PeakAL: Protons I Have Known and Loved — Fifty Shades of Grey-Market Spectra

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Supplementary Data: http://dx.doi.org/10.16889/isomerdesign-1-supp

> *"Once you get a serious spectrum collection, the tendency is to push it as far as you can."*
> *pace* Hunter S. Thompson

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Supplementary Data for *PeakAL*: Protons I Have Known and Loved — Fifty Shades of Grey-Market Spectra

Page	Analyte	Alleged	Found	Acquired
4	P0	PEA HCl	PEA HCl	2014-08-19
7	P1	2C-H	2C-H	2013-01-16
10	P1 as HCl	2C-H	2C-H HCl	2013-11-08
13	P2	2C-D	2C-D	2012-11-20
16	P3	2C-E	2C-E	2012-11-24
19	P4	2C-P	2C-P	2012-11-24
22	P4 in DMF-d_7	2C-P	2C-P	2013-05-07
25	P5	2C-IP	2C-IP	2012-11-24
28	P6a	2C-C	2C-E	2012-11-24
31	P6b	2C-C	2C-C	2013-03-26
34	P7	2C-I	2C-I	2012-11-24
37	P8	2C-T	2C-T	2012-11-24
40	P9	2C-T-2	2C-T-2	2012-11-24
43	P10	2C-T-4	2C-T-4	2012-11-24
46	P11	2C-T-7	2C-T-7	2012-11-24
49	P12	Escaline	Escaline	2013-01-16
52	P13a	Proscaline	Proscaline	2012-11-24
55	P13b	Proscaline	Proscaline	2013-03-26
58	P14	AL	AL	2012-11-24
61	P15	MAL	MAL	2012-11-24
64	P16	BOD	BOD	2012-11-24
67	P17	bk-2C-B	bk-2C-B	2013-11-29

Page	Analyte	Alleged	Found	Acquired
70	B1	25B-NBOMe	25B-NBOMe	2013-01-16
73	B2	25C-NBOMe	25C-NBOMe	2013-01-16
76	B3	25I-NBOMe	25I-NBOMe	2013-01-16
79	B4	25I-NBOH	25I-NBOH	2013-01-16
82	B5	25I-NBMD	25I-NBMD	2013-05-07
85	B6	25D-NBOMe	25D-NBOMe	2013-01-16
88	B7	25E-NBOMe	25E-NBOMe	2013-01-16
91	B8	25IP-NBOMe	25IP-NBOMe	2013-03-26
94	B9	25G-NBOMe	25G-NBOMe	2013-05-07
97	B10	M-NBOMe	M-NBOMe	2013-01-16
100	IM1	25H-NBOMe imine	25H-NBOMe imine	2013-11-08
104	IM2	25I-NBOMe imine	25I-NBOMe imine	2013-11-08

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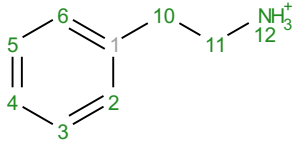
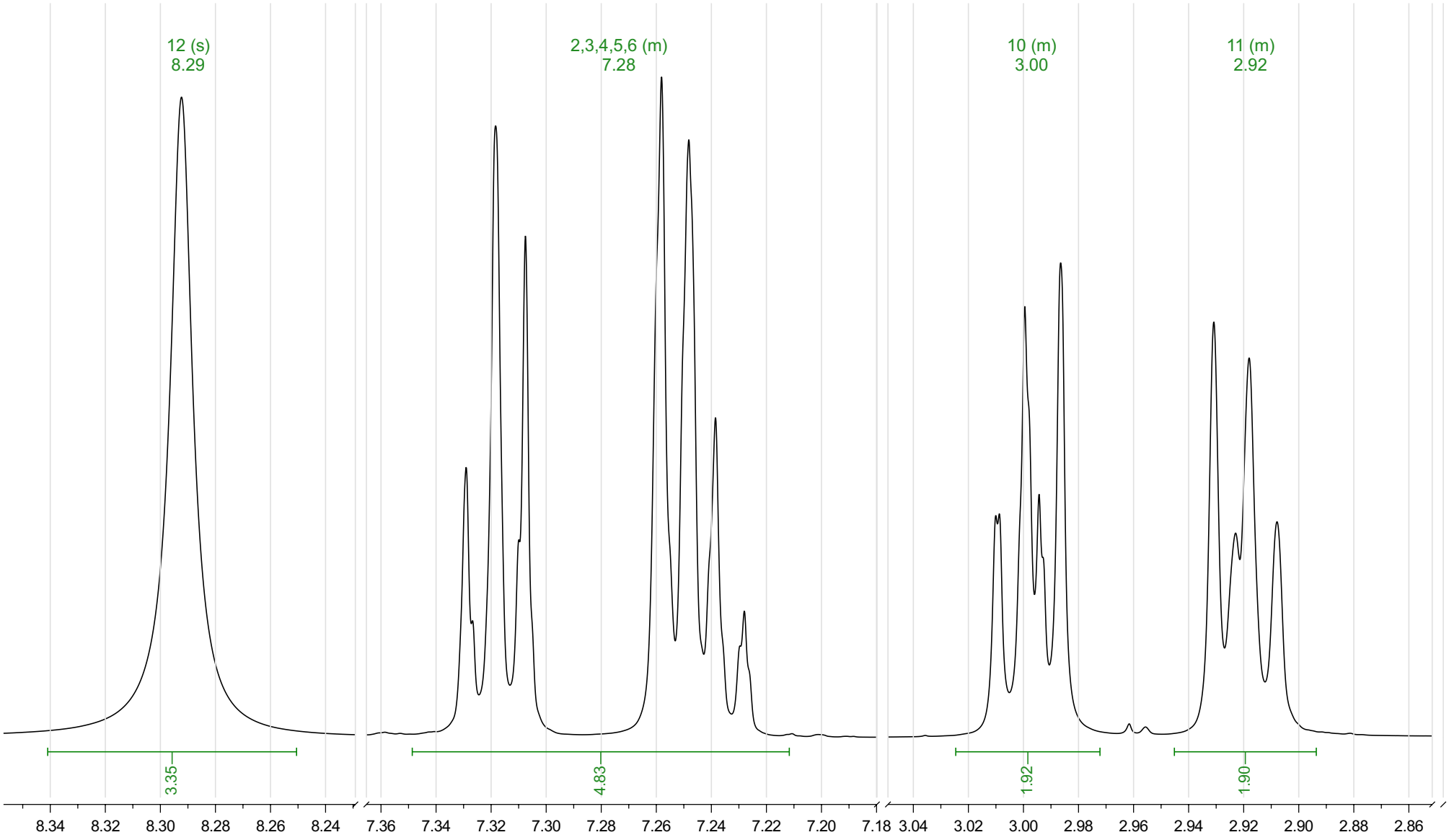
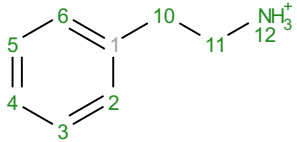
Analyte	P0: PEA; 2-Phenylethan-1-amine HCl
Acquisition Date	2014-08-19T02:01:52
Solvent	dmso
Temperature	27
Number of Scans	64
Relaxation Delay	5
Spectrometer Frequency	699.81
Spectral Width	11160.7
Nucleus	1H
Acquired Size	50223



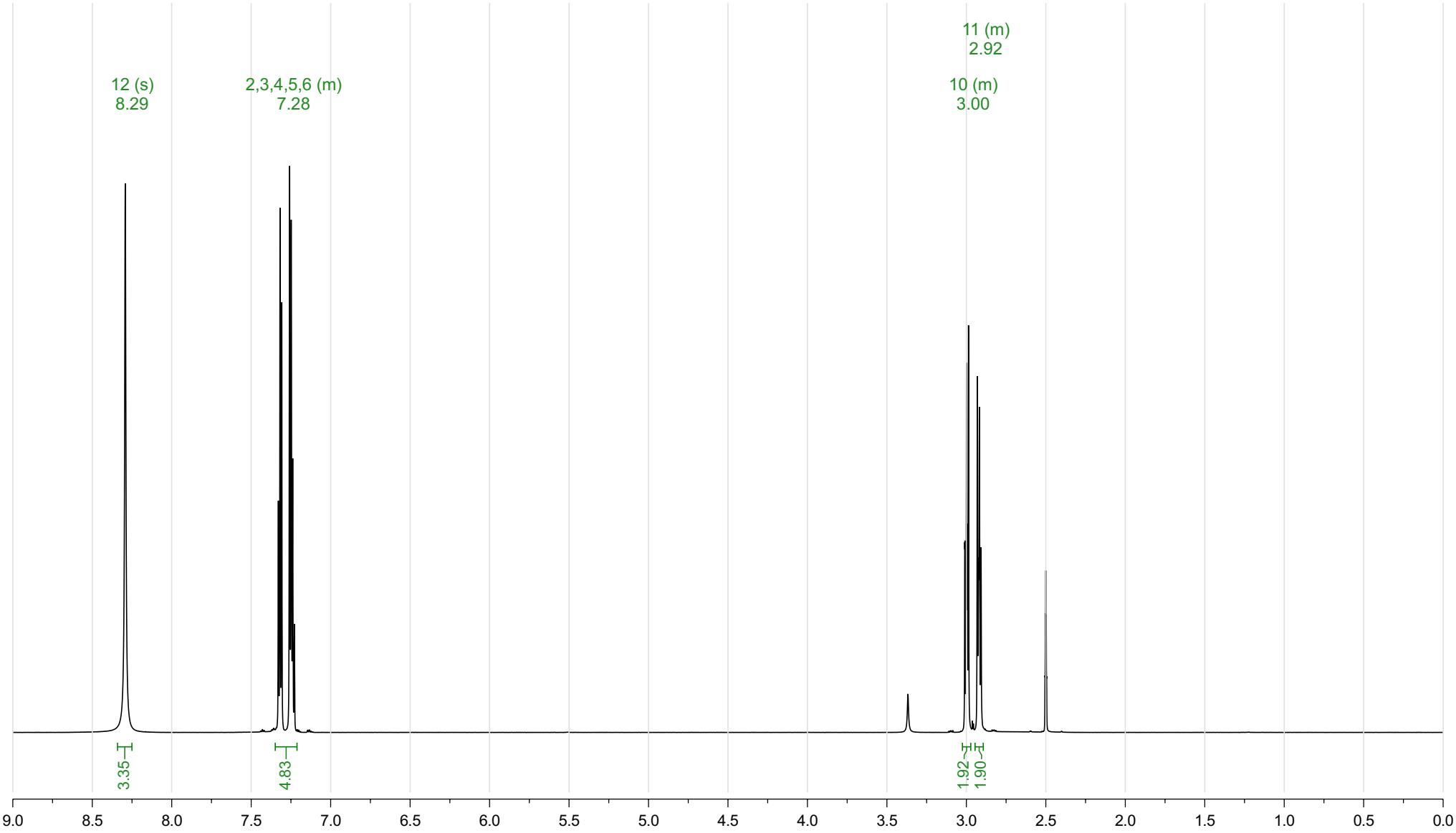
^{1}H NMR (700 MHz, DMSO-d_6) δ 8.29 (s, 3H), 7.34 – 7.21 (m, 5H), 3.02 – 2.97 (m, 2H), 2.95 – 2.89 (m, 2H).



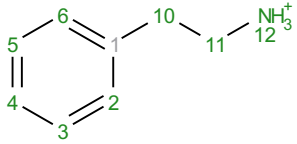
Analyte	P0: PEA; 2-Phenylethan-1-amine HCl
Acquisition Date	2014-08-19T02:01:52
Solvent	dmso
Temperature	27
Number of Scans	64
Relaxation Delay	5
Spectrometer Frequency	699.81
Spectral Width	11160.7
Nucleus	1H
Acquired Size	50223



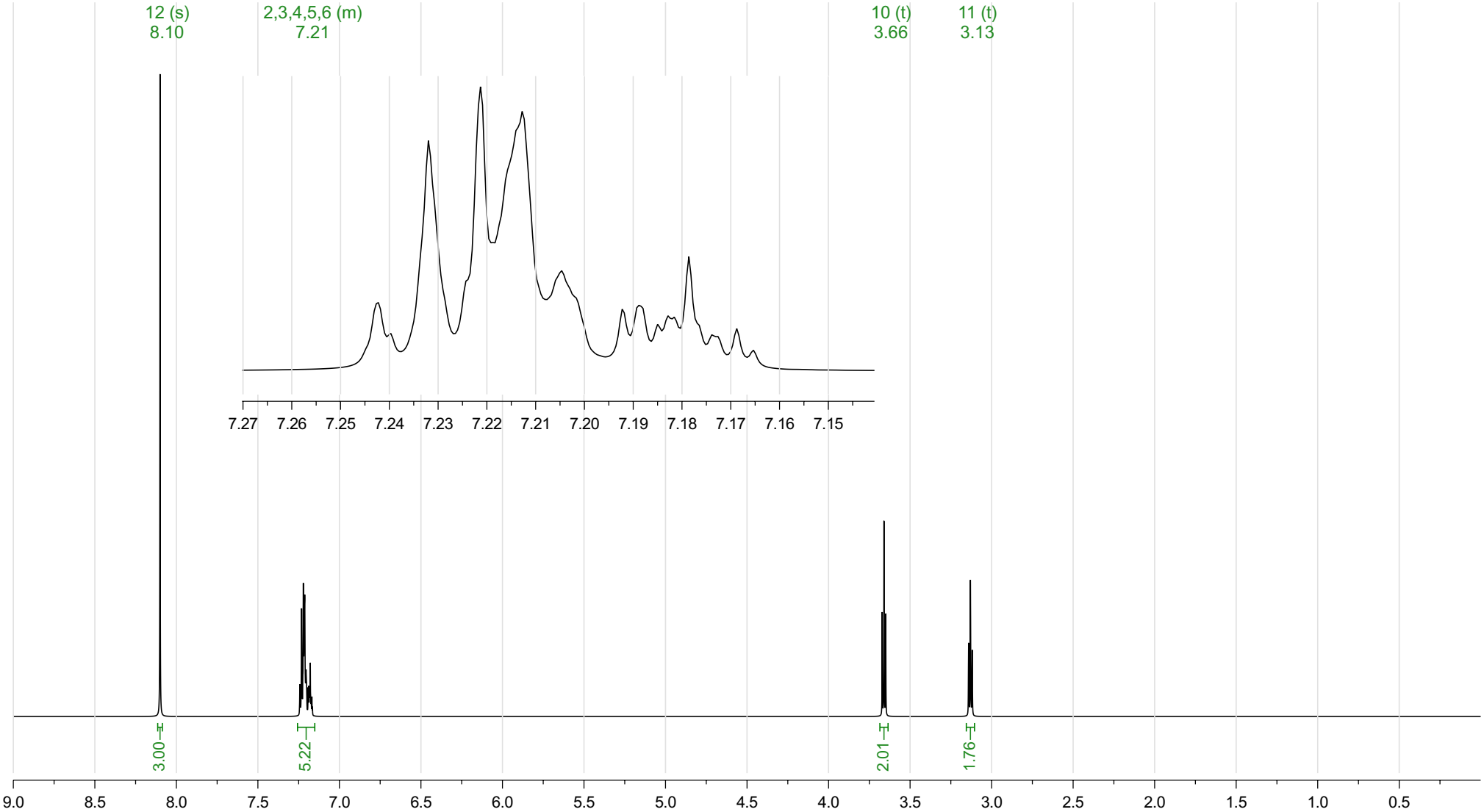
^{1}H NMR (700 MHz, DMSO-d_6) δ 8.29 (s, 3H), 7.34 – 7.21 (m, 5H), 3.02 – 2.97 (m, 2H), 2.95 – 2.89 (m, 2H).



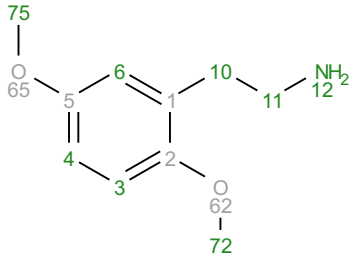
Prediction	2-Phenylethan-1-amine H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	12489
Frequency	700.00
Nucleus	1H



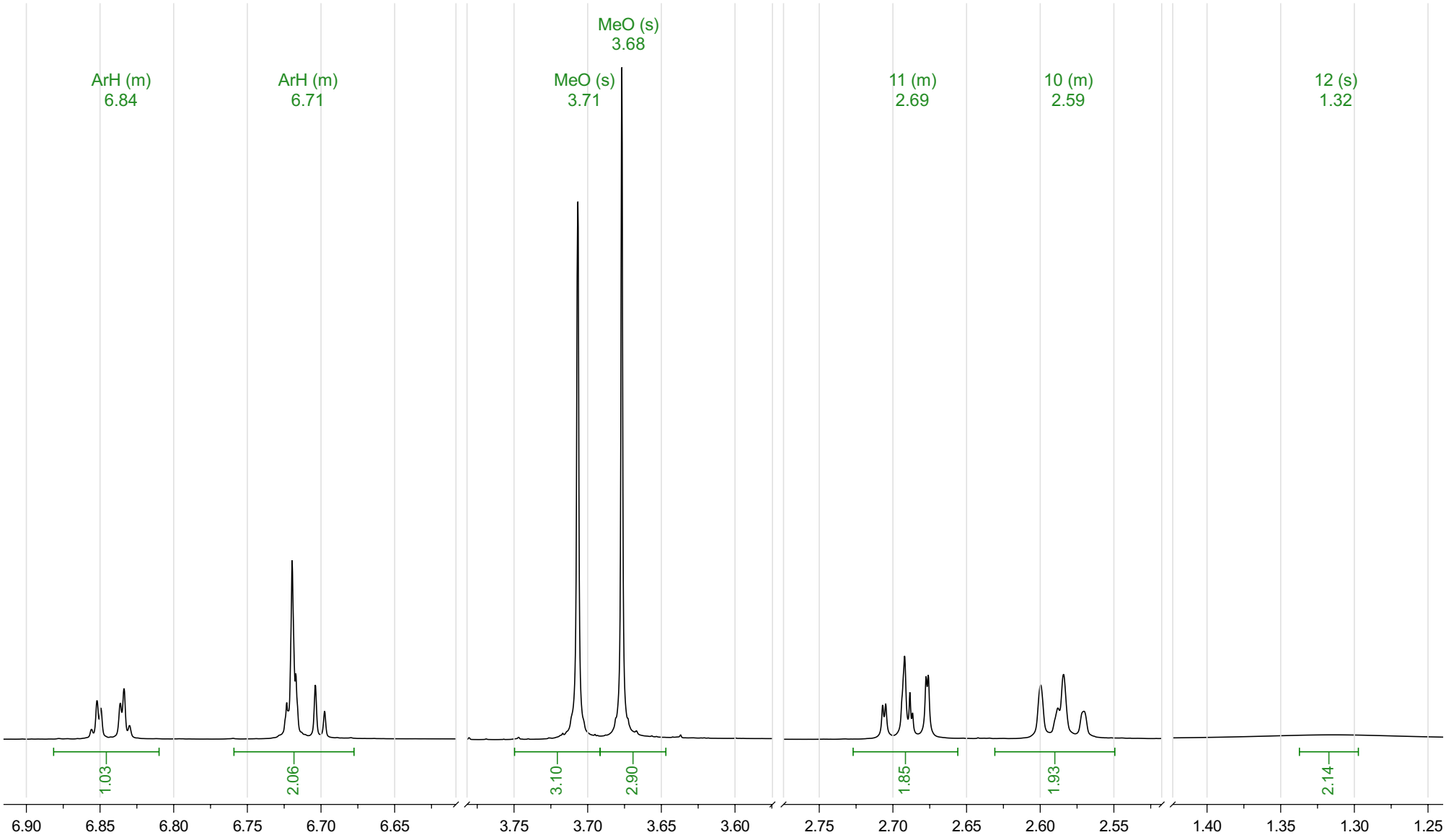
^{1}H NMR (700 MHz, DMSO-d_6) δ 8.10 (s, 3H), 7.26 – 7.15 (m, 5H), 3.66 (t, J = 7.6 Hz, 2H), 3.13 (t, J = 7.6 Hz, 2H).



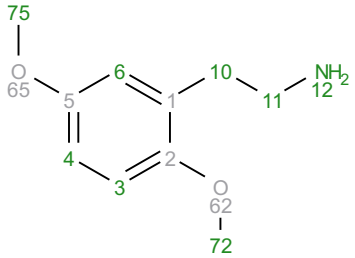
Analyte	P1: 2C-H freebase
Acquisition Date	2013-01-17T02:00:25
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



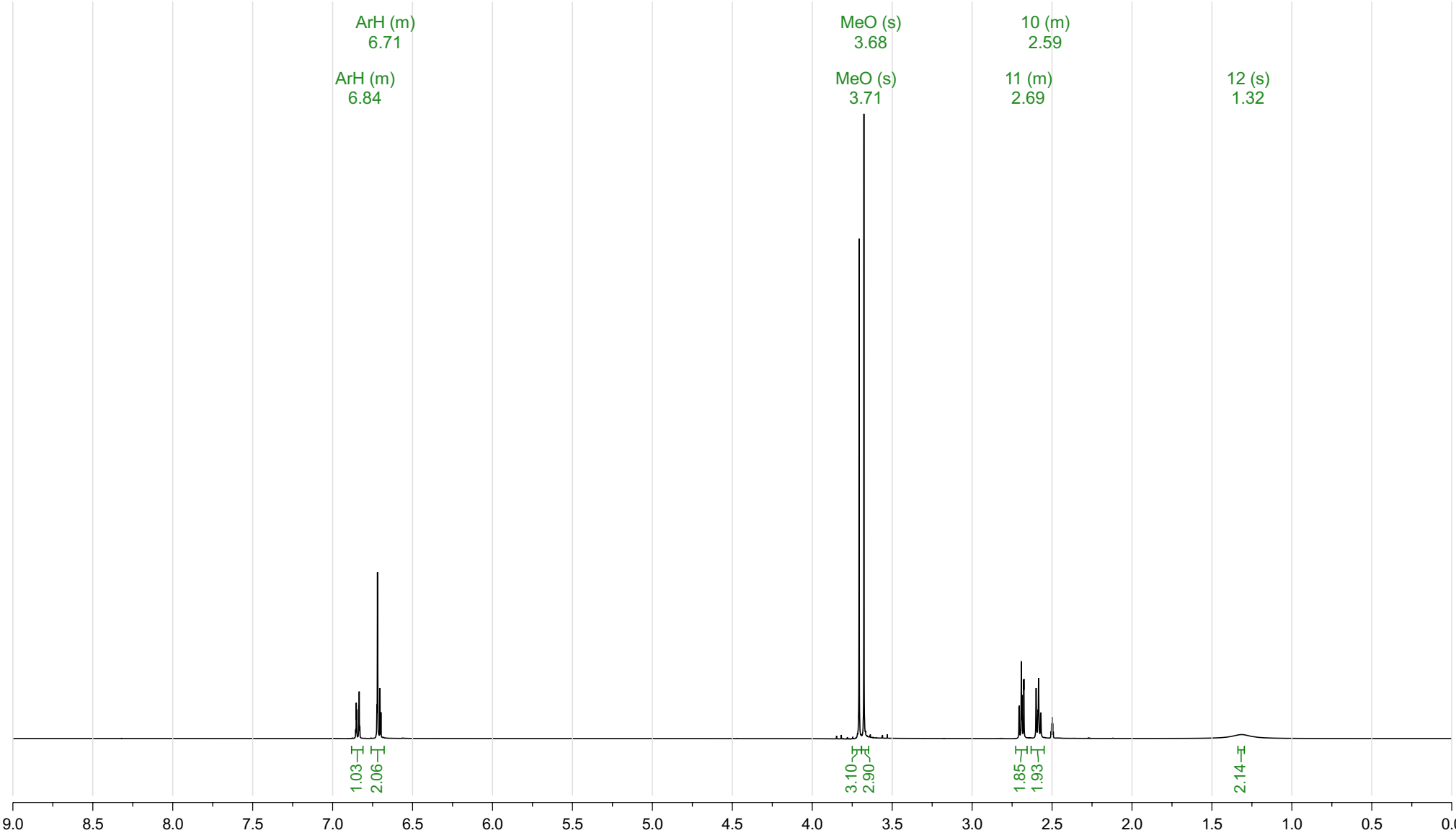
^{1}H NMR (500 MHz, DMSO-d_6) δ 6.88 – 6.81 (m, 1H), 6.76 – 6.68 (m, 2H), 3.71 (s, 3H), 3.68 (s, 3H), 2.73 – 2.66 (m, 2H), 2.63 – 2.55 (m, 2H), 1.32 (s, 2H).



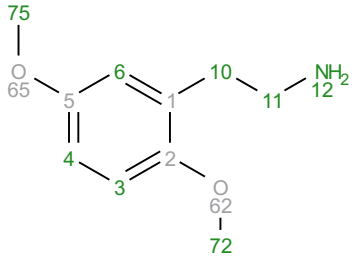
Analyte	P1: 2C-H freebase
Acquisition Date	2013-01-17T02:00:25
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



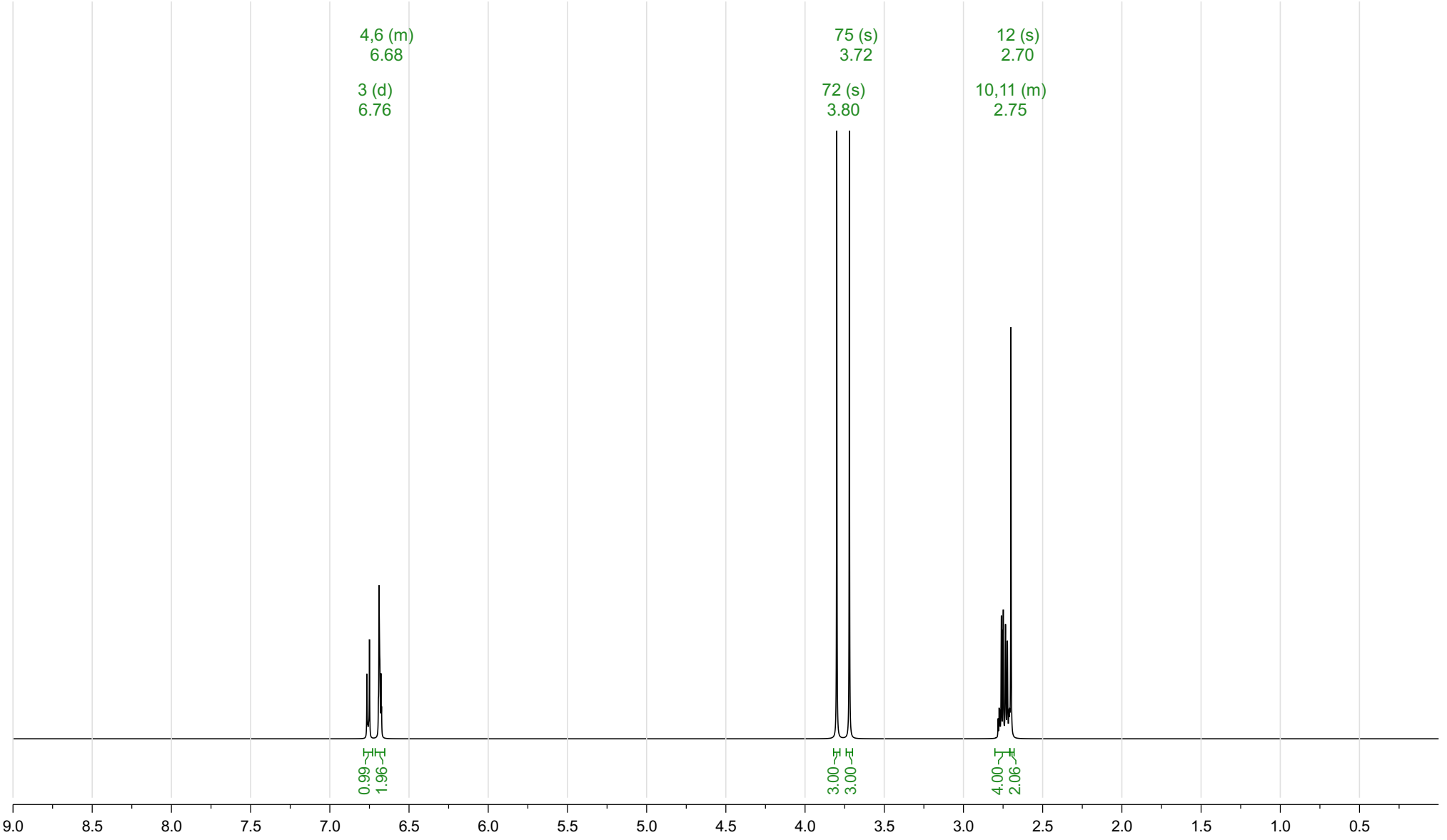
^{1}H NMR (500 MHz, DMSO-d_6) δ 6.88 – 6.81 (m, 1H), 6.76 – 6.68 (m, 2H), 3.71 (s, 3H), 3.68 (s, 3H), 2.73 – 2.66 (m, 2H), 2.63 – 2.55 (m, 2H), 1.32 (s, 2H).



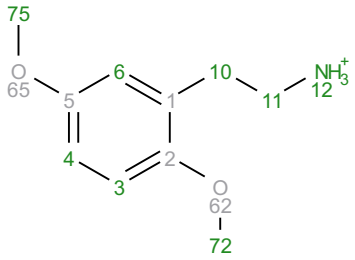
Prediction	2C-H freebase
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



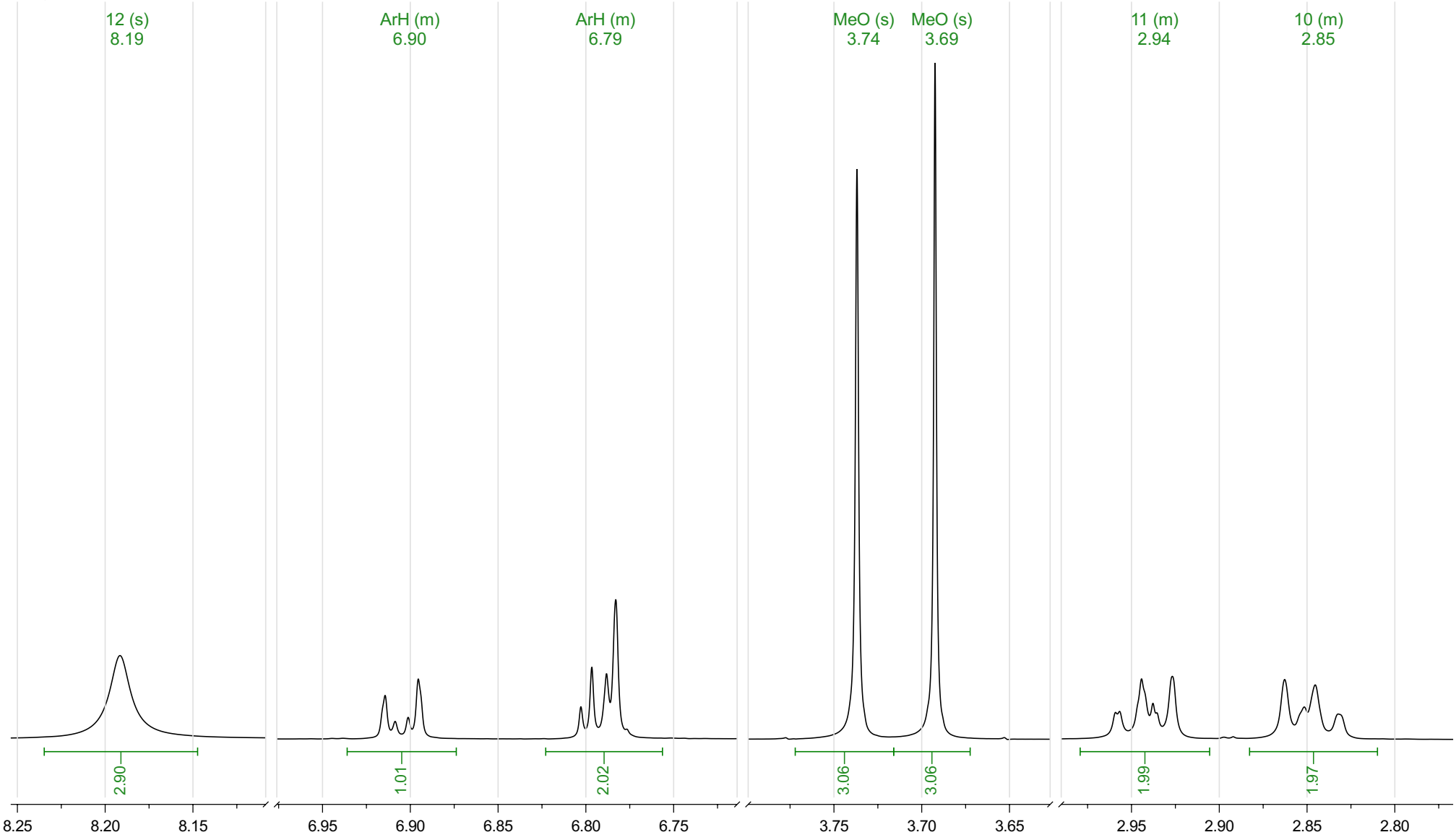
^{1}H NMR (500 MHz, DMSO-d_6) δ 6.76 (d, J = 7.9 Hz, 1H), 6.71 – 6.65 (m, 2H), 3.80 (s, 3H), 3.72 (s, 3H), 2.80 – 2.69 (m, 4H), 2.70 (s, 2H).



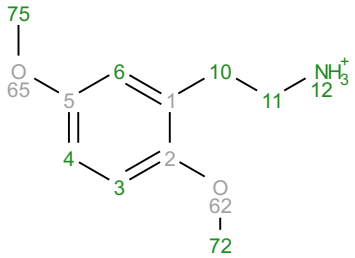
Analyte	P1 HCl: 2C-H H+
Acquisition Date	2013-11-08T20:55:22
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	1
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	36058



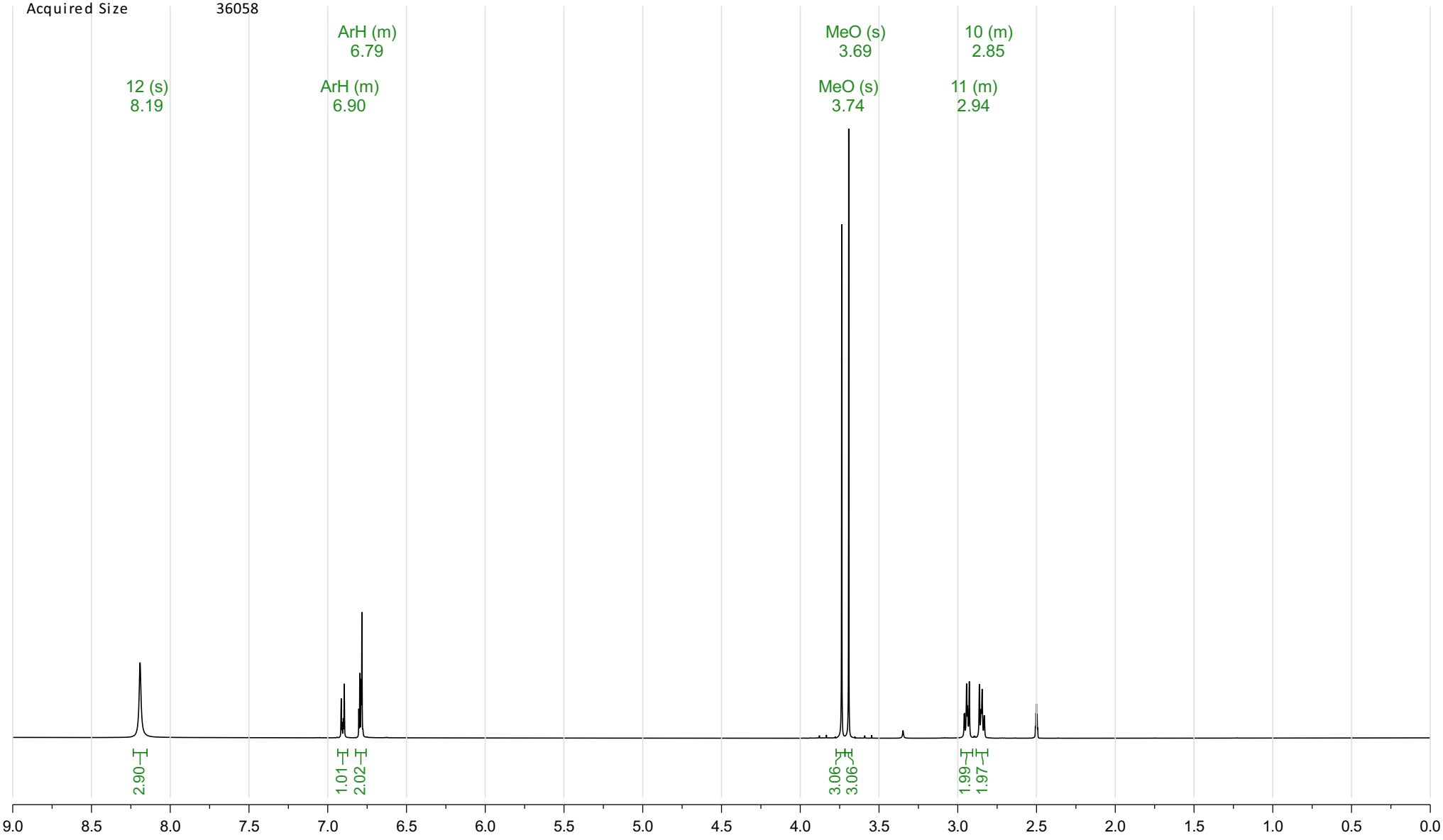
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.19 (s, 3H), 6.94 – 6.87 (m, 1H), 6.82 – 6.76 (m, 2H), 3.74 (s, 3H), 3.69 (s, 3H), 2.98 – 2.91 (m, 2H), 2.88 – 2.81 (m, 2H).



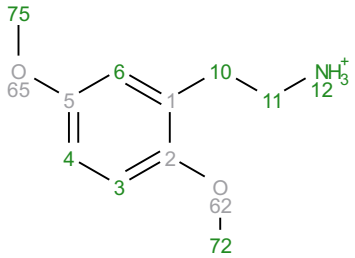
Analyte	P1 HCl: 2C-H H+
Acquisition Date	2013-11-08T20:55:22
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	1
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	36058



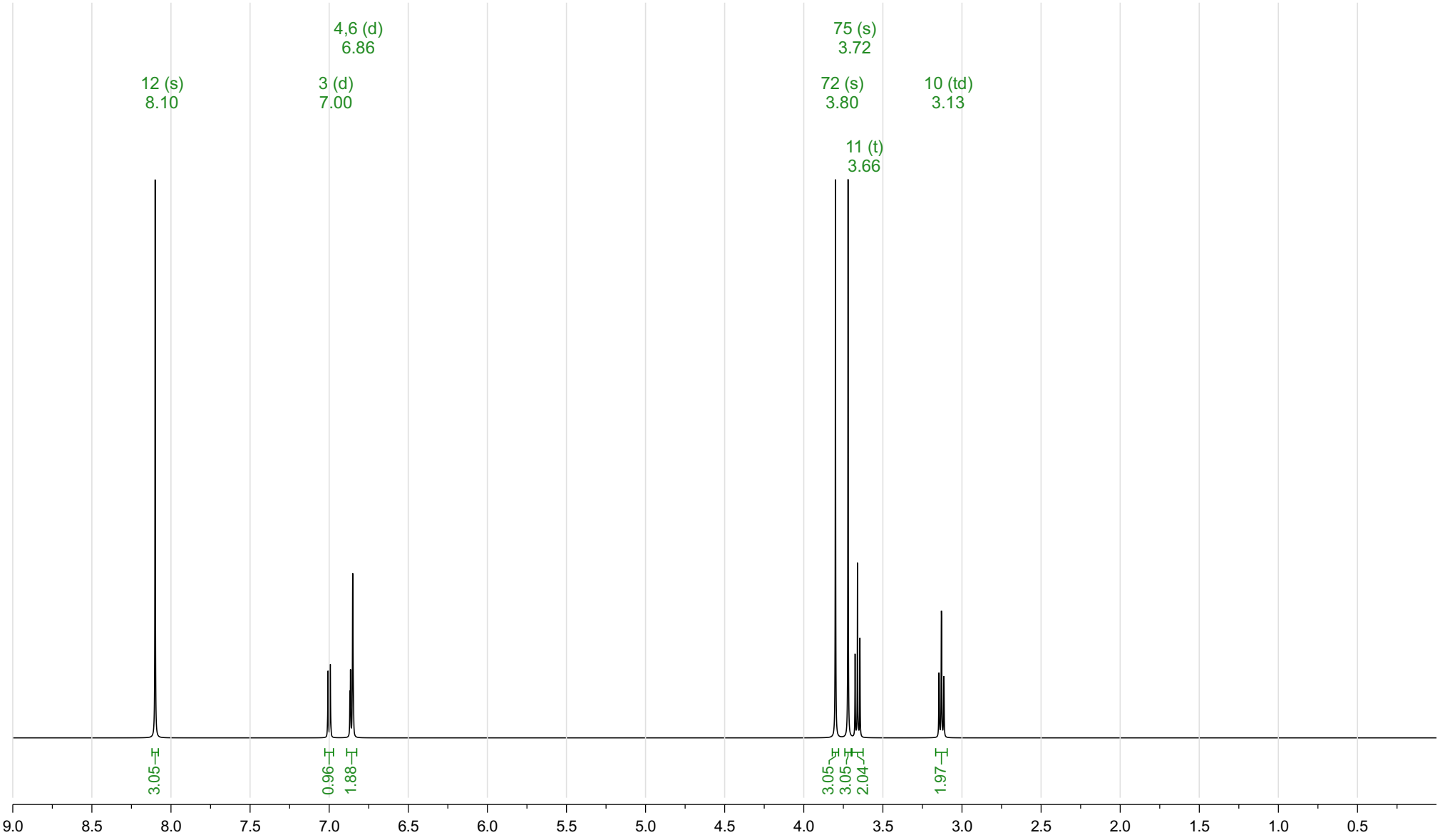
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.19 (s, 3H), 6.94 – 6.87 (m, 1H), 6.82 – 6.76 (m, 2H), 3.74 (s, 3H), 3.69 (s, 3H), 2.98 – 2.91 (m, 2H), 2.88 – 2.81 (m, 2H).



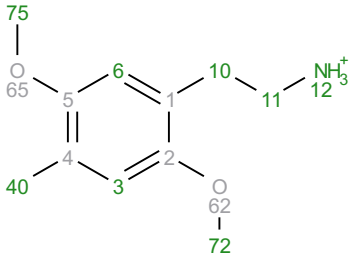
Prediction	2C-H H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



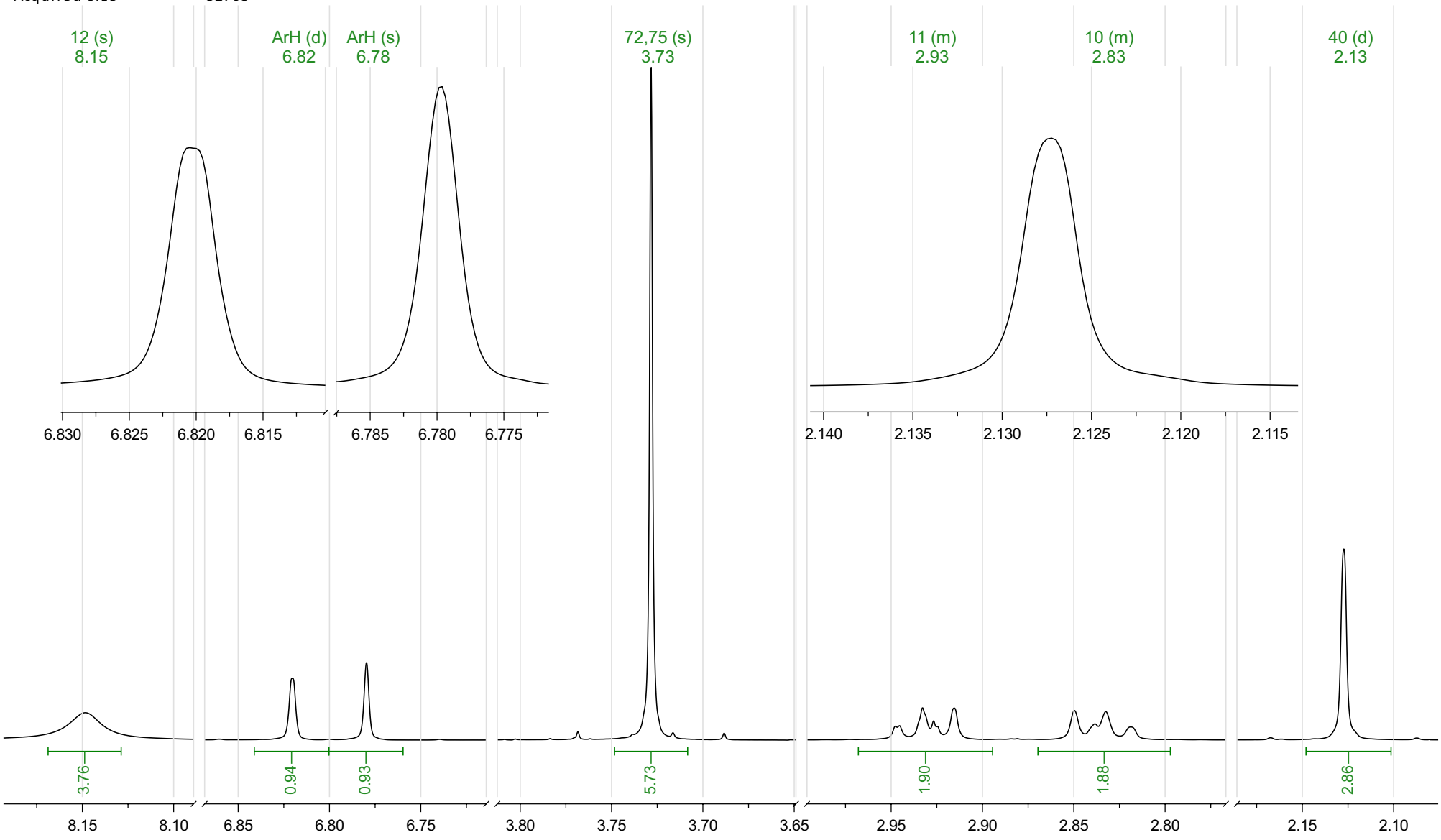
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.10 (s, 3H), 7.00 (d, J = 7.2 Hz, 1H), 6.86 (d, J = 7.0 Hz, 2H), 3.80 (s, 3H), 3.72 (s, 3H), 3.66 (t, J = 7.6 Hz, 2H), 3.13 (td, J = 7.7, 0.9 Hz, 2H).



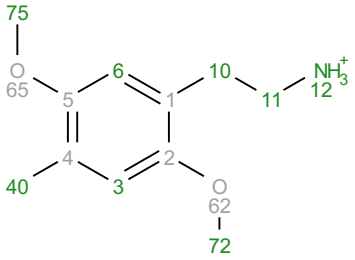
Analyte	P2: 2C-D H+
Acquisition Date	2012-11-20T16:56:00
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



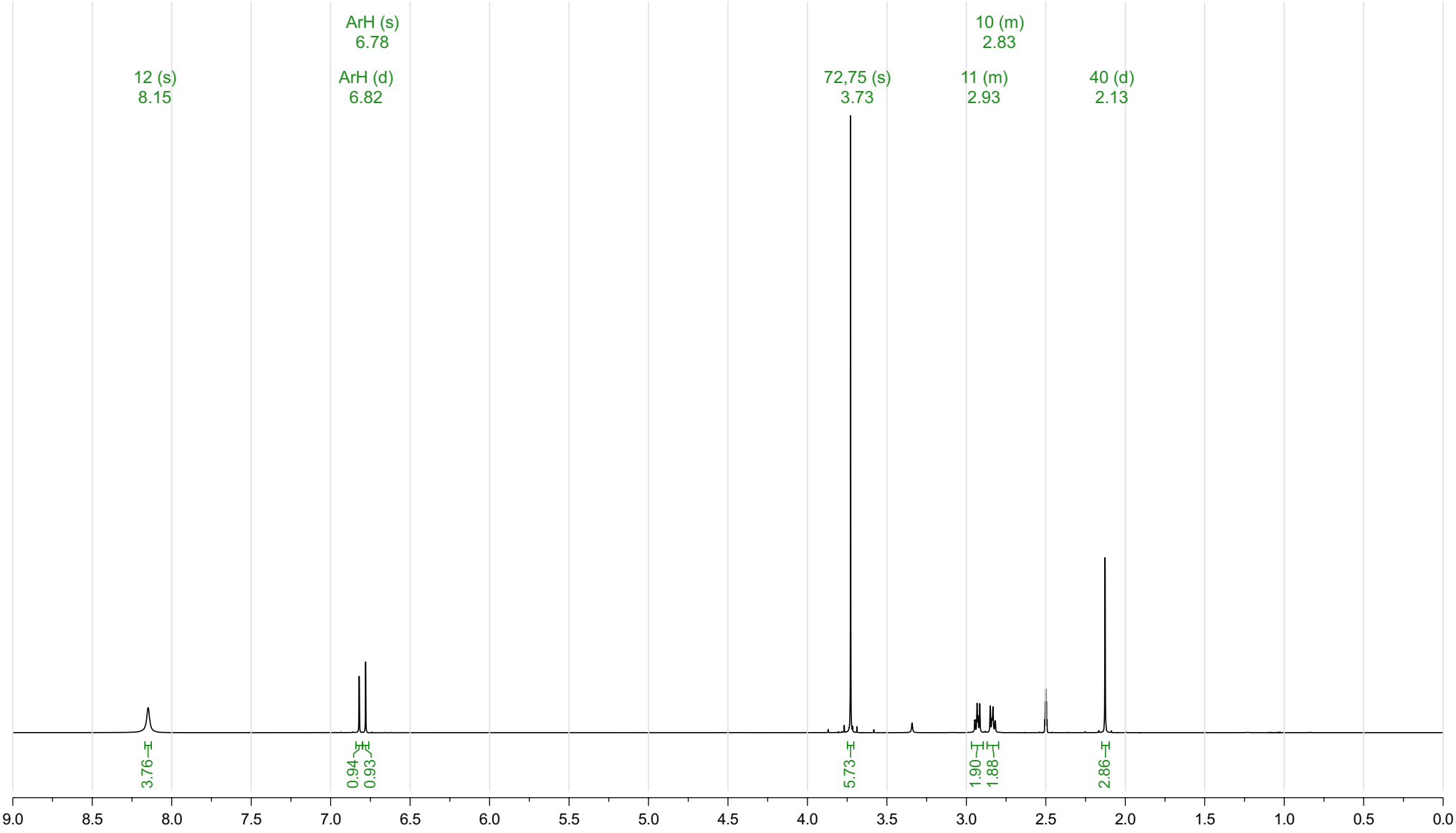
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.15 (s, 3H), 6.82 (d, J = 0.8 Hz, 1H), 6.78 (s, 1H), 3.73 (s, 6H), 2.97 – 2.89 (m, 2H), 2.87 – 2.80 (m, 2H), 2.13 (d, J = 0.7 Hz, 3H).



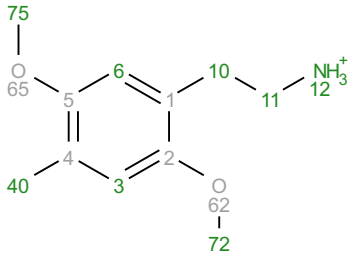
Analyte	P2: 2C-D H+
Acquisition Date	2012-11-20T16:56:00
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



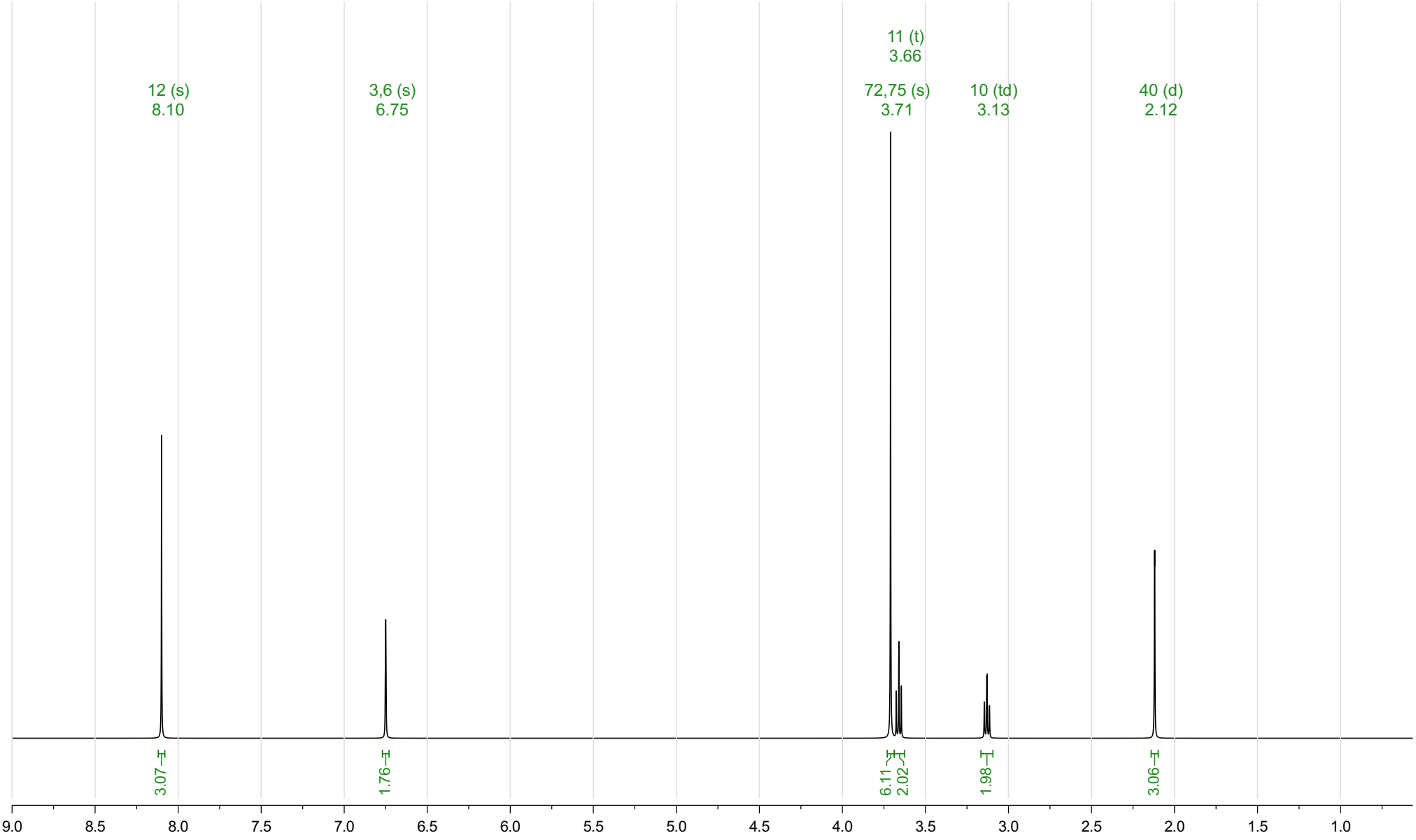
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.15 (s, 3H), 6.82 (d, J = 0.8 Hz, 1H), 6.78 (s, 1H), 3.73 (s, 6H), 2.97 – 2.89 (m, 2H), 2.87 – 2.80 (m, 2H), 2.13 (d, J = 0.7 Hz, 3H).



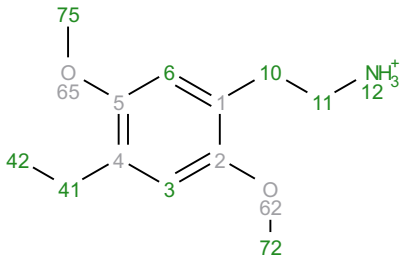
Prediction	2C-D H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



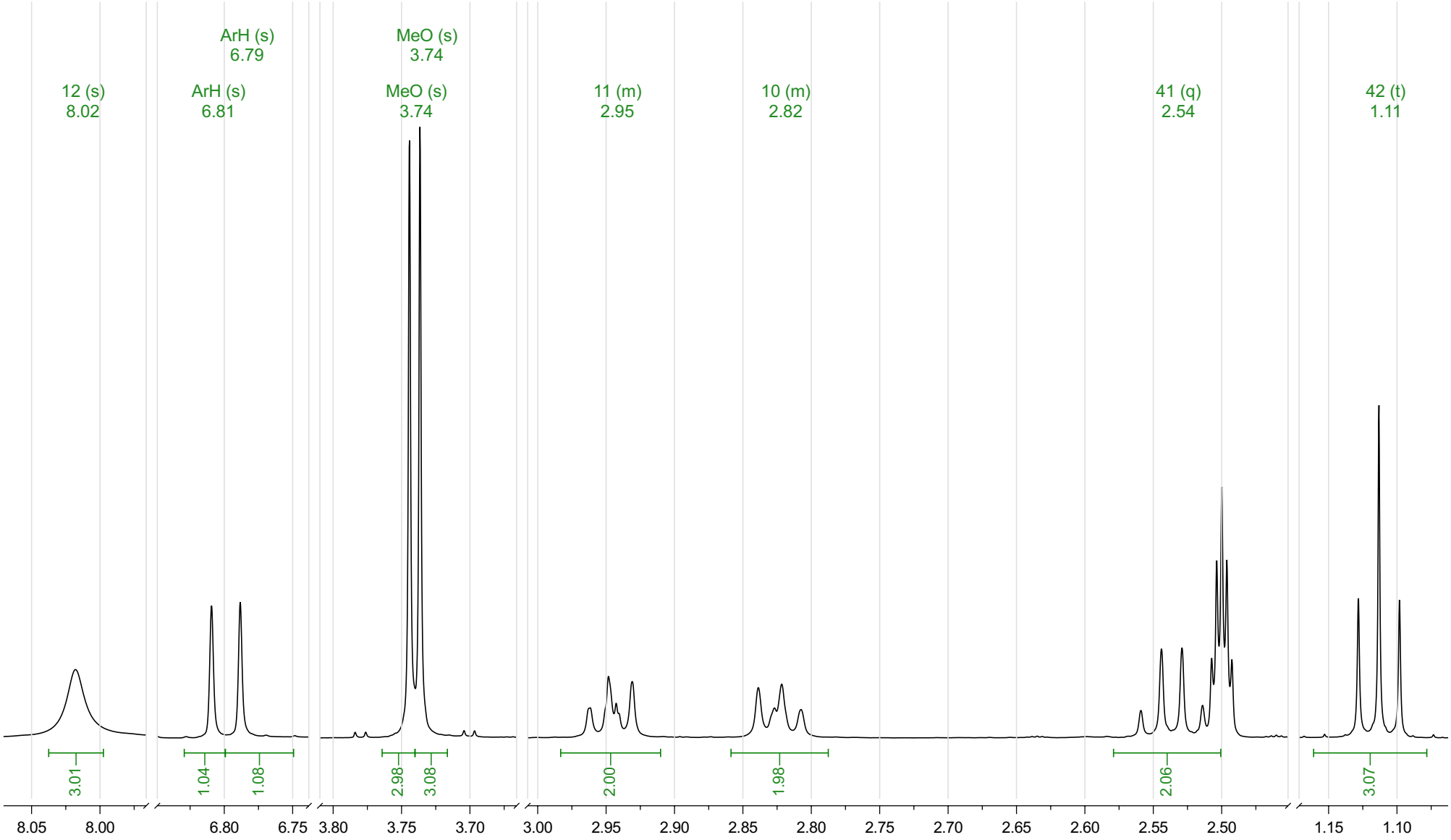
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.10 (s, 3H), 6.75 (s, 2H), 3.71 (s, 6H), 3.66 (t, J = 7.6 Hz, 2H), 3.13 (td, J = 7.6, 1.0 Hz, 2H), 2.12 (d, J = 1.1 Hz, 3H).



