Electronic Supplementary Material (ESI) for RSC Medicinal Chemistry.
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Supporting information for:

AiZynth Impact on Medicinal Chemistry Practice at AstraZeneca

Jason D. Shields,* Rachel Howells, Gillian Lamont, Yin Leilei, Andrew Madin, Christopher E. Reimann, Hadi Rezaei, Tristan Reuillon, Bryony Smith, Clare Thomson, Yuting Zheng, Robert E. Ziegler

Snapshots of the AiZynth GUI

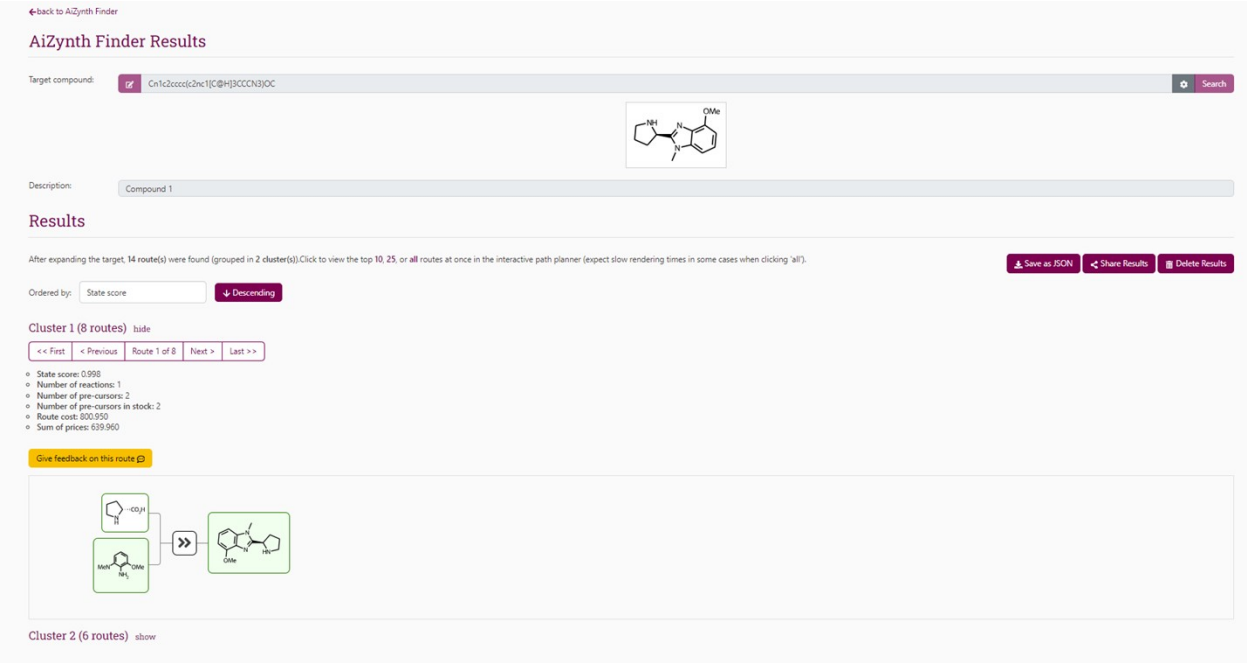


Figure S1. A snapshot of the AiZynthFinder search results for compound **1**. Results are clustered together by similarity and can be viewed individually by the chemist. This example was the highest ranking route and is therefore Cluster 1 Route 1. Compounds have a green border if they are found within our inventory or a commercial catalogue. They have green shading within the boxes if they are reported as products in our internal ELN database.

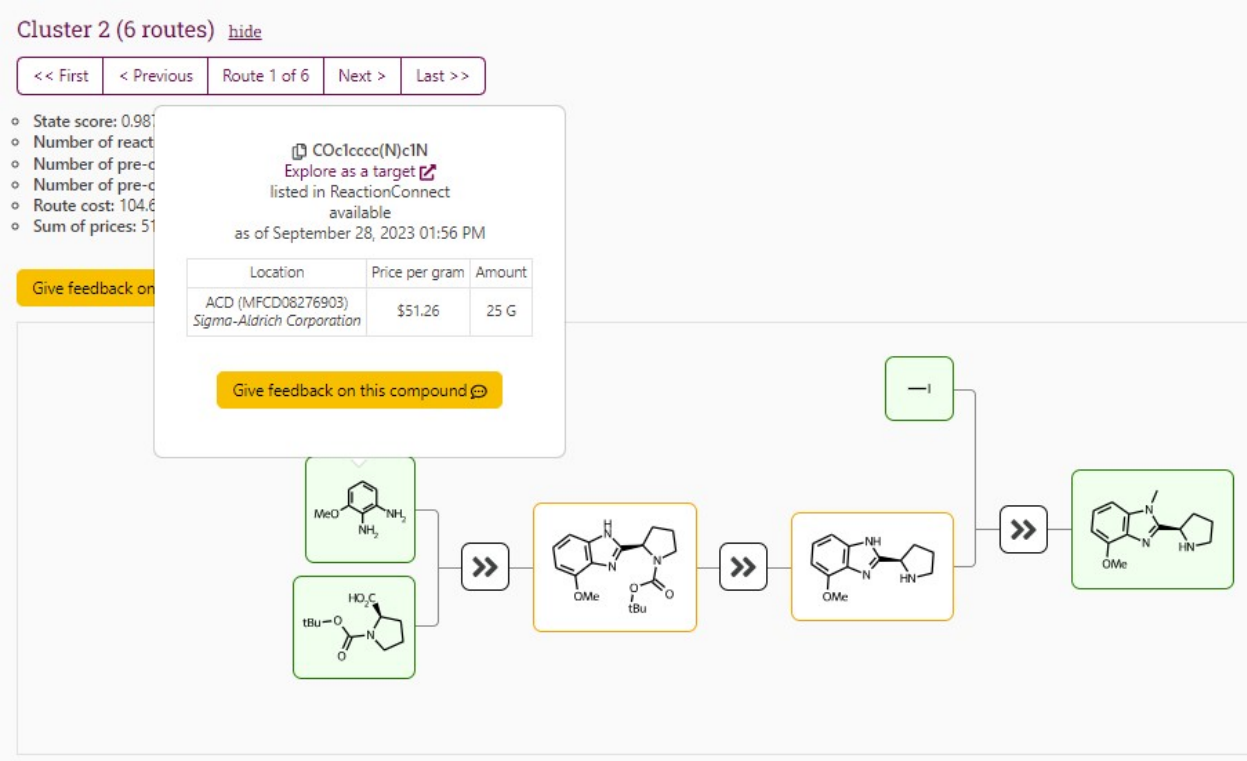


Figure S2. A view of one of the AiZynthFinder routes to compound **1** from Cluster 2. This route is less efficient (and indeed it may suffer from regioselectivity of methylation on the final step) but can still be viewed by the chemist for completeness. Note the mouseover on 3-methoxybenzene-1,2-diamine which provides basic information about commercial availability, including the MFCD number, a unique identifier that can be copy-pasted into online commercial catalogues for easy searching. Note also the feedback buttons that are available for chemists to indicate if a reaction or compound are unsuitable, which can be taken into account in future development of AiZynth.

