

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

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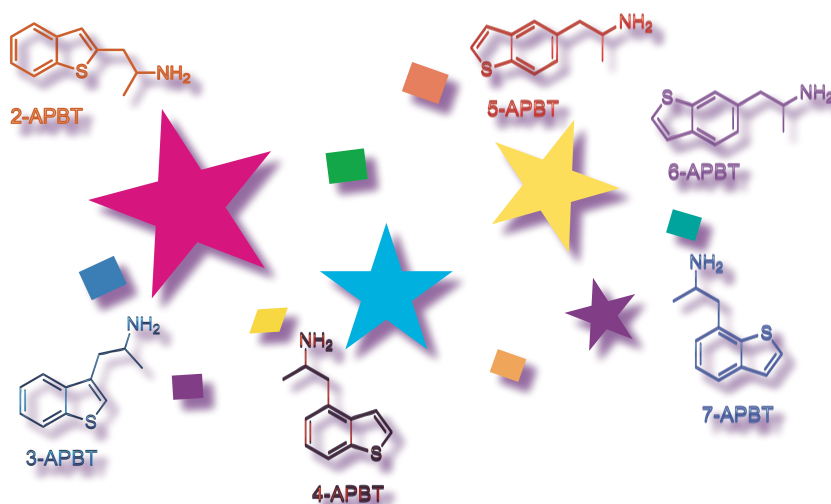
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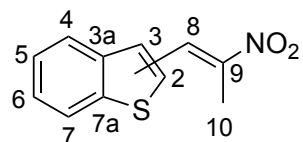
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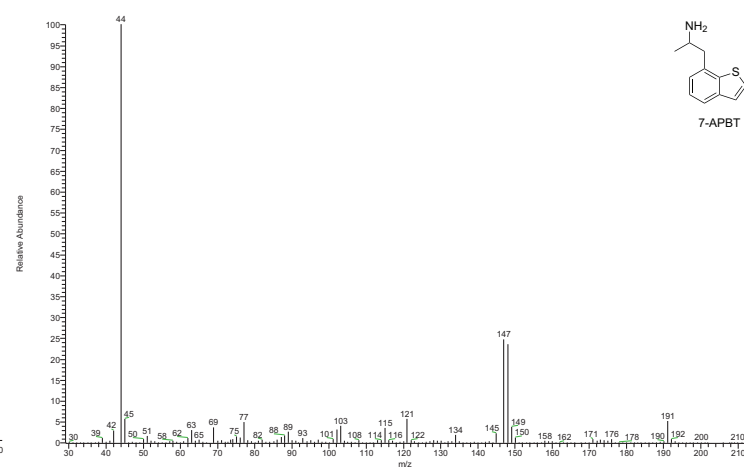
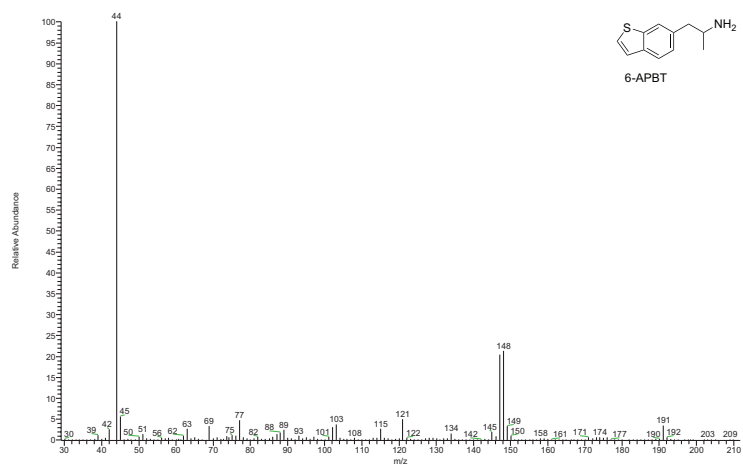
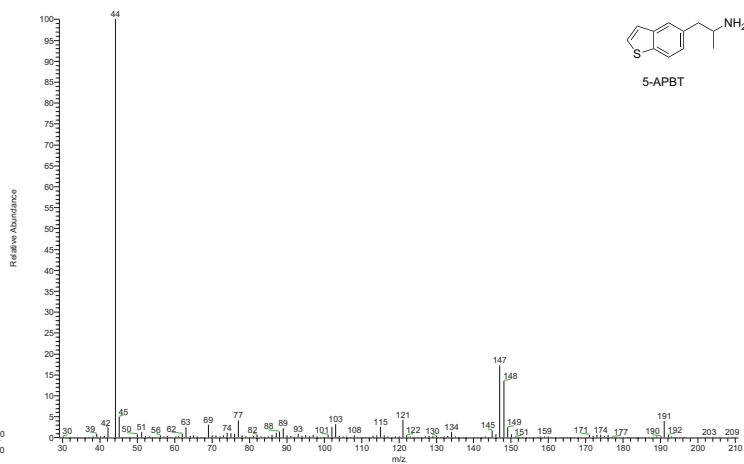
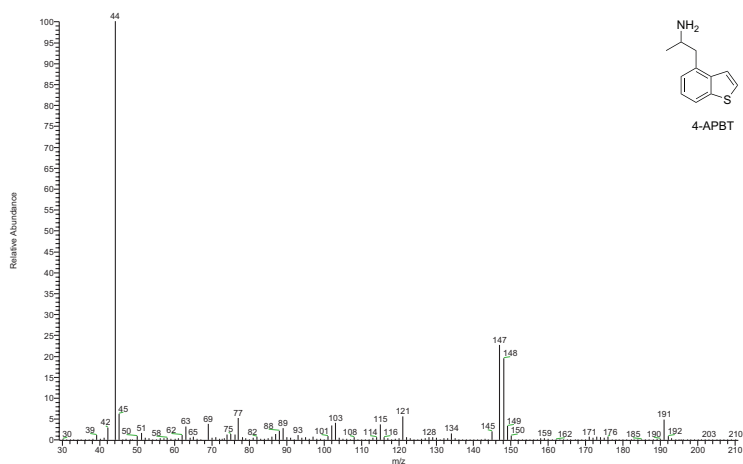
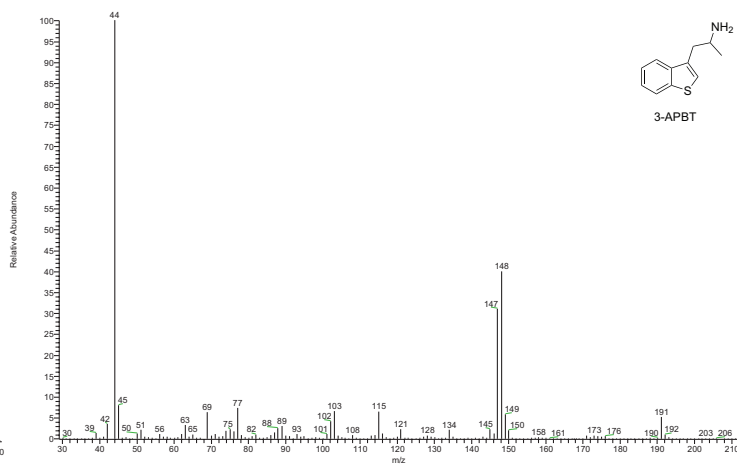
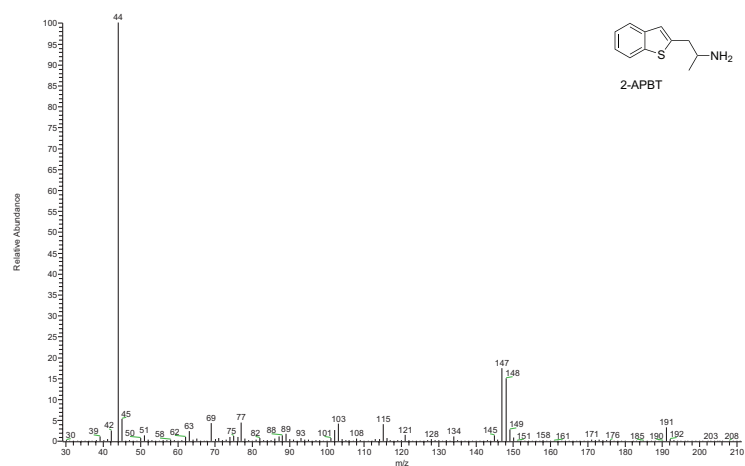


Isomer	2		3		5		6	
Position	¹ H	¹³ C	¹ H	¹³ C	¹ H	¹³ C	¹ H	¹³ C
2	-	134.90	7.70 (s)	129.03	7.56 (d, <i>J</i> = 5.4 Hz)	128.06	7.59 (d, <i>J</i> = 5.4 Hz)	129.28
3	7.68 (s)	132.07	-	128.23	7.42 (d, <i>J</i> = 5.4 Hz)	124.00	7.38 (d, <i>J</i> = 5.4 Hz)	123.82
3a	-	138.62 or 141.94	-	138.30	-	139.92	-	140.23
4	7.91–7.86 (m)	124.75	7.91 (dist. d, <i>J</i> = 7.8 Hz)	121.77	7.91 (s)	125.46 or 125.48	7.88 (d, <i>J</i> = 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, <i>J</i> = 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, <i>J</i> = 8.4, 1.6 Hz)	125.46 or 125.48	-	128.43
7	7.91–7.86 (m)	122.35	7.94 (dist. d, <i>J</i> = 7.8 Hz)	122.92	7.97 (d, <i>J</i> = 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, <i>J</i> = 0.4 Hz)	14.28	2.57 (d, <i>J</i> = 0.8 Hz)	14.70	2.54 (d, <i>J</i> = 1.0 Hz)	14.19	2.53 (d, <i>J</i> = 0.9 Hz)	14.26

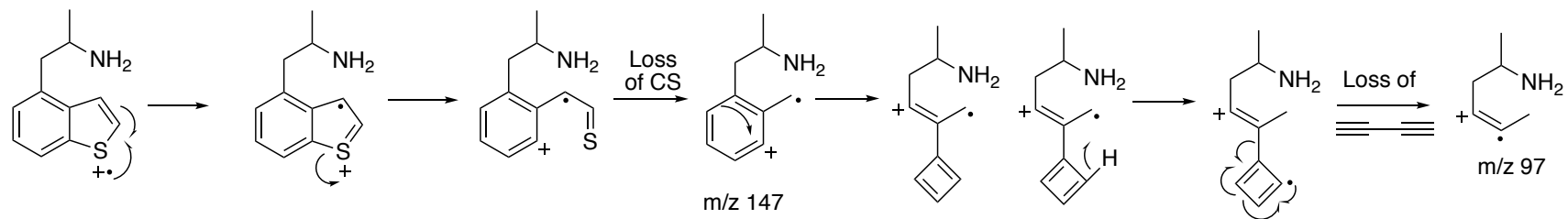
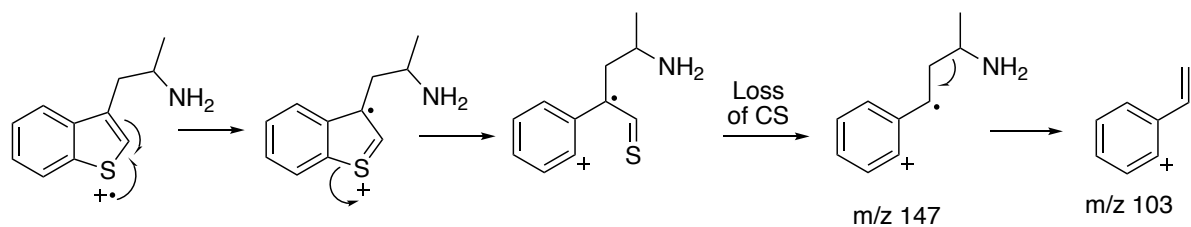
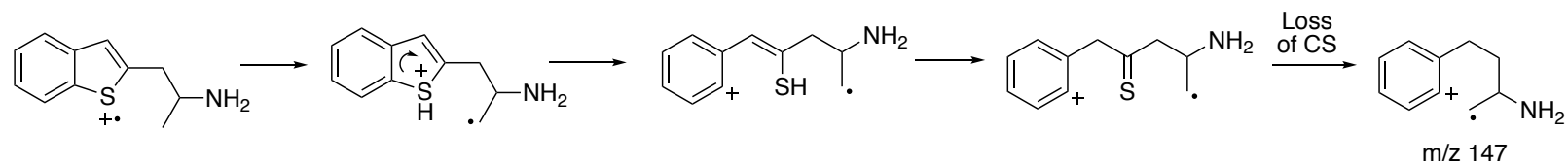
Table 1. NMR data for nitrostyrene intermediates (CDCl₃, 600/150 MHz).

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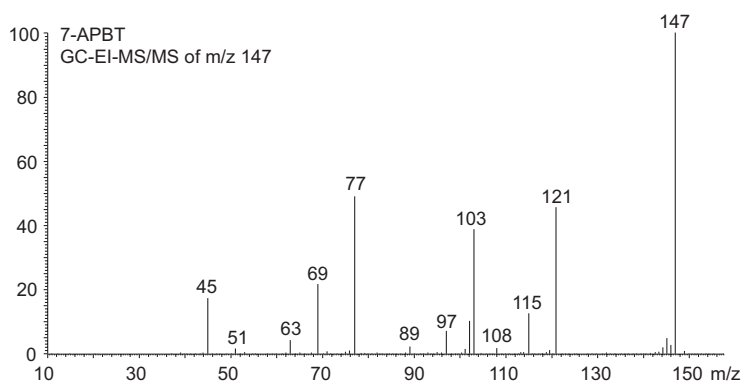
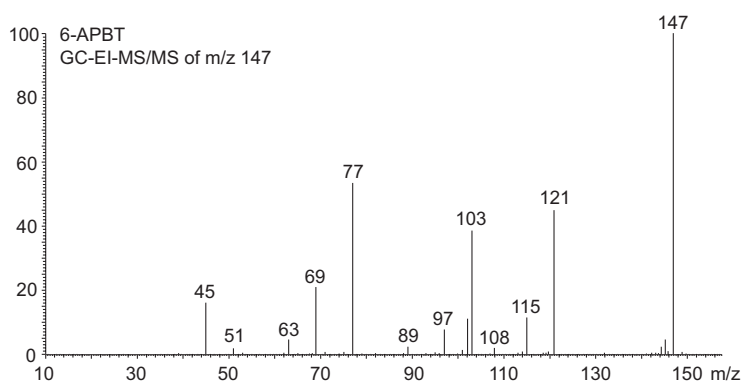
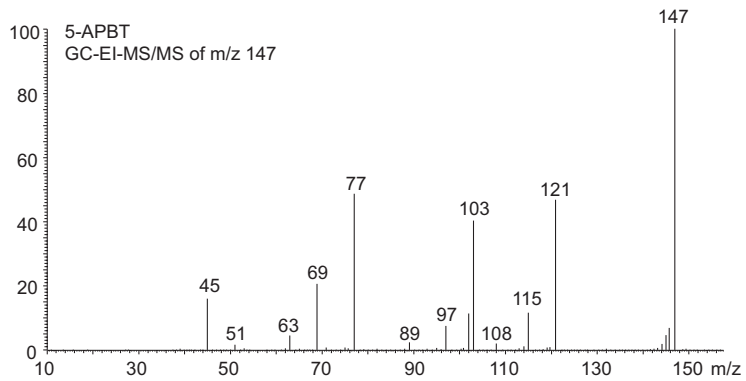
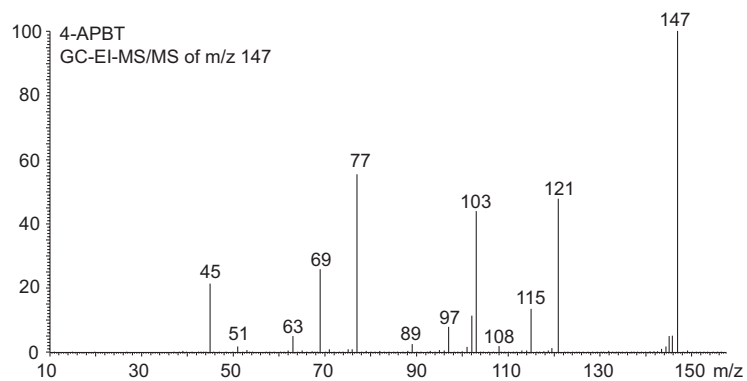
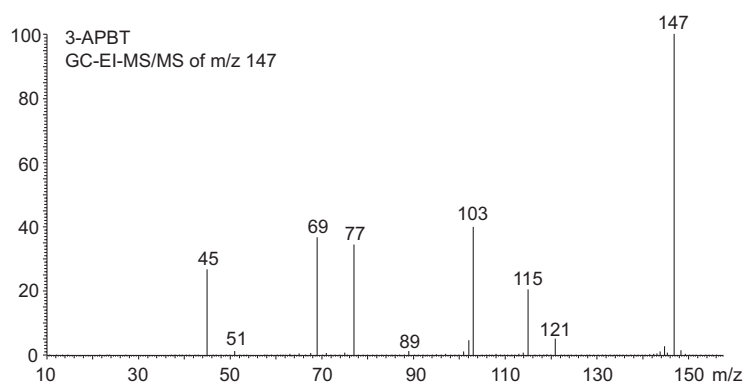
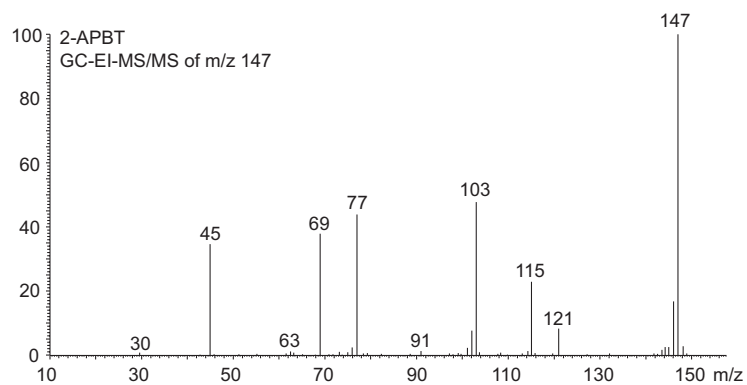
Electron ionization mass spectra of APBT isomers



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



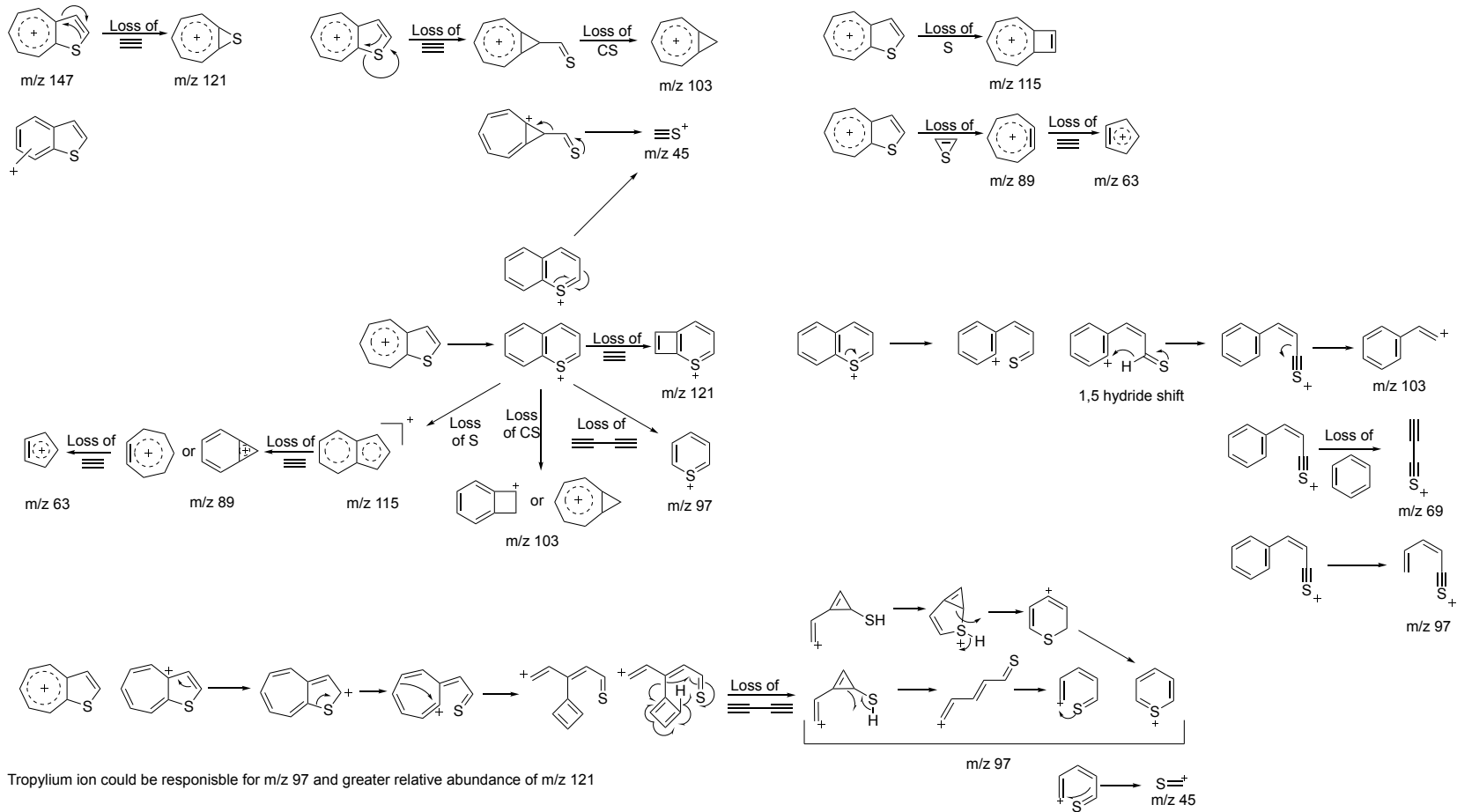
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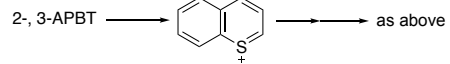
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EI-MS/MS of m/z 147

4-, 5-, 6-, 7-APBT

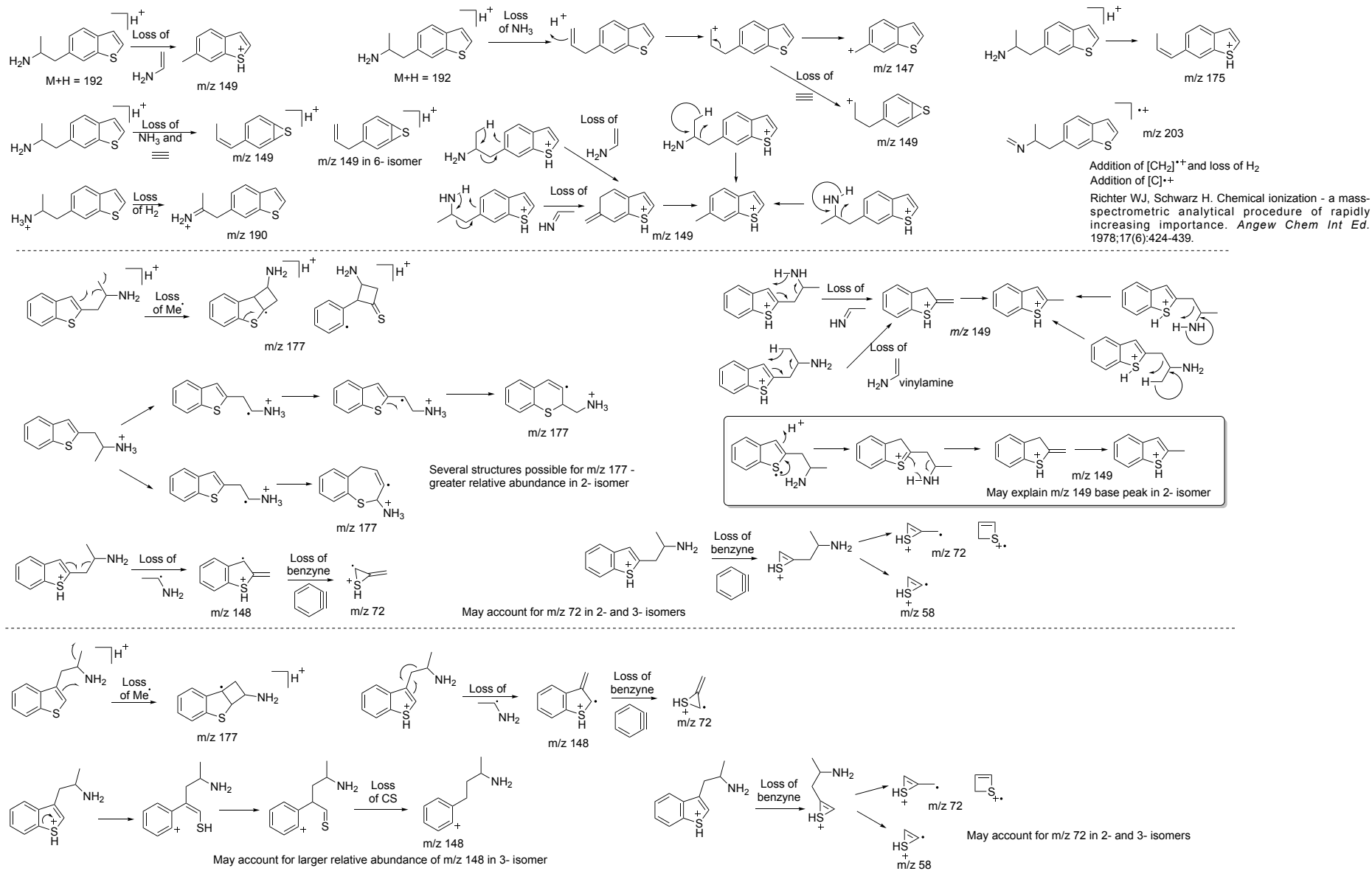


Tropylium ion could be responsible for m/z 97 and greater relative abundance of m/z 121

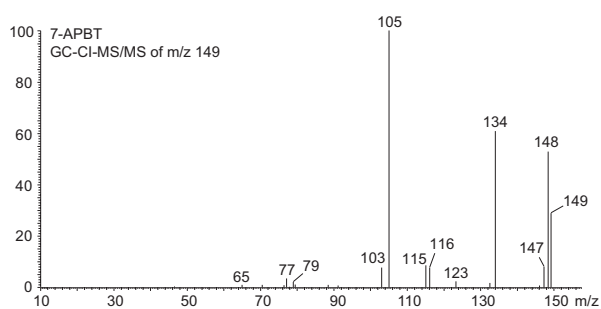
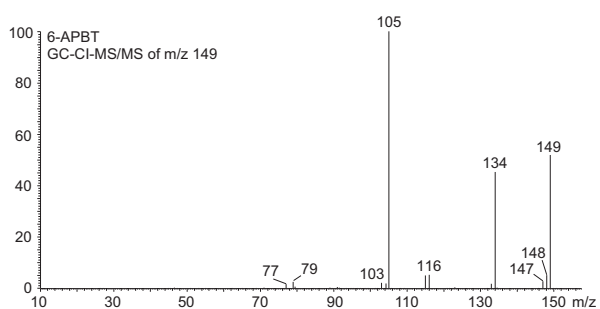
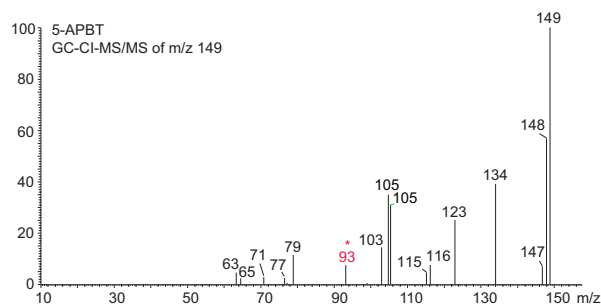
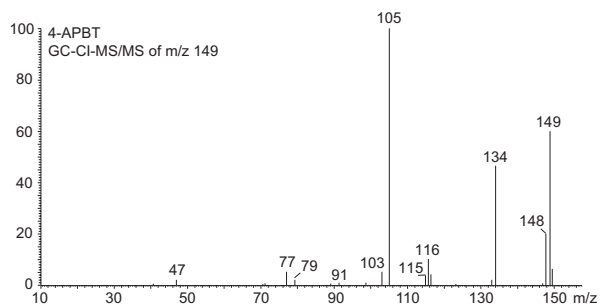
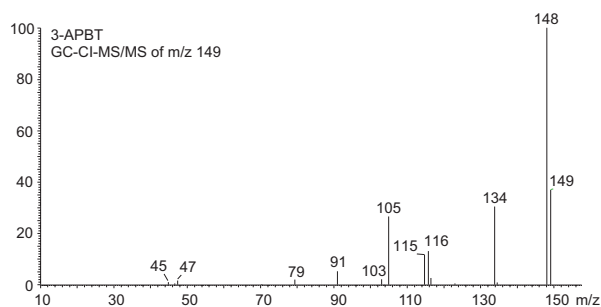
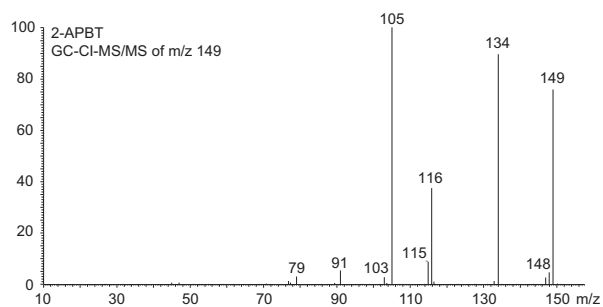


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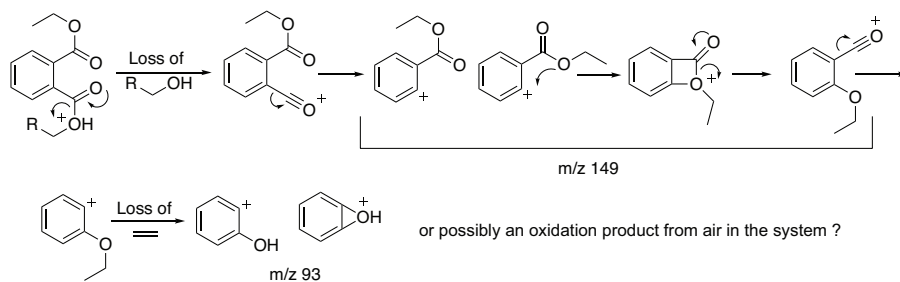
CI-MS analysis



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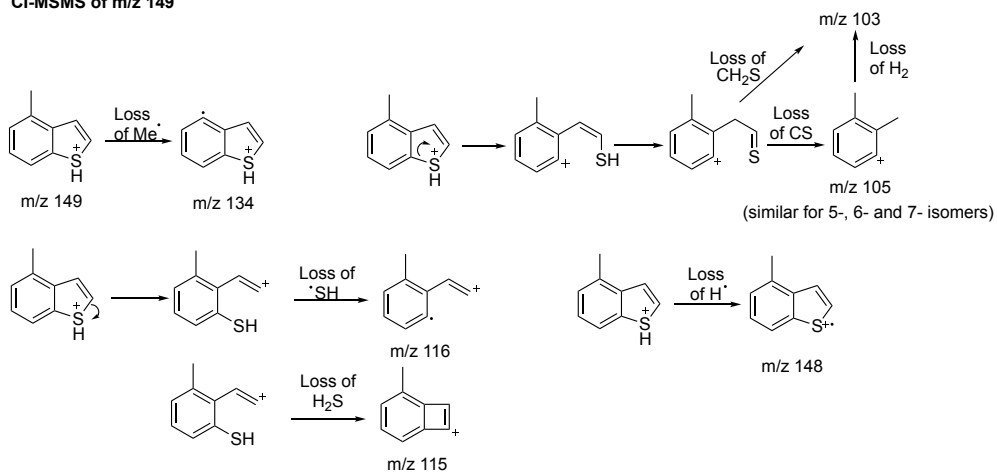


* m/z 93: possibly from an ethyl phthalate?

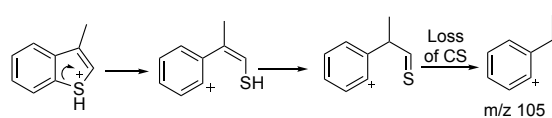
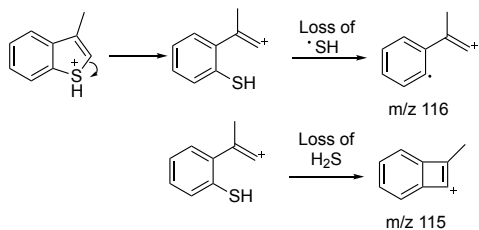
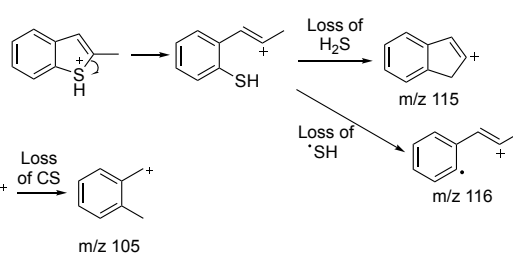
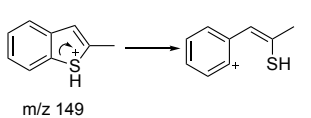
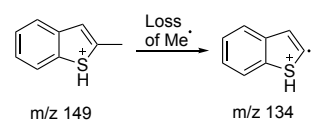
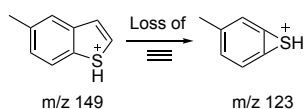


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CI-MSMS of m/z 149

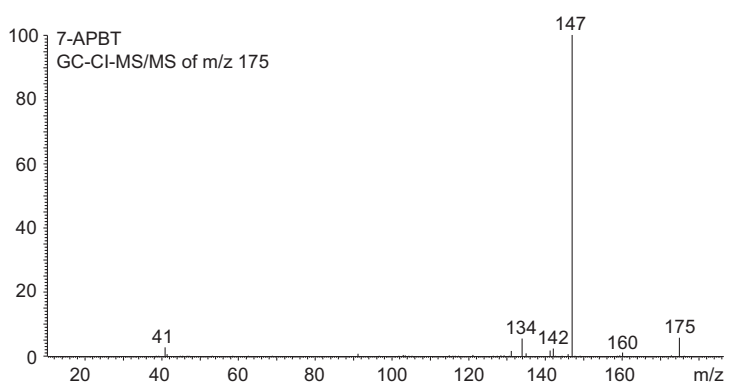
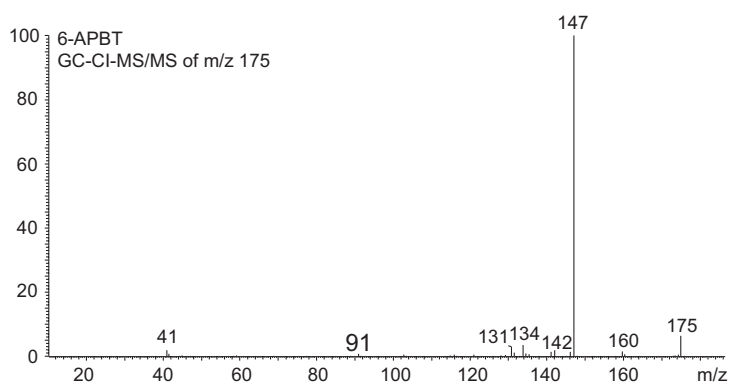
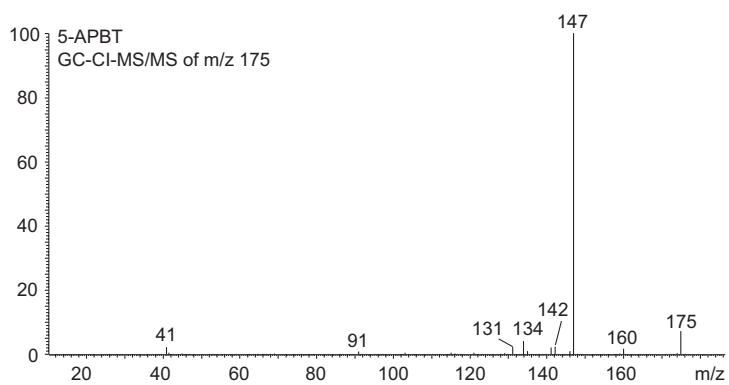
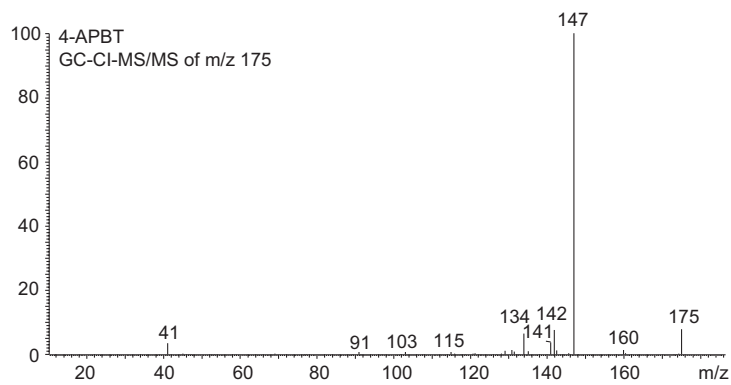
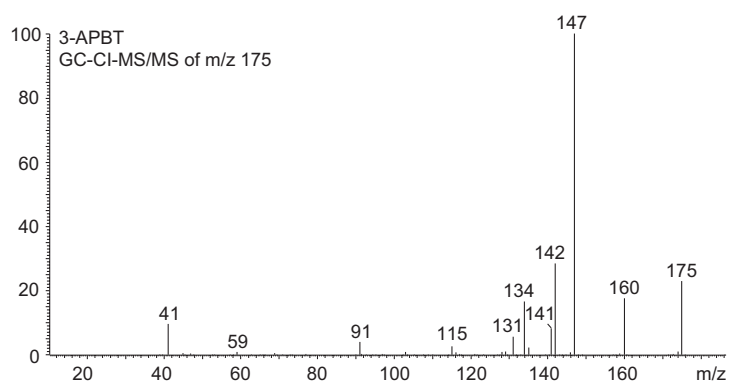
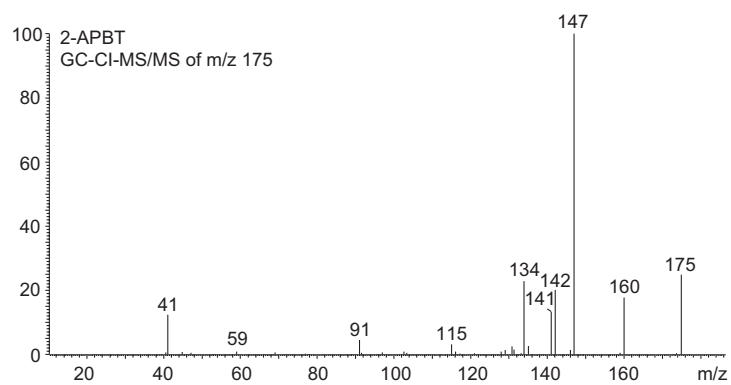


