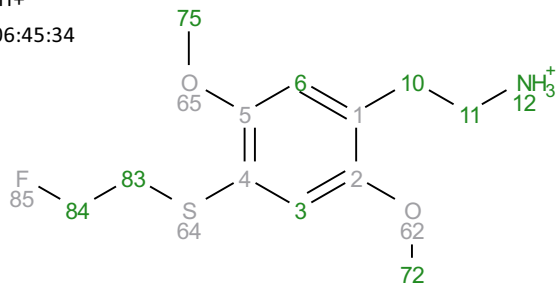
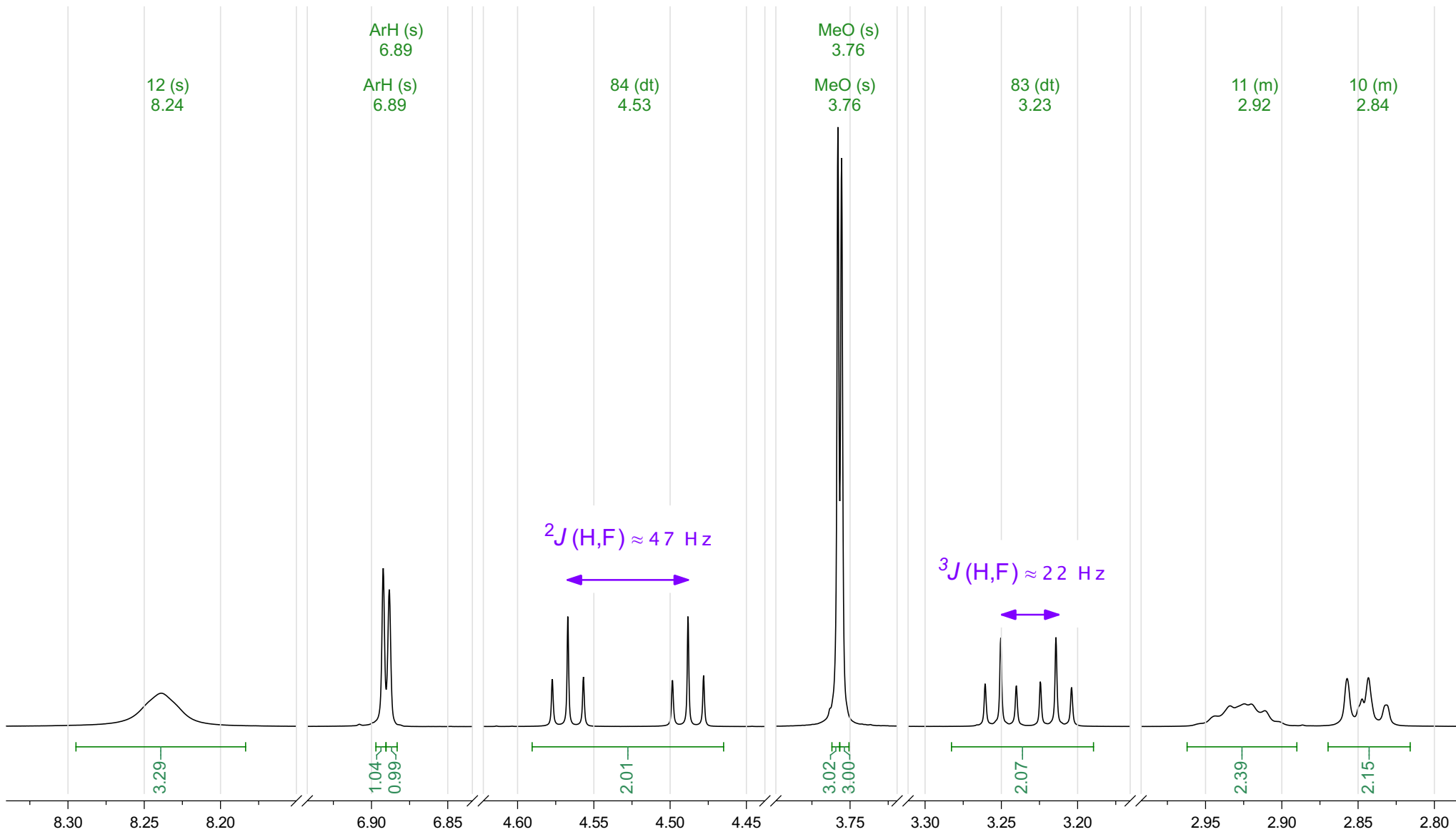


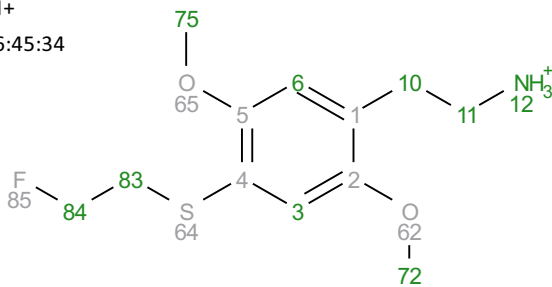
Analyte P21: 2C-T-21 H+
 Acquisition Date 2017-09-12T06:45:34
 Solvent dmso
 Temperature 25
 Number of Scans 16
 Relaxation Delay 1
 Spectrometer Frequency 599.82
 Spectral Width 9615.4
 Nucleus 1H
 Acquired Size 43269



