

Supporting Information

for

**Skeletal Rearrangement of Cyano-Substituted Iminoisobenzofurans into Alkyl
2-Cyanobenzoates Catalyzed by B(C₆F₅)₃**

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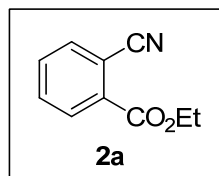
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1. General.

All the reactions were carried out under argon atmosphere using standard Schlenk techniques. Glassware was dried in an oven (130 °C) and heated under reduced pressure before use. For thin layer chromatography (TLC) analyses throughout this work, Merck precoated TLC plates (silica gel 60 GF254, 0.25 mm) were used. Silica gel column chromatography was carried out using Silica gel 60 N (spherical, neutral, 40-100 μ m) from Kanto Chemicals Co., Ltd. NMR spectra (^1H , $^{13}\text{C}\{^1\text{H}\}$) were recorded on Varian INOVA-600 (600 MHz) spectrometers. GC/MS analyses were carried out on a SHIMADZU GC-17A equipped with a SHIMADZU QP-5050 GC-MS system. Infrared spectra were recorded on a Shimadzu IRPrestige-21 spectrophotometer. Elemental analyses were carried out with a Perkin-Elmer 2400 CHN elemental analyzer at Okayama University. High resolution mass spectra (HRMS) were obtained by fast atom bombardment (FAB) using a double focusing magnetic sector mass spectrometer.

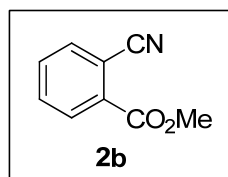
Cyano-substituted iminoisobenzofurans **1** and α -iminonitrile **3** were prepared by the palladium-catalyzed three-component coupling of arynes, isocyanides, and cyanoformates.¹⁾ 1-Adamantanyl isocyanide was prepared according to the literature procedures.²⁾ Unless otherwise noted, commercially available reagents were used without purification.

2. Experimental Procedures and Spectroscopic Data for the New Compounds.

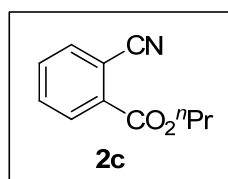


Ethyl 2-cyanobenzoate (2a).³⁾ A flame-dried 25 mL Schlenk with a magnetic stir bar was charged with $\text{B}(\text{C}_6\text{F}_5)_3$ (2.6 mg, 0.055 mmol, 5 mol %) in THF (1 mL) under argon. To this solution were added *N*-[3-Cyano-3-ethoxy-1(3*H*)-isobenzofuranylidene]-2,4,4-trimethyl-2-pentanamine (**1a**) (31.4 mg, 0.1 mmol). The reaction mixture was heated to 70 °C for 8 h, then cooled to ambient temperature, quenched with water, and extracted with diethyl ether (5 mL $\times$ 3). The combined extracts were washed with brine and dried over anhydrous sodium sulfate. The volatiles were removed under reduced pressure to give crude products, which were purified by silica gel column chromatography (eluent: hexane/ethyl acetate, 10:1) gave **2a** in 90% yield (15.8 mg, 0.09 mmol) as a white solid. From **1h**, **2a** was isolated in 88% yield (15.4 mg, 0.09 mmol). From **1i**, **2a** was isolated in 50% yield (8.8 mg, 0.05 mmol). From **3a**, **2a** was isolated in 97% yield (17.0 mg, 0.1

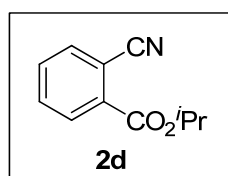
mmol). ^1H NMR (600 MHz, CDCl_3 , rt): δ 1.45 (t, $J = 7.2$ Hz, 3H), 4.47 (q, $J = 7.2$ Hz, 2H), 7.65-7.68 (m, 2H), 7.80-7.81 (m, 1H), 8.14-8.16 (m, 1H); ^{13}C NMR (150 MHz, CDCl_3 , rt): δ 14.1, 62.3, 112.9, 117.5, 131.1, 132.4, 132.5, 132.7, 134.7, 164.0. MS (EI, m/z (relative intensity)): 175 (M^+ , 25), 148 (10), 147 (17), 131 (13), 130 (100), 105 (16), 103 (41), 102 (41), 76 (16), 75 (18).



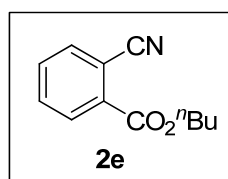
Methyl 2-cyanobenzoate (2b).⁴⁾ Isolated in 99% yield (15.9 mg, 0.099 mmol) as a white solid. ^1H NMR (600 MHz, CDCl_3 , rt): δ 4.00 (s, 3H), 7.66-7.69 (m, 2H), 7.80-7.82 (m, 1H), 8.13-8.15 (m, 1H); ^{13}C NMR (150 MHz, CDCl_3 , rt): δ 52.8, 112.9, 117.5, 131.1, 132.38, 132.44, 132.7, 134.8, 164.5. MS (EI, m/z (relative intensity)): 161 (M^+ , 23), 131 (23), 130 (100), 103 (13), 102 (41), 76 (10), 75 (16).



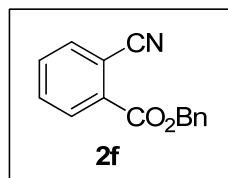
Propyl 2-cyanobenzoate (2c). Isolated in 89% yield (16.8 mg, 0.089 mmol) as a white solid. IR (KBr, cm^{-1}): 2972 (s), 2878 (s), 2228 (m, CN), 1719 (s), 1595 (m), 1446 (m), 1389 (m), 1273 (s), 1138 (s), 1080 (s), 935 (m), 760 (s), 694 (m), 662 (w). ^1H NMR (600 MHz, CDCl_3 , rt): δ 1.05 (t, $J = 7.2$ Hz, 3H), 1.85 (m, $J = 7.2$ Hz, 2H), 4.37 (t, $J = 6.6$ Hz, 2H), 7.65-7.69 (m, 2H), 7.80-7.81 (m, 1H), 8.14-8.16 (m, 1H); ^{13}C NMR (150 MHz, CDCl_3 , rt): δ 10.5, 21.9, 67.9, 112.9, 117.6, 131.2, 132.4, 132.5, 132.7, 134.8, 164.1. MS (EI, m/z (relative intensity)): 189 (M^+ , 0.04), 148 (36), 131 (10), 130 (100), 103 (15), 102 (29), 76 (9), 75 (10). Anal. Calc for $\text{C}_{11}\text{H}_{11}\text{NO}_2$: C 69.83; H 5.86; N 7.40%. Found: C 69.84; H 6.04; N 7.47%.



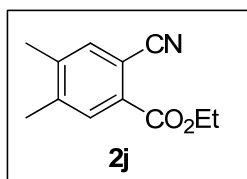
Isopropyl 2-cyanobenzoate (2d). Isolated in 94% yield (17.8 mg, 0.094 mmol) as a colorless oil. IR (KBr, cm^{-1}): 2982 (s), 2855 (m), 2230 (m, CN), 1722 (s), 1595 (m), 1447 (m), 1352 (m), 1182 (s), 1143 (s), 1107 (s), 1080 (s), 916 (m), 760 (s), 694 (m). ^1H NMR (600 MHz, CDCl_3 , rt): δ 1.43 (d, J = 6.6 Hz, 6H), 5.32 (m, J = 6.6 Hz, 1H), 7.64-7.68 (m, 2H), 7.79-7.80 (m, 1H), 8.12-8.14 (m, 1H); ^{13}C NMR (150 MHz, CDCl_3 , rt): δ 21.7, 70.4, 112.9, 117.6, 131.1, 132.3, 132.4, 133.1, 134.7, 163.6. MS (EI, m/z (relative intensity)): 189 (M^+ , 2), 148 (31), 131 (10), 130 (100), 103 (34), 102 (26), 76 (10), 75 (10). Anal. Calc for $\text{C}_{11}\text{H}_{11}\text{NO}_2$: C 69.83; H 5.86; N 7.40%. Found: C 69.82; H 5.98; N 7.47%.



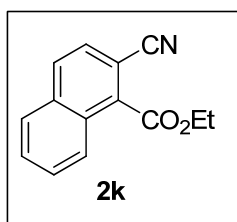
Butyl 2-cyanobenzoate (2e).⁵⁾ Isolated in 88% yield (17.9 mg, 0.088 mmol) as a colorless oil. ^1H NMR (600 MHz, CDCl_3 , rt): δ 0.98 (t, J = 7.2 Hz, 3H), 1.46-1.55 (m, 2H), 1.78-1.83 (m, 2H), 4.42 (t, J = 6.6 Hz, 2H), 7.65-7.69 (m, 2H), 7.80-7.81 (m, 1H), 8.14-8.16 (m, 1H); ^{13}C NMR (150 MHz, CDCl_3 , rt): δ 13.7, 19.2, 30.5, 66.1, 112.9, 117.6, 131.2, 132.4, 132.5, 132.7, 134.8, 164.1. MS (EI, m/z (relative intensity)): 203 (M^+ , 0.5), 148 (37), 131 (10), 130 (100), 103 (15), 102 (30), 76 (9), 75 (10).



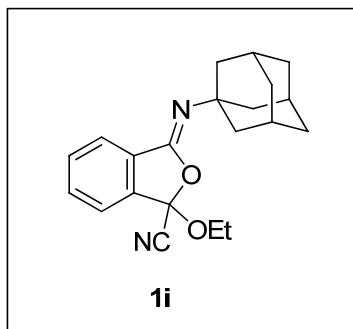
Benzyl 2-cyanobenzoate (2f). Isolated in 82% yield (19.4 mg, 0.082 mmol) as a colorless oil. IR (KBr, cm^{-1}): 2970 (w), 2891 (w), 2228 (m, CN), 1728 (s), 1595 (m), 1487 (m), 1454 (m), 1377 (m), 1271 (s), 1138 (s), 1076 (s), 964 (m), 760 (s), 696 (m), 662 (w). ^1H NMR (600 MHz, CDCl_3 , rt): δ 5.45 (s, 2H), 7.36-7.42 (m, 3H), 7.50-7.51 (m, 2H), 7.65-7.67 (m, 2H), 7.81-7.82 (m, 1H), 8.15-8.17 (m, 1H); ^{13}C NMR (150 MHz, CDCl_3 , rt): δ 67.8, 113.1, 117.5, 128.6, 128.66, 128.72, 131.2, 132.39, 132.42, 132.7, 134.8, 135.1, 163.8. MS (EI, m/z (relative intensity)): 237 (M^+ , 15), 209 (19), 148 (36), 131 (11), 130 (52), 107 (100), 104 (13), 103 (32), 102 (26), 91 (90), 90 (14), 89 (12), 79 (14), 77 (14), 75 (11), 65 (25). Anal. Calc for $\text{C}_{15}\text{H}_{11}\text{NO}_2$: C 75.94; H 4.67; N 5.90%. Found: C 75.56; H 4.69; N 5.85%.



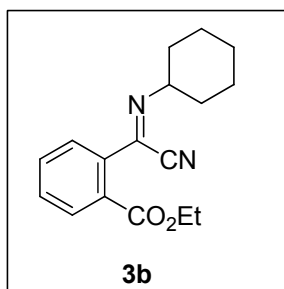
4,5-Dimethyl ethyl 2-cyanobenzoate (2j). Isolated in 89% yield (18.1 mg, 0.089 mmol) as a white solid. IR (KBr, cm^{-1}): 2976 (s), 2864 (s), 2228 (w, CN), 1728 (s), 1606 (w), 1560 (w), 1444 (m), 1382 (s), 1279 (s), 1121 (s), 1045 (m), 845 (w), 787 (w). ^1H NMR (600 MHz, CDCl_3 , rt): δ 1.44 (t, $J = 7.2$ Hz, 3H), 2.34 (s, 3H), 2.36 (s, 3H), 4.44 (q, $J = 7.2$ Hz, 2H), 7.54 (s, 1H), 7.89 (s, 1H); ^{13}C NMR (150 MHz, CDCl_3 , rt): δ 14.1, 19.6, 20.0, 62.0, 110.1, 117.9, 130.0, 132.2, 135.6, 142.1, 142.3, 164.3. MS (EI, m/z (relative intensity)): 203 (M^+ , 23), 175 (44), 159 (14), 158 (100), 131 (46), 130 (24), 104 (11), 103 (29), 77 (23). Anal. Calc for $\text{C}_{11}\text{H}_{11}\text{NO}_2$: C 69.83; H 5.86; N 7.40%. Found: C 69.83; H 6.08; N 7.40%.



Ethyl 2-cyano-1-naphthoate (2k). Isolated in 83% yield (18.7 mg, 0.083 mmol) as a white solid. IR (KBr, cm^{-1}): 2978 (s), 2866 (s), 2216 (w, CN), 1730 (m), 1383 (m), 1286 (m), 1253 (m), 1124 (s), 777 (m). ^1H NMR (600 MHz, CDCl_3 , rt): δ 1.50 (t, $J = 7.2$ Hz, 3H), 4.54 (q, $J = 7.2$ Hz, 2H), 7.71-7.78 (m, 2H), 7.95-7.98 (m, 1H), 8.12 (s, 2H), 8.46-8.49 (m, 1H); ^{13}C NMR (150 MHz, CDCl_3 , rt): δ 14.1, 62.4, 111.4, 115.9, 125.6, 126.7, 128.5, 129.2, 129.3, 132.5, 132.7, 132.8, 134.5, 164.6. MS (EI, m/z (relative intensity)): 225 (M^+ , 62), 197 (58), 181 (16), 180 (100), 153 (50), 152 (67), 126 (22), 125 (28), 75 (10). Anal. Calc for $\text{C}_{14}\text{H}_{11}\text{NO}_2$: C 74.65; H 4.92; N 6.22%. Found: C 74.65; H 4.74; N 6.18%.



