

The Optimal DFT Approach in DP4 NMR Structure Analysis – Pushing the Limits of Relative Configuration Elucidation

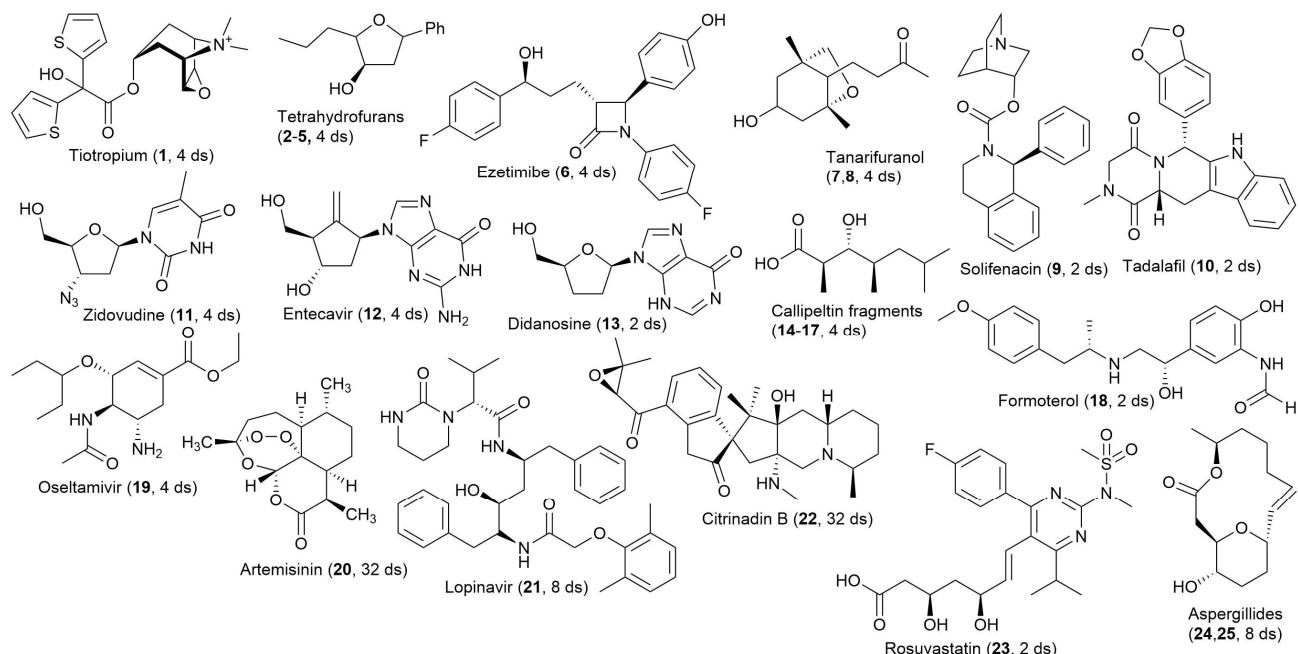
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S-1. Compounds used in the study



S-2. Statistical models to be used with the top performing DFT conditions

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

S-2.1. mPW1PW91, 6-311G* for shifts, mPW1PW91, 6-311G* for energies, MMFF geometries

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

Mean1: -0.131388

StDev1: 1.953609

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

Mean1: 0.008310

StDev1: 0.15584

S-2.2. mPW1PW91, 6-311G* for shifts, M06-2X, 6-31G for energies, MMFF geometries**

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

Mean1: -0.138097

StDev1: 1.970539

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

Mean1: 0.007649

StDev1: 0.165801

S-2.3. mPW1PW91, 6-311G* for shifts, M06-2X, 6-31G for energies, B3LYP, 6-31G** geometries**

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

Mean1: -0.134853

StDev1: 1.496604

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

Mean1: 0.008159

StDev1: 0.146512

S-3. Per compound overview of structure elucidation in-sample results from the top 3 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; linear internal correction is done by plotting the predicted shifts vs. the experimental, estimating the

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	mPW1	mPW1	Geometries				
		PW91	PW91	MMFF				
		DP4 probability	Rank	C Corr	H Corr	Carbon MAE	Proton MAE	
Compounds						Carbon CMAE	Proton CMAE	
Ezetimibe (6)		39.1	2	0.9985	0.9966	5.84	0.20	1.73
Formoterol (18)		100.0	1	0.9984	0.9974	3.93	0.23	1.94
Rosuvastatin (23)		100.0	1	0.9986	0.9941	5.08	0.20	2.31
Solifenacin (9)		100.0	1	0.9996	0.9986	4.21	0.17	1.10
Tadalafil (10)		75.7	1	0.9980	0.9948	5.12	0.17	1.90
Tiotropium (1)		31.2	3	0.9982	0.9938	6.92	0.18	2.08
Tanarifuranonol, reass. (7)		82.1	1	0.9997	0.9962	3.69	0.08	0.90
Tanarifuranonol, proposed (8)		98.9	1	0.9997	0.9958	3.73	0.08	1.03
Tetrahydrofuran 1 (2)		98.5	1	0.9994	0.9994	4.03	0.12	1.31
Tetrahydrofuran 2 (3)		77.9	1	0.9991	0.9979	4.05	0.15	1.55
Tetrahydrofuran 3 (4)		35.8	2	0.9994	0.9970	4.03	0.15	1.32
Tetrahydrofuran 4 (5)		91.3	1	0.9991	0.9982	4.27	0.18	1.52
Didanosine (13)		56.2	1	0.9983	0.9959	4.83	0.24	2.32
Zidovudine (11)		0.0	2	0.9972	0.9847	8.96	0.32	2.84
Entecavir (12)		100.0	1	0.9971	0.9942	7.19	0.42	2.39
Citrinadin B (22)		0.0	5	0.9988	0.9835	4.40	0.34	1.81
Callipeltin frag. RRR (14)		0.7	3	0.9995	0.9830	2.78	0.14	1.26
Callipeltin frag. SRR (15)		48.6	1	0.9996	0.9925	2.38	0.13	1.15
Callipeltin frag. SRS (16)		61.8	1	0.9994	0.9976	2.38	0.07	1.34
Callipeltin frag. RRS (17)		79.1	1	0.9991	0.9968	2.90	0.09	1.65
Oseltamivir (19)		100.0	1	0.9993	0.9839	4.21	0.18	1.41
Lopinavir (21)		0.0	3	0.9994	0.9947	4.98	0.37	1.55
Artemisinin (20)		99.9	1	0.9997	0.9956	4.27	0.09	0.82
Aspergillide A (24)		100.0	1	0.9990	0.9962	4.14	0.14	1.55
Aspergillide B (25)		100.0	1	0.9995	0.9938	4.96	0.30	1.15
Average		0.9989	0.9941	4.53	0.19	1.60	0.13	
Percentage of correct identification				72				

In sample data	Shifts	mPW1						
		PW91	Energies	M06-2X	Geometries	MMFF		
		DP4			Carbon	Proton	Carbon	Proton
Compounds		probability	Rank	C Corr	H Corr	MAE	MAE	CMAE
Ezetimibe (6)		99.8	1	0.9984	0.9963	5.81	0.20	1.76
Formoterol (18)		96.6	1	0.9987	0.9912	4.03	0.26	1.67
Rosuvastatin (23)		99.9	1	0.9983	0.9878	5.24	0.27	2.56
Solifenacin (9)		95.3	1	0.9996	0.9981	4.30	0.17	1.13
Tadalafil (10)		67.1	1	0.9980	0.9948	5.12	0.17	1.90
Tiotropium (1)		39.6	1	0.9982	0.9937	6.92	0.18	2.07
Tanarifuranonol, reass. (7)		82.7	1	0.9998	0.9967	3.61	0.08	0.83
Tanarifuranonol, proposed (8)		98.1	1	0.9998	0.9951	3.55	0.09	0.90
Tetrahydrofuran 1 (2)		96.4	1	0.9994	0.9991	4.35	0.16	1.21
Tetrahydrofuran 2 (3)		59.9	1	0.9991	0.9981	3.91	0.15	1.49
Tetrahydrofuran 3 (4)		47.5	2	0.9994	0.9971	3.85	0.15	1.27
Tetrahydrofuran 4 (5)		98.7	1	0.9991	0.9982	4.20	0.19	1.50
Didanosine (13)		40.8	2	0.9983	0.9960	4.82	0.24	2.30
Zidovudine (11)		0.0	3	0.9971	0.9839	9.04	0.33	2.92
Entecavir (12)		100.0	1	0.9971	0.9942	7.18	0.41	2.39
Citrinadin B (22)		0.0	6	0.9988	0.9835	4.40	0.34	1.81
Callipeltin frag. RRR (14)		9.0	2	0.9996	0.9889	2.83	0.13	1.08
Callipeltin frag. SRR (15)		44.7	1	0.9996	0.9915	2.36	0.14	1.15
Callipeltin frag. SRS (16)		66.7	1	0.9994	0.9971	2.35	0.08	1.32
Callipeltin frag. RRS (17)		74.6	1	0.9992	0.9959	2.88	0.10	1.64
Oseltamivir (19)		99.6	1	0.9992	0.9833	4.20	0.20	1.55
Lopinavir (21)		0.0	4	0.9990	0.9960	5.24	0.32	1.90
Artemisinin (20)		99.8	1	0.9997	0.9956	4.27	0.09	0.82
Aspergillide A (24)		100.0	1	0.9990	0.9963	3.94	0.14	1.54
Aspergillide B (25)		100.0	1	0.9993	0.9932	5.28	0.31	1.36
Average				0.9989	0.9937	4.52	0.19	1.61
Percentage of correct identification				76				