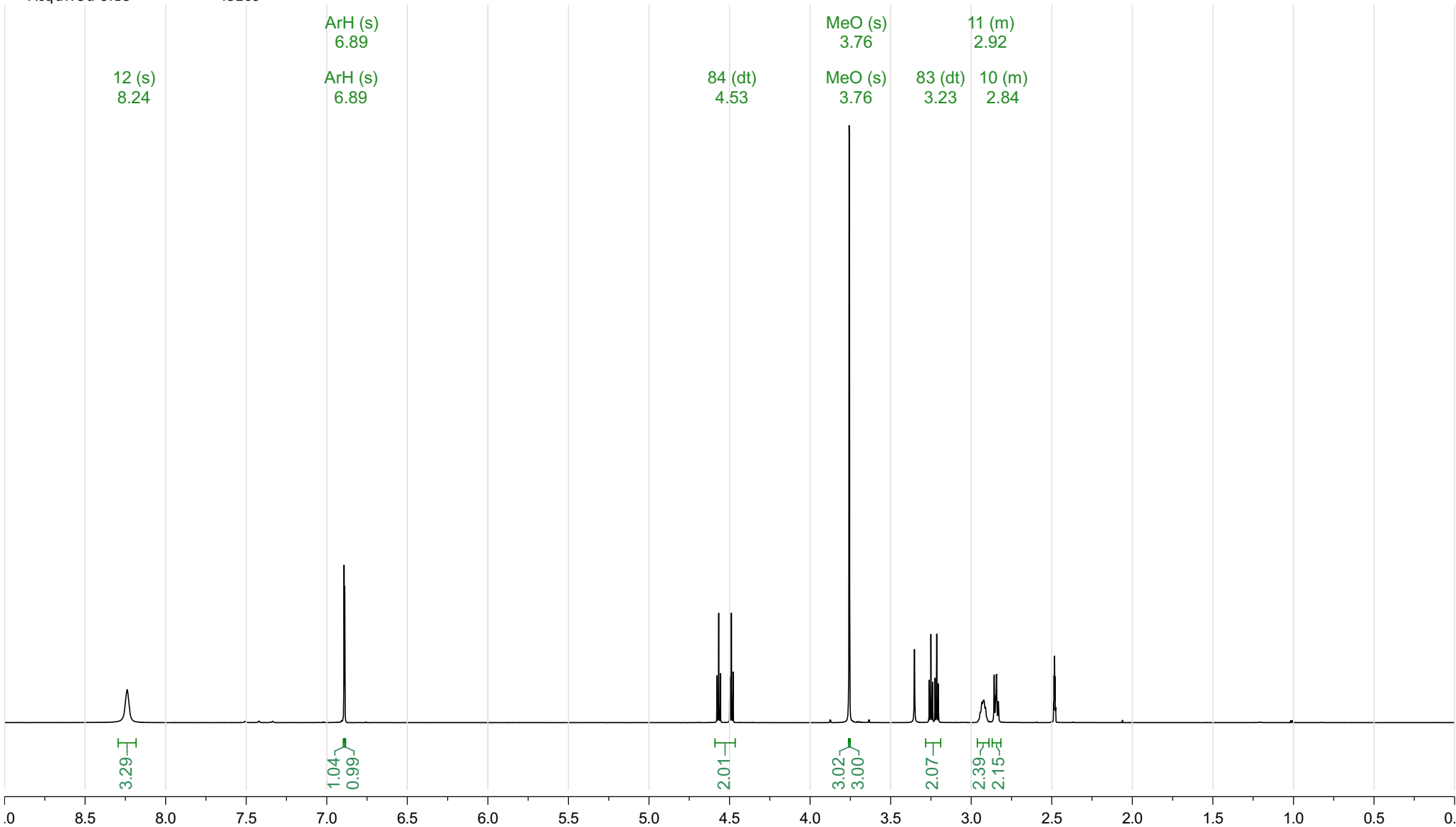
¹H NMR (600 MHz, DMSO-*d*₆) δ 8.24 (s, 3H), 6.89 (s, 1H), 6.89 (s, 1H), 4.53 (dt, *J* = 47.3, 6.1 Hz, 2H), 3.76 (s, 3H), 3.76 (s, 3H), 3.23 (dt, *J* = 21.7, 6.1 Hz, 2H), 2.96 – 2.89 (m, 2H), 2.87 – 2.82 (m, 2H).



Analyte P21: 2C-T-21 H+
 Acquisition Date 2017-09-12T06:45:34
 Solvent dmso
 Temperature 25
 Number of Scans 16
 Relaxation Delay 1
 Spectrometer Frequency 599.82
 Spectral Width 9615.4
 Nucleus 1H
 Acquired Size 43269



$^1\text{H NMR}$ (600 MHz, $\text{DMSO-}d_6$) δ 8.24 (s, 3H), 6.89 (s, 1H), 6.89 (s, 1H), 4.53 (dt, $J = 47.3, 6.1$ Hz, 2H), 3.76 (s, 3H), 3.76 (s, 3H), 3.23 (dt, $J = 21.7, 6.1$ Hz, 2H), 2.96 – 2.89 (m, 2H), 2.87 – 2.82 (m, 2H).



Prediction 2C-T-21 H+
Origin Modgraph NMRPredict Desktop
Solvent DMSO-d6
Algorithm Best
GMMX Cycles 5
Version 15465
Frequency 600.00
Nucleus 1H

^1H NMR (600 MHz, DMSO- d_6) δ 7.80 (s, 3H), 6.76 (s, 1H), 6.73 (s, 1H), 4.49 (dt, $J = 46.3, 7.7$ Hz, 2H), 3.79 (s, 3H), 3.74 (s, 3H), 3.66 (t, $J = 7.6$ Hz, 2H), 3.13 (td, $J = 7.6, 1.1$ Hz, 2H), 2.99 (dt, $J = 25.4, 7.7$ Hz, 2H).

