Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.
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Supporting Information

General: ^{1}H and ^{13}C NMR spectra of synthetic target compounds and intermediates were recorded on a Bruker 400 MHz spectrometer. NMR solvent signals were calibrated to 7.26 ppm ($CDCl_3$), 4.79 ppm (D_2O), 3.31 ppm (CD_3OD) and 2.50 ppm ([D_6]-dmso).

^{1}H and ^{13}C-NMR spectra:

Sodium nitromalonaldehyde monohydrate **5**

[2,6-$^{13}C_2$] 4-Nitrophenol **6**

5-([2,6-$^{13}C_2$] 4-Nitrophenoxy)-1-phenyl-1*H*-tetrazole **7**

[3,5-$^{13}C_2$] Aniline **8**

[3,5-$^{13}C_2$] 2,4,6-Trideuterioaniline **9**

[3,5-$^{13}C_2$] 2,4,6-Trideuteriobenzonitrile **10**

[3,5-$^{13}C_2$] 2,4,6-Trideuteriobenzaldehyde **11**

5-([3,5-$^{13}C_2$] 2,4,6-Trideuteriobenzylidene)hydantoin **12**

Sodium 3,3-dideuterio([3,5-$^{13}C_2$] 2,4,6-trideuteriophenyl)pyruvate **1**

[1-^{13}C] 4-Nitrophenol **14**

[1-^{13}C] 4-Aminophenol **15**

[1-^{13}C] 2,3,5,6-Tetradeuterio-4-aminophenol **16**

5-([1-^{13}C]-2,3,5,6-Tetradeuterio-4-aminophenoxy)-1-phenyl-1*H*-tetrazole **17**

[4-^{13}C] 2,3,5,6-Tetradeuterioaniline **18**

[4-^{13}C] 2,3,5,6-Tetradeuteriobenzonitrile **19**

[4-^{13}C] 2,3,5,6-Tetradeuteriobenzaldehyde **20**

5-([4-^{13}C] 2,3,5,6-Tetradeuteriobenzylidene)hydantoin **21**

Sodium 3,3-dideuterio([4-^{13}C] 2,3,5,6-tetradeuteriophenyl)pyruvate **2**

[2,6-$^{13}C_2$] 4-Aminophenol **22**

[2,6-$^{13}C_2$] 3,5-Dideuterio-4-aminophenol **23**

[3,5-$^{13}C_2$] 2,6-Dideuteriohydroxybenzonitrile **24**

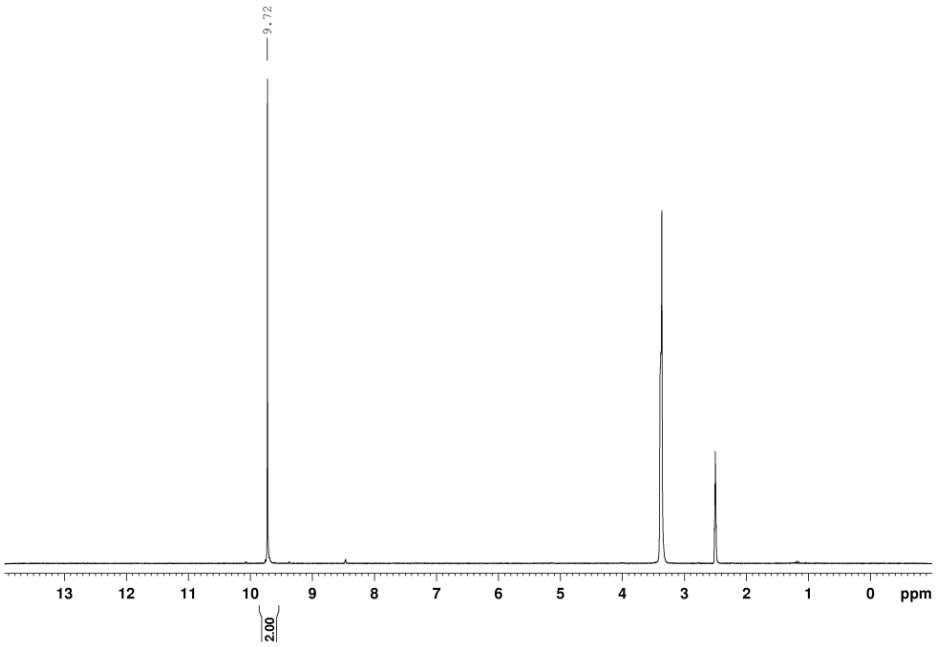
[3,5-$^{13}C_2$] 2,6-Dideuteriohydroxybenzaldehyde **25**

5-([3,5-$^{13}C_2$] 2,6-Dideuterio-4-hydroxybenzylidene)hydantoin **26**

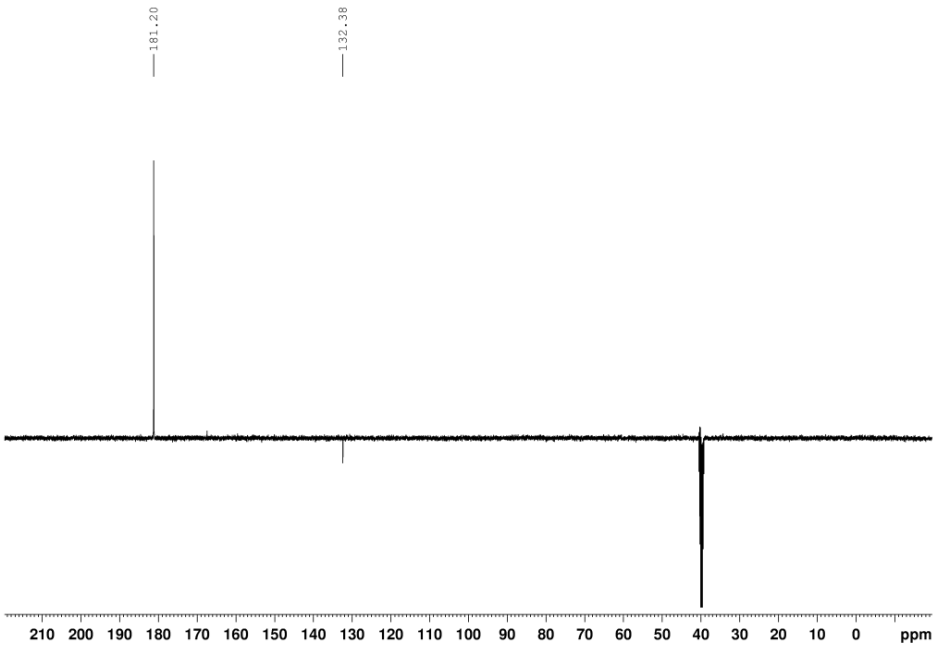
Sodium 3,3-dideuterio([3,5-$^{13}C_2$] 2,6-dideuterio-4-hydroxyphenyl)pyruvate **3**

3,5-Dideuterio-4-aminophenol **30**

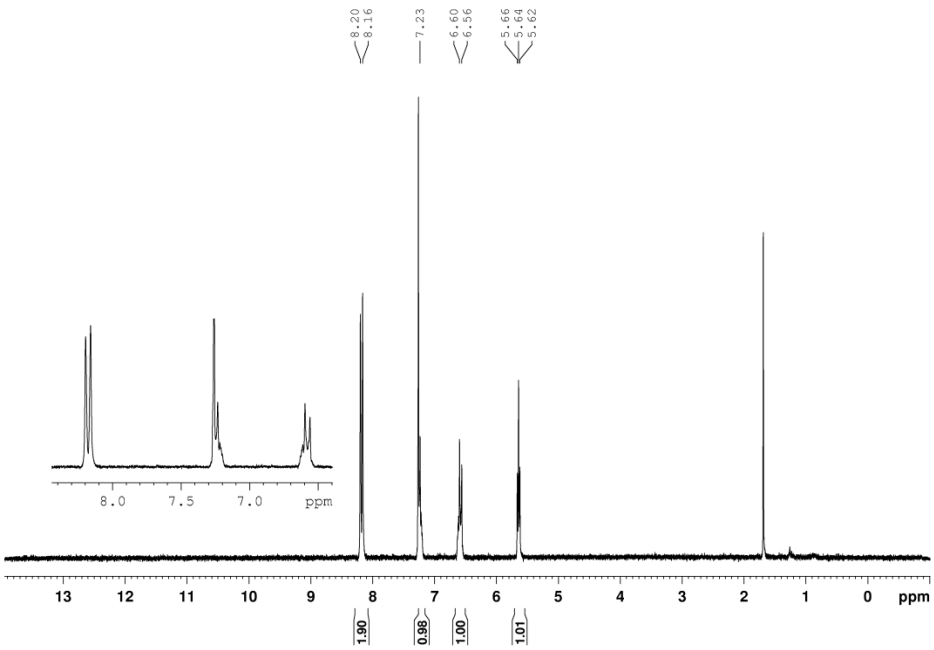
Sodium nitromalonaldehyde monohydrate **5** (^{1}H, 400 MHz, DMSO-6d)



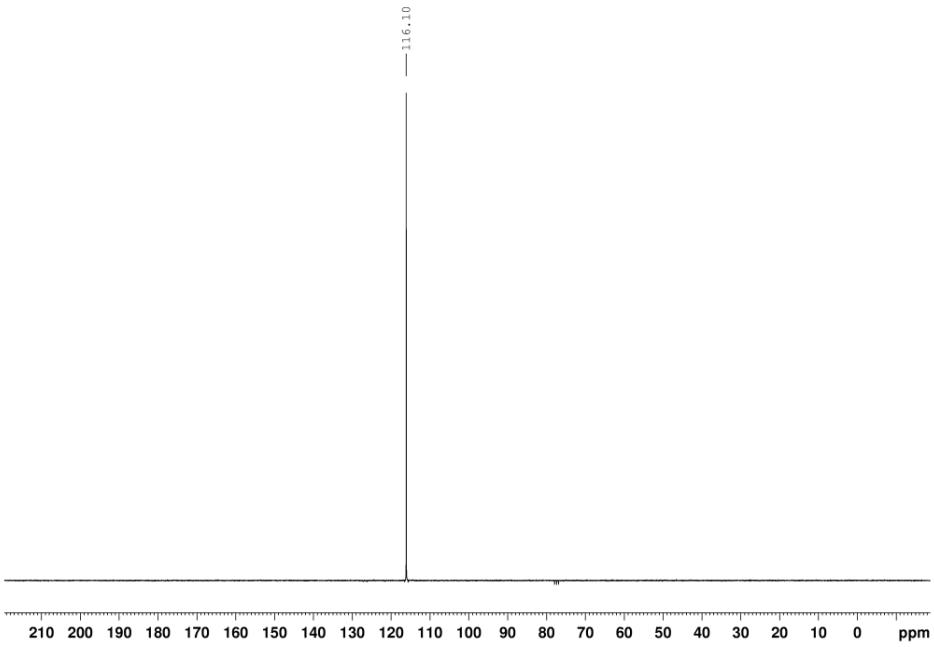
Sodium nitromalonaldehyde monohydrate **5** (^{13}C, 100.6 MHz, DMSO-6d)



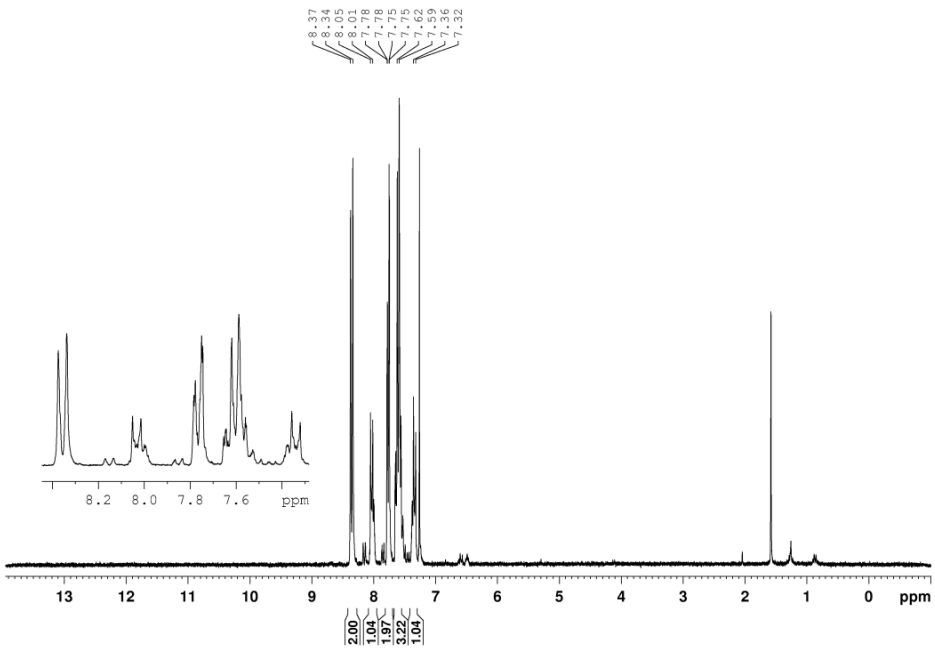
[2,6-$^{13}C_2$] 4-Nitrophenol **6** (^{1}H, 400 MHz, $CDCl_3$)