In sample data	Shifts	mPW1			Energies M06-2X 6-31G**	Geometries		B3LYP	
		PW91						6-31G**	
		6-31G*							
Compounds	DP4 probability	Rank	C Corr	H Corr	Carbon MAE	Proton MAE	Carbon CMAE	Proton CMAE	
Ezetimibe (6)	100.0	1	0.9993	0.9961	5.90	0.20	1.32	0.18	
Formoterol (18)	99.4	1	0.9991	0.9956	4.31	0.20	1.36	0.18	
Rosuvastatin (23)	99.9	1	0.9987	0.9923	5.03	0.27	2.02	0.23	
Solifenacin (9)	100.0	1	0.9997	0.9985	4.32	0.16	0.77	0.09	
Tadalafil (10)	100.0	1	0.9996	0.9968	4.81	0.14	0.86	0.11	
Tiotropium (1)	95.8	1	0.9993	0.9939	6.22	0.20	1.53	0.17	
Tanarifuranonol, reass. (7)	99.3	1	0.9998	0.9983	3.55	0.05	0.80	0.04	
Tanarifuranonol, proposed (8)	96.1	1	0.9997	0.9979	3.56	0.05	0.92	0.05	
Tetrahydrofuran 1 (2)	99.9	1	0.9995	0.9990	4.93	0.17	1.19	0.07	
Tetrahydrofuran 2 (3)	43.5	2	0.9997	0.9970	4.62	0.19	0.99	0.13	
Tetrahydrofuran 3 (4)	98.7	1	0.9996	0.9978	4.18	0.12	1.07	0.11	
Tetrahydrofuran 4 (5)	83.1	1	0.9992	0.9982	4.49	0.19	1.35	0.08	
Didanosine (13)	82.2	1	0.9992	0.9959	5.81	0.28	1.59	0.15	
Zidovudine (11)	0.0	4	0.9976	0.9855	9.09	0.31	2.54	0.26	
Entecavir (12)	46.8	2	0.9991	0.9902	7.05	0.39	1.55	0.20	
Citrinadin B (22)	94.9	1	0.9988	0.9863	5.16	0.35	1.56	0.27	
Callipeltin frag. RRR (14)	77.9	1	0.9996	0.9958	2.31	0.10	1.18	0.07	
Callipeltin frag. SRR (15)	59.9	1	0.9997	0.9933	2.22	0.12	0.96	0.08	
Callipeltin frag. SRS (16)	61.5	1	0.9997	0.9973	1.96	0.07	0.97	0.05	
Callipeltin frag. RRS (17)	88.0	1	0.9995	0.9975	2.38	0.09	1.19	0.04	
Oseltamivir (19)	100.0	1	0.9991	0.9880	3.75	0.20	1.59	0.19	
Lopinavir (21)	0.0	2	0.9993	0.9969	4.81	0.34	1.46	0.12	
Artemisinin (20)	100.0	1	0.9999	0.9982	2.95	0.06	0.58	0.06	
Aspergillide A (24)	100.0	1	0.9998	0.9963	4.23	0.12	0.87	0.11	
Aspergillide B (25)	100.0	1	0.9997	0.9934	5.10	0.29	1.05	0.13	
Average			0.9994	0.9951	4.49	0.18	1.26	0.13	
Percentage of correct identification			84						

S-4. Per compound detailed DP4 results from the top 3 performing workflows

Ezetimibe (6)	Shifts	mPW1		mPW1		mPW1	
		PW91	6-311G*	PW91	6-311G*	PW91	6-311G*
		mPW1		M06-2X		M06-2X	
Energy Geom.	PW91	6-311G*	MMFF	MMFF	M06-2X	6-31G**	B3LYP
	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
	Carbon shifts	24.50	28.25	23.41	27.88	23.24	26.42
Carbon shifts	36.36	42.92	37.92	43.06	38.22	42.98	39.39
	59.40	64.52	59.28	64.52	59.40	64.96	60.69
	59.58	66.83	61.56	66.82	61.68	65.83	61.54
	71.05	73.75	68.41	73.21	67.98	73.16	68.64
	114.64	119.92	114.06	119.81	113.97	119.48	113.53
	115.71	117.39	111.56	117.41	111.60	118.95	113.02
	115.79	121.44	115.57	121.47	115.62	120.83	114.85
	118.22	123.62	117.72	123.68	117.79	123.49	117.42
	127.50	133.35	127.34	133.29	127.29	132.05	125.72
	127.52	134.76	128.73	134.76	128.73	133.79	127.41
	127.88	140.62	134.54	140.58	134.48	134.48	128.08
	133.98	138.19	132.13	138.17	132.10	140.49	133.90
	142.14	150.68	144.48	150.80	144.57	148.58	141.74
	157.42	160.63	154.32	160.67	154.31	164.33	157.00
	158.00	165.72	159.35	165.78	159.35	166.91	159.51
	161.02	167.88	161.49	167.75	161.29	169.41	161.93
	167.33	172.62	166.18	172.94	166.42	178.06	170.31
Proton shifts	1.73	2.01	1.85	1.98	1.82	1.90	1.80
	1.73	1.62	1.46	1.58	1.42	1.66	1.55
	1.73	1.83	1.66	1.82	1.67	1.70	1.59
	1.83	2.27	2.11	2.32	2.17	2.21	2.10
	3.09	3.10	2.95	3.09	2.94	3.13	3.01
	4.50	4.95	4.81	4.95	4.82	5.04	4.91
	4.81	4.74	4.59	4.74	4.60	4.59	4.47
	6.76	6.89	6.76	6.89	6.76	6.91	6.77
	7.11	7.03	6.90	7.02	6.89	7.09	6.95
	7.13	7.02	6.89	7.03	6.90	7.01	6.87
	7.18	7.40	7.28	7.40	7.28	7.51	7.36
	7.22	7.49	7.36	7.49	7.36	7.49	7.34
	7.32	7.64	7.51	7.63	7.50	7.56	7.41
C MAE		5.84	1.73	5.81	1.76	5.90	1.32
H MAE		0.20	0.18	0.20	0.18	0.20	0.18
C CorrCoef		0.9985		0.9984		0.9993	
H CorrCoef		0.9966		0.9963		0.9961	
PROBABILITIES							
DP4 combined		10.6%		99.9%		100.0%	
DP4 C only		14.7%		12.5%		35.4%	
DP4 H only		25.1%		100.0%		99.9%	

Gaussian combined	39.1%	99.8%	100.0%	
Gaussian C only	14.7%	7.0%	70.1%	
Gaussian H only	48.4%	100.0%	100.0%	

Formoterol (18)	Shifts	mPW1	mPW1	mPW1	mPW1 PW91 6-311G*
		PW91	6-311G*	PW91	
		mPW1		mPW1	
Energy	PW91 6-311G*	M06-2X 6-31G**	M06-2X 6-31G**	B3LYP 6-31G**	
Geom.	MMFF	MMFF			
Exp	Calc.	Corr.	Calc.	Corr.	Calc.
Carbon	19.40	21.15	17.23	20.38	21.18
shifts	42.00	46.68	42.76	41.30	41.07
	53.60	54.97	51.05	49.67	49.02
	54.70	60.72	56.80	55.73	54.78
	55.30	61.22	57.29	55.83	54.87
	71.30	75.95	72.02	73.92	72.07
	114.00	118.25	114.33	118.85	114.77
	117.80	118.47	114.55	123.62	119.30
	119.50	121.54	117.62	125.65	121.23
	123.70	127.32	123.39	127.16	122.67
	125.70	128.31	124.38	131.57	126.86
	130.20	135.80	131.87	135.20	130.32
	130.60	137.73	133.80	136.49	131.54
	133.40	143.05	139.12	144.08	138.75
	147.70	147.87	143.95	151.09	145.42
	158.30	161.90	157.97	162.99	156.72
	160.20	163.21	159.28	163.10	156.83
					164.81
					157.89
Proton	1.02	1.06	1.08	1.24	0.97
shifts	2.67	2.59	2.52	2.49	2.31
	2.67	2.74	2.66	2.53	2.35
	2.67	2.75	2.66	2.60	2.43
	2.67	2.75	2.66	3.05	2.91
	2.67	2.93	2.83	3.38	3.26
	3.74	3.72	3.58	3.64	3.54
	4.46	4.79	4.58	4.97	4.97
	6.80	6.88	6.54	6.28	6.37
	6.80	6.90	6.56	6.65	6.76
	6.80	7.40	7.03	6.95	7.09
	6.99	7.44	7.06	6.99	7.13
	7.46	8.18	7.76	7.28	7.44
	8.11	8.45	8.01	7.80	8.00
C MAE	3.93	1.94	4.03	1.67	4.31
H MAE	0.23	0.13	0.26	0.25	0.20
C CorrCoef	0.9984		0.9987		0.9991
H CorrCoef	0.9974		0.9912		0.9956
PROBABILITIES					
DP4 combined	99.7%		91.6%		97.5%
DP4 C only	0.5%		8.1%		1.6%
DP4 H only	100.0%		99.2%		100.0%
Gaussian combined	100.0%		96.6%		99.4%
Gaussian C only	0.6%		3.4%		0.1%

Gaussian H only | 100.0% | 99.9% | 100.0% |

Rosuvastatin (23)	Shifts	mPW1		mPW1		mPW1	
		PW91	6-311G*	PW91	6-311G*	PW91	6-311G*
		mPW1		mPW1		mPW1	
		Energy	PW91 6-311G*	M06-2X 6-31G**	M06-2X 6-31G**	B3LYP	6-31G**
Carbon	Geom.	MMFF		MMFF		B3LYP	6-31G**
	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
shifts	22.60	22.99	22.10	23.09	22.56	22.91	22.05
	33.70	37.71	36.22	37.75	36.57	38.70	37.23
	34.30	34.52	33.16	33.78	32.78	33.92	32.63
	42.80	49.42	47.45	50.54	48.81	50.50	48.57
	44.70	42.87	41.16	40.89	39.58	40.69	39.14
	45.40	41.08	39.45	40.53	39.23	41.57	39.99
	69.10	74.44	71.43	73.88	71.13	74.70	71.84
	72.10	75.45	72.40	74.96	72.17	75.32	72.44
	116.60	120.78	115.86	121.43	116.62	120.74	116.12
	123.60	131.39	126.03	130.74	125.52	130.26	125.28
	124.40	128.14	122.93	127.78	122.69	128.81	123.88
	134.00	138.96	133.30	138.57	133.01	139.72	134.38
	136.60	144.05	138.18	145.22	139.37	142.75	137.28
	142.30	151.80	145.61	151.85	145.71	149.46	143.74
	159.30	167.93	161.08	168.21	161.36	164.92	158.61
	163.60	173.70	166.61	173.82	166.73	172.05	165.46
	165.20	169.37	162.46	168.77	161.90	171.47	164.90
	176.90	184.50	176.96	184.15	176.61	184.73	177.66
	182.40	184.76	177.22	184.83	177.26	185.49	178.39
Proton	1.27	1.38	1.52	1.40	1.67	1.35	1.57
shifts	1.50	1.15	1.29	0.50	0.83	0.90	1.16
	1.65	1.18	1.33	0.83	1.14	0.95	1.21
	2.27	2.50	2.59	2.44	2.64	2.33	2.47
	2.37	2.50	2.59	2.66	2.85	2.63	2.76
	3.48	3.39	3.44	3.41	3.54	3.34	3.40
	3.51	3.22	3.28	3.25	3.40	3.24	3.31
	3.53	3.08	3.15	3.15	3.30	3.30	3.37
	4.01	4.22	4.24	4.03	4.12	4.17	4.16
	4.35	4.50	4.51	4.57	4.63	4.74	4.69
	5.55	5.55	5.52	5.50	5.50	5.46	5.35
	6.62	6.91	6.82	6.83	6.74	7.09	6.85
	7.16	7.24	7.14	7.27	7.15	7.36	7.09
	7.70	7.69	7.57	7.63	7.48	7.87	7.56
C MAE		5.08	2.31	5.24	2.56	5.03	2.02
H MAE		0.20	0.20	0.27	0.26	0.27	0.23
C CorrCoef		0.9986		0.9983		0.9987	
H CorrCoef		0.9941		0.9878		0.9923	
PROBABILITIES							
DP4 combined		100.0%		98.0%		95.8%	
DP4 C only		89.8%		14.4%		58.4%	
DP4 H only		100.0%		99.7%		94.1%	

