Brandt, SD, Carlino, L, Kavanagh, PV, Westphal, F, Dreiseitel, W, Dowling, G, Baumann, MH, Sitte, HH and Halberstadt, AL

Syntheses and analytical characterizations of novel (2-aminopropyl)benzo[b]thiophene (APBT) based stimulants

Syntheses and analytical characterizations of novel (2-aminopropyl)benzo[*b*]thiophene (APBT) based stimulants

Simon D. Brandt,[1,*] Laura Carlino,[1,2] Pierce V. Kavanagh,[3] Folker Westphal,[4] Wolfgang Dreiseitel,[5] Geraldine Dowling,[3,6] Michael H. Baumann,[7] Harald H. Sitte,[8] Adam L. Halberstadt [9,10]

[1] *School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, Byrom Street, Liverpool L3 3AF, UK*

[2] *School of Chemical Engineers, University of Upper Alsace, 68093 Mulhouse, France*

[3] *Department of Pharmacology and Therapeutics, School of Medicine, Trinity Centre for Health Sciences, St. James Hospital, Dublin 8, Ireland*

[4] *State Bureau of Criminal Investigation Schleswig-Holstein, Section Narcotics/Toxicology, Mühlenweg 166, D-24116 Kiel, Germany*

[5] *Hessian State Bureau of Criminal Investigation, Hölderlinstraße 1–5, Wiesbaden, Germany*

[6] *Department of Life Sciences, School of Science, Sligo Institute of Technology, Ash Lane, Sligo, F91YW50, Ireland*

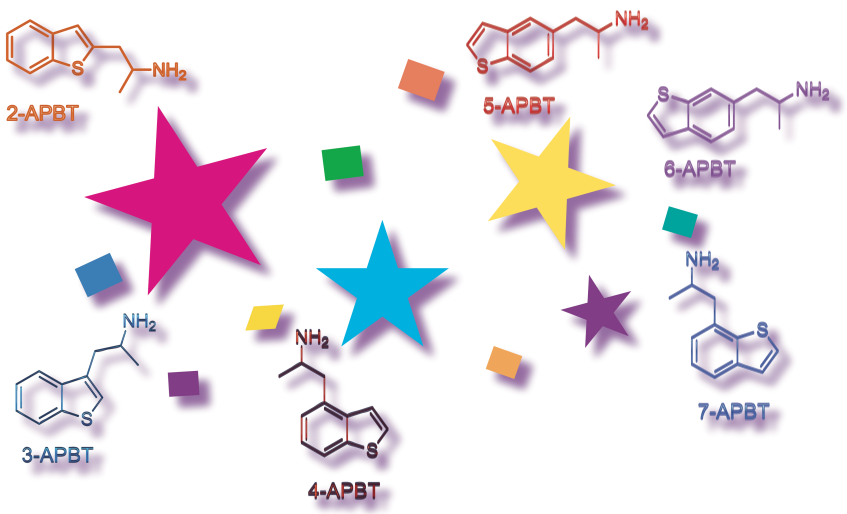
[7] *Designer Drug Research Unit, Intramural Research Program, National Institute on Drug Abuse, National Institutes of Health, Baltimore, MD 21224, USA*

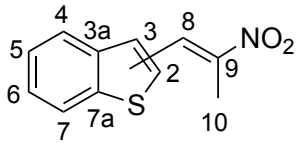
[8] *Medical University of Vienna, Center for Physiology and Pharmacology, Institute of Pharmacology, Währinger Straße 13a, A-1090 Vienna, Austria.*

[9] *Department of Psychiatry, University of California San Diego, La Jolla, CA 92093-0804, USA*

[10] *Research Service, VA San Diego Healthcare System, La Jolla, CA, USA*

* Correspondence to: Simon D. Brandt, School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, Byrom Street, Liverpool, L3 3AF, UK. E-Mail: s.brandt@ljmu.ac.uk

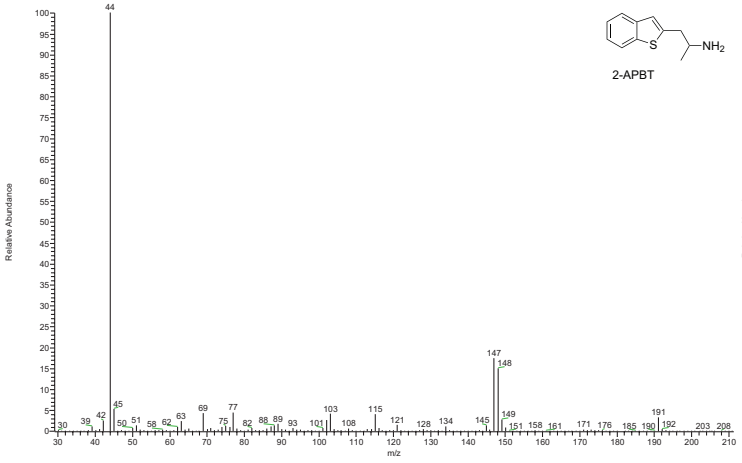


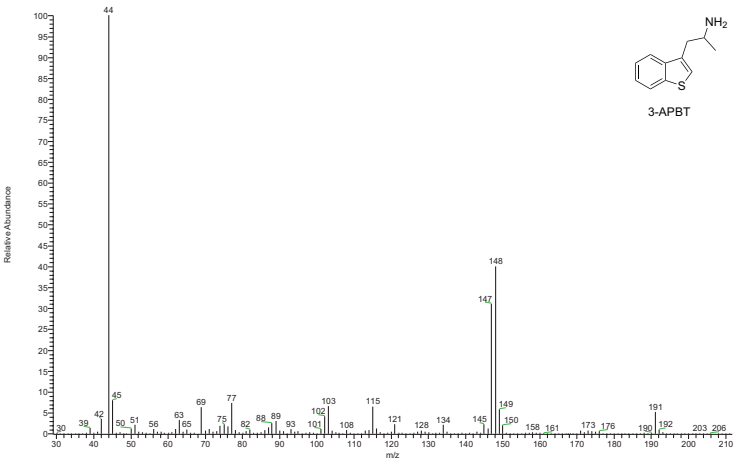


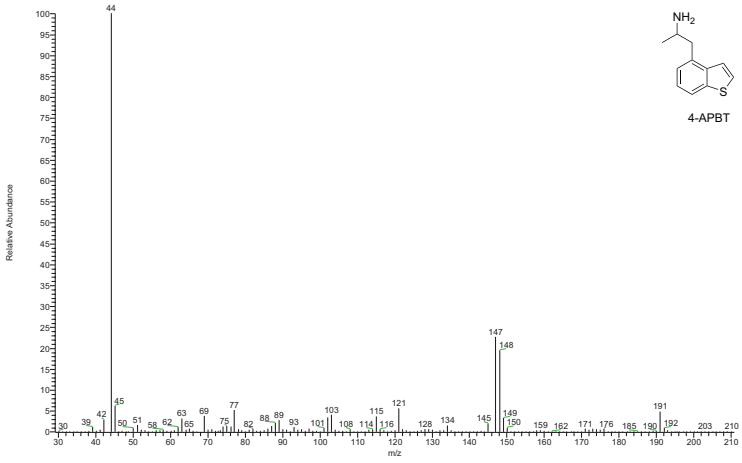
Isomer	**2**		**3**		**5**		**6**	
Position	^{1}H	^{13}C	^{1}H	^{13}C	^{1}H	^{13}C	^{1}H	^{13}C
2	-	134.90	7.70 (s)	129.03	7.56 (d, *J* = 5.4 Hz)	128.06	7.59 (d, *J* = 5.4 Hz)	129.28
3	7.68 (s)	132.07	-	128.23	7.42 (d, *J* = 5.4 Hz)	124.00	7.38 (d, J = 5.4 Hz)	123.82
3a	-	138.62 or 141.94	-	138.30	-	139.92	-	140.23
4	7.91–7.86 (m)	124.75	7.91 (dist. d, *J* = 7.8 Hz)	121.77	7.91 (s)	125.46 or 125.48	7.88 (d, *J* = 8.3 Hz)	123.98
5	7.49–7.43 (m)	126.66 or 125.28	7.54–7.51 (m)	125.14 or 125.15	-	128.56	7.44 (dd, *J* = 8.3, 1.4 Hz)	125.95
6	7.49–7.43 (m)	126.66 or 125.28	7.50–7.47 (m)	125.52	7.42 (dd, *J* = 8.4, 1.6 Hz)	125.46 or 125.48	-	128.43
7	7.91–7.86 (m)	122.35	7.94 (dist. d, *J* = 7.8 Hz)	122.92	7.97 (d, *J* = 8.4 Hz)	123.01	7.97 (s)	124.43
7a	-	138.62 or 141.94	-	139.51	-	141.29	-	140.63
8	8.37–8.36 (m)	127.73	8.38–8.37 (m)	125.14 or 125.15	8.25 (s)	133.98	8.22 (s)	133.83
9	-	146.17	-	148.28	-	147.37	-	147.37
10	2.66 (d, *J* = 0.4 Hz)	14.28	2.57 (d, *J* = 0.8 Hz)	14.70	2.54 (d, *J* = 1.0 Hz)	14.19	2.53 (d, *J* = 0.9 Hz)	14.26

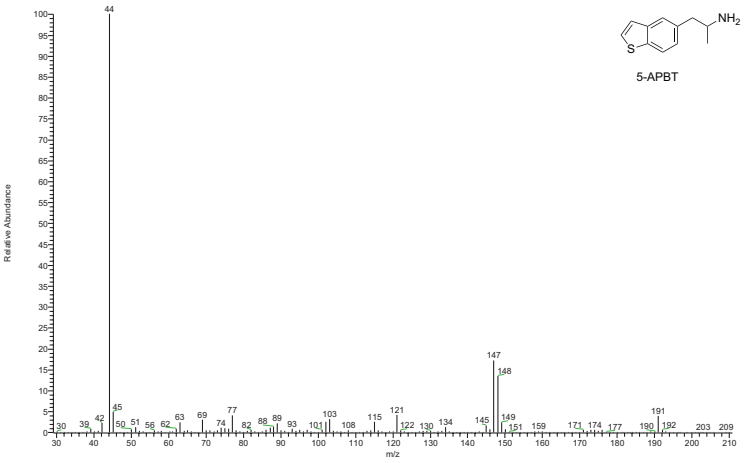
Table 1. NMR data for nitrostyrene intermediates ($CDCl_3$, 600/150 MHz).

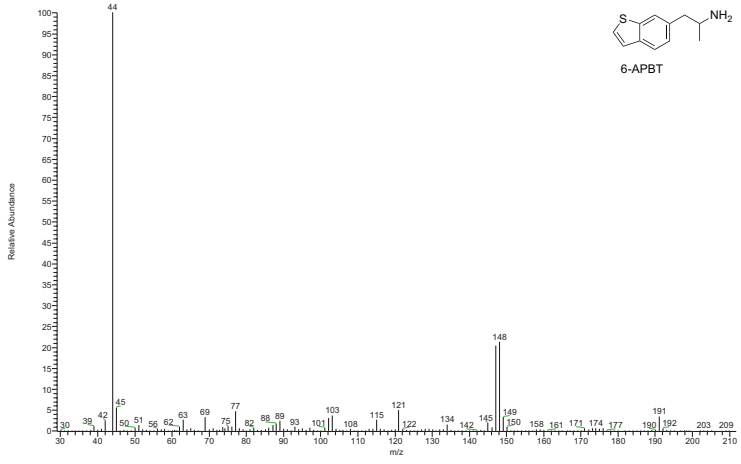
Electron ionization mass spectra of APBT isomers

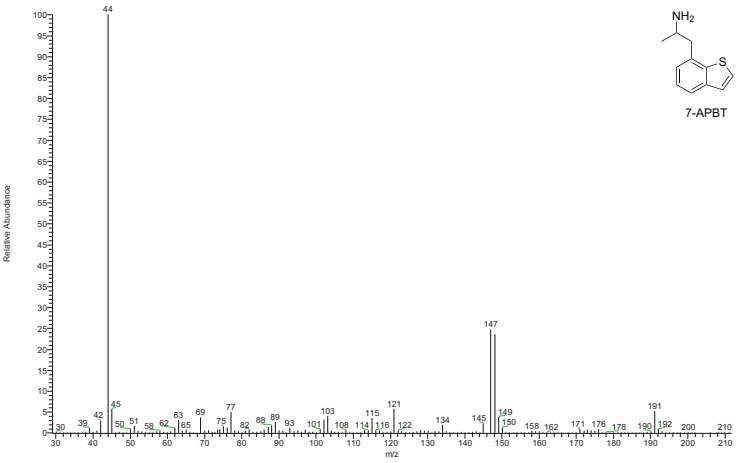




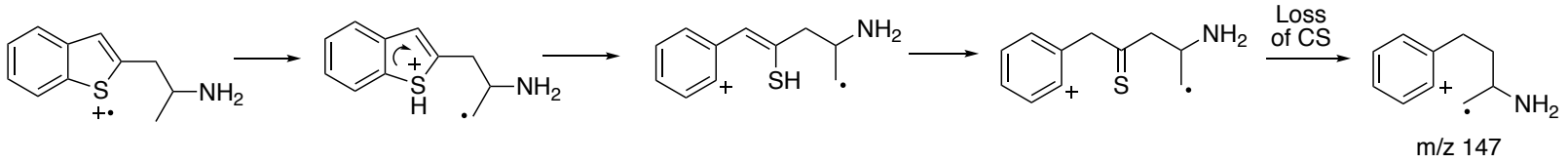


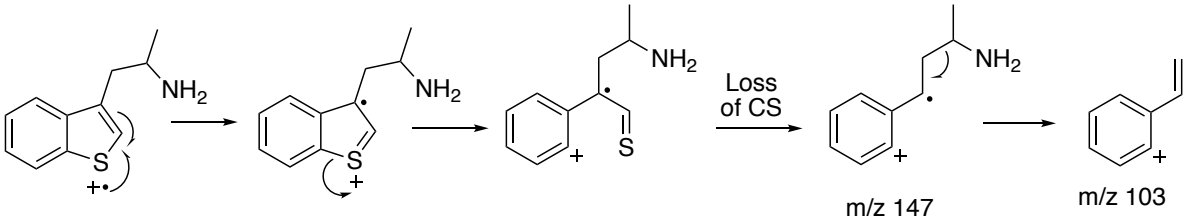


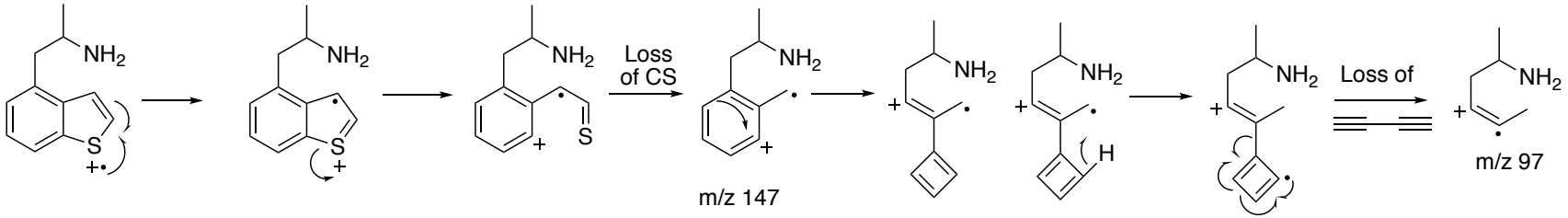


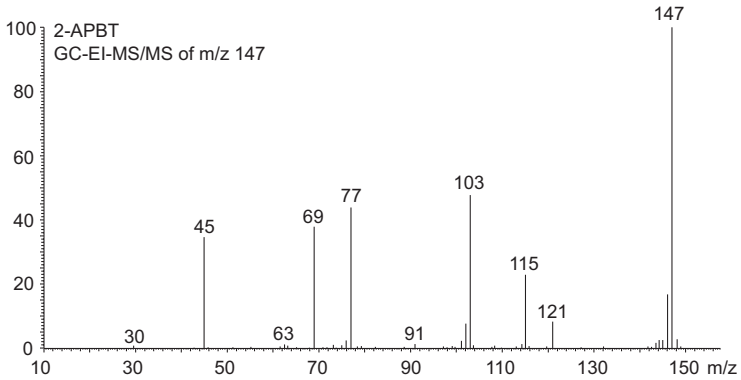


Alternative suggestions for m/z 147 and m/z 97 (EI-MS)





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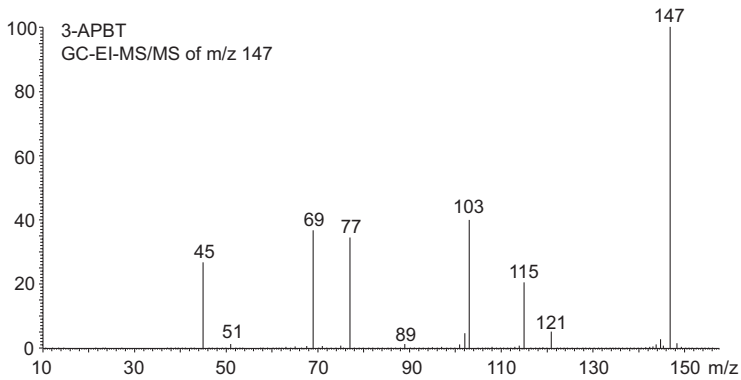
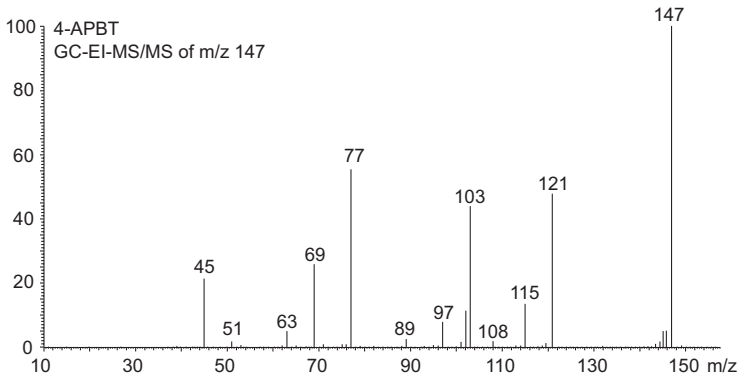
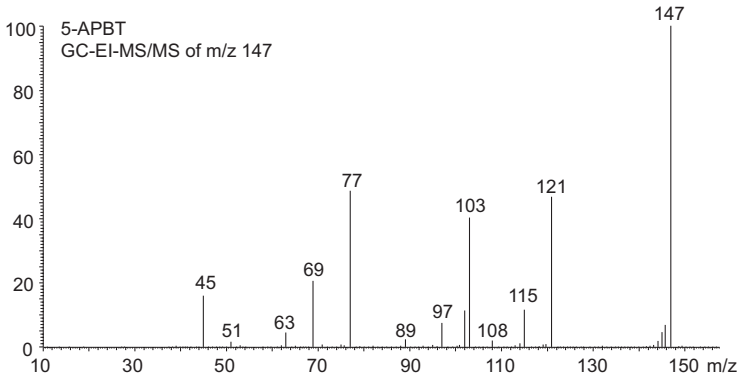
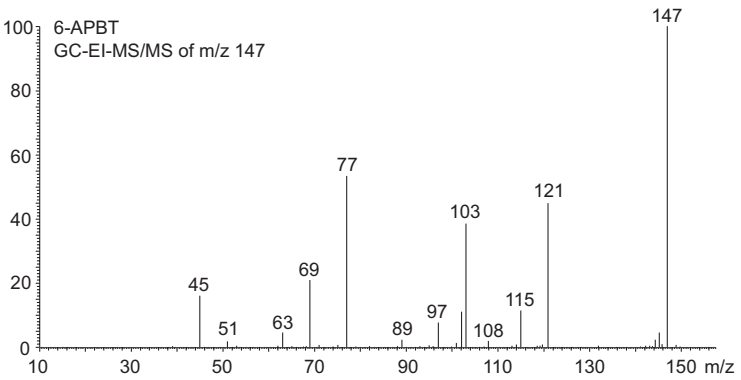
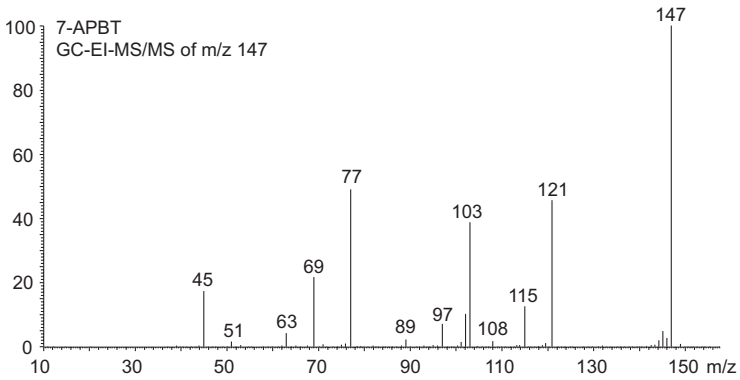
GC-EI-MS/MS of m/z 147
147
103
77
69
45
115
121
30
63
91
m/z


3-APBT
GC-EI-MS/MS of m/z 147
147
103
69
77
45
115
121
51
89
m/z

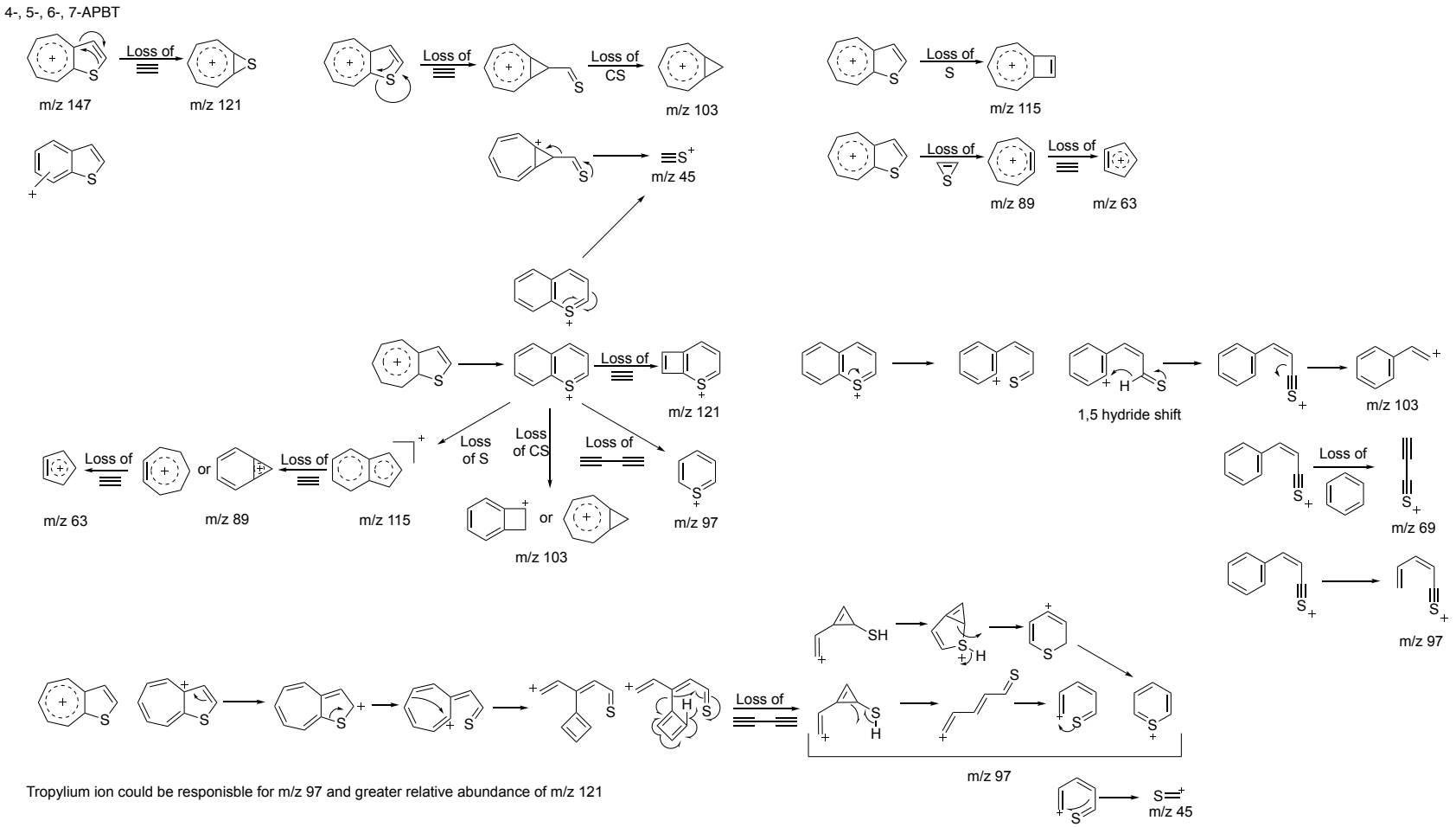

4-APBT
GC-EI-MS/MS of m/z 147
147
77
103
121
45
69
115
51
63
89
97
108
m/z


5-APBT
GC-EI-MS/MS of m/z 147
147
77
121
103
45
69
115
51
63
89
97
108
m/z

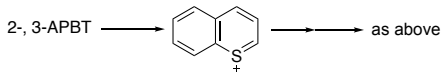

6-APBT
GC-EI-MS/MS of m/z 147
147
77
121
103
45
69
115
51
63
89
97
108
m/z


7-APBT
GC-EI-MS/MS of m/z 147
147
77
121
103
45
69
115
51
63
89
97
108
m/z

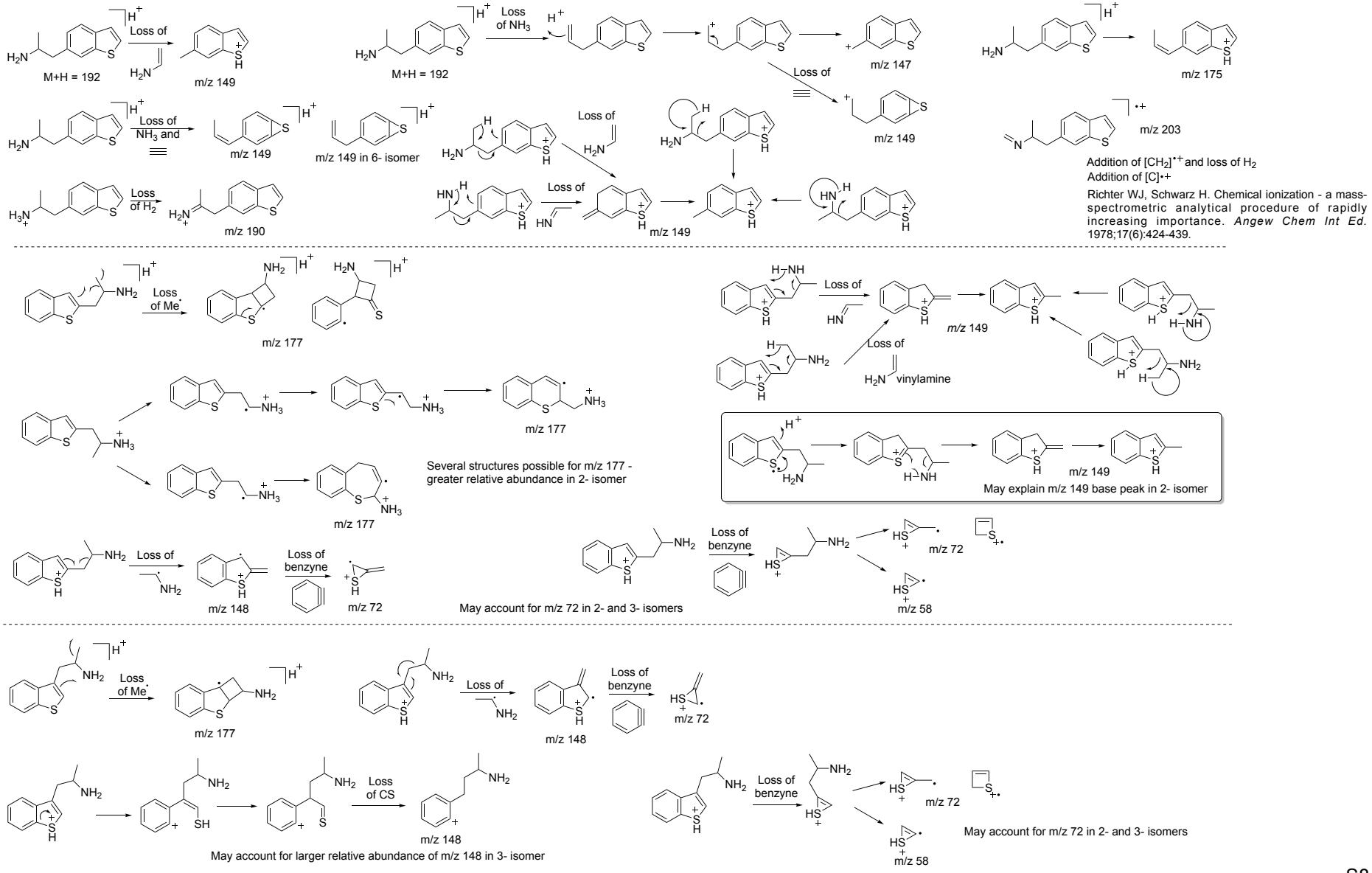
EI-MS/MS of m/z 147

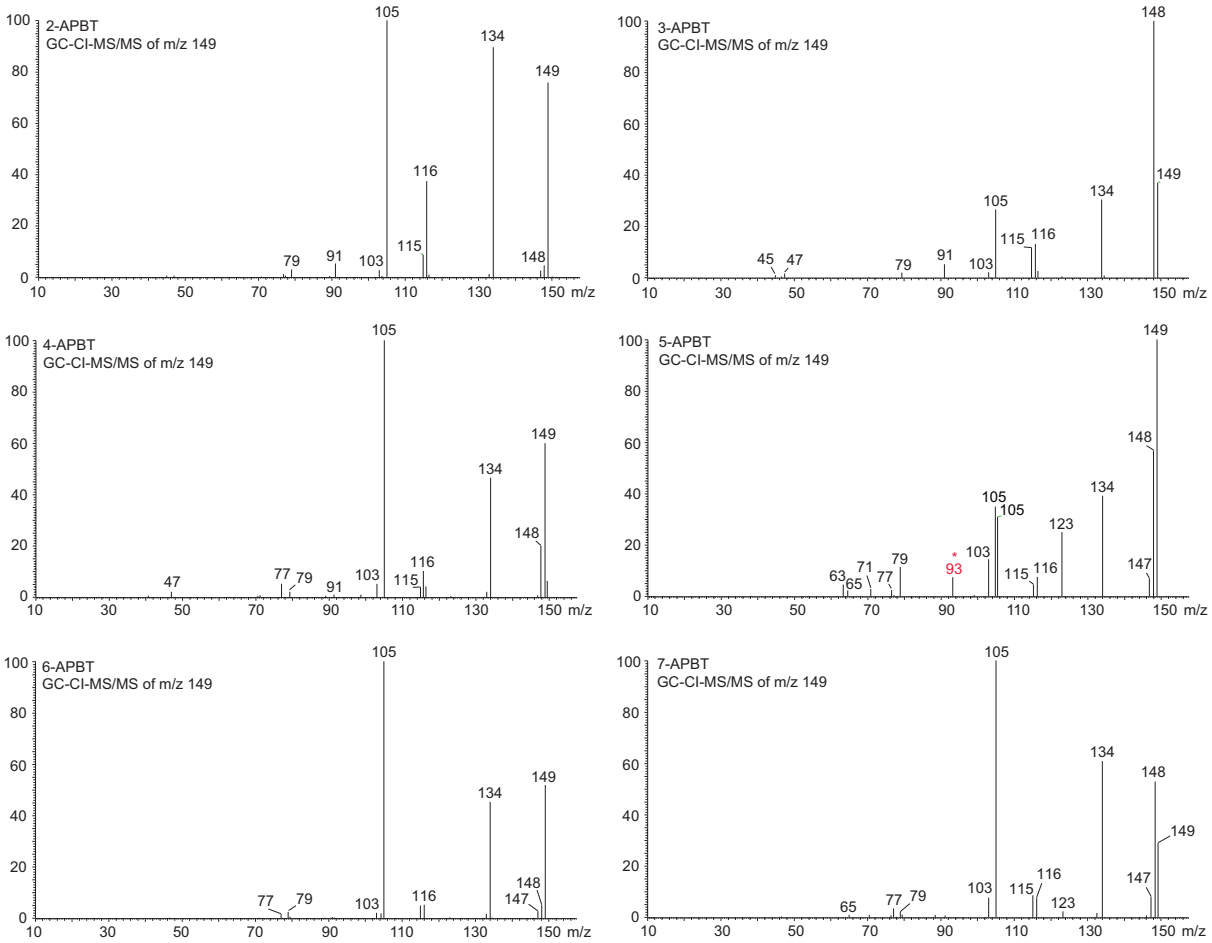


Tropylium ion could be responisble for m/z 97 and greater relative abundance of m/z 121

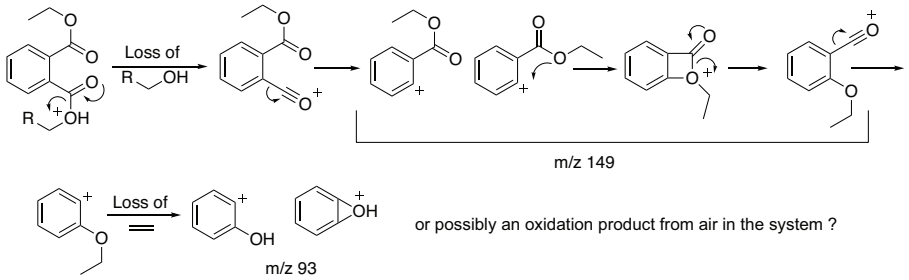


CI-MS analysis



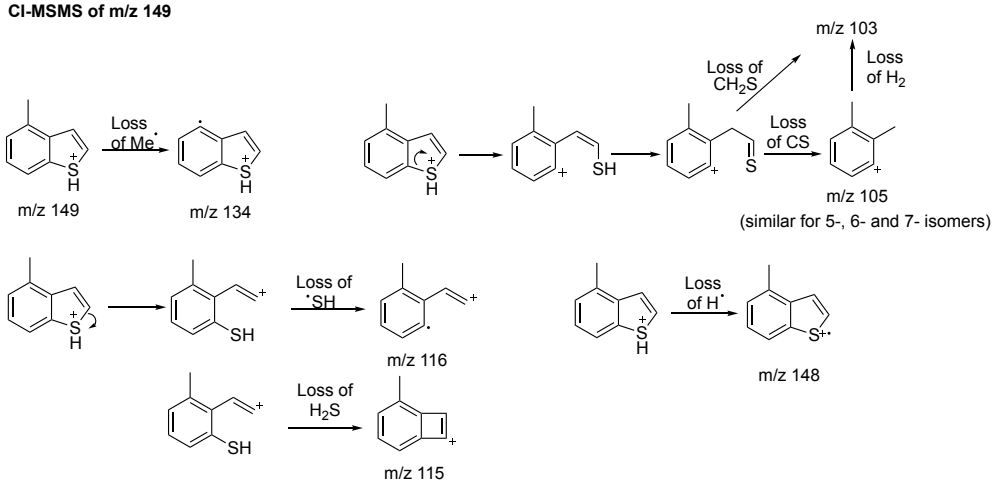


* m/z 93: possibly from an ethyl phthalate?

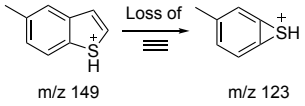


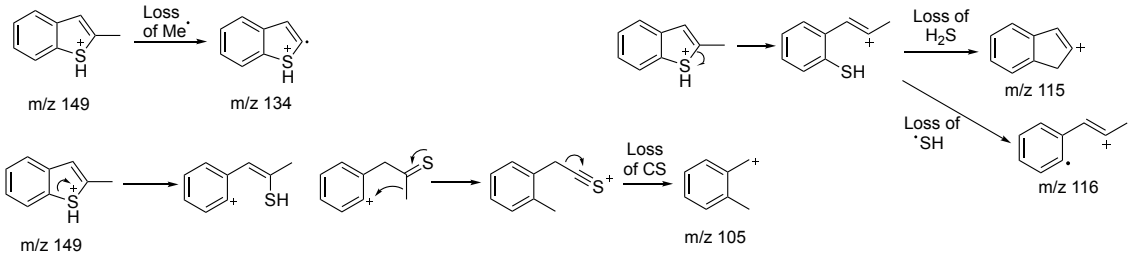
or possibly an oxidation product from air in the system ?