5-APBT

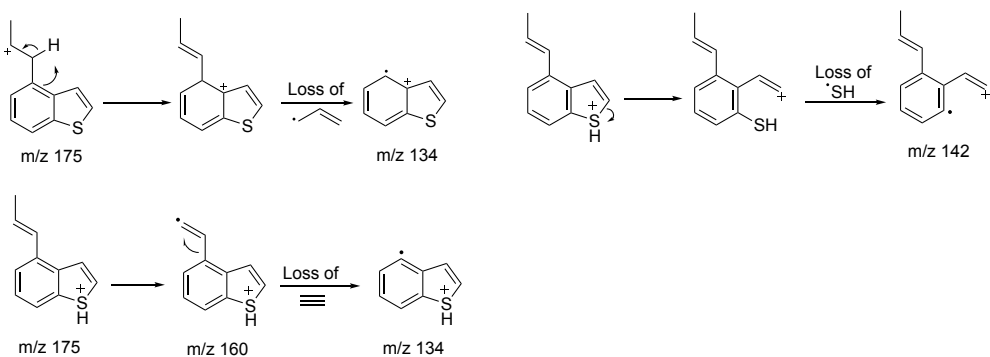
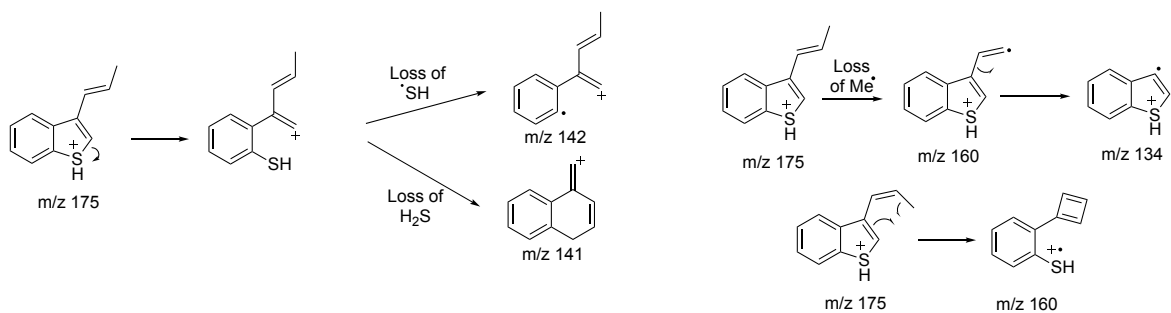
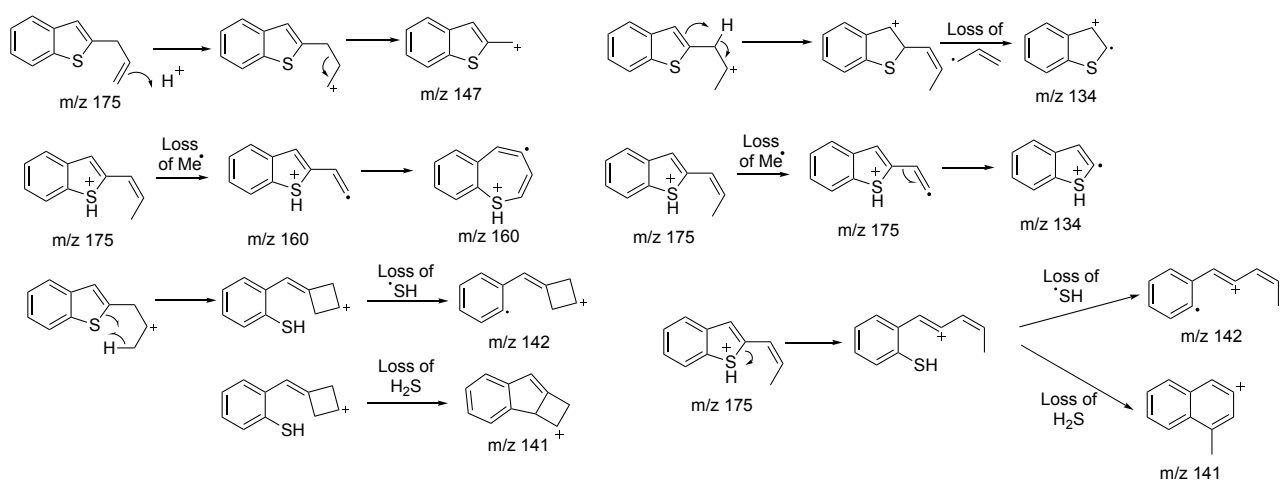


Pathways to m/z 105 for 2-/3- different to 4-/5-/6-/7-APBT

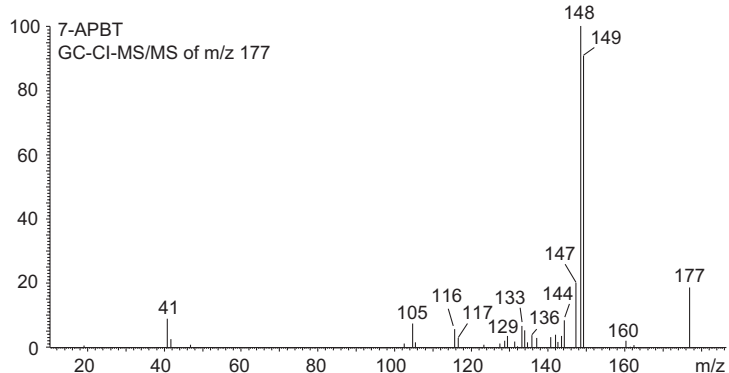
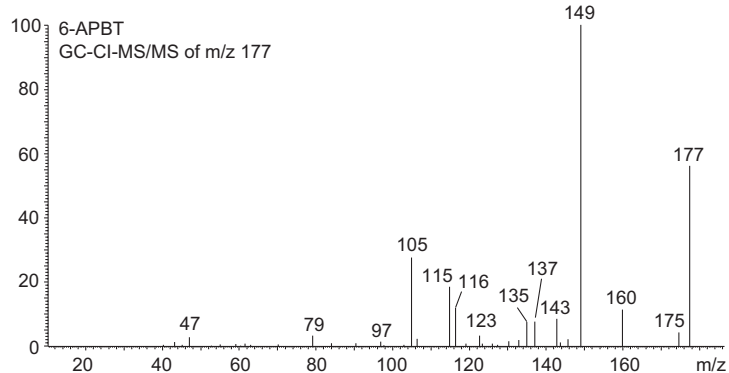
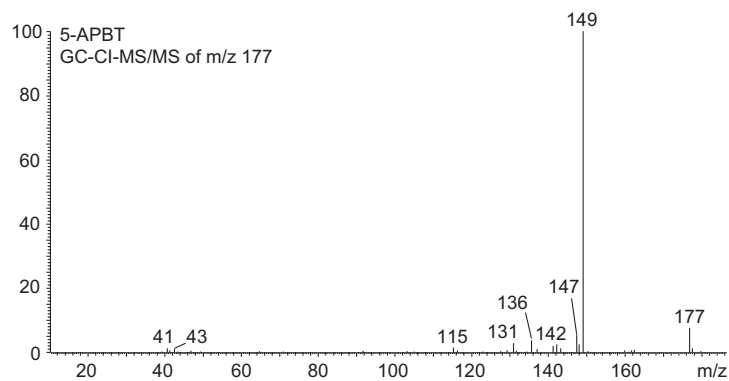
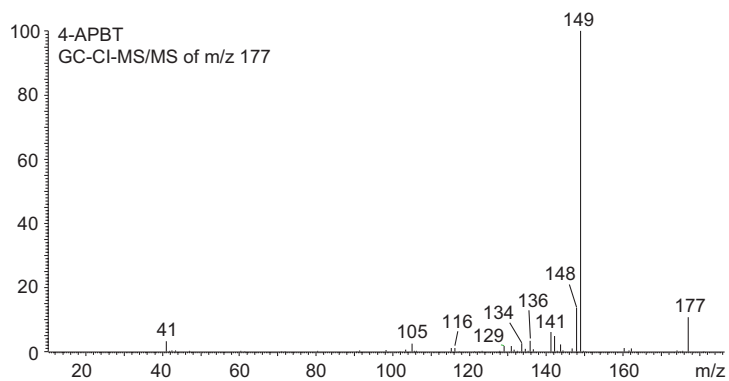
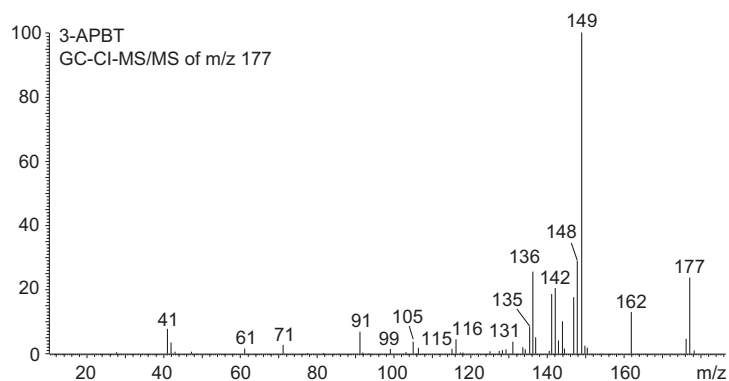
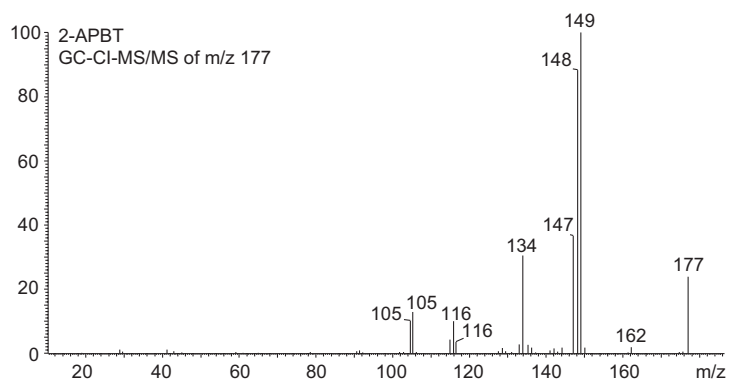
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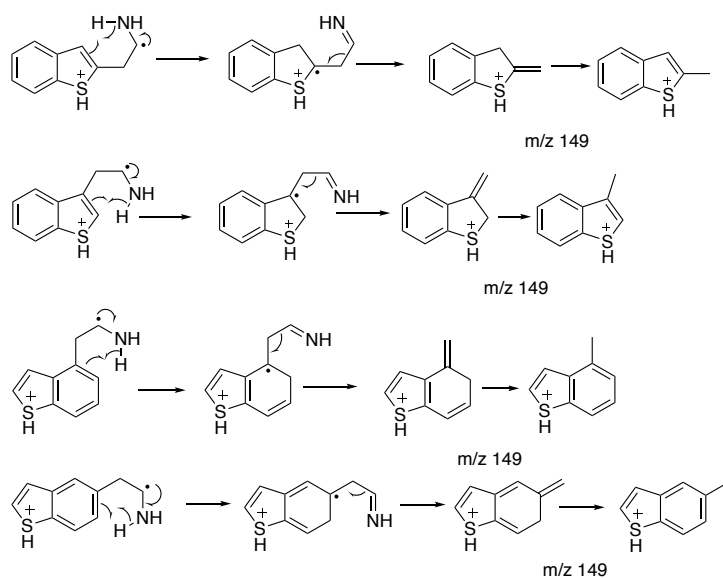
CI-MSMS of m/z 175



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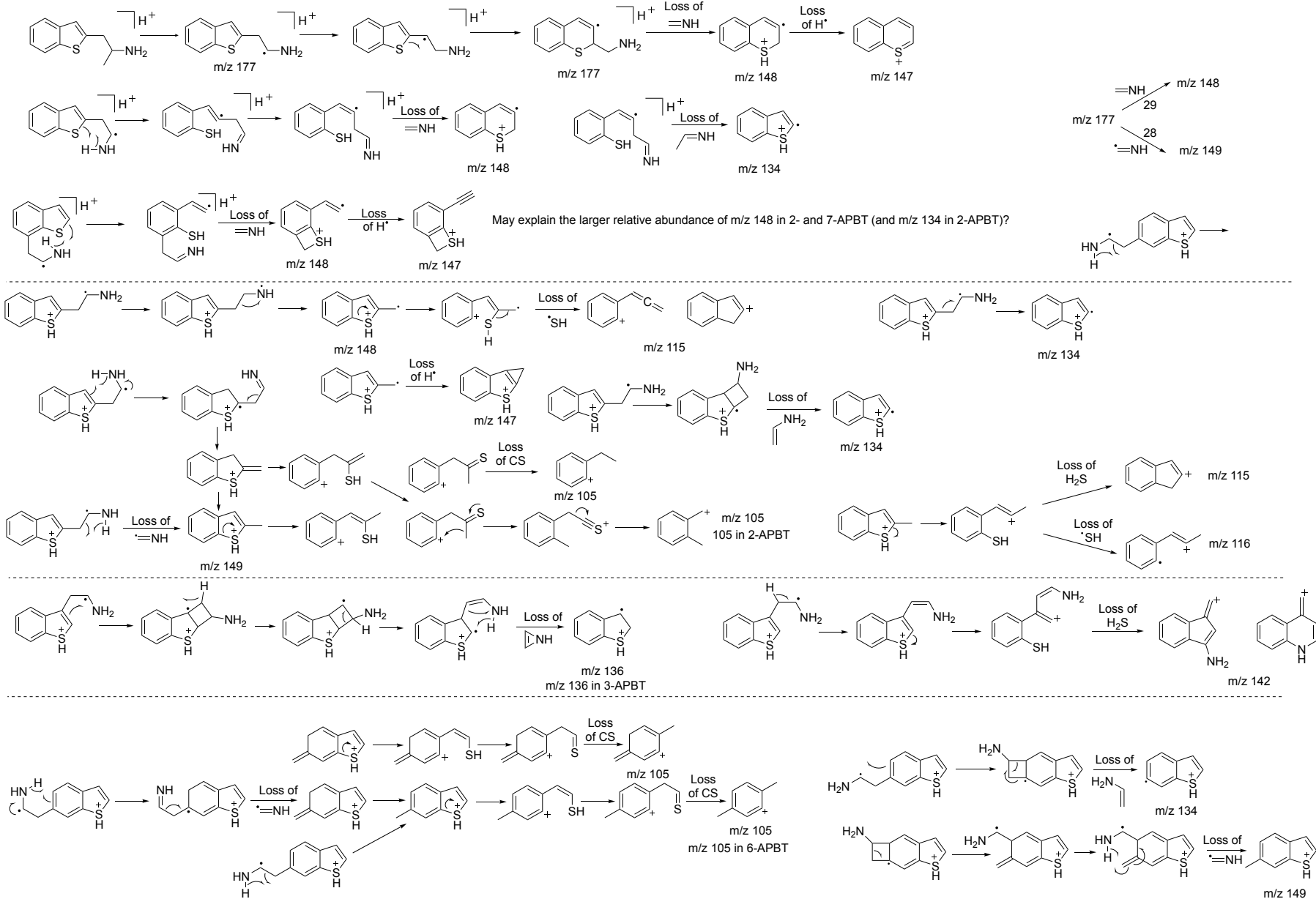


CI-MSMS m/z 149 from m/z 177

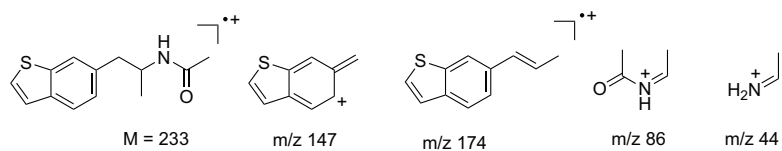


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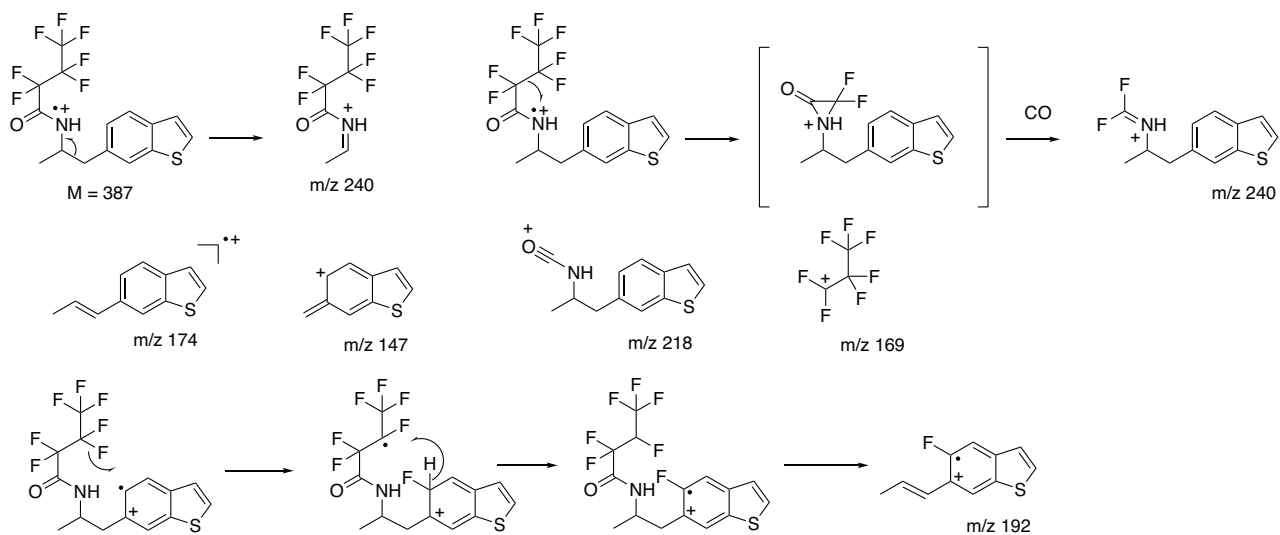
CI-MSMS m/z 177



AC derivatives

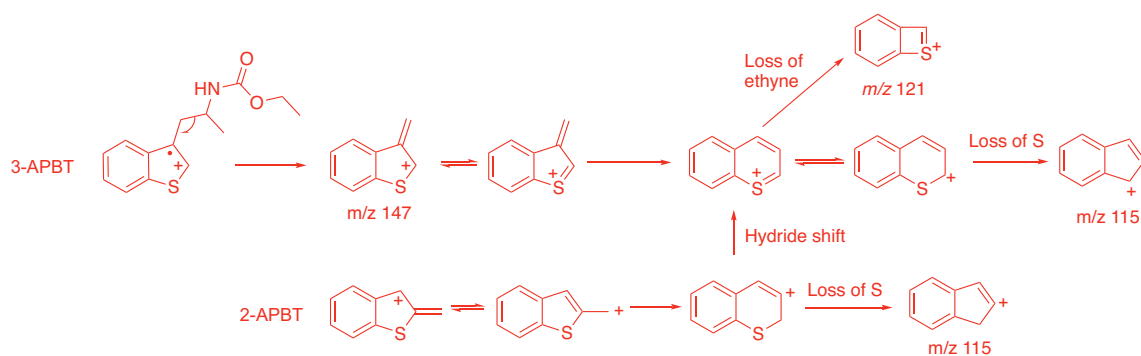
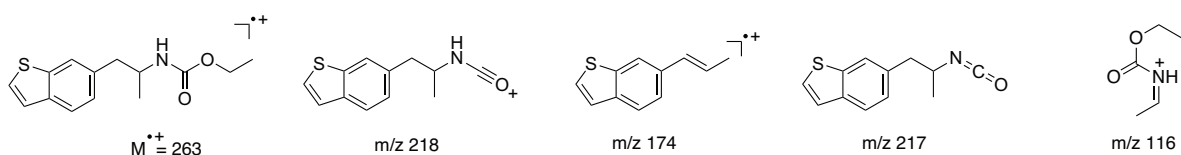


HFB derivatives



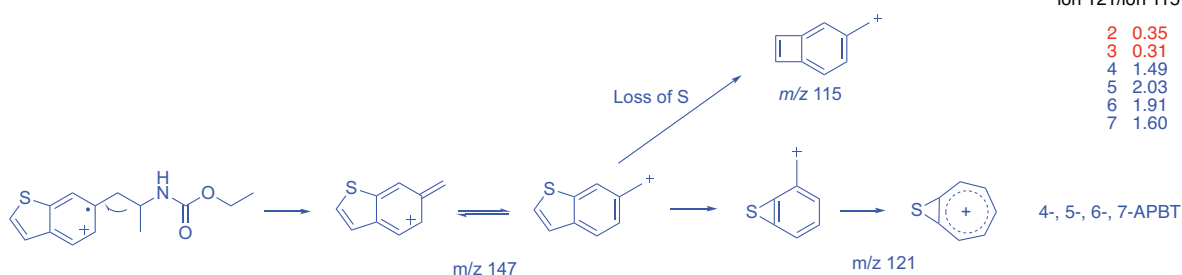
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EC derivatives

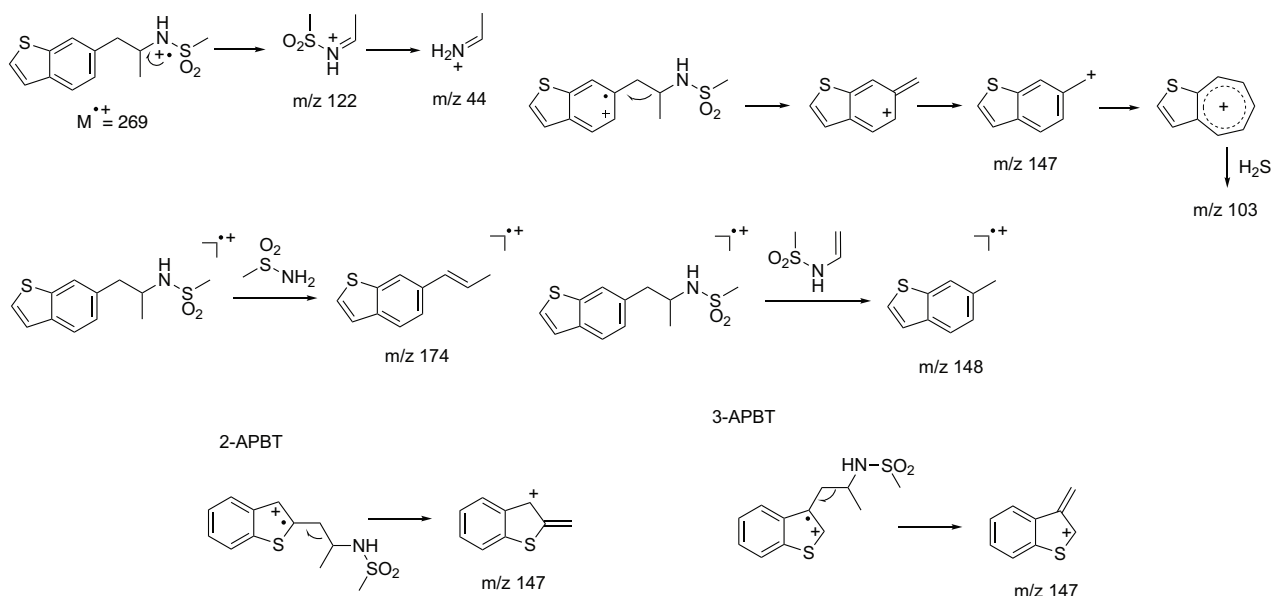


ion 121/ion 115 ratio

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

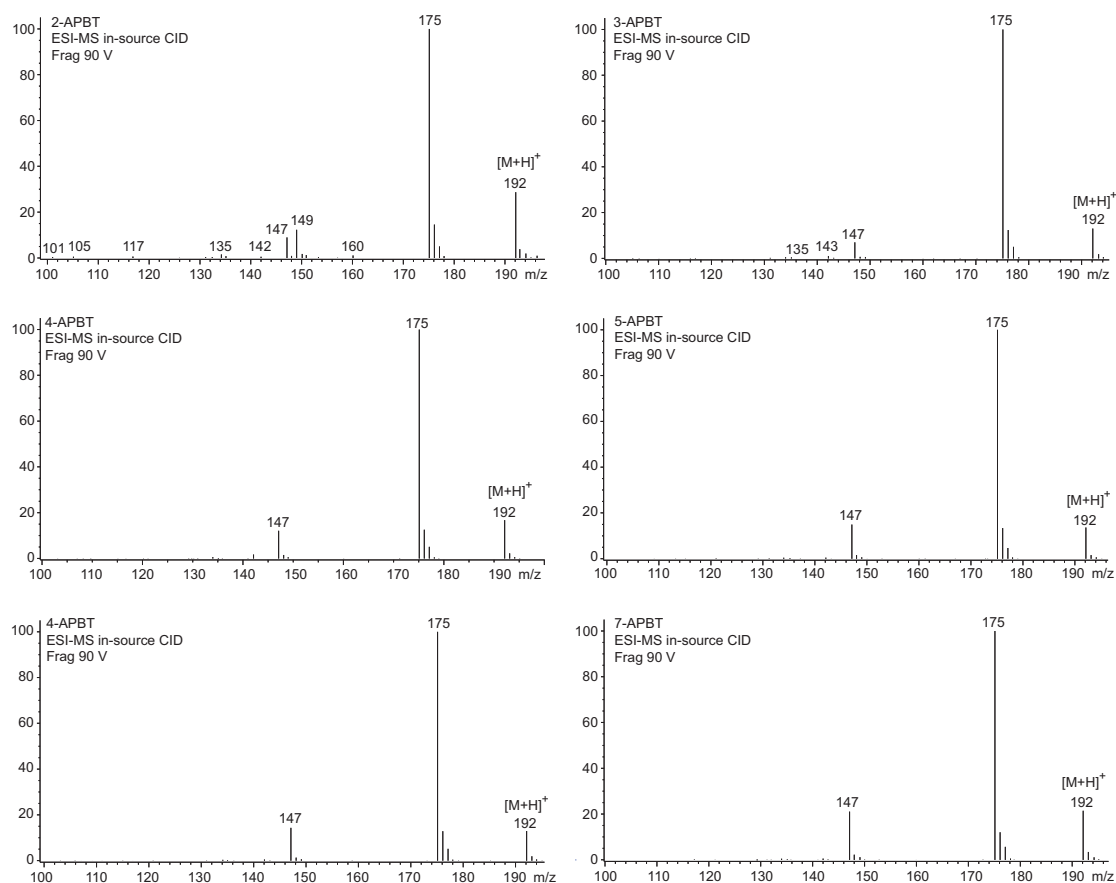


MSA derivatives

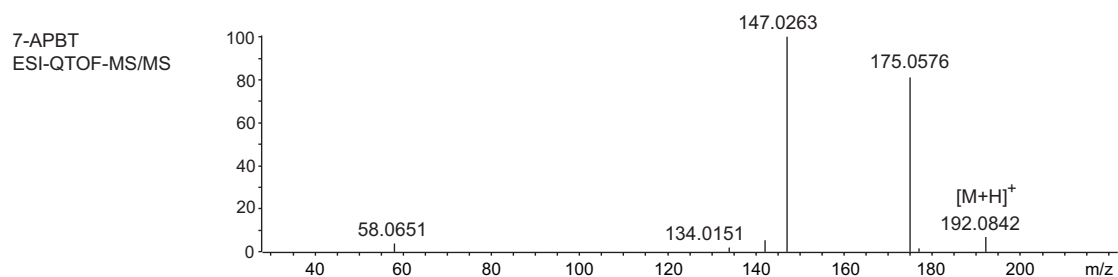
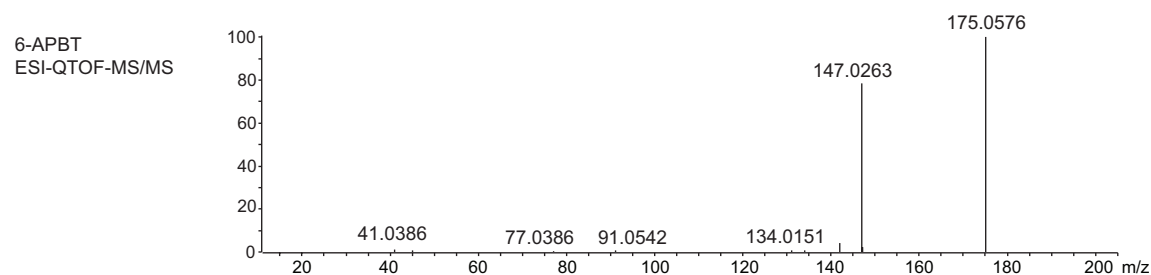
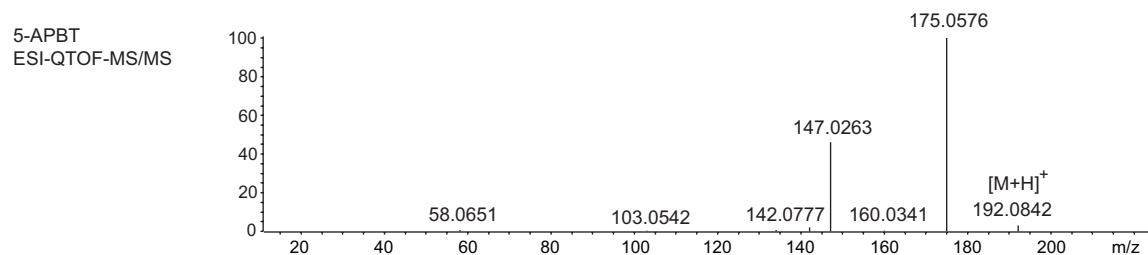
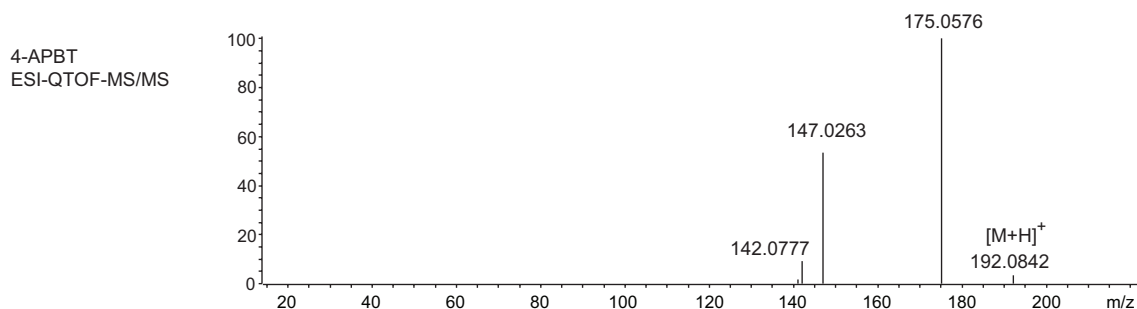
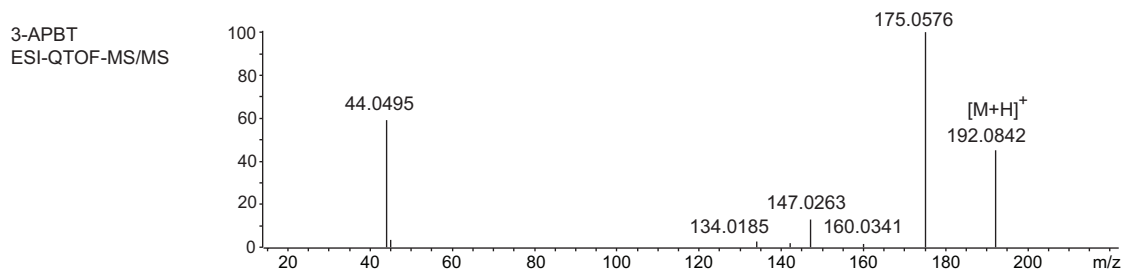
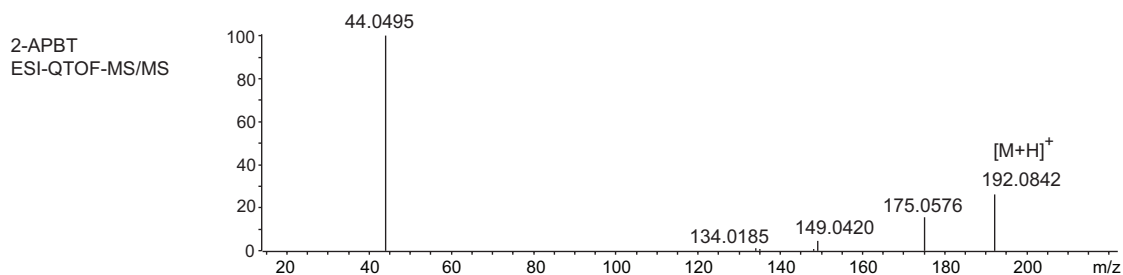


In-source CID mass spectra - liquid chromatography electrospray ionization mass spectrometry

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 μ m, 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 μ L/min, 10 μ L of a 50 μ g/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).

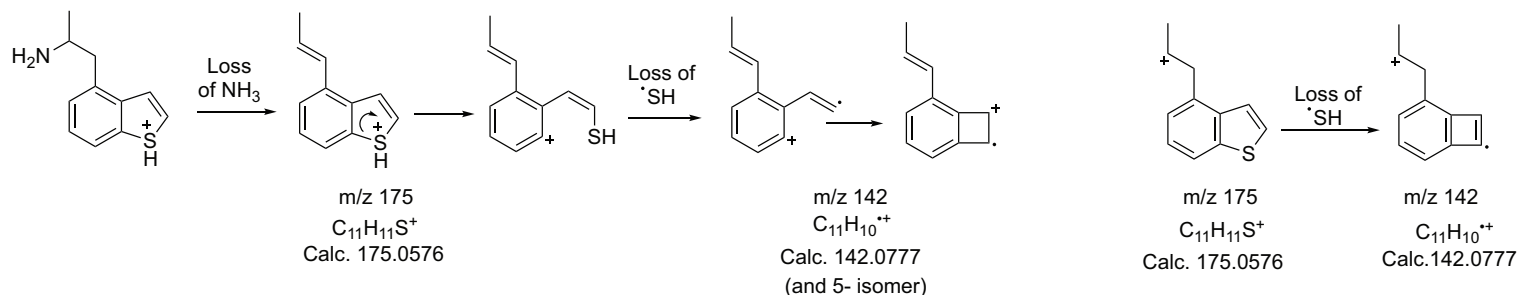


Supporting Information – Drug Testing and Analysis

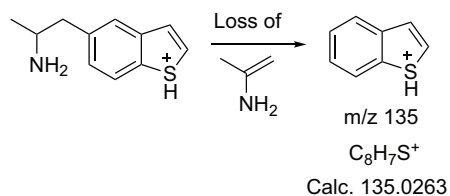


Calc. m/z	Formula	2-APBT		3-APBT		4-APBT		5-APBT		6-APBT		7-APBT	
		Obs. m/z	Δ (ppm)	Obs. m/z	Δ (ppm)	Obs. m/z	Δ (ppm)	Obs. m/z	Δ (ppm)	Obs. m/z	Δ (ppm)	Obs. m/z	Δ (ppm)
192.0842	$C_{11}H_{14}NS^+$	192.0842	0	192.0842	0	192.0842	0	192.0842	0	No $[M+H]^+$		192.0842	0
175.0576	$C_{11}H_{11}S^+$	175.0576	0	175.0576	0	175.0576	0	175.0576	0	175.0576	0	175.0576	0
160.03412	$C_{10}H_8S^{+*}$	–	–	160.03412	0	–	–	–	–	–	–	–	–
149.0420	$C_9H_9S^+$	149.0420	0	–	–	–	–	–	–	–	–	–	–
147.0263	$C_9H_7S^+$	–	–	147.0263	0	147.0263	0	147.0263	0	147.0263	0	147.0263	0
142.0777	$C_{11}H_{10}^{+*}$	–	–	–	–	142.0777	0	142.0777	0	–	–	–	–
135.0263	$C_8H_7S^+$	–	–	–	–	–	–	135.0263	0	–	–	–	–
134.0185	$C_8H_6S^{+*}$	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	–	–	–	–	–	–	–	–

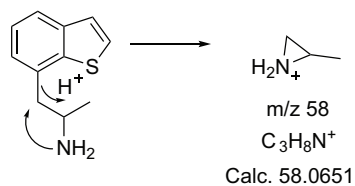
4- and 5-APBT



5-APBT



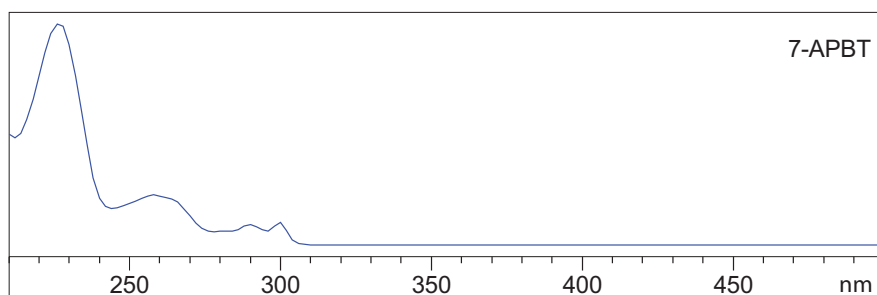
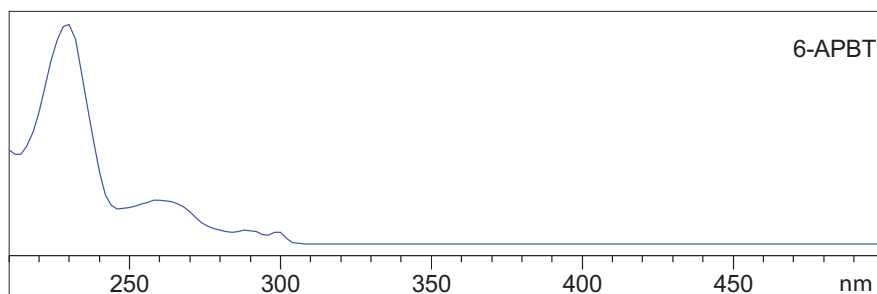
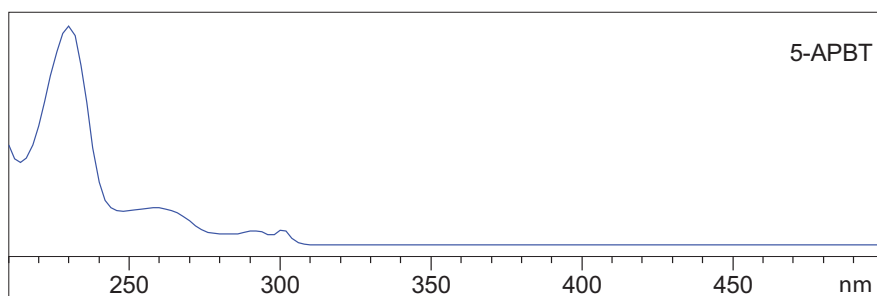
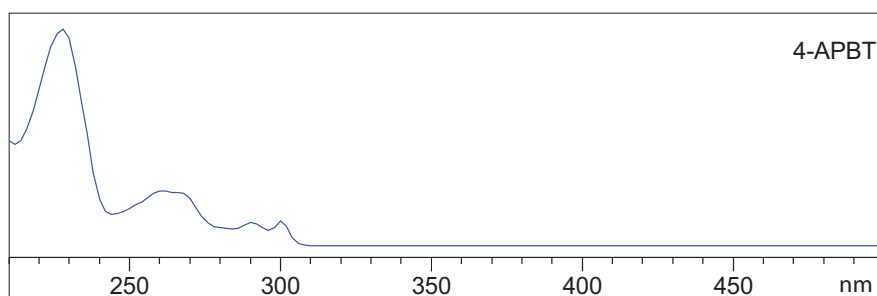
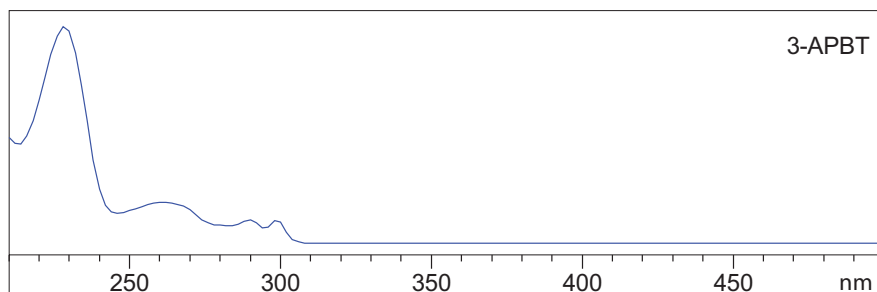
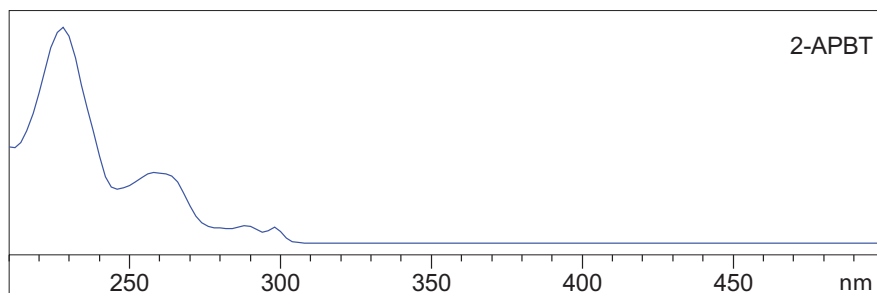
7-APBT



