.04	27.82	27.54	27.48	27.35	27.64	27.65	27.45
H 13	30.38	29.83	30.12	29.76	29.50	30.14	29.11	29.78
H 14a	29.05	28.94	29.61	29.68	29.58	29.49	29.54	29.79
H 14b	29.89	29.24	28.96	29.02	29.28	29.08	29.25	28.73
H 16	25.92	25.88	25.87	25.83	25.82	25.92	25.93	25.91
H 18	28.77	29.47	29.57	29.61	29.56	29.31	29.53	29.52
H 19a	28.64	29.06	28.75	29.14	28.75	28.78	29.07	29.23
H 19b	29.71	29.48	29.71	29.46	29.65	29.62	29.31	29.50
H 21	28.33	28.64	29.06	28.97	29.75	29.49	29.30	29.24
H 23	24.59	24.67	24.97	24.72	25.17	25.42	25.83	25.14
H 25a-c	30.51	30.28	30.40	30.57	30.80	30.33	30.67	30.34
H 27a-c	29.97	29.93	29.92	29.91	29.92	29.94	30.03	29.99
H 28a-c	31.01	30.93	30.95	30.83	31.01	30.64	30.66	30.45
H 29a-c	30.55	30.57	30.75	30.51	30.70	30.45	30.70	30.47

Isotropic shielding constants								
Nuclei	Isomer 17	Isomer 18	Isomer 19	Isomer 20	Isomer 21	Isomer 22	Isomer 23	Isomer 24
C 7	6.71	7.18	7.36	7.63	7.85	8.14	7.60	7.64
C 8	144.65	147.94	145.38	144.74	146.25	147.84	145.56	147.45
C 9	134.78	138.51	134.51	139.22	138.14	136.11	137.56	136.37
C 10	-18.15	-21.23	-21.68	-23.79	-24.40	-19.72	-22.39	-16.55
C 11	113.01	113.22	121.71	118.59	115.41	115.14	118.91	115.00
C 12	142.88	146.35	138.05	145.32	145.45	138.53	146.76	142.58
C 13	140.98	149.87	140.60	142.66	136.21	138.85	140.61	145.98
C 14	159.25	154.80	155.35	157.03	156.84	157.95	160.11	160.90
C 15	34.03	31.39	30.97	31.67	32.99	32.83	34.03	33.82
C 16	68.04	68.69	68.94	68.90	68.63	69.03	67.94	68.12
C 17	2.89	2.72	4.28	3.09	3.51	3.65	3.48	3.59
C 18	142.67	147.84	144.84	148.06	146.78	147.74	146.99	147.63
C 19	149.39	153.87	148.71	147.47	147.65	147.12	147.30	147.09
C 20	-12.12	-14.30	-13.40	-15.11	-12.59	-12.78	-14.30	-13.80
C 21	127.85	132.54	126.50	130.20	129.82	135.05	132.02	137.27
C 22	145.66	141.33	145.51	147.03	147.96	143.60	146.59	143.76
C 23	56.52	65.62	56.77	63.72	60.67	64.63	59.36	63.77
C 24	49.51	46.73	49.93	45.17	47.89	46.93	48.27	47.03
C 25	155.44	166.66	157.03	167.02	154.42	169.80	154.53	170.11
C 27	165.88	166.20	165.69	165.53	165.86	165.83	165.81	165.73
C 28	162.07	154.38	162.96	162.91	174.32	177.78	172.89	175.44
C 29	165.59	166.72	165.67	168.43	163.11	168.98	163.24	166.64
H 8a	29.50	29.04	29.60	29.11	29.05	29.10	29.11	29.01
H 8b	29.12	29.74	28.95	29.48	29.51	29.64	29.38	29.76
H 11	28.02	27.71	27.46	27.11	27.57	27.77	28.14	28.13
H 13	30.05	29.79	30.08	30.43	29.60	29.89	29.12	29.13
H 14a	29.02	29.92	29.33	29.32	29.51	29.46	29.89	29.84
H 14b	29.72	29.16	29.20	29.35	29.17	29.21	29.38	29.68
H 16	25.85	25.98	25.84	25.90	25.90	25.88	25.87	25.86
H 18	28.70	29.23	29.59	29.21	29.38	29.51	29.44	29.51
H 19a	28.73	29.23	28.70	28.72	28.99	28.78	28.94	28.73
H 19b	29.85	29.46	29.89	29.61	29.57	29.83	29.59	29.81
H 21	29.75	29.34	29.59	29.45	29.13	29.22	28.81	28.75
H 23	25.11	25.99	25.24	25.45	25.07	24.74	24.89	24.69
H 25a-c	30.37	30.49	30.35	30.76	30.62	30.53	30.38	30.50
H 27a-c	29.93	30.08	29.91	29.94	29.93	29.94	29.94	29.95
H 28a-c	30.77	30.56	30.73	30.97	30.99	31.01	31.09	31.02
H 29a-c	30.27	30.68	30.53	30.67	30.49	30.77	30.58	30.55

Isotropic shielding constants								
Nuclei	Isomer 25	Isomer 26	Isomer 27	Isomer 28	Isomer 29	Isomer 30	Isomer 31	Isomer 32
C 7	5.74	8.86	6.88	10.17	8.20	8.01	6.66	9.28
C 8	147.00	145.14	147.84	147.40	146.66	146.99	147.54	146.02
C 9	132.81	136.15	133.16	135.60	135.00	137.87	133.08	136.97
C 10	-16.91	-15.82	-20.96	-19.92	-22.03	-21.03	-20.51	-20.02
C 11	111.14	111.55	118.67	118.23	115.58	114.64	112.67	112.55
C 12	145.67	146.52	144.24	144.71	146.67	143.19	141.07	142.10
C 13	140.45	141.23	141.76	141.66	143.08	143.26	152.65	151.68
C 14	162.07	161.84	155.30	156.06	157.23	157.61	155.87	155.73
C 15	33.75	34.43	33.20	32.92	33.20	32.46	33.00	32.96
C 16	67.92	67.82	67.86	68.08	68.17	68.41	69.33	69.20
C 17	3.21	3.00	3.18	3.38	4.82	3.86	3.36	3.29
C 18	147.76	147.95	146.68	147.39	148.17	148.48	147.92	147.79
C 19	146.50	146.36	152.42	151.11	152.03	148.49	149.57	149.19
C 20	-15.08	-15.50	-12.96	-13.04	-13.74	-13.99	-12.96	-12.23
C 21	142.65	140.81	140.69	136.98	134.49	129.55	133.68	130.98
C 22	145.67	145.40	144.29	144.11	147.15	145.46	144.60	144.57
C 23	57.93	63.15	56.80	60.24	58.59	61.62	61.15	62.22
C 24	46.56	47.97	47.26	47.60	46.58	47.79	46.63	47.73
C 25	161.58	168.66	163.96	169.67	164.29	167.38	161.65	166.86
C 27	165.78	165.71	165.86	165.81	165.73	165.66	165.97	165.88
C 28	165.90	167.66	163.63	164.79	169.77	170.63	165.08	166.27
C 29	167.25	170.93	169.20	171.51	169.17	167.62	168.24	170.73
H 8a	29.51	29.93	29.63	29.13	29.10	29.30	29.63	29.07
H 8b	28.97	28.31	28.74	29.91	29.26	29.38	28.75	29.88
H 11	28.00	28.01	27.31	27.38	27.73	27.65	27.27	27.37
H 13	30.30	30.34	29.91	30.02	29.95	29.80	29.35	29.62
H 14a	28.78	28.96	29.64	29.63	29.47	29.55	29.48	29.46
H 14b	29.82	29.85	29.04	28.98	29.32	29.19	28.79	29.01
H 16	25.93	25.92	25.81	25.84	25.79	25.86	25.92	25.92
H 18	28.89	28.81	29.69	29.66	29.45	29.43	29.49	29.51
H 19a	28.60	28.64	28.83	28.80	29.15	28.84	28.98	28.97
H 19b	29.77	29.76	29.72	29.75	29.04	29.50	29.46	29.50
H 21	28.37	28.08	28.90	28.70	29.33	29.47	29.13	29.00
H 23	24.89	25.21	24.61	24.78	24.91	25.90	25.03	25.84
H 25a-c	30.09	30.47	30.30	30.71	30.33	30.51	30.37	30.84
H 27a-c	29.96	29.96	29.91	29.91	29.93	29.93	30.00	30.00
H 28a-c	30.99	31.01	30.89	30.95	30.68	30.84	30.55	30.60
H 29a-c	30.40	30.68	30.59	30.57	30.55	30.55	30.55	30.61

Isotropic shielding constants

Nuclei	Isomer 44
C 7	7.83
C 8	145.73
C 9	138.61
C 10	-23.22
C 11	111.94
C 12	148.78
C 13	144.30
C 14	160.47
C 15	32.66
C 16	68.52
C 17	4.83
C 18	148.31
C 19	152.61
C 20	-12.23
C 21	134.16
C 22	147.27
C 23	59.75
C 24	48.01
C 25	153.74
C 27	165.65
C 28	173.57
C 29	162.54
H 8a	29.51
H 8b	29.02
H 11	27.51
H 13	29.34
H 14a	29.23
H 14b	29.56
H 16	25.81
H 18	29.10
H 19a	28.78
H 19b	29.49
H 21	28.99
H 23	24.69
H 25a-c	30.55
H 27a-c	29.94
H 28a-c	30.94
H 29a-c	30.44

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8	Isomer 9	Isomer 10	Isomer 11	Isomer 12	Isomer 13	Isomer 14	Isomer 15	Isomer 16	Isomer 17
$J_{13,14a}$	9.73	9.37	9.94	10.25	9.37	9.48	9.89	9.86	10.47	9.79	9.85	9.52	9.47	10.15	8.57	8.61	9.83
$J_{13,14b}$	2.78	4.35	2.30	3.21	4.22	4.03	3.16	2.93	3.71	3.24	3.58	3.23	3.52	3.26	4.42	2.55	2.51
$J_{13,18}$	11.60	12.99	11.11	10.97	11.33	11.34	11.50	11.50	11.42	11.70	11.89	11.76	11.60	10.83	12.00	12.11	11.45
$J_{18,19a}$	11.54	11.93	11.88	9.97	10.85	10.66	11.05	10.91	9.58	10.27	10.52	10.38	9.92	9.38	9.12	11.88	11.63
$J_{18,19b}$	4.27	3.97	4.08	6.27	4.78	4.97	4.73	4.95	5.98	4.06	4.10	3.83	5.31	7.15	6.68	4.87	4.09

	Isomer 18	Isomer 19	Isomer 20	Isomer 21	Isomer 22	Isomer 23	Isomer 24	Isomer 25	Isomer 26	Isomer 27	Isomer 28	Isomer 29	Isomer 30	Isomer 31	Isomer 32	Isomer 44
$J_{13,14a}$	9.68	9.81	10.19	9.15	9.28	9.54	9.89	10.65	10.54	9.66	9.74	9.46	9.79	8.50	8.63	3.72
$J_{13,14b}$	2.96	2.37	3.00	4.09	4.28	3.52	3.32	3.63	3.68	3.30	3.46	3.26	3.46	4.88	4.62	11.53
$J_{13,18}$	12.66	11.07	10.98	11.69	11.38	11.86	11.55	11.25	11.30	12.06	11.97	11.93	11.59	11.95	11.86	8.46
$J_{18,19a}$	12.00	11.99	10.11	9.77	10.99	10.07	11.16	9.61	9.54	11.03	10.79	6.20	8.96	9.98	9.80	11.53
$J_{18,19b}$	4.04	3.65	6.13	5.81	4.67	5.68	4.56	5.56	5.95	3.14	3.56	7.93	6.34	5.99	5.94	4.79

Table S59. Studied Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) and coupling constants of isomers calculated at the PCM/B3LYP/6-31G**//MM3 level of theory after elimination of conformations incompatible with experimental $^3J_{\text{HH}}$ of Zoarenone according to iJ/dJ-DP4.

Isotropic shielding constants								
Nuclei	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 7	9.79	9.46	10.07	9.72	12.18	9.08	10.60	8.19
C 8	143.50	144.24	144.48	144.74	145.18	146.03	143.90	145.48
C 9	136.36	136.48	136.52	136.94	135.03	133.98	135.38	134.42
C 10	-13.29	-17.28	-15.90	-18.57	-14.23	-15.31	-11.77	-13.51
C 11	111.64	115.91	119.29	118.42	114.01	114.62	113.35	113.37
C 12	140.01	148.22	136.16	145.05	138.22	137.11	141.36	140.87
C 13	138.88	139.75	137.69	140.33	134.60	134.29	142.50	141.89
C 14	156.57	157.34	152.52	154.57	154.92	154.69	157.41	157.30
C 15	39.56	39.43	34.86	36.24	37.12	37.24	38.73	38.41
C 16	68.11	68.27	69.63	69.16	69.07	69.06	68.29	68.42
C 17	5.37	4.51	6.75	5.57	6.33	6.19	6.23	6.14
C 18	141.44	147.78	144.72	148.18	145.57	145.18	145.74	145.46
C 19	146.47	144.00	145.19	144.44	145.91	146.06	145.70	145.95
C 20	-8.65	-11.69	-10.08	-11.01	-8.00	-8.25	-9.01	-9.13
C 21	127.16	132.24	125.24	130.80	131.00	134.78	134.33	137.08
C 22	143.73	148.08	144.02	149.78	145.25	145.22	144.84	145.16
C 23	61.32	67.07	61.89	68.24	65.72	65.28	67.47	65.08
C 24	55.64	52.85	55.51	52.39	53.40	52.95	53.69	52.89
C 25	163.96	163.65	164.13	161.14	165.67	161.61	164.78	159.91
C 27	163.08	162.93	163.07	162.91	162.83	162.94	162.96	163.05
C 28	160.63	155.47	162.81	159.31	172.19	171.89	170.54	169.99
C 29	161.58	165.89	160.86	165.76	168.50	165.86	168.23	165.21
H 8a	29.09	28.61	29.02	28.71	29.35	28.22	29.42	28.34
H 8b	28.57	28.54	28.64	28.55	28.50	29.16	27.27	29.11
H 11	27.56	27.63	26.90	26.92	27.05	26.90	27.73	27.74
H 13	29.45	29.63	29.46	29.72	29.27	29.21	28.37	28.39
H 14a	28.86	28.12	28.09	28.62	28.81	28.79	29.15	29.16
H 14b	29.05	29.11	28.79	28.81	28.47	28.58	29.15	29.03
H 16	25.54	25.58	25.58	25.56	25.56	25.56	25.54	25.53
H 18	27.87	27.58	28.93	28.80	28.95	28.91	28.97	28.94
H 19a	28.29	28.12	28.18	28.18	28.40	28.41	28.35	28.36
H 19b	29.29	28.97	29.37	28.99	29.29	29.23	29.25	29.22
H 21	29.24	28.53	29.12	28.46	28.31	28.43	27.85	28.07
H 23	25.87	24.99	25.86	25.19	24.96	25.12	25.01	25.12
H 25a-c	29.51	29.49	29.63	29.82	29.95	29.67	29.94	29.66
H 27a-c	29.44	29.45	29.43	29.41	29.42	29.41	29.44	29.44
H 28a-c	30.11	30.11	30.02	30.06	30.32	30.30	30.37	30.37
H 29a-c	29.68	29.93	29.95	29.87	30.01	29.96	30.08	29.73

Isotropic shielding constants								
Nuclei	Isomer 9	Isomer 10	Isomer 11	Isomer 12	Isomer 13	Isomer 14	Isomer 15	Isomer 16
C 7	10.43	9.68	10.81	9.80	9.20	9.50	10.05	9.06
C 8	145.35	143.05	146.24	143.80	143.51	144.41	145.88	143.33
C 9	136.21	137.97	136.33	138.23	137.32	136.50	136.59	138.20
C 10	-11.92	-16.99	-15.16	-19.70	-17.99	-16.03	-15.42	-17.44
C 11	110.51	115.12	115.96	114.65	112.40	113.49	110.89	110.15
C 12	143.86	150.65	141.81	149.44	141.36	137.43	140.44	144.40
C 13	138.71	133.56	138.26	136.08	141.74	135.48	149.87	146.58
C 14	158.61	149.42	153.21	153.69	154.33	156.89	152.31	152.07
C 15	38.54	36.99	37.27	38.54	36.80	36.58	36.94	36.61
C 16	68.31	68.28	68.47	67.60	68.96	68.63	69.01	69.31
C 17	5.52	5.90	5.98	5.85	6.56	5.63	6.04	6.59
C 18	145.87	142.35	145.30	142.02	146.21	149.17	144.79	145.48
C 19	143.96	149.78	148.15	150.20	147.24	144.26	147.70	149.97
C 20	-11.82	-10.16	-9.87	-8.96	-9.20	-10.82	-8.72	-10.84
C 21	139.90	134.73	137.11	133.21	128.74	126.15	129.52	126.69
C 22	145.30	148.10	144.33	149.00	147.31	145.50	144.59	148.24
C 23	66.75	64.23	69.62	66.54	66.96	64.59	71.67	68.02
C 24	53.49	55.01	53.38	54.19	52.49	55.30	53.80	52.47
C 25	167.24	151.48	165.77	151.25	165.66	154.85	164.86	148.90
C 27	162.97	162.98	162.97	163.03	162.93	162.83	163.07	163.08
C 28	163.63	155.06	162.36	156.70	166.60	165.64	164.02	161.22
C 29	163.46	158.75	165.22	159.23	165.28	162.30	164.15	160.29
H 8a	29.19	28.85	29.06	28.94	28.74	28.33	29.13	28.81
H 8b	28.53	28.56	28.65	28.57	28.91	29.17	28.67	28.62
H 11	27.64	27.52	26.89	26.94	26.66	27.07	27.03	26.84
H 13	29.69	29.21	29.41	29.08	28.88	29.54	28.34	28.84
H 14a	28.44	28.28	29.03	29.13	28.91	28.83	29.00	29.03
H 14b	29.31	28.66	28.26	28.44	28.58	28.45	28.17	27.89
H 16	25.59	25.58	25.54	25.52	25.49	25.55	25.60	25.60
H 18	28.16	28.82	28.96	28.94	28.92	28.68	28.84	28.86
H 19a	28.14	28.56	28.30	28.65	28.34	28.32	28.57	28.58
H 19b	29.19	28.93	29.15	28.91	28.97	28.98	28.63	28.77
H 21	27.55	27.97	28.32	28.27	29.06	28.80	28.65	28.65
H 23	24.53	24.59	24.96	24.72	25.06	25.67	25.58	25.26
H 25a-c	29.90	29.61	29.75	30.00	30.16	29.92	30.10	29.84
H 27a-c	29.46	29.44	29.42	29.42	29.42	29.43	29.53	29.53
H 28a-c	30.34	30.22	30.25	30.10	30.29	29.90	30.03	29.87
H 29a-c	29.94	29.96	30.14	29.91	30.12	29.88	30.11	29.83

