C-H Functionalization of azines. Anodic dehydroaromatization of 9-(hetero)aryl-9,10-dihydroacridines

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Supporting Information

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1. Crystallographic experiments

Crystallographic description of 2a: T = 120.01(10) K, crystal system is monoclinic, a = 5.48181(13) Å, b = 10.7977(2) Å, c = 24.0126(6) Å, β = 95.443(2)°, V = 1414.92(6) Å^3, space group $P2_1/c$, Z = 4, μ = 0.074 mm^{-1}, 8836 reflections measured, 4628 unique (R_{int} = 0.0236) which were used in all calculations. The final wR_2 was 0.1459 (all data) and R_1 was 0.0473 (>2σ(I)). GooF= 1.000. Largest diff. peak and hole: 0.46/-0.22 ēÅ^{-3}.

Crystallographic description of 2c: T = 150.01(10) K crystal system is monoclinic, a= 8.4601(3) Å, b= 10.9097(5) Å, c= 16.1704(6) Å, β= 94.110(3)°, space group $P2_1/c$, volume 1488.65(10) Å^3, Z= 4, μ= 0.075 mm^{-1}. Reflections collected/independent/with [I>2σ(I)] 6286/3487/2779, R_{int}= 0.0245, completeness to θ= 28.22° 99.97 %. Final R indices: R_1= 0.044, wR_2= 0.0393 [I>2σ(I)], R_1= 0.058, wR_2= 0.1336 (all data), GooF= 1.055. Largest diff. peak and hole: 0.289 and -0.255 ēÅ^{-3}.

Crystallographic description of 2p: T = 150.01(10) K crystal system is triclinic, a = 10.7236(3) Å, b = 12.3739(3) Å, c = 14.3134(4) Å, α = 109.830(2)°, β = 111.959(3)°, γ = 90.014(2)°, V = 1639.36(8) Å^3, space group P-1, Z = 2, μ = 0.104 mm^{-1}, 16154 reflections measured, 8885 unique (R_{int} = 0.0166) which were used in all calculations. The final R_1 = 0.0596, wR_2 = 0.1700 (all data) and R_1 = 0.0491, wR_2 = 0.1554 [I>2σ(I)], GooF= 1.021. Largest diff. peak and hole: 0.54/-0.40 ēÅ^{-3}.

Crystallographic description of 3n: T= 295(2) K crystal system is monoclinic, a= 10.467(5) Å, b= 10.928(8) Å, c= 13.713(7) Å, β= 99.78(4)°, space group $P2_1/n$, volume 1545.7(15) Å^3, Z= 4, μ= 0.124 mm^{-1}. Reflections collected/independent/with [I>2σ(I)] 12228/3151/931, R_{int}= 0.0667, completeness to θ= 26.39° 99.8 %. Final R indices: R_1= 0.0449, wR_2= 0.0393 [I>2σ(I)], R_1= 0.1589, wR_2= 0.0417 (all data), GooF= 0.966. Largest diff. peak and hole: 0.198 and -0.147 ēÅ^{-3}.

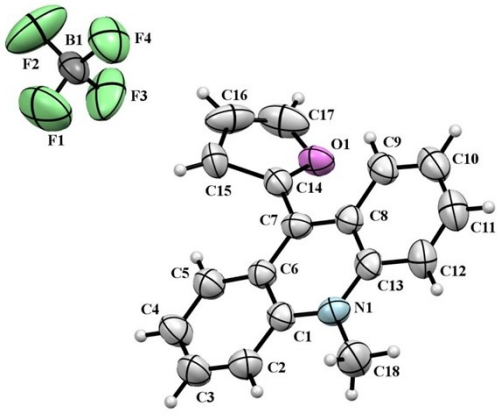
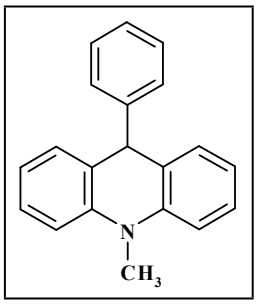


Figure 1 The compound **3n** in according XRD data in the thermal ellipsoids of the 50% probability. Components of the disordering are omitted for the clarity.

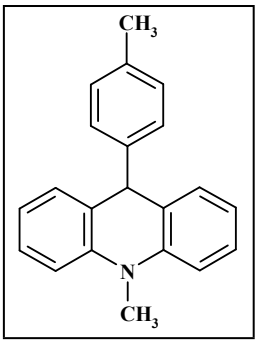
2. Characterizations of all compounds

10-Methyl-9-phenyl-9,10-dihydroacridine[1] *(2a)*



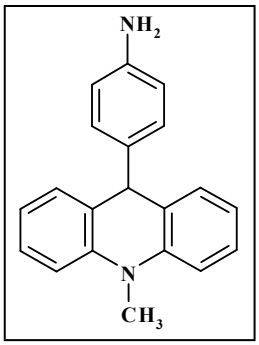
Colorless crystals. 676 mg (80%). M.p.: 109 °C. ^{1}H NMR (500 MHz, [D$_6$]DMSO): δ 7.27-7.22 (m, 4H), 7.19-7.16 (m, 2H), 7.10-7.06 (m, 5H), 6.94-6.92 (m, 2H), 5.28 (s, 1H), 3.37 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D$_6$]DMSO): δ 145.5, 141.9, 128.4, 128.3, 127.3, 126.8, 126.3, 126.1, 120.5, 112.6, 47.3, 32.9 ppm. Elem. Anal. Calcd. For $C_{20}H_{17}N$: C 88.52, H 6.31, N 5.16 Found: C 88.47, H 6.41, N 5.06. FT-IR (DRA, cm^{-1}): 937, 968, 1033, 1043, 1061, 1077, 1100, 1129, 1141, 1162, 1184, 1201, 1269, 1312, 1343, 1427, 1442, 1460, 1473, 1491, 1504, 1592, 1739, 1901, 1931, 1955, 2651, 2822, 2877, 2906, 2981, 3019, 3058, 3078.

10-Methyl-9-(4-methylphenyl)-9,10-dihydroacridine *(2b)*



Colorless crystals. 693 mg (78%). M.p.: 144-145 °C. ^{1}H NMR (500 MHz, [D$_6$]DMSO): δ 7.24-7.20 (m, 4H), 7.06-7.04 (m, 2H), 6.98-6.90 (m, 6H), 5.21 (s, 1H), 3.35 (s, 3H), 2.16 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D$_6$]DMSO): δ 142.5, 141.9, 135.1, 128.8, 128.4, 127.2, 126.7, 126.4, 120.5, 112.6, 46.9, 32.9, 20.4 ppm. Elem. Anal. Calcd. For $C_{21}H_{19}N$: C 88.38, H 6.71, N 4.19 Found: C 88.25, H 6.69, N 4.96. FT-IR (DRA, cm^{-1}): 933, 1020, 1039, 1062, 1098, 1132, 1141, 1163, 1188, 1202, 1242, 1269, 1311, 1342, 1428, 1459, 1471, 1509, 1591, 1737, 1893, 1931, 2826, 2893, 2907, 2973, 3020, 3032, 3071.

10-Methyl-9-(4-aminophenyl)-9,10-dihydroacridine *(2c)*[2]

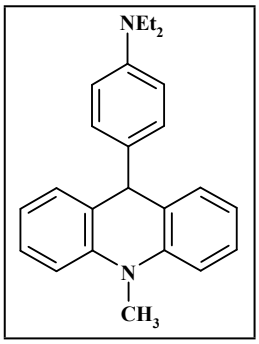


Colorless crystals. 482 mg (54%). M.p.: 148-149 °C. ^{1}H NMR (500 MHz, [D$_6$]DMSO): δ 7.21-7.17 (m, 4H), 7.02 (d, 2H, J=8.0 Hz), 6.90 (t, 2H, J=7.3 Hz), 6.70 (d, 2H, J=8.3 Hz), 6.37 (d, 2H, J=8.4 Hz) 5.03 (s, 1H), 4.82 (s,2H), 3.34 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D$_6$]DMSO): δ 146.8, 141.9, 132.8, 128.2, 127.5, 127.2, 126.9, 120.3, 113.7, 112.4, 46.6, 32.9 ppm. Elem. Anal. Calcd. For $C_{20}H_{18}N_2$: C 83.88, H 6.34, N 9.78 Found: C 83.70, H 6.36, N 9.81. FT-IR (DRA, cm^{-1}): 505, 522, 541, 577, 589, 618, 637, 710, 727, 747, 760, 801, 818, 843, 867, 897, 939, 1044, 1064, 1100, 1130, 1146, 1163, 1171, 1182, 1199, 1236, 1266, 1281, 1317, 1348, 1434, 1456, 1477, 1511, 1591, 1607, 1623, 1874, 1949, 2826, 2881, 2968, 3031, 3214, 3355, 3432.

10-Methyl-9-(4-diethylaminophenyl)-9,10-dihydroacridine *(2d)*[2]

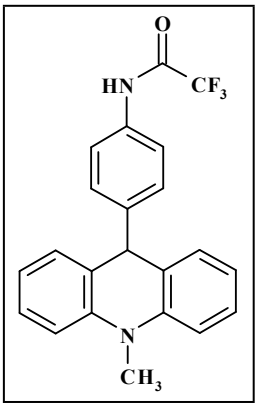
[1] X. Yang, J. Walpita, D. Zhou, Hoi Ling Luk, S. Vyas, R. S. Khnayzer, S. C. Tiwari, K. Diri, C. M. Hadad, F. N. Castellano, A. I. Krylov, K. D. Glusac, *J. Phys. Chem. B*, 2013, **117**, 15290–15296.

2 V. N. Charushin, O. N. Chupakhin, E. O. Sidorov, Yu. I. Beilis, I. A. Terent´eva, Zh. Org. Khim., 1978, 14, 140-146 (in English Russ. J. Org. Chem.).



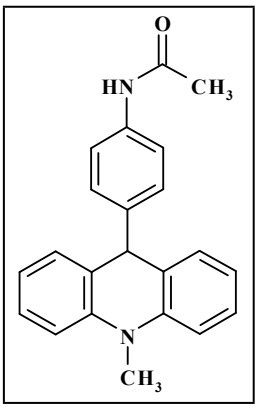
Colorless crystals. 470 mg (44%). M.p.: 116 °C. ^{1}H NMR (500 MHz, [D$_6$]DMSO): δ 7.21-7.19 (m, 4H), 7.03 (d, 2H, J=8.4 Hz), 6.91 (t, 2H, J=7.3 Hz), 6.83 (d, 2H, J=8.5 Hz), 6.45 (d, 2H, J=8.6 Hz) 5.07 (s, 1H), 3.35 (s, 3H), 3.22-3.17 (m, 4H), 0.99-0.96 (m, 6H) ppm. ^{13}C NMR (126 MHz, [D$_6$]DMSO): δ 145.8, 141.9, 132.1, 128.3, 127.6, 127.1, 126.9, 120.4, 112.4, 111.4, 46.4, 43.5, 32.9, 12.4 ppm. Elem. Anal. Calcd. For $C_{24}H_{26}N_2$: C 84.17, H 7.65, N 8.18 Found: C 83.08, H 7.79, N 8.16.

10-Methyl-9-[4-(2,2,2-trifluoroacetylamino)phenyl]-9,10-dihydroacridine *(2e)*



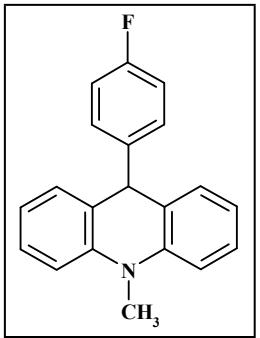
Light yellow crystalline powder. 340 mg (89%). M.p.: 179-181 °C. ^{1}H NMR (500 MHz, [D$_6$]DMSO): δ 11.16 (s, 1H), 7.46 (d, 2H, J=7.8 Hz), 7.27-7.23 (m, 4H), 7.09-7.06 (m, 4H), 6.95-6.92 (m, 2H), 5.28 (s, 1H), 3.37 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D$_6$]DMSO): δ 154.3 (d, $^{2}J_{CF}$=36.7 Hz), 142.9, 141.9, 134.3, 128.4, 127.4, 127.3, 126.1, 121.2, 120.1, 115.8 (d, $^{1}J_{CF}$=288.9 Hz), 112.7, 46.8, 32.9 ppm. ^{19}F NMR (470.5 MHz, [D$_6$]DMSO): δ 88.7 ppm. Elem. Anal. Calcd. For $C_{22}H_{17}F_3N_2O$: C 69.10, H 4.48, N 7.33 Found: C 68.91, H 4.47, N 7.24. FT-IR (DRA, cm^{-1}): 474, 495, 519, 574, 609, 654, 698, 715, 727, 742, 755, 798, 832, 847, 866, 895, 905, 934, 953, 1019, 1042, 1065, 1124, 1156, 1169, 1202,1246, 1270, 1285, 1313, 1344, 1412, 1461, 1475, 1509, 1551, 1593, 1609, 1706, 1727, 1781, 1932, 2825, 2892, 3037, 3073, 3144, 3208, 3324.

10-Methyl-9-[4-(acetylamino)phenyl]-9,10-dihydroacridine *(2f)*



Colorless crystalline powder. 302 mg (92%). M.p.: 242 °C. ^{1}H NMR (500 MHz, [D$_6$]DMSO): δ 9.81 (s, 1H), 7.35 (d, 2H, J=8.6 Hz), 7.24-7.21 (m, 4H), 7.05 (d, 2H, J=8.0 Hz), 6.98-6.91 (m, 4H), 5.20 (s, 1H), 3.36 (s, 3H), 1.97 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D$_6$]DMSO): δ 168.0, 141.9, 140.1, 137.4, 128.3, 127.2, 127.0, 126.4, 120.5, 119.1, 112.6, 46.8, 32.9, 23.8 ppm. Elem. Anal. Calcd. For $C_{22}H_{20}N_2O$: C 80.46, H 6.14, N 8.53 Found: C 80.47, H 6.08, N 8.63. FT-IR (DRA, cm^{-1}): 460, 518, 540, 570, 592, 607, 617, 629, 651, 660, 746, 808, 821, 857, 900, 932, 944, 974, 1021, 1044, 1063, 1131, 1145, 1166, 1265, 1287, 1315, 1349, 1370, 1409, 1475, 1509, 1536, 1591, 1661, 1891, 2828, 2892, 3035, 3118, 3188, 3279.

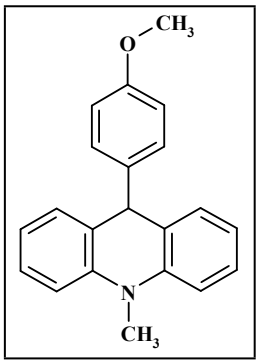
10-Methyl-9-(4-fluorophenyl)-9,10-dihydroacridine *(2g)*



Light yellow crystals. 721 mg (80%). M.p.: 112 °C. ^{1}H NMR (500 MHz, [D$_6$]DMSO): δ 7.28-7.22 (m, 4H), 7.10-7.06 (m, 4H), 7.03-6.99 (m, 2H), 6.96-6.93 (m, 2H), 5.30 (s, 1H), 3.36 (s, 3H) ppm. ^{13}C NMR (126

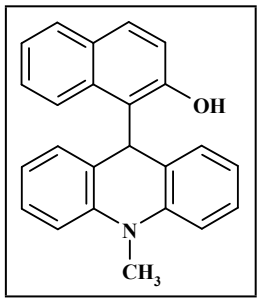
MHz, [D_6]DMSO): δ 160.6 (d, $^1J_{CF}$=242.2 Hz), 141.9, 141.7 (d, $^4J_{CF}$=3.0 Hz), 128.5 (d, $^3J_{CF}$=8.0 Hz), 128.4, 127.4, 126.1, 120.6, 115.0 (d, $^2J_{CF}$=21.1 Hz), 112.7, 46.4, 32.9 ppm. ^{19}F NMR (470.5 MHz, [D_6]DMSO): δ 45.6-45.5 (m) ppm. Elem. Anal. Calcd. For $C_{20}H_{16}NF$: C 83.02, H 5.57, N 4.84 Found: C 82.91, H 5.55, N 4.71. FT-IR (DRA, cm^{-1}): 495, 526, 549, 581, 616, 635, 654, 696, 724, 752, 792, 814, 827, 834, 844, 864, 896, 935, 1012, 1041, 1064, 1095, 1130, 1143, 1158, 1166, 1181, 1197, 1218, 1273, 1317, 1346, 1457, 1474, 1501, 1594, 1894, 1934, 2824, 2881, 2983, 3025, 3064.

10-Methyl-9-(4-methoxyphenyl)-9,10-dihydroacridine[3] *(2h)*



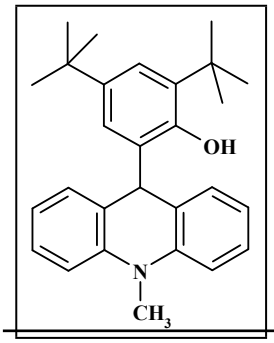
Colorless needles. 760 mg (81%). M.p.: 143-144 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 7.24-7.20 (m, 4H), 7.05 (d, 2H, J=8.0 Hz), 6.98-6.91 (m, 4H), 6.74 (d, 2H, J=8.8 Hz), 5.20 (s, 1H), 3.63 (s, 3H), 3.35 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D_6]DMSO): δ 157.6, 141.9, 137.6, 128.3, 127.8, 127.1, 126.6, 120.5, 113.7, 112.6, 54.9, 46.4, 32.8 ppm. Elem. Anal. Calcd. For $C_{21}H_{19}NO$: C 83.69, H 6.35, N 4.65 Found: C 83.54, H 6.31, N 4.55. FT-IR (DRA, cm^{-1}): 502, 523, 557, 586, 635, 652, 699, 725, 757, 785, 806, 841, 861, 870, 897, 936, 1037, 1062, 1098, 1131, 1141, 1160, 1181, 1245, 1269, 1300, 1310, 1344, 1428, 1458, 1472, 1507, 1592, 1605, 1903, 2824, 2839, 2878, 2904, 2958, 3031, 3060.

10-Methyl-9-(2-hydroxy-1-naphthyl)-9,10-dihydroacridine *(2i)*



Colorless crystals. 893 mg (85%). M.p.: 127 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 10.01 (s, 1H), 7.84-7.80 (m, 2H), 7.37 (d, 1H, J=8.6 Hz), 7.28 (d, 1H, J=8.2 Hz), 7.14-7.11 (m, 3H), 7.04-6.97 (m, 3H), 6.62 (t, 2H, J=7.3 Hz), 6.35 (d, 2H, J=6.9 Hz), 6.19 (s, 1H), 3.46 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D_6]DMSO): δ 154.3, 142.2, 132.2, 129.4, 129.0, 128.6, 126.8, 126.6, 124.7, 121.9, 120.0, 117.9, 117.0, 112.1, 36.5, 33.4 ppm. Elem. Anal. Calcd. For $C_{24}H_{19}NO$: C 85.43, H 5.68, N 4.15 Found: C 85.61, H 5.78, N 4.33.

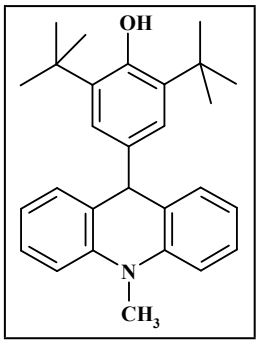
10-Methyl-9-(2-hydroxy-3,5-di-tertbutyl-phenyl)-9,10-dihydroacridine *(2j)*



Colorless crystalline powder. 1058 mg (85%). M.p.: 177 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 8.32 (s, 1H), 7.20-7.17 (m, 4H), 7.04 (d, 2H, J=8.0 Hz), 6.97 (d, 1H, J=2.4 Hz), 6.88-6.85 (m, 2H), 6.70 (d, 1H, J=2.4 Hz), 5.78 (s, 1H), 3.40 (s, 3H), 1.38 (s, 9H), 1.01 (s, 9H) ppm. ^{13}C

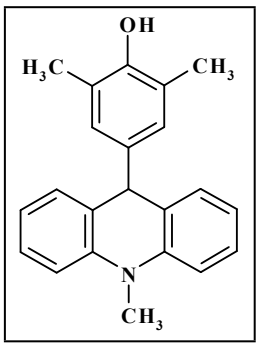
[3] In-Sook Han Lee, Kim-Hung Chow, Maurice M. Kreevoy, *J. Am. Chem. Soc.*, 2002, **124**, 7755–7761.

NMR (126 MHz, [D_6]DMSO): δ 149.1, 142.4, 141.0, 137.0, 132.9, 127.9, 127.5, 126.9, 123.3, 120.8, 120.3, 112.5, 34.8, 33.7, 33.0, 31.2, 30.0 ppm. Elem. Anal. Calcd. For $C_{28}H_{33}NO$: C 84.17, H 8.32, N 3.51 Found: C 83.98, H 8.36, N 3.51. FT-IR (DRA, cm^{-1}): 569, 636, 654, 696, 758, 795, 826, 877, 888, 936, 968, 1047, 1094, 1131, 1157, 1180, 1206, 1231, 1267, 1286, 1300, 1344, 1362, 1390, 1418, 1464, 1499, 1588, 1605, 2824, 2873, 2957, 2996, 3036, 3072, 3546.



10-Methyl-9-(4-hydroxy-3,5-di-tertbutyl-phenyl)-9,10-dihydroacridine *(*2k*)*

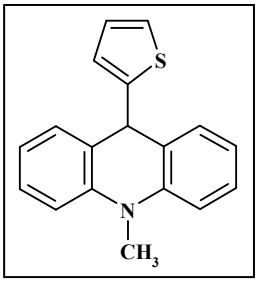
Colorless crystalline powder. 983 mg (79%). M.p.: 183 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 7.25-7.19 (m, 4H), 7.04 (d, 2H, J=7.9 Hz), 6.93-6.90 (m, 2H), 6.84 (s, 2H), 6.69 (s, 1H), 5.11 (s, 1H), 3.36 (s, 3H), 1.24 (s, 18H) ppm. ^{13}C NMR (126 MHz, [D_6]DMSO): δ 152.0, 142.0, 138.7, 136.3, 128.1, 127.3, 127.0, 122.8, 120.5, 112.5, 47.4, 34.4, 32.9, 30.2 ppm. Elem. Anal. Calcd. For $C_{28}H_{33}NO$: C 84.17, H 8.32, N 3.51 Found: C 84.08, H 8.24, N 3.27.



10-Methyl-9-(4-hydroxy-3,5-dimethyl-phenyl)-9,10-dihydroacridine *(*2l*)*

Colorless crystalline powder. 668 mg (68%). M.p.: 141 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 8.03 (s, 1H), 7.27-7.21 (m, 4H), 7.08 (d, 2H, J=8.0 Hz), 6.96-6.93 (m, 2H), 6.65 (s, 2H), 5.10 (s, 1H), 3.41 (s, 3H), 2.07 (s, 6H) ppm. ^{13}C NMR (126 MHz, [D_6]DMSO): δ 151.5, 141.9, 136.2, 128.3, 127.0, 126.9, 126.7, 123.8, 120.4, 112.5, 46.7, 32.8, 16.8 ppm. Elem. Anal. Calcd. For $C_{22}H_{21}NO$: C 83.78, H 6.71, N 4.44 Found: C 83.59, H 6.66, N 4.39.

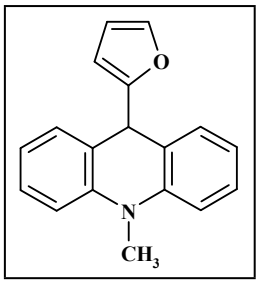
10-Methyl-9-(thiophen-2-yl)-9,10-dihydroacridine *(*2m*)*



Colorless needles. 665 mg (77%). M.p.: 121-122 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 7.34-7.33 (m, 2H), 7.28-7.25 (m, 2H), 7.19-7.17 (m, 1H), 7.07 (d, 2H, J=8.2 Hz), 6.99-6.96 (m, 2H), 6.79-6.78 (m, 1H), 6.54 (m, 1H), 5.54 (s, 1H), 3.36 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D_6]DMSO): δ 149.8, 141.7, 128.2, 127.6, 126.4, 125.9, 124.3, 123.3, 120.5, 112.8, 42.8, 32.9 ppm. Elem. Anal. Calcd. For $C_{18}H_{15}NS$: C 77.94, H 5.45, N 5.05 Found:

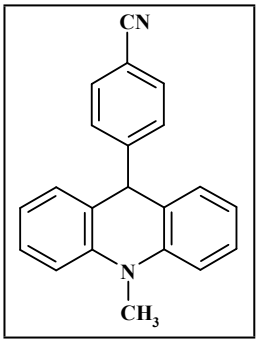
C 77.91, H 5.47, N 5.04. FT-IR (DRA, cm^{-1}): 474, 562, 610, 622, 655, 684, 702, 713, 753, 788, 824, 845, 897, 932, 1040, 1064, 1099, 1132, 1166, 1187, 1200, 1216, 1233, 1247, 1270, 1281, 1314, 1344, 1422, 1474, 1505, 1524, 1592, 1895, 1929, 2819, 2875, 2971, 3036, 3056, 3089.

10-Methyl-9-(furan-2-yl)-9,10-dihydroacridine *(2n)*



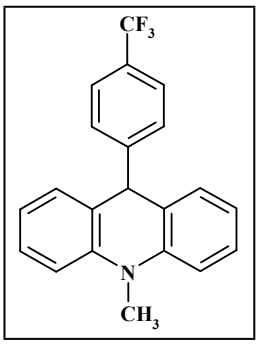
Colorless needles. 561 mg (69%). M.p.: 148 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 7.45 (d, 1H, J=0.7 Hz), 7.28-7.24 (m, 4H), 7.05 (d, 2H, J=8.0 Hz), 6.97-6.94 (m, 2H), 6.23-6.22 (m, 1H), 5.59 (d, 1H, J=3.1 Hz), 5.36 (s, 1H), 3.34 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D_6]DMSO): δ 156.5, 142.0, 141.9, 128.5, 127.7, 123.2, 120.4, 112.6, 110.2, 105.4, 41.4, 32.9 ppm. Elem. Anal. Calcd. For $C_{18}H_{15}NO$: C 82.73, H 5.79, N 5.36 Found: C 82.59, H 5.95, N 5.29.

10-Methyl-9-(4-cyanophenyl)-9,10-dihydroacridine *(2o)*



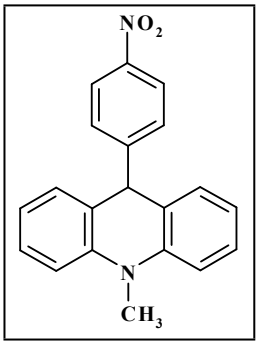
Colorless crystals. 145 mg (49%). M.p.: 126-127 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 7.66 (d, 2H, J=8.4 Hz), 7.32 (d, 2H, J=7.4 Hz), 7.27-7.24 (m, 4H), 7.13-7.07 (m, 2H), 6.97-6.94 (m, 2H), 5.45 (s, 1H), 3.37 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D_6]DMSO): δ 150.9, 141.9, 132.4, 128.5, 127.4, 127.7, 125.1, 126.8, 118.8, 112.9, 109.0, 47.1, 32.9 ppm. Elem. Anal. Calcd. For $C_{21}H_{16}N_2$: C 85.11, H 5.44, N 9.54 Found: C 85.28, H 4.49, N 9.50.

10-Methyl-9-(4-trifluoromethylphenyl)-9,10-dihydroacridine *(2p)*



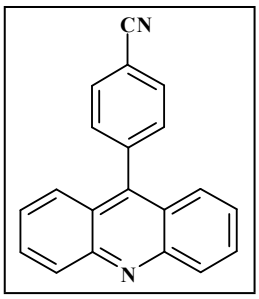
Colorless crystals. 149 mg (44%). M.p.: 132-133 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 7.55 (d, 2H, J=8.3 Hz), 7.32-7.24 (m, 6H), 7.10 (d, 2H, J=8.1 Hz), 6.97-6.94 (m, 2H), 5.44 (s, 1H), 3.38 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D_6]DMSO): δ 150.0, 141.9, 128.5, 127.6, 127.5, 126.8 (d, $^{2}J_{CF}$=31.7 Hz), 125.3, 125.3 (q, $^{2}J_{CF}$=3.7 Hz), 123.1, 120.7, 112.8, 46.9, 32.9 ppm. ^{19}F NMR (470.5 MHz, [D_6]DMSO): δ 101.8 ppm. Elem. Anal. Calcd. For $C_{21}H_{16}F_3N$: C 74.33, H 4.75, N 4.13 Found: C 74.21, H 4.78, N 4.15.

10-Methyl-9-(4-nitrophenyl)-9,10-dihydroacridine *(2q)*



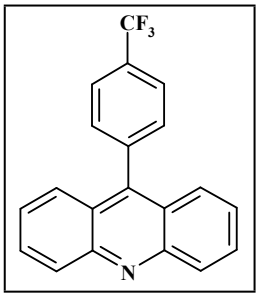
Yellow crystals. 164 mg (52%). M.p.: 148-149 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 8.07-8.05 (m, 2H), 7.34-7.32 (m, 4H), 7.29-7.26 (m, 2H), 7.11 (d, 2H, J=8.0 Hz), 6.98-6.95 (m, 2H), 5.52 (s, 1H), 3.38 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D_6]DMSO): δ 152.9, 145.9, 141.9, 128.5, 127.9, 127.8, 124.9, 123.7, 120.8, 112.9, 46.9, 32.9 ppm.. Elem. Anal. Calcd. For $C_{20}H_{16}N_2O_2$: C 75.93, H 5.10, N 8.85 Found: C 75.96, H 5.05, N 8.90. FT-IR (DRA, cm^{-1}): 493, 507, 617, 642, 660, 693, 711, 742, 757, 819, 846, 854, 863, 898, 938, 1013, 1043, 1063, 1108, 1131, 1142, 1169, 1269, 1285, 1318, 1339, 1431, 1474, 1505, 1519, 1591, 1796, 1931, 2830, 2894, 2974, 3040, 3072, 3102.

9-(4-Cyanophenyl)-acridine *(6o)*



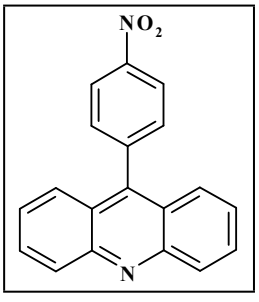
Yellow crystalline powder. 118 mg (90%). M.p.: 223-224 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 8.25 (d, 2H, J=8.8 Hz), 8.16 (d, 2H, J=7.9 Hz), 7.91-7.87 (m, 2H), 7.75 (d, 2H, J=8.0 Hz), 7.59-7.54 (m, 4H) ppm. ^{13}C NMR (126 MHz, [D_6]DMSO): δ 148.1, 144.5, 140.4, 132.6, 131.4, 130.4, 129.4, 126.6, 125.9, 123.8, 118.7, 111.6 ppm. Elem. Anal. Calcd. For $C_{20}H_{12}N_2$: C 85.69, H 4.31, N 9.99 Found: C 85.70, H 4.43, N 9.84. GC t_R 31.60 min; MS m/z (rel intensity) 280 (M^+, 100).

9-(4-Trifluoromethylphenyl)-acridine *(6p)*



Yellow crystalline powder. 140 mg (92%). M.p.: 264-265 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 8.25 (d, 2H, J=8.8 Hz), 8.05 (d, 2H, J=7.9 Hz), 7.90-7.87 (m, 2H), 7.77 (d, 2H, J=8.0 Hz), 7.60-7.55 (m, 4H) ppm. ^{13}C NMR (126 MHz, [D_6]DMSO): δ 148.1, 144.7, 139.6, 131.2, 130.3, 129.4, 126.5, 126.0, 125.8, 125.6, 125.5, 124.0 ppm. ^{19}F NMR (470.5 MHz, [D_6]DMSO): δ 101.6 ppm. Elem. Anal. Calcd. For $C_{20}H_{12}F_3N$: C 74.30, H 3.74, N 4.33 Found: C 74.18, H 3.75, N 4.33. GC t_R 26.51 min; MS m/z (rel intensity) 323 (M^+, 100).

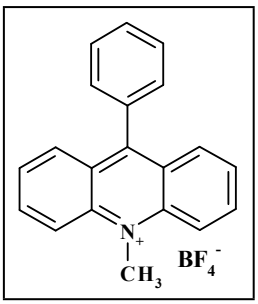
9-(4-Nitrophenyl)-acridine *(6q)*



Yellow crystalline powder. 122 mg (87%). M.p.: 291-292 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.49 (d, 2H, J=7.6 Hz), 8.32 (d, 2H, J=8.3 Hz), 7.83-7.80 (m, 2H), 7.66 (d, 2H, J=7.7 Hz), 7.57-7.56 (m, 2H), 7.49-7.48 (m, 2H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$): δ 148.6, 148.0, 143.1, 131.6, 130.2, 129.9, 128.3, 126.5, 125.8, 124.4, 123.8 ppm. Elem. Anal. Calcd. For $C_{19}H_{12}N_2O_2$: C 75.99, H 4.09, N 9.33 Found: C 75.68, H 4.10, N 9.32. GC t_R 33.26 min; MS m/z (rel intensity) 330 (M^+, 100). FT-IR (DRA, cm^{-1}): 457, 574,

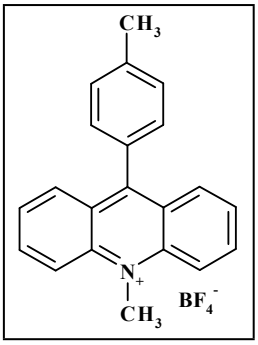
605, 614, 638, 653, 689, 703, 747, 757, 769, 816, 832, 854, 878, 934, 1014, 1032, 1104, 1146, 1162, 1211, 1284, 1313, 1344, 1413, 1438, 1460, 1477, 1517, 1545, 1557, 1600, 1626, 1830, 1943, 2849, 3028, 3072.

9-Phenyl-10-methylacridinium tetrafluoroborate (3a)



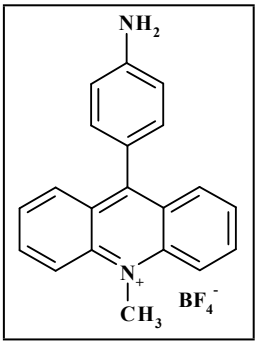
Yellow crystals. 628 mg (88%). M.p.: 247 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 8.88 (d, 2H, J=9.3 Hz), 8.49-8.44 (m, 2H), 7.95 (d, 4H, J=4.2 Hz),7.80-7.78 (m, 3H), 7.60-7.59 (m, 2H), 4.95 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D_6]DMSO): δ 160.4, 141.2, 138.4, 133.1, 130.1, 129.8, 129.5, 128.8, 127.9, 125.5, 119.2, 38.9 ppm. Elem. Anal. Calcd. For $C_{20}H_{16}NBF_4$: C 67.25, H 4.52, N 3.92, F 21.28 Found: C 67.27, H 4.55, N 4.02, F 21.22. FT-IR (DRA, cm^{-1}): 464, 520, 546, 570, 599, 619, 629, 665, 677, 702, 747, 765, 797, 860, 924, 937, 971, 1024, 1042, 1061, 1104, 1161, 1170, 1182, 1197, 1277, 1381, 1413, 1442, 1460, 1550, 1579, 1612, 1831, 3058, 3134.

9-(4-Methylphenyl)-10-methylacridinium tetrafluoroborate (3b)



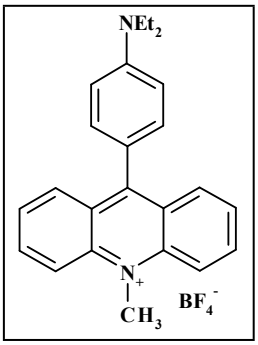
Yellow crystals. 683 mg (92%). M.p.: 271 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 8.86 (d, 2H, J=9.2 Hz), 8.47-8.44 (m, 2H), 8.00-7.92 (m, 4H), 7.60 (d, 2H, J=7.8 Hz),7.49 (d, 2H, J=8.0 Hz), 4.93 (s, 3H), 2.55 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D_6]DMSO): δ 160.8, 141.2, 139.9, 138.3, 130.1, 129.9, 129.6, 129.4, 127.8, 125.6, 119.1, 38.9, 20.9 ppm. Elem. Anal. Calcd. For $C_{21}H_{18}NBF_4$: C 67.94, H 4.90, N 3.77, F 20.47 Found: C 67.98, H 4.88, N 3.82, F 20.52. FT-IR (DRA, cm^{-1}): 442, 507, 519, 567, 600, 618, 627, 669, 725, 767, 794, 815, 866, 925, 971, 1032, 1171, 1188, 1218, 1245, 1279, 1379, 1390, 1412, 1448, 1460, 1495, 1551, 1580, 1612, 2922, 3055, 3137.

9-(4-Aminophenyl)-10-methyl-acridinium tetrafluoroborate (3c)



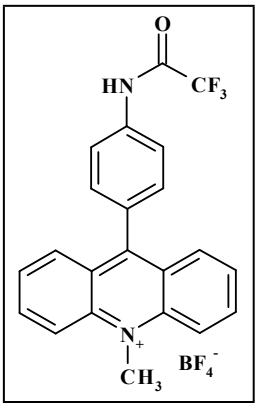
Dark needles. 677 mg (91%). M.p.: 233 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 8.76 (d, 2H, J=9.2 Hz), 8.42-8.38 (m, 2H), 8.24-8.22 (m, 2H), 7.93-7.90 (m, 2H),7.31-7.29 (m, 2H), 6.92-6.90 (m, 2H), 6.02 (s, 2H), 4.83 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D_6]DMSO): δ 162.0, 151.3, 141.2, 137.8, 132.6, 130.3, 127.2, 125.4, 119.1, 118.9, 113.5, 38.5 ppm. Elem. Anal. Calcd. For $C_{20}H_{17}N_2BF_4$: C 64.54, H 4.61, N 7.52, F 20.42 Found: C 64.69, H 4.55, N 7.53, F 20.26. FT-IR (DRA, cm^{-1}): 410, 429, 470, 524, 570, 588, 602, 615, 630, 668, 732, 766, 794, 824, 865, 922, 997, 1038, 1064, 1176, 1199, 1272, 1317, 1374, 1407, 1446, 1458, 1523, 1546, 1574, 1606, 1641, 1741, 2925, 3038, 3139, 3256, 3381, 3466.

9-(4-Diethylaminophenyl)-10-methyl-acridinium tetrafluoroborate (3d)



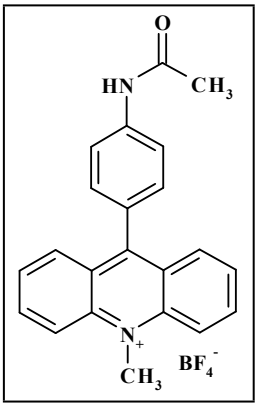
Dark violet crystals. 728 mg (85%). M.p.: 236 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 8.77 (d, 2H, J=9.2 Hz), 8.42-8.38 (m, 2H), 8.25-8.23 (m, 2H), 7.93-7.90 (m, 2H),7.44 (d, 2H, J=8.8 Hz), 7.03 (d, 2H, J=8.9 Hz), 4.83 (s, 3H), 3.55-3.51 (m, 4H), 1.24-1.21 (m, 6H) ppm. ^{13}C NMR (126 MHz,[D_6]DMSO): δ 161.6, 149.0, 141.2, 137.8, 132.9, 130.3, 127.2, 125.4, 118.9, 118.5, 111.0, 43.8, 38.5, 12.4 ppm. Elem. Anal. Calcd. For $C_{24}H_{25}N_2BF_4$: C 67.30, H 5.90, N 6.54, F 17.74 Found: C 67.15, H 5.74, N 6.35, F 17.86. FT-IR (DRA, cm^{-1}): 414, 470, 520, 565, 578, 601, 616, 628, 662, 733, 763, 793, 821, 863, 925, 968, 1049, 1152, 1184, 1210, 1263, 1283, 1359, 1415, 1488, 1530, 1564, 1598, 1825, 1988, 2600, 2872, 2973, 3064, 3137.

9-[4-(2,2,2-Trifluoroacetylamino)phenyl]-10-methyl-acridinium tetrafluoroborate (3e)

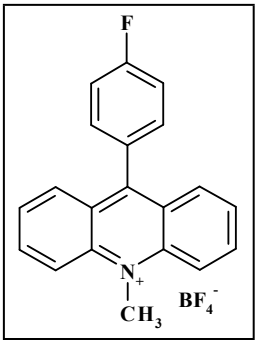


Yellow crystals. 796 mg (85%). M.p.: 270 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 11.71 (s,1H), 8.77 (d, 2H, J=9.3 Hz), 8.48-8.45 (m, 2H), 8.10 (d, 2H, J=8.6 Hz), 8.01-7.93 (m, 4H),7.66 (d, 2H, J=8.6 Hz), 4.94 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D_6]DMSO): δ 159.9, 154.9 (d, $^{2}J_{CF}$=37.4 Hz), 141.2, 138.4, 138.1, 130.9, 130.0. 129.6, 128.0, 125.6, 120.9, 119.2, 115.7 (d, $^{1}J_{CF}$=288.7 Hz), 39.0 ppm. ^{19}F NMR ([D_6]DMSO): δ 88.8, 14.3, 14.2 ppm. Elem. Anal. Calcd. For $C_{22}H_{16}N_2BF_7O$: C 56.43, H 3.45, N 5.98, F 28.41 Found: C 56.17, H 3.52, N 5.93, F 28.30.

9-[4-(Acetylamino)phenyl]-10-methyl-acridinium tetrafluoroborate (3f)



Red crystals. 712 mg (86%). M.p.: 306-307 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 10.39 (s,1H), 8.85 (d, 2H, J=9.3 Hz), 8.47-8.44 (m, 2H), 8.06-8.04 (m, 2H), 7.99-7.93 (m, 4H),7.54 (d, 2H, J=8.6 Hz), 4.92 (s, 3H), 2.16 (s,3H) ppm. ^{13}C NMR (126 MHz, [D_6]DMSO): δ 169.0, 160.6, 141.2, 141.1, 138.3, 130.9, 129.8, 127.8, 127.2, 125.6, 119.2, 118.8, 38.9, 24.2 ppm. Elem. Anal. Calcd. For $C_{22}H_{19}N_2BF_4$: C 63.79, H 4.63, N 6.76 Found: C 63.54, H 4.60, N 6.75. FT-IR (DRA, cm^{-1}): 405, 518, 531, 567, 603, 622, 653, 664, 710, 732, 745, 760, 793, 840, 867, 925, 1012, 1056, 1121, 1181, 1201, 1254, 1274, 1313, 1374, 1405, 1449, 1460, 1521, 1550, 1578, 1609, 1690, 3130, 3354.

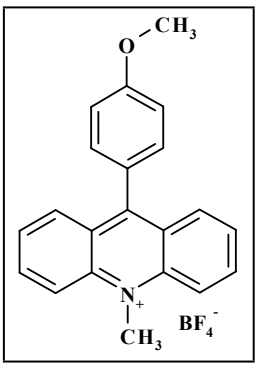


9-(4-Fluorophenyl)-10-methyl-acridinium tetrafluoroborate (3g)

Yellow crystals. 727 mg (97%). M.p.: 313 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 8.88 (d, 2H, J=9.3 Hz), 8.49-8.45 (m, 2H), 7.98-7.93 (m,

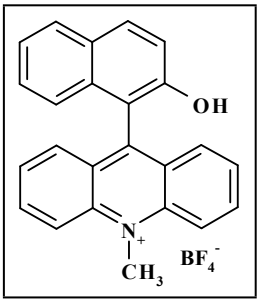
4H), 7.68-7.62 (m, 4H), 4.95 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D_6]DMSO): δ 163.1 (d, $^{1}J_{CF}$=247.8 Hz), 159.6, 141.2, 138.5, 132.3 (d, $^{3}J_{CF}$=8.7 Hz), 129.5, 129.4 (d, $^{4}J_{CF}$=3.2 Hz), 128.0, 125.7, 119.2, 116.1 (d, $^{2}J_{CF}$=22.1 Hz), 39.0 ppm. ^{19}F NMR ([D_6]DMSO): δ 51.67-51.6 (m), 14.3, 14.3 (m) ppm. Elem. Anal. Calcd. For $C_{20}H_{15}NBF_5$: C 64.03, H 4.04, N 3.73, F 25.32 Found: C 64.12, H 3.91, N 3.74, F 24.99. FT-IR (DRA, cm^{-1}): 443, 520, 568, 587, 599, 616, 671, 730, 767, 795, 831, 866, 926, 976, 1049, 1085, 1168, 1201, 1232, 1279, 1380, 1413, 1450, 1462, 1514, 1551, 1581, 1602, 1612, 3118.

9-(4-Methoxyphenyl)-10-methyl-acridinium tetrafluoroborate (3h)



Orange crystals. 704 mg (91%). M.p.: 243-244 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 8.85 (d, 2H, J=9.2 Hz), 8.47-8.44 (m, 2H), 8.06-8.04 (m, 2H), 7.96-7.93 (m, 2H), 7.56-7.53 (m, 2H), 7.36-7.33 (m, 2H), 4.92 (s, 3H), 3.96 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D_6]DMSO): δ 160.8, 160.7, 141.2, 138.3, 131.8, 129.7, 127.7, 125.7, 124.9, 119.1, 114.4, 55.5, 38.8 ppm. Elem. Anal. Calcd. For $C_{21}H_{18}NBF_4O$: C 65.14, H 4.70, N 3.62, F 19.63 Found: C 64.99, H 4.49, N 3.65, F 19.45. FT-IR (DRA, cm^{-1}): 411, 445, 469, 519, 567, 592, 618, 671, 729, 768, 795, 832, 865, 925, 1047, 1184, 1255, 1278, 1294, 1379, 1413, 1447, 1461, 1519, 1550, 1579, 1608, 2847, 2942, 3022, 3048, 3065, 3118, 3141.

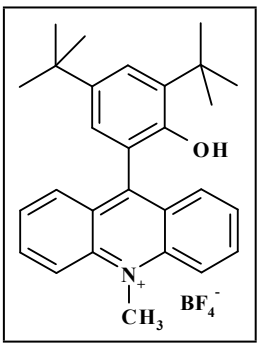
9-(2-Hydroxy-1-naphthyl)-10-methyl-acridinium tetrafluoroborate (3i)



Red needles. 778 mg (92%). M.p.: 311-313 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 13.32 (s,1H), 8.91 (d, 2H, J=9.3 Hz), 8.45-8.42 (m, 2H), 8.22 (d, 1H, J=9.0 Hz), 8.05 (d, 1H, J=8.1 Hz),7.85-7.77 (m, 4H), 7.52 (d, 1H, J=9.0 Hz), 7.38-7.35(m, 1H), 7.23-7.20(m, 1H), 6.69 (d, 1H, J=8.5Hz), 4.99 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D_6]DMSO): δ 158.7, 153.0, 141.3, 138.5, 133.2, 132.2, 129.1, 128.3, 128.0, 127.6, 127.5, 126.6, 123.7, 123.5, 119.5, 118.2, 111.8, 38.9 ppm. Elem. Anal. Calcd. For $C_{24}H_{18}NBF_4O$: C 68.10, H 4.30, N 3.31, F 17.96 Found: C 68.00, H 4.16, N 3.30, F 18.08. FT-IR (DRA, cm^{-1}): 526, 557, 566, 599, 625, 657, 687, 711, 755, 781, 824, 866, 910, 974, 993, 1028, 1078, 1169, 1193, 1216, 1261, 1278, 1346, 1385, 1438, 1460, 1515, 1549, 1583, 1610, 1626, 3079, 3408.

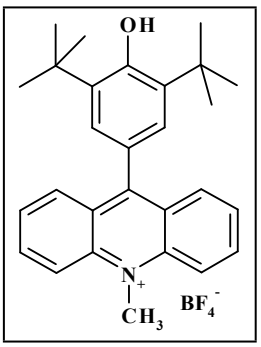
9-(2-Hydroxy-3,5-di-tertbutyl-phenyl)-10-methyl-acridinium tetrafluoroborate (3j)

Yellow crystals. 845 mg (87%). M.p.: 305-306°C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 8.85 (d, 2H, J=9.3 Hz), 8.48-8.42 (m, 2H), 8.32 (s, 1H), 7.98-7.94 (m, 4H), 7.58 (d, 1H, J=2.4 Hz), 7.10 (d, 1H, J=2.4 Hz), 4.97 (s, 3H), 1.47 (s, 9H), 1.30 (s, 9H) ppm. ^{13}C NMR (126 MHz,



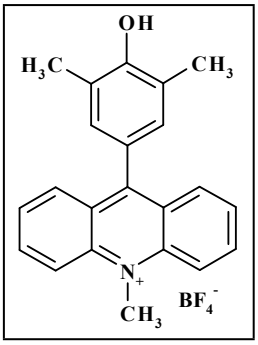
[D$_6$]DMSO): δ 159.5, 150.3, 141.3, 141.2, 138.3, 137.3, 129.6, 127.9, 126.7, 125.5, 125.4, 120.7, 119.0, 38.7, 35.0, 34.1, 31.3, 29.5 ppm. Elem. Anal. Calcd. For $C_{28}H_{32}NOBF_4$: C 69.28, H 6.66, N 2.88, F 15.66 Found: C 69.07, H 6.79, N 3.01, F 15.54. FT-IR (DRA, cm^{-1}): 411, 517, 554, 600, 645, 674, 693, 760, 795, 822, 835, 882, 984, 1006, 1069, 1154, 1173, 1198, 1214, 1254, 1273, 1321, 1361, 1388, 1446, 1477, 1550, 1584, 1611, 2865, 2955, 3141, 3400.

9-(4-Hydroxy-3,5-di-tertbutyl-phenyl)-10-methyl-acridinium tetrafluoroborate (3k)



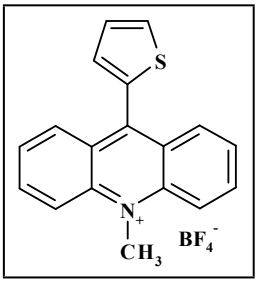
Yellow crystals. 845 mg (87%). M.p.: 285-286°C. ^{1}H NMR (500 MHz, [D$_6$]DMSO): δ 8.82 (d, 2H, J=9.2 Hz), 8.45-8.41 (m, 2H), 8.08 (d, 2H, J=8.6Hz), 7.97-7.94 (m, 2H), 7.79 (s, 1H), 7.31 (s, 2H), 4.89 (s, 3H), 1.46 (s, 18H) ppm. ^{13}C NMR (126 MHz, [D$_6$]DMSO): δ 141.3, 139.3, 138.1, 130.0, 127.7, 127.3, 125.7, 124.2, 119.0, 38.8, 34.8, 30.2 ppm. Elem. Anal. Calcd. For $C_{28}H_{32}NOBF_4$: C 69.28, H 6.66, N 2.88, F 15.66 Found: C 69.19, H 6.64, N 2.98, F 15.79.

9-(4-Hydroxy-3,5-dimethyl-phenyl)-10-methyl-acridinium tetrafluoroborate (3l)



Orange needles. 722 mg (90%). M.p.: 280-281 °C. ^{1}H NMR (500 MHz, [D$_6$]DMSO): δ 9.09 (s, 1H), 8.82 (d, 2H, J=9.2 Hz), 8.45-8.42 (m, 2H), 8.12-8.10 (m, 2H), 7.94-7.91 (m, 2H), 7.16 (s, 2H), 4.90 (s, 3H), 2.33 (s, 6H) ppm. ^{13}C NMR (126 MHz, [D$_6$]DMSO): δ 161.5, 155.2, 141.2, 138.2, 130.3, 130.1, 127.6, 125.7, 124.8, 123.5, 119.0, 38.8, 16.6 ppm. Elem. Anal. Calcd. For $C_{22}H_{20}NBF_4O$: C 65.85, H 5.03, N 3.49, F 18.94 Found: C 65.66, H 5.09, N 3.52, F 19.13. FT-IR (DRA, cm^{-1}): 411, 420, 467, 522, 562, 600, 649, 671, 739, 750, 765, 797, 892, 928, 951, 975, 1010, 1032, 1071, 1113, 1147, 1170, 1218, 1242, 1273, 1290, 1334, 1384, 1411, 1448, 1486, 1546, 1575, 1609, 2921, 3137, 3485.

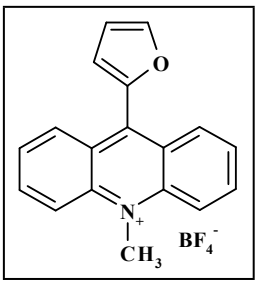
9-(Thiophen-2-yl)-10-methyl-acridinium tetrafluoroborate (3m)



Red needles. 690 mg (95%). M.p.: 203-204 °C. ^{1}H NMR (500 MHz, [D$_6$]DMSO): δ 8.86 (d, 2H, J=9.2 Hz), 8.48-8.45 (m, 2H), 8.25-8.21 (m, 3H), 8.01-7.98 (m, 2H),7.66 (d, 1H, J=3.3 Hz), 7.56-7.54 (m, 1H), 4.93 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D$_6$]DMSO): δ 153.6, 141.1, 138.4, 133.0, 131.5, 129.2, 128.2, 128.1, 126.5, 119.2, 39.1 ppm. Elem. Anal. Calcd. For $C_{18}H_{14}NBF_4S$: C 59.52, H 3.89, N 3.85, F 20.93, S 8.83 Found: C 59.55, H 3.96, N 3.88, F 21.12, S 8.74. FT-IR (DRA, cm^{-1}): 472, 492, 520, 569, 603, 638, 652, 671, 719,

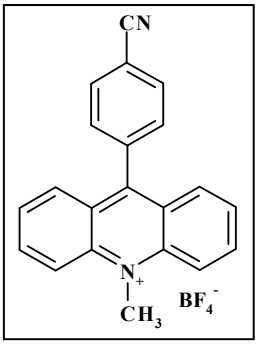
736, 767, 791, 845, 870, 1035, 1045, 1079, 1100, 1172, 1198, 1269, 1373, 1422, 1449, 1511, 1525, 1548, 1574, 1607, 2000, 3116.

9-(Furan-2-yl)-10-methyl-acridinium tetrafluoroborate (3n)



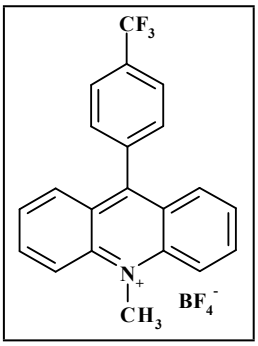
Red needles. 631 mg (91%). M.p.: 244-245 °C. ^{1}H NMR (500 MHz, [D$_6$]DMSO): δ 8.81 (d, 2H, J=9.2 Hz), 8.50-8.42 (m, 5H), 8.02-7.99 (m, 2H), 7.54 (d, 1H, J=3.5 Hz),7.14-7.13 (m, 1H), 4.87 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D$_6$]DMSO): δ 148.7, 146.3, 144.9, 141.5, 138.1, 129.2, 128.2, 124.5, 121.1, 119.2, 113.3, 39.3 ppm. Elem. Anal. Calcd. For $C_{18}H_{14}NBF_4O$: C 62.28, H 4.07, N 4.03, F 21.89 Found: C 62.12, H 4.26, N 4.07, F 21.99.

9-(4-Cyanophenyl)-10-methyl-acridinium tetrafluoroborate (3o)



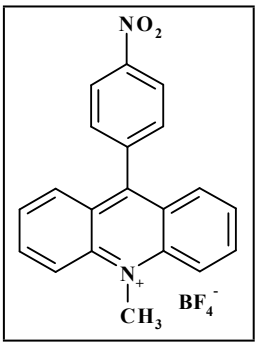
Yellow crystals. 680 mg (89%). M.p.: 324-325 °C. ^{1}H NMR (500 MHz, [D$_6$]DMSO): δ 8.90 (d, 2H, J=9.1 Hz), 8.48 (t, 2H, J=7.6 Hz), 8.27 (d, 2H, J=7.7 Hz), 7.96-7.82 (m, 6H), 4.97 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D$_6$]DMSO): δ 158.3, 141.2, 138.6, 138.0, 132.8, 130.8, 129.3, 128.2, 125.3, 119.3, 118.4, 113.0 39.6 ppm. Elem. Anal. Calcd. For $C_{21}H_{15}N_2BF_4$: C 65.99, H 3.96, N 7.33, F 19.89 Found: C 65.96, H 4.01, N 7.20, F 20.02. FT-IR (DRA, cm^{-1}): 424, 520, 543, 561, 585, 609, 628, 668, 732, 765, 799, 831, 873, 933, 1054, 1153, 1178, 1246, 1276, 1369, 1397, 1411, 1429, 1463, 1581, 1641, 2001, 2233, 2252, 2925, 3013, 3095, 3282, 3572.

9-(4-Trifluoromethylphenyl)-10-methyl-acridinium tetrafluoroborate (3p)



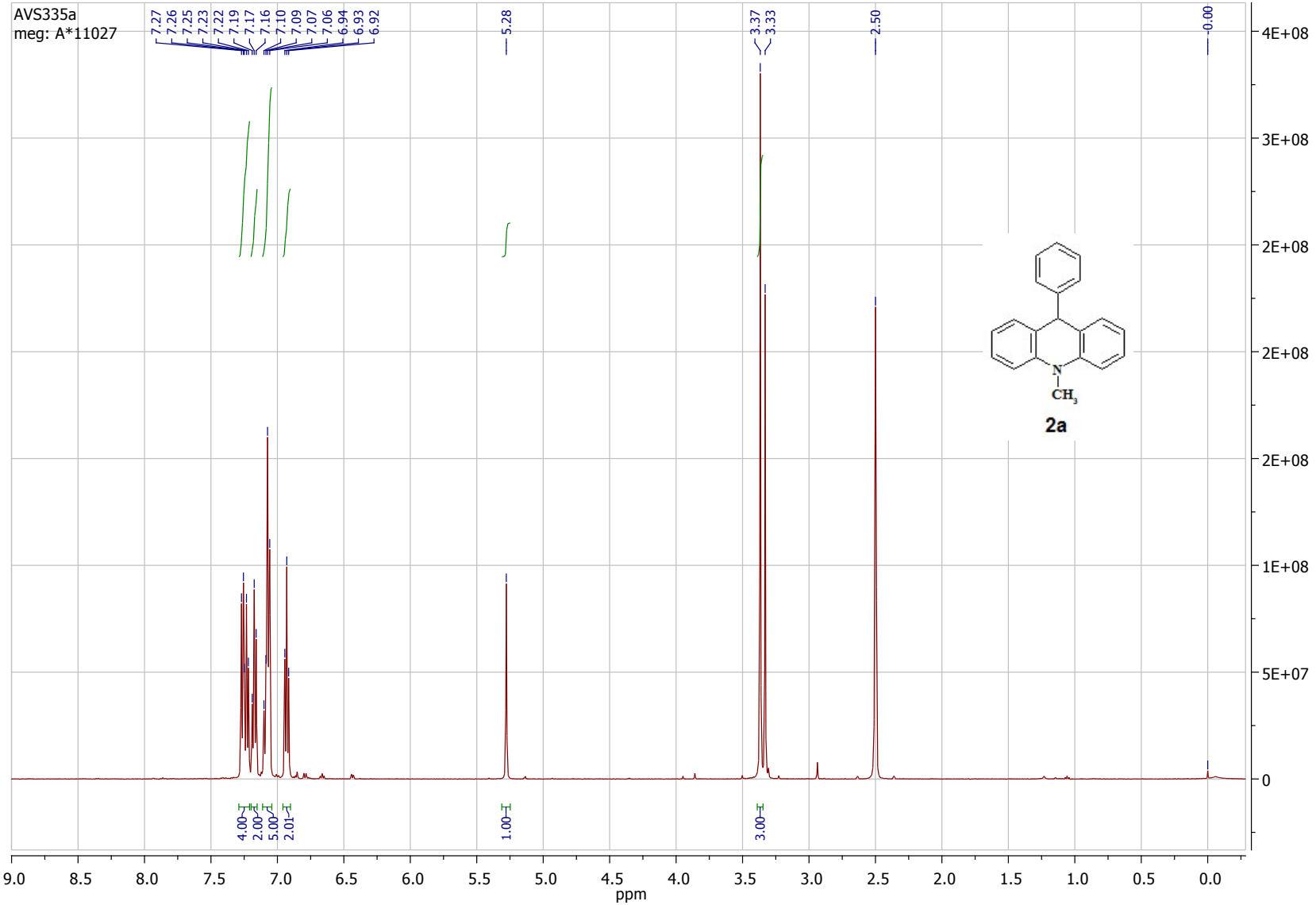
Yellow crystals. 782 mg (92%). M.p.: 244-245 °C. ^{1}H NMR (500 MHz, [D$_6$]DMSO): δ 8.90 (d, 2H, J=9.2 Hz), 8.50-8.47 (m, 2H), 8.16 (d, 2H, J=8.2 Hz), 7.96-7.89 (m, 4H), 7.85 (d, 2H, J=8.0 Hz), 4.97 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D$_6$]DMSO): δ 158.6, 141.2, 138.5, 137.4, 130.7, 130.4 (d, $^{2}J_{CF}$=32.3 Hz), 129.3, 128.2, 125.8 (d, $^{3}J_{CF}$=3.6 Hz), 125.4, 124.0 (d, $^{1}J_{CF}$=272.3 Hz), 119.2, 39.1 ppm. ^{19}F NMR ([D$_6$]DMSO): δ 101.4, 14.3, 14.3 (m) ppm. Elem. Anal. Calcd. For $C_{21}H_{15}NBF_7$: C 59.32, H 3.56, N 3.29, F 31.28 Found: C 59.21, H 3.47, N 3.42, F 31.46. FT-IR (DRA, cm^{-1}): 427, 443, 520, 554, 565, 600, 632, 667, 681, 747, 762, 785, 798, 839, 872, 926, 1049, 1064, 1123, 1162, 1197, 1275, 1323, 1375, 1406, 1458, 1550, 1578, 1609, 3134.

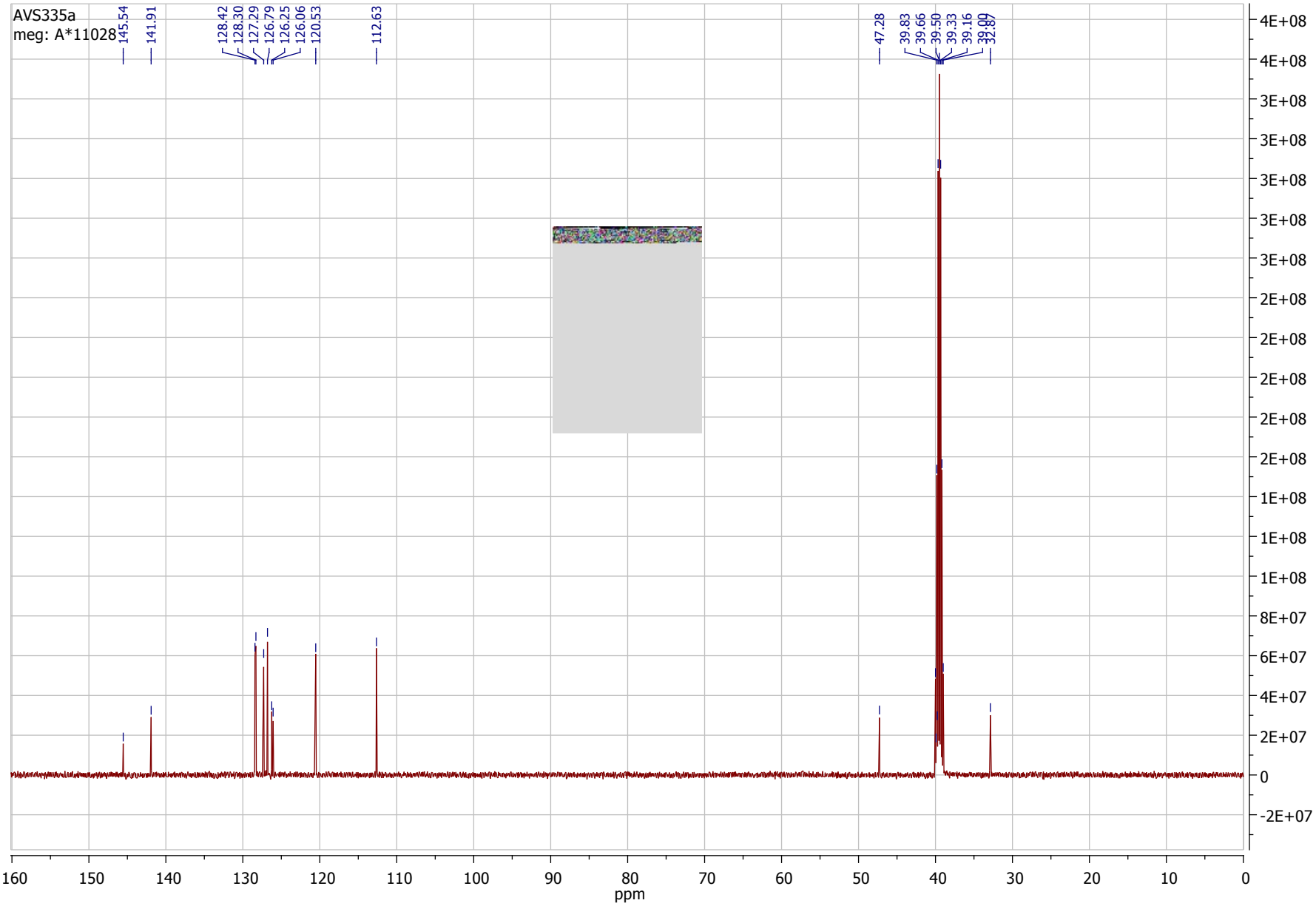
9-(4-Nitrophenyl)-10-methyl-acridinium tetrafluoroborate (3q)



Brown needles. 755 mg (94%). M.p.: 281-282 °C. ^{1}H NMR (500 MHz, [D_6]DMSO): δ 8.91 (d, 2H, J=9.3 Hz), 8.63-8.60 (m, 2H), 8.51-8.47 (m, 2H), 7.97-7.90 (m, 6H), 4.98 (s, 3H) ppm. ^{13}C NMR (126 MHz, [D_6]DMSO): δ 158.0, 148.6, 141.2, 139.8, 138.7, 131.5, 129.3, 128.3, 125.3, 124.0, 119.3, 39.2 ppm. Elem. Anal. Calcd. For $C_{20}H_{15}N_2O_2BF_4$: C 59.73, H 3.77, N 6.96, F 18.90 Found: C 59.83, H 3.73, N 7.02.