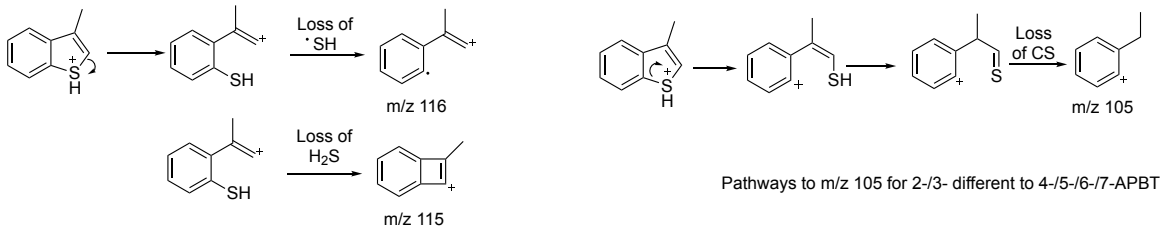
CI-MSMS of m/z 149



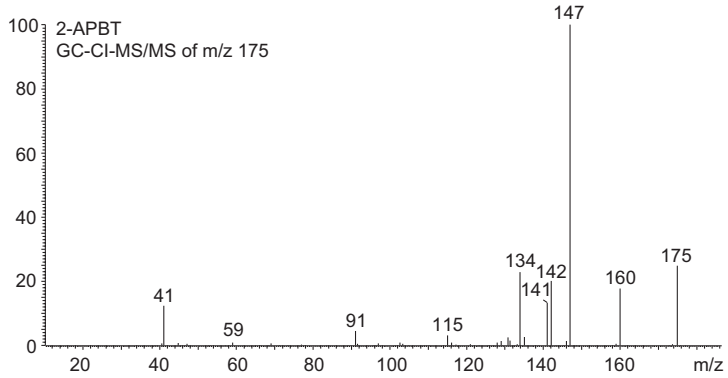
5-APBT

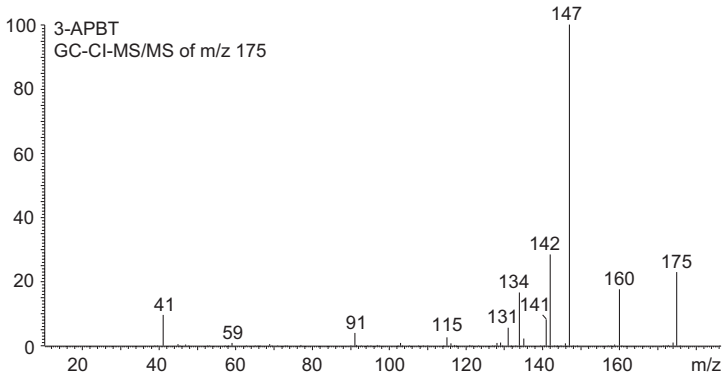


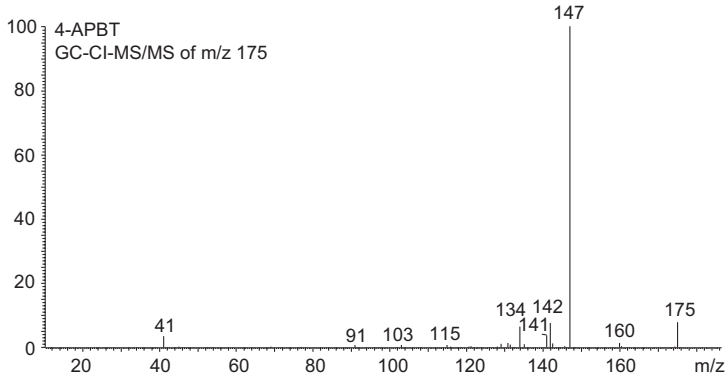




Pathways to m/z 105 for 2-/3- different to 4-/5-/6-/7-APBT


2-APBT
GC-CI-MS/MS of m/z 175
147
175
134
142
141
160
41
59
91
115
m/z


3-APBT
GC-CI-MS/MS of m/z 175
147
142
175
134
160
141
131
41
59
91
115
m/z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GC-CI-MS/MS of m/z 175
147
134
142
175
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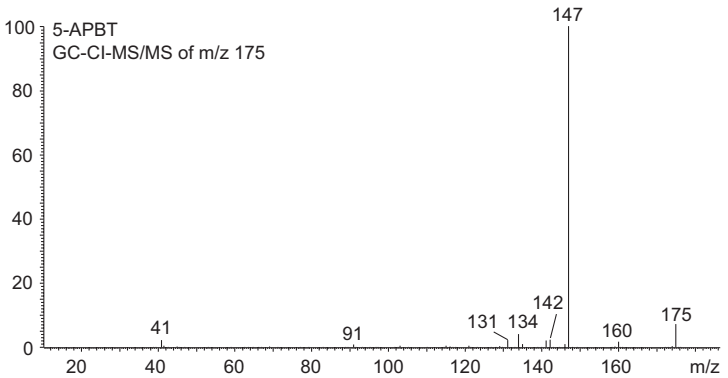
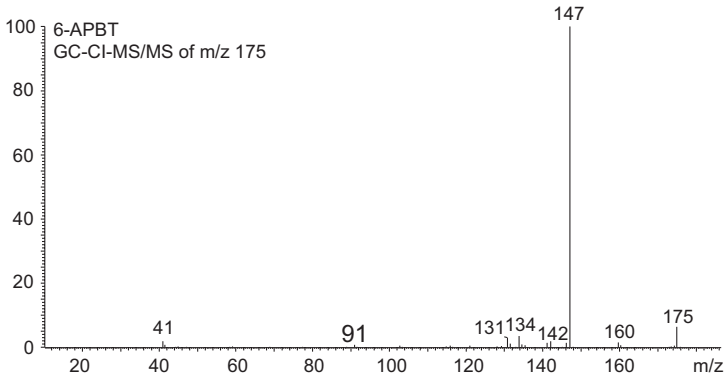
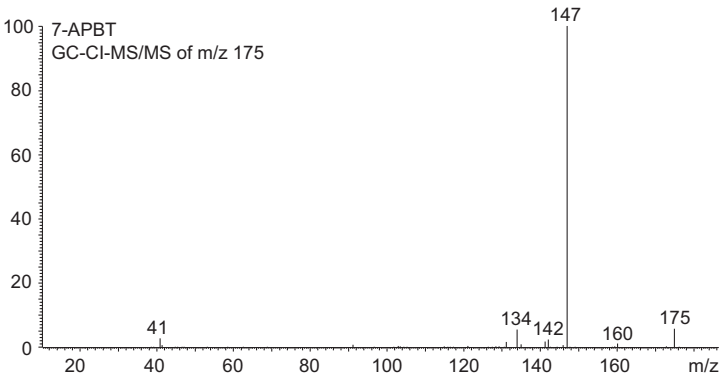
91
103
115
160
m/z


5-APBT
GC-CI-MS/MS of m/z 175
147
142
131
134
175
41
91
160
m/z


6-APBT
GC-CI-MS/MS of m/z 175
147
175
41
91
131
134
142
160
m/z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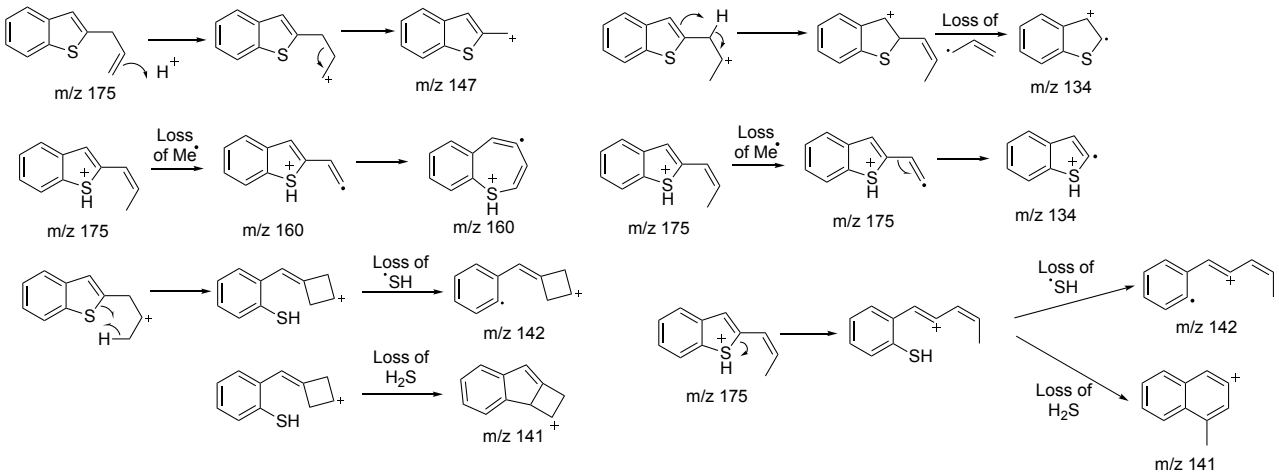
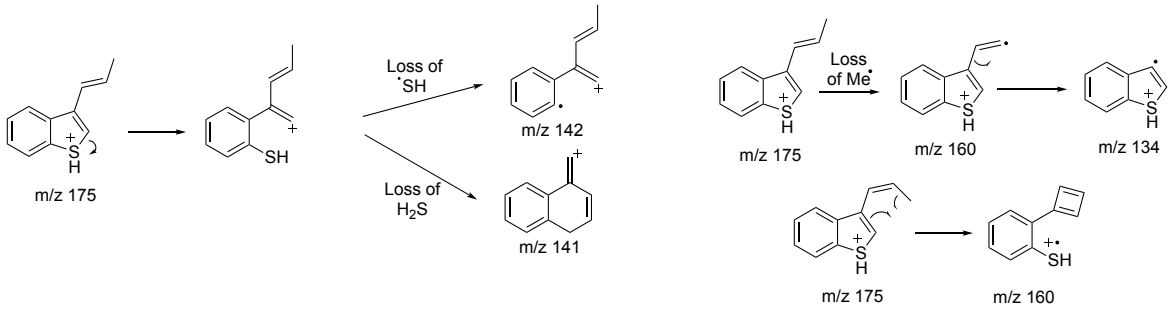
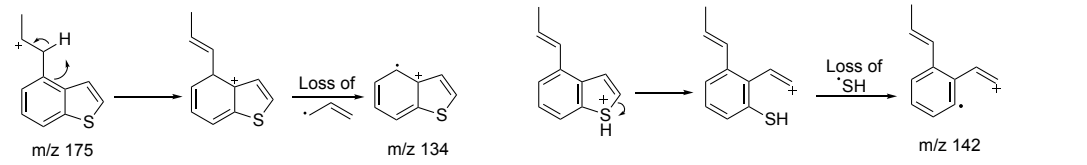
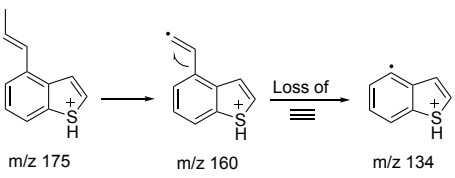
GC-CI-MS/MS of m/z 175
147
134
142
175
41
160
m/z

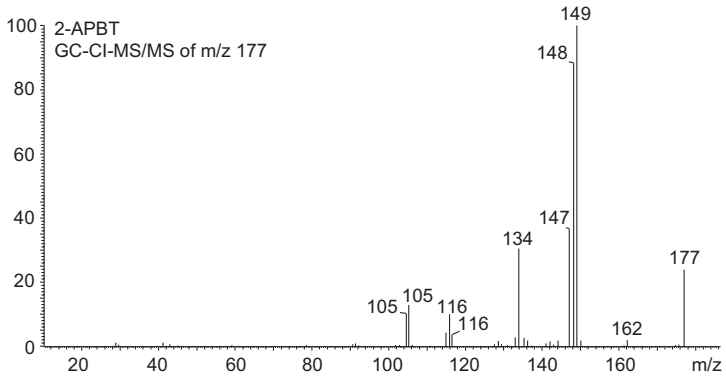
CI-MSMS of m/z 175

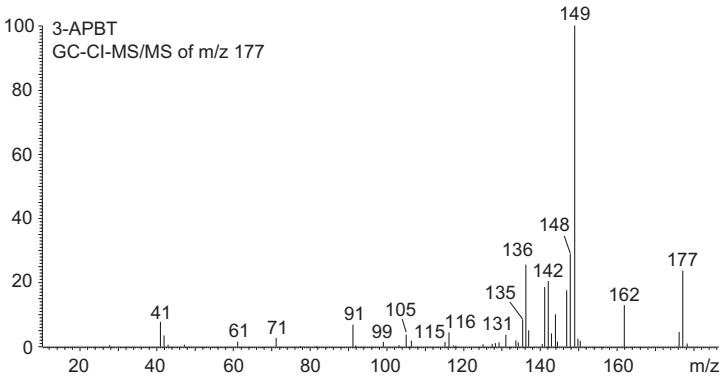


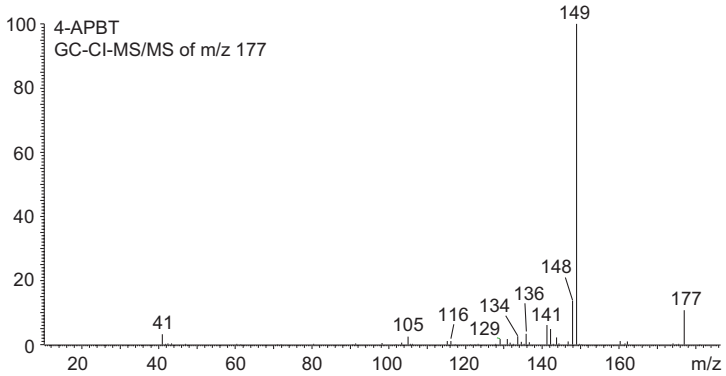


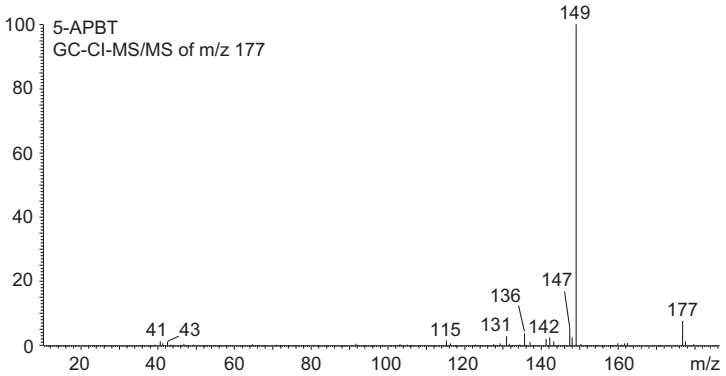


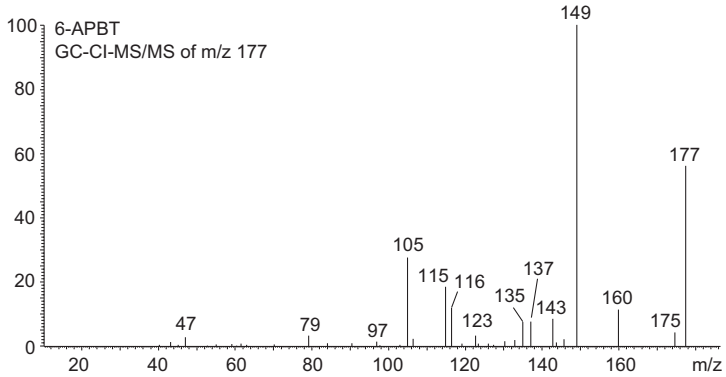


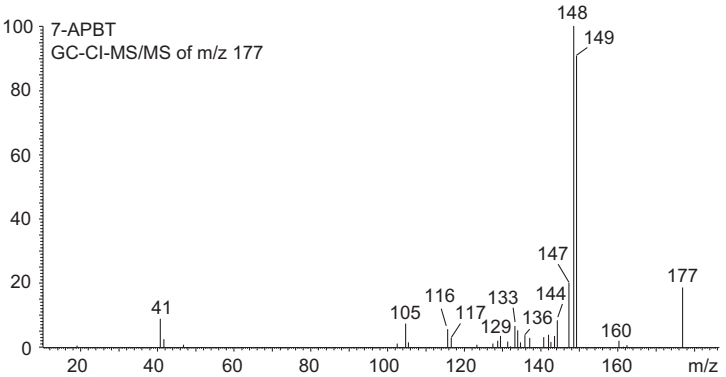




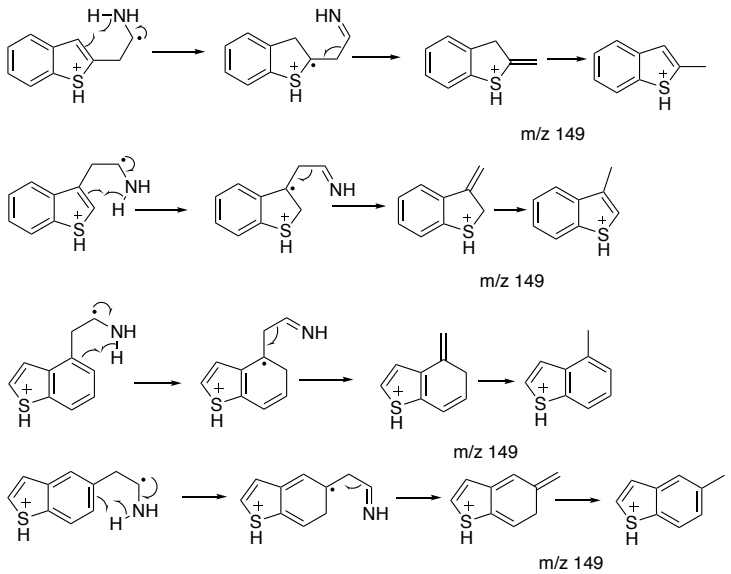




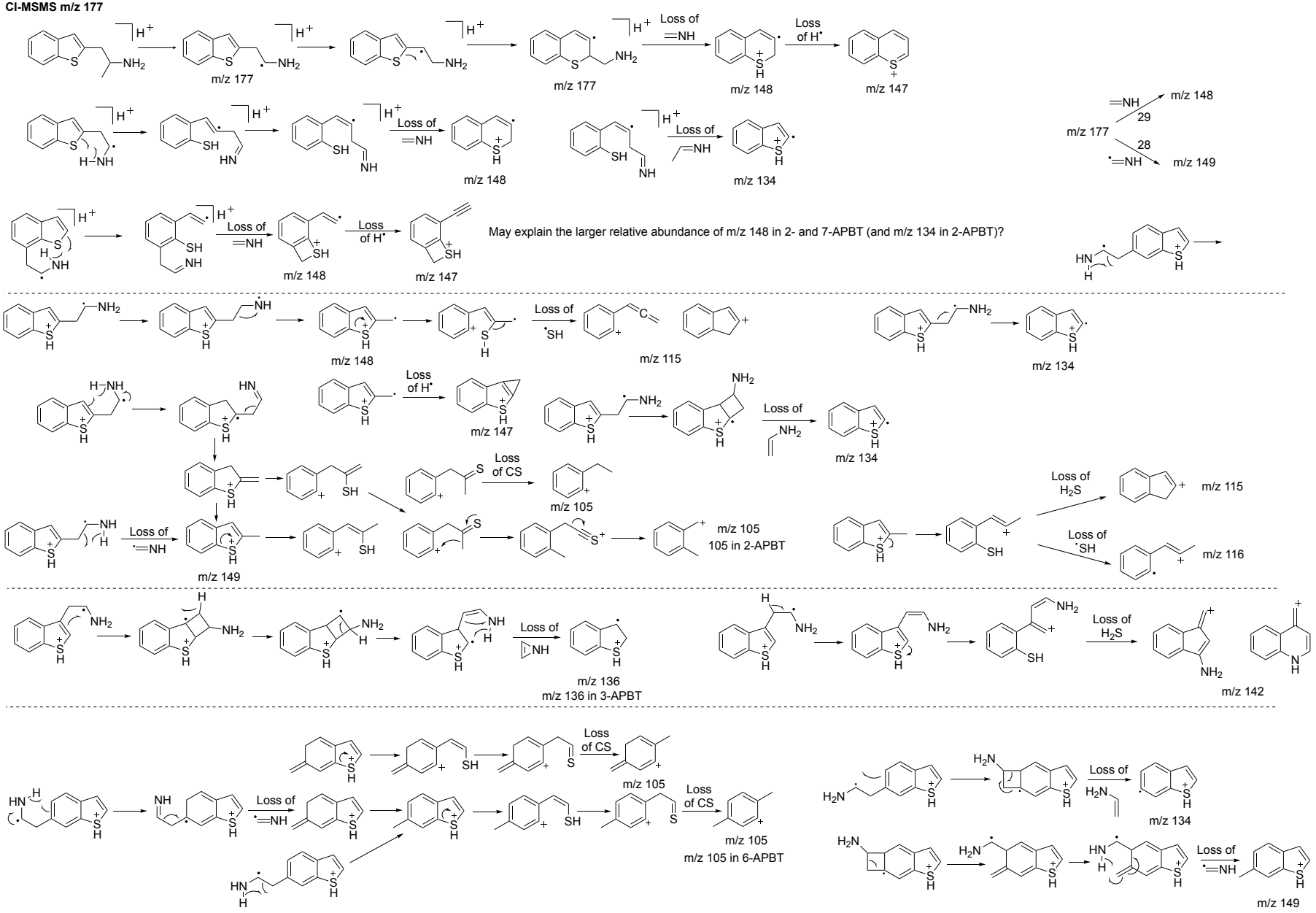




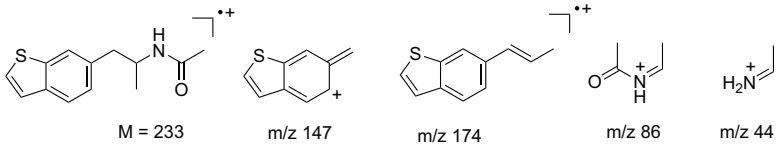
CI-MSMS m/z 149 from m/z 177



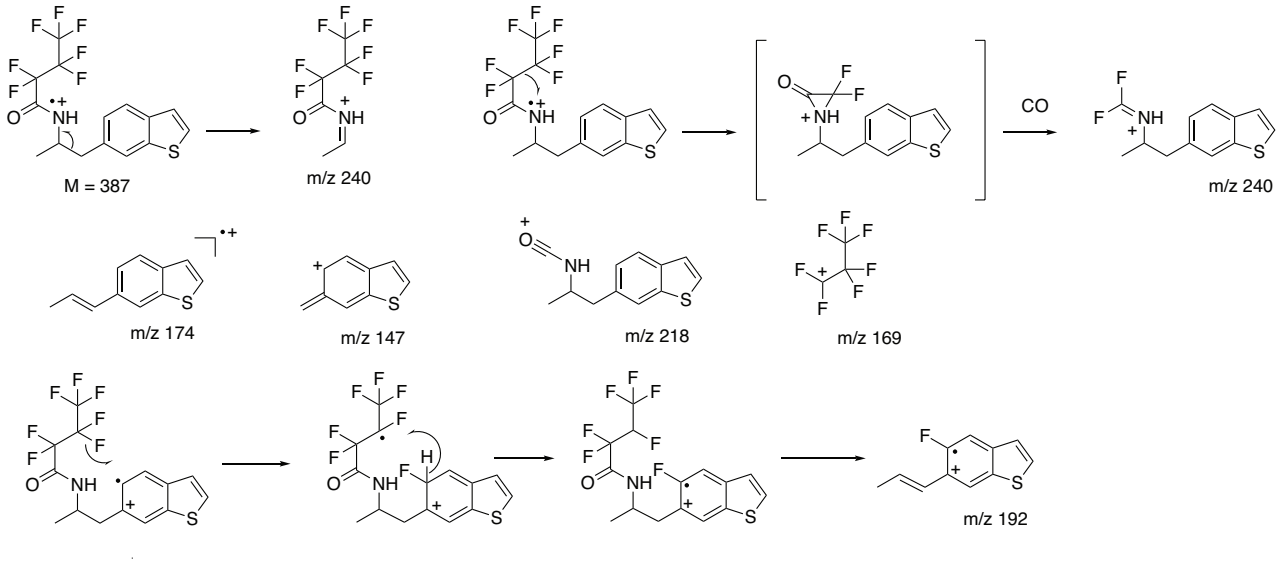
CI-MSMS m/z 177



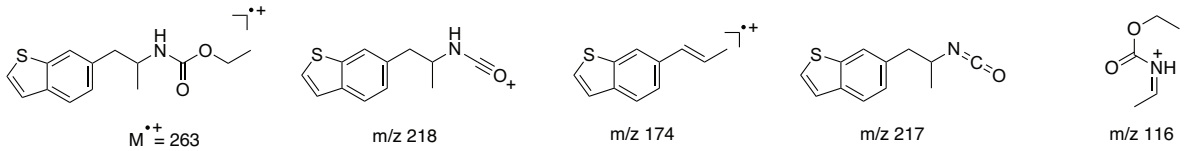
AC derivatives

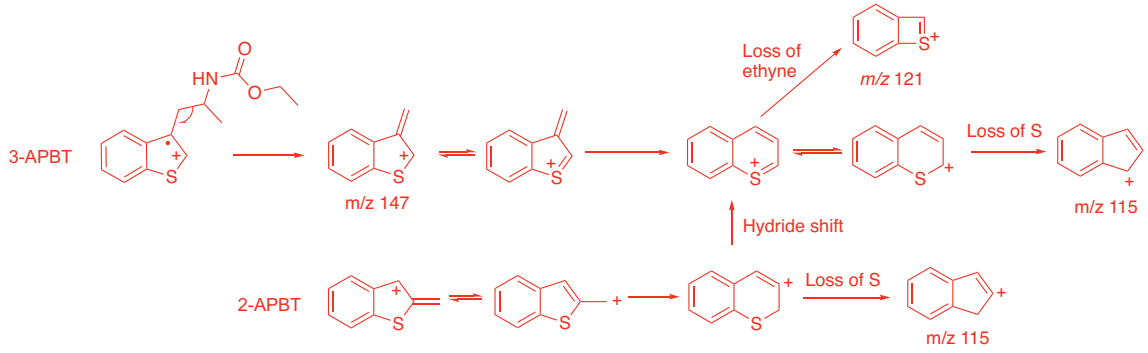


HFB derivatives



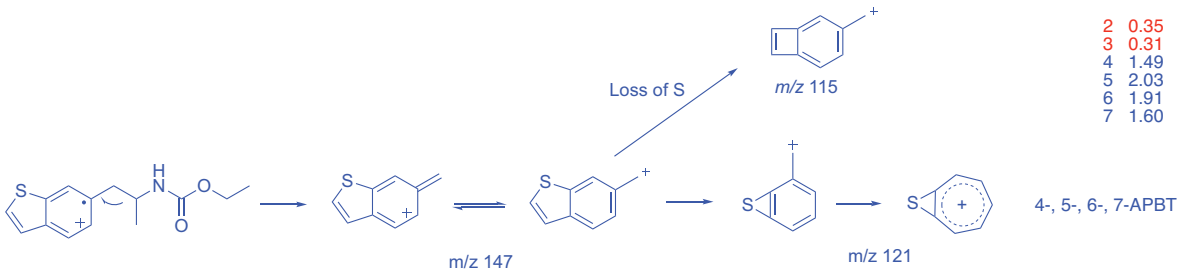
EC derivatives



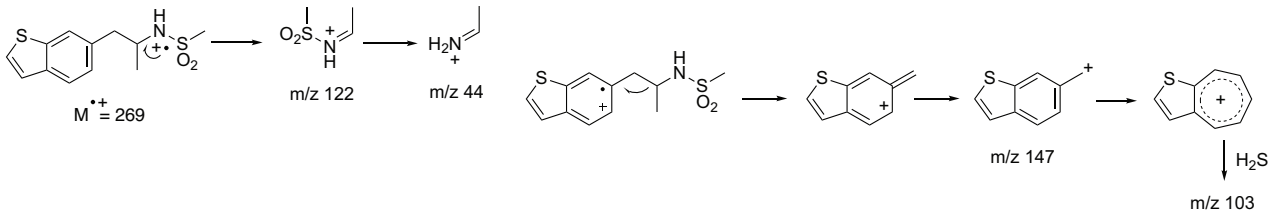


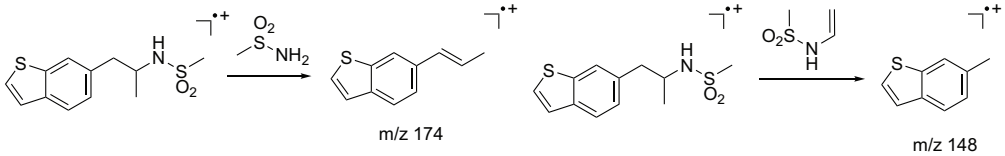
ion 121/ion 115 ratio

2	0.35
3	0.31
4	1.49
5	2.03
6	1.91
7	1.60

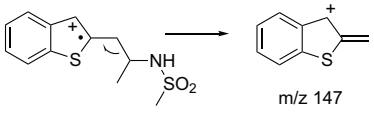


MSA derivatives

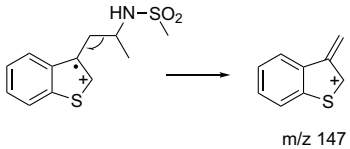




2-APBT

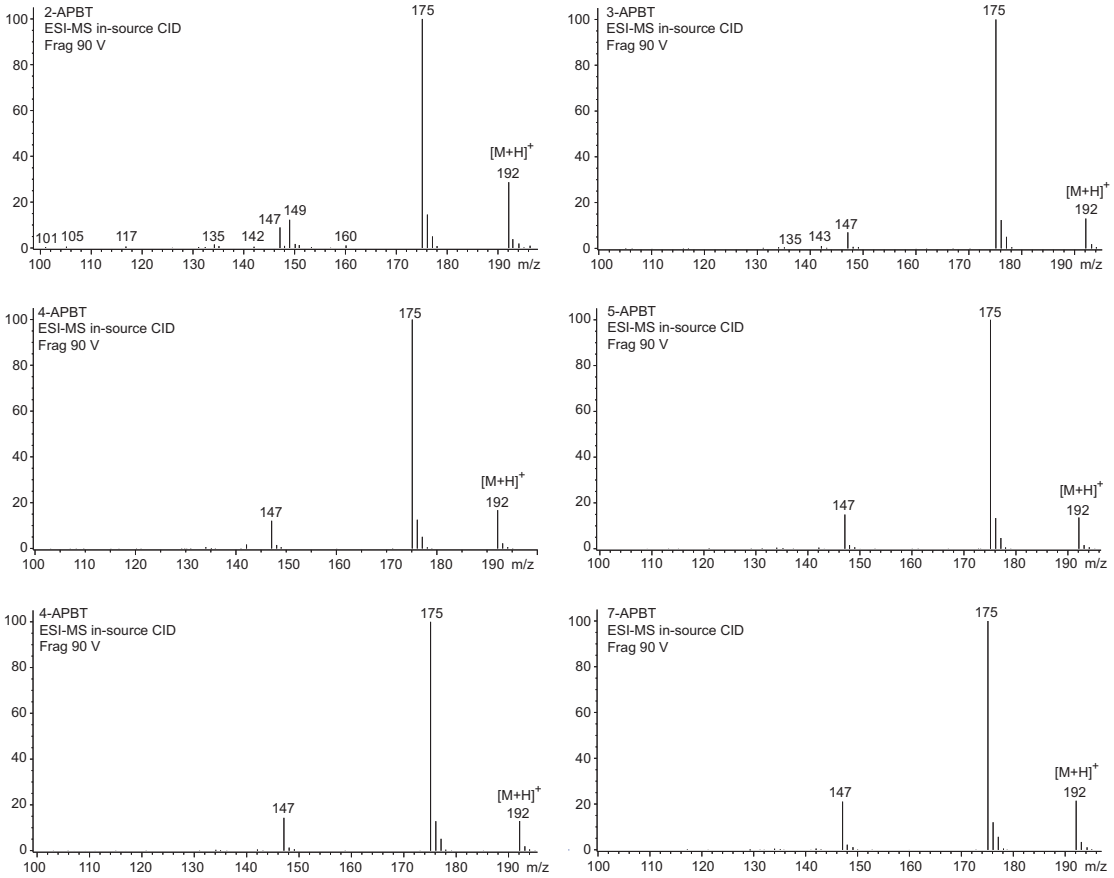


3-APBT

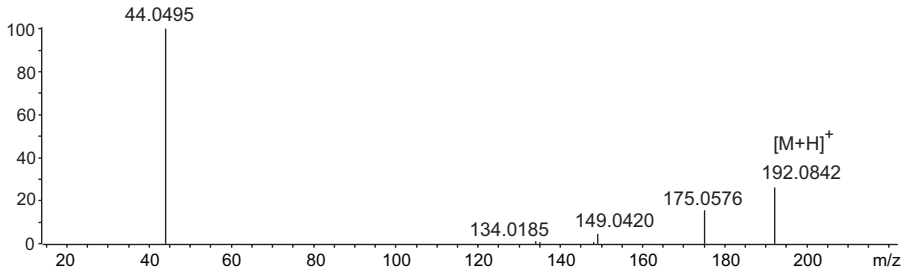


In-source CID mass spectra - liquid chromatography electrospray ionization mass spectrometry

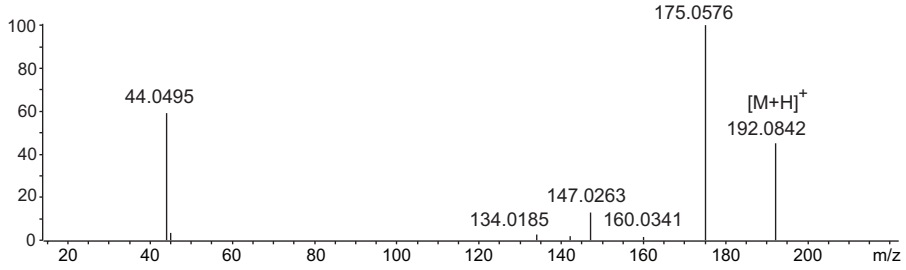
This consisted of an Agilent 1100 LC system coupled to a Hewlett Packard/Agilent 1100 MSD (Santa Clara, CA, USA). The following conditions were used: capillary voltage 3500 V, drying gas (N_2) 12 L/min at 350 °C and nebulizer (N_2) pressure 50 psig. The mass spectrometer was tuned according to the manufacturer's instructions using ESI Tuning Mix G2421A (Agilent Technologies). Chromatography was performed using an Allure PFP Propyl column (5 µm, 50 x 2.1 mm; Restek, Bellefonte, PA, USA): eluent A – methanol containing 0.1% formic acid, eluent B – water containing 0.1% formic acid); 20 % A (0 - 2 min.) followed by a linear gradient up to 80 % A at 22 min, 80 % A for 1 min, linear gradient down to 20 % A at 25 min, 20 % A for 5 min (run-time 30 min); flow rate of 600 µL/min, 10 µL of a 50 µg/mL injected. The mass spectrometer was run in ESI mode (m/z 70–500, with a fragmentor voltage set at 90 V for in-source CID).