1i: Isolated in 39% yield (65.5 mg, 0.20 mmol) as a yellow solid. IR (KBr, cm^{-1}): 2330 (w, $\text{C}\equiv\text{N}$), 1717 (s, $\text{C}=\text{N}$). ^1H NMR (300 MHz, CDCl_3 , rt): δ 1.33 (t, $J = 7.2$ Hz, 3H), 1.72 (s, 6H), 2.05 (s, 6H), 2.12 (s, 3H), 4.00 (m, 2H), 7.56-7.62 (m, 3H), 7.82-7.84 (m, 1H); ^{13}C NMR (150 MHz, CDCl_3 , rt): δ 14.9, 29.7, 36.5, 42.6, 55.7, 63.5, 98.9, 114.8, 122.5, 124.1, 131.6, 131.7, 132.3, 139.1. MS (EI, m/z (relative intensity)): 336 (M^+ , 3), 308 (1), 307 (6), 233 (3), 224 (1), 158 (2), 136 (11), 135 (100), 107 (10), 105 (4), 104 (2), 103 (3), 102 (5), 94 (2), 93 (18), 92 (2), 91 (8). HRMS (FAB $^+$): m/z Calcd for $\text{C}_{21}\text{H}_{24}\text{N}_2\text{O}_2$: ($\text{M}+\text{H}$) $^+$ 337.1916. Found: 337.1923.



3b: Isolated in 57% yield (81 mg, 0.29 mmol) as a yellow oil. IR (KBr, cm^{-1}): 2216 (w, $\text{C}\equiv\text{N}$), 1715 (s, $\text{C}=\text{N}$), 1622 (s, $\text{C}=\text{O}$). ^1H NMR (300 MHz, CDCl_3 , rt): δ 1.25-1.31 (m, 1H), 1.39 (t, $J = 6.6$ Hz, 3H), 1.42-1.88 (m, 9H), 3.81-3.88 (m, 1H), 4.39 (q, $J = 7.2$ Hz, 2H), 7.54-7.62 (m, 3H), 7.92-7.94 (m, 1H); ^{13}C NMR (150 MHz, CDCl_3 , rt): δ 14.1, 24.1, 25.3, 33.1, 61.8, 67.5, 110.2, 129.9, 130.2, 130.3, 130.7, 132.3, 135.7, 139.8, 166.4. MS (EI, m/z (relative intensity)): 284 (M^+ , 25), 256 (20), 255 (54), 238 (22), 211 (100), 183 (22), 159 (30), 158 (82), 157 (61), 148 (53), 130 (78), 104 (24), 103 (37), 102 (64), 81 (62), 67 (32). Anal. Calc for $\text{C}_{17}\text{H}_{20}\text{N}_2\text{O}_2$: C, 71.81; H, 7.09; N, 9.85%. Found: C, 71.89; H, 6.80; N, 9.46%.

3. Time-Course Experiment.

An NMR tube was charged with $\text{B}(\text{C}_6\text{F}_5)_3$ (0.6 mg, 0.001 mmol, 5 mol %) in $\text{THF-}d_8$ (1 mL) under argon. To this solution were added *N*-[3-cyano-3-ethoxy-1(3*H*)-isobenzofuranylidene]-2,4,4-trimethyl-2-pentanamine (**1a**) (7.9 mg, 0.025 mmol) and CH_2Br_2 (4.3 mg, 0.025 mmol). The reaction mixture was heated to 70 °C or room temperature at different reaction time, conversion of **1a** and yields of **2a** and **3a** were determined by the ^1H NMR spectra using CH_2Br_2 as an internal standard.

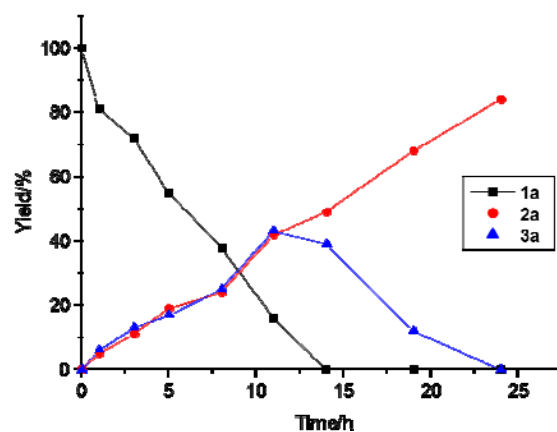
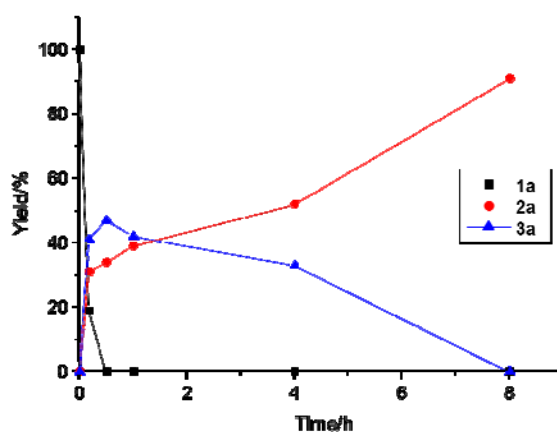
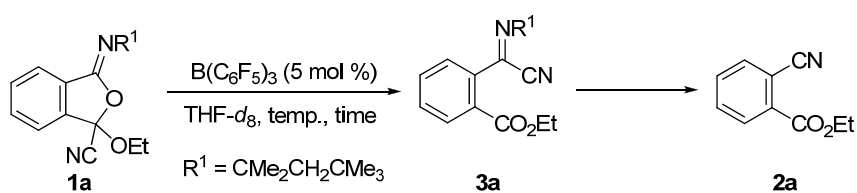


Figure S1. Time-Course Experiment (a) At 70 °C. (b) At room temperature.

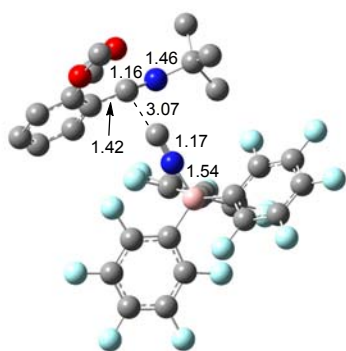
4. Theoretical Information

Table S1. Calculated energies and correction values to thermal energies of stationary points (a.u.) at the B3LYP/6-31G(d) level.

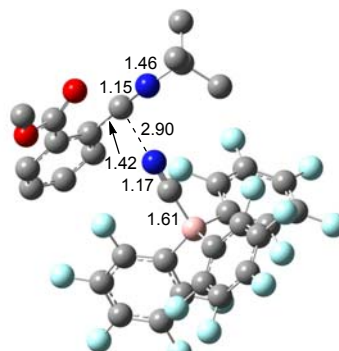
Structure	Total electronic energy	Zero-point correction	Thermal correction to Energy	Thermal correction to Enthalpy	Thermal correction to Gibbs Free Energy
1	-803.027026868	0.277189	0.294708	0.295652	0.232116
B(C ₆ F ₅) ₃	-2208.20630652	0.154298	0.183198	0.184142	0.093012
INT1	-3011.24899942	0.433226	0.480989	0.481934	0.34695
TS1	-3011.22053569	0.430526	0.479041	0.479986	0.345491
INT2	-3011.22891293	0.430416	0.480373	0.481317	0.342085
INT2'	-3011.24696076	0.430945	0.480659	0.481603	0.343609
TS2	-3011.19654125	0.425772	0.475936	0.47688	0.335471
TS2'	-3011.21083673	0.425452	0.475968	0.476912	0.334345
(INT3)	—	—	—	—	—
INT3'	-3011.21631565	0.425555	0.475879	0.476823	0.337710
TS3	-3011.1974242	0.424551	0.475041	0.475985	0.334365
TS3'	-3011.21631565	0.425555	0.475879	0.476823	0.337710
2 + 'BuCN–B(C₆F₅)₃	-3011.28576717	0.43103	0.481231	0.482175	0.337129
2 + 'BuNC–B(C₆F₅)₃	-3011.26669607	0.430807	0.481058	0.482003	0.336803

Table S2. Uncorrected energies of stationary points (a.u.) at the B3LYP(PCM)/6-311+G(d)//B3LYP/6-31G(d) level.

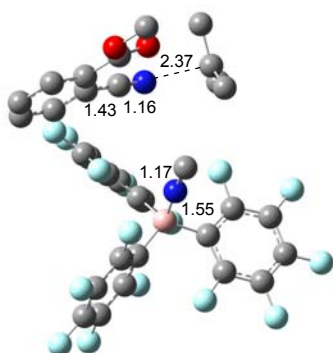
Structure	Total electronic energy
1	-803.242641743
B(C ₆ F ₅) ₃	-2208.93331756
INT1	-3012.18776740
TS1	-3012.16820719
INT2	-3012.18364757
INT2'	-3012.20020726
TS2	-3012.15566885
TS2'	-3012.17240632
(INT3)	—
INT3'	-3012.17364671
TS3	-3012.15371077
TS3'	-3012.17380538
2 + 'BuCN–B(C₆F₅)₃	-3012.23416486
2 + 'BuNC–B(C₆F₅)₃	-3012.21739235



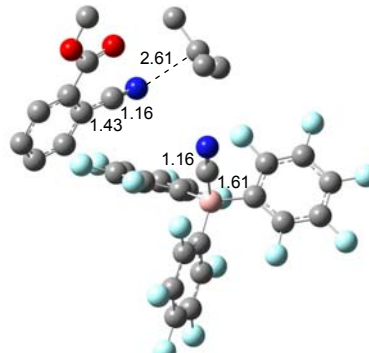
INT2



INT2'



TS2



TS2'

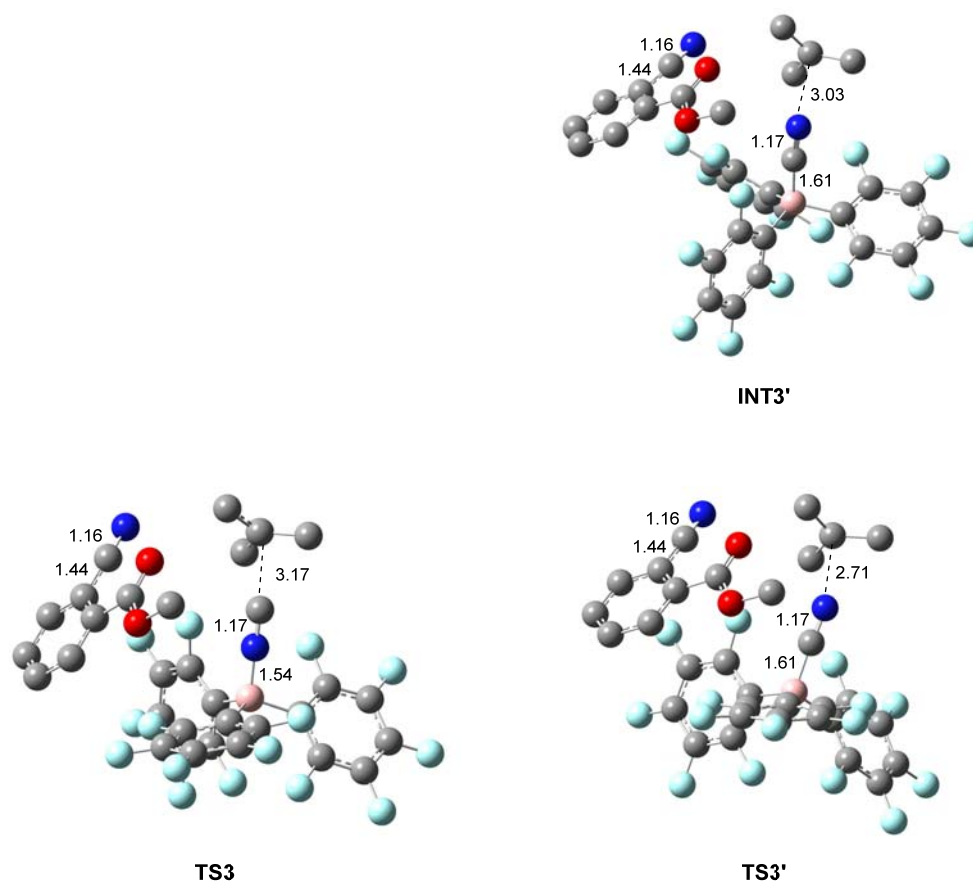


Figure S2. Representative structures of stationary points at the B3LYP/6-31G(d) level. Atomic distances are also shown in angstrom unit. Hydrogen atoms are omitted for clarity.

Table S3. Cartesian Coordinates for Optimized Structures and Imaginary Frequencies shown for TSs.