3. Spectra of all compounds




AVS335a
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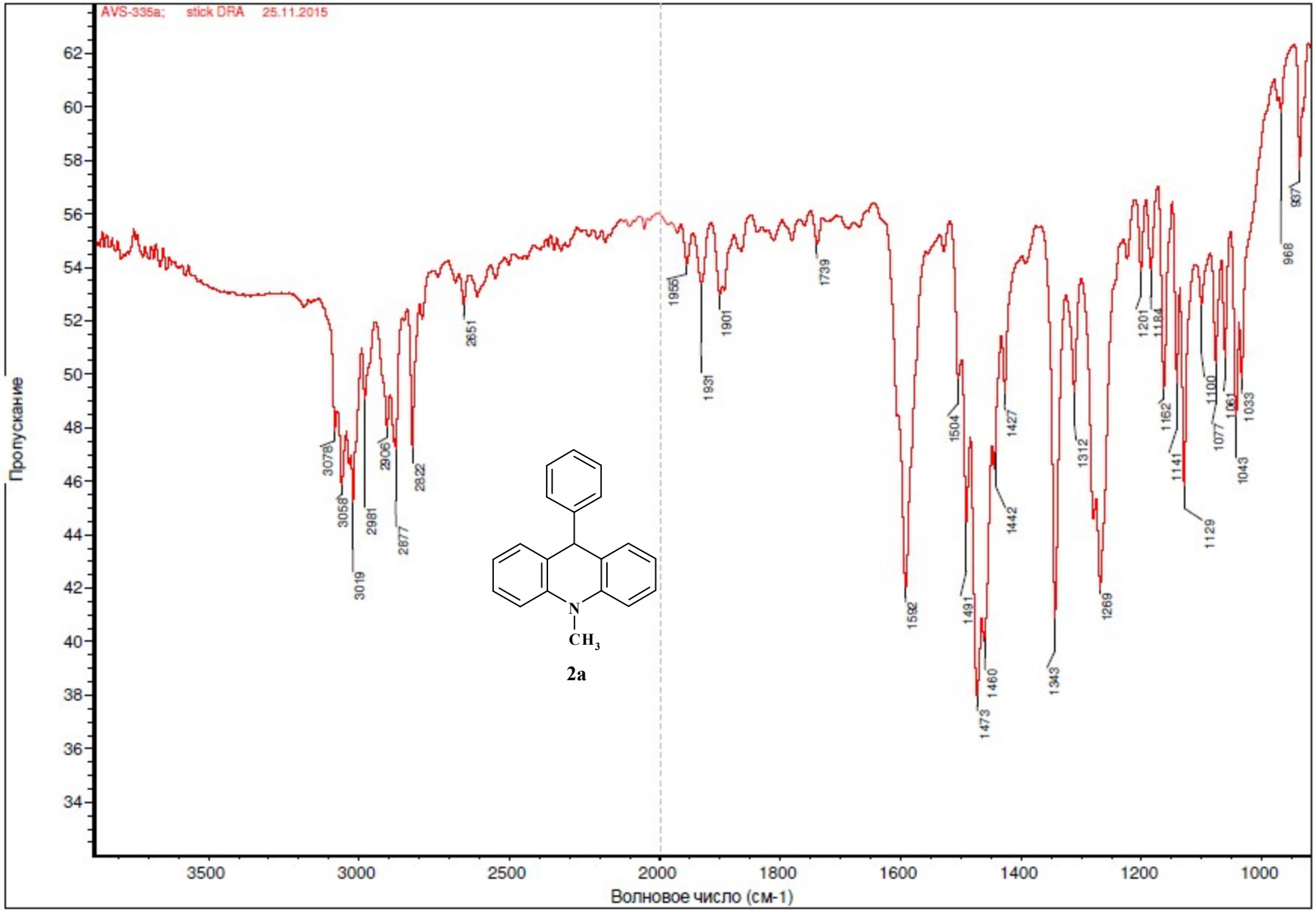
128.42
128.30
127.29
126.79
126.25
126.06
120.53
112.63
47.28
39.83
39.66
39.50
39.33
39.16
32.87
4E+08
3E+08
2E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


AVS-335a; stick DRA 25.11.2015
Пропускание
Волновое число (см-1)
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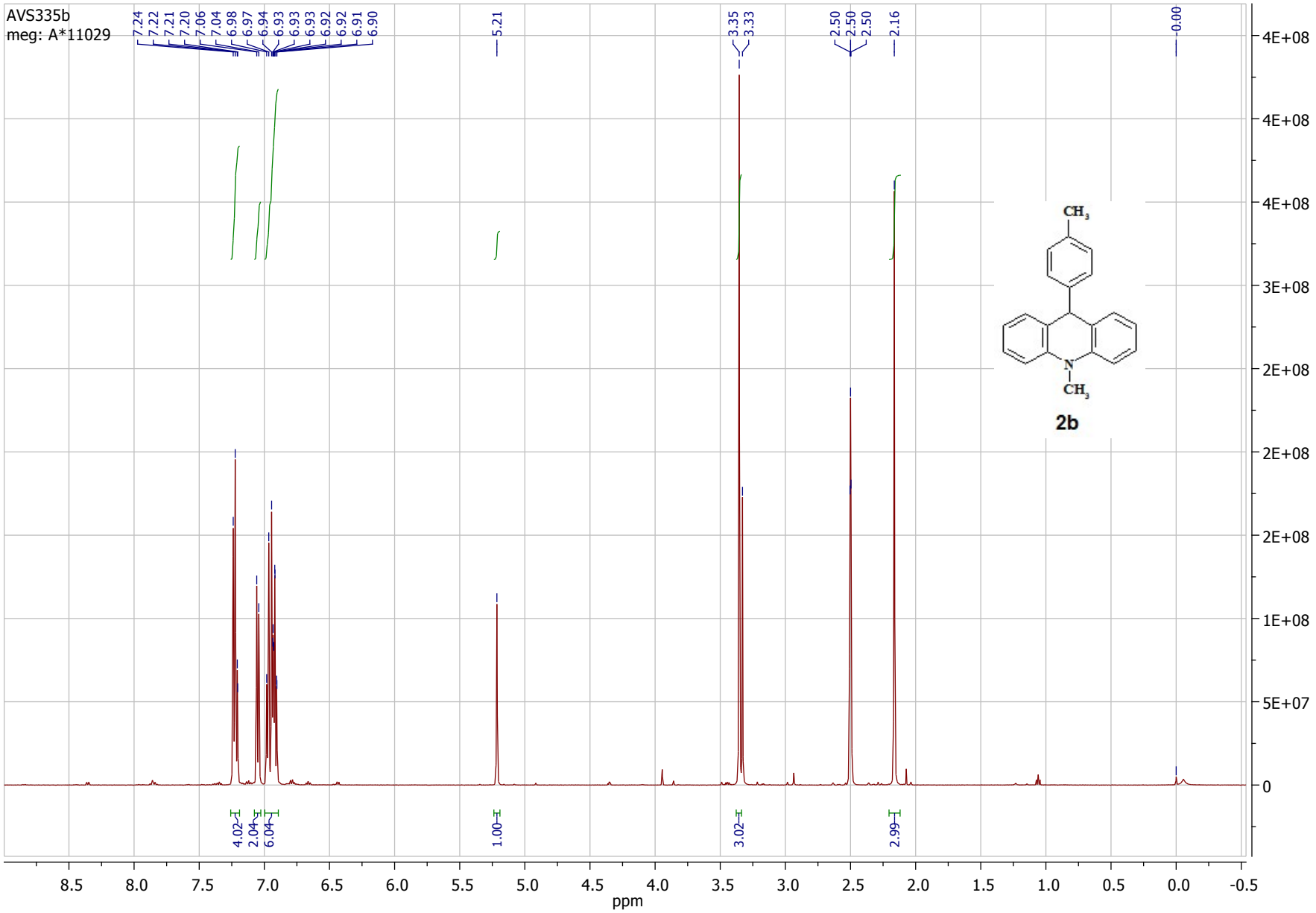
3058
3019
2981
2905
2877
2822
2651
1955
1931
1901
1739
1592
1504
1491
1473
1460
1442
1427
1343
1312
1269
1201
1184
1162
1141
1129
1100
1077
1061
1043
1033
968
907
N
CH3

2a


AVS335b
meg: A*11029
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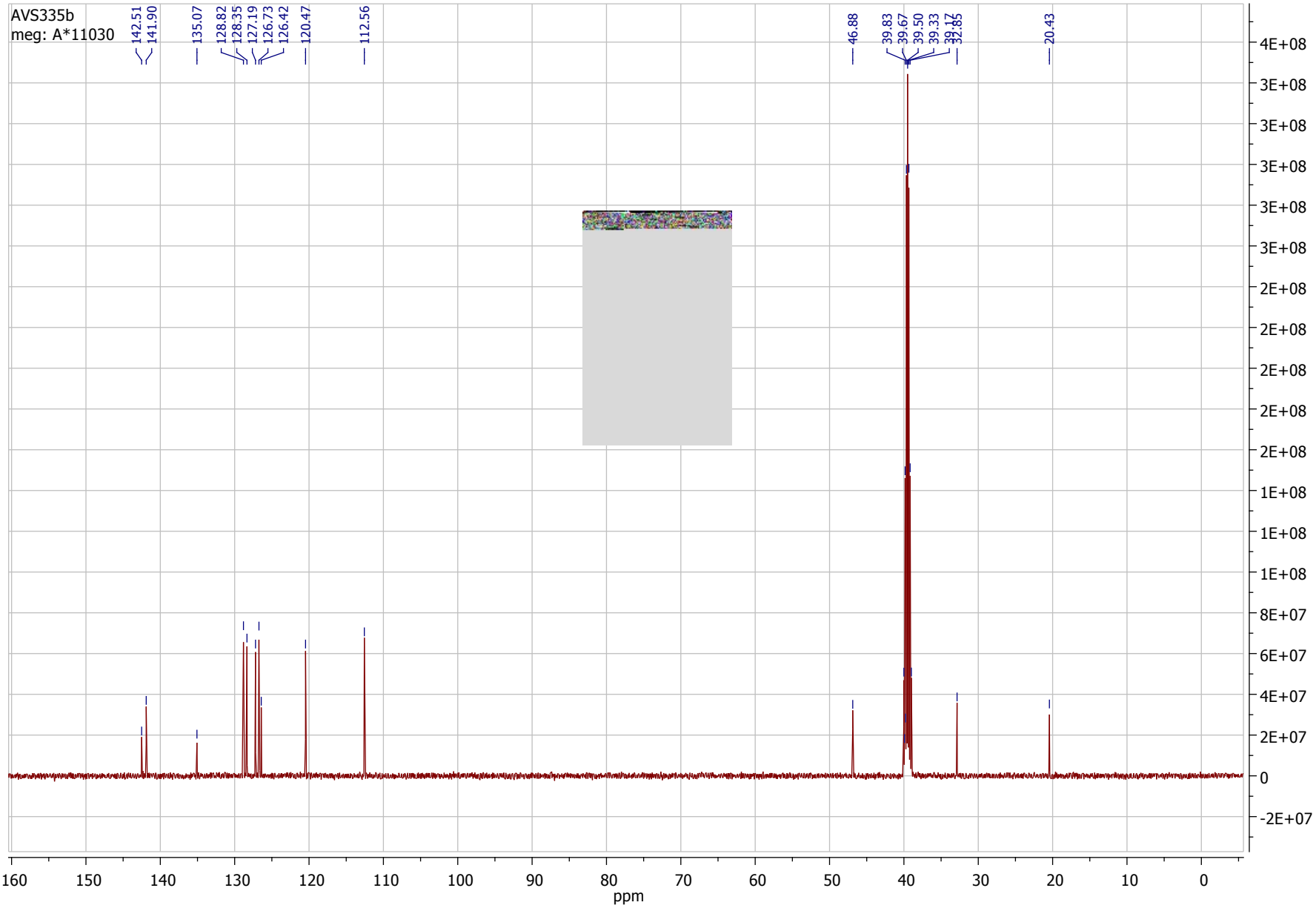
7.22
7.21
7.20
7.06
7.04
6.98
6.97
6.94
6.93
6.93
6.93
6.92
6.92
6.91
6.90
5.21
3.35
3.33
2.50
2.50
2.50
2.16
0.00
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
4.02
2.04
6.04
1.00
3.02
2.99
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm
CH3
N
CH3
2b


AVS335b
meg: A*11030
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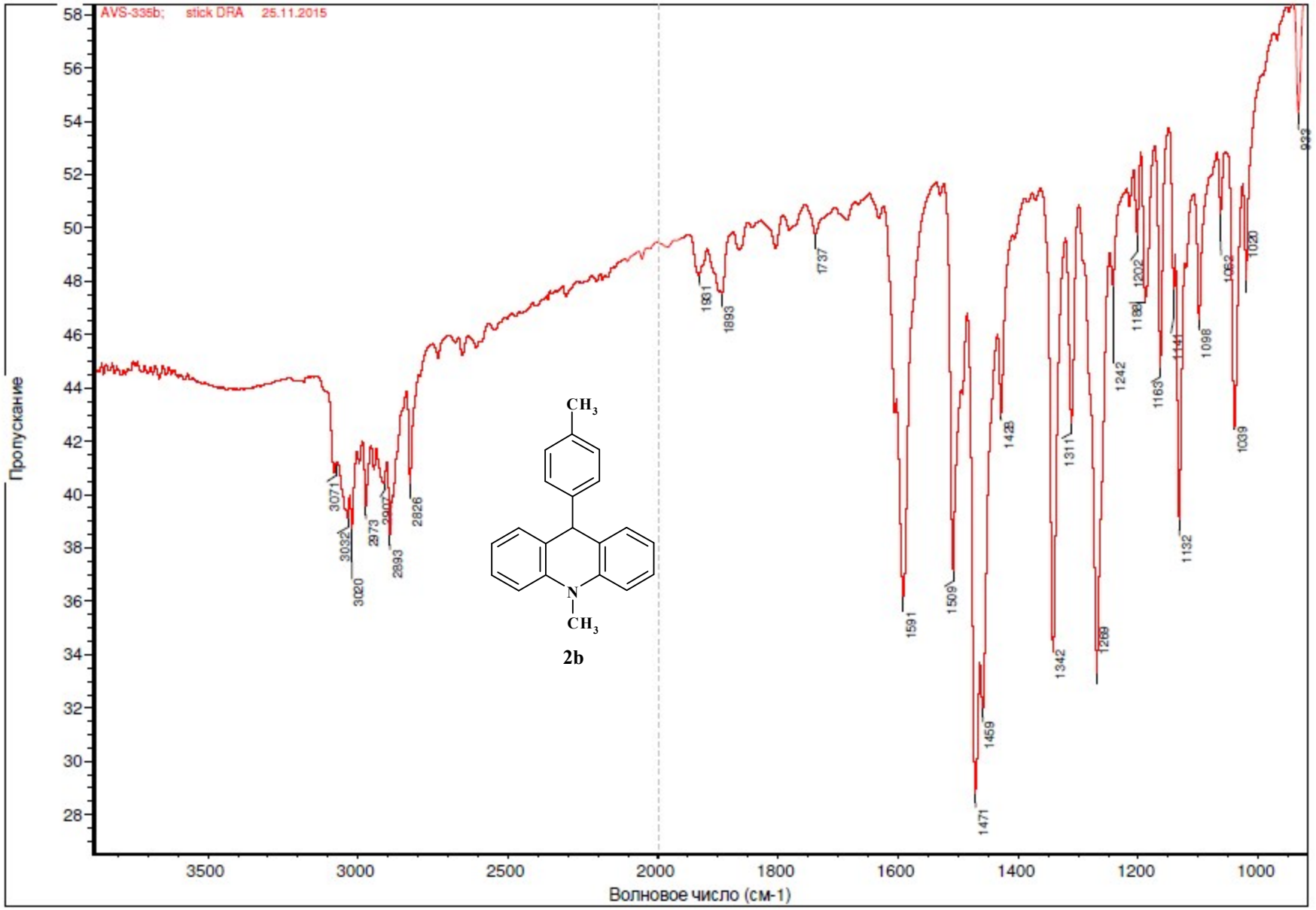
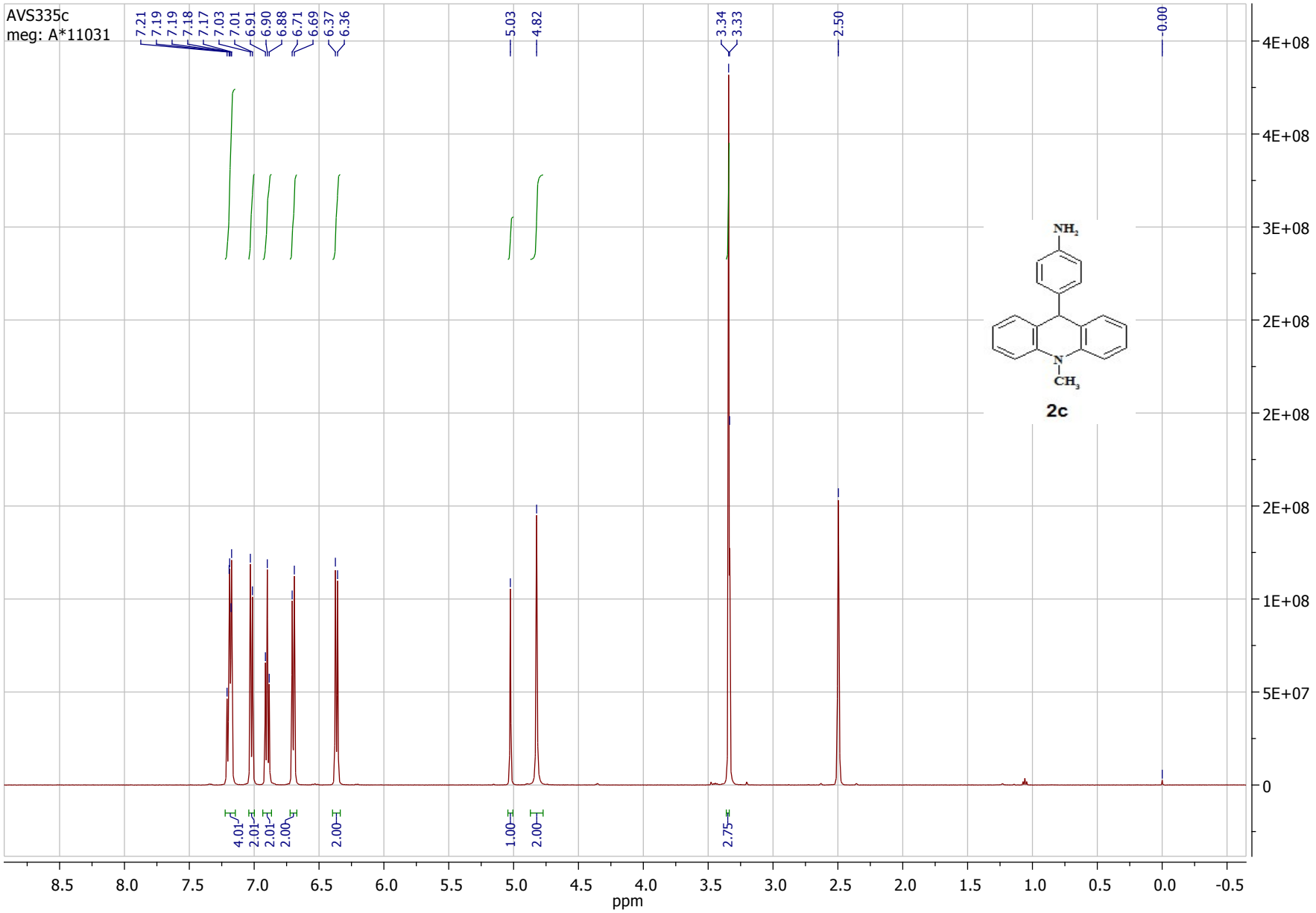
128.82
128.35
127.19
126.73
126.42
120.47
112.56
46.88
39.83
39.67
39.50
39.33
39.17
32.85
20.43
4E+08
3E+08
3E+08
3E+08
3E+08
2E+08
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


AVS-335b; stick DRA 25.11.2015
Пропускание
Волновое число (см-1)
3500
3000
2500
2000
1800
1600
1400
1200
1000
3071
3032
3020
2973
2907
2893
2826
1931
1893
1737
1591
1509
1471
1459
1428
1342
1311
1269
1242
1202
1188
1163
1141
1132
1098
1062
1039
1020
933
CH3
N
CH3

2b


AVS335c
meg: A*11031
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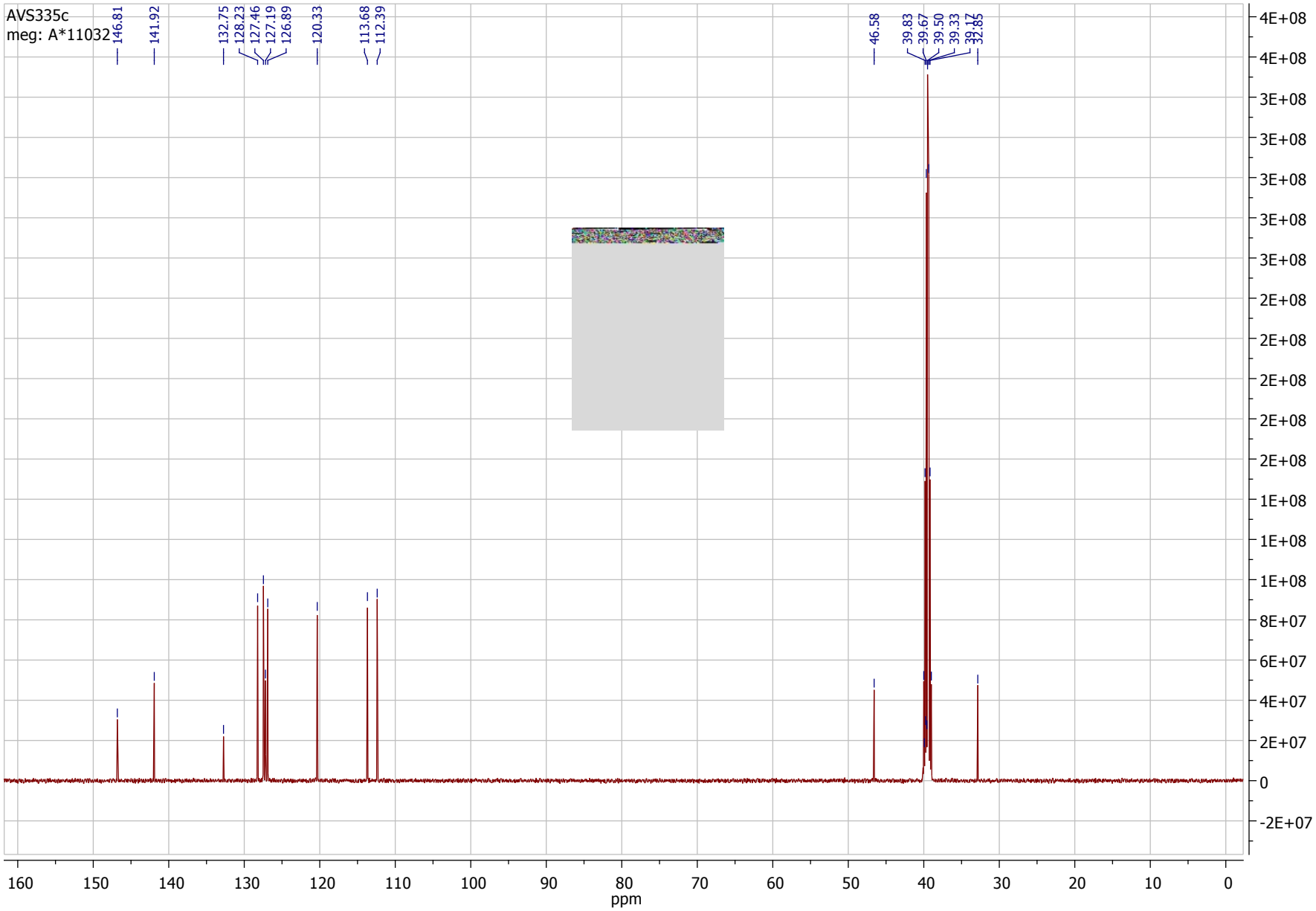
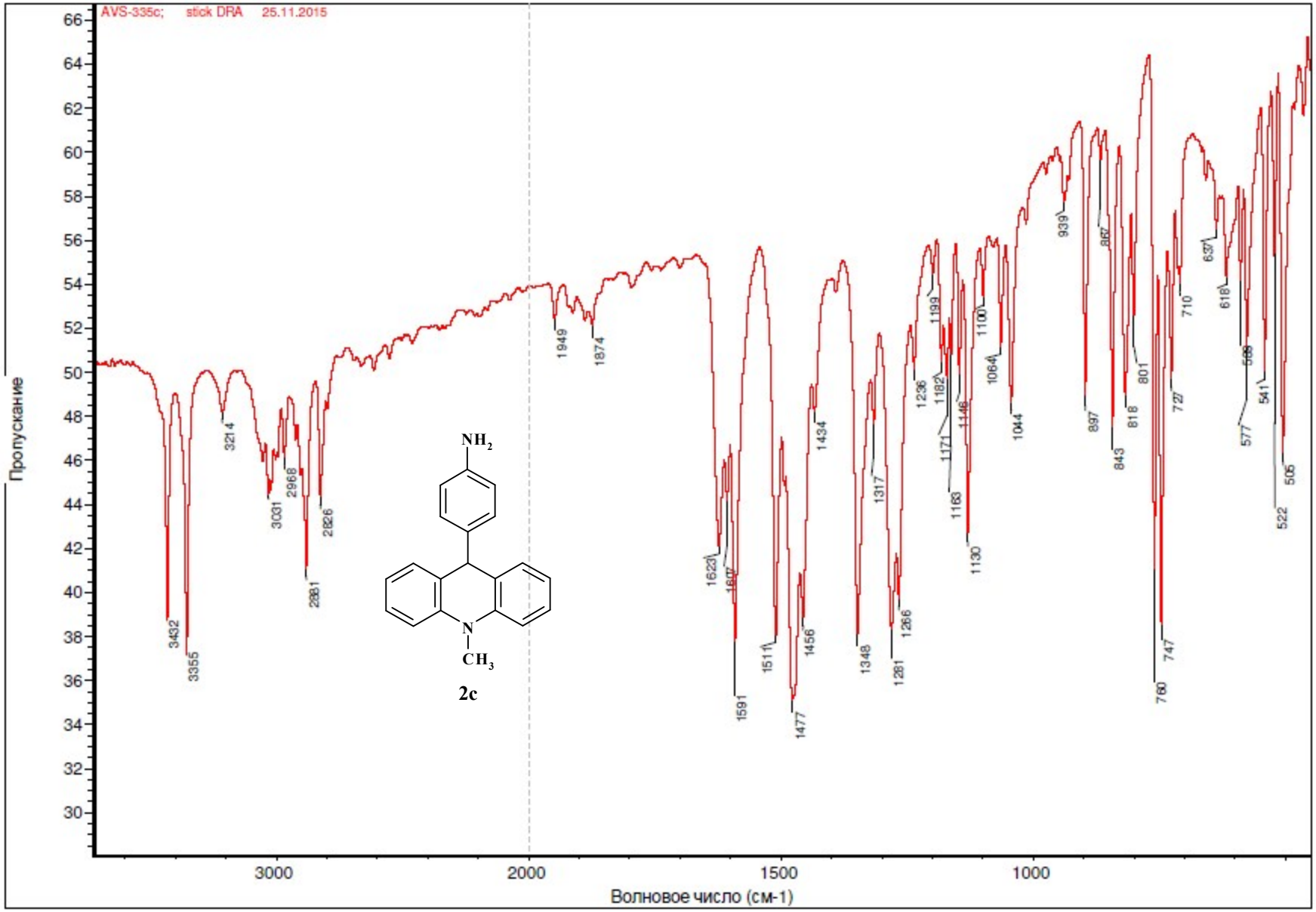
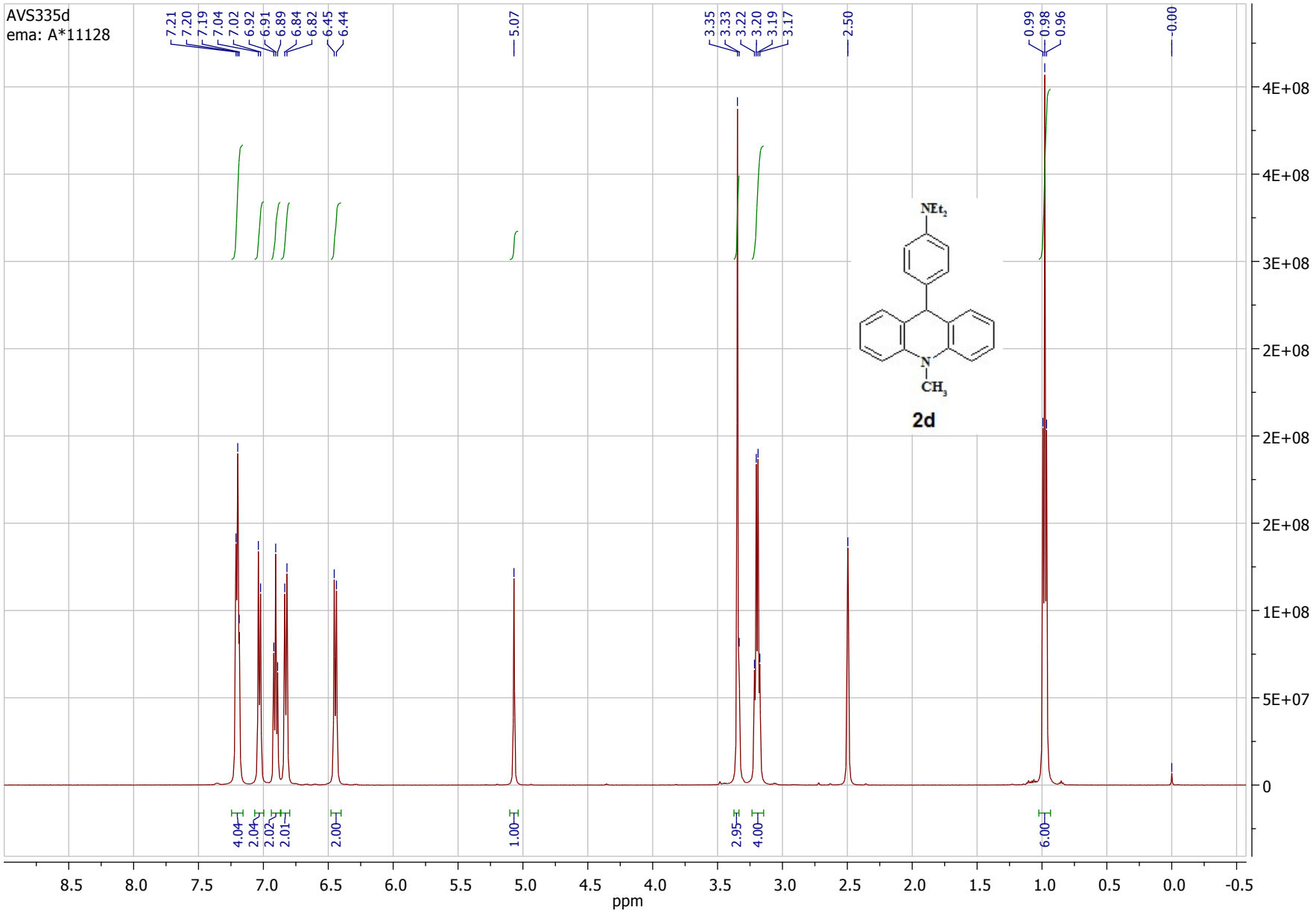
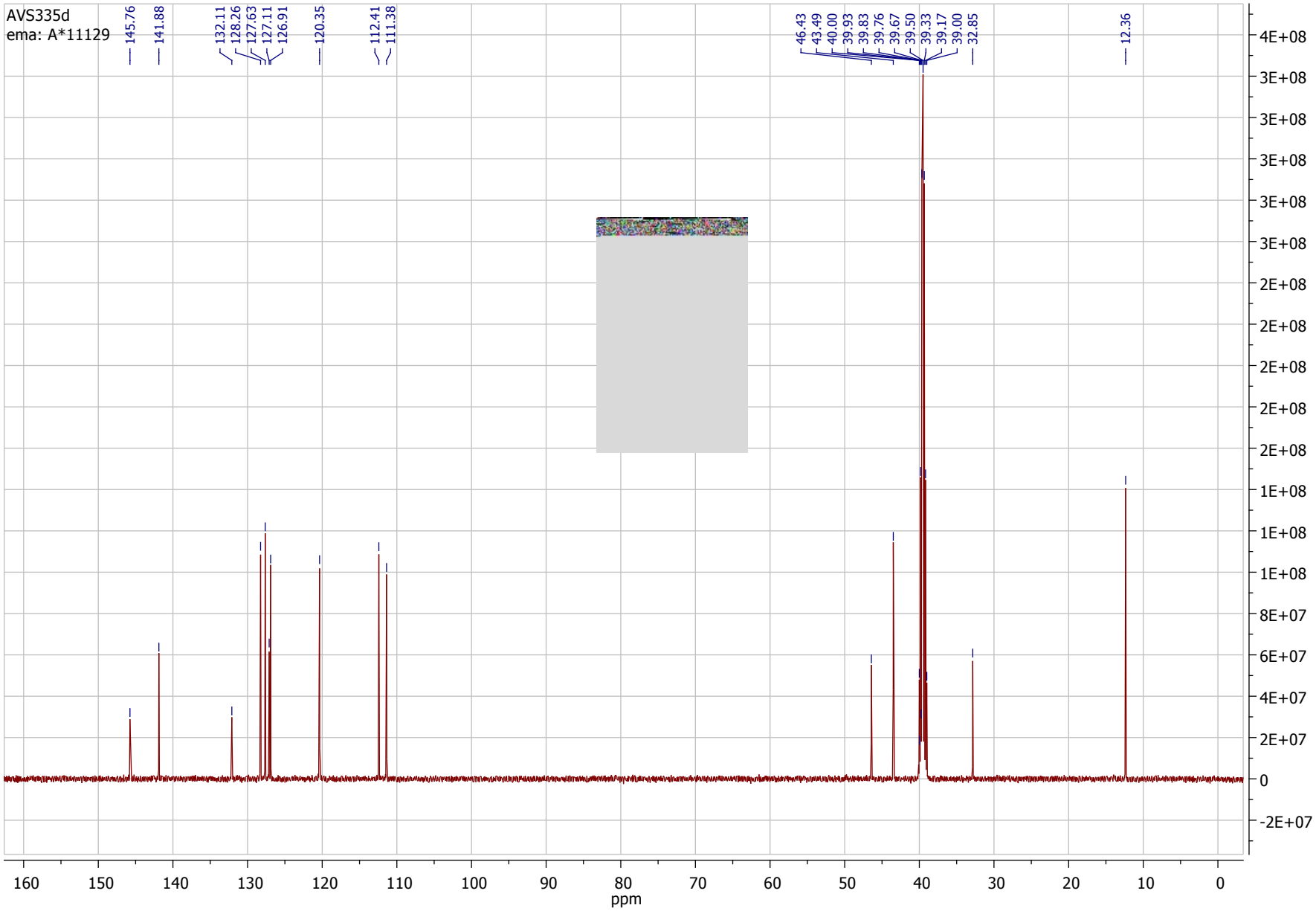
7.19
7.19
7.18
7.17
7.03
7.01
6.91
6.90
6.88
6.71
6.69
6.37
6.36
5.03
4.82
3.34
3.33
2.50
0.00
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
NH2
N
CH3
2c
4.01
2.01
2.01
2.00
2.00
1.00
2.00
2.75
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm

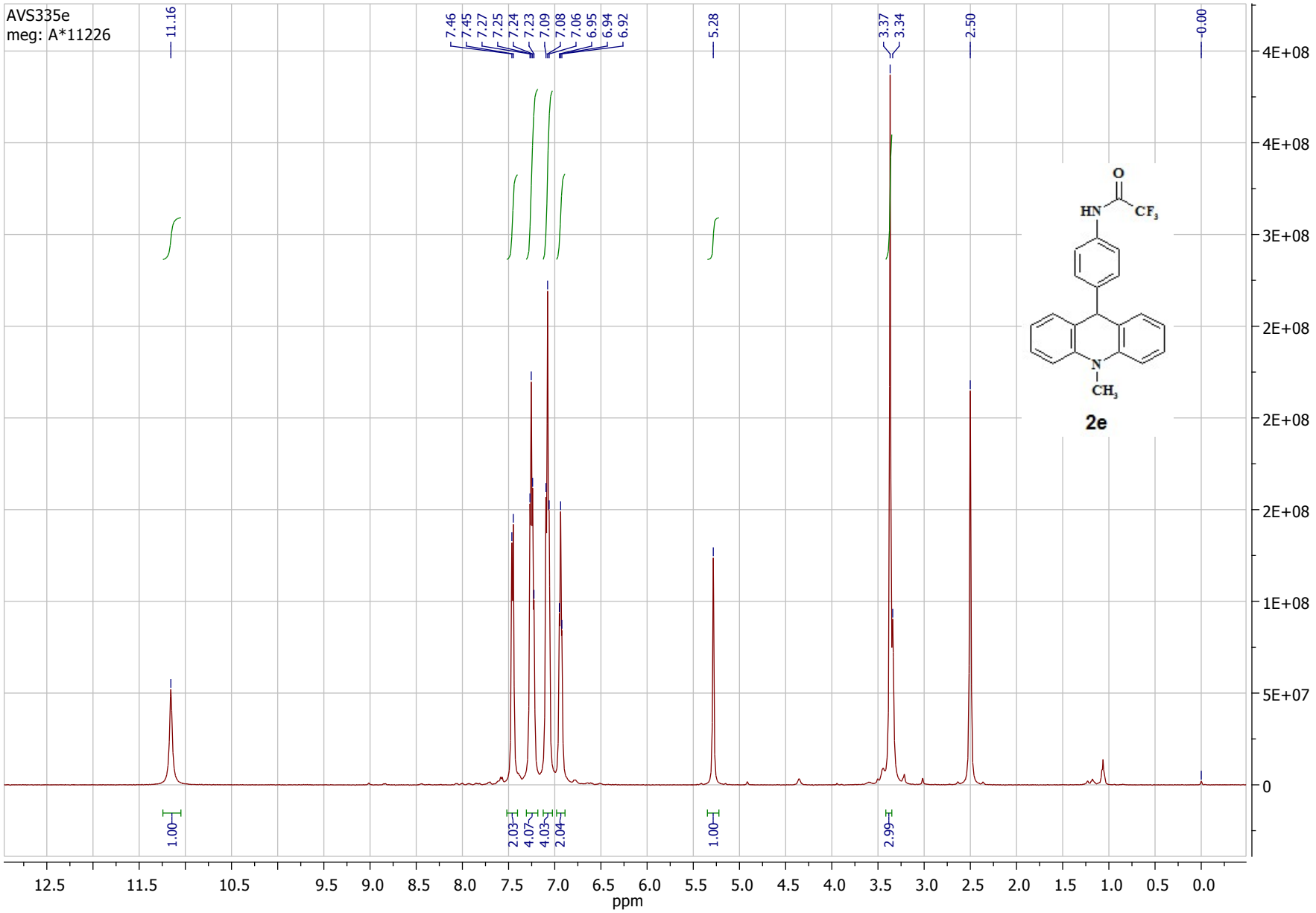

AVS335c
meg: A*11032
146.81
141.92
132.75
128.23
127.46
127.19
126.89
120.33
113.68
112.39
46.58
39.83
39.67
39.50
39.33
39.17
32.85
4E+08
3E+08
2E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

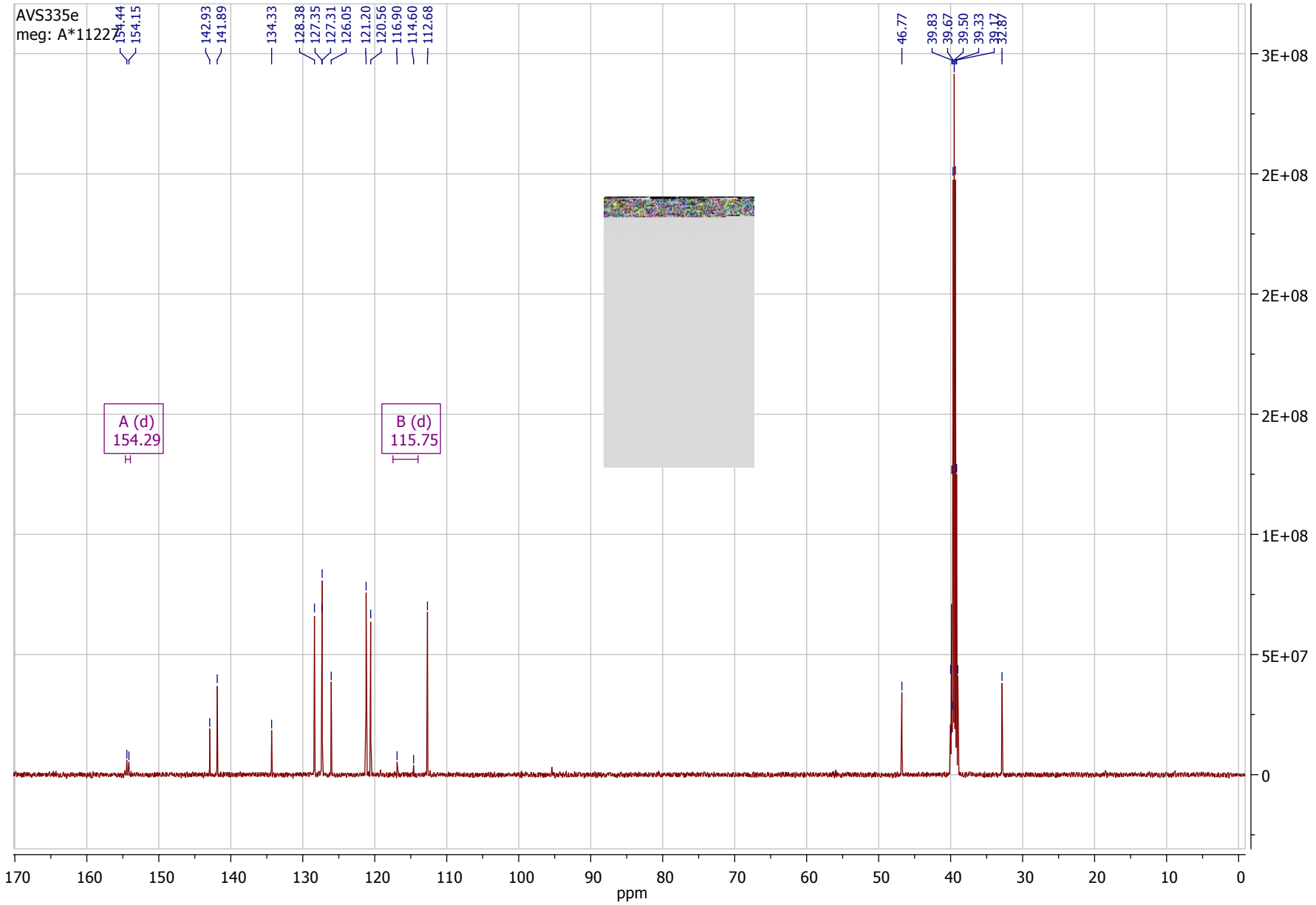

AVS-335c; stick DRA 25.11.2015
Пропускание
Волновое число (см-1)
3000
2000
1500
1000
66
64
62
60
58
56
54
52
50
48
46
44
42
40
38
36
34
32
30
3432
3355
3214
3031
2968
2881
2826
1949
1874
1623
1607
1591
1511
1477
1456
1434
1348
1317
1281
1266
1236
1199
1182
1171
1163
1146
1130
1100
1064
1044
939
897
867
843
818
801
760
747
727
710
637
618
588
577
541
522
505
NH2
N
CH3

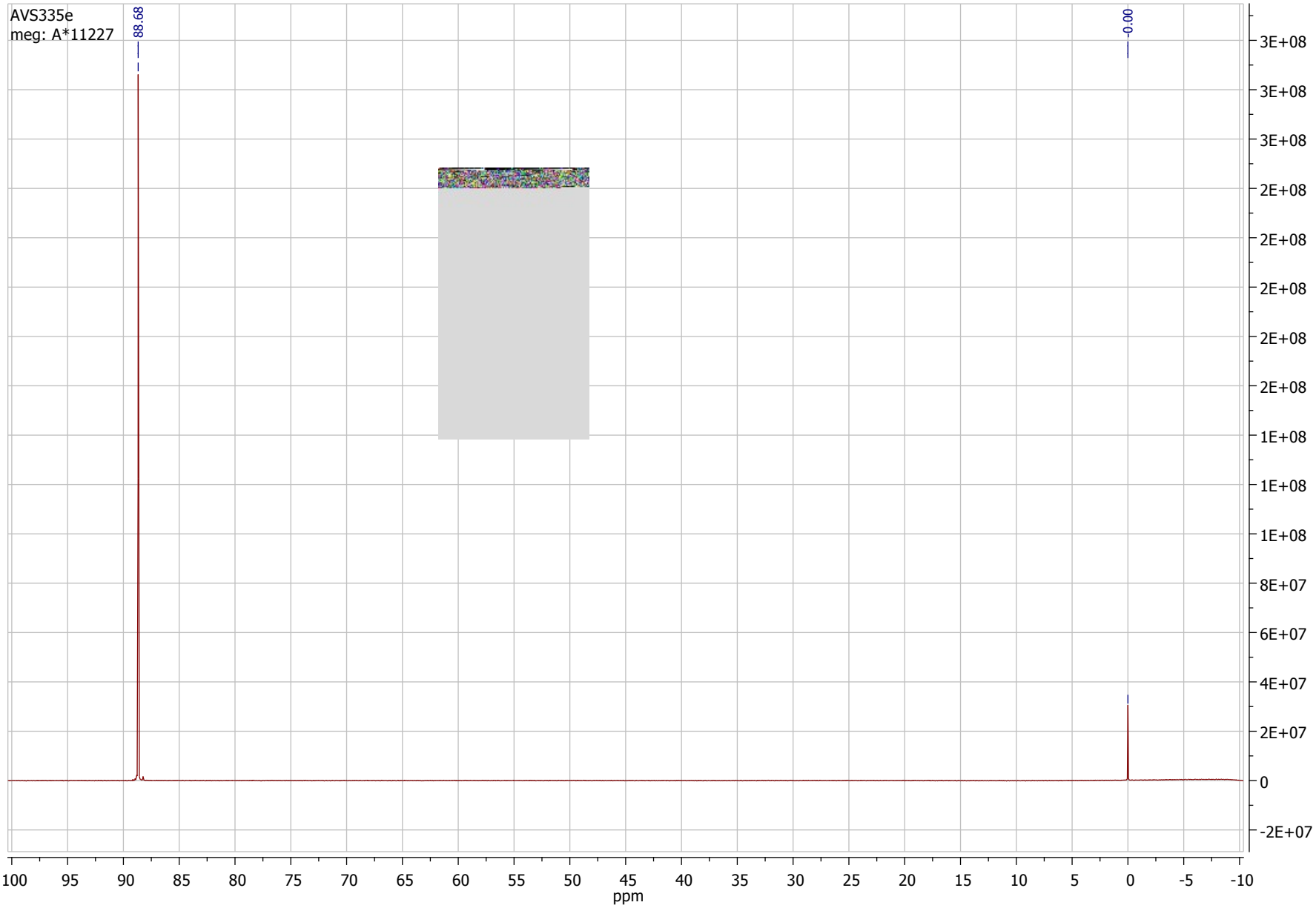
2c

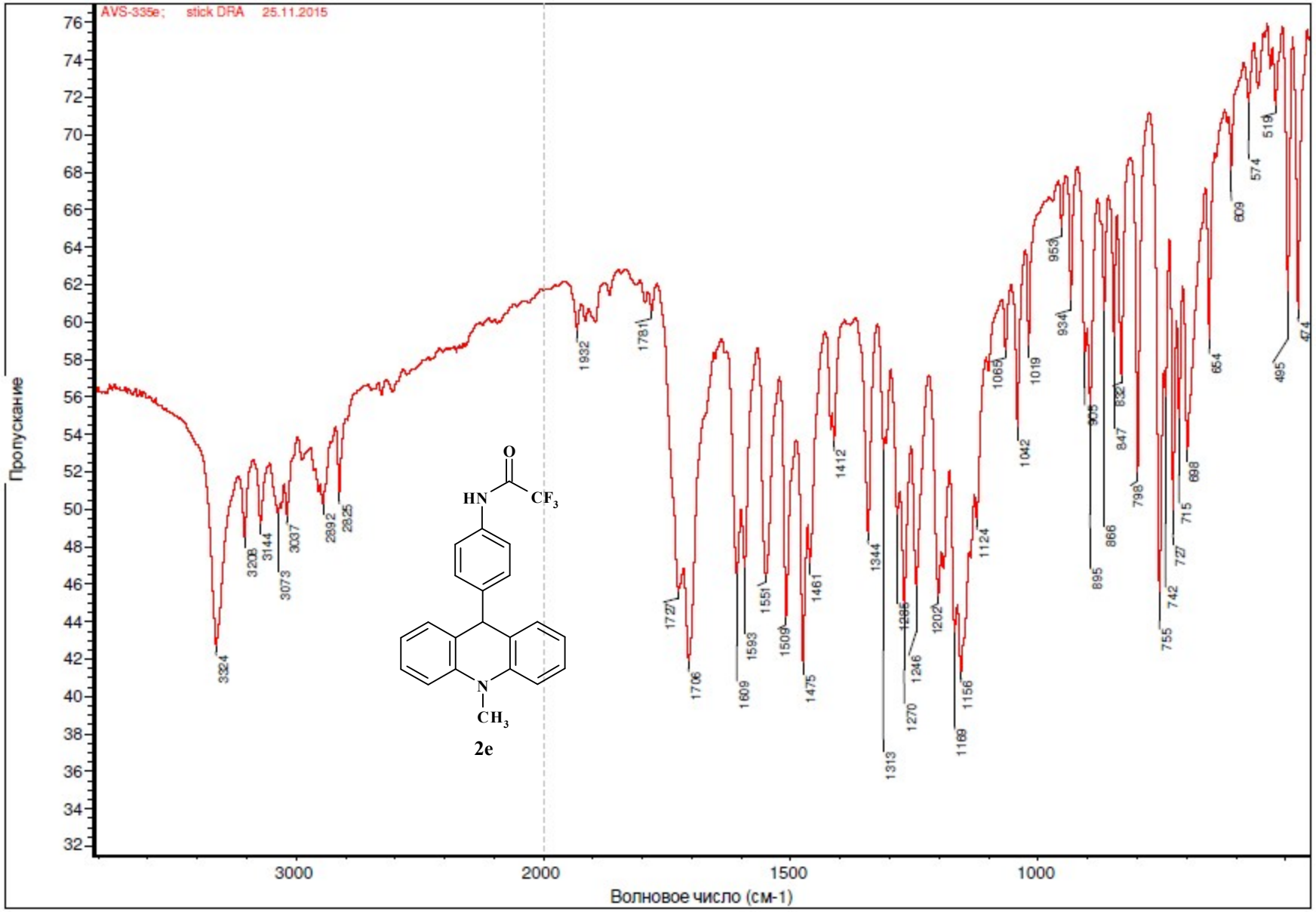

AVS335d
ema: A*11128
7.21
7.20
7.19
7.04
7.02
6.92
6.91
6.89
6.84
6.82
6.45
6.44
5.07
3.35
3.33
3.22
3.20
3.19
3.17
2.50
0.99
0.98
0.96
-0.00
NEt2
N
CH3
2d
4.04
2.04
2.02
2.01
2.00
1.00
2.95
4.00
6.00
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm


AVS335d
ema: A*11129
145.76
141.88
132.11
128.26
127.63
127.11
126.91
120.35
112.41
111.38
46.43
43.49
40.00
39.93
39.83
39.76
39.67
39.50
39.33
39.17
39.00
32.85
12.36
4E+08
3E+08
3E+08
3E+08
3E+08
3E+08
2E+08
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

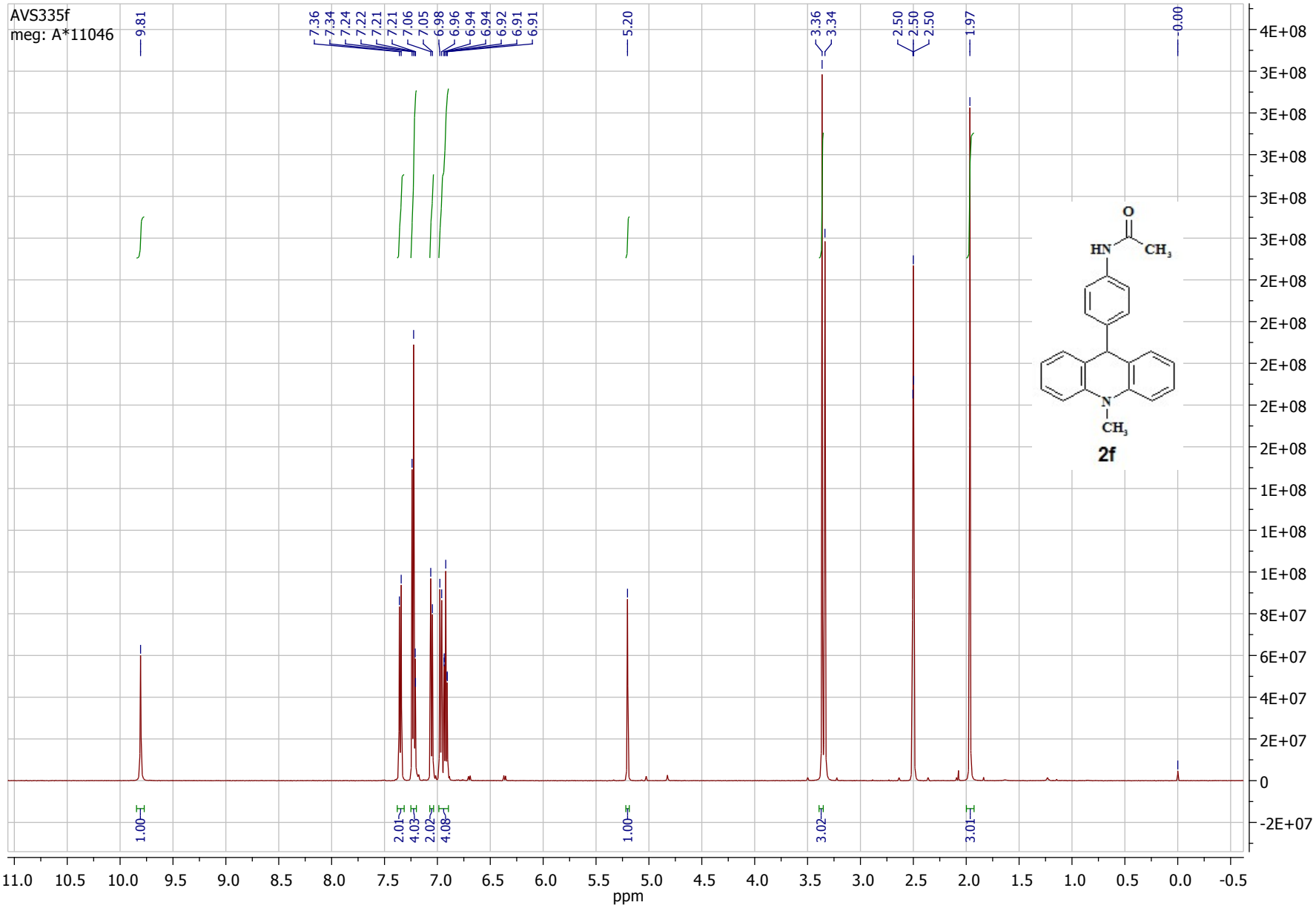

AVS335e
meg: A*11226
11.16
7.46
7.45
7.27
7.25
7.24
7.23
7.09
7.08
7.06
6.95
6.94
6.92
5.28
3.37
3.34
2.50
0.00
HN
O
CF3
N
CH3
2e
1.00
2.03
4.07
4.03
2.04
1.00
2.99
ppm

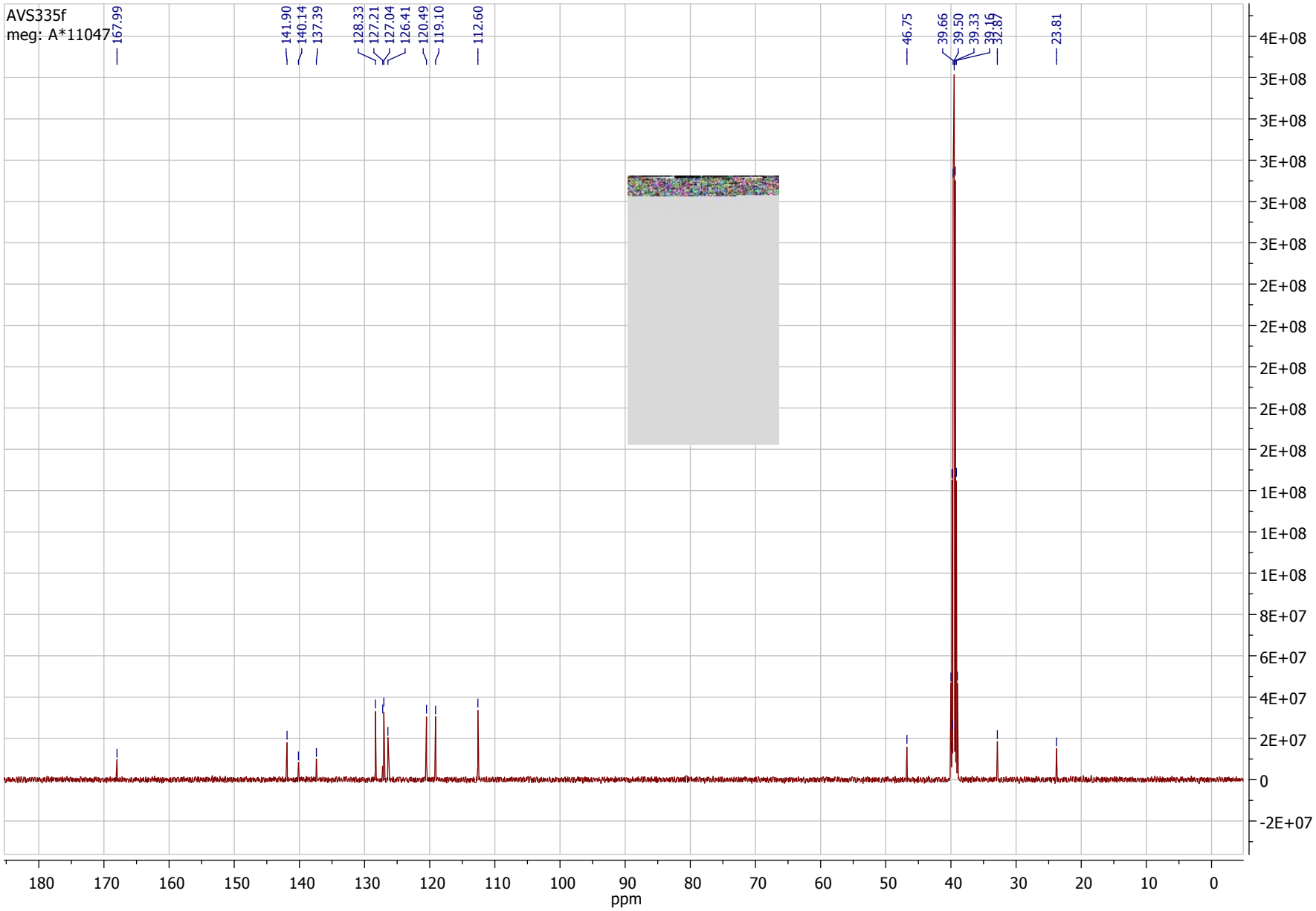

AVS335e
meg: A*11227
154.44
154.15
142.93
141.89
134.33
128.38
127.35
127.31
126.05
121.20
120.56
116.90
114.60
112.68
46.77
39.83
39.67
39.50
39.33
39.17
32.87
A (d)
154.29
H
B (d)
115.75
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

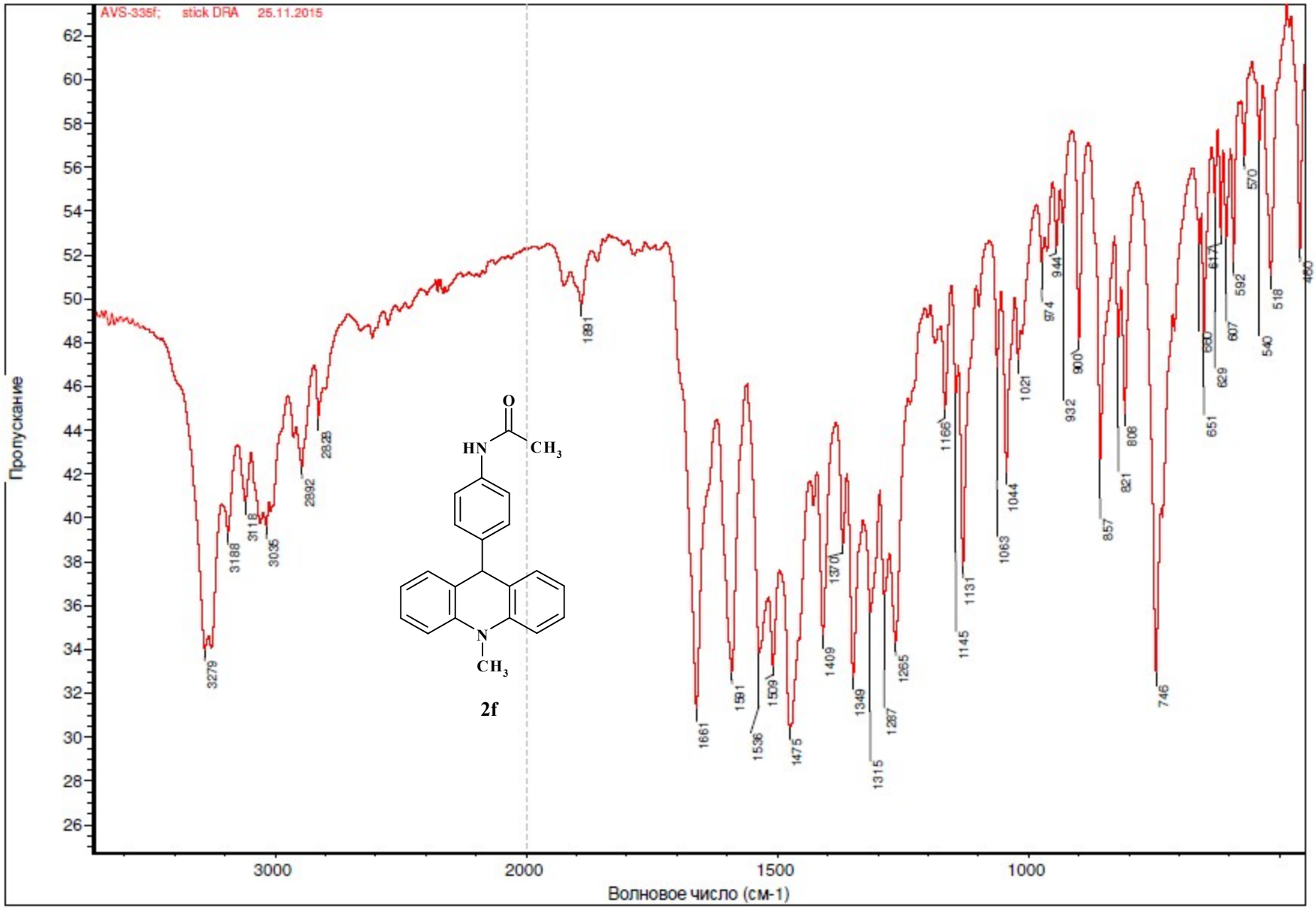

AVS335e
meg: A*11227
88.68
0.00
3E+08
3E+08
3E+08
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
-10
ppm


AVS-335e; stick DRA 25.11.2015
Пропускание
Волновое число (см-1)
3000
2000
1500
1000
3324
3208
3144
3073
3037
2892
2825
1932
1781
1727
1706
1609
1593
1551
1509
1475
1461
1412
1344
1313
1285
1270
1246
1202
1188
1156
1124
1065
1042
1019
953
934
905
895
866
847
832
798
755
742
727
715
698
654
609
574
519
495
474
HN
O
CF3
N
CH3

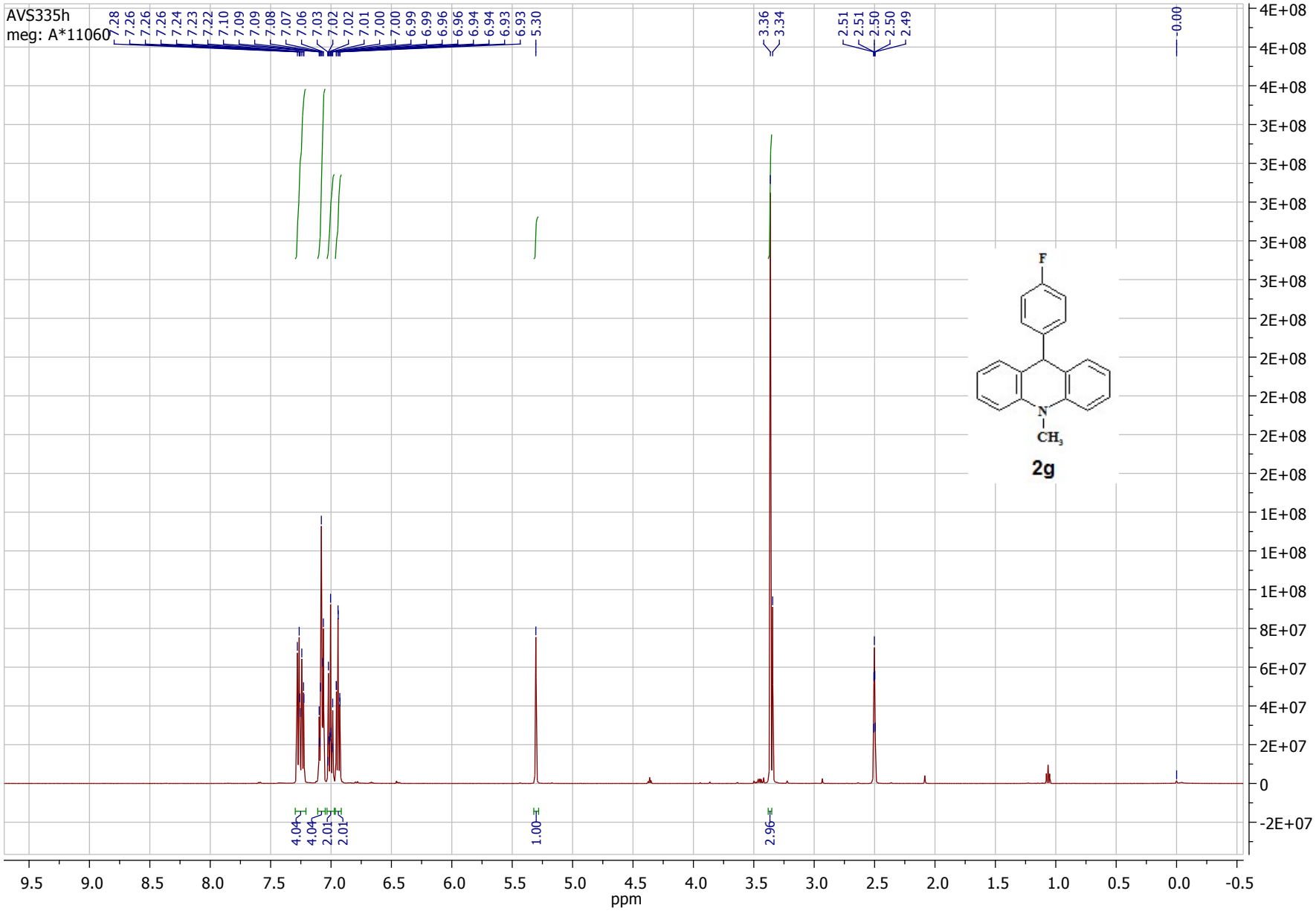
2e

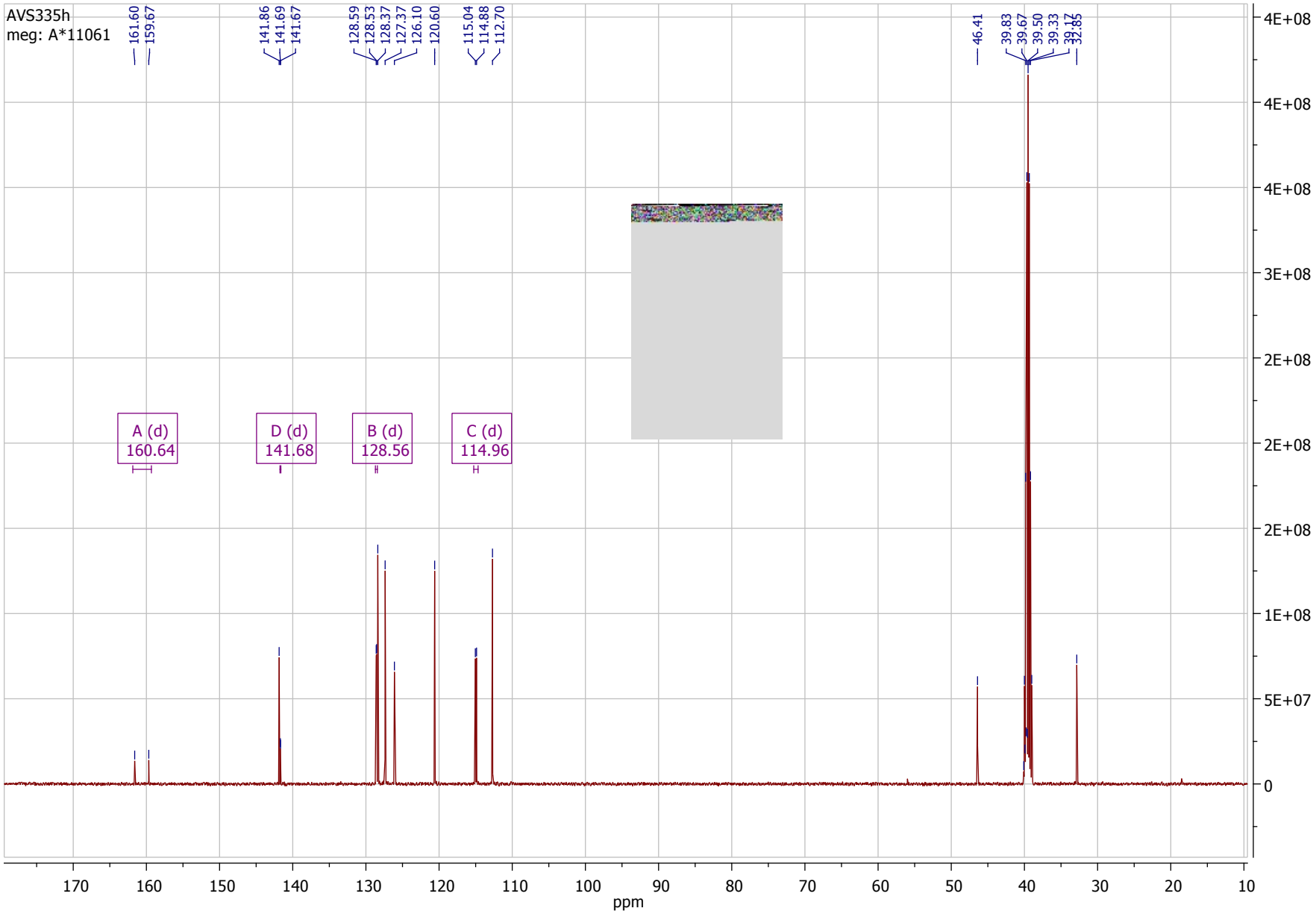

AVS335f
meg: A*11046
9.81
7.36
7.34
7.24
7.22
7.21
7.21
7.06
7.05
6.98
6.96
6.94
6.94
6.92
6.91
6.91
5.20
3.36
3.34
2.50
2.50
2.50
1.97
0.00
HN
O
CH3
N
CH3
2f
1.00
2.01
4.03
2.02
4.08
1.00
3.02
3.01
ppm

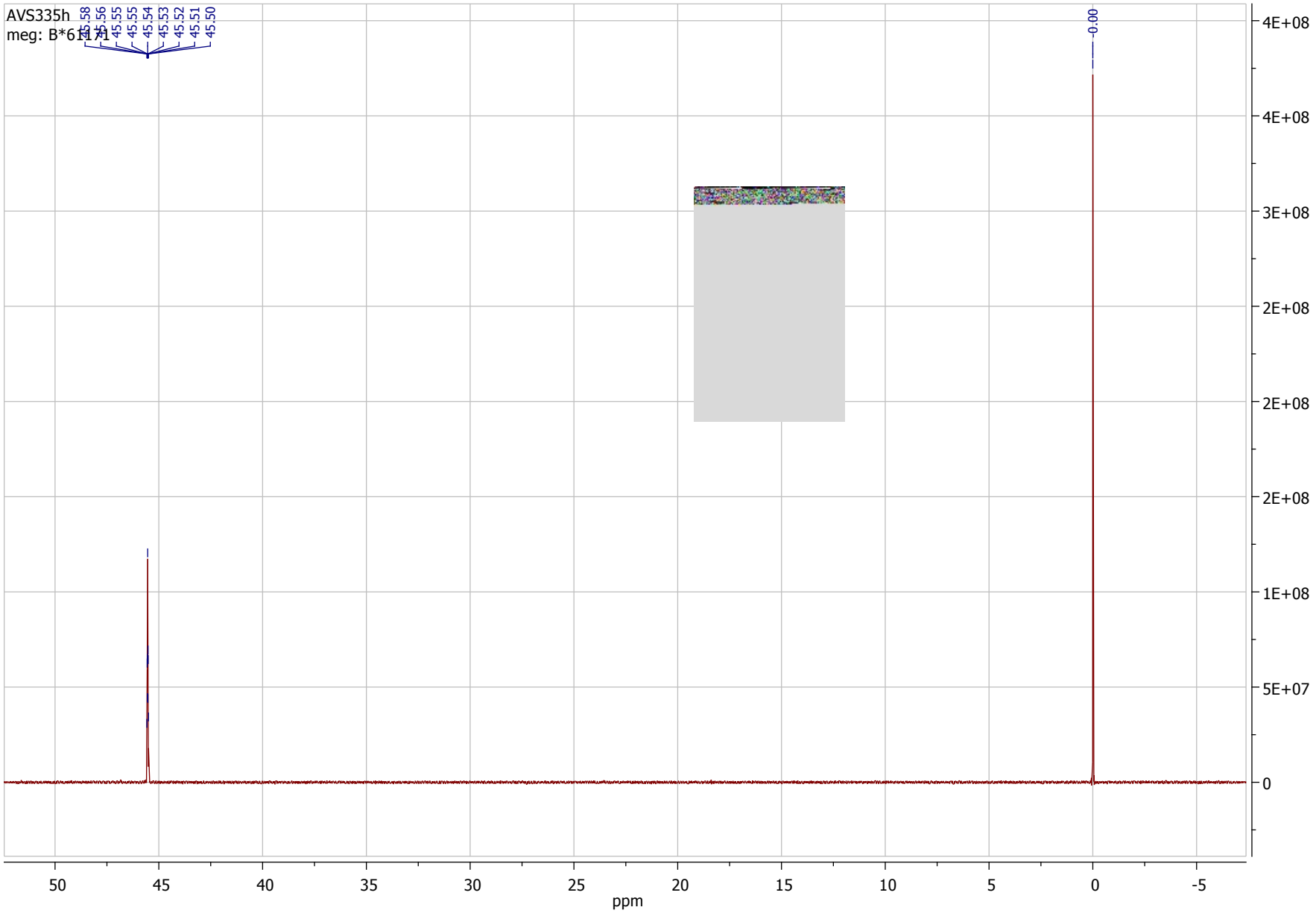

AVS335f
meg: A*11047
167.99
141.90
140.14
137.39
128.33
127.21
127.04
126.41
120.49
119.10
112.60
46.75
39.66
39.50
39.33
39.16
32.87
23.81
4E+08
3E+08
3E+08
3E+08
3E+08
3E+08
2E+08
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

