

Supporting Information

Gold-Catalyzed 1,2-Iminonitrations of Electron-deficient Alkynes with Nitrosoarenes to Afford α -Imidoyl Nitrones

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(I) Experimental Procedure for the synthesis of ethyl propiolate:

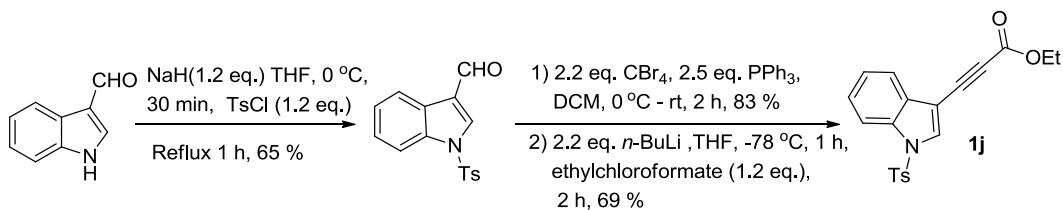
(a) General Information

Unless otherwise noted, all the reactions for the preparation of the substrates were performed in oven-dried glassware under nitrogen atmosphere with freshly distilled solvents. The catalytic reactions were performed in dry solvent. DCE was distilled from CaH_2 under nitrogen. THF was distilled from Na metal under nitrogen. All other commercial reagents were used without further purification, unless otherwise indicated. ^1H NMR and ^{13}C NMR spectra were recorded on a Bruker 400 MHz, Varian 500 MHz, 600 MHz and 700 MHz Spectrometers using chloroform-d as the internal standards. Ethyl propiolate were prepared according to the literature procedures ^[S1]. Ethyl propiolate with variable substituents (**1a-1m**) were prepared according to literature procedures ^[S2].

Reference:

- [S1] H. Gao, J. Zhang, *Chem. Eur. J.*, 2012, **18**, 2777.
[S2] (a) S.T. Gadge, B. M. Bhanage, *Synlett*, 2013, **24**, 981. (b) J. G. Kim, D. H. Kang, D.O. Jang, *Synlett*, **2008**, 3, 443.
[S3] A. Duschek, S. F. Kirsch, *Chem. Eur. J.* 2009, **15**, 10713

(b) Representative Synthetic Procedures:



(1) Synthesis of 1-tosyl-1H-indole-3-carbaldehyde.

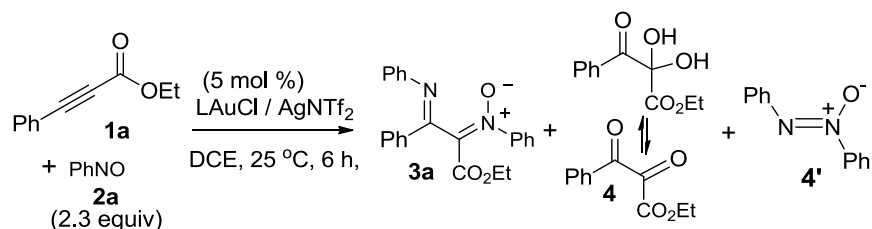
Sodium hydride (35 mmol) was added at 0 °C to a solution of indole-3-carbaldehyde (5 g, 35 mmol) in anhydrous THF (100 mL) under an argon atmosphere. The resulting mixture was stirred 30 min at 0 °C, to this solution was added THF solution (20 mL) of sulfonyl chloride (35 mmol) at room temperature. The resulting mixture was refluxed for 1 h, cooled, poured into water (100 mL). The organic layer was extracted with DCM, washed with brine, dried over MgSO_4 , and concentrated. The crude product was chromatographed through a silica gel column to afford 1-tosyl-1H-indole-3-carbaldehyde (6.69 g, 22 mmol, 65 %) as brownish solid.

(I) Synthesis of ethyl 3-(1-tosyl-1H-indol-3-yl) propiolate (**1j**).

To a dichloromethane solution (DCM, 20 ml) of carbon tetrabromide (9.88 g, 29.3 mmol) was added a DCM solution (20 ml) of triphenylphosphine (8.5 g, 32.5 mmol) slowly at 0 °C; the resulting mixture was stirred for 10 min at 0 °C, to this solution was added a DCM (30 mL) solution of compound 1-tosyl-1H-indole-3-carbaldehyde (4.00 g, 13.30 mmol). The resulting solution was stirred for 1 hour at room temperature before quenching with water. The organic layer was extracted with DCM, washed with brine, dried over MgSO₄, and concentrated. The crude product was chromatographed on a silica column to afford 3-(2,2-dibromovinyl)-1-tosyl-1H-indole (5.0 g, 11 mmol, 83 %) as a white solid.

To a THF solution of 3-(2,2-dibromovinyl)-1-tosyl-1H-indole (2.0 g, 20.14 mmol) was added *n*-BuLi (5.0 mL, 2.5 M in hexane, 11.0 mmol) drop wise at -78 °C for 30 min and allow to stir for 1 hour at -78 °C. To this solution was added a THF (5 mL) solution of ethyl chloroformate (0.57 g, 5.3 mmol). The resulting solution was stirred at -78 °C for 2 hours and monitored by TLC. After completion of reaction it was quenched by saturated solution of NH₄Cl at room temperature. The aqueous layer was separated and extracted with (3 x 20 mL) of ether. The organic layer is washed with water (50 ml), brine (50 mL), dried over MgSO₄, and concentrated. The crude product was chromatographed on a silica column to afford **1j** (1.10 g, 3.0 mmol, 69 %) as white solid.

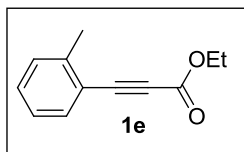
(II) Standard Catalytic Procedure for Gold-catalyzed 1,2-iminonitronation reactions:



A reaction tube was charged with P(*t*-Bu)₂(*o*-biphenyl)AuCl(I) (15.1 mg, 0.029 mmol) and Silver(I) Bis(trifluoromethanesulfonyl)imide (11.0 mg, 0.029 mmol), and to this mixture was added dry Dichloroethane (DCE) (1.0 mL). The resulting solution was stirred at room temperature for 5 min. To this solution was added a Dichloroethane (DCE) solution (2 mL) of compound **1a** (100 mg, 0.57 mmol) and Nitrosobenzene (141 mg, 1.3 mmol). The mixture was kept stirring at 25 °C for 6 h before it was filtered over a short silica bed. The solvent was concentrated, and the crude product was chromatographed through a silica gel column to afford compound **3a** as yellow oil (101 mg, 0.27 mmol, 77 %) together with α,β -dioxo ester **4** (13%) and diazene oxide **4'** (0.14 equiv) in minor proportion .

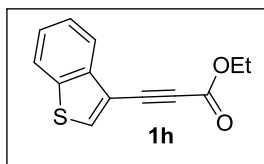
(III) Spectral data :

Spectral data for ethyl 3-(*o*-tolyl)propiolate (**1e**).



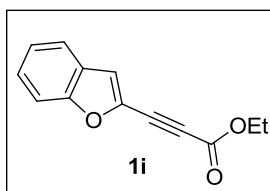
Light yellow liquid ; ^1H NMR (600 MHz, CDCl_3): δ 7.52 (d, $J = 7.7$ Hz, 1 H), 7.31 (t, $J = 7.6$ Hz, 1 H), 7.21 (d, $J = 7.7$ Hz, 1 H), 7.16 (t, $J = 7.6$ Hz, 1 H), 4.27 (q, $J = 7.1$ Hz, 2 H), 2.47 (s, 3H) 1.34 (t, $J = 7.1$ Hz, 3 H); ^{13}C NMR (150 MHz, CDCl_3): 154.2, 142.2, 133.3, 130.5, 129.7, 125.7, 119.5, 85.1, 84.4, 61.9, 20.5, 14.1 ; HRMS: calcd. for $\text{C}_{12}\text{H}_{12}\text{O}_2$: 188.0837; Found: 188.0833.

Spectral data for ethyl 3-(benzo[*b*]thiophen-3-yl) propiolate (**1h**).



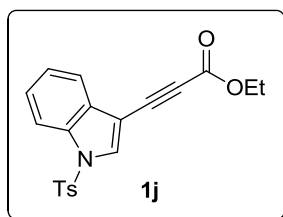
Dark Brown liquid ; ^1H NMR (600 MHz, CDCl_3): δ 7.99~7.97 (m, 1 H), 7.90 (s, 1 H), 7.83 (t, $J = 8.0$ Hz, 1 H), 7.46 ~ 7.44 (m, 1 H), 7.21 (t, $J = 7.8$ Hz, 1 H), 4.31 (q, $J = 7.1$ Hz, 2 H), 1.36 (t, $J = 7.1$ Hz, 3 H); ^{13}C NMR (150 MHz, CDCl_3): 154.0, 138.7, 138.5, 135.6, 125.5, 125.2, 122.9, 122.6, 114.9, 83.4, 79.9, 62.0, 14.0; HRMS: calcd. for $\text{C}_{13}\text{H}_{10}\text{O}_2\text{S}$: 230.0402; Found: 230.0397.

Spectral data for ethyl 3-(benzofuran-2-yl) propiolate (**1i**).



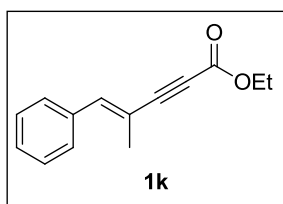
Yellow liquid ; ^1H NMR (600 MHz, CDCl_3): δ 7.57 (d, $J = 7.8$ Hz, 1 H), 7.44 (d, $J = 8.3$ Hz, 1 H), 7.37 (t, $J = 7.2$ Hz, 1 H), 7.26 ~ 7.22 (m, 2 H), 4.29 (q, $J = 7.1$ Hz, 2 H), 1.33 (t, $J = 7.1$ Hz, 3 H); ^{13}C NMR (150 MHz, CDCl_3): 155.5, 153.2, 135.7, 127.1, 123.7, 121.8, 116.9, 111.5, 86.3, 76.0, 62.3, 13.9; HRMS: calcd. for $\text{C}_{13}\text{H}_{10}\text{O}_3$: 214.0630; Found: 214.0626.

Spectral data for ethyl 3-(1-tosyl-1H-indol-3-yl) propiolate (1j).



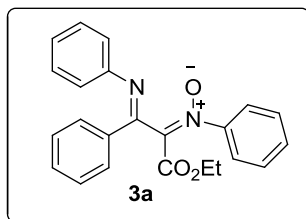
White solid; ^1H NMR (600 MHz, CDCl_3): δ 7.96 ~ 7.94 (m, 2 H), 7.76 (dd, $J = 6.7, 1.8$ Hz, 2 H), 7.68 ~ 7.66 (m, 1 H), 7.37 ~ 7.34 (m, 1 H), 7.31 ~ 7.28 (m, 1 H), 7.23 (d, $J = 8.1$ Hz, 2 H), 4.28 (q, $J = 7.1$ Hz, 2H), 2.33 (s, 3H), 1.34 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 153.9, 145.8, 134.5, 134.0, 132.6, 130.1, 130.0, 127.0, 125.9, 124.2, 120.6, 113.6, 101.6, 85.1, 78.4, 62.0, 21.5, 14.0, (one carbon merged with others); HRMS: calcd. for $\text{C}_{20}\text{H}_{17}\text{NO}_4\text{S}$: 367.0878; Found: 367.0879.

Spectral data for (*E*)-ethyl 4-methyl-5-phenylpent-4-en-2-ynoate (1k).



Pale Yellow liquid ; ^1H NMR (600 MHz, CDCl_3): δ 7.36 ~ 7.33 (m, 3 H), 7.28 ~ 7.26 (m, 2 H), 7.08 (s, 1 H), 4.24 (q, $J = 7.1$ Hz, 2H), 2.01 (s, 3 H), 1.31 (t, $J = 7.1$ Hz, 3 H); ^{13}C NMR (150 MHz, CDCl_3): δ 153.9, 141.6, 135.5, 129.0, 128.3, 128.1, 116.6, 89.8, 79.3, 61.7, 18.1, 13.9; HRMS: calcd. for $\text{C}_{14}\text{H}_{14}\text{O}_2$: 214.0994; Found: 214.0992.

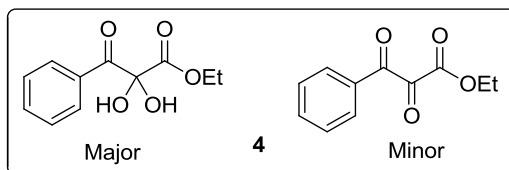
Spectral data for (*E*)-*N*-((*E*)-1-ethoxy-1-oxo-3-phenyl-3-(phenylimino) propan-2-ylidene) aniline oxide (3a)



Pale Yellow liquid; ^1H NMR (400 MHz, CDCl_3): δ 7.90 (dd, $J = 7.2, 1.7$ Hz, 2 H), 7.52 ~ 7.45 (m, 3 H), 7.42 (d, $J = 7.3$ Hz, 1 H), 7.38 ~ 7.30 (m, 4 H), 7.15 (t, $J = 7.5$ Hz, 1 H), 7.08~7.05 (m, 4 H),

3.89 (q, $J = 7.12$ Hz, 2 H), 0.94 (t, $J = 7.2$ Hz, 3 H); ^{13}C NMR (150 MHz, CDCl_3): δ 159.3, 159.7, 150.4, 147.5, 137.6, 135.4, 131.4, 130.3, 128.9, 128.8, 128.7, 127.3, 125.2, 122.7, 118.5, 61.9, 13.6; ESI-MS: calcd. for $\text{C}_{23}\text{H}_{20}\text{N}_2\text{O}_3$: 372.1474; Found: 372.1472.

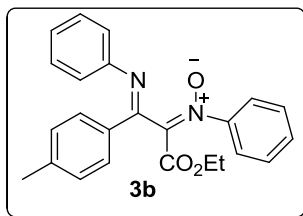
Spectral data ethyl 2,3-dioxo-3-phenylpropanoate (4)



Yellow liquid; (1:2 mixture of ketone and hydrate) *Ketone* : ^1H NMR (600 MHz, CDCl_3): δ 7.97 (dd, $J = 7.2, 1.2$ Hz, 2 H), 7.70 ~ 7.67 (m, 1 H), 7.54 ~ 7.52 (m, 2 H), 4.41 (q, $J = 7.2$ Hz, 2 H), 1.37 (t, $J = 7.2$ Hz, 3 H); ^{13}C NMR (175 MHz, CDCl_3): δ 190.2, 183.7, 160.5, 135.5, 131.5, 130.0, 129.1, 63.3, 13.9; *Hydrate*: ^1H NMR (600 MHz, CDCl_3): δ 8.05 (dd, $J = 8.9, 0.6$ Hz, 2 H), 7.62 ~ 7.59 (m, 1 H), 7.47 ~ 7.44 (m, 2 H), 4.19 (q, $J = 7.2$ Hz, 2 H), 1.06 (t, $J = 7.2$ Hz, 3 H); ^{13}C NMR (150 MHz, CDCl_3): δ 191.5, 169.9, 134.7, 131.3, 130.1, 128.8, 91.5, 63.2, 13.6 ; HRMS: calcd. for $\text{C}_{11}\text{H}_{12}\text{O}_5$: 224.0685; Found: 224.0685.

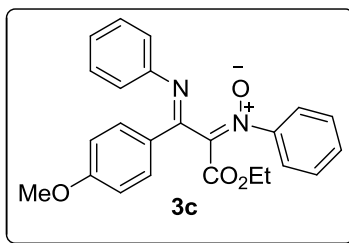
The spectral data are in agreement with the values reported previously in the literature.^[S3]

Spectral data for (*E*)-*N*-((*E*)-1-ethoxy-1-oxo-3-(phenylimino)-3-(*p*-tolyl) propan-2-ylidene) aniline oxide (3b)



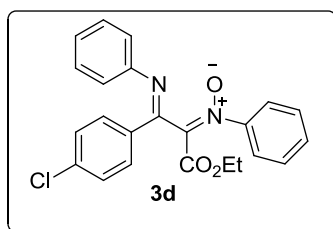
Light Yellow liquid; ^1H NMR (600 MHz, CDCl_3): δ 7.80 (dd, $J = 6.5, 1.7$ Hz, 2 H), 7.40 (t, $J = 6.5$ Hz, 1 H), 7.37 ~ 7.27(m, 6 H), 7.14 (t, $J = 6.3$ Hz, 1 H), 7.07 ~ 7.05(m, 4 H), 3.94 (q, $J = 7.1$ Hz, 2 H), 2.41 (s, 3 H), 0.94 (t, $J = 7.1$ Hz, 3 H); ^{13}C NMR (150 MHz, CDCl_3): δ 159.4, 158.5, 150.6, 147.6, 141.9, 137.8, 132.7, 130.3, 129.6, 128.9, 128.7, 127.3, 125.0, 122.7, 118.6, 61.9, 21.5, 13.6; HRMS: calcd. for $\text{C}_{24}\text{H}_{22}\text{N}_2\text{O}_3$: 386.1630; Found: 386.1628.

Spectral data for (*E*)-*N*-((*E*)-1-ethoxy-3-(4-methoxyphenyl)-1-oxo-3-(phenylimino) propan-2-ylidene) aniline oxide (3c).



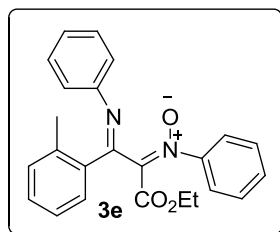
Yellow liquid; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.85 (dd, $J = 6.9, 2.0$ Hz, 2 H), 7.43 ~ 7.29 (m, 5 H), 7.13 (t, $J = 7.4$ Hz, 1 H), 7.05 (dd, $J = 8.3, 1.2$ Hz, 4 H), 6.97 (dd, $J = 6.9, 2.0$ Hz, 2 H), 3.89 (q, $J = 6.9$ Hz, 2 H), 3.86 (s, 3 H), 0.95 (t, $J = 7.4$ Hz, 3 H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 162.3, 159.5, 157.8, 150.6, 147.6, 137.8, 130.3, 129.1, 128.9, 128.7, 128.1, 124.9, 122.7, 118.6, 114.3, 61.9, 55.4, 13.7; HRMS: calcd. for $\text{C}_{24}\text{H}_{22}\text{N}_2\text{O}_4$: 402.1580; Found: 402.1581.

Spectral data for (*E*)-*N*-((*E*)-1-(4-chlorophenyl)-3-ethoxy-3-oxo-1-(phenylimino)propan-2-ylidene)aniline oxide (3d).



Pale Yellow liquid; $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.85 (d, $J = 8.5$ Hz, 2 H), 7.45 ~ 7.42 (m, 3 H), 7.37 (t, $J = 8.1$ Hz, 2 H), 7.33 (t, $J = 7.6$ Hz, 2 H), 7.16 (t, $J = 7.4$ Hz, 1 H), 7.08 (d, $J = 9.3$ Hz, 2 H), 7.04 (d, $J = 8.4$ Hz, 2 H), 3.88 (q, $J = 7.1$ Hz, 2 H), 0.94 (t, $J = 7.1$ Hz, 3 H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 159.1, 157.6, 150.1, 147.3, 137.5, 137.1, 133.8, 130.5, 129.2, 129.0, 128.8, 128.6, 125.4, 122.6, 118.4, 62.0, 13.6; HRMS: calcd. for $\text{C}_{23}\text{H}_{19}\text{ClN}_2\text{O}_3$: 406.1084; Found: 406.1070.

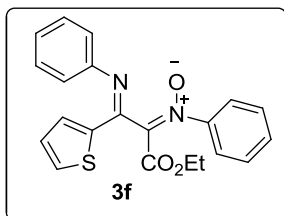
Spectral data for ((*E*)-*N*-((*E*)-1-ethoxy-1-oxo-3-(phenylimino)-3-(4-(trifluoromethyl)phenyl)propan-2-ylidene)aniline oxide (3e).



Yellow liquid; $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.55 (d, $J = 7.8$ Hz, 1 H), 7.41 ~ 7.38 (m, 1 H), 7.34 ~ 7.29 (m, 6 H), 7.26 ~ 7.23 (m, 1 H), 7.16 ~ 7.13 (m, 1 H), 7.09 ~ 7.06 (m, 4 H), 3.84 (q, $J =$

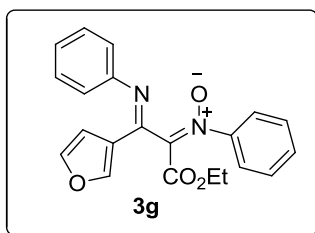
7.2 Hz, 2 H), 2.67 (s, 3H), 0.92 (t, $J = 7.2$ Hz, 3 H); ^{13}C NMR (150 MHz, CDCl_3): δ 159.8, 159.7, 150.4, 147.5, 138.9, 138.7, 135.7, 131.6, 130.4, 130.0, 128.9, 128.7, 128.0, 125.7, 125.3, 122.7, 118.7, 61.9, 20.2, 13.5; HRMS: calcd. for $\text{C}_{24}\text{H}_{22}\text{F}_3\text{N}_2\text{O}_3$: 386.1630, Found: 386.1623.

Spectral data for (*E*)-*N*-((*Z*)-1-ethoxy-1-oxo-3-(phenylimino)-3-(thiophen-2-yl) propan-2-ylidene) aniline oxide (3f).



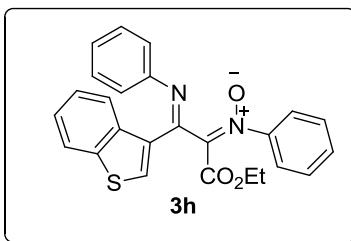
Brownish liquid; ^1H NMR (400 MHz, CDCl_3): δ 7.53 (dd, $J = 5.0, 1.0$ Hz, 1 H), 7.45 ~ 7.39 (m, 3 H), 7.37 (s, 1 H), 7.35 ~ 7.29 (m, 2 H), 7.16 (t, $J = 8.5$ Hz, 1 H), 7.10 ~ 7.07 (m, 5 H), 3.92 (q, $J = 7.0$ Hz, 2 H), 0.96 (t, $J = 7.1$ Hz, 3 H); ^{13}C NMR (100 MHz, CDCl_3): δ 159.1, 152.8, 149.7, 147.6, 141.2, 136.8, 130.7, 130.4, 129.1, 129.0, 128.7, 127.7, 125.4, 122.6, 118.9, 62.0, 13.6; HRMS: calcd. for $\text{C}_{21}\text{H}_{18}\text{N}_2\text{O}_3\text{S}$: 378.1038; Found: 378.1028

Spectral data for (*E*)-*N*-((*E*)-1-ethoxy-3-(furan-3-yl)-1-oxo-3-(phenylimino) propan-2-ylidene) aniline oxide (3g).



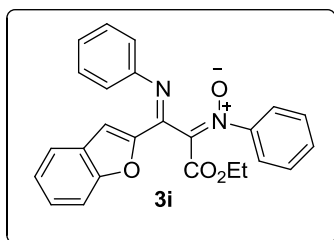
Light Yellow liquid; ^1H NMR (600 MHz, CDCl_3): δ 7.84 (s, 1 H), 7.49 (t, $J = 1.5$ Hz, 1 H), 7.43 ~ 7.40 (m, 1 H), 7.37 ~ 7.34 (m, 2 H), 7.32 ~ 7.29 (m, 2 H), 7.15 ~ 7.12 (m, 1 H), 7.06 ~ 7.04 (m, 4 H), 6.93 (dd, $J = 3.2, 0.8$ Hz, 1 H), 3.92 (q, $J = 7.1$ Hz, 2 H), 0.96 (t, $J = 7.1$ Hz, 3 H); ^{13}C NMR (150 MHz, CDCl_3): δ 159.2, 152.0, 150.1, 147.6, 144.3, 144.2, 130.5, 129.2, 129.0, 128.7, 125.3, 124.7, 122.6, 118.7, 108.8, 62.0, 13.6; ESI-MS: calcd. for $\text{C}_{21}\text{H}_{18}\text{N}_2\text{O}_4$: 362.1267; Found: 362.1265.