1				C	-0.36139200	-5.95688200	-0.06302200
C	-5.68487900	0.16519600	2.43698000	C	-2.49389800	-5.02662700	-0.70022800
C	-4.45238000	0.03120900	3.06377800	C	-1.26803700	-5.58679200	-1.05449900
C	-4.27168900	0.35814100	4.40215500	F	-3.98957300	-4.30147900	0.92672400
C	-5.38449800	0.82621600	5.10685300	F	-3.36028900	-4.66417800	-1.65119000
C	-6.63268500	0.96076200	4.47888400	F	-0.96360200	-5.76808500	-2.33796800
C	-6.79818700	0.63328400	3.13264600	F	0.81102800	-6.50157200	-0.40223400
H	-3.30399400	0.25525200	4.88332700	F	0.21564400	-6.13507300	2.18309800
H	-5.28187600	1.09036400	6.15545200	F	-0.09507400	-3.12294100	2.62838400
H	-7.48071300	1.32561400	5.05147300	F	1.79442000	-2.37881400	4.37478700
H	-7.75414700	0.73305500	2.62891600	F	1.79672100	-3.38652800	6.90835700
O	-4.21939600	-0.63324400	0.83305900	F	-0.13165300	-5.15239500	7.68138600
C	-3.45062400	-0.46254000	2.03974000	F	-2.04349300	-5.90097700	5.96139000
C	-5.55755600	-0.24531400	1.02948900	F	-4.09887700	-7.06114700	2.23423600
N	-6.47297000	-0.25788300	0.16578100	F	-6.60539000	-7.43685700	3.09932000
C	-6.31356700	-0.68079800	-1.23918100	F	-3.64195600	-3.39723700	5.23281400
C	-5.88363400	-2.16044300	-1.31474000	F	-6.15715300	-3.78585200	6.06667800
C	-7.69973000	-0.51606700	-1.88818900	F	-7.65664800	-5.80546200	5.01463100
C	-5.29696300	0.22143800	-1.96832400				
H	-4.89001400	-2.31134700	-0.88483100	INT1			
H	-6.59515500	-2.79327600	-0.77276000	C	-5.68020700	0.21019200	2.43038000
H	-5.86251000	-2.49201000	-2.35943500	C	-4.44939400	0.06103300	3.05942100
H	-8.03047000	0.52641000	-1.82734200	C	-4.26693300	0.32243700	4.41186700
H	-7.67492800	-0.81227000	-2.94322000	C	-5.38164900	0.76719400	5.12818100
H	-8.44068100	-1.13480900	-1.37074300	C	-6.62573000	0.93374900	4.49926500
H	-5.26287800	-0.03561500	-3.03341500	C	-6.79302000	0.65447000	3.14181900
H	-5.58827400	1.27424500	-1.88224500	H	-3.30584100	0.17073300	4.89320700
H	-4.29171200	0.10529700	-1.55442900	H	-5.28499200	0.98205800	6.18812200
O	-2.44254100	0.48044600	1.88918600	H	-7.47432200	1.27789400	5.08325600
C	-1.45093700	0.18965300	0.89557900	H	-7.75084700	0.76838500	2.64504200
H	-0.74006100	1.01577000	0.94256900	O	-4.19527100	-0.54639000	0.81506100
H	-0.93467100	-0.75285100	1.11503100	C	-3.45083500	-0.39472200	2.01843100
H	-1.89959700	0.14197000	-0.10154200	C	-5.55798600	-0.18393900	1.01849600
C	-2.88882700	-1.80178100	2.38534300	N	-6.46341800	-0.23117300	0.15283500
N	-2.43384300	-2.82631000	2.68511500	C	-6.30440400	-0.68839700	-1.24338500
				C	-5.90499500	-2.17903300	-1.26709200
B(C₆F₅)₃				C	-7.68435400	-0.51567500	-1.90271200
B	-2.27566400	-4.98649100	3.19432300	C	-5.26760400	0.17229700	-1.99323600
C	-3.74685500	-5.21033100	3.69160200	H	-4.92307800	-2.34883900	-0.81620600
C	-4.56797300	-6.22506200	3.17461200	H	-6.64242800	-2.78043300	-0.72432700
C	-4.33326300	-4.40982300	4.68489000	H	-5.87239000	-2.53849700	-2.30175100
C	-5.86967600	-6.44500700	3.61049400	H	-7.99320400	0.53495900	-1.87950400
C	-5.63809400	-4.58662700	5.13091300	H	-7.66023600	-0.84752500	-2.94668600
C	-6.40834800	-5.61544800	4.59216200	H	-8.44013600	-1.10144700	-1.36915800
C	-1.16241500	-4.54882500	4.20973800	H	-5.24865900	-0.10796900	-3.05239400
C	-1.12170600	-5.02481600	5.52990400	H	-5.53019500	1.23410300	-1.92841100
C	-0.13806400	-3.65432600	3.86098200	H	-4.26221200	0.03706200	-1.58596700
C	-0.13741200	-4.65681000	6.44013600	O	-2.40301100	0.49733100	1.91628700
C	0.85045700	-3.24748600	4.74987200	C	-1.45102200	0.24141000	0.87059300
C	0.85187600	-3.75762100	6.04670800	H	-0.68793200	1.01227000	0.97837900
C	-1.91710800	-5.20031900	1.68186300	H	-0.98903700	-0.74725200	0.98953400
C	-0.69239000	-5.75061600	1.27140900	H	-1.92475000	0.31408600	-0.11204200
C	-2.79855600	-4.85439400	0.64524700	C	-2.93575800	-1.76706700	2.35748700

N	-2.56071100	-2.79534200	2.70622000	H	-3.72980100	-0.20196400	-1.64486700
B	-2.07998900	-4.24596400	3.12896900	H	-3.39363400	-1.89043400	-1.19275300
C	-3.46630000	-5.08125900	3.40147600	H	-3.90858000	-1.50259700	-2.84314900
C	-3.70519100	-6.38712700	2.96700000	H	-6.97804400	-3.06393900	-1.32509500
C	-4.48019400	-4.52607300	4.18708300	H	-5.84809500	-3.14912700	-2.69507200
C	-4.87211600	-7.08790900	3.27081500	H	-5.29450200	-3.58992600	-1.06995600
C	-5.66076900	-5.18769100	4.51032500	H	-6.35131000	-0.69019400	-3.24194400
C	-5.85821800	-6.48421400	4.04436200	H	-7.48027500	-0.61718100	-1.87348500
C	-1.25919500	-4.12778600	4.53827600	H	-6.14958400	0.55900200	-1.99626500
C	-0.85066600	-5.31589200	5.15336100	O	-2.59717200	1.55822500	2.36067400
C	-0.98177100	-2.97008000	5.26487900	C	-1.49278800	1.69857700	1.42705100
C	-0.21386900	-5.36999700	6.38766800	H	-0.85049200	2.46044600	1.86434400
C	-0.34893400	-2.97656600	6.50814400	H	-0.99430300	0.72753100	1.37980300
C	0.03711900	-4.18464300	7.07542900	H	-1.86438300	2.00696100	0.44846800
C	-1.22614900	-4.71981600	1.81307200	C	-1.96095400	-1.38912400	2.64427600
C	0.12351400	-5.07813600	1.79354300	N	-1.98047600	-2.52115700	2.93625500
C	-1.86087400	-4.76016200	0.56618400	B	-2.06155200	-4.04069400	3.18994100
C	0.79127300	-5.46972000	0.63132900	C	-3.62155900	-4.38369700	3.64264500
C	-1.23415600	-5.13900000	-0.61485300	C	-4.38898400	-5.45113800	3.16942400
C	0.10996600	-5.50224500	-0.57957700	C	-4.24149600	-3.62474400	4.64032700
F	-3.16466900	-4.40708000	0.47198900	C	-5.67817900	-5.73648300	3.62157600
F	-1.90291800	-5.15291300	-1.77591800	C	-5.52241600	-3.87896300	5.12376600
F	0.73891600	-5.86801400	-1.70062500	C	-6.25415700	-4.94071800	4.60450900
F	2.08735900	-5.80391400	0.67516900	C	-1.11214400	-4.49922400	4.45033700
F	0.87155100	-5.05459700	2.91179500	C	-1.12239300	-5.84019900	4.84727300
F	-1.31278600	-1.74250500	4.78966800	C	-0.33139700	-3.66299900	5.25049600
F	-0.11360900	-1.82577900	7.15495000	C	-0.42327400	-6.33635800	5.94109700
F	0.64613200	-4.20973300	8.26523200	C	0.38533900	-4.11833000	6.35980400
F	0.15789100	-6.54144400	6.91817800	C	0.33950000	-5.46130900	6.70996400
F	-1.06142700	-6.48839500	4.52337900	C	-1.63865100	-4.69026700	1.72852100
F	-2.79645300	-7.04617900	2.22706300	C	-0.50220200	-5.45355700	1.45513000
F	-5.04964400	-8.33808000	2.82504100	C	-2.41227200	-4.39971300	0.60236100
F	-4.33670700	-3.27233300	4.68154200	C	-0.16776900	-5.90998600	0.17680000
F	-6.59817400	-4.59329200	5.26185600	C	-2.11774000	-4.82548100	-0.68532600
F	-6.98275200	-7.14336700	4.34103400	C	-0.97967500	-5.59509400	-0.90488700
TS1 Imaginary frequency = 187.7115i cm ⁻¹				F	-3.53767000	-3.64431100	0.73095800
				F	-2.91587800	-4.49089200	-1.72084500
				F	-0.67165500	-6.01552100	-2.13894100
C	-5.54496700	-0.40330700	2.39865600	F	0.94061300	-6.64020200	-0.01490100
C	-4.56073100	0.36308700	3.03155100	F	0.36903400	-5.78868000	2.42541900
C	-4.61532500	0.63511500	4.39380700	F	-0.21753100	-2.34498600	4.99382800
C	-5.69581600	0.12209500	5.11488400	F	1.11864000	-3.26305500	7.09196100
C	-6.69038400	-0.63619700	4.48190300	F	1.02231000	-5.91104400	7.77188900
C	-6.62694000	-0.91401300	3.11400100	F	-0.47437800	-7.63885000	6.26135300
H	-3.83107800	1.20739700	4.87674700	F	-1.83536300	-6.73672300	4.13048600
H	-5.76024900	0.29938700	6.18346300	F	-3.91338000	-6.28502300	2.22560800
H	-7.50791800	-1.03933900	5.06932300	F	-6.36808000	-6.76950000	3.11345300
H	-7.38235600	-1.51763600	2.62290100	F	-3.59636000	-2.57992800	5.20494400
O	-3.77425400	0.33802000	0.86097000	F	-6.06584200	-3.09841100	6.08115000
C	-3.55152200	0.74176000	2.04156600	F	-7.49500500	-5.19147400	5.04810800
C	-5.27579200	-0.61470500	0.98749000	INT2			
N	-5.72467100	-1.16803400	0.02294500				
C	-5.51098400	-1.44855800	-1.40143700				
C	-4.03818400	-1.24066900	-1.78798900	C	-4.90336600	0.06889700	3.02543300
C	-5.93847700	-2.90966400	-1.63079900	C	-3.86353100	1.02524500	3.05754400
C	-6.43534900	-0.48366300	-2.17033300	C	-3.51998600	1.59678700	4.27873900
				C	-4.21110100	1.24129500	5.44132100

C	-5.23977400	0.29831100	5.39950300	F	-0.36640700	-5.25633100	7.92924100
C	-5.58686600	-0.30563800	4.19350300	F	-1.02633400	-7.32898700	6.26208600
H	-2.71133800	2.31745200	4.31466300	F	-1.86438800	-6.83361600	3.76033600
H	-3.93452000	1.69673700	6.38734700	F	-3.52181500	-6.92852600	1.47524500
H	-5.75958100	0.01397700	6.30855800	F	-6.05843400	-7.66055800	1.75499300
H	-6.33605000	-1.08788600	4.15846400	F	-4.46154800	-2.89912700	3.83044400
O	-3.74122100	1.23513900	0.68991800	F	-7.01425000	-3.62160300	4.03671600
C	-3.20168800	1.39581500	1.76982600	F	-7.85854300	-6.03642100	3.02322200
C	-5.23262200	-0.58246400	1.80522600				
N	-5.61280000	-1.16403500	0.88257500	INT2'			
C	-5.90772500	-1.75193500	-0.42550800	C	-4.47107900	-0.04047100	3.09550300
C	-4.61195900	-1.64310100	-1.25113700	C	-3.39130000	0.87136700	3.08323500
C	-6.32465100	-3.21467400	-0.20592300	C	-2.76371300	1.18102300	4.28670100
C	-7.04875000	-0.91804900	-1.03598100	C	-3.20498300	0.60695900	5.48186600
H	-4.28973200	-0.60184800	-1.33250400	C	-4.27834500	-0.28453500	5.48711600
H	-3.81196800	-2.22911400	-0.79504600	C	-4.91291000	-0.62237600	4.29469500
H	-4.81376400	-2.03836900	-2.25188100	H	-1.92491900	1.86692600	4.28136100
H	-7.20852600	-3.28486400	0.43558300	H	-2.69749700	0.84581300	6.41055900
H	-6.56991400	-3.65018300	-1.17933900	H	-4.60851400	-0.73681600	6.41654400
H	-5.50910500	-3.79295100	0.23298500	H	-5.71346600	-1.35194700	4.27702900
H	-7.28361400	-1.32348500	-2.02470200	O	-3.66579700	1.39541200	0.77566500
H	-7.95217900	-0.96831900	-0.41992200	C	-2.98222700	1.47256300	1.78034600
H	-6.75119700	0.12843100	-1.15119000	C	-5.11308800	-0.43435000	1.88951300
O	-1.99749000	1.93503200	1.95089100	N	-5.76294400	-0.81026900	1.01255000
C	-1.25310100	2.21275600	0.74665800	C	-6.30824400	-1.33746400	-0.23609700
H	-0.31190400	2.64503000	1.08405200	C	-5.31866500	-0.92635600	-1.34219100
H	-1.08151800	1.27965000	0.20569500	C	-6.38924500	-2.86653900	-0.08646700
H	-1.80093700	2.91467100	0.11350900	C	-7.69753800	-0.70911700	-0.43525100
C	-2.37575700	-1.70327300	1.70991400	H	-5.25681900	0.16219000	-1.42764700
N	-2.33519700	-2.81372600	2.08397100	H	-4.32385100	-1.32108200	-1.12146500
B	-2.28033400	-4.29646700	2.50165100	H	-5.67440100	-1.33910900	-2.29170300
C	-3.84909600	-4.84671700	2.59820600	H	-7.00974600	-3.14947300	0.76873100
C	-4.33023600	-6.06814700	2.11650400	H	-6.84118300	-3.27642100	-0.99525800
C	-4.80730600	-4.08422500	3.26859400	H	-5.39159300	-3.29478500	0.03409600
C	-5.65815700	-6.48123500	2.25138100	H	-8.11503700	-1.07779300	-1.37688600
C	-6.14280300	-4.44643800	3.41276600	H	-8.37913800	-0.98721800	0.37482000
C	-6.57781800	-5.66268400	2.89909000	H	-7.63410400	0.38206300	-0.48953100
C	-1.66462400	-4.48350300	4.01628000	O	-1.80843300	2.10689900	1.84990100
C	-1.54990600	-5.77561500	4.53923100	C	-1.33581900	2.68257900	0.61483600
C	-1.31977700	-3.46539600	4.90733200	H	-0.37483200	3.13434800	0.85776500
C	-1.11797500	-6.06205300	5.82893600	H	-1.21890900	1.90124400	-0.13933300
C	-0.88414300	-3.70759800	6.21238600	H	-2.04036600	3.43609400	0.25436700
C	-0.78146700	-5.01151900	6.67846400	B	-2.44835900	-4.45770500	2.32289400
C	-1.40270100	-5.00801100	1.29823000	C	-3.89121400	-5.28360400	2.33839000
C	-0.10879500	-5.51795800	1.41734300	C	-4.04547600	-6.64794600	2.06729400
C	-1.90800800	-5.03214000	-0.00369700	C	-5.08083100	-4.63996700	2.67850300
C	0.61756500	-6.03454800	0.34185200	C	-5.27451800	-7.30845700	2.10191800
C	-1.22463600	-5.53172200	-1.10526000	C	-6.33006400	-5.25057900	2.70896300
C	0.05726000	-6.04425600	-0.92900300	C	-6.43239400	-6.60477500	2.41650400
F	-3.15071700	-4.53860000	-0.25672000	C	-2.00140900	-4.26988100	3.89816200
F	-1.78329100	-5.52232000	-2.32736300	C	-1.82792300	-5.39752100	4.70823900
F	0.74171600	-6.53160100	-1.97241700	C	-1.82856600	-3.05616400	4.56244100
F	1.85779700	-6.51179800	0.52587500	C	-1.52719400	-5.34527300	6.06577400
F	0.53538700	-5.52520200	2.60119000	C	-1.53575900	-2.95505200	5.92295000
F	-1.38926100	-2.16491200	4.55897300	C	-1.38459300	-4.10608200	6.68425300
F	-0.56868800	-2.68257300	7.02356800	C	-1.30687500	-5.15919600	1.36143300

