

Doubling the Power of DP4 for Computational Structure Elucidation

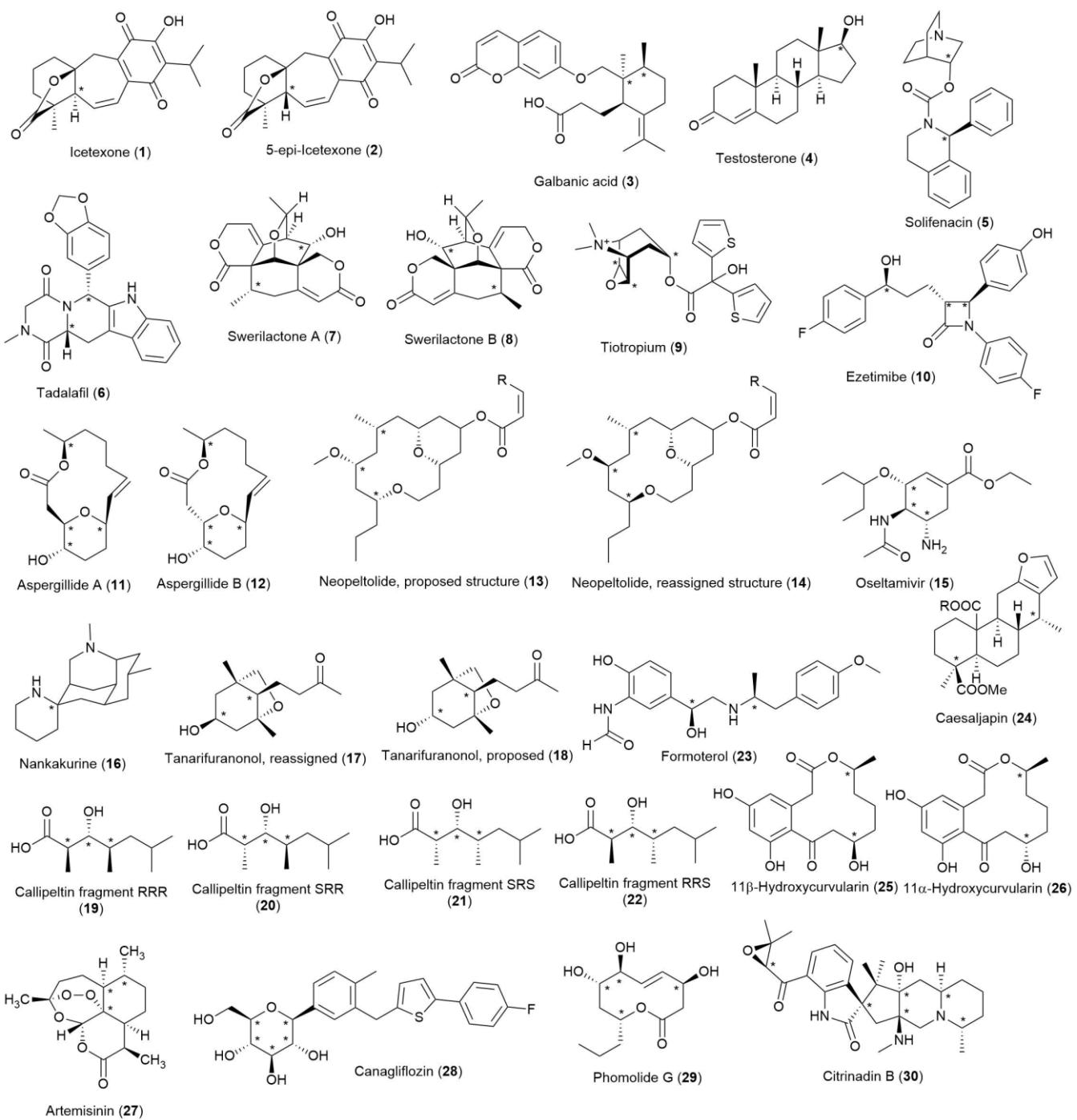
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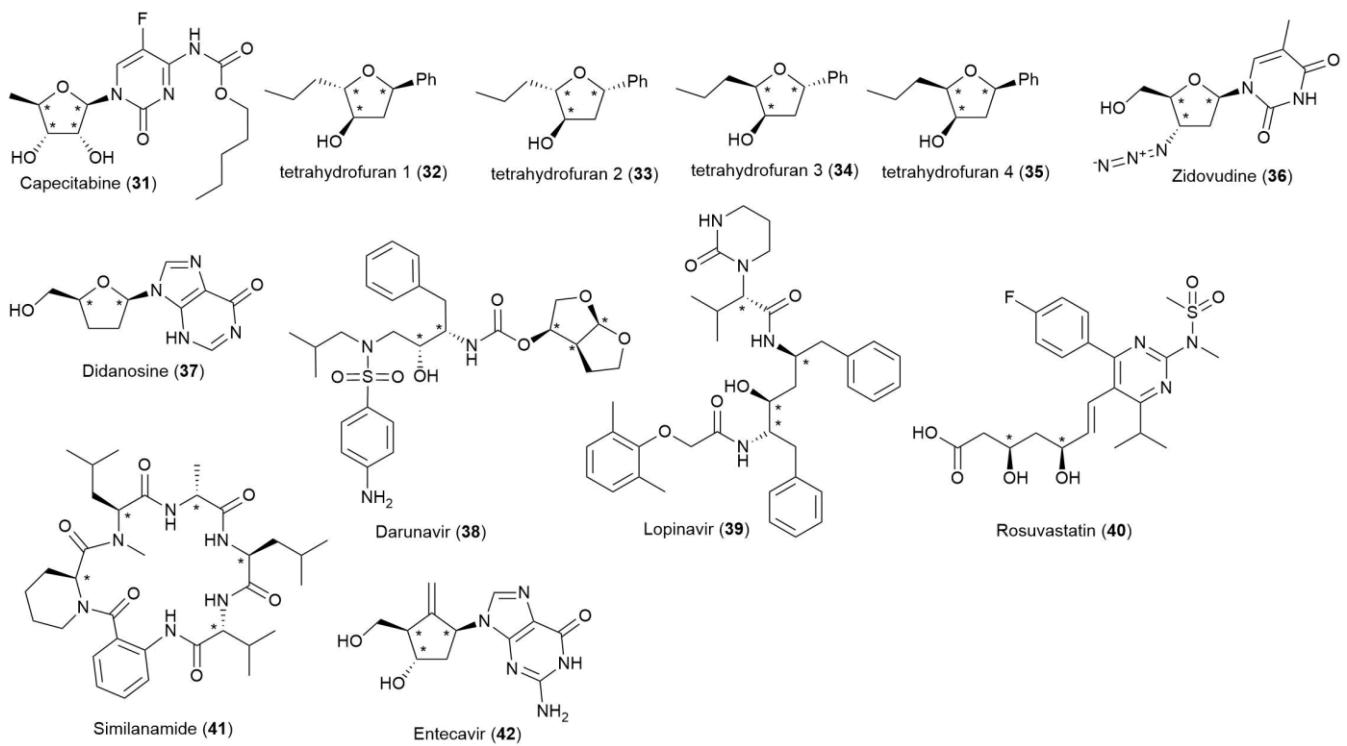
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S-1. Compounds used in the study

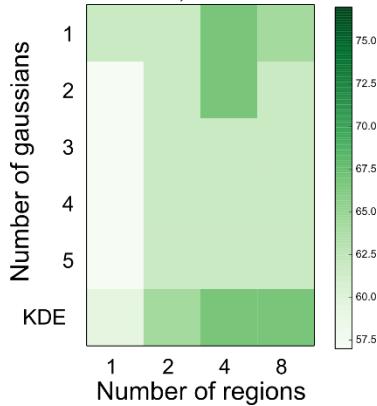




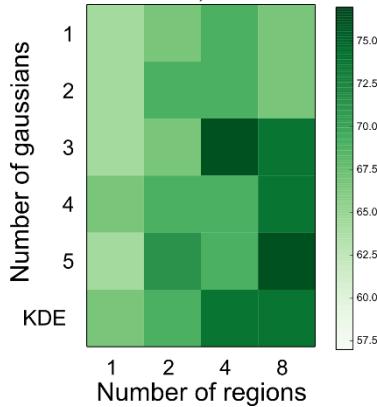
S-2. Statistical model scans for the various DFT conditions

Graphs of in sample performance, in percent, showing dependence on the number of spectral regions and the number of Gaussian functions used to model energies in each region

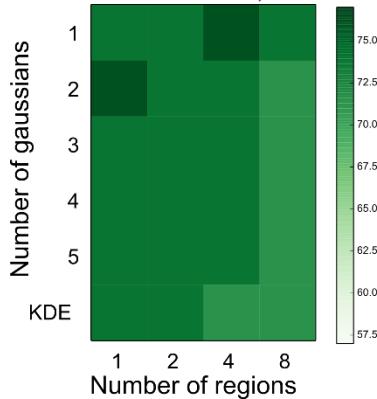
S-2.1 B3LYP, 6-31G** for shifts and energies



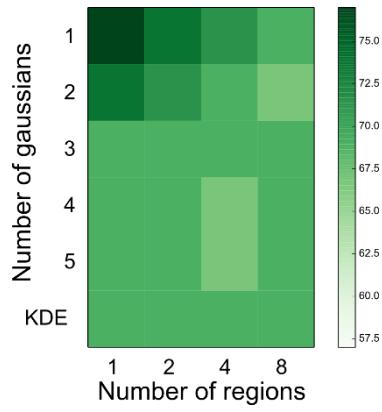
S-2.2 M06-2X, 6-31G** for shifts and energies



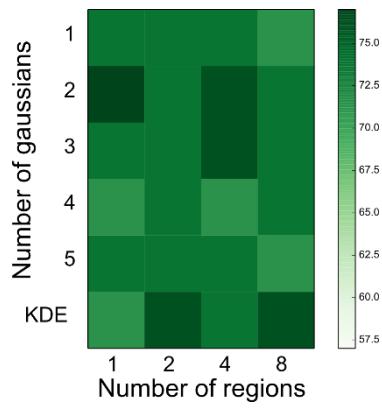
S-2.3 mPW1PW91, 6-311G* for shifts and energies



S-2.4 mPW1PW91, 6-311G* for shifts, B3LYP, 6-31G** for energies



S-2.5 mPW1PW91, 6-311G* for shifts, M06-2X, 6-31G** for energies



S-3. Cross-validated statistical models to be used with the top performing DFT conditions

All of the parameters are for Gaussian functions, all values in ppm

S-3.1. mPW1PW91, 6-311G*, used for both shifts and energies

For carbon NMR - 1 region spanning all of the spectrum, composed of sum of 2 gaussians:

Mean1: 0.099563

StDev1: 2.716966

Mean2: -0.043505

StDev2: 1.380371

For proton NMR - 1 region spanning all of the spectrum, composed of sum of 2 gaussians:

Mean1: 0.002012

StDev1: 0.100944

Mean2: 0.002164

StDev2: 0.255732

S-3.2. mPW1PW91, 6-311G* for shifts, B3LYP, 6-31G for energies**

For carbon NMR - 1 region spanning all of the spectrum, composed of 1 Gaussian:

Mean1: -0.081750

StDev1: 1.910708

For proton NMR - 1 region spanning all of the spectrum, composed of 1 Gaussian:

Mean1: 0.003744

StDev1: 0.154878

S-3.3. mPW1PW91, 6-311G* for shifts, M06-2X, 6-31G for energies**

For carbon NMR - 1 region spanning all of the spectrum, composed of sum of 2 gaussians:

Mean1: -0.012304

StDev1: 2.821282

Mean2: 0.000950

StDev2: 1.361471

For proton NMR - 1 region spanning all of the spectrum, composed of sum of 2 gaussians:

Mean1: -0.003345

StDev1: 0.108534

Mean2: 0.001826

StDev2: 0.259742

S-4. Per compound overview of structure elucidation in-sample results from the top 4 performing workflows

Columns:

1. Compound name;
 2. Probability of the actual structure being the correct one as given by the denoted statistical model;
 3. Rank – 1, if the correct structure had the highest relative probability, 2 – if it was the second most likely, etc.;
 4. C Corr – Pearson correlation coefficient between calculated and measured C₁₃ chemical shifts;
 5. H Corr – Pearson correlation coefficient between calculated and measured H₁ chemical shifts;
 6. Carbon and Proton MAE – mean absolute errors between the measured and uncorrected calculated chemical shifts;
 7. Carbon and Proton CMAE – mean absolute errors between the measured and calculated chemical shifts after linear internal correction;

Color schemes were chosen so as to facilitate not only comparison between a particular parameter within one workflow's results, but among all four. So, a dark green shaded cell represents a good result both in the particular set and overall.

In sample data	Shifts	B3LYP	6-	En-	B3LYP	6-	Pro-	Car-	Pro-
			31G**			31G**		bon	ton
Compounds	DP4 prob.	Rank	C Corr	H Corr	MAE	MAE	CMAE	CMAE	CMAE
Ezetimibe (10)	1.7	2	0.9980	0.9954	4.32	0.21	2.11	0.21	0.21
Formoterol (23)	81.9	1	0.9981	0.9974	4.56	0.20	2.10	0.13	0.13
Rosuvastatin (40)	0.3	2	0.9976	0.9899	3.66	0.26	3.24	0.24	0.24
Solifenacin (5)	99.9	1	0.9996	0.9986	3.33	0.16	1.03	0.09	0.09
Tadalafil (6)	38.8	2	0.9975	0.9938	17.66	0.23	2.18	0.15	0.15
Testosterone (4)	100	1	0.9997	0.9947	3.06	0.09	0.91	0.09	0.09
Tiotropium (9)	14.7	2	0.9977	0.9948	2.97	0.18	2.60	0.18	0.18
Capecitabine (31)	0.4	2	0.9989	0.9931	3.81	0.17	1.74	0.16	0.16
Oseltamivir (15)	0.1	3	0.9990	0.9828	2.47	0.20	1.59	0.22	0.22
Swerilactone A (7)	100	1	0.9994	0.9969	2.22	0.11	1.40	0.10	0.10
Swerilactone B (8)	100	1	0.9994	0.9879	2.36	0.17	1.40	0.15	0.15
Tanarifuranonol, reass. (17)	99.9	1	0.9998	0.9977	1.43	0.07	0.70	0.05	0.05
Tanarifuranonol, proposed (18)	97.5	1	0.9997	0.9966	1.42	0.07	0.94	0.07	0.07
Galbanic acid (3)	100	1	0.9986	0.9976	3.25	0.16	2.29	0.12	0.12
Icetexone (1)	100	1	0.9993	0.9969	3.08	0.13	1.81	0.11	0.11
5-epi-Icetexone (2)	100	1	0.9998	0.9957	2.40	0.13	1.04	0.13	0.13
Tetrahydrofuran 1 (32)	92.5	1	0.9992	0.9992	2.87	0.10	1.46	0.07	0.07
Tetrahydrofuran 2 (33)	39.5	2	0.9989	0.9982	2.80	0.12	1.77	0.08	0.08
Tetrahydrofuran 3 (34)	4.1	2	0.9991	0.9968	2.93	0.13	1.78	0.12	0.12
Tetrahydrofuran 4 (35)	99.1	1	0.9987	0.9980	2.68	0.14	1.83	0.11	0.11
Artemisinin (27)	100	1	0.9996	0.9969	2.39	0.08	0.93	0.07	0.07
Didanosine (37)	90	1	0.9975	0.9967	4.37	0.20	2.76	0.13	0.13
Zidovudine (36)	0	3	0.9950	0.9836	6.09	0.30	3.80	0.28	0.28
Entecavir (42)	100	1	0.9972	0.9945	4.51	0.35	2.52	0.14	0.14
Canagliflozin (28)	2.6	4	0.9987	0.9939	2.37	0.24	1.65	0.17	0.17
Similanamide (41)	0	3	0.9982	0.9895	3.17	0.24	2.77	0.22	0.22
Lopinavir (39)	0	3	0.9988	0.9957	3.26	0.28	2.15	0.16	0.16
CitrinadinB (30)	0	5	0.9984	0.9849	2.54	0.36	2.15	0.28	0.28
Darunavir (38)	0	6	0.9990	0.9914	2.89	0.23	1.55	0.21	0.21
Nankakurine (16)	100	1	0.9982	0.9882	1.07	0.08	0.61	0.07	0.07
Aspergillide A (11)	100	1	0.9995	0.9964	1.79	0.13	1.22	0.11	0.11
Aspergillide B (12)	100	1	0.9997	0.9938	1.96	0.26	1.01	0.12	0.12
Callipeltin frag. RRR (19)	0	4	0.9990	0.9672	2.65	0.17	1.75	0.19	0.19
Callipeltin frag. SRR (20)	27.4	2	0.9994	0.9880	2.10	0.12	1.51	0.12	0.12
Callipeltin frag. SRS (21)	99.9	1	0.9993	0.9940	2.40	0.09	1.52	0.08	0.08
Callipeltin frag. RRS (22)	1.1	3	0.9982	0.9885	3.48	0.12	2.23	0.12	0.12
Neopeltolide, proposed (13)	100	1	0.9990	0.9929	1.85	0.10	1.16	0.11	0.11
Neopeltolide, reass. (14)	100	1	0.9993	0.9902	1.73	0.14	0.88	0.14	0.14
Caesaljapin (24)	100	1	0.9993	0.9963	3.34	0.11	1.47	0.09	0.09
11 β -hydroxycurvularin (25)	0	2	0.9967	0.9860	4.36	0.22	3.86	0.22	0.22
11 α -hydroxycurvularin (26)	100	1	0.9983	0.9821	3.11	0.23	2.83	0.22	0.22
Phomolide G (29)	99.7	1	0.9997	0.9962	1.54	0.23	0.86	0.09	0.09
Average			0.9987	0.9926	3.24	0.17	1.79	0.14	
Percentage of correct identification				57.1					

In sample data	Shifts	mPW1	6-	En- ergy	mPW1	6-311G*		
		PW91	311G*		PW91	Car- bon MAE	Pro- ton MAE	Car- bon CMAE
Compounds	Gauss- ian prob.	Rank	C Corr	H Corr				
Ezetimibe (10)	38.5	2	0.9985	0.9966	5.84	0.20	1.73	0.18
Formoterol (23)	100	1	0.9984	0.9974	3.93	0.23	1.94	0.13
Rosuvastatin (40)	100	1	0.9986	0.9941	5.08	0.20	2.31	0.20
Solifenacin (5)	100	1	0.9996	0.9986	4.21	0.17	1.10	0.09
Tadalafil (6)	73.5	1	0.9980	0.9948	5.12	0.17	1.90	0.14
Testosterone (4)	100	1	0.9997	0.9968	4.34	0.09	0.96	0.06
Tiotropium (9)	33.6	3	0.9982	0.9938	6.92	0.18	2.08	0.18
Capecitabine (31)	4.6	2	0.9994	0.9915	5.21	0.21	1.48	0.19
Oseltamivir (15)	100	1	0.9993	0.9839	4.21	0.18	1.41	0.18
Swerilactone A (7)	100	1	0.9995	0.9959	6.24	0.11	1.28	0.11
Swerilactone B (8)	100	1	0.9995	0.9853	6.49	0.17	1.33	0.17
Tanarifuranonol, reass. (17)	82.6	1	0.9997	0.9962	3.69	0.08	0.90	0.06
Tanarifuranonol, proposed (18)	99	1	0.9997	0.9958	3.73	0.08	1.03	0.07
Galbanic acid (3)	99.8	1	0.9988	0.9982	5.16	0.13	2.05	0.10
Icetexone (1)	100	1	0.9992	0.9976	4.84	0.12	1.68	0.10
5-epi-Icetexone (2)	100	1	0.9997	0.9977	4.29	0.10	0.95	0.10
Tetrahydrofuran 1 (32)	98.8	1	0.9994	0.9994	4.03	0.12	1.31	0.07
Tetrahydrofuran 2 (33)	79	1	0.9991	0.9979	4.05	0.15	1.55	0.10
Tetrahydrofuran 3 (34)	37	2	0.9994	0.9970	4.03	0.15	1.32	0.11
Tetrahydrofuran 4 (35)	92.5	1	0.9991	0.9982	4.27	0.18	1.52	0.10
Artemisinin (27)	99.9	1	0.9997	0.9956	4.27	0.09	0.82	0.09
Didanosine (37)	52.5	1	0.9983	0.9959	4.83	0.24	2.32	0.15
Zidovudine (36)	0	3	0.9972	0.9847	8.96	0.32	2.84	0.27
Entecavir (42)	100	1	0.9971	0.9942	7.19	0.42	2.39	0.14
Canagliflozin (28)	99.5	1	0.9992	0.9935	6.28	0.33	1.12	0.18
Similanamide (41)	0	3	0.9983	0.9903	5.33	0.23	2.57	0.22
Lopinavir (39)	0	3	0.9994	0.9947	4.98	0.37	1.55	0.17
CitrinadinB (30)	0	5	0.9988	0.9835	4.40	0.34	1.81	0.29
Darunavir (38)	0	6	0.9996	0.9914	4.52	0.23	1.00	0.21
Nankakurine (16)	98.5	1	0.9980	0.9915	1.77	0.06	0.61	0.06
Aspergillide A (11)	100	1	0.9990	0.9962	4.14	0.14	1.55	0.10
Aspergillide B (12)	100	1	0.9995	0.9938	4.96	0.30	1.15	0.12
Callipeltin frag. RRR (19)	0.6	3	0.9995	0.9830	2.78	0.14	1.26	0.12
Callipeltin frag. SRR (20)	49.7	1	0.9996	0.9925	2.38	0.13	1.15	0.09
Callipeltin frag. SRS (21)	62.1	1	0.9994	0.9976	2.38	0.07	1.34	0.05
Callipeltin frag. RRS (22)	80	1	0.9991	0.9968	2.90	0.09	1.65	0.06
Neopeltolide, proposed (13)	100	1	0.9988	0.9924	3.37	0.14	1.45	0.12
Neopeltolide, reass. (14)	99.7	1	0.9989	0.9899	3.30	0.17	1.27	0.14
Caesaljapin (24)	100	1	0.9995	0.9968	4.53	0.13	1.29	0.10
11 β -hydroxycurvularin (25)	0	2	0.9973	0.9848	5.85	0.25	3.60	0.24
11 α -hydroxycurvularin (26)	100	1	0.9984	0.9839	5.35	0.21	2.76	0.22
Phomolide G (29)	99.2	1	0.9995	0.9937	5.18	0.32	1.34	0.11
Average			0.9990	0.9934	4.65	0.18	1.59	0.14
Percentage of correct identification			73.8					

In sample data	Shifts	mPW1	6-	En-	B3LYP	6-	En-	
		PW91	311G*			Pro-	Car-	Pro-
Compounds	2gaus prob.	Rank	C Corr	H Corr	Car-bon MAE	Pro-ton MAE	Car-bon CMAE	Pro-ton CMAE
Ezetimibe (10)	23.2	2	0.9984	0.9964	5.82	0.20	1.74	0.18
Formoterol (23)	99.3	1	0.9986	0.9979	3.90	0.21	1.80	0.13
Rosuvastatin (40)	75.1	1	0.9983	0.9884	5.23	0.27	2.54	0.26
Solifenacin (5)	98.9	1	0.9996	0.9987	4.21	0.17	1.09	0.09
Tadalafil (6)	79.6	1	0.9980	0.9948	5.12	0.17	1.90	0.14
Testosterone (4)	100	1	0.9997	0.9967	4.34	0.09	0.96	0.06
Tiotropium (9)	11.4	3	0.9982	0.9939	6.93	0.18	2.09	0.18
Capecitabine (31)	61	1	0.9994	0.9915	5.21	0.21	1.49	0.18
Oseltamivir (15)	99.7	1	0.9993	0.9836	4.29	0.18	1.44	0.18
Swerilactone A (7)	100	1	0.9995	0.9959	6.24	0.11	1.28	0.11
Swerilactone B (8)	100	1	0.9995	0.9853	6.49	0.17	1.33	0.17
Tanarifuranonol, reass. (17)	86.7	1	0.9997	0.9961	3.69	0.08	0.91	0.06
Tanarifuranonol, proposed (18)	98.6	1	0.9997	0.9957	3.69	0.08	1.00	0.07
Galbanic acid (3)	99.7	1	0.9988	0.9982	5.16	0.14	2.05	0.10
Icetexone (1)	100	1	0.9992	0.9974	4.86	0.12	1.74	0.11
5-epi-Icetexone (2)	100	1	0.9997	0.9977	4.28	0.10	0.95	0.10
Tetrahydrofuran 1 (32)	97.8	1	0.9993	0.9994	4.08	0.12	1.31	0.07
Tetrahydrofuran 2 (33)	72.3	1	0.9991	0.9981	4.05	0.14	1.55	0.10
Tetrahydrofuran 3 (34)	36.4	2	0.9994	0.9970	4.05	0.14	1.31	0.11
Tetrahydrofuran 4 (35)	83.3	1	0.9991	0.9981	4.33	0.19	1.54	0.10
Artemisinin (27)	99.9	1	0.9997	0.9956	4.27	0.09	0.82	0.09
Didanosine (37)	56.1	1	0.9983	0.9959	4.83	0.24	2.31	0.14
Zidovudine (36)	0	3	0.9972	0.9848	8.98	0.32	2.87	0.27
Entecavir (42)	99.9	1	0.9970	0.9942	7.19	0.42	2.39	0.14
Canagliflozin (28)	99	1	0.9992	0.9933	6.30	0.33	1.13	0.18
Similanamide (41)	0	3	0.9983	0.9905	5.32	0.23	2.54	0.22
Lopinavir (39)	0	3	0.9993	0.9958	5.07	0.35	1.64	0.16
CitrinadinB (30)	0.9	4	0.9988	0.9835	4.40	0.34	1.81	0.29
Darunavir (38)	0.1	5	0.9996	0.9917	4.55	0.23	1.00	0.20
Nankakurine (16)	99.9	1	0.9982	0.9929	1.79	0.05	0.55	0.05
Aspergillide A (11)	100	1	0.9990	0.9961	4.22	0.14	1.58	0.10
Aspergillide B (12)	100	1	0.9995	0.9938	4.96	0.30	1.15	0.12
Callipeltin frag. RRR (19)	0.1	4	0.9995	0.9709	2.94	0.17	1.22	0.16
Callipeltin frag. SRR (20)	64.8	1	0.9996	0.9911	2.38	0.13	1.15	0.09
Callipeltin frag. SRS (21)	97.4	1	0.9994	0.9973	2.40	0.07	1.35	0.05
Callipeltin frag. RRS (22)	4.3	3	0.9987	0.9912	3.30	0.11	2.03	0.10
Neopektolide, proposed (13)	100	1	0.9988	0.9922	3.38	0.14	1.46	0.12
Neopektolide, reass. (14)	98.7	1	0.9989	0.9907	3.32	0.17	1.29	0.13
Caesaljapin (24)	100	1	0.9995	0.9968	4.54	0.13	1.29	0.10
11 β -hydroxycurvularin (25)	0	2	0.9973	0.9850	5.83	0.25	3.57	0.24
11 α -hydroxycurvularin (26)	100	1	0.9984	0.9834	5.37	0.21	2.78	0.22
Phomolide G (29)	98.7	1	0.9995	0.9941	5.22	0.32	1.35	0.11
Average			0.9990	0.9929	4.68	0.19	1.60	0.14
Percentage of correct identification			73.8					

In sample data	Shifts	mPW1	6-	En-	M06-	6-	Pro-	Car-	Pro-	
		PW91	311G*		2X	31G**				
Compounds	2gaus.	Rank	C	H	Car-	Pro-	ton	ton	CMAE	CMAE
	prob.		Corr	Corr	MAE	MAE	ton	ton		
Ezetimibe (10)	97.7	1	0.9984	0.9963	5.81	0.20	1.76	0.18		
Formoterol (23)	52.4	1	0.9987	0.9912	4.03	0.26	1.67	0.25		
Rosuvastatin (40)	64.7	1	0.9983	0.9878	5.24	0.27	2.56	0.26		
Solifenacin (5)	66.2	1	0.9996	0.9981	4.30	0.17	1.13	0.10		
Tadalafil (6)	80.1	1	0.9980	0.9948	5.12	0.17	1.90	0.14		
Testosterone (4)	100	1	0.9997	0.9968	4.34	0.09	0.96	0.06		
Tiotropium (9)	13.1	3	0.9982	0.9937	6.92	0.18	2.07	0.18		
Capecitabine (31)	57.1	1	0.9994	0.9915	5.22	0.22	1.50	0.18		
Oseltamivir (15)	91.3	1	0.9992	0.9833	4.20	0.20	1.55	0.20		
Swerilactone A (7)	100	1	0.9995	0.9958	6.24	0.11	1.29	0.11		
Swerilactone B (8)	100	1	0.9995	0.9853	6.49	0.17	1.33	0.17		
Tanarifuranonol, reass. (17)	90.1	1	0.9998	0.9967	3.61	0.08	0.83	0.06		
Tanarifuranonol, proposed (18)	97.6	1	0.9998	0.9951	3.55	0.09	0.90	0.08		
Galbanic acid (3)	99.8	1	0.9988	0.9981	5.17	0.14	2.02	0.10		
Icetexone (1)	100	1	0.9994	0.9979	4.82	0.11	1.56	0.10		
5-epi-Icetexone (2)	100	1	0.9997	0.9977	4.31	0.10	0.95	0.10		
Tetrahydrofuran 1 (32)	93.5	1	0.9994	0.9991	4.35	0.16	1.21	0.08		
Tetrahydrofuran 2 (33)	56.6	1	0.9991	0.9981	3.91	0.15	1.49	0.10		
Tetrahydrofuran 3 (34)	43	2	0.9994	0.9971	3.85	0.15	1.27	0.10		
Tetrahydrofuran 4 (35)	94.2	1	0.9991	0.9982	4.20	0.19	1.50	0.10		
Artemisinin (27)	99.9	1	0.9997	0.9956	4.27	0.09	0.82	0.09		
Didanosine (37)	67.4	1	0.9983	0.9960	4.82	0.24	2.30	0.15		
Zidovudine (36)	0	4	0.9971	0.9839	9.04	0.33	2.92	0.28		
Entecavir (42)	99.7	1	0.9971	0.9942	7.18	0.41	2.39	0.14		
Canagliflozin (28)	99.4	1	0.9993	0.9932	6.26	0.33	1.05	0.18		
Similanamide (41)	0	3	0.9983	0.9900	5.32	0.24	2.62	0.23		
Lopinavir (39)	0	4	0.9990	0.9960	5.24	0.32	1.90	0.16		
CitrinadinB (30)	6.3	5	0.9988	0.9835	4.40	0.34	1.81	0.29		
Darunavir (38)	1.4	5	0.9996	0.9930	4.64	0.20	1.04	0.18		
Nankakurine (16)	99.9	1	0.9981	0.9925	1.78	0.05	0.57	0.05		
Aspergillide A (11)	100	1	0.9990	0.9963	3.94	0.14	1.54	0.10		
Aspergillide B (12)	100	1	0.9993	0.9932	5.28	0.31	1.36	0.13		
Callipeltin frag. RRR (19)	4.3	2	0.9996	0.9889	2.83	0.13	1.08	0.11		
Callipeltin frag. SRR (20)	44.9	1	0.9996	0.9915	2.36	0.14	1.15	0.09		
Callipeltin frag. SRS (21)	77.8	1	0.9994	0.9971	2.35	0.08	1.32	0.05		
Callipeltin frag. RRS (22)	75.3	1	0.9992	0.9959	2.88	0.10	1.64	0.06		
Neopektolide, proposed (13)	100	1	0.9983	0.9919	2.91	0.15	1.56	0.12		
Neopektolide, reass. (14)	98.5	1	0.9989	0.9908	3.08	0.18	1.29	0.13		
Caesaljapin (24)	100	1	0.9995	0.9968	4.52	0.13	1.29	0.10		
11 β -hydroxycurvularin (25)	0.7	2	0.9973	0.9914	5.46	0.20	3.59	0.20		
11 α -hydroxycurvularin (26)	82.7	1	0.9983	0.9818	5.45	0.22	2.83	0.23		
Phomolide G (29)	99.1	1	0.9995	0.9947	5.17	0.32	1.34	0.10		
Average			0.9990	0.9934	4.64	0.19	1.59	0.14		
Percentage of correct identification				78.6						

