

**Synthesis of Nitriles from Aldehydes with Trimethylphenylammonium
Tribromide and Ammonium Acetate**

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Supporting Information

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General Information:

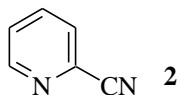
IR spectra were recorded on a Perkin Elmer Spectrum One FT-IR spectrometer.

^1H and ^{13}C NMR spectra were recorded with a JEOL JNM-EX270 spectrometer at room temperature and the chemical shifts (δ) are given relative to internal standard SiMe_4 in CDCl_3 .

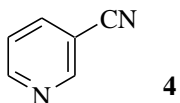
A number of IR and ^1H NMR spectra of aromatic and heterocyclic nitriles were in good agreement with those of corresponding compounds in the Aldrich Library of IR and ^1H NMR spectra. The Aldrich Library of Infrared spectra (Edition III) and The Aldrich Library of ^1H NMR Spectra (Edition II, vol. 2) were edited by Charles J. Pouchert.

The Aldrich library of IR spectra and ^1H NMR was published by Aldrich Chemical Company, Inc., 1981, 1983, USA.

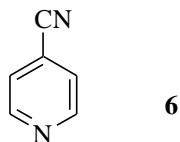
Physical data of nitriles



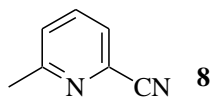
IR (neat, cm^{-1}) 3059, 3021, 2926, 2236, 1597, 1581, 1571, 1462, 1432, 1287, 1248, 1217, 1154, 1091, 1045, 992, 780, 756, 667, 631. ^1H NMR(CDCl_3) δ 7.53-7.58(1H, m), 7.73(1H, d, $J=8.1$ Hz), 7.88(1H, dd, $J=8.1, 2.7$ Hz), 8.75(1H, d, $J=2.7$ Hz). ^{13}C NMR(CDCl_3) δ 117.16, 126.89, 128.49, 133.93, 136.99, 151.08.



IR(neat, cm^{-1}) 3092, 3061, 2917, 2230, 1588, 1563, 1472, 1419, 1213, 1185, 1023, 1034, 972, 933, 810, 780, 699, 631. ^1H NMR(CDCl_3) δ 7.44-7.49(1H, m), 7.97-8.01(1H, m), 8.83-8.87(1H, m), 8.91(1H, brs). ^{13}C NMR(CDCl_3) δ 110.04, 116.43, 123.57, 139.19, 152.41, 152.94.



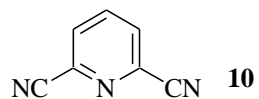
IR (neat, cm^{-1}) 3102, 3083, 3028, 2242, 1593, 1545, 1497, 1416, 1239, 1208, 1193, 1085, 1077, 990, 827, 776, 753. ^1H NMR(CDCl_3) δ 7.55(2H, d, $J=5.4$ Hz), 8.83(2H, $J=5.4$ Hz), ^{13}C NMR(CDCl_3) δ 116.28, 120.27, 125.14, 150.65.



IR (neat, cm^{-1}) 3064, 2234, 1589, 1459, 1447, 1379, 1279, 1210, 1166, 1096, 1039, 985, 916, 798, 730, 703. ^1H

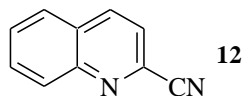
NMR(CDCl_3) δ 2.62(3H, s), 7.40(1H, d, $J=8.1$ Hz), 7.53(1H, d, $J=8.1$ Hz), 7.74(1H, t, $J=8.1$ Hz). ^{13}C NMR(CDCl_3)

δ 24.29, 117.32, 125.62, 126.84, 133.13, 137.03, 160.59.

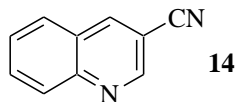


IR (neat, cm^{-1}) 3152, 3081, 3027, 2246, 1575, 1442, 1261, 1198, 1157, 1084, 987. ^1H NMR(CDCl_3) δ 7.93-7.962H,

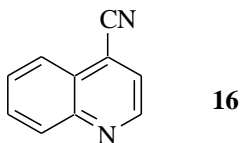
m), 8.07-8.13(1H, m). ^{13}C NMR(CDCl_3) δ 115.39 131.10, 135.24, 138.86.



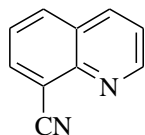
IR (neat, cm^{-1}) 3075, 3060, 2234, 1617, 1588, 1500, 1457, 1426, 1378, 1335, 1303, 1214, 1152, 1120, 1197, 974, 870, 827, 785, 748. ^1H NMR(CDCl_3) δ 7.68-7.74(2H, m), 7.82-7.92(2H, m), 8.15(1H, d, $J=8.1$ Hz), 8.31(1H, d, $J=8.1$ Hz). ^{13}C NMR(CDCl_3) δ 117.50, 123.25, 127.74, 128.60, 129.40, 129.90, 131.20, 133.54, 137.45, 148.13.



IR (neat, cm^{-1}) 3064, 2229, 1620, 1597, 1567, 1489, 1371, 1128, 981, 961, 922, 862, 784, 7461. ^1H NMR(CDCl_3) δ 7.70(1H, t, $J=8.1$ Hz), 7.87-7.93(2H, m), 8.17(1H, d, $J=8.1$ Hz), 8.54(1H, brs), 9.03(1H, brs). ^{13}C NMR(CDCl_3) δ 106.49, 117.03, 126.11, 128.19, 128.42, 129.77, 132.71, 141.39, 148.70, 149.65.

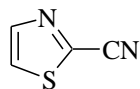


IR (neat, cm^{-1}) 3066, 3040, 2227, 1614, 1584, 1502, 1465, 1391, 1360, 1161, 1141, 1074, 865, 853, 759. ^1H NMR(CDCl_3) δ 7.74-7.80(2H, m), 7.90(1H, t, $J=5.4$ Hz), 8.19-8.23(2H, m), 9.04(1H, d, $J=2.7$ Hz). ^{13}C NMR(CDCl_3) δ 115.49, 118.62, 124.79, 124.90, 125.71, 129.18, 130.35, 131.15, 148.10, 149.39.



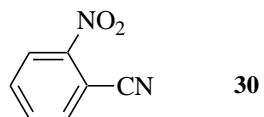
18

IR (neat, cm^{-1}) 3047, 2227, 1611, 1593, 1572, 1496, 1389, 1315, 1142, 1071, 864, 831, 795, 769. ^1H NMR(CDCl_3) δ 7.55-7.66(2H, m), 8.12(2H, m), 8.27(1H, dd, $J=8.1, 2.7$ Hz), 9.10(1H, dd, $J=5.4, 2.7$ Hz). ^{13}C NMR(CDCl_3) δ 113.37, 117.18, 122.71, 125.79, 128.05, 132.86, 135.45, 136.43, 147.38, 152.42.

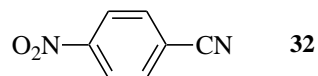


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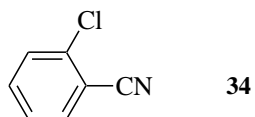
IR (neat, cm^{-1}) 3119, 3096, 2233, 1470, 1375, 1321, 1191, 1123, 1060, 822, 768, 750. ^1H NMR(CDCl_3) δ 7.73(1H, d, $J=2.7$ Hz), 8.08(1H, d, $J=2.7$ Hz). ^{13}C NMR(CDCl_3) δ 112.61, 124.96, 136.75, 145.23.



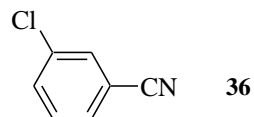
IR (neat, cm^{-1}) 3111, 2232, 1611, 1569, 1530, 1344, 858, 791, 743. $^1\text{H NMR}(\text{CDCl}_3)$ δ 7.84-7.97(3H, m), 8.33-8.39(1H, m). $^{13}\text{C NMR}(\text{CDCl}_3)$ δ 108.07, 109.79, 114.84, 125.52, 133.70, 134.31, 135.55.



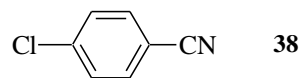
IR (neat, cm^{-1}) 3107, 3053, 2232, 1600, 1526, 1488, 1348, 1294, 858, 747. $^1\text{H NMR}(\text{CDCl}_3)$ δ 7.90(2H, d, $J=8.1\text{ Hz}$), 8.37(2H, d, $J=8.1\text{ Hz}$). $^{13}\text{C NMR}(\text{CDCl}_3)$ δ 116.80, 118.51, 118.52, 124.25, 133.44.



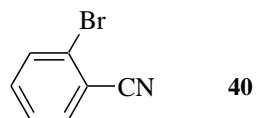
IR (neat, cm^{-1}) 3068, 2230, 1591, 1472, 1437, 1056, 757. $^1\text{H NMR}(\text{CDCl}_3)$ δ 7.37(1H, t, $J=8.1\text{ Hz}$), 7.51-7.57(2H, m), 7.68(1H, d, $J=8.1\text{ Hz}$). $^{13}\text{C NMR}(\text{CDCl}_3)$ δ 113.46, 116.03, 127.11, 130.03, 133.83, 133.99, 136.89.



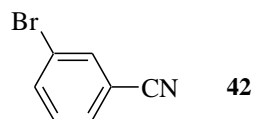
IR (neat, cm^{-1}) 2924, 2233, 1571, 1471, 1414, 1195, 790. $^1\text{H NMR}(\text{CDCl}_3)$ δ 7.43(1H, t, $J=8.1\text{ Hz}$), 7.55-7.66(3H, m). $^{13}\text{C NMR}(\text{CDCl}_3)$ δ 113.96, 117.47, 130.28, 130.46, 131.92, 133.23, 135.24.



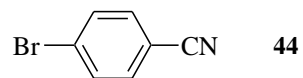
IR (neat, cm^{-1}) 3091, 3040, 2226, 1593, 1484, 1398, 1089, 1016, 828, 779. $^1\text{H NMR}(\text{CDCl}_3)$ δ 7.47(2H, d, $J=8.1$ Hz), 7.61(2H, d, $J=8.1$ Hz). $^{13}\text{C NMR}(\text{CDCl}_3)$ δ 110.78, 117.95, 129.67, 133.35, 139.67.



IR (neat, cm^{-1}) 3088, 2225, 1584, 1465, 1434, 1044, 756. $^1\text{H NMR}(\text{CDCl}_3)$ δ 7.40-7.4851(2H, m), 7.65-7.72(2H, m). $^{13}\text{C NMR}(\text{CDCl}_3)$ δ 115.80, 117.09, 125.26, 127.60, 133.15, 133.87, 134.28.



IR (neat, cm^{-1}) 3068, 2232, 1561, 1472, 1409, 1190, 1076, 788. $^1\text{H NMR}(\text{CDCl}_3)$ δ 7.37(1H, t, $J=8.1$ Hz), 7.60(1H, d, $J=8.1$ Hz), 7.73-7.80(2H, m). $^{13}\text{C NMR}(\text{CDCl}_3)$ δ 114.16, 117.19, 122.86, 130.57, 130.67, 134.72, 136.09.



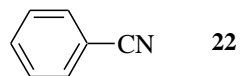
IR (neat, cm^{-1}) 2225, 1585, 1479, 1068, 1014, 822. ^1H NMR(CDCl_3) δ 7.53(2H, d, $J=8.1\text{Hz}$), 7.64(2H, $J=8.1\text{ Hz}$). ^{13}C NMR(CDCl_3) δ 111.15, 117.91, 127.96, 132.59, 133.36.



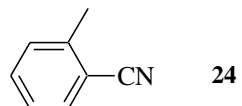
IR (neat, cm^{-1}) 3030, 2985, 2935, 2242, 1601, 1496, 1452, 1378, 761. ^1H NMR(CDCl_3) δ 1.65(3H, d, $J=8.1\text{ Hz}$), 3.89(1H, q, $J=8.1\text{ Hz}$), 7.31-7.39(5H, m). ^{13}C NMR(CDCl_3) δ 21.45, 31.23, 121.70, 126.67, 128.02, 129.12, 137.10.



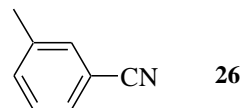
IR (neat, cm^{-1}) 3029, 2931, 2247, 1603, 1496, 1454, 1424, 1078, 748, 699. ^1H NMR(CDCl_3) δ 2.61(2H, t, $J=8.1\text{Hz}$), 2.95(2H, t, $J=8.1\text{Hz}$), 7.21-7.36(5H, m). ^{13}C NMR(CDCl_3) δ 19.30, 31.52, 119.10, 127.19, 128.21, 128.83, 138.00.



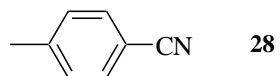
IR (neat, cm^{-1}) 3066, 2229, 1598, 1490, 1447, 1287, 1178, 1071, 1026, 926, 758, 687. $^1\text{H NMR}(\text{CDCl}_3)$
 δ 7.45-7.51(2H, m), 7.59-7.68(3H, m). $^{13}\text{C NMR}(\text{CDCl}_3)$ δ 112.33, 118.98, 129.05, 132.06, 132.71.



$^1\text{H NMR}(\text{CDCl}_3)$ δ 2.54(3H, s), 7.24-7.36(2H, m), 7.48(1H, t, $J=8.1$ Hz), 7.58(1H, d, $J=8.1$ Hz).



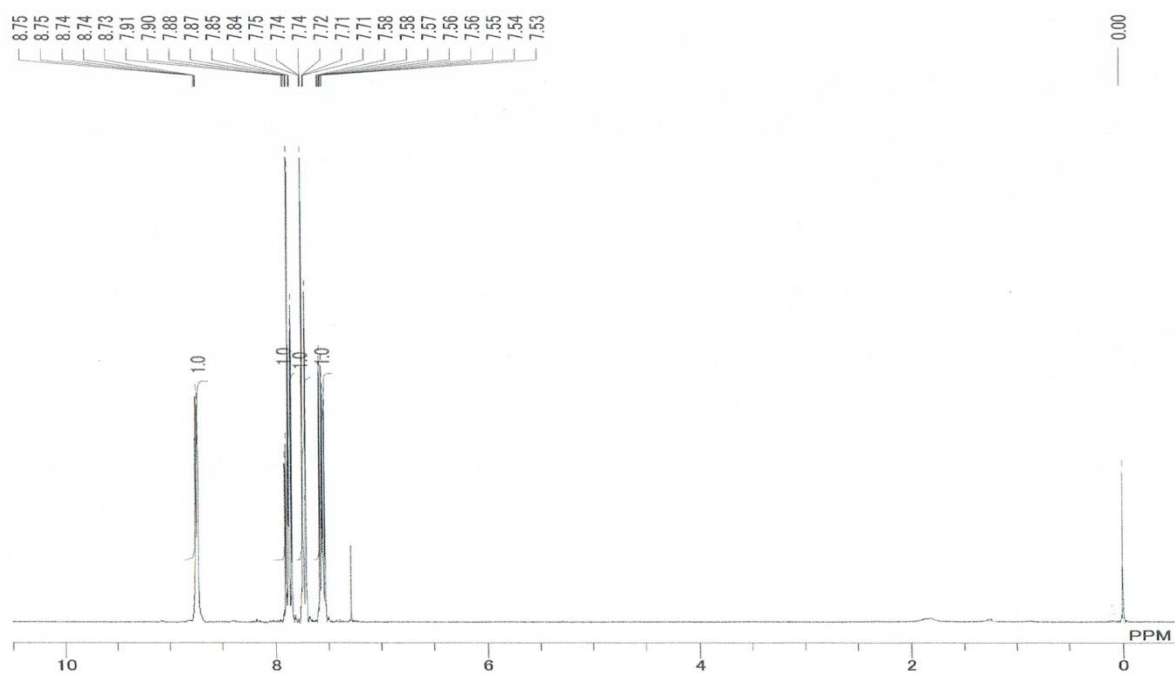
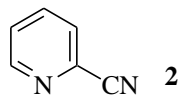
$^1\text{H NMR}(\text{CDCl}_3)$ δ 2.38(3H, s), 7.34-7.39(3H, m), 7.44(1H, s).