Spectral data for (*E*)-*N*-((*E*)-1-(benzo[*b*]thiophen-3-yl)-3-ethoxy-3-oxo-1-(phenylimino) propan-2-ylidene) aniline oxide (3h).



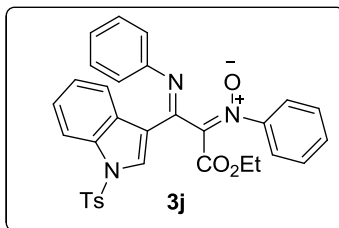
Brownish liquid; $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 8.98 (d, $J = 8.2$ Hz, 1 H), 7.89 ~ 7.87 (m, 2 H), 7.50 ~ 7.41 (m, 3 H), 7.38 ~ 7.35 (m, 4 H), 7.19 ~ 7.14 (m, 3 H), 7.06 (d, $J = 7.9$ Hz, 2 H), 3.93 (q, $J = 7.1$ Hz, 2 H), 0.94 (t, $J = 7.1$ Hz, 3 H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 159.5, 154.1, 150.3, 147.6, 140.5, 137.7, 136.7, 132.3, 131.9, 130.4, 129.0, 128.7, 125.9, 125.4, 125.3, 125.1, 122.6, 122.3, 118.5, 62.0, 13.6; HRMS: calcd. for $\text{C}_{25}\text{H}_{20}\text{N}_2\text{O}_3\text{S}$: 428.1195; Found: 428.1186.

Spectral data for (*E*)-*N*-((*Z*)-1-(benzofuran-2-yl)-3-ethoxy-3-oxo-1-(phenylimino)propan-2-ylidene)aniline oxide (3i).



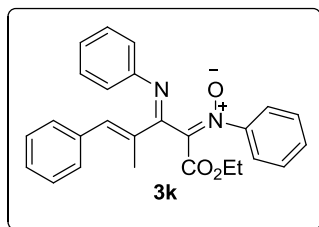
Light yellow liquid; $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.65 (d, $J = 7.8$ Hz, 1 H), 7.57 (d, $J = 8.3$ Hz, 1 H), 7.45 (t, $J = 6.5$ Hz, 1 H), 7.41 ~ 7.38 (m, 3 H), 7.34 (t, $J = 7.5$ Hz, 3 H), 7.27 (t, $J = 7.5$ Hz, 1 H), 7.19 ~ 7.17 (m, 3 H), 7.13 (d, $J = 7.4$ Hz, 2 H), 3.92 (q, $J = 7.0$ Hz, 2 H), 0.95 (t, $J = 7.0$ Hz, 3 H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 159.1, 155.7, 151.5, 149.8, 149.7, 147.7, 135.7, 130.6, 129.0, 128.7, 127.8, 126.8, 125.8, 123.6, 122.7, 122.3, 118.9, 112.1, 110.4, 62.0, 13.6; HRMS: calcd. for $\text{C}_{25}\text{H}_{20}\text{N}_2\text{O}_4$: 412.1423; Found: 412.1433.

Spectral data for (*E*)-*N*-((*E*)-1-ethoxy-1-oxo-3-(phenylimino)-3-(1-tosyl-1H-indol-3-yl)propan-2-ylidene)aniline oxide (3j).



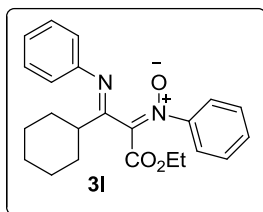
White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.49 (d, $J = 7.7$ Hz, 1 H), 7.95 ~ 7.92 (m, 2 H), 7.78 (d, $J = 8.4$ Hz, 2 H), 7.45 ~ 7.34 (m, 4 H), 7.33 ~ 7.31 (m, 3 H), 7.23 (d, $J = 8.5$ Hz, 2 H), 7.16 (t, $J = 7.4$ Hz, 1 H), 7.11 ~ 7.07 (m, 4 H), 3.87 (q, $J = 7.1$ Hz, 2 H), 2.33 (s, 3 H), 0.94 (t, $J = 6.1$ Hz, 3 H); ^{13}C NMR (150 MHz, CDCl_3): δ 159.3, 153.1, 150.4, 147.6, 145.5, 137.1, 135.5, 134.6, 130.4, 130.1, 129.1, 128.9, 128.7, 128.1, 127.0, 125.7, 125.2, 124.4, 123.6, 122.6, 119.1, 118.6, 113.2, 62.0, 21.5, 13.7; HRMS: calcd. for $\text{C}_{32}\text{H}_{27}\text{N}_3\text{O}_5\text{S}$: 565.1671; Found: 565.1674.

Spectral data for (*E*)-*N*-((3*E*,4*E*)-1-ethoxy-4-methyl-1-oxo-5-phenyl-3-(phenylimino) pent-4-en-2-ylidene) aniline oxide (3k)



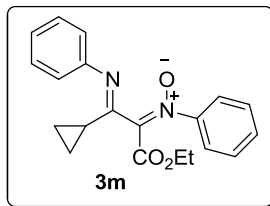
Yellow liquid; ^1H NMR (600 MHz, CDCl_3): δ 7.42 ~ 7.38 (m, 5 H), 7.34 ~ 7.29 (m, 5 H), 7.12 (t, $J = 7.1$ Hz, 1 H), 7.04 (s, 1 H), 7.10 (dd, $J = 8.5, 1.0$ Hz, 2 H), 6.93 (d, $J = 7.4$ Hz, 2 H), 3.96 (q, $J = 7.1$ Hz, 2 H), 2.37 (s, 3 H), 1.01 (t, $J = 7.1$ Hz, 3 H); ^{13}C NMR (150 MHz, CDCl_3): δ 161.5, 159.6, 150.7, 147.7, 137.8, 136.4, 135.9, 135.7, 130.2, 129.7, 128.9, 128.6, 128.3, 127.9, 124.7, 122.6, 118.1, 61.9, 14.4, 13.7; HRMS: calcd. for $\text{C}_{26}\text{H}_{24}\text{N}_2\text{O}_3$: 412.1787; Found: 412.1777.

Spectral data for (*E*)-*N*-((*E*)-1-cyclohexyl-3-ethoxy-3-oxo-1-(phenylimino) propan-2-ylidene) aniline oxide (3l)



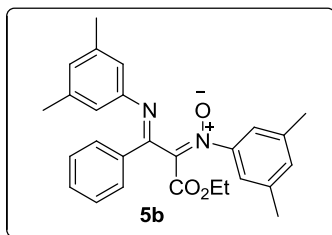
Yellow liquid; ^1H NMR (600 MHz, CDCl_3): δ 7.39 ~ 7.37 (m, 2 H), 7.35 ~ 7.33 (m, 1 H), 7.24 ~ 7.21 (m, 2 H), 7.19 ~ 7.17 (m, 2 H), 6.92 ~ 6.91 (m, 2 H), 6.89 ~ 6.87 (m, 1 H), 3.96 (q, $J = 7.1$ Hz, 2 H), 2.27 (t, $J = 6.4$ Hz, 2H), 2.18 (t, $J = 6.2$ Hz, 2H), 1.75 ~ 1.71 (m, 3 H), 1.65 ~ 1.61 (m, 4 H), 0.88 (t, $J = 7.1$ Hz, 3 H); ^{13}C NMR (150 MHz, CDCl_3): δ 161.7, 143.9, 139.8, 137.3, 128.8, 128.4, 127.8, 127.3, 120.4, 118.3, 111.6, 58.9, 23.3, 23.2, 23.1, 22.7, 13.8; HRMS: calcd. For $\text{C}_{23}\text{H}_{26}\text{N}_2\text{O}_3$: 378.1943; Found: 378.1938.

Spectral data for (*E*)-*N*-((*E*)-1-cyclopropyl-3-ethoxy-3-oxo-1-(phenylimino) propan-2-ylidene) aniline oxide (3m).



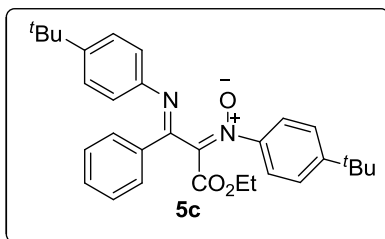
Light Yellow liquid; ^1H NMR (600 MHz, CDCl_3): δ 7.41 ~ 7.38 (m, 1 H), 7.34 (t, $J = 7.4$ Hz, 2 H); 7.24 ~ 7.22 (m, 2 H), 7.07 ~ 7.03 (m, 3 H), 6.88 (d, $J = 7.4$ Hz, 2 H), 3.84 (q, $J = 7.1$ Hz, 2 H), 2.03 ~ 2.00 (m, 1 H), 1.23 ~ 1.20 (m, 2 H), 1.06 ~ 1.04 (m, 2 H), 0.99 (t, $J = 7.1$ Hz, 3 H); ^{13}C NMR (150 MHz, CDCl_3): δ 164.7, 159.1, 150.1, 147.5, 138.3, 130.3, 128.9, 128.6, 124.8, 122.9, 118.9, 61.8, 17.3, 13.3, 9.5; HRMS: calcd. for $\text{C}_{20}\text{H}_{20}\text{N}_2\text{O}_3$: 336.1474; Found: 336.1474.

Spectral data for (*E*)-*N*-((*E*)-1-((3,5-dimethylphenyl)imino)-3-ethoxy-3-oxo-1-phenylpropan-2-ylidene)-3,5-dimethylaniline oxide (5b).



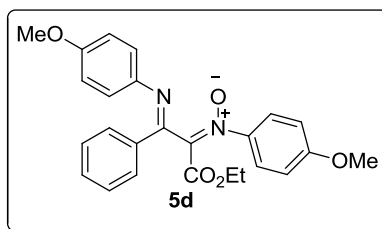
Pale Yellow liquid; ^1H NMR (600 MHz, CDCl_3): δ 7.90 ~ 7.89 (m, 2 H), 7.48 ~ 7.46 (m, 3 H), 7.04 (m, 1 H), 6.80 (s, 1 H), 6.70 (t, $J = 0.7$ Hz, 4 H), 3.89 (q, $J = 6.8$ Hz, 2H), 2.30 (d, $J = 5.6$ Hz, 12 H) 0.96 (t, $J = 6.9$ Hz, 3 H); ^{13}C NMR (150 MHz, CDCl_3): δ 159.3, 158.4, 150.4, 147.7, 138.9, 138.2, 137.4, 135.6, 131.8, 131.2, 128.8, 127.4, 126.8, 120.3, 116.4, 61.7, 21.3, 21.1, 13.7; ESI-MS: calcd. for $\text{C}_{27}\text{H}_{28}\text{N}_2\text{O}_3$: 428.2100; Found: 428.2094.

Spectral data for (*E*)-4-(*tert*-butyl)-*N*-((*E*)-1-((4-(*tert*-butyl)phenyl)imino)-3-ethoxy-3-oxo-1-phenylpropan-2-ylidene) aniline oxide (5c).



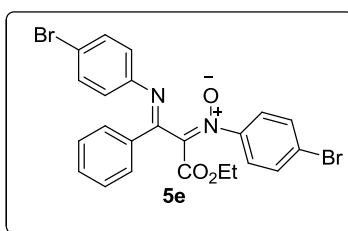
Yellow liquid; ^1H NMR (600 MHz, CDCl_3): δ 7.88 (dd, $J = 7.9, 1.6$ Hz, 2 H), 7.49 ~ 7.44 (m, 3 H), 7.35 ~ 7.31 (m, 4 H), 7.00 ~ 6.97 (m, 4 H), 3.88 (q, $J = 7.1$ Hz, 2H), 1.29 (s, 9 H), 1.28 (s, 9 H), 0.89 (t, $J = 7.1$ Hz, 3 H); ^{13}C NMR (150 MHz, CDCl_3): 159.7, 158.8, 154.0, 148.1, 147.9, 145.3, 137.5, 135.6, 131.2, 128.4, 127.4, 125.8, 125.5, 122.4, 118.3, 61.8, 34.9, 34.4, 31.4, 13.1, 13.6; ESI-MS: calcd. for $\text{C}_{31}\text{H}_{36}\text{N}_2\text{O}_3$: 484.2726; Found: 484.2732.

Spectral data for (*E*)-*N*-((*E*)-1-ethoxy-3-((4-methoxyphenyl)imino)-1-oxo-3-phenylpropan-2-ylidene)-4-methoxyaniline oxide (5d).



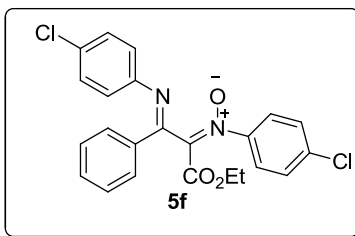
Light Yellow liquid; ^1H NMR (400 MHz, CDCl_3): δ 7.87 (dd, $J = 7.2, 2.1$ Hz, 2 H), 7.46 ~ 7.44 (m, 3 H), 7.16 (dd, $J = 8.0, 0.9$ Hz, 2 H), 7.02 (dd, $J = 7.9, 0.9$ Hz, 2 H), 6.87 ~ 6.83 (m, 4 H), 3.88 (q, $J = 7.1$ Hz, 2H), 3.80 (s, 3 H), 3.77 (s, 3 H), 0.94 (t, $J = 7.1$ Hz, 3 H); ^{13}C NMR (100 MHz, CDCl_3): δ 161.2, 159.8, 158.7, 157.6, 143.8, 140.7, 137.3, 135.8, 131.1, 128.8, 127.3, 124.4, 120.2, 114.0, 113.9, 61.9, 55.6, 55.4, 13.7; ESI-MS: calcd. for $\text{C}_{25}\text{H}_{24}\text{N}_2\text{O}_5$: 432.1685; Found: 432.1687.

Spectral data for (*E*)-4-bromo-*N*-((*E*)-1-((4-bromophenyl)imino)-3-ethoxy-3-oxo-1-phenylpropan-2-ylidene) aniline oxide (5e).



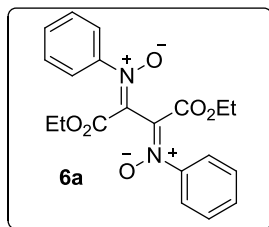
Brown liquid; ^1H NMR (600 MHz, CDCl_3): δ 7.85 (dd, $J = 8.3, 1.4$ Hz, 2 H), 7.54 ~ 7.50 (m, 3 H), 7.48 ~ 7.45 (m, 2 H), 7.43 (dd, $J = 6.6, 2.1$ Hz, 2 H), 6.95 (dd, $J = 6.7, 2.0$ Hz, 2 H), 6.92 (dd, $J = 6.7, 2.0$ Hz, 2 H), 3.94 (q, $J = 7.1$ Hz, 2 H), 0.98 (t, $J = 7.1$ Hz, 3 H); ^{13}C NMR (150 MHz, CDCl_3): δ 159.1, 158.9, 149.3, 146.2, 137.6, 135.0, 132.3, 131.8, 129.0, 127.4, 124.7, 124.3, 120.3, 118.4, 62.3, 13.7 (one carbon merged with others); ESI-MS: calcd. for $\text{C}_{23}\text{H}_{18}\text{Br}_2\text{N}_2\text{O}_3$: 527.9684; Found: 527.9687.

Spectral data for (*E*)-4-chloro-*N*-((*E*)-1-((4-chlorophenyl)imino)-3-ethoxy-3-oxo-1-phenylpropan-2-ylidene) aniline oxide (5f**).**



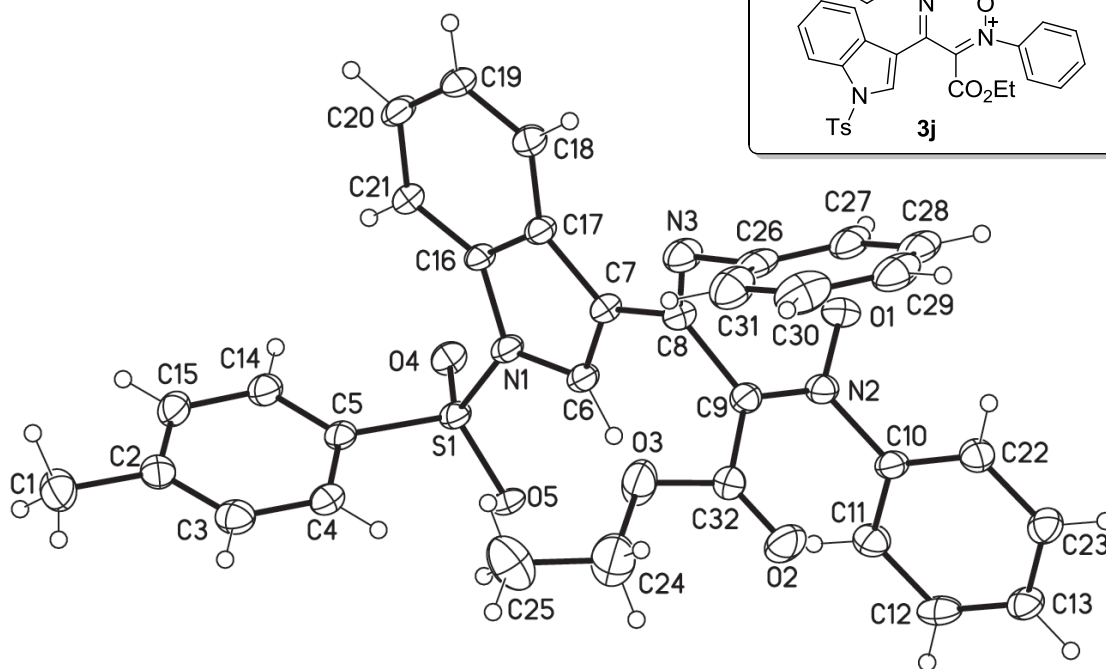
Yellow liquid; ^1H NMR (400 MHz, CDCl_3): δ 7.86 (dd, $J = 8.1, 1.2$ Hz, 2 H), 7.52 ~ 7.45 (m, 3 H), 7.37 (d, $J = 8.6$ Hz, 2 H), 7.29 (d, $J = 8.5$ Hz, 2 H), 7.04 (d, $J = 8.8$ Hz, 2 H), 6.99 (d, $J = 8.5$ Hz, 2 H), 3.94 (q, $J = 7.1$ Hz, 2 H), 0.97 (t, $J = 7.1$ Hz, 3 H); ^{13}C NMR (100 MHz, CDCl_3): δ 159.0, 158.9, 148.8, 145.6, 137.6, 136.6, 134.9, 131.8, 130.6, 129.3, 128.9, 128.8, 127.3, 124.0, 119.9, 62.3, 13.7; ESI-MS: calcd. for $\text{C}_{23}\text{H}_{18}\text{Cl}_2\text{N}_2\text{O}_3$: 440.0694; Found: 440.0690.

Spectral data for (*N,N'E,N,N'E*)-*N,N'*-(1,4-diethoxy-1,4-dioxobutane-2,3-diylidene) bis (aniline oxide) (6a**).**



Yellow solid; ^1H NMR (600 MHz, CDCl_3): δ 7.50 ~ 7.42 (m, 10 H), 4.10 (q, $J = 7.1$ Hz, 4 H), 1.01 (t, $J = 7.1$ Hz, 6 H); ^{13}C NMR (150 MHz, CDCl_3): δ 160.0, 147.5, 135.3, 131.1, 129.1, 123.5, 62.4, 13.6; HRMS: calcd. for $\text{C}_{20}\text{H}_{20}\text{Cl}_2\text{N}_2\text{O}_6$: 384.1321; Found: 384.1359.

(IV) X-ray data for compound 3j



:

Table 1. Crystal data and structure refinement for mo_130802lt_0m.

Identification code	mo_130802lt_0m	
Empirical formula	C ₃₂ H ₂₇ N ₃ O ₅ S	
Formula weight	565.63	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.1408(17) Å	α = 103.814(4)°.
	b = 10.8111(18) Å	β = 92.891(4)°.
	c = 13.136(2) Å	γ = 95.161(4)°.
Volume	1389.0(4) Å ³	
Z	2	
Density (calculated)	1.352 Mg/m ³	
Absorption coefficient	0.164 mm ⁻¹	
F(000)	592	
Crystal size	0.25 x 0.20 x 0.20 mm ³	
Theta range for data collection	1.60 to 26.53°.	
Index ranges	-12 ≤ h ≤ 12, -13 ≤ k ≤ 13, -7 ≤ l ≤ 16	

Reflections collected	19602
Independent reflections	5725 [R(int) = 0.0530]
Completeness to theta = 26.53°	98.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9486 and 0.7194
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5725 / 0 / 372
Goodness-of-fit on F ²	1.042
Final R indices [I>2sigma(I)]	R1 = 0.0574, wR2 = 0.1466
R indices (all data)	R1 = 0.0776, wR2 = 0.1619
Largest diff. peak and hole	0.663 and -0.712 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for mo_130802lt_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	6325(1)	8107(1)	8617(1)	20(1)
O(1)	7810(2)	9853(2)	4683(1)	28(1)
O(2)	6047(2)	6199(2)	3127(2)	38(1)
O(3)	7165(2)	5558(2)	4386(2)	41(1)
O(4)	6568(2)	9238(2)	9444(1)	25(1)
O(5)	5128(2)	7862(2)	7945(1)	24(1)
N(1)	7539(2)	8141(2)	7802(2)	21(1)
N(2)	7146(2)	8769(2)	4274(2)	22(1)
N(3)	9854(2)	7565(2)	4827(2)	29(1)
C(1)	6991(3)	3605(3)	10485(2)	37(1)
C(2)	6823(2)	4718(2)	10003(2)	27(1)
C(3)	6344(2)	4534(2)	8958(2)	29(1)
C(4)	6200(2)	5567(2)	8518(2)	24(1)
C(5)	6554(2)	6788(2)	9138(2)	21(1)
C(6)	7338(2)	7935(2)	6721(2)	21(1)
C(7)	8534(2)	7981(2)	6288(2)	21(1)
C(8)	8713(2)	7763(2)	5175(2)	23(1)
C(9)	7497(2)	7694(2)	4452(2)	22(1)
C(10)	5982(2)	8826(2)	3588(2)	22(1)

C(11)	4732(2)	8715(2)	3949(2)	28(1)
C(12)	3644(2)	8790(2)	3290(2)	30(1)
C(13)	3825(2)	8988(2)	2303(2)	27(1)
C(14)	7028(2)	7002(2)	10181(2)	26(1)
C(15)	7153(2)	5962(3)	10608(2)	29(1)
C(16)	8916(2)	8323(2)	8079(2)	20(1)
C(17)	9559(2)	8233(2)	7149(2)	21(1)
C(18)	10949(2)	8396(2)	7197(2)	24(1)
C(19)	11638(2)	8628(2)	8172(2)	26(1)
C(20)	10974(2)	8710(2)	9087(2)	25(1)
C(21)	9596(2)	8566(2)	9062(2)	22(1)
C(22)	6191(2)	9039(2)	2618(2)	25(1)
C(23)	5096(2)	9118(2)	1965(2)	27(1)
C(24)	6613(4)	4246(3)	3895(3)	58(1)
C(25)	6827(4)	3458(3)	4627(3)	52(1)
C(26)	9997(2)	7361(3)	3730(2)	32(1)
C(27)	9942(2)	8354(3)	3229(2)	32(1)
C(28)	10145(2)	8137(3)	2164(2)	38(1)
C(29)	10408(3)	6954(3)	1605(2)	43(1)
C(30)	10472(3)	5968(3)	2108(2)	46(1)
C(31)	10279(3)	6165(3)	3172(2)	40(1)
C(32)	6808(2)	6433(2)	3894(2)	26(1)

Table 3. Bond lengths [\AA] and angles [$^\circ$] for mo_130802lt_0m.