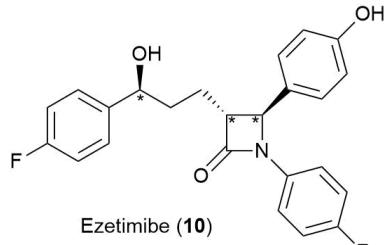
S-5. Per compound overview of structure elucidation cross-validation results from the top 4 performing workflows

Columns:

1. Compound name;
2. Probability of the actual structure being the correct one as given by the denoted statistical model;
3. Rank – 1, if the correct structure had the highest relative probability, 2 – if it was the second most likely, etc.;

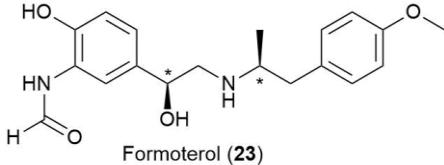
Shifts	B3LYP	6-31G**	mPW1 PW91	6-311G*	mPW1 PW91	6-311G*	mPW1 PW91	6-311G*
Energy	B3LYP	6-31G**	mPW1 PW91	6-311G*	B3LYP	6-31G**	M06-2X	6-31G**
Compounds	DP4 prob.	Rank	Gauss-ian prob.	Rank	2gaus prob.	Rank	2gaus. prob.	Rank
Ezetimibe (10)	1.7	2	38.4	2	23	2	98	1
Formoterol (23)	81.9	1	100	1	99.1	1	64.6	1
Rosuvastatin (40)	0.3	2	100	1	74.1	1	67	1
Solifenacin (5)	99.9	1	100	1	98.9	1	65.9	1
Tadalafil (6)	38.8	2	71.1	1	65.3	1	76.3	1
Testosterone (4)	100	1	100	1	100	1	100	1
Tiotropium (9)	14.7	2	32.7	2	15	2	12.9	3
Capecitabine (31)	0.4	2	4.5	2	61.8	2	57.1	1
Oseltamivir (15)	0.1	3	100	1	99.7	1	92.3	1
Swerilactone A (7)	100	1	100	1	100	1	100	1
Swerilactone B (8)	100	1	100	1	100	1	100	1
Tanarifuranonol, reass. (17)	99.9	1	82.1	1	85.5	1	89.8	1
Tanarifuranonol, proposed (18)	97.5	1	98.9	1	98.5	1	97.6	1
Galbanic acid (3)	100	1	99.8	1	99.7	1	99.9	1
Icetexone (1)	100	1	100	1	100	1	100	1
5-epi-Icetexone (2)	100	1	100	1	100	1	100	1
Tetrahydrofuran 1 (32)	92.5	1	98.7	1	97.7	1	93.4	1
Tetrahydrofuran 2 (33)	39.5	2	79	1	71.8	1	56.5	1
Tetrahydrofuran 3 (34)	4.1	2	36.4	2	36.3	2	42.3	2
Tetrahydrofuran 4 (35)	99.1	1	92.5	1	83.5	1	94.1	1
Artemisinin (27)	100	1	99.9	1	99.9	1	99.9	1
Didanosine (37)	90	1	48.9	2	54.5	2	67.8	1
Zidovudine (36)	0	3	0	2	0	2	0	4
Entecavir (42)	100	1	100	1	99.8	1	99.7	1
Canagliflozin (28)	2.6	4	99.6	1	98.8	1	99.4	1
Similanamide (41)	0	3	0	3	0	3	0	3
Lopinavir (39)	0	3	0	3	0	3	0	3
CitrinadinB (30)	0	5	0	5	0.4	5	4.4	5
Darunavir (38)	0	6	0	5	0	5	1.3	5
Nankakurine (16)	100	1	98.1	1	99.9	1	99.9	1
Aspergillide A (11)	100	1	100	1	100	1	100	1
Aspergillide B (12)	100	1	100	1	100	1	100	1
Callipeltin frag. RRR (19)	0	4	0.7	3	0.1	3	4.2	2
Callipeltin frag. SRR (20)	27.4	2	49.5	1	64.7	1	45	1
Callipeltin frag. SRS (21)	99.9	1	61.7	1	97.4	1	77.8	1
Callipeltin frag. RRS (22)	1.1	3	79.5	1	4.2	1	75.1	1
Neopeltolide, proposed (13)	100	1	100	1	100	1	100	1
Neopeltolide, reass. (14)	100	1	99.6	1	98.6	1	98.4	1
Caesalapin (24)	100	1	100	1	100	1	100	1
11 β -hydroxycurvularin (25)	0	2	0	2	0	2	0.4	2
11 α -hydroxycurvularin (26)	100	1	100	1	100	1	84	1
Phomolide G (29)	99.7	1	99.2	1	98.8	1	99.1	1
Percentage of correct identification	57.1		71.4		73.8		78.6	

S-6. Per compound detailed DP4 results from the top 4 performing workflows



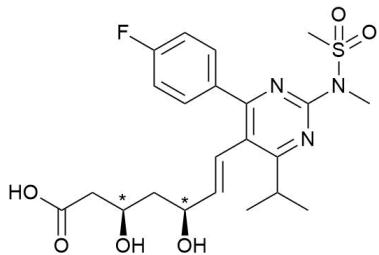
	Shifts	En-	Shifts	En-	Shifts	En-	Shifts	En-
	Func.	B3LYP	B3LYP	mPW1	mPW1	mPW1	mPW1	M06-
	Basis	6-	6-	PW91	PW91	PW91	PW91	PW91
	s.	31G**	31G**	6-	6-	6-	6-	6-
	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.
Ezetimibe (10)								
Carbon shifts	24.50	27.88	22.20	28.25	23.41	28.11	23.38	27.88
	36.36	42.45	38.13	42.92	37.92	42.99	38.08	43.06
	59.40	62.29	59.83	64.52	59.28	64.45	59.27	64.52
	59.58	65.06	62.87	66.83	61.56	66.81	61.60	66.82
	71.05	71.03	69.40	73.75	68.41	73.46	68.17	73.21
	114.64	111.20	113.34	119.92	114.06	119.87	114.03	119.81
	115.71	109.17	111.11	117.39	111.56	117.40	111.58	117.41
	115.79	112.73	115.01	121.44	115.57	121.46	115.60	121.47
	118.22	114.59	117.05	123.62	117.72	123.65	117.76	123.68
	127.50	123.64	126.94	133.35	127.34	133.36	127.36	133.29
	127.52	124.86	128.28	134.76	128.73	134.75	128.72	134.76
	127.88	130.65	134.62	140.62	134.54	140.61	134.52	140.58
	133.98	128.03	131.74	138.19	132.13	138.19	132.12	138.17
	142.14	140.11	144.96	150.68	144.48	150.71	144.50	150.80
	157.42	147.98	153.57	160.63	154.32	160.65	154.31	160.67
	158.00	153.95	160.10	165.72	159.35	165.75	159.35	165.78
	161.02	155.79	162.12	167.88	161.49	167.83	161.41	167.75
	167.33	160.04	166.77	172.62	166.18	172.76	166.28	172.94
Proton shifts	1.73	1.92	1.87	2.01	1.85	1.97	1.82	1.98
	1.73	1.47	1.42	1.62	1.46	1.58	1.43	1.58
	1.73	1.67	1.62	1.83	1.66	1.84	1.69	1.82
	1.83	2.28	2.23	2.27	2.11	2.29	2.14	2.32
	3.09	3.01	2.95	3.10	2.95	3.10	2.95	3.09
	4.50	4.85	4.78	4.95	4.81	4.95	4.81	4.95
	4.81	4.58	4.50	4.74	4.59	4.73	4.59	4.74
	6.76	6.84	6.74	6.89	6.76	6.89	6.76	6.89
	7.11	6.98	6.88	7.03	6.90	7.02	6.90	7.02
	7.13	7.00	6.91	7.02	6.89	7.02	6.90	7.03
	7.18	7.39	7.28	7.40	7.28	7.40	7.28	7.40
	7.22	7.56	7.45	7.49	7.36	7.49	7.36	7.49
	7.32	7.60	7.50	7.64	7.51	7.63	7.51	7.63
C MAE	4.32	2.11	5.84	1.73	5.82	1.74	5.81	1.76
H MAE	0.21	0.21	0.20	0.18	0.20	0.18	0.20	0.18
C CorrCoef	0.9980		0.9985		0.9984		0.9984	
H CorrCoef	0.9954		0.9966		0.9964		0.9963	
PROBABILITIES								
DP4 combined	1.7%		10.6%		38.4%		99.9%	
DP4 C only	9.3%		14.7%		24.2%		12.5%	
DP4 H only	2.9%		25.1%		34.6%		100.0%	
Gaussian combined	10.1%		38.5%		57.9%		99.9%	
Gaussian C only	8.4%		14.2%		18.9%		6.1%	
Gaussian H only	11.7%		48.4%		45.2%		100.0%	
KDE combined	2.0%		8.4%		27.7%		98.5%	
KDE C only	25.8%		22.7%		35.7%		32.8%	
KDE H only	3.3%		19.9%		33.4%		96.3%	

RKDE combined	0.3%	2.2%	8.8%	96.0%	
RKDE C only	18.1%	27.9%	43.8%	31.0%	
RKDE H only	1.0%	4.7%	8.4%	85.5%	
URKDE combined	23.7%	83.0%	77.8%	97.9%	
URKDE C only	29.4%	44.2%	50.0%	10.5%	
URKDE H only	9.6%	54.8%	45.6%	98.7%	
2gaus combined	2.2%	4.4%	23.2%	97.7%	
2gaus C only	23.7%	19.0%	27.8%	21.2%	
2gaus H only prob.	4.3%	13.0%	33.2%	97.4%	



	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
	B3LYP	B3LYP	mPW1 PW91	mPW1 PW91	mPW1 PW91	B3LYP	mPW1 PW91	M06- 2X
Formoterol	Func.	B3LYP	6-	6-	6-	6-	6-	6-
	Basis	31G**	31G**	311G*	311G*	311G*	31G**	31G**
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	
42.00	45.26	42.66	46.68	42.76	46.32	42.66	41.30	41.07
53.60	52.83	50.98	54.97	51.05	55.04	51.34	49.67	49.02
54.70	58.52	57.23	60.72	56.80	60.37	56.65	55.73	54.78
55.30	58.71	57.44	61.22	57.29	60.38	56.66	55.83	54.87
71.30	73.66	73.88	75.95	72.02	75.84	72.06	73.92	72.07
114.00	110.00	113.83	118.25	114.33	118.30	114.35	118.85	114.77
117.80	111.51	115.49	118.47	114.55	119.07	115.13	123.62	119.30
119.50	113.55	117.73	121.54	117.62	121.62	117.67	125.65	121.23
123.70	118.74	123.44	127.32	123.39	127.71	123.73	127.16	122.67
125.70	119.85	124.66	128.31	124.38	128.23	124.25	131.57	126.86
130.20	125.74	131.14	135.80	131.87	135.76	131.75	135.20	130.32
130.60	127.86	133.47	137.73	133.80	137.64	133.62	136.49	131.54
133.40	133.37	139.52	143.05	139.12	143.09	139.05	144.08	138.75
147.70	136.83	143.32	147.87	143.95	148.14	144.08	151.09	145.42
158.30	150.48	158.33	161.90	157.97	161.99	157.88	162.99	156.72
160.20	150.69	158.57	163.21	159.28	163.19	159.08	163.10	156.83
Proton shifts	1.02	0.99	1.14	1.06	1.08	1.07	1.24	0.97
	2.67	2.52	2.55	2.59	2.52	2.60	2.52	2.31
	2.67	2.54	2.57	2.74	2.66	2.71	2.63	2.35
	2.67	2.58	2.60	2.75	2.66	2.74	2.65	2.43
	2.67	2.63	2.65	2.75	2.66	2.75	2.66	3.05
	2.67	2.85	2.85	2.93	2.83	2.96	2.86	3.38
	3.74	3.72	3.67	3.72	3.58	3.71	3.57	3.64
	4.46	4.67	4.54	4.79	4.58	4.80	4.61	4.97
	6.80	6.81	6.53	6.88	6.54	6.88	6.57	6.37
	6.80	6.83	6.54	6.90	6.56	6.91	6.61	6.65
	6.80	7.33	7.01	7.40	7.03	7.36	7.03	6.95
	6.99	7.34	7.01	7.44	7.06	7.40	7.07	7.13
	7.46	8.17	7.79	8.18	7.76	8.02	7.65	7.28
	8.11	8.47	8.07	8.45	8.01	8.41	8.02	7.80
C MAE	4.56	2.10	3.93	1.94	3.90	1.80	4.03	1.67
H MAE	0.20	0.13	0.23	0.13	0.21	0.13	0.26	0.25
C CorrCoef	0.9981		0.9984		0.9986		0.9987	
H CorrCoef	0.9974		0.9974		0.9979		0.9912	
PROBABILITIES								
DP4 combined	81.9%		99.7%		100.0%		91.6%	
DP4 C only	0.2%		0.5%		2.7%		8.1%	
DP4 H only	99.9%		100.0%		100.0%		99.2%	
Gaussian combined	97.4%		100.0%		100.0%		97.7%	
Gaussian C only	0.4%		0.4%		2.2%		2.6%	
Gaussian H only	100.0%		100.0%		100.0%		99.9%	
KDE combined	57.3%		83.8%		99.2%		42.1%	
KDE C only	1.7%		1.5%		7.3%		22.8%	
KDE H only	98.7%		99.7%		99.9%		71.1%	
RKDE combined	87.4%		99.7%		100.0%		97.2%	
RKDE C only	4.1%		0.9%		2.6%		19.7%	
RKDE H only	99.4%		100.0%		100.0%		99.3%	
URKDE combined	86.6%		15.3%		50.1%		0.1%	
URKDE C only	16.7%		0.3%		1.2%		2.8%	
URKDE H only	97.0%		98.5%		98.8%		3.5%	

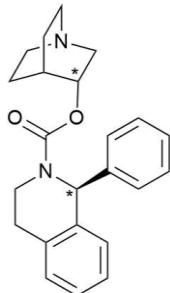
2gaus combined	52.9%	76.9%	99.3%	52.4%
2gaus C only	1.8%	1.3%	5.4%	19.6%
2gaus H only	98.4%	99.6%	100.0%	81.9%



Rosuvastatin (**40**)

		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
Rosuvastatin	Func.	B3LYP	B3LYP	mPW1	mPW1	mPW1	mPW1	mPW1	M06-
Basis	s.	6-	6-	PW91	PW91	PW91	PW91	PW91	2X
Carbon shifts	Exp	31G**	31G**	6-	6-	6-	6-	6-	6-
	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.
33.70	36.31	36.61	37.71	36.22	37.71	36.51	37.75	36.57	
34.30	32.35	32.52	34.52	33.16	33.72	32.70	33.78	32.78	
42.80	46.36	47.02	49.42	47.45	50.65	48.90	50.54	48.81	
44.70	39.24	39.65	42.87	41.16	40.98	39.65	40.89	39.58	
45.40	38.87	39.27	41.08	39.45	40.56	39.25	40.53	39.23	
69.10	71.53	73.09	74.44	71.43	73.91	71.16	73.88	71.13	
72.10	71.42	72.98	75.45	72.40	74.98	72.18	74.96	72.17	
116.60	112.13	115.14	120.78	115.86	121.39	116.59	121.43	116.62	
123.60	123.44	126.85	131.39	126.03	130.58	125.38	130.74	125.52	
124.40	118.67	121.91	128.14	122.93	127.81	122.73	127.78	122.69	
134.00	128.24	131.82	138.96	133.30	138.59	133.05	138.57	133.01	
136.60	135.68	139.52	144.05	138.18	145.16	139.33	145.22	139.37	
142.30	140.43	144.44	151.80	145.61	151.84	145.73	151.85	145.71	
159.30	158.59	163.25	167.93	161.08	168.20	161.38	168.21	161.36	
163.60	164.16	169.02	173.70	166.61	173.71	166.65	173.82	166.73	
165.20	156.25	160.83	169.37	162.46	168.80	161.96	168.77	161.90	
176.90	172.56	177.72	184.50	176.96	184.12	176.61	184.15	176.61	
182.40	170.04	175.10	184.76	177.22	184.82	177.29	184.83	177.26	
Proton shifts									
	1.27	1.33	1.66	1.38	1.52	1.40	1.66	1.40	1.67
	1.50	0.58	0.97	1.15	1.29	0.54	0.85	0.50	0.83
	1.65	0.73	1.11	1.18	1.33	0.85	1.14	0.83	1.14
	2.27	2.26	2.53	2.50	2.59	2.44	2.63	2.44	2.64
	2.37	2.51	2.76	2.50	2.59	2.65	2.83	2.66	2.85
	3.48	3.36	3.55	3.39	3.44	3.41	3.54	3.41	3.54
	3.51	3.31	3.50	3.22	3.28	3.25	3.39	3.25	3.40
	3.53	3.16	3.36	3.08	3.15	3.16	3.30	3.15	3.30
	4.01	3.97	4.11	4.22	4.24	4.04	4.13	4.03	4.12
	4.35	4.47	4.58	4.50	4.51	4.57	4.62	4.57	4.63
	5.55	5.35	5.39	5.55	5.52	5.51	5.50	5.50	5.50
	6.62	6.96	6.89	6.91	6.82	6.83	6.74	6.83	6.74
	7.16	7.21	7.12	7.24	7.14	7.27	7.15	7.27	7.15
	7.70	7.57	7.45	7.69	7.57	7.63	7.48	7.63	7.48
	C MAE	3.66	3.24	5.08	2.31	5.23	2.54	5.24	2.56
	H MAE	0.26	0.24	0.20	0.20	0.27	0.26	0.27	0.26
	C CorrCoef	0.9976		0.9986		0.9983		0.9983	
	H CorrCoef	0.9899		0.9941		0.9884		0.9878	
PROBABILITIES									
DP4 combined		0.3%		100.0%		99.2%		98.0%	
DP4 C only		0.1%		89.8%		19.2%		14.4%	
DP4 H only		76.8%		100.0%		99.8%		99.7%	
Gaussian combined		4.2%		100.0%		100.0%		99.9%	
Gaussian C only		0.2%		94.9%		17.7%		12.1%	
Gaussian H only		95.9%		100.0%		100.0%		100.0%	
KDE combined		9.5%		99.3%		16.3%		7.9%	
KDE C only		2.9%		83.2%		21.6%		18.7%	
KDE H only		77.7%		96.8%		41.5%		27.1%	

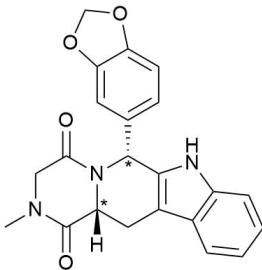
RKDE combined	5.3%	99.2%	1.4%	0.6%	
RKDE C only	19.1%	97.3%	40.0%	33.2%	
RKDE H only	19.3%	77.4%	2.0%	1.3%	
URKDE combined	82.9%	99.1%	44.4%	43.4%	
URKDE C only	26.7%	89.2%	35.8%	33.4%	
URKDE H only	93.0%	92.9%	58.9%	60.5%	
2gaus combined	0.7%	100.0%	75.1%	64.7%	
2gaus C only	2.1%	82.6%	19.7%	16.7%	
2gaus H only	26.2%	99.9%	92.5%	90.2%	



Solifenacin (5)

	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	
Solifenacin	B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06-	
Func.			PW91	PW91	PW91		PW91	2X	
Basis	6-	6-	6-	6-	6-		6-	6-	
s.	31G**	31G**	311G*	311G*	311G*		311G*	31G**	
Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	
Carbon shifts	24.80	27.49	24.81	27.60	25.40	27.60	25.39	27.79	25.47
	25.80	28.52	25.92	29.50	27.24	29.50	27.24	29.79	27.41
	28.60	32.27	29.93	32.98	30.62	32.99	30.62	32.93	30.46
	38.90	37.90	35.97	38.82	36.28	38.83	36.29	38.60	35.96
	46.70	47.55	46.33	48.89	46.05	48.89	46.05	48.82	45.88
	47.70	47.90	46.70	49.29	46.43	49.29	46.43	49.30	46.34
	56.10	58.09	57.64	60.03	56.85	60.01	56.83	60.35	57.07
	58.30	59.25	58.88	60.22	57.03	60.24	57.05	60.47	57.19
	72.40	72.90	73.52	75.11	71.48	75.12	71.48	75.24	71.52
	126.30	121.29	125.44	130.98	125.66	130.98	125.66	130.97	125.62
	127.20	121.96	126.15	132.06	126.72	132.06	126.72	132.11	126.72
	127.50	122.07	126.27	132.07	126.72	132.07	126.72	132.15	126.76
	128.20	123.22	127.51	132.98	127.60	132.99	127.61	133.04	127.62
	128.40	124.30	128.66	133.85	128.45	133.85	128.45	133.95	128.51
	128.60	124.32	128.68	134.31	128.89	134.30	128.88	134.19	128.74
	129.00	125.03	129.45	135.27	129.83	135.26	129.82	135.17	129.69
	135.10	128.47	133.14	138.35	132.81	138.35	132.81	138.36	132.79
	135.70	132.99	137.98	143.19	137.51	143.19	137.51	143.37	137.65
	143.00	140.18	145.69	151.23	145.31	151.25	145.32	151.33	145.38
	155.40	148.54	154.66	162.04	155.79	162.04	155.79	162.05	155.78
Proton shifts	1.41	1.17	1.35	1.32	1.38	1.32	1.38	1.41	1.43
	1.57	1.42	1.58	1.51	1.56	1.51	1.56	1.52	1.53
	1.69	1.47	1.63	1.59	1.63	1.59	1.63	1.63	1.64
	1.83	1.81	1.95	1.87	1.90	1.87	1.90	1.96	1.95
	2.04	1.93	2.06	1.93	1.96	1.93	1.96	2.01	1.99
	2.79	2.53	2.62	2.66	2.65	2.67	2.65	2.68	2.63
	2.79	2.60	2.69	2.73	2.71	2.73	2.71	2.77	2.71
	2.79	2.68	2.76	2.84	2.81	2.84	2.81	2.83	2.77
	2.79	2.68	2.76	2.85	2.83	2.86	2.83	2.88	2.82
	2.79	2.71	2.80	2.88	2.85	2.88	2.85	2.90	2.84
	2.79	2.79	2.87	2.96	2.93	2.96	2.93	3.05	2.98
	2.79	3.02	3.09	3.12	3.08	3.12	3.08	3.10	3.03
	3.31	3.17	3.23	3.29	3.24	3.29	3.24	3.25	3.18
	3.31	3.27	3.32	3.31	3.26	3.31	3.26	3.34	3.26
	4.03	4.16	4.16	4.23	4.13	4.23	4.13	4.20	4.08
	4.82	4.65	4.62	4.69	4.56	4.69	4.56	4.72	4.57
	6.32	6.44	6.30	6.57	6.34	6.57	6.34	6.59	6.36
	7.07	7.11	6.93	7.16	6.89	7.16	6.89	7.16	6.89
	7.20	7.28	7.09	7.38	7.11	7.38	7.11	7.28	7.01
	7.20	7.33	7.14	7.44	7.17	7.44	7.17	7.38	7.10
	7.20	7.36	7.17	7.45	7.17	7.44	7.17	7.45	7.17
	7.20	7.38	7.18	7.48	7.20	7.48	7.20	7.49	7.21
	7.20	7.41	7.21	7.50	7.22	7.50	7.22	7.49	7.21
	7.20	7.44	7.24	7.50	7.22	7.50	7.22	7.51	7.23
	7.20	7.47	7.27	7.57	7.28	7.57	7.29	7.62	7.33
	7.20	7.72	7.50	7.76	7.46	7.76	7.47	7.91	7.61
C MAE	3.33	1.03	4.21	1.10	4.21	1.09	4.30	1.13	
H MAE	0.16	0.09	0.17	0.09	0.17	0.09	0.17	0.10	
C CorrCoef	0.9996		0.9996		0.9996		0.9996		

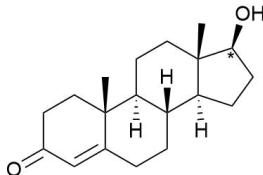
H CorrCoef	0.9986	0.9986	0.9987	0.9981	
PROBABILITIES					
DP4 combined	99.9%	99.9%	99.9%	85.9%	
DP4 C only	48.8%	47.6%	47.2%	21.6%	
DP4 H only	100.0%	99.9%	99.9%	95.7%	
Gaussian combined	99.9%	100.0%	100.0%	96.6%	
Gaussian C only	46.2%	47.2%	46.9%	29.5%	
Gaussian H only	99.9%	100.0%	100.0%	98.5%	
KDE combined	99.3%	99.5%	99.6%	69.8%	
KDE C only	45.3%	47.2%	46.8%	28.2%	
KDE H only	99.5%	99.6%	99.6%	85.4%	
RKDE combined	96.7%	98.4%	98.6%	63.0%	
RKDE C only	45.5%	47.5%	47.7%	23.1%	
RKDE H only	97.2%	98.6%	98.7%	85.1%	
URKDE combined	96.1%	94.1%	98.8%	92.2%	
URKDE C only	49.9%	47.3%	47.7%	30.4%	
URKDE H only	96.1%	94.7%	98.9%	96.4%	
2gaus combined	98.9%	99.1%	98.9%	66.2%	
2gaus C only	45.8%	47.1%	46.9%	26.0%	
2gaus H only	99.1%	99.2%	99.0%	84.8%	



Tadalafil (6)

		Shifts	En-	Shifts	En-	Shifts	En-	Shifts	En-
		B3LYP	ergy	B3LYP	ergy	mPW1	ergy	B3LYP	ergy
		6-		6-		6-		6-	
Tadalafil	Func.	B3LYP		mPW1		mPW1		mPW1	M06-
	Basis	6-		PW91		PW91		PW91	2X
	s.	31G**		31G*		31G*		31G*	6-
Carbon shifts	Exp	31G**		31G*		31G*		31G**	31G**
	Calc.	33.60	45.68	33.20	34.55	32.98	34.55	32.98	34.55
	Corr.	52.10	67.97	54.07	55.82	53.31	55.82	53.31	55.82
		56.20	68.28	54.35	57.73	55.13	57.74	55.13	57.73
		56.70	72.83	58.61	61.32	58.56	61.32	58.56	61.32
		101.20	121.33	104.01	107.40	102.57	107.40	102.57	107.40
		106.60	122.13	104.76	109.90	104.97	109.90	104.96	109.90
		107.50	125.97	108.35	113.97	108.86	113.98	108.87	113.97
		108.20	127.21	109.51	114.71	109.56	114.71	109.56	114.71
		111.20	128.36	110.59	116.31	111.09	116.33	111.10	116.30
		118.60	136.14	117.87	123.46	117.92	123.46	117.92	123.46
		120.10	137.35	119.00	124.45	118.87	124.45	118.87	124.45
		120.70	138.65	120.23	126.12	120.46	126.12	120.46	126.12
		122.50	138.88	120.44	126.35	120.68	126.35	120.68	126.35
		126.20	143.89	125.13	130.98	125.10	130.96	125.08	130.99
		132.80	150.79	131.59	138.37	132.16	138.37	132.16	138.37
		135.40	151.55	132.30	139.12	132.88	139.12	132.88	139.12
		136.60	157.52	137.89	144.09	137.63	144.10	137.63	144.09
		147.10	162.46	142.51	149.42	142.71	149.41	142.71	149.42
		147.90	162.96	142.98	149.75	143.03	149.74	143.03	149.76
		166.40	194.24	172.26	179.68	171.62	179.68	171.62	179.67
		166.80	195.55	173.49	181.15	173.02	181.15	173.03	181.15
Proton shifts		3.04	3.13	3.06	2.83	2.94	2.83	2.94	2.83
		3.21	3.65	3.56	3.48	3.57	3.48	3.57	3.48
		3.78	3.85	3.74	3.64	3.71	3.64	3.71	3.64
		3.94	3.92	3.81	3.76	3.83	3.76	3.83	3.76
		4.10	4.00	3.89	3.82	3.89	3.82	3.89	3.82
		4.31	4.15	4.03	4.15	4.20	4.15	4.20	4.15
		5.85	5.97	5.76	6.00	5.98	6.00	5.98	6.00
		5.88	6.30	6.08	6.02	5.99	6.02	6.00	6.02
		6.15	6.32	6.10	6.06	6.04	6.06	6.04	6.06
		6.69	7.10	6.84	6.77	6.72	6.77	6.72	6.77
		6.73	7.11	6.85	6.84	6.78	6.84	6.79	6.84
		6.85	7.37	7.09	7.21	7.14	7.21	7.14	7.21
		7.12	7.52	7.24	7.27	7.20	7.27	7.20	7.27
		7.28	7.55	7.27	7.40	7.32	7.40	7.32	7.40
		7.60	7.61	7.32	7.45	7.37	7.45	7.37	7.45
		7.81	7.99	7.69	7.74	7.65	7.74	7.65	7.74
C MAE		17.66	2.18	5.12	1.90	5.12	1.90	5.12	1.90
H MAE		0.23	0.15	0.17	0.14	0.17	0.14	0.17	0.14
C CorrCoef		0.9975		0.9980		0.9980		0.9980	
H CorrCoef		0.9938		0.9948		0.9948		0.9948	
PROBABILITIES									
DP4 combined		38.8%		56.4%		53.4%		61.1%	
DP4 C only		1.5%		9.5%		9.2%		9.8%	
DP4 H only		97.6%		92.5%		91.9%		93.5%	
Gaussian combined		77.3%		73.5%		71.0%		69.9%	
Gaussian C only		2.0%		4.6%		4.7%		4.7%	
Gaussian H only		99.4%		98.3%		98.0%		97.9%	

