Exercises: NMR Crystallography

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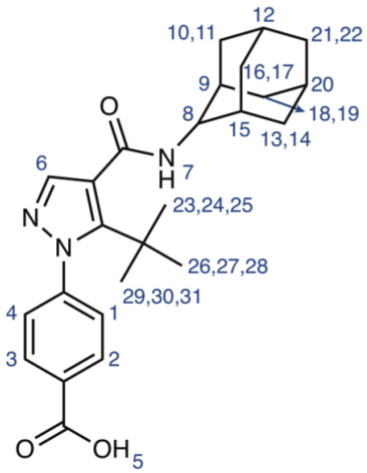
a) AZD8329 is a pharmaceutical compound with potential for the treatment of type 2 diabetes. Accurate ^{1}H chemical shifts for AZD8329 are given below. You can find the structures of four different polymorphs of AZD8329 on Moodle. Determine the correct polymorph using the chemical shifts predicted by https://tools.materialscloud.org/shiftml/. For this, calculate the root-mean-square deviation between experimental and calculated chemical shifts for the polymorphs A-D.



Atom Label	^{1}H δ (ppm)
1	6.92
2	8.69
3	9.01
4	8.47
5	15.37
6	7.73
7	9.64
8	2.90
9	1.78
10,11	1.88

Atom Label	^{1}H δ (ppm)
12	1.8
13	1.6
14	0.44
15	1.54
16,17	1.88
18,19	0.8
20	1
21,22	1.74
23,24,25, 26,27,28, 29,30,31	0.73

b) What would (should) you do for chemically equivalent atoms and/or exchanging protons?

c) When using the program, you can choose between chemical shieldings and chemical shifts. What is the difference? How do you get from one property to the other?