S(1)-O(4)	1.4213(17)
S(1)-O(5)	1.4301(16)
S(1)-N(1)	1.676(2)
S(1)-C(5)	1.751(2)
O(1)-N(2)	1.279(2)
O(2)-C(32)	1.200(3)
O(3)-C(32)	1.331(3)
O(3)-C(24)	1.457(3)
N(1)-C(6)	1.384(3)

N(1)-C(16)	1.410(3)
N(2)-C(9)	1.315(3)
N(2)-C(10)	1.463(3)
N(3)-C(8)	1.282(3)
N(3)-C(26)	1.422(3)
C(1)-C(2)	1.506(3)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-C(15)	1.391(4)
C(2)-C(3)	1.394(4)
C(3)-C(4)	1.390(3)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.380(3)
C(4)-H(4)	0.9500
C(5)-C(14)	1.387(3)
C(6)-C(7)	1.367(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.448(3)
C(7)-C(17)	1.455(3)
C(8)-C(9)	1.504(3)
C(9)-C(32)	1.478(3)
C(10)-C(22)	1.370(3)
C(10)-C(11)	1.381(3)
C(11)-C(12)	1.388(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.382(4)
C(12)-H(12)	0.9500
C(13)-C(23)	1.390(4)
C(13)-H(13)	0.9500
C(14)-C(15)	1.384(3)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-C(21)	1.389(3)
C(16)-C(17)	1.400(3)
C(17)-C(18)	1.401(3)

C(18)-C(19)	1.384(3)
C(18)-H(18)	0.9500
C(19)-C(20)	1.395(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.391(3)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-C(23)	1.390(3)
C(22)-H(22)	0.9500
C(23)-H(23)	0.9500
C(24)-C(25)	1.450(4)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-C(31)	1.388(4)
C(26)-C(27)	1.391(4)
C(27)-C(28)	1.391(4)
C(27)-H(27)	0.9500
C(28)-C(29)	1.371(4)
C(28)-H(28)	0.9500
C(29)-C(30)	1.386(4)
C(29)-H(29)	0.9500
C(30)-C(31)	1.389(4)
C(30)-H(30)	0.9500
C(31)-H(31)	0.9500
O(4)-S(1)-O(5)	120.74(10)
O(4)-S(1)-N(1)	107.13(10)
O(5)-S(1)-N(1)	104.38(10)
O(4)-S(1)-C(5)	108.48(11)
O(5)-S(1)-C(5)	110.20(10)
N(1)-S(1)-C(5)	104.65(10)
C(32)-O(3)-C(24)	115.2(2)
C(6)-N(1)-C(16)	108.62(18)

C(6)-N(1)-S(1)	124.69(16)
C(16)-N(1)-S(1)	126.64(15)
O(1)-N(2)-C(9)	122.3(2)
O(1)-N(2)-C(10)	114.60(18)
C(9)-N(2)-C(10)	123.13(19)
C(8)-N(3)-C(26)	119.2(2)
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(15)-C(2)-C(3)	118.9(2)
C(15)-C(2)-C(1)	119.6(2)
C(3)-C(2)-C(1)	121.5(2)
C(4)-C(3)-C(2)	121.1(2)
C(4)-C(3)-H(3A)	119.4
C(2)-C(3)-H(3A)	119.4
C(5)-C(4)-C(3)	118.5(2)
C(5)-C(4)-H(4)	120.8
C(3)-C(4)-H(4)	120.8
C(4)-C(5)-C(14)	121.8(2)
C(4)-C(5)-S(1)	119.32(17)
C(14)-C(5)-S(1)	118.83(19)
C(7)-C(6)-N(1)	109.9(2)
C(7)-C(6)-H(6)	125.1
N(1)-C(6)-H(6)	125.1
C(6)-C(7)-C(8)	125.4(2)
C(6)-C(7)-C(17)	107.0(2)
C(8)-C(7)-C(17)	127.6(2)
N(3)-C(8)-C(7)	120.7(2)
N(3)-C(8)-C(9)	122.0(2)
C(7)-C(8)-C(9)	117.2(2)
N(2)-C(9)-C(32)	122.0(2)
N(2)-C(9)-C(8)	118.0(2)
C(32)-C(9)-C(8)	119.7(2)

C(22)-C(10)-C(11)	122.7(2)
C(22)-C(10)-N(2)	117.8(2)
C(11)-C(10)-N(2)	119.5(2)
C(10)-C(11)-C(12)	118.4(2)
C(10)-C(11)-H(11)	120.8
C(12)-C(11)-H(11)	120.8
C(13)-C(12)-C(11)	120.1(2)
C(13)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9
C(12)-C(13)-C(23)	120.3(2)
C(12)-C(13)-H(13)	119.8
C(23)-C(13)-H(13)	119.8
C(15)-C(14)-C(5)	119.0(2)
C(15)-C(14)-H(14)	120.5
C(5)-C(14)-H(14)	120.5
C(14)-C(15)-C(2)	120.8(2)
C(14)-C(15)-H(15)	119.6
C(2)-C(15)-H(15)	119.6
C(21)-C(16)-C(17)	122.9(2)
C(21)-C(16)-N(1)	129.8(2)
C(17)-C(16)-N(1)	107.29(19)
C(16)-C(17)-C(18)	119.4(2)
C(16)-C(17)-C(7)	107.25(19)
C(18)-C(17)-C(7)	133.3(2)
C(19)-C(18)-C(17)	118.2(2)
C(19)-C(18)-H(18)	120.9
C(17)-C(18)-H(18)	120.9
C(18)-C(19)-C(20)	121.3(2)
C(18)-C(19)-H(19)	119.3
C(20)-C(19)-H(19)	119.3
C(21)-C(20)-C(19)	121.7(2)
C(21)-C(20)-H(20)	119.2
C(19)-C(20)-H(20)	119.2
C(16)-C(21)-C(20)	116.5(2)
C(16)-C(21)-H(21)	121.8
C(20)-C(21)-H(21)	121.8

C(10)-C(22)-C(23)	118.5(2)
C(10)-C(22)-H(22)	120.7
C(23)-C(22)-H(22)	120.7
C(13)-C(23)-C(22)	119.9(2)
C(13)-C(23)-H(23)	120.0
C(22)-C(23)-H(23)	120.0
C(25)-C(24)-O(3)	108.8(3)
C(25)-C(24)-H(24A)	109.9
O(3)-C(24)-H(24A)	109.9
C(25)-C(24)-H(24B)	109.9
O(3)-C(24)-H(24B)	109.9
H(24A)-C(24)-H(24B)	108.3
C(24)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(31)-C(26)-C(27)	119.9(2)
C(31)-C(26)-N(3)	118.8(2)
C(27)-C(26)-N(3)	121.2(2)
C(26)-C(27)-C(28)	119.8(3)
C(26)-C(27)-H(27)	120.1
C(28)-C(27)-H(27)	120.1
C(29)-C(28)-C(27)	120.5(3)
C(29)-C(28)-H(28)	119.7
C(27)-C(28)-H(28)	119.7
C(28)-C(29)-C(30)	119.6(3)
C(28)-C(29)-H(29)	120.2
C(30)-C(29)-H(29)	120.2
C(29)-C(30)-C(31)	120.8(3)
C(29)-C(30)-H(30)	119.6
C(31)-C(30)-H(30)	119.6
C(26)-C(31)-C(30)	119.3(3)
C(26)-C(31)-H(31)	120.3
C(30)-C(31)-H(31)	120.3

O(2)-C(32)-O(3)	124.0(2)
O(2)-C(32)-C(9)	127.3(2)
O(3)-C(32)-C(9)	108.7(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for mo_130802lt_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
S(1)	14(1)	25(1)	22(1)	6(1)	-1(1)	2(1)
O(1)	23(1)	25(1)	32(1)	5(1)	-2(1)	-5(1)
O(2)	40(1)	32(1)	38(1)	5(1)	-16(1)	-3(1)
O(3)	60(1)	28(1)	34(1)	10(1)	-17(1)	-3(1)
O(4)	21(1)	27(1)	26(1)	5(1)	0(1)	4(1)
O(5)	11(1)	32(1)	29(1)	10(1)	-4(1)	1(1)
N(1)	14(1)	28(1)	22(1)	7(1)	-2(1)	1(1)
N(2)	18(1)	27(1)	22(1)	6(1)	1(1)	-1(1)
N(3)	20(1)	40(1)	26(1)	7(1)	1(1)	3(1)
C(1)	28(1)	44(2)	47(2)	25(1)	8(1)	9(1)
C(2)	13(1)	38(1)	36(1)	18(1)	8(1)	7(1)
C(3)	22(1)	28(1)	36(1)	7(1)	2(1)	4(1)
C(4)	18(1)	28(1)	27(1)	7(1)	-1(1)	3(1)
C(5)	13(1)	29(1)	22(1)	9(1)	2(1)	3(1)
C(6)	17(1)	26(1)	20(1)	6(1)	-1(1)	1(1)
C(7)	16(1)	24(1)	23(1)	7(1)	-3(1)	2(1)
C(8)	19(1)	24(1)	24(1)	6(1)	-2(1)	0(1)
C(9)	18(1)	29(1)	19(1)	8(1)	2(1)	0(1)
C(10)	16(1)	22(1)	26(1)	6(1)	-2(1)	0(1)
C(11)	20(1)	37(1)	28(1)	10(1)	5(1)	0(1)
C(12)	14(1)	34(1)	40(2)	5(1)	1(1)	1(1)
C(13)	20(1)	26(1)	37(1)	9(1)	-3(1)	4(1)
C(14)	20(1)	34(1)	24(1)	8(1)	1(1)	1(1)
C(15)	20(1)	44(2)	27(1)	17(1)	2(1)	4(1)
C(16)	13(1)	22(1)	26(1)	8(1)	-3(1)	2(1)

C(17)	17(1)	21(1)	24(1)	6(1)	-4(1)	1(1)
C(18)	18(1)	29(1)	28(1)	9(1)	1(1)	4(1)
C(19)	14(1)	32(1)	34(1)	12(1)	-3(1)	2(1)
C(20)	19(1)	28(1)	28(1)	7(1)	-8(1)	2(1)
C(21)	18(1)	25(1)	22(1)	7(1)	-3(1)	2(1)
C(22)	20(1)	27(1)	29(1)	8(1)	4(1)	4(1)
C(23)	28(1)	27(1)	28(1)	9(1)	-1(1)	6(1)
C(24)	88(3)	29(2)	52(2)	9(1)	-26(2)	-9(2)
C(25)	68(2)	36(2)	53(2)	13(2)	16(2)	2(2)
C(26)	12(1)	52(2)	28(1)	6(1)	1(1)	1(1)
C(27)	15(1)	52(2)	29(1)	12(1)	0(1)	2(1)
C(28)	15(1)	67(2)	32(1)	16(1)	0(1)	-1(1)
C(29)	22(1)	79(2)	27(1)	11(2)	2(1)	2(1)
C(30)	30(2)	63(2)	37(2)	-4(1)	4(1)	10(1)
C(31)	29(2)	54(2)	35(2)	10(1)	3(1)	10(1)
C(32)	24(1)	29(1)	24(1)	9(1)	0(1)	0(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for mo_130802lt_0m.

	x	y	z	U(eq)
H(1A)	7937	3570	10654	55
H(1B)	6626	2807	9985	55
H(1C)	6521	3714	11128	55
H(3A)	6112	3688	8540	35
H(4)	5866	5437	7808	29
H(6)	6496	7784	6338	25
H(11)	4619	8590	4632	34
H(12)	2773	8705	3517	36
H(13)	3078	9036	1853	33
H(14)	7263	7850	10596	31
H(15)	7468	6100	11324	34
H(18)	11406	8349	6577	29

H(19)	12581	8735	8219	32
H(20)	11478	8868	9743	30
H(21)	9143	8629	9686	26
H(22)	7065	9130	2398	30
H(23)	5216	9261	1288	32
H(24A)	5651	4220	3709	70
H(24B)	7052	3918	3243	70
H(25A)	7778	3517	4831	78
H(25B)	6499	2565	4292	78
H(25C)	6348	3758	5254	78
H(27)	9766	9178	3612	38
H(28)	10101	8814	1821	45
H(29)	10546	6811	878	51
H(30)	10650	5147	1720	55
H(31)	10339	5489	3514	48

(V) X-ray data for compound 5a :

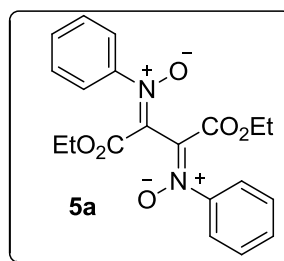
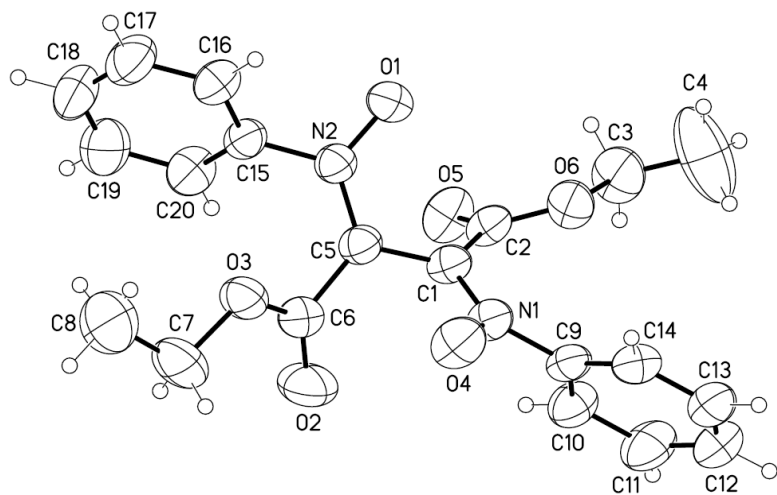


Table 7. Crystal data and structure refinement for mo_140816_0m_a.

Identification code	mo_140816_0m_a	
Empirical formula	C ₂₀ H ₂₀ N ₂ O ₆	
Formula weight	384.38	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 11.8424(8) Å	α = 90°.
	b = 10.9091(8) Å	β = 105.318(2)°.
	c = 16.0091(11) Å	γ = 90°.
Volume	1994.7(2) Å ³	
Z	4	
Density (calculated)	1.280 Mg/m ³	
Absorption coefficient	0.096 mm ⁻¹	
F(000)	808	
Crystal size	0.20 x 0.18 x 0.08 mm ³	
Theta range for data collection	1.783 to 26.402°.	
Index ranges	-14 ≤ h ≤ 14, -13 ≤ k ≤ 13, -19 ≤ l ≤ 20	
Reflections collected	15944	
Independent reflections	4076 [R(int) = 0.0463]	
Completeness to theta = 25.242°	99.8 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9485 and 0.8871
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4076 / 0 / 255
Goodness-of-fit on F ²	1.030
Final R indices [I>2sigma(I)]	R1 = 0.0480, wR2 = 0.1198
R indices (all data)	R1 = 0.0857, wR2 = 0.1396
Extinction coefficient	n/a
Largest diff. peak and hole	0.344 and -0.230 e.Å ⁻³

Table 8. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for mo_140816_0m_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3015(2)	2787(2)	5043(1)	45(1)
C(2)	3945(2)	1858(2)	5368(1)	47(1)
C(3)	5994(2)	1491(2)	5839(2)	74(1)
C(4)	7053(2)	2127(4)	5833(3)	141(2)
C(5)	1915(2)	2409(2)	4467(1)	45(1)
C(6)	813(2)	2783(2)	4674(1)	53(1)
C(7)	-1169(2)	3356(3)	4099(2)	96(1)
C(8)	-2045(3)	3187(4)	3297(3)	150(2)
C(9)	4019(2)	4375(2)	6037(1)	45(1)
C(10)	4181(2)	3793(2)	6818(1)	58(1)
C(11)	5035(2)	4229(3)	7516(2)	72(1)
C(12)	5707(2)	5224(3)	7422(2)	74(1)
C(13)	5510(2)	5813(2)	6640(2)	67(1)
C(14)	4650(2)	5401(2)	5937(1)	53(1)
C(15)	916(2)	1043(2)	3308(1)	46(1)
C(16)	570(2)	1209(2)	2428(1)	56(1)
C(17)	-416(2)	612(2)	1954(2)	70(1)
C(18)	-1014(2)	-149(3)	2356(2)	79(1)
C(19)	-648(2)	-337(2)	3230(2)	79(1)
C(20)	335(2)	262(2)	3722(2)	60(1)
N(1)	3117(1)	3946(2)	5294(1)	47(1)

N(2)	1943(1)	1694(2)	3806(1)	45(1)
O(1)	2893(1)	1489(2)	3592(1)	61(1)
O(2)	754(2)	2861(2)	5406(1)	83(1)
O(3)	-34(1)	3030(1)	3975(1)	59(1)
O(4)	2372(1)	4752(1)	4916(1)	67(1)
O(5)	3713(1)	832(1)	5532(1)	64(1)
O(6)	5008(1)	2291(1)	5430(1)	55(1)

Table 9. Bond lengths [\AA] and angles [$^\circ$] for mo_140816_0m_a.

C(1)-N(1)	1.322(2)
C(1)-C(5)	1.443(3)
C(1)-C(2)	1.486(3)
C(2)-O(5)	1.199(2)
C(2)-O(6)	1.323(2)
C(3)-C(4)	1.435(4)
C(3)-O(6)	1.466(2)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-H(4A)	0.9600
C(4)-H(4B)	0.9600
C(4)-H(4C)	0.9600
C(5)-N(2)	1.322(2)
C(5)-C(6)	1.487(3)
C(6)-O(2)	1.196(2)
C(6)-O(3)	1.318(3)
C(7)-C(8)	1.433(4)
C(7)-O(3)	1.453(3)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(9)-C(10)	1.370(3)
C(9)-C(14)	1.378(3)

C(9)-N(1)	1.451(2)
C(10)-C(11)	1.379(3)
C(10)-H(10)	0.9300
C(11)-C(12)	1.378(4)
C(11)-H(11)	0.9300
C(12)-C(13)	1.372(4)
C(12)-H(12)	0.9300
C(13)-C(14)	1.378(3)
C(13)-H(13)	0.9300
C(14)-H(14)	0.9300
C(15)-C(20)	1.371(3)
C(15)-C(16)	1.372(3)
C(15)-N(2)	1.452(2)
C(16)-C(17)	1.377(3)
C(16)-H(16)	0.9300
C(17)-C(18)	1.358(4)
C(17)-H(17)	0.9300
C(18)-C(19)	1.366(4)
C(18)-H(18)	0.9300
C(19)-C(20)	1.385(3)
C(19)-H(19)	0.9300
C(20)-H(20)	0.9300
N(1)-O(4)	1.280(2)
N(2)-O(1)	1.2787(19)
N(1)-C(1)-C(5)	117.57(17)
N(1)-C(1)-C(2)	123.07(17)
C(5)-C(1)-C(2)	119.25(17)
O(5)-C(2)-O(6)	125.83(19)
O(5)-C(2)-C(1)	121.48(19)
O(6)-C(2)-C(1)	112.69(17)
C(4)-C(3)-O(6)	107.7(2)
C(4)-C(3)-H(3A)	110.2
O(6)-C(3)-H(3A)	110.2
C(4)-C(3)-H(3B)	110.2
O(6)-C(3)-H(3B)	110.2
H(3A)-C(3)-H(3B)	108.5

C(3)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
N(2)-C(5)-C(1)	118.09(16)
N(2)-C(5)-C(6)	123.38(17)
C(1)-C(5)-C(6)	118.44(17)
O(2)-C(6)-O(3)	126.1(2)
O(2)-C(6)-C(5)	121.4(2)
O(3)-C(6)-C(5)	112.52(17)
C(8)-C(7)-O(3)	108.8(2)
C(8)-C(7)-H(7A)	109.9
O(3)-C(7)-H(7A)	109.9
C(8)-C(7)-H(7B)	109.9
O(3)-C(7)-H(7B)	109.9
H(7A)-C(7)-H(7B)	108.3
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(10)-C(9)-C(14)	122.2(2)
C(10)-C(9)-N(1)	119.62(18)
C(14)-C(9)-N(1)	118.09(18)
C(9)-C(10)-C(11)	118.4(2)
C(9)-C(10)-H(10)	120.8
C(11)-C(10)-H(10)	120.8
C(12)-C(11)-C(10)	120.2(2)
C(12)-C(11)-H(11)	119.9
C(10)-C(11)-H(11)	119.9
C(13)-C(12)-C(11)	120.4(2)
C(13)-C(12)-H(12)	119.8
C(11)-C(12)-H(12)	119.8

C(12)-C(13)-C(14)	120.2(2)
C(12)-C(13)-H(13)	119.9
C(14)-C(13)-H(13)	119.9
C(13)-C(14)-C(9)	118.5(2)
C(13)-C(14)-H(14)	120.8
C(9)-C(14)-H(14)	120.8
C(20)-C(15)-C(16)	121.8(2)
C(20)-C(15)-N(2)	119.57(18)
C(16)-C(15)-N(2)	118.63(18)
C(15)-C(16)-C(17)	118.9(2)
C(15)-C(16)-H(16)	120.6
C(17)-C(16)-H(16)	120.6
C(18)-C(17)-C(16)	120.0(2)
C(18)-C(17)-H(17)	120.0
C(16)-C(17)-H(17)	120.0
C(17)-C(18)-C(19)	120.9(2)
C(17)-C(18)-H(18)	119.6
C(19)-C(18)-H(18)	119.6
C(18)-C(19)-C(20)	120.2(2)
C(18)-C(19)-H(19)	119.9
C(20)-C(19)-H(19)	119.9
C(15)-C(20)-C(19)	118.2(2)
C(15)-C(20)-H(20)	120.9
C(19)-C(20)-H(20)	120.9
O(4)-N(1)-C(1)	121.12(16)
O(4)-N(1)-C(9)	115.62(15)
C(1)-N(1)-C(9)	123.14(16)
O(1)-N(2)-C(5)	121.83(16)
O(1)-N(2)-C(15)	115.85(15)
C(5)-N(2)-C(15)	122.25(16)
C(6)-O(3)-C(7)	117.25(19)
C(2)-O(6)-C(3)	116.84(17)

Symmetry transformations used to generate equivalent atoms:

Table 10. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for mo_140816_0m_a. The anisotropic

displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(1)	50(1)	45(1)	38(1)	-4(1)	9(1)	4(1)
C(2)	55(1)	44(1)	38(1)	-6(1)	5(1)	3(1)
C(3)	58(1)	64(2)	88(2)	-1(1)	3(1)	22(1)
C(4)	57(2)	143(3)	216(4)	73(3)	24(2)	24(2)
C(5)	47(1)	48(1)	38(1)	-3(1)	9(1)	3(1)
C(6)	54(1)	58(1)	48(1)	-7(1)	16(1)	1(1)
C(7)	51(1)	135(3)	103(2)	-27(2)	23(2)	25(2)
C(8)	55(2)	213(5)	169(4)	-87(4)	5(2)	25(2)
C(9)	52(1)	43(1)	41(1)	-9(1)	11(1)	6(1)
C(10)	71(1)	58(1)	45(1)	-2(1)	14(1)	-6(1)
C(11)	88(2)	84(2)	40(1)	-4(1)	9(1)	-6(2)
C(12)	71(2)	90(2)	56(2)	-26(1)	10(1)	-10(1)
C(13)	71(2)	65(2)	68(2)	-22(1)	26(1)	-15(1)
C(14)	64(1)	49(1)	49(1)	-6(1)	20(1)	2(1)
C(15)	46(1)	45(1)	44(1)	-6(1)	8(1)	4(1)
C(16)	61(1)	59(1)	44(1)	-5(1)	9(1)	-3(1)
C(17)	70(2)	78(2)	54(1)	-14(1)	0(1)	-1(1)
C(18)	67(2)	79(2)	83(2)	-29(2)	6(1)	-18(1)
C(19)	82(2)	66(2)	92(2)	-9(2)	31(2)	-25(1)
C(20)	68(1)	55(1)	54(1)	2(1)	14(1)	-5(1)
N(1)	50(1)	46(1)	42(1)	-1(1)	6(1)	9(1)
N(2)	43(1)	52(1)	39(1)	-4(1)	9(1)	3(1)
O(1)	48(1)	80(1)	57(1)	-17(1)	18(1)	4(1)
O(2)	79(1)	124(2)	51(1)	-9(1)	28(1)	11(1)
O(3)	47(1)	74(1)	57(1)	-8(1)	13(1)	14(1)
O(4)	68(1)	54(1)	67(1)	-3(1)	-1(1)	22(1)
O(5)	73(1)	46(1)	63(1)	6(1)	3(1)	-1(1)
O(6)	50(1)	47(1)	65(1)	1(1)	8(1)	10(1)

Table 11. Hydrogen coordinates (x 10⁴) and isotropic displacement parameters (Å²x 10⁻³) for mo_140816_0m_a.

	x	y	z	U(eq)
H(3A)	5983	1304	6429	88
H(3B)	5943	728	5520	88
H(4A)	7092	2235	5247	212
H(4B)	7716	1656	6147	212
H(4C)	7061	2913	6104	212
H(7A)	-1342	2843	4544	115
H(7B)	-1162	4204	4282	115
H(8A)	-1823	3627	2845	225
H(8B)	-2782	3491	3353	225
H(8C)	-2115	2331	3156	225
H(10)	3726	3120	6876	70
H(11)	5158	3850	8053	87
H(12)	6298	5497	7891	88
H(13)	5958	6493	6583	80
H(14)	4499	5806	5408	64
H(16)	995	1716	2155	67
H(17)	-674	729	1359	84
H(18)	-1682	-546	2033	95
H(19)	-1060	-869	3495	94
H(20)	594	138	4317	71

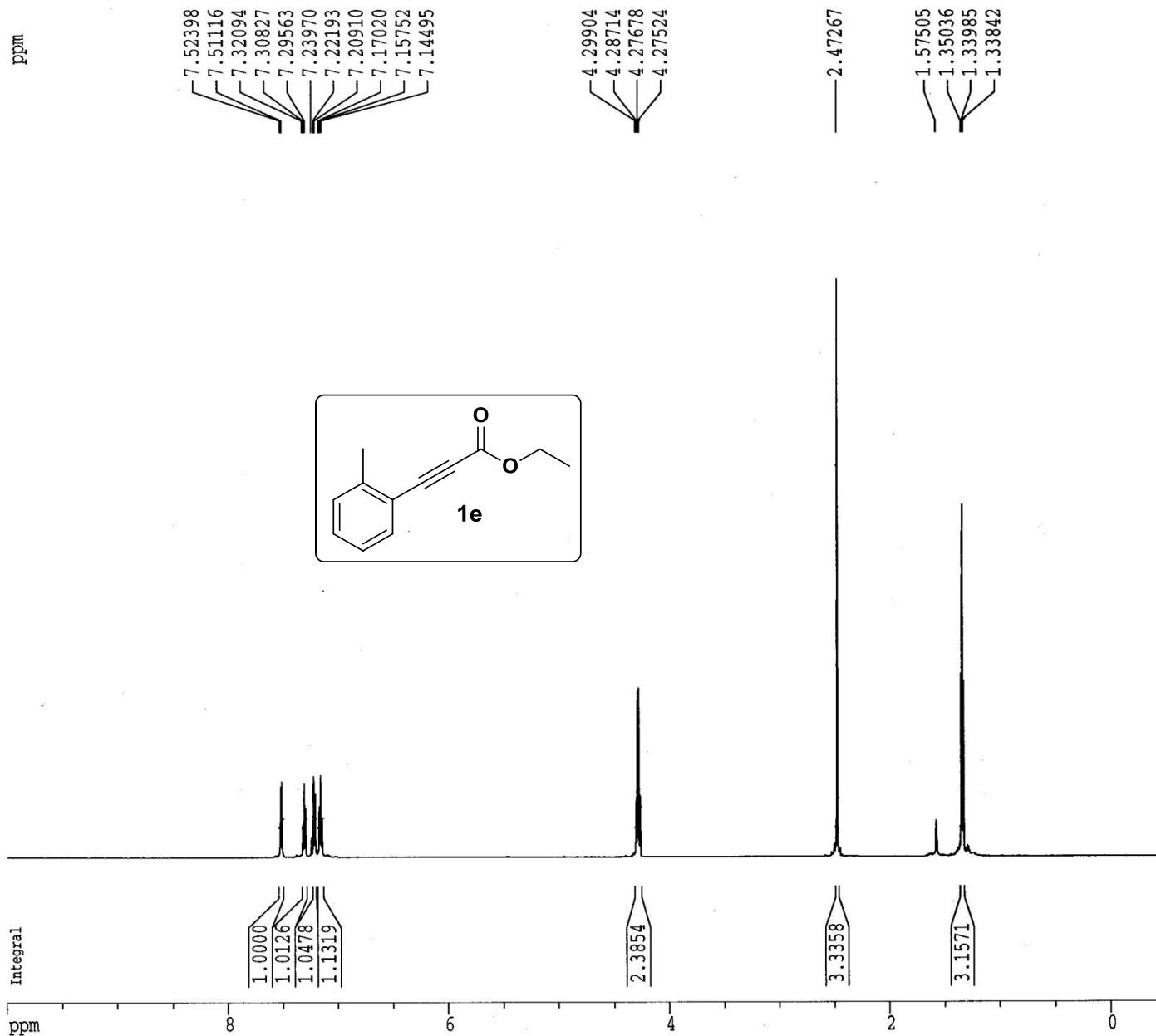
Current Data Parameters
NAME RKS-2-155
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140925
Time 14.16
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.250008 Hz
AQ 1.9999876 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 303.8 K
D1 2.0000000 sec
MCREST 0.0000000 sec
MCMRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.7029935 MHz

F2 - Processing parameters
SI 32768
SF 598.7000255 MHz
WDW EM
SSB 0
LB 0.40 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 5987.00 Hz
F2P -0.500 ppm
F2 -299.35 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.31750 Hz/cm



Current Data Parameters
NAME RKS-2-155
EXPNO 2
PROCNO 1

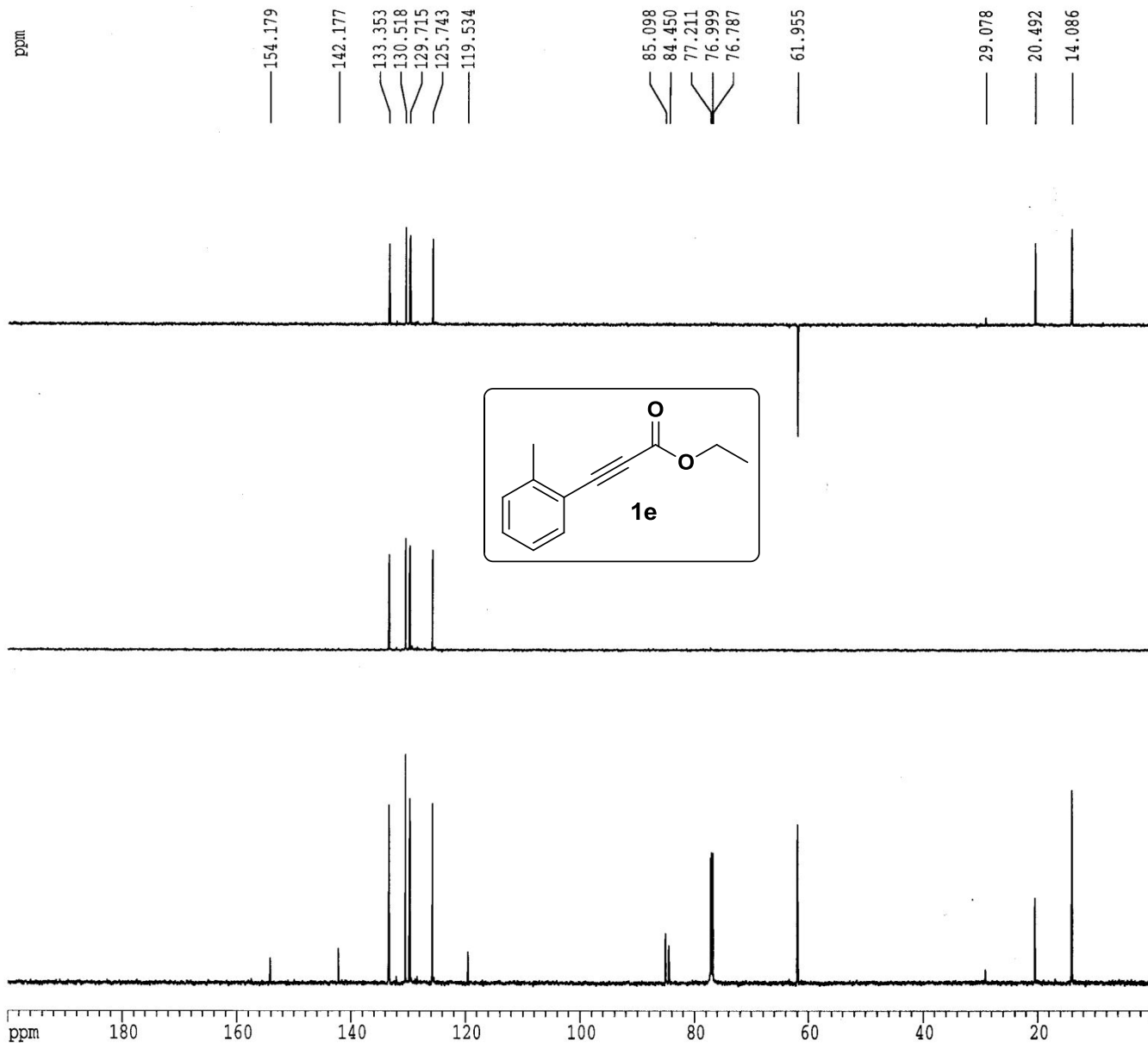
F2 - Acquisition Parameters
Date_ 20140925
Time 14.36
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 300
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 305.7 K
D1 3.5000000 sec
d11 0.0300000 sec
DELTA 3.4000010 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5597948 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.7029935 MHz

F2 - Processing parameters
SI 65536
SF 150.5432363 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
FIP 200.000 ppm
F1 30108.65 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.43237 Hz/cm



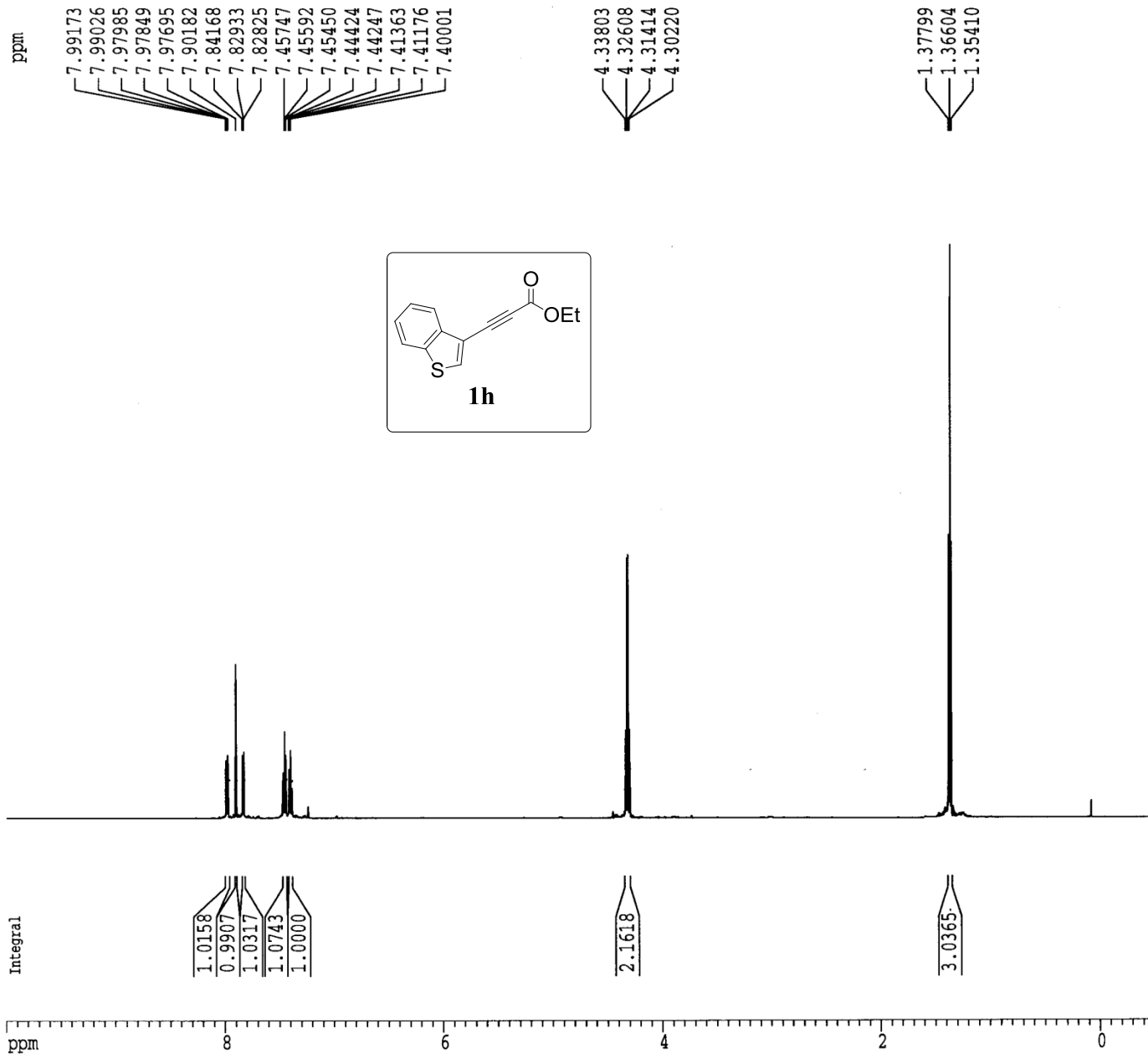
Current Data Parameters
NAME RKS-1-147
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130729
Time 15.29
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8382.229 Hz
FIDRES 0.255805 Hz
AQ 1.9546613 sec
RG 256
DW 59.650 usec
DE 6.50 usec
TE 300.9 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFOL 598.8026946 MHz

F2 - Processing parameters
SI 32768
SF 598.8000284 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 5988.00 Hz
F2P -0.500 ppm
F2 -299.40 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.37003 Hz/cm



Current Data Parameters
NAME RKS-1-147
EXPNO 2
PROCNO 1

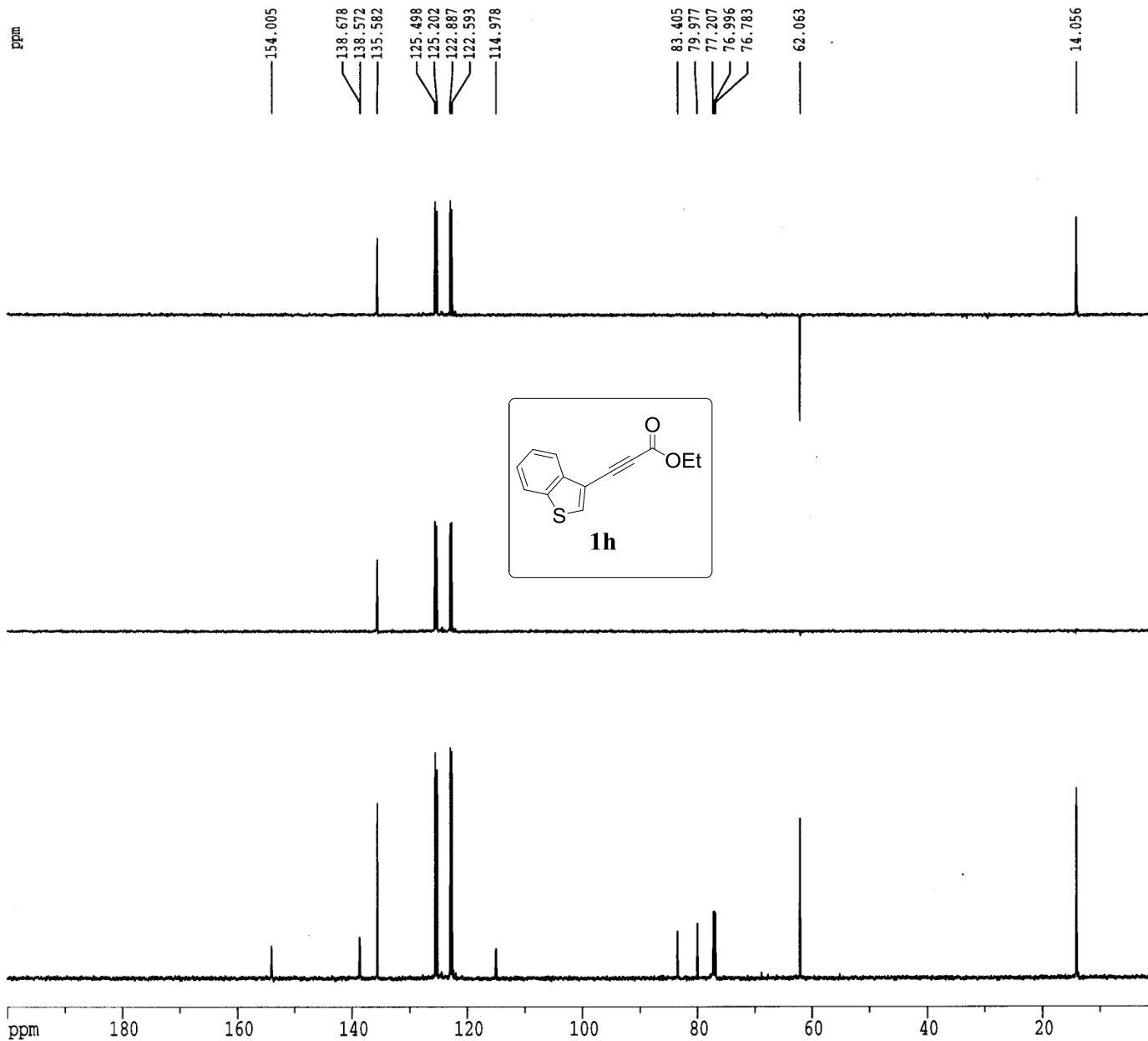
F2 - Acquisition Parameters
Date_ 20130729
Time 15.29
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDC13
NS 39
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 300.9 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

=====
CHANNEL f1
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5849425 MHz

=====
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.8029940 MHz

F2 - Processing parameters
SI 65536
SF 150.5683965 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30113.68 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.68384 Hz/cm



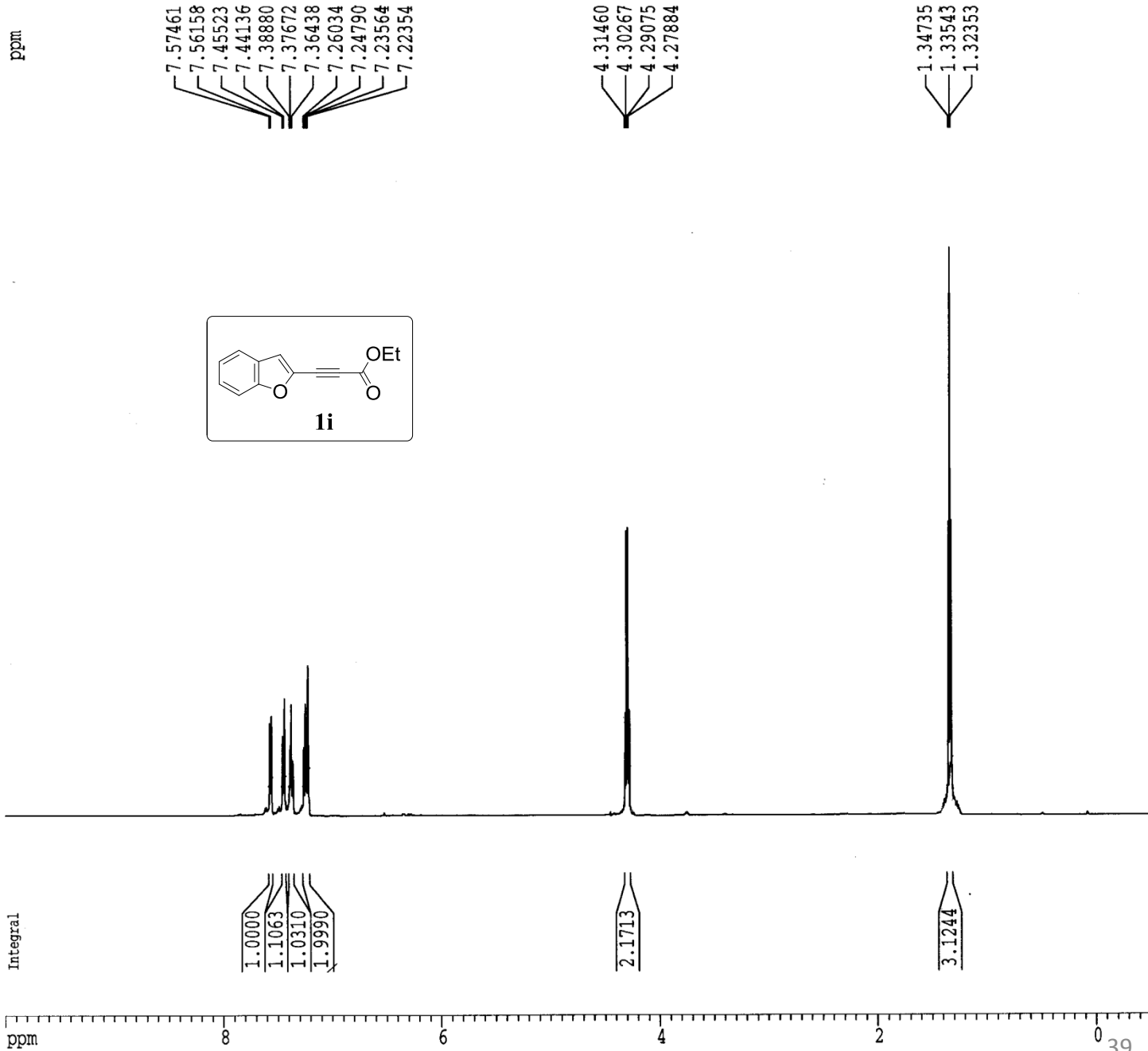
Current Data Parameters
 NAME RKS-1-164
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130806
 Time 21.42
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8382.229 Hz
 FIDRES 0.255805 Hz
 AQ 1.9546613 sec
 RG 32
 DW 59.650 usec
 DE 6.50 usec
 TE 298.3 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SF01 598.8026946 MHz

