Supporting Information

for

Base-mediated self-propagative Lossen rearrangement of hydroxamic acids for the efficient and facile synthesis of aromatic and aliphatic primary amines

Naoya Ohtsuka, Moriaki Okuno, Yujiro Hoshino* and Kiyoshi Honda*

Graduate School of Environment and Information Sciences, Yokohama National University, Tokiwadai, Hodogaya-ku, Yokohama 240-8501, Japan.

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Synthesis of Hydroxamic Acids 1a-1v

Separate solutions of hydroxylamine hydrochloride (4.17 g, 0.060 mol) in 30 mL of MeOH, and of potassium hydroxide (6.72 g 0.12 mol) in 30 mL of MeOH, were prepared. Both were cooled in ice bath, and the one containing alkali was added with shaking to the hydroxylamine solution. After all the alkali was added, the mixture was allowed to stand in an ice bath for five minutes to ensure complete precipitation of potassium chloride. The mixture was filtered with suction and the filtrate was added to Methyl 4-methylbenzoate (4.77 mL, 0.030 mol) in 100 mL flask. Additional potassium hydroxide was added to become a basic solution (pH 10). After 12 hours with stirring at room temperature, MeOH was evaporated in vacuo and to the residue was added 20 mL of water in order to become a clear solution, which was acidified with 2 M HCl to be pH <4. The solid appeared was collected by filtration to give the title compound. Additionally, the filtrate was extracted with ethyl acetate and the organic phase was evaporated and purified by recrystallization from ethyl acetate/hexane to give the additional desired product.

***N*-hydroxy-4-methylbenzamide (1a)**[1,2]**:** Yield 88%. White crystalline solid. IR (KBr) ν 3295, 2760, 1650, 1614, 1564, 1508, 1331, 1038, 839, 739, 538 cm^{-1}; ^1H NMR (270 MHz, DMSO-d_6) δ 2.34 (s, 3H), 7.24 (d, J = 8.4 Hz, 2H), 7.65 (d, J = 8.4 Hz, 2H), 8.95 (s, 1H), 11.13 (s, 1H).

***N*-hydroxy-2-methylbnzamide (1b)**[2]**:** Yield 55%. White crystalline solid. IR (KBr) ν 3303, 3212, 1625, 1595, 1527, 1482, 1316, 1165, 1022, 901 cm^{-1}; ^1H

NMR (270 MHz, DMSO-d_6) δ 2.33 (s, 3H), 7.18-7.35 (m, 4H), 9.04 (s, 1H), 10.08 (s, 1H).

***N*-hydroxy-3-methylbnzamide (1c)[2]:** Yield 61%. White crystalline solid. IR (KBr) ν 3307, 3064, 2914, 1651, 1624, 1580, 1561, 1485, 1459, 810, 725 cm^{-1}; ^1H NMR (270 MHz, DMSO-d_6) δ 2.34 (s, 3H), 7.33 (d, J = 4.6 Hz, 2H), 7.54 (t, J = 4.6 Hz, 2H), 9.01 (s, 1H), 11.13 (s, 1H).

***N*-hydroxybenzamide (1d)[1]:** Yield 90%. White crystalline solid. IR (KBr) ν 3299, 3060, 2758, 1648, 1312, 1532, 1491, 1453, 1435, 1328, 706, 691 cm^{-1}; ^1H NMR (270 MHz, DMSO-d_6) δ 7.42-7.55 (m, 3H), 7.74-7.77 (m, 2H), 9.04 (s, 1H), 11.12 (s, 1H).

4-*tert*-buty- *N*-hydroxylbenzamide (1e)[3]: Yield 98%. White crystalline solid. IR (neat) ν 3153, 2953, 1608, 1542, 1452, 1163, 1106, 1012, 846, 667 cm^{-1}; ^1H NMR (270 MHz, DMSO-d_6) δ 1.29 (s, 9H), 7.46 (d, J = 7.6 Hz, 2H), 7.68 (d, J = 7.6 Hz, 2H), 8.97 (s, 1H), 11.13 (s, 1H).

***N*-hydroxy-4-methoxylbenzamide (1f)[1]:** Yield 81%. White crystalline solid. IR (KBr) ν 3285, 2971, 2755, 1644, 1610, 1568, 1507, 1443, 1305, 1254, 1024 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 3.80 (s, 3H), 6.98 (d, J = 8.4 Hz, 2H), 7.73 (d, J = 8.4 Hz, 2H), 8.91 (s, 1H), 11.06 (s, 1H).

4-chloro-*N*-hydroxybenzamide (1g)[1,2]**:** Yield 95%. White crystalline solid. IR (KBr) ν 3292, 3067, 2745, 1651, 1598, 1561, 1487, 1097, 1013, 847, 746, 538 cm^{-1}: ^1H NMR (270 MHz, DMSO-d_6) δ 7.53 (d, J = 8.6 Hz, 2H), 7.77 (d, J = 8.6 Hz, 2H), 9.11 (s, 1H), 11.30 (s, 1H).

4-bromo-*N*-hydroxybenzamide (1h)[4]**:** Yield 98%. White crystalline solid. IR (KBr) ν 3290, 3066, 2748, 1649, 1614, 1591, 1558, 1483, 1075, 1011, 526 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 7.65-7.72 (m, 4H), 9.13 (s, 1H), 11.24 (s, 1H).

***N*-hydroxy-2-iodobenzamide (1i):** Yield 71%. White solid. IR (KBr) ν 3237, 3039, 2876, 1622, 1542, 1467, 1170, 904, 744 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 7.18 (dt, J = 8.0, 1.6 Hz, 1H), 7.29 (dd, J = 8.0, 1.6 Hz, 1H), 7.43 (dt, J = 8.0, 0.8 Hz, 1H), 7.88 (dd, J = 8.0, 0.8 Hz, 1H), 9.20 (s, 1H), 10.91 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 99.4, 127.9, 128.6, 131.1, 139.2, 140.6, 165.7. Anal. Calcd for $C_7H_6INO_2$: C, 31.96; H, 2.30; N, 5.33. Found: C, 31.98; H, 2.39; N, 5.30.

***N*-hydroxy-4-nitrobenzamide (1j)**[5]**:** Yield 90%. Yellow Crystalline solid. IR (KBr) ν 3249, 2856, 1654, 1600, 1516, 1358, 1034, 850, 550 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 7.99 (d, J = 5.4 Hz, 2H), 8.31 (d, J = 5.4 Hz, 2H), 9.37 (s, 1H), 11.58 (s, 1H).

***N*-hydroxy-2,6-dimethoxybenzamide (1k)**[6a]**:** Yield 50%. White Crystalline solid. Mp. 201.2-201.5 °C (AcOEt) (lit.[6b] 200-201 °C). IR (KBr) ν 3260, 2887,

2835, 1619, 1600, 1475, 1257, 1119, 898, 791, cm^{-1}: ^1H NMR (270 MHz, DMSO-d_6) δ 3.36 (s, 3H), 6.66 (d, J = 9.5 Hz, 2H), 7.30 (t, J = 9.5 Hz, 1H), 8.96 (s, 1H), 10.52 (s, 1H).

***N*-hydroxy-2,3-dimethoxybenzamide (1l):** Yield 70%. White Crystalline solid. IR (KBr) ν 3345, 3321, 3089, 2838, 1644, 1577, 1267, 988, 812, 757 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 3.75 (s, 3H), 3.82 (s, 3H), 6.94 (dd, J = 7.2, 1.2 Hz, 1H), 7.07-7.14 (m, 2H), 9.08 (s, 1H), 10.68 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 55.9, 61.0, 114.4, 120.2, 124.0, 129.3, 146.1, 152.5, 163.5. Anal. Calcd for $C_9H_{11}NO_4$: C, 54.82; H, 5.62; N, 7.10. Found: C, 54.97; H, 5.59; N, 6.95.

***N*-hydroxy-3,5-dimethylbenzamide (1m)[7]:** Yield 98%. White Crystalline solid. IR (neat) ν 3208, 2919, 1625, 1592, 1528, 1400, 1144, 944, 862, 782, 684, 637 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 2.29 (s, 6H), 7.14 (s, 1H), 7.35 (s, 1H), 8.97 (s, 1H), 11.13 (s, 1H).

***N*-hydroxy-2-pyridinecarboxamide (1n)[8]:** Yield 27%. White solid. IR (ATR) ν 3340, 3152, 2835, 1645, 1511, 1428, 1177, 1026, 906, 746. ^1H NMR (270 MHz, DMSO-d_6) δ 7.58 (q, J = 4.40 Hz, 1H), 7.98 (d, J = 4.14 Hz, 2H), 8.54-8.65 (m, 2H), 9.10 (s, 1H), 11.42 (s, 1H).

***N*-hydroxy-2-quinolinecarboxamide (1o)[9]:** Yield 52%. White solid. IR (ATR) ν 3142, 2855, 1645, 1623, 1504, 1145, 1041, 916. 769. ^1H NMR (270 MHz,

DMSO-d_6) δ 7.67-7.74 (m, 1H), 7.86 (ddd, J = 1.5, 6.9, 8.5 Hz, 1H), 8.09 (dd, J = 6.2, 8.5 Hz, 3H), 8.52-8.59 (m, 1H), 9.22 (s, 1H), 11.55 (s, 1H).

***N*-hydroxy-2-phenylacetamide (1p)[4]:** Yield 90%. White Crystalline solid. IR (KBr) ν 3189, 3031, 1632, 1548, 1455, 1418, 1365, 1054, 979, 693, 542 cm^{-1}: ^1H NMR (270 MHz, DMSO-d_6) δ 3.26 (s, 2H), 7.19-7.30 (m, 5H), 8.85 (s, 1H), 10.63 (s, 1H).

N-hydroxy-3-phenylpropaneamide (1q)[1]: Yield 89%. Yellow Crystalline solid. IR (KBr) ν 3297, 3030, 2797, 1665, 1629, 1562, 1454, 1371, 718, 697, 483 cm^{-1}: ^1H NMR (270 MHz, DMSO-d_6) δ 2.41 (t, J = 7.3 Hz, 2H), 2.93 (t, J = 7.3 Hz, 2H), 7.15-7.31 (m, 5H).

***N*-hydroxy-2-cyclohexylacetamide (1r):** Yield 74%. White crystalline solid. IR (KBr) ν 3190, 3006, 2924, 2850, 1630, 1542, 1448, 1038, 980, 735, 808, 539 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 0.83-0.92 (m, 2H), 1.04-1.24 (m, 3H), 1.58-1.65 (m, 6H), 1.81 (d, J = 6.4 Hz, 2H), 8.66 (s, 1H), 10.30 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 25.5, 25.8, 32.4, 34.4, 168.2. HRMS (ESI) *m/z* 158.1178 (158.1176 calcd for $C_8H_{16}NO_2$ [MH^+])

***N*-hydroxycyclohexanecarboxamide (1s)[10]:** Yield 63%. White crystalline solid. IR (KBr) ν 3202, 3037, 2922, 2852, 1628, 1543, 1447, 1060, 1018, 963, 808 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 1.06-1.37 (m, 6H), 1.57-1.69 (m, 4H), 1.90-1.98 (m, 1H), 8.62 (s, 1H), 10.32 (s, 1H).

***N*-hydroxy-adamantane-1-carboxamide (1t)[11]:** Yield 91%. White crystalline solid. IR (KBr) ν 3448, 3278, 3153, 2906, 2849, 1694, 1604, 1477, 1451, 1287, 1124, 1022, 928, 812, 628 cm^{-1}: ^1H NMR (270 MHz, DMSO-d_6) δ 1.60-1.80 (m, 12H), 1.94 (s, 3H), 8.50 (s, 1H), 10.22 (s, 1H).

(9*Z*)-*N*-hydroxy-octadecenecarboxamide (1u): Yield 61%. White crystalline solid. IR (KBr) ν 3283, 2918, 2850, 1666, 1623, 1465, 1428, 1068, 968, 725, 545, 481 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 0.86 (t, J = 6.8 Hz, 3H), 1.24 (brs, 20H), 1.45-1.50 (m, 2H), 1.90-2.02 (m, 6H), 5.28-5.36 (m, 2H), 8.65 (s, 1H), 10.32 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 13.9, 22.1, 25.1, 26.6, 28.5, 28.6, 28.7, 28.8, 29.1, 31.2, 32.2, 129.6, 169.1. HRMS (ESI) *m/z* 298.2752 (298.2741 calcd for $C_{18}H_{36}NO_2$ [MH^+])

1*N*,8*N*-dihydroxyoctanediamide (1v)[12]: Yield 22%. White crystalline solid. IR (KBr) ν 3259, 3067, 2945, 2757, 1664, 1621, 1466, 1426, 1000, 979, 556 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 1.21 (brs, 4H), 1.46 (brs, 4H), 1.92 (t, J = 7.2 Hz, 2H), 8.65 (s, 1H), 10.35 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 25.0, 28.3, 32.2, 169.1.

***N*,4-dihydroxynonanecarboxamide (1w):** Yield 35%. IR (KBr) ν 3195, 3078, 2934, 1773, 1626, 1457, 1342, 970, 767, 673, 617 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 0.86 (t, J = 7.2 Hz, 3H), 1.24-1.60 (m, 10H), 1.94-2.07 (m, 2H),

8.65 (s, 1H), 10.34 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 14.0, 22.2, 24.9, 28.9, 31.4, 33.0, 37.0, 69.1, 169.5.

(2*S*)-*N*-hydroxy-2-(6-methoxynapthyl)propanecarboxamide (1x): The reaction time is 72 h, and purified by recrystallization with EtOAc. Yield 56%. White crystalline solid. $[\alpha]_D^{25}$ = 17.1 (c. = 1.0 in acetone). IR (KBr) ν 3196, 3023, 2906, 1634, 1607, 1392, 1264, 1214, 1028, 810, 619, 474 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ 1.42 (d, J = 7.2 Hz, 3H), 3.57 (q, J = 6.8 Hz, 1H), 3.86 (s, 3H), 7.14 (dd, J = 2.4, 8.8 Hz, 1H), 7.27 (d, J = 2.8 Hz, 1H), 7.45 (dd, J = 2.0, 8.8 Hz, 1H), 7.17-7.79 (m, 3H), 8.82 (s, 1H), 10.7 (s, 1H). LC-MS (ESI) found [M+Na$^+$] 268.2 (calcd. 268.1).

Synthesis of *N,O*-bis(methoxymethyl)-*N*-hydroxy-2-(6-methoxynapthyl) propanecarboxamide

(2*S*)-*N*-hydroxy-2-(6-methoxynapthyl)propanecarboxamide **1x** (245 mg, 1.0 mmol) was suspension in CH_2Cl_2 (1 mL). The reaction mixture was cooled in ice bath, then (^{i}Pr)$_2$EtN (0.520 mL, 3.0 mmol), MOMCl (0.166 mL, 2.2 mmol) were added to mixture and stirred for 4 hour at rt. The mixture was quenched by sat. NH_4Cl aq. and extracted with CH_2Cl_2 (5.0 mL × 3). The combined organic layer was dried over anhydrous Na_2SO_4, filtered and evaporated under reduced pressure. The residue was purified by silica gel column chromatography (EtOAc) to yield the pure title compound (69.0 mg, 21%, 93% ee) as a Yellow oil.

IR (ATR) ν 2935, 2635, 2606, 1264, 1153, 997, 921, 728 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.54 (d, J = 7.2 Hz, 3H), 3.23 (s, 3H), 3.51 (s, 3H), 3.91-3.95 (m,

4H), 5.01 (d, J = 6.0 Hz, 1H), 5.08 (s, 2H), 5.20 (d, J = 6.0 Hz, 1H), 7.10-7.16 (m, 2H), 7.39-7.47 (m, 1H), 7.66-7.72 (m, 3H). HPLC [Chiralpak IA, *n*-hexane/2-propanol = 98/2, λ = 254 nm, retention time: (major) 21.8 min, (minor) 25.1 min].

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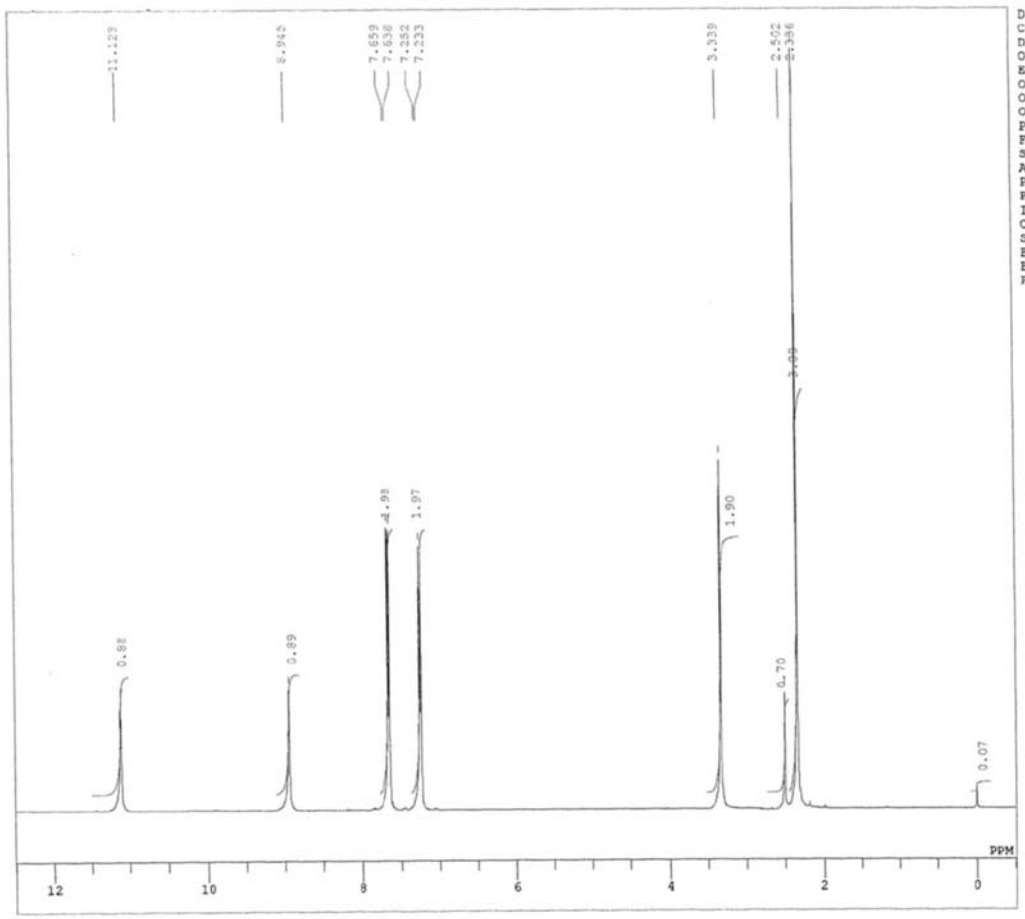


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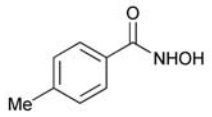

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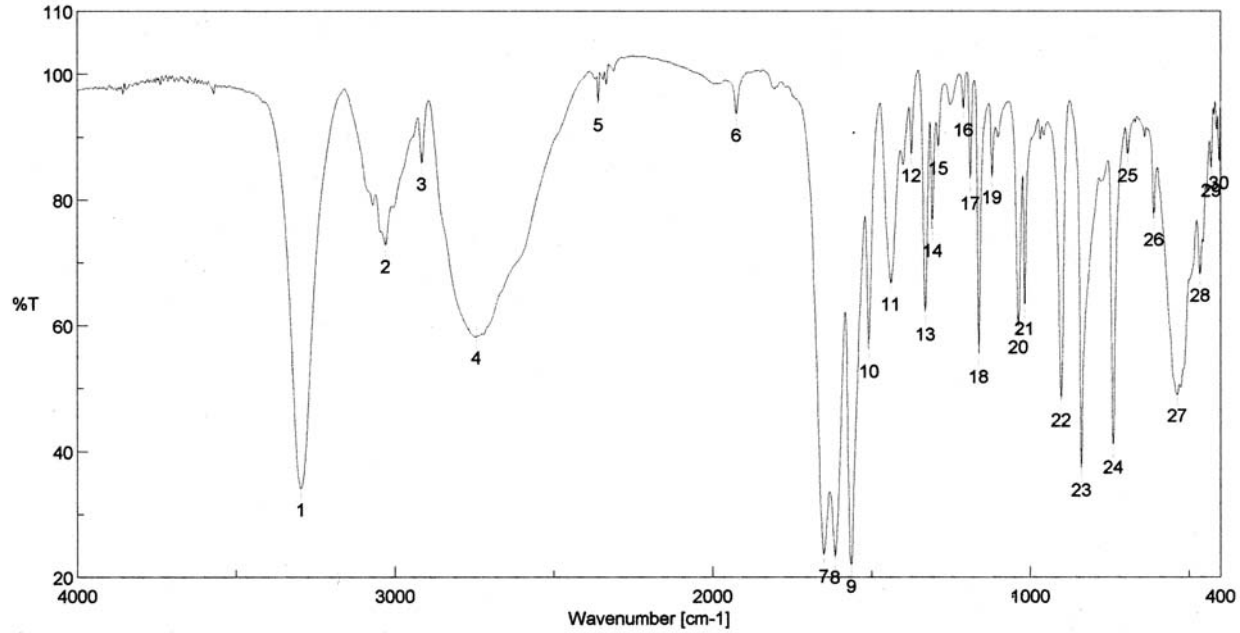

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9	1563.99	21.8803	10	1508.06	55.9871	11	1438.64	66.6992	12	1374.03	87.1544
13	1330.64	61.8933	14	1308.46	75.1979	15	1290.14	88.301	16	1210.11	94.4635
17	1188.9	82.7462	18	1161.9	55.1657	19	1120.44	83.711	20	1037.52	59.8628
21	1017.27	62.7985	22	901.558	48.2415	23	838.883	37.2239	24	738.603	40.846
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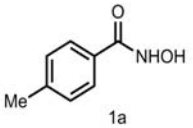

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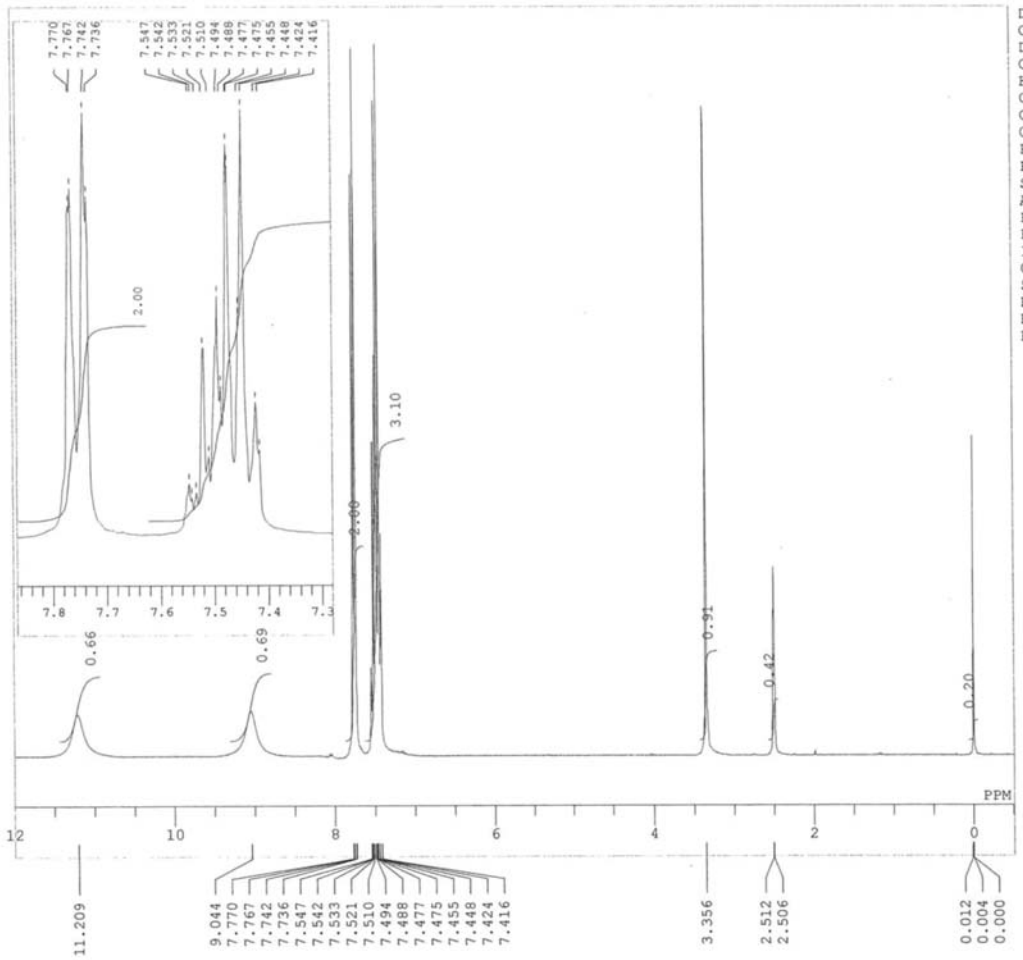

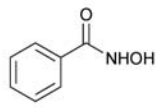

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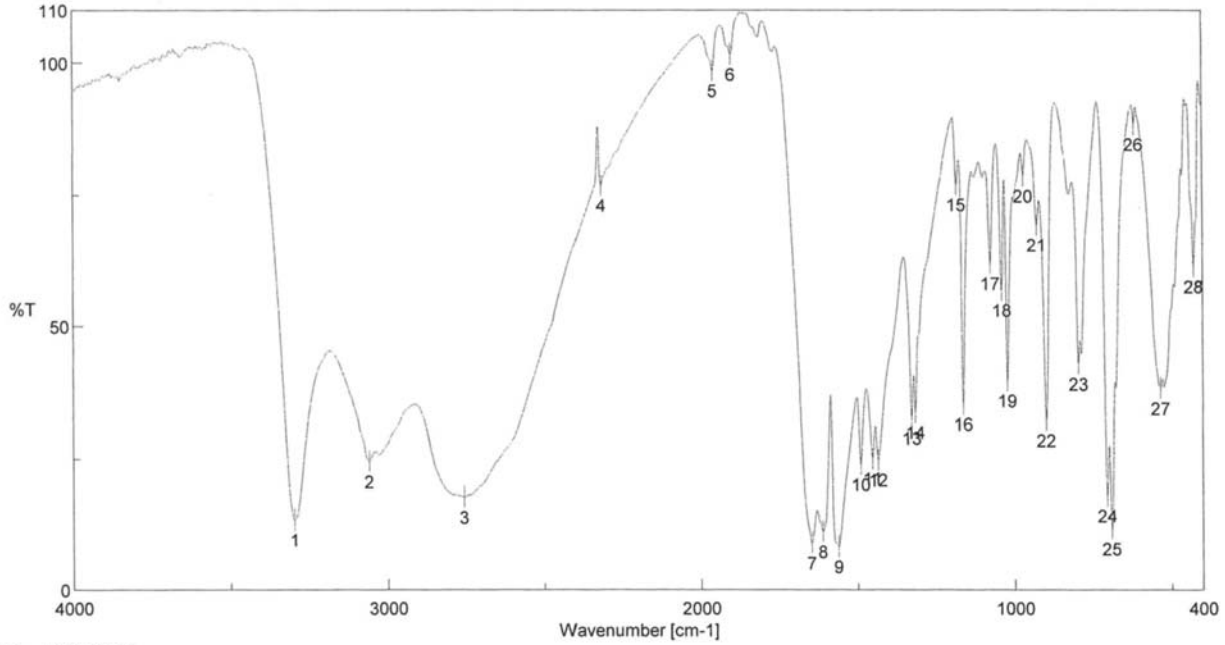

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9	1562.06	8.27254	10	1490.7	24.0758	11	1453.1	25.1948	12	1434.78	24.9187
13	1327.75	32.8786	14	1316.18	33.9553	15	1184.08	77.1947	16	1162.87	35.4638
17	1077.05	62.03	18	1040.41	56.966	19	1023.05	39.8485	20	970.983	78.835
21	928.557	69.4171	22	898.666	32.4131	23	796.457	42.9754	24	705.819	18.064
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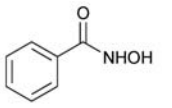

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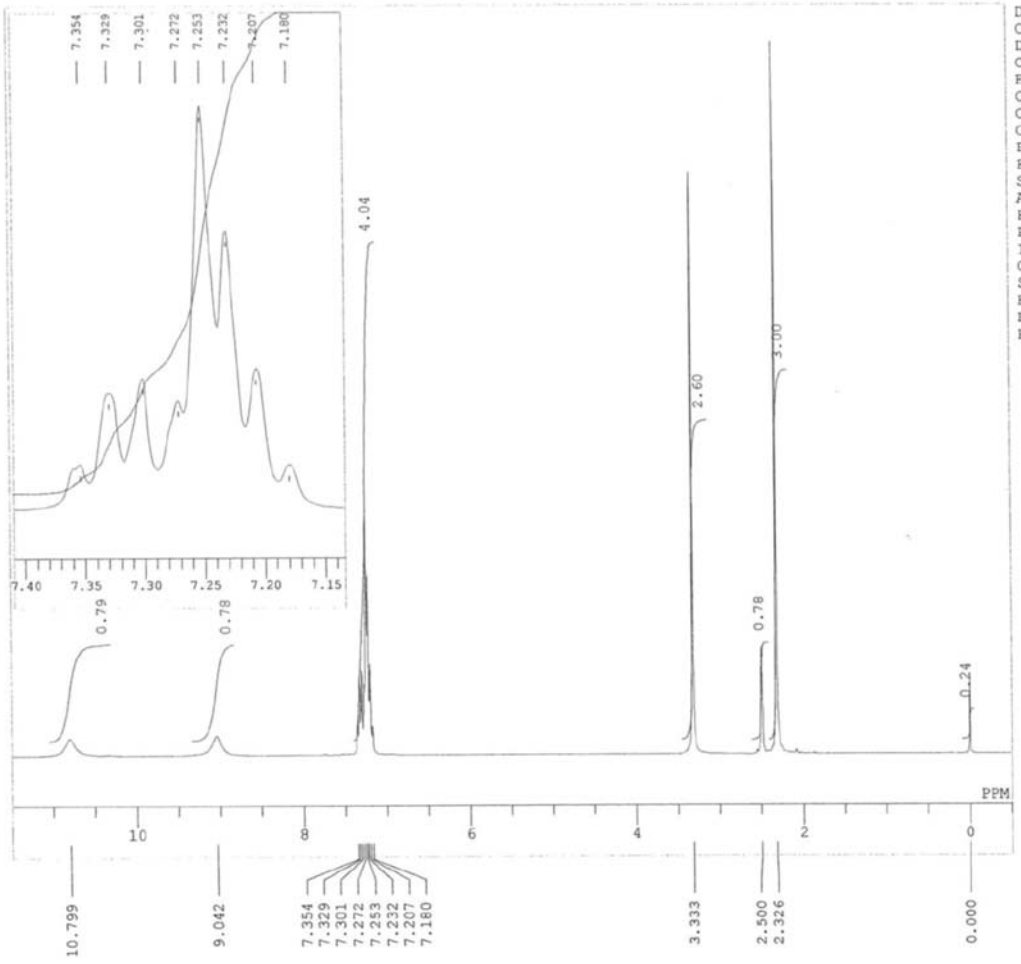

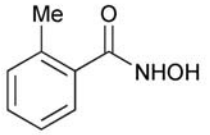

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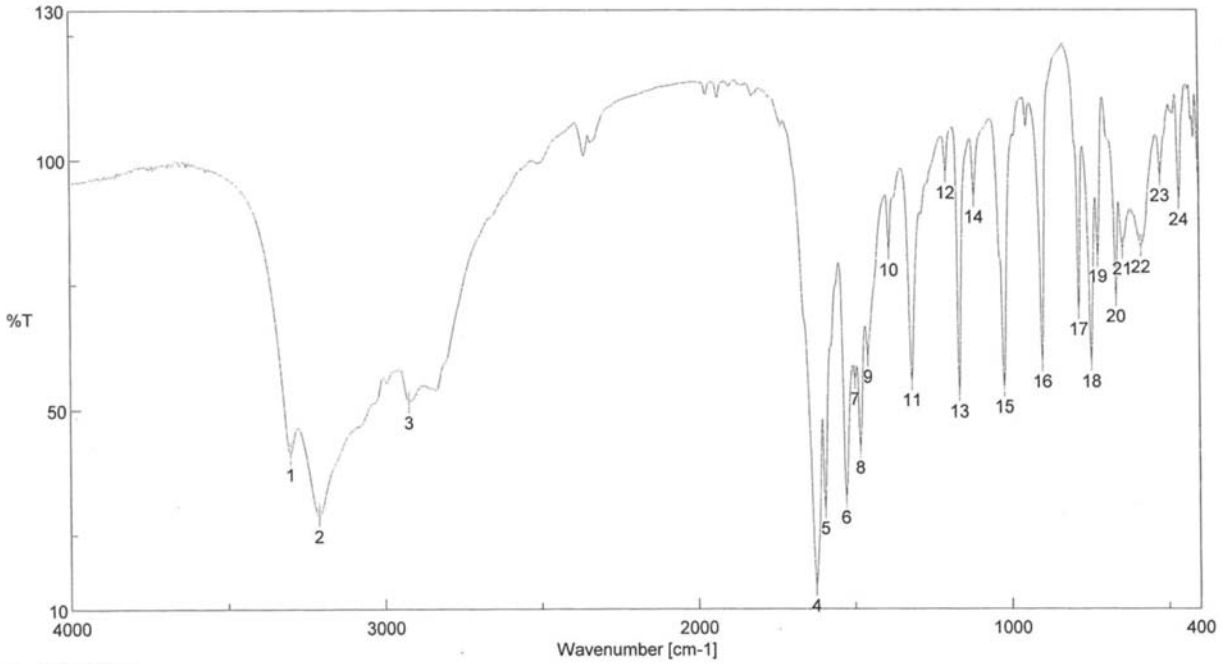

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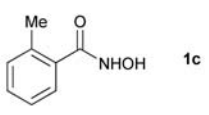
9	1456.96	60.7231	10	1388.5	82.086	11	1316.18	56.0238	12	1206.26	97.5924
13	1164.79	53.8218	14	1116.58	92.7699	15	1022.09	54.7626	16	900.594	59.7379
17	783.922	70.2049	18	744.388	59.7976	19	723.175	80.7907	20	665.321	72.7734
21	644.108	82.3307	22	585.29	82.7092	23	523.579	97.0428	24	463.796	92.2891



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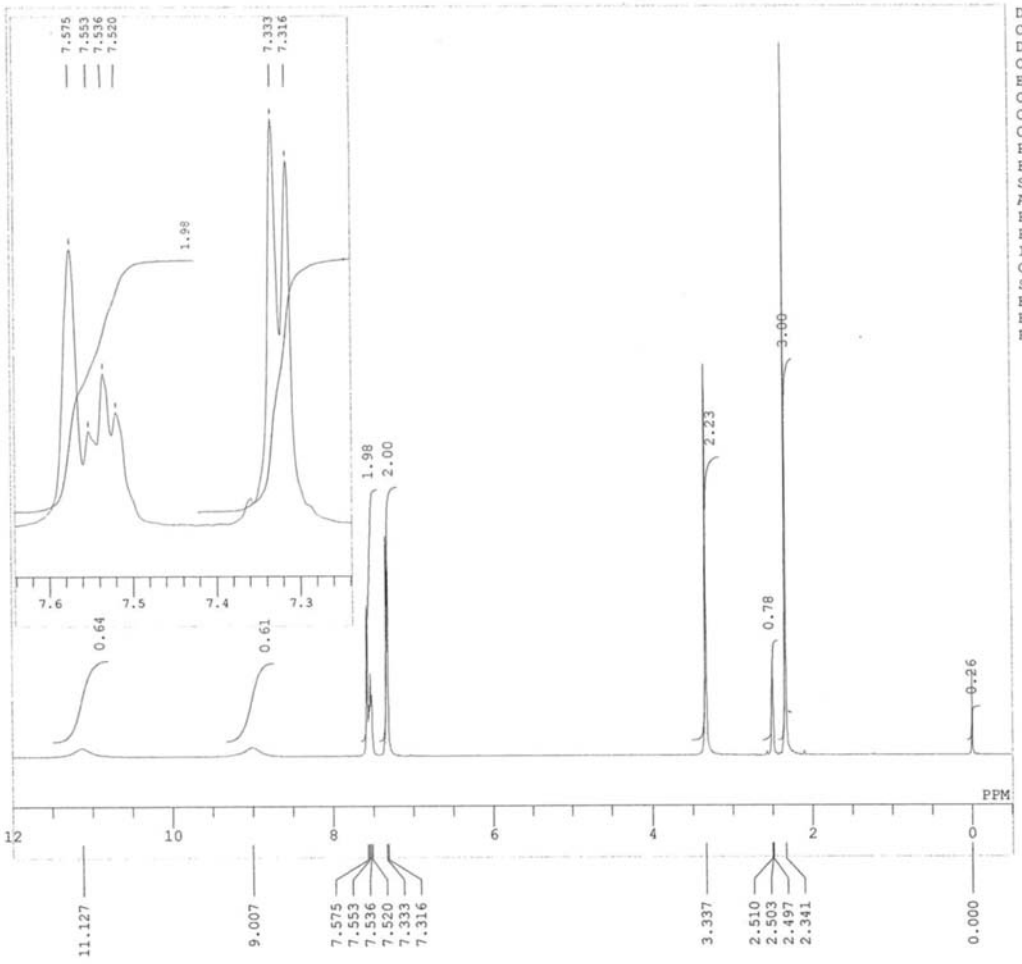


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EXMOD   NON
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OBSET       112.00 KHz
OBFIN       5800.0 Hz
POINT        16384
FREQU       5405.4 Hz
SCANS             8
ACQTM         3.031 sec
PD            3.969 sec
PW1             4.9 us
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EXREF          0.00 ppm
BF             1.00 Hz
RGAIN            19
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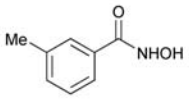

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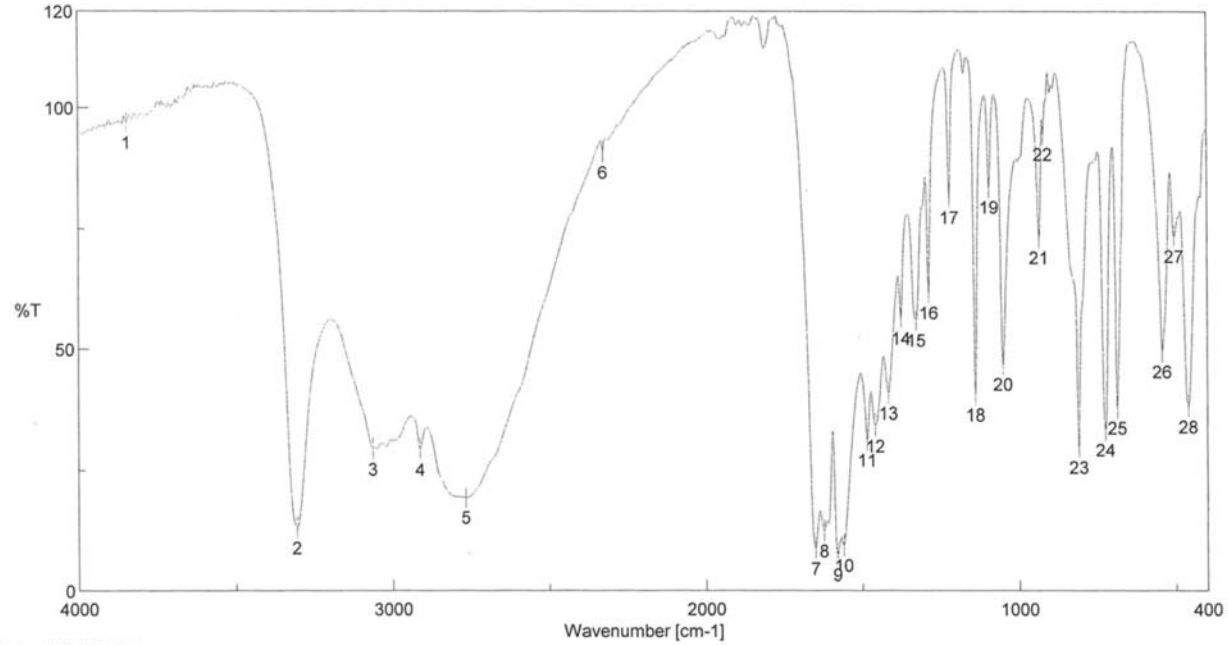
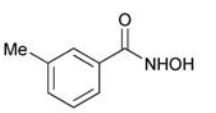


[ピーク検出結果]

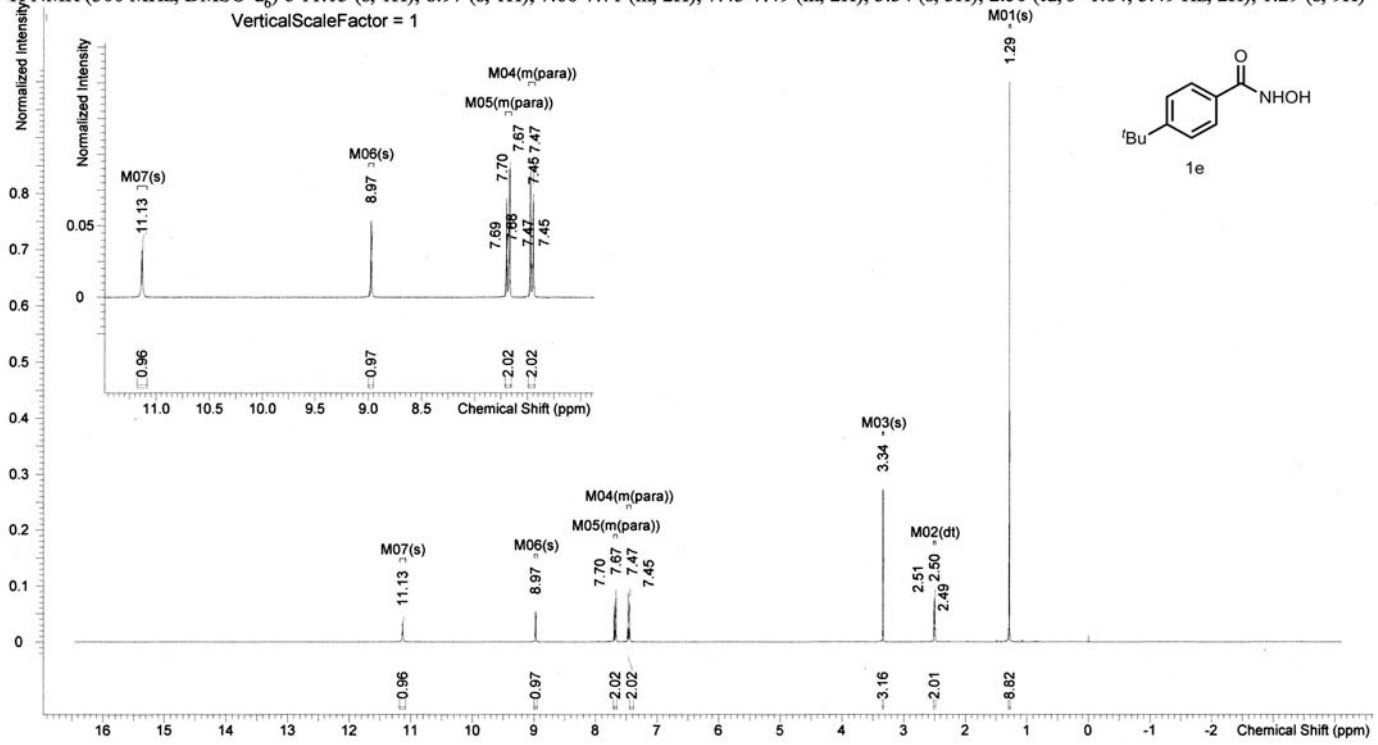
No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3846.33	97.1835	2	3307.32	13.101	3	3064.33	29.5108	4	2913.91	29.413
5	2767.35	19.4413	6	2327.66	90.9766	7	1650.77	8.85626	8	1623.77	12.4825
9	1580.38	7.53744	10	1561.09	9.46756	11	1484.92	31.4042	12	1458.89	34.3242
13	1416.46	41.0039	14	1375.96	56.4732	15	1327.75	56.0863	16	1287.25	61.8245
17	1220.72	81.652	18	1138.76	40.7243	19	1094.4	83.7963	20	1051.01	46.992
21	935.306	73.267	22	921.807	94.8284	23	809.956	29.9881	24	725.104	33.5781
25	687.498	38.0692	26	543.828	49.6069	27	505.258	73.5723	28	460.904	38.3689

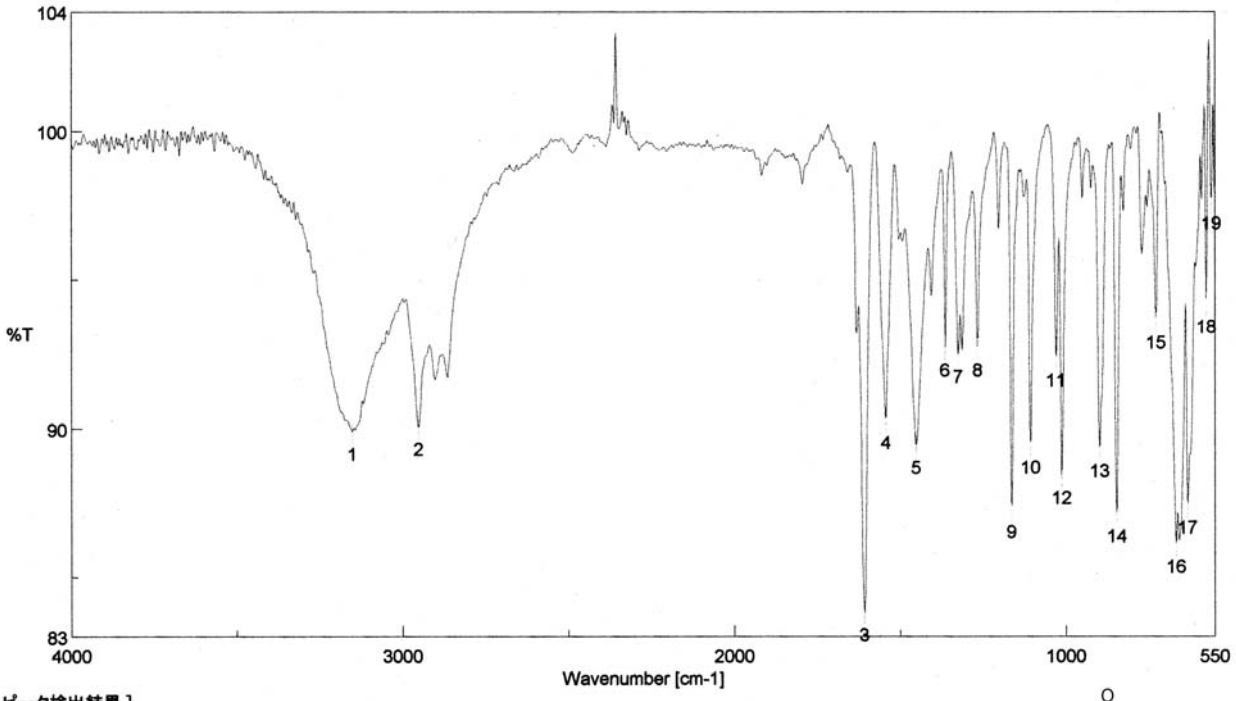


1d

OriginalDateForRelativeTime				Multiplets Integrals Sum	19.98	Number of Nuclei	20 H's		
Acquisition Time (sec)	2.6542	Comment	5 mm QNP 1H/13C/31P/19F Z3333/0001			Date			
Date Stamp				File Name				Frequency (MHz)	300.13
Nucleus	1H	Number of Transients	8	Origin	spect	Original Points Count	16384	Owner	DRX300
Points Count	16384	Pulse Sequence	zg30	Receiver Gain	645.10	SW(cyclical) (Hz)	6172.84	Solvent	DMSO-d6
Spectrum Offset (Hz)	1853.5107	Spectrum Type	STANDARD	Sweep Width (Hz)	6172.46	Temperature (degree C)	27.000		