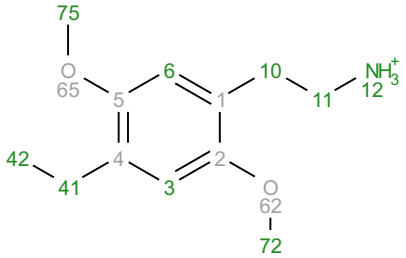
Analyte	P3: 2C-E H+
Acquisition Date	2012-11-24T13:37:16
Solvent	dmso
Temperature	25
Number of Scans	1
Relaxation Delay	1
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



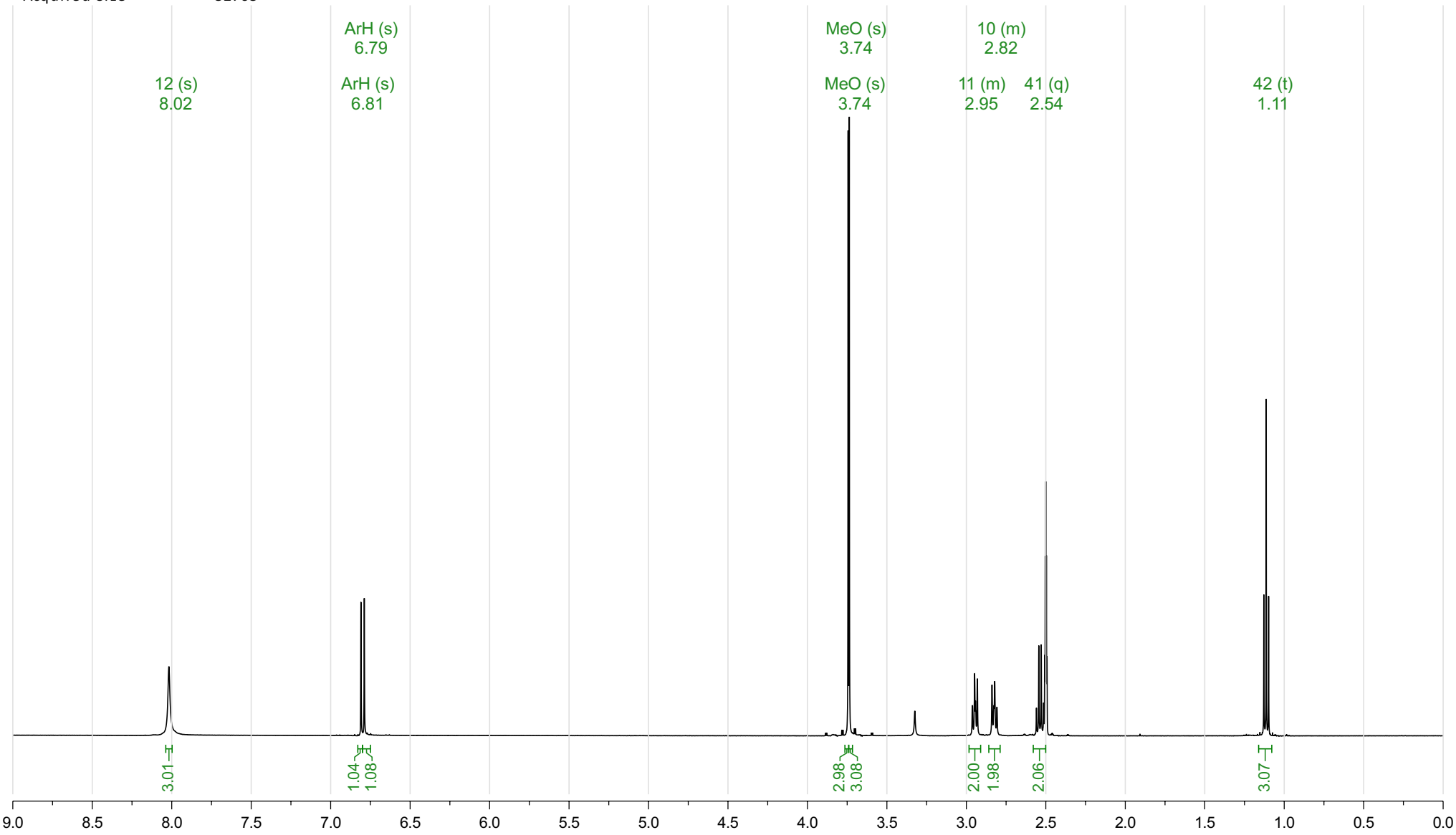
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.02 (s, 3H), 6.81 (s, 1H), 6.79 (s, 1H), 3.74 (s, 3H), 3.74 (s, 3H), 3.00 – 2.91 (m, 2H), 2.86 – 2.79 (m, 2H), 2.54 (q, J = 7.5 Hz, 2H), 1.11 (t, J = 7.5 Hz, 3H).



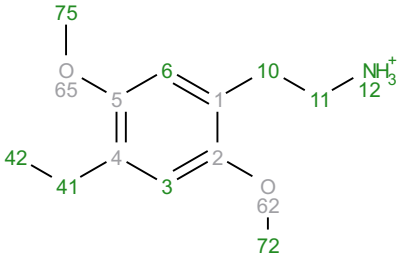
Analyte	P3: 2C-E H+
Acquisition Date	2012-11-24T13:37:16
Solvent	dmso
Temperature	25
Number of Scans	1
Relaxation Delay	1
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



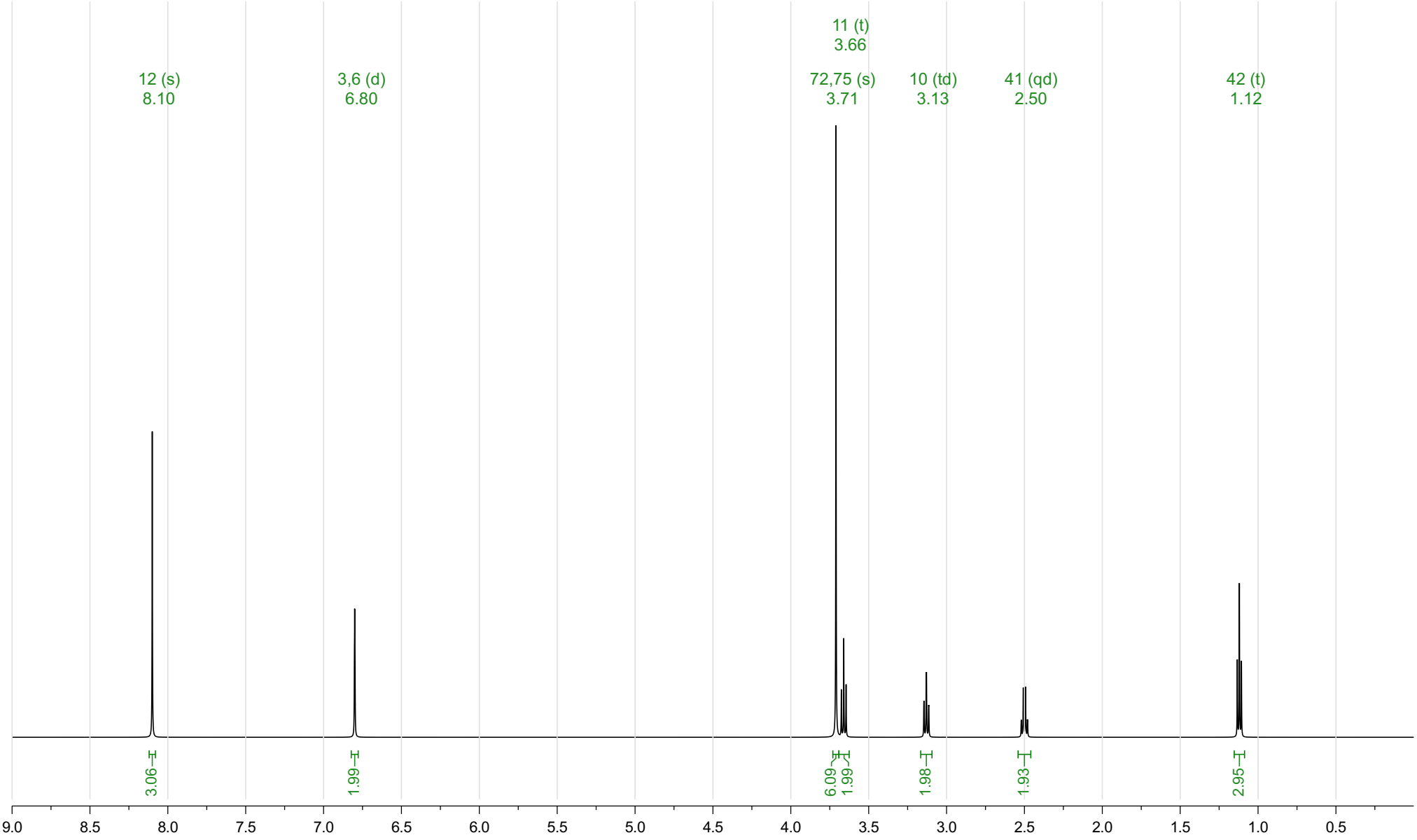
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.02 (s, 3H), 6.81 (s, 1H), 6.79 (s, 1H), 3.74 (s, 3H), 3.74 (s, 3H), 3.00 – 2.91 (m, 2H), 2.86 – 2.79 (m, 2H), 2.54 (q, J = 7.5 Hz, 2H), 1.11 (t, J = 7.5 Hz, 3H).



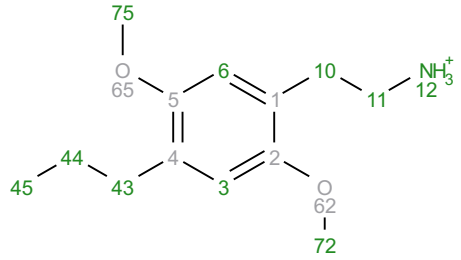
Prediction	2C-E H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



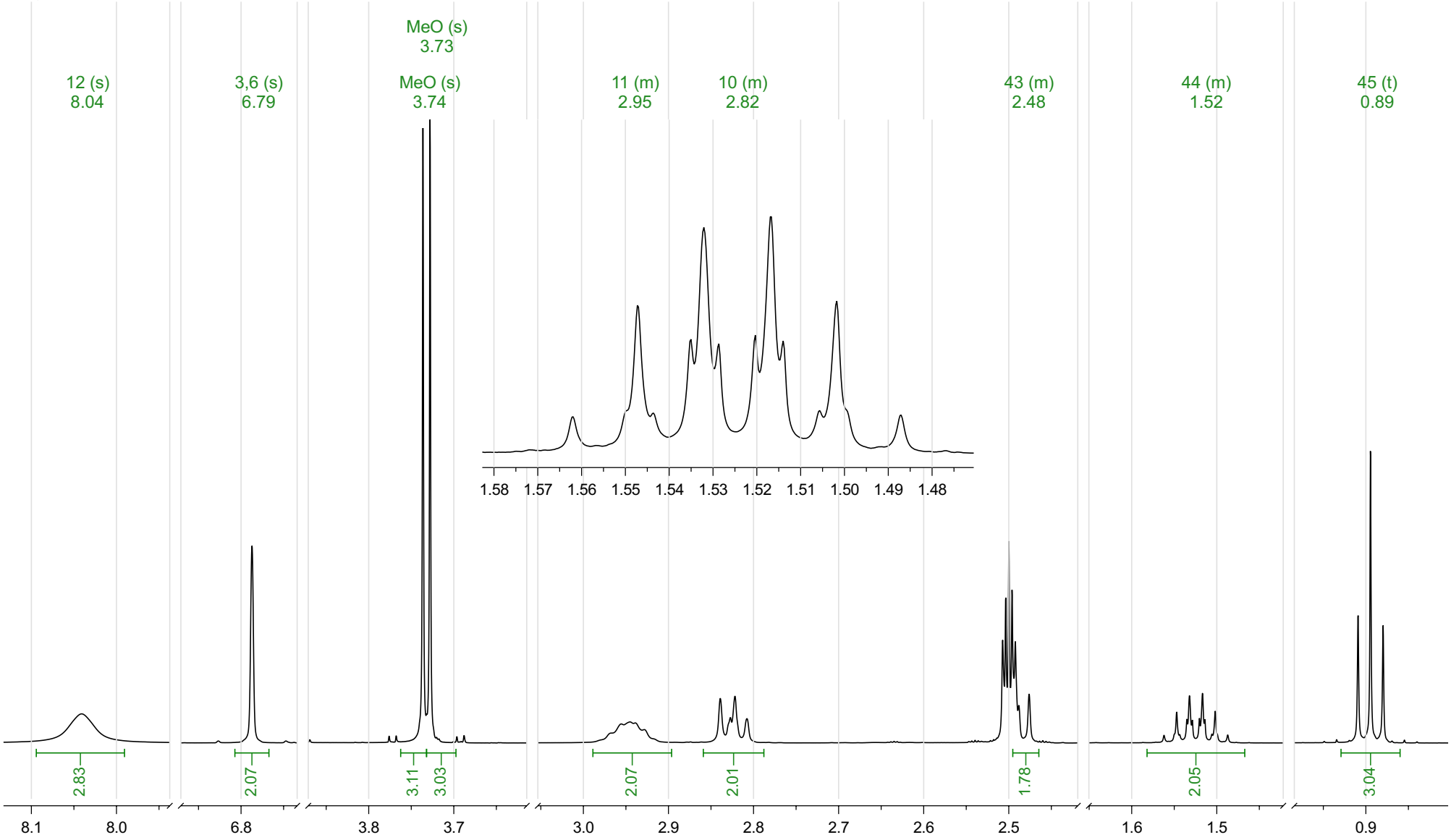
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.10 (s, 3H), 6.80 (d, J = 1.2 Hz, 2H), 3.71 (s, 6H), 3.66 (t, J = 7.6 Hz, 2H), 3.13 (td, J = 7.6, 1.0 Hz, 2H), 2.50 (qd, J = 6.6, 1.0 Hz, 2H), 1.12 (t, J = 6.6 Hz, 3H).



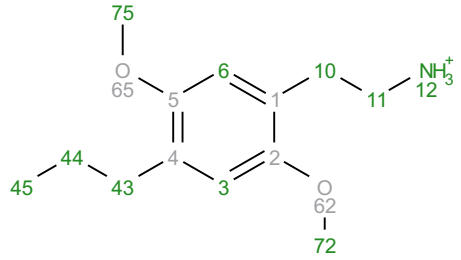
Analyte	P4: 2C-P H+
Acquisition Date	2012-11-24T13:58:43
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



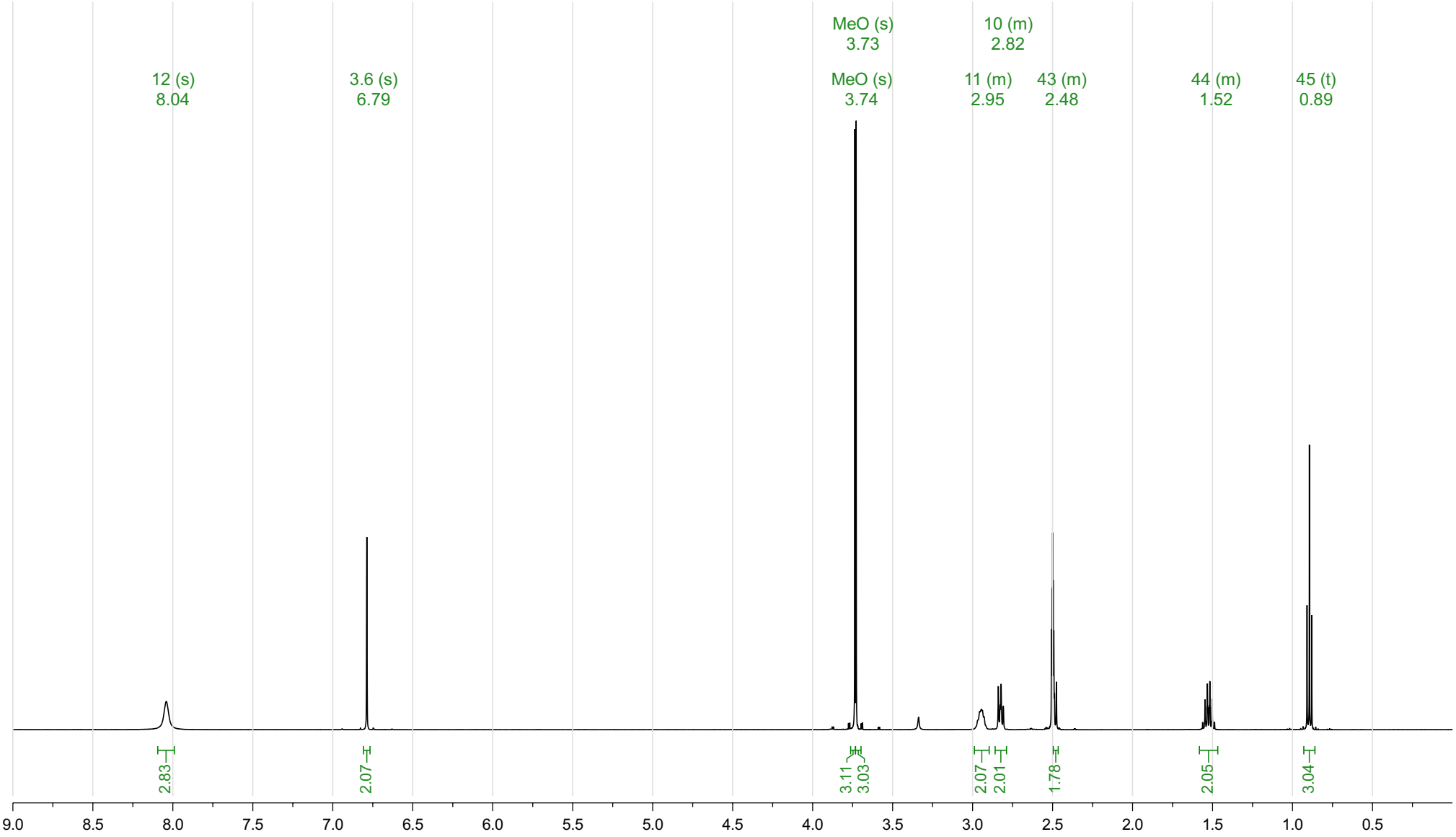
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.04 (s, 3H), 6.79 (s, 2H), 3.74 (s, 3H), 3.73 (s, 3H), 2.99 – 2.90 (m, 2H), 2.86 – 2.79 (m, 2H), 2.51 – 2.45 (m, 2H), 1.60 – 1.45 (m, 2H), 0.89 (t, J = 7.4 Hz, 3H).



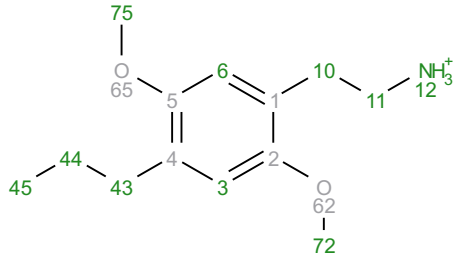
Analyte	P4: 2C-P H+
Acquisition Date	2012-11-24T13:58:43
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



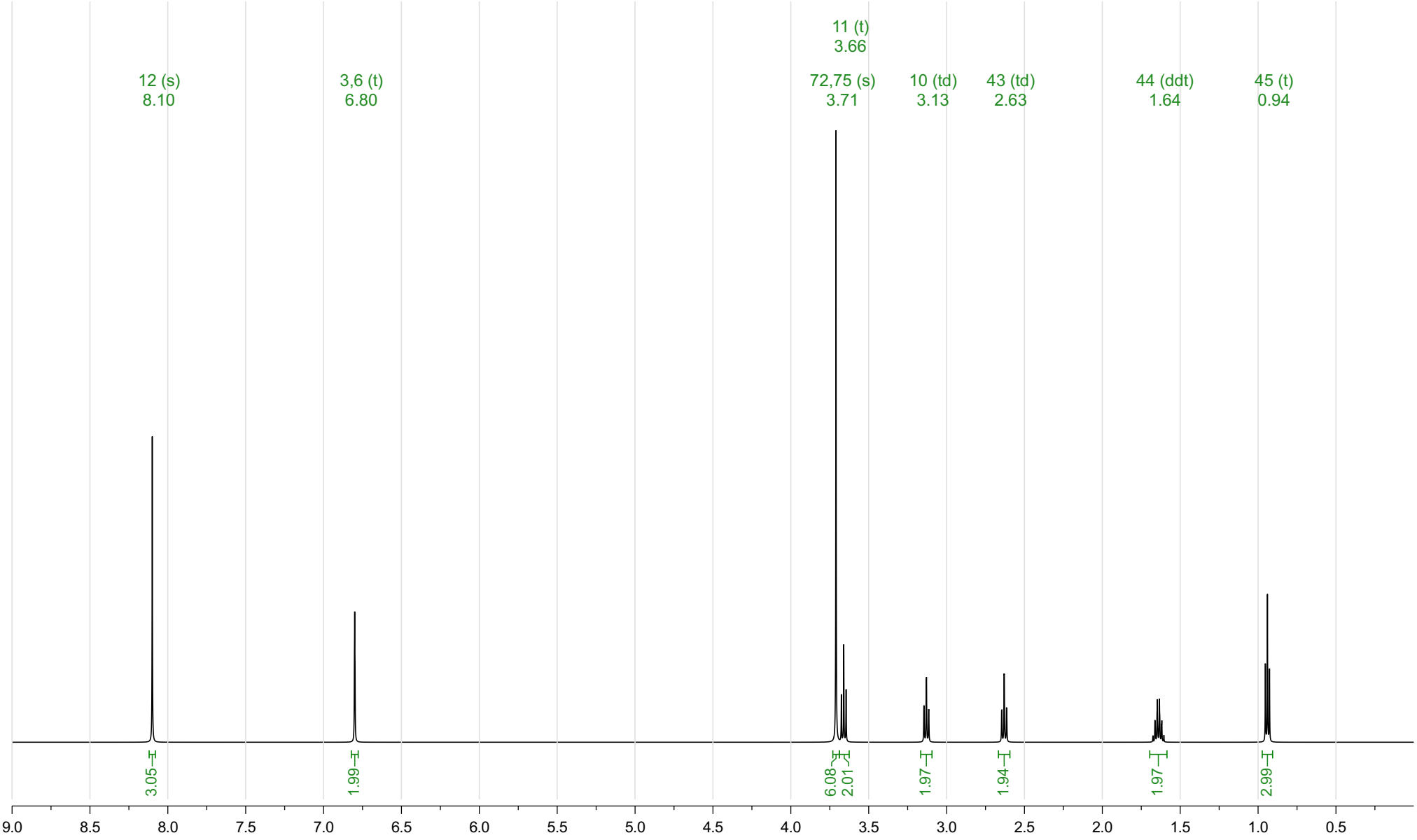
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.04 (s, 3H), 6.79 (s, 2H), 3.74 (s, 3H), 3.73 (s, 3H), 2.99 – 2.90 (m, 2H), 2.86 – 2.79 (m, 2H), 2.51 – 2.45 (m, 2H), 1.60 – 1.45 (m, 2H), 0.89 (t, J = 7.4 Hz, 3H).



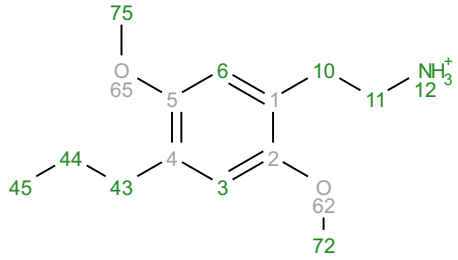
Prediction	2C-P H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



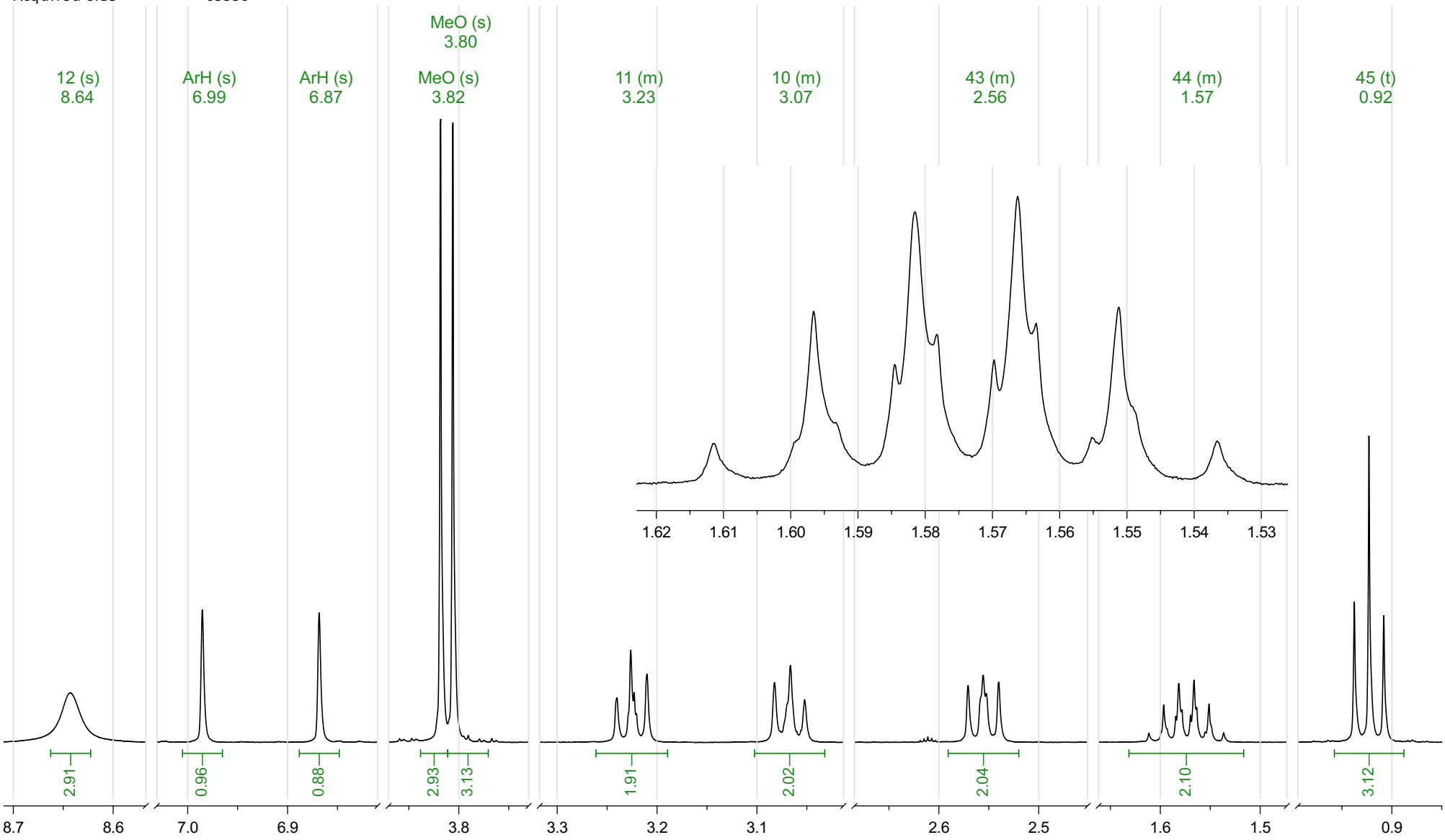
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.10 (s, 3H), 6.80 (t, J = 1.0 Hz, 2H), 3.71 (s, 6H), 3.66 (t, J = 7.6 Hz, 2H), 3.13 (td, J = 7.6, 1.0 Hz, 2H), 2.63 (td, J = 7.9, 1.1 Hz, 2H), 1.64 (ddt, J = 14.4, 7.8, 6.6 Hz, 2H), 0.94 (t, J = 6.6 Hz, 3H).



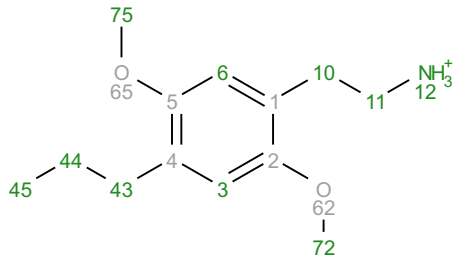
Analyte	P4 in DMF: 2C-P H+
Acquisition Date	2013-05-07T20:17:09
Solvent	dmf
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	10000.0
Nucleus	1H
Acquired Size	65536



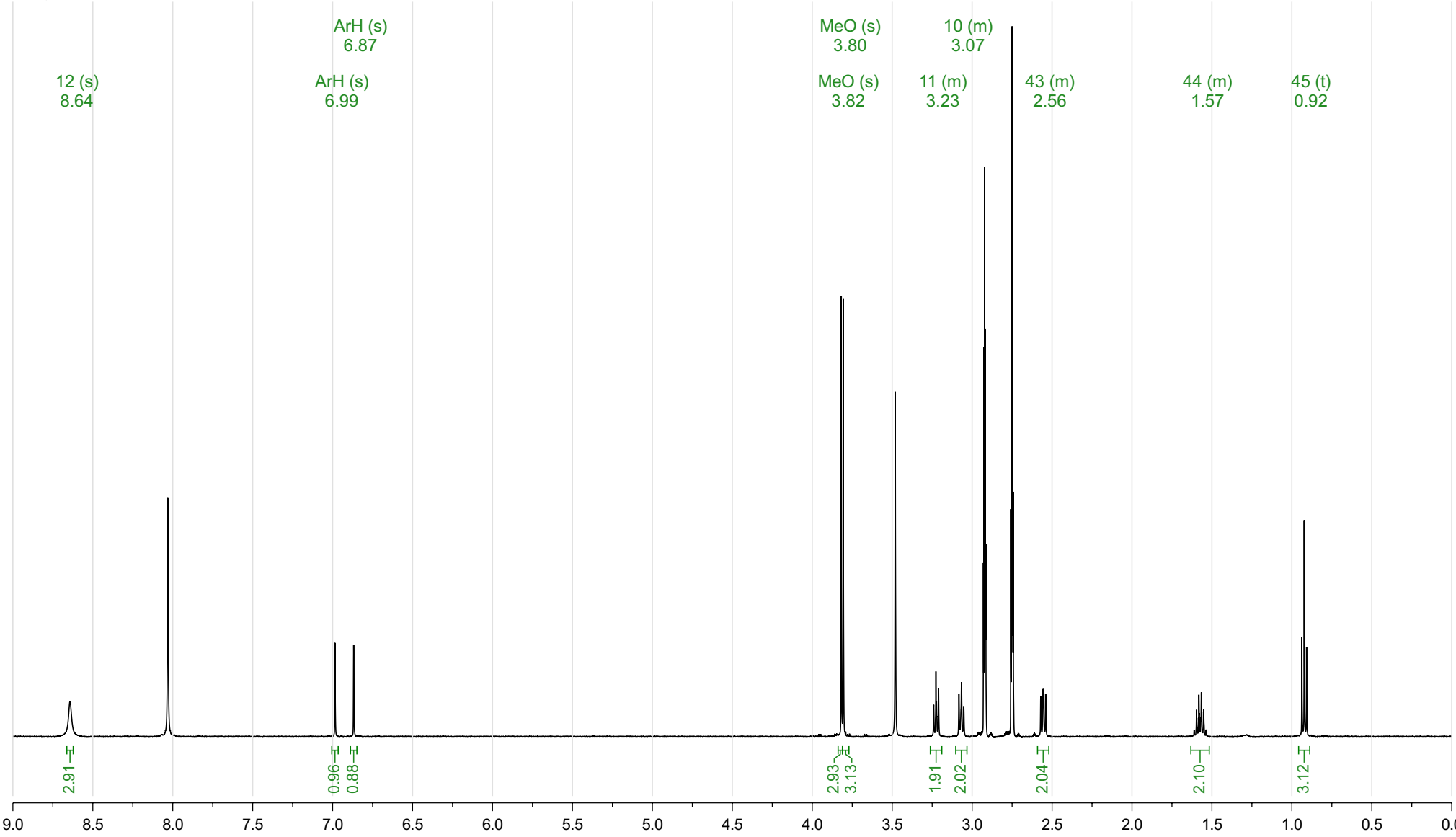
^{1}H NMR (500 MHz, DMF-d_7) δ 8.64 (s, 3H), 6.99 (s, 1H), 6.87 (s, 1H), 3.82 (s, 3H), 3.80 (s, 3H), 3.26 – 3.19 (m, 2H), 3.10 – 3.03 (m, 2H), 2.59 – 2.52 (m, 2H), 1.63 – 1.52 (m, 2H), 0.92 (t, J = 7.4 Hz, 3H).



Analyte	P4 in DMF: 2C-P H+
Acquisition Date	2013-05-07T20:17:09
Solvent	dmf
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	10000.0
Nucleus	1H
Acquired Size	65536



^{1}H NMR (500 MHz, DMF-d_7) δ 8.64 (s, 3H), 6.99 (s, 1H), 6.87 (s, 1H), 3.82 (s, 3H), 3.80 (s, 3H), 3.26 – 3.19 (m, 2H), 3.10 – 3.03 (m, 2H), 2.59 – 2.52 (m, 2H), 1.63 – 1.52 (m, 2H), 0.92 (t, J = 7.4 Hz, 3H).



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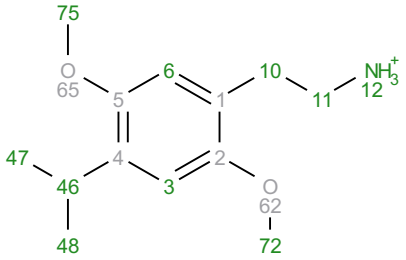
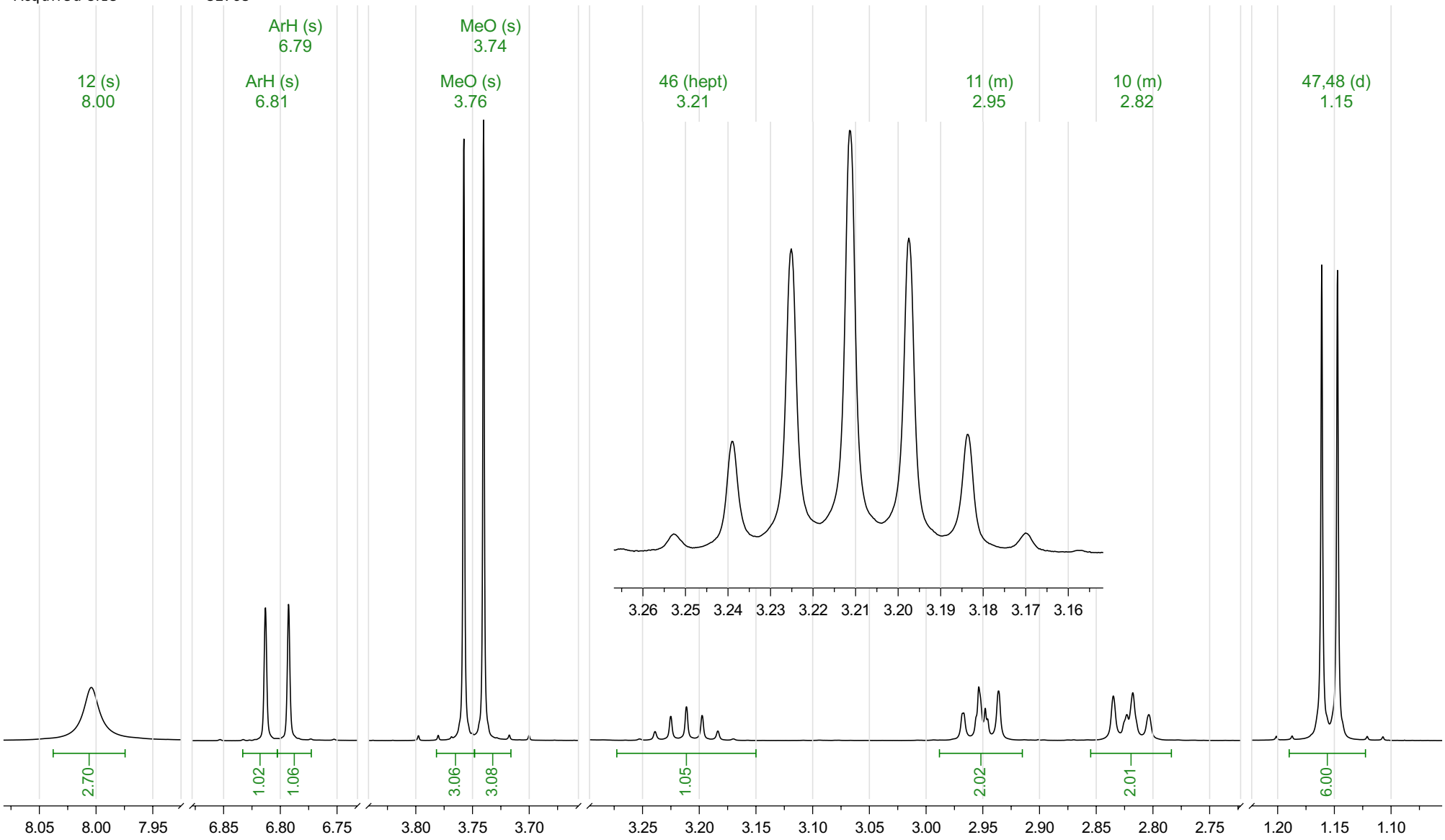
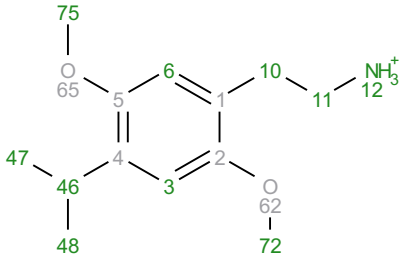
Analyte	P5: 2C-IP H+
Acquisition Date	2012-11-24T13:26:15
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



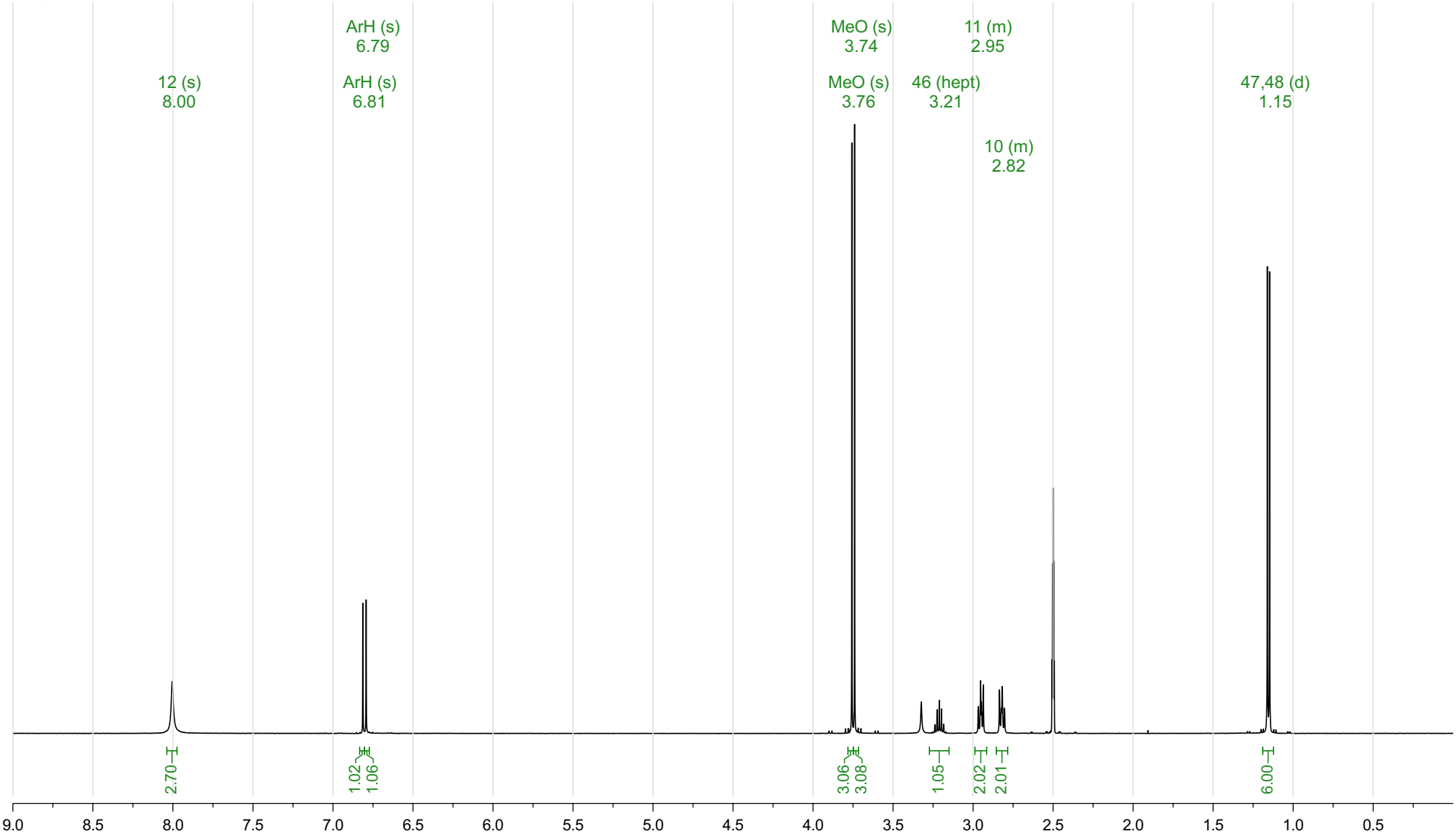
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.00 (s, 3H), 6.81 (s, 1H), 6.79 (s, 1H), 3.76 (s, 3H), 3.74 (s, 3H), 3.21 (hept, J = 6.9 Hz, 1H), 2.99 – 2.92 (m, 2H), 2.85 – 2.78 (m, 2H), 1.15 (d, J = 6.9 Hz, 6H).



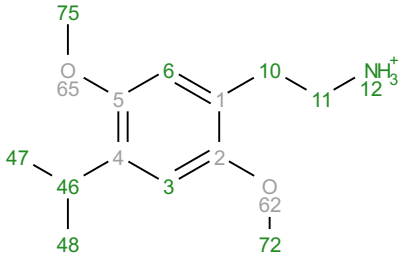
Analyte	P5: 2C-IP H+
Acquisition Date	2012-11-24T13:26:15
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



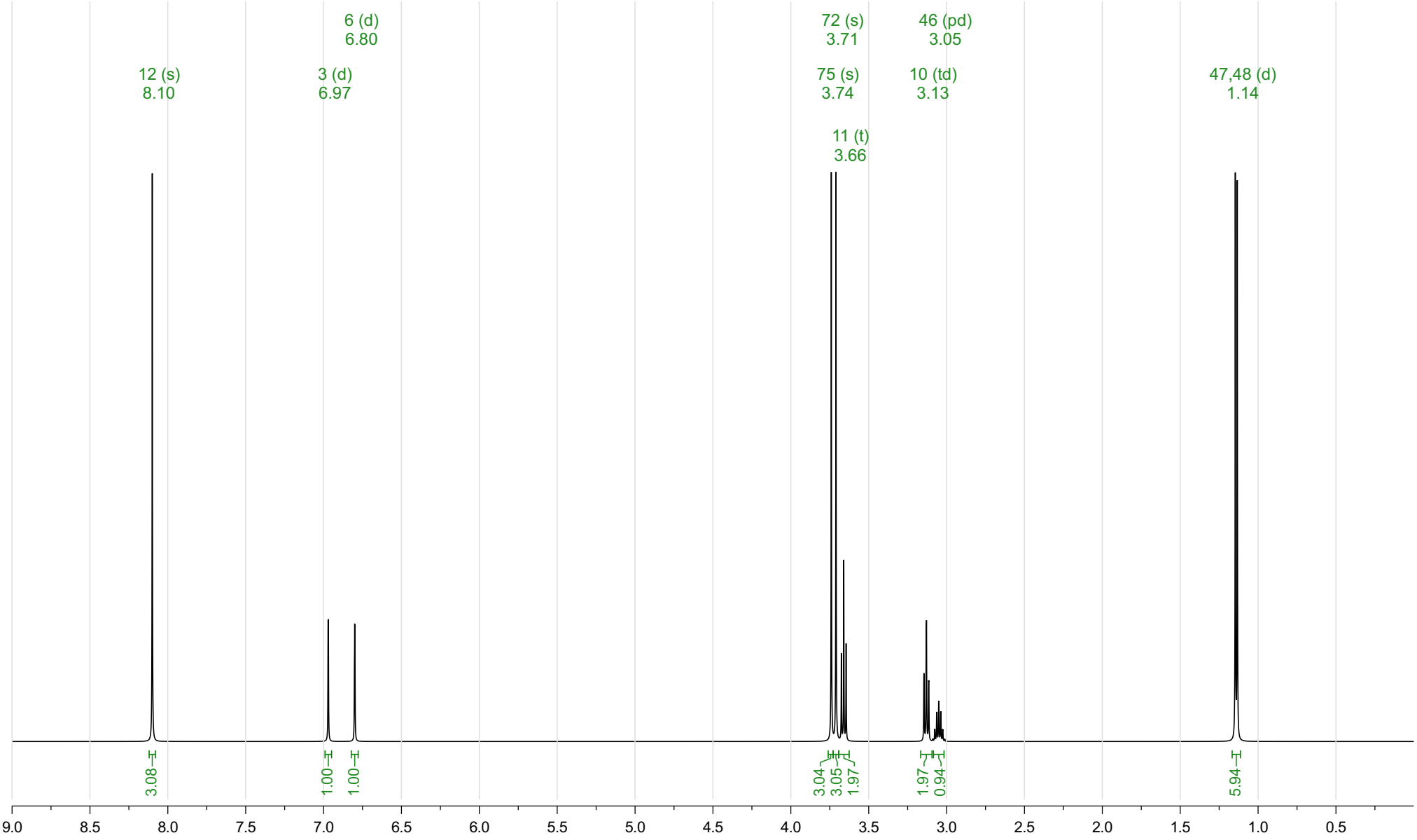
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.00 (s, 3H), 6.81 (s, 1H), 6.79 (s, 1H), 3.76 (s, 3H), 3.74 (s, 3H), 3.21 (hept, J = 6.9 Hz, 1H), 2.99 – 2.92 (m, 2H), 2.85 – 2.78 (m, 2H), 1.15 (d, J = 6.9 Hz, 6H).



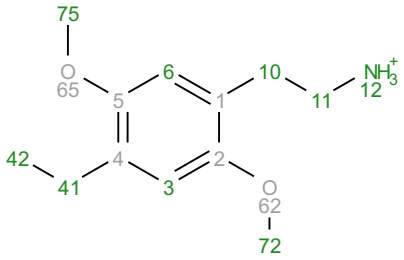
Prediction	2C-IP H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



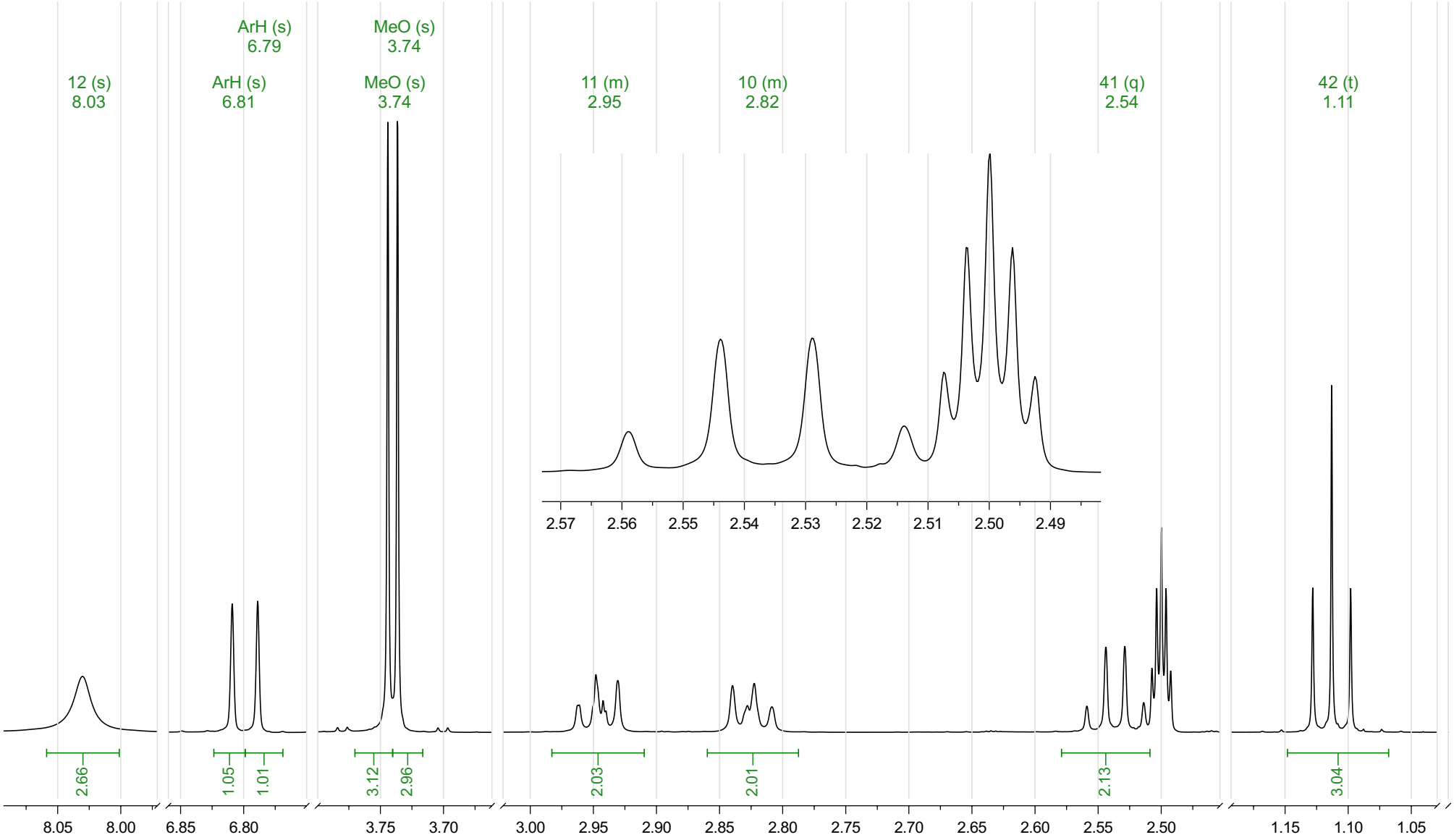
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.10 (s, 3H), 6.97 (d, J = 1.0 Hz, 1H), 6.80 (d, J = 1.1 Hz, 1H), 3.74 (s, 3H), 3.71 (s, 3H), 3.66 (t, J = 7.6 Hz, 2H), 3.13 (td, J = 7.6, 1.0 Hz, 2H), 3.05 (pd, J = 6.4, 1.0 Hz, 1H), 1.14 (d, J = 6.4 Hz, 6H).



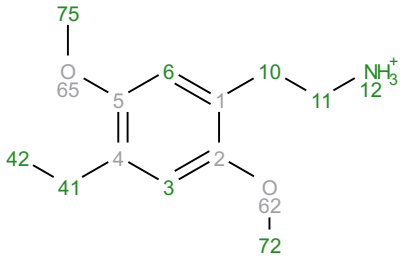
Analyte	P6a: 2C-E H+
Acquisition Date	2012-11-24T13:50:28
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



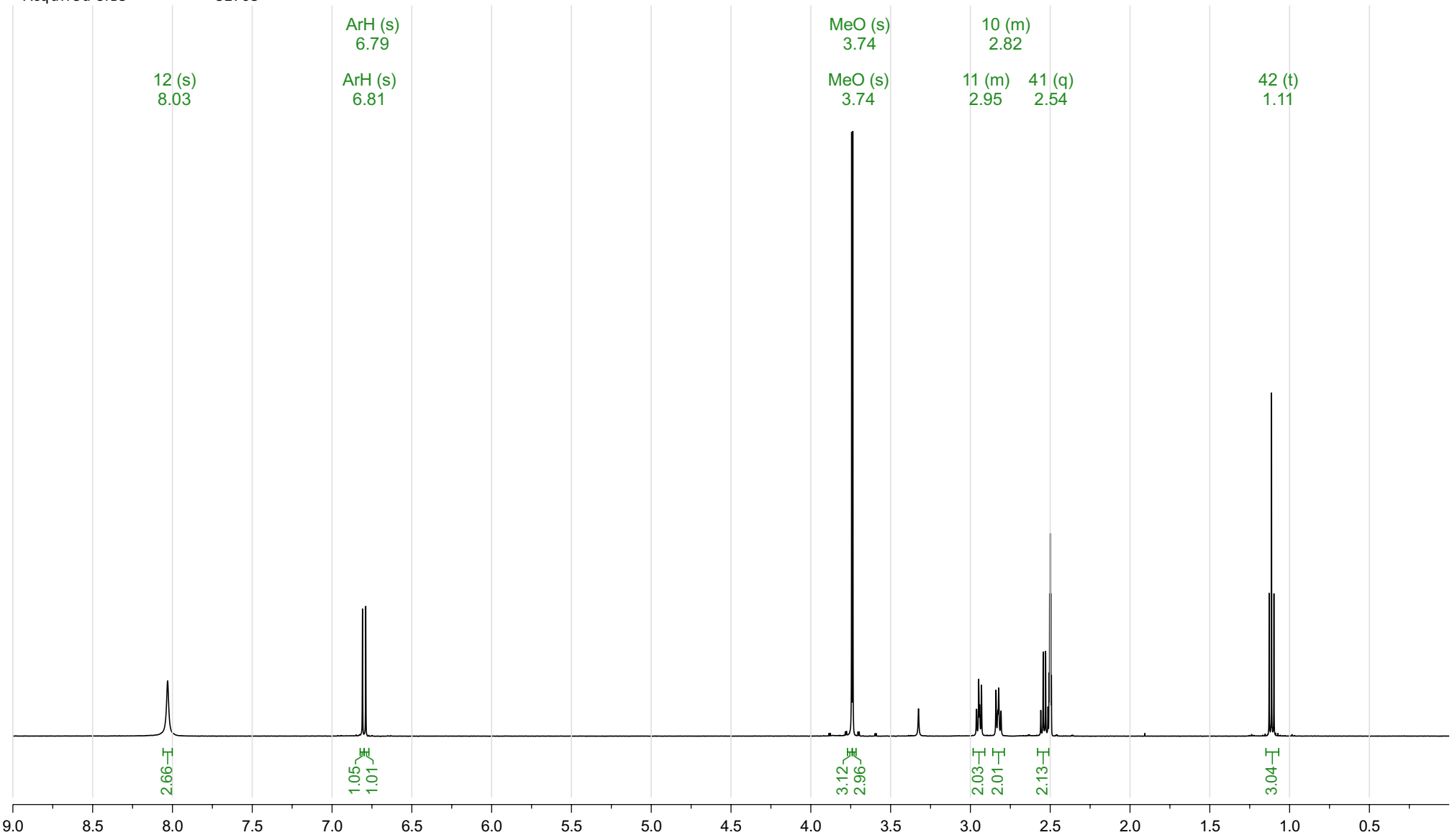
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.03 (s, 3H), 6.81 (s, 1H), 6.79 (s, 1H), 3.74 (s, 3H), 3.74 (s, 3H), 2.98 – 2.91 (m, 2H), 2.86 – 2.79 (m, 2H), 2.54 (q, J = 7.5 Hz, 2H), 1.11 (t, J = 7.5 Hz, 3H).



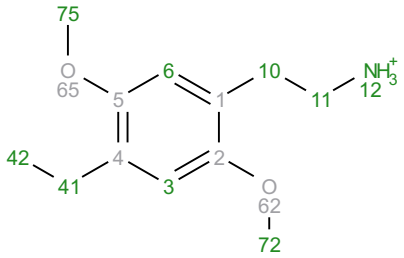
Analyte	P6a: 2C-E H+
Acquisition Date	2012-11-24T13:50:28
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



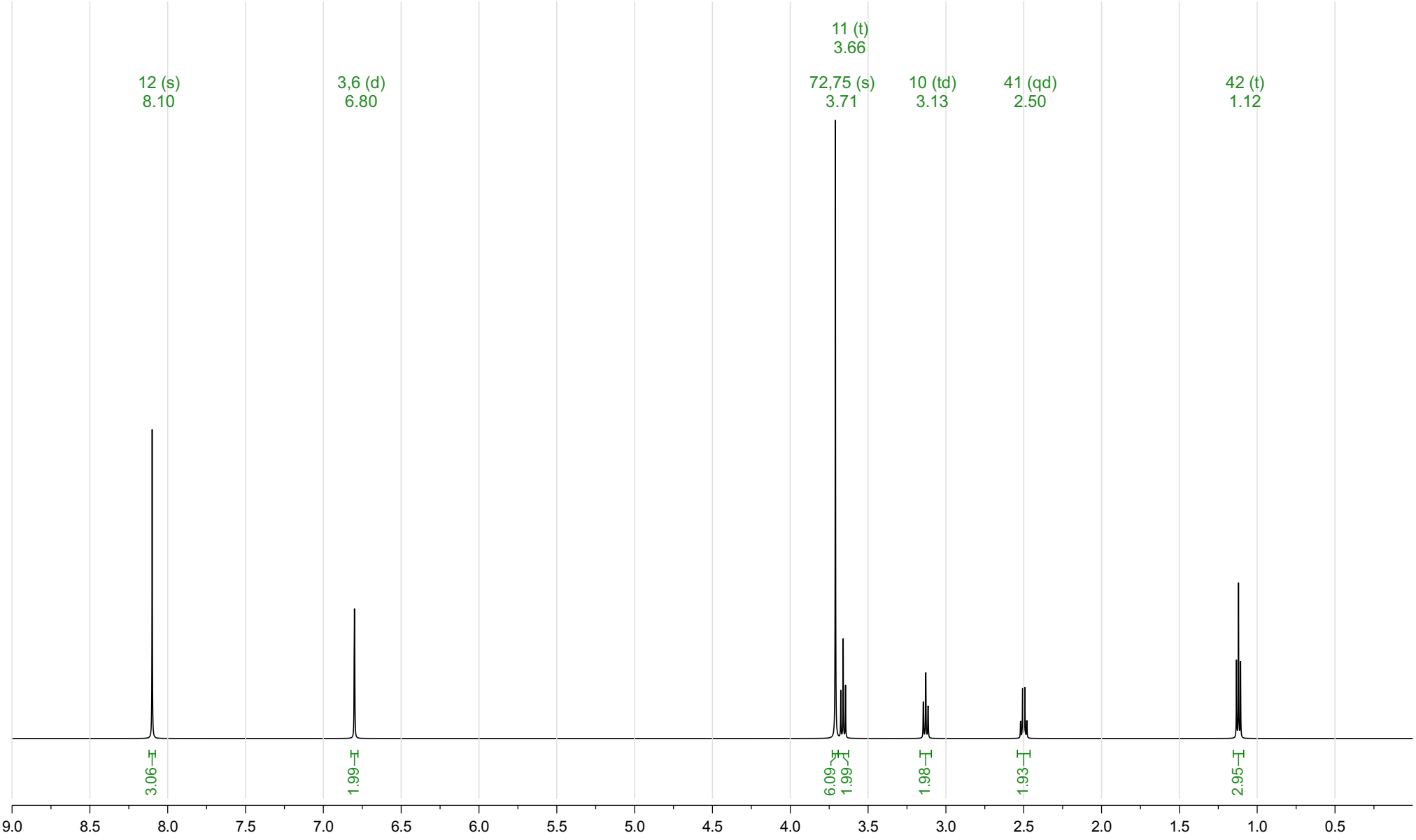
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.03 (s, 3H), 6.81 (s, 1H), 6.79 (s, 1H), 3.74 (s, 3H), 3.74 (s, 3H), 2.98 – 2.91 (m, 2H), 2.86 – 2.79 (m, 2H), 2.54 (q, J = 7.5 Hz, 2H), 1.11 (t, J = 7.5 Hz, 3H).



