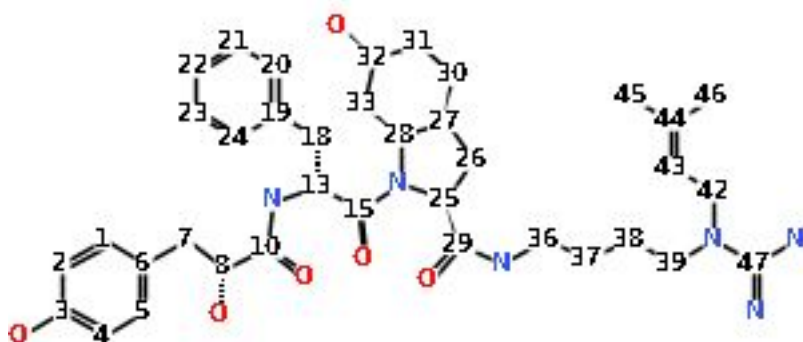












nmrshiftdb2 Quality Report - ¹³C

Atom	δ [ppm]	Deviation from prediction	Prediction		HOSE Code
			No. Spheres	No. shift values	
1	130.3	1.00	4.0	1.0	<u>3D</u>
2	115.0	0.80	5.0	1.0	<u>3D</u>
3	155.8	0.80	6.0	1.0	<u>3D</u>
4	115.0	Symmetric to atom 2	5.0	1.0	<u>3D</u>
5	130.3	Symmetric to atom 1	4.0	1.0	<u>3D</u>
6	128.6	1.50	3.0	1.0	<u>3D</u>
7	40.0	2.37  ¹	2.0	3.0	<u>3D</u>
8	72.4	3.59  ¹	2.0	14.0	<u>2D</u>
10	173.5	2.30  ^{1, 2}	2.0	27.0	<u>2D</u>
13	51.4	1.74	3.0	4.0	<u>2D</u>
15	170.0	2.10  ¹	2.0	1.0	<u>3D</u>
18	36.6	0.80	4.0	1.0	<u>3D</u>
19	138.2	0.83	5.0	3.0	<u>2D</u>
20	129.3	0.24	6.0	2.0	<u>2D</u>
21	128.2	0.49	6.0	6.0	<u>3D</u>
22	126.4	0.51	6.0	19.0	<u>3D</u>
23	128.2	Symmetric to atom 21	6.0	6.0	<u>3D</u>
24	129.3	Symmetric to atom 20	6.0	2.0	<u>2D</u>
25	59.7	0.70  ¹	2.0	1.0	<u>3D</u>
26	32.8	4.33  ¹	2.0	5.0	<u>3D</u>
27	32.2	4.60  ¹	2.0	1.0	<u>3D</u>
28	56.8	8.88  ^{1, 2}	2.0	5.0	<u>3D</u>
29	172.4	0.50	3.0	1.0	<u>3D</u>

30	22.8	3.80  ^{1, 2}	2.0	957.0	<u>3D</u>
31	29.9	3.25	3.0	2.0	<u>3D</u>
32	67.0	1.77	3.0	4.0	<u>3D</u>
33	36.2	0.77  ²	3.0	3.0	<u>3D</u>
36	38.6	2.70	4.0	1.0	<u>2D</u>
37	26.4	0.90	3.0	7.0	<u>2D</u>
38	24.7	1.09	3.0	4.0	<u>2D</u>
39	47.3	1.84  ^{1, 2}	2.0	220.0	<u>2D</u>
42	45.9	4.55  ^{1, 2}	2.0	56.0	<u>2D</u>
43	118.6	1.33	3.0	4.0	<u>2D</u>
44	137.1	1.52	4.0	4.0	<u>2D</u>
45	25.7	1.92	5.0	4.0	<u>3D</u>
46	18.0	Symmetric to atom 45	5.0	4.0	<u>3D</u>
47	155.8	12.50  ¹	2.0	1.0	<u>2D</u>

Overall mark 9 (out of 1 to 10, 10 being best)

Mean deviation from prediction: 2.38 ppm → 1.19 Points

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

No. of yellow shifts: 0.0 → 0.0 Points

Result: 9/accept

1 yellow shift(s) and 1 red shift(s) not taken into account because the underlying prediction was unreliable.

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