Gaussian combined	100.0%	99.9%	99.9%	
Gaussian C only	94.0%	13.7%	54.7%	
Gaussian H only	100.0%	100.0%	99.9%	

Solifenacin (9)	Shifts	mPW1		mPW1		mPW1		
		PW91	6-311G*	PW91	6-311G*	PW91	6-311G*	
		mPW1		M06-2X		M06-2X		
	Energy	PW91	6-311G*	MMFF	6-31G**	B3LYP	6-31G**	
	Geom.	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
Carbon shifts	20.10	23.19	21.12	23.43	21.24	22.74	20.25	
	24.80	27.60	25.40	27.79	25.47	28.20	25.58	
	25.80	29.50	27.24	29.79	27.41	29.94	27.26	
	28.60	32.98	30.62	32.93	30.46	31.90	29.17	
	38.90	38.82	36.28	38.60	35.96	39.72	36.79	
	46.70	48.89	46.05	48.82	45.88	49.57	46.40	
	47.70	49.29	46.43	49.30	46.34	50.39	47.19	
	56.10	60.03	56.85	60.35	57.07	59.38	55.95	
	58.30	60.22	57.03	60.47	57.19	61.26	57.78	
	72.40	75.11	71.48	75.24	71.52	76.84	72.96	
	126.30	130.98	125.66	130.97	125.62	131.04	125.77	
	127.20	132.06	126.72	132.11	126.72	132.24	126.94	
	127.50	132.07	126.72	132.15	126.76	132.57	127.27	
	128.20	132.98	127.60	133.04	127.62	132.76	127.45	
	128.40	133.85	128.45	133.95	128.51	133.91	128.57	
	128.60	134.31	128.89	134.19	128.74	134.05	128.71	
	129.00	135.27	129.83	135.17	129.69	134.38	129.03	
	135.10	138.35	132.81	138.36	132.79	137.86	132.42	
	135.70	143.19	137.51	143.37	137.65	143.16	137.59	
	143.00	151.23	145.31	151.33	145.38	150.93	145.15	
	155.40	162.04	155.79	162.05	155.78	161.61	155.56	
Proton shifts	1.41	1.32	1.38	1.41	1.43	1.28	1.39	
	1.57	1.51	1.56	1.52	1.53	1.48	1.58	
	1.69	1.59	1.63	1.63	1.64	1.58	1.67	
	1.83	1.87	1.90	1.96	1.95	1.86	1.93	
	2.04	1.93	1.96	2.01	1.99	1.96	2.02	
	2.79	2.66	2.65	2.68	2.63	2.64	2.67	
	2.79	2.73	2.71	2.77	2.71	2.70	2.72	
	2.79	2.84	2.81	2.83	2.77	2.75	2.77	
	2.79	2.85	2.83	2.88	2.82	2.79	2.81	
	2.79	2.88	2.85	2.90	2.84	2.84	2.85	
	2.79	2.96	2.93	3.05	2.98	2.95	2.96	
	2.79	3.12	3.08	3.10	3.03	3.04	3.04	
	3.31	3.29	3.24	3.25	3.18	3.18	3.17	
	3.31	3.31	3.26	3.34	3.26	3.31	3.29	
	4.03	4.23	4.13	4.20	4.08	3.96	3.90	
	4.82	4.69	4.56	4.72	4.57	4.71	4.61	
	6.32	6.57	6.34	6.59	6.36	6.64	6.43	
	7.07	7.16	6.89	7.16	6.89	7.13	6.88	
	7.20	7.38	7.11	7.28	7.01	7.26	7.01	
	7.20	7.44	7.17	7.38	7.10	7.43	7.17	
	7.20	7.45	7.17	7.45	7.17	7.46	7.19	
	7.20	7.48	7.20	7.49	7.21	7.46	7.19	

	7.20	7.50	7.22	7.49	7.21	7.51	7.24	
	7.20	7.50	7.22	7.51	7.23	7.51	7.24	
	7.20	7.57	7.28	7.62	7.33	7.59	7.32	
	7.20	7.76	7.46	7.91	7.61	7.77	7.49	
C MAE		4.21	1.10	4.30	1.13	4.32	0.77	
H MAE		0.17	0.09	0.17	0.10	0.16	0.09	
C CorrCoef		0.9996		0.9996		0.9997		
H CorrCoef		0.9986		0.9981		0.9985		
PROBABILITIES								
DP4 combined		99.9%		85.9%		99.9%		
DP4 C only		47.6%		21.6%		63.3%		
DP4 H only		99.9%		95.7%		99.7%		
Gaussian combined		100.0%		95.3%		100.0%		
Gaussian C only		47.4%		30.8%		59.7%		
Gaussian H only		100.0%		97.9%		100.0%		

Tadalafil (10)		Shifts	mPW1		mPW1		mPW1	
			PW91	6-311G*	PW91	6-311G*	PW91	6-311G*
Energy		mPW1		M06-2X	6-31G**	M06-2X	6-31G**	
Geom.		MMFF		MMFF		B3LYP	6-31G**	
Carbon	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	
shifts	23.90	26.39	25.19	26.39	25.19	27.04	25.10	
	33.60	34.55	32.98	34.55	32.98	32.94	30.80	
	52.10	55.82	53.31	55.82	53.31	53.84	51.03	
	56.20	57.73	55.13	57.73	55.13	60.07	57.06	
	56.70	61.32	58.56	61.32	58.56	61.60	58.54	
	101.20	107.40	102.57	107.40	102.57	106.06	101.56	
	106.60	109.90	104.97	109.90	104.97	111.04	106.38	
	107.50	113.97	108.86	113.97	108.85	111.99	107.30	
	108.20	114.71	109.56	114.71	109.56	114.20	109.44	
	111.20	116.31	111.09	116.30	111.08	114.49	109.72	
	118.60	123.46	117.92	123.46	117.92	123.24	118.19	
	120.10	124.45	118.87	124.45	118.87	124.14	119.06	
	120.70	126.12	120.46	126.12	120.46	126.72	121.55	
	122.50	126.35	120.68	126.35	120.68	128.13	122.92	
	126.20	130.98	125.10	130.99	125.11	130.88	125.58	
	132.80	138.37	132.16	138.37	132.16	140.50	134.89	
	135.40	139.12	132.88	139.12	132.88	141.04	135.41	
	136.60	144.09	137.63	144.09	137.62	142.71	137.03	
	147.10	149.42	142.71	149.42	142.71	153.19	147.17	
	147.90	149.75	143.03	149.76	143.04	153.38	147.35	
	166.40	179.68	171.62	179.67	171.62	172.01	165.38	
	166.80	181.15	173.02	181.15	173.02	173.56	166.87	
Proton	3.04	2.83	2.94	2.83	2.94	2.92	3.03	
shifts	3.21	3.48	3.57	3.48	3.57	3.27	3.36	
	3.78	3.64	3.71	3.64	3.71	3.66	3.74	
	3.94	3.76	3.83	3.76	3.83	3.72	3.79	
	4.10	3.82	3.89	3.82	3.89	3.93	4.00	
	4.31	4.15	4.20	4.15	4.20	4.19	4.25	
	5.85	6.00	5.98	6.00	5.98	6.01	5.99	
	5.88	6.02	5.99	6.02	5.99	6.04	6.02	
	6.15	6.06	6.04	6.06	6.04	6.04	6.02	
	6.69	6.77	6.72	6.77	6.72	6.73	6.69	
	6.73	6.84	6.78	6.84	6.78	6.87	6.82	
	6.85	7.21	7.14	7.21	7.14	7.08	7.02	
	7.12	7.27	7.20	7.27	7.20	7.32	7.25	
	7.28	7.40	7.32	7.40	7.32	7.39	7.31	
	7.60	7.45	7.37	7.45	7.37	7.39	7.32	
	7.81	7.74	7.65	7.74	7.65	7.81	7.72	
C MAE		5.12	1.90	5.12	1.90	4.81	0.86	
H MAE		0.17	0.14	0.17	0.14	0.14	0.11	
C CorrCoef		0.998		0.998		0.9996		
H CorrCoef		0.9948		0.9948		0.9968		

PROBABILITIES				
DP4 combined	56.4%	61.1%	100.0%	
DP4 C only	9.5%	9.8%	100.0%	
DP4 H only	92.5%	93.5%	99.3%	
Gaussian combined	75.7%	67.1%	100.0%	
Gaussian C only	5.5%	5.8%	100.0%	
Gaussian H only	98.2%	97.0%	99.9%	

Tiotropium (1)	Shifts	mPW1		mPW1		mPW1	
		PW91	6-311G*	PW91	6-311G*	PW91	6-311G*
		mPW1		mPW1		mPW1	
Energy	PW91	6-311G*	M06-2X	6-31G**	M06-2X	6-31G**	
Geom.	MMFF		MMFF		B3LYP	6-31G**	
Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	
Carbon	28.20	34.33	30.84	34.32	30.84	32.34	29.35
shifts	47.10	50.45	46.08	50.44	46.08	48.72	44.90
	53.60	55.11	50.49	55.12	50.50	56.54	52.33
	55.50	59.25	54.40	59.24	54.40	58.10	53.81
	63.60	68.63	63.27	68.63	63.28	70.90	65.97
	64.40	73.22	67.61	73.22	67.61	70.92	65.99
	76.20	83.78	77.59	83.76	77.58	82.41	76.90
	125.70	132.42	123.57	132.42	123.58	131.83	123.83
	126.10	135.27	126.26	135.24	126.25	133.23	125.16
	126.70	135.79	126.75	135.73	126.71	137.67	129.38
	146.60	151.68	141.78	151.71	141.82	154.52	145.39
	169.70	186.57	174.75	186.55	174.75	180.85	170.39
Proton	1.91	2.27	2.29	2.27	2.29	2.13	2.28
shifts	2.69	2.79	2.82	2.79	2.82	2.63	2.76
	3.07	3.06	3.08	3.06	3.08	2.78	2.92
	3.27	3.06	3.08	3.06	3.09	3.23	3.35
	3.52	3.23	3.26	3.23	3.26	3.24	3.36
	4.16	3.76	3.78	3.76	3.78	3.63	3.73
	5.14	5.20	5.22	5.20	5.22	5.02	5.08
	7.02	7.17	7.19	7.19	7.20	7.14	7.14
	7.14	7.26	7.27	7.26	7.27	7.39	7.37
	7.53	7.45	7.46	7.44	7.45	7.48	7.46
C MAE	6.92	2.08	6.92	2.07	6.22	1.53	
H MAE	0.18	0.18	0.18	0.18	0.20	0.17	
C CorrCoef	0.9982		0.9982		0.9993		
H CorrCoef	0.9938		0.9937		0.9939		
PROBABILITIES							
DP4 combined	16.4%		18.2%		88.1%		
DP4 C only	72.6%		76.5%		88.6%		
DP4 H only	3.5%		3.3%		2.3%		
Gaussian combined	31.2%		39.6%		95.8%		
Gaussian C only	82.2%		83.7%		95.0%		
Gaussian H only	4.2%		5.3%		1.1%		