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

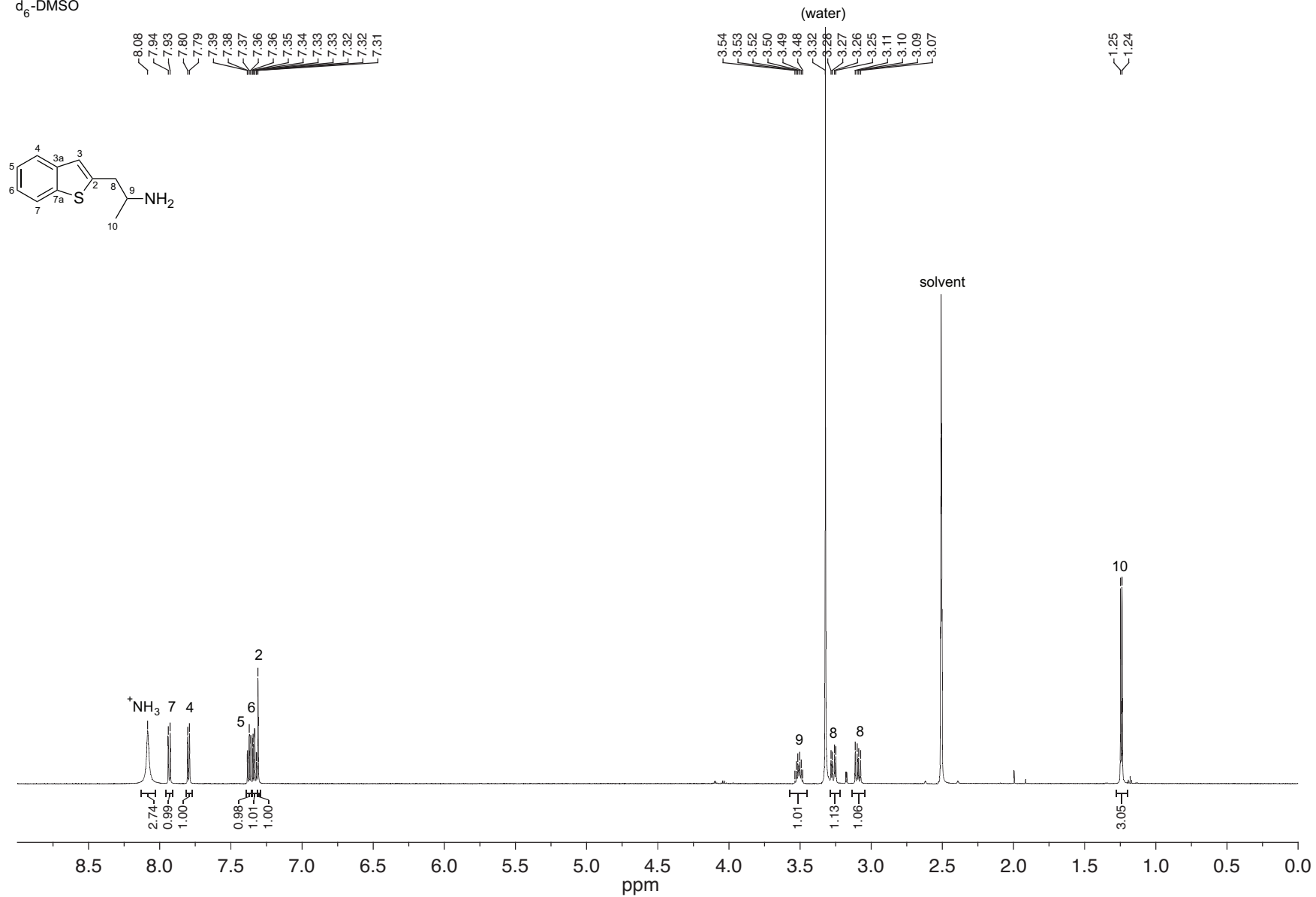
Supporting Information – Drug Testing and Analysis

HPLC-DAD UV spectra



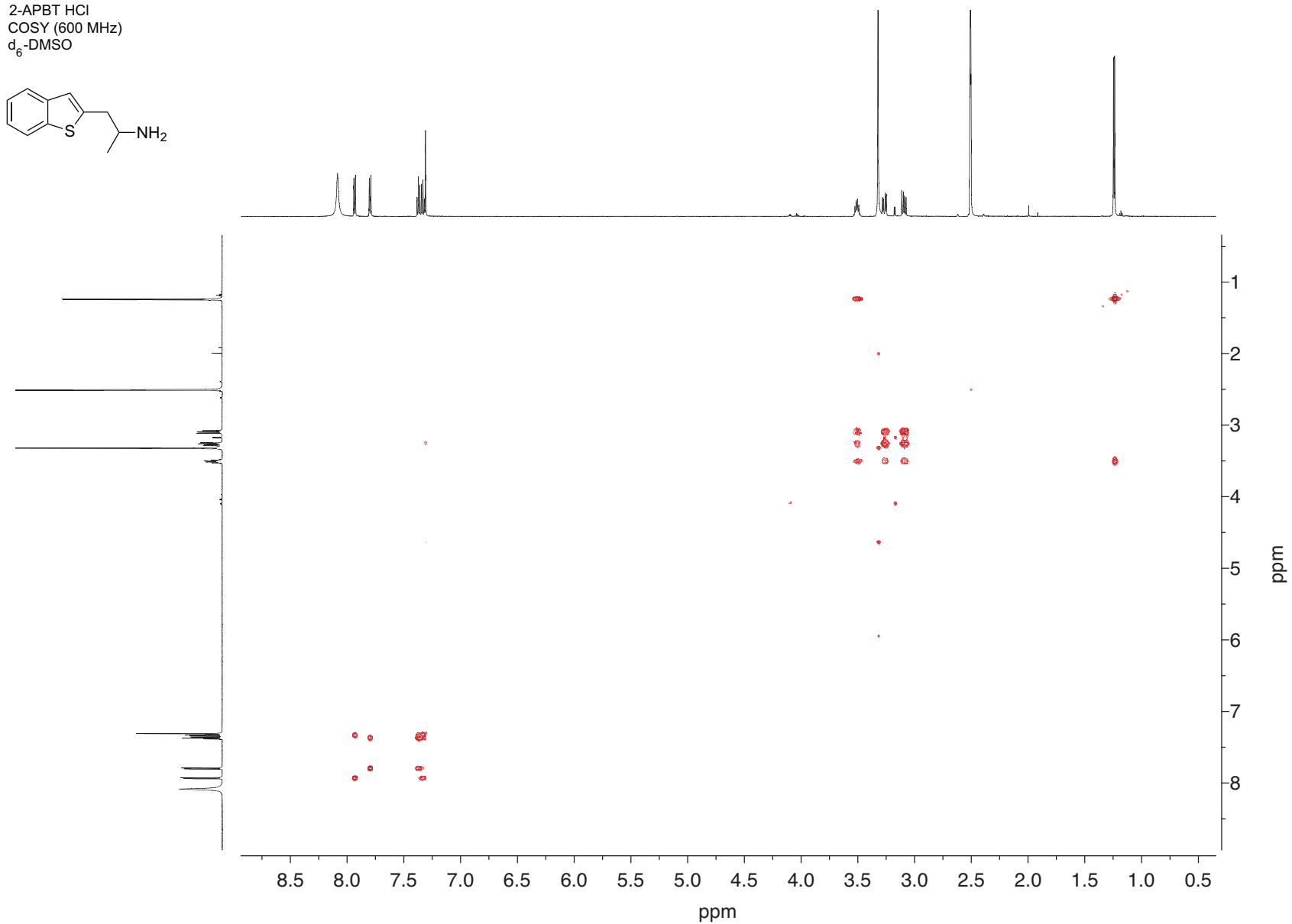
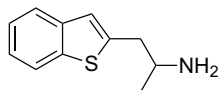
Supporting Information – Drug Testing and Analysis

2-APBT HCl
¹H-NMR (600 MHz)
 d₆-DMSO

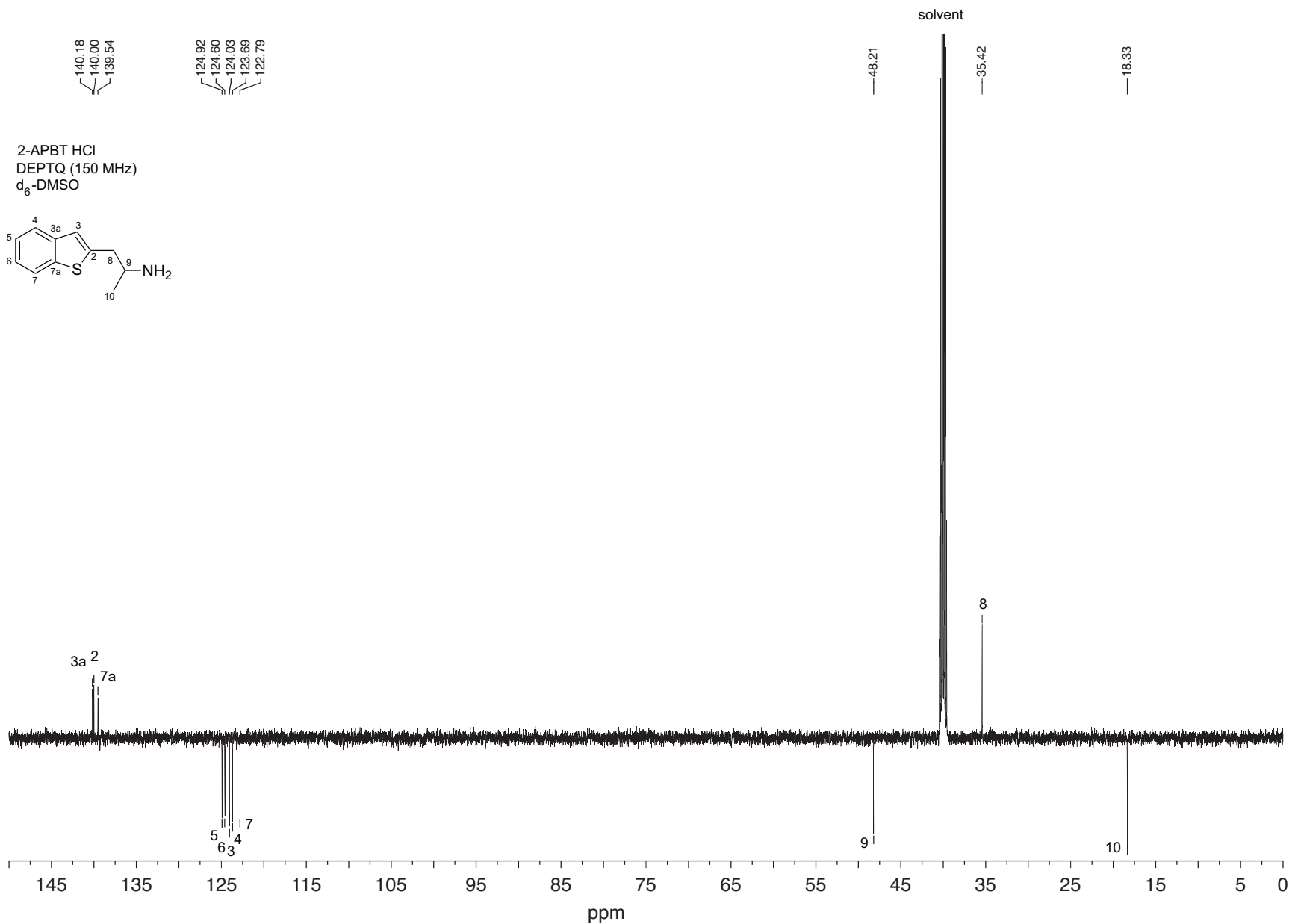


Supporting Information – Drug Testing and Analysis

2-APBT HCl
COSY (600 MHz)
d₆-DMSO

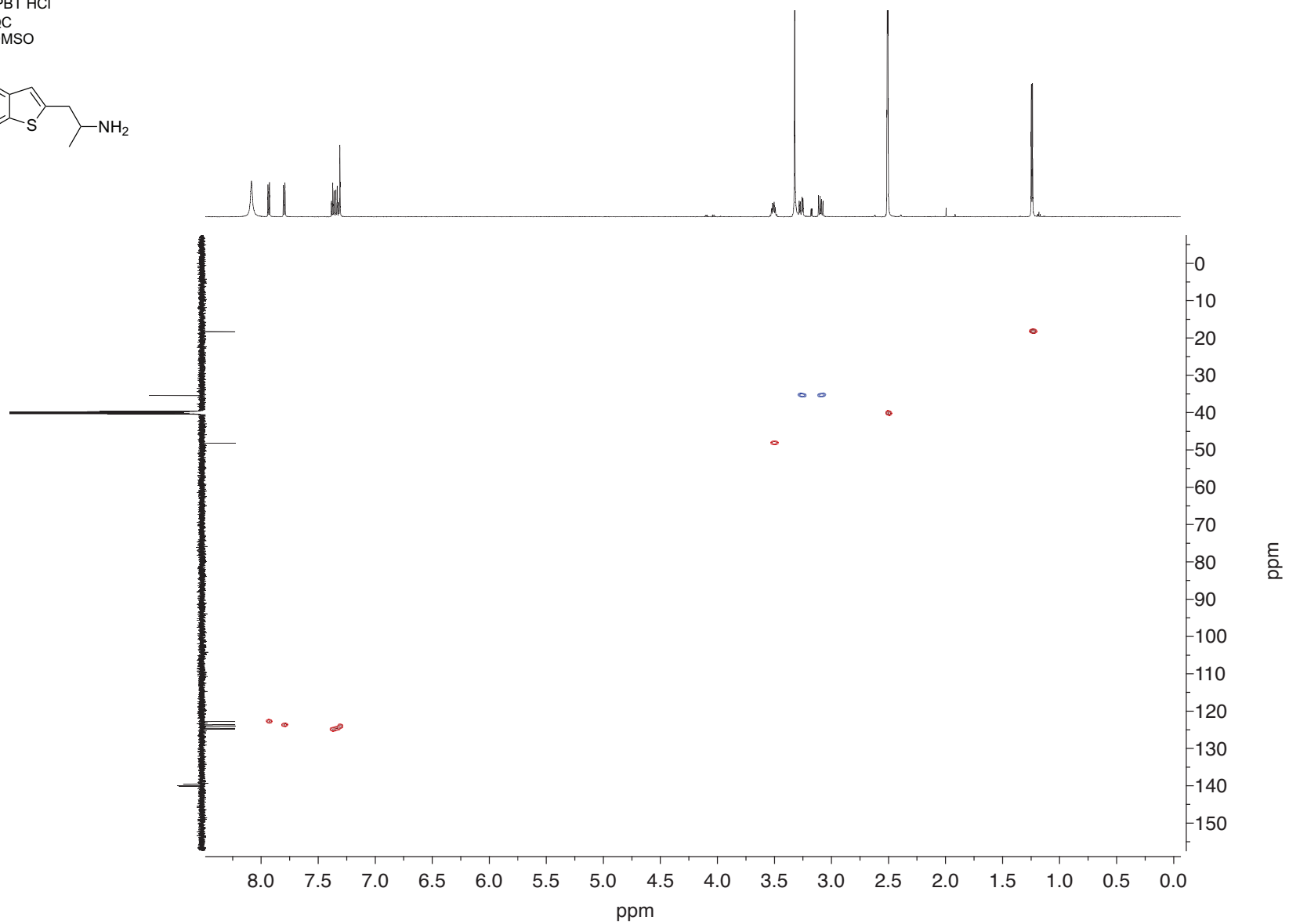
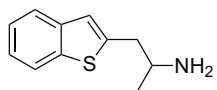


Supporting Information – Drug Testing and Analysis



Supporting Information – Drug Testing and Analysis

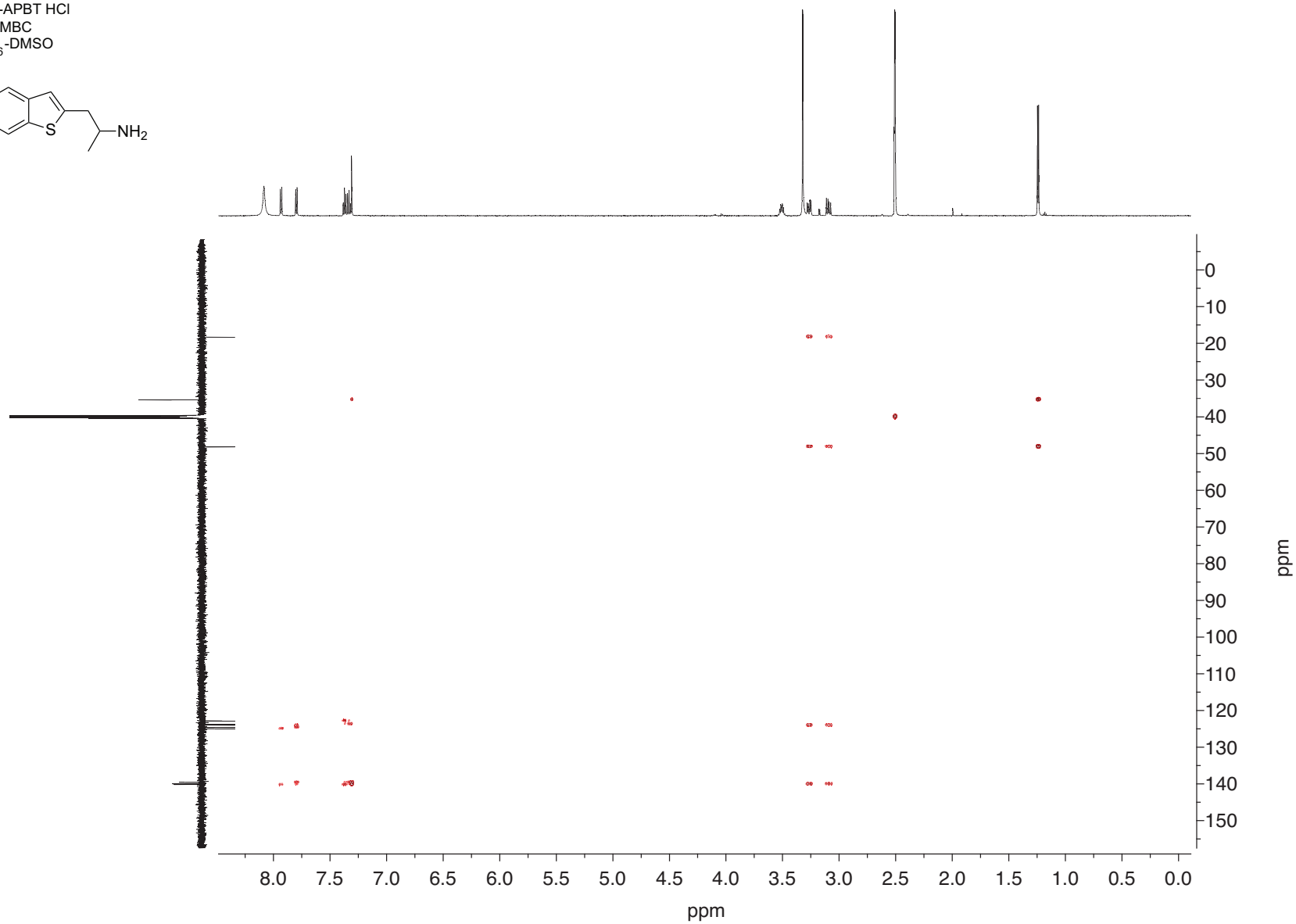
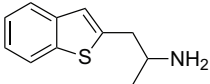
2-APBT HCl
HSQC
d₆-DMSO



Supporting Information – Drug Testing and Analysis

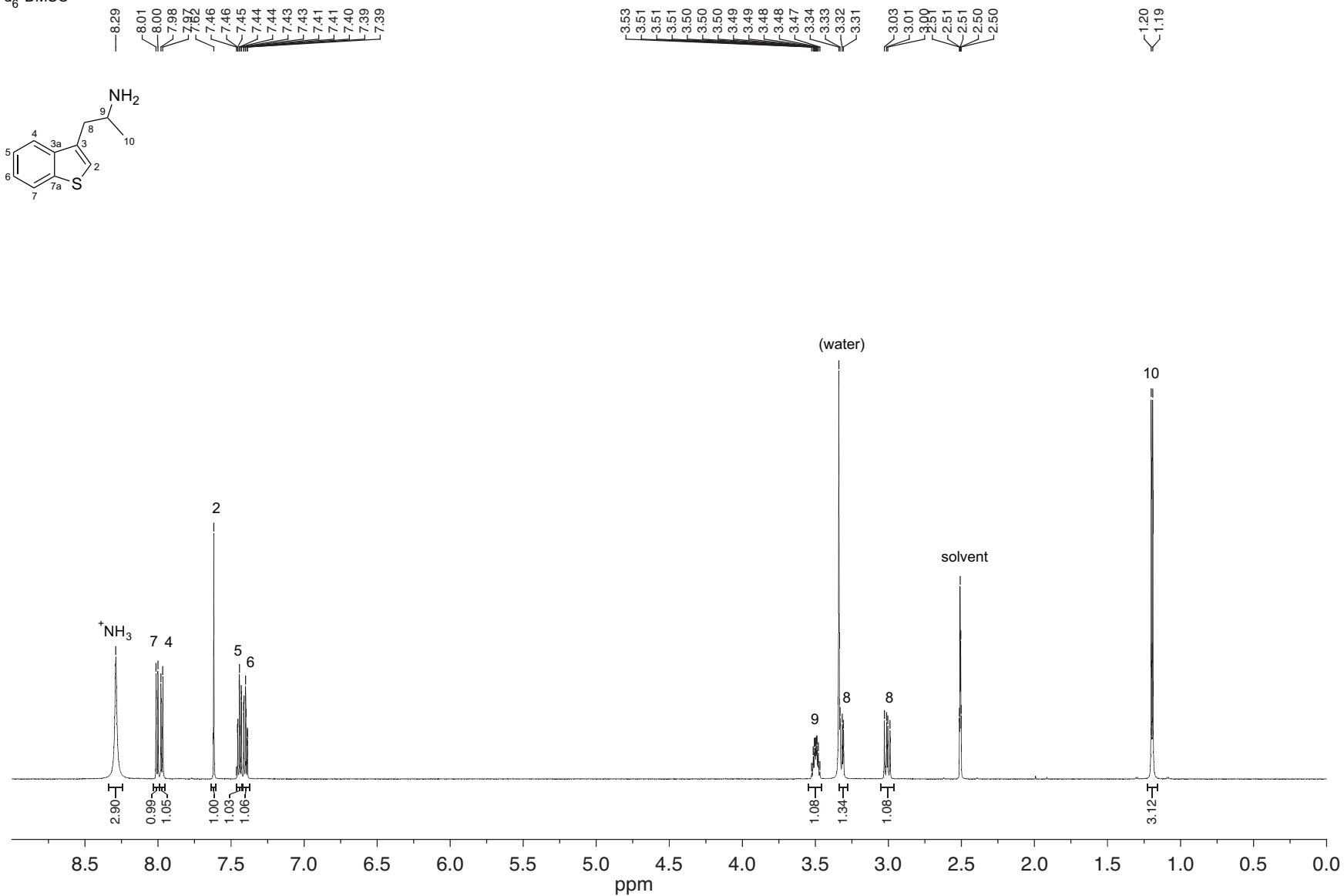
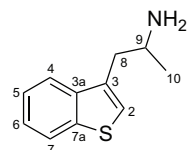
2-APBT HCl

HMBC

d₆-DMSO

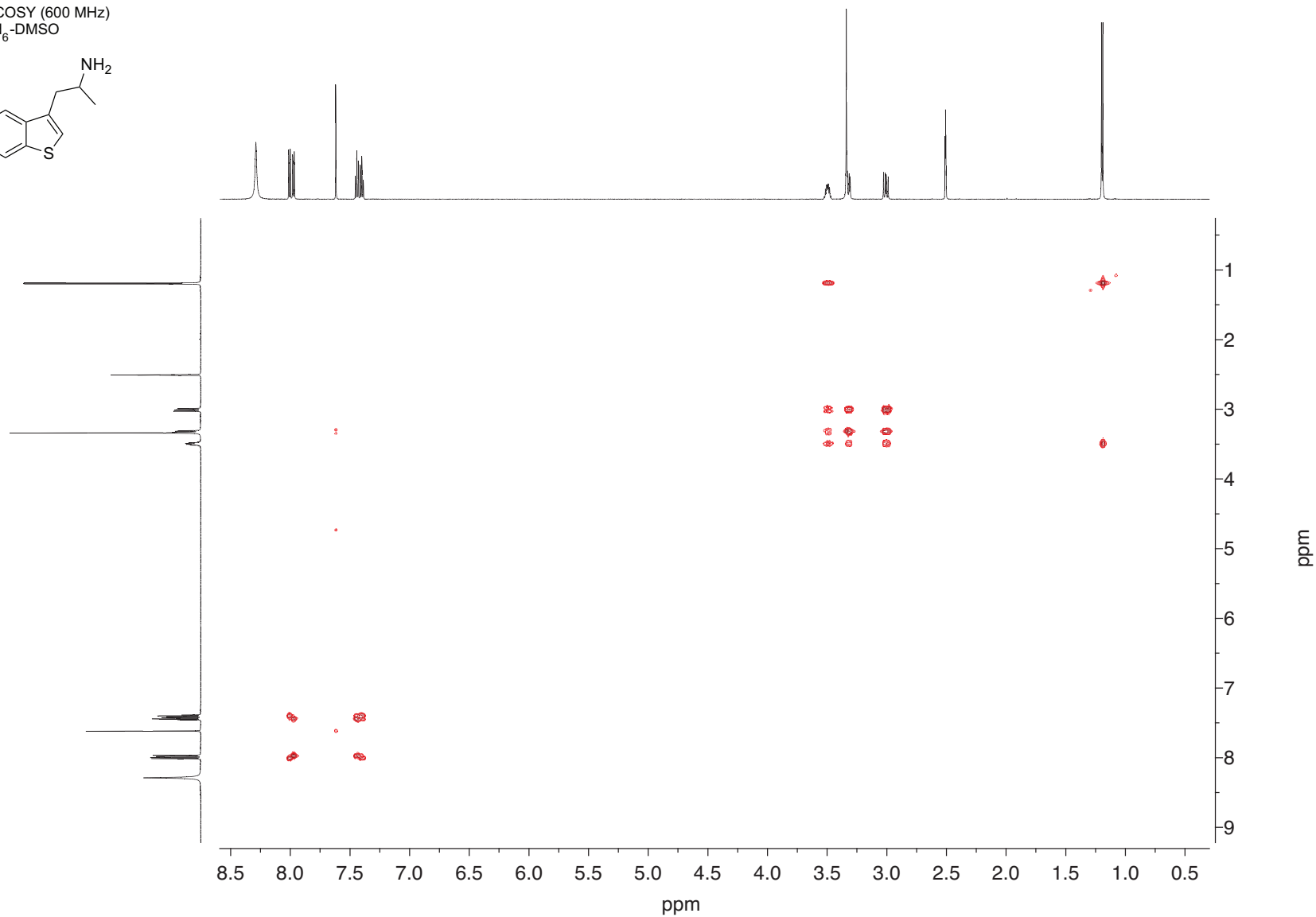
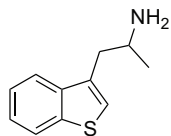
Supporting Information – Drug Testing and Analysis

3-APBT HCl
¹H-NMR (600 MHz)
d₆-DMSO

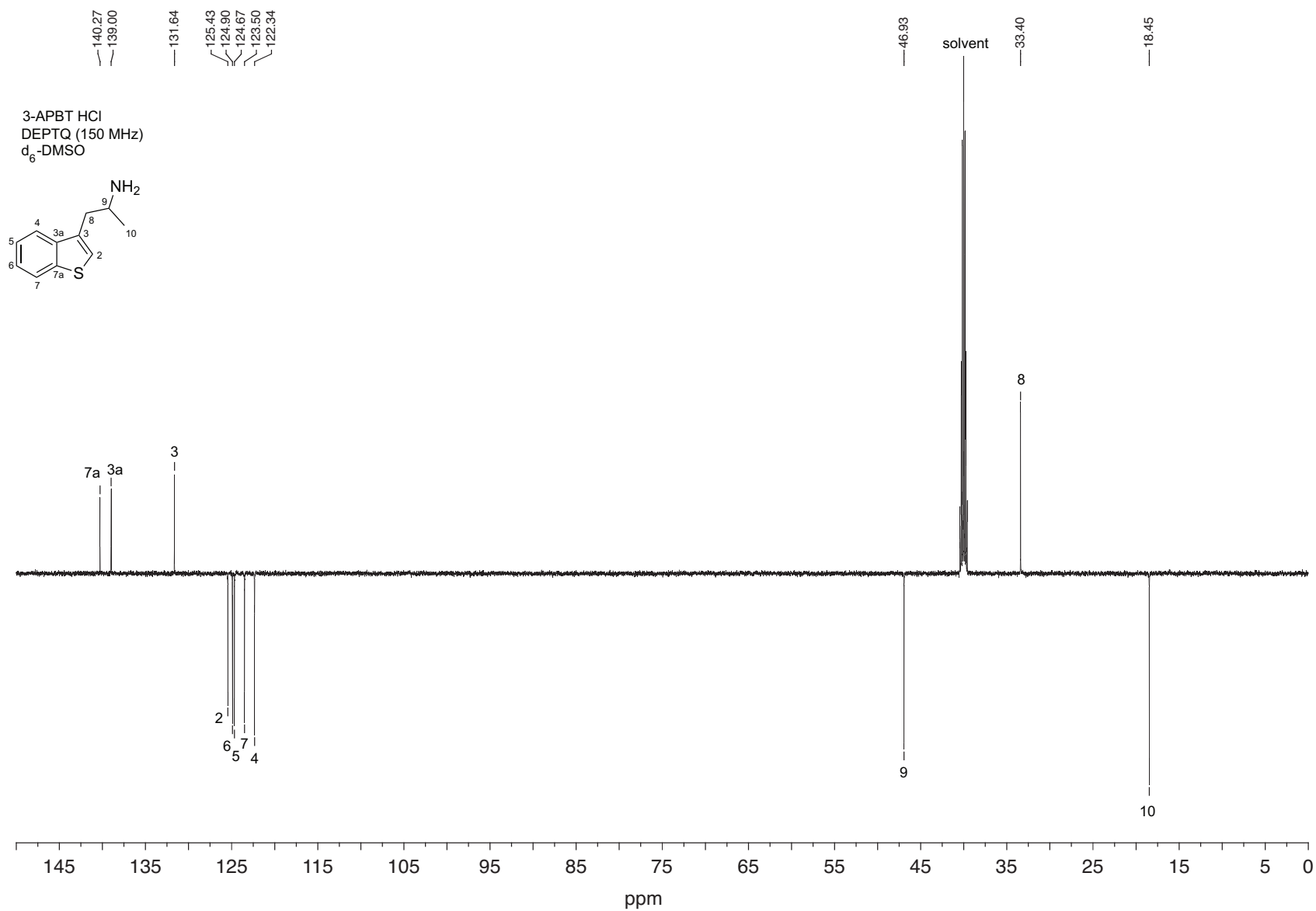


Supporting Information – Drug Testing and Analysis

3-APBT HCl
COSY (600 MHz)
d₆-DMSO

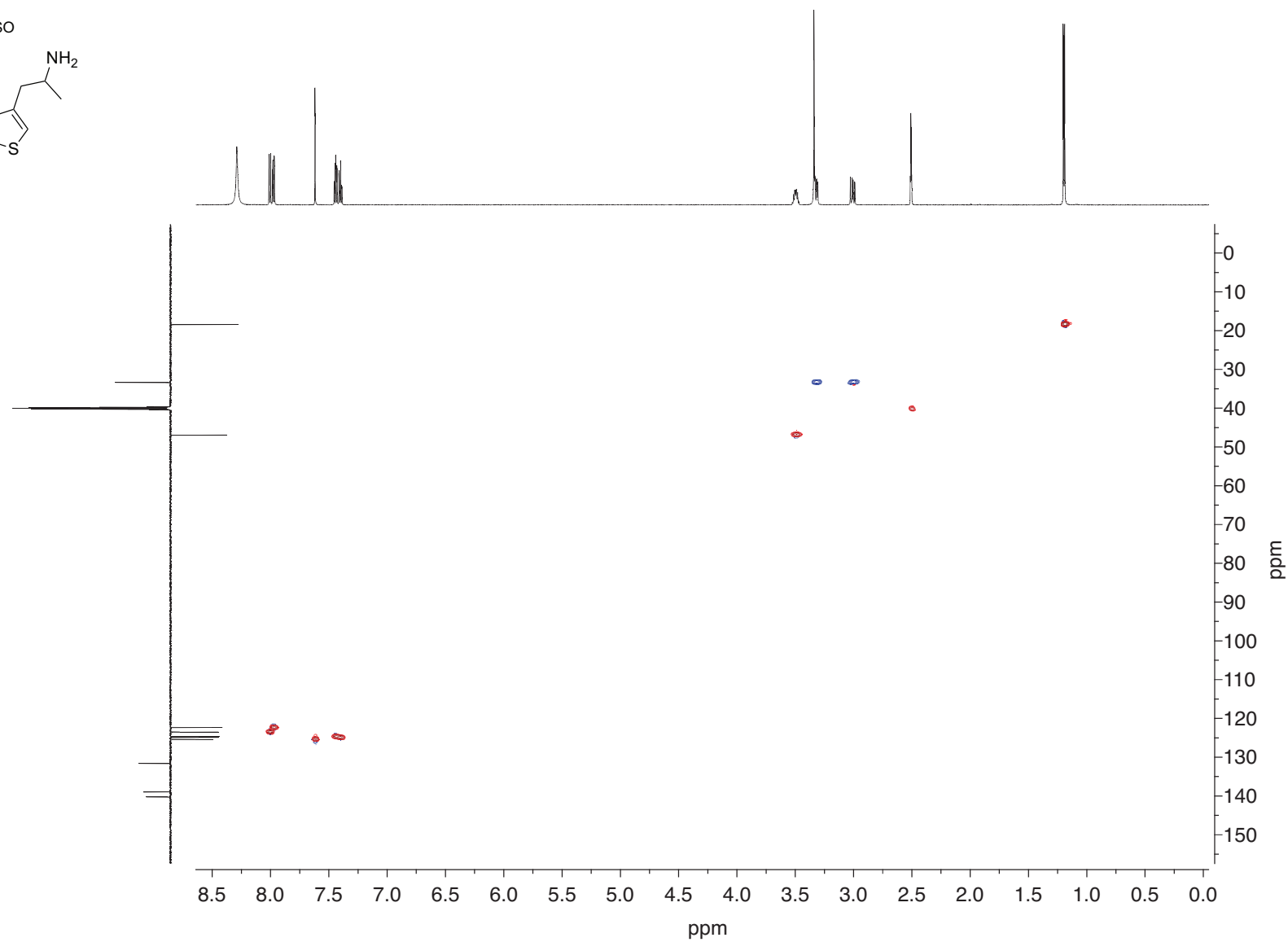
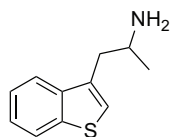