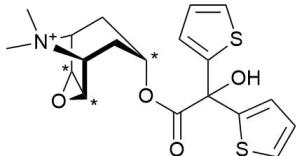
KDE combined	53.2%	82.7%	88.1%	89.6%	
KDE C only	14.5%	44.5%	45.6%	52.0%	
KDE H only	87.0%	85.6%	89.8%	88.9%	
RKDE combined	98.9%	94.7%	95.1%	96.0%	
RKDE C only	66.2%	47.3%	47.6%	50.3%	
RKDE H only	97.8%	95.2%	95.5%	95.9%	
URKDE combined	99.8%	97.7%	97.7%	96.8%	
URKDE C only	85.7%	80.9%	81.1%	69.2%	
URKDE H only	98.9%	91.1%	90.6%	93.0%	
2gaus combined	47.4%	69.5%	79.6%	80.1%	
2gaus C only	12.4%	36.6%	34.1%	40.0%	
2gaus H only	86.4%	79.8%	88.3%	85.8%	



Testosterone (4)

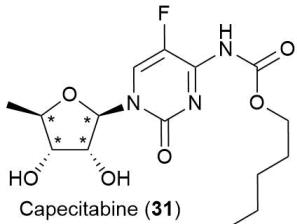
		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
Testosterone	Func. Basis s.	B3LYP 6- 31G**	B3LYP 6- 31G**	mPW1 PW91 311G*	mPW1 PW91 311G*	mPW1 PW91 311G*	mPW1 B3LYP 311G*	mPW1 PW91 311G*	M06- 2X 31G**
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
	17.14	19.68	15.76	19.35	15.96	19.35	15.96	19.35	15.96
	20.39	24.03	20.36	24.44	20.93	24.43	20.92	24.43	20.93
	23.08	26.25	22.71	26.57	23.01	26.59	23.03	26.57	23.02
	29.83	32.62	29.44	33.40	29.68	33.28	29.57	33.34	29.63
	31.31	34.01	30.91	35.17	31.41	35.17	31.42	35.17	31.42
	32.59	35.54	32.52	36.94	33.14	36.94	33.14	36.94	33.14
	33.62	34.10	31.00	35.95	32.18	35.95	32.18	35.95	32.18
	35.34	38.84	36.01	39.84	35.98	39.83	35.97	39.84	35.98
	35.38	39.53	36.74	40.07	36.20	40.08	36.21	40.07	36.21
	36.18	38.71	35.87	39.52	35.66	39.51	35.65	39.50	35.65
	38.43	43.31	40.74	44.56	40.59	44.56	40.59	44.56	40.59
	42.53	46.93	44.55	47.89	43.84	47.89	43.85	47.89	43.85
	50.21	51.56	49.45	52.68	48.52	52.70	48.54	52.67	48.52
	53.68	56.66	54.84	58.06	53.78	58.06	53.78	58.06	53.78
	80.93	81.27	80.84	84.80	79.90	84.78	79.88	84.81	79.91
	123.41	122.60	124.52	131.23	125.26	131.23	125.26	131.23	125.26
	171.80	166.28	170.66	179.91	172.81	179.91	172.82	179.91	172.81
	199.70	193.59	199.51	205.61	197.92	205.61	197.93	205.61	197.92
Proton shifts	0.80	0.91	0.86	0.81	0.73	0.81	0.73	0.81	0.73
	0.93	1.08	1.04	1.18	1.10	1.18	1.10	1.18	1.10
	0.98	1.15	1.11	1.25	1.17	1.25	1.17	1.25	1.17
	1.01	1.04	1.00	1.13	1.05	1.13	1.05	1.13	1.05
	1.09	1.06	1.02	1.22	1.14	1.22	1.14	1.22	1.14
	1.20	1.34	1.31	1.29	1.22	1.29	1.22	1.29	1.22
	1.31	1.46	1.42	1.41	1.34	1.42	1.34	1.41	1.34
	1.44	1.52	1.49	1.51	1.44	1.51	1.44	1.51	1.44
	1.46	1.47	1.44	1.49	1.41	1.51	1.43	1.49	1.41
	1.58	1.77	1.74	1.69	1.61	1.69	1.61	1.69	1.61
	1.61	1.61	1.58	1.54	1.46	1.54	1.46	1.54	1.46
	1.63	1.60	1.57	1.66	1.58	1.66	1.58	1.66	1.58
	1.70	1.72	1.69	1.78	1.70	1.78	1.70	1.78	1.70
	1.85	1.78	1.75	1.86	1.78	1.86	1.78	1.86	1.78
	1.86	1.78	1.75	1.83	1.75	1.82	1.75	1.83	1.75
	2.04	1.96	1.94	2.06	1.99	2.06	1.99	2.06	1.99
	2.08	2.05	2.03	2.16	2.08	2.15	2.07	2.16	2.09
	2.27	2.18	2.15	2.37	2.29	2.37	2.29	2.37	2.29
	2.34	2.06	2.03	2.27	2.19	2.27	2.19	2.27	2.19
	2.37	2.43	2.41	2.44	2.37	2.45	2.37	2.44	2.37
	2.41	2.44	2.42	2.48	2.40	2.48	2.40	2.48	2.40
	3.65	3.76	3.76	3.84	3.76	3.85	3.77	3.84	3.76
	5.74	5.82	5.84	5.86	5.78	5.86	5.78	5.86	5.78
C MAE	3.06	0.91	4.34	0.96	4.34	0.96	4.34	0.96	
H MAE	0.09	0.09	0.09	0.06	0.09	0.06	0.09	0.06	
C CorrCoef	0.9997		0.9997		0.9997		0.9997		
H CorrCoef	0.9947		0.9968		0.9967		0.9968		
PROBABILITIES									
DP4 combined	100.0%		100.0%		100.0%		100.0%		
DP4 C only	100.0%		100.0%		100.0%		100.0%		
DP4 H only	100.0%		100.0%		100.0%		100.0%		
Gaussian combined	100.0%		100.0%		100.0%		100.0%		
Gaussian C only	99.9%		100.0%		100.0%		100.0%		
Gaussian H only	100.0%		100.0%		100.0%		100.0%		

KDE combined	100.0%	100.0%	100.0%	100.0%	
KDE C only	99.7%	100.0%	100.0%	100.0%	
KDE H only	100.0%	100.0%	100.0%	100.0%	
RKDE combined	100.0%	100.0%	100.0%	100.0%	
RKDE C only	100.0%	100.0%	100.0%	100.0%	
RKDE H only	100.0%	100.0%	100.0%	100.0%	
URKDE combined	100.0%	100.0%	100.0%	100.0%	
URKDE C only	100.0%	100.0%	100.0%	100.0%	
URKDE H only	100.0%	100.0%	100.0%	100.0%	
2gaus combined	100.0%	100.0%	100.0%	100.0%	
2gaus C only	99.8%	100.0%	100.0%	100.0%	
2gaus H only	99.9%	100.0%	100.0%	100.0%	



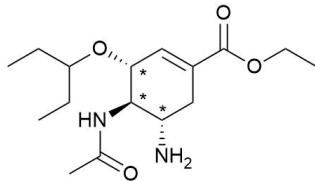
Tiotropium (9)

		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
Tiotropium	Func. Basis s.	B3LYP 6- 31G**	B3LYP 6- 31G**	mPW1 PW91 311G*	mPW1 PW91 311G*	mPW1 PW91 311G*	B3LYP 6- 31G**	mPW1 PW91 311G*	M06- 2X 311G* 31G**
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
47.10	48.39	45.77		50.45	46.08	50.45	46.08	50.44	46.08
53.60	52.25	49.74		55.11	50.49	55.11	50.49	55.12	50.50
55.50	56.95	54.57		59.25	54.40	59.25	54.40	59.24	54.40
63.60	66.43	64.32		68.63	63.27	68.63	63.27	68.63	63.28
64.40	70.54	68.54		73.22	67.61	73.22	67.61	73.22	67.61
76.20	81.53	79.84		83.78	77.59	83.78	77.59	83.76	77.58
125.70	122.01	121.45		132.42	123.57	132.42	123.56	132.42	123.58
126.10	124.53	124.04		135.27	126.26	135.28	126.27	135.24	126.25
126.70	125.88	125.43		135.79	126.75	135.80	126.76	135.73	126.71
146.60	144.66	144.73		151.68	141.78	151.68	141.77	151.71	141.82
169.70	174.19	175.09		186.57	174.75	186.57	174.75	186.55	174.75
Proton shifts									
1.91	2.21	2.21		2.27	2.29	2.27	2.29	2.27	2.29
2.69	2.78	2.77		2.79	2.82	2.79	2.82	2.79	2.82
3.07	3.11	3.10		3.06	3.08	3.06	3.08	3.06	3.08
3.27	3.14	3.13		3.06	3.08	3.06	3.08	3.06	3.09
3.52	3.33	3.32		3.23	3.26	3.24	3.26	3.23	3.26
4.16	3.82	3.79		3.76	3.78	3.76	3.78	3.76	3.78
5.14	5.32	5.28		5.20	5.22	5.20	5.22	5.20	5.22
7.02	7.30	7.24		7.17	7.19	7.17	7.19	7.19	7.20
7.14	7.31	7.25		7.26	7.27	7.26	7.27	7.26	7.27
7.53	7.44	7.37		7.45	7.46	7.45	7.46	7.44	7.45
C MAE	2.97	2.60		6.92	2.08	6.93	2.09	6.92	2.07
H MAE	0.18	0.18		0.18	0.18	0.18	0.18	0.18	0.18
C CorrCoef	0.9977			0.9982		0.9982		0.9982	
H CorrCoef	0.9948			0.9938		0.9939		0.9937	
PROBABILITIES									
DP4 combined	14.7%			16.4%		17.5%		18.2%	
DP4 C only	55.5%			72.6%		74.4%		76.5%	
DP4 H only	7.2%			3.5%		3.5%		3.3%	
Gaussian combined	43.2%			33.6%		35.1%		39.0%	
Gaussian C only	66.8%			84.4%		84.9%		86.3%	
Gaussian H only	13.1%			4.0%		4.1%		4.3%	
KDE combined	11.7%			8.1%		8.6%		10.6%	
KDE C only	35.7%			55.5%		54.8%		56.4%	
KDE H only	9.2%			2.9%		3.1%		3.7%	
RKDE combined	22.0%			10.4%		15.5%		15.8%	
RKDE C only	40.4%			51.1%		53.9%		56.4%	
RKDE H only	16.1%			4.9%		6.7%		6.2%	
URKDE combined	17.4%			17.2%		17.8%		17.6%	
URKDE C only	22.1%			21.6%		19.4%		23.6%	
URKDE H only	29.0%			24.3%		27.9%		22.2%	
2gaus combined	12.8%			12.5%		11.4%		13.1%	
2gaus C only	38.8%			55.2%		57.3%		54.9%	
2gaus H only	9.1%			4.8%		4.2%		5.0%	



		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
		B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06-
	Func.			PW91	PW91	PW91		PW91	2X
	Basis	6-	6-	6-	6-	6-	6-	6-	6-
	s.	31G**	31G**	311G*	311G*	311G*	31G**	311G*	31G**
Capecitabine	Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.
	18.70	22.53	17.50	22.59	17.98	22.59	18.01	22.59	17.96
	22.20	27.16	22.47	28.21	23.55	28.20	23.56	28.21	23.52
	27.90	31.65	27.29	32.54	27.84	32.45	27.77	32.73	28.01
	28.30	33.09	28.83	34.01	29.29	34.02	29.32	34.09	29.35
	65.90	66.41	64.61	68.87	63.82	68.84	63.81	68.70	63.64
	73.90	77.67	76.70	80.17	75.02	80.17	75.02	80.16	75.00
	74.60	78.72	77.82	81.55	76.39	81.55	76.39	81.56	76.39
	79.70	80.75	80.01	84.17	78.98	84.17	78.99	84.18	78.98
	91.10	95.28	95.61	98.84	93.51	98.84	93.51	98.85	93.51
	129.60	122.12	124.43	131.05	125.41	131.04	125.39	131.03	125.41
	138.00	135.32	138.60	144.94	139.17	144.93	139.14	144.93	139.17
	152.20	148.12	152.35	156.61	150.73	156.60	150.70	156.60	150.74
	152.20	146.30	150.39	158.51	152.62	158.63	152.71	158.53	152.65
	152.20	148.62	152.88	159.98	154.06	159.97	154.04	159.97	154.07
Proton shifts									
	0.89	0.95	0.89	1.04	0.90	1.04	0.90	1.04	0.89
	1.36	1.17	1.11	1.25	1.10	1.25	1.10	1.25	1.10
	1.36	1.32	1.25	1.36	1.21	1.36	1.21	1.38	1.23
	1.36	1.33	1.26	1.37	1.22	1.36	1.22	1.40	1.25
	1.36	1.37	1.30	1.43	1.28	1.43	1.29	1.42	1.27
	1.36	1.38	1.31	1.44	1.30	1.44	1.30	1.43	1.28
	1.61	1.64	1.56	1.72	1.57	1.72	1.57	1.69	1.54
	1.61	1.66	1.58	1.74	1.59	1.74	1.59	1.74	1.59
	3.68	4.31	4.16	4.41	4.25	4.41	4.25	4.42	4.25
	3.90	4.58	4.42	4.59	4.43	4.59	4.43	4.59	4.42
	4.08	4.30	4.15	4.34	4.18	4.34	4.18	4.34	4.17
	4.08	4.13	3.99	4.16	3.99	4.16	4.00	4.17	4.00
	4.08	4.17	4.03	4.18	4.02	4.19	4.02	4.24	4.07
	5.69	6.01	5.82	6.05	5.87	6.05	5.87	6.05	5.86
	8.00	7.82	7.58	7.69	7.50	7.69	7.50	7.69	7.49
	C MAE	3.81	1.74	5.21	1.48	5.21	1.49	5.22	1.50
	H MAE	0.17	0.16	0.21	0.19	0.21	0.18	0.22	0.18
PROBABILITIES	C CorrCoef	0.9989		0.9994		0.9994		0.9994	
	H CorrCoef	0.9931		0.9915		0.9915		0.9915	
	DP4 combined	0.4%		24.5%		27.7%		19.0%	
	DP4 C only	0.2%		16.5%		18.3%		20.3%	
	DP4 H only	0.0%		0.0%		0.0%		0.0%	
	Gaussian combined	0.1%		4.6%		5.4%		3.6%	
	Gaussian C only	0.5%		18.4%		20.5%		20.3%	
	Gaussian H only	0.0%		0.0%		0.0%		0.0%	
	KDE combined	3.1%		57.9%		52.3%		64.9%	
	KDE C only	1.2%		21.9%		25.4%		26.2%	
	KDE H only	0.3%		0.2%		0.2%		0.6%	
	RKDE combined	8.2%		65.5%		57.1%		60.8%	
	RKDE C only	3.3%		14.1%		13.7%		11.6%	
	RKDE H only	0.3%		0.5%		0.4%		1.0%	
	URKDE combined	15.7%		8.1%		11.2%		8.1%	
	URKDE C only	5.8%		2.1%		2.6%		1.7%	

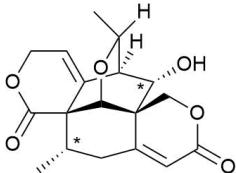
URKDE H only	1.9%	3.3%	3.6%	3.5%	
2gaus combined	5.8%	63.6%	61.0%	57.1%	
2gaus C only	1.1%	21.5%	25.0%	26.0%	
2gaus H only	0.4%	0.3%	0.3%	0.4%	



Oseltamivir (15)

		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
		B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06- 2X
		6-	6-	PW91	PW91	PW91		PW91	
		31G**	31G**	311G*	311G*	311G*		311G*	31G**
		Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.
Oseltamivir	Func.	B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06- 2X
	Basis	6-	6-	PW91	PW91	PW91		PW91	
	s.	31G**	31G**	311G*	311G*	311G*		311G*	31G**
	Carbon shifts	9.50	12.79	9.96	12.23	10.54	12.48	10.69	12.84
		14.20	15.67	12.95	16.24	14.38	16.25	14.30	16.35
		23.70	22.84	20.41	24.25	22.04	24.26	21.97	24.33
		25.80	28.03	25.81	28.57	26.17	28.65	26.17	27.97
		26.30	28.73	26.54	29.24	26.82	29.38	26.88	29.30
		33.60	36.19	34.30	36.72	33.98	36.75	33.93	36.76
		49.20	50.00	48.67	51.87	48.48	52.02	48.55	52.16
		59.00	59.70	58.76	62.23	58.40	62.23	58.33	62.09
		60.80	67.43	66.80	68.20	64.11	68.57	64.40	68.87
		74.80	74.95	74.63	76.61	72.16	76.63	72.11	76.71
		81.70	80.30	80.19	83.19	78.46	83.10	78.31	82.24
		129.60	128.50	130.34	137.39	130.35	137.48	130.37	137.62
		137.50	139.79	142.08	149.72	142.16	149.71	142.08	149.57
		166.30	161.77	164.95	174.77	166.13	174.80	166.11	174.75
		170.90	164.00	167.26	177.37	168.63	177.51	168.70	177.64
Proton shifts									
	0.89	0.92	0.98	0.93	0.91	0.93	0.92	0.95	0.93
	0.90	0.96	1.02	1.00	0.98	1.00	0.99	1.02	1.00
	1.29	1.22	1.28	1.31	1.30	1.31	1.30	1.30	1.28
	1.50	1.51	1.57	1.53	1.52	1.53	1.53	1.42	1.41
	1.50	1.51	1.57	1.54	1.53	1.54	1.53	1.45	1.44
	1.50	1.53	1.59	1.56	1.55	1.54	1.54	1.63	1.63
	1.50	1.55	1.61	1.58	1.57	1.56	1.56	1.65	1.64
	2.04	1.80	1.86	1.86	1.86	1.86	1.86	1.87	1.86
	2.15	1.88	1.94	2.05	2.05	2.04	2.05	2.04	2.04
	2.75	2.50	2.56	2.68	2.69	2.71	2.72	2.72	2.73
	3.24	2.54	2.60	2.77	2.78	2.74	2.76	2.74	2.75
	3.34	3.36	3.41	3.38	3.39	3.37	3.39	3.44	3.46
	3.52	4.15	4.19	4.15	4.18	4.15	4.18	4.10	4.13
	4.18	4.16	4.21	4.18	4.21	4.15	4.19	4.19	4.22
	4.20	4.19	4.24	4.20	4.23	4.19	4.23	4.21	4.24
	5.62	4.99	5.03	4.83	4.87	4.83	4.87	4.81	4.85
	6.78	7.23	7.26	7.19	7.27	7.20	7.28	7.20	7.28
	C MAE	2.47	1.59	4.21	1.41	4.29	1.44	4.20	1.55
	H MAE	0.20	0.22	0.18	0.18	0.18	0.18	0.20	0.20
	C CorrCoef	0.9990		0.9993		0.9993		0.9992	
	H CorrCoef	0.9828		0.9839		0.9836		0.9833	
PROBABILITIES									
	DP4 combined	0.1%		100.0%		100.0%		99.4%	
	DP4 C only	0.6%		91.7%		92.7%		76.6%	
	DP4 H only	13.2%		95.8%		95.4%		77.9%	
	Gaussian combined	0.1%		100.0%		100.0%		99.8%	
	Gaussian C only	0.3%		68.1%		69.1%		44.1%	
	Gaussian H only	16.0%		99.3%		98.8%		96.8%	
	KDE combined	3.5%		94.8%		91.8%		38.6%	
	KDE C only	4.5%		78.1%		76.6%		65.9%	
	KDE H only	2.1%		23.2%		23.5%		5.3%	
	RKDE combined	79.4%		100.0%		100.0%		99.5%	
	RKDE C only	42.8%		76.6%		75.8%		60.9%	

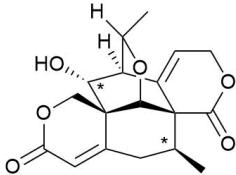
RKDE H only	81.3%	99.0%	98.8%	86.6%	
URKDE combined	94.8%	99.9%	99.8%	88.5%	
URKDE C only	51.6%	87.9%	87.3%	71.8%	
URKDE H only	36.2%	76.0%	77.6%	28.3%	
2gaus combined	5.7%	99.8%	99.7%	91.3%	
2gaus C only	4.7%	84.3%	83.4%	70.5%	
2gaus H only	19.2%	84.8%	82.8%	48.9%	



Swerilactone A (7)

		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
SwerilactoneA	Func. Basis s.	B3LYP 6- 31G**	B3LYP 6- 31G**	mPW1 PW91 311G*	mPW1 PW91 311G*	mPW1 PW91 311G*	mPW1 B3LYP 6- 31G**	mPW1 PW91 311G*	M06- 2X 6- 31G**
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
20.40	22.38	18.86		22.99	20.31	22.99	20.31	22.99	20.32
38.30	41.24	38.38		42.64	38.92	42.64	38.92	42.65	38.93
41.30	44.62	41.87		46.21	42.30	46.21	42.30	46.21	42.30
46.40	49.73	47.17		50.93	46.77	50.94	46.78	50.97	46.81
50.60	52.57	50.10		54.83	50.46	54.80	50.44	54.70	50.35
55.20	58.43	56.17		59.75	55.13	59.75	55.13	59.74	55.12
69.20	69.35	67.47		72.75	67.43	72.75	67.44	72.75	67.44
72.60	77.05	75.43		79.96	74.27	79.97	74.27	79.97	74.28
73.40	74.49	72.79		76.77	71.25	76.78	71.25	76.80	71.28
75.90	77.28	75.68		79.97	74.27	79.97	74.27	79.97	74.28
77.00	82.04	80.61		84.30	78.38	84.30	78.38	84.30	78.38
115.80	116.63	116.40		124.95	116.88	124.95	116.88	124.96	116.89
127.30	126.67	126.79		137.75	129.01	137.75	129.00	137.74	129.00
133.80	134.78	135.18		145.14	136.00	145.13	135.99	145.11	135.98
161.30	157.63	158.84		169.85	159.41	169.85	159.41	169.86	159.41
165.00	161.15	162.48		172.75	162.15	172.74	162.15	172.74	162.14
172.50	172.55	174.28		185.30	174.03	185.30	174.03	185.30	174.04
Proton shifts	1.00	0.95	0.99	0.98	0.98	0.98	0.98	0.99	0.98
	1.08	1.06	1.11	1.11	1.10	1.11	1.10	1.11	1.10
	2.22	2.16	2.20	2.35	2.34	2.35	2.34	2.35	2.34
	2.28	2.31	2.34	2.34	2.34	2.34	2.34	2.34	2.34
	2.70	2.80	2.83	2.84	2.83	2.84	2.84	2.85	2.84
	3.02	2.78	2.81	2.69	2.68	2.69	2.68	2.69	2.68
	4.10	4.21	4.22	4.10	4.10	4.10	4.10	4.10	4.10
	4.33	4.18	4.19	4.16	4.16	4.16	4.16	4.16	4.16
	4.55	4.48	4.49	4.53	4.53	4.53	4.53	4.53	4.52
	4.60	4.62	4.63	4.64	4.64	4.64	4.64	4.64	4.64
	4.63	4.52	4.54	4.57	4.56	4.57	4.56	4.56	4.56
	4.82	4.88	4.88	4.97	4.96	4.97	4.96	4.97	4.96
	5.09	5.22	5.22	5.21	5.21	5.21	5.21	5.21	5.21
	6.09	5.86	5.86	5.87	5.87	5.87	5.87	5.87	5.87
	6.24	6.46	6.45	6.45	6.45	6.45	6.45	6.45	6.45
C MAE	2.22	1.40	6.24	1.28	6.24	1.28	6.24	1.29	
H MAE	0.11	0.10	0.11	0.11	0.11	0.11	0.11	0.11	
C CorrCoef	0.9994		0.9995		0.9995		0.9995		
H CorrCoef	0.9969		0.9959		0.9959		0.9958		
PROBABILITIES									
DP4 combined	100.0%		100.0%		100.0%		100.0%		
DP4 C only	99.5%		100.0%		100.0%		100.0%		
DP4 H only	5.1%		0.6%		0.6%		0.6%		
Gaussian combined	100.0%		100.0%		100.0%		100.0%		
Gaussian C only	99.3%		100.0%		100.0%		100.0%		
Gaussian H only	11.3%		1.2%		1.2%		1.4%		
KDE combined	99.7%		100.0%		100.0%		100.0%		
KDE C only	98.0%		99.9%		99.9%		99.9%		
KDE H only	6.0%		0.8%		0.8%		0.9%		
RKDE combined	100.0%		100.0%		100.0%		100.0%		
RKDE C only	97.5%		99.8%		99.8%		99.7%		
RKDE H only	28.4%		14.4%		13.8%		10.1%		

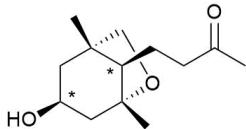
URKDE combined	99.8%	100.0%	100.0%	100.0%	
URKDE C only	95.8%	96.4%	96.6%	91.1%	
URKDE H only	32.9%	34.6%	34.4%	23.3%	
 2gaus combined	 99.8%	 100.0%	 100.0%	 100.0%	
2gaus C only	97.7%	99.9%	99.9%	99.9%	
2gaus H only	6.7%	0.9%	0.7%	1.1%	



Swerilactone B (8)

		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
SwerilactoneB	Func. Basis s.	B3LYP 6- 31G**	B3LYP 6- 31G**	mPW1 PW91 311G*	mPW1 PW91 311G*	mPW1 PW91 311G*	mPW1 B3LYP 6- 31G**	mPW1 PW91 311G*	M06- 2X 6- 31G**
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
	20.70	22.34	18.41	23.08	19.91	23.08	19.91	23.07	19.92
	30.70	35.39	31.96	36.36	32.52	36.36	32.53	36.36	32.54
	37.30	40.31	37.08	41.88	37.77	41.88	37.77	41.88	37.78
	47.30	50.60	47.76	51.69	47.10	51.70	47.11	51.75	47.15
	49.20	51.11	48.30	53.34	48.66	53.30	48.62	53.18	48.51
	53.80	57.63	55.07	59.11	54.15	59.11	54.14	59.10	54.14
	67.60	67.60	65.42	71.31	65.73	71.31	65.73	71.31	65.74
	71.50	76.75	74.93	78.59	72.65	78.59	72.65	78.59	72.65
	73.10	74.39	72.47	76.54	70.70	76.54	70.70	76.58	70.74
	73.70	78.33	76.57	81.38	75.30	81.39	75.30	81.40	75.32
	75.80	77.34	75.54	80.09	74.07	80.09	74.07	80.09	74.08
	118.20	118.61	118.42	127.21	118.84	127.21	118.84	127.21	118.84
	124.80	124.60	124.63	135.49	126.71	135.49	126.70	135.48	126.69
	139.00	139.50	140.11	150.25	140.73	150.25	140.72	150.23	140.70
	160.80	157.32	158.63	169.81	159.31	169.81	159.31	169.83	159.33
	164.70	160.81	162.25	172.37	161.74	172.37	161.74	172.37	161.73
	170.50	170.69	172.52	183.85	172.64	183.85	172.64	183.85	172.64
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Proton shifts	1.03	0.92	0.99	0.97	0.98	0.97	0.98	0.97	0.98
	1.05	0.98	1.05	0.98	1.00	0.98	0.99	0.98	0.99
	2.21	2.14	2.19	2.33	2.33	2.33	2.33	2.33	2.33
	2.69	2.45	2.49	2.48	2.49	2.48	2.49	2.48	2.48
	2.69	2.73	2.76	2.77	2.77	2.77	2.78	2.78	2.78
	3.41	3.16	3.19	3.09	3.10	3.09	3.10	3.09	3.10
	4.03	4.86	4.85	4.92	4.92	4.92	4.92	4.92	4.92
	4.13	4.21	4.22	4.14	4.14	4.14	4.14	4.14	4.14
	4.53	4.35	4.35	4.29	4.29	4.29	4.29	4.29	4.29
	4.63	4.55	4.54	4.59	4.59	4.59	4.59	4.59	4.59
	4.63	4.65	4.65	4.65	4.65	4.65	4.65	4.65	4.65
	4.70	4.62	4.62	4.66	4.65	4.66	4.65	4.65	4.65
	5.33	5.26	5.24	5.21	5.21	5.21	5.21	5.21	5.21
	6.16	5.96	5.92	5.95	5.94	5.95	5.94	5.95	5.94
	6.18	6.38	6.33	6.34	6.34	6.34	6.34	6.34	6.34
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C MAE	2.36	1.40	6.49	1.33	6.49	1.33	6.49	1.33	
H MAE	0.17	0.15	0.17	0.17	0.17	0.17	0.17	0.17	
C CorrCoef	0.9994		0.9995		0.9995		0.9995		
H CorrCoef	0.9879		0.9853		0.9853		0.9853		
<hr/>									
PROBABILITIES									
DP4 combined	100.0%		100.0%		100.0%		100.0%		
DP4 C only	100.0%		100.0%		100.0%		100.0%		
DP4 H only	94.7%		89.9%		89.8%		89.3%		
<hr/>									
Gaussian combined	100.0%		100.0%		100.0%		100.0%		
Gaussian C only	99.9%		100.0%		100.0%		100.0%		
Gaussian H only	76.0%		71.5%		71.3%		70.3%		
<hr/>									
KDE combined	100.0%		100.0%		100.0%		100.0%		
KDE C only	99.6%		100.0%		100.0%		100.0%		
KDE H only	96.7%		96.4%		95.0%		94.4%		
<hr/>									
RKDE combined	100.0%		100.0%		100.0%		100.0%		
RKDE C only	99.6%		100.0%		100.0%		100.0%		
RKDE H only	91.8%		92.6%		91.7%		91.2%		

