Supporting Information

Induction of One-handed Helical Oligo (*p*-Benzamide)s by Domino Effect Based on the Planar-Axial-Helical Chirality Relay

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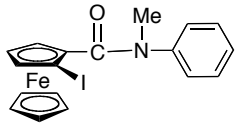
Japan

(*S*)-Iodoferrocene (**2**)[1] and *p*-oligobenzamide[2] were prepared by reported procedure.

Generaral Procedure for Ferrocenyloligoamide

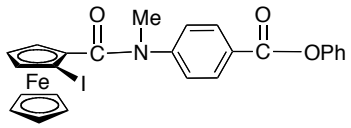
To a solution of (*S*)-iodoferroncecarboxylic acid (50 mg, 0.14 mmol) in CH_2Cl_2 (1.0 mL), $(COCl)_2$ (24 μl, 0.28 mmol) was added at 25 °C under argon. The resulting solution was stirred for 0.5 h and concentrated under reduced pressure. The residue was diluted with CH_2Cl_2 (2.0 mL). Oligo (*p*-benzamide) (0.14 mmol) and Et_3N (39 ml, 0.28 mmol) were dissolved in CH_2Cl_2 (1.0 mL) and added to the solution. The resulting mixture was stirred 15 h at 25 °C. The reaction mixture was extracted with $CHCl_3$ and organic layer was washed with $NaHCO_3$ aq. and brine. The organic layer was dried over $MgSO_4$, filtrated and concentrated under reduced pressure. The crude product was recrystalized from diethylether to give yellow crystals of **3** (73-80% yield).



Ferrocenylamide **1**

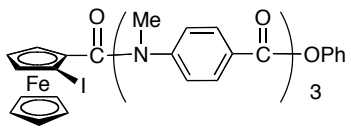
mp 110°C; $[\alpha]_D^{21}$ = –41.5 (*c* 1.1, $CHCl_3$); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 3.41 (3H, s), 3.73 (1H, d, *J* = 2.5Hz), 3.96 (1H, t, *J* = 2.5 Hz), 4.25 (5H, s), 4.41-4.42 (1H, m), 7.01 (2H, d, *J* = 7.2 Hz), 7.16 (1H, d, *J* = 7.2 Hz), 7.20-7.26 (2H, m)); ^{13}C-NMR (100 MHz,

$CDCl_3$) δ 68.6, 68.9, 72.9, 75.6, 76.7, 77.0, 77.3, 126.5, 126.9, 128.9; IR ($CHCl_3$) 3006, 2958, 1637, 1595, 1558 cm^{-1}; MS (relative intensity) *m/z* 445 (M^+, 100), 318 (48), 262 (35); HRMS calcd for $C_{18}H_{16}NOIFe$, 444.9626. found 444.9627.



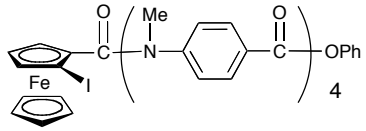
Ferrocenylamide **3a**.

$[\alpha]_D^{23}$ = –6.0 (*c* 0.2, $CHCl_3$); ^{1}H-NMR(400 MHz, $CDCl_3$) δ 3.47 (3H, s), 3.87 (1H, d, *J* = 2.5Hz), 4.06 (1H, d, *J* = 2.5Hz), 4.27 (5H, s), 4.48 (1H, d, *J* = 2.5Hz), 7.12 (2H, d, *J* =8.8Hz), 7.18 (2H, d, *J* = 7.7Hz), 7.27 (2H, d, *J* = 7.7Hz), 7.42 (2H, d, *J* = 7.7Hz), 8.05 (2H, d, *J* = 8.8Hz); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 37.7, 68.9, 69.2, 72.8, 73.0, 75.9, 77.2, 111.1, 121.5, 121.9, 125.9, 126.3, 126.9, 129.3, 129.4, 130.8, 132.2, 149.2, 150.7, 164.3, 168.5; IR ($CHCl_3$) 3352, 1728, 1604, 1443, 1268, 1075, 939cm^{-1}; MS (relative intensity) *m/z* 565 (M^+, 100), 437 (48), 339 (53); HRMS calcd for $C_{25}H_{21}NO_3IFe$, 564.9838. found 564.9838



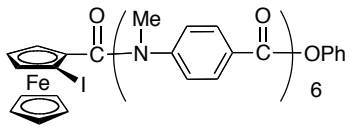
Ferrocenylamide **3b**

mp 132°C; $[\alpha]_D^{26}$ = +47.0 (*c* 0.2, $CHCl_3$); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 3.33 (3H, s), 3.41 (3H, s), 3.55 (3H, s), 3.71 (1H, d, *J* = 2.5Hz), 4.03(1H, t, *J* = 2.5Hz), 4.24 (5H, s), 4.42 (1H, d, *J* = 2.5Hz), 6.81 (2H, d, *J* = 8.3Hz), 6.83 (2H, d, *J* = 8.5Hz), 7.08 (2H, d, *J* = 8.3Hz), 7.10 (2H, d, *J* = 8.5Hz), 7.20 (4H, d, *J* = 8.5Hz), 7.29 (1H, t, *J* = 7.8Hz), 7.44 (2H, t, *J* = 7.8Hz), 8.07 (2H, d, *J* = 8.5Hz); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 37.8, 38.1, 38.2, 68.9, 69.0, 73.0, 73.3, 75.7, 77.2, 121.5, 125.8, 125.9, 126.1, 126.4, 127.3, 129.5, 131.2, 132.9, 133.0, 146.0, 146.2, 149.3, 150.6, 164.1, 168.2, 169.3, 169.4; IR($CHCl_3$) 3361, 1793, 1642, 1599, 1294, 1095 cm^{-1}; MS (relative intensity) *m/z* 831 (M^+, 23), 705 (61), 548 (17), 497 (16), 368 (17), 213 (18), 185 (15), 134 (100); HRMS calcd for $C_{41}H_{34}N_3O_5IFe$, 831.0893. found. 831.0889



Ferrocenylamide **3c**

mp 125°C; $[\alpha]_D^{26}$ = +36.0 (*c* 0.1, $CHCl_3$); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 3.35 (3H, s), 3.36 (3H, s), 3.44 (3H, s), 3.55 (3H, s), 3.68 (1H, s), 4.01 (1H, t, *J* = 2.4Hz), 4.23 (5H, s), 4.40-4.41 (1H, m), 6.76 (4H, d, *J* = 8.8Hz), 6.82 (2H, d, *J* = 8.5Hz), 7.01 (2H, d, *J* = 8.5Hz), 7.08 (2H, d, *J* = 8.8Hz), 7.12 (2H, d, *J* = 8.5Hz), 7.17 (1H, d, *J* = 8.0Hz), 7.20 (2H, d, *J* = 8.5Hz), 7.29 (1H, t, *J* = 8.0Hz), 7.44 (2H, t, *J* = 8.0Hz); ^{13}C-NMR (100 MHz, $CDCl_3$) δ; 37.8, 38.1, 38.2, 38.3, 66.1, 68.9, 69.2, 73.0, 75.8, 77.2, 121.5, 125.7, 125.9, 126.0, 126.1, 126.4, 127.3, 129.5, 129.6, 129.8, 129.9, 131.2, 132.9, 133.0, 133.5, 145.9, 146.1, 146.2, 149.3, 150.6, 164.1, 168.3, 169.2; IR($CHCl_3$) 3414, 1733, 1603, 1372, 1193, 1059, 909 cm^{-1}; MS (relative intensity) *m/z* 964 (M^+, 41), 899 (3), 831 (7), 544 (8), 472 (9), 339 (67), 154 (100)