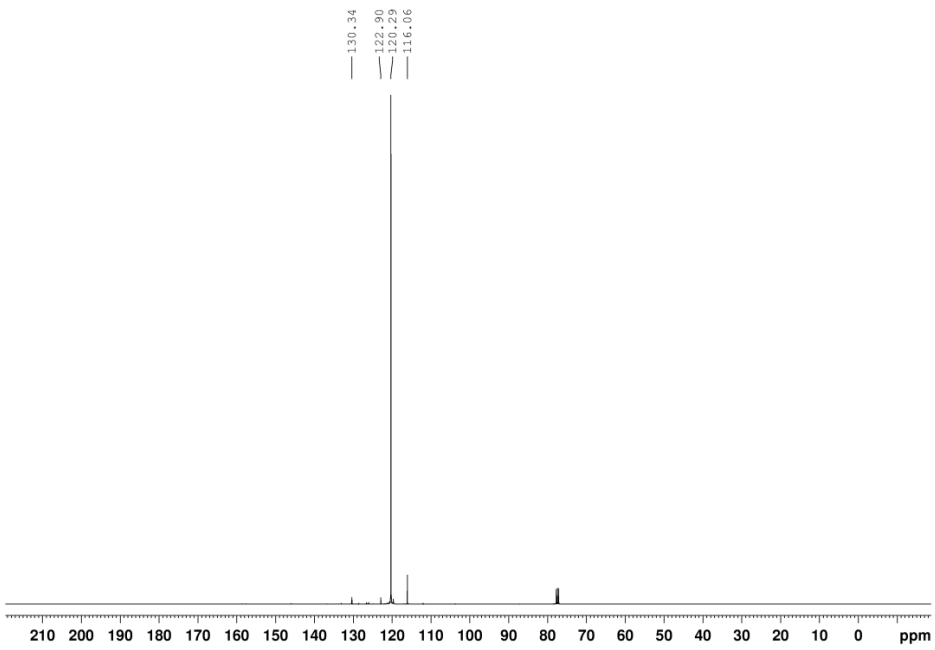
[2,6-$^{13}C_2$] 4-Nitrophenol **6** (^{13}C, 100.6 MHz, $CDCl_3$)



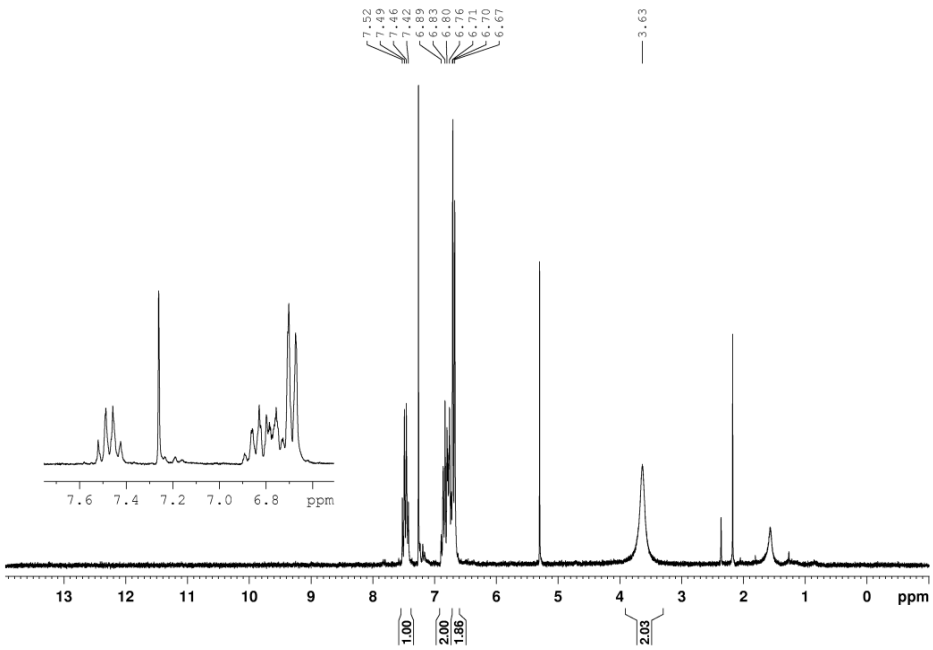
5-([2,6-$^{13}C_2$] 4-Nitrophenoxy)-1-phenyl-1*H*-tetrazole **7** (^{1}H, 400 MHz, $CDCl_3$)



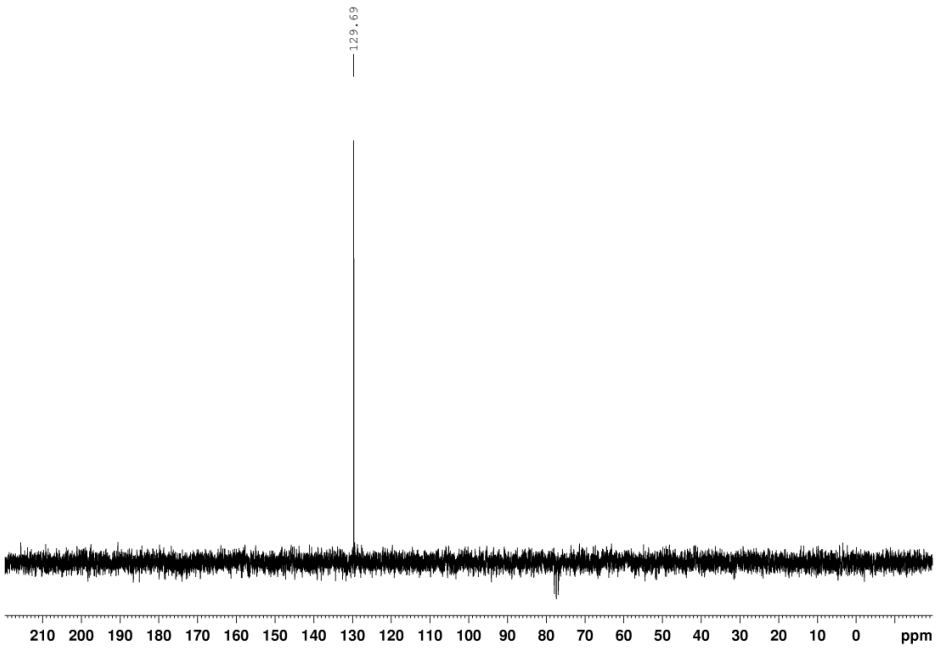
5-([2,6-$^{13}C_2$] 4-Nitrophenoxy)-1-phenyl-1*H*-tetrazole **7** (^{13}C, 100.6 MHz, $CDCl_3$)



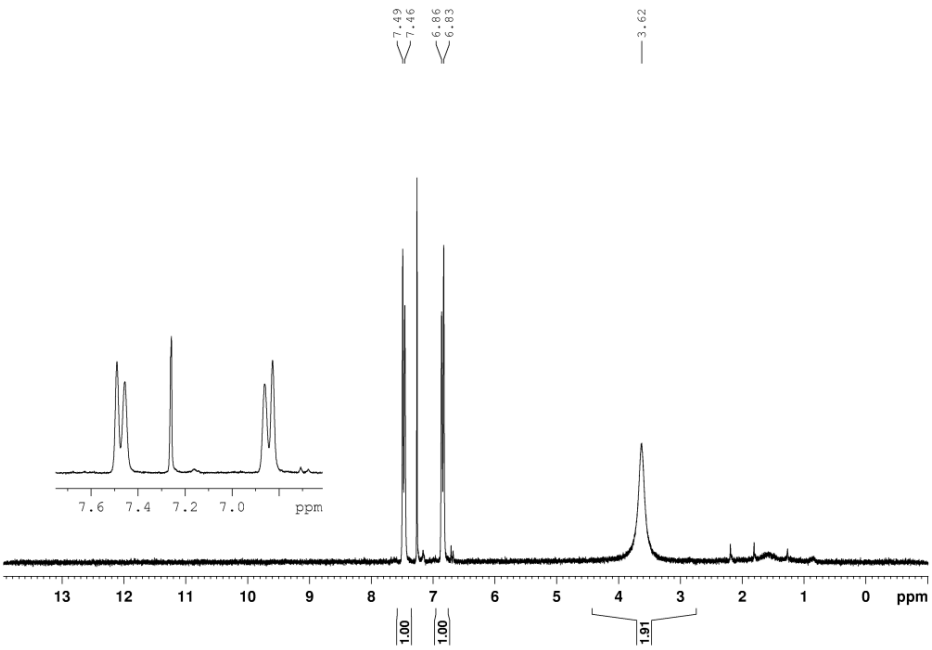
[3,5-$^{13}C_2$] Aniline **8** (^{1}H, 400 MHz, $CDCl_3$)



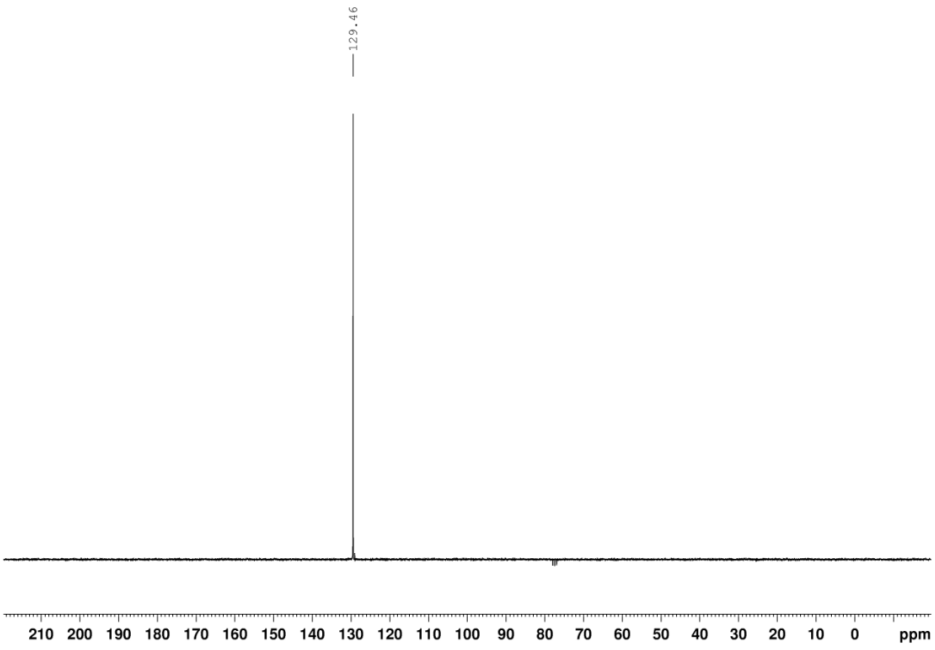
[3,5-$^{13}C_2$] Aniline **8** (^{13}C, 100.6 MHz, $CDCl_3$)



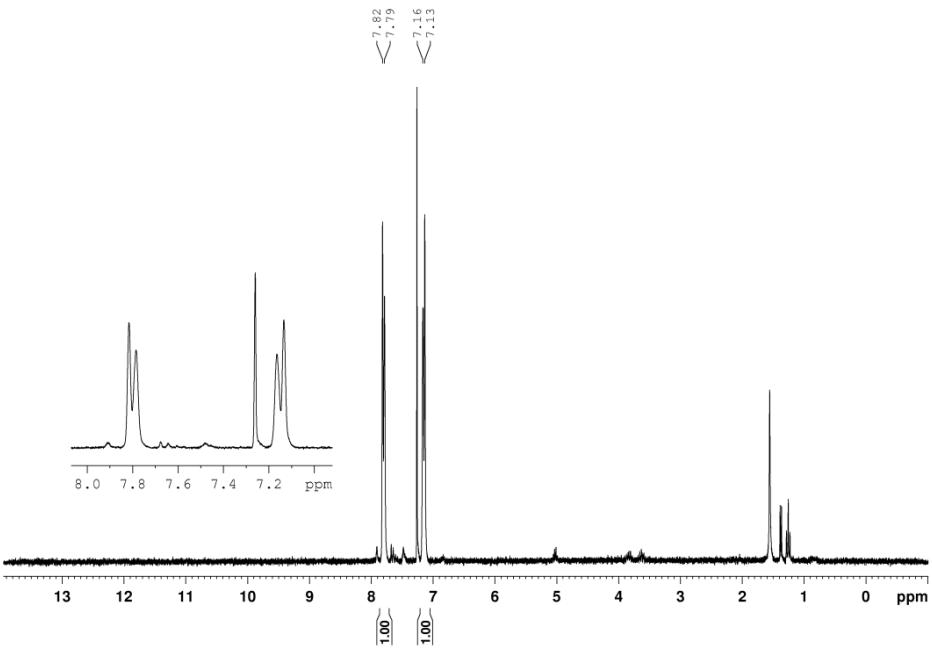
[3,5-$^{13}C_2$] 2,4,6-Trideuterioaniline **9** (^{1}H, 400 MHz, $CDCl_3$)