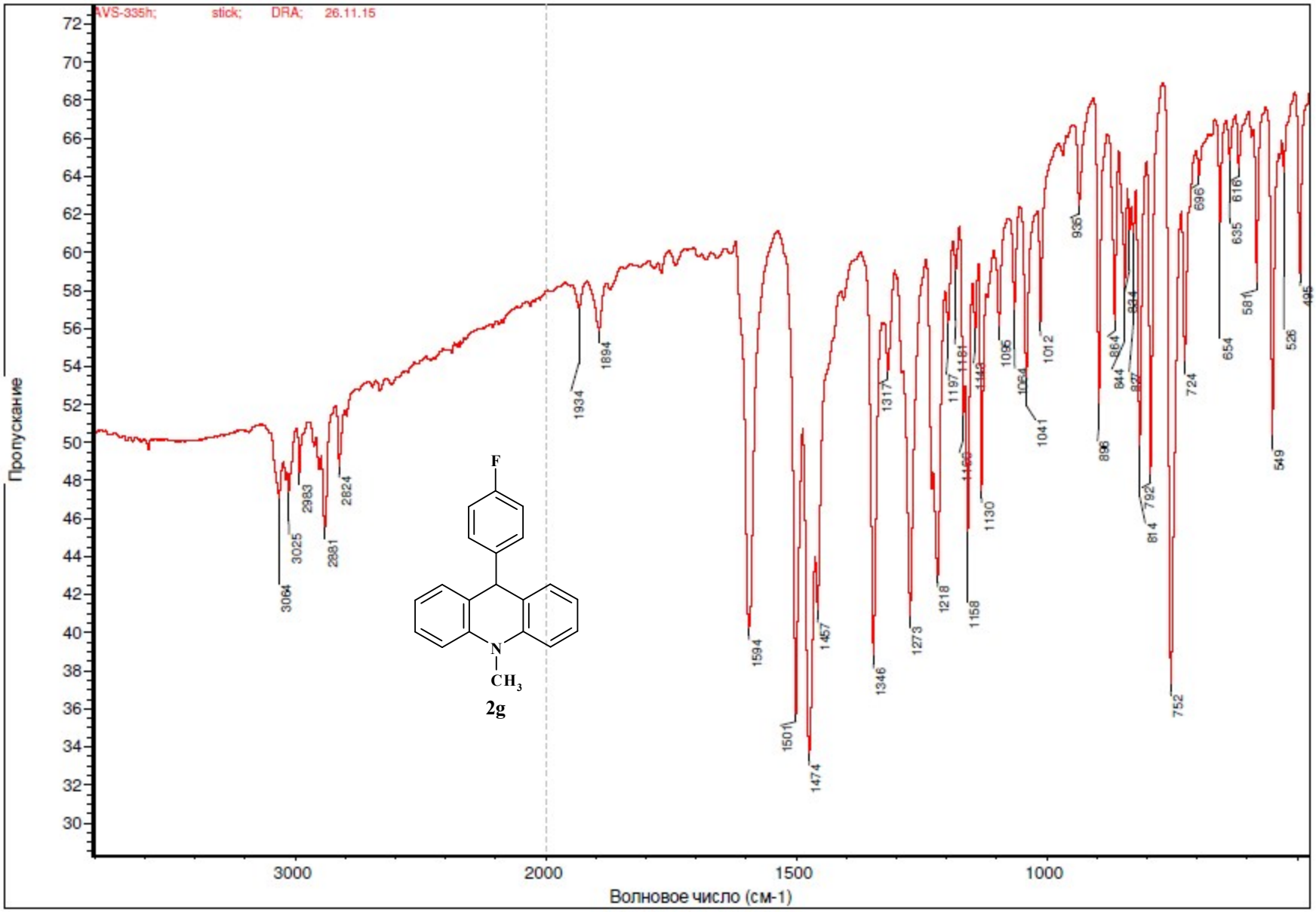

AVS-335f; stick DRA 25.11.2015
Пропускание
Волновое число (см-1)
3000
2000
1500
1000
3279
3188
3118
3035
2892
2828
1891
1661
1591
1536
1509
1475
1409
1370
1349
1315
1287
1265
1166
1145
1131
1063
1044
1021
974
944
932
900
857
821
808
746
680
651
629
617
607
592
570
540
518
480
HN
O
CH3
N
CH3

2f

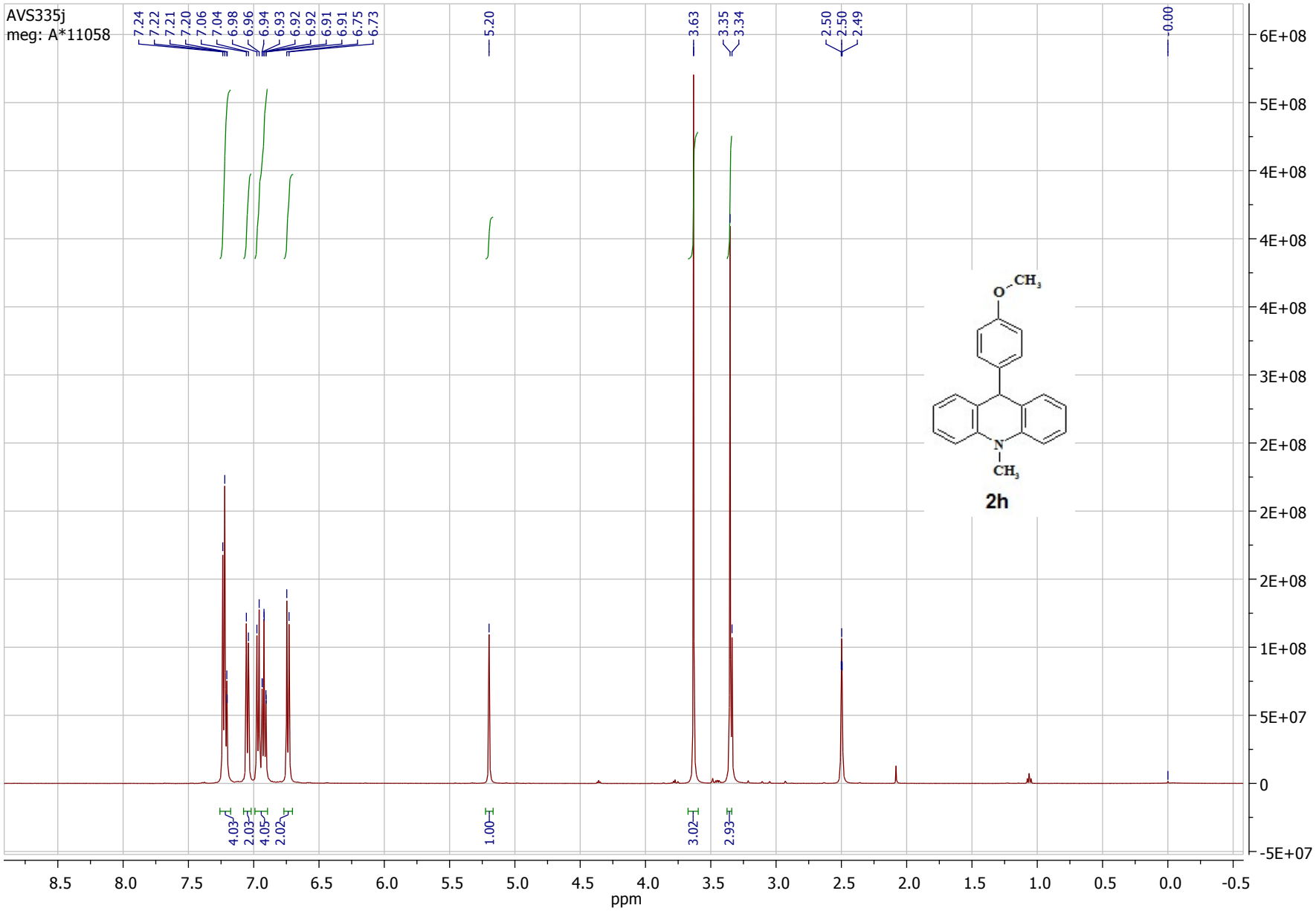

AVS335h
meg: A*11060
7.28
7.26
7.26
7.26
7.24
7.23
7.22
7.10
7.09
7.09
7.08
7.07
7.06
7.03
7.02
7.02
7.01
7.00
7.00
6.99
6.99
6.96
6.96
6.94
6.94
6.93
6.93
5.30
3.36
3.34
2.51
2.51
2.50
2.50
2.49
0.00
F
N
CH3
2g
4.04
4.04
2.01
2.01
1.00
2.96
ppm

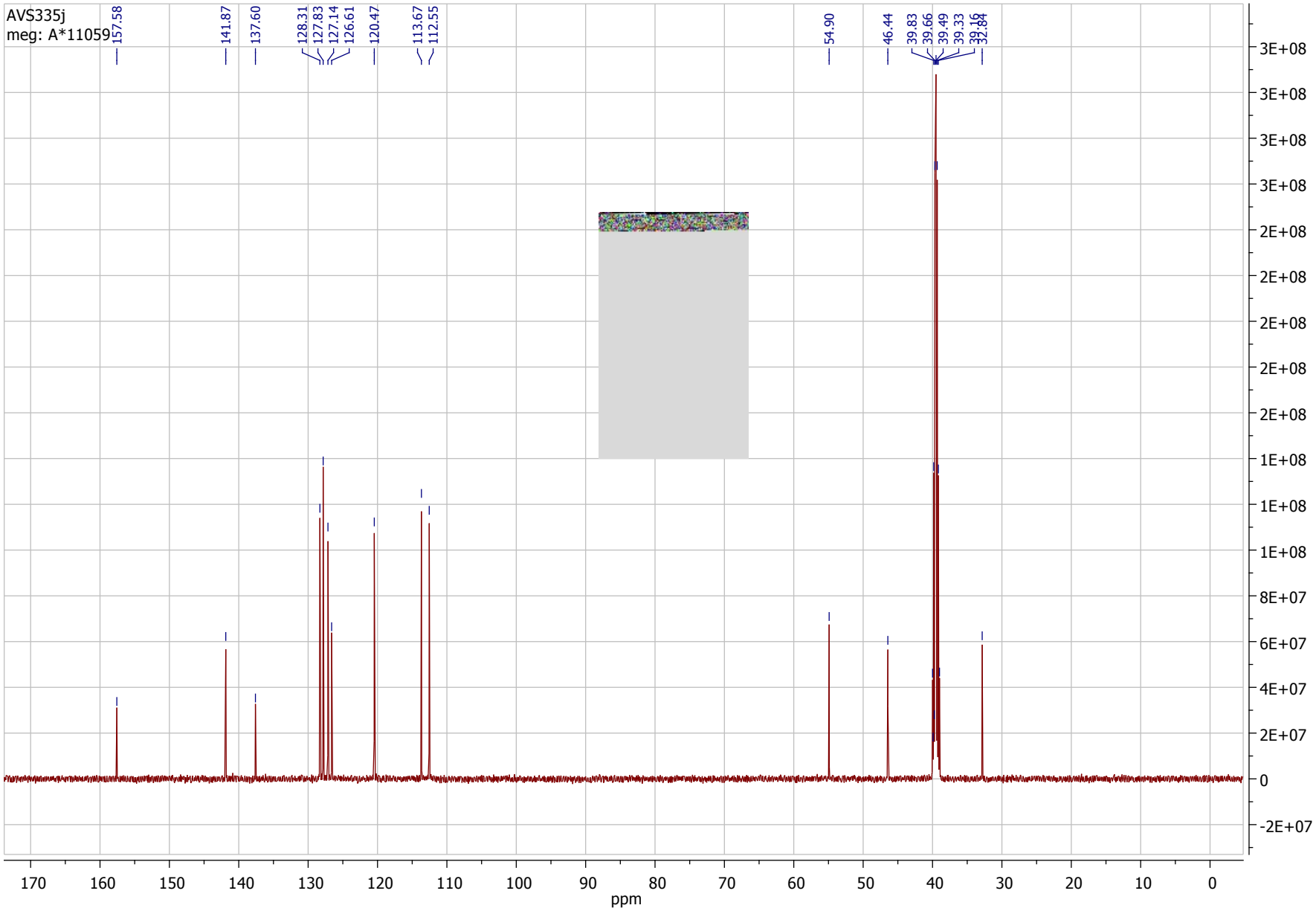

AVS335h
meg: A*11061
161.60
159.67
141.86
141.69
141.67
128.59
128.53
128.37
127.37
126.10
120.60
115.04
114.88
112.70
46.41
39.83
39.67
39.50
39.33
39.17
32.85
A (d)
160.64
D (d)
141.68
B (d)
128.56
C (d)
114.96
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

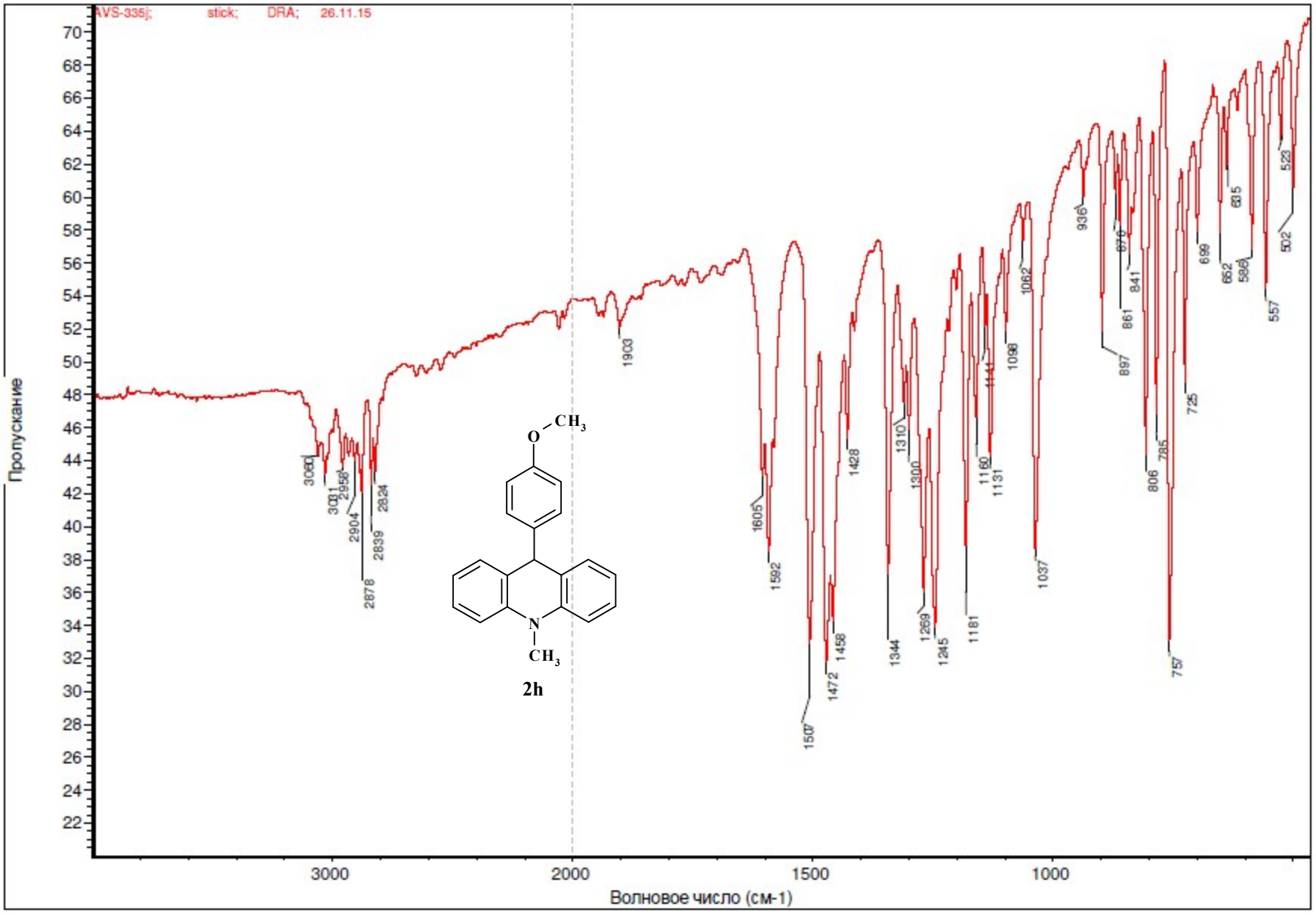

AVS335h
meg: B*6.1 71
45.58
45.56
45.55
45.55
45.54
45.53
45.52
45.51
45.50
0.00
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
50
45
40
35
30
25
20
15
10
5
0
-5
ppm


AVS-335h; stick; DRA; 26.11.15
Пропускание
Волновое число (см-1)
3064
3025
2983
2881
2824
1934
1894
1594
1501
1474
1457
1346
1317
1273
1218
1197
1181
1158
1130
1096
1064
1041
1012
935
896
864
844
824
814
792
752
724
696
654
635
616
581
549
526
495
F
N
CH3

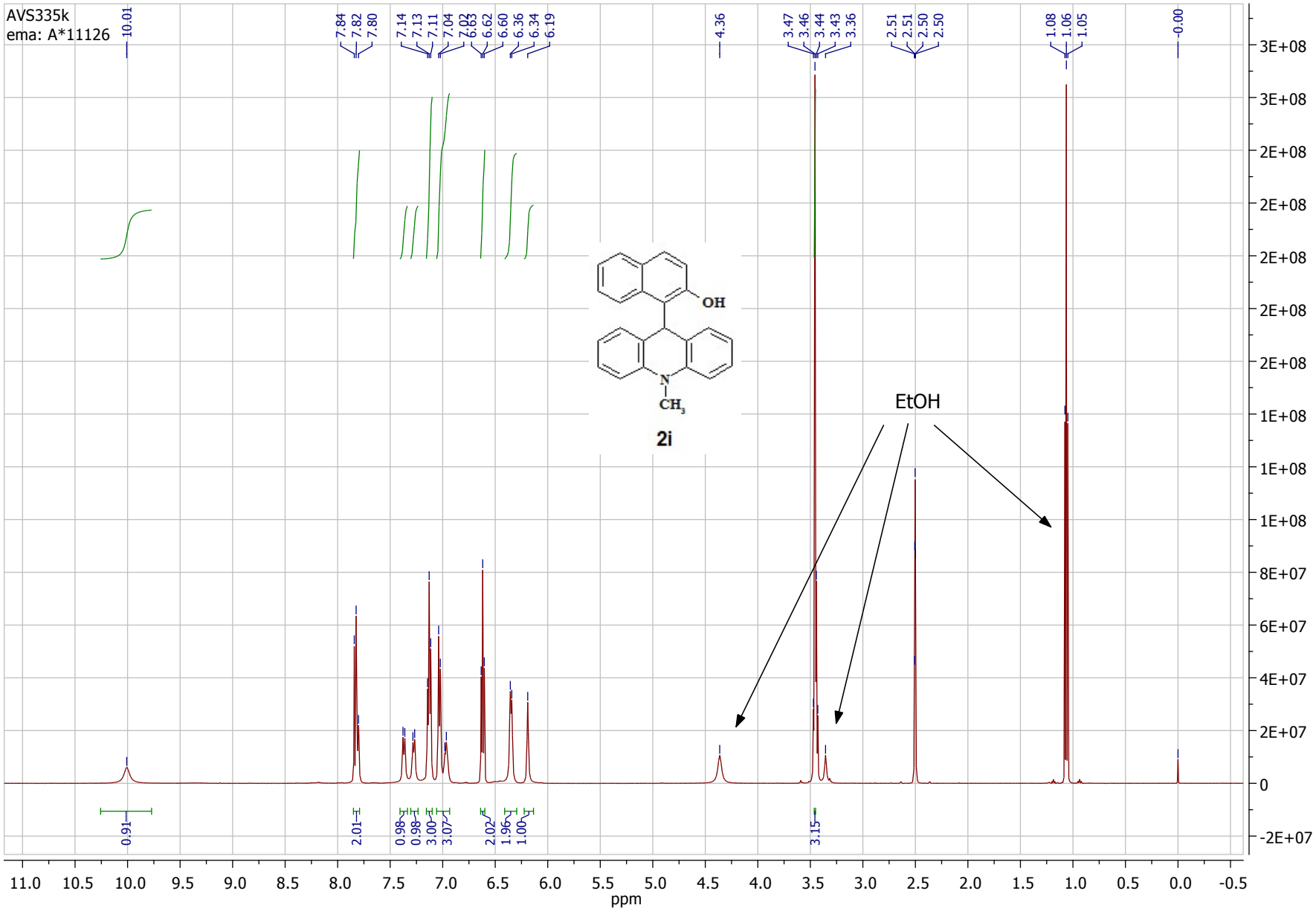
2g

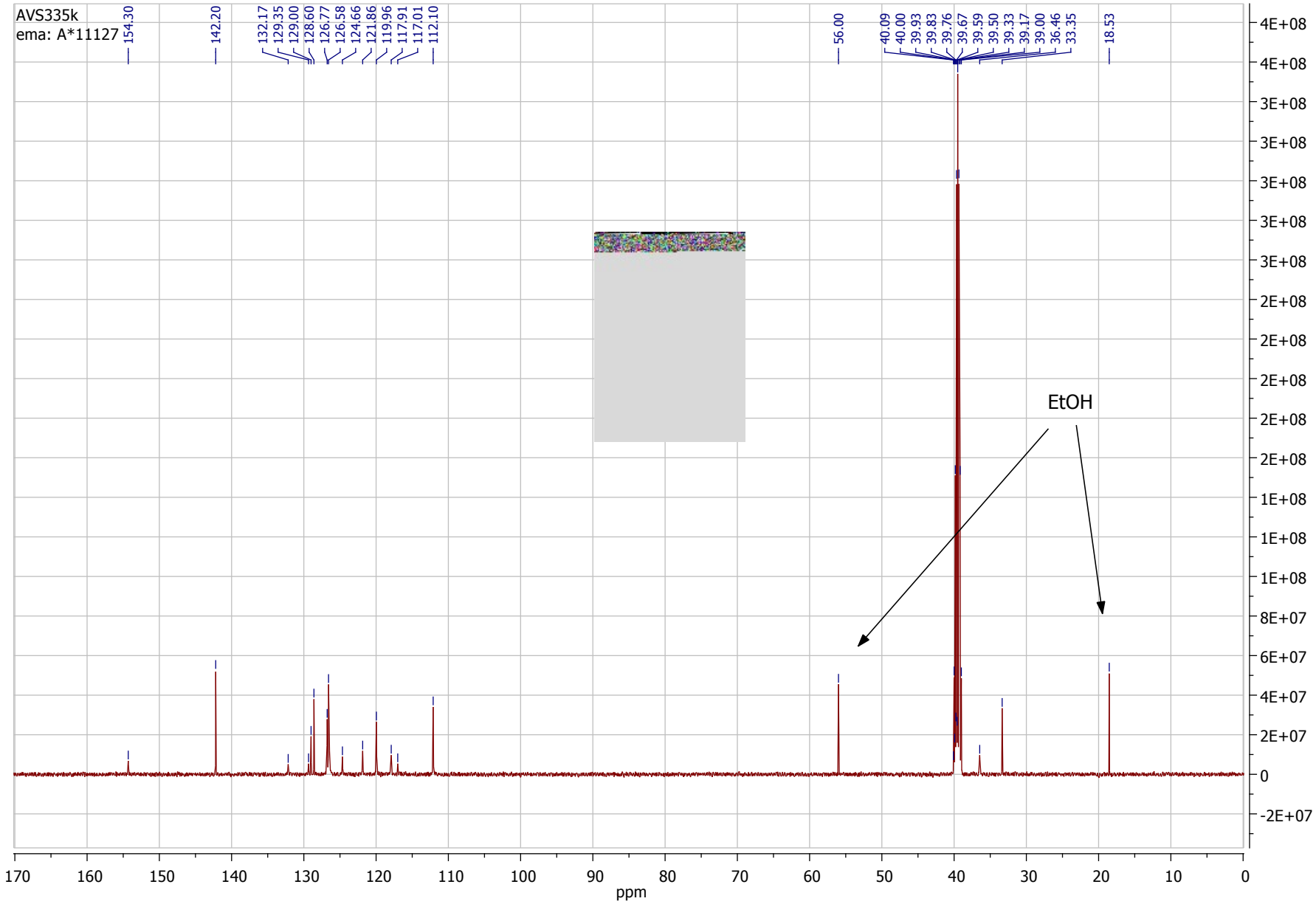

AVS335j
meg: A*11058
7.24
7.22
7.21
7.20
7.06
7.04
6.98
6.96
6.94
6.93
6.92
6.92
6.91
6.91
6.75
6.73
5.20
3.63
3.35
3.34
2.50
2.50
2.49
0.00
4.03
2.03
4.05
2.02
1.00
3.02
2.93
ppm
2h

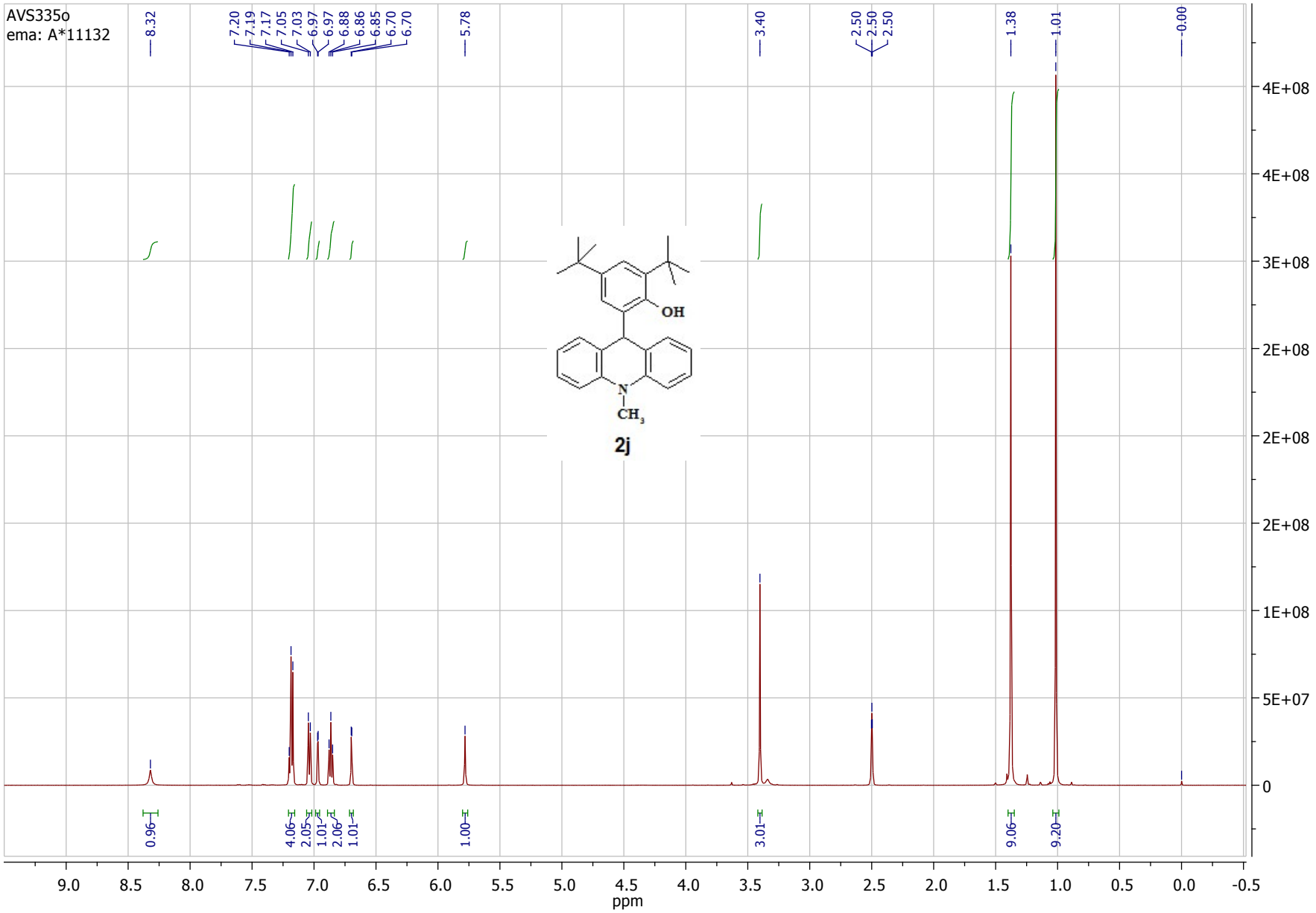

AVS335j
meg: A*11059
157.58
141.87
137.60
128.31
127.83
127.14
126.61
120.47
113.67
112.55
54.90
46.44
39.83
39.66
39.49
39.33
39.16
32.84
3E+08
2E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

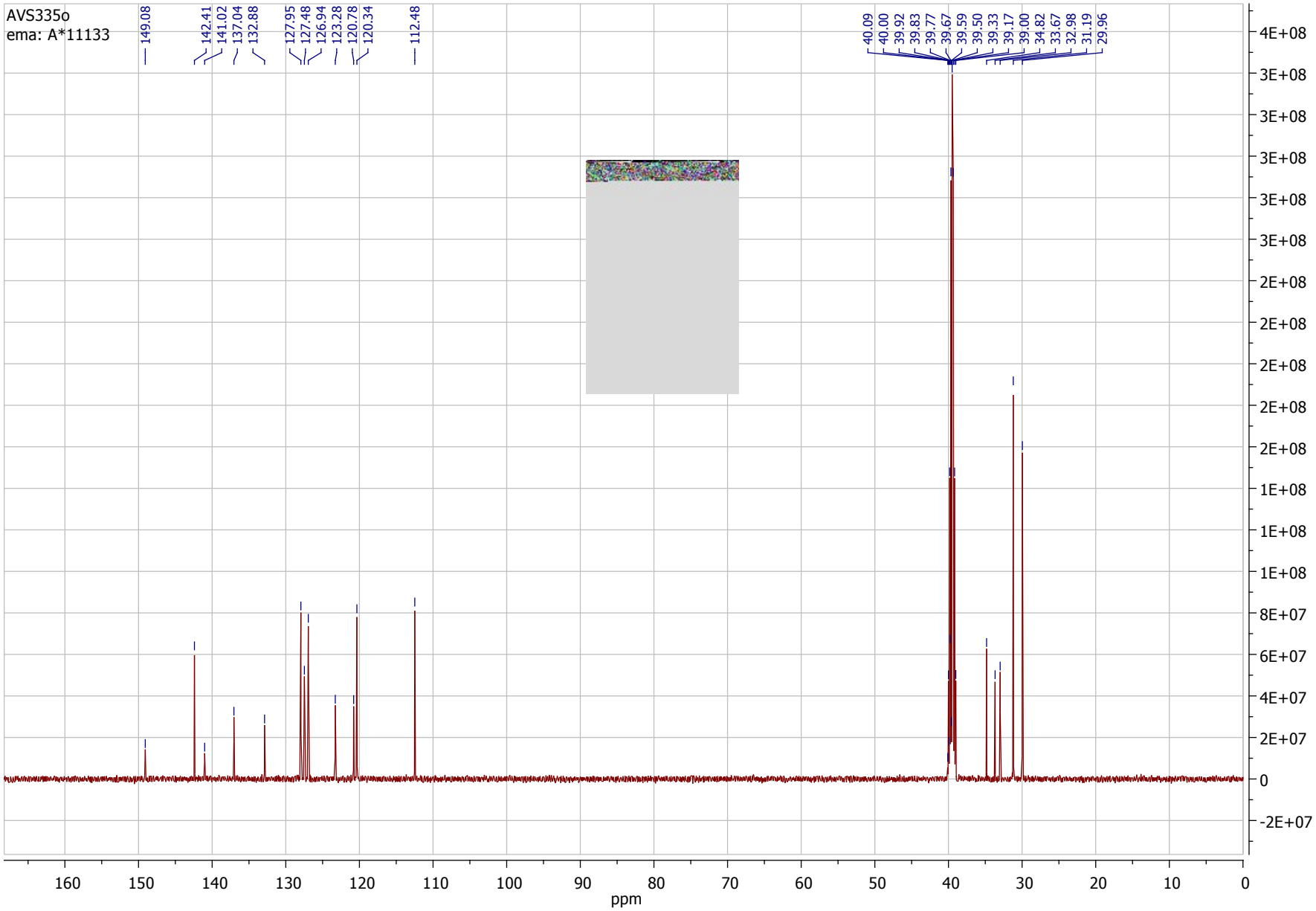

AVS-335j; stick; DRA; 26.11.15
Пропускание
Волновое число (см-1)
3000
2000
1500
1000
3060
3031
2958
2904
2878
2839
2824
1903
1605
1592
1507
1472
1458
1428
1344
1310
1300
1269
1245
1181
1160
1131
1098
1062
1037
936
897
861
841
806
785
757
725
699
662
635
596
557
523
502
O
CH3
N
CH3

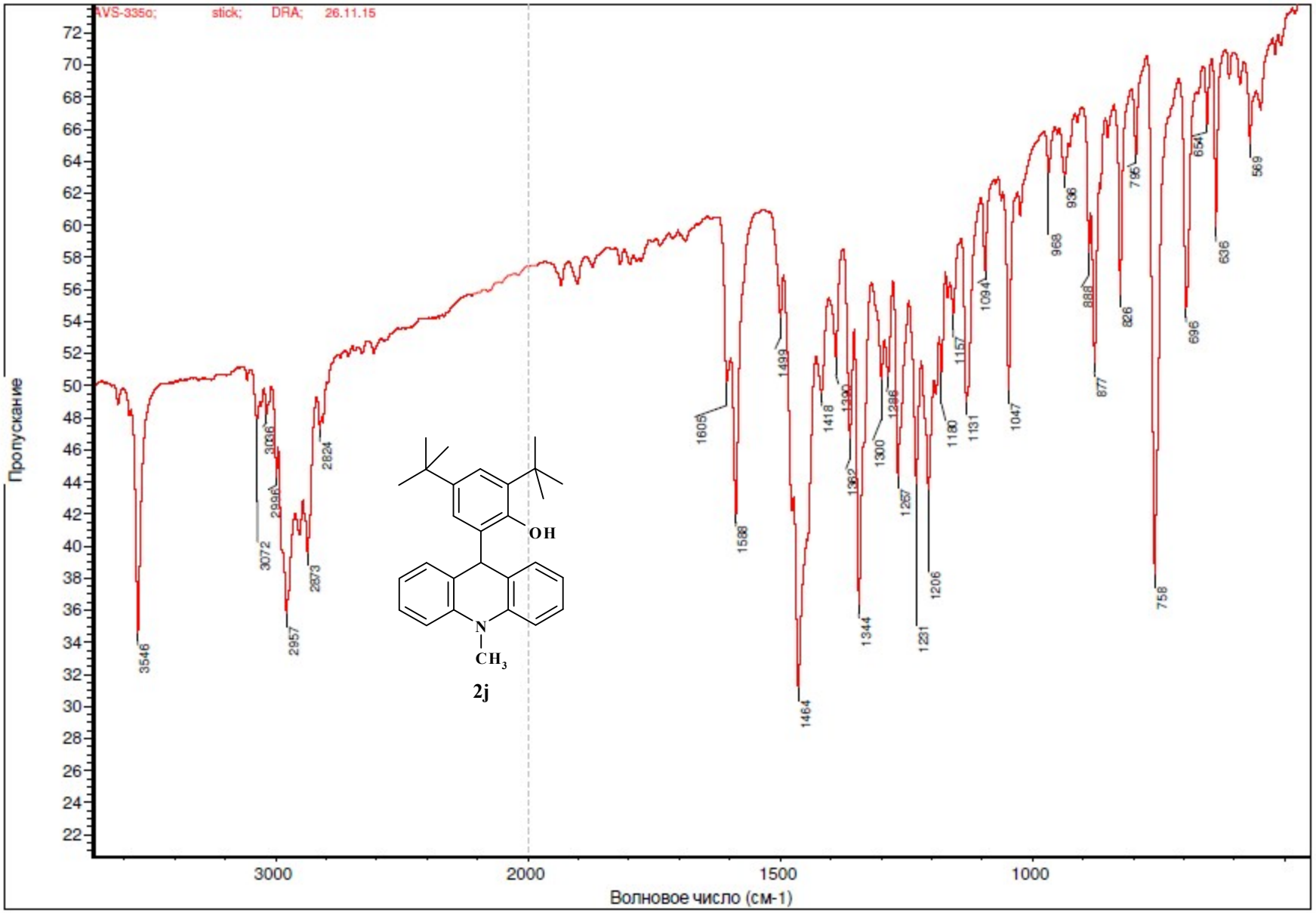
2h


AVS335k
ema: A*11126
10.01
7.84
7.82
7.80
7.14
7.13
7.11
7.04
7.02
6.83
6.62
6.60
6.36
6.34
6.19
4.36
3.47
3.46
3.44
3.43
3.36
2.51
2.51
2.50
2.50
1.08
1.06
1.05
0.00
OH
N
CH3
2i
EtOH
0.91
2.01
0.98
0.98
3.00
3.07
2.02
1.96
1.00
3.15
3E+08
2E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
11.0
10.5
10.0
9.5
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
-0.5
ppm

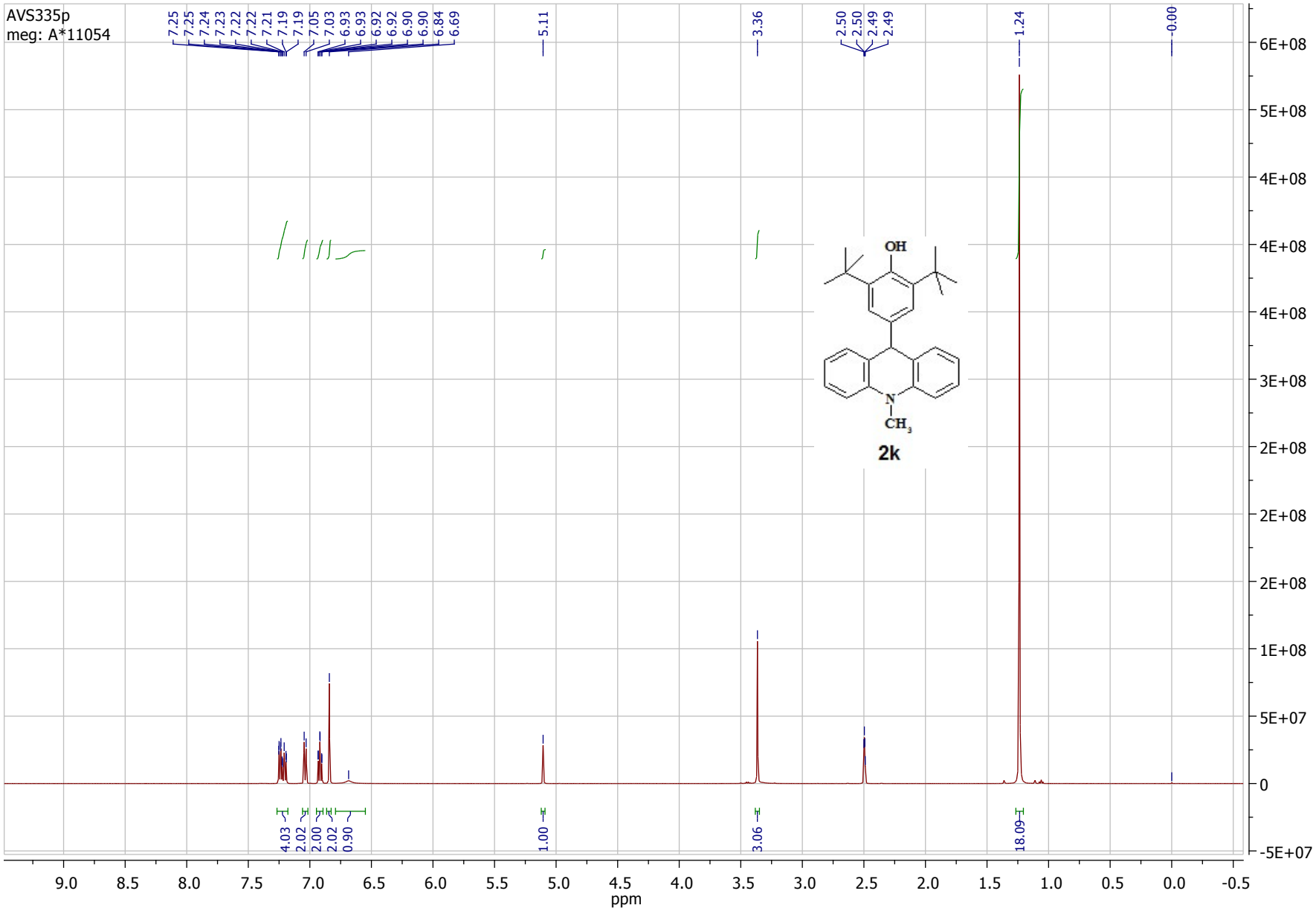

AVS335k
ema: A*11127
154.30
142.20
132.17
129.35
129.00
128.60
126.77
126.58
124.66
121.86
119.96
117.91
117.01
112.10
56.00
40.09
40.00
39.93
39.83
39.76
39.67
39.59
39.50
39.33
39.17
39.00
36.46
33.35
18.53
EtOH
4E+08
4E+08
3E+08
3E+08
3E+08
3E+08
3E+08
2E+08
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

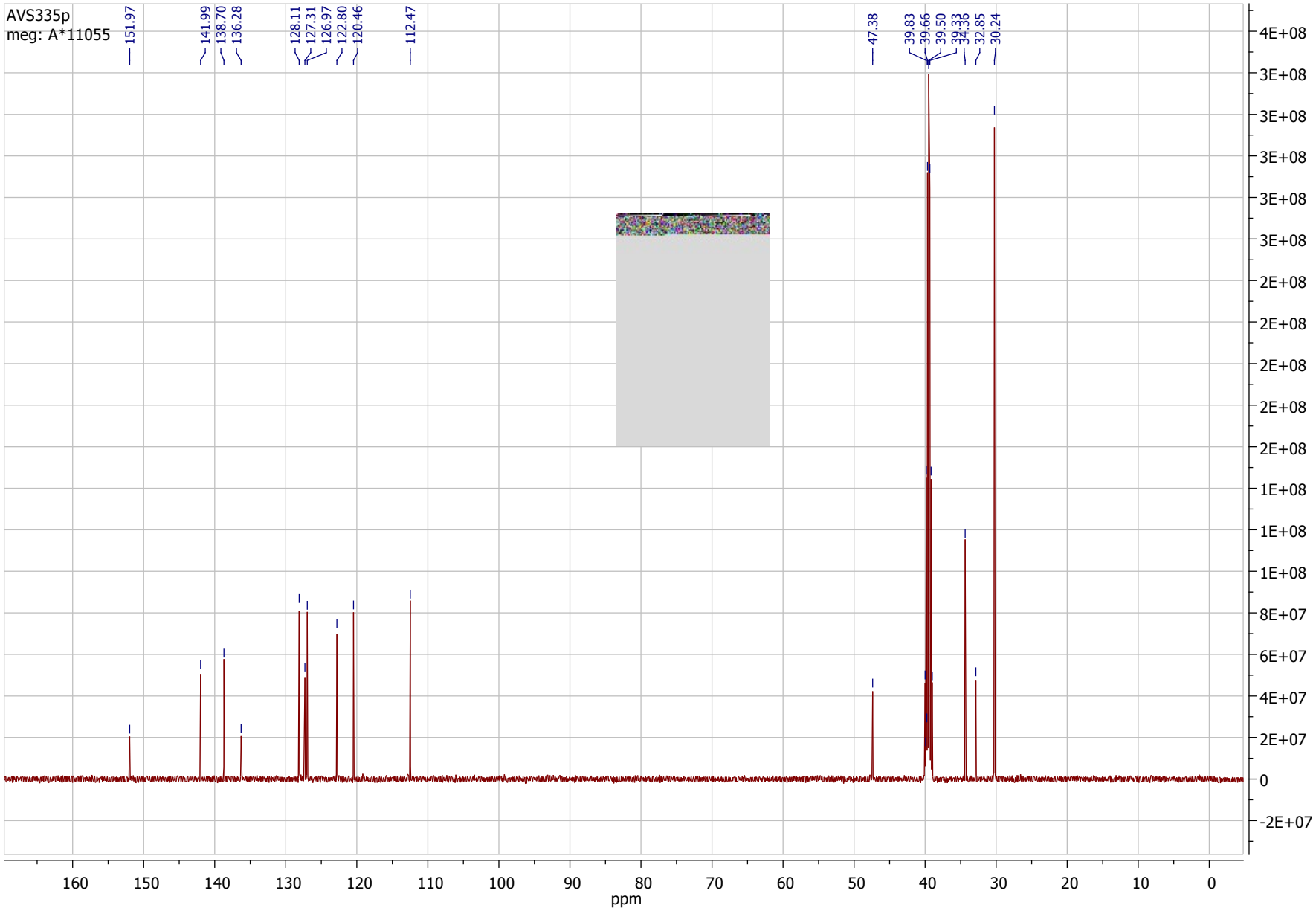

AVS335o
ema: A*11132
8.32
7.20
7.19
7.17
7.05
7.03
6.97
6.97
6.88
6.86
6.85
6.70
6.70
5.78
3.40
2.50
2.50
2.50
1.38
1.01
-0.00
OH
N
CH3
2j
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
0.96
4.06
2.05
1.01
2.06
1.01
1.00
3.01
9.06
9.20
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm

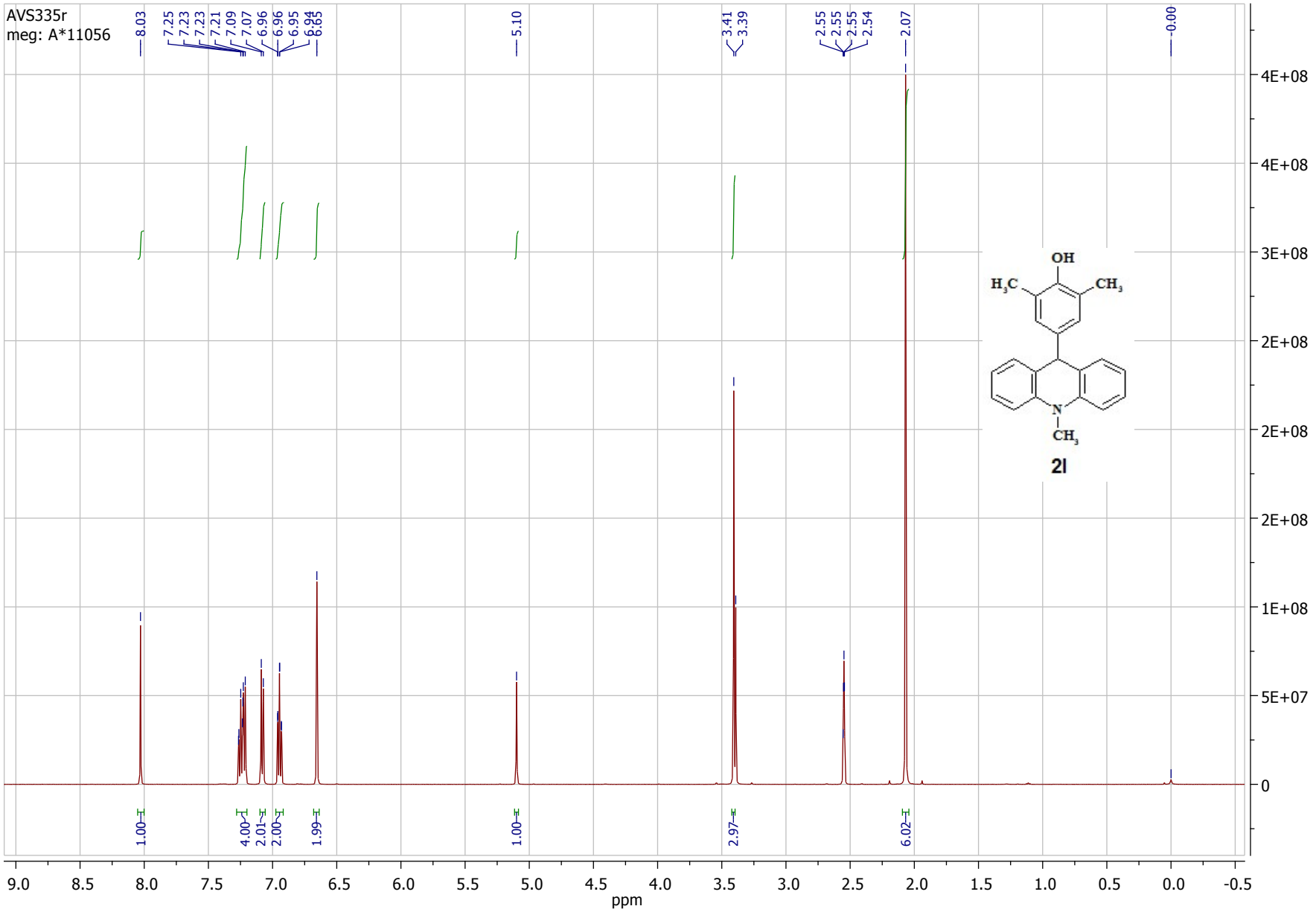

AVS335o
ema: A*11133
149.08
142.41
141.02
137.04
132.88
127.95
127.48
126.94
123.28
120.78
120.34
112.48
40.09
40.00
39.92
39.83
39.77
39.67
39.59
39.50
39.33
39.17
39.00
34.82
33.67
32.98
31.19
29.96
4E+08
3E+08
3E+08
3E+08
3E+08
3E+08
2E+08
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

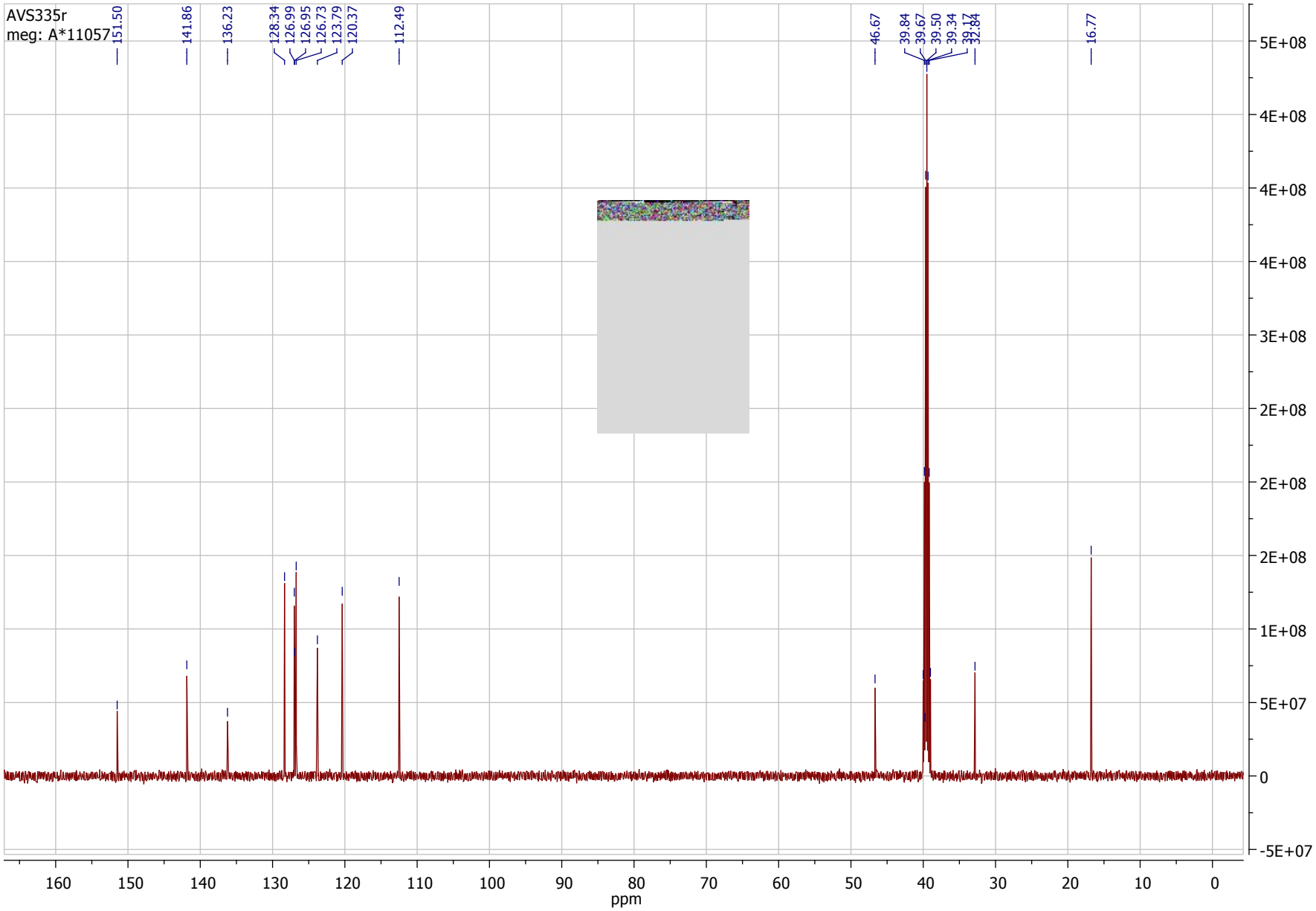

AVS-335o; stick; DRA; 26.11.15
Пропускание
Волновое число (см-1)
3000
2000
1500
1000
3546
3072
3036
2996
2957
2873
2824
1605
1588
1499
1464
1418
1390
1382
1344
1300
1286
1257
1231
1206
1180
1157
1131
1094
1047
968
936
888
877
826
796
758
696
654
636
569
OH
N
CH3

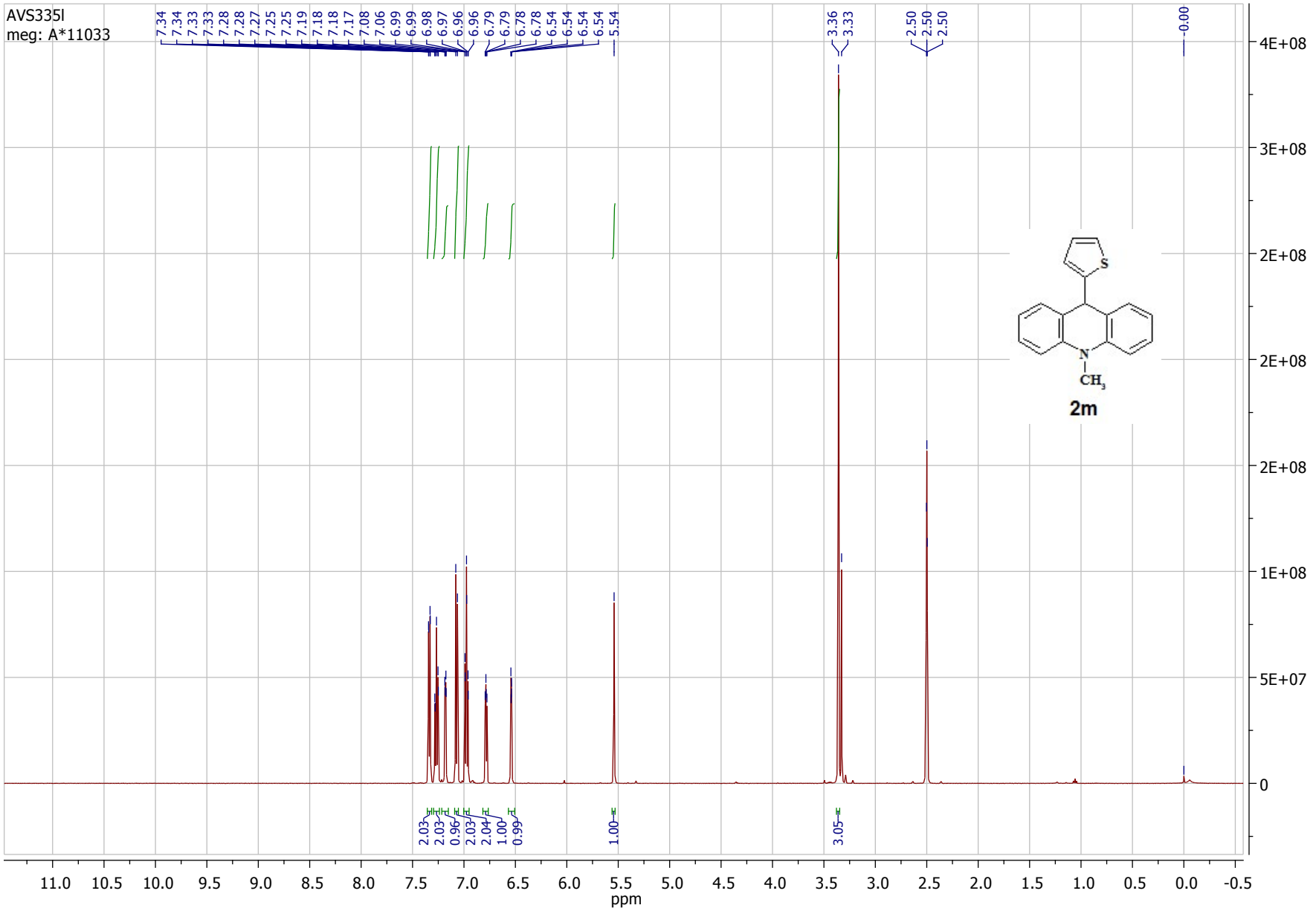
2j

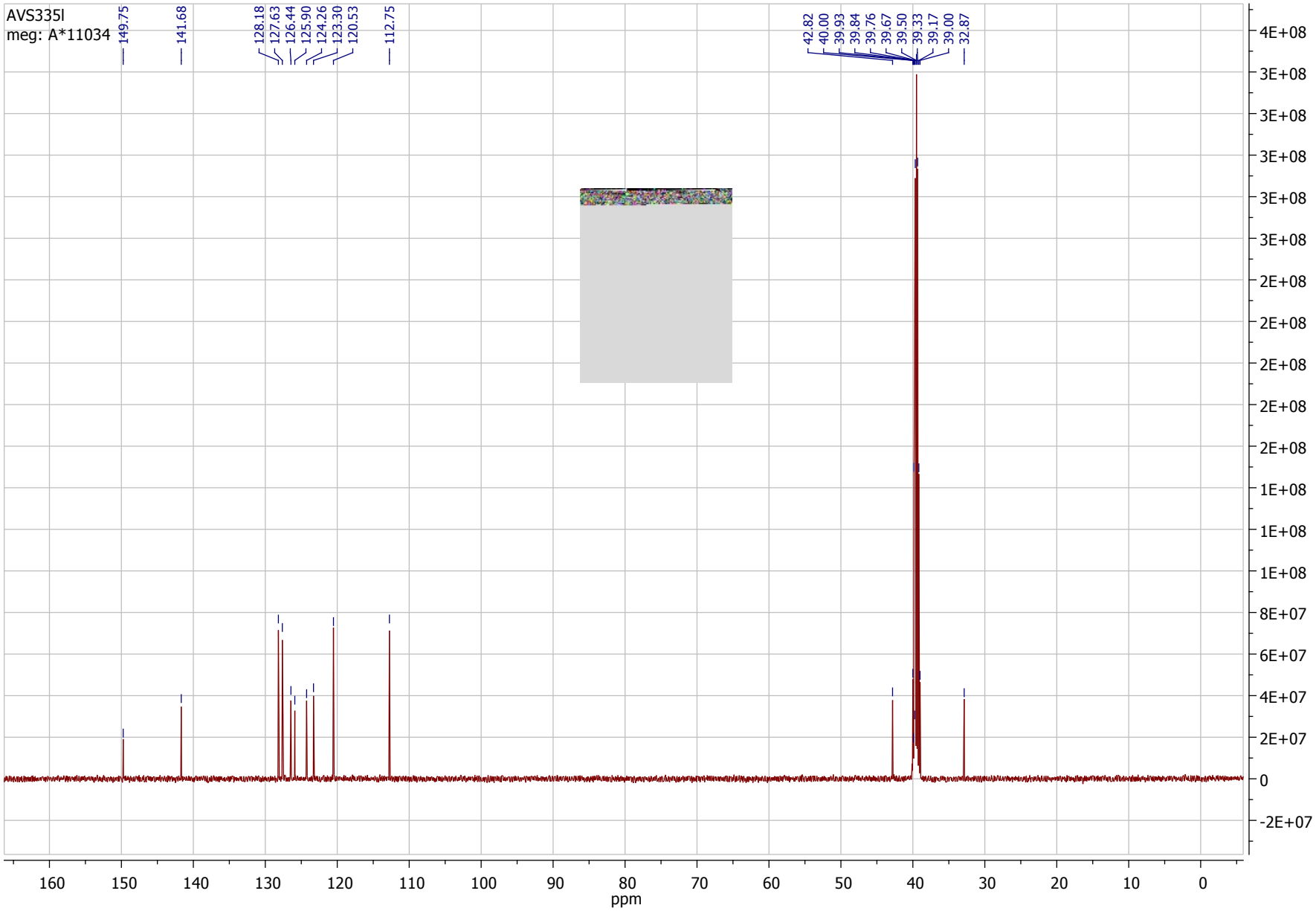

AVS335p
meg: A*11054
7.25
7.25
7.24
7.23
7.22
7.22
7.21
7.19
7.19
7.05
7.03
6.93
6.93
6.92
6.92
6.90
6.90
6.84
6.69
5.11
3.36
2.50
2.50
2.49
2.49
1.24
-0.00
OH
N
CH3
2k
4.03
2.02
2.00
2.02
0.90
1.00
3.06
18.09
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
9.0
8.5
8.0
7.5
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
-0.5
ppm

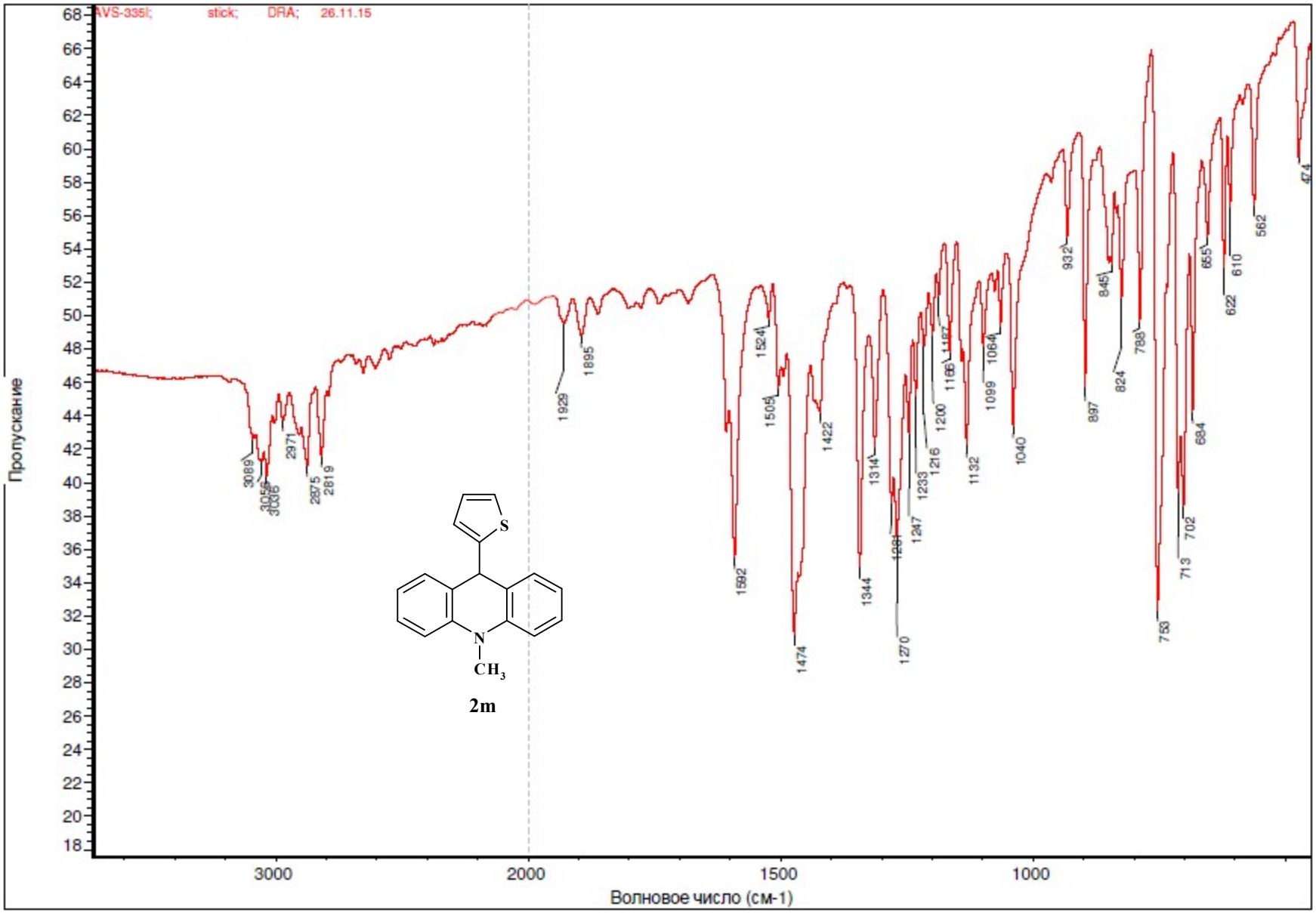

AVS335p
meg: A*11055
151.97
141.99
138.70
136.28
128.11
127.31
126.97
122.80
120.46
112.47
47.38
39.83
39.66
39.50
39.33
34.36
32.85
30.24
4E+08
3E+08
3E+08
3E+08
3E+08
3E+08
2E+08
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


AVS335r
meg: A*11056
8.03
7.25
7.23
7.23
7.21
7.09
7.07
6.96
6.96
6.95
6.94
6.85
5.10
3.41
3.39
2.55
2.55
2.55
2.54
2.07
-0.00
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
1.00
4.00
2.01
2.00
1.99
1.00
2.97
6.02
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
-0.5
ppm
OH
H3C
CH3
N
CH3
2l

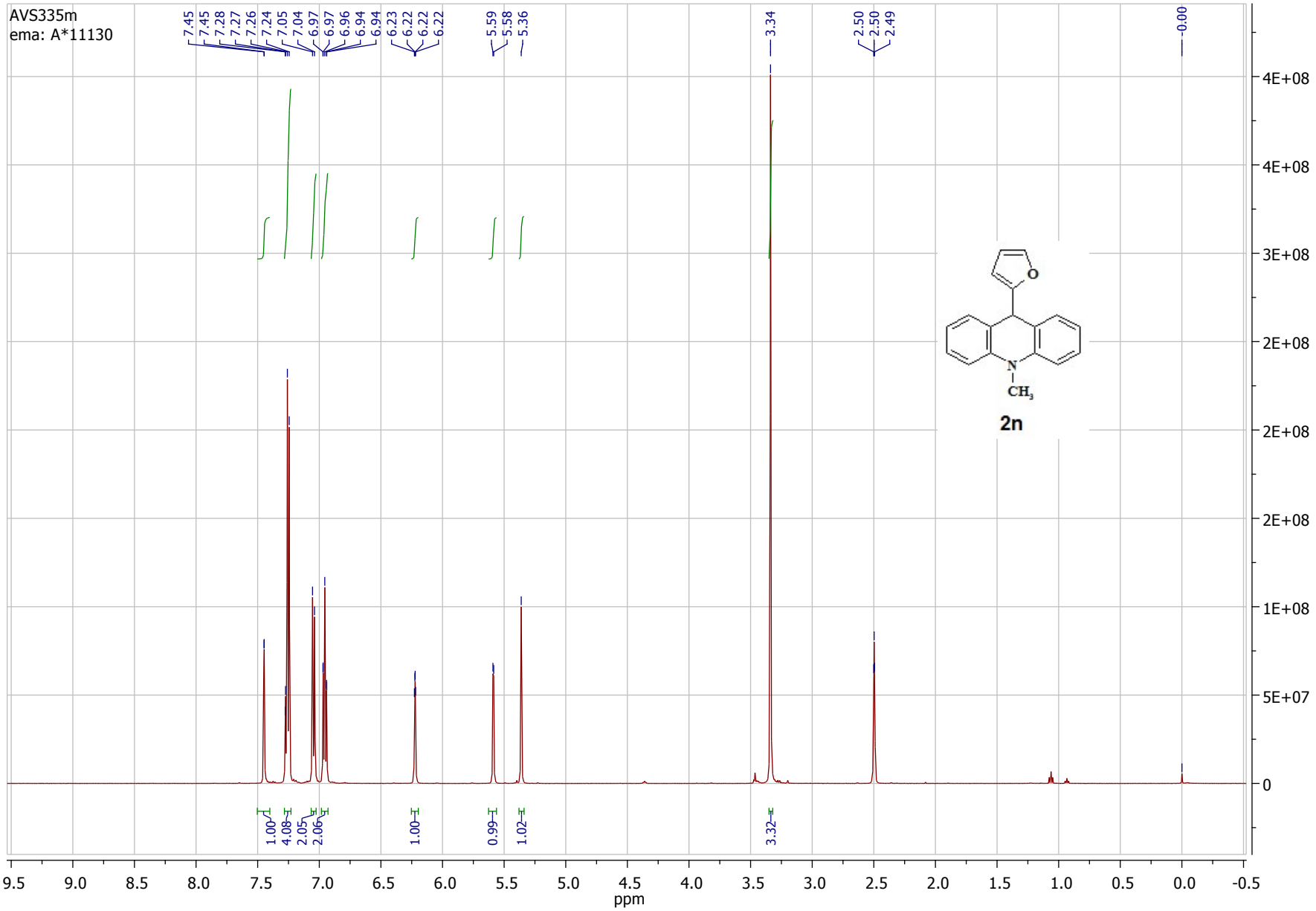

AVS335r
meg: A*11057
151.50
141.86
136.23
128.34
126.99
126.95
126.73
123.79
120.37
112.49
46.67
39.84
39.67
39.50
39.34
39.17
32.84
16.77
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

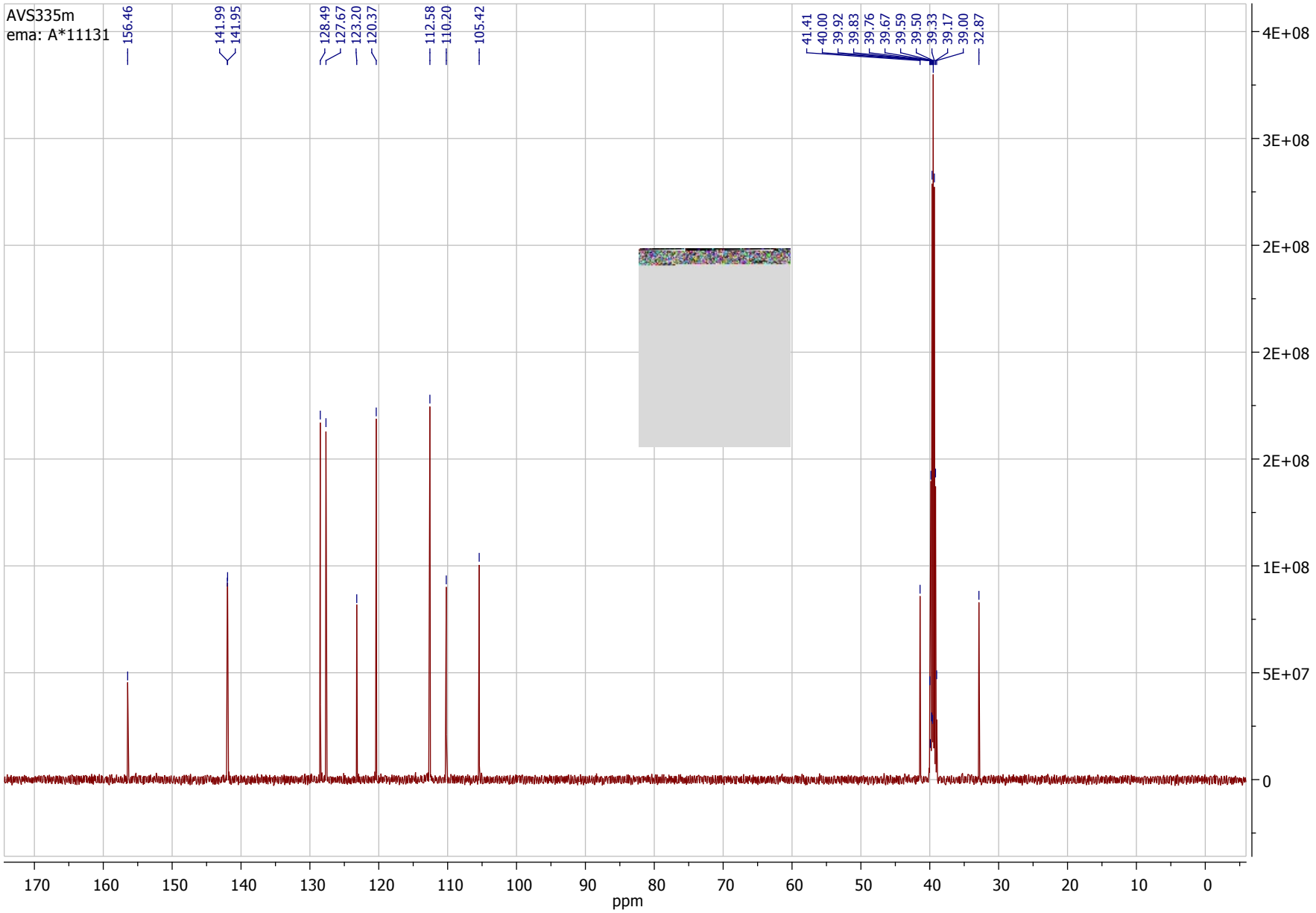

AVS335I
meg: A*11033
7.34 7.34 7.33 7.33 7.28 7.28 7.27 7.25 7.25 7.19 7.18 7.18 7.17 7.08 7.06 6.99 6.99 6.98 6.97 6.96 6.96 6.79 6.79 6.78 6.78 6.54 6.54 6.54 6.54 5.54
3.36 3.33
2.50 2.50 2.50
0.00
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
2.03 2.03 0.96 2.03 2.04 1.00 0.99
1.00
3.05
11.0 10.5 10.0 9.5 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 -0.5
ppm
S
N
CH3
2m