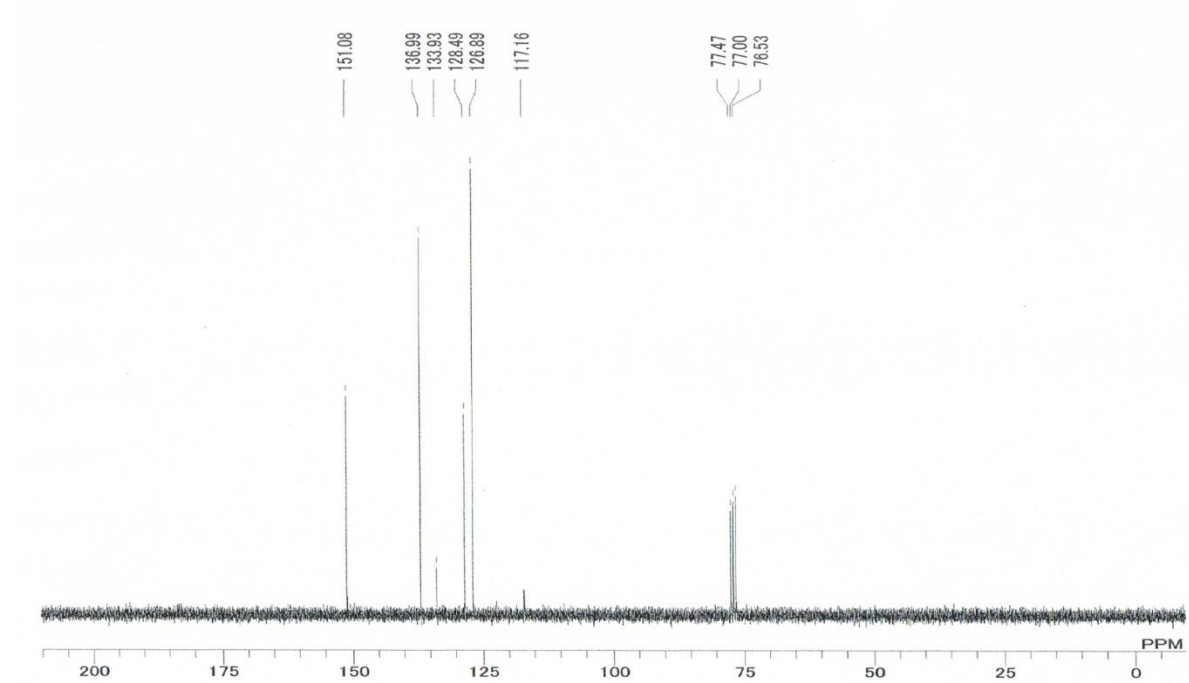
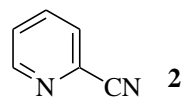
$^1\text{H NMR}(\text{CDCl}_3)$ δ 2.42(3H, s), 7.26(2H, d, $J=8.1$ Hz), 7.53(2H, d, $J=8.1$ Hz). $^{13}\text{C NMR}(\text{CDCl}_3)$ δ
21.73, 109.15, 119.07, 129.73, 131.92, 143.62.

The $^1\text{H NMR}$ and IR spectra of benzonitrile(**22**), *o*-, *m*-, and *p*-tolunitrile(**24**) (**26**) (**28**) were coincident with those of the Aldrich library of $^1\text{H NMR}$ spectra (Edition II Vol 2) and IR spectra (Edition III) edited by Charles J. Pouchert. The Aldrich library of $^1\text{H NMR}$ and IR spectra was published by Aldrich Chemical Company, Inc., 1981, 1983, USA.

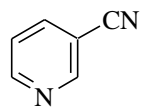
^1H NMR (CDCl_3 , 270.05 MHz)



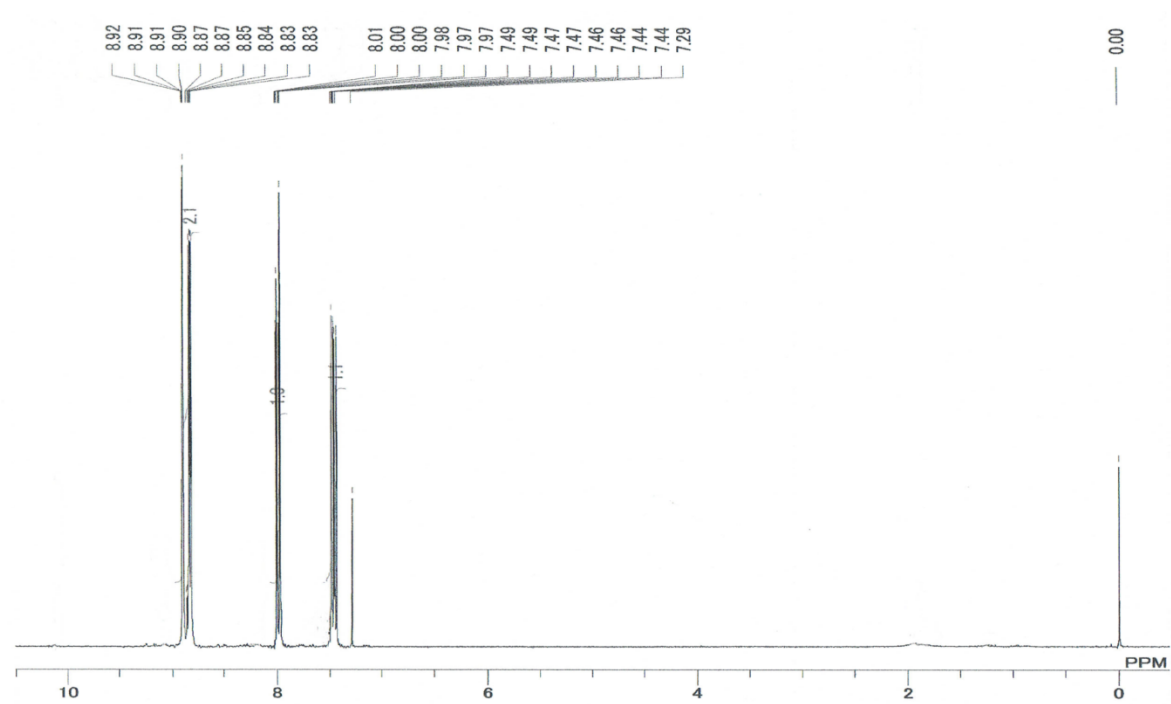
^{13}C NMR (CDCl_3 , 67.80 MHz)



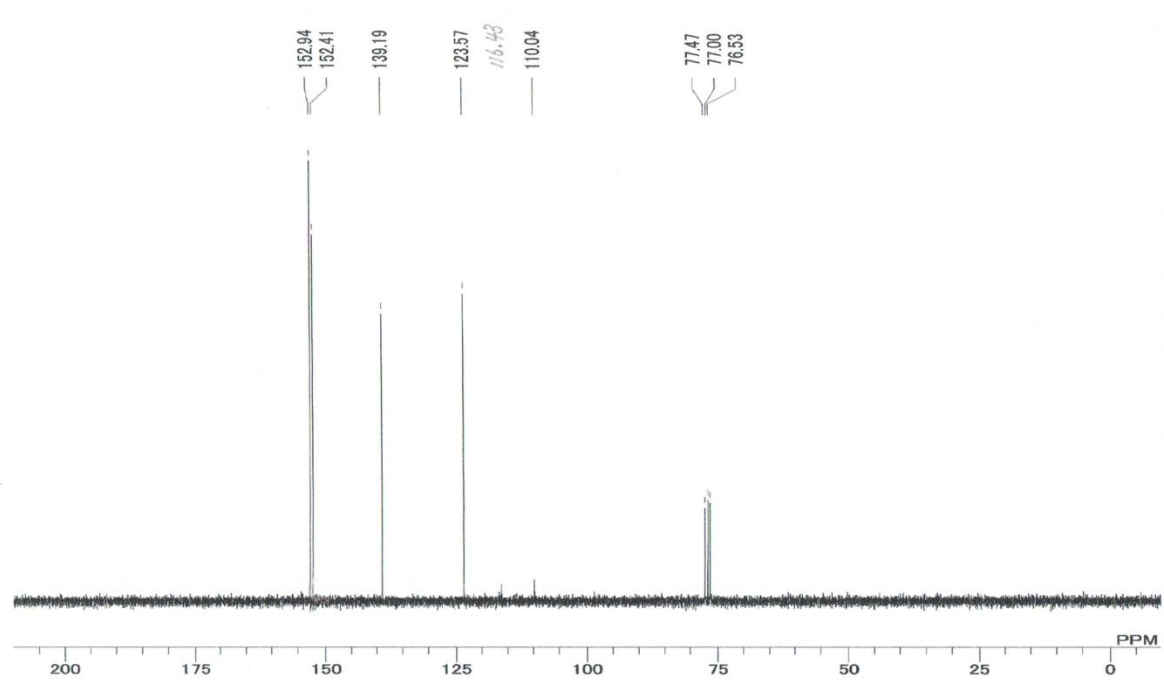
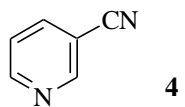
$^1\text{H NMR}$ (CDCl_3 , 270.05 MHz)



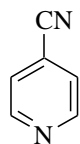
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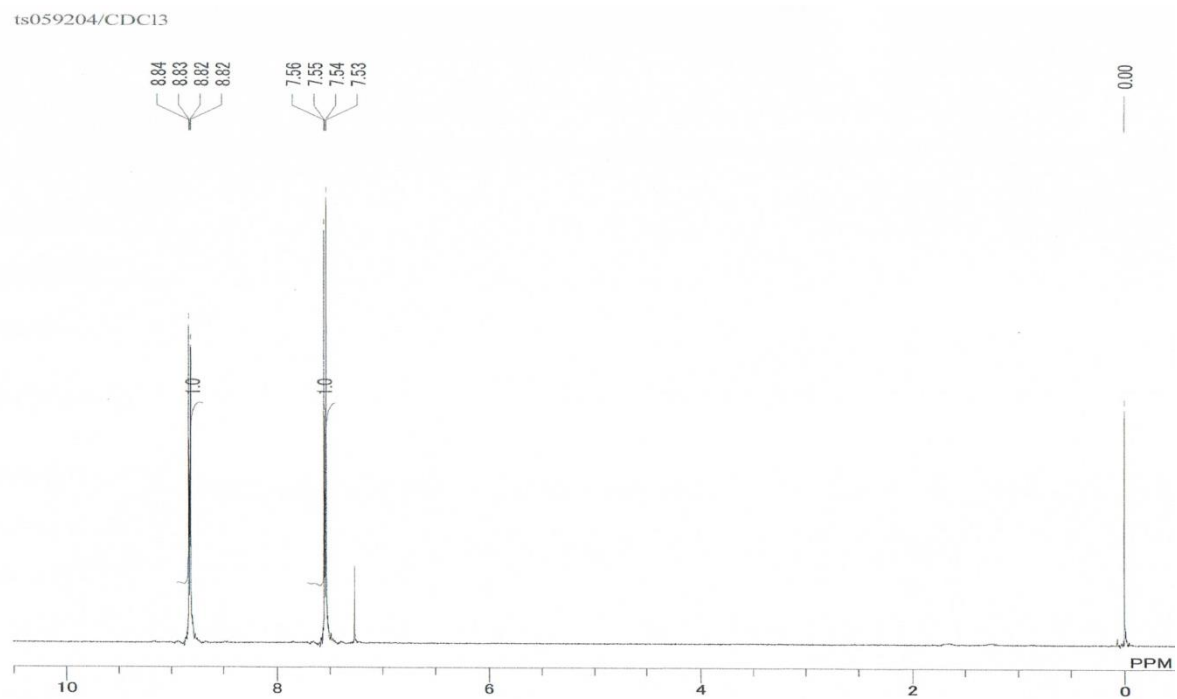
^{13}C NMR (CDCl_3 , 67.80 MHz)



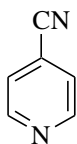
$^1\text{H NMR}$ (CDCl_3 , 270.05 MHz)



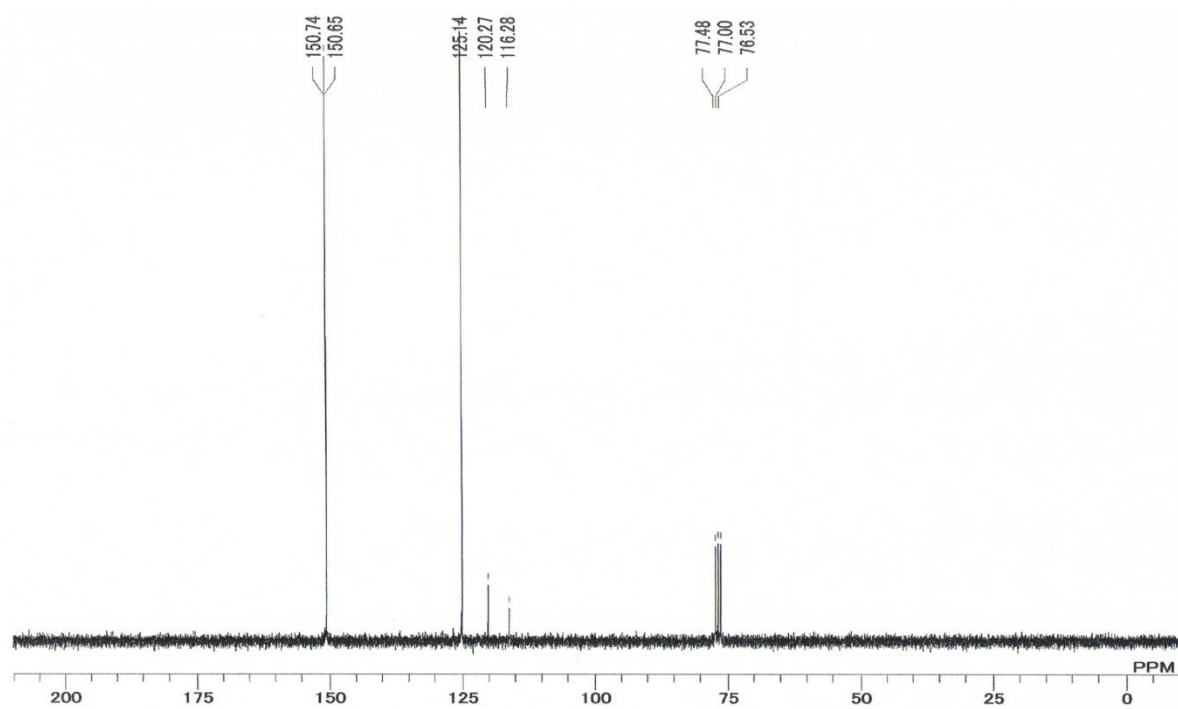
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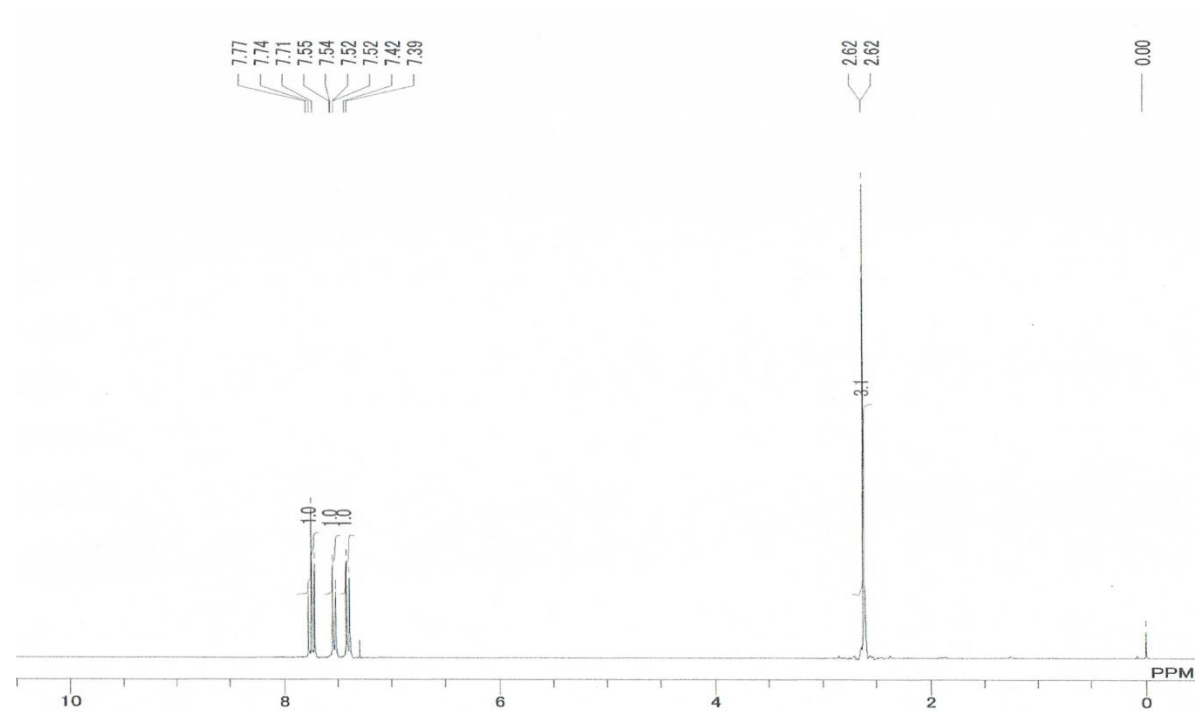
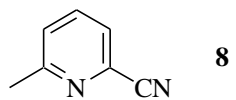
^{13}C NMR (CDCl_3 , 67.80 MHz)