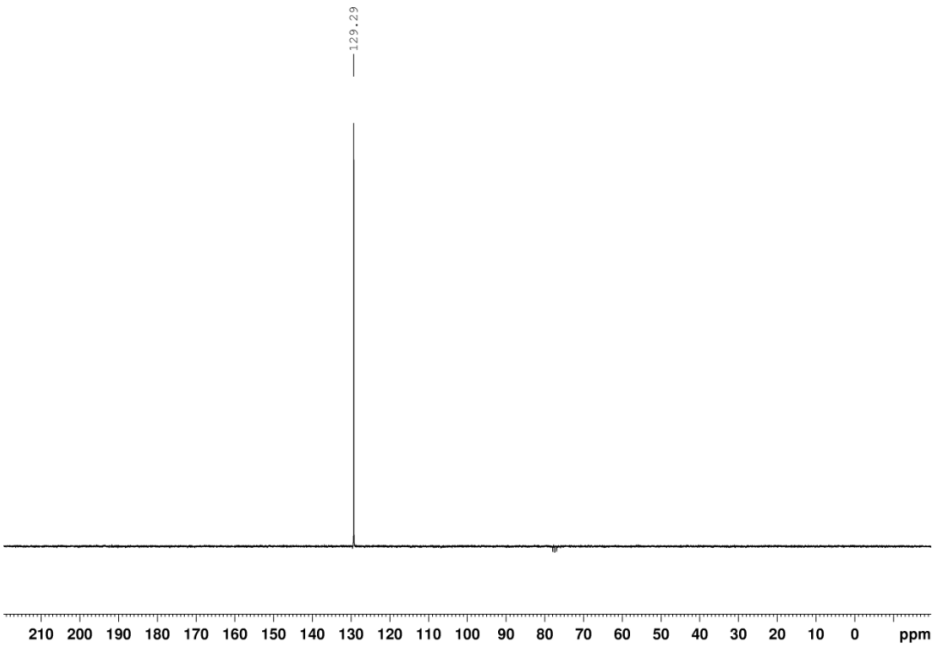
[3,5-$^{13}C_2$] 2,4,6-Trideuterioaniline **9** (^{13}C, 100.6 MHz, $CDCl_3$)



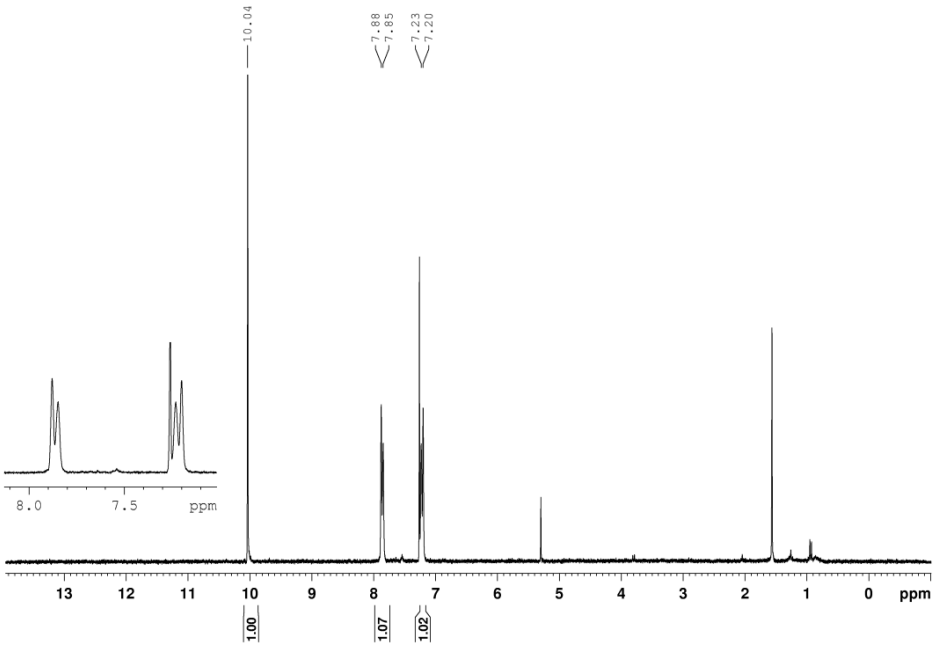
[3,5-$^{13}C_2$] 2,4,6-Trideuteriobenzonitrile **10** (^{1}H, 400 MHz, $CDCl_3$)



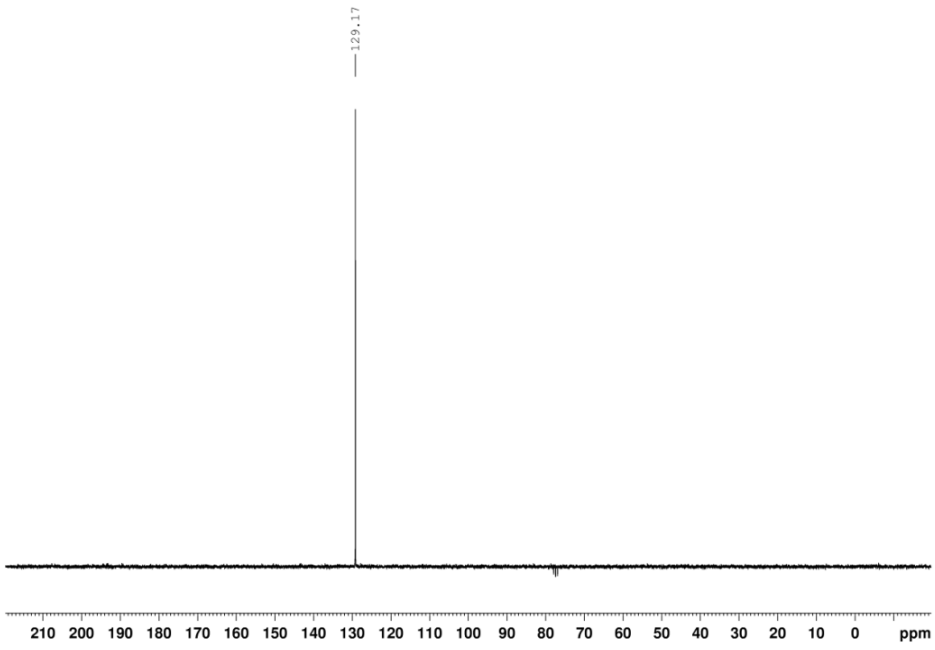
[3,5-$^{13}C_2$] 2,4,6-Trideuteriobenzonitrile **10** (^{1}H, 100.6 MHz, $CDCl_3$)



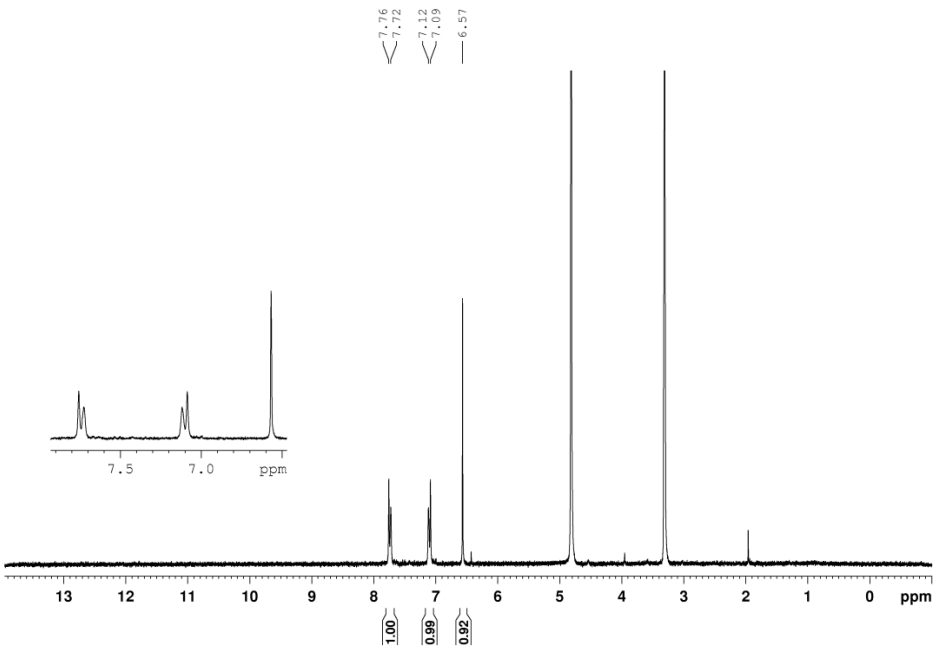
[3,5-$^{13}C_2$] 2,4,6-Trideuteriobenzaldehyde **11** (^{1}H, 400 MHz, $CDCl_3$)



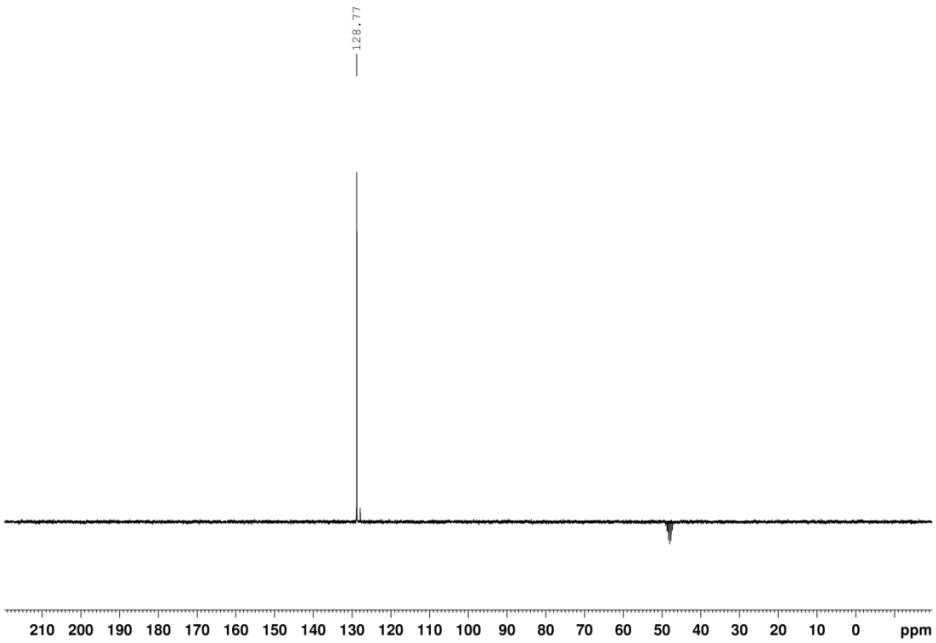
[3,5-$^{13}C_2$] 2,4,6-Trideuteriobenzaldehyde **11** (^{13}C, 100.6 MHz, $CDCl_3$)



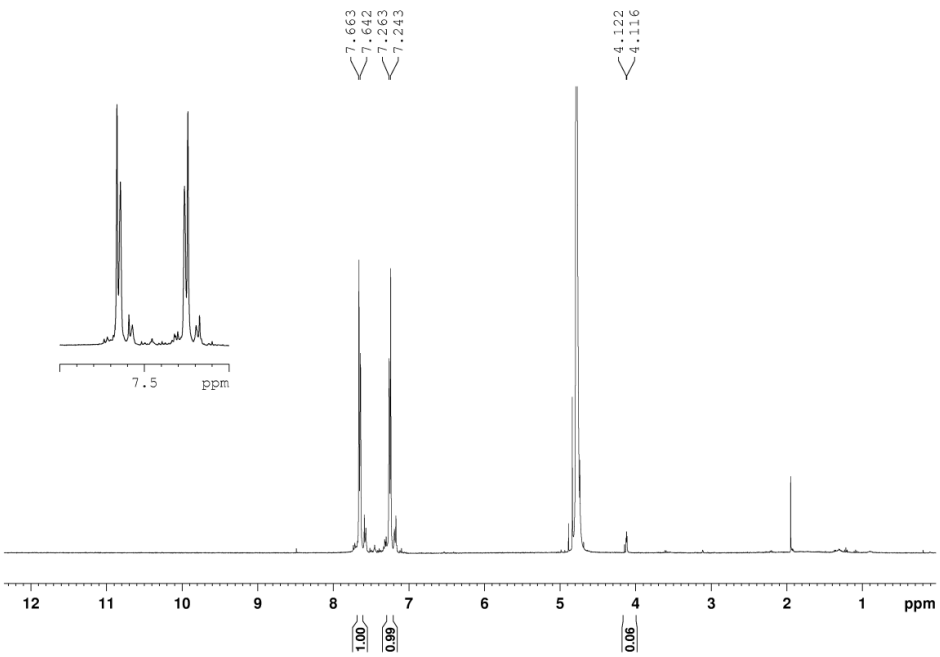
5-([3,5-$^{13}C_2$] 2,4,6-Trideuteriobenzylidene)hydantoin **12** (^{1}H, 400 MHz, methanol-d4)



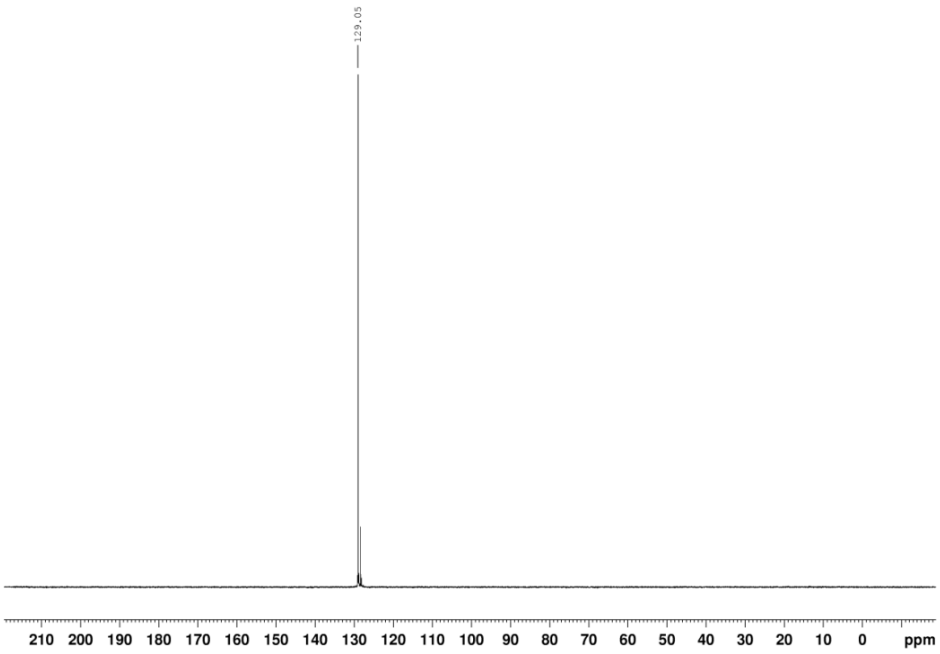
5-([3,5-$^{13}C_2$] 2,4,6-Trideuteriobenzylidene)hydantoin **12** (^{13}C, 100.6 MHz, methanol-d4)