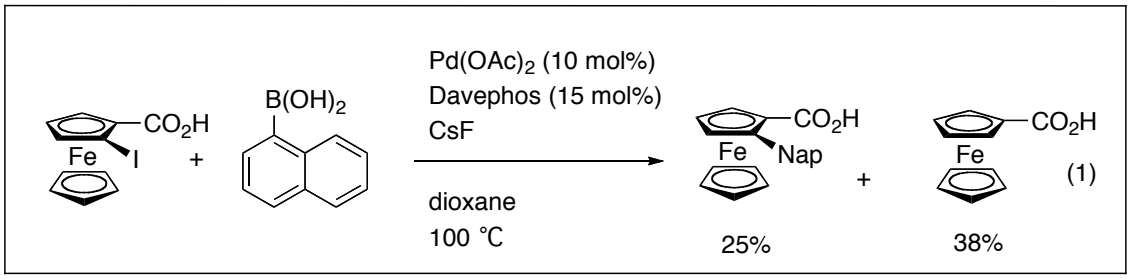


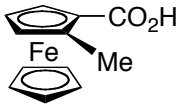
Ferrocenylamide **3d**

mp 135°C; $[\alpha]_D^{24}$ = +26.7 (*c* 0.06, $CHCl_3$) ^{1}H-NMR (400 MHz, $CDCl_3$) δ 3.35 (3H, s), 3.39 (6H, s), 3.41 (3H, s), 3.42 (3H, s), 3.54 (3H, s), 3.67 (1H, s), 4.00-4.01 (1H, m), 4.23 (5H, s), 4.40 (1H, s), 6.75-6.78 (6H, m), 6.80 (2H, d, *J* = 8.3Hz), 6.85 (2H, d, *J* = 8.3Hz), 7.02 (2H, d, *J* = 8.5Hz), 7.05-7.12 (8H, m), 7.18 (2H, d, *J* = 7.8Hz), 7.20 (2H, d, *J* = 8.5Hz), 7.29 (1H, t, *J* = 7.8Hz), 7.43 (2H, t, *J* = 7.8Hz), 8.05 (2H, d, *J* = 8.3Hz),; ^{13}C-NMR (100 MHz, $CDCl_3$) δ 37.8, 38.1, 38.2, 38.3, 38.4, 42.3, 65.8, 68.9, 69.1, 73.0, 75.8, 77.2, 121.5, 125.8, 125.9, 126.0, 126.1, 126.2, 126.4, 127.4, 129.5, 129.6, 129.7, 129.8, 129.9, 130.0, 131.1, 133.0, 133.1, 133.4, 133.6, 145.8, 145.9, 146.0, 146.0, 146.1, 149.3, 150.6, 164.1, 168.2, 169.1, 169.2, 169.3, 169.4; IR($CHCl_3$) 3387, 1737, 1640, 1603, 1367, 1268, 1174, 909 cm^{-1}; MS (relative intensity) *m/z* 1231 (M^+, 15), 1165 (3), 1097 (4), 893 (3), 810 (5), 760 (4), 472 (13), 444 (4), 339 (60), 316 (10), 134 (100), 132 (43) ; HRMS calcd for $C_{65}H_{55}N_6O_8IFe$, 1231.2556. found. 1231.2551

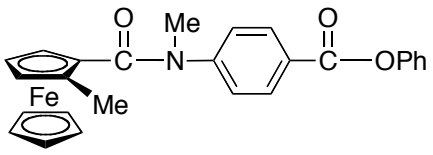
Synthesis of planar chiral 2-methyl or 2-naphtyl ferrocenecarboxylic acid

2-Naphtyl ferrocenecarboxylic acids were prepared by a conventional Suzuki-Miyaura cross-coupling reaction. 2-Naphtyl ferrocenyloligoamides were prepared by the procedure mentioned in S1.



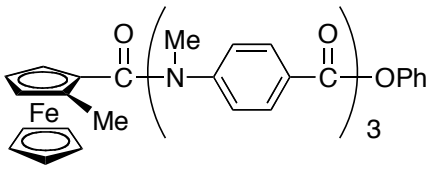


$[\alpha]_D^{27}$ = 11.1 (*c* 0.13, $CHCl_3$); ^{1}H-NMR(500 MHz, $CDCl_3$) δ 2.30 (3H, s), 4.18 (5H, s), 4.31 (1H, t, *J* = 2.3Hz), 4.38 (1H, s), 4.79 (1H, s); ^{13}C-NMR (100 MHz, $CDCl_3$) 14.6, 68.1, 69.5, 70.6, 70.7, 74.3, 87.5, 179.4; IR ($CHCl_3$) 3099, 1712, 1289, 1214, 894, 767cm^{-1}; MS (relative intensity) *m/z* 244 (M^+, 100), 179 (18), 149 (6), 138 (37), 106(26) ; HRMS calcd for $C_{12}H_{12}FeO_2$, 244.0187. found 244.0193



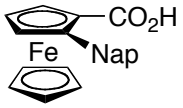
Ferrocenylamide **4a**

$[\alpha]_D^{25}$= 142.0 (*c* 0.28, $CHCl_3$); ^{1}H-NMR (500 MHz, $CDCl_3$) δ 2.07 (3H, s), 3.46 (3H, s), 3.81 (1H, s), 3.97 (1H, s), 4.21 (5H, s), 4.21 (1H, s), 7.14 (2H, d, *J* = 7.8Hz), 7.19 (2H, d, *J* = 7.8Hz), 7.27(1H, t, *J* = 7.8Hz), 7.42 (2H, t, *J* = 7.8Hz), 8.07 (2H, d, *J* = 7.8Hz) ; ^{13}C-NMR (100 MHz, $CDCl_3$) 14.0, 37.7, 66.9, 69.4, 70.7, 70.9, 78.9, 86.8, 121.6, 126.0, 126.1, 126.5, 129.5, 130.8, 150.0, 150.8, 164.4, 171.2 ; IR ($CHCl_3$) 3055, 1732, 1600, 1270, 1186, 760.7cm^{-1}; MS (relative intensity) *m/z* 453 (M^+, 100), 451 (7), 332(8), 227(90), 199(38), 180(11), 149(13), 132(10) ; HRMS calcd for $C_{26}H_{23}FeNO_3$, 453.1027. found 457.1031