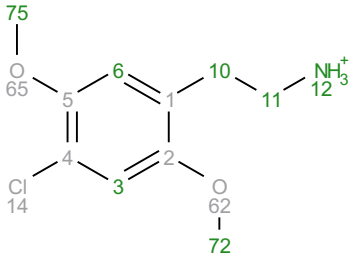
Prediction	2C-E H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



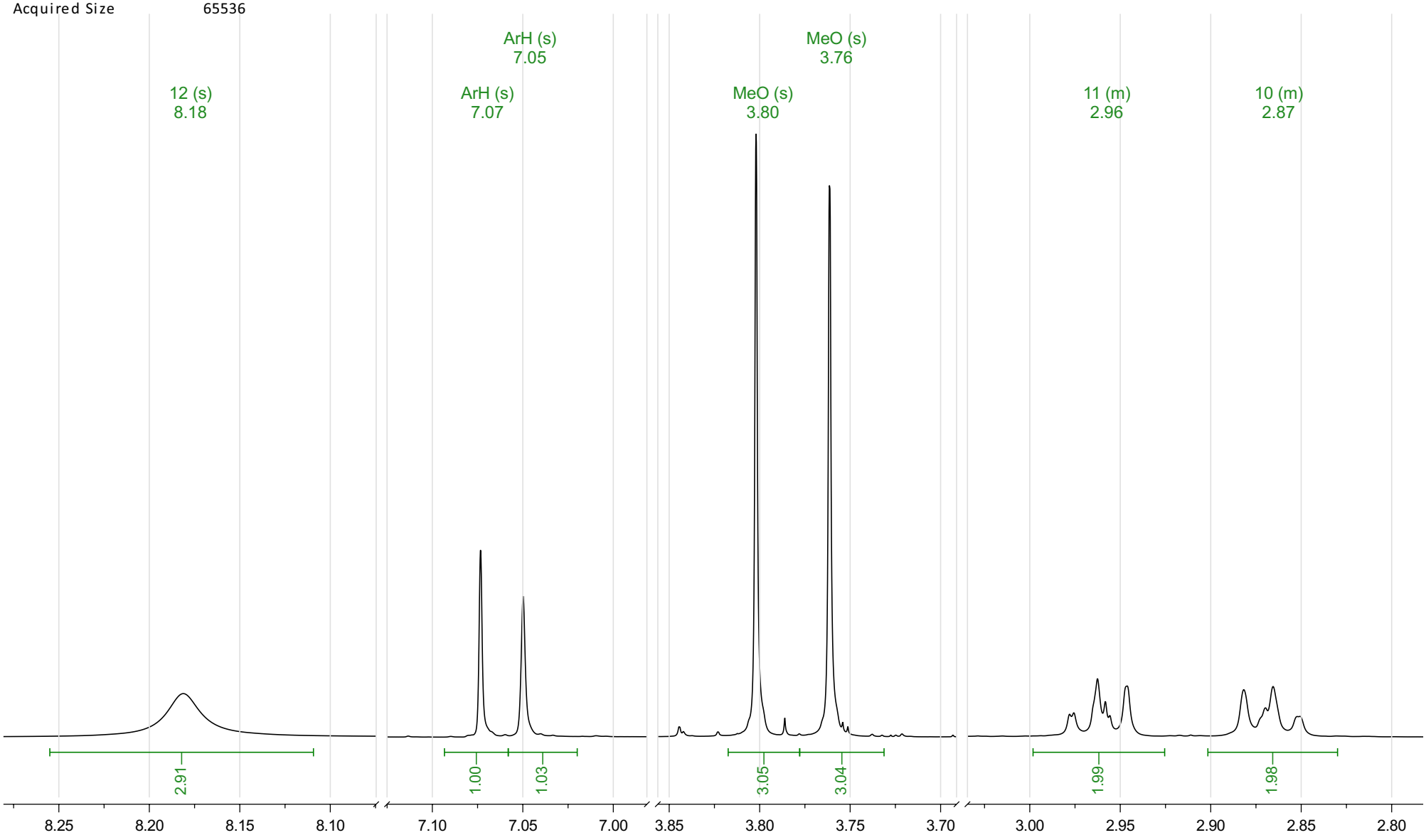
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.10 (s, 3H), 6.80 (d, J = 1.2 Hz, 2H), 3.71 (s, 6H), 3.66 (t, J = 7.6 Hz, 2H), 3.13 (td, J = 7.6, 1.0 Hz, 2H), 2.50 (qd, J = 6.6, 1.0 Hz, 2H), 1.12 (t, J = 6.6 Hz, 3H).



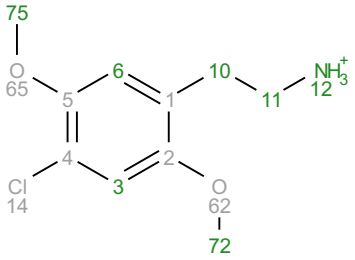
Analyte	P6b: 2C-C H+
Acquisition Date	2013-03-26T19:35:22
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	10964.9
Nucleus	1H
Acquired Size	65536



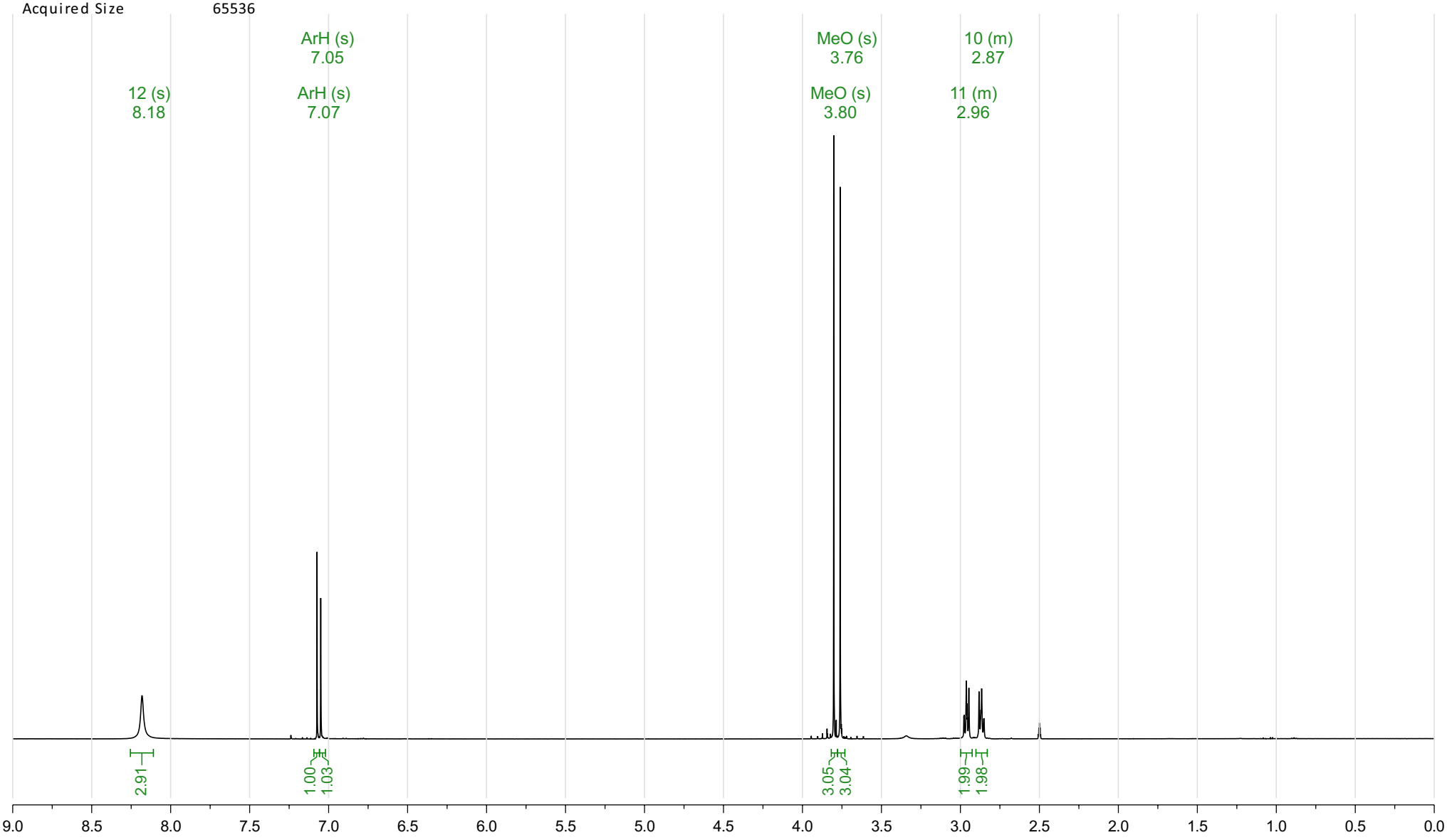
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.18 (s, 3H), 7.07 (s, 1H), 7.05 (s, 1H), 3.80 (s, 3H), 3.76 (s, 3H), 3.00 – 2.93 (m, 2H), 2.90 – 2.83 (m, 2H).



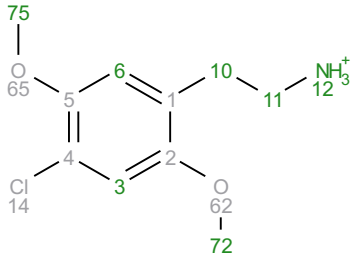
Analyte	P6b: 2C-C H+
Acquisition Date	2013-03-26T19:35:22
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	10964.9
Nucleus	1H
Acquired Size	65536



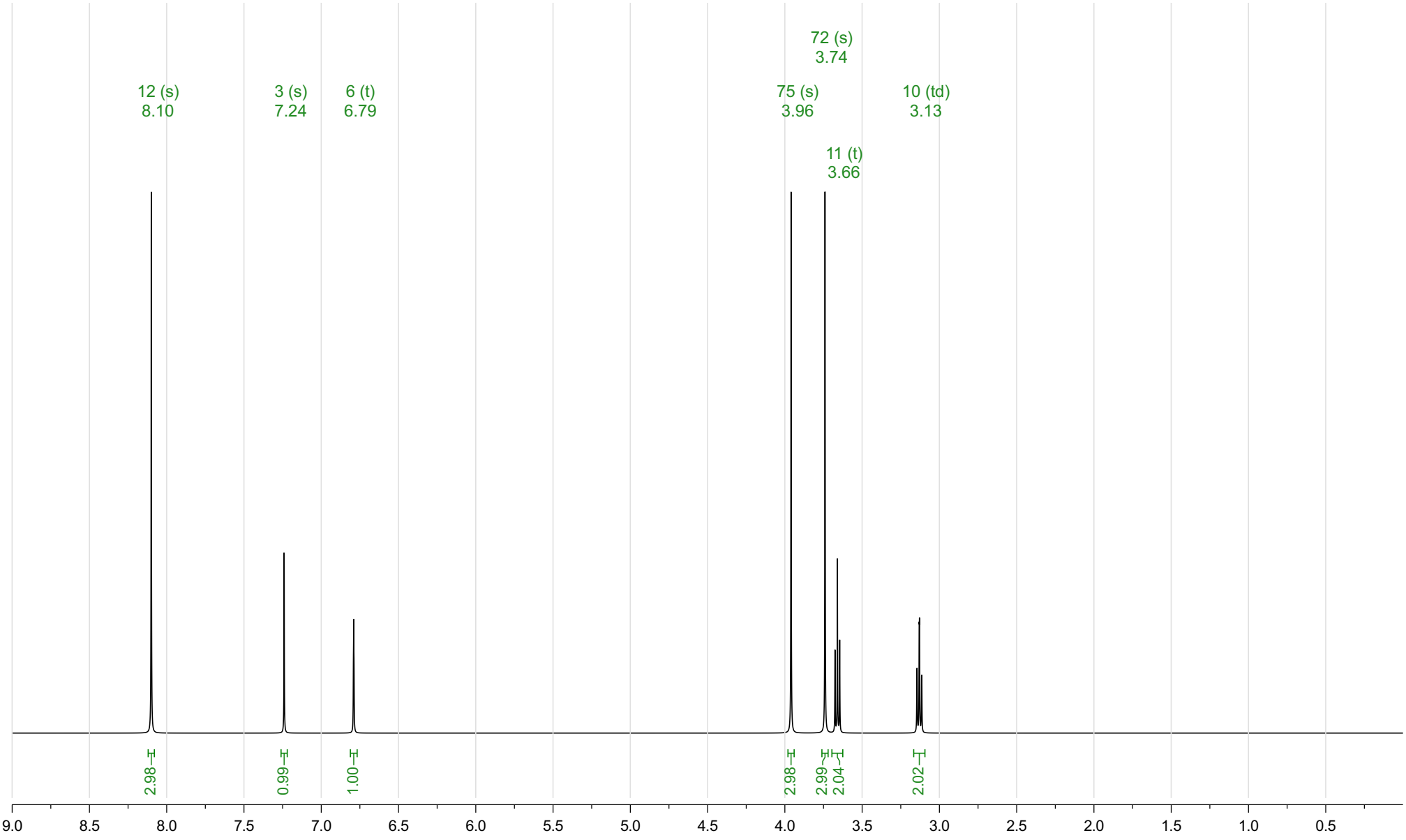
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.18 (s, 3H), 7.07 (s, 1H), 7.05 (s, 1H), 3.80 (s, 3H), 3.76 (s, 3H), 3.00 – 2.93 (m, 2H), 2.90 – 2.83 (m, 2H).



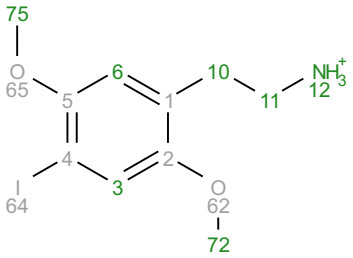
Prediction	2C-C H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



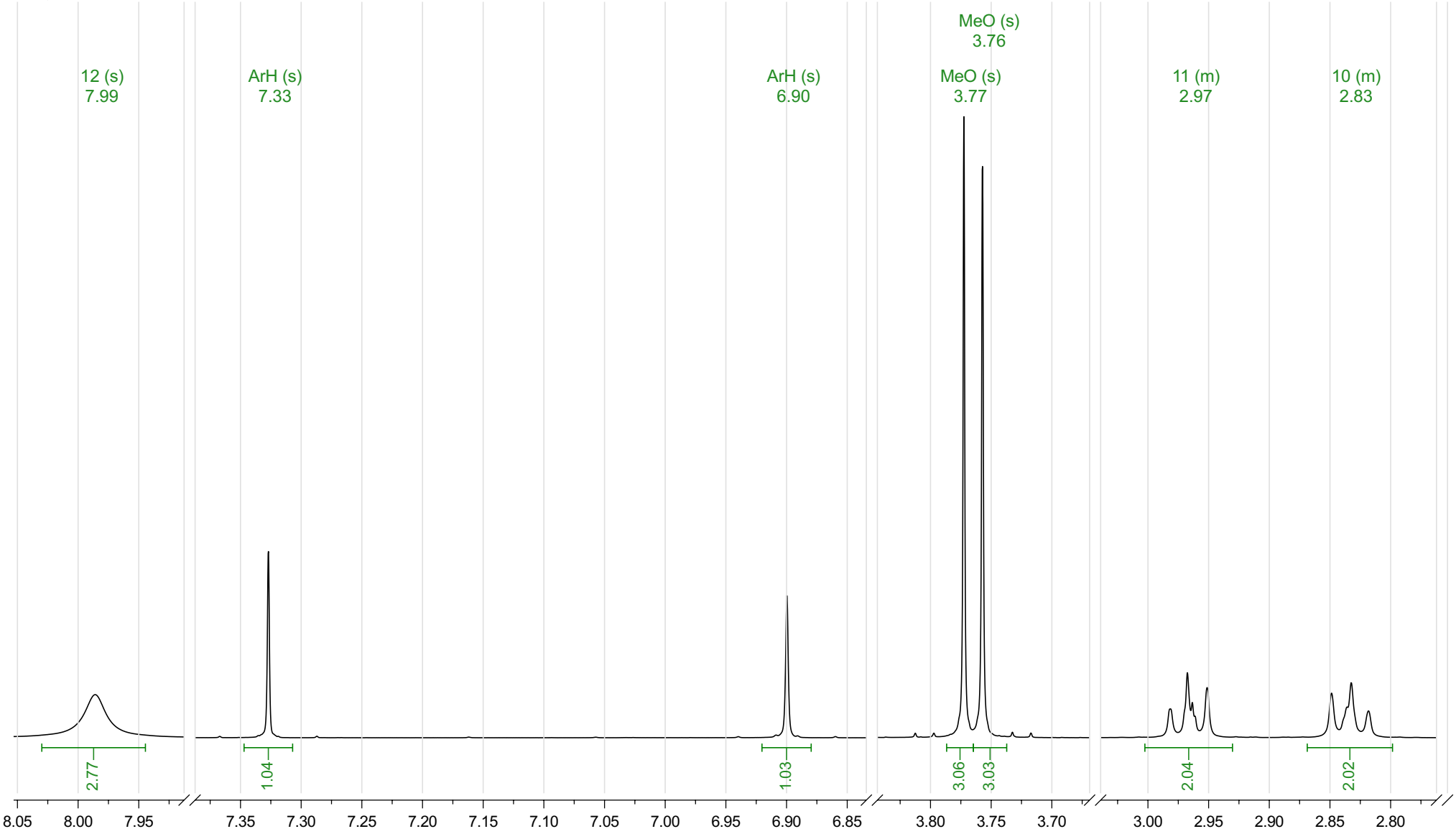
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.10 (s, 3H), 7.24 (s, 1H), 6.79 (t, J = 1.0 Hz, 1H), 3.96 (s, 3H), 3.74 (s, 3H), 3.66 (t, J = 7.6 Hz, 2H), 3.13 (td, J = 7.6, 1.0 Hz, 2H).



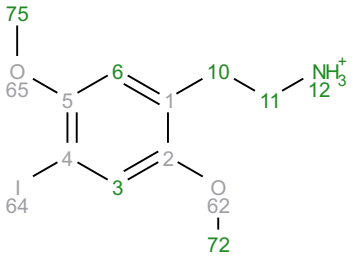
Analyte	P7: 2C-I H+
Acquisition Date	2012-11-24T13:42:12
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



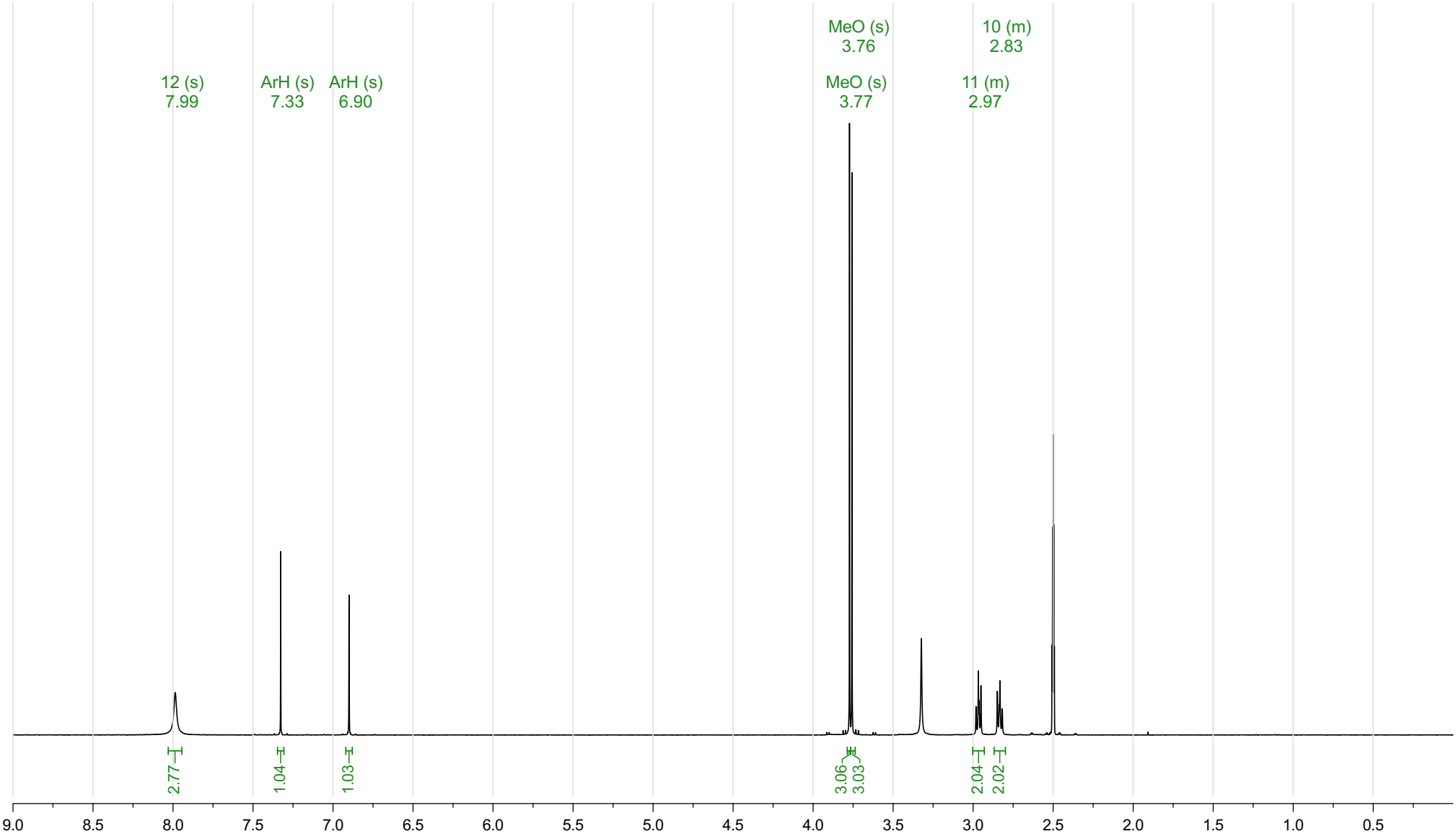
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.99 (s, 3H), 7.33 (s, 1H), 6.90 (s, 1H), 3.77 (s, 3H), 3.76 (s, 3H), 3.00 – 2.93 (m, 2H), 2.87 – 2.80 (m, 2H).



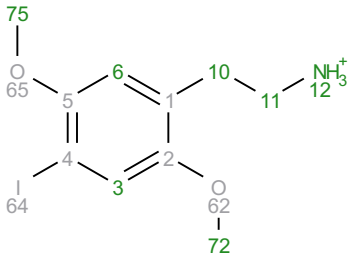
Analyte	P7: 2C-I H+
Acquisition Date	2012-11-24T13:42:12
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



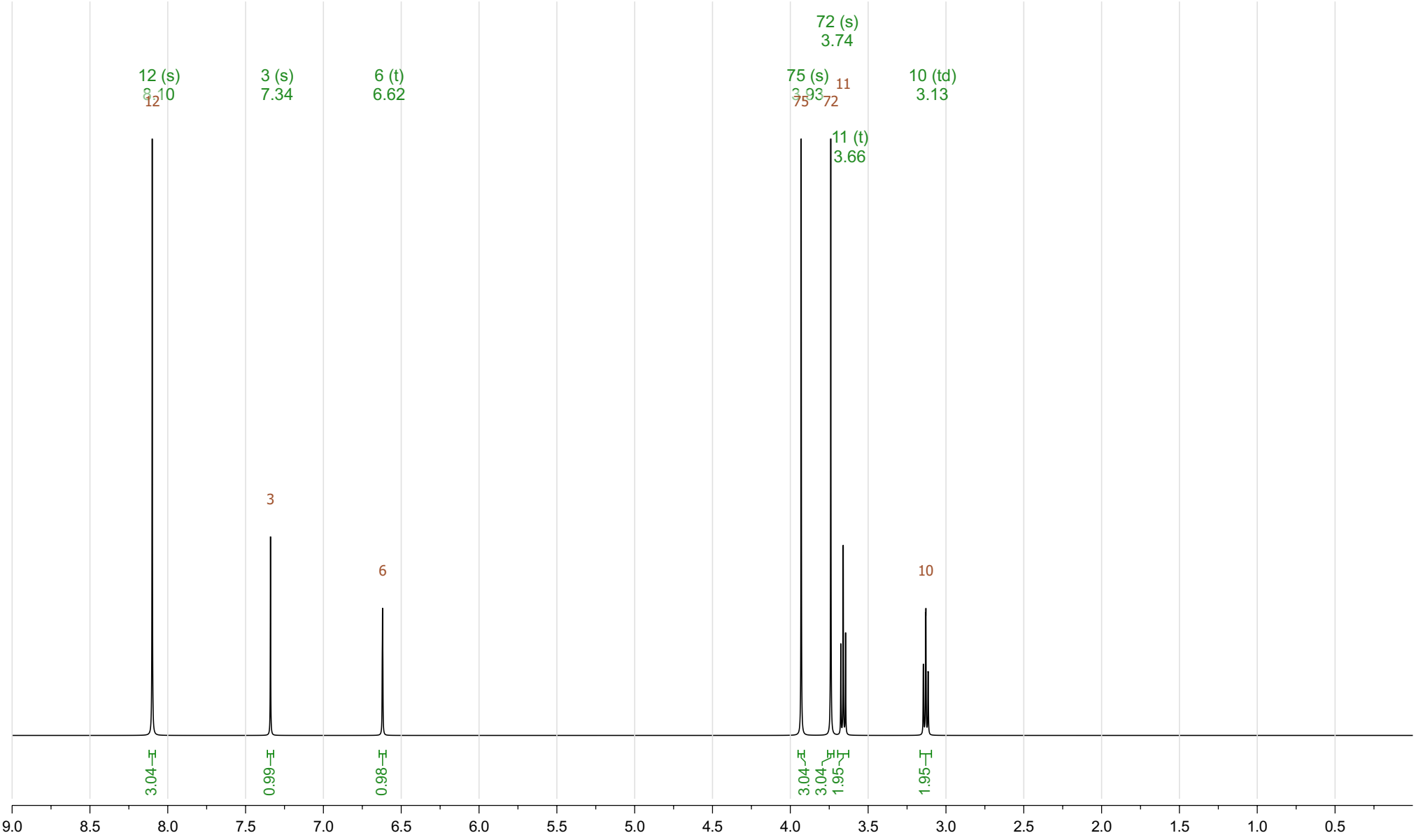
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.99 (s, 3H), 7.33 (s, 1H), 6.90 (s, 1H), 3.77 (s, 3H), 3.76 (s, 3H), 3.00 – 2.93 (m, 2H), 2.87 – 2.80 (m, 2H).



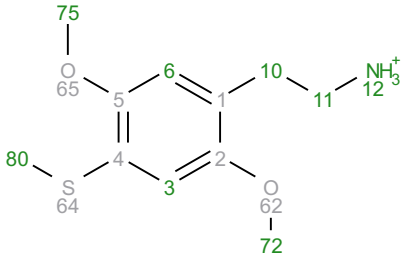
Prediction	2C-C H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



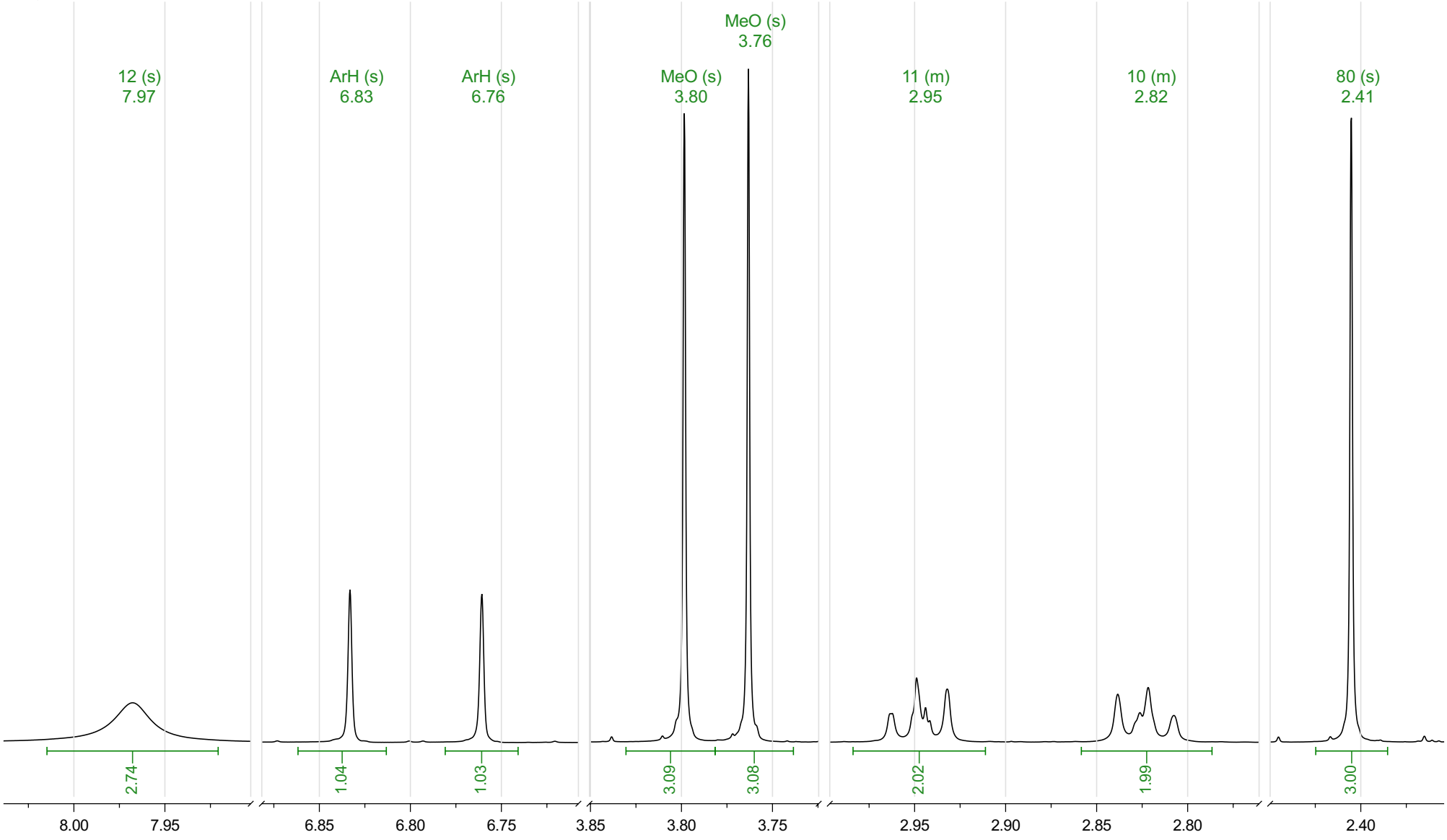
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.10 (s, 3H), 7.34 (s, 1H), 6.62 (t, J = 1.0 Hz, 1H), 3.93 (s, 3H), 3.74 (s, 3H), 3.66 (t, J = 7.6 Hz, 2H), 3.13 (td, J = 7.6, 1.0 Hz, 2H).



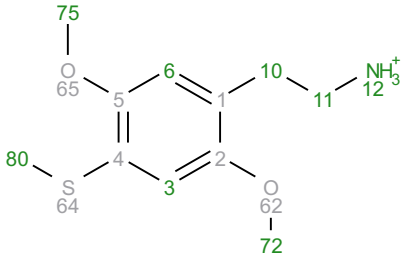
Analyte	P8: 2C-T H+
Acquisition Date	2012-11-24T14:06:55
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



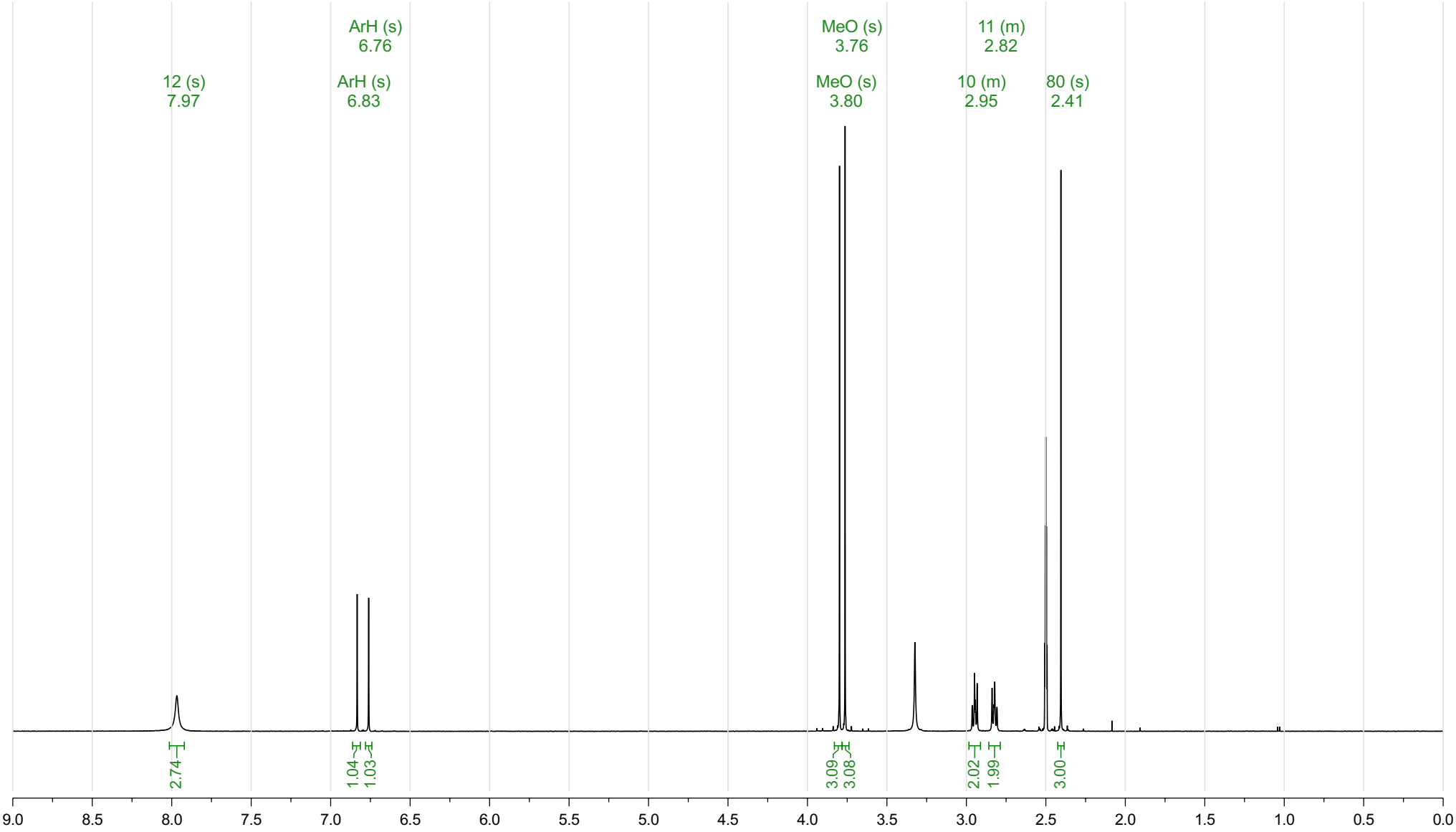
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.97 (s, 3H), 6.83 (s, 1H), 6.76 (s, 1H), 3.80 (s, 3H), 3.76 (s, 3H), 2.98 – 2.91 (m, 2H), 2.86 – 2.79 (m, 2H), 2.41 (s, 3H).



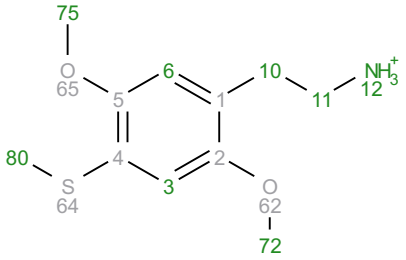
Analyte	P8: 2C-T H+
Acquisition Date	2012-11-24T14:06:55
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



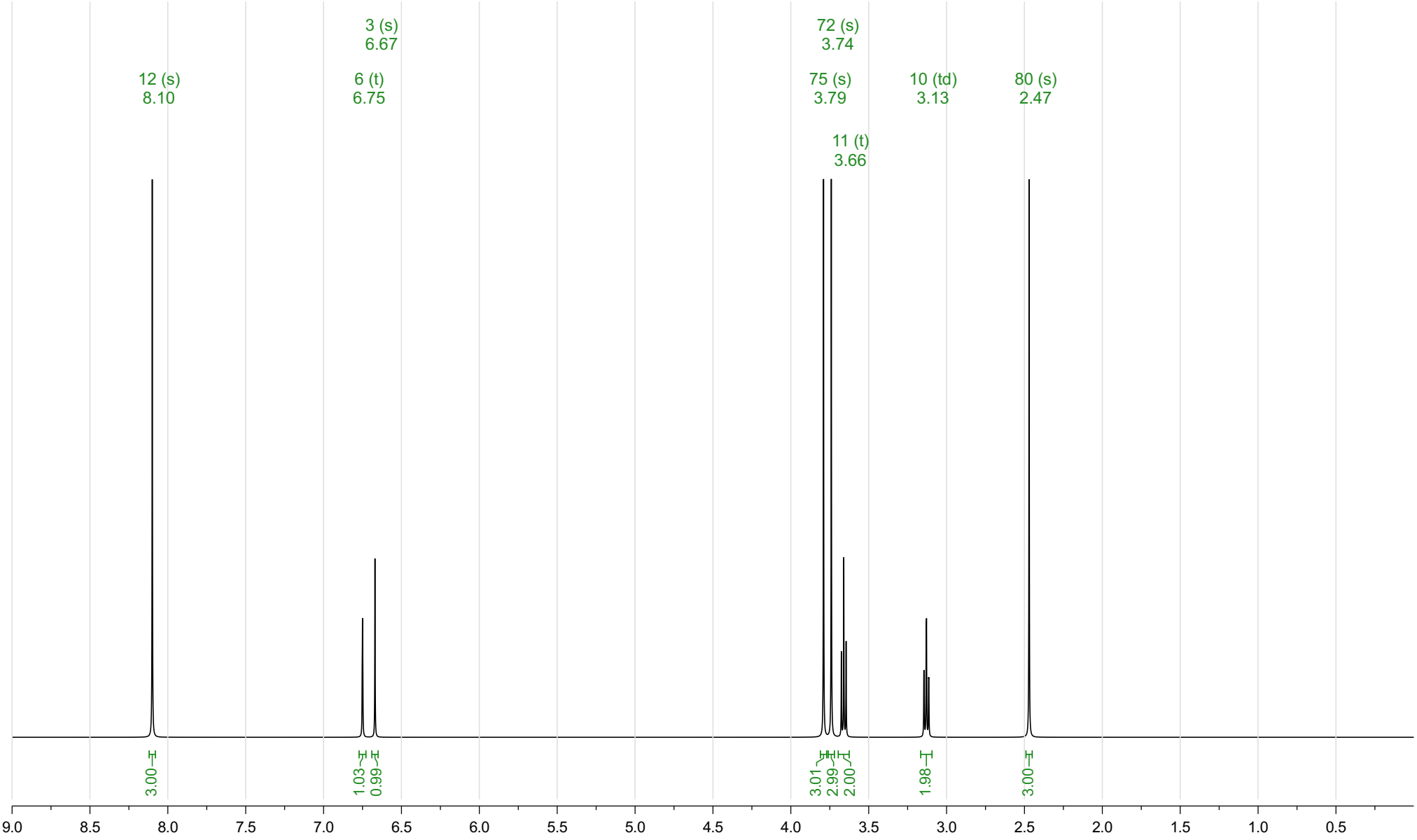
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.97 (s, 3H), 6.83 (s, 1H), 6.76 (s, 1H), 3.80 (s, 3H), 3.76 (s, 3H), 2.98 – 2.91 (m, 2H), 2.86 – 2.79 (m, 2H), 2.41 (s, 3H).



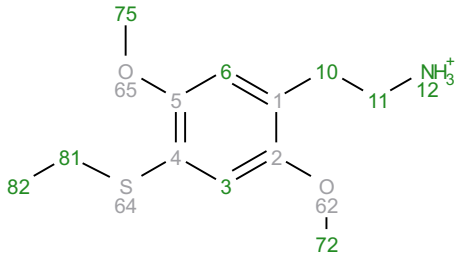
Prediction	2C-T H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



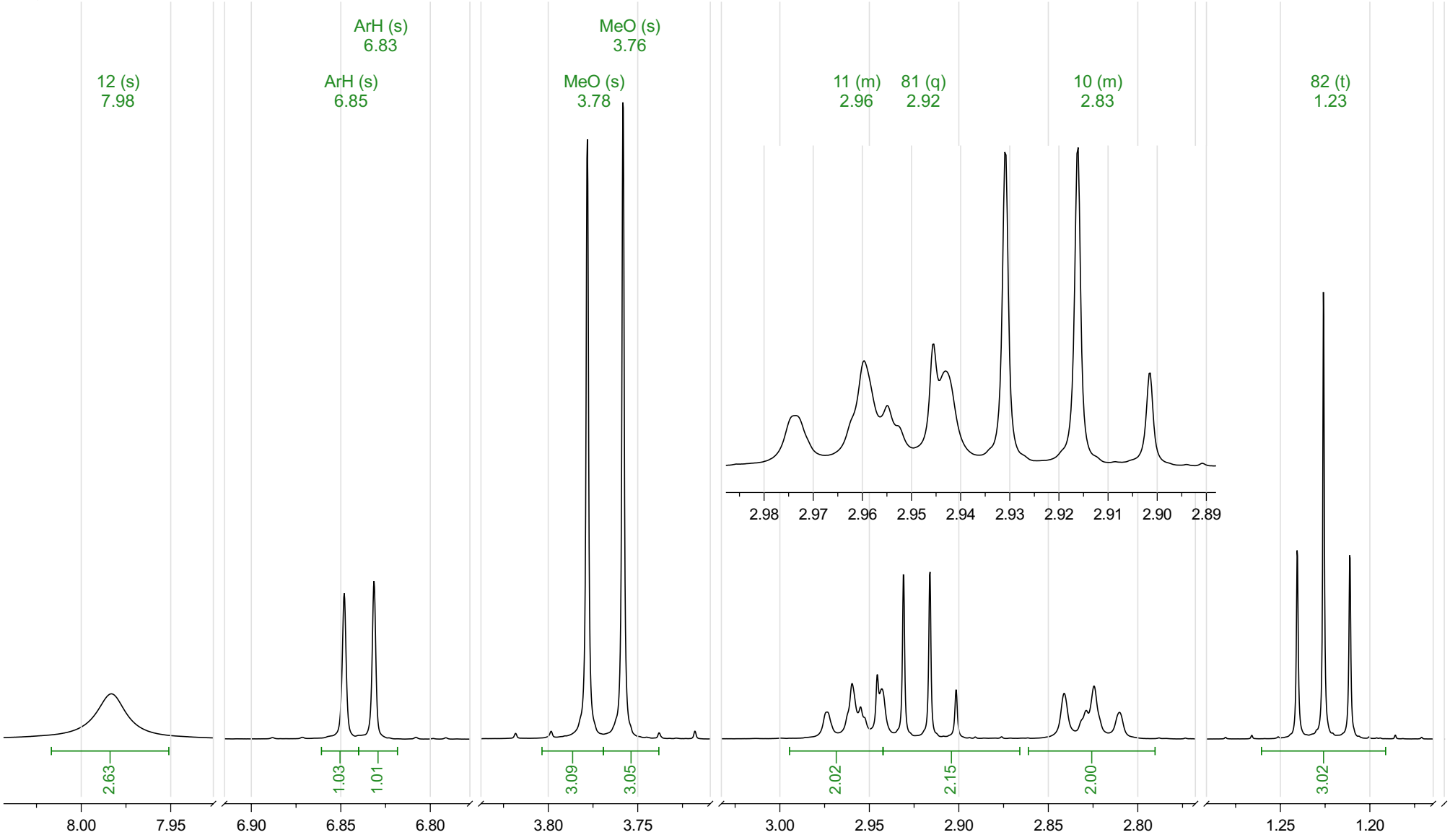
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.10 (s, 3H), 6.75 (t, J = 0.9 Hz, 1H), 6.67 (s, 1H), 3.79 (s, 3H), 3.74 (s, 3H), 3.66 (t, J = 7.6 Hz, 2H), 3.13 (td, J = 7.6, 1.0 Hz, 2H), 2.47 (s, 3H).



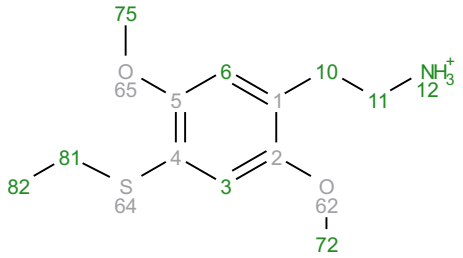
Analyte	P9: 2C-T-2 H+
Acquisition Date	2012-11-24T13:18:04
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



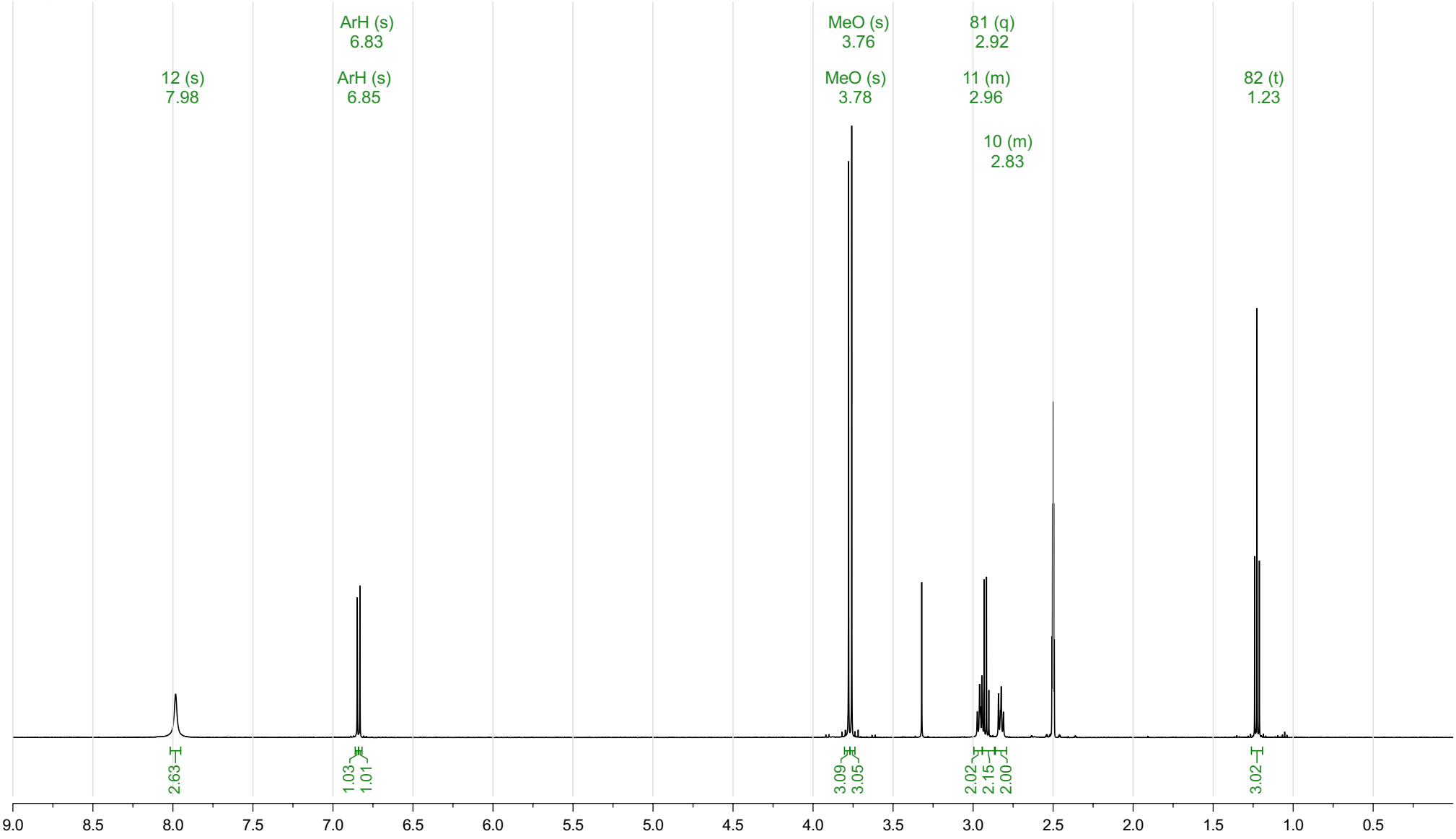
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.98 (s, 3H), 6.85 (s, 1H), 6.83 (s, 1H), 3.78 (s, 3H), 3.76 (s, 3H), 3.01 – 2.92 (m, 2H), 2.92 (q, J = 7.3 Hz, 2H), 2.86 – 2.79 (m, 2H), 1.23 (t, J = 7.3 Hz, 3H).



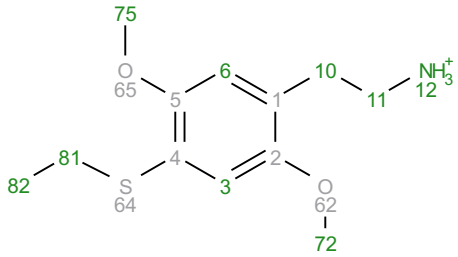
Analyte	P9: 2C-T-2 H+
Acquisition Date	2012-11-24T13:18:04
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



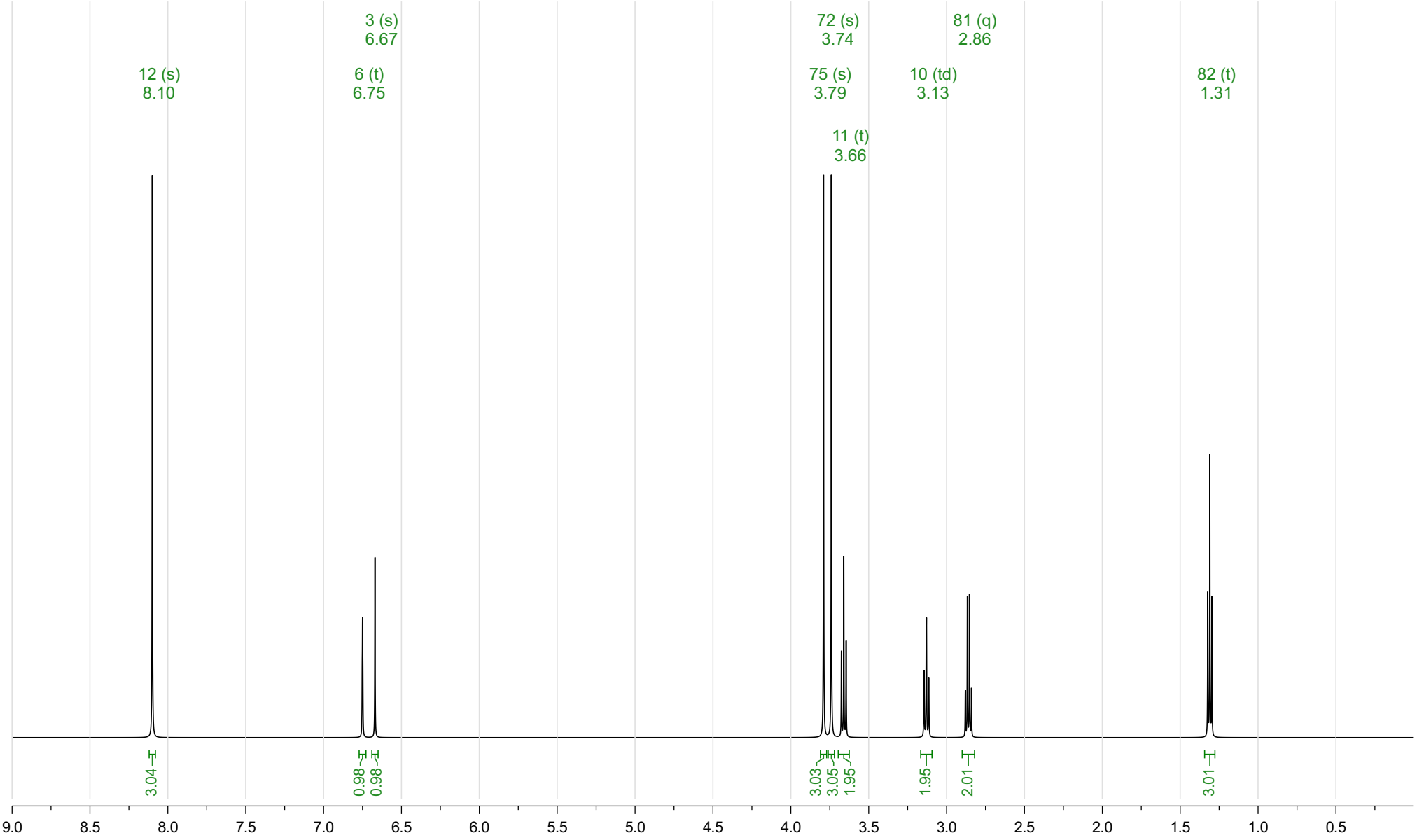
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.98 (s, 3H), 6.85 (s, 1H), 6.83 (s, 1H), 3.78 (s, 3H), 3.76 (s, 3H), 3.01 – 2.92 (m, 2H), 2.92 (q, J = 7.3 Hz, 2H), 2.86 – 2.79 (m, 2H), 1.23 (t, J = 7.3 Hz, 3H).



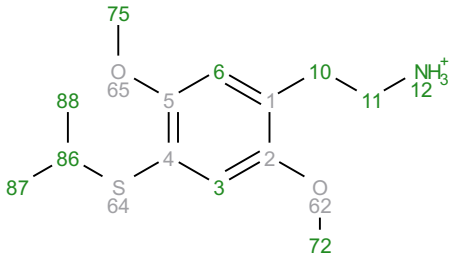
Prediction	2C-T-2 H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



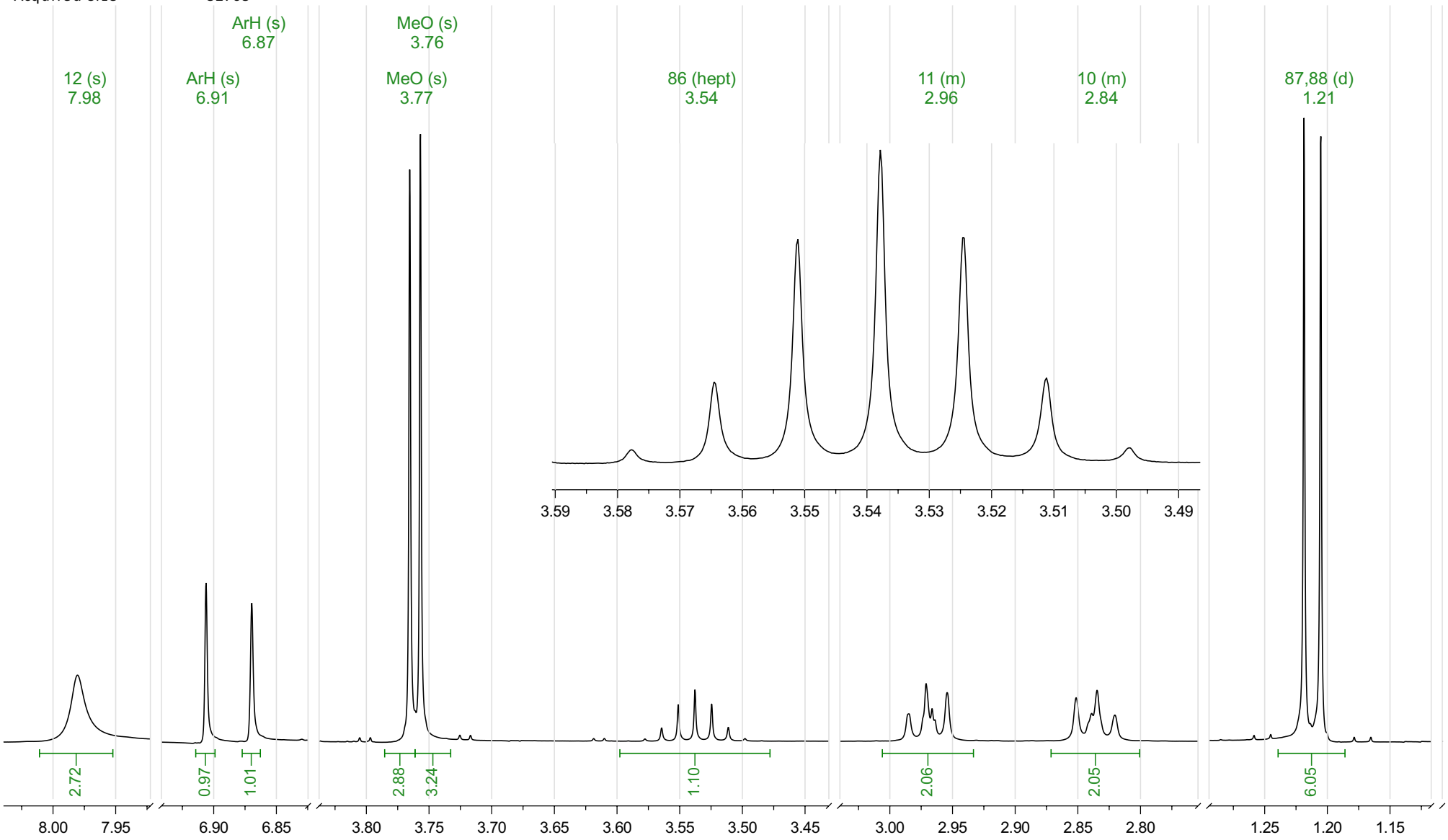
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.10 (s, 3H), 6.75 (t, J = 0.9 Hz, 1H), 6.67 (s, 1H), 3.79 (s, 3H), 3.74 (s, 3H), 3.66 (t, J = 7.6 Hz, 2H), 3.13 (td, J = 7.6, 1.0 Hz, 2H), 2.86 (q, J = 6.6 Hz, 2H), 1.31 (t, J = 6.6 Hz, 3H).