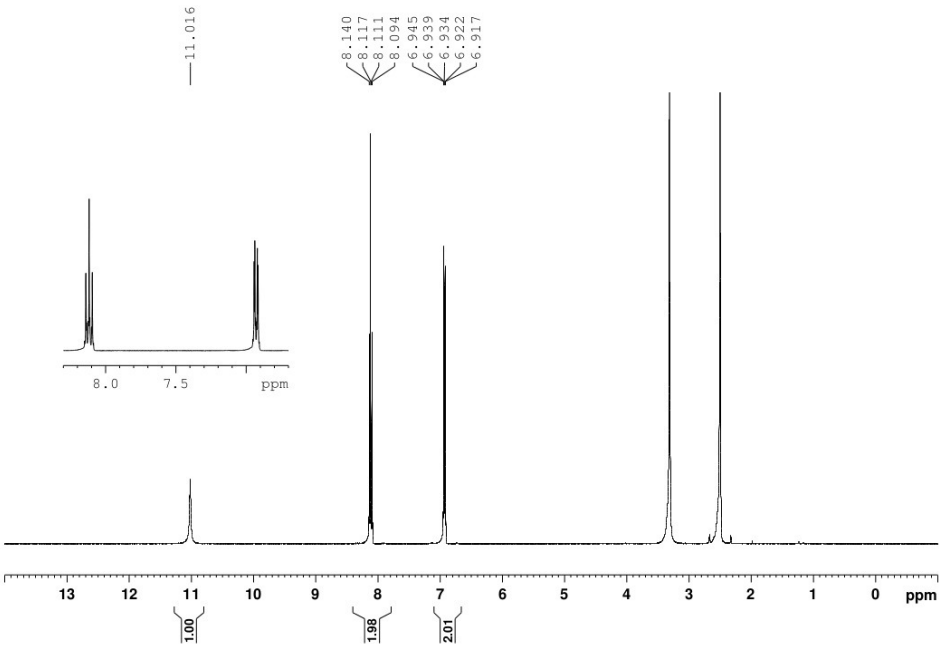
Sodium 3,3-dideuterio([3,5-$^{13}C_2$] 2,4,6-trideuteriophenyl)pyruvate **1** (^{1}H, 400 MHz, D_2O)



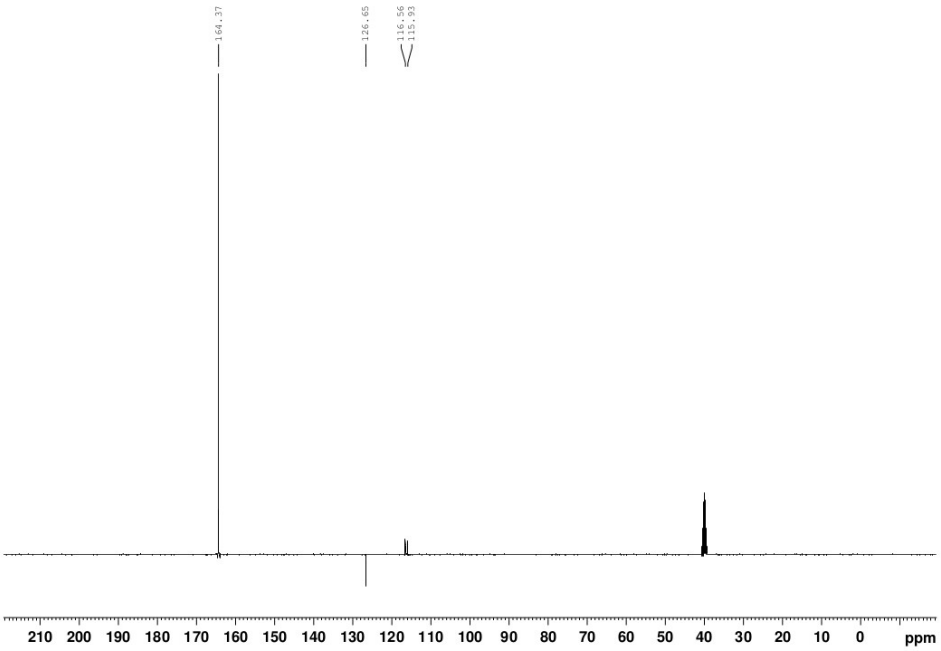
Sodium 3,3-dideuterio([3,5-$^{13}C_2$] 2,4,6-trideuteriophenyl)pyruvate **1** (^{13}C, 100.6 MHz, D_2O)



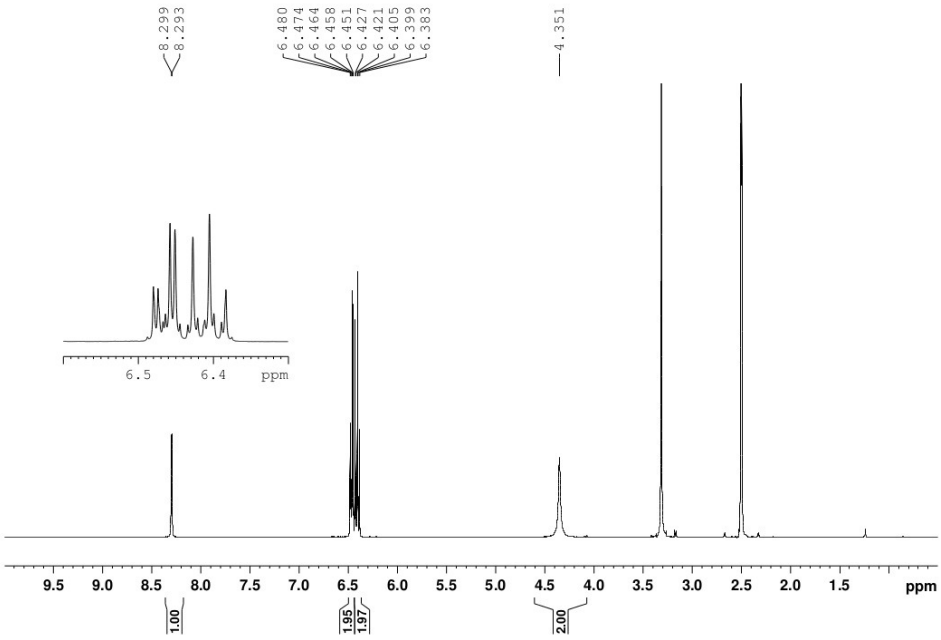
[1-^{13}C] 4-Nitrophenol **14** (^{1}H, 400 MHz, DMSO-6d)



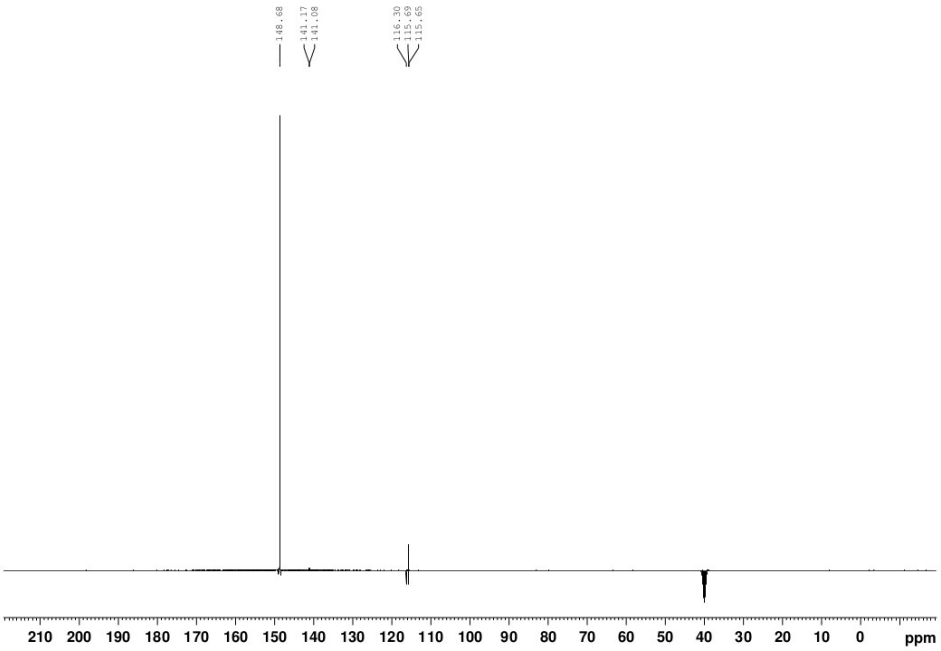
[1-^{13}C] 4-Nitrophenol **14** (^{13}C, 100.6 MHz, DMSO-6d)



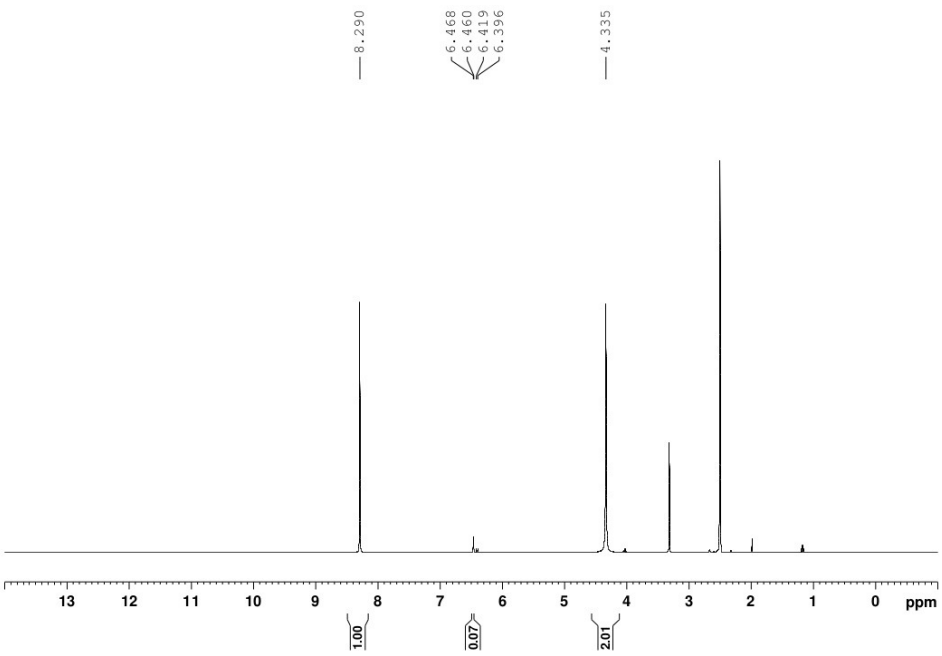
[1-^{13}C] 4-Aminophenol **15** (^{1}H, 400 MHz, DMSO-6d)



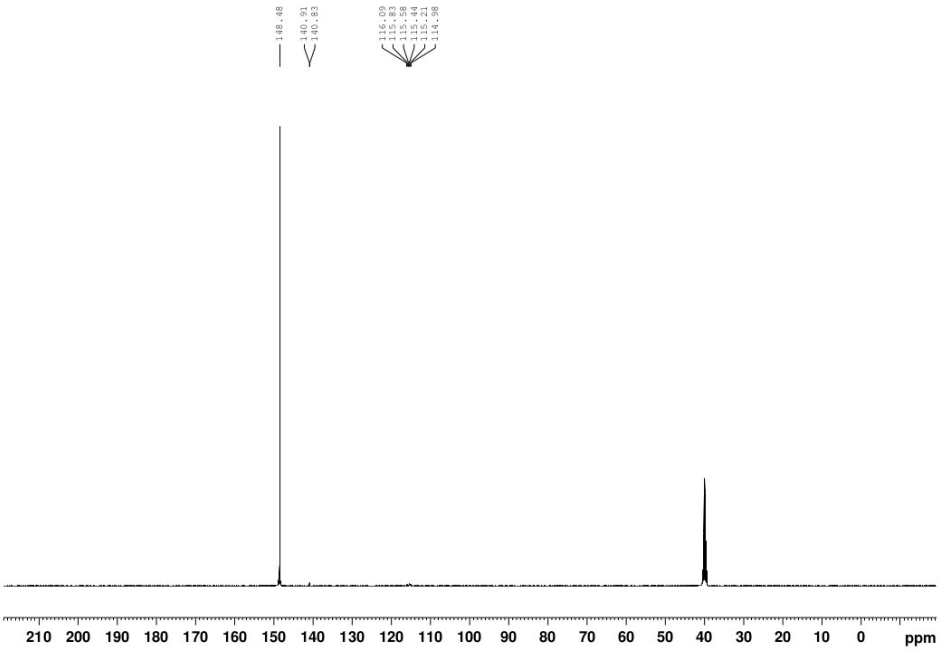
[1-^{13}C] 4-Aminophenol **15** (^{13}C, 100.6 MHz, DMSO-6d)