C	0.01940900	-5.41103700	1.71380800	H	-4.31820900	4.36312600	0.17464700
C	-1.62311400	-5.47172700	0.03541400	C	-2.23205700	-2.58420600	1.21604100
C	0.95907900	-5.95096900	0.83340000	N	-2.24077500	-3.59311800	1.80560000
C	-0.72194400	-6.01062700	-0.87518600	B	-2.29826800	-4.99007600	2.46498900
C	0.58730000	-6.25483000	-0.46993100	C	-3.89061500	-5.29488900	2.81754200
F	-2.87759000	-5.25097100	-0.42247900	C	-4.56494200	-6.49835100	2.59520600
F	-1.09702800	-6.29209600	-2.13347300	C	-4.65590900	-4.31967300	3.46052300
F	1.47718600	-6.77073300	-1.32864700	C	-5.89952500	-6.71056000	2.94543700
F	2.22066700	-6.17120300	1.23575700	C	-5.98892500	-4.48599100	3.82097400
F	0.48168700	-5.12807800	2.95012600	C	-6.62299500	-5.69510800	3.56072000
F	-1.93989700	-1.87808800	3.90756600	C	-1.50647500	-5.01907300	3.90426100
F	-1.40462000	-1.74497600	6.50570800	C	-1.48085500	-6.21352400	4.63095800
F	-1.10478000	-4.02517700	7.99240100	C	-0.91345500	-3.93282100	4.54989400
F	-1.37597600	-6.46893500	6.78194700	C	-0.91190300	-6.34780600	5.89197700
F	-1.94164800	-6.62742700	4.16937200	C	-0.33309400	-4.02216900	5.81742800
F	-2.98938800	-7.41385600	1.74676200	C	-0.33145400	-5.23470000	6.49426900
F	-5.35137200	-8.61768900	1.82532300	C	-1.66540000	-5.97798600	1.30199900
F	-5.07896100	-3.31343900	2.99419600	C	-0.42929000	-6.62411000	1.35856700
F	-7.43476600	-4.52678300	2.98596300	C	-2.33317900	-6.12832700	0.08388800
F	-7.62275300	-7.21850500	2.43559600	C	0.09454700	-7.37853700	0.30577700
C	-2.71376600	-3.04724000	1.59338500	C	-1.85143300	-6.86260800	-0.99256900
N	-2.89918000	-2.07474900	0.97861400	C	-0.61995900	-7.50093200	-0.87882700
TS2				F	-3.53993800	-5.53089100	-0.10338400
Imaginary frequency = 103.5237i cm ⁻¹				F	-2.55613500	-6.95842500	-2.13377700
C	-4.95047500	0.30423900	3.21924300	F	-0.12961000	-8.21504800	-1.90102100
C	-4.52094500	1.65303800	3.16543700	F	1.28967800	-7.97592200	0.42647500
C	-4.37931900	2.36130200	4.36288300	F	0.35642900	-6.54067300	2.44999400
C	-4.66142700	1.75609600	5.58773800	F	-0.86468100	-2.71312600	3.97888800
C	-5.08721300	0.42867700	5.63235700	F	0.22113400	-2.93895200	6.38876900
C	-5.23001200	-0.30177800	4.45382000	F	0.22111100	-5.33327000	7.71172800
H	-4.04593100	3.39119400	4.32583600	F	-0.91775400	-7.52802500	6.53132300
H	-4.54469500	2.32325700	6.50625600	F	-2.02629200	-7.32597500	4.09293900
H	-5.30322600	-0.04705000	6.58388900	F	-3.94867400	-7.54154900	2.01074000
H	-5.54443600	-1.33740900	4.47956800	F	-6.49283000	-7.88675100	2.69159500
O	-4.43259000	1.79126300	0.76580900	F	-4.10477000	-3.12316700	3.78177400
C	-4.23271900	2.30392800	1.85377200	F	-6.66816400	-3.48596800	4.42546400
C	-5.10520200	-0.49960400	2.04268800	F	-7.90661700	-5.87790100	3.89962500
N	-5.26681600	-1.21607400	1.14205700	TS2'			
C	-4.77674500	-1.37478700	-1.17459100	Imaginary frequency = 75.6507i cm ⁻¹			
C	-3.38448300	-0.94943600	-1.14260100	C	-4.92806900	0.42475100	3.25694000
C	-5.06916900	-2.82557100	-1.26924100	C	-4.71270400	1.82035100	3.14152000
C	-5.84712000	-0.38522500	-1.45242400	C	-4.60506700	2.58309100	4.30983000
H	-3.24769300	0.13088900	-1.19577300	C	-4.70776700	1.98540000	5.56564900
H	-2.90135800	-1.37478700	-0.21373700	C	-4.91996200	0.61084600	5.67159000
H	-2.82953600	-1.47025100	-1.93727600	C	-5.02922200	-0.17178600	4.52346400
H	-6.08347700	-3.06463000	-0.94582000	H	-4.43793000	3.64983200	4.22515100
H	-4.98480800	-3.08855300	-2.33763800	H	-4.61932200	2.59535900	6.45960600
H	-4.33743400	-3.43263600	-0.73002000	H	-4.99728000	0.14058300	6.64700300
H	-5.80201300	-0.20465100	-2.54105500	H	-5.18867800	-1.24032700	4.59445800
H	-6.84392400	-0.75522300	-1.20729300	O	-4.67662400	1.87775700	0.73446400
H	-5.64433200	0.56683100	-0.95671800	C	-4.59792400	2.46461600	1.80080900
O	-3.72484600	3.53900400	1.99940800	C	-5.05098400	-0.43899500	2.11889700
C	-3.41727700	4.23873900	0.78076700	N	-5.17270800	-1.20757200	1.25523000
H	-3.02692900	5.20650500	1.09425800	C	-4.31113000	-1.33577900	-1.21021900
H	-2.66774000	3.68869100	0.20638800	C	-3.04367900	-0.65071300	-0.94999800

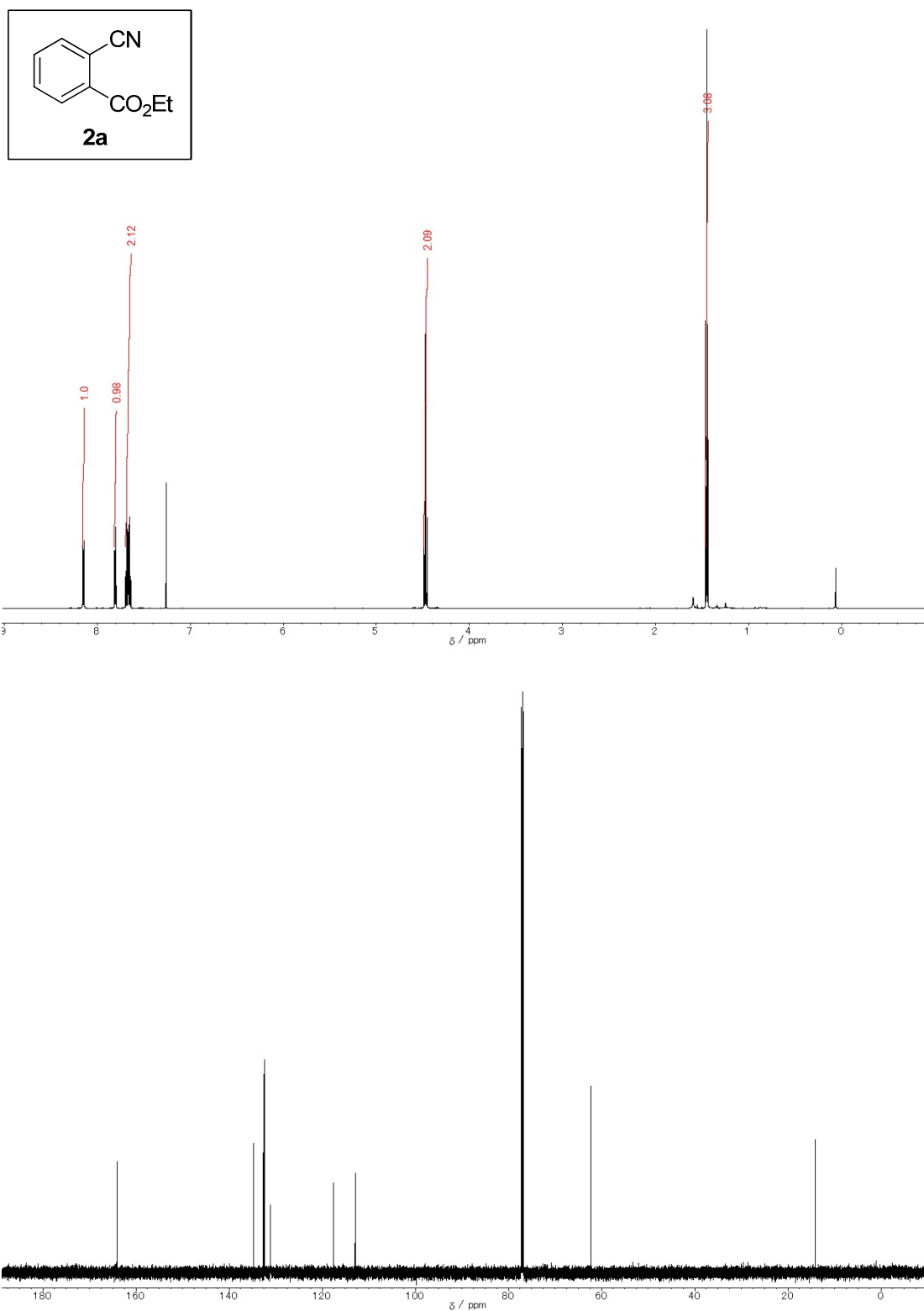
C	-4.30773300	-2.80103600	-1.30337700	C	-4.57350600	0.64279300	5.85137500
C	-5.52392800	-0.55999800	-1.53226800	C	-5.36774600	0.38463700	6.96815300
H	-3.15055400	0.42383500	-0.80532800	C	-6.67478900	-0.07701600	6.80630500
H	-2.56420500	-1.15274000	-0.08030400	C	-7.18638700	-0.28184200	5.52717000
H	-2.35187000	-0.87067700	-1.77865300	H	-3.55461800	0.99073600	5.97153800
H	-5.27054100	-3.23017800	-1.58188100	H	-4.96242200	0.53904000	7.96366500
H	-3.51539300	-3.14078700	-1.98353700	H	-7.29469500	-0.28593900	7.67292600
H	-3.98606400	-3.18856300	-0.32199500	H	-8.19348500	-0.65995700	5.38889200
H	-5.43861600	-0.35752700	-2.61767400	O	-4.66860800	0.82348900	2.22601600
H	-6.44322800	-1.12593500	-1.37302400	C	-4.22839500	0.75294800	3.36165400
H	-5.54330500	0.40281800	-1.01783700	C	-6.98432300	-0.27721000	3.11526200
O	-4.39355100	3.79053800	1.88917400	N	-7.55527900	-0.53493300	2.13471200
C	-4.26590100	4.49075500	0.63991300	C	-5.32348500	-1.57494100	-0.89590800
H	-4.11609000	5.53608400	0.90859900	C	-4.35536300	-1.98311500	-1.91264300
H	-3.40931300	4.11169500	0.07665200	C	-6.03967600	-2.60140800	-0.12624600
H	-5.17280200	4.37206900	0.04163500	C	-5.53102400	-0.16970900	-0.58609500
B	-2.30668300	-5.11519600	2.47228600	H	-4.28148300	-1.28378300	-2.74928000
C	-3.90566100	-5.29874700	2.87031700	H	-3.40574900	-1.90924500	-1.33410400
C	-4.67205300	-6.45062200	2.67288200	H	-4.45160900	-3.02370200	-2.22811700
C	-4.57549000	-4.27208500	3.53891500	H	-6.83863500	-2.96052900	-0.80255300
C	-6.00374400	-6.56751800	3.07452000	H	-5.40101400	-3.46833900	0.06918100
C	-5.90099300	-4.34401700	3.95306600	H	-6.51242400	-2.20859200	0.77535100
C	-6.62832500	-5.50494800	3.71817500	H	-5.21634500	0.51791900	-1.37319800
C	-1.47744500	-5.23119400	3.88363600	H	-6.53573900	0.03295700	-0.20030200
C	-1.49966000	-6.43622200	4.59211200	H	-4.88354200	0.00395100	0.30728500
C	-0.80469100	-4.19043100	4.52383300	O	-2.94977000	0.95786000	3.68254900
C	-0.89808300	-6.61960200	5.83198300	C	-2.05083000	1.23124900	2.58626000
C	-0.18905200	-4.32840000	5.76939300	H	-1.06150700	1.27793600	3.03906900
C	-0.23540300	-5.55000700	6.42885200	H	-2.10349700	0.42622900	1.85200600
C	-1.79028800	-6.13087100	1.27269900	H	-2.31233000	2.18664000	2.12266800
C	-0.59712600	-6.85660500	1.27639900	B	-2.43998300	-4.06406600	2.15864500
C	-2.51479300	-6.23267400	0.08215200	C	-3.95842400	-4.59478700	2.56445600
C	-0.16886200	-7.64119000	0.20283600	C	-4.42977900	-5.90178800	2.40816500
C	-2.12779200	-6.99407700	-1.01351700	C	-4.85241900	-3.73221700	3.20640700
C	-0.93811300	-7.71322700	-0.95144500	C	-5.69154500	-6.32055200	2.83344000
F	-3.68243500	-5.54972300	-0.05708700	C	-6.11819500	-4.10751800	3.64836700
F	-2.88228700	-7.03467500	-2.12610200	C	-6.54540300	-5.41730300	3.45667900
F	-0.53826900	-8.45453400	-1.99348700	C	-1.61706600	-3.92517100	3.57225000
F	0.98778500	-8.31677900	0.27420900	C	-1.41641400	-5.06189800	4.36173800
F	0.23721700	-6.82704400	2.33382400	C	-1.15451500	-2.73755000	4.13762300
F	-0.71296500	-2.96960300	3.95903500	C	-0.80608200	-5.04294300	5.61077100
F	0.44377700	-3.28717700	6.33620400	C	-0.53946600	-2.66929400	5.38857900
F	0.34964000	-5.69849800	7.62573600	C	-0.36429700	-3.82928600	6.13218300
F	-0.95062400	-7.80617500	6.45711300	C	-1.69773400	-4.98429200	1.00039000
F	-2.12750600	-7.50599700	4.05922000	C	-0.39558200	-5.48631100	1.06361300
F	-4.15330000	-7.53307700	2.06559400	C	-2.34504200	-5.24380400	-0.20980500
F	-6.68850000	-7.69800700	2.84475600	C	0.20512300	-6.20482700	0.02680900
F	-3.92636300	-3.11677300	3.83005100	C	-1.79056700	-5.94705000	-1.27095300
F	-6.48235500	-3.30039300	4.58270500	C	-0.49466900	-6.43969900	-1.14999600
F	-7.90693900	-5.59780200	4.10813100	F	-3.61467100	-4.78621800	-0.41391600
N	-2.08289200	-2.69846300	1.14002100	F	-2.48655000	-6.14447400	-2.40363900
C	-2.15336700	-3.67260700	1.77356400	F	0.06900300	-7.11983200	-2.15571800
				F	1.45887600	-6.66062200	0.15629700
INT3'				F	0.37964800	-5.28763300	2.14669400
C	-6.39655500	-0.01401100	4.39826400	F	-1.27722200	-1.56099100	3.48463500
C	-5.07279600	0.45519700	4.55850400	F	-0.11914200	-1.49044000	5.87758600