Tanarifuranonol, reassigned (7)	Shifts	mPW1 PW91 6-311G*	mPW1 PW91 6-311G*	mPW1 PW91 6-311G*	
	Energy Geom.	PW91 6-311G* MMFF	M06-2X 6-31G** MMFF	M06-2X 6-31G** B3LYP 6-31G**	
	Exp	Calc.	Corr.	Calc.	Corr.
Carbon	18.30	22.59	20.91	21.72	20.21
shifts	21.40	23.18	21.48	23.12	21.54
	25.20	27.03	25.13	26.89	25.10
	29.80	32.23	30.06	32.27	30.20
	39.50	43.20	40.45	43.18	40.53
	41.30	43.52	40.76	43.43	40.77
	42.75	44.32	41.52	44.81	42.07
	42.80	46.54	43.62	46.52	43.69
	53.40	55.89	52.48	55.58	52.27
	65.60	69.35	65.24	69.37	65.33
	76.90	80.09	75.42	80.06	75.45
	83.40	87.17	82.13	87.14	82.15
	208.20	221.39	209.35	221.38	209.25
Proton	0.97	0.95	0.94	0.94	0.93
shifts	1.22	1.21	1.19	1.19	1.17
	1.28	1.39	1.36	1.38	1.36
	1.42	1.46	1.44	1.46	1.43
	1.42	1.50	1.47	1.46	1.43
	1.67	1.53	1.50	1.56	1.53
	1.67	1.70	1.67	1.67	1.64
	1.67	1.79	1.75	1.82	1.78
	1.87	2.01	1.96	2.02	1.98
	2.14	2.15	2.10	2.15	2.10
	2.53	2.54	2.48	2.60	2.54
	2.53	2.58	2.52	2.61	2.55
	3.41	3.51	3.43	3.50	3.42
	3.60	3.55	3.46	3.55	3.47
	4.05	4.28	4.17	4.24	4.14
C MAE		3.69	0.90	3.61	0.83
H MAE		0.08	0.06	0.08	0.06
C CorrCoef		0.9997		0.9998	
H CorrCoef		0.9962		0.9967	
PROBABILITIES					
DP4 combined		86.2%		89.5%	
DP4 C only		48.2%		48.0%	
DP4 H only		69.1%		73.0%	
Gaussian combined		82.1%		82.7%	
Gaussian C only		53.5%		50.2%	
Gaussian H only		57.9%		57.8%	

Tanarifuranonol, proposed (8)	Shifts	mPW1 PW91 6-311G*	mPW1 PW91 6-311G*	mPW1 PW91 6-311G*	
	Energy Geom.	PW91 6-311G* MMFF	M06-2X 6-31G** MMFF	M06-2X 6-31G** B3LYP 6-31G**	
	Exp	Calc.	Corr.	Calc.	Corr.
Carbon shifts	18.60	22.74	21.05	21.50	20.11
	21.10	22.95	21.25	22.79	21.32
	25.90	27.35	25.41	27.25	25.55
	30.00	32.30	30.11	32.27	30.29
	39.20	42.99	40.23	42.98	40.42
	39.50	43.75	40.95	43.31	40.74
	42.30	44.23	41.40	44.12	41.50
	42.90	46.02	43.10	45.94	43.22
	53.10	55.32	51.90	55.21	51.98
	66.30	69.29	65.14	69.34	65.34
Proton shifts	77.00	79.74	75.03	79.72	75.16
	84.70	88.94	83.75	88.96	83.90
	208.00	221.49	209.27	221.34	209.08
				217.52	207.55
	0.93	0.91	0.84	0.88	0.80
	1.23	1.19	1.13	1.20	1.12
	1.33	1.36	1.31	1.45	1.39
	1.41	1.50	1.45	1.49	1.42
	1.61	1.51	1.46	1.50	1.44
	1.61	1.72	1.68	1.70	1.65
C MAE	1.61	1.82	1.79	1.84	1.80
	1.74	1.87	1.83	1.88	1.83
	1.81	1.88	1.84	1.90	1.85
	2.13	2.14	2.11	2.14	2.10
	2.51	2.47	2.46	2.57	2.55
	2.51	2.56	2.55	2.57	2.55
	3.43	3.50	3.52	3.48	3.49
	3.88	3.78	3.82	3.77	3.80
	3.92	3.83	3.87	3.83	3.86
				3.87	3.88
C CorrCoef	3.73	1.03	3.55	0.90	3.56
H CorrCoef	0.08	0.07	0.09	0.08	0.05
PROBABILITIES	0.9997		0.9998		0.9997
DP4 combined	0.9958		0.9951		0.9979
DP4 C only	98.4%		98.6%		95.6%
DP4 H only	67.3%		75.7%		47.9%
Gaussian combined	91.3%		82.0%		86.2%
Gaussian C only	98.9%		98.1%		96.1%
Gaussian H only	60.8%		68.3%		49.5%
	85.4%		67.3%		75.6%

Tetrahydro-furan 1 (2)	Shifts	mPW1	mPW1	mPW1	
		PW91 6-311G*	PW91 6-311G*	PW91 6-311G*	
		mPW1	M06-2X 6-31G**	M06-2X 6-31G**	
Carbon shifts	Energy	PW91 6-311G*	M06-2X 6-31G**	MMFF	B3LYP 6-31G**
	Geom.	MMFF	MMFF		
	Exp	Calc.	Corr.	Calc.	Corr.
	14.10	16.32	13.58	16.11	13.62
	19.10	23.69	20.81	22.94	20.26
	35.30	40.15	36.95	40.31	37.15
	43.40	46.15	42.84	44.97	41.69
	76.80	79.36	75.42	80.20	75.96
	78.30	81.68	77.69	82.70	78.38
	85.60	88.08	83.96	90.09	85.58
Proton shifts	125.60	129.27	124.37	129.64	124.04
	127.30	130.98	126.05	131.28	125.64
	128.40	133.42	128.44	133.69	127.98
	143.30	152.43	147.09	153.12	146.88
	0.98	1.09	1.04	1.07	0.98
	1.50	1.61	1.55	1.55	1.44
	1.96	2.01	1.94	2.26	2.14
	2.66	2.65	2.57	2.66	2.53
	3.99	4.06	3.94	4.06	3.91
	4.15	4.15	4.03	4.27	4.11
PROBABILITIES	5.05	5.38	5.24	5.41	5.23
	7.26	7.41	7.22	7.41	7.19
	7.34	7.56	7.37	7.60	7.38
	7.39	7.59	7.40	7.61	7.38
	7.62	7.62	7.62	7.62	7.37
	C MAE	4.03	1.31	4.35	1.21
	H MAE	0.12	0.07	0.16	0.08
	C CorrCoef	0.9994		0.9994	0.9995
	H CorrCoef	0.9994		0.9991	0.999
	DP4 combined	99.1%		98.4%	99.4%
Gaussian combined	DP4 C only	69.2%		71.5%	24.5%
	DP4 H only	79.4%		65.9%	60.9%
	Gaussian C only	58.2%		56.2%	27.7%
Gaussian combined	Gaussian H only	70.0%		55.9%	54.2%

Tetrahydro-furan 2 (3)	Shifts	mPW1		mPW1		mPW1	
		PW91	6-311G*	PW91	6-311G*	PW91	6-311G*
		mPW1		mPW1		mPW1	
	Energy	PW91	6-311G*	M06-2X	6-31G**	M06-2X	6-31G**
	Geom.	MMFF		MMFF		B3LYP	6-31G**
	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
Carbon shifts	14.10	16.23	13.75	16.08	13.88	15.53	12.44
	19.10	23.69	21.04	23.42	21.04	22.83	19.58
	36.50	41.30	38.24	40.86	38.04	39.19	35.58
	44.00	45.13	41.98	45.08	42.15	49.90	46.05
	76.80	79.62	75.67	79.54	75.74	82.06	77.50
	79.50	83.94	79.90	83.64	79.74	85.06	80.43
	87.10	89.90	85.72	89.60	85.55	91.59	86.81
	125.90	129.59	124.50	129.64	124.58	130.71	125.07
	127.40	130.72	125.60	130.73	125.64	132.22	126.55
	128.30	133.02	127.85	133.02	127.88	133.09	127.39
	142.10	152.16	146.55	152.18	146.55	149.47	143.41
Proton shifts	0.99	1.07	1.06	1.07	1.04	1.10	1.17
	1.56	1.56	1.52	1.57	1.52	1.66	1.70
	1.97	1.89	1.84	1.93	1.86	1.63	1.68
	2.21	2.33	2.25	2.38	2.29	2.01	2.04
	3.91	4.08	3.92	4.08	3.92	4.12	4.03
	4.17	4.22	4.06	4.18	4.02	4.24	4.14
	5.12	5.64	5.40	5.60	5.38	5.34	5.18
	7.30	7.51	7.19	7.51	7.21	7.55	7.28
C MAE		4.05	1.55	3.91	1.49	4.62	0.99
H MAE		0.15	0.10	0.15	0.10	0.19	0.13
C CorrCoef		0.9991		0.9991		0.9997	
H CorrCoef		0.9979		0.9981		0.997	
PROBABILITIES							
DP4 combined		69.5%		59.8%		10.1%	
DP4 C only		65.3%		48.7%		79.3%	
DP4 H only		44.8%		49.2%		2.1%	
Gaussian combined		77.9%		59.9%		43.5%	
Gaussian C only		71.1%		52.6%		94.4%	
Gaussian H only		43.7%		42.0%		3.0%	

Tetrahydro-furan 3 (4)	Shifts	mPW1		mPW1		mPW1	
		PW91	6-311G*	PW91	6-311G*	PW91	6-311G*
	Energy						
	Geom.	MMFF		MMFF		B3LYP	6-31G**
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
14.30	16.51	13.88		16.32	13.97	15.69	13.20
19.70	24.30	21.51		23.95	21.43	23.48	20.80
31.30	35.09	32.07		34.90	32.13	33.84	30.90
44.70	45.73	42.49		45.96	42.95	48.89	45.57
73.70	77.22	73.32		76.96	73.24	78.85	74.78
78.20	83.86	79.82		83.37	79.51	82.78	78.61
83.10	86.16	82.07		85.44	81.53	85.92	81.68
125.30	129.04	124.05		128.98	124.09	129.35	124.02
127.20	130.61	125.58		130.65	125.72	131.52	126.13
128.40	133.15	128.07		133.19	128.20	133.20	127.77
143.80	152.32	146.84		152.36	146.94	152.16	146.25
Proton shifts	1.01	1.11	1.10	1.11	1.09	1.11	1.07
1.47	1.47	1.46		1.57	1.53	1.64	1.59
1.56	1.53	1.51		1.58	1.55	1.64	1.59
1.64	1.74	1.71		1.66	1.63	1.67	1.62
1.64	1.84	1.81		1.84	1.80	1.84	1.78
2.08	1.86	1.83		1.88	1.83	1.94	1.89
2.45	2.48	2.43		2.53	2.47	2.46	2.40
4.06	4.18	4.06		4.18	4.07	4.06	3.97
4.36	4.22	4.10		4.18	4.07	4.20	4.11
5.26	5.69	5.52		5.63	5.48	5.50	5.39
7.29	7.52	7.28		7.52	7.31	7.52	7.39
C MAE	4.03	1.32		3.85	1.27	4.18	1.07
H MAE	0.15	0.11		0.15	0.10	0.12	0.11
C CorrCoef	0.9994			0.9994		0.9996	
H CorrCoef	0.997			0.9971		0.9978	
PROBABILITIES							
DP4 combined	36.6%			53.9%		88.8%	
DP4 C only	58.0%			62.3%		56.3%	
DP4 H only	7.9%			7.9%		3.9%	
Gaussian combined	35.8%			47.5%		98.7%	
Gaussian C only	62.3%			65.5%		84.7%	
Gaussian H only	6.7%			6.6%		6.2%	