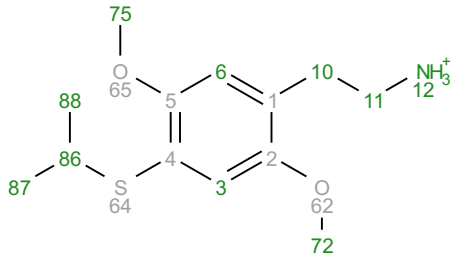
Analyte	P10: 2C-T-4 H+
Acquisition Date	2012-11-24T13:09:47
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



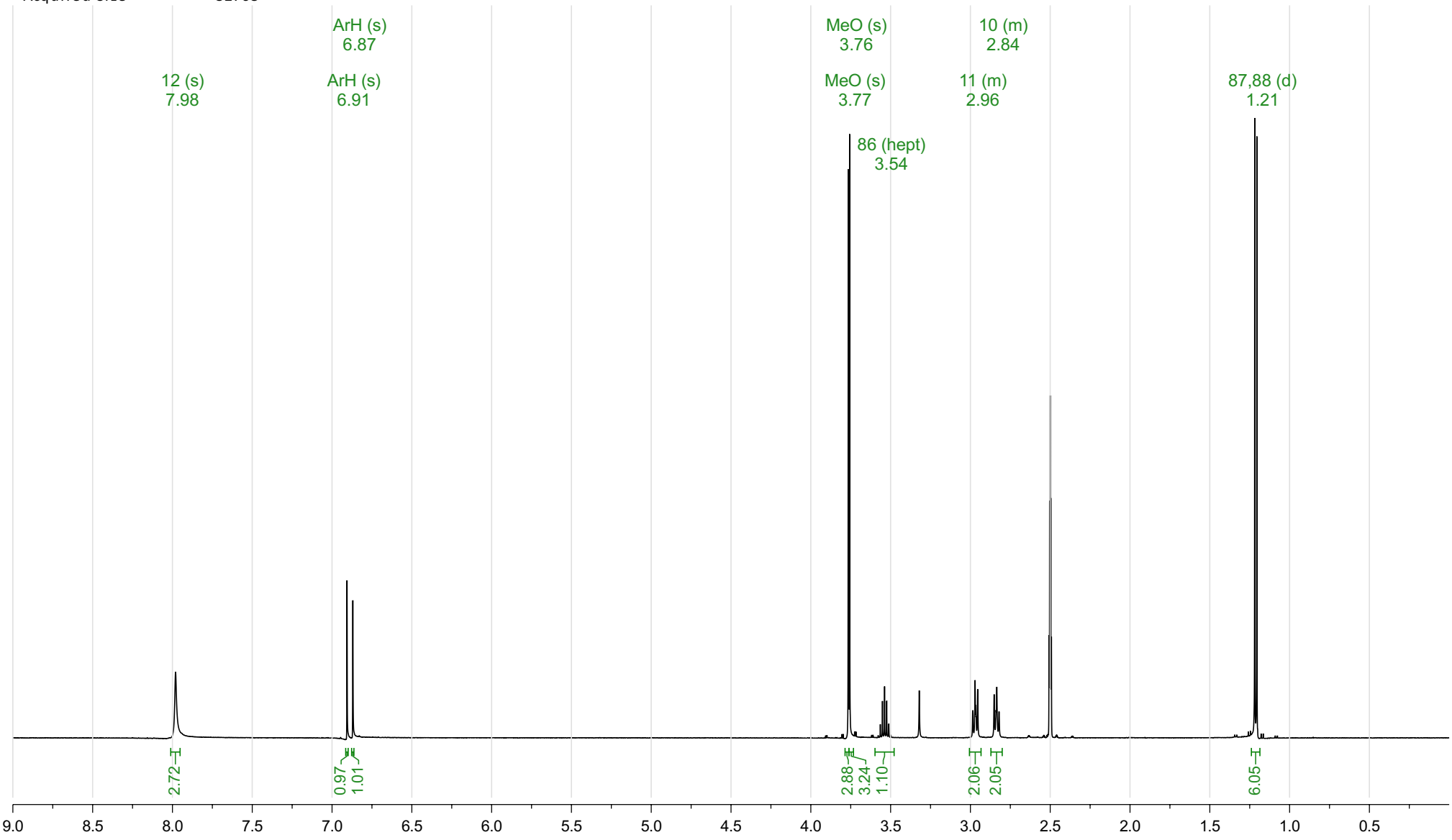
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.98 (s, 3H), 6.91 (s, 1H), 6.87 (s, 1H), 3.77 (s, 3H), 3.76 (s, 3H), 3.54 (hept, J = 6.6 Hz, 1H), 3.01 – 2.93 (m, 2H), 2.87 – 2.80 (m, 2H), 1.21 (d, J = 6.6 Hz, 6H).



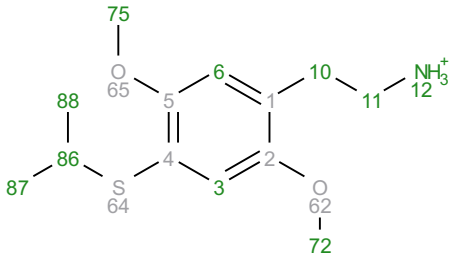
Analyte	P10: 2C-T-4 H+
Acquisition Date	2012-11-24T13:09:47
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



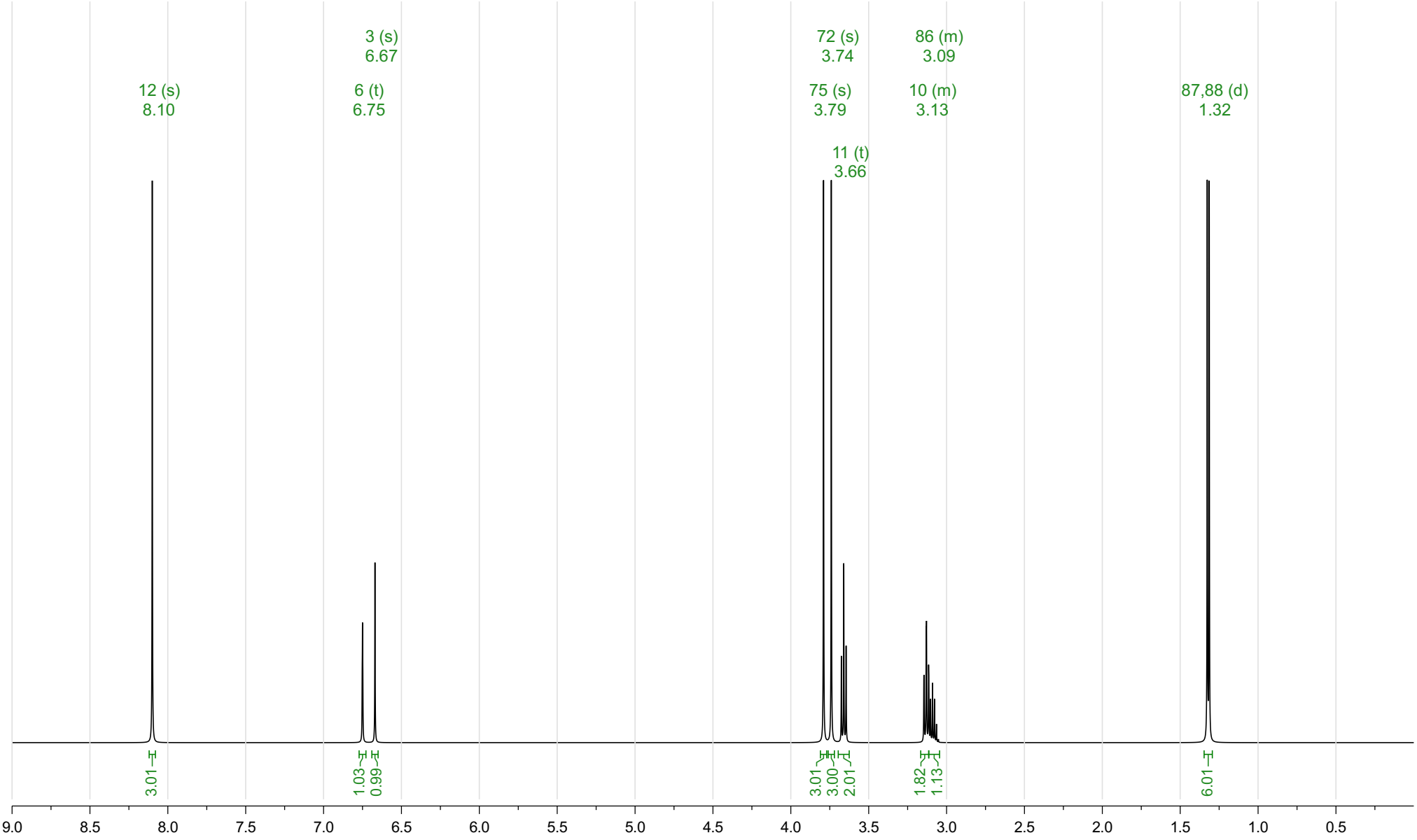
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.98 (s, 3H), 6.91 (s, 1H), 6.87 (s, 1H), 3.77 (s, 3H), 3.76 (s, 3H), 3.54 (hept, J = 6.6 Hz, 1H), 3.01 – 2.93 (m, 2H), 2.87 – 2.80 (m, 2H), 1.21 (d, J = 6.6 Hz, 6H).



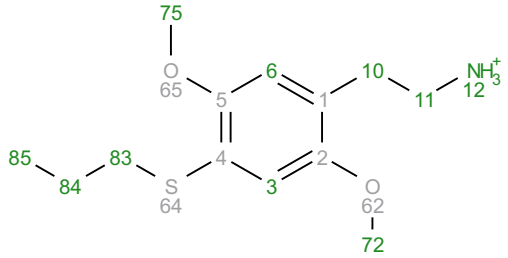
Prediction	2C-T-4 H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



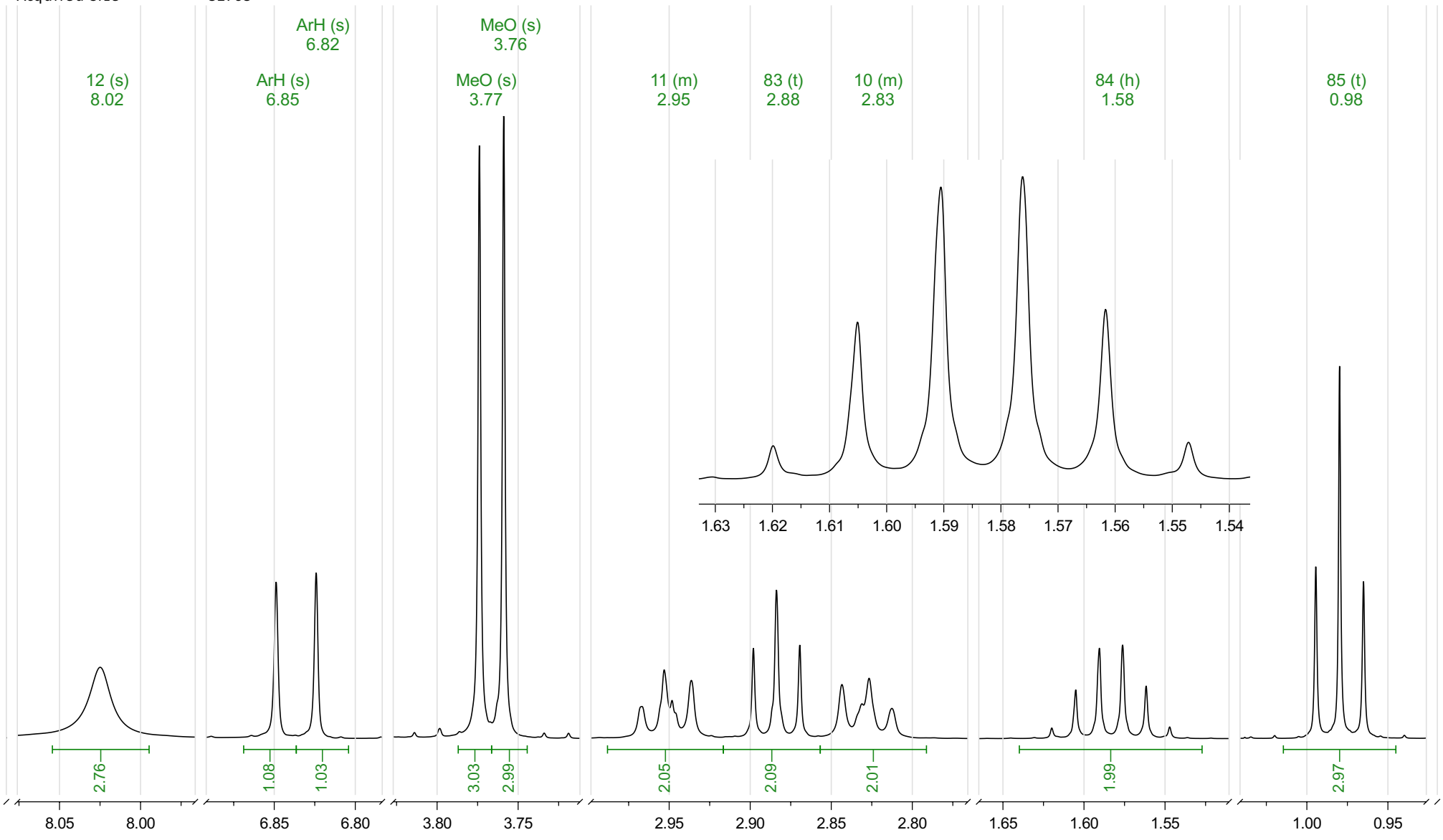
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.10 (s, 3H), 6.75 (t, J = 0.9 Hz, 1H), 6.67 (s, 1H), 3.79 (s, 3H), 3.74 (s, 3H), 3.66 (t, J = 7.6 Hz, 2H), 3.17 – 3.10 (m, 2H), 3.13 – 3.03 (m, 1H), 1.32 (d, J = 6.4 Hz, 6H).



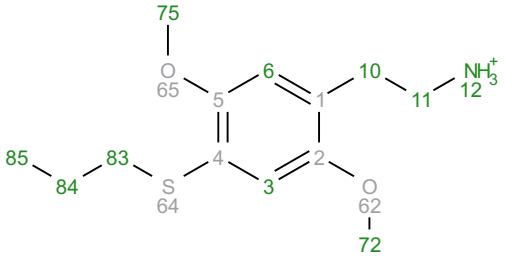
Analyte	P11: 2C-T-7 H+
Acquisition Date	2012-11-24T14:15:22
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



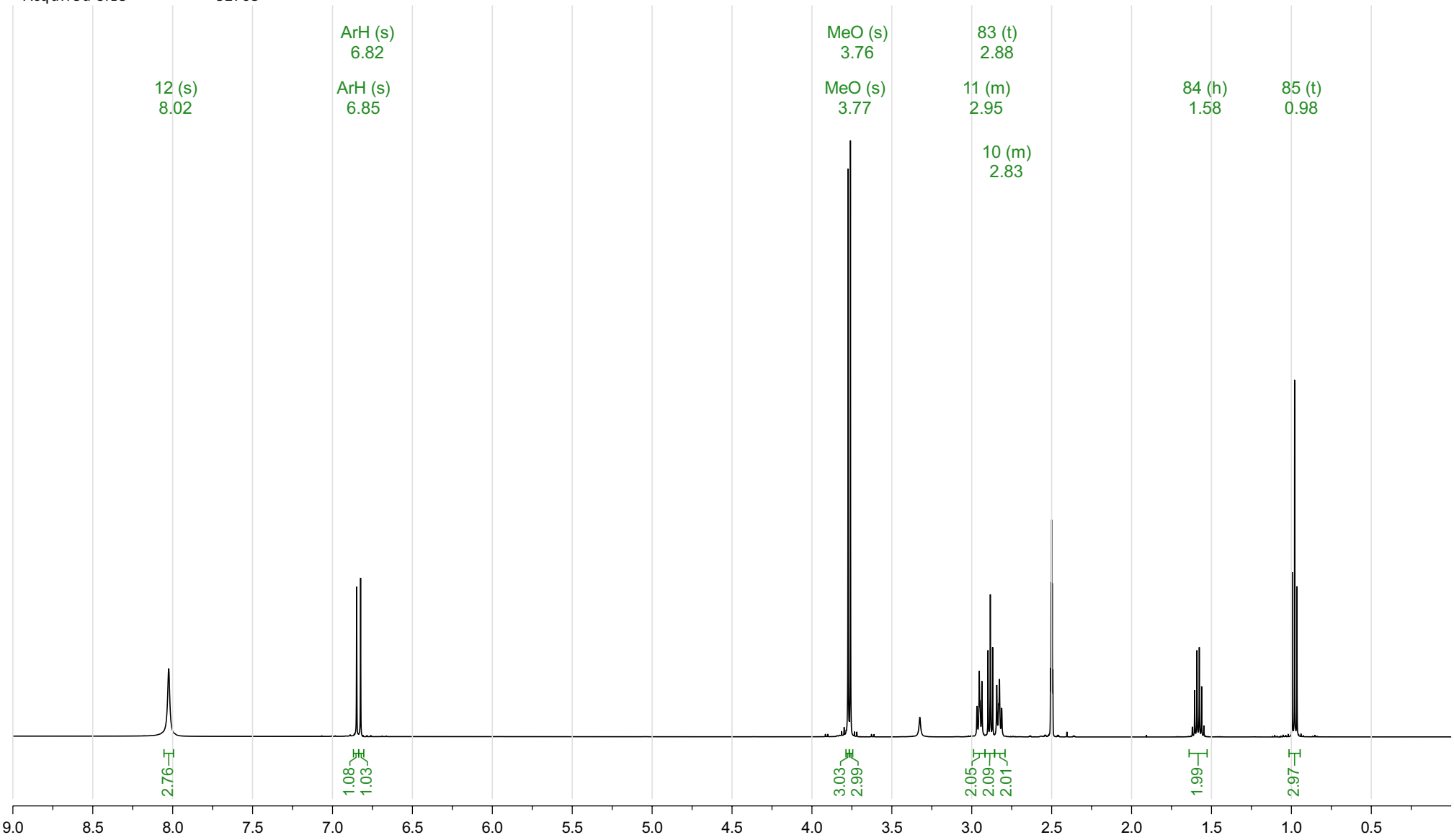
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.02 (s, 3H), 6.85 (s, 1H), 6.82 (s, 1H), 3.77 (s, 3H), 3.76 (s, 3H), 2.99 – 2.92 (m, 2H), 2.88 (t, J = 7.1 Hz, 2H), 2.86 – 2.79 (m, 2H), 1.58 (h, J = 7.3 Hz, 2H), 0.98 (t, J = 7.3 Hz, 3H).



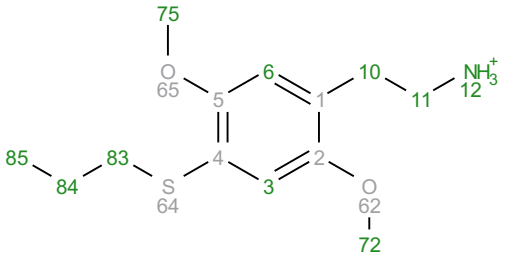
Analyte	P11: 2C-T-7 H+
Acquisition Date	2012-11-24T14:15:22
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



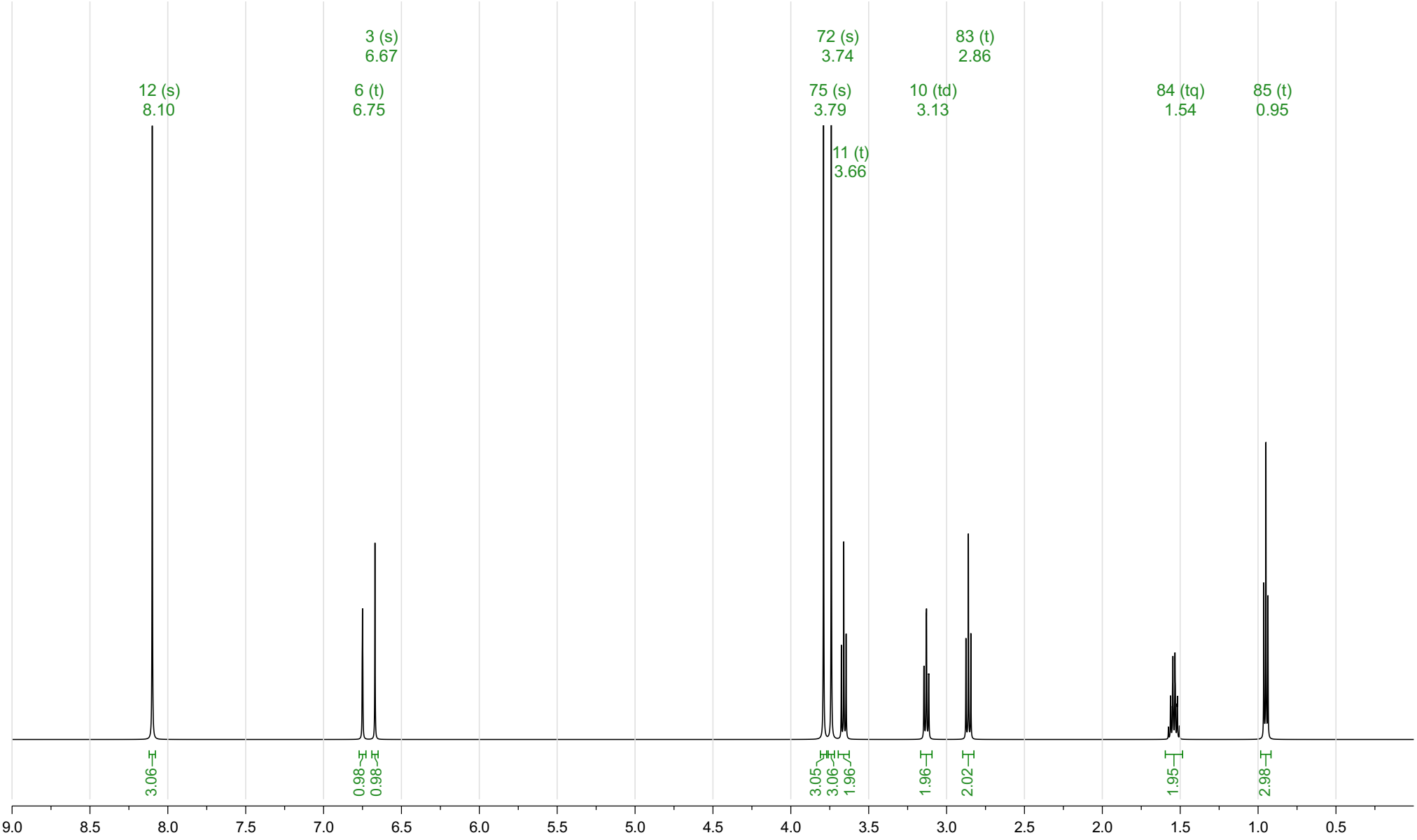
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.02 (s, 3H), 6.85 (s, 1H), 6.82 (s, 1H), 3.77 (s, 3H), 3.76 (s, 3H), 2.99 – 2.92 (m, 2H), 2.88 (t, J = 7.1 Hz, 2H), 2.86 – 2.79 (m, 2H), 1.58 (h, J = 7.3 Hz, 2H), 0.98 (t, J = 7.3 Hz, 3H).



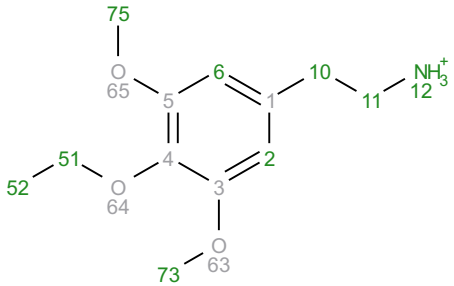
Prediction	2C-T-7 H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



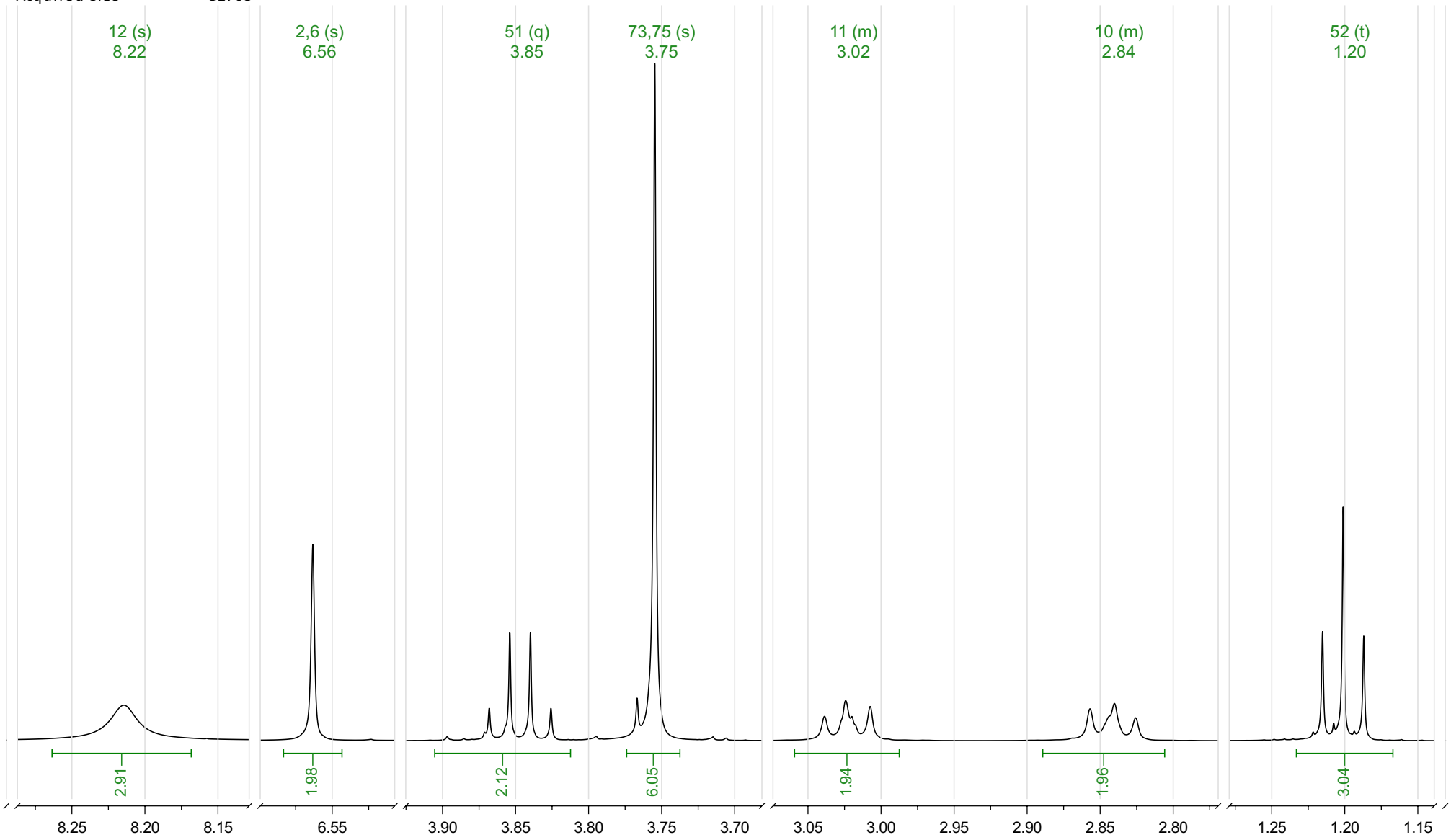
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.10 (s, 3H), 6.75 (t, J = 0.9 Hz, 1H), 6.67 (s, 1H), 3.79 (s, 3H), 3.74 (s, 3H), 3.66 (t, J = 7.6 Hz, 2H), 3.13 (td, J = 7.6, 1.0 Hz, 2H), 2.86 (t, J = 7.9 Hz, 2H), 1.54 (tq, J = 7.9, 6.6 Hz, 2H), 0.95 (t, J = 6.6 Hz, 3H).



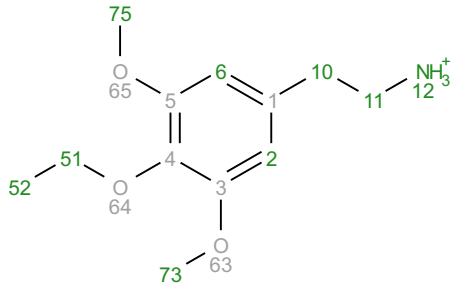
Analyte	P12: Escaline H+
Acquisition Date	2013-01-17T01:53:27
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



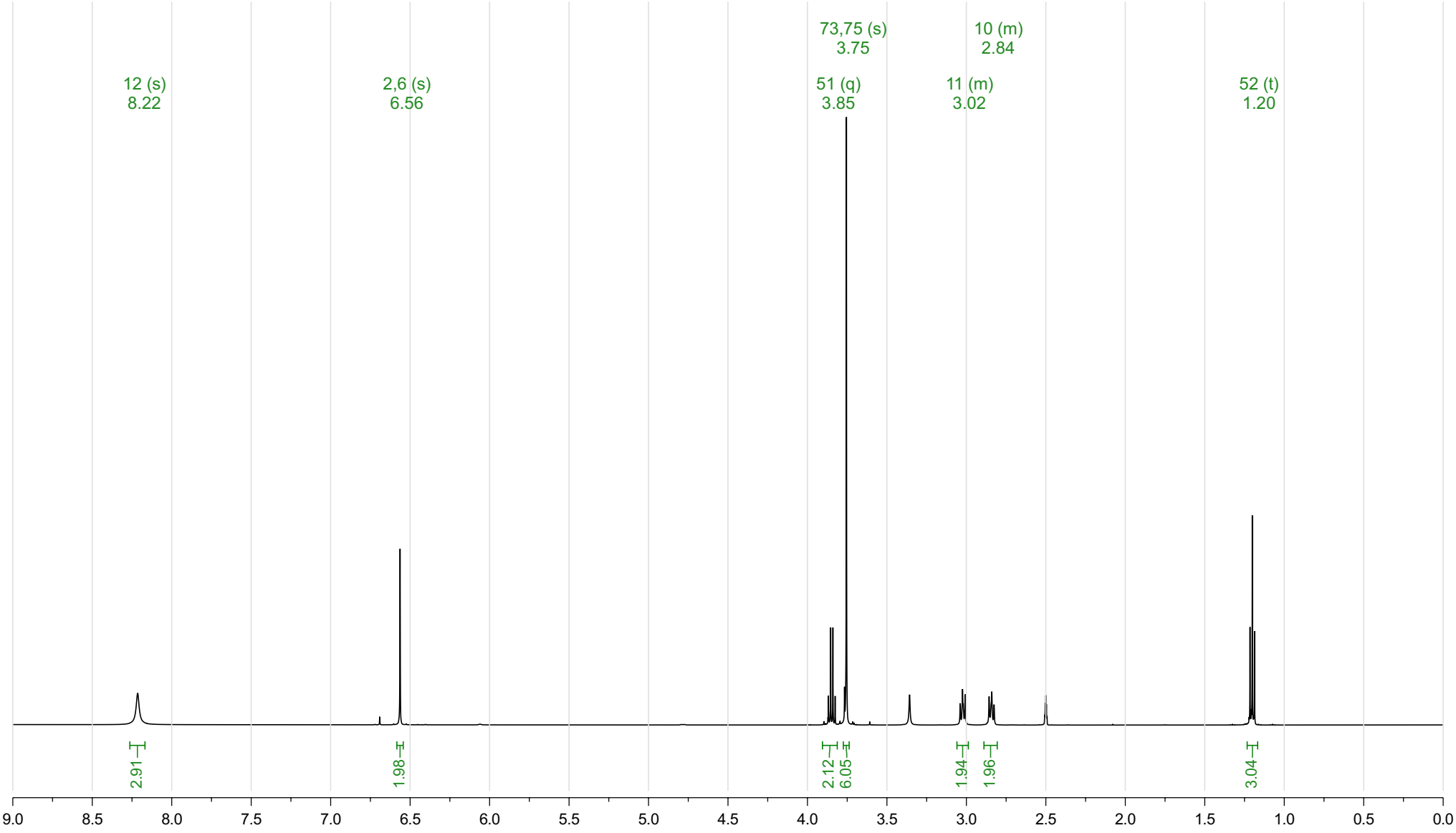
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.22 (s, 3H), 6.56 (s, 2H), 3.85 (q, J = 7.0 Hz, 2H), 3.75 (s, 6H), 3.06 – 2.99 (m, 2H), 2.89 – 2.81 (m, 2H), 1.20 (t, J = 7.0 Hz, 3H).



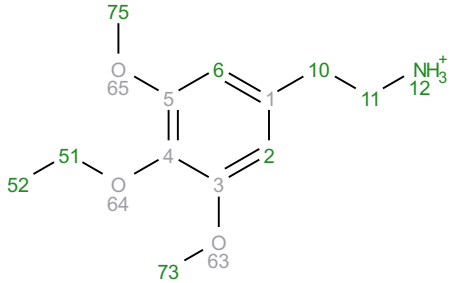
Analyte	P12: Escaline H+
Acquisition Date	2013-01-17T01:53:27
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



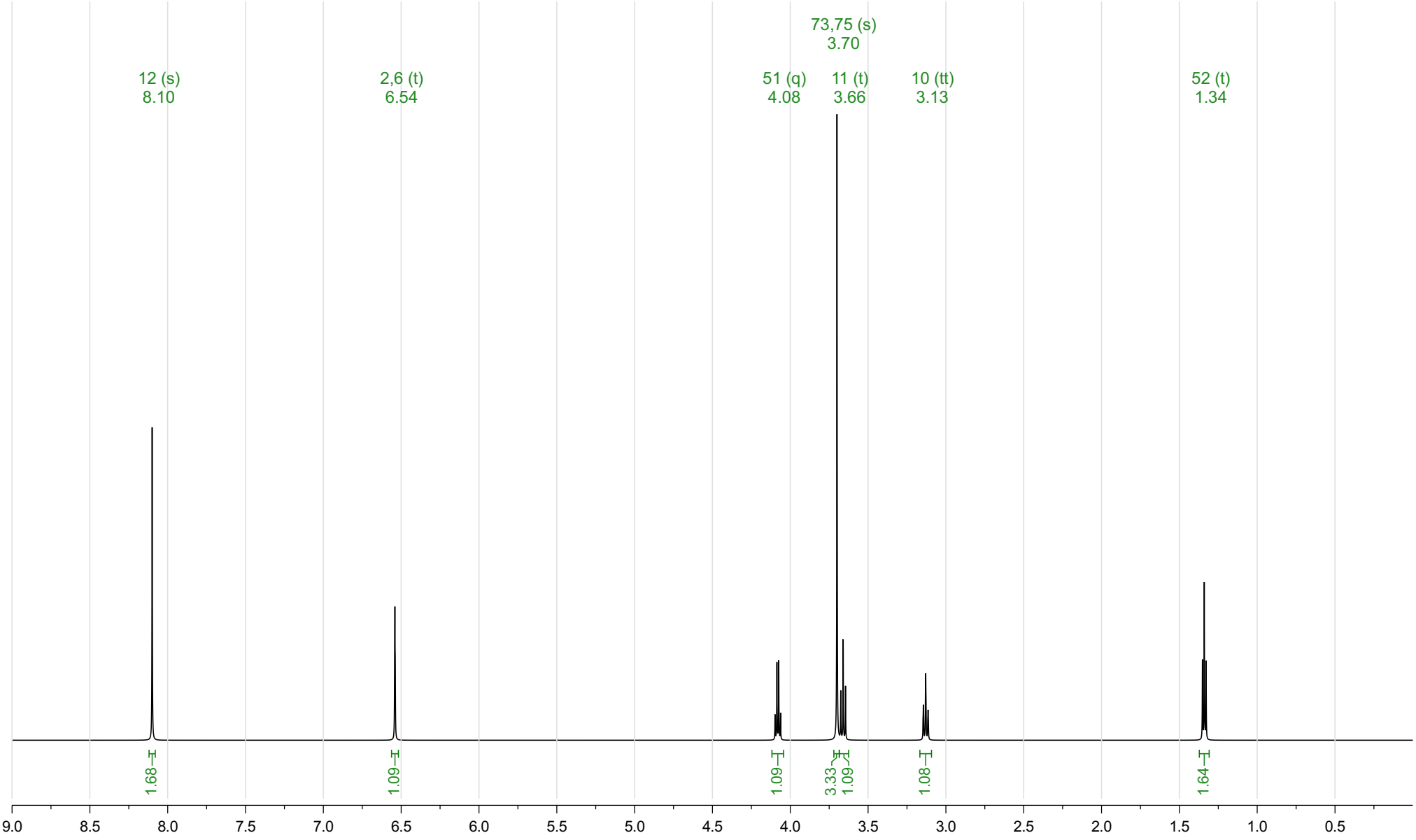
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.22 (s, 3H), 6.56 (s, 2H), 3.85 (q, J = 7.0 Hz, 2H), 3.75 (s, 6H), 3.06 – 2.99 (m, 2H), 2.89 – 2.81 (m, 2H), 1.20 (t, J = 7.0 Hz, 3H).



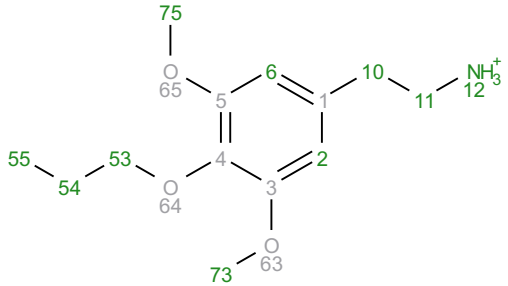
Prediction	Escaline H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



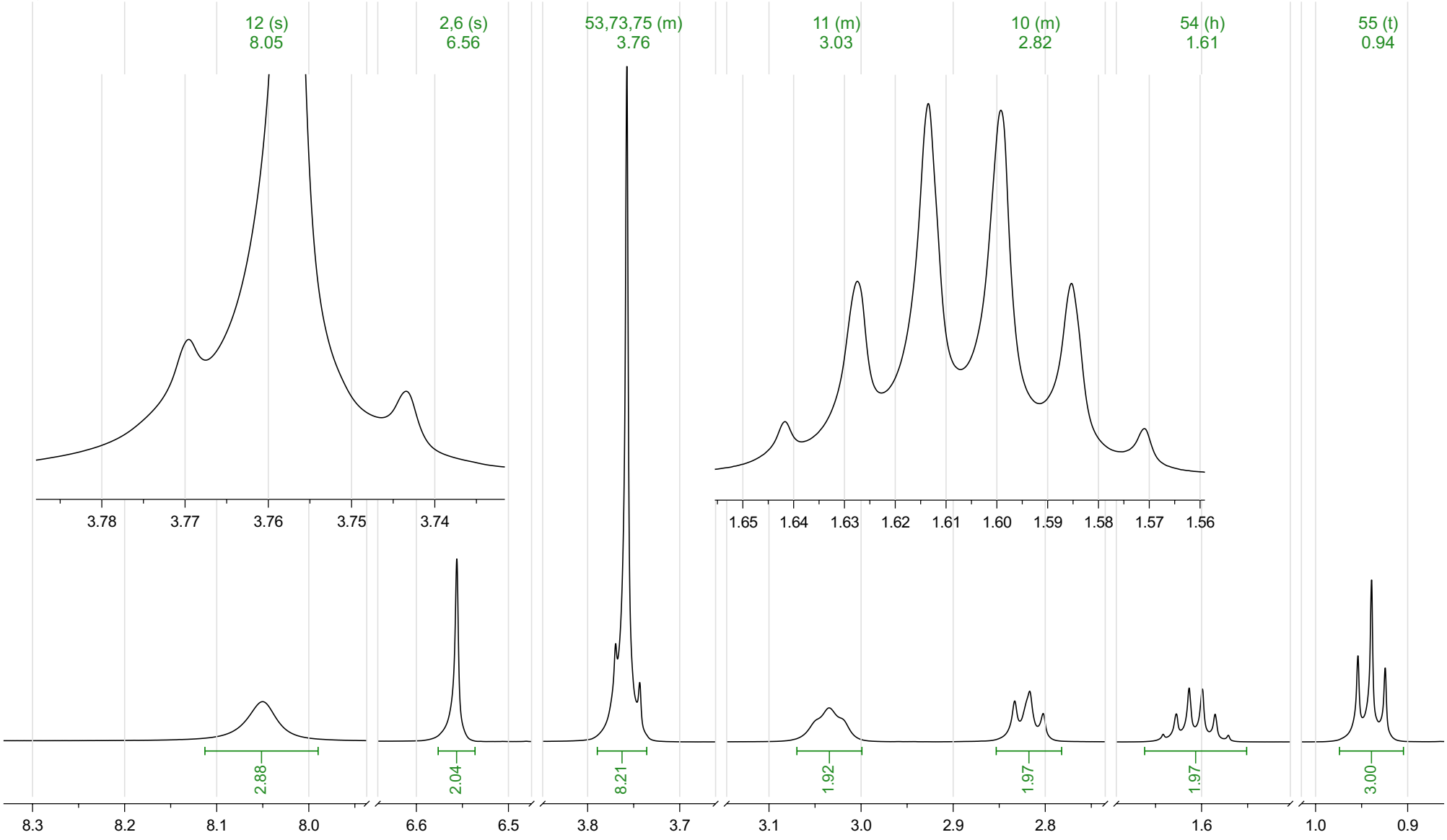
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.10 (s, 3H), 6.54 (t, J = 1.0 Hz, 2H), 4.08 (q, J = 5.9 Hz, 2H), 3.70 (s, 6H), 3.66 (t, J = 7.6 Hz, 2H), 3.13 (tt, J = 7.5, 1.1 Hz, 2H), 1.34 (t, J = 5.8 Hz, 3H).



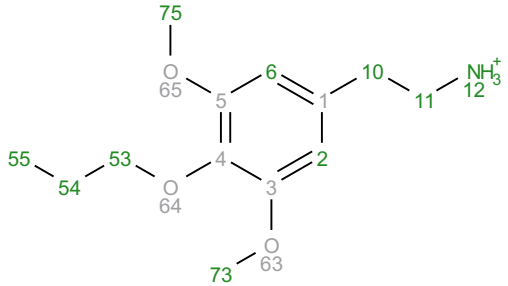
Analyte	P13a: Proscaline H+
Acquisition Date	2012-11-24T12:58:57
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



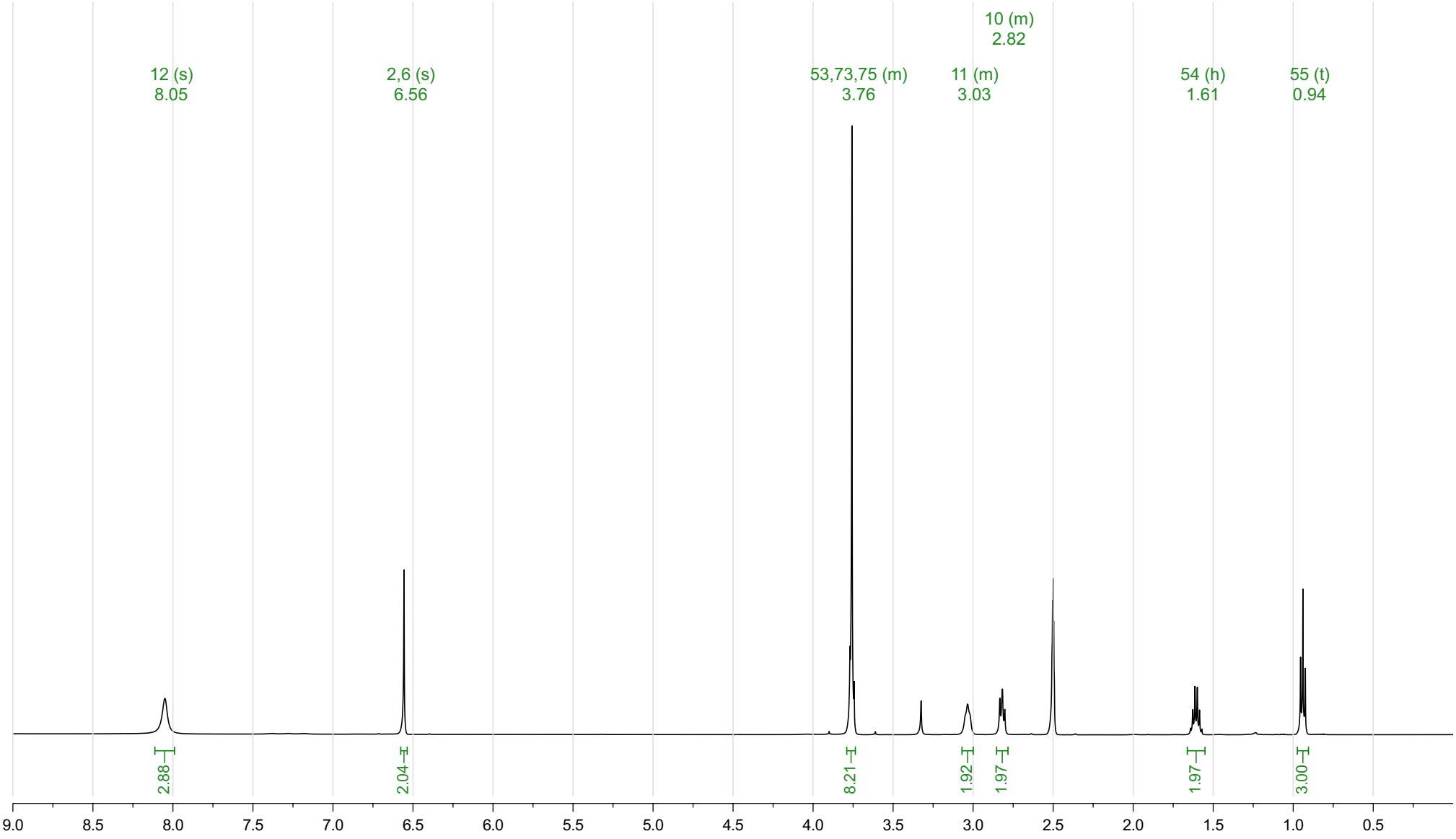
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.05 (s, 3H), 6.56 (s, 2H), 3.79 – 3.72 (m, 8H), 3.07 – 3.00 (m, 2H), 2.85 – 2.78 (m, 2H), 1.61 (h, J = 7.1 Hz, 2H), 0.94 (t, J = 7.4 Hz, 3H).



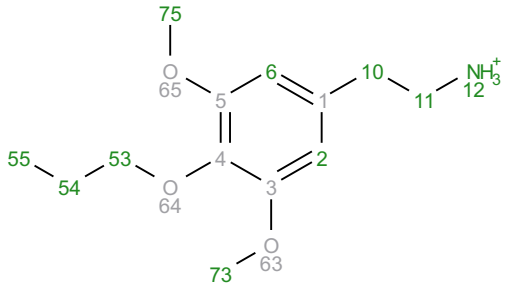
Analyte	P13a: Proscaline H+
Acquisition Date	2012-11-24T12:58:57
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



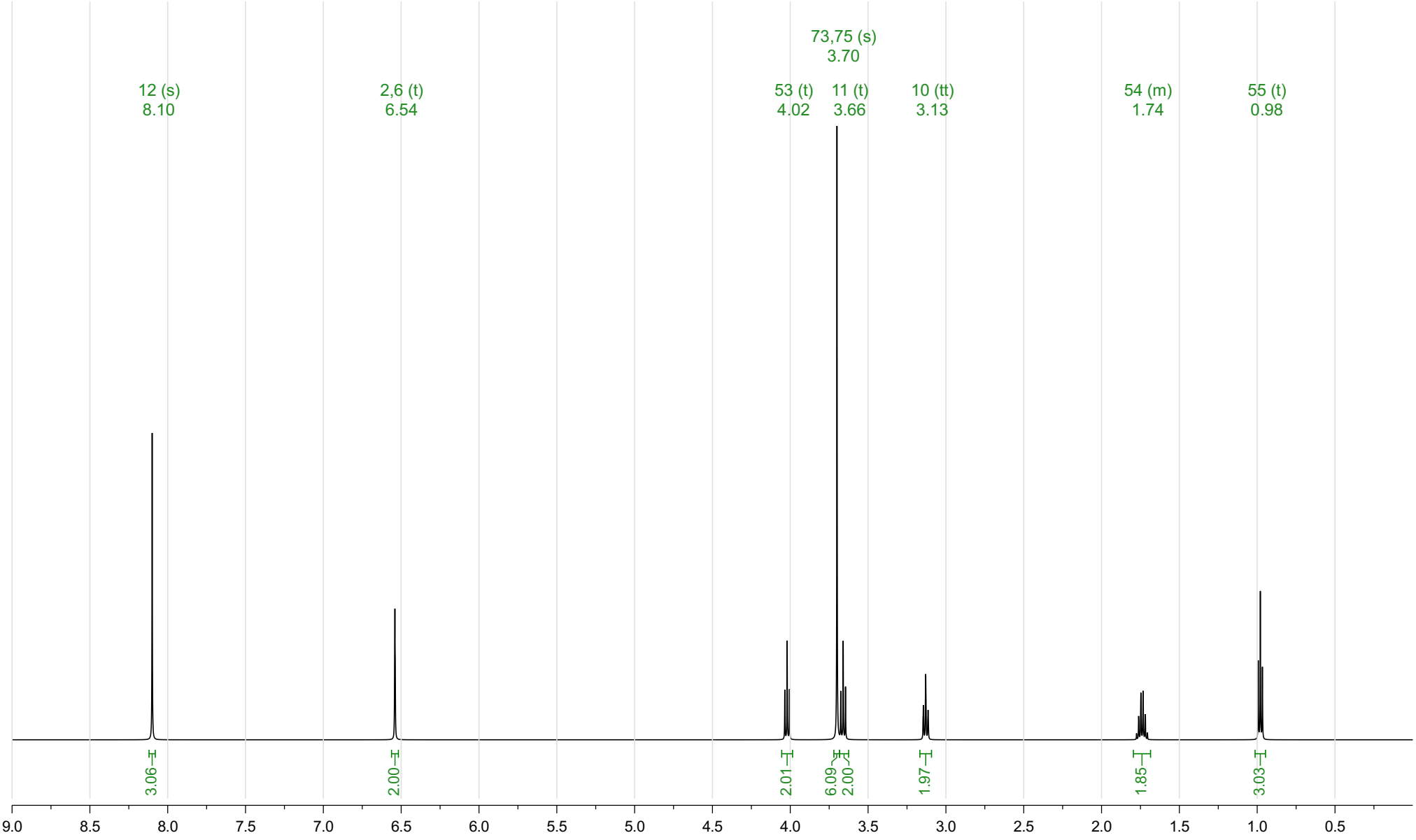
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.05 (s, 3H), 6.56 (s, 2H), 3.79 – 3.72 (m, 8H), 3.07 – 3.00 (m, 2H), 2.85 – 2.78 (m, 2H), 1.61 (h, J = 7.1 Hz, 2H), 0.94 (t, J = 7.4 Hz, 3H).



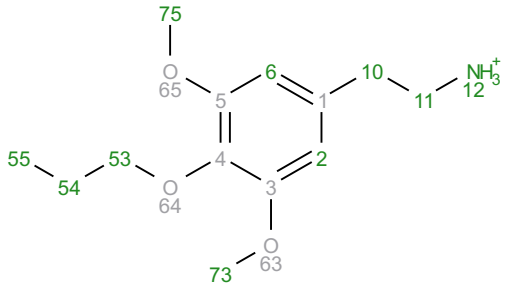
Prediction	Proscaline H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11880
Frequency	500.00
Nucleus	1H



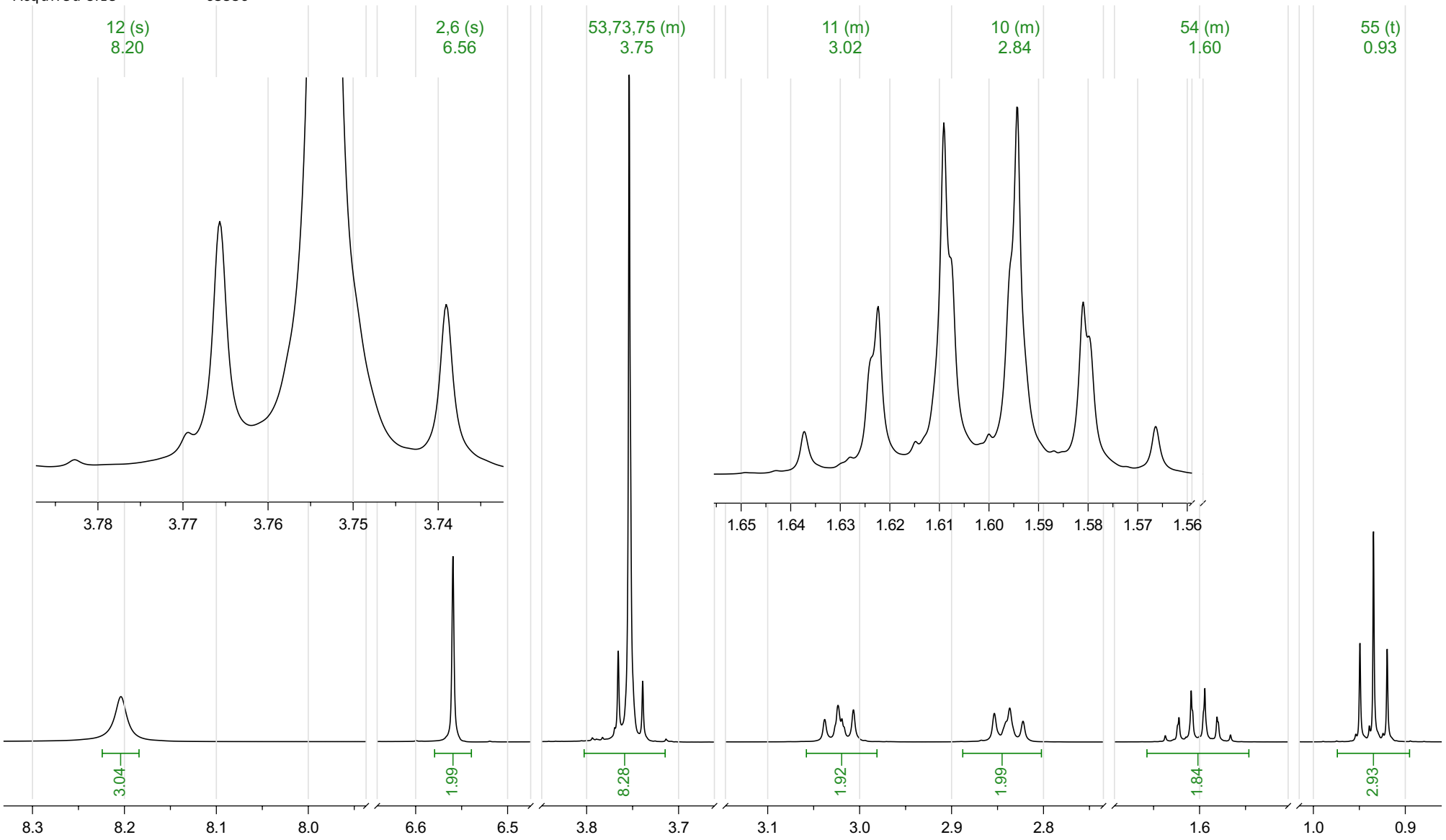
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.10 (s, 3H), 6.54 (t, *J* = 1.0 Hz, 2H), 4.02 (t, *J* = 7.5 Hz, 2H), 3.70 (s, 6H), 3.66 (t, *J* = 7.6 Hz, 2H), 3.13 (tt, *J* = 7.5, 1.1 Hz, 2H), 1.80 – 1.69 (m, 2H), 0.98 (t, *J* = 6.7 Hz, 3H).



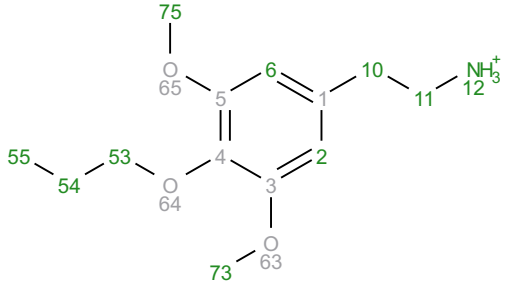
Analyte	P13b: Proscaline H+
Acquisition Date	2013-03-26T19:44:08
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	10964.9
Nucleus	1H
Acquired Size	65536



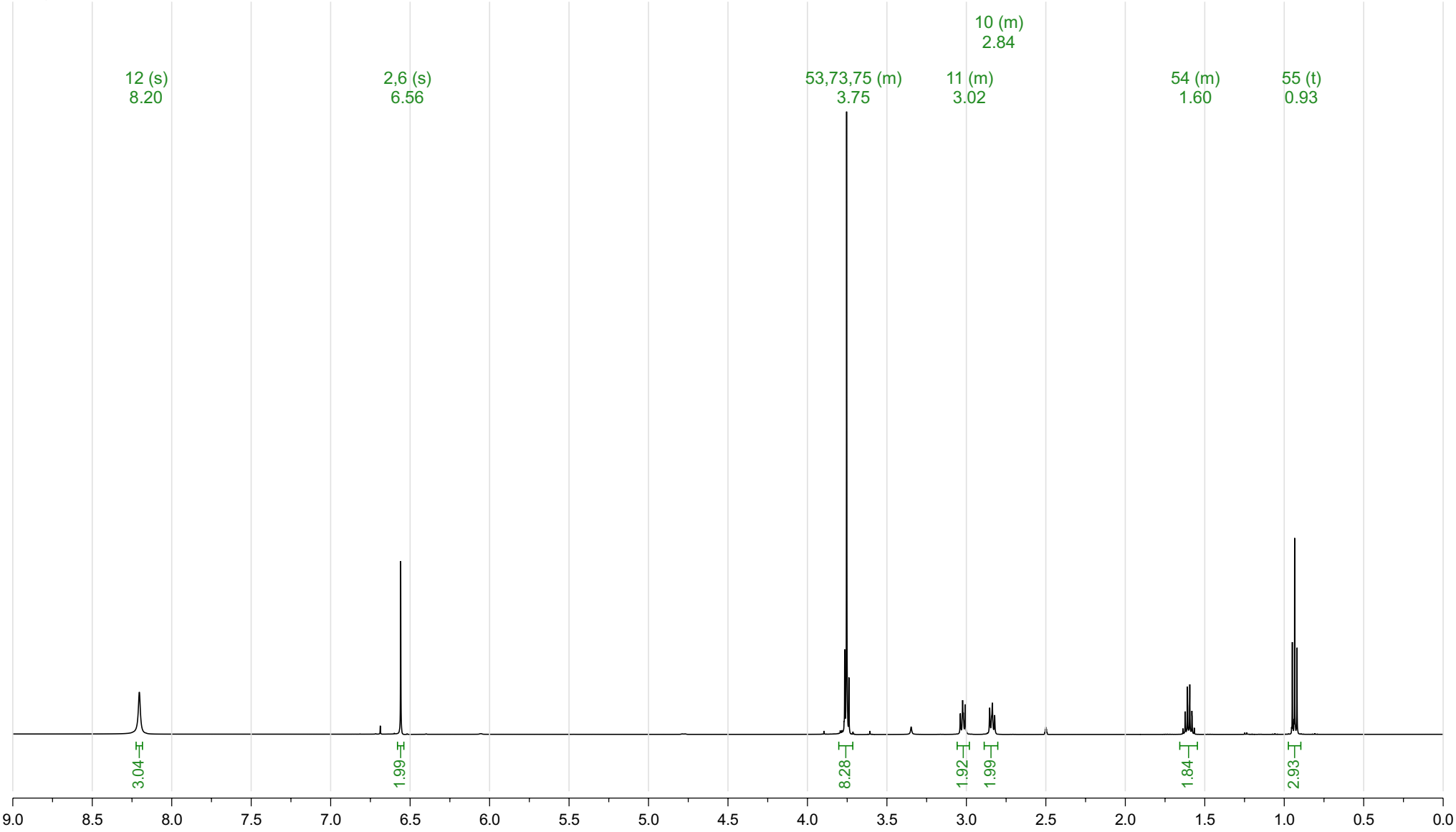
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.20 (s, 3H), 6.56 (s, 2H), 3.80 – 3.71 (m, 8H), 3.06 – 2.98 (m, 2H), 2.89 – 2.80 (m, 2H), 1.66 – 1.55 (m, 2H), 0.93 (t, *J* = 7.4 Hz, 3H).