Isotropic shielding constants								
Nuclei	Isomer 17	Isomer 18	Isomer 19	Isomer 20	Isomer 21	Isomer 22	Isomer 23	Isomer 24
C 7	8.98	9.40	9.74	10.12	9.70	10.65	9.48	10.25
C 8	143.45	145.86	144.25	142.99	143.58	145.99	142.98	145.04
C 9	135.60	137.31	135.42	138.13	138.53	136.24	138.11	136.39
C 10	-14.02	-16.62	-16.44	-18.88	-19.65	-14.53	-18.20	-12.75
C 11	111.85	111.72	120.13	117.01	113.53	113.32	118.21	113.66
C 12	139.97	144.01	135.86	143.99	144.47	136.66	146.15	140.53
C 13	138.74	145.70	138.08	140.23	132.05	135.08	137.23	143.57
C 14	156.89	151.76	152.69	153.68	153.45	154.42	156.98	157.76
C 15	39.40	36.55	35.36	35.65	37.18	36.79	38.75	38.62
C 16	68.25	68.81	69.43	69.27	69.10	69.33	68.35	68.41
C 17	5.76	5.59	7.00	5.59	6.07	6.19	5.99	6.06
C 18	142.20	145.83	145.44	147.94	144.17	145.14	144.69	145.55
C 19	146.99	151.08	146.21	144.53	145.91	145.47	145.70	145.50
C 20	-8.27	-11.01	-9.09	-10.73	-8.32	-9.04	-9.69	-9.77
C 21	126.43	130.83	124.61	128.92	126.34	133.77	129.02	136.34
C 22	145.36	141.49	145.28	147.96	149.05	144.71	147.79	144.14
C 23	62.57	70.28	62.31	67.93	66.86	69.57	65.55	68.84
C 24	56.37	52.99	56.62	51.75	54.00	53.35	54.45	53.73
C 25	152.24	163.75	153.48	165.04	151.06	166.24	151.38	166.62
C 27	163.01	163.33	162.97	162.91	163.00	162.97	163.02	162.95
C 28	158.48	149.93	159.88	159.46	169.29	173.82	168.15	171.76
C 29	162.80	163.40	161.50	165.42	159.41	165.82	159.02	164.16
H 8a	29.13	28.64	29.19	28.60	28.56	28.64	28.61	28.60
H 8b	28.50	29.10	28.39	28.81	28.92	29.06	28.80	29.15
H 11	27.62	27.10	26.81	26.29	27.02	27.13	27.78	27.74
H 13	29.41	29.10	29.44	29.76	29.07	29.30	28.55	28.41
H 14a	28.58	29.17	28.43	28.43	28.87	28.84	29.22	29.17
H 14b	29.04	28.27	28.66	28.85	28.40	28.36	28.90	29.22
H 16	25.53	25.66	25.53	25.57	25.59	25.56	25.55	25.54
H 18	27.93	28.39	29.06	28.64	28.77	28.90	28.84	28.93
H 19a	28.16	28.69	28.09	28.17	28.62	28.39	28.57	28.34
H 19b	29.40	28.81	29.46	28.95	28.96	29.27	29.00	29.25
H 21	29.12	28.65	29.00	28.75	28.46	28.54	28.15	28.07
H 23	25.18	25.89	25.31	25.27	25.08	24.71	24.86	24.71
H 25a-c	29.83	29.87	29.84	30.16	30.06	29.89	29.76	29.86
H 27a-c	29.42	29.59	29.40	29.42	29.43	29.43	29.44	29.45
H 28a-c	30.10	29.89	30.00	30.28	30.25	30.31	30.37	30.35
H 29a-c	29.66	30.10	29.98	30.10	29.89	30.17	29.97	29.92

Isotropic shielding constants								
Nuclei	Isomer 25	Isomer 26	Isomer 27	Isomer 28	Isomer 29	Isomer 30	Isomer 31	Isomer 32
C 7	7.47	10.54	8.95	12.14	10.16	9.80	8.76	11.15
C 8	145.70	143.44	146.39	144.78	144.89	144.96	146.17	143.20
C 9	134.19	135.18	134.50	135.24	136.13	137.24	134.61	136.38
C 10	-12.88	-11.51	-15.71	-14.80	-17.33	-15.48	-15.65	-15.62
C 11	109.80	109.93	116.91	116.53	114.65	112.33	111.04	110.76
C 12	143.05	144.02	142.10	142.57	144.17	139.17	138.82	140.91
C 13	137.34	138.07	137.14	137.24	140.41	138.05	148.07	147.75
C 14	158.85	158.54	152.28	152.91	153.67	155.18	152.18	152.34
C 15	38.29	38.80	38.51	37.91	37.78	35.95	36.65	36.60
C 16	68.33	68.20	68.03	68.25	68.62	68.84	69.47	69.47
C 17	5.84	5.66	5.70	5.92	7.82	6.17	5.88	5.90
C 18	145.94	146.08	144.13	144.88	146.27	147.70	145.34	145.64
C 19	143.90	143.87	150.21	148.96	152.29	144.35	146.99	147.04
C 20	-10.90	-11.01	-9.38	-9.30	-10.13	-11.08	-9.12	-8.29
C 21	141.11	139.35	139.25	134.76	133.31	126.73	131.68	128.35
C 22	145.91	145.66	144.76	144.62	148.01	144.72	145.56	145.41
C 23	65.04	68.61	63.74	64.97	64.64	64.62	68.51	66.06
C 24	52.46	54.02	53.24	53.77	52.66	54.44	52.69	53.59
C 25	158.64	164.52	161.28	165.61	163.50	164.47	159.15	162.98
C 27	162.96	163.00	163.01	162.97	162.92	162.87	162.99	162.97
C 28	161.87	163.13	159.05	160.15	165.27	167.20	162.01	162.93
C 29	163.82	168.13	165.52	168.61	166.21	162.16	164.38	167.15
H 8a	29.09	29.46	29.17	28.46	28.59	28.72	29.19	28.43
H 8b	28.36	27.34	28.18	29.33	28.68	29.01	28.18	29.29
H 11	27.62	27.61	26.70	26.78	27.12	27.03	26.71	26.76
H 13	29.64	29.67	29.24	29.35	29.50	29.38	28.63	28.84
H 14a	28.08	28.32	29.06	29.05	28.80	28.97	28.95	28.94
H 14b	29.25	29.27	28.43	28.32	28.77	28.33	27.61	27.90
H 16	25.60	25.59	25.49	25.52	25.46	25.56	25.61	25.61
H 18	28.28	28.22	29.04	29.03	28.78	28.79	28.83	28.86
H 19a	28.11	28.13	28.41	28.35	28.91	28.28	28.47	28.46
H 19b	29.22	29.22	29.12	29.17	28.05	29.05	28.86	28.87
H 21	27.54	27.33	28.21	28.05	28.59	28.92	28.49	28.47
H 23	25.10	25.19	24.78	24.69	24.94	25.95	25.15	25.89
H 25a-c	29.56	29.83	29.79	30.07	29.82	29.83	29.86	30.18
H 27a-c	29.45	29.45	29.41	29.41	29.44	29.44	29.51	29.49
H 28a-c	30.34	30.37	30.19	30.24	29.88	30.05	29.93	29.97
H 29a-c	29.74	30.10	29.95	30.00	29.92	29.86	29.92	30.02

Isotropic shielding constants			
Nuclei	Isomer 34	Isomer 44	Isomer 50
C 7	9.30	9.63	9.50
C 8	146.48	143.35	145.66
C 9	135.38	138.74	137.57
C 10	-15.44	-18.72	-15.50
C 11	112.49	110.08	111.78
C 12	141.35	147.67	142.15
C 13	151.09	140.85	153.84
C 14	155.12	156.97	155.33
C 15	36.58	36.86	37.26
C 16	68.10	68.23	68.19
C 17	7.55	7.40	7.40
C 18	148.33	146.12	148.59
C 19	151.89	149.70	151.65
C 20	-11.01	-8.42	-11.04
C 21	132.58	131.53	130.16
C 22	143.14	148.64	142.00
C 23	68.25	66.32	74.03
C 24	52.73	53.99	53.41
C 25	160.89	150.41	163.82
C 27	163.05	163.08	163.23
C 28	154.82	168.71	157.14
C 29	164.79	158.56	163.80
H 8a	28.18	28.93	28.72
H 8b	29.23	28.54	29.12
H 11	26.90	26.94	27.11
H 13	28.86	28.70	29.16
H 14a	28.27	28.53	28.18
H 14b	28.97	28.94	29.06
H 16	25.49	25.46	25.52
H 18	28.57	28.41	28.31
H 19a	28.39	28.28	28.26
H 19b	28.90	28.95	28.92
H 21	28.39	28.23	28.68
H 23	24.26	24.71	25.94
H 25a-c	30.04	29.98	29.91
H 27a-c	29.44	29.42	29.50
H 28a-c	29.81	30.17	29.92
H 29a-c	29.91	29.83	30.10

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8	Isomer 9	Isomer 10	Isomer 11	Isomer 12	Isomer 13	Isomer 14	Isomer 15	Isomer 16	Isomer 17
$J_{13,14a}$	10.97	11.29	11.27	11.43	10.57	10.62	10.89	10.84	11.56	11.06	11.00	10.80	10.56	11.10	9.97	10.14	10.97
$J_{13,14b}$	3.30	4.12	2.81	3.35	4.01	3.92	3.42	3.35	4.03	3.38	3.66	3.34	3.65	3.78	4.18	3.70	3.25
$J_{13,18}$	13.00	12.89	12.45	12.44	12.62	12.63	13.06	13.05	13.02	12.72	13.26	12.67	13.08	12.37	13.27	13.21	12.92
$J_{18,19a}$	12.75	10.22	13.23	10.51	12.10	11.89	12.27	12.12	10.31	11.56	11.80	11.73	10.24	9.47	10.35	10.94	13.01
$J_{18,19b}$	4.33	7.92	4.16	7.38	5.13	5.31	4.96	5.15	6.41	4.09	4.08	3.87	6.23	8.63	7.13	6.35	4.03

	Isomer 18	Isomer 19	Isomer 20	Isomer 21	Isomer 22	Isomer 23	Isomer 24	Isomer 25	Isomer 26	Isomer 27	Isomer 28	Isomer 29	Isomer 30	Isomer 31	Isomer 32	Isomer 34	Isomer 44	Isomer 50
$J_{13,14a}$	11.03	11.15	11.52	10.47	10.52	10.75	10.93	11.64	11.58	10.85	10.93	10.47	11.09	10.03	10.11	3.70	4.05	3.85
$J_{13,14b}$	3.20	2.75	3.23	4.00	4.05	3.55	3.45	4.03	4.01	3.47	3.61	3.45	3.65	4.33	4.23	12.43	12.72	12.75
$J_{13,18}$	13.76	12.36	12.36	12.81	12.65	13.10	13.10	12.98	12.99	13.30	13.28	13.52	12.71	13.16	13.13	8.37	8.69	9.04
$J_{18,19a}$	13.89	13.39	10.55	10.75	12.27	11.06	12.41	10.38	10.29	12.40	12.07	4.02	9.97	11.47	11.21	15.78	13.03	14.94
$J_{18,19b}$	3.91	3.69	7.31	6.29	4.98	6.10	4.81	5.91	6.29	3.27	3.71	10.67	7.25	6.12	6.17	3.91	5.05	4.60

Table S60. Studied Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) and coupling constants of isomers calculated at the PCM/B3LYP/6-31G**//MMFF level of theory after elimination of conformations incompatible with experimental $^3J_{\text{HH}}$ of Zoarenone according to iJ/dJ-DP4.

Isotropic shielding constants								
Nuclei	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
C 7	3.23	2.27	3.35	2.92	5.67	2.25	4.42	1.38
C 8	146.72	148.43	147.41	146.99	147.28	148.46	145.77	147.90
C 9	134.57	133.74	135.06	135.20	133.68	131.64	133.84	131.80
C 10	-22.11	-24.48	-24.59	-26.78	-23.42	-23.04	-21.38	-21.22
C 11	111.55	112.23	118.89	117.67	113.41	113.88	113.01	112.27
C 12	137.43	141.98	132.88	144.20	136.67	135.17	139.44	138.51
C 13	139.76	144.53	138.01	140.55	136.09	135.79	143.53	142.72
C 14	158.95	155.86	154.96	157.00	157.28	157.13	159.85	159.45
C 15	40.15	38.23	35.54	37.38	37.98	38.15	39.51	39.04
C 16	66.81	67.63	68.37	68.30	67.94	67.83	67.04	67.18
C 17	-0.91	-0.59	0.44	-1.44	-0.03	-0.23	-0.11	-0.30
C 18	143.01	148.30	143.97	149.70	147.45	147.02	147.41	146.99
C 19	148.55	152.31	147.45	147.70	147.50	147.92	147.36	147.84
C 20	-16.22	-18.64	-18.18	-18.50	-14.81	-14.68	-16.14	-15.87
C 21	125.73	132.40	124.08	131.48	130.70	134.18	133.41	136.07
C 22	142.08	141.39	142.43	147.27	143.41	143.63	143.41	143.89
C 23	64.77	70.15	65.69	71.46	68.33	68.31	69.53	68.05
C 24	51.73	48.80	51.32	48.45	49.90	49.15	50.30	49.03
C 25	166.37	163.22	167.01	165.19	169.39	164.91	168.40	163.42
C 27	166.52	166.60	166.47	166.17	166.23	166.36	166.35	166.44
C 28	164.56	152.25	165.91	163.03	176.29	175.75	174.27	173.22
C 29	164.24	167.04	163.77	168.33	170.56	168.58	170.10	167.75
H 8a	29.51	28.60	29.41	29.09	29.63	28.61	29.63	28.74
H 8b	28.52	29.32	28.61	28.76	28.99	29.40	27.91	29.32
H 11	27.71	27.10	27.20	27.25	27.32	27.17	27.87	27.88
H 13	29.71	29.45	29.72	30.04	29.52	29.44	28.69	28.72
H 14a	29.25	29.43	28.72	29.07	29.25	29.23	29.59	29.60
H 14b	29.52	28.30	29.24	29.23	28.95	29.09	29.52	29.37
H 16	25.65	25.71	25.68	25.68	25.67	25.66	25.65	25.63
H 18	28.41	28.97	29.27	29.19	29.30	29.24	29.32	29.27
H 19a	28.61	28.75	28.55	28.61	28.69	28.73	28.64	28.69
H 19b	29.66	29.36	29.70	29.13	29.64	29.55	29.61	29.54
H 21	29.43	28.70	29.21	28.72	28.69	28.79	28.26	28.47
H 23	26.05	24.73	26.07	25.50	25.23	25.24	25.29	25.26
H 25a-c	30.01	30.41	30.21	30.39	30.37	30.13	30.36	30.09
H 27a-c	29.92	29.98	29.91	29.88	29.90	29.88	29.92	29.92
H 28a-c	30.66	30.31	30.57	30.55	30.81	30.78	30.87	30.85
H 29a-c	30.14	30.46	30.38	30.39	30.43	30.50	30.49	30.25