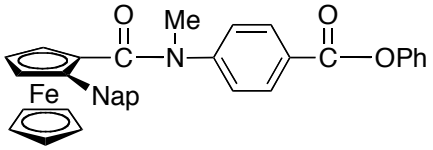


Ferrocenylamide **4b**

$[\alpha]_D^{26}$= 93.8 (*c* 0.16,$CHCl_3$); ^{1}H-NMR(500 MHz,$CDCl_3$) δ 2.02(3H, s), 3.32(3H, s), 3.42(3H, s), 3.55(3H, s), 3.55(1H, s), 3.86(1H, t, *J* = 2.3Hz), 4.07(1H, s), 4.11(5H, s), 6.81(2H, d, *J* = 8.2Hz), 6.85(2H, d, *J* = 8.2Hz), 7.07-7.09(4H, m), 7.20(2H, d, *J* = 8.2Hz), 7.29(1H, t, *J* = 8.2Hz), 7.44(2H, t, *J* = 8.2Hz), 8.03(2H, d, *J* = 8.2Hz); ^{13}C-NMR(100 MHz, $CDCl_3$) 14.0, 37.8, 38.2, 66.6, 69.4, 70.7, 70.8, 78.7, 86.8, 121.5, 125.7, 125.9, 126.4, 127.3, 129.5, 129.6, 129.9, 131.1, 132.6, 133.1, 146.3, 146.7, 149.3, 150.7, 164.1, 169.4, 169.5, 170.9 IR ($CHCl_3$) 3136, 1733, 1604, 1356, 1212, 1104, 851, 771 cm^{-1} ; MS (relative intensity) *m/z* 719 (M^+, 91), 548 (10), 493(38), 400(11), 277(75), 267(24), 227(24), 201(17), 199(29), 170(25), 167(22) ; HRMS calcd for $C_{42}H_{37}FeN_3O_5$, 719.2083. found 719.2073

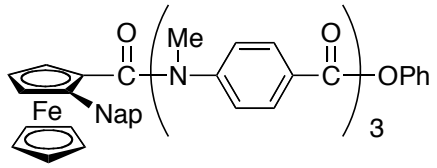


$[\alpha]_D^{30}$ = -101.3 (*c* 0.31, $CHCl_3$); ^{1}H-NMR(500 MHz, $CDCl_3$) δ 4.38 (5H, s), 4.57 (1H, s), 4.62 (1H, t, *J* = 2.8Hz), 5.06 (1H, t, *J* = 2.8Hz), 7.30 (1H, t, *J* = 6.9Hz), 7.40 (1H, t, *J* = 6.9Hz) , 7.52 (2H, d, *J* = 7.4Hz) , 7.82 (2H, dd, *J* = 7.4, 3.2Hz) , 8.09 (2H, d, *J* = 6.9Hz); ^{13}C-NMR(100 MHz, $CDCl_3$) 70.2, 70.9, 71.3, 71.5, 76.9, 91.9, 124.9, 125.4, 125.6, 125.7, 127.7, 128.1, 129.3, 133.0, 133.3, 133.6, 177.1; IR ($CHCl_3$) 3017, 2603, 1717, 1286, 1118, 905, 833 cm^{-1} ; MS (relative intensity) *m/z* 356 (M^+, 16), 218 (16), 192 (28), 189 (17), 149 (34), 137 (18); HRMS calcd for $C_{21}H_{16}FeO_2$, 356.0500. found 306.0499.



Ferrocenylamide **5a**

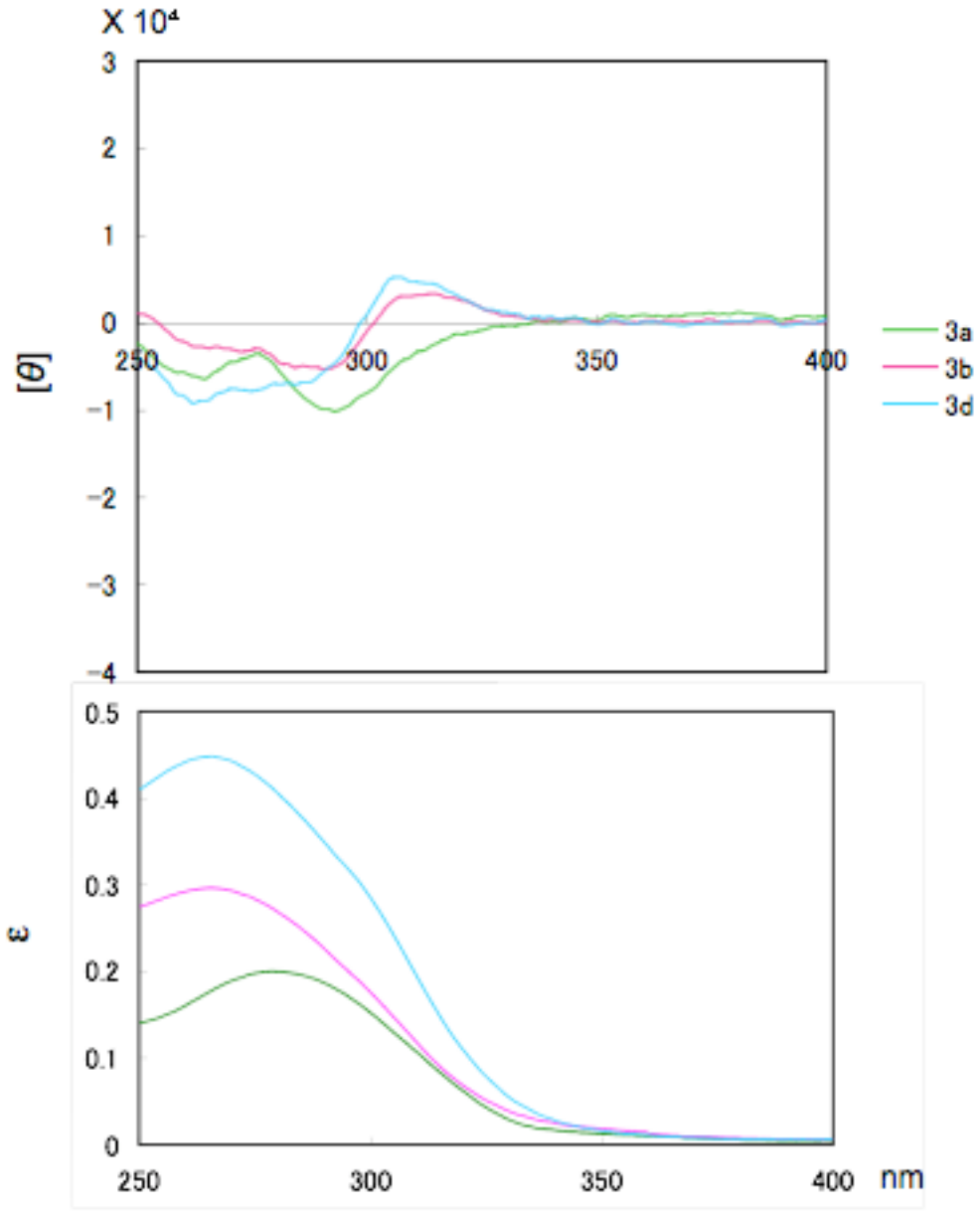
$[\alpha]_D^{28}$ = -31.9 (*c* 0.27,$CHCl_3$); ^{1}H-NMR (500 MHz, $CDCl_3$) δ 3.21 (3H, s), 4.29 (5H, s), 4.48 (1H, t, *J* = 2.3Hz), 4.55 (1H, dd, *J* = 2.3, 1.4Hz), 4.92 (1H, dd, *J* = 2.3, 1.4Hz), 6.16 (2H, d, *J* = 8.7Hz), 7.12-7.28 (5H, m), 7.35 (1H, t, *J* = 8.2Hz), 7.42-7.47 (4H, m), 7.54 (1H, d, *J* = 8.7Hz), 7.76 (1H, t, *J* = 8.3Hz), 7.87 (1H, d, *J* = 6.8Hz); ^{13}C-NMR (100 MHz, $CDCl_3$) 37.1, 67.8, 69.9, 71.4, 71.8, 84.8, 86.1, 121.5, 124.5, 124.7, 125.0, 125.2, 125.5, 125.8, 127.3, 128.0, 129.0, 129.4, 129.5, 131.7, 133.5, 134.2, 147.9, 150.8, 163.9, 169.9; IR ($CHCl_3$) 1731, 1600, 1351, 1270, 1079, 831, 750 cm^{-1}; MS (relative intensity) *m/z* 565 (M^+, 2), 386 (2), 368 (5), 341 (4), 279 (8), 257 (7), 236 (10), 229 (7), 167 (23) ; HRMS calcd for $C_{35}H_{27}FeNO_3$, 565.1340. found 565.1340