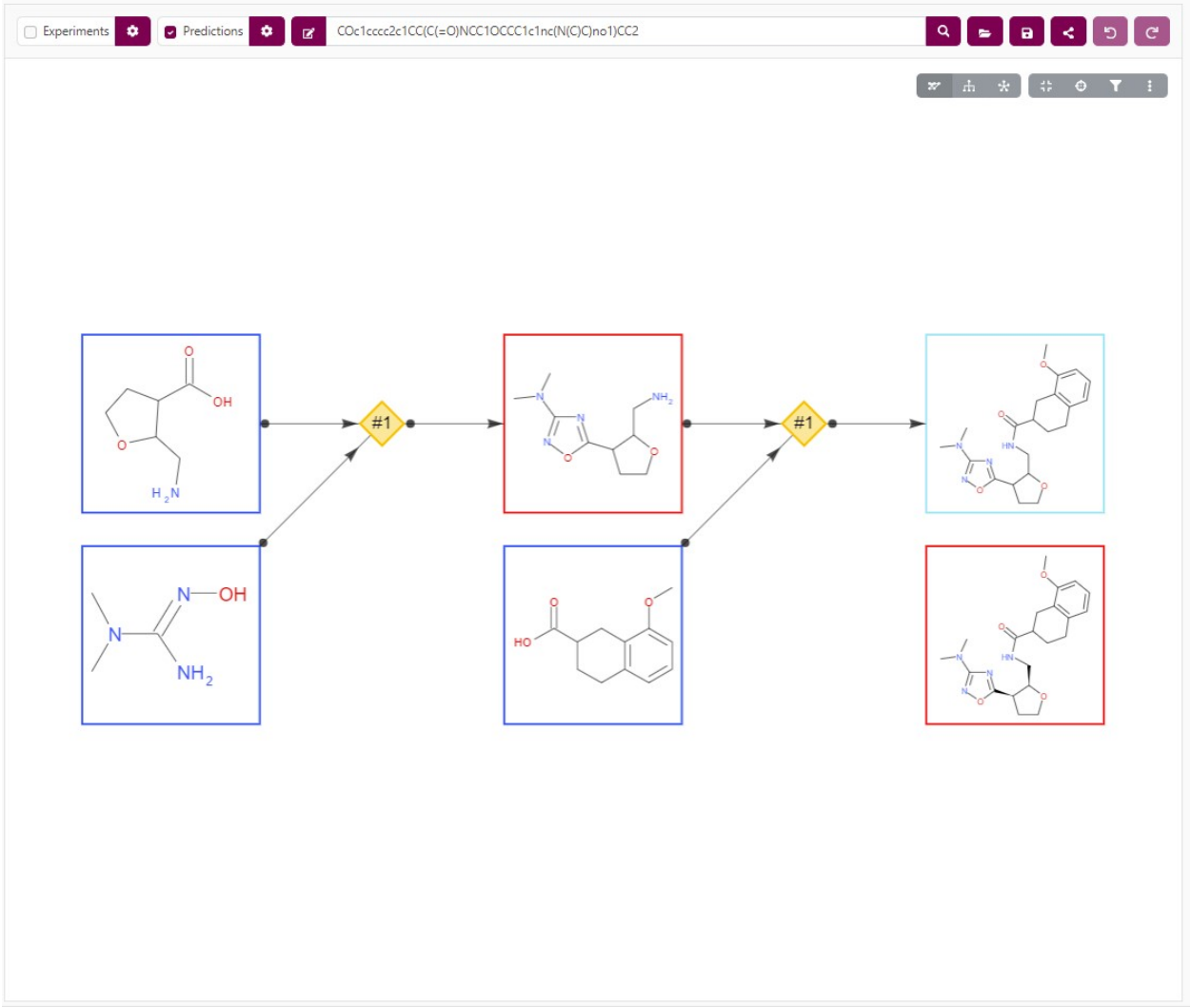
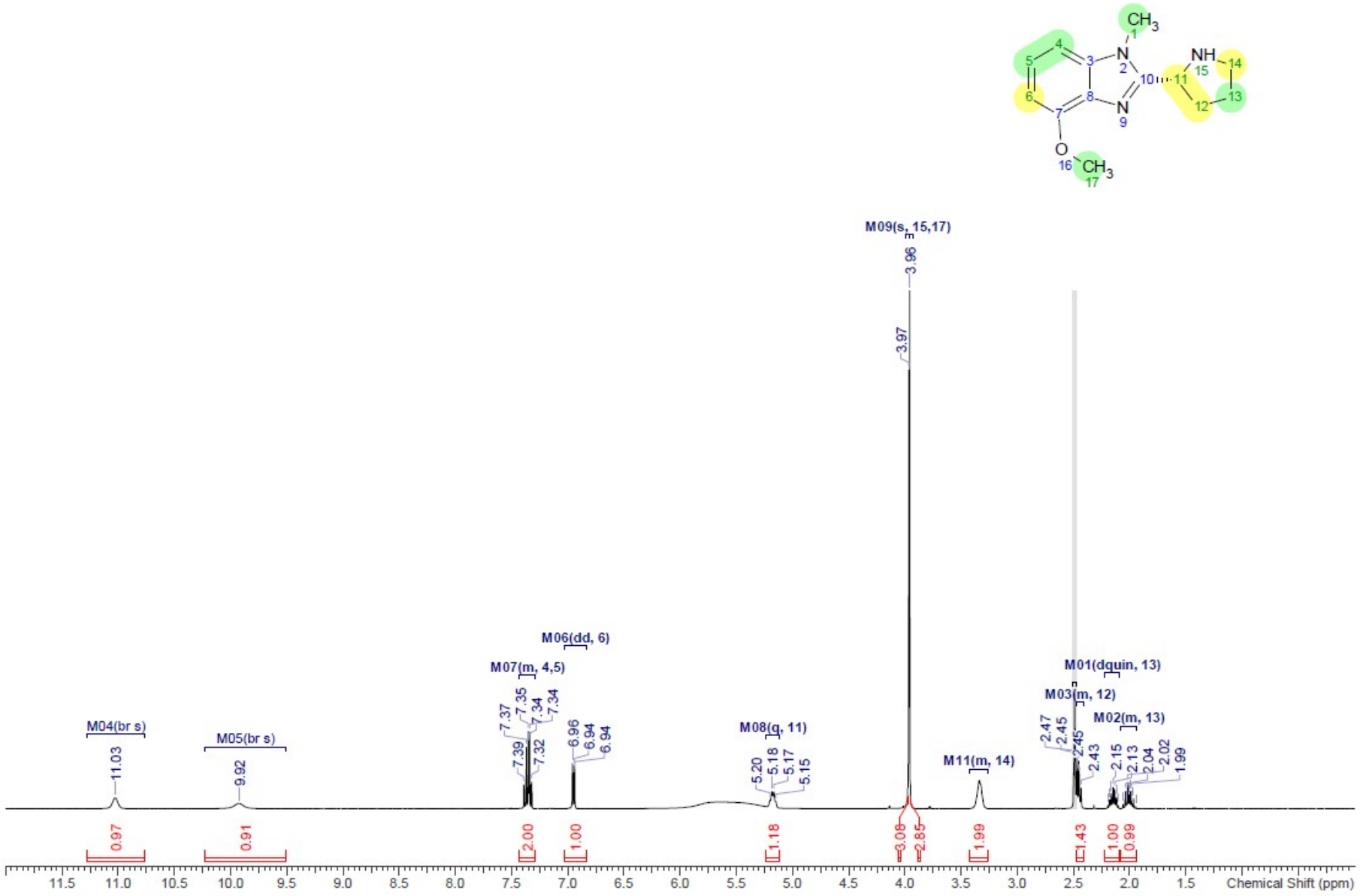