F	0.22318200	-3.78248800	7.33517300	C	1.08849100	-3.04005800	3.71934700
F	-0.64025900	-6.17230000	6.31501600	C	0.77535800	-2.56476600	4.99063400
F	-1.81807400	-6.26567700	3.90274000	C	-2.16646000	-5.19305600	1.16947300
F	-3.67016500	-6.84811200	1.82820100	C	-1.29050100	-6.24765400	1.43975800
F	-6.08772200	-7.58760000	2.64649900	C	-2.87845800	-5.33480100	-0.02318900
F	-4.49997200	-2.44419100	3.43904500	C	-1.09937400	-7.32943000	0.58031400
F	-6.92910700	-3.22087600	4.25426300	C	-2.72065100	-6.39162900	-0.91425500
F	-7.75981300	-5.80151000	3.86949800	C	-1.81674300	-7.40297100	-0.60903000
N	-2.76898300	-1.71326100	0.73134200	F	-3.81452500	-4.40627800	-0.38382100
C	-2.61301900	-2.65345500	1.40280800	F	-3.43757400	-6.44498100	-2.05037000
TS3				F	-1.64564500	-8.43478600	-1.44493100
Imaginary frequency = 126.5480i cm ⁻¹				F	-0.23430900	-8.30403500	0.89361600
C	-6.06093400	0.03931500	4.24051300	F	-0.57271300	-6.27208200	2.57626900
C	-4.67509600	0.03050500	4.52640600	F	0.43870400	-3.87989400	1.65143200
C	-4.24826100	-0.36180000	5.80014600	F	2.36393600	-3.03687700	3.30353900
C	-5.17226200	-0.71623000	6.78269600	F	1.73888500	-2.10784700	5.80104600
C	-6.53898400	-0.69149100	6.50315100	F	-0.88753000	-2.06697000	6.60453600
C	-6.98276200	-0.32364600	5.23493700	F	-2.80044900	-2.97055400	5.02270200
H	-3.18737500	-0.40917100	6.01066400	F	-3.10955200	-6.22223500	3.76469000
H	-4.82063600	-1.02015900	7.76392600	F	-5.47206100	-6.86962500	4.84029700
H	-7.26070400	-0.97046100	7.26497100	F	-4.98648800	-2.14794500	2.17397400
H	-8.04107800	-0.32567800	4.99770800	F	-7.32508900	-2.83030000	3.20878500
O	-3.99911100	0.87582300	2.38484500	F	-7.62252200	-5.19206200	4.57904500
C	-3.68958700	0.43883500	3.48076200	C	-2.43013900	-1.69796100	0.57761400
C	-6.59941800	0.35497100	2.94701700	N	-2.48926100	-2.64912800	1.25867500
N	-7.15028100	0.55898600	1.94231300	TS3'			
C	-5.06946400	-1.02564400	-1.04517800	Imaginary frequency = 107.0395i cm ⁻¹			
C	-4.91360700	0.32313400	-0.54777800	C	-6.01774800	-0.08894800	4.26197800
C	-4.17080300	-1.57719700	-2.07344500	C	-4.63812000	-0.09870200	4.57840200
C	-6.15815700	-1.87487500	-0.53072000	C	-4.23510500	-0.51159200	5.85309800
H	-4.20686300	0.16748900	0.30950300	C	-5.17847900	-0.88312200	6.81076500
H	-4.39686900	0.99460600	-1.23781700	C	-6.53875700	-0.85907300	6.50178000
H	-5.81138400	0.74116300	-0.08455400	C	-6.95784900	-0.47391800	5.22982500
H	-3.73055200	-2.50803300	-1.69183800	H	-3.17818600	-0.55787100	6.08395600
H	-4.78760300	-1.87400100	-2.93784700	H	-4.84723800	-1.20003900	7.79495900
H	-3.38845700	-0.88621400	-2.38501300	H	-7.27533200	-1.15365100	7.24318900
H	-5.90878500	-2.93820600	-0.56357600	H	-8.01061500	-0.48086000	4.96983100
H	-6.50235800	-1.56111100	0.45630600	O	-3.92188300	0.88068700	2.51107600
H	-7.00024500	-1.70480300	-1.22792900	C	-3.63443600	0.33348400	3.56283200
O	-2.42364700	0.30126500	3.89402300	C	-6.52375800	0.24221000	2.95878000
C	-1.40198100	0.70512200	2.95854000	N	-7.03699300	0.45854800	1.93712600
H	-0.45855200	0.50067400	3.46397100	C	-4.62733900	-0.73279300	-1.11151700
H	-1.48606200	0.12461100	2.03795200	C	-4.67349700	0.57026700	-0.46194400
H	-1.49902000	1.77143700	2.73730600	C	-3.71609400	-0.97141700	-2.24834000
B	-2.45641400	-3.90153300	2.16132900	C	-5.57791000	-1.78067100	-0.71456100
C	-3.92517700	-4.18270200	2.86051200	H	-4.13124000	0.45199100	0.50011200
C	-4.13148600	-5.36220800	3.58397000	H	-4.19518800	1.36854000	-1.03261700
C	-5.04532600	-3.35879600	2.79025000	H	-5.68735800	0.82591200	-0.12880500
C	-5.34664700	-5.72030100	4.16227100	H	-3.98599100	-1.85307300	-2.83434800
C	-6.28516000	-3.67718600	3.34093900	H	-3.60708200	-0.08340000	-2.87850100
C	-6.44136400	-4.86951000	4.03571900	H	-2.73827100	-1.16700000	-1.78017500
C	-1.28086700	-3.53305400	3.25809200	H	-5.17319400	-2.78420500	-0.86071300
C	-1.53893400	-3.04340900	4.53906500	H	-5.97343200	-1.64352800	0.29183300
C	0.06765200	-3.49136200	2.88760400	H	-6.41792100	-1.65786800	-1.42706100
C	-0.55221300	-2.56100500	5.39814700	O	-2.37563000	0.08010500	3.94236300

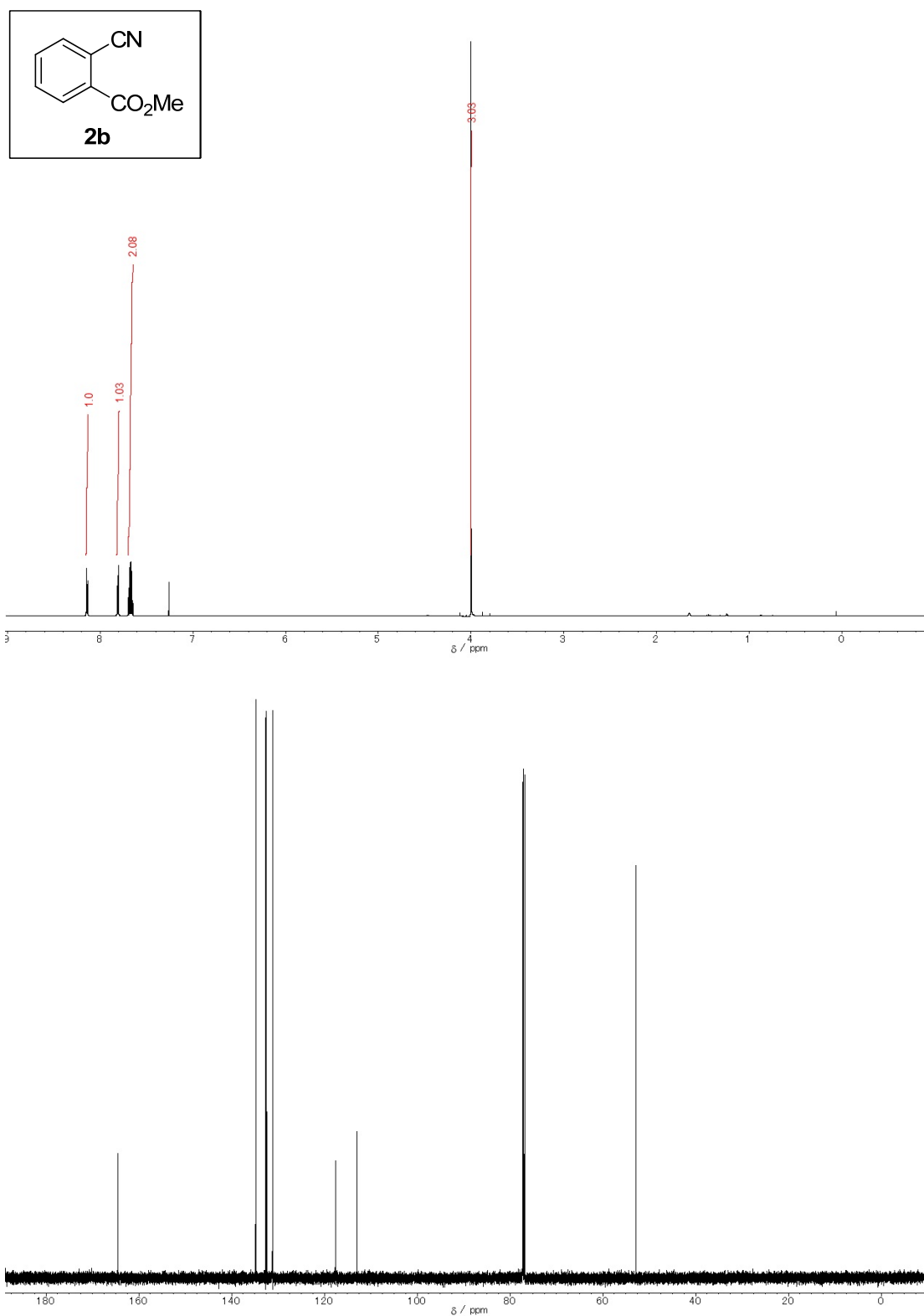
C	-1.34577400	0.47114500	3.01160700	C	-4.13726900	-2.33657400	-1.39950600
H	-0.40799500	0.20254300	3.49631600	C	-2.85132600	-1.62855900	-1.89275700
H	-1.46781000	-0.07362700	2.07330000	C	-4.49173800	-3.54529600	-2.30404100
H	-1.39361600	1.54764100	2.82847000	C	-5.31913100	-1.34344300	-1.30911300
B	-2.59008700	-4.00889900	2.25628700	H	-2.62889300	-0.75880400	-1.27030100
C	-3.96790900	-4.34194500	3.09326200	H	-1.99617600	-2.31149100	-1.87711600
C	-4.01955300	-5.47998500	3.90485900	H	-3.01484200	-1.29579700	-2.92330500
C	-5.14991200	-3.60743200	3.06174600	H	-5.34108600	-4.10812600	-1.90616300
C	-5.14909100	-5.87633100	4.61486700	H	-4.75226100	-3.16829300	-3.29832000
C	-6.30742200	-3.96344900	3.75163400	H	-3.64084400	-4.22622500	-2.40440800
C	-6.30915600	-5.10988600	4.53593900	H	-5.51349800	-0.94965900	-2.31232900
C	-1.33842800	-3.52399700	3.21885700	H	-6.22833600	-1.83841300	-0.95254600
C	-1.47568600	-3.08359400	4.53600600	H	-5.07331400	-0.50988600	-0.64721900
C	-0.04661800	-3.38629900	2.69864700	O	-0.88347600	5.10082500	1.79312100
C	-0.42464900	-2.56508000	5.29212000	C	-0.22050900	5.65737000	0.64535100
C	1.03599500	-2.89445200	3.42133600	H	0.24871800	6.57577900	0.99830600
C	0.84521800	-2.47596900	4.73648700	H	0.53069200	4.96118100	0.26373300
C	-2.29352600	-5.32165300	1.29701000	H	-0.94301600	5.87157000	-0.14637500
C	-1.31260700	-6.29169400	1.51692600	C	-3.86669200	-2.88506200	-0.06309700
C	-3.11356200	-5.57233900	0.19485200	N	-3.64072500	-3.40387100	0.93867600
C	-1.13026000	-7.39982900	0.68966900	B	-3.24834600	-4.24511400	2.22851900
C	-2.96989900	-6.66141500	-0.65914500	C	-4.34814300	-3.83424200	3.36995100
C	-1.96160300	-7.58627200	-0.40964800	C	-5.04395000	-4.74045900	4.17329800
F	-4.14418600	-4.73028800	-0.08837900	C	-4.62767200	-2.49087900	3.63163800
F	-3.79386300	-6.82742200	-1.70742600	C	-5.96141400	-4.35019100	5.15066200
F	-1.79924100	-8.64504100	-1.21310000	C	-5.53098900	-2.05891500	4.59477000
F	-0.16327700	-8.29149200	0.94881900	C	-6.20917600	-2.99929500	5.36422200
F	-0.47916800	-6.20458900	2.56910600	C	-1.71697900	-3.76523600	2.56726600
F	0.19722200	-3.72693900	1.41660300	C	-1.25250400	-3.44094300	3.84379000
F	2.25206100	-2.80196600	2.86235100	C	-0.75299500	-3.68209600	1.55840600
F	1.86840400	-1.98488800	5.44775200	C	0.05758600	-3.04013100	4.10310900
F	-0.64565700	-2.12763100	6.54452000	C	0.56342000	-3.28491900	1.77058100
F	-2.67324100	-3.10161500	5.16275700	C	0.97286500	-2.95828300	3.05956500
F	-2.92125400	-6.24879500	4.04488800	C	-3.34292100	-5.81063700	1.74953700
F	-5.13043100	-6.97898400	5.37690300	C	-2.43467200	-6.79148700	2.15695000
F	-5.22859200	-2.45290100	2.34953700	C	-4.37436300	-6.27860900	0.93113800
F	-7.41237400	-3.19978100	3.67267600	C	-2.51646000	-8.12555900	1.76000800
F	-7.40807000	-5.46861500	5.21285400	C	-4.49252100	-7.59839200	0.50619100
N	-2.79479000	-1.82720800	0.55359000	C	-3.55070300	-8.53302200	0.92438400
C	-2.76699600	-2.74871800	1.26744900	F	-5.34667800	-5.43143100	0.50843500
				F	-5.50311400	-7.97348800	-0.29140900
				F	-3.64293300	-9.80794400	0.53198900
2 + 'BuCN-B(C₆F₅)₃				F	-1.61037000	-9.01734200	2.18160300
C	-2.91669200	2.20610800	2.77160100	F	-1.42113500	-6.48919300	2.99087600
C	-2.19682400	3.42301900	2.80910600	F	-1.07844500	-4.00636300	0.28229500
C	-2.11729100	4.12475600	4.01721300	F	1.43326500	-3.21960800	0.75279200
C	-2.73659200	3.63947400	5.16848500	F	2.23257300	-2.57381700	3.29207900
C	-3.44616500	2.43864700	5.12689500	F	0.44141000	-2.73676800	5.35091200
C	-3.53648500	1.72218800	3.93548900	F	-2.06437700	-3.51578700	4.91699900
H	-1.56421000	5.05580000	4.04407500	F	-4.85194400	-6.06723100	4.05450400
H	-2.66310600	4.19950600	6.09606200	F	-6.60073600	-5.26821000	5.88683900
H	-3.93063700	2.05326500	6.01897600	F	-3.98114200	-1.52631400	2.93393500
H	-4.08105600	0.78665600	3.89573100	F	-5.74656200	-0.74504000	4.79884900
O	-1.57654700	3.39170000	0.49108800	F	-7.08253400	-2.60637200	6.29732900
C	-1.53701000	3.94053800	1.57318000				
C	-3.06552200	1.40424500	1.58878000				
N	-3.27333600	0.65767000	0.72249700	2 + 'BuNC-B(C₆F₅)₃			