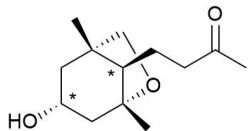
URKDE combined	99.8%	100.0%	100.0%	100.0%	
URKDE C only	96.4%	94.4%	94.3%	86.6%	
URKDE H only	67.2%	63.2%	63.2%	59.2%	
2gaus combined	100.0%	100.0%	100.0%	100.0%	
2gaus C only	99.6%	100.0%	100.0%	100.0%	
2gaus H only	93.5%	88.9%	89.5%	86.2%	



Tanarifuranonol, reassigned (17)

	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
Tanarifuranol1	B3LYP	B3LYP	mpW1	mpW1	mPW1	B3LYP	mPW1	M06- 2X
Func.	6-	6-	PW91	PW91	PW91		PW91	6-
Basis	31G**	31G**	311G*	311G*	311G*	31G**	311G*	31G**
s.								
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.
21.40	23.45	21.51	23.18	21.48	23.15	21.44	23.12	21.54
25.20	26.86	25.01	27.03	25.13	27.04	25.13	26.89	25.10
29.80	29.62	27.82	32.23	30.06	32.29	30.10	32.27	30.20
39.50	41.57	40.04	43.20	40.45	43.39	40.63	43.18	40.53
41.30	42.36	40.85	43.52	40.76	43.44	40.67	43.43	40.77
42.75	43.79	42.32	44.32	41.52	44.54	41.71	44.81	42.07
42.80	44.95	43.50	46.54	43.62	46.57	43.64	46.52	43.69
53.40	54.78	53.55	55.89	52.48	55.82	52.41	55.58	52.27
65.60	65.83	64.85	69.35	65.24	69.37	65.25	69.37	65.33
76.90	77.08	76.35	80.09	75.42	80.07	75.40	80.06	75.45
83.40	83.80	83.22	87.17	82.13	87.13	82.09	87.14	82.15
208.20	206.47	208.67	221.39	209.35	221.37	209.34	221.38	209.25
Proton shifts								
0.97	0.91	0.95	0.95	0.94	0.95	0.94	0.94	0.93
1.22	1.12	1.15	1.21	1.19	1.20	1.18	1.19	1.17
1.28	1.36	1.37	1.39	1.36	1.37	1.35	1.38	1.36
1.42	1.39	1.40	1.46	1.44	1.46	1.43	1.46	1.43
1.42	1.41	1.42	1.50	1.47	1.47	1.44	1.46	1.43
1.67	1.64	1.64	1.53	1.50	1.52	1.50	1.56	1.53
1.67	1.68	1.68	1.70	1.67	1.70	1.67	1.67	1.64
1.67	1.80	1.79	1.79	1.75	1.81	1.77	1.82	1.78
1.87	1.90	1.89	2.01	1.96	2.03	1.99	2.02	1.98
2.14	2.07	2.04	2.15	2.10	2.15	2.10	2.15	2.10
2.53	2.55	2.50	2.54	2.48	2.55	2.49	2.60	2.54
2.53	2.58	2.53	2.58	2.52	2.59	2.53	2.61	2.55
3.41	3.57	3.45	3.51	3.43	3.51	3.43	3.50	3.42
3.60	3.62	3.50	3.55	3.46	3.55	3.47	3.55	3.47
4.05	4.28	4.12	4.28	4.17	4.26	4.15	4.24	4.14
C MAE	1.43	0.70	3.69	0.90	3.69	0.91	3.61	0.83
H MAE	0.07	0.05	0.08	0.06	0.08	0.06	0.08	0.06
C CorrCoef	0.9998		0.9997		0.9997		0.9998	
H CorrCoef	0.9977		0.9962		0.9961		0.9967	
PROBABILITIES								
DP4 combined	99.90%		86.20%		86.80%		89.50%	
DP4 C only	85.60%		48.20%		46.70%		48.00%	
DP4 H only	87.00%		69.10%		69.10%		73.00%	
Gaussian combined	97.90%		82.60%		80.70%		84.80%	
Gaussian C only	71.00%		53.70%		51.70%		50.20%	
Gaussian H only	68.60%		58.30%		57.00%		60.50%	
KDE combined	99.50%		88.90%		88.10%		91.10%	
KDE C only	74.20%		56.80%		54.90%		53.60%	
KDE H only	82.60%		62.10%		59.00%		62.20%	
RKDE combined	99.10%		83.00%		80.60%		89.80%	
RKDE C only	73.40%		56.90%		57.60%		58.10%	
RKDE H only	88.50%		65.50%		58.10%		60.20%	
URKDE combined	98.20%		81.60%		74.10%		83.30%	
URKDE C only	82.80%		71.30%		71.50%		69.60%	
URKDE H only	84.30%		54.20%		42.50%		55.20%	
2gaus combined	99.50%		88.60%		86.70%		90.10%	
2gaus C only	74.40%		52.90%		50.70%		49.80%	

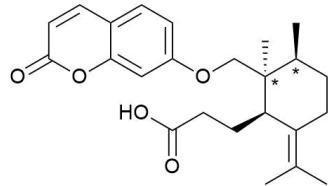
2gaus H only | 79.70% | 69.00% | 61.20% | 67.10% |



Tanarifuranonol, proposed (18)

	Shifts	En-	Shifts	En-	Shifts	En-	Shifts	En-
	B3LYP	Energy	mPW1	Energy	mPW1	Energy	mPW1	Energy
	6-		PW91	6-	PW91	6-	M06-	
Tanarifuranolol2	Func.	B3LYP	B3LYP	mPW1	mPW1	mPW1	mPW1	
	Basis	6-	6-	PW91	PW91	PW91	PW91	
	s.	31G**	31G**	311G*	311G*	311G*	311G*	
	Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
	21.10	23.26	21.49	22.95	21.25	22.91	21.26	22.79
	25.90	27.09	25.40	27.35	25.41	27.37	25.48	27.25
	30.00	29.64	28.00	32.30	30.11	32.33	30.17	32.27
	39.20	41.57	40.17	42.99	40.23	42.99	40.27	42.98
	39.50	41.76	40.37	43.75	40.95	43.62	40.87	43.31
	42.30	42.24	40.86	44.23	41.40	44.20	41.42	44.12
	42.90	44.63	43.30	46.02	43.10	46.03	43.15	45.94
	53.10	54.12	52.98	55.32	51.90	55.26	51.89	55.21
	66.30	65.98	65.08	69.29	65.14	69.30	65.19	69.34
	77.00	76.80	76.13	79.74	75.03	79.72	75.06	79.72
	84.70	85.65	85.17	88.94	83.75	88.93	83.77	88.96
	208.00	206.51	208.49	221.49	209.27	221.43	209.24	221.34
								209.08
Proton shifts	0.93	0.89	0.85	0.91	0.84	0.91	0.83	0.88
	1.23	1.14	1.10	1.19	1.13	1.19	1.13	1.20
	1.33	1.43	1.39	1.36	1.31	1.37	1.31	1.45
	1.41	1.51	1.47	1.50	1.45	1.50	1.44	1.49
	1.61	1.60	1.56	1.51	1.46	1.52	1.47	1.50
	1.61	1.65	1.61	1.72	1.68	1.72	1.68	1.70
	1.61	1.73	1.69	1.82	1.79	1.84	1.80	1.84
	1.74	1.90	1.85	1.87	1.83	1.86	1.82	1.88
	1.81	1.91	1.87	1.88	1.84	1.88	1.84	1.90
	2.13	2.07	2.03	2.14	2.11	2.14	2.11	2.14
	2.51	2.50	2.46	2.47	2.46	2.48	2.47	2.57
	2.51	2.58	2.54	2.56	2.55	2.57	2.56	2.57
	3.43	3.57	3.53	3.50	3.52	3.49	3.52	3.48
	3.88	3.87	3.84	3.78	3.82	3.78	3.81	3.77
	3.92	3.91	3.87	3.83	3.87	3.83	3.87	3.83
								3.86
C MAE	1.42	0.94	3.73	1.03	3.69	1.00	3.55	0.90
H MAE	0.07	0.07	0.08	0.07	0.08	0.07	0.09	0.08
C CorrCoef	0.9997		0.9997		0.9997		0.9998	
H CorrCoef	0.9966		0.9958		0.9957		0.9951	
PROBABILITIES								
DP4 combined	97.5%		98.4%		98.9%		98.6%	
DP4 C only	61.1%		67.3%		70.3%		75.7%	
DP4 H only	92.1%		91.3%		90.6%		82.0%	
Gaussian combined	96.1%		99.0%		99.2%		98.7%	
Gaussian C only	54.4%		61.5%		64.6%		69.6%	
Gaussian H only	85.4%		85.9%		83.5%		70.0%	
KDE combined	97.1%		97.6%		98.6%		98.1%	
KDE C only	58.6%		63.0%		66.8%		73.1%	
KDE H only	90.3%		89.4%		88.9%		73.9%	
RKDE combined	89.4%		84.5%		91.6%		88.4%	
RKDE C only	55.9%		58.0%		60.8%		64.4%	
RKDE H only	78.0%		72.4%		77.2%		57.0%	
URKDE combined	76.1%		77.5%		88.6%		87.1%	
URKDE C only	38.6%		47.7%		50.7%		55.1%	
URKDE H only	75.6%		68.7%		77.0%		69.1%	
2gaus combined	96.6%		97.3%		98.6%		97.6%	
2gaus C only	57.9%		64.1%		67.0%		73.4%	

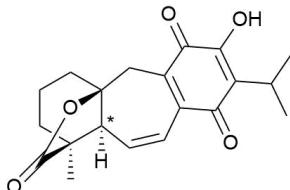
2gaus H only | 90.5% | 89.7% | 89.2% | 74.6% |



Galbanic acid (3)

		Shifts	En-	Shifts	En-	Shifts	En-	Shifts	En-
		B3LYP	Energy	mPW1	Energy	mPW1	Energy	mPW1	Energy
		6-	6-	6-	6-	6-	6-	6-	6-
1109E	Func.	B3LYP	B3LYP	PW91	PW91	PW91	B3LYP	M06-	
	Basis	6-	6-	6-	6-	6-	6-	PW91	2X
	s.	31G**	31G**	311G*	311G*	311G*	31G**	311G*	31G**
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
20.20		21.13	17.61	22.20	18.99	22.24	19.03	22.41	19.17
20.20		20.26	16.68	21.05	17.88	21.06	17.88	21.03	17.83
22.00		26.00	22.77	25.83	22.52	25.76	22.44	25.50	22.17
22.40		25.14	21.86	24.62	21.34	24.58	21.30	24.63	21.32
24.40		27.39	24.24	28.28	24.89	28.30	24.91	28.39	24.97
31.90		30.73	27.76	31.73	28.25	31.70	28.21	31.81	28.29
31.90		34.80	32.07	35.84	32.24	35.85	32.24	35.88	32.24
34.80		39.02	36.54	39.94	36.22	39.94	36.21	39.95	36.20
40.70		48.38	46.44	49.33	45.33	49.34	45.33	49.29	45.27
42.60		46.18	44.11	46.86	42.93	46.90	42.97	47.02	43.06
71.60		71.77	71.20	73.81	69.10	73.84	69.13	73.88	69.15
101.10		98.24	99.21	105.61	99.97	105.66	100.02	105.91	100.26
112.20		110.85	112.55	117.61	111.62	117.60	111.62	117.59	111.60
112.80		111.24	112.96	119.72	113.67	119.65	113.60	119.40	113.36
113.10		114.81	116.74	122.88	116.73	122.87	116.73	122.86	116.71
126.20		128.50	131.23	138.45	131.85	138.51	131.91	138.94	132.33
128.60		126.47	129.08	135.40	128.89	135.40	128.89	135.40	128.90
129.50		131.63	134.54	141.75	135.05	141.70	135.01	141.41	134.73
143.50		136.77	139.98	146.67	139.84	146.68	139.84	146.69	139.85
155.90		152.58	156.71	163.13	155.81	163.13	155.81	163.12	155.82
161.30		158.79	163.28	169.71	162.20	169.71	162.20	169.70	162.20
162.80		155.31	159.60	167.48	160.04	167.48	160.04	167.52	160.09
179.50		168.29	173.33	182.75	174.86	182.72	174.83	182.59	174.72
Proton shifts		0.91	0.97	0.85	0.99	0.88	0.99	0.99	0.87
		1.15	1.33	1.22	1.34	1.24	1.34	1.23	1.23
		1.19	1.40	1.29	1.40	1.30	1.40	1.29	1.28
		1.44	1.53	1.42	1.62	1.52	1.62	1.51	1.49
		1.60	1.62	1.51	1.69	1.59	1.69	1.59	1.58
		1.61	1.37	1.25	1.44	1.33	1.44	1.34	1.31
		1.89	2.05	1.94	1.91	1.81	1.91	1.81	1.82
		1.89	1.95	1.84	1.95	1.84	1.96	1.85	1.89
		1.89	2.09	1.98	2.11	2.01	2.10	2.00	1.97
		1.89	2.03	1.93	2.01	1.91	2.01	1.91	1.93
		2.17	2.28	2.18	2.26	2.16	2.28	2.18	2.34
		2.23	2.31	2.21	2.30	2.20	2.31	2.21	2.24
		2.50	2.41	2.31	2.49	2.39	2.48	2.38	2.46
		2.94	3.32	3.23	3.29	3.20	3.29	3.19	3.32
		3.70	3.92	3.84	3.78	3.69	3.79	3.70	3.78
		3.87	4.08	4.00	3.89	3.80	3.88	3.79	3.88
		6.23	6.18	6.12	6.17	6.09	6.17	6.09	6.17
		6.75	6.81	6.76	6.81	6.74	6.82	6.74	6.83
		6.81	7.00	6.95	7.05	6.97	7.04	6.96	7.03
		7.33	7.56	7.51	7.65	7.57	7.65	7.57	7.65
		7.62	7.33	7.28	7.46	7.38	7.46	7.38	7.38
	C MAE	3.25	2.29	5.16	2.05	5.16	2.05	5.17	2.02
	H MAE	0.16	0.12	0.13	0.10	0.14	0.10	0.14	0.10
	C CorrCoef	0.9986		0.9988		0.9988		0.9988	
	H CorrCoef	0.9976		0.9982		0.9982		0.9981	
PROBABILITIES									
DP4 combined		100.0%		99.9%		99.9%		100.0%	
DP4 C only		99.5%		94.4%		94.7%		98.0%	
DP4 H only		76.3%		93.8%		93.6%		89.2%	

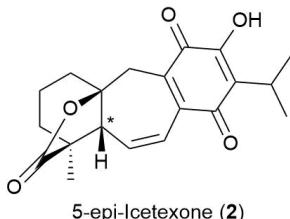
Gaussian combined	99.5%	99.8%	99.8%	99.9%	
Gaussian C only	98.0%	95.2%	94.9%	96.9%	
Gaussian H only	49.0%	82.3%	80.2%	73.7%	
 KDE combined	99.5%	99.8%	99.7%	99.8%	
KDE C only	96.6%	90.7%	89.0%	94.4%	
KDE H only	67.5%	94.3%	93.0%	86.9%	
 RKDE combined	99.6%	100.0%	100.0%	100.0%	
RKDE C only	98.6%	98.9%	98.4%	98.9%	
RKDE H only	57.2%	93.9%	92.0%	80.2%	
 URKDE combined	90.0%	100.0%	100.0%	100.0%	
URKDE C only	96.9%	98.6%	98.8%	98.6%	
URKDE H only	17.9%	81.0%	76.3%	70.2%	
 2gaus combined	99.6%	99.8%	99.7%	99.8%	
2gaus C only	96.7%	90.8%	90.6%	95.1%	
2gaus H only	72.5%	93.4%	92.3%	87.9%	



Icetexone (1)

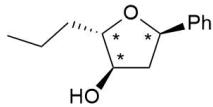
		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
C Ma	Func.	B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06-
	Basis	6-	6-	PW91	PW91	PW91		PW91	2X
	s.	31G**	31G**	311G*	311G*	311G*	31G**	311G*	31G**
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
	19.70	21.28	18.63	21.61	18.98	21.62	18.98	21.61	18.89
	20.10	21.73	19.09	21.79	19.15	21.85	19.21	21.85	19.12
	20.10	22.04	19.42	22.94	20.27	22.96	20.29	22.90	20.15
	24.60	30.00	27.74	30.44	27.57	30.42	27.55	30.77	27.81
	29.90	33.74	31.66	34.29	31.32	34.24	31.28	34.41	31.35
	32.90	36.88	34.94	38.14	35.07	38.16	35.09	38.11	34.96
	36.10	39.14	37.30	39.94	36.82	40.03	36.92	39.68	36.48
	47.90	48.14	46.72	49.31	45.95	49.36	46.01	49.14	45.69
	57.90	60.57	59.72	62.70	58.98	62.84	59.13	62.31	58.51
	92.50	86.11	86.43	89.13	84.72	88.67	84.30	90.46	85.91
	125.30	120.56	122.46	129.17	123.71	129.00	123.58	129.63	124.03
	125.50	124.50	126.58	132.20	126.65	132.19	126.68	132.23	126.57
	133.80	130.57	132.93	138.79	133.07	138.71	133.03	138.95	133.11
	138.90	132.71	135.17	141.65	135.85	141.49	135.74	142.16	136.23
	140.70	138.43	141.15	149.79	143.78	149.79	143.82	149.79	143.66
	151.10	147.48	150.62	157.24	151.04	157.25	151.10	157.06	150.74
	179.00	177.82	182.35	188.93	181.89	188.94	181.96	188.86	181.69
	183.00	179.27	183.87	190.54	183.46	190.57	183.55	190.48	183.27
	185.80	183.36	188.14	193.58	186.42	193.59	186.49	193.65	186.35
Proton shifts	1.24	1.16	1.21	1.20	1.18	1.20	1.18	1.21	1.19
	1.27	1.28	1.32	1.36	1.33	1.36	1.32	1.36	1.34
	1.80	1.71	1.73	1.77	1.73	1.77	1.73	1.76	1.72
	1.80	1.72	1.74	1.81	1.77	1.81	1.76	1.80	1.76
	1.80	1.73	1.75	1.82	1.77	1.82	1.77	1.81	1.77
	1.80	1.75	1.77	1.82	1.77	1.82	1.77	1.82	1.78
	1.80	1.90	1.91	1.94	1.89	1.94	1.89	1.93	1.89
	1.80	1.91	1.92	1.99	1.93	1.99	1.94	1.98	1.93
	2.56	2.35	2.34	2.45	2.38	2.43	2.36	2.52	2.45
	2.80	2.63	2.60	2.72	2.64	2.73	2.65	2.69	2.62
	3.16	3.35	3.30	3.37	3.26	3.37	3.26	3.36	3.27
	3.22	3.56	3.50	3.54	3.43	3.57	3.46	3.44	3.34
	6.44	6.76	6.55	6.81	6.58	6.80	6.57	6.84	6.61
	6.86	6.93	6.72	6.94	6.70	6.94	6.70	6.92	6.70
C MAE		3.08	1.81	4.84	1.68	4.86	1.74	4.82	1.56
H MAE		0.13	0.11	0.12	0.10	0.12	0.11	0.11	0.10
C CorrCoef		0.9993		0.9992		0.9992		0.9994	
H CorrCoef		0.9969		0.9976		0.9974		0.9979	
PROBABILITIES									
DP4 combined		100.0%		100.0%		100.0%		100.0%	
DP4 C only		100.0%		100.0%		100.0%		100.0%	
DP4 H only		67.0%		95.3%		93.3%		97.7%	
Gaussian combined		100.0%		100.0%		100.0%		100.0%	
Gaussian C only		100.0%		100.0%		100.0%		100.0%	
Gaussian H only		60.4%		96.2%		94.5%		97.6%	
KDE combined		100.0%		100.0%		100.0%		100.0%	
KDE C only		100.0%		100.0%		100.0%		100.0%	
KDE H only		62.5%		94.7%		92.4%		96.6%	
RKDE combined		100.0%		100.0%		100.0%		100.0%	
RKDE C only		100.0%		100.0%		100.0%		100.0%	
RKDE H only		78.1%		97.6%		96.1%		98.1%	

URKDE combined	100.0%	100.0%	100.0%	100.0%	
URKDE C only	100.0%	100.0%	100.0%	100.0%	
URKDE H only	95.0%	99.8%	99.7%	99.9%	
2gaus combined	100.0%	100.0%	100.0%	100.0%	
2gaus C only	100.0%	100.0%	100.0%	100.0%	
2gaus H only	62.8%	95.2%	91.3%	96.9%	



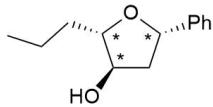
	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
CMb	B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06-
Func.	6-	6-	PW91	PW91	PW91	PW91	PW91	2X
Basis	31G**	31G**	311G*	311G*	311G*	31G**	311G*	6-
s.								6-
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.
19.30	20.92	18.95	21.31	19.36	21.31	19.36	21.35	19.34
20.10	21.00	19.03	21.35	19.40	21.34	19.39	21.51	19.50
20.10	22.21	20.29	21.95	19.98	21.95	19.98	21.95	19.92
25.00	28.64	26.96	28.88	26.68	28.88	26.68	28.87	26.61
27.50	28.82	27.14	29.65	27.42	29.65	27.43	29.66	27.37
27.80	30.05	28.41	30.47	28.21	30.45	28.20	30.70	28.38
38.80	41.48	40.28	42.30	39.64	42.30	39.65	42.28	39.58
46.90	48.10	47.14	49.33	46.44	49.33	46.44	49.33	46.40
54.70	56.77	56.13	58.65	55.45	58.65	55.45	58.65	55.41
82.10	79.61	79.83	82.27	78.28	82.27	78.28	82.27	78.25
124.10	119.96	121.70	127.78	122.26	127.78	122.26	127.74	122.22
125.50	123.99	125.87	131.60	125.95	131.60	125.96	131.59	125.94
133.00	130.33	132.46	139.29	133.38	139.29	133.39	139.25	133.35
133.70	130.89	133.03	139.35	133.44	139.34	133.44	139.39	133.48
137.80	134.13	136.40	145.20	139.10	145.20	139.10	145.20	139.10
150.80	147.29	150.05	157.00	150.50	157.01	150.51	156.90	150.41
179.00	178.08	182.00	189.89	182.29	189.89	182.29	189.86	182.28
184.00	180.06	184.05	190.30	182.69	190.30	182.69	190.30	182.72
185.80	182.75	186.84	192.94	185.23	192.93	185.23	193.01	185.33
Proton shifts								
1.25	1.13	1.14	1.21	1.16	1.21	1.16	1.21	1.16
1.27	1.28	1.28	1.36	1.32	1.36	1.32	1.37	1.32
1.61	1.55	1.55	1.59	1.55	1.59	1.55	1.59	1.55
1.61	1.56	1.55	1.62	1.57	1.62	1.57	1.62	1.57
1.61	1.60	1.60	1.63	1.58	1.63	1.58	1.63	1.58
1.61	1.62	1.62	1.63	1.58	1.63	1.58	1.63	1.58
1.61	1.82	1.81	1.77	1.72	1.77	1.72	1.77	1.72
1.61	1.88	1.88	1.82	1.77	1.82	1.77	1.82	1.77
2.86	2.66	2.63	2.78	2.72	2.78	2.72	2.78	2.72
2.94	2.74	2.71	2.86	2.80	2.86	2.80	2.86	2.80
3.24	3.42	3.37	3.44	3.37	3.44	3.37	3.43	3.37
3.58	3.58	3.53	3.66	3.59	3.66	3.59	3.66	3.59
6.18	6.61	6.49	6.53	6.43	6.53	6.43	6.53	6.43
7.14	7.09	6.96	7.06	6.95	7.06	6.95	7.06	6.95
C MAE	2.40	1.04	4.29	0.95	4.28	0.95	4.31	0.95
H MAE	0.13	0.13	0.10	0.10	0.10	0.10	0.10	0.10
C CorrCoef	0.9998		0.9997		0.9997		0.9997	
H CorrCoef	0.9957		0.9977		0.9977		0.9977	
PROBABILITIES								
DP4 combined	100.0%		100.0%		100.0%		100.0%	
DP4 C only	100.0%		100.0%		100.0%		100.0%	
DP4 H only	100.0%		100.0%		100.0%		100.0%	
Gaussian combined	100.0%		100.0%		100.0%		100.0%	
Gaussian C only	100.0%		100.0%		100.0%		100.0%	
Gaussian H only	100.0%		100.0%		100.0%		100.0%	
KDE combined	100.0%		100.0%		100.0%		100.0%	
KDE C only	100.0%		100.0%		100.0%		100.0%	
KDE H only	99.8%		100.0%		100.0%		100.0%	
RKDE combined	100.0%		100.0%		100.0%		100.0%	
RKDE C only	100.0%		100.0%		100.0%		100.0%	
RKDE H only	99.9%		100.0%		100.0%		100.0%	

URKDE combined	100.0%	100.0%	100.0%	100.0%	
URKDE C only	100.0%	100.0%	100.0%	100.0%	
URKDE H only	99.9%	100.0%	100.0%	100.0%	
 2gaus combined	 100.0%	 100.0%	 100.0%	 100.0%	
2gaus C only	100.0%	100.0%	100.0%	100.0%	
2gaus H only	99.7%	100.0%	100.0%	100.0%	



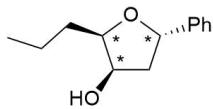
tetrahydrofuran 1 (32)

		tetrahydrofuran 1 (32)							
		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
1166A	Func. Basis s.	B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06- 2X
Carbon shifts	Exp	6- 31G**	6- 31G**	6- 311G*	6- 311G*	6- 311G*	6- 31G**	6- 311G*	6- 31G**
	Calc.	19.10	23.18	19.86	23.69	20.81	23.80	20.83	22.94
		35.30	39.37	37.25	40.15	36.95	40.23	36.96	40.31
		43.40	44.59	42.85	46.15	42.84	46.18	42.80	44.97
		76.80	75.94	76.52	79.36	75.42	79.40	75.40	80.20
		78.30	78.26	79.01	81.68	77.69	81.68	77.63	82.70
		85.60	85.07	86.32	88.08	83.96	88.28	84.12	90.09
		125.60	119.63	123.43	129.27	124.37	129.27	124.34	129.64
		127.30	120.98	124.88	130.98	126.05	130.98	126.02	131.28
		128.40	123.49	127.58	133.42	128.44	133.43	128.42	133.69
		143.30	141.75	147.19	152.43	147.09	152.47	147.11	153.12
Proton shifts		0.98	0.99	1.02	1.09	1.04	1.09	1.04	1.07
		1.50	1.53	1.55	1.61	1.55	1.61	1.55	1.55
		1.96	1.86	1.87	2.01	1.94	2.00	1.93	2.26
		2.66	2.58	2.57	2.65	2.57	2.66	2.58	2.66
		3.99	4.06	4.02	4.06	3.94	4.05	3.93	4.06
		4.15	4.12	4.07	4.15	4.03	4.14	4.03	4.27
		5.05	5.36	5.28	5.38	5.24	5.38	5.24	5.41
		7.26	7.30	7.17	7.41	7.22	7.41	7.22	7.41
		7.34	7.48	7.34	7.56	7.37	7.56	7.37	7.60
		7.39	7.53	7.39	7.59	7.40	7.59	7.40	7.61
	C MAE	2.87	1.46	4.03	1.31	4.08	1.31	4.35	1.21
	H MAE	0.10	0.07	0.12	0.07	0.12	0.07	0.16	0.08
	C CorrCoef	0.9992		0.9994		0.9993		0.9994	
	H CorrCoef	0.9992		0.9994		0.9994		0.9991	
PROBABILITIES									
	DP4 combined	92.5%		99.1%		99.0%		98.4%	
	DP4 C only	72.1%		69.2%		69.2%		71.5%	
	DP4 H only	70.6%		79.4%		81.1%		65.9%	
Gaussian combined		85.8%		98.8%		98.7%		97.4%	
	Gaussian C only	61.9%		59.3%		59.8%		57.0%	
	Gaussian H only	56.5%		70.3%		72.8%		57.2%	
KDE combined		82.2%		98.4%		98.3%		94.7%	
	KDE C only	56.5%		66.8%		66.9%		60.8%	
	KDE H only	64.6%		79.0%		80.1%		60.8%	
RKDE combined		88.2%		98.4%		98.5%		91.9%	
	RKDE C only	57.1%		80.7%		81.3%		59.5%	
	RKDE H only	73.6%		78.6%		79.7%		53.0%	
URKDE combined		95.3%		97.7%		97.3%		91.9%	
	URKDE C only	70.6%		71.4%		70.3%		66.1%	
	URKDE H only	68.3%		83.7%		84.1%		59.0%	
2gaus combined		79.7%		98.0%		97.8%		93.5%	
	2gaus C only	54.8%		66.8%		66.2%		62.9%	
	2gaus H only	63.4%		77.1%		79.1%		56.9%	



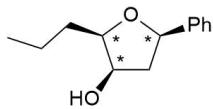
tetrahydrofuran 2 (33)