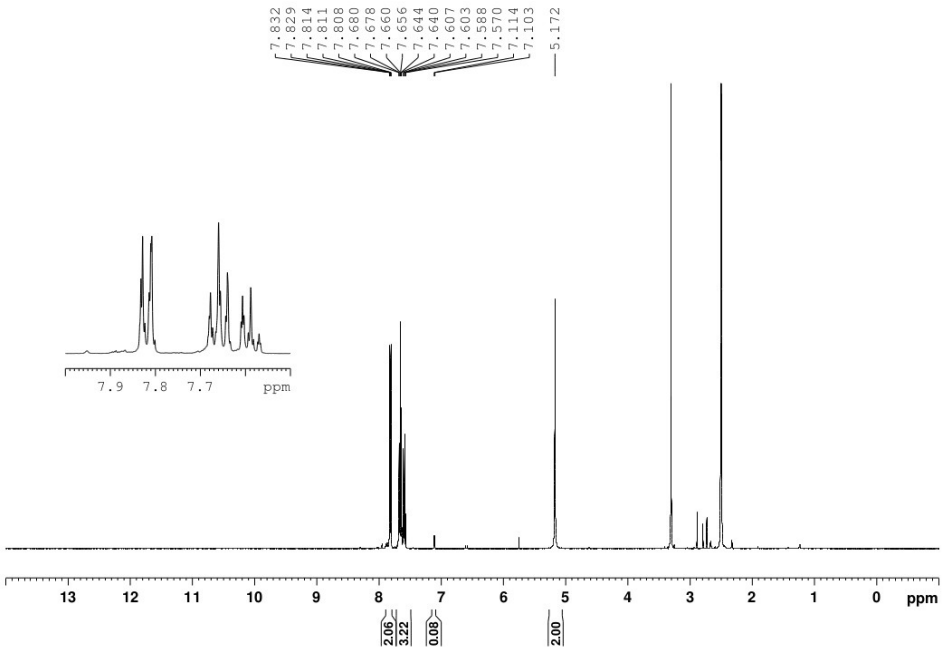
[1-^{13}C] 2,3,5,6-Tetradeuterio-4-aminophenol **16** (^{1}H, 400 MHz, DMSO-6d)



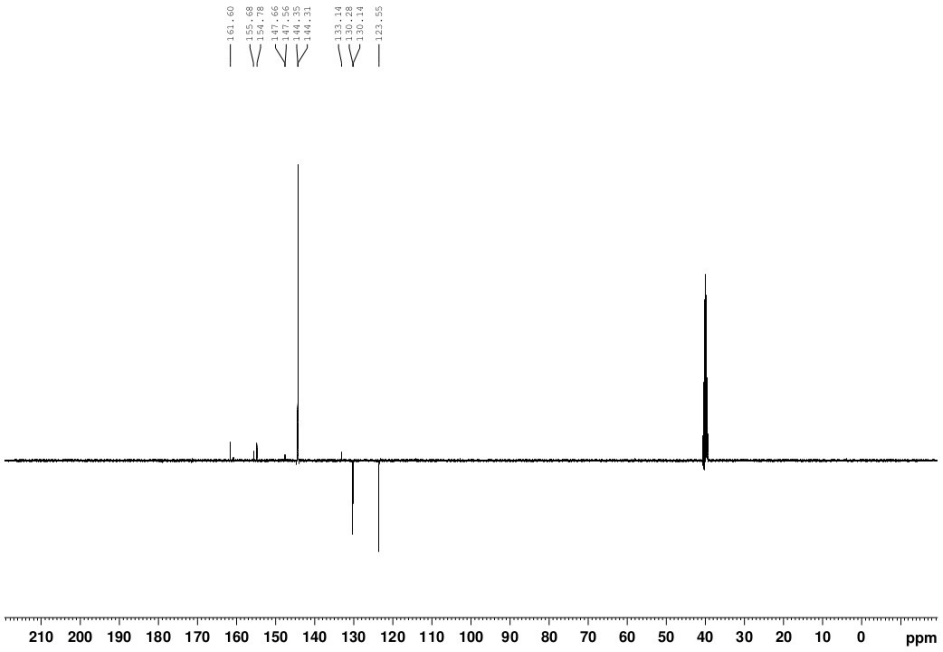
[1-^{13}C] 2,3,5,6-Tetradeuterio-4-aminophenol **16** (^{13}C, 100.6 MHz, DMSO-6d)



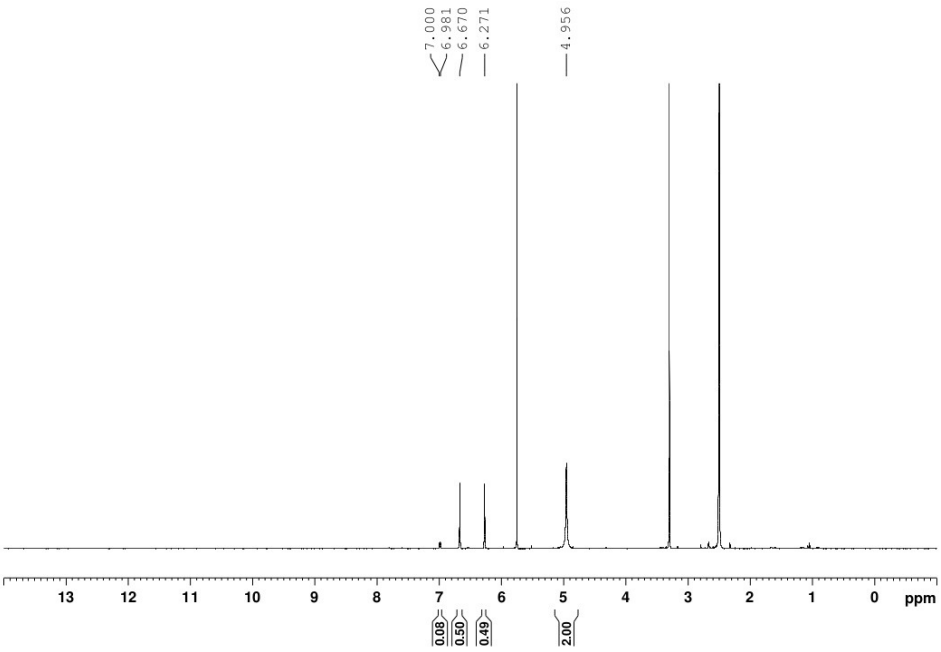
5-([1-^{13}C]-2,3,5,6-Tetradeuterio-4-aminophenoxy)-1-phenyl-1*H*-tetrazole **17** (^{1}H, 400 MHz, DMSO-6d)



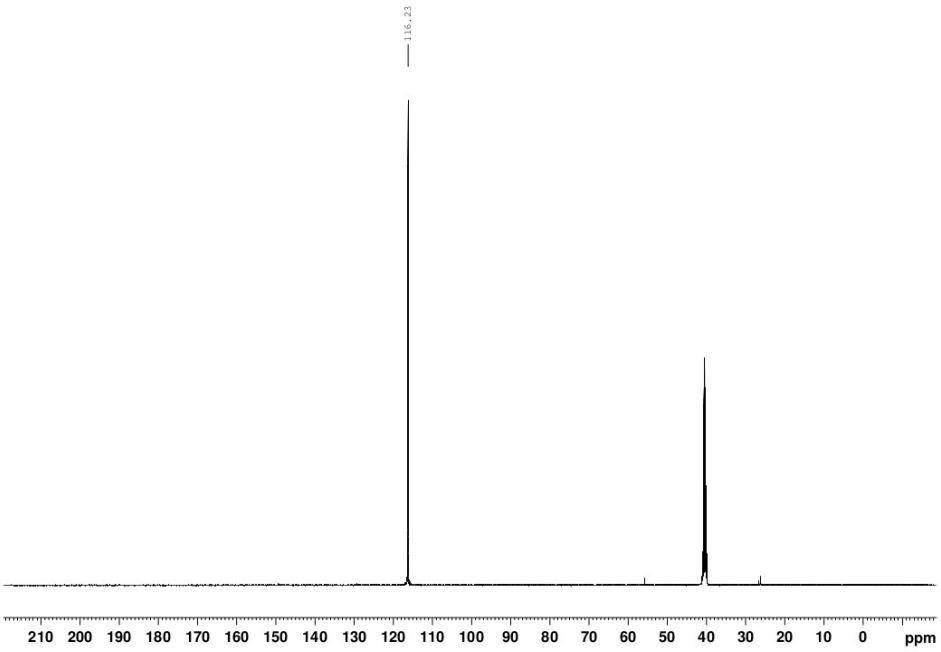
5-([1-^{13}C]-2,3,5,6-Tetradeuterio-4-aminophenoxy)-1-phenyl-1*H*-tetrazole **17** (^{13}C, 100.6 MHz, DMSO-6d)



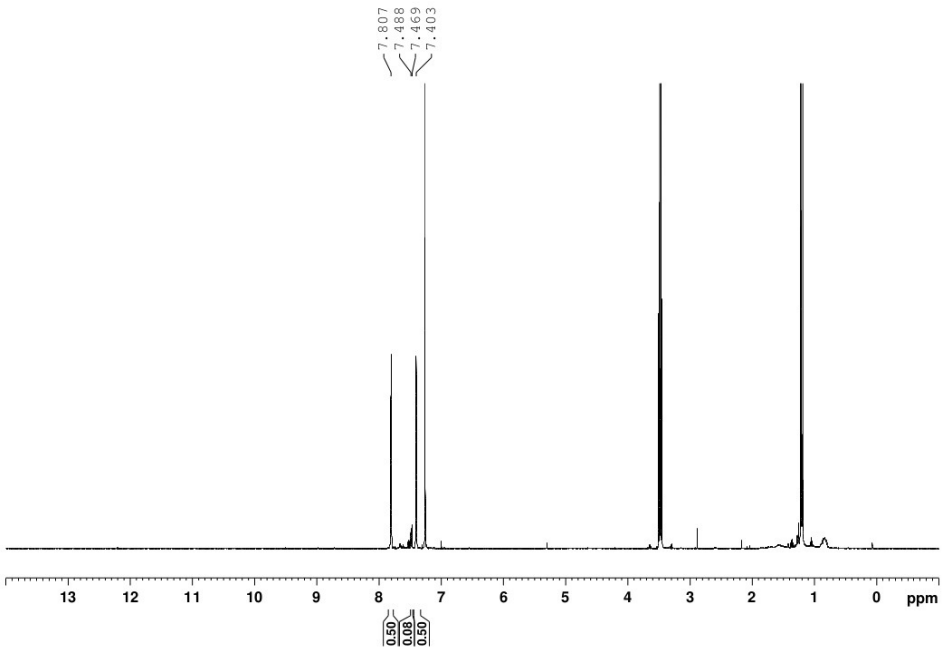
[4-^{13}C] 2,3,5,6-Tetradeuterioaniline **18** (^{1}H, 400 MHz, DMSO-6d)



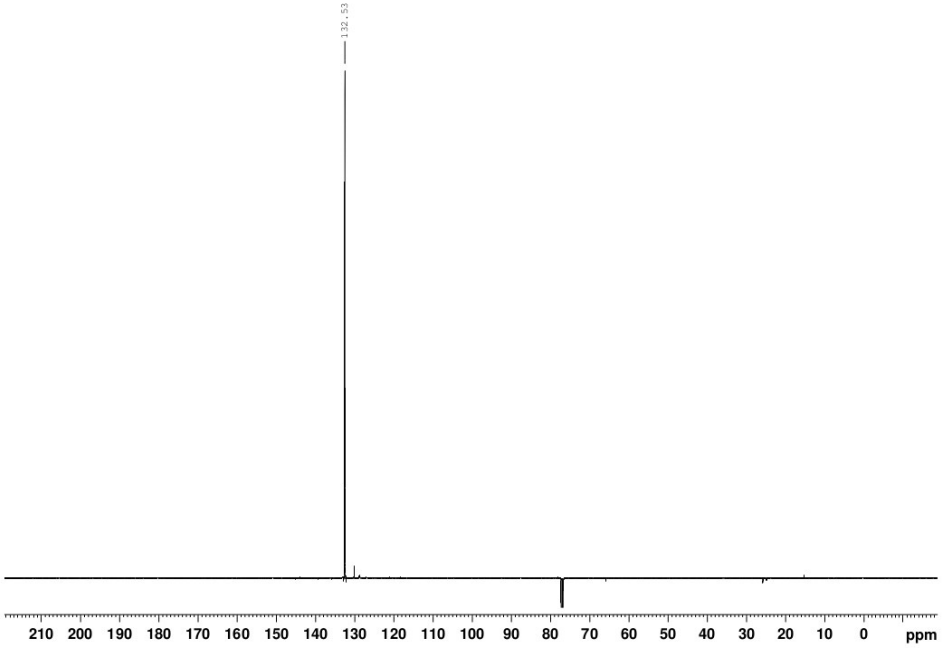
[4-^{13}C] 2,3,5,6-Tetradeuterioaniline **18** (^{13}C, 100.6 MHz, DMSO-6d)