F2 - Processing parameters
 SI 32768
 SF 598.8000292 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 F1P 10.000 ppm
 F1 5988.00 Hz
 F2P -0.500 ppm
 F2 -299.40 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 314.37003 Hz/cm



Current Data Parameters
 NAME RKS-1-164
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20130806
 Time 21.45
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg
 TD 32768
 SOLVENT CDCl3
 NS 55
 DS 0
 SWH 45045.047 Hz
 FIDRES 1.374666 Hz
 AQ 0.3637748 sec
 RG 2048
 DW 11.100 usec
 DE 6.50 usec
 TE 299.4 K
 D1 3.50000000 sec
 d11 0.03000000 sec
 DELTA 3.40000010 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 4.80 usec
 PL1 0.00 dB
 SFO1 150.5849425 MHz

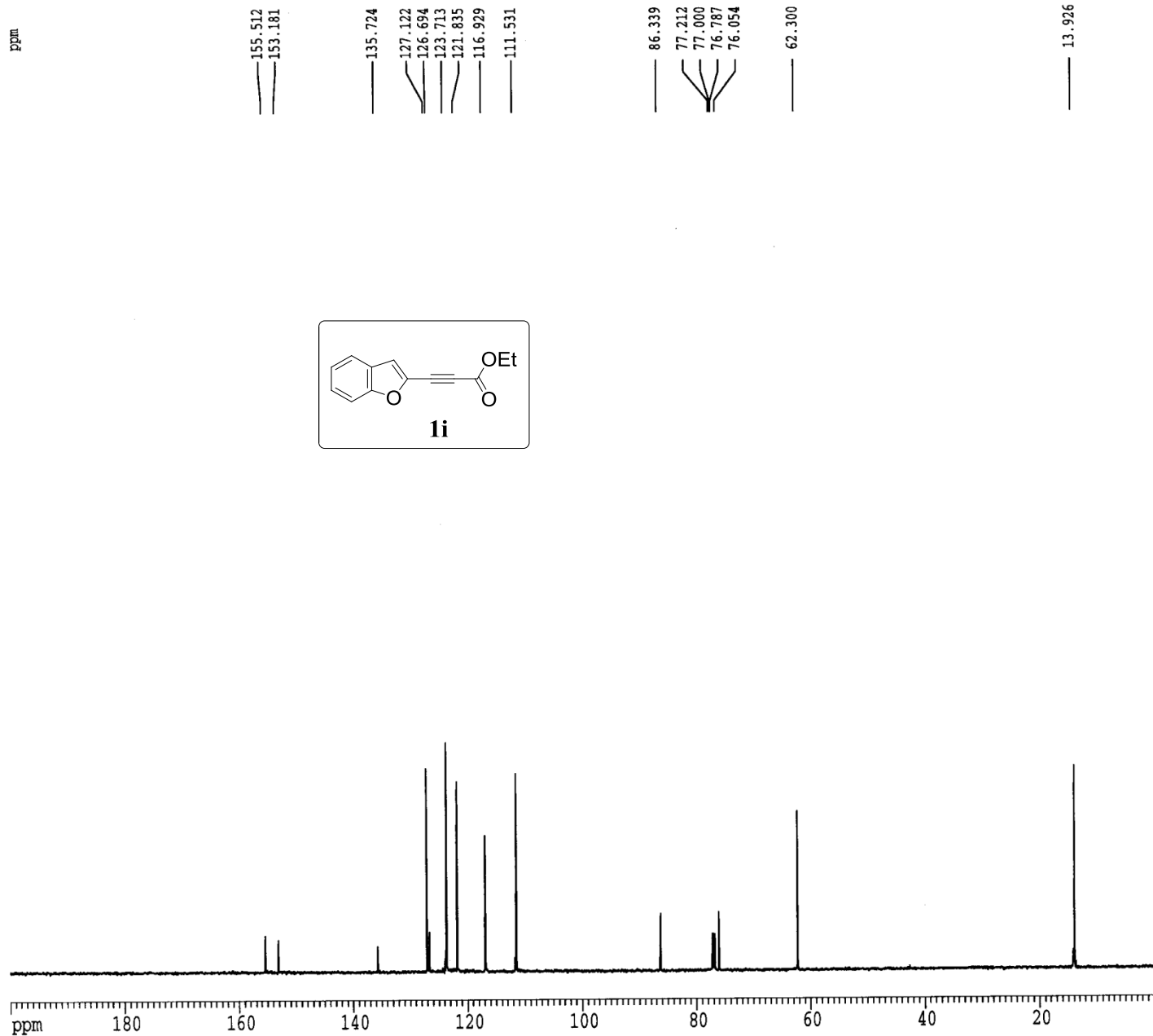
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 92.00 usec
 PL2 120.00 dB
 PL12 9.00 dB
 PL13 14.00 dB
 SFO2 598.8029940 MHz

F2 - Processing parameters

SI 65536
 SF 150.5683993 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 0.50

1D NMR plot parameters

CX 20.00 cm
 CY 4.00 cm
 F1P 200.000 ppm
 F1 30113.68 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 10.00000 ppm/cm
 HZCM 1505.68408 Hz/cm



Current Data Parameters
 NAME RKS-1-145
 EXPNO 1
 PROCNO 1

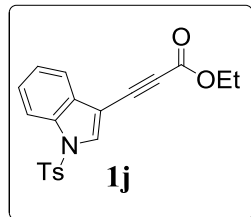
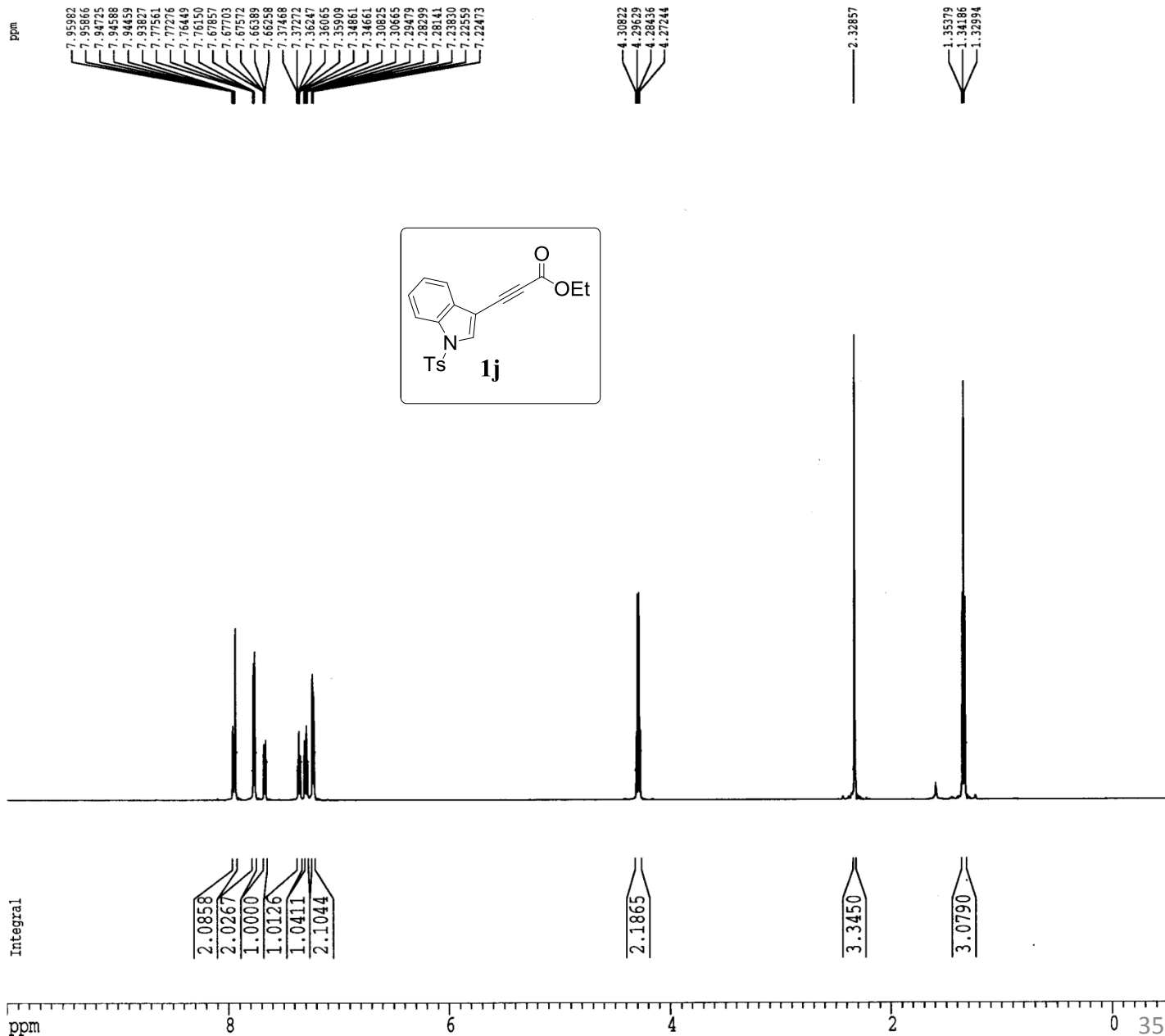
F2 - Acquisition Parameters

Date_ 20130804
 Time 17.22
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8382.229 Hz
 FIDRES 0.255805 Hz
 AQ 1.9546613 sec
 RG 128
 DW 59.650 usec
 DE 6.50 usec
 TE 302.4 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 598.8029940 MHz

F2 - Processing parameters
 SI 32768
 SF 598.8000301 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 8.00 cm
 F1P 10.000 ppm
 F1 5988.00 Hz
 F2P -0.500 ppm
 F2 -299.40 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 314.37003 Hz/cm



Current Data Parameters
NAME RKS-1-145
EXPNO 2
PROCNO 1

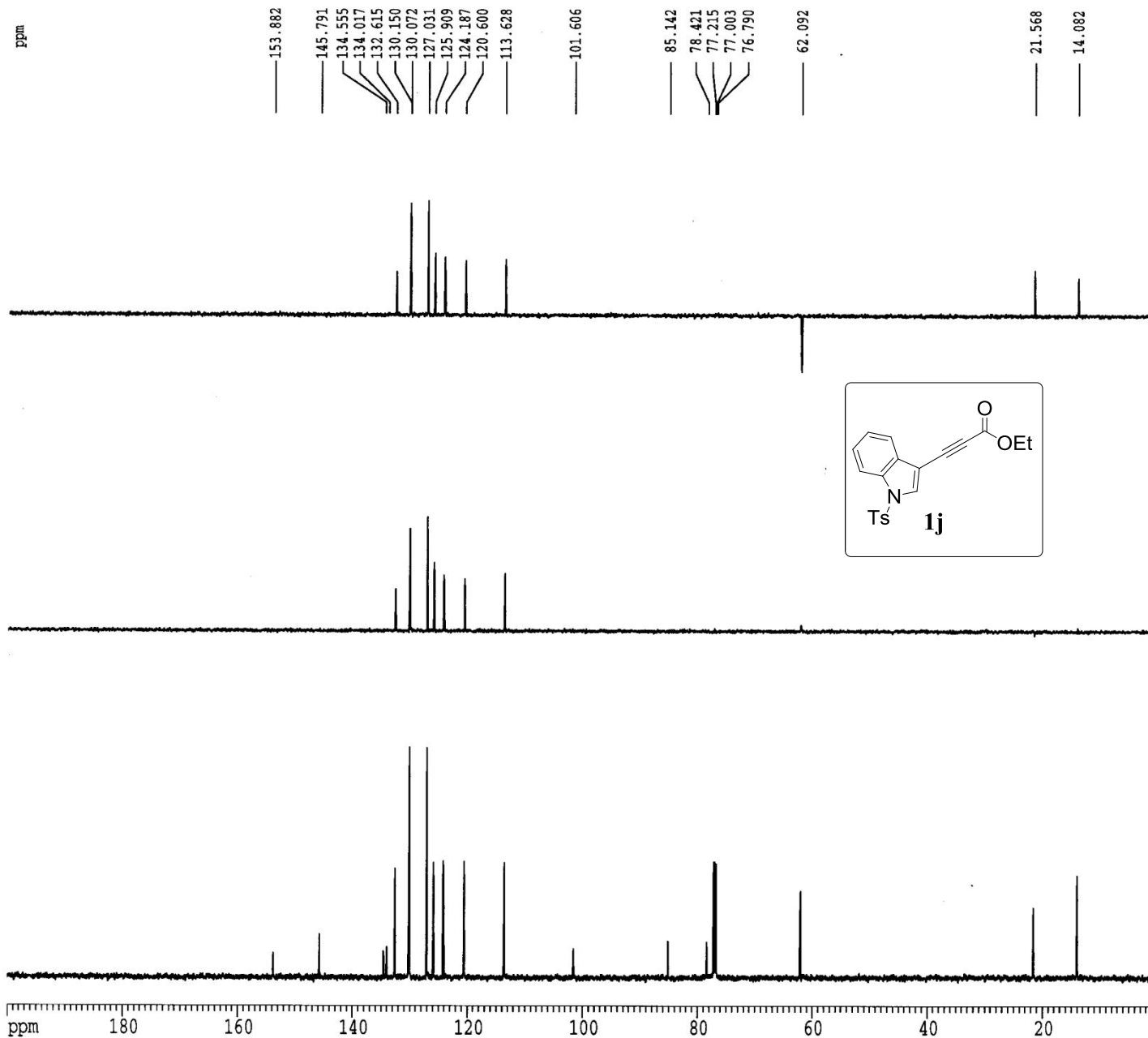
F2 - Acquisition Parameters
Date_ 20130804
Time 17.23
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 46
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 302.4 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5849425 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.8029940 MHz

F2 - Processing parameters
SI 65536
SF 150.5683862 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30113.68 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.68384 Hz/cm



Current Data Parameters
NAME RKS-1-1-106
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

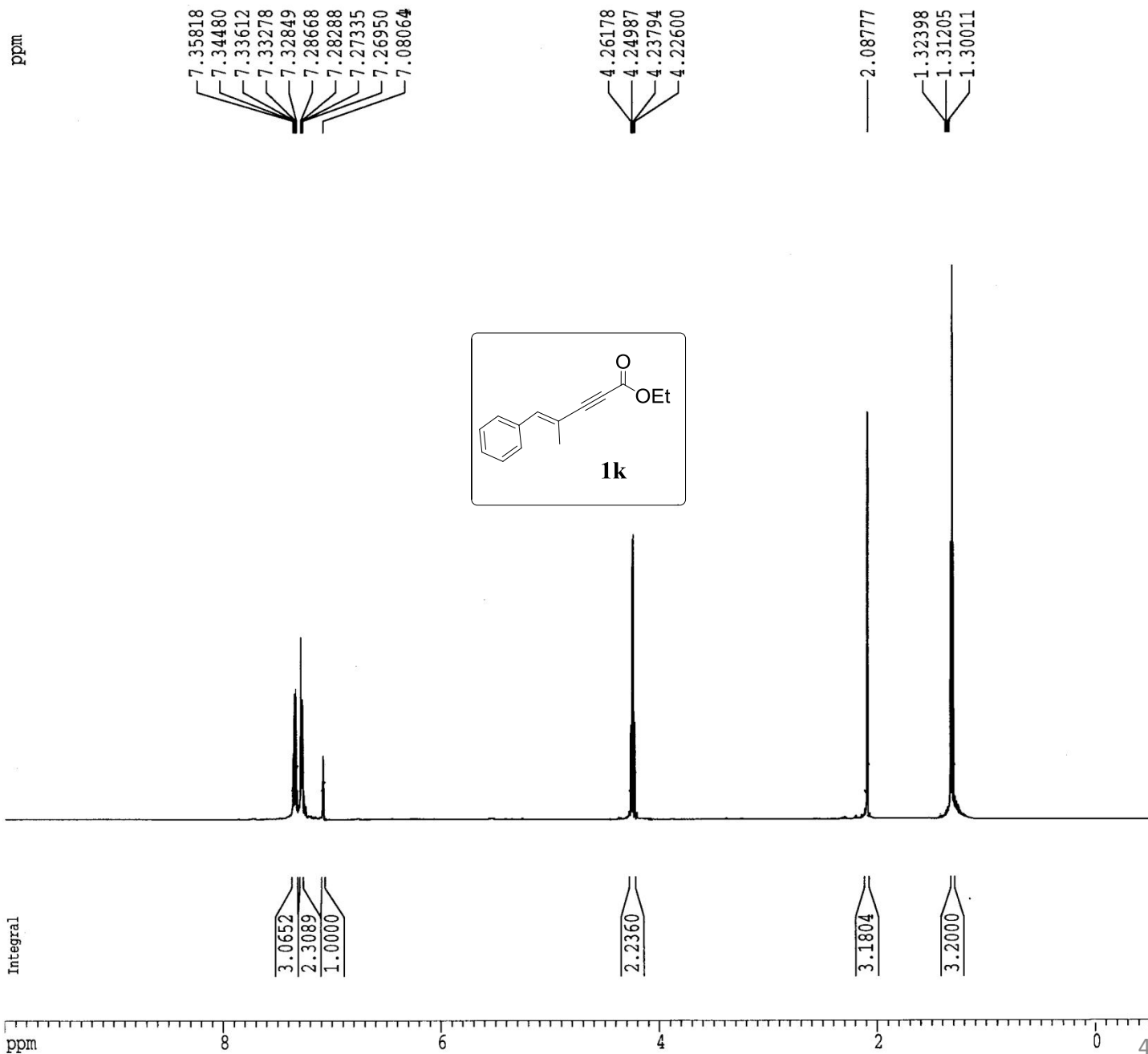
Date_ 20130612
Time 19.46
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8382.229 Hz
FIDRES 0.255805 Hz
AQ 1.9546613 sec
RG 32
DW 59.650 usec
DE 6.50 usec
TE 299.6 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.8026946 MHz

F2 - Processing parameters

SI 32768
SF 598.8000284 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 5988.00 Hz
F2P -0.500 ppm
F2 -299.40 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.37003 Hz/cm



Current Data Parameters
NAME RKS-1-1-106
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

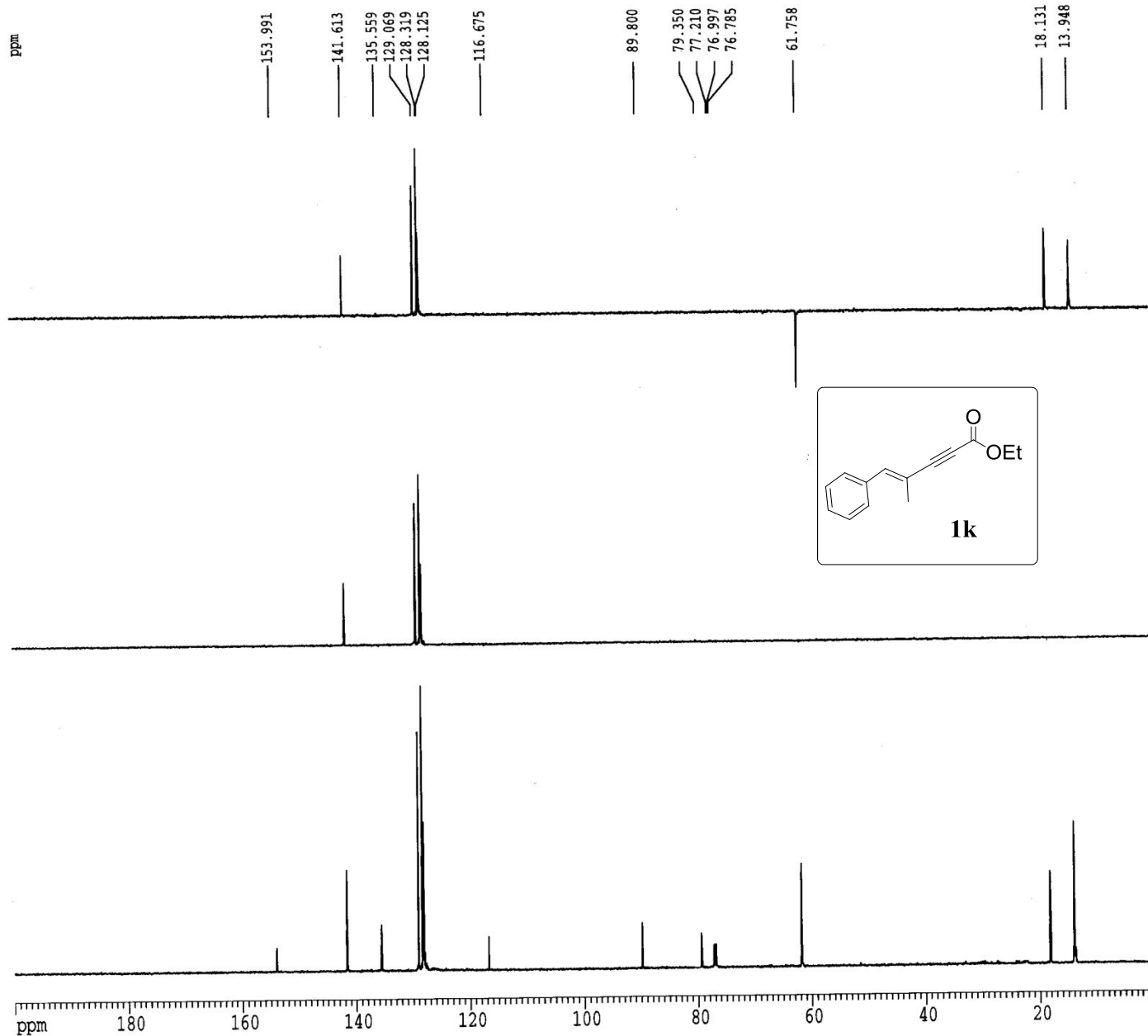
Date_ 20130612
Time 19.51
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 65
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 300.4 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5849425 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.8029940 MHz

F2 - Processing parameters
SI 65536
SF 150.5684034 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 200.000 ppm
F1 30113.68 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.68408 Hz/cm



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7.5084
7.5067
7.4953
7.4899
7.4697
7.4587
7.4543
7.4479
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7.4313
7.4242
7.4185
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7.4035
7.3833
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7.0822
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7.0558

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3.8623

1.5510

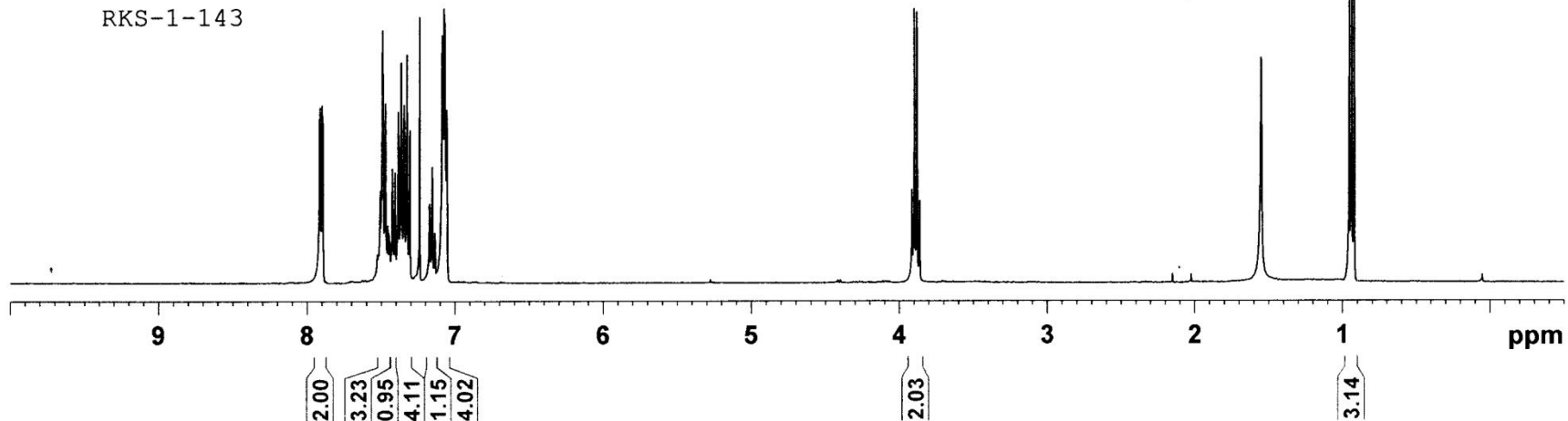
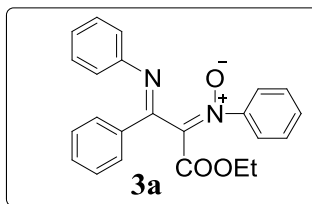
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Current Data Parameters
NAME 20140820
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140820
Time 23.12
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 23
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 287
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz