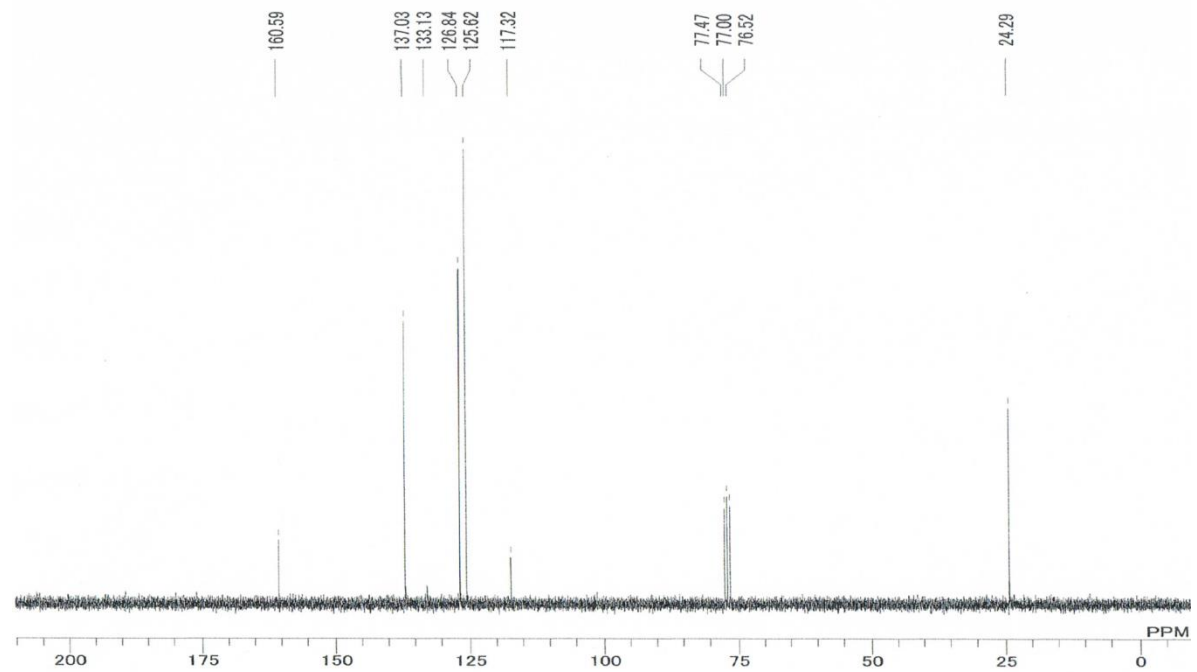
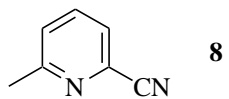
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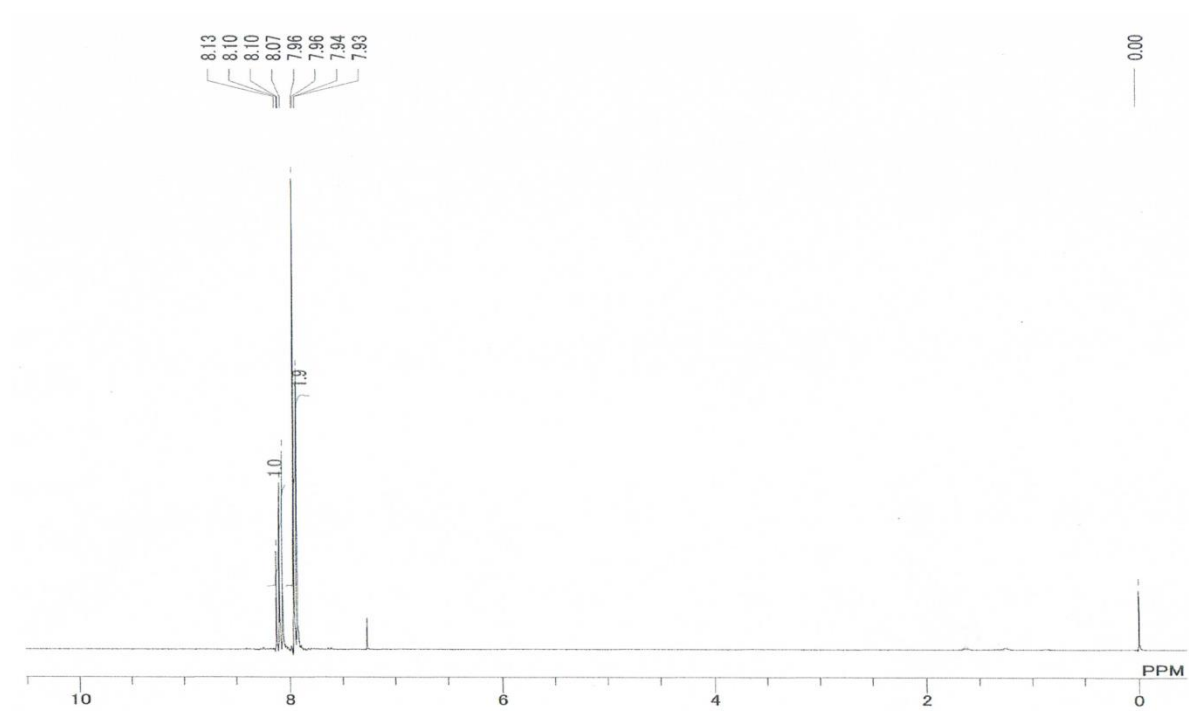
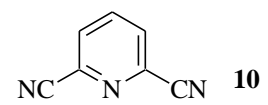
^1H NMR (CDCl_3 , 270.05 MHz)



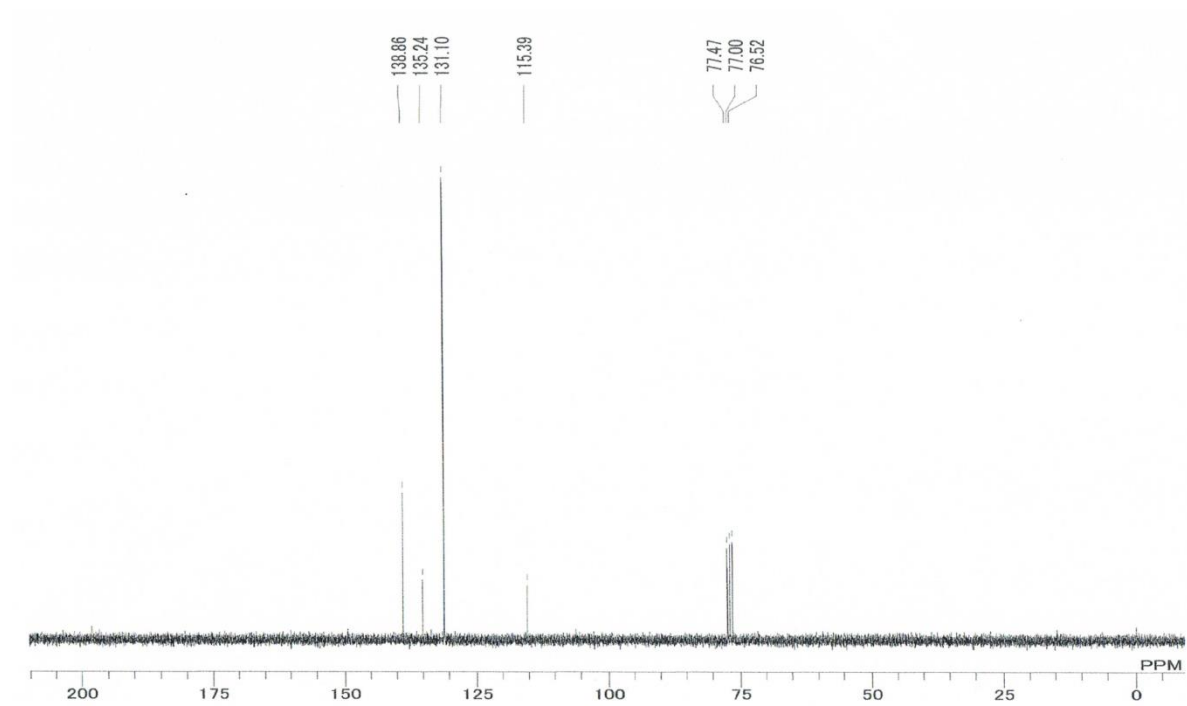
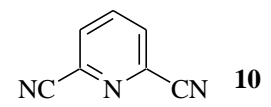
^{13}C NMR (CDCl_3 , 67.80 MHz)



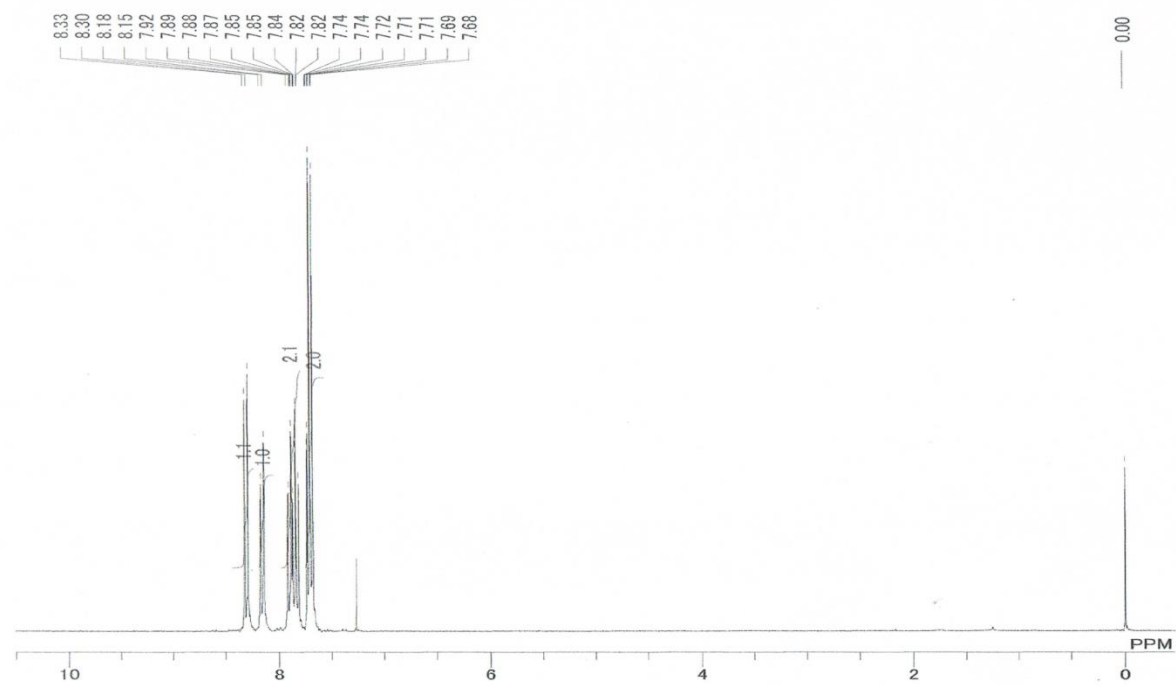
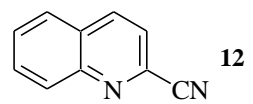
^1H NMR (CDCl_3 , 270.05 MHz)



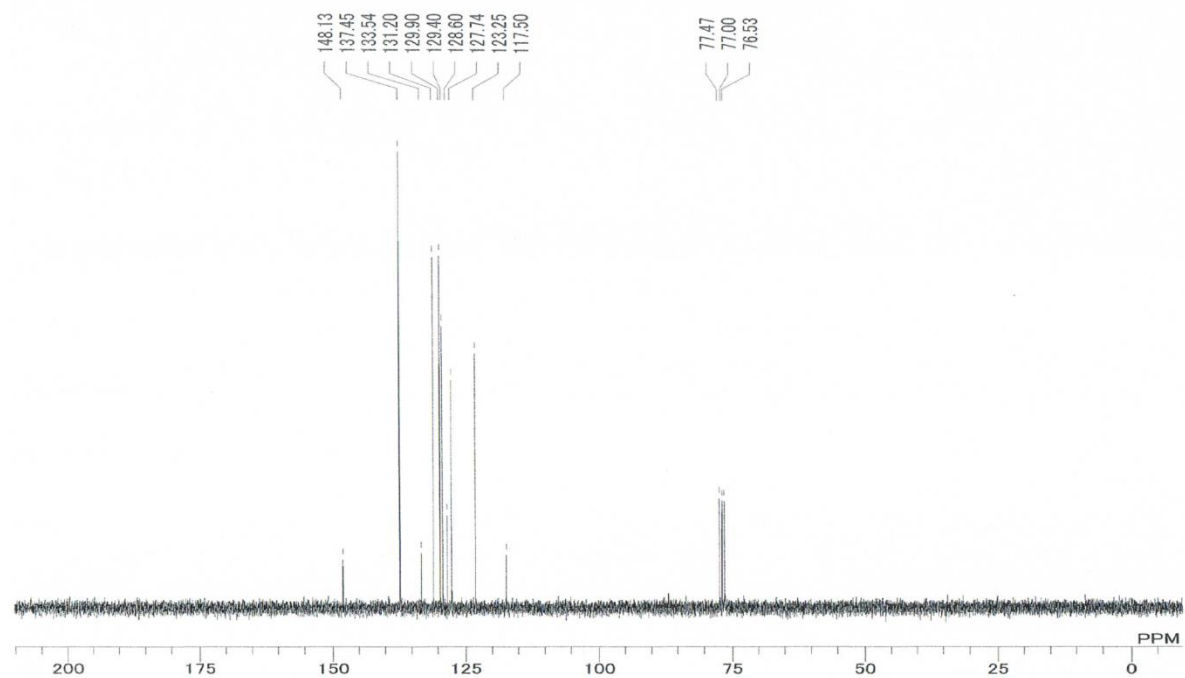
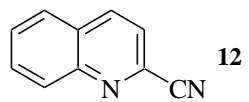
^{13}C NMR (CDCl_3 , 67.80 MHz)



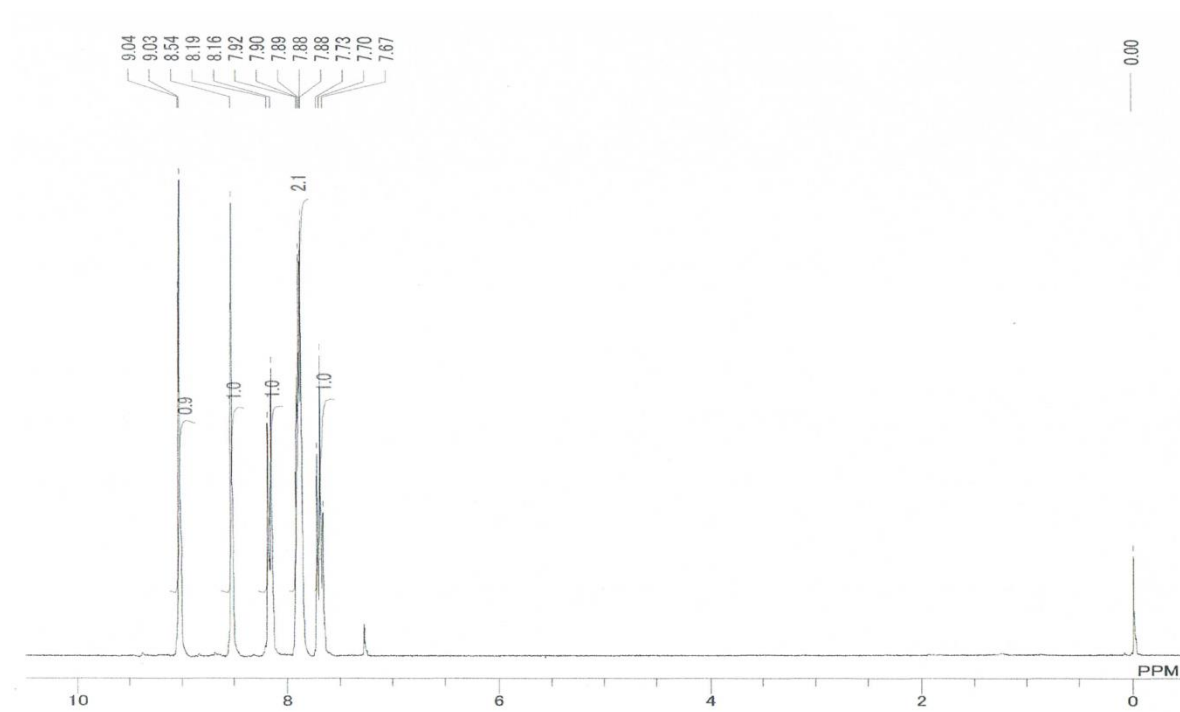
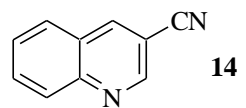
^1H NMR (CDCl_3 , 270.05 MHz)



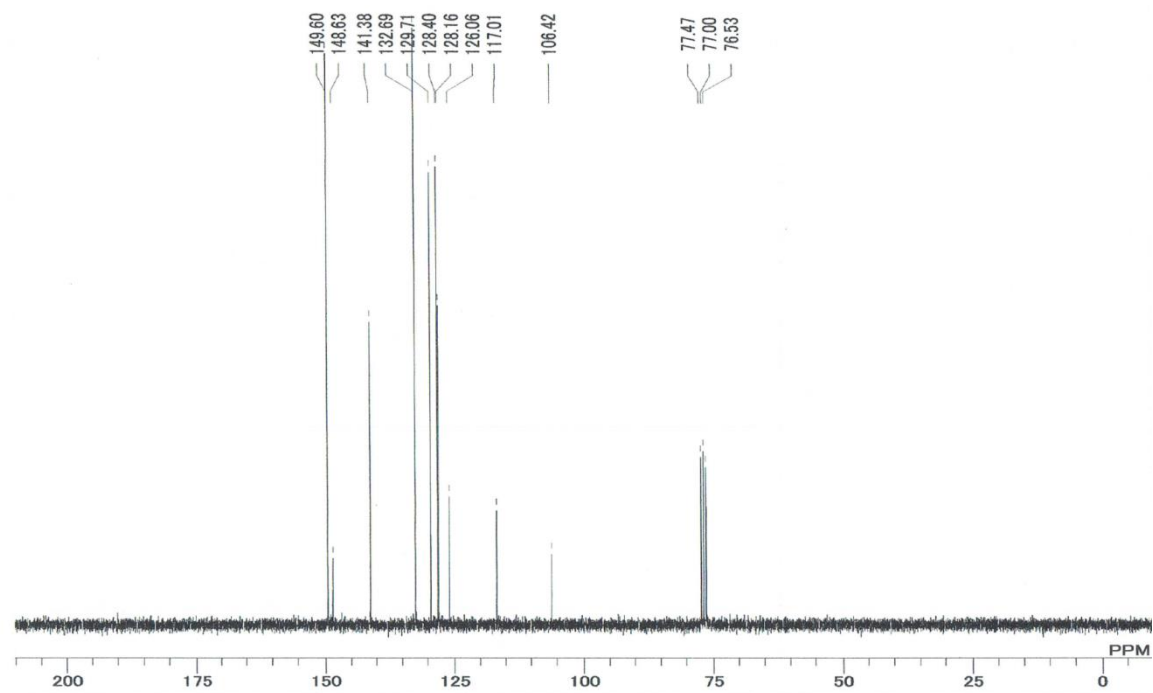
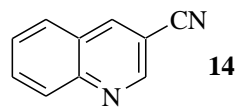
^{13}C NMR (CDCl_3 , 67.80 MHz)