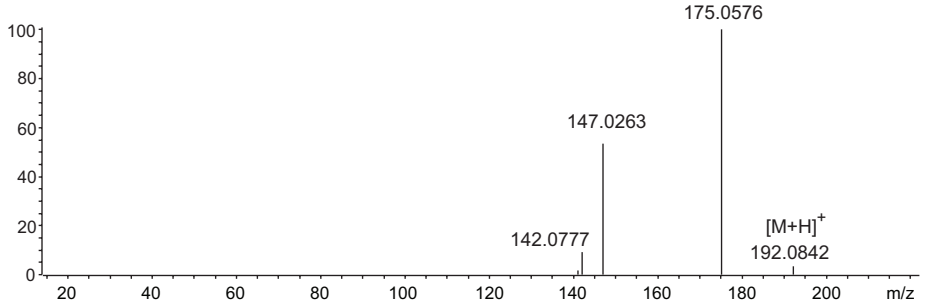
2-APBT
ESI-QTOF-MS/MS



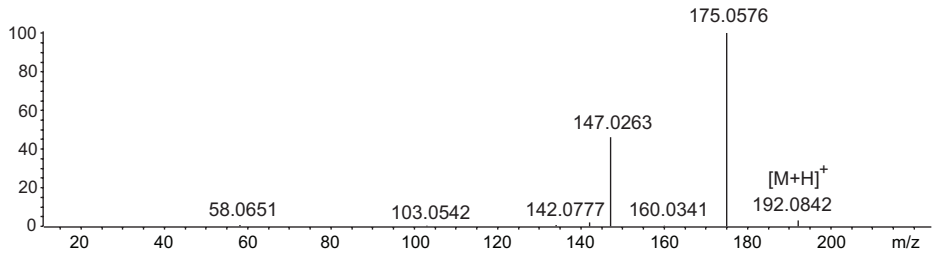
3-APBT
ESI-QTOF-MS/MS



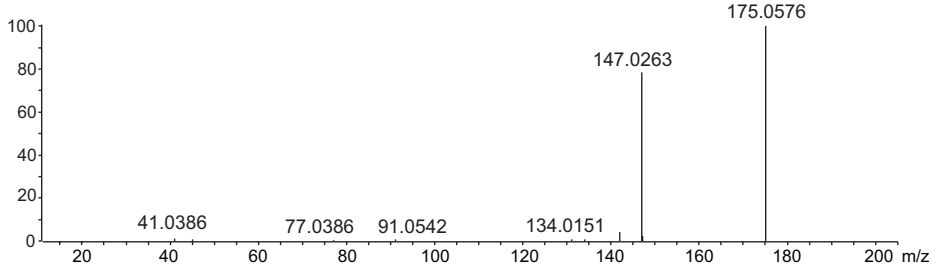
4-APBT
ESI-QTOF-MS/MS



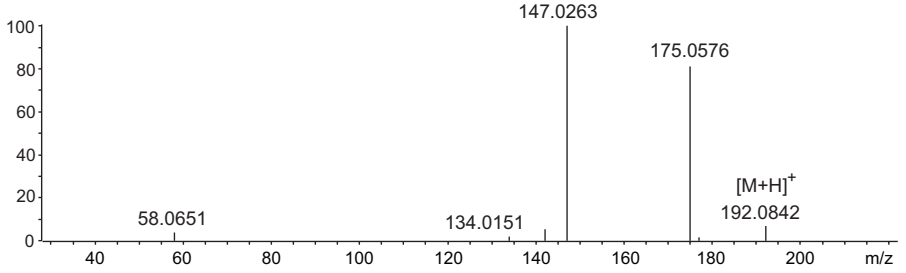
5-APBT
ESI-QTOF-MS/MS



6-APBT
ESI-QTOF-MS/MS

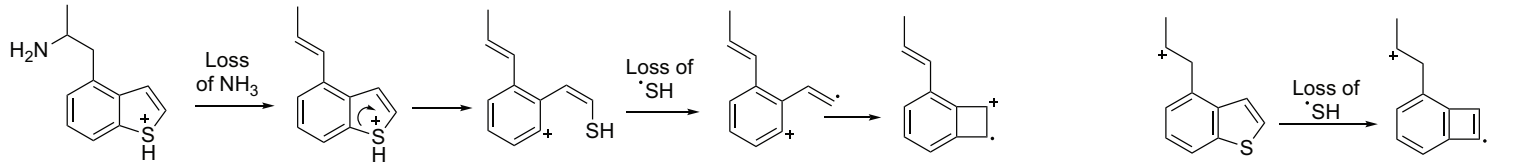


7-APBT
ESI-QTOF-MS/MS



		2-APBT		3-APBT		4-APBT		5-APBT		6-APBT		7-APBT	
Calc. m/z	Formula	Obs. m/z	Δ (ppm)	Obs. m/z	Δ (ppm)	Obs. m/z	Δ (ppm)	Obs. m/z	Δ (ppm)	Obs. m/z	Δ (ppm)	Obs. m/z	Δ (ppm)
192.0842	$C_{11}H_{14}NS^+$	192.0842	0	192.0842	0	192.0842	0	192.0842	0	No $[M+H]^+$		192.0842	0
175.0576	$C_{11}H_{11}S^+$	175.0576	0	175.0576	0	175.0576	0	175.0576	0	175.0576	0	175.0576	0
160.03412	$C_{10}H_8S^{\bullet+}$	–	–	160.03412	0	–	–	–	–	–	–	–	–
149.0420	$C_9H_9S^+$	149.0420	0	–	–	–	–	–	–	–	–	–	–
147.0263	$C9H7_S^+$	–	–	147.0263	0	147.0263	0	147.0263	0	147.0263	0	147.0263	0
142.0777	$C_{11}H_{10}^{\bullet+}$	–	–	–	–	142.0777	0	142.0777	0	–	–	–	–
135.0263	$C_8H_7S^+$	–	–	–	–	–	–	135.0263	0	–	–	–	–
134.0185	$C8H6S^{\bullet+}$	134.0185	0	134.0185	0	–	–	–	–	–	–	–	–
58.0651	$C_3H_8N^+$	–	–	–	–	–	–	–	–	–	–	58.0651	0
44.0495	$C_2H_6N^+$	44.0495	0	44.0495	0	–	–	–	–	–	–	–	–

4- and 5-APBT



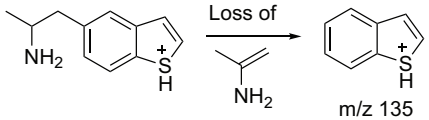
m/z 175
$C_{11}H_{11}S^+$
Calc. 175.0576

m/z 142
$C_{11}H_{10}^{\bullet+}$
Calc. 142.0777
(and 5- isomer)

m/z 175
$C_{11}H_{11}S^+$
Calc. 175.0576

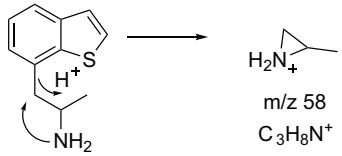
m/z 142
$C_{11}H_{10}^{\bullet+}$
Calc.142.0777

5-APBT



m/z 135
$C_8H_7S^+$
Calc. 135.0263

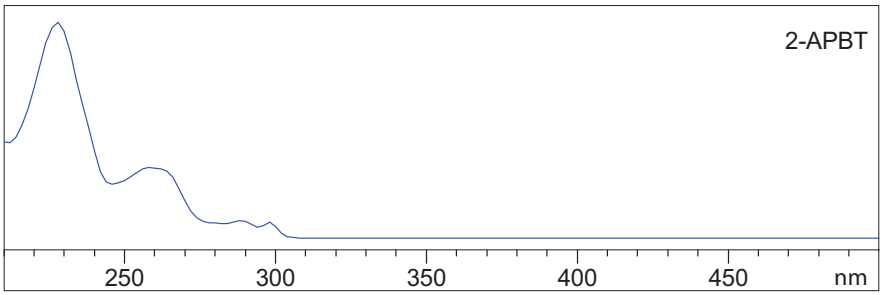
7-APBT

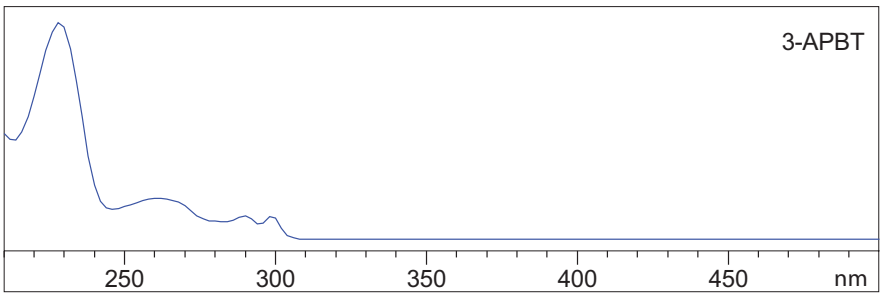


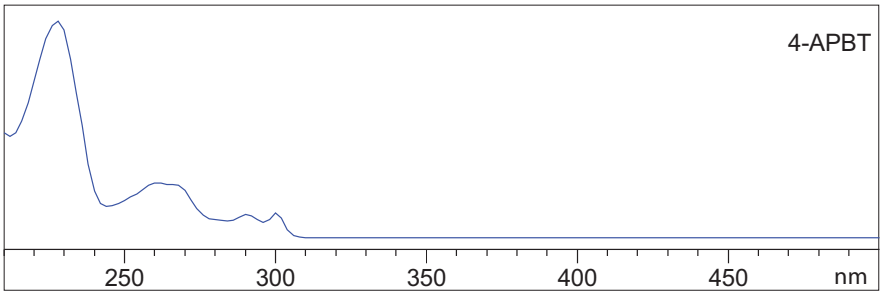
m/z 58
$C_3H_8N^+$
Calc. 58.0651

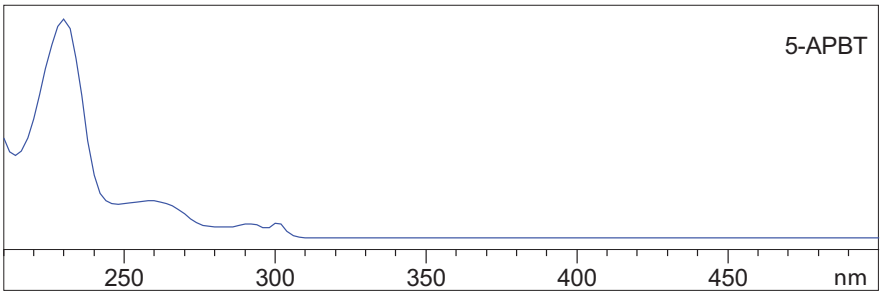
Proposed fragments related to 2-APBT and 3-APBT shown in main text of manuscript

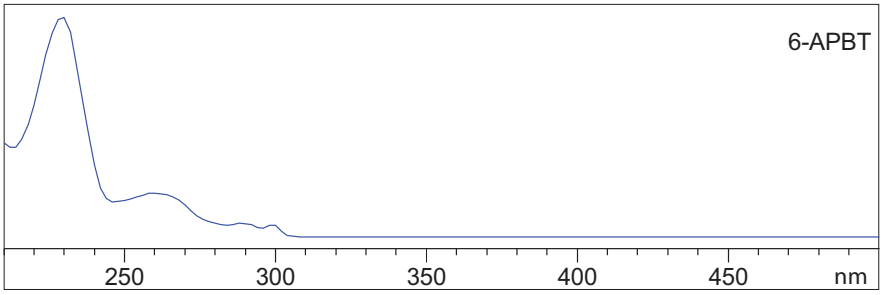
HPLC-DAD UV spectra

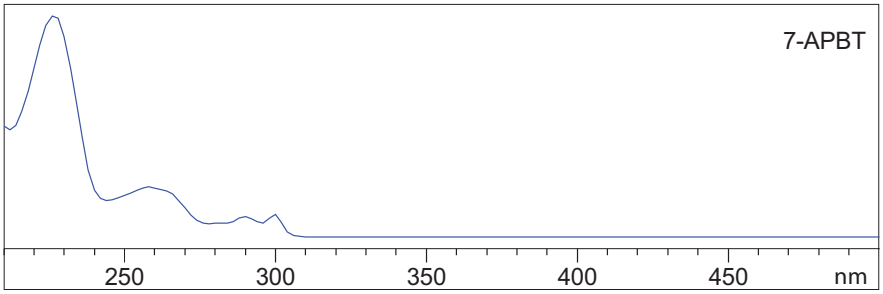


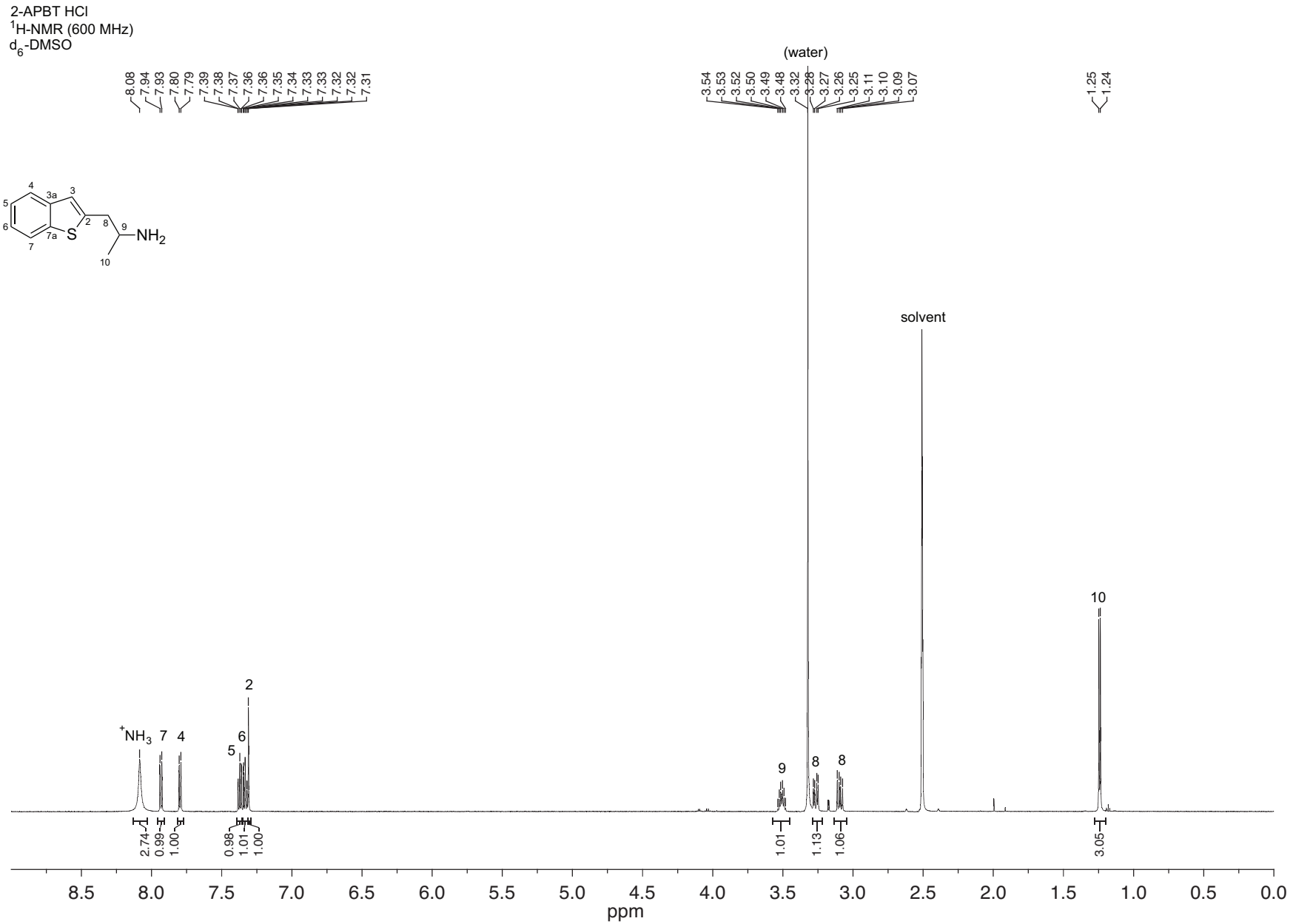




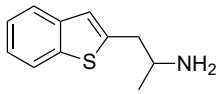


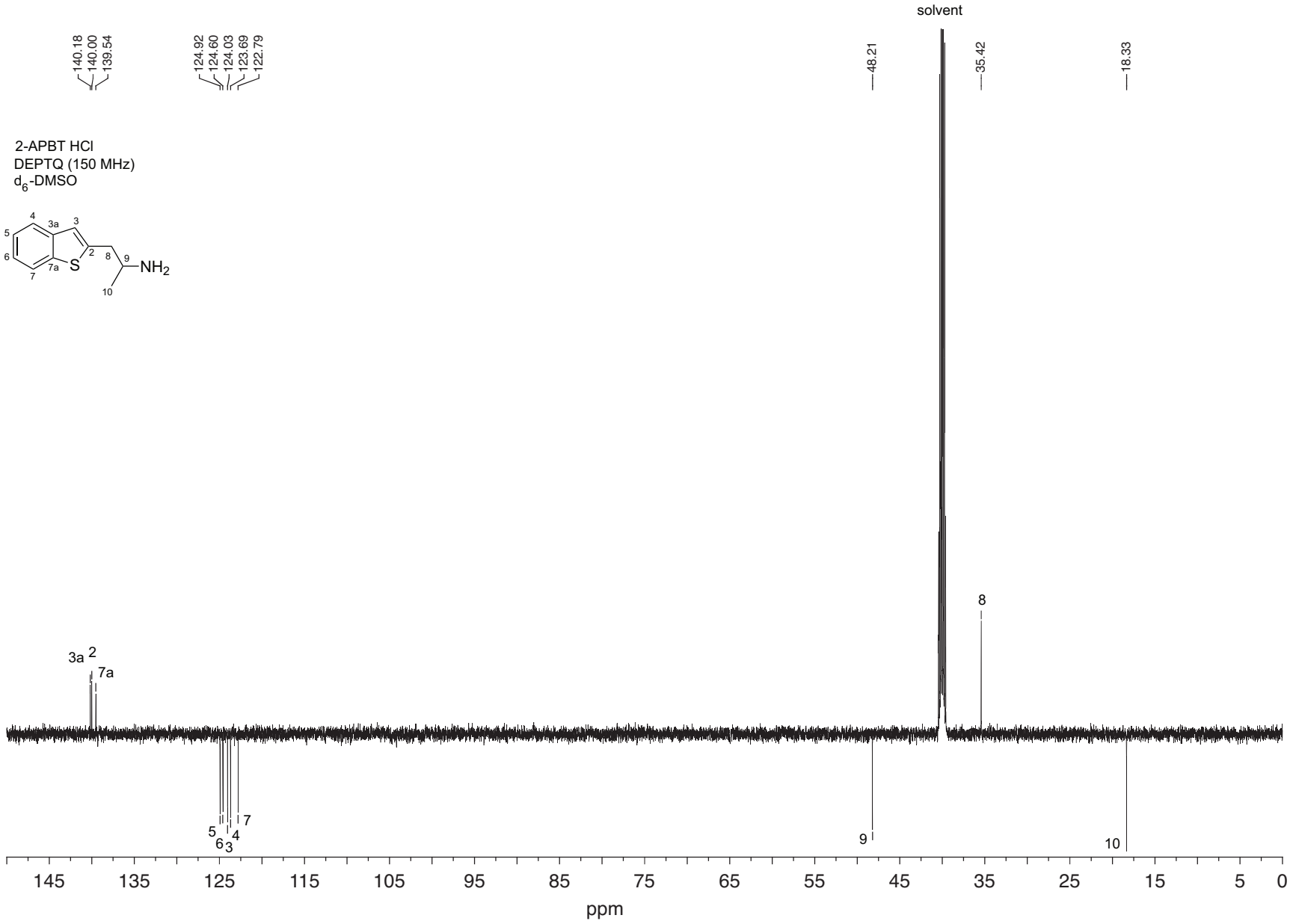




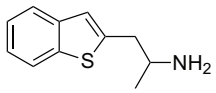

2-APBT HCl
1H-NMR (600 MHz)
d6-DMSO
(water)
solvent
+NH3
NH2
ppm

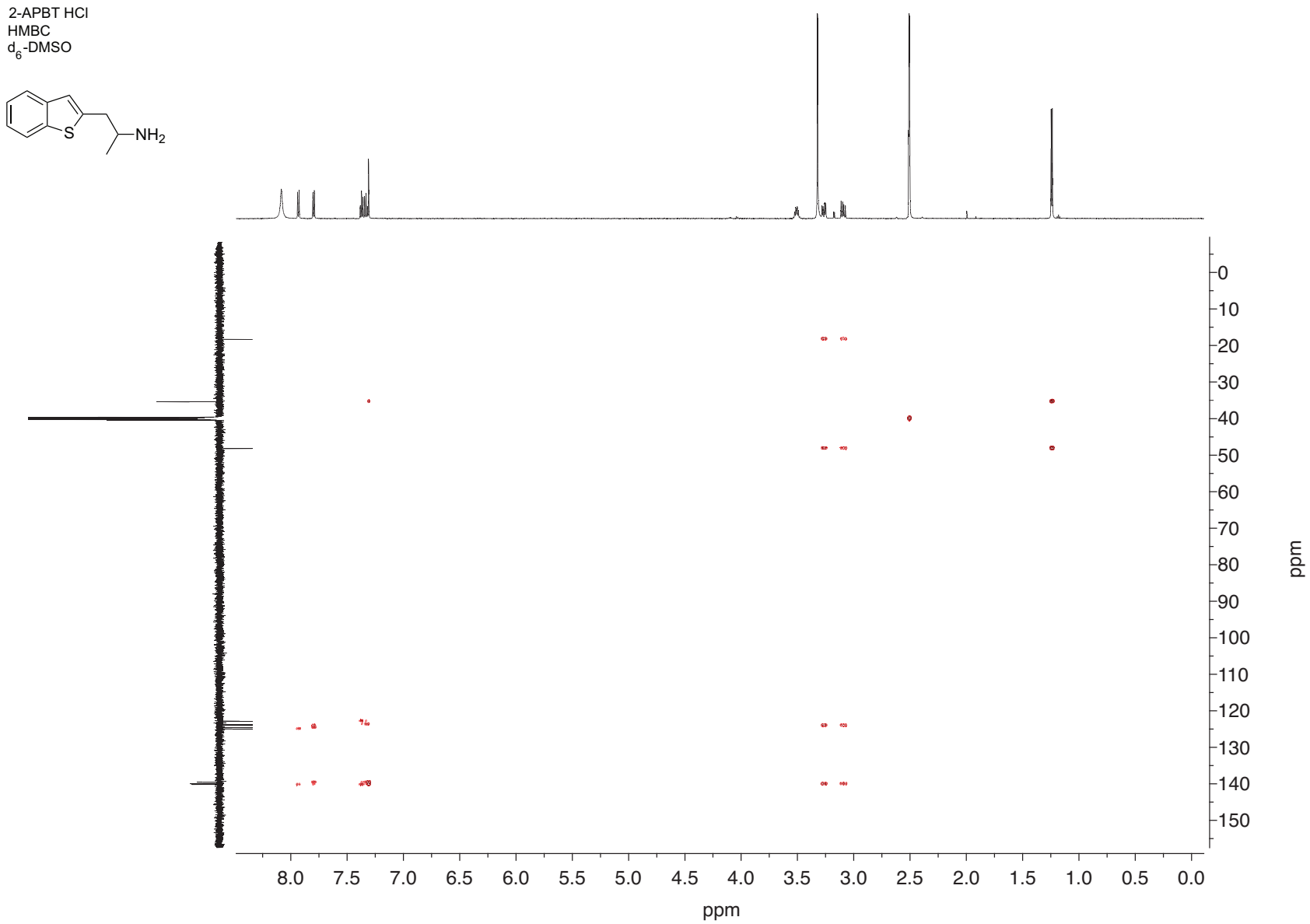
2-APBT HCl
COSY (600 MHz)
d_6-DMSO



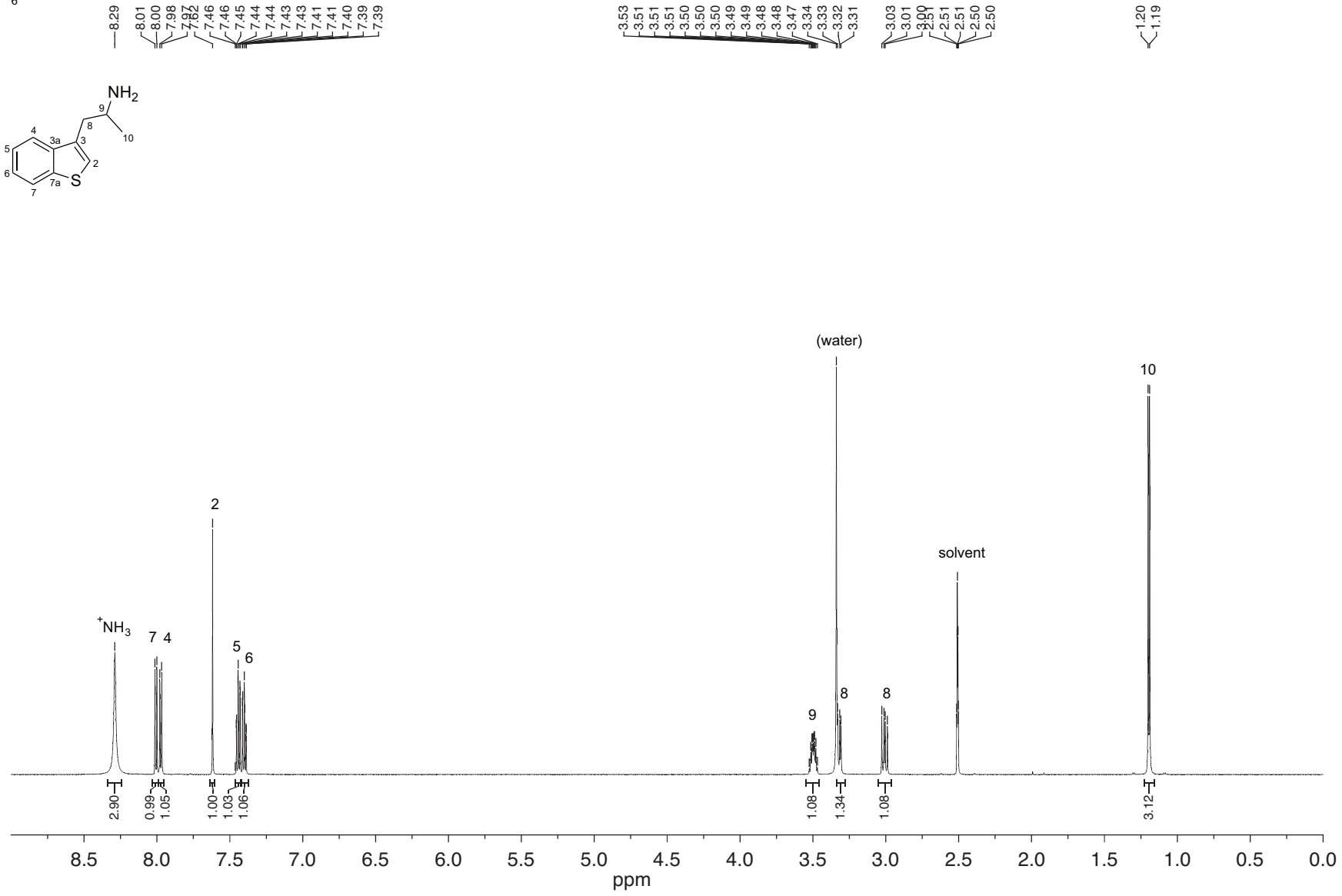

solvent
140.18
140.00
139.54
124.92
124.60
124.03
123.69
122.79
48.21
35.42
18.33
2-APBT HCl
DEPTQ (150 MHz)
d6-DMSO
NH2
3a
2
7a
8
5
6
3
4
7
9
10
145
135
125
115
105
95
85
75
65
55
45
35
25
15
5
0
ppm

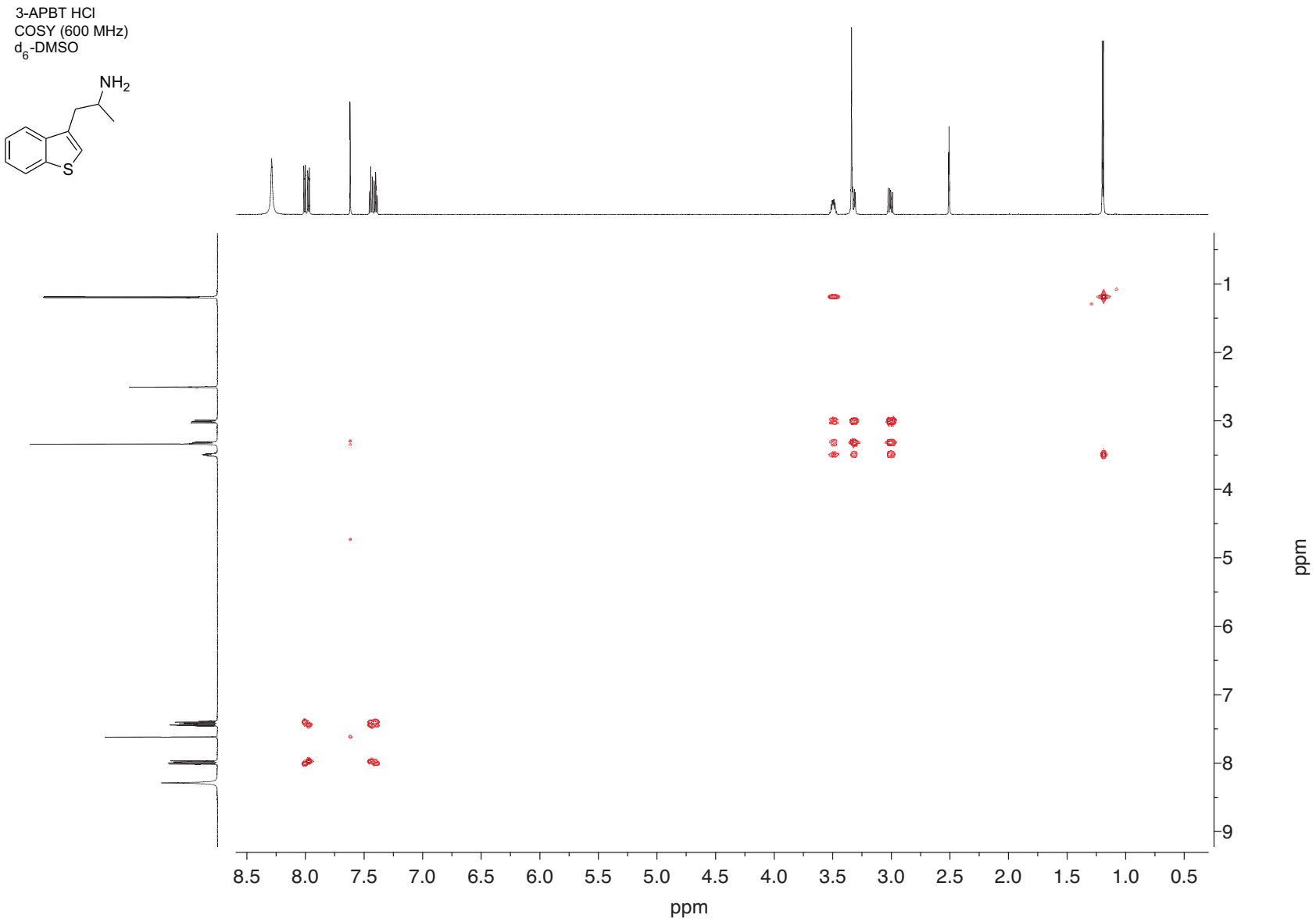
2-APBT HCl
HSQC
d_6-DMSO

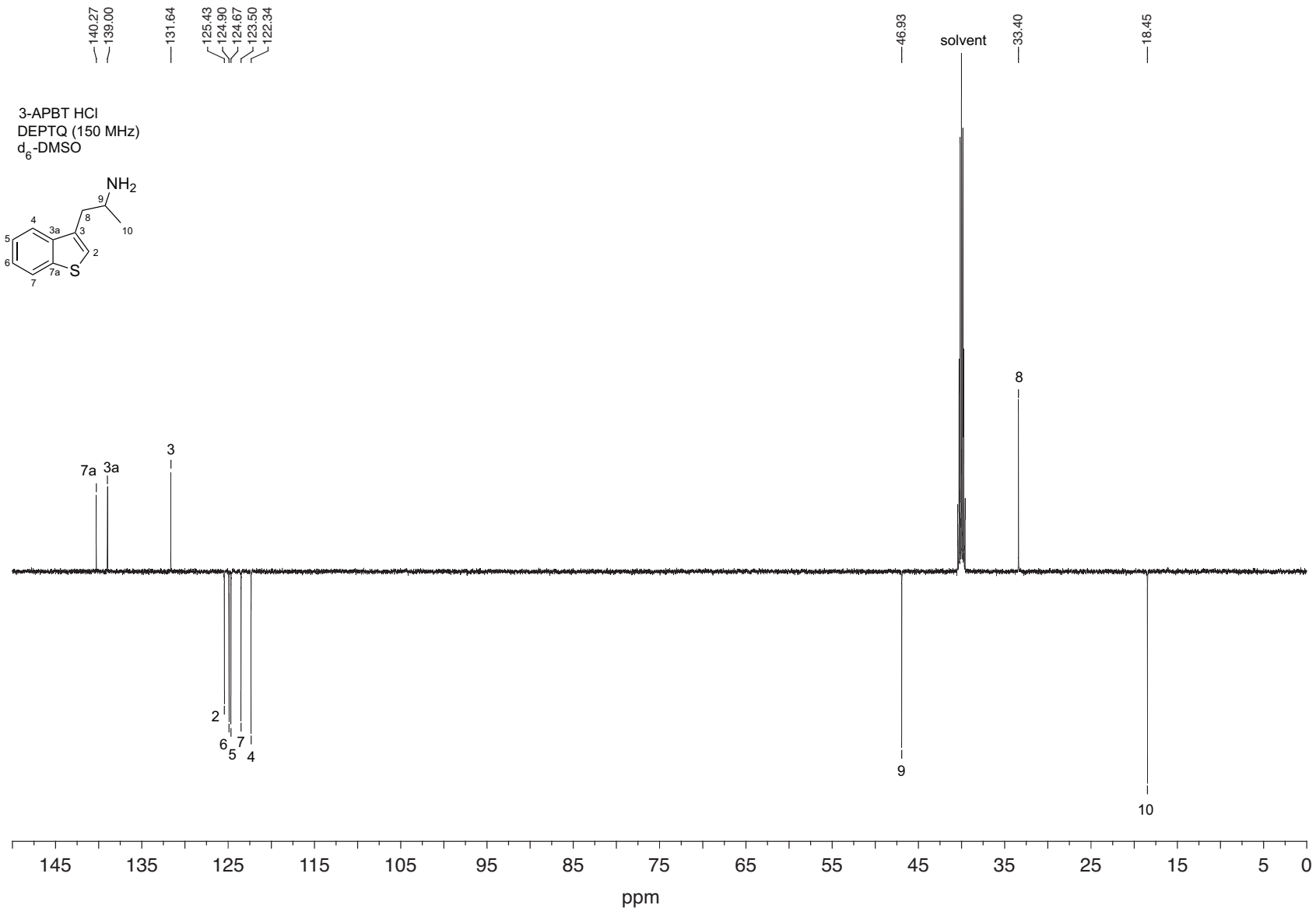



2-APBT HCl
HMBC
d6-DMSO
S
NH2
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
ppm
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

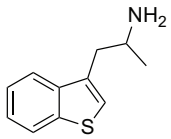
3-APBT HCl
^{1}H-NMR (600 MHz)
d_6-DMSO

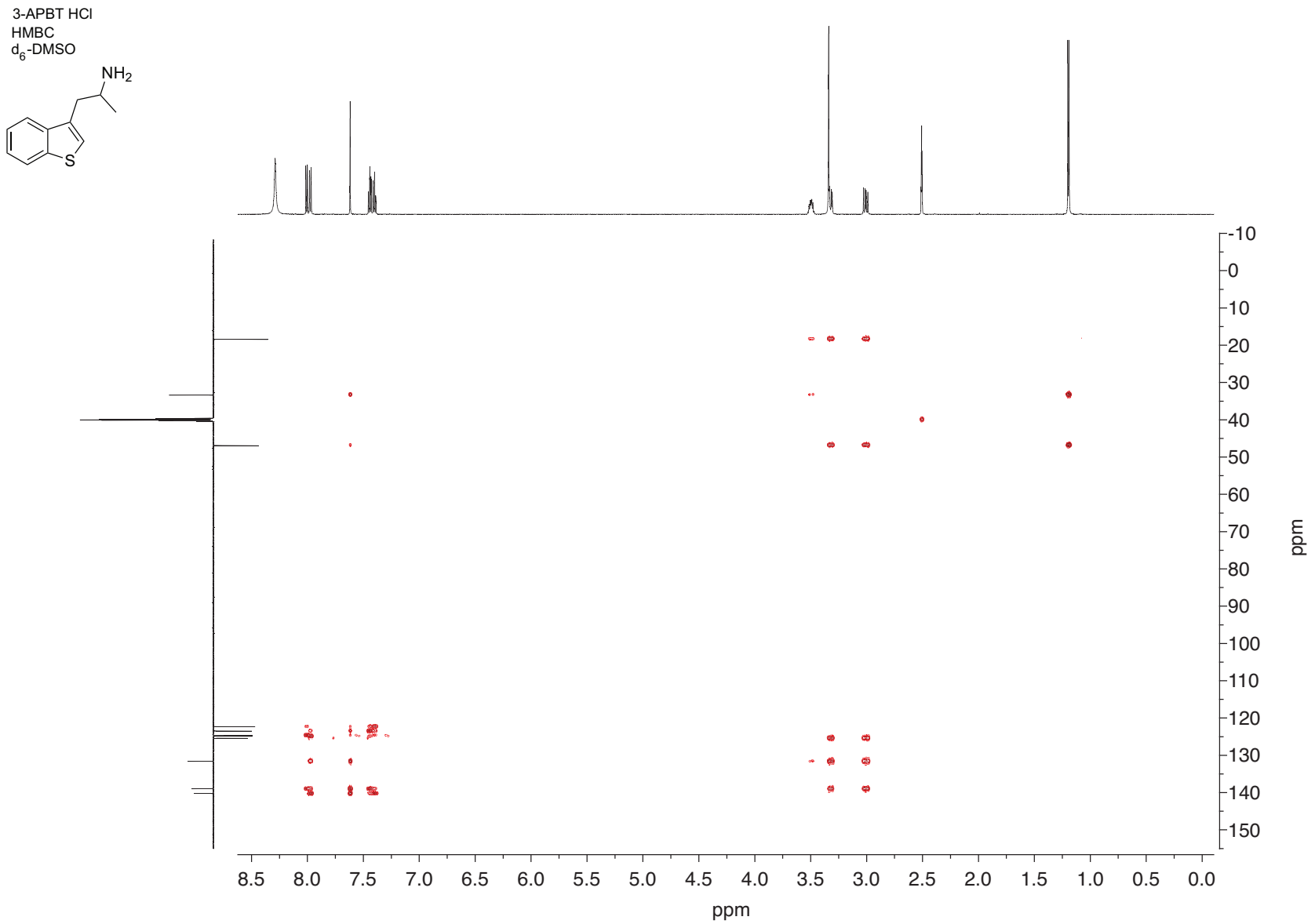



3-APBT HCl
COSY (600 MHz)
d6-DMSO
NH2
S
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1
2
3
4
5
6
7
8
9
ppm