Isotropic shielding constants								
Nuclei	Isomer 9	Isomer 10	Isomer 11	Isomer 12	Isomer 13	Isomer 14	Isomer 15	Isomer 16
C 7	3.94	2.46	4.21	2.70	4.01	2.54	3.74	2.86
C 8	148.26	144.74	148.96	145.38	145.89	146.53	148.53	144.99
C 9	134.44	136.29	134.77	136.60	135.78	134.78	135.10	136.39
C 10	-20.62	-25.38	-23.71	-28.44	-27.35	-23.49	-23.74	-24.73
C 11	110.07	114.16	115.24	113.91	111.50	113.23	110.87	110.49
C 12	141.81	147.70	139.40	147.37	140.66	135.48	138.92	142.78
C 13	139.87	134.24	138.85	136.37	142.45	137.51	150.82	146.93
C 14	160.90	152.15	156.43	155.85	156.83	158.99	154.50	154.28
C 15	39.44	36.90	37.31	38.46	37.67	38.08	37.50	37.22
C 16	67.25	67.02	67.65	66.39	67.73	67.61	67.89	67.96
C 17	-1.16	0.06	-0.19	0.09	0.14	-1.23	-0.26	0.06
C 18	147.60	144.55	148.11	144.42	148.51	150.37	147.34	147.27
C 19	146.01	151.55	148.63	151.93	149.11	147.57	150.47	151.93
C 20	-17.85	-16.31	-16.48	-14.88	-16.77	-17.10	-16.48	-18.19
C 21	138.46	133.49	135.42	132.33	129.09	125.70	129.63	127.13
C 22	143.52	145.65	142.56	146.53	145.54	143.76	141.76	145.88
C 23	70.13	66.97	72.13	69.50	70.18	67.85	74.82	70.74
C 24	49.72	50.52	49.59	49.82	49.34	50.80	49.68	49.05
C 25	169.11	154.00	168.03	154.13	167.58	157.96	166.63	154.08
C 27	166.35	166.50	166.23	166.53	166.25	166.17	166.51	166.51
C 28	167.70	159.37	166.58	161.08	169.84	168.92	166.53	161.83
C 29	166.07	162.94	168.16	162.88	168.20	164.98	167.38	165.75
H 8a	29.62	29.16	29.50	29.29	29.18	28.67	29.55	29.10
H 8b	28.46	28.79	28.63	28.77	28.96	29.39	28.69	28.87
H 11	27.79	27.66	27.18	27.30	27.14	27.34	27.26	27.28
H 13	29.96	29.50	29.82	29.38	29.26	29.77	28.98	29.22
H 14a	28.89	28.62	29.38	29.49	29.33	29.30	29.39	29.47
H 14b	29.70	29.18	28.75	28.81	29.02	29.01	28.72	28.56
H 16	25.70	25.70	25.68	25.64	25.60	25.66	25.72	25.70
H 18	28.59	29.16	29.24	29.26	29.32	28.99	29.25	29.25
H 19a	28.57	28.88	28.59	28.97	28.54	28.90	28.84	28.89
H 19b	29.38	29.32	29.46	29.31	29.42	28.93	29.07	29.25
H 21	28.01	28.33	28.70	28.65	29.28	29.09	28.91	28.95
H 23	24.66	24.98	24.93	25.08	25.35	25.92	25.97	25.53
H 25a-c	30.37	30.11	30.30	30.49	30.61	30.39	30.51	30.32
H 27a-c	29.94	29.91	29.89	29.90	29.90	29.91	30.00	29.98
H 28a-c	30.86	30.71	30.78	30.57	30.75	30.38	30.48	30.30
H 29a-c	30.38	30.44	30.60	30.37	30.55	30.36	30.56	30.35

Isotropic shielding constants								
Nuclei	Isomer 17	Isomer 18	Isomer 19	Isomer 20	Isomer 21	Isomer 22	Isomer 23	Isomer 24
C 7	1.94	3.54	2.69	4.12	2.59	4.00	2.34	3.68
C 8	145.69	148.53	146.31	145.39	145.36	148.75	144.66	148.00
C 9	132.95	135.86	133.22	136.69	136.70	134.79	136.38	134.69
C 10	-22.10	-24.85	-24.29	-27.75	-28.46	-23.01	-26.57	-20.94
C 11	111.21	111.75	118.97	116.48	112.88	113.00	117.12	113.10
C 12	137.53	142.63	133.14	142.18	142.32	134.87	143.36	138.58
C 13	139.41	146.68	137.97	140.42	133.01	136.43	137.88	144.21
C 14	159.40	154.43	155.55	156.16	155.84	156.93	159.19	160.13
C 15	40.21	36.24	36.41	36.77	38.05	37.68	39.41	39.36
C 16	66.90	67.64	68.10	68.32	67.85	68.20	67.07	67.15
C 17	-0.59	-0.29	0.68	-1.22	-0.30	-0.28	-0.33	-0.35
C 18	144.24	147.66	145.75	148.71	146.02	147.03	146.42	147.31
C 19	149.05	153.48	148.43	147.43	147.59	147.28	147.27	147.35
C 20	-15.49	-18.44	-16.24	-18.65	-13.93	-15.39	-15.74	-16.51
C 21	124.69	130.26	123.04	128.92	126.79	132.63	128.70	134.54
C 22	143.60	139.30	143.45	145.62	146.89	142.53	145.61	142.27
C 23	64.98	73.75	65.37	71.51	69.87	72.39	68.24	71.78
C 24	52.16	49.45	52.01	48.18	49.63	49.49	50.06	49.83
C 25	156.07	165.33	157.22	166.35	154.00	168.19	153.98	168.54
C 27	166.40	166.84	166.28	166.25	166.45	166.39	166.43	166.34
C 28	162.16	152.18	162.82	162.48	173.83	177.67	172.50	175.32
C 29	165.28	166.85	164.37	168.00	163.23	168.67	163.62	166.82
H 8a	29.34	28.62	29.41	28.63	28.77	28.65	28.85	28.57
H 8b	28.86	29.54	28.74	29.27	29.27	29.49	29.11	29.61
H 11	27.76	27.28	27.11	26.94	27.38	27.38	27.92	27.87
H 13	29.66	29.44	29.69	30.05	29.32	29.53	28.79	28.74
H 14a	28.99	29.77	28.98	28.93	29.30	29.27	29.66	29.62
H 14b	29.50	28.62	29.13	29.25	28.93	28.91	29.26	29.58
H 16	25.63	25.77	25.64	25.70	25.69	25.67	25.66	25.64
H 18	28.49	29.00	29.44	29.05	29.11	29.24	29.18	29.27
H 19a	28.43	28.91	28.40	28.59	28.98	28.68	28.92	28.63
H 19b	29.78	29.33	29.83	29.17	29.28	29.61	29.33	29.60
H 21	29.40	28.89	29.24	28.97	28.74	28.85	28.44	28.43
H 23	25.43	26.12	25.59	25.64	25.42	24.81	25.24	24.76
H 25a-c	30.28	30.30	30.30	30.58	30.55	30.38	30.24	30.37
H 27a-c	29.91	30.06	29.87	29.90	29.90	29.91	29.91	29.93
H 28a-c	30.59	30.35	30.47	30.71	30.74	30.81	30.88	30.85
H 29a-c	30.18	30.55	30.45	30.50	30.37	30.64	30.45	30.39

Isotropic shielding constants								
Nuclei	Isomer 25	Isomer 26	Isomer 27	Isomer 28	Isomer 29	Isomer 30	Isomer 31	Isomer 32
C 7	0.72	4.61	2.19	5.74	3.48	3.20	2.20	5.15
C 8	147.93	145.13	148.67	146.92	147.30	147.75	148.37	145.77
C 9	131.20	133.56	132.08	133.77	135.09	135.84	132.44	134.77
C 10	-20.74	-21.73	-23.23	-24.01	-25.20	-23.87	-23.04	-24.16
C 11	108.75	109.86	116.12	115.73	114.16	112.55	110.62	111.05
C 12	140.52	142.12	140.14	140.99	142.98	136.80	136.99	138.99
C 13	138.66	139.66	137.96	138.02	140.99	139.34	148.92	149.08
C 14	161.02	160.81	155.24	156.32	156.04	157.62	154.32	154.22
C 15	39.04	39.79	38.50	37.84	38.72	37.10	37.24	37.31
C 16	67.27	67.06	66.82	67.37	67.25	67.87	68.37	68.35
C 17	-0.77	-1.07	-0.15	-0.09	1.76	-0.72	-0.48	-0.57
C 18	147.49	147.73	146.54	147.85	148.43	148.94	147.64	147.70
C 19	145.91	145.78	151.99	149.91	154.17	146.55	149.94	149.96
C 20	-17.01	-17.48	-16.33	-16.02	-16.69	-18.26	-16.74	-15.99
C 21	140.40	138.49	137.38	133.66	131.91	126.61	131.57	128.85
C 22	144.45	144.25	142.84	142.78	145.75	142.84	143.12	142.57
C 23	67.99	70.22	66.62	67.70	69.27	67.09	71.36	68.40
C 24	48.62	50.63	49.40	50.21	48.69	50.71	48.95	50.18
C 25	162.37	168.32	164.61	169.32	168.28	167.47	163.61	166.62
C 27	166.33	166.36	166.44	166.31	166.35	166.23	166.48	166.41
C 28	165.31	167.32	162.40	164.46	169.06	170.84	164.32	165.86
C 29	166.46	170.07	168.28	170.50	168.67	164.96	167.67	169.54
H 8a	29.30	29.62	29.40	28.96	28.81	28.76	29.43	28.85
H 8b	28.76	27.99	28.56	29.60	29.05	29.42	28.55	29.58
H 11	27.78	27.78	27.01	27.11	27.43	27.29	26.99	27.09
H 13	29.91	29.95	29.57	29.75	29.72	29.62	29.07	29.34
H 14a	28.55	28.84	29.43	29.42	29.22	29.42	29.33	29.32
H 14b	29.65	29.68	28.84	28.68	29.17	28.87	28.20	28.52
H 16	25.71	25.70	25.61	25.66	25.56	25.68	25.70	25.71
H 18	28.68	28.60	29.38	29.34	29.15	29.04	29.21	29.23
H 19a	28.52	28.57	28.63	28.58	29.29	28.76	28.76	28.80
H 19b	29.43	29.38	29.54	29.56	28.38	29.15	29.29	29.22
H 21	28.03	27.81	28.60	28.53	28.94	29.12	28.75	28.76
H 23	25.24	25.41	24.83	25.02	25.13	26.11	25.46	25.96
H 25a-c	30.01	30.25	30.24	30.44	30.36	30.35	30.44	30.70
H 27a-c	29.93	29.93	29.89	29.90	29.91	29.92	29.98	29.96
H 28a-c	30.83	30.85	30.66	30.74	30.34	30.55	30.37	30.45
H 29a-c	30.25	30.51	30.48	30.41	30.43	30.30	30.43	30.45

Isotropic shielding constants		
Nuclei	Isomer 44	Isomer 50
C 7	2.50	3.65
C 8	144.71	148.30
C 9	137.14	136.30
C 10	-27.43	-23.87
C 11	109.88	112.01
C 12	144.69	140.23
C 13	141.10	154.55
C 14	160.04	158.53
C 15	37.62	37.69
C 16	67.96	67.82
C 17	1.65	1.44
C 18	148.65	150.92
C 19	150.68	153.56
C 20	-13.85	-18.40
C 21	131.15	129.59
C 22	146.18	139.54
C 23	69.38	76.55
C 24	49.60	49.43
C 25	153.34	165.17
C 27	166.10	166.23
C 28	173.80	159.64
C 29	162.62	167.32
H 8a	29.27	28.73
H 8b	28.72	29.55
H 11	27.31	27.35
H 13	28.98	29.39
H 14a	29.02	28.79
H 14b	29.35	29.47
H 16	25.62	25.69
H 18	28.73	28.93
H 19a	28.58	28.55
H 19b	29.33	29.43
H 21	28.62	28.87
H 23	25.08	26.14
H 25a-c	30.47	30.31
H 27a-c	29.91	29.98
H 28a-c	30.69	30.36
H 29a-c	30.28	30.54

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8	Isomer 9	Isomer 10	Isomer 11	Isomer 12	Isomer 13	Isomer 14	Isomer 15	Isomer 16	Isomer 17
$J_{13,14a}$	9.98	9.68	10.31	10.31	9.56	9.66	10.05	9.99	10.67	10.28	10.18	9.83	9.57	10.09	8.89	9.10	9.97
$J_{13,14b}$	3.49	4.34	2.88	3.42	4.37	4.20	3.69	3.54	4.18	3.39	4.08	3.50	3.95	3.91	4.32	3.44	3.57
$J_{13,18}$	12.27	13.43	11.74	12.19	12.06	12.07	12.24	12.23	12.43	11.97	12.42	11.94	12.41	12.46	12.60	12.63	12.20
$J_{18,19a}$	12.69	12.45	12.98	9.72	11.73	11.35	11.97	11.68	9.52	10.80	10.63	10.98	10.43	7.47	9.71	11.08	12.91
$J_{18,19b}$	4.25	4.61	3.89	7.84	4.99	5.33	4.85	5.19	6.71	4.14	4.86	3.83	5.79	10.33	7.13	6.14	3.89

	Isomer 18	Isomer 19	Isomer 20	Isomer 21	Isomer 22	Isomer 23	Isomer 24	Isomer 25	Isomer 26	Isomer 27	Isomer 28	Isomer 29	Isomer 30	Isomer 31	Isomer 32	Isomer 44	Isomer 50
$J_{13,14a}$	9.93	10.18	10.41	9.55	9.53	9.84	10.05	10.80	10.68	9.86	10.03	9.49	10.17	8.73	8.85	4.81	4.29
$J_{13,14b}$	3.34	2.95	3.33	4.23	4.37	3.81	3.71	4.16	4.14	3.65	4.02	3.66	3.80	4.57	4.41	11.92	11.71
$J_{13,18}$	13.18	11.66	12.04	12.17	12.08	12.32	12.29	12.34	12.39	12.46	12.47	13.07	12.43	12.54	12.56	8.96	8.55
$J_{18,19a}$	13.28	13.20	10.08	10.00	11.80	10.46	12.01	9.58	9.42	11.81	11.08	3.83	8.88	11.08	10.52	12.24	14.99
$J_{18,19b}$	3.92	3.35	7.27	6.32	4.92	6.10	4.80	6.23	6.85	3.22	4.15	10.58	8.36	6.13	6.42	5.04	4.17

Table S61. Studied Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) and coupling constants of isomers calculated at the PCM/B3LYP/6-31G**//AMBER level of theory after elimination of conformations incompatible with experimental $^3J_{\text{HH}}$ of Zoaramine according to iJ/dJ-DP4.

Isotropic shielding constants				
Nuclei	Isomer 1	Isomer 2	Isomer 3	Isomer 4
C 1	145.9	146	143.1	142
C 2	128.2	128.1	128.8	129.5
C 3	145.4	145.4	144.3	143.3
C 4	161.5	161.6	163.8	163.5
C 5	154.8	154.7	154.4	152.1
C 6	31.2	31.24	25.35	26.88
C 7	76.07	75.18	79.6	75.11
C 8	155.1	155.1	155.5	155.2
C 9	139.5	139.5	138.8	139.7
C 10	-19.6	-17	-20.3	-17.2
C 11	115.6	114.7	116.2	114.7
C 12	138.4	142.3	139	142.4
C 13	138.6	146.1	137.7	146
C 14	158	161	158.2	161
C 15	32.75	33.77	33.2	33.84
C 16	68.97	68.18	68.81	68.19
C 17	3.36	3.23	3.5	3.23
C 18	147.8	147.5	147.9	147.6
C 19	147.7	147.6	147.7	147.7
C 20	-12.9	-14.1	-12.5	-14
C 21	133.2	135.7	133	135.8
C 22	147	147.6	145.6	147.3
C 23	143.5	142.7	145.5	142.2
C 24	2.89	2.41	1.92	0.72
C 25	164.1	163.1	167.8	163.2
C 27	165.7	165.8	165.7	165.8
C 28	178.3	175.9	177.3	176
C 29	168.2	166.2	168.5	166.1
C 30	166.2	166.1	166.1	165.1
H 1a	28.88	28.91	28.59	28.86
H 1b	28.79	28.81	28.88	28.96
H 2	28.04	28.07	28.27	28.38
H 3a	30.33	30.33	31.09	30.97
H 3b	30.23	30.23	29.91	29.94
H 4	30.01	30.01	29.89	29.75
H 5a	29.31	29.3	29.84	29.78
H 5b	29.56	29.52	29.54	29.44
H 8a	29.26	29.25	29.05	29.31
H 8b	29.31	29.37	29.5	29.36
H 11	27.76	28.2	27.58	28.23
H 13	29.88	29.15	29.83	29.16
H 14a	29.45	29.85	29.45	29.87
H 14b	29.23	29.7	29.33	29.72
H 16	25.9	25.88	25.9	25.88

H 18	29.52	29.53	29.52	29.52
H 19a	28.87	28.83	28.88	28.82
H 19b	29.87	29.84	29.84	29.84
H 21	29.39	28.88	29.39	28.89
H 23a	28.85	28.68	29.58	28.72
H 23b	29.39	29.52	28.9	29.56
H 25a-c	30.68	30.63	30.67	30.63
H 27a-c	29.94	29.97	29.94	29.97
H 28a-c	31.05	31.07	31.07	31.09
H 29a-c	30.82	30.61	30.77	30.6
H 30a-c	30.96	30.95	30.95	30.91

	Isomer 1	Isomer 2	Isomer 3	Isomer 4
$J_{3a,4}$	10.02	10.07	9.8	9.8
$J_{3b,4}$	4.29	4.24	2.65	1.63
$J_{3a,2}$	0.9	0.94	1.12	1.38
$J_{3b,2}$	5.21	5.3	4.8	4.08
$J_{4,5a}$	10.33	10.29	10.51	10.12
$J_{4,5b}$	1.3	1.49	1.17	1.15
$J_{13,14a}$	9.28	9.89	9.3	9.89
$J_{13,14b}$	4.27	3.33	4.28	3.32
$J_{13,18}$	11.4	11.57	11.39	11.56
$J_{18,19a}$	4.78	4.65	4.86	4.66
$J_{18,19b}$	10.85	11.05	10.73	11.04

Table S62. Studied Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) and coupling constants of isomers calculated at the PCM/B3LYP/6-31G**//MM3 level of theory after elimination of conformations incompatible with experimental $^3J_{\text{HH}}$ of Zoaramine according to iJ/dJ-DP4.