Tetrahydro-furan 4 (5)	Shifts	mPW1		mPW1		mPW1	
		PW91	6-311G*	PW91	6-311G*	PW91	6-311G*
	Energy	mPW1	PW91 6-311G*	M06-2X 6-31G**	M06-2X 6-31G**	B3LYP 6-31G**	
	Geom.	MMFF		MMFF		B3LYP	6-31G**
Carbon shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
14.30	16.52	14.05	16.33	14.04	15.75	13.37	
19.60	23.61	20.94	23.50	21.00	23.39	20.77	
30.90	36.19	33.19	35.84	32.99	34.21	31.25	
44.20	45.92	42.66	45.94	42.80	48.02	44.63	
73.10	76.94	72.84	76.90	72.88	78.43	74.10	
78.70	82.03	77.80	82.06	77.89	82.21	77.76	
83.60	86.25	81.91	86.07	81.79	87.65	83.03	
125.90	129.57	124.06	129.59	124.06	128.82	122.92	
127.30	131.26	125.71	131.27	125.70	131.79	125.80	
128.40	133.73	128.11	133.74	128.10	133.94	127.88	
143.00	153.90	147.74	153.97	147.75	154.17	147.48	
Proton shifts	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
1.00	1.10	0.97	1.10	0.95	1.12	0.99	
1.52	1.61	1.47	1.62	1.47	1.64	1.50	
1.52	1.64	1.50	1.63	1.48	1.68	1.54	
1.52	1.68	1.54	1.73	1.57	1.75	1.62	
1.72	1.82	1.68	1.85	1.70	1.90	1.77	
1.92	2.30	2.16	2.32	2.16	2.05	1.91	
2.70	2.70	2.55	2.71	2.54	2.71	2.57	
3.76	4.02	3.86	4.01	3.84	3.96	3.80	
4.27	4.15	3.98	4.17	3.99	4.06	3.91	
4.87	5.33	5.15	5.33	5.15	5.34	5.18	
7.26	7.40	7.20	7.40	7.20	7.46	7.27	
7.34	7.56	7.36	7.57	7.36	7.53	7.34	
7.40	7.60	7.39	7.60	7.39	7.59	7.40	
C MAE	4.27	1.52	4.20	1.50	4.49	1.35	
H MAE	0.18	0.10	0.19	0.10	0.19	0.08	
C CorrCoef	0.9991		0.9991		0.9992		
H CorrCoef	0.9982		0.9982		0.9982		
PROBABILITIES							
DP4 combined	91.3%		99.2%		94.9%		
DP4 C only	26.4%		25.3%		28.7%		
DP4 H only	37.6%		84.0%		76.4%		
Gaussian combined	91.3%		98.7%		83.1%		
Gaussian C only	23.8%		25.9%		11.2%		
Gaussian H only	44.4%		75.4%		54.7%		

Didanosine (13)	Shifts	mPW1		mPW1		mPW1	
		PW91	6-311G*	PW91	6-311G*	PW91	6-311G*
		mPW1		mPW1		mPW1	
	Energy	PW91	6-311G*	M06-2X	6-31G**	M06-2X	6-31G**
	Geom.	MMFF		MMFF		B3LYP	6-31G**
	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
Carbon	25.52	29.75	24.93	29.72	24.92	30.02	24.14
shifts	32.21	34.91	30.08	34.94	30.13	36.79	30.92
	62.71	70.00	65.17	69.89	65.07	69.02	63.18
	82.11	82.95	78.12	83.01	78.19	87.04	81.21
	84.52	93.75	88.91	93.74	88.91	94.26	88.44
	124.38	132.37	127.53	132.36	127.53	132.58	126.79
	138.25	144.67	139.84	144.66	139.83	145.16	139.39
	145.68	150.20	145.36	150.19	145.36	150.03	144.26
	147.66	148.50	143.66	148.50	143.66	153.18	147.41
	156.68	160.95	156.11	160.95	156.12	159.73	153.97
Proton	2.03	2.37	2.13	2.39	2.14	2.42	2.13
shifts	2.03	2.42	2.18	2.41	2.16	2.34	2.05
	2.40	2.58	2.35	2.57	2.34	2.62	2.36
	2.40	2.22	1.96	2.23	1.97	2.27	1.97
	3.51	3.52	3.38	3.53	3.39	3.57	3.43
	3.63	4.14	4.06	4.14	4.06	4.14	4.07
	4.11	4.17	4.09	4.17	4.09	4.30	4.24
	6.20	6.10	6.20	6.10	6.20	5.98	6.13
	8.06	7.72	7.97	7.72	7.96	7.61	7.96
	8.34	8.10	8.38	8.10	8.39	7.99	8.38
C MAE	4.83	2.32		4.82	2.30	5.81	1.59
H MAE	0.24	0.15		0.24	0.15	0.28	0.15
C CorrCoef	0.9983			0.9983		0.9992	
H CorrCoef	0.9959			0.996		0.9959	
PROBABILITIES							
DP4 combined	54.5%			58.7%		83.0%	
DP4 C only	2.1%			10.0%		30.6%	
DP4 H only	98.2%			92.7%		91.7%	
Gaussian combined	56.2%			40.8%		82.2%	
Gaussian C only	3.7%			11.7%		35.4%	
Gaussian H only	97.1%			83.9%		89.4%	

Zidovudine (11)	Shifts	mPW1		mPW1		mPW1	
		PW91	6-311G*	PW91	6-311G*	PW91	6-311G*
		mPW1		mPW1		mPW1	
	Energy	PW91	6-311G*	M06-2X	6-31G**	M06-2X	6-31G**
	Geom.	MMFF		MMFF		B3LYP	6-31G**
	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
Carbon	10.24	15.76	7.05	15.76	6.99	15.53	7.85
shifts	34.33	38.65	29.87	38.51	29.67	38.71	30.62
	58.27	68.01	59.13	68.17	59.22	67.93	59.34
	58.90	68.72	59.84	68.83	59.88	67.59	59.00
	81.56	91.90	82.95	92.03	83.00	91.75	82.75
	82.11	98.90	89.93	99.18	90.13	98.04	88.93
	107.59	119.82	110.79	119.89	110.77	117.13	107.69
	134.10	142.91	133.81	143.09	133.89	147.51	137.54
	148.48	155.03	145.89	155.04	145.81	156.64	146.51
	161.78	167.26	158.09	167.26	157.98	167.43	157.12
Proton	1.73	1.84	1.45	1.84	1.44	1.85	1.53
shifts	2.22	2.06	1.70	2.04	1.68	1.99	1.69
	2.33	2.75	2.51	2.77	2.53	2.78	2.56
	3.55	3.63	3.53	3.62	3.52	3.69	3.58
	3.61	4.08	4.05	4.07	4.05	4.07	4.00
	3.77	4.25	4.25	4.26	4.26	4.17	4.11
	4.35	4.44	4.47	4.44	4.48	4.51	4.49
	6.05	5.58	5.80	5.57	5.80	5.52	5.61
	7.62	7.02	7.47	7.01	7.47	7.35	7.65
C MAE		8.96	2.84	9.04	2.92	9.09	2.54
H MAE		0.32	0.27	0.33	0.28	0.31	0.26
C CorrCoef		0.9972		0.9971		0.9976	
H CorrCoef		0.9847		0.9839		0.9855	
PROBABILITIES							
DP4 combined		0.0%		0.0%		0.0%	
DP4 C only		0.0%		0.0%		0.0%	
DP4 H only		1.1%		3.4%		0.0%	
Gaussian combined		0.0%		0.0%		0.0%	
Gaussian C only		0.0%		0.0%		0.0%	
Gaussian H only		0.6%		3.2%		0.0%	

Entecavir (12)	Shifts	mPW1		mPW1		mPW1	
		PW91	6-311G*	PW91	6-311G*	PW91	6-311G*
		mPW1		mPW1		mPW1	
	Energy	PW91	6-311G*	M06-2X	6-31G**	M06-2X	6-31G**
	Geom.	MMFF		MMFF		B3LYP	6-31G**
	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
Carbon	39.20	44.13	36.69	44.13	36.70	43.80	35.81
shifts	54.10	60.46	53.19	60.46	53.20	60.36	52.59
	55.20	62.20	54.94	62.18	54.93	64.66	56.95
	63.10	70.31	63.13	70.27	63.10	70.99	63.38
	70.40	78.74	71.64	78.72	71.63	79.98	72.49
	109.30	121.01	114.33	121.03	114.36	118.71	111.75
	116.20	125.15	118.51	125.15	118.51	124.19	117.31
	136.00	143.79	137.32	143.78	137.33	144.05	137.45
	151.30	148.85	142.43	148.85	142.44	154.40	147.94
	151.50	156.05	149.71	156.05	149.72	157.03	150.61
	153.50	160.86	154.56	160.86	154.57	160.07	153.69
	156.90	166.48	160.24	166.45	160.21	163.07	156.73
Proton	2.04	2.40	1.85	2.40	1.85	2.25	1.74
shifts	2.22	2.73	2.21	2.72	2.20	2.62	2.13
	2.52	2.83	2.32	2.83	2.32	2.74	2.27
	3.53	3.94	3.51	3.94	3.51	4.03	3.67
	3.53	4.10	3.68	4.10	3.68	4.15	3.80
	4.23	4.69	4.32	4.69	4.32	4.70	4.40
	4.84	5.27	4.94	5.27	4.94	5.21	4.95
	4.87	5.51	5.20	5.51	5.20	5.41	5.17
	5.36	5.70	5.40	5.70	5.40	5.60	5.37
	7.66	7.53	7.37	7.53	7.37	7.36	7.29
C MAE		7.19	2.39	7.18	2.39	7.05	1.55
H MAE		0.42	0.14	0.41	0.14	0.39	0.20
C CorrCoef		0.9971		0.9971		0.9991	
H CorrCoef		0.9942		0.9942		0.9902	
PROBABILITIES							
DP4 combined		100.0%		100.0%		23.2%	
DP4 C only		21.7%		54.4%		16.4%	
DP4 H only		99.8%		75.4%		26.4%	
Gaussian combined		100.0%		100.0%		46.8%	
Gaussian C only		5.3%		14.7%		17.3%	
Gaussian H only		99.8%		74.0%		47.0%	