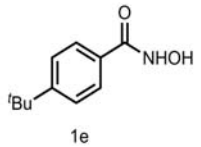
^{1}H NMR (300 MHz, DMSO-d_6) δ 11.13 (s, 1H), 8.97 (s, 1H), 7.66-7.71 (m, 2H), 7.43-7.49 (m, 2H), 3.34 (s, 3H), 2.50 (td, *J*=1.84, 3.49 Hz, 2H), 1.29 (s, 9H)

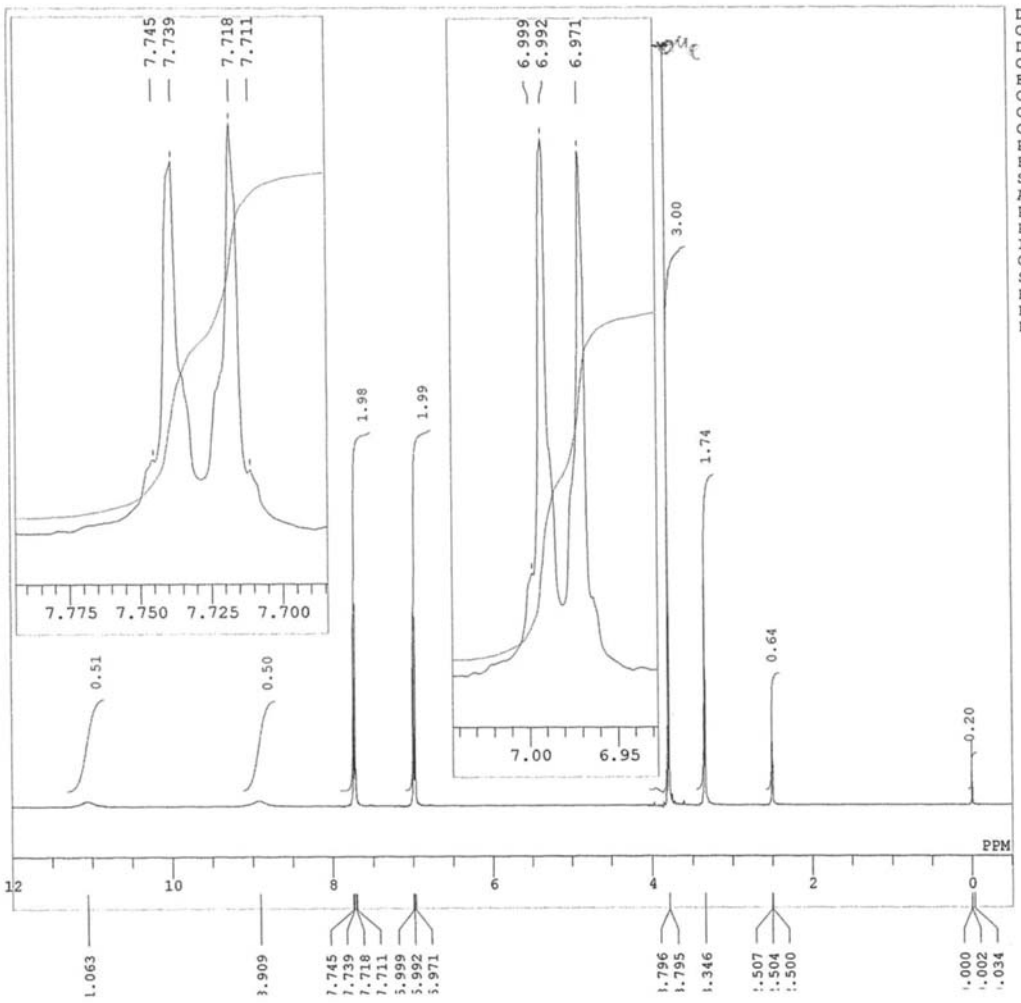




[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3153.04	89.8979	2	2953.45	90.0661	3	1608.34	83.8065	4	1542.77	90.2886
5	1452.14	89.4359	6	1364.39	92.6935	7	1324.86	92.4826	8	1267	92.6944
9	1163.83	87.284	10	1106.94	89.4605	11	1029.8	92.3633	12	1012.45	88.4279
13	898.666	89.3347	14	846.597	87.1352	15	728.961	93.6345	16	667.25	86.1146
17	632.537	87.4158	18	576.612	94.158	19	561.184	97.6463			



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EXMOD   NON
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OBSET         124.00 KHz
OBFIN       10500.00 Hz
POINT         32768
FREQU         7992.01 Hz
SCANS             8
ACQTM           4.1001 sec
PD              2.9000 sec
PW1             6.20 usec
IRNUC   1H
CTEMP            23.1 c
SLVNT   DMSO
EXREF             0.00 ppm
BF                0.12 Hz
RGAIN               18
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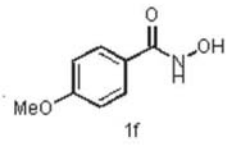

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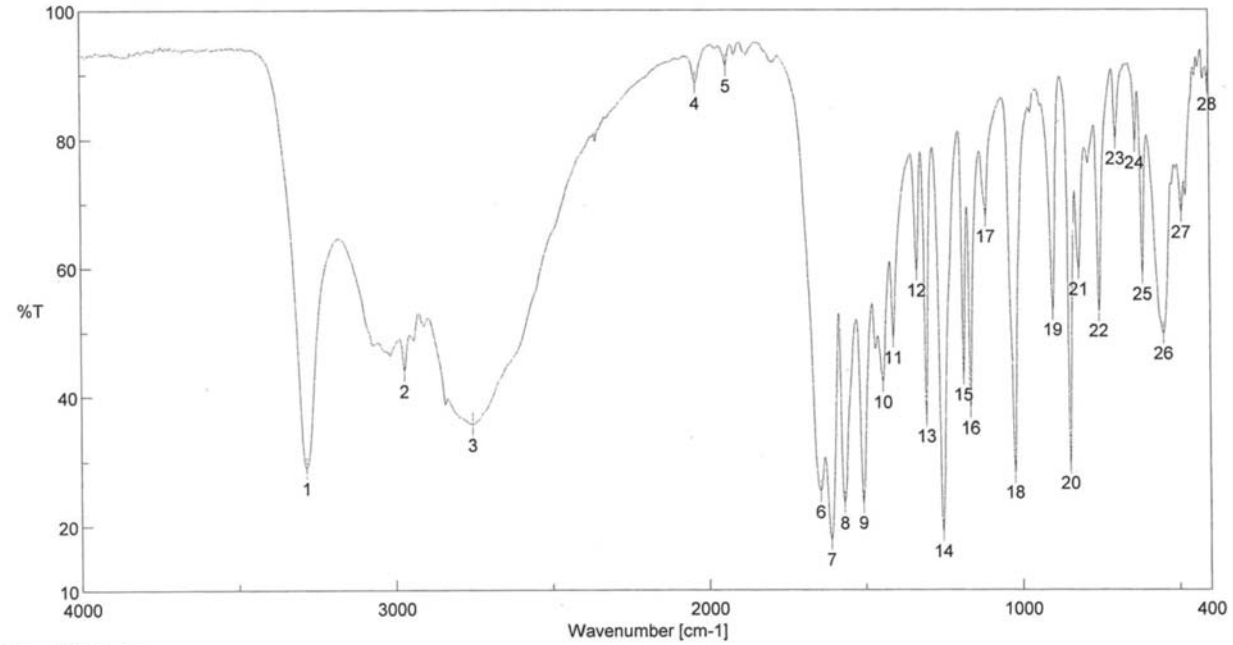
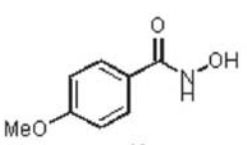


[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3285.14	29.0713	2	2971.77	44.0308	3	2754.82	35.7383	4	2039.35	88.7158
5	1941	91.378	6	1644.02	25.3244	7	1610.27	17.9133	8	1567.84	23.5914
9	1507.1	23.6351	10	1443.46	42.2785	11	1409.71	49.1923	12	1334.5	59.6476
13	1304.61	37.0814	14	1253.5	19.2421	15	1186.01	43.475	16	1163.83	38.3106
17	1113.69	68.062	18	1024.02	28.3649	19	901.558	53.5446	20	846.597	29.8126
21	818.634	59.8342	22	754.031	53.3969	23	699.069	80.1965	24	637.358	79.5465
25	615.181	59.0992	26	548.649	49.8338	27	490.795	68.701	28	404.978	88.5485



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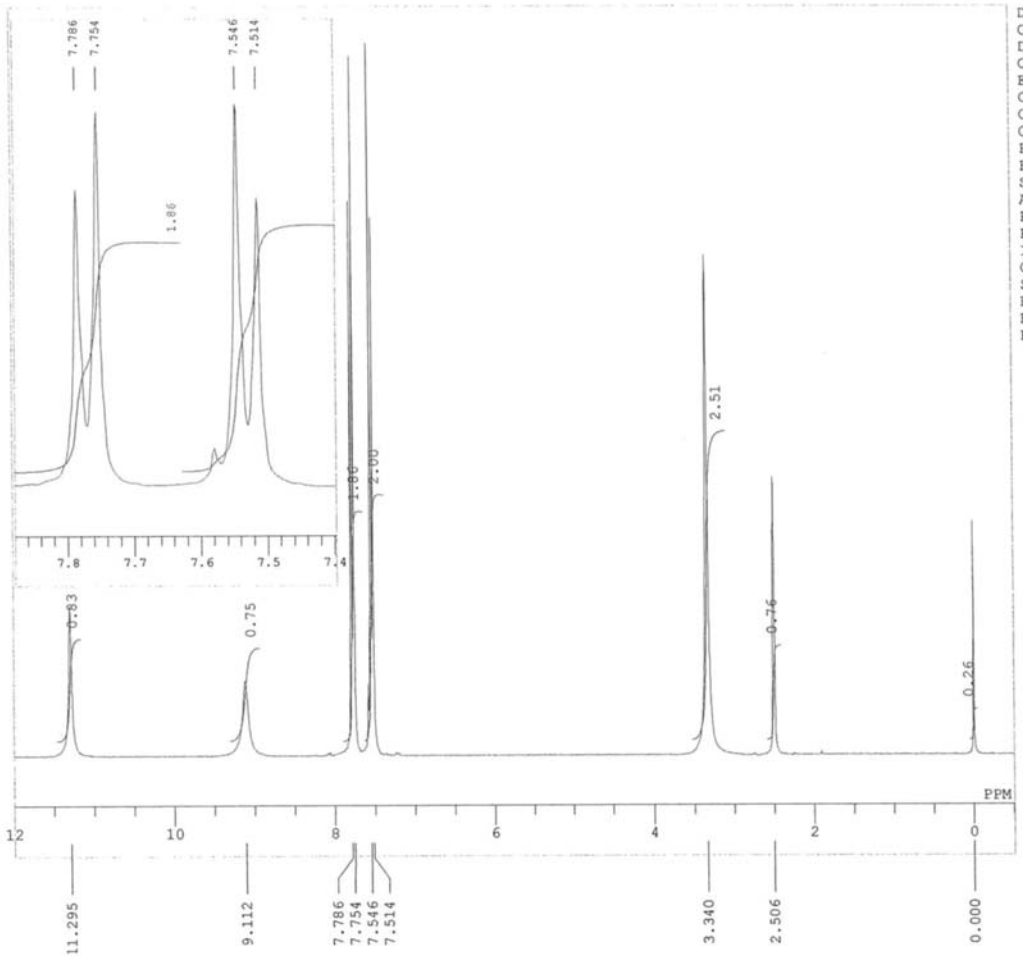

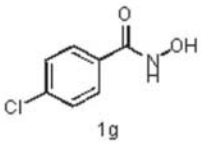

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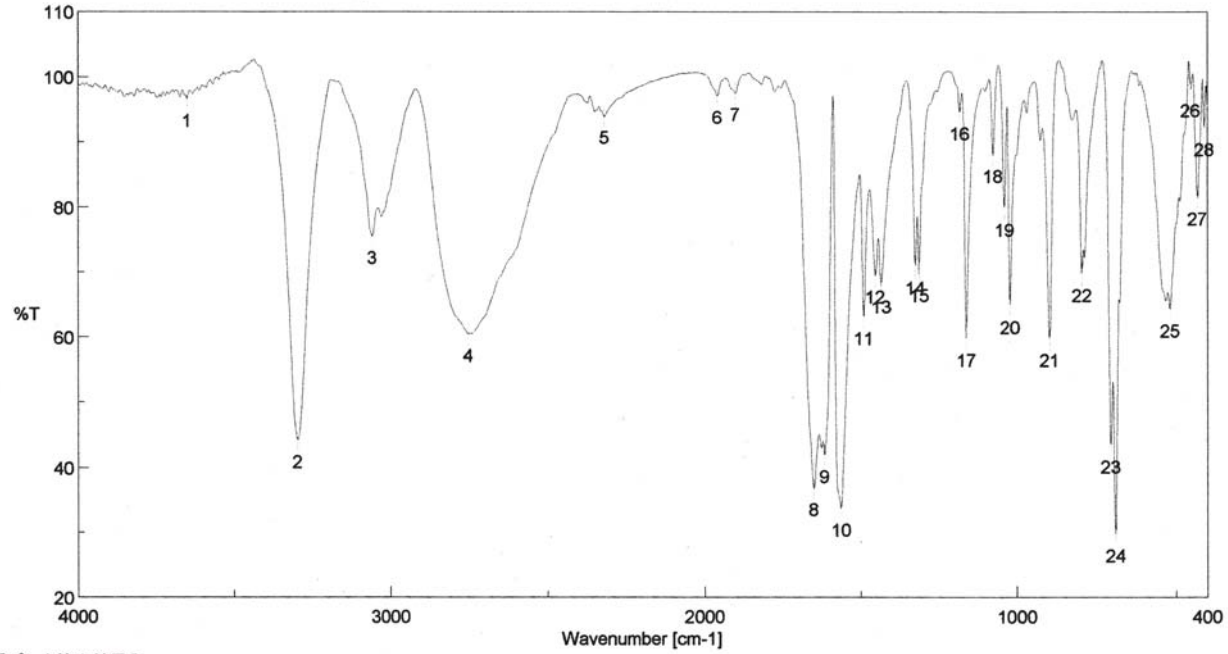
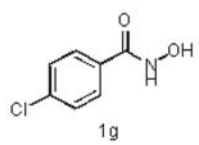


［ピーク検出結果］

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3649.62	96.5198	2	3297.68	44.1495	3	3060.48	75.4547	4	2753.85	60.3946
5	2317.05	93.9101	6	1960.29	97.0593	7	1901.47	97.477	8	1647.88	36.7857
9	1614.13	41.8949	10	1562.06	33.6482	11	1490.7	63.027	12	1454.06	69.4554
13	1435.74	67.9062	14	1327.75	70.7958	15	1315.21	69.6889	16	1184.08	94.5507
17	1162.87	59.7016	18	1078.01	88.0332	19	1041.37	79.713	20	1022.09	64.732
21	898.666	59.6933	22	796.457	69.6641	23	705.819	43.3886	24	690.391	29.7108
25	519.722	64.1796	26	454.154	98.118	27	431.977	81.4172	28	410.763	92.0406



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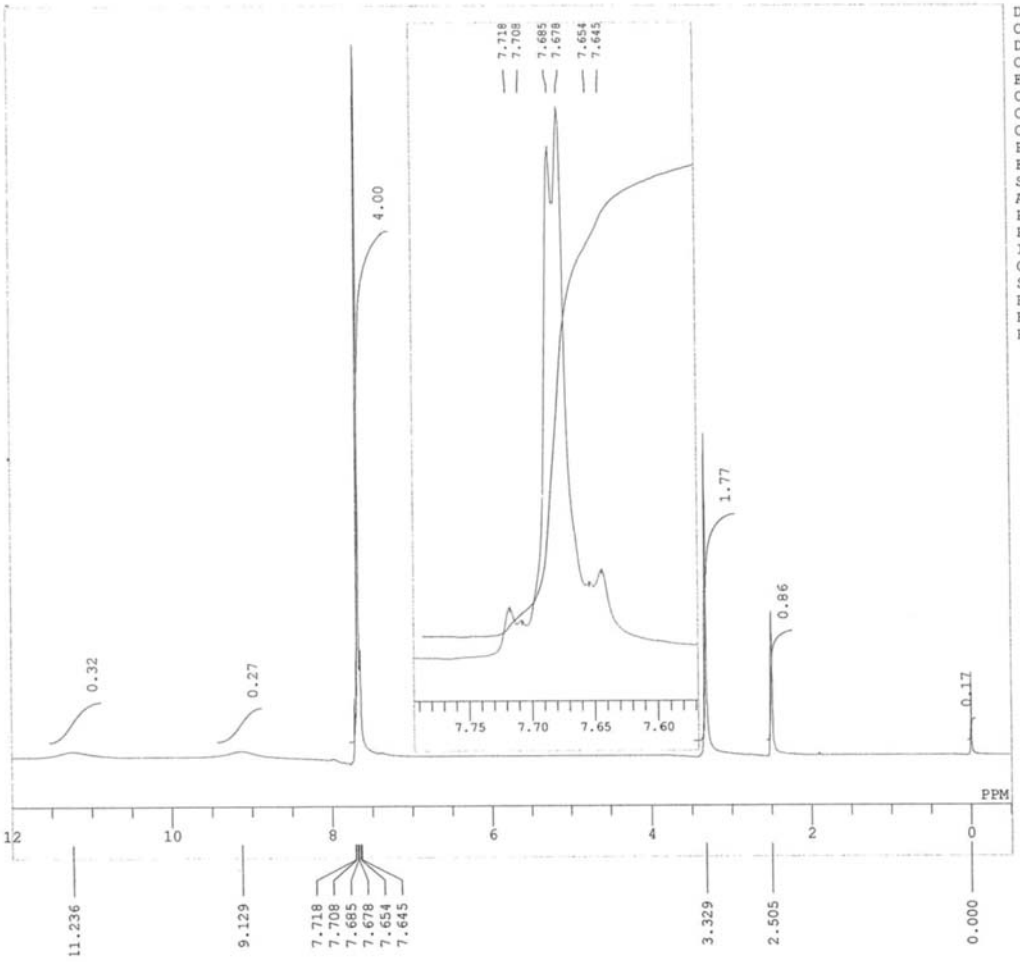

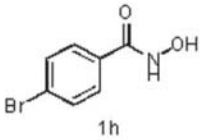

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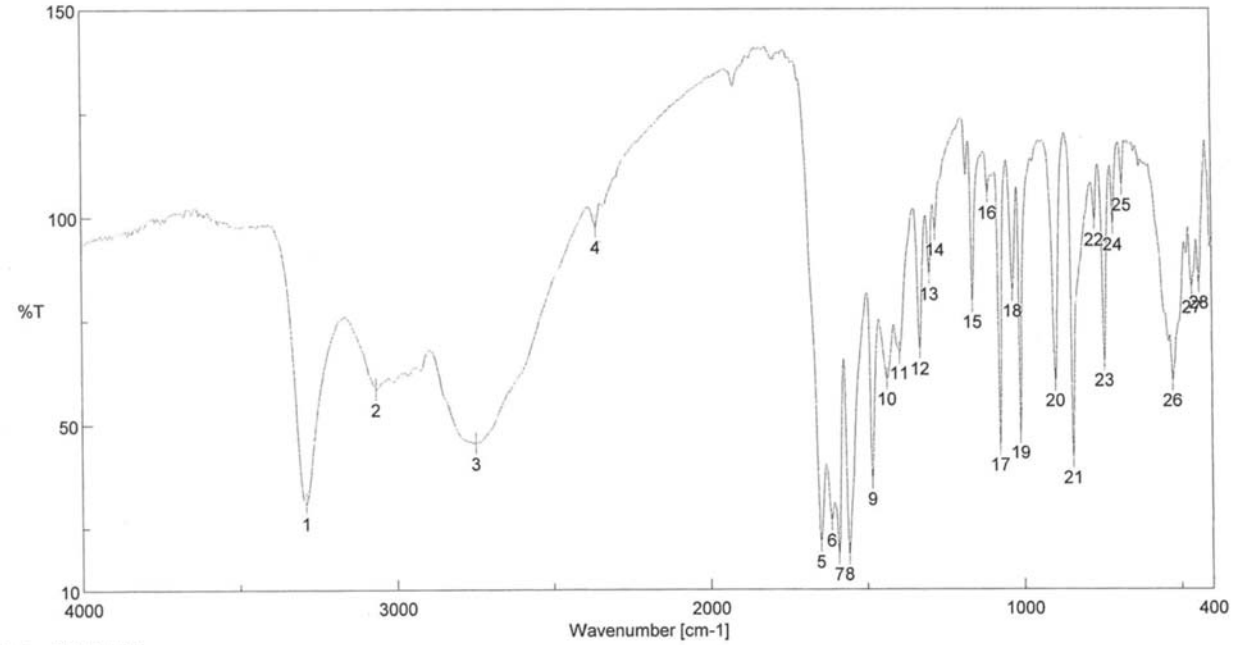
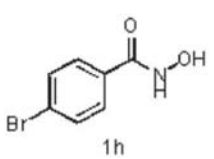
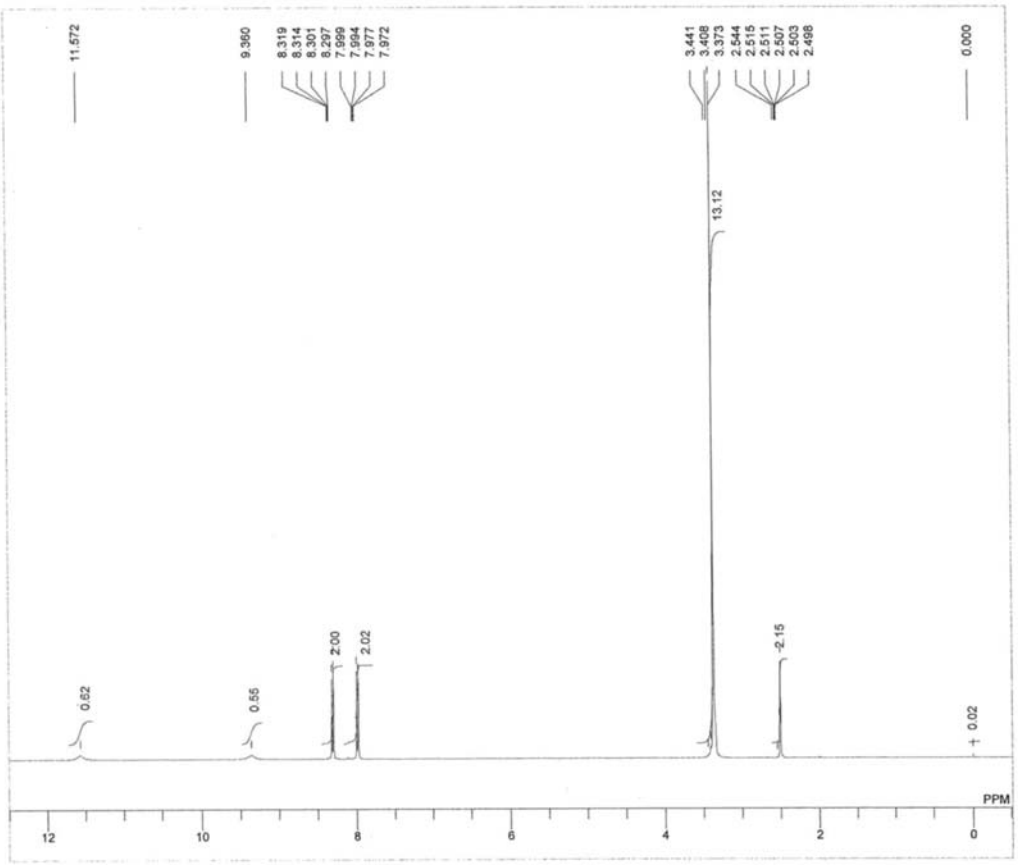


[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3290.93	30.9516	2	3066.26	58.4979	3	2748.07	45.3989	4	2363.34	97.6378
5	1648.84	21.6637	6	1614.13	26.7682	7	1590.99	18.6493	8	1558.2	18.7163
9	1482.99	36.7415	10	1435.74	60.8594	11	1395.25	67.0944	12	1329.68	68.1706
13	1298.82	86.206	14	1279.54	96.9032	15	1160.94	79.5128	16	1111.76	105.799
17	1075.12	45.0318	18	1034.62	82.0992	19	1010.52	48.0154	20	898.666	60.5343
21	842.74	41.9021	22	772.351	99.3471	23	742.46	65.397	24	713.533	98.2285
25	684.606	107.733	26	525.507	60.4515	27	463.796	82.9676	28	440.655	84.0753



1h



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OBFIN 10500.00 Hz
POINT 32768
FREQU 8000.00 Hz
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ACQTM 4.0960 sec
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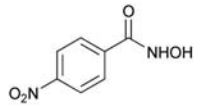
RGAIN 18



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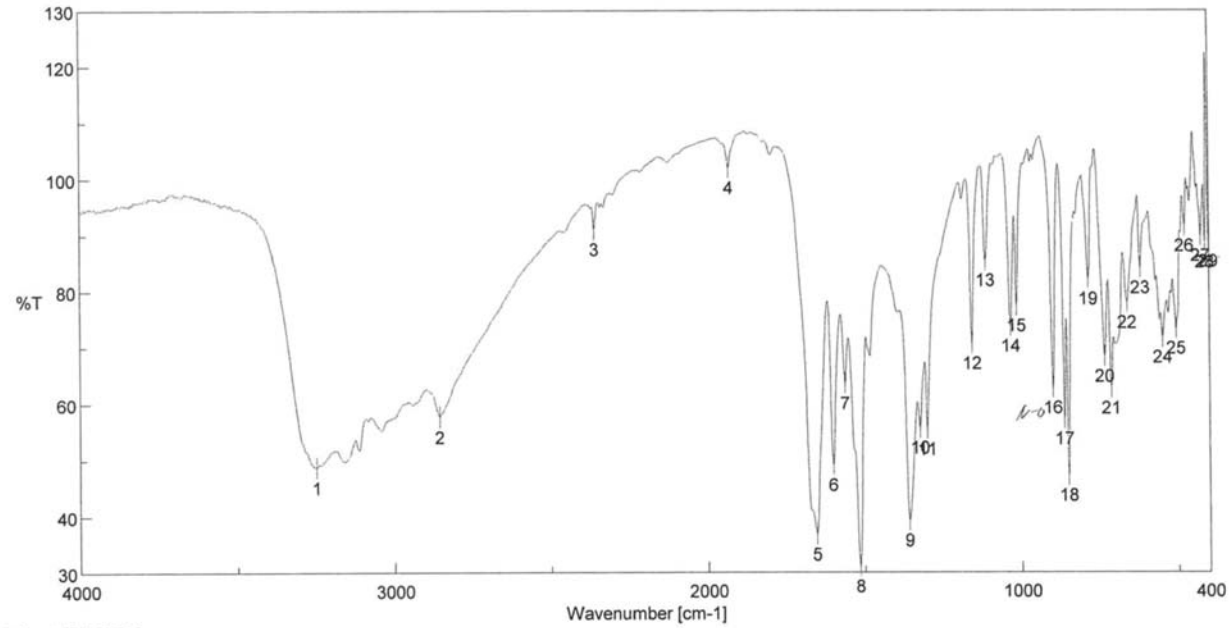
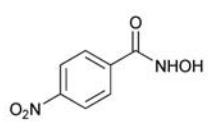


[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3249.47	48.7941	2	2856.06	57.7787	3	2361.41	91.1236	4	1931.36	102.129
5	1653.66	36.8537	6	1599.66	49.2375	7	1562.06	63.7482	8	1515.78	31.1656
9	1357.64	39.3051	10	1322.93	55.8588	11	1299.79	55.5926	12	1156.12	70.7906
13	1112.73	85.5563	14	1033.66	73.8819	15	1014.37	77.5341	16	898.666	62.9294
17	862.989	57.4537	18	850.454	47.3882	19	785.85	82.2743	20	734.746	68.5106
21	713.533	62.8785	22	662.428	78.1029	23	620.002	84.2507	24	549.613	71.9037
25	506.223	73.4914	26	478.26	91.7813	27	427.155	89.9767	28	413.656	88.8216
29	402.085	88.9889									



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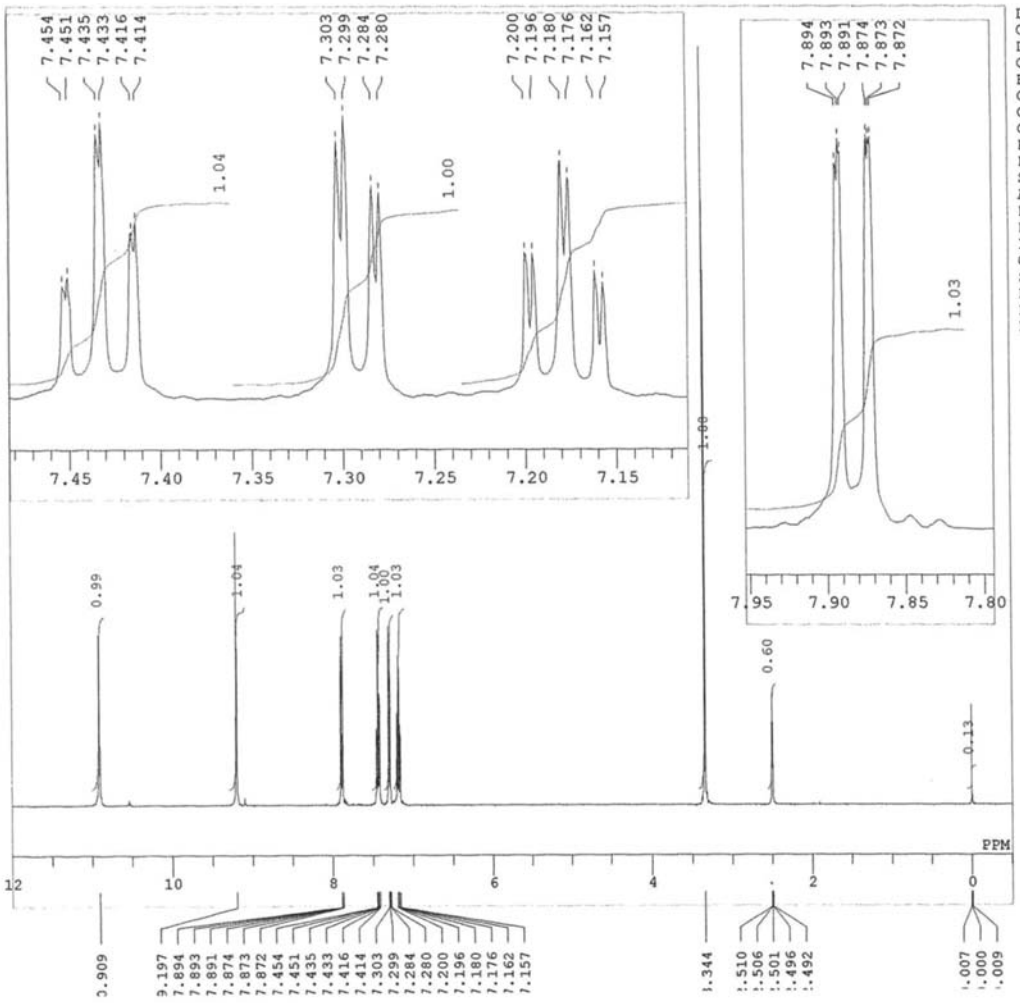
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OBFIN 10500.00 Hz
POINT 32768
FREQU 7992.01 Hz
SCANS 8
ACQTM 4.1001 sec
PD 2.9000 sec
PW1 6.20 usec
IRNUC 1H
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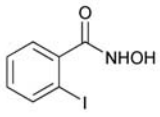
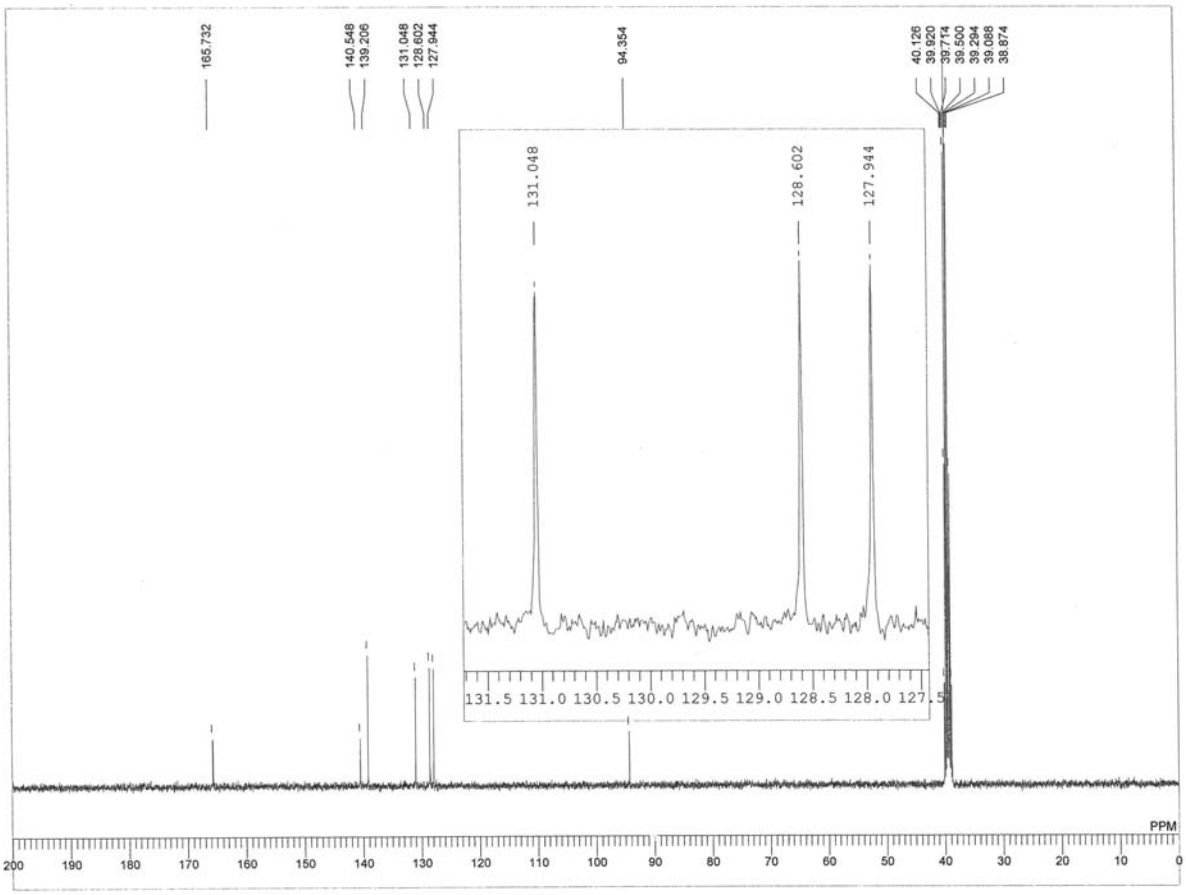
BF 0.12 Hz
RGAIN 19
PPM


O
NHOH
I

1j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PD 1.7920 sec
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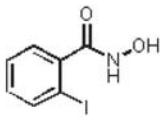
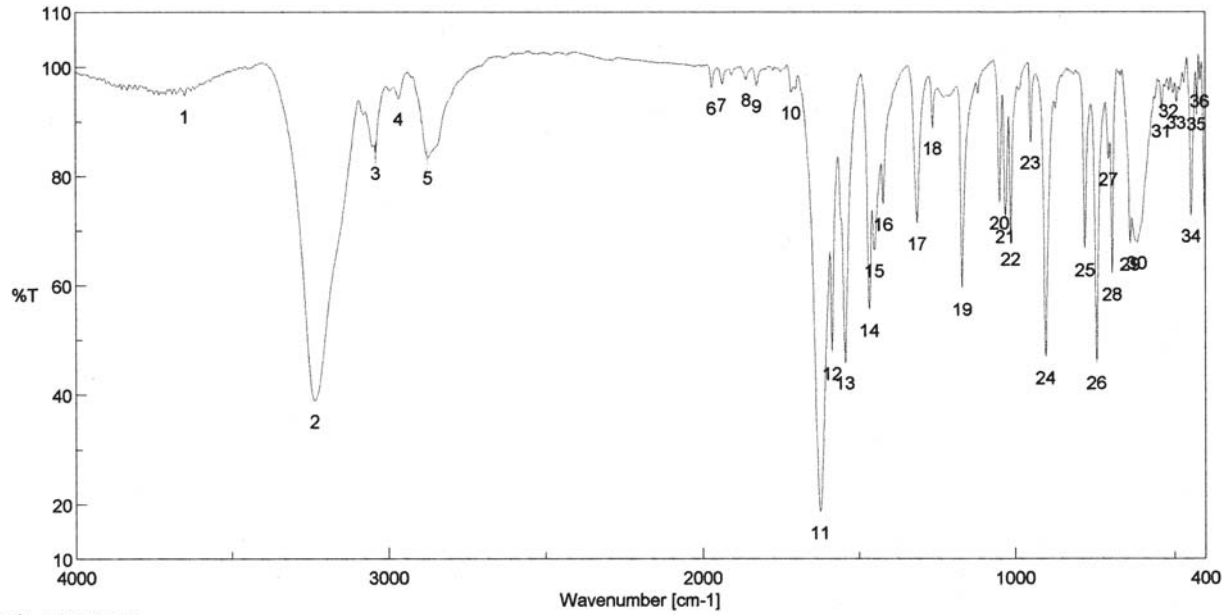
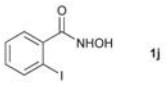

O
N
OH
H
I

1j

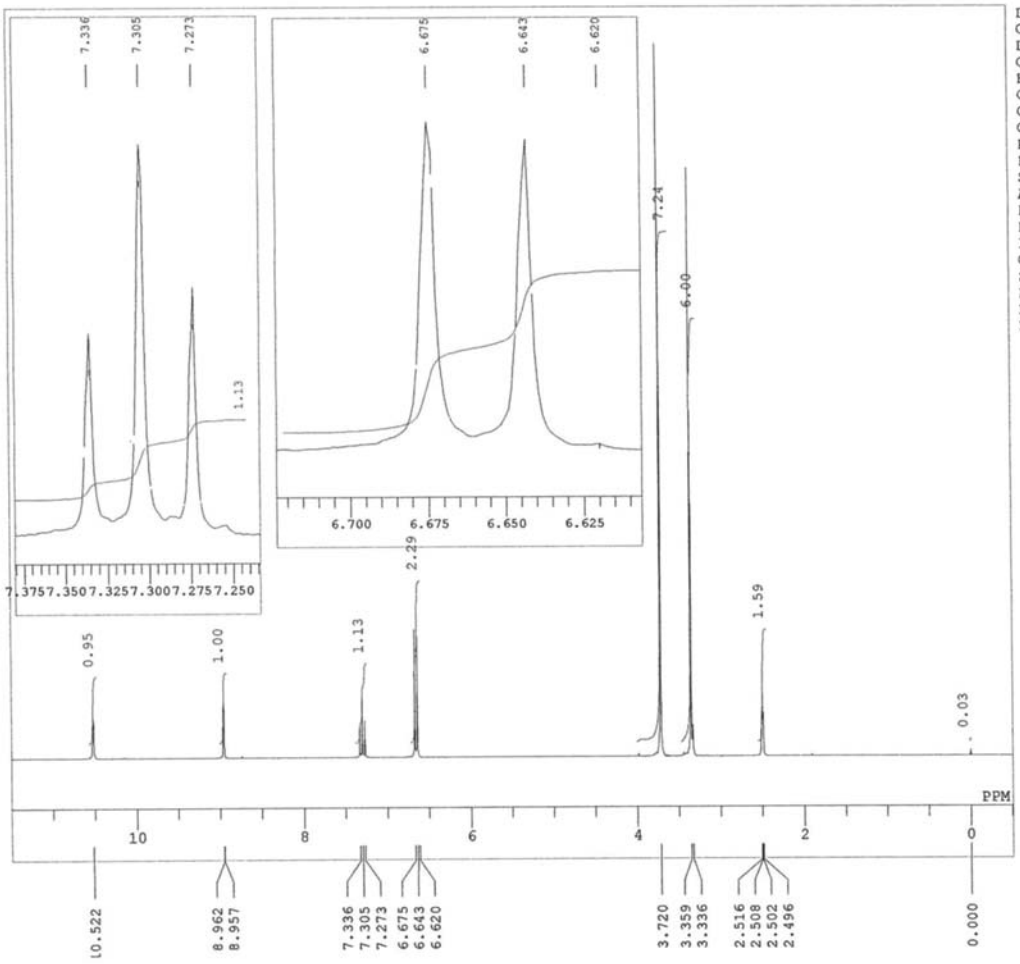


[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3648.66	94.6602	2	3238.86	38.8441	3	3039.26	84.3032	4	2967.91	94.1861
5	2874.38	83.4312	6	1970.89	96.1554	7	1935.22	96.7533	8	1856.15	97.69
9	1822.4	96.5577	10	1714.41	95.343	11	1621.84	18.5538	12	1584.24	47.5531
13	1542.77	45.8755	14	1466.6	55.5044	15	1451.17	66.4098	16	1423.21	74.8736
17	1315.21	71.363	18	1265.07	88.8292	19	1169.62	59.3398	20	1049.09	75.1261
21	1030.77	72.684	22	1014.37	68.4927	23	951.698	86.2001	24	904.451	46.7819
25	781.029	66.5155	26	744.388	45.8486	27	705.819	83.1494	28	694.248	62.0435
29	638.323	67.5766	30	616.145	67.8138	31	540.935	91.9079	32	517.793	95.6546
33	492.723	93.5282	34	445.476	72.6967	35	427.155	93.2224	36	417.513	97.4395



1j

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OBSET       112.00 KHz
OBFIN       5800.0 Hz
POINT        16384
FREQU       5405.4 Hz
SCANS            8
ACQTM        3.031 sec
PD           3.969 sec
PW1            4.9 us
IRNUC   1H
CTEMP        18.6 c
SLVNT   DMSO
EXREF        0.00 ppm
BF           0.12 Hz
RGAIN          19
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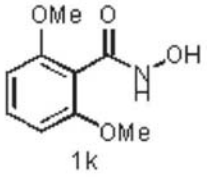
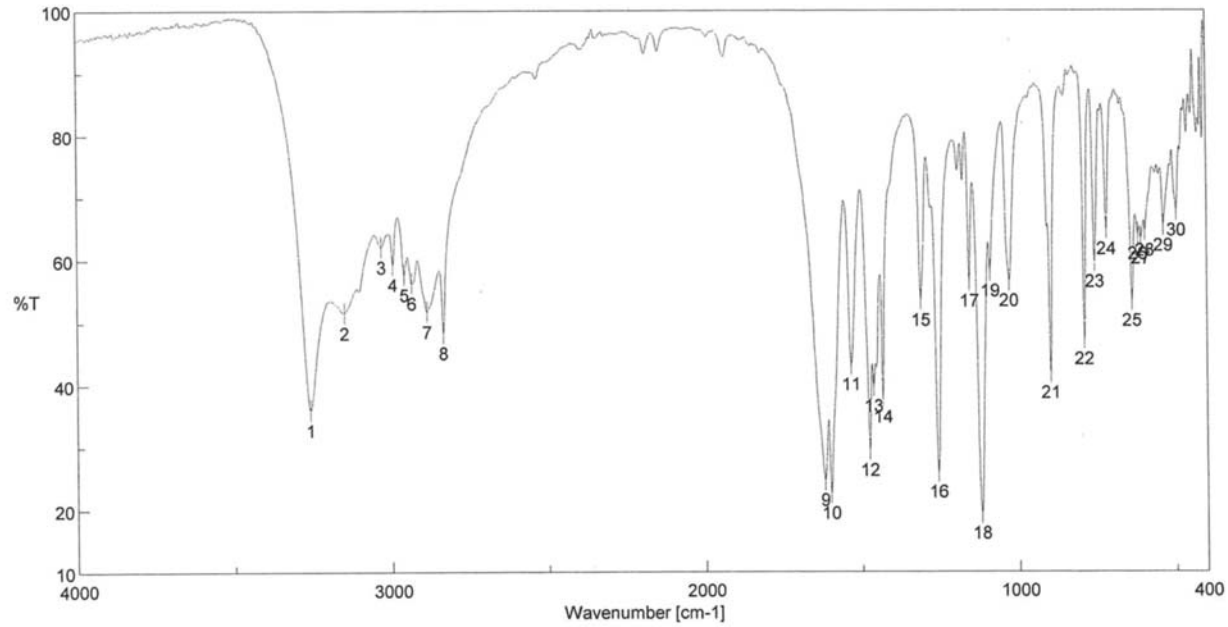
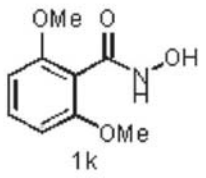


1k



[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3260.07	36.0458	2	3151.11	51.5826	3	3032.51	62.1129	4	2995.87	59.3325
5	2959.23	57.7041	6	2936.09	56.3341	7	2886.92	51.7704	8	2834.85	48.4069
9	1618.95	24.7539	10	1599.66	22.6925	11	1534.1	43.3796	12	1475.28	29.5834
13	1462.74	39.8485	14	1432.85	38.1931	15	1311.36	53.6683	16	1257.36	26.0722
17	1156.12	56.6994	18	1119.48	19.4426	19	1089.58	58.3074	20	1029.8	56.7366
21	897.701	42.0288	22	790.671	47.4611	23	756.923	59.7854	24	719.318	65.0063
25	638.323	53.6002	26	619.038	64.2237	27	609.396	63.5295	28	596.861	64.7716
29	538.042	65.5718	30	496.58	68.0009						