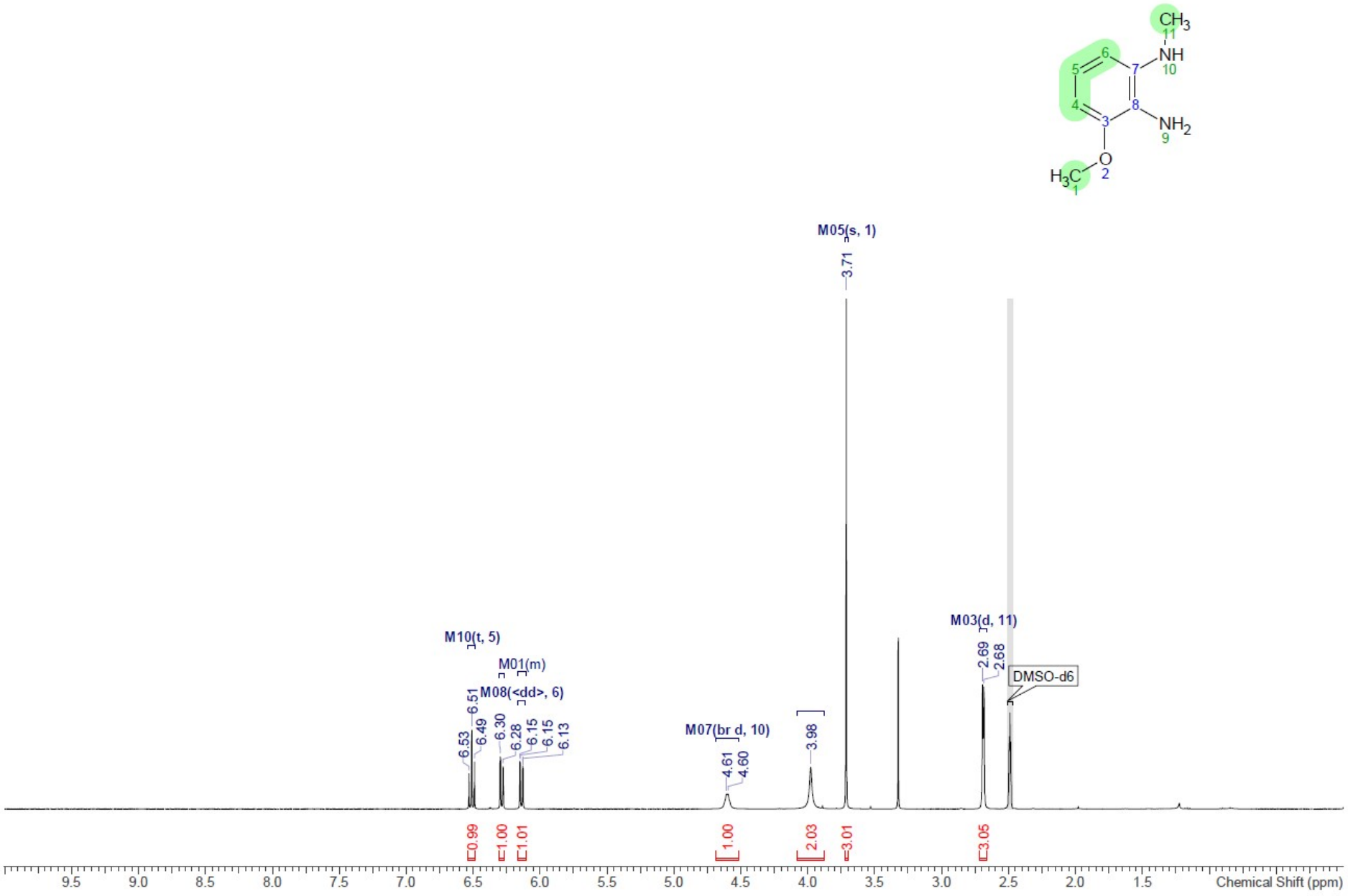
Figure S3. A snapshot of the AiZynth single-step retrosynthesis tool. Here, the view can be changed to read from left-to-right to any desired direction (e.g. for a bottom-to-top view see Figure 7B in the paper). Chemists can hide and add AI suggestions to the reaction network in order to get a sense of multiple alternative routes at once. Additional, unconnected compounds can also be added for the user to refer to visually, e.g. the *cis* isomer at the bottom right. Here, a blue border indicates commercial or inventory availability, while a red border indicates the opposite. The light blue border indicates the target molecule.

Figure S4. A side panel that can be viewed within the AiZynth single-step retrosynthesis interface. Here, a chemist can get a quick sense of the price and scale of the availability of a given molecule.

