

SUPPLEMENTARY MATERIAL TO
Theoretical study *via* DFT for the prediction of ^{13}C - and ^1H -NMR data for two diterpenoids derived from the root of *Salvia grandifolia*

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TABLE S-I. Experimental (Exp), theoretical (Theo-DFT), residues and predicted (by linear models) NMR data (δ_{H} and δ_{C}) for diterpene **1**

Position	B3LPY/cc-pVDZ				B3PW91/DGDZVP				B3LPY/cc-pVDZ				B3PW91/DGDZVP			
	^{13}C								^1H							
	δ / ppm								δ / ppm							
	Exp	Theo	Res	Pred	Theo	Res	Pred	Exp	Theo	Res	Pred	Theo	Res	Pred		
1 α	31.4	31.6	0.2	29.4	32.3	0.9	30.1	1.07	1.22	0.35	2.34	2.21	0.28	2.20		
1 β	–	–	–	–	–	–	–	2.49	2.14	0.15	1.34	1.07	0.35	1.37		
2 α	19.3	21.7	2.4	19.5	22.1	2.8	20.5	1.61	1.59	0.02	1.74	1.65	0.04	1.61		
2 β	–	–	–	–	–	–	–	1.41	1.42	0.01	1.56	1.59	0.18	1.55		
3 α	42.1	38.4	3.6	36.2	38.8	3.2	36.2	1.11	1.15	0.07	1.26	1.56	0.19	1.52		
3 β	–	–	–	–	–	–	–	1.37	1.44	0.04	1.58	1.41	0.30	1.36		
4	34.1	37.9	3.8	35.8	34.3	0.2	31.9	–	–	–	–	–	–	–		
5	51.5	49.1	1.9	46.9	48.6	2.4	45.4	1.31	1.26	0.05	1.38	1.73	0.42	1.70		
6 α	18.7	22.4	3.7	20.2	22.3	3.6	20.7	1.93	1.61	0.32	1.76	1.73	0.20	1.70		
6 β	–	–	–	–	–	–	–	1.71	1.48	0.23	1.62	1.60	0.11	1.56		
7 α	35.2	38.1	2.9	35.9	38.3	3.1	35.7	1.85	1.43	0.48	1.99	2.04	0.26	2.02		

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TABLE S-I. Continued

Position	B3LPY/cc-pVDZ				B3PW91/DGDZVP				B3LPY/cc-pVDZ				B3PW91/DGDZVP			
	¹³ C								¹ H							
	δ / ppm								δ / ppm							
	Exp	Theo	Res	Pred	Theo	Res	Pred	Exp	Theo	Res	Pred	Theo	Res	Pred		
7 β	–	–	–	–	–	–	–	2.30	1.82	0.42	1.57	1.63	0.22	1.60		
8	82.6	87.0	4.4	85.0	89.2	6.6	83.5	–	–	–	–	–	–	–		
9	160.6	166.7	6.1	165.0	175.8	15.2	164.9	–	–	–	–	–	–	–		
10	45.3	51.9	6.6	49.8	50.3	5.0	46.9	–	–	–	–	–	–	–		
11	120.0	122.2	2.2	120.3	129.2	9.2	121.1	6.28	5.55	0.73	6.02	5.78	0.50	1.93		
12	103.5	102.5	1.0	100.5	105.5	2.0	98.8	–	–	–	–	–	–	–		
13	193.3	189.4	3.8	187.8	201.4	8.1	188.9	–	–	–	–	–	–	–		
14	135.7	136.0	0.3	134.2	141.4	5.7	132.6	–	–	–	–	–	–	–		
15	145.9	152.8	6.9	151.0	163.1	17.2	153.0	6.93	6.94	0.01	7.52	7.22	0.29	7.44		
16	18.8	21.1	2.3	18.9	23.1	4.3	21.4	1.93	1.81	0.12	1.98	1.82	0.11	1.79		
17	34.1	31.7	2.3	29.5	33.3	0.7	31.0	0.89	0.79	0.10	0.88	0.90	0.01	0.83		
18	23.7	28.7	5.0	26.5	30.4	6.7	28.3	0.89	0.89	0.00	0.98	0.98	0.09	0.91		
19	59.8	63.8	4.0	61.7	68.0	8.2	63.6	4.16	3.56	0.60	3.88	3.60	0.56	3.65		
19	–	–	–	–	–	–	–	3.68	3.22	0.46	3.51	3.28	0.40	3.32		