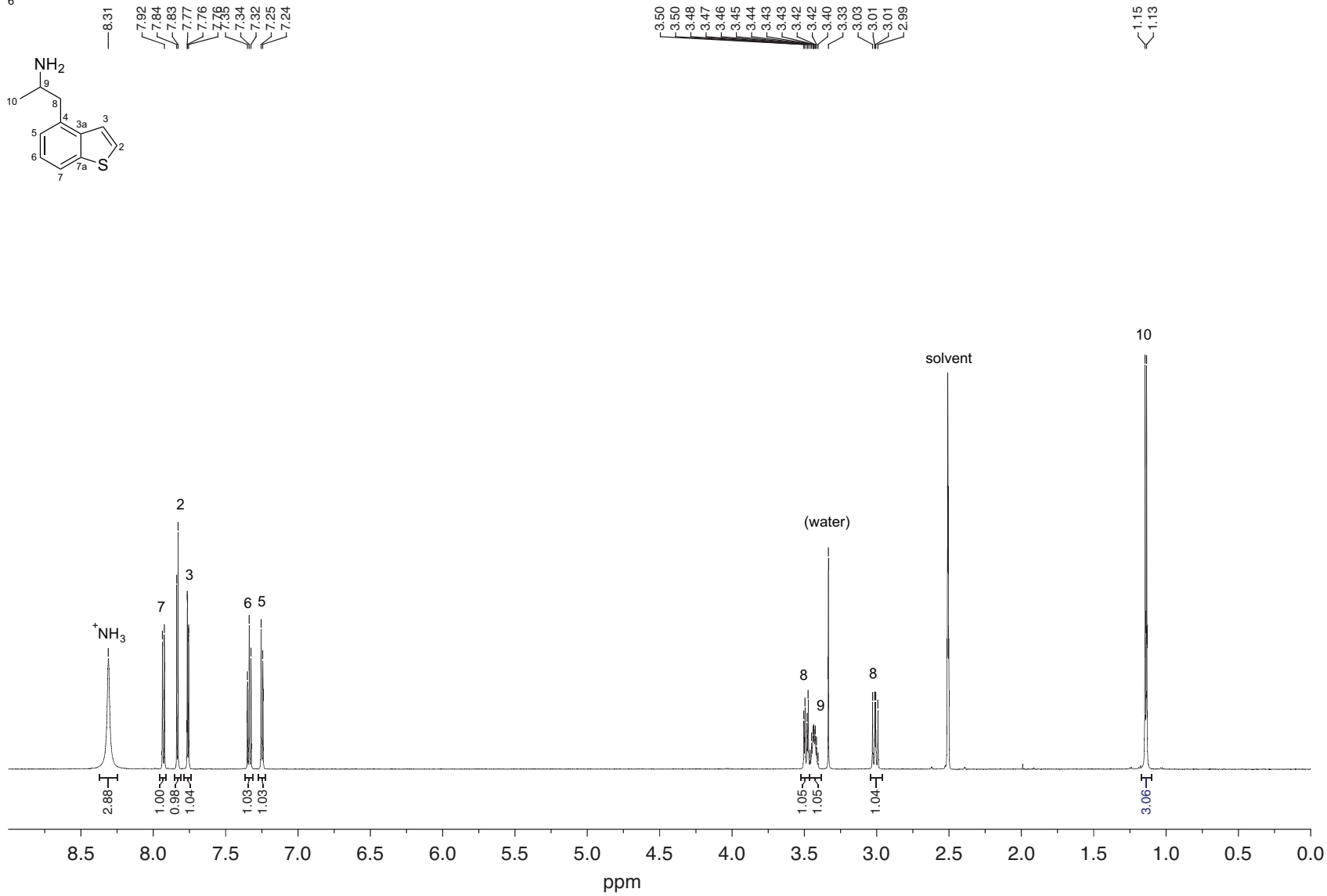

140.27
139.00
131.64
125.43
124.90
124.67
123.50
122.34
46.93
solvent
33.40
18.45
3-APBT HCl
DEPTQ (150 MHz)
d6-DMSO
NH2
9
8
10
4
3a
3
5
2
6
7a
S
7
7a
3a
3
8
2
6
5
7
4
9
10
145
135
125
115
105
95
85
75
65
55
45
35
25
15
5
0
ppm

3-APBT HCl
HSQC
d_6-DMSO

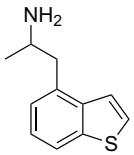


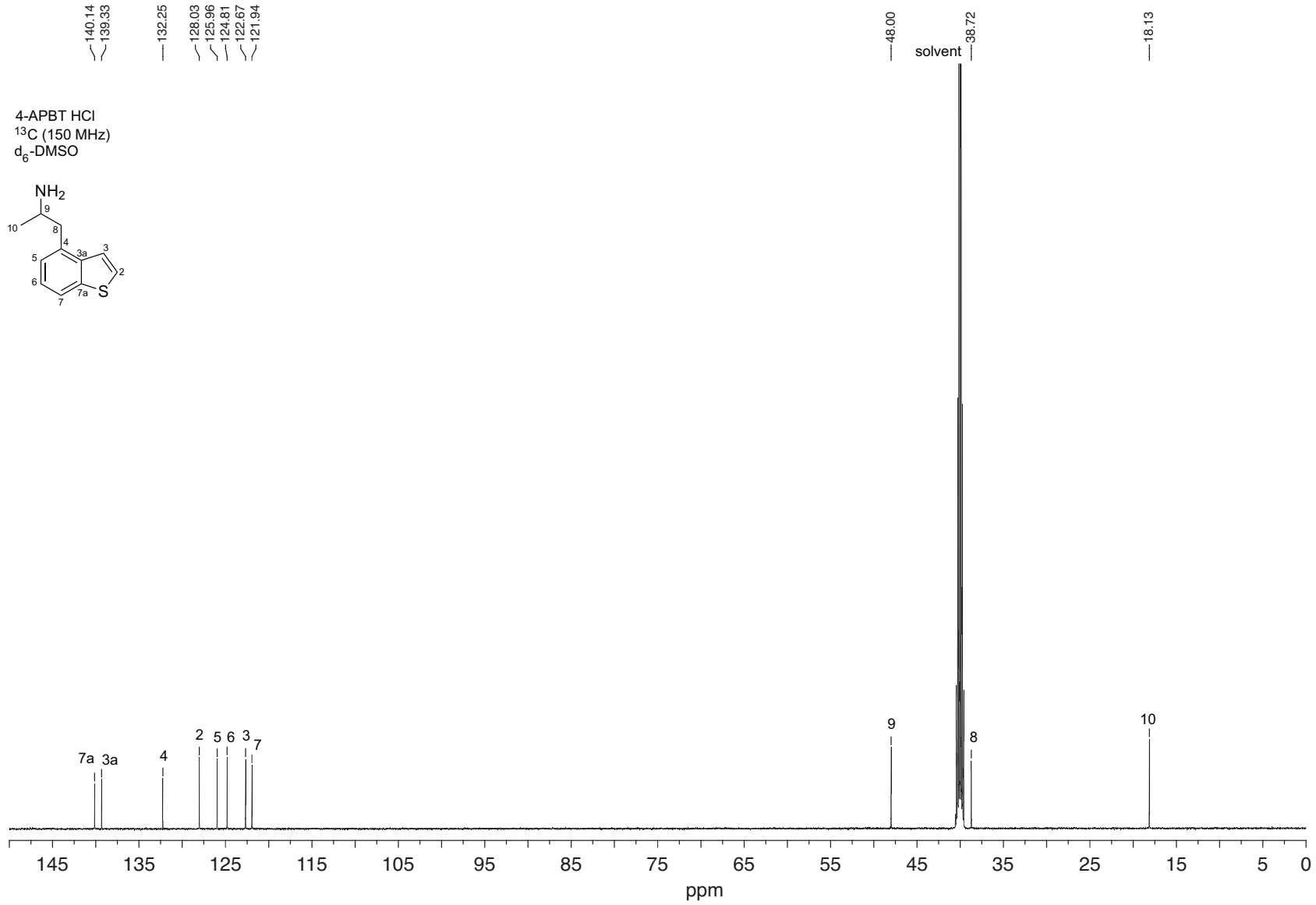

3-APBT HCl
HMBC
d6-DMSO
NH2
S
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
ppm
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

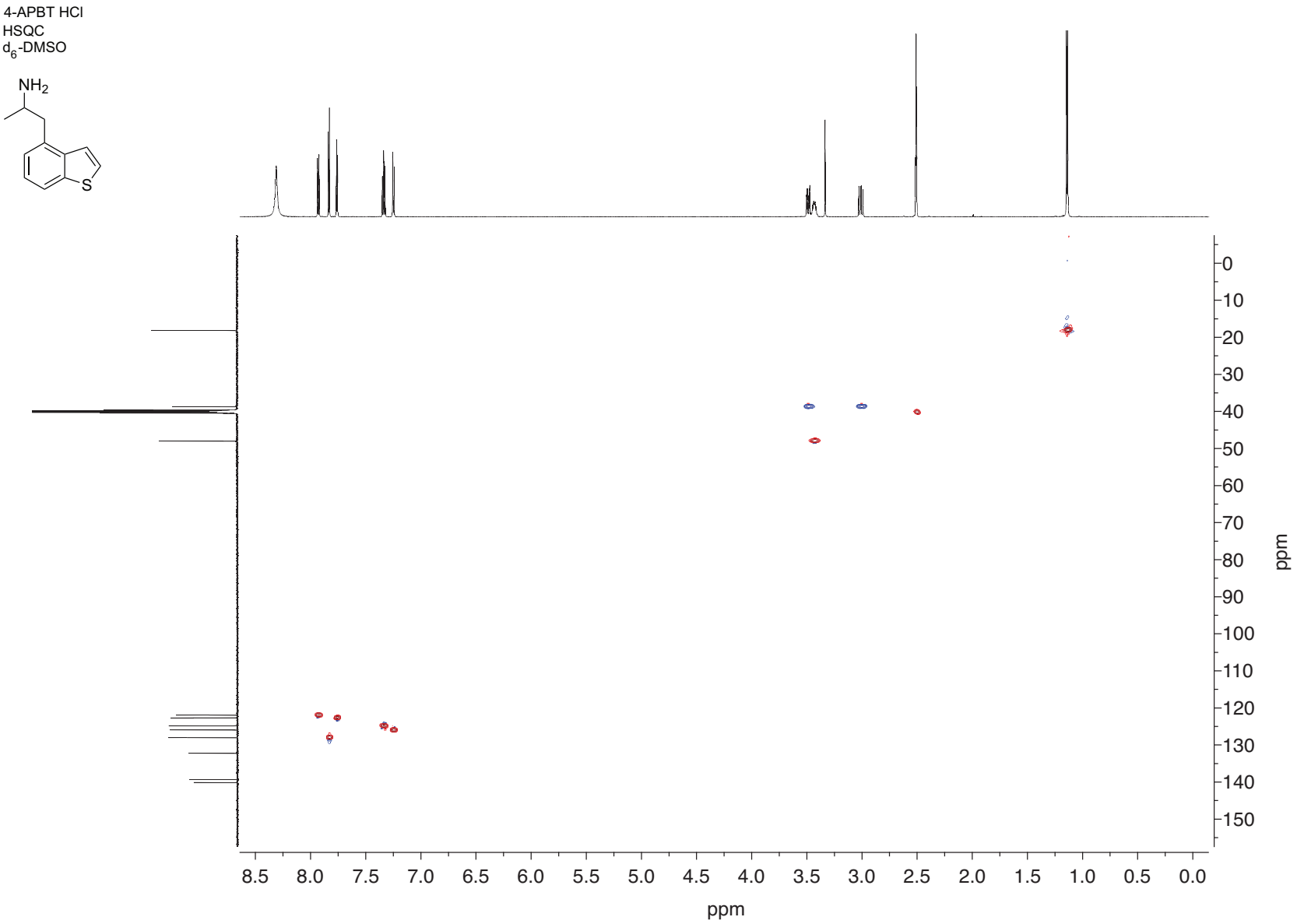
4-APBT HCl
^{1}H-NMR (600 MHz)
d_6-DMSO

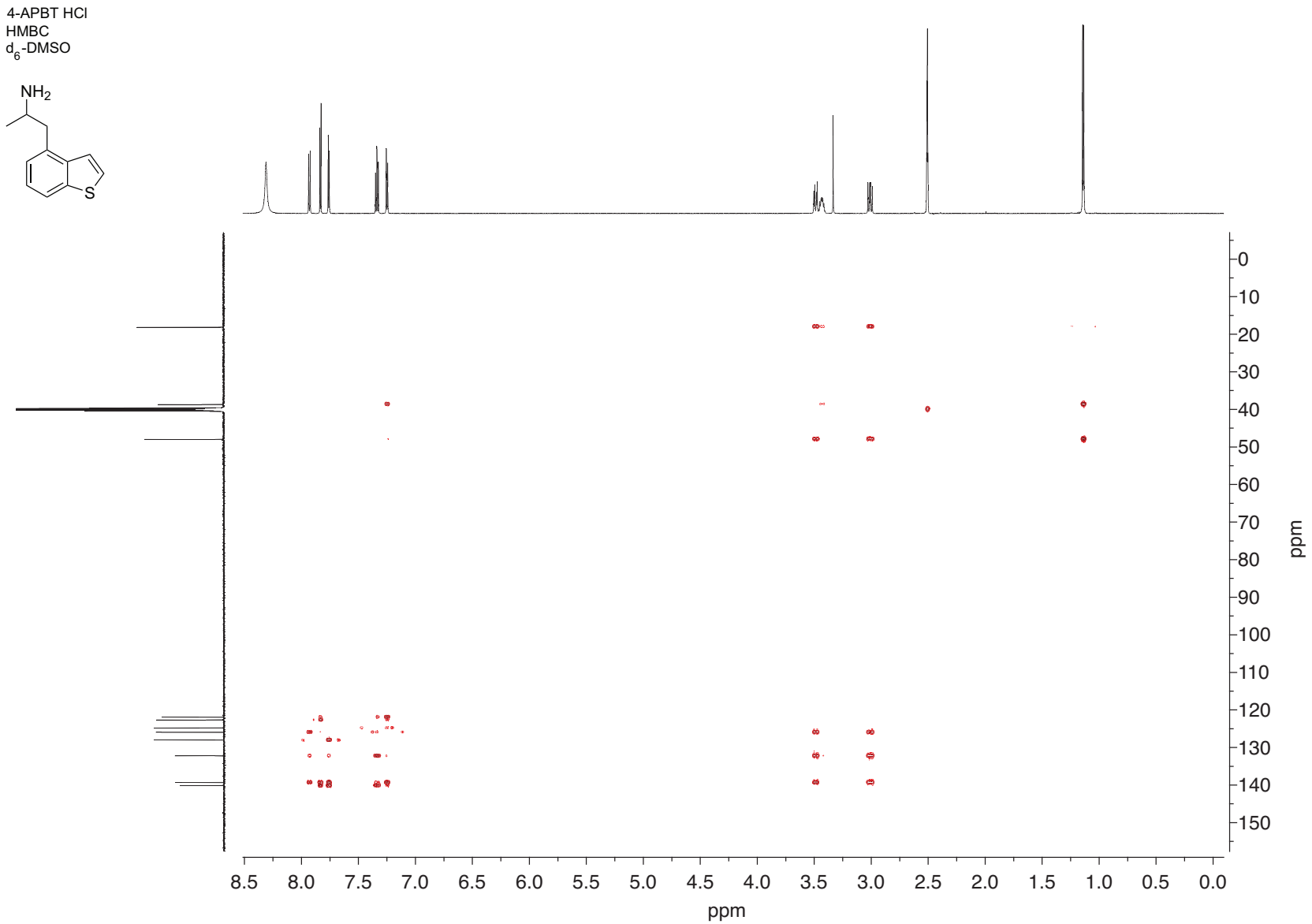


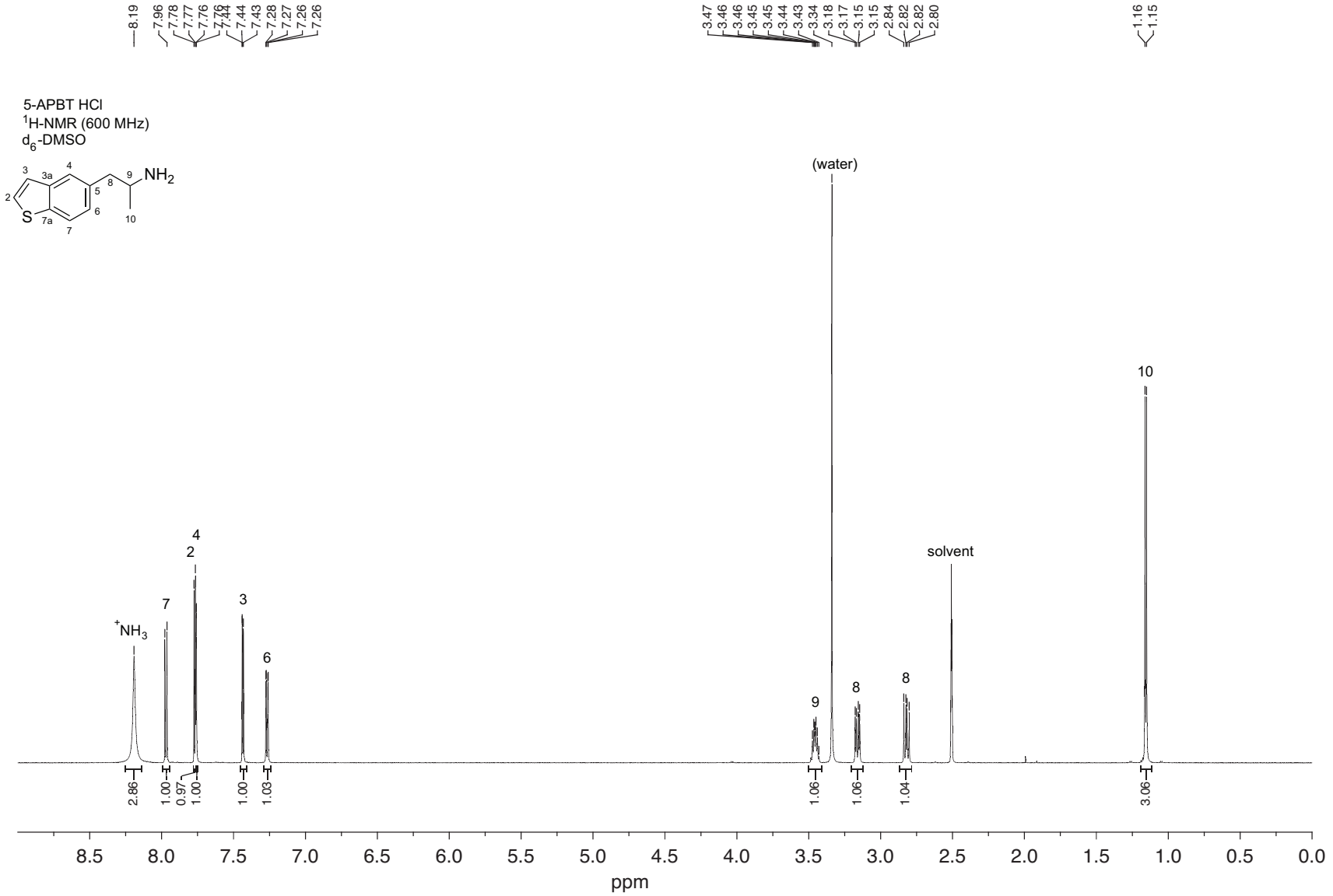
4-APBT HCl
COSY (600 MHz)
d_6-DMSO



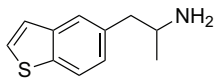

140.14
139.33
132.25
128.03
125.96
124.81
122.67
121.94
48.00
solvent
38.72
18.13
4-APBT HCl
13C (150 MHz)
d6-DMSO
NH2
9
10
8
4
3a
3
5
2
6
7a
S
7
7a 3a 4 2 5 6 3 7 9 8 10
145 135 125 115 105 95 85 75 65 55 45 35 25 15 5 0
ppm

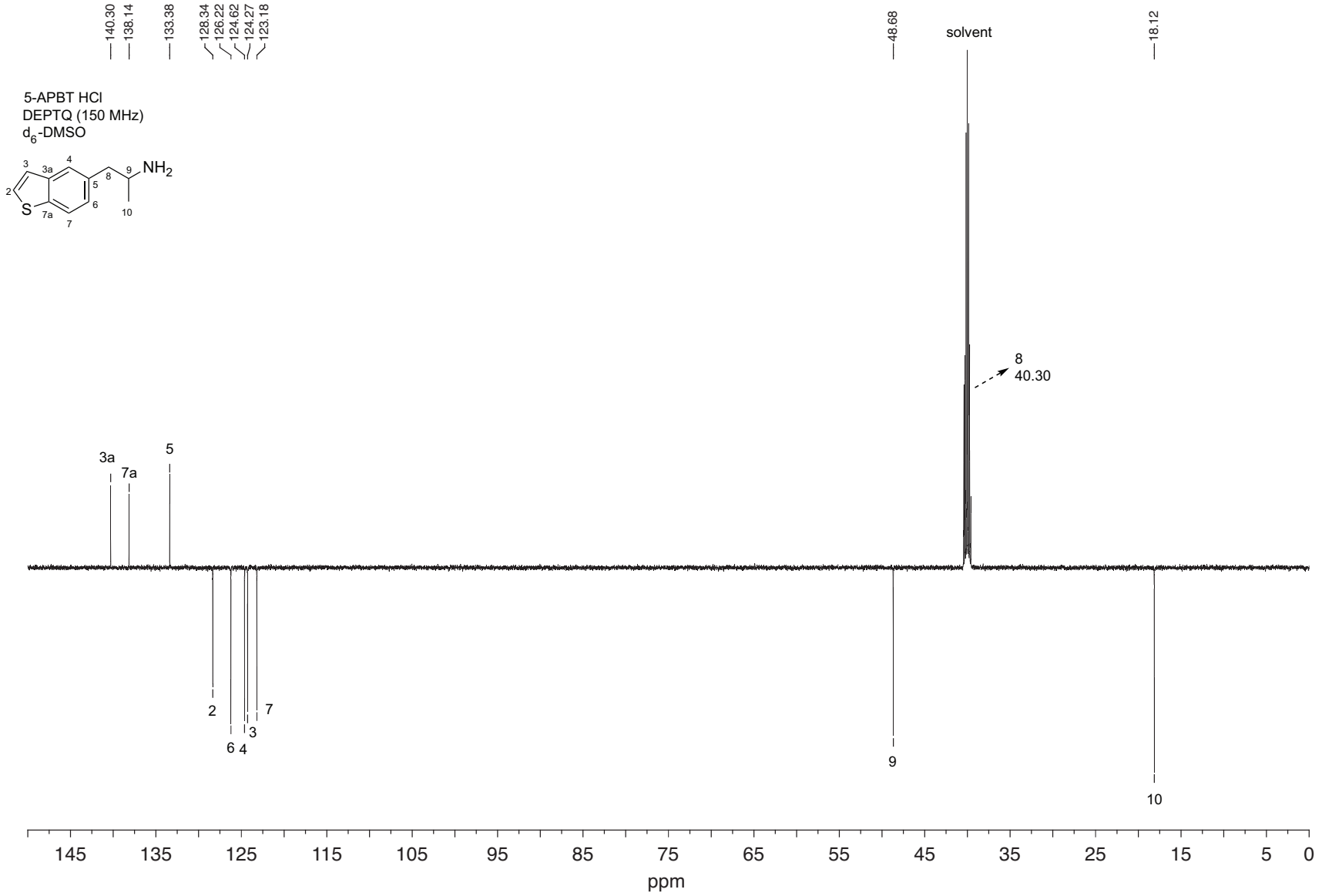

4-APBT HCl
HSQC
d6-DMSO
NH2
S
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
ppm
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm


4-APBT HCl
HMBC
d6-DMSO
NH2
S
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
ppm

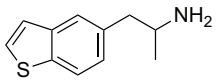

8.19
7.96
7.78
7.77
7.76
7.44
7.43
7.28
7.27
7.26
3.47
3.46
3.46
3.45
3.45
3.44
3.43
3.34
3.18
3.17
3.15
3.15
2.84
2.82
2.82
2.80
1.16
1.15
5-APBT HCl
1H-NMR (600 MHz)
d6-DMSO
NH2
(water)
solvent
+NH3
ppm

5-APBT HCl
COSY (600 MHz)
d_6-DMSO

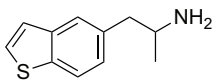



140.30
138.14
133.38
128.34
126.22
124.62
124.27
123.18
48.68
solvent
18.12
5-APBT HCl
DEPTQ (150 MHz)
d6-DMSO
NH2
8
40.30
3a
7a
5
2
6
4
3
7
9
10
145
135
125
115
105
95
85
75
65
55
45
35
25
15
5
0
ppm