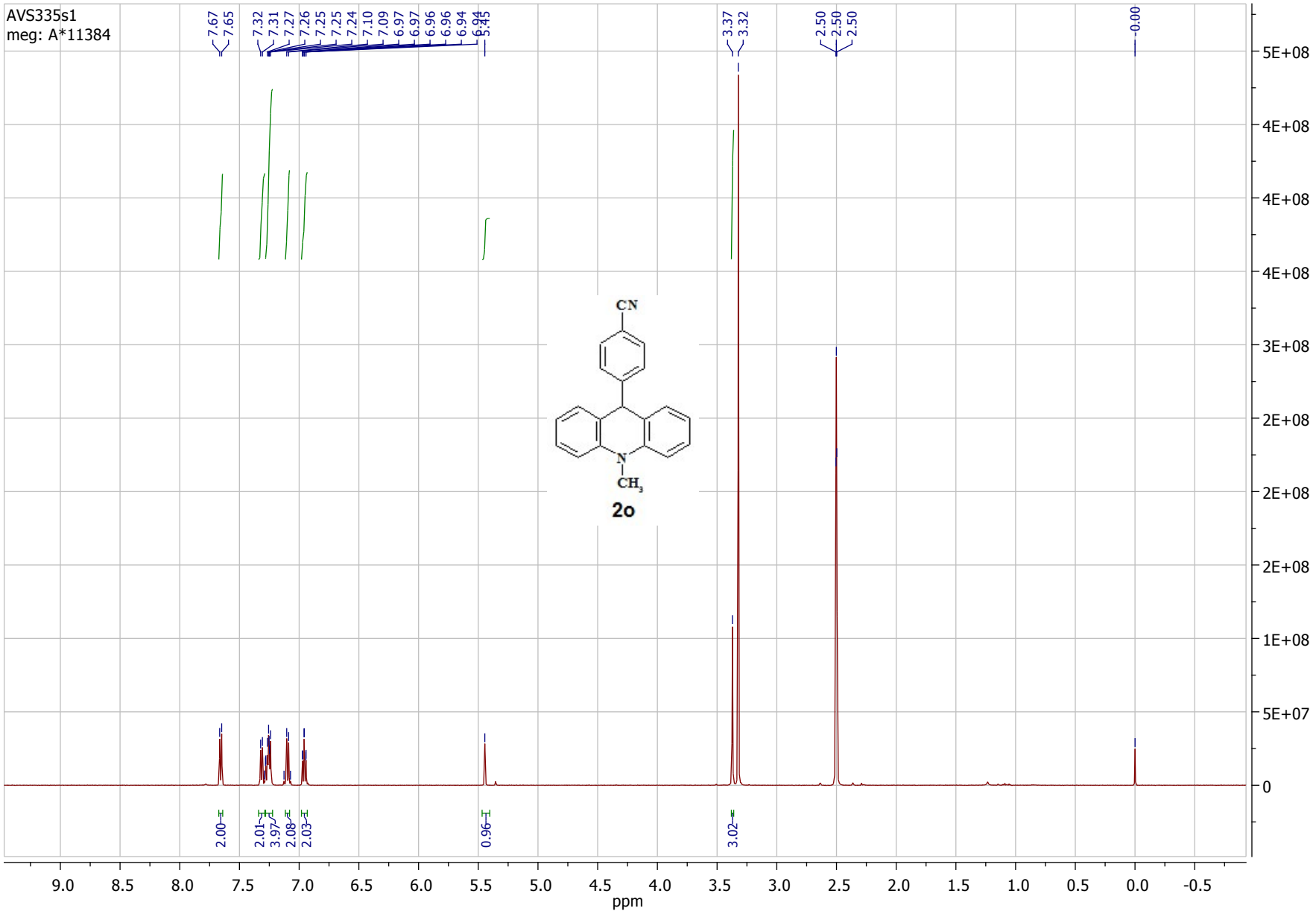

AVS335I
meg: A*11034
149.75
141.68
128.18
127.63
126.44
125.90
124.26
123.30
120.53
112.75
42.82
40.00
39.93
39.84
39.76
39.67
39.50
39.33
39.17
39.00
32.87
4E+08
3E+08
3E+08
3E+08
3E+08
3E+08
2E+08
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

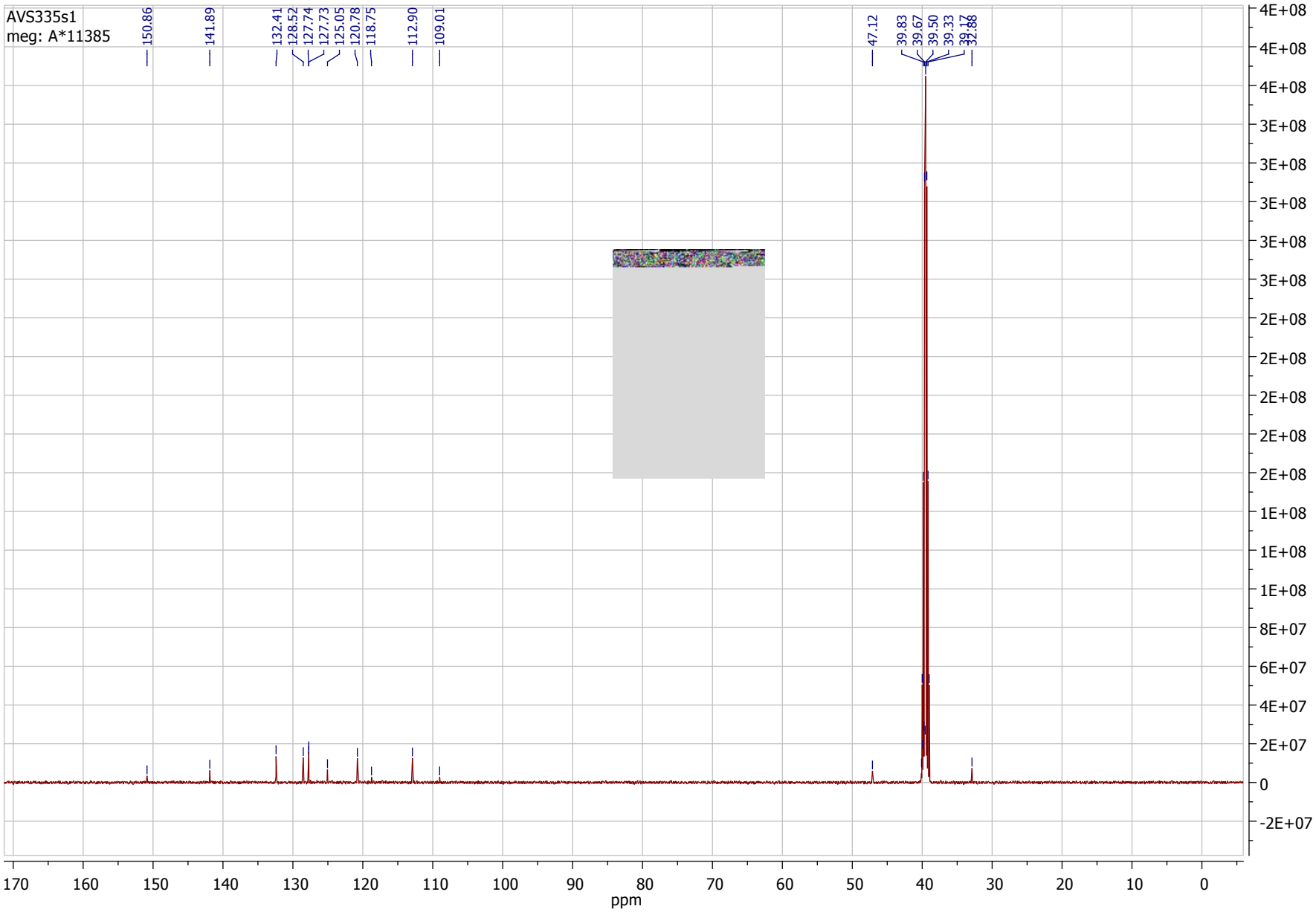

AVS-335l; stick; DRA; 26.11.15
Пропускание
Волновое число (см-1)
3089
3058
3036
2971
2875
2819
1929
1895
1592
1524
1505
1474
1422
1344
1314
1270
1247
1233
1216
1200
1187
1166
1132
1099
1064
1040
932
897
845
824
793
753
713
702
684
655
622
610
562
474
S
N
CH3

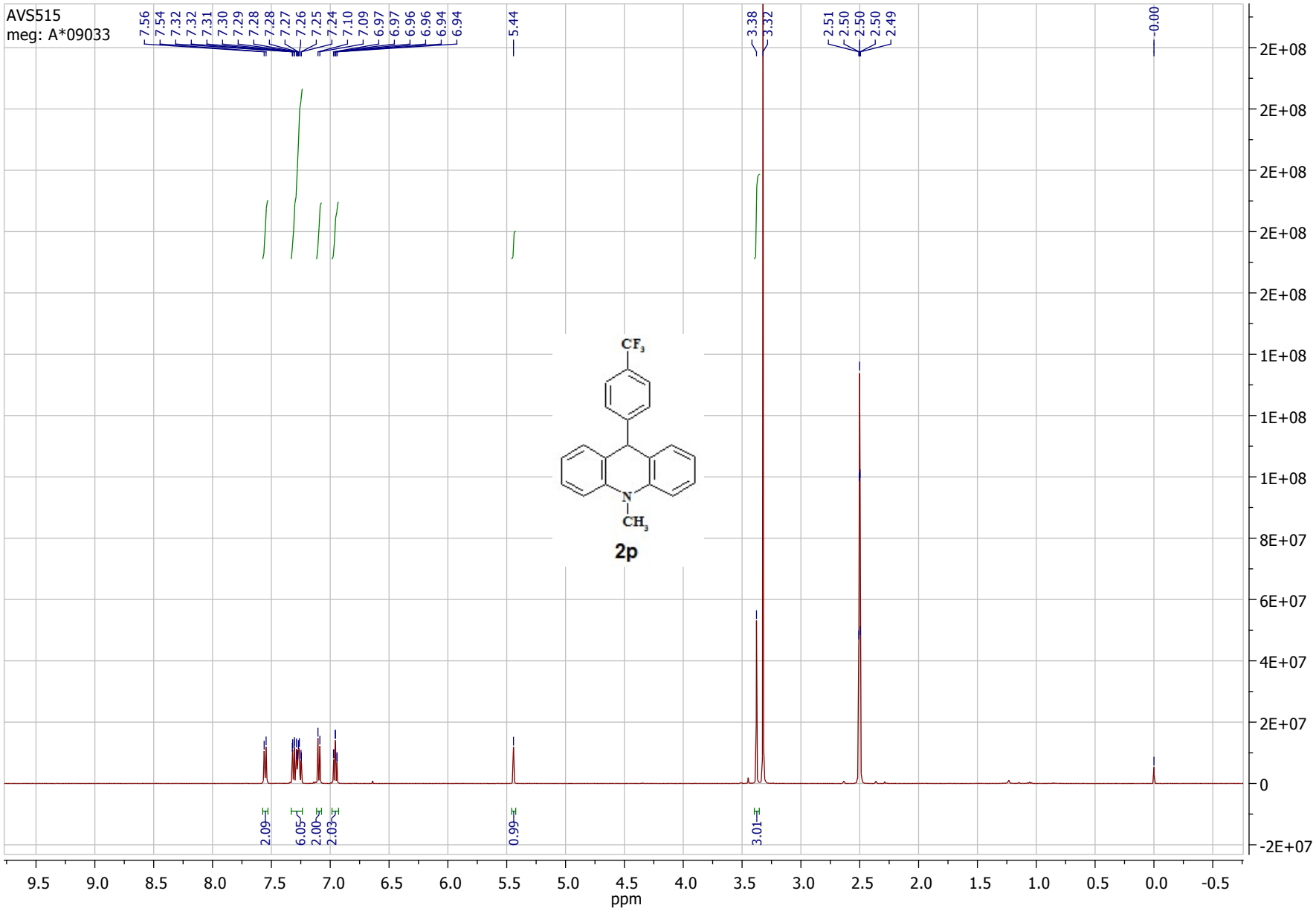
2m

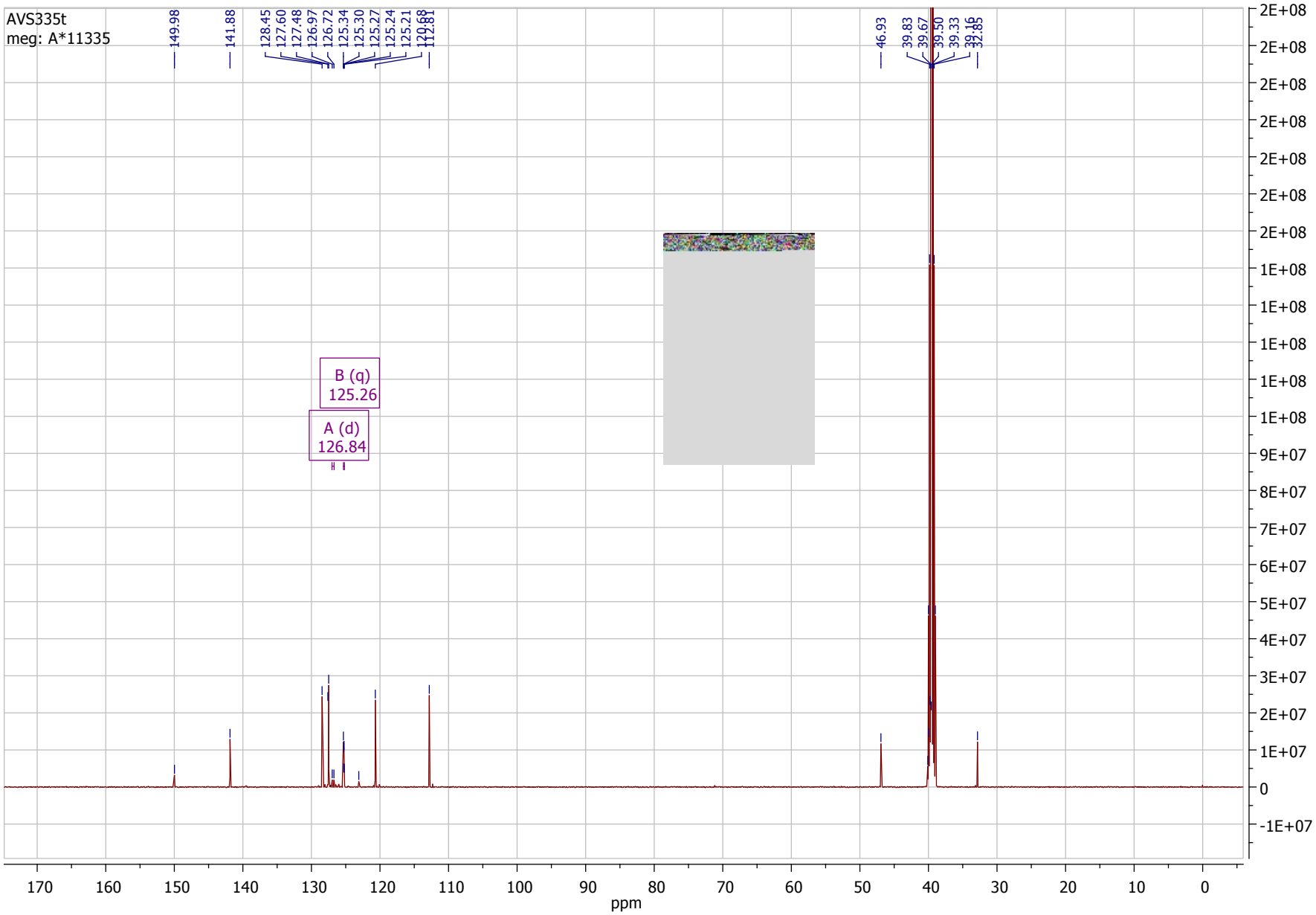

AVS335m
ema: A*11130
7.45
7.45
7.28
7.27
7.26
7.24
7.05
7.04
6.97
6.97
6.96
6.94
6.94
6.23
6.22
6.22
6.22
5.59
5.58
5.36
3.34
2.50
2.50
2.49
0.00
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
1.00
4.08
2.05
2.06
1.00
0.99
1.02
3.32
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm
O
N
CH3
2n

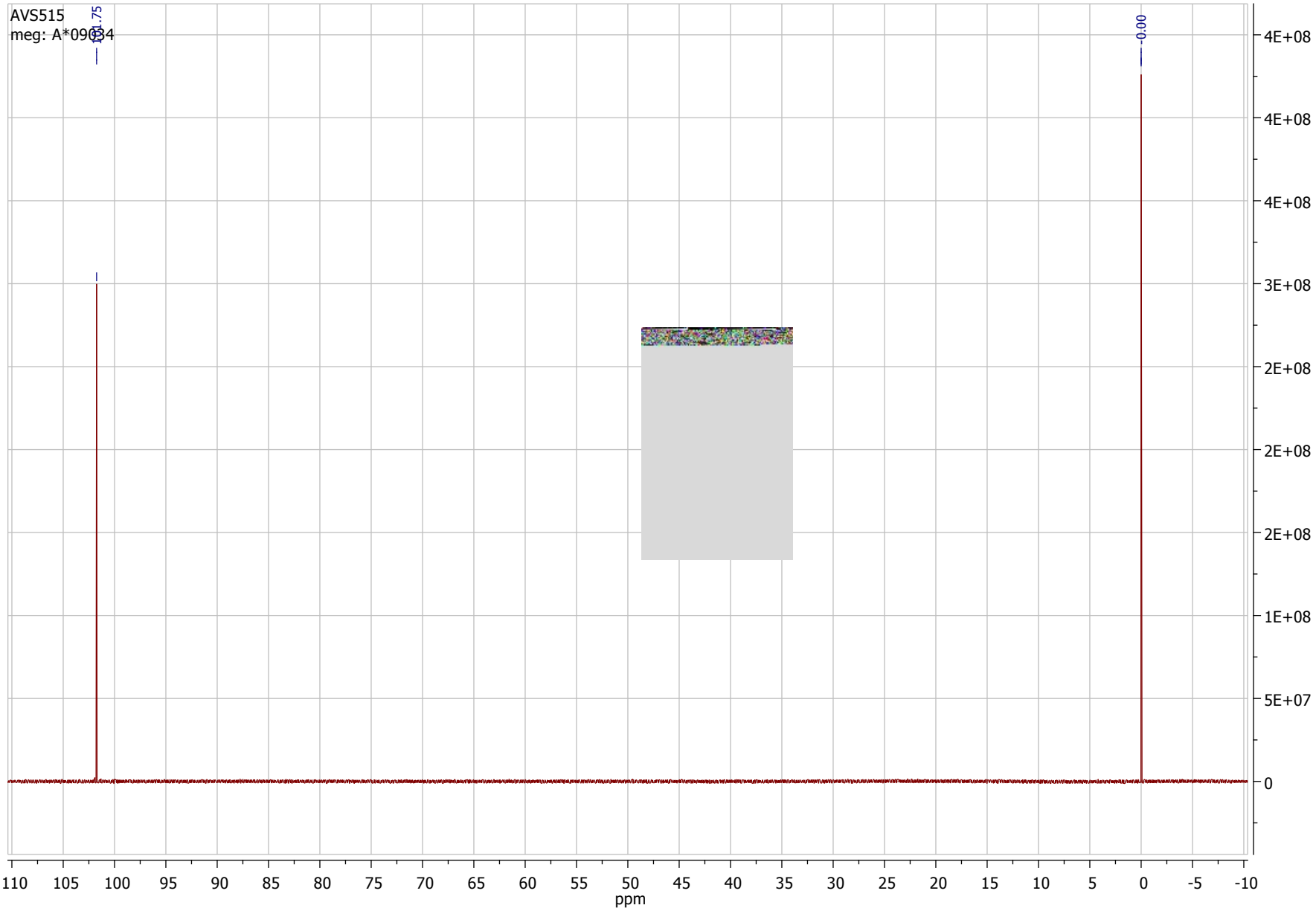

AVS335m
ema: A*11131
156.46
141.99
141.95
128.49
127.67
123.20
120.37
112.58
110.20
105.42
41.41
40.00
39.92
39.83
39.76
39.67
39.59
39.50
39.33
39.17
39.00
32.87
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

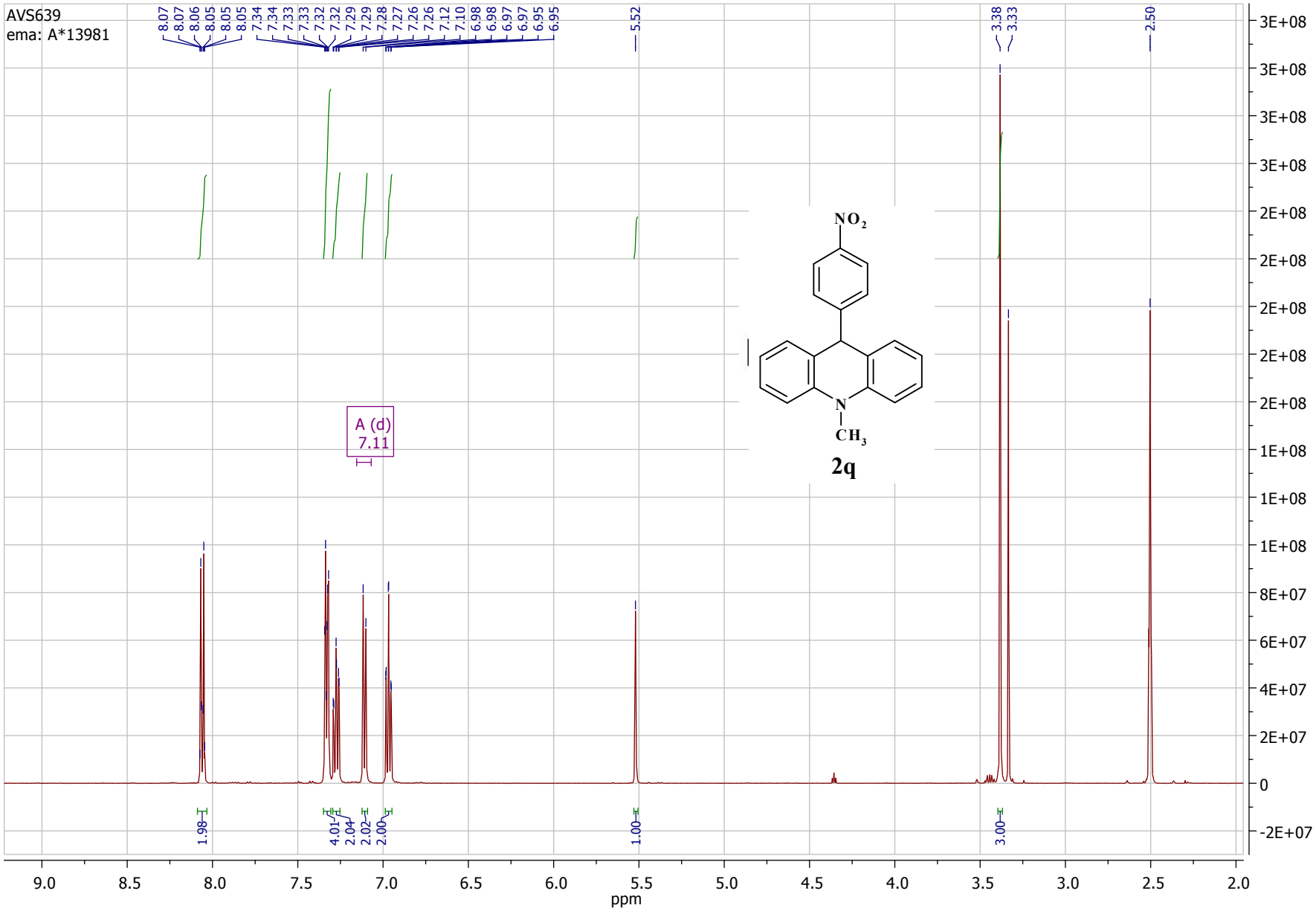

AVS335s1
meg: A*11384
7.67
7.65
7.32
7.31
7.27
7.26
7.25
7.25
7.24
7.10
7.09
6.97
6.97
6.96
6.96
6.94
6.94
5.45
3.37
3.32
2.50
2.50
2.50
-0.00
CN
N
CH3
2o
2.00
2.01
3.97
2.08
2.03
0.96
3.02
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm

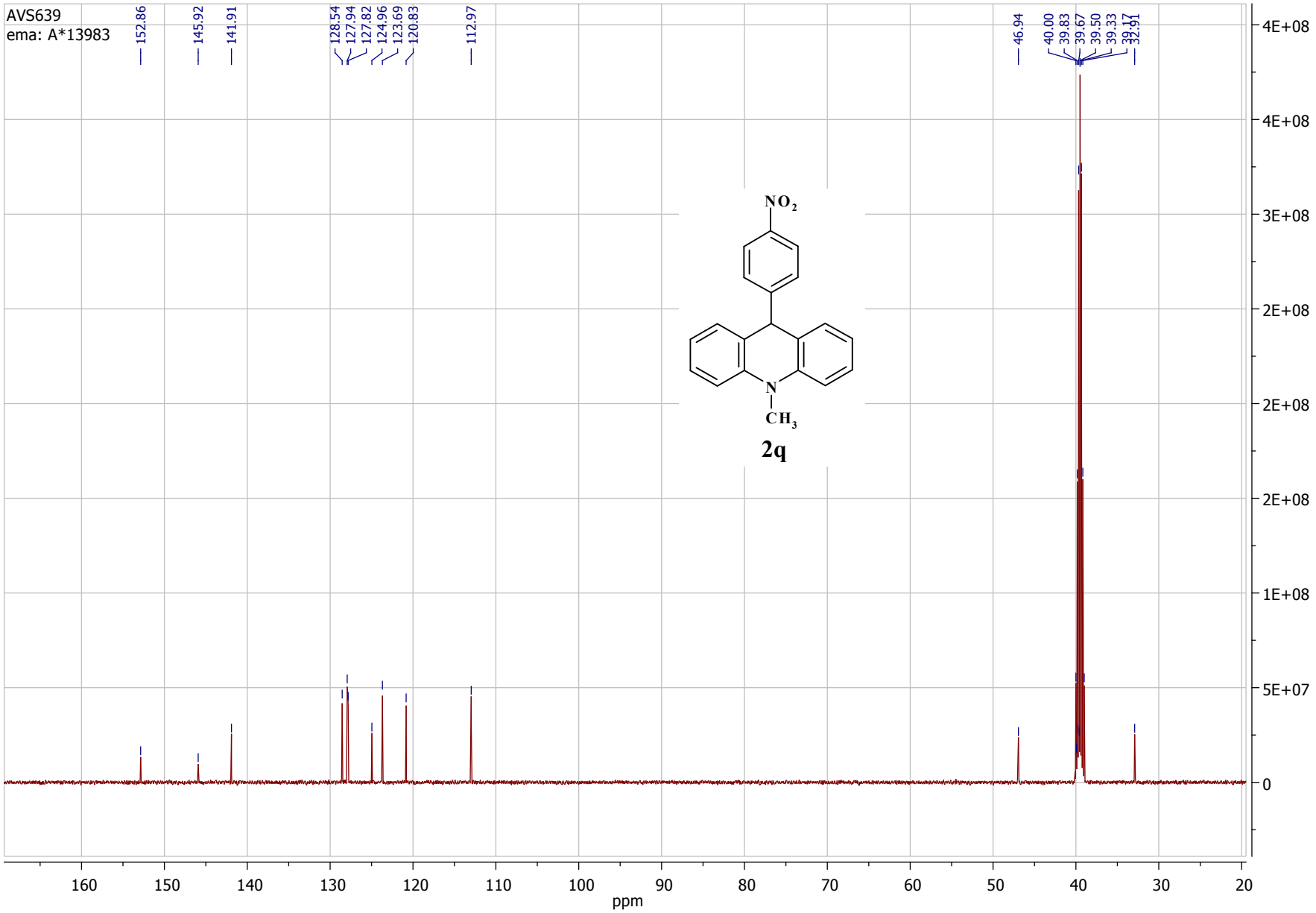

AVS335s1
meg: A*11385
150.86
141.89
132.41
128.52
127.74
127.73
125.05
120.78
118.75
112.90
109.01
47.12
39.83
39.67
39.50
39.33
39.17
32.88
4E+08
4E+08
4E+08
3E+08
3E+08
3E+08
3E+08
3E+08
3E+08
2E+08
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

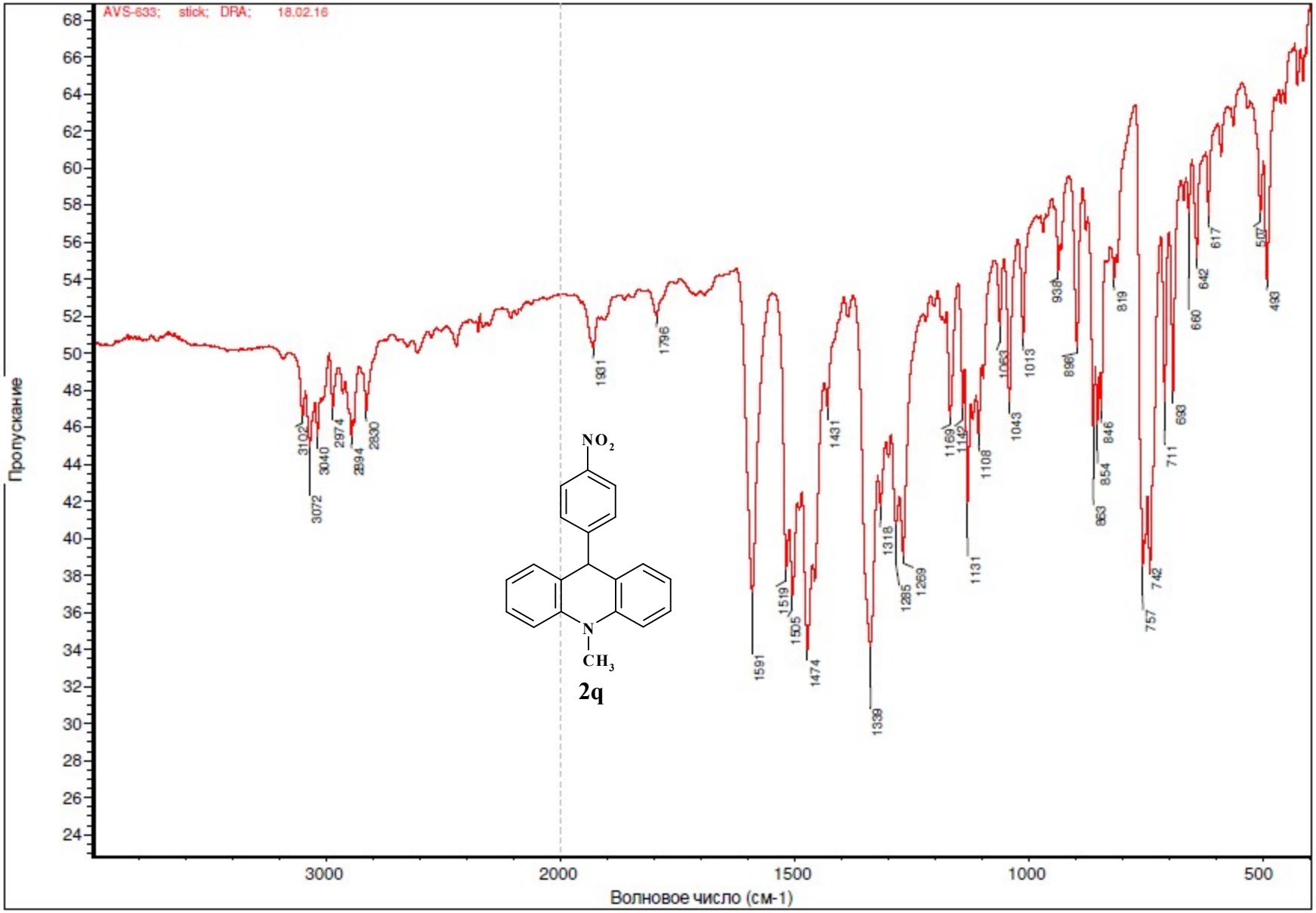

AVS515
meg: A*09033
7.56
7.54
7.32
7.32
7.31
7.30
7.29
7.28
7.28
7.27
7.26
7.25
7.24
7.10
7.09
6.97
6.97
6.96
6.96
6.94
6.94
5.44
3.38
3.32
2.51
2.50
2.50
2.50
2.49
0.00
CF3
N
CH3
2p
2.09
6.05
2.00
2.03
0.99
3.01
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
9.5
9.0
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
-0.5
ppm

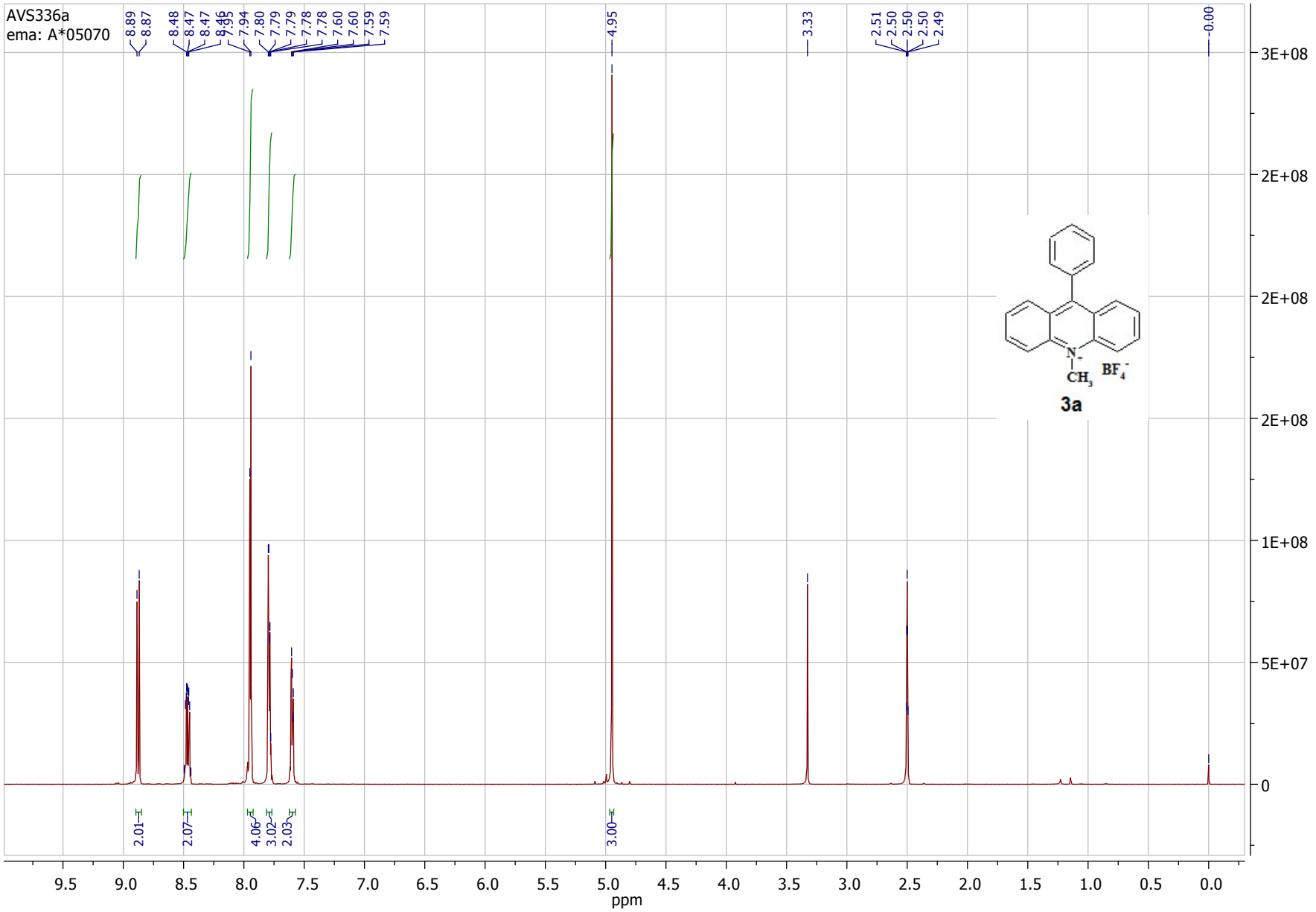

AVS335t
meg: A*11335
149.98
141.88
128.45
127.60
127.48
126.97
126.72
125.34
125.30
125.27
125.24
125.21
120.68
112.81
46.93
39.83
39.67
39.50
39.33
39.16
32.85
B (q)
125.26
A (d)
126.84
ppm

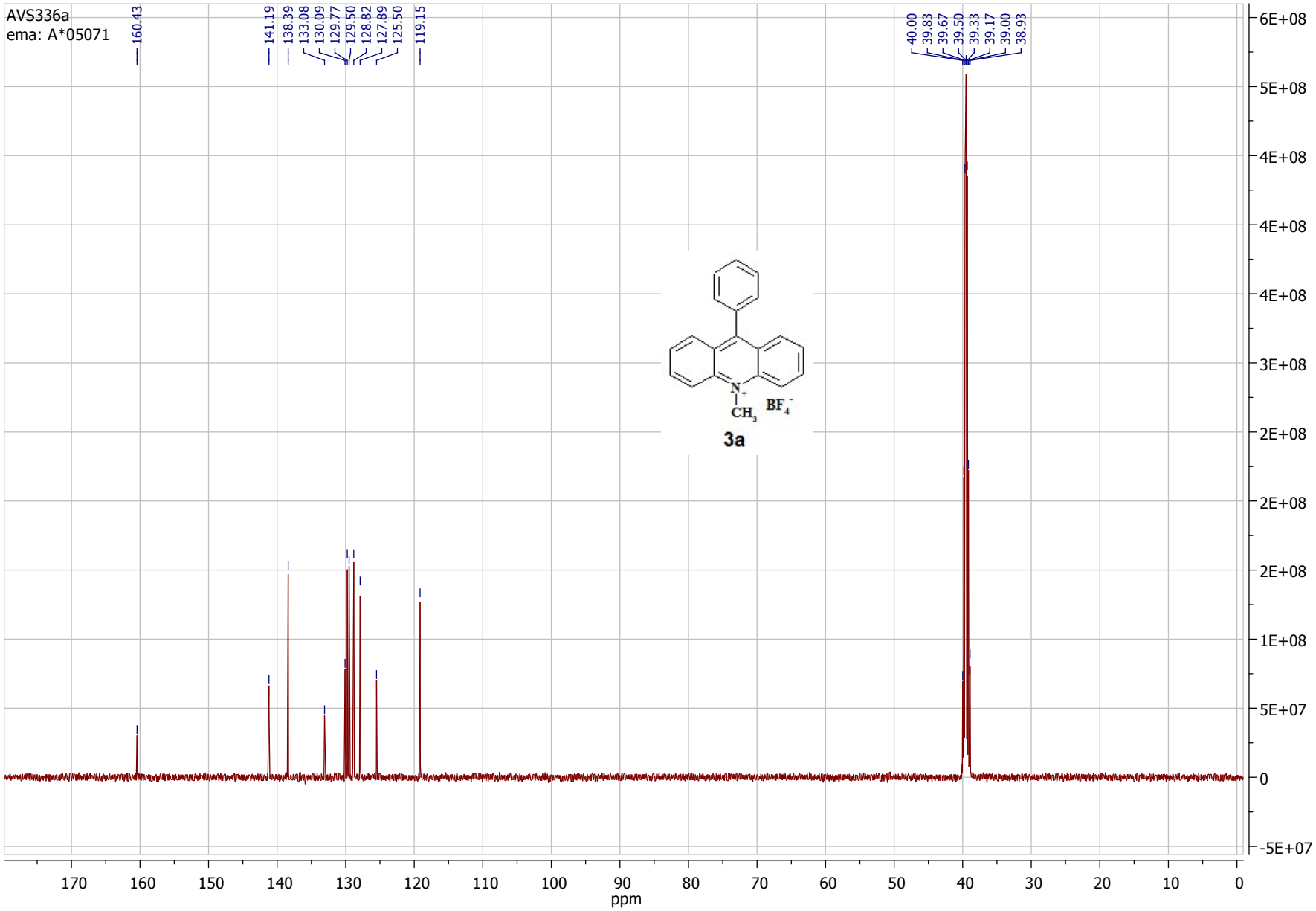

AVS515
meg: A*09034
101.75
0.00
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10
ppm

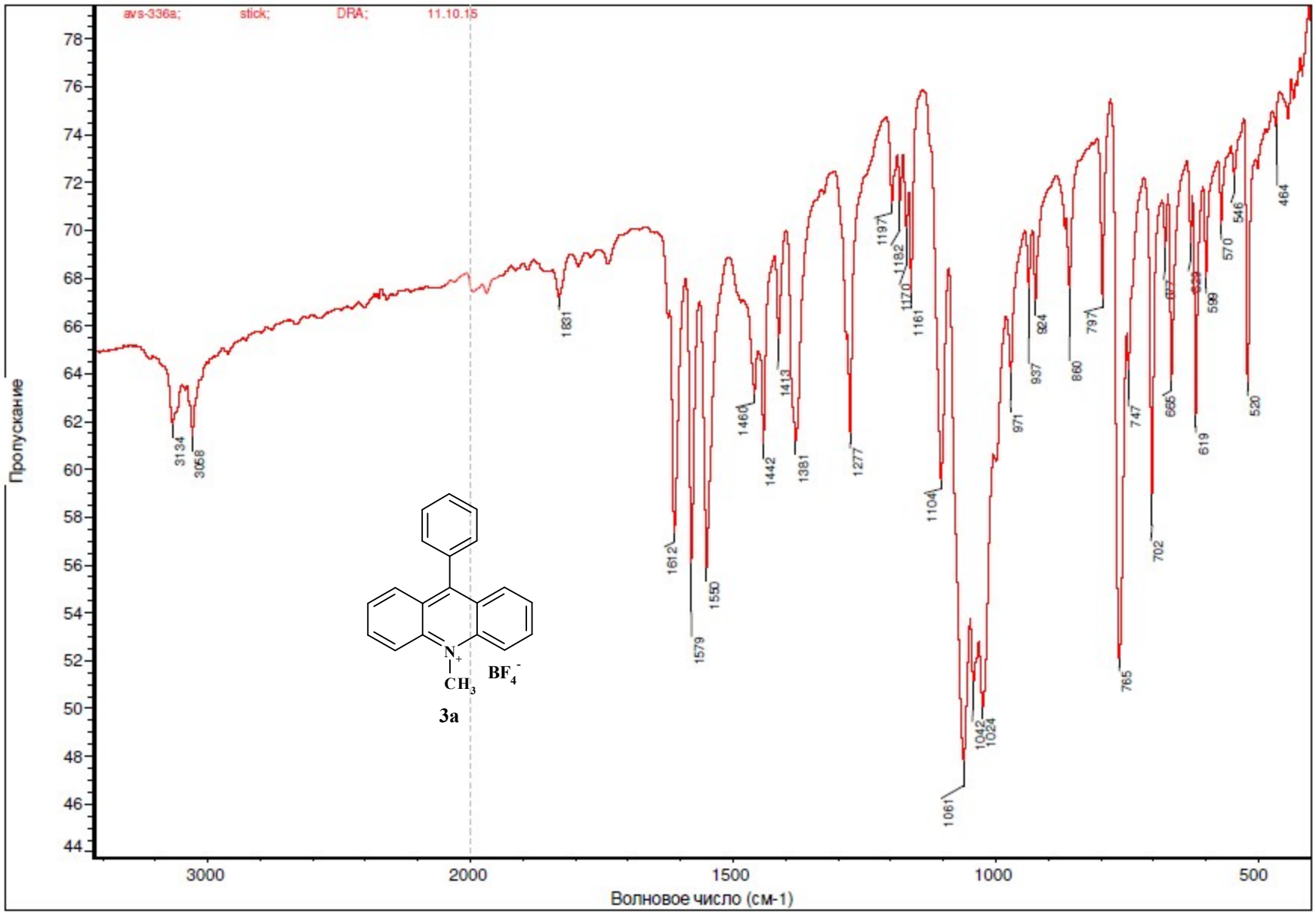

AVS639
ema: A*13981
8.07 8.07 8.06 8.05 8.05 8.05 7.34 7.34 7.33 7.33 7.32 7.32 7.29 7.29 7.28 7.27 7.26 7.26 7.12 7.10 6.98 6.98 6.97 6.97 6.95 6.95
5.52
3.38 3.33
2.50
A (d)
7.11
NO2
N
CH3
2q
1.98 4.01 2.04 2.02 2.00 1.00 3.00
ppm


AVS639
ema: A*13983
152.86
145.92
141.91
128.54
127.94
127.82
124.96
123.69
120.83
112.97
46.94
40.00
39.83
39.67
39.50
39.33
39.17
32.91
NO2
N
CH3
2q
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

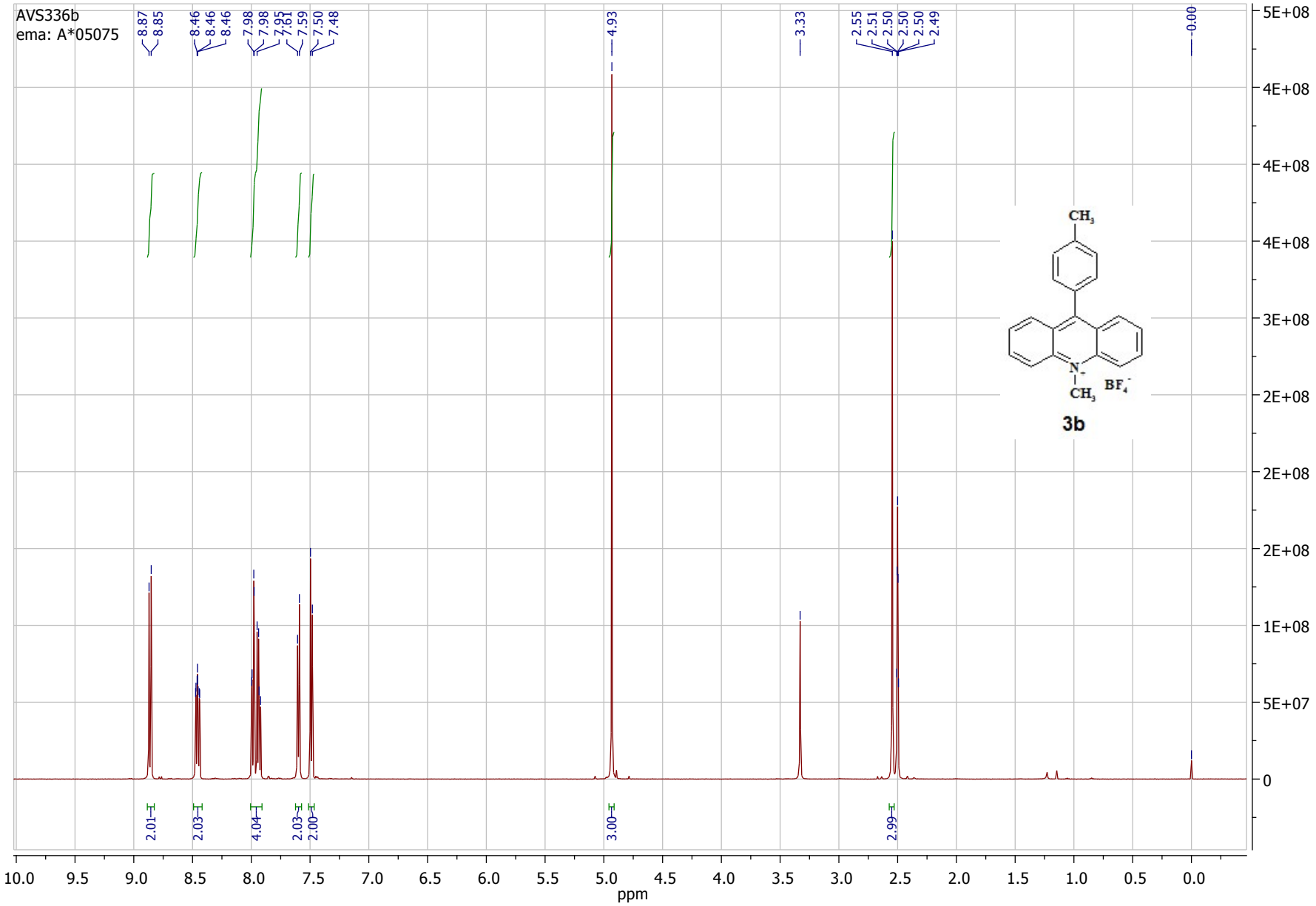

AVS-633; stick; DRA; 18.02.16
Пропускание
Волновое число (см-1)
3000
2000
1500
1000
500
3102
3072
3040
2974
2894
2830
1931
1796
1591
1519
1505
1474
1431
1339
1318
1285
1269
1169
1149
1131
1108
1063
1043
1013
938
896
863
854
846
819
757
742
711
693
660
642
617
507
493
NO2
N
CH3
2q

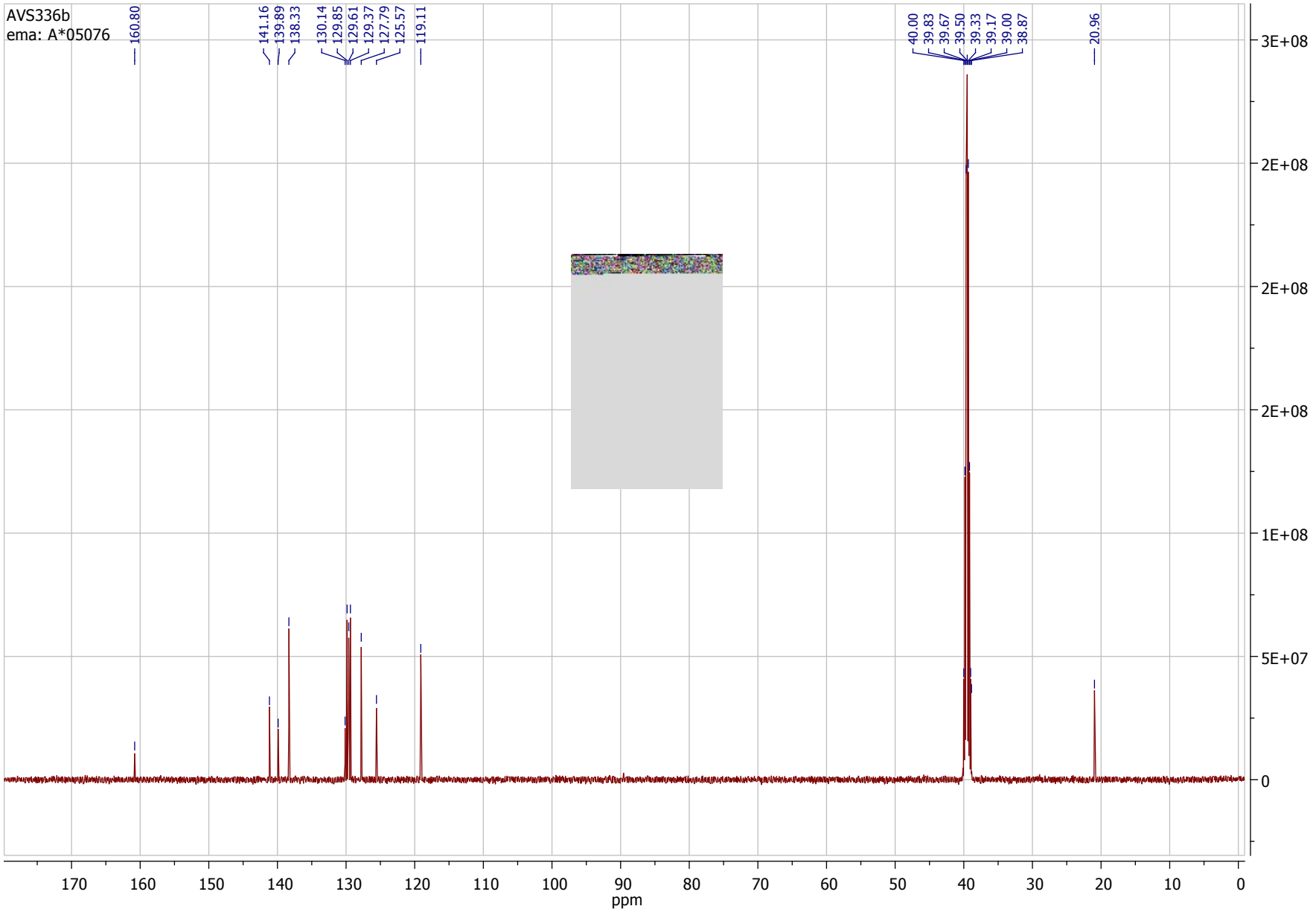

AVS336a
ema: A*05070
8.89
8.87
8.48
8.47
8.47
8.46
7.95
7.94
7.80
7.79
7.79
7.78
7.78
7.60
7.59
7.59
4.95
3.33
2.51
2.50
2.50
2.50
2.49
0.00
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
2.01
2.07
4.06
3.02
2.03
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
N
CH3
BF4
3a

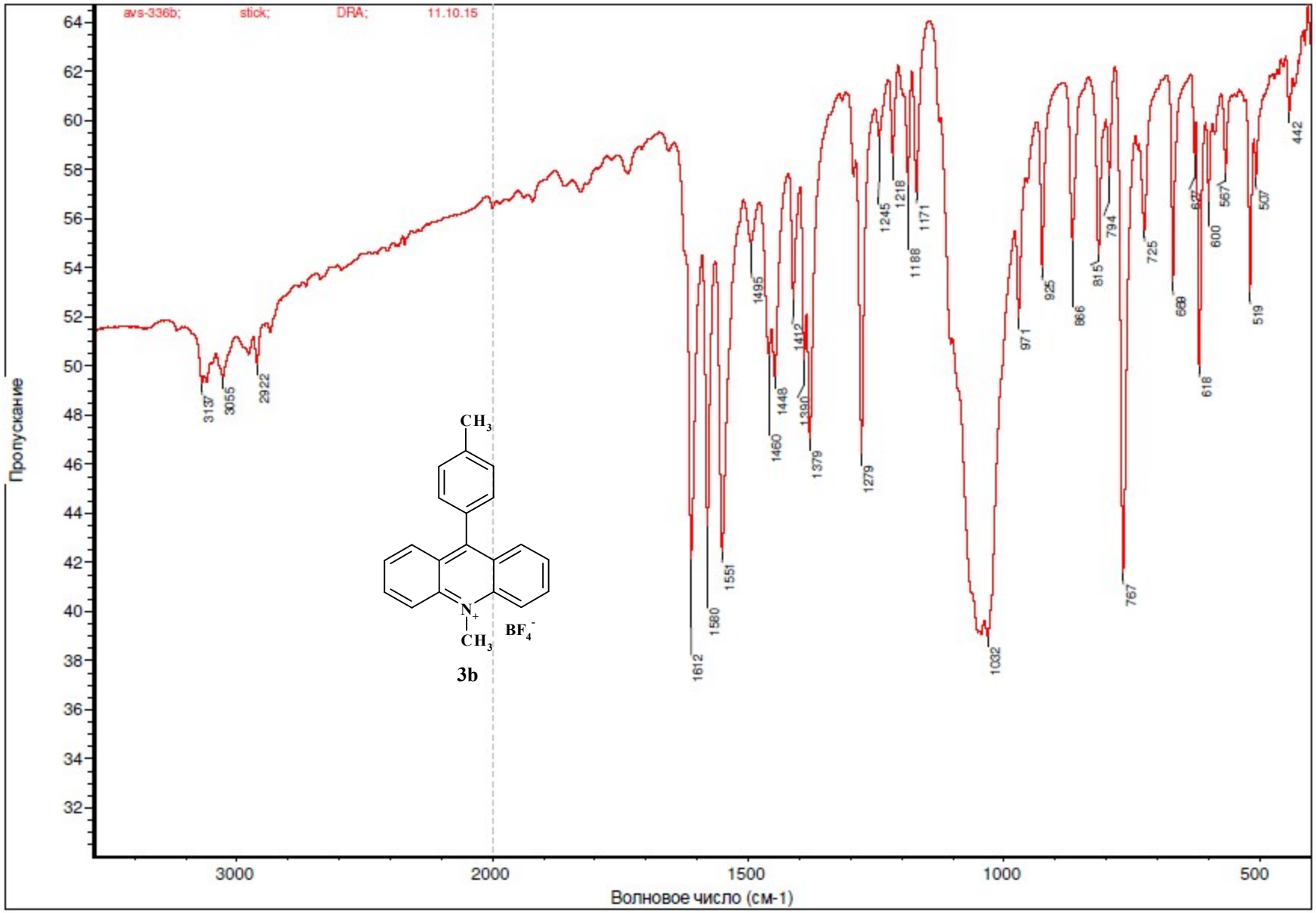

AVS336a
ema: A*05071
160.43
141.19
138.39
133.08
130.09
129.77
129.50
128.82
127.89
125.50
119.15
40.00
39.83
39.67
39.50
39.33
39.17
39.00
38.93
3a
ppm


avs-336a; stick; DRA; 11.10.15
Пропускание
Волновое число (см-1)
3134
3058
1631
1612
1579
1550
1460
1442
1413
1381
1277
1197
1182
1170
1161
1104
1061
1042
1024
971
937
924
860
797
765
747
702
665
627
619
599
570
546
520
464
3000
2000
1500
1000
500
78
76
74
72
70
68
66
64
62
60
58
56
54
52
50
48
46
44
CH3
BF4-

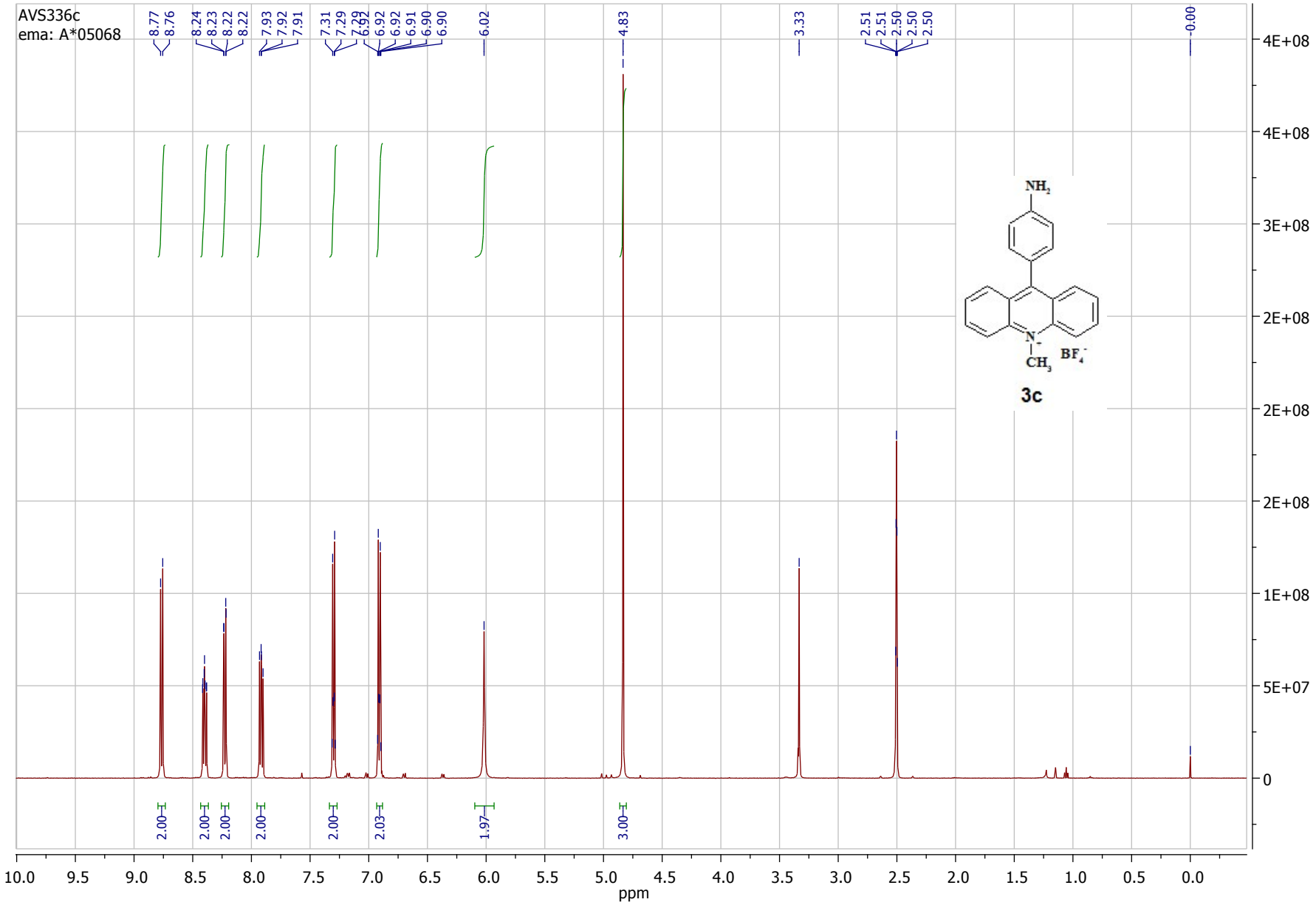
3a

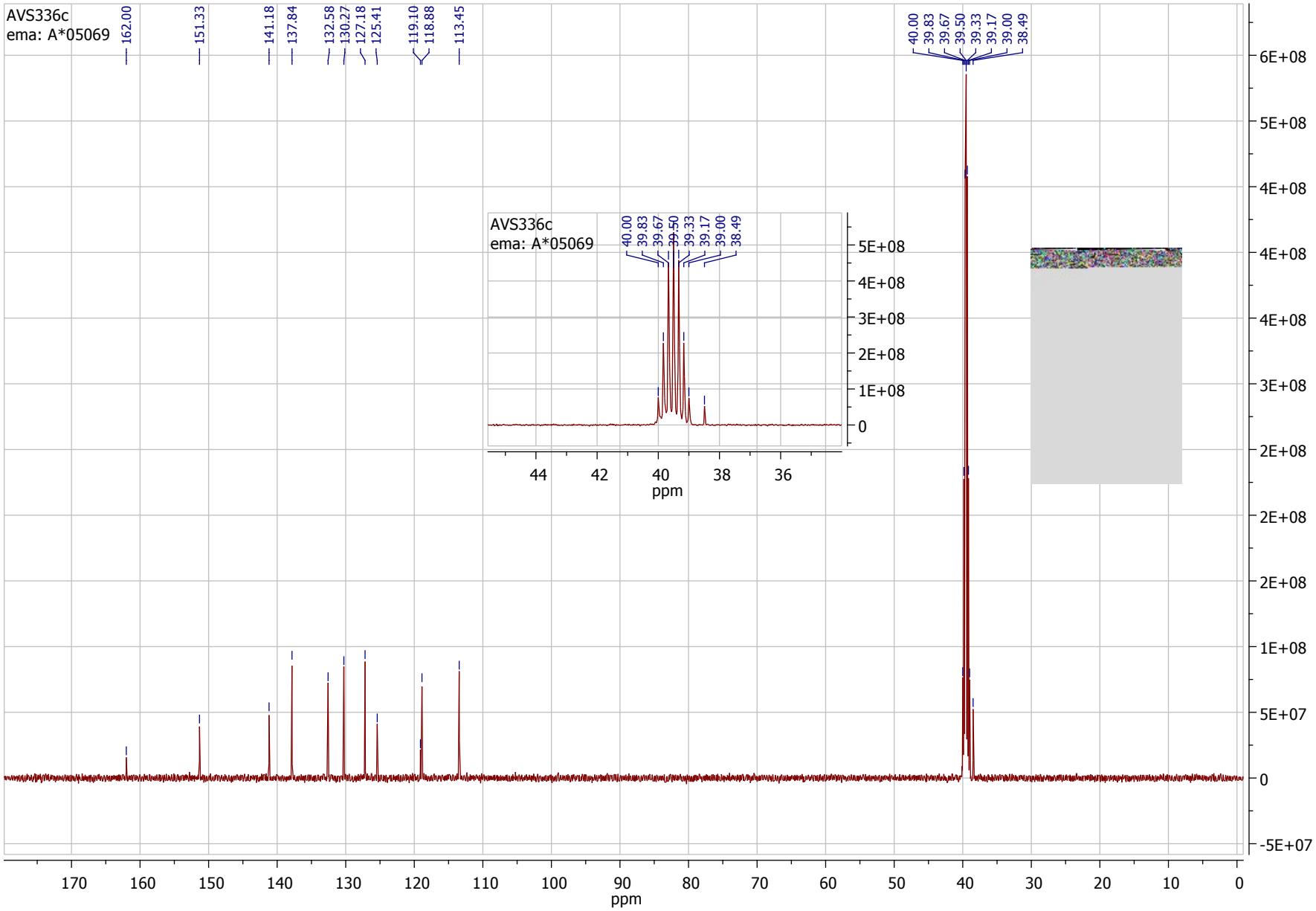

AVS336b
ema: A*05075
8.87
8.85
8.46
8.46
8.46
7.98
7.98
7.95
7.81
7.59
7.50
7.48
4.93
3.33
2.55
2.51
2.50
2.50
2.50
2.49
0.00
2.01
2.03
4.04
2.03
2.00
3.00
2.99
ppm
CH3
N
CH3
BF4-
3b

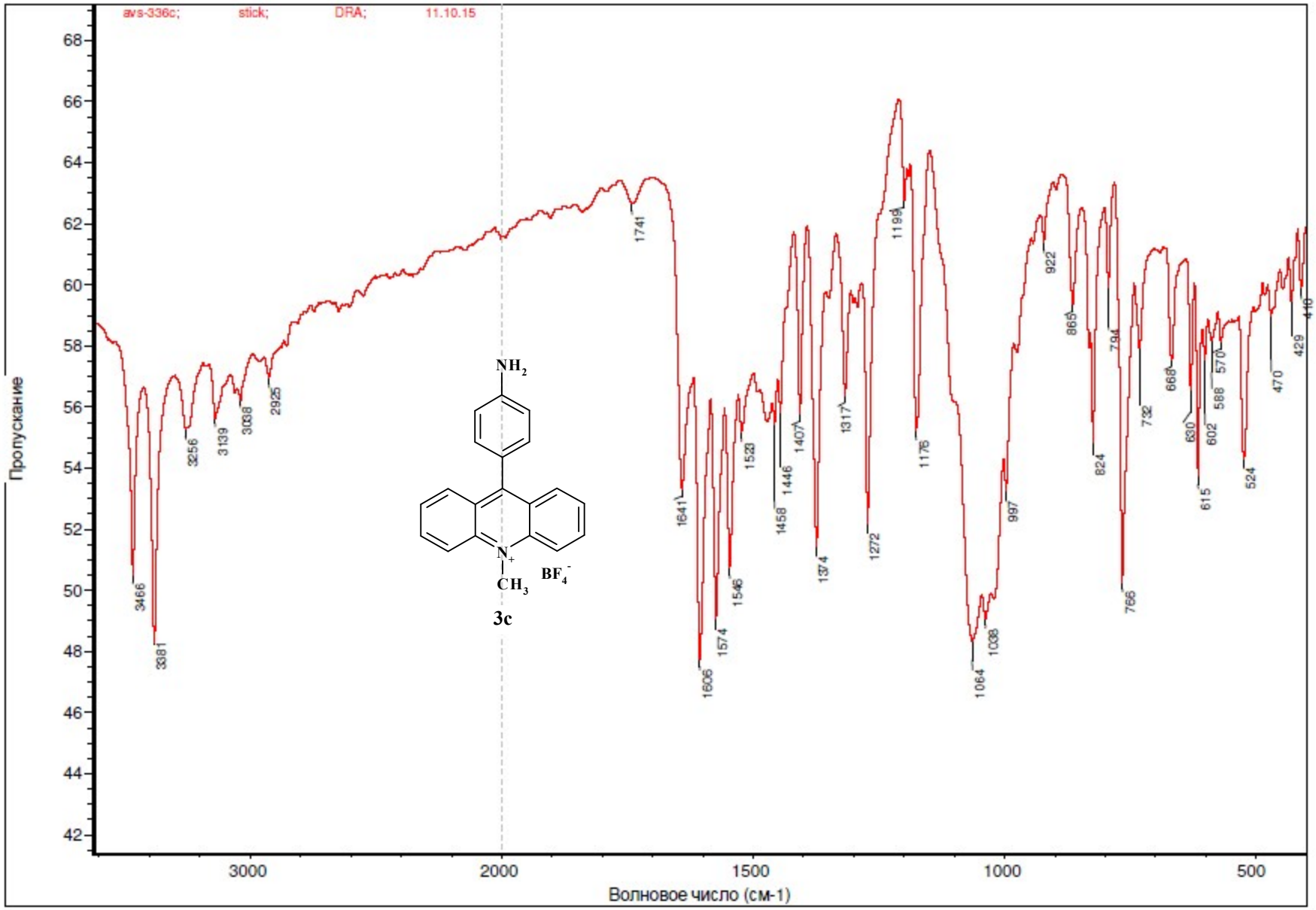

AVS336b
ema: A*05076
160.80
141.16
139.89
138.33
130.14
129.85
129.61
129.37
127.79
125.57
119.11
40.00
39.83
39.67
39.50
39.33
39.17
39.00
38.87
20.96
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


avs-336b; stick; DRA; 11.10.15
Пропускание
Волновое число (см-1)
3000
2000
1500
1000
500
64
62
60
58
56
54
52
50
48
46
44
42
40
38
36
34
32
3137
3055
2922
1612
1580
1551
1495
1460
1448
1412
1390
1379
1279
1245
1218
1188
1171
1032
971
925
866
815
794
767
725
688
637
618
600
567
537
519
442
CH3
N+
CH3
BF4-