Citrinadin B (22)	Shifts	mPW1	mPW1	mPW1			
		PW91	6-311G*	PW91			
		mPW1		M06-2X			
		PW91	6-311G*	6-31G**			
Energy	Geom.	MMFF	MMFF	B3LYP			
				6-31G**			
Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	
Carbon	10.40	11.18	9.82	11.18	9.82	11.14	9.11
shifts	18.60	22.73	20.83	22.73	20.83	20.57	18.09
	18.90	23.17	21.25	23.17	21.25	22.51	19.93
	22.10	23.59	21.65	23.59	21.65	22.55	19.97
	24.30	23.70	21.75	23.70	21.75	25.88	23.14
	28.20	29.10	26.90	29.10	26.90	29.11	26.22
	29.30	30.11	27.86	30.11	27.86	31.71	28.68
	32.70	35.73	33.22	35.73	33.22	35.63	32.42
	34.70	36.77	34.21	36.77	34.21	37.27	33.98
	35.40	40.12	37.40	40.12	37.40	38.95	35.58
	40.80	43.34	40.48	43.34	40.48	43.98	40.36
	46.90	50.73	47.52	50.73	47.51	50.41	46.49
	50.30	52.33	49.05	52.33	49.05	52.21	48.20
	52.00	56.29	52.82	56.29	52.82	59.76	55.39
	55.20	57.36	53.84	57.36	53.84	60.06	55.67
	60.80	60.79	57.11	60.79	57.11	66.87	62.15
	61.50	63.17	59.38	63.19	59.40	67.87	63.10
	64.10	65.71	61.80	65.71	61.80	70.65	65.75
	68.70	75.15	70.80	75.15	70.80	73.55	68.51
	84.00	92.11	86.96	92.11	86.96	89.63	83.81
	105.00	120.92	114.43	120.93	114.44	122.42	115.03
	121.80	128.02	121.20	128.03	121.21	125.39	117.85
	127.00	136.17	128.97	136.17	128.97	136.45	128.38
	133.30	139.23	131.88	139.23	131.89	140.26	132.00
	134.60	141.48	134.03	141.49	134.04	142.16	133.81
	142.60	147.33	139.60	147.32	139.60	152.26	143.42
	185.80	193.82	183.92	193.82	183.93	193.35	182.53
	194.70	205.47	195.03	205.44	195.01	205.52	194.11
Proton	0.99	0.92	1.23	0.92	1.23	0.87	1.23
shifts	1.06	1.11	1.41	1.11	1.41	1.06	1.41
	1.30	1.27	1.56	1.27	1.56	1.21	1.54
	1.36	1.35	1.64	1.35	1.64	1.27	1.60
	1.44	1.38	1.68	1.38	1.68	1.35	1.68
	1.61	1.45	1.74	1.45	1.74	1.46	1.77
	1.63	1.47	1.76	1.47	1.76	1.50	1.81
	1.63	1.58	1.87	1.58	1.87	1.51	1.82
	1.63	1.59	1.88	1.59	1.88	1.51	1.82
	1.74	1.61	1.90	1.61	1.90	1.54	1.85
	2.02	1.63	1.92	1.63	1.92	1.59	1.90
	2.06	1.72	2.00	1.72	2.00	1.74	2.04
	2.23	1.91	2.18	1.90	2.18	1.85	2.14
	2.53	1.99	2.26	1.99	2.26	2.01	2.29

2.87	2.06	2.33	2.06	2.33	2.17	2.43
3.00	2.27	2.54	2.27	2.54	2.32	2.58
3.06	2.67	2.92	2.67	2.92	2.60	2.83
3.35	3.12	3.36	3.12	3.36	3.01	3.22
3.65	3.13	3.37	3.13	3.37	3.14	3.34
4.05	3.19	3.42	3.19	3.42	3.28	3.47
4.52	3.28	3.52	3.28	3.52	3.74	3.90
7.15	7.38	7.50	7.38	7.50	7.28	7.19
7.71	7.99	8.09	7.99	8.09	7.95	7.82
7.75	8.16	8.26	8.16	8.26	8.82	8.63
C MAE	4.40	1.81	4.40	1.81	5.16	1.56
H MAE	0.34	0.29	0.34	0.29	0.35	0.27
C CorrCoef	0.9988		0.9988		0.9988	
H CorrCoef	0.9835		0.9835		0.9863	
PROBABILITIES						
DP4 combined	0.0%		0.2%		64.3%	
DP4 C only	47.9%		48.1%		71.7%	
DP4 H only	0.0%		0.0%		0.0%	
Gaussian combined	0.0%		0.0%		94.9%	
Gaussian C only	54.4%		54.3%		84.0%	
Gaussian H only	0.0%		0.0%		0.0%	

Callipeltin fragment RRR (14)		Shifts	mPW1 PW91 6-311G*	mPW1 PW91 6-311G*	mPW1 PW91 6-311G*	
		Energy Geom.	PW91 6-311G*	M06-2X 6-31G** MMFF	M06-2X 6-31G** B3LYP 6-31G**	
		Exp	Calc.	Corr.	Calc.	Corr.
Carbon shifts	14.60	15.70	13.82	16.45	14.42	16.53
	16.60	17.85	15.92	17.80	15.74	16.81
	21.30	20.99	18.98	21.69	19.53	21.19
	24.30	25.54	23.41	25.07	22.83	24.96
	25.20	28.88	26.68	29.01	26.68	29.31
	33.40	39.10	36.65	38.98	36.41	37.89
	39.40	42.50	39.97	42.33	39.68	41.06
	42.30	43.83	41.27	44.27	41.59	43.78
	78.20	82.72	79.22	82.44	78.85	82.01
	181.40	186.81	180.79	187.01	180.96	186.00
Proton shifts	0.84	0.83	0.68	0.85	0.70	0.89
	0.92	0.85	0.70	0.87	0.72	0.92
	0.95	0.99	0.85	0.99	0.85	1.00
	1.15	1.28	1.15	1.30	1.17	1.31
	1.18	1.44	1.32	1.43	1.31	1.36
	1.23	1.68	1.57	1.59	1.47	1.43
	1.64	1.77	1.66	1.83	1.72	1.77
	1.69	1.81	1.71	1.86	1.75	1.84
	2.74	2.84	2.80	2.82	2.74	2.70
	3.48	3.39	3.37	3.46	3.40	3.55
C MAE		2.78	1.26	2.83	1.08	2.31
H MAE		0.14	0.12	0.13	0.11	0.10
C CorrCoef	0.9995			0.9996		0.9996
H CorrCoef	0.983			0.9889		0.9958
PROBABILITIES						
DP4 combined		0.2%		3.4%		62.0%
DP4 C only		31.0%		48.7%		56.7%
DP4 H only		0.3%		1.9%		27.1%
Gaussian combined		0.7%		9.0%		77.9%
Gaussian C only		28.9%		39.7%		71.3%
Gaussian H only		0.9%		6.8%		34.6%

Callipeltin fragment SRR (15)		Shifts	mPW1 PW91 6-311G*	mPW1 PW91 6-311G*	mPW1 PW91 6-311G*	
		Energy Geom.	PW91 6-311G*	M06-2X 6-31G** MMFF	M06-2X 6-31G** B3LYP 6-31G**	
		Exp	Calc.	Corr.	Calc.	Corr.
Carbon shifts	9.90	11.91	11.08	11.90	10.83	12.59
	15.70	14.45	13.53	15.10	13.93	15.68
	21.30	20.89	19.77	21.57	20.20	21.59
	24.30	25.63	24.35	25.16	23.68	24.83
	25.30	28.91	27.53	29.16	27.56	29.65
	33.50	36.25	34.63	36.08	34.26	35.69
	41.60	41.51	39.73	41.53	39.54	43.29
	41.80	44.20	42.34	45.09	42.99	43.54
	76.30	79.94	76.93	80.07	76.89	79.86
	181.90	188.17	181.72	188.25	181.71	187.06
Proton shifts	0.85	0.77	0.67	0.78	0.67	0.81
	0.85	0.89	0.79	0.89	0.78	0.92
	0.93	1.00	0.89	1.00	0.89	1.01
	1.04	1.18	1.07	1.18	1.07	1.15
	1.22	1.31	1.21	1.31	1.20	1.25
	1.49	1.80	1.69	1.81	1.69	1.70
	1.62	1.84	1.73	1.88	1.76	1.82
	1.67	1.87	1.76	1.89	1.77	1.94
	2.74	2.73	2.61	2.72	2.59	2.68
	3.67	3.78	3.66	3.80	3.66	3.76
C MAE		2.38	1.15	2.36	1.15	2.22
H MAE		0.13	0.09	0.14	0.09	0.12
C CorrCoef	0.9996		0.9996		0.9997	
H CorrCoef	0.9925		0.9915		0.9933	
PROBABILITIES						
DP4 combined		60.2%		46.5%		35.4%
DP4 C only		48.7%		47.8%		53.5%
DP4 H only		31.4%		15.3%		11.3%
Gaussian combined		48.6%		44.7%		59.9%
Gaussian C only		44.1%		47.9%		55.7%
Gaussian H only		27.7%		19.0%		17.1%

Callipeltin fragment SRS (16)		Shifts	mPW1 PW91 6-311G*	mPW1 PW91 6-311G*	mPW1 PW91 6-311G*	
		Energy Geom.	PW91 6-311G*	M06-2X 6-31G** MMFF	M06-2X 6-31G** B3LYP 6-31G**	
		Exp	Calc.	Corr.	Calc.	Corr.
Carbon shifts	11.10	12.27	11.40	12.16	11.33	12.65
	14.50	15.88	14.90	16.04	15.09	15.39
	21.60	20.87	19.74	20.99	19.90	21.40
	23.60	25.47	24.21	25.36	24.13	24.47
	25.00	29.05	27.68	29.04	27.70	29.35
	33.30	36.52	34.93	36.42	34.86	35.96
	42.10	41.29	39.56	41.22	39.52	42.34
	42.60	42.05	40.30	42.00	40.28	43.28
	75.60	79.37	76.51	79.17	76.33	78.53
	181.60	187.85	181.77	187.94	181.85	186.82
Proton shifts	0.85	0.90	0.85	0.91	0.86	0.93
	0.89	0.97	0.92	0.97	0.92	0.97
	0.95	1.00	0.95	1.01	0.96	1.01
	1.07	1.04	0.98	1.01	0.96	1.04
	1.07	1.04	0.98	1.04	0.99	1.08
	1.22	1.30	1.25	1.30	1.24	1.23
	1.66	1.79	1.74	1.79	1.73	1.78
	1.66	1.83	1.77	1.84	1.78	1.86
	2.72	2.72	2.65	2.72	2.65	2.71
	3.68	3.76	3.68	3.77	3.69	3.74
C MAE		2.38	1.34	2.35	1.32	1.96
H MAE		0.07	0.05	0.08	0.05	0.07
C CorrCoef		0.9994		0.9994	0.9997	
H CorrCoef		0.9976		0.9971	0.9973	
PROBABILITIES						
DP4 combined		81.3%		87.8%	78.8%	
DP4 C only		21.4%		14.8%	34.0%	
DP4 H only		73.8%		81.4%	68.7%	
Gaussian combined		61.8%		66.7%	61.5%	
Gaussian C only		23.5%		21.1%	30.8%	
Gaussian H only		59.7%		62.7%	55.3%	