Supporting Information – Drug Testing and Analysis



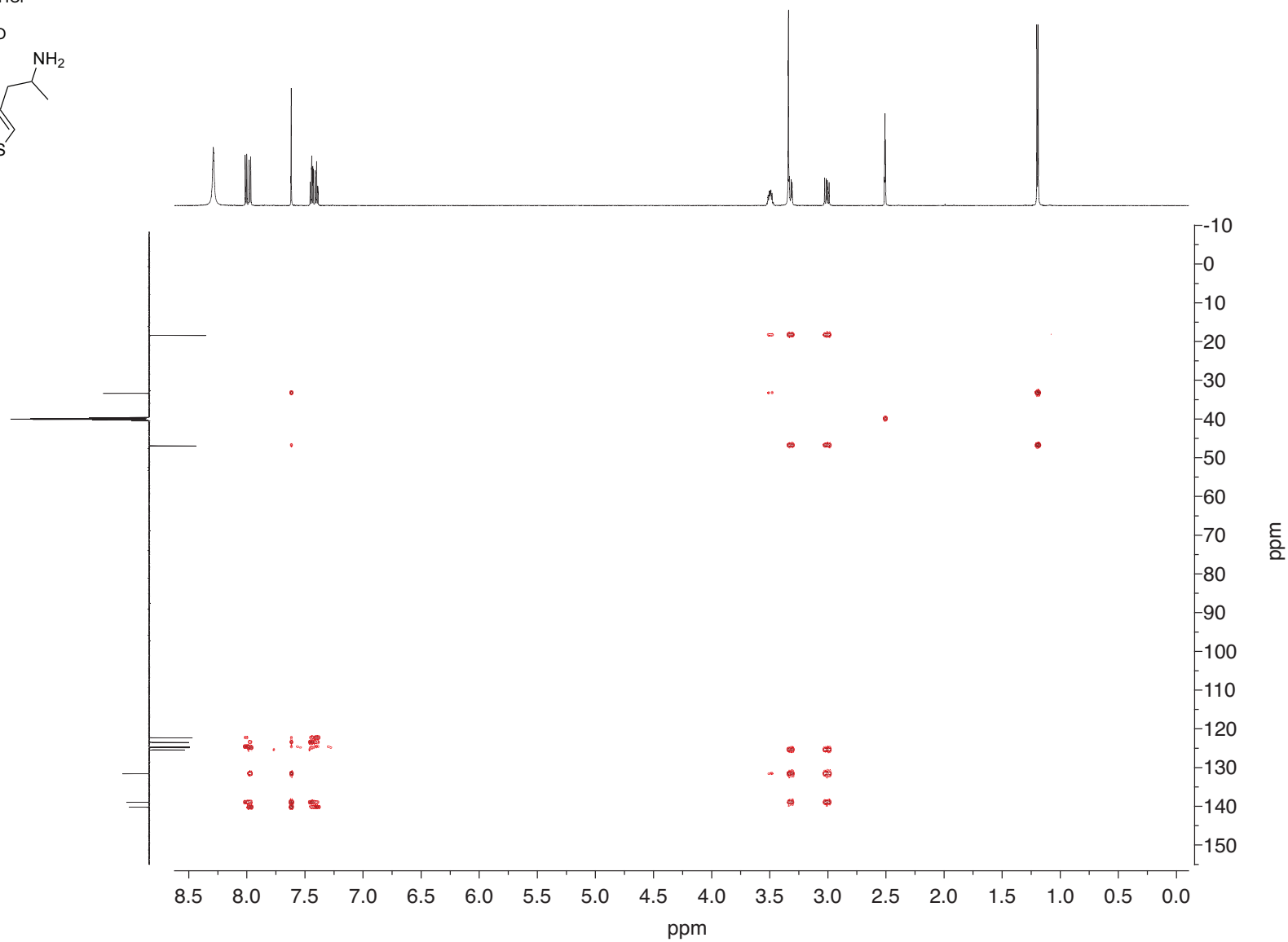
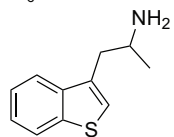
Supporting Information – Drug Testing and Analysis

3-APBT HCl
HSQC
d₆-DMSO



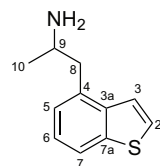
Supporting Information – Drug Testing and Analysis

3-APBT HCl
HMBC
d₆-DMSO



Supporting Information – Drug Testing and Analysis

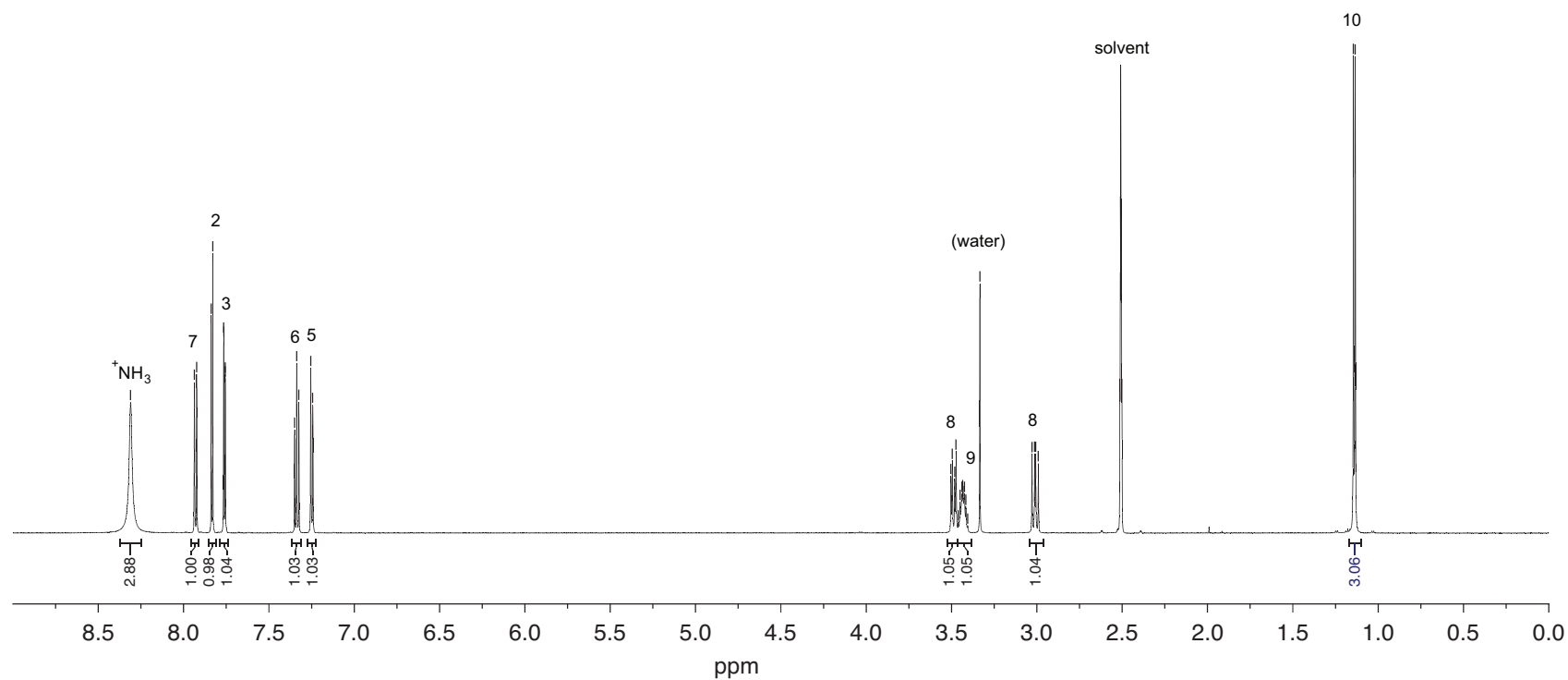
4-APBT HCl
¹H-NMR (600 MHz)
d₆-DMSO



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7.32
7.25
7.24

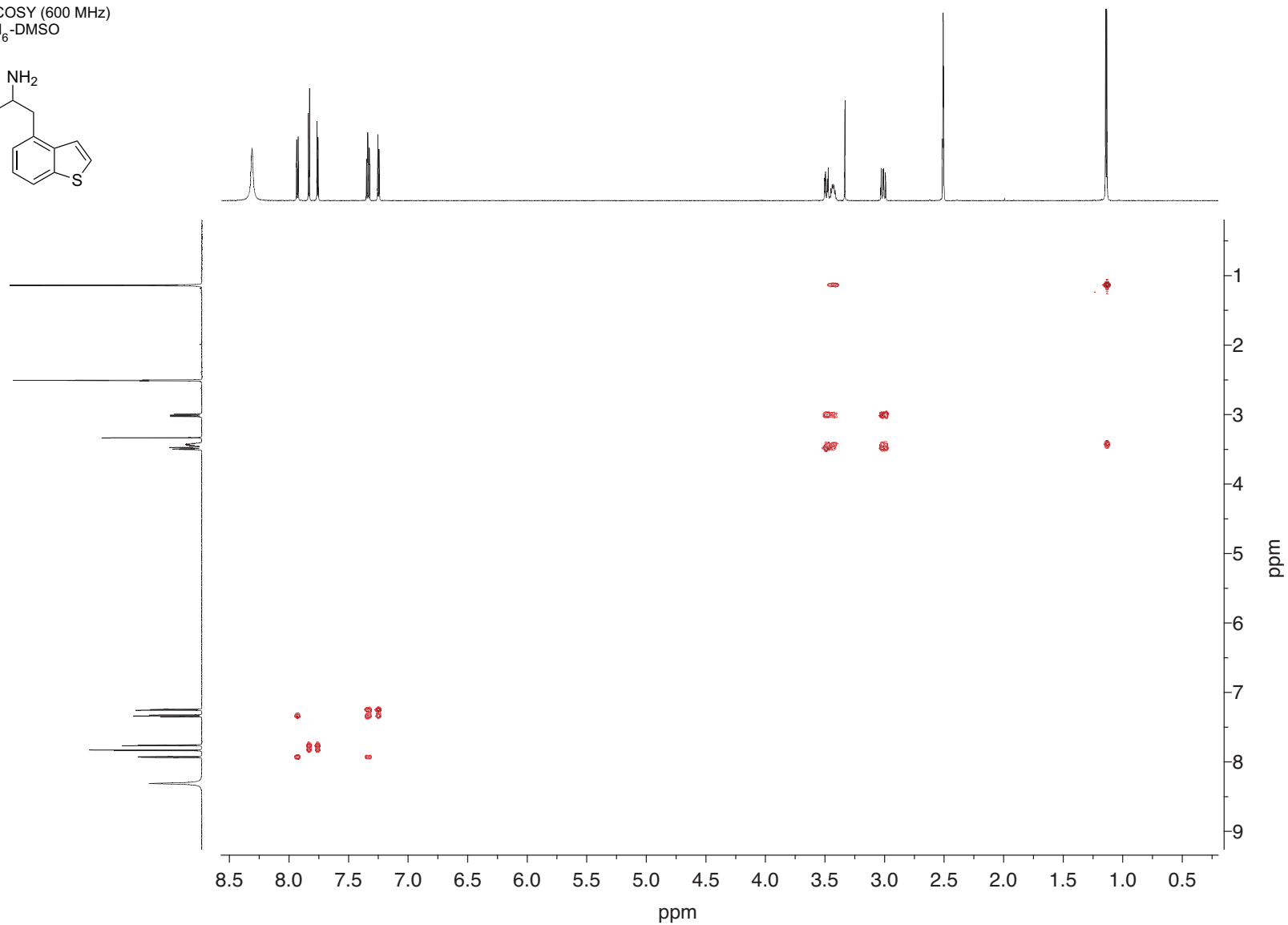
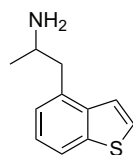
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2.99

1.15
1.13

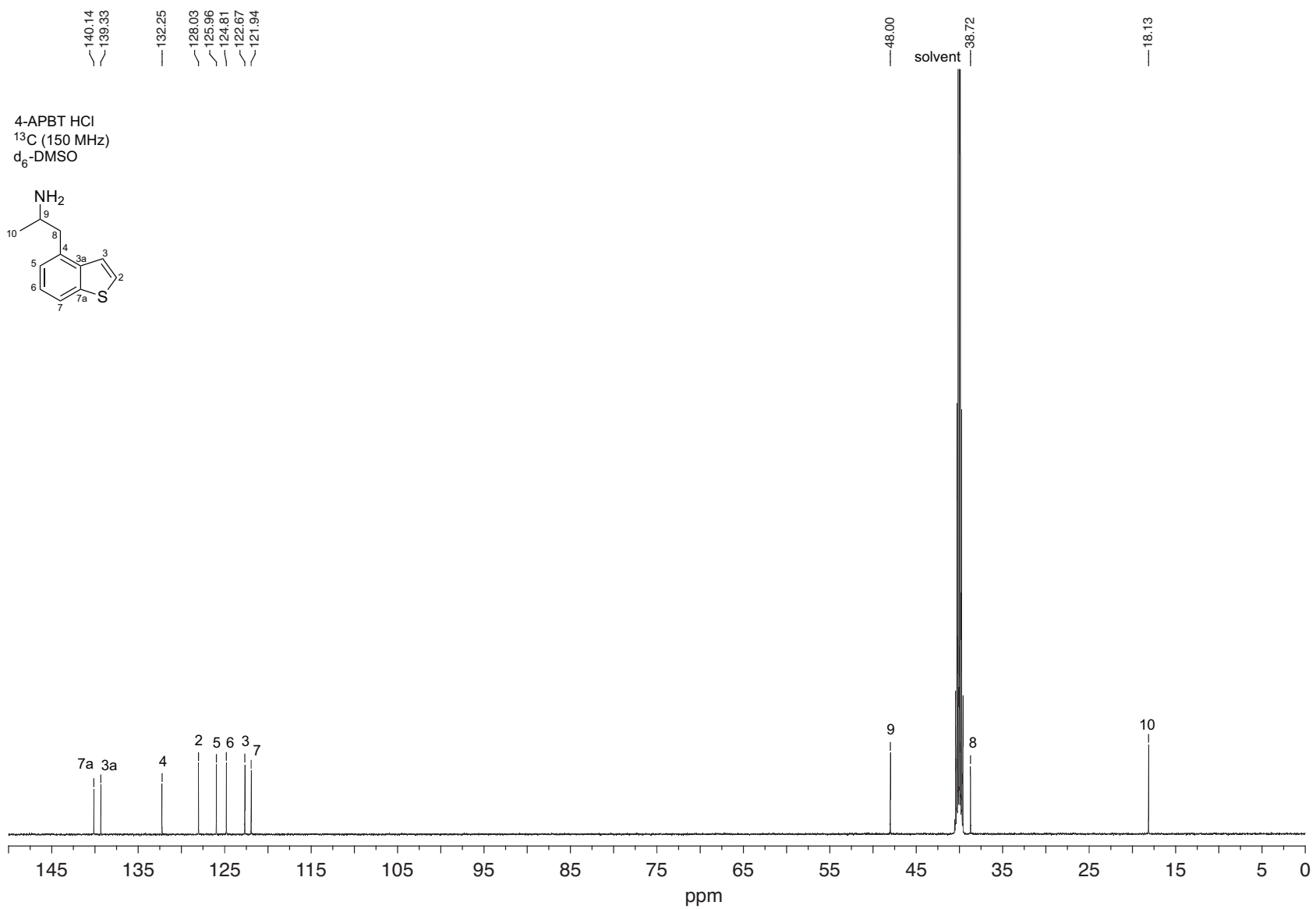


Supporting Information – Drug Testing and Analysis

4-APBT HCl
COSY (600 MHz)
d₆-DMSO

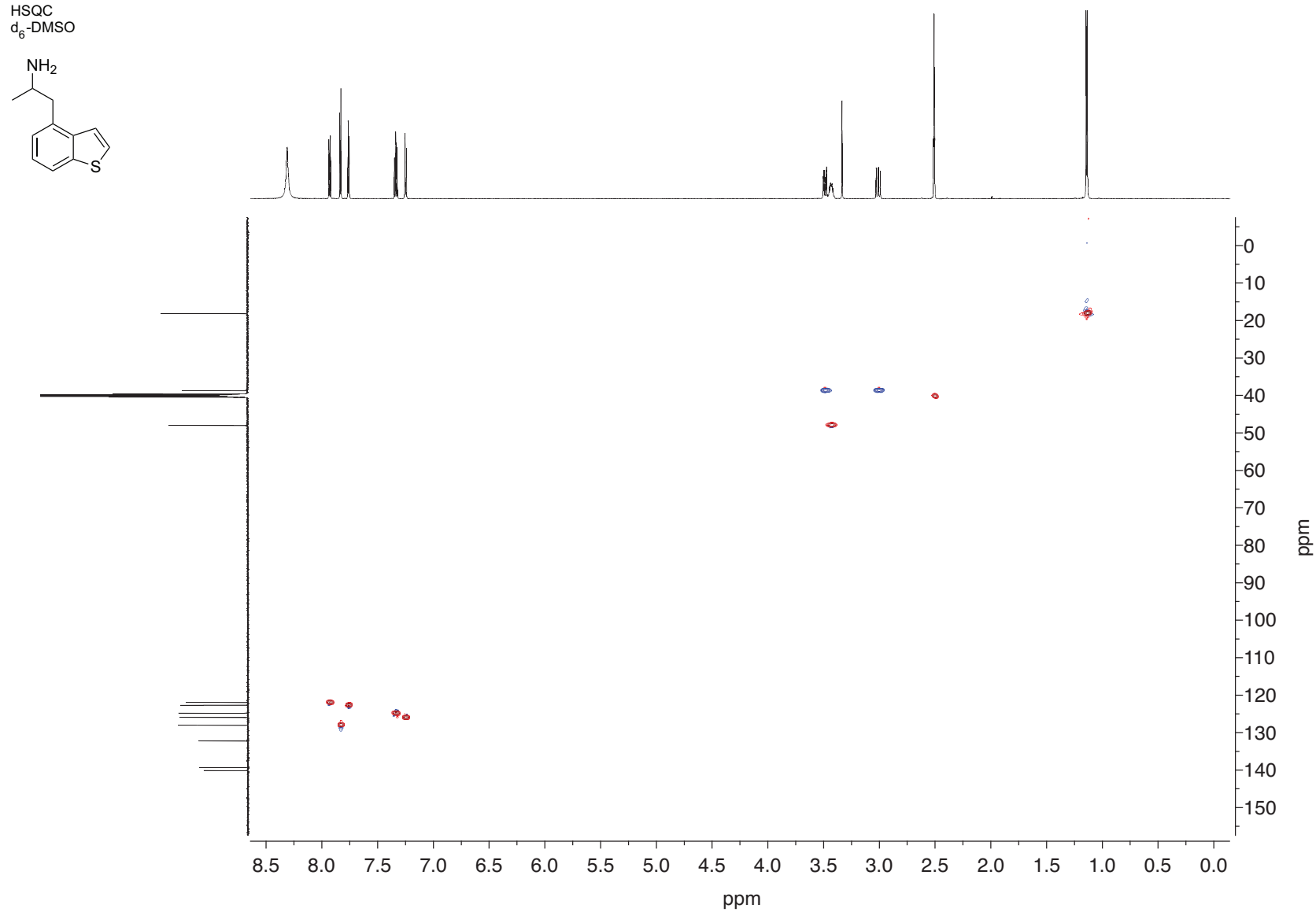
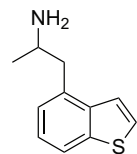


Supporting Information – Drug Testing and Analysis



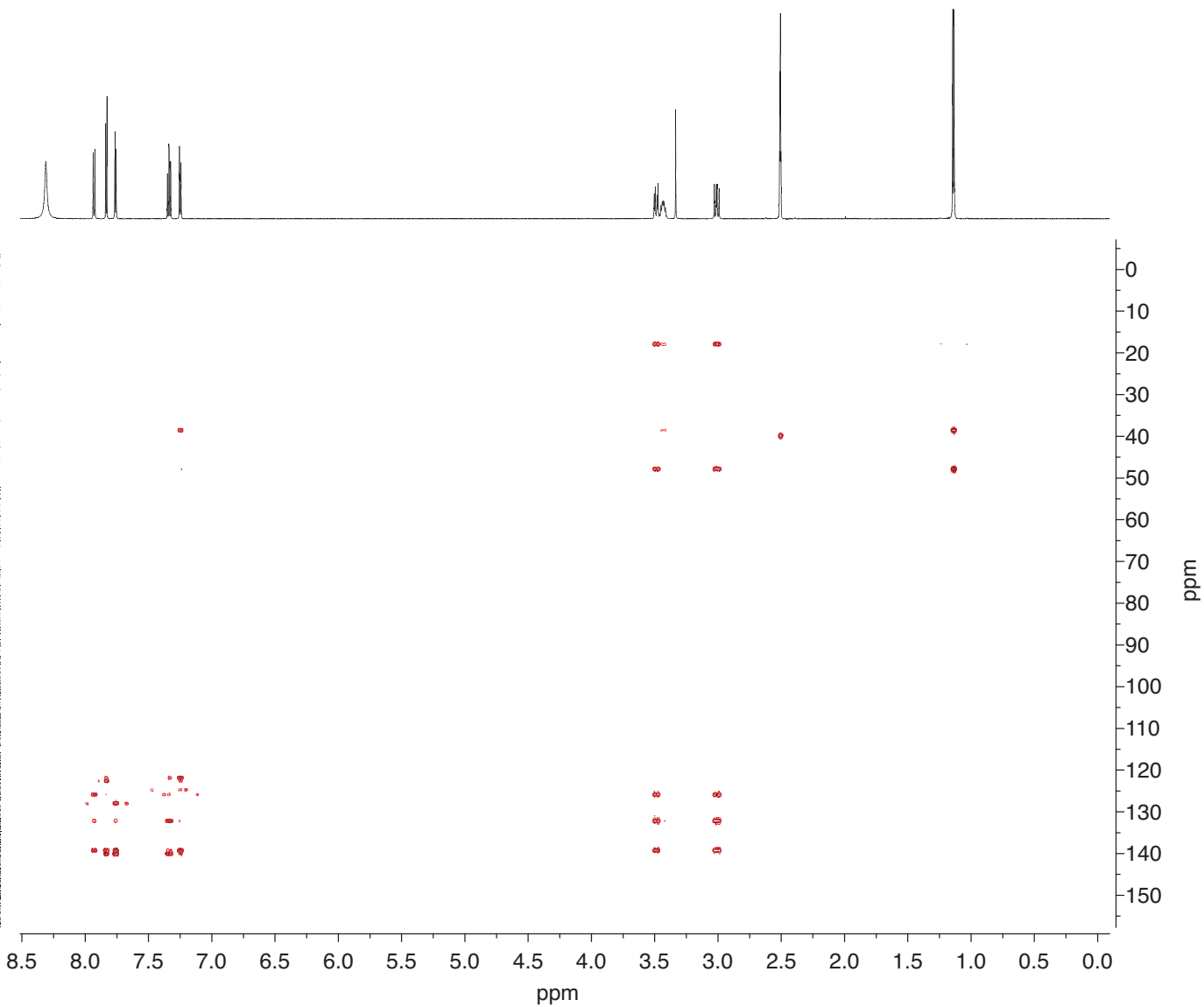
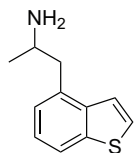
Supporting Information – Drug Testing and Analysis

4-APBT HCl
HSQC
d₆-DMSO

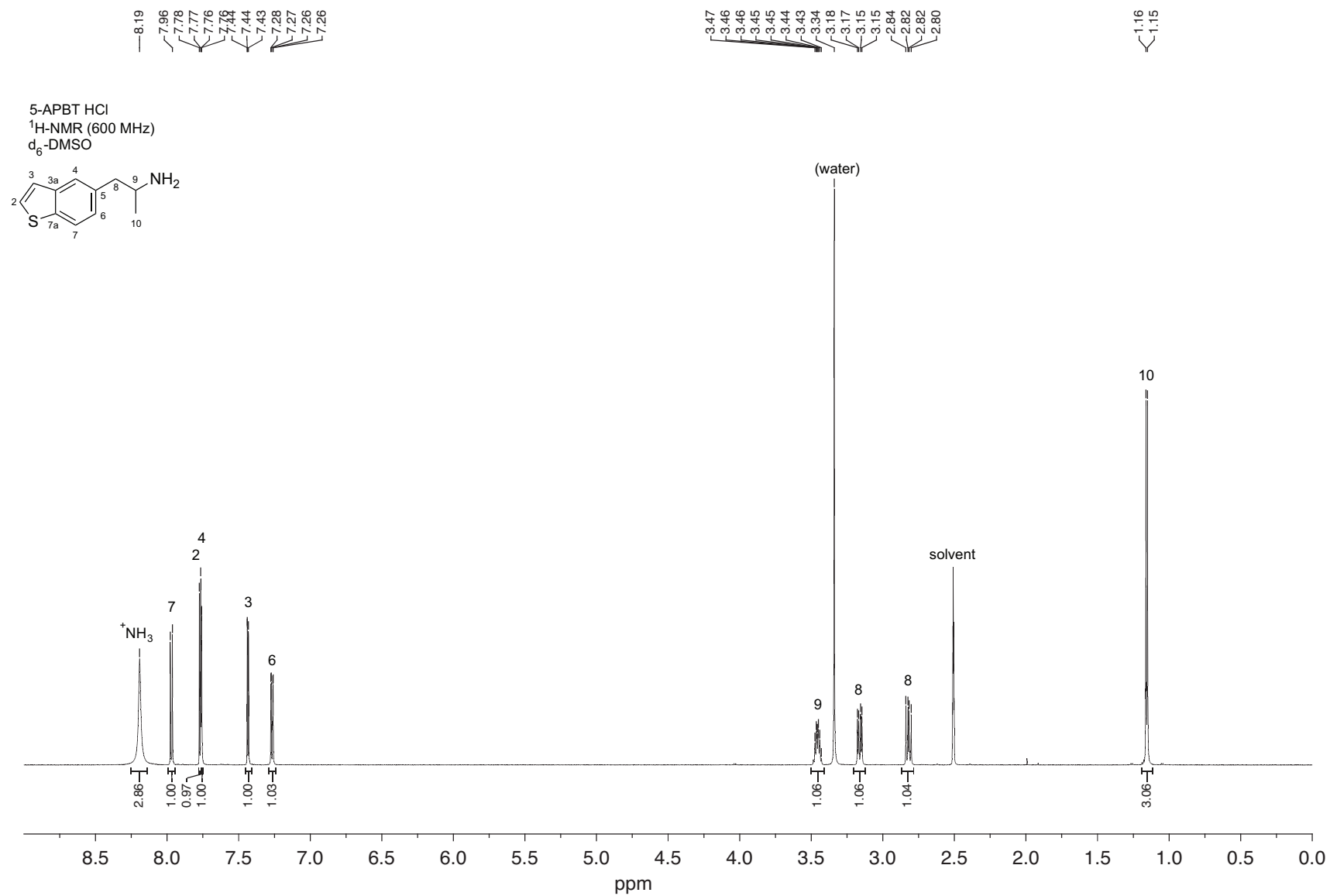


Supporting Information – Drug Testing and Analysis

4-APBT HCl
HMBC
d₆-DMSO

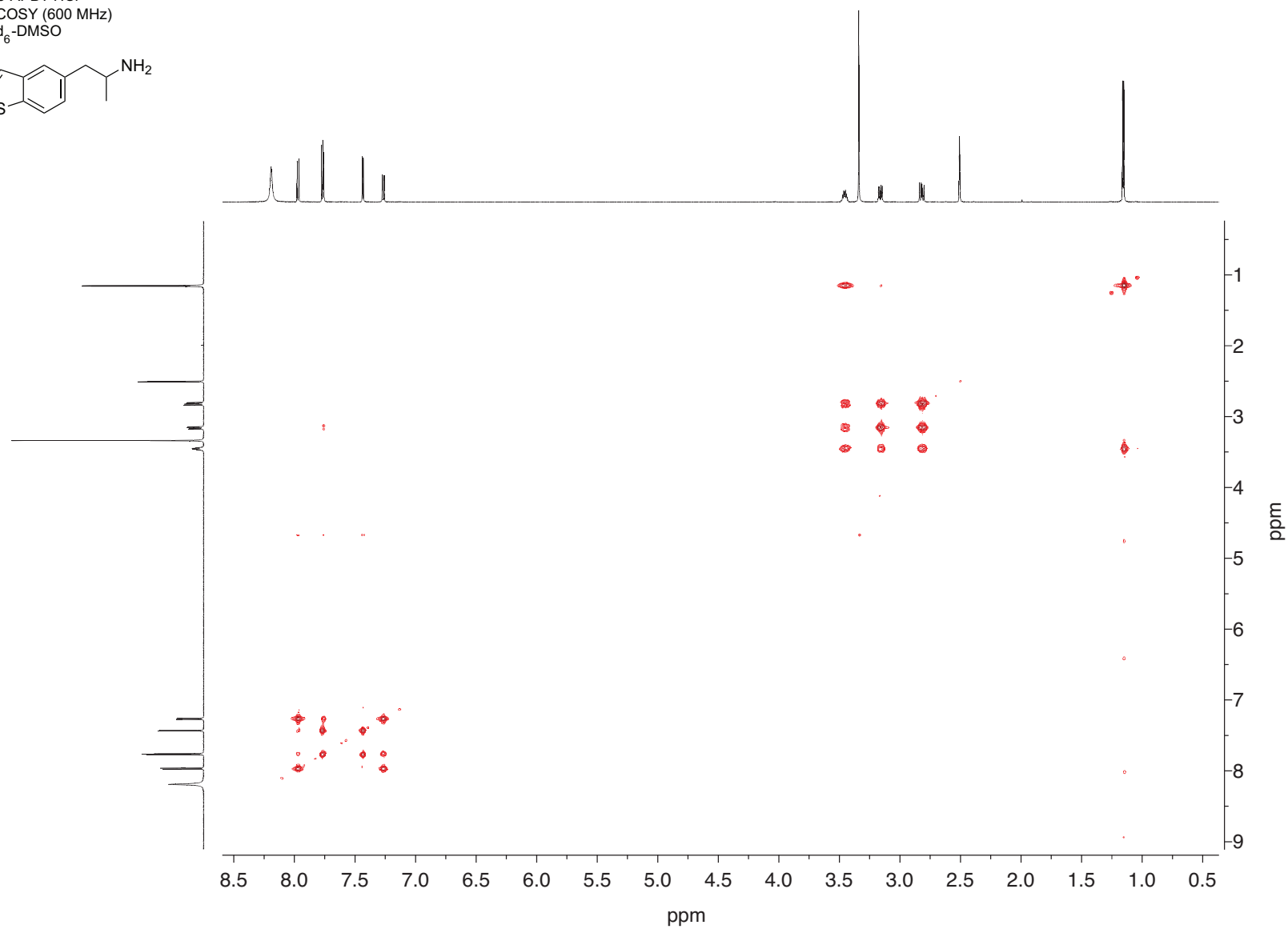
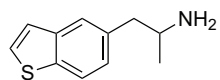


Supporting Information – Drug Testing and Analysis

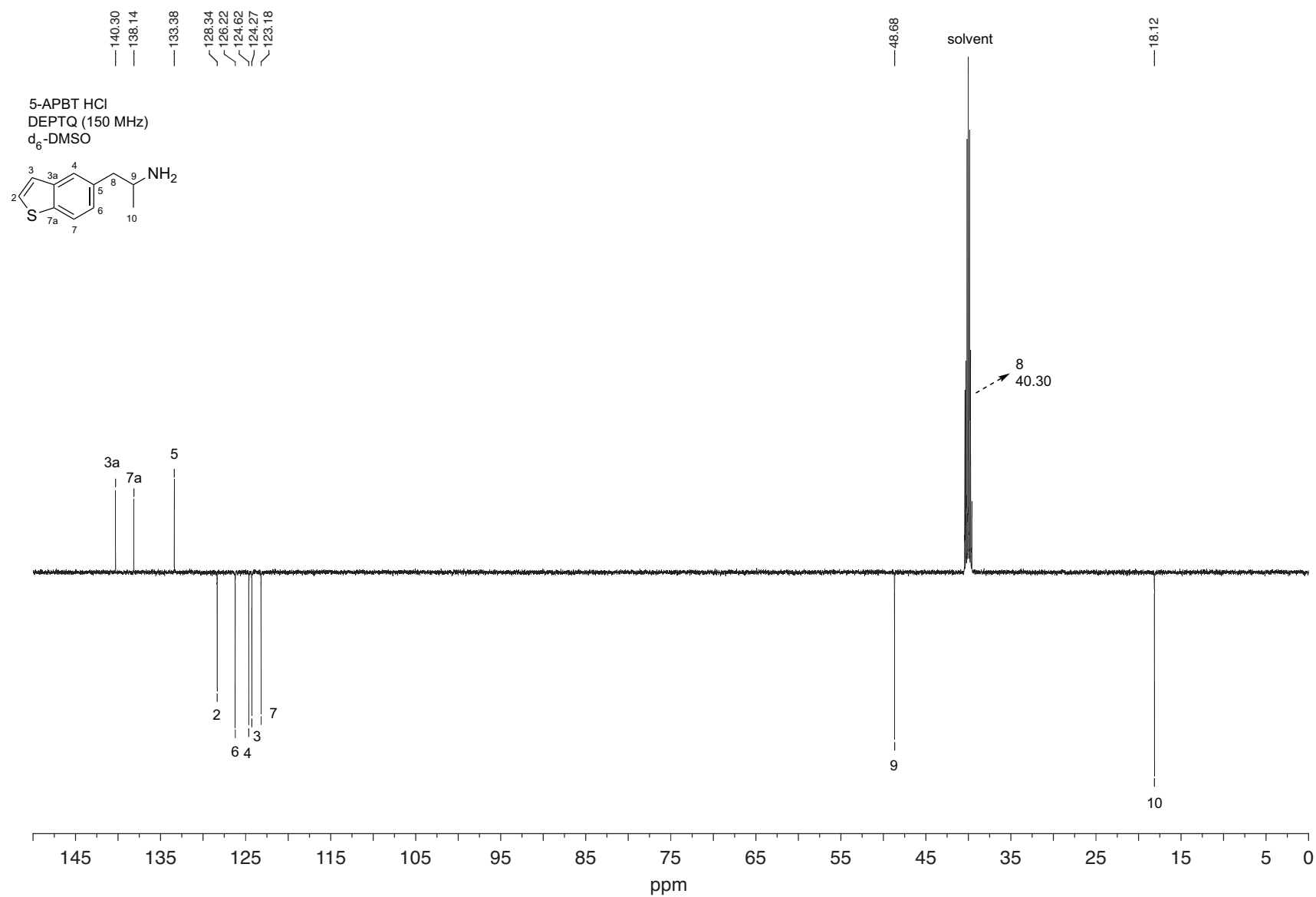


Supporting Information – Drug Testing and Analysis

5-APBT HCl
COSY (600 MHz)
d₆-DMSO

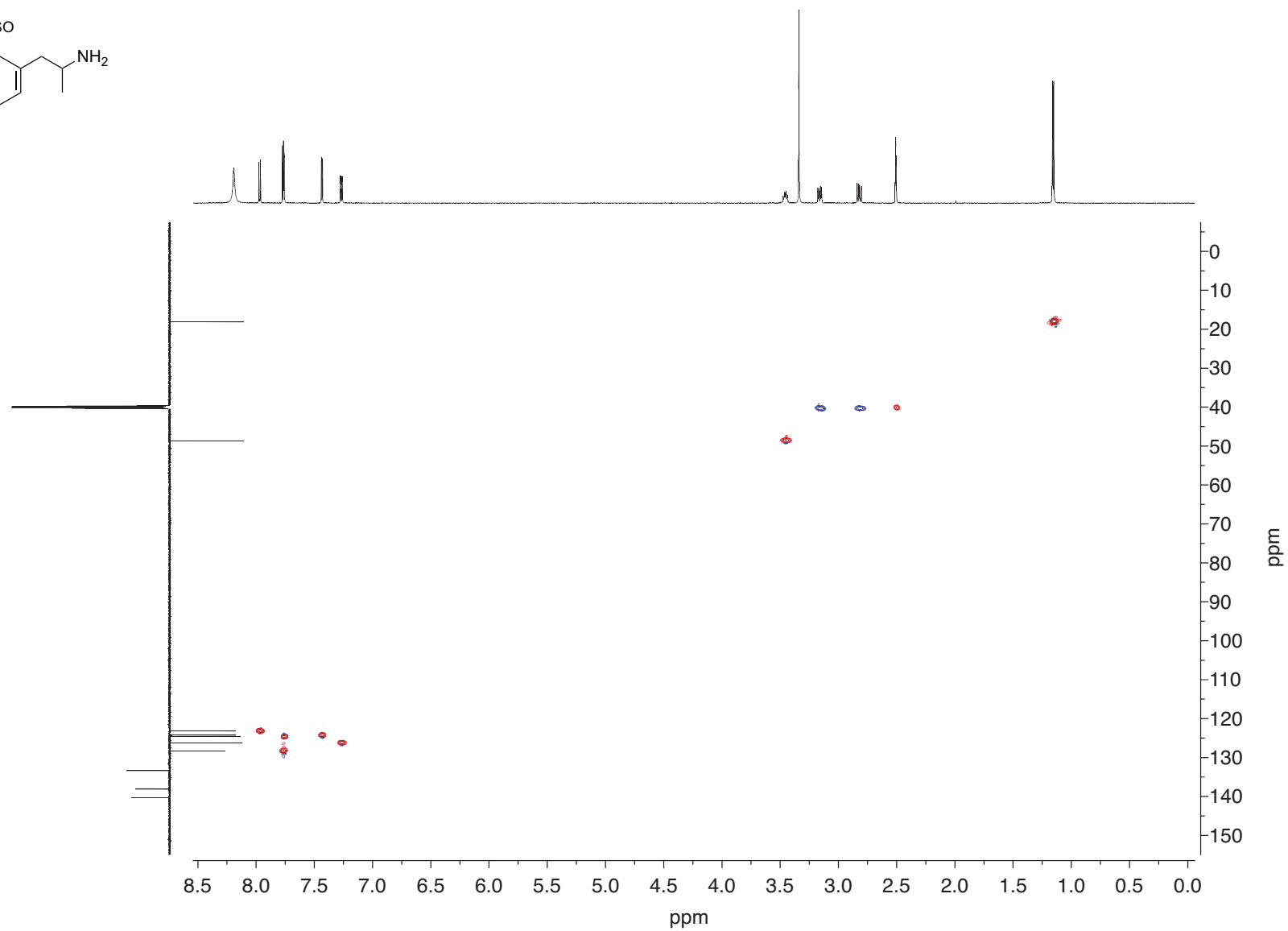
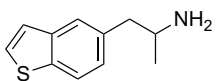


Supporting Information – Drug Testing and Analysis



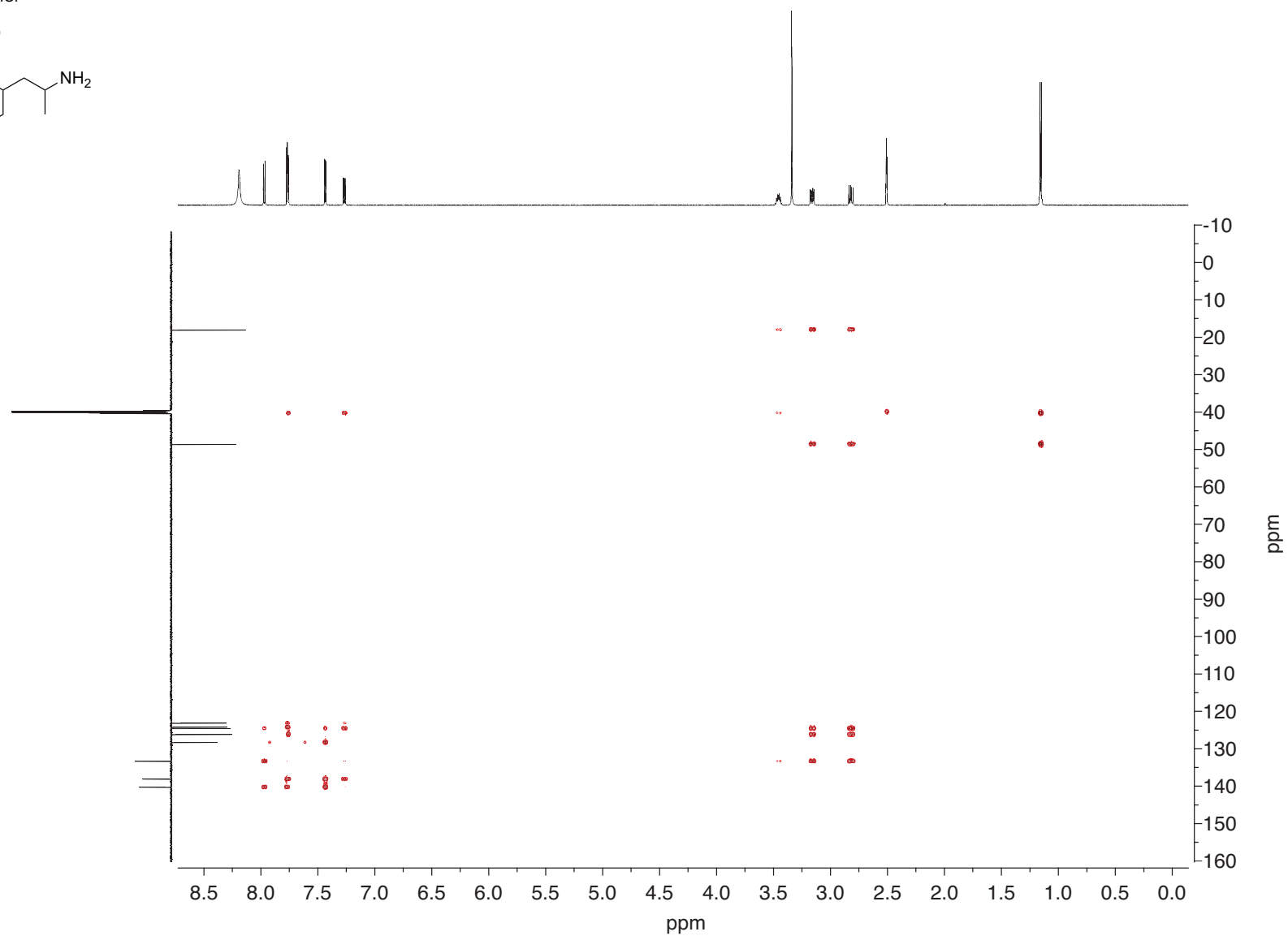
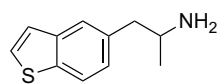
Supporting Information – Drug Testing and Analysis