Ferrocenylamide **5b**

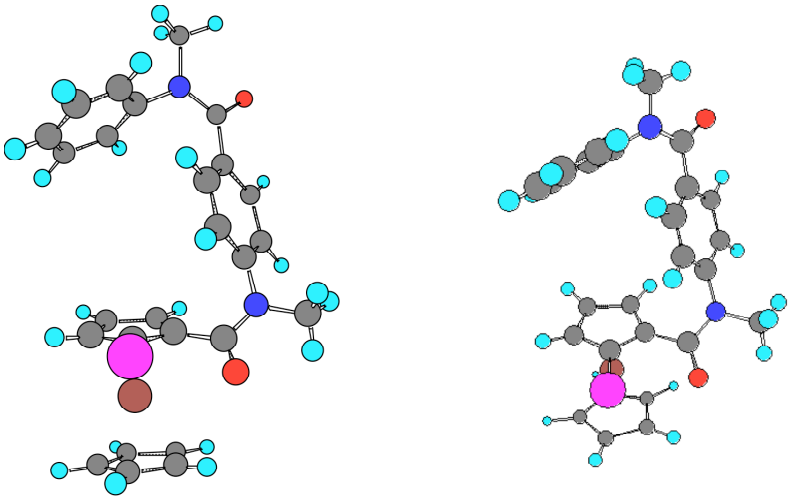
$[\alpha]_D^{28}$= -30.7 (*c* 0.5, $CHCl_3$); ^{1}H-NMR (500 MHz, $CDCl_3$) δ 2.99 (3H, s), 3.35 (3H, s), 3.51 (3H, s), 4.28 (5H, s), 4.30 (1H, t, *J* = 2.3Hz), 4.48 (1H, s), 4.52 (1H, s), 5.99 (2H, d, *J* = 7.3Hz), 6.56 (2H, d, *J* = 8.3Hz), 6.77 (2H, d, *J* = 8.3Hz), 7.08 (2H, d, *J* = 8.2Hz), 7.17-7.20 (4H, m), 7.29 (2H, t, *J* = 7.3Hz), 7.39-7.46 (4H, m), 7.67 (1H, d, *J* = 8.2Hz), 7.72 (1H, d, *J* = 8.2Hz), 7.78 (1H, d, *J* = 8.3Hz), 7.87 (1H, d, *J* = 8.3Hz), 8.03 (2H, d, *J* = 7.3Hz); ^{13}C-NMR (100 MHz, $CDCl_3$) 37.2, 38.2, 67.2, 69.6, 71.1, 71.3, 71.4, 86.1, 86.4, 121.5, 124.8, 125.0, 125.2, 125.3, 125.5, 125.7, 126.0, 126.3, 127.2, 127.2, 128.0, 128.9, 129.4, 129.5, 129.8, 131.1, 131.9, 132.1, 132.7, 133.3, 133.9, 145.1, 146.4, 149.3, 150.7, 164.0, 169.1, 169.3, 169.5; IR ($CHCl_3$) 3148, 2830. 1602, 1353, 1110, 853, 695cm^{-1}; MS (relative intensity) *m/z* 781 (M^+, 100), 648 (48), 548 (16), 493 (29), 368 (37), 353 (11), 313 (11), 289 (47), 267 (20), 260 (55), 218 (28), 213 (18) ; HRMS calcd for $C_{47}H_{39}FeN_3O_5$, 831.2396. found 831.2401

CD and UV of 3a, 3b and 3d in CH_3CN solution

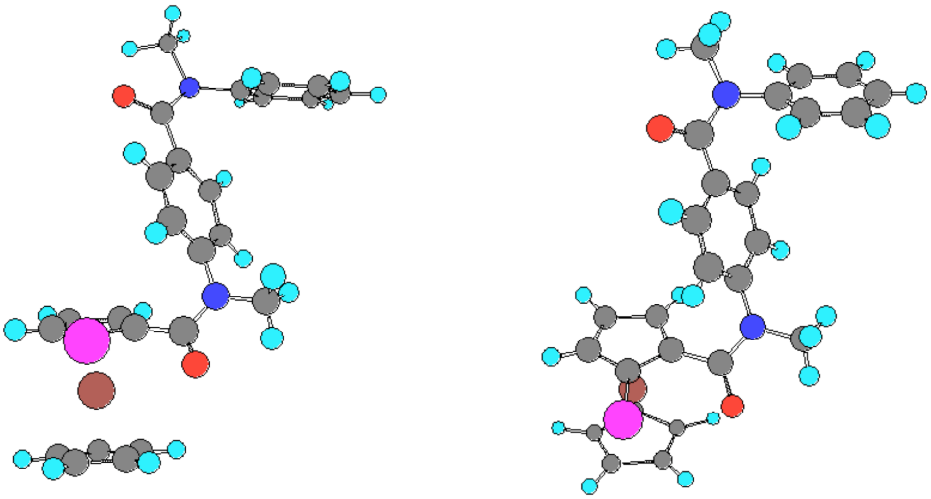


Computational work and Cartesian coordinate

Geometry optimization calculations were carried out for estimating **3d** structure by Gaussian 98 program[3]. RHF level of theory in conjunction with 3-21(d) basis sets has been used. Total energy difference between two structures which were right-hand helical structure (**3d-I**) and not helical structure (**3d-II**) was compared.



