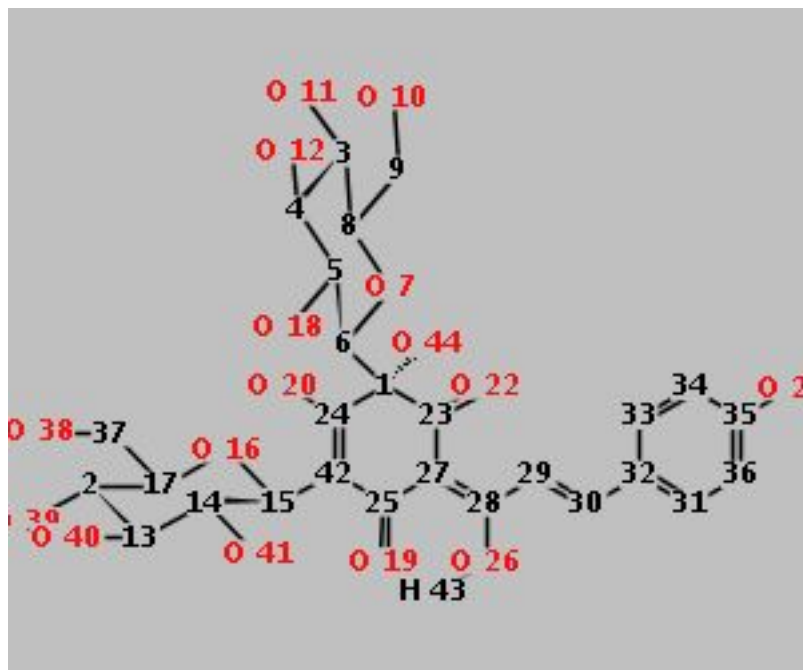




Atom number	Shift	Deviation from prediction
2	3.04	0,02
3	2.88	0,02
4	3.08	0,15
5	3.32	0,54
6	3.64	1,14
8	2.94	0,05
9	3.46	0,07
9	3.46	0,41, prediction not reliable
13	3.11	0,48
14	4.13	0,10
15	4.2	1,41
17	3.03	0,49
29	7.4	0,71
30	7.29	0,32
31	7.41	0,16
33	7.41	0,16
34	6.78	0,01
36	6.78	0,01
37	3.47	0,39
37	3.47	0,40, prediction not reliable

Overall mark 5 (out of 1 to 10, 10 being best), recommendation: revision

Mean deviation from prediction: 0,35 ppm -> 0,18 Points

No. of red or missing shifts: 0.0 -> 0.0 Points

No. of yellow shifts: 2.0 -> 5.0 Points

Result: 5/revision