		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
1166B	Func. Basis s.	B3LYP	B3LYP	mPW1	mPW1	mPW1	mPW1	mPW1	M06- 2X
Carbon shifts	Exp	6- 31G**	6- 31G**	PW91	PW91	PW91	B3LYP	PW91	6- 31G*
		Calc.	Corr.	311G*	311G*	311G*	31G**	311G*	31G**
				Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
	19.10	23.23	19.99	23.69	21.04	23.82	21.14	23.42	21.04
	36.50	40.79	38.82	41.30	38.24	41.31	38.23	40.86	38.04
	44.00	44.07	42.34	45.13	41.98	45.17	42.00	45.08	42.15
	76.80	76.22	76.79	79.62	75.67	79.47	75.53	79.54	75.74
	79.50	80.09	80.94	83.94	79.90	83.78	79.74	83.64	79.74
	87.10	86.48	87.78	89.90	85.72	89.85	85.67	89.60	85.55
	125.90	119.98	123.69	129.59	124.50	129.64	124.56	129.64	124.58
	127.40	120.78	124.55	130.72	125.60	130.72	125.62	130.73	125.64
	128.30	123.11	127.04	133.02	127.85	133.02	127.86	133.02	127.88
	142.10	141.28	146.51	152.16	146.55	152.22	146.63	152.18	146.55
Proton shifts									
	0.99	0.98	1.03	1.07	1.06	1.07	1.05	1.07	1.04
	1.56	1.51	1.54	1.56	1.52	1.57	1.53	1.57	1.52
	1.97	1.84	1.85	1.89	1.84	1.93	1.87	1.93	1.86
	2.21	2.22	2.21	2.33	2.25	2.34	2.26	2.38	2.29
	3.91	4.03	3.93	4.08	3.92	4.04	3.89	4.08	3.92
	4.17	4.22	4.11	4.22	4.06	4.20	4.04	4.18	4.02
	5.12	5.58	5.40	5.64	5.40	5.62	5.40	5.60	5.38
	7.30	7.44	7.16	7.51	7.19	7.51	7.20	7.51	7.21
	C MAE	2.80	1.77	4.05	1.55	4.05	1.55	3.91	1.49
	H MAE	0.12	0.08	0.15	0.10	0.14	0.10	0.15	0.10
	C CorrCoef	0.9989		0.9991		0.9991		0.9991	
	H CorrCoef	0.9982		0.9979		0.9981		0.9981	
PROBABILITIES									
	DP4 combined	39.5%		69.5%		74.4%		59.8%	
	DP4 C only	15.0%		65.3%		63.0%		48.7%	
	DP4 H only	54.2%		44.8%		51.9%		49.2%	
Gaussian combined		50.0%		79.0%		81.1%		60.9%	
Gaussian C only		31.3%		72.4%		68.4%		52.8%	
Gaussian H only		40.5%		44.0%		50.1%		43.7%	
KDE combined		36.6%		65.8%		72.2%		55.9%	
KDE C only		17.9%		61.2%		58.9%		45.0%	
KDE H only		49.1%		44.9%		53.5%		48.4%	
RKDE combined		66.0%		47.9%		58.4%		77.3%	
RKDE C only		24.3%		34.4%		33.0%		44.9%	
RKDE H only		69.7%		53.0%		63.3%		64.4%	
URKDE combined		85.3%		57.9%		65.6%		80.8%	
URKDE C only		49.7%		44.0%		40.0%		33.1%	
URKDE H only		75.0%		55.1%		66.1%		73.8%	
2gaus combined		34.6%		67.5%		72.3%		56.6%	
2gaus C only		17.2%		63.0%		60.1%		46.0%	
2gaus H only		47.7%		44.1%		52.7%		47.7%	



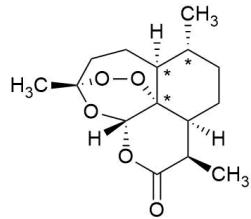
tetrahydrofuran 3 (34)

		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
1166C	Func. Basis s.	B3LYP 6- 31G**	B3LYP 6- 31G**	mPW1 6- 311G*	mPW1 6- 311G*	mPW1 6- 311G*	mPW1 B3LYP 6- 311G*	mPW1 M06- PW91 6- 311G*	M06- 2X 6- 31G**
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
		19.70	23.72	20.51	24.30	21.51	24.40	21.54	23.95
		31.30	34.74	32.32	35.09	32.07	35.21	32.13	34.90
		44.70	44.29	42.57	45.73	42.49	45.82	42.52	45.96
		73.70	74.38	74.85	77.22	73.32	77.27	73.34	76.96
		78.20	80.03	80.92	83.86	79.82	83.74	79.67	83.37
		83.10	83.07	84.18	86.16	82.07	86.16	82.05	85.44
		125.30	119.49	123.24	129.04	124.05	129.02	124.04	128.98
		127.20	120.65	124.49	130.61	125.58	130.62	125.60	130.65
		128.40	123.23	127.25	133.15	128.07	133.16	128.09	133.19
		143.80	141.49	146.84	152.32	146.84	152.33	146.87	152.36
Proton shifts		1.01	1.01	1.09	1.11	1.10	1.11	1.10	1.09
		1.47	1.43	1.49	1.47	1.46	1.48	1.46	1.57
		1.56	1.47	1.52	1.53	1.51	1.54	1.52	1.58
		1.64	1.69	1.73	1.74	1.71	1.75	1.72	1.66
		1.64	1.74	1.78	1.84	1.81	1.83	1.80	1.84
		2.08	1.72	1.77	1.86	1.83	1.87	1.84	1.88
		2.45	2.39	2.40	2.48	2.43	2.49	2.44	2.53
		4.06	4.18	4.12	4.18	4.06	4.17	4.05	4.18
		4.36	4.24	4.17	4.22	4.10	4.21	4.09	4.18
		5.26	5.66	5.53	5.69	5.52	5.68	5.51	5.63
		7.29	7.43	7.22	7.52	7.28	7.52	7.29	7.52
C MAE		2.93	1.78	4.03	1.32	4.05	1.31	3.85	1.27
H MAE		0.13	0.12	0.15	0.11	0.14	0.11	0.15	0.10
C CorrCoef		0.9991		0.9994		0.9994		0.9994	
H CorrCoef		0.9968		0.9970		0.9970		0.9971	
PROBABILITIES									
DP4 combined		4.1%		36.6%		45.7%		53.9%	
DP4 C only		56.2%		58.0%		61.3%		62.3%	
DP4 H only		2.0%		7.9%		11.0%		7.9%	
Gaussian combined		12.6%		37.0%		45.6%		47.4%	
Gaussian C only		64.1%		63.5%		65.5%		66.9%	
Gaussian H only		3.7%		6.6%		8.4%		5.6%	
KDE combined		7.0%		33.6%		42.7%		41.9%	
KDE C only		50.2%		57.6%		61.0%		60.4%	
KDE H only		4.0%		7.7%		9.2%		5.8%	
RKDE combined		17.7%		22.2%		26.2%		34.5%	
RKDE C only		73.9%		53.3%		55.9%		56.3%	
RKDE H only		4.3%		5.9%		6.3%		5.8%	
URKDE combined		18.4%		15.0%		20.8%		26.3%	
URKDE C only		64.8%		37.3%		39.7%		39.7%	
URKDE H only		8.5%		6.5%		9.0%		13.6%	
2gaus combined		6.3%		25.9%		36.4%		43.0%	
2gaus C only		49.8%		54.8%		59.0%		60.2%	
2gaus H only		3.6%		6.3%		8.1%		6.3%	



tetrahydrofuran 4 (35)

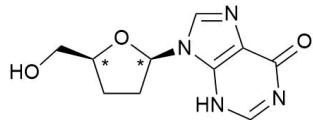
		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
1166D	Func. Basis s.	B3LYP 6- 31G**	B3LYP 6- 31G**	mPW1 mPW1 PW91 PW91	mPW1 mPW1 PW91 PW91	mPW1 mPW1 PW91 PW91	mPW1 mPW1 B3LYP B3LYP	mPW1 mPW1 PW91 PW91	M06- 2X 6- 31G**
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
		19.60	23.20	20.14	23.61	20.94	23.81	21.04	23.50
		30.90	35.88	33.64	36.19	33.19	36.28	33.18	35.84
		44.20	44.01	42.30	45.92	42.66	45.91	42.56	45.94
		73.10	73.95	74.18	76.94	72.84	77.12	72.95	76.90
		78.70	78.65	79.19	82.03	77.80	82.08	77.78	82.06
		83.60	82.87	83.68	86.25	81.91	86.36	81.96	86.07
		125.90	119.81	123.02	129.57	124.06	129.58	124.04	129.59
		127.30	121.27	124.58	131.26	125.71	131.27	125.69	131.27
		128.40	123.86	127.34	133.73	128.11	133.73	128.09	133.74
		143.00	143.36	148.11	153.90	147.74	153.92	147.74	153.97
Proton shifts		1.00	1.00	0.94	1.10	0.97	1.10	0.97	1.10
		1.52	1.52	1.45	1.61	1.47	1.61	1.46	1.62
		1.52	1.59	1.52	1.64	1.50	1.66	1.52	1.63
		1.52	1.62	1.55	1.68	1.54	1.68	1.54	1.73
		1.72	1.72	1.65	1.82	1.68	1.82	1.67	1.85
		1.92	2.22	2.14	2.30	2.16	2.31	2.16	2.32
		2.70	2.59	2.51	2.70	2.55	2.70	2.55	2.71
		3.76	4.02	3.91	4.02	3.86	4.01	3.84	4.01
		4.27	4.16	4.05	4.15	3.98	4.14	3.97	4.17
		4.87	5.31	5.18	5.33	5.15	5.34	5.15	5.33
		7.26	7.32	7.15	7.40	7.20	7.41	7.20	7.40
		7.34	7.51	7.34	7.56	7.36	7.57	7.36	7.57
		7.40	7.58	7.40	7.60	7.39	7.60	7.39	7.60
C MAE		2.68	1.83	4.27	1.52	4.33	1.54	4.20	1.50
H MAE		0.14	0.11	0.18	0.10	0.19	0.10	0.19	0.10
C CorrCoef		0.9987		0.9991		0.9991		0.9991	
H CorrCoef		0.9980		0.9982		0.9981		0.9982	
PROBABILITIES									
DP4 combined		99.1%		91.3%		89.5%		99.2%	
DP4 C only		34.9%		26.4%		24.5%		25.3%	
DP4 H only		43.9%		37.6%		33.6%		84.0%	
Gaussian combined		98.1%		92.5%		90.6%		99.2%	
Gaussian C only		24.2%		22.6%		21.9%		24.4%	
Gaussian H only		58.9%		44.3%		39.1%		77.5%	
KDE combined		95.6%		91.1%		88.0%		95.5%	
KDE C only		46.1%		35.6%		32.7%		38.6%	
KDE H only		37.6%		42.8%		34.5%		73.7%	
RKDE combined		90.8%		95.9%		95.3%		92.9%	
RKDE C only		18.7%		44.2%		41.3%		41.3%	
RKDE H only		19.9%		31.9%		24.7%		75.5%	
URKDE combined		89.3%		93.4%		90.3%		77.6%	
URKDE C only		27.4%		53.7%		51.8%		55.9%	
URKDE H only		27.0%		18.1%		14.2%		53.8%	
2gaus combined		94.3%		86.9%		83.3%		94.2%	
2gaus C only		45.0%		31.7%		28.8%		32.2%	
2gaus H only		35.1%		35.7%		29.9%		73.9%	



Artemisinin (27)

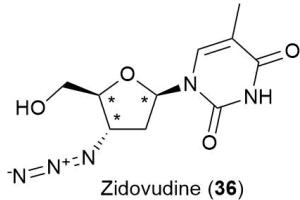
		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
Artemisinin	Func. Basis s.	B3LYP 6- 31G**	B3LYP 6- 31G**	mPW1 6- 311G*	mPW1 6- 311G*	mPW1 6- 311G*	B3LYP 6- 31G**	mPW1 6- 311G*	M06- PW91 2X 6- 31G**
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
20.50	21.49	18.74		21.35	18.90	21.35	18.90	21.35	18.90
24.00	26.49	23.81		27.58	24.81	27.58	24.81	27.58	24.81
25.50	26.84	24.16		27.60	24.83	27.60	24.83	27.60	24.83
25.80	28.67	26.02		29.42	26.56	29.42	26.56	29.42	26.56
33.50	35.67	33.10		36.67	33.45	36.67	33.45	36.67	33.45
34.20	37.57	35.02		38.75	35.43	38.75	35.43	38.75	35.43
36.50	38.99	36.47		40.34	36.94	40.34	36.94	40.34	36.94
38.20	40.30	37.78		41.54	38.08	41.54	38.08	41.54	38.08
45.60	48.55	46.14		49.39	45.53	49.39	45.53	49.39	45.53
50.70	52.70	50.35		53.93	49.85	53.93	49.85	53.93	49.85
80.10	83.93	81.97		85.89	80.22	85.89	80.22	85.89	80.22
94.30	98.83	97.06		101.56	95.10	101.56	95.10	101.56	95.10
106.00	106.62	104.95		110.08	103.20	110.08	103.20	110.08	103.20
172.70	172.13	171.29		184.49	173.90	184.49	173.90	184.49	173.90
Proton shifts									
0.98	0.90	0.90		0.97	0.90	0.97	0.90	0.97	0.90
1.05	1.05	1.05		0.97	0.90	0.97	0.90	0.97	0.90
1.05	1.07	1.06		1.11	1.05	1.11	1.05	1.11	1.05
1.18	1.08	1.07		1.16	1.10	1.16	1.10	1.16	1.10
1.42	1.39	1.37		1.42	1.37	1.42	1.37	1.42	1.37
1.42	1.45	1.43		1.49	1.43	1.49	1.43	1.49	1.43
1.42	1.51	1.49		1.63	1.58	1.63	1.58	1.63	1.58
1.42	1.63	1.61		1.69	1.64	1.69	1.64	1.69	1.64
1.75	1.73	1.71		1.71	1.66	1.71	1.66	1.71	1.66
1.75	1.75	1.72		1.84	1.79	1.84	1.79	1.84	1.79
1.86	1.90	1.87		1.88	1.84	1.88	1.84	1.88	1.84
1.99	1.93	1.90		1.95	1.91	1.95	1.91	1.95	1.91
1.99	2.09	2.06		2.11	2.07	2.11	2.07	2.11	2.07
2.41	2.64	2.59		2.63	2.60	2.63	2.60	2.63	2.60
3.38	3.29	3.21		3.26	3.24	3.26	3.24	3.26	3.24
5.84	6.03	5.87		5.78	5.84	5.78	5.84	5.78	5.84
C MAE	2.39	0.93		4.27	0.82	4.27	0.82	4.27	0.82
H MAE	0.08	0.07		0.09	0.09	0.09	0.09	0.09	0.09
C CorrCoef	0.9996			0.9997		0.9997		0.9997	
H CorrCoef	0.9969			0.9956		0.9956		0.9956	
PROBABILITIES									
DP4 combined	100.0%			100.0%		100.0%		100.0%	
DP4 C only	98.1%			82.2%		82.1%		82.2%	
DP4 H only	93.3%			97.5%		97.5%		97.5%	
Gaussian combined	99.9%			99.9%		99.9%		99.9%	
Gaussian C only	93.5%			69.6%		68.9%		69.5%	
Gaussian H only	81.5%			93.6%		93.5%		92.7%	
KDE combined	99.9%			99.9%		99.9%		99.9%	
KDE C only	87.2%			73.3%		72.9%		72.9%	
KDE H only	91.4%			93.5%		92.9%		93.4%	
RKDE combined	100.0%			99.1%		99.4%		99.8%	
RKDE C only	92.7%			86.5%		87.5%		87.7%	
RKDE H only	93.1%			82.9%		85.6%		91.5%	

URKDE combined	100.0%	99.7%	99.8%	99.6%	
URKDE C only	94.2%	92.5%	93.3%	90.0%	
URKDE H only	97.0%	87.4%	88.9%	87.0%	
 2gaus combined	 99.9%	 99.9%	 99.9%	 99.9%	
2gaus C only	87.3%	74.9%	75.0%	76.1%	
2gaus H only	89.1%	92.4%	94.8%	91.7%	

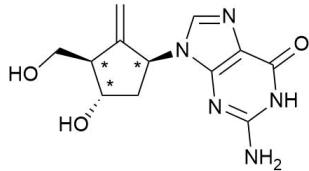


Didanosine (37)

		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
Didanosine	Func. Basis s.	B3LYP 6- 31G**	B3LYP 6- 31G**	mPW1 311G*	mPW1 311G*	mPW1 311G*	mPW1 311G**	mPW1 311G*	M06- 2X 31G**
Carbon shifts	Exp	32.21	34.01	29.37	34.91	30.08	34.91	30.09	34.94
		62.71	66.75	64.95	70.00	65.17	69.98	65.16	69.89
		82.11	79.69	79.01	82.95	78.12	82.96	78.13	83.01
		84.52	90.70	90.97	93.75	88.91	93.74	88.91	78.19
		124.38	125.70	129.00	132.37	127.53	132.36	127.53	132.36
		138.25	134.66	138.73	144.67	139.84	144.67	139.83	144.66
		145.68	139.98	144.52	150.20	145.36	150.19	145.36	139.83
		147.66	138.85	143.29	148.50	143.66	148.50	143.67	145.36
		156.68	150.43	155.87	160.95	156.11	160.95	156.12	143.66
Proton shifts		2.03	2.28	2.14	2.37	2.13	2.37	2.13	2.39
		2.03	2.29	2.15	2.42	2.18	2.42	2.18	2.41
		2.40	2.58	2.45	2.58	2.35	2.58	2.35	2.57
		2.40	2.12	1.97	2.22	1.96	2.22	1.97	2.23
		3.51	3.43	3.35	3.52	3.38	3.52	3.38	3.53
		3.63	3.99	3.94	4.14	4.06	4.14	4.06	4.06
		4.11	4.19	4.16	4.17	4.09	4.17	4.09	4.17
		6.20	6.10	6.19	6.10	6.20	6.10	6.20	6.20
		8.06	7.84	8.02	7.72	7.97	7.72	7.97	7.72
		8.34	8.15	8.35	8.10	8.38	8.10	8.38	7.96
	C MAE	4.37	2.76	4.83	2.32	4.83	2.31	4.82	2.30
	H MAE	0.20	0.13	0.24	0.15	0.24	0.14	0.24	0.15
PROBABILITIES	C CorrCoef	0.9975		0.9983		0.9983		0.9983	
	H CorrCoef	0.9967		0.9959		0.9959		0.9960	
DP4 combined		90.0%		54.5%		58.2%		58.7%	
DP4 C only		3.9%		2.1%		2.3%		10.0%	
DP4 H only		99.5%		98.2%		98.3%		92.7%	
Gaussian combined		90.4%		52.5%		58.9%		41.0%	
Gaussian C only		7.2%		3.0%		3.5%		10.1%	
Gaussian H only		99.2%		97.3%		97.5%		86.0%	
KDE combined		77.1%		40.6%		44.7%		54.0%	
KDE C only		6.8%		3.4%		4.0%		14.2%	
KDE H only		97.9%		95.1%		95.1%		87.7%	
RKDE combined		55.8%		31.1%		28.2%		35.8%	
RKDE C only		9.2%		4.3%		4.2%		16.5%	
RKDE H only		92.6%		91.0%		89.9%		73.8%	
URKDE combined		34.0%		32.7%		41.9%		50.6%	
URKDE C only		43.4%		50.6%		52.8%		62.4%	
URKDE H only		40.2%		32.2%		39.2%		38.2%	
2gaus combined		83.8%		50.8%		56.1%		67.4%	
2gaus C only		7.6%		3.4%		3.9%		14.1%	
2gaus H only		98.4%		96.7%		96.9%		92.7%	

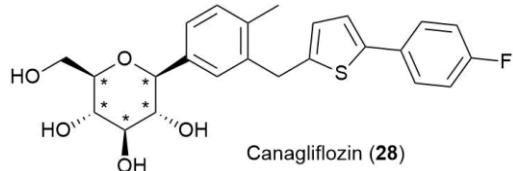


		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
Zidovudine	Func. Basis s.	B3LYP 6- 31G**	B3LYP 6- 31G**	mPW1 PW91 311G*	mPW1 PW91 311G*	mPW1 PW91 311G*	B3LYP 6- 31G**	mPW1 PW91 311G*	M06- 2X 6- 31G**
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
	34.33	37.67	29.13	38.65	29.87	38.61	29.81	38.51	29.67
	58.27	65.73	59.63	68.01	59.13	68.06	59.17	68.17	59.22
	58.90	65.38	59.25	68.72	59.84	68.75	59.85	68.83	59.88
	81.56	89.09	85.02	91.90	82.95	91.93	82.97	92.03	83.00
	82.11	96.28	92.84	98.90	89.93	98.97	89.99	99.18	90.13
	107.59	112.71	110.70	119.82	110.79	119.84	110.79	119.89	110.77
	134.10	133.44	133.24	142.91	133.81	142.95	133.83	143.09	133.89
	148.48	143.68	144.37	155.03	145.89	155.03	145.87	155.04	145.81
	161.78	156.02	157.79	167.26	158.09	167.26	158.06	167.26	157.98
Proton shifts	1.73	1.79	1.46	1.84	1.45	1.84	1.45	1.84	1.44
	2.22	1.96	1.65	2.06	1.70	2.06	1.70	2.04	1.68
	2.33	2.82	2.63	2.75	2.51	2.75	2.51	2.77	2.53
	3.55	3.57	3.49	3.63	3.53	3.62	3.52	3.62	3.52
	3.61	3.93	3.91	4.08	4.05	4.07	4.05	4.07	4.05
	3.77	4.29	4.33	4.25	4.25	4.25	4.25	4.26	4.26
	4.35	4.39	4.44	4.44	4.47	4.44	4.47	4.44	4.48
	6.05	5.61	5.85	5.58	5.80	5.58	5.80	5.57	5.80
	7.62	7.03	7.47	7.02	7.47	7.02	7.47	7.01	7.47
	C MAE	6.09	3.80	8.96	2.84	8.98	2.87	9.04	2.92
	H MAE	0.30	0.28	0.32	0.27	0.32	0.27	0.33	0.28
	C CorrCoef	0.9950		0.9972		0.9972		0.9971	
	H CorrCoef	0.9836		0.9847		0.9848		0.9839	
PROBABILITIES									
	DP4 combined	0.0%		0.0%		0.0%		0.0%	
	DP4 C only	0.0%		0.0%		0.0%		0.0%	
	DP4 H only	0.3%		1.1%		0.9%		3.4%	
	Gaussian combined	0.0%		0.0%		0.0%		0.0%	
	Gaussian C only	0.0%		0.0%		0.0%		0.0%	
	Gaussian H only	0.2%		0.6%		0.5%		2.3%	
	KDE combined	0.0%		0.0%		0.0%		0.0%	
	KDE C only	0.0%		0.0%		0.0%		0.0%	
	KDE H only	3.5%		8.5%		6.8%		23.0%	
	RKDE combined	0.0%		0.0%		0.0%		0.1%	
	RKDE C only	0.0%		0.0%		0.0%		0.0%	
	RKDE H only	3.9%		12.9%		13.3%		41.5%	
	URKDE combined	0.5%		0.8%		0.5%		0.7%	
	URKDE C only	6.1%		3.4%		2.7%		3.4%	
	URKDE H only	2.7%		8.2%		7.1%		6.9%	
	2gaus combined	0.0%		0.0%		0.0%		0.0%	
	2gaus C only	0.0%		0.0%		0.0%		0.0%	
	2gaus H only	2.7%		8.2%		5.9%		15.7%	



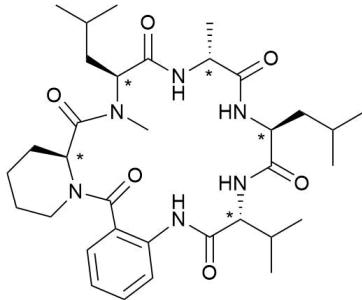
Entecavir (42)

	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
Entecavir	B3LYP	B3LYP	mPW1	mPW1	PW91	B3LYP	mPW1	M06-
Func.							PW91	2X
Basis	6-	6-	6-	6-	6-	6-	6-	6-
s.	31G**	31G**	311G*	311G*	311G*	31G**	311G*	31G**
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.
54.10	58.17	53.00	60.46	53.19	60.49	53.21	60.46	53.20
55.20	60.49	55.57	62.20	54.94	62.20	54.94	62.18	54.93
63.10	67.30	63.13	70.31	63.13	70.32	63.14	70.27	63.10
70.40	75.52	72.27	78.74	71.64	78.74	71.64	78.72	71.63
109.30	111.38	112.13	121.01	114.33	121.02	114.34	121.03	114.36
116.20	118.65	120.22	125.15	118.51	125.15	118.51	125.15	118.51
136.00	134.13	137.42	143.79	137.32	143.79	137.32	143.78	137.33
151.30	139.21	143.07	148.85	142.43	148.85	142.43	148.85	142.44
151.50	144.38	148.82	156.05	149.71	156.05	149.71	156.05	149.72
153.50	150.43	155.54	160.86	154.56	160.86	154.56	160.86	154.57
156.90	153.92	159.42	166.48	160.24	166.50	160.25	166.45	160.21
Proton shifts	2.04	2.19	1.77	2.40	1.85	2.40	1.85	2.40
	2.22	2.72	2.32	2.73	2.21	2.73	2.21	2.72
	2.52	2.74	2.34	2.83	2.32	2.83	2.32	2.83
	3.53	3.90	3.54	3.94	3.51	3.94	3.51	3.94
	3.53	3.98	3.63	4.10	3.68	4.10	3.68	4.10
	4.23	4.59	4.26	4.69	4.32	4.69	4.32	4.69
	4.84	5.30	4.99	5.27	4.94	5.27	4.94	5.27
	4.87	5.44	5.13	5.51	5.20	5.51	5.20	5.51
	5.36	5.72	5.42	5.70	5.40	5.70	5.40	5.70
	7.66	7.62	7.39	7.53	7.37	7.53	7.37	7.37
C MAE	4.51	2.52	7.19	2.39	7.19	2.39	7.18	2.39
H MAE	0.35	0.14	0.42	0.14	0.42	0.14	0.41	0.14
C CorrCoef	0.9972		0.9971		0.9970		0.9971	
H CorrCoef	0.9945		0.9942		0.9942		0.9942	
PROBABILITIES								
DP4 combined	100.0%		100.0%		100.0%		100.0%	
DP4 C only	73.9%		21.7%		24.4%		54.4%	
DP4 H only	99.7%		99.8%		99.7%		75.4%	
Gaussian combined	100.0%		100.0%		100.0%		100.0%	
Gaussian C only	66.5%		4.5%		5.5%		13.0%	
Gaussian H only	99.7%		99.9%		99.8%		76.1%	
KDE combined	99.8%		99.8%		99.8%		99.6%	
KDE C only	71.4%		81.9%		83.8%		85.1%	
KDE H only	96.6%		97.0%		96.8%		64.7%	
RKDE combined	97.9%		96.9%		96.6%		96.0%	
RKDE C only	49.8%		39.5%		40.5%		49.5%	
RKDE H only	92.1%		94.6%		93.8%		62.2%	
URKDE combined	24.3%		14.0%		15.4%		33.4%	
URKDE C only	18.6%		15.3%		14.5%		12.4%	
URKDE H only	15.0%		13.0%		13.4%		38.5%	
2gaus combined	99.6%		99.8%		99.9%		99.7%	
2gaus C only	59.2%		44.7%		47.9%		70.4%	
2gaus H only	97.0%		97.6%		97.1%		68.9%	



	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
Canagliflozin	B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06-
Func.	6-	6-	PW91	PW91	PW91	6-	6-	2X
Basis	31G**	31G**	311G*	311G*	311G*	31G**	311G*	6-
s.			Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.
	33.44	35.25	31.95	35.95	33.05	35.98	33.02	36.13
	61.43	65.13	63.46	67.84	63.56	68.02	63.69	67.41
	70.42	74.72	73.57	76.56	71.89	76.91	72.19	76.03
	74.67	78.17	77.21	80.18	75.36	80.06	75.21	80.22
	78.48	79.18	78.27	81.35	76.48	81.30	76.40	81.43
	81.21	79.46	78.57	81.76	76.87	81.78	76.85	81.76
	81.32	83.58	82.92	85.74	80.68	85.78	80.68	85.71
	115.88	112.65	113.58	121.51	114.89	121.52	114.89	121.51
	123.39	120.93	122.31	131.30	124.25	131.31	124.26	131.28
	126.25	121.45	122.86	132.00	124.92	131.96	124.88	132.09
	126.36	122.31	123.76	132.07	124.99	132.08	124.99	132.17
	126.95	126.02	127.68	135.80	128.56	135.78	128.54	135.82
	129.06	126.79	128.48	136.41	129.14	136.47	129.19	136.38
	129.65	127.71	129.46	137.04	129.74	137.08	129.78	137.03
	130.52	128.50	130.29	138.19	130.84	138.19	130.84	138.20
	134.93	133.79	135.86	143.25	135.68	143.24	135.67	143.25
	137.36	134.05	136.14	144.57	136.95	144.61	136.98	144.71
	138.24	137.56	139.84	147.99	140.22	147.94	140.17	147.95
	140.22	140.55	142.99	148.01	140.24	147.95	140.18	148.06
	143.63	143.80	146.43	152.72	144.74	152.70	144.73	152.64
	161.37	157.18	160.53	169.23	160.53	169.23	160.55	169.24
Proton shifts	2.27	2.30	1.90	2.43	1.84	2.42	1.83	2.41
	3.16	3.49	3.17	3.54	3.06	3.55	3.07	3.56
	3.18	3.59	3.27	3.75	3.29	3.75	3.29	3.73
	3.22	3.86	3.56	4.00	3.56	4.00	3.56	4.01
	3.27	3.92	3.63	4.07	3.64	4.08	3.64	4.07
	3.45	3.99	3.69	4.08	3.65	4.08	3.65	4.11
	3.71	4.01	3.71	4.16	3.74	4.17	3.74	4.16
	3.97	4.05	3.76	4.25	3.84	4.25	3.83	4.25
	4.10	4.07	3.78	4.26	3.84	4.26	3.85	4.26
	4.15	4.24	3.96	4.46	4.07	4.47	4.07	4.47
	6.80	6.98	6.87	6.86	6.69	6.84	6.68	6.85
	7.12	7.05	6.94	6.97	6.82	6.97	6.82	6.97
	7.15	7.12	7.02	7.16	7.03	7.16	7.03	7.17
	7.20	7.31	7.22	7.34	7.23	7.35	7.23	7.34
	7.23	7.43	7.34	7.54	7.45	7.54	7.45	7.54
	7.28	7.58	7.50	7.60	7.51	7.61	7.52	7.61
	7.59	7.60	7.53	7.68	7.60	7.68	7.59	7.68
C MAE	2.37	1.65	6.28	1.12	6.30	1.13	6.26	1.05
H MAE	0.24	0.17	0.33	0.18	0.33	0.18	0.33	0.18
C CorrCoef	0.9987		0.9992		0.9992		0.9993	
H CorrCoef	0.9939		0.9935		0.9933		0.9932	
PROBABILITIES								
DP4 combined	2.6%		99.7%		99.8%		99.9%	
DP4 C only	1.1%		78.2%		84.5%		88.7%	
DP4 H only	1.7%		20.8%		16.1%		15.3%	
Gaussian combined	6.7%		99.5%		99.7%		99.9%	
Gaussian C only	3.6%		73.6%		81.7%		80.8%	
Gaussian H only	2.4%		19.4%		15.2%		14.6%	
KDE combined	2.4%		98.5%		98.9%		99.4%	
KDE C only	2.2%		75.8%		80.3%		85.6%	
KDE H only	2.3%		20.8%		20.0%		18.4%	