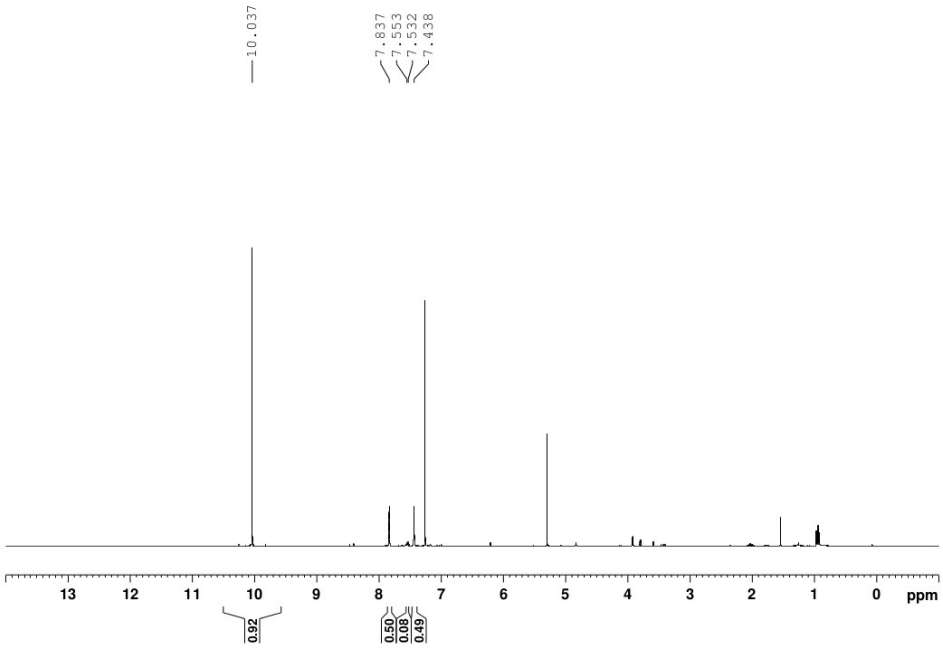
[4-^{13}C] 2,3,5,6-Tetradeuteriobenzonitrile **19** (^{1}H, 400 MHz, $CDCl_3$)



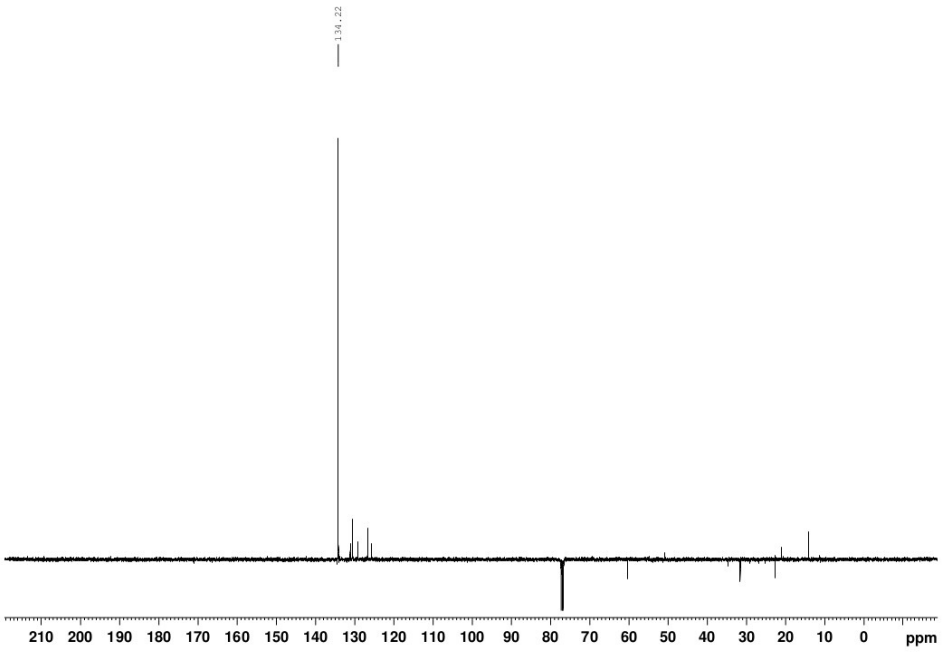
[4-^{13}C] 2,3,5,6-Tetradeuteriobenzonitrile **19** (^{13}C, 100.6 MHz, $CDCl_3$)



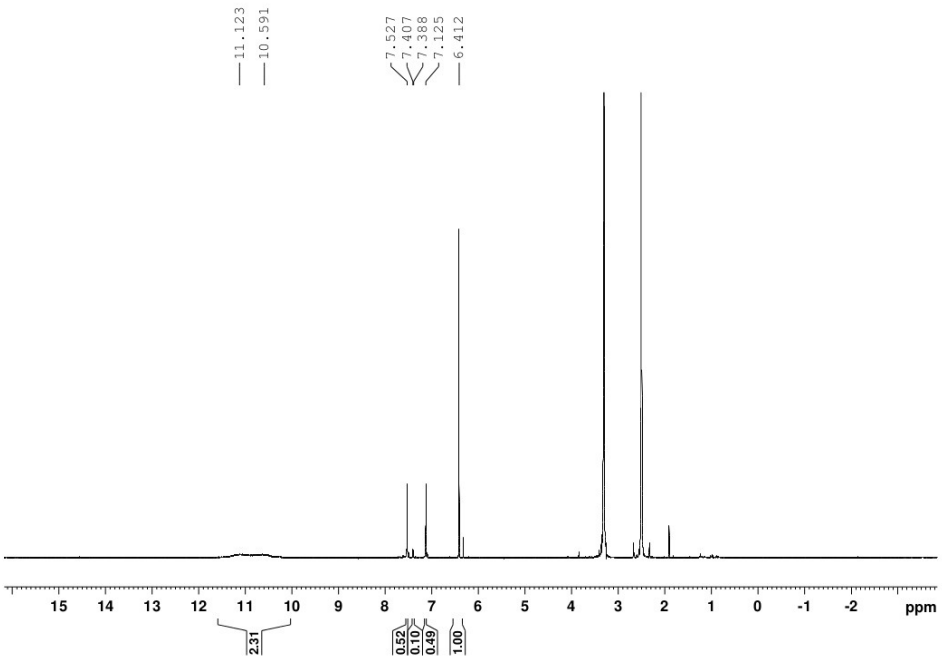
[4-^{13}C] 2,3,5,6-Tetradeuteriobenzaldehyde **20** (^{1}H, 400 MHz, $CDCl_3$)



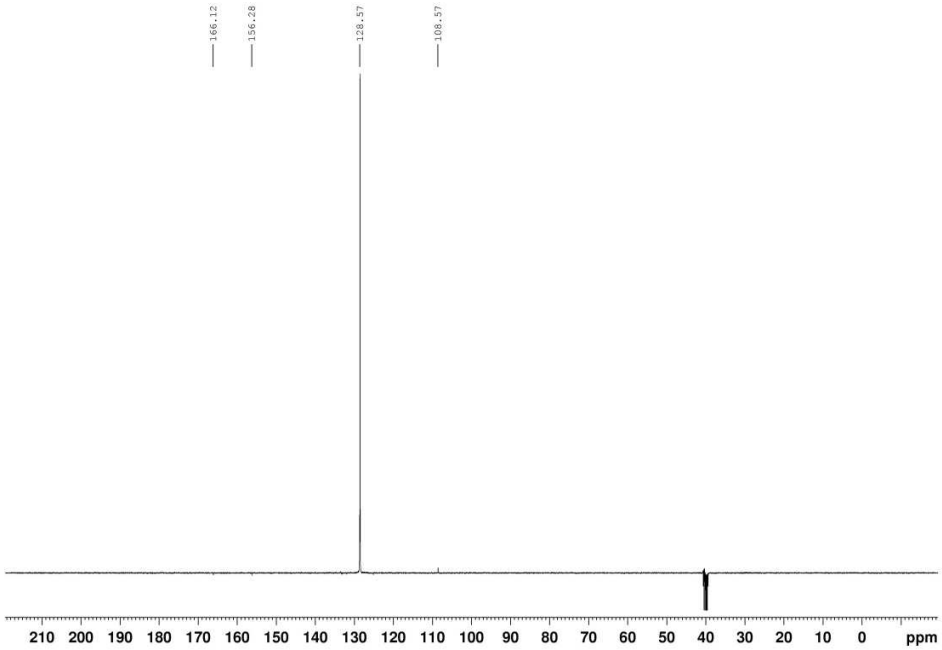
[4-^{13}C] 2,3,5,6-Tetradeuteriobenzaldehyde **20** (^{13}C, 100.6 MHz, $CDCl_3$)



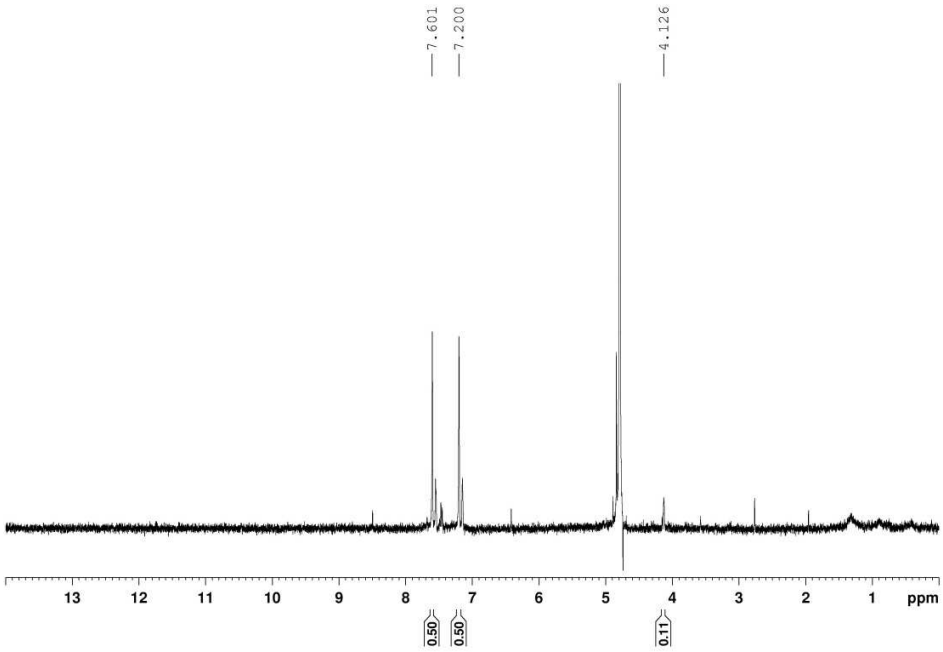
5-([4-^{13}C] 2,3,5,6-Tetradeuteriobenzylidene)hydantoin **21** (^{1}H, 400 MHz, DMSO-6d)



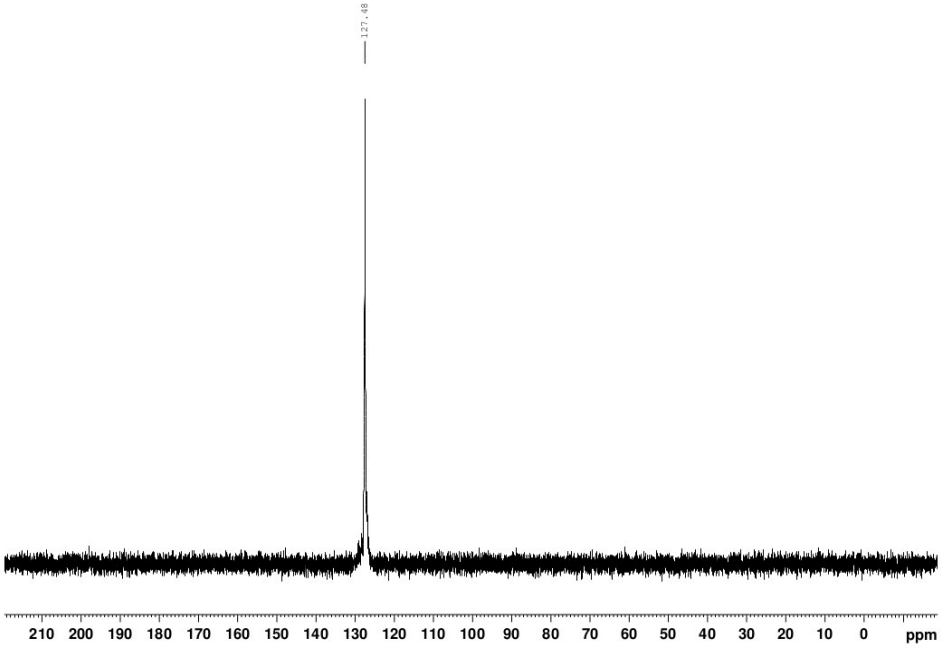
5-([4-^{13}C] 2,3,5,6-Tetradeuteriobenzylidene)hydantoin **21** (^{13}C, 100.6 MHz, DMSO-6d)



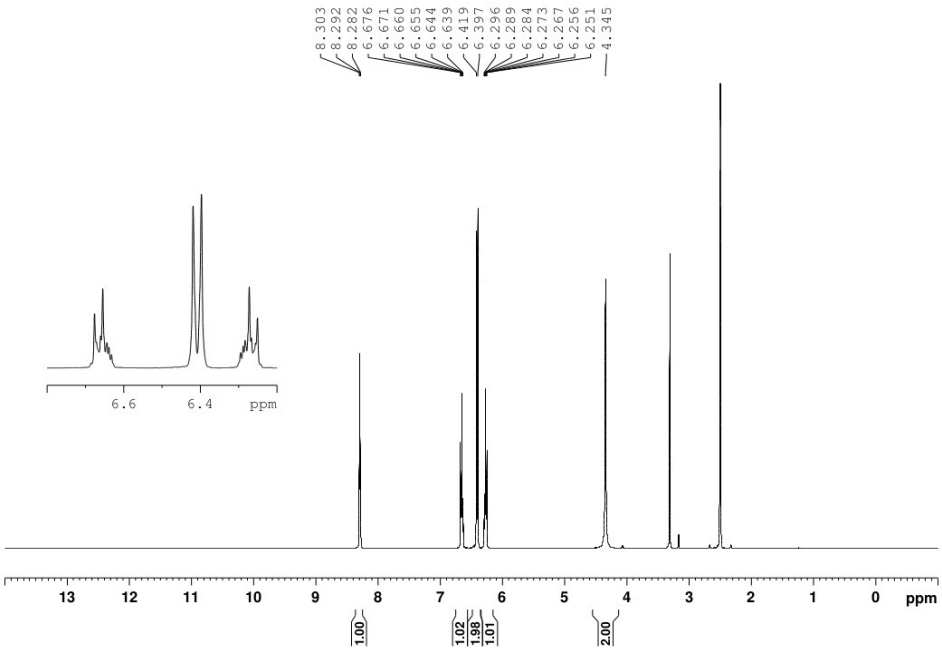
Sodium 3,3-dideuterio([4-^{13}C] 2,3,5,6-tetradeuteriophenyl)pyruvate **2** (^{1}H, 400 MHz, D_2O)