Callipeltin fragment RRS (17)		Shifts	mPW1 PW91 6-311G*	mPW1 PW91 6-311G*	mPW1 PW91 6-311G*	
		Energy Geom.	PW91 6-311G*	M06-2X 6-31G** MMFF	M06-2X 6-31G** B3LYP 6-31G**	
		Exp	Calc.	Corr.	Calc.	Corr.
Carbon shifts	12.50	15.40	13.29	15.73	13.59	14.42
	14.20	16.93	14.79	16.99	14.82	16.22
	22.20	21.57	19.34	21.79	19.53	22.35
	23.10	24.99	22.70	24.80	22.48	23.67
	25.00	28.85	26.48	28.82	26.43	29.16
	32.10	38.28	35.73	38.30	35.72	37.15
	43.10	43.19	40.55	43.18	40.52	43.56
	43.20	43.52	40.87	43.52	40.84	44.63
	75.60	80.73	77.36	80.43	77.05	79.18
	181.40	186.70	181.28	186.81	181.41	185.88
Proton shifts	0.85	0.87	0.77	0.87	0.76	0.92
	0.86	0.95	0.86	0.95	0.85	0.96
	0.89	1.01	0.92	1.02	0.92	0.98
	1.16	1.19	1.11	1.14	1.05	1.14
	1.18	1.22	1.14	1.28	1.19	1.28
	1.24	1.37	1.29	1.38	1.30	1.42
	1.66	1.77	1.71	1.78	1.71	1.71
	1.70	1.78	1.72	1.78	1.72	1.87
	2.66	2.82	2.80	2.83	2.80	2.72
	3.61	3.50	3.50	3.50	3.50	3.57
C MAE		2.90	1.65	2.88	1.64	2.38
H MAE		0.09	0.06	0.10	0.06	0.09
C CorrCoef		0.9991		0.9992		0.9995
H CorrCoef		0.9968		0.9959		0.9975
PROBABILITIES						
DP4 combined		87.3%		83.1%		91.2%
DP4 C only		34.9%		19.7%		50.7%
DP4 H only		72.2%		67.4%		48.8%
Gaussian combined		79.1%		74.6%		88.0%
Gaussian C only		31.7%		25.8%		54.4%
Gaussian H only		65.0%		56.6%		40.9%

Oseltamivir (19)	Shifts	mPW1		mPW1		mPW1	
		PW91	6-311G*	PW91	6-311G*	PW91	6-311G*
		mPW1		mPW1		mPW1	
Energy	PW91	6-311G*	M06-2X	6-31G**	M06-2X	6-31G**	B3LYP
Geom.	MMFF	MMFF					6-31G**
Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.	
Carbon	9.30	11.03	9.39	10.25	8.69	9.96	8.64
shifts	9.50	12.23	10.54	12.84	11.17	11.99	10.60
	14.20	16.24	14.38	16.35	14.52	15.74	14.19
	23.70	24.25	22.04	24.33	22.15	24.93	23.03
	25.80	28.57	26.17	27.97	25.64	28.13	26.10
	26.30	29.24	26.82	29.30	26.91	29.43	27.36
	33.60	36.72	33.98	36.76	34.05	35.87	33.55
	49.20	51.87	48.48	52.16	48.78	50.62	47.73
	59.00	62.23	58.40	62.09	58.29	64.44	61.02
	60.80	68.20	64.11	68.87	64.77	67.11	63.59
	74.80	76.61	72.16	76.71	72.27	74.10	70.30
	81.70	83.19	78.46	82.24	77.56	82.96	78.82
	129.60	137.39	130.35	137.62	130.54	135.60	129.44
	137.50	149.72	142.16	149.57	141.98	149.64	142.93
	166.30	174.77	166.13	174.75	166.07	173.61	165.97
	170.90	177.37	168.63	177.64	168.83	176.68	168.92
Proton	0.89	0.93	0.91	0.95	0.93	0.96	0.96
shifts	0.90	1.00	0.98	1.02	1.00	1.02	1.03
	1.29	1.31	1.30	1.30	1.28	1.31	1.32
	1.50	1.53	1.52	1.42	1.41	1.46	1.46
	1.50	1.54	1.53	1.45	1.44	1.47	1.48
	1.50	1.56	1.55	1.63	1.63	1.59	1.59
	1.50	1.58	1.57	1.65	1.64	1.69	1.69
	2.04	1.86	1.86	1.87	1.86	1.85	1.85
	2.15	2.05	2.05	2.04	2.04	1.94	1.94
	2.75	2.68	2.69	2.72	2.73	2.64	2.63
	3.24	2.77	2.78	2.74	2.75	2.70	2.69
	3.34	3.38	3.39	3.44	3.46	3.56	3.54
	3.52	4.15	4.18	4.10	4.13	4.00	3.98
	4.18	4.18	4.21	4.19	4.22	4.25	4.22
	4.20	4.20	4.23	4.21	4.24	4.28	4.25
	5.62	4.83	4.87	4.81	4.85	5.15	5.12
	6.78	7.19	7.27	7.20	7.28	7.22	7.16
C MAE	4.21	1.41	4.20	1.55	3.75	1.59	
H MAE	0.18	0.18	0.20	0.20	0.20	0.19	
C CorrCoef	0.9993		0.9992		0.9991		
H CorrCoef	0.9839		0.9833		0.988		
PROBABILITIES							
DP4 combined	100.0%		99.4%		100.0%		
DP4 C only	91.7%		76.6%		70.4%		
DP4 H only	95.8%		77.9%		99.9%		

Gaussian combined	100.0%	99.6%	100.0%	
Gaussian C only	66.9%	44.4%	51.5%	
Gaussian H only	99.3%	95.4%	100.0%	

		mPW1		mPW1		mPW1	
		PW91	6-311G*	PW91	6-311G*	PW91	6-311G*
		mPW1		mPW1		mPW1	
		PW91	6-311G*	M06-2X	6-31G**	M06-2X	6-31G**
		MMFF		MMFF		B3LYP	
		Exp	Calc.	Corr.	Calc.	Corr.	Calc.
Lopinavir (21)	Shifts	16.10	19.22	17.00	19.02	16.59	18.81
	Energy	18.70	20.43	18.16	20.51	18.03	19.17
Carbon shifts		19.60	21.01	18.72	20.73	18.24	20.62
		21.70	23.68	21.30	23.39	20.80	24.60
		25.40	29.63	27.03	29.82	27.00	28.95
		38.20	39.40	36.44	40.66	37.43	40.60
		40.00	40.60	37.60	41.19	37.94	40.88
		40.80	41.88	38.83	41.91	38.63	41.02
		41.10	43.08	39.99	42.00	38.72	42.88
		41.80	43.61	40.50	43.96	40.60	42.96
		48.70	55.42	51.88	54.87	51.11	55.52
		54.40	63.10	59.27	65.30	61.15	65.04
		63.10	68.06	64.05	68.76	64.48	65.43
		69.70	74.00	69.77	74.70	70.20	72.16
		70.20	75.75	71.47	77.45	72.85	74.43
		124.60	130.71	124.41	130.19	123.63	129.57
		126.00	130.72	124.42	130.54	123.97	131.41
		126.30	131.43	125.11	131.48	124.88	131.60
		128.20	133.67	127.26	133.45	126.77	133.15
		128.40	133.94	127.52	133.60	126.92	133.57
		129.00	134.42	127.98	134.54	127.82	133.66
		129.20	134.58	128.14	134.68	127.95	135.16
		129.30	134.98	128.53	135.22	128.48	135.59
		130.30	138.55	131.96	138.77	131.89	138.85
		138.00	146.85	139.96	147.17	139.98	147.25
		138.10	147.78	140.86	149.19	141.93	148.00
		154.20	160.00	152.62	158.98	151.35	161.92
		156.50	160.23	152.85	160.62	152.93	162.29
		168.80	179.17	171.10	180.13	171.71	177.50
		170.70	180.48	172.35	181.60	173.13	178.80
							170.70
Proton shifts	0.83	0.73	0.34	0.54	0.31	0.69	0.35
	1.28	1.73	1.34	1.28	1.04	1.65	1.31
	1.28	1.81	1.43	1.52	1.28	1.80	1.46
	1.53	1.87	1.49	1.99	1.74	1.95	1.61
	1.74	2.09	1.72	2.10	1.85	1.96	1.62
	1.74	2.31	1.94	2.18	1.93	2.11	1.78
	1.83	2.38	2.01	2.24	1.99	2.18	1.84
	2.18	3.00	2.64	2.69	2.42	2.87	2.53
	2.23	3.02	2.66	2.71	2.45	2.89	2.55
	2.68	3.04	2.67	2.77	2.50	3.00	2.67
	2.81	3.17	2.81	2.79	2.53	3.10	2.77
	2.88	3.18	2.82	3.04	2.78	3.16	2.83
	2.97	3.28	2.92	3.09	2.82	3.20	2.86

2.97	3.29	2.93	3.12	2.85	3.24	2.91
3.06	3.52	3.17	3.45	3.17	3.33	2.99
3.06	3.62	3.27	3.78	3.50	3.41	3.07
3.12	3.64	3.29	3.94	3.66	3.96	3.63
3.78	3.88	3.53	4.08	3.80	4.14	3.80
4.19	3.97	3.62	4.10	3.81	4.17	3.84
4.19	4.04	3.69	4.34	4.05	4.17	3.84
4.25	4.11	3.77	4.38	4.09	4.54	4.21
6.97	7.14	6.84	7.14	6.81	7.15	6.83
6.97	7.22	6.92	7.23	6.90	7.15	6.84
6.97	7.26	6.97	7.25	6.91	7.18	6.87
7.21	7.40	7.11	7.45	7.11	7.48	7.17
7.21	7.41	7.12	7.46	7.12	7.53	7.21
7.21	7.48	7.18	7.54	7.20	7.53	7.22
7.21	7.52	7.23	7.58	7.24	7.55	7.24
7.21	7.55	7.26	7.60	7.26	7.56	7.24
7.21	7.56	7.27	7.61	7.26	7.56	7.25
7.21	7.57	7.28	7.63	7.29	7.61	7.29
7.21	7.62	7.33	7.64	7.30	7.61	7.30
7.21	7.68	7.39	7.64	7.30	7.66	7.34
7.21	7.96	7.67	7.71	7.36	7.67	7.35
C MAE	4.98	1.55	5.24	1.90	4.81	1.46
H MAE	0.37	0.17	0.32	0.16	0.34	0.12
C CorrCoef	0.9994		0.999		0.9993	
H CorrCoef	0.9947		0.996		0.9969	
PROBABILITIES						
DP4 combined	0.0%		0.0%		0.0%	
DP4 C only	0.0%		0.0%		0.0%	
DP4 H only	0.0%		0.0%		44.5%	
Gaussian combined	0.0%		0.0%		0.0%	
Gaussian C only	0.1%		0.0%		0.0%	
Gaussian H only	0.0%		0.0%		7.1%	