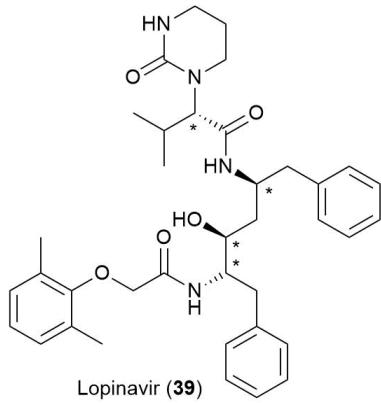
RKDE combined	24.0%	93.1%	95.4%	95.6%	
RKDE C only	14.7%	59.5%	68.6%	70.5%	
RKDE H only	8.1%	35.6%	34.5%	33.8%	
URKDE combined	82.0%	68.8%	76.8%	65.7%	
URKDE C only	23.4%	17.9%	26.6%	17.3%	
URKDE H only	65.1%	66.5%	64.3%	64.1%	
2gaus combined	3.2%	98.6%	99.0%	99.4%	
2gaus C only	2.4%	71.9%	78.0%	83.1%	
2gaus H only	2.9%	28.6%	30.1%	22.7%	



Similanamide (41)

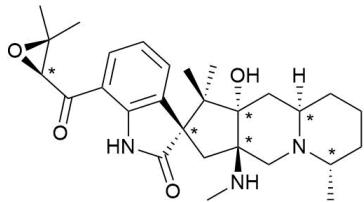
		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
Similanamide	Func. Basis s.	B3LYP 6- 31G**	B3LYP 6- 31G**	mPW1 PW91 311G*	mPW1 PW91 311G*	mPW1 PW91 311G*	B3LYP 6- 31G**	mPW1 PW91 311G*	M06- 2X 31G**
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
	18.40	19.12	17.85	19.39	18.54	19.28	18.45	19.44	18.61
	19.70	21.55	20.33	21.92	20.92	22.00	21.01	22.20	21.21
	21.70	20.31	19.06	20.41	19.50	20.51	19.61	20.37	19.49
	22.10	22.72	21.53	22.53	21.49	22.85	21.81	22.01	21.03
	23.10	25.00	23.86	25.17	23.97	25.13	23.95	25.15	23.98
	23.30	24.30	23.15	24.76	23.59	24.43	23.30	25.31	24.13
	24.40	26.53	25.43	27.42	26.09	27.47	26.15	27.39	26.08
	24.50	28.43	27.38	28.96	27.54	28.93	27.52	29.09	27.68
	25.60	28.35	27.29	29.27	27.83	29.45	28.02	28.99	27.58
	27.30	26.18	25.07	26.99	25.69	27.02	25.73	26.94	25.66
	28.10	23.02	21.83	23.98	22.86	23.93	22.82	24.00	22.90
	29.90	34.90	33.99	36.25	34.39	36.20	34.36	36.27	34.43
	36.20	38.95	38.14	39.32	37.27	39.37	37.34	39.30	37.27
	37.77	39.77	38.98	39.57	37.51	40.04	37.96	38.74	36.75
	37.82	38.19	37.36	39.64	37.58	39.39	37.36	39.84	37.78
	47.80	52.62	52.13	54.30	51.36	54.20	51.27	54.37	51.43
	50.90	55.52	55.10	57.13	54.01	57.05	53.95	57.11	54.01
	52.50	45.43	44.77	46.58	44.10	46.54	44.08	46.59	44.12
	59.20	65.64	65.45	67.39	63.66	67.32	63.60	67.41	63.69
	61.50	56.53	56.13	58.26	55.07	58.13	54.97	58.37	55.19
	65.10	67.60	67.46	69.27	65.42	68.98	65.16	69.54	65.69
	122.70	118.67	119.72	126.45	119.16	126.49	119.20	126.42	119.13
	123.30	118.44	119.49	127.80	120.43	127.82	120.46	127.78	120.41
	123.90	116.31	117.31	124.44	117.27	124.46	117.30	124.44	117.27
	127.10	125.03	126.24	135.05	127.25	134.97	127.17	135.06	127.25
	131.60	128.92	130.21	139.29	131.23	139.22	131.17	139.30	131.24
	137.10	134.04	135.45	144.26	135.90	144.18	135.83	144.29	135.92
	168.80	172.87	175.19	185.87	175.01	186.16	175.28	185.80	174.93
	169.20	166.59	168.76	179.44	168.96	179.52	169.05	179.29	168.81
	170.10	173.48	175.81	186.57	175.67	186.54	175.64	186.58	175.66
	170.60	166.75	168.93	178.26	167.85	178.40	167.99	178.42	168.00
	174.10	174.51	176.87	188.39	177.38	188.20	177.20	188.44	177.41
	174.30	170.34	172.60	183.95	173.20	183.86	173.12	183.95	173.19
Proton shifts	0.87	0.84	0.83	0.86	0.85	0.86	0.85	0.86	0.84
	0.93	0.99	0.97	1.05	1.04	1.05	1.03	1.04	1.02
	0.96	0.94	0.93	0.98	0.96	0.98	0.97	0.97	0.96
	0.97	0.99	0.97	1.04	1.02	1.03	1.01	1.04	1.03
	0.97	1.06	1.04	1.08	1.06	1.07	1.06	1.08	1.07
	1.06	1.12	1.10	1.17	1.15	1.18	1.16	1.18	1.16
	1.26	1.51	1.48	1.55	1.52	1.55	1.52	1.54	1.51
	1.29	1.49	1.46	1.57	1.54	1.56	1.53	1.57	1.54
	1.52	1.97	1.92	2.02	1.98	2.01	1.97	2.04	1.99
	1.55	1.59	1.56	1.65	1.62	1.64	1.61	1.65	1.62
	1.64	1.85	1.81	1.67	1.63	1.73	1.70	1.55	1.51
	1.76	1.69	1.65	1.71	1.67	1.71	1.67	1.70	1.67
	1.77	2.04	2.00	1.90	1.86	1.90	1.86	1.89	1.85
	1.94	2.24	2.19	2.11	2.07	2.10	2.05	1.96	1.91
	2.00	2.18	2.13	2.24	2.19	2.23	2.18	2.24	2.19
	2.04	1.67	1.64	1.69	1.65	1.68	1.65	1.69	1.66
	2.04	1.47	1.45	1.48	1.45	1.48	1.45	1.47	1.44

2.08	2.12	2.08	2.15	2.10	2.14	2.09	2.16	2.12
2.20	2.26	2.21	2.24	2.19	2.20	2.16	2.48	2.42
2.68	2.33	2.28	2.38	2.33	2.41	2.35	2.40	2.35
3.15	3.28	3.20	3.15	3.08	3.15	3.08	3.16	3.09
3.20	3.17	3.10	3.12	3.05	3.11	3.03	3.13	3.06
3.48	3.79	3.70	3.75	3.66	3.74	3.65	3.79	3.70
3.70	4.60	4.49	4.53	4.42	4.54	4.43	4.54	4.43
4.13	3.78	3.69	3.61	3.53	3.62	3.53	3.61	3.52
4.32	3.80	3.71	3.96	3.86	3.98	3.89	3.95	3.86
4.57	4.36	4.25	4.31	4.21	4.32	4.21	4.31	4.21
4.82	4.66	4.54	4.65	4.54	4.65	4.53	4.65	4.54
7.13	7.11	6.92	7.20	7.02	7.20	7.02	7.21	7.02
7.19	7.57	7.37	7.57	7.38	7.57	7.38	7.57	7.38
7.46	7.63	7.43	7.77	7.57	7.77	7.57	7.76	7.56
8.30	9.10	8.87	9.01	8.78	9.00	8.77	9.01	8.77
C MAE	3.17	2.77	5.33	2.57	5.32	2.54	5.32	2.62
H MAE	0.24	0.22	0.23	0.22	0.23	0.22	0.24	0.23
C CorrCoef	0.9982		0.9983		0.9983		0.9983	
H CorrCoef	0.9895		0.9903		0.9905		0.9900	
PROBABILITIES								
DP4 combined	0.0%		0.0%		0.0%		0.0%	
DP4 C only	0.0%		0.0%		0.0%		0.0%	
DP4 H only	0.0%		0.0%		0.0%		0.0%	
Gaussian combined	0.0%		0.0%		0.0%		0.0%	
Gaussian C only	0.0%		0.0%		0.0%		0.0%	
Gaussian H only	0.0%		0.0%		0.0%		0.0%	
KDE combined	0.0%		0.0%		0.0%		0.0%	
KDE C only	0.0%		0.0%		0.0%		0.0%	
KDE H only	0.1%		0.1%		0.0%		0.0%	
RKDE combined	0.0%		0.0%		0.0%		0.0%	
RKDE C only	0.0%		0.0%		0.0%		0.0%	
RKDE H only	1.0%		15.1%		0.4%		0.1%	
URKDE combined	0.0%		0.0%		0.0%		0.0%	
URKDE C only	0.0%		0.0%		0.0%		0.0%	
URKDE H only	0.5%		21.1%		2.7%		0.4%	
2gaus combined	0.0%		0.0%		0.0%		0.0%	
2gaus C only	0.0%		0.0%		0.0%		0.0%	
2gaus H only	0.0%		0.1%		0.0%		0.0%	



		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
Lopinavir	Func.	B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06-
	Basis	6-	6-	PW91	PW91	PW91		PW91	PW91
	s.	31G**	31G**	311G*	311G*	311G*	31G**	311G*	31G**
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
	18.70	20.46	17.23	20.43	18.16	20.42	18.08	20.51	18.03
	19.60	20.88	17.68	21.01	18.72	20.98	18.61	20.73	18.24
	21.70	22.86	19.78	23.68	21.30	23.54	21.08	23.39	20.80
	25.40	29.01	26.31	29.63	27.03	29.64	26.95	29.82	27.00
	38.20	39.50	37.44	39.40	36.44	40.51	37.42	40.66	37.43
	40.00	39.95	37.91	40.60	37.60	40.60	37.51	41.19	37.94
	40.80	40.46	38.46	41.88	38.83	41.71	38.59	41.91	38.63
	41.10	41.99	40.08	43.08	39.99	42.93	39.76	42.00	38.72
	41.80	42.54	40.67	43.61	40.50	43.58	40.38	43.96	40.60
	48.70	53.99	52.81	55.42	51.88	55.22	51.60	54.87	51.11
	54.40	62.50	61.84	63.10	59.27	64.00	60.06	65.30	61.15
	63.10	66.47	66.06	68.06	64.05	68.09	63.99	68.76	64.48
	69.70	71.64	71.55	74.00	69.77	74.19	69.87	74.70	70.20
	70.20	72.80	72.78	75.75	71.47	76.24	71.85	77.45	72.85
	124.60	120.52	123.41	130.71	124.41	130.60	124.21	130.19	123.63
	126.00	120.54	123.43	130.72	124.42	130.64	124.25	130.54	123.97
	126.30	121.52	124.48	131.43	125.11	131.43	125.01	131.48	124.88
	128.20	123.51	126.58	133.67	127.26	133.65	127.14	133.45	126.77
	128.40	123.63	126.71	133.94	127.52	133.78	127.28	133.60	126.92
	129.00	124.39	127.51	134.42	127.98	134.45	127.91	134.54	127.82
	129.20	124.75	127.90	134.58	128.14	134.61	128.07	134.68	127.95
	129.30	124.96	128.12	134.98	128.53	135.01	128.46	135.22	128.48
	130.30	128.55	131.93	138.55	131.96	138.62	131.93	138.77	131.89
	138.00	136.38	140.24	146.85	139.96	147.01	140.01	147.17	139.98
	138.10	137.20	141.11	147.78	140.86	148.07	141.04	149.19	141.93
	154.20	146.58	151.06	160.00	152.62	159.81	152.34	158.98	151.35
	156.50	148.94	153.57	160.23	152.85	160.34	152.86	160.62	152.93
	168.80	165.92	171.59	179.17	171.10	179.52	171.33	180.13	171.71
	170.70	167.65	173.43	180.48	172.35	180.89	172.65	181.60	173.13
Proton shifts	0.83	0.67	0.38	0.73	0.34	0.69	0.35	0.54	0.31
	1.28	1.46	1.18	1.73	1.34	1.54	1.21	1.28	1.04
	1.28	1.67	1.39	1.81	1.43	1.75	1.42	1.52	1.28
	1.53	1.80	1.52	1.87	1.49	1.94	1.61	1.99	1.74
	1.74	2.06	1.79	2.09	1.72	2.13	1.80	2.10	1.85
	1.74	2.09	1.82	2.31	1.94	2.22	1.89	2.18	1.93
	1.83	2.33	2.05	2.38	2.01	2.24	1.91	2.24	1.99
	2.18	2.90	2.63	3.00	2.64	2.85	2.53	2.69	2.42
	2.23	2.91	2.64	3.02	2.66	2.87	2.54	2.71	2.45
	2.68	2.92	2.65	3.04	2.67	2.95	2.62	2.77	2.50
	2.81	2.94	2.68	3.17	2.81	3.11	2.78	2.79	2.53
	2.88	2.97	2.70	3.18	2.82	3.11	2.78	3.04	2.78
	2.97	3.07	2.81	3.28	2.92	3.15	2.82	3.09	2.82
	2.97	3.14	2.88	3.29	2.93	3.29	2.97	3.12	2.85
	3.06	3.46	3.20	3.52	3.17	3.60	3.28	3.45	3.17
	3.06	3.51	3.25	3.62	3.27	3.61	3.28	3.78	3.50
	3.12	3.73	3.47	3.64	3.29	3.80	3.47	3.94	3.66
	3.78	3.98	3.72	3.88	3.53	3.98	3.65	4.08	3.80
	4.19	4.00	3.74	3.97	3.62	4.02	3.70	4.10	3.81

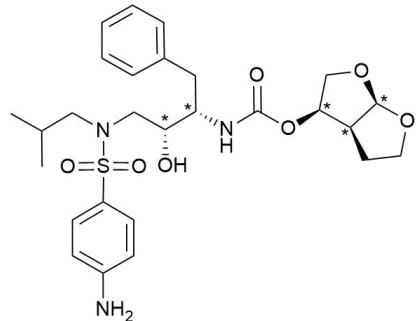
4.19	4.06	3.81	4.04	3.69	4.04	3.72	4.34	4.05
4.25	4.19	3.94	4.11	3.77	4.20	3.88	4.38	4.09
6.97	7.07	6.85	7.14	6.84	7.14	6.83	7.14	6.81
6.97	7.15	6.93	7.22	6.92	7.22	6.91	7.23	6.90
6.97	7.17	6.95	7.26	6.97	7.25	6.94	7.25	6.91
7.21	7.29	7.07	7.40	7.11	7.42	7.11	7.45	7.11
7.21	7.37	7.15	7.41	7.12	7.45	7.15	7.46	7.12
7.21	7.38	7.16	7.48	7.18	7.47	7.17	7.54	7.20
7.21	7.41	7.20	7.52	7.23	7.52	7.21	7.58	7.24
7.21	7.45	7.23	7.55	7.26	7.57	7.26	7.60	7.26
7.21	7.47	7.25	7.56	7.27	7.57	7.26	7.61	7.26
7.21	7.49	7.27	7.57	7.28	7.58	7.28	7.63	7.29
7.21	7.56	7.34	7.62	7.33	7.65	7.35	7.64	7.30
7.21	7.57	7.35	7.68	7.39	7.67	7.36	7.64	7.30
7.21	7.80	7.59	7.96	7.67	7.86	7.56	7.71	7.36
C MAE	3.26	2.15	4.98	1.55	5.07	1.64	5.24	1.90
H MAE	0.28	0.16	0.37	0.17	0.35	0.16	0.32	0.16
C CorrCoef	0.9988		0.9994		0.9993		0.9990	
H CorrCoef	0.9957		0.9947		0.9958		0.9960	
PROBABILITIES								
DP4 combined	0.0%		0.0%		0.0%		0.0%	
DP4 C only	0.0%		0.0%		0.0%		0.0%	
DP4 H only	0.0%		0.0%		0.0%		0.0%	
Gaussian combined	0.0%		0.0%		0.0%		0.0%	
Gaussian C only	0.0%		0.1%		0.0%		0.0%	
Gaussian H only	0.0%		0.0%		0.0%		0.0%	
KDE combined	0.0%		0.0%		0.0%		0.0%	
KDE C only	0.0%		0.1%		0.0%		0.0%	
KDE H only	0.0%		0.0%		0.0%		0.0%	
RKDE combined	0.0%		0.0%		0.0%		0.0%	
RKDE C only	0.0%		0.0%		0.0%		0.0%	
RKDE H only	0.0%		0.0%		0.0%		0.0%	
URKDE combined	0.0%		0.0%		0.0%		0.0%	
URKDE C only	0.4%		0.5%		0.1%		0.1%	
URKDE H only	0.0%		0.0%		0.0%		0.0%	
2gaus combined	0.0%		0.0%		0.0%		0.0%	
2gaus C only	0.0%		0.1%		0.0%		0.0%	
2gaus H only	0.0%		0.0%		0.0%		0.0%	



Citrinadin B (30)

	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
	B3LYP 6- 31G**	B3LYP 6- 31G**	mPW1 PW91 311G*	mPW1 PW91 311G*	mPW1 PW91 311G*	B3LYP 6- 31G**	mPW1 M06- PW91 2X 6- 311G*	mPW1 M06- PW91 2X 6- 31G**
CitrinadinB	Func.	B3LYP	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
Basis	6-	6-	6-	6-	6-	6-	6-	6-
s.								
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.
18.60	22.04	19.71	22.73	20.83	22.73	20.83	22.73	20.83
18.90	22.60	20.29	23.17	21.25	23.17	21.25	23.17	21.25
22.10	22.65	20.35	23.59	21.65	23.59	21.65	23.59	21.65
24.30	24.07	21.81	23.70	21.75	23.70	21.75	23.70	21.75
28.20	28.92	26.81	29.10	26.90	29.10	26.90	29.10	26.90
29.30	29.86	27.77	30.11	27.86	30.11	27.86	30.11	27.86
32.70	34.26	32.31	35.73	33.22	35.73	33.22	35.73	33.22
34.70	35.72	33.81	36.77	34.21	36.77	34.21	36.77	34.21
35.40	39.67	37.88	40.12	37.40	40.12	37.40	40.12	37.40
40.80	42.38	40.67	43.34	40.48	43.34	40.48	43.34	40.48
46.90	49.67	48.19	50.73	47.52	50.73	47.52	50.73	47.51
50.30	51.80	50.38	52.33	49.05	52.33	49.05	52.33	49.05
52.00	54.90	53.58	56.29	52.82	56.29	52.82	56.29	52.82
55.20	56.16	54.88	57.36	53.84	57.36	53.84	57.36	53.84
60.80	58.89	57.68	60.79	57.11	60.79	57.11	60.79	57.11
61.50	60.03	58.86	63.17	59.38	63.16	59.37	63.19	59.40
64.10	63.50	62.44	65.71	61.80	65.71	61.80	65.71	61.80
68.70	74.11	73.37	75.15	70.80	75.15	70.80	75.15	70.80
84.00	89.59	89.32	92.11	86.96	92.11	86.96	92.11	86.96
105.00	114.22	114.70	120.92	114.43	120.92	114.43	120.93	114.44
121.80	119.78	120.42	128.02	121.20	128.02	121.20	128.03	121.21
127.00	126.85	127.71	136.17	128.97	136.17	128.97	136.17	128.97
133.30	128.58	129.49	139.23	131.88	139.23	131.88	139.23	131.89
134.60	132.66	133.70	141.48	134.03	141.48	134.03	141.49	134.04
142.60	137.33	138.51	147.33	139.60	147.33	139.60	147.32	139.60
185.80	181.08	183.59	193.82	183.92	193.82	183.92	193.82	183.93
194.70	193.65	196.54	205.47	195.03	205.47	195.03	205.44	195.01
Proton shifts	0.99	0.93	1.27	0.92	1.23	0.92	1.23	1.23
	1.06	1.11	1.45	1.11	1.41	1.11	1.41	1.41
	1.30	1.16	1.49	1.27	1.56	1.27	1.56	1.56
	1.36	1.31	1.64	1.35	1.64	1.35	1.64	1.64
	1.44	1.36	1.68	1.38	1.68	1.38	1.68	1.68
	1.61	1.36	1.69	1.45	1.74	1.45	1.74	1.74
	1.63	1.43	1.76	1.47	1.76	1.47	1.76	1.76
	1.63	1.47	1.80	1.58	1.87	1.58	1.87	1.87
	1.63	1.50	1.83	1.59	1.88	1.59	1.88	1.88
	1.74	1.60	1.92	1.61	1.90	1.61	1.90	1.90
	2.02	1.61	1.93	1.63	1.92	1.63	1.92	1.92
	2.06	1.65	1.97	1.72	2.00	1.72	2.00	2.00
	2.23	1.78	2.09	1.91	2.18	1.91	2.18	2.18
	2.53	2.07	2.38	1.99	2.26	1.99	2.26	2.26
	2.87	2.12	2.43	2.06	2.33	2.06	2.33	2.33
	3.00	2.29	2.59	2.27	2.54	2.27	2.54	2.54
	3.06	2.63	2.93	2.67	2.92	2.67	2.92	2.92
	3.35	3.00	3.28	3.12	3.36	3.12	3.36	3.36
	3.65	3.14	3.41	3.13	3.37	3.13	3.37	3.37
	4.05	3.20	3.48	3.19	3.42	3.19	3.42	3.42
	4.52	3.22	3.50	3.28	3.52	3.28	3.52	3.52
	7.15	7.32	7.48	7.38	7.50	7.38	7.50	7.50
	7.71	7.94	8.08	7.99	8.09	7.99	8.09	8.09
	7.75	8.11	8.25	8.16	8.26	8.16	8.26	8.26
C MAE	2.54	2.15	4.40	1.81	4.40	1.81	4.40	1.81

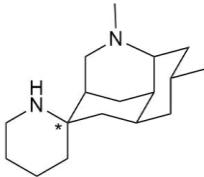
H MAE	0.36	0.28	0.34	0.29	0.34	0.29	0.34	0.29
C CorrCoef	0.9984		0.9988		0.9988		0.9988	
H CorrCoef	0.9849		0.9835		0.9835		0.9835	
PROBABILITIES								
DP4 combined	0.0%		0.0%		0.0%		0.2%	
DP4 C only	29.5%		47.9%		48.0%		48.1%	
DP4 H only	0.0%		0.0%		0.0%		0.0%	
Gaussian combined	0.0%		0.0%		0.0%		0.0%	
Gaussian C only	26.7%		55.1%		55.2%		55.0%	
Gaussian H only	0.0%		0.0%		0.0%		0.0%	
KDE combined	12.7%		6.5%		4.5%		26.8%	
KDE C only	24.7%		47.7%		47.5%		44.3%	
KDE H only	0.0%		0.0%		0.0%		0.0%	
RKDE combined	5.0%		1.0%		3.8%		21.8%	
RKDE C only	29.5%		41.0%		40.6%		37.2%	
RKDE H only	0.0%		0.0%		0.0%		0.0%	
URKDE combined	1.4%		0.2%		1.3%		32.4%	
URKDE C only	30.7%		38.2%		42.0%		33.5%	
URKDE H only	0.0%		0.0%		0.0%		0.0%	
2gaus combined	0.1%		0.4%		0.9%		6.3%	
2gaus C only	31.9%		49.0%		49.3%		49.0%	
2gaus H only	0.0%		0.0%		0.0%		0.0%	



Darunavir (38)

		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
Darunavir	Func.	B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06-
	Basis	6-	6-	PW91	PW91	PW91		PW91	PW91
	s.	31G**	31G**	6-	6-	6-		6-	2X
Carbon shifts	Exp	Calc.	Corr.	311G*	311G*	311G*	31G**	311G*	31G**
		Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
	20.20	21.80	18.11	22.04	19.56	22.07	19.58	21.92	19.39
	25.80	27.19	23.86	28.04	25.38	28.07	25.39	28.09	25.36
	27.30	30.51	27.41	31.38	28.62	31.46	28.68	32.24	29.38
	35.70	38.10	35.52	39.18	36.17	39.27	36.25	39.40	36.31
	45.40	45.65	43.59	47.37	44.11	47.36	44.09	47.15	43.82
	53.70	56.39	55.06	56.97	53.42	57.15	53.57	57.48	53.83
	55.10	60.82	59.79	62.22	58.51	62.11	58.38	62.20	58.39
	58.90	61.39	60.40	62.62	58.89	62.78	59.03	62.55	58.74
	69.60	68.17	67.64	71.12	67.14	71.10	67.10	71.07	66.98
	70.80	71.20	70.88	73.32	69.27	73.21	69.14	73.57	69.41
	72.80	74.30	74.20	77.81	73.61	77.64	73.44	77.50	73.21
	73.40	75.92	75.92	78.27	74.06	78.29	74.07	78.30	73.98
	109.30	110.99	113.39	116.67	111.28	116.62	111.21	116.67	111.15
	114.10	111.98	114.44	119.93	114.44	119.98	114.47	120.06	114.42
	126.00	121.60	124.72	131.40	125.56	131.36	125.49	131.64	125.65
	126.50	123.90	127.18	131.69	125.84	131.69	125.81	131.67	125.67
	126.50	124.22	127.52	133.78	127.86	133.79	127.85	133.85	127.79
	128.50	124.47	127.79	133.90	127.98	133.88	127.93	133.87	127.80
	129.40	125.26	128.63	135.58	129.61	135.57	129.57	135.52	129.40
	137.70	131.81	135.63	142.31	136.14	142.34	136.13	142.56	136.22
	150.80	145.87	150.65	158.37	151.70	158.52	151.81	159.04	152.17
	155.40	147.94	152.86	161.36	154.60	161.57	154.77	161.73	154.78
Proton shifts	0.81	0.86	0.81	0.91	0.89	0.91	0.89	0.99	0.94
	0.90	1.13	1.08	1.11	1.09	1.13	1.10	1.11	1.06
	1.44	1.86	1.81	1.76	1.72	1.78	1.74	1.78	1.73
	1.61	2.03	1.98	2.10	2.06	2.09	2.05	2.07	2.01
	1.82	2.10	2.04	2.12	2.09	2.10	2.06	2.07	2.01
	2.78	2.16	2.10	2.20	2.16	2.20	2.16	2.34	2.28
	2.78	2.56	2.50	2.42	2.37	2.44	2.39	2.39	2.33
	2.92	2.62	2.56	2.67	2.62	2.69	2.64	2.75	2.69
	2.92	2.63	2.57	2.76	2.71	2.75	2.70	2.76	2.70
	2.92	2.75	2.69	2.80	2.75	2.86	2.80	2.86	2.80
	3.10	3.00	2.94	2.86	2.81	2.87	2.82	3.06	2.99
	3.10	3.59	3.52	3.66	3.60	3.60	3.53	3.55	3.48
	3.67	3.67	3.60	3.69	3.63	3.71	3.65	3.72	3.65
	3.67	3.77	3.70	3.75	3.69	3.77	3.70	3.78	3.71
	3.85	3.84	3.77	3.81	3.75	3.79	3.72	3.81	3.74
	3.85	4.00	3.92	3.92	3.86	3.92	3.85	3.89	3.81
	3.85	4.19	4.11	4.01	3.94	3.99	3.92	3.93	3.85
	3.94	4.24	4.16	4.09	4.02	4.13	4.05	4.13	4.06
	4.99	4.72	4.64	4.69	4.61	4.67	4.59	4.66	4.58
	5.63	5.74	5.66	5.65	5.56	5.64	5.55	5.62	5.54
	6.67	6.79	6.70	6.88	6.77	6.87	6.76	6.76	6.67
	7.23	7.42	7.32	7.36	7.24	7.37	7.25	7.37	7.26
	7.23	7.44	7.34	7.53	7.41	7.54	7.42	7.54	7.44
	7.23	7.53	7.43	7.64	7.52	7.65	7.52	7.65	7.55
	7.53	7.58	7.48	7.69	7.56	7.69	7.57	7.69	7.58
C MAE	2.89	1.55	4.52	1.00	4.55	1.00	4.64	1.04	

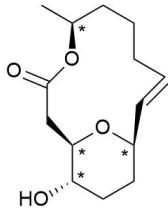
H MAE	0.23	0.21	0.23	0.21	0.23	0.20	0.20	0.18
C CorrCoef	0.9990		0.9996		0.9996		0.9996	
H CorrCoef	0.9914		0.9914		0.9917		0.9930	
PROBABILITIES								
DP4 combined	0.0%		0.0%		0.0%		0.4%	
DP4 C only	89.7%		36.5%		44.9%		47.2%	
DP4 H only	0.0%		0.0%		0.0%		0.0%	
Gaussian combined	0.0%		0.0%		0.0%		0.1%	
Gaussian C only	82.1%		31.6%		43.6%		39.1%	
Gaussian H only	0.0%		0.0%		0.0%		0.0%	
KDE combined	0.7%		0.0%		0.1%		1.6%	
KDE C only	83.9%		34.1%		42.8%		41.7%	
KDE H only	0.0%		0.0%		0.0%		0.0%	
RKDE combined	0.0%		0.0%		0.0%		0.4%	
RKDE C only	74.7%		46.0%		47.3%		34.7%	
RKDE H only	0.0%		0.0%		0.0%		0.0%	
URKDE combined	0.1%		2.9%		0.5%		2.6%	
URKDE C only	43.6%		72.1%		77.5%		81.9%	
URKDE H only	0.0%		0.3%		0.1%		0.2%	
2gaus combined	0.3%		0.0%		0.1%		1.4%	
2gaus C only	81.9%		36.9%		44.8%		41.2%	
2gaus H only	0.0%		0.0%		0.0%		0.0%	



Nankakurine (**16**)