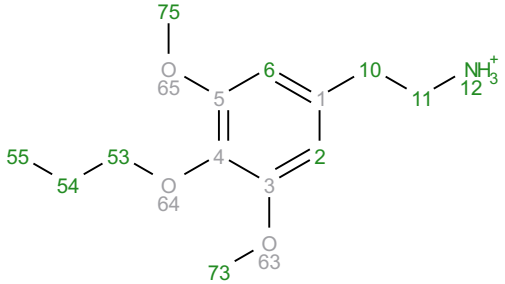
Analyte	P13b: Proscaline H+
Acquisition Date	2013-03-26T19:44:08
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	10964.9
Nucleus	1H
Acquired Size	65536



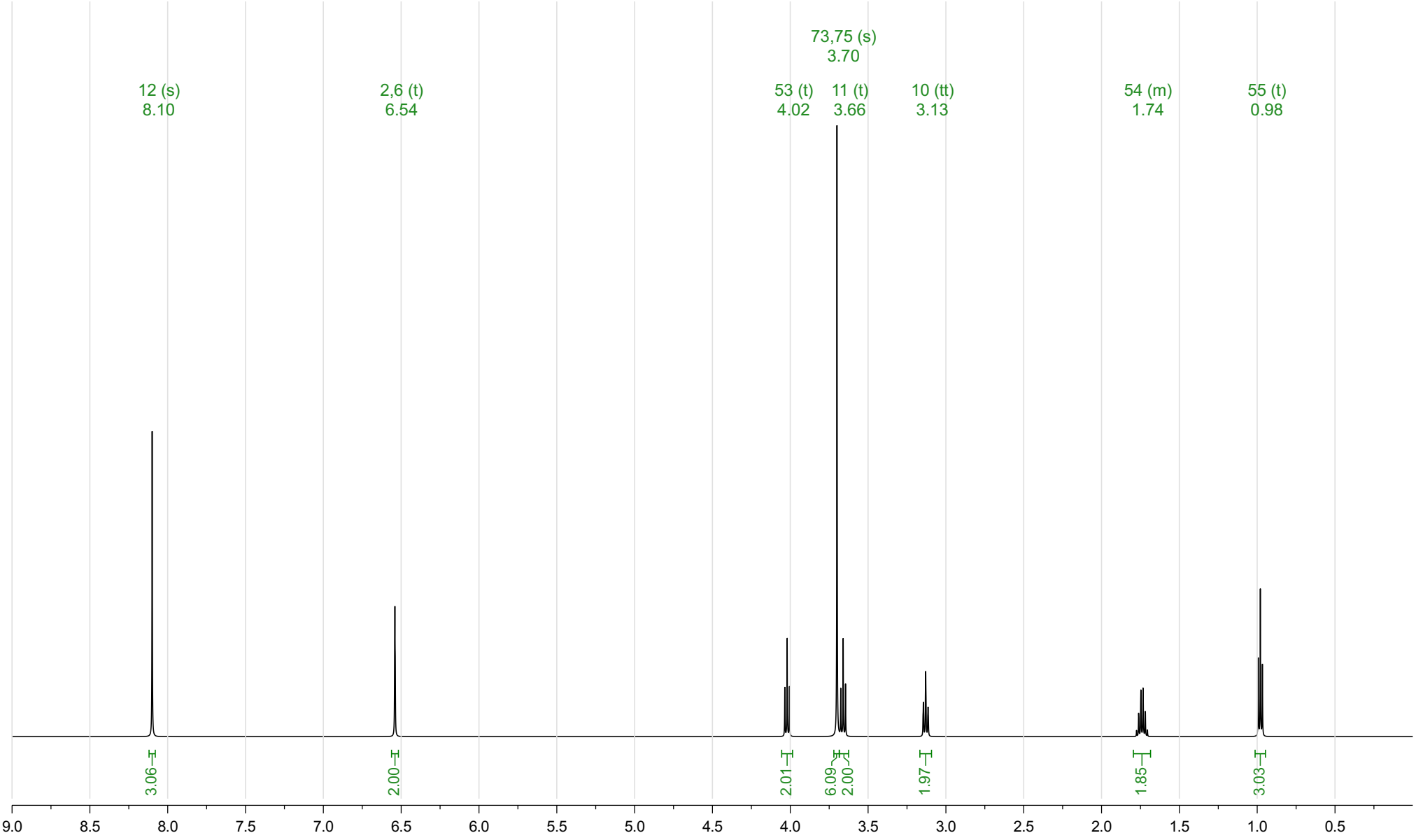
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.20 (s, 3H), 6.56 (s, 2H), 3.80 – 3.71 (m, 8H), 3.06 – 2.98 (m, 2H), 2.89 – 2.80 (m, 2H), 1.66 – 1.55 (m, 2H), 0.93 (t, *J* = 7.4 Hz, 3H).



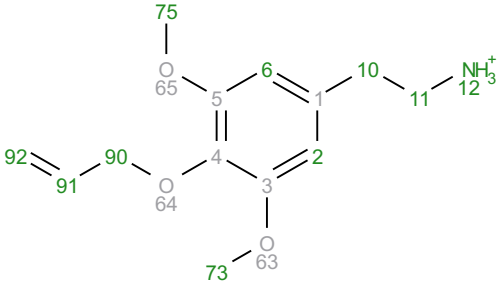
Prediction	Proscaline H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



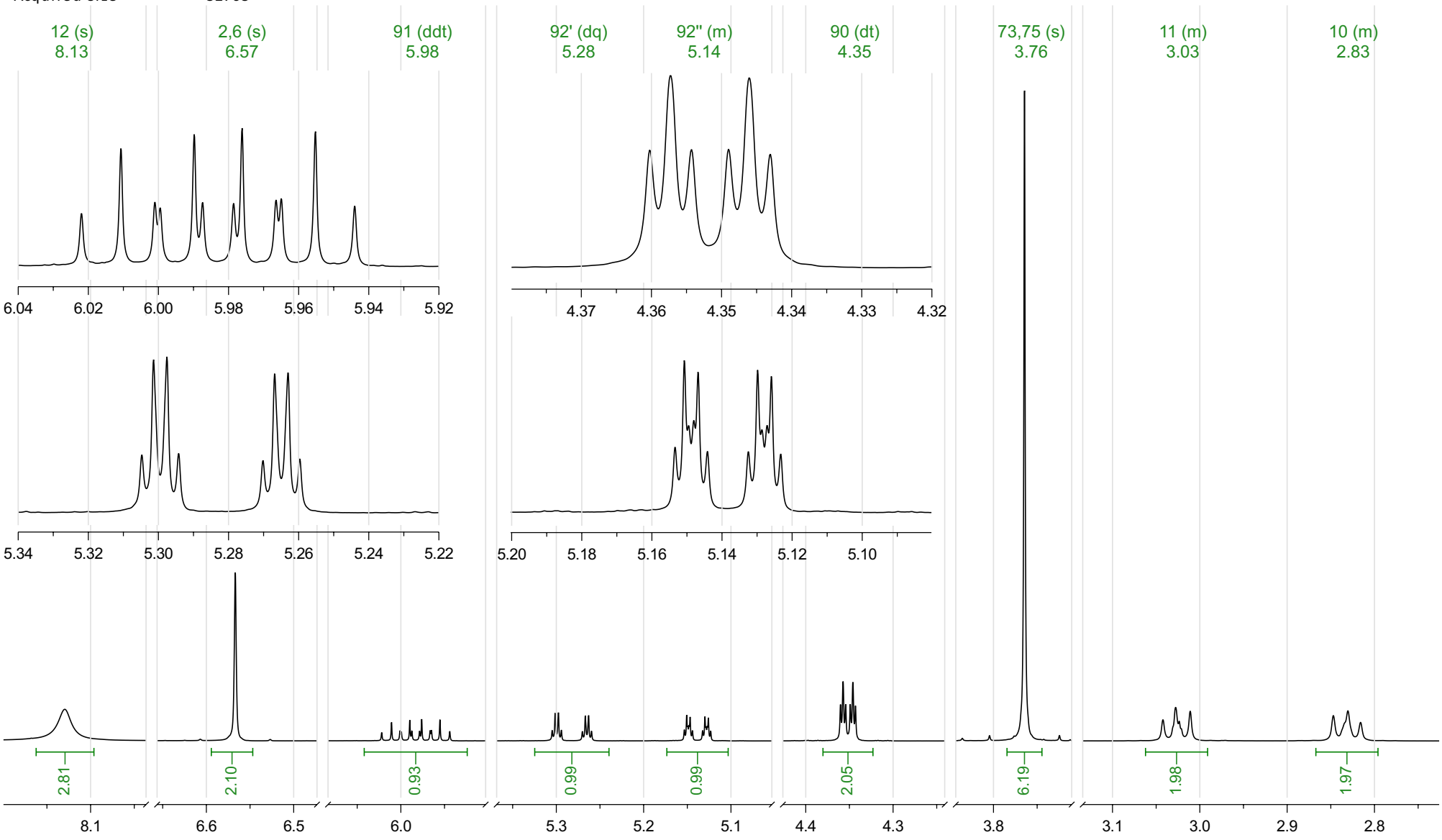
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.10 (s, 3H), 6.54 (t, J = 1.0 Hz, 2H), 4.02 (t, J = 7.5 Hz, 2H), 3.70 (s, 6H), 3.66 (t, J = 7.6 Hz, 2H), 3.13 (tt, J = 7.5, 1.1 Hz, 2H), 1.80 – 1.69 (m, 2H), 0.98 (t, J = 6.7 Hz, 3H).



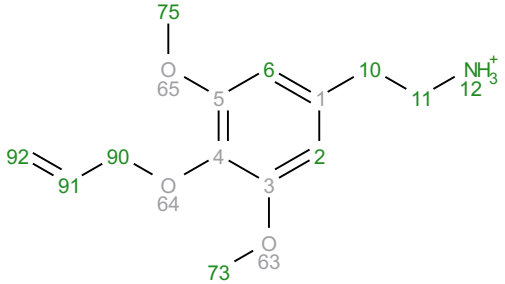
Analyte	P14: AL H+
Acquisition Date	2012-11-24T14:23:49
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



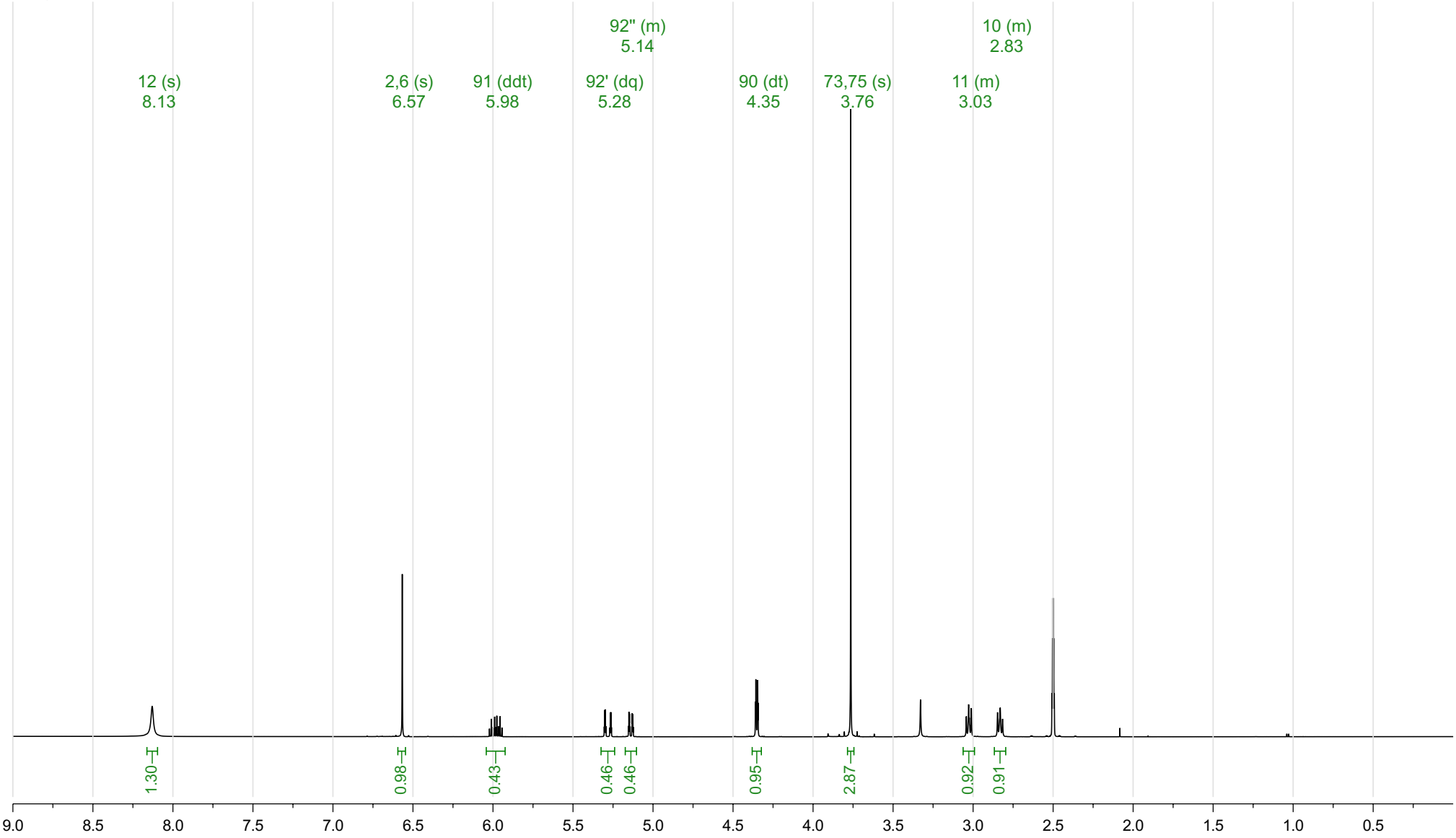
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.13 (s, 3H), 6.57 (s, 2H), 5.98 (ddt, J = 17.3, 10.4, 5.6 Hz, 1H), 5.28 (dq, J = 17.3, 1.8 Hz, 1H), 5.17 – 5.10 (m, 1H), 4.35 (dt, J = 5.6, 1.6 Hz, 2H), 3.76 (s, 6H), 3.06 – 2.99 (m, 2H), 2.87 – 2.80 (m, 2H).



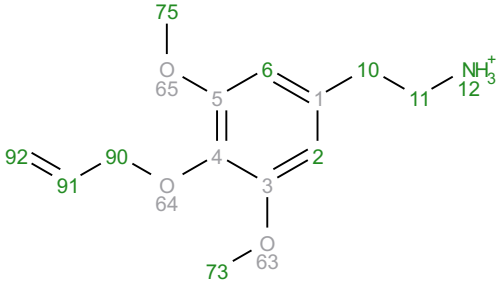
Analyte	P14: AL H+
Acquisition Date	2012-11-24T14:23:49
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



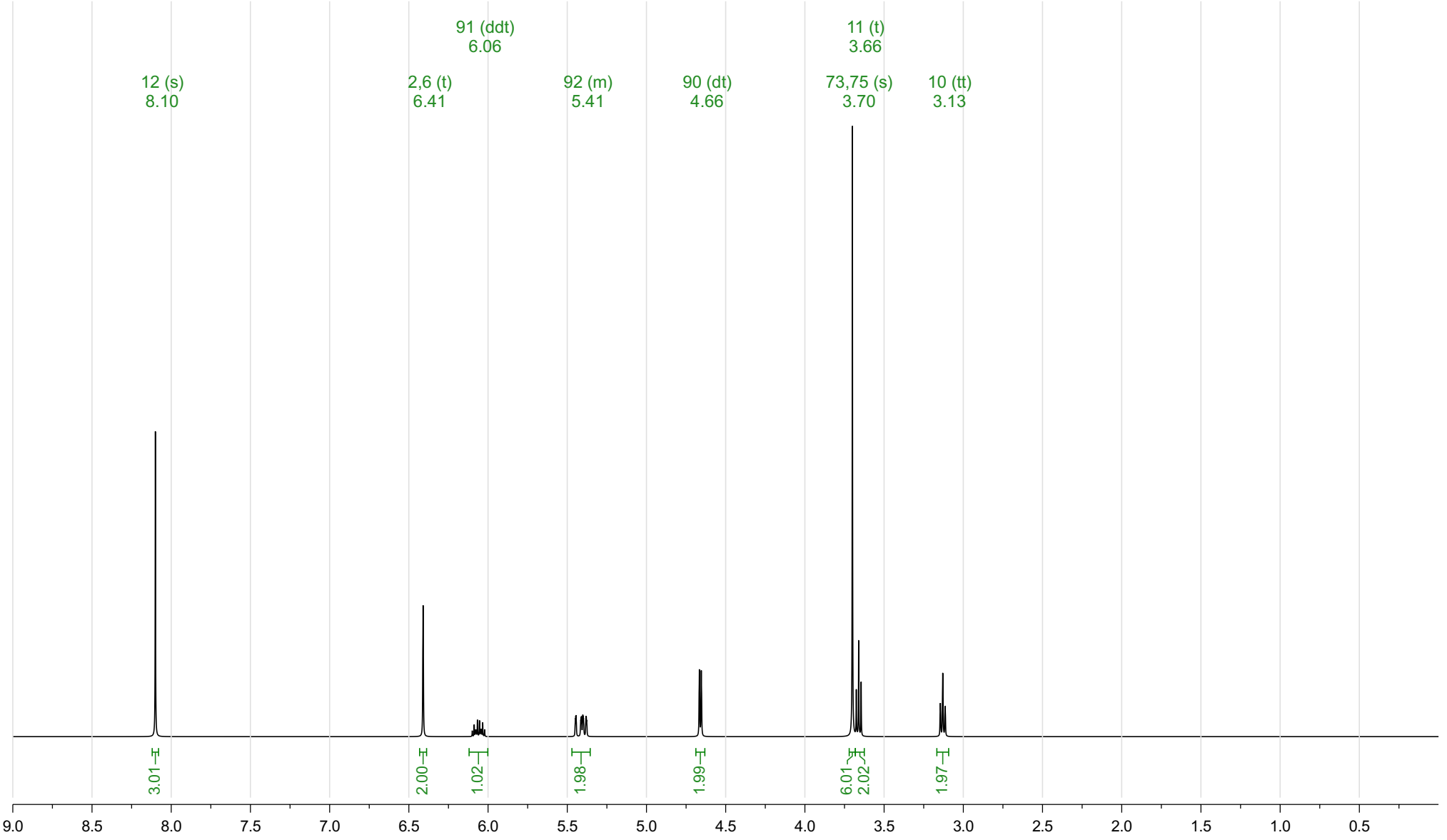
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.13 (s, 3H), 6.57 (s, 2H), 5.98 (ddt, J = 17.3, 10.4, 5.6 Hz, 1H), 5.28 (dq, J = 17.3, 1.8 Hz, 1H), 5.17 – 5.10 (m, 1H), 4.35 (dt, J = 5.6, 1.6 Hz, 2H), 3.76 (s, 6H), 3.06 – 2.99 (m, 2H), 2.87 – 2.80 (m, 2H).



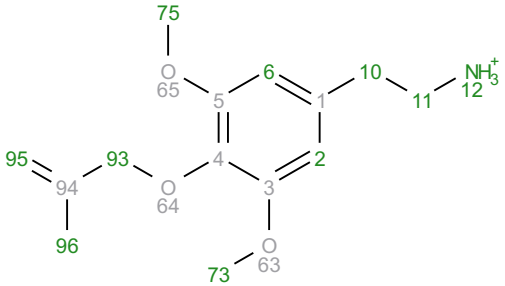
Prediction	AL H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	12489
Frequency	500.00
Nucleus	1H



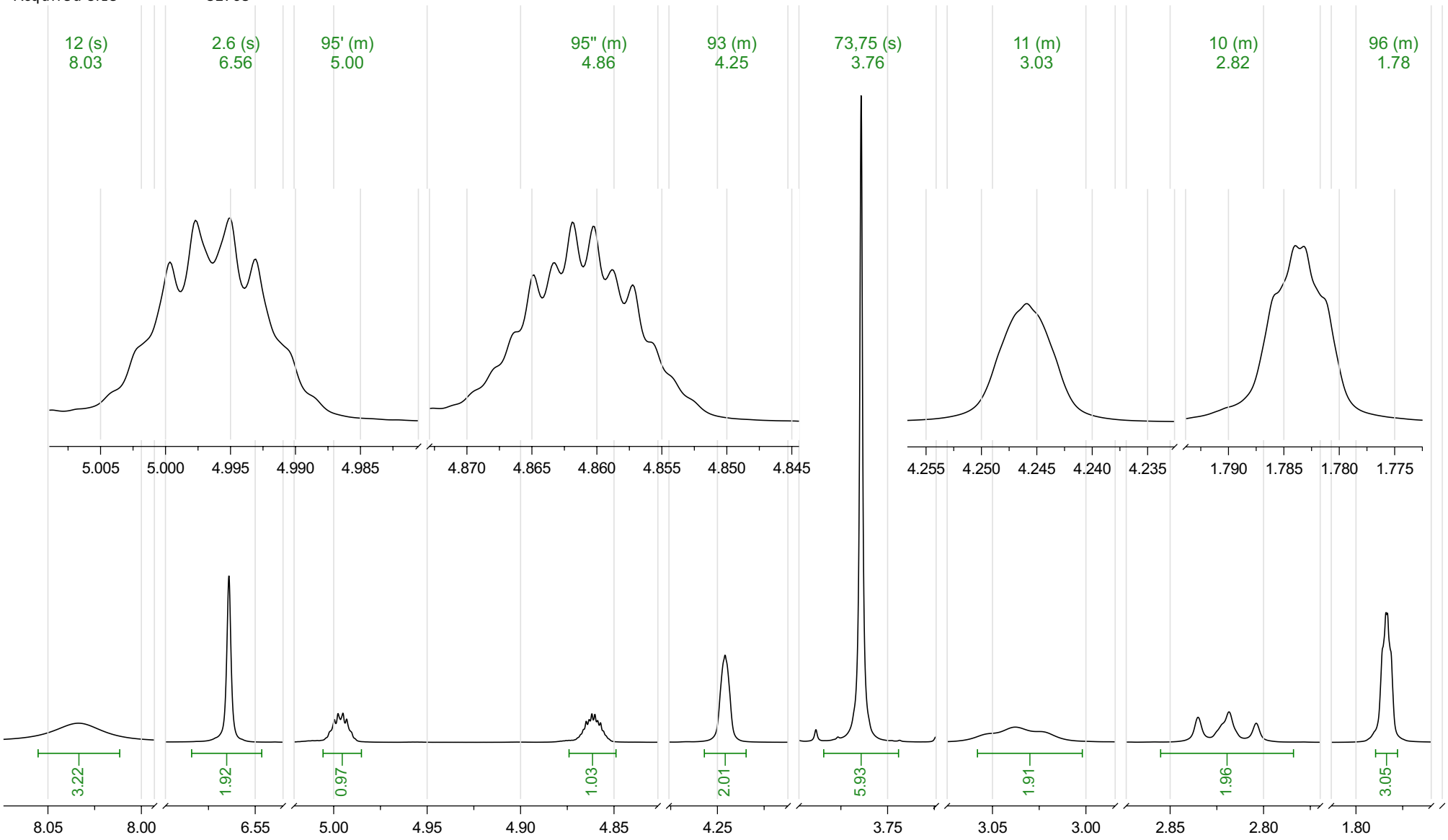
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.10 (s, 3H), 6.41 (t, J = 1.0 Hz, 2H), 6.06 (ddt, J = 16.3, 10.0, 6.1 Hz, 1H), 5.47 – 5.36 (m, 2H), 4.66 (dt, J = 6.2, 1.1 Hz, 2H), 3.70 (s, 6H), 3.66 (t, J = 7.6 Hz, 2H), 3.13 (tt, J = 7.6, 1.2 Hz, 2H).



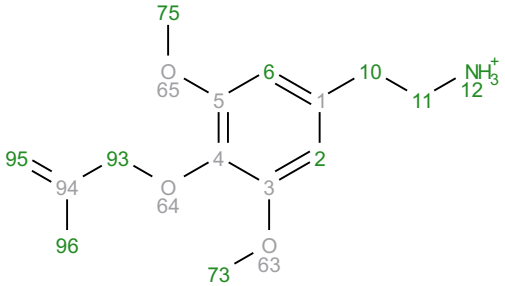
Analyte	P15: MAL H+
Acquisition Date	2012-11-24T12:41:39
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



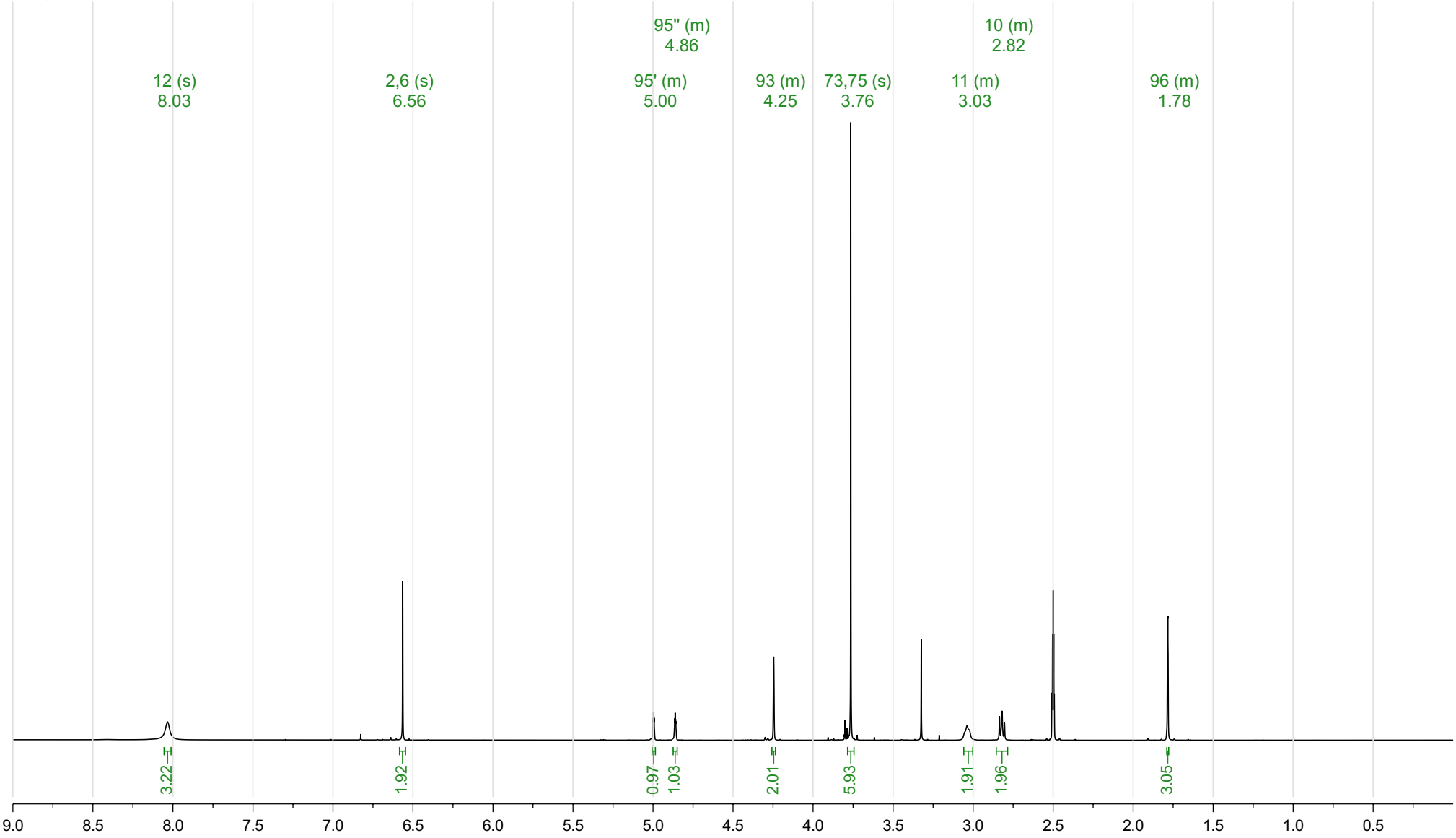
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.03 (s, 3H), 6.56 (s, 2H), 5.02 – 4.97 (m, 1H), 4.89 – 4.83 (m, 1H), 4.27 – 4.22 (m, 2H), 3.76 (s, 6H), 3.06 – 3.00 (m, 2H), 2.86 – 2.78 (m, 2H), 1.81 – 1.76 (m, 3H).



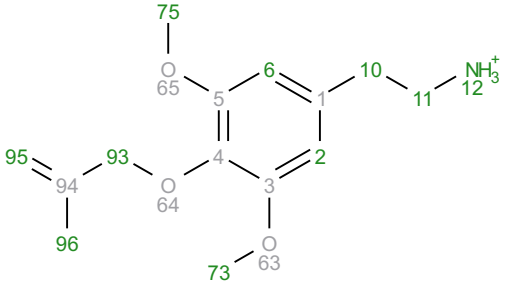
Analyte	P15: MAL H+
Acquisition Date	2012-11-24T12:41:39
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



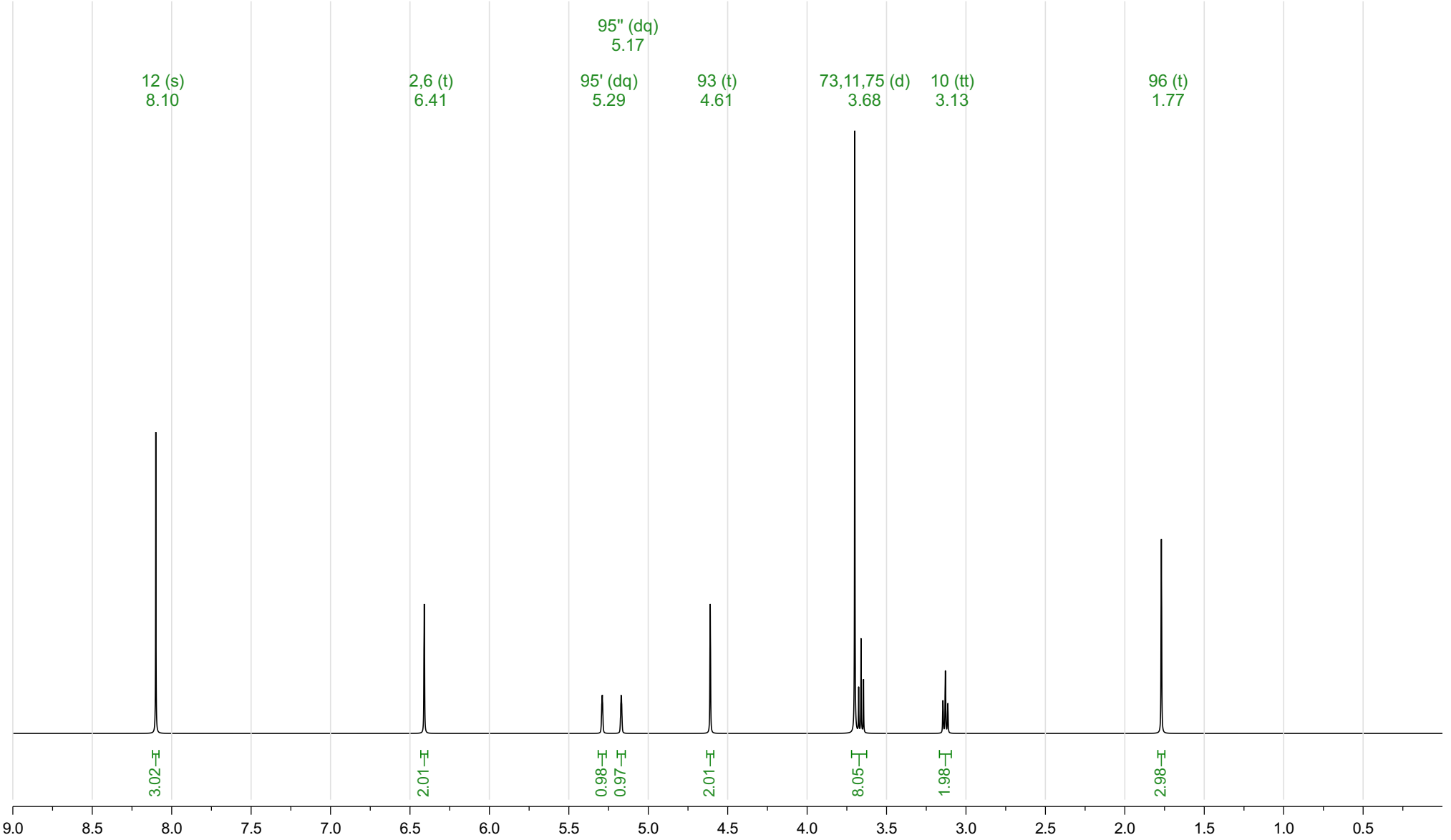
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.03 (s, 3H), 6.56 (s, 2H), 5.02 – 4.97 (m, 1H), 4.89 – 4.83 (m, 1H), 4.27 – 4.22 (m, 2H), 3.76 (s, 6H), 3.06 – 3.00 (m, 2H), 2.86 – 2.78 (m, 2H), 1.81 – 1.76 (m, 3H).



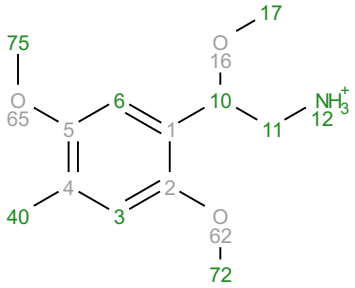
Prediction	MAL H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	12489
Frequency	500.00
Nucleus	1H



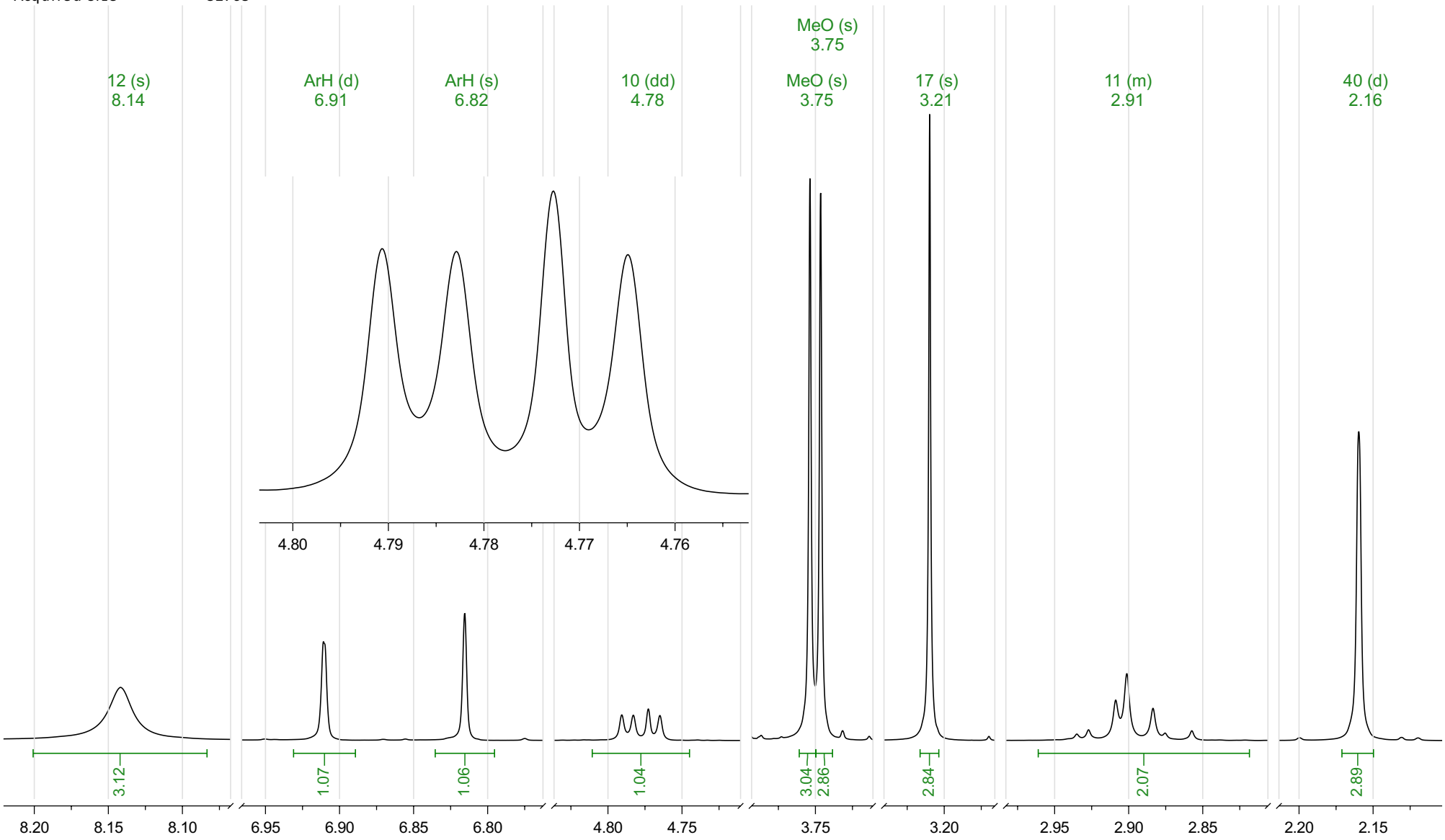
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.10 (s, 3H), 6.41 (t, J = 1.0 Hz, 2H), 5.29 (dq, J = 2.2, 1.1 Hz, 1H), 5.17 (dq, J = 2.2, 1.1 Hz, 1H), 4.61 (t, J = 1.0 Hz, 2H), 3.68 (d, J = 19.9 Hz, 8H), 3.13 (tt, J = 7.6, 1.2 Hz, 2H), 1.77 (t, J = 1.0 Hz, 3H).



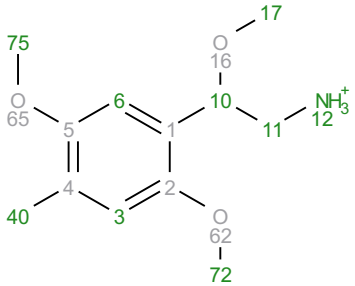
Analyte	P16: BOD H+
Acquisition Date	2012-11-24T12:49:33
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



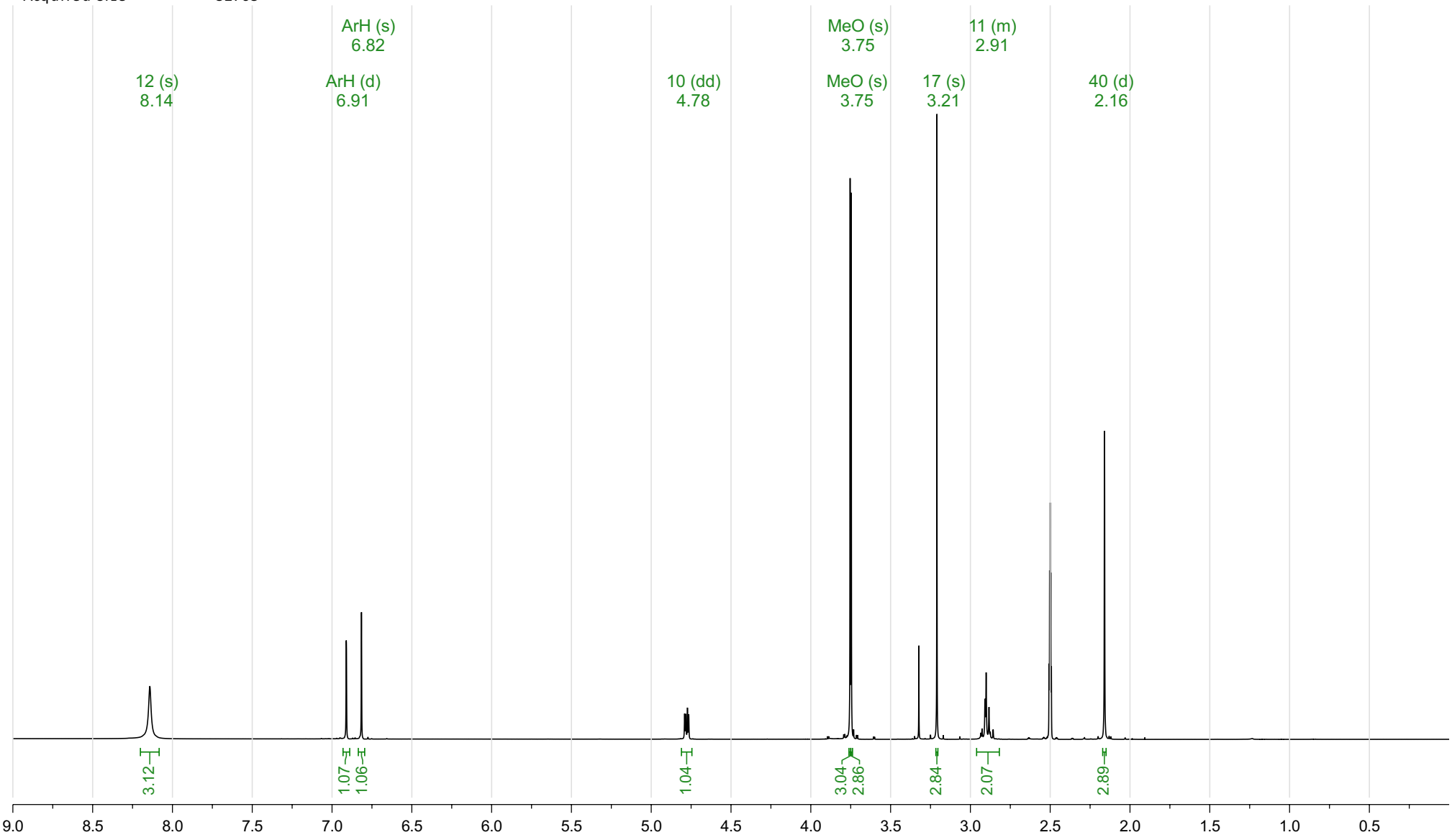
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.14 (s, 3H), 6.91 (d, J = 0.9 Hz, 1H), 6.82 (s, 1H), 4.78 (dd, J = 8.9, 3.9 Hz, 1H), 3.75 (s, 3H), 3.75 (s, 3H), 3.21 (s, 3H), 2.96 – 2.82 (m, 2H), 2.16 (d, J = 0.9 Hz, 3H).



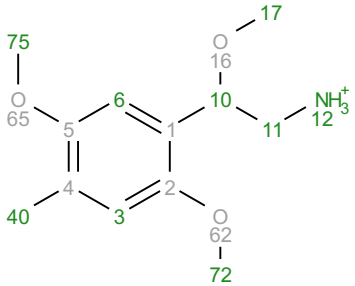
Analyte	P16: BOD H+
Acquisition Date	2012-11-24T12:49:33
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



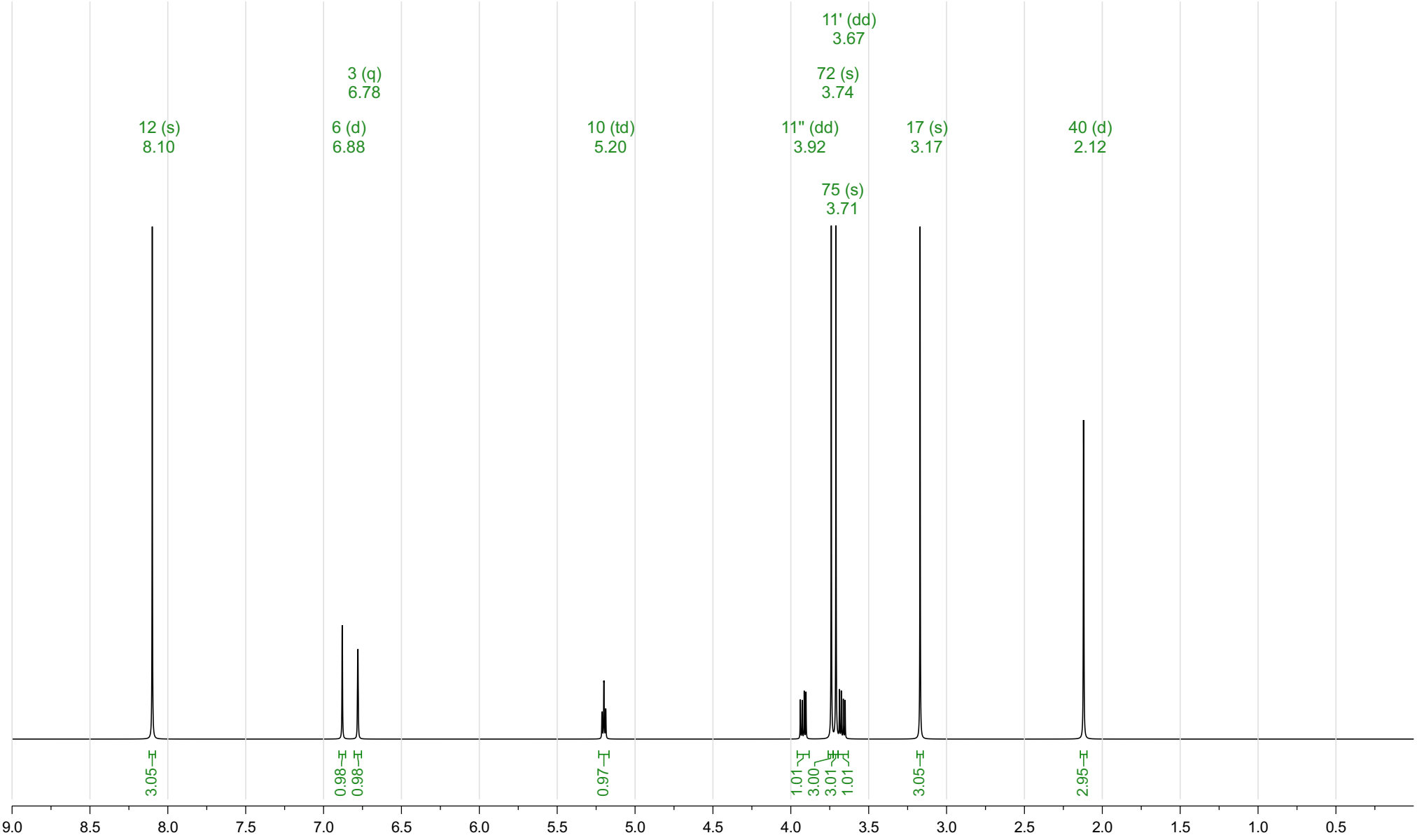
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.14 (s, 3H), 6.91 (d, J = 0.9 Hz, 1H), 6.82 (s, 1H), 4.78 (dd, J = 8.9, 3.9 Hz, 1H), 3.75 (s, 3H), 3.75 (s, 3H), 3.21 (s, 3H), 2.96 – 2.82 (m, 2H), 2.16 (d, J = 0.9 Hz, 3H).



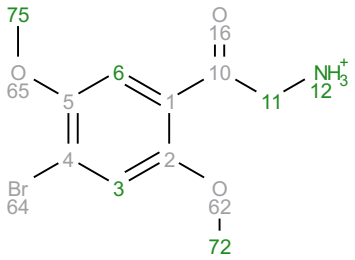
Prediction	BOD H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



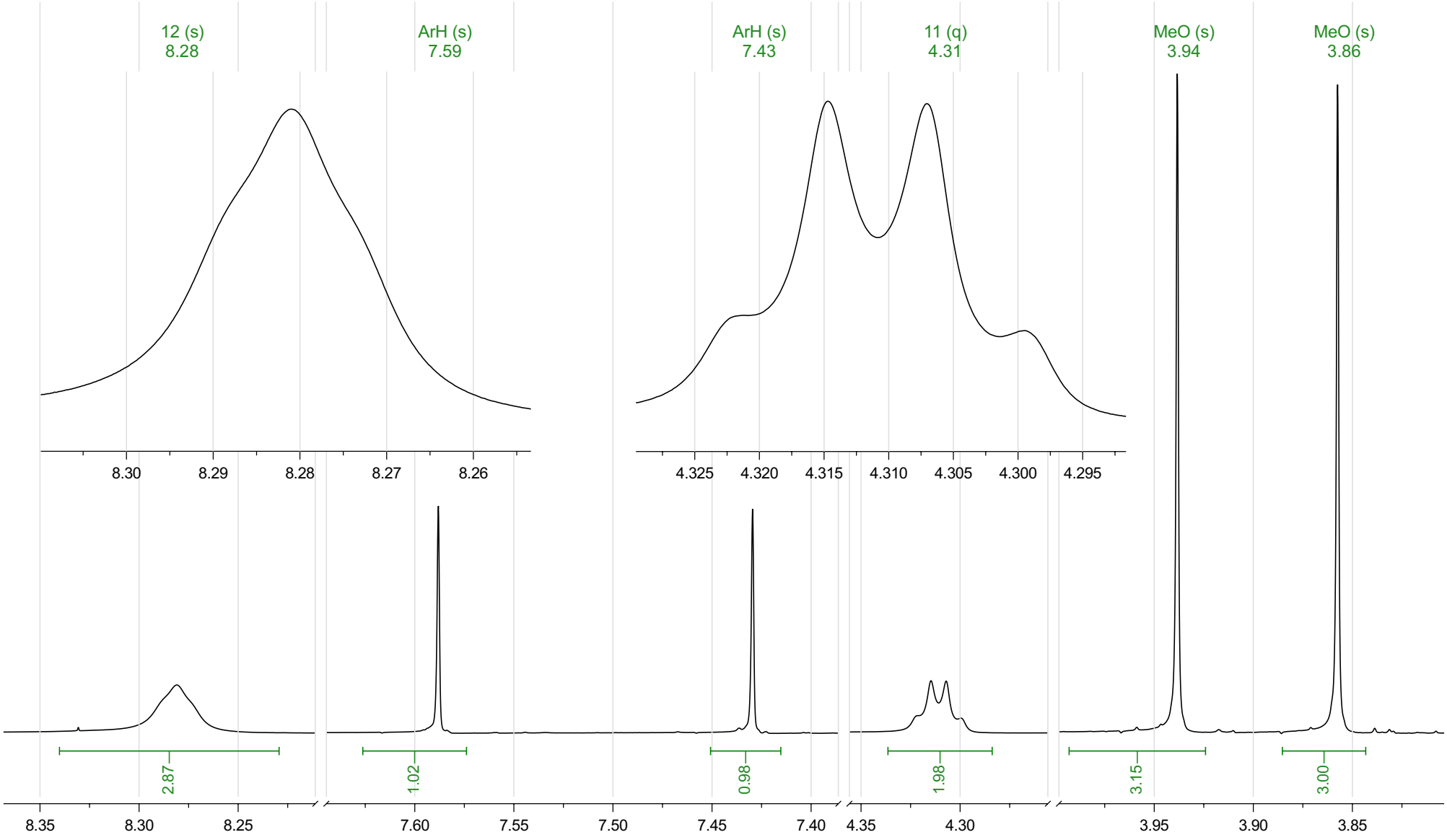
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.10 (s, 3H), 6.88 (d, *J* = 1.0 Hz, 1H), 6.78 (q, *J* = 1.1 Hz, 1H), 5.20 (td, *J* = 6.0, 1.0 Hz, 1H), 3.92 (dd, *J* = 12.4, 5.8 Hz, 1H), 3.74 (s, 3H), 3.71 (s, 3H), 3.67 (dd, *J* = 12.4, 5.9 Hz, 1H), 3.17 (s, 3H), 2.12 (d, *J* = 1.1 Hz, 3H).



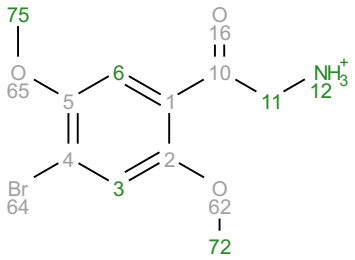
Analyte	P17: bk-2C-B H+
Acquisition Date	2013-11-29T14:34:40
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	699.82
Spectral Width	11160.7
Nucleus	1H
Acquired Size	50223



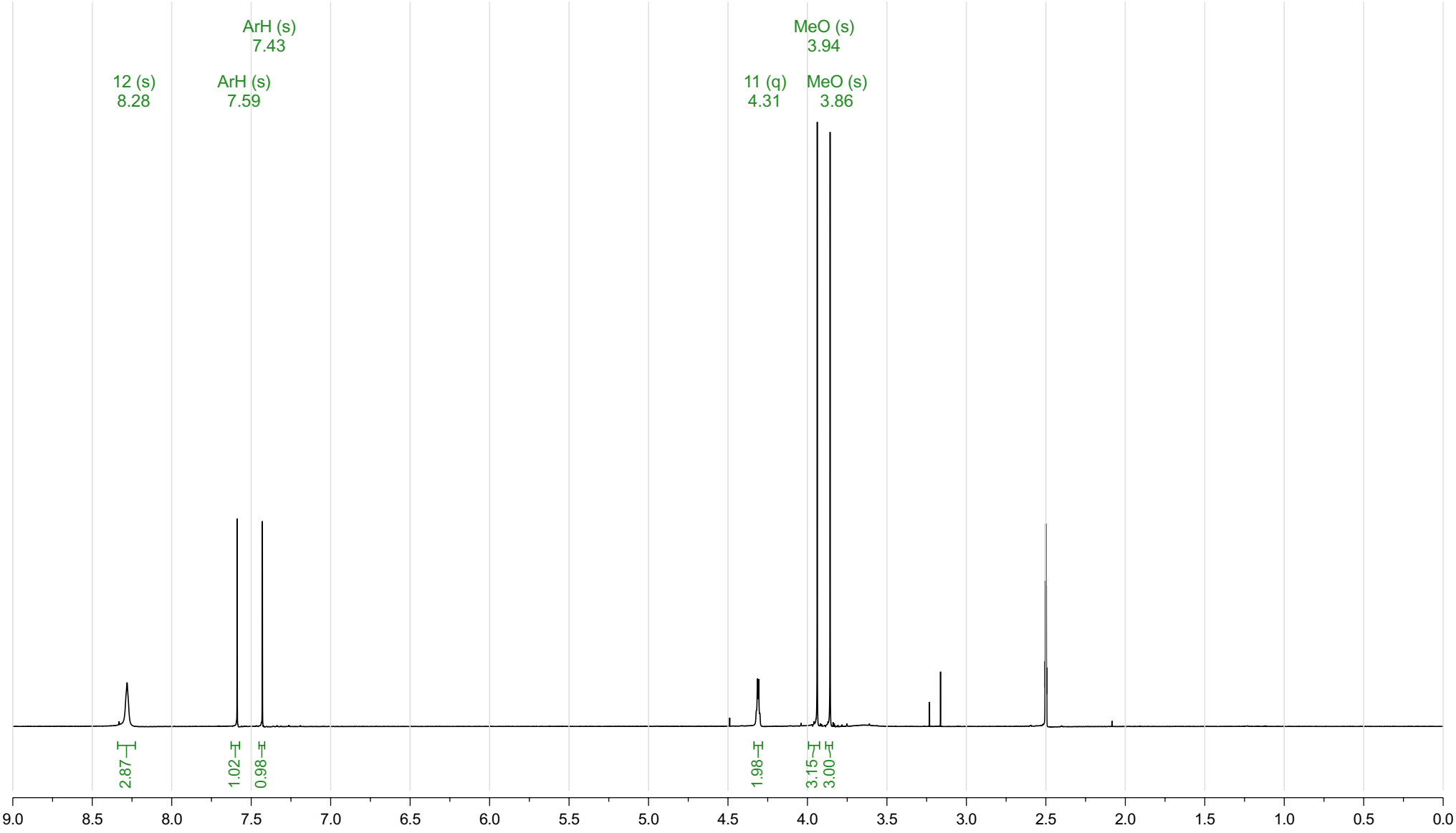
^{1}H NMR (700 MHz, DMSO-d_6) δ 8.28 (s, 3H), 7.59 (s, 1H), 7.43 (s, 1H), 4.31 (q, J = 5.2 Hz, 2H), 3.94 (s, 3H), 3.86 (s, 3H).