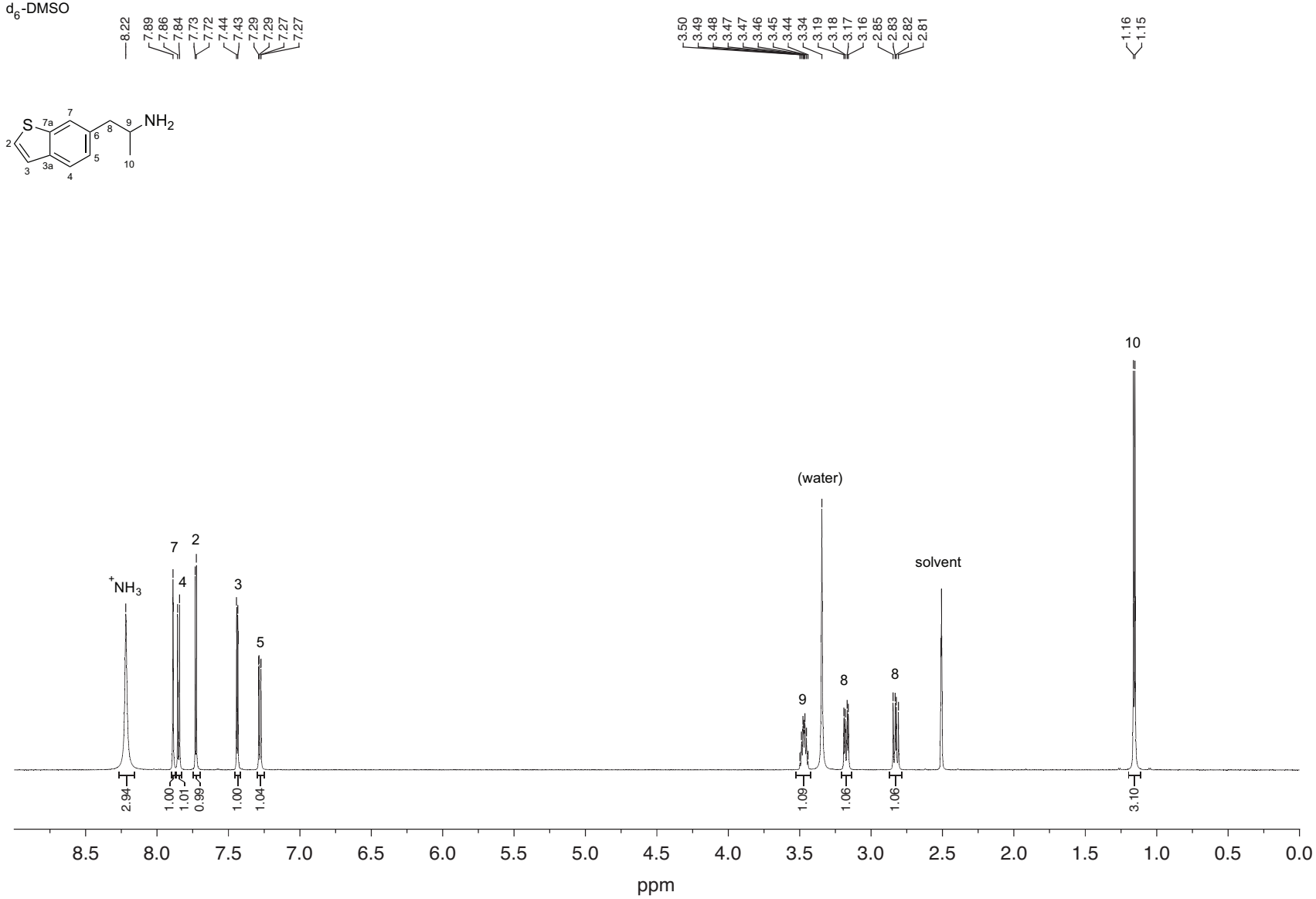
5-APBT HCl
HSQC
d_6-DMSO



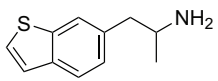
5-APBT HCl
HMBC
d_6-DMSO

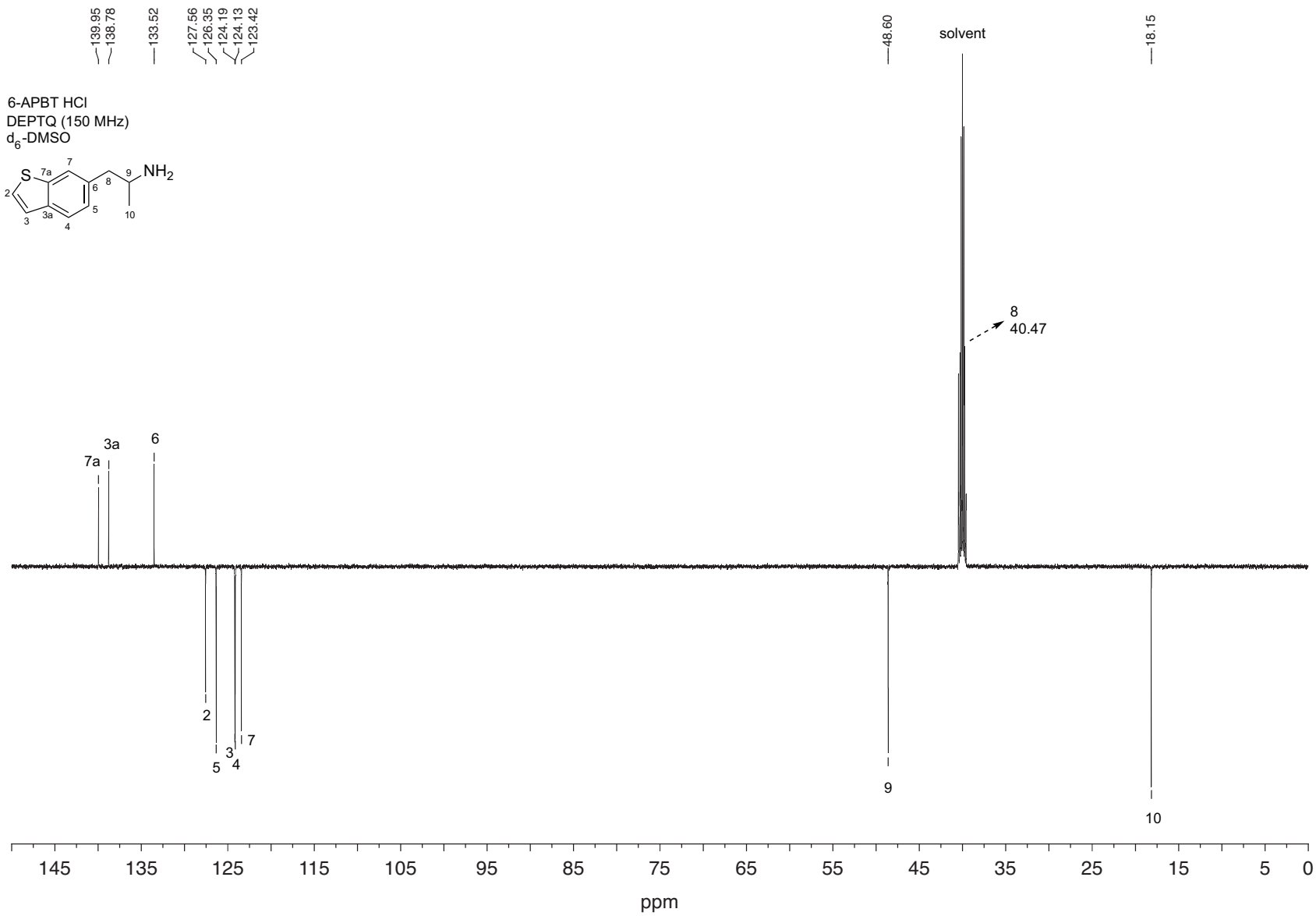


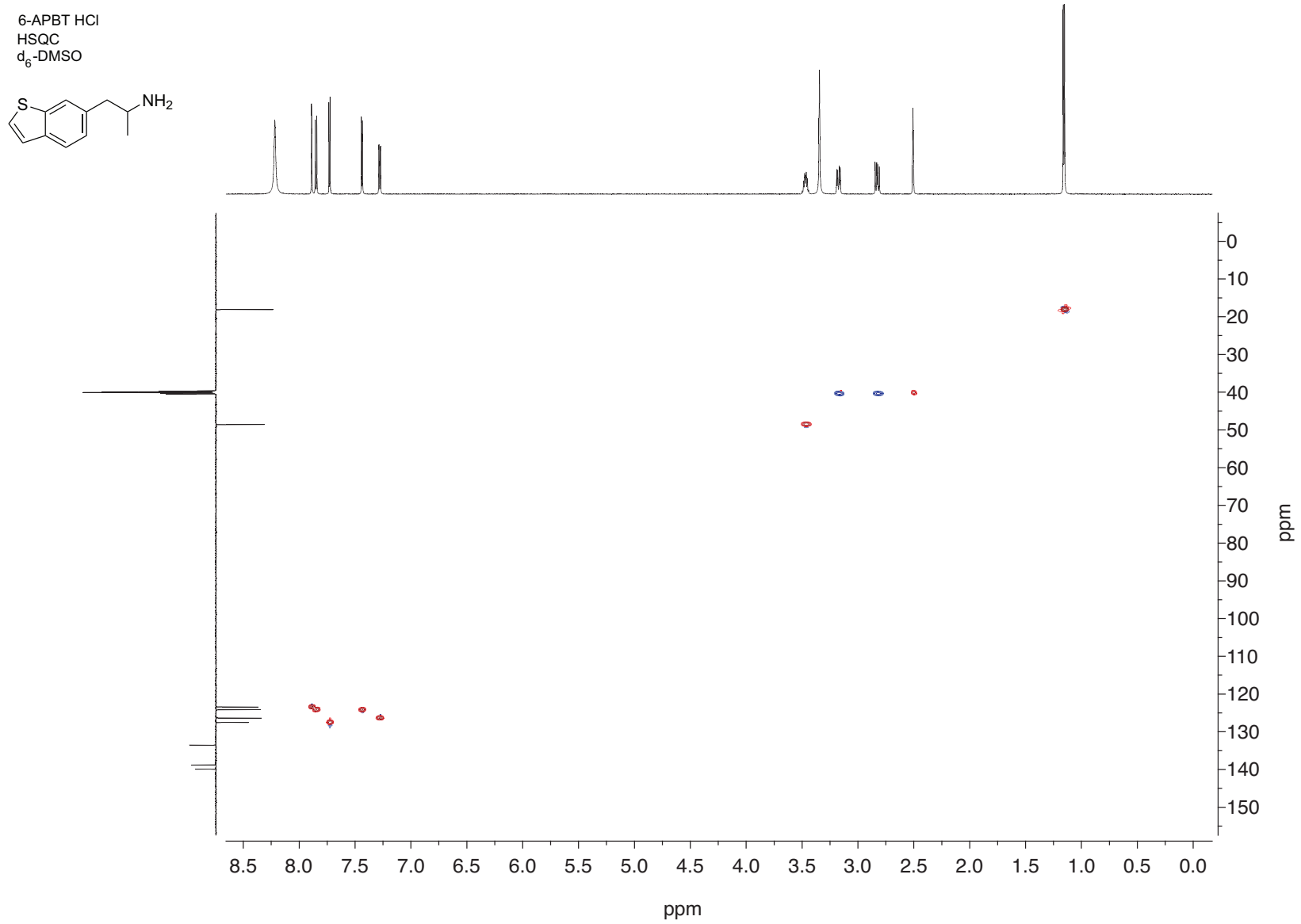
6-APBT HCl
^{1}H-NMR (600 MHz)
d_6-DMSO

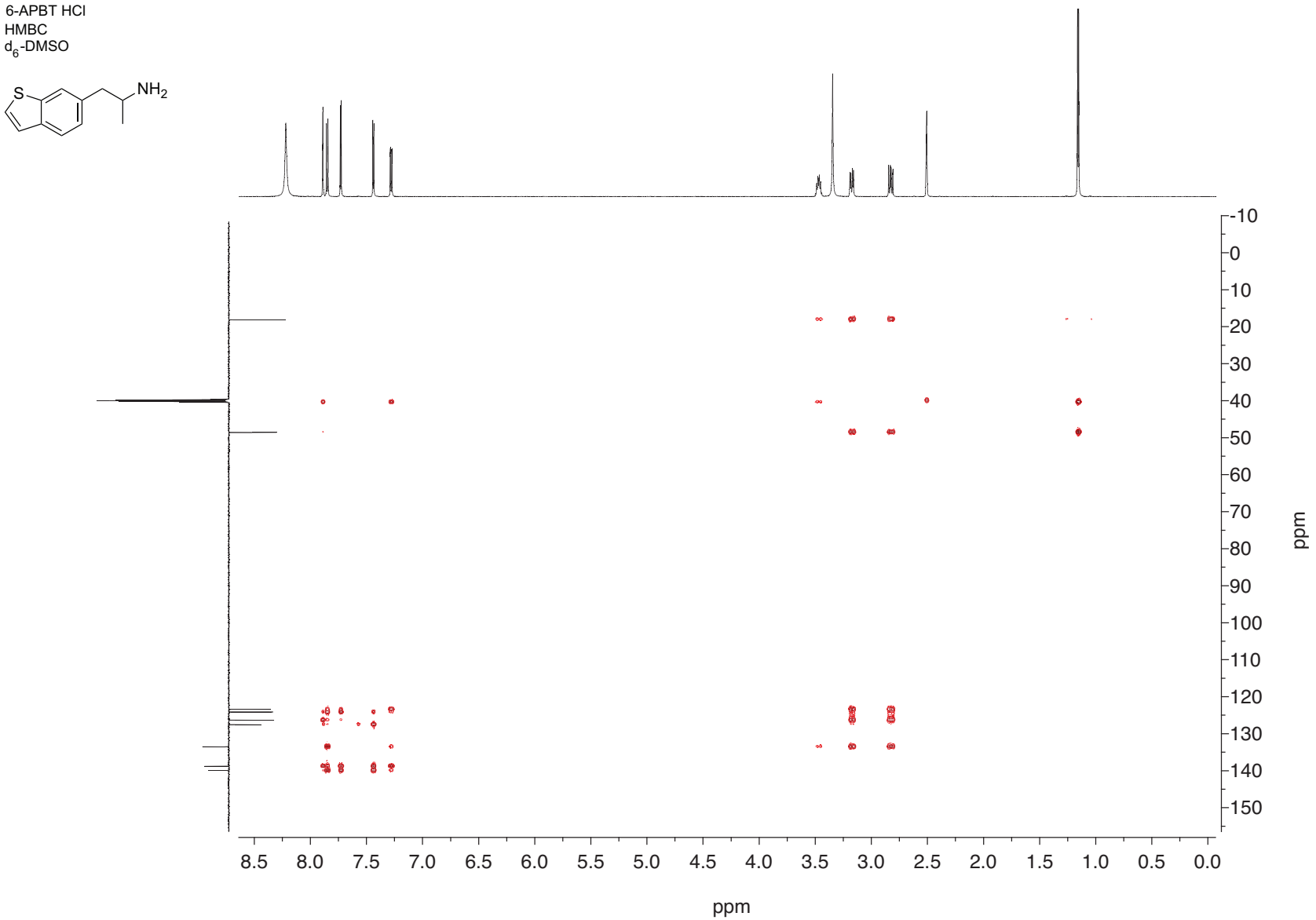


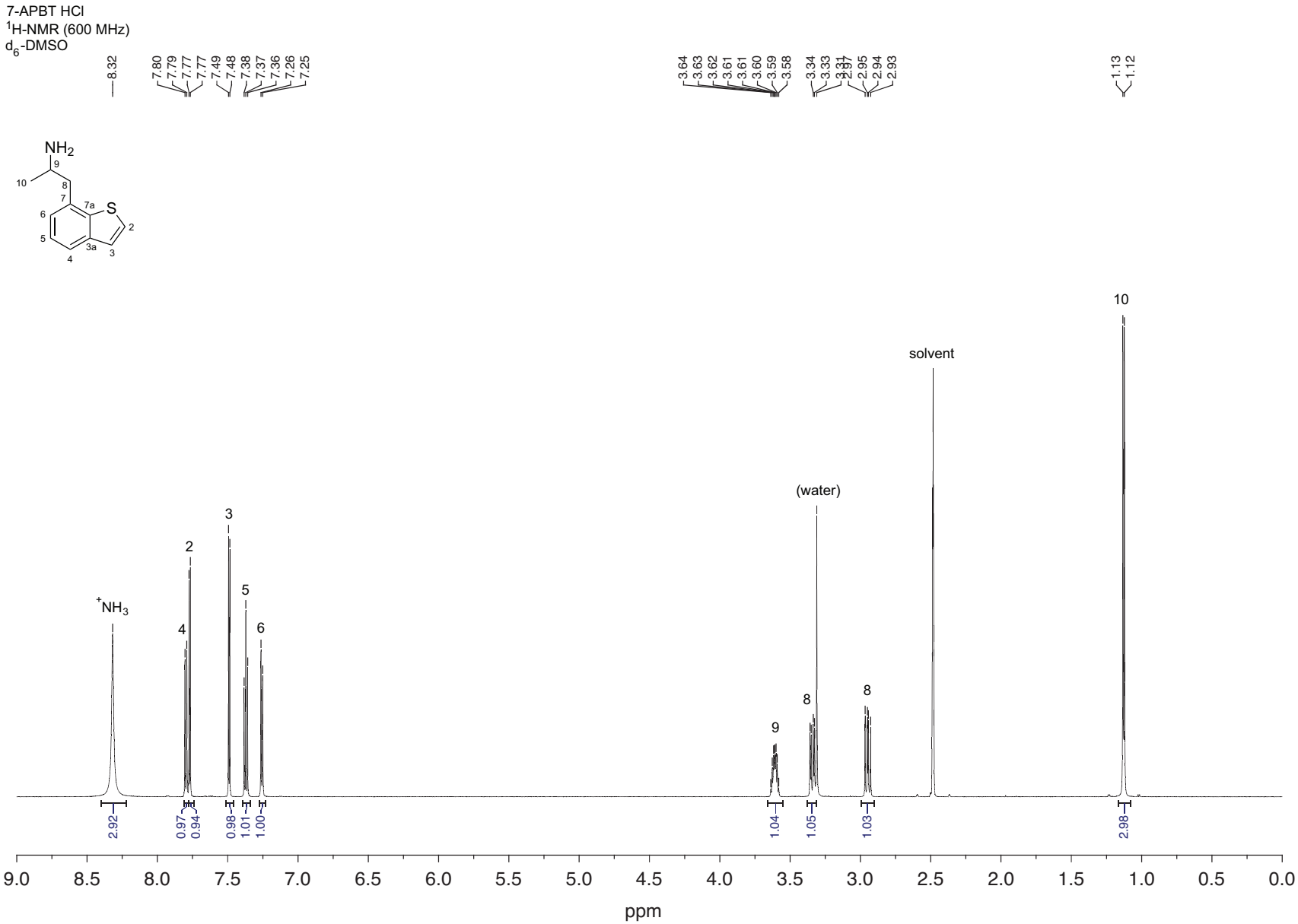
6-APBT HCl
COSY (600 MHz)
d_6-DMSO



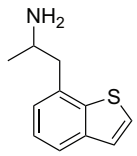

139.95
138.78
133.52
127.56
126.35
124.19
124.13
123.42
48.60
solvent
18.15
6-APBT HCl
DEPTQ (150 MHz)
d6-DMSO
S
NH2
8
40.47
7a
3a
6
2
5
3
4
7
9
10
145
135
125
115
105
95
85
75
65
55
45
35
25
15
5
0
ppm

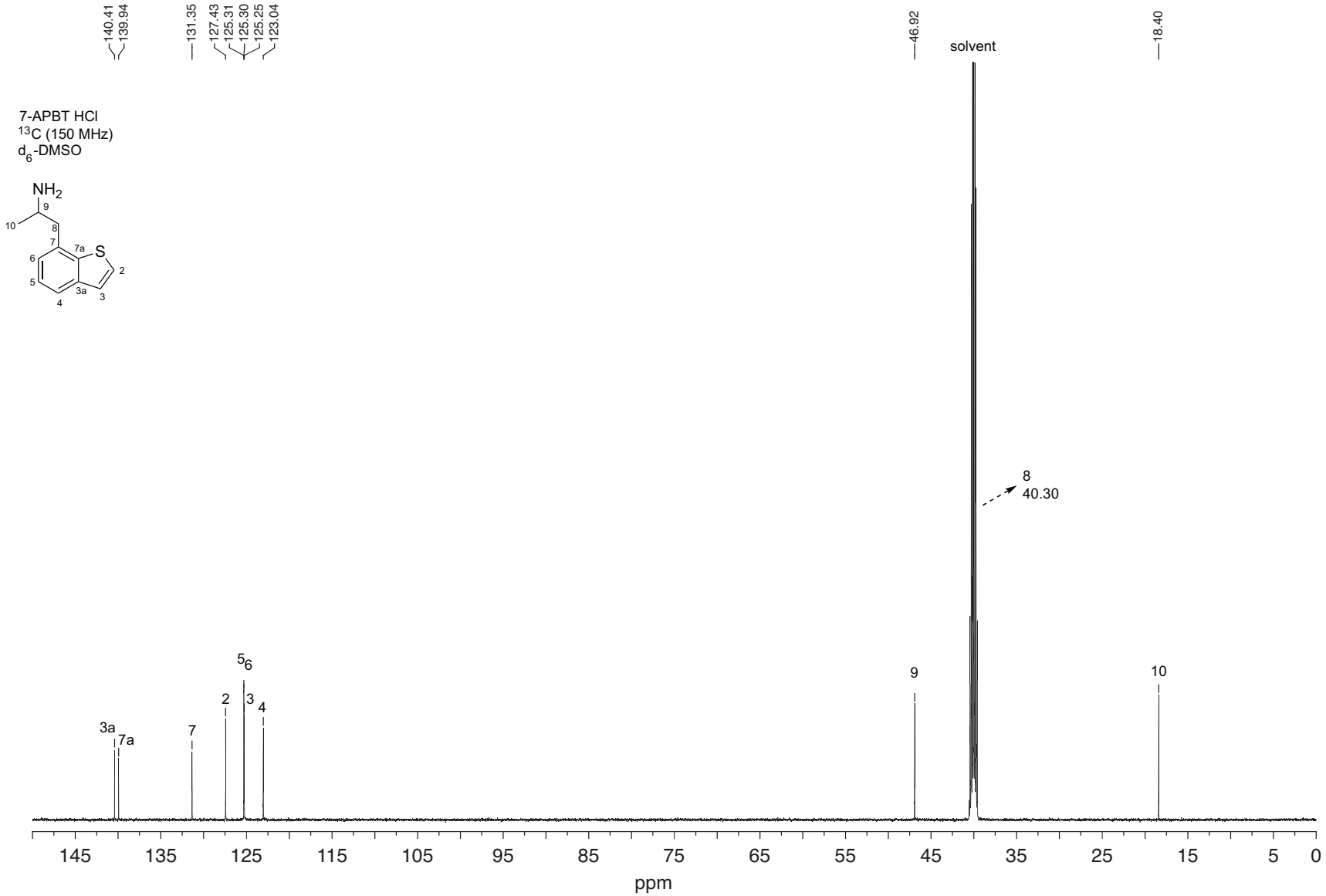

6-APBT HCl
HSQC
d6-DMSO
S
NH2
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
ppm
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

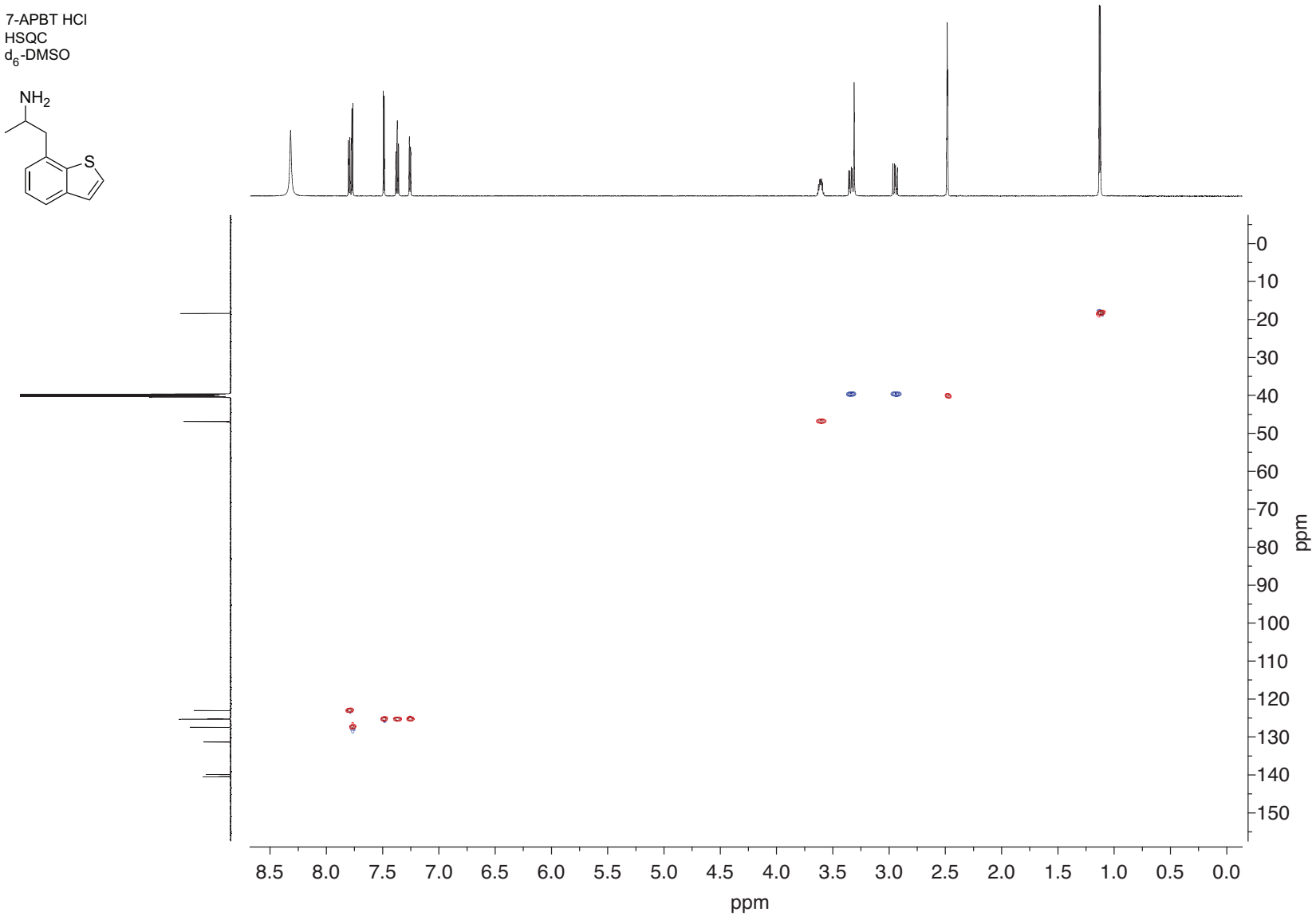

6-APBT HCl
HMBC
d6-DMSO
S
NH2
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
ppm
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

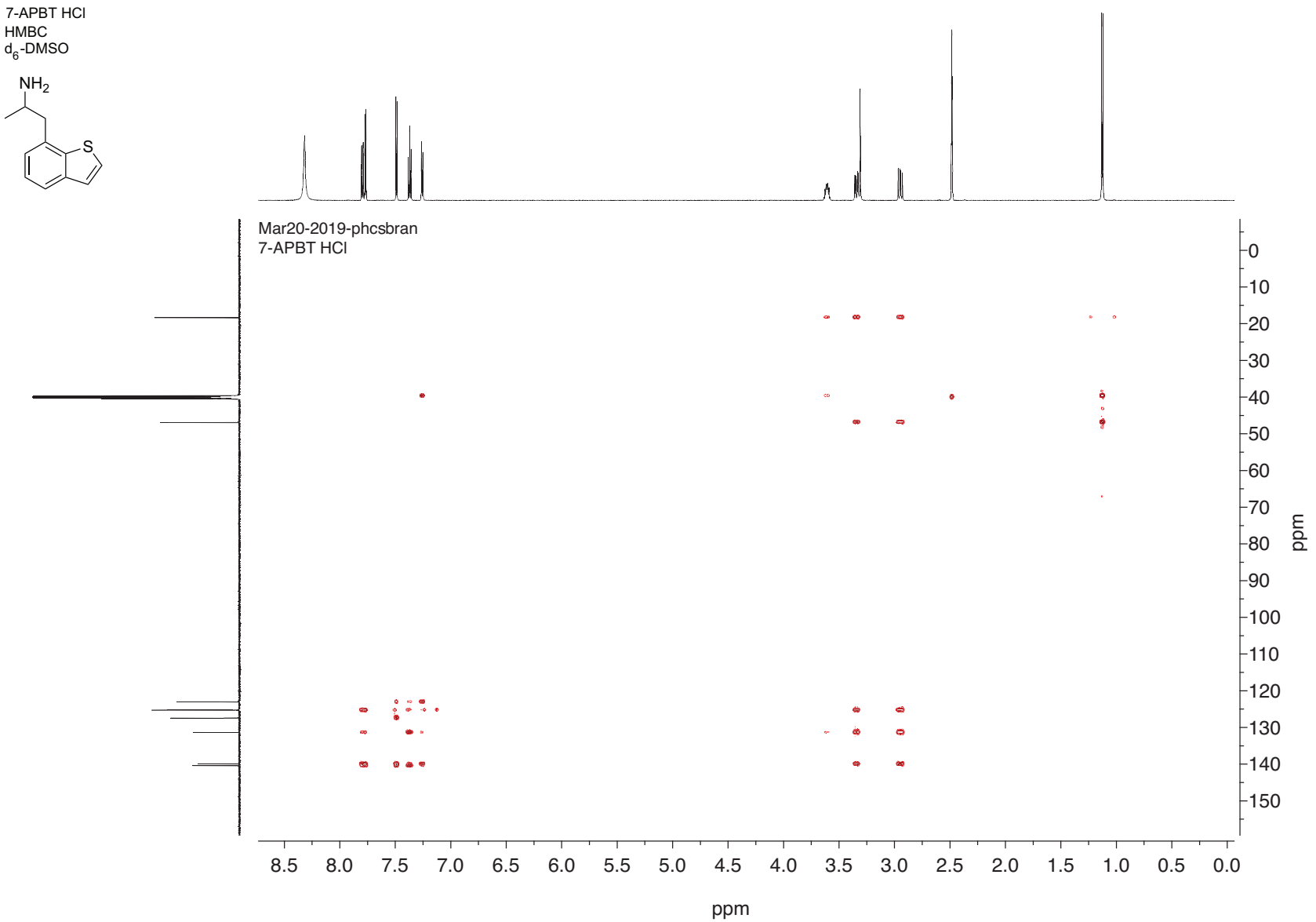

7-APBT HCl
1H-NMR (600 MHz)
d6-DMSO
8.32
7.80
7.79
7.77
7.77
7.49
7.48
7.38
7.37
7.36
7.26
7.25
3.64
3.63
3.62
3.61
3.61
3.60
3.59
3.58
3.34
3.33
3.31
2.95
2.94
2.93
1.13
1.12
NH2
9
10
8
7
7a
S
6
2
5
3a
3
4
10
solvent
(water)
3
2
5
+NH3
4
6
9
8
8
2.92
0.97
0.94
0.98
1.01
1.00
1.04
1.05
1.03
2.98
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

7-APBT HCl
COSY (600 MHz)
d_6-DMSO

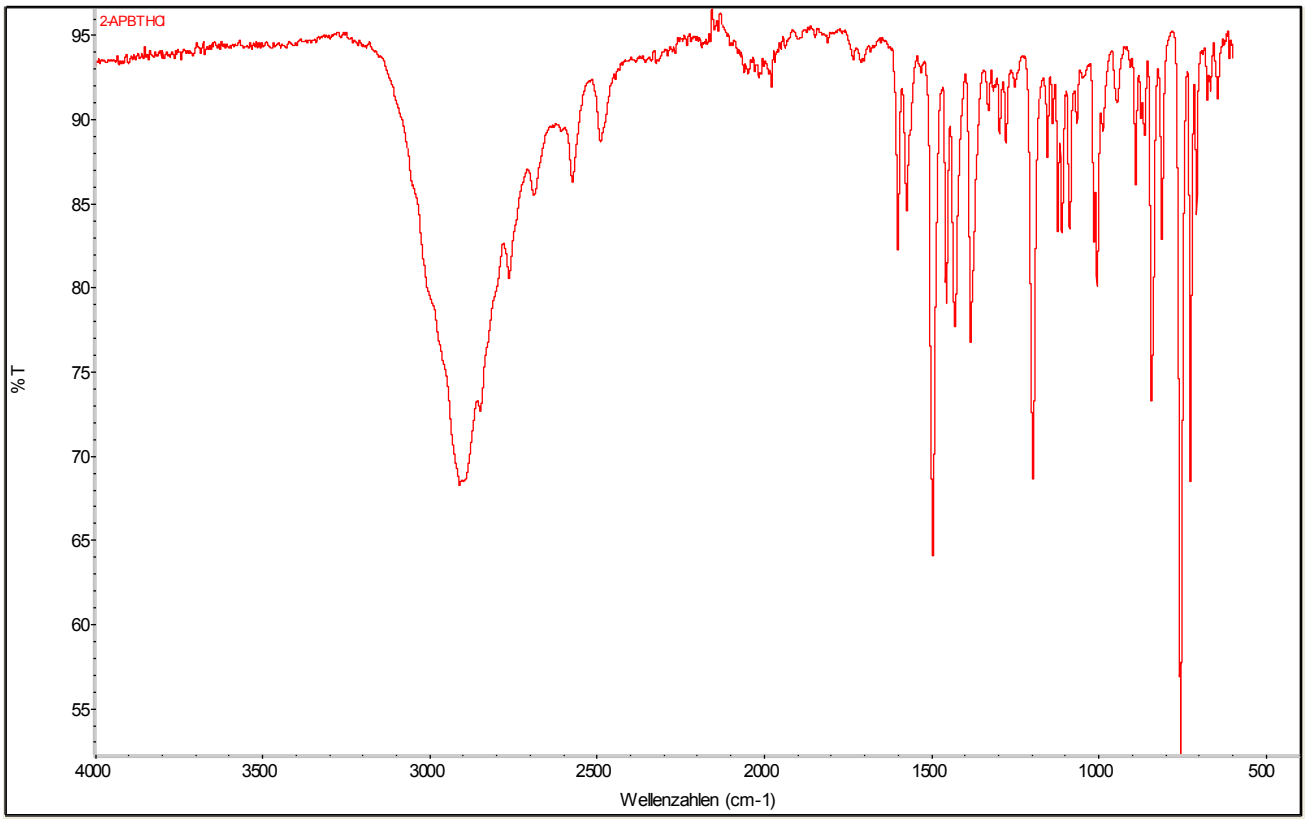


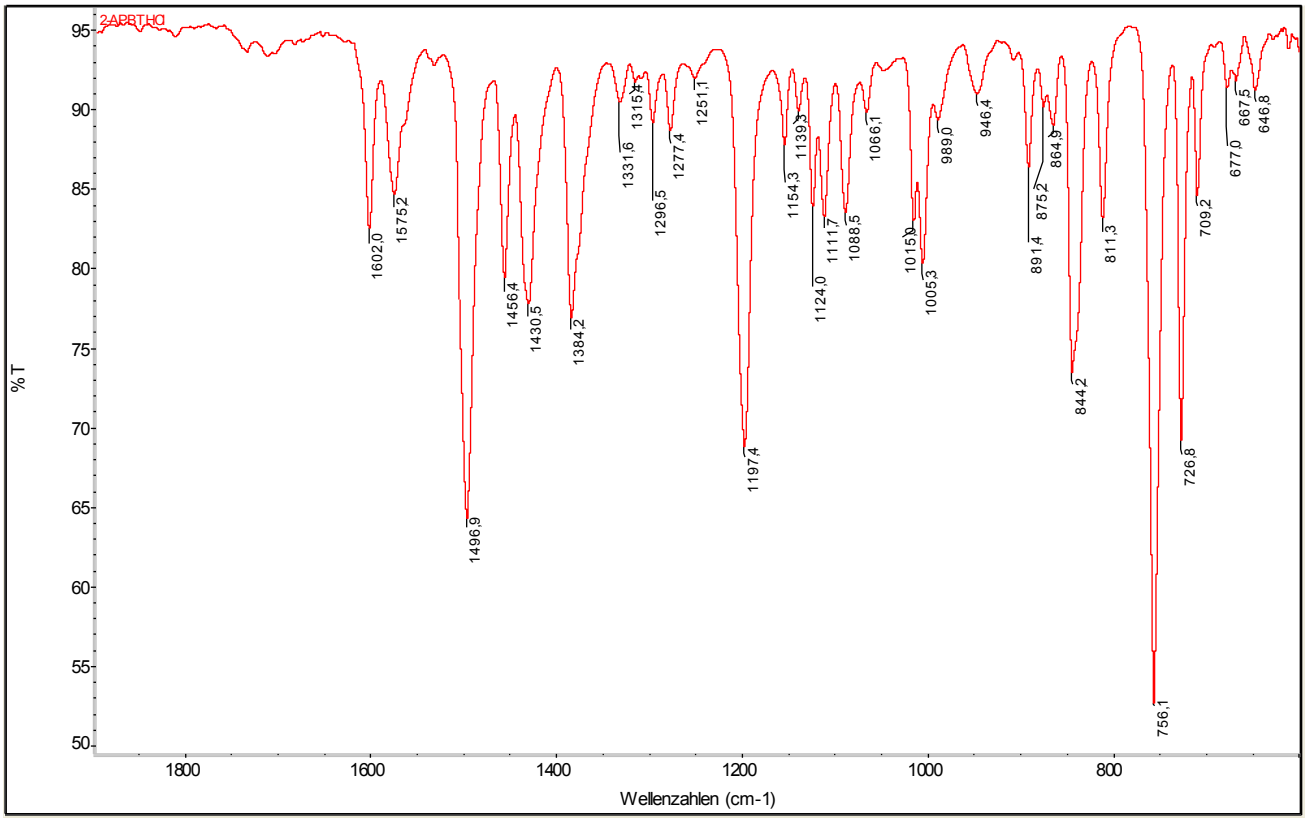

140.41
139.94
131.35
127.43
125.31
125.30
125.25
123.04
46.92
solvent
18.40
7-APBT HCl
13C (150 MHz)
d6-DMSO
NH2
9
10
8
7
7a
S
6
5
3a
4
3
2
8
40.30
5
6
3a
7a
7
2
3
4
9
10
145
135
125
115
105
95
85
75
65
55
45
35
25
15
5
0
ppm


7-APBT HCl
HSQC
d6-DMSO
NH2
S
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
ppm

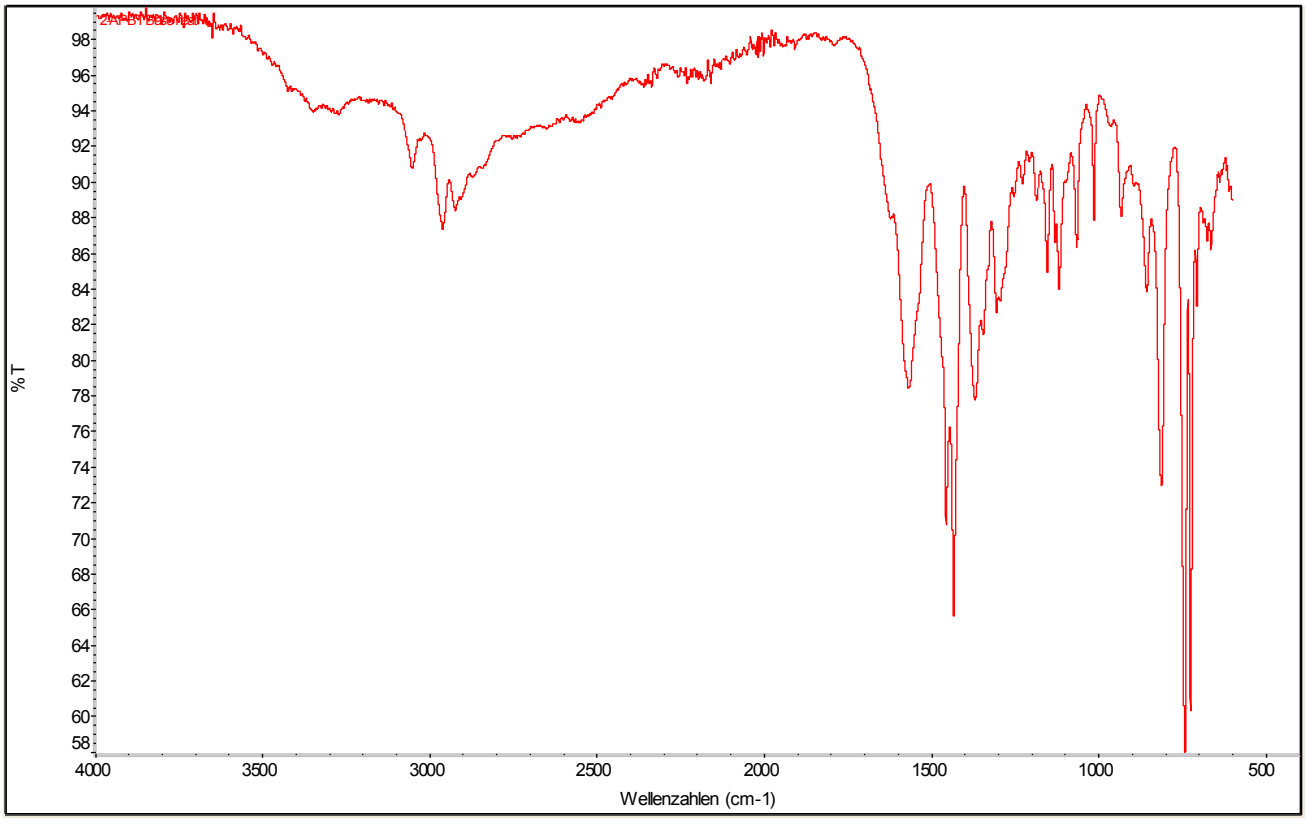

7-APBT HCl
HMBC
d6-DMSO
NH2
S
Mar20-2019-phcsbran
7-APBT HCl
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
ppm
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