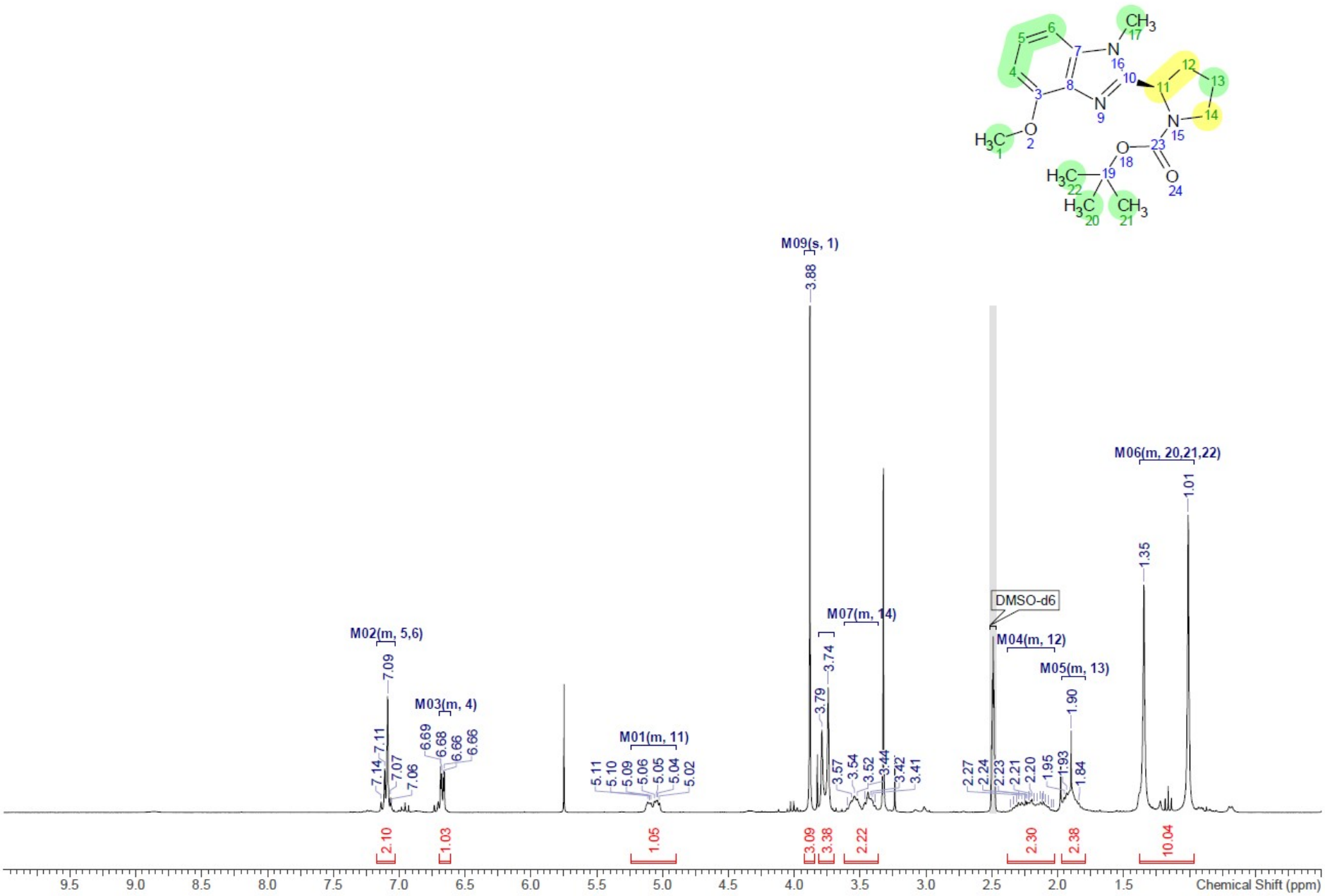
^{1}H NMR spectra of previously unreported compounds