Molecular structure of **3d-I** -9393.7652087H



Molecular structure of **3d-II** -9393.757785H

Cartesian coordinate for **3d-I**

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.408077646737
C	1.362814262795	0.000000000000	-0.436749785148
H	-0.858706698087	0.070780737657	-0.628627821268
Fe	0.991181438547	-1.909938820804	0.689790925059
C	1.349146449730	-0.033442028144	1.857067676070
C	2.183466352105	0.000176380133	0.705678555952
H	-0.864753068793	0.039630174089	2.032954667065
H	1.696610376758	0.052368248156	-1.448127457758
C	0.370090801336	-3.859402693610	-0.300445920743
C	-0.077521531001	-3.894270390773	1.056534156603
C	1.046855112066	-3.851928540271	1.887026145684
C	2.207845423282	-3.756590349130	1.070226651439
C	1.772056240656	-3.786169860386	-0.285676200956
H	1.675589831927	0.027617351644	2.870003584340
H	3.250255160099	-0.009729907870	0.708339161740
C	3.600872143057	-3.583223557549	1.512392586003
I	2.968556030213	-3.838128067797	-2.018638893870
H	-0.239453296752	-3.956546663104	-1.168451098149
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References

1. Riant, O. Samuel, T. Flessner, S. Taudien, H. B. Kagan, *J. Org. Chem.* 1997, **62**, 6733.
2. A. Tanatani, A. Yokoyama, I. Azuma, Y. Takakura, C. Mitsui, M. Shiro, M. Uchiyama, A. Muranaka, N. Kobayashi and T. Yokozawa, *J. Am. Chem. Soc.*, 2005, **127**, 8553