		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	
		B3LYP 6- s. Exp	B3LYP 6- 31G**	mPW1 6- 311G*	mPW1 6- 311G*	mPW1 6- 311G*	B3LYP 6- 31G**	mPW1 6- 311G*	M06- 2X	
Nankakurine	Func.	B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06-	
	Basis			PW91	PW91	PW91		PW91	2X	
Carbon shifts		6-	6-	6-	6-	6-	6-	6-	6-	
	Exp	31G**	31G**	311G*	311G*	311G*	31G**	311G*	31G**	
	Calc.			Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	
22.20		24.23	22.50	24.25	22.00	24.25	21.96	24.25	21.99	
23.20		25.11	23.43	25.61	23.40	25.62	23.37	25.61	23.39	
26.50		27.47	25.93	28.78	26.66	28.83	26.68	28.78	26.65	
32.70		34.42	33.31	34.95	33.02	34.93	32.97	34.95	33.01	
34.60		35.94	34.92	36.75	34.87	36.70	34.79	36.69	34.80	
34.80		36.52	35.54	37.57	35.72	37.57	35.69	37.58	35.71	
37.60		38.24	37.36	38.35	36.52	38.92	37.08	38.68	36.85	
37.60		39.59	38.78	40.56	38.79	40.56	38.78	40.56	38.79	
40.10		39.87	39.08	40.63	38.87	40.65	38.86	40.64	38.87	
40.10		40.63	39.89	42.03	40.31	42.09	40.35	42.06	40.33	
41.40		41.44	40.75	42.09	40.37	42.11	40.37	42.09	40.37	
42.00		41.50	40.81	42.55	40.84	42.55	40.83	42.55	40.84	
43.60		44.21	43.68	45.70	44.08	45.35	43.71	45.49	43.86	
56.00		57.10	57.35	58.65	57.42	58.67	57.45	58.67	57.44	
58.70		58.76	59.11	59.83	58.63	59.82	58.63	59.82	58.63	
65.20		63.70	64.35	65.85	64.83	65.84	64.84	65.85	64.84	
Proton shifts		0.84	0.77	0.85	0.87	0.83	0.87	0.84	0.87	0.83
		0.89	0.86	0.94	0.99	0.96	0.99	0.96	0.99	0.96
		1.20	1.19	1.26	1.30	1.28	1.30	1.28	1.30	1.28
		1.55	1.38	1.44	1.51	1.49	1.50	1.49	1.50	1.49
		1.55	1.40	1.46	1.51	1.50	1.52	1.50	1.51	1.50
		1.55	1.40	1.47	1.53	1.52	1.53	1.52	1.53	1.52
		1.55	1.43	1.49	1.53	1.52	1.53	1.52	1.53	1.52
		1.55	1.45	1.51	1.53	1.52	1.54	1.52	1.54	1.53
		1.55	1.45	1.51	1.54	1.53	1.55	1.54	1.55	1.53
		1.55	1.47	1.53	1.56	1.55	1.56	1.55	1.56	1.55
		1.68	1.53	1.58	1.59	1.58	1.59	1.58	1.59	1.58
		1.68	1.59	1.64	1.59	1.58	1.62	1.61	1.61	1.60
		1.68	1.79	1.83	1.80	1.79	1.80	1.80	1.80	1.80
		1.83	1.85	1.89	1.89	1.89	1.85	1.85	1.86	1.86
		1.83	1.89	1.94	1.94	1.94	1.90	1.90	1.92	1.92
		1.83	1.92	1.96	1.96	1.96	1.95	1.95	1.95	1.96
		1.96	1.95	1.99	1.97	1.97	1.97	1.97	1.97	1.97
		2.04	1.95	1.99	1.97	1.97	1.97	1.98	1.97	1.98
		2.04	1.96	2.00	2.00	2.00	2.00	2.01	2.00	2.00
		2.11	1.98	2.02	2.04	2.04	2.04	2.04	2.04	2.04
		2.13	2.19	2.22	2.05	2.05	2.04	2.05	2.04	2.05
		2.28	2.41	2.43	2.26	2.27	2.26	2.28	2.26	2.27
		2.80	2.72	2.73	2.79	2.83	2.81	2.84	2.80	2.84
		2.80	2.80	2.81	2.86	2.89	2.85	2.88	2.85	2.89
		3.00	2.97	2.97	2.95	2.99	2.96	3.00	2.95	2.99
	C MAE	1.07	0.61	1.77	0.61	1.79	0.55	1.78	0.57	
	H MAE	0.08	0.07	0.06	0.06	0.05	0.05	0.05	0.05	
	C CorrCoef	0.9982		0.9980		0.9982		0.9981		
	H CorrCoef	0.9882		0.9915		0.9929		0.9925		
PROBABILITIES										
DP4 combined		100.0%		99.8%		100.0%		100.0%		
DP4 C only		81.2%		89.5%		87.3%		81.9%		
DP4 H only		100.0%		98.1%		99.8%		99.9%		
Gaussian combined		100.0%		98.5%		99.5%		99.5%		
Gaussian C only		69.8%		79.9%		74.8%		72.1%		
Gaussian H only		99.9%		94.4%		98.5%		98.7%		

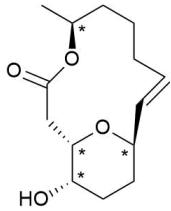
KDE combined	100.0%	99.7%	99.9%	99.9%	
KDE C only	74.8%	81.7%	76.7%	73.4%	
KDE H only	100.0%	98.7%	99.8%	99.7%	
RKDE combined	100.0%	100.0%	100.0%	100.0%	
RKDE C only	77.9%	89.2%	82.4%	76.7%	
RKDE H only	100.0%	99.7%	100.0%	99.9%	
URKDE combined	100.0%	99.7%	99.9%	99.9%	
URKDE C only	56.6%	68.3%	61.7%	52.3%	
URKDE H only	100.0%	99.3%	99.9%	99.9%	
2gaus combined	100.0%	99.6%	99.9%	99.9%	
2gaus C only	73.1%	84.6%	79.9%	77.2%	
2gaus H only	100.0%	98.1%	99.8%	99.7%	



Aspergillide A (11)

		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
		B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06-
		6- 31G**	6- 31G**	PW91	PW91	PW91		PW91	PW91
		311G*	311G*	311G*	311G*	311G*	31G**	311G*	2X
AspergillideAC-DCI3	Func.	B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06-
	Basis	6- 31G**	6- 31G**	PW91	PW91	PW91		PW91	PW91
	s.			311G*	311G*	311G*	31G**	311G*	2X
Carbon shifts	Exp	21.70	24.35	22.79	24.33	23.15	24.34	23.05	24.34
	Calc.	21.90	23.68	22.10	23.88	22.72	23.90	22.64	23.84
	Corr.	23.60	26.51	25.00	27.02	25.66	27.22	25.75	26.47
		31.00	33.21	31.86	34.88	33.02	35.05	33.08	34.40
		32.10	33.28	31.93	34.09	32.29	34.46	32.53	33.11
		40.50	42.08	40.95	42.93	40.56	42.92	40.46	42.90
		66.70	67.77	67.27	69.84	65.75	69.84	65.67	69.84
		71.30	68.23	67.73	70.72	66.58	70.67	66.45	70.85
		71.50	69.01	68.54	71.43	67.24	71.59	67.31	71.01
		74.00	76.01	75.71	77.67	73.08	77.69	73.03	77.59
		132.10	132.48	133.55	143.19	134.43	143.10	134.31	143.47
		137.00	135.06	136.20	146.62	137.64	146.83	137.81	145.97
		170.10	168.95	170.92	182.58	171.31	182.61	171.33	182.50
Proton shifts		1.19	1.21	1.28	1.26	1.23	1.26	1.23	1.28
		1.38	1.28	1.35	1.41	1.38	1.41	1.37	1.42
		1.49	1.39	1.44	1.45	1.41	1.46	1.42	1.42
		1.50	1.51	1.56	1.68	1.63	1.67	1.62	1.70
		1.71	1.61	1.65	1.79	1.73	1.79	1.73	1.79
		1.81	1.83	1.86	1.92	1.86	1.92	1.86	1.91
		1.88	2.02	2.03	2.00	1.94	1.99	1.93	2.02
		1.95	1.69	1.73	1.79	1.74	1.79	1.74	1.79
		2.10	2.32	2.32	2.41	2.33	2.42	2.34	2.39
		2.21	2.21	2.21	2.28	2.21	2.28	2.21	2.29
		2.28	2.37	2.36	2.47	2.39	2.46	2.38	2.50
		2.39	2.24	2.24	2.27	2.20	2.27	2.20	2.28
		2.63	2.74	2.70	2.72	2.63	2.72	2.63	2.72
		3.58	3.47	3.38	3.56	3.43	3.56	3.43	3.56
		4.21	4.25	4.11	4.30	4.14	4.30	4.14	4.30
		4.23	4.31	4.16	4.36	4.19	4.36	4.20	4.36
		4.94	5.02	4.82	4.92	4.73	4.90	4.72	4.97
		5.69	6.07	5.80	6.12	5.88	6.13	5.89	6.11
		5.79	6.25	5.97	6.15	5.91	6.14	5.91	6.17
	C MAE	1.79	1.22	4.14	1.55	4.22	1.58	3.94	1.54
	H MAE	0.13	0.11	0.14	0.10	0.14	0.10	0.14	0.10
	C CorrCoef	0.9995		0.9990		0.9990		0.9990	
	H CorrCoef	0.9964		0.9962		0.9961		0.9963	
PROBABILITIES									
DP4 combined		100.0%		100.0%		100.0%		100.0%	
DP4 C only		99.7%		99.8%		99.8%		99.8%	
DP4 H only		99.6%		99.7%		99.7%		99.7%	
Gaussian combined		100.0%		100.0%		100.0%		100.0%	
Gaussian C only		98.8%		99.4%		99.5%		99.6%	
Gaussian H only		99.2%		99.5%		99.4%		99.3%	
KDE combined		100.0%		100.0%		100.0%		100.0%	
KDE C only		96.0%		99.4%		99.4%		99.6%	
KDE H only		99.2%		99.2%		99.2%		99.3%	
RKDE combined		100.0%		100.0%		100.0%		100.0%	
RKDE C only		97.8%		97.7%		98.0%		99.1%	
RKDE H only		99.6%		99.5%		99.4%		99.5%	

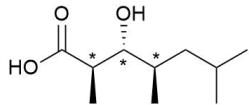
URKDE combined	100.0%	100.0%	100.0%	100.0%	
URKDE C only	96.9%	67.3%	81.9%	94.0%	
URKDE H only	99.5%	99.6%	99.5%	99.4%	
 2gaus combined	 100.0%	 100.0%	 100.0%	 100.0%	
2gaus C only	96.0%	99.4%	99.4%	99.5%	
2gaus H only	99.3%	99.1%	99.1%	99.2%	



Aspergillide B (12)

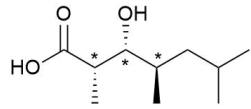
		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
		B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06-
		6- s. 31G**	6- 31G**	PW91	PW91	PW91	PW91	PW91	PW91
Asper-	gillideBC6D6	Func.	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06-
Basis		6-	6-	PW91	PW91	PW91	PW91	PW91	PW91
s.		31G**	31G**	311G*	311G*	311G*	31G**	311G*	2X
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
22.60	26.07	23.56		26.32	24.05	26.32	24.05	26.42	23.67
25.30	28.74	26.30		29.30	26.84	29.31	26.85	30.60	27.61
27.80	30.36	27.96		30.78	28.24	30.78	28.24	30.86	27.85
30.70	33.05	30.72		34.77	31.98	34.77	31.98	34.75	31.52
32.10	34.96	32.69		35.67	32.83	35.69	32.84	37.79	34.38
39.90	41.87	39.79		43.27	39.96	43.27	39.96	43.16	39.45
67.20	69.26	67.93		71.18	66.16	71.18	66.16	70.89	65.58
69.60	69.00	67.66		71.48	66.44	71.48	66.44	71.64	66.29
69.80	72.77	71.54		73.97	68.78	73.97	68.78	74.01	68.52
71.50	71.03	69.74		73.97	68.78	73.98	68.78	74.16	68.66
129.00	128.16	128.44		138.37	129.23	138.36	129.23	138.12	128.95
138.20	136.22	136.73		148.51	138.75	148.51	138.75	148.82	139.04
169.80	170.26	171.70		183.49	171.59	183.49	171.59	183.69	171.90
Proton shifts									
0.99	1.18	1.01		1.35	1.06	1.35	1.06	1.34	1.03
1.07	1.17	1.00		1.24	0.95	1.24	0.95	1.26	0.96
1.31	1.62	1.44		1.70	1.42	1.71	1.43	1.78	1.49
1.34	1.56	1.38		1.53	1.25	1.53	1.25	1.60	1.30
1.37	1.56	1.38		1.69	1.41	1.69	1.41	1.68	1.39
1.52	1.90	1.71		1.97	1.69	1.97	1.69	1.99	1.70
1.55	1.63	1.45		1.81	1.53	1.81	1.53	1.80	1.51
1.61	1.91	1.71		1.93	1.65	1.93	1.65	1.83	1.54
1.74	1.95	1.76		2.06	1.78	2.06	1.78	2.07	1.78
1.78	2.04	1.84		2.15	1.88	2.15	1.88	2.15	1.87
2.04	2.18	1.98		2.34	2.07	2.34	2.07	2.40	2.12
2.12	2.32	2.11		2.37	2.10	2.37	2.10	2.36	2.09
2.71	2.51	2.30		2.59	2.32	2.59	2.32	2.62	2.34
3.22	3.40	3.16		3.46	3.20	3.46	3.20	3.46	3.21
4.08	4.59	4.31		4.38	4.14	4.38	4.14	4.40	4.18
4.30	4.56	4.28		4.57	4.32	4.57	4.33	4.57	4.35
5.09	4.95	4.66		4.85	4.61	4.85	4.61	4.77	4.55
5.38	5.78	5.46		5.74	5.51	5.74	5.51	5.71	5.52
6.19	6.83	6.47		6.72	6.50	6.72	6.50	6.66	6.49
C MAE	1.96	1.01		4.96	1.15	4.96	1.15	5.28	1.36
H MAE	0.26	0.12		0.30	0.12	0.30	0.12	0.31	0.13
C CorrCoef	0.9997			0.9995		0.9995		0.9993	
H CorrCoef	0.9938			0.9938		0.9938		0.9932	
PROBABILITIES									
DP4 combined	100.0%			100.0%		100.0%		100.0%	
DP4 C only	95.5%			86.5%		86.6%		49.5%	
DP4 H only	97.3%			99.0%		99.4%		99.5%	
Gaussian combined	100.0%			100.0%		100.0%		100.0%	
Gaussian C only	87.3%			83.8%		83.5%		47.1%	
Gaussian H only	84.6%			97.4%		98.4%		98.8%	
KDE combined	100.0%			100.0%		100.0%		100.0%	
KDE C only	89.3%			87.3%		86.7%		42.9%	
KDE H only	97.0%			99.0%		99.2%		99.0%	
RKDE combined	100.0%			100.0%		100.0%		100.0%	
RKDE C only	82.6%			90.3%		90.2%		57.9%	
RKDE H only	98.6%			97.8%		98.3%		99.0%	

URKDE combined	100.0%	100.0%	100.0%	100.0%	
URKDE C only	92.6%	96.3%	96.7%	74.5%	
URKDE H only	47.3%	52.3%	37.8%	78.9%	
 2gaus combined	 100.0%	 100.0%	 100.0%	 100.0%	
2gaus C only	89.5%	84.3%	84.9%	46.4%	
2gaus H only	96.0%	99.0%	98.6%	99.0%	



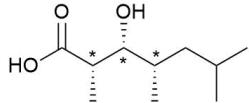
Callipeltin fragment RRR
(19)

	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
	B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06-
	6-	6-	PW91	PW91	PW91		PW91	2X
	31G**	31G**	311G*	311G*	311G*	31G**	311G*	6-
	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	31G**
CallipeltinRRR								
Carbon shifts								
16.60	18.21	15.43	17.85	15.92	18.30	16.16	17.80	15.74
21.30	21.10	18.49	20.99	18.98	21.17	18.97	21.69	19.53
24.30	25.26	22.91	25.54	23.41	25.43	23.12	25.07	22.83
25.20	27.84	25.65	28.88	26.68	28.94	26.55	29.01	26.68
33.40	38.89	37.39	39.10	36.65	39.55	36.90	38.98	36.41
39.40	41.26	39.89	42.50	39.97	42.18	39.48	42.33	39.68
42.30	43.86	42.66	43.83	41.27	44.83	42.06	44.27	41.59
78.20	80.60	81.67	82.72	79.22	83.07	79.38	82.44	78.85
181.40	172.91	179.67	186.81	180.79	186.85	180.66	187.01	180.96
Proton shifts								
0.84	0.80	0.65	0.83	0.68	0.80	0.62	0.85	0.70
0.92	0.84	0.69	0.85	0.70	0.85	0.68	0.87	0.72
0.95	0.92	0.77	0.99	0.85	0.99	0.83	0.99	0.85
1.15	1.11	0.99	1.28	1.15	1.22	1.08	1.30	1.17
1.18	1.41	1.31	1.44	1.32	1.48	1.36	1.43	1.31
1.23	1.76	1.69	1.68	1.57	1.79	1.69	1.59	1.47
1.64	1.87	1.81	1.77	1.66	1.80	1.70	1.83	1.72
1.69	1.88	1.82	1.81	1.71	1.80	1.70	1.86	1.75
2.74	2.81	2.82	2.84	2.80	2.87	2.85	2.82	2.74
3.48	3.22	3.27	3.39	3.37	3.29	3.31	3.46	3.40
C MAE	2.65	1.75	2.78	1.26	2.94	1.22	2.83	1.08
H MAE	0.17	0.19	0.14	0.12	0.17	0.16	0.13	0.11
C CorrCoef	0.9990		0.9995		0.9995		0.9996	
H CorrCoef	0.9672		0.9830		0.9709		0.9889	
PROBABILITIES								
DP4 combined	0.0%		0.2%		0.0%		3.4%	
DP4 C only	11.5%		31.0%		34.3%		48.7%	
DP4 H only	0.0%		0.3%		0.0%		1.9%	
Gaussian combined	0.0%		0.6%		0.0%		7.5%	
Gaussian C only	11.0%		29.0%		29.4%		40.8%	
Gaussian H only	0.1%		0.8%		0.0%		5.6%	
KDE combined	0.0%		0.3%		0.1%		3.7%	
KDE C only	21.1%		31.0%		32.5%		42.3%	
KDE H only	0.1%		0.4%		0.1%		3.0%	
RKDE combined	0.0%		0.1%		0.0%		1.9%	
RKDE C only	38.9%		27.8%		29.6%		38.6%	
RKDE H only	0.0%		0.2%		0.0%		1.9%	
URKDE combined	2.1%		2.6%		1.1%		9.7%	
URKDE C only	67.6%		66.8%		66.3%		76.5%	
URKDE H only	0.8%		1.3%		0.5%		3.1%	
2gaus combined	0.1%		0.4%		0.1%		4.3%	
2gaus C only	18.1%		32.1%		32.3%		44.9%	
2gaus H only	0.1%		0.5%		0.1%		2.8%	



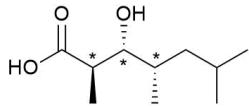
Callipeltin fragment SRR
(20)

	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
CallipeltinSRR	B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06-
Func.	6-	6-	PW91	PW91	PW91		PW91	2X
Basis	31G**	31G**	311G*	311G*	311G*	31G**	311G*	6-
s.								
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.
15.70	14.94	13.01	14.45	13.53	14.53	13.59	15.10	13.93
21.30	20.98	19.35	20.89	19.77	21.10	19.95	21.57	20.20
24.30	25.25	23.84	25.63	24.35	25.49	24.19	25.16	23.68
25.30	27.96	26.69	28.91	27.53	28.98	27.57	29.16	27.56
33.50	35.95	35.09	36.25	34.63	36.17	34.52	36.08	34.26
41.60	40.99	40.39	41.51	39.73	41.43	39.61	41.53	39.54
41.80	43.73	43.26	44.20	42.34	44.65	42.72	45.09	42.99
76.30	77.94	79.21	79.94	76.93	79.90	76.83	80.07	76.89
181.90	174.46	180.64	188.17	181.72	188.34	181.72	188.25	181.71
Proton shifts	0.85	0.78	0.70	0.77	0.67	0.77	0.66	0.67
	0.85	0.86	0.78	0.89	0.79	0.89	0.78	0.78
	0.93	0.91	0.83	1.00	0.89	1.00	0.89	1.00
	1.04	1.05	0.97	1.18	1.07	1.17	1.06	1.18
	1.22	1.31	1.23	1.31	1.21	1.32	1.21	1.31
	1.49	1.82	1.73	1.80	1.69	1.83	1.71	1.81
	1.62	1.90	1.81	1.84	1.73	1.86	1.75	1.88
	1.67	1.93	1.83	1.87	1.76	1.88	1.77	1.77
	2.74	2.69	2.59	2.73	2.61	2.72	2.60	2.72
	3.67	3.75	3.63	3.78	3.66	3.78	3.65	3.80
C MAE	2.10	1.51	2.38	1.15	2.38	1.15	2.36	1.15
H MAE	0.12	0.12	0.13	0.09	0.13	0.09	0.14	0.09
C CorrCoef	0.9994		0.9996		0.9996		0.9996	
H CorrCoef	0.9880		0.9925		0.9911		0.9915	
PROBABILITIES								
DP4 combined	27.4%		60.2%		62.9%		46.5%	
DP4 C only	26.9%		48.7%		53.3%		47.8%	
DP4 H only	39.8%		31.4%		39.4%		15.3%	
Gaussian combined	39.2%		49.7%		55.5%		45.7%	
Gaussian C only	32.6%		44.7%		51.3%		49.0%	
Gaussian H only	42.0%		27.7%		32.6%		18.2%	
KDE combined	40.0%		55.3%		64.8%		48.9%	
KDE C only	29.3%		43.9%		50.8%		49.2%	
KDE H only	48.3%		32.1%		40.6%		17.9%	
RKDE combined	51.6%		67.8%		77.3%		60.7%	
RKDE C only	33.0%		54.6%		58.9%		54.1%	
RKDE H only	47.1%		25.6%		31.1%		14.2%	
URKDE combined	69.5%		5.7%		26.7%		6.7%	
URKDE C only	65.1%		20.7%		44.5%		34.8%	
URKDE H only	24.4%		12.1%		13.0%		7.3%	
2gaus combined	33.1%		51.2%		64.8%		44.9%	
2gaus C only	28.4%		45.5%		52.8%		50.2%	
2gaus H only	43.1%		27.6%		38.5%		16.1%	



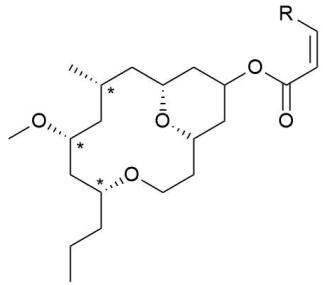
Callipeltin fragment SRS
(21)

	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
CallipeltinSRS	B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06- 2X
Func.	6-	6-	PW91	PW91	PW91		PW91	6-
Basis	31G**	31G**	311G*	311G*	311G*	31G**	311G*	31G**
s.			Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.
14.50	16.47	14.60	15.88	14.90	15.87	14.91	16.04	15.09
21.60	20.80	19.16	20.87	19.74	20.83	19.72	20.99	19.90
23.60	25.33	23.94	25.47	24.21	25.51	24.25	25.36	24.13
25.00	27.98	26.73	29.05	27.68	29.05	27.70	29.04	27.70
33.30	36.28	35.49	36.52	34.93	36.51	34.93	36.42	34.86
42.10	40.86	40.32	41.29	39.56	41.27	39.55	41.22	39.52
42.60	41.15	40.62	42.05	40.30	42.02	40.28	42.00	40.28
75.60	77.41	78.86	79.37	76.51	79.41	76.54	79.17	76.33
181.60	174.05	180.75	187.85	181.77	187.90	181.77	187.94	181.85
Proton shifts								
0.85	0.89	0.84	0.90	0.85	0.90	0.85	0.91	0.86
0.89	0.90	0.85	0.97	0.92	0.97	0.92	0.97	0.92
0.95	1.01	0.96	1.00	0.95	0.99	0.94	1.01	0.96
1.07	1.01	0.96	1.04	0.98	1.03	0.98	1.01	0.96
1.07	1.01	0.97	1.04	0.98	1.04	0.98	1.04	0.99
1.22	1.30	1.25	1.30	1.25	1.30	1.25	1.30	1.24
1.66	1.88	1.83	1.79	1.74	1.80	1.74	1.79	1.73
1.66	1.88	1.83	1.83	1.77	1.83	1.77	1.84	1.78
2.72	2.67	2.61	2.72	2.65	2.71	2.65	2.72	2.65
3.68	3.73	3.67	3.76	3.68	3.75	3.68	3.77	3.69
C MAE	2.40	1.52	2.38	1.34	2.40	1.35	2.35	1.32
H MAE	0.09	0.08	0.07	0.05	0.07	0.05	0.08	0.05
C CorrCoef	0.9993		0.9994		0.9994		0.9994	
H CorrCoef	0.9940		0.9976		0.9973		0.9971	
PROBABILITIES								
DP4 combined	99.9%		81.3%		99.2%		87.8%	
DP4 C only	49.7%		21.4%		19.5%		14.8%	
DP4 H only	92.9%		73.8%		92.0%		81.4%	
Gaussian combined	99.1%		62.1%		97.6%		68.5%	
Gaussian C only	45.7%		22.9%		25.6%		20.2%	
Gaussian H only	80.9%		59.8%		83.6%		64.2%	
KDE combined	98.9%		68.1%		97.5%		73.2%	
KDE C only	41.8%		19.4%		20.7%		15.7%	
KDE H only	88.8%		68.3%		89.8%		71.6%	
RKDE combined	99.5%		69.9%		98.6%		72.1%	
RKDE C only	34.8%		18.7%		15.9%		12.5%	
RKDE H only	84.0%		63.2%		86.4%		67.3%	
URKDE combined	96.8%		9.4%		68.0%		11.5%	
URKDE C only	21.9%		8.2%		22.1%		6.2%	
URKDE H only	75.4%		46.7%		58.7%		53.4%	
2gaus combined	98.7%		71.0%		97.4%		77.8%	
2gaus C only	42.1%		21.7%		22.2%		17.6%	
2gaus H only	88.7%		65.8%		90.1%		71.0%	



Callipeltin fragment RRS
(22)

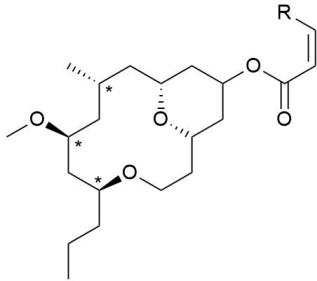
	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
	B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06- 2X
	6- s.	6-	PW91	PW91	PW91		PW91	6- 6-
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.
14.20	17.44	14.31	16.93	14.79	17.54	15.19	16.99	14.82
22.20	21.00	18.12	21.57	19.34	21.09	18.68	21.79	19.53
23.10	25.17	22.56	24.99	22.70	25.38	22.89	24.80	22.48
25.00	27.90	25.49	28.85	26.48	28.92	26.36	28.82	26.43
32.10	38.62	36.93	38.28	35.73	39.04	36.29	38.30	35.72
43.10	41.71	40.23	43.19	40.55	42.59	39.78	43.18	40.52
43.20	42.20	40.76	43.52	40.87	43.12	40.29	43.52	40.84
75.60	79.44	80.53	80.73	77.36	81.69	78.14	80.43	77.05
181.40	172.74	180.19	186.70	181.28	186.71	181.20	186.81	181.41
Proton shifts	0.85	0.83	0.75	0.87	0.77	0.85	0.74	0.87
	0.86	0.89	0.80	0.95	0.86	0.96	0.86	0.95
	0.89	1.02	0.94	1.01	0.92	1.04	0.95	1.02
	1.16	1.11	1.04	1.19	1.11	1.14	1.06	1.14
	1.18	1.11	1.05	1.22	1.14	1.15	1.07	1.28
	1.24	1.36	1.31	1.37	1.29	1.42	1.36	1.38
	1.66	1.83	1.82	1.77	1.71	1.76	1.72	1.78
	1.70	1.85	1.83	1.78	1.72	1.76	1.72	1.78
	2.66	2.79	2.84	2.82	2.80	2.84	2.88	2.83
	3.61	3.32	3.42	3.50	3.50	3.37	3.45	3.50
C MAE	3.48	2.23	2.90	1.65	3.30	2.03	2.88	1.64
H MAE	0.12	0.12	0.09	0.06	0.11	0.10	0.10	0.06
C CorrCoef	0.9982		0.9991		0.9987		0.9992	
H CorrCoef	0.9885		0.9968		0.9912		0.9959	
PROBABILITIES								
DP4 combined	1.1%		87.3%		3.9%		83.1%	
DP4 C only	1.9%		34.9%		2.5%		19.7%	
DP4 H only	14.0%		72.2%		18.6%		67.4%	
Gaussian combined	1.8%		80.0%		4.8%		77.5%	
Gaussian C only	1.4%		31.4%		2.5%		25.1%	
Gaussian H only	30.7%		65.4%		25.9%		58.6%	
KDE combined	6.2%		85.4%		4.1%		76.3%	
KDE C only	6.4%		32.2%		2.9%		22.5%	
KDE H only	24.2%		75.7%		22.7%		66.4%	
RKDE combined	11.4%		96.5%		8.3%		92.2%	
RKDE C only	4.7%		43.3%		2.0%		25.5%	
RKDE H only	40.9%		87.3%		37.4%		78.8%	
URKDE combined	41.9%		99.5%		88.6%		98.7%	
URKDE C only	5.9%		84.8%		30.9%		72.6%	
URKDE H only	60.4%		88.1%		65.8%		83.7%	
2gaus combined	5.9%		83.0%		4.3%		75.3%	
2gaus C only	6.9%		33.5%		3.6%		23.7%	
2gaus H only	21.6%		70.5%		20.9%		63.2%	



Neopeltolide, proposed structure (13)