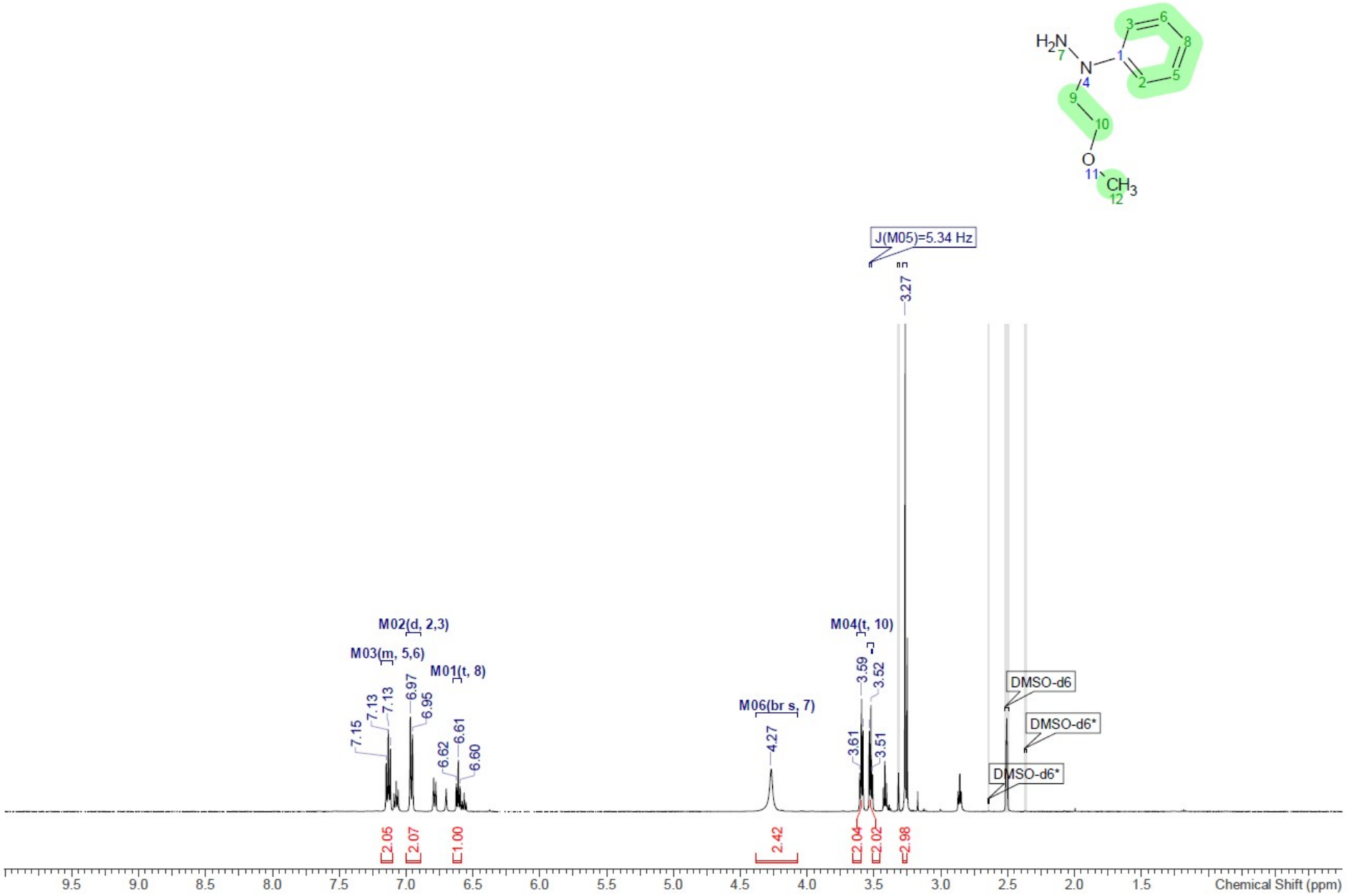
Compound **1** ^{1}H NMR



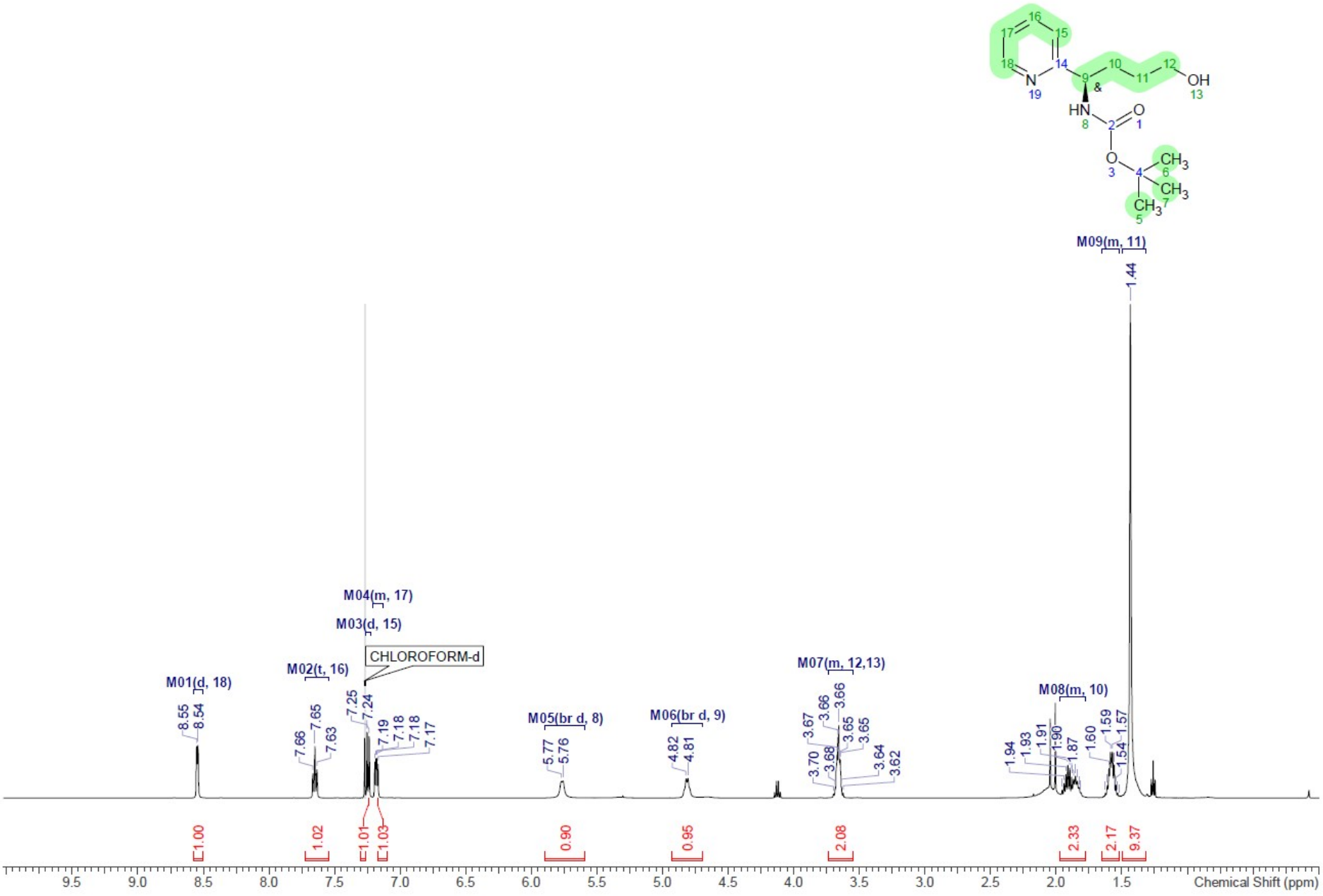
Compound **3** ^{1}H NMR



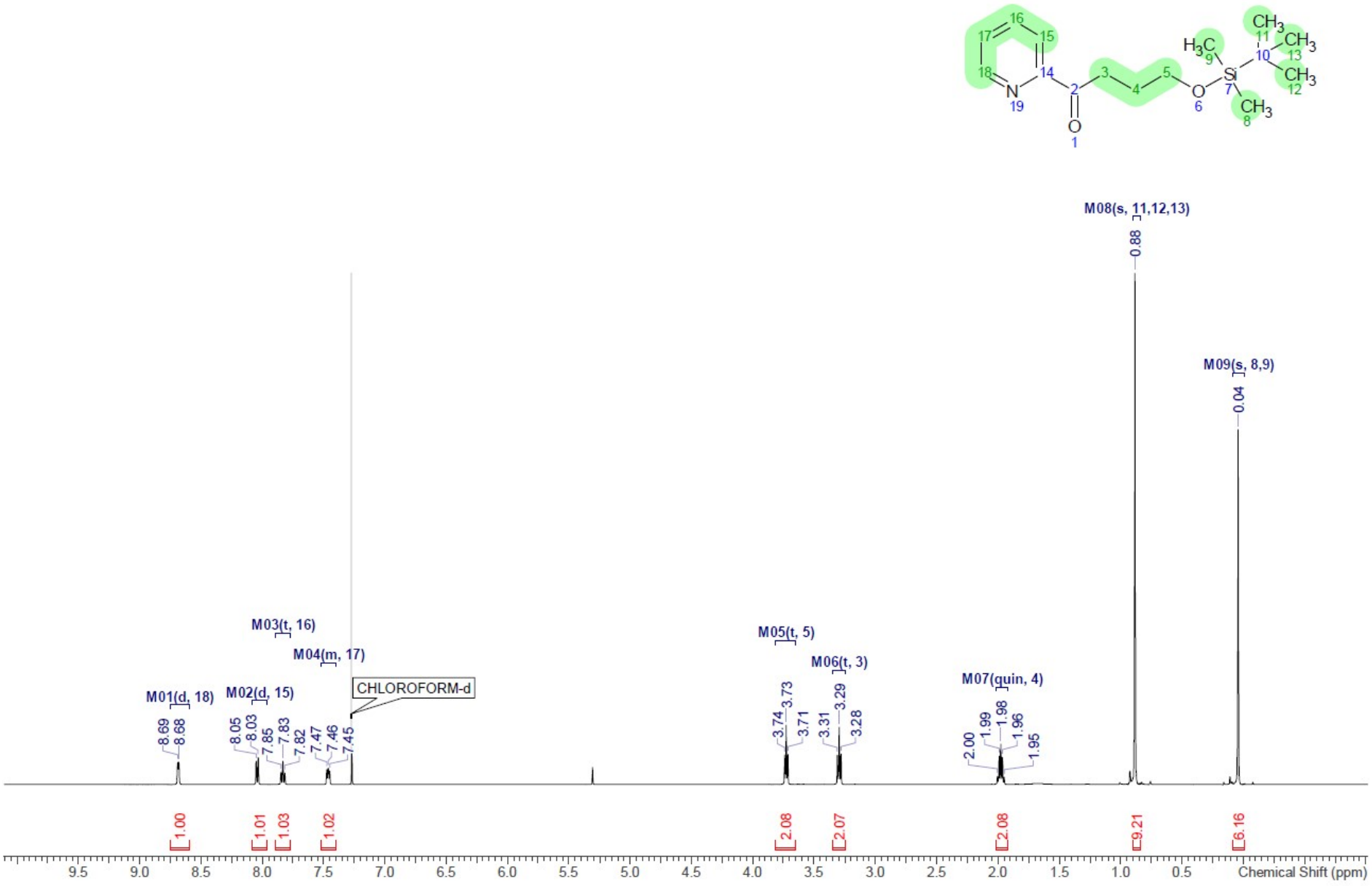