5-APBT HCl
HSQC
d₆-DMSO



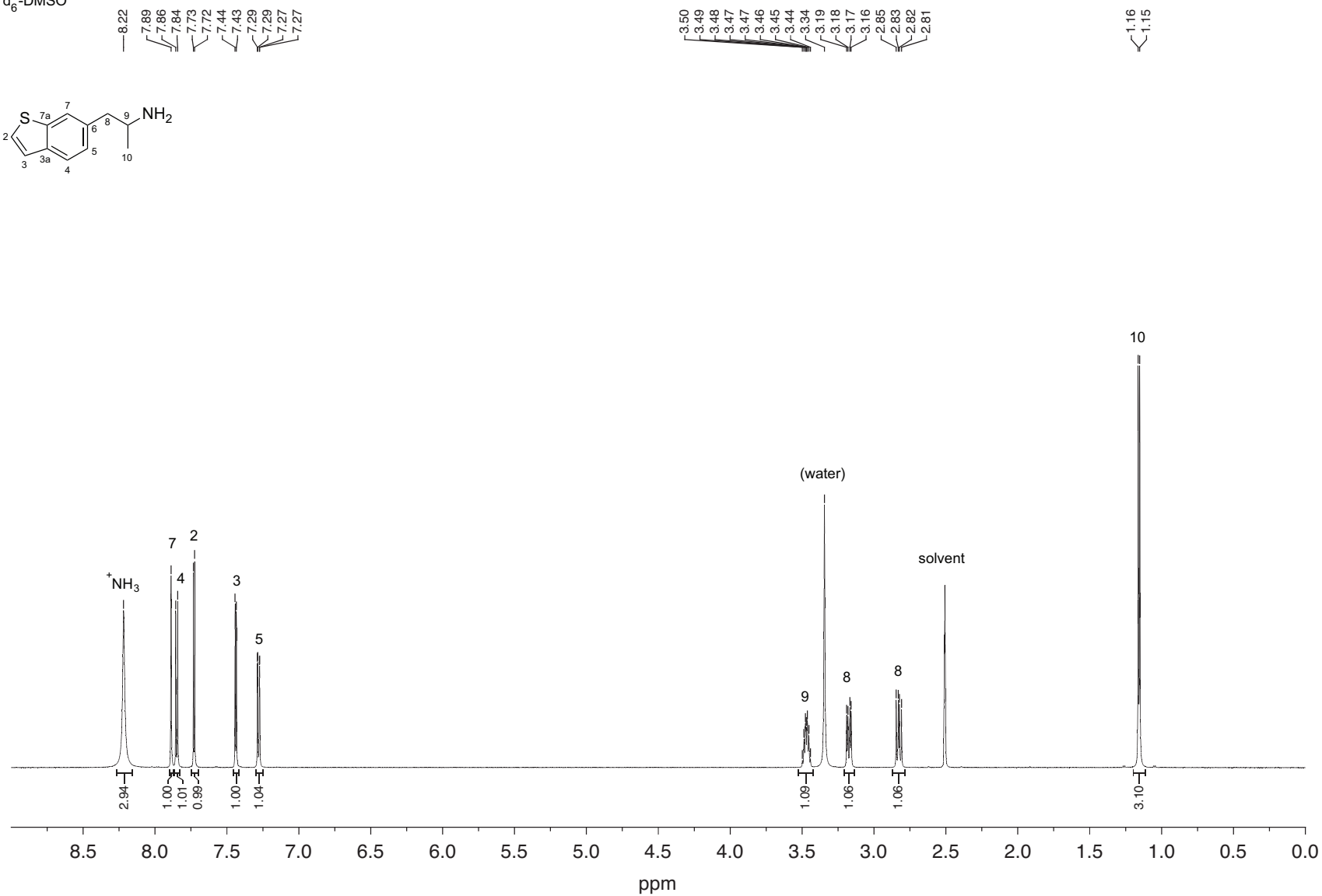
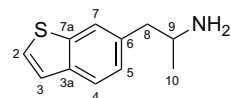
Supporting Information – Drug Testing and Analysis

5-APBT HCl
HMBC
d₆-DMSO



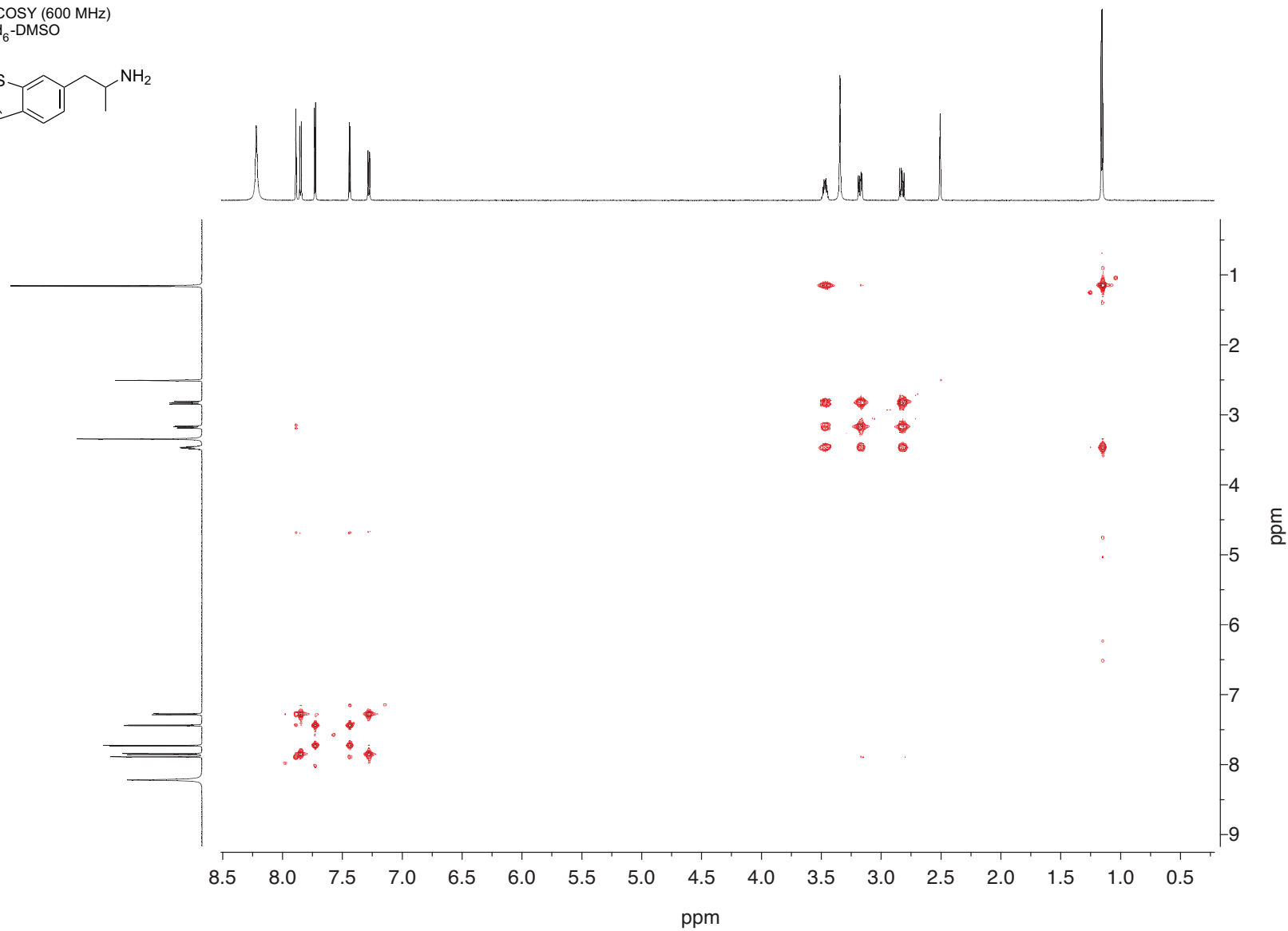
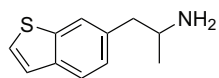
Supporting Information – Drug Testing and Analysis

6-APBT HCl
¹H-NMR (600 MHz)
d₆-DMSO

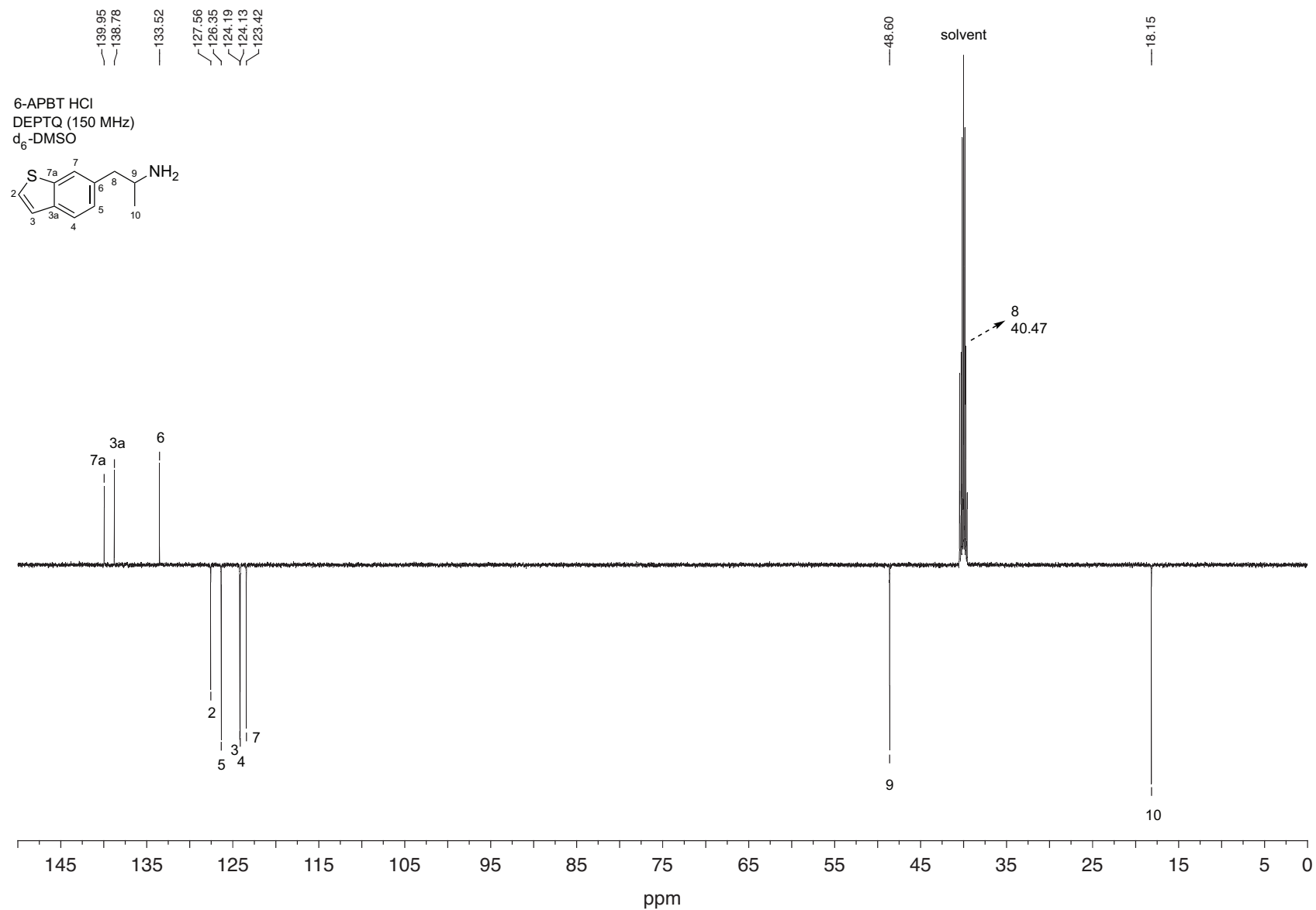


Supporting Information – Drug Testing and Analysis

6-APBT HCl
COSY (600 MHz)
d₆-DMSO

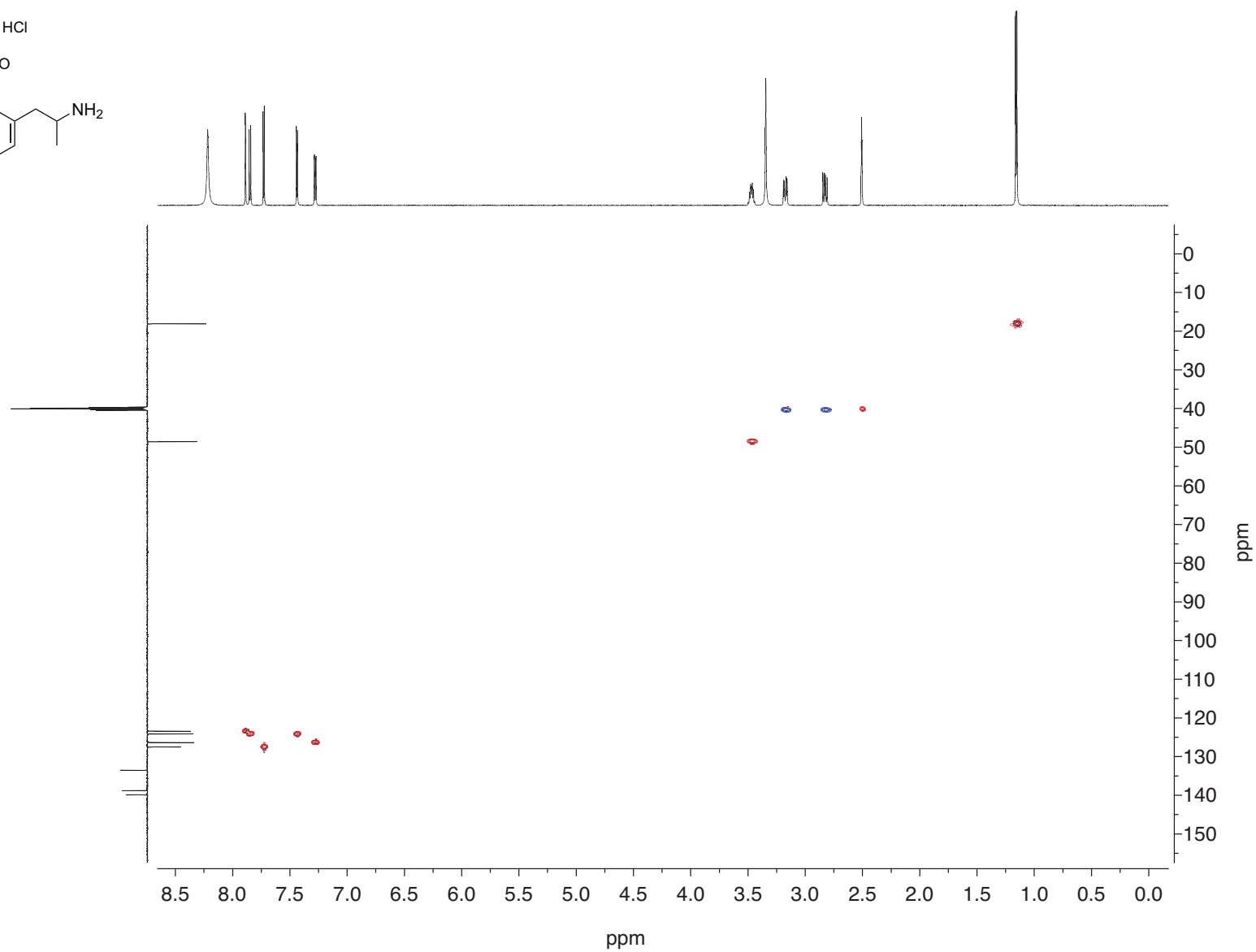
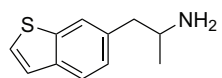


Supporting Information – Drug Testing and Analysis



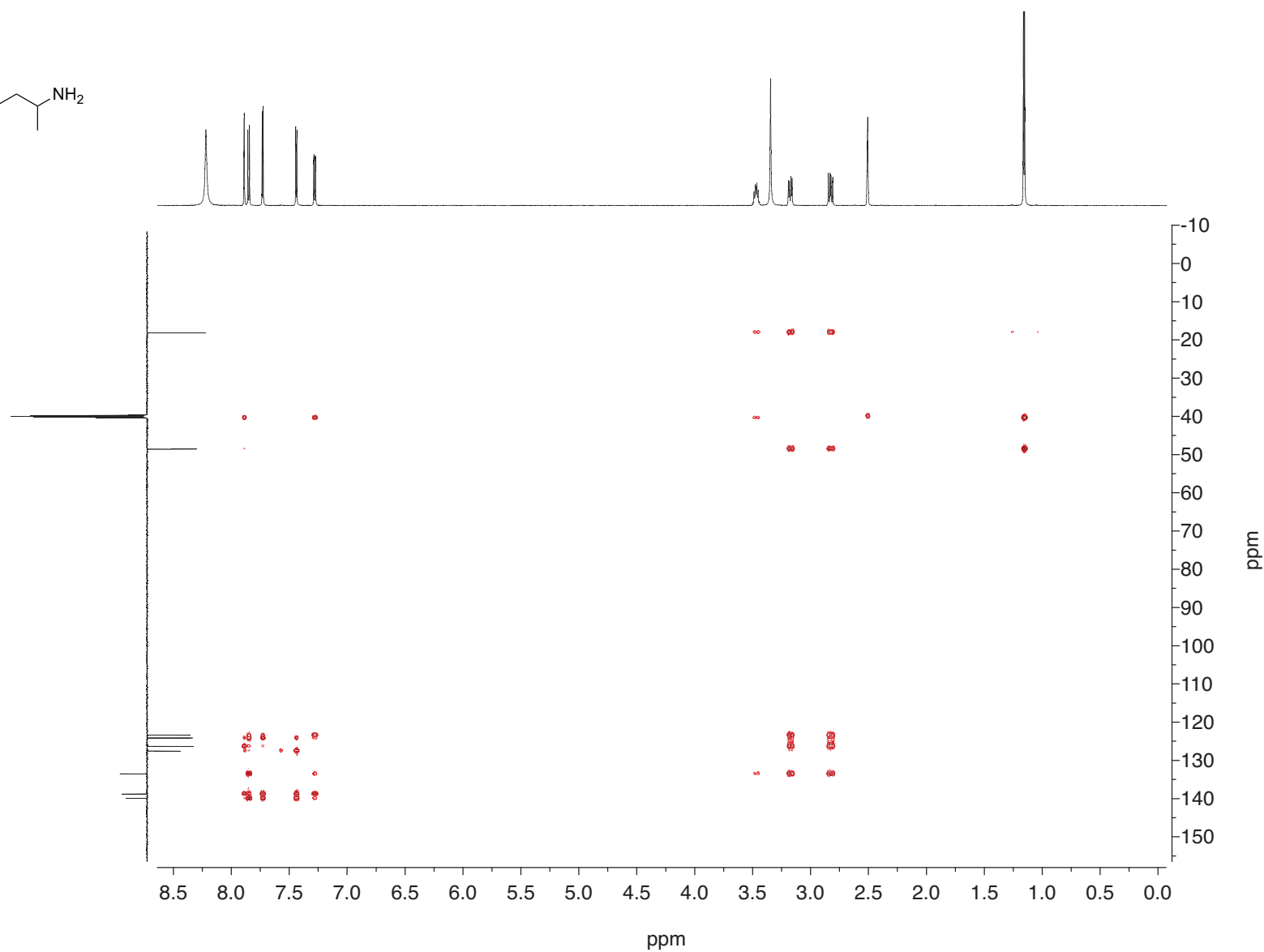
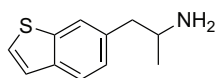
Supporting Information – Drug Testing and Analysis

6-APBT HCl
HSQC
d₆-DMSO



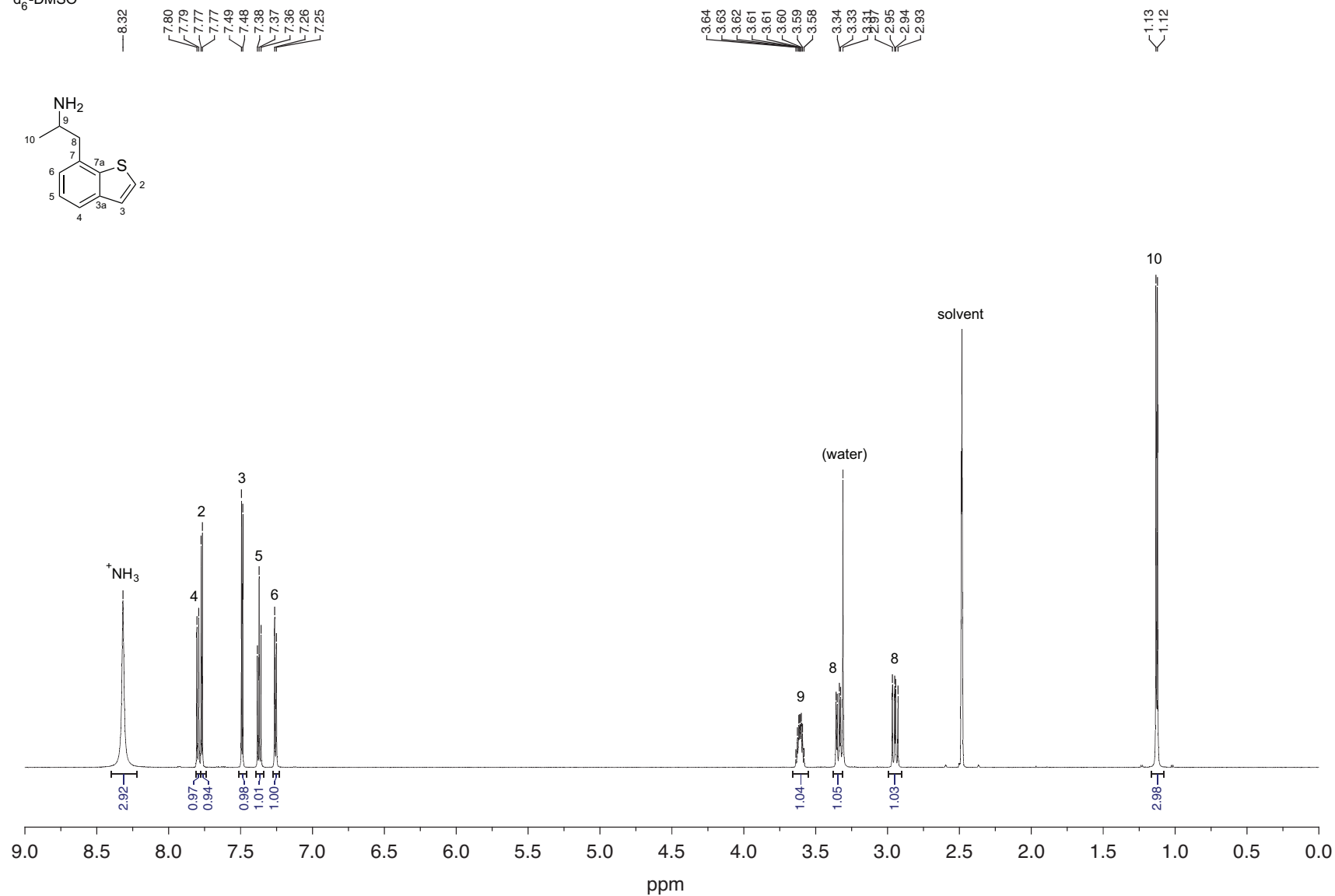
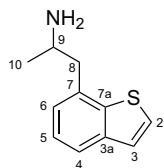
Supporting Information – Drug Testing and Analysis

6-APBT HCl
HMBC
d₆-DMSO



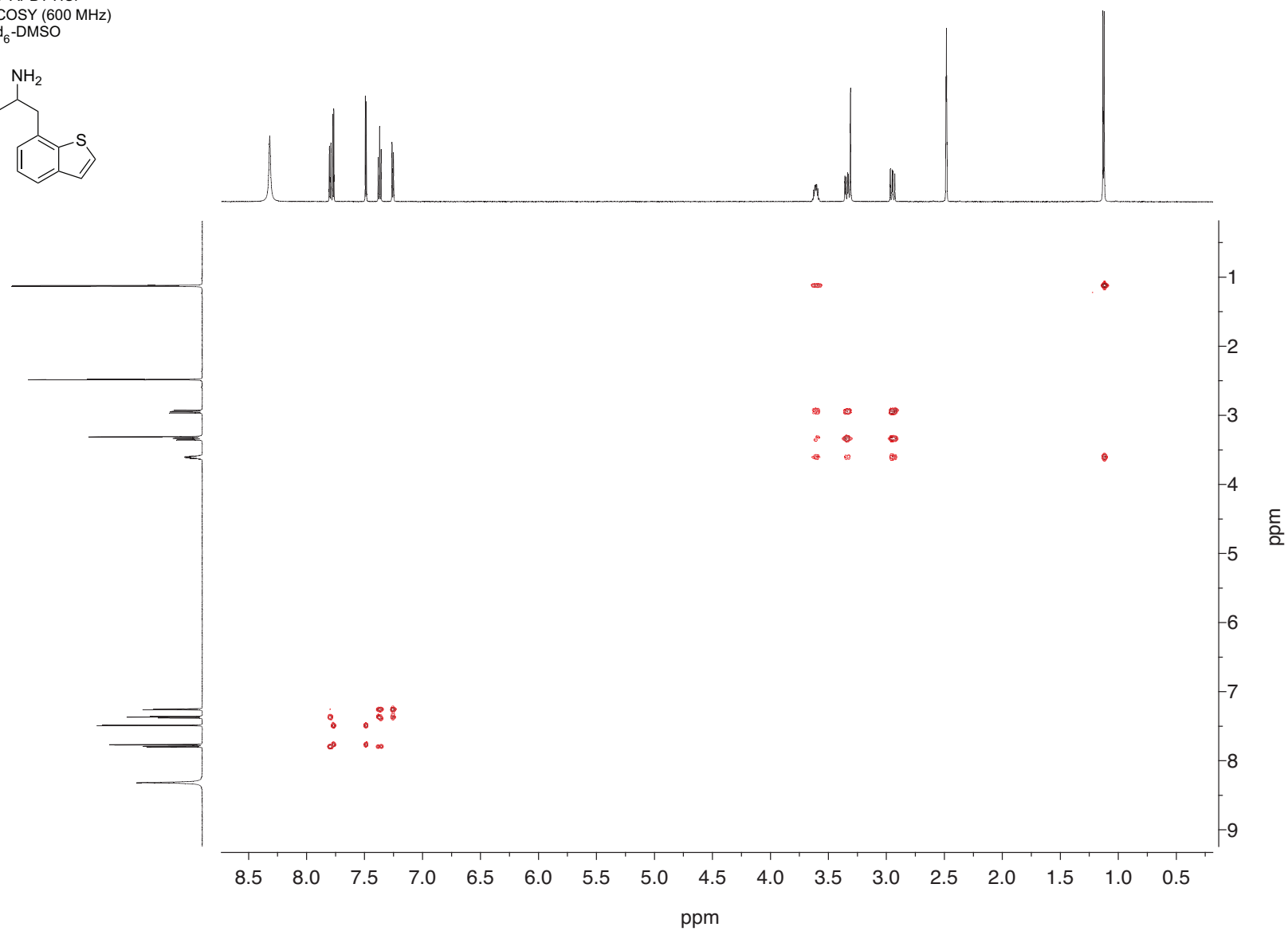
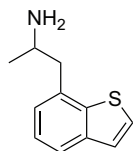
Supporting Information – Drug Testing and Analysis

7-APBT HCl
¹H-NMR (600 MHz)
d₆-DMSO



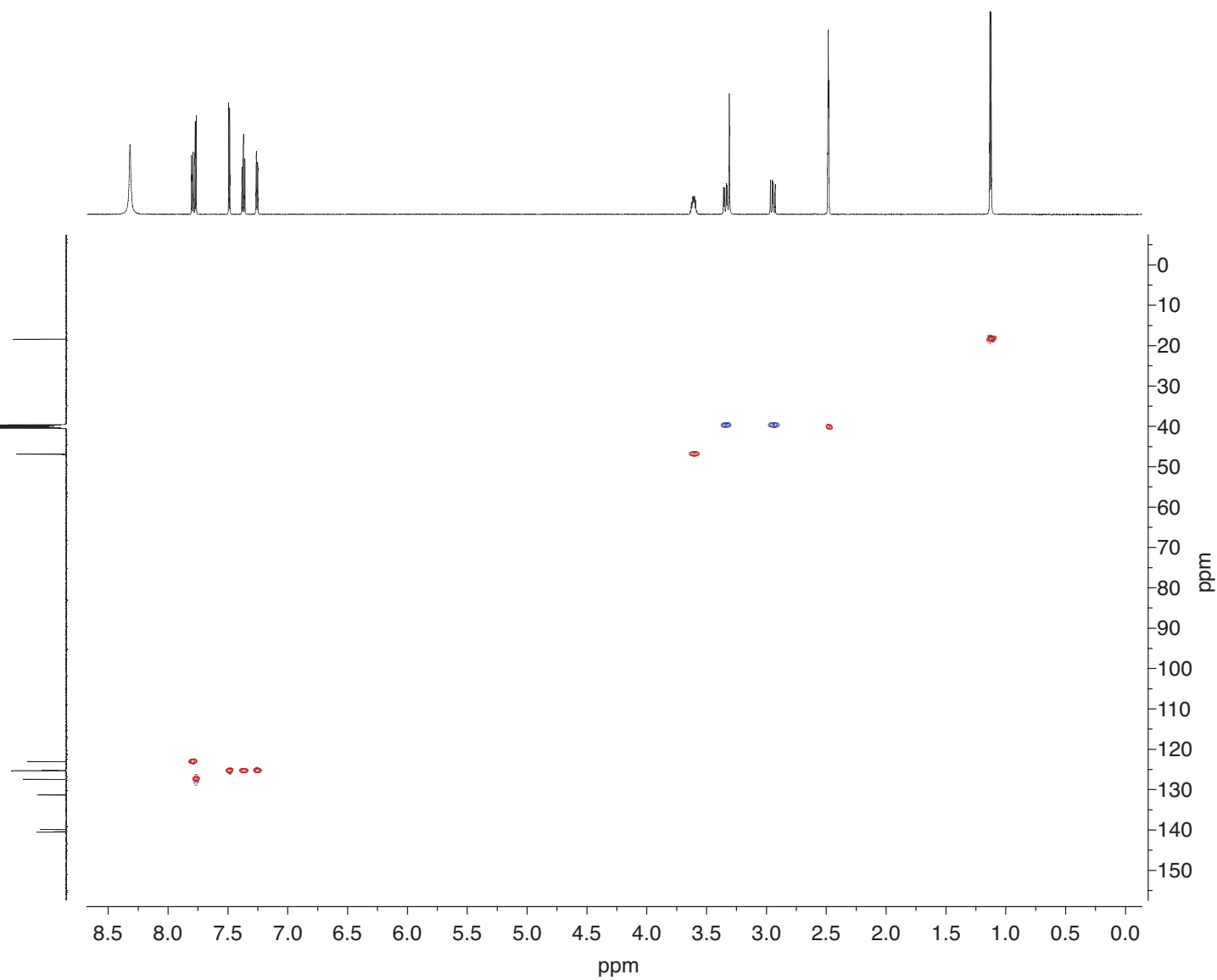
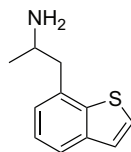
Supporting Information – Drug Testing and Analysis

7-APBT HCl
COSY (600 MHz)
d₆-DMSO



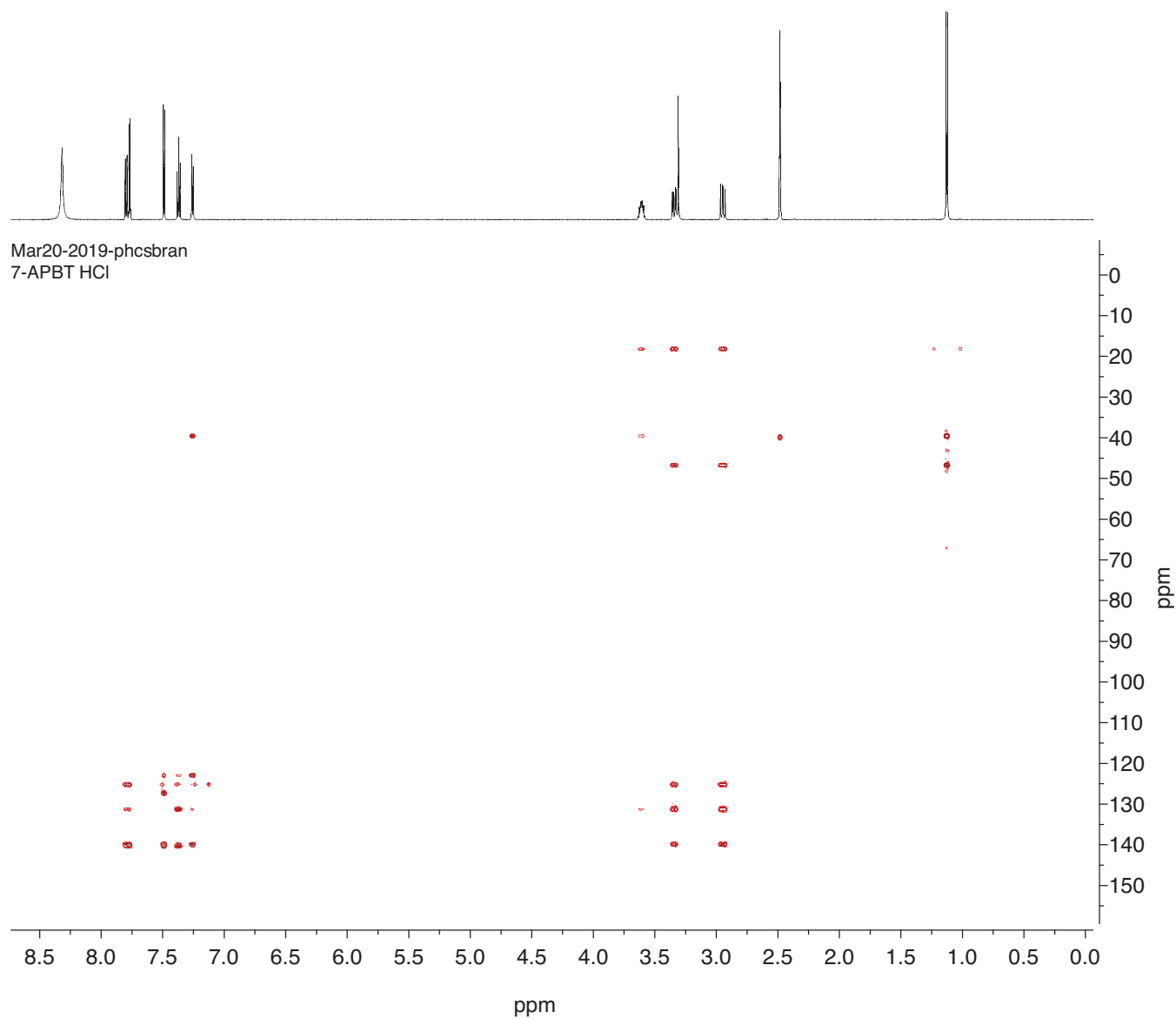
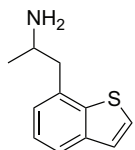
Supporting Information – Drug Testing and Analysis