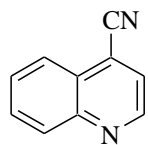
^1H NMR (CDCl_3 , 270.05 MHz)



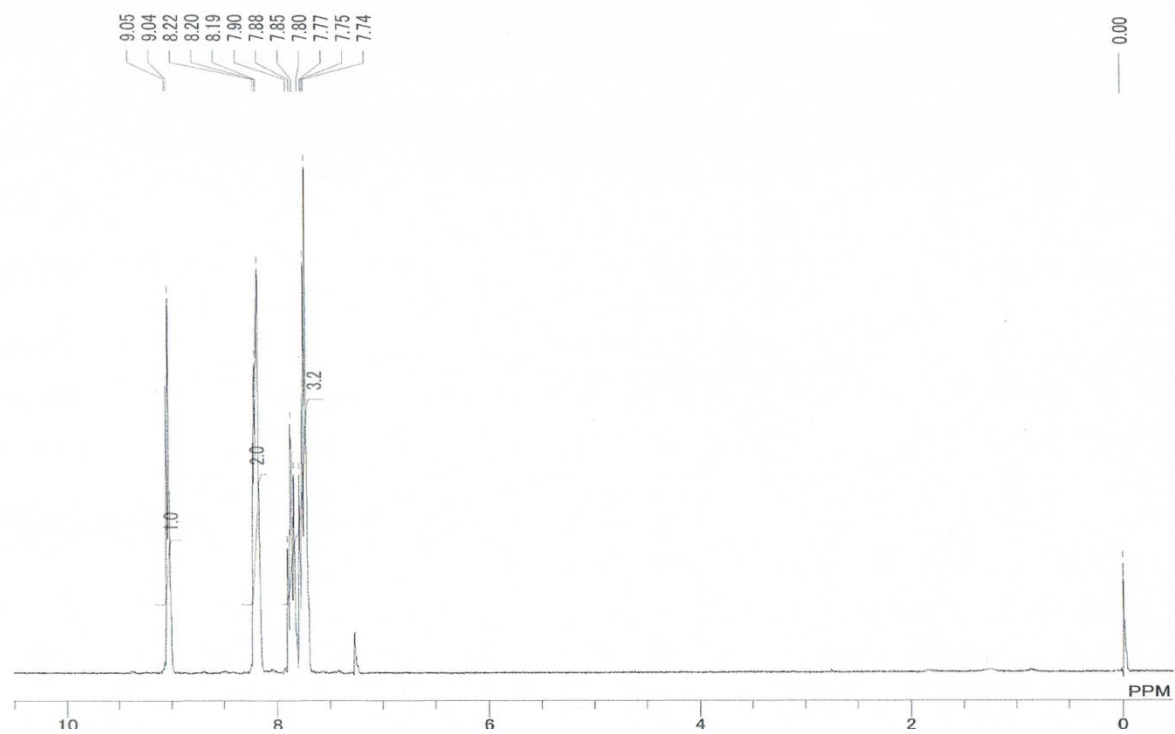
^{13}C NMR (CDCl_3 , 67.80 MHz)



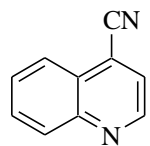
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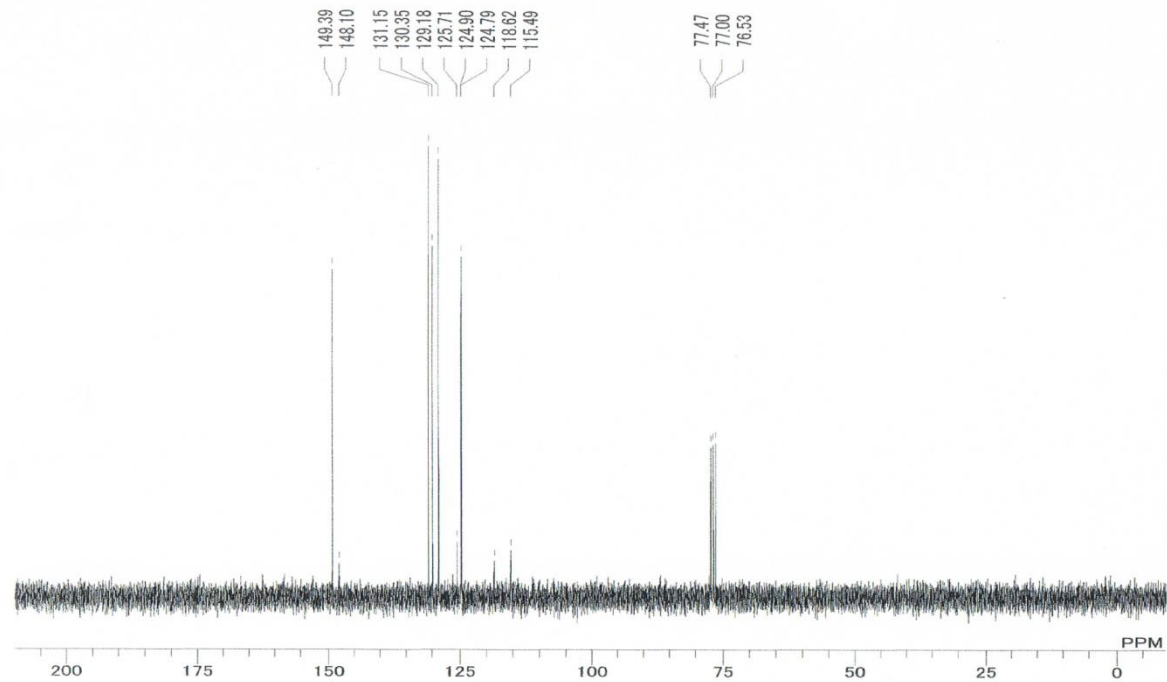
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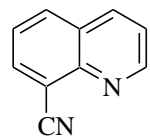
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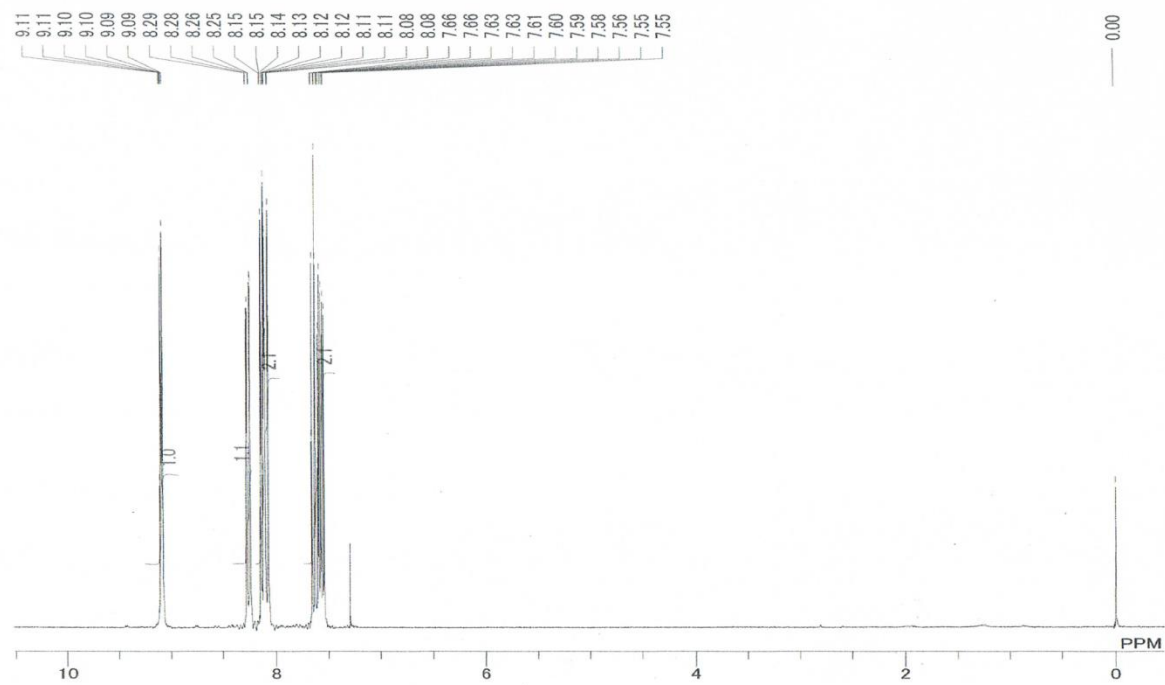
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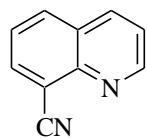
^1H NMR (CDCl_3 , 270.05 MHz)