Compound **6** ^{1}H NMR



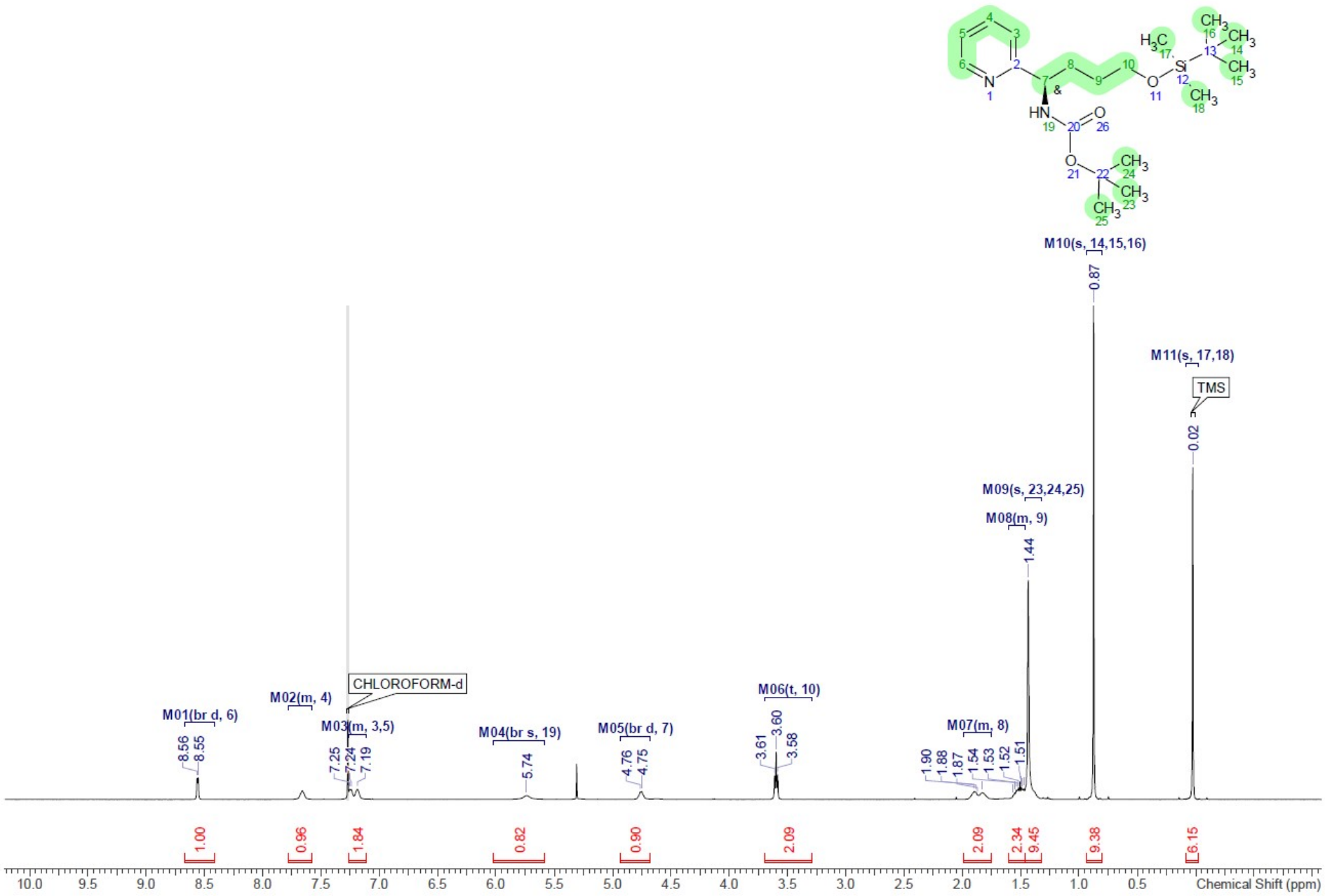
Compound **19** ^{1}H NMR. ~3:1 mixture with N2-alkylated regioisomer