7-APBT HCl
HSQC
d₆-DMSO

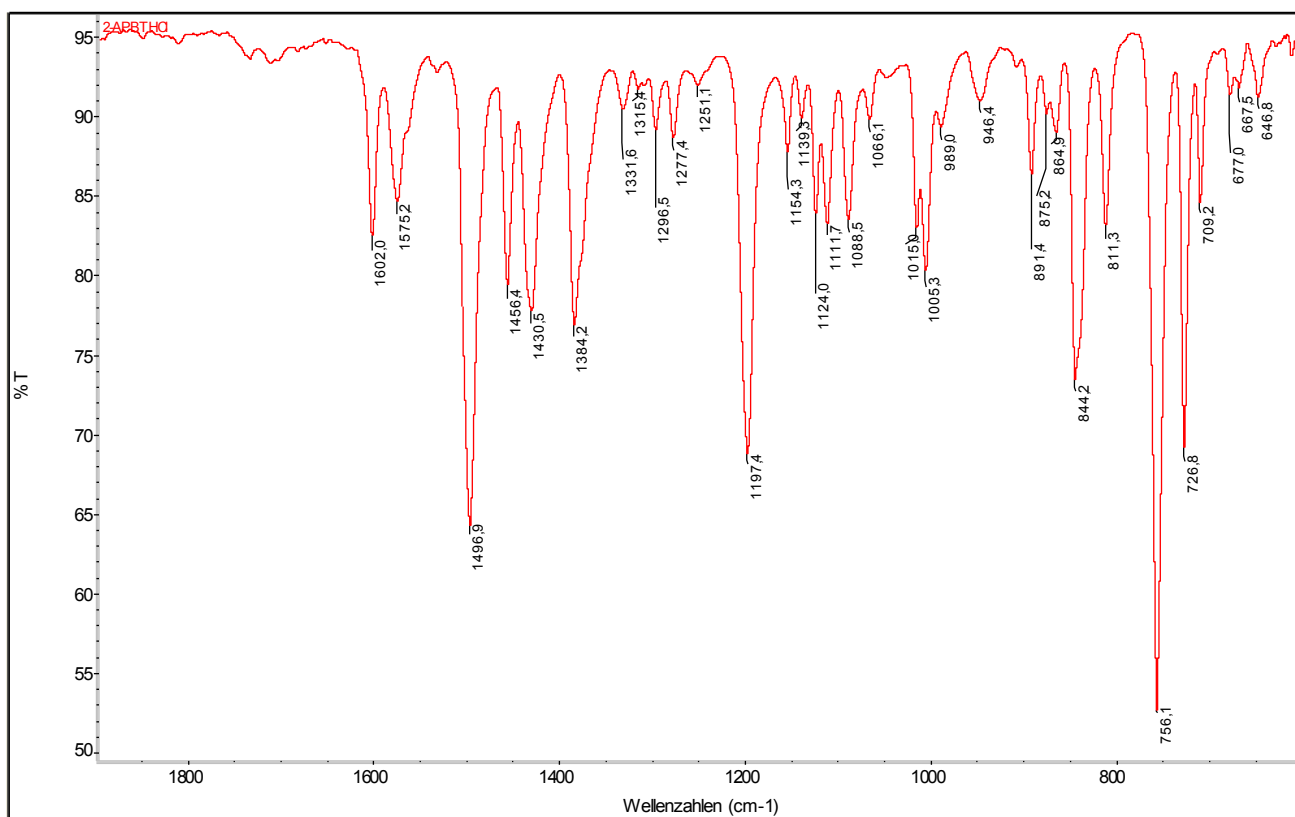
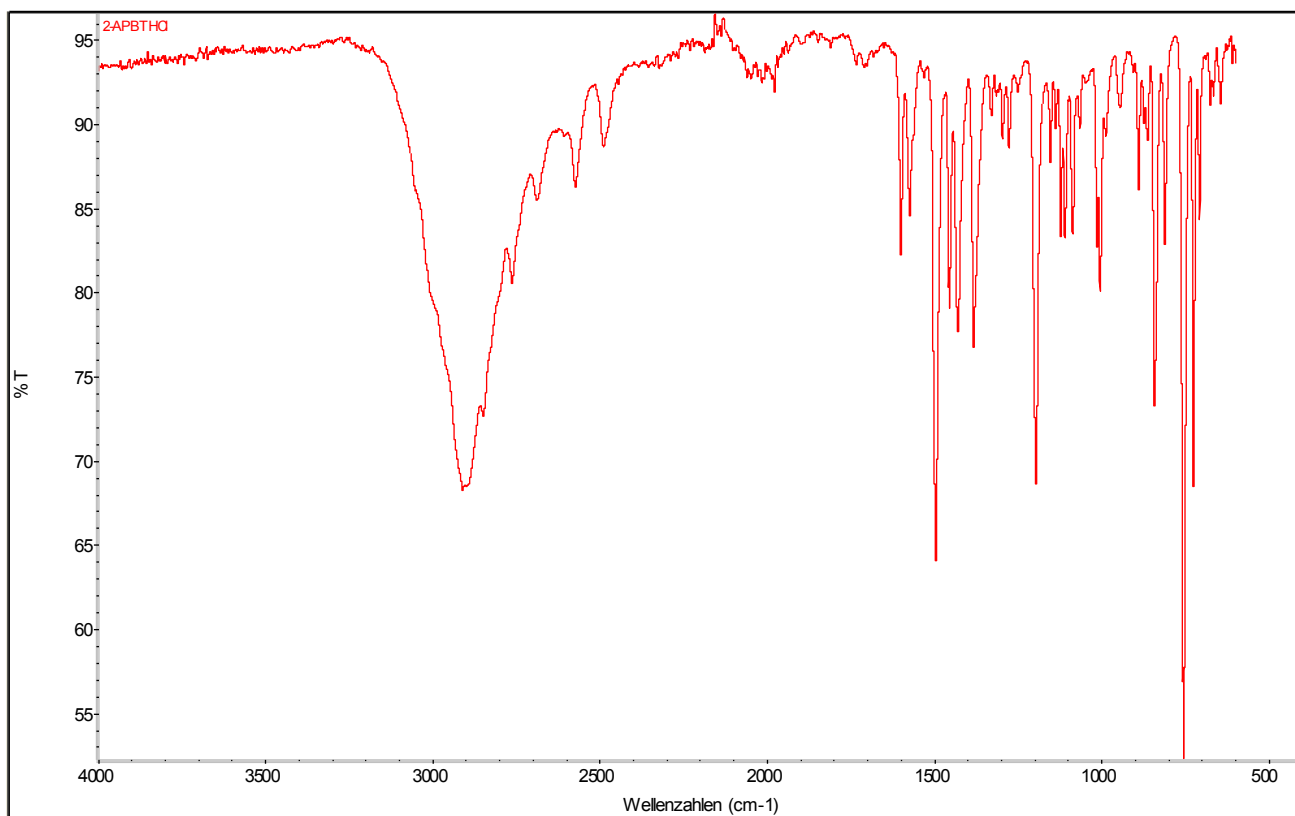


Supporting Information – Drug Testing and Analysis

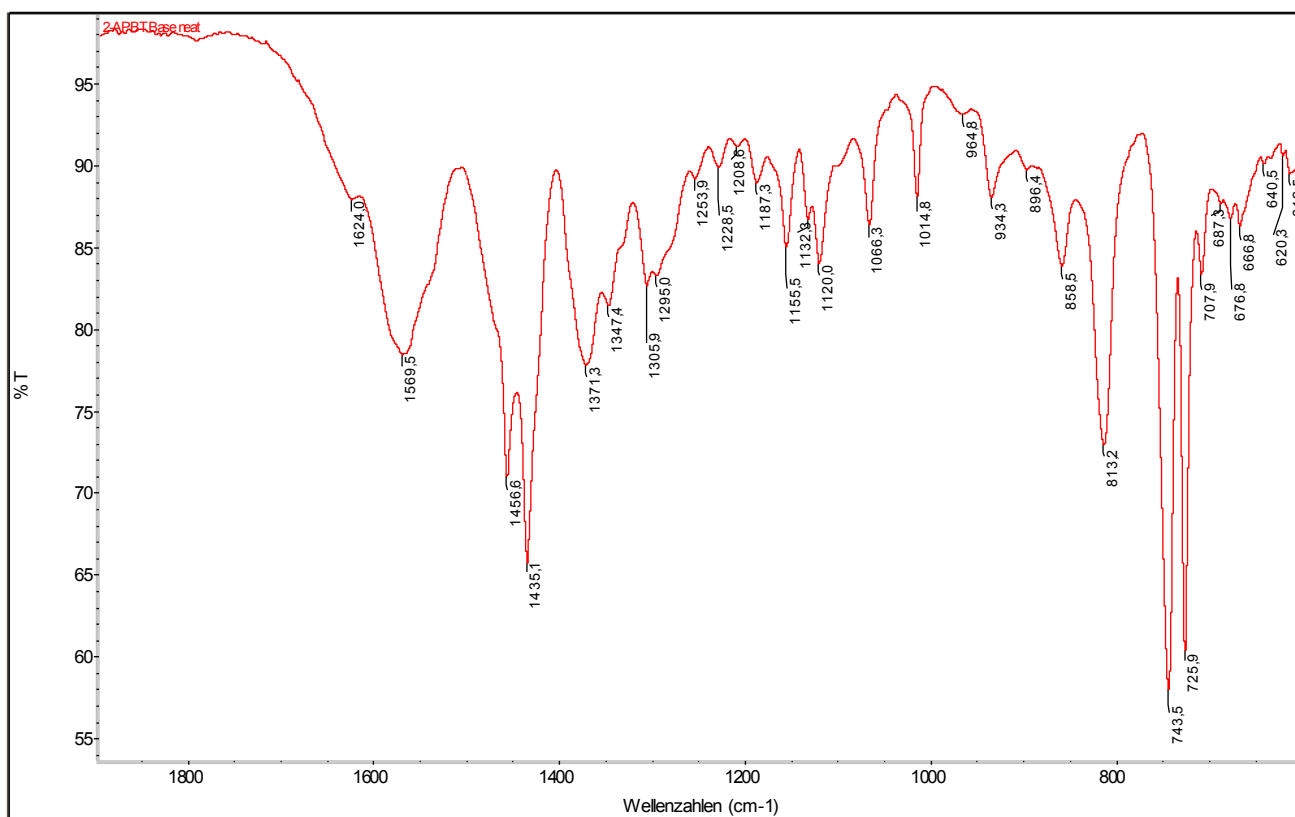
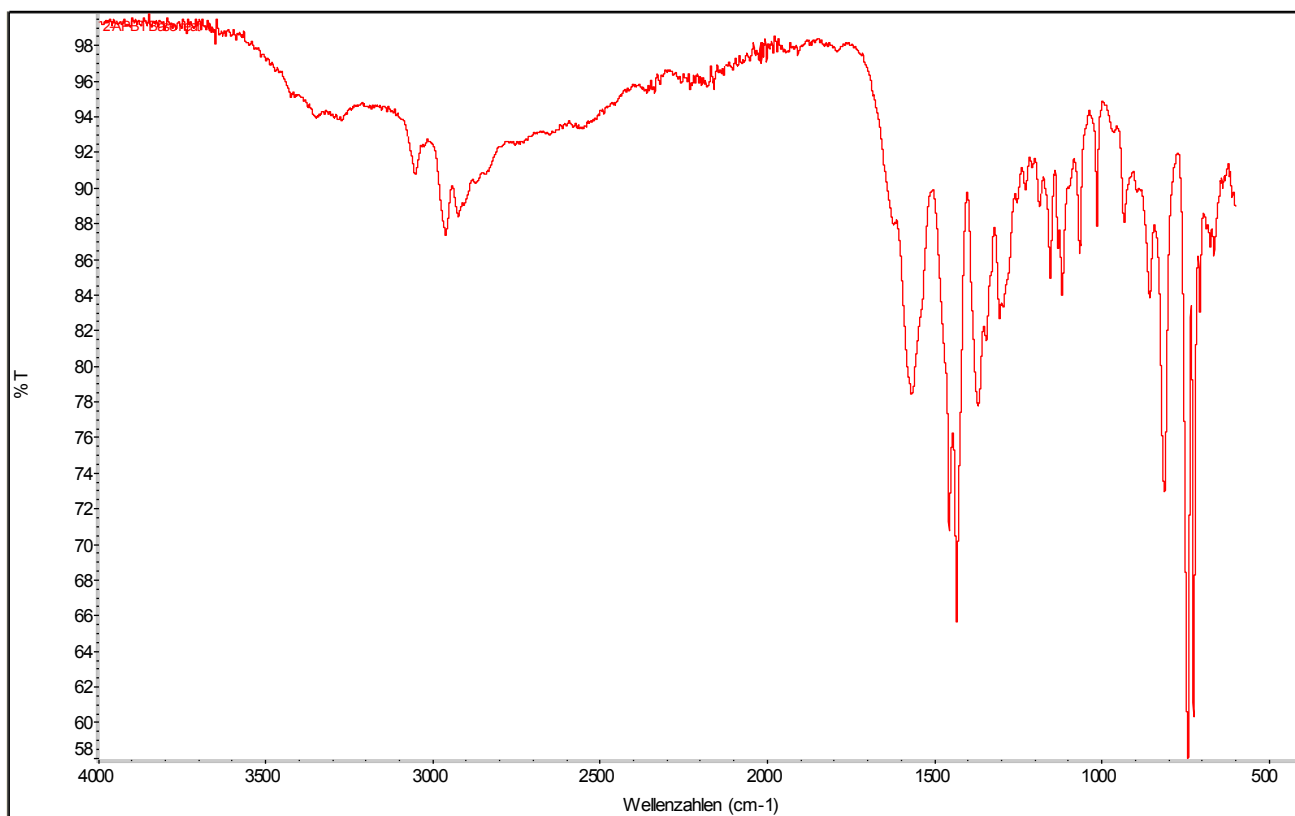
7-APBT HCl
HMBC
d₆-DMSO



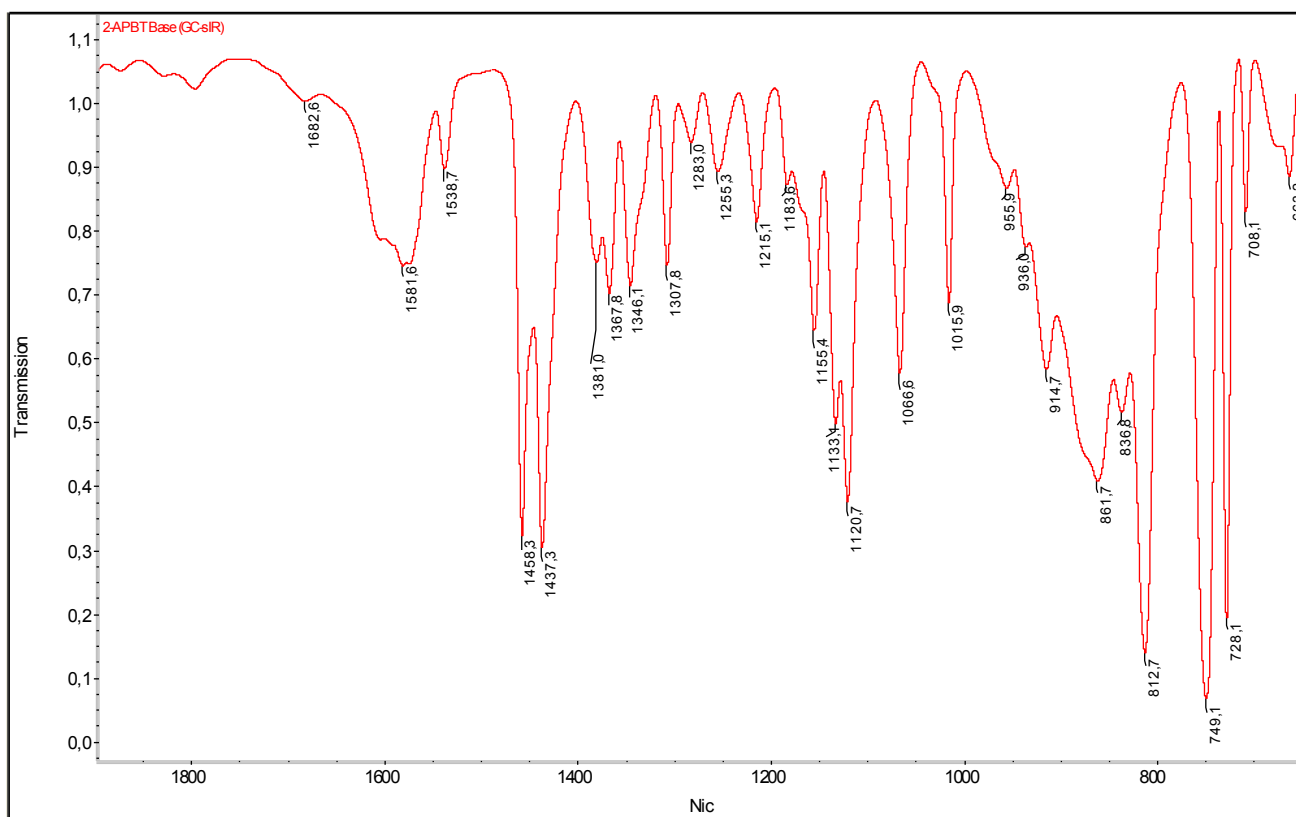
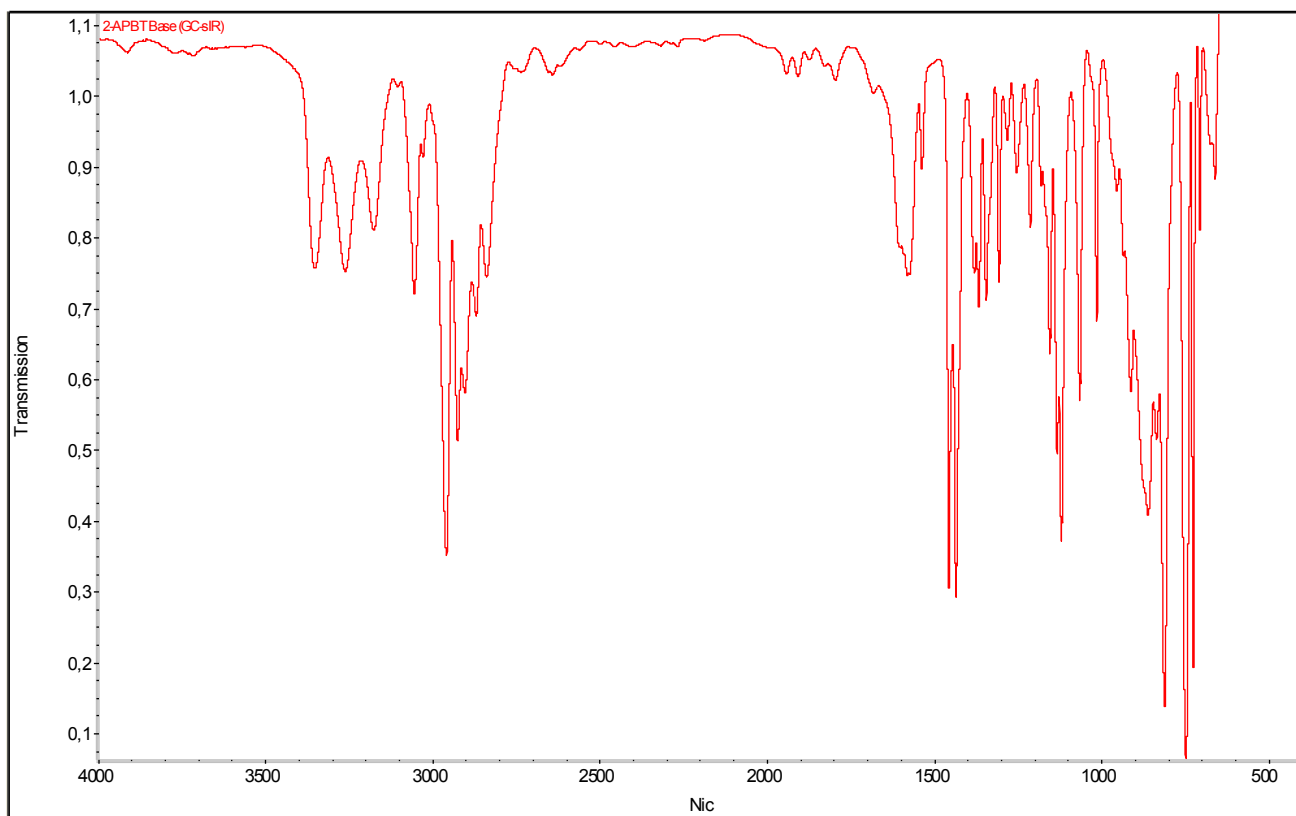
2-APBT HCl – ATR-IR



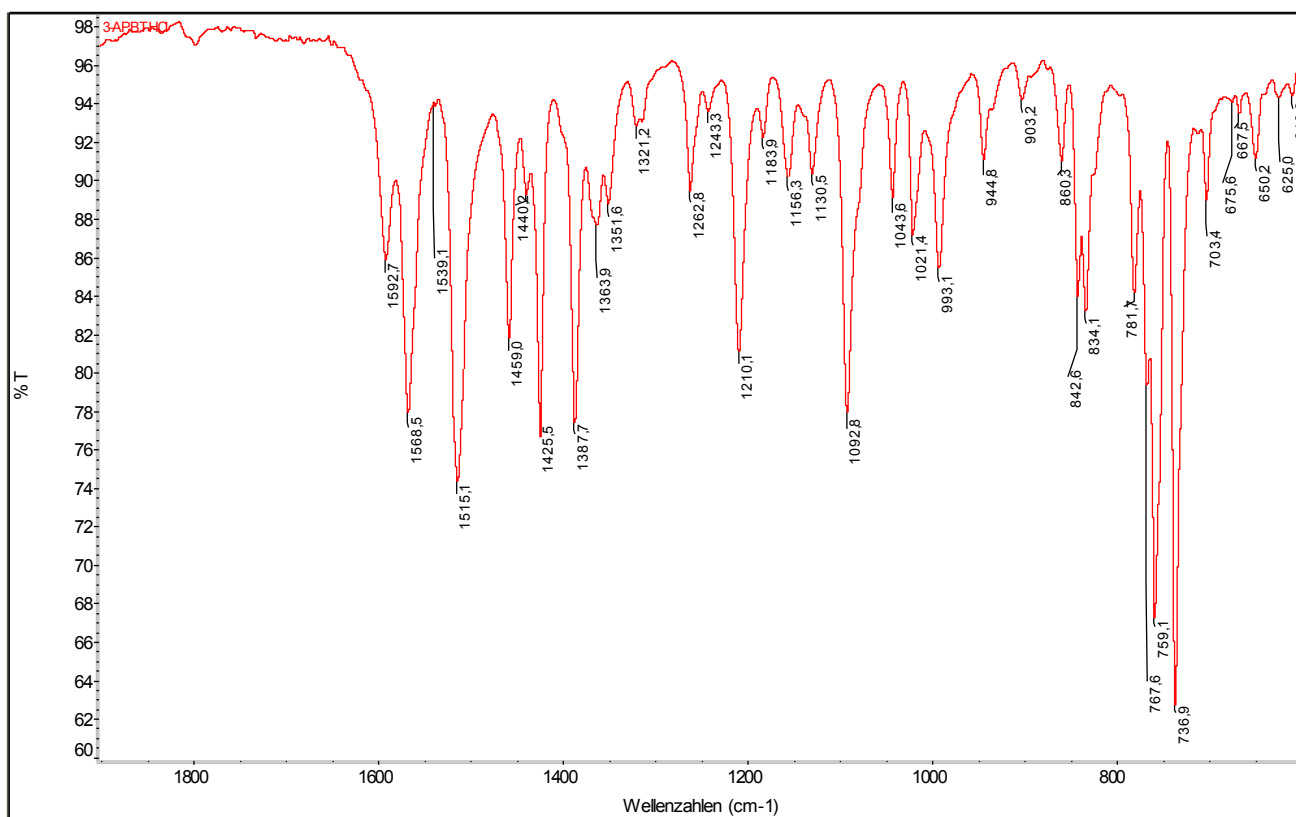
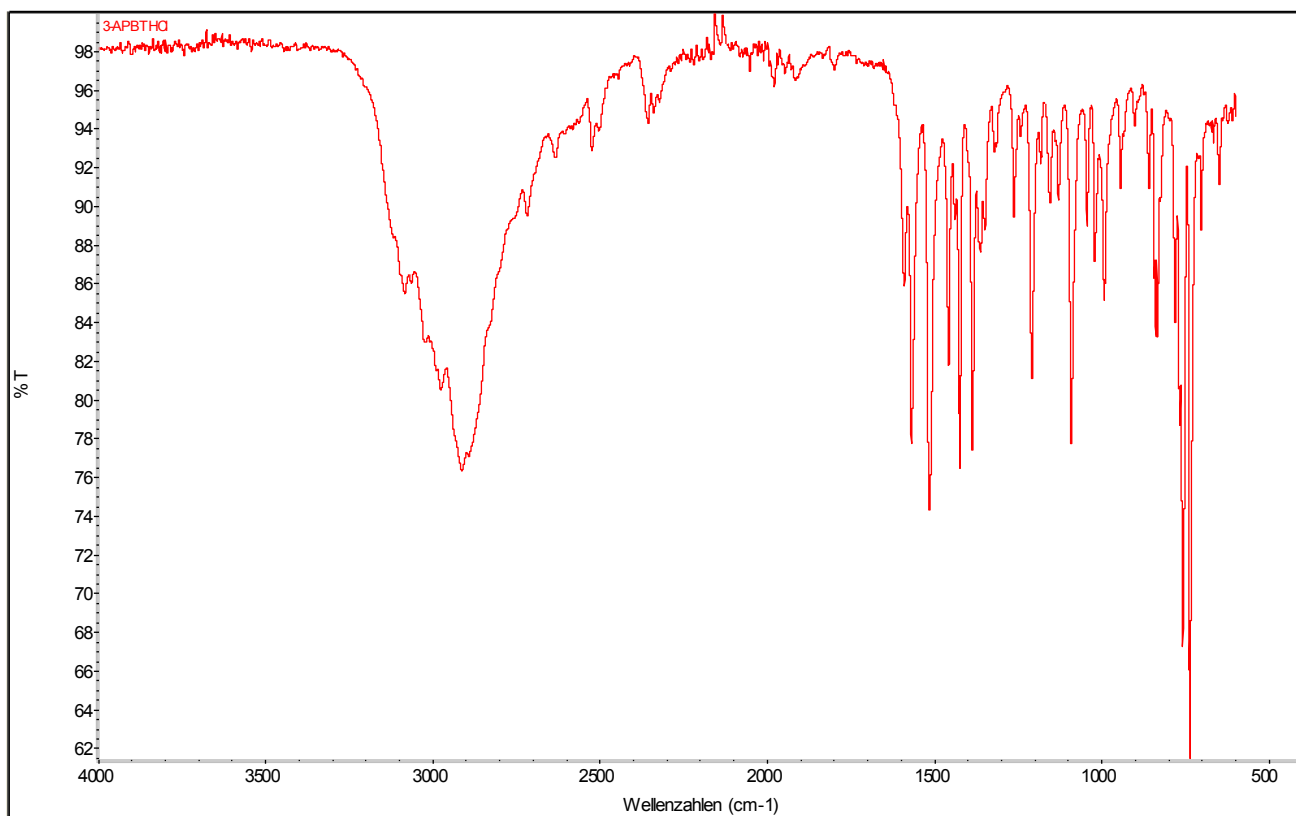
2-APBT base – ATR-IR



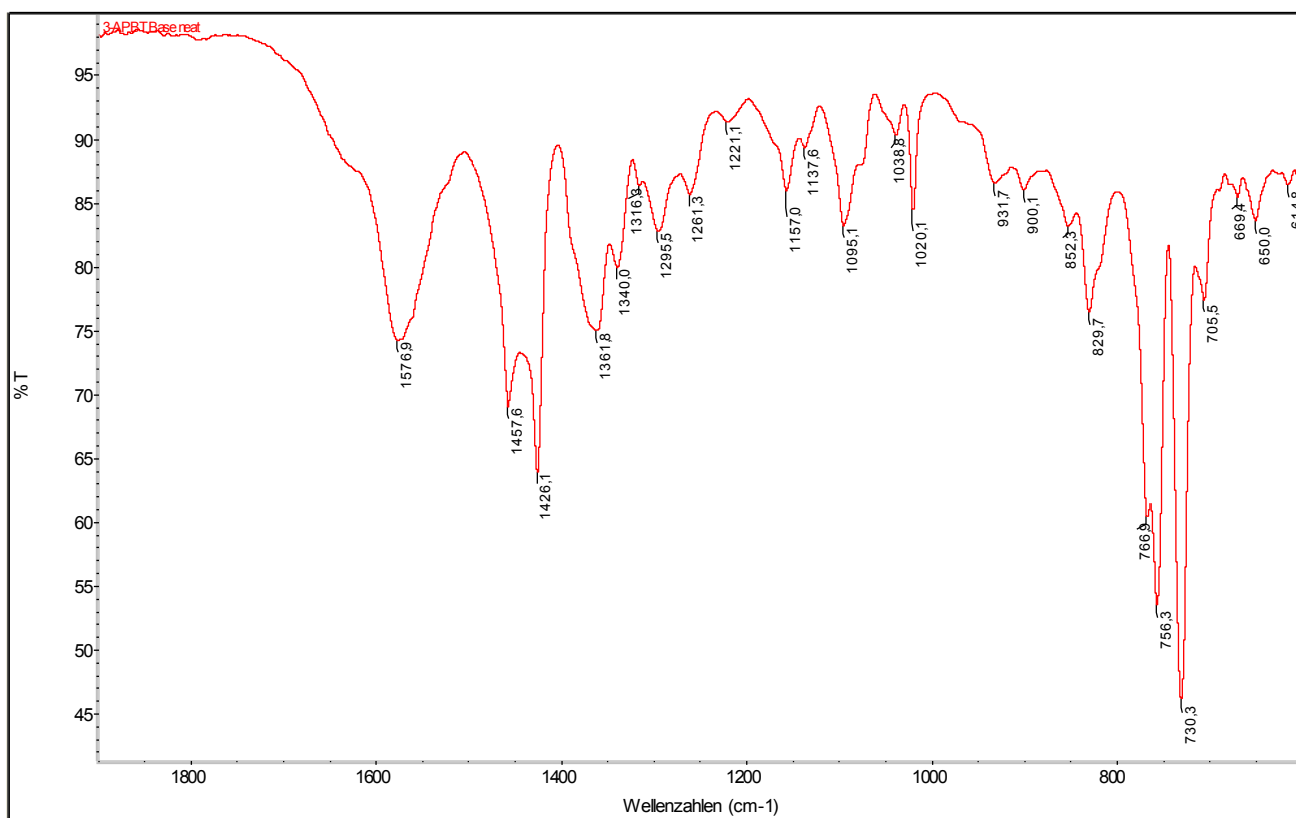
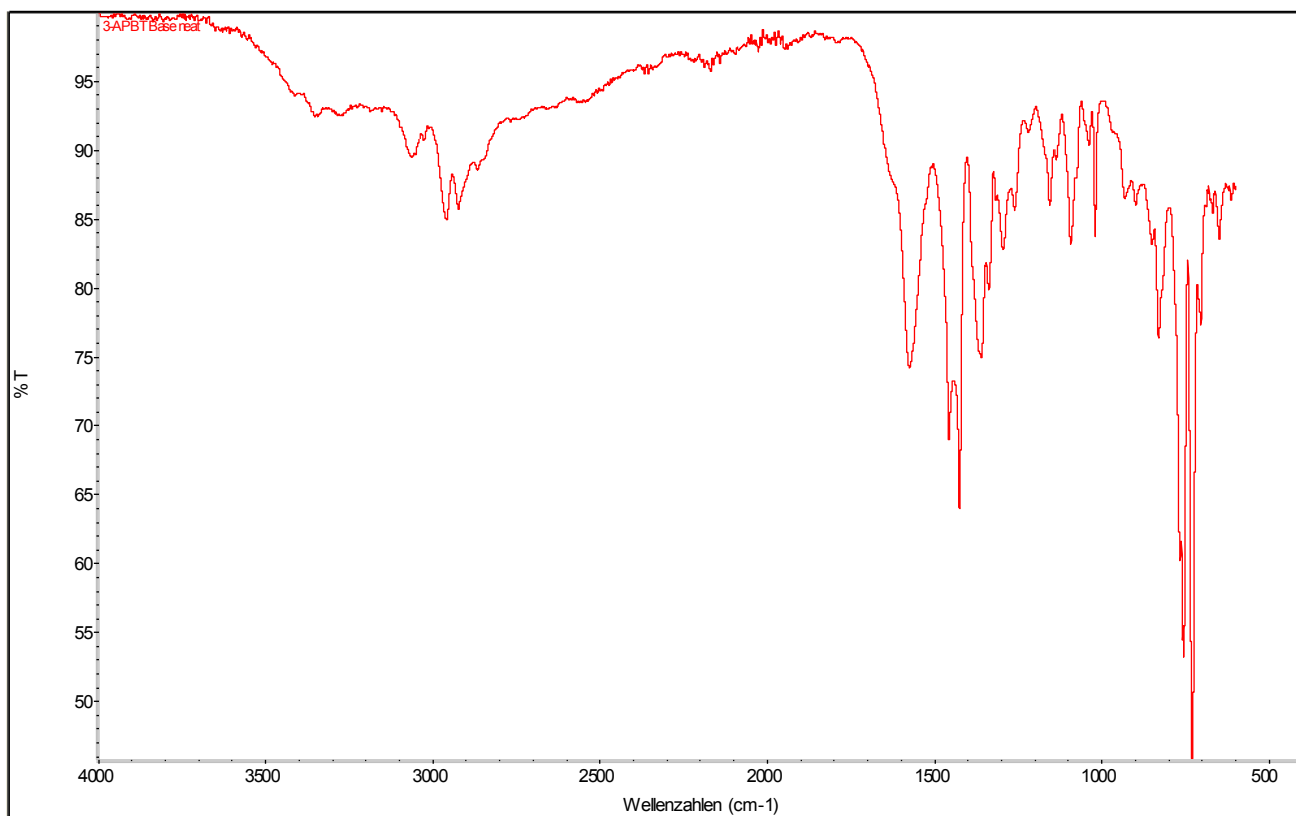
2-APBT base – GC-sIR



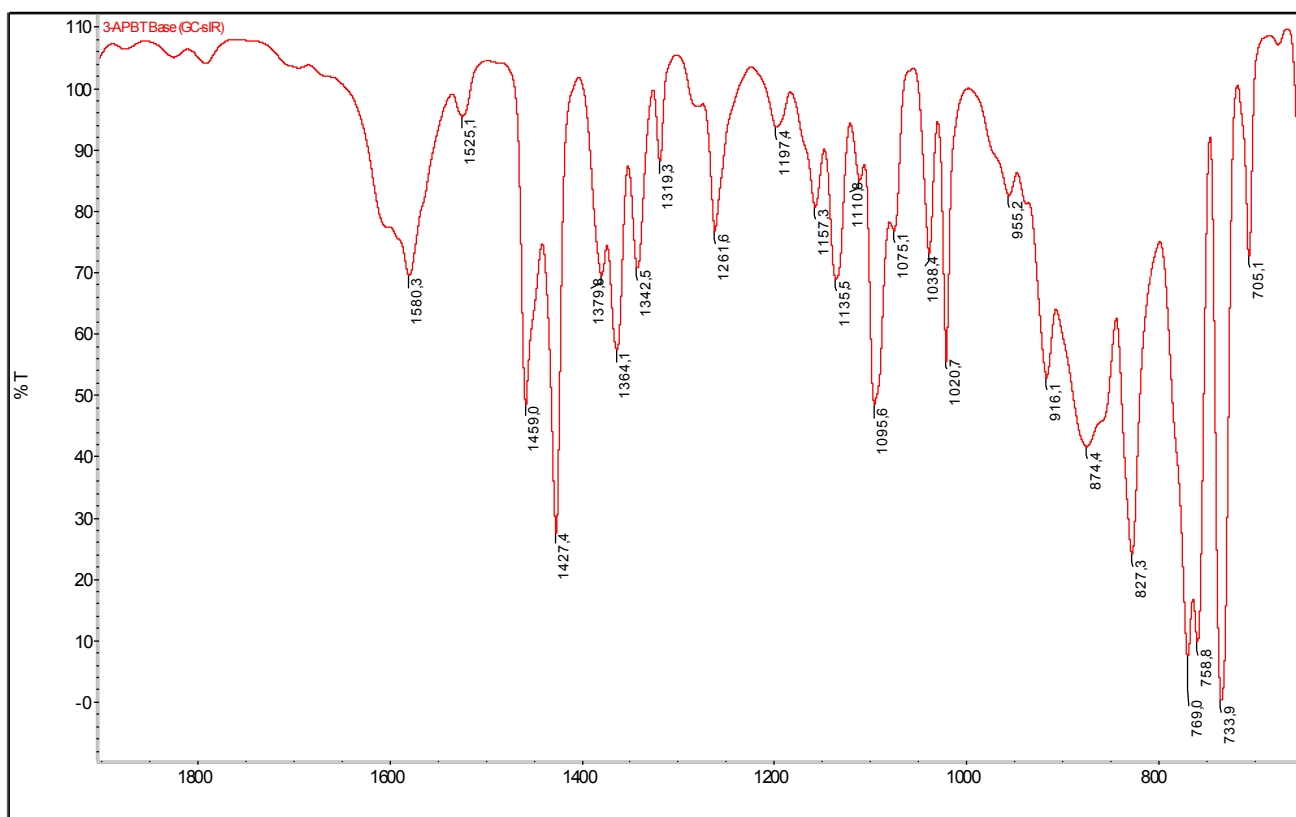
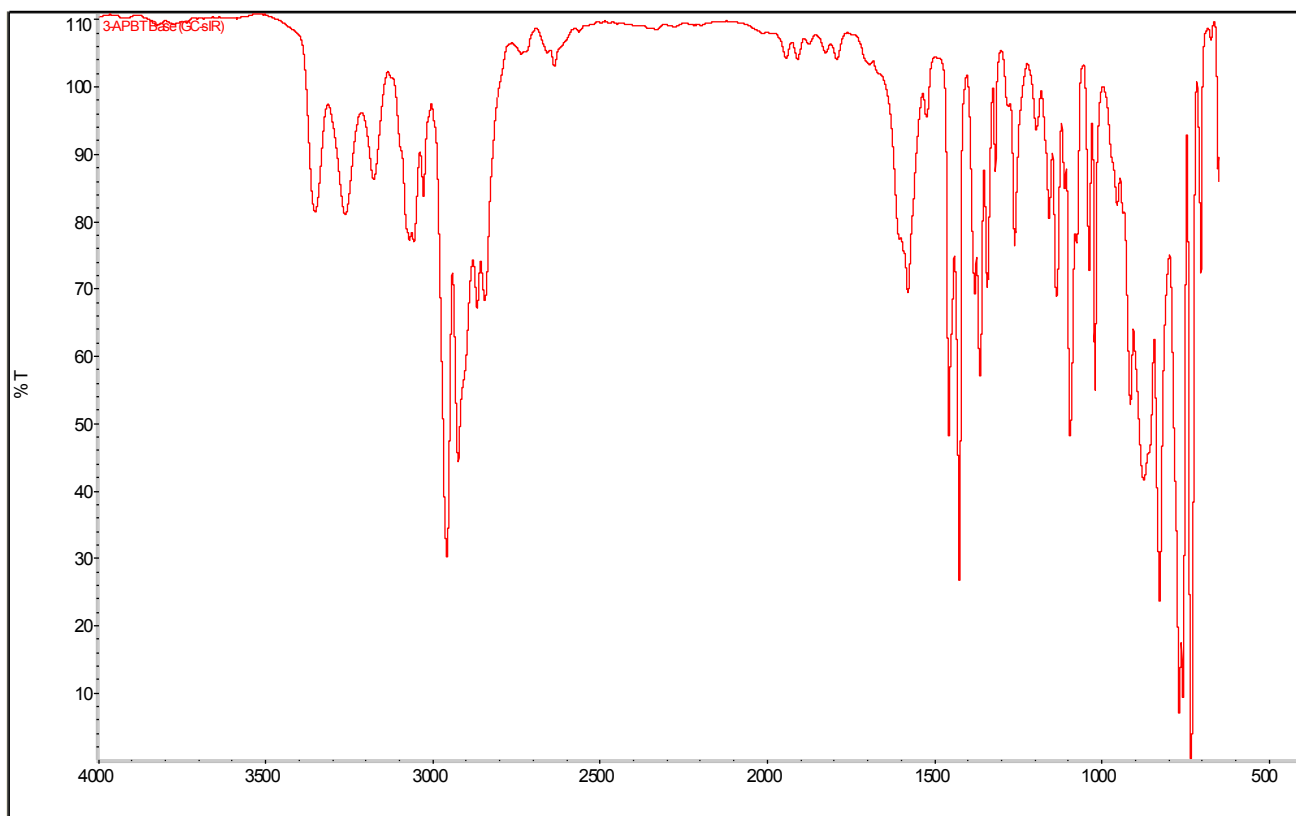
3-APBT HCl – ATR-IR