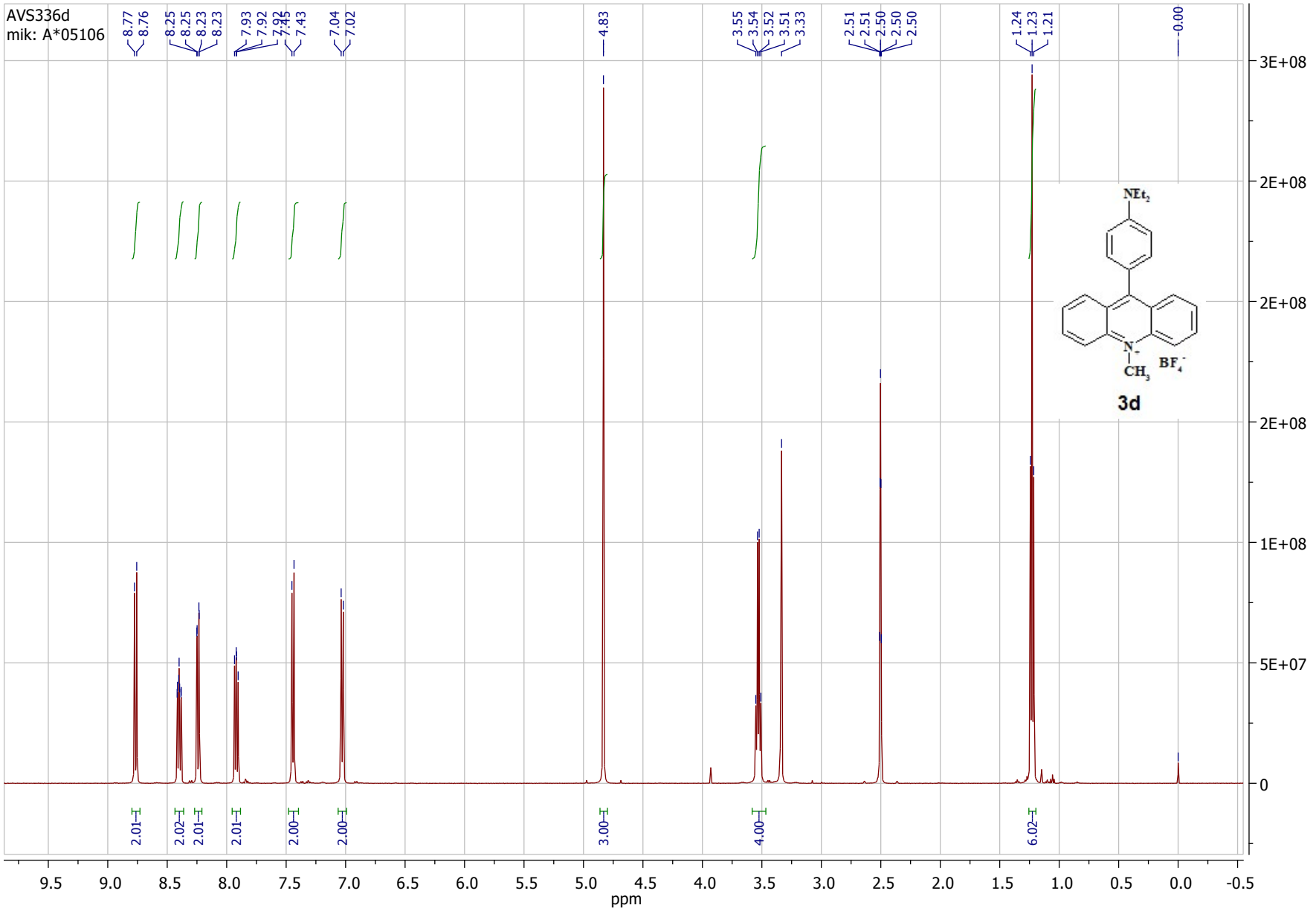
3b

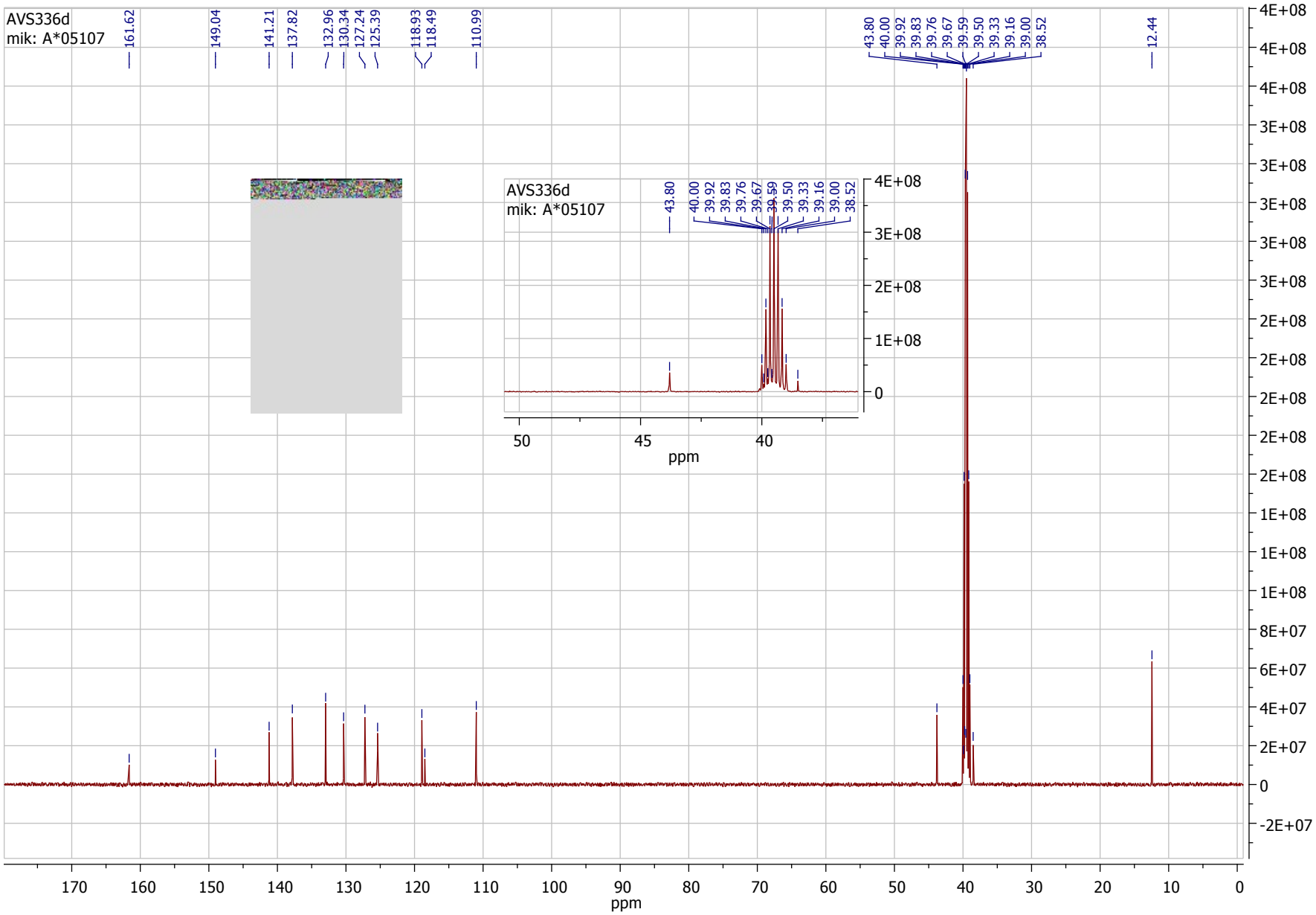

AVS336c
ema: A*05068
8.77
8.76
8.24
8.23
8.22
8.22
7.93
7.92
7.91
7.31
7.29
6.92
6.92
6.91
6.90
6.90
6.02
4.83
3.33
2.51
2.51
2.50
2.50
2.50
0.00
NH2
N
CH3
BF4-
3c
2.00
2.00
2.00
2.00
2.00
2.03
1.97
3.00
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

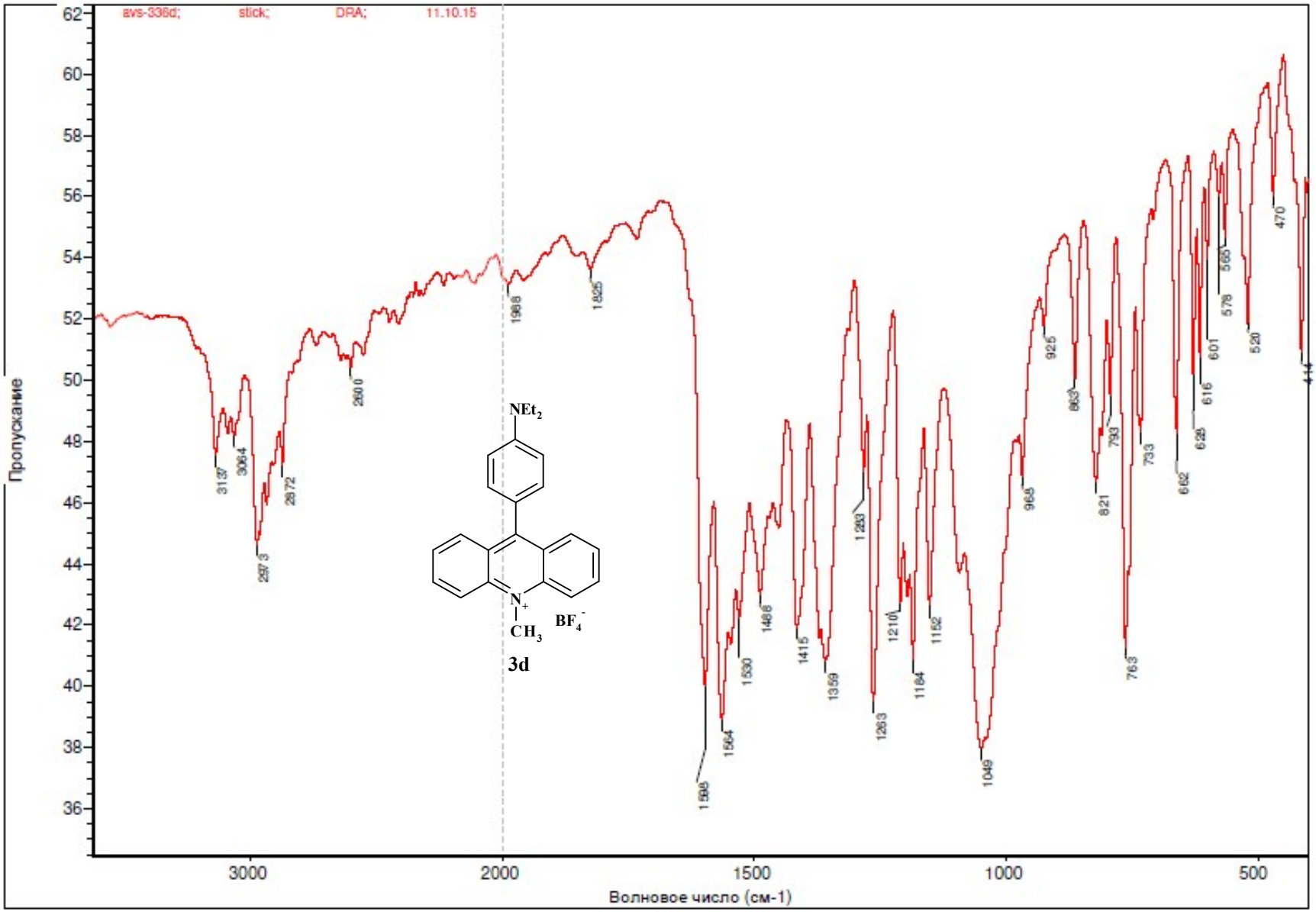

AVS336c
ema: A*05069
162.00
151.33
141.18
137.84
132.58
130.27
127.18
125.41
119.10
118.88
113.45
40.00
39.83
39.67
39.50
39.33
39.17
39.00
38.49
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm
AVS336c
ema: A*05069
40.00
39.83
39.67
39.50
39.33
39.17
39.00
38.49
5E+08
4E+08
3E+08
2E+08
1E+08
0
44
42
40
38
36
ppm


avs-336c; stick; DRA; 11.10.15
Пропускание
Волновое число (см-1)
3000
2000
1500
1000
500
68
66
64
62
60
58
56
54
52
50
48
46
44
42
3466
3381
3256
3139
3038
2925
1741
1641
1606
1574
1546
1528
1458
1446
1407
1374
1317
1272
1199
1176
1064
1038
997
922
865
824
794
766
732
668
630
615
602
588
570
524
470
429
416
NH2
N+
CH3
BF4-

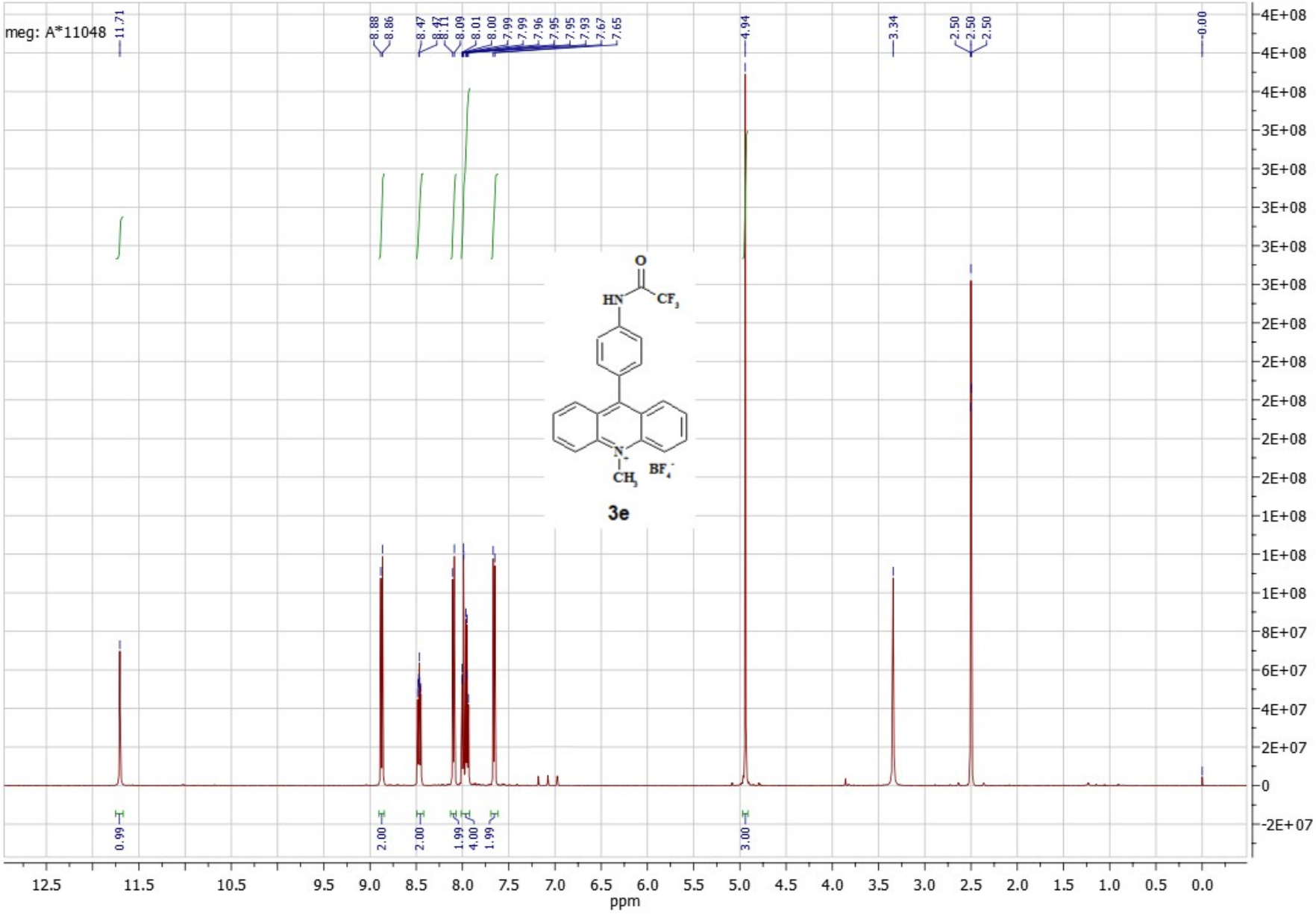
3c

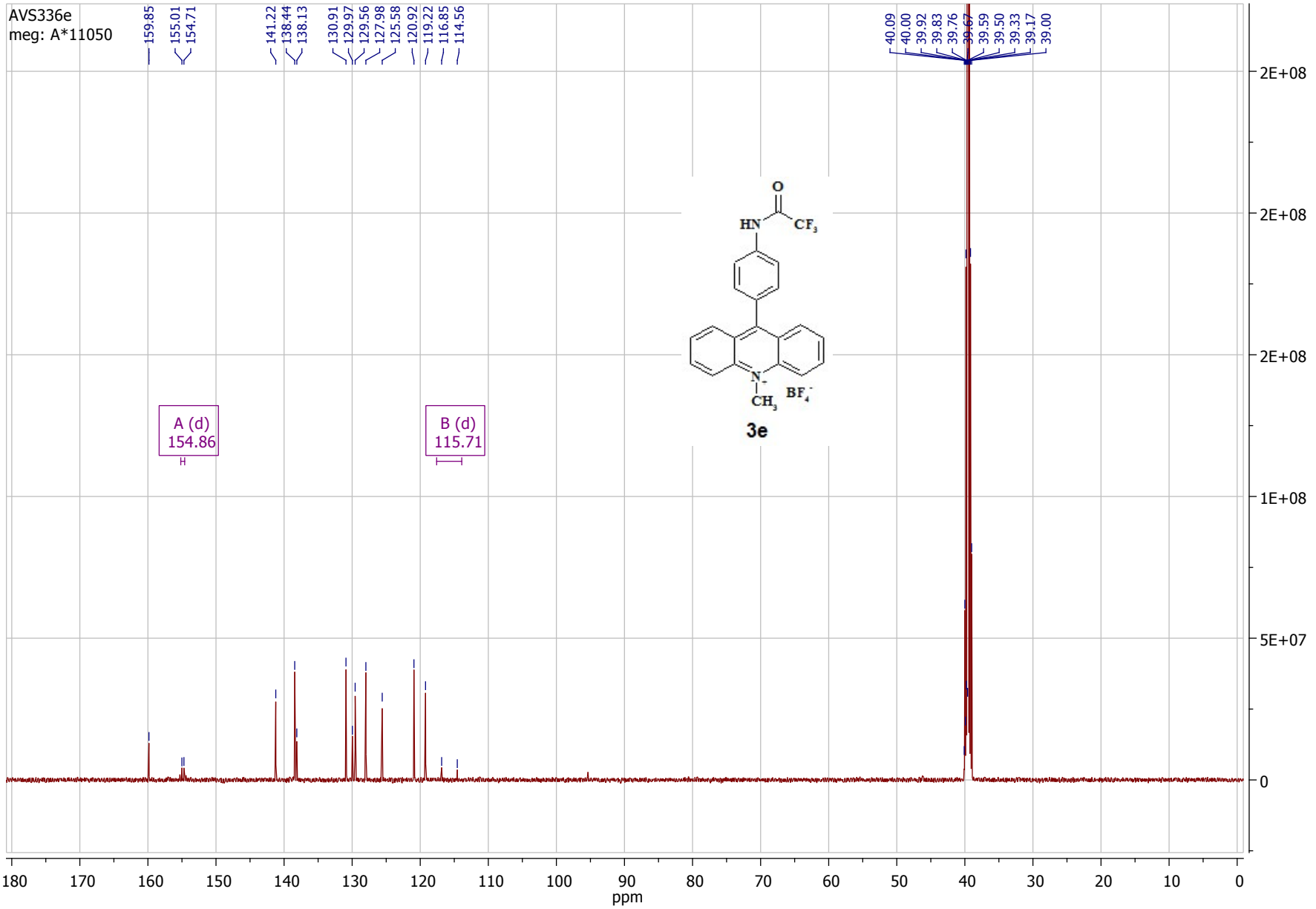

AVS336d
mik: A*05106
8.77
8.76
8.25
8.25
8.23
8.23
7.93
7.92
7.45
7.43
7.04
7.02
4.83
3.55
3.54
3.52
3.51
3.33
2.51
2.51
2.50
2.50
2.50
1.24
1.23
1.21
0.00
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
2.01
2.02
2.01
2.01
2.00
2.00
3.00
4.00
6.02
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm
NEt2
N
CH3
BF4
3d

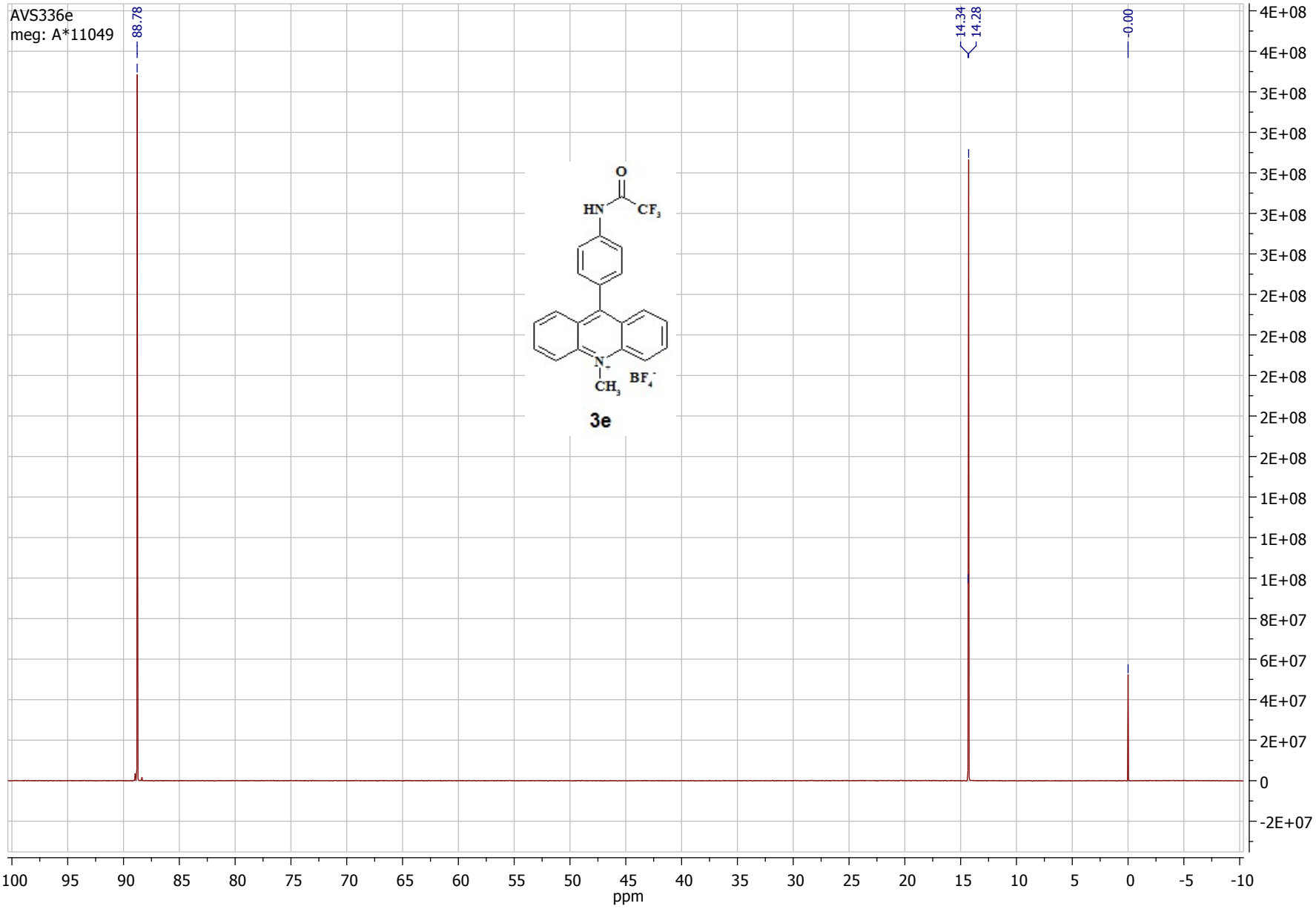

AVS336d
mik: A*05107
161.62
149.04
141.21
137.82
132.96
130.34
127.24
125.39
118.93
118.49
110.99
43.80
40.00
39.92
39.83
39.76
39.67
39.59
39.50
39.33
39.16
39.00
38.52
12.44
ppm

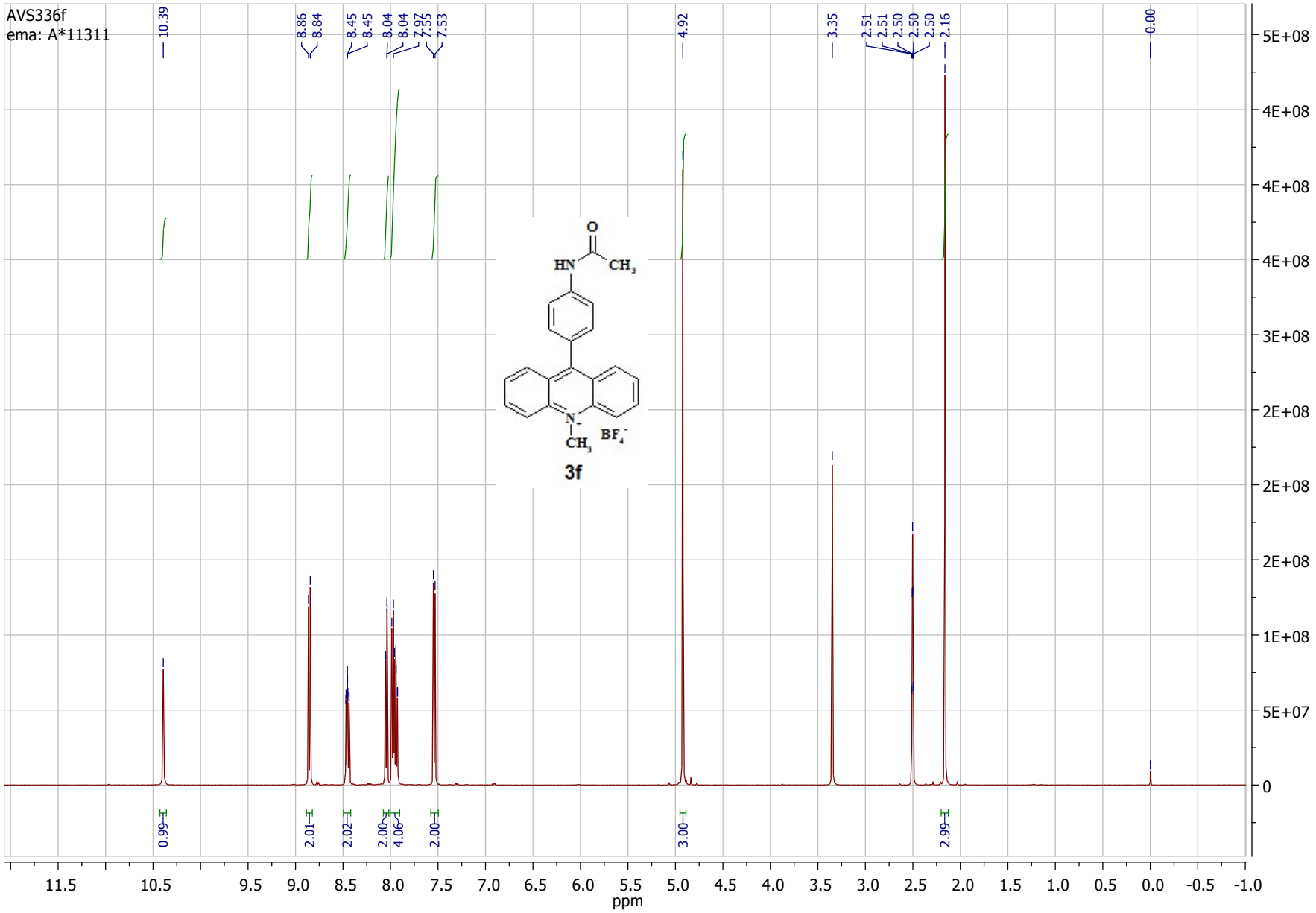

avs-338d; stick; DRA; 11.10.15
Пропускание
Волновое число (см-1)
3000
2000
1500
1000
500
62
60
58
56
54
52
50
48
46
44
42
40
38
36
3137
3064
2972
2872
2600
1988
1925
1598
1564
1530
1468
1415
1359
1293
1263
1210
1184
1152
1049
964
925
863
821
793
763
733
662
625
616
601
578
565
520
470
414
NEt2
N+
CH3
BF4-

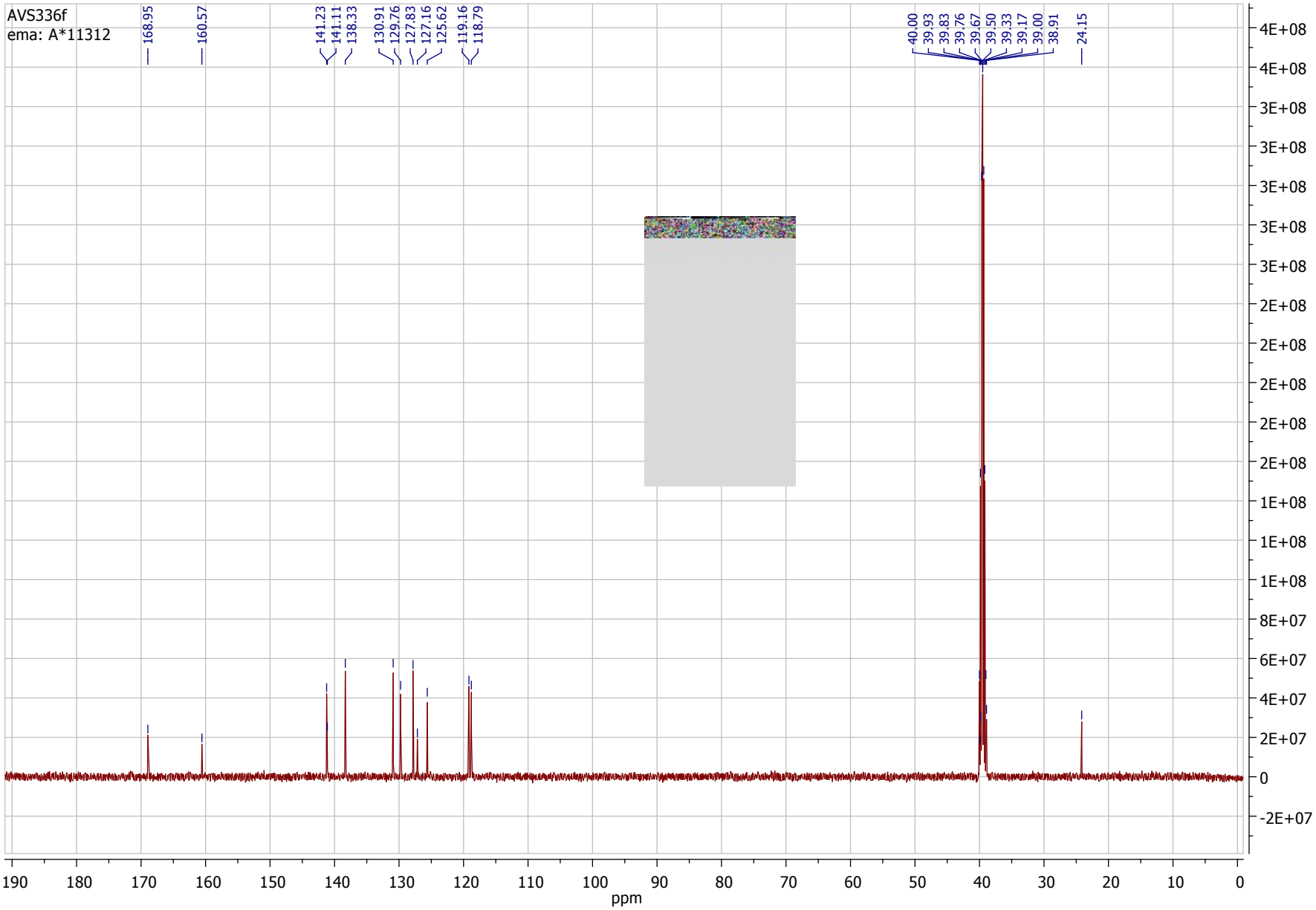
3d

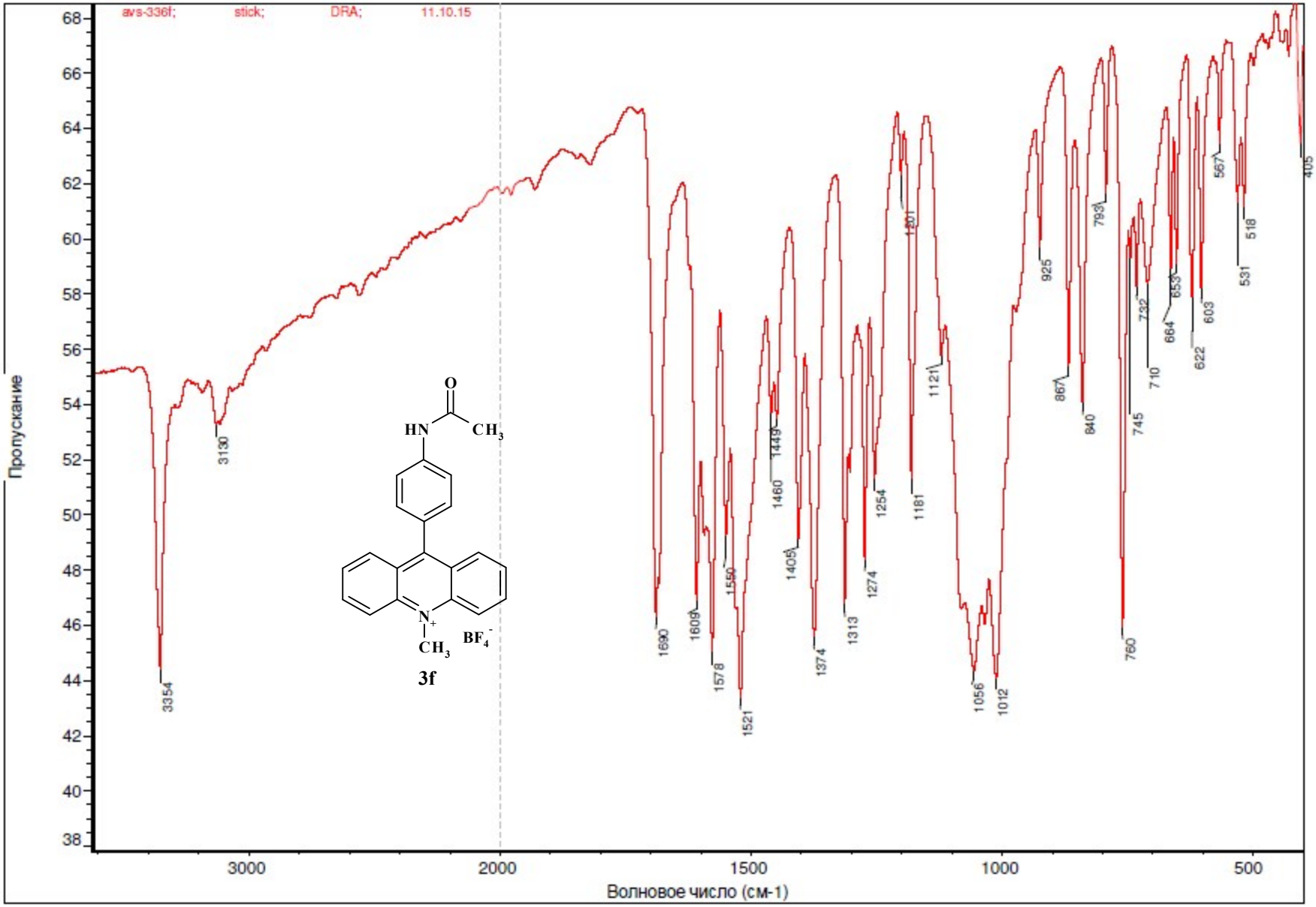

meg: A*11048
11.71
8.88
8.86
8.47
8.41
8.09
8.01
8.00
7.99
7.99
7.96
7.95
7.95
7.93
7.67
7.65
4.94
3.34
2.50
2.50
2.50
0.00
HN
O
CF3
N+
CH3
BF4-
3e
0.99
2.00
2.00
1.99
4.00
1.99
3.00
ppm


AVS336e
meg: A*11050
159.85
155.01
154.71
141.22
138.44
138.13
130.91
129.97
129.56
127.98
125.58
120.92
119.22
116.85
114.56
40.09
40.00
39.92
39.83
39.76
39.67
39.59
39.50
39.33
39.17
39.00
A (d)
154.86
B (d)
115.71
HN
O
CF3
N
CH3
BF4-
3e
2E+08
2E+08
2E+08
1E+08
5E+07
0
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

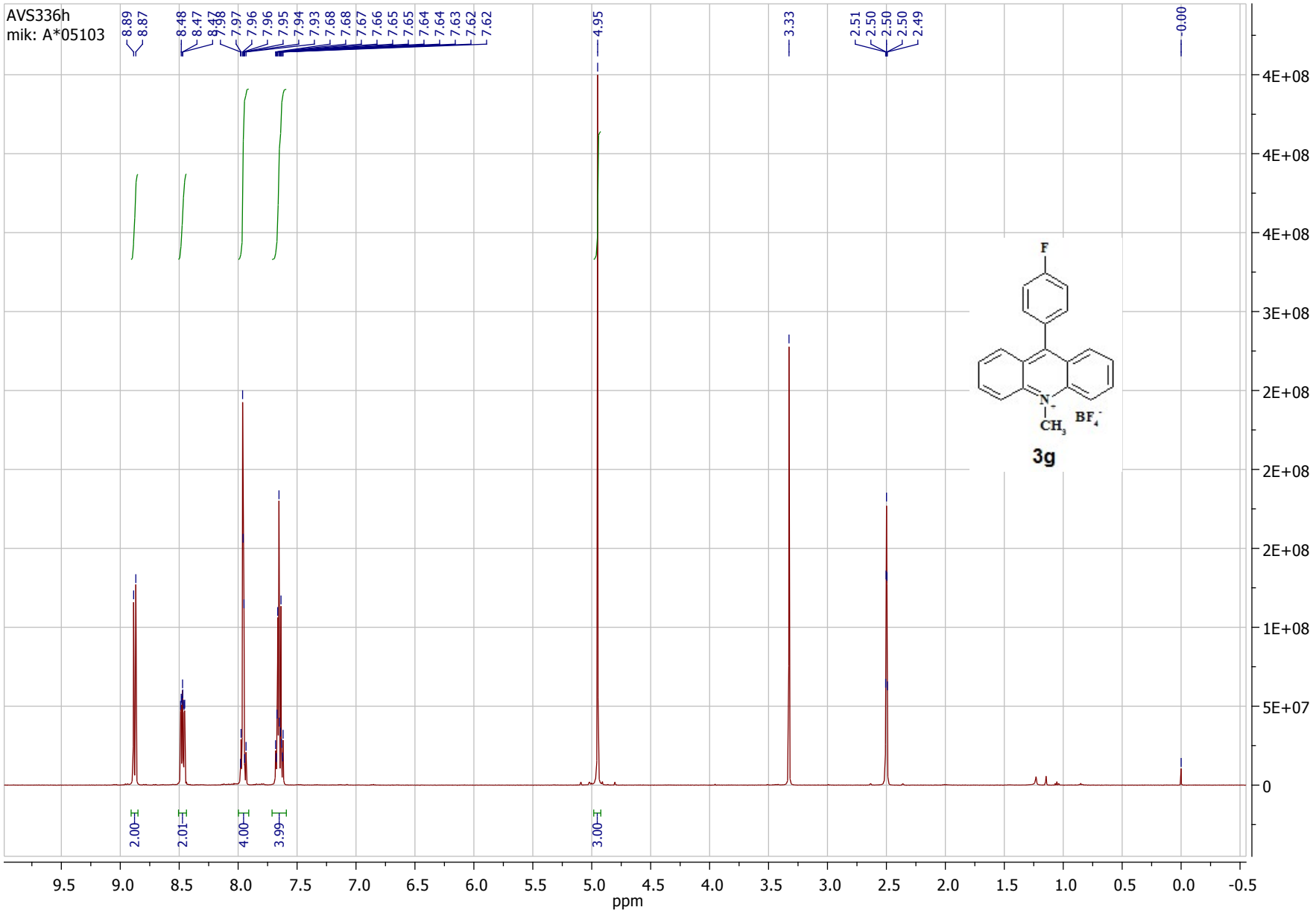

AVS336e
meg: A*11049
88.78
14.34
14.28
0.00
HN
O
CF3
N
CH3
BF4-
3e
4E+08
4E+08
3E+08
3E+08
3E+08
3E+08
3E+08
2E+08
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10
ppm

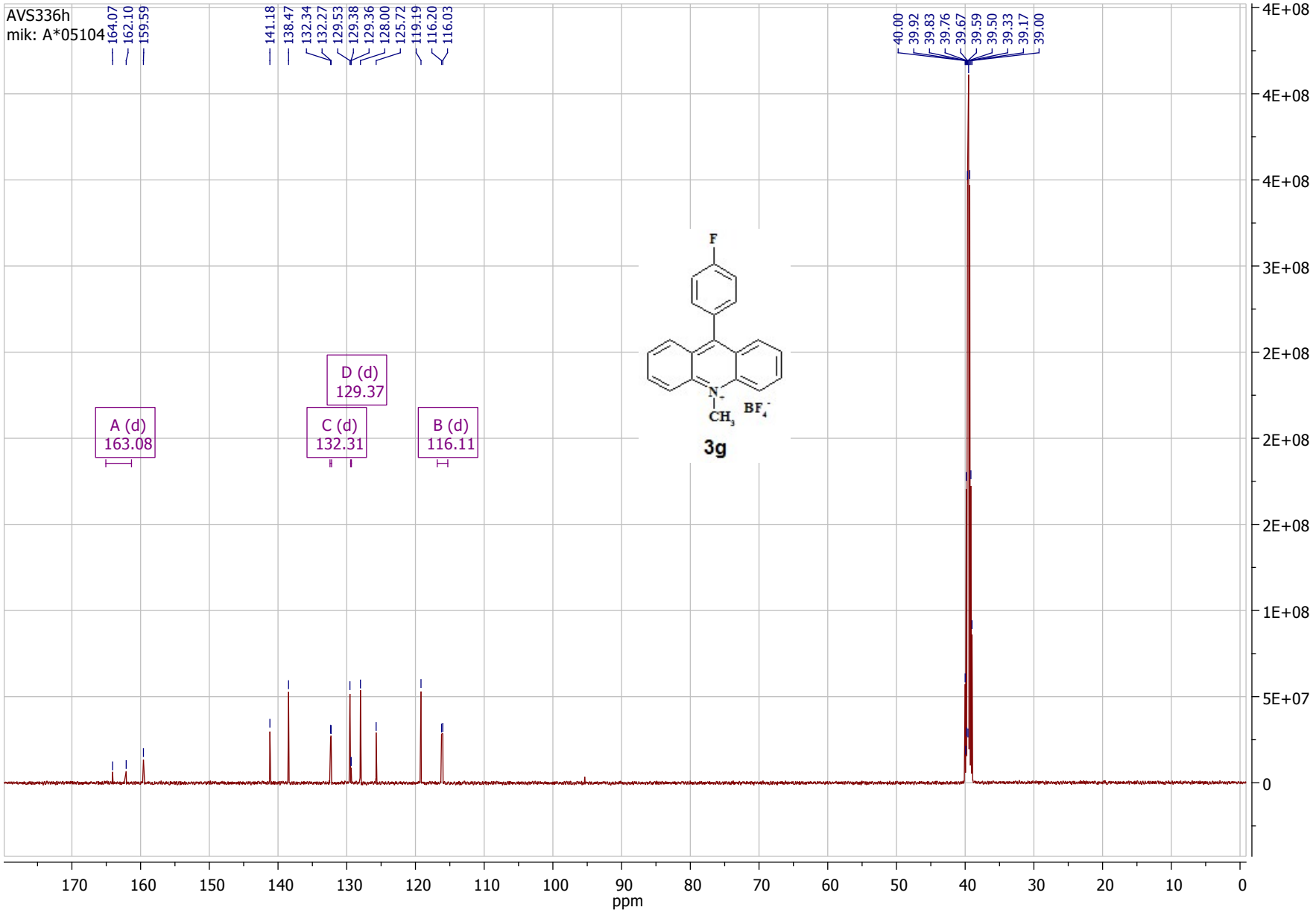

AVS336f
ema: A*11311
10.39
8.86
8.84
8.45
8.45
8.04
8.04
7.97
7.55
7.53
4.92
3.35
2.51
2.51
2.50
2.50
2.50
2.16
0.00
HN
O
CH3
N
CH3
BF4-
3f
0.99
2.01
2.02
2.00
4.06
2.00
3.00
2.99
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
ppm

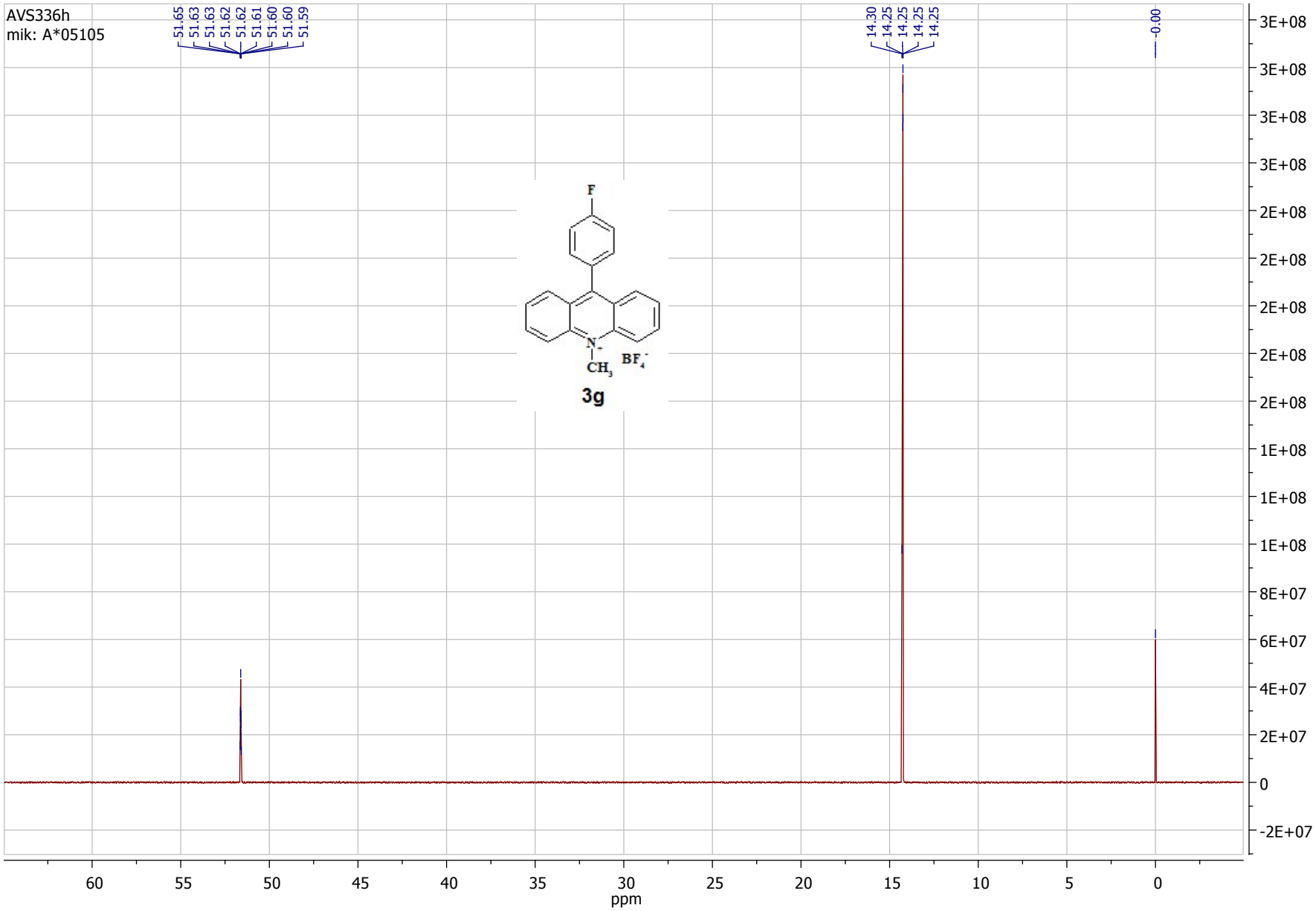

AVS336f
ema: A*11312
168.95
160.57
141.23
141.11
138.33
130.91
129.76
127.83
127.16
125.62
119.16
118.79
40.00
39.93
39.83
39.76
39.67
39.50
39.33
39.17
39.00
38.91
24.15
4E+08
4E+08
3E+08
3E+08
3E+08
3E+08
3E+08
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

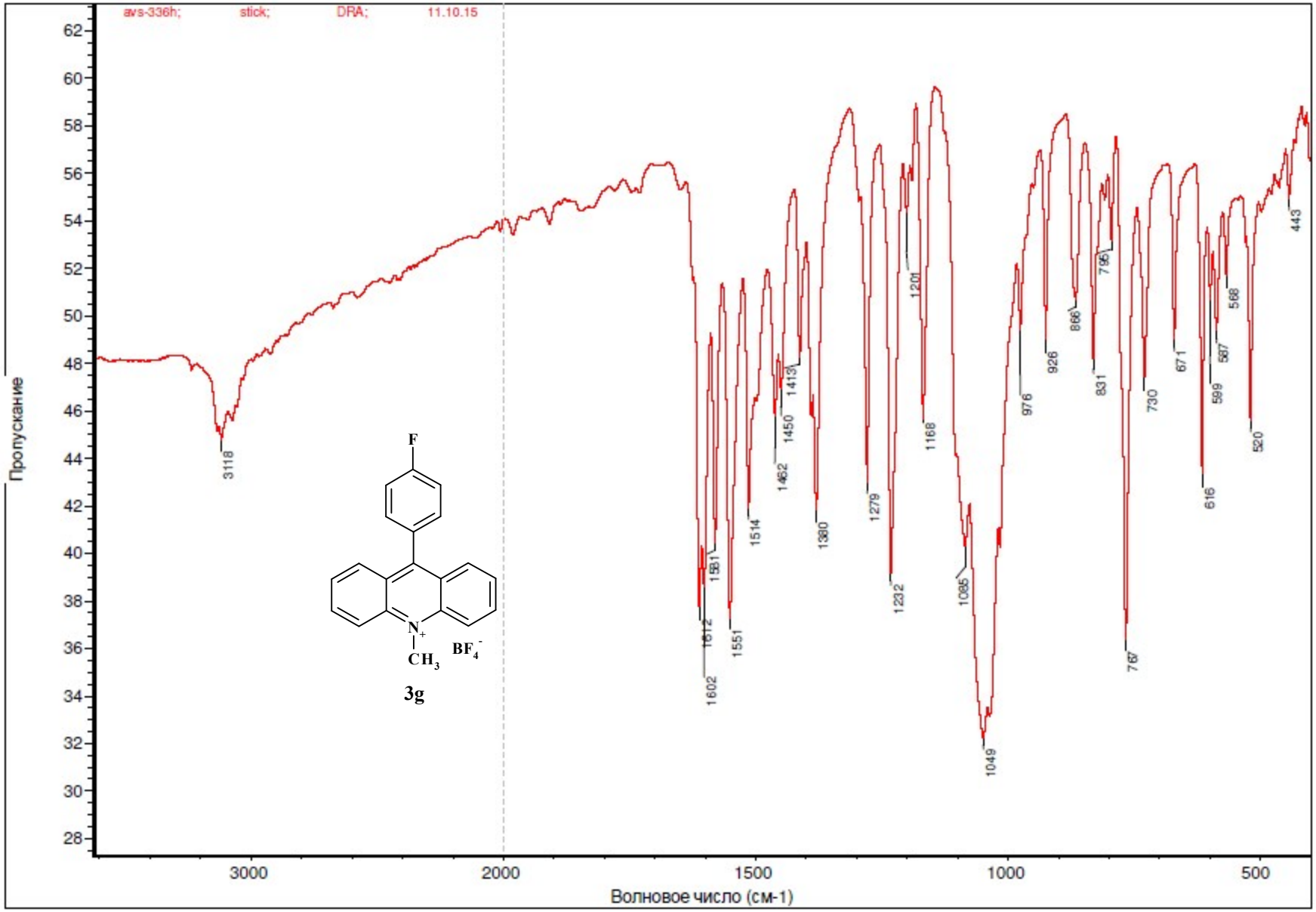

avs-336f; stick; DRA; 11.10.15
Пропускание
Волновое число (см-1)
3000
2000
1500
1000
500
3354
3130
1690
1609
1578
1550
1521
1460
1449
1405
1374
1313
1274
1254
1181
1121
1056
1012
925
867
840
793
760
745
732
710
664
653
622
603
567
531
518
405
HN
O
CH3
N+
CH3
BF4-

3f

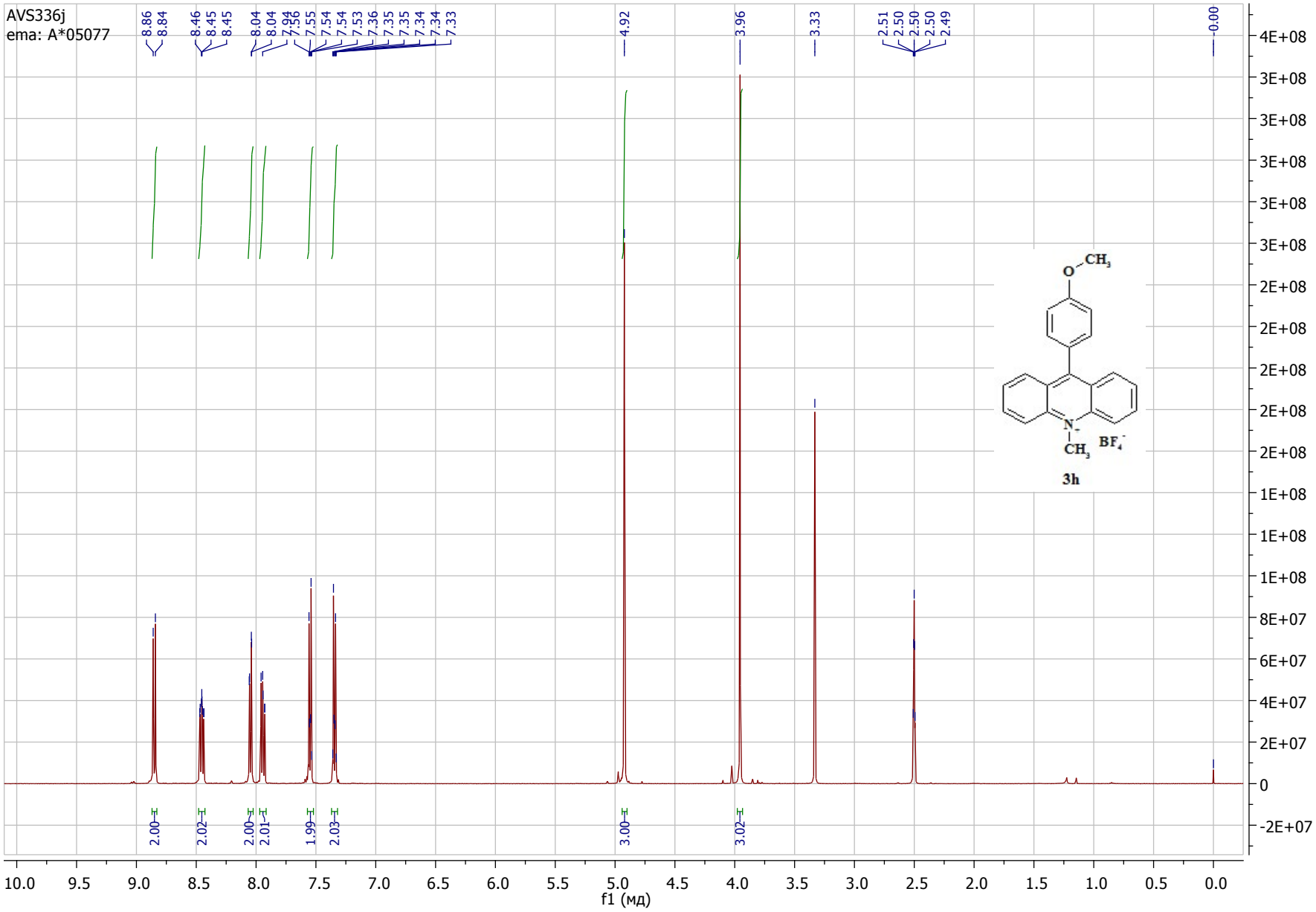

AVS336h
mik: A*05103
8.89
8.87
8.48
8.47
8.47
8.47
7.98
7.97
7.96
7.96
7.95
7.94
7.93
7.68
7.68
7.67
7.66
7.65
7.65
7.64
7.64
7.63
7.62
7.62
4.95
3.33
2.51
2.50
2.50
2.50
2.49
0.00
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
2.00
2.01
4.00
3.99
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm
F
N
CH3
BF4-
3g

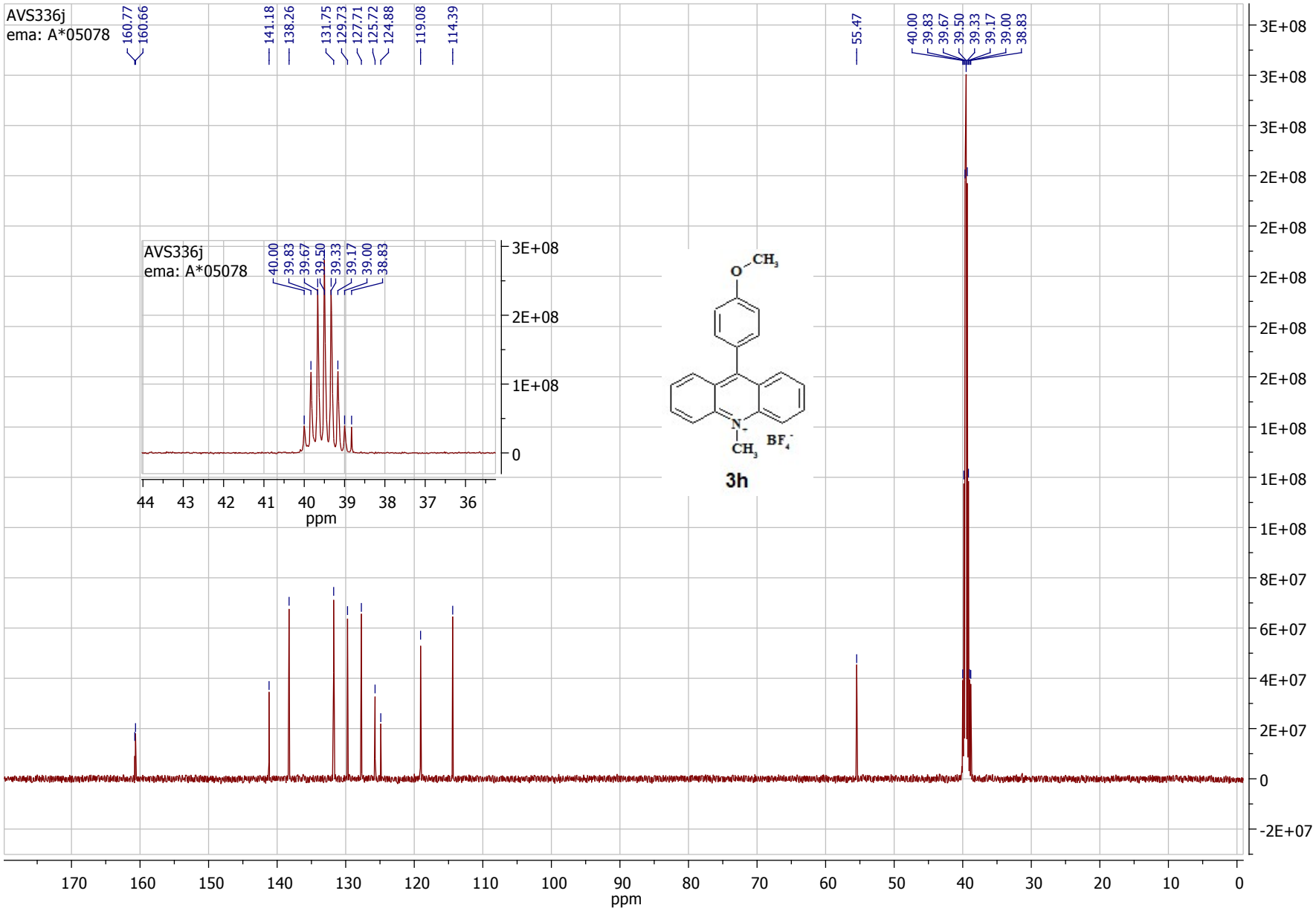

AVS336h
mik: A*05104
164.07
162.10
159.59
141.18
138.47
132.34
132.27
129.53
129.38
129.36
128.00
125.72
119.19
116.20
116.03
40.00
39.92
39.83
39.76
39.67
39.59
39.50
39.33
39.17
39.00
A (d)
163.08
C (d)
132.31
D (d)
129.37
B (d)
116.11
F
N
CH3
BF4
3g
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

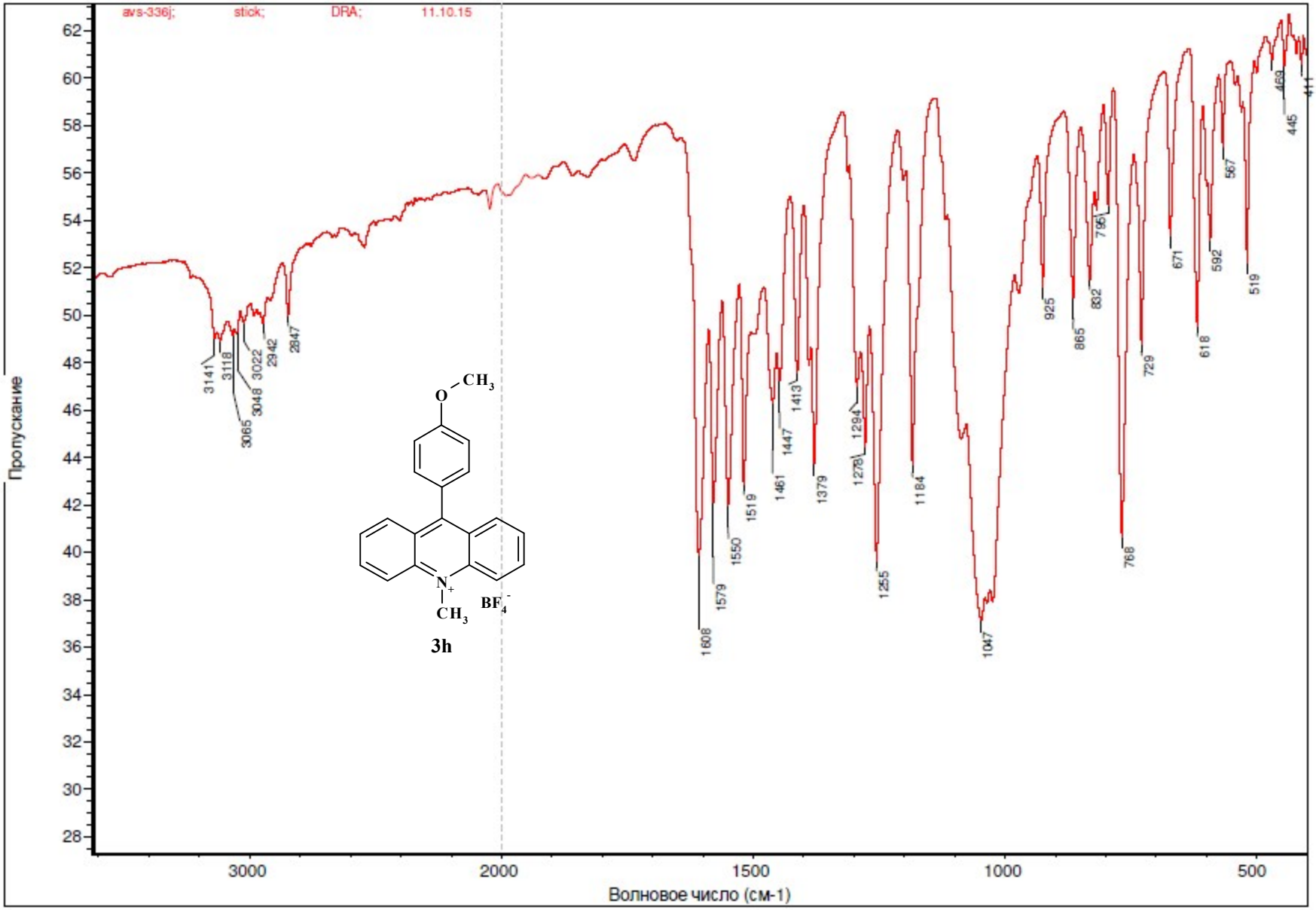

AVS336h
mik: A*05105
51.65
51.63
51.63
51.62
51.62
51.61
51.60
51.60
51.59
14.30
14.25
14.25
14.25
14.25
0.00
F
N
CH3
BF4-
3g
3E+08
3E+08
3E+08
3E+08
2E+08
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
60
55
50
45
40
35
30
25
20
15
10
5
0
ppm


avs-336h; stick; DRA; 11.10.15
Пропускание
Волновое число (см-1)
3118
1602
1581
1551
1514
1462
1450
1413
1380
1279
1232
1201
1168
1085
1049
976
926
866
831
795
767
730
671
616
599
587
568
520
443
F
N+
CH3
BF4-

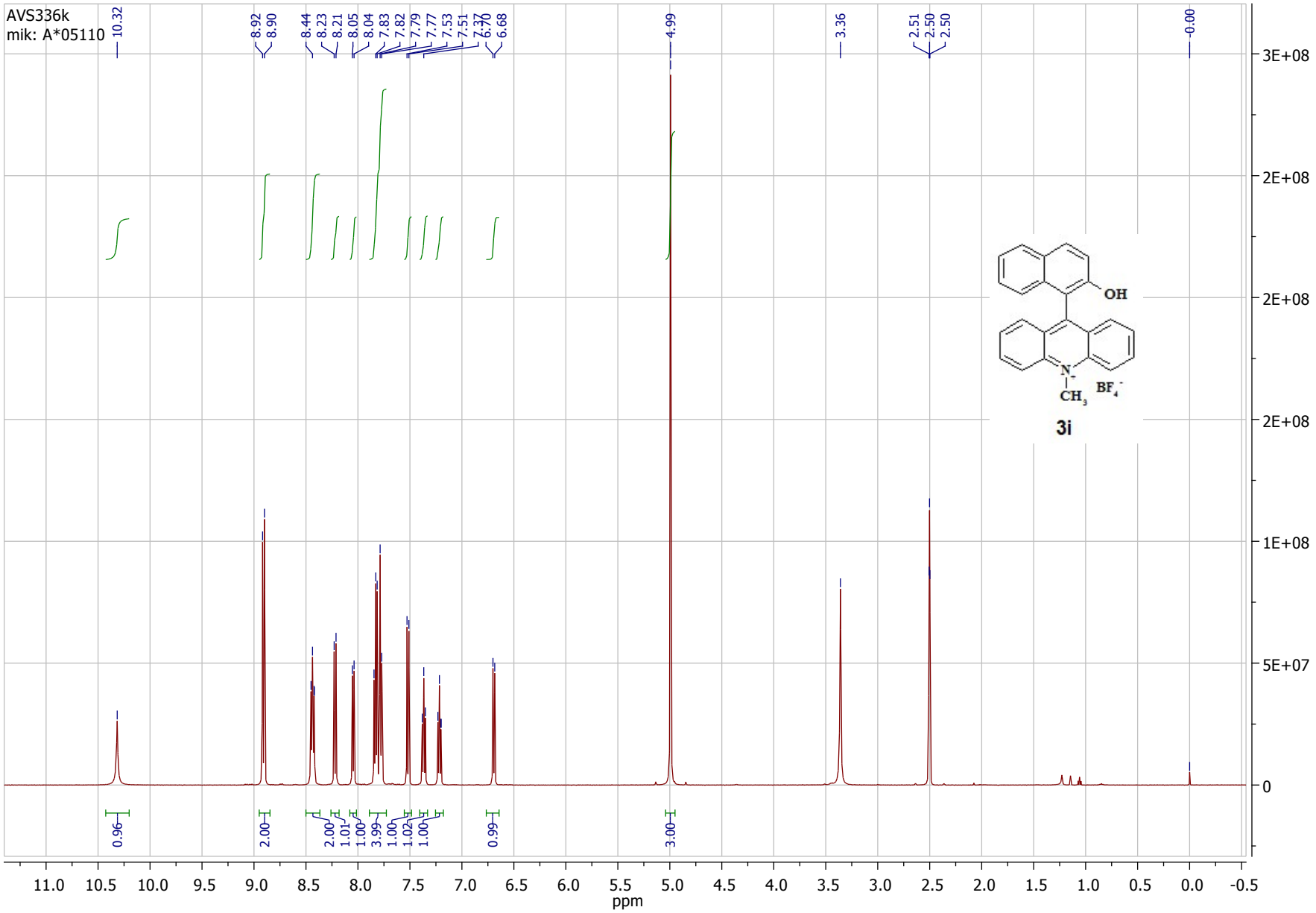
3g

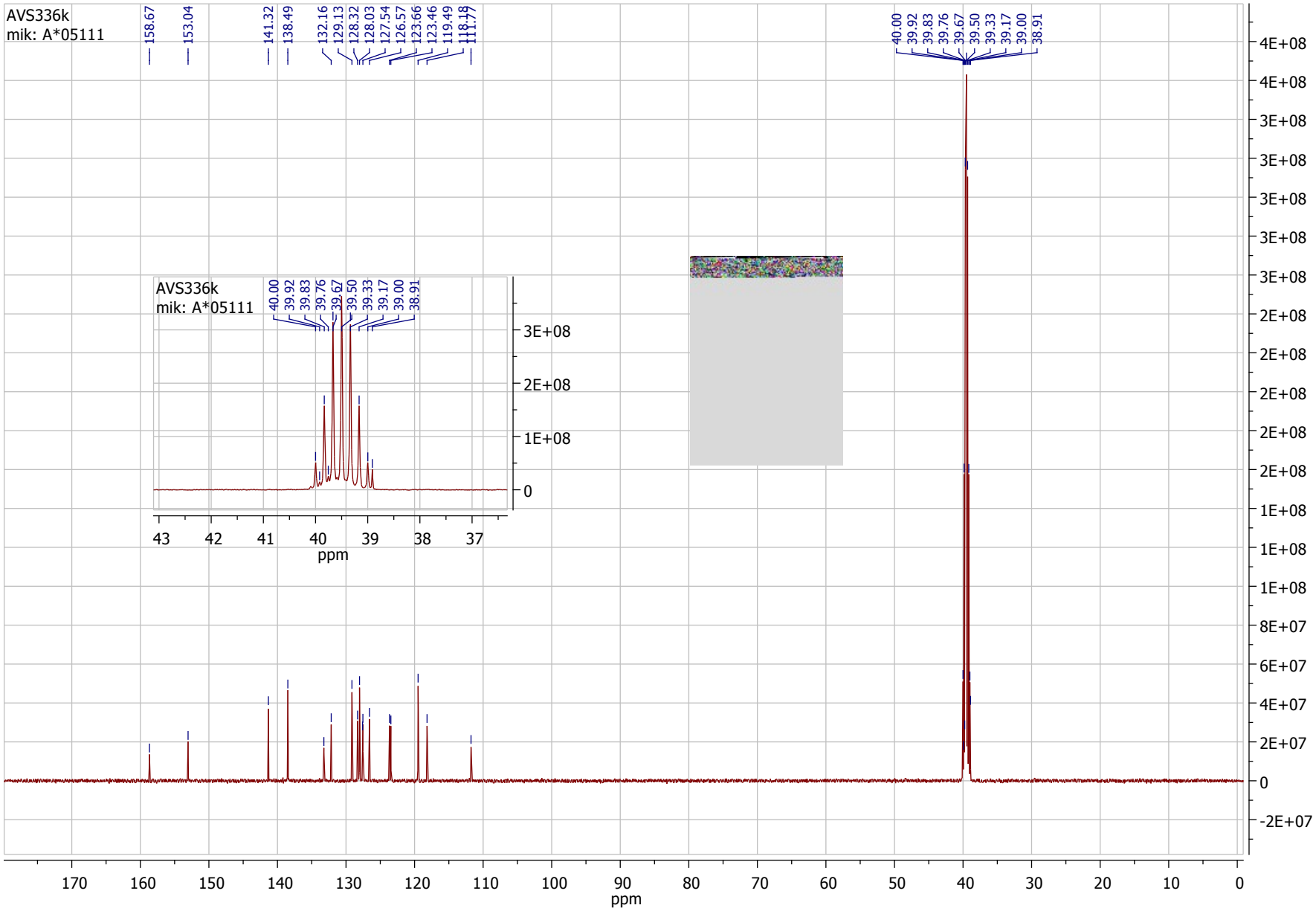

AVS336j
ema: A*05077
8.86
8.84
8.46
8.45
8.45
8.04
8.04
7.94
7.56
7.55
7.54
7.54
7.53
7.36
7.35
7.35
7.34
7.34
7.33
4.92
3.96
3.33
2.51
2.50
2.50
2.50
2.49
0.00
2.00
2.02
2.00
2.01
1.99
2.03
3.00
3.02
f1 (мд)
3h