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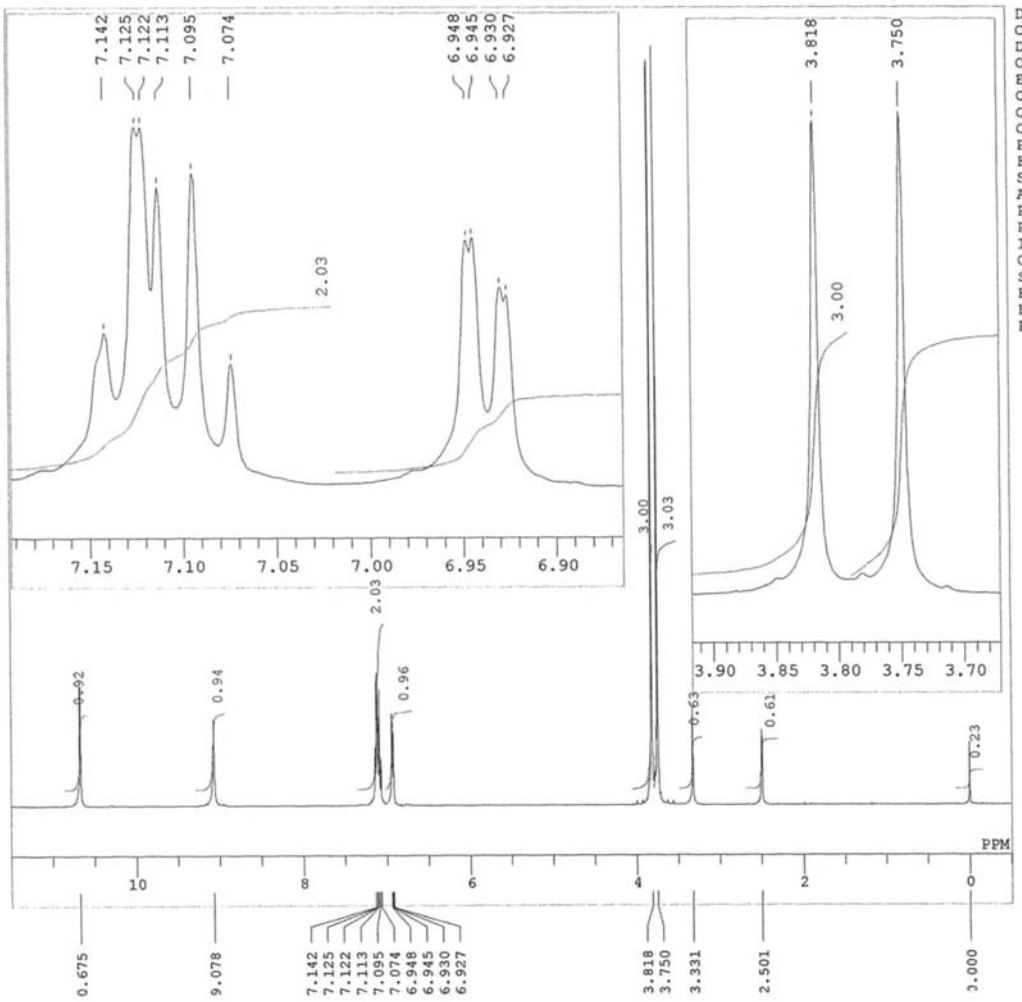
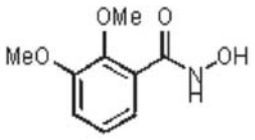
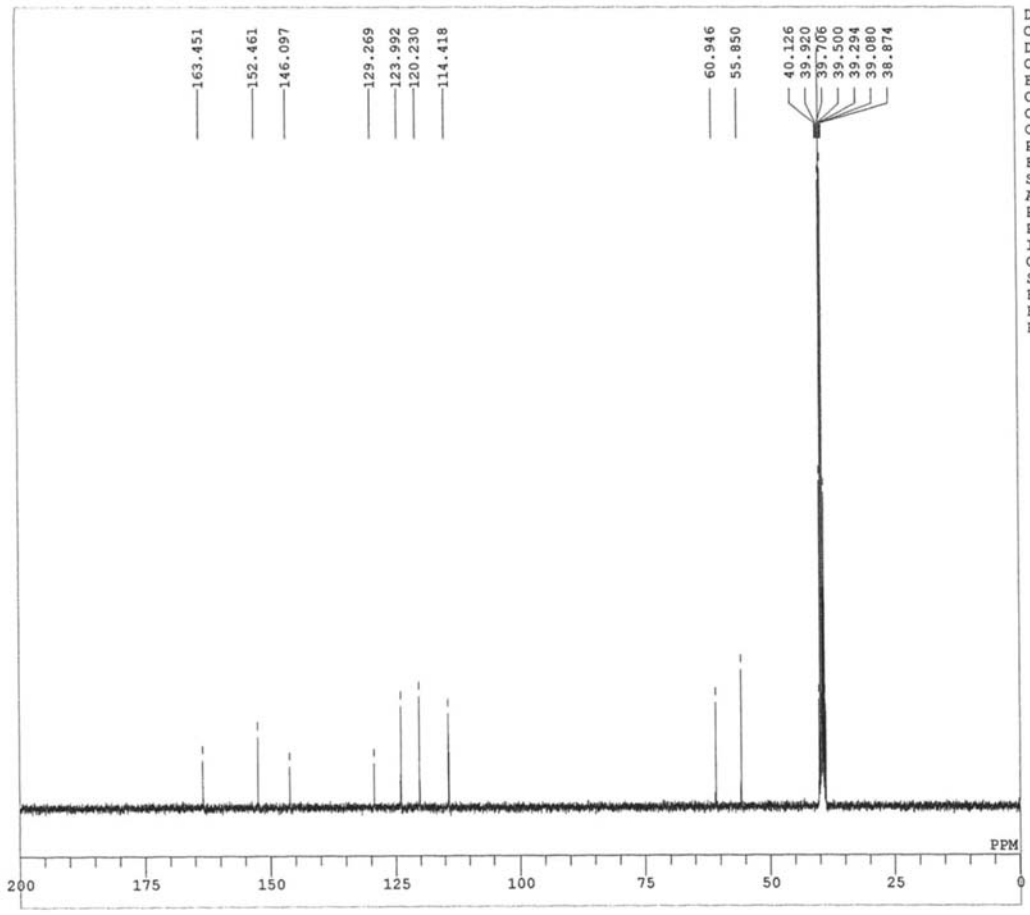


DFILE
COMNT
DATIM
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 7992.01 Hz
SCANS 16
ACQTM 4.1001 sec
PD 2.9000 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 24.1 c
SLVNT DMSO
EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 17



1l



DFILE
COMNT
DATIM
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 400
ACQTM 1.2083 sec
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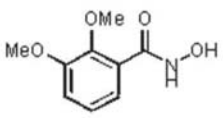
IRNUC 1H
CTEMP 24.7 c
SLVNT DMSO
EXREF 39.50 ppm
BF 1.00 Hz
RGAIN 26



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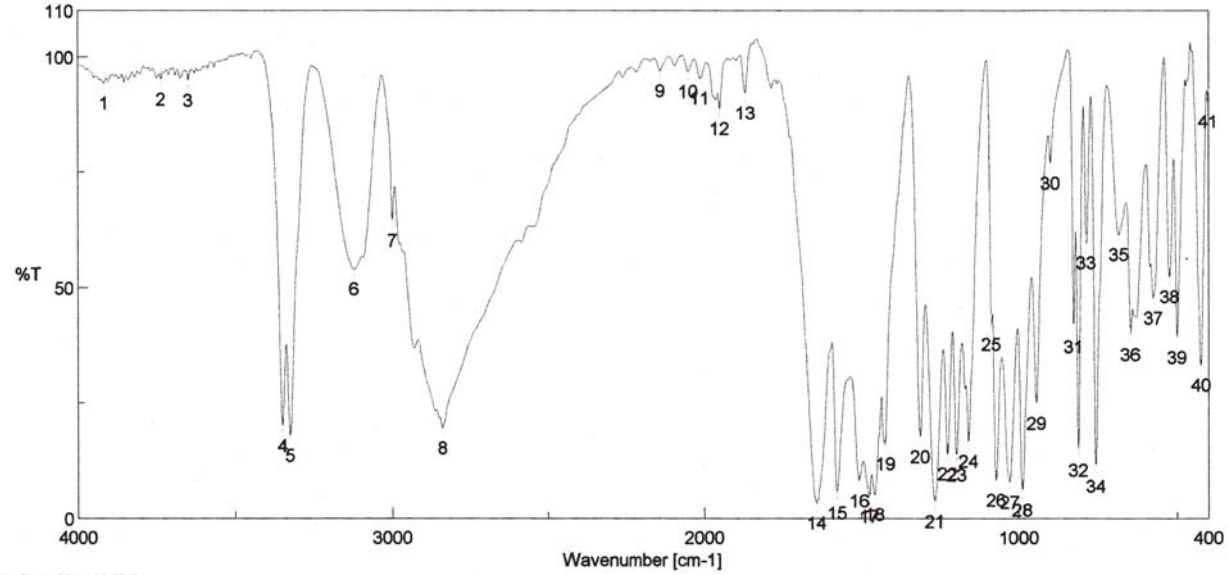
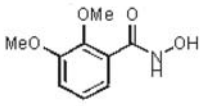


[ピーク検出結果]

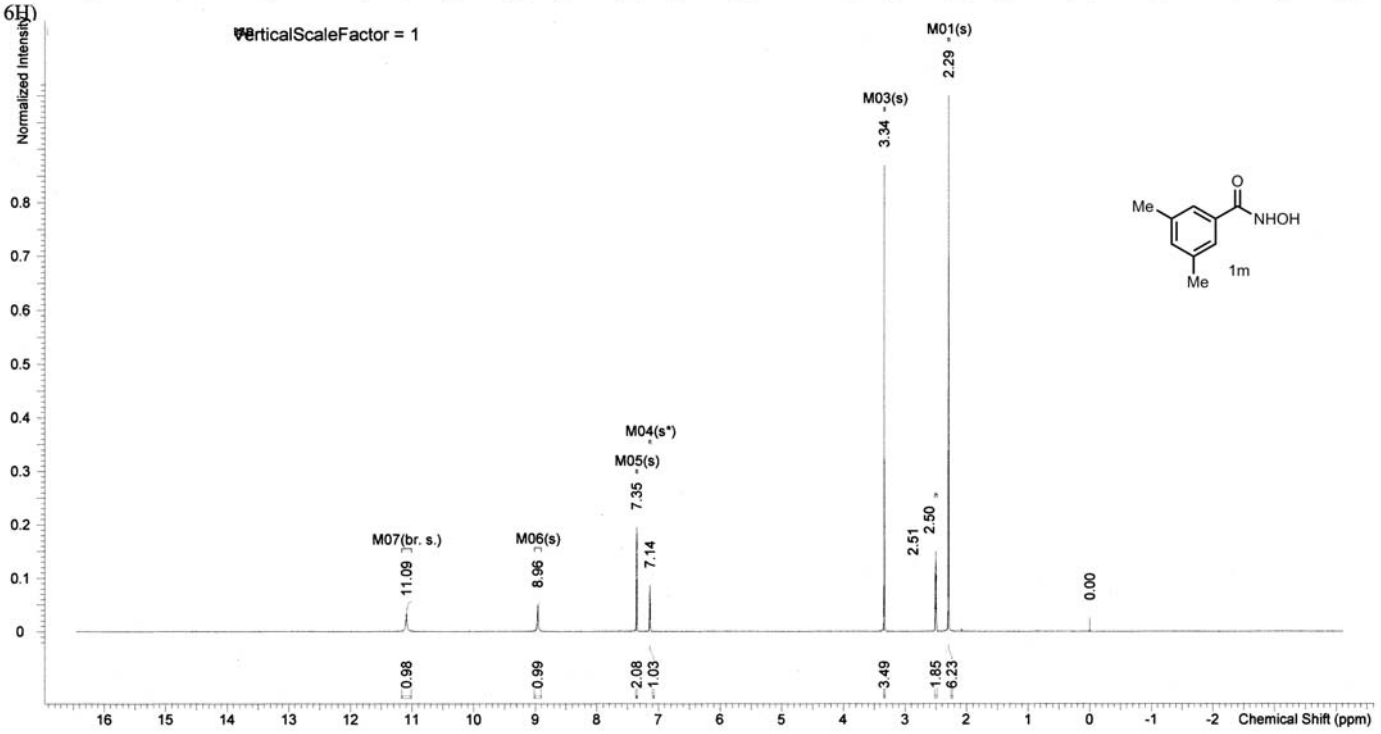
No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3915.75	94.2769	2	3734.48	95.0449	3	3648.66	94.8636	4	3345.89	20.0812
5	3321.78	17.987	6	3119.3	53.9514	7	2999.73	64.4053	8	2836.77	19.5998
9	2140.6	96.9204	10	2050.92	96.7797	11	2013.32	95.38	12	1951.61	88.7385
13	1870.61	92.1138	14	1644.02	3.35593	15	1577.49	5.53394	16	1508.06	8.14088
17	1476.24	4.7798	18	1458.89	5.13486	19	1425.14	16.1519	20	1313.29	17.6989
21	1267	3.67593	22	1226.5	14.0079	23	1198.54	13.8086	24	1160.94	16.7334
25	1087.66	41.9341	26	1072.23	8.25996	27	1027.87	7.85493	28	988.339	6.09631
29	944.949	24.9165	30	899.63	76.8629	31	826.348	41.4229	32	811.885	14.7841
33	786.815	59.5832	34	756.923	11.286	35	684.606	61.3485	36	647.965	39.7206
37	576.612	47.6119	38	524.543	52.264	39	500.437	39.1025	40	424.263	33.101
41	402.085	90.2778									

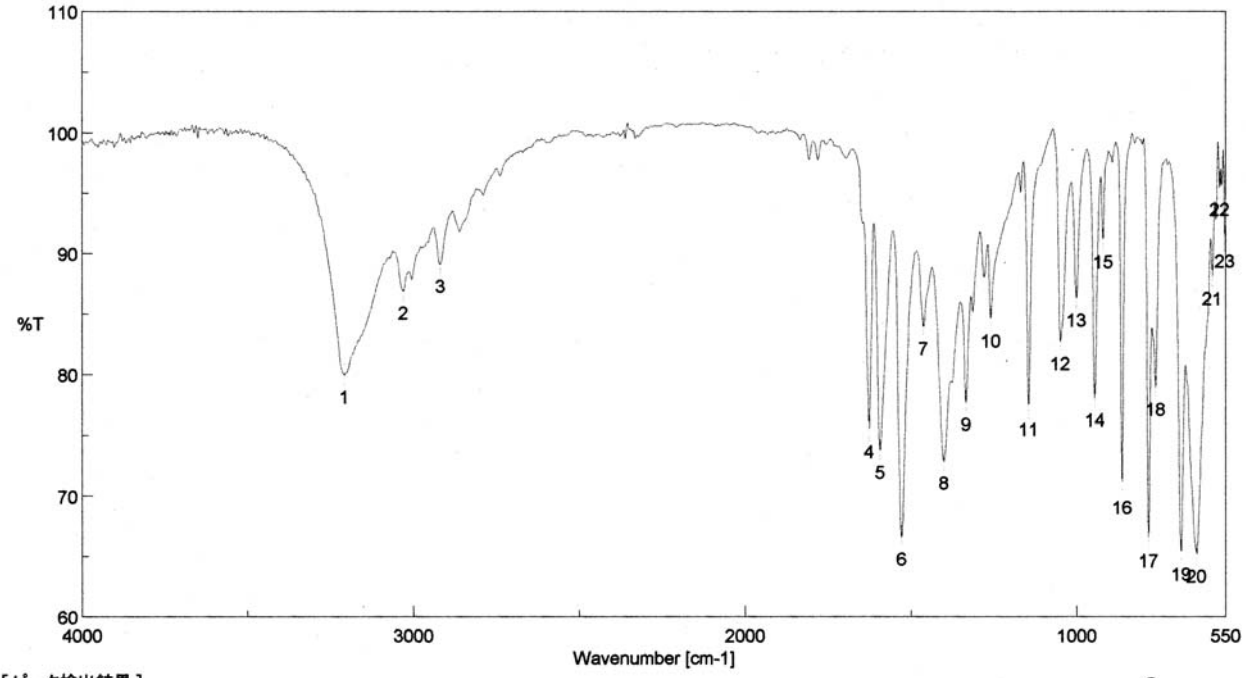


1l

OriginalDateForRelativeTime				Multiplets Integrals Sum	16.65	Number of Nuclei	16 H's		
Acquisition Time (sec)	2.6542	Comment	5 mm QNP 1H/13C/31P/19F Z3333/0001			Date			
Date Stamp				File Name				Frequency (MHz)	300.13
Nucleus	1H	Number of Transients	8	Origin	spect	Original Points Count	16384	Owner	DRX300
Points Count	16384	Pulse Sequence	zg30	Receiver Gain	724.10	SW(cyclical) (Hz)	6172.84	Solvent	DMSO-d6
Spectrum Offset (Hz)	1853.3876	Spectrum Type	STANDARD	Sweep Width (Hz)	6172.46	Temperature (degree C)	27.000		

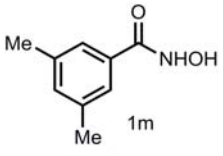
^{1}H NMR (300 MHz, DMSO-d_6) δ 11.09 (br. s., 1H), 8.96 (s, 1H), 7.35 (s, 2H), 7.14 (s, *J*=3.16 Hz, 1H), 3.34 (s, 3H), 2.50 (td, *J*=1.74, 3.67 Hz, 2H), 2.29 (s, 6H)





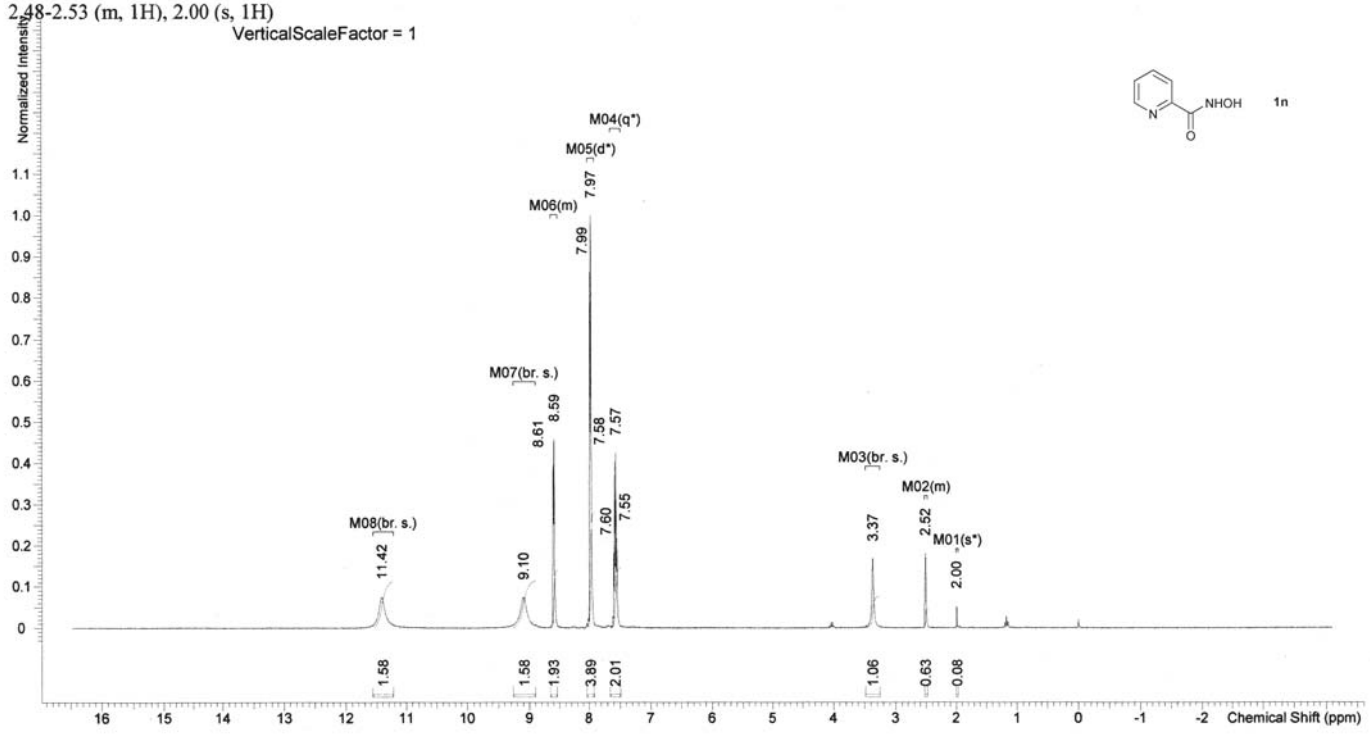
[ピーク検出結果]

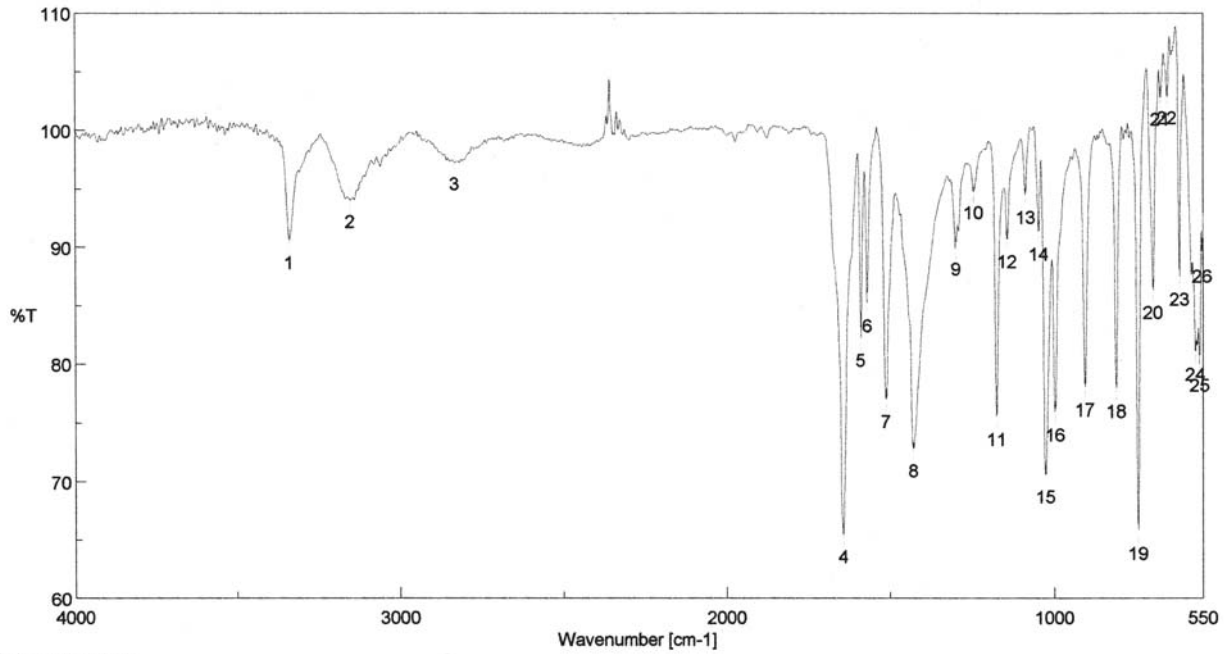
No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3208.97	79.9345	2	3030.59	86.8842	3	2919.7	89.0892	4	1625.7	75.4525
5	1592.91	73.7278	6	1528.31	66.5545	7	1461.78	83.9184	8	1400.07	72.843
9	1333.53	77.6891	10	1259.29	84.5555	11	1144.55	77.2905	12	1049.09	82.6642
13	1000.87	86.2823	14	944.949	78.0477	15	919.879	91.0865	16	862.989	70.8432
17	782.958	66.4123	18	761.744	78.9001	19	684.606	65.3235	20	637.358	65.142
21	590.111	88.0474	22	567.934	95.4183	23	552.506	91.1529			



OriginalDateForRelativeTime				Multiplets Integrals Sum	12.75	Number of Nuclei	15 H's		
Acquisition Time (sec)	2.6542	Comment	5 mm QNP 1H/13C/31P/19F Z3333/0001			Date			
Date Stamp				File Name				Frequency (MHz)	300.13
Nucleus	1H	Number of Transients	8	Origin	spect	Original Points Count	16384	Owner	DRX300
Points Count	16384	Pulse Sequence	zg30	Receiver Gain	362.00	SW(cyclical) (Hz)	6172.84	Solvent	DMSO-d6
Spectrum Offset (Hz)	1856.9833	Spectrum Type	STANDARD	Sweep Width (Hz)	6172.46	Temperature (degree C)	27.000		

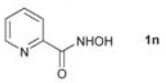
^{1}H NMR (300 MHz, DMSO-d_6) δ 11.42 (br. s., 2H), 9.10 (br. s., 2H), 8.54-8.65 (m, 2H), 7.98 (d, *J*=4.14 Hz, 4H), 7.58 (q, *J*=4.40 Hz, 2H), 3.37 (br. s., 1H), 2.48-2.53 (m, 1H), 2.00 (s, 1H)





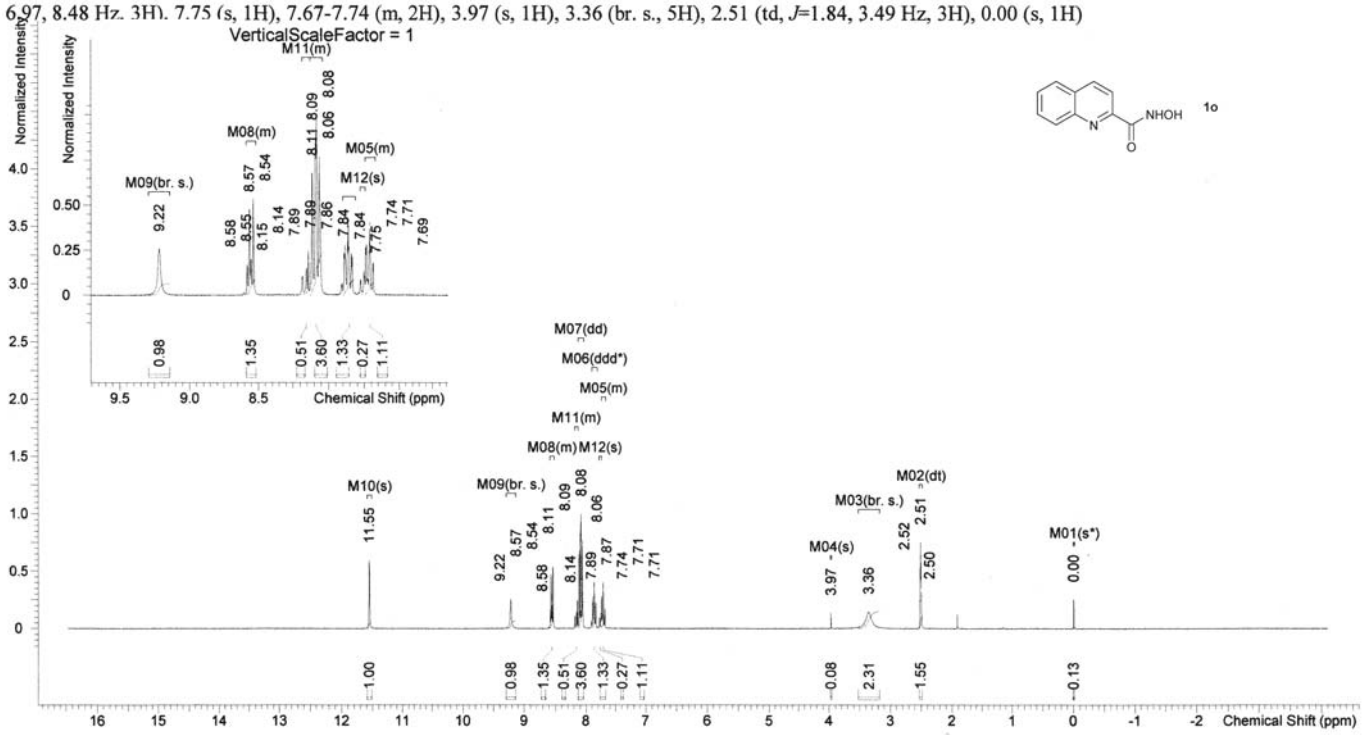
[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3340.1	90.4909	2	3152.08	94.0079	3	2835.81	97.2459	4	1645.95	65.3821
5	1590.02	82.144	6	1569.77	85.0905	7	1511.92	76.942	8	1428.99	72.7426
9	1300.75	89.9398	10	1246.75	94.767	11	1177.33	75.4327	12	1145.51	90.5901
13	1088.62	94.35	14	1048.12	91.2217	15	1026.91	70.531	16	997.982	75.821
17	906.379	77.9434	18	811.885	77.7982	19	746.317	65.663	20	701.962	86.2158
21	678.82	102.761	22	658.571	102.868	23	620.966	87.3497	24	572.755	80.9637
25	560.22	79.9881	26	552.506	89.3344						



OriginalDateForRelativeTime				Multiplets Integrals Sum	14.22	Number of Nuclei	31 H's		
Acquisition Time (sec)	2.6542	Comment	5 mm QNP 1H/13C/31P/19F Z3333/0001	Date					
Date Stamp		File Name						Frequency (MHz)	300.13
Nucleus	1H	Number of Transients	8	Origin	spect	Original Points Count	16384	Owner	DRX300
Points Count	16384	Pulse Sequence	zg30	Receiver Gain	724.10	SW(cyclical) (Hz)	6172.84	Solvent	DMSO-d6
Spectrum Offset (Hz)	1855.8727	Spectrum Type	STANDARD	Sweep Width (Hz)	6172.46	Temperature (degree C)	27.000		

^{1}H NMR (300 MHz, DMSO-d_6) δ 11.55 (s, 2H), 9.22 (br. s., 2H), 8.52-8.59 (m, 3H), 8.13-8.19 (m, 1H), 8.09 (dd, *J*=6.22, 8.48 Hz, 7H), 7.86 (ddd, *J*=1.51, 6.97, 8.48 Hz, 3H), 7.75 (s, 1H), 7.67-7.74 (m, 2H), 3.97 (s, 1H), 3.36 (br. s., 5H), 2.51 (td, *J*=1.84, 3.49 Hz, 3H), 0.00 (s, 1H)



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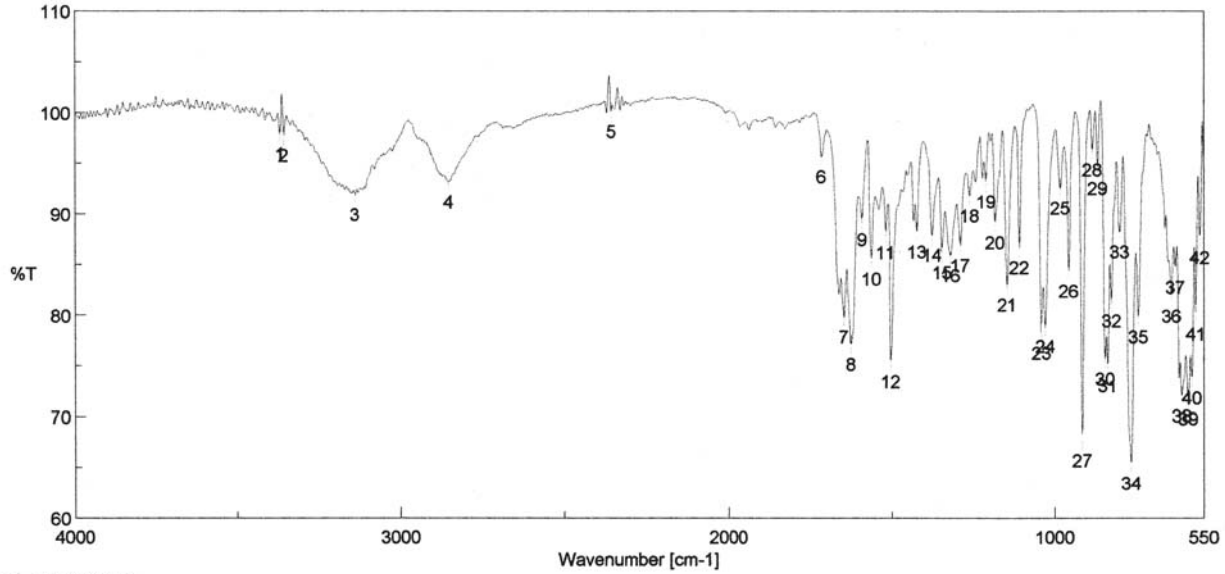
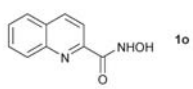


[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3370.96	97.835	2	3359.39	97.6831	3	3142.44	91.8429	4	2855.1	93.1145
5	2356.59	100.039	6	1713.44	95.6022	7	1645.95	79.7885	8	1623.77	77.0774
9	1590.99	89.3667	10	1562.06	85.5054	11	1518.67	88.1278	12	1504.2	75.3841
13	1423.21	88.1958	14	1376.93	87.8622	15	1346.07	86.1625	16	1319.07	85.8609
17	1290.14	86.8578	18	1262.18	91.764	19	1212.04	93.1552	20	1183.11	89.0994
21	1145.51	82.9256	22	1108.87	86.6317	23	1041.37	78.1962	24	1028.84	78.8459
25	983.518	92.5141	26	957.484	84.3194	27	916.986	67.6313	28	887.095	96.2678
29	871.667	94.4444	30	848.525	75.6276	31	840.812	74.9674	32	829.241	81.3389
33	804.171	88.1897	34	769.458	65.3937	35	748.245	79.7666	36	647.965	81.8154
37	635.43	84.6535	38	616.145	71.9969	39	596.861	71.7127	40	586.254	73.7453
41	574.683	80.0655	42	562.148	87.6361						



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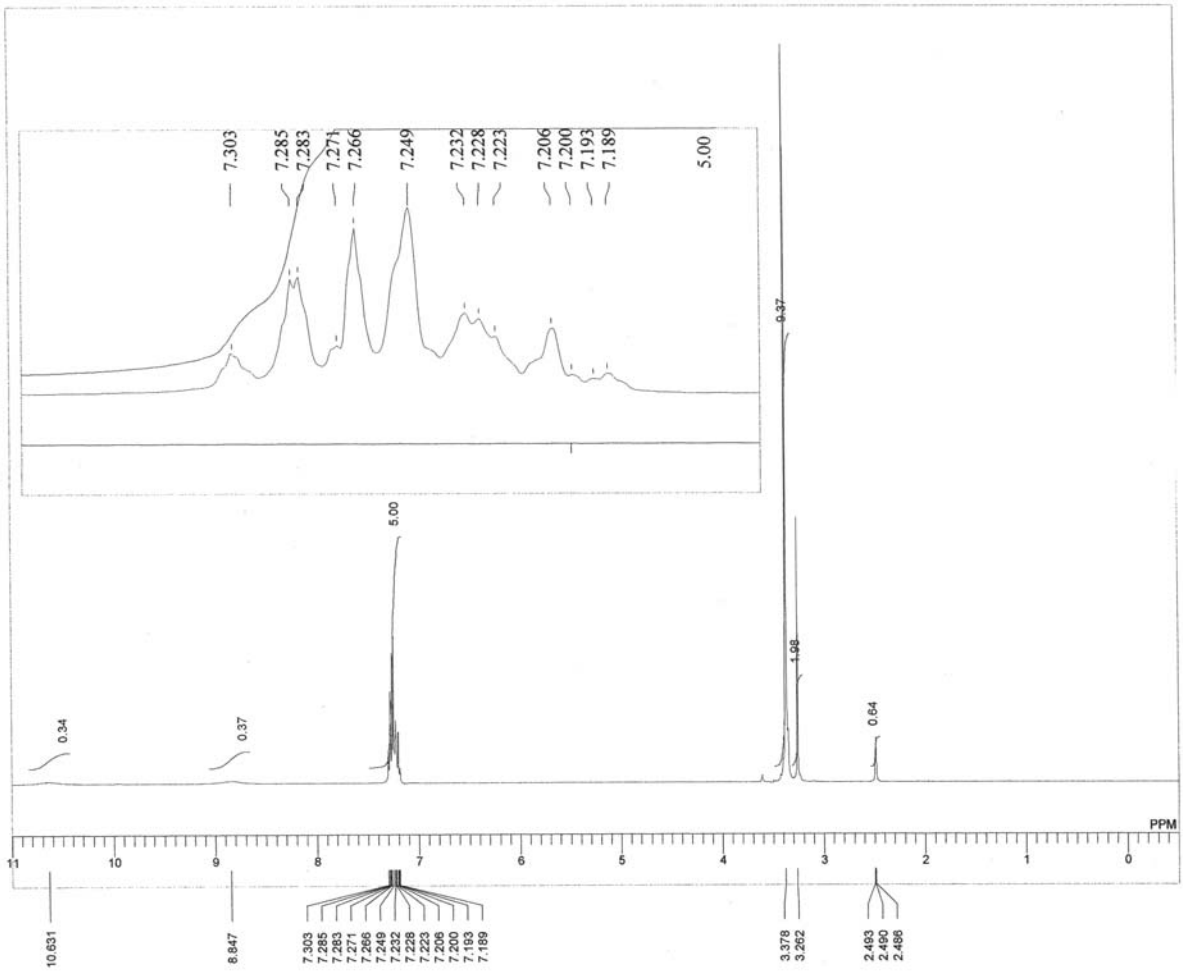
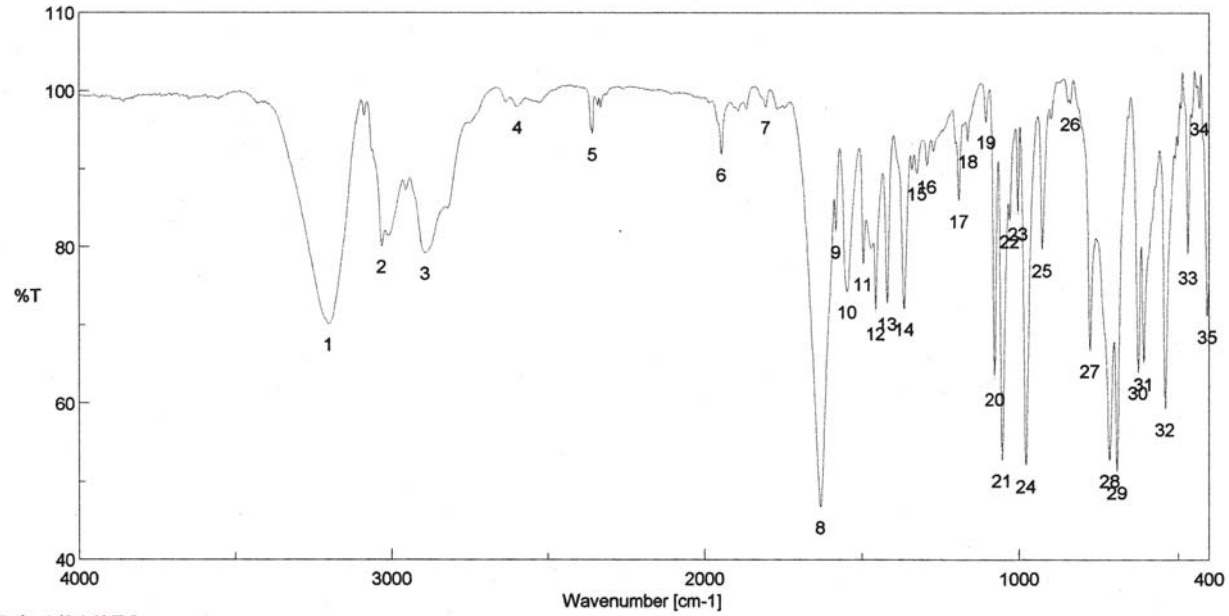
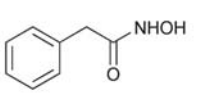
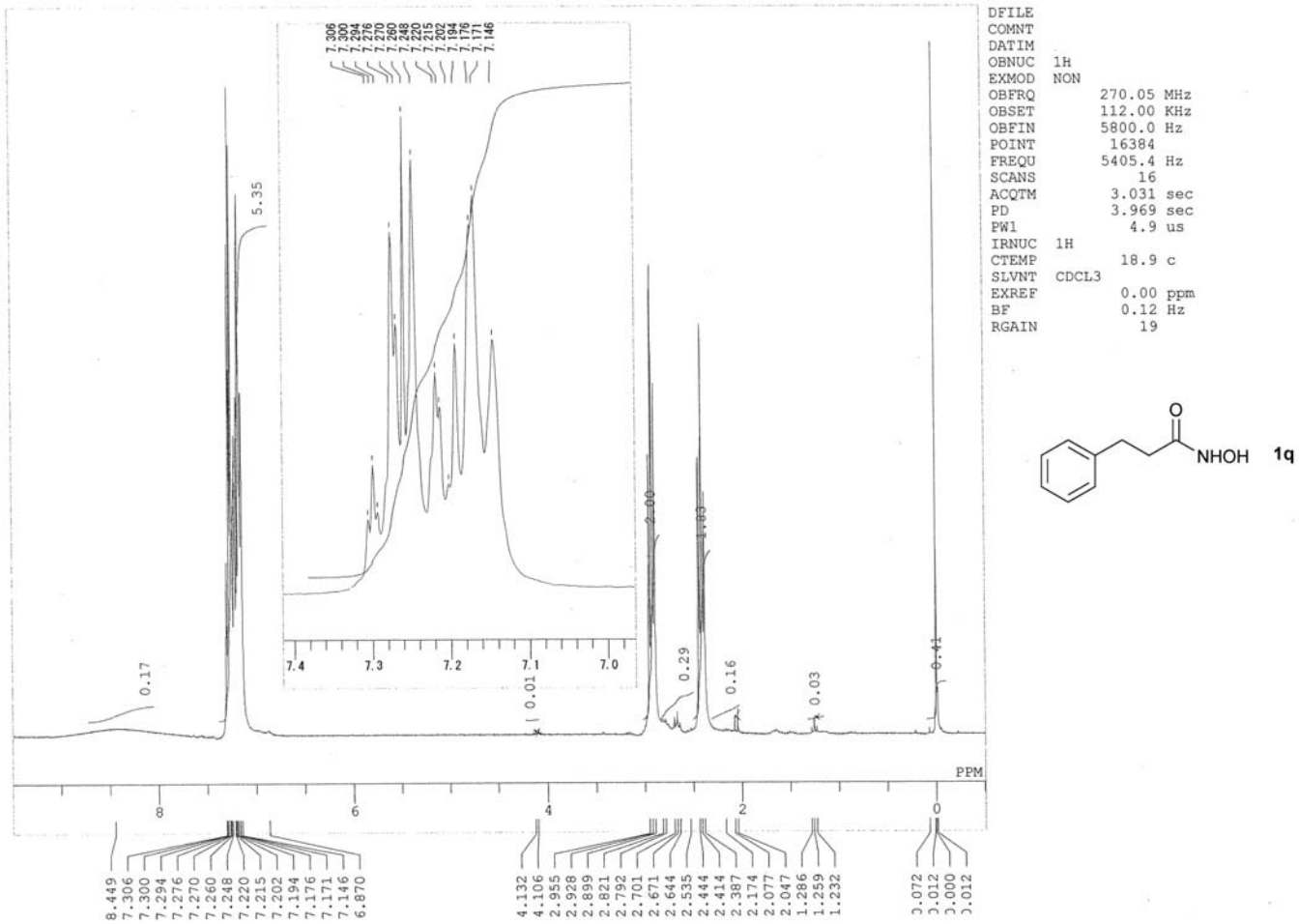


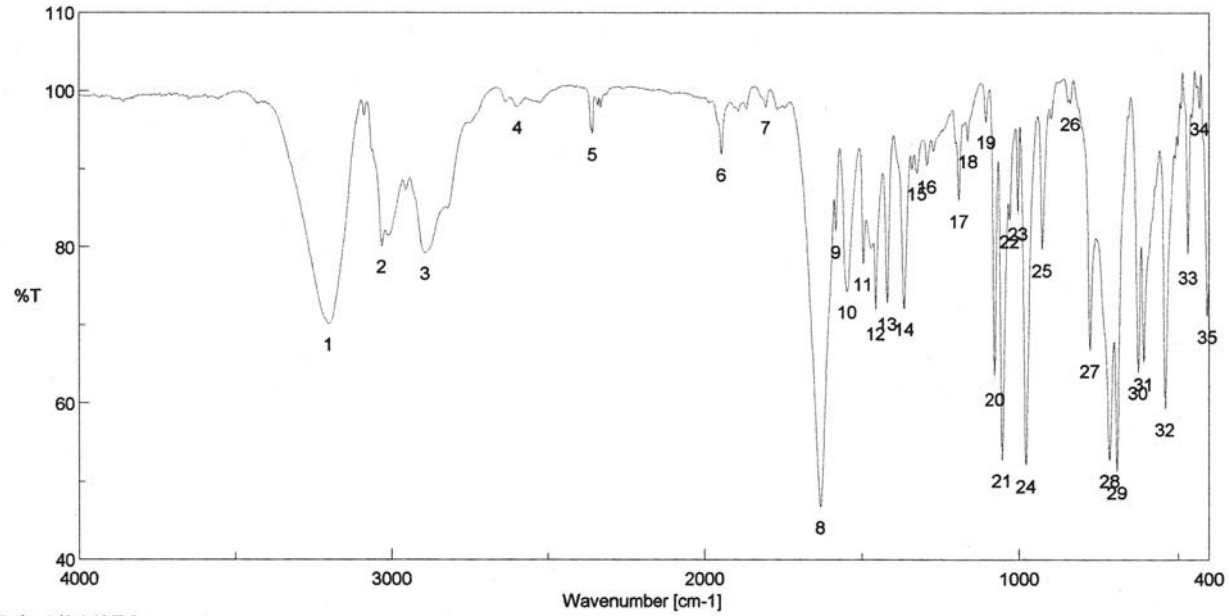


[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3202.22	70.1002	2	3030.59	80.0978	3	2894.63	79.2566	4	2596.68	97.9574
5	2359.48	94.4973	6	1945.82	91.8766	7	1804.08	97.9371	8	1633.41	46.7502
9	1584.24	81.9682	10	1547.59	74.2971	11	1495.53	77.8706	12	1455.03	71.5718
13	1418.39	72.7731	14	1365.35	72.1092	15	1324.86	89.4714	16	1293.04	90.375
17	1190.83	85.9302	18	1162.87	93.5713	19	1105.01	96.0677	20	1077.05	63.1304
21	1053.91	52.7921	22	1029.8	83.3725	23	1003.77	84.3167	24	978.697	52.0652
25	927.593	79.6207	26	837.919	98.4268	27	777.172	66.7689	28	716.425	52.7494
29	693.284	51.2422	30	627.716	63.9258	31	609.396	65.0644	32	541.899	59.3282
33	468.617	78.727	34	431.012	97.7998	35	405.942	71.123			