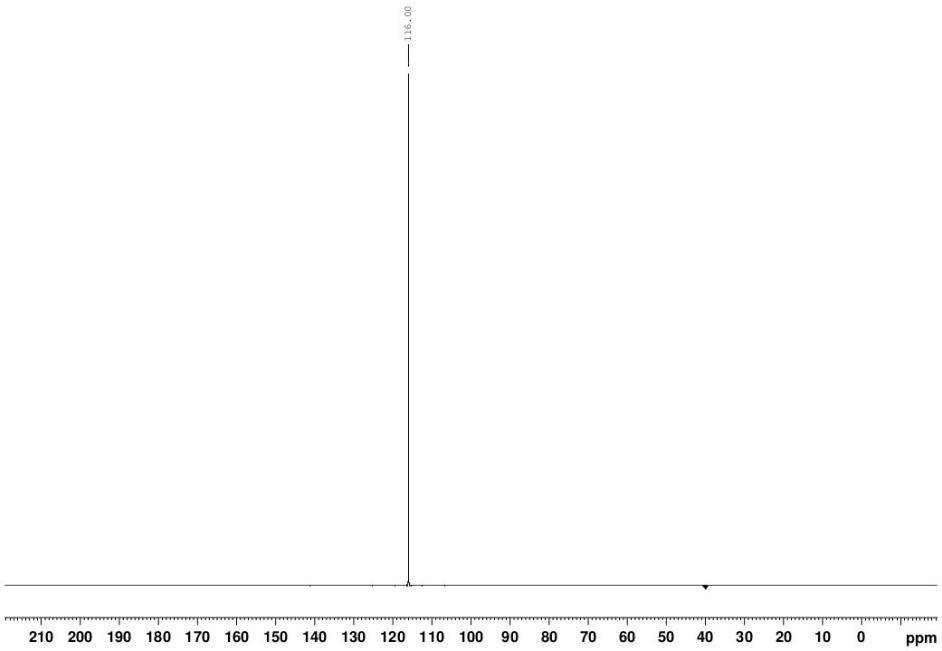
Sodium 3,3-dideuterio([4-^{13}C] 2,3,5,6-tetradeuteriophenyl)pyruvate **2** (^{13}C, 100.6 MHz, D_2O)



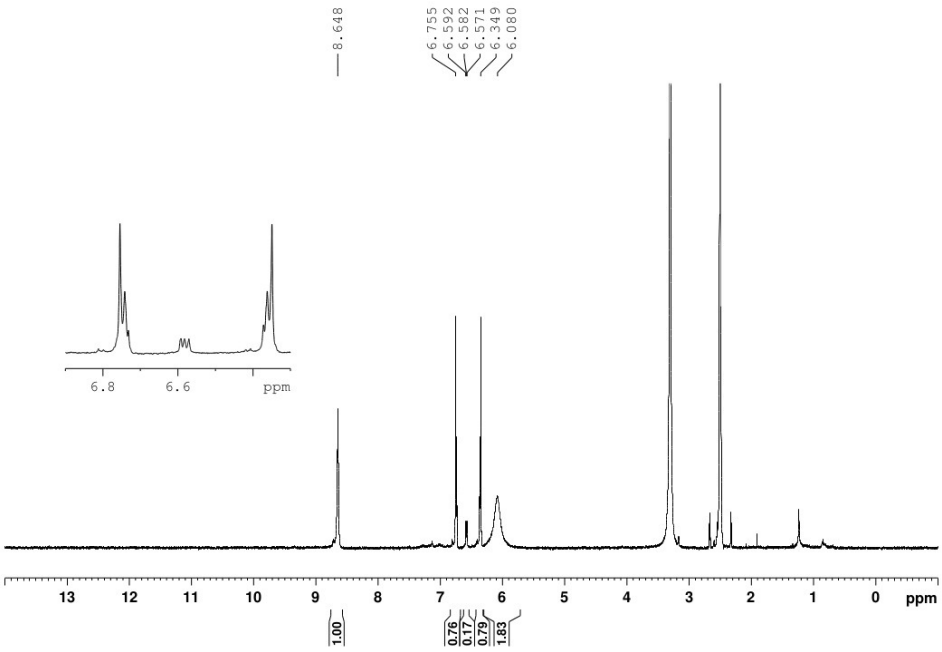
[2,6-$^{13}C_2$] 4-Aminophenol **22** (^{1}H, 400 MHz, DMSO-6d)



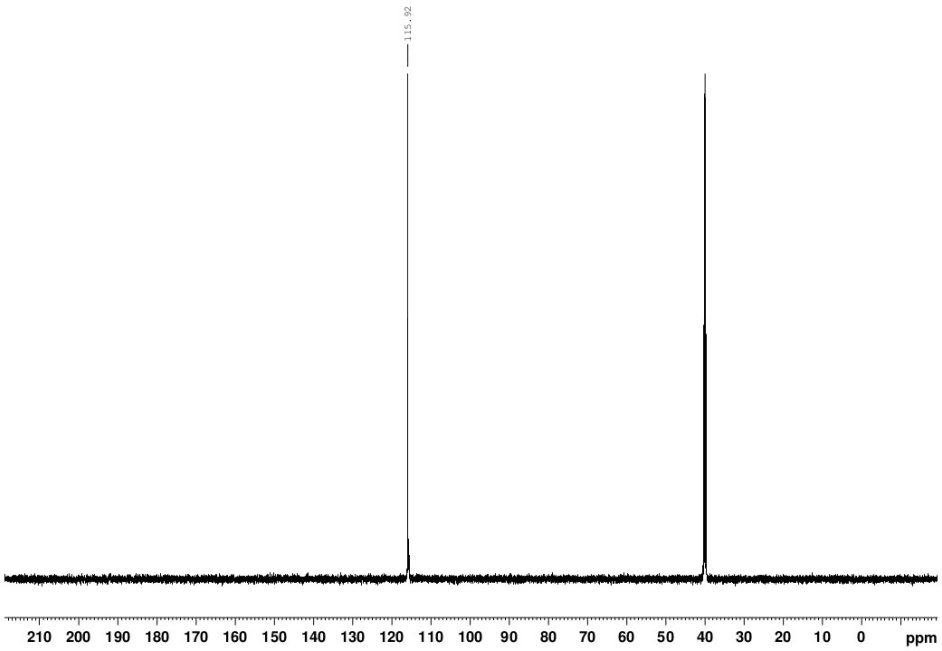
[2,6-$^{13}C_2$] 4-Aminophenol **22** (^{13}C, 100.6 MHz, DMSO-6d)



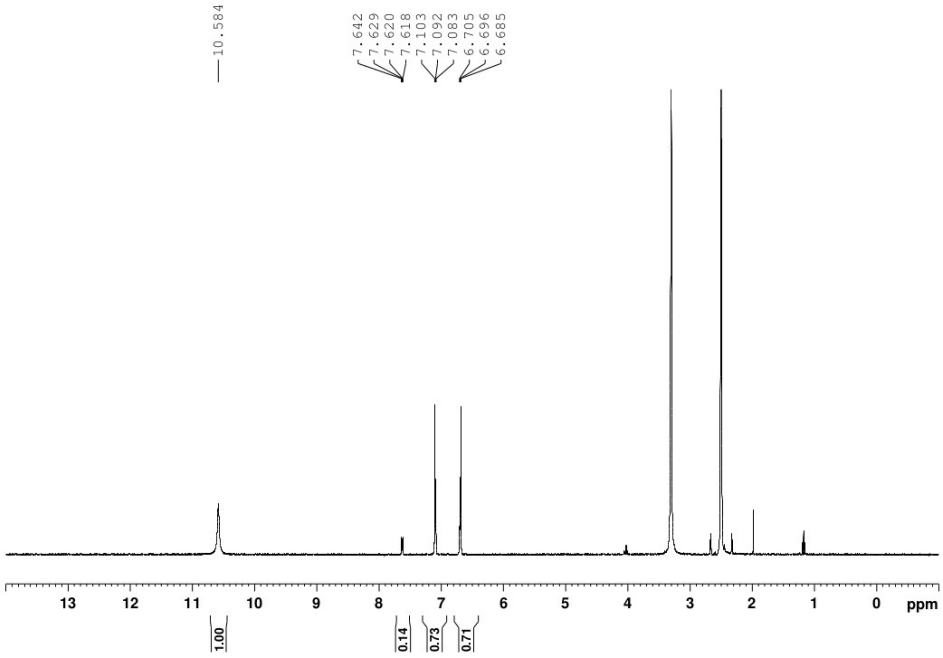
[2,6-$^{13}C_2$] 3,5-Dideuterio-4-aminophenol **23** [2,6-$^{13}C_2$] (^{1}H, 400 MHz, DMSO-6d)



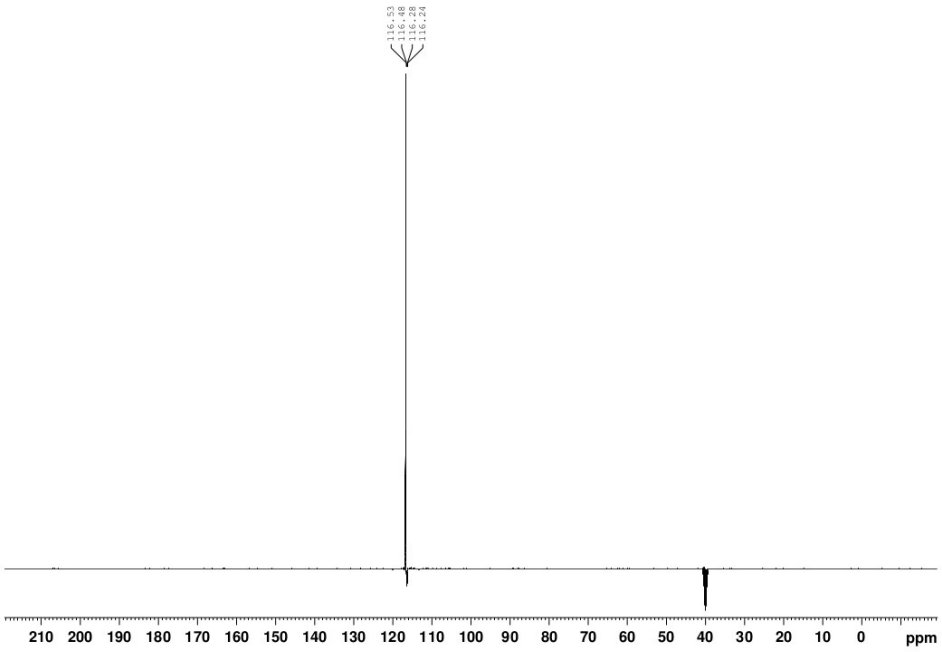
[2,6-$^{13}C_2$] 3,5-Dideuterio-4-aminophenol **23** [2,6-$^{13}C_2$] (^{13}C, 100.6 MHz, DMSO-6d)



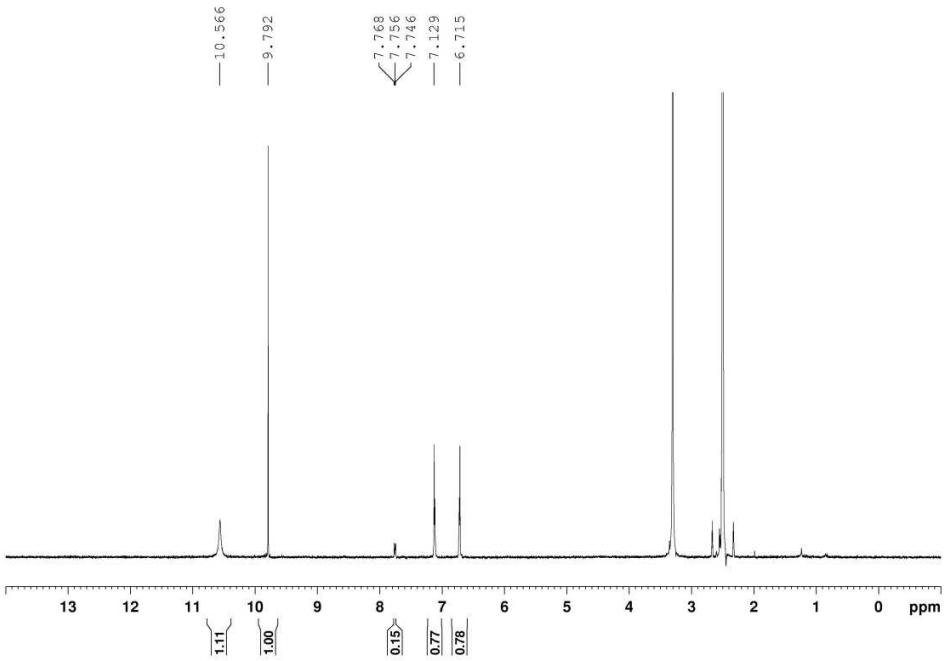
[3,5-$^{13}C_2$] 2,6-Dideuteriohydroxybenzonitrile **24** (^{1}H, 400 MHz, DMSO-6d)