Artemisinin (20)	Shifts	mPW1		mPW1		mPW1	
		PW91	6-311G*	PW91	6-311G*	PW91	6-311G*
		mPW1		M06-2X	6-31G**	M06-2X	6-31G**
		Energy	PW91 6-311G*	MMFF	MMFF	B3LYP	6-31G**
	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
Carbon	13.20	16.20	14.00	16.20	14.00	14.20	12.43
shifts	20.50	21.35	18.90	21.35	18.90	21.04	19.08
	24.00	27.58	24.81	27.58	24.81	26.34	24.23
	25.50	27.60	24.83	27.60	24.83	26.69	24.57
	25.80	29.42	26.56	29.42	26.56	28.51	26.34
	33.50	36.67	33.45	36.67	33.45	36.16	33.78
	34.20	38.75	35.43	38.75	35.43	37.23	34.82
	36.50	40.34	36.94	40.34	36.94	38.69	36.23
	38.20	41.54	38.08	41.54	38.08	41.49	38.95
	45.60	49.39	45.53	49.39	45.53	48.95	46.21
	50.70	53.93	49.85	53.93	49.85	53.98	51.10
	80.10	85.89	80.22	85.89	80.22	84.76	81.02
	94.30	101.56	95.10	101.56	95.10	97.92	93.82
	106.00	110.08	103.20	110.08	103.20	110.47	106.02
	172.70	184.49	173.90	184.49	173.90	178.57	172.22
Proton	0.98	0.97	0.90	0.97	0.90	1.01	0.98
shifts	1.05	0.97	0.90	0.97	0.90	1.09	1.06
	1.05	1.11	1.05	1.11	1.05	1.12	1.09
	1.18	1.16	1.10	1.16	1.10	1.20	1.17
	1.42	1.42	1.37	1.42	1.37	1.39	1.37
	1.42	1.49	1.43	1.49	1.43	1.49	1.47
	1.42	1.63	1.58	1.63	1.58	1.54	1.51
	1.42	1.69	1.64	1.69	1.64	1.59	1.57
	1.75	1.71	1.66	1.71	1.66	1.70	1.68
	1.75	1.84	1.79	1.84	1.79	1.75	1.74
	1.86	1.88	1.84	1.88	1.84	1.76	1.75
	1.99	1.95	1.91	1.95	1.91	1.94	1.92
	1.99	2.11	2.07	2.11	2.07	1.99	1.98
	2.41	2.63	2.60	2.63	2.60	2.43	2.43
	3.38	3.26	3.24	3.26	3.24	3.25	3.27
	5.84	5.78	5.84	5.78	5.84	5.84	5.92
C MAE	4.27	0.82	4.27	0.82	2.95	0.58	
H MAE	0.09	0.09	0.09	0.09	0.06	0.06	
C CorrCoef	0.9997		0.9997		0.9999		
H CorrCoef	0.9956		0.9956		0.9982		
PROBABILITIES							
DP4 combined	100.0%		100.0%		100.0%		
DP4 C only	82.2%		82.2%		95.3%		
DP4 H only	97.5%		97.5%		95.5%		
Gaussian combined	99.9%		99.8%		100.0%		
Gaussian C only	67.1%		66.5%		97.0%		

Gaussian H only | 93.3% | 90.6% | 89.6% |

Aspergillide A (24)	Shifts	mPW1		mPW1		mPW1	
		PW91	6-311G*	PW91	6-311G*	PW91	6-311G*
		mPW1		mPW1		mPW1	
		Energy	PW91 6-311G*	Geom.	M06-2X 6-31G**	Geom.	M06-2X 6-31G**
		MMFF		MMFF		B3LYP	6-31G**
	Exp	Calc.	Corr.	Calc.	Corr.	Calc.	Corr.
Carbon	18.50	19.42	18.55	19.05	18.49	18.55	16.71
shifts	21.70	24.33	23.15	24.34	23.44	24.52	22.40
	21.90	23.88	22.72	23.84	22.97	24.83	22.69
	23.60	27.02	25.66	26.47	25.43	27.07	24.83
	31.00	34.88	33.02	34.40	32.84	35.40	32.76
	32.10	34.09	32.29	33.11	31.63	33.02	30.50
	40.50	42.93	40.56	42.90	40.79	43.28	40.28
	66.70	69.84	65.75	69.84	65.97	69.79	65.54
	71.30	70.72	66.58	70.85	66.92	75.88	71.34
	71.50	71.43	67.24	71.01	67.06	75.16	70.66
	74.00	77.67	73.08	77.59	73.22	78.93	74.25
	132.10	143.19	134.43	143.47	134.80	140.51	132.94
	137.00	146.62	137.64	145.97	137.14	145.31	137.51
	170.10	182.58	171.31	182.50	171.29	178.97	169.59
Proton	1.19	1.26	1.23	1.28	1.24	1.28	1.25
shifts	1.38	1.41	1.38	1.42	1.38	1.38	1.35
	1.49	1.45	1.41	1.42	1.38	1.45	1.41
	1.50	1.68	1.63	1.70	1.65	1.72	1.67
	1.71	1.79	1.73	1.79	1.73	1.73	1.69
	1.81	1.92	1.86	1.91	1.85	1.93	1.88
	1.88	2.00	1.94	2.02	1.96	2.07	2.01
	1.95	1.79	1.74	1.79	1.74	1.88	1.83
	2.10	2.41	2.33	2.39	2.31	2.41	2.34
	2.21	2.28	2.21	2.29	2.21	2.21	2.15
	2.28	2.47	2.39	2.50	2.41	2.43	2.36
	2.39	2.27	2.20	2.28	2.20	2.31	2.24
	2.63	2.72	2.63	2.72	2.62	2.55	2.48
	3.58	3.56	3.43	3.56	3.42	3.51	3.40
	4.21	4.30	4.14	4.30	4.13	4.23	4.09
	4.23	4.36	4.19	4.36	4.19	4.32	4.17
	4.94	4.92	4.73	4.97	4.77	5.04	4.87
	5.69	6.12	5.88	6.11	5.86	6.06	5.85
	5.79	6.15	5.91	6.17	5.92	6.14	5.93
C MAE		4.14	1.55	3.94	1.54	4.23	0.87
H MAE		0.14	0.10	0.14	0.10	0.12	0.11
C CorrCoef		0.999		0.999		0.9998	
H CorrCoef		0.9962		0.9963		0.9963	
PROBABILITIES							
DP4 combined		100.0%		100.0%		100.0%	
DP4 C only		99.8%		99.8%		100.0%	
DP4 H only		99.7%		99.7%		98.6%	

Gaussian combined	100.0%	100.0%	100.0%	
Gaussian C only	99.2%	99.3%	100.0%	
Gaussian H only	99.4%	98.9%	99.5%	

		mPW1		mPW1		mPW1			
		PW91	6-311G*	PW91	6-311G*	PW91	6-311G*		
		mPW1		M06-2X		M06-2X			
		PW91	6-311G*	M06-2X	6-31G**	M06-2X	6-31G**		
		MMFF		MMFF		B3LYP			
		Exp	Calc.	Corr.	Calc.	Corr.	Calc.		
Aspergillide B (25)	Shifts	Carbon shifts	19.20	21.01	19.07	21.76	19.28	21.52	18.14
			22.60	26.32	24.05	26.42	23.67	26.68	23.12
			25.30	29.30	26.84	30.60	27.61	30.75	27.04
			27.80	30.78	28.24	30.86	27.85	31.31	27.58
			30.70	34.77	31.98	34.75	31.52	35.68	31.80
			32.10	35.67	32.83	37.79	34.38	38.03	34.07
			39.90	43.27	39.96	43.16	39.45	42.33	38.22
			67.20	71.18	66.16	70.89	65.58	70.21	65.12
			69.60	71.48	66.44	71.64	66.29	74.65	69.40
			69.80	73.97	68.78	74.01	68.52	74.33	69.09
			71.50	73.97	68.78	74.16	68.66	76.17	70.87
			129.00	138.37	129.23	138.12	128.95	135.64	128.24
			138.20	148.51	138.75	148.82	139.04	147.70	139.88
			169.80	183.49	171.59	183.69	171.90	179.05	170.12
Proton shifts	Proton shifts	0.99	1.35	1.06	1.34	1.03	1.33	1.03	
		1.07	1.24	0.95	1.26	0.96	1.30	0.99	
		1.31	1.70	1.42	1.78	1.49	1.71	1.43	
		1.34	1.53	1.25	1.60	1.30	1.67	1.39	
		1.37	1.69	1.41	1.68	1.39	1.68	1.40	
		1.52	1.97	1.69	1.99	1.70	1.87	1.60	
		1.55	1.81	1.53	1.80	1.51	1.81	1.53	
		1.61	1.93	1.65	1.83	1.54	1.84	1.56	
		1.74	2.06	1.78	2.07	1.78	2.22	1.95	
		1.78	2.15	1.88	2.15	1.87	2.10	1.83	
		2.04	2.34	2.07	2.40	2.12	2.37	2.12	
		2.12	2.37	2.10	2.36	2.09	2.23	1.97	
		2.71	2.59	2.32	2.62	2.34	2.46	2.21	
		3.22	3.46	3.20	3.46	3.21	3.48	3.27	
		4.08	4.38	4.14	4.40	4.18	4.27	4.11	
		4.30	4.57	4.32	4.57	4.35	4.55	4.39	
		5.09	4.85	4.61	4.77	4.55	4.82	4.68	
		5.38	5.74	5.51	5.71	5.52	5.62	5.51	
		6.19	6.72	6.50	6.66	6.49	6.51	6.45	
		C MAE	4.96	1.15	5.28	1.36	5.10	1.05	
		H MAE	0.30	0.12	0.31	0.13	0.29	0.13	
		C CorrCoef	0.9995		0.9993		0.9997		
		H CorrCoef	0.9938		0.9932		0.9934		
PROBABILITIES									
		DP4 combined	100.0%		100.0%		99.8%		
		DP4 C only	86.5%		49.5%		94.7%		
		DP4 H only	99.0%		99.5%		73.2%		

Gaussian combined	100.0%	100.0%	100.0%	
Gaussian C only	82.4%	47.2%	99.2%	
Gaussian H only	97.2%	98.2%	43.2%	

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