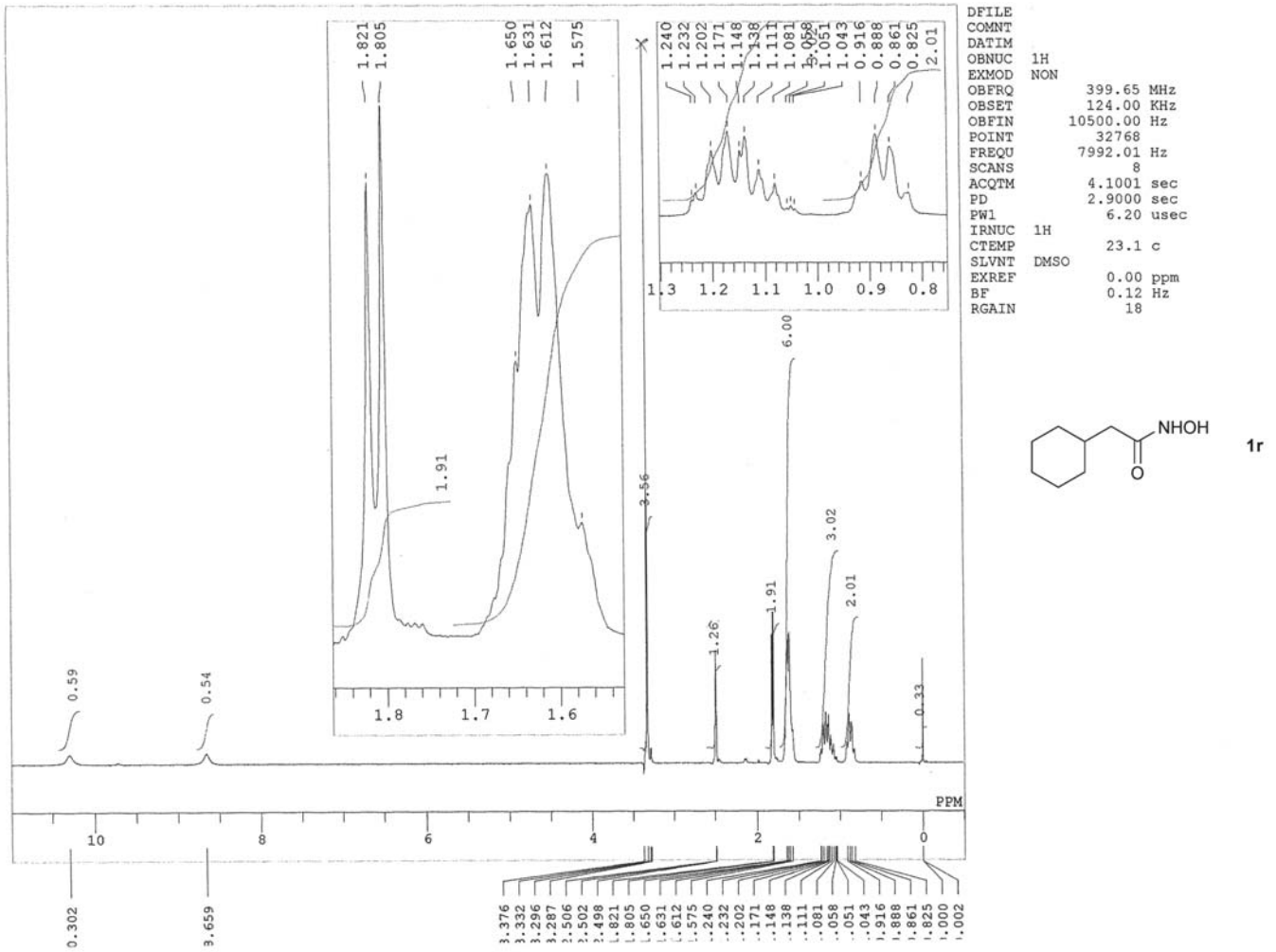






[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3202.22	70.1002	2	3030.59	80.0978	3	2894.63	79.2566	4	2596.68	97.9574
5	2359.48	94.4973	6	1945.82	91.8766	7	1804.08	97.9371	8	1633.41	46.7502
9	1584.24	81.9682	10	1547.59	74.2971	11	1495.53	77.8706	12	1455.03	71.5718
13	1418.39	72.7731	14	1365.35	72.1092	15	1324.86	89.4714	16	1293.04	90.375
17	1190.83	85.9302	18	1162.87	93.5713	19	1105.01	96.0677	20	1077.05	63.1304
21	1053.91	52.7921	22	1029.8	83.3725	23	1003.77	84.3167	24	978.697	52.0652
25	927.593	79.6207	26	837.919	98.4268	27	777.172	66.7689	28	716.425	52.7494
29	693.284	51.2422	30	627.716	63.9258	31	609.396	65.0644	32	541.899	59.3282
33	468.617	78.727	34	431.012	97.7998	35	405.942	71.123			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COMNT
DATIM
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 7992.01 Hz
SCANS 8
ACQTM 4.1001 sec
PD 2.9000 sec
PW1 6.20 usec
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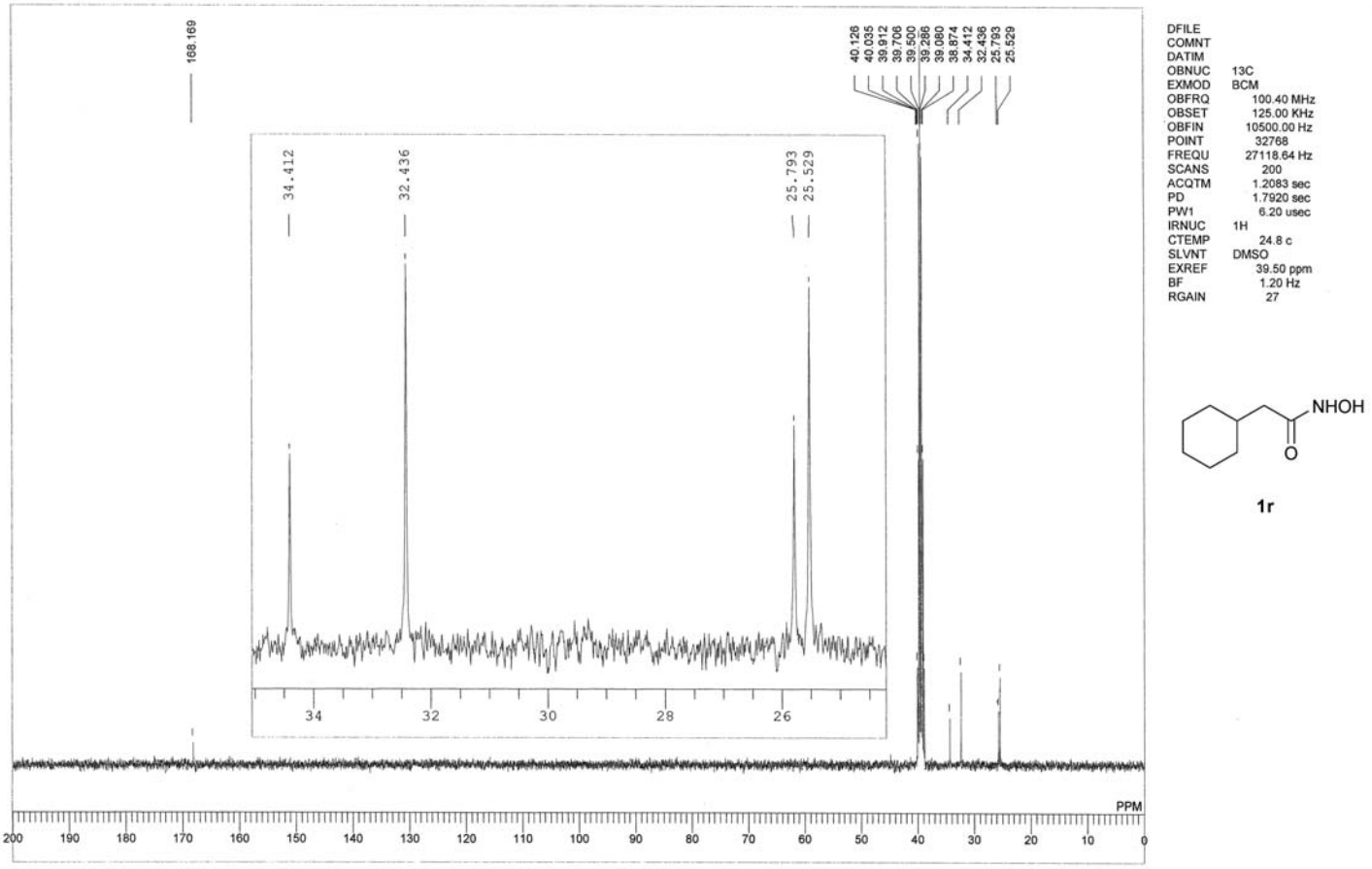
CTEMP 23.1 c
SLVNT DMSO
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 18
NHOH
O
1r
PPM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DATIM
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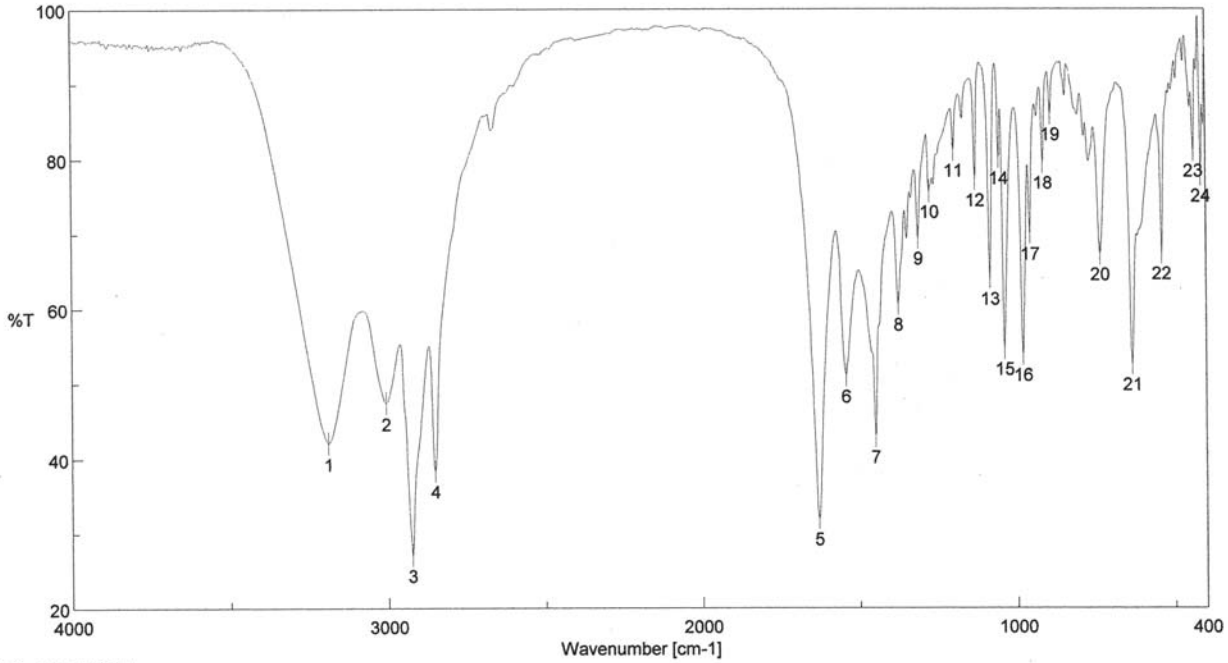
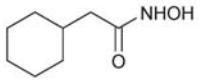
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 200
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 24.8 c
SLVNT DMSO
EXREF 39.50 ppm
BF 1.20 Hz
RGAIN 27
NHOH
O
1r
PPM



[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3189.68	42.0722	2	3005.52	47.4241	3	2923.56	27.1645	4	2850.27	38.4636
5	1629.55	32.033	6	1541.81	51.0878	7	1448.28	43.0277	8	1375	60.6659
9	1311.36	69.4793	10	1275.68	75.7461	11	1198.54	81.2376	12	1130.08	77.284
13	1083.8	64.1022	14	1054.87	80.2428	15	1038.48	54.7322	16	979.661	53.941
17	956.52	70.1055	18	915.058	79.599	19	890.952	86.101	20	734.746	67.3625
21	633.501	52.6726	22	539.007	67.4894	23	437.762	81.2251	24	414.62	77.8807



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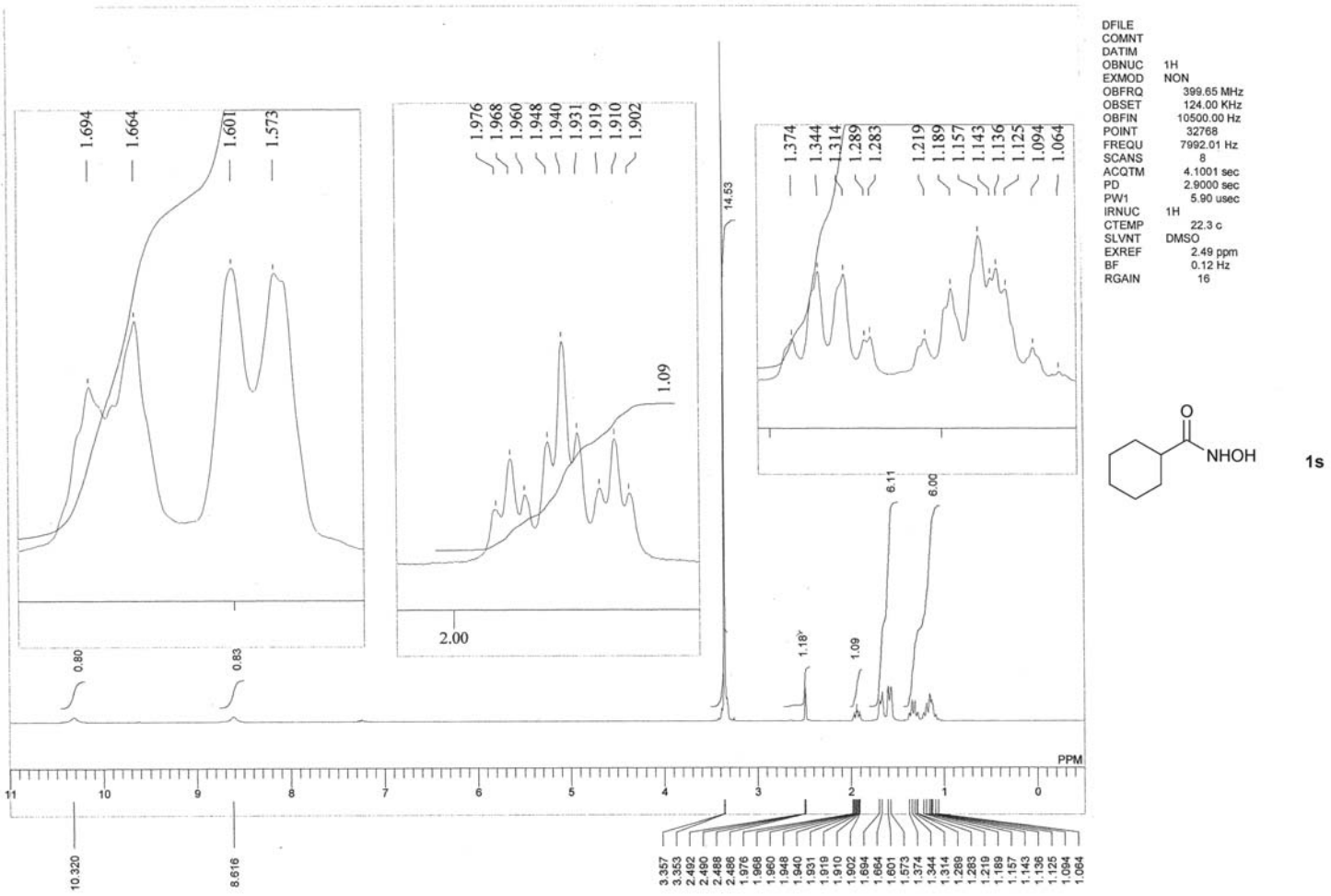
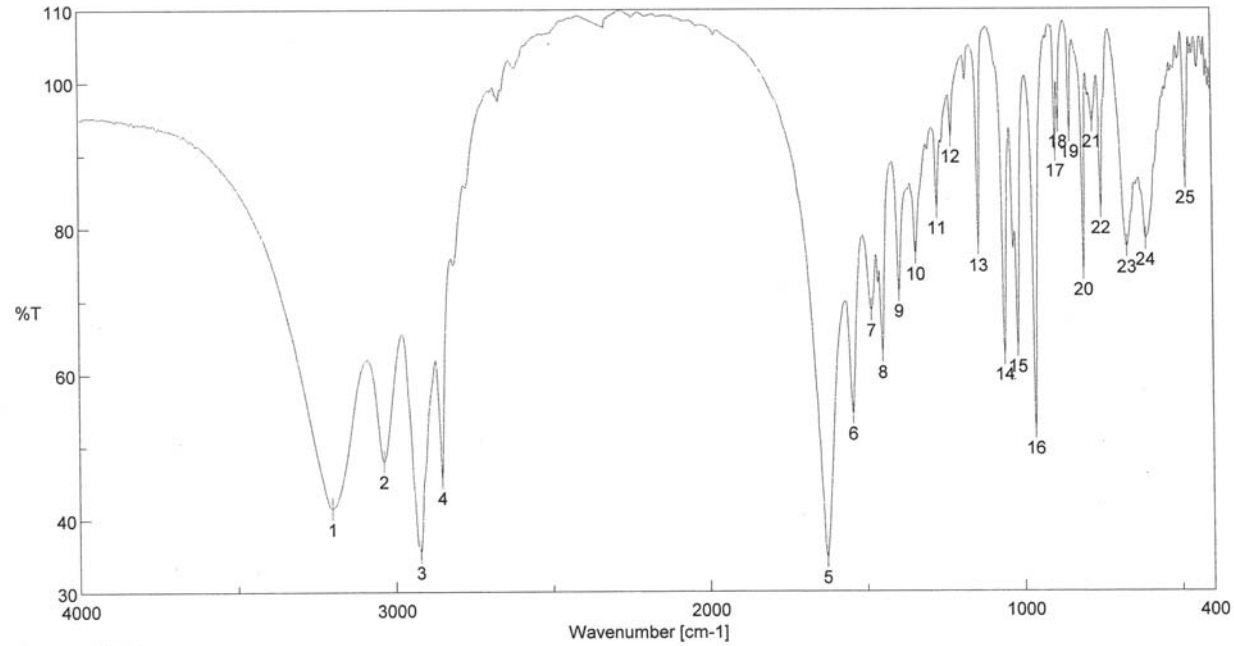
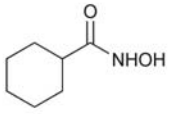
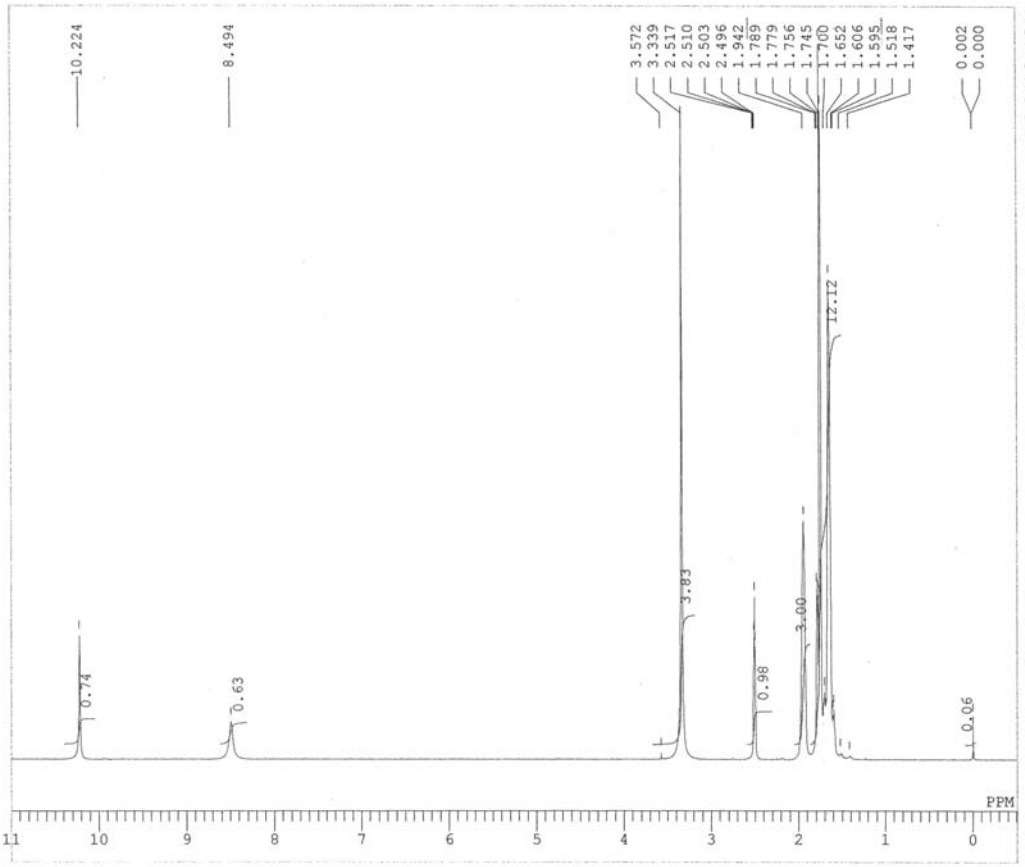




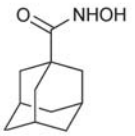
[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3202.22	41.4692	2	3037.34	47.9989	3	2921.63	35.5216	4	2852.2	45.752
5	1627.63	34.775	6	1542.77	54.5109	7	1482.99	68.6833	8	1447.31	62.9768
9	1394.28	71.3537	10	1341.25	76.4632	11	1272.79	82.751	12	1227.47	92.5723
13	1141.65	77.592	14	1059.69	62.6894	15	1018.23	63.7705	16	963.269	52.4959
17	895.773	90.6028	18	887.095	94.5744	19	850.454	93.225	20	808.028	74.3089
21	778.136	94.6106	22	752.102	82.7676	23	671.106	77.3664	24	611.324	78.3907
25	484.045	86.8937									





DFILE
COMNT
DATIM
OBNUC 1H
EXMOD NON
OBFRQ 270.05 MHz
OBSET 112.00 KHz
OBFIN 5800.0 Hz
POINT 16384
FREQU 5405.4 Hz
SCANS 16
ACQTM 3.031 sec
PD 3.969 sec
PW1 4.9 us
IRNUC 1H
CTEMP 22.7 c
SLVNT DMSO
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 17



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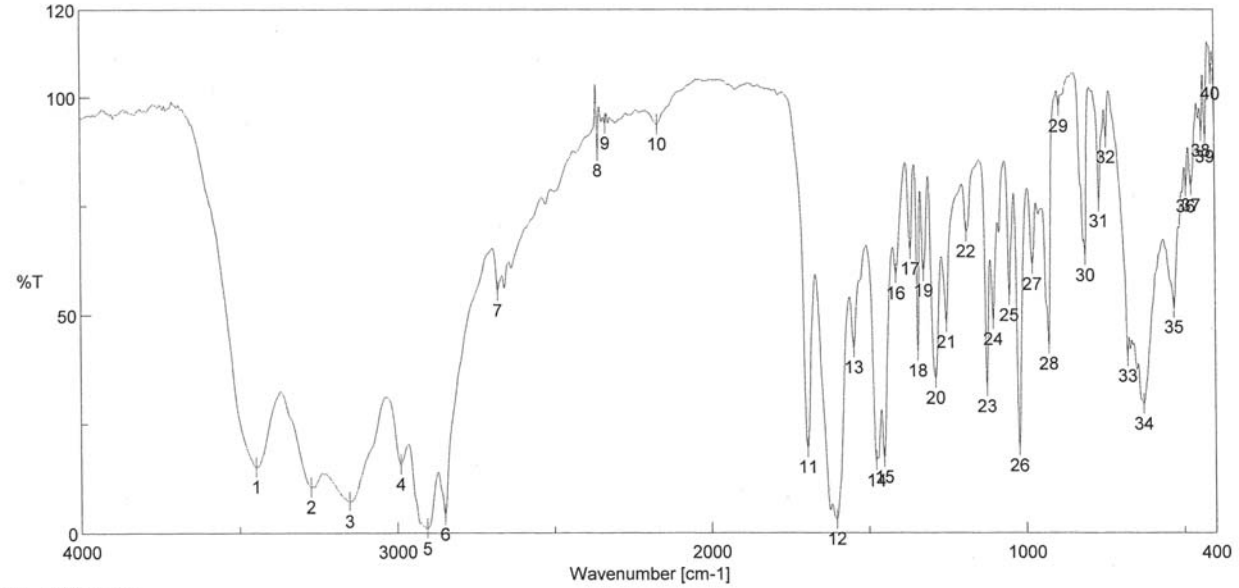
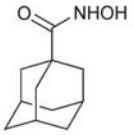
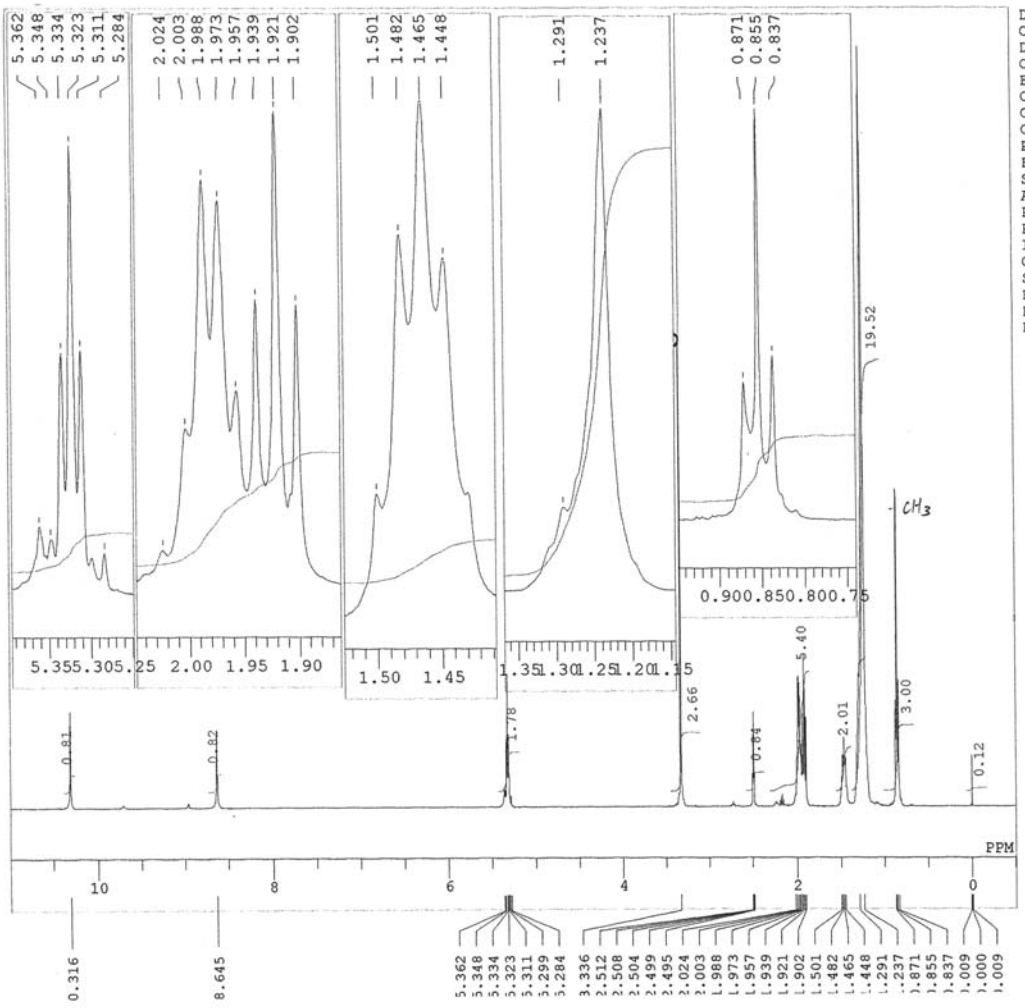


[ピーク検出結果]

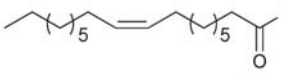
No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3448.1	15.1575	2	3274.54	10.4589	3	3153.04	7.20731	4	2989.12	15.7252
5	2906.2	1.03112	6	2849.31	4.30517	7	2679.6	55.5766	8	2359.48	87.6978
9	2334.41	93.986	10	2169.53	93.7761	11	1694.16	19.6352	12	1603.52	3.19718
13	1546.63	42.4894	14	1477.21	16.5511	15	1451.17	17.3329	16	1412.6	59.4669
17	1366.32	65.1122	18	1343.18	41.7757	19	1324.86	60.1333	20	1287.25	35.4827
21	1252.54	48.2979	22	1188.9	69.1139	23	1124.3	33.6041	24	1104.05	48.9698
25	1052.94	54.4635	26	1022.09	20.0015	27	979.661	61.6929	28	927.593	43.3972
29	892.88	97.8851	30	811.885	63.677	31	767.53	76.0797	32	744.388	90.7205
33	677.856	40.5429	34	627.716	29.5908	35	531.293	51.7252	36	491.759	79.5041
37	475.367	79.7292	38	442.583	92.3059	39	430.048	90.9099	40	410.763	105.274



1t




```
DFILE
COMNT
DATIM
OBNUC   1H
EXMOD   NON
OBFRQ         399.65 MHz
OBSET         124.00 KHz
OBFIN       10500.00 Hz
POINT         32768
FREQU          7992.01 Hz
SCANS             8
ACQTM          4.1001 sec
PD             2.9000 sec
PW1              6.20 usec
IRNUC   1H
CTEMP            23.1 c
SLVNT   DMSO
EXREF             0.00 ppm
BF                0.12 Hz
RGAIN               13
```



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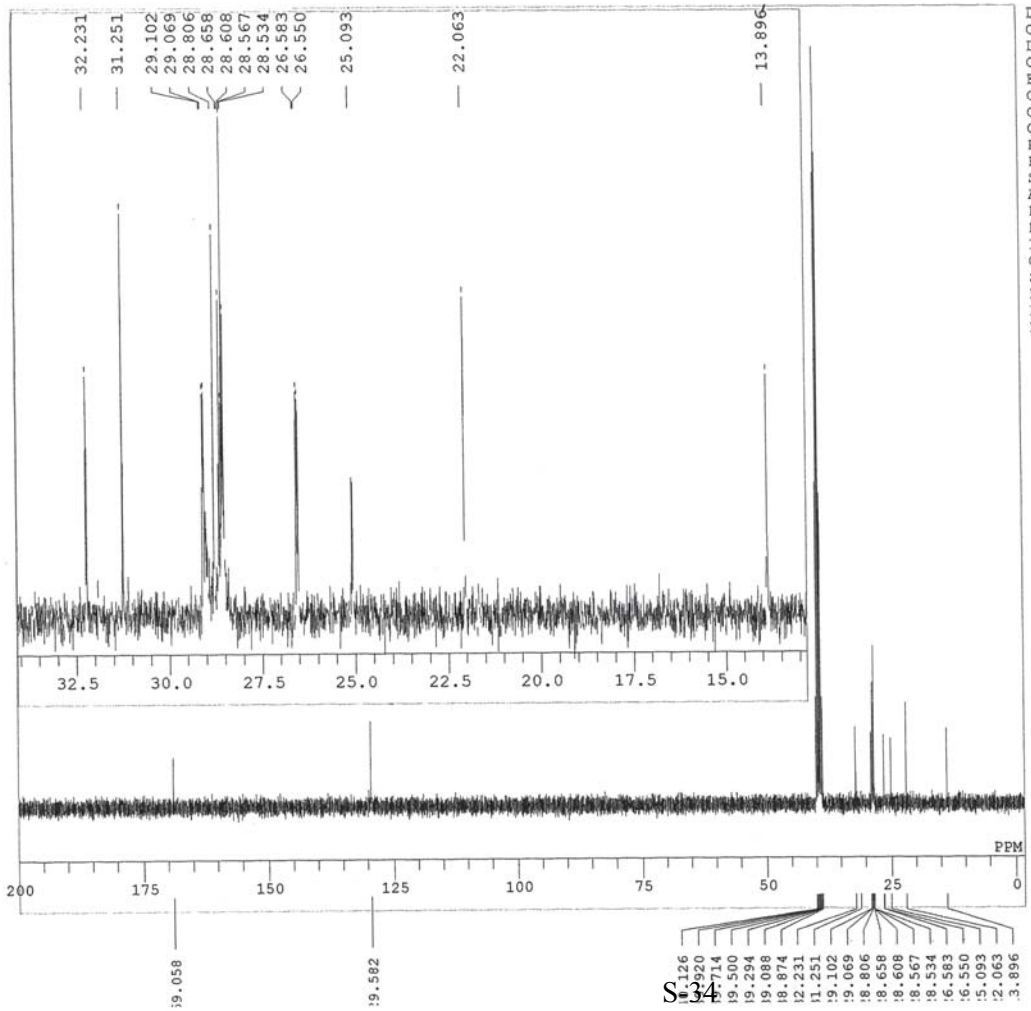