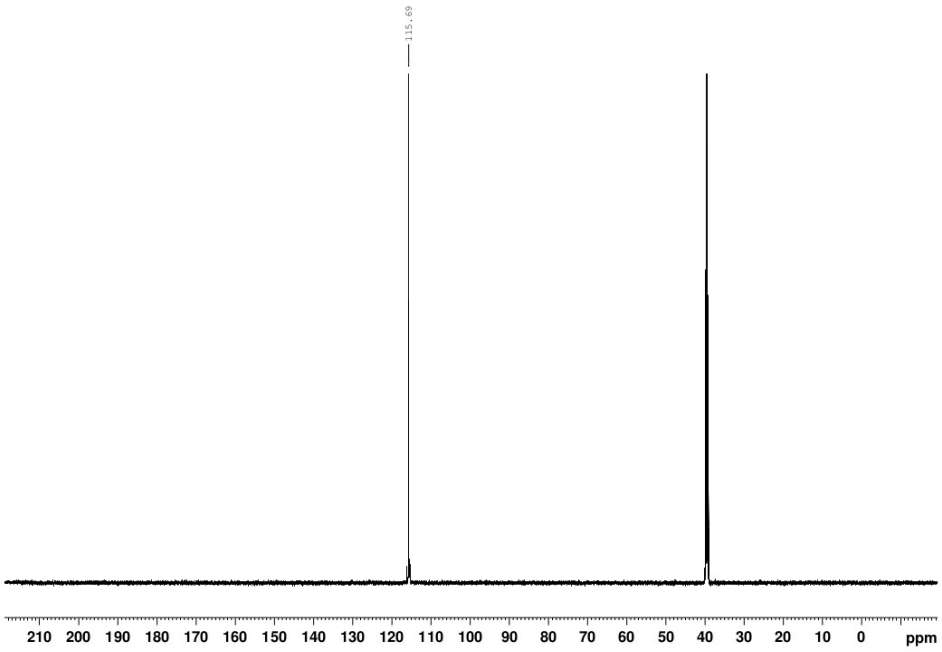
[3,5-$^{13}C_2$] 2,6-Dideuteriohydroxybenzonitrile **24** (^{13}C, 100.6 MHz, DMSO-6d)



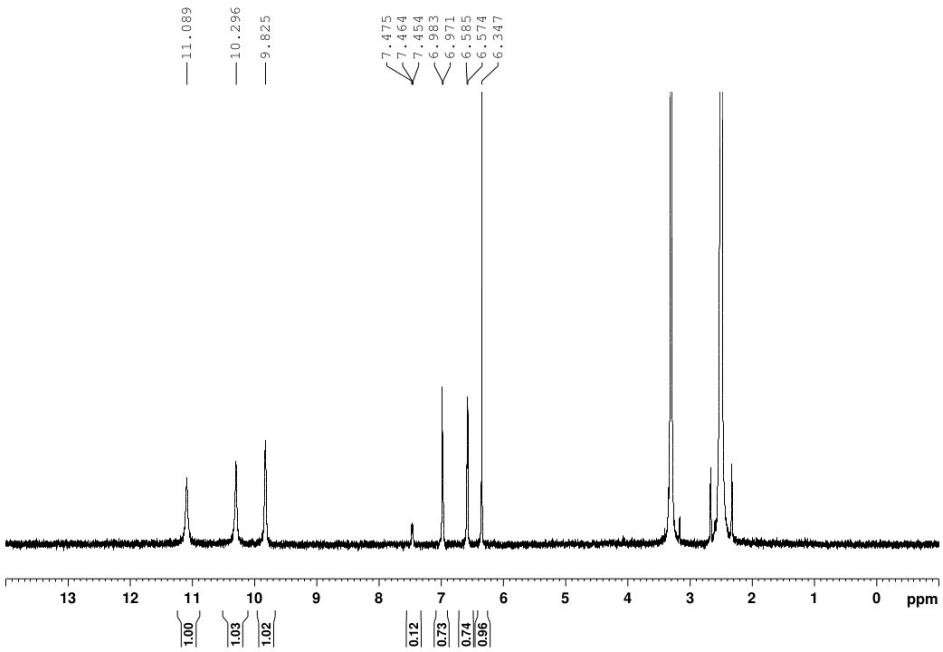
[3,5-$^{13}C_2$] 2,6-Dideuteriohydroxybenzaldehyde **25** (^{1}H, 400 MHz, DMSO-6d)



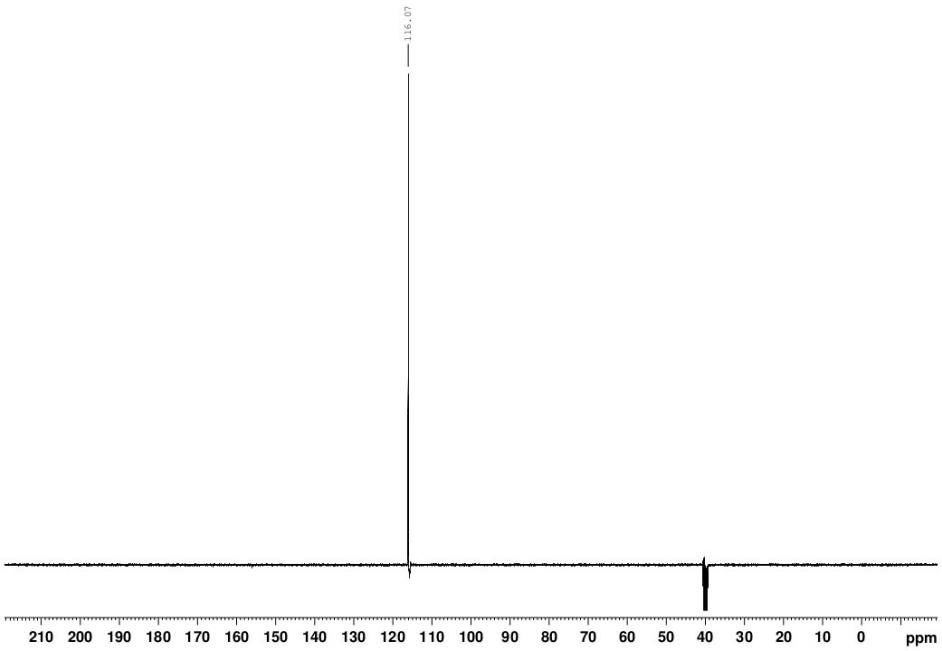
[3,5-$^{13}C_2$] 2,6-Dideuteriohydroxybenzaldehyde **25** (^{13}C, 100.6 MHz, DMSO-6d)



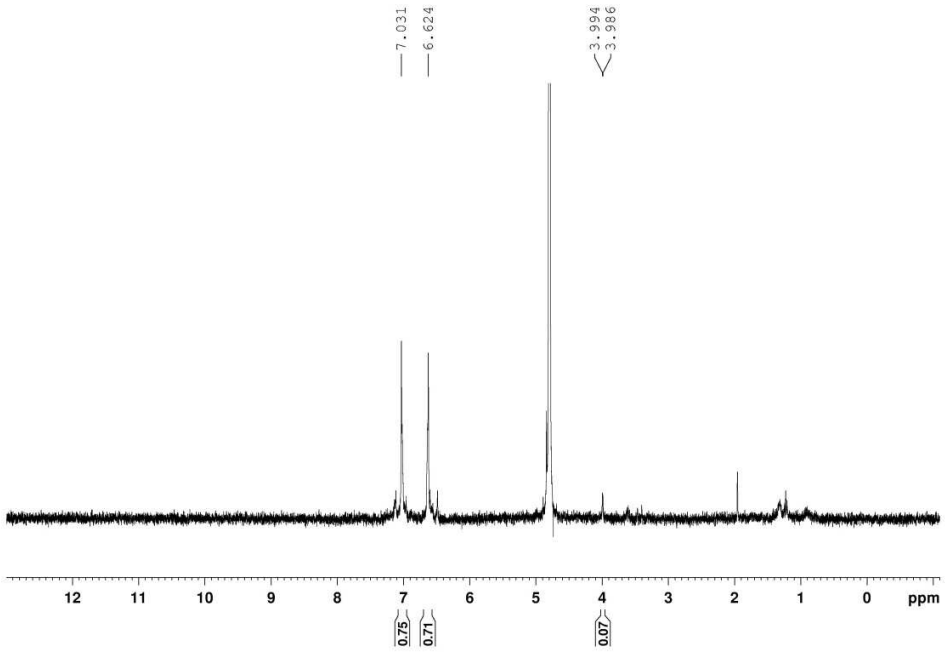
5-([3,5-$^{13}C_2$] 2,6-Dideuterio-4-hydroxybenzylidene)hydantoin **26** (^{1}H, 400 MHz, DMSO-6d)



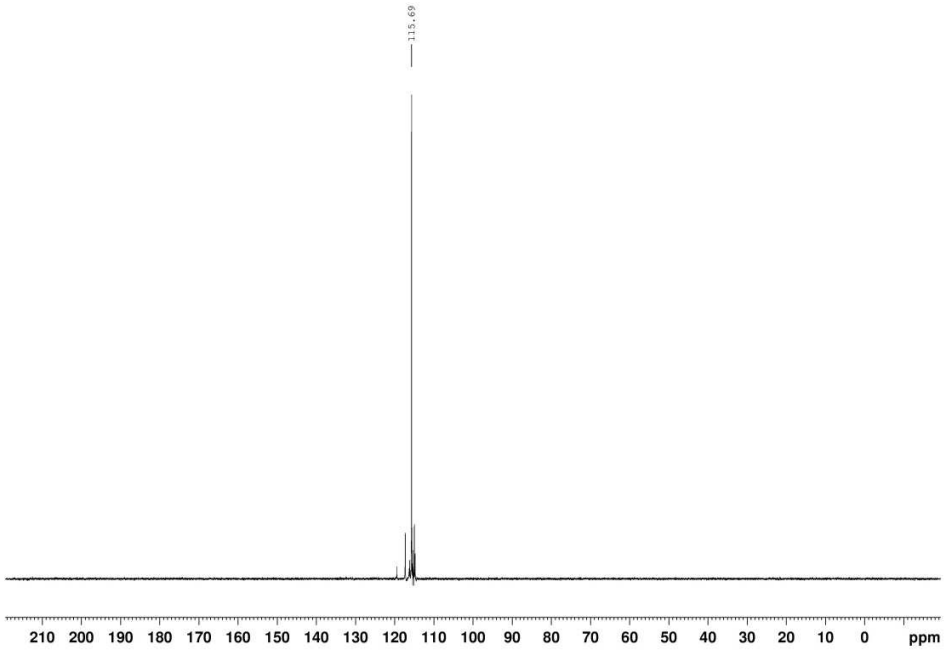
5-([3,5-$^{13}C_2$] 2,6-Dideuterio-4-hydroxybenzylidene)hydantoin **26** (^{13}C, 100.6 MHz, DMSO-6d)



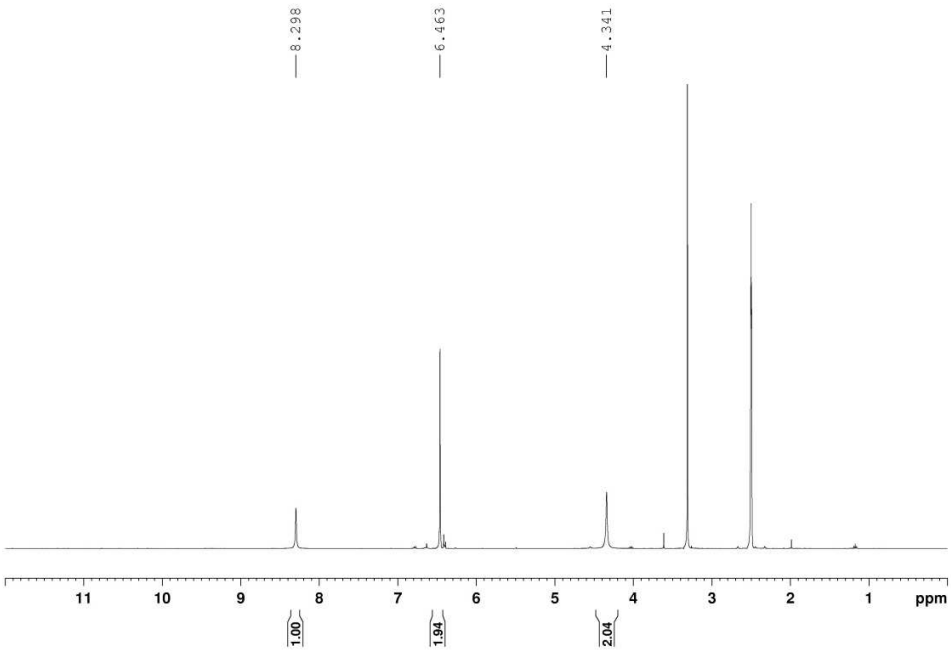
Sodium 3,3-dideuterio([3,5-$^{13}C_2$] 2,6-dideuterio-4-hydroxyphenyl)pyruvate **3** (^{1}H, 400 MHz, D_2O)



Sodium 3,3-dideuterio([3,5-$^{13}C_2$] 2,6-dideuterio-4-hydroxyphenyl)pyruvate **3** (^{13}C, 100.6 MHz, D_2O)



3,5-Dideuterio-4-aminophenol **30** (^{1}H, 400 MHz, DMSO-6d)



3,5-Dideuterio-4-aminophenol **30** (^{13}C, 100.6 MHz, DMSO-6d)