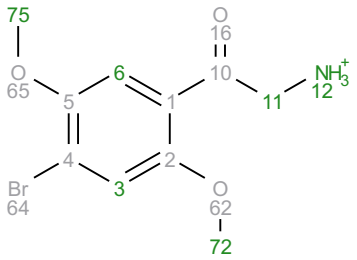
Analyte	P17: bk-2C-B H+
Acquisition Date	2013-11-29T14:34:40
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	699.82
Spectral Width	11160.7
Nucleus	1H
Acquired Size	50223



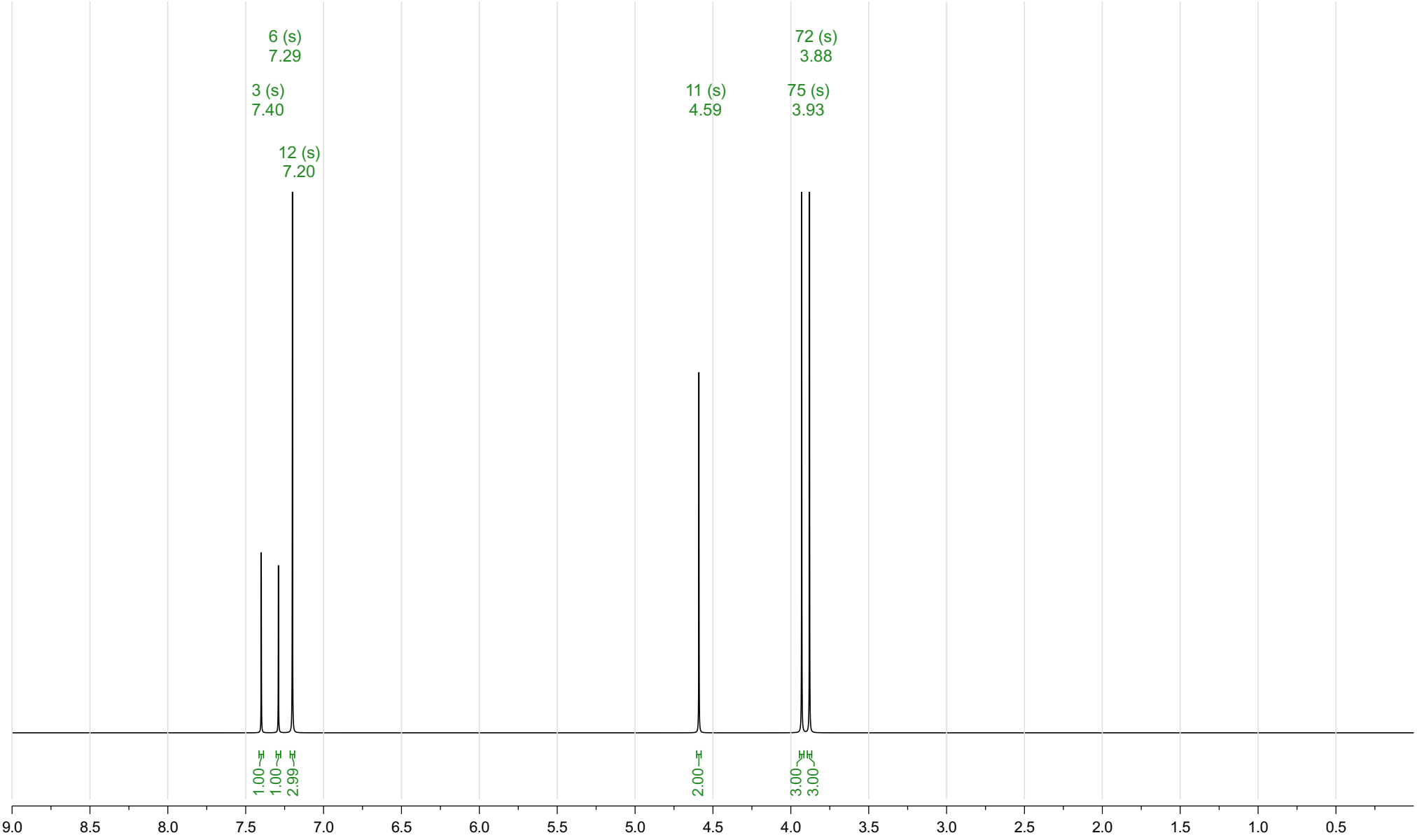
^{1}H NMR (700 MHz, DMSO-d_6) δ 8.28 (s, 3H), 7.59 (s, 1H), 7.43 (s, 1H), 4.31 (q, J = 5.2 Hz, 2H), 3.94 (s, 3H), 3.86 (s, 3H).



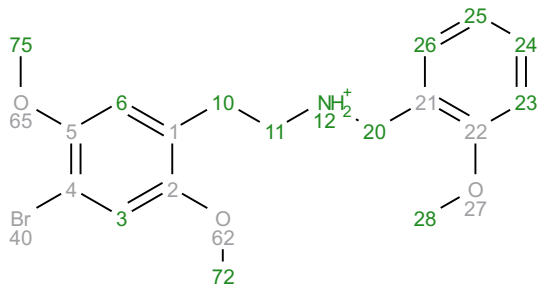
Prediction	bk-2C-B H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	12489
Frequency	700.00
Nucleus	1H



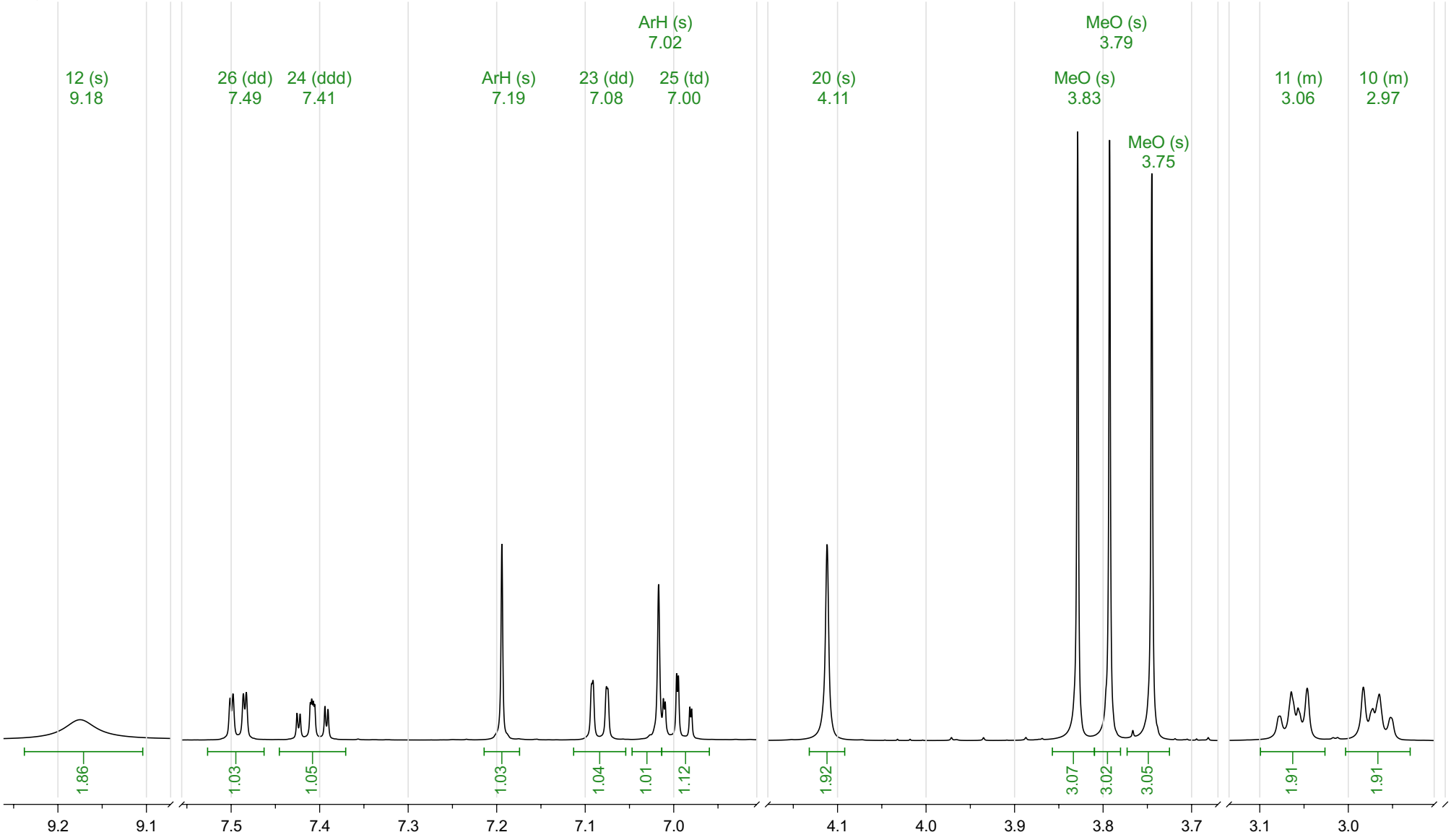
^{1}H NMR (700 MHz, DMSO-d_6) δ 7.40 (s, 1H), 7.29 (s, 1H), 7.20 (s, 3H), 4.59 (s, 2H), 3.93 (s, 3H), 3.88 (s, 3H).



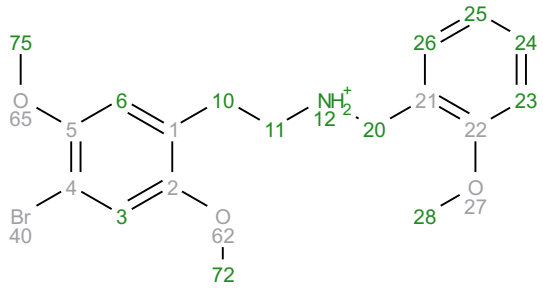
Analyte	B1: 25B-NBOMe H+
Acquisition Date	2013-01-17T02:31:12
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



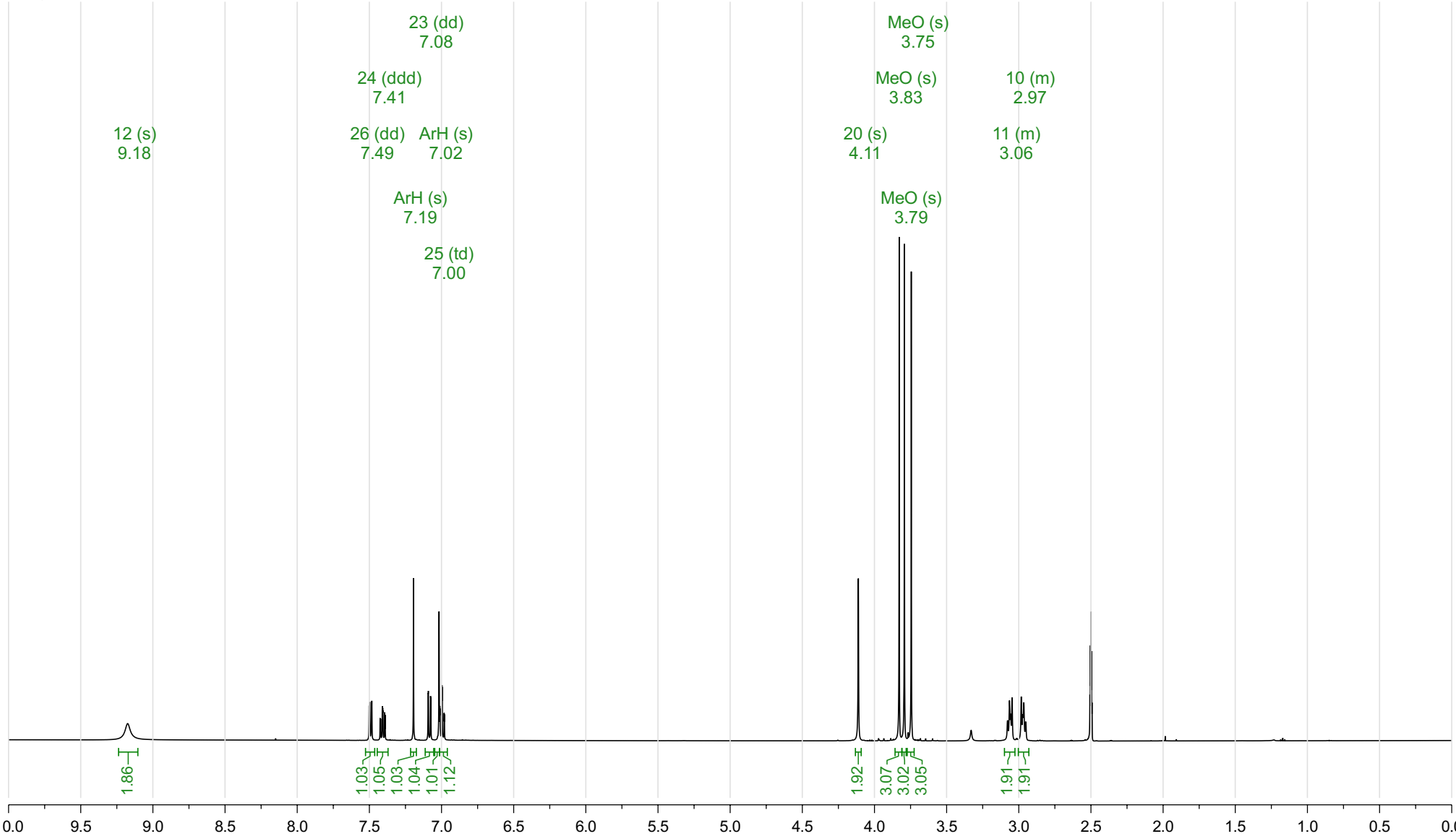
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.18 (s, 2H), 7.49 (dd, J = 7.5, 1.7 Hz, 1H), 7.41 (ddd, J = 8.3, 7.5, 1.7 Hz, 1H), 7.19 (s, 1H), 7.08 (dd, J = 8.4, 1.0 Hz, 1H), 7.02 (s, 1H), 7.00 (td, J = 7.4, 1.1 Hz, 1H), 4.11 (s, 2H), 3.83 (s, 3H), 3.79 (s, 3H), 3.75 (s, 3H), 3.10 – 3.03 (m, 2H), 3.00 – 2.93 (m, 2H).



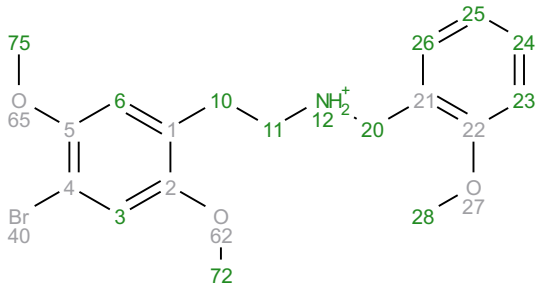
Analyte	B1: 25B-NBOMe H+
Acquisition Date	2013-01-17T02:31:12
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



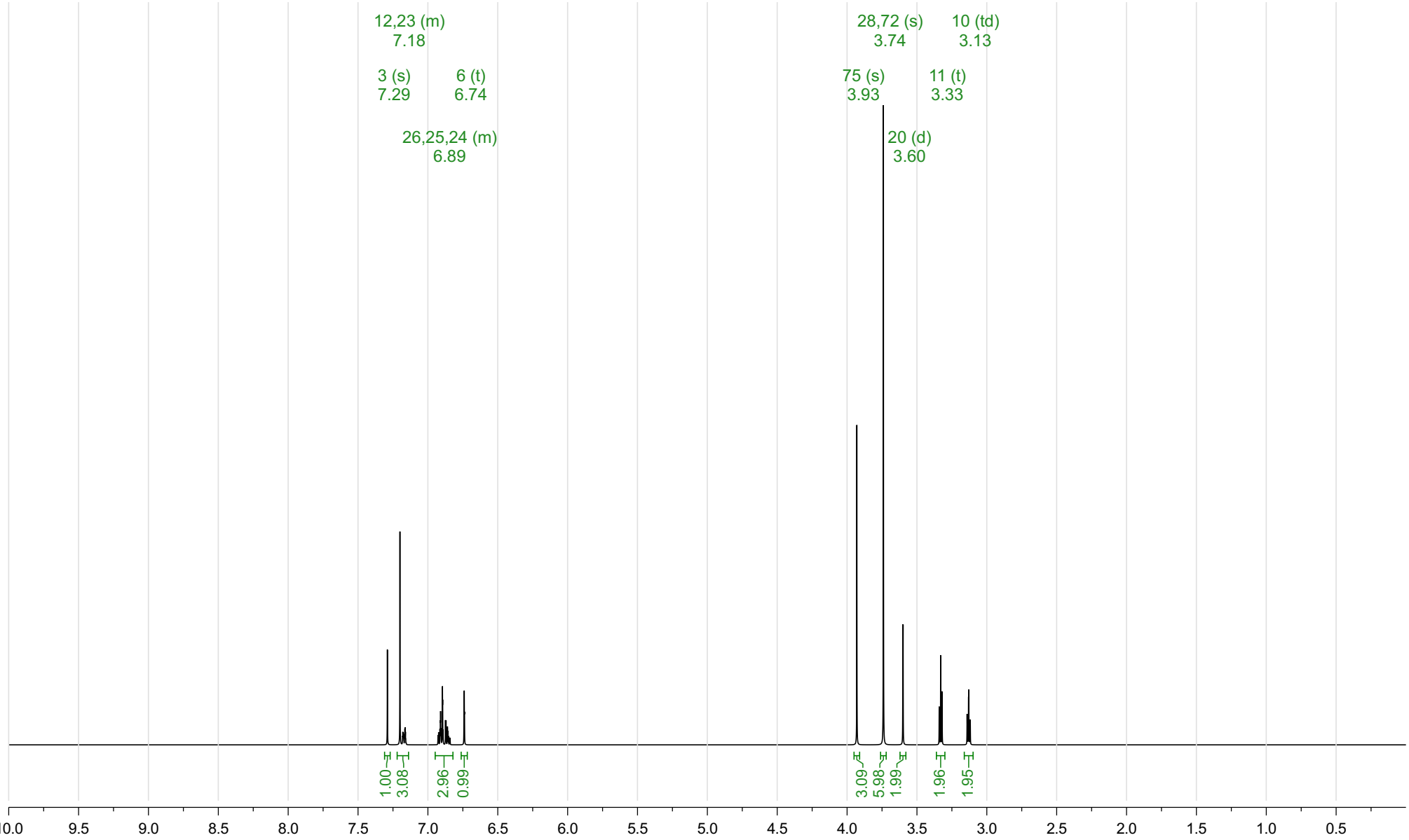
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.18 (s, 2H), 7.49 (dd, J = 7.5, 1.7 Hz, 1H), 7.41 (ddd, J = 8.3, 7.5, 1.7 Hz, 1H), 7.19 (s, 1H), 7.08 (dd, J = 8.4, 1.0 Hz, 1H), 7.02 (s, 1H), 7.00 (td, J = 7.4, 1.1 Hz, 1H), 4.11 (s, 2H), 3.83 (s, 3H), 3.79 (s, 3H), 3.75 (s, 3H), 3.10 – 3.03 (m, 2H), 3.00 – 2.93 (m, 2H).



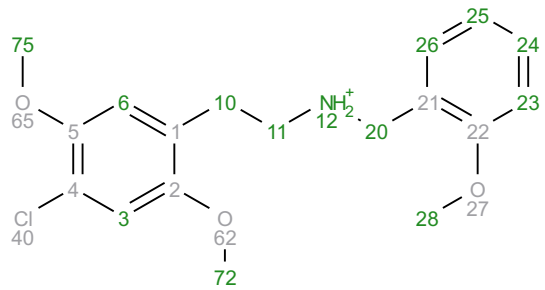
Prediction	25B-NBOMe H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



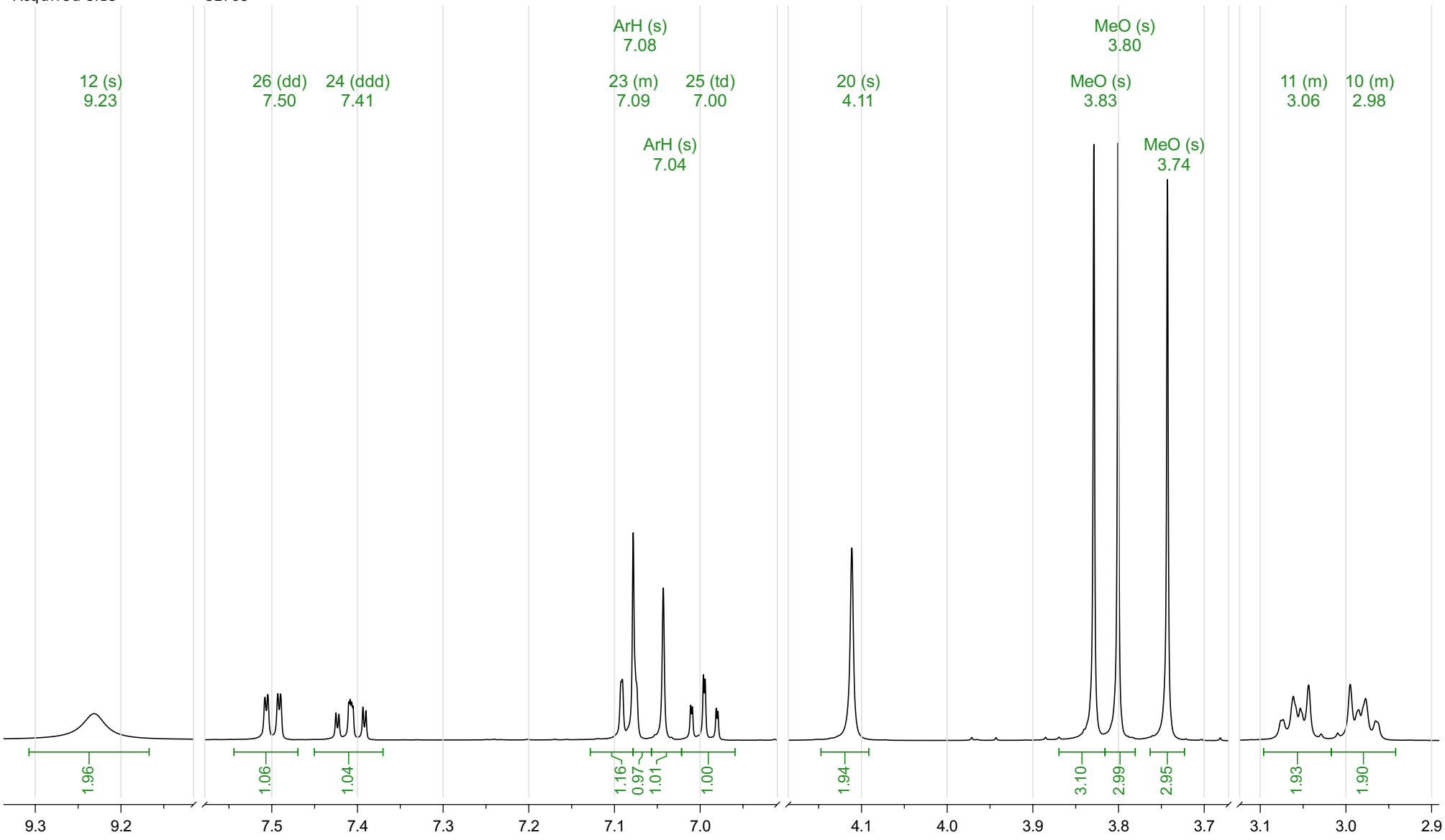
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.29 (s, 1H), 7.22 – 7.13 (m, 3H), 6.95 – 6.82 (m, 3H), 6.74 (t, J = 1.0 Hz, 1H), 3.93 (s, 3H), 3.74 (s, 6H), 3.60 (d, J = 0.9 Hz, 2H), 3.33 (t, J = 5.2 Hz, 2H), 3.13 (td, J = 5.3, 1.0 Hz, 2H).



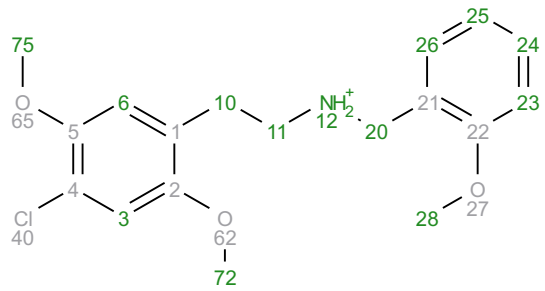
Analyte	B2: 25C-NBOMe H+
Acquisition Date	2013-01-17T02:39:37
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



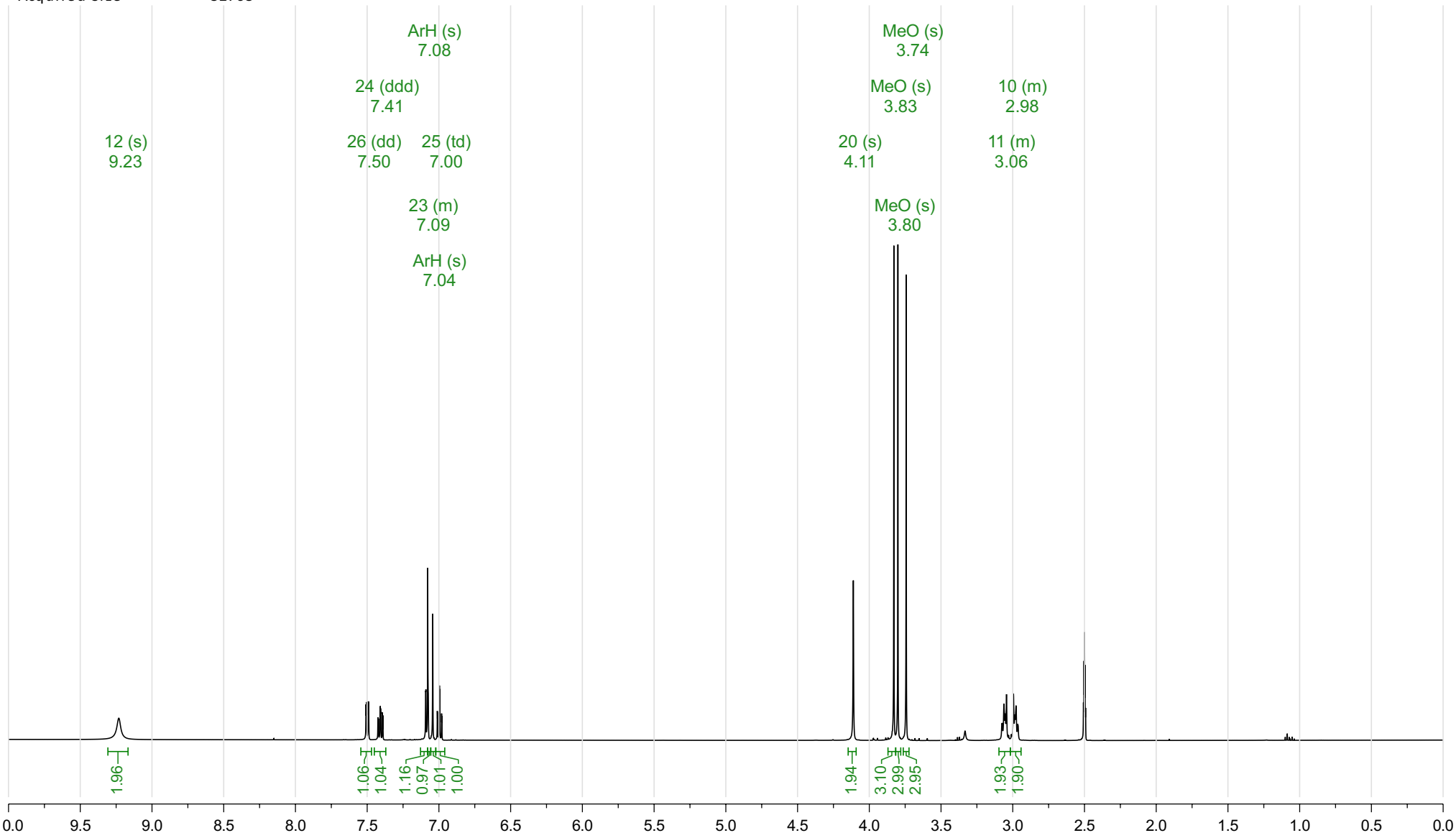
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.23 (s, 2H), 7.50 (dd, J = 7.5, 1.7 Hz, 1H), 7.41 (ddd, J = 8.2, 7.4, 1.7 Hz, 1H), 7.14 – 7.05 (m, 1H), 7.08 (s, 1H), 7.04 (s, 1H), 7.00 (td, J = 7.5, 1.1 Hz, 1H), 4.11 (s, 2H), 3.83 (s, 3H), 3.80 (s, 3H), 3.74 (s, 3H), 3.10 – 3.01 (m, 2H), 3.03 – 2.94 (m, 2H).



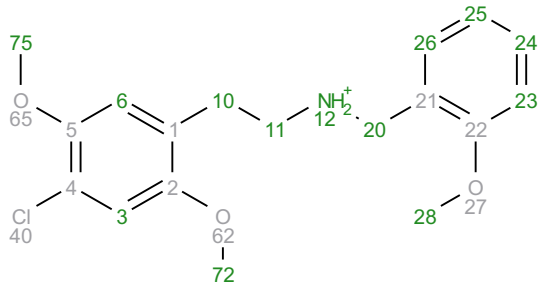
Analyte	B2: 25C-NBOMe H+
Acquisition Date	2013-01-17T02:39:37
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



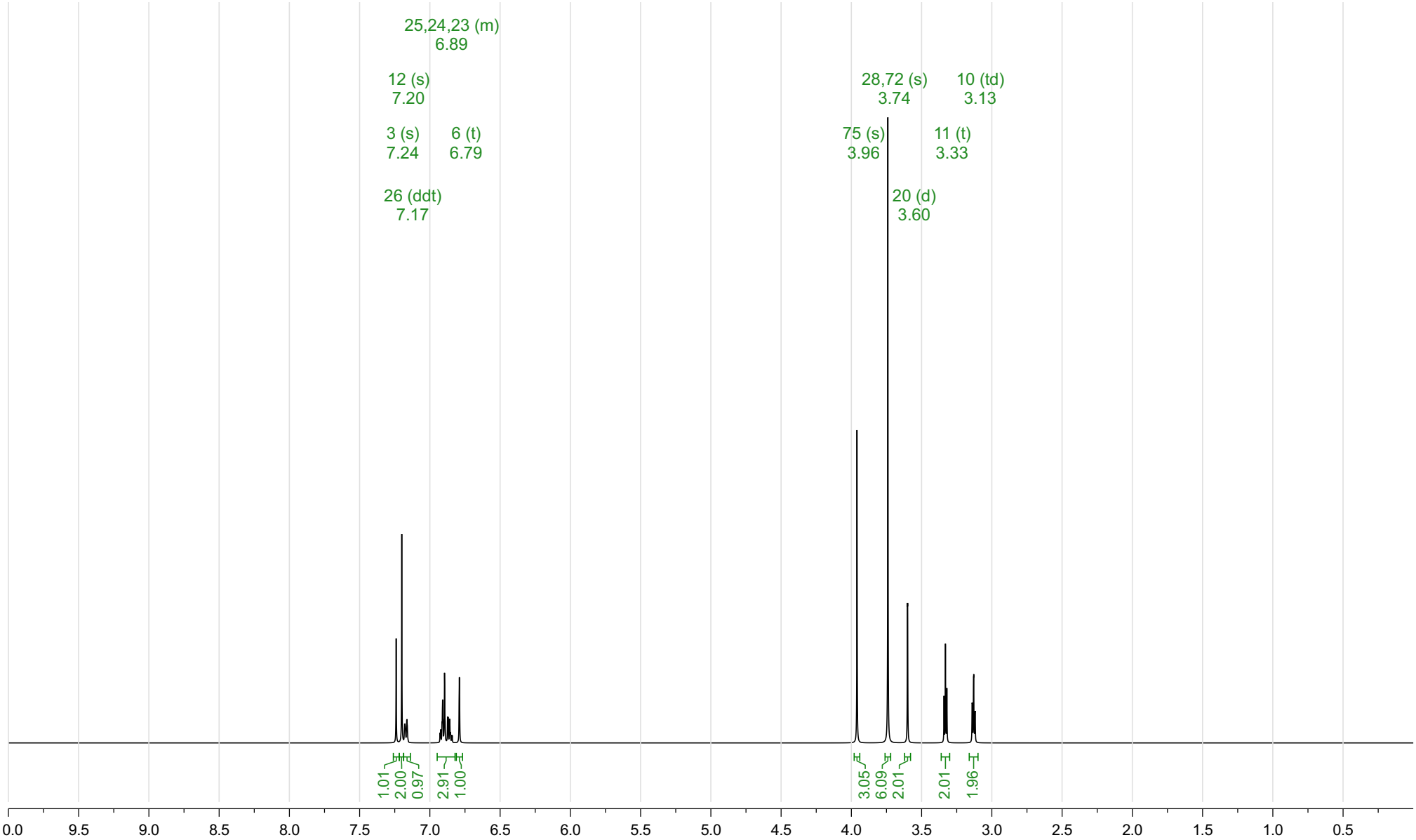
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.23 (s, 2H), 7.50 (dd, J = 7.5, 1.7 Hz, 1H), 7.41 (ddd, J = 8.2, 7.4, 1.7 Hz, 1H), 7.14 – 7.05 (m, 1H), 7.08 (s, 1H), 7.04 (s, 1H), 7.00 (td, J = 7.5, 1.1 Hz, 1H), 4.11 (s, 2H), 3.83 (s, 3H), 3.80 (s, 3H), 3.74 (s, 3H), 3.10 – 3.01 (m, 2H), 3.03 – 2.94 (m, 2H).



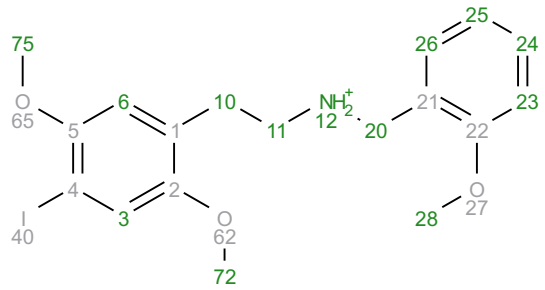
Prediction	25C-NBOMe H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



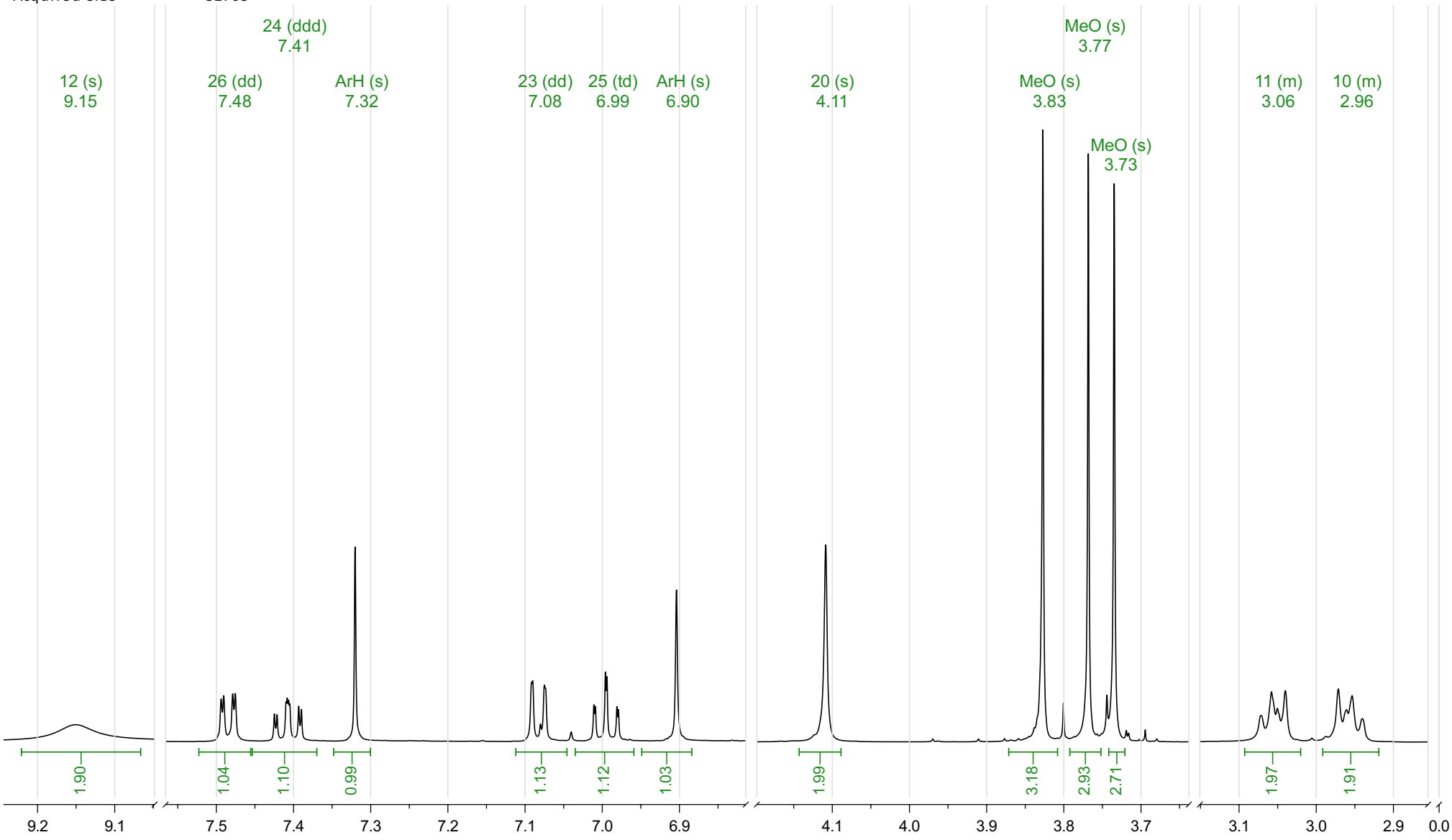
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.24 (s, 1H), 7.20 (s, 2H), 7.17 (ddt, J = 7.7, 2.1, 1.1 Hz, 1H), 6.95 – 6.82 (m, 3H), 6.79 (t, J = 1.0 Hz, 1H), 3.96 (s, 3H), 3.74 (s, 6H), 3.60 (d, J = 0.9 Hz, 2H), 3.33 (t, J = 5.1 Hz, 2H), 3.13 (td, J = 5.1, 1.0 Hz, 2H).



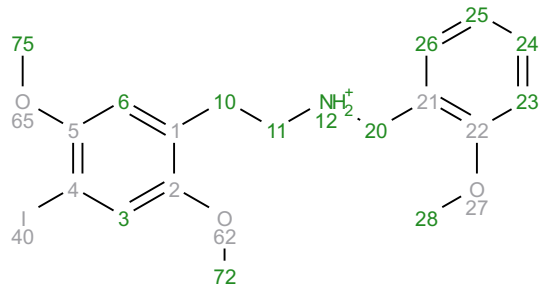
Analyte	B3: 25I-NBOMe H+
Acquisition Date	2013-01-17T02:47:03
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



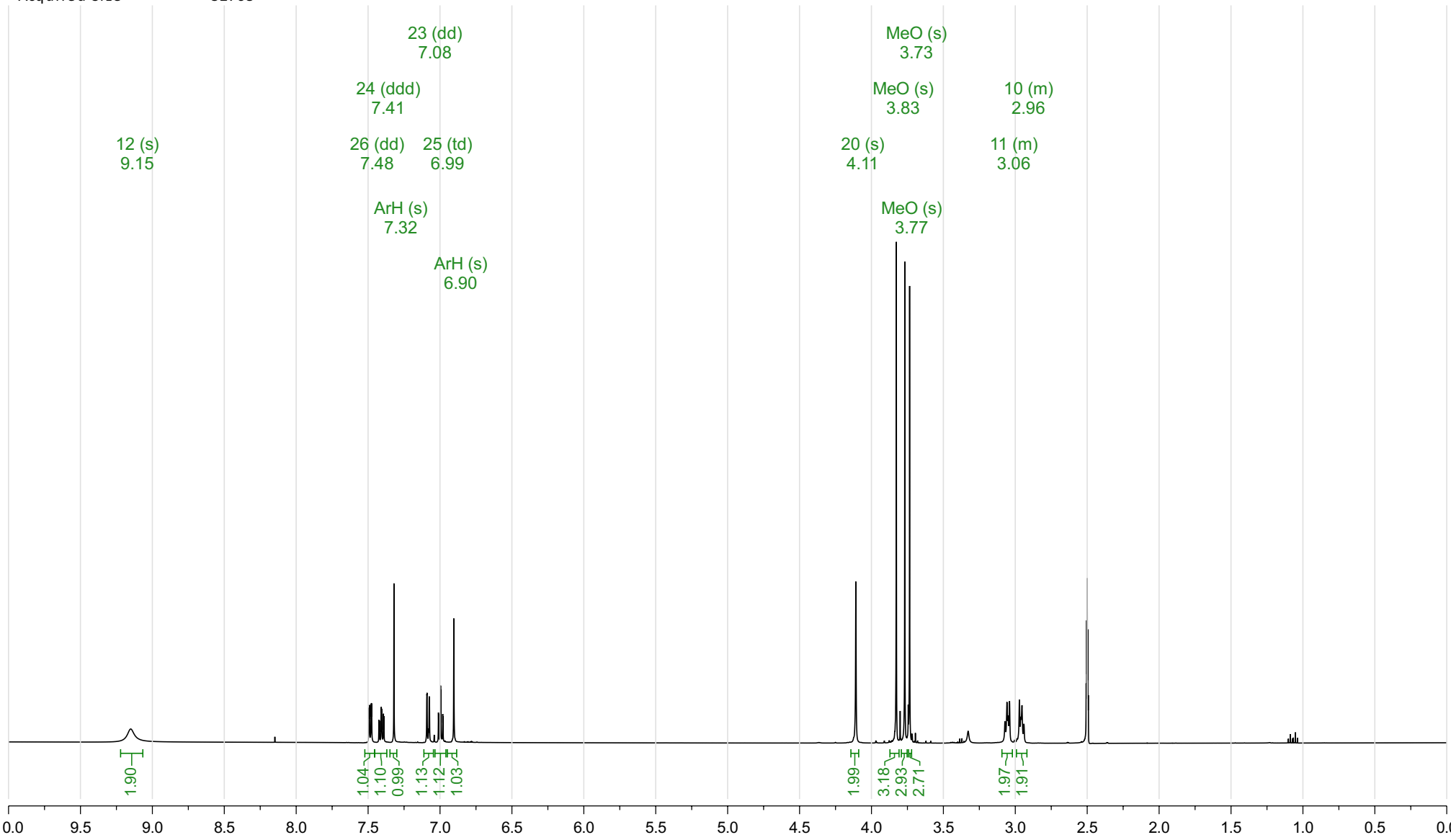
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.15 (s, 2H), 7.48 (dd, J = 7.5, 1.8 Hz, 1H), 7.41 (ddd, J = 8.3, 7.5, 1.7 Hz, 1H), 7.32 (s, 1H), 7.08 (dd, J = 8.3, 1.0 Hz, 1H), 6.99 (td, J = 7.4, 1.1 Hz, 1H), 6.90 (s, 1H), 4.11 (s, 2H), 3.83 (s, 3H), 3.77 (s, 3H), 3.73 (s, 2H), 3.09 – 3.00 (m, 2H), 2.99 – 2.92 (m, 2H).



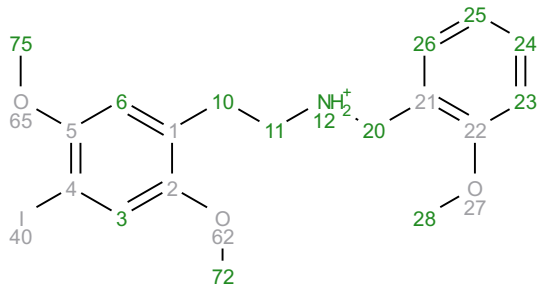
Analyte	B3: 25I-NBOMe H+
Acquisition Date	2013-01-17T02:47:03
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



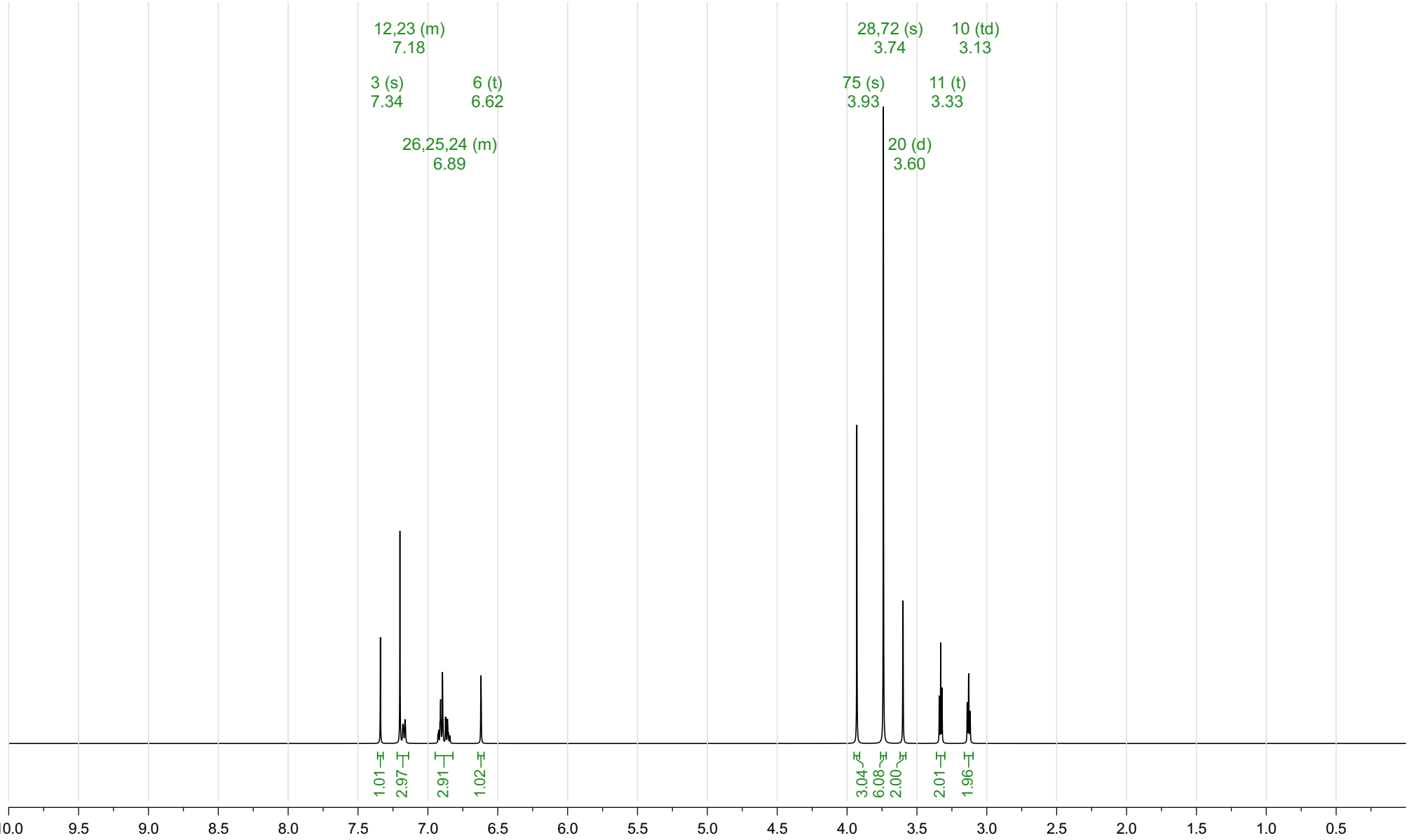
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.15 (s, 2H), 7.48 (dd, J = 7.5, 1.8 Hz, 1H), 7.41 (ddd, J = 8.3, 7.5, 1.7 Hz, 1H), 7.32 (s, 1H), 7.08 (dd, J = 8.3, 1.0 Hz, 1H), 6.99 (td, J = 7.4, 1.1 Hz, 1H), 6.90 (s, 1H), 4.11 (s, 2H), 3.83 (s, 3H), 3.77 (s, 3H), 3.73 (s, 2H), 3.09 – 3.00 (m, 2H), 2.99 – 2.92 (m, 2H).



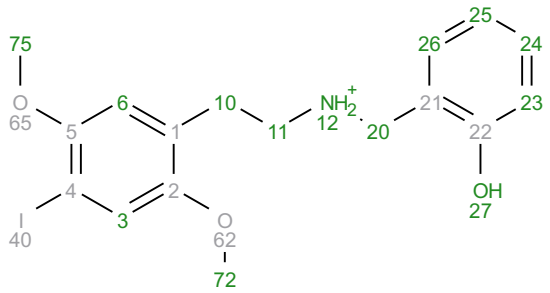
Prediction	25I-NBOMe H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	12489
Frequency	500.00
Nucleus	1H



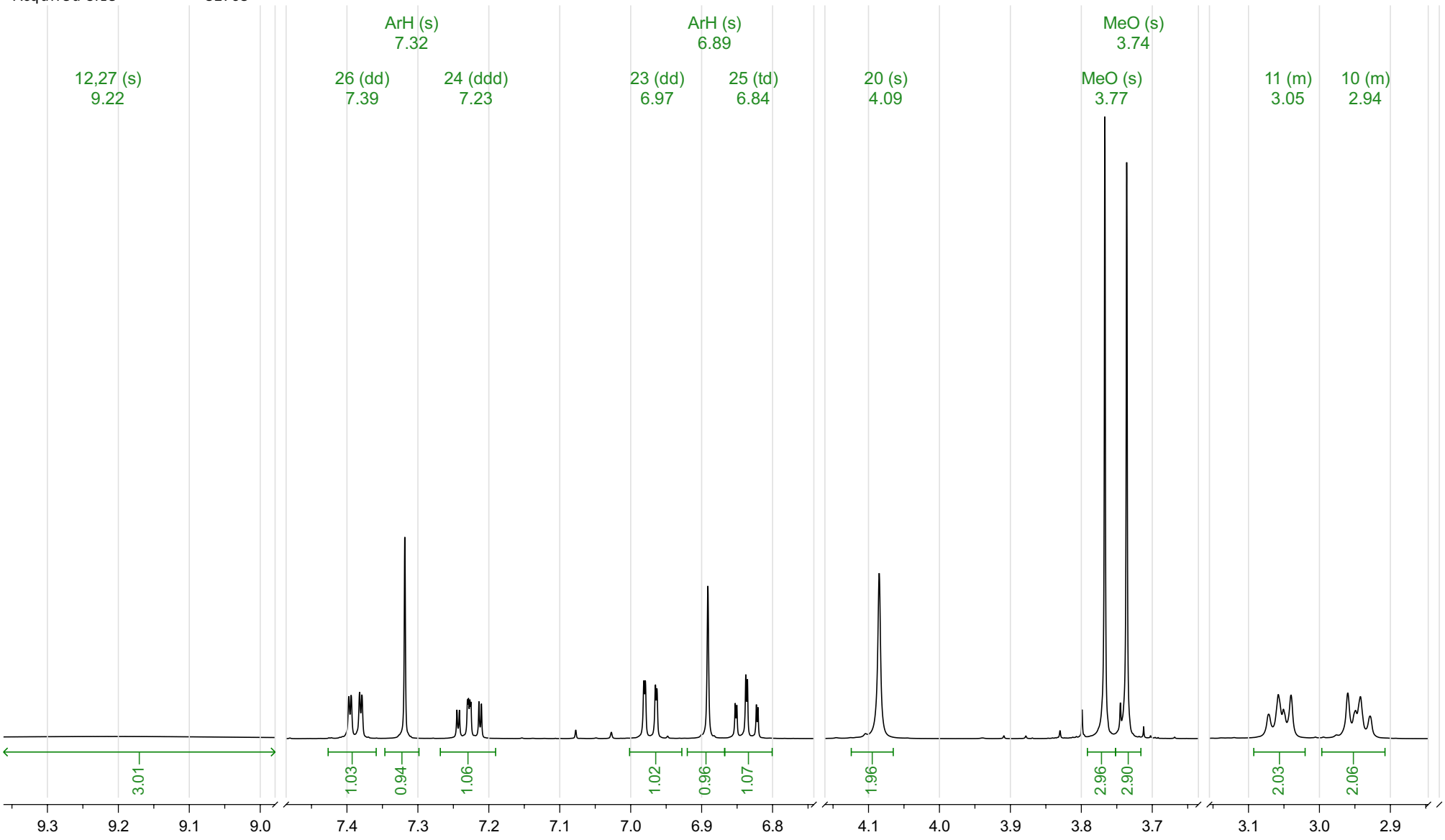
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.34 (s, 1H), 7.22 – 7.13 (m, 3H), 6.95 – 6.82 (m, 3H), 6.62 (t, *J* = 0.9 Hz, 1H), 3.93 (s, 3H), 3.74 (s, 6H), 3.60 (d, *J* = 0.9 Hz, 2H), 3.33 (t, *J* = 5.1 Hz, 2H), 3.13 (td, *J* = 5.1, 1.0 Hz, 2H).



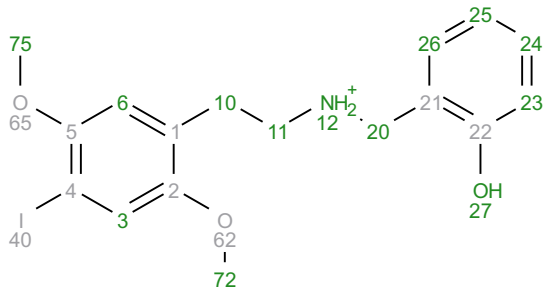
Analyte	B4: 25I-NBOH H+
Acquisition Date	2013-01-17T03:09:57
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



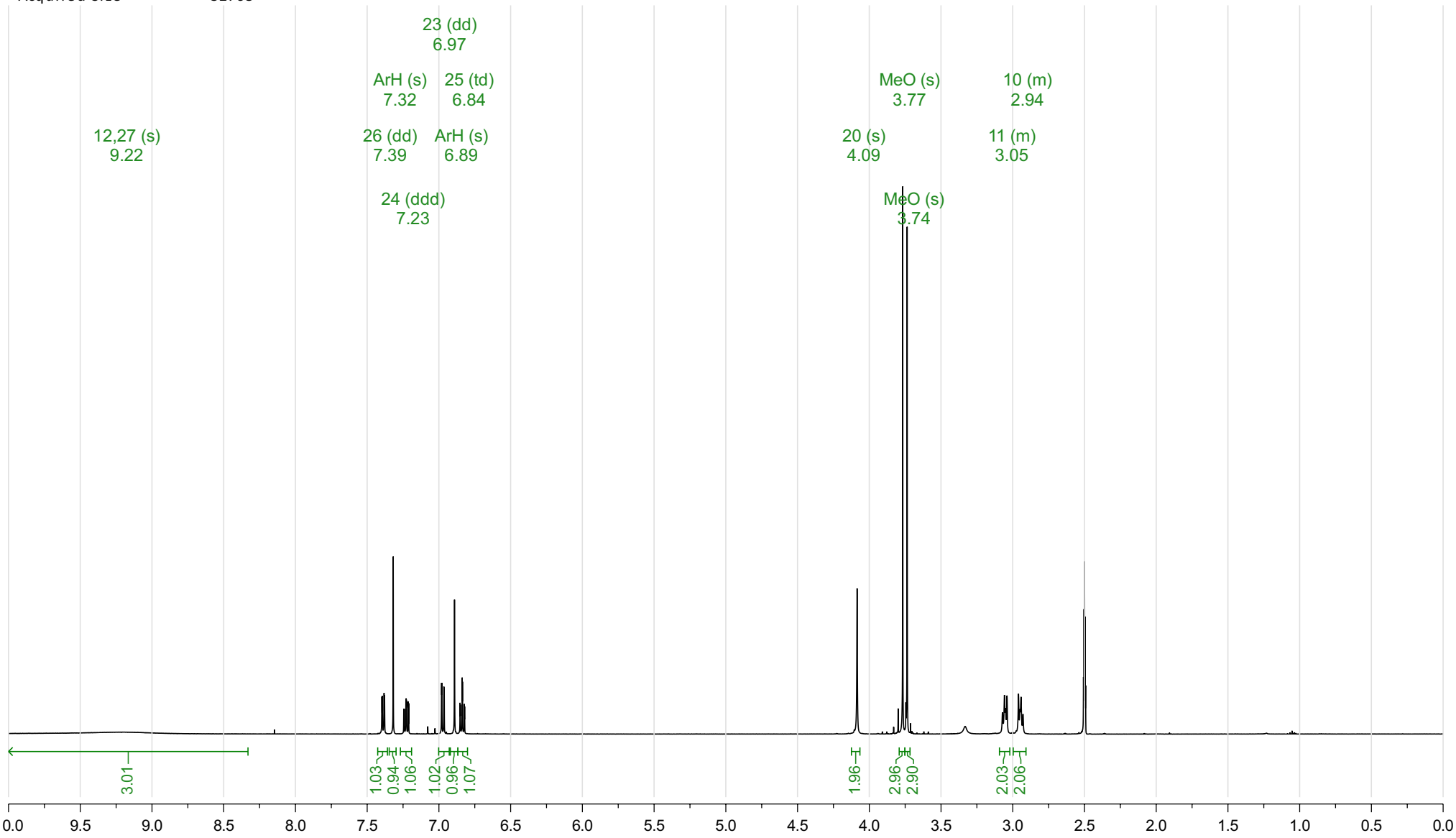
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.22 (s, 3H), 7.39 (dd, J = 7.6, 1.7 Hz, 1H), 7.32 (s, 1H), 7.23 (ddd, J = 8.1, 7.3, 1.7 Hz, 1H), 6.97 (dd, J = 8.2, 1.1 Hz, 1H), 6.89 (s, 1H), 6.84 (td, J = 7.4, 1.1 Hz, 1H), 4.09 (s, 2H), 3.77 (s, 3H), 3.74 (s, 3H), 3.09 – 3.02 (m, 2H), 3.00 – 2.91 (m, 2H).



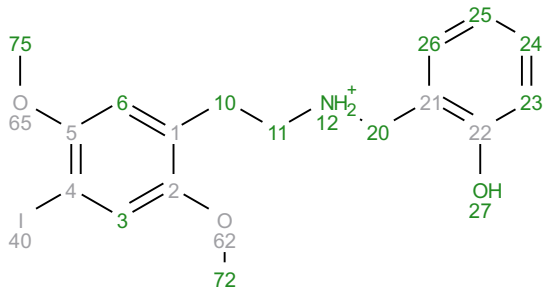
Analyte	B4: 25I-NBOH H+
Acquisition Date	2013-01-17T03:09:57
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



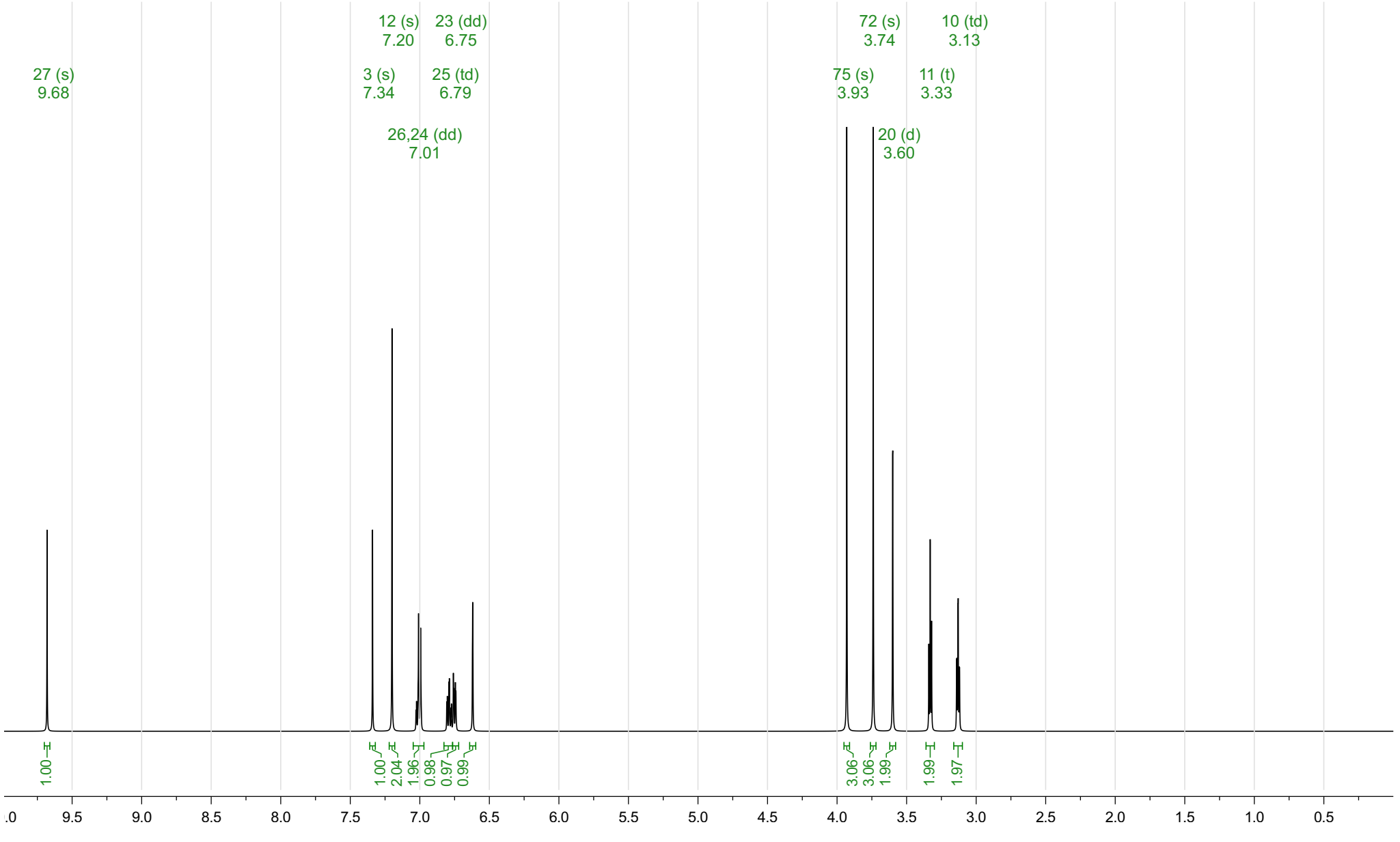
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.22 (s, 3H), 7.39 (dd, J = 7.6, 1.7 Hz, 1H), 7.32 (s, 1H), 7.23 (ddd, J = 8.1, 7.3, 1.7 Hz, 1H), 6.97 (dd, J = 8.2, 1.1 Hz, 1H), 6.89 (s, 1H), 6.84 (td, J = 7.4, 1.1 Hz, 1H), 4.09 (s, 2H), 3.77 (s, 3H), 3.74 (s, 3H), 3.09 – 3.02 (m, 2H), 3.00 – 2.91 (m, 2H).