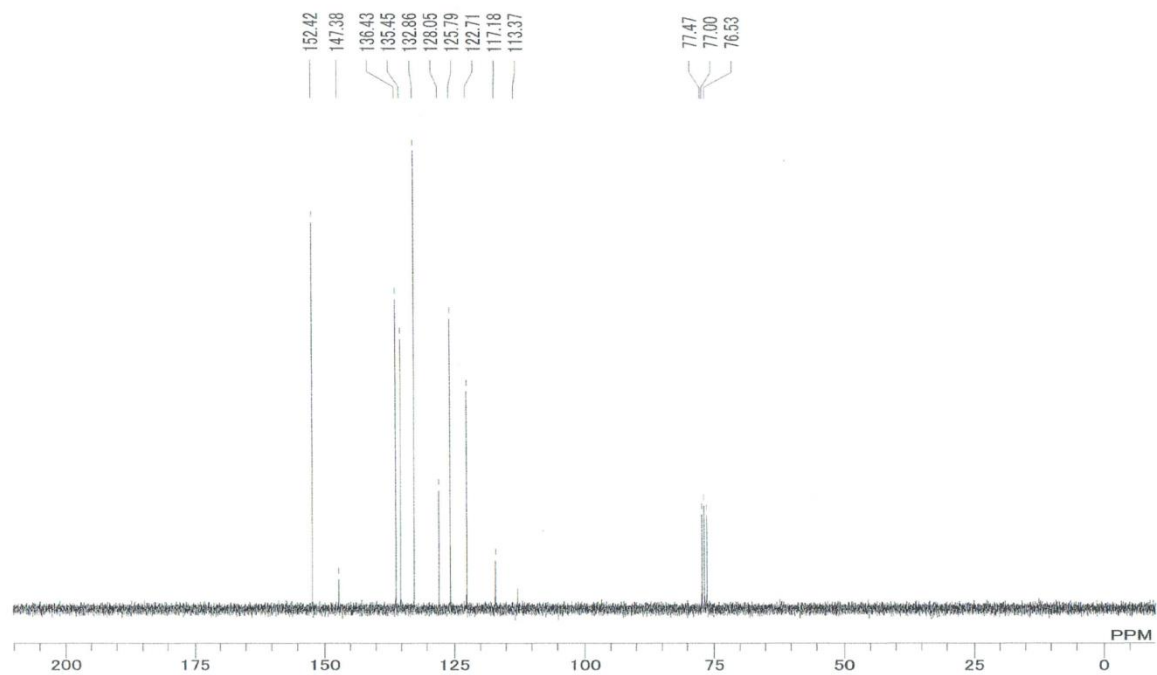
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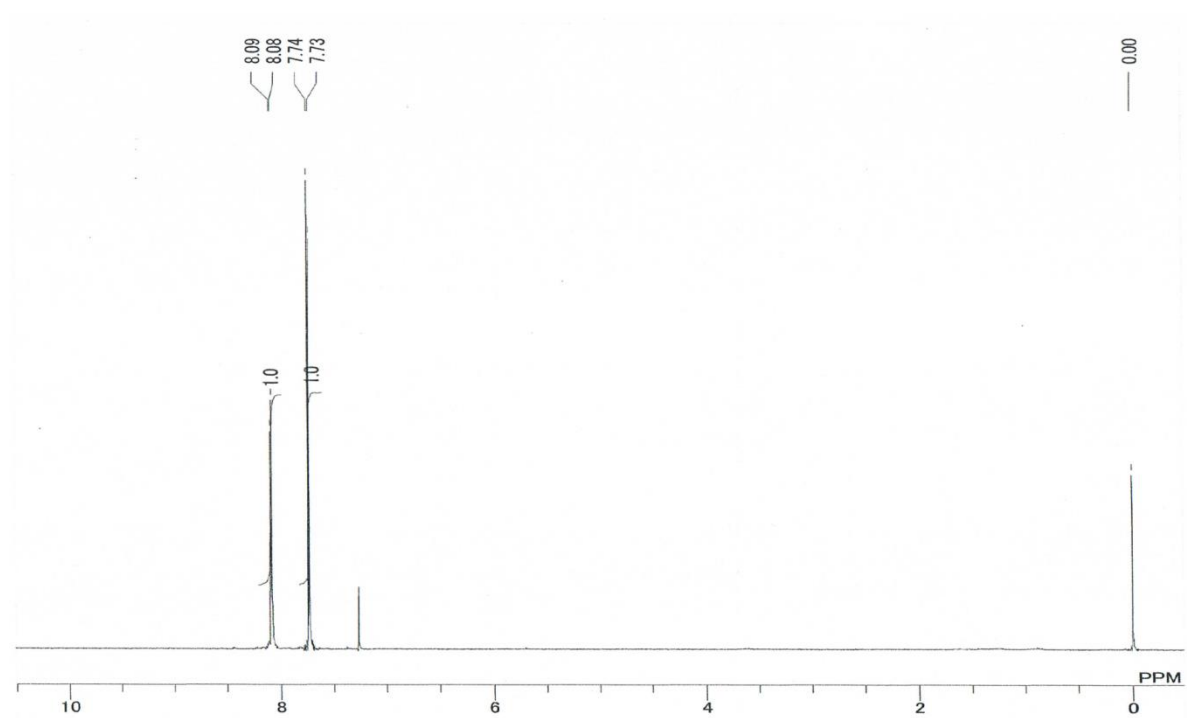
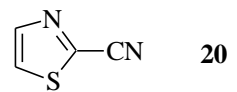
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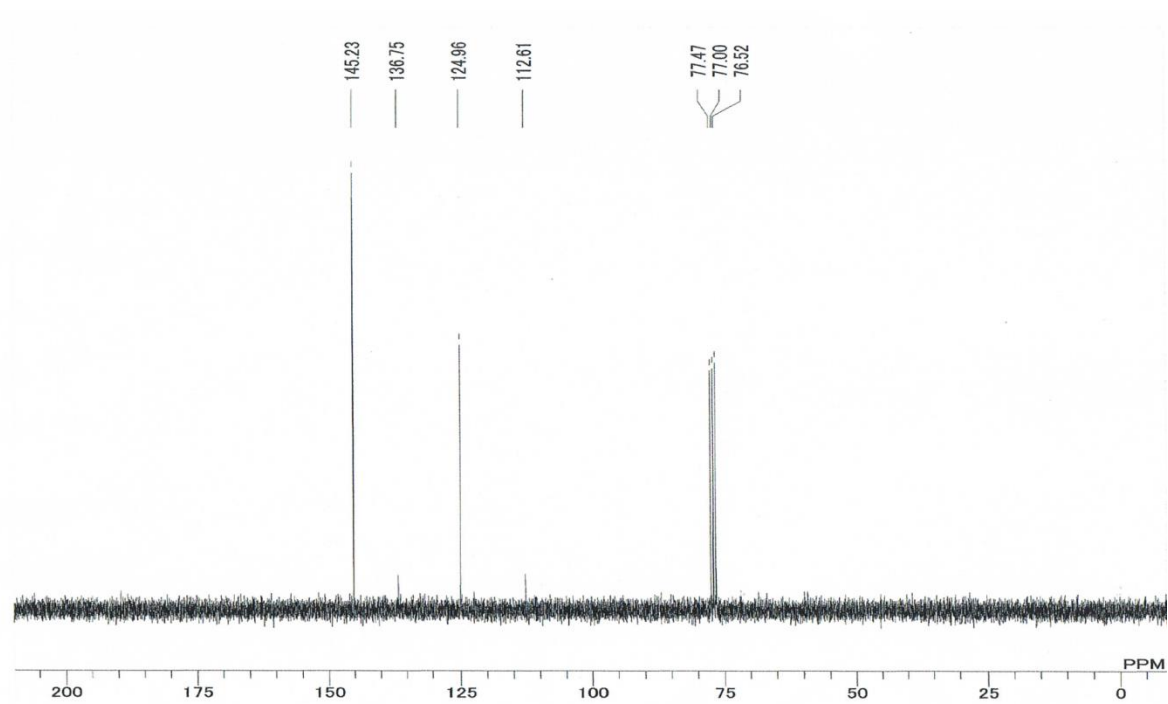
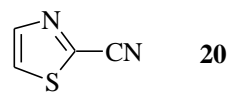
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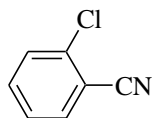
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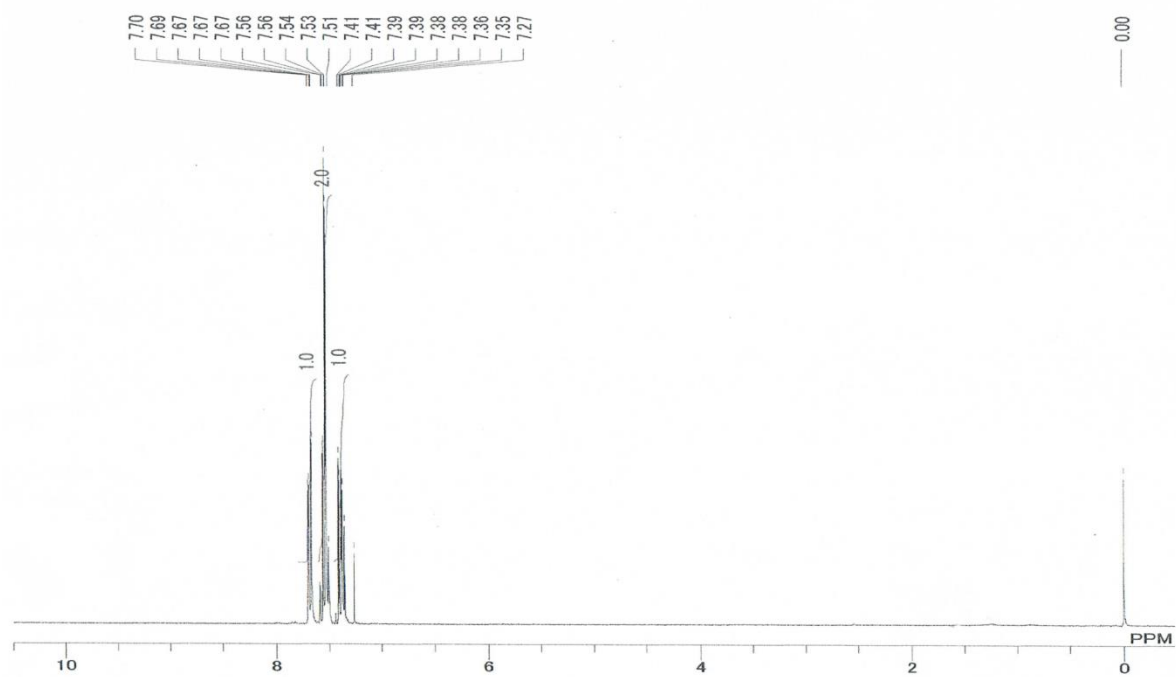
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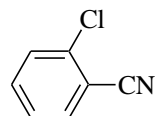
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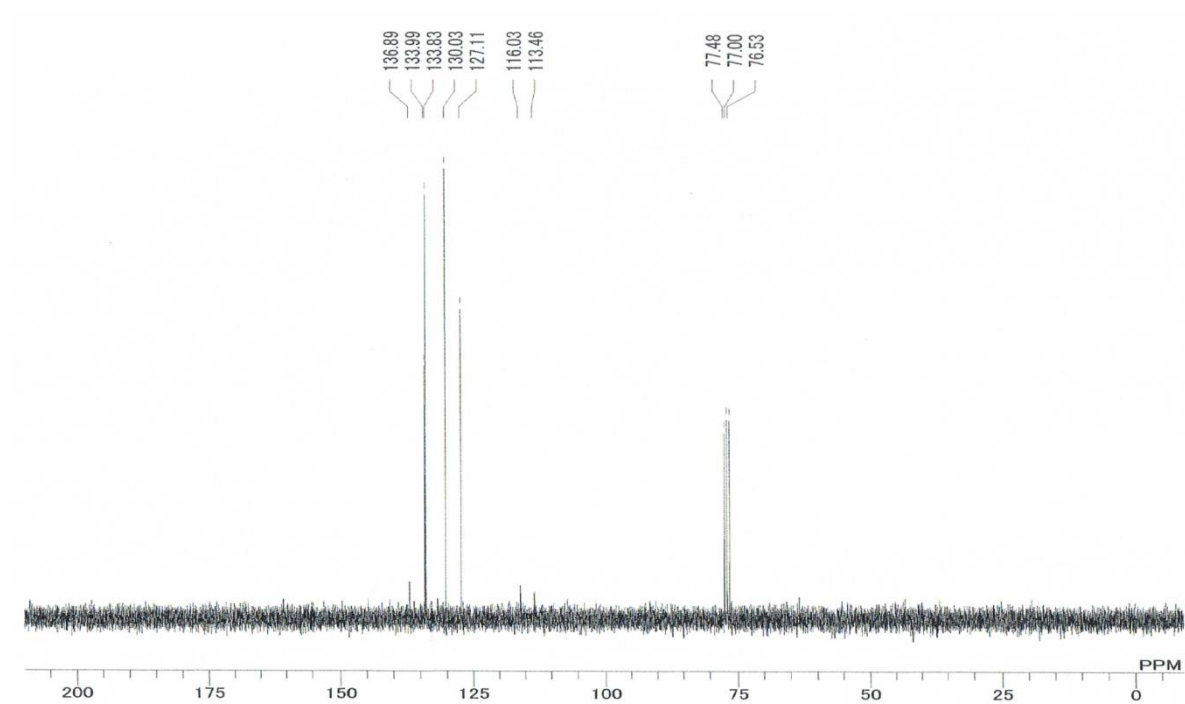
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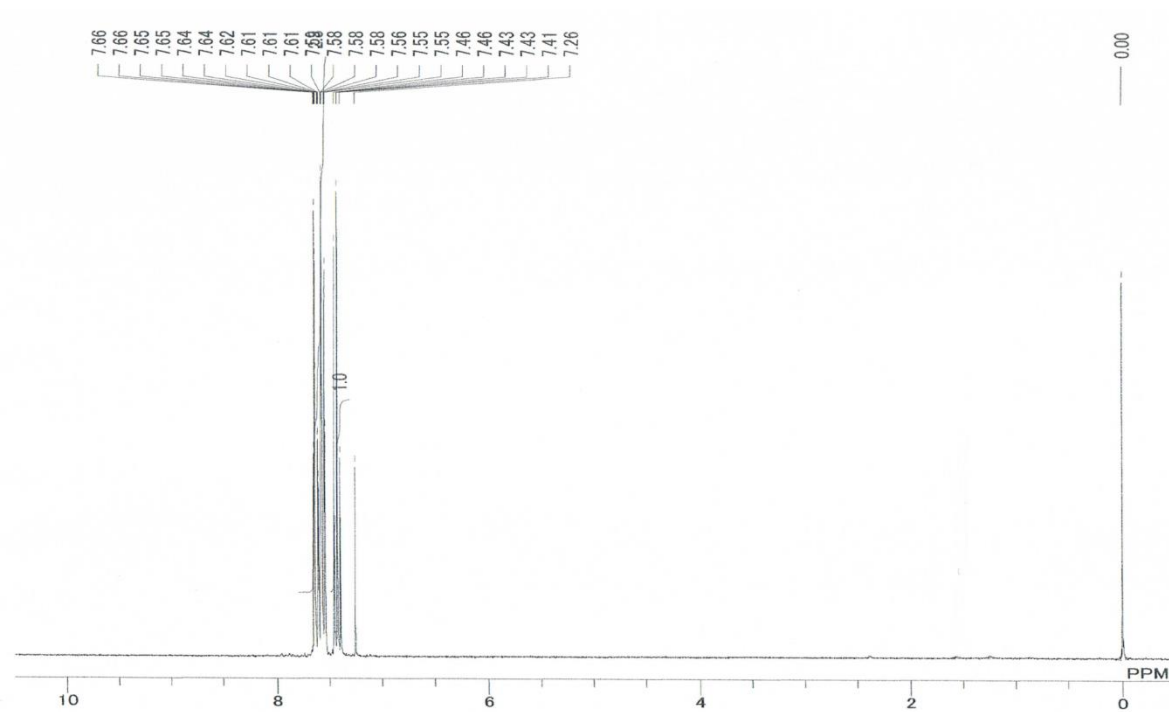
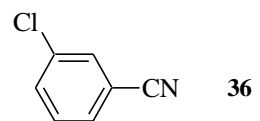
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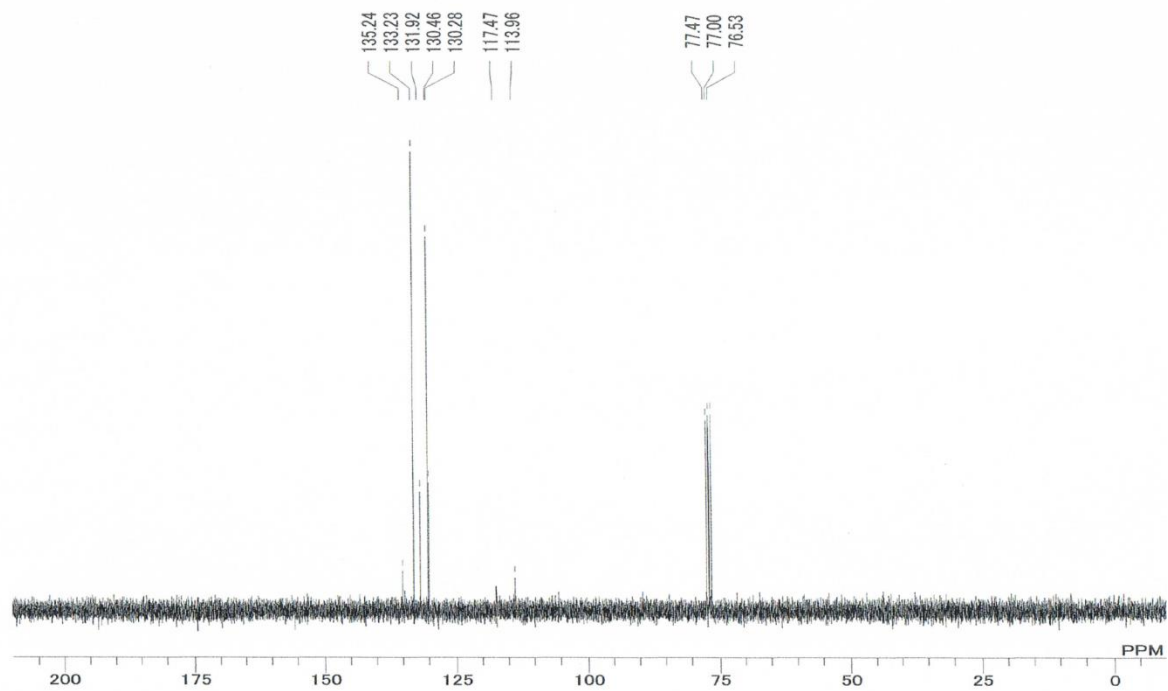
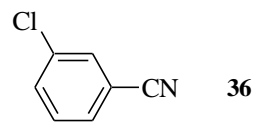
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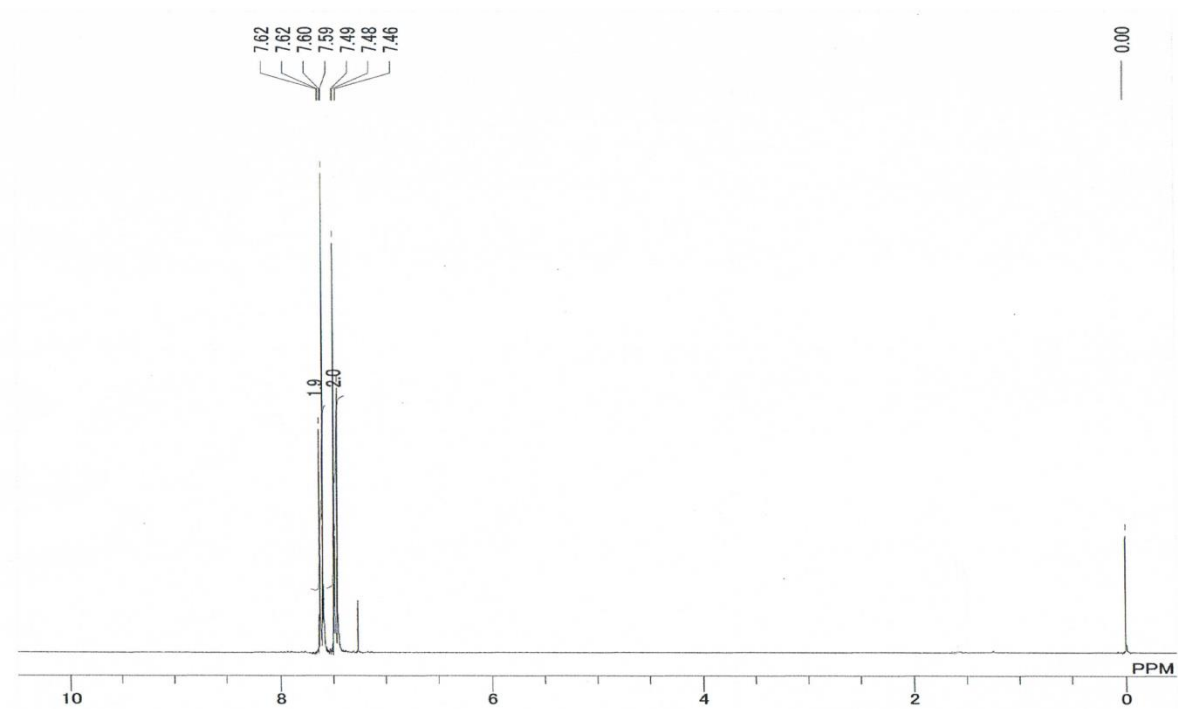