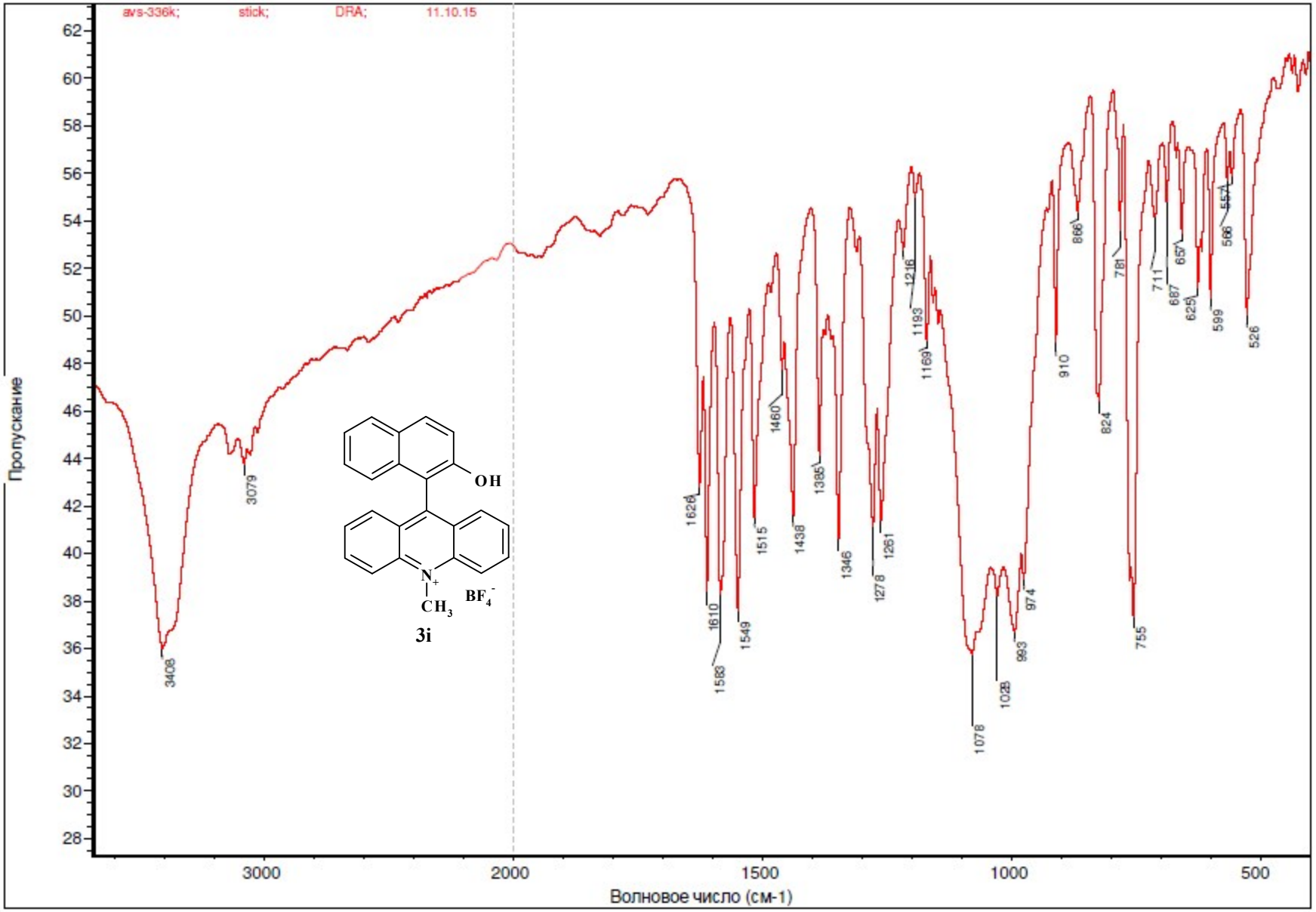

AVS336j
ema: A*05078
160.77
160.66
141.18
138.26
131.75
129.73
127.71
125.72
124.88
119.08
114.39
55.47
40.00
39.83
39.67
39.50
39.33
39.17
39.00
38.83
3E+08
2E+08
1E+08
0
-2E+07
8E+07
6E+07
4E+07
2E+07
ppm
AVS336j
ema: A*05078
44
43
42
41
40
39
38
37
36
O
CH3
N
CH3
BF4-
3h


avs-336j; stick; DRA; 11.10.15
Пропускание
Волновое число (см-1)
3000
2000
1500
1000
500
62
60
58
56
54
52
50
48
46
44
42
40
38
36
34
32
30
28
3141
3118
3065
3048
3022
2942
2847
1608
1579
1550
1519
1461
1447
1413
1379
1294
1278
1255
1184
1047
925
865
832
796
768
729
671
618
592
567
519
469
445
411
O
CH3
N+
CH3
BF4-

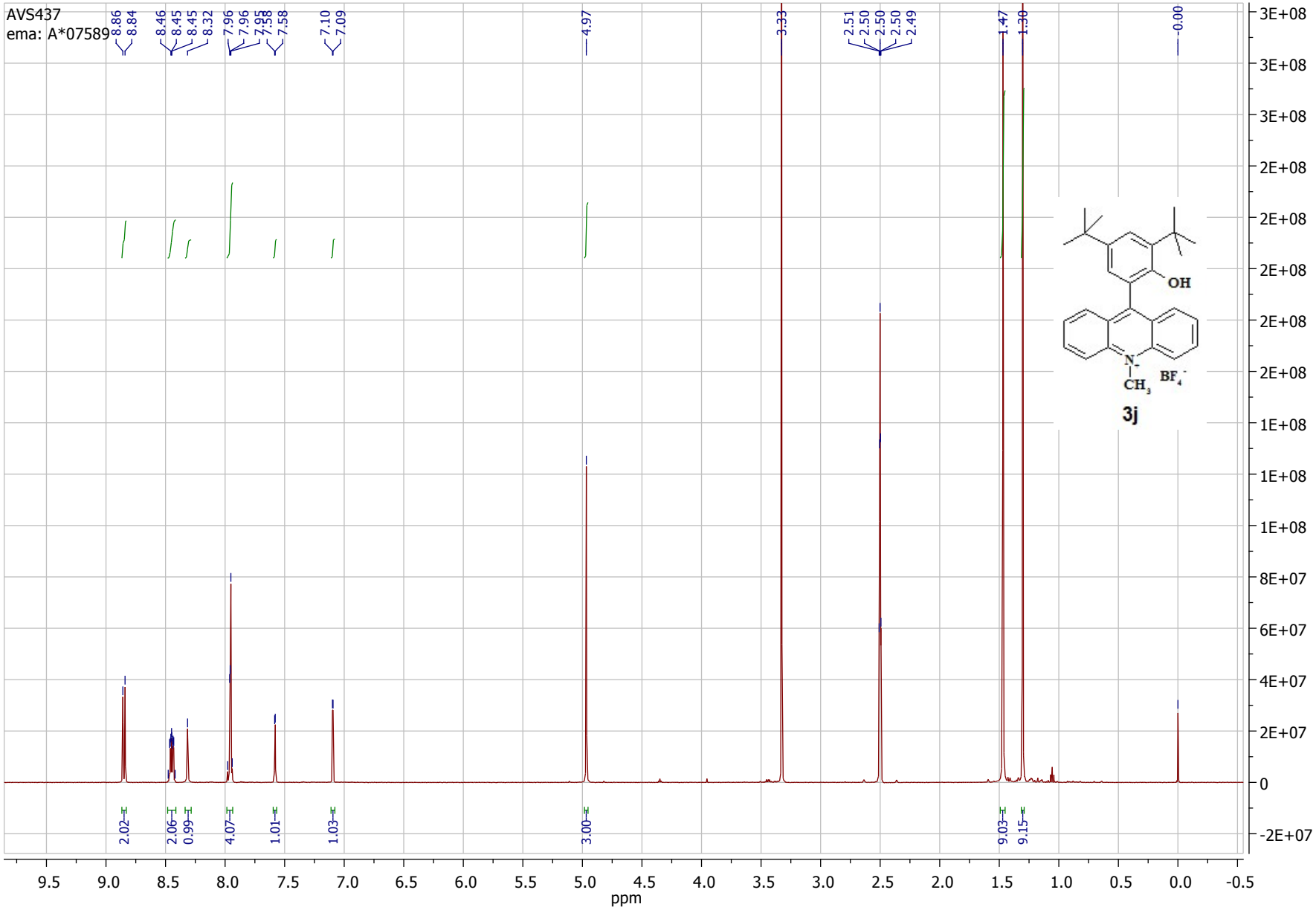
3h

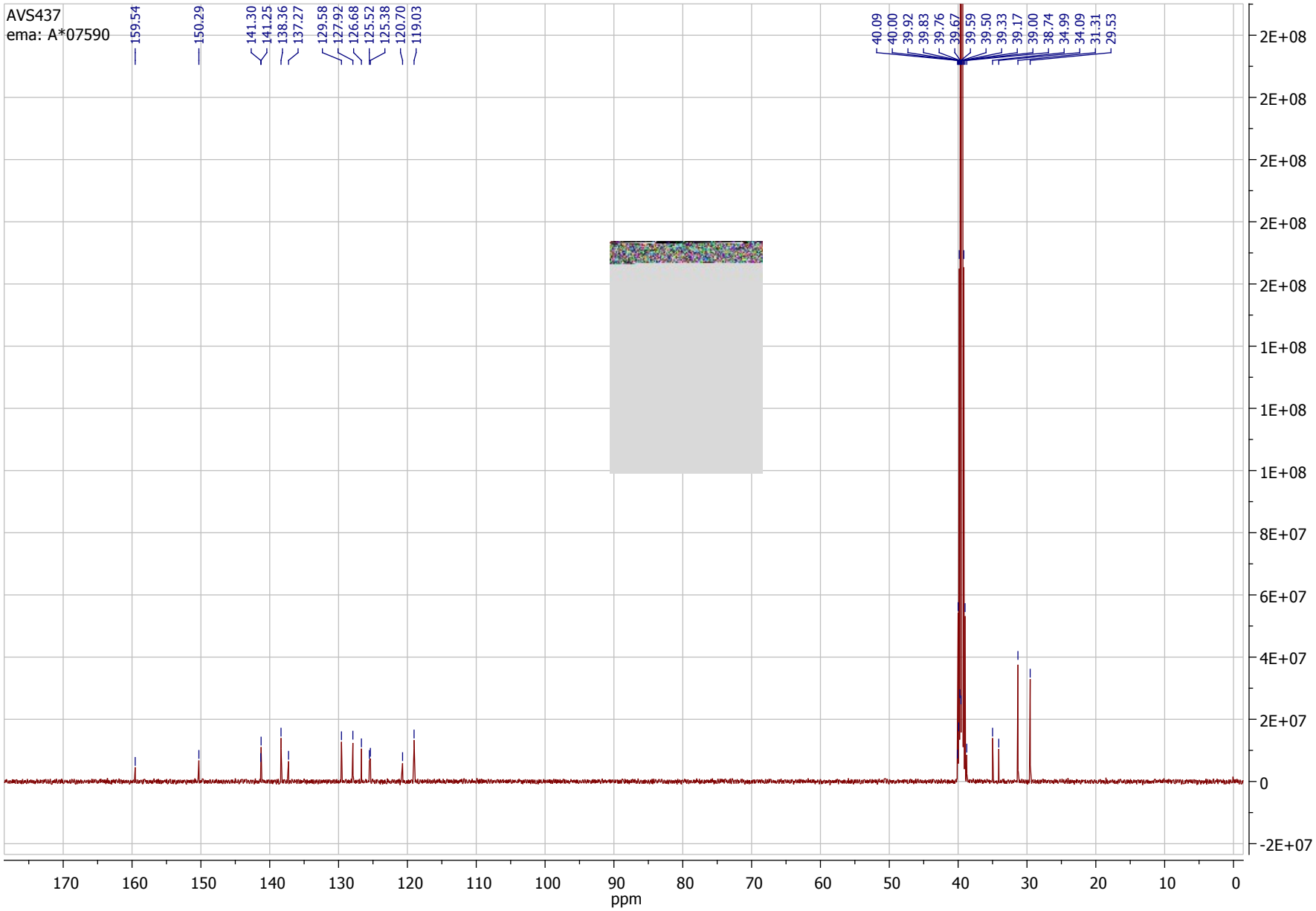

AVS336k
mik: A*05110
10.32
8.92
8.90
8.44
8.23
8.21
8.05
8.04
7.83
7.82
7.79
7.77
7.53
7.51
7.37
7.35
6.68
4.99
3.36
2.51
2.50
2.50
0.00
OH
N
CH3
BF4-
3i
0.96
2.00
2.00
1.01
1.00
3.99
1.00
1.02
1.00
0.99
3.00
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm

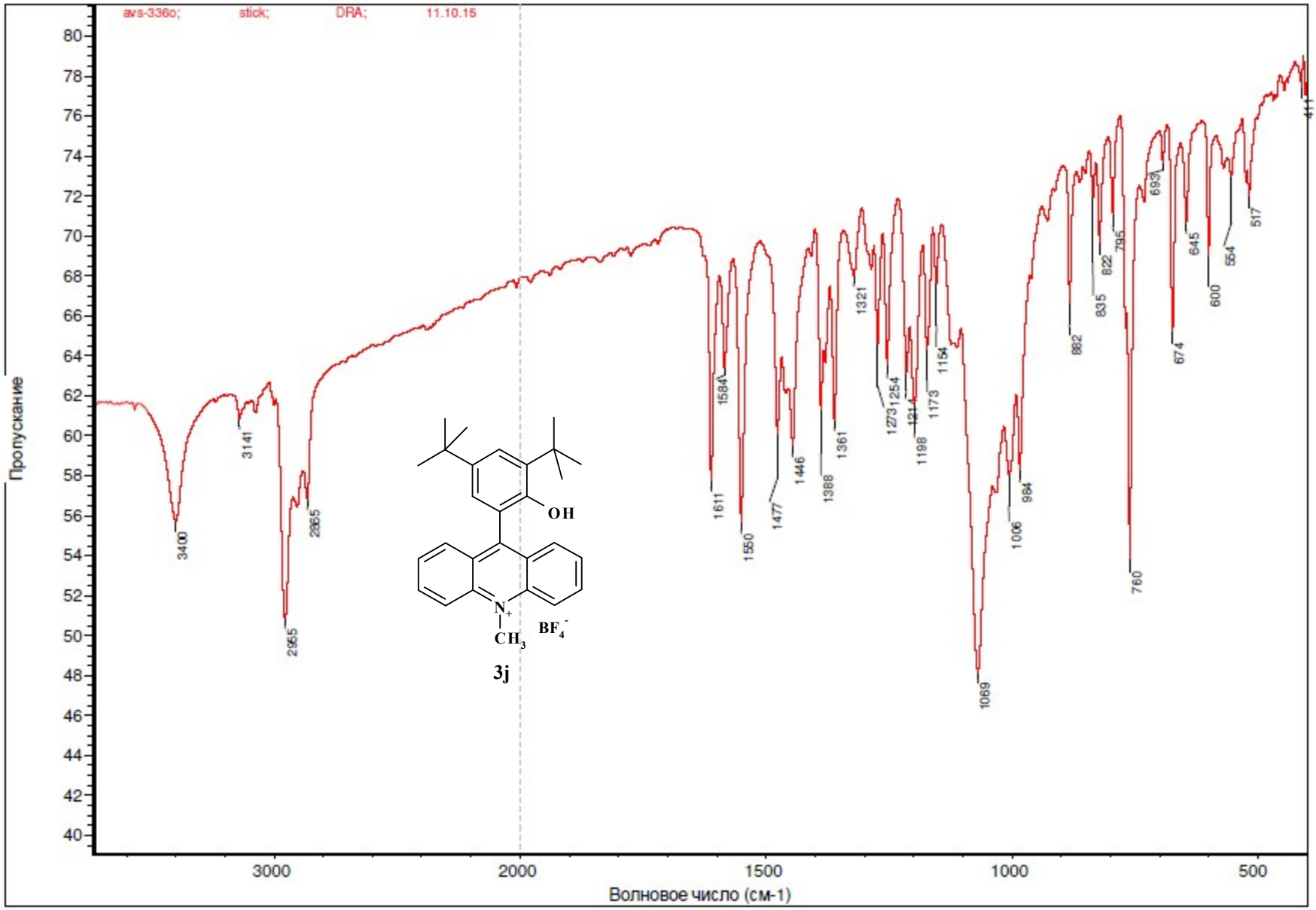

AVS336k
mik: A*05111
158.67
153.04
141.32
138.49
132.16
129.13
128.32
128.03
127.54
126.57
123.66
123.46
119.49
118.18
111.77
40.00
39.92
39.83
39.76
39.67
39.50
39.33
39.17
39.00
38.91
4E+08
4E+08
3E+08
3E+08
3E+08
3E+08
3E+08
2E+08
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm
AVS336k
mik: A*05111
40.00
39.92
39.83
39.76
39.67
39.50
39.33
39.17
39.00
38.91
3E+08
2E+08
1E+08
0
43
42
41
40
39
38
37
ppm


avs-336k; stick; DRA; 11.10.15
Пропускание
Волновое число (см-1)
3408
3079
1626
1610
1583
1549
1515
1460
1438
1385
1346
1278
1261
1216
1193
1169
1078
1028
993
974
910
866
824
781
755
711
687
657
625
599
566
557
526
OH
N+
CH3
BF4-

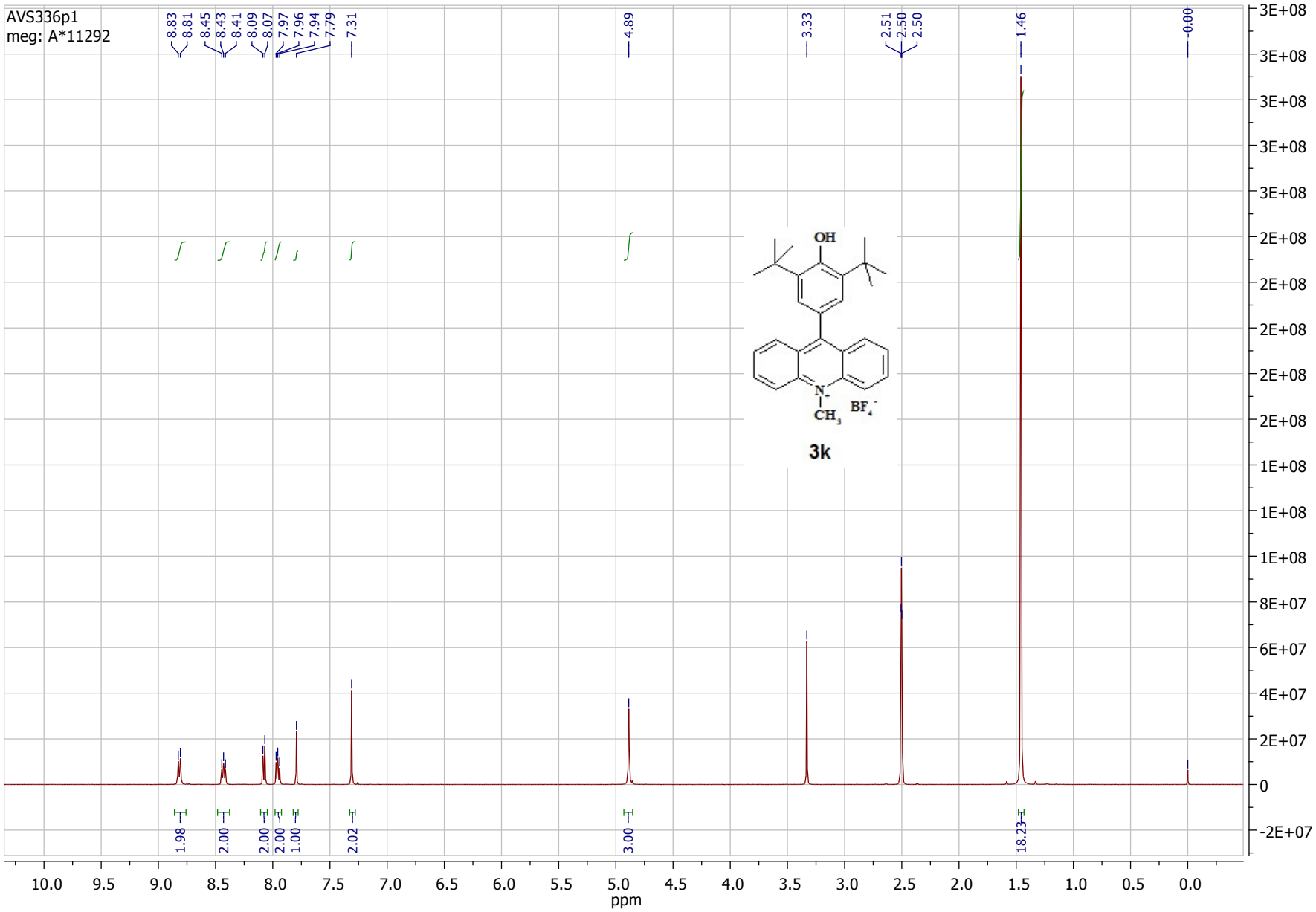
3i

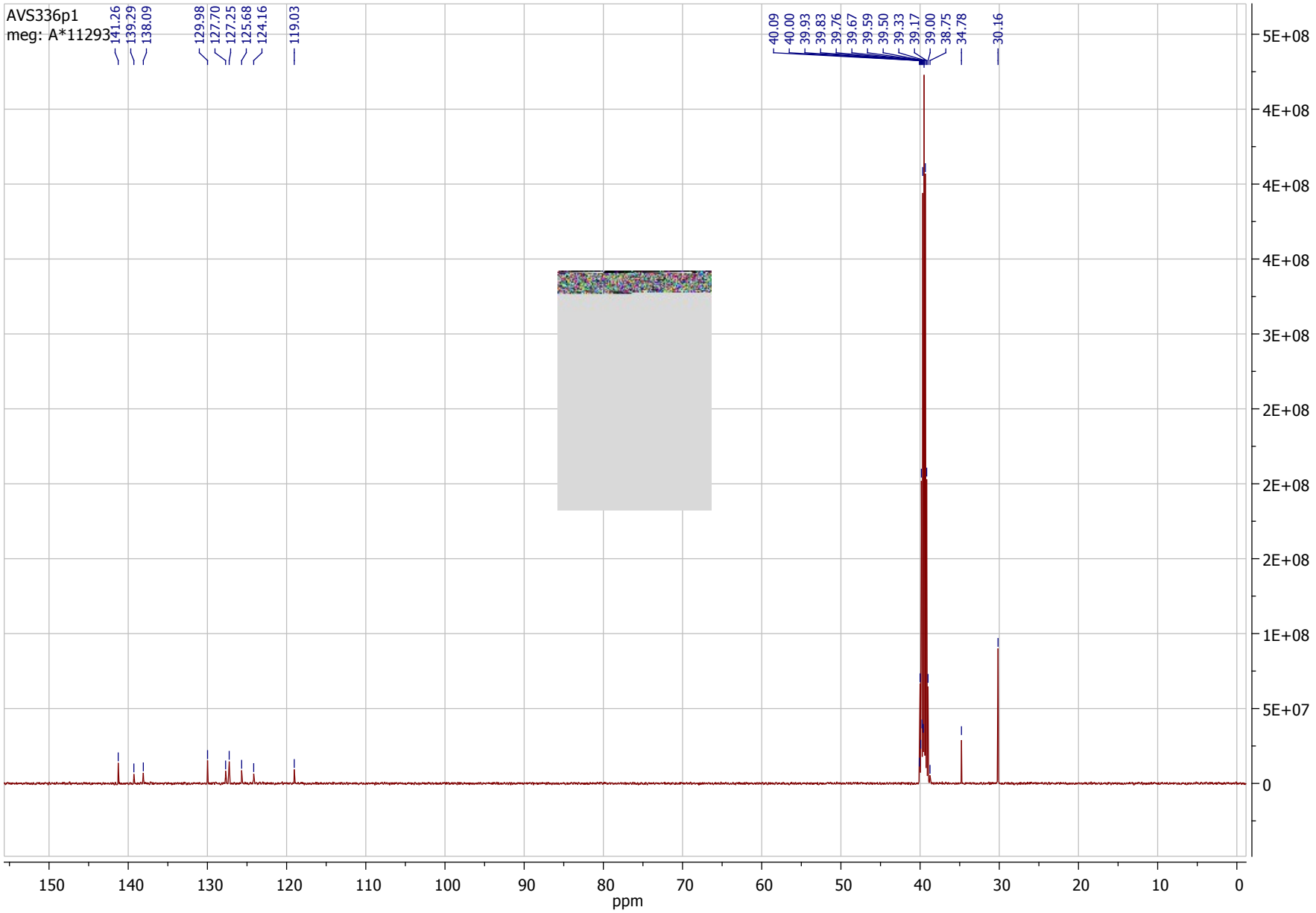

AVS437
ema: A*07589
8.86
8.84
8.46
8.45
8.45
8.32
7.96
7.96
7.95
7.58
7.58
7.10
7.09
4.97
3.33
2.51
2.50
2.50
2.50
2.49
1.47
1.30
0.00
OH
N
CH3
BF4-
3j
2.02
2.06
0.99
4.07
1.01
1.03
3.00
9.03
9.15
ppm

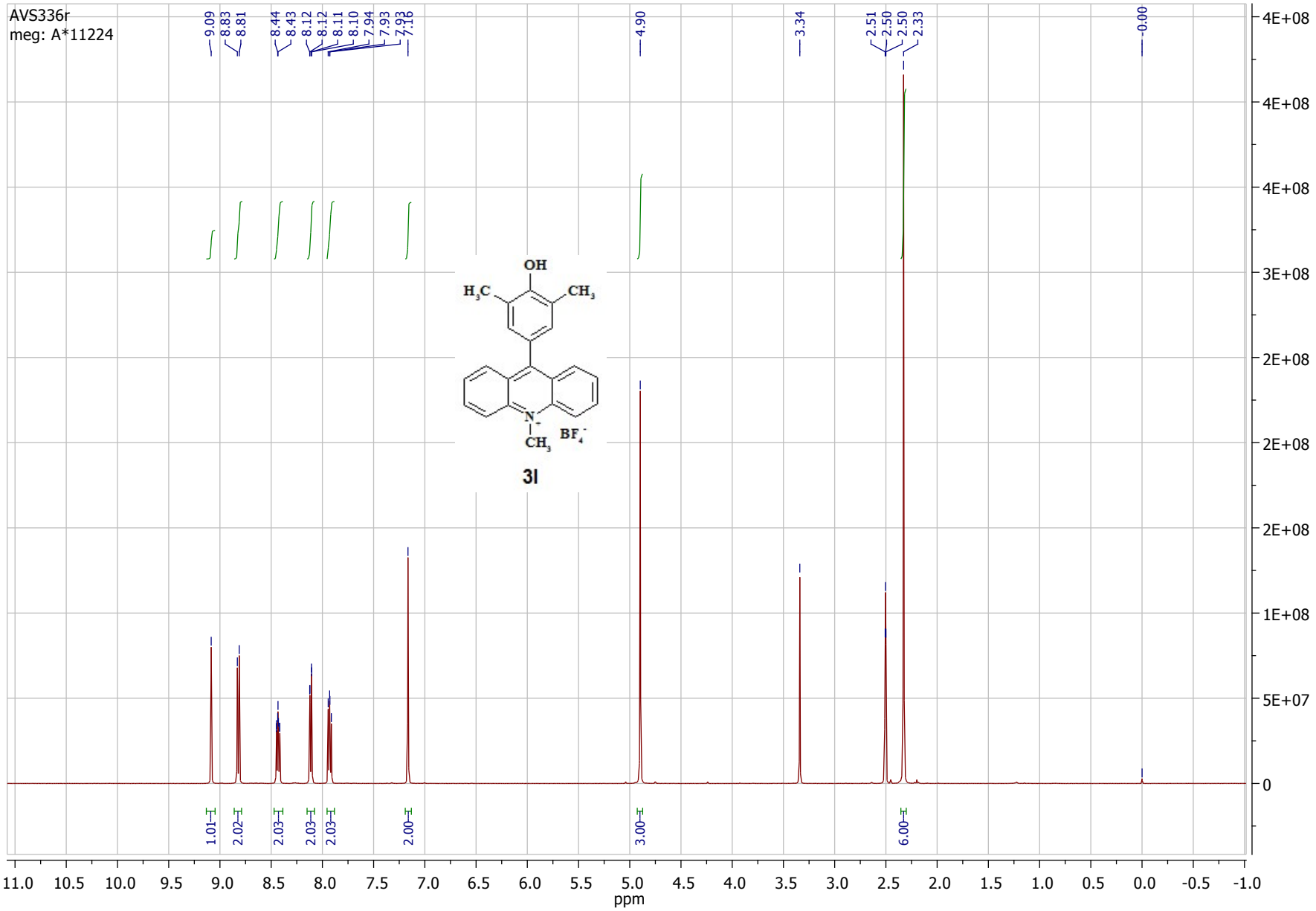

AVS437
ema: A*07590
159.54
150.29
141.30
141.25
138.36
137.27
129.58
127.92
126.68
125.52
125.38
120.70
119.03
40.09
40.00
39.92
39.83
39.76
39.67
39.59
39.50
39.33
39.17
39.00
38.74
34.99
34.09
31.31
29.53
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

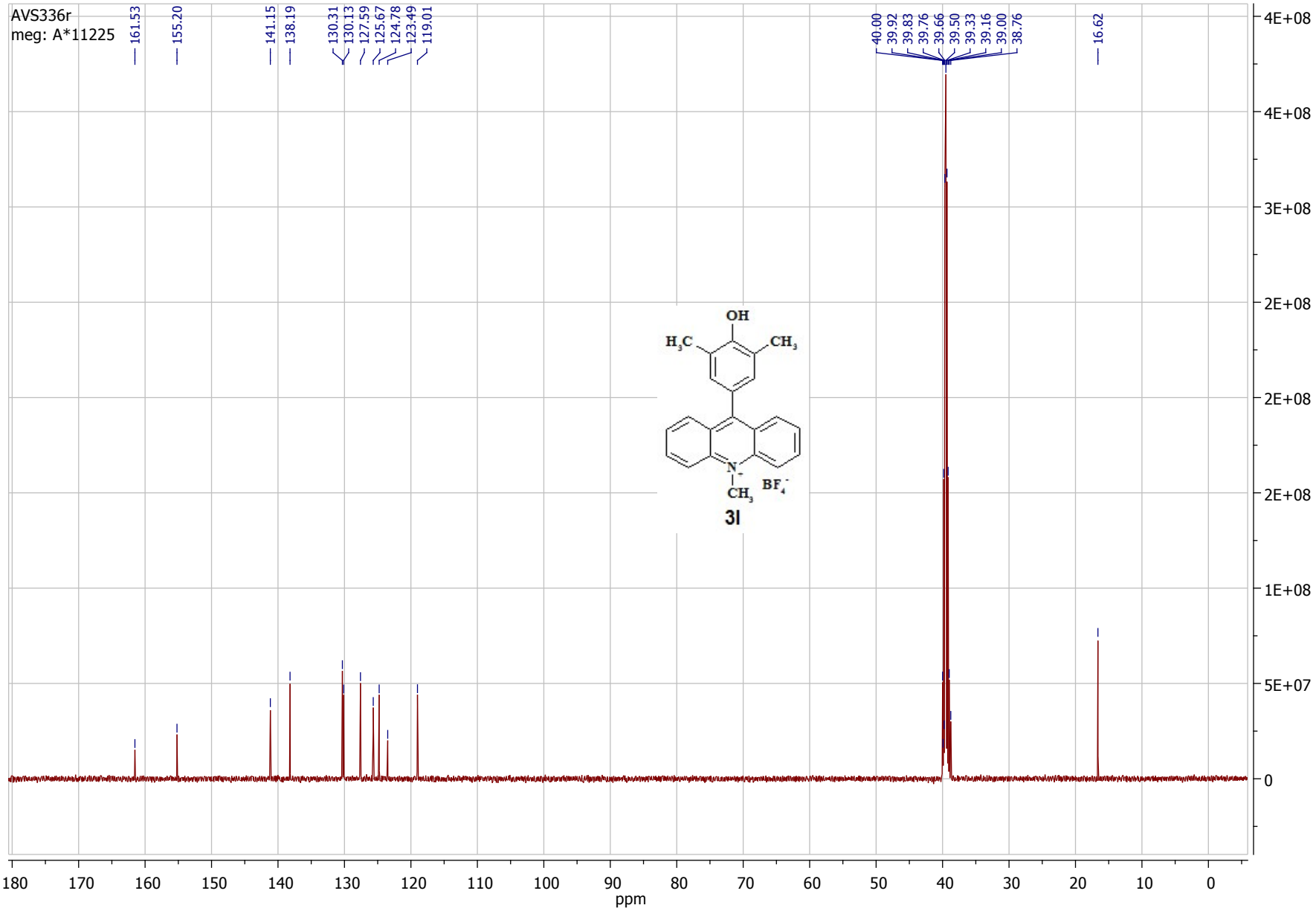

avs-336o; stick; DRA; 11.10.15
Пропускание
Волновое число (см-1)
3400
3141
2955
2865
1611
1584
1550
1477
1446
1388
1361
1321
1273
1254
1214
1198
1173
1154
1069
1006
964
862
835
822
795
760
693
674
645
600
564
517
OH
N+
CH3
BF4-

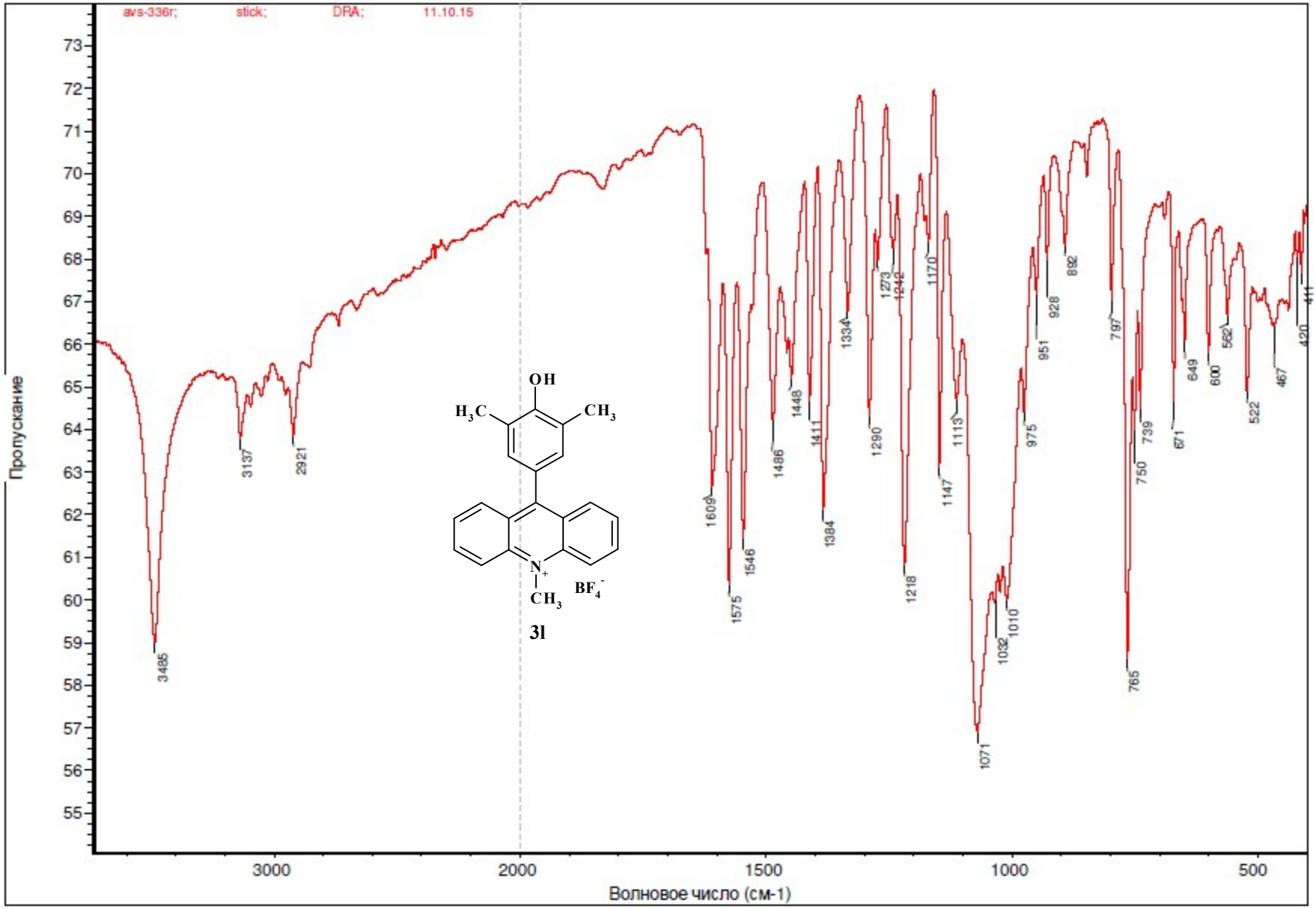
3j


AVS336p1
meg: A*11292
8.83
8.81
8.45
8.43
8.41
8.09
8.07
7.97
7.96
7.94
7.79
7.31
4.89
3.33
2.51
2.50
2.50
1.46
0.00
OH
N
CH3
BF4
3k
1.98
2.00
2.00
2.00
1.00
2.02
3.00
18.23
ppm

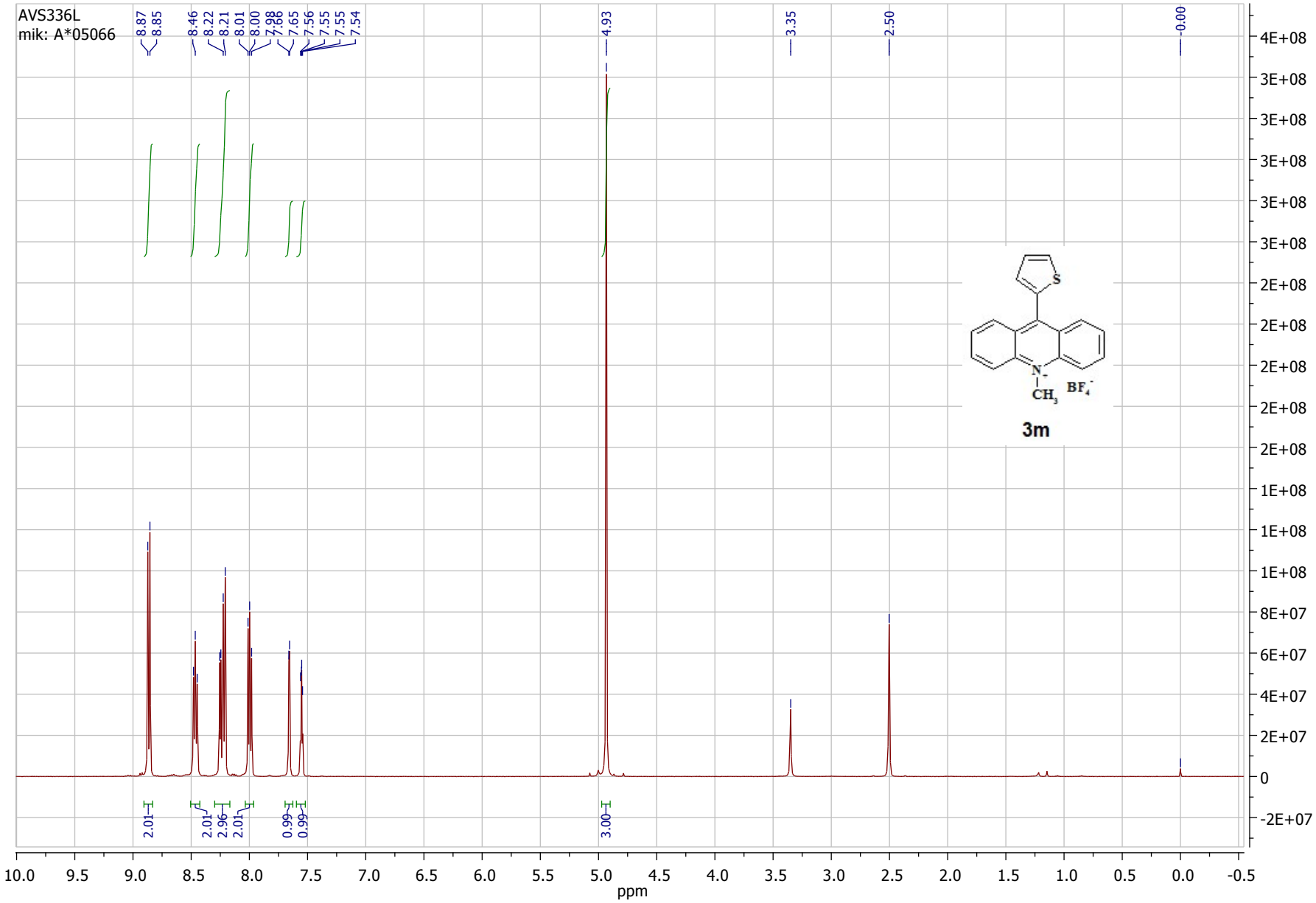

AVS336p1
meg: A*11293
141.26
139.29
138.09
129.98
127.70
127.25
125.68
124.16
119.03
40.09
40.00
39.93
39.83
39.76
39.67
39.59
39.50
39.33
39.17
39.00
38.75
34.78
30.16
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

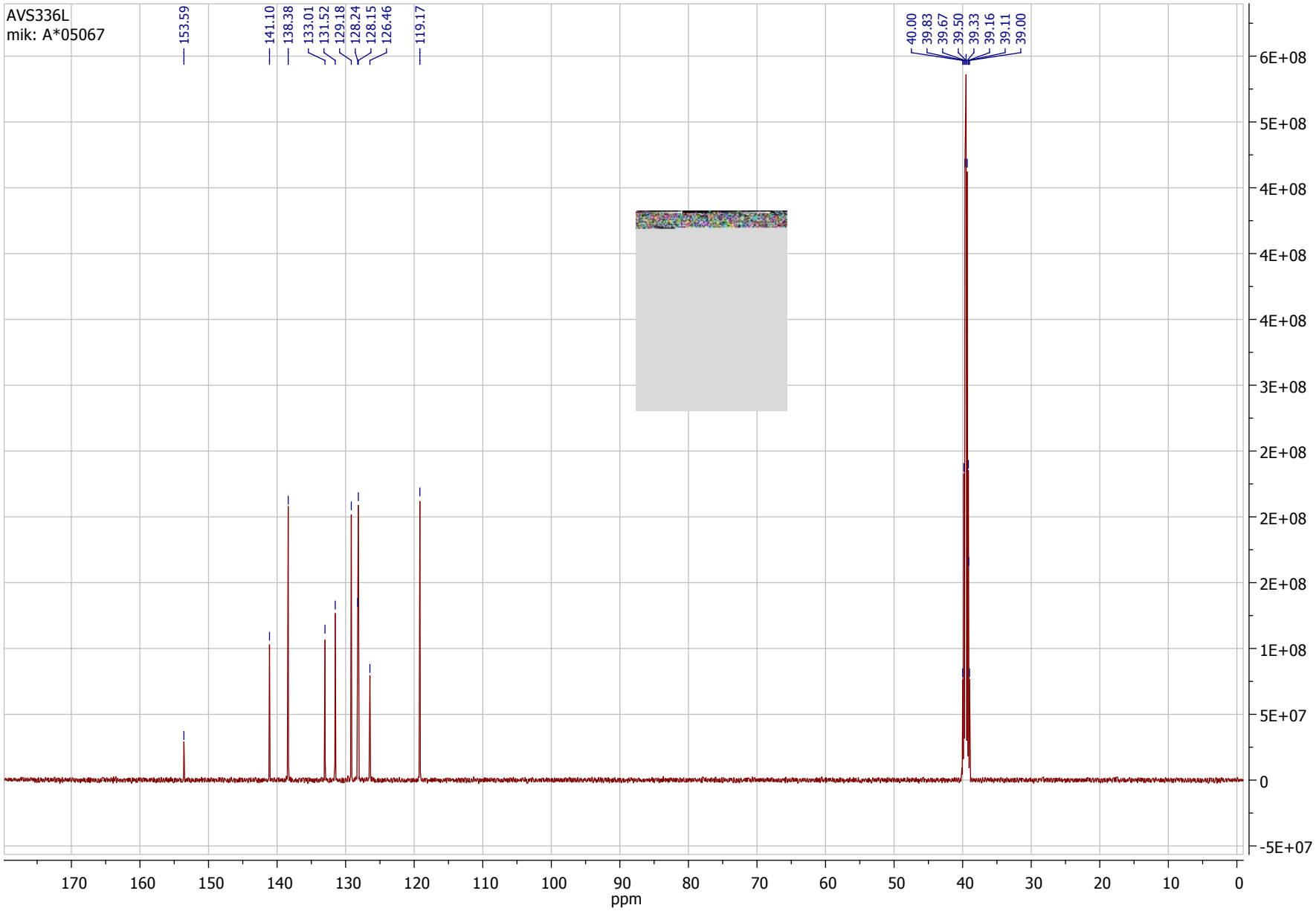

AVS336r
meg: A*11224
9.09
8.83
8.81
8.44
8.43
8.12
8.12
8.11
8.10
7.94
7.93
7.93
7.16
4.90
3.34
2.51
2.50
2.50
2.33
-0.00
OH
H3C
CH3
N
CH3
BF4-
3l
1.01
2.02
2.03
2.03
2.03
2.00
3.00
6.00
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
ppm

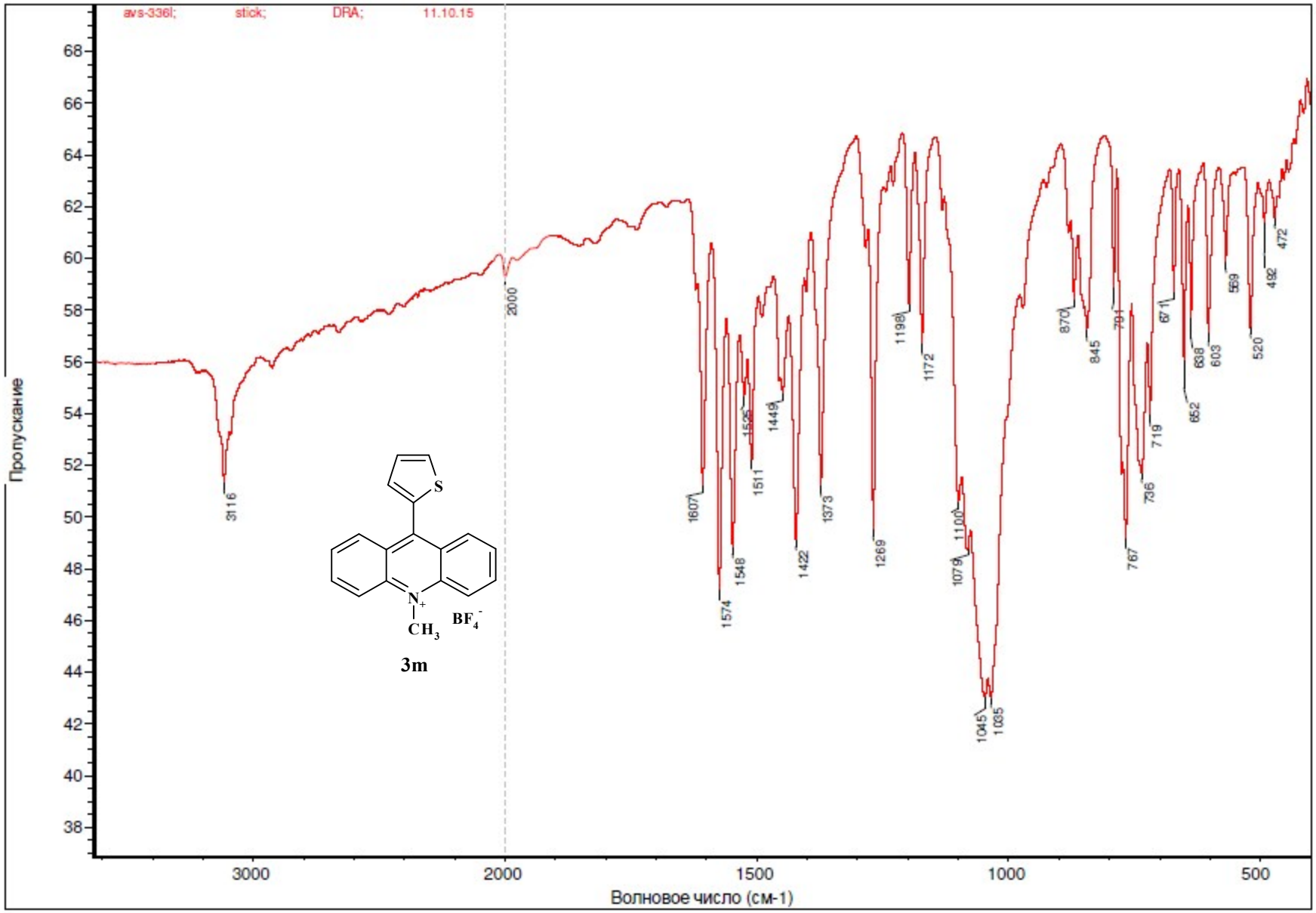

AVS336r
meg: A*11225
161.53
155.20
141.15
138.19
130.31
130.13
127.59
125.67
124.78
123.49
119.01
40.00
39.92
39.83
39.76
39.66
39.50
39.33
39.16
39.00
38.76
16.62
OH
H3C
CH3
N
CH3
BF4-
3l
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


avs-336r; stick; DRA; 11.10.15
Пропускание
Волновое число (см-1)
3000
2000
1500
1000
500
3485
3137
2921
1609
1575
1546
1486
1448
1411
1384
1334
1290
1273
1242
1218
1170
1147
1113
1071
1032
1010
975
951
928
892
797
765
750
739
671
649
600
562
522
467
420
411
OH
H3C
CH3
N+
CH3
BF4-

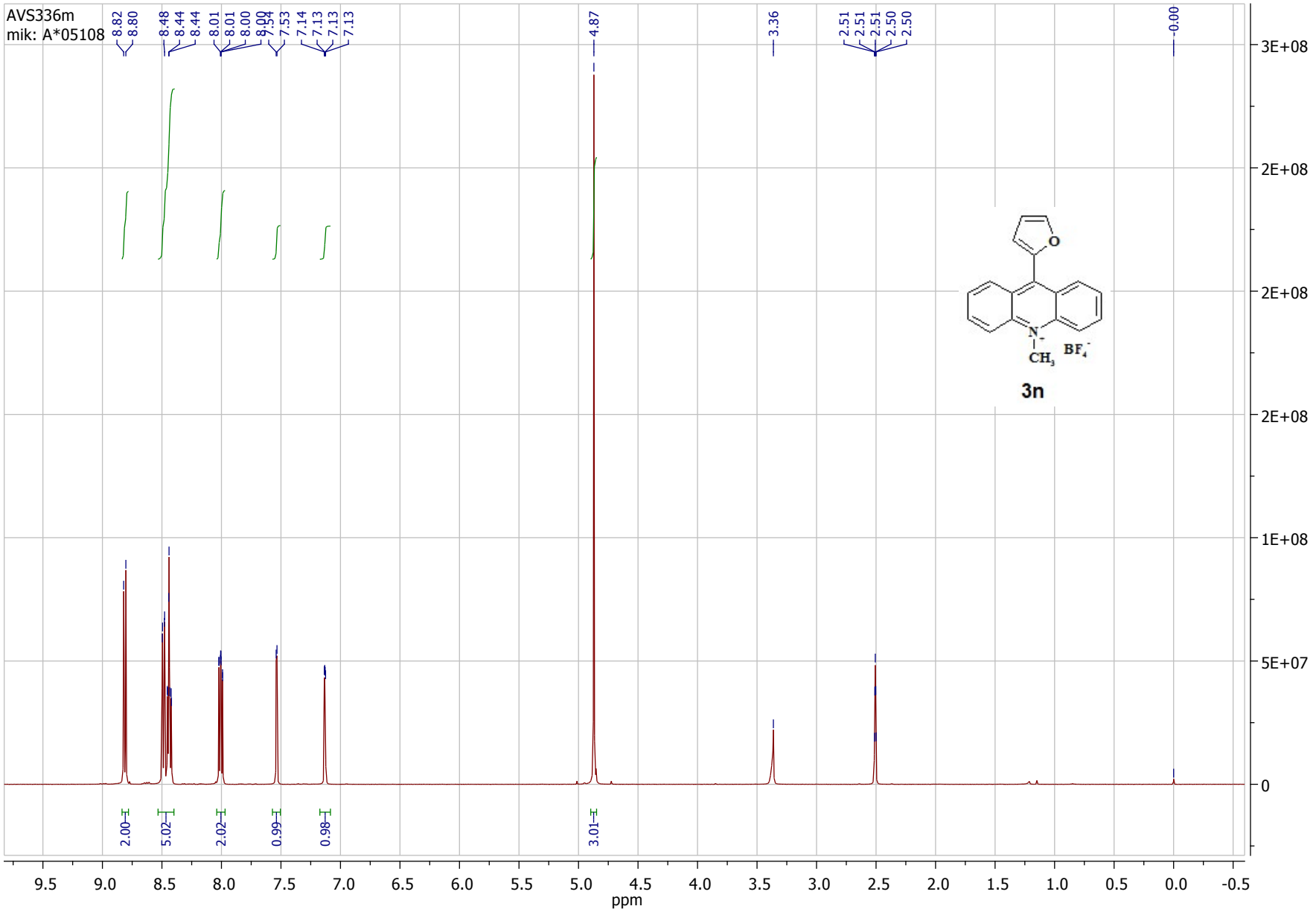
3l

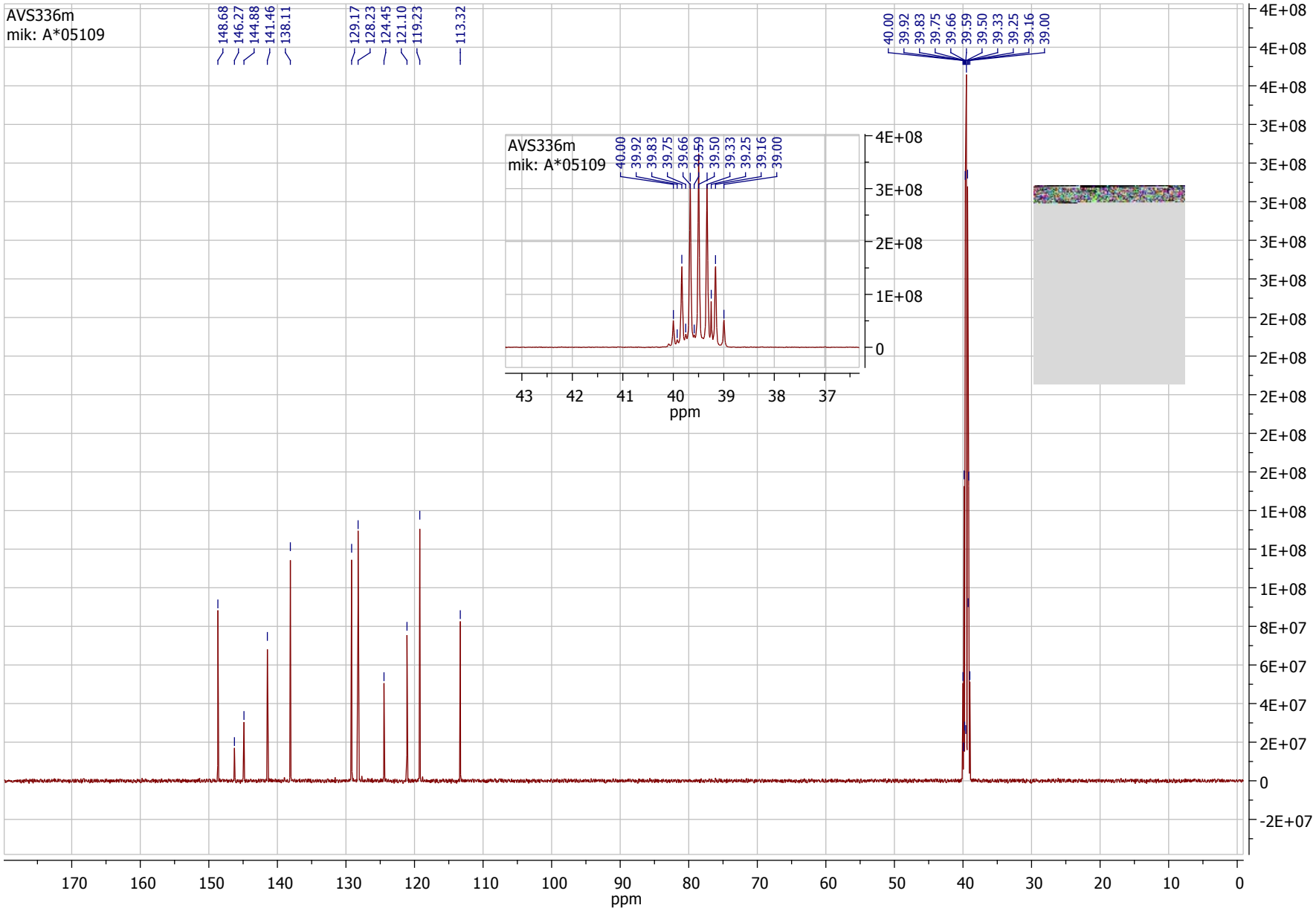

AVS336L
mik: A*05066
8.87
8.85
8.46
8.22
8.21
8.01
8.00
7.98
7.66
7.65
7.56
7.55
7.55
7.54
4.93
3.35
2.50
0.00
2.01
2.01
2.96
2.01
0.99
0.99
3.00
4E+08
3E+08
3E+08
3E+08
3E+08
3E+08
2E+08
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
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
-0.5
ppm
S
N
CH3
BF4
3m

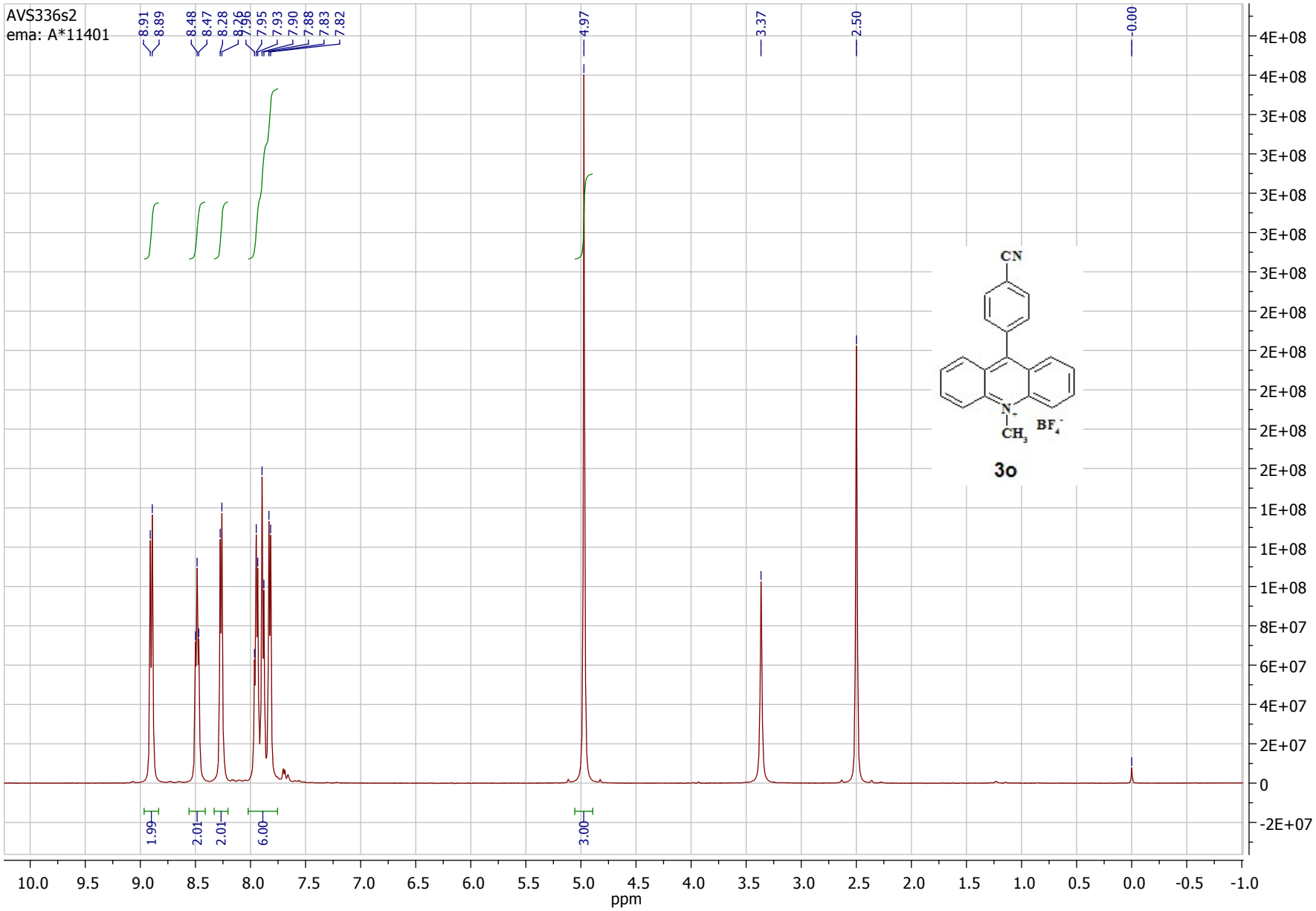

AVS336L
mik: A*05067
153.59
141.10
138.38
133.01
131.52
129.18
128.24
128.15
126.46
119.17
40.00
39.83
39.67
39.50
39.33
39.16
39.11
39.00
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

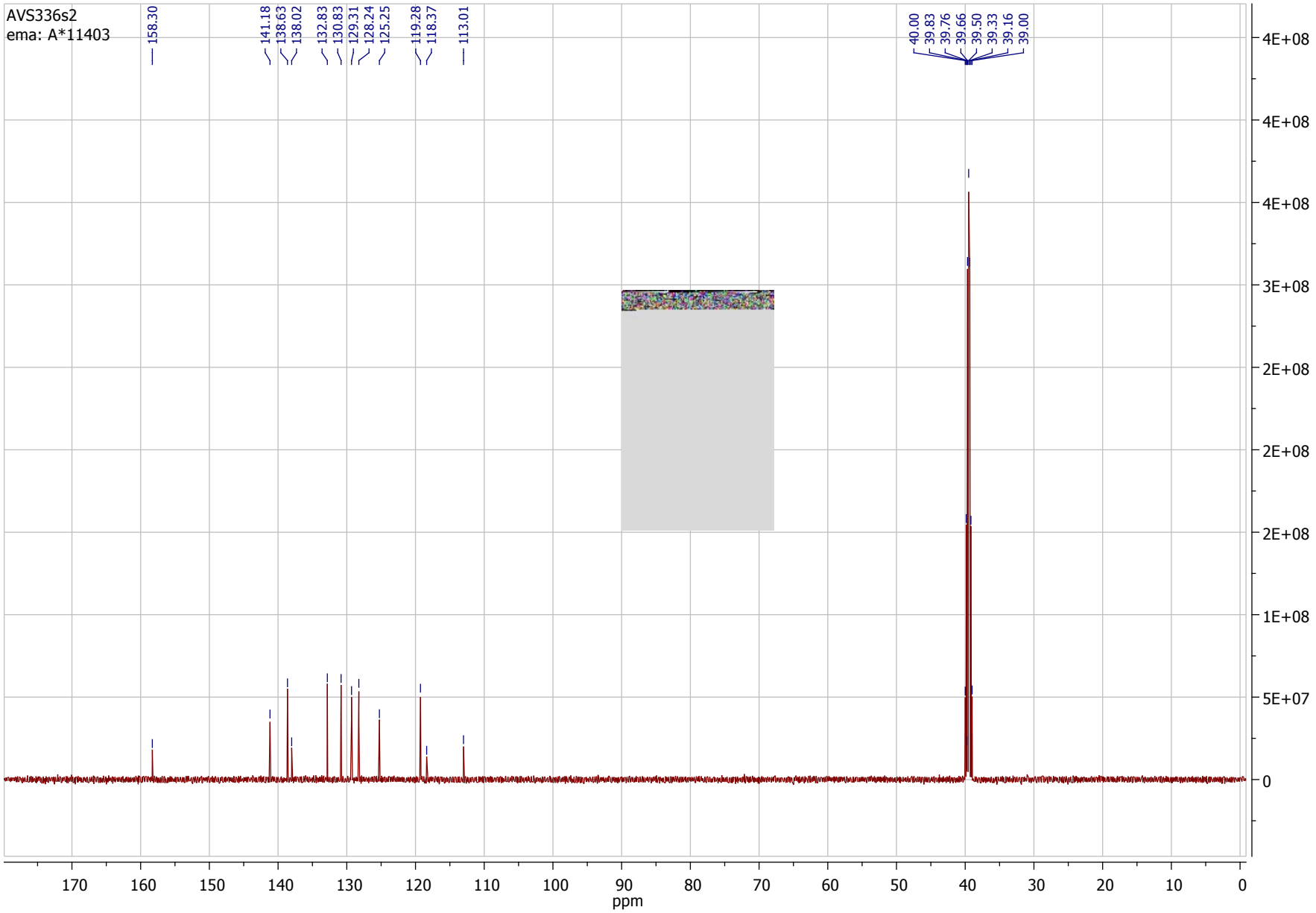

avs-336l; stick; DRA; 11.10.15
Пропускание
Волновое число (см-1)
3000
2000
1500
1000
500
3116
2000
1607
1574
1548
1511
1526
1449
1422
1373
1269
1198
1172
1100
1079
1045
1035
870
845
791
767
736
719
671
652
638
603
559
520
492
472
S
N+
CH3
BF4-

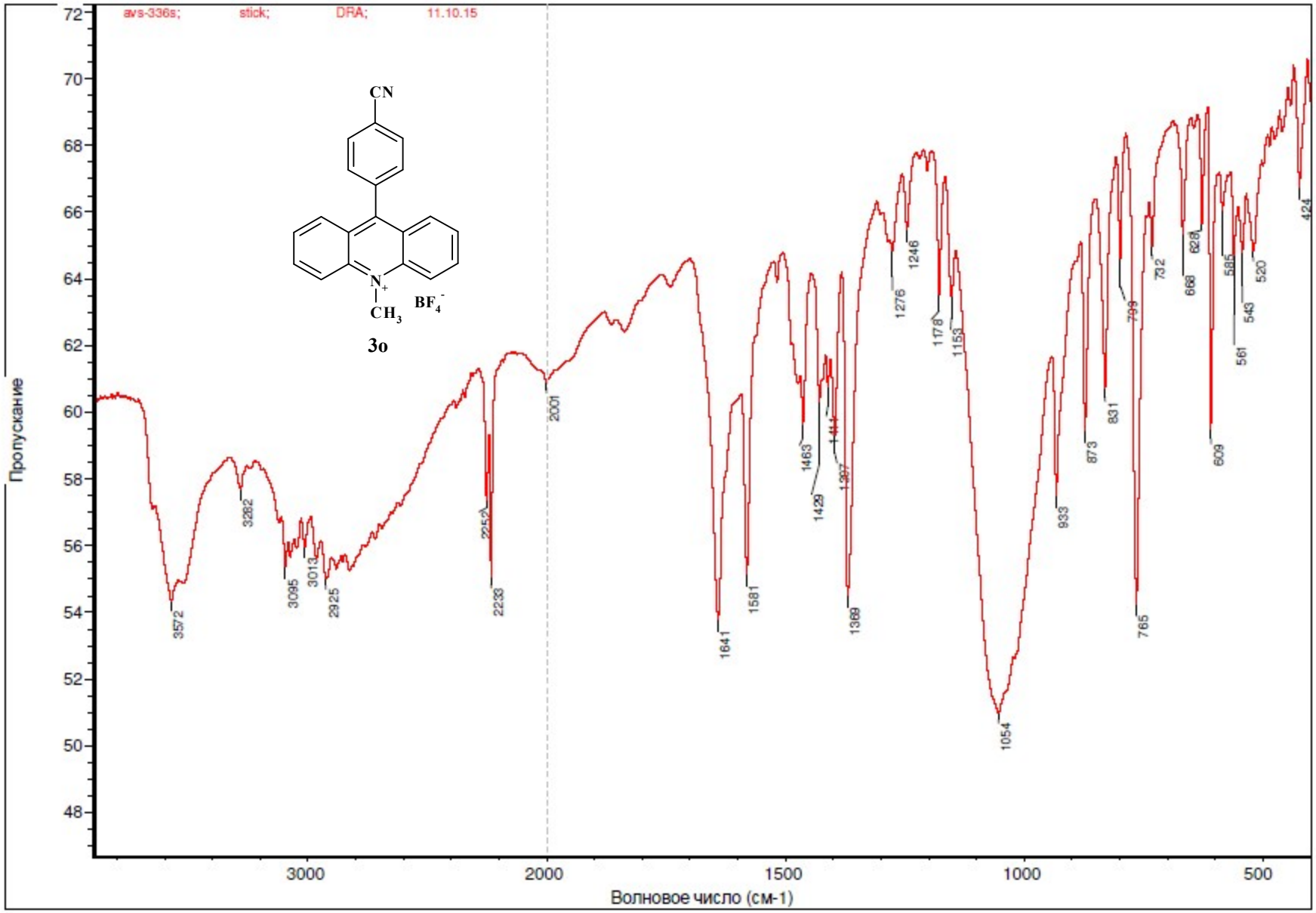
3m

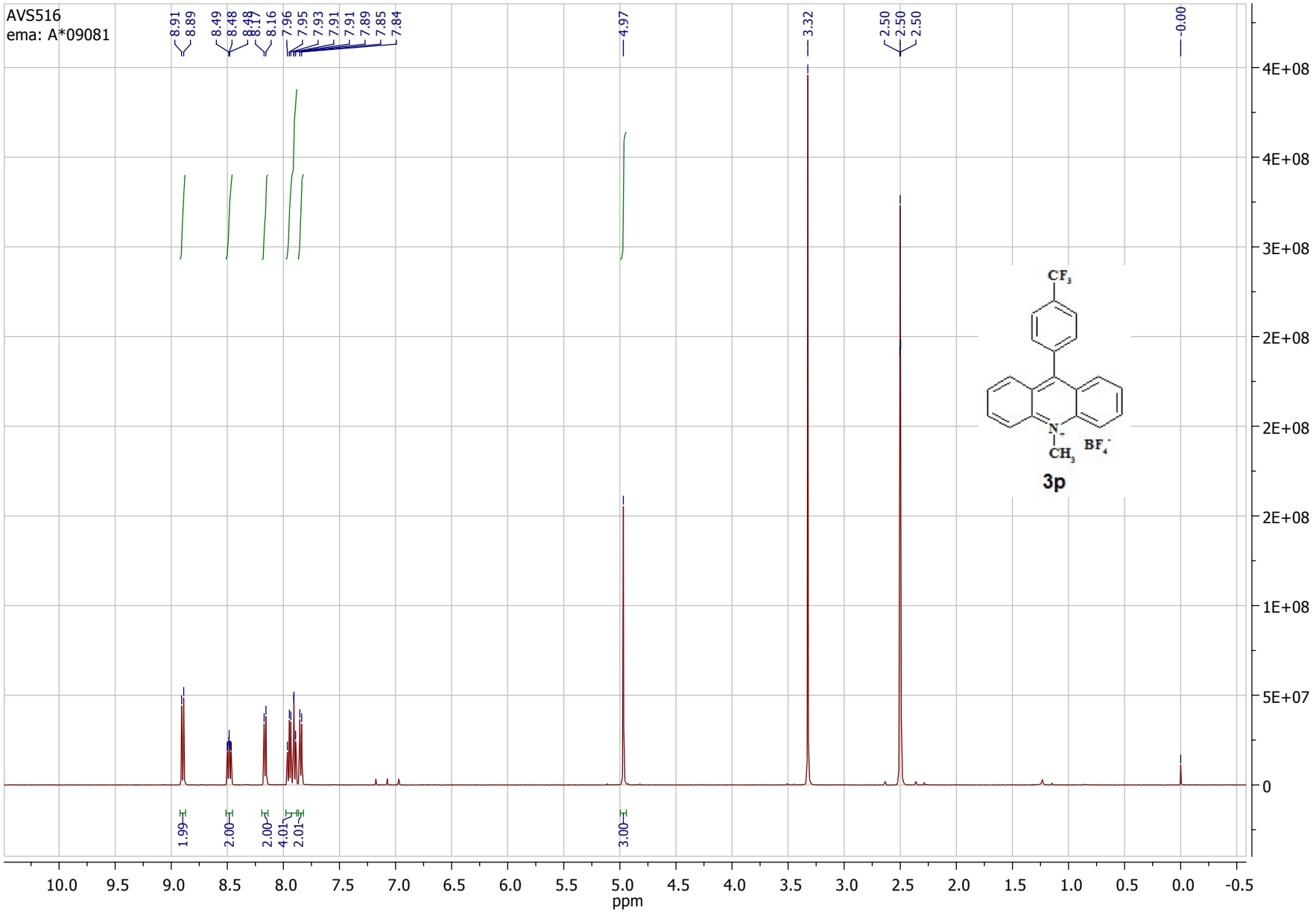

AVS336m
mik: A*05108
8.82
8.80
8.48
8.44
8.44
8.01
8.01
8.00
8.00
7.54
7.53
7.14
7.13
7.13
7.13
4.87
3.36
2.51
2.51
2.51
2.50
2.50
-0.00
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
2.00
5.02
2.02
0.99
0.98
3.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm
O
N
CH3
BF4
3n