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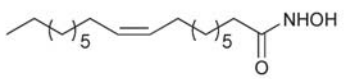
DFILE
COMNT
DATIM
OBNUC   13C
EXMOD   BCM
OBFRQ         100.40 MHz
OBSET         125.00 KHz
OBFIN       10500.00 Hz
POINT         32768
FREQU       27118.64 Hz
SCANS           200
ACQTM          1.2083 sec
PD             1.7920 sec
PW1              6.20 usec
IRNUC   1H
CTEMP            24.5 c
SLVNT   DMSO
EXREF            39.50 ppm
BF                0.12 Hz
RGAIN               27
```



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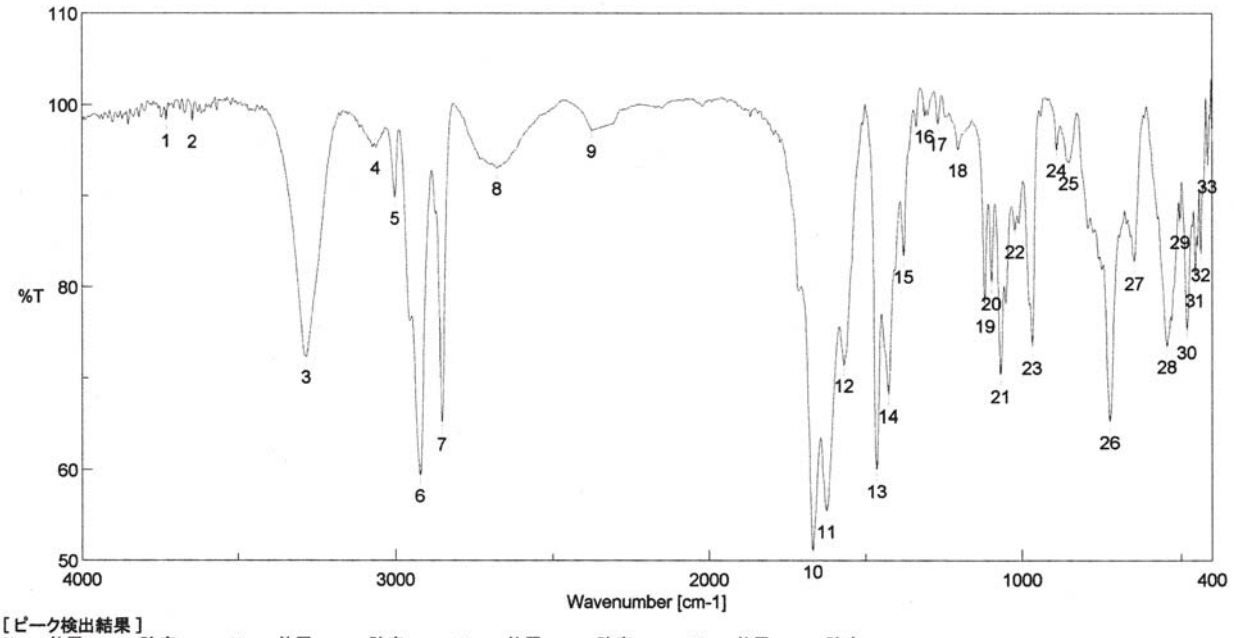
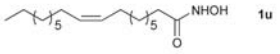
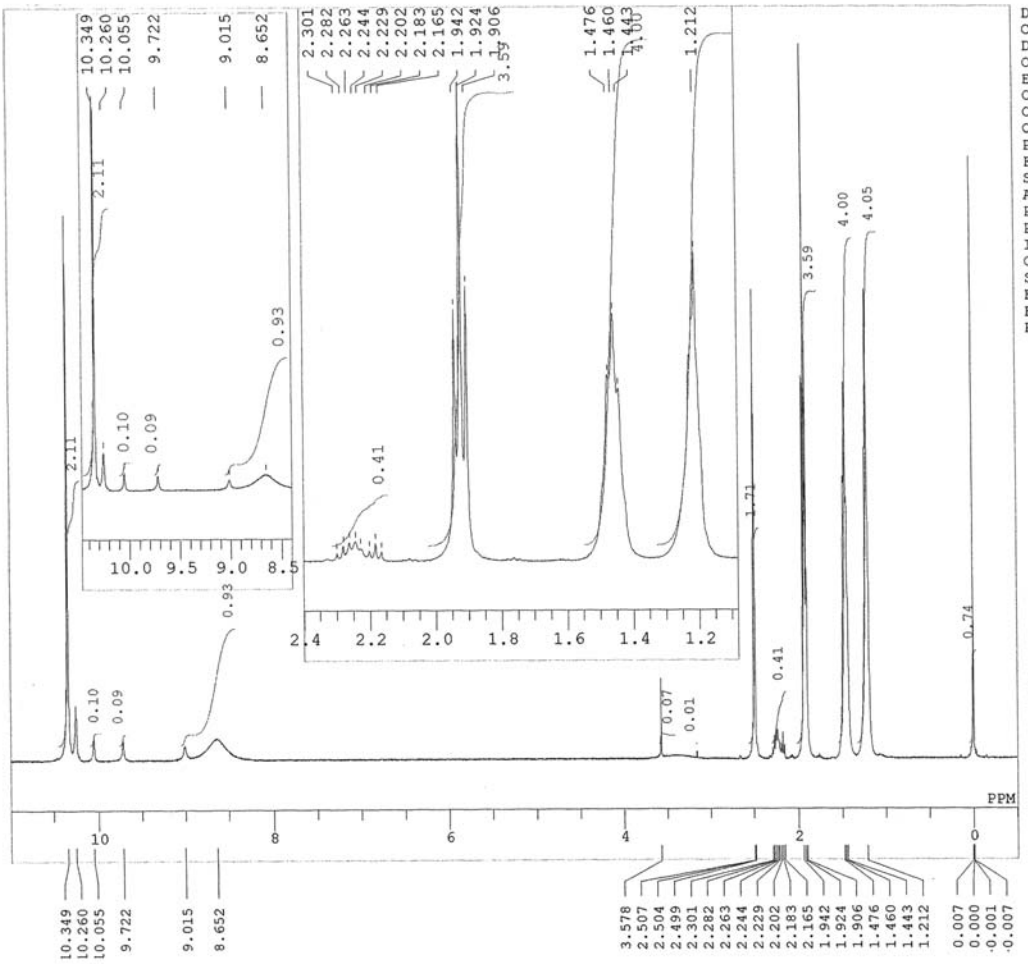


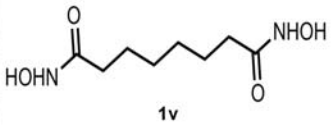
[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3733.51	98.2684	2	3647.7	98.175	3	3284.18	72.3238	4	3064.33	95.2645
5	3002.62	89.7629	6	2919.7	59.366	7	2849.31	64.9872	8	2674.78	92.9911
9	2372.01	97.1374	10	1666.2	51.067	11	1622.8	55.4288	12	1566.88	71.4079
13	1464.67	59.8907	14	1428.03	68.0736	15	1379.82	83.3473	16	1313.29	98.7489
17	1270.86	97.8967	18	1205.29	95.04	19	1117.55	77.9423	20	1096.33	80.425
21	1068.37	70.2093	22	1023.05	86.0957	23	968.09	73.3461	24	891.916	95.0288
25	853.347	93.6244	26	725.104	65.2492	27	648.929	82.6002	28	544.792	73.4472
29	503.33	87.173	30	481.153	75.0376	31	454.154	80.766	32	436.798	83.6076
33	414.62	93.2612									

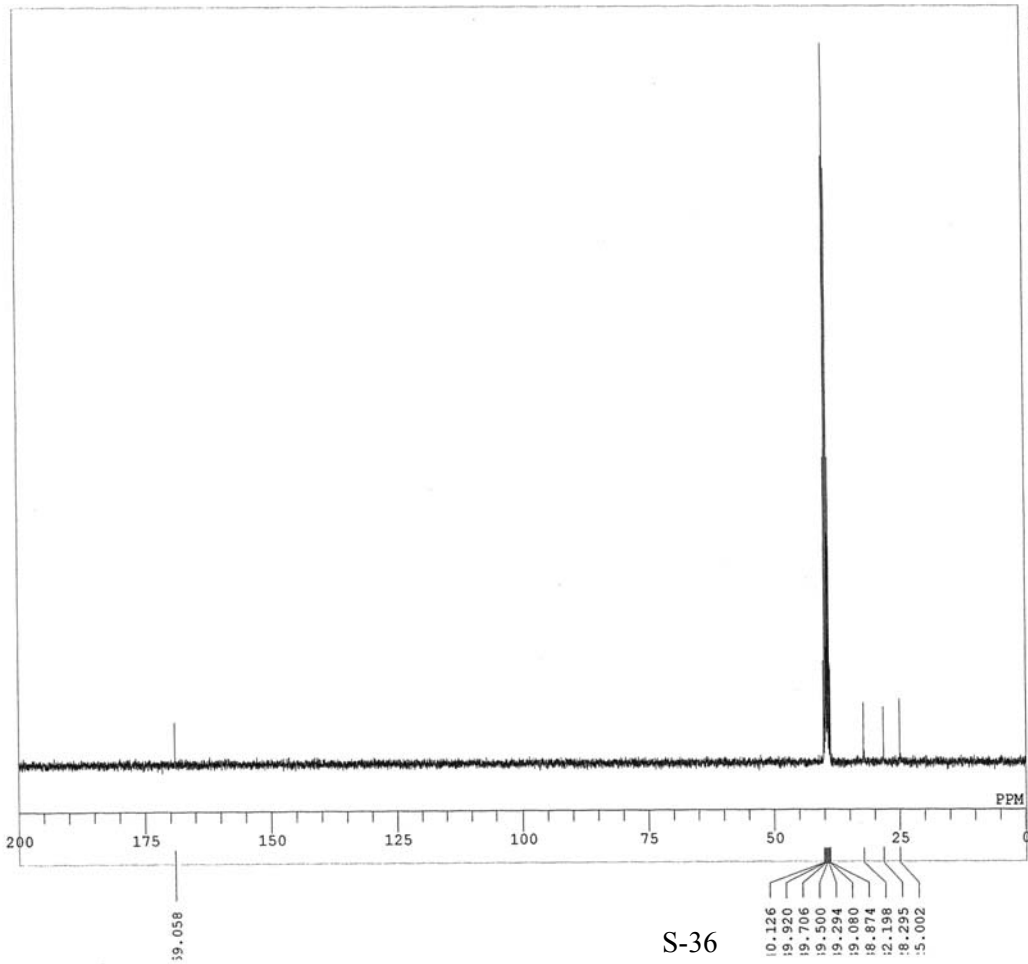


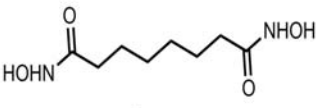
1u


DFILE
COMNT
DATIM
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 7992.01 Hz
SCANS 16
ACQTM 4.1001 sec
PD 2.9000 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 22.4 c
SLVNT DMSO
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 17
PPM

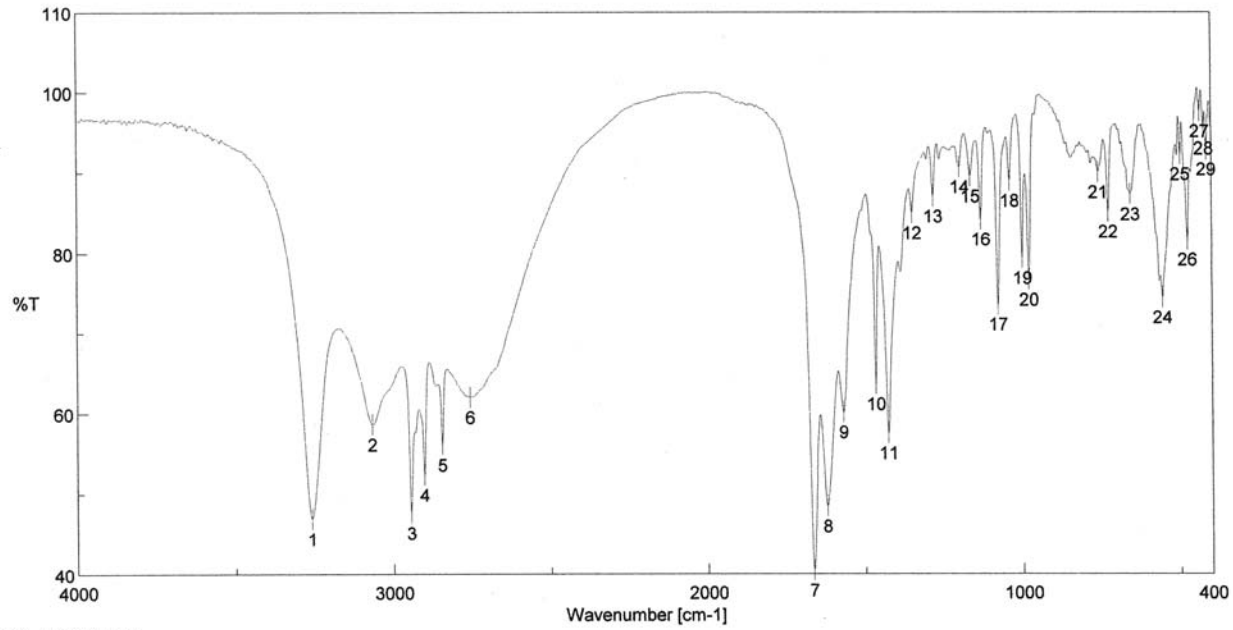

HOHN
NHOH
O
O

1v


DFILE
COMNT
DATIM
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 209
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 23.8 c
SLVNT DMSO
EXREF 39.50 ppm
BF 1.22 Hz
RGAIN 26
PPM

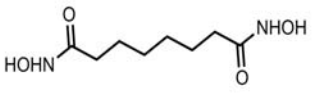

HOHN
NHOH
O
O

1v

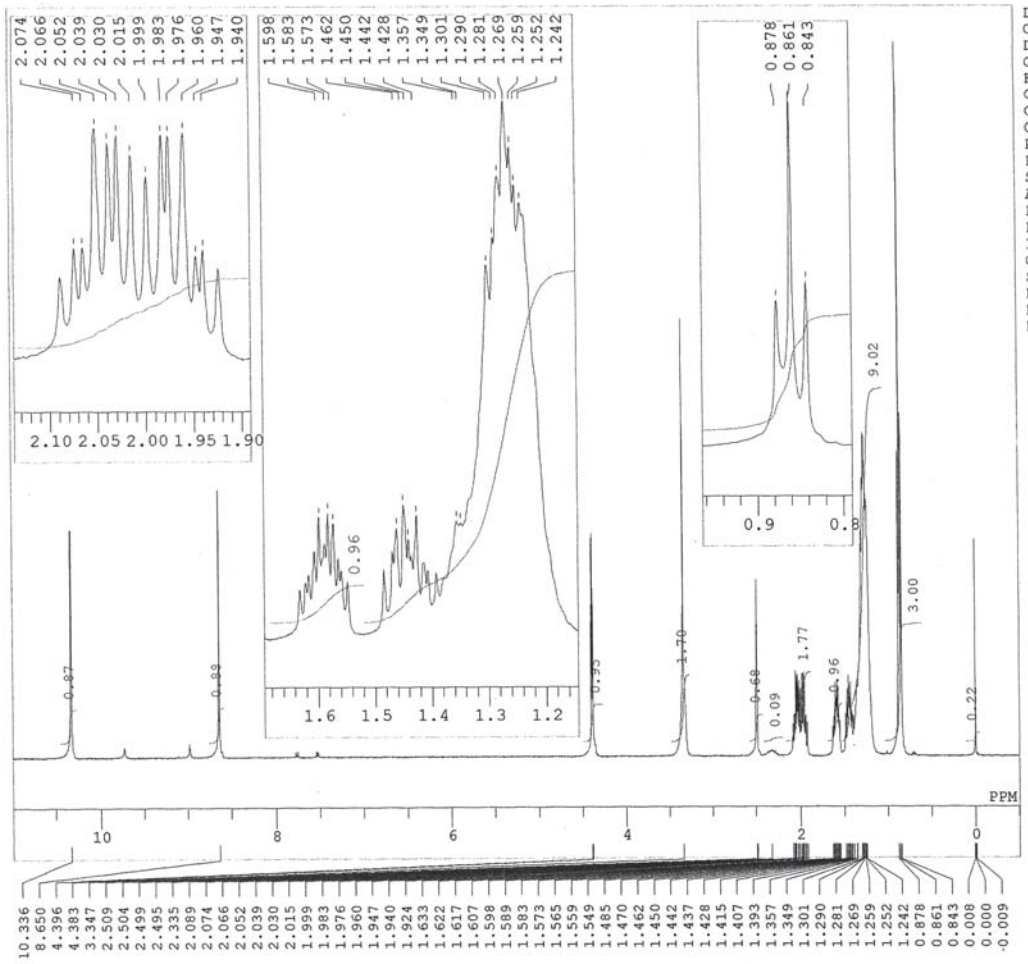


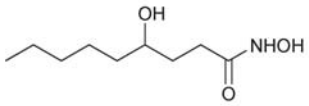
[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3259.11	46.9401	2	3067.23	58.6328	3	2944.77	47.6658	4	2902.34	52.3995
5	2845.45	56.1035	6	2756.74	62.0527	7	1664.27	40.5091	8	1620.88	48.5027
9	1568.81	60.1751	10	1465.63	63.6927	11	1426.1	57.573	12	1348.96	85.0805
13	1282.43	87.1741	14	1198.54	90.7881	15	1163.83	89.6375	16	1131.05	84.2933
17	1077.05	73.6722	18	1039.44	89.1134	19	999.91	79.4652	20	978.697	76.7371
21	758.852	90.1649	22	727.032	85.2803	23	656.643	87.4484	24	556.363	74.5309
25	498.509	92.3886	26	476.331	81.7671	27	436.798	97.6922	28	424.263	95.5749
29	416.549	92.9916									

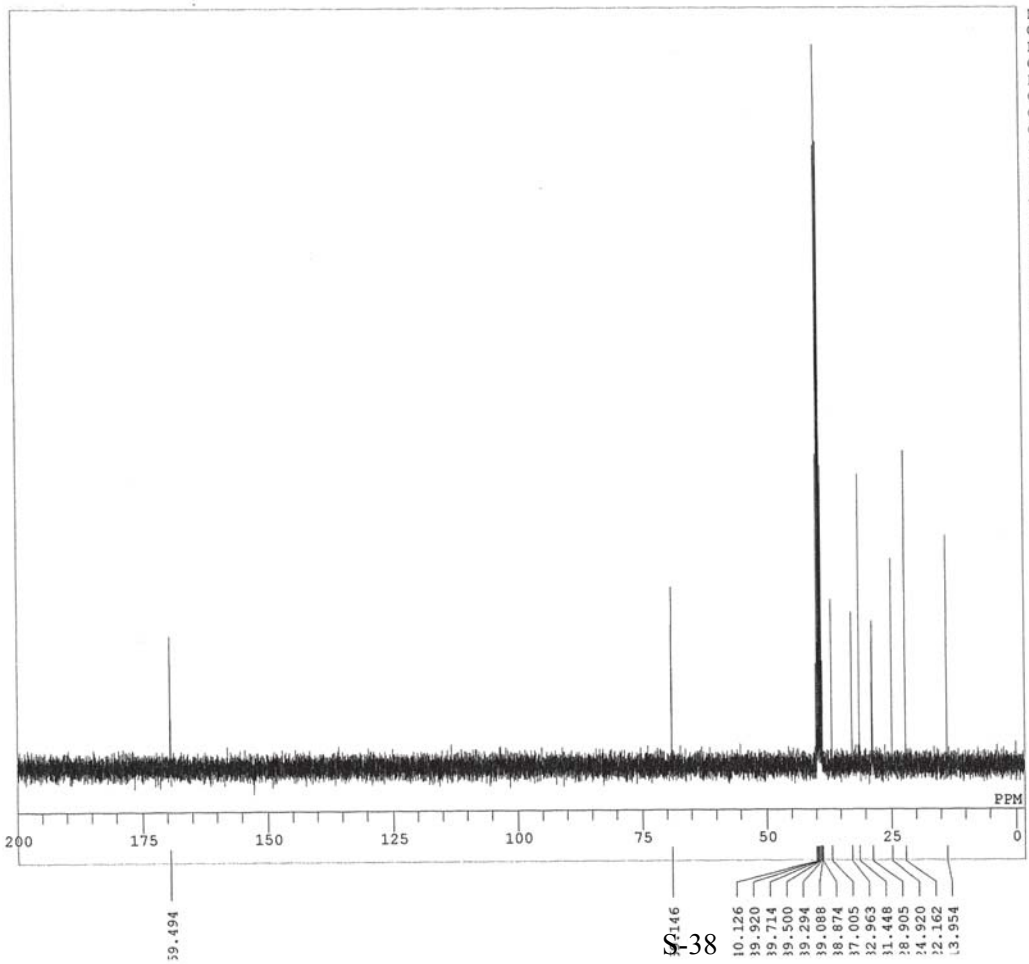


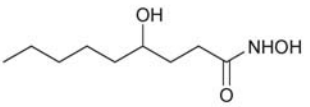
1v


DFILE
COMNT
DATIM
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 7992.01 Hz
SCANS 8
ACQTM 4.1001 sec
PD 2.9000 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 20.8 c
SLVNT DMSO
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 14
PPM

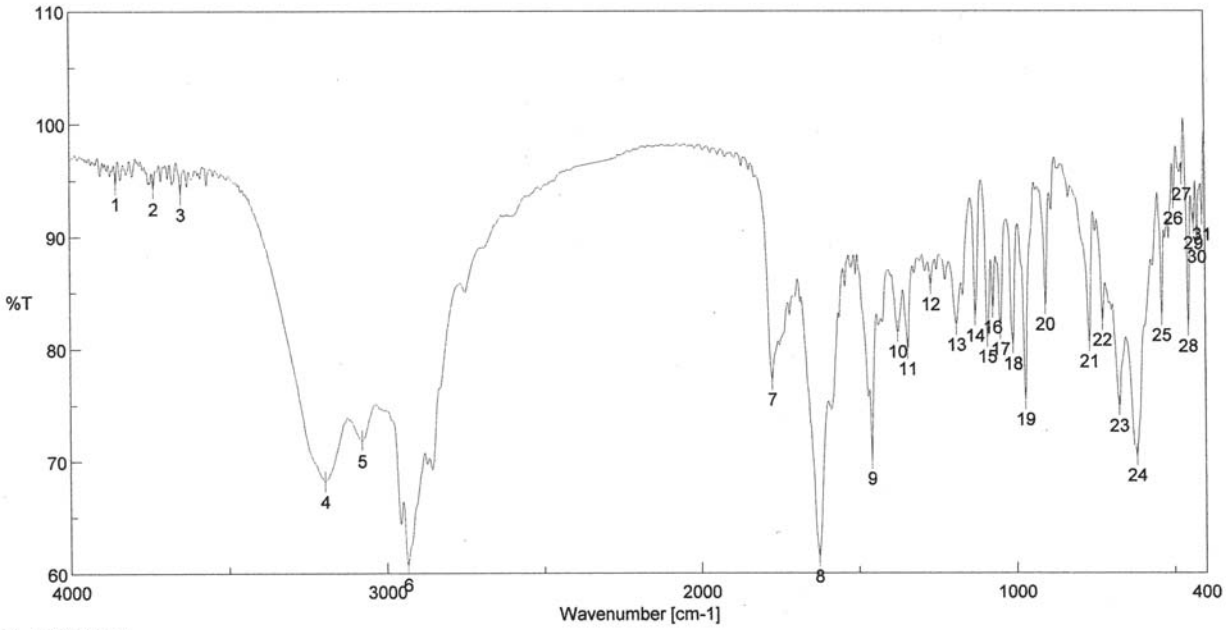

OH
NHOH
O

1w


DFILE
COMNT
DATIM
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 100
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 22.4 c
SLVNT DMSO
EXREF 39.50 ppm
BF 0.12 Hz
RGAIN 27
PPM

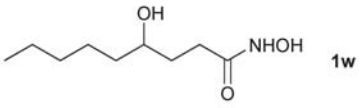

OH
NHOH
O

1w

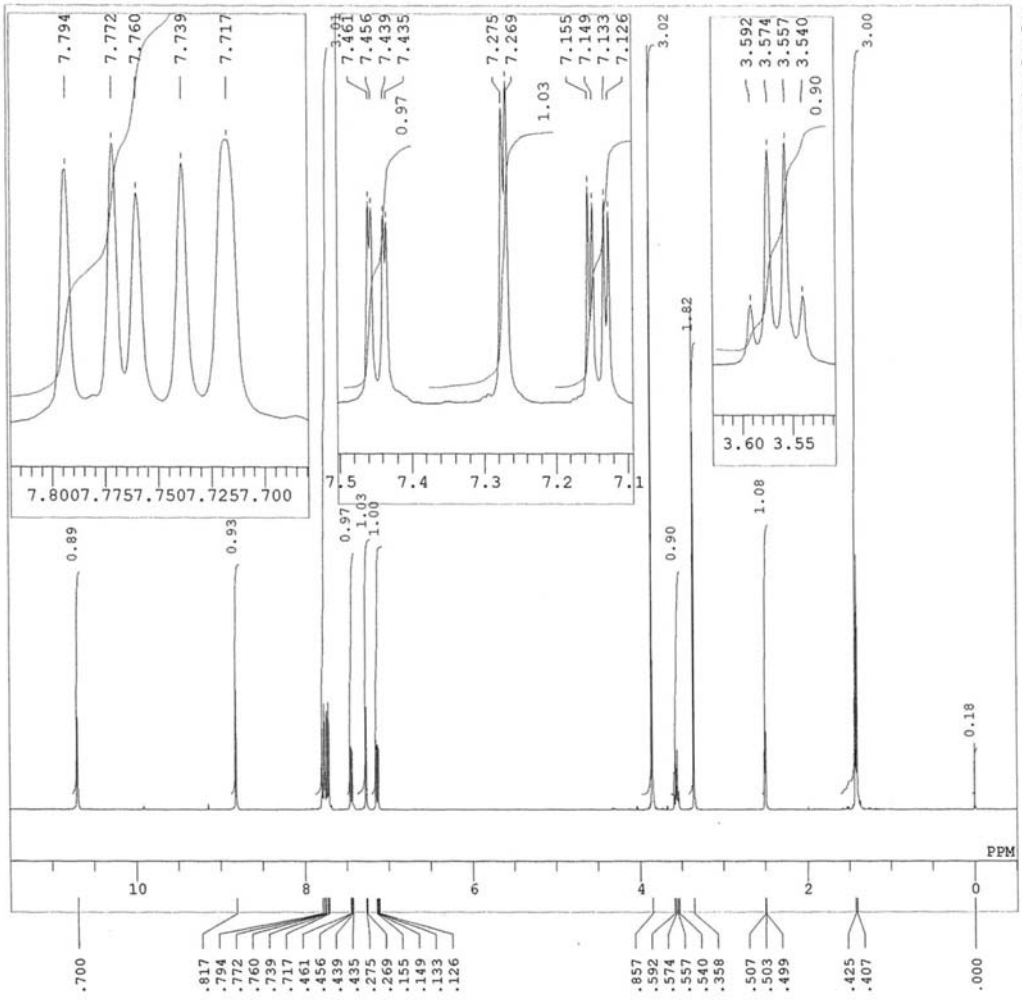


[ピーク検出結果]

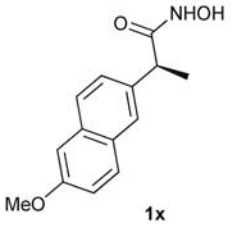
No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3854.04	94.7333	2	3734.48	94.289	3	3648.66	93.7873	4	3195.47	68.1749
5	3077.83	71.8094	6	2934.16	60.7937	7	1773.23	77.3019	8	1625.7	61.5258
9	1456.96	70.2201	10	1374.03	81.527	11	1342.21	80.0076	12	1268.93	85.7427
13	1187.94	82.1558	14	1128.15	82.969	15	1089.58	81.0978	16	1072.23	83.7082
17	1048.12	81.7834	18	1008.59	80.4777	19	970.019	75.5157	20	905.415	83.997
21	766.566	80.6788	22	725.104	82.6091	23	673.035	74.9362	24	617.109	70.5251
25	537.078	83.0183	26	498.509	93.3907	27	472.474	95.5612	28	453.19	82.0477
29	435.834	91.1783	30	425.227	89.9864	31	408.835	91.9734			



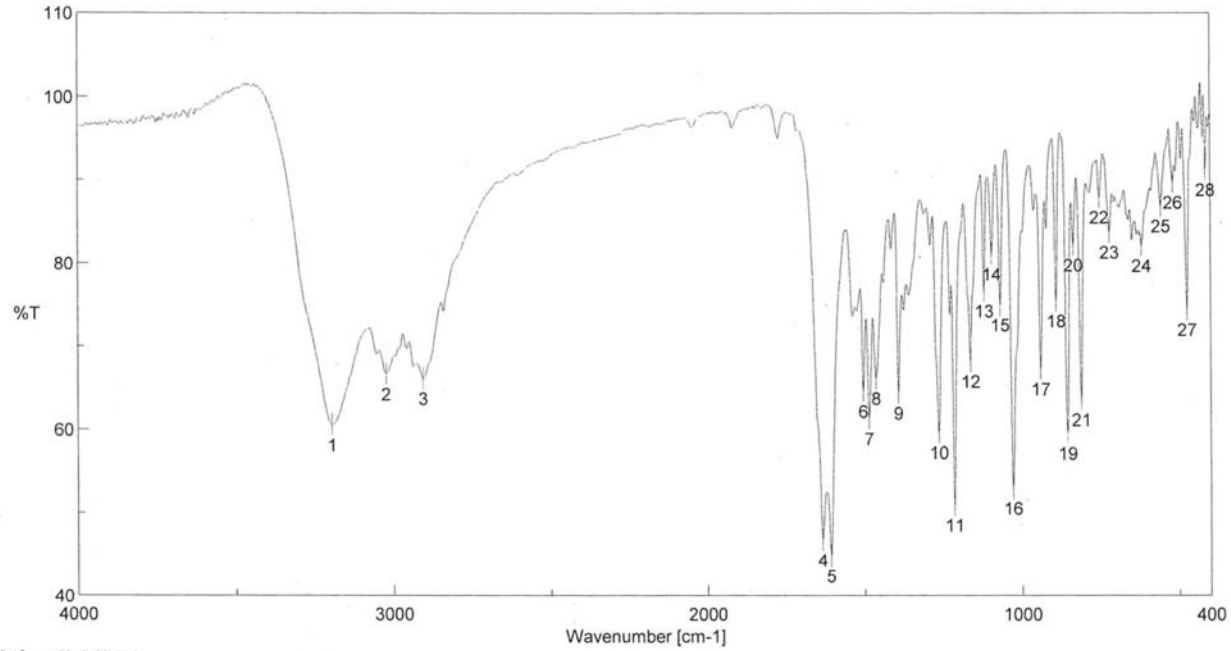
1w