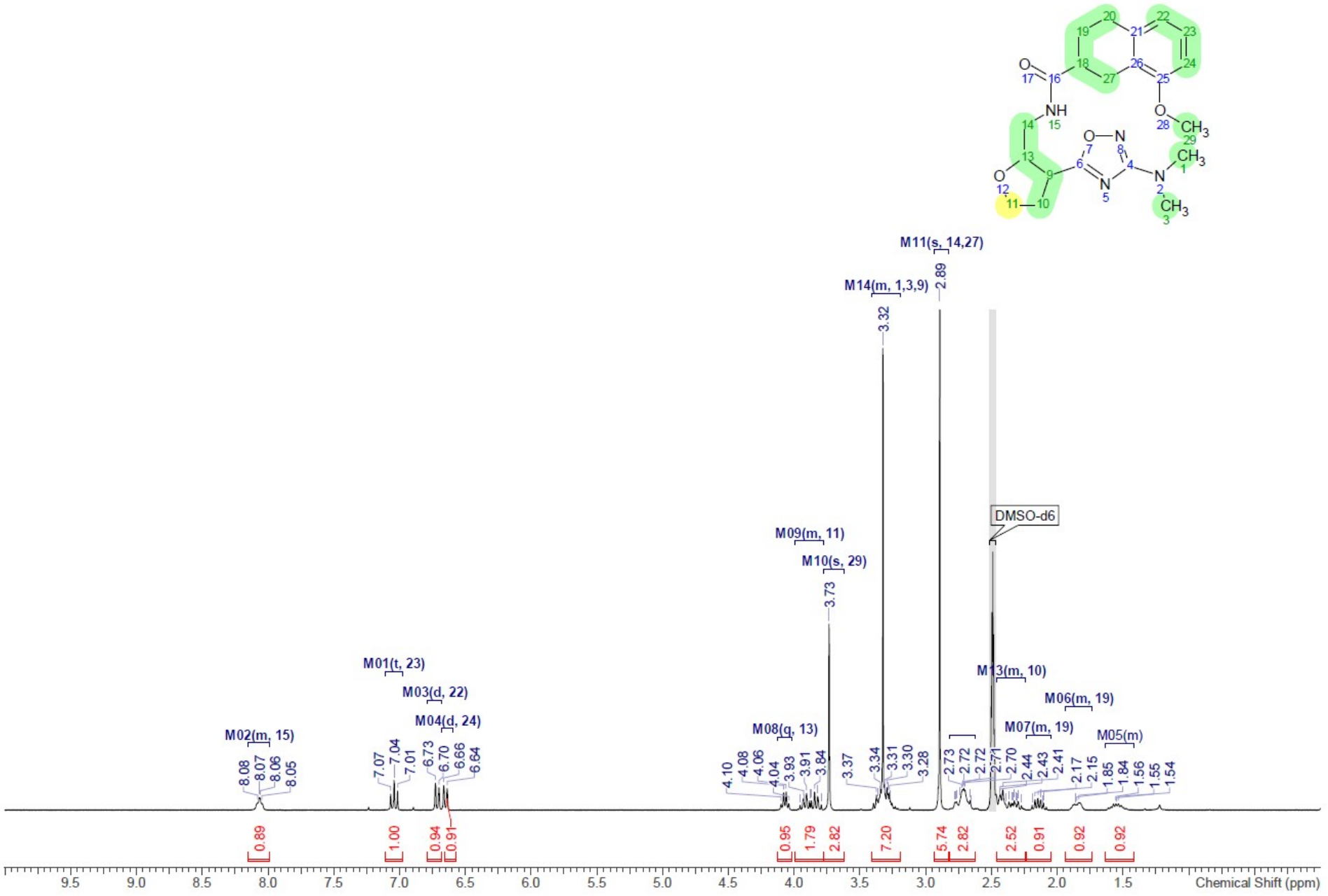
Compound **20** ^{1}H NMR



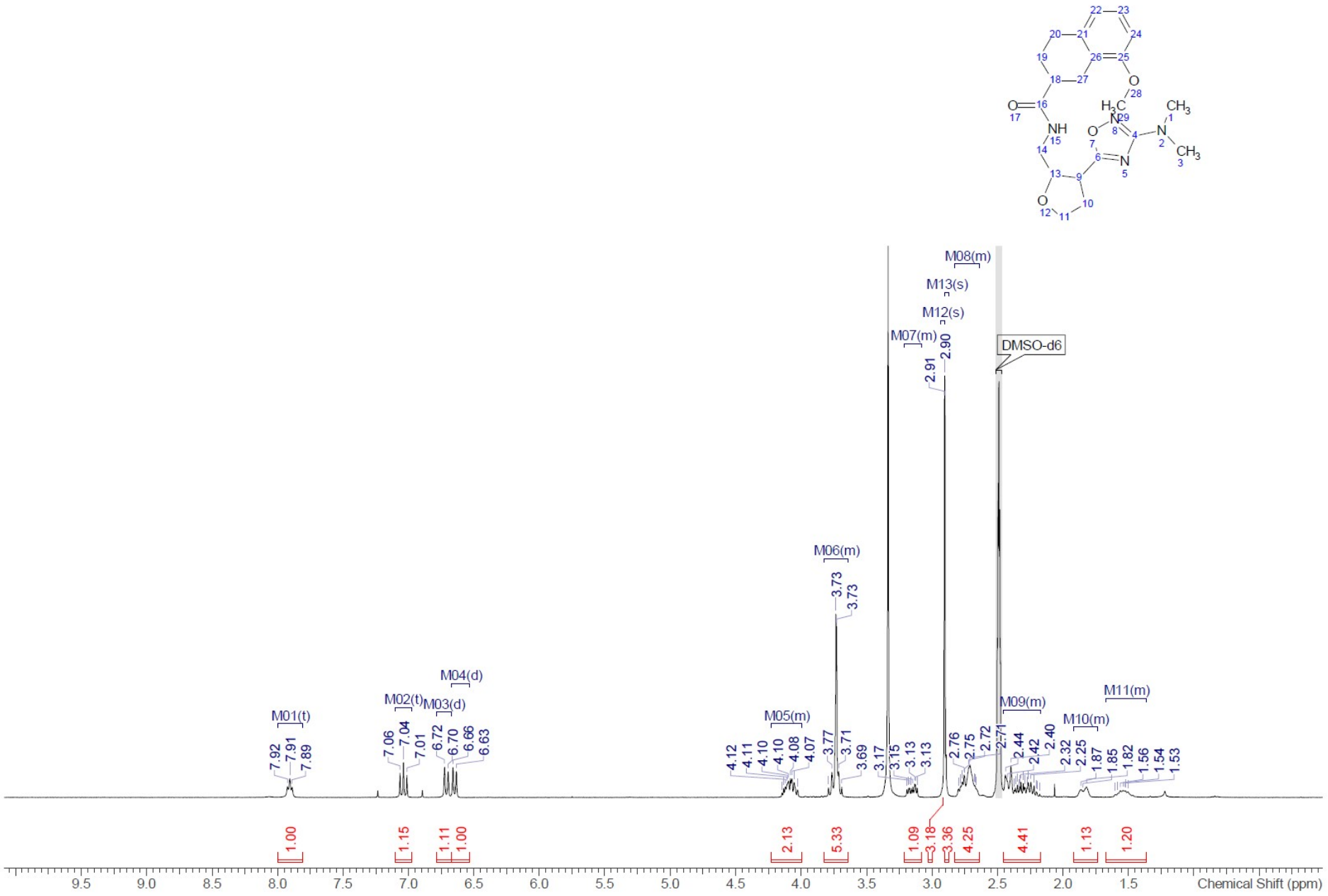
Compound **23** ^{1}H NMR



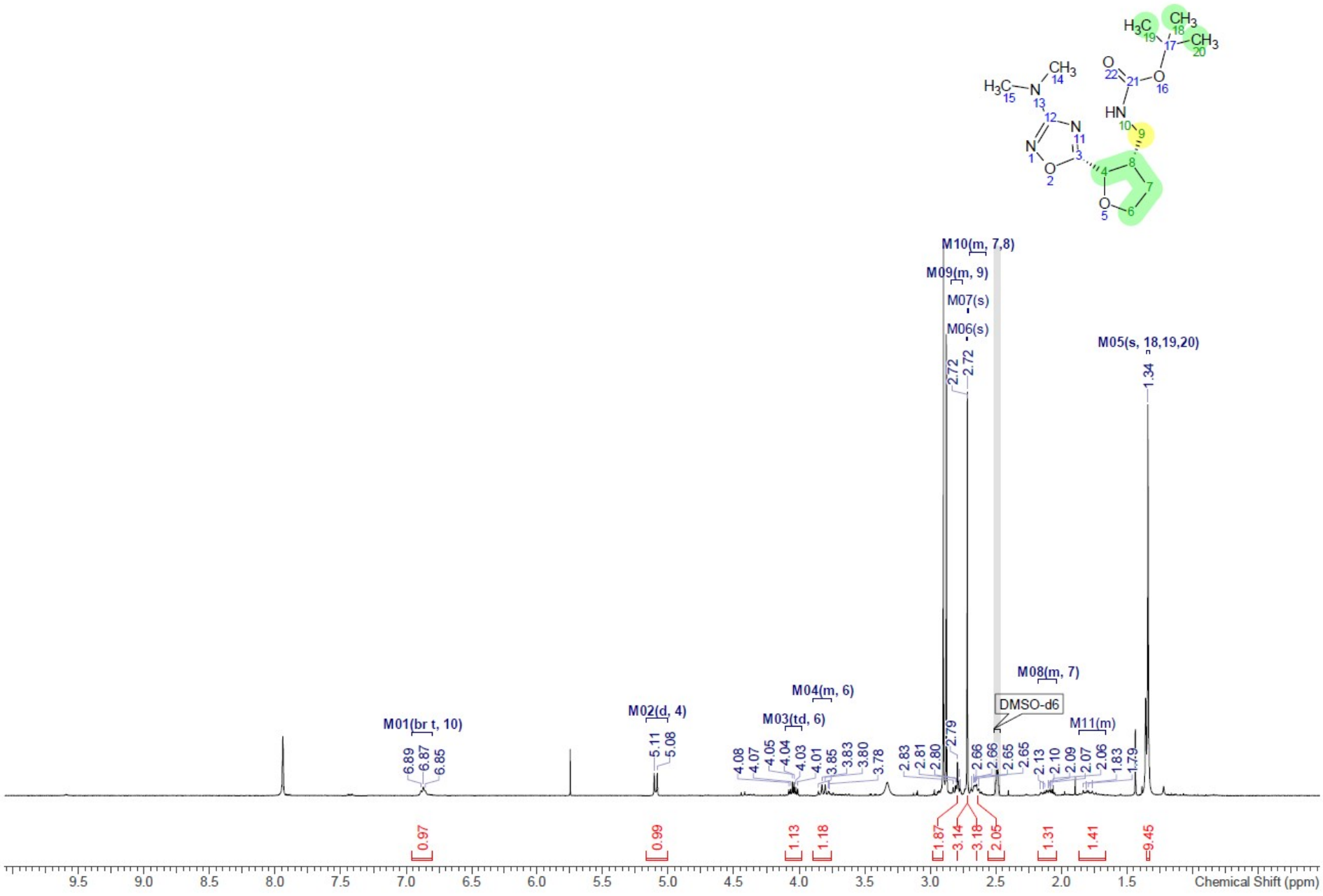
Compound **25** ^{1}H NMR