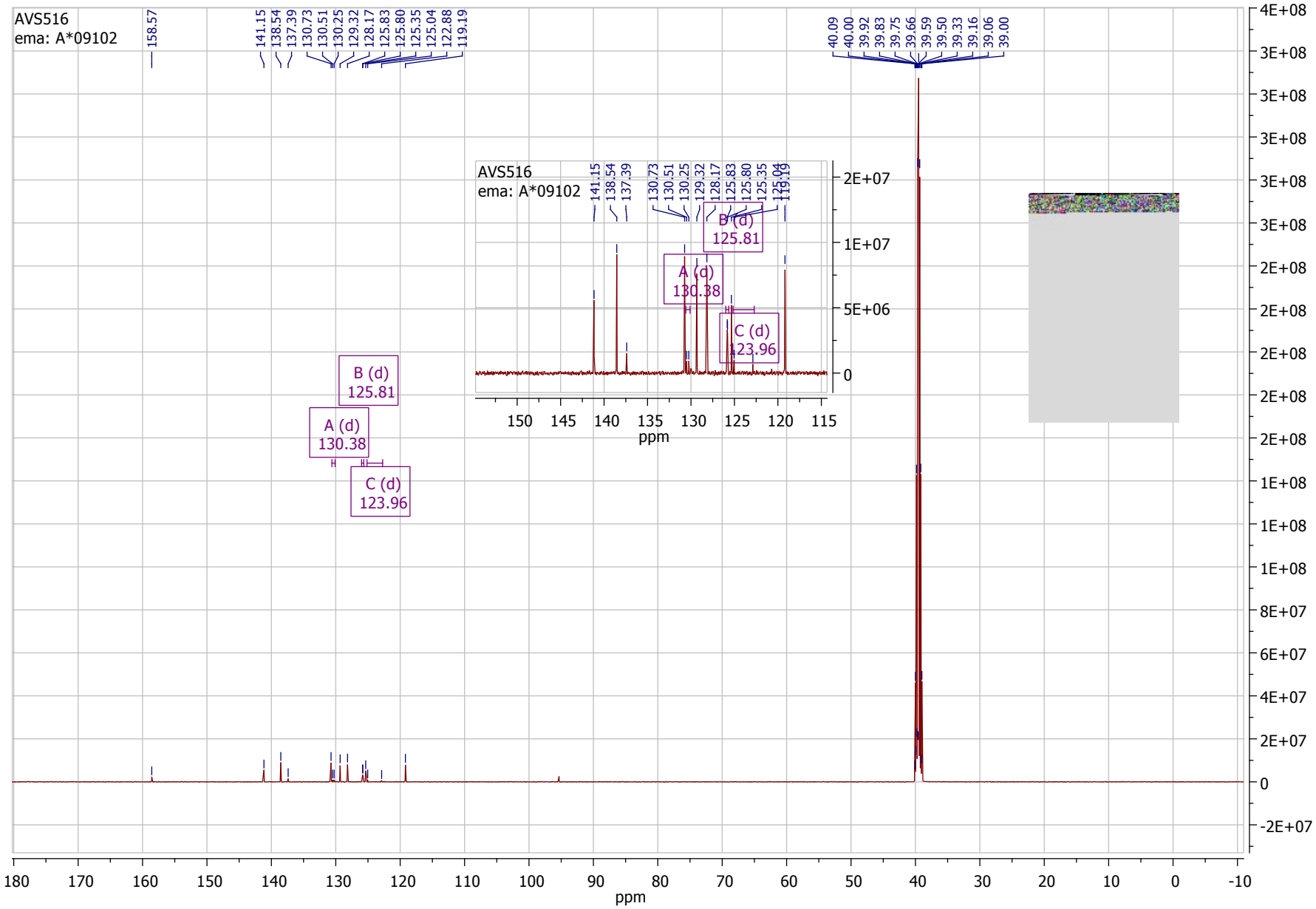

AVS336m
mik: A*05109
148.68
146.27
144.88
141.46
138.11
129.17
128.23
124.45
121.10
119.23
113.32
40.00
39.92
39.83
39.75
39.66
39.59
39.50
39.33
39.25
39.16
39.00
ppm

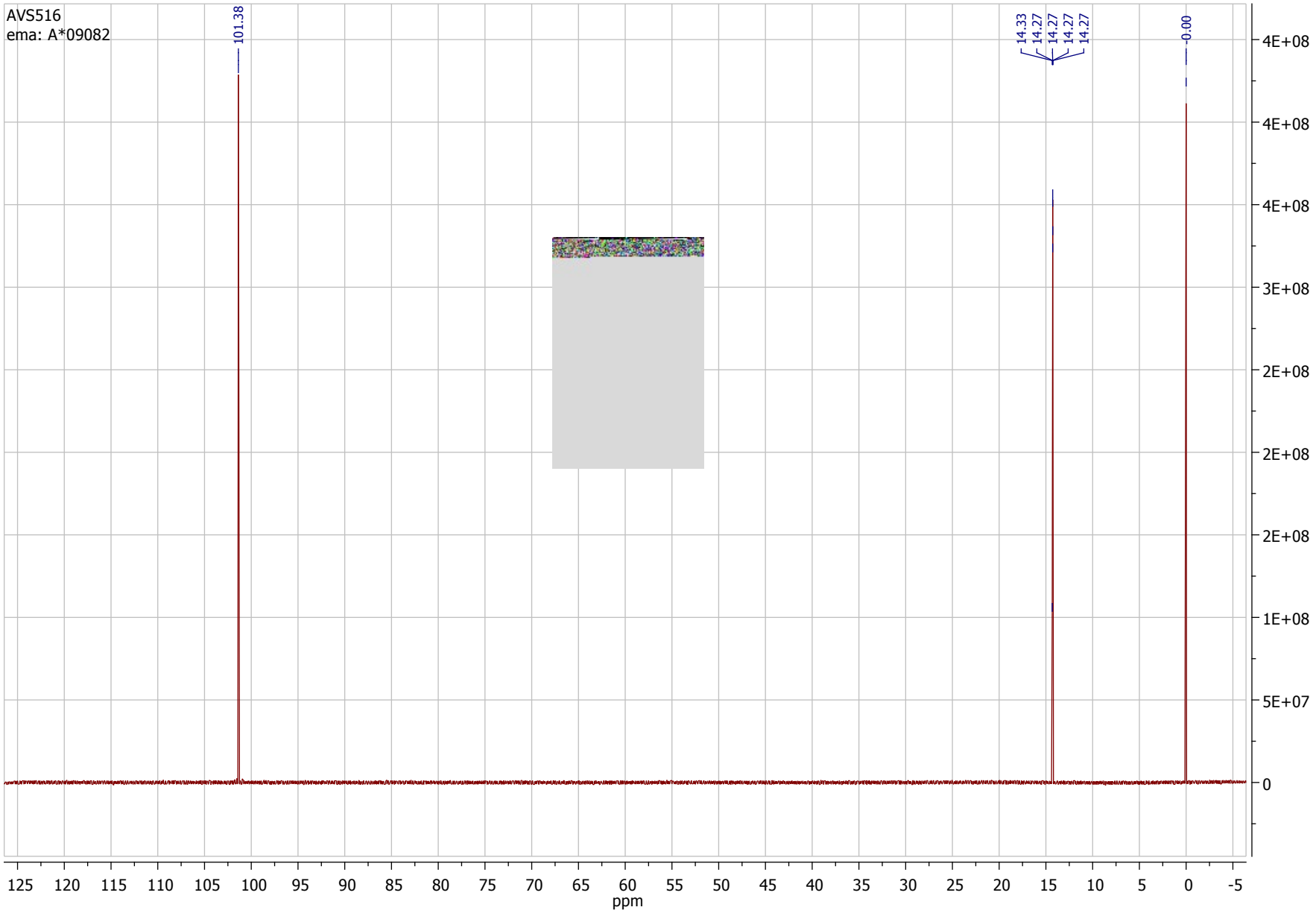

AVS336s2
ema: A*11401
8.91
8.89
8.48
8.47
8.28
8.26
7.96
7.95
7.93
7.90
7.88
7.83
7.82
4.97
3.37
2.50
0.00
1.99
2.01
2.01
6.00
3.00
CN
N
CH3
BF4-
3o
ppm

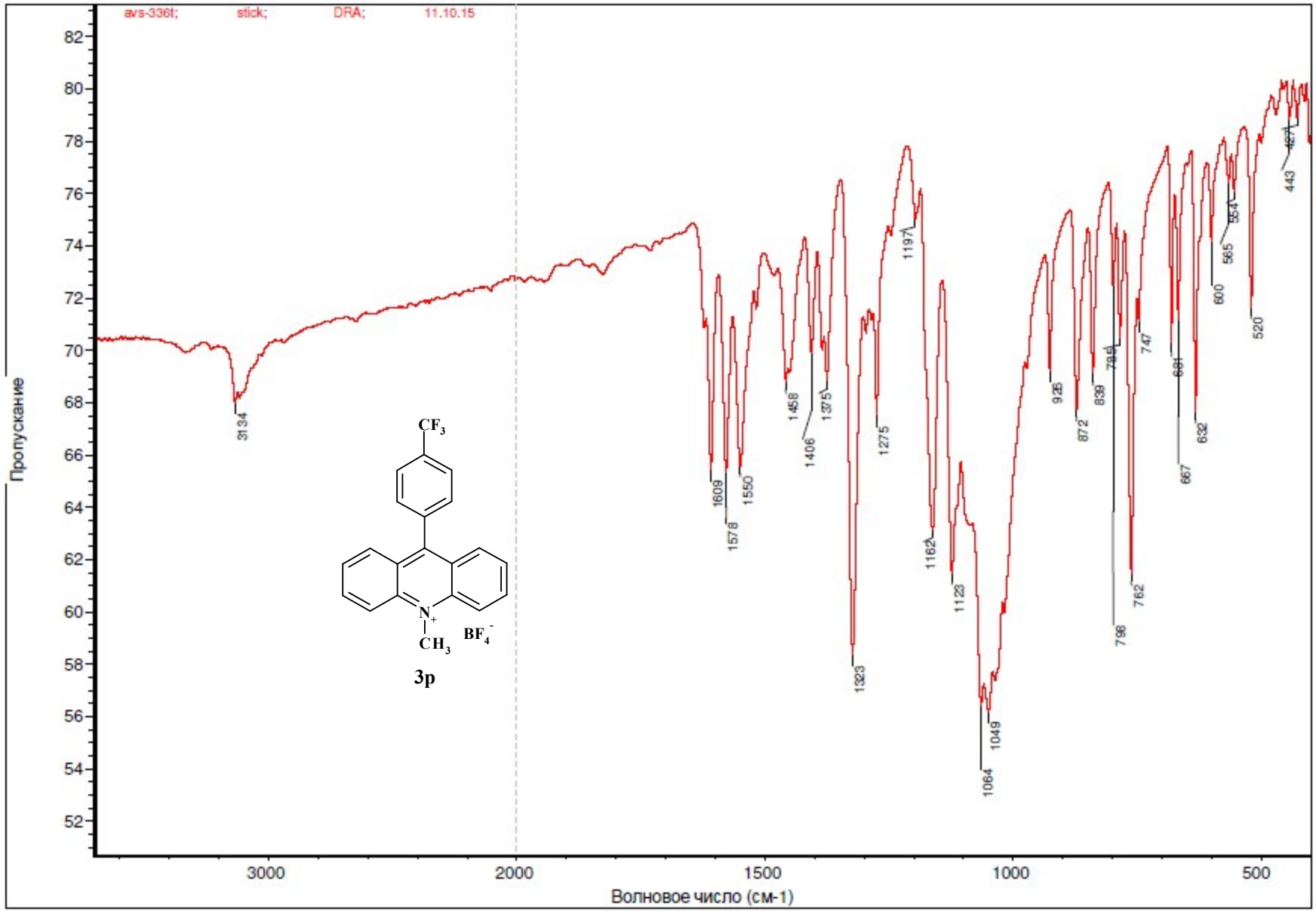

AVS336s2
ema: A*11403
158.30
141.18
138.63
138.02
132.83
130.83
129.31
128.24
125.25
119.28
118.37
113.01
40.00
39.83
39.76
39.66
39.50
39.33
39.16
39.00
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


avs-336s; stick; DRA; 11.10.15
CN
N+
CH3
BF4-
3o
Пропускание
Волновое число (см-1)
72
70
68
66
64
62
60
58
56
54
52
50
48
3000
2000
1500
1000
500
3572
3282
3095
3013
2925
2252
2233
2001
1641
1581
1463
1429
1414
1397
1369
1276
1246
1178
1153
1054
933
873
831
799
765
732
668
628
609
585
561
543
520
424

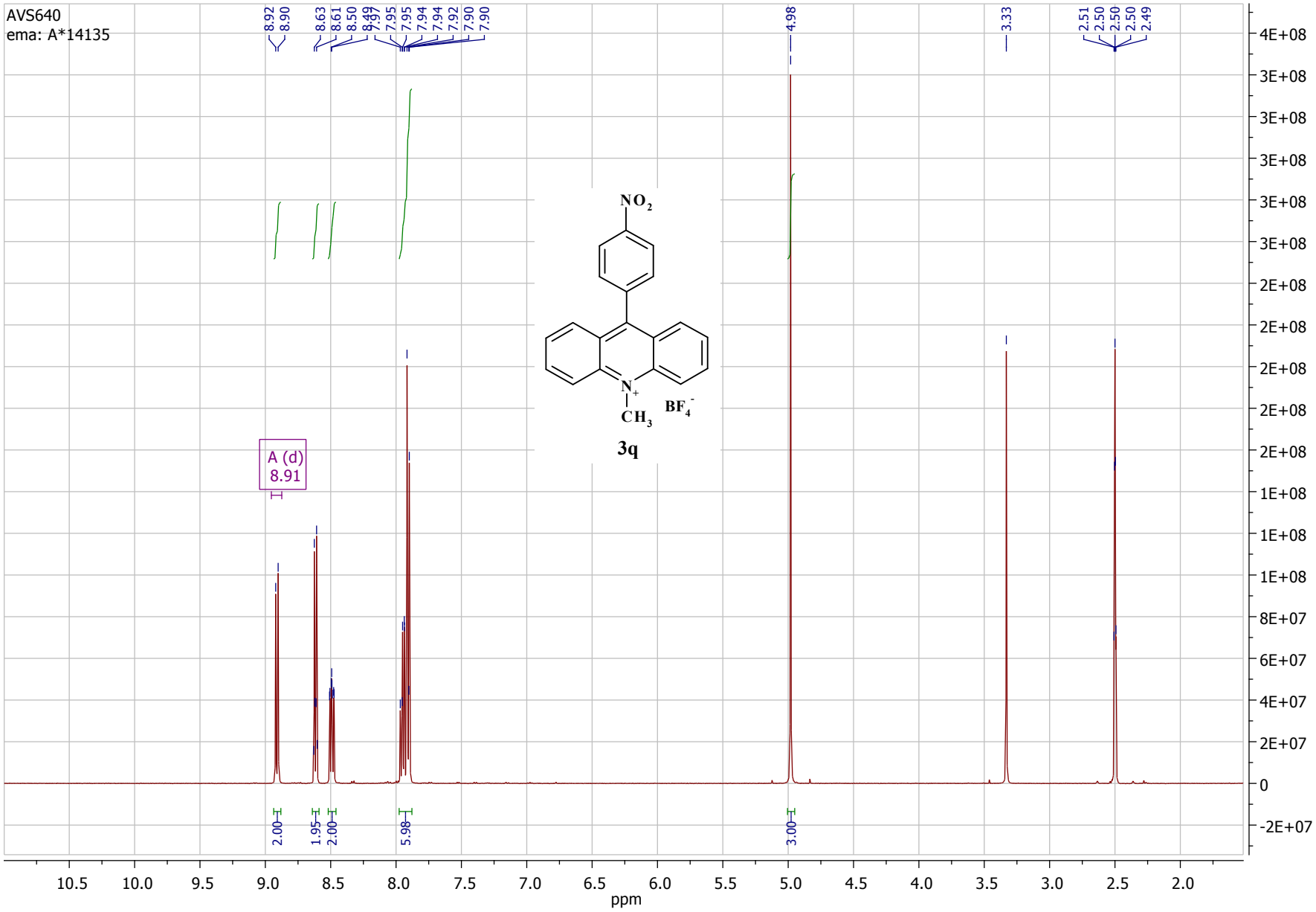

AVS516
ema: A*09081
8.91
8.89
8.49
8.48
8.48
8.17
8.16
7.96
7.95
7.93
7.91
7.91
7.89
7.85
7.84
4.97
3.32
2.50
2.50
2.50
0.00
1.99
2.00
2.00
4.01
2.01
3.00
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm
CF3
N
CH3
BF4
3p

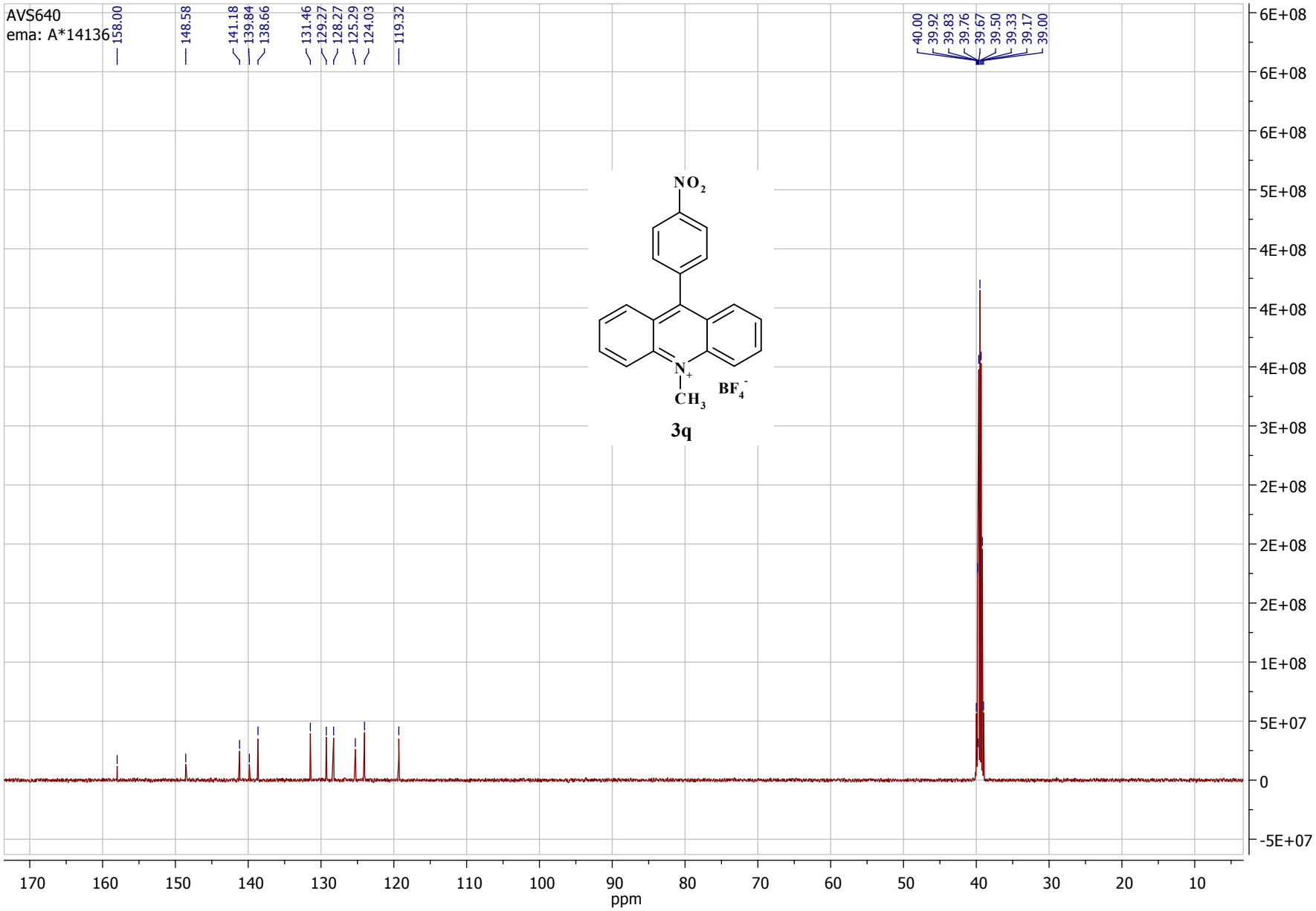

AVS516
ema: A*09102
158.57
141.15
138.54
137.39
130.73
130.51
130.25
129.32
128.17
125.83
125.80
125.35
125.04
122.88
119.19
40.09
40.00
39.92
39.83
39.75
39.66
39.59
39.50
39.33
39.16
39.06
39.00
B (d)
125.81
A (d)
130.38
C (d)
123.96
ppm
AVS516
ema: A*09102
B (d)
125.81
A (d)
130.38
C (d)
123.96
ppm

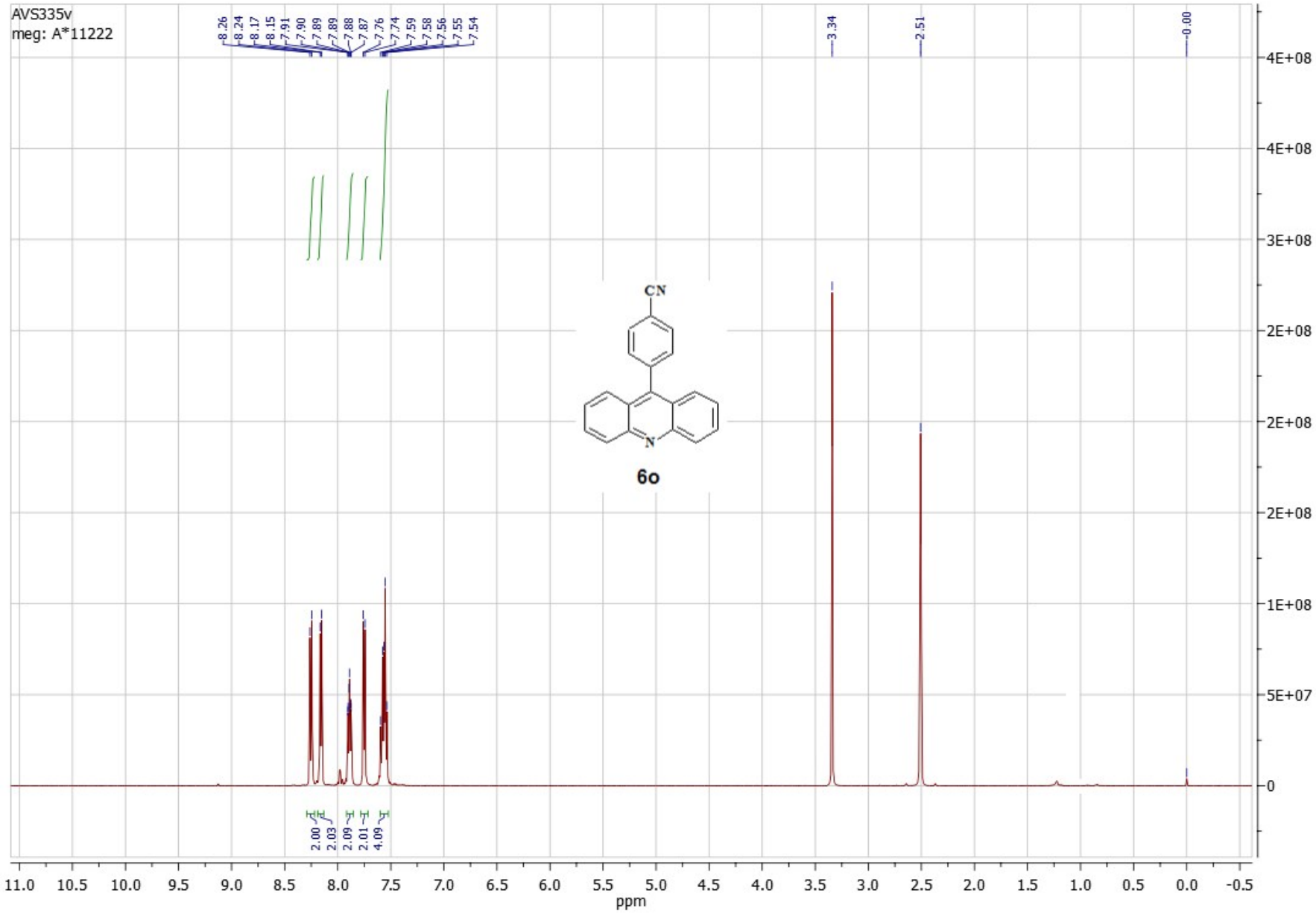

AVS516
ema: A*09082
101.38
14.33
14.27
14.27
14.27
14.27
0.00
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5
ppm

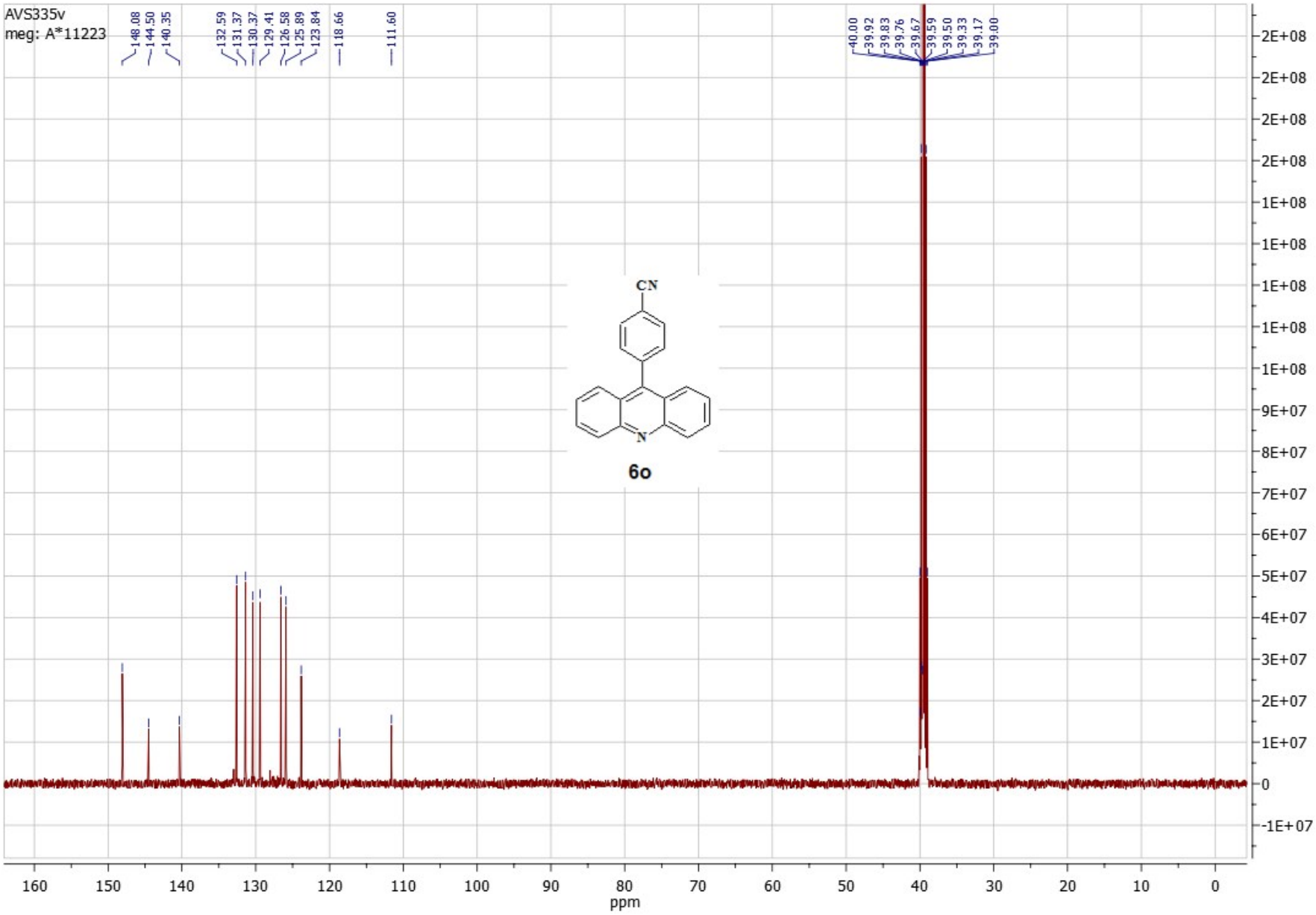

avs-336t; stick; DRA; 11.10.15
Пропускание
Волновое число (см-1)
3000
2000
1500
1000
500
82
80
78
76
74
72
70
68
66
64
62
60
58
56
54
52
3134
1609
1578
1550
1458
1406
1375
1323
1275
1197
1162
1123
1064
1049
925
872
839
796
762
747
681
667
632
600
565
554
520
443
CF3
N+
CH3
BF4-

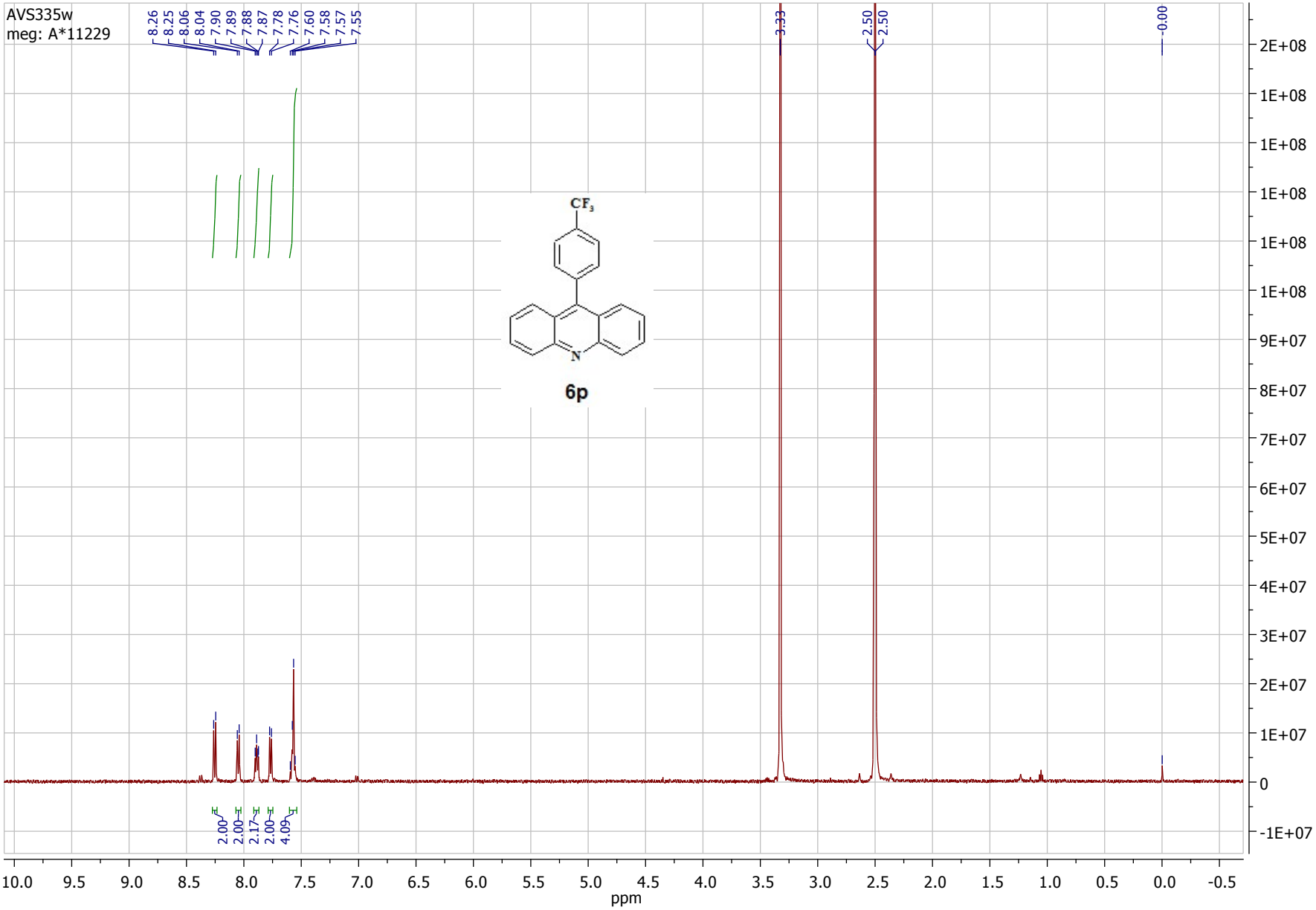
3p

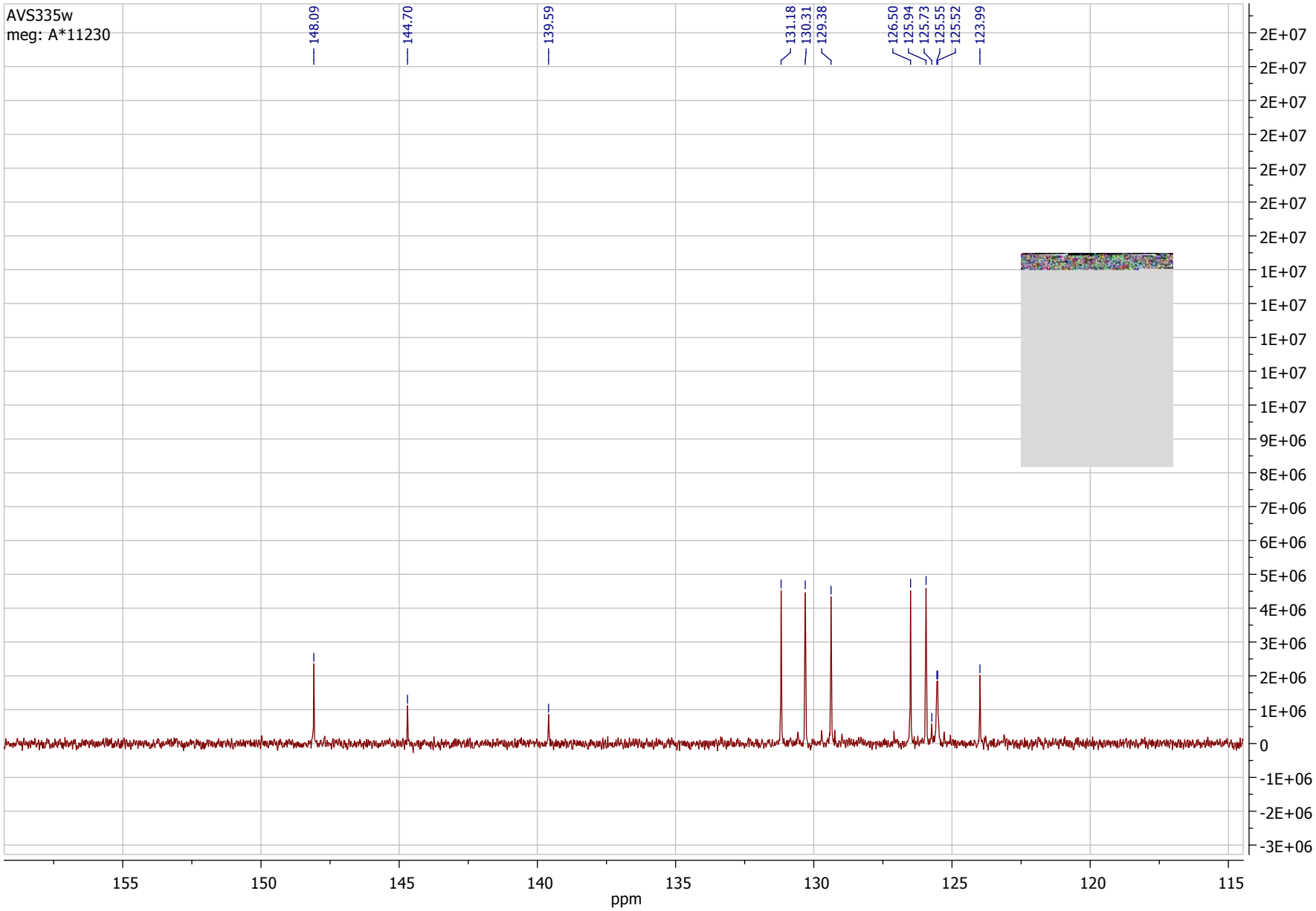

AVS640
ema: A*14135
8.92
8.90
8.63
8.61
8.50
8.49
7.97
7.95
7.95
7.94
7.94
7.92
7.90
7.90
4.98
3.33
2.51
2.50
2.50
2.50
2.49
A (d)
8.91
2.00
1.95
2.00
5.98
3.00
NO2
CH3
BF4-
3q
ppm

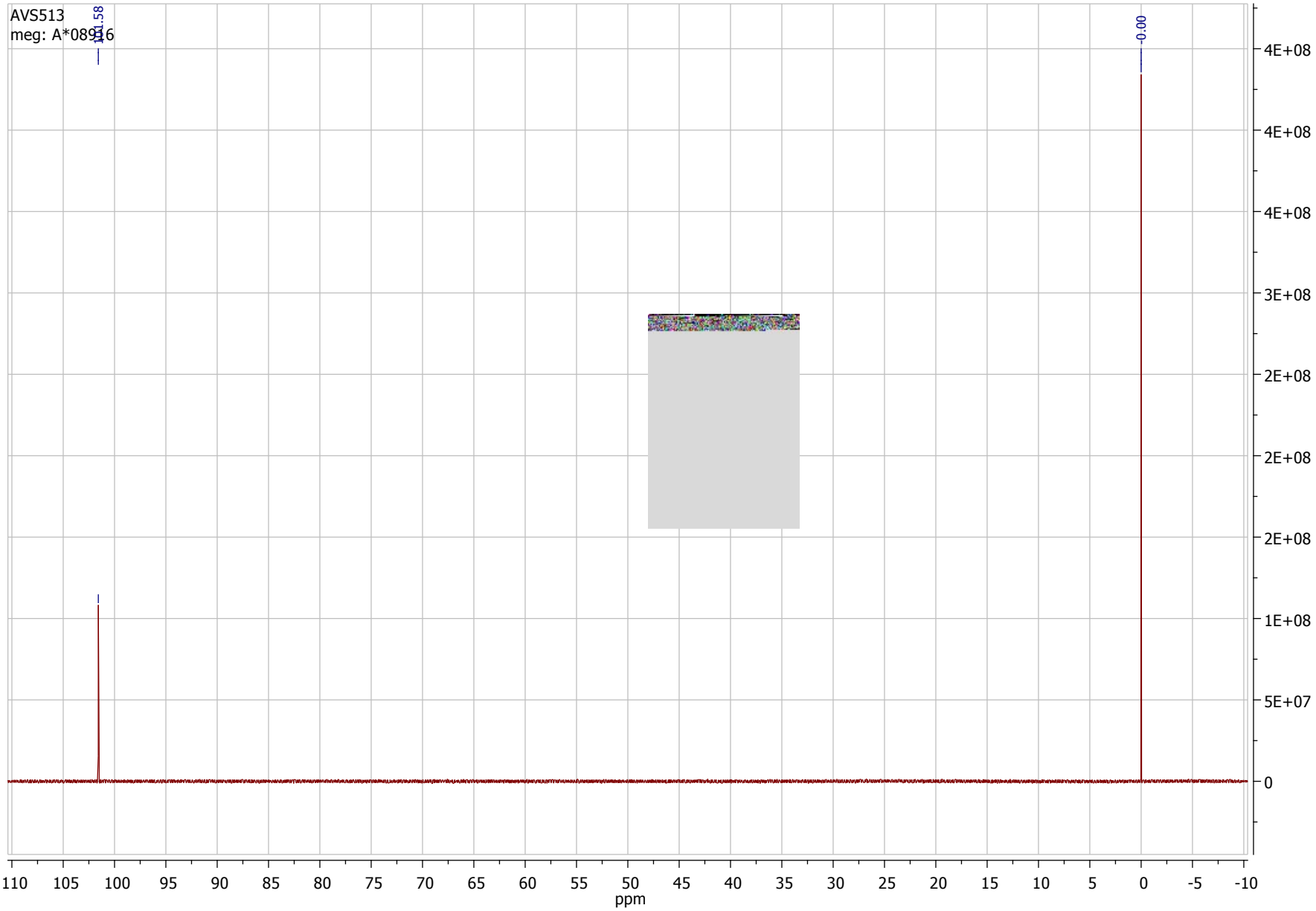

AVS640
ema: A*14136
158.00
148.58
141.18
139.84
138.66
131.46
129.27
128.27
125.29
124.03
119.32
40.00
39.92
39.83
39.76
39.67
39.50
39.33
39.17
39.00
NO2
N+
CH3
BF4-
3q
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

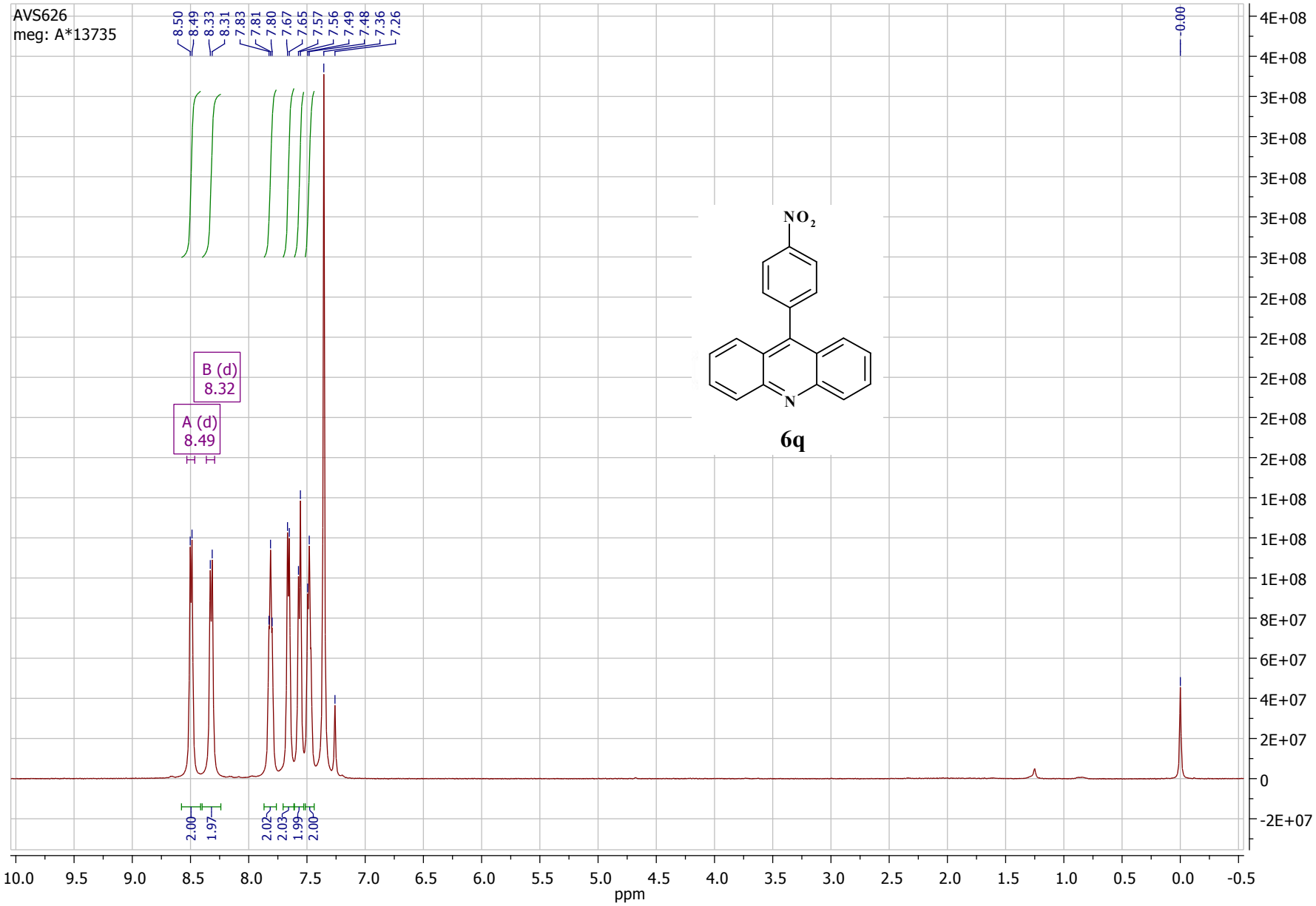

AVS335v
meg: A*11222
8.26
8.24
8.17
8.15
7.91
7.90
7.89
7.89
7.88
7.87
7.76
7.74
7.59
7.58
7.56
7.55
7.54
3.34
2.51
0.00
CN
N
6o
2.00
2.03
2.09
2.01
4.09
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm

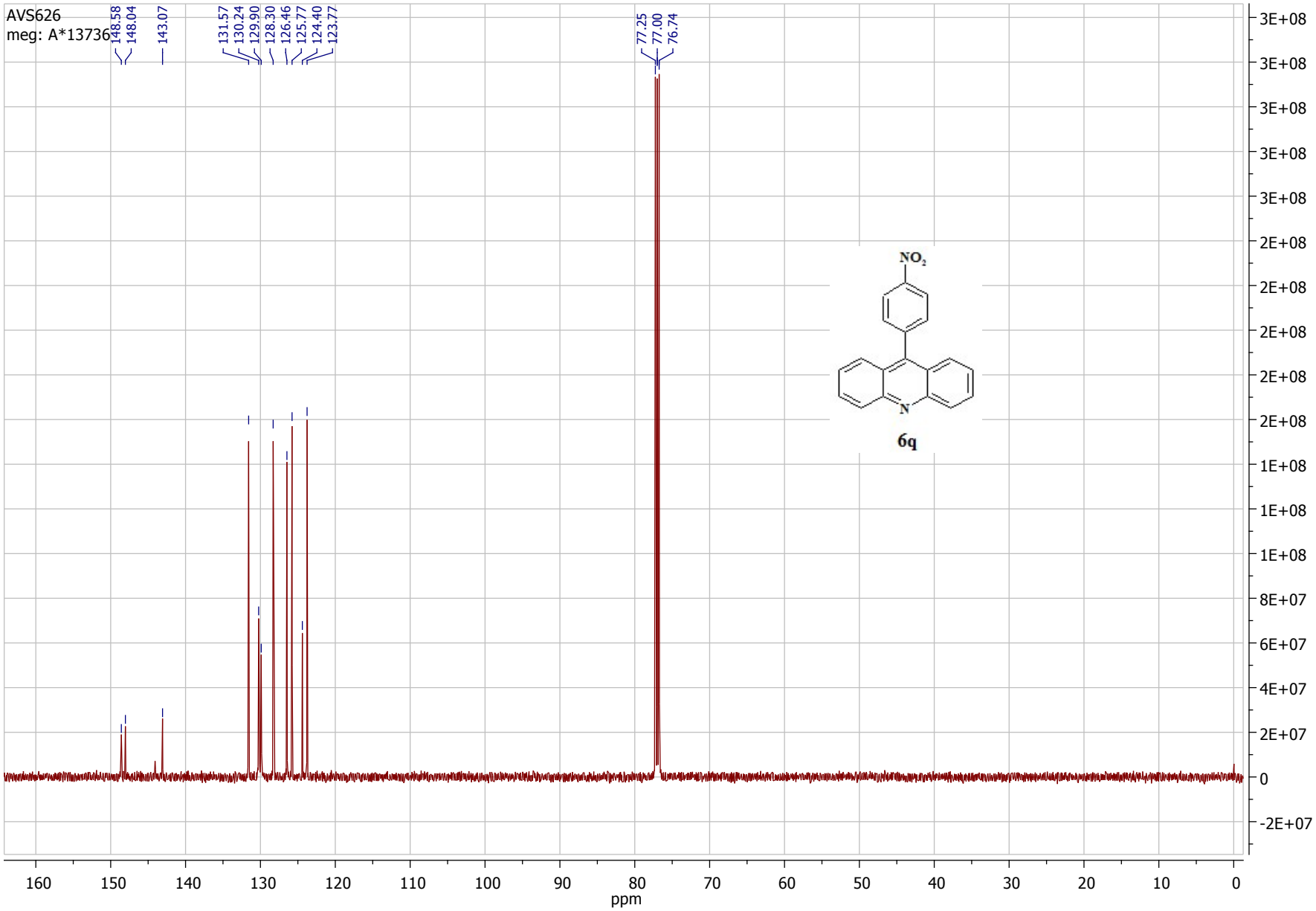

AVS335v
meg: A*11223
148.08
144.50
140.35
132.59
131.37
130.37
129.41
126.58
125.89
123.84
118.66
111.60
40.00
39.92
39.83
39.76
39.67
39.59
39.50
39.33
39.17
39.00
CN
N
6o
ppm

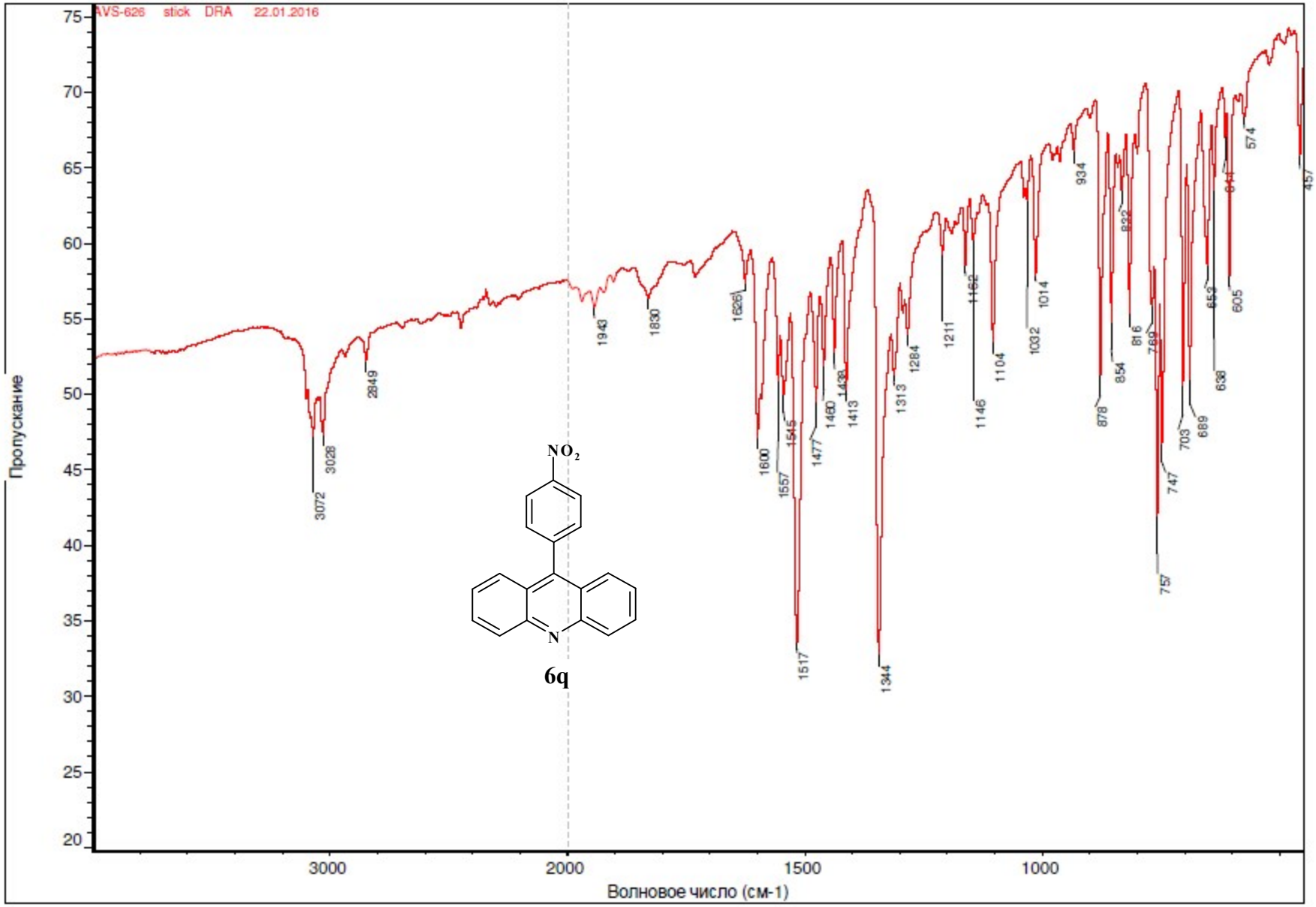

AVS335w
meg: A*11229
8.26
8.25
8.06
8.04
7.90
7.89
7.88
7.87
7.78
7.76
7.60
7.58
7.57
7.55
3.33
2.50
2.50
-0.00
CF3
N
6p
2.00
2.00
2.17
2.00
4.09
ppm


AVS335w
meg: A*11230
148.09
144.70
139.59
131.18
130.31
129.38
126.50
125.94
125.73
125.55
125.52
123.99
2E+07
2E+07
2E+07
2E+07
2E+07
2E+07
2E+07
1E+07
1E+07
1E+07
1E+07
1E+07
1E+07
9E+06
8E+06
7E+06
6E+06
5E+06
4E+06
3E+06
2E+06
1E+06
0
-1E+06
-2E+06
-3E+06
155
150
145
140
135
130
125
120
115
ppm


AVS513
meg: A*08916
101.58
-0.00
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10
ppm

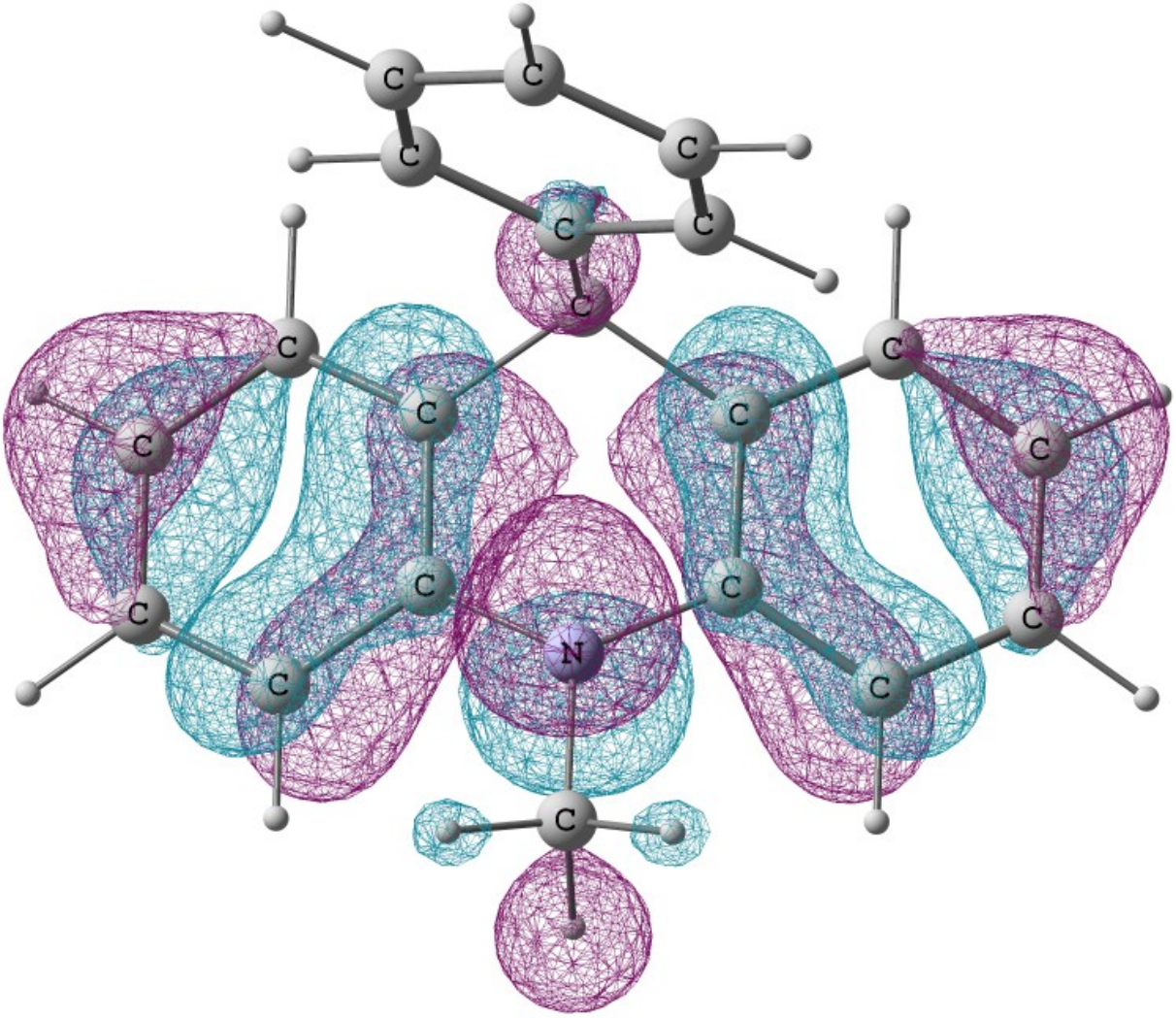

AVS626
meg: A*13735
8.50
8.49
8.33
8.31
7.83
7.81
7.80
7.67
7.65
7.57
7.56
7.49
7.48
7.36
7.26
-0.00
B (d)
8.32
A (d)
8.49
NO2
N
6q
2.00
1.97
2.02
2.03
1.99
2.00
ppm


AVS626
meg: A*13736
148.58
148.04
143.07
131.57
130.24
129.90
128.30
126.46
125.77
124.40
123.77
77.25
77.00
76.74
NO2
N
6q
3E+08
2E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

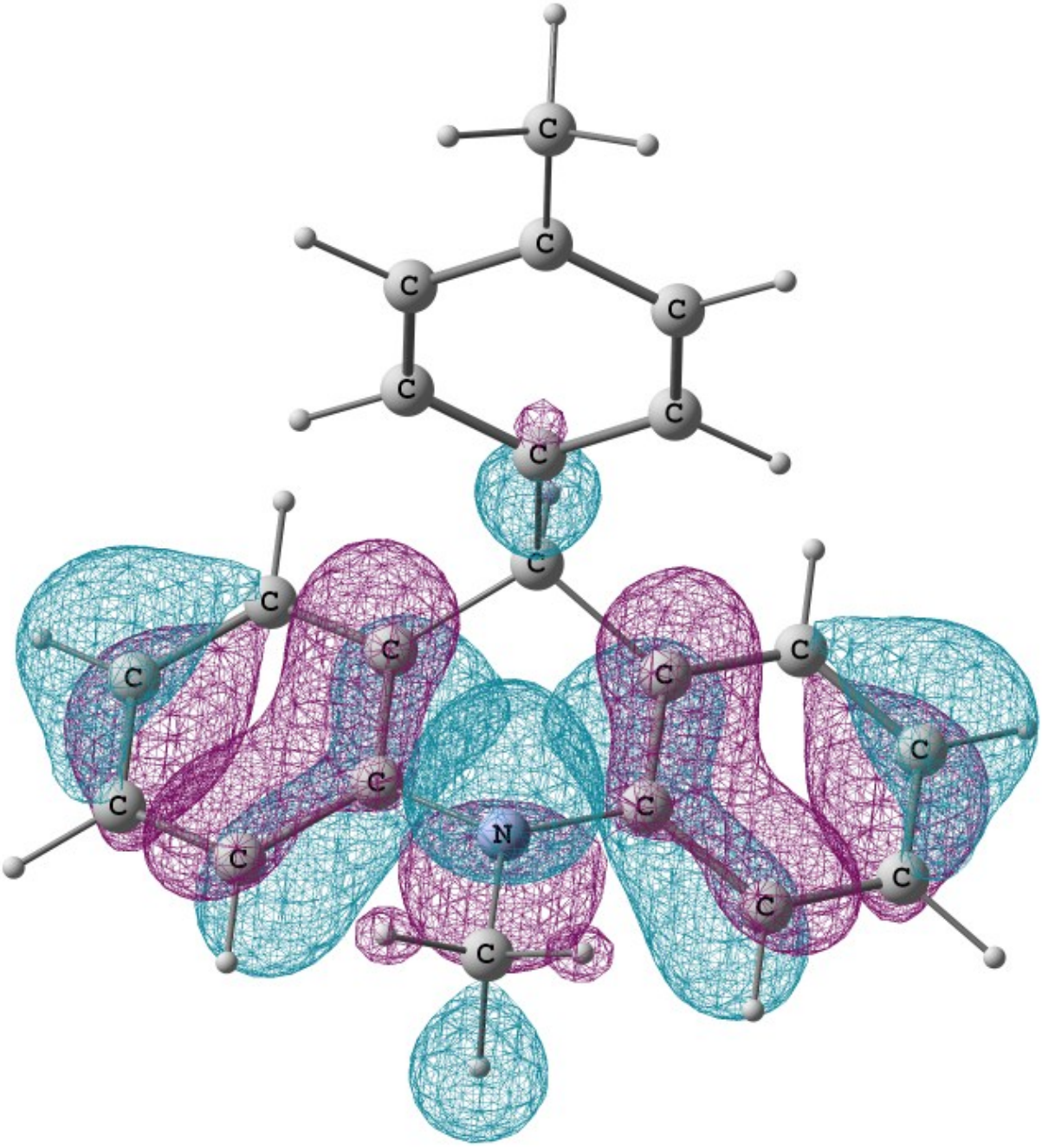

AVS-626 stick DRA 22.01.2016
Пропускание
Волновое число (см-1)
3072
3028
2849
1943
1830
1626
1600
1557
1545
1517
1477
1460
1438
1413
1344
1313
1284
1211
1162
1146
1104
1032
1014
934
878
854
832
816
769
757
747
703
689
653
638
605
574
457
NO2
N

6q

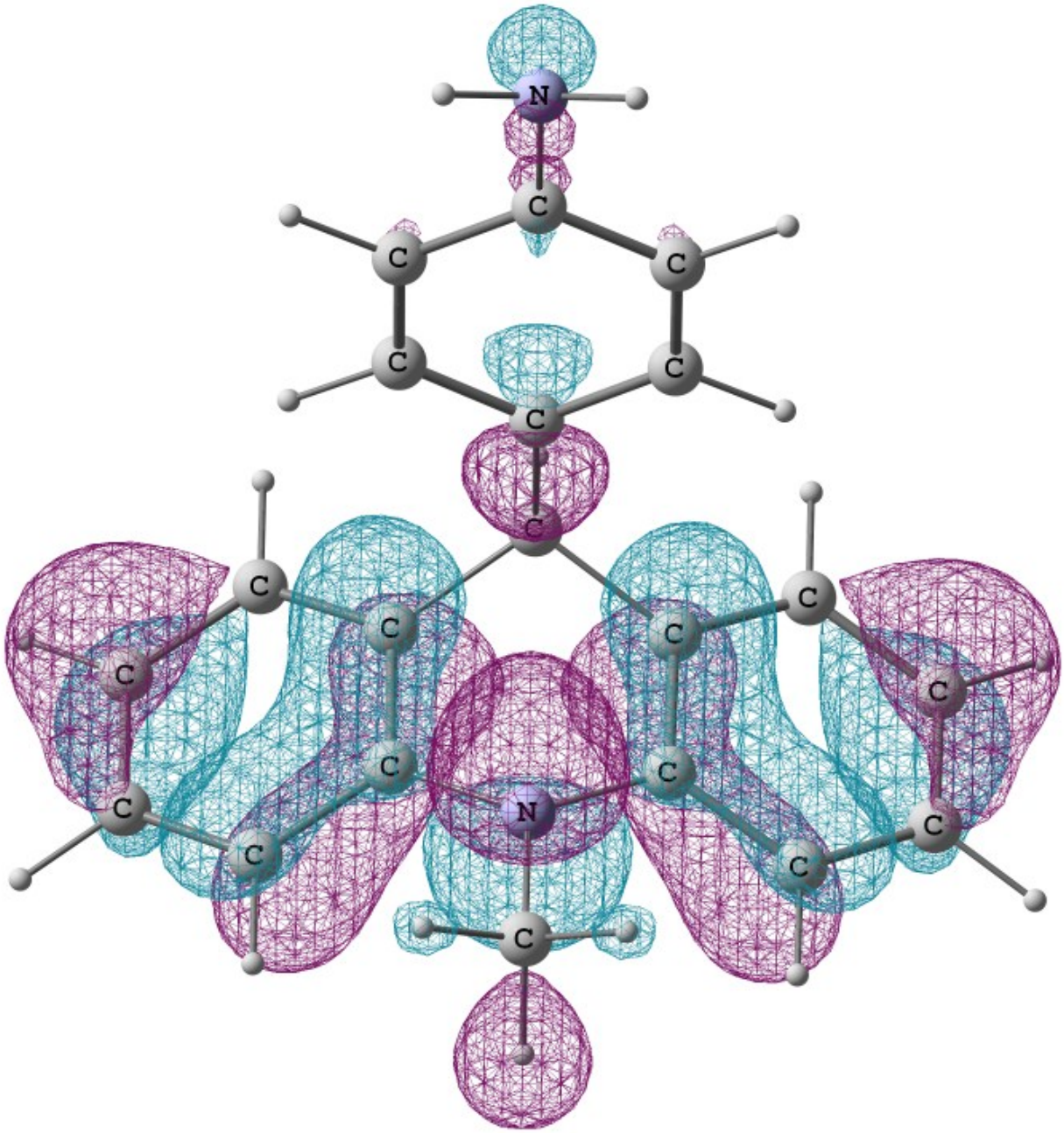
4. Visual representation of the HOMO obtained in the approximation of B3LYP/6-311+G (3df, 2p) for σ^H-adducts 2



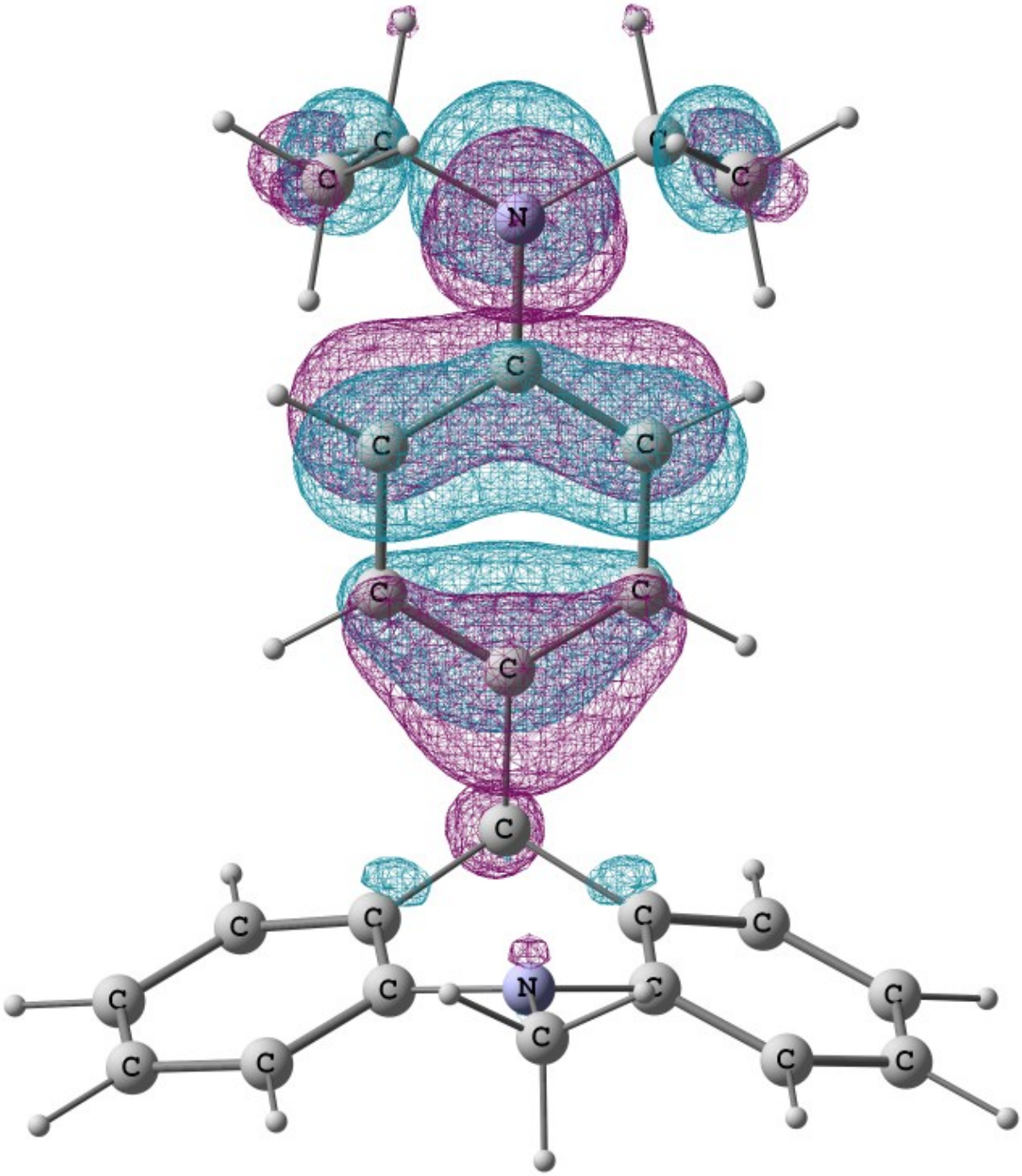
Visual representation of the HOMO for ***2a***