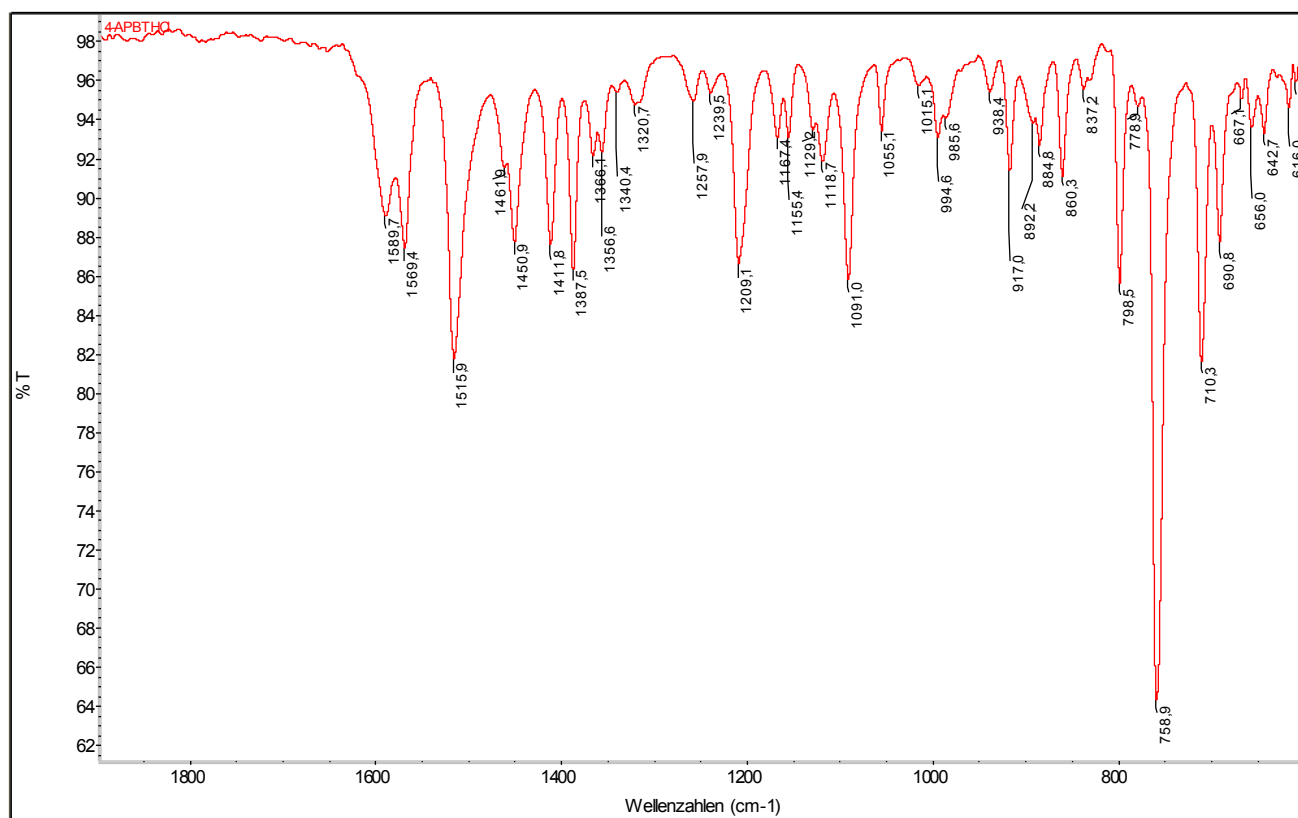
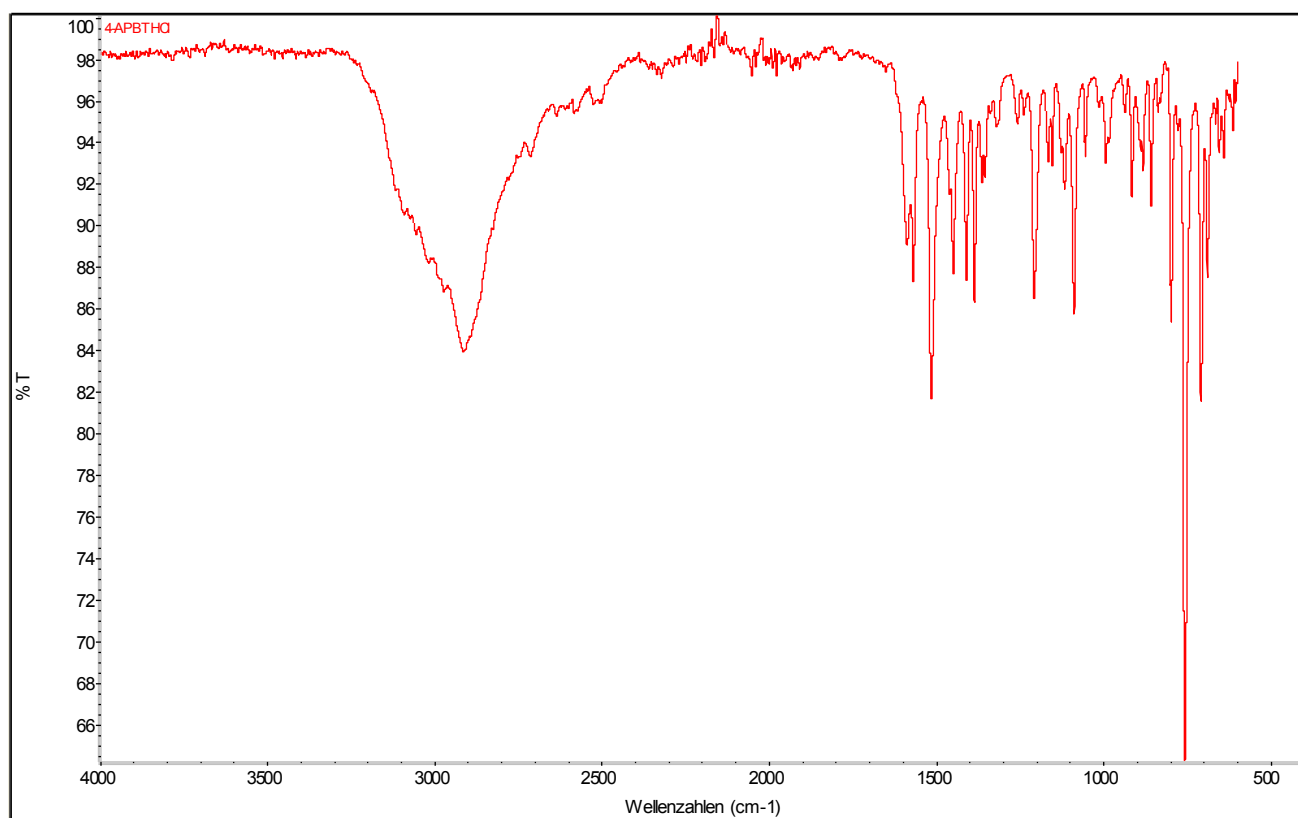
3-APBT base – ATR-IR



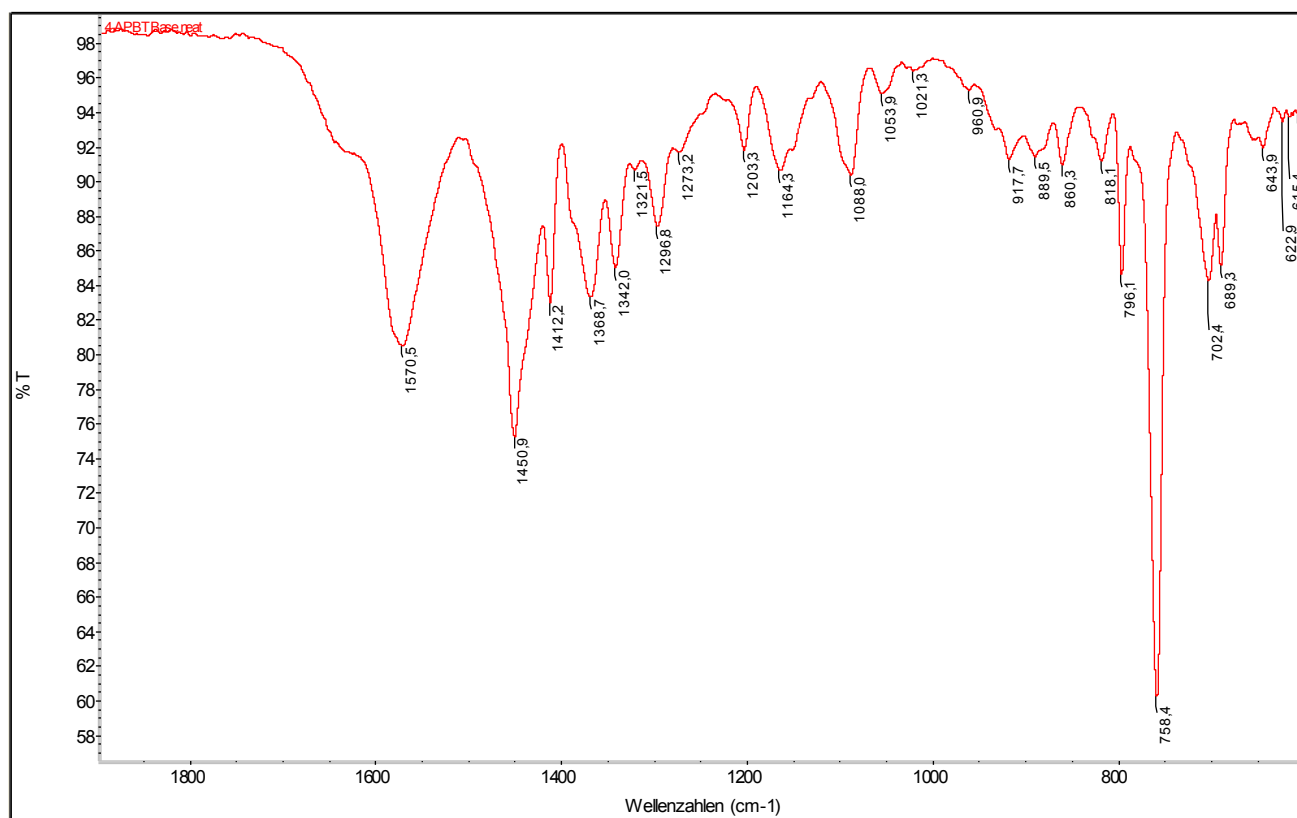
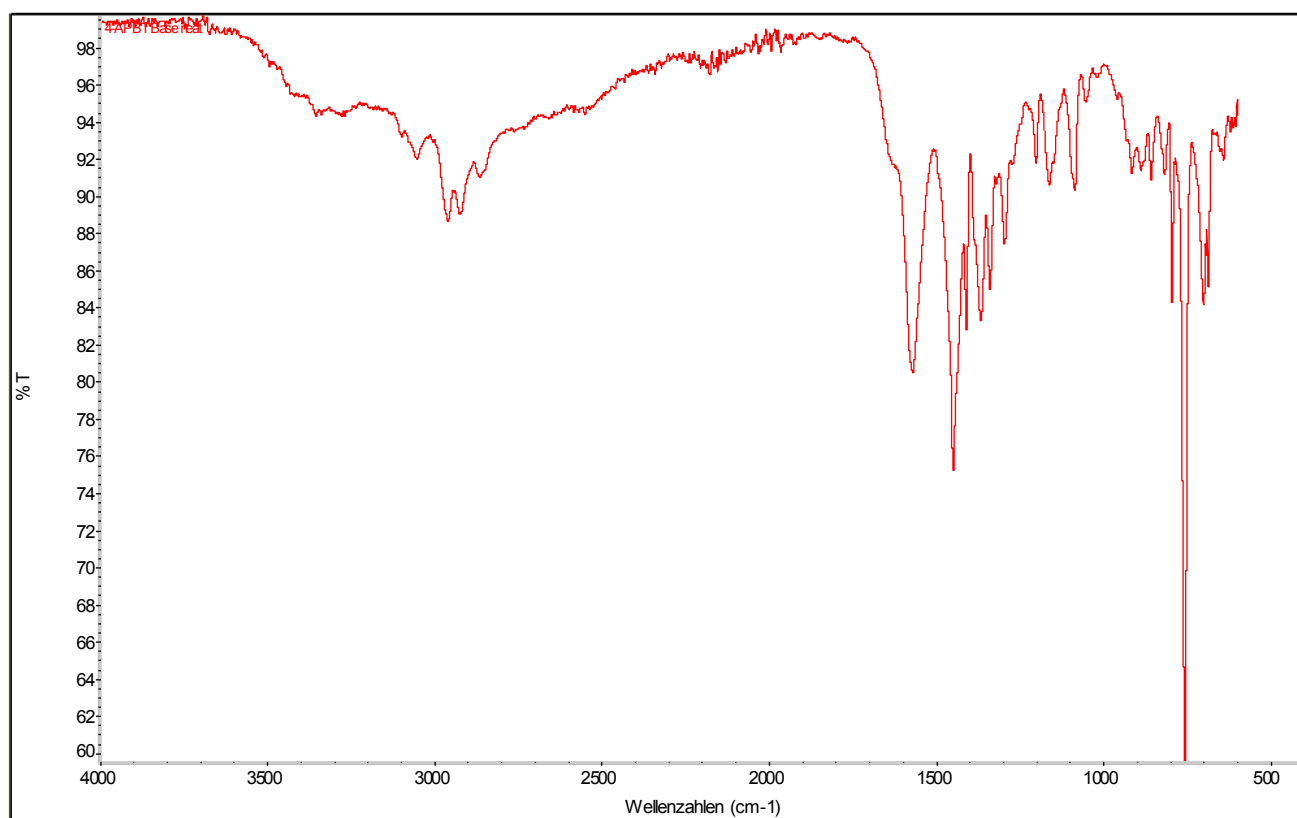
3-APBT base – GC-sIR



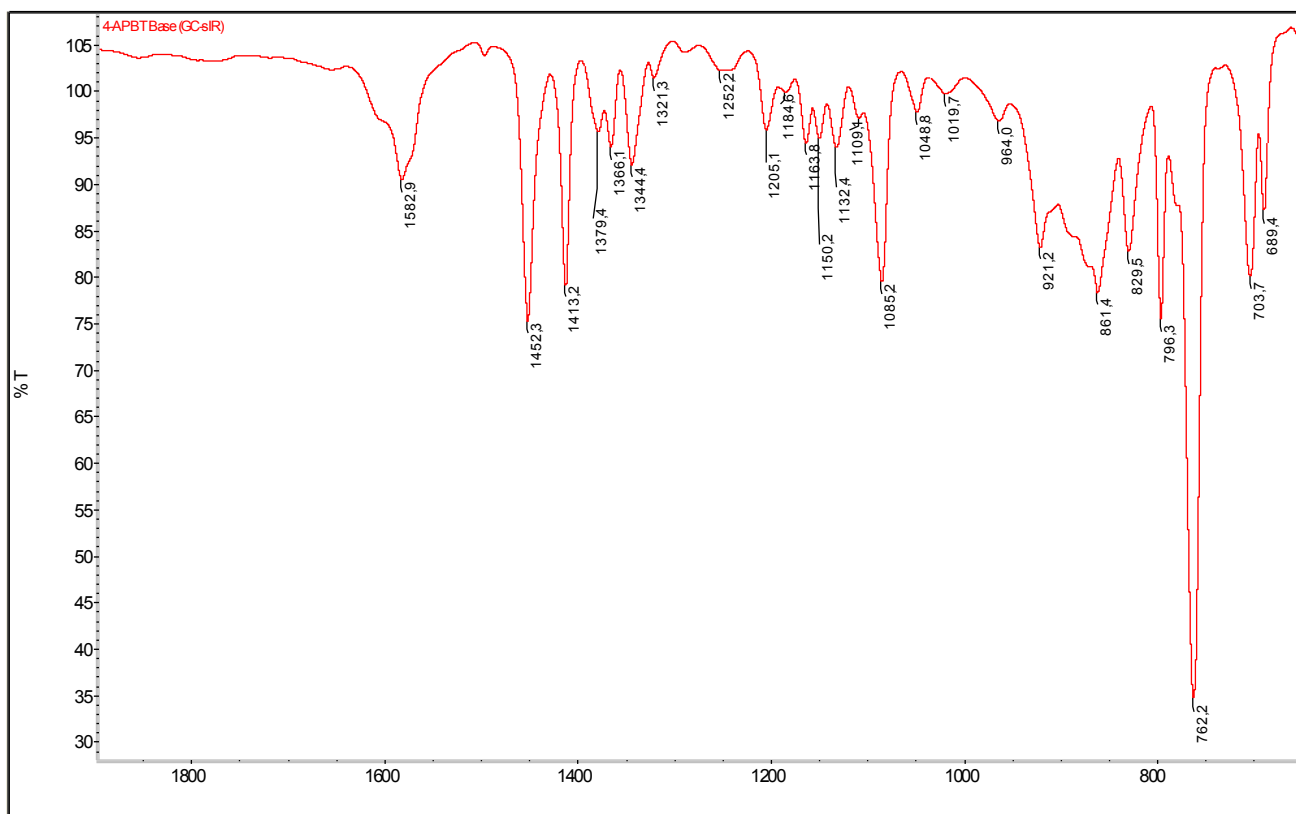
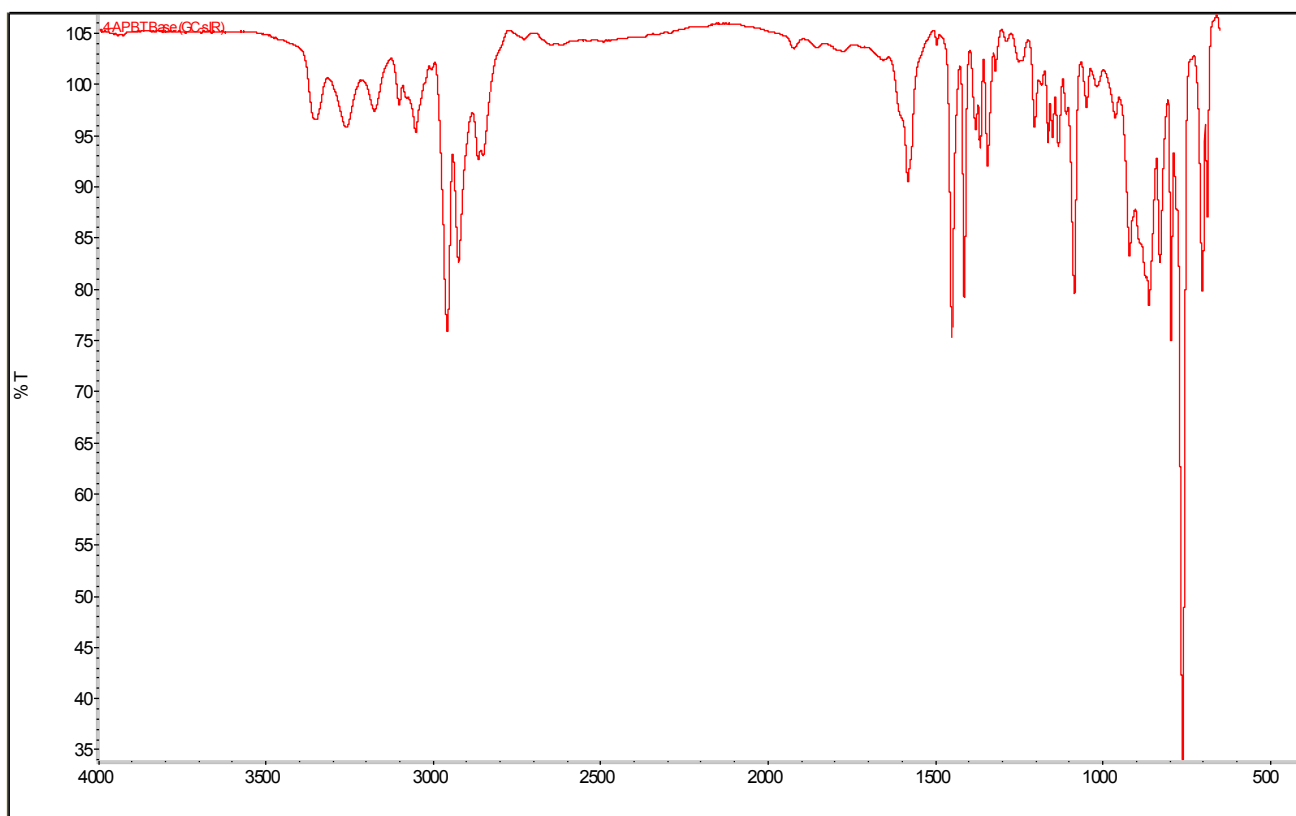
4-APBT HCl – ATR-IR



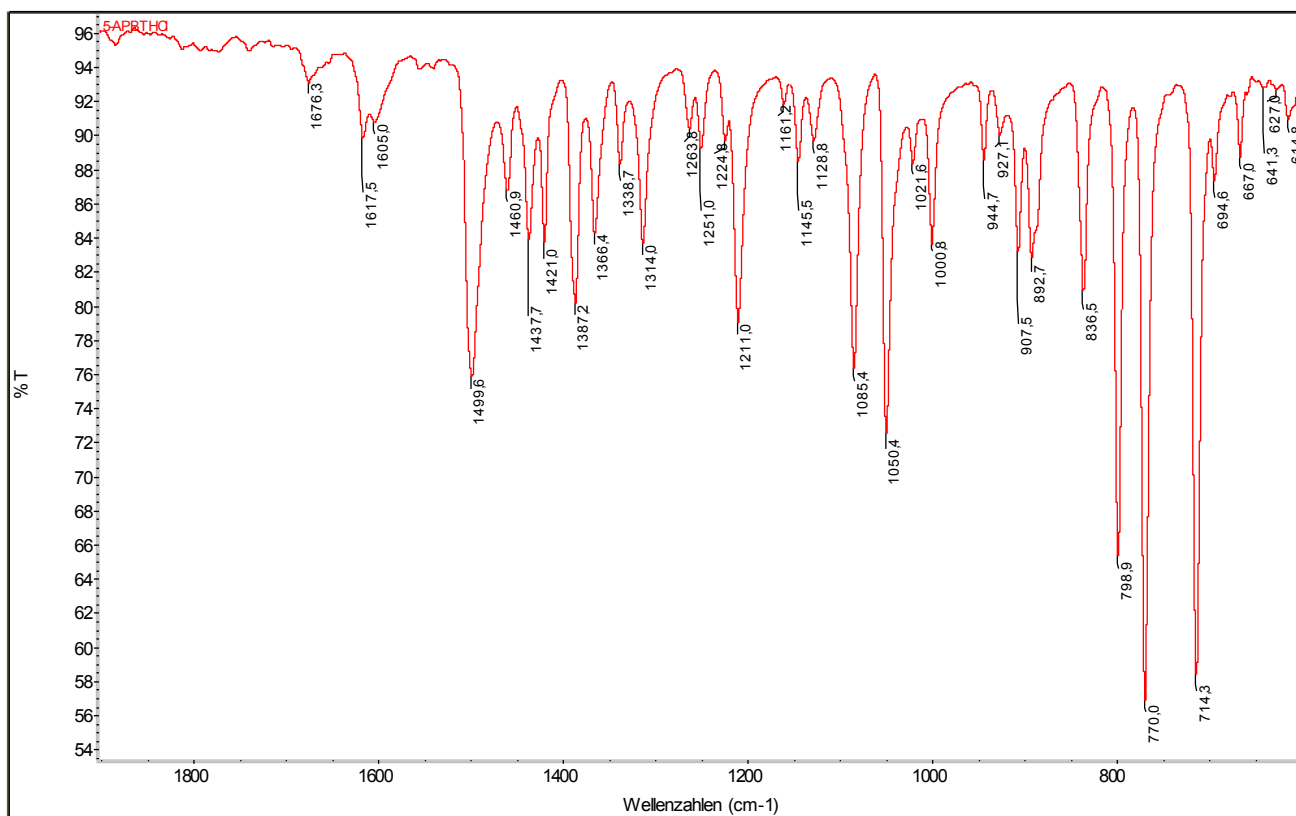
4-APBT base – ATR-IR



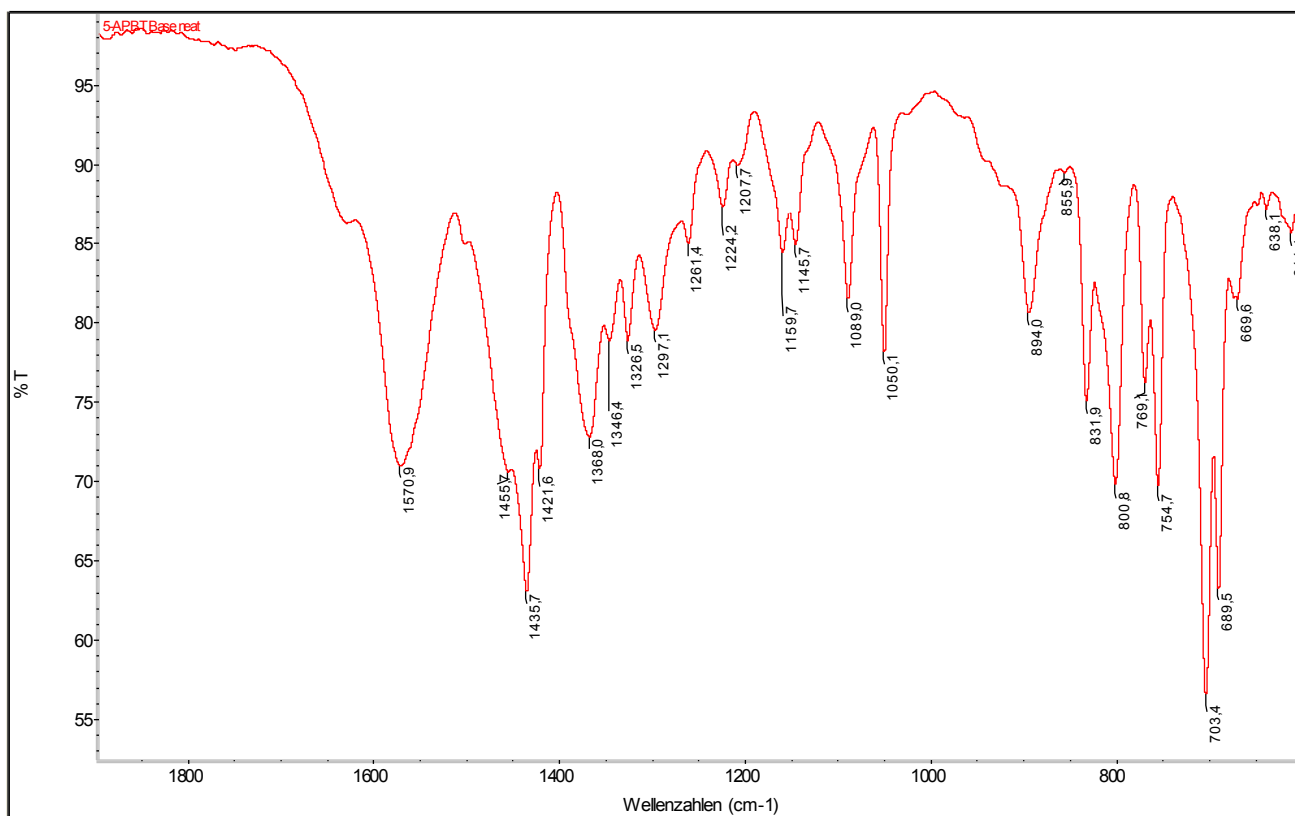
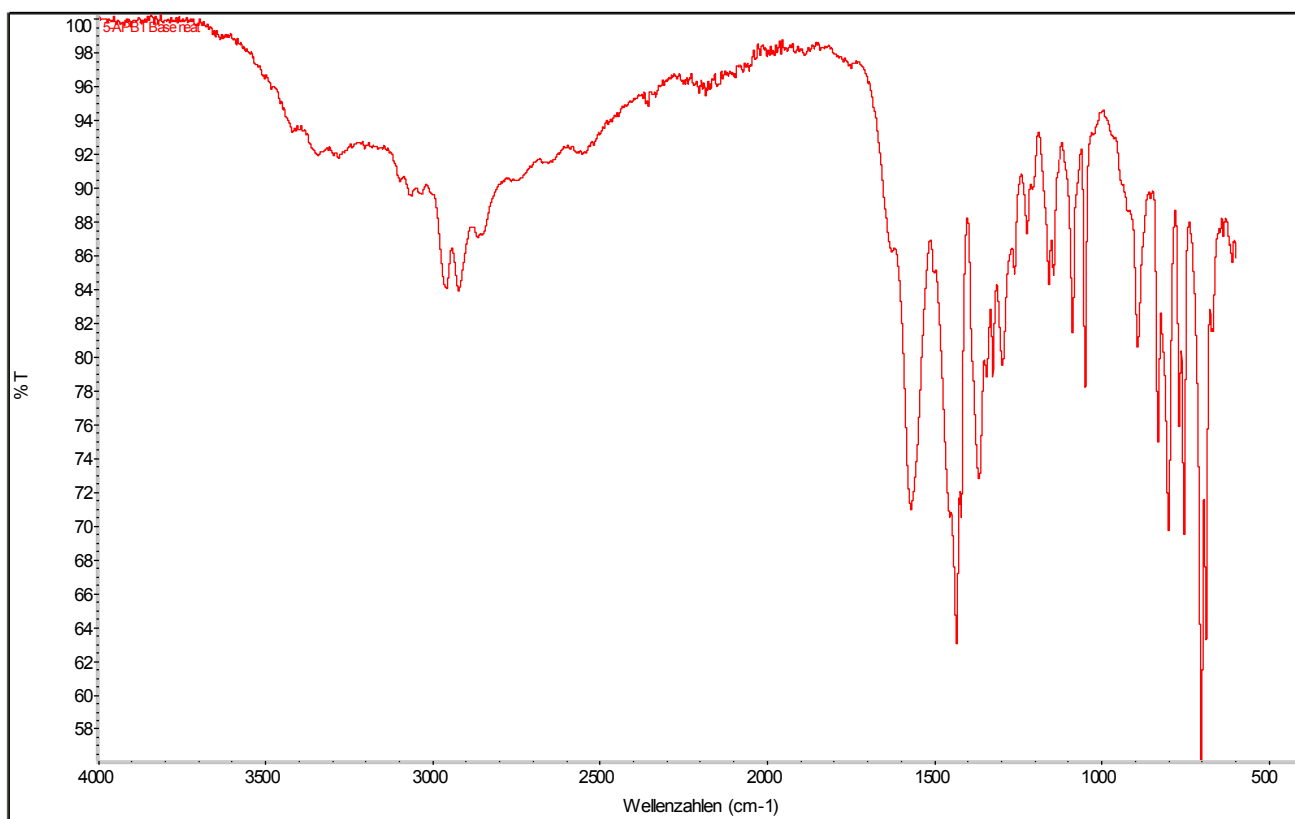
4-APBT base – GC-sIR



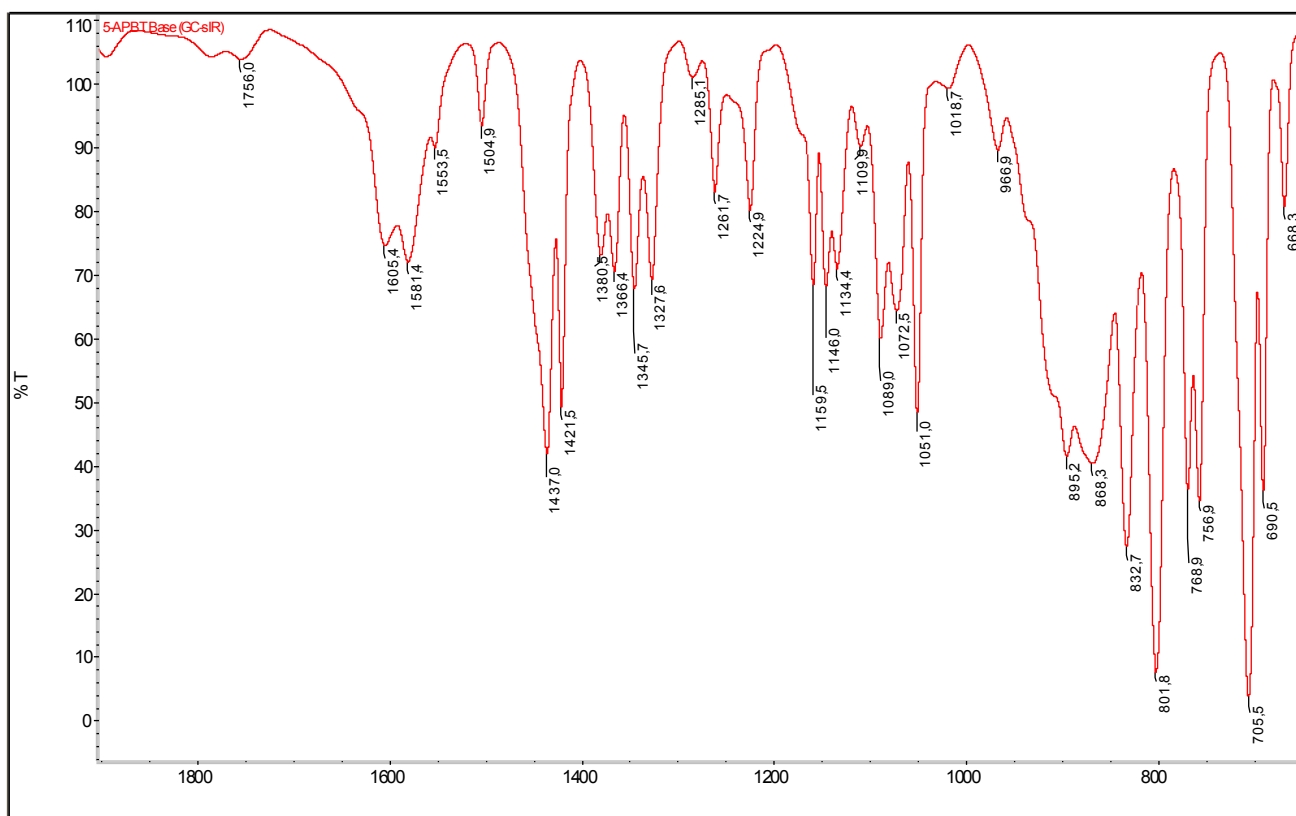
5-APBT HCl – ATR-IR



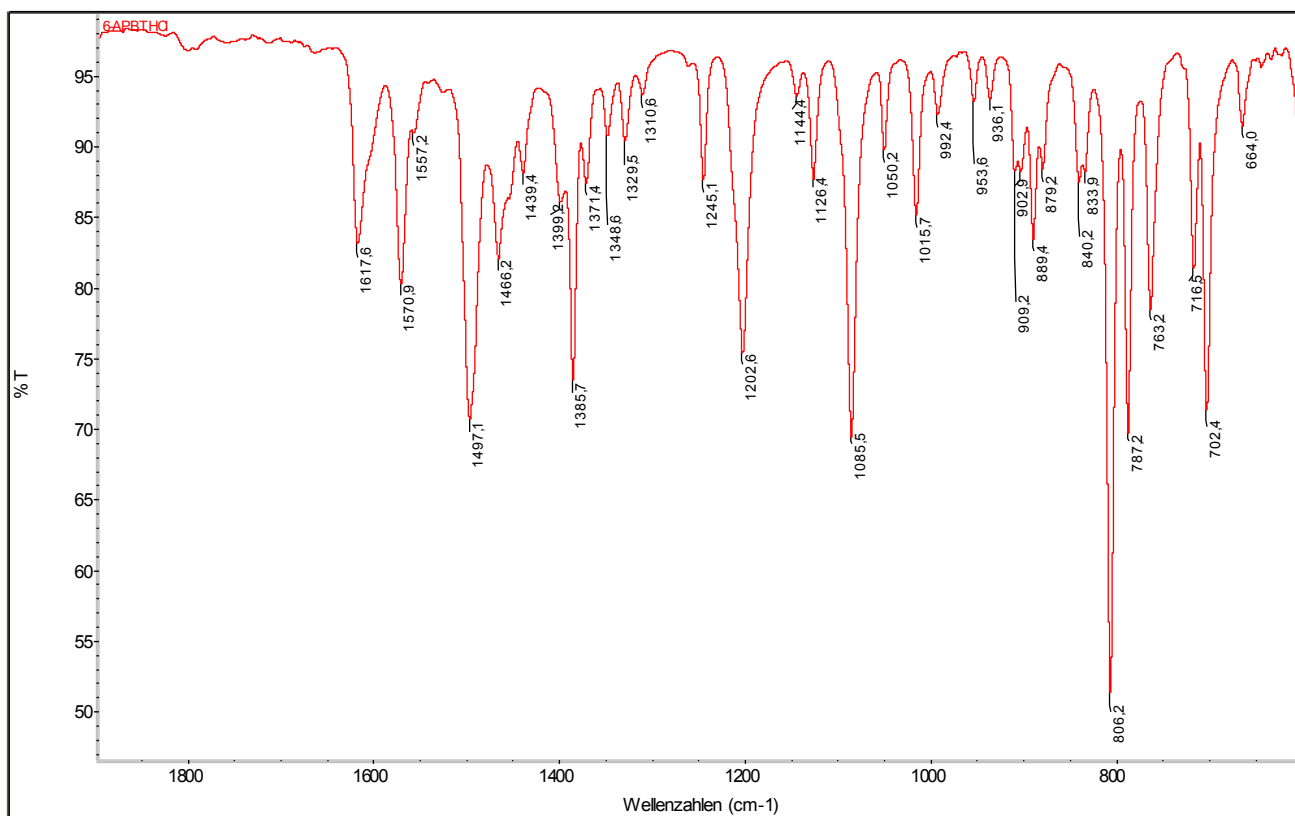
5-APBT base – ATR-IR



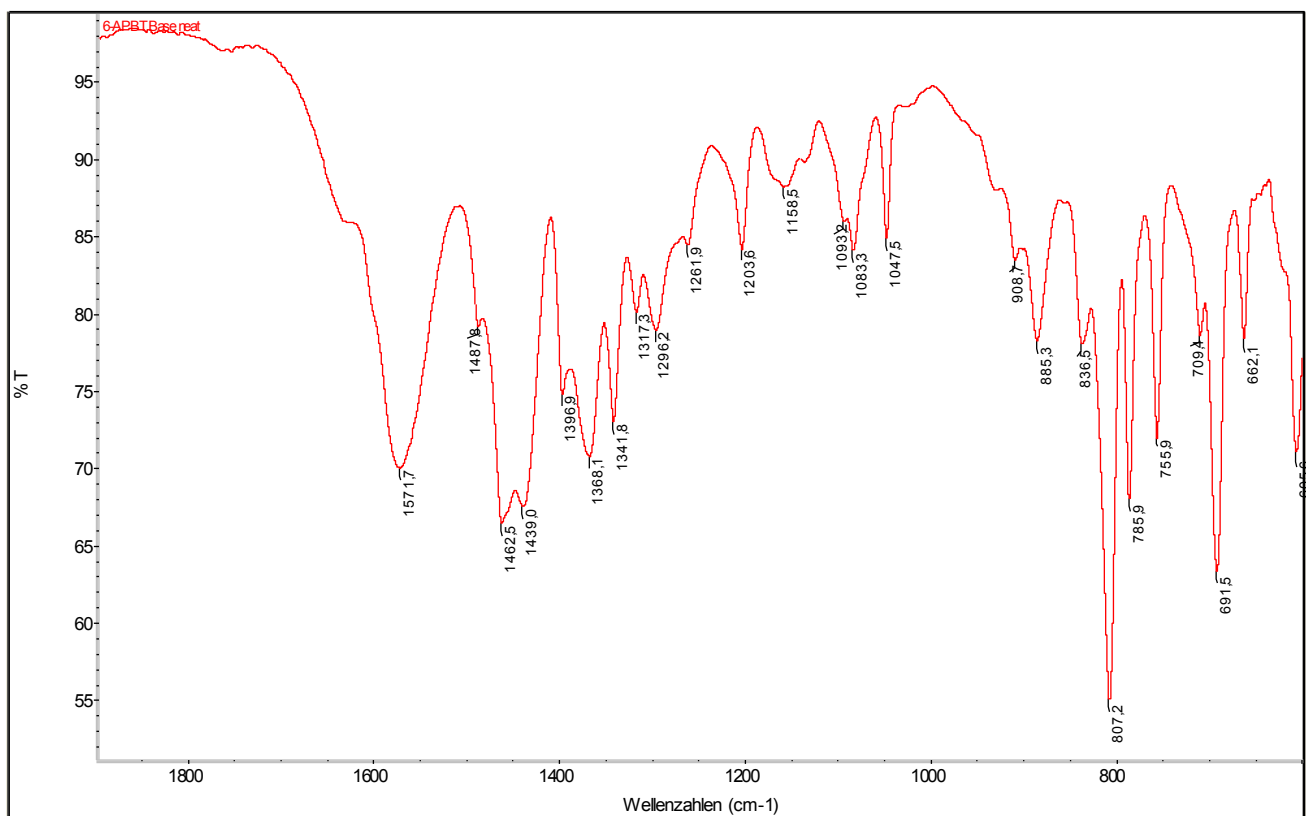
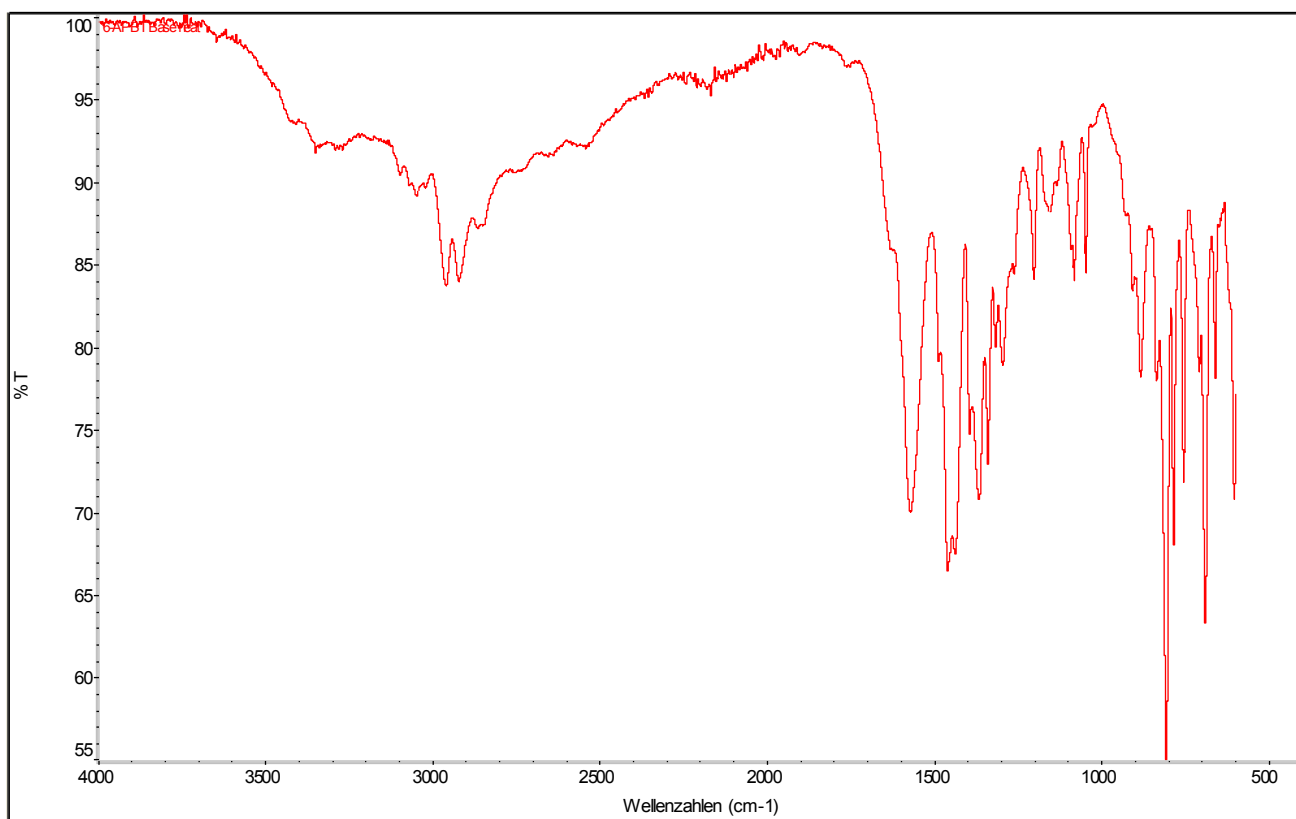
5-APBT base – GC-sIR