Isotropic shielding constants				
Nuclei	Isomer 1	Isomer 2	Isomer 3	Isomer 4
C 1	137.30	137.34	142.23	141.97
C 2	119.04	118.96	122.49	123.10
C 3	138.70	138.93	141.29	141.28
C 4	155.96	155.74	159.95	158.26
C 5	152.86	152.74	152.19	153.46
C 6	50.89	49.55	49.88	50.10
C 7	89.29	88.95	87.64	91.66
C 8	154.10	153.42	154.43	151.74
C 9	139.10	138.98	139.28	138.30
C 10	-15.19	-14.82	-14.79	-16.87
C 11	113.20	114.36	113.28	114.55
C 12	137.40	141.24	137.22	141.15
C 13	134.72	143.63	134.74	143.97
C 14	154.49	158.08	154.50	158.27
C 15	36.70	38.71	36.75	39.05
C 16	69.40	68.52	69.34	68.33
C 17	5.95	5.79	5.96	6.04
C 18	145.19	145.87	145.13	146.00
C 19	145.70	145.70	145.80	145.37
C 20	-9.08	-9.87	-9.10	-9.61
C 21	131.55	134.72	131.54	135.01
C 22	145.90	146.00	145.99	145.70
C 23	141.87	142.85	140.96	146.25
C 24	3.64	4.15	3.50	1.49
C 25	160.89	161.01	160.42	162.48
C 27	162.85	162.93	162.88	162.94
C 28	174.36	172.14	174.52	172.24
C 29	164.22	162.60	164.18	163.00
C 30	162.63	162.70	162.81	163.01
H 1a	28.02	28.03	27.91	27.95
H 1b	28.35	28.31	28.22	28.13
H 2	27.94	27.96	27.58	27.61
H 3a	30.12	30.14	30.41	30.47
H 3b	29.22	29.28	29.20	29.30
H 4	29.70	29.70	29.31	29.33
H 5a	29.46	29.51	29.47	29.66
H 5b	29.09	28.97	29.06	28.94
H 8a	28.77	28.75	28.81	28.57
H 8b	28.79	28.95	28.63	29.15
H 11	27.26	27.86	27.25	27.72
H 13	29.35	28.46	29.35	28.41
H 14a	28.86	29.20	28.86	29.22
H 14b	28.35	29.26	28.39	29.25
H 16	25.60	25.55	25.60	25.53

H 18	28.92	28.97	28.91	29.01
H 19a	28.44	28.39	28.44	28.35
H 19b	29.33	29.31	29.31	29.31
H 21	28.72	28.20	28.69	28.14
H 23a	28.42	28.63	28.18	29.27
H 23b	28.68	28.35	28.90	27.31
H 25a-c	30.04	30.02	30.01	30.09
H 27a-c	29.45	29.46	29.45	29.44
H 28a-c	30.34	30.44	30.32	30.47
H 29a-c	30.22	29.98	30.21	29.89
H 30a-c	30.27	30.28	30.30	30.32

	Isomer 1	Isomer 2	Isomer 3	Isomer 4
$J_{3a,4}$	11.24	11.23	11.24	11.18
$J_{3b,4}$	3.07	3.11	3.03	2.83
$J_{3a,2}$	10.44	10.45	1.50	1.54
$J_{3b,2}$	2.73	2.70	4.42	4.30
$J_{4,5a}$	11.00	10.94	11.14	10.75
$J_{4,5b}$	1.11	1.11	1.08	0.92
$J_{13,14a}$	10.49	10.95	10.51	10.98
$J_{13,14b}$	4.08	3.50	4.06	3.58
$J_{13,18}$	12.68	13.10	12.66	13.10
$J_{18,19a}$	5.01	4.77	5.06	4.62
$J_{18,19b}$	12.22	12.42	12.18	12.57

Table S63. Studied Boltzmann averaged GIAO isotropic magnetic shielding constants (σ) and coupling constants of isomers calculated at the PCM/B3LYP/6-31G**//MMFF level of theory after elimination of conformations incompatible with experimental $^3J_{\text{HH}}$ of Zoaramine according to iJ/dJ-DP4.

Isotropic shielding constants			
Nuclei	Isomer 1	Isomer 3	Isomer 4
C 1	139.32	142.60	142.46
C 2	118.86	126.21	126.48
C 3	143.85	143.86	143.65
C 4	157.89	162.34	162.15
C 5	157.31	154.39	154.53
C 6	50.96	47.34	46.82
C 7	88.49	88.01	87.04
C 8	153.88	155.23	154.80
C 9	135.78	137.26	137.05
C 10	-23.84	-22.95	-22.42
C 11	113.52	113.26	113.91
C 12	135.71	135.47	139.35
C 13	135.25	136.16	143.97
C 14	157.28	157.05	160.43
C 15	37.93	37.64	39.28
C 16	68.12	68.24	67.28
C 17	-0.26	-0.52	-0.59
C 18	147.25	147.02	147.50
C 19	147.44	147.82	147.84
C 20	-15.23	-15.34	-16.68
C 21	131.30	130.59	132.83
C 22	139.86	143.10	143.20
C 23	143.57	142.13	142.28
C 24	-11.83	-8.21	-8.56
C 25	167.58	163.40	163.21
C 27	166.20	166.31	166.28
C 28	176.41	177.89	175.44
C 29	167.42	166.87	164.96
C 30	166.26	165.52	165.53
H 1a	28.48	28.43	28.43
H 1b	29.12	28.86	28.86
H 2	28.02	28.14	28.12
H 3a	30.48	30.80	30.79
H 3b	29.91	29.75	29.73
H 4	30.17	29.76	29.75
H 5a	29.83	29.88	29.92
H 5b	29.10	29.47	29.49
H 8a	28.93	28.75	28.72
H 8b	29.52	29.08	29.13
H 11	27.33	27.44	28.01
H 13	29.51	29.56	28.79
H 14a	29.27	29.28	29.62
H 14b	29.01	28.95	29.58
H 16	25.68	25.70	25.65

H 18	29.33	29.26	29.29
H 19a	28.79	28.77	28.71
H 19b	29.64	29.64	29.64
H 21	29.00	29.01	28.59
H 23a	29.45	28.67	28.71
H 23b	28.05	29.10	29.00
H 25a-c	30.57	30.44	30.41
H 27a-c	29.91	29.91	29.94
H 28a-c	30.83	30.82	30.91
H 29a-c	30.71	30.68	30.43
H 30a-c	30.76	30.79	30.81

	Isomer 1	Isomer 3	Isomer 4
$J_{3a,4}$	10.85	10.41	10.4
$J_{3b,4}$	3.15	2.32	2.24
$J_{3a,2}$	9.97	1.7	1.71
$J_{3b,2}$	2.59	4.12	4.08
$J_{4,5a}$	10.79	10.18	10.1
$J_{4,5b}$	1.04	0.75	0.74
$J_{13,14a}$	9.53	9.53	10.04
$J_{13,14b}$	4.39	4.36	3.71
$J_{13,18}$	12.11	12.1	12.3
$J_{18,19a}$	5.08	5.07	4.88
$J_{18,19b}$	11.61	11.64	11.92

Table S64. Conformer contribution and energy for each conformer of Zoarenone at AMBER 12 kJ/mol MAD 0.5 Å.

Name	Energy (Hartree)	Boltzmann population
01-Zoarenone-miniAMBER-1	-1305.323053	1.00
02-Zoarenone-miniAMBER-3	-1305.31163	0.89
02-Zoarenone-miniAMBER-2	-1305.309651	0.11
03-Zoarenone-miniAMBER-4	-1305.330064	1.00
04-Zoarenone-miniAMBER-5	-1305.316487	0.50
04-Zoarenone-miniAMBER-6	-1305.316477	0.50
05-Zoarenone-miniAMBER-7	-1305.338395	1.00
06-Zoarenone-miniAMBER-8	-1305.33226	1.00
07-Zoarenone-miniAMBER-9	-1305.330265	1.00
08-Zoarenone-miniAMBER-10	-1305.322105	1.00
09-Zoarenone-miniAMBER-11	-1305.326736	1.00
10-Zoarenone-miniAMBER-12	-1305.29435	1.00
10-Zoarenone-miniAMBER-13	-1305.288056	0.00
11-Zoarenone-miniAMBER-15	-1305.334134	0.56
11-Zoarenone-miniAMBER-14	-1305.333907	0.44
12-Zoarenone-miniAMBER-16	-1305.306248	0.50
12-Zoarenone-miniAMBER-17	-1305.306244	0.50
13-Zoarenone-miniAMBER-18	-1305.333289	0.89
13-Zoarenone-miniAMBER-19	-1305.331356	0.11
13-Zoarenone-miniAMBER-21	-1305.325584	0.00
13-Zoarenone-miniAMBER-20	-1305.323866	0.00
14-Zoarenone-miniAMBER-22	-1305.318539	1.00
15-Zoarenone-miniAMBER-23	-1305.332735	1.00
15-Zoarenone-miniAMBER-24	-1305.319699	0.00
16-Zoarenone-miniAMBER-25	-1305.307784	0.02
16-Zoarenone-miniAMBER-27	-1305.310674	0.49
16-Zoarenone-miniAMBER-28	-1305.310668	0.48
16-Zoarenone-miniAMBER-26	-1305.306743	0.01
17-Zoarenone-miniAMBER-29	-1305.309995	1.00
18-Zoarenone-miniAMBER-30	-1305.317711	0.00
18-Zoarenone-miniAMBER-32	-1305.323627	1.00
18-Zoarenone-miniAMBER-33	-1305.316273	0.00
18-Zoarenone-miniAMBER-31	-1305.314881	0.00
19-Zoarenone-miniAMBER-34	-1305.318288	1.00
20-Zoarenone-miniAMBER-36	-1305.327062	0.85
20-Zoarenone-miniAMBER-35	-1305.325427	0.15
21-Zoarenone-miniAMBER-37	-1305.313078	1.00
22-Zoarenone-miniAMBER-38	-1305.342592	1.00
23-Zoarenone-miniAMBER-39	-1305.308134	0.50
23-Zoarenone-miniAMBER-40	-1305.308132	0.50

24-Zoarenone-miniAMBER-41	-1305.334492	1.00
25-Zoarenone-miniAMBER-42	-1305.310445	1.00
26-Zoarenone-miniAMBER-43	-1305.322907	1.00
27-Zoarenone-miniAMBER-44	-1305.323627	1.00
28-Zoarenone-miniAMBER-46	-1305.330489	0.38
28-Zoarenone-miniAMBER-47	-1305.330493	0.38
28-Zoarenone-miniAMBER-45	-1305.330026	0.23
29-Zoarenone-miniAMBER-48	-1305.321281	0.52
29-Zoarenone-miniAMBER-49	-1305.320564	0.24
29-Zoarenone-miniAMBER-50	-1305.320558	0.24
30-Zoarenone-miniAMBER-52	-1305.330551	0.44
30-Zoarenone-miniAMBER-51	-1305.330475	0.41
30-Zoarenone-miniAMBER-53	-1305.329515	0.15
31-Zoarenone-miniAMBER-54	-1305.319891	1.00
32-Zoarenone-miniAMBER-55	-1305.326373	0.93
32-Zoarenone-miniAMBER-58	-1305.323942	0.07
32-Zoarenone-miniAMBER-59	-1305.319862	0.00
32-Zoarenone-miniAMBER-56	-1305.31858	0.00
32-Zoarenone-miniAMBER-57	-1305.317424	0.00
44-Zoarenone-miniAMBER-86	-1305.301367	1.00

Table S65. Conformer contribution and energy for each conformer of Zoarenone at MM3 12 kJ/mol MAD 0.5 Å.

Name	Energy (Hartree)	Boltzmann population
01-Zoarenone-miniMM3-1	-1305.320444	1.00
02-Zoarenone-miniMM3-2	-1305.307115	1.00
03-Zoarenone-miniMM3-4	-1305.327047	1.00
04-Zoarenone-miniMM3-5	-1305.31292	0.50
04-Zoarenone-miniMM3-6	-1305.312907	0.50
05-Zoarenone-miniMM3-7	-1305.33366	1.00
06-Zoarenone-miniMM3-8	-1305.328427	1.00
07-Zoarenone-miniMM3-9	-1305.326132	1.00
08-Zoarenone-miniMM3-10	-1305.318217	1.00
09-Zoarenone-miniMM3-11	-1305.323895	1.00
10-Zoarenone-miniMM3-12	-1305.291683	1.00
11-Zoarenone-miniMM3-15	-1305.331098	0.69
11-Zoarenone-miniMM3-14	-1305.330352	0.31
12-Zoarenone-miniMM3-16	-1305.303093	0.50
12-Zoarenone-miniMM3-17	-1305.303084	0.50
13-Zoarenone-miniMM3-18	-1305.328782	0.79
13-Zoarenone-miniMM3-19	-1305.327531	0.21
14-Zoarenone-miniMM3-22	-1305.31669	1.00
15-Zoarenone-miniMM3-23	-1305.329589	1.00
16-Zoarenone-miniMM3-26	-1305.307152	0.15
16-Zoarenone-miniMM3-27	-1305.308043	0.40
16-Zoarenone-miniMM3-28	-1305.308024	0.39
16-Zoarenone-miniMM3-25	-1305.306288	0.06
17-Zoarenone-miniMM3-29	-1305.307729	1.00
18-Zoarenone-miniMM3-32	-1305.320046	1.00
19-Zoarenone-miniMM3-34	-1305.315546	1.00
20-Zoarenone-miniMM3-36	-1305.323203	0.97
20-Zoarenone-miniMM3-35	-1305.320054	0.03
21-Zoarenone-miniMM3-37	-1305.309738	1.00
22-Zoarenone-miniMM3-38	-1305.338858	1.00
23-Zoarenone-miniMM3-39	-1305.304663	0.50
23-Zoarenone-miniMM3-40	-1305.30466	0.50
24-Zoarenone-miniMM3-41	-1305.330693	1.00
25-Zoarenone-miniMM3-42	-1305.307577	1.00
26-Zoarenone-miniMM3-43	-1305.319341	1.00
27-Zoarenone-miniMM3-44	-1305.320078	1.00
28-Zoarenone-miniMM3-46	-1305.326036	0.39
28-Zoarenone-miniMM3-47	-1305.326027	0.38
28-Zoarenone-miniMM3-45	-1305.325539	0.23
29-Zoarenone-miniMM3-48	-1305.317592	0.83

29-Zoarenone-miniMM3-49	-1305.316113	0.17
30-Zoarenone-miniMM3-51	-1305.3281	0.84
30-Zoarenone-miniMM3-52	-1305.326185	0.11
30-Zoarenone-miniMM3-53	-1305.325342	0.05
31-Zoarenone-miniMM3-54	-1305.317372	1.00
32-Zoarenone-miniMM3-55	-1305.32239	0.84
32-Zoarenone-miniMM3-58	-1305.320852	0.16
34-Zoarenone-miniMM3-65	-1305.312407	1.00
44-Zoarenone-miniMM3-86	-1305.298507	1.00
50-Zoarenone-miniMM3-106	-1305.320197	0.50
50-Zoarenone-miniMM3-108	-1305.320182	0.50

Table S66. Conformer contribution and energy for each conformer of Zoarenone at MMFF 12 kJ/mol MAD 0.5 Å.