3 Gaussian 98, Revision A.11.3, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E.

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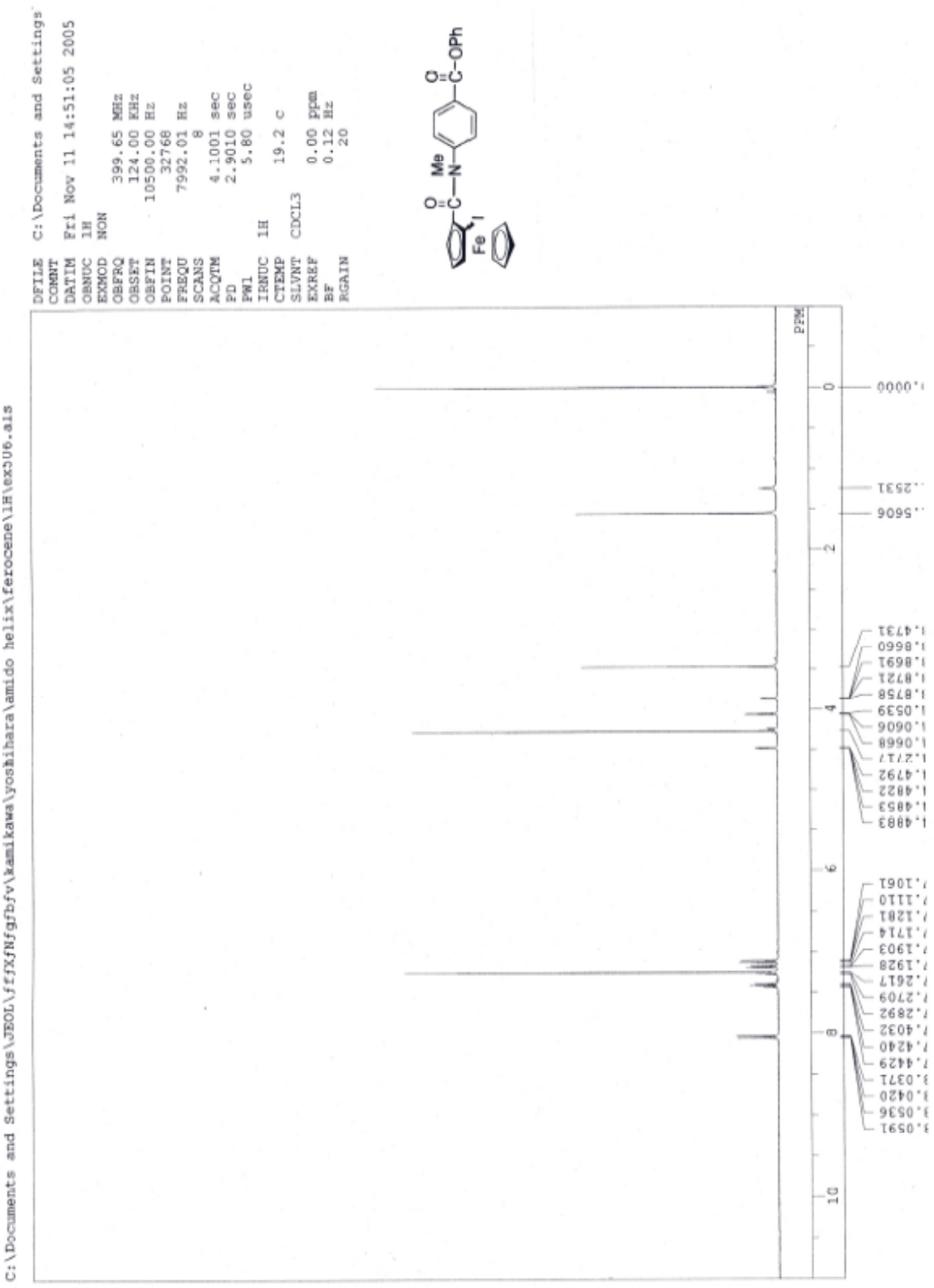
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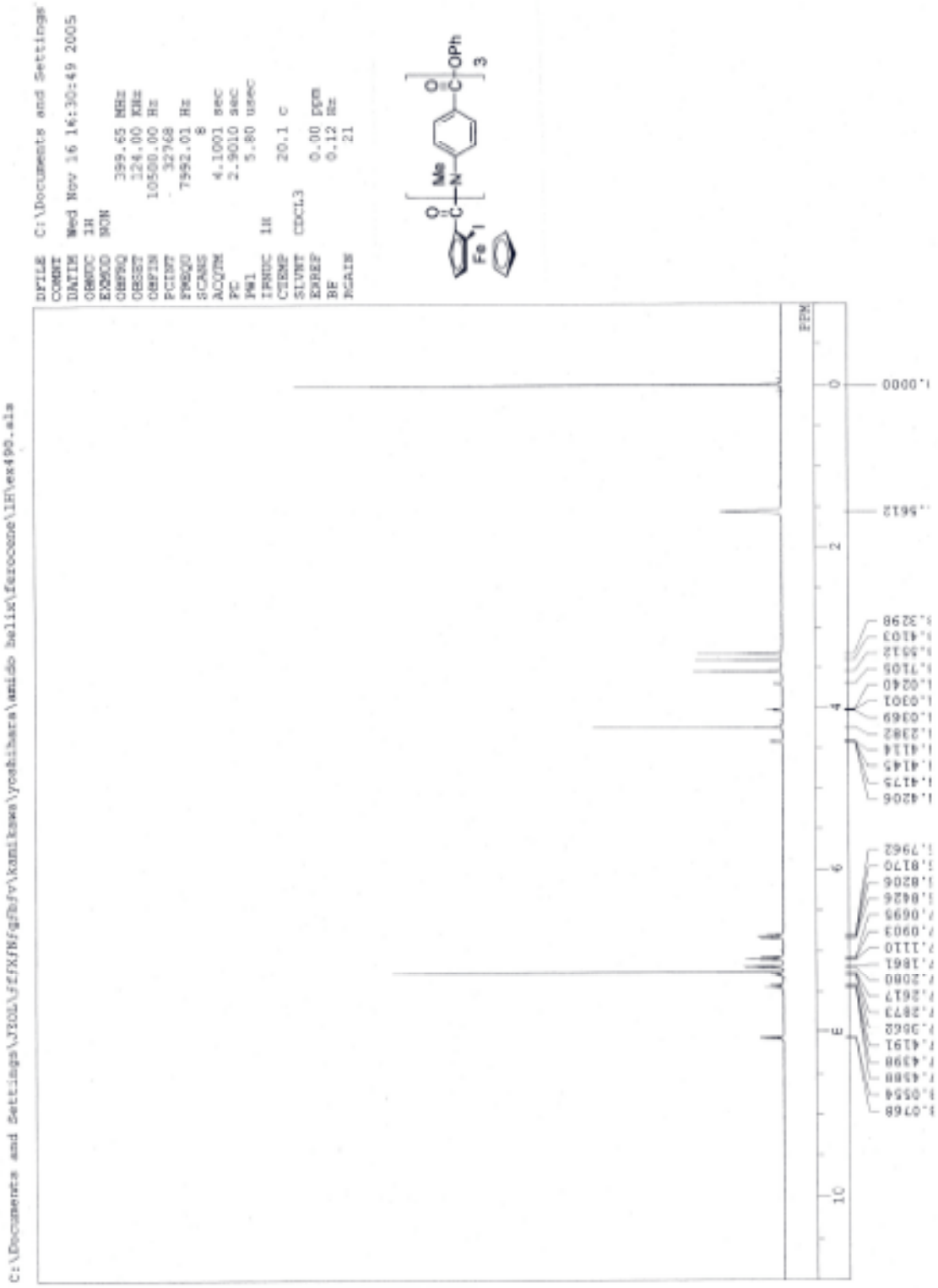