F2 - Processing parameters
SI 16384
SF 400.1500175 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME RKS-1-143
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

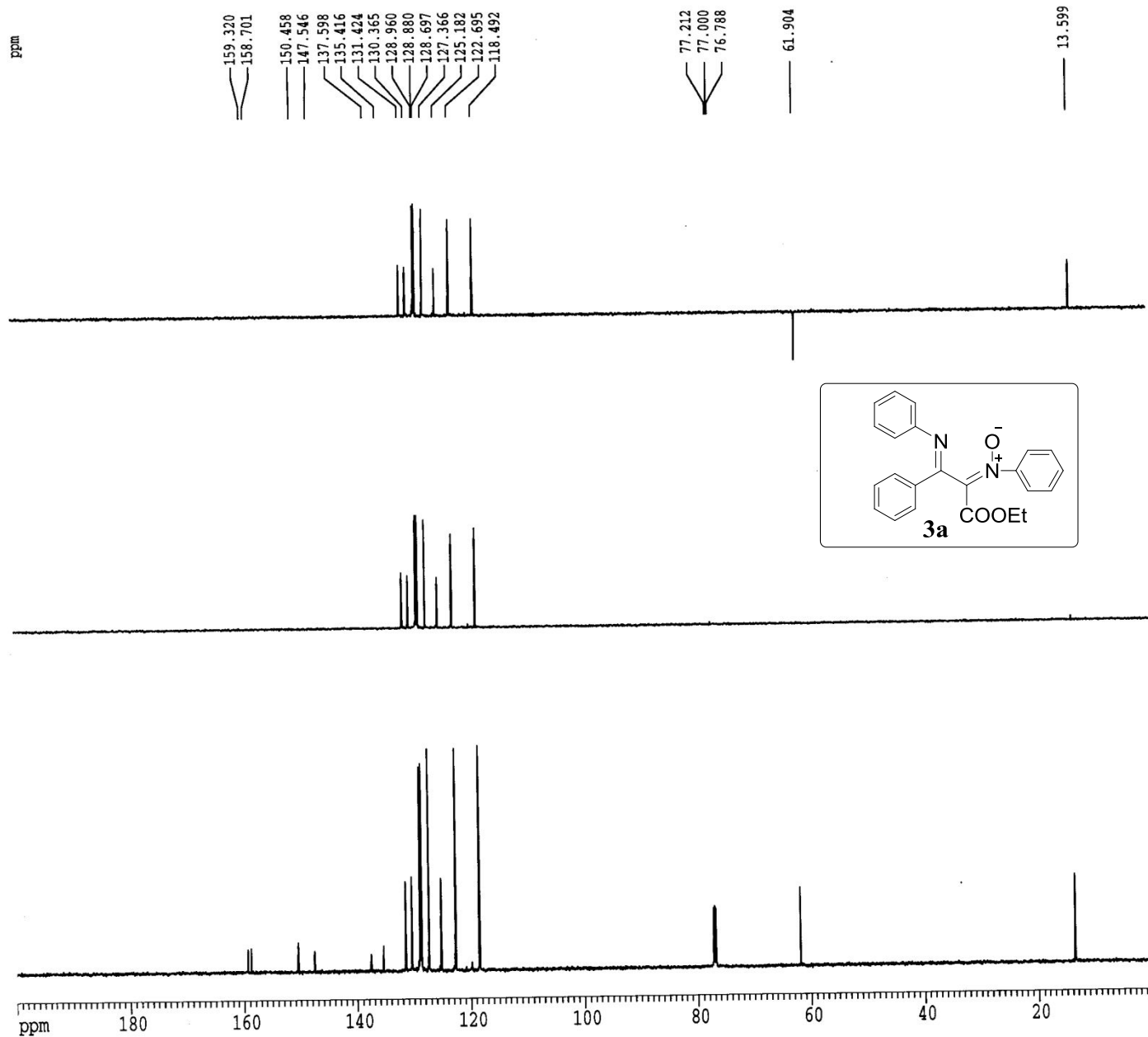
Date_ 20130723
 Time 20.52
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg
 TD 32768
 SOLVENT CDCl3
 NS 100
 DS 0
 SWH 45045.047 Hz
 FIDRES 1.374666 Hz
 AQ 0.3637748 sec
 RG 2048
 DW 11.100 usec
 DE 6.50 usec
 TE 302.4 K
 D1 3.50000000 sec
 d11 0.03000000 sec
 DELTA 3.40000010 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 4.80 usec
 PL1 0.00 dB
 SFO1 150.5849425 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 92.00 usec
 PL2 120.00 dB
 PL12 9.00 dB
 PL13 14.00 dB
 SFO2 598.8029940 MHz

F2 - Processing parameters
 SI 65536
 SF 150.5683910 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 0.50

1D NMR plot parameters
 CX 20.00 cm
 CY 4.00 cm
 FIP 200.000 ppm
 F1 30113.68 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 10.00000 ppm/cm
 HZCM 1505.68384 Hz/cm



8.059
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8.049
8.046
8.043
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7.978
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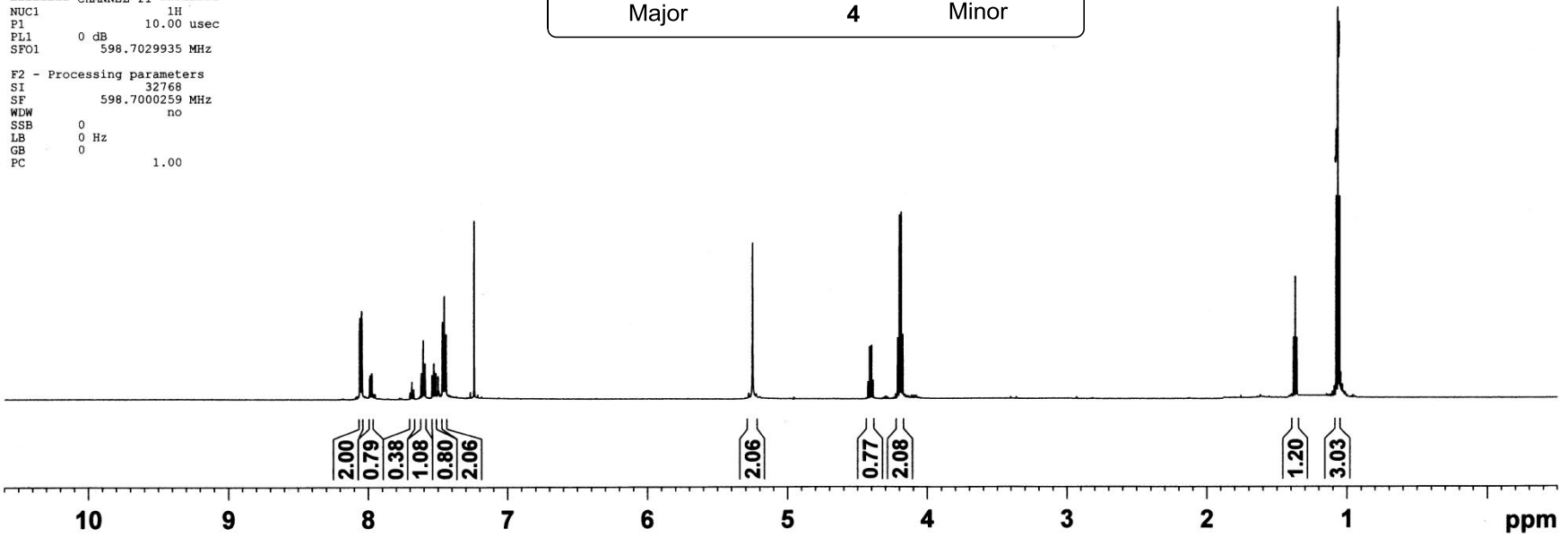
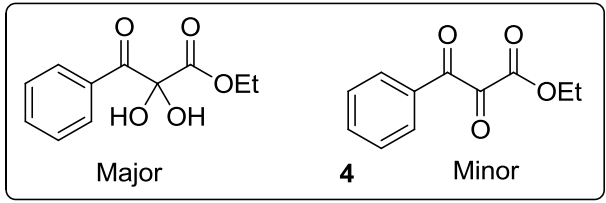
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Current Data Parameters
 NAME SNK-Triketo
 EXFNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141001
 Time_ 13.58
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 33556
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8389.262 Hz
 FIDRES 0.250008 Hz
 AQ 1.9999876 sec
 RG 128
 DW 59.600 usec
 DE 6.50 usec
 TE 303.1 K
 D1 2.00000000 sec
 MCREST 0 sec
 MCWRK 0.01500000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 10.00 usec
 PL1 0 dB
 SF01 598.7029935 MHz

F2 - Processing parameters
 SI 32768
 SF 598.7000259 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



191.50
190.18
183.73
169.88
160.51

135.51
134.66
131.51
131.35
130.13
130.02
129.14
128.77

91.52

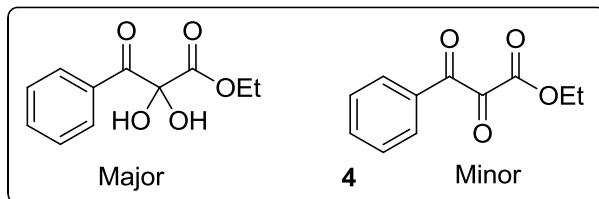
77.18
77.00
76.82

63.31
63.22

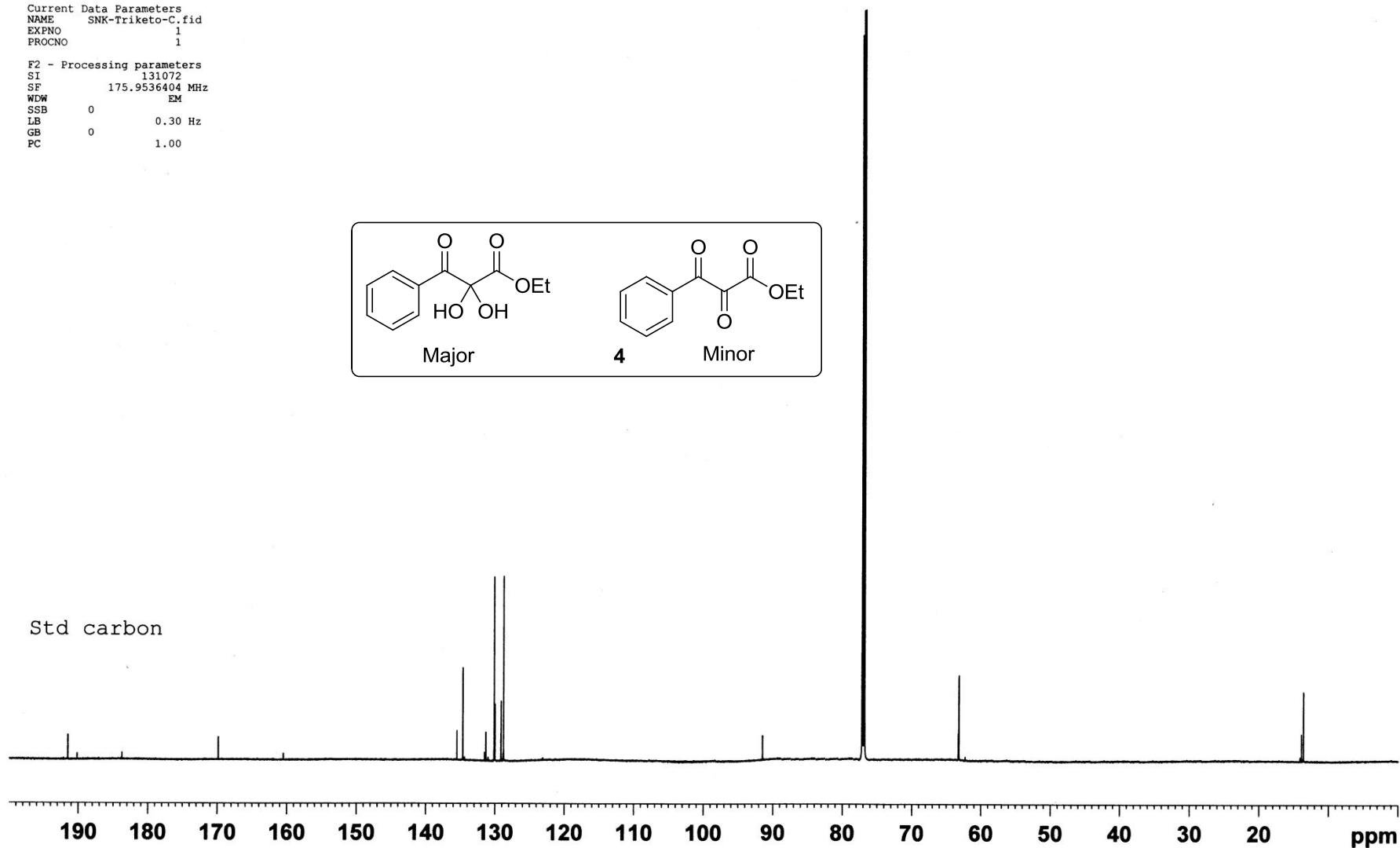
13.94
13.64

Current Data Parameters
NAME SNK-Triketo-C.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 131072
SF 175.9536404 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Std carbon



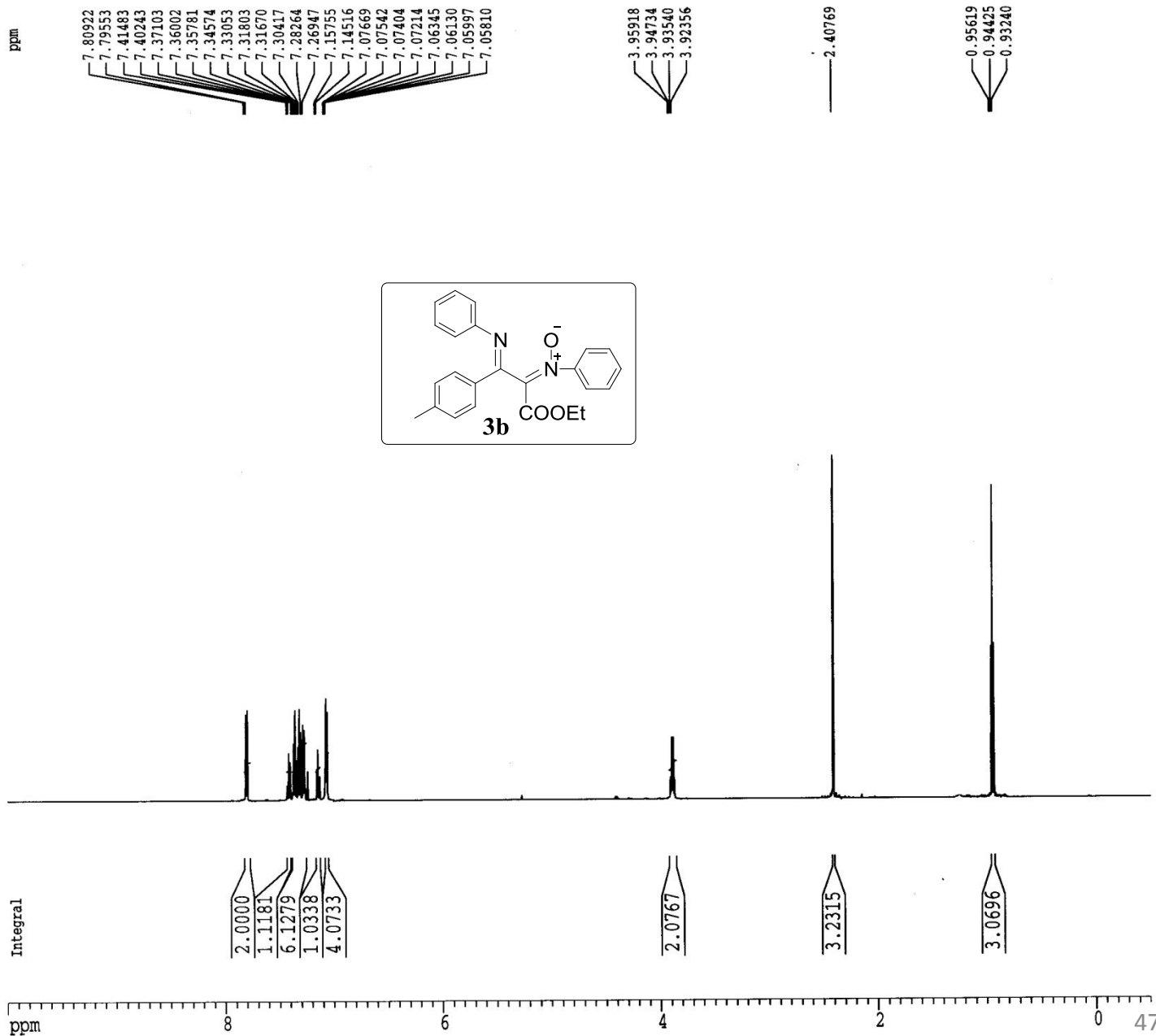
Current Data Parameters
 NAME RKS-1-168
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130825
 Time 21.12
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 9578.544 Hz
 FIDRES 0.292314 Hz
 AQ 1.7105396 sec
 RG 32
 DW 52.200 usec
 DE 6.50 usec
 TE 303.3 K
 DI 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 598.8041916 MHz

F2 - Processing parameters
 SI 32768
 SF 598.8000288 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 6.00 cm
 FLP 10.000 ppm
 F1 5988.00 Hz
 F2P -0.500 ppm
 F2 -299.40 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 314.37003 Hz/cm



Current Data Parameters
 NAME RKS-1-168
 EXPNO 2
 PROCNO 1

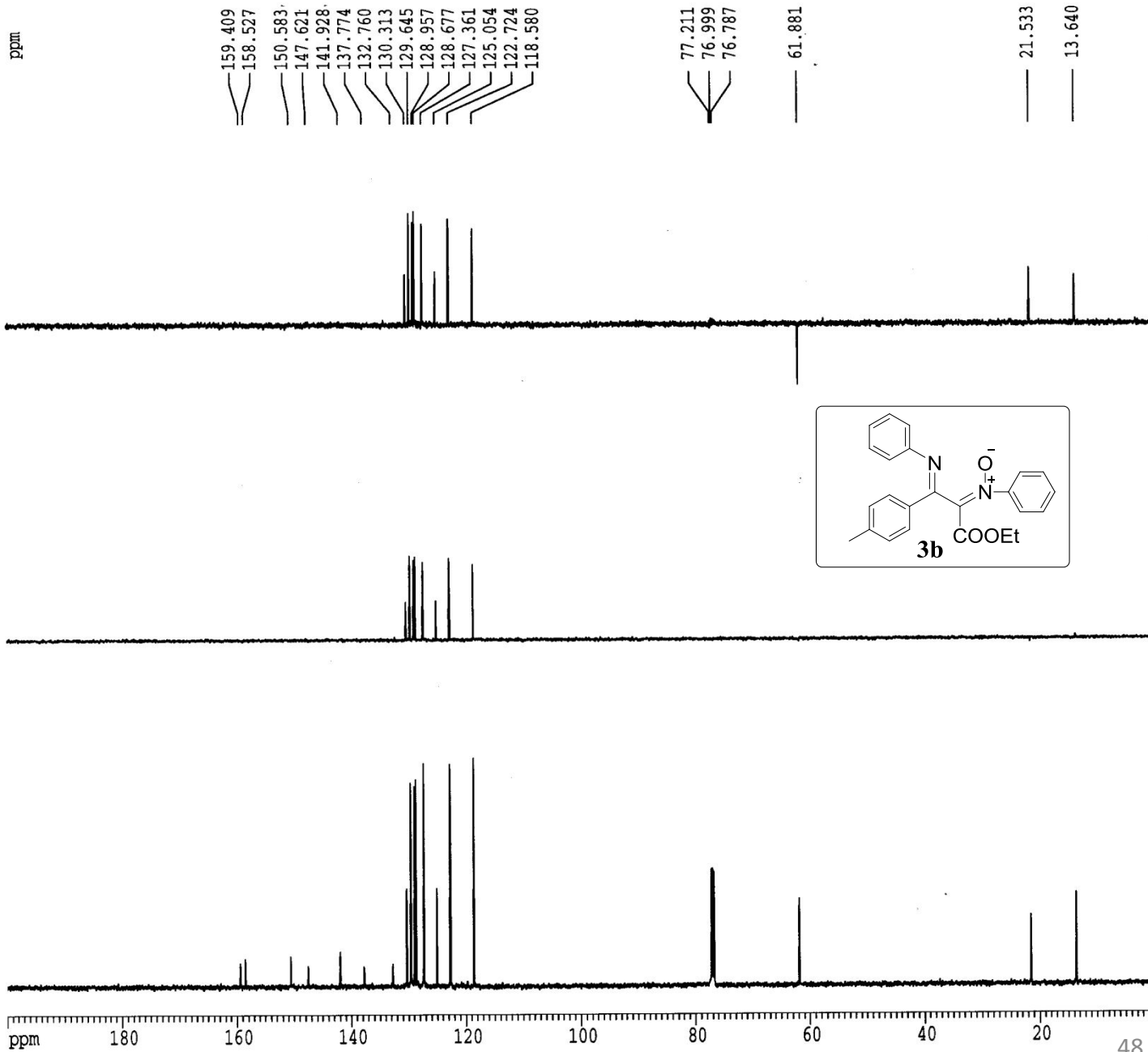
F2 - Acquisition Parameters
 Date_ 20130825
 Time 21.19
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg
 TD 32768
 SOLVENT DMSO
 NS 100
 DS 0
 SWH 45045.047 Hz
 FIDRES 1.374666 Hz
 AQ 0.3637748 sec
 RG 2048
 DW 11.100 usec
 DE 6.50 usec
 TE 304.3 K
 D1 3.50000000 sec
 d11 0.03000000 sec
 DELTA 3.40000010 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 4.80 usec
 PL1 0.00 dB
 SFO1 150.5849425 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 92.00 usec
 PL2 120.00 dB
 PL12 9.00 dB
 PL13 14.00 dB
 SFO2 598.8029940 MHz

F2 - Processing parameters
 SI 65536
 SF 150.5683862 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 0.50

1D NMR plot parameters
 CX 20.00 cm
 CY 4.00 cm
 F1P 200.000 ppm
 F1 30113.68 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 10.00000 ppm/cm
 HZCM 1505.68384 Hz/cm



7.8687
7.8638
7.8517
7.8465
7.4347
7.4319
7.4229
7.4161
7.4104
7.4013
7.3981
7.3949
7.3744
7.3591
7.3550
7.3417
7.3375
7.3312
7.3264
7.3121
7.3109
7.2919
7.2407
7.1552
7.1525
7.1366
7.1181
7.0690
7.0653
7.0482
7.0451
6.9966
6.9894
6.9843
6.9722
6.9672
6.9599
3.9216
3.9042
3.8864
3.8569