C	-4.85957900	0.64071200	3.28930100	C	-6.31311900	-4.47894100	3.29947800
C	-4.46214800	1.86603100	3.87328600	C	-6.69541600	-5.75896300	3.68794800
C	-4.80628700	2.12463000	5.20494700	C	-1.85311600	-4.28449100	2.62327300
C	-5.53223300	1.19611600	5.94973900	C	-1.54074700	-4.94193700	3.81639200
C	-5.92312000	-0.01149700	5.36992800	C	-1.34398700	-2.99220200	2.51095900
C	-5.58803400	-0.29148300	4.04705900	C	-0.78300400	-4.37149600	4.83291500
H	-4.49852600	3.06306800	5.64996300	C	-0.58160600	-2.37880800	3.50502500
H	-5.79026100	1.41660200	6.98137000	C	-0.30081700	-3.07369500	4.67558700
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H	-5.88039600	-1.23084700	3.59351700	C	-0.86323800	-6.79336900	0.89886300
O	-3.39710800	2.72566600	1.90164500	C	-2.90818100	-6.96186800	-0.25190500
C	-3.69102100	2.86280000	3.07109300	C	-0.35969500	-7.88041400	0.18145100
C	-4.55982800	0.27066000	1.93360400	C	-2.44713100	-8.04433100	-0.99097700
N	-4.39729400	-0.15757800	0.86540500	C	-1.15484100	-8.51217100	-0.76735700
C	-3.81985300	-2.77677700	-1.88794600	F	-4.16723500	-6.53853500	-0.52336400
C	-2.89622900	-1.55474400	-2.03167700	F	-3.22457700	-8.63067300	-1.91202300
C	-3.61545600	-3.79567600	-3.02421200	F	-0.68259700	-9.54992500	-1.46501200
C	-5.29430700	-2.35302500	-1.76340800	F	0.88902100	-8.31366500	0.39763100
H	-3.04123200	-0.86622800	-1.19571700	F	-0.01102000	-6.23654000	1.77863600
H	-1.84624400	-1.86135200	-2.07280200	F	-1.57266900	-2.25851400	1.39829800
H	-3.14319100	-1.03767700	-2.96452100	F	-0.12121700	-1.13062300	3.34011000
H	-3.93003100	-3.34292600	-3.96949600	F	0.42850700	-2.50380300	5.64171400
H	-2.56233800	-4.08140900	-3.11071500	F	-0.51197000	-5.05274800	5.95434200
H	-4.21004600	-4.69783800	-2.85005400	F	-1.97095400	-6.20501100	4.00887000
H	-5.58917900	-1.83957000	-2.68412100	F	-3.93236800	-7.70869500	2.43995000
H	-5.94204800	-3.22556400	-1.63067600	F	-6.22357300	-8.07123200	3.75006000
H	-5.42312000	-1.66854500	-0.92159900	F	-4.79561800	-3.03769200	2.26074900
O	-3.35376000	3.94883900	3.79873200	F	-7.08961300	-3.42170800	3.60310200
C	-2.60570300	4.95127400	3.09030100	F	-7.83743100	-5.95004700	4.35655900
H	-2.41918400	5.74193200	3.81719400	N	-3.45918300	-3.45583300	-0.65340400
H	-1.66477300	4.53518900	2.72138700	C	-3.17562600	-4.02319200	0.31237500
H	-3.18325800	5.33210600	2.24400700				
B	-2.81944900	-5.02404300	1.53370200				
C	-4.25921000	-5.35328400	2.26505700				
C	-4.67936500	-6.61851800	2.68187900				
C	-5.12056700	-4.30905000	2.60561700				
C	-5.87069200	-6.83512400	3.37557600				

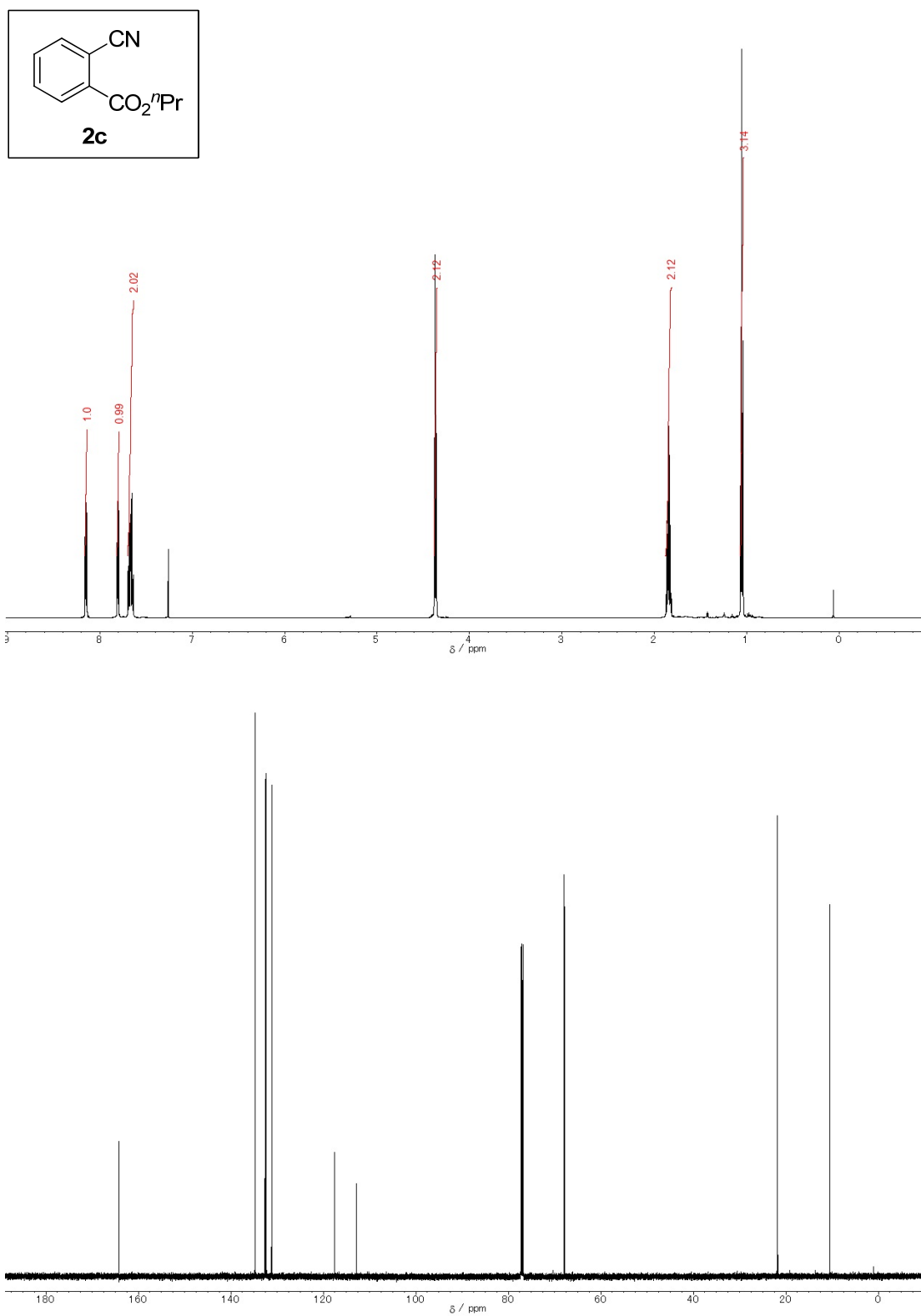
5. Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR Charts for the New Compounds

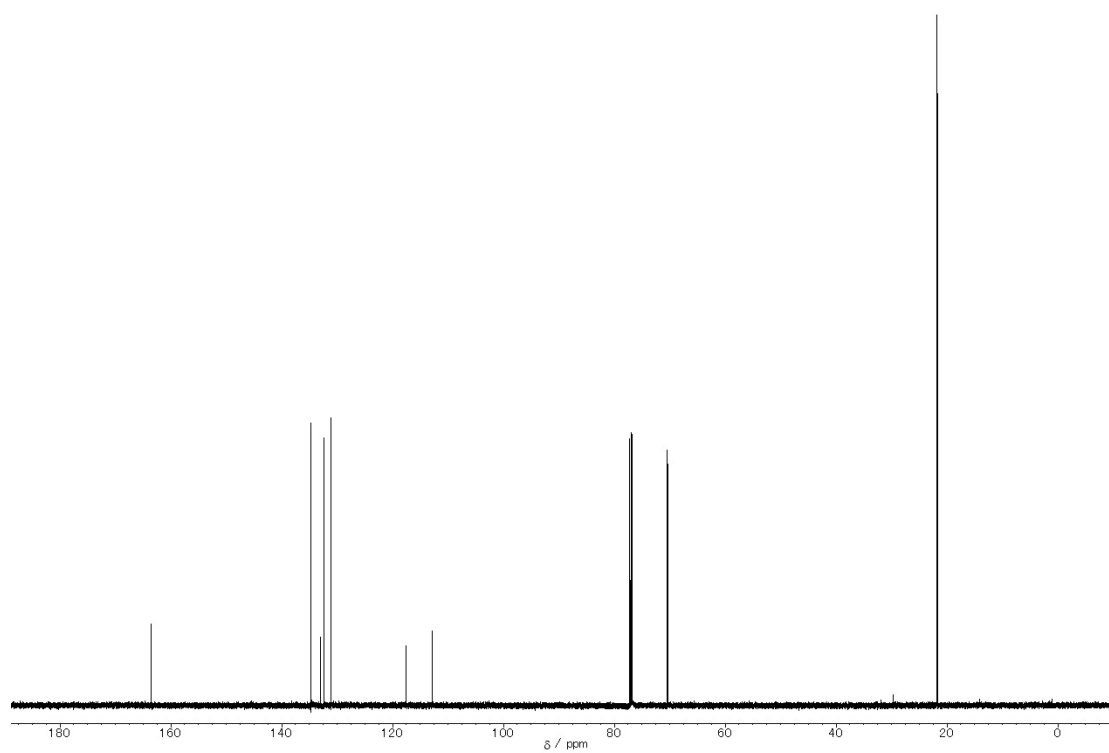
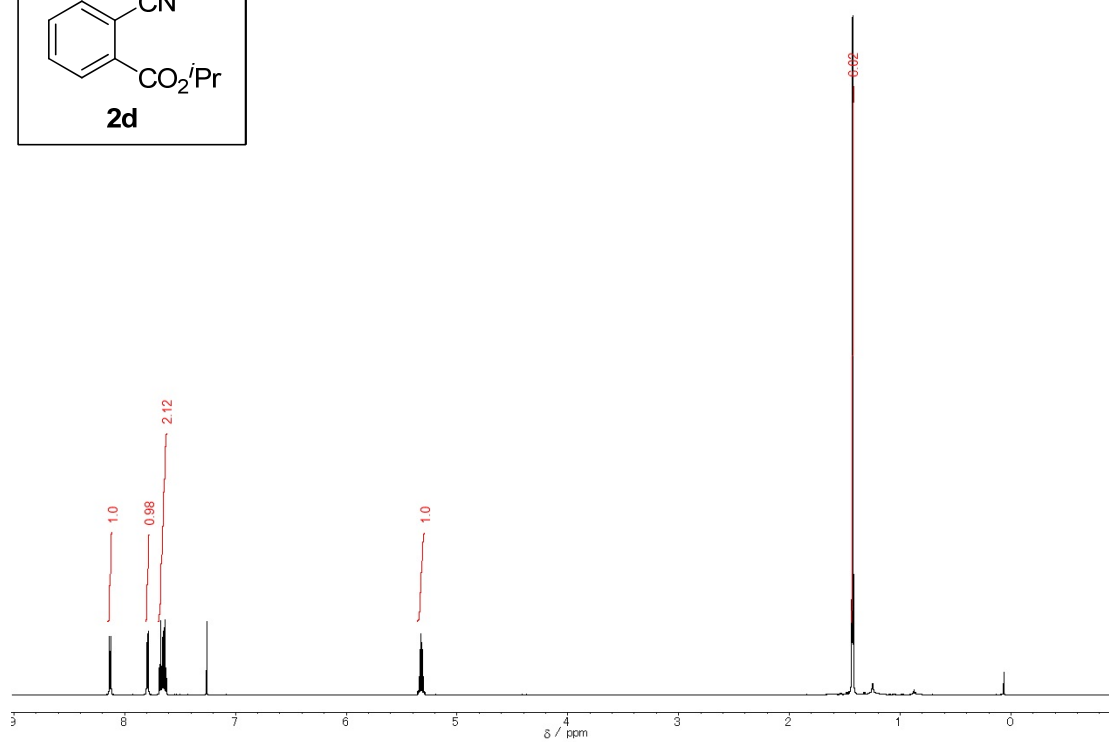
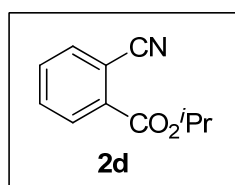


^1H NMR (600 MHz) and $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz) spectra of **2a** (rt, CDCl₃).