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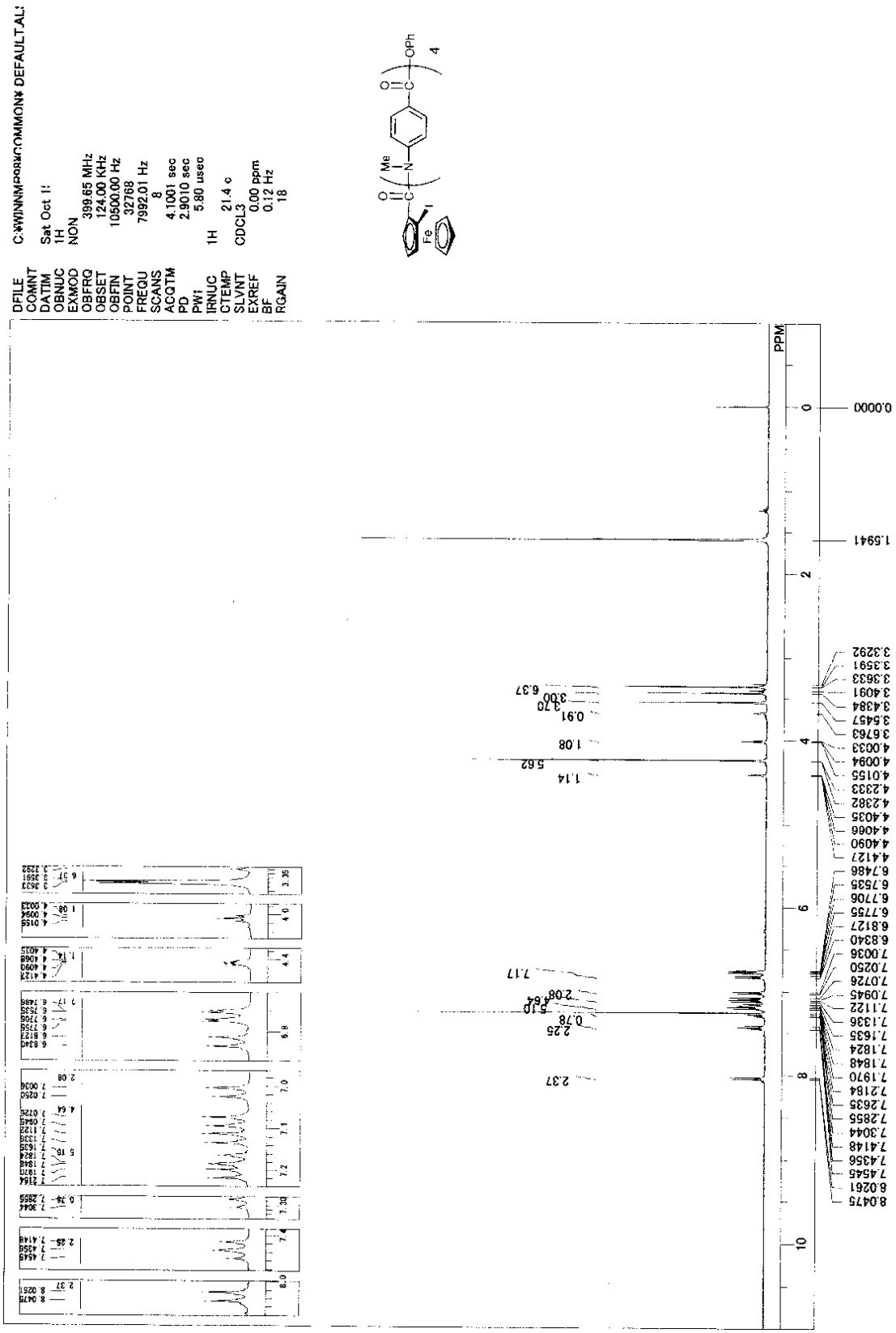
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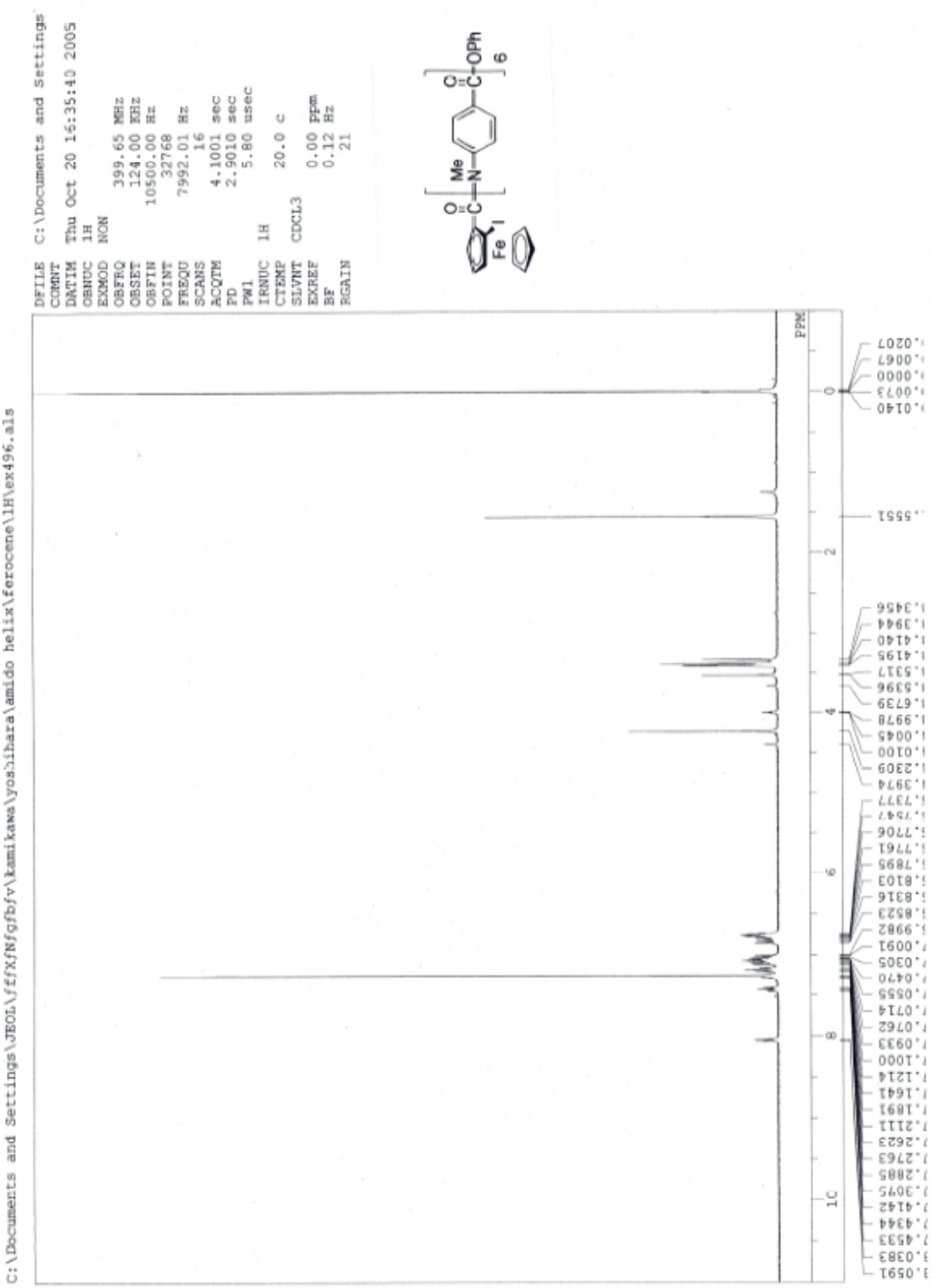
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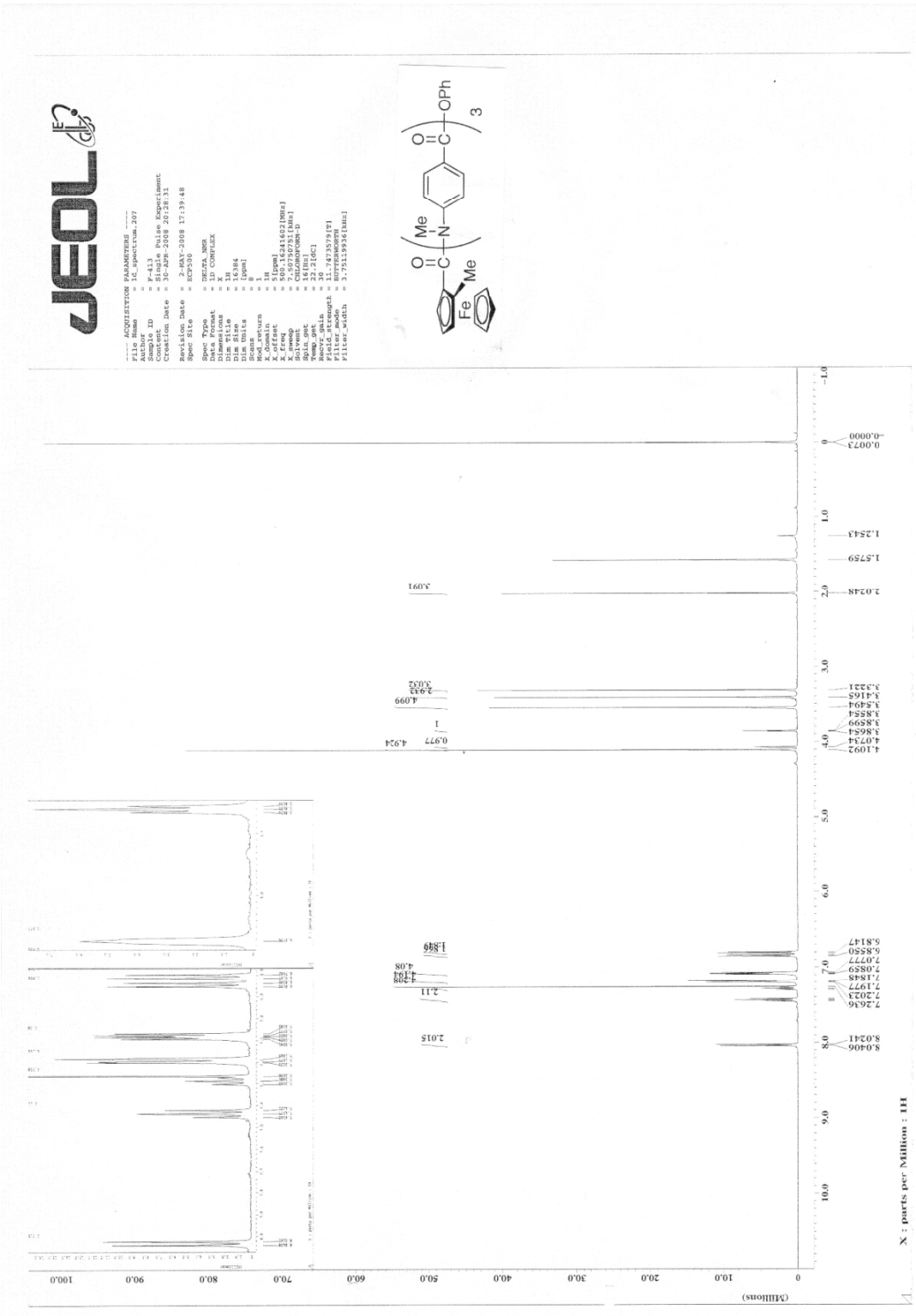