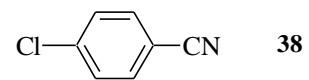
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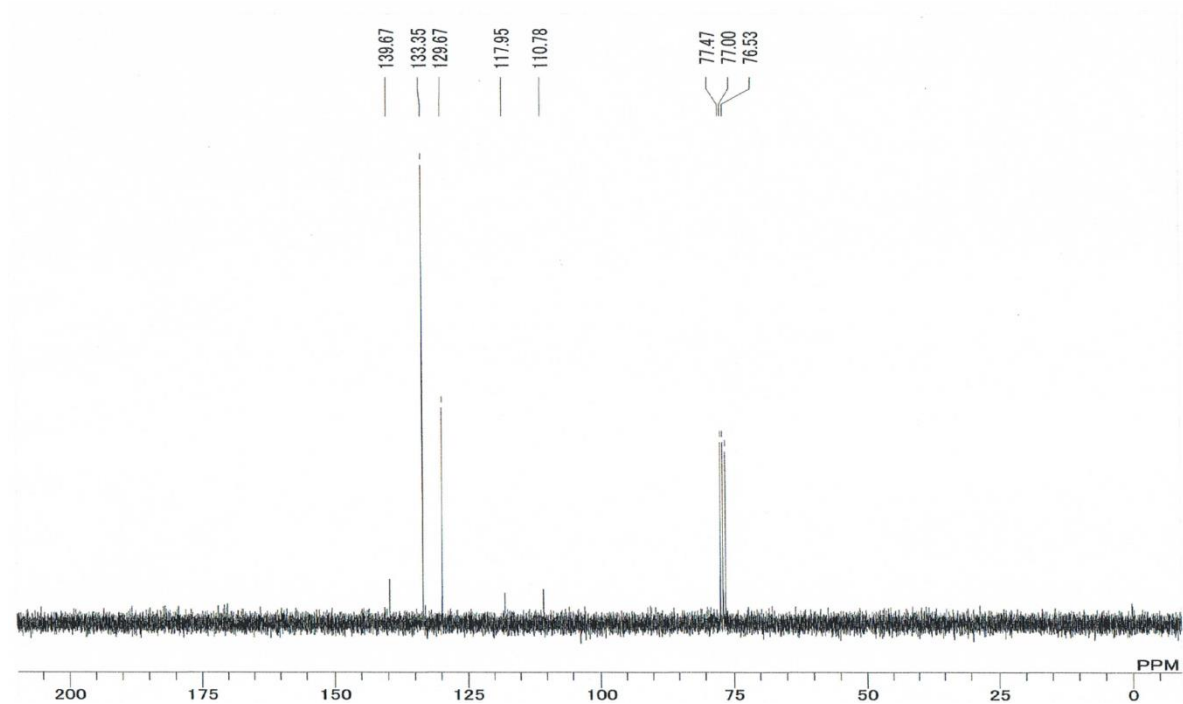
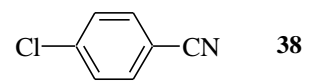
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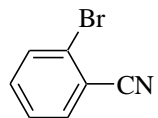
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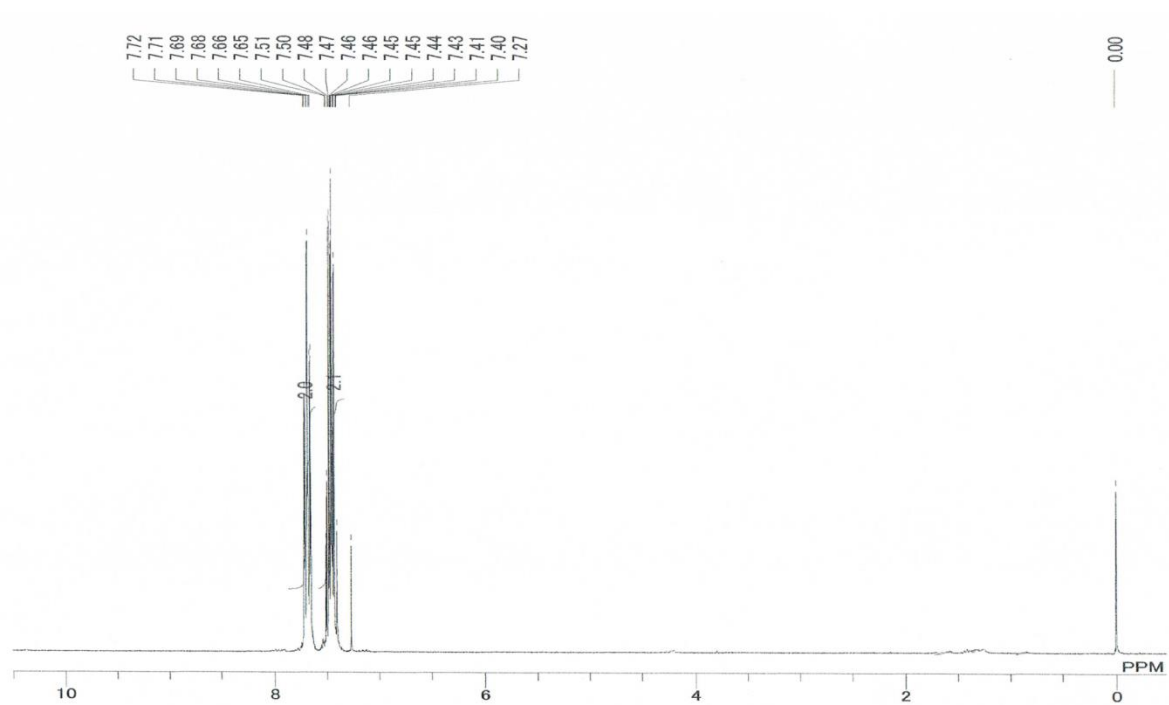
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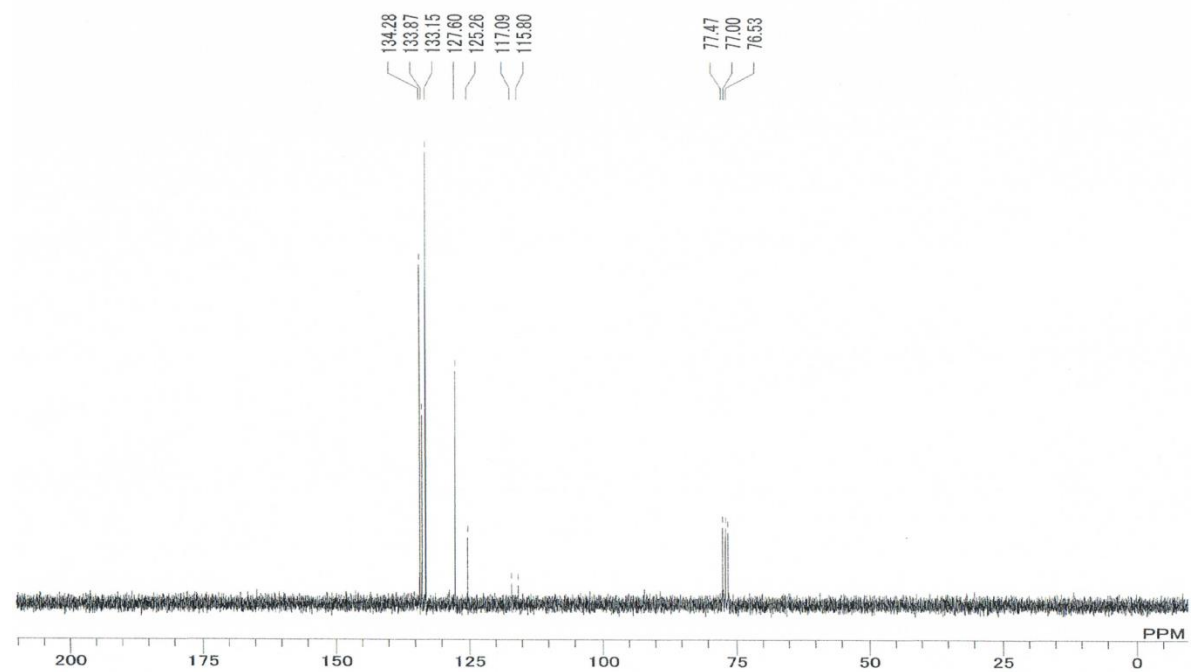
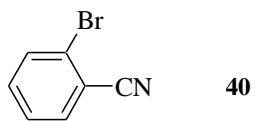
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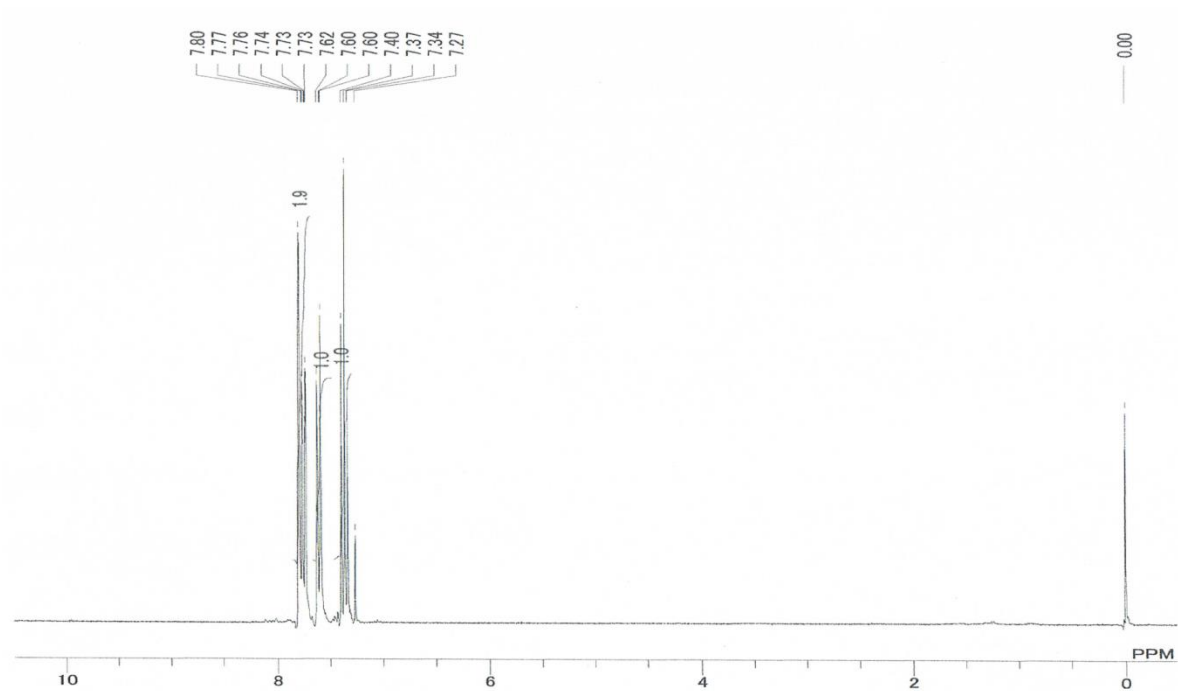
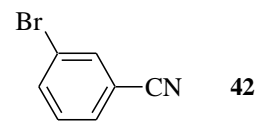
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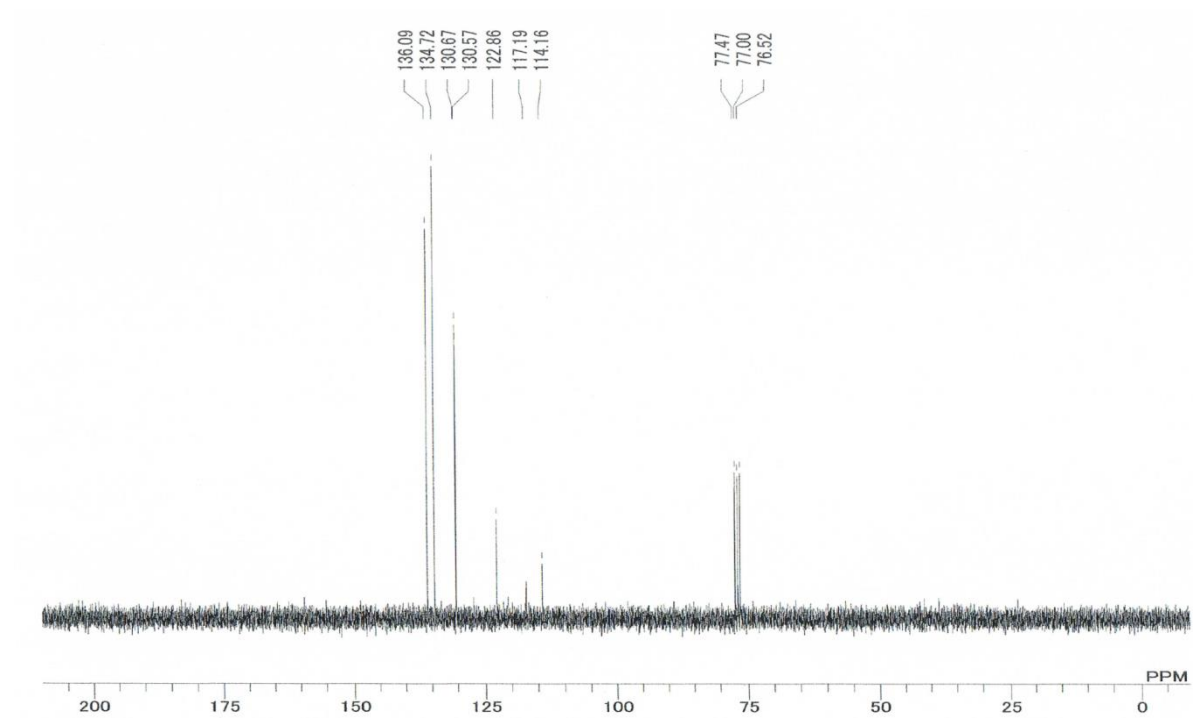
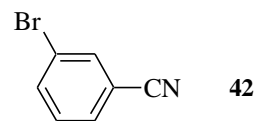
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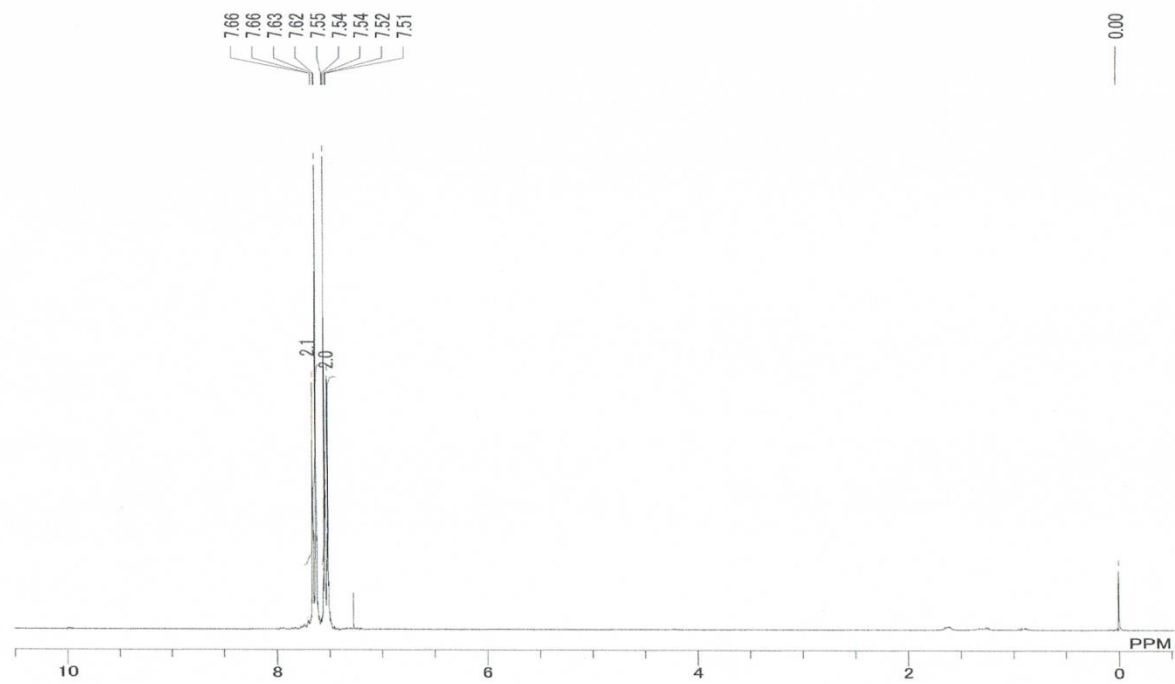
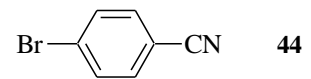
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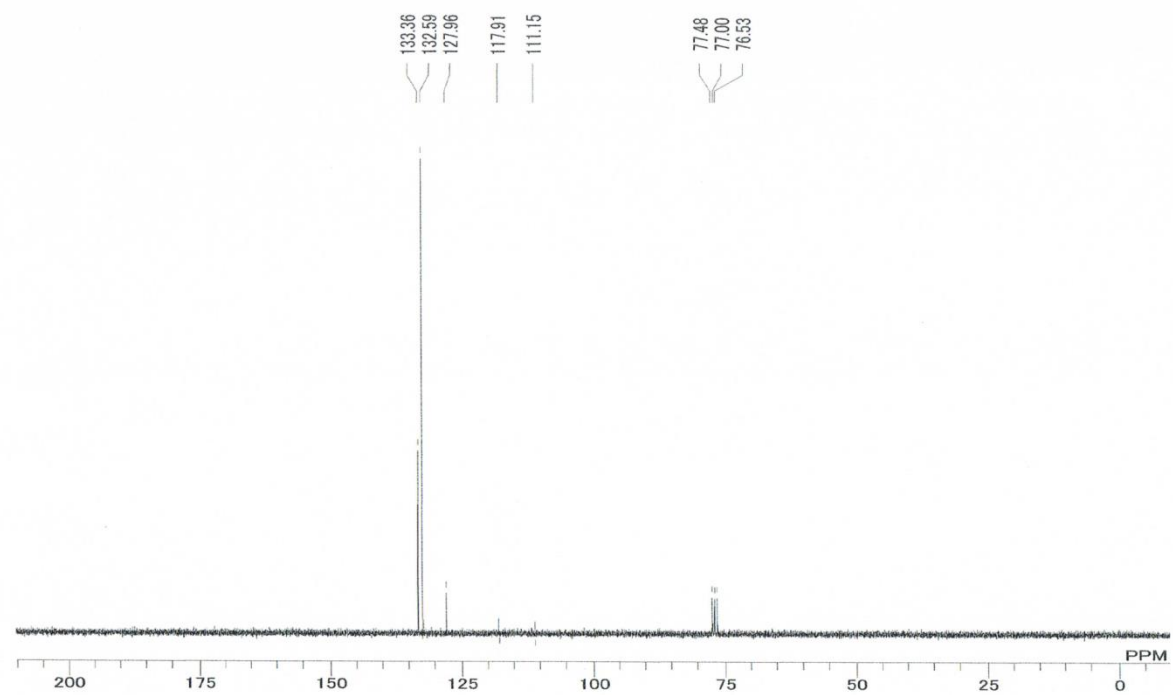