```
DFILE
COMNT
DATIM
OBNUC   1H
EXMOD   NON
OBFRQ         399.65 MHz
OBSET         124.00 KHz
OBFIN       10500.00 Hz
POINT          32768
FREQU        7992.01 Hz
SCANS             16
ACQTM          4.1001 sec
PD             2.9000 sec
PW1               6.20 usec
IRNUC   1H
CTEMP            20.2 c
SLVNT   DMSO
EXREF             0.00 ppm
BF                0.12 Hz
RGAIN               16
```

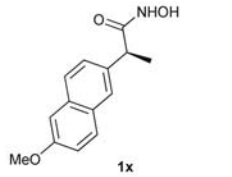


1x



[ピーク検出結果]

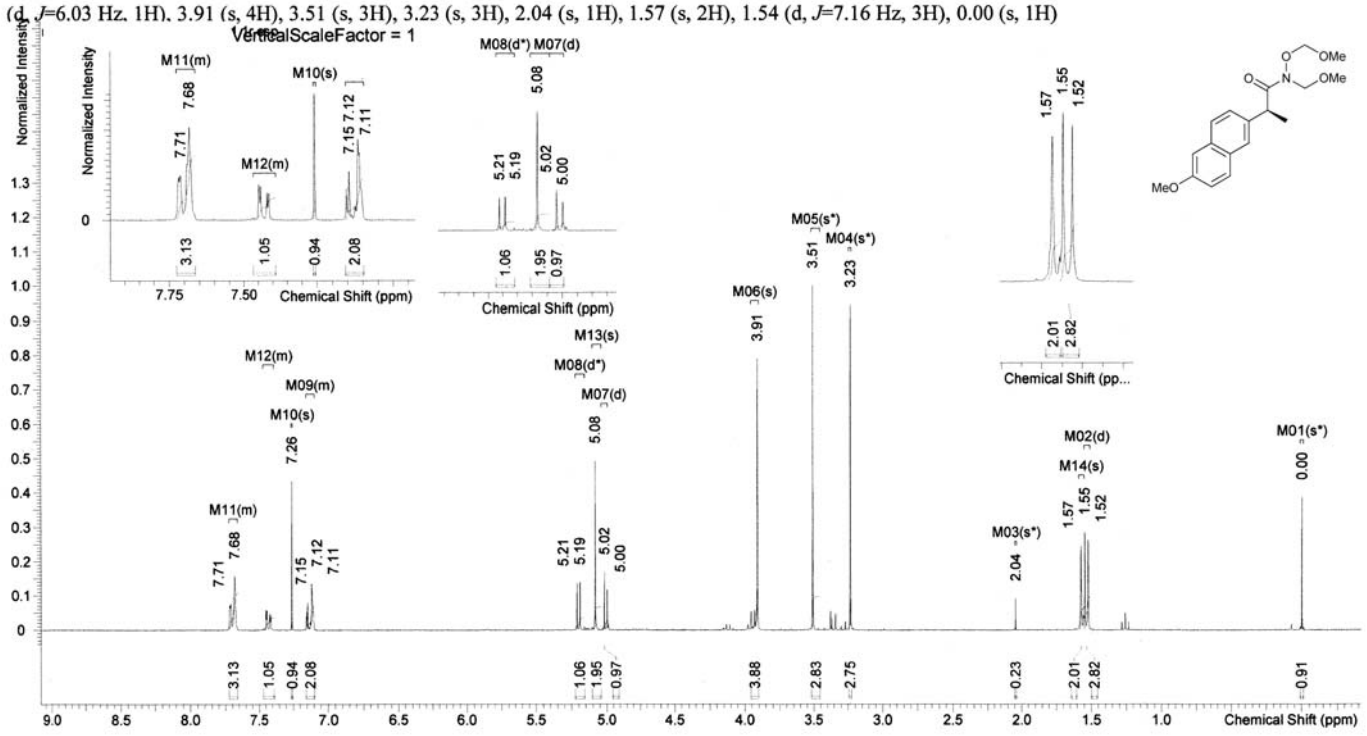
No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3196.43	60.5684	2	3023.84	66.6991	3	2906.2	66.1629	4	1634.38	46.8077
5	1607.38	44.8757	6	1504.2	64.6295	7	1485.88	61.3434	8	1463.71	66.1761
9	1392.35	64.4264	10	1264.11	59.7048	11	1214.93	50.9834	12	1162.87	68.223
13	1119.48	76.7112	14	1095.37	81.1565	15	1068.37	75.0241	16	1028.84	53.0169
17	940.128	67.3024	18	890.952	75.5186	19	855.275	59.6075	20	835.99	82.2533
21	810.92	63.6181	22	753.066	87.9801	23	721.247	83.8025	24	619.038	82.1909
25	557.327	86.9204	26	518.758	89.7424	27	474.403	74.4402	28	415.585	91.2583

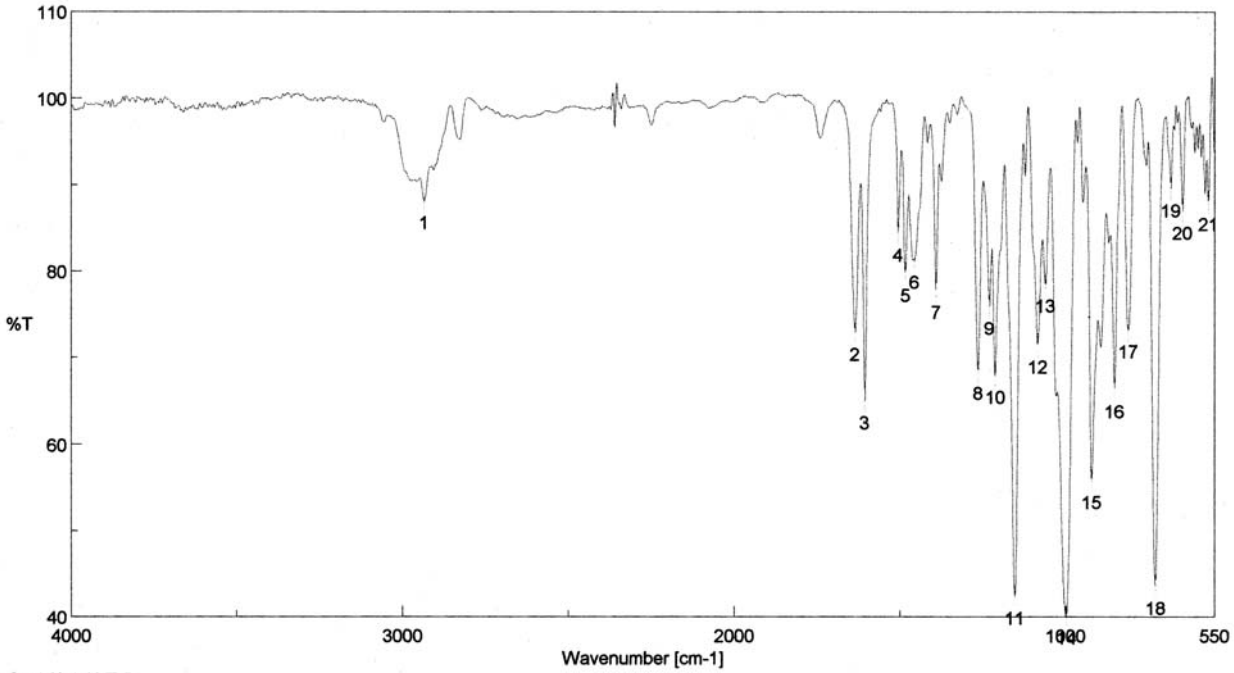


1x

OriginalDateForRelativeTime			Multiplets Integrals Sum	26.60	Number of Nuclei	28 H's	
Acquisition Time (sec)	2.6542	Comment	5 mm QNP 1H/13C/31P/19F Z3333/0001		Date		
Date Stamp			File Name			Frequency (MHz)	300.13
Nucleus	1H	Number of Transients	8	Origin	spect	Original Points Count	16384	Owner	DRX300
Points Count	16384	Pulse Sequence	zg30	Receiver Gain	812.70	SW(cyclical) (Hz)	6172.84	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	1847.2979	Spectrum Type	STANDARD	Sweep Width (Hz)	6172.46	Temperature (degree C)	27.000		

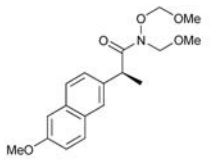
^{1}H NMR (300 MHz, CHLOROFORM-d) δ 7.66-7.72 (m, 3H), 7.39-7.47 (m, 1H), 7.26 (s, 1H), 7.10-7.16 (m, 2H), 5.20 (d, *J*=6.03 Hz, 1H), 5.08 (s, 2H), 5.01 (d, *J*=6.03 Hz, 1H), 3.91 (s, 4H), 3.51 (s, 3H), 3.23 (s, 3H), 2.04 (s, 1H), 1.57 (s, 2H), 1.54 (d, *J*=7.16 Hz, 3H), 0.00 (s, 1H)

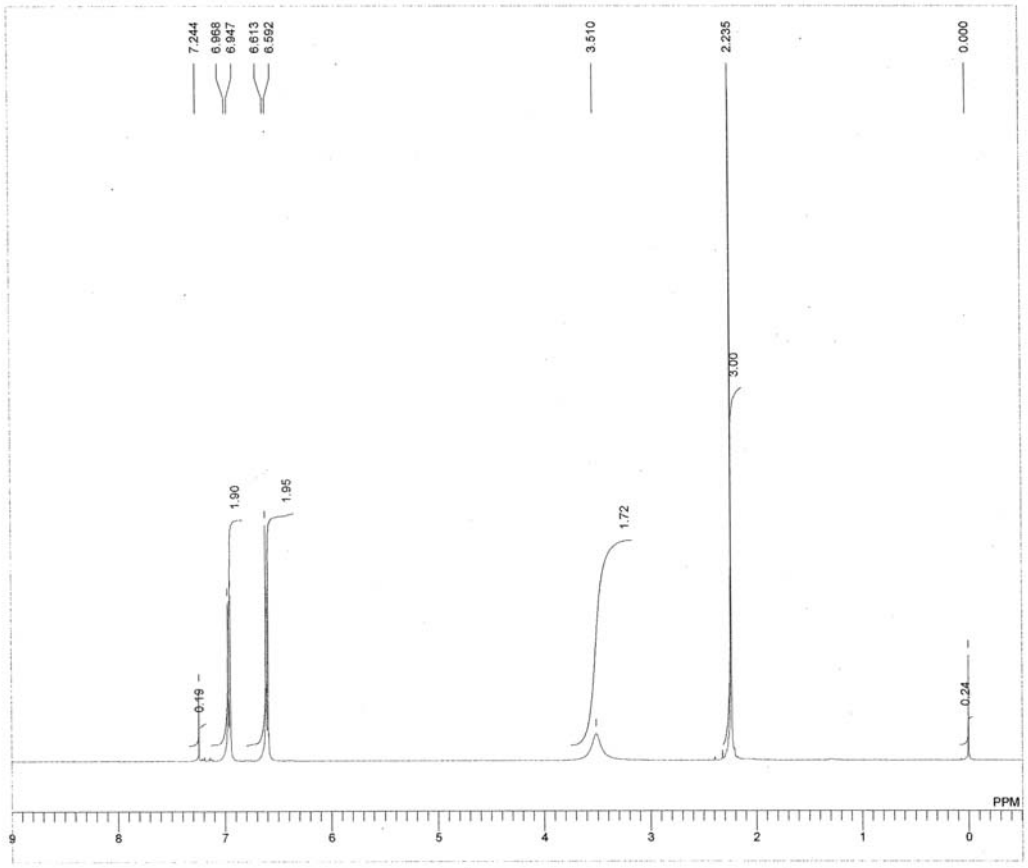




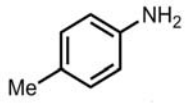
[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	2935.13	88.0973	2	1635.34	72.8436	3	1606.41	64.9704	4	1506.13	84.3528
5	1483.96	79.6747	6	1456.96	81.202	7	1391.39	77.7441	8	1264.11	68.3568
9	1230.36	75.8924	10	1213.01	67.8933	11	1153.22	42.3792	12	1083.8	71.4452
13	1061.62	78.481	14	997.982	40.103	15	921.807	55.8286	16	852.382	66.251
17	810.92	73.2107	18	728.961	43.5504	19	682.677	89.5217	20	647.001	86.9298
21	568.898	87.9668									

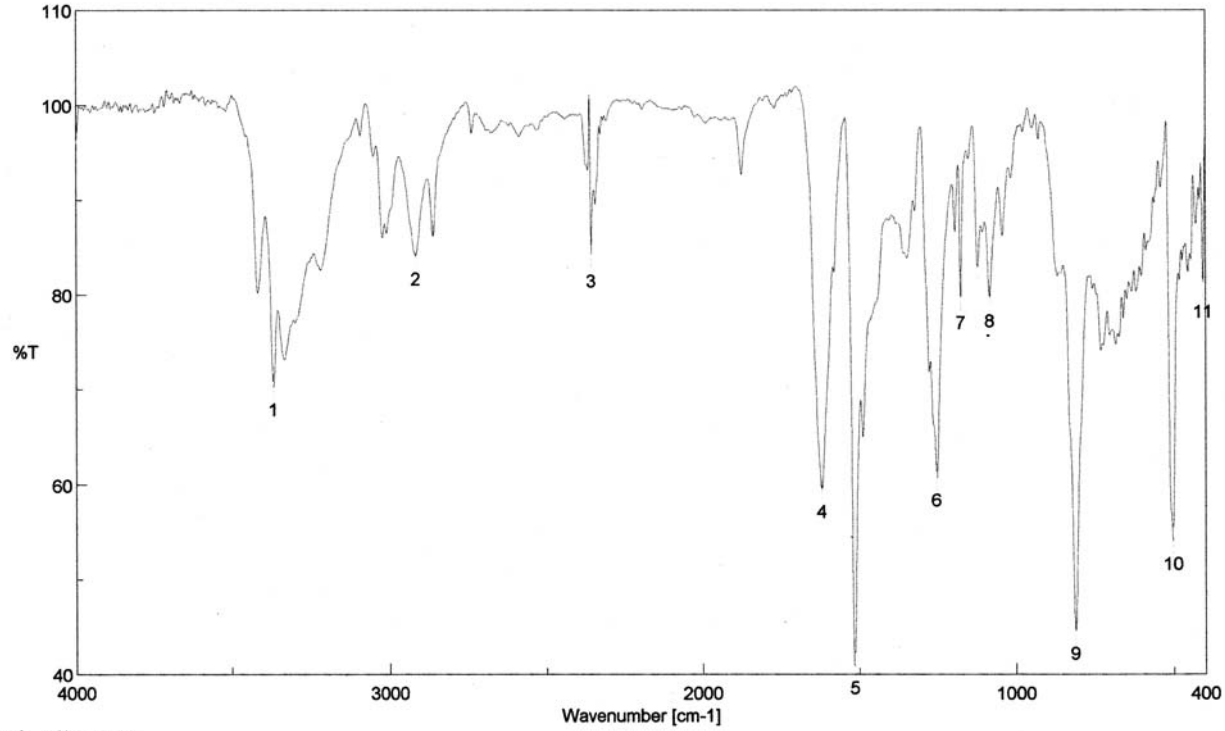




DFILE
COMNT
DATIM
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 7993.60 Hz
SCANS 16
ACQTM 4.0993 sec
PD 2.9010 sec
PW1 6.60 usec
IRNUC 1H
CTEMP 20.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 16

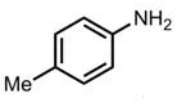


2a

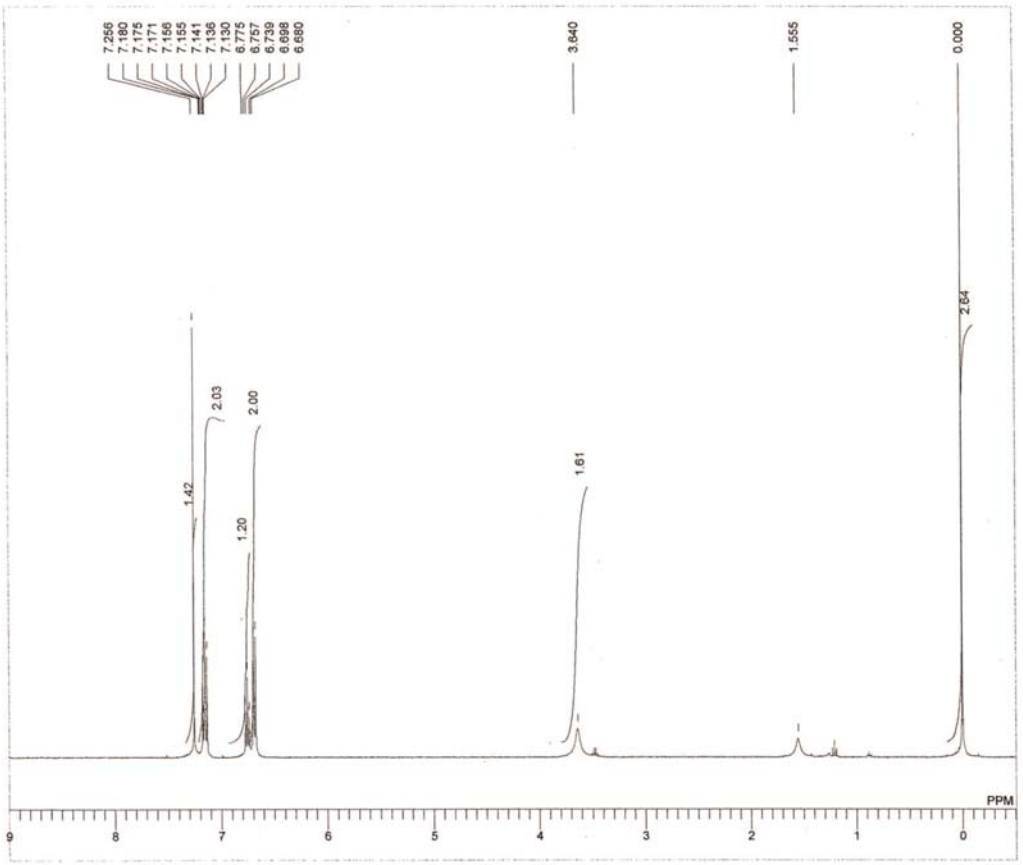


[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3369.03	70.2513	2	2914.88	84.0564	3	2355.62	83.8493	4	1619.91	59.5854
5	1514.81	40.9422	6	1255.43	60.7579	7	1177.33	79.4411	8	1082.83	79.6209
9	812.849	44.6213	10	502.366	54.0532	11	407.871	80.6043			



2a

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DFILE
COMNT
DATIM
OBNUC   1H
EXMOD   NON
OBFRQ     399.65 MHz
OBSET     124.00 KHz
OBFIN     10500.00 Hz
POINT     32768
FREQU     7993.60 Hz
SCANS     16
ACQTM     4.0993 sec
PD        2.9007 sec
PW1       6.60 usec
IRNUC   1H
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SLVNT   CDCL3
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BF        0.12 Hz
RGAIN     24
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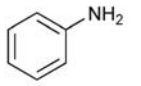
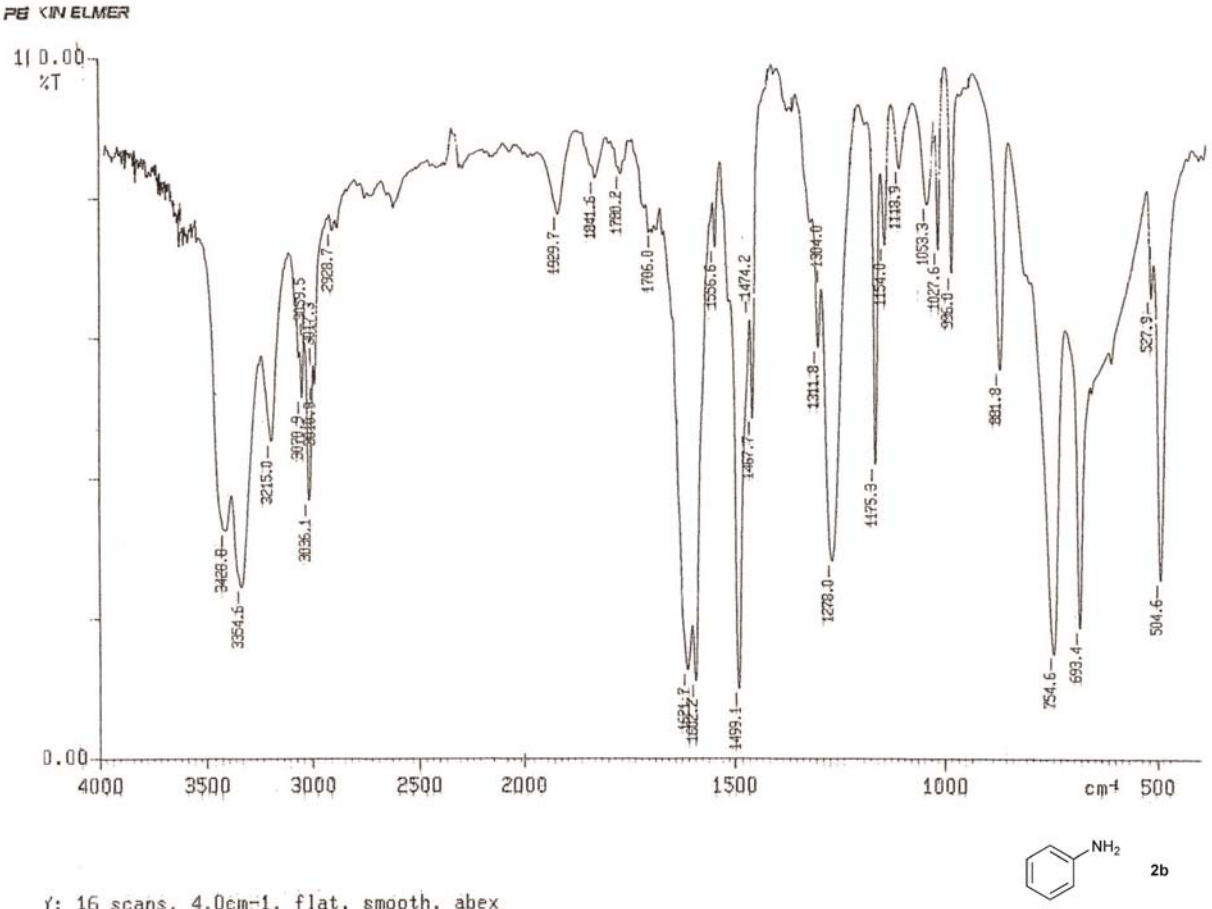
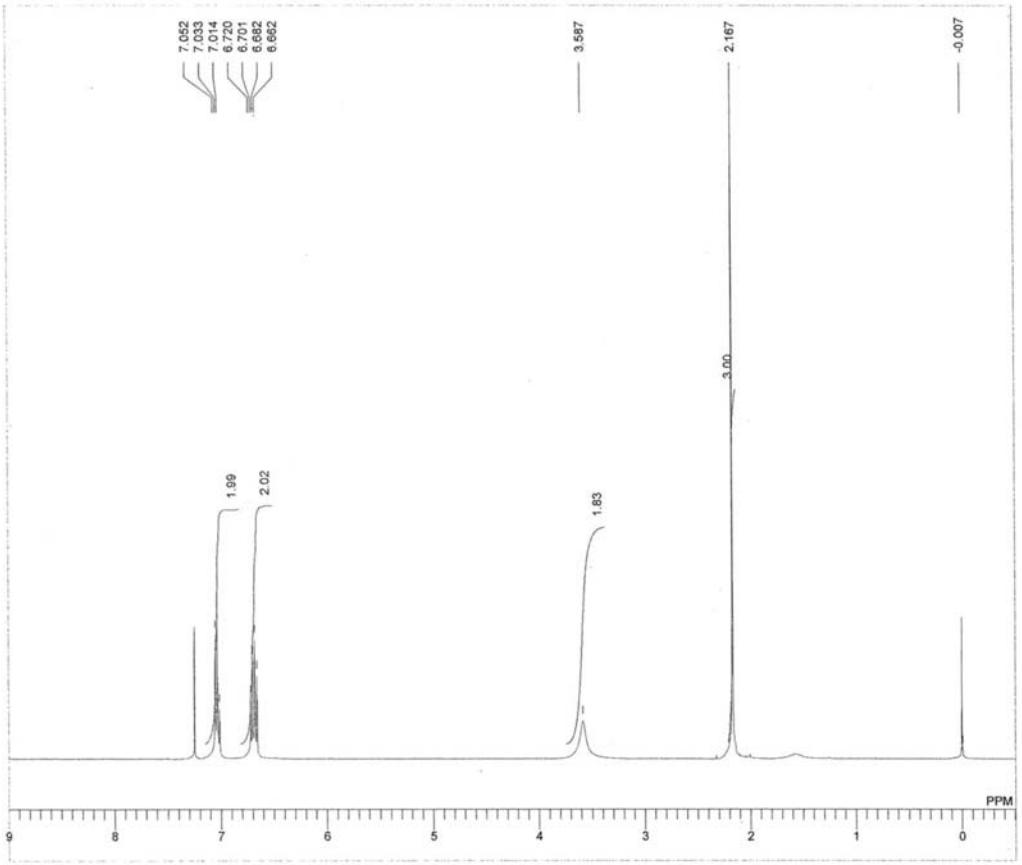


2b

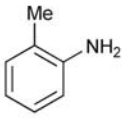


2b

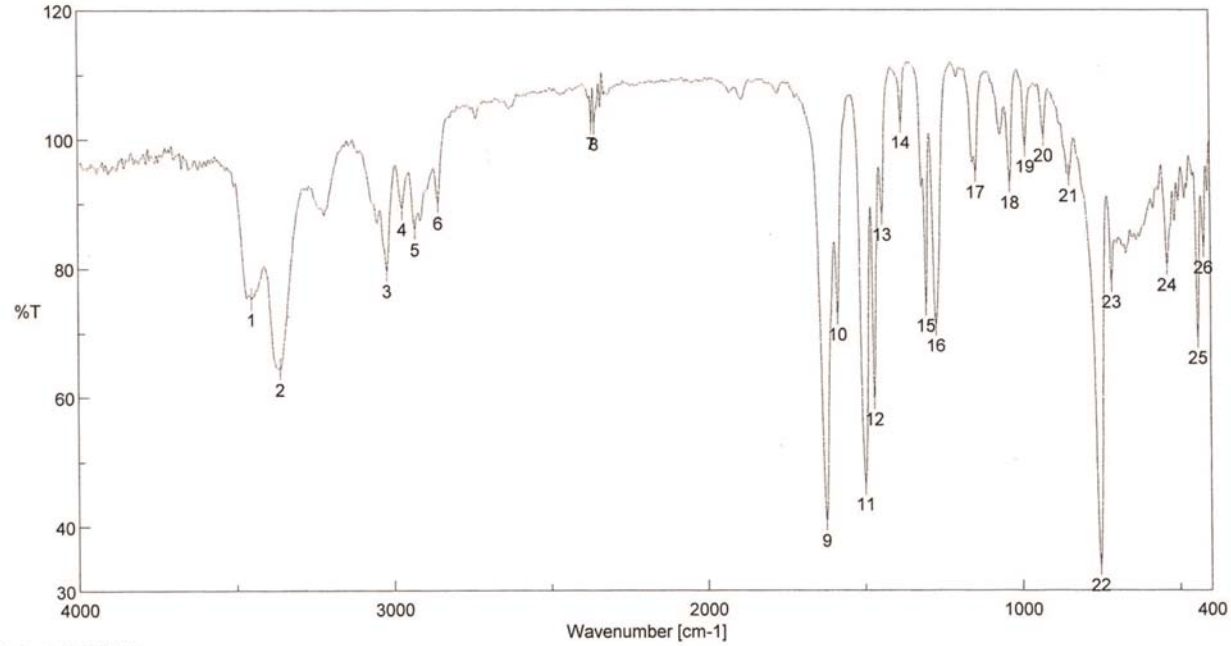
Y: 16 scans, 4.0cm-1, flat, smooth, abex



DFILE
COMNT
DATIM
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 7993.60 Hz
SCANS 16
ACQTM 4.0993 sec
PD 2.9010 sec
PW1 6.60 usec
IRNUC 1H
CTEMP 20.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 20

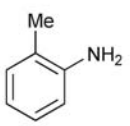


2c

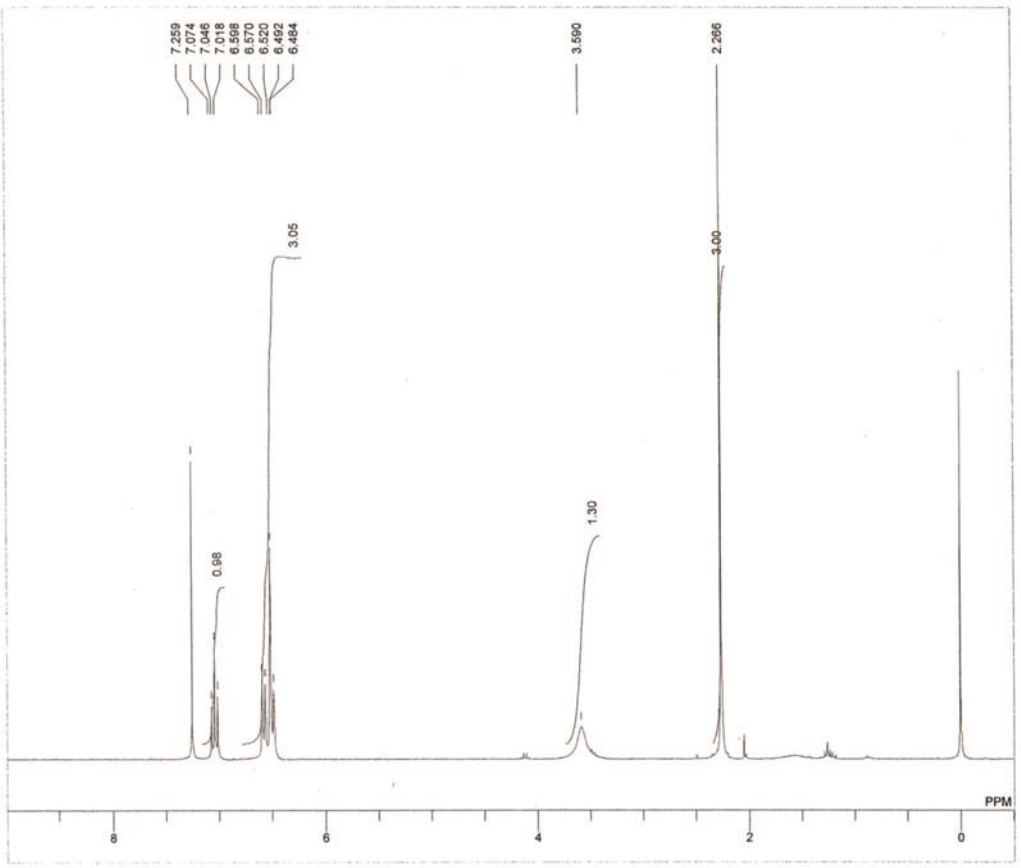


[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3451.96	75.309	2	3361.32	64.3987	3	3020.94	79.6854	4	2971.77	89.2011
5	2931.27	86.0566	6	2857.02	90.1533	7	2367.19	102.531	8	2357.55	102.429
9	1622.8	40.9372	10	1585.2	72.9563	11	1498.42	46.5855	12	1468.53	59.7332
13	1442.49	88.3309	14	1380.78	102.69	15	1303.64	74.3481	16	1271.82	71.2299
17	1144.55	94.9426	18	1035.59	93.3046	19	986.411	98.9309	20	927.593	100.638
21	847.561	94.3993	22	753.066	34.0367	23	714.497	78.0074	24	538.042	80.6278
25	440.655	69.3256	26	422.334	83.3195						



2c



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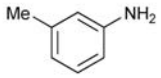
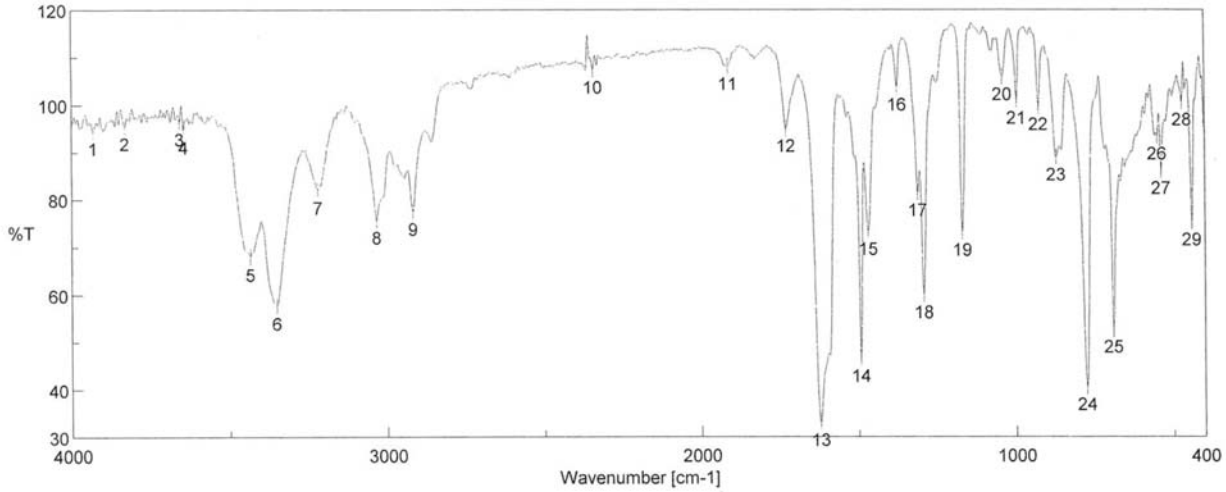
COMNT
DATIM
OBNUC 1H
EXMOD NON
OBFRQ 270.05 MHz
OBSET 112.00 KHz
OBFIN 5800.00 Hz
POINT 16384
FREQU 5405.40 Hz
SCANS 16
ACQTM 3.0310 sec
PD 20.0000 sec
PW1 4.90 usec
IRNUC 1H
CTEMP 19.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 22

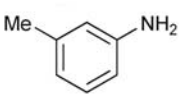


2d



[ピーク検出結果]

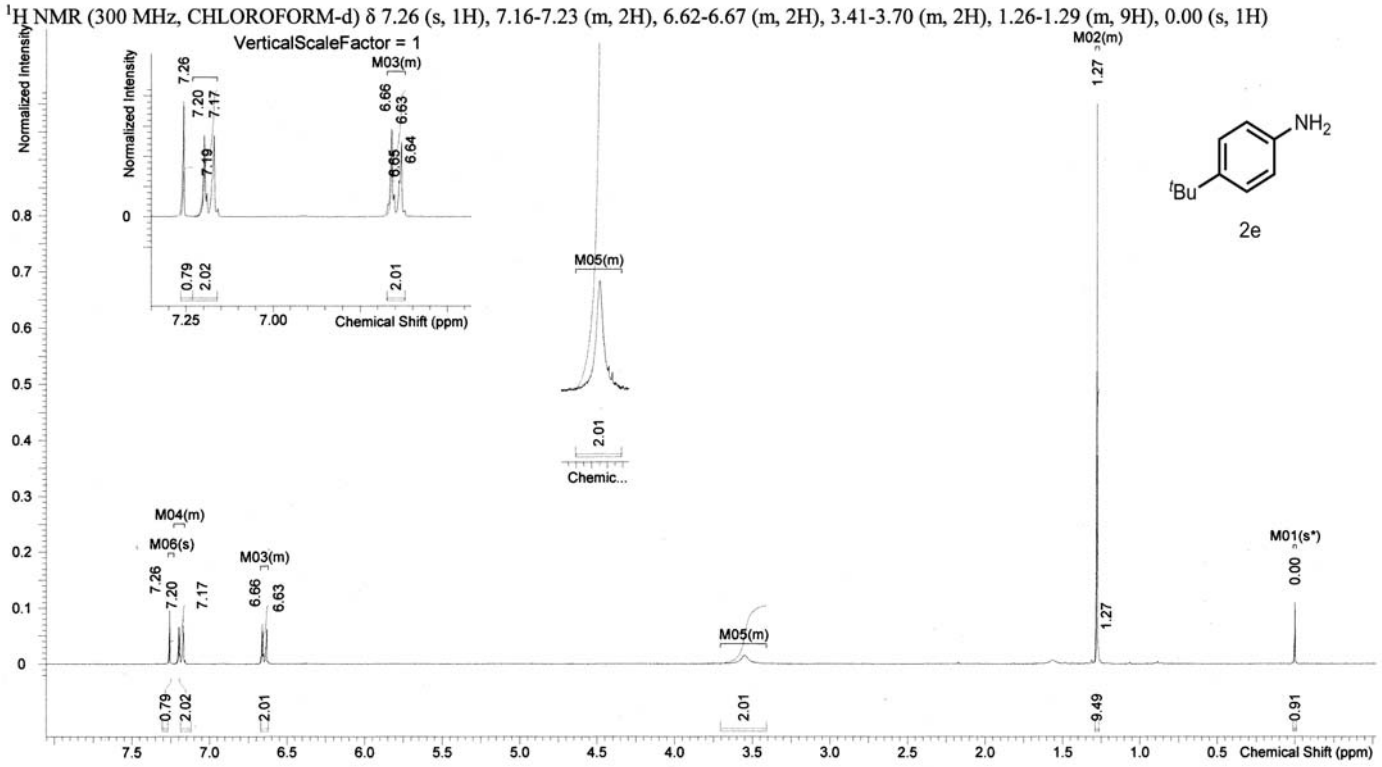
No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3932.14	94.5162	2	3831.86	95.5667	3	3658.3	96.4745	4	3645.77	94.8117
5	3435.56	67.9498	6	3351.68	57.6597	7	3221.5	81.9734	8	3034.44	75.7108
9	2918.73	77.4741	10	2344.05	107.424	11	1914	108.124	12	1729.83	95.0531
13	1622.8	33.0695	14	1493.6	46.5738	15	1469.49	73.3513	16	1375.96	103.791
17	1312.32	81.4915	18	1293.04	60.0609	19	1170.58	73.1441	20	1041.37	105.93
21	996.053	100.948	22	926.628	99.6201	23	871.667	88.9601	24	776.208	40.5837
25	691.355	52.7497	26	551.542	93.3824	27	539.007	86.1698	28	472.474	100.594
29	442.583	75.3542									

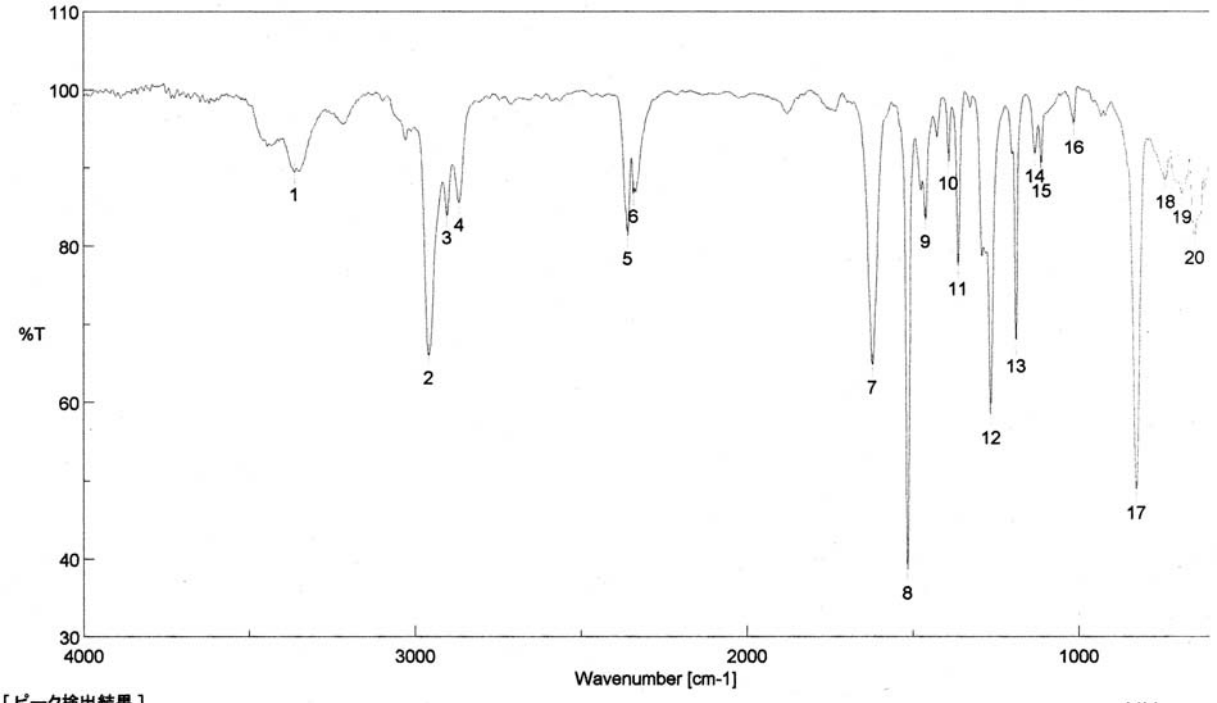


2d

OriginalDateForRelativeTime			Multiplets Integrals Sum	17.24	Number of Nuclei	17 H's	
Acquisition Time (sec)	2.6542	Comment	5 mm QNP 1H/13C/31P/19F Z3333/0001		Date		
Date Stamp			File Name			Frequency (MHz)	300.13
Nucleus	1H	Number of Transients	8	Origin	spect	Original Points Count 16384	Owner DRX300
Points Count	16384	Pulse Sequence	zg30	Receiver Gain	812.70	SW(cyclical) (Hz) 6172.84	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	1846.8896	Spectrum Type	STANDARD	Sweep Width (Hz)	6172.46	Temperature (degree C) 27.000	

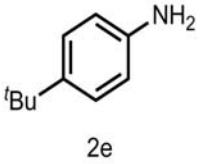
^{1}H NMR (300 MHz, CHLOROFORM-d) δ 7.26 (s, 1H), 7.16-7.23 (m, 2H), 6.62-6.67 (m, 2H), 3.41-3.70 (m, 2H), 1.26-1.29 (m, 9H), 0.00 (s, 1H)



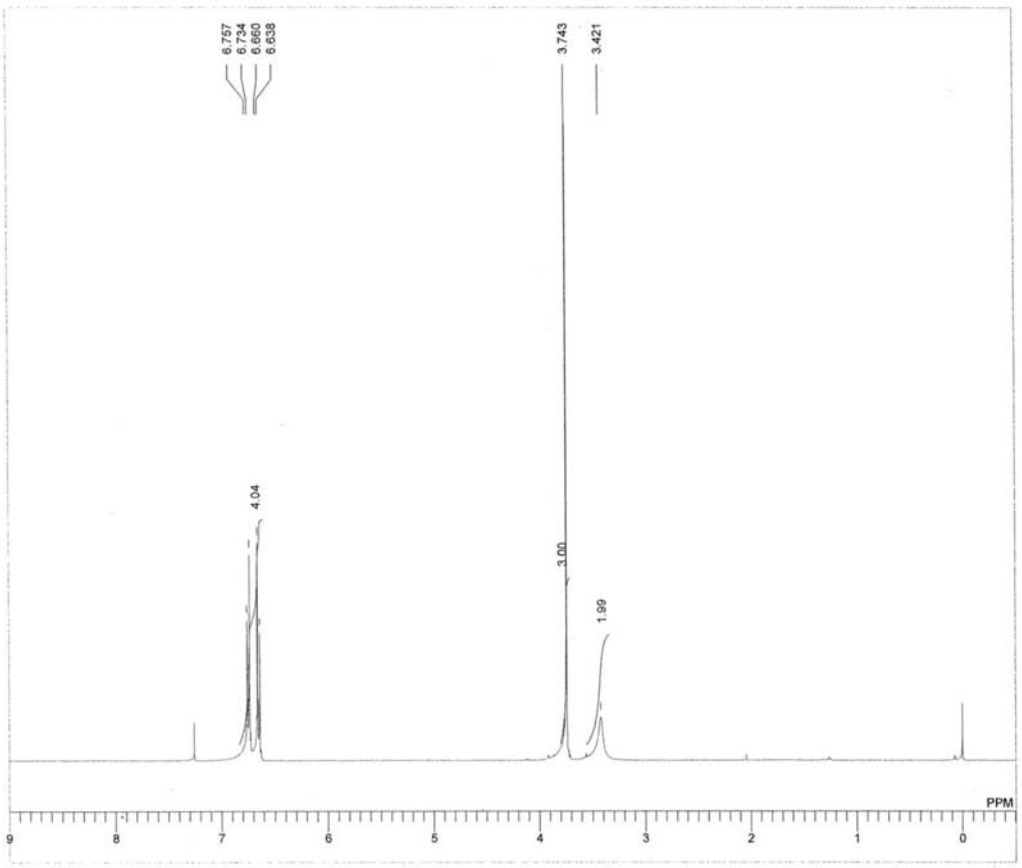


[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3363.25	89.4329	2	2959.23	65.9743	3	2904.27	83.879	4	2867.63	85.5432
5	2359.48	81.2195	6	2341.16	86.6632	7	1621.84	64.7438	8	1515.78	38.4438
9	1461.78	83.4215	10	1392.35	90.877	11	1363.43	77.3727	12	1265.07	58.3835
13	1188.9	67.4997	14	1132.01	91.8014	15	1112.73	89.904	16	1014.37	95.4749
17	826.348	48.7576	18	738.603	88.4815	19	688.463	86.5466	20	649.893	81.3651



2e



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COMNT
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EXMOD NON
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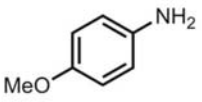
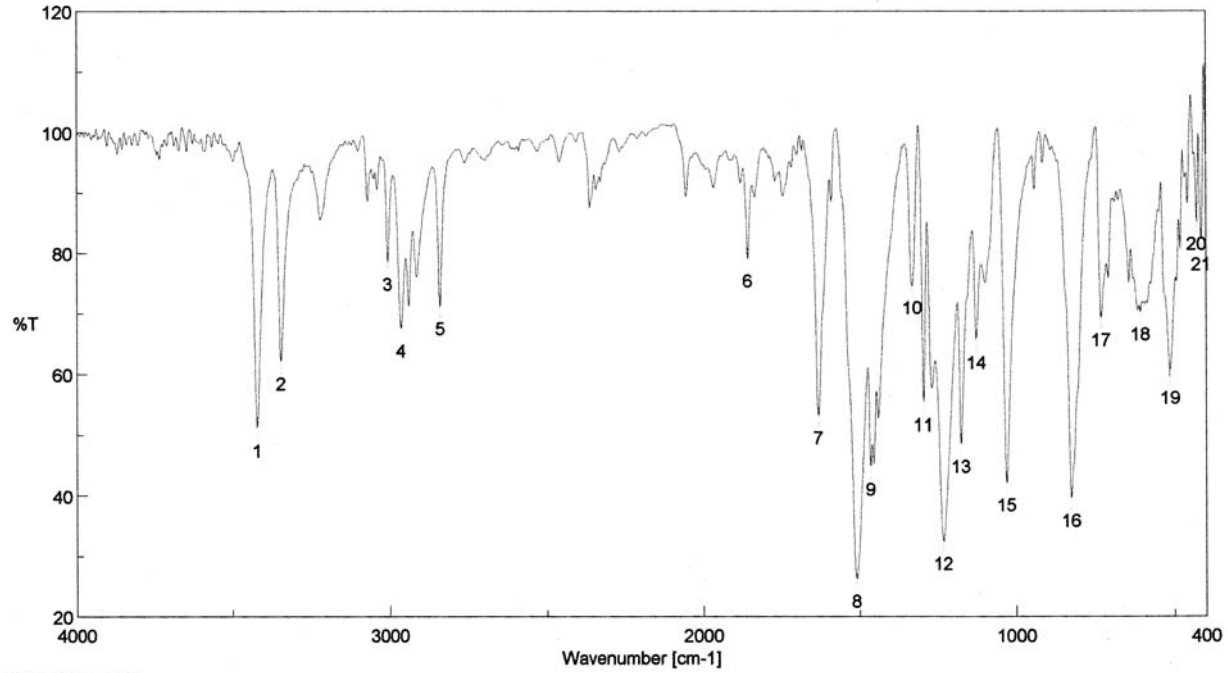
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 20000.00 Hz
SCANS 16
ACQTM 1.6384 sec
PD 2.9010 sec
PW1 6.60 usec
IRNUC 1H
CTEMP 19.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 17

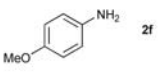


2f

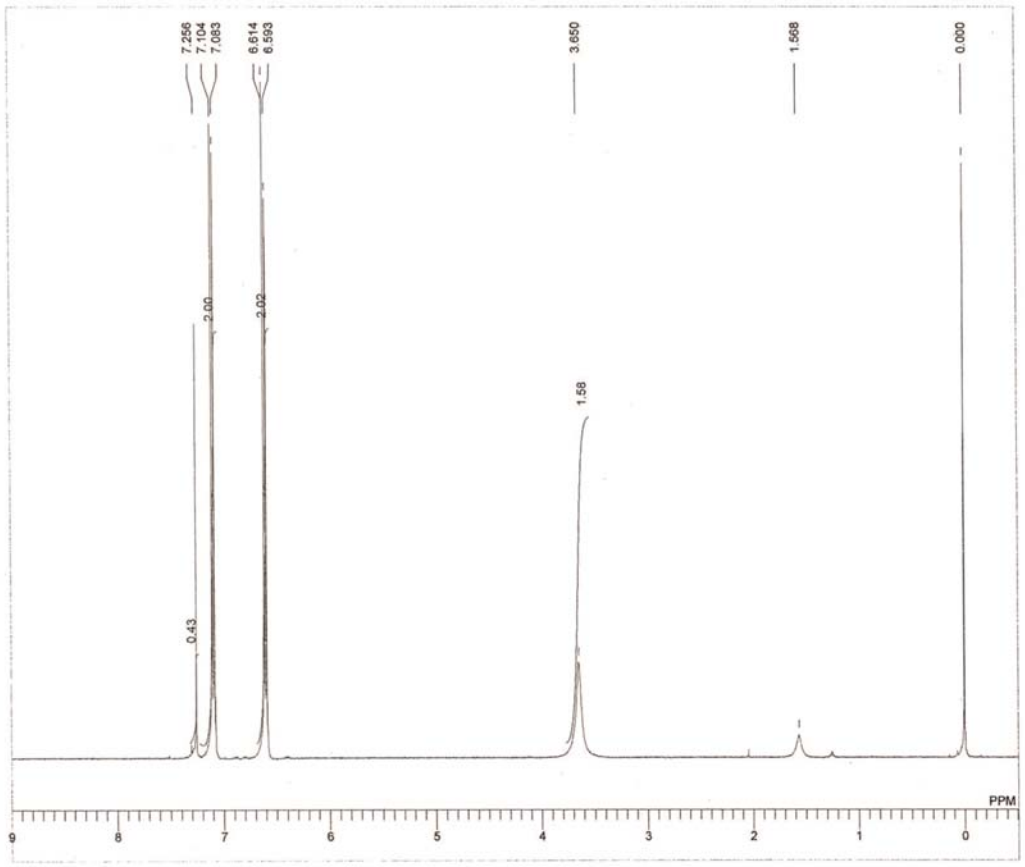


[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3422.06	51.0296	2	3346.85	62.0281	3	3007.44	78.4734	4	2964.05	67.4326
5	2838.7	71.0649	6	1860.01	78.9877	7	1631.48	53.1049	8	1509.03	26.0837
9	1464.67	44.6432	10	1333.53	74.6011	11	1298.82	55.2875	12	1235.18	32.3586
13	1178.29	48.3959	14	1129.12	65.4976	15	1031.73	42.0513	16	826.348	39.4542
17	731.853	69.2203	18	607.467	70.1353	19	513.936	59.627	20	430.048	85.1052
21	414.62	81.6916									



2f

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COMNT
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EXMOD    NON
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OBSET    124.00 KHz
OBFIN    10500.00 Hz
POINT    32768
FREQU    7993.60 Hz
SCANS    8
ACQTM    4.0993 sec
PD       2.9010 sec
PW1      6.60 usec
IRNUC    1H
CTEMP    18.9 c
SLVNT    CDCL3
EXREF    0.00 ppm
BF       0.12 Hz
RGAIN    21
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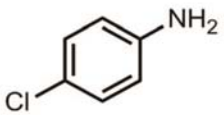
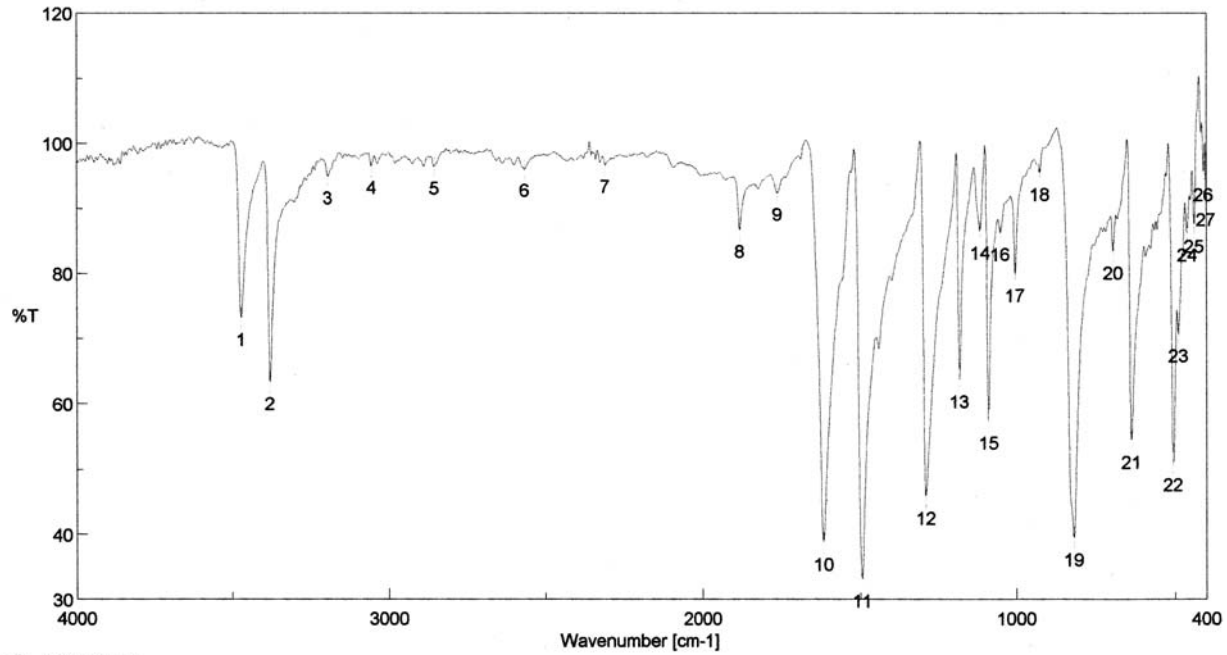
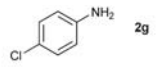


2g

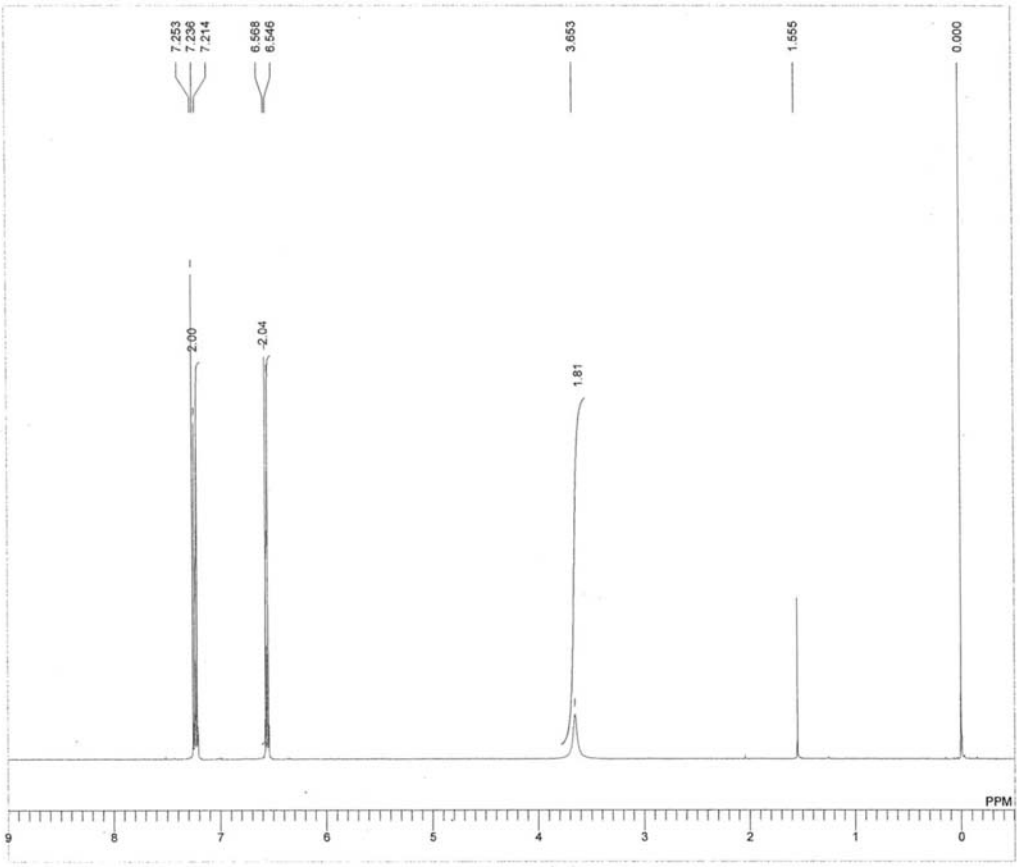


[ピーク検出結果]

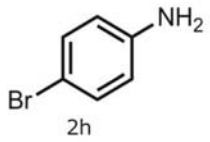
No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3472.2	73.0941	2	3381.57	63.2391	3	3196.43	94.8567	4	3056.62	96.4812
5	2857.99	96.3777	6	2566.79	96.0328	7	2310.3	96.6437	8	1880.26	86.6412
9	1760.69	92.3653	10	1616.06	38.6788	11	1493.6	32.9945	12	1288.22	45.7171
13	1181.19	63.5741	14	1115.62	86.382	15	1088.62	57.3402	16	1051.98	86.1971