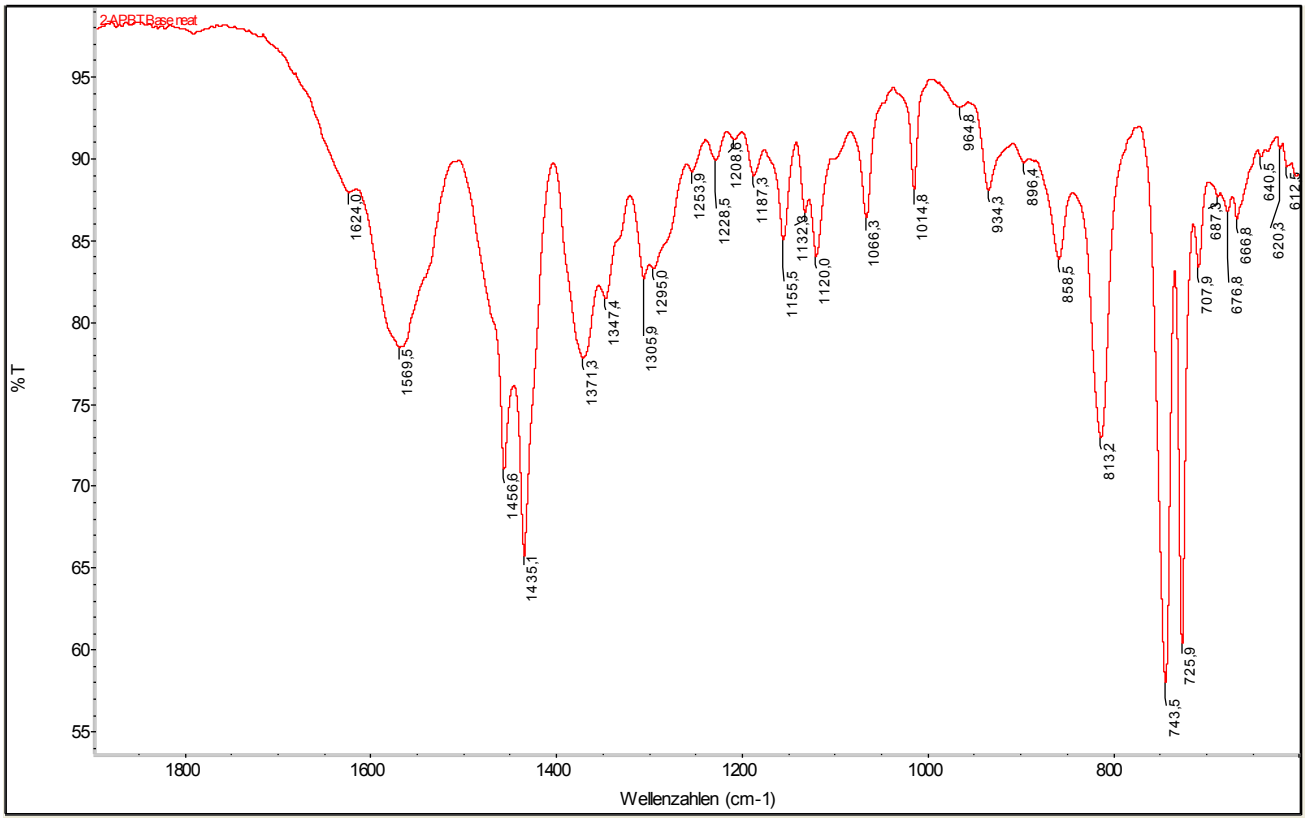
2-APBT HCl – ATR-IR



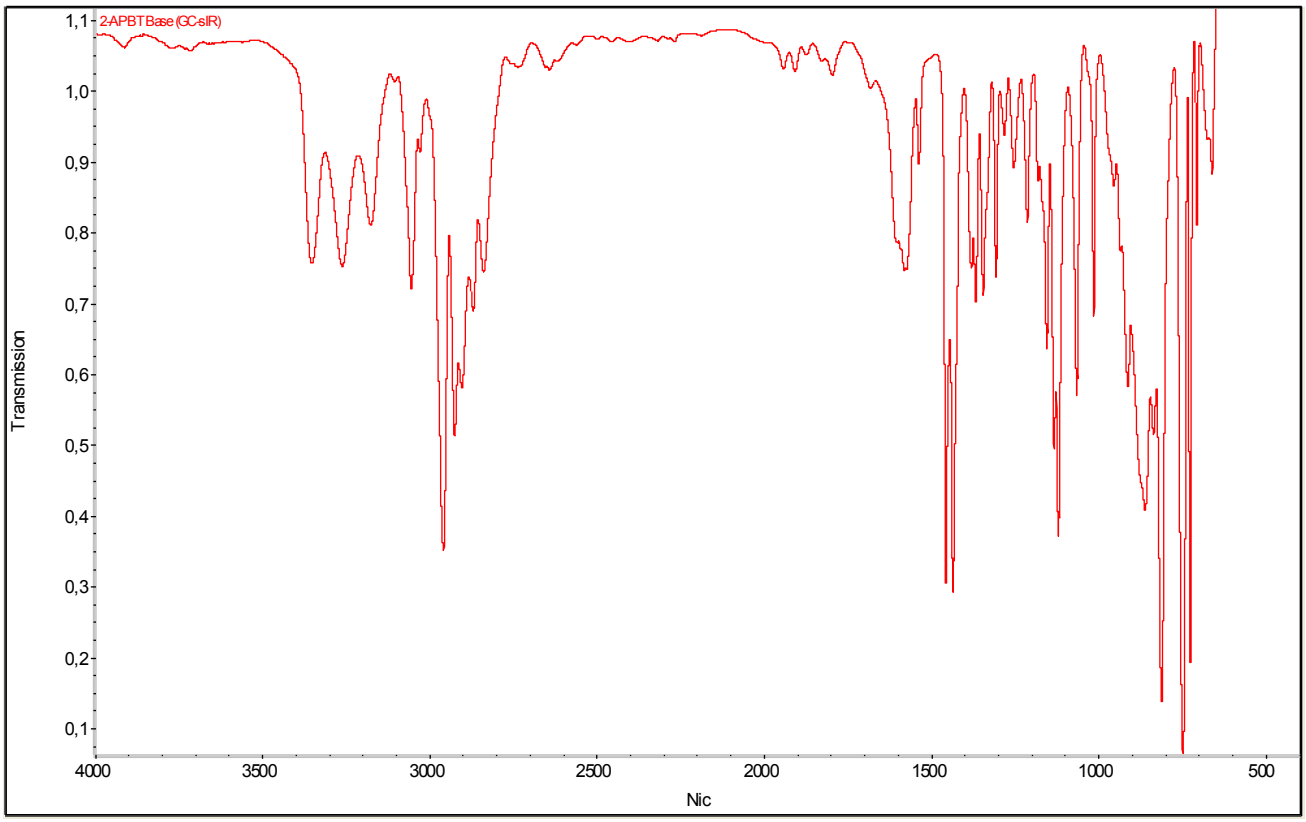


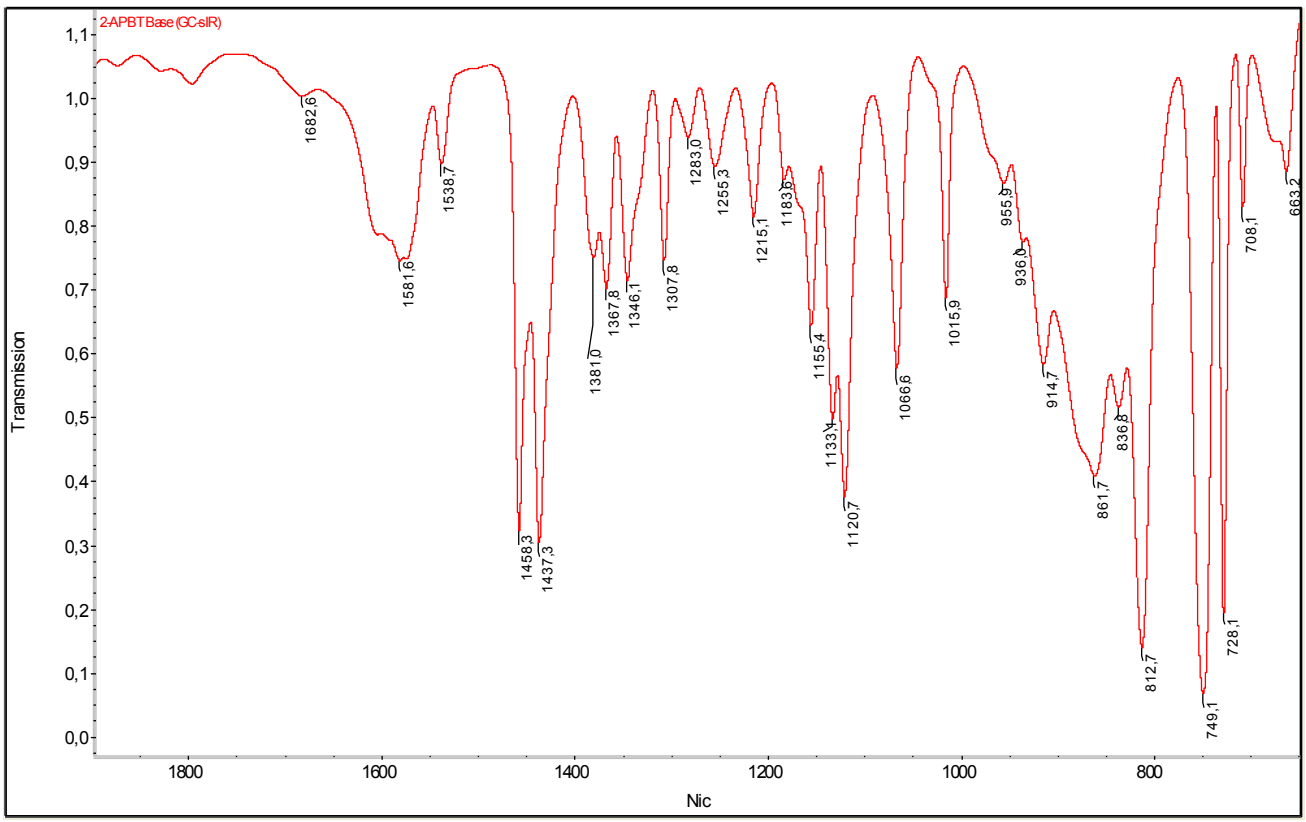
2-APBT base – ATR-IR



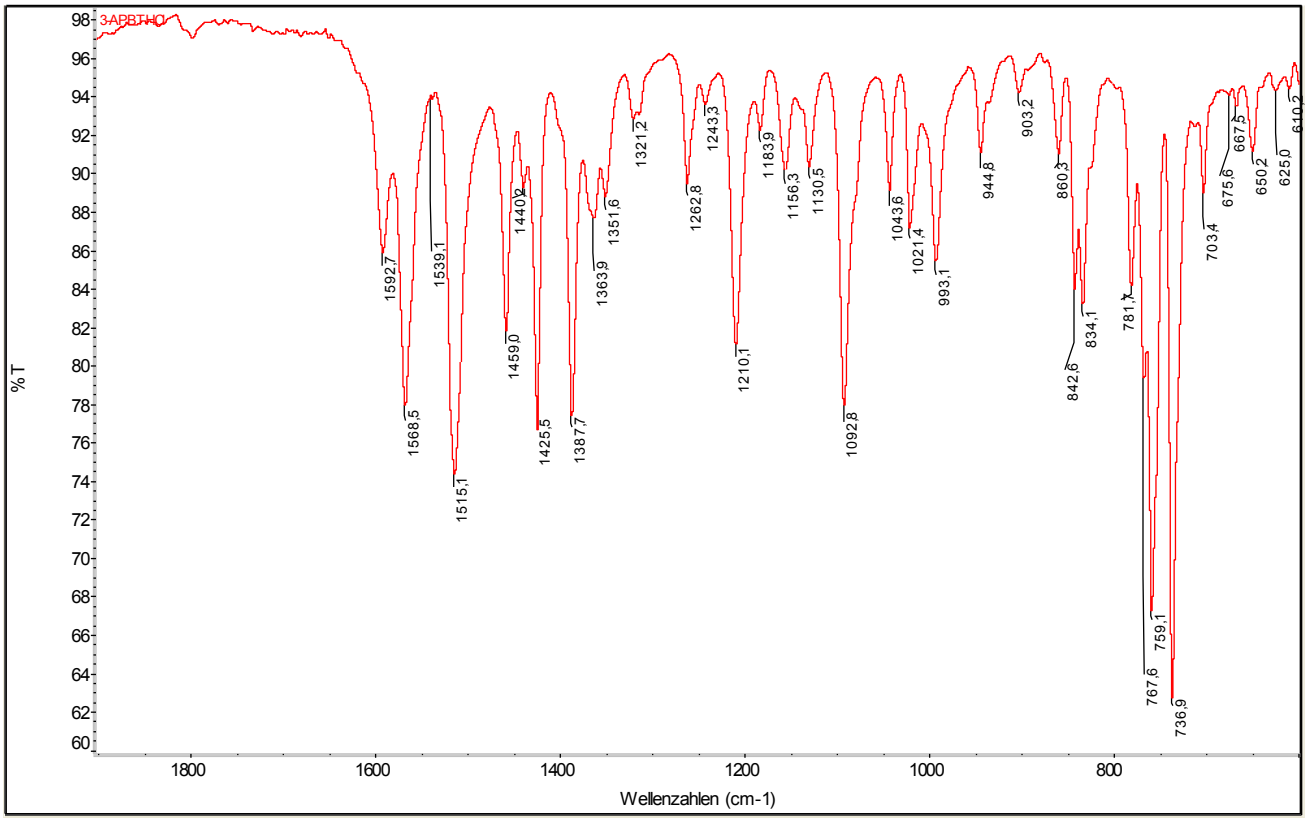


2-APBT base – GC-sIR

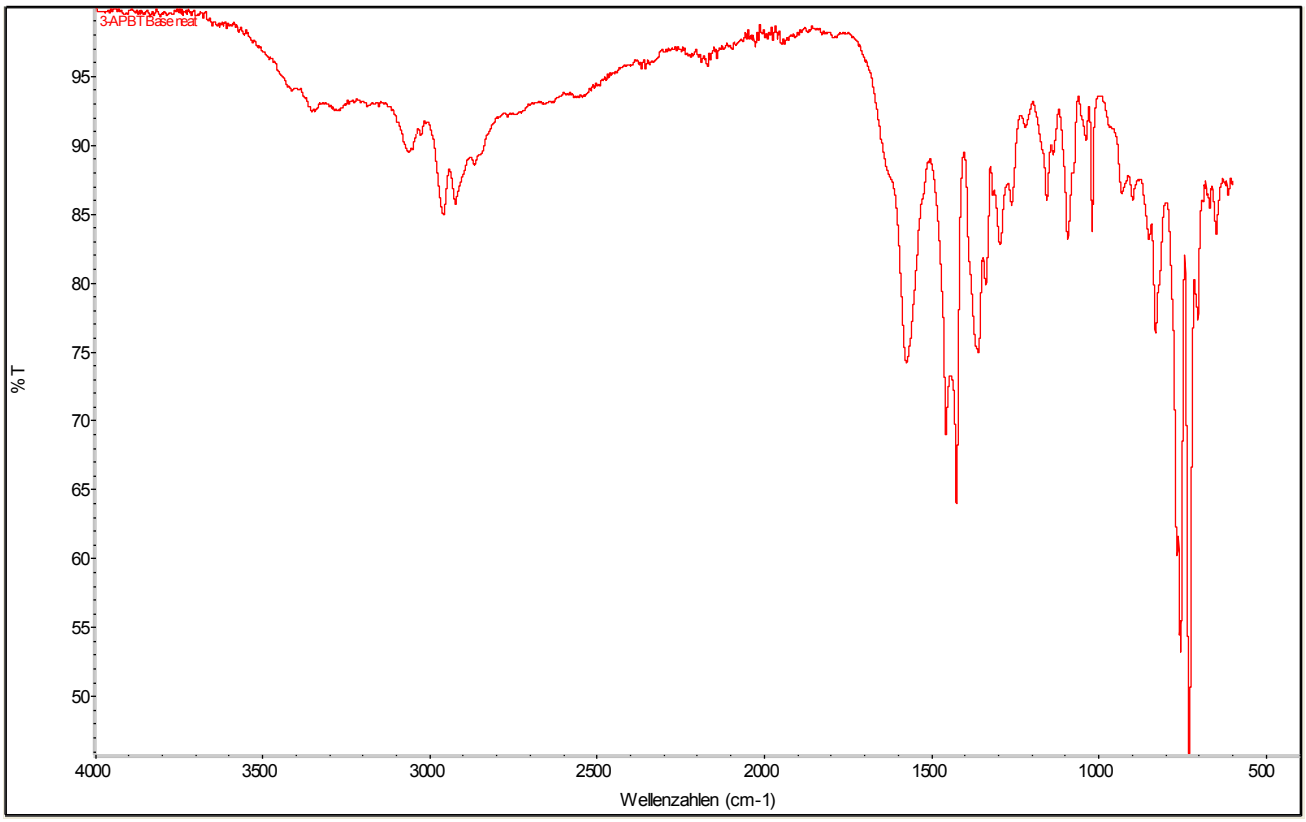


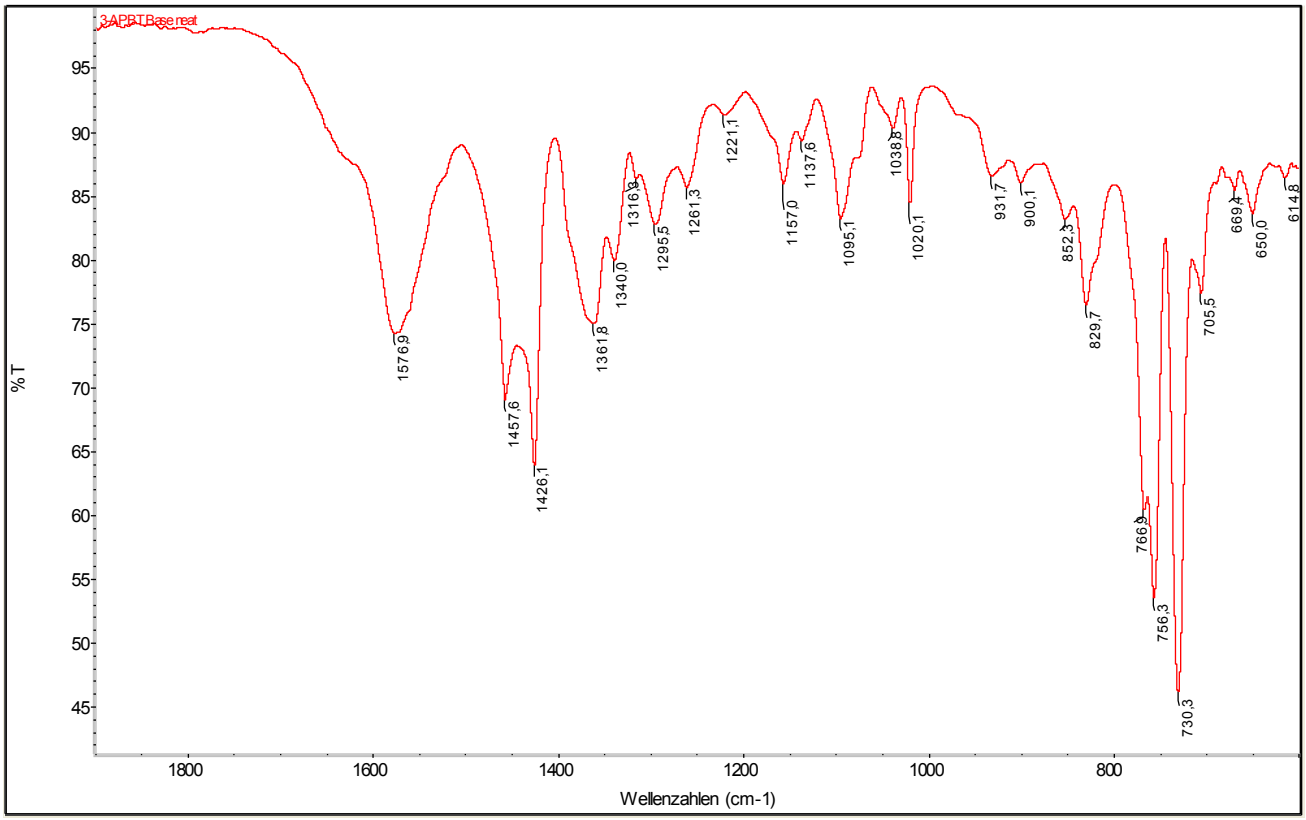


3-APBT HCl – ATR-IR

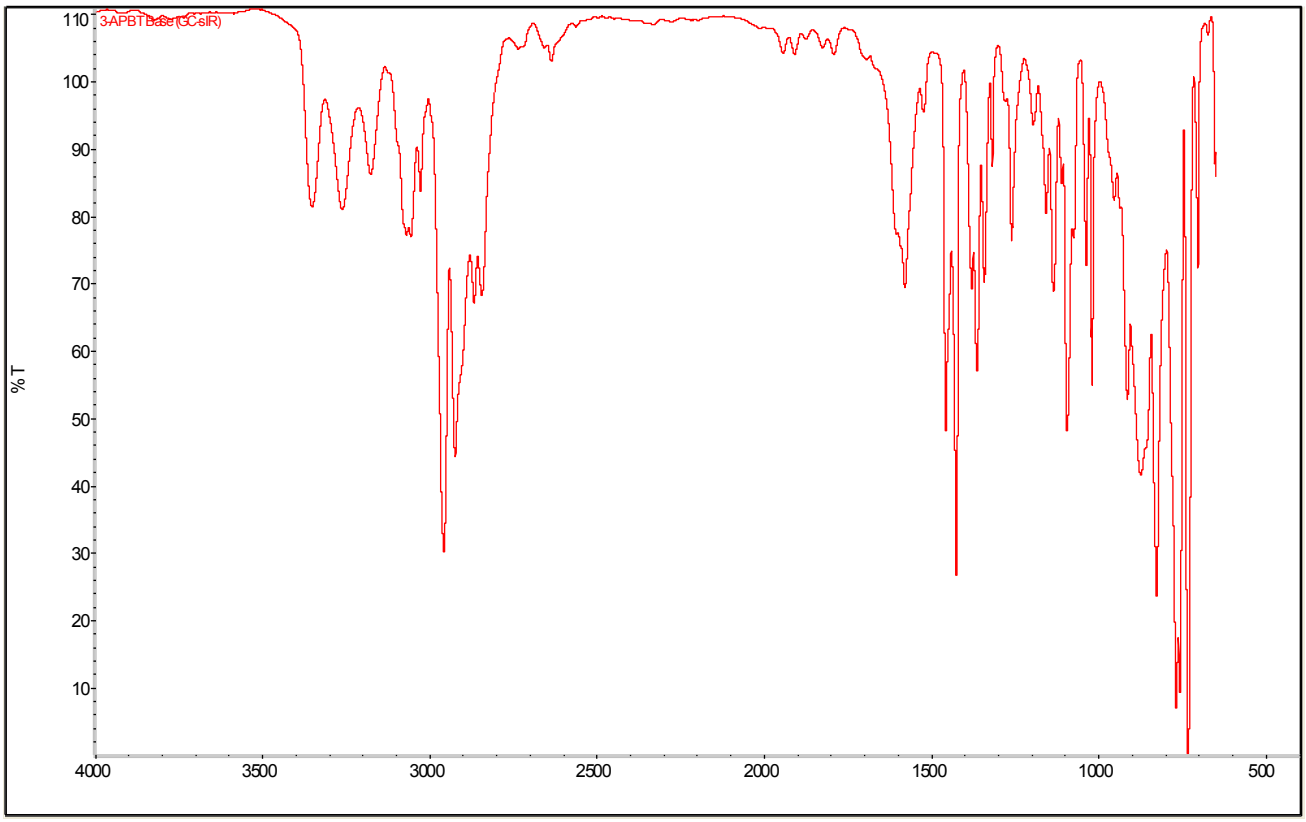


3-APBT base – ATR-IR

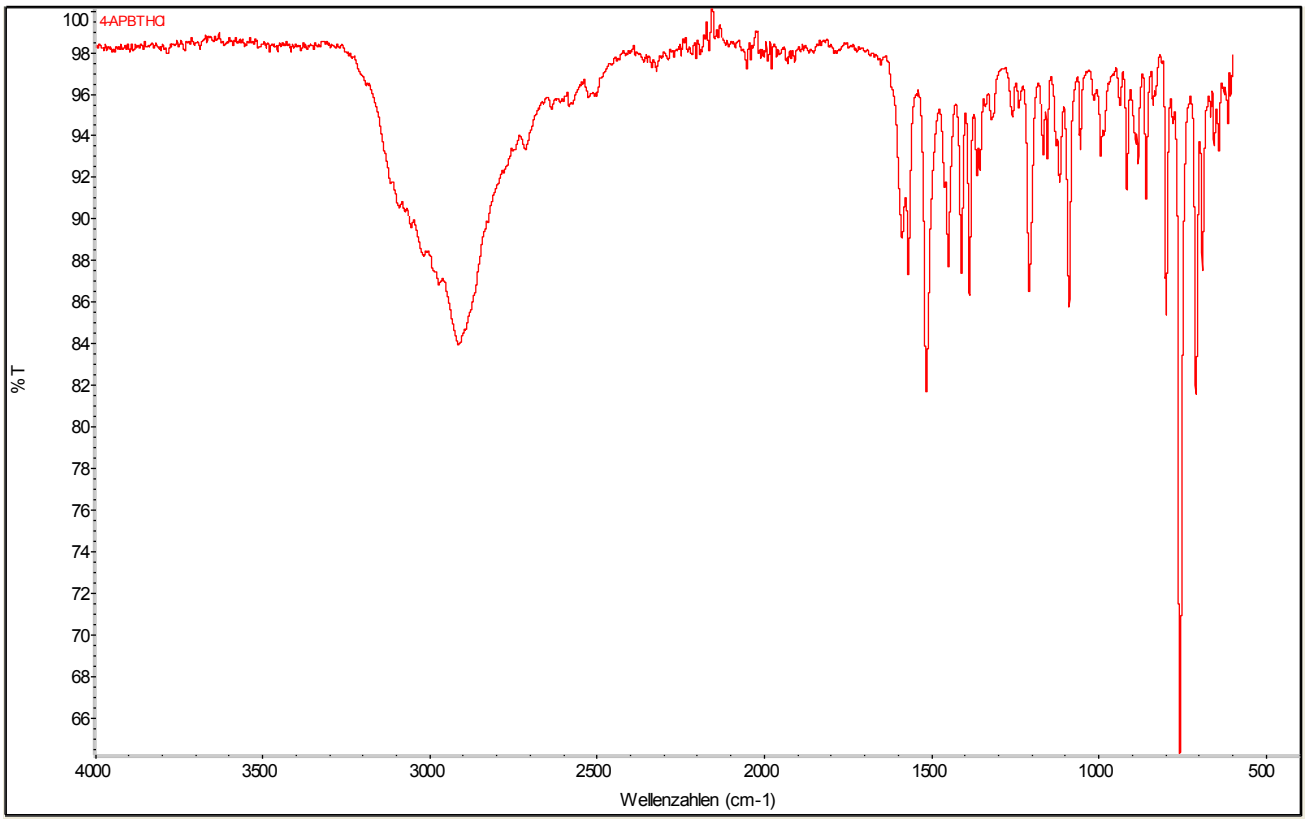


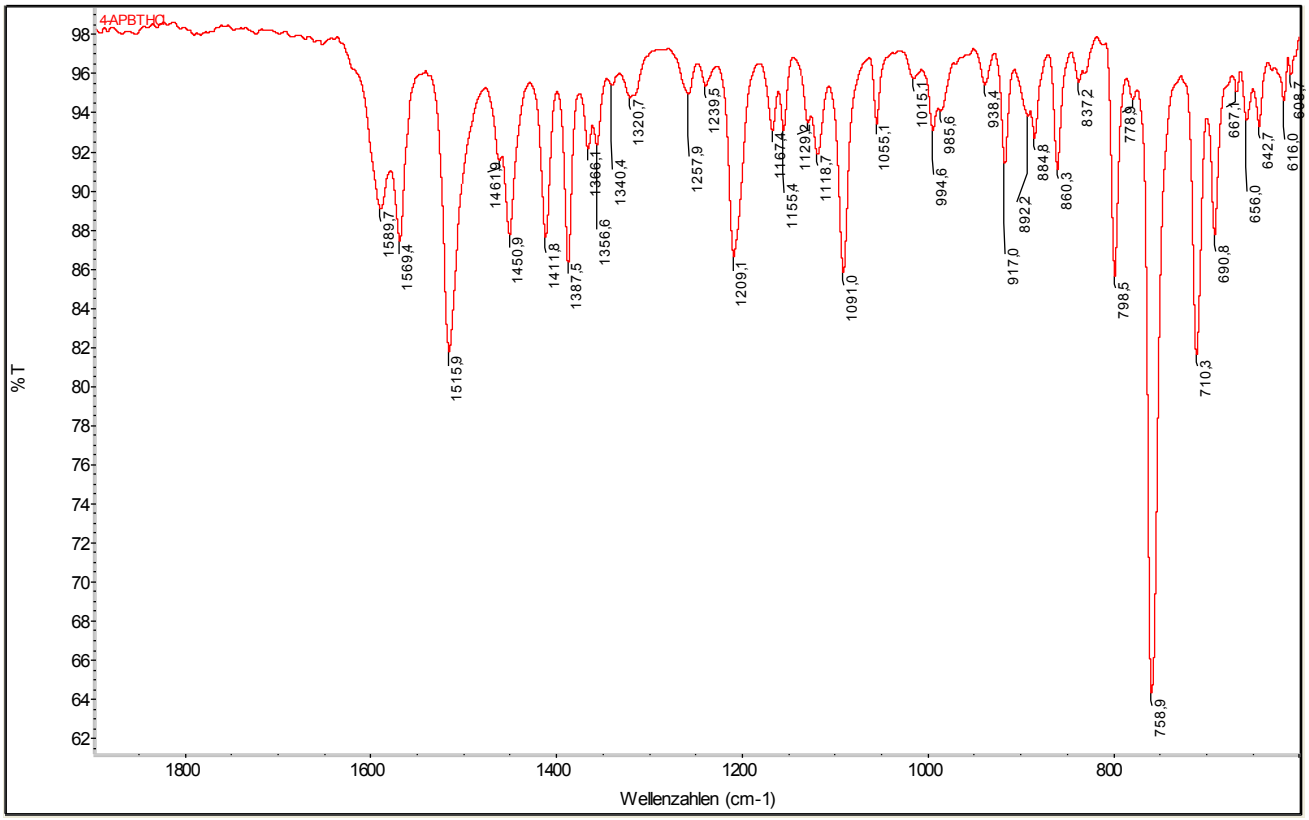


3-APBT base – GC-sIR

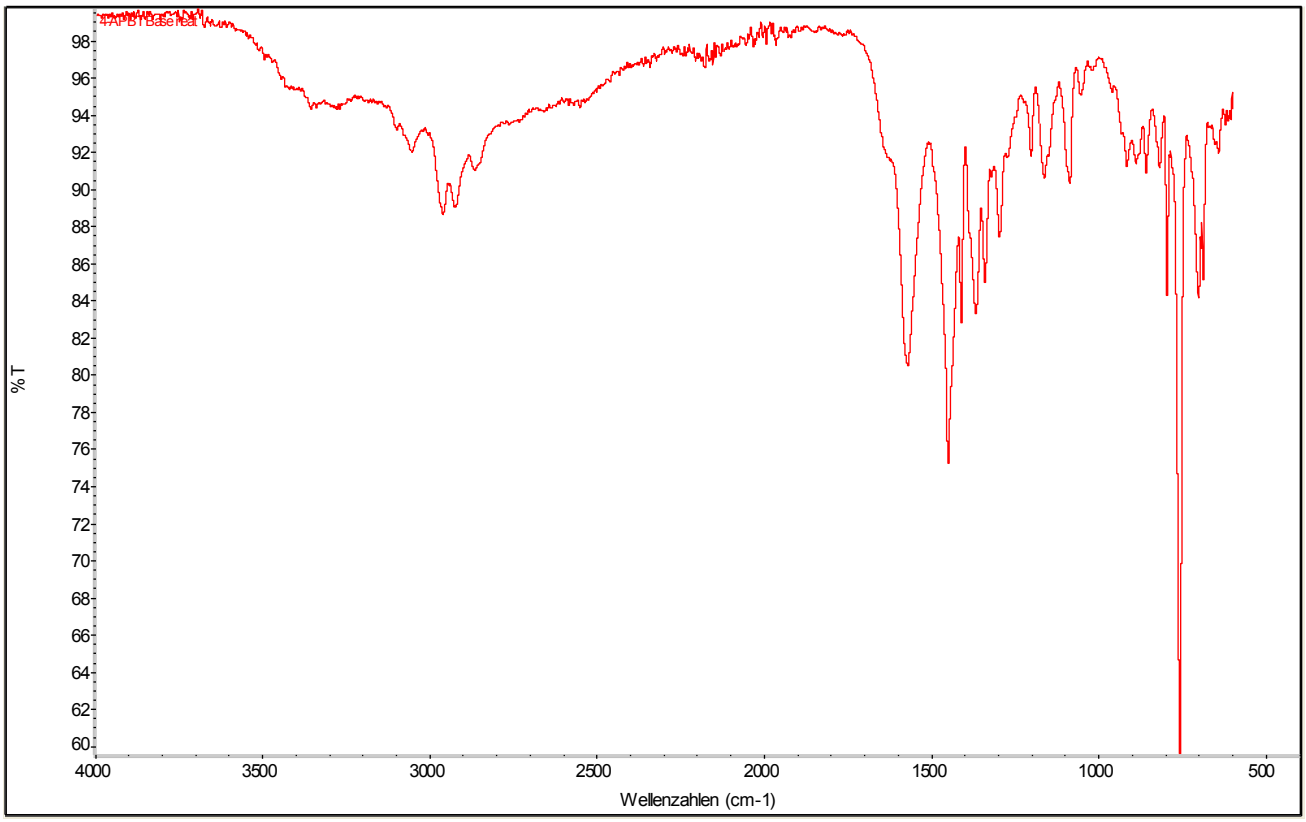


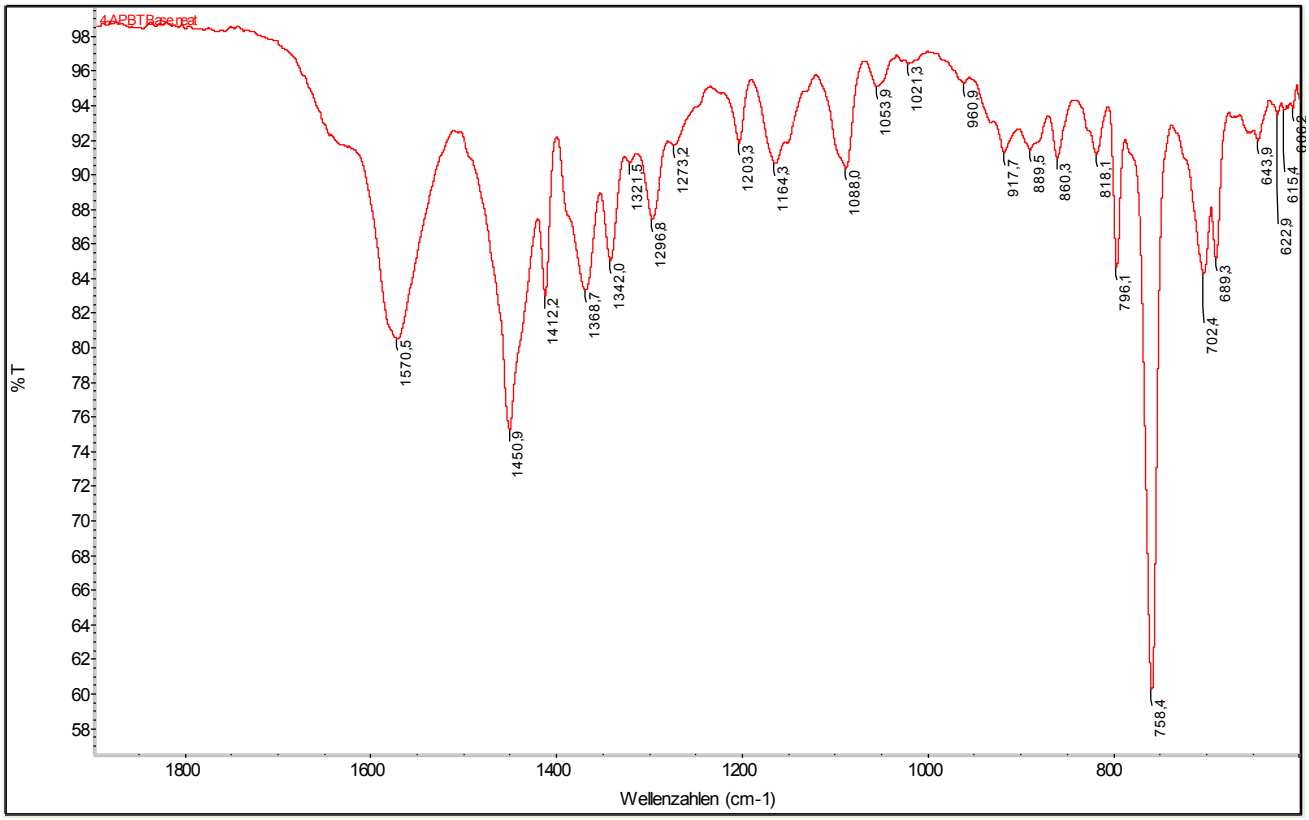
4-APBT HCl – ATR-IR



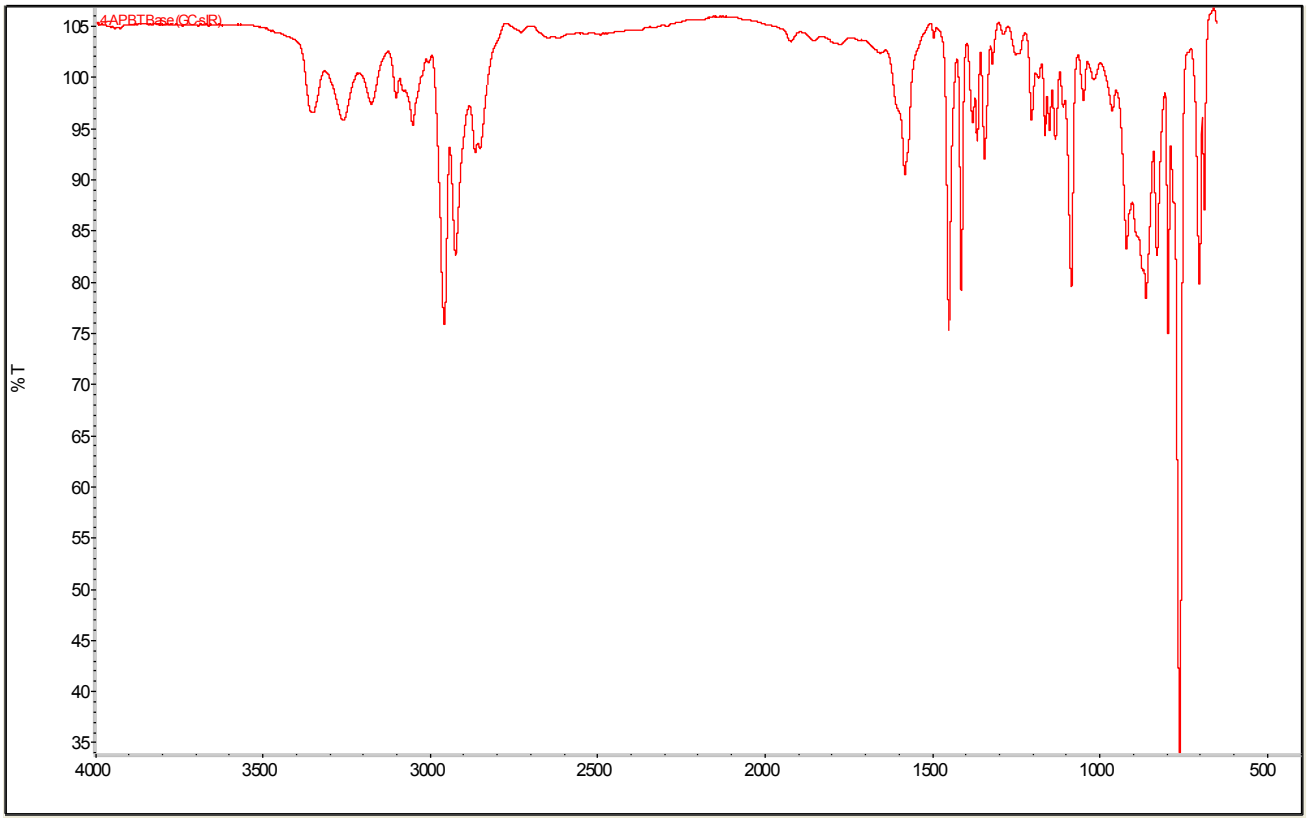


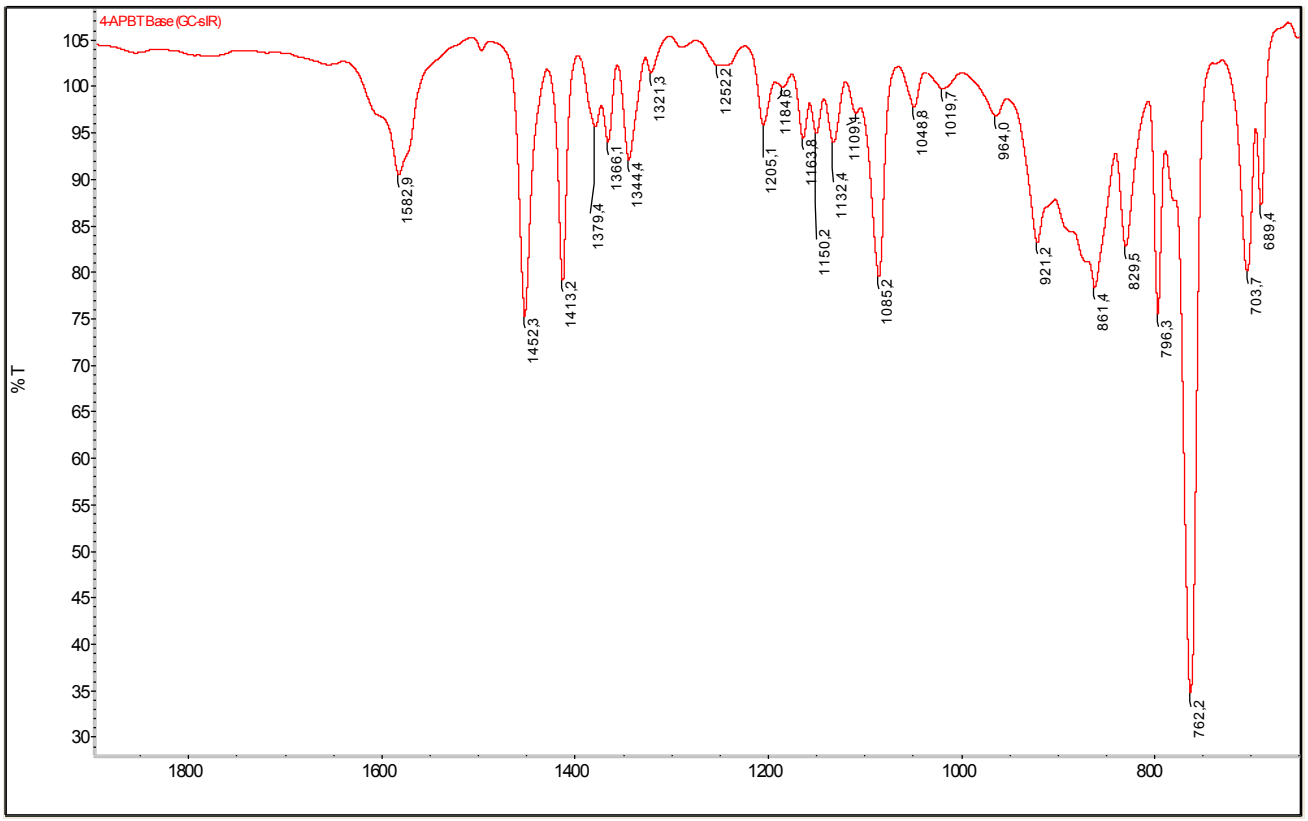
4-APBT base – ATR-IR



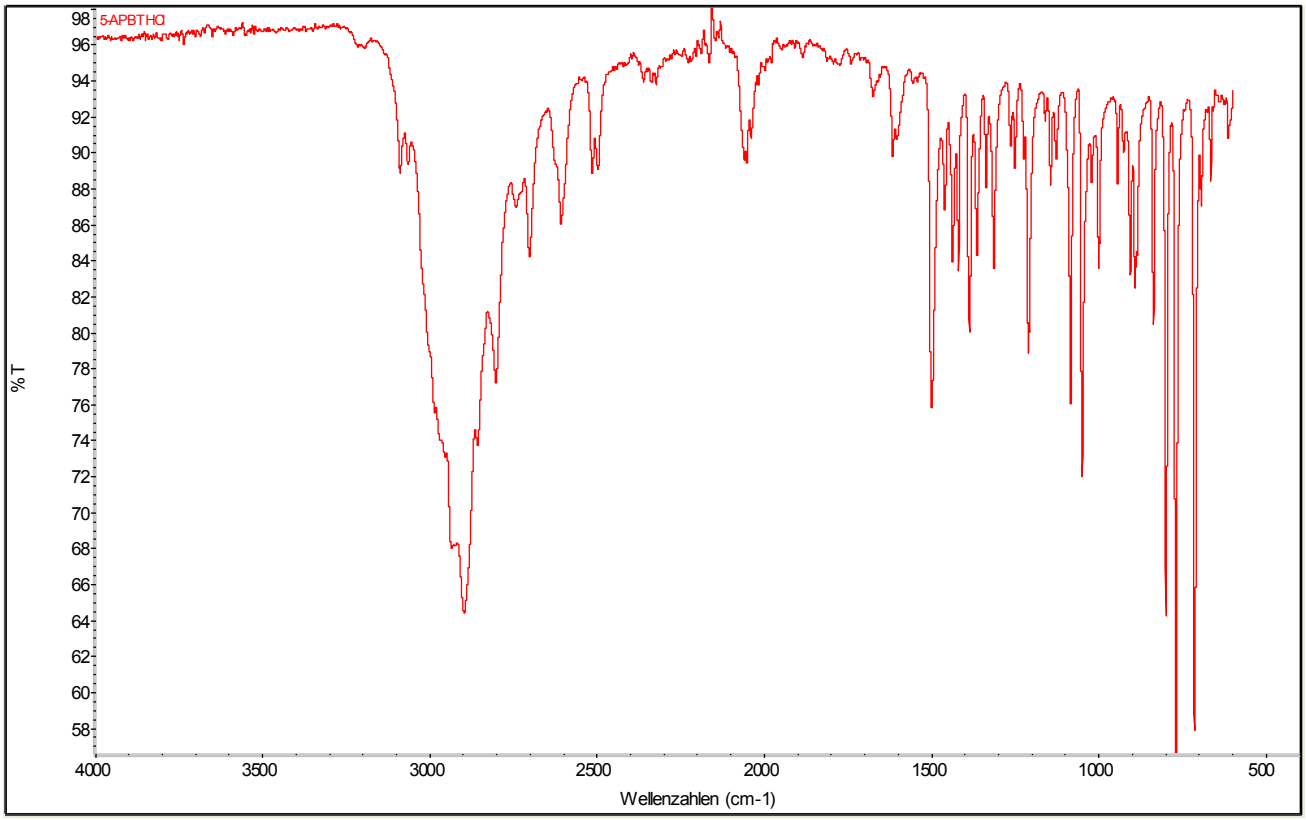


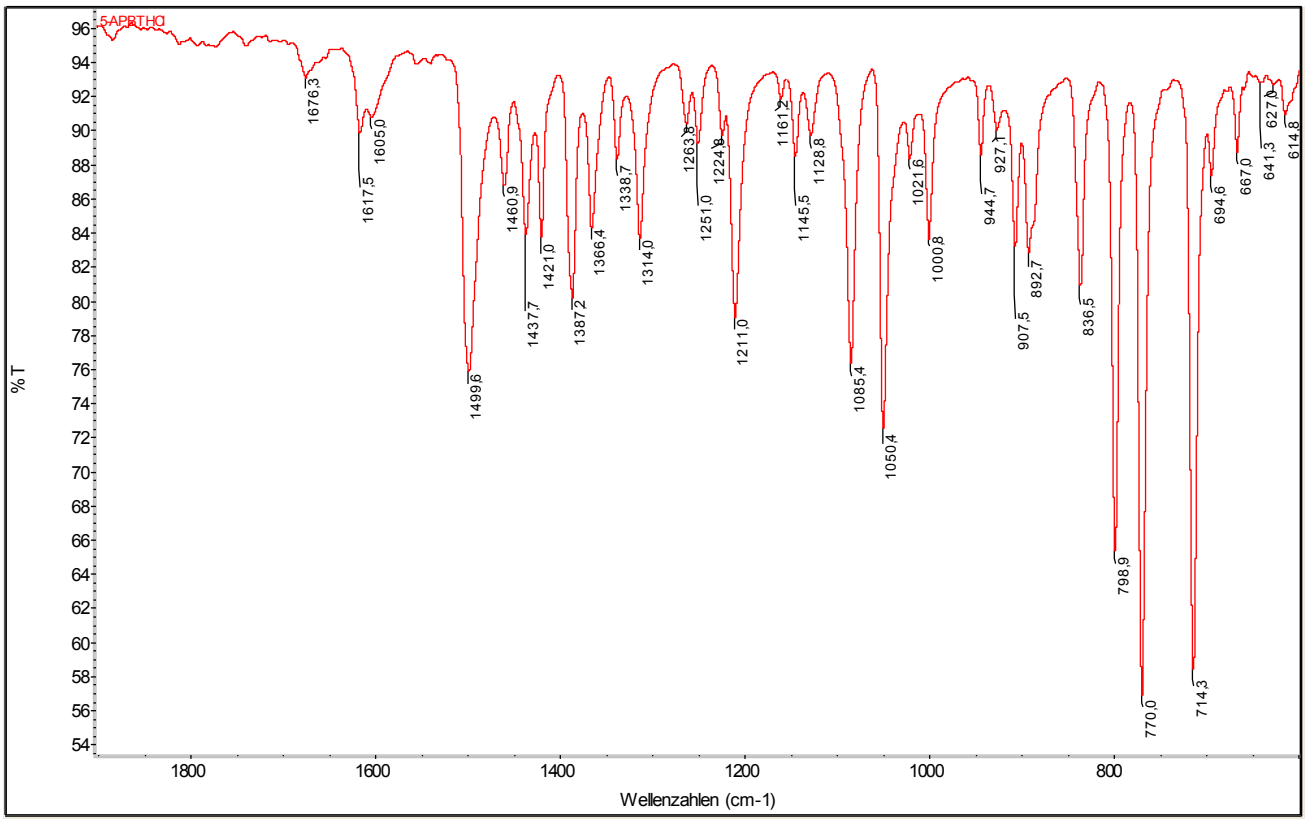
4-APBT base – GC-sIR



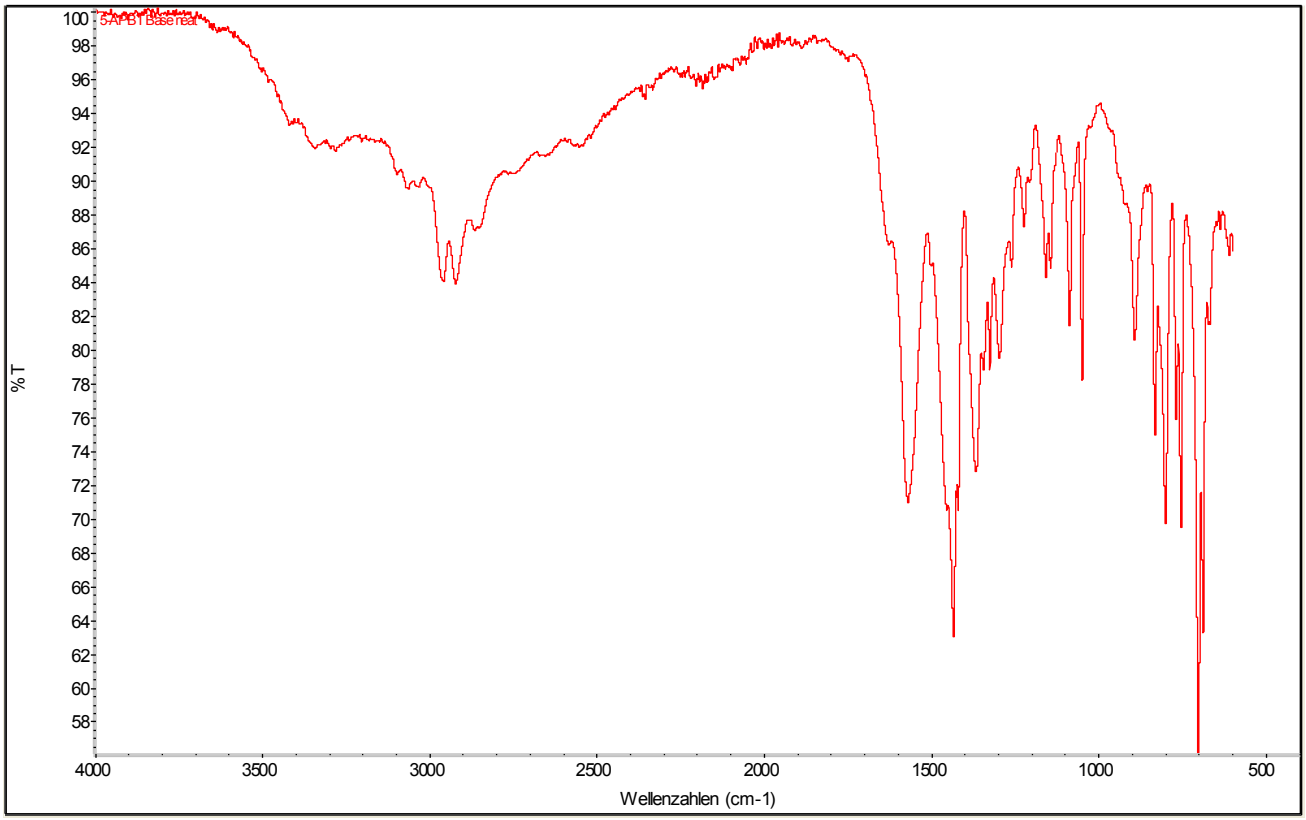


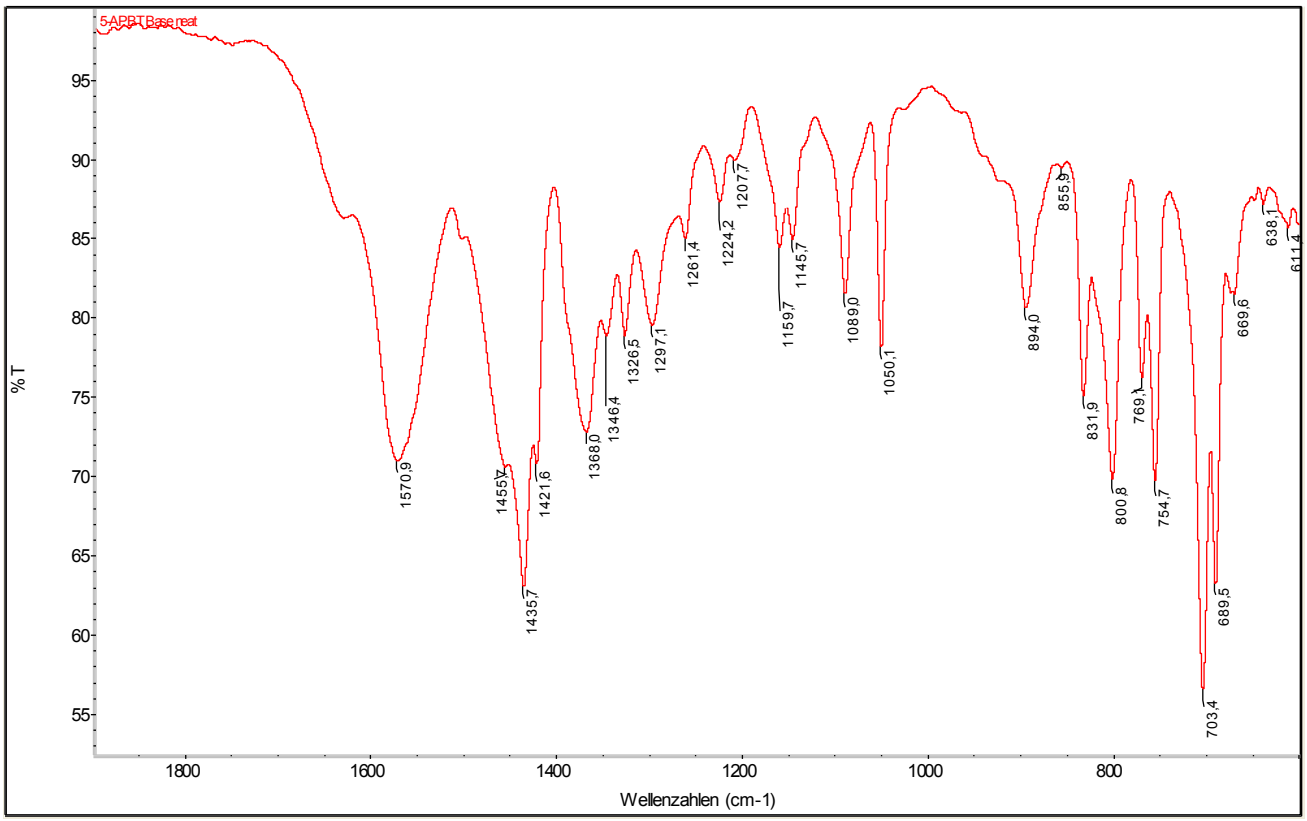
5-APBT HCl – ATR-IR



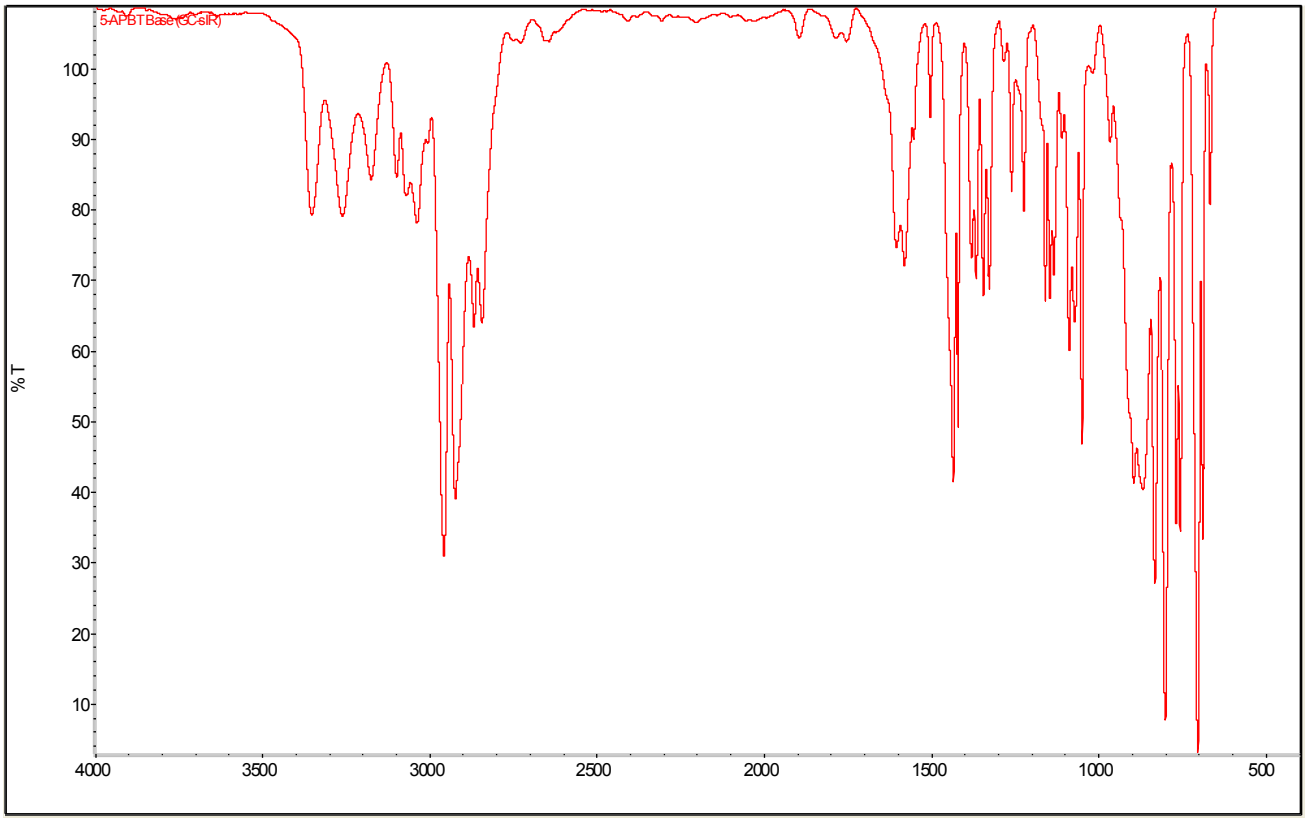


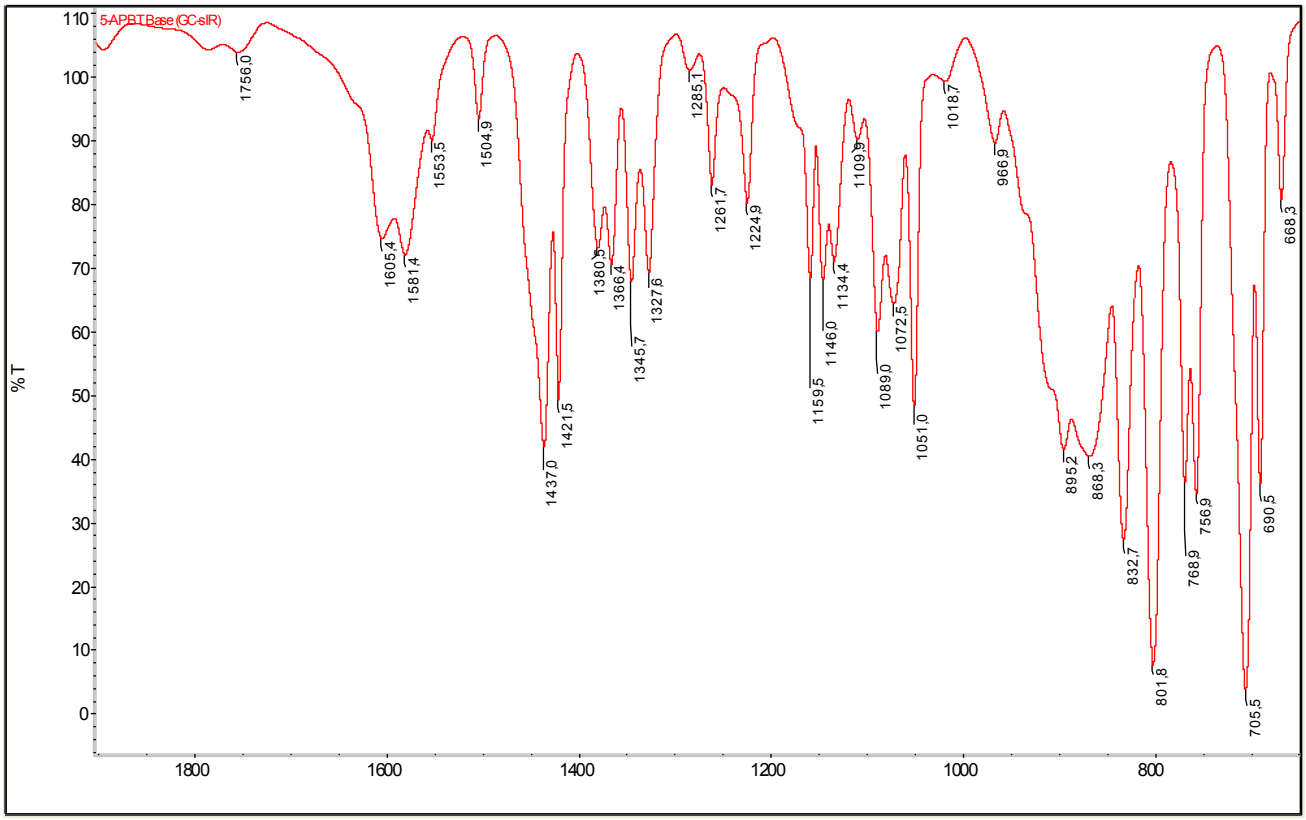
5-APBT base – ATR-IR



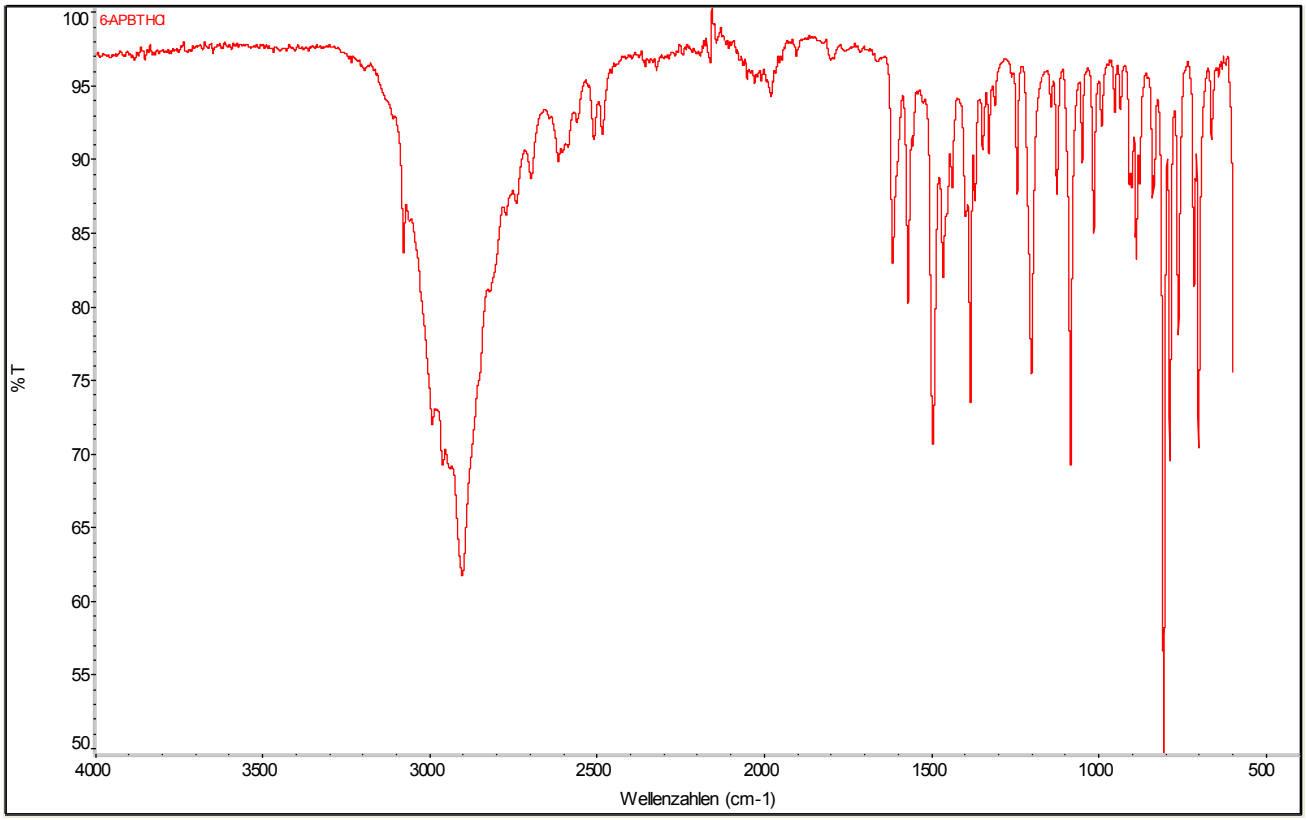


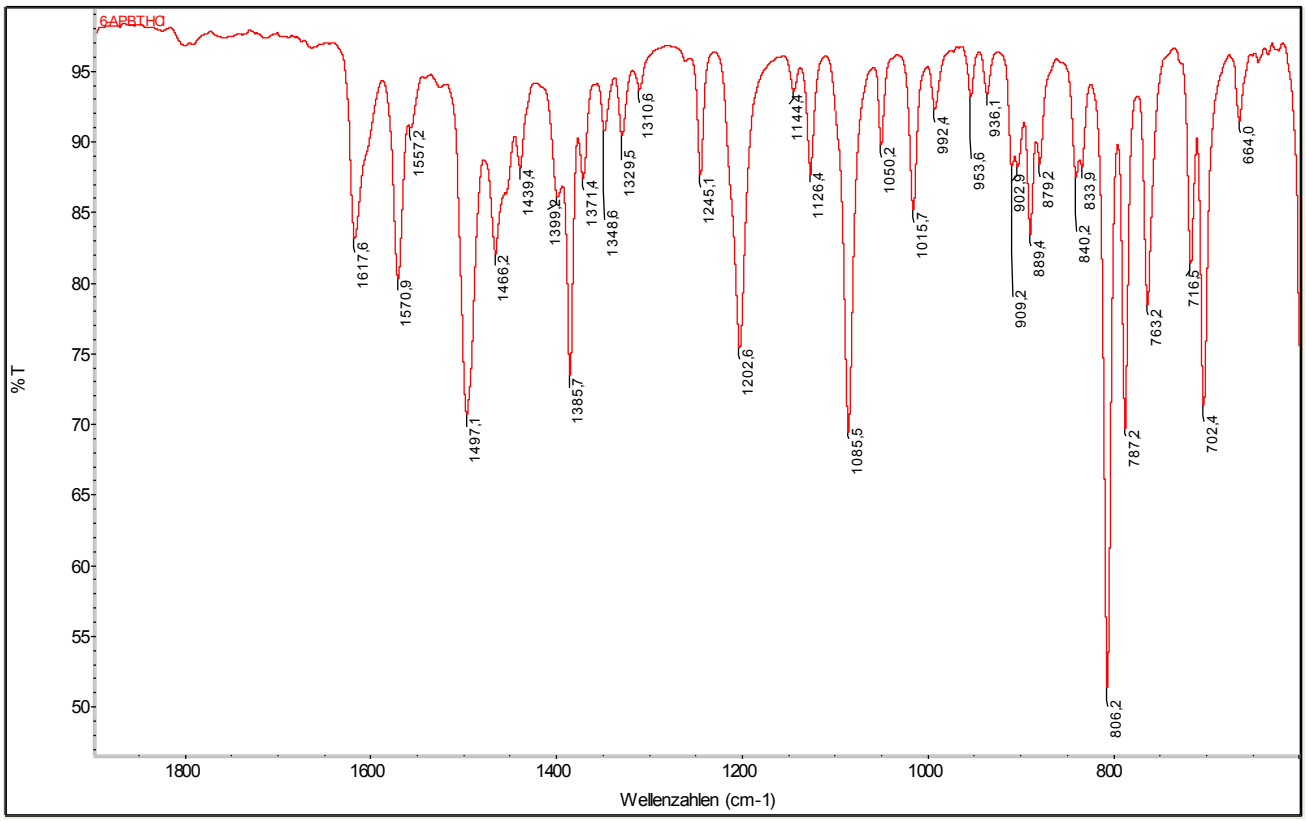
5-APBT base – GC-sIR



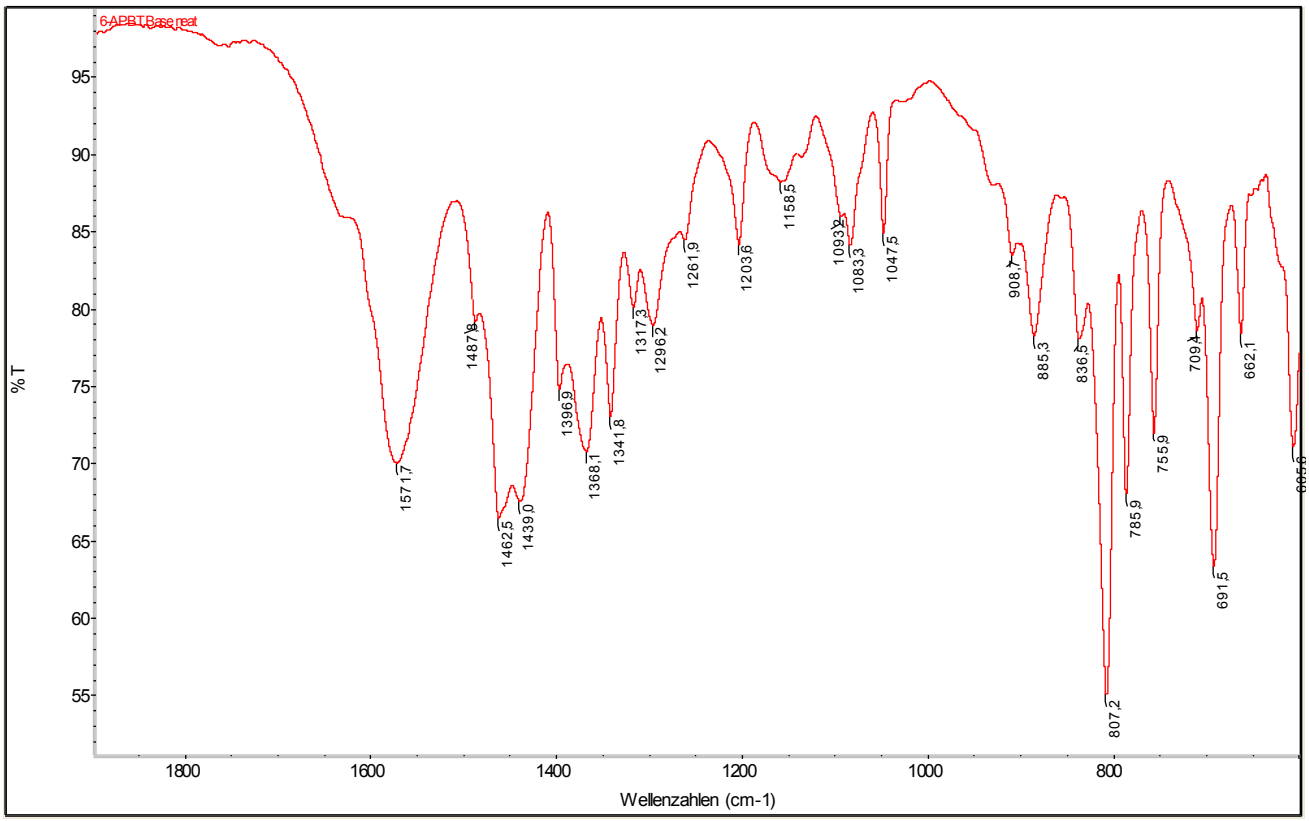


6-APBT HCl – ATR-IR

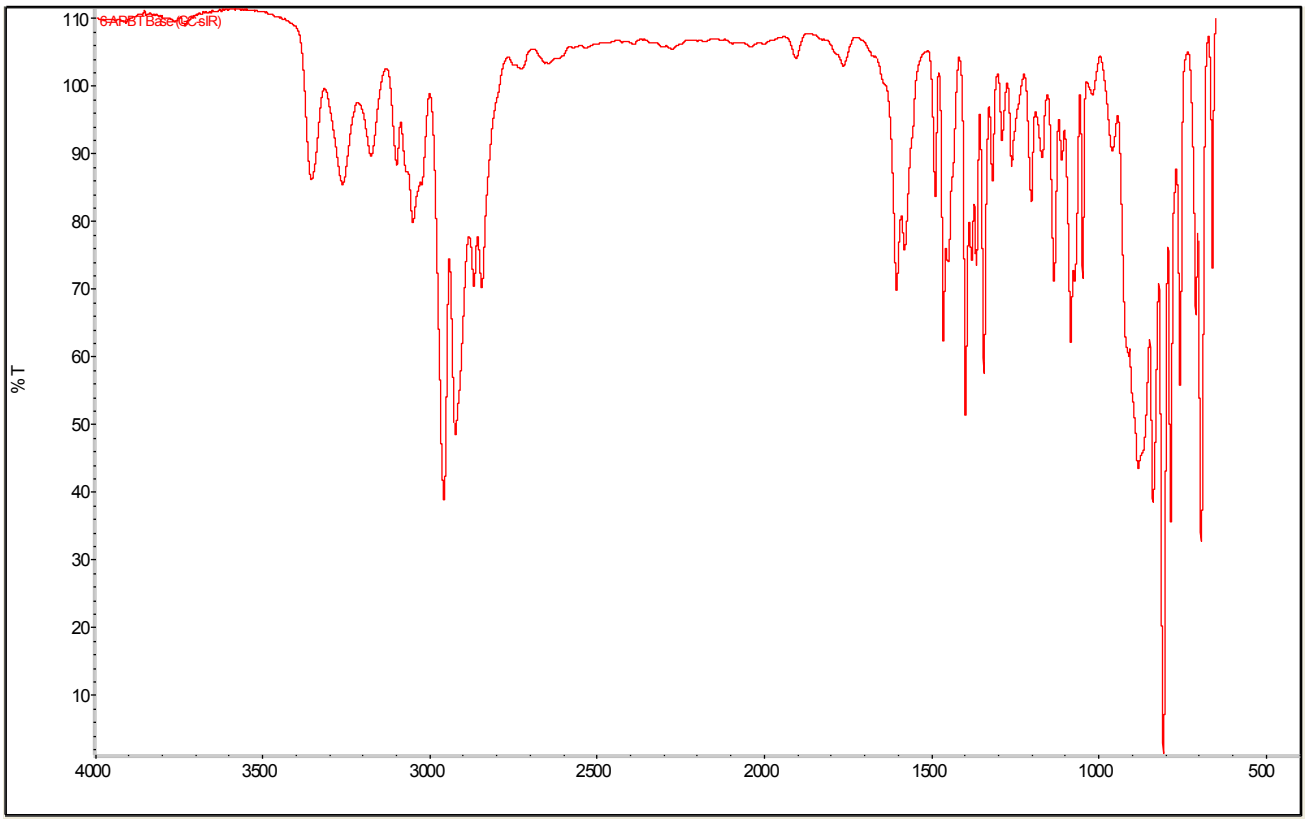


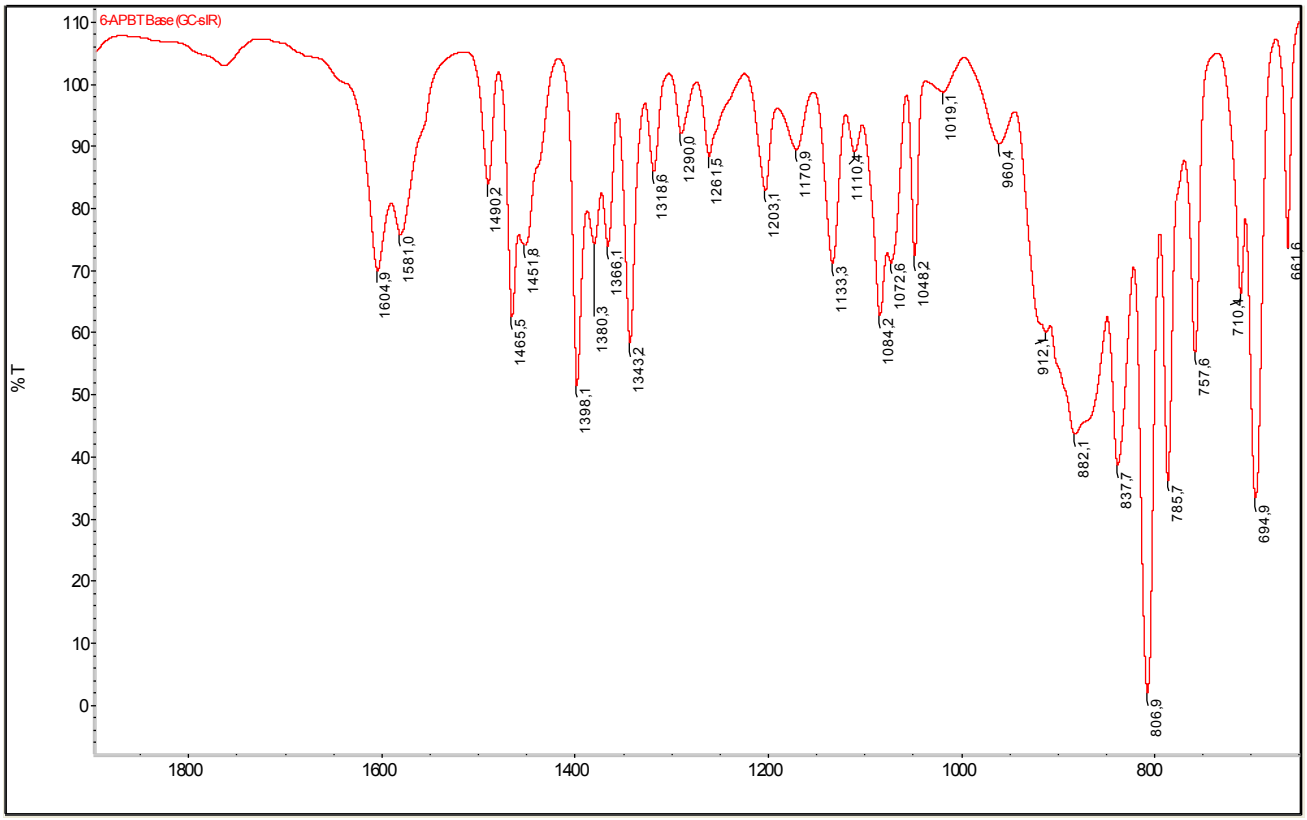


6-APBT base – ATR-IR

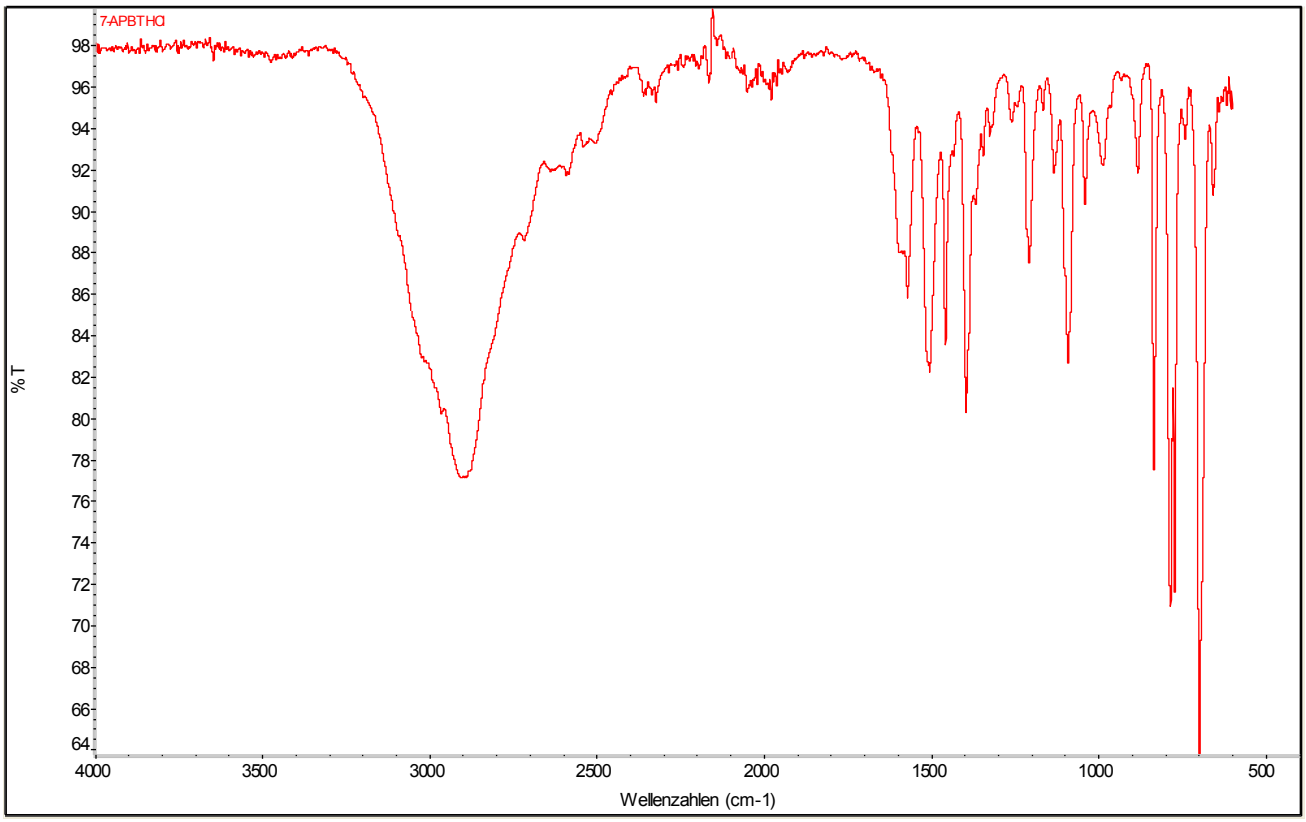


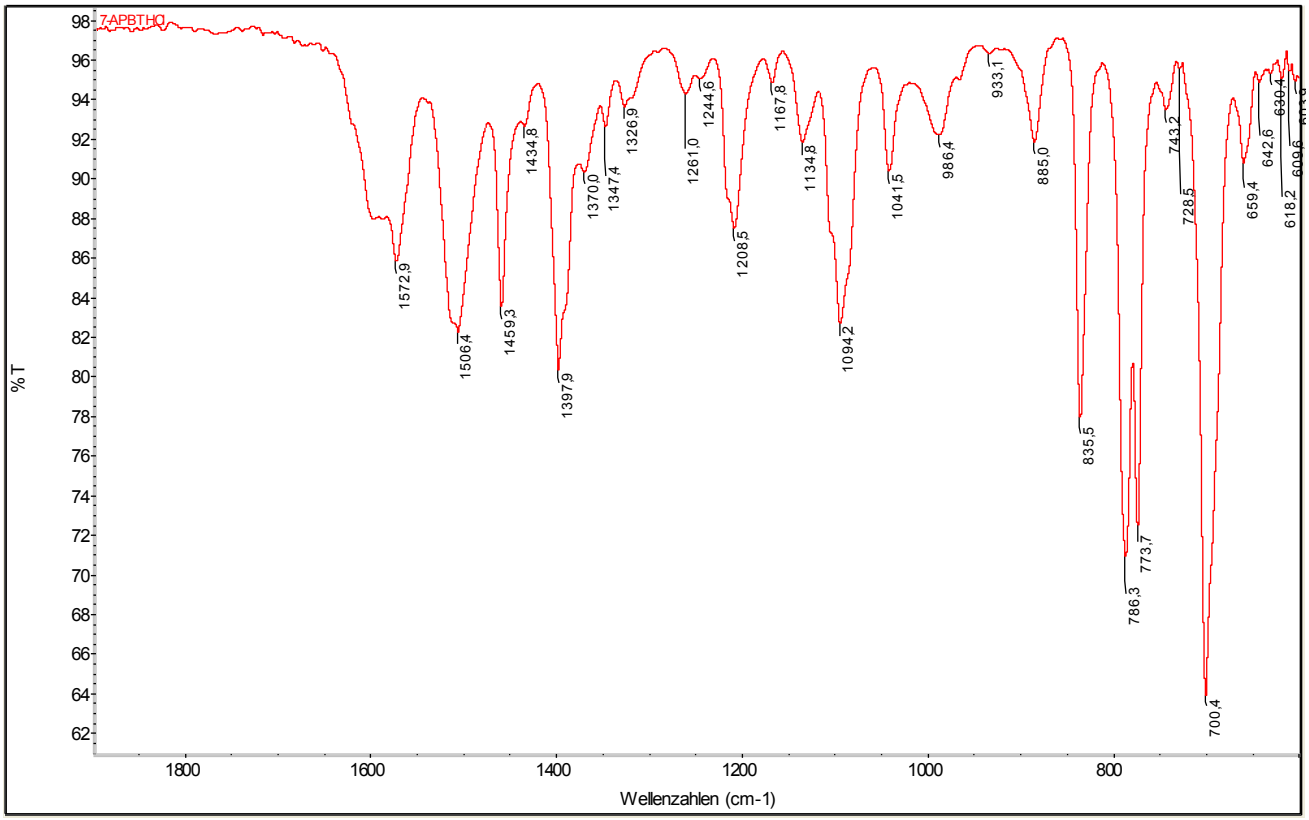
6-APBT base – GC-sIR



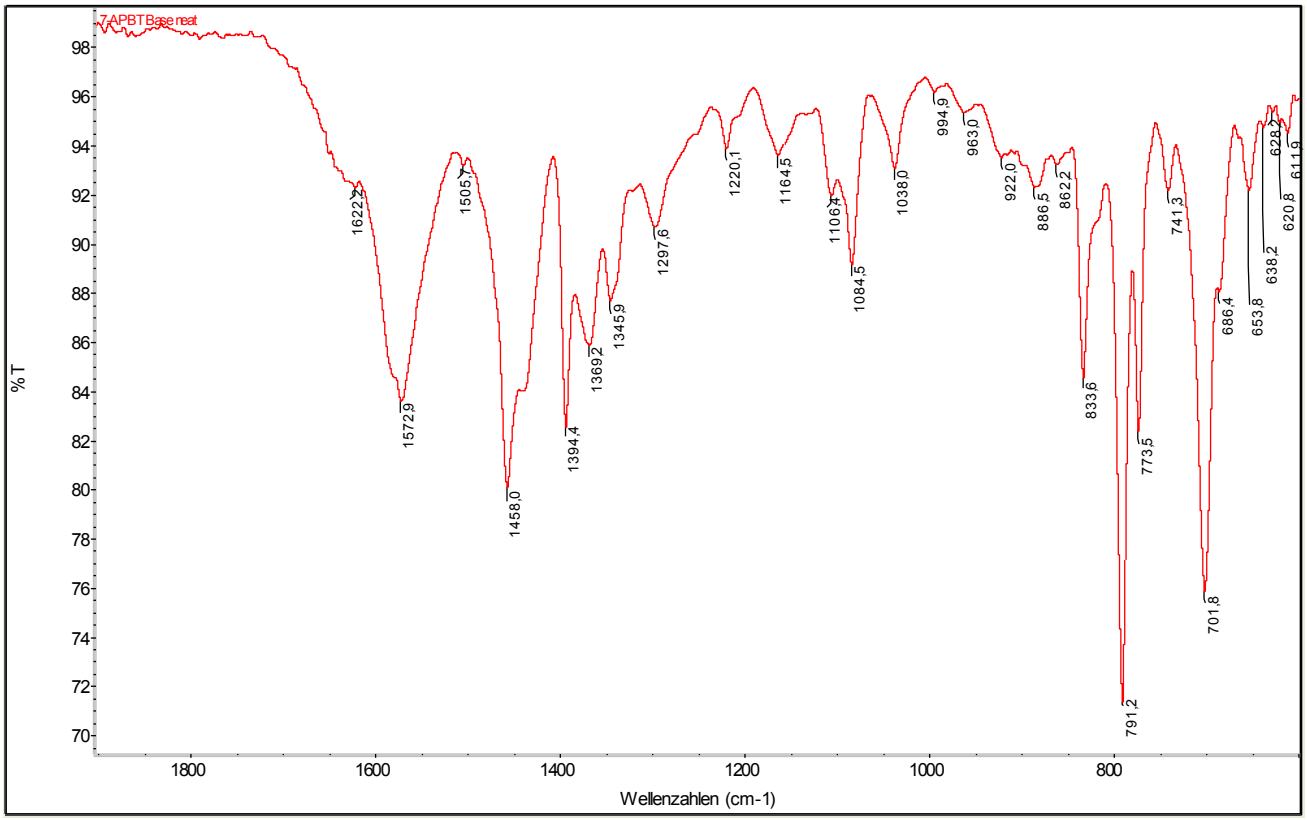


7-APBT HCl – ATR-IR

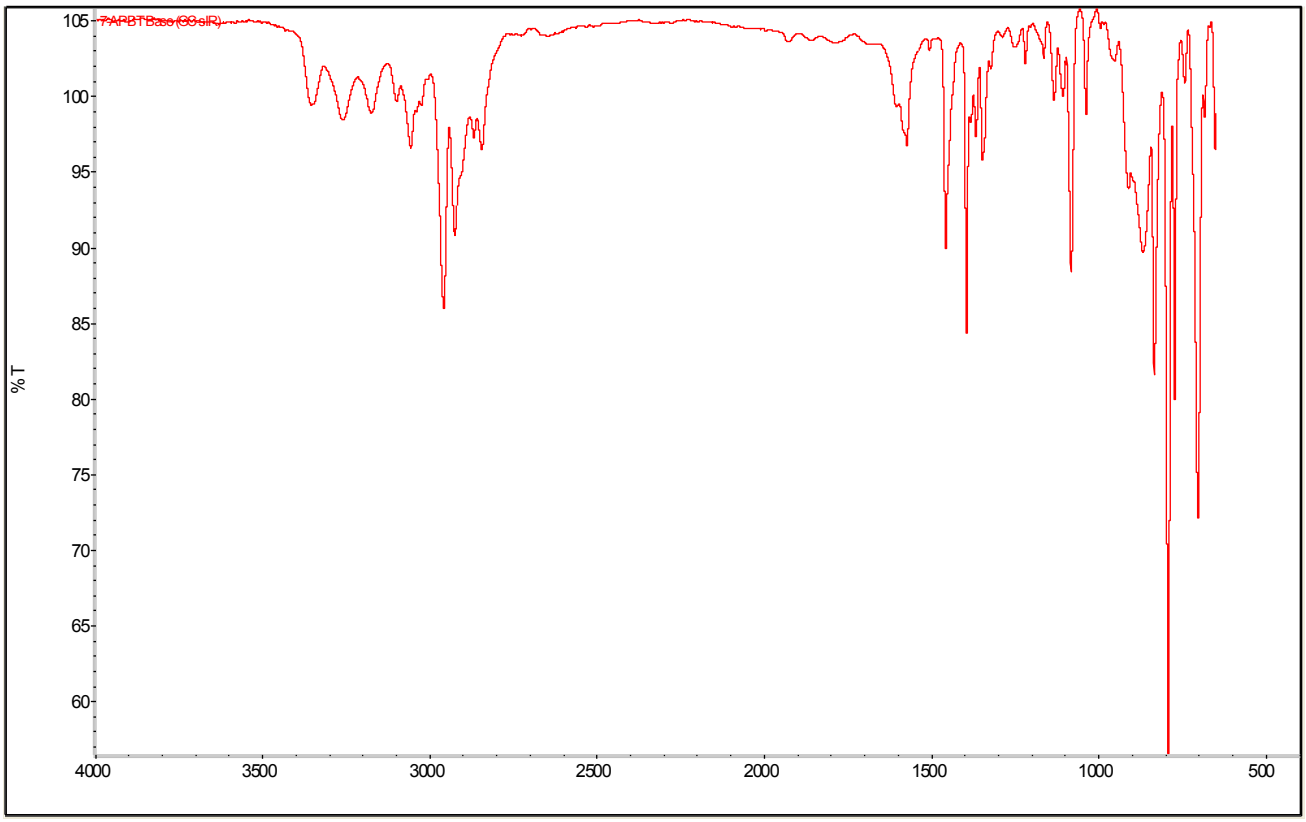


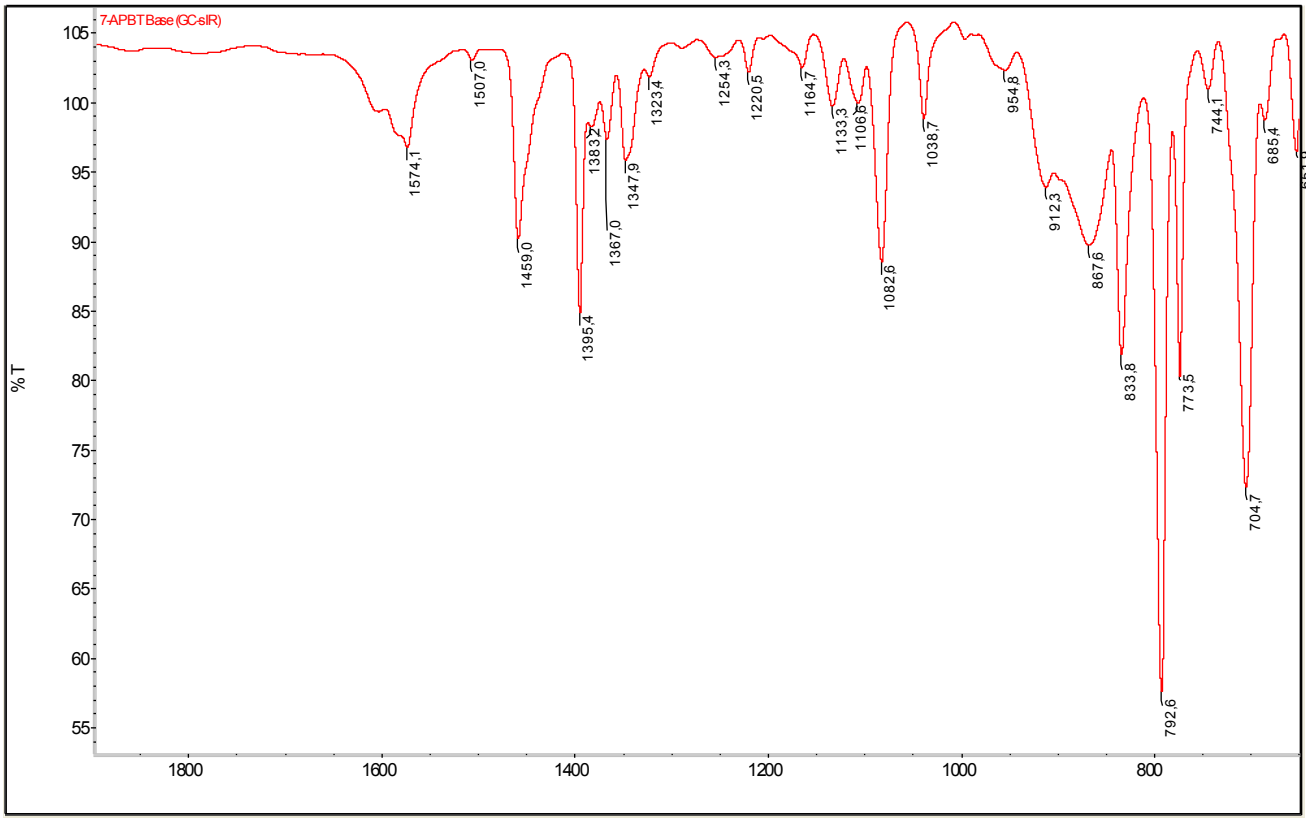


7-APBT base – ATR-IR



7-APBT base – GC-sIR





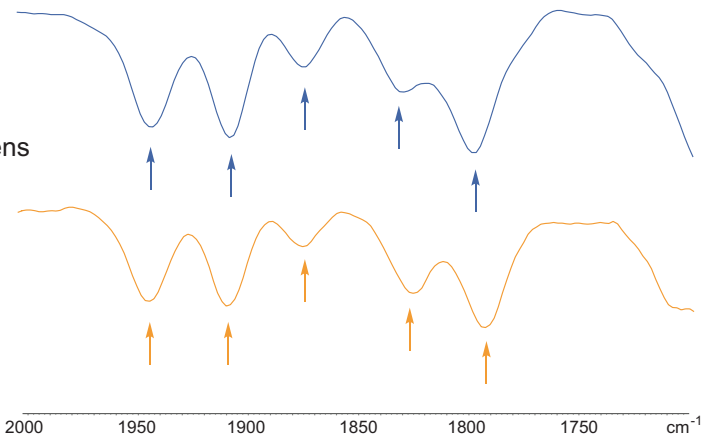