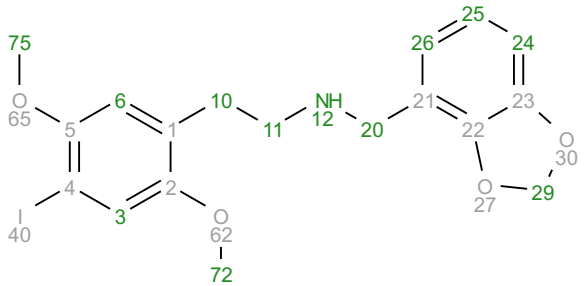
Prediction	25I-NBOH H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



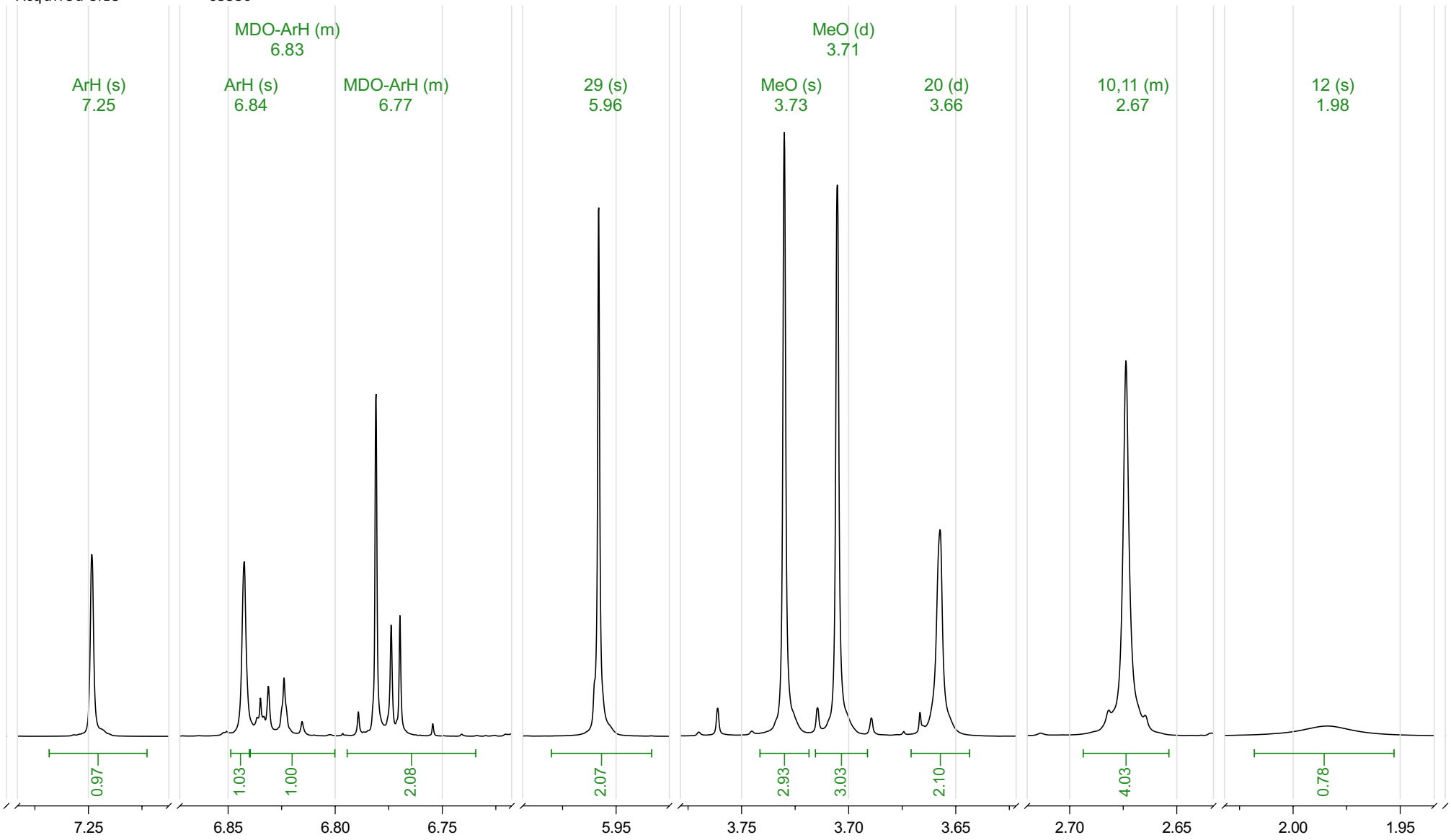
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.68 (s, 1H), 7.34 (s, 1H), 7.20 (s, 2H), 7.01 (dd, *J* = 8.2, 6.4 Hz, 2H), 6.79 (td, *J* = 7.4, 2.0 Hz, 1H), 6.75 (dd, *J* = 7.2, 2.0 Hz, 1H), 6.62 (t, *J* = 0.9 Hz, 1H), 3.93 (s, 3H), 3.74 (s, 3H), 3.60 (d, *J* = 0.9 Hz, 2H), 3.33 (t, *J* = 5.0 Hz, 2H), 3.13 (td, *J* = 5.0, 1.1 Hz, 2H).



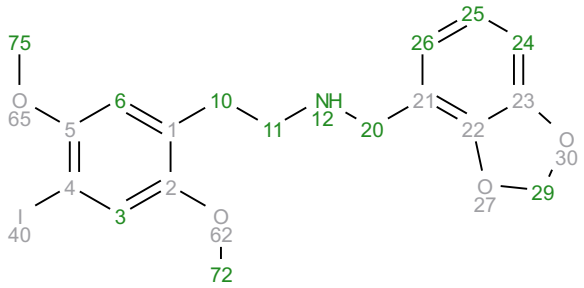
Analyte	B5: 25I-NBMD
Acquisition Date	2013-05-07T19:21:56
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	10000.0
Nucleus	1H
Acquired Size	65536



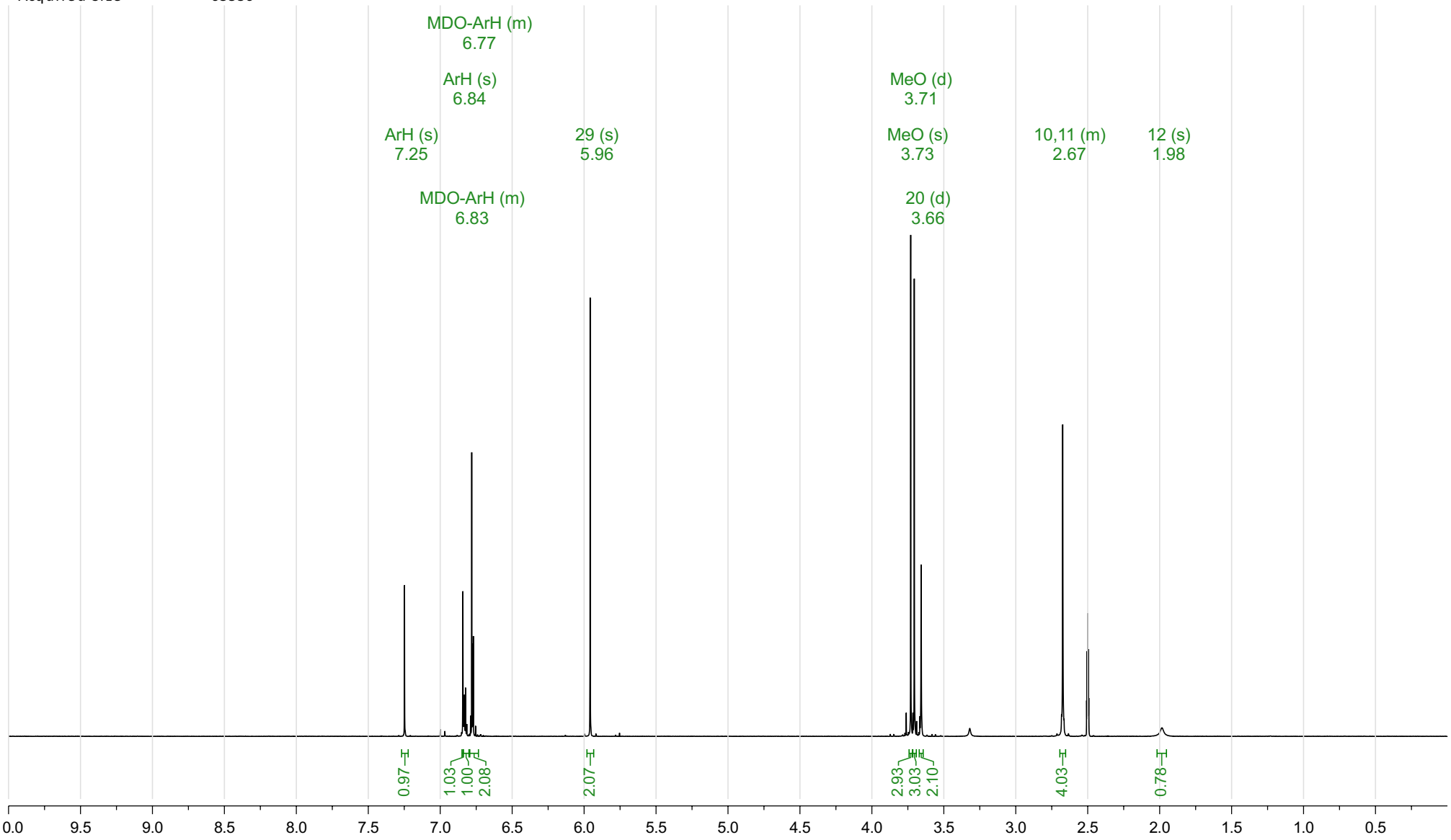
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.25 (s, 1H), 6.84 (s, 1H), 6.86 – 6.78 (m, 1H), 6.81 – 6.72 (m, 2H), 5.96 (s, 2H), 3.73 (s, 3H), 3.71 (d, *J* = 0.3 Hz, 3H), 3.66 (d, *J* = 0.6 Hz, 2H), 2.69 – 2.65 (m, 4H), 1.98 (s, 1H).



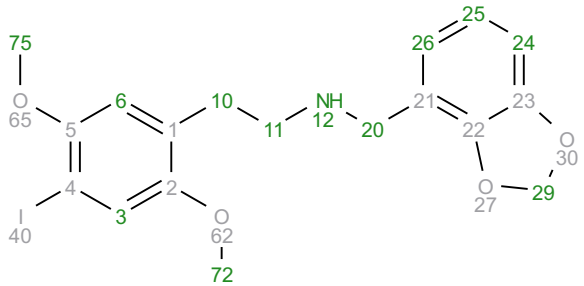
Analyte	B5: 25I-NBMD
Acquisition Date	2013-05-07T19:21:56
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	10000.0
Nucleus	1H
Acquired Size	65536



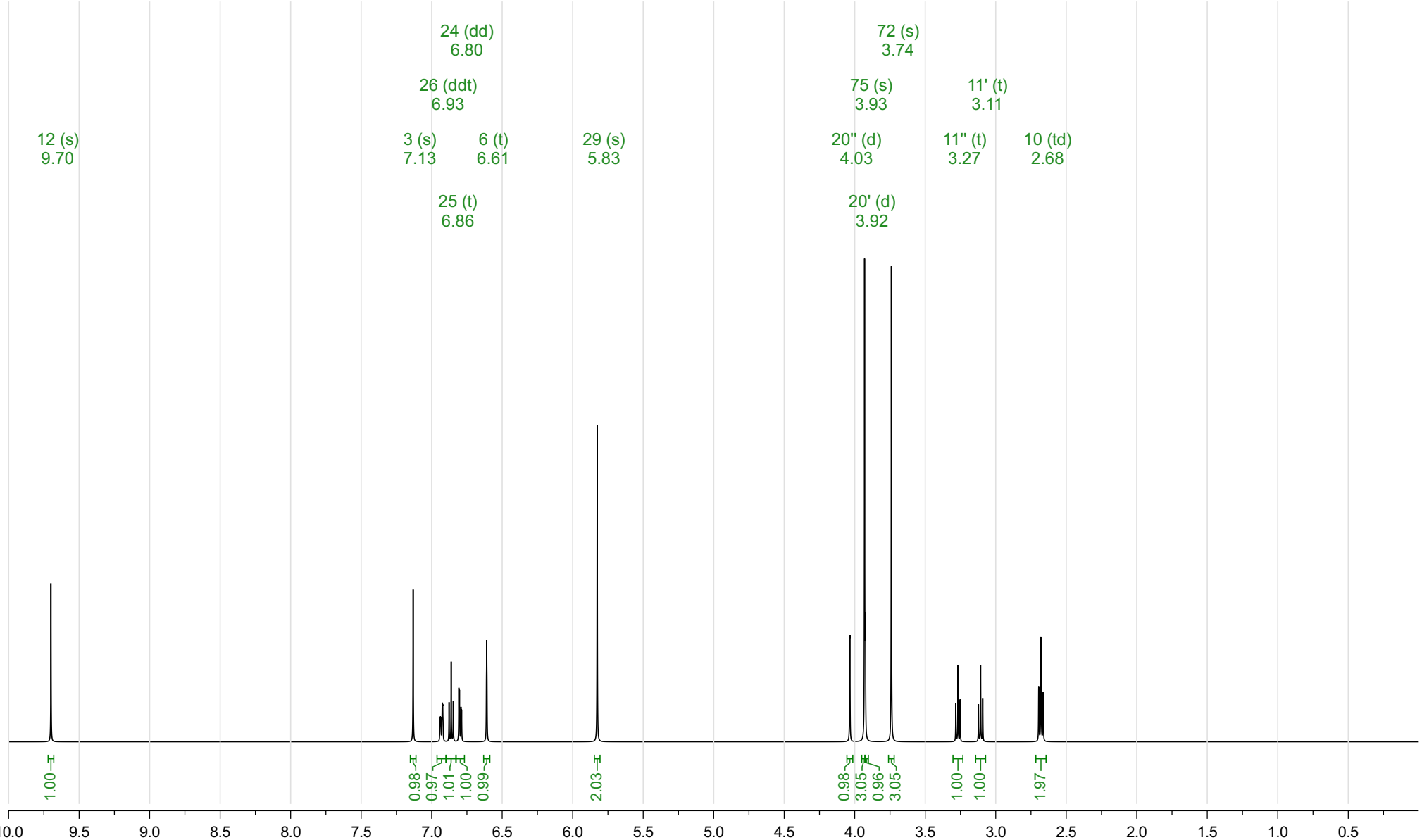
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.25 (s, 1H), 6.84 (s, 1H), 6.86 – 6.78 (m, 1H), 6.81 – 6.72 (m, 2H), 5.96 (s, 2H), 3.73 (s, 3H), 3.71 (d, *J* = 0.3 Hz, 3H), 3.66 (d, *J* = 0.6 Hz, 2H), 2.69 – 2.65 (m, 4H), 1.98 (s, 1H).



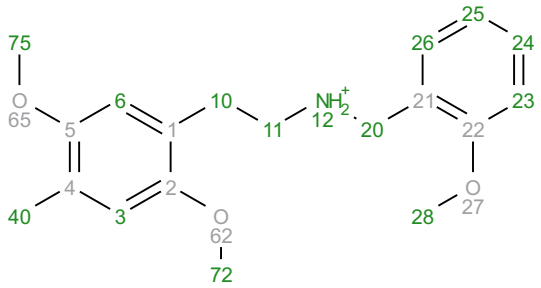
Prediction	25I-NBMD
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



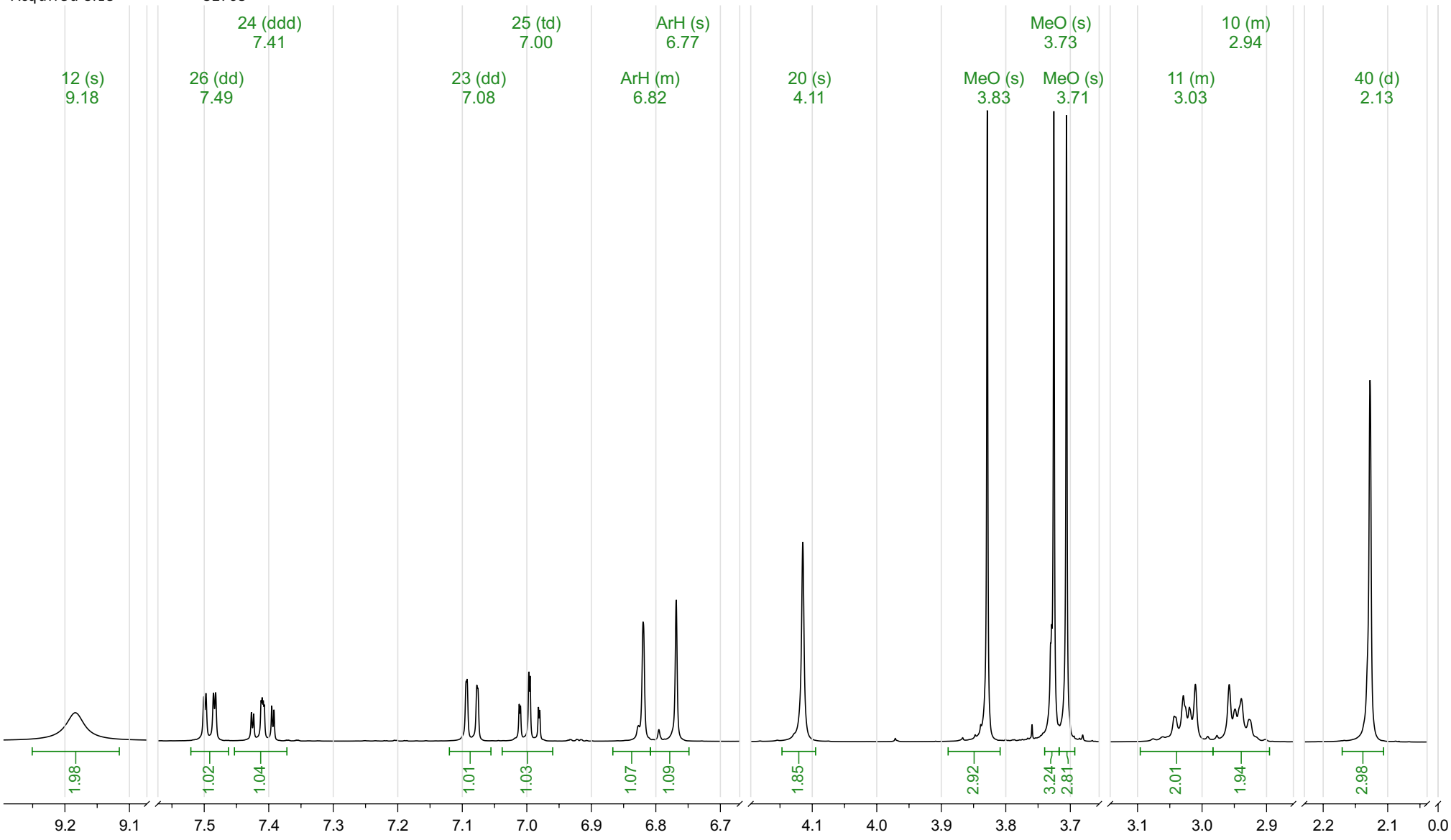
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.70 (s, 1H), 7.13 (s, 1H), 6.93 (ddt, *J* = 7.5, 2.1, 1.0 Hz, 1H), 6.86 (t, *J* = 7.5 Hz, 1H), 6.80 (dd, *J* = 7.5, 2.2 Hz, 1H), 6.61 (t, *J* = 1.0 Hz, 1H), 5.83 (s, 2H), 4.03 (d, *J* = 0.9 Hz, 1H), 3.93 (s, 3H), 3.92 (d, *J* = 1.1 Hz, 1H), 3.74 (s, 3H), 3.27 (t, *J* = 7.6 Hz, 1H), 3.11 (t, *J* = 7.6 Hz, 1H), 2.68 (td, *J* = 7.6, 1.0 Hz, 2H).



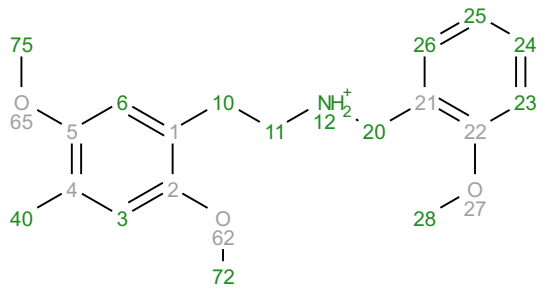
Analyte	B6: 25D-NBOMe H+
Acquisition Date	2013-01-17T02:54:51
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



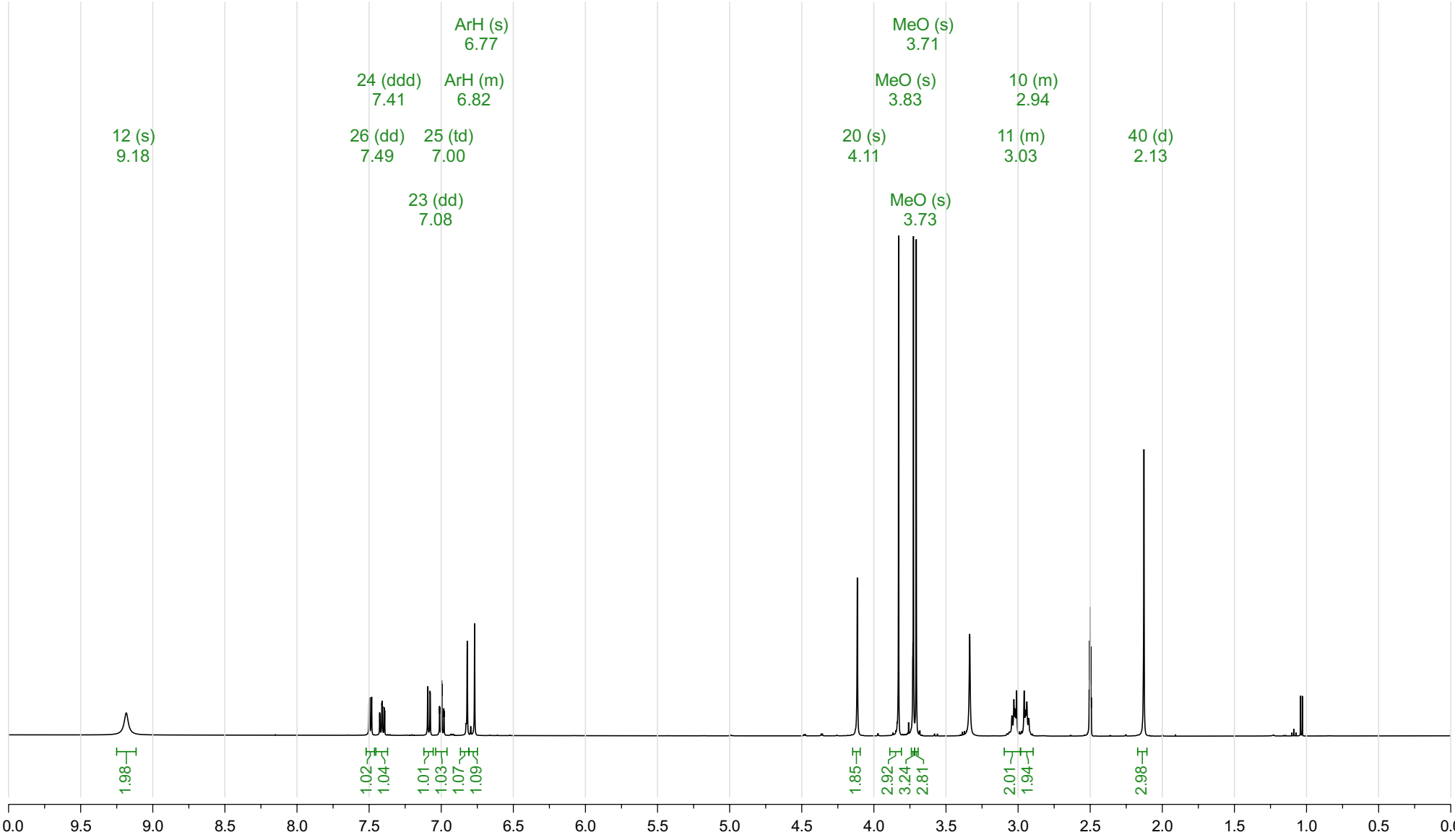
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.18 (s, 2H), 7.49 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.41 (ddd, *J* = 8.3, 7.5, 1.7 Hz, 1H), 7.08 (dd, *J* = 8.3, 1.0 Hz, 1H), 7.00 (td, *J* = 7.5, 1.1 Hz, 1H), 6.88 – 6.79 (m, 1H), 6.77 (s, 1H), 4.11 (s, 2H), 3.83 (s, 3H), 3.73 (s, 3H), 3.71 (s, 3H), 3.10 – 2.96 (m, 2H), 3.00 – 2.88 (m, 2H), 2.13 (d, *J* = 0.7 Hz, 3H).



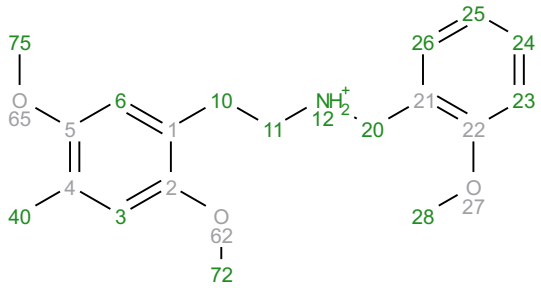
Analyte	B6: 25D-NBOMe H+
Acquisition Date	2013-01-17T02:54:51
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



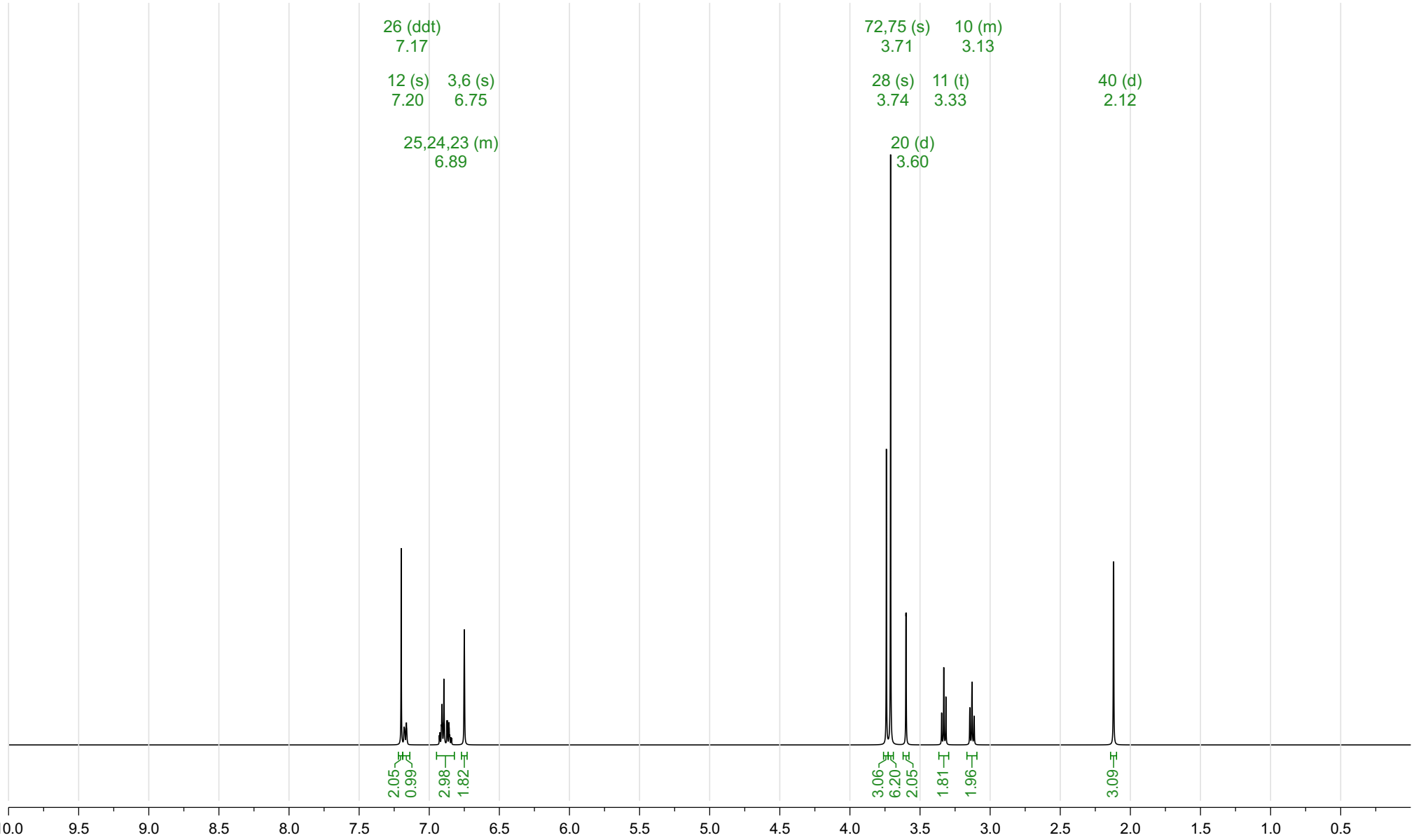
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.18 (s, 2H), 7.49 (dd, J = 7.5, 1.7 Hz, 1H), 7.41 (ddd, J = 8.3, 7.5, 1.7 Hz, 1H), 7.08 (dd, J = 8.3, 1.0 Hz, 1H), 7.00 (td, J = 7.5, 1.1 Hz, 1H), 6.88 – 6.79 (m, 1H), 6.77 (s, 1H), 4.11 (s, 2H), 3.83 (s, 3H), 3.73 (s, 3H), 3.71 (s, 3H), 3.10 – 2.96 (m, 2H), 3.00 – 2.88 (m, 2H), 2.13 (d, J = 0.7 Hz, 3H).



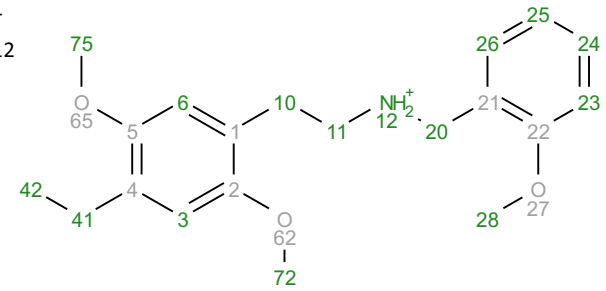
Prediction	25D-NBOMe H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



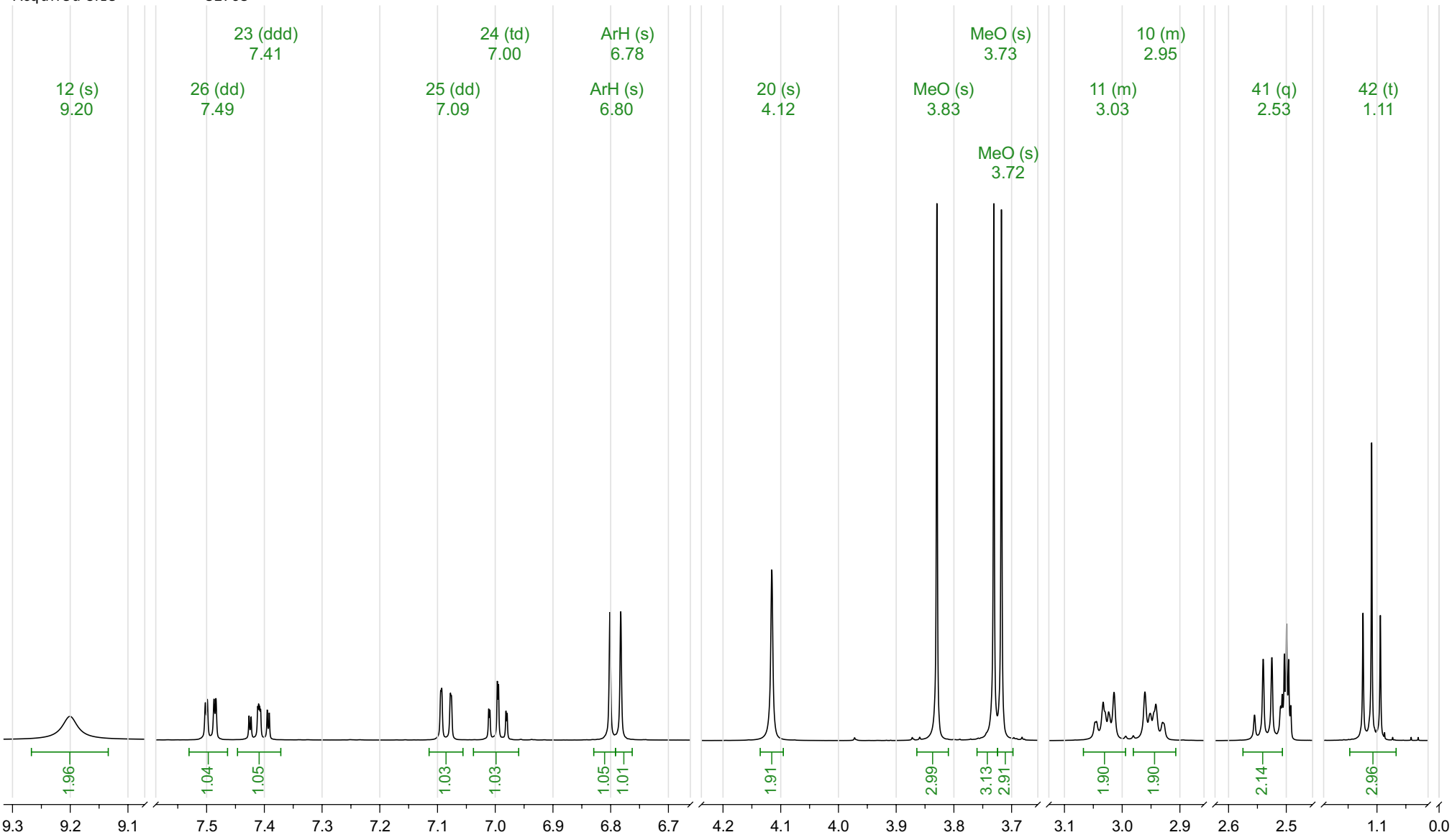
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.20 (s, 2H), 7.17 (ddt, J = 7.6, 2.1, 1.0 Hz, 1H), 6.95 – 6.82 (m, 3H), 6.75 (s, 2H), 3.74 (s, 3H), 3.71 (s, 6H), 3.60 (d, J = 0.9 Hz, 2H), 3.33 (t, J = 7.5 Hz, 2H), 3.17 – 3.09 (m, 2H), 2.12 (d, J = 1.1 Hz, 3H).



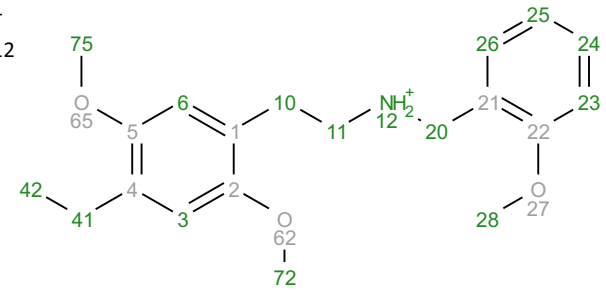
Analyte	B7: 25E-NBOMe H+
Acquisition Date	2013-01-17T03:02:12
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



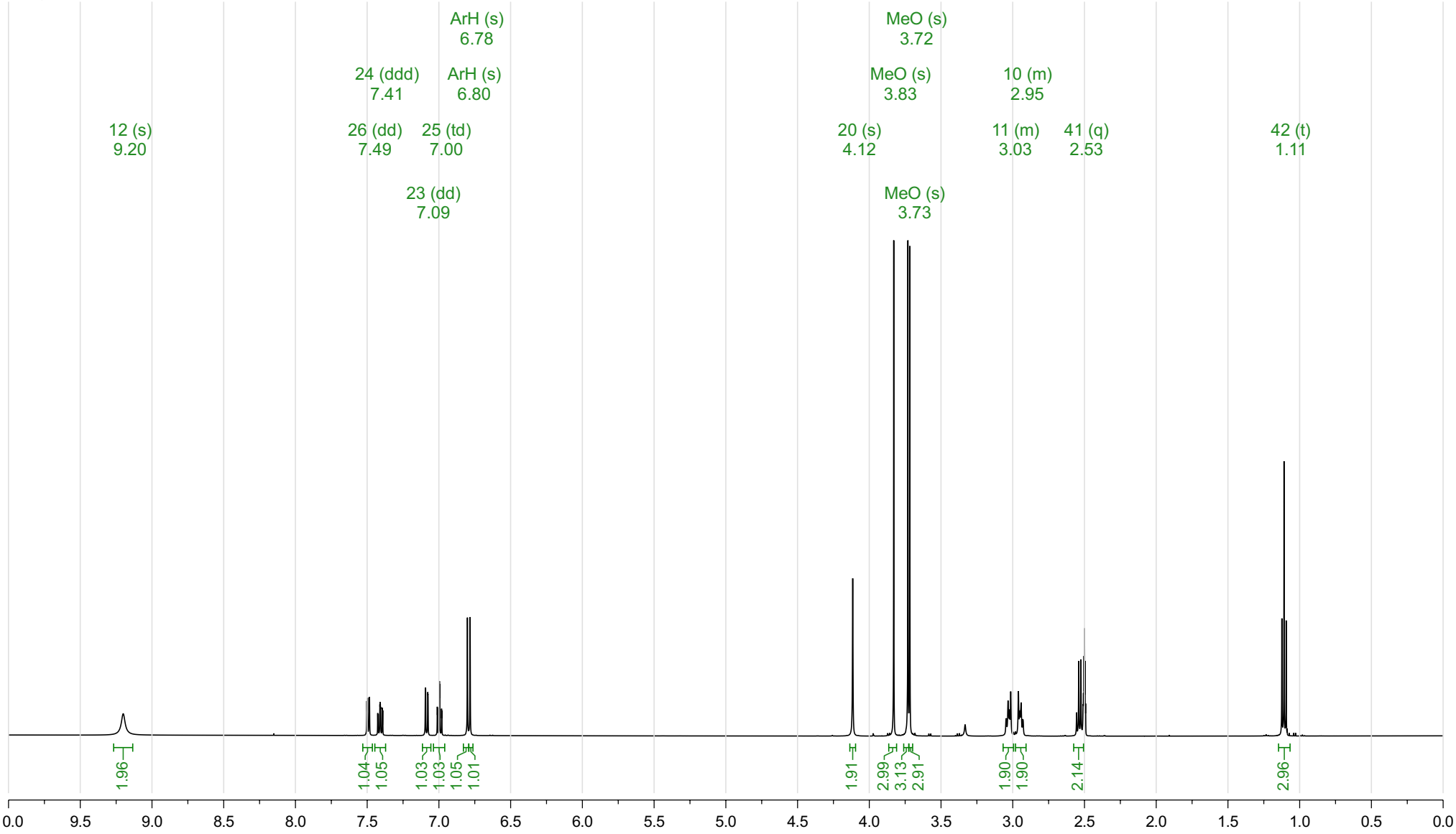
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.20 (s, 2H), 7.49 (dd, J = 7.5, 1.7 Hz, 1H), 7.41 (ddd, J = 8.3, 7.5, 1.7 Hz, 1H), 7.09 (dd, J = 8.3, 1.0 Hz, 1H), 7.00 (td, J = 7.5, 1.0 Hz, 1H), 6.80 (s, 1H), 6.78 (s, 1H), 4.12 (s, 2H), 3.83 (s, 3H), 3.73 (s, 3H), 3.72 (s, 3H), 3.07 – 2.99 (m, 2H), 2.98 – 2.91 (m, 2H), 2.53 (q, J = 7.4 Hz, 2H), 1.11 (t, J = 7.5 Hz, 3H).



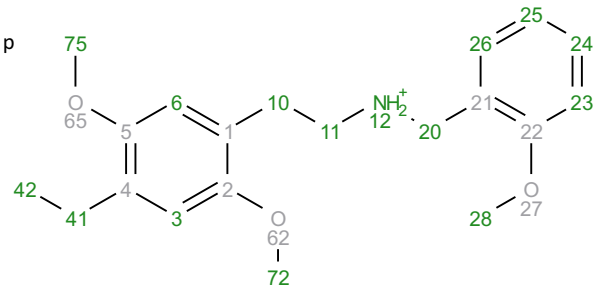
Analyte	B7: 25E-NBOMe H+
Acquisition Date	2013-01-17T03:02:12
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



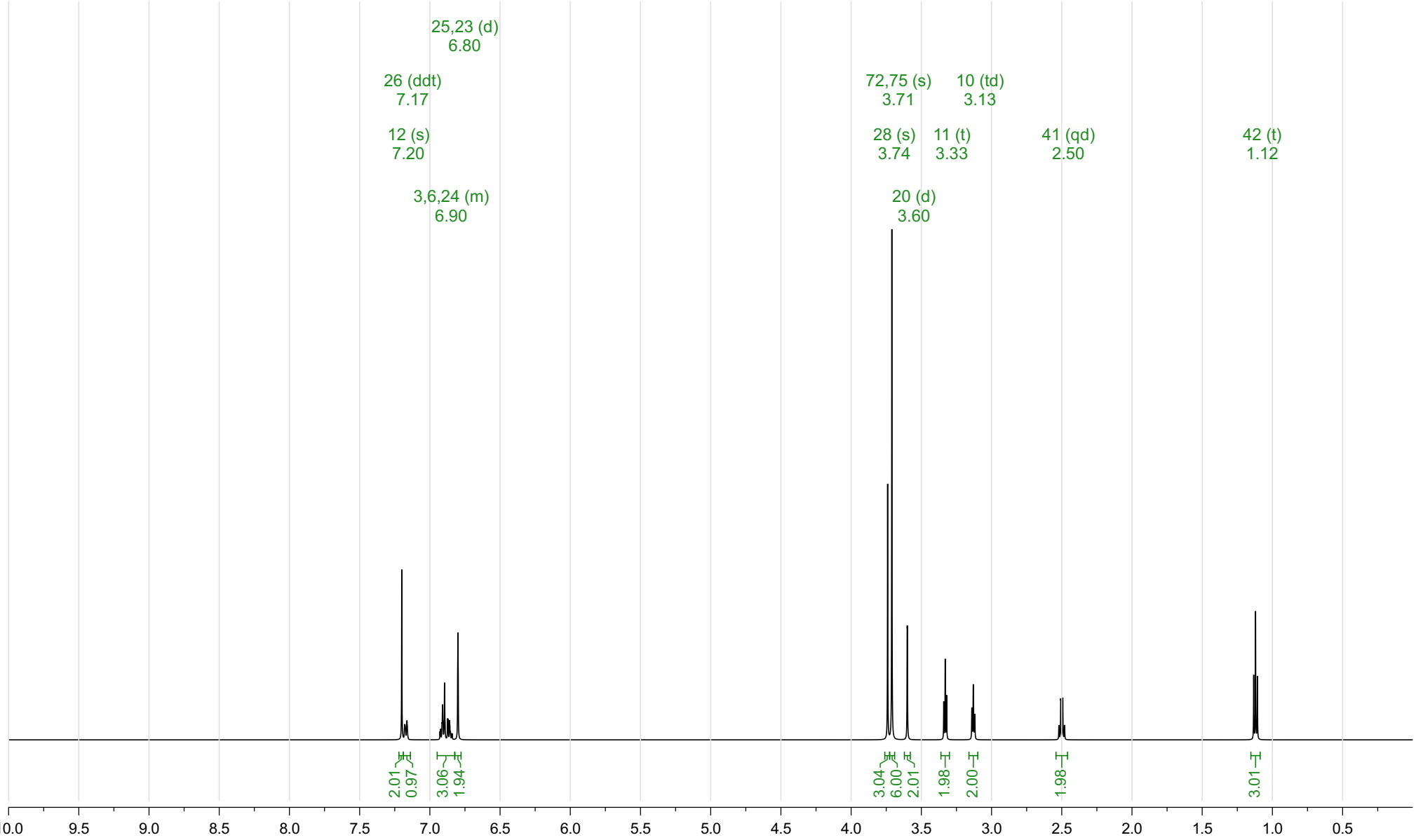
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.20 (s, 2H), 7.49 (dd, J = 7.5, 1.7 Hz, 1H), 7.41 (ddd, J = 8.3, 7.5, 1.7 Hz, 1H), 7.09 (dd, J = 8.3, 1.0 Hz, 1H), 7.00 (td, J = 7.5, 1.0 Hz, 1H), 6.80 (s, 1H), 6.78 (s, 1H), 4.12 (s, 2H), 3.83 (s, 3H), 3.73 (s, 3H), 3.72 (s, 3H), 3.07 – 2.99 (m, 2H), 2.98 – 2.91 (m, 2H), 2.53 (q, J = 7.4 Hz, 2H), 1.11 (t, J = 7.5 Hz, 3H).



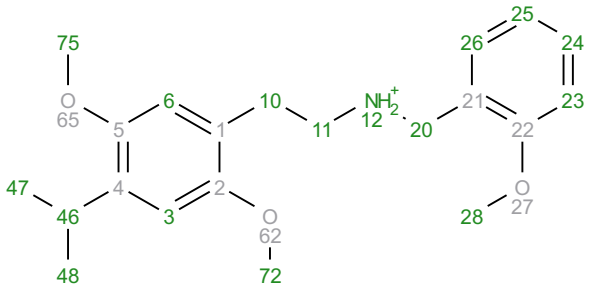
Prediction	25E-NBOMe H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



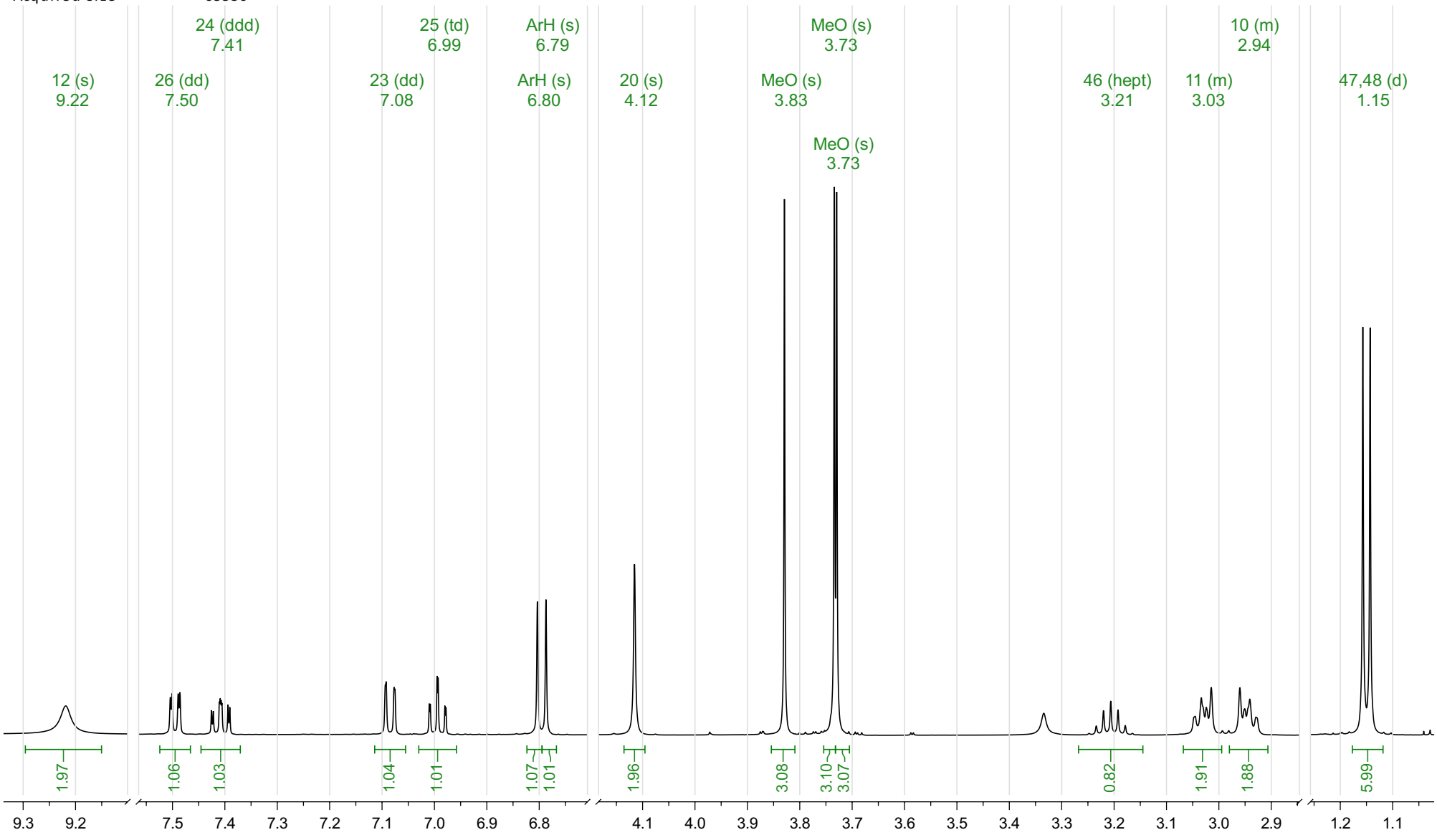
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.20 (s, 2H), 7.17 (ddt, *J* = 7.6, 2.1, 1.1 Hz, 1H), 6.95 – 6.82 (m, 3H), 6.80 (d, *J* = 1.2 Hz, 2H), 3.74 (s, 3H), 3.71 (s, 6H), 3.60 (d, *J* = 0.9 Hz, 2H), 3.33 (t, *J* = 5.1 Hz, 2H), 3.13 (td, *J* = 5.1, 1.1 Hz, 2H), 2.50 (qd, *J* = 6.6, 1.0 Hz, 2H), 1.12 (t, *J* = 6.6 Hz, 3H).



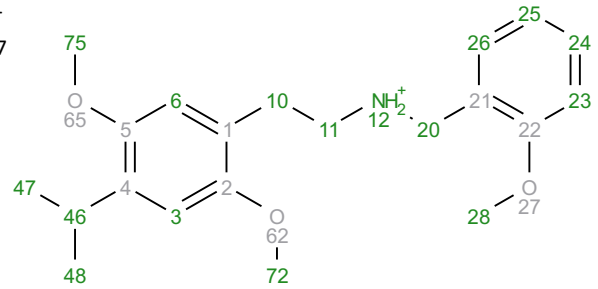
Analyte	B8: 25IP-NBOMe H+
Acquisition Date	2013-03-26T19:52:57
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	10964.9
Nucleus	1H
Acquired Size	65536



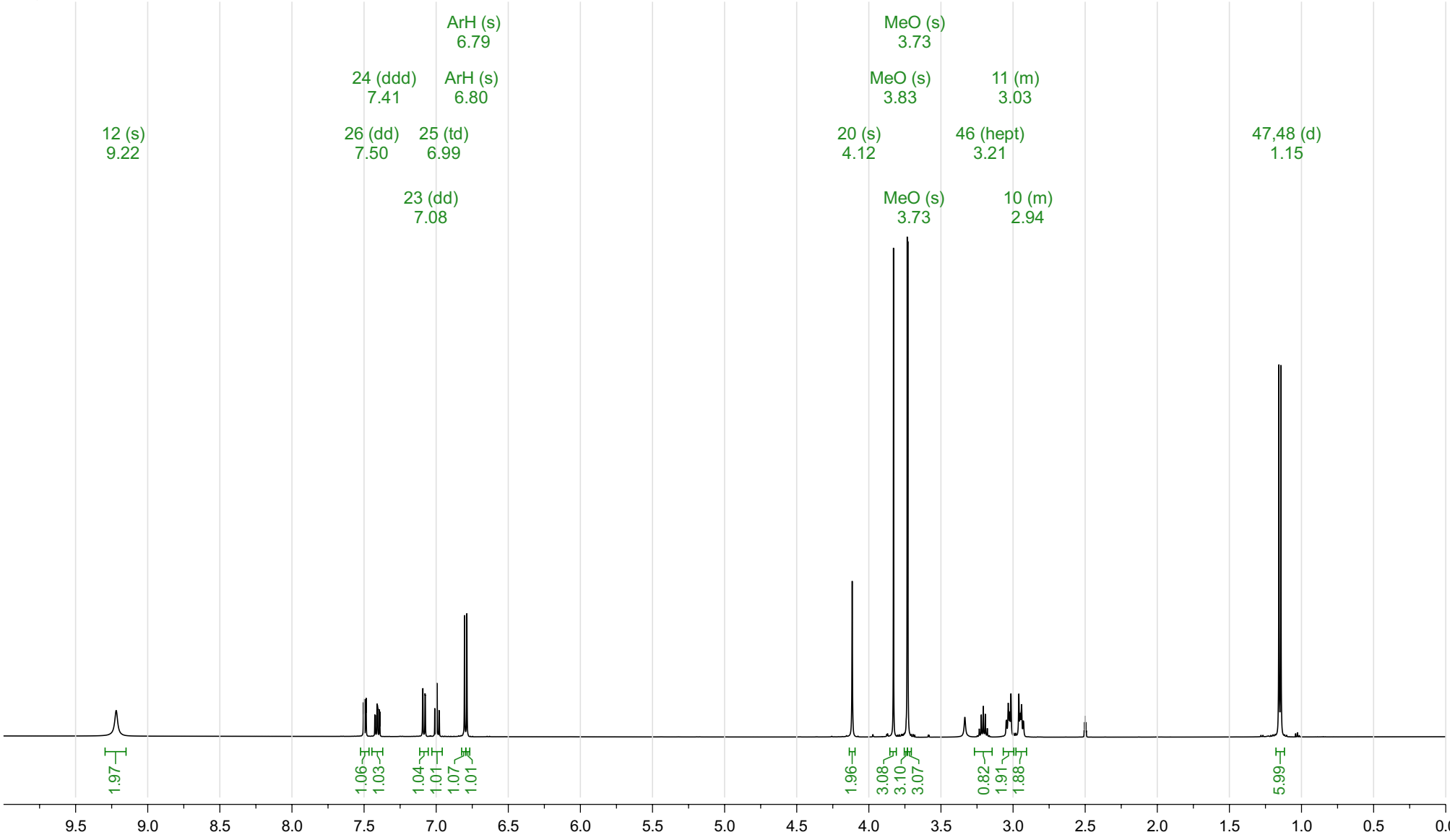
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.22 (s, 2H), 7.50 (dd, J = 7.5, 1.7 Hz, 1H), 7.41 (ddd, J = 8.3, 7.4, 1.7 Hz, 1H), 7.08 (dd, J = 8.4, 1.0 Hz, 1H), 6.99 (td, J = 7.4, 1.0 Hz, 1H), 6.80 (s, 1H), 6.79 (s, 1H), 4.12 (s, 2H), 3.83 (s, 3H), 3.73 (s, 3H), 3.73 (s, 3H), 3.21 (hept, J = 6.9 Hz, 1H), 3.07 – 2.99 (m, 2H), 2.98 – 2.91 (m, 2H), 1.15 (d, J = 6.9 Hz, 6H).



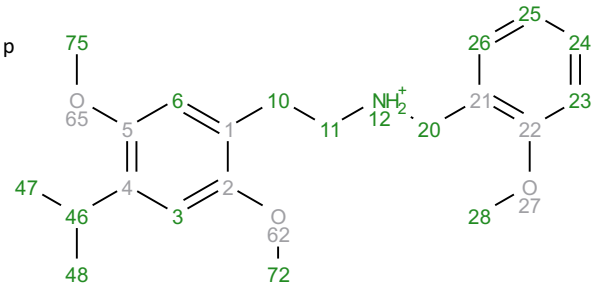
Analyte	B8: 25IP-NBOMe H+
Acquisition Date	2013-03-26T19:52:57
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	10964.9
Nucleus	1H
Acquired Size	65536



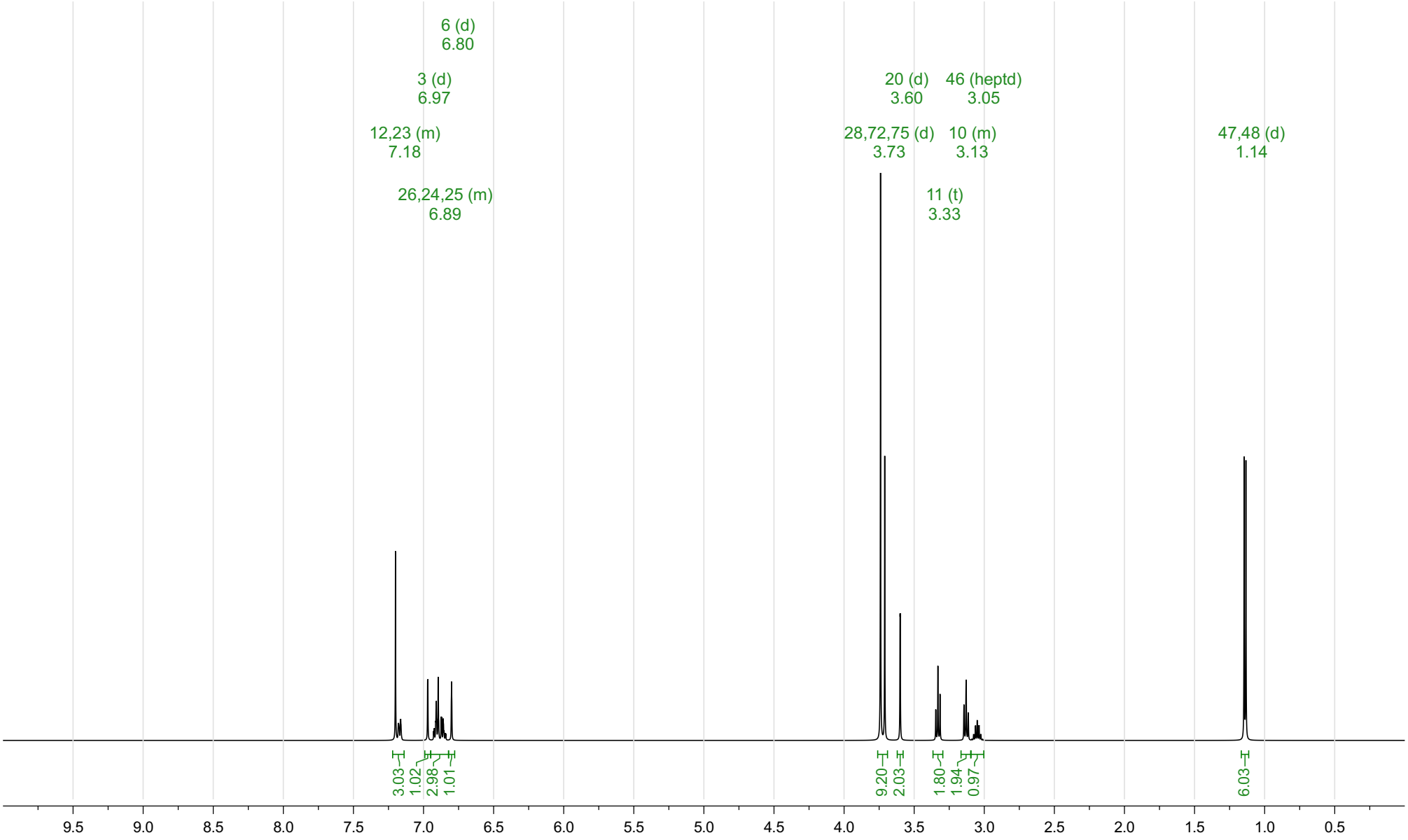
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.22 (s, 2H), 7.50 (dd, J = 7.5, 1.7 Hz, 1H), 7.41 (ddd, J = 8.3, 7.4, 1.7 Hz, 1H), 7.08 (dd, J = 8.4, 1.0 Hz, 1H), 6.99 (td, J = 7.4, 1.0 Hz, 1H), 6.80 (s, 1H), 6.79 (s, 1H), 4.12 (s, 2H), 3.83 (s, 3H), 3.73 (s, 3H), 3.73 (s, 3H), 3.21 (hept, J = 6.9 Hz, 1H), 3.07 – 2.99 (m, 2H), 2.98 – 2.91 (m, 2H), 1.15 (d, J = 6.9 Hz, 6H).