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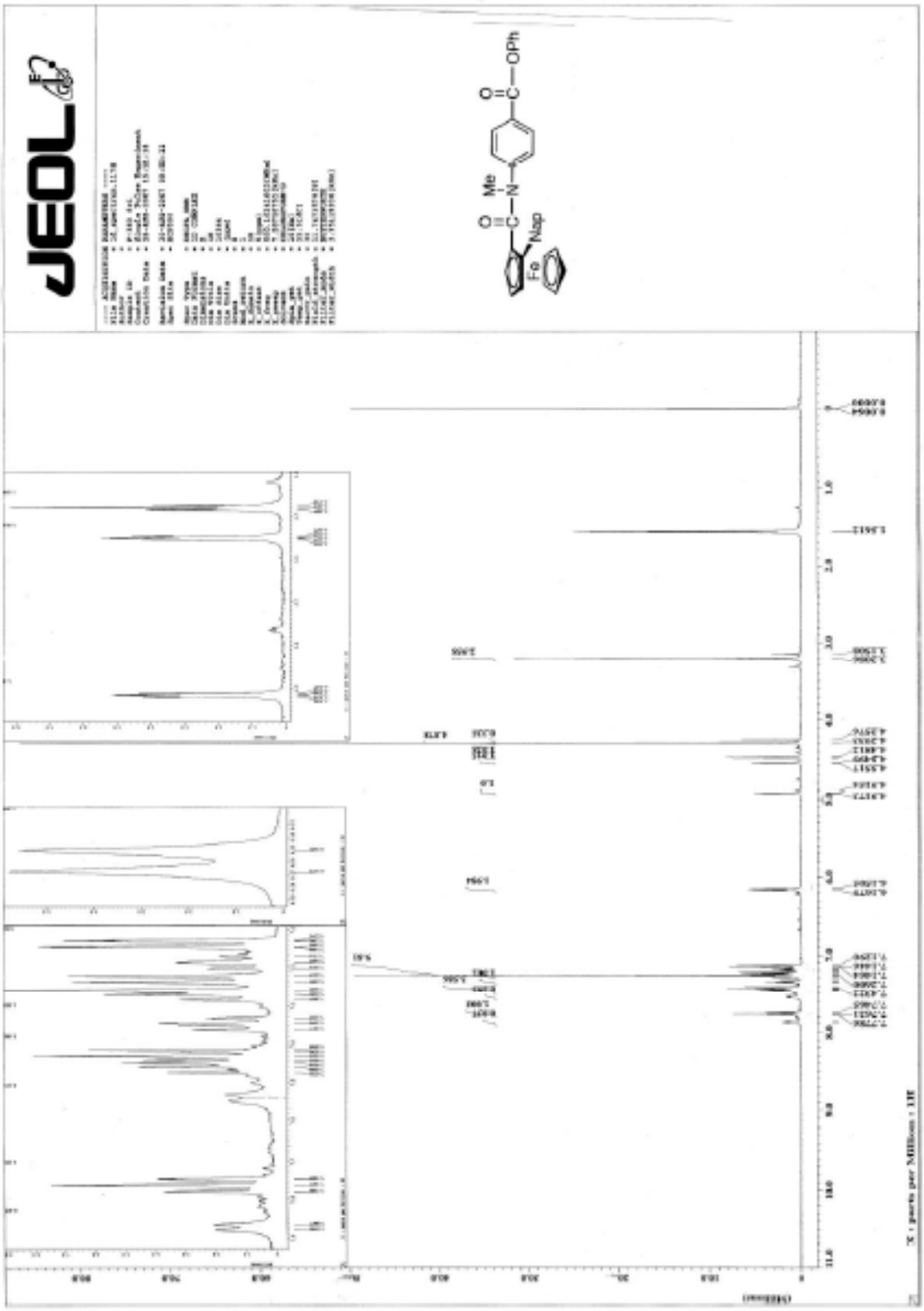
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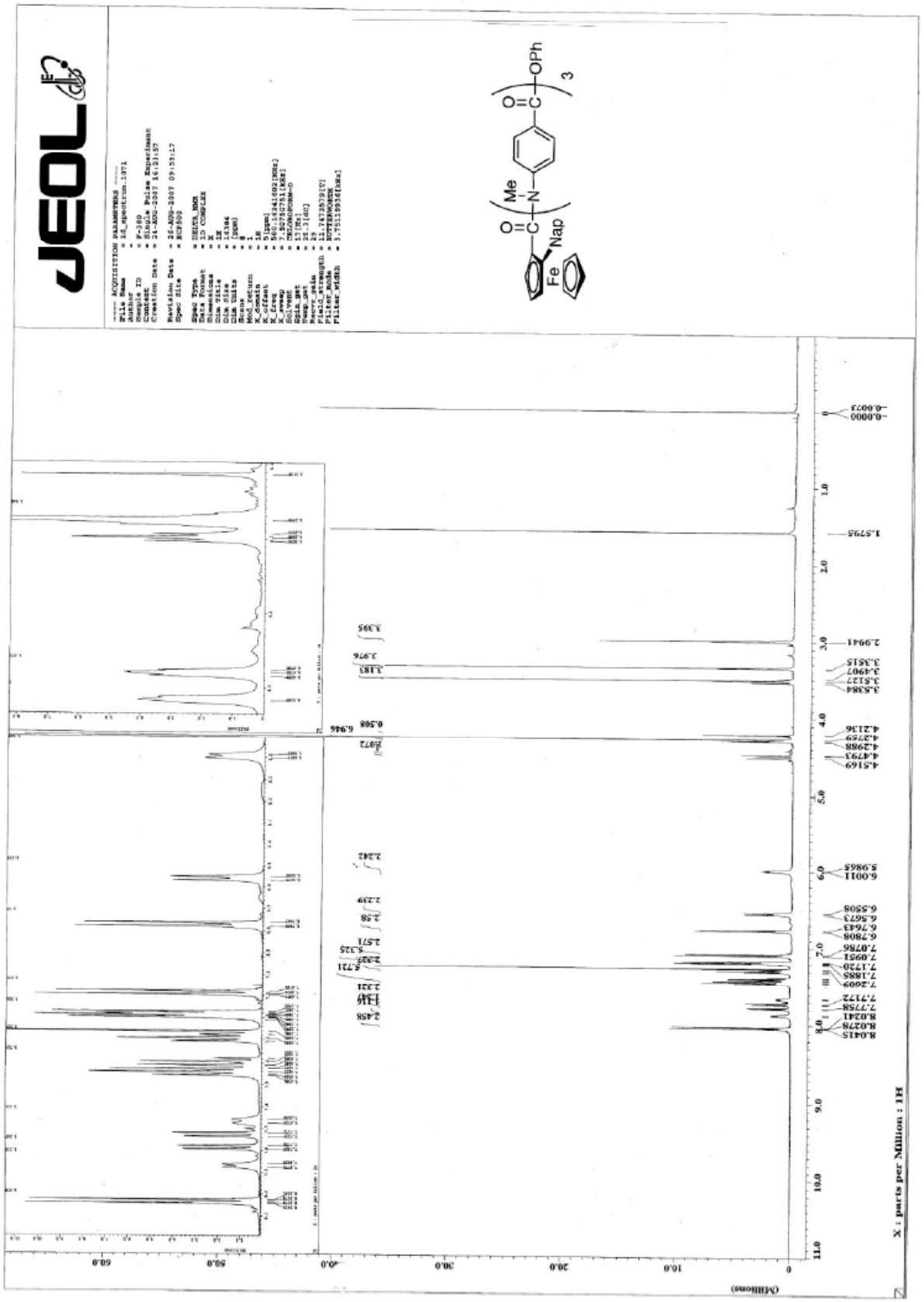
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