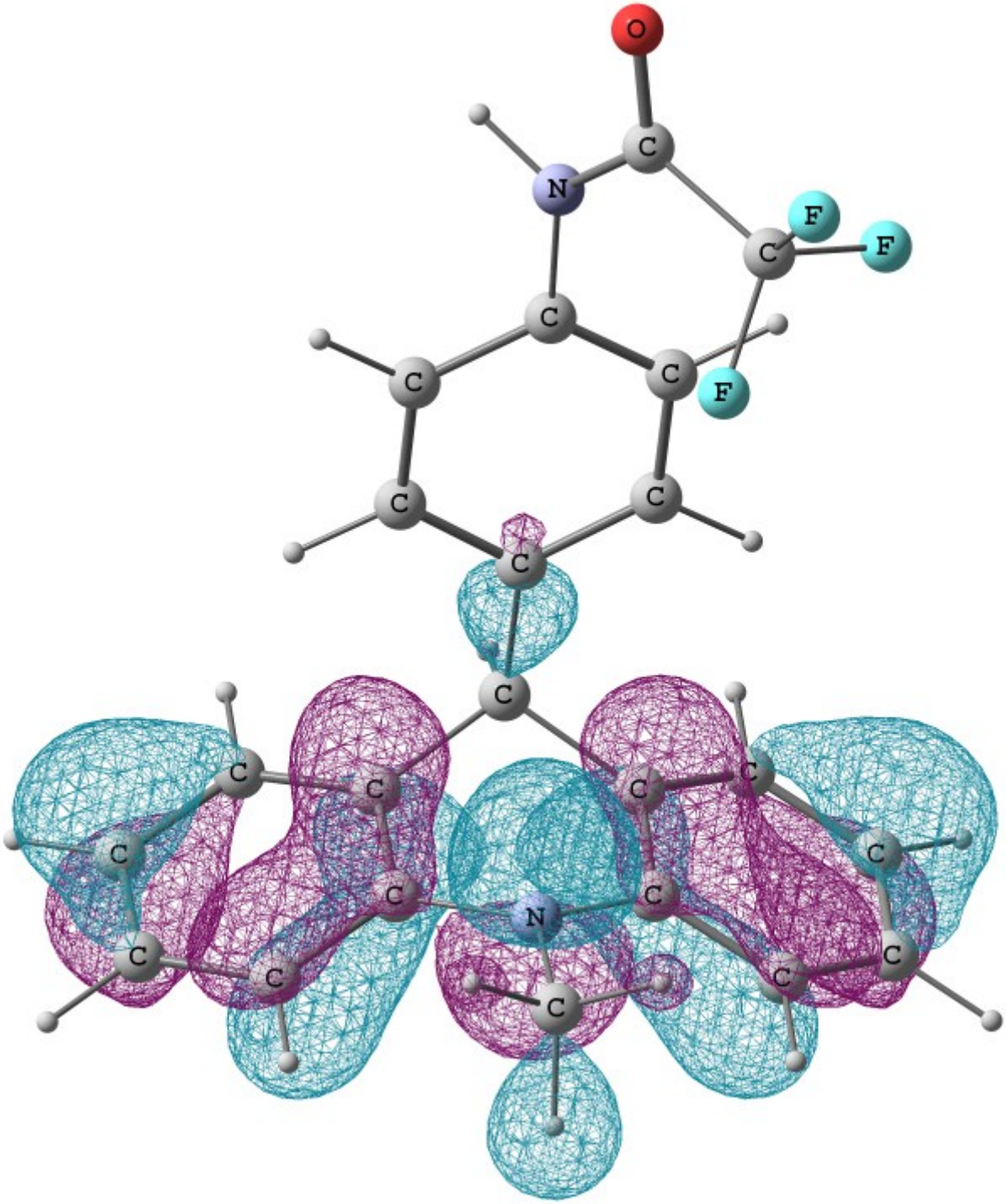
Visual representation of the HOMO for ***2b***



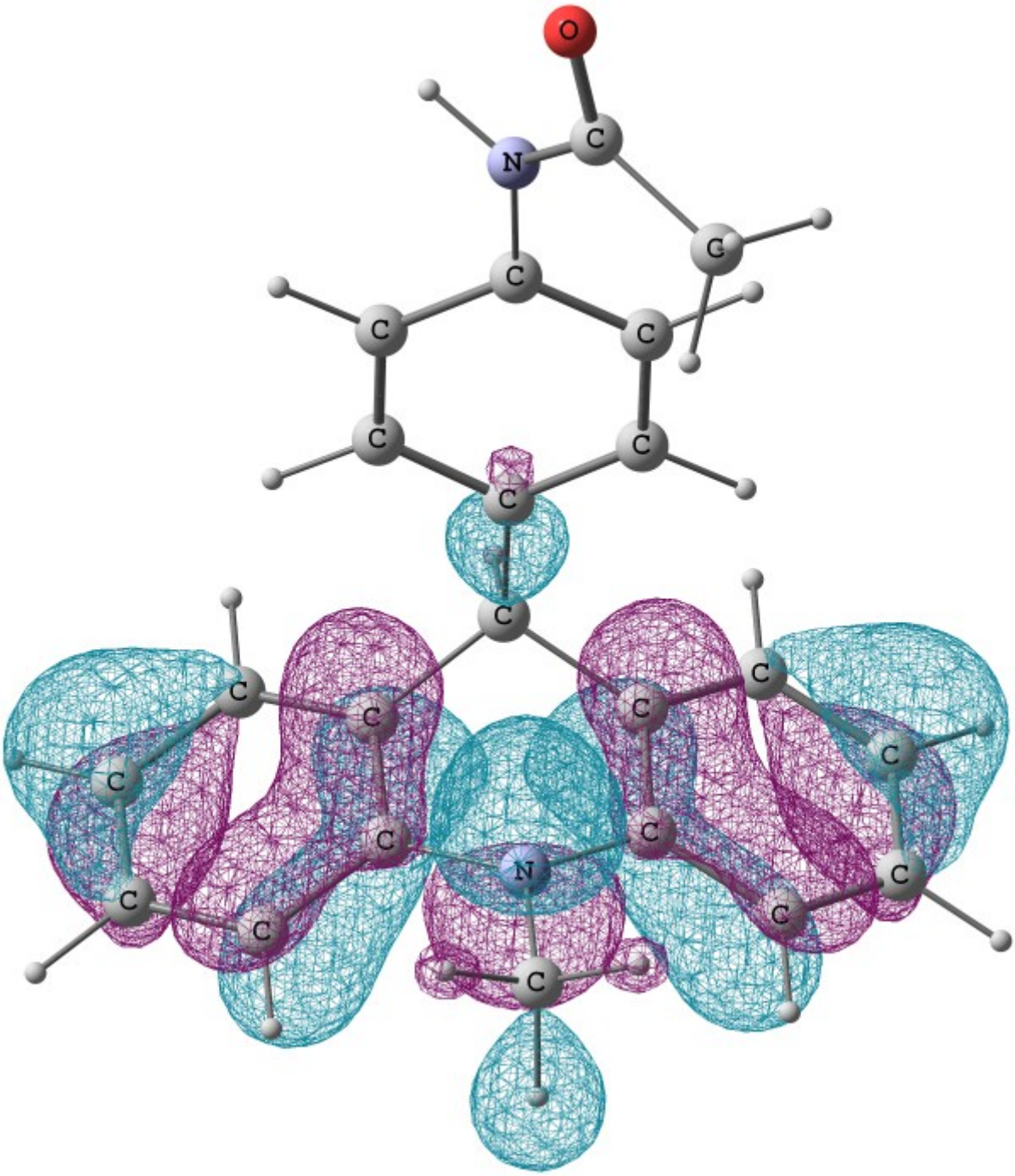
Visual representation of the HOMO for ***2c***



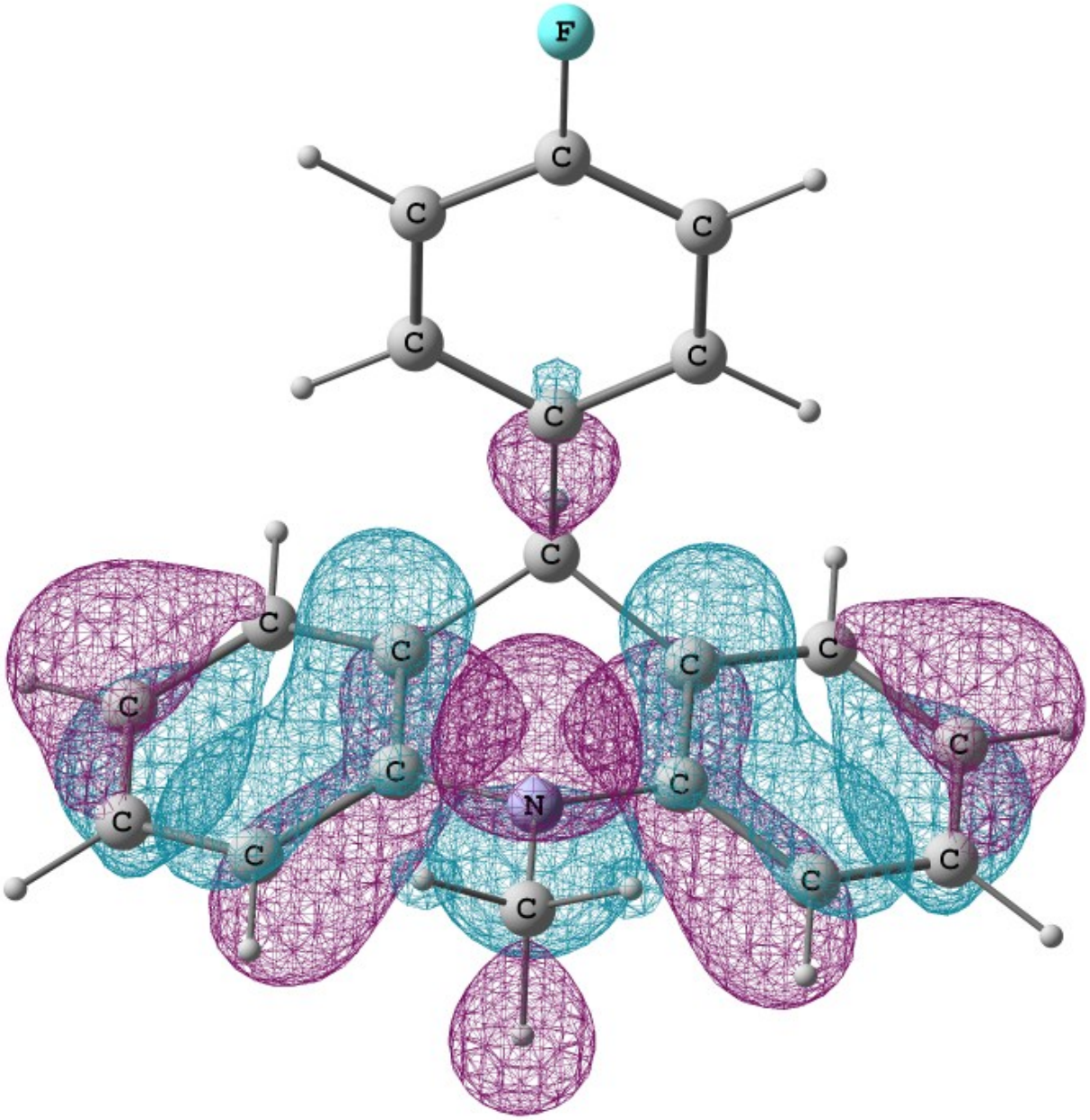
Visual representation of the HOMO for ***2d***



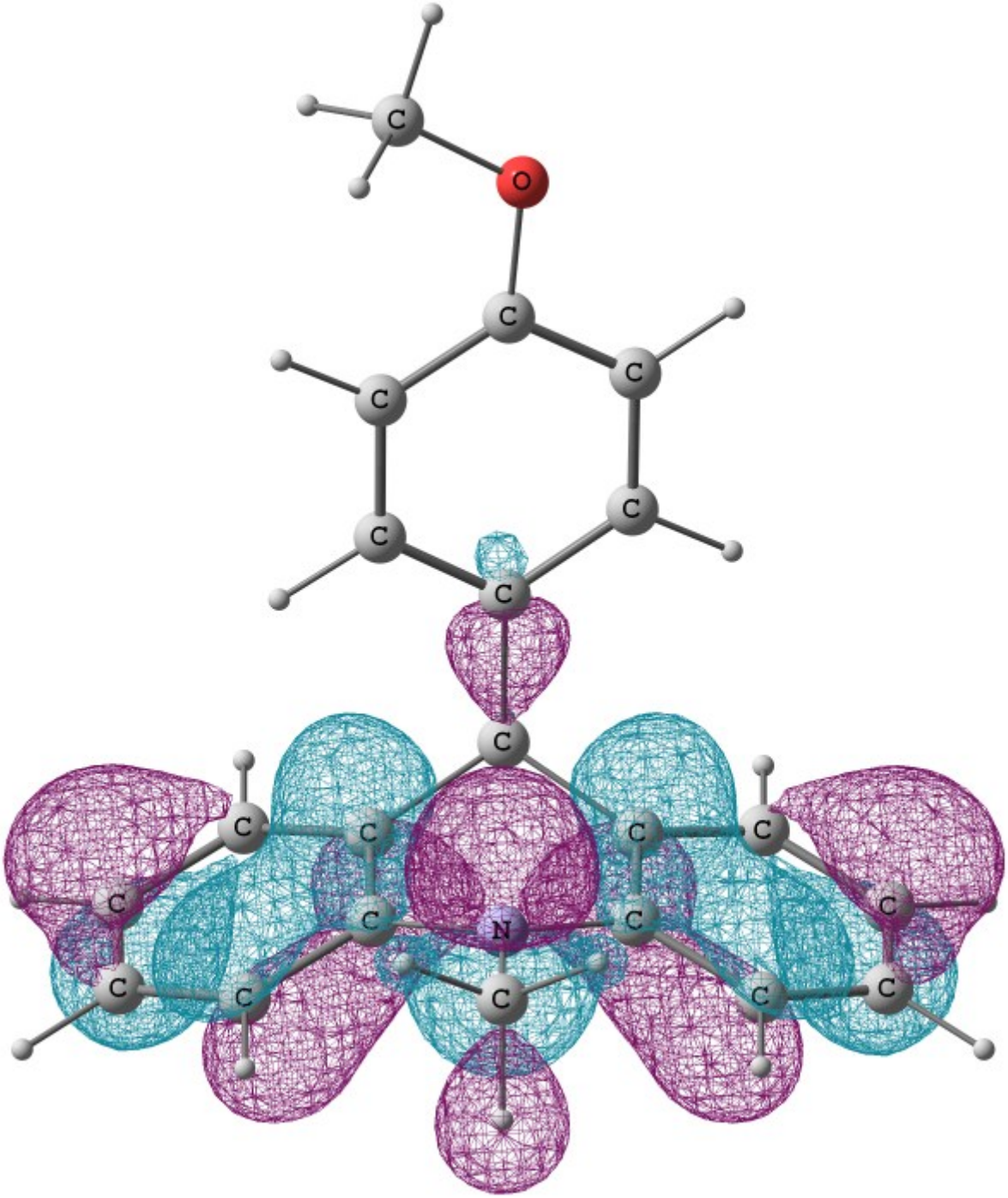
Visual representation of the HOMO for ***2e***



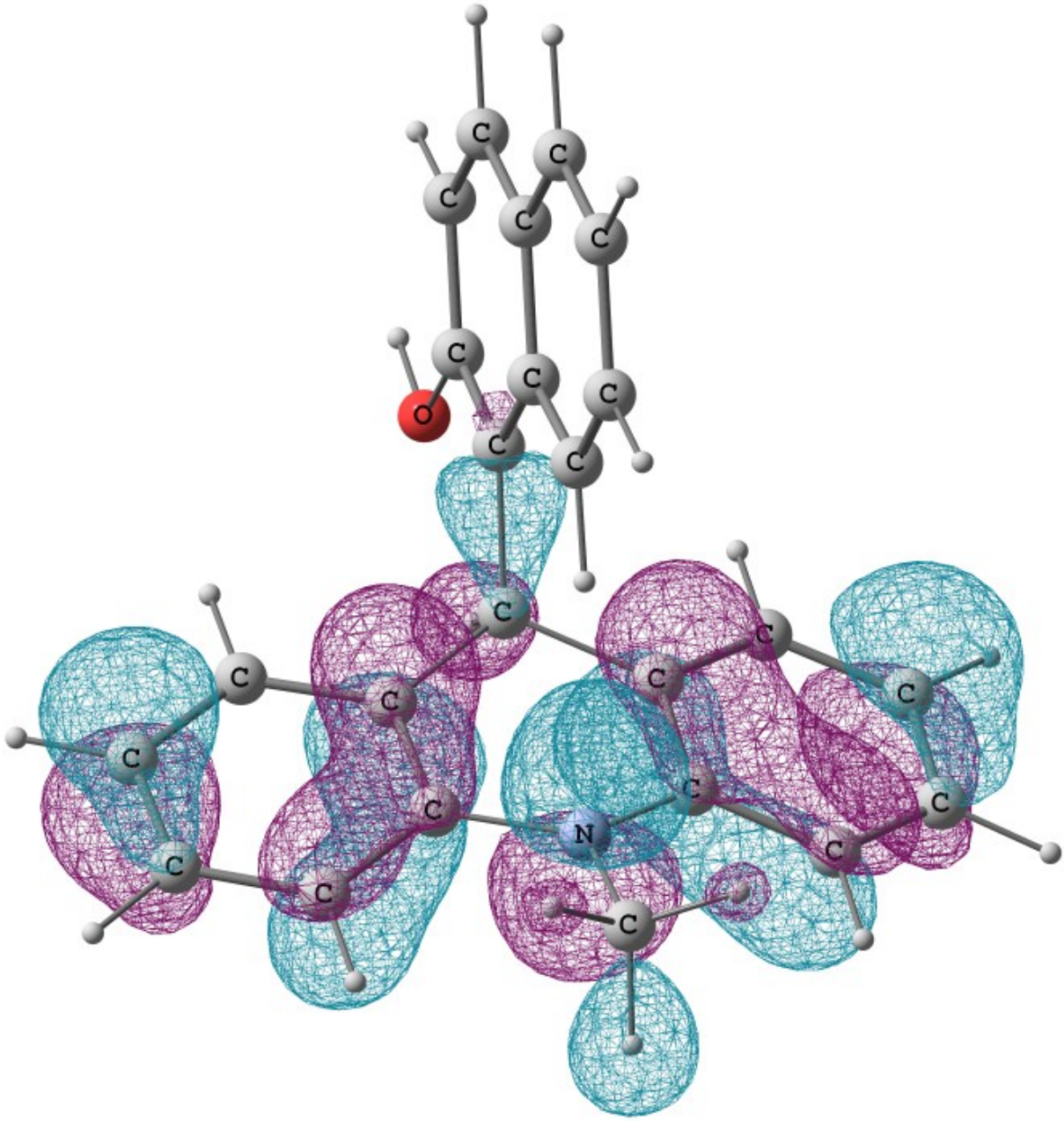
Visual representation of the HOMO for ***2f***



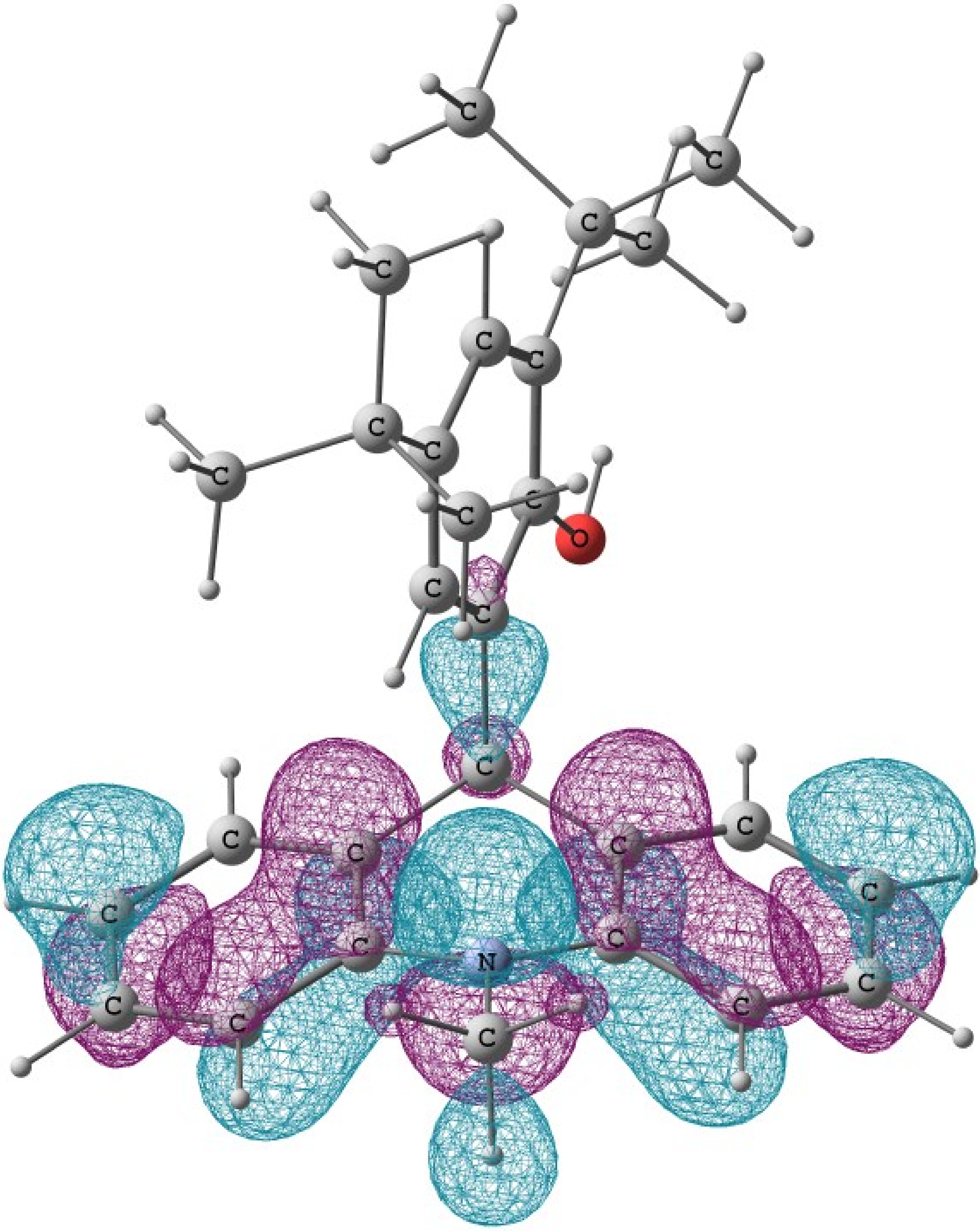
Visual representation of the HOMO for ***2g***



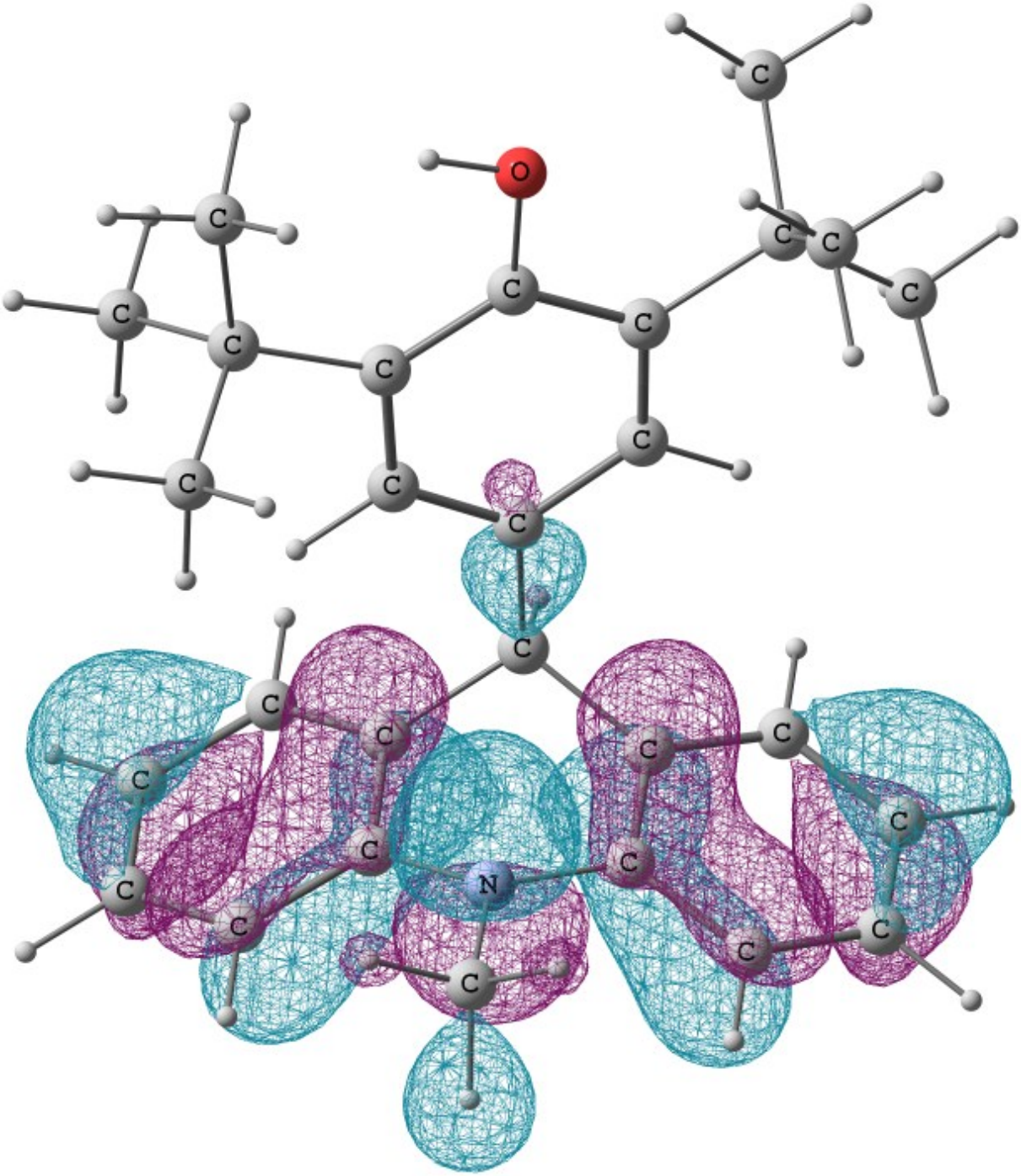
Visual representation of the HOMO for ***2h***



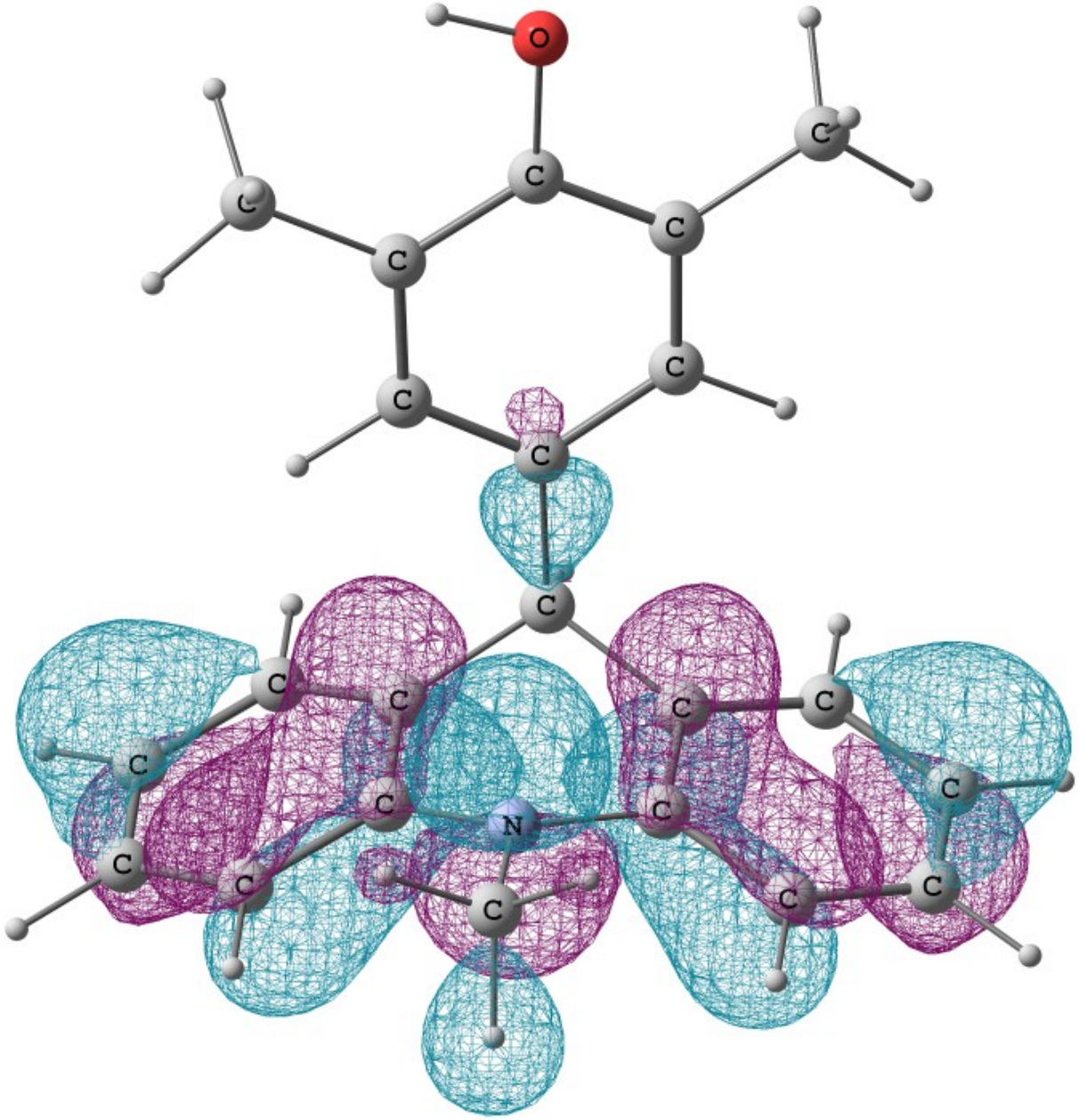
Visual representation of the HOMO for ***2i***



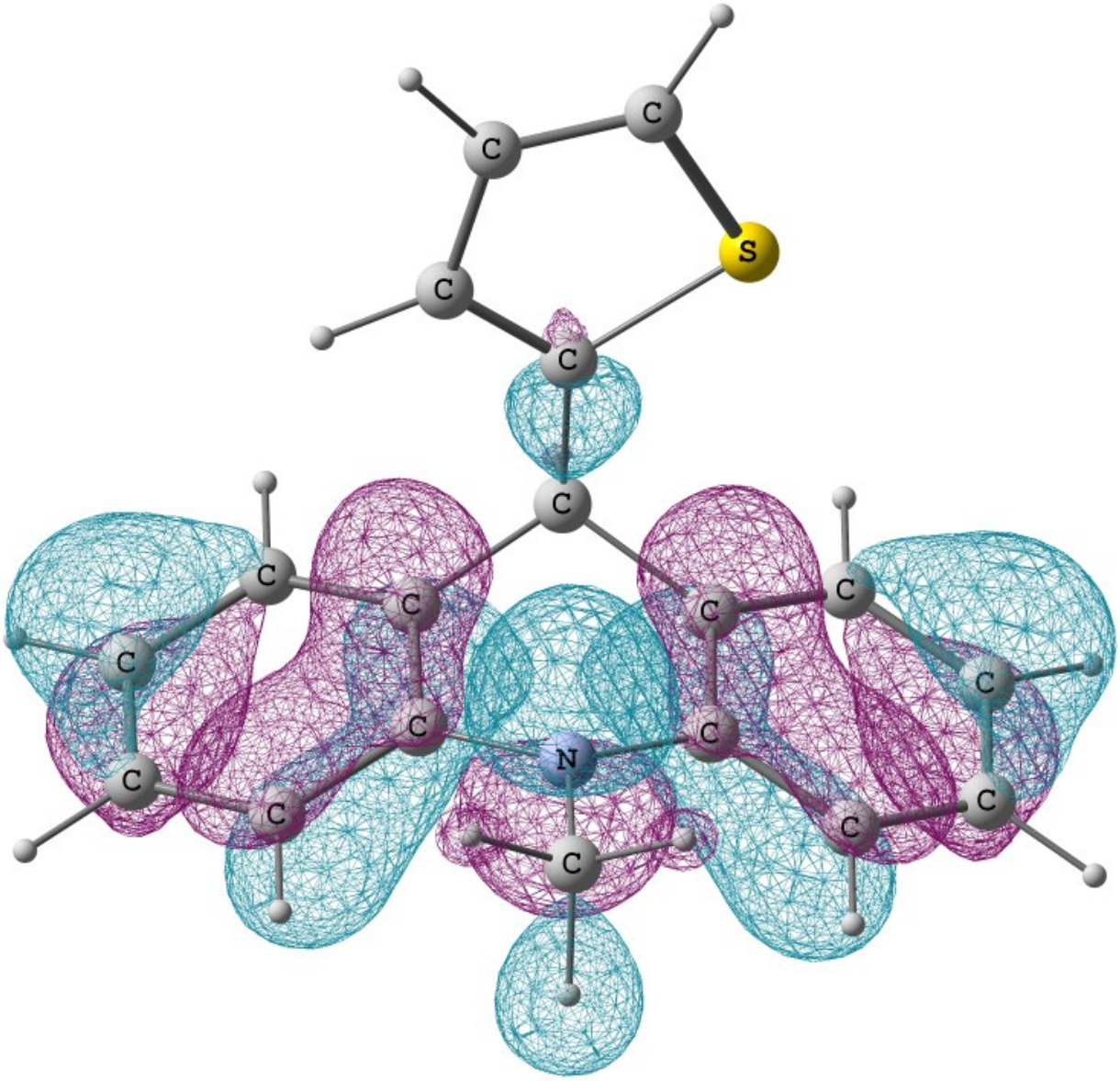
Visual representation of the HOMO for ***2j***



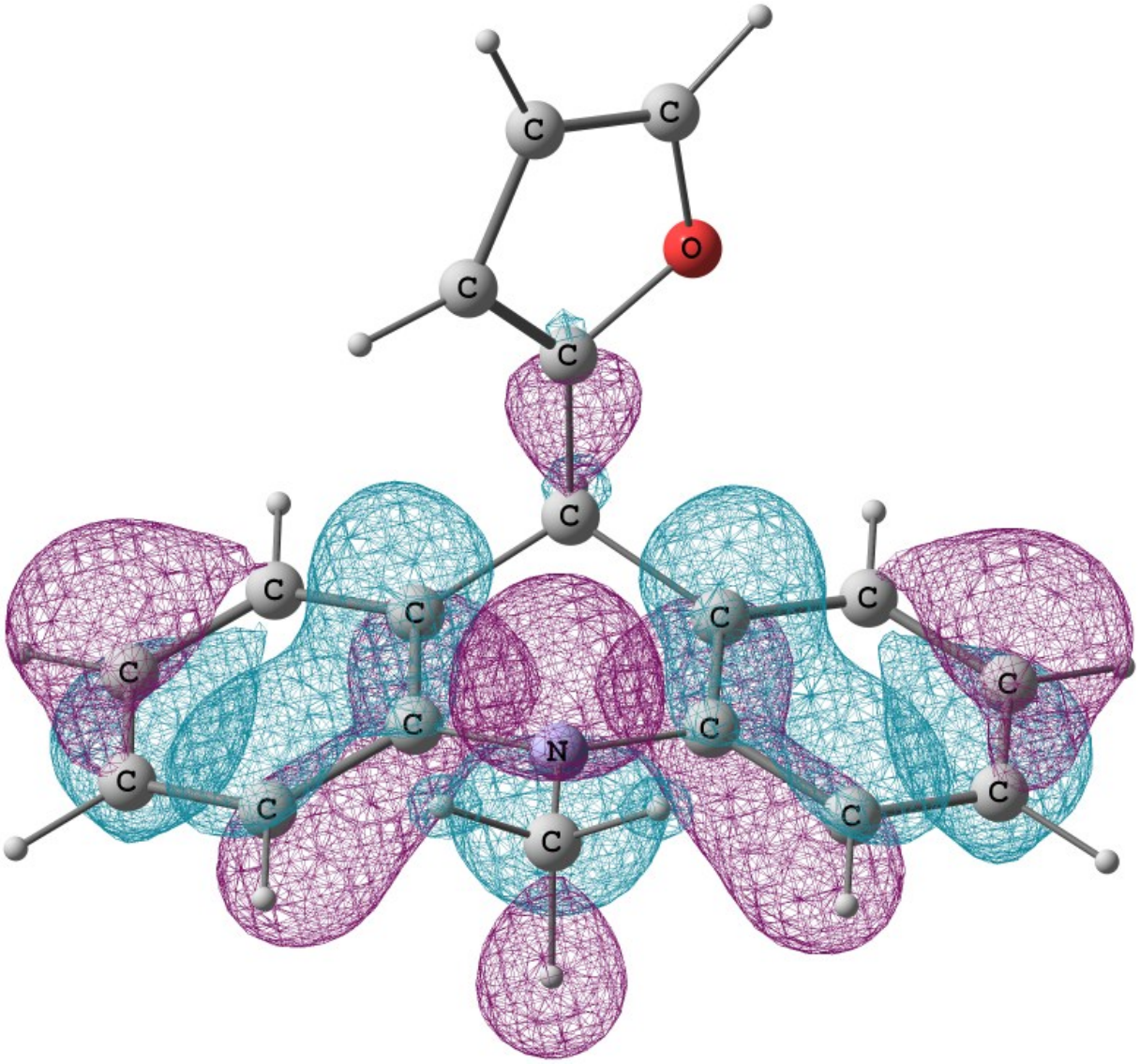
Visual representation of the HOMO for ***2k***



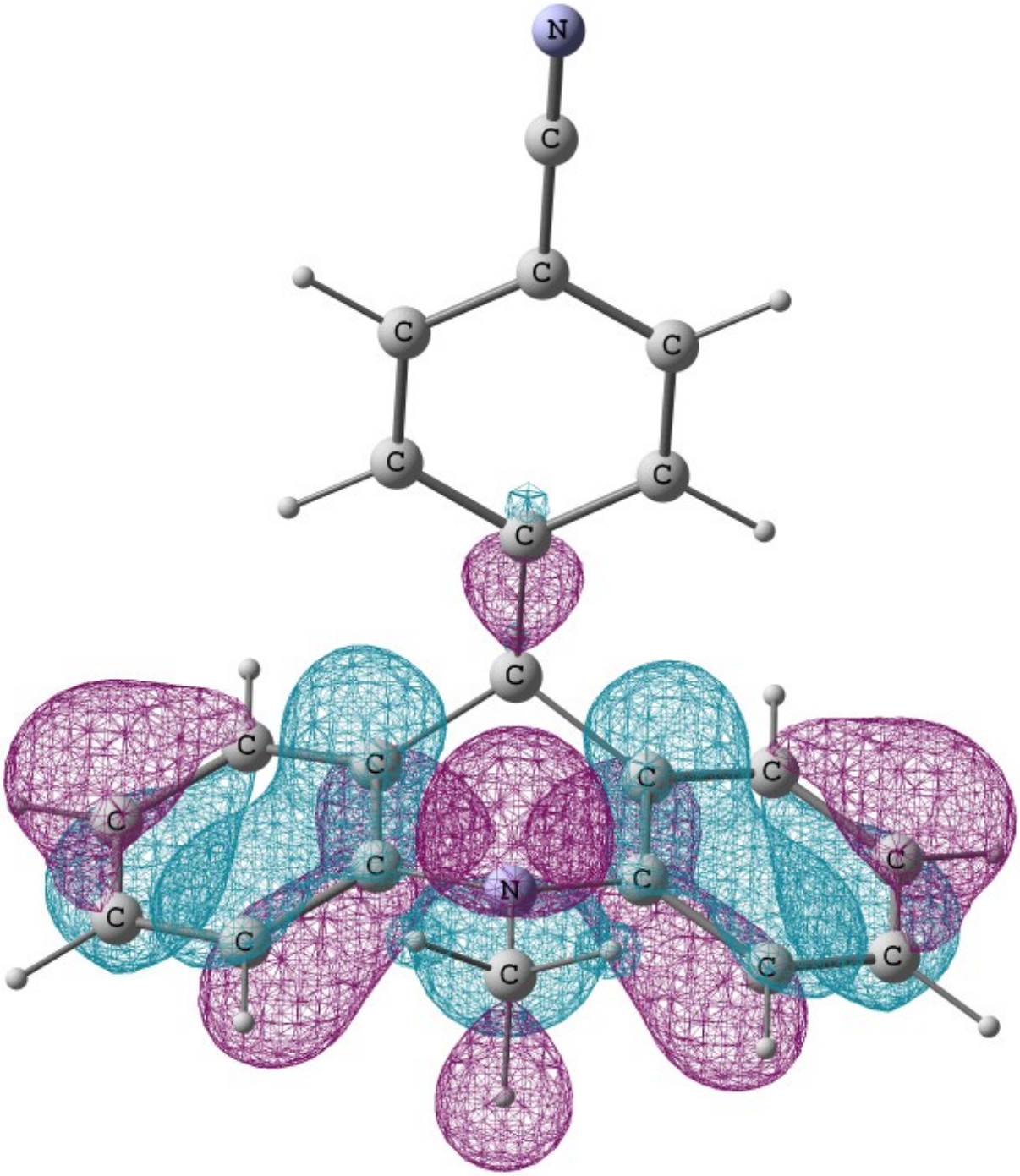
Visual representation of the HOMO for ***2l***



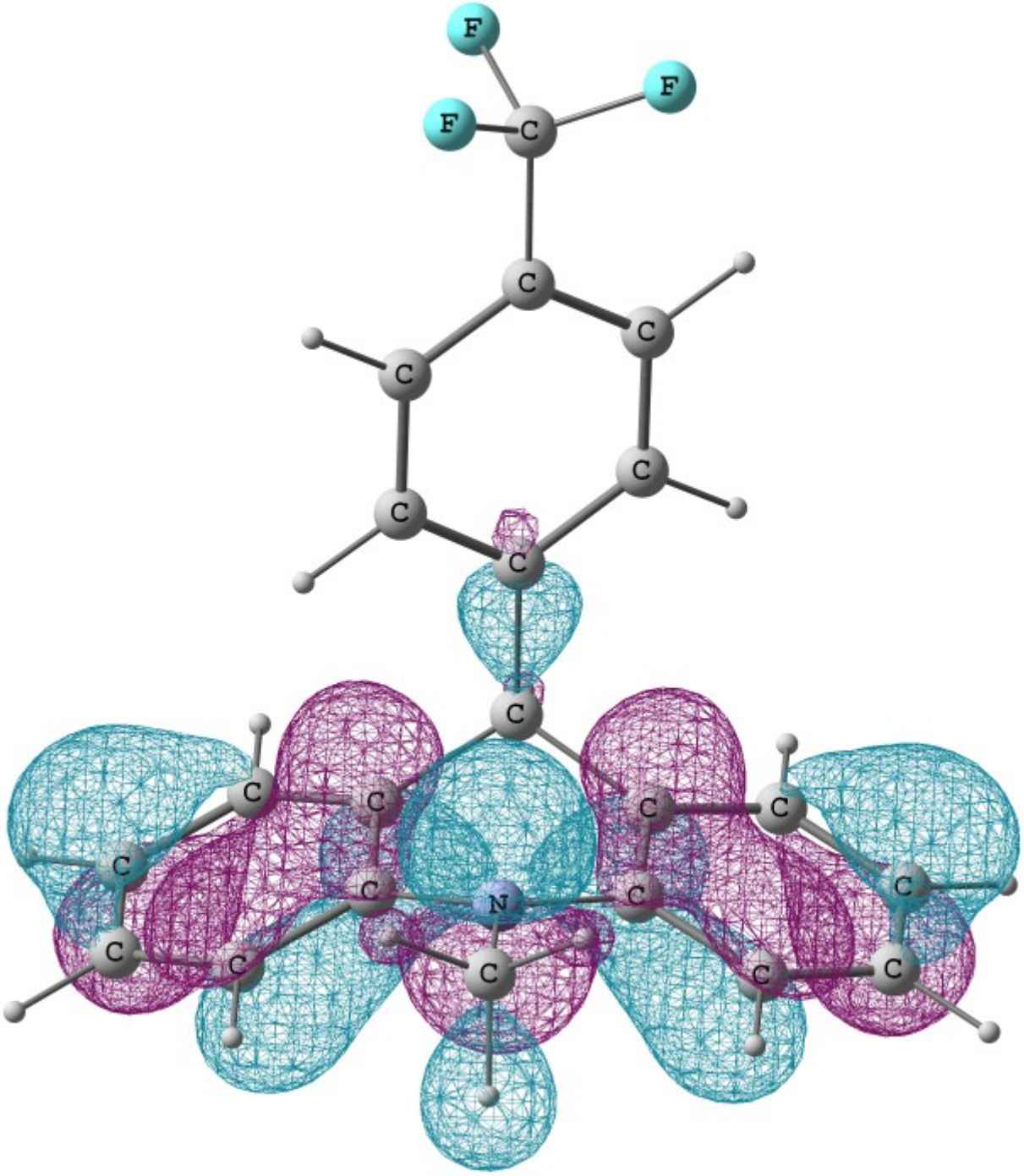
Visual representation of the HOMO for ***2m***



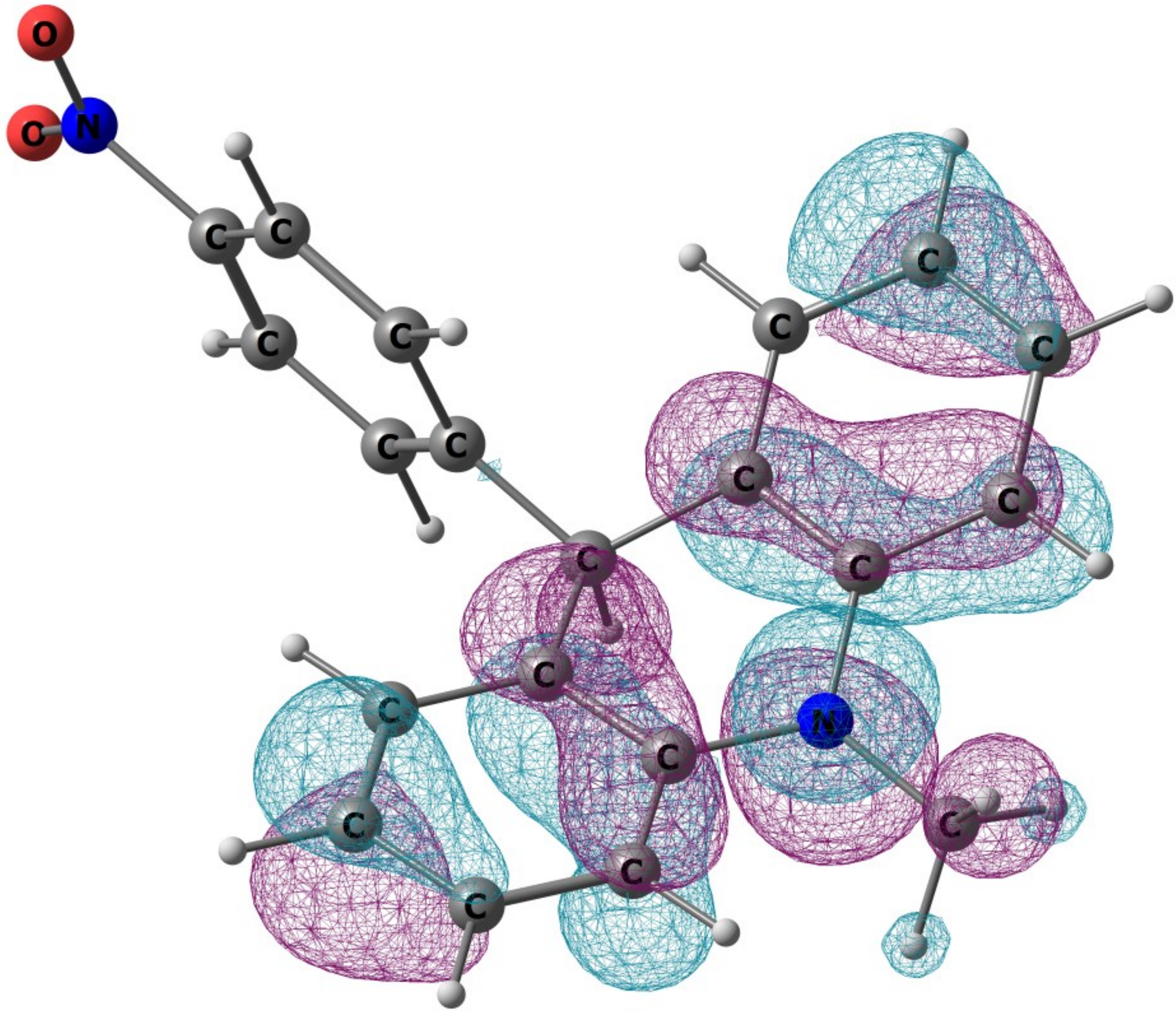
Visual representation of the HOMO for ***2n***



Visual representation of the HOMO for ***2o***

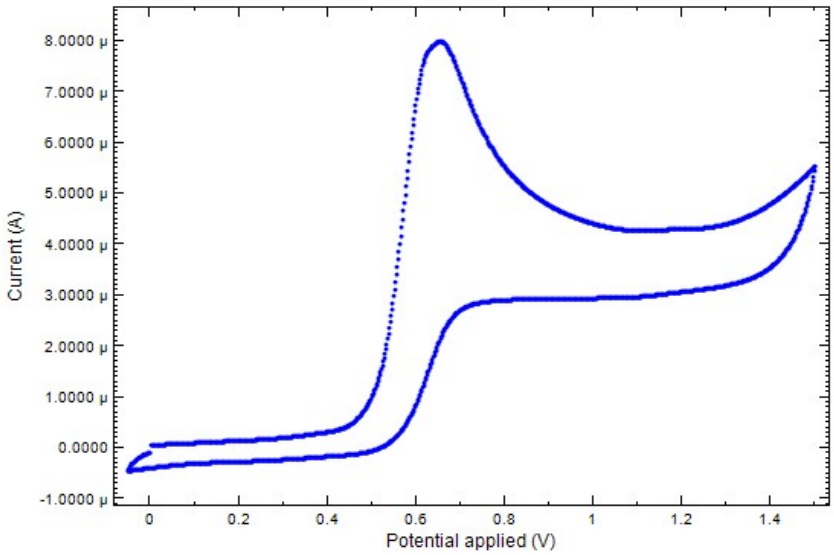


Visual representation of the HOMO for ***2p***

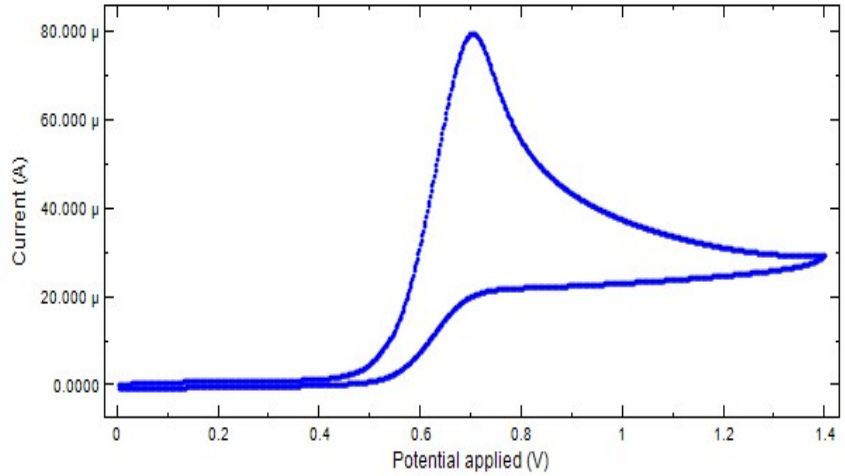


Visual representation of the HOMO for ***2q***

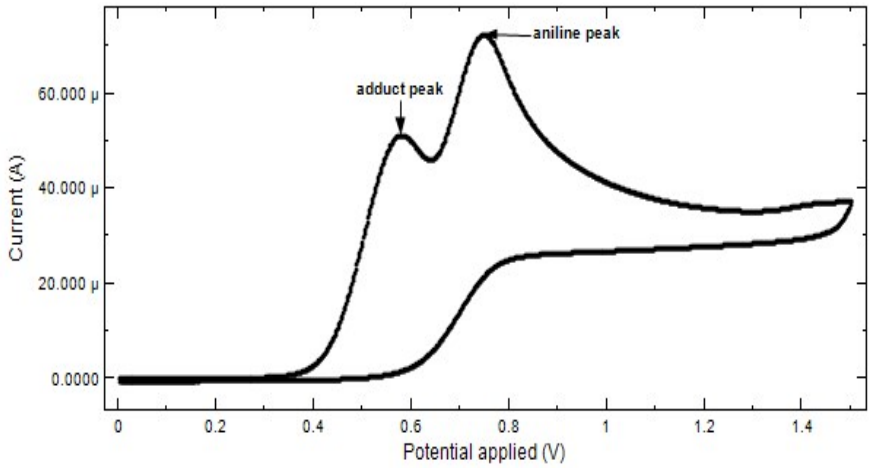
5. Cyclic voltammogrames



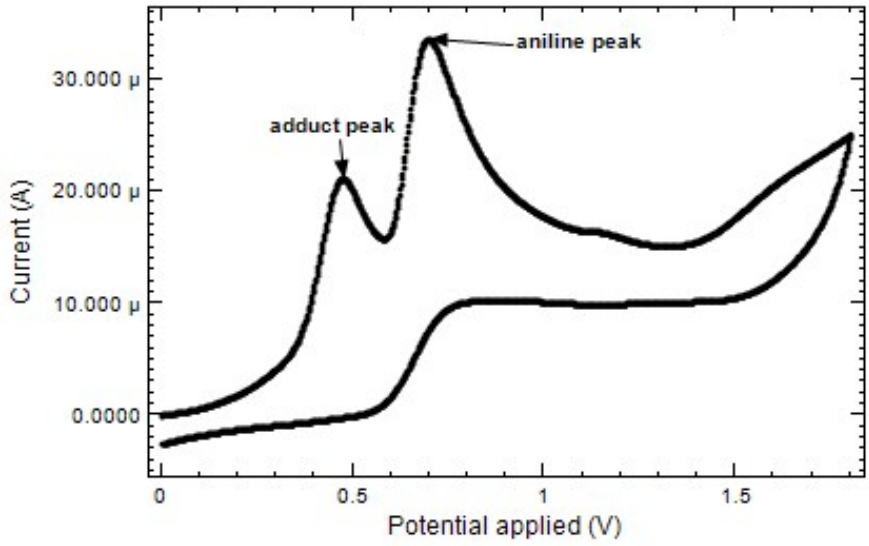
Cyclic voltammogram of **2a**



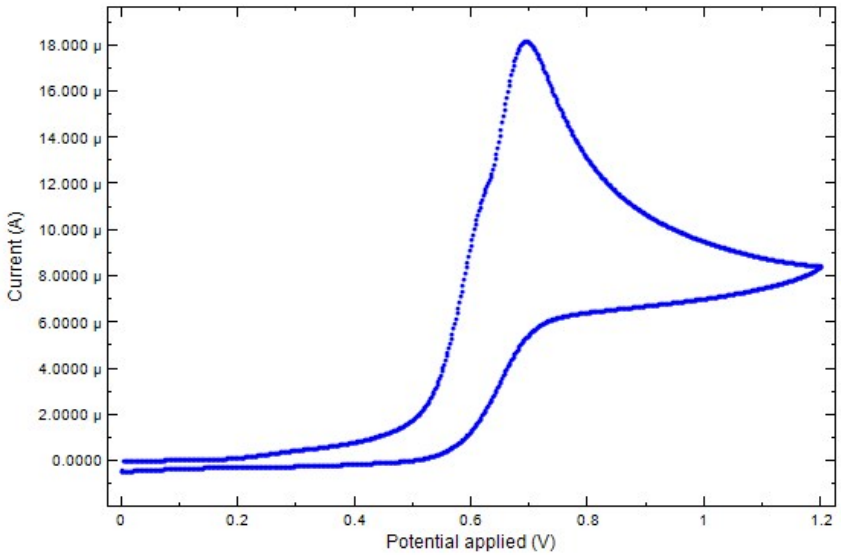
Cyclic voltammogram of **2b**



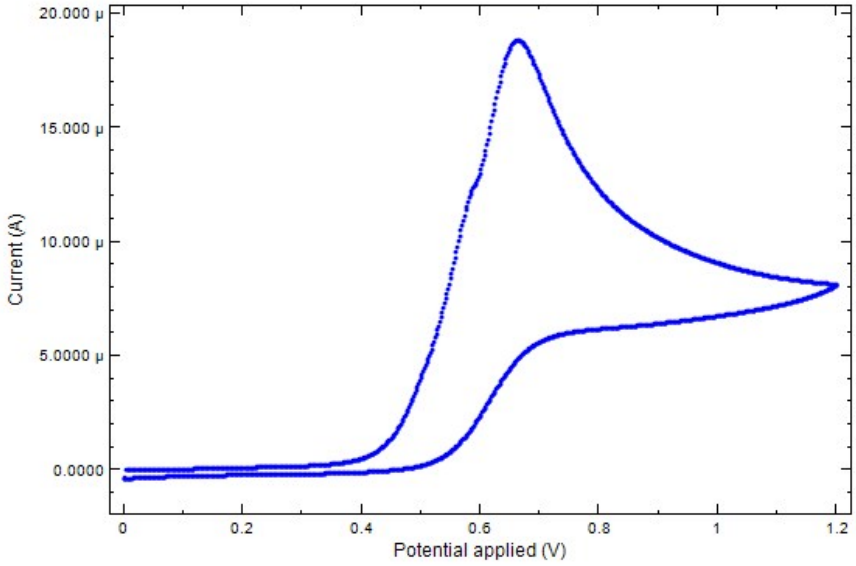
Cyclic voltammogram of **2c**



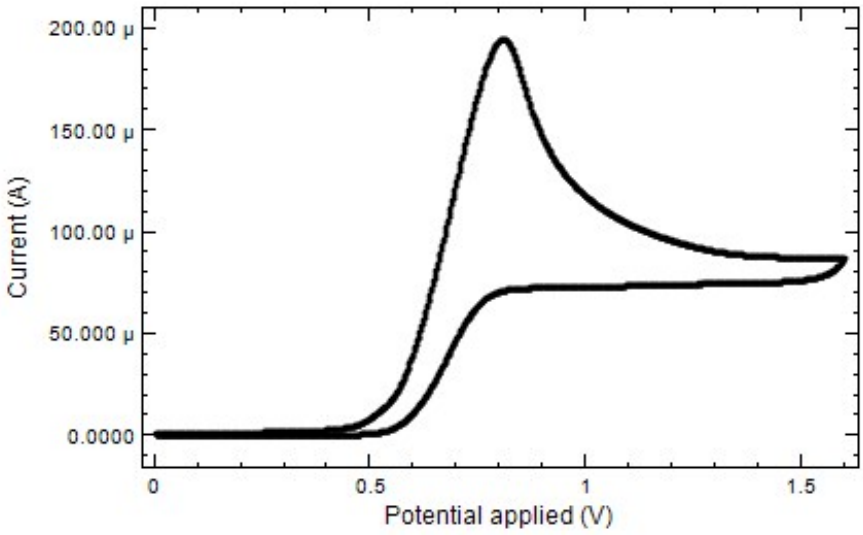
Cyclic voltammogram of **2d**



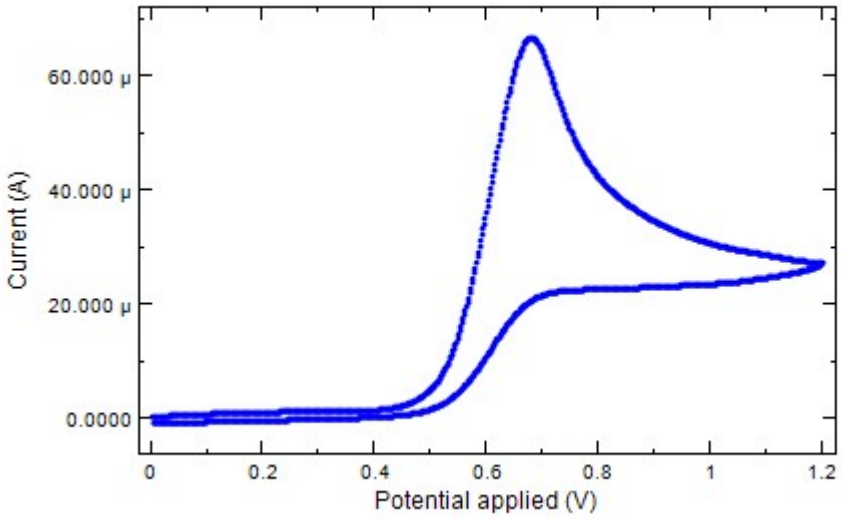
Cyclic voltammogram of **2e**



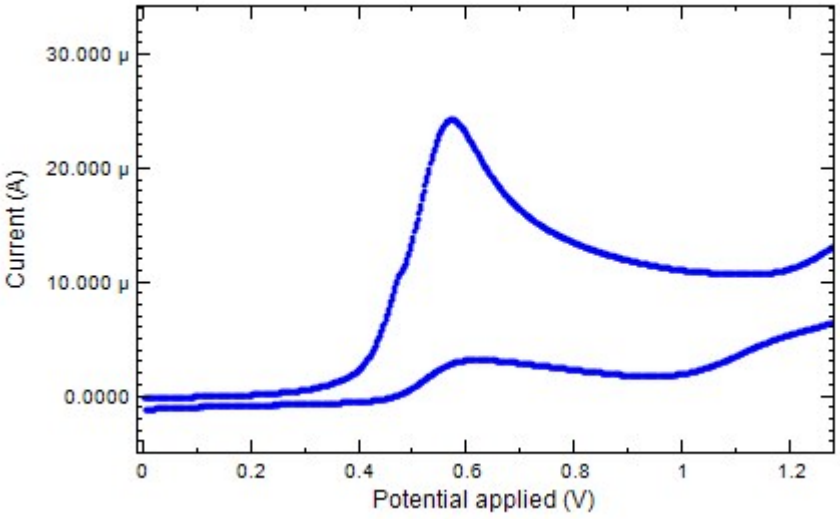
Cyclic voltammogram of **2f**



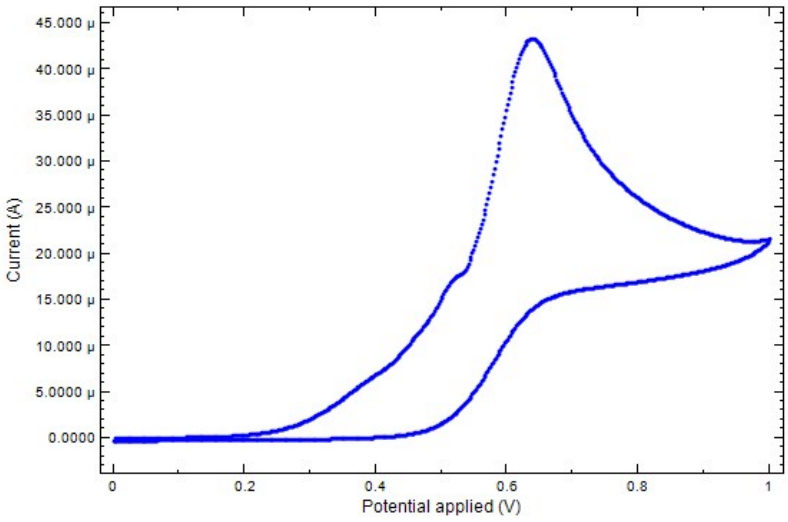
Cyclic voltammogram of **2g**



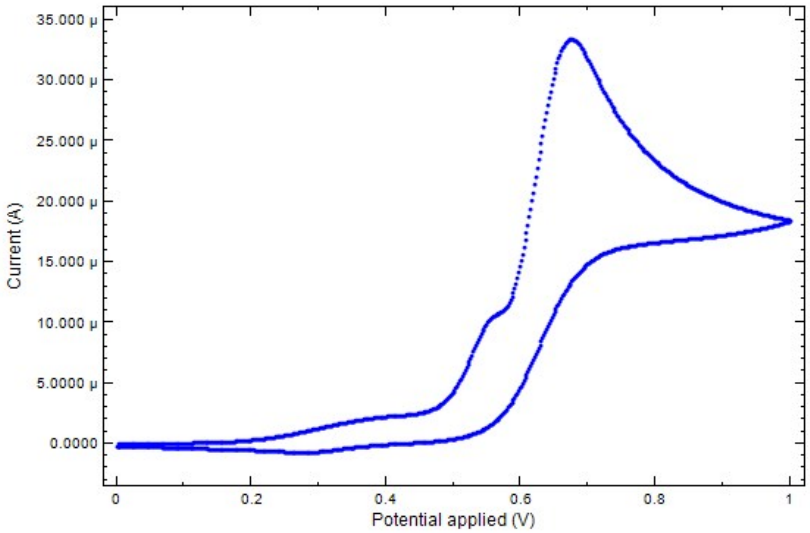
Cyclic voltammogram of **2h**



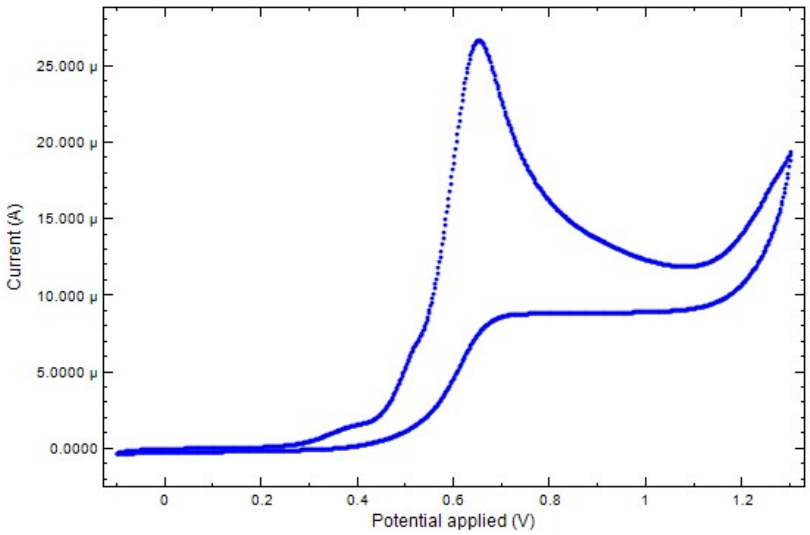
Cyclic voltammogram of **2i**



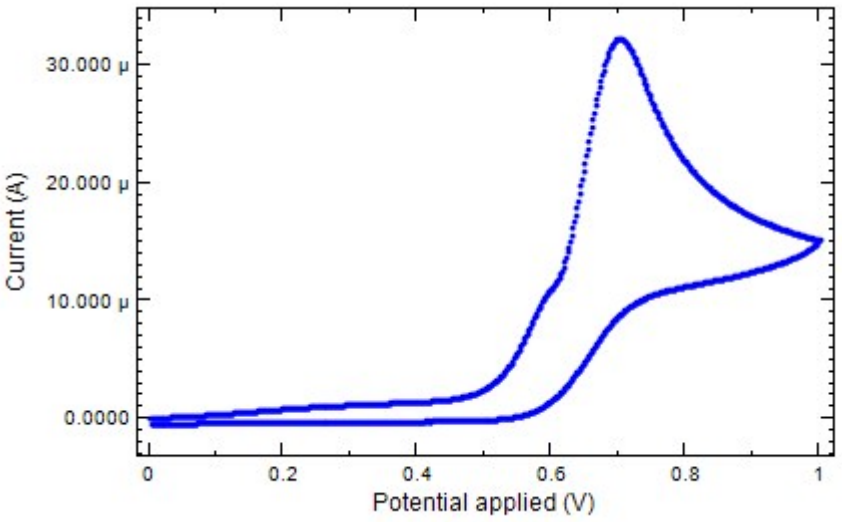
Cyclic voltammogram of **2j**



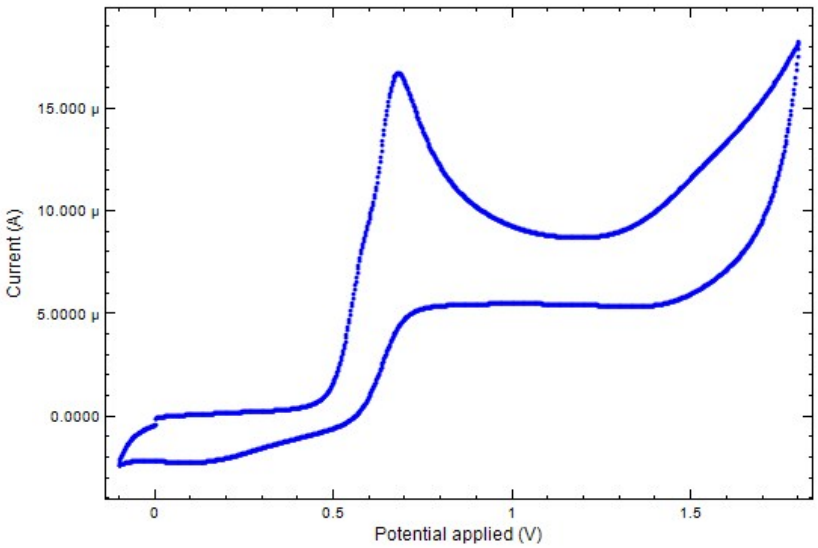
Cyclic voltammogram of **2k**



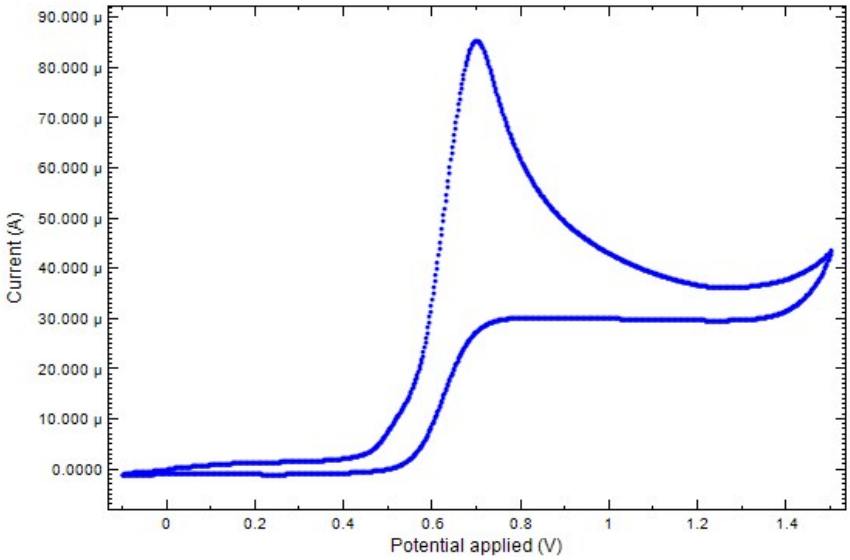
Cyclic voltammogram of **2l**



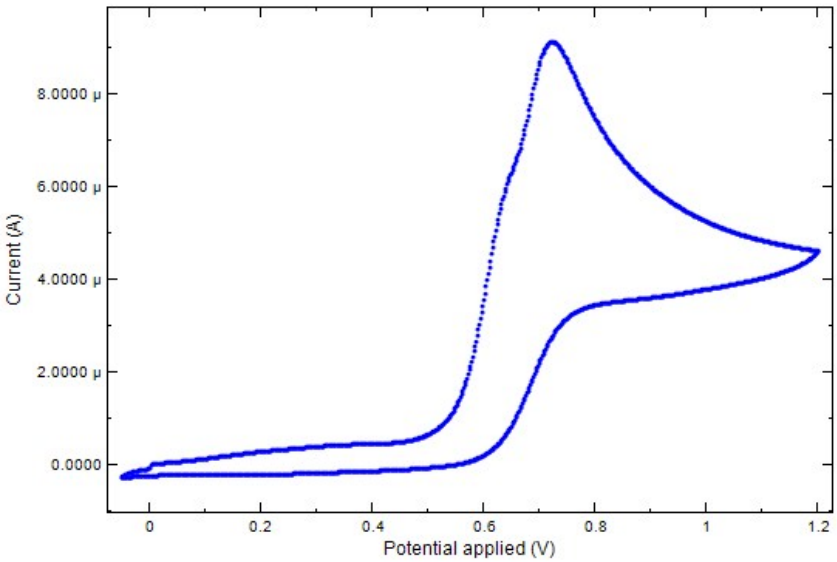
Cyclic voltammogram of **2n**



Cyclic voltammogram of **2o**



Cyclic voltammogram of **2p**



Cyclic voltammogram of **2q**