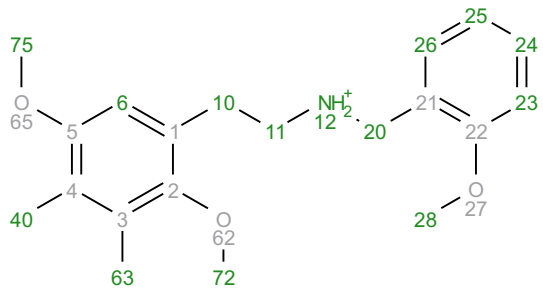
Prediction	25IP-NBOMe H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



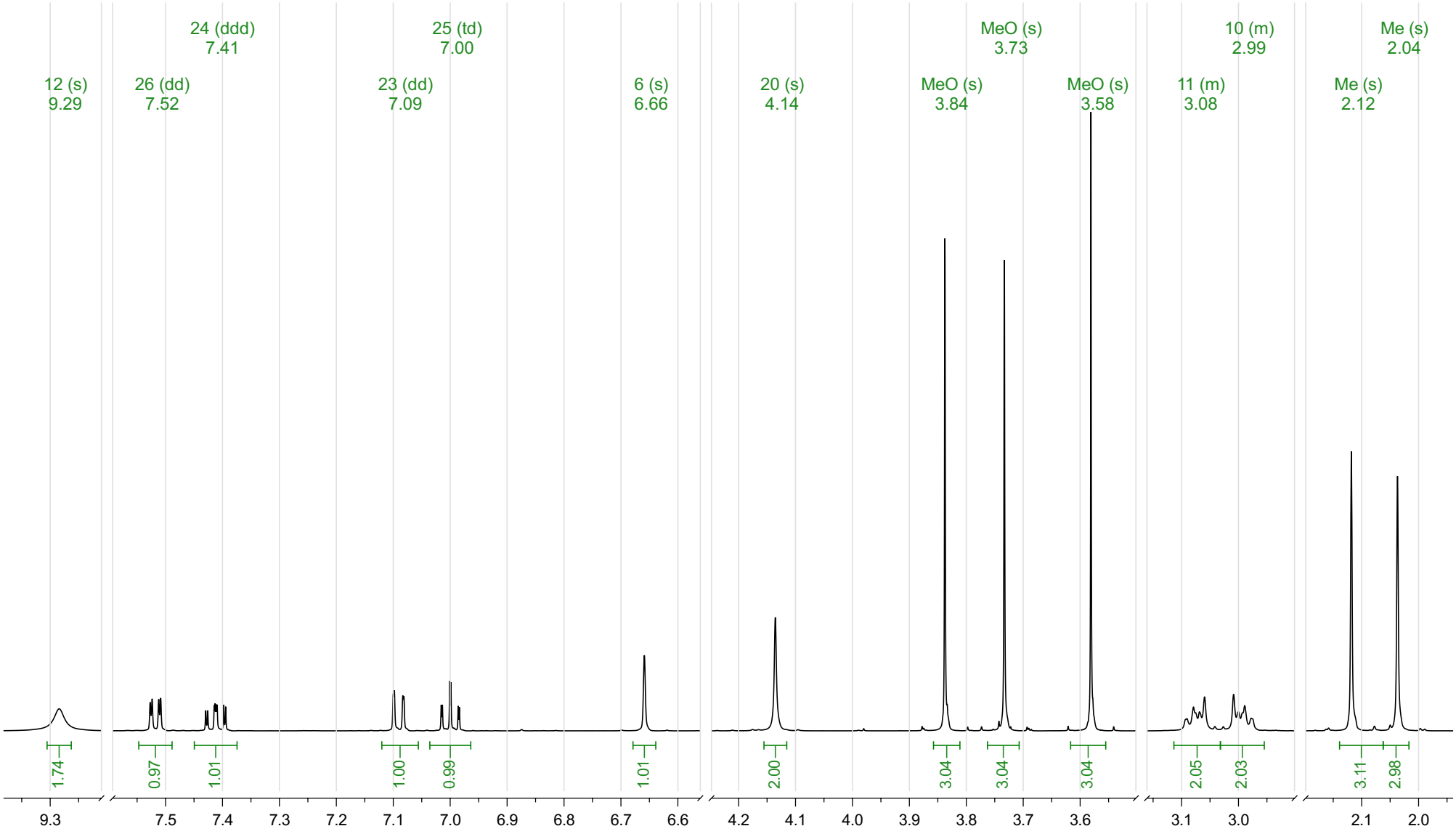
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.22 – 7.14 (m, 3H), 6.97 (d, J = 1.0 Hz, 1H), 6.95 – 6.82 (m, 3H), 6.80 (d, J = 1.0 Hz, 1H), 3.73 (d, J = 15.0 Hz, 9H), 3.60 (d, J = 0.9 Hz, 2H), 3.33 (t, J = 7.5 Hz, 2H), 3.17 – 3.09 (m, 2H), 3.05 (heptd, J = 6.4, 1.0 Hz, 1H), 1.14 (d, J = 6.4 Hz, 6H).



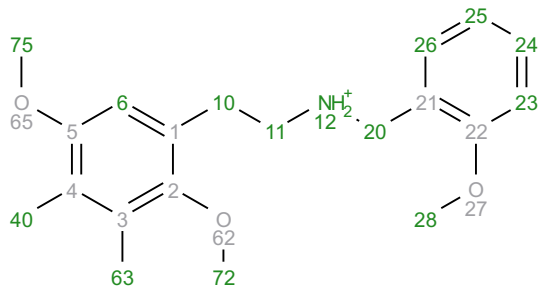
Analyte	B9: 25G-NBOMe H+
Acquisition Date	2013-05-07T19:40:05
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	10000.0
Nucleus	1H
Acquired Size	65536



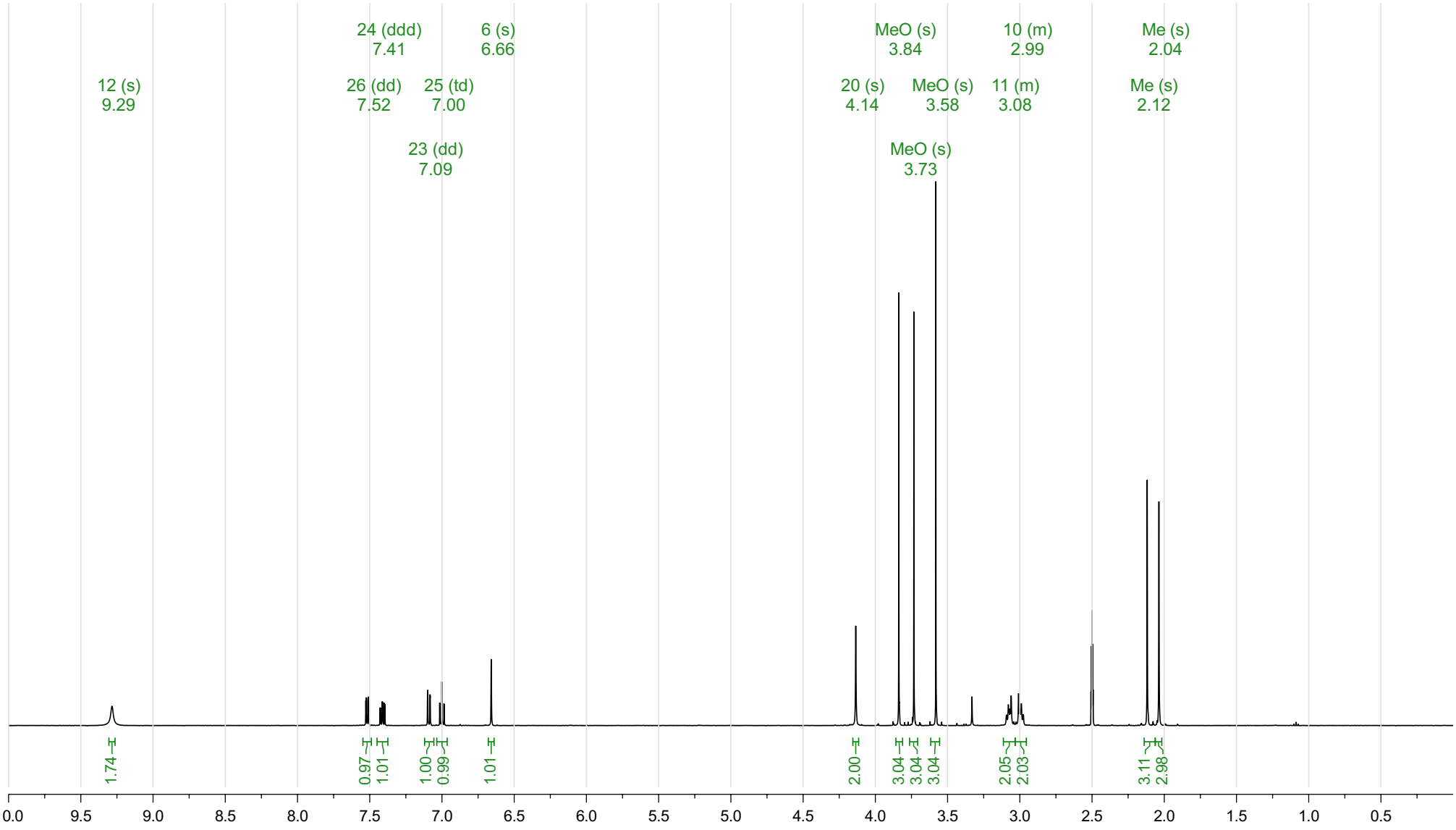
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.29 (s, 2H), 7.52 (dd, J = 7.5, 1.7 Hz, 1H), 7.41 (ddd, J = 8.3, 7.5, 1.7 Hz, 1H), 7.09 (dd, J = 8.4, 1.0 Hz, 1H), 7.00 (td, J = 7.5, 7.4, 1.0 Hz, 1H), 6.66 (s, 1H), 4.14 (s, 2H), 3.84 (s, 3H), 3.73 (s, 3H), 3.58 (s, 3H), 3.11 – 3.02 (m, 2H), 3.05 – 2.95 (m, 2H), 2.12 (s, 3H), 2.04 (s, 3H).



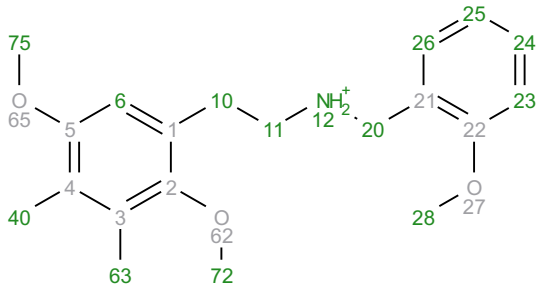
Analyte	B9: 25G-NBOMe H+
Acquisition Date	2013-05-07T19:40:05
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	10000.0
Nucleus	1H
Acquired Size	65536



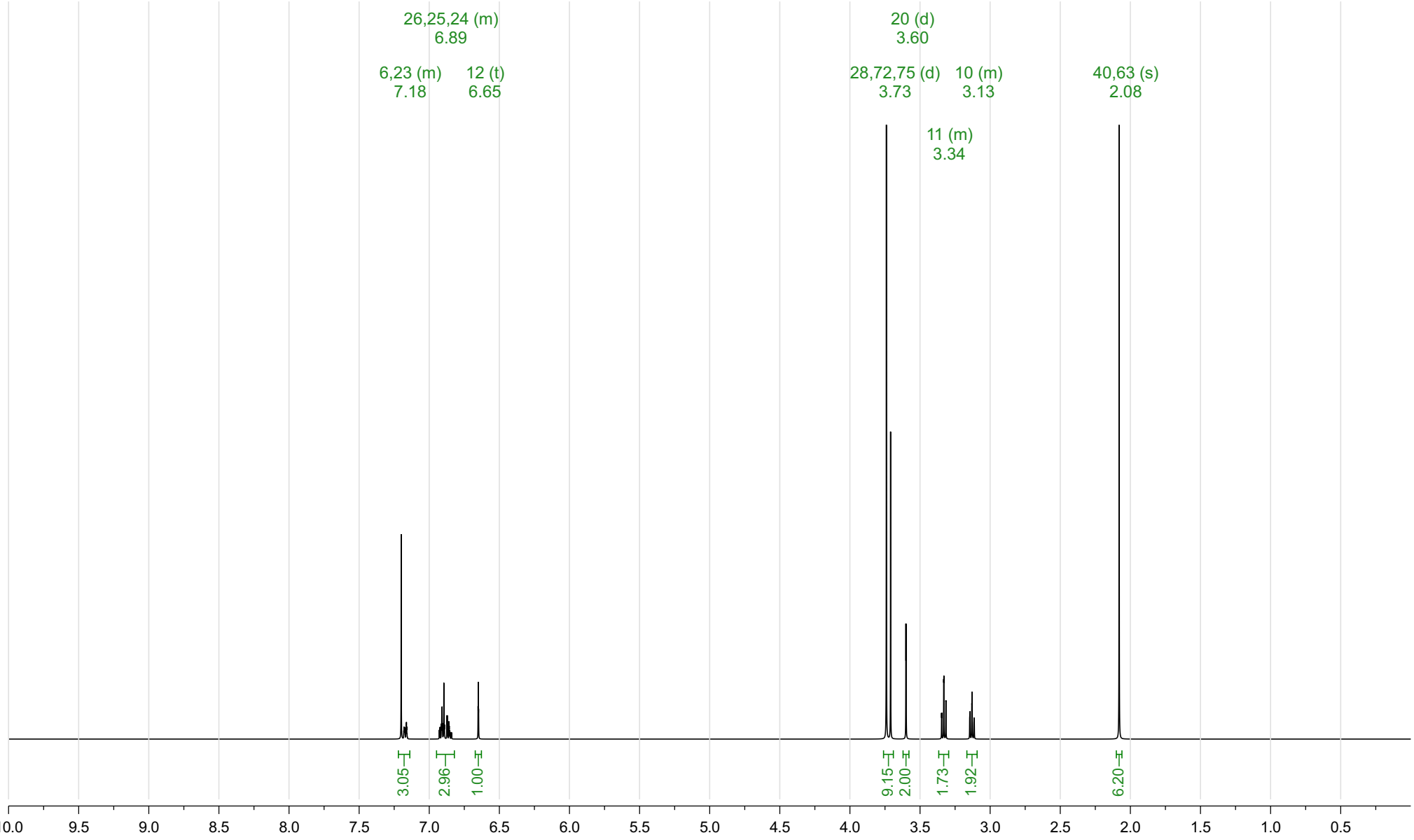
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.29 (s, 2H), 7.52 (dd, J = 7.5, 1.7 Hz, 1H), 7.41 (ddd, J = 8.3, 7.5, 1.7 Hz, 1H), 7.09 (dd, J = 8.4, 1.0 Hz, 1H), 7.00 (td, J = 7.5, 1.0 Hz, 1H), 6.66 (s, 1H), 4.14 (s, 2H), 3.84 (s, 3H), 3.73 (s, 3H), 3.58 (s, 3H), 3.11 – 3.02 (m, 2H), 3.05 – 2.95 (m, 2H), 2.12 (s, 3H), 2.04 (s, 3H).



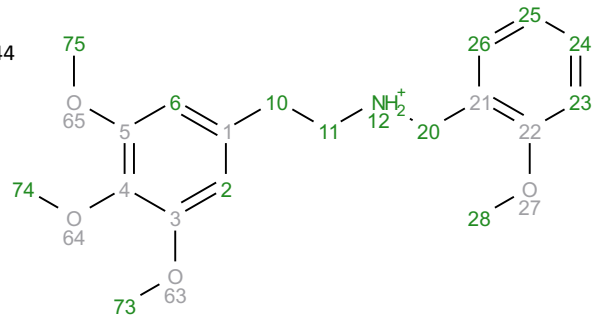
Prediction	25G-NBOMe H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11591
Frequency	500.00
Nucleus	1H



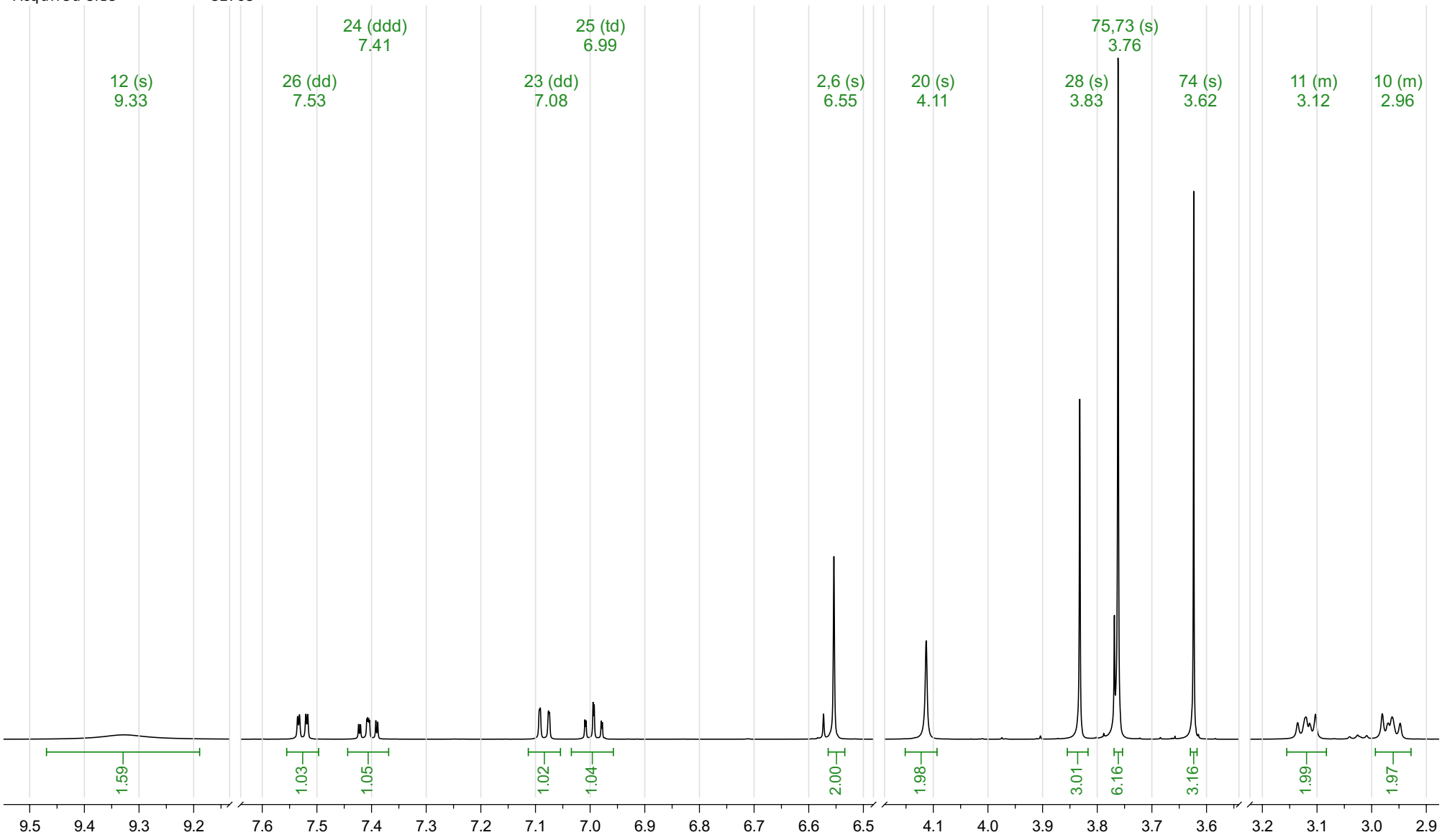
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.22 – 7.13 (m, 3H), 6.95 – 6.82 (m, 3H), 6.65 (t, J = 1.0 Hz, 1H), 3.73 (d, J = 15.0 Hz, 9H), 3.60 (d, J = 0.9 Hz, 2H), 3.37 – 3.30 (m, 2H), 3.17 – 3.09 (m, 2H), 2.08 (s, 6H).



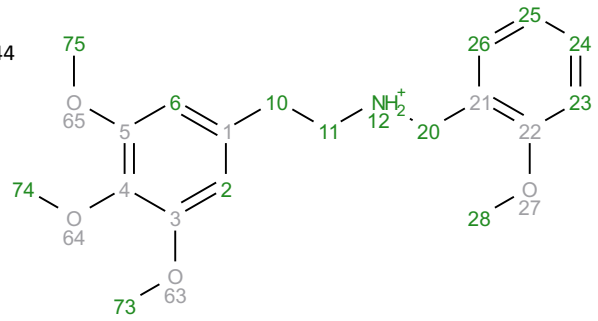
Analyte	B10: M-NBOMe H+
Acquisition Date	2013-01-17T03:17:44
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



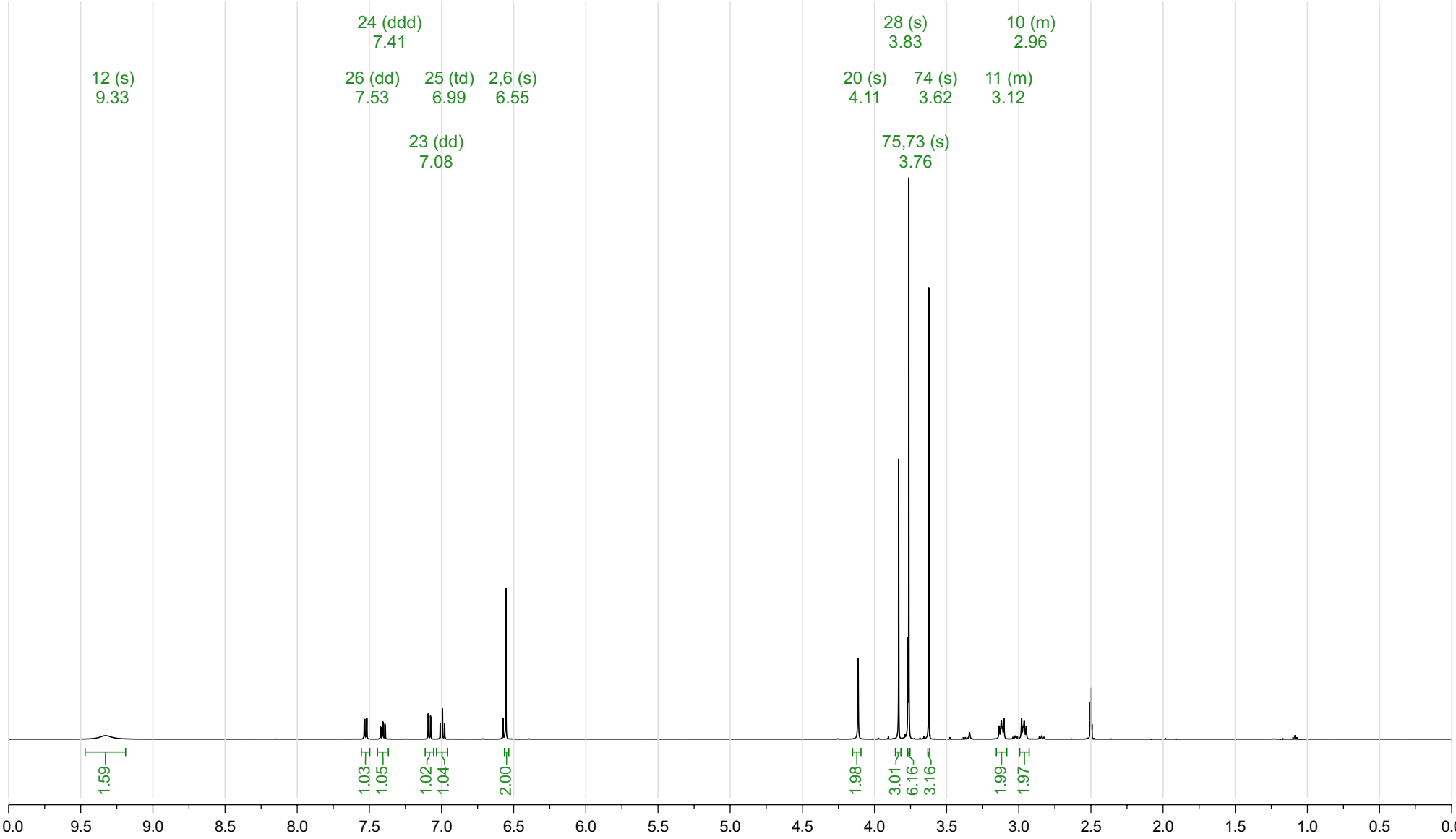
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.33 (s, 2H), 7.53 (dd, J = 7.5, 1.7 Hz, 1H), 7.41 (ddd, J = 8.2, 7.4, 1.7 Hz, 1H), 7.08 (dd, J = 8.4, 1.0 Hz, 1H), 6.99 (td, J = 7.5, 1.0 Hz, 1H), 6.55 (s, 2H), 4.11 (s, 2H), 3.83 (s, 3H), 3.76 (s, 6H), 3.62 (s, 3H), 3.16 – 3.08 (m, 2H), 3.00 – 2.93 (m, 2H).



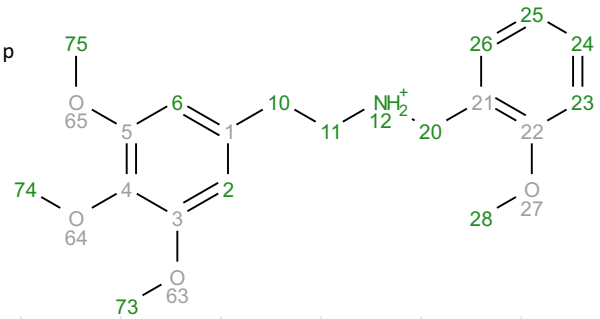
Analyte	B10: M-NBOMe H+
Acquisition Date	2013-01-17T03:17:44
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	32768



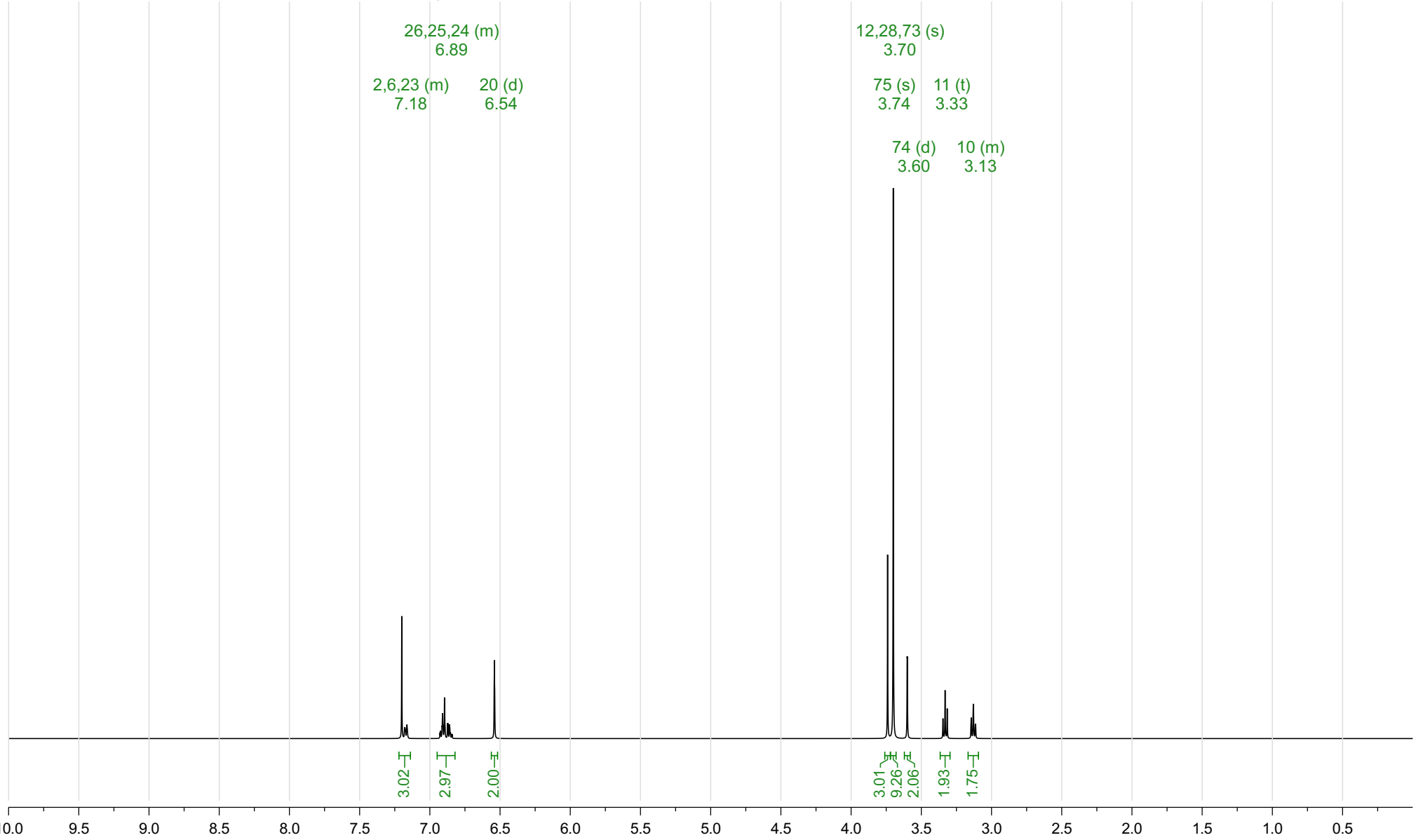
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.33 (s, 2H), 7.53 (dd, J = 7.5, 1.7 Hz, 1H), 7.41 (ddd, J = 8.2, 7.4, 1.7 Hz, 1H), 7.08 (dd, J = 8.4, 1.0 Hz, 1H), 6.99 (td, J = 7.5, 1.0 Hz, 1H), 6.55 (s, 2H), 4.11 (s, 2H), 3.83 (s, 3H), 3.76 (s, 6H), 3.62 (s, 3H), 3.16 – 3.08 (m, 2H), 3.00 – 2.93 (m, 2H).



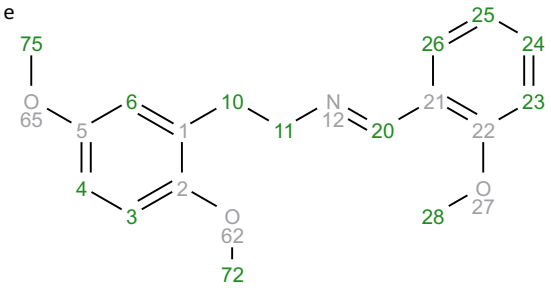
Prediction	M-NBOMe H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	11880
Frequency	500.00
Nucleus	1H



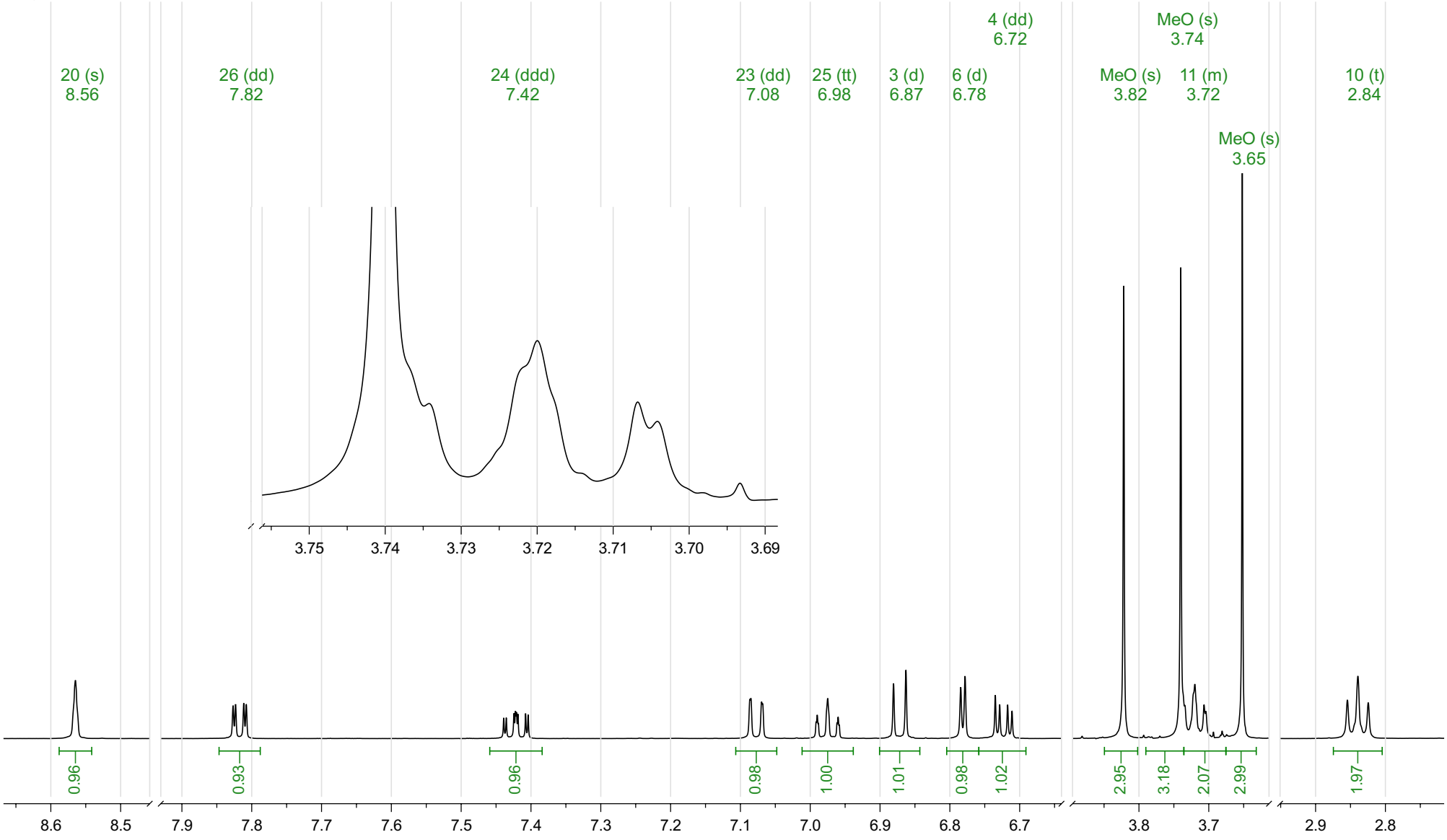
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.22 – 7.13 (m, 3H), 6.95 – 6.82 (m, 3H), 6.54 (d, J = 1.2 Hz, 2H), 3.74 (s, 3H), 3.70 (s, 9H), 3.60 (d, J = 0.9 Hz, 2H), 3.33 (t, J = 7.5 Hz, 2H), 3.17 – 3.09 (m, 2H).



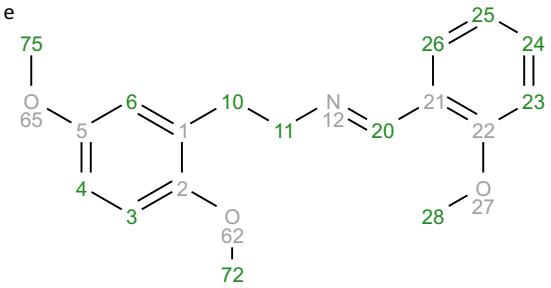
Analyte	IM1: 25H-NBOMe imine
Acquisition Date	2013-11-08T17:11:08
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	1
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	36058



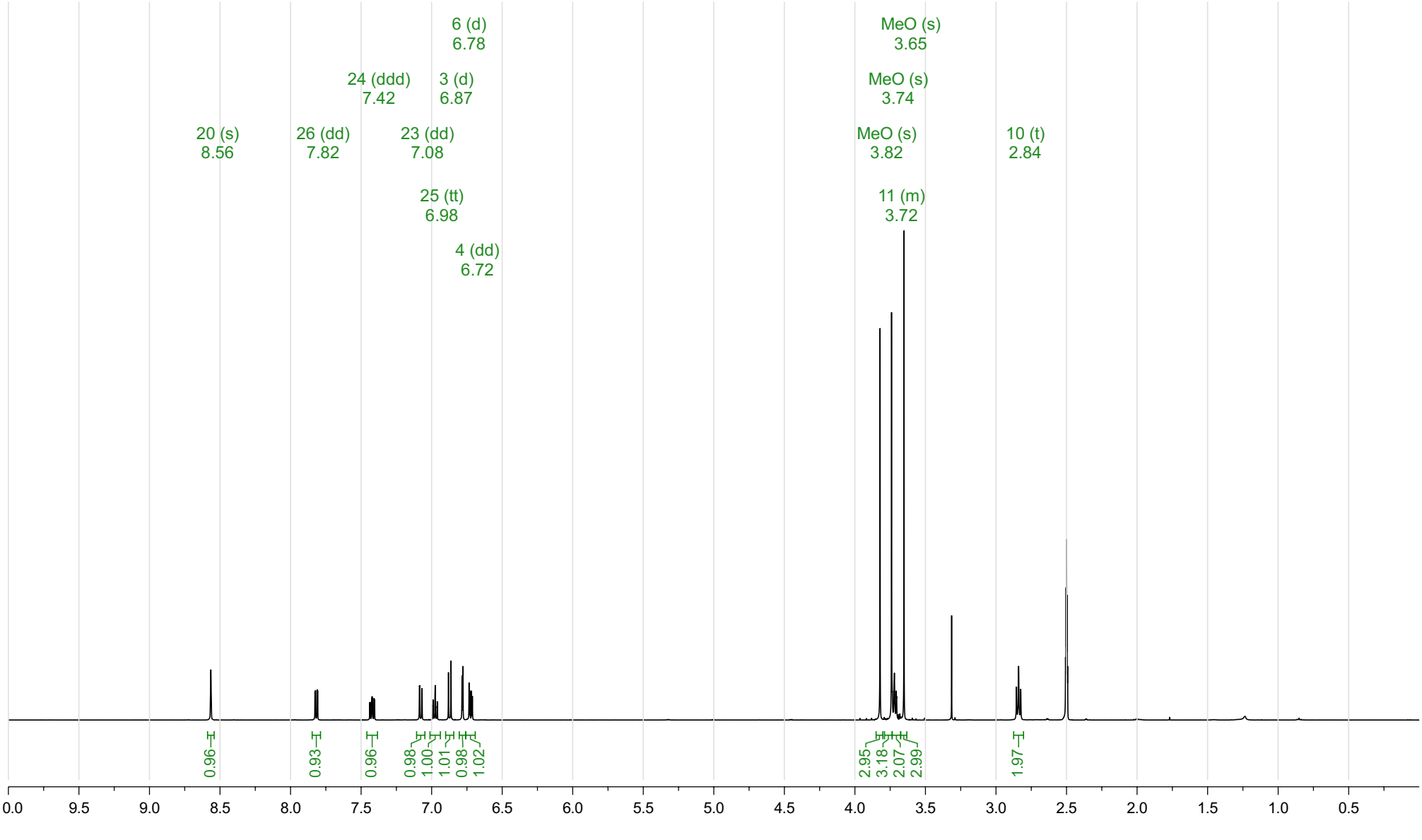
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.56 (s, 1H), 7.82 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.42 (ddd, *J* = 8.3, 7.3, 1.8 Hz, 1H), 7.08 (dd, *J* = 8.4, 1.0 Hz, 1H), 6.98 (tt, *J* = 7.5, 0.8 Hz, 1H), 6.87 (d, *J* = 8.8 Hz, 1H), 6.78 (d, *J* = 3.1 Hz, 1H), 6.72 (dd, *J* = 8.8, 3.1 Hz, 1H), 3.82 (s, 3H), 3.74 (s, 3H), 3.75 – 3.68 (m, 2H), 3.65 (s, 3H), 2.84 (t, *J* = 7.5 Hz, 2H).



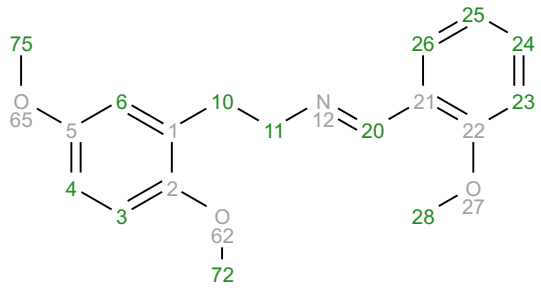
Analyte	IM1: 25H-NBOMe imine
Acquisition Date	2013-11-08T17:11:08
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	1
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	36058



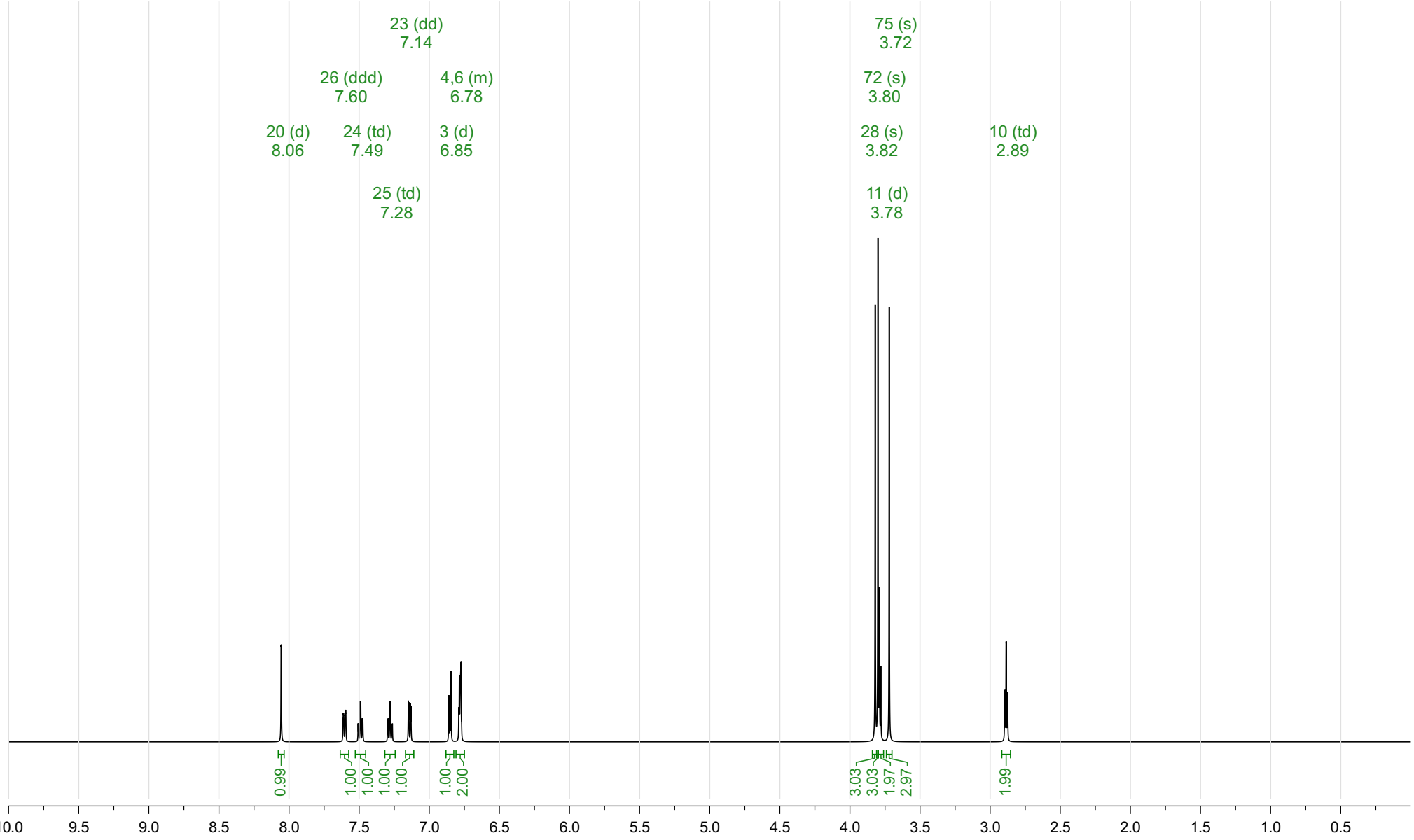
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.56 (s, 1H), 7.82 (dd, J = 7.7, 1.8 Hz, 1H), 7.42 (ddd, J = 8.3, 7.3, 1.8 Hz, 1H), 7.08 (dd, J = 8.4, 1.0 Hz, 1H), 6.98 (tt, J = 7.5, 0.8 Hz, 1H), 6.87 (d, J = 8.8 Hz, 1H), 6.78 (d, J = 3.1 Hz, 1H), 6.72 (dd, J = 8.8, 3.1 Hz, 1H), 3.82 (s, 3H), 3.74 (s, 3H), 3.75 – 3.68 (m, 2H), 3.65 (s, 3H), 2.84 (t, J = 7.5 Hz, 2H).



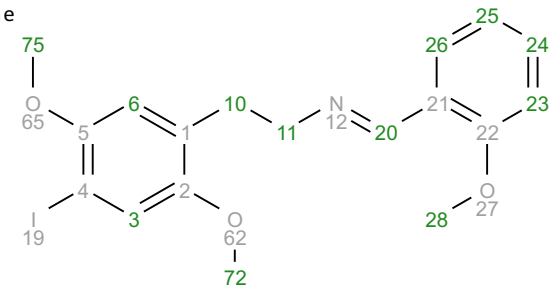
Prediction	25H-NBOMe imine
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	12489
Frequency	500.00
Nucleus	1H



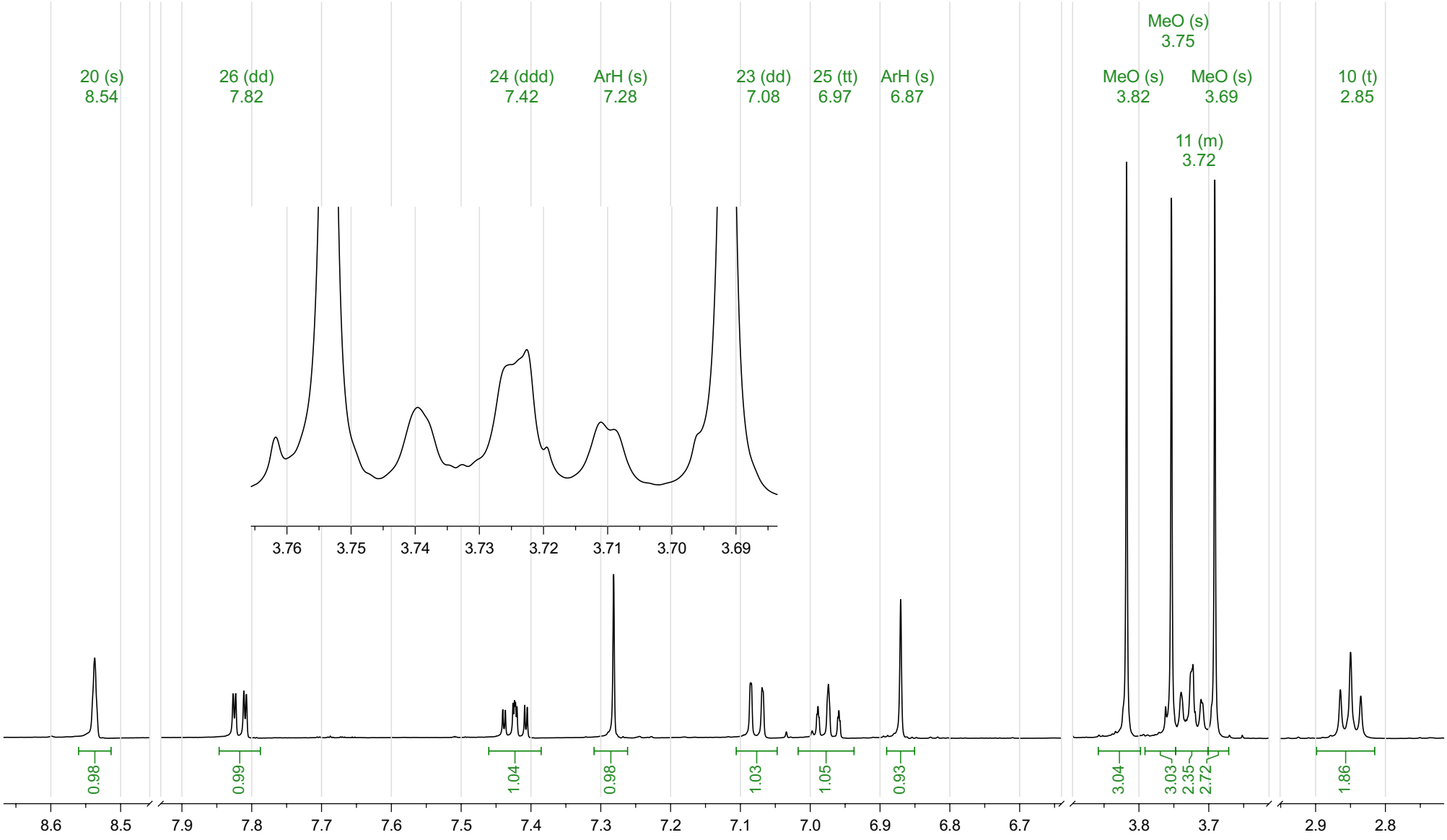
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.06 (d, J = 1.0 Hz, 1H), 7.60 (ddd, J = 7.4, 2.0, 1.0 Hz, 1H), 7.49 (td, J = 7.5, 2.0 Hz, 1H), 7.28 (td, J = 7.5, 2.0 Hz, 1H), 7.14 (dd, J = 7.5, 2.1 Hz, 1H), 6.85 (d, J = 8.0 Hz, 1H), 6.81 – 6.75 (m, 2H), 3.82 (s, 3H), 3.80 (s, 3H), 3.78 (d, J = 5.0 Hz, 2H), 3.72 (s, 3H), 2.89 (td, J = 5.0, 1.0 Hz, 2H).



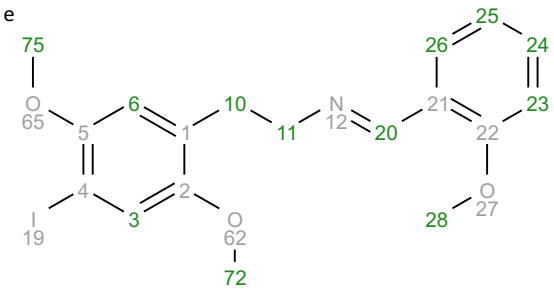
Analyte	IM2: 25I-NBOMe imine
Acquisition Date	2013-11-08T17:17:35
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	1
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	36058



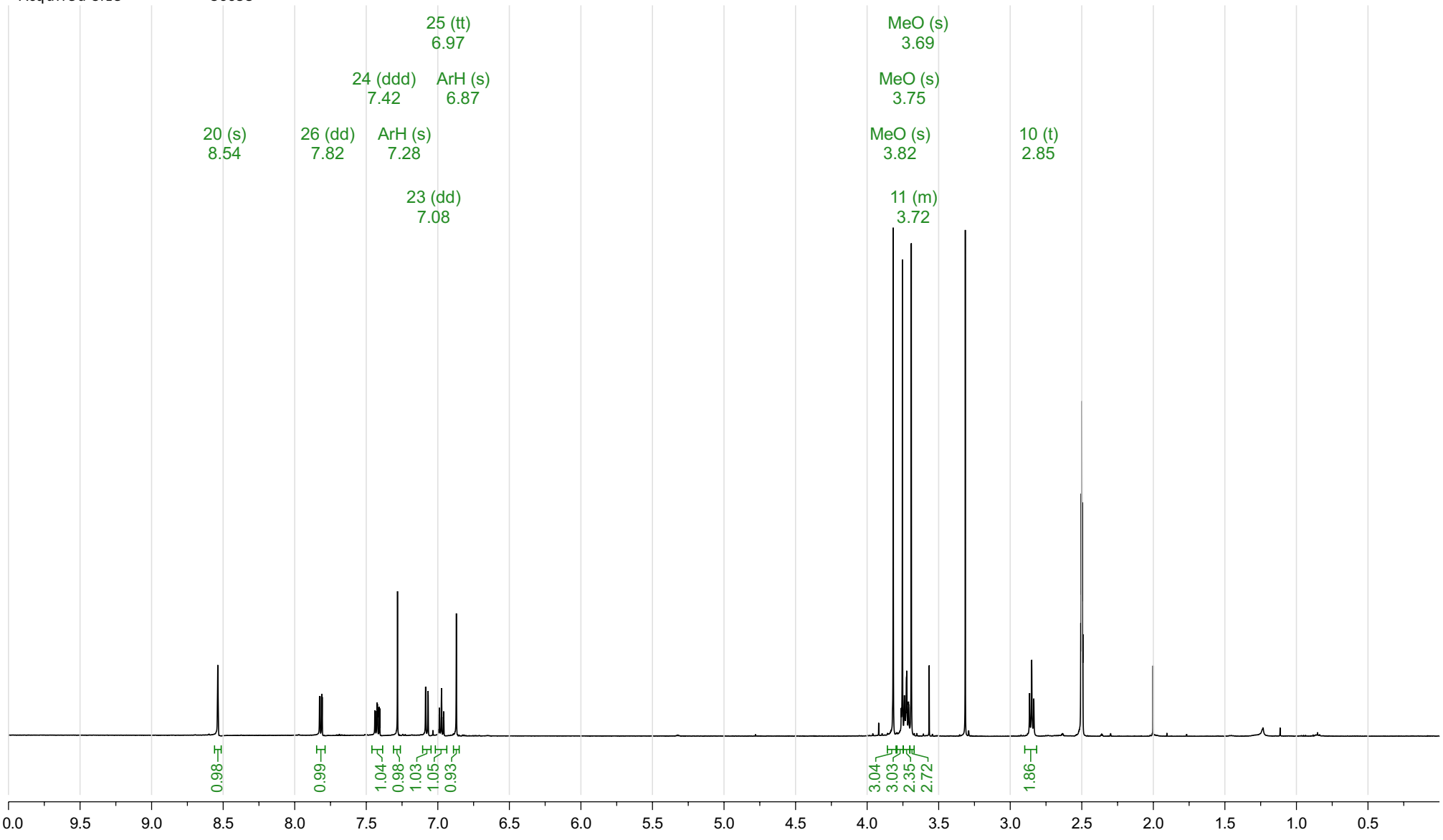
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.54 (s, 1H), 7.82 (dd, J = 7.7, 1.8 Hz, 1H), 7.42 (ddd, J = 8.3, 7.3, 1.8 Hz, 1H), 7.28 (s, 1H), 7.08 (dd, J = 8.3, 1.0 Hz, 1H), 6.97 (tt, J = 7.5, 0.8 Hz, 1H), 6.87 (s, 1H), 3.82 (s, 3H), 3.75 (s, 3H), 3.76 – 3.69 (m, 2H), 3.69 (s, 3H), 2.85 (t, J = 7.3 Hz, 2H).



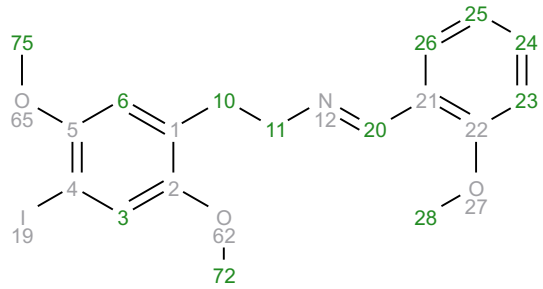
Analyte	IM2: 25I-NBOMe imine
Acquisition Date	2013-11-08T17:17:35
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	1
Spectrometer Frequency	499.67
Spectral Width	8012.8
Nucleus	1H
Acquired Size	36058



^{1}H NMR (500 MHz, DMSO-d_6) δ 8.54 (s, 1H), 7.82 (dd, J = 7.7, 1.8 Hz, 1H), 7.42 (ddd, J = 8.3, 7.3, 1.8 Hz, 1H), 7.28 (s, 1H), 7.08 (dd, J = 8.3, 1.0 Hz, 1H), 6.97 (tt, J = 7.5, 0.8 Hz, 1H), 6.87 (s, 1H), 3.82 (s, 3H), 3.75 (s, 3H), 3.76 – 3.69 (m, 2H), 3.69 (s, 3H), 2.85 (t, J = 7.3 Hz, 2H).



Prediction	25I-NBOMe imine
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	50
Version	12489
Frequency	500.00
Nucleus	1H



^{1}H NMR (500 MHz, DMSO-d_6) δ 7.99 (d, J = 1.2 Hz, 1H), 7.58 (ddd, J = 7.5, 2.0, 0.9 Hz, 1H), 7.49 (td, J = 7.5, 2.0 Hz, 1H), 7.28 (td, J = 7.5, 2.0 Hz, 1H), 7.22 (s, 1H), 7.14 (dd, J = 7.5, 2.0 Hz, 1H), 6.72 (t, J = 1.0 Hz, 1H), 3.93 (s, 3H), 3.82 (s, 3H), 3.78 (t, J = 5.1 Hz, 2H), 3.74 (s, 3H), 2.87 (td, J = 5.1, 1.0 Hz, 2H).