17	1004.73	79.8841	18	926.628	95.4334	19	820.563	39.3473	20	697.141	83.3262
21	639.287	54.378	22	506.223	50.8792	23	489.831	70.5788	24	461.868	86.0928
25	439.69	87.3784	26	409.799	95.387	27	401.121	91.5083			



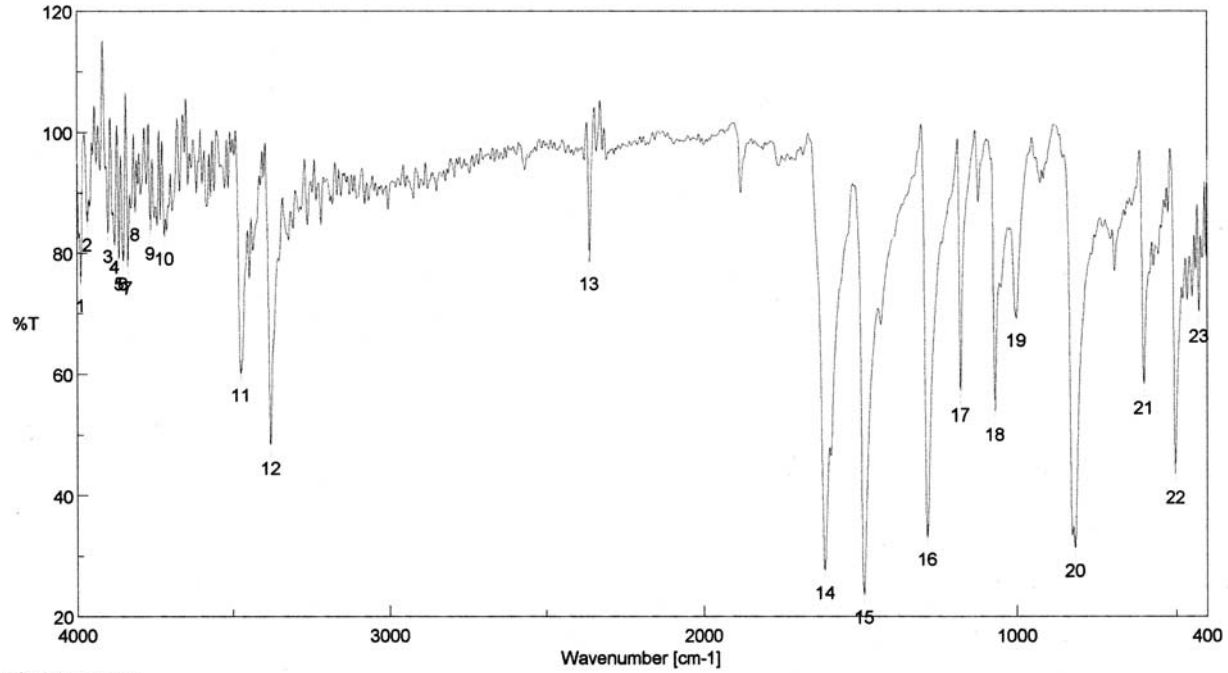
2g



DFILE
COMNT
DATIM
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 7993.60 Hz
SCANS 16
ACQTM 4.0993 sec
PD 2.9010 sec
PW1 6.60 usec
IRNUC 1H
CTEMP 22.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 22

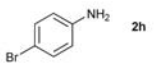


2h

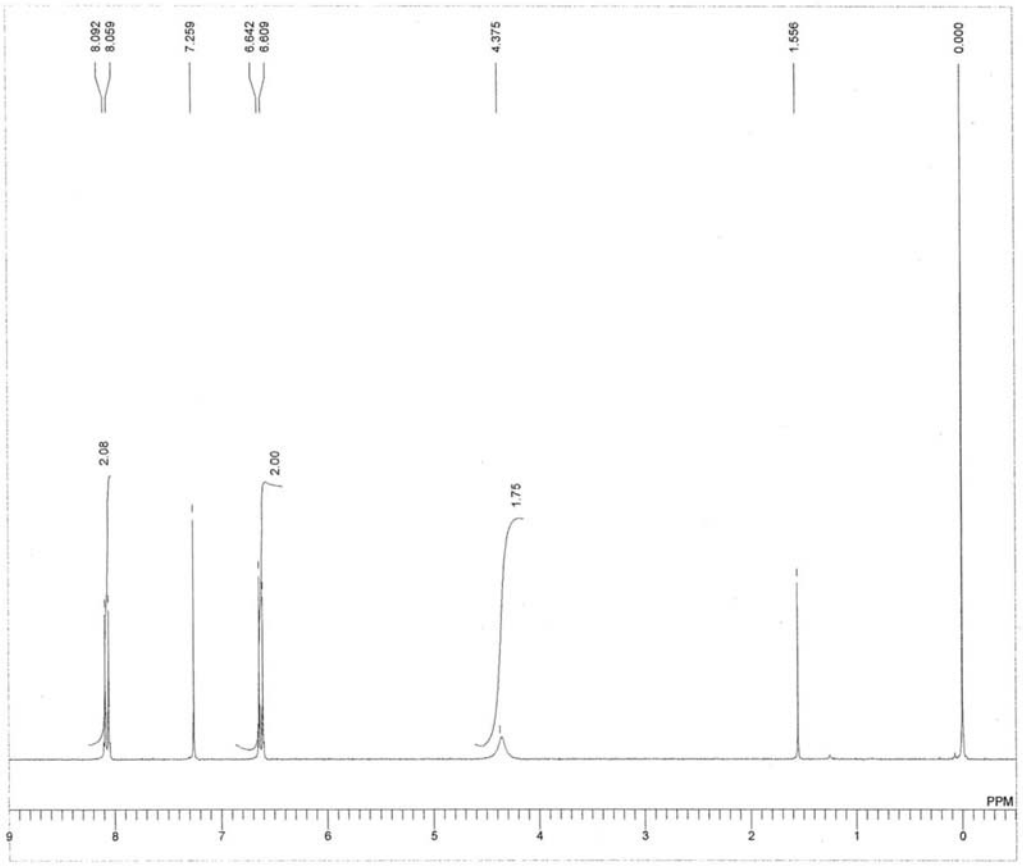


[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3987.11	74.9369	2	3965.89	84.9607	3	3900.32	83.0866	4	3880.08	81.2741
5	3865.61	78.5506	6	3852.11	78.5574	7	3835.72	77.8884	8	3813.54	86.653
9	3764.37	83.534	10	3719.05	82.6721	11	3474.13	60.1095	12	3381.57	48.116
13	2362.37	78.5198	14	1612.2	27.5397	15	1488.78	23.4734	16	1286.29	33.0592
17	1180.22	56.8718	18	1069.33	53.6625	19	1001.84	69.1497	20	817.67	31.1887
21	603.61	57.9939	22	502.366	43.3062	23	426.191	69.8598			



2h

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DATIM
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EXMOD   NON
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OBSET     112.00 KHz
OBFIN     5800.00 Hz
POINT     16384
FREQU     5402.40 Hz
SCANS     8
ACQTM     3.0327 sec
PD        3.9690 sec
PW1       4.90 usec
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CTEMP     19.6 c
SLVNT   CDCL3
EXREF     0.00 ppm
BF        0.12 Hz
RGAIN     25
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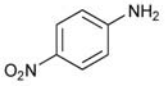
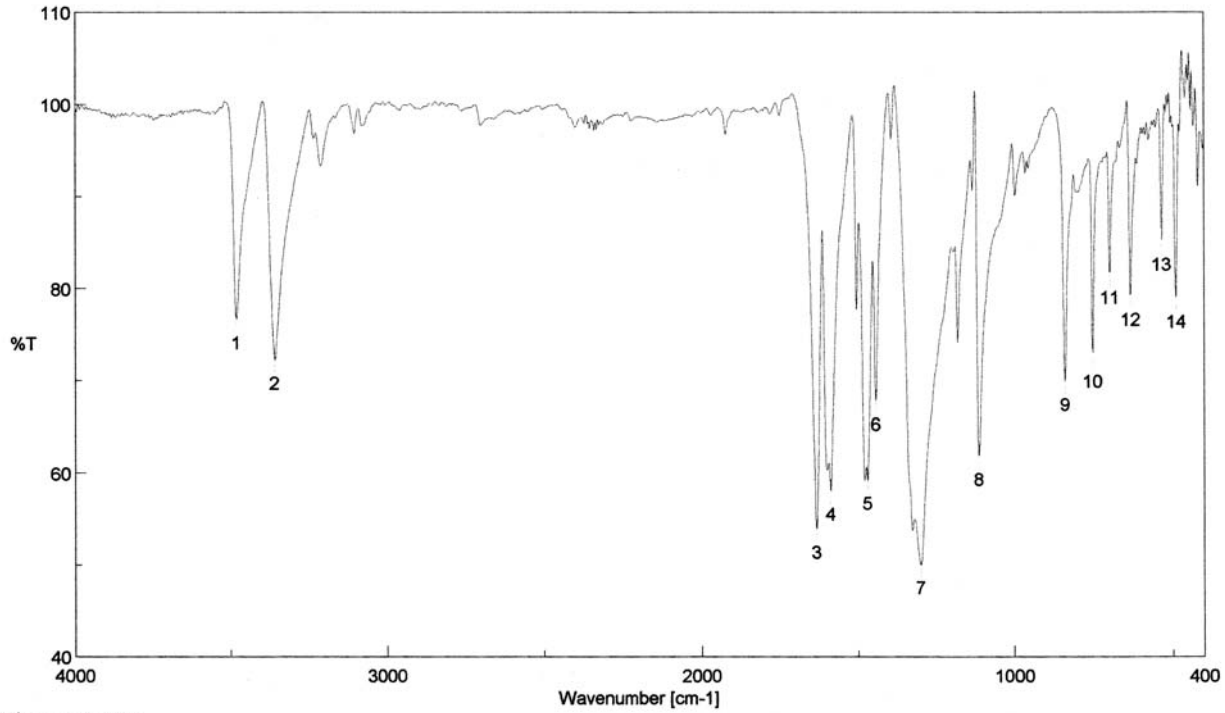
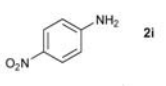


2i



[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3481.85	76.5516	2	3361.32	72.1449	3	1631.48	53.8235	4	1587.13	57.9544
5	1471.42	59.1322	6	1444.42	67.7209	7	1298.82	49.9968	8	1113.69	61.7443
9	839.847	69.8087	10	753.066	72.3376	11	698.105	81.4646	12	632.537	79.0597
13	535.15	85.0621	14	489.831	78.8199						



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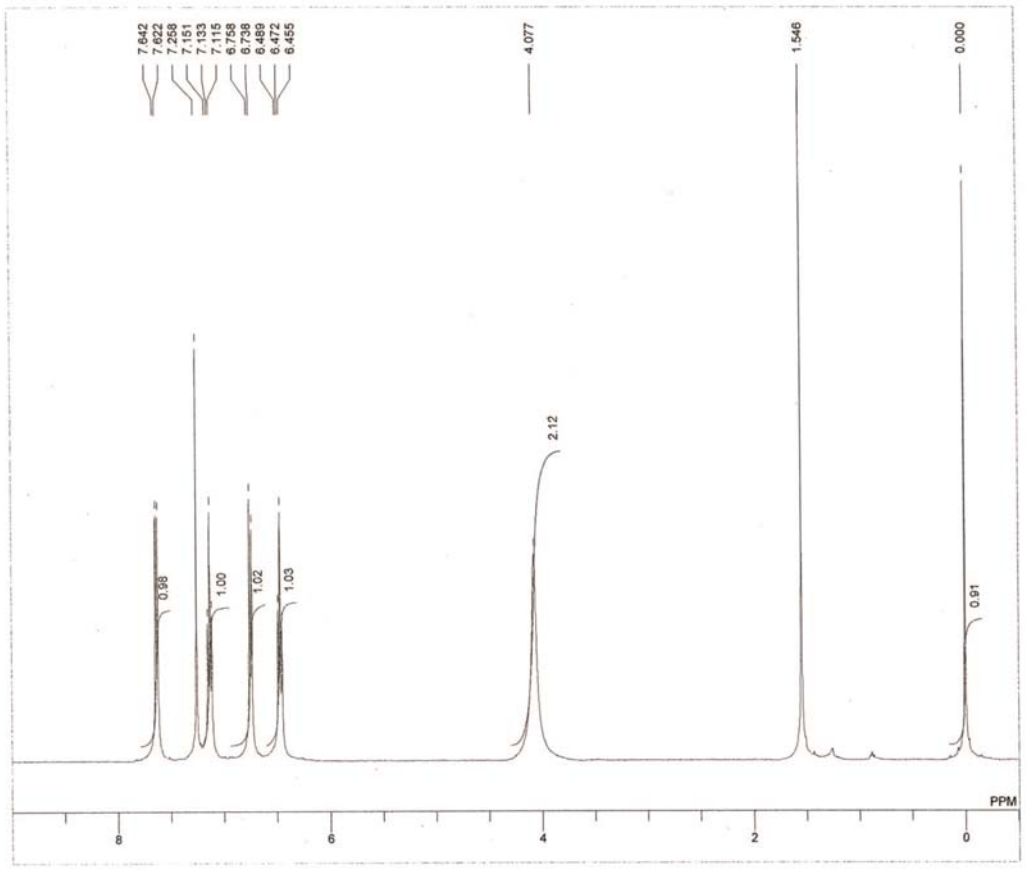

DFILE
COMNT
DATIM
OBNUC 1H
EXMOD NON
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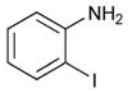
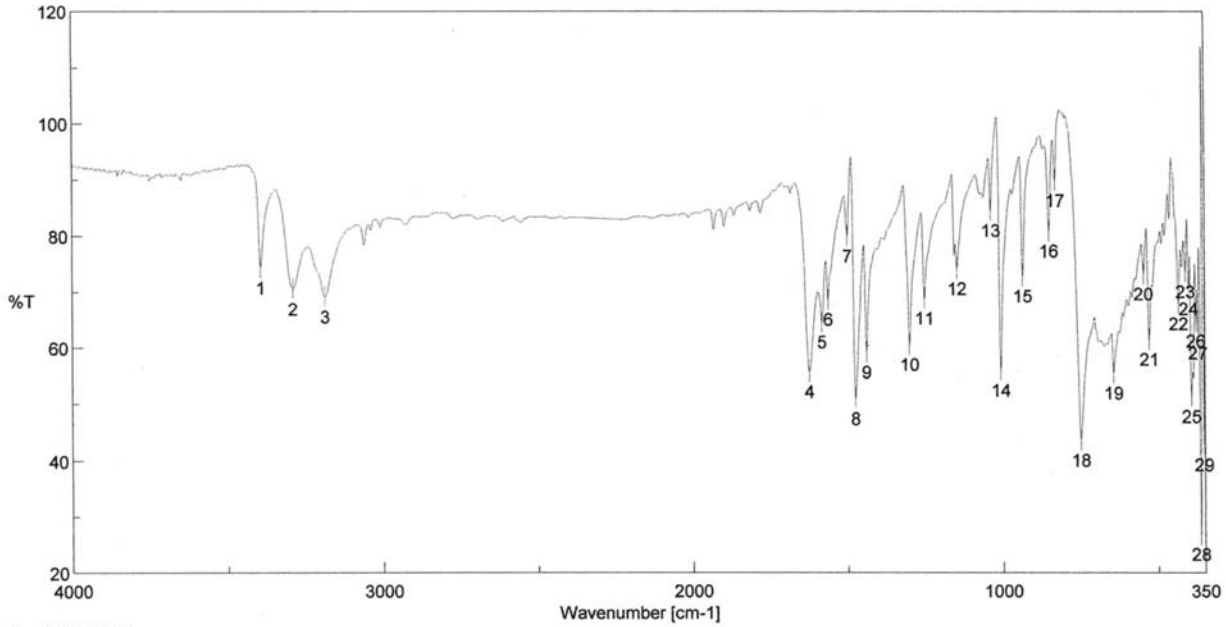
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 7992.01 Hz
SCANS 16
ACQTM 4.1001 sec
PD 2.9000 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 25.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 22

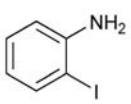


2j

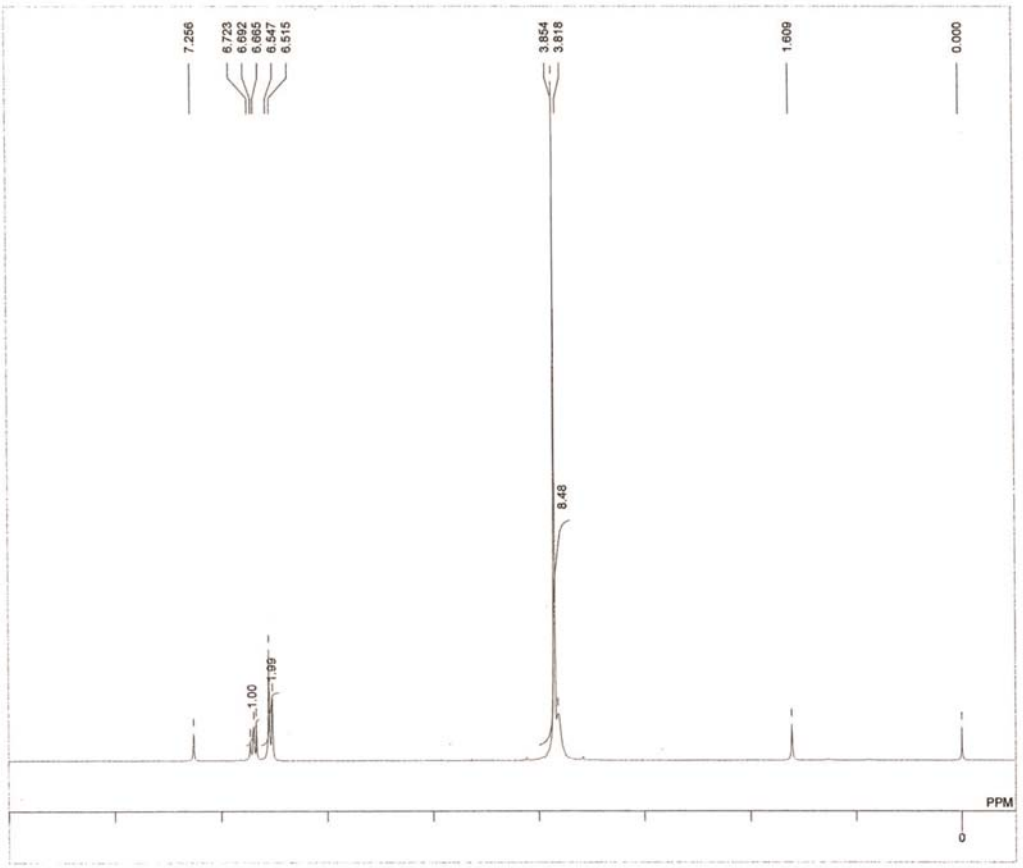


[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3394.1	74.3297	2	3289.96	70.5124	3	3186.79	69.1143	4	1622.8	55.7675
5	1582.31	64.627	6	1562.06	68.666	7	1500.35	80.004	8	1474.31	50.9699
9	1438.64	59.2303	10	1299.79	60.5907	11	1251.58	68.8688	12	1146.47	74.2298
13	1037.52	84.6047	14	1005.7	56.0443	15	935.306	72.8893	16	850.454	80.9308
17	830.205	89.9679	18	749.209	43.716	19	643.144	55.54	20	546.72	73.3225
21	528.4	61.5527	22	433.905	67.9409	23	411.728	73.7206	24	401.121	70.6334
25	392.443	51.4293	26	377.98	64.8487	27	372.194	62.6935	28	363.516	26.9125
29	352.909	42.9453									



2j



DFILE
COMNT
DATIM
OBNUC 1H
EXMOD NON
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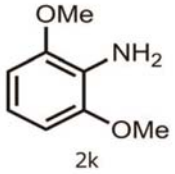
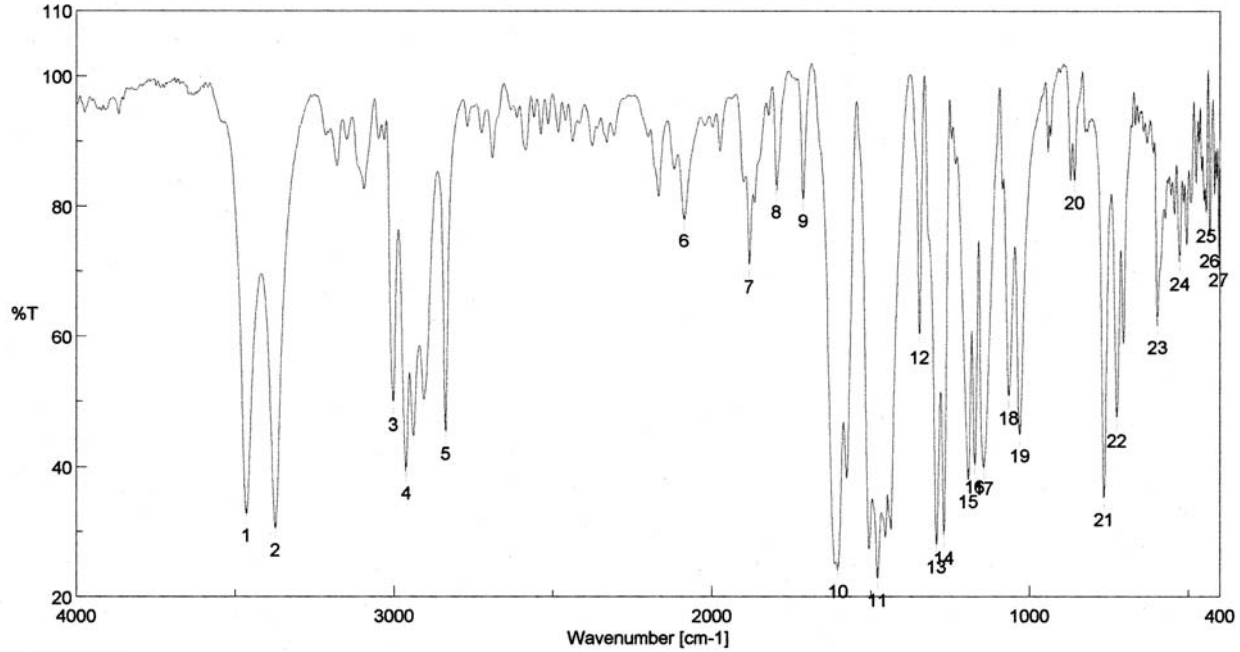
OBSET 112.00 KHz
OBFIN 5800.00 Hz
POINT 16384
FREQU 20000.00 Hz
SCANS 8
ACQTM 0.8192 sec
PD 3.9690 sec
PW1 4.90 usec
IRNUC 1H
CTEMP 18.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 17

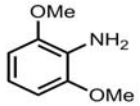


2k

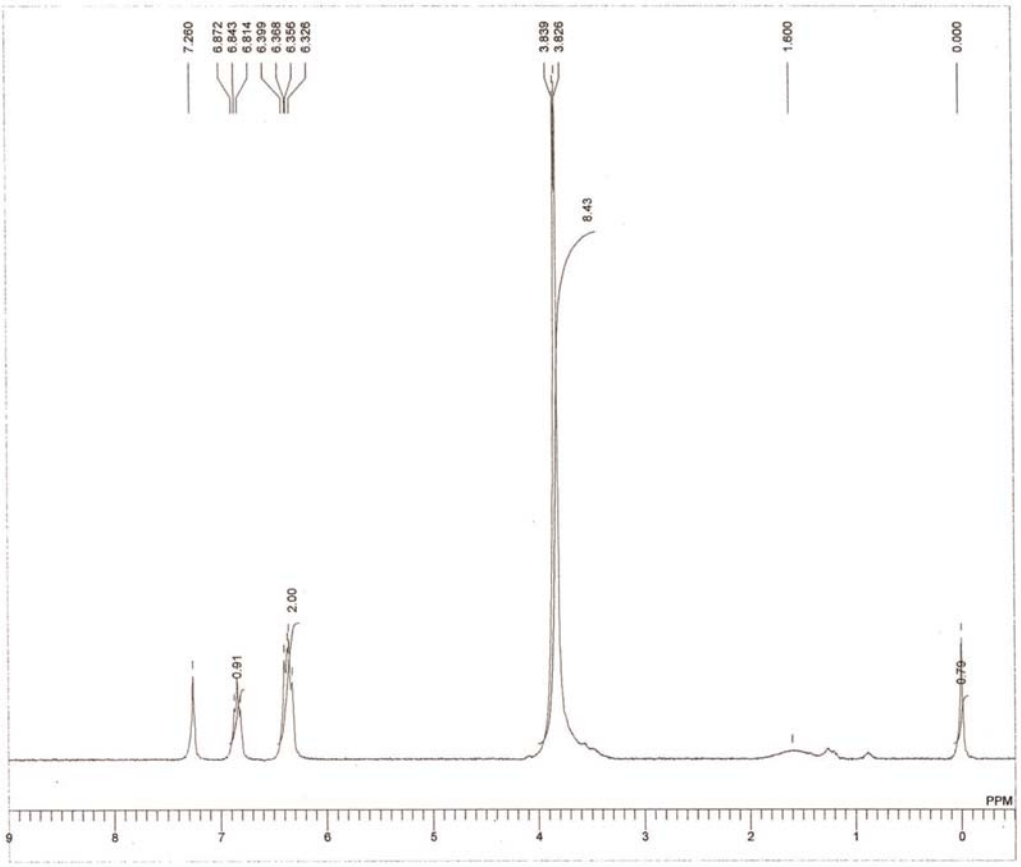


[ピーク検出結果]

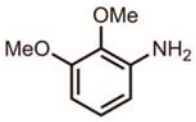
No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3463.53	32.7179	2	3372.89	30.4886	3	3001.66	49.7546	4	2962.13	39.2274
5	2837.74	45.2782	6	2086.6	77.9663	7	1881.22	70.8917	8	1796.37	82.3939
9	1712.48	81.0267	10	1602.56	24.1031	11	1478.17	22.7415	12	1346.07	60.0176
13	1293.04	27.9212	14	1269.9	29.2012	15	1192.76	37.9361	16	1172.51	40.1886
17	1143.58	39.9489	18	1065.48	50.7345	19	1030.77	44.9423	20	858.168	83.8154
21	765.601	35.11	22	725.104	47.2772	23	596.861	61.5526	24	527.436	71.3206
25	443.547	78.7259	26	431.977	74.8735	27	403.05	71.967			



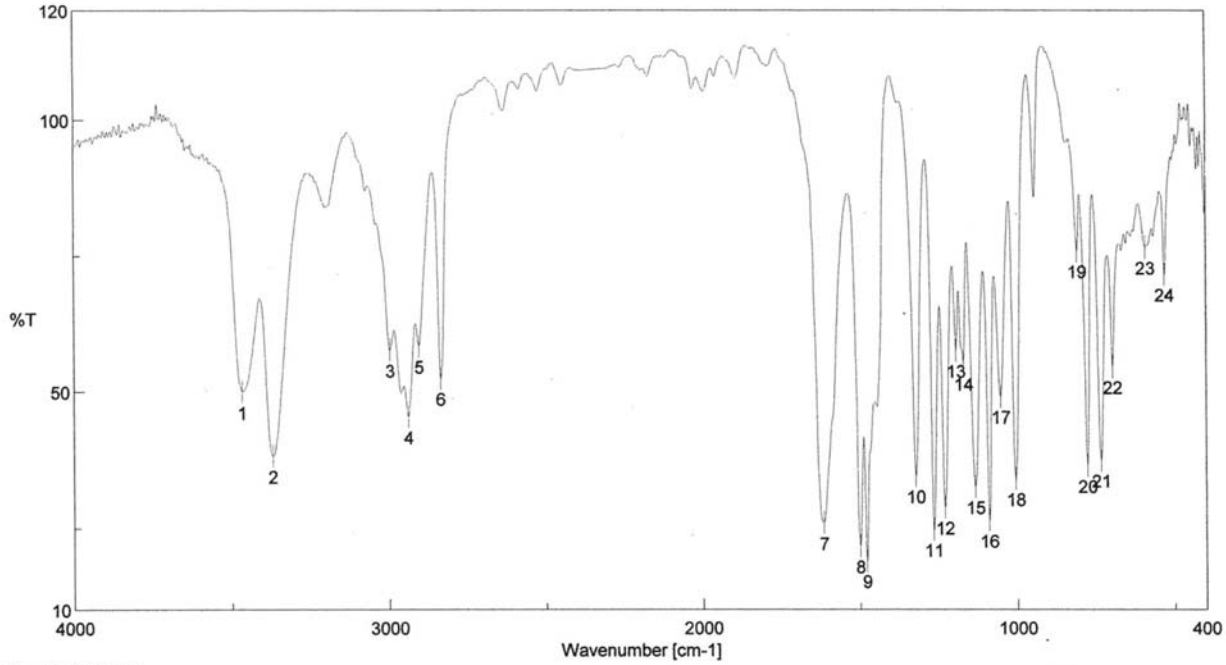
2k



DFILE
COMNT
DATIM
OBNUC 1H
EXMOD NON
OBFRQ 270.05 MHz
OBSET 112.00 KHz
OBFIN 5800.00 Hz
POINT 16384
FREQU 5405.40 Hz
SCANS 16
ACQTM 3.0310 sec
PD 3.9690 sec
PW1 4.90 usec
IRNUC 1H
CTEMP 25.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 21

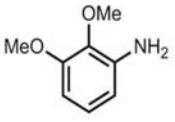


2l



[ピーク検出結果]

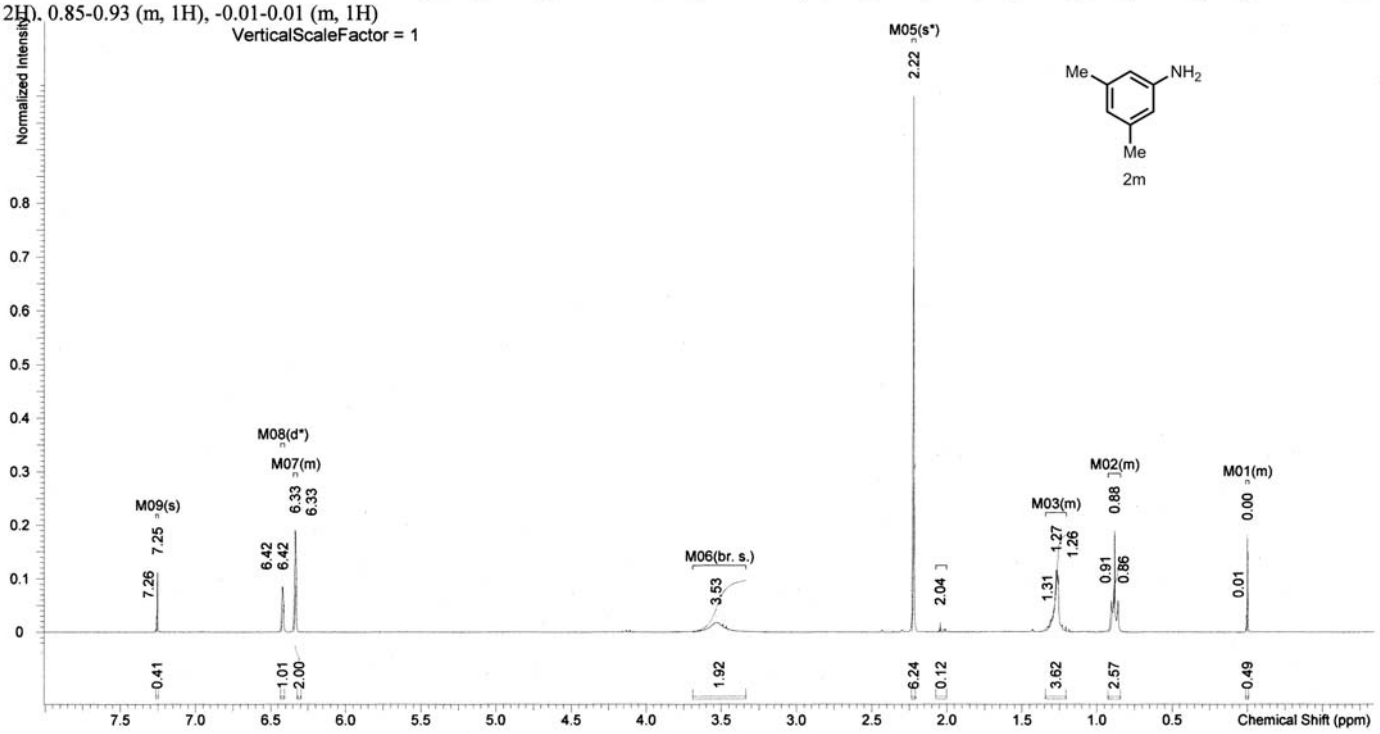
No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3466.42	49.9528	2	3369.03	38.2687	3	2996.84	57.6241	4	2938.02	45.4675
5	2904.27	58.345	6	2834.85	52.4518	7	1615.09	25.9899	8	1499.38	21.6967
9	1478.17	19.0293	10	1321.96	34.5881	11	1265.07	24.7881	12	1229.4	28.8141
13	1193.72	57.5567	14	1169.62	55.1904	15	1132.97	32.6068	16	1088.62	26.4565
17	1051.98	49.1432	18	1004.73	34.054	19	808.028	75.8872	20	776.208	36.493
21	732.817	37.4996	22	696.177	54.5843	23	591.075	76.5502	24	530.328	71.5848

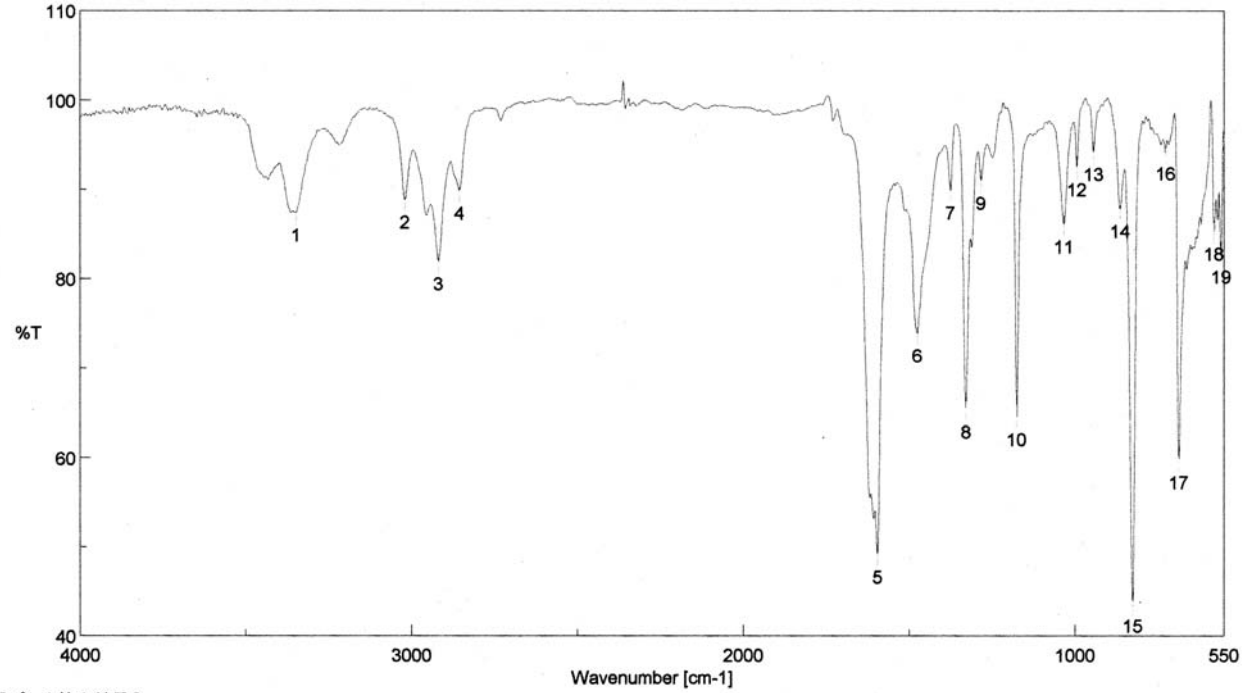


2l

OriginalDateForRelativeTime				Multiplets Integrals Sum	18.37	Number of Nuclei	12 H's		
Acquisition Time (sec)	2.6542	Comment	5 mm QNP 1H/13C/31P/19F Z3333/0001	Date					
Date Stamp		File Name						Frequency (MHz)	300.13
Nucleus	1H	Number of Transients	8	Origin	spect	Original Points Count	16384	Owner	DRX300
Points Count	16384	Pulse Sequence	zg30	Receiver Gain	512.00	SW(cyclical) (Hz)	6172.84	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	1845.7345	Spectrum Type	STANDARD	Sweep Width (Hz)	6172.46	Temperature (degree C)	27.000		

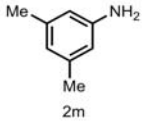
^{1}H NMR (300 MHz, CHLOROFORM-d) δ 7.26 (s, 1H), 6.42 (d, *J*=2.59 Hz, 1H), 6.32-6.35 (m, 1H), 3.53 (br. s., 1H), 2.22 (s, 3H), 2.04 (s, 1H), 1.21-1.34 (m, 2H), 0.85-0.93 (m, 1H), -0.01-0.01 (m, 1H)





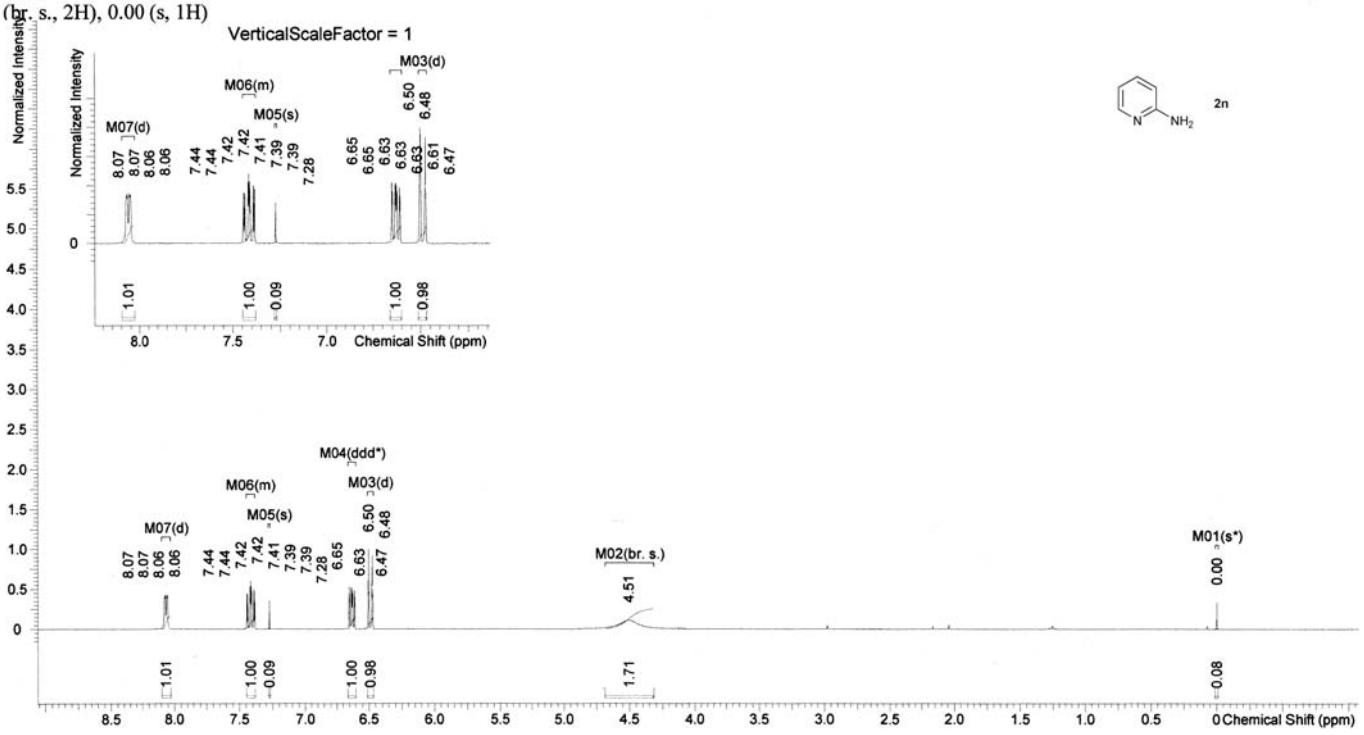
[ピーク検出結果]

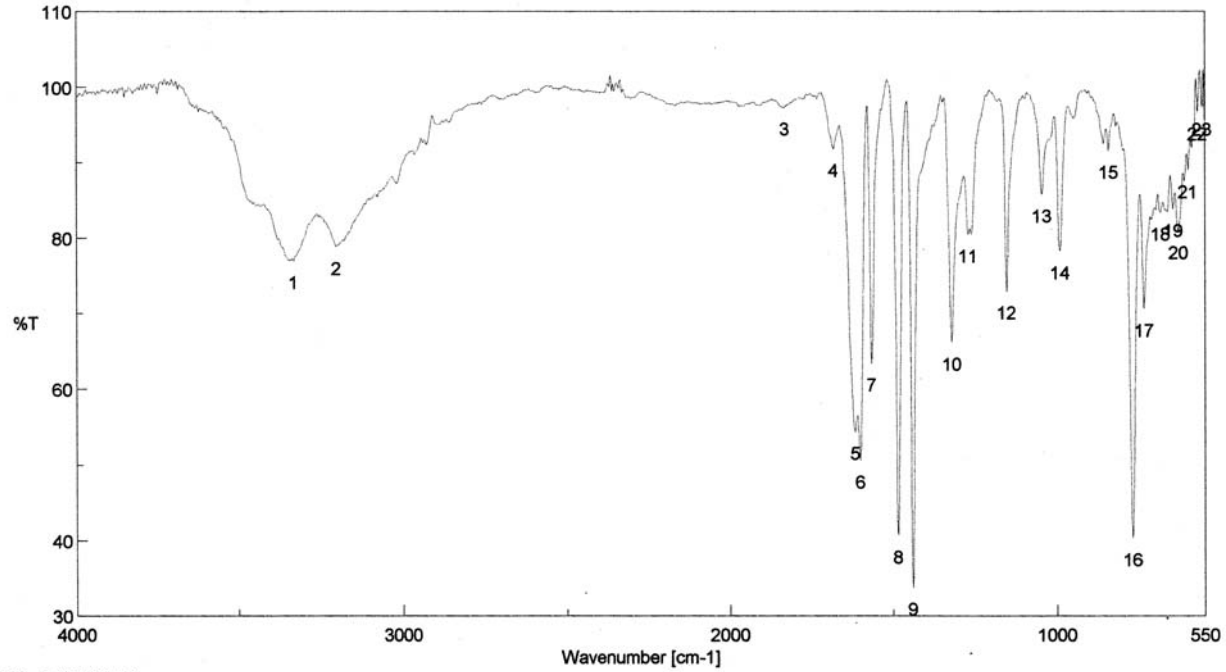
No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3348.78	87.3624	2	3019.98	88.8145	3	2918.73	81.8753	4	2856.06	89.8292
5	1594.84	49.1031	6	1475.28	73.8326	7	1375	89.8354	8	1328.71	65.3467
9	1283.39	90.9307	10	1175.4	64.4952	11	1033.66	86.0509	12	994.125	92.4405
13	943.985	94.1965	14	863.953	87.8213	15	825.384	43.6192	16	727.032	94.2381
17	686.534	59.7243	18	580.469	85.2361	19	559.255	82.6797			



OriginalDateForRelativeTime				Multiplets Integrals Sum	5.88	Number of Nuclei	8 H's
Acquisition Time (sec)	2.6542	Comment	5 mm QNP 1H/13C/31P/19F Z3333/0001	Date			
Date Stamp				File Name		Frequency (MHz)	300.13
Nucleus	1H	Number of Transients	8	Origin	spect	Original Points Count	16384	Owner	DRX300
Points Count	16384	Pulse Sequence	zg30	Receiver Gain	406.40	SW(cyclical) (Hz)	6172.84	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	1852.1483	Spectrum Type	STANDARD	Sweep Width (Hz)	6172.46	Temperature (degree C)	27.000		

^{1}H NMR (300 MHz, CHLOROFORM-d) δ 8.06 (d, *J*=5.02 Hz, 1H), 7.38-7.45 (m, 1H), 7.28 (s, 1H), 6.63 (t, *J*=6.20 Hz, 1H), 6.49 (d, *J*=8.36 Hz, 1H), 4.51 (br. s., 2H), 0.00 (s, 1H)



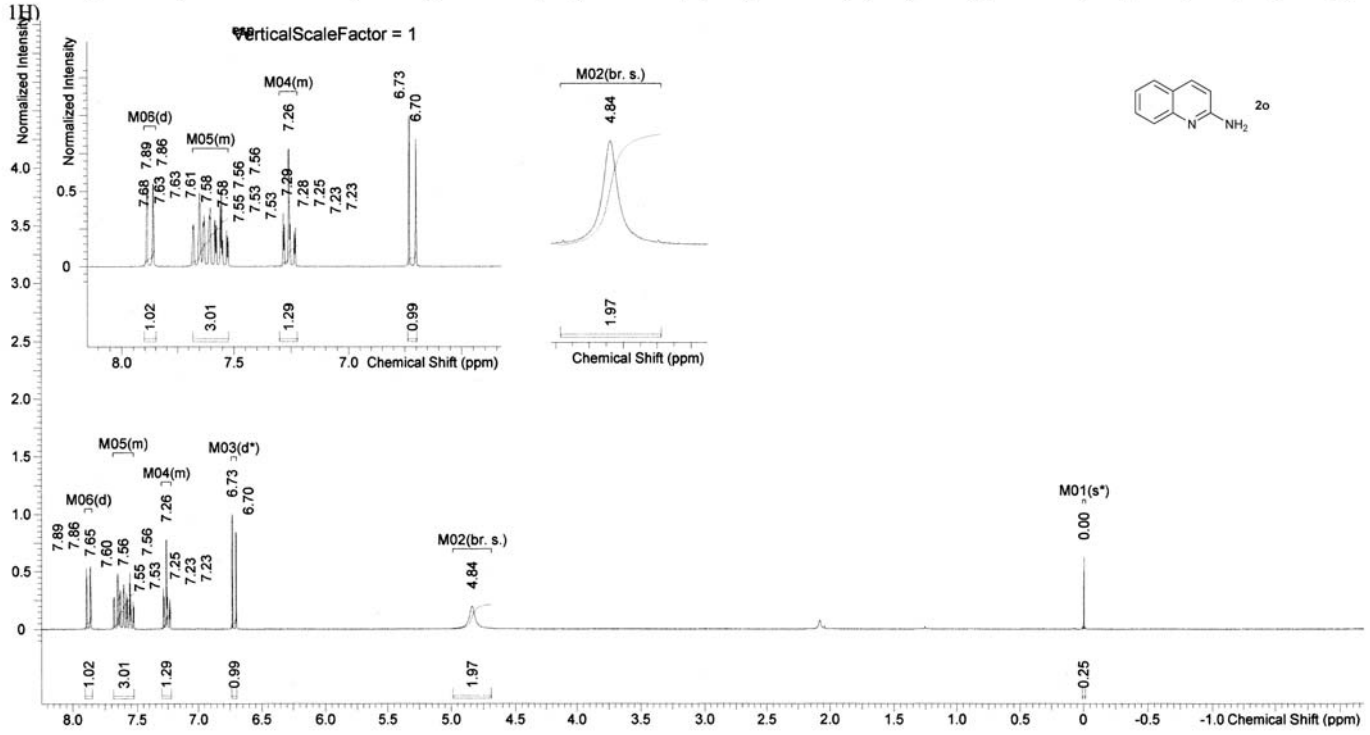


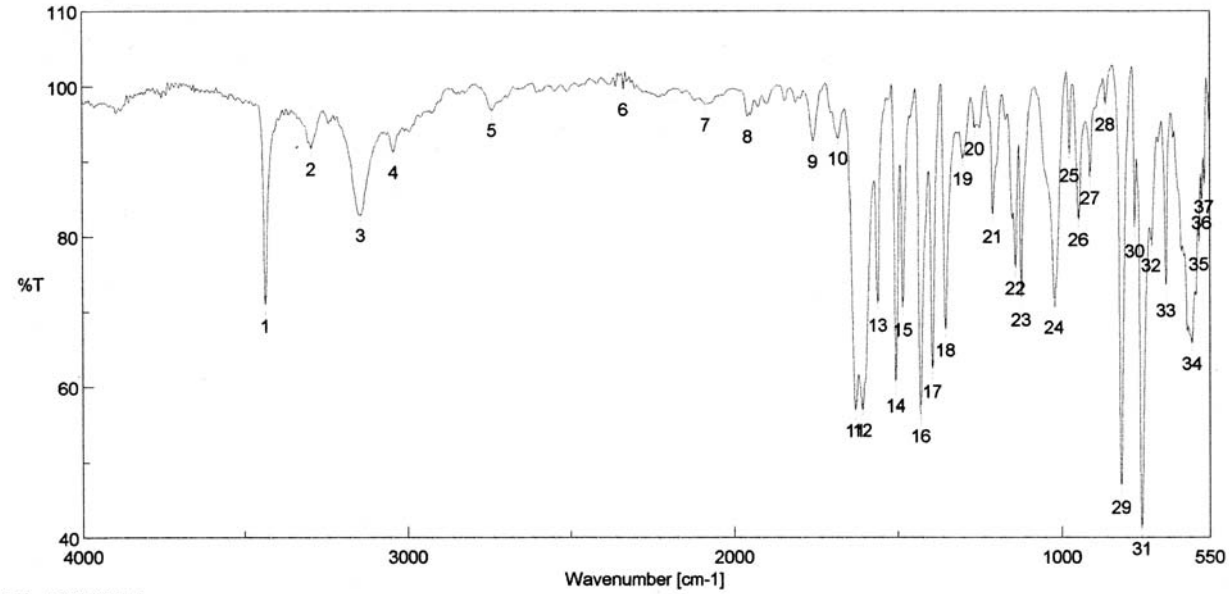
[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3334.32	76.955	2	3206.08	78.8399	3	1832.04	97.2689	4	1682.59	91.7837
5	1617.02	54.3847	6	1600.63	50.6165	7	1565.92	63.4152	8	1484.92	40.6672
9	1440.56	33.7796	10	1321.96	66.1516	11	1270.86	80.4529	12	1152.26	72.9588
13	1046.19	85.7746	14	991.232	78.2648	15	845.633	91.5386	16	770.423	40.3159
17	736.674	70.5986	18	686.534	83.3473	19	647.965	83.8242	20	631.573	80.9006
21	601.682	88.966	22	572.755	96.6353	23	559.255	97.2213			

OriginalDateForRelativeTime			Multiplets Integrals Sum	8.53	Number of Nuclei	9 H's	
Acquisition Time (sec)	2.6542	Comment	5 mm QNP 1H/13C/31P/19F Z3333/0001		Date		
Date Stamp			File Name			Frequency (MHz)	300.13
Nucleus	1H	Number of Transients	8	Origin	spect	Original Points Count 16384	Owner DRX300
Points Count	16384	Pulse Sequence	zg30	Receiver Gain	724.10	SW(cyclical) (Hz) 6172.84	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	1847.5984	Spectrum Type	STANDARD	Sweep Width (Hz)	6172.46	Temperature (degree C) 27.000	

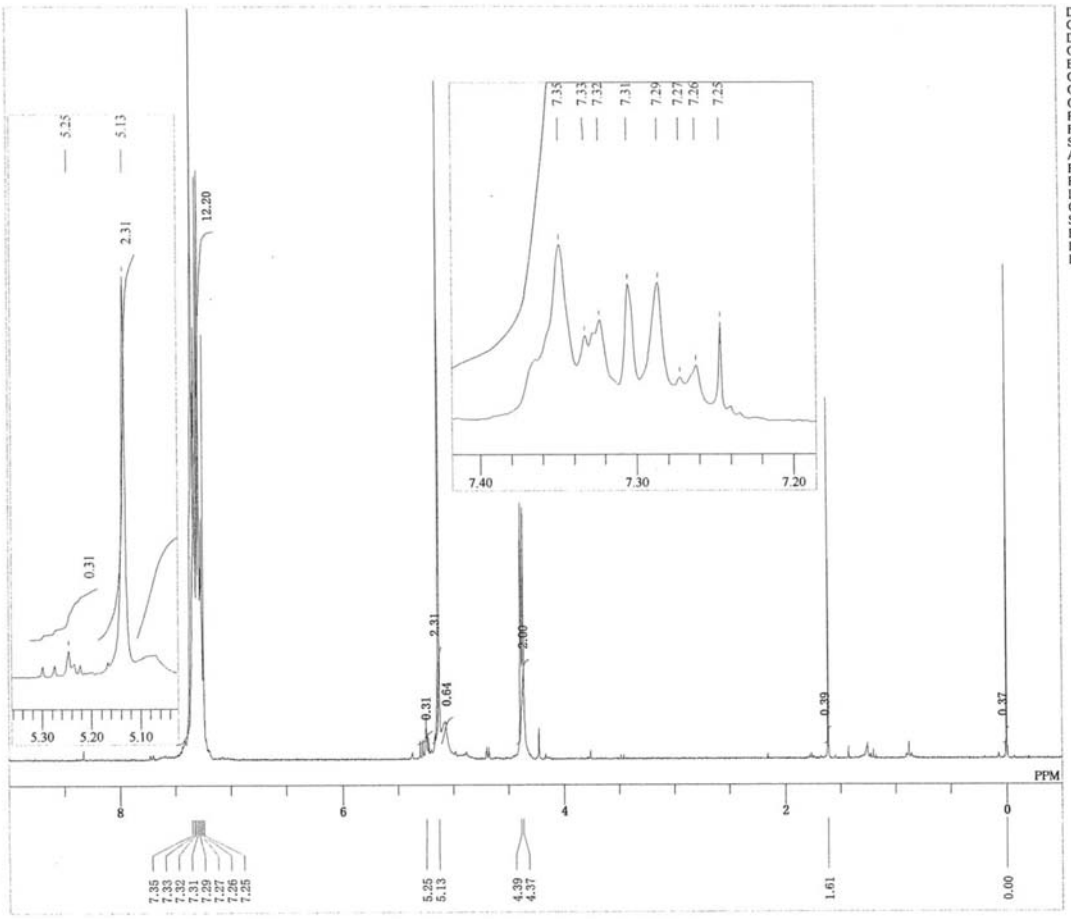
^{1}H NMR (300 MHz, CHLOROFORM-d) δ 7.88 (d, *J*=8.67 Hz, 1H), 7.53-7.68 (m, 3H), 7.22-7.30 (m, 1H), 6.72 (d, *J*=8.77 Hz, 1H), 4.84 (br. s., 2H), 0.00 (s, 1H)

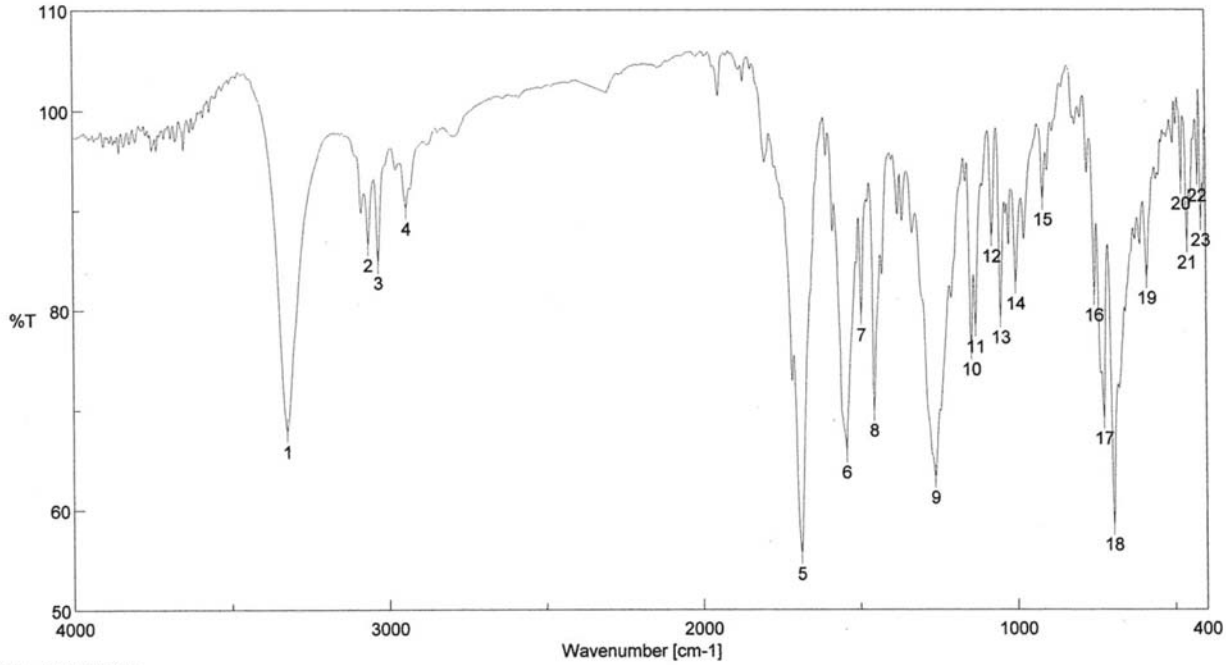




[ピーク検出結果]

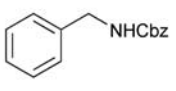
No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3436.53	70.8015	2	3294.79	91.6811	3	3144.37	82.8155	4	3043.12	91.2346
5	2744.21	96.7703	6	2340.19	99.5819	7	2086.6	97.5729	8	1958.36	95.9646
9	1758.76	92.6656	10	1684.52	93.0821	11	1632.45	56.946	12	1611.23	56.9722
13	1563.02	70.8558	14	1506.13	60.1991	15	1483.96	70.2602	16	1428.99	56.2392
17	1393.32	62.0569	18	1352.82	67.5667	19	1300.75	90.3444	20	1264.11	94.3618
21	1209.15	82.7112	22	1141.65	75.8065	23	1123.33	71.5859	24	1023.05	70.6061