Isomer		Aromatic ring C-C stretches (1400–1500, 1585–1600 cm^{-1})	Aromatic ring C-H in-plane bends (1000–1250 cm^{-1})*	Aromatic C-H out-of-plane bends (675–900 cm^{-1})**
2	HCl (ATR-IR)	1430.5, 1456.4, 1496.9, 1575.2, 1602.0	1005.3, 1015.0, 1066.1, 1088.5, 1111.7, 1124.0, 1154.3, 1197.4, 1251.1, 1228.5, 1253.9	709.2, 726.8, 756.1, 811.3, 844.2
	Base (ATR-IR)	1435.1, 1456.6, 1569.5	1014.8, 1066.3, 1120.0, 1132.8, 1155.5, 1187.3	707.9, 725.9, 743.5, 813.2, 858.5
	Base (GC-sIR)	1437.3, 1458.3, 1538.7, 1581.6	1015.9, 1066.6, 1120.7, 1133.4, 1155.4, 1183.6, 1215.1, 1255.3	708.1, 728.1, 749.1, 812.7, 861.7
3	HCl (ATR-IR)	1425.5, 1459.0, 1515.1, 1539.1, 1568.5, 1592.7	1021.4, 1043.6, 1092.8, 1130.5, 1156.3, 1210.1, 1243.3, 1262.8	703.4, 736.9, 759.1, 767.6, 781.7, 834.1, 842.6
	Base (ATR-IR)	1426.1, 1457.6, 1576.9	1020.1, 1038.8, 1095.1, 1137.6, 1157.0, 1221.0, 1261.3	705.5, 730.3, 756.3, 766.9, 829.7
	Base (GC-sIR)	1427.4, 1459.0, 1580.3	1020.7, 1038.4, 1075.1, 1095.6, 1110.8, 1135.5, 1157.3, 1197.4, 1261.6	705.1, 733.9, 758.8, 769.0, 827.3, 874.4
4	HCl (ATR-IR)	1411.8, 1450.9, 1461.9, 1515.9, 1569.4, 1589.7	1055.1, 1091.0, 1117.7, 1129.2, 1155.4, 1167.4, 1209.1, 1239.5, 1257.9	690.8, 710.3, 758.9, 798.5, 860.3
	Base (ATR-IR)	1412.2, 1450.9, 1570.5	1053.9, 1088.0, 1164.3, 1203.3	689.3, 702.4, 758.4, 796.1, 818.1, 860.3
	Base (GC-sIR)	1413.2, 1452.3, 1582.9	1048.8, 1085.2, 1132.4, 1150.2, 1163.8, 1205.1, 1252.2	689.4, 703.7, 762.2, 796.3, 829.5, 861.4
5	HCl (ATR-IR)	1421.0, 1437.7, 1499.6, 1605.0	1000.8, 1021.6, 1050.4, 1085.4, 1128.8, 1145.5, 1211.0, 1224.8, 1251.0	694.6, 714.3, 770.0, 798.9, 836.5
	Base (ATR-IR)	1421.6, 1435.7, 1455.7, 1570.9	1050.1, 1089.0, 1145.7, 1159.7, 1224.2, 1261.4	689.5, 703.4, 754.7, 769.1, 800.8, 831.9, 894.0
