

Correction to Advanced Structural Determination of Diterpene Esters Using Molecular Modeling and NMR Spectroscopy

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Page 2428: Some of the calculated chemical shifts shown in Table 4 do not correspond to the indicated positions. Table 4 should be replaced by Table 4 below. The authors

greatly apologize to the scientific community for the inconvenience caused by these errors.

Table 4. Comparison of ¹H NMR Data from Experimental Chemical Shifts (δ_{exp}) for 3 vs Calculated Chemical Shifts by DFT-NMR (δ_{calcd}) for 3a–3d (δ_{H} in ppm)

position	δ_{exp} (3)	δ_{calcd} (3a)	δ_{calcd} (3b)	δ_{calcd} (3c)	δ_{calcd} (3d)
1 α	2.03 dd (15.3, 6.2)	1.82	2.32	2.21	2.17
1 β	1.79 m	1.82	2.35	2.31	1.77
2	1.91 m	1.88	1.87	1.64	2.12
3	5.88 br dd (3.0, 2.6)	5.63	5.61	5.46	5.39
4	2.49 dd (3.0, 2.2)	2.60	3.06	2.41	3.61
5	6.0 br d (2.2)	5.87	4.92	5.16	6.03
7	5.07 d (9.5)	4.89	5.95	5.11	4.85
8	5.41 d (9.5)	5.29	5.73	5.41	5.56
11	5.79 d (15.7)	5.78	6.02	5.74	6.39
12	5.86 dd (15.7, 8.5)	5.94	5.65	5.63	5.55
13	3.01 dt (8.5, 7.0)	3.04	2.96	2.85	3.14
14	5.08 br s	4.82	5.37	5.32	4.95
16	0.90 d (6.6)	0.92	0.91	0.86	1.01
17 α	3.81 d (12.2)	3.62	4.96	5.08	3.59
17 β	3.75 d (12.2)	3.74	3.72	3.82	3.22
18	1.11 s	1.20	1.33	1.40	1.40
19	0.88 s	0.88	1.13	1.03	1.04
20	1.03 d (7.0)	0.99	1.13	1.09	1.05
OH-6	3.45 br s	2.11	4.27	2.27	4.77
OH-9	3.21 br s	3.32	1.76	2.62	1.79
OH-15	2.17 br s	0.67	4.77	3.90	0.65
OBz-3					
2', 6'	8.09 dd (8.1, 1.1)	8.00	7.89	7.90	7.97
3', 5'	7.44 t (7.7)	7.19	7.18	7.22	7.22
4'	7.57 t (7.5)	7.31	7.26	7.29	7.33
OAc-5	1.78 s	2.08	1.83	1.94	1.39
OAc-7	1.84 s	1.74	1.99	1.82	2.05
OAc-8	1.97 s	1.91	2.10	1.96	2.01
OAc-14	2.18 s	2.11	2.20	2.13	2.15
r^a		0.983	0.941	0.964	0.962
r^2		0.9973	0.9663	0.9751	0.9878
MAE		0.12	0.31	0.24	0.25
MaxErr		0.30	1.15	1.27	1.12
CMAE		0.09	0.39	0.37	0.28
CMaxErr		0.32	1.22	1.16	1.13

^aThe best agreements are highlighted in bold type. r = Pearson product-moment correlation coefficient; r^2 = correlation coefficient; MAE = mean average error; MaxErr = maximum error; CMAE = corrected mean average error; CMaxErr = corrected maximum error.

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