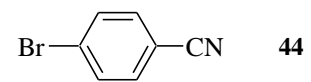
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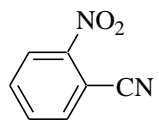
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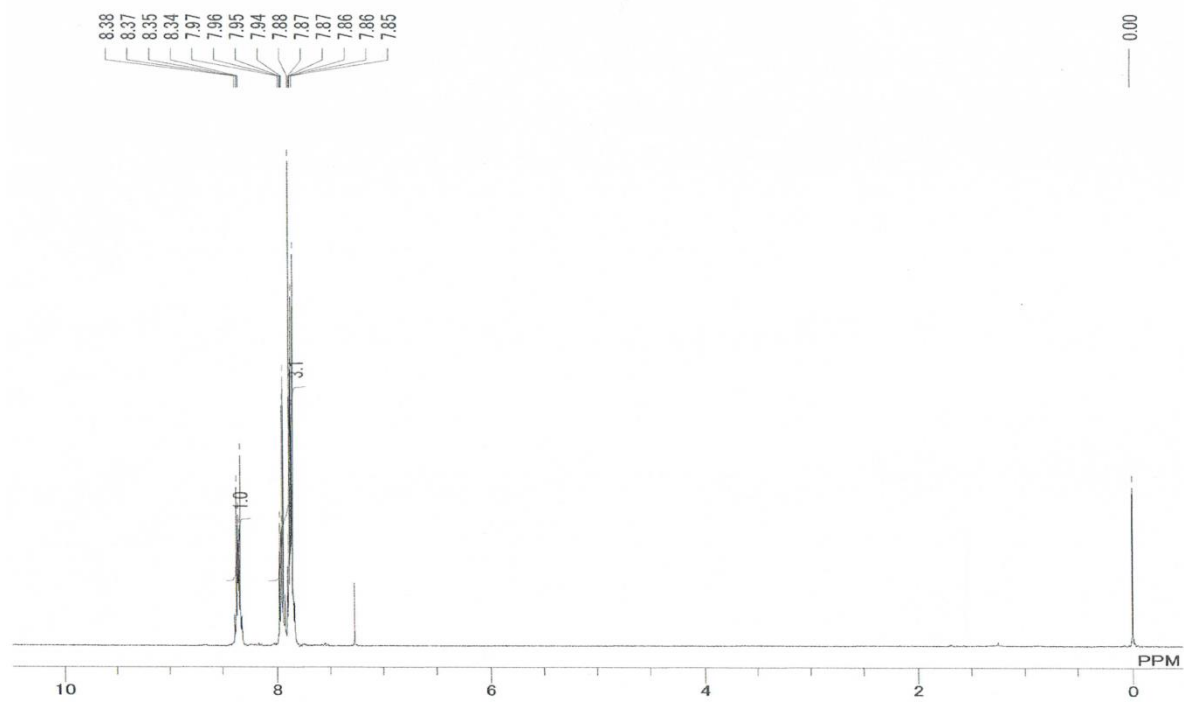
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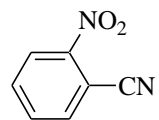
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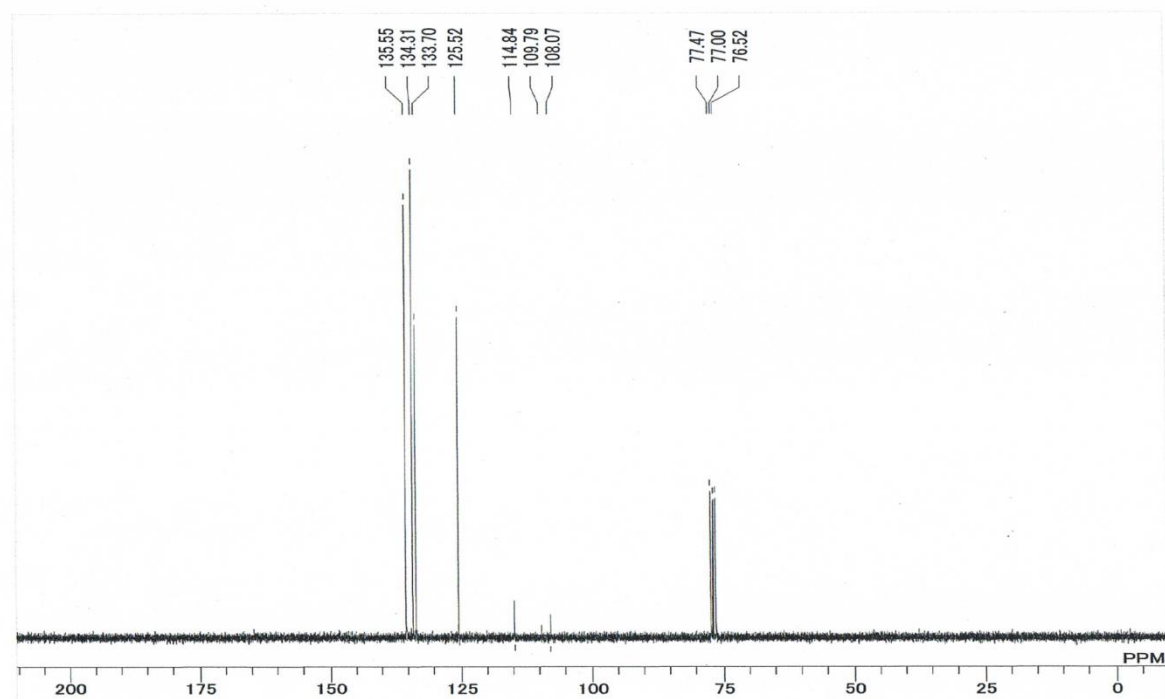
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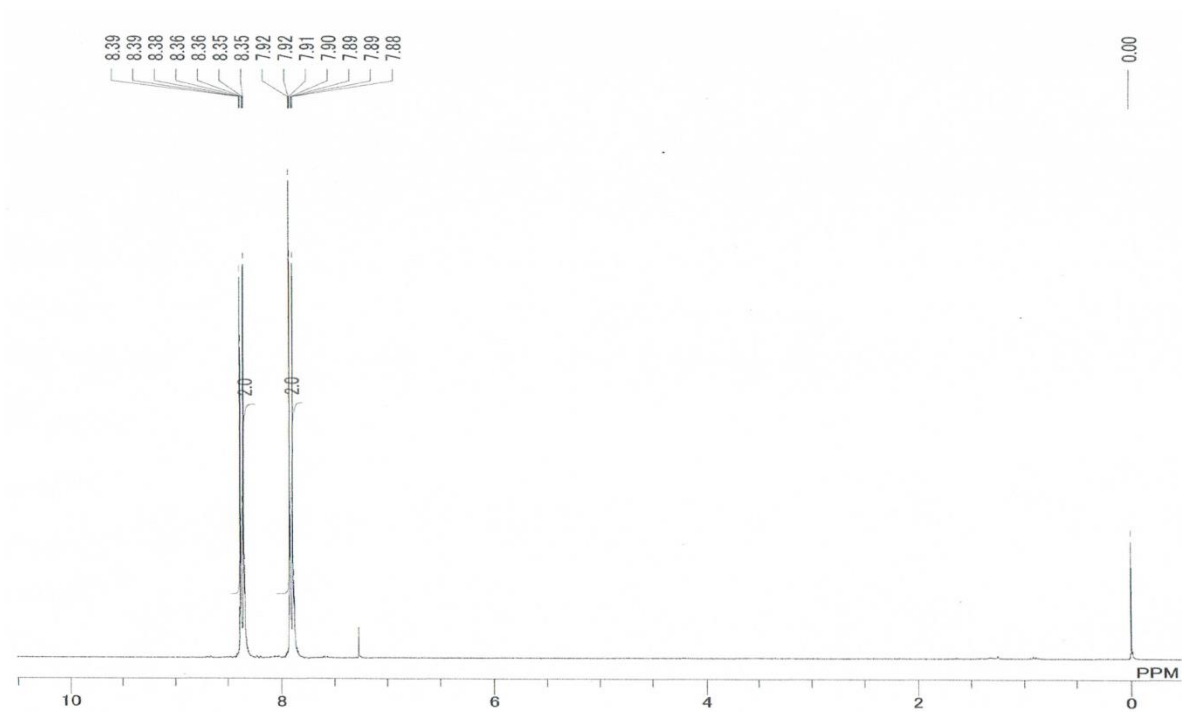
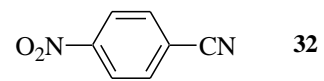
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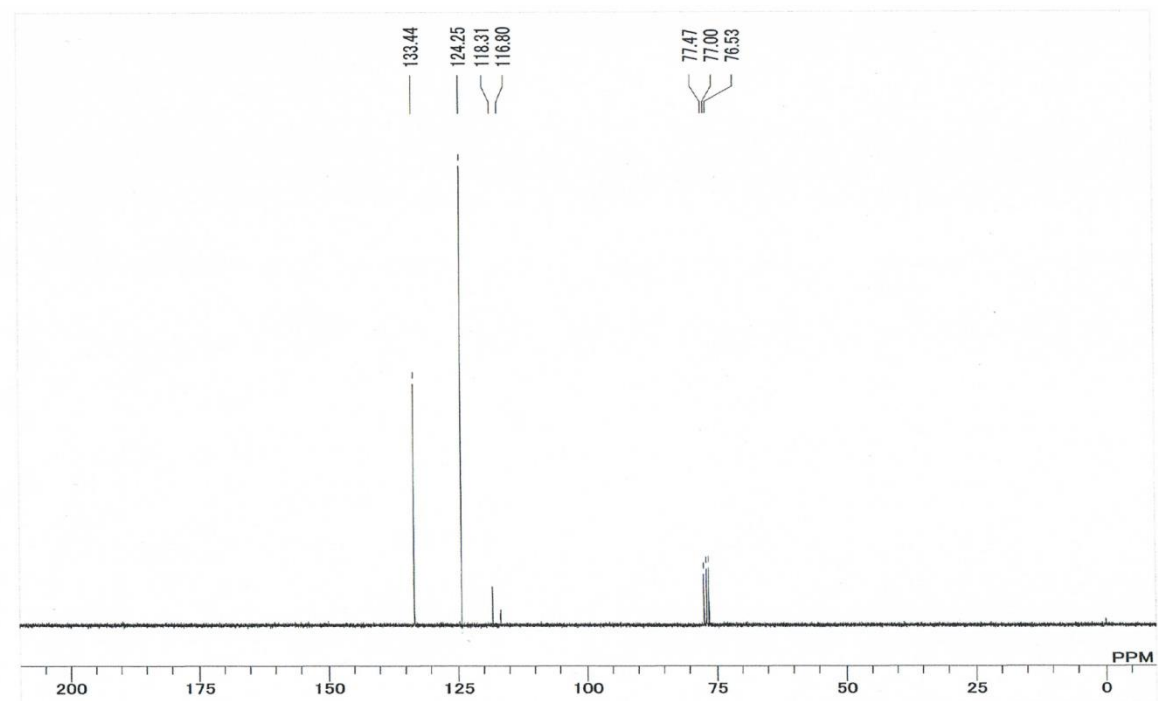
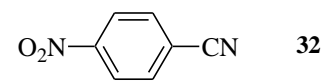
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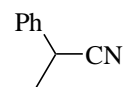
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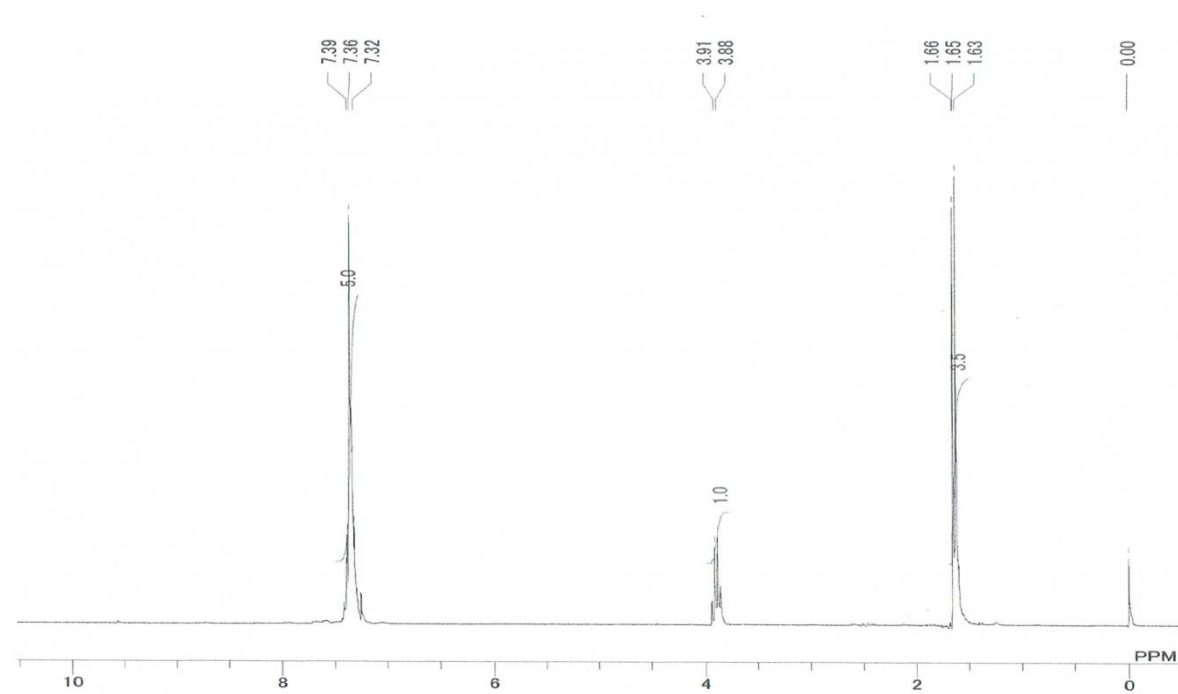
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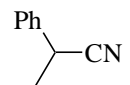
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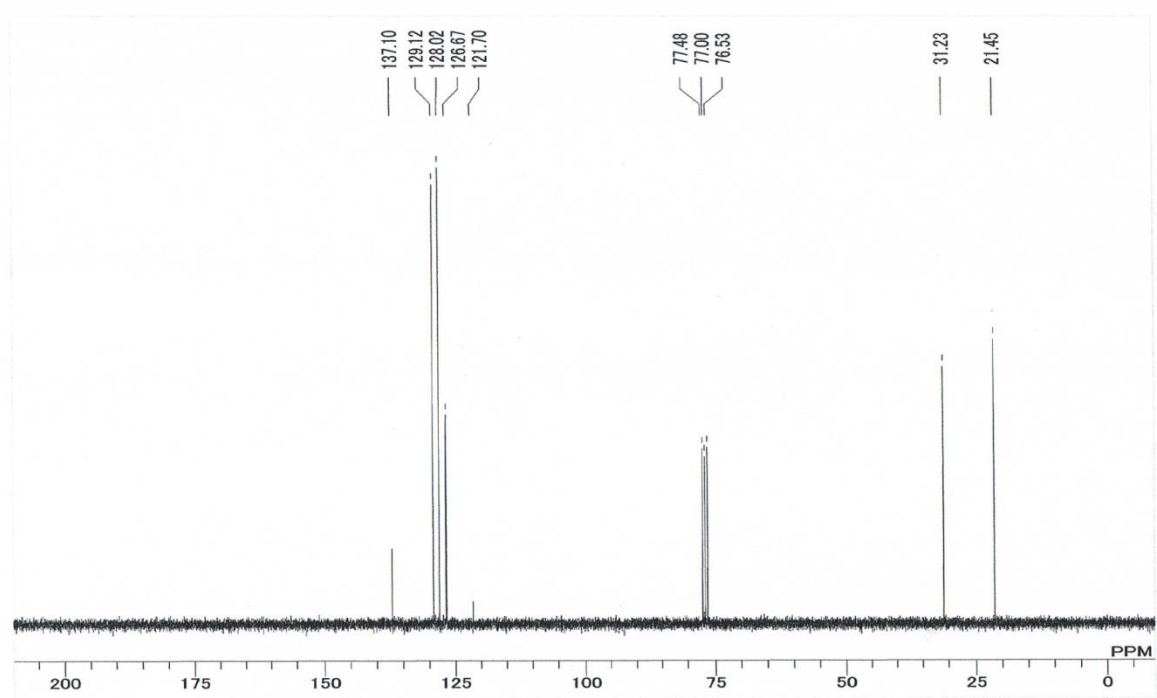