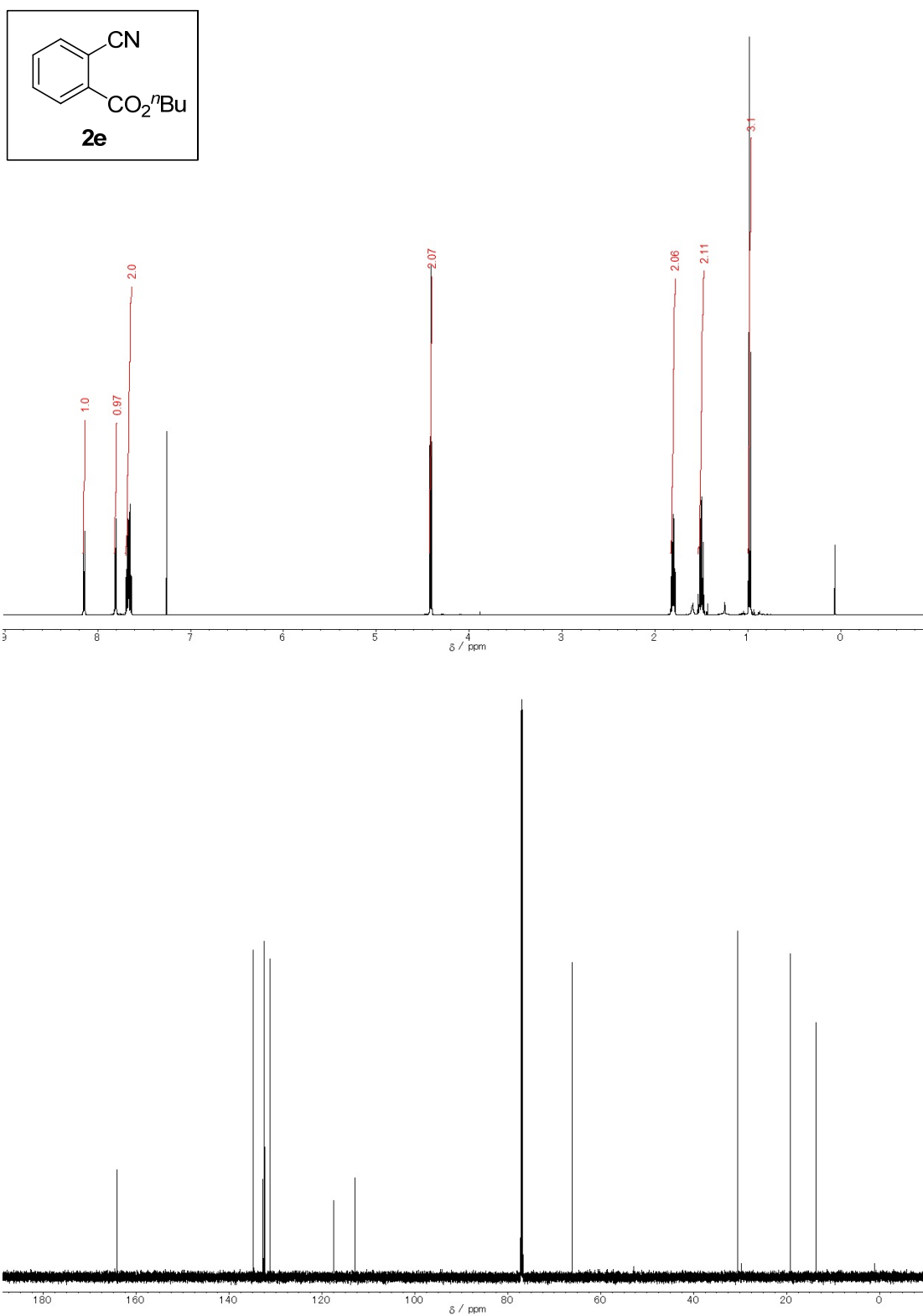


¹H NMR (600 MHz) and ¹³C{¹H} NMR (150 MHz) spectra of **2b** (rt, CDCl₃).

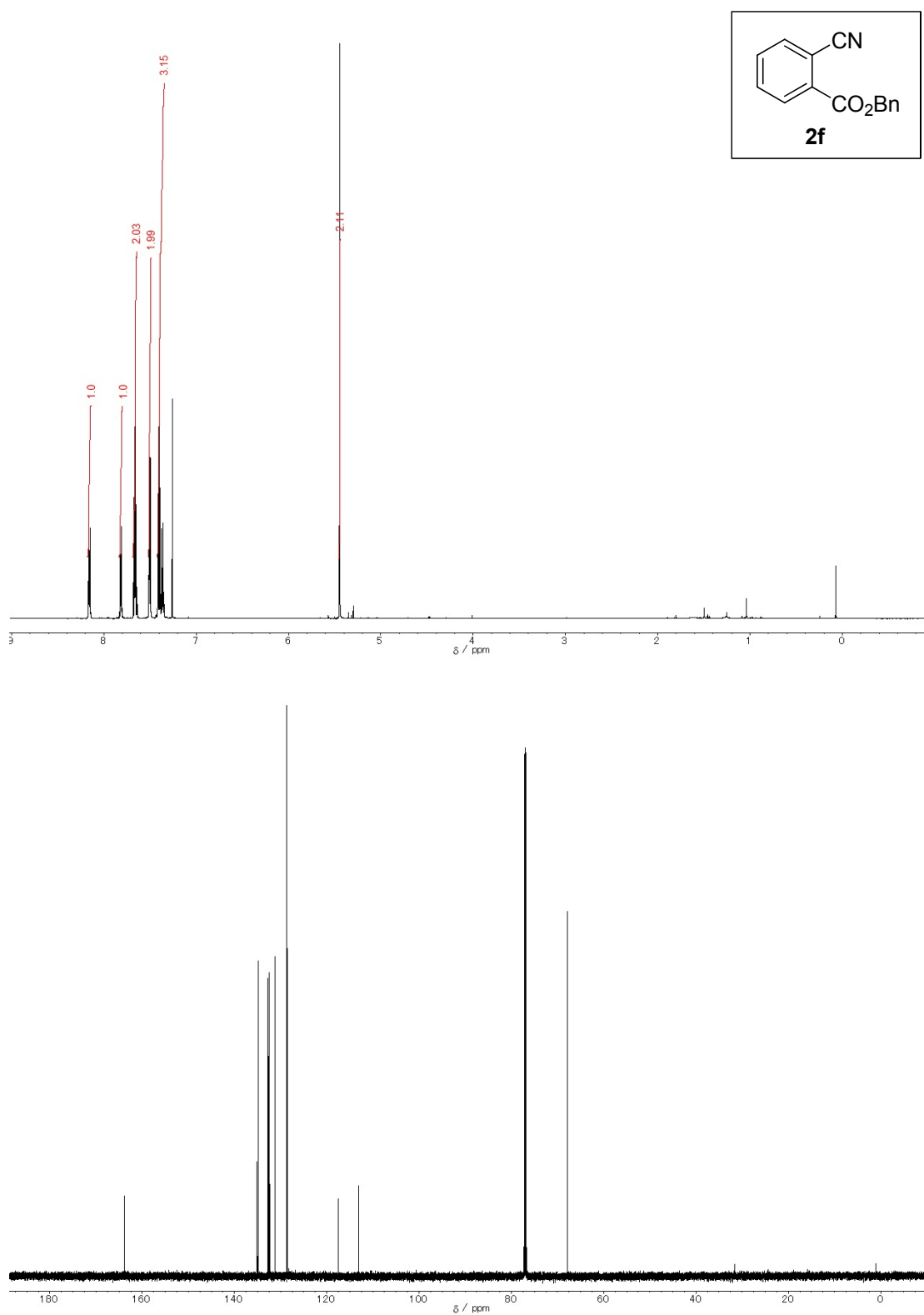




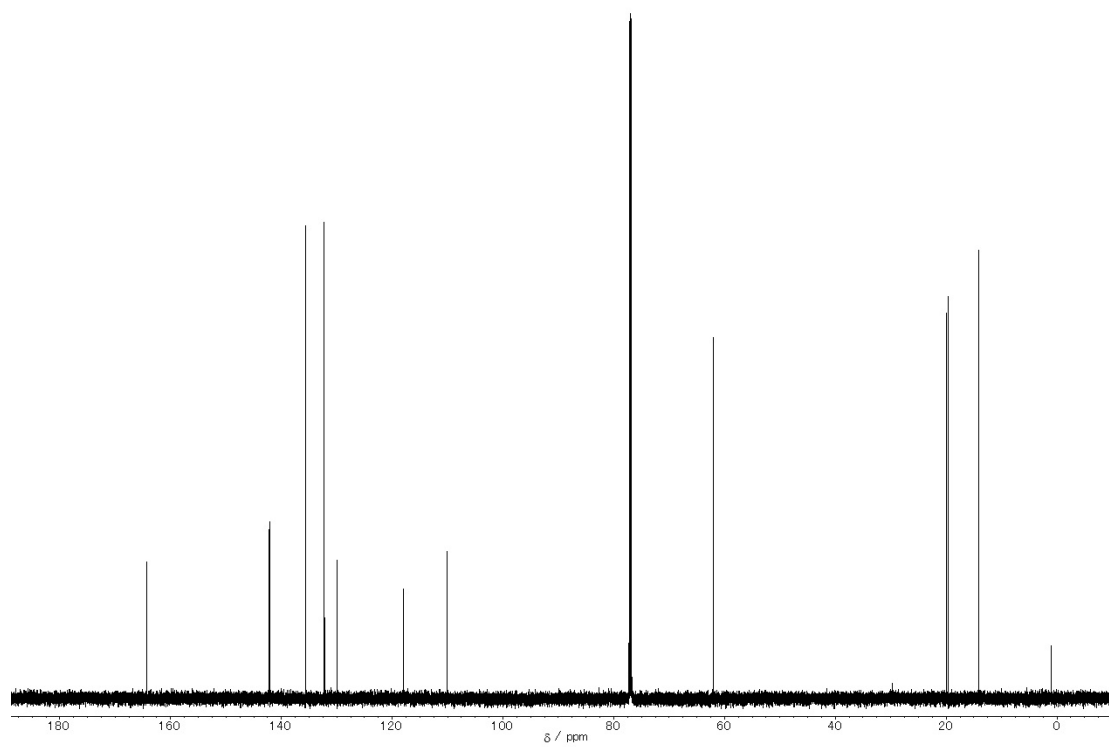
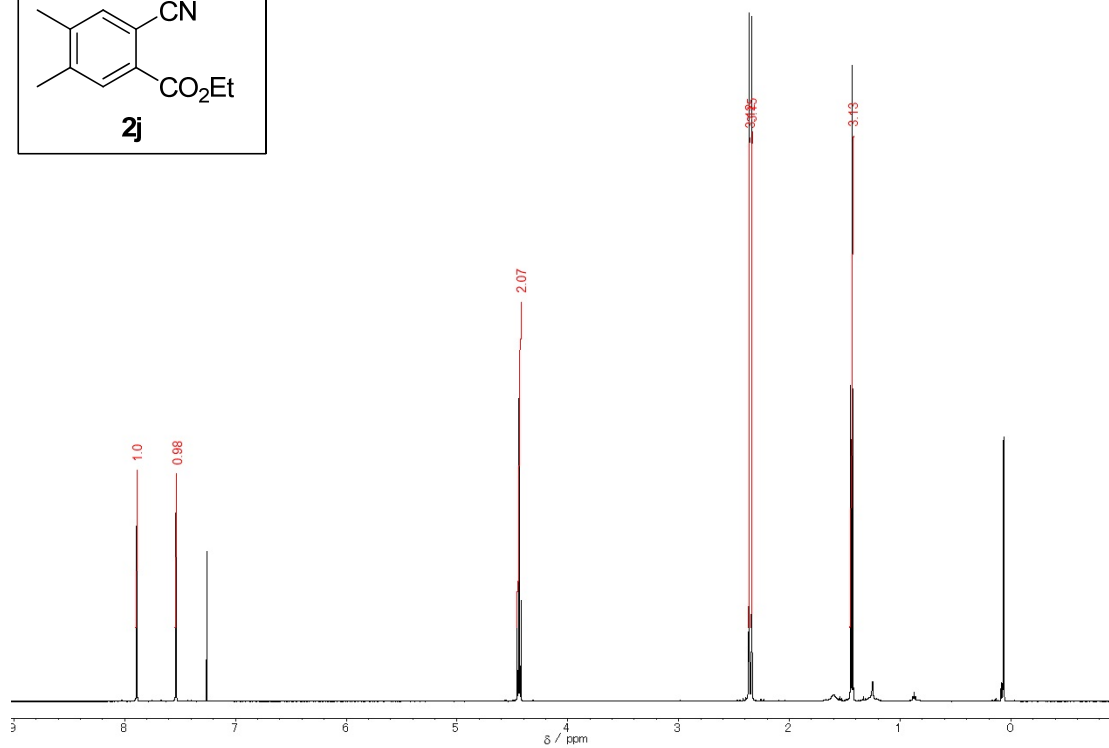
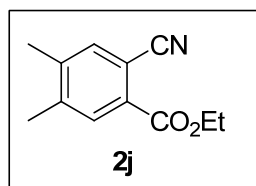
^1H NMR (600 MHz) and $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz) spectra of **2d** (rt, CDCl_3).