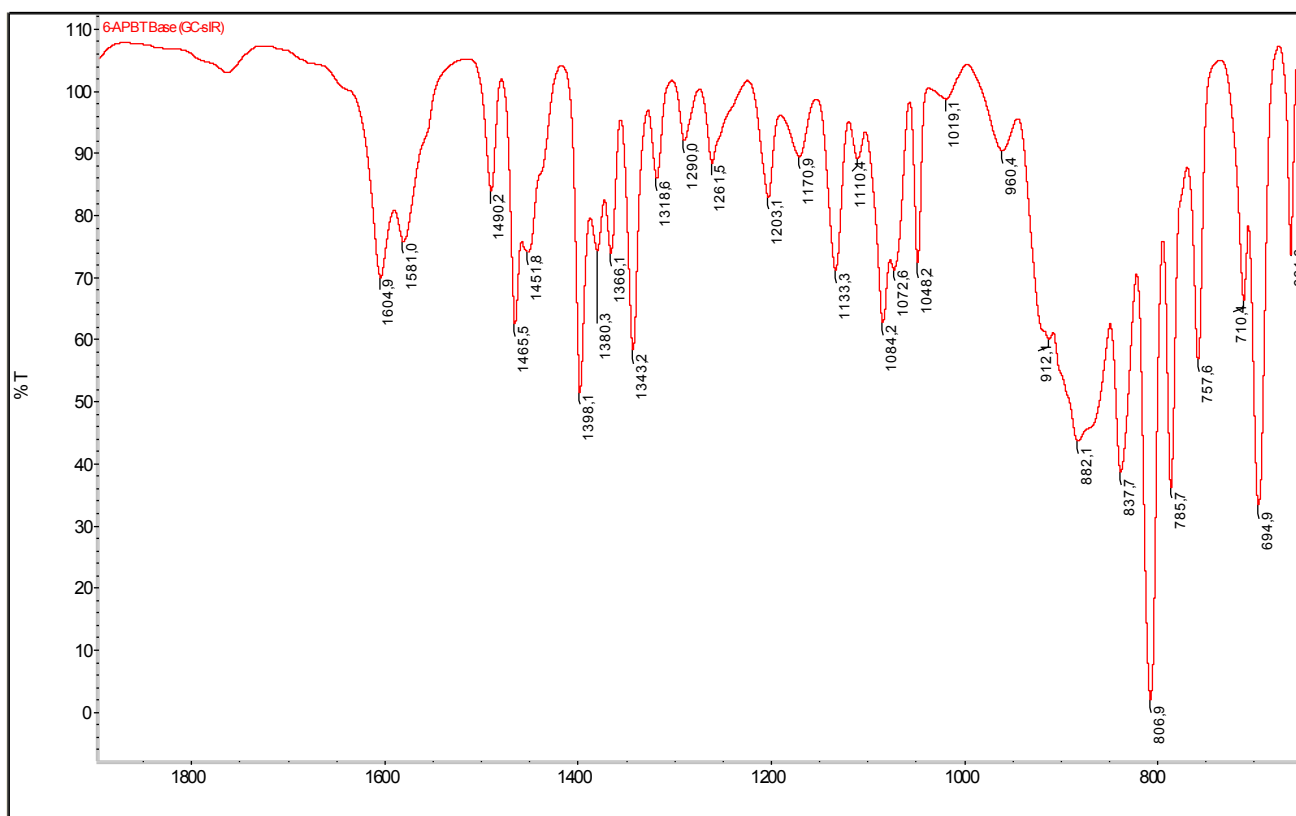
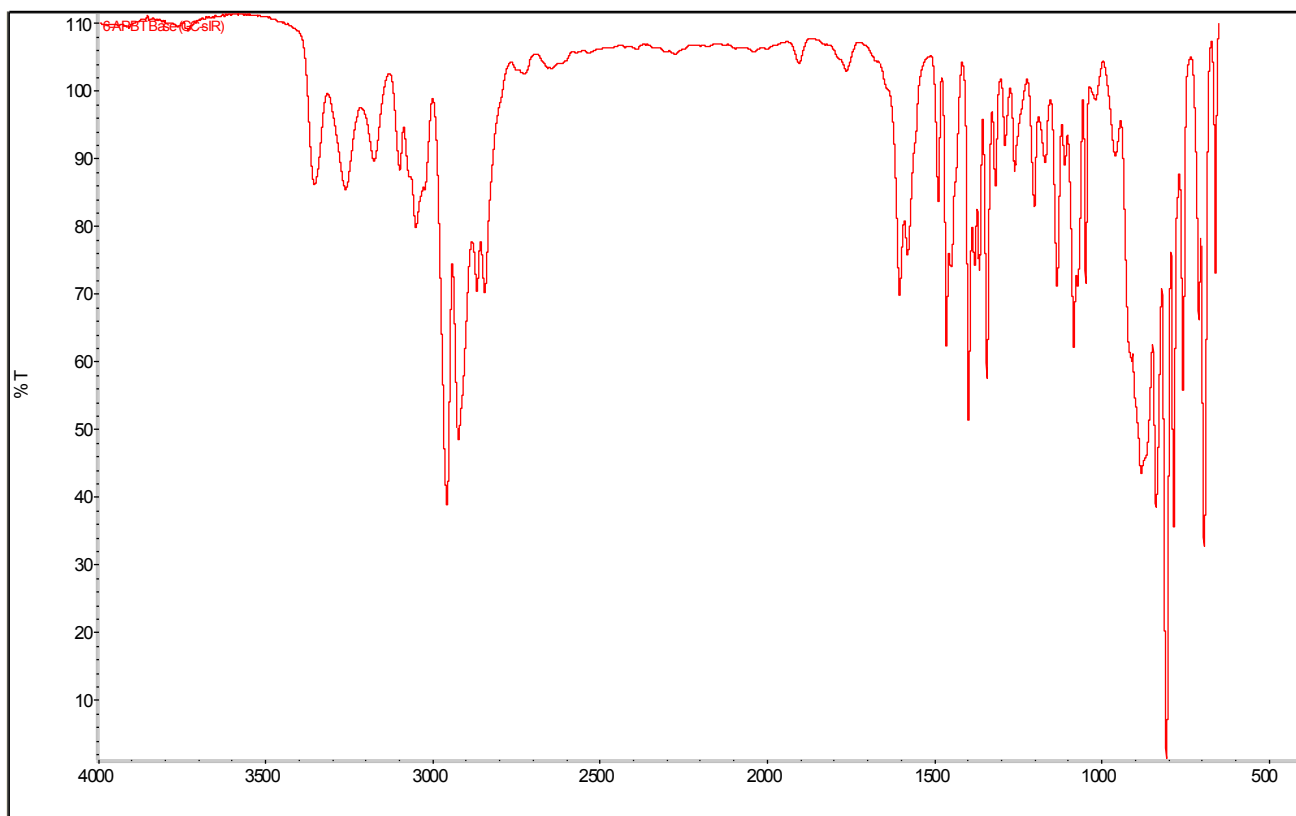
6-APBT HCl – ATR-IR



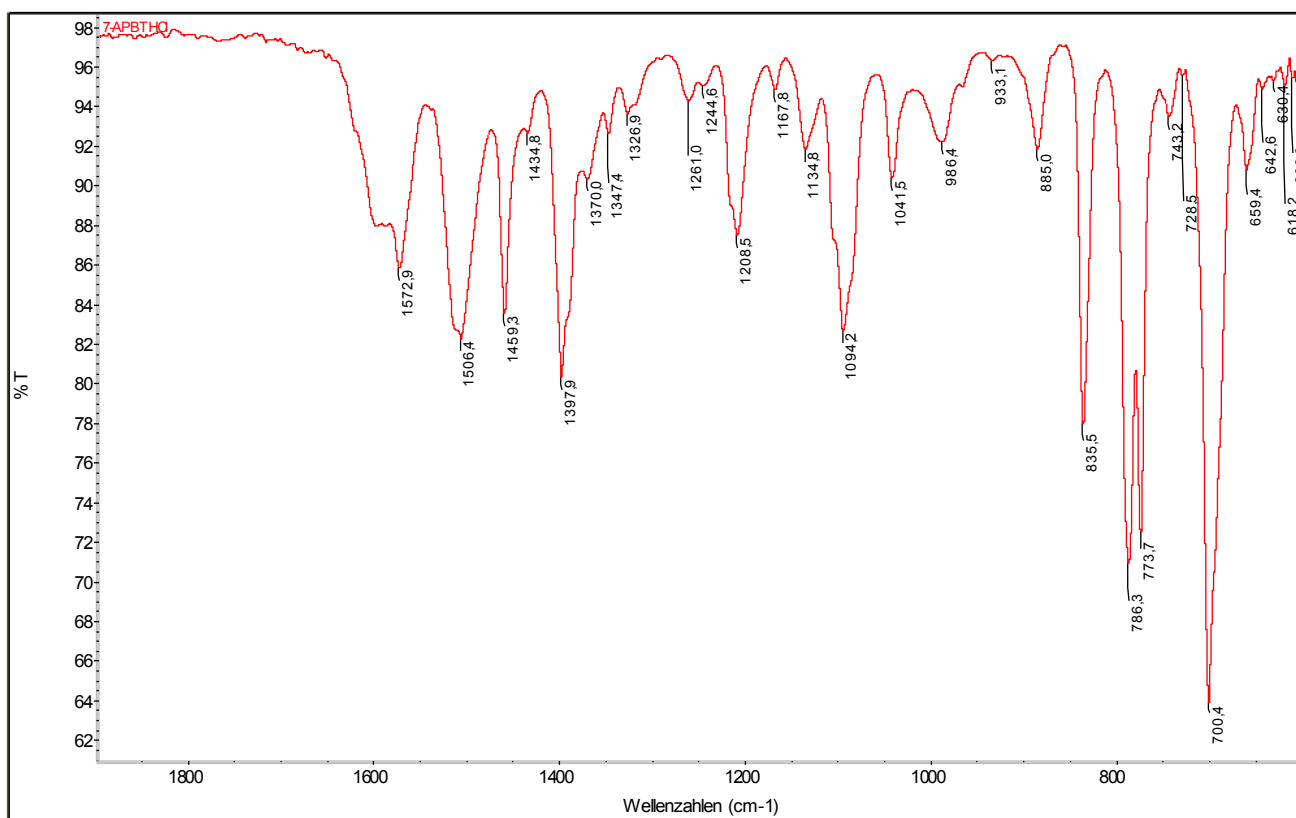
6-APBT base – ATR-IR



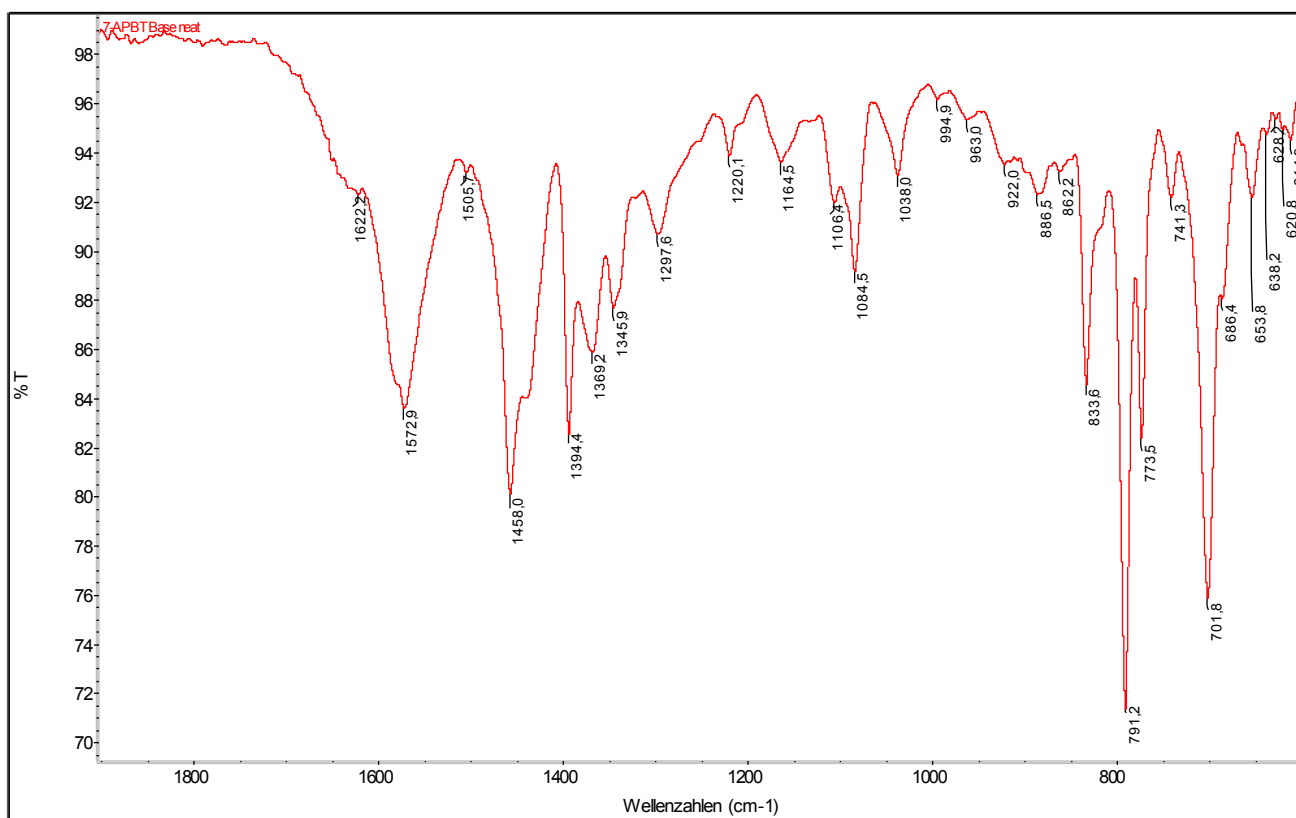
6-APBT base – GC-sIR



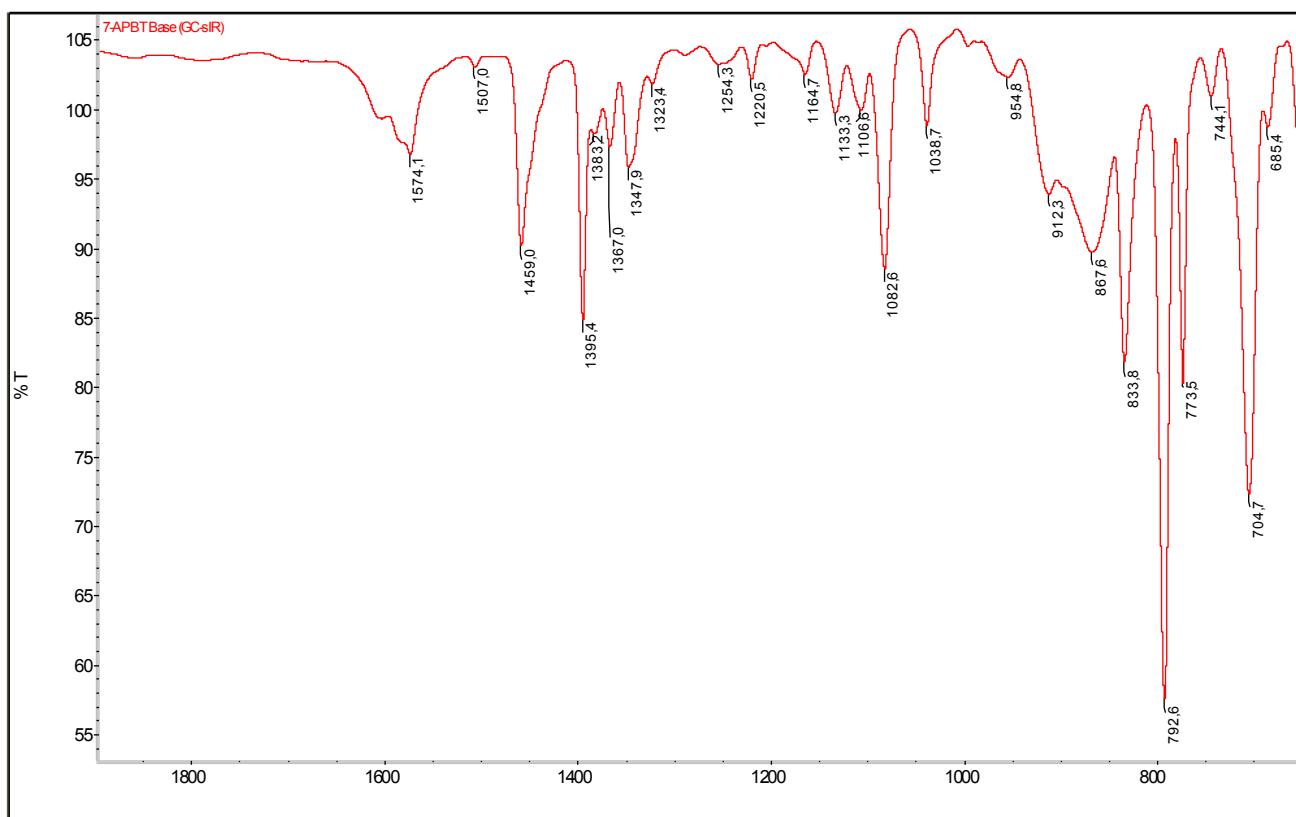
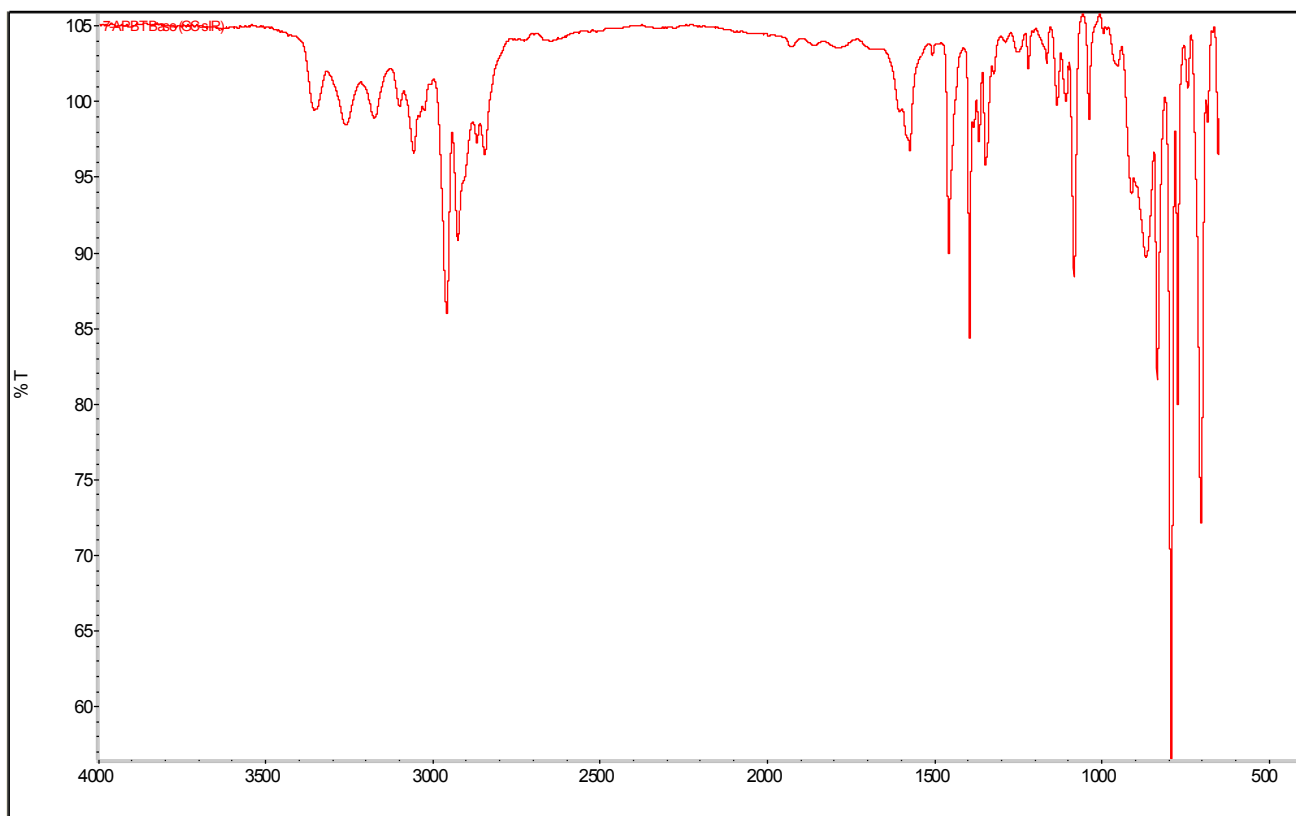
7-APBT HCl – ATR-IR



7-APBT base – ATR-IR



7-APBT base – GC-sIR



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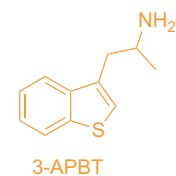
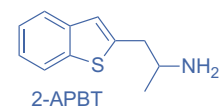
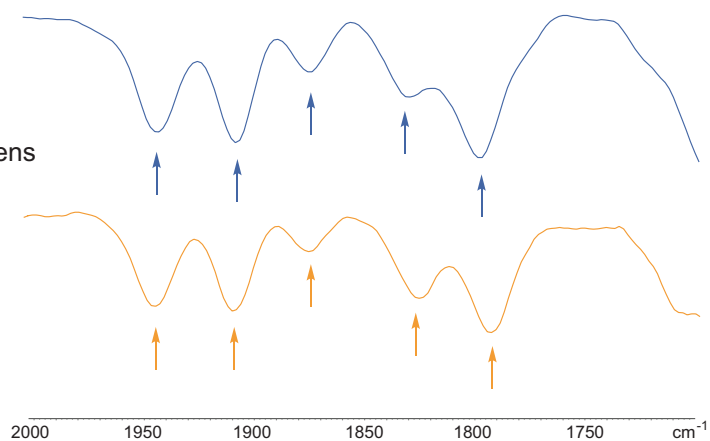
Isomer		Aromatic ring C-C stretches (1400–1500, 1585–1600 cm ⁻¹)	Aromatic ring C-H in-plane bends (1000–1250 cm ⁻¹)*	Aromatic C-H out-of-plane bends (675–900 cm ⁻¹)**
2	HCl (ATR-IR)	1430.5, 1456.4, 1496.9, 1575.2, 1602.0	1005.3, 1015.0, 1066.1, 1088.5, 1111.7, 1124.0, 1154.3, 1197.4, 1251.1, 1228.5, 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

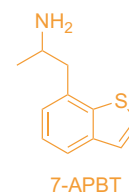
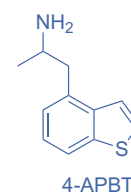
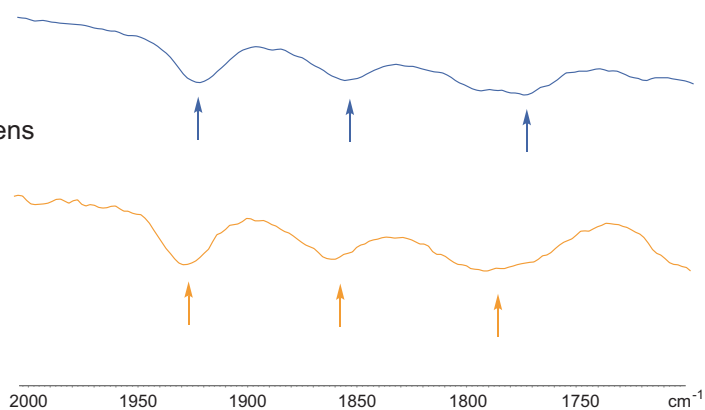
** Also C–S stretches in this region

GC-sIR partial spectrum - overtone bands

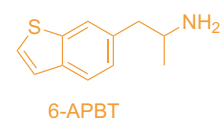
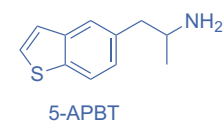
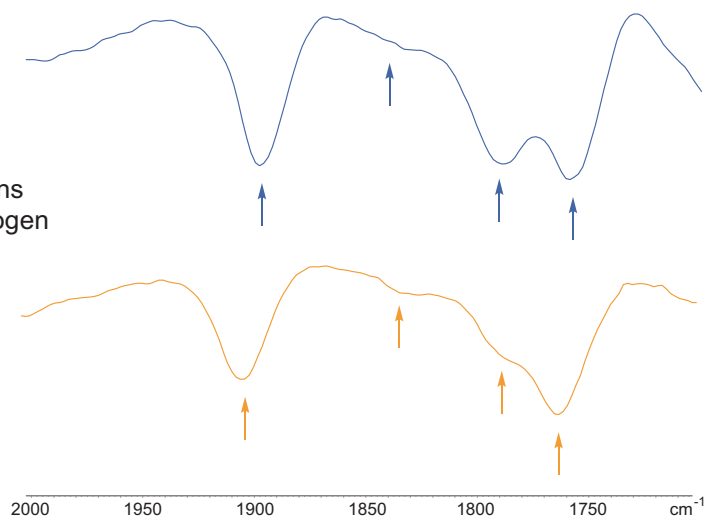
Four adjacent hydrogens
on benzene ring



Three adjacent hydrogens
on benzene ring

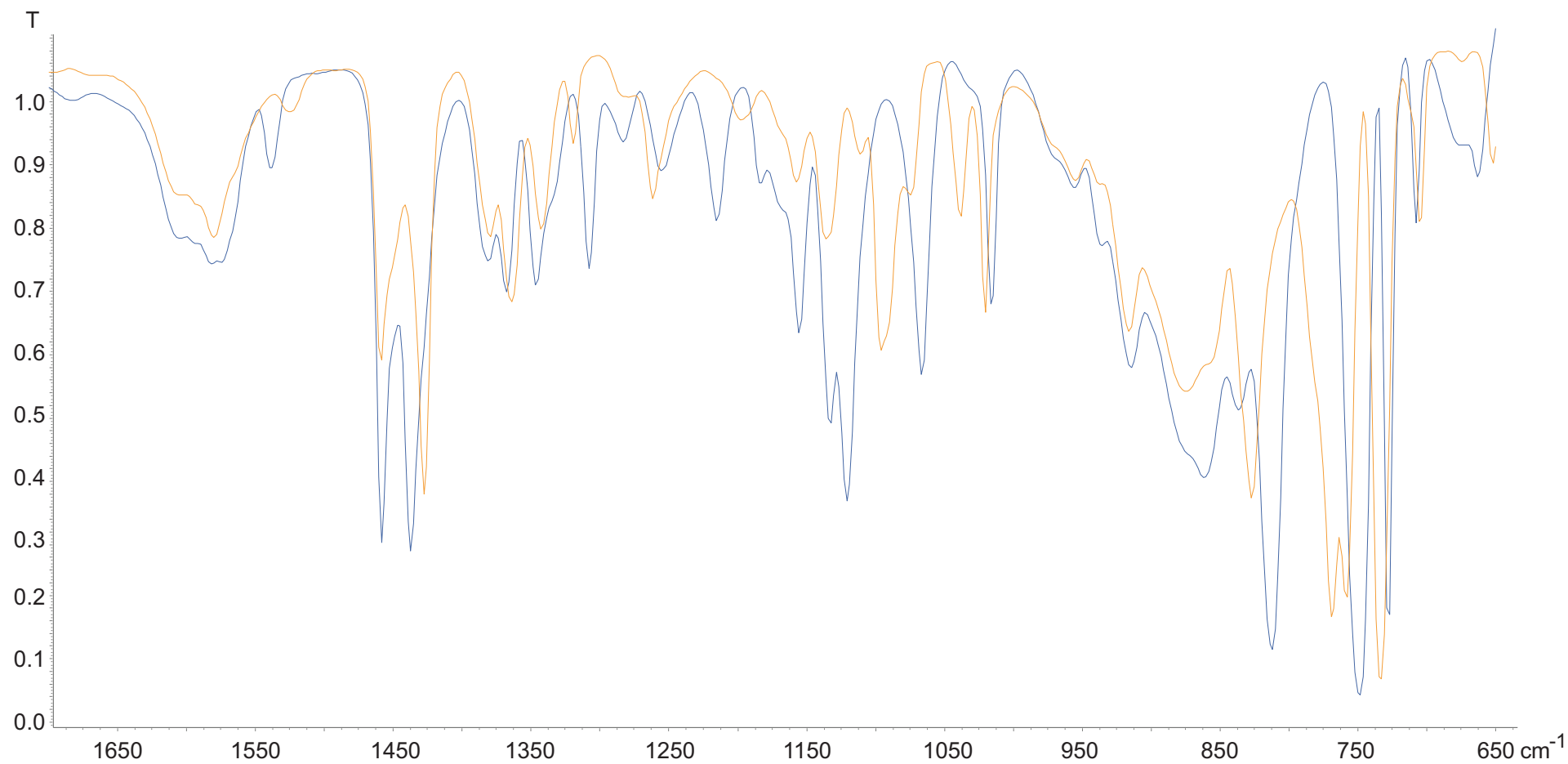
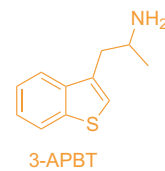
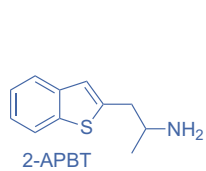


Two adjacent hydrogens
and one isolated hydrogen
on benzene ring



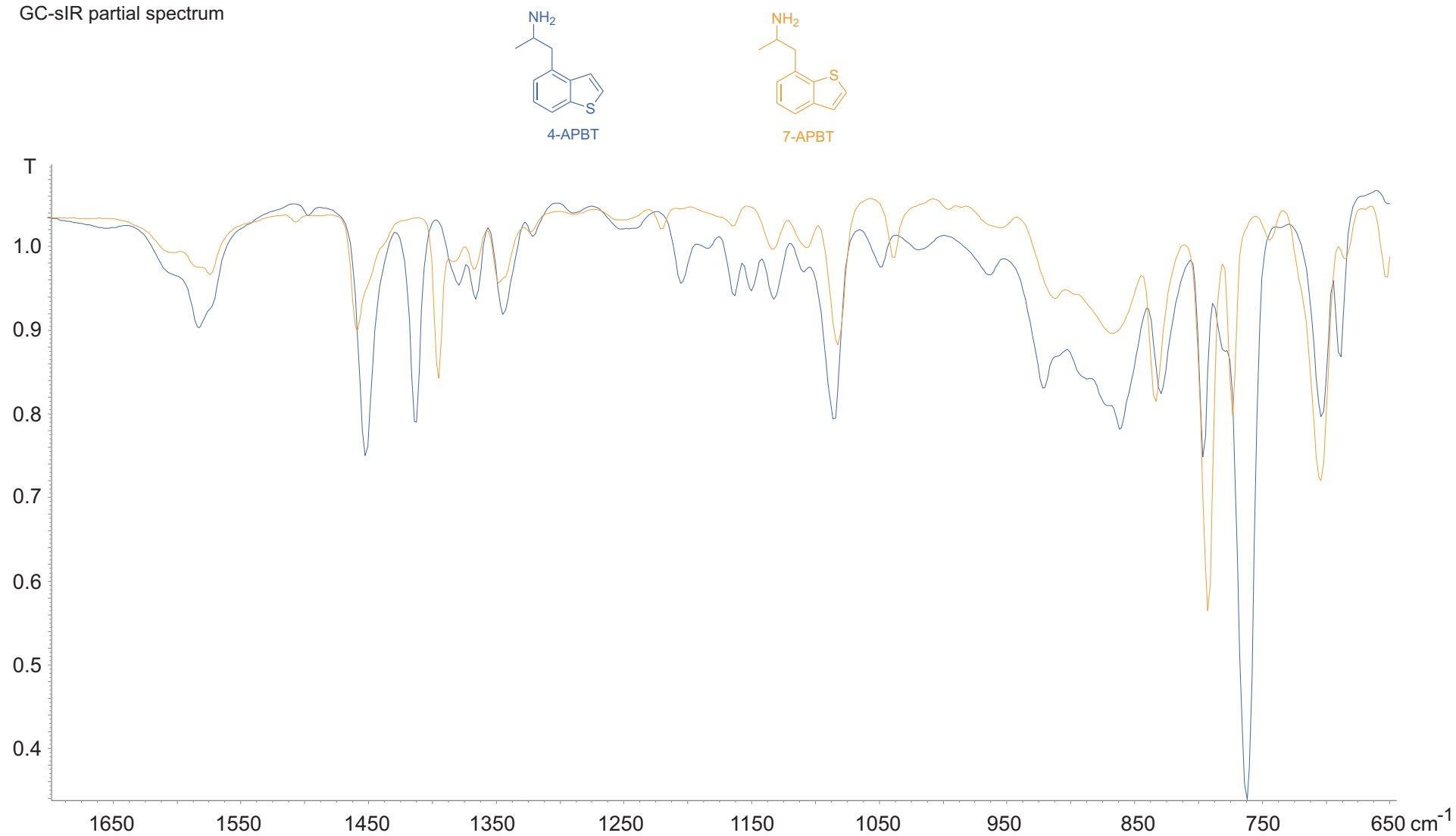
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GC-sIR partial spectrum

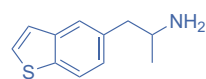


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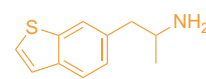
GC-sIR partial spectrum



GC-sIR partial spectrum



5-APBT



6-APBT

