nmrshiftdb2 Quality Report - ^{1}H
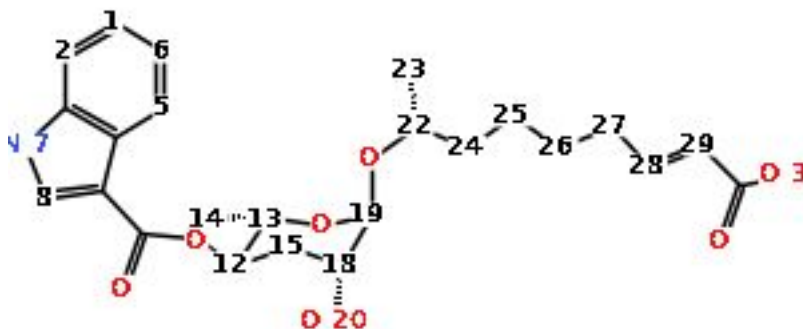
Atom	δ [ppm]	Deviation from prediction	Prediction		HOSE Code
			No. Spheres	No. shift values	
1	7.18	0.02	6.0	11.0	2D
2	7.42	0.04	5.0	11.0	2D
5	7.99	0.07	4.0	4.0	2D
6	7.15	0.04	5.0	4.0	2D
8	7.94	0.60	3.0	19.0	2D
12	5.09	1.12	3.0	13.0	2D
13	4.02	0.15	3.0	40.0	2D
14	1.21	0.01	4.0	40.0	2D
15a	2.19	0.24, calculated from average of shifts	3.0	5.0	2D
15b	1.98	0.24, calculated from average of shifts	3.0	5.0	2D
18	3.77	0.41 ⚠ [1]	2.0	277.0	3D
19	4.73	0.17	3.0	119.0	2D
22	3.83	0.73	3.0	13.0	2D
23	1.15	0.11	4.0	4.0	3D
24a	1.54	0.09, calculated from average of shifts	4.0	2.0	3D
24b	1.53	0.09, calculated from average of shifts	4.0	2.0	3D
25a	1.51	0.27, calculated from average of shifts	4.0	2.0	3D
25b	1.51	0.27, calculated from average of shifts	4.0	2.0	3D
26a	1.54	0.17, calculated from average of shifts	4.0	10.0	2D

26b	1.54	0.17, calculated from average of shifts	4.0	10.0	2D
27a	2.23	0.20, calculated from average of shifts	4.0	4.0	3D
27b	2.23	0.20, calculated from average of shifts	4.0	4.0	3D
28	6.79	0.00	4.0	1.0	3D
29	5.82	0.05	5.0	1.0	3D

Overall mark 7 (out of 1 to 10, 10 being best)

Mean deviation from prediction: 0.08 ppm → 0.04 Points

No. of red or missing shifts: 0.0 → 0.0 Points

No. of yellow shifts: 1.0 → 2.5 Points

Result: 7/accept

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