Name	Energy (Hartree)	Boltzmann population
01-Zoarenone-miniMMFF-1	-1305.326685	1.00
02-Zoarenone-miniMMFF-3	-1305.314846	0.80
02-Zoarenone-miniMMFF-2	-1305.313526	0.20
03-Zoarenone-miniMMFF-4	-1305.333759	1.00
04-Zoarenone-miniMMFF-5	-1305.319694	0.96
04-Zoarenone-miniMMFF-6	-1305.316777	0.04
05-Zoarenone-miniMMFF-7	-1305.340318	1.00
06-Zoarenone-miniMMFF-8	-1305.334962	1.00
07-Zoarenone-miniMMFF-9	-1305.332915	1.00
08-Zoarenone-miniMMFF-10	-1305.324948	1.00
09-Zoarenone-miniMMFF-11	-1305.331161	1.00
10-Zoarenone-miniMMFF-12	-1305.298992	1.00
11-Zoarenone-miniMMFF-14	-1305.33799	0.65
11-Zoarenone-miniMMFF-15	-1305.337423	0.35
12-Zoarenone-miniMMFF-16	-1305.30967	0.94
12-Zoarenone-miniMMFF-17	-1305.307135	0.06
13-Zoarenone-miniMMFF-18	-1305.335927	0.85
13-Zoarenone-miniMMFF-19	-1305.334323	0.15
14-Zoarenone-miniMMFF-22	-1305.322619	1.00
15-Zoarenone-miniMMFF-23	-1305.335405	1.00
16-Zoarenone-miniMMFF-25	-1305.31289	0.15
16-Zoarenone-miniMMFF-28	-1305.314094	0.53
16-Zoarenone-miniMMFF-27	-1305.313247	0.22
16-Zoarenone-miniMMFF-26	-1305.312506	0.10
17-Zoarenone-miniMMFF-29	-1305.313152	1.00
18-Zoarenone-miniMMFF-32	-1305.326817	1.00
19-Zoarenone-miniMMFF-34	-1305.321009	1.00
20-Zoarenone-miniMMFF-36	-1305.330344	0.89
20-Zoarenone-miniMMFF-35	-1305.328379	0.11
21-Zoarenone-miniMMFF-37	-1305.316429	1.00
22-Zoarenone-miniMMFF-38	-1305.345542	1.00
23-Zoarenone-miniMMFF-39	-1305.311763	0.98
23-Zoarenone-miniMMFF-40	-1305.308122	0.02
24-Zoarenone-miniMMFF-41	-1305.337329	1.00
25-Zoarenone-miniMMFF-42	-1305.314281	1.00
26-Zoarenone-miniMMFF-43	-1305.326466	1.00
27-Zoarenone-miniMMFF-44	-1305.326533	1.00
28-Zoarenone-miniMMFF-46	-1305.332671	0.38
28-Zoarenone-miniMMFF-47	-1305.332512	0.32
28-Zoarenone-miniMMFF-45	-1305.332464	0.30

29-Zoarenone-miniMMFF-48	-1305.324371	0.81
29-Zoarenone-miniMMFF-49	-1305.323007	0.19
30-Zoarenone-miniMMFF-51	-1305.334629	0.89
30-Zoarenone-miniMMFF-52	-1305.332286	0.07
30-Zoarenone-miniMMFF-53	-1305.331615	0.04
31-Zoarenone-miniMMFF-54	-1305.32337	1.00
32-Zoarenone-miniMMFF-55	-1305.328862	0.91
32-Zoarenone-miniMMFF-58	-1305.32669	0.09
44-Zoarenone-miniMMFF-86	-1305.305464	1.00
50-Zoarenone-miniMMFF-106	-1305.327043	1.00

Table S67. Conformer contribution and energy for each conformer of Zoaramine at AMBER 12 kJ/mol MAD 0.5 Å.

Name	Energy (Hartree)	Boltzmann population
01-Zoaramine_miniAMBER_RRSRSRSRS_5	-1634.676535	0.11
01-Zoaramine_miniAMBER_RRSRSRSRS_13	-1634.678448	0.85
01-Zoaramine_miniAMBER_RRSRSRSRS_8	-1634.675508	0.04
02-Zoaramine_miniAMBER_RRSSRSRSRS_69	-1634.670451	0.95
02-Zoaramine_miniAMBER_RRSSRSRSRS_65	-1634.667714	0.05
03-Zoaramine_miniAMBER_SRSRSRSRS_144	-1634.683399	0.64
03-Zoaramine_miniAMBER_SRSRSRSRS_145	-1634.682855	0.36
04-Zoaramine_miniAMBER_SRSSRSRSRS_191	-1634.674918	0.96
04-Zoaramine_miniAMBER_SRSSRSRSRS_192	-1634.671802	0.04

Table S68. Conformer contribution and energy for each conformer of Zoaramine at MM3 12 kJ/mol MAD 0.5 Å.

Name	Energy (Hartree)	Boltzmann population
01-Zoaramine_miniMM3_RRSRSRSRS_3	-1634.672988	0.02
01-Zoaramine_miniMM3_RRSRSRSRS_10	-1634.675938	0.42
01-Zoaramine_miniMM3_RRSRSRSRS_14	-1634.675314	0.21
01-Zoaramine_miniMM3_RRSRSRSRS_11	-1634.675094	0.17
01-Zoaramine_miniMM3_RRSRSRSRS_17	-1634.674628	0.10
01-Zoaramine_miniMM3_RRSRSRSRS_19	-1634.673821	0.04
01-Zoaramine_miniMM3_RRSRSRSRS_7	-1634.673233	0.02
01-Zoaramine_miniMM3_RRSRSRSRS_4	-1634.67234	0.01
02-Zoaramine_miniMM3_RRSSRSRSRS_66	-1634.668543	0.27
02-Zoaramine_miniMM3_RRSSRSRSRS_74	-1634.66856	0.27
02-Zoaramine_miniMM3_RRSSRSRSRS_71	-1634.668305	0.21
02-Zoaramine_miniMM3_RRSSRSRSRS_67	-1634.667926	0.14
02-Zoaramine_miniMM3_RRSSRSRSRS_75	-1634.667761	0.12
02-Zoaramine_miniMM3_RRSSRSRSRS_68	-1634.662837	0.00
02-Zoaramine_miniMM3_RRSSRSRSRS_127	-1634.662415	0.00
02-Zoaramine_miniMM3_RRSSRSRSRS_62	-1634.661927	0.00
03-Zoaramine_miniMM3_SRSRSRSRS_145	-1634.676646	0.97
03-Zoaramine_miniMM3_SRSRSRSRS_190	-1634.673419	0.03
03-Zoaramine_miniMM3_SRSRSRSRS_166	-1634.65836	0.00
04-Zoaramine_miniMM3_SRSSRSRSRS_226	-1634.670259	1.00
04-Zoaramine_miniMM3_SRSSRSRSRS_192	-1634.663147	0.00

Table S69. Conformer contribution and energy for each conformer of Zoaramine at MMFF 12 kJ/mol MAD 0.5 Å.

Name	Energy (Hartree)	Boltzmann population
01-Zoaramine_miniMMFF_RRSRSRSRS_3	-1634.6807	0.69
01-Zoaramine_miniMMFF_RRSRSRSRS_4	-1634.68	0.31
03-Zoaramine_miniMMFF_SRSRSRSRS_145	-1634.6858	0.90
03-Zoaramine_miniMMFF_SRSRSRSRS_144	-1634.6837	0.10
04-Zoaramine_miniMMFF_SRSSRSRS_191	-1634.6782	0.99
04-Zoaramine_miniMMFF_SRSSRSRS_192	-1634.6733	0.01

Table S70. CMAE (corrected mean absolute error) values for the isomers of Zoarenone at the PCM/B3LYP/6-31G**//AMBER

	Absoluted Error Scaled																
	Isomer1	Isomer2	Isomer3	Isomer4	Isomer5	Isomer6	Isomer7	Isomer8	Isomer9	Isomer10	Isomer11	Isomer12	Isomer13	Isomer14	Isomer15	Isomer16	Isomer17
C 7	3.04	3.24	4.19	4.65	6.23	3.61	4.27	2.65	3.81	3.81	4.21	4.26	4.36	4.07	3.08	4.51	2.35
C 8	2.07	0.07	1.59	2.76	2.08	1.81	4.51	2.58	2.22	2.05	1.55	1.81	4.69	2.13	1.74	3.62	1.88
C 9	1.17	1.63	1.34	1.27	2.72	4.74	2.75	4.97	1.10	2.24	1.38	1.82	0.50	0.98	0.02	2.04	0.07
C 10	2.44	6.84	5.31	7.13	4.25	4.64	1.17	1.85	0.55	6.32	5.26	9.38	6.82	5.25	5.25	6.06	3.88
C 11	1.10	1.36	9.54	6.54	2.08	3.44	0.31	1.04	2.06	3.16	3.56	3.99	0.67	2.91	1.64	0.33	1.58
C 12	5.61	9.41	0.72	10.54	1.49	1.25	4.05	4.62	7.98	15.94	5.46	13.98	5.44	3.63	3.91	10.84	7.74
C 13	6.44	12.38	4.89	4.40	0.35	0.01	5.94	6.24	3.45	2.36	3.71	3.89	6.27	1.93	15.18	13.52	5.62
C 14	4.65	2.22	0.42	2.24	1.72	2.13	3.38	3.80	5.38	1.43	0.07	1.32	1.39	5.71	0.47	1.96	6.45
C 15	2.71	2.08	1.07	1.05	1.04	1.75	1.24	1.51	2.12	0.02	0.25	1.52	1.27	1.04	0.95	0.04	2.40
C 16	0.24	1.17	2.08	0.98	0.06	0.69	1.11	0.10	0.65	0.45	0.22	0.38	0.65	1.56	0.06	1.48	0.76
C 17	4.52	5.34	6.97	6.10	5.94	6.51	5.38	6.13	4.97	5.25	5.57	5.38	7.08	6.41	5.35	6.51	4.59
C 18	0.64	5.68	1.05	5.17	3.42	3.63	2.18	2.48	2.90	2.50	3.34	1.61	3.67	7.89	2.90	2.09	1.02
C 19	4.09	7.59	3.10	0.42	0.29	1.37	0.36	1.00	0.73	7.93	2.83	7.66	1.71	1.84	3.24	7.45	5.76
C 20	2.49	3.18	3.35	2.86	0.71	0.04	2.55	1.65	4.82	2.94	2.31	1.15	0.70	2.58	1.82	4.68	1.57
C 21	1.44	5.30	2.85	1.89	0.93	5.36	3.57	7.41	8.64	7.30	6.34	5.03	2.33	1.81	1.19	0.56	1.54
C 22	0.33	2.97	0.28	2.23	2.03	1.49	2.09	1.00	2.01	2.60	3.17	2.90	0.19	0.99	3.04	4.07	2.40
C 23	15.40	11.72	13.67	11.09	11.81	13.45	11.05	14.29	10.87	14.18	8.06	12.14	9.59	13.94	5.66	9.89	15.49
C 24	0.75	2.31	1.21	2.51	2.36	1.87	2.52	2.21	2.91	0.23	2.73	0.60	2.62	1.23	2.54	1.77	0.86
C 25	2.51	5.73	2.53	4.97	1.71	2.93	0.18	4.94	2.69	10.64	1.36	12.01	1.31	9.25	0.05	13.34	9.31
C 27	3.42	3.02	3.29	0.89	0.41	1.17	0.08	0.89	0.60	3.56	0.71	2.67	0.72	2.75	1.17	3.26	4.70
C 28	12.52	25.23	11.28	15.50	1.85	1.52	4.40	4.52	11.74	16.88	12.71	14.49	8.27	5.55	11.33	15.09	13.26
C 29	2.92	0.73	1.93	0.96	2.84	1.58	2.08	0.36	2.87	2.90	0.02	4.03	0.16	0.48	1.18	1.49	0.79
Average	3.66	5.42	3.76	4.37	2.56	2.95	2.96	3.47	3.87	5.21	3.40	5.09	3.20	3.82	3.26	5.21	4.27

H 8a	0.56	0.18	0.42	0.18	0.78	0.26	0.86	0.10	0.71	0.41	0.53	0.45	0.17	0.20	0.66	0.24	0.43
H 8b	0.64	0.21	0.50	0.39	0.36	0.16	1.23	0.11	0.48	0.33	0.38	0.38	0.13	0.16	0.40	0.29	0.34
H 11	0.34	0.10	0.14	0.05	0.14	0.08	0.64	0.64	0.65	0.48	0.11	0.13	0.11	0.09	0.00	0.01	0.50
H 13	0.67	0.32	0.66	0.93	0.26	0.29	0.42	0.37	0.87	0.40	0.57	0.26	0.07	0.70	0.44	0.35	0.60
H 14a	0.31	0.23	0.51	0.19	0.21	0.15	0.24	0.28	0.50	0.55	0.01	0.11	0.07	0.07	0.04	0.28	0.57
H 14b	0.70	0.33	0.22	0.30	0.15	0.28	0.53	0.44	0.83	0.25	0.13	0.02	0.15	0.00	0.15	0.31	0.68
H 16	0.75	0.16	0.56	0.15	0.15	0.09	0.22	0.23	0.01	0.02	0.10	0.04	0.19	0.33	0.48	0.20	0.39
H 18	0.89	0.02	0.01	0.04	0.07	0.10	0.12	0.11	0.61	0.13	0.12	0.20	0.07	0.10	0.11	0.16	0.75
H 19a	0.29	0.09	0.36	0.35	0.31	0.23	0.28	0.24	0.37	0.10	0.31	0.12	0.35	0.30	0.03	0.23	0.35
H 19b	0.25	0.19	0.28	0.17	0.27	0.31	0.31	0.30	0.21	0.05	0.16	0.03	0.06	0.14	0.23	0.05	0.38
H 21	0.92	0.32	0.70	0.27	0.00	0.30	0.36	0.03	0.50	0.15	0.16	0.13	0.79	0.63	0.39	0.41	0.90
H 23	0.05	0.45	0.24	0.15	0.15	0.17	0.18	0.29	0.47	0.40	0.17	0.30	0.01	0.05	0.22	0.19	0.36
H 25a-c	0.27	0.09	0.16	0.19	0.06	0.37	0.02	0.37	0.07	0.22	0.23	0.03	0.12	0.17	0.21	0.14	0.13
H 27a-c	0.04	0.11	0.01	0.02	0.11	0.04	0.01	0.02	0.01	0.04	0.08	0.05	0.12	0.03	0.12	0.11	0.01
H 28a-c	0.13	0.65	0.26	0.33	0.20	0.15	0.07	0.05	0.18	0.17	0.28	0.37	0.26	0.42	0.39	0.61	0.30
H 29a-c	0.25	0.04	0.04	0.10	0.14	0.07	0.04	0.22	0.12	0.02	0.03	0.17	0.06	0.12	0.16	0.08	0.32
Average	0.44	0.22	0.32	0.24	0.21	0.19	0.35	0.24	0.41	0.23	0.21	0.17	0.17	0.22	0.25	0.23	0.44

	Absoluted Error Scaled															
	Isomer18	Isomer19	Isomer20	Isomer21	Isomer22	Isomer23	Isomer24	Isomer25	Isomer26	Isomer27	Isomer28	Isomer29	Isomer30	Isomer31	Isomer32	Isomer44
C 7	3.32	3.60	4.77	4.57	4.37	4.07	3.34	2.17	4.45	3.34	6.02	4.84	4.58	2.89	5.04	4.10
C 8	0.69	1.23	4.36	1.72	1.93	3.03	2.96	1.72	4.89	1.09	2.27	3.05	2.35	1.11	3.36	3.51
C 9	1.77	0.43	2.24	2.10	1.77	0.93	2.12	4.19	1.93	4.04	2.24	2.79	0.51	3.89	0.49	1.39
C 10	6.13	6.94	7.52	8.92	4.26	7.00	1.48	1.21	0.99	5.39	5.05	6.18	5.30	5.25	5.30	7.97
C 11	0.18	10.82	5.70	3.15	1.32	6.29	0.58	1.94	2.68	5.70	4.51	1.95	1.24	0.37	1.14	1.52
C 12	9.15	2.51	7.74	8.94	0.07	9.72	3.51	8.40	8.04	6.67	6.43	8.46	5.22	3.65	4.06	11.16
C 13	12.72	5.11	4.89	0.81	0.16	3.21	6.92	2.87	2.44	4.00	3.16	4.65	5.19	15.62	13.94	6.40
C 14	0.74	2.12	1.15	2.14	1.33	4.94	3.76	6.77	5.25	0.54	0.47	0.67	1.46	0.38	0.44	4.61
C 15	0.42	0.42	0.63	1.84	0.93	2.62	1.42	2.32	2.01	1.69	0.66	1.67	0.91	1.35	0.71	0.90
C 16	0.71	1.97	1.32	1.28	0.60	0.16	0.91	0.08	1.11	0.09	0.60	0.02	0.35	1.44	0.68	0.36
C 17	4.97	6.64	6.37	6.34	6.03	6.07	5.45	5.83	4.66	5.80	5.26	7.65	6.58	5.74	5.09	7.28
C 18	4.20	3.20	4.08	3.83	2.97	3.46	2.23	4.07	3.02	2.71	2.72	3.51	4.20	4.29	3.49	4.17
C 19	8.09	4.90	1.07	2.34	0.08	1.38	0.73	0.36	1.03	6.27	4.18	5.10	1.81	3.61	2.55	6.24
C 20	2.99	2.28	2.65	0.68	1.18	2.66	2.74	3.40	4.75	1.18	2.00	1.72	2.11	1.47	1.28	0.65
C 21	1.44	3.01	1.19	0.69	3.03	1.06	4.71	11.96	8.81	9.68	5.10	2.58	2.21	2.64	0.83	2.67
C 22	4.39	2.11	1.21	3.26	3.12	1.24	3.57	0.10	1.42	1.58	2.49	0.66	0.73	0.97	1.67	1.29
C 23	6.50	14.91	8.03	11.04	7.96	12.78	9.41	14.32	9.96	15.59	12.75	13.91	10.68	11.09	10.59	12.75
C 24	2.41	1.65	3.42	0.59	2.48	0.54	2.92	2.35	1.93	1.70	2.08	2.52	1.21	2.43	1.89	1.15
C 25	0.06	7.80	0.22	12.09	1.90	12.58	1.58	5.44	0.64	3.24	1.97	3.74	0.12	5.29	0.54	14.09
C 27	2.36	4.27	1.14	2.77	0.69	2.08	0.05	1.83	0.47	1.64	0.86	0.65	1.00	2.11	1.34	1.19
C 28	23.87	12.52	15.47	2.30	0.84	4.44	3.91	11.95	11.40	14.58	14.10	9.08	7.76	12.72	12.15	4.48
C 29	0.70	0.65	0.54	3.71	0.35	4.20	2.71	0.24	2.29	1.51	3.18	0.60	0.57	0.88	2.79	5.64
Average	4.44	4.50	3.90	3.87	2.15	4.29	3.04	4.25	3.83	4.45	4.01	3.91	3.00	4.05	3.61	4.71
H 8a	0.17	0.50	0.03	0.03	0.03	0.02	0.10	0.52	0.91	0.57	0.03	0.05	0.16	0.67	0.06	0.51