	Base (GC-sIR)	1421.5, 1437.0, 1504.9, 1581.4, 1605.4	1051.0, 1072.5, 1089.0, 1109.9, 1134.4, 1146.0, 1159.5, 1224.9, 1261.7	690.5, 705.5, 756.9, 768.9, 801.8, 832.7, 868.3, 895.2
6	HCl (ATR-IR)	1466.2, 1497.1, 1570.9, 1617.6	1015.7, 1050.2, 1085.5, 1126.4, 1144.4, 1202.6, 1245.1	702.4, 716.5, 763.2, 787.2, 806.2, 840.2, 889.4
	Base (ATR-IR)	1439.0, 1462.5, 1478.8, 1571.7	1047.5, 1083.3, 1093.2, 1185.5, 1203.6, 1261.9	691.5, 755.9, 785.9, 807.2, 836.5, 885.3
	Base (GC-sIR)	1451.8, 1465.5, 1490.2, 1581.0, 1604.9	1019.1, 1048.2, 1072.6, 1084.2, 1104.4, 1133.3, 1170.9, 1203.1, 1261.5	694.9, 710.4, 757.6, 785.7, 806.9, 837.7, 882.1
7	HCl (ATR-IR)	1459.3, 1506.4, 1572.9	1041.5, 1094.2, 1134.8, 1167.8, 1208.5, 1261.0	700.4, 773.7, 786.3, 835.5, 885.0
	Base (ATR-IR)	1458.0, 1572.9	1038.0, 1084.5, 1106.4, 1164.5, 1220.1	686.4, 701.8, 773.5, 791.2, 833.6
	Base (GC-sIR)	1395.4, 1459.0, 1574.1	1038.7, 1082.6, 1106.6, 1113.3, 1164.7, 1220.5, 1254.3	704.7, 773.5, 792.6, 833.6, 867.6

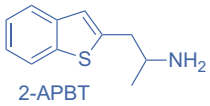
* Also C–N stretch (aliphatic amines) from 1250–1020 cm^{-1}

** Also C-S stretches in this region

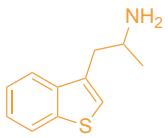
GC-sIR partial spectrum - overtone bands

Four adjacent hydrogens on benzene ring



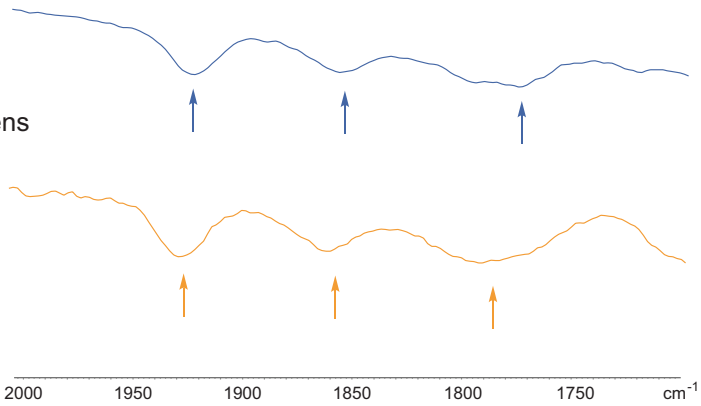


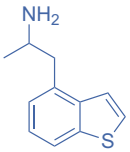
2-APBT



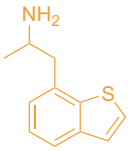
3-APBT

Three adjacent hydrogens on benzene ring



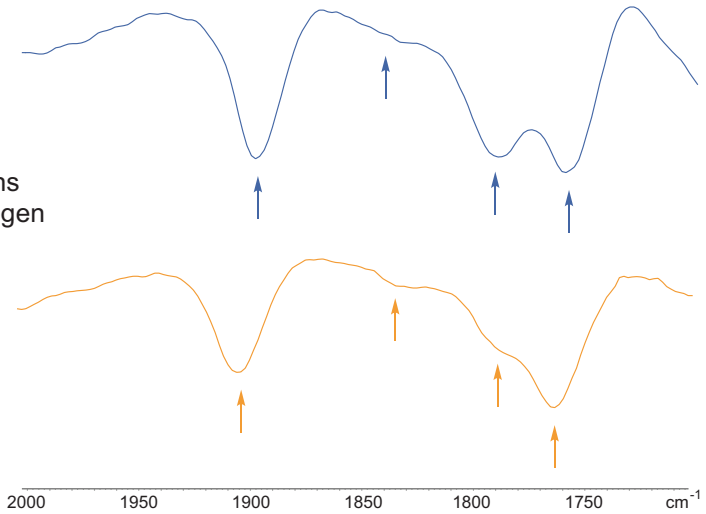


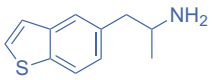
4-APBT



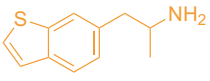
7-APBT

Two adjacent hydrogens and one isolated hydrogen on benzene ring



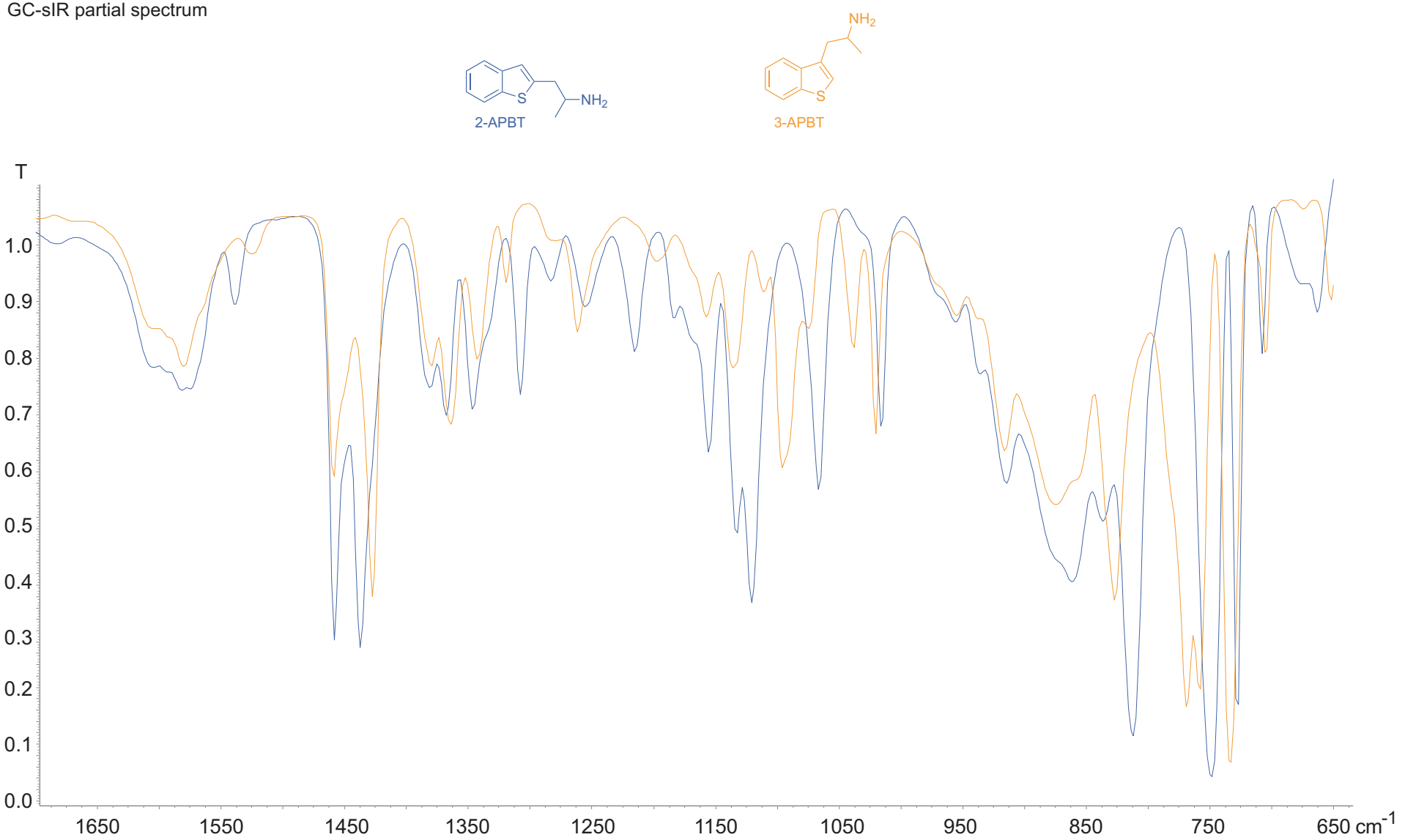


5-APBT

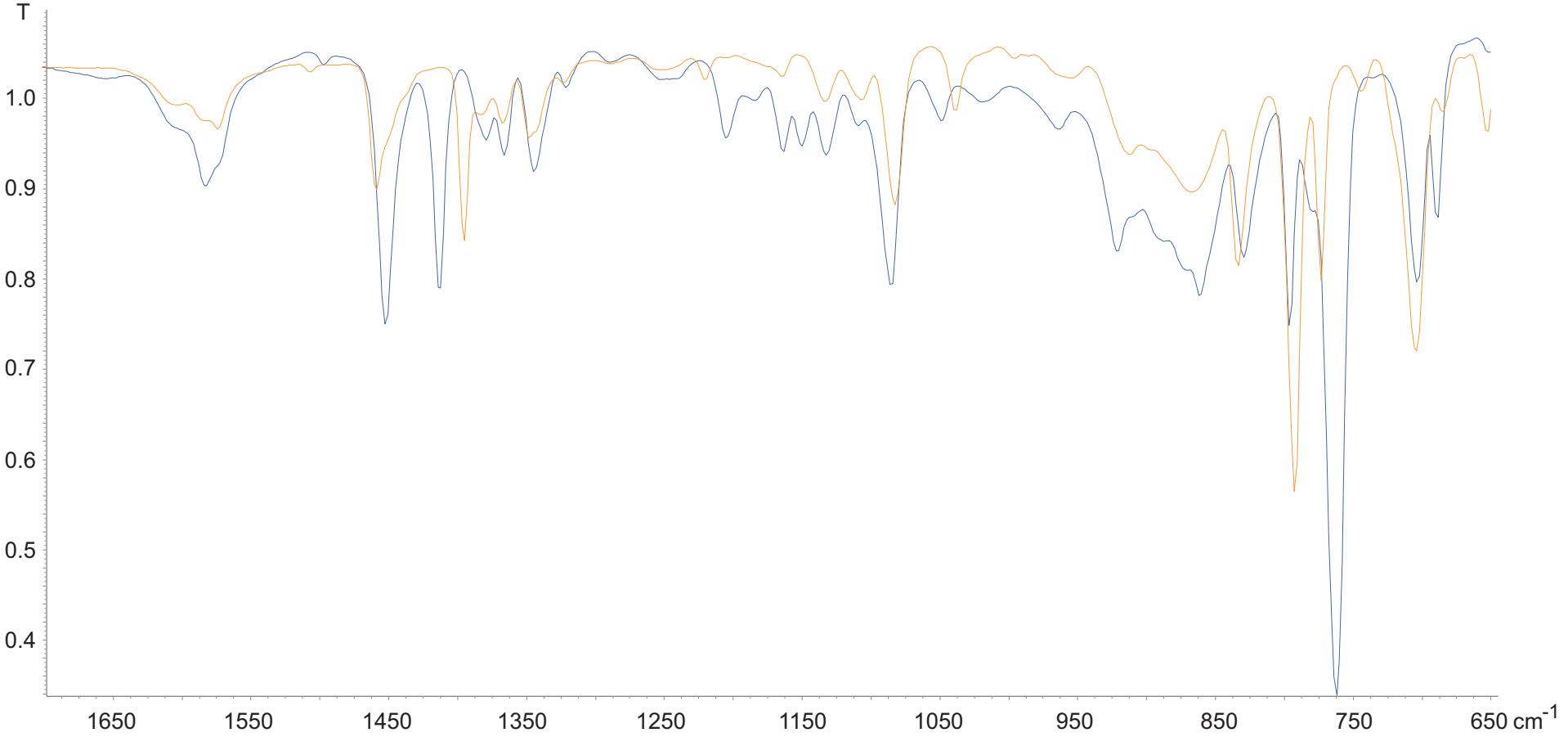


6-APBT

GC-sIR partial spectrum



GC-sIR partial spectrum



GC-sIR partial spectrum