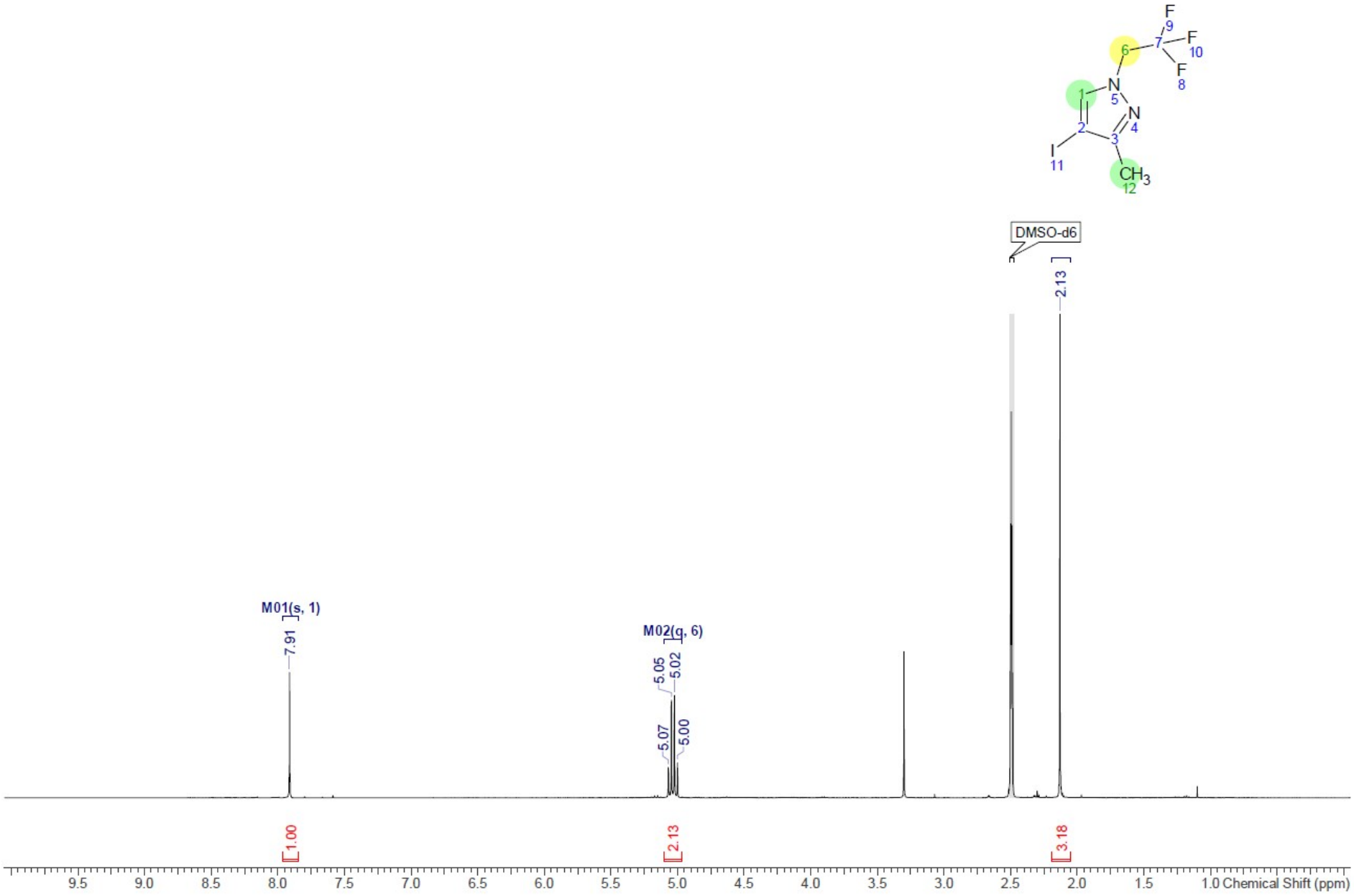
Compound **27** Isomer 1 ^{1}H NMR



Compound **27** Isomer 2 ^{1}H NMR



Compound **32** ^{1}H NMR. Heavily contaminated with DMF



Compound **38** ^{1}H NMR