H 8b	0.24	0.54	0.04	0.06	0.11	0.08	0.26	0.41	1.13	0.64	0.39	0.16	0.12	0.60	0.44	0.34
H 11	0.03	0.05	0.38	0.14	0.34	0.70	0.69	0.61	0.57	0.02	0.04	0.31	0.01	0.10	0.24	0.21
H 13	0.26	0.58	0.87	0.10	0.31	0.38	0.39	0.92	0.93	0.42	0.45	0.50	0.30	0.02	0.12	0.07
H 14a	0.32	0.27	0.31	0.06	0.18	0.31	0.22	0.72	0.58	0.09	0.00	0.07	0.05	0.03	0.13	0.25
H 14b	0.02	0.11	0.22	0.11	0.09	0.31	0.57	0.86	0.85	0.03	0.09	0.29	0.06	0.17	0.10	0.58
H 16	0.56	0.30	0.18	0.11	0.04	0.15	0.10	0.11	0.18	0.02	0.01	0.23	0.56	0.07	0.38	0.02
H 18	0.29	0.16	0.26	0.03	0.03	0.02	0.06	0.45	0.57	0.30	0.19	0.07	0.03	0.20	0.08	0.22
H 19a	0.08	0.38	0.38	0.05	0.30	0.11	0.33	0.38	0.38	0.14	0.24	0.14	0.30	0.05	0.12	0.16
H 19b	0.12	0.38	0.04	0.06	0.24	0.08	0.26	0.37	0.32	0.24	0.19	0.43	0.04	0.08	0.02	0.07
H 21	0.37	0.70	0.51	0.26	0.29	0.06	0.14	0.44	0.79	0.09	0.16	0.49	0.56	0.37	0.08	0.22
H 23	0.26	0.10	0.19	0.12	0.32	0.32	0.42	0.36	0.11	0.30	0.17	0.31	0.29	0.16	0.35	0.30
H 25a-c	0.03	0.21	0.13	0.05	0.15	0.19	0.14	0.37	0.01	0.28	0.02	0.19	0.01	0.05	0.36	0.04
H 27a-c	0.12	0.05	0.08	0.03	0.10	0.02	0.06	0.11	0.08	0.04	0.11	0.02	0.02	0.18	0.07	0.06
H 28a-c	0.54	0.41	0.25	0.18	0.29	0.07	0.22	0.03	0.04	0.31	0.34	0.43	0.22	0.46	0.49	0.18
H 29a-c	0.11	0.11	0.04	0.16	0.01	0.07	0.17	0.13	0.13	0.08	0.19	0.05	0.03	0.05	0.03	0.15
Average	0.22	0.30	0.25	0.10	0.18	0.18	0.26	0.42	0.47	0.22	0.16	0.23	0.17	0.20	0.19	0.21

Table S71. CMAE (corrected mean absolute error) values for the isomers of Zoarenone at the PCM/B3LYP/6-31G**//MM3

	Absoluted Error Scaled																	
	Isomer1	Isomer2	Isomer3	Isomer4	Isomer5	Isomer6	Isomer7	Isomer8	Isomer9	Isomer10	Isomer11	Isomer12	Isomer13	Isomer14	Isomer15	Isomer16	Isomer17	Isomer18
C 7	1.41	1.98	2.45	2.44	4.17	1.42	1.94	0.18	2.27	1.34	2.48	1.65	2.04	2.09	1.60	1.27	0.13	1.37
C 8	2.30	3.45	1.31	2.96	2.52	1.16	4.72	2.42	2.65	2.32	1.49	2.19	4.37	1.42	1.76	2.75	1.47	0.55
C 9	2.14	0.47	2.28	0.94	1.22	1.91	1.64	2.07	0.24	4.37	0.06	4.00	1.27	2.24	0.45	3.94	2.11	2.42
C 10	3.79	6.68	5.78	7.85	4.27	4.79	2.07	3.07	1.72	7.91	5.50	10.52	7.01	5.60	5.87	7.52	5.21	6.84
C 11	0.27	3.07	8.22	5.78	0.78	1.92	0.68	0.01	3.24	3.95	2.76	2.92	0.74	1.90	2.66	1.94	0.54	0.72
C 12	5.36	12.34	1.08	8.88	1.44	0.68	4.03	4.10	7.24	17.57	5.20	15.50	4.81	2.45	3.84	9.92	6.17	8.93
C 13	4.01	3.10	2.66	3.69	2.59	2.48	5.16	5.10	1.57	1.39	1.25	0.74	5.12	0.22	13.98	12.21	4.70	10.68
C 14	4.88	3.49	0.29	0.44	0.84	1.02	2.70	3.15	4.50	2.48	1.13	1.47	0.07	5.01	1.97	0.38	6.25	1.31
C 15	5.18	5.33	0.59	2.02	2.21	2.92	3.37	3.82	3.68	2.49	2.18	4.20	2.73	2.68	1.81	2.41	4.90	2.01
C 16	1.19	1.35	0.85	0.31	0.95	0.42	2.44	1.56	1.91	0.77	1.77	1.71	0.47	0.11	1.15	0.38	0.87	0.57
C 17	2.85	2.94	5.12	4.27	4.12	4.59	3.51	4.26	3.25	3.46	3.54	3.62	5.50	4.17	3.54	4.87	2.85	3.51
C 18	0.43	5.37	3.95	5.75	2.91	2.92	2.27	2.56	2.92	1.91	2.49	0.86	3.53	8.78	2.06	4.61	2.14	4.42
C 19	3.57	1.11	2.07	0.68	0.87	1.47	0.17	0.69	1.55	7.71	3.18	7.44	2.24	1.01	2.82	7.12	5.06	7.75
C 20	2.78	4.75	3.50	3.80	1.61	1.24	3.18	2.43	5.71	4.47	3.86	2.83	1.65	4.01	2.69	4.40	2.93	4.81
C 21	2.09	1.80	4.17	0.22	0.31	4.85	3.12	6.71	9.66	6.70	6.80	4.39	2.06	3.17	1.33	2.75	2.17	1.24
C 22	1.15	3.89	1.39	5.67	0.76	1.16	0.50	0.43	0.50	6.46	0.36	6.72	2.91	2.97	0.04	5.83	3.85	2.12
C 23	12.66	6.64	11.62	5.30	8.58	8.51	7.33	9.17	7.59	9.24	4.52	6.88	6.62	8.52	2.27	5.03	11.17	2.96
C 24	4.88	1.81	5.20	1.42	1.86	1.93	1.56	1.46	1.86	4.38	1.66	3.37	1.61	5.13	2.12	1.76	5.74	1.96
C 25	1.32	1.40	1.30	4.18	0.80	3.19	1.03	5.73	2.14	11.91	0.80	12.91	0.55	8.92	0.04	15.55	10.61	0.08
C 27	3.25	0.72	3.04	0.62	0.62	1.15	0.10	0.56	0.42	3.69	0.66	2.92	0.52	2.70	0.92	2.86	4.25	2.52
C 28	13.35	21.23	11.14	17.16	3.13	3.06	5.80	5.84	12.77	18.96	13.90	17.93	9.43	8.13	11.95	13.08	14.68	26.01
C 29	2.00	0.32	2.98	0.10	3.17	0.71	2.01	0.71	2.65	4.58	0.50	4.85	0.55	1.48	1.51	3.79	0.41	1.00
Average	3.68	4.24	3.68	3.84	2.26	2.43	2.70	3.00	3.64	5.82	3.00	5.44	2.99	3.76	3.02	5.20	4.46	4.26

H 8a	0.60	0.20	0.52	0.21	0.81	0.35	0.98	0.25	0.70	0.41	0.54	0.44	0.17	0.29	0.69	0.39	0.65	0.05
H 8b	0.45	0.26	0.32	0.34	0.46	0.31	1.79	0.26	0.36	0.27	0.27	0.32	0.03	0.34	0.22	0.20	0.47	0.25
H 11	0.25	0.69	0.46	0.16	0.00	0.15	0.74	0.71	0.71	0.61	0.12	0.02	0.37	0.16	0.14	0.24	0.51	0.21
H 13	0.66	0.98	0.65	0.93	0.32	0.32	0.60	0.60	0.82	0.39	0.50	0.18	0.10	0.74	0.65	0.02	0.57	0.21
H 14a	0.19	0.87	1.12	0.38	0.25	0.22	0.19	0.20	0.58	0.70	0.01	0.15	0.15	0.19	0.05	0.15	0.49	0.21
H 14b	0.57	0.80	0.25	0.34	0.10	0.07	0.70	0.56	0.85	0.23	0.29	0.06	0.02	0.13	0.42	0.65	0.56	0.39
H 16	0.95	0.31	0.68	0.28	0.17	0.20	0.30	0.41	0.05	0.09	0.14	0.09	0.19	0.56	0.40	0.26	0.55	0.58
H 18	1.31	1.34	0.07	0.02	0.06	0.08	0.15	0.11	0.71	0.05	0.10	0.11	0.02	0.21	0.02	0.12	1.10	0.59
H 19a	0.40	0.34	0.48	0.35	0.16	0.10	0.17	0.19	0.37	0.14	0.23	0.18	0.21	0.27	0.07	0.17	0.46	0.15
H 19b	0.44	0.20	0.53	0.10	0.33	0.33	0.37	0.34	0.28	0.08	0.21	0.01	0.01	0.06	0.32	0.08	0.54	0.16
H 21	1.00	0.31	0.85	0.14	0.08	0.09	0.56	0.35	0.82	0.33	0.04	0.05	0.71	0.48	0.34	0.42	0.84	0.27
H 23	0.28	0.20	0.47	0.12	0.00	0.13	0.08	0.07	0.36	0.35	0.06	0.12	0.17	0.39	0.38	0.16	0.15	0.52
H 25a-c	0.34	0.25	0.21	0.03	0.03	0.25	0.09	0.22	0.03	0.24	0.21	0.07	0.17	0.13	0.35	0.10	0.01	0.09
H 27a-c	0.18	0.31	0.15	0.12	0.02	0.08	0.14	0.14	0.12	0.18	0.05	0.07	0.01	0.15	0.29	0.35	0.12	0.35
H 28a-c	0.15	0.11	0.32	0.35	0.22	0.15	0.02	0.00	0.15	0.17	0.28	0.41	0.28	0.49	0.32	0.46	0.28	0.48
H 29a-c	0.20	0.19	0.10	0.05	0.04	0.01	0.16	0.22	0.06	0.06	0.12	0.10	0.05	0.00	0.28	0.01	0.29	0.29
Average	0.50	0.46	0.45	0.24	0.19	0.18	0.44	0.29	0.44	0.27	0.20	0.15	0.17	0.29	0.31	0.23	0.47	0.30

	Absoluted Error Scaled																
	Isomer19	Isomer20	Isomer21	Isomer22	Isomer23	Isomer24	Isomer25	Isomer26	Isomer27	Isomer28	Isomer29	Isomer30	Isomer31	Isomer32	Isomer34	Isomer44	Isomer50
C 7	1.43	3.13	2.13	2.71	1.56	1.79	0.43	1.95	0.94	3.86	2.59	2.65	0.74	3.12	1.11	1.77	0.81
C 8	0.62	4.59	2.28	1.84	3.82	3.74	1.20	4.62	0.55	2.70	3.49	1.80	0.55	4.14	0.92	3.90	2.47
C 9	1.91	2.47	4.49	0.08	3.17	0.77	1.40	1.29	1.18	0.78	0.60	2.14	0.83	0.74	0.67	3.39	1.06
C 10	7.34	7.92	9.78	4.32	8.41	2.82	2.33	1.80	5.67	5.26	6.76	4.54	5.64	5.79	5.54	8.82	6.09
C 11	9.79	4.51	1.94	0.07	6.28	0.48	3.09	3.91	4.50	3.65	1.11	0.06	1.70	2.33	0.71	2.93	2.10
C 12	1.59	7.99	10.19	0.43	11.14	2.90	7.42	7.51	6.29	6.39	7.24	3.43	2.95	4.86	5.01	12.29	5.22
C 13	3.95	3.83	3.50	2.24	1.32	6.08	1.12	0.95	0.79	0.49	3.10	2.11	12.92	12.20	15.48	4.78	17.79
C 14	1.52	0.27	1.31	0.08	4.24	2.78	5.88	4.58	1.35	1.06	1.25	2.08	1.20	1.40	1.26	3.69	0.81
C 15	0.78	1.64	3.20	1.98	4.47	3.38	4.04	3.64	4.07	2.90	3.28	1.98	2.11	1.81	1.71	2.34	1.91
C 16	0.68	0.07	0.32	0.64	1.07	2.29	1.13	2.23	1.63	1.88	1.37	0.18	0.04	0.24	1.88	1.39	2.36
C 17	4.70	4.55	4.46	4.19	4.05	3.57	4.10	2.95	3.71	3.39	6.38	5.01	3.90	3.71	5.51	5.65	4.84
C 18	5.69	5.74	3.36	2.24	3.05	1.81	4.06	3.25	1.99	2.41	3.00	6.17	3.55	3.51	6.09	4.11	5.70
C 19	4.15	0.33	2.86	0.20	1.75	0.64	0.56	1.55	6.20	4.45	7.07	0.14	2.95	2.63	7.55	5.60	6.62
C 20	3.31	3.24	1.48	2.48	3.24	3.71	4.28	5.36	2.89	3.37	3.12	3.88	2.63	1.92	4.83	1.73	5.35
C 21	4.16	1.55	2.95	3.15	0.83	5.08	12.01	9.14	9.89	4.59	2.27	3.35	1.88	2.10	2.20	1.46	1.08
C 22	3.72	3.96	6.90	0.02	4.63	1.51	2.23	0.99	0.88	0.32	3.07	1.14	1.99	1.46	1.34	5.04	3.24
C 23	11.20	5.37	6.13	4.38	8.12	5.82	8.70	5.79	10.30	9.45	9.65	8.75	5.00	7.95	5.72	7.46	0.03
C 24	6.31	0.99	3.60	1.88	3.58	1.68	1.43	2.17	2.09	2.16	1.28	4.02	1.57	2.29	1.24	2.95	1.42
C 25	9.31	0.27	13.00	1.16	13.56	0.64	6.05	0.63	3.26	1.06	2.38	0.44	5.31	1.53	4.18	15.13	1.69
C 27	4.09	0.87	2.96	0.52	2.03	0.42	1.54	0.62	1.52	1.09	0.11	1.61	1.77	1.36	1.06	1.53	0.57
C 28	13.23	16.74	4.05	1.64	6.28	4.82	13.54	13.14	16.69	15.88	11.48	7.60	13.20	12.58	21.77	6.26	19.93
C 29	1.13	0.02	4.56	0.01	5.93	2.71	1.12	2.59	0.65	3.63	0.17	2.76	0.32	2.31	0.65	6.98	2.41
Average	4.57	3.64	4.34	1.65	4.66	2.70	3.99	3.67	3.96	3.67	3.67	2.99	3.31	3.64	4.38	4.96	4.25