		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
		B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06- 2X
		6- s. 31G**	6- 31G**	PW91	PW91	PW91	B3LYP	PW91	6- 31G**
NeopeltolideProp	Func. Basis	B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06- 2X
Carbon shifts	Exp	6- s. 31G**	6- 31G**	PW91	PW91	PW91	B3LYP	PW91	6- 6- 31G**
	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	
19.70	21.93	19.54	22.73	20.85	22.65	20.78	22.83	21.44	
25.20	27.18	24.96	27.59	25.51	27.59	25.51	27.38	25.80	
35.60	38.70	36.87	39.42	36.84	39.41	36.84	37.58	35.59	
36.20	39.30	37.48	40.40	37.79	40.38	37.77	40.39	38.28	
37.10	40.68	38.91	41.73	39.06	41.72	39.05	41.50	39.35	
38.80	39.34	37.52	40.33	37.72	40.31	37.69	40.47	38.36	
41.30	44.13	42.48	44.96	42.16	45.19	42.37	43.00	40.78	
43.20	43.54	41.87	45.02	42.22	45.02	42.21	44.92	42.63	
45.60	46.29	44.70	47.99	45.06	47.99	45.06	47.63	45.23	
46.00	47.68	46.14	48.83	45.86	48.87	45.90	48.57	46.13	
56.60	55.95	54.68	57.97	54.62	57.96	54.61	58.00	55.18	
69.10	73.97	73.30	76.91	72.76	76.91	72.75	76.94	73.34	
72.80	74.01	73.34	75.69	71.60	75.75	71.64	75.57	72.03	
75.70	73.77	73.10	76.48	72.35	76.34	72.22	74.91	71.39	
76.50	76.78	76.21	78.82	74.60	78.86	74.63	77.91	74.27	
84.50	84.24	83.91	87.18	82.61	87.17	82.59	85.06	81.13	
174.70	172.17	174.75	185.54	176.86	185.60	176.88	185.54	177.50	
Proton shifts									
0.92	0.90	0.85	0.98	0.82	0.98	0.82	0.99	0.79	
0.94	0.92	0.87	1.04	0.88	1.04	0.88	1.03	0.83	
1.08	1.06	1.01	1.22	1.08	1.23	1.08	1.26	1.09	
1.24	1.57	1.53	1.63	1.51	1.63	1.51	1.76	1.62	
1.25	1.17	1.13	1.27	1.13	1.27	1.13	1.38	1.21	
1.30	1.50	1.47	1.59	1.46	1.59	1.46	1.61	1.46	
1.33	1.31	1.27	1.36	1.22	1.36	1.22	1.38	1.21	
1.33	1.36	1.32	1.41	1.27	1.41	1.27	1.44	1.28	
1.36	1.39	1.35	1.49	1.36	1.49	1.36	1.46	1.30	
1.45	1.55	1.51	1.65	1.53	1.65	1.53	1.65	1.50	
1.48	1.45	1.41	1.54	1.42	1.55	1.42	1.56	1.41	
1.49	1.66	1.62	1.78	1.67	1.80	1.69	1.63	1.49	
1.55	1.48	1.44	1.59	1.47	1.59	1.47	1.73	1.59	
1.69	1.58	1.54	1.64	1.52	1.64	1.52	1.63	1.48	
1.79	1.71	1.68	1.77	1.66	1.78	1.66	1.77	1.63	
1.83	1.83	1.80	1.87	1.76	1.85	1.74	2.13	2.02	
2.26	2.25	2.23	2.31	2.23	2.31	2.24	2.28	2.18	
2.28	2.45	2.43	2.46	2.40	2.45	2.39	2.37	2.28	
2.40	2.41	2.39	2.52	2.46	2.53	2.46	2.52	2.44	
3.23	3.09	3.09	3.14	3.12	3.14	3.11	3.15	3.12	
3.30	3.34	3.34	3.29	3.28	3.29	3.28	3.31	3.29	
3.69	3.98	4.00	4.00	4.04	4.00	4.04	4.00	4.04	
4.02	4.19	4.21	4.19	4.24	4.20	4.24	4.19	4.24	
5.19	4.78	4.82	4.74	4.82	4.73	4.81	4.78	4.87	
5.24	5.28	5.33	5.18	5.29	5.20	5.31	5.14	5.26	
C MAE	1.85	1.16	3.37	1.45	3.38	1.46	2.91	1.56	
H MAE	0.10	0.11	0.14	0.12	0.14	0.12	0.15	0.12	
C CorrCoef	0.9990		0.9988		0.9988		0.9983		
H CorrCoef	0.9929		0.9924		0.9922		0.9919		
PROBABILITIES									
DP4 combined	100.0%		100.0%		100.0%		100.0%		
DP4 C only	99.9%		100.0%		100.0%		99.9%		

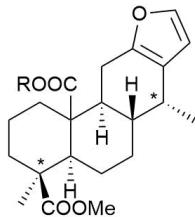
DP4 H only	100.0%	100.0%	100.0%	100.0%	
Gaussian combined	100.0%	100.0%	100.0%	100.0%	
Gaussian C only	99.0%	100.0%	100.0%	100.0%	
Gaussian H only	100.0%	100.0%	100.0%	100.0%	
KDE combined	100.0%	100.0%	100.0%	100.0%	
KDE C only	98.8%	99.7%	99.7%	96.3%	
KDE H only	100.0%	99.6%	99.5%	99.0%	
RKDE combined	100.0%	100.0%	100.0%	100.0%	
RKDE C only	95.4%	99.9%	99.8%	98.4%	
RKDE H only	100.0%	99.7%	99.4%	98.1%	
URKDE combined	100.0%	100.0%	100.0%	100.0%	
URKDE C only	99.5%	99.8%	99.8%	99.0%	
URKDE H only	100.0%	99.9%	99.9%	99.6%	
2gaus combined	100.0%	100.0%	100.0%	100.0%	
2gaus C only	99.0%	99.9%	99.9%	97.9%	
2gaus H only	100.0%	99.7%	99.7%	99.2%	



Neopeltolide, reassigned structure (14)

		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
Neopeltolide	Func. Basis	B3LYP 6- s. 31G**	B3LYP 6- 31G**	mPW1 6- 311G*	mPW1 6- 311G*	mPW1 6- 311G*	mPW1 6- 31G**	mPW1 6- 311G*	mPW1 M06- 2X
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
	20.00	22.87	20.72	23.59	22.07	23.60	22.00	23.21	22.00
	26.00	27.44	25.41	27.65	25.92	27.75	25.94	27.37	25.93
	32.60	34.91	33.08	35.30	33.16	35.56	33.36	35.37	33.49
	36.20	38.53	36.80	39.56	37.20	39.49	37.09	39.41	37.31
	37.40	39.63	37.92	40.69	38.27	40.74	38.27	40.53	38.37
	37.90	39.85	38.16	40.96	38.53	41.16	38.67	40.44	38.28
	41.00	42.32	40.69	42.71	40.19	42.91	40.33	42.70	40.42
	43.20	44.06	42.47	45.56	42.89	45.54	42.83	44.98	42.58
	43.50	45.03	43.47	45.91	43.22	45.91	43.18	45.94	43.48
	45.20	46.11	44.58	47.53	44.75	47.54	44.73	46.69	44.19
	56.40	55.06	53.77	57.25	53.97	57.23	53.93	57.12	54.04
	69.20	74.02	73.23	76.91	72.59	76.92	72.62	76.91	72.74
	71.30	73.39	72.59	75.24	71.01	75.06	70.85	74.77	70.72
	73.90	74.43	73.66	77.33	72.98	77.02	72.71	77.23	73.04
	77.00	77.11	76.40	78.60	74.19	78.77	74.37	77.89	73.67
	77.10	76.31	75.59	78.46	74.06	78.48	74.09	79.18	74.89
	173.00	171.05	172.84	185.08	175.07	184.91	175.12	185.15	175.02
Proton shifts	0.92	0.95	0.85	1.04	0.84	1.04	0.84	1.03	0.80
	0.94	0.94	0.83	1.06	0.86	1.06	0.86	1.07	0.84
	1.08	1.29	1.19	1.40	1.23	1.43	1.26	1.39	1.20
	1.25	1.30	1.21	1.35	1.18	1.36	1.19	1.36	1.16
	1.28	1.20	1.11	1.30	1.12	1.31	1.14	1.39	1.19
	1.33	1.42	1.33	1.46	1.29	1.45	1.29	1.48	1.29
	1.33	1.47	1.38	1.51	1.35	1.51	1.35	1.51	1.32
	1.36	1.57	1.49	1.61	1.45	1.61	1.46	1.62	1.44
	1.38	1.60	1.52	1.56	1.40	1.58	1.42	1.62	1.44
	1.46	1.47	1.38	1.55	1.40	1.55	1.40	1.62	1.44
	1.48	1.61	1.52	1.67	1.52	1.68	1.54	1.61	1.43
	1.49	1.50	1.42	1.57	1.42	1.57	1.42	1.56	1.37
	1.54	1.37	1.29	1.51	1.34	1.50	1.34	1.75	1.59
	1.64	1.60	1.52	1.66	1.51	1.67	1.52	1.66	1.48
	1.68	1.99	1.92	2.13	2.02	2.05	1.93	2.18	2.06
	1.78	1.65	1.57	1.72	1.58	1.72	1.58	1.71	1.54
	1.83	2.21	2.14	2.20	2.09	2.16	2.05	2.18	2.05
	2.26	2.36	2.30	2.48	2.40	2.48	2.39	2.43	2.33
	2.66	2.53	2.47	2.54	2.46	2.56	2.49	2.56	2.47
	3.23	3.24	3.21	3.22	3.19	3.21	3.18	3.23	3.20
	3.55	3.82	3.81	3.80	3.83	3.81	3.83	3.82	3.85
	3.64	3.71	3.69	3.64	3.65	3.63	3.63	3.64	3.65
	4.04	4.37	4.38	4.36	4.42	4.37	4.43	4.31	4.39
	5.14	5.11	5.14	4.95	5.07	5.01	5.12	4.88	5.02
	5.17	4.78	4.79	4.73	4.83	4.72	4.81	4.76	4.89
C MAE		1.73	0.88	3.30	1.27	3.32	1.29	3.08	1.29
H MAE		0.14	0.14	0.17	0.14	0.17	0.13	0.18	0.13
C CorrCoef		0.9993		0.9989		0.9989		0.9989	
H CorrCoef		0.9902		0.9899		0.9907		0.9908	
PROBABILITIES									
DP4 combined		100.0%		99.4%		99.8%		99.5%	
DP4 C only		93.9%		97.1%		97.1%		95.4%	

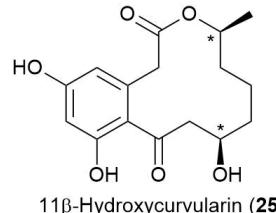
DP4 H only	54.7%	0.4%	1.1%	1.1%	
Gaussian combined	100.0%	99.7%	99.9%	99.8%	
Gaussian C only	69.6%	94.6%	95.0%	92.0%	
Gaussian H only	61.9%	0.7%	2.2%	2.4%	
KDE combined	100.0%	96.3%	98.4%	98.2%	
KDE C only	88.1%	93.1%	93.6%	89.7%	
KDE H only	44.4%	0.9%	2.3%	3.1%	
RKDE combined	100.0%	99.5%	99.9%	99.9%	
RKDE C only	96.7%	97.7%	98.5%	93.4%	
RKDE H only	20.7%	0.3%	1.0%	1.3%	
URKDE combined	100.0%	100.0%	100.0%	100.0%	
URKDE C only	99.5%	99.6%	99.7%	95.9%	
URKDE H only	26.5%	2.8%	6.0%	3.7%	
2gaus combined	99.9%	97.8%	98.7%	98.5%	
2gaus C only	87.7%	93.3%	93.6%	91.0%	
2gaus H only	37.8%	1.2%	2.3%	3.3%	



Caesaljapin (24)

	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
	B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06- 2X
	6- 31G**	6- 31G**	PW91	PW91	PW91	PW91	PW91	6- 31G**
Caesaljapin1	Func.	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06- 2X
	Basis	6-						
	s.	31G**	31G**	311G*	311G*	311G*	31G**	31G**
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.
17.20	19.82	16.00	19.59	16.51	19.60	16.51	19.59	16.51
19.20	22.75	19.11	23.52	20.32	23.53	20.33	23.52	20.33
23.30	26.70	23.33	27.38	24.07	27.36	24.05	27.39	24.08
24.20	26.16	22.75	27.09	23.79	27.09	23.79	27.09	23.79
30.00	31.89	28.86	32.78	29.33	32.78	29.33	32.79	29.34
31.30	35.40	32.60	35.91	32.36	35.91	32.36	35.89	32.35
35.50	37.44	34.78	37.79	34.19	37.76	34.16	37.79	34.19
35.50	39.51	36.98	40.74	37.06	40.73	37.04	40.73	37.05
36.70	37.78	35.14	38.74	35.12	38.77	35.14	38.65	35.03
43.70	47.21	45.20	47.78	43.90	47.79	43.91	47.79	43.91
47.90	52.12	50.44	53.46	49.43	53.47	49.43	53.44	49.41
48.60	52.06	50.37	53.68	49.63	53.69	49.64	53.66	49.61
50.30	52.68	51.03	53.48	49.44	53.54	49.49	53.57	49.53
52.00	51.19	49.44	53.38	49.34	53.38	49.33	53.37	49.34
109.60	106.72	108.65	115.10	109.32	115.10	109.31	115.10	109.33
122.70	120.11	122.93	129.17	122.99	129.18	122.99	129.16	122.99
140.60	135.32	139.15	146.22	139.55	146.21	139.54	146.22	139.57
148.10	143.83	148.22	155.33	148.41	155.33	148.39	155.33	148.42
178.40	177.04	183.63	191.29	183.35	191.33	183.38	191.24	183.32
181.00	170.55	176.72	184.73	176.98	184.73	176.96	184.70	176.97
Proton shifts	0.98	1.03	0.97	1.07	0.92	1.07	0.92	0.92
	1.07	1.13	1.07	1.15	1.01	1.15	1.01	1.14
	1.09	1.16	1.10	1.31	1.17	1.32	1.17	1.32
	1.11	1.04	0.99	1.14	1.00	1.14	1.00	1.13
	1.46	1.58	1.52	1.68	1.54	1.68	1.54	1.67
	1.59	1.50	1.44	1.58	1.44	1.58	1.44	1.57
	1.63	1.51	1.45	1.63	1.50	1.63	1.50	1.50
	1.69	2.09	2.01	2.10	1.97	2.10	1.97	2.10
	1.73	1.68	1.62	1.78	1.65	1.78	1.65	1.65
	1.84	1.91	1.84	2.03	1.90	2.03	1.90	2.05
	1.94	1.97	1.90	1.99	1.86	1.99	1.86	1.99
	1.95	2.24	2.17	2.36	2.23	2.35	2.23	2.34
	2.17	2.21	2.14	2.20	2.07	2.21	2.08	2.20
	2.18	2.21	2.14	2.24	2.11	2.23	2.10	2.23
	2.25	2.65	2.57	2.56	2.44	2.57	2.45	2.57
	2.52	2.58	2.50	2.66	2.54	2.66	2.54	2.66
	2.63	2.67	2.59	2.76	2.64	2.76	2.64	2.76
	2.82	2.79	2.71	2.88	2.76	2.88	2.76	2.88
	3.69	3.69	3.60	3.67	3.57	3.67	3.56	3.67
	6.17	6.33	6.19	6.25	6.18	6.25	6.18	6.25
	7.20	7.36	7.20	7.26	7.21	7.26	7.21	7.21
C MAE	3.34	1.47	4.53	1.29	4.54	1.29	4.52	1.29
H MAE	0.11	0.09	0.13	0.10	0.13	0.10	0.13	0.10
C CorrCoef	0.9993		0.9995		0.9995		0.9995	
H CorrCoef	0.9963		0.9968		0.9968		0.9968	
PROBABILITIES								
DP4 combined	100.0%		100.0%		100.0%		100.0%	
DP4 C only	100.0%		100.0%		100.0%		100.0%	
DP4 H only	100.0%		100.0%		100.0%		100.0%	
Gaussian combined	100.0%		100.0%		100.0%		100.0%	

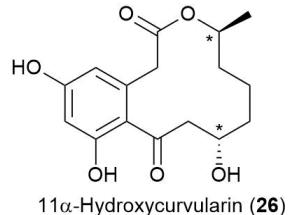
Gaussian C only	100.0%	100.0%	100.0%	100.0%	
Gaussian H only	100.0%	100.0%	100.0%	100.0%	
KDE combined	100.0%	100.0%	100.0%	100.0%	
KDE C only	99.8%	99.9%	99.9%	99.9%	
KDE H only	100.0%	100.0%	100.0%	100.0%	
RKDE combined	100.0%	100.0%	100.0%	100.0%	
RKDE C only	100.0%	100.0%	100.0%	100.0%	
RKDE H only	100.0%	100.0%	100.0%	100.0%	
URKDE combined	100.0%	100.0%	100.0%	100.0%	
URKDE C only	99.9%	100.0%	100.0%	100.0%	
URKDE H only	100.0%	100.0%	100.0%	100.0%	
2gaus combined	100.0%	100.0%	100.0%	100.0%	
2gaus C only	99.9%	100.0%	100.0%	100.0%	
2gaus H only	100.0%	100.0%	100.0%	100.0%	



11 β -Hydroxycurvularin (25)

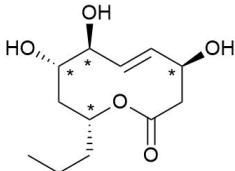
	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	
hydroxycur- vularin1	Func. Basis s.	B3LYP 6- 31G**	B3LYP 6- 31G**	mPW1 PW91 311G*	mPW1 PW91 311G*	mPW1 PW91 311G*	B3LYP 6- 31G**	mPW1 PW91 311G*	M06- 2X 6- 31G**
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
	19.40	25.55	23.79	25.79	23.94	25.79	23.95	24.76	23.42
	32.00	37.01	35.66	38.10	35.68	38.12	35.71	38.58	36.55
	35.10	39.98	38.75	40.77	38.23	40.65	38.13	38.48	36.45
	40.00	38.02	36.71	39.33	36.85	39.33	36.87	40.60	38.46
	53.90	46.93	45.95	49.54	46.60	49.63	46.69	51.11	48.44
	67.80	71.80	71.72	74.73	70.64	74.69	70.61	73.74	69.93
	71.50	71.99	71.92	74.98	70.87	74.93	70.84	71.96	68.24
	102.80	97.46	98.31	104.22	98.78	104.22	98.79	104.05	98.71
	112.50	109.31	110.61	116.54	110.53	116.55	110.55	116.10	110.14
	120.60	118.66	120.29	126.14	119.69	126.13	119.69	126.20	119.74
	137.60	135.01	137.23	144.53	137.24	144.55	137.27	145.13	137.71
	159.30	149.98	152.75	161.62	153.54	161.64	153.58	161.28	153.04
	160.70	151.86	154.70	164.21	156.02	164.21	156.03	164.21	155.83
	170.70	170.25	173.76	183.41	174.34	183.39	174.32	184.03	174.64
	204.40	210.00	214.96	224.46	213.51	224.41	213.47	225.69	214.19
Proton shifts	1.14	1.10	1.06	1.18	1.05	1.18	1.05	1.23	1.08
	1.41	1.61	1.60	1.83	1.74	1.83	1.73	1.71	1.58
	1.41	1.38	1.36	1.51	1.40	1.52	1.40	1.60	1.46
	1.49	1.52	1.50	1.56	1.45	1.56	1.45	1.50	1.36
	1.49	1.01	0.97	0.97	0.83	0.98	0.84	1.37	1.22
	1.72	2.26	2.27	2.27	2.20	2.27	2.20	2.07	1.96
	1.72	1.75	1.74	1.83	1.74	1.82	1.73	1.76	1.63
	3.10	3.10	3.14	3.15	3.13	3.15	3.13	3.06	3.00
	3.32	3.41	3.47	3.63	3.63	3.63	3.64	3.63	3.60
	3.71	3.17	3.22	3.30	3.29	3.30	3.29	3.38	3.33
	3.84	4.19	4.28	4.20	4.24	4.20	4.24	4.30	4.30
	4.02	3.58	3.65	3.68	3.69	3.69	3.70	3.82	3.80
	4.97	4.87	4.99	4.75	4.83	4.75	4.82	5.13	5.17
	6.36	6.41	6.60	6.42	6.59	6.42	6.59	6.36	6.46
	6.43	6.10	6.28	6.17	6.32	6.17	6.32	6.09	6.18
	C MAE	4.36	3.86	5.85	3.60	5.83	3.57	5.46	3.59
	H MAE	0.22	0.22	0.25	0.24	0.25	0.24	0.20	0.20
	C CorrCoef	0.9967		0.9973		0.9973		0.9973	
	H CorrCoef	0.9860		0.9848		0.9850		0.9914	
PROBABILITIES									
DP4 combined		0.0%		0.0%		0.0%		3.0%	
DP4 C only		0.0%		0.0%		0.0%		0.0%	
DP4 H only		91.6%		4.1%		13.3%		100.0%	
Gaussian combined		0.0%		0.0%		0.0%		15.6%	
Gaussian C only		0.0%		0.0%		0.0%		0.0%	
Gaussian H only		98.0%		17.5%		51.8%		100.0%	
KDE combined		0.0%		0.0%		0.0%		0.2%	
KDE C only		0.0%		0.1%		0.1%		0.4%	
KDE H only		1.6%		0.2%		0.5%		27.6%	
RKDE combined		0.0%		0.0%		0.0%		0.6%	
RKDE C only		0.0%		0.1%		0.1%		0.3%	
RKDE H only		0.6%		1.1%		3.6%		65.7%	
URKDE combined		0.0%		0.1%		0.1%		71.2%	
URKDE C only		0.1%		0.4%		0.6%		1.6%	

URKDE H only	26.0%	21.9%	17.7%	99.3%	
2gaus combined	0.0%	0.0%	0.0%	0.7%	
2gaus C only	0.0%	0.0%	0.0%	0.0%	
2gaus H only	56.3%	3.4%	4.5%	96.5%	



	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
hydroxycurvularin2	B3LYP 6- s. Exp	B3LYP 6- 31G** Calc.	mPW1 PW91 311G* Calc.	mPW1 PW91 311G* Corr.	mPW1 PW91 311G* Calc.	mPW1 B3LYP 311G** Corr.	mPW1 PW91 311G* Calc.	M06- 2X 6- 31G** Corr.
Carbon shifts								
22.70	24.07	23.92	24.65	24.39	24.60	24.37	24.76	24.45
32.50	35.26	35.35	36.42	35.49	36.45	35.54	36.62	35.64
35.60	35.63	35.73	36.75	35.80	36.73	35.80	36.23	35.28
39.50	41.91	42.14	43.16	41.84	43.22	41.92	43.54	42.17
54.50	48.33	48.71	50.72	48.98	50.62	48.90	50.65	48.88
67.10	71.99	72.87	75.09	71.97	75.15	72.04	75.22	72.05
73.50	68.06	68.86	70.41	67.55	70.31	67.46	69.97	67.10
102.70	98.45	99.91	105.07	100.24	105.04	100.22	105.16	100.30
112.10	109.51	111.20	116.75	111.26	116.76	111.27	116.97	111.44
121.20	117.50	119.37	124.60	118.66	124.53	118.60	124.28	118.33
137.00	138.43	140.75	148.33	141.05	148.36	141.07	148.73	141.40
158.50	154.23	156.89	165.63	157.37	165.69	157.41	166.02	157.71
160.40	152.67	155.30	164.99	156.77	165.01	156.77	165.10	156.84
170.90	169.42	172.41	182.45	173.24	182.44	173.21	182.61	173.36
204.90	205.75	209.53	219.26	207.96	219.31	207.98	218.84	207.53
Proton shifts								
1.12	1.04	1.01	1.10	1.01	1.10	1.01	1.12	1.05
1.21	1.25	1.24	1.20	1.12	1.19	1.10	1.17	1.10
1.41	1.59	1.58	1.74	1.67	1.74	1.67	1.73	1.67
1.41	1.38	1.37	1.36	1.27	1.36	1.28	1.29	1.22
1.41	1.52	1.51	1.62	1.54	1.62	1.54	1.62	1.56
1.59	1.57	1.56	1.66	1.58	1.66	1.58	1.65	1.58
1.71	1.32	1.31	1.31	1.23	1.31	1.23	1.28	1.21
2.90	2.89	2.90	3.15	3.11	3.15	3.11	3.11	3.07
3.55	3.42	3.44	3.53	3.49	3.53	3.49	3.54	3.50
3.71	3.38	3.40	3.56	3.53	3.55	3.52	3.56	3.53
3.83	4.86	4.90	4.83	4.82	4.85	4.85	4.92	4.91
4.12	3.78	3.81	3.89	3.86	3.88	3.85	3.89	3.86
4.85	5.08	5.13	4.90	4.89	4.90	4.90	4.90	4.89
6.36	6.22	6.29	6.30	6.32	6.30	6.32	6.29	6.30
6.42	6.09	6.16	6.14	6.16	6.14	6.15	6.14	6.15
C MAE	3.11	2.83	5.35	2.76	5.37	2.78	5.45	2.83
H MAE	0.23	0.22	0.21	0.22	0.21	0.22	0.22	0.23
C CorrCoef	0.9983		0.9984		0.9984		0.9983	
H CorrCoef	0.9821		0.9839		0.9834		0.9818	
PROBABILITIES								
DP4 combined	100.0%		100.0%		100.0%		37.5%	
DP4 C only	100.0%		100.0%		100.0%		100.0%	
DP4 H only	97.2%		96.7%		88.0%		0.0%	
Gaussian combined	100.0%		100.0%		100.0%		6.8%	
Gaussian C only	100.0%		100.0%		100.0%		100.0%	
Gaussian H only	70.5%		84.4%		49.0%		0.0%	
KDE combined	100.0%		100.0%		100.0%		99.8%	
KDE C only	99.9%		99.8%		99.7%		99.5%	
KDE H only	99.8%		99.9%		99.7%		77.3%	
RKDE combined	100.0%		100.0%		100.0%		97.4%	
RKDE C only	99.4%		98.5%		97.8%		95.3%	
RKDE H only	100.0%		100.0%		100.0%		65.4%	
URKDE combined	100.0%		100.0%		100.0%		96.6%	
URKDE C only	96.0%		93.9%		90.6%		89.4%	

URKDE H only	99.8%	99.4%	100.0%	76.9%	
2gaus combined	100.0%	100.0%	100.0%	82.7%	
2gaus C only	99.9%	99.8%	99.7%	99.6%	
2gaus H only	96.2%	95.7%	93.9%	1.7%	



Phomolide G (29)

		Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy	Shifts	En- ergy
		B3LYP	B3LYP	mPW1	mPW1	mPW1	B3LYP	mPW1	M06-
	Func.	6-	6-	6-	6-	6-	6-	PW91	2X
	Basis	s.	31G**	31G**	311G*	311G*	311G*	311G*	6-
	Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Calc.	6-
PhomolideG1	Func.	18.10	21.33	19.21	21.86	20.51	21.96	20.53	21.89
	Basis	39.00	41.77	39.98	42.70	39.97	42.87	40.06	42.90
	Carbon shifts	41.10	42.16	40.38	42.45	39.73	42.77	39.97	43.09
	Exp	45.20	44.14	42.39	45.92	42.97	45.91	42.90	45.97
	Calc.	71.60	72.61	71.32	75.93	70.98	75.92	70.92	75.91
	Corr.	72.50	72.88	71.60	75.26	70.35	75.19	70.24	74.71
	18.10	76.00	78.49	77.30	81.15	75.84	81.18	75.84	81.08
	39.00	78.10	79.43	78.26	81.93	76.57	81.92	76.53	81.91
	41.10	128.10	129.44	129.08	138.31	129.19	138.29	129.17	138.26
	45.20	136.40	136.77	136.53	147.38	137.65	147.34	137.63	147.21
	71.60	169.80	169.04	169.33	182.28	170.22	182.32	170.29	182.33
	72.50	76.00	78.10	79.43	81.93	76.57	81.92	76.53	81.91
	77.00	128.10	129.44	129.08	138.31	129.19	138.29	129.17	138.26
	78.10	136.40	136.77	136.53	147.38	137.65	147.34	137.63	147.21
	128.10	169.80	169.04	169.33	182.28	170.22	182.32	170.29	182.33
Proton shifts	0.79	0.86	0.79	0.96	0.78	0.96	0.78	0.96	0.78
	1.19	1.35	1.24	1.38	1.18	1.38	1.17	1.37	1.16
	1.19	1.33	1.22	1.37	1.17	1.36	1.16	1.37	1.16
	1.39	1.52	1.39	1.63	1.41	1.62	1.40	1.62	1.39
	1.39	1.46	1.34	1.55	1.33	1.56	1.34	1.61	1.38
	1.71	1.81	1.66	1.91	1.67	1.91	1.67	1.90	1.66
	1.71	1.94	1.78	2.02	1.77	2.02	1.78	2.04	1.79
	2.21	2.38	2.20	2.51	2.23	2.51	2.24	2.51	2.23
	2.51	2.47	2.28	2.61	2.33	2.61	2.33	2.62	2.33
	3.22	3.71	3.43	3.84	3.48	3.83	3.47	3.84	3.47
	3.57	3.97	3.66	4.16	3.78	4.15	3.77	4.15	3.76
	4.22	4.63	4.28	4.73	4.32	4.74	4.32	4.74	4.31
	4.68	4.68	4.33	4.57	4.17	4.59	4.18	4.64	4.22
	5.06	5.61	5.19	5.64	5.17	5.64	5.17	5.64	5.15
	5.61	6.11	5.65	6.17	5.67	6.17	5.66	6.17	5.65
	C MAE	1.54	0.86	5.18	1.34	5.22	1.35	5.17	1.34
	H MAE	0.23	0.09	0.32	0.11	0.32	0.11	0.32	0.10
	C CorrCoef	0.9997		0.9995		0.9995		0.9995	
	H CorrCoef	0.9962		0.9937		0.9941		0.9947	
PROBABILITIES									
	DP4 combined	99.7%		99.1%		99.3%		99.6%	
	DP4 C only	98.7%		98.3%		99.0%		99.2%	
	DP4 H only	72.6%		64.6%		55.9%		64.2%	
	Gaussian combined	98.4%		99.2%		99.2%		99.2%	
	Gaussian C only	91.8%		98.1%		98.7%		99.1%	
	Gaussian H only	70.7%		69.4%		59.9%		51.1%	
	KDE combined	98.5%		98.0%		98.5%		99.1%	
	KDE C only	96.0%		97.4%		98.2%		98.4%	
	KDE H only	57.6%		54.4%		52.5%		60.3%	
	RKDE combined	97.1%		96.8%		97.5%		96.9%	
	RKDE C only	95.1%		96.1%		97.5%		97.1%	
	RKDE H only	51.8%		51.1%		45.9%		42.2%	
	URKDE combined	100.0%		100.0%		100.0%		99.9%	
	URKDE C only	86.3%		83.0%		85.3%		73.5%	
	URKDE H only	99.8%		99.8%		99.4%		99.2%	
	2gaus combined	98.7%		98.7%		98.7%		99.1%	
	2gaus C only	95.2%		97.3%		98.1%		98.4%	
	2gaus H only	65.1%		64.7%		54.7%		59.5%	

S-7. References for the sources of NMR data used in the study

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