TABLE S-II. Experimental (Exp), theoretical (Theo-DFT), residues and predicted (by linear models) NMR data (δ_H and δ_C) for diterpene 2

Position	B3LPY/cc-Pvdz				B3PW91/DGDZVP				B3LPY/cc-pVDZ				B3PW91/DGDZVP			
	¹³ C								¹ H							
	δ / ppm								δ / ppm							
	Exp	Theo	Res	Pred	Theo	Res	Pred	Exp	Theo	Res	Pred	Theo	Res	Pred		
1 α	33.8	27.5	6.2	24.4	28.0	5.7	24.8	2.93	2.42	0.51	2.56	2.49	0.44	2.43		
1 β	–	–	–	–	–	–	–	1.16	1.57	0.41	1.68	1.72	0.56	1.65		
2 α	19.6	21.8	2.5	18.6	21.7	2.4	18.8	1.66	1.47	0.12	1.67	1.76	0.07	1.69		
2 β	–	–	–	–	–	–	–	1.69	1.57	0.19	1.57	1.55	0.11	1.49		
3 α	40.7	41.1	0.4	38.5	41.6	0.9	37.9	1.26	1.26	0.18	1.40	1.54	0.05	1.48		
3 β	–	–	–	–	–	–	–	1.49	1.31	0.00	1.34	1.46	0.20	1.39		
4	34.0	38.7	4.7	36.1	35.3	1.3	31.9	–	–	–	–	–	–	–		
5	51.0	49.6	1.4	47.3	50.8	0.1	46.8	1.58	1.36	0.22	1.45	1.70	0.12	1.63		
6 α	18.2	23.7	5.5	20.6	23.2	5.0	20.2	2.06	1.68	0.21	2.45	2.33	0.23	2.27		
6 β	–	–	–	–	–	–	–	2.10	2.31	0.38	1.78	1.88	0.18	1.82		
7 α	35.5	36.7	0.8	35.9	37.9	2.1	34.4	3.03	2.50	0.53	2.67	2.85	0.18	2.81		
7 β	–	–	–	–	–	–	–	3.03	2.75	0.28	2.92	2.67	0.36	2.63		
8	138.8	141.2	2.4	142.0	149.3	10.5	141.4	–	–	–	–	–	–	–		
9	141.4	147.5	6.1	148.6	154.4	13.0	146.2	–	–	–	–	–	–	–		
10	55.8	62.4	6.6	60.6	63.4	7.6	58.8	–	–	–	–	–	–	–		
11	117.0	109.2	7.7	109.0	119.6	2.6	112.8	7.29	7.25	0.04	7.63	7.76	0.47	7.77		
12	159.1	161.0	1.9	162.5	168.9	9.8	160.2	–	–	–	–	–	–	–		
13	176.4	171.5	4.8	173.4	179.8	3.4	170.7	–	–	–	–	–	–	–		
14	140.8	141.8	1.0	142.7	151.6	10.8	143.6	–	–	–	–	–	–	–		
15	142.8	142.1	0.6	143.1	152.2	9.4	144.2	7.45	7.36	0.09	7.74	7.88	0.43	7.89		
16	22.6	26.4	3.8	23.3	28.7	6.2	25.5	2.41	2.12	0.29	2.25	2.39	0.02	2.33		

TABLE S-II. Continued

Position	B3LPY/cc-Pvdz			B3PW91/DGDZVP			B3LPY/cc-pVDZ			B3PW91/DGDZVP				
	^{13}C						^1H							
	δ / ppm						δ / ppm							
	Exp	Theo	Res	Pred	Theo	Res	Pred	Exp	Theo	Res	Pred	Theo	Res	Pred
17	31.6	34.35	2.7	31.5	31.4	0.1	28.1	1.02	0.98	0.04	1.05	1.09	0.07	1.01
18	20.8	29.79	8.9	26.8	36.5	15.7	33.0	0.84	0.83	0.01	0.90	0.95	0.11	0.87
19	200.0	193.5	6.4	196.2	210.3	10.3	199.9	9.94	9.19	0.75	9.66	9.46	0.48	9.49