H 8a	0.69	0.05	0.02	0.06	0.04	0.01	0.71	1.11	0.70	0.08	0.10	0.13	0.88	0.13	0.23	0.54	0.19
H 8b	0.59	0.10	0.04	0.12	0.12	0.23	0.51	1.69	0.70	0.43	0.17	0.12	0.63	0.52	0.48	0.25	0.32
H 11	0.36	0.76	0.02	0.14	0.77	0.73	0.64	0.63	0.23	0.13	0.10	0.31	0.29	0.48	0.11	0.06	0.17
H 13	0.56	0.87	0.16	0.33	0.43	0.61	0.94	0.94	0.36	0.41	0.70	0.53	0.17	0.06	0.06	0.12	0.33
H 14a	0.66	0.62	0.13	0.22	0.23	0.13	0.96	0.68	0.10	0.02	0.15	0.05	0.12	0.02	0.62	0.38	0.97
H 14b	0.11	0.34	0.14	0.21	0.38	0.69	0.92	0.92	0.05	0.20	0.32	0.33	0.89	0.74	0.60	0.57	0.63
H 16	0.39	0.11	0.17	0.07	0.27	0.22	0.30	0.27	0.08	0.01	0.34	0.70	0.12	0.44	0.07	0.10	0.74
H 18	0.21	0.24	0.08	0.00	0.03	0.03	0.56	0.64	0.24	0.16	0.02	0.11	0.14	0.05	0.16	0.35	0.65
H 19a	0.52	0.36	0.12	0.16	0.04	0.23	0.39	0.37	0.05	0.15	0.50	0.37	0.10	0.06	0.03	0.11	0.34
H 19b	0.57	0.00	0.03	0.29	0.05	0.28	0.44	0.42	0.23	0.21	0.92	0.11	0.08	0.03	0.09	0.14	0.02
H 21	0.68	0.42	0.12	0.17	0.25	0.35	0.88	1.12	0.09	0.28	0.31	0.59	0.30	0.12	0.20	0.00	0.35
H 23	0.17	0.38	0.08	0.13	0.22	0.30	0.07	0.08	0.01	0.01	0.10	0.59	0.17	0.71	0.37	0.08	0.59
H 25a-c	0.06	0.23	0.17	0.13	0.17	0.12	0.22	0.06	0.13	0.06	0.01	0.01	0.15	0.47	0.20	0.17	0.19
H 27a-c	0.05	0.05	0.10	0.01	0.09	0.05	0.26	0.23	0.08	0.01	0.18	0.14	0.37	0.26	0.19	0.19	0.29
H 28a-c	0.47	0.24	0.21	0.29	0.09	0.19	0.09	0.09	0.31	0.36	0.53	0.31	0.36	0.37	0.63	0.22	0.39
H 29a-c	0.02	0.08	0.09	0.08	0.02	0.14	0.09	0.29	0.05	0.09	0.02	0.03	0.14	0.20	0.02	0.07	0.35
Average	0.38	0.30	0.11	0.15	0.20	0.27	0.50	0.60	0.21	0.16	0.28	0.28	0.31	0.29	0.25	0.21	0.41

Table S72. CMAE (corrected mean absolute error) values for the isomers of Zoarenone at the PCM/B3LYP/6-31G**//MMFF

	Absoluted Error Scaled																
	Isomer1	Isomer2	Isomer3	Isomer4	Isomer5	Isomer6	Isomer7	Isomer8	Isomer9	Isomer10	Isomer11	Isomer12	Isomer13	Isomer14	Isomer15	Isomer16	Isomer17
C 7	0.21	0.46	1.13	0.92	2.81	0.37	1.15	1.44	0.80	0.57	1.10	0.20	1.99	0.03	0.51	0.09	1.50
C 8	0.39	0.82	0.47	2.26	1.90	0.20	4.09	1.21	1.03	1.93	0.10	1.95	3.36	0.80	0.51	2.57	0.49
C 9	0.81	2.18	0.11	2.05	3.64	5.28	4.08	5.51	3.00	1.49	2.47	1.17	1.44	0.75	2.11	0.76	1.66
C 10	6.13	8.11	7.81	9.33	7.02	6.31	5.24	4.55	4.37	9.63	7.58	12.56	9.98	6.89	7.74	8.48	6.70
C 11	0.13	0.23	7.83	4.77	0.24	1.17	0.75	0.86	3.37	3.03	2.13	2.25	1.54	1.59	2.39	1.45	0.17
C 12	1.38	5.60	3.18	6.38	1.35	2.43	0.89	0.61	3.81	12.68	1.52	11.63	2.77	0.82	1.04	6.62	2.38
C 13	3.72	8.16	2.07	2.53	2.05	1.89	5.00	4.85	1.71	1.57	0.85	0.03	4.51	1.20	13.26	10.85	4.27
C 14	5.22	1.35	1.14	0.80	1.22	1.56	3.22	3.51	4.83	1.34	0.43	1.79	0.66	4.98	1.53	0.08	6.79
C 15	9.88	7.98	5.70	7.25	7.17	7.72	8.31	8.41	8.47	6.63	6.33	8.18	7.52	8.07	6.45	6.93	9.94
C 16	0.01	0.79	2.14	1.15	0.30	0.59	1.12	0.37	0.60	0.48	0.09	0.43	0.56	1.05	0.11	1.19	0.35
C 17	2.17	2.86	4.39	2.75	3.23	3.36	2.78	3.13	1.83	3.21	2.85	3.37	4.32	2.40	2.67	3.47	2.13
C 18	0.73	5.68	1.88	5.52	3.27	3.31	2.60	2.85	3.29	2.87	4.02	2.04	4.32	8.20	3.26	4.81	2.97
C 19	4.13	7.46	3.11	1.07	0.93	1.84	0.15	1.33	0.75	7.83	2.16	7.49	2.54	2.88	4.10	7.27	5.66
C 20	4.06	6.13	5.22	4.94	2.23	1.77	3.94	3.13	5.61	4.20	4.20	2.48	3.23	4.34	4.32	5.76	3.81
C 21	4.17	2.33	5.66	0.03	0.82	3.24	1.37	4.79	7.05	4.44	4.10	2.60	2.40	4.31	1.87	3.00	4.48
C 22	2.05	3.31	1.52	1.22	2.70	1.99	3.32	2.14	2.72	2.22	3.52	2.45	0.52	0.49	4.32	1.56	0.50
C 23	6.13	0.59	4.66	0.39	3.30	2.92	2.56	3.47	1.63	3.57	0.54	1.17	0.93	2.70	3.29	0.09	5.68
C 24	4.01	0.98	4.16	0.60	1.47	1.09	1.43	0.71	1.09	2.94	1.03	2.05	1.49	3.33	1.06	1.27	4.57
C 25	1.29	2.68	2.01	2.50	2.02	2.10	0.33	4.10	1.61	11.10	0.73	11.71	0.01	7.79	0.67	11.99	8.43
C 27	4.35	3.74	4.35	1.40	1.66	2.30	1.12	1.92	1.66	4.94	1.77	4.16	1.52	3.67	2.10	3.87	5.39
C 28	11.60	25.10	10.14	15.72	1.85	1.90	4.62	4.99	10.84	16.46	11.77	15.44	8.70	7.37	11.78	14.91	12.99
C 29	1.64	0.59	2.07	0.02	2.53	0.99	1.38	0.33	2.23	2.40	0.16	3.26	0.08	1.17	0.60	0.52	0.61
Average	3.37	4.42	3.67	3.35	2.44	2.47	2.70	2.92	3.29	4.80	2.70	4.47	2.93	3.40	3.44	4.43	4.16

H 8a	0.65	0.17	0.53	0.21	0.69	0.28	0.77	0.17	0.75	0.34	0.59	0.41	0.24	0.28	0.71	0.26	0.44
H 8b	0.90	0.16	0.76	0.51	0.33	0.15	1.41	0.08	0.76	0.41	0.63	0.48	0.35	0.16	0.62	0.36	0.45
H 11	0.14	0.01	0.36	0.11	0.01	0.11	0.56	0.56	0.59	0.43	0.03	0.04	0.17	0.15	0.22	0.09	0.35
H 13	0.48	0.25	0.47	0.81	0.17	0.15	0.63	0.60	0.68	0.29	0.50	0.09	0.09	0.55	0.34	0.02	0.38
H 14a	0.15	0.15	0.75	0.30	0.19	0.15	0.24	0.25	0.46	0.71	0.01	0.13	0.10	0.06	0.04	0.18	0.43
H 14b	0.68	0.45	0.35	0.38	0.02	0.22	0.67	0.52	0.85	0.39	0.12	0.05	0.10	0.12	0.20	0.31	0.64
H 16	0.90	0.04	0.69	0.37	0.27	0.23	0.37	0.41	0.07	0.19	0.08	0.22	0.31	0.64	0.54	0.40	0.57
H 18	0.99	0.14	0.04	0.01	0.02	0.02	0.11	0.06	0.59	0.01	0.01	0.05	0.05	0.25	0.05	0.10	0.82
H 19a	0.38	0.01	0.42	0.26	0.22	0.12	0.23	0.18	0.24	0.09	0.25	0.13	0.36	0.02	0.04	0.07	0.51
H 19b	0.41	0.15	0.44	0.17	0.28	0.25	0.33	0.26	0.10	0.09	0.13	0.01	0.06	0.41	0.24	0.01	0.50
H 21	0.76	0.14	0.51	0.03	0.05	0.11	0.46	0.24	0.63	0.31	0.02	0.02	0.55	0.40	0.21	0.31	0.72
H 23	0.39	0.11	0.57	0.25	0.10	0.15	0.06	0.01	0.28	0.13	0.01	0.02	0.24	0.47	0.55	0.22	0.02
H 25a-c	0.24	0.12	0.04	0.12	0.04	0.22	0.06	0.22	0.01	0.15	0.11	0.15	0.20	0.18	0.31	0.11	0.01
H 27a-c	0.27	0.31	0.23	0.18	0.09	0.13	0.20	0.21	0.20	0.25	0.10	0.16	0.10	0.25	0.35	0.35	0.20
H 28a-c	0.05	0.56	0.21	0.30	0.19	0.15	0.00	0.01	0.09	0.12	0.23	0.36	0.25	0.42	0.31	0.50	0.26
H 29a-c	0.16	0.09	0.08	0.04	0.06	0.07	0.11	0.13	0.06	0.11	0.11	0.06	0.06	0.07	0.29	0.07	0.20
Average	0.47	0.18	0.40	0.25	0.17	0.16	0.39	0.24	0.40	0.25	0.18	0.15	0.20	0.28	0.31	0.21	0.41

	Absoluted Error Scaled																
	Isomer18	Isomer19	Isomer20	Isomer21	Isomer22	Isomer23	Isomer24	Isomer25	Isomer26	Isomer27	Isomer28	Isomer29	Isomer30	Isomer31	Isomer32	Isomer44	Isomer50
C 7	0.57	0.36	2.30	0.17	1.12	0.31	0.35	2.05	1.44	0.68	2.67	0.79	1.25	0.65	2.28	0.37	0.03
C 8	0.70	0.31	3.30	2.00	0.45	3.41	1.90	0.28	4.27	0.38	2.02	2.59	0.50	0.10	2.96	3.92	1.13
C 9	0.20	1.20	0.05	1.27	2.55	0.29	3.31	5.33	3.92	4.53	3.34	2.81	0.49	4.12	2.05	0.53	1.25
C 10	8.81	8.63	10.28	11.97	6.55	10.13	4.81	4.11	5.57	6.84	7.94	8.43	6.48	6.64	7.89	11.19	8.25
C 11	0.51	8.56	4.06	1.26	0.23	5.09	0.75	3.81	3.61	3.71	2.78	0.52	0.28	1.96	1.82	2.91	1.59
C 12	6.05	2.09	4.89	6.33	3.27	6.74	0.11	3.54	4.12	3.03	3.33	4.48	0.29	0.20	1.52	7.56	2.02
C 13	10.17	2.91	2.98	3.47	1.76	0.95	5.59	1.51	1.48	0.67	0.16	2.34	2.23	12.08	11.87	3.74	16.74
C 14	0.35	2.87	0.57	1.71	0.79	4.48	3.39	6.10	4.73	0.01	0.51	0.82	2.49	0.92	1.40	4.76	2.26
C 15	5.63	6.23	6.88	8.11	6.86	9.19	8.10	8.69	8.79	7.99	6.91	7.93	7.23	6.70	6.59	7.01	6.27
C 16	0.54	1.87	1.53	1.35	0.55	0.11	1.08	0.17	0.83	0.43	0.30	0.60	1.18	1.20	0.95	0.65	0.34
C 17	2.88	3.82	3.10	3.46	3.00	3.22	2.50	2.70	1.87	3.20	2.93	5.32	3.50	2.87	2.65	5.04	4.05
C 18	4.79	4.72	5.11	3.68	2.78	3.42	2.39	4.26	3.42	3.17	3.94	3.57	5.73	4.35	4.04	5.16	6.59
C 19	8.46	5.15	1.39	2.92	0.64	1.90	0.03	0.23	1.00	6.42	3.67	7.06	0.87	4.33	3.98	4.86	6.92
C 20	6.23	4.24	5.02	0.93	2.79	2.99	4.35	4.34	5.28	3.79	3.76	3.80	4.79	4.21	3.52	1.22	6.69
C 21	0.13	6.04	2.04	3.15	1.12	1.78	2.43	10.11	7.07	6.87	2.44	0.17	4.11	0.87	2.28	0.23	2.30
C 22	5.71	0.50	0.13	2.79	3.66	0.78	4.60	0.69	1.98	2.47	3.11	0.98	2.36	2.14	3.07	0.80	7.00
C 23	2.90	5.01	0.81	0.54	0.87	2.67	0.31	3.09	1.57	4.64	3.96	2.53	3.63	0.30	3.00	1.88	4.70
C 24	1.39	4.69	0.61	2.17	1.05	2.25	0.88	0.63	1.99	1.30	1.72	0.16	3.27	0.85	1.92	1.43	0.42
C 25	0.70	7.07	0.65	11.90	0.71	12.63	0.35	4.20	0.79	1.99	2.27	0.03	0.95	2.98	0.26	13.88	2.56
C 27	3.77	5.39	2.15	3.96	1.75	3.20	0.99	2.80	1.67	2.81	2.06	0.95	2.57	2.89	2.42	2.24	1.43
C 28	25.40	12.16	15.63	2.25	0.51	4.39	3.66	12.16	11.24	15.28	13.76	10.17	6.57	13.25	12.04	3.68	19.29
C 29	0.18	0.23	0.35	2.99	0.51	3.32	2.12	0.66	1.90	1.12	2.80	0.27	2.34	0.53	2.07	4.97	1.04
Average	4.37	4.28	3.36	3.56	1.98	3.78	2.45	3.70	3.57	3.70	3.47	3.02	2.87	3.37	3.66	4.00	4.68

H 8a	0.38	0.50	0.30	0.14	0.26	0.07	0.34	0.50	0.82	0.54	0.05	0.05	0.21	0.67	0.07	0.48	0.23
H 8b	0.30	0.58	0.00	0.01	0.18	0.16	0.31	0.45	1.30	0.65	0.30	0.17	0.18	0.63	0.35	0.45	0.36
H 11	0.27	0.31	0.42	0.05	0.16	0.60	0.61	0.51	0.49	0.14	0.11	0.15	0.25	0.28	0.36	0.12	0.19
H 13	0.15	0.39	0.77	0.02	0.18	0.54	0.59	0.75	0.77	0.29	0.41	0.49	0.36	0.12	0.05	0.22	0.13
H 14a	0.44	0.45	0.48	0.08	0.15	0.29	0.20	0.80	0.50	0.08	0.01	0.11	0.06	0.08	0.05	0.26	0.65
H 14b	0.36	0.22	0.37	0.04	0.01	0.38	0.67	0.90	0.91	0.02	0.20	0.35	0.06	0.61	0.42	0.59	0.65
H 16	0.59	0.47	0.30	0.31	0.07	0.36	0.17	0.31	0.33	0.08	0.11	0.39	0.68	0.24	0.46	0.20	0.70
H 18	0.28	0.20	0.19	0.12	0.02	0.05	0.02	0.50	0.60	0.19	0.09	0.02	0.22	0.11	0.01	0.40	0.32
H 19a	0.01	0.54	0.30	0.11	0.19	0.05	0.24	0.30	0.26	0.17	0.28	0.49	0.17	0.00	0.09	0.18	0.39
H 19b	0.01	0.53	0.16	0.03	0.24	0.02	0.25	0.22	0.15	0.25	0.21	0.92	0.18	0.11	0.09	0.13	0.17
H 21	0.14	0.53	0.27	0.03	0.14	0.29	0.27	0.65	0.91	0.03	0.16	0.30	0.41	0.16	0.04	0.03	0.15
H 23	0.62	0.28	0.45	0.22	0.09	0.02	0.22	0.01	0.16	0.03	0.08	0.02	0.62	0.31	0.62	0.05	0.63
H 25a-c	0.06	0.03	0.25	0.23	0.08	0.09	0.05	0.22	0.02	0.13	0.01	0.09	0.13	0.27	0.47	0.23	0.13
H 27a-c	0.39	0.12	0.15	0.16	0.08	0.17	0.12	0.31	0.29	0.14	0.09	0.23	0.25	0.39	0.27	0.27	0.36
H 28a-c	0.47	0.44	0.20	0.16	0.25	0.01	0.17	0.08	0.08	0.31	0.29	0.52	0.23	0.40	0.39	0.13	0.40
H 29a-c	0.26	0.05	0.09	0.04	0.09	0.05	0.12	0.04	0.22	0.02	0.10	0.08	0.01	0.18	0.12	0.04	0.32
Average	0.30	0.35	0.29	0.11	0.14	0.20	0.27	0.41	0.49	0.19	0.16	0.27	0.25	0.29	0.24	0.24	0.36

Table S73. CMAE (corrected mean absolute error) values for the isomers of Zoaremine at the PCM/B3LYP/6-31G**//AMBER