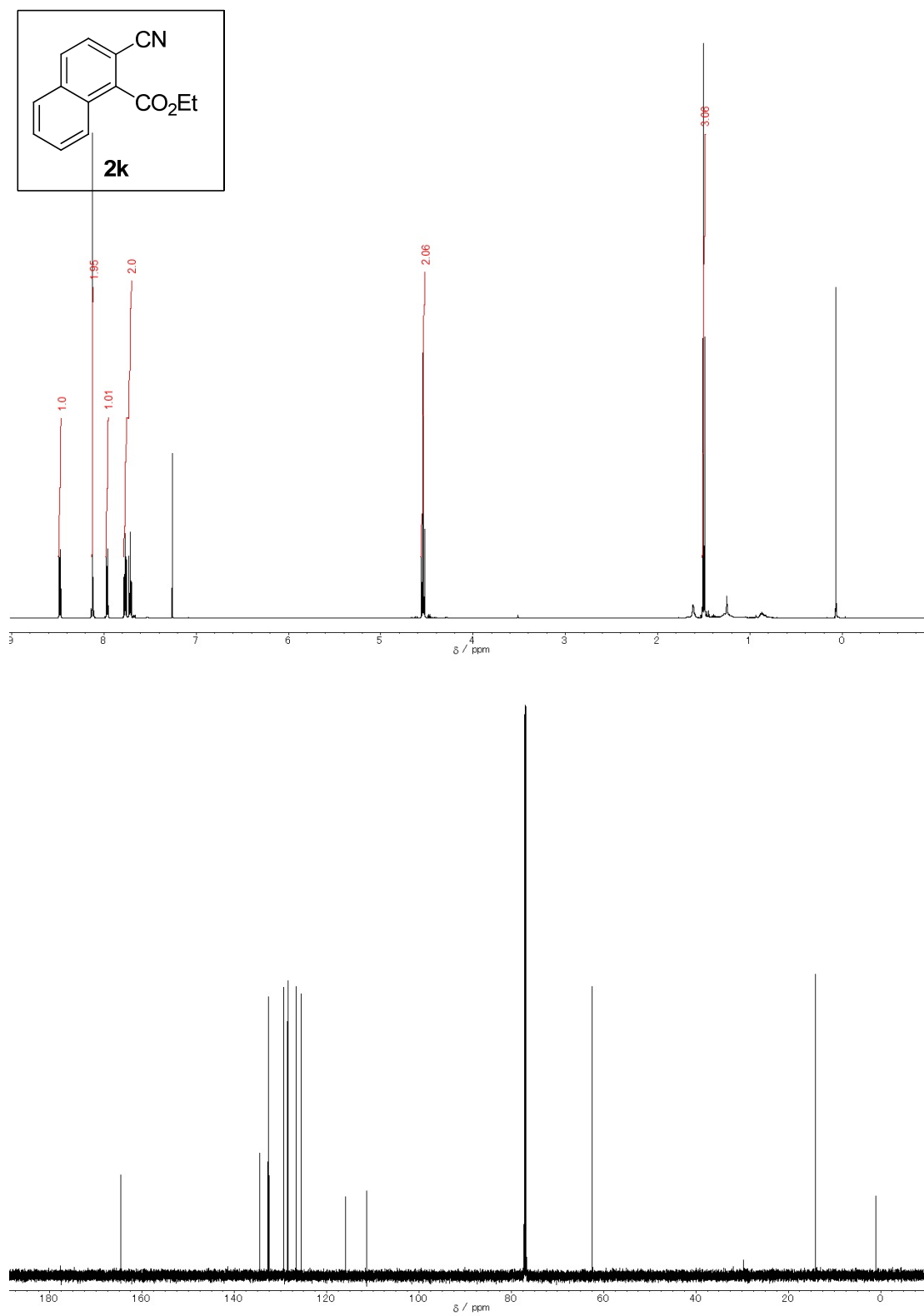
¹H NMR (600 MHz) and ¹³C{¹H} NMR (150 MHz) spectra of **2e** (rt, CDCl₃).



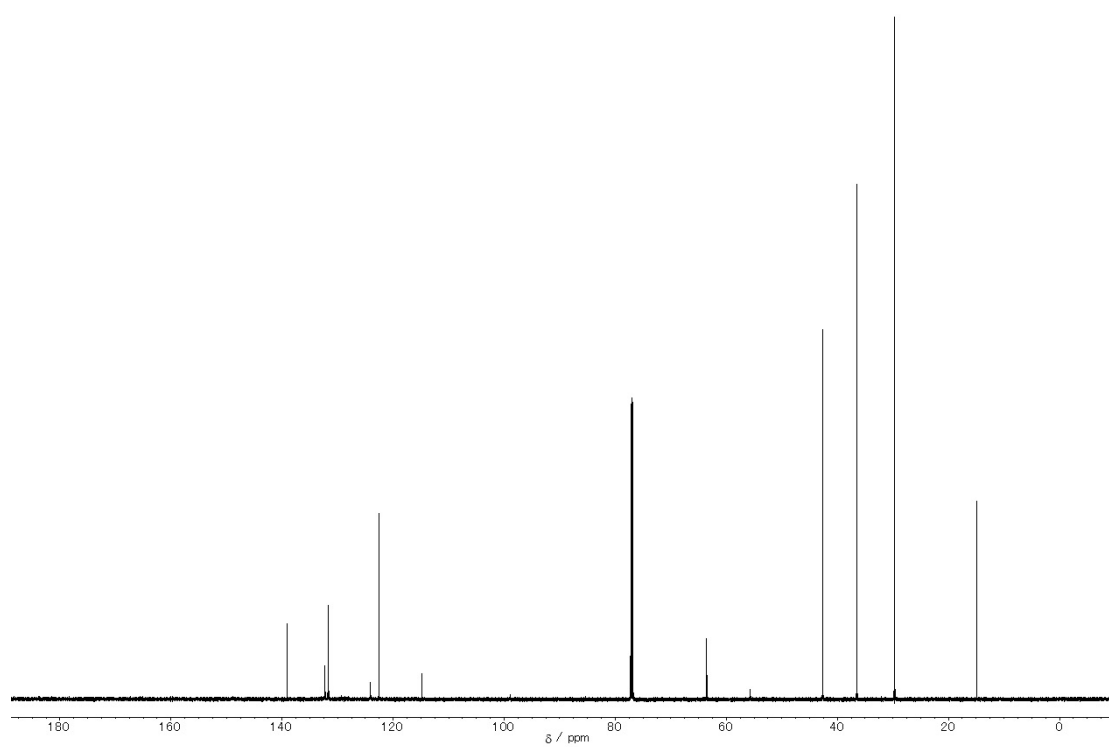
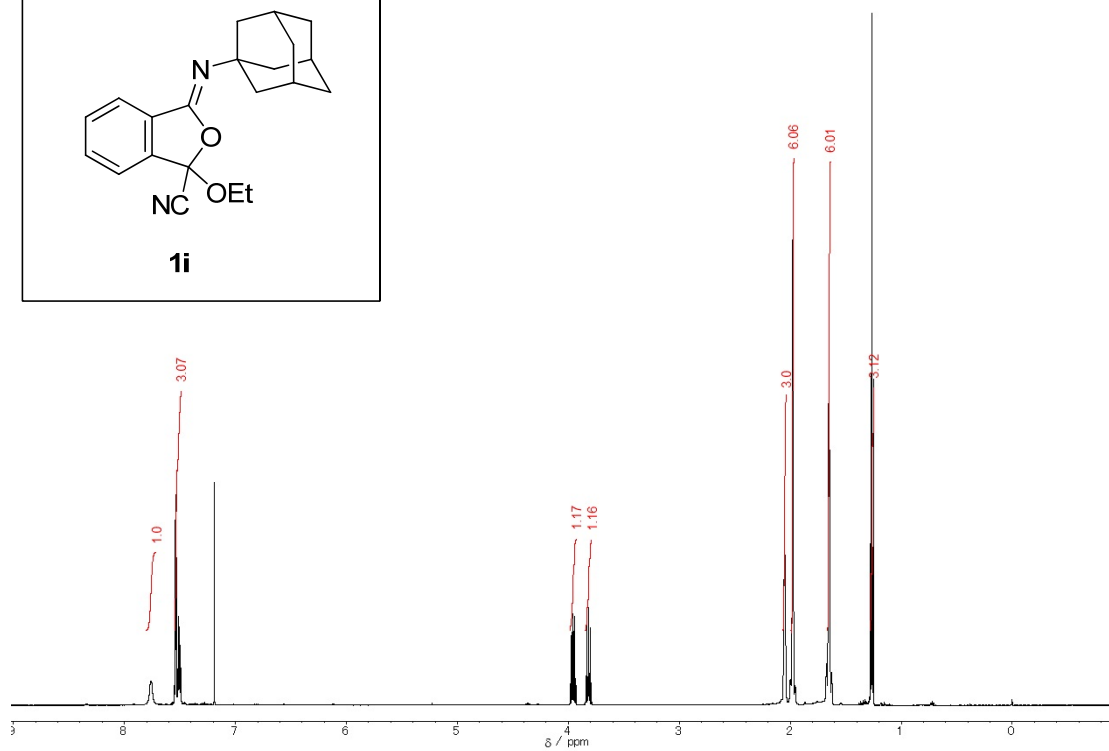
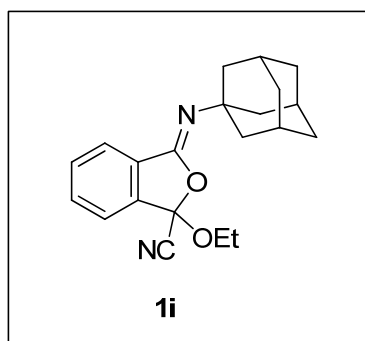
^1H NMR (600 MHz) and $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz) spectra of **2f** (rt, CDCl_3).



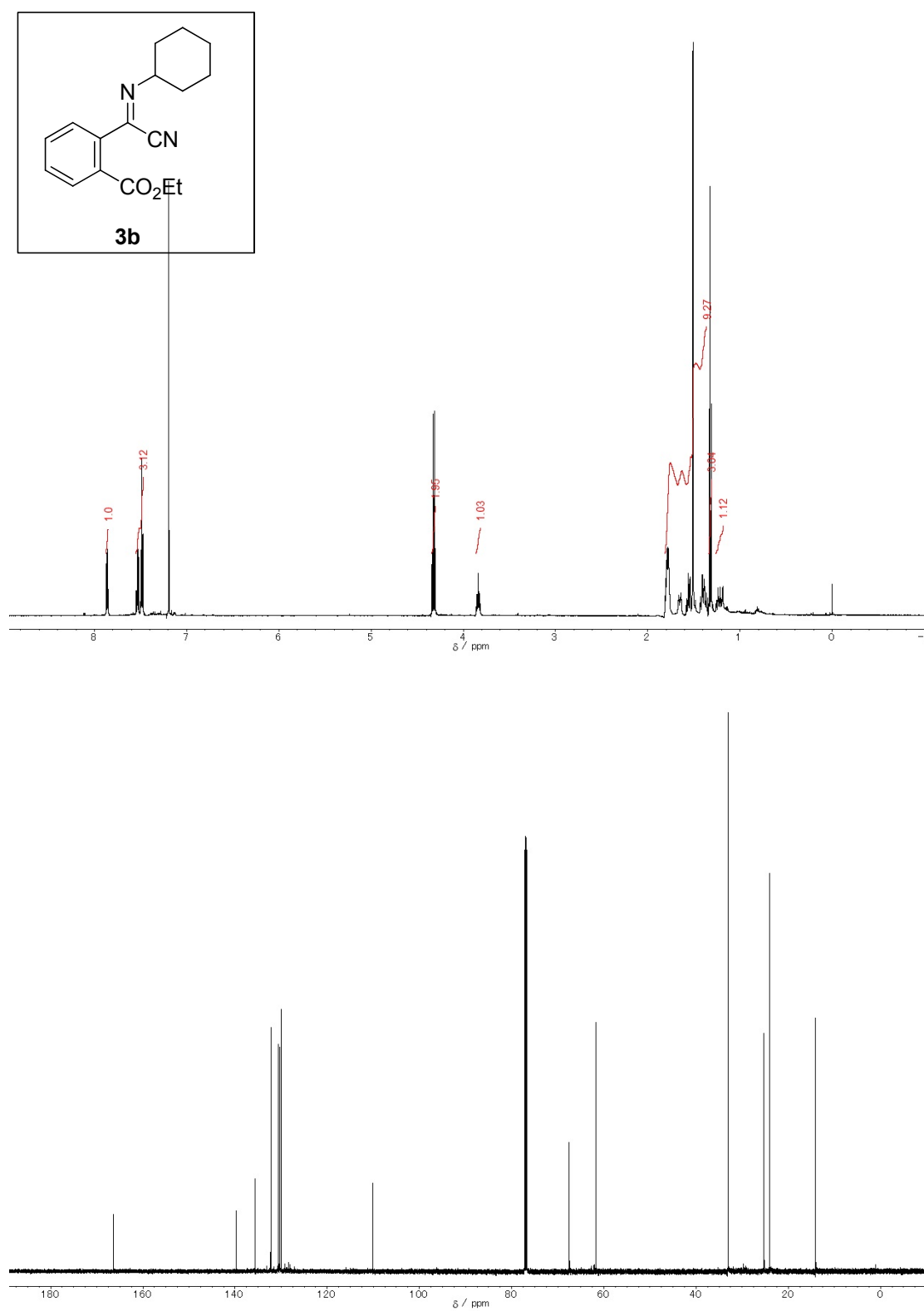
^1H NMR (600 MHz) and $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz) spectra of **2j** (rt, CDCl_3).



¹H NMR (600 MHz) and ¹³C{¹H} NMR (150 MHz) spectra of **2k** (rt, CDCl₃).



¹H NMR (600 MHz) and ¹³C{¹H} NMR (150 MHz) spectra of **1i** (rt, CDCl₃).



¹H NMR (600 MHz) and ¹³C{¹H} NMR (150 MHz) spectra of **3b** (rt, CDCl₃).

6. References

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