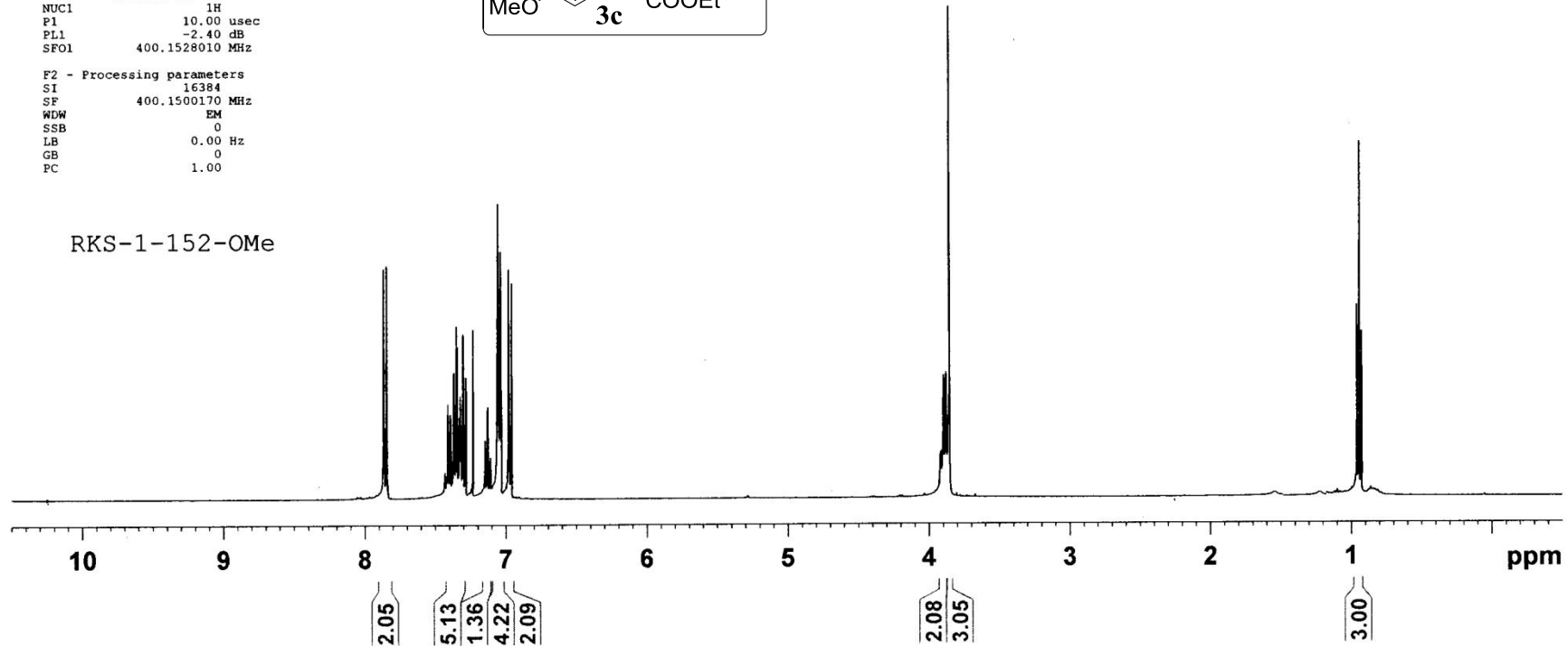
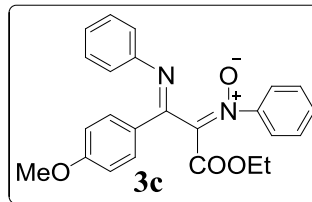
0.9657
0.9479
0.9300

Current Data Parameters
NAME 20140804
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140804
Time 15.59
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 36
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 287
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz

F2 - Processing parameters
SI 16384
SF 400.1500170 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



Current Data Parameters

NAME 20140807
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20140807
 Time 18.09
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1000
 DS 0
 SWH 22727.273 Hz
 FIDRES 0.346791 Hz
 AQ 1.4418420 sec
 RG 57
 DW 22.000 usec
 DE 8.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====

NUC1 13C
 P1 9.70 usec
 PL1 -0.50 dB
 SFO1 100.6288660 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -2.40 dB
 PL12 15.10 dB
 PL13 18.10 dB
 SFO2 400.1514010 MHz

F2 - Processing parameters

SI 32768
 SF 100.6178000 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.00

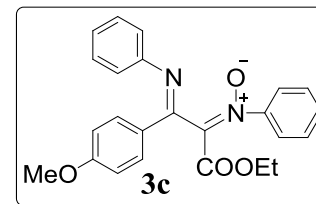
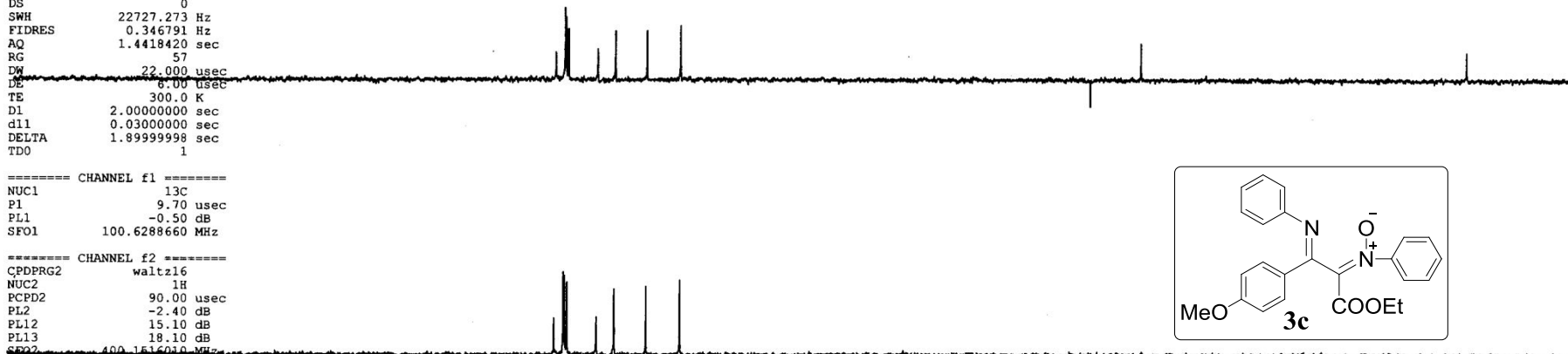
162.35
 159.47
 157.84
 150.64
 147.64
 137.80
 130.33
 129.14
 128.98
 128.69
 128.10
 124.96
 122.72
 118.66
 114.36

77.32
 77.00
 76.68

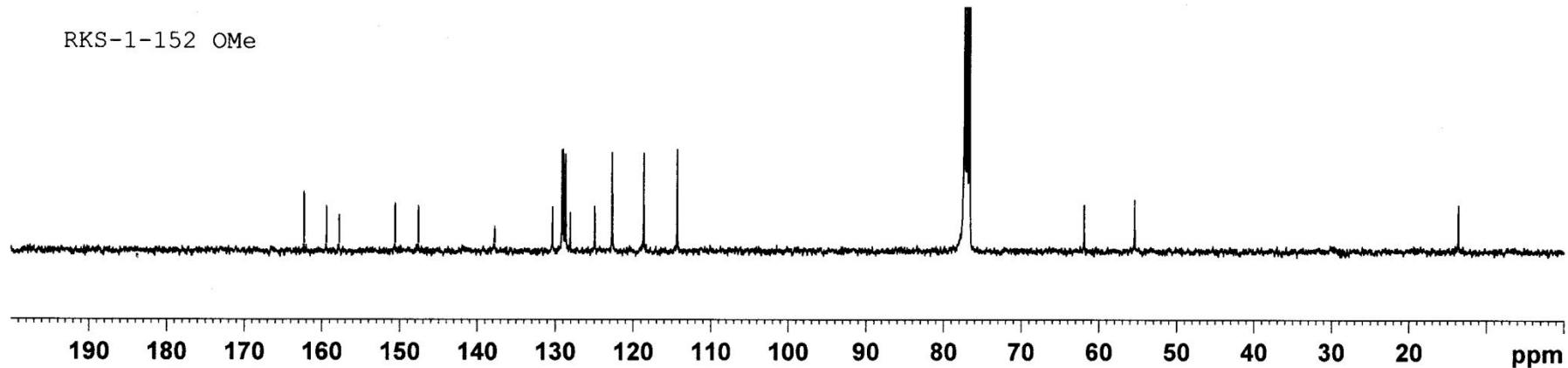
61.91

55.44

13.68



RKS-1-152 OMe



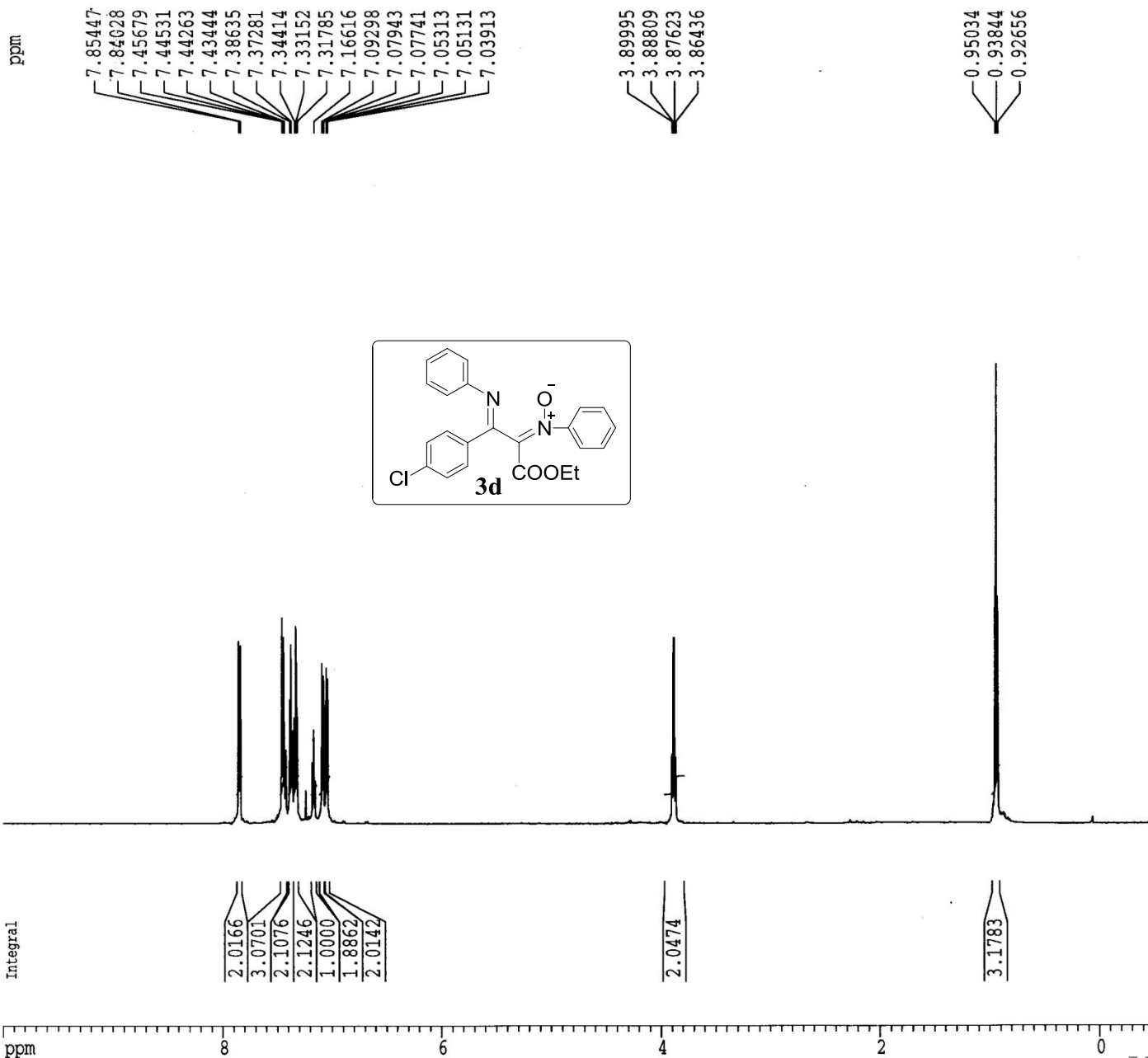
Current Data Parameters
 NAME RKS-1-162
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130806
 Time 21.14
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8382.229 Hz
 FIDRES 0.255805 Hz
 AQ 1.9546613 sec
 RG 128
 DW 59.650 usec
 DE 6.50 usec
 TE 296.6 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 598.8026946 MHz

F2 - Processing parameters
 SI 32768
 SF 598.8000292 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 8.00 cm
 F1P 10.000 ppm
 F1 5988.00 Hz
 F2P -0.500 ppm
 F2 -299.40 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 314.37003 Hz/cm



Current Data Parameters
NAME RKS-1-162
EXPNO 2
PROCNO 1

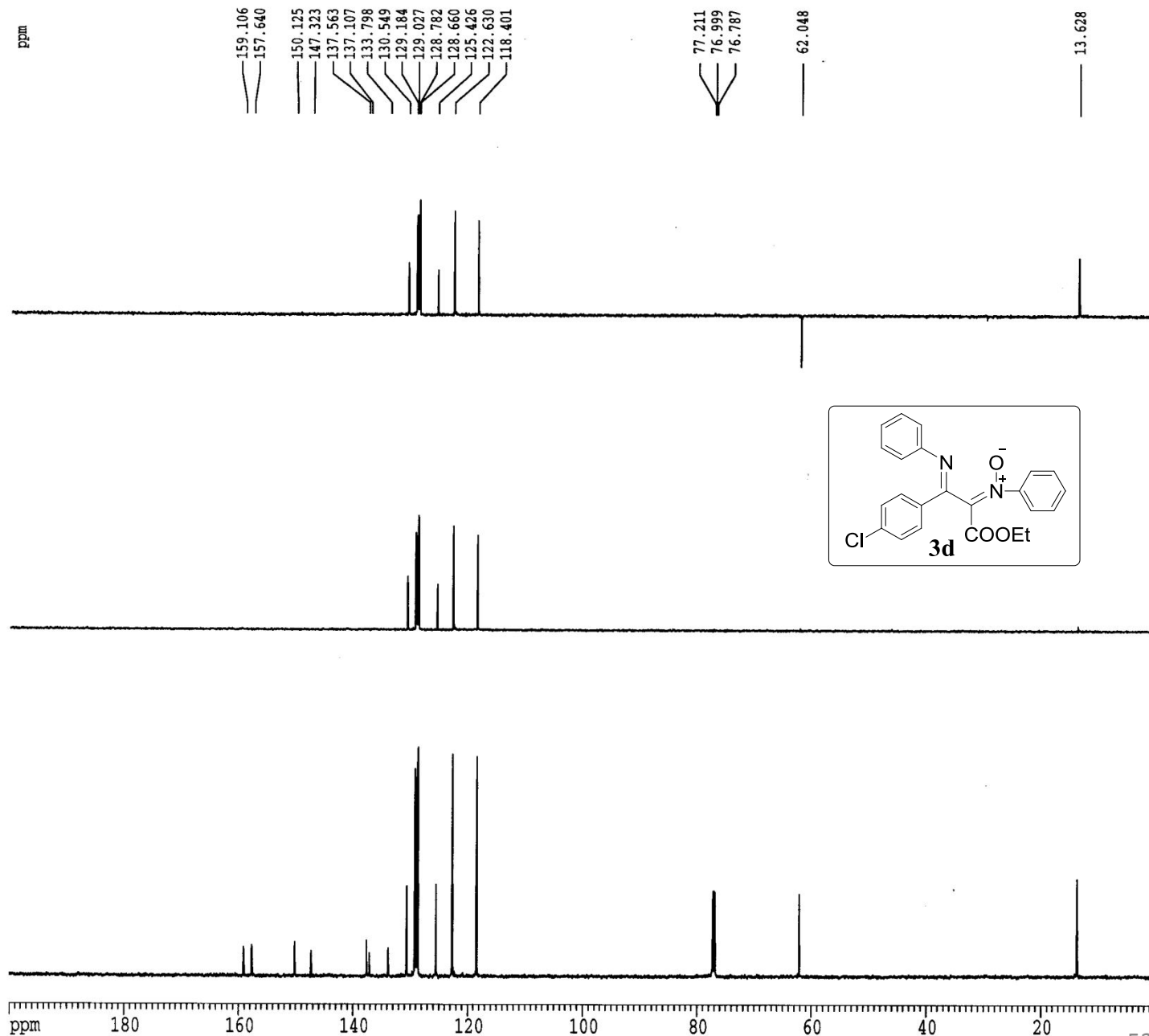
F2 - Acquisition Parameters
Date_ 20130806
Time 19.50
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 173
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 290.0 K
D1 3.5000000 sec
d11 0.0300000 sec
DELTA 3.4000010 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

=====
CHANNEL f1
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5849425 MHz

=====
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.8029940 MHz

F2 - Processing parameters
SI 65536
SF 150.5683945 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30113.68 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.68384 Hz/cm



7.566
7.553
7.408
7.407
7.394
7.391
7.383
7.383
7.382
7.380
7.346
7.343
7.338
7.335
7.333
7.326
7.321
7.320
7.319
7.315
7.313
7.300
7.299
7.288
7.258
7.246
7.243
7.241
7.240
7.234
7.233
7.233
7.159
7.147
7.146
7.135
7.133
7.089
7.087
7.075
7.073
7.070
7.058
7.056

3.859
3.847
3.835
3.823

2.671

1.547

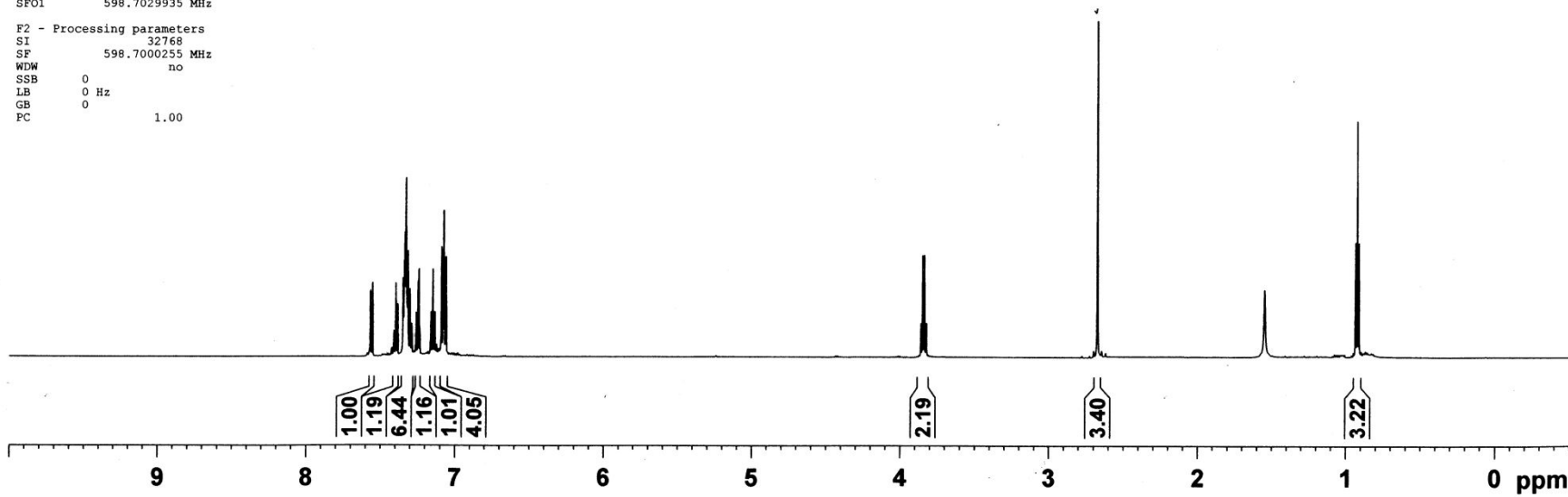
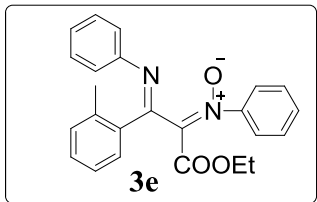
0.934
0.922
0.910

Current Data Parameters
NAME RKS-2-156
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140925
Time 11.46
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.250008 Hz
AQ 1.9999876 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 301.7 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.7029935 MHz

F2 - Processing parameters
SI 32768
SF 598.7000255 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



159.87
 159.70
 150.40
 147.54
 138.97
 138.75
 135.75
 131.61
 130.41
 130.03
 128.92
 128.76
 128.03
 125.72
 125.35
 122.72
 118.75

77.21
 77.00
 76.79

61.94

20.19
 13.55

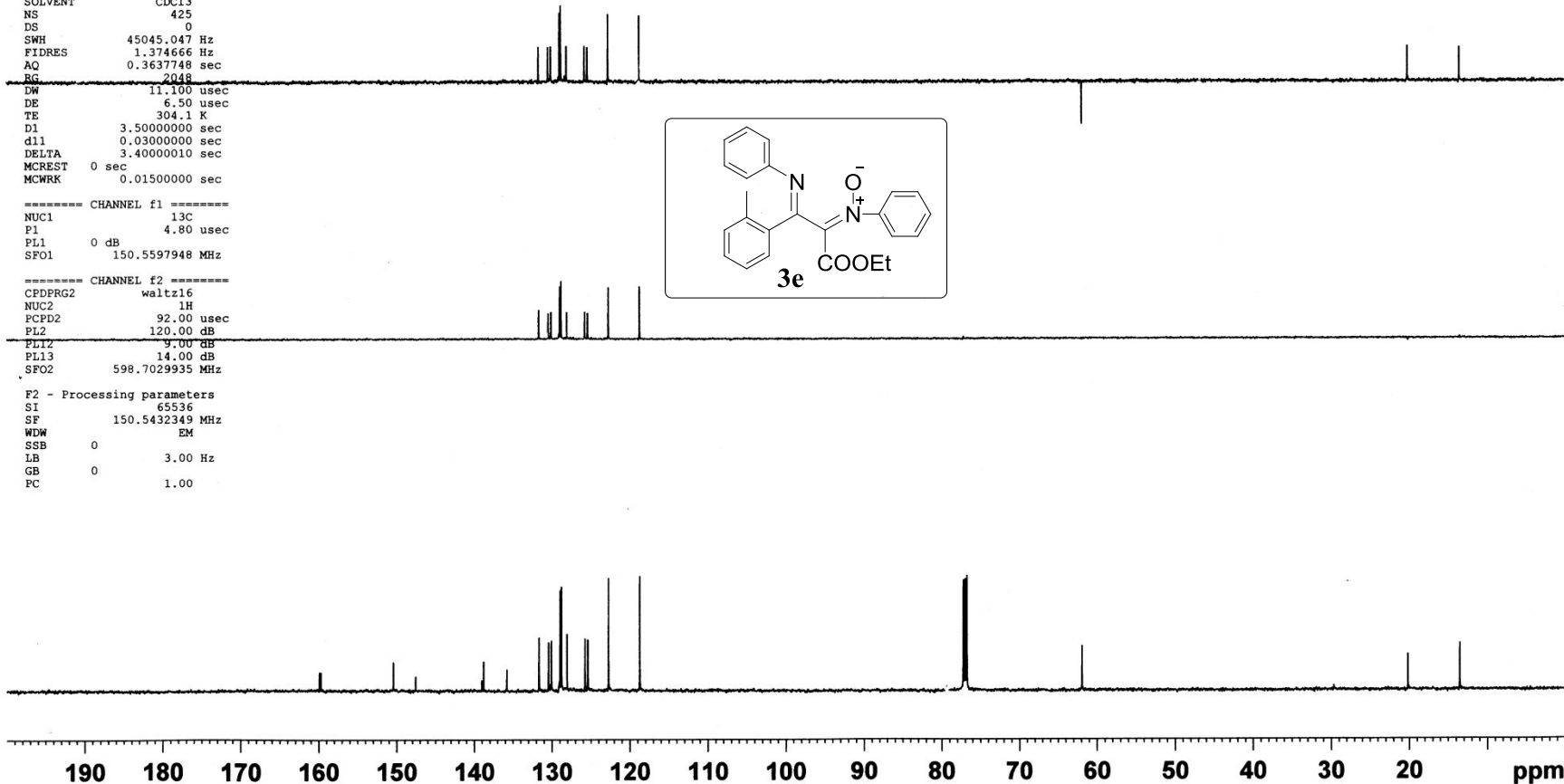
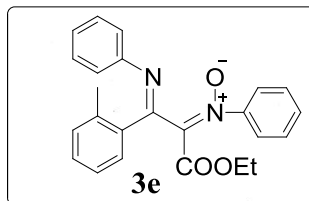
Current Data Parameters
 NAME RKS-2-156
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date 20140925
 Time 11.53
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg
 TD 32768
 SOLVENT CDCl3
 NS 425
 DS 0
 SWH 45045.047 Hz
 FIDRES 1.374666 Hz
 AQ 0.3637748 sec
 RG 2048
 DW 11.100 usec
 DE 6.50 usec
 TE 304.1 K
 D1 3.5000000 sec
 d11 0.0300000 sec
 DELTA 3.4000010 sec
 MCREST 0 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 4.80 usec
 PL1 0 dB
 SFO1 150.5597948 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 92.00 usec
 PL2 120.00 dB
 PL12 9.00 dB
 PL13 14.00 dB
 SFO2 598.7029935 MHz