25	975.804	90.7953	26	948.806	82.2573	27	915.058	87.7996	28	868.774	97.5998
29	819.598	46.7159	30	779.101	80.7747	31	756.923	41.2169	32	727.996	78.8571
33	683.642	72.8231	34	603.61	65.7506	35	582.397	78.972	36	573.719	84.4915
37	566.005	86.6357									

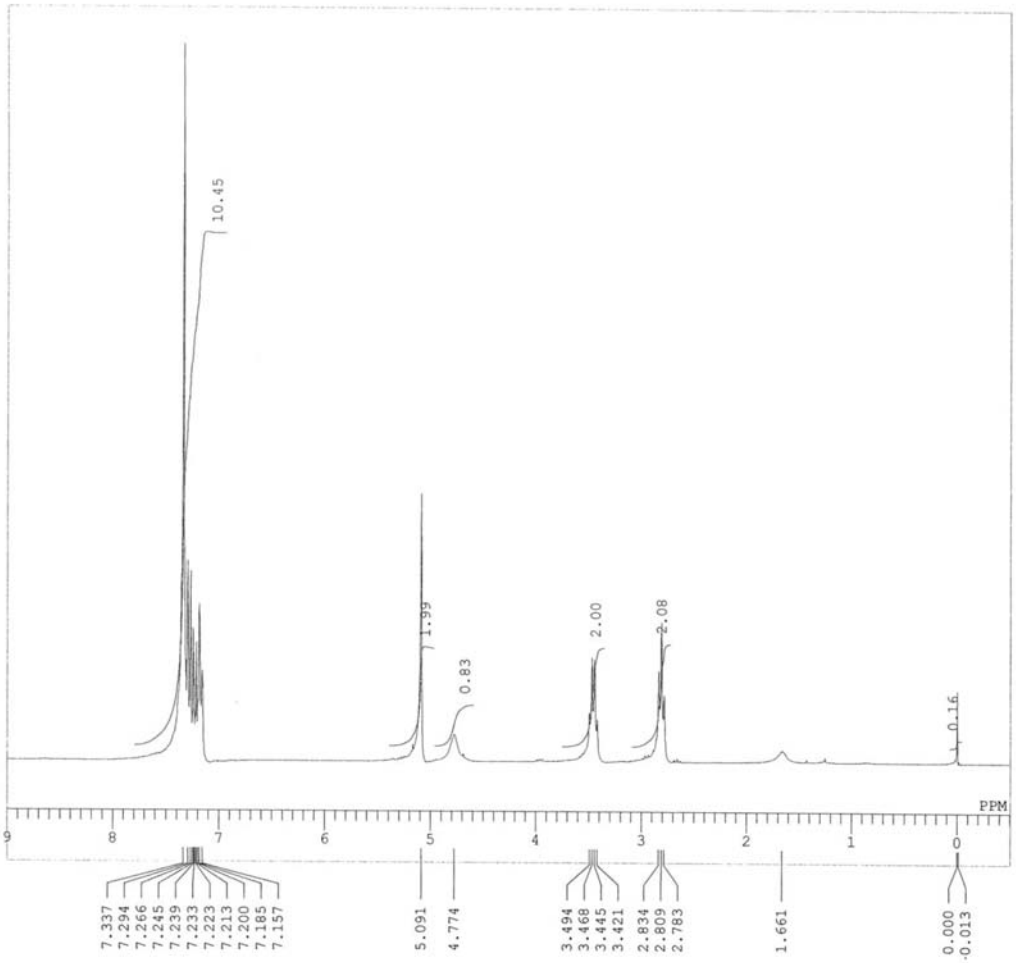


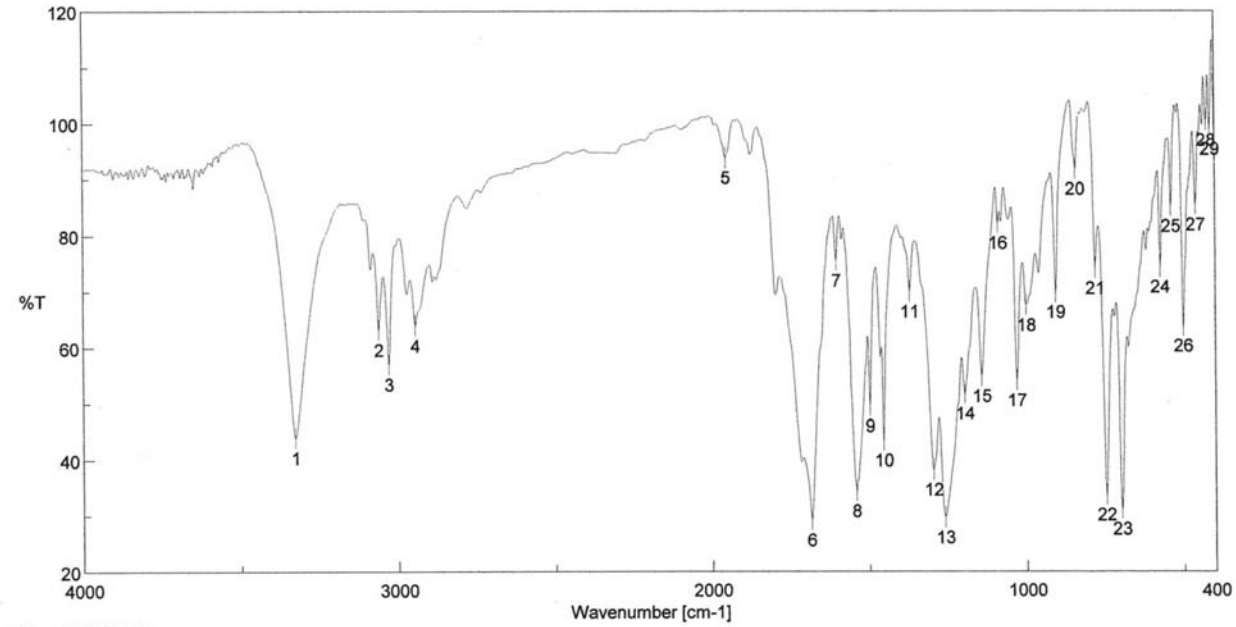


[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3322.75	67.9566	2	3063.37	86.6346	3	3031.55	84.8511	4	2942.84	90.2763
5	1686.44	55.7177	6	1541.81	65.8905	7	1494.56	79.5992	8	1454.06	70.086
9	1260.25	63.3521	10	1144.55	76.1743	11	1131.05	78.4517	12	1078.98	87.502
13	1051.01	79.3685	14	1002.8	82.7643	15	916.022	91.1786	16	754.031	81.6057
17	724.139	69.3037	18	694.248	58.6254	19	587.218	83.326	20	477.296	92.7709
21	458.975	86.8862	22	425.227	93.5526	23	414.62	89.1271			

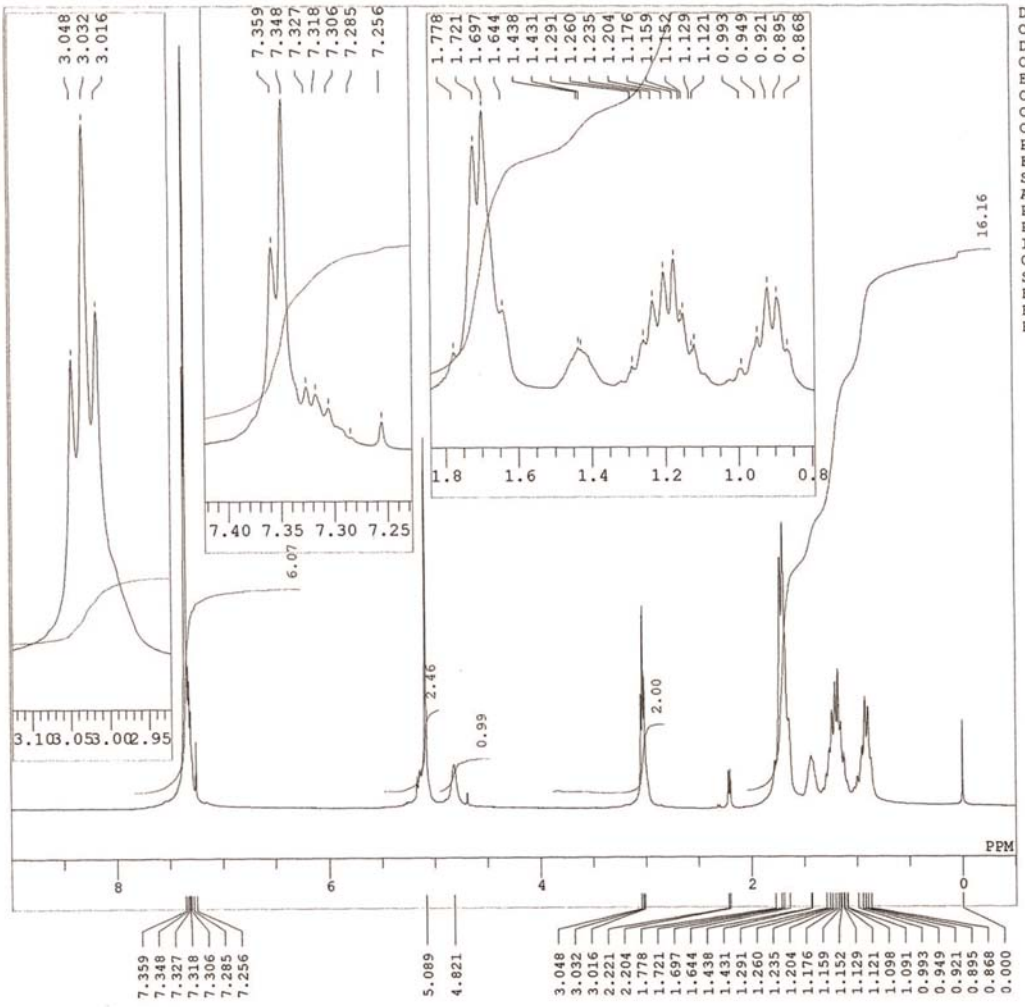






[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3327.57	43.9368	2	3061.44	63.1884	3	3029.62	56.9831	4	2945.73	63.9484
5	1954.5	93.8646	6	1683.55	29.2109	7	1603.52	75.5631	8	1540.85	34.3797
9	1497.45	49.5781	10	1454.06	43.4455	11	1370.18	70.0313	12	1295.93	38.2616
13	1259.29	29.7141	14	1195.65	51.7695	15	1141.65	54.8993	16	1088.62	82.2412
17	1029.8	54.1595	18	999.91	67.583	19	905.415	69.9252	20	842.74	91.8878
21	780.065	74.2058	22	746.317	33.7603	23	697.141	31.228	24	573.719	74.4825
25	539.007	85.2853	26	500.437	63.8875	27	460.904	85.5646	28	426.191	100.573
29	414.62	99.0097									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DATIM
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EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 7992.01 Hz
SCANS 16
ACQTM 4.1001 sec
PD 2.9000 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 22.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.00 Hz
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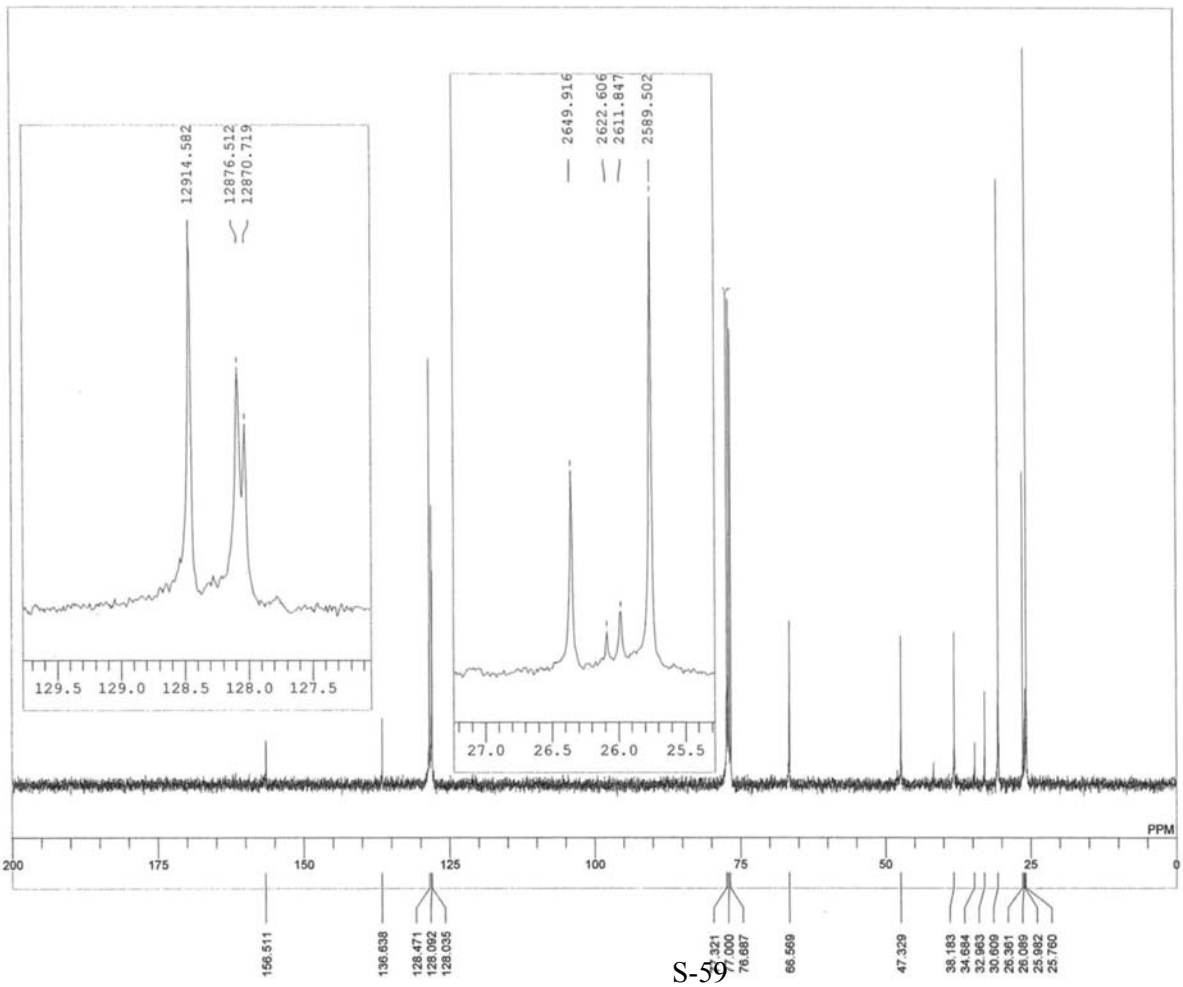
NHCbz
2r
PPM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DATIM
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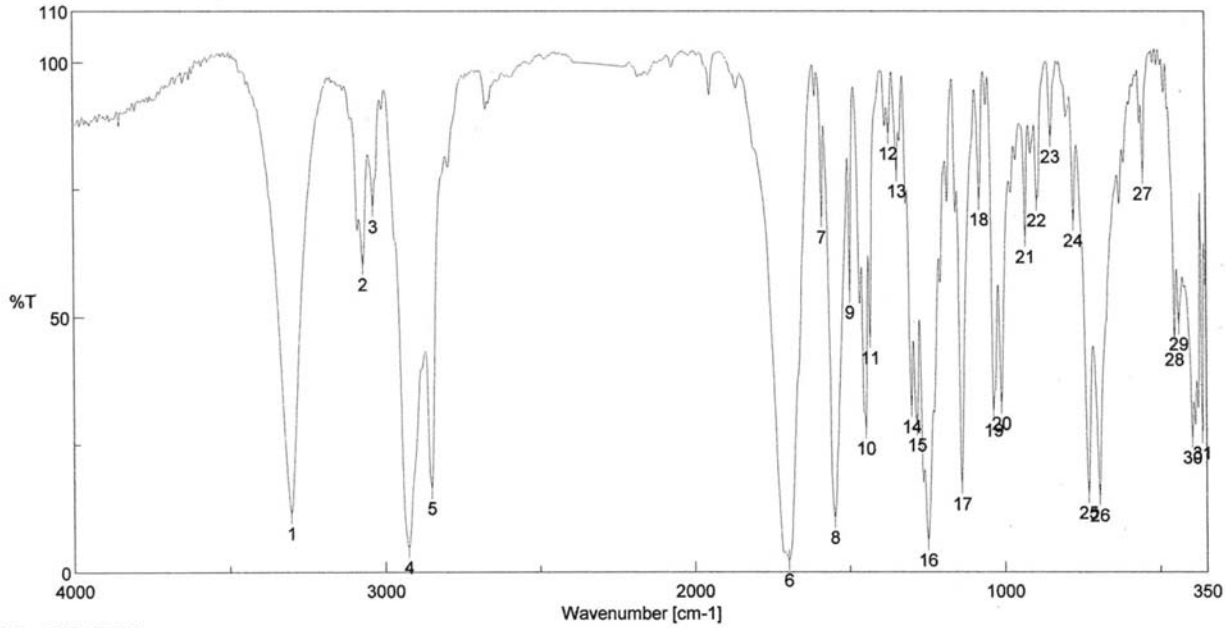
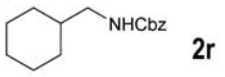
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 500
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 23.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 26
NHCbz
2r
PPM



[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3302.5	11.652	2	3069.16	60.3519	3	3036.37	71.6776	4	2924.52	4.92568
5	2849.31	16.548	6	1697.05	2.42527	7	1587.13	69.6205	8	1547.59	10.8238
9	1496.49	54.8964	10	1446.35	28.2413	11	1431.89	45.9866	12	1370.18	86.0374
13	1344.14	78.6363	14	1298.82	32.5036	15	1281.47	28.9266	16	1247.72	6.36982
17	1137.8	17.388	18	1078.98	73.0864	19	1034.62	31.8249	20	1009.55	33.131
21	931.45	65.7842	22	893.844	72.9124	23	848.525	85.4246	24	776.208	68.9855
25	729.925	15.6606	26	694.248	15.1784	27	551.542	78.1721	28	452.225	45.7033
29	437.762	48.7644	30	395.336	26.5688	31	363.516	27.3959			



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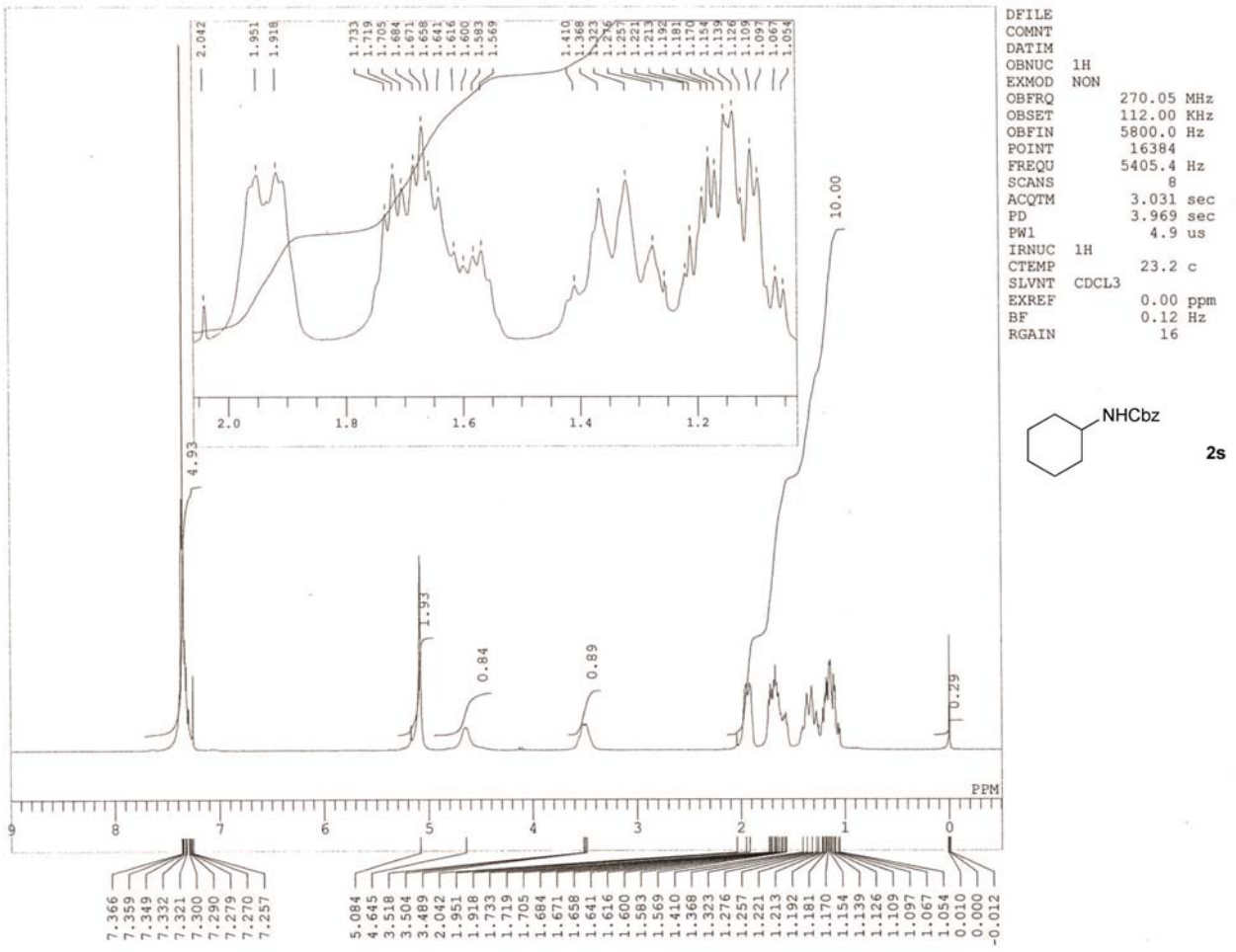
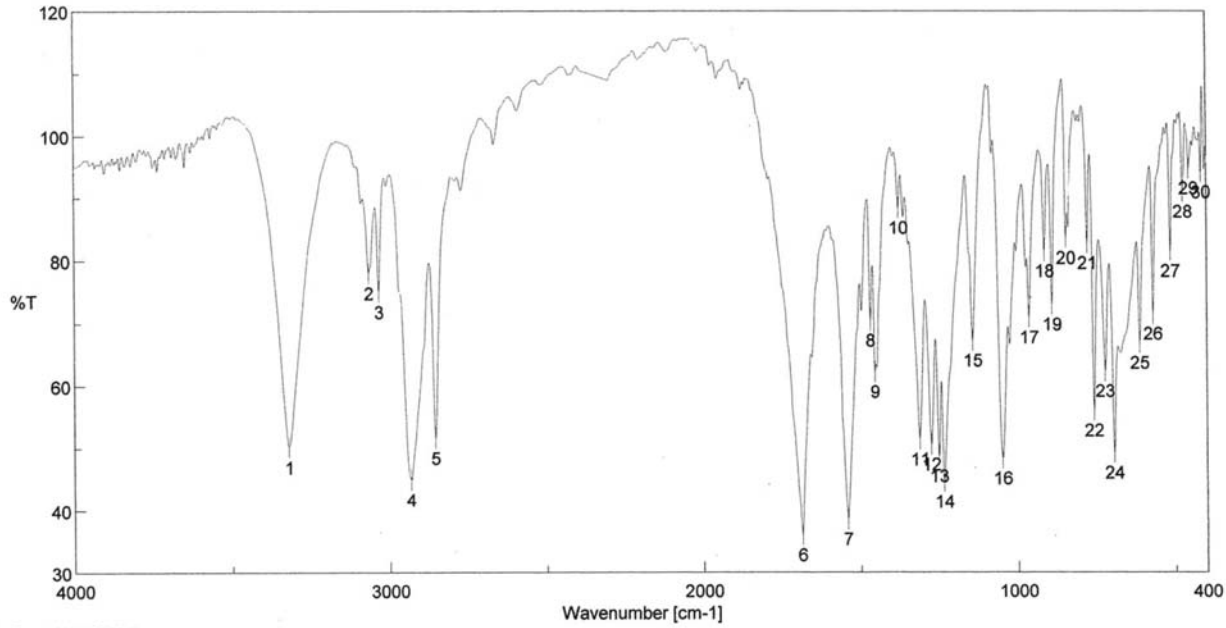
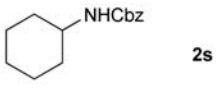
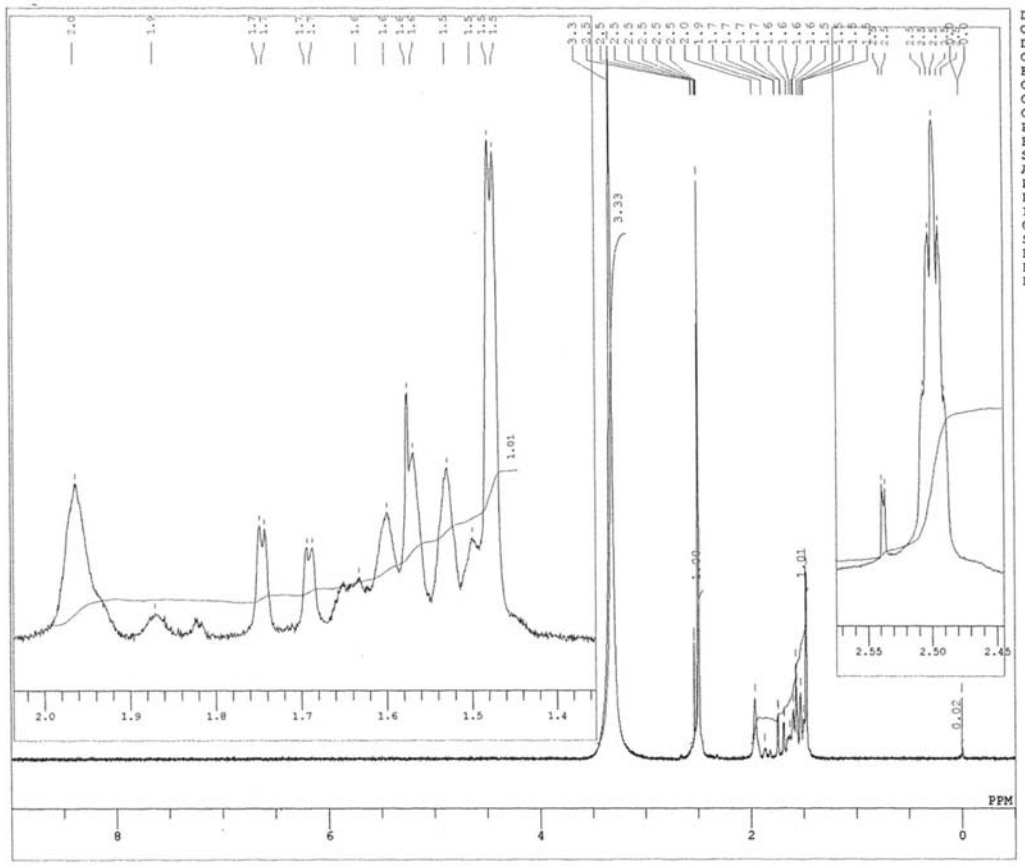


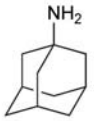


[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3319.86	50.1535	2	3065.3	78.0047	3	3033.48	75.0019	4	2932.23	44.9105
5	2854.13	51.6076	6	1685.48	36.0381	7	1540.85	38.5918	8	1467.56	70.491
9	1453.1	62.2132	10	1377.89	88.4909	11	1311.36	51.4179	12	1274.72	50.6041
13	1250.61	48.7195	14	1234.22	44.6126	15	1142.62	67.2509	16	1048.12	48.3809
17	963.269	70.9952	18	914.093	81.5862	19	889.987	73.0716	20	845.633	83.649
21	778.136	82.8557	22	757.888	56.0355	23	722.211	62.3455	24	693.284	49.296
25	612.288	66.8969	26	569.862	71.5895	27	513.936	81.6118	28	474.403	91.0961
29	455.118	94.8286	30	416.549	94.2409						







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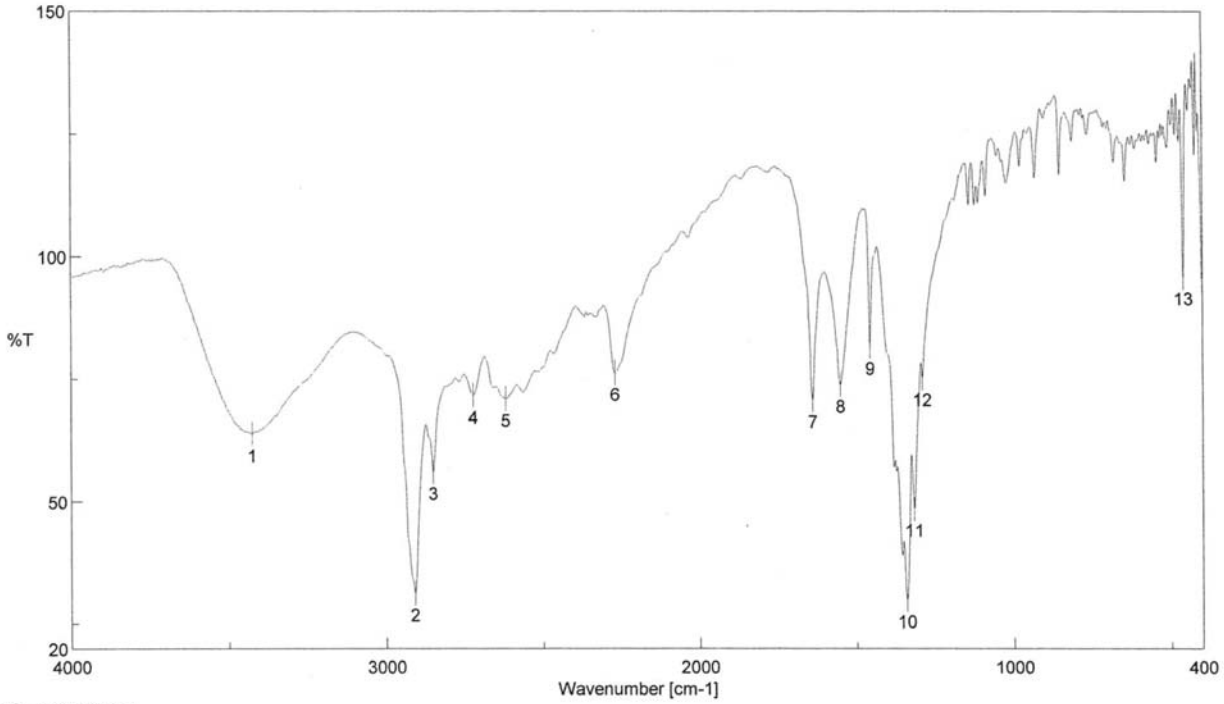
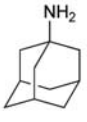


[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3426.89	63.8685	2	2909.09	31.2725	3	2851.24	56.1159	4	2723	71.6428
5	2619.82	70.9779	6	2269.81	76.2886	7	1640.16	70.7685	8	1551.45	73.8975
9	1456.96	81.6572	10	1341.25	29.9423	11	1317.14	48.5936	12	1291.11	75.2099
13	460.904	95.9702									



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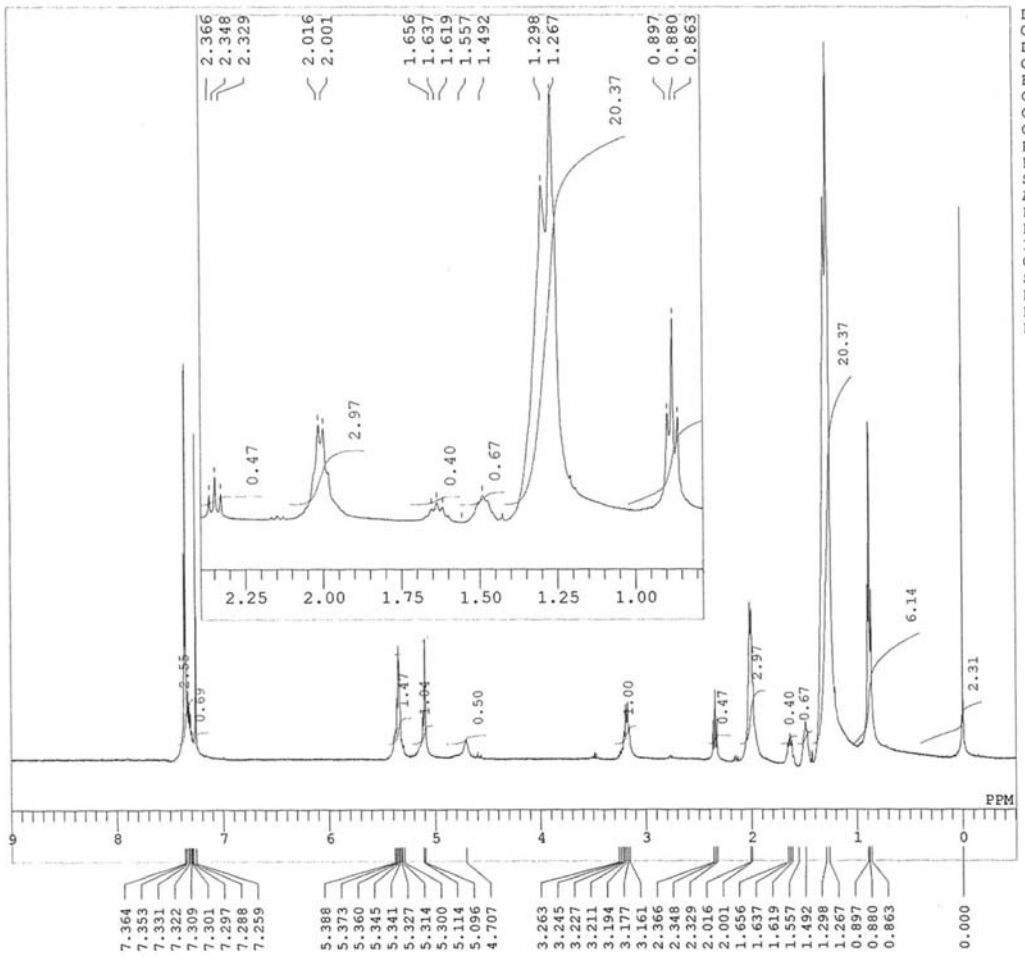


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DFILE
COMNT
DATIM
OBNUC   1H
EXMOD   NON
OBFRQ       399.65 MHz
OBSET       124.00 KHz
OBFIN     10500.00 Hz
POINT        32768
FREQU      7992.01 Hz
SCANS           16
ACQTM       4.1001 sec
PD          2.9000 sec
PW1            6.20 usec
IRNUC   1H
CTEMP         24.4 c
SLVNT   CDCL3
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            18
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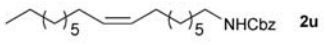

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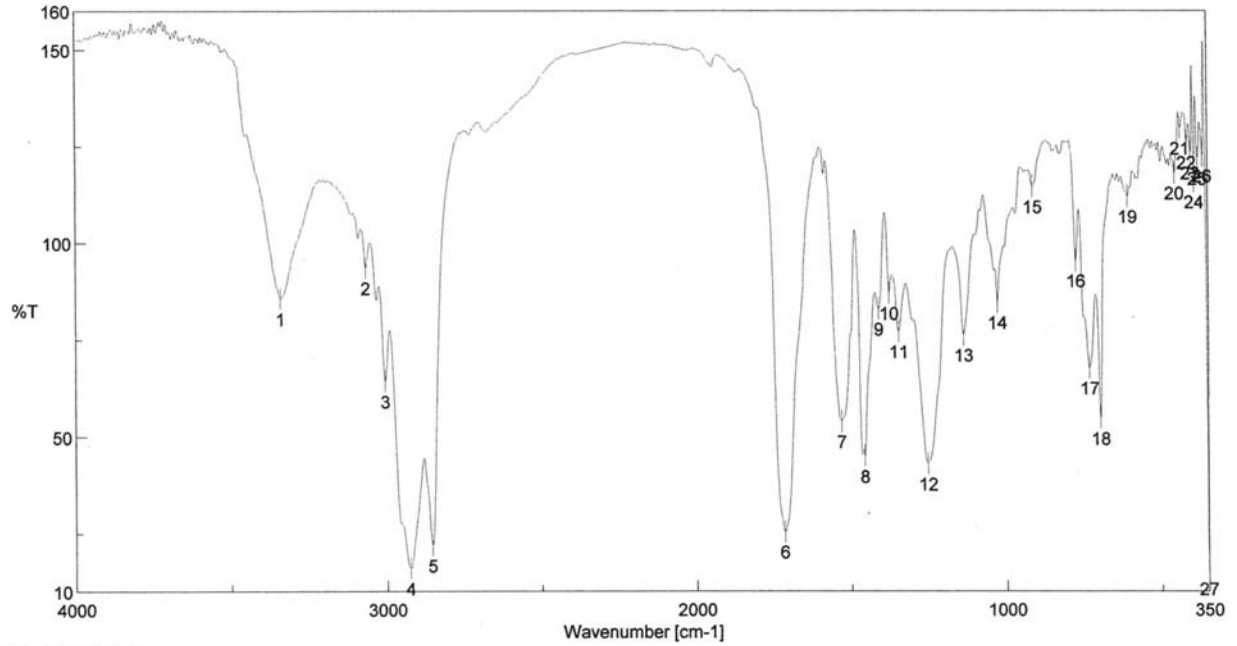
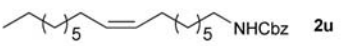


[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3341.07	85.6726	2	3066.26	93.6152	3	3004.55	64.3002	4	2925.48	16.0398
5	2854.13	21.9261	6	1715.37	25.4415	7	1531.2	53.9889	8	1455.99	45.0126
9	1410.67	83.0022	10	1376.93	87.0794	11	1346.07	77.2153	12	1252.54	43.0247
13	1136.83	76.3069	14	1027.87	84.7279	15	913.129	114.622	16	775.244	95.5341
17	731.853	67.8131	18	697.141	54.8294	19	607.467	112.092	20	456.082	118.181
21	436.798	129.709	22	416.549	126.054	23	404.014	123.335	24	393.407	115.888
25	381.836	121.926	26	366.409	122.573	27	350.981	15.9271			



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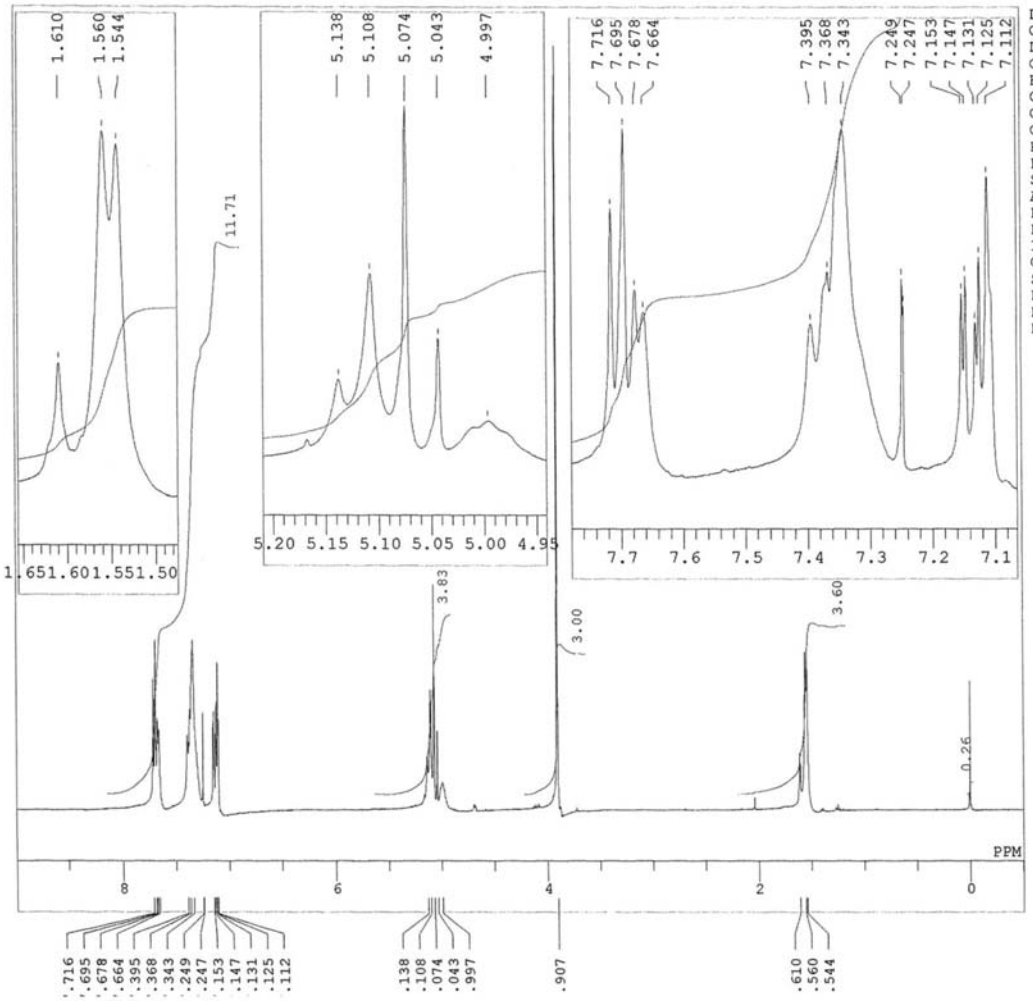


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EXMOD   NON
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OBSET        124.00 KHz
OBFIN      10500.00 Hz
POINT         65536
FREQU       7992.01 Hz
SCANS            16
ACQTM         8.2002 sec
PD            2.9000 sec
PW1             6.20 usec
IRNUC   1H
CTEMP           21.0 c
SLVNT   CDCL3
EXREF            0.00 ppm
BF               0.10 Hz
RGAIN              15
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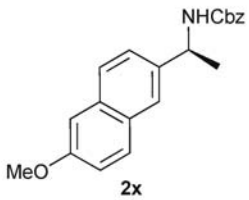

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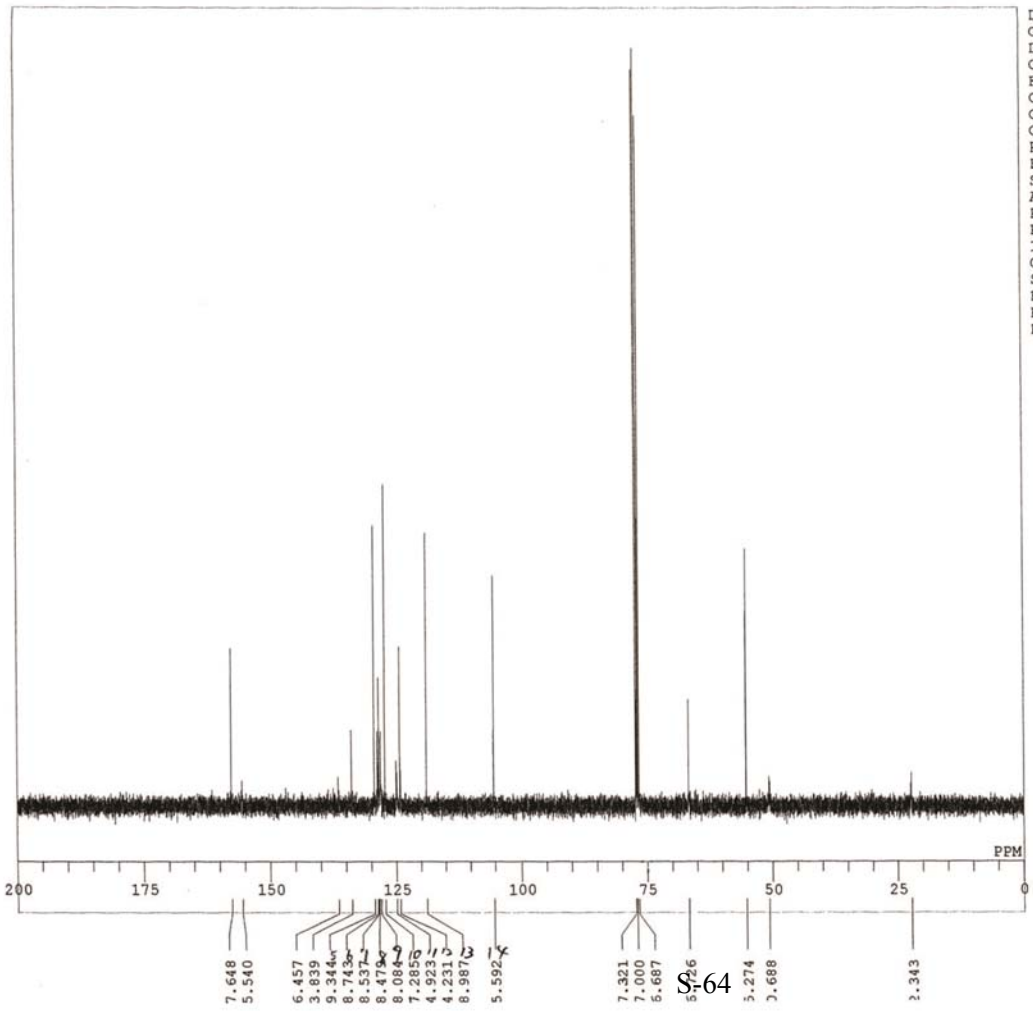


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EXMOD   BCM
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OBSET        125.00 KHz
OBFIN      10500.00 Hz
POINT         32768
FREQU      27118.64 Hz
SCANS           700
ACQTM         1.2083 sec
PD            1.7920 sec
PW1             6.20 usec
IRNUC   1H
CTEMP           21.9 c
SLVNT   CDCL3
EXREF           77.00 ppm
BF               0.10 Hz
RGAIN              27
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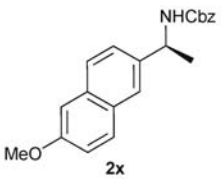

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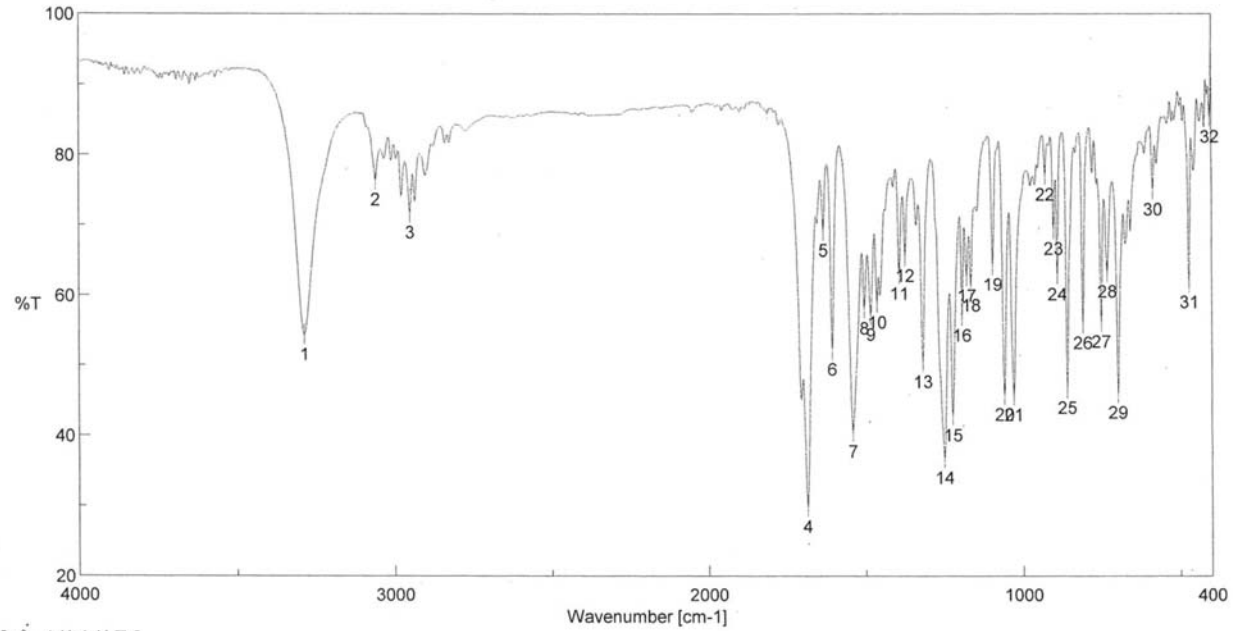
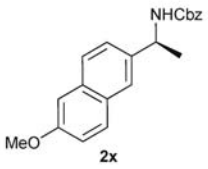


[ピーク検出結果]

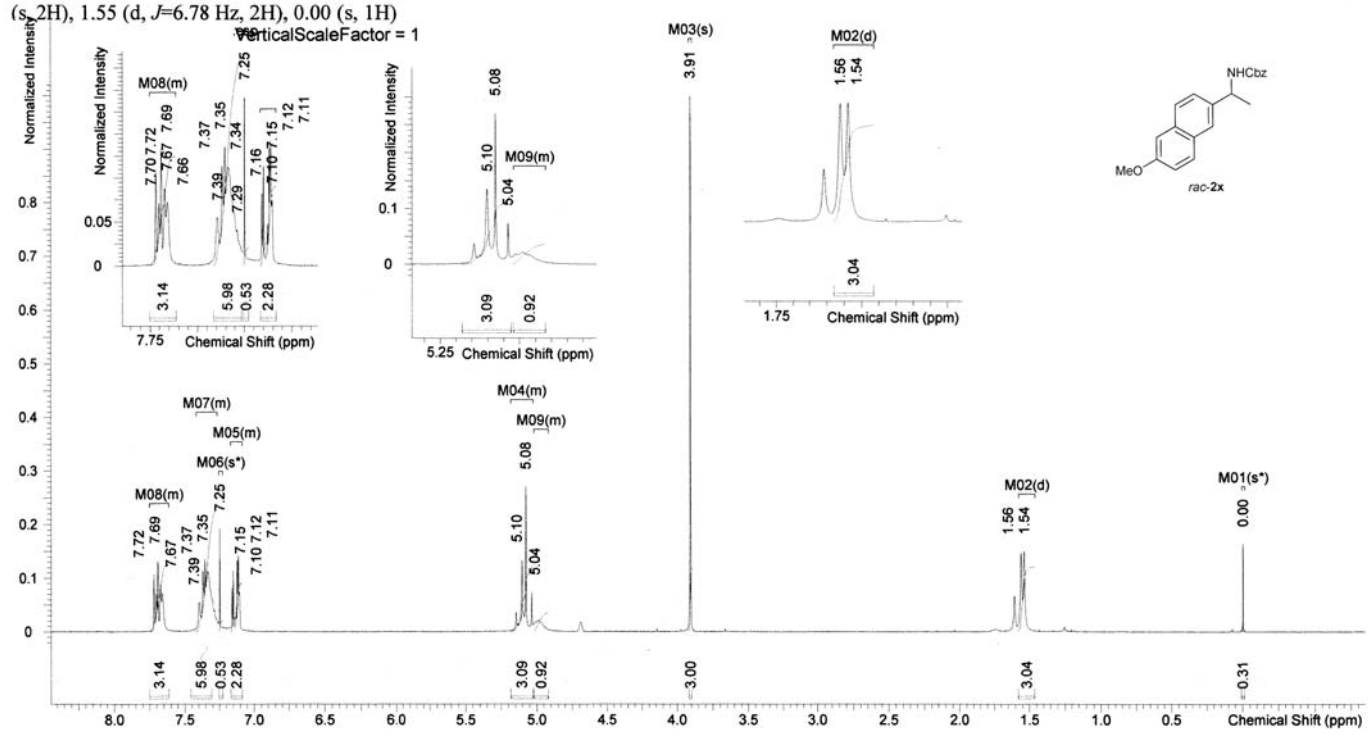
No.	位置	強度	No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3287.07	54.4849	2	3059.51	76.5061	3	2950.55	71.8367	4	1685.48	29.9975
5	1634.38	69.337	6	1606.41	52.3006	7	1540.85	40.6794	8	1504.2	58.2363
9	1483.96	57.3354	10	1463.71	59.0899	11	1392.35	63.17	12	1374.03	65.7355
13	1318.11	50.549	14	1249.65	36.9913	15	1223.61	42.979	16	1193.72	57.2104
17	1178.29	62.88	18	1164.79	61.5104	19	1095.37	64.4844	20	1058.73	45.8566
21	1028.84	45.8538	22	928.557	77.2327	23	901.558	69.5755	24	889.987	63.0696
25	859.132	46.832	26	808.992	56.1309	27	751.138	56.2942	28	731.853	63.451
29	698.105	46.1501	30	586.254	75.1133	31	471.51	61.9632	32	404.978	85.5007



2x

OriginalDateForRelativeTime				Multiplets Integrals Sum	22.29	Number of Nuclei	21 H's		
Acquisition Time (sec)	2.6542	Comment	5 mm QNP 1H/13C/31P/19F Z3333/0001	Date					
Date Stamp				File Name				Frequency (MHz)	300.13
Nucleus	1H	Number of Transients	8	Origin	spect	Original Points Count	16384	Owner	DRX300
Points Count	16384	Pulse Sequence	zg30	Receiver Gain	456.10	SW(cyclical) (Hz)	6172.84	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	1843.9907	Spectrum Type	STANDARD	Sweep Width (Hz)	6172.46	Temperature (degree C)	27.000		

^{1}H NMR (300 MHz, CHLOROFORM-d) δ 7.61-7.75 (m, 3H), 7.27-7.42 (m, 6H), 7.25 (s, 1H), 7.08-7.17 (m, 2H), 5.03-5.18 (m, 3H), 4.92-5.02 (m, 1H), 3.91 (s, 2H), 1.55 (d, *J*=6.78 Hz, 2H), 0.00 (s, 1H)



OriginalDateForRelativeTime				Multiplets Integrals Sum	264.40	Number of Nuclei	258 H's		
Acquisition Time (sec)	2.6542	Comment	5 mm QNP 1H/13C/31P/19F Z3333/0001	Date					
Date Stamp				File Name				Frequency (MHz)	300.13
Nucleus	1H	Number of Transients	8	Origin	spect	Original Points Count	16384	Owner	DRX300
Points Count	16384	Pulse Sequence	zg30	Receiver Gain	143.70	SW(cyclical) (Hz)	6172.84	Solvent	DEUTERIUM OXIDE
Spectrum Offset (Hz)	1853.4569	Spectrum Type	STANDARD	Sweep Width (Hz)	6172.46	Temperature (degree C)	27.000		

^{1}H NMR (300 MHz, DEUTERIUM OXIDE) δ 7.72-7.81 (m, 1H), 7.37-7.51 (m, 1H), 7.20-7.31 (m, 1H), 7.02-7.15 (m, 1H), 4.59-4.83 (m, 251H), 4.48-4.58 (m, 1H), 3.82 (s, 1H), 1.59 (d, *J*=6.78 Hz, 1H)