	Absoluted Error Scaled			
	Isomer1	Isomer2	Isomer3	Isomer4
C 1	5.25	4.97	2.19	1.22
C 2	6.67	6.21	7.25	8.02
C 3	2.90	2.53	1.58	0.71
C 4	0.55	0.29	2.62	2.53
C 5	0.40	0.83	1.04	3.17
C 6	4.16	3.80	1.24	0.05
C 7	21.49	22.80	17.57	22.27
C 8	3.10	3.37	2.95	3.00
C 9	0.46	0.81	1.29	0.25
C 10	3.40	1.16	3.15	0.46
C 11	0.81	0.44	1.50	0.00
C 12	0.81	2.89	0.33	3.33
C 13	1.73	9.09	0.64	9.37
C 14	1.08	3.88	1.09	4.19
C 15	0.67	1.32	1.72	2.12
C 16	0.88	0.33	1.05	0.30
C 17	6.61	6.06	7.54	6.89
C 18	2.57	1.97	2.46	2.34
C 19	0.14	0.35	0.13	0.08
C 20	1.10	2.75	0.23	1.75
C 21	2.77	5.08	2.56	5.50
C 22	1.87	1.62	3.44	1.51
C 23	3.40	4.64	1.60	4.80
C 24	0.98	1.89	1.18	2.79
C 25	4.89	6.23	1.42	5.84
C 27	0.49	0.21	0.19	0.48
C 28	1.84	1.02	0.38	0.68
C 29	1.81	0.69	1.74	0.45
C 30	0.97	0.59	0.59	0.17
Average	2.89	3.37	2.44	3.25
H 1a	0.28	0.29	0.02	0.19
H 1b	0.18	0.18	0.27	0.30
H 2	0.35	0.37	0.08	0.08
H 3a	0.20	0.15	0.47	0.51
H 3b	0.43	0.48	0.03	0.11
H 4	0.25	0.22	0.44	0.55
H 5a	0.40	0.41	0.10	0.08
H 5b	0.18	0.14	0.11	0.01
H 8a	0.29	0.28	0.05	0.30
H 8b	0.60	0.53	0.44	0.59

H 11	0.20	0.62	0.08	0.61
H 13	0.38	0.39	0.27	0.43
H 14a	0.09	0.36	0.13	0.34
H 14b	0.07	0.44	0.00	0.42
H 16	0.38	0.55	0.21	0.60
H 18	0.08	0.11	0.04	0.05
H 19a	0.35	0.41	0.34	0.46
H 19b	0.36	0.36	0.27	0.31
H 21	0.40	0.16	0.36	0.20
H 23a	0.94	1.14	0.21	1.14
H 23b	0.49	0.63	0.04	0.63
H 25a-c	0.07	0.06	0.19	0.11
H 27a-c	0.00	0.06	0.07	0.02
H 28a-c	0.02	0.12	0.09	0.10
H 29a-c	0.23	0.07	0.06	0.01
H 30a-c	0.19	0.25	0.05	0.16
Average	0.28	0.34	0.17	0.32

Table S74. CMAE (corrected mean absolute error) values for the isomers of Zoaramine at the PCM/B3LYP/6-31G**//MM3

	Absoluted Error Scaled			
	Isomer1	Isomer2	Isomer3	Isomer4
C 1	1.40	2.09	3.43	2.06
C 2	1.71	2.47	1.60	1.33
C 3	1.67	2.15	0.61	0.49
C 4	1.75	2.79	1.96	1.11
C 5	0.85	0.07	0.50	0.30
C 6	21.31	19.41	20.09	19.98
C 7	8.61	9.55	10.72	7.02
C 8	0.79	2.32	1.06	5.16
C 9	1.47	0.60	1.12	1.02
C 10	6.20	6.01	5.56	7.63
C 11	0.91	0.29	1.25	0.73
C 12	0.41	3.87	0.33	2.87
C 13	0.23	8.78	0.74	8.22
C 14	0.83	3.97	0.22	3.11
C 15	0.66	2.47	0.66	2.92
C 16	0.71	2.17	0.98	2.58
C 17	3.26	2.81	3.37	3.48
C 18	2.64	2.63	2.00	1.82
C 19	0.80	0.04	0.33	1.26
C 20	4.11	5.20	3.96	4.37
C 21	3.00	5.75	2.47	5.22
C 22	0.18	0.83	0.66	2.10
C 23	2.59	2.27	4.15	0.49
C 24	6.37	6.08	6.41	8.55
C 25	4.45	5.13	5.62	4.64
C 27	1.40	0.66	0.76	0.44
C 28	2.31	0.98	1.76	2.07
C 29	1.60	1.00	0.88	1.67
C 30	1.15	0.41	0.68	0.36
Average	2.88	3.54	2.89	3.55
H 1a	0.12	0.15	0.19	0.11
H 1b	0.24	0.17	0.15	0.08
H 2	0.05	0.03	0.29	0.21
H 3a	0.18	0.23	0.52	0.52
H 3b	0.07	0.00	0.05	0.03
H 4	0.01	0.02	0.39	0.39
H 5a	0.34	0.40	0.38	0.55
H 5b	0.24	0.10	0.24	0.11
H 8a	0.32	0.28	0.40	0.15
H 8b	0.60	0.44	0.74	0.18

H 11	0.15	0.77	0.20	0.76
H 13	0.39	0.61	0.43	0.58
H 14a	0.17	0.21	0.13	0.25
H 14b	0.48	0.52	0.39	0.53
H 16	0.29	0.45	0.21	0.14
H 18	0.00	0.05	0.03	0.13
H 19a	0.27	0.35	0.22	0.30
H 19b	0.36	0.34	0.37	0.35
H 21	0.23	0.37	0.24	0.33
H 23a	0.86	0.65	1.08	0.09
H 23b	0.28	0.11	0.56	1.11
H 25a-c	0.15	0.15	0.15	0.12
H 27a-c	0.05	0.07	0.09	0.05
H 28a-c	0.11	0.03	0.11	0.02
H 29a-c	0.20	0.04	0.22	0.18
H 30a-c	0.07	0.11	0.12	0.08
Average	0.24	0.26	0.30	0.28

Table S75. CMAE (corrected mean absolute error) values for the isomers of Zoaramine at the PCM/B3LYP/6-31G**//MMFF

	Absoluted Error Scaled		
	Isomer1	Isomer3	Isomer4
C 1	0.44	2.50	1.87
C 2	1.94	5.22	5.06
C 3	2.45	2.00	1.29
C 4	2.00	2.14	1.40
C 5	3.40	0.10	0.47
C 6	25.41	21.25	20.50
C 7	7.71	8.63	9.96
C 8	3.16	2.23	3.19
C 9	3.21	2.13	2.82
C 10	7.20	6.64	6.10
C 11	0.27	0.99	0.72
C 12	2.48	3.19	0.35
C 13	0.66	0.17	7.43
C 14	1.57	0.86	3.82
C 15	6.81	6.11	7.62
C 16	0.89	0.59	0.67
C 17	3.54	2.89	2.74
C 18	3.17	2.47	2.47
C 19	0.97	0.90	0.42
C 20	2.87	3.36	4.77
C 21	1.95	0.76	2.62
C 22	8.08	5.19	5.57
C 23	2.24	4.19	4.52
C 24	15.55	12.17	12.59
C 25	0.06	4.87	5.61
C 27	2.21	1.85	1.26
C 28	1.09	2.14	0.98
C 29	2.17	1.13	1.40
C 30	2.27	1.03	0.49
Average	3.99	3.71	4.09
H 1a	0.08	0.01	0.02
H 1b	0.70	0.45	0.43
H 2	0.11	0.03	0.09
H 3a	0.02	0.42	0.45
H 3b	0.20	0.08	0.08
H 4	0.01	0.36	0.35
H 5a	0.26	0.36	0.42
H 5b	0.14	0.25	0.27
H 8a	0.12	0.06	0.11
H 8b	0.24	0.66	0.62

H 11	0.06	0.11	0.64
H 13	0.13	0.21	0.59
H 14a	0.12	0.10	0.26
H 14b	0.13	0.18	0.47
H 16	0.16	0.28	0.45
H 18	0.04	0.02	0.01
H 19a	0.23	0.26	0.34
H 19b	0.25	0.28	0.29
H 21	0.16	0.18	0.28
H 23a	0.16	0.93	0.91
H 23b	0.68	0.36	0.25
H 25a-c	0.13	0.19	0.19
H 27a-c	0.07	0.12	0.17
H 28a-c	0.18	0.10	0.04
H 29a-c	0.15	0.20	0.02
H 30a-c	0.01	0.13	0.19
Average	0.18	0.24	0.31

Table S76. *u*/*dJ*-DP4 results of Zoarenone with AMBER 12 kJ/mol MAD 0.5 Å.


Settings		Type of data (shifts)			Default settings						Custom settings						Most Likely Isomers		
Default		Shielding tensors															Rank	Isomer	Probability
					TMS	σ	ν			TMS	σ	ν			1 st	22	100.00		
					H	31.830573	0.185	14.18		H	31.830573	0.185	14.18		2 nd	5	0.00		
					C	192.29325	2.306	11.38		C	192.29325	2.306	11.38		3 rd	6	0.00		
					J	-	0.992	3.06		J	-	0.992	3.06		4 th	30	0.00		
					Slope scaling J			0.9509		Slope scaling J			0.9509						
					Intercept scaling J			-0.1405		Intercept scaling J			-0.1405						
Isomer N ^o		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15			
DP4 (%)	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00			
	C	0.00	0.00	0.00	0.00	0.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00			
	H+C	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00			
	J	11.22	0.58	5.05	0.85	2.27	2.19	16.50	9.33	0.71	3.13	2.83	1.96	1.36	0.15	0.01			
	all data	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00			
 /pe	Exp	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15			
16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33		
0.00	0.00	0.00	0.00	0.00	99.96	0.01	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00			
0.00	0.00	0.00	0.00	0.00	0.00	99.67	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00			
0.00	0.00	0.00	0.00	0.00	0.00	100.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00			
2.21	8.02	3.21	2.59	0.96	0.24	2.40	0.91	15.93	0.93	0.62	1.54	1.95	0.01	0.26	0.04	0.06			
0.00	0.00	0.00	0.00	0.00	0.00	100.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00			
16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33		

Table S77. *u*/*dJ*-DP4 results of Zoarenone with MM3 12 kJ/mol MAD 0.5 Å.


Settings		Type of data (shifts)		Default settings						Custom settings						Most Likely Isomers			
Default		Shielding tensors														Rank	Isomer	Probability	
				H	31.830573	0.185	14.18			H	31.830573	0.185	14.18		1 st	22	100.00		
				C	192.29325	2.306	11.38			C	192.29325	2.306	11.38		2 nd	6	0.00		
				J	-	0.992	3.06			J	-	0.992	3.06		3 rd	5	0.00		
				Slope scaling J			0.9509			Slope scaling J			0.9509		4 th	13	0.00		
				Intercept scaling J			-0.1405			Intercept scaling J			-0.1405						
Isomer N°		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15			
DP4 (%)	H	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.23	0.01	0.00	0.00			
	C	0.00	0.00	0.00	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00			
	H+C	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00			
	J	4.31	0.05	2.21	0.33	9.31	9.77	7.56	8.30	0.15	9.14	4.56	11.97	0.71	0.04	0.13			
	all data	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00			
 /pe	Exp	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15			
16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35
0.00	0.00	0.00	0.00	0.00	99.26	0.44	0.00	0.00	0.00	0.00	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	99.96	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	100.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1.18	2.69	0.38	1.32	0.40	1.17	8.77	1.83	6.64	0.27	0.18	1.41	2.65	0.00	0.17	1.25	1.14	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	100.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35

Table S78. *u*/*dJ*-DP4 results of Zoarenone with MMFF 12 kJ/mol MAD 0.5 Å.

Settings		Type of data (shifts)		Default settings						Custom settings						Most Likely Isomers		
Default		Shielding tensors														Rank	Isomer	Probability
				TMS	σ	ν				TMS	σ	ν			1 ^o	22	99.98	
				H	31.830573	0.185	14.18			H	31.830573	0.185	14.18		2 ^o	6	0.02	
				C	192.29325	2.306	11.38			C	192.29325	2.306	11.38		3 ^o	5	0.00	
				J	-	0.992	3.06			J	-	0.992	3.06		4 ^o	11	0.00	
				Slope scaling J			0.9509			Slope scaling J			0.9509					
				Intercept scaling J			-0.1405			Intercept scaling J			-0.1405					
Isomer N ^o		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15		
DP4 (%)	H	0.00	0.01	0.00	0.00	0.00	0.02	0.87	0.00	0.00	0.00	0.00	0.33	0.00	0.00	0.00		
	C	0.00	0.00	0.00	0.00	0.00	0.44	0.24	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
	H+C	0.00	0.00	0.00	0.00	0.00	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
	J	5.45	0.82	6.06	0.18	5.14	3.47	14.11	13.01	0.10	9.52	3.29	5.09	0.63	0.00	0.02		
	all data	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
Type	Exp	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15		
16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34
0.00	0.00	0.00	0.00	0.00	91.69	6.68	0.00	0.00	0.00	0.00	0.00	0.38	0.00	0.00	0.00	0.00	0.00	
0.00	0.00	0.00	0.00	0.00	99.19	0.00	0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
0.00	0.00	0.00	0.00	0.00	99.97	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
0.69	2.86	0.79	2.66	0.50	0.21	5.04	0.79	13.17	0.18	0.09	2.63	3.23	0.00	0.03	0.15	0.08	0.00	
0.00	0.00	0.00	0.00	0.00	99.98	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34

Table S79. *i*/*d*J-DP4 results of Zoaramine with AMBER 12 kJ/mol MAD 0.5 Å.

Settings		Type of data (shifts)		Default settings						Custom settings						Most Likely Isomers		
Default		Shielding tensors			TMS	σ	ν				TMS	σ	ν			Rank	Isomer	Probability
				H	31.830573	0.185	14.18	H	31.830573	0.185	14.18					1 st	3	100.00
				C	192.29325	2.306	11.38	C	192.29325	2.306	11.38					2 nd	1	0.00
				J	-	0.992	3.06	J	-	0.992	3.06					3 rd	4	0.00
				Slope scaling J			0.9509	Slope scaling J			0.9509	Slope scaling J			0.9509	4 th	2	0.00
				Intercept scaling J			-0.1405	Intercept scaling J			-0.1405	Intercept scaling J			-0.1405			
Isomer N ^o		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15		
DP4 (%)	H	0.00	0.00	100.00	0.00	-	-	-	-	-	-	-	-	-	-	-		
	C	0.05	0.00	99.95	0.00	-	-	-	-	-	-	-	-	-	-	-		
	H+C	0.00	0.00	100.00	0.00	-	-	-	-	-	-	-	-	-	-	-		
	J	3.74	2.22	17.64	76.40	-	-	-	-	-	-	-	-	-	-	-		
	all data	0.00	0.00	100.00	0.00	-	-	-	-	-	-	-	-	-	-	-		
Type	Exp	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15		

Table S80. *i*/*d*J-DP4 results of Zoaramine with MM3 12 kJ/mol MAD 0.5 Å.

Settings		Type of data (shifts)		Default settings						Custom settings						Most Likely Isomers		
Default		Shielding tensors			TMS	σ	ν				TMS	σ	ν			Rank	Isomer	Probability
				H	31.830573	0.185	14.18	H	31.830573	0.185	14.18					1 st	1	100.00
				C	192.29325	2.306	11.38	C	192.29325	2.306	11.38					2 nd	2	0.00
				J	-	0.992	3.06	J	-	0.992	3.06					3 rd	3	0.00
				Slope scaling J			0.9509	Slope scaling J			0.9509	Slope scaling J			0.9509	4 th	4	0.00
				Intercept scaling J			-0.1405	Intercept scaling J			-0.1405	Intercept scaling J			-0.1405			
Isomer N ^o		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15		
DP4 (%)	H	99.48	0.52	0.00	0.00	-	-	-	-	-	-	-	-	-	-	-		
	C	78.71	0.00	21.29	0.00	-	-	-	-	-	-	-	-	-	-	-		
	H+C	100.00	0.00	0.00	0.00	-	-	-	-	-	-	-	-	-	-	-		
	J	86.89	13.05	0.05	0.01	-	-	-	-	-	-	-	-	-	-	-		
	all data	100.00	0.00	0.00	0.00	-	-	-	-	-	-	-	-	-	-	-		
Type	Exp	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15		

Table S81. *i*/*d*J-DP4 results of Zoaramine with MMFF 12 kJ/mol MAD 0.5 Å.

Settings		Type of data (shifts)		Default settings						Custom settings						Most Likely Isomers		
Default		Shielding tensors			TMS	σ	ν				TMS	σ	ν			Rank	Isomer	Probability
				H	31.830573	0.185	14.18	H	31.830573	0.185	14.18					1 st	1	100.00
				C	192.29325	2.306	11.38	C	192.29325	2.306	11.38					2 nd	2	0.00
				J	-	0.992	3.06	J	-	0.992	3.06					3 rd	3	0.00
				Slope scaling J			0.9509	Slope scaling J			0.9509	Slope scaling J			0.9509	4 th	-	-
				Intercept scaling J			-0.1405	Intercept scaling J			-0.1405	Intercept scaling J			-0.1405			
Isomer N ^o		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15		
DP4 (%)	H	100.00	0.00	0.00	-	-	-	-	-	-	-	-	-	-	-	-		
	C	1.57	98.41	0.03	-	-	-	-	-	-	-	-	-	-	-	-		
	H+C	100.00	0.00	0.00	-	-	-	-	-	-	-	-	-	-	-	-		
	J	99.76	0.15	0.09	-	-	-	-	-	-	-	-	-	-	-	-		
	all data	100.00	0.00	0.00	-	-	-	-	-	-	-	-	-	-	-	-		
Type	Exp	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15		