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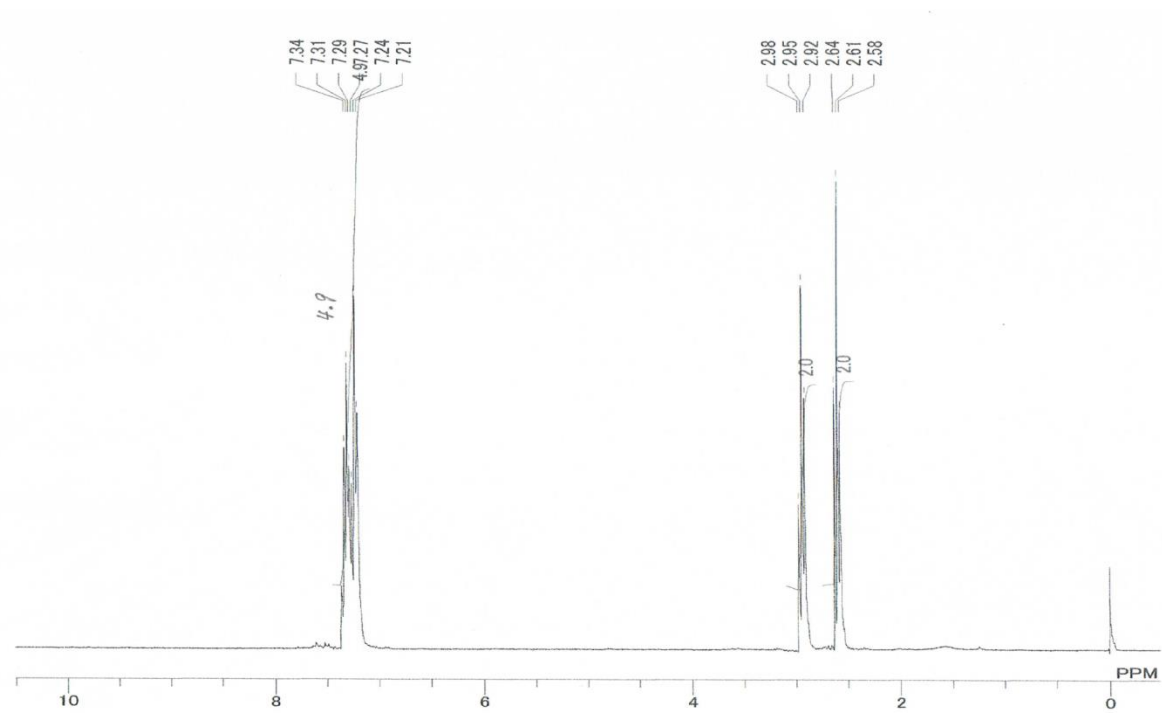
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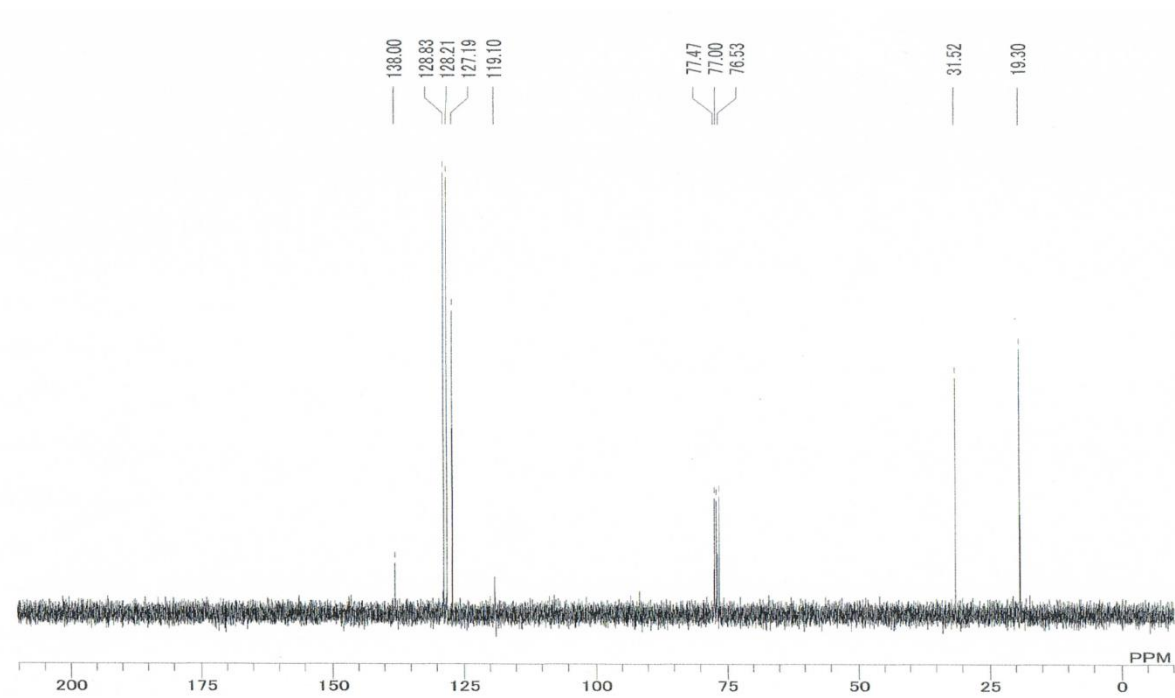
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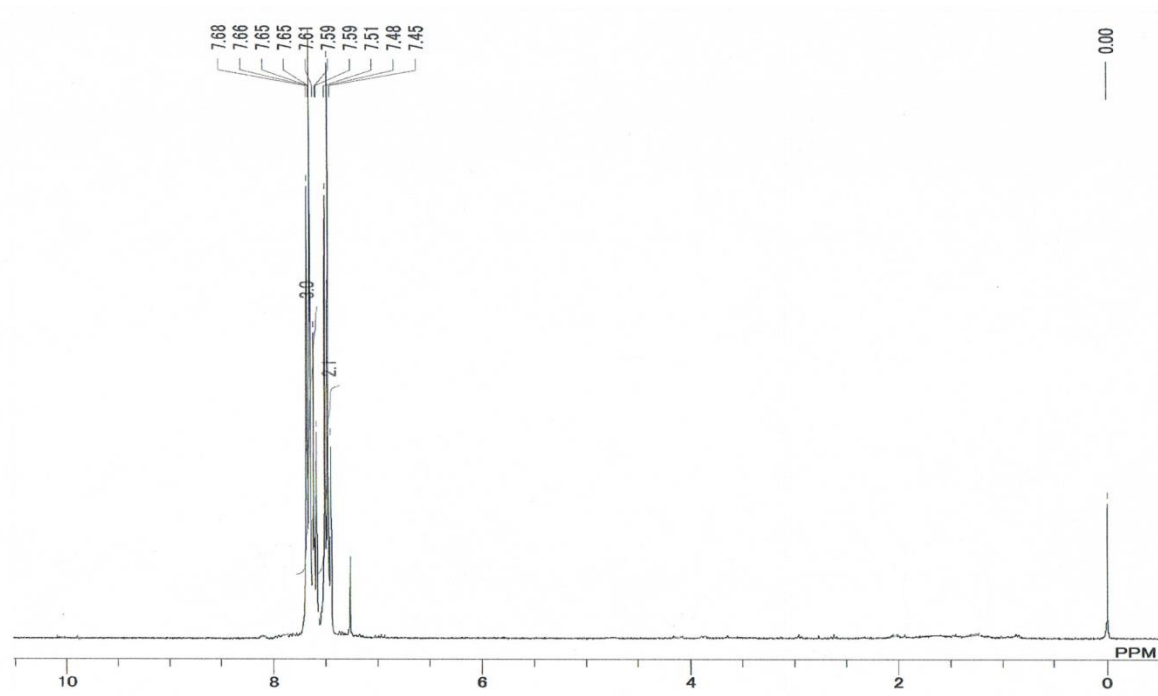
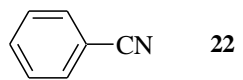
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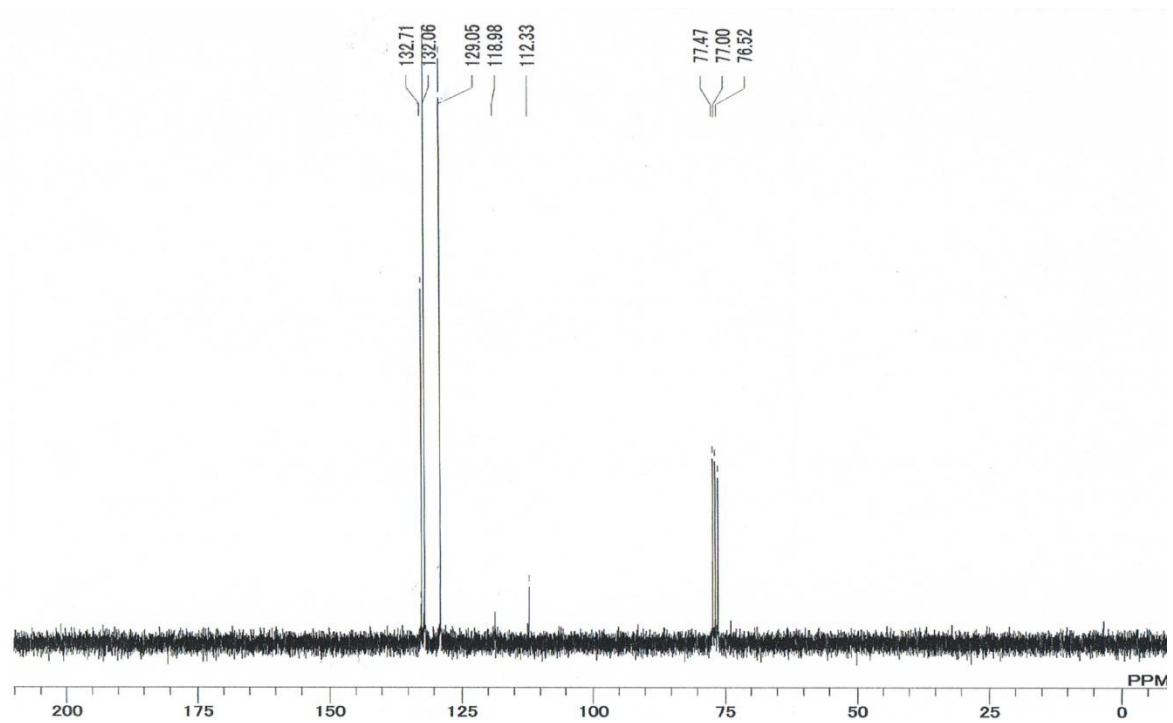
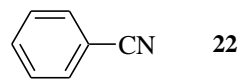
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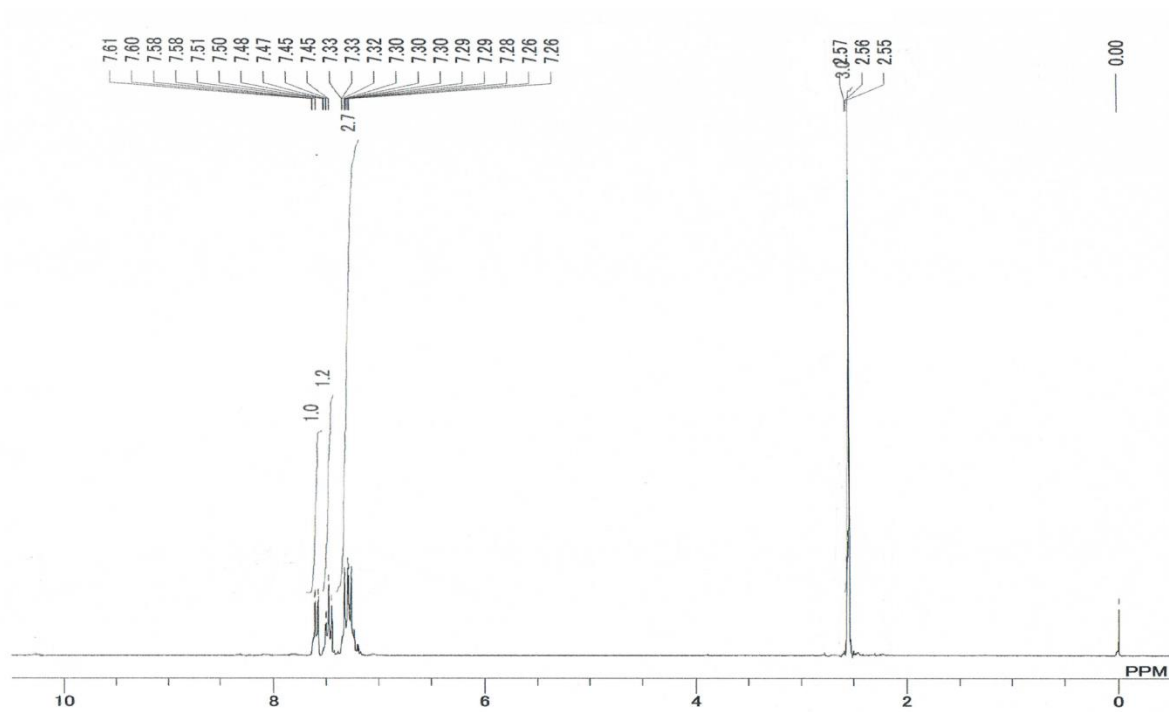
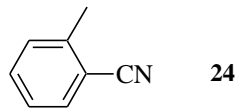
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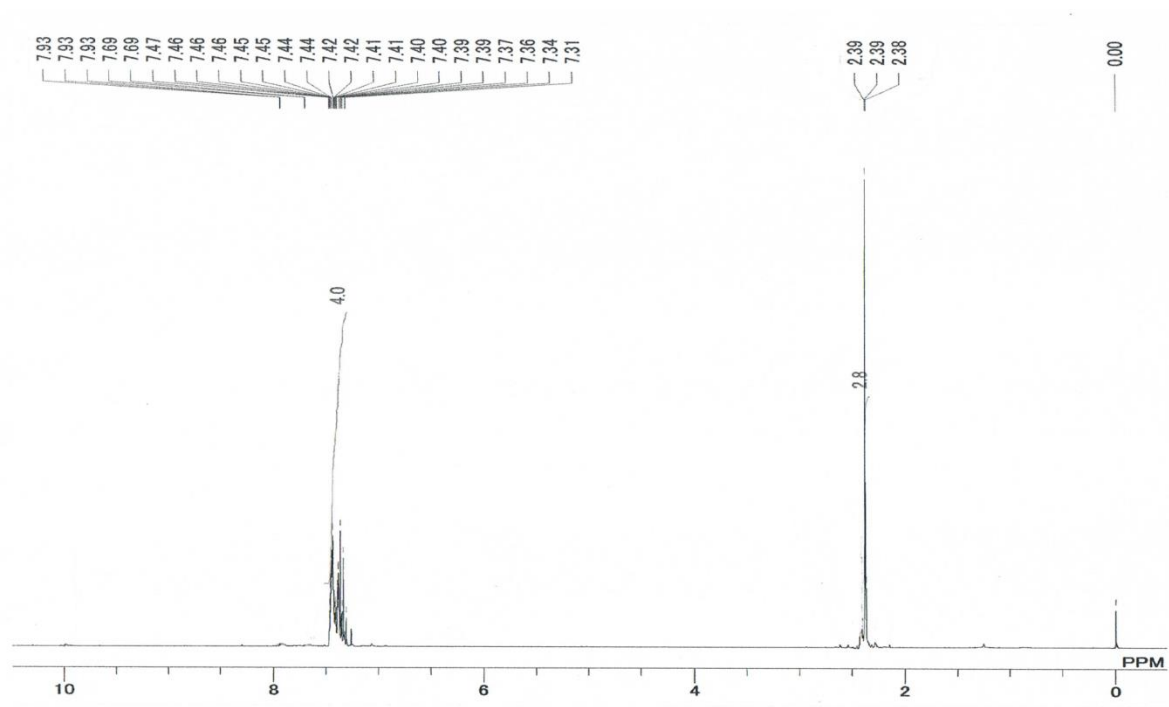
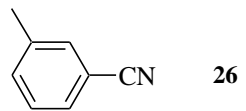
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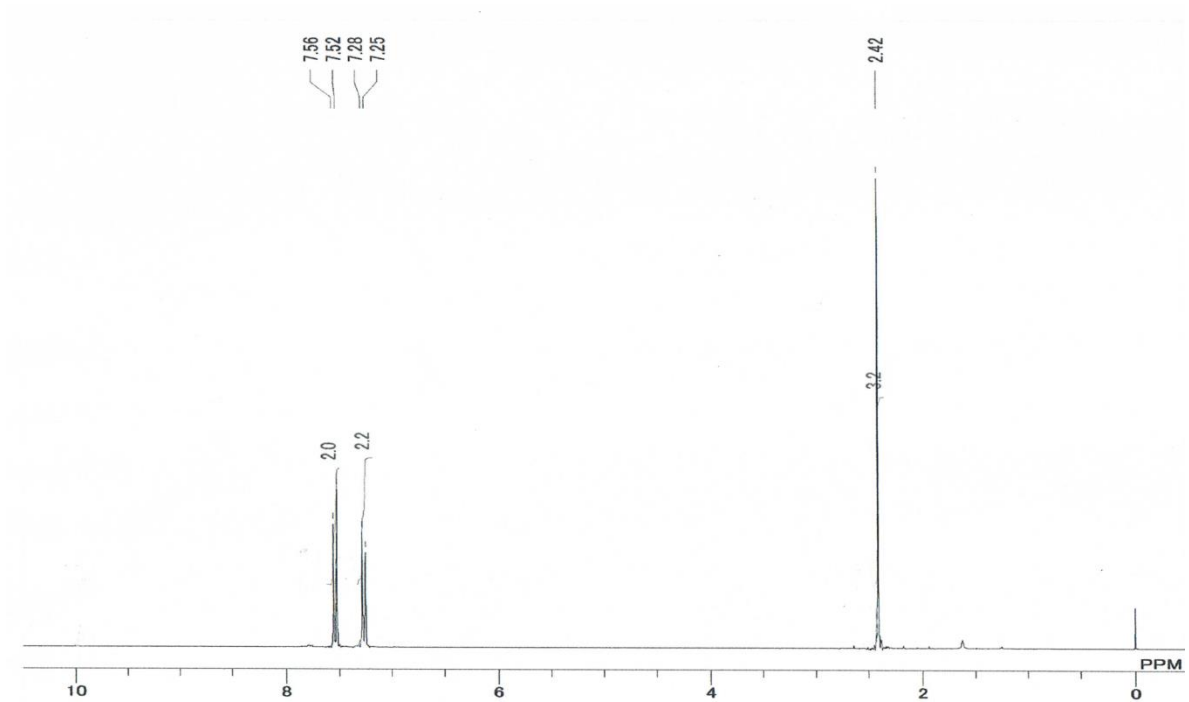
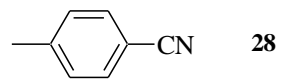
^1H NMR (CDCl_3 , 270.05 MHz)



$^1\text{H NMR}$ (CDCl_3 , 270.05 MHz)



^1H NMR (CDCl_3 , 270.05 MHz)



^{13}C NMR (CDCl_3 , 67.80 MHz)