F2 - Processing parameters
 SI 65536
 SF 150.5432349 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.00



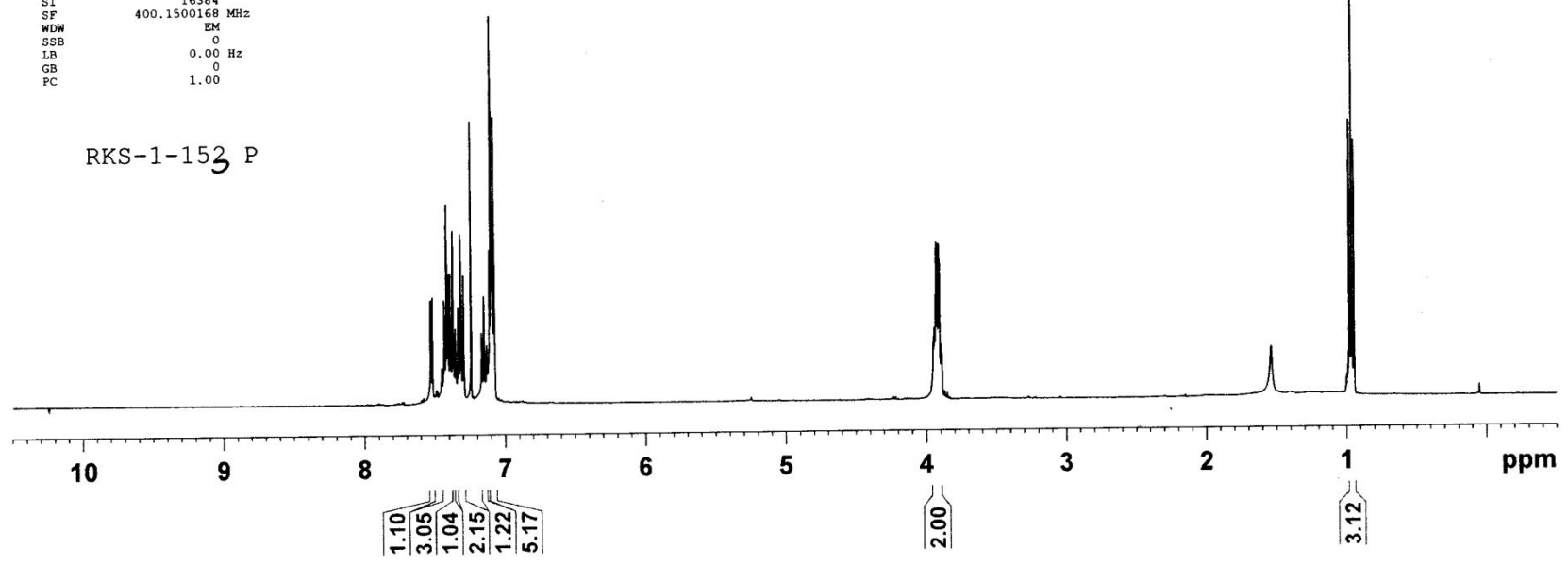
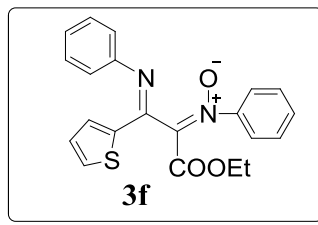
7.5311
7.5284
7.5185
7.5160
7.4515
7.4396
7.4328
7.4270
7.4172
7.4147
7.4121
7.4056
7.4029
7.3963
7.3904
7.3750
7.3707
7.3577
7.3533
7.3500
7.3333
7.3285
7.3145
7.2983
7.2941
7.2407
7.1670
7.1642
7.1484
7.1298
7.1270
7.1093
7.0971
7.0950
7.0877
7.0770
7.0738
3.9327
3.9260
3.9150
3.9083

Current Data Parameters
 NAME 20140801
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140801
 Time_ 19.23
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 6410.256 Hz
 FIDRES 0.195625 Hz
 AQ 2.5559540 sec
 RG 512
 DW 78.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 TDO 1

----- CHANNEL f1 -----
 NUC1 1H
 P1 10.00 usec
 PL1 -2.40 dB
 SFO1 400.1528010 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1500168 MHz
 WDW EM
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



1.5388
0.9800
0.9622
0.9445

Current Data Parameters
NAME RKS-1-152-1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20140302
Time 19.48
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 209
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 293.7 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

==== CHANNEL f1 =====
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5597948 MHz

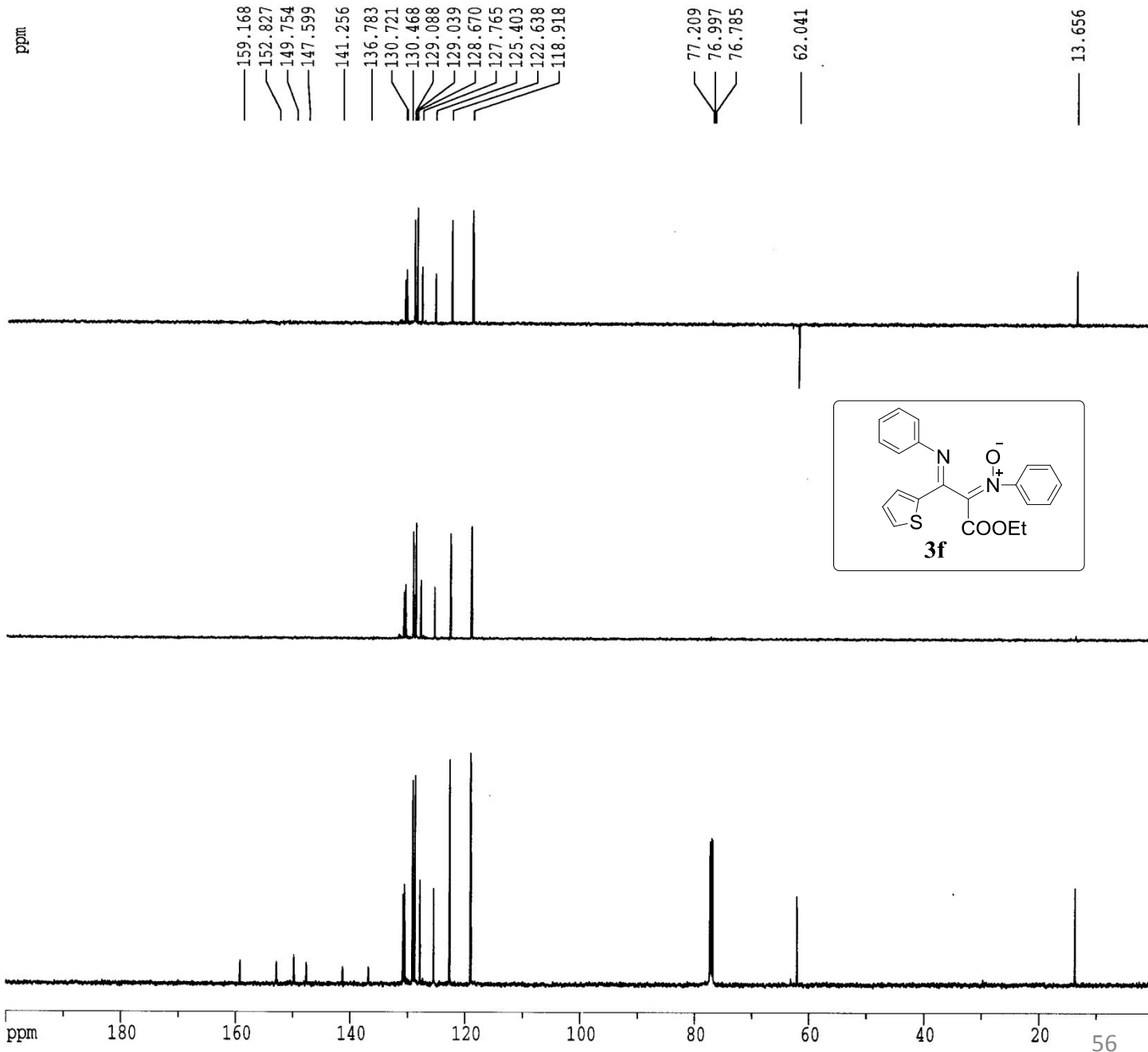
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.7029935 MHz

F2 - Processing parameters

SI 65536
SF 150.5432431 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50

1D NMR plot parameters

CX 20.00 cm
CY 4.00 cm
FIP 200.000 ppm
F1 30108.65 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.43237 Hz/cm



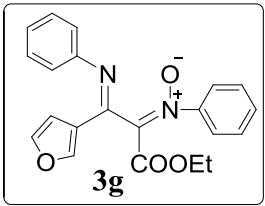
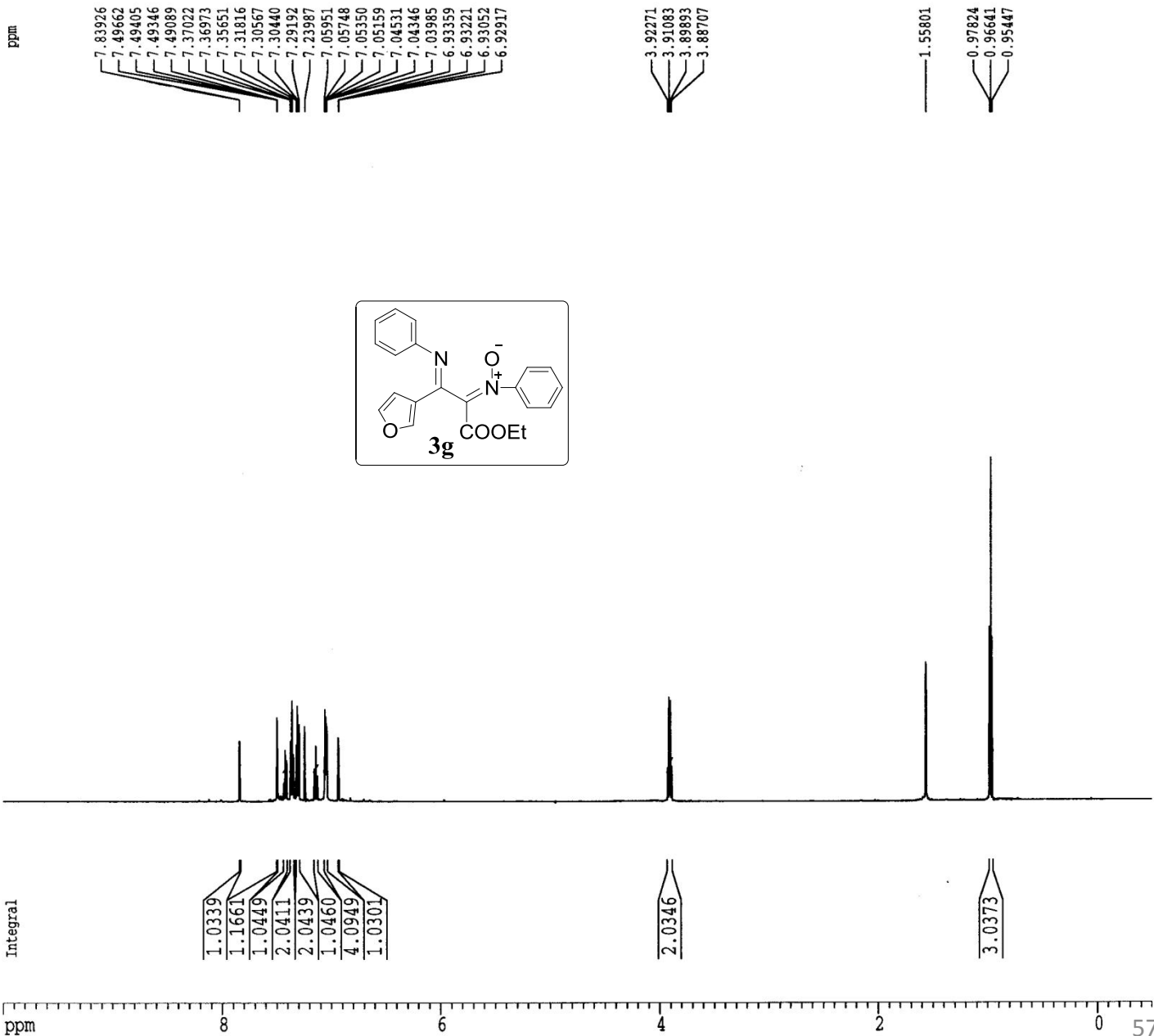
Current Data Parameters
 NAME RKS-1-192
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130912
 Time 16.34
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 47890
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 7183.908 Hz
 FIDRES 0.150009 Hz
 AQ 3.3331940 sec
 RG 128
 DW 69.600 usec
 DE 6.50 usec
 TE 302.4 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 598.8029940 MHz

F2 - Processing parameters
 SI 32768
 SF 598.8000287 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 6.00 cm
 F1P 10.000 ppm
 F1 5988.00 Hz
 F2P -0.500 ppm
 F2 -299.40 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 314.37003 Hz/cm



Current Data Parameters
NAME RKS-1-192
EXPNO 2
PROCNO 1

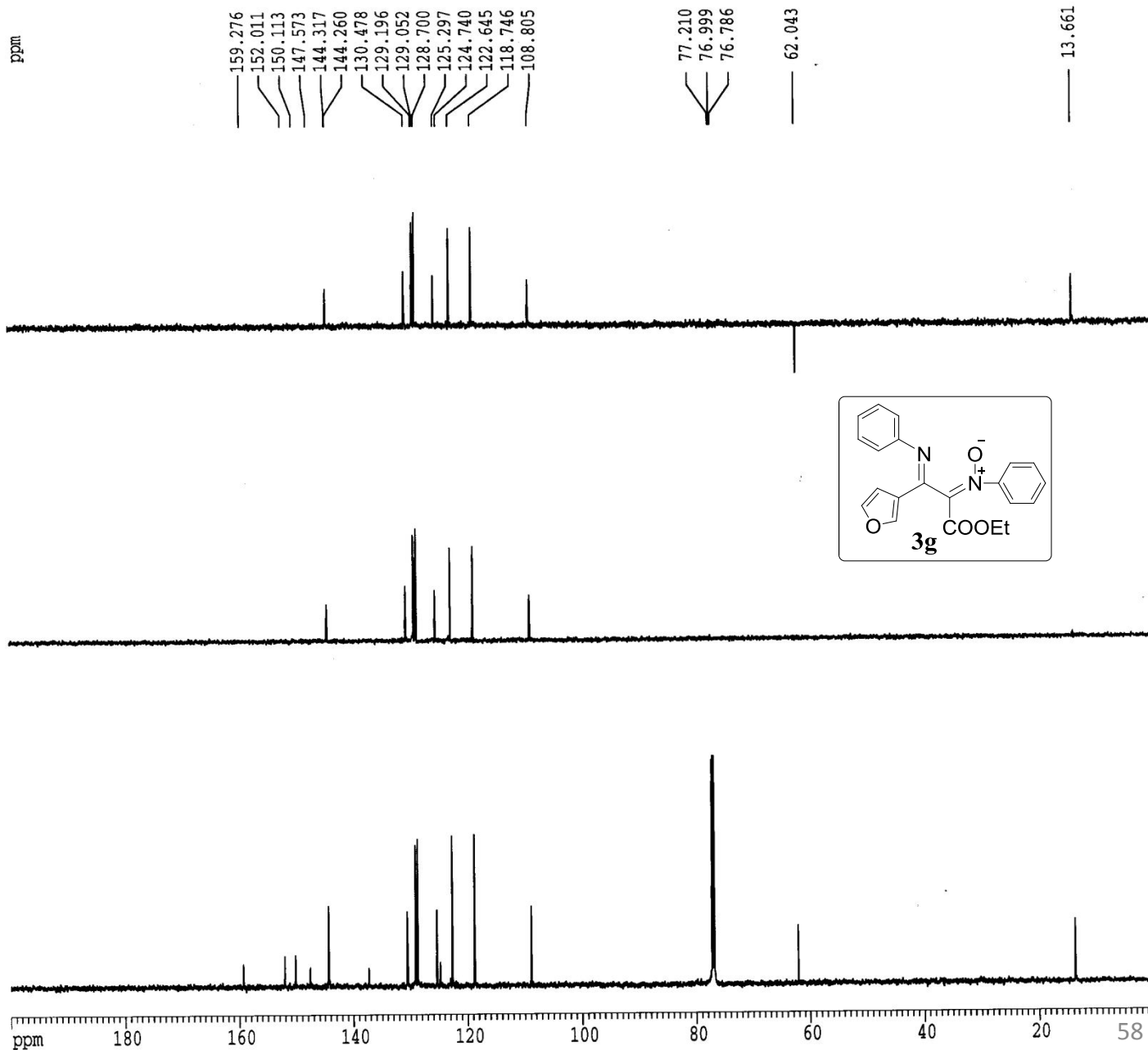
F2 - Acquisition Parameters
Date_ 20130912
Time 16.35
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 410
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 302.5 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5849425 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.8029940 MHz

F2 - Processing parameters
SI 65536
SF 150.5683821 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30113.68 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.68372 Hz/cm



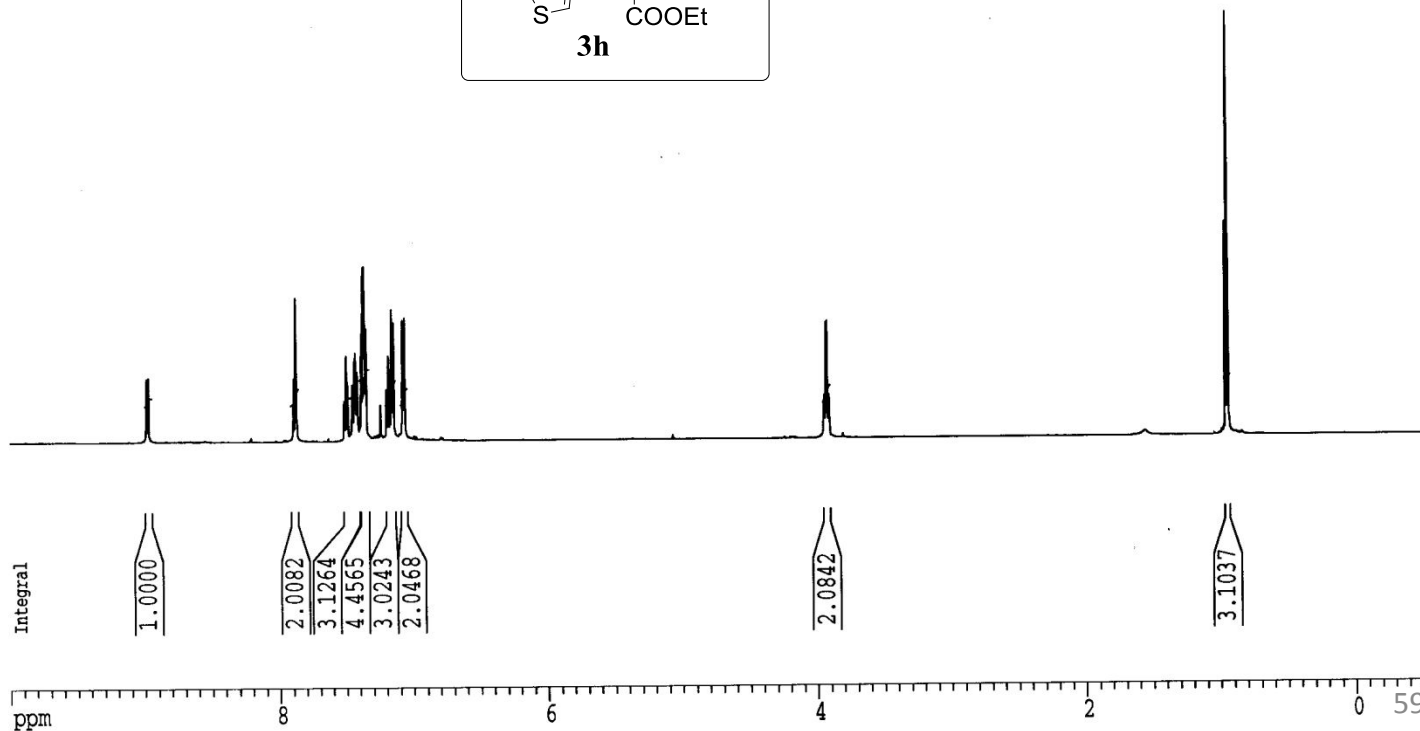
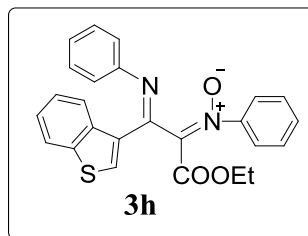
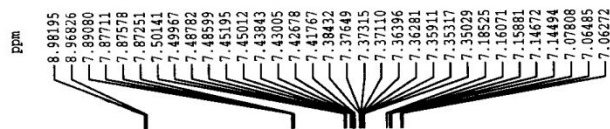
Current Data Parameters
NAME RKS-1-148
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130730
Time 20.53
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDC13
NS 16
DS 0
SWH 8382.229 Hz
FIDRES 0.255805 Hz
AQ 1.9546613 sec
RG 128
DW 59.650 usec
DE 6.50 usec
TE 301.9 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.8029940 MHz

F2 - Processing parameters
SI 32768
SF 598.8000275 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
FLP 10.000 ppm
F1 5988.00 Hz
F2P -0.500 ppm
F2 -299.40 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.37003 Hz/cm



Current Data Parameters
 NAME RKS-1-148
 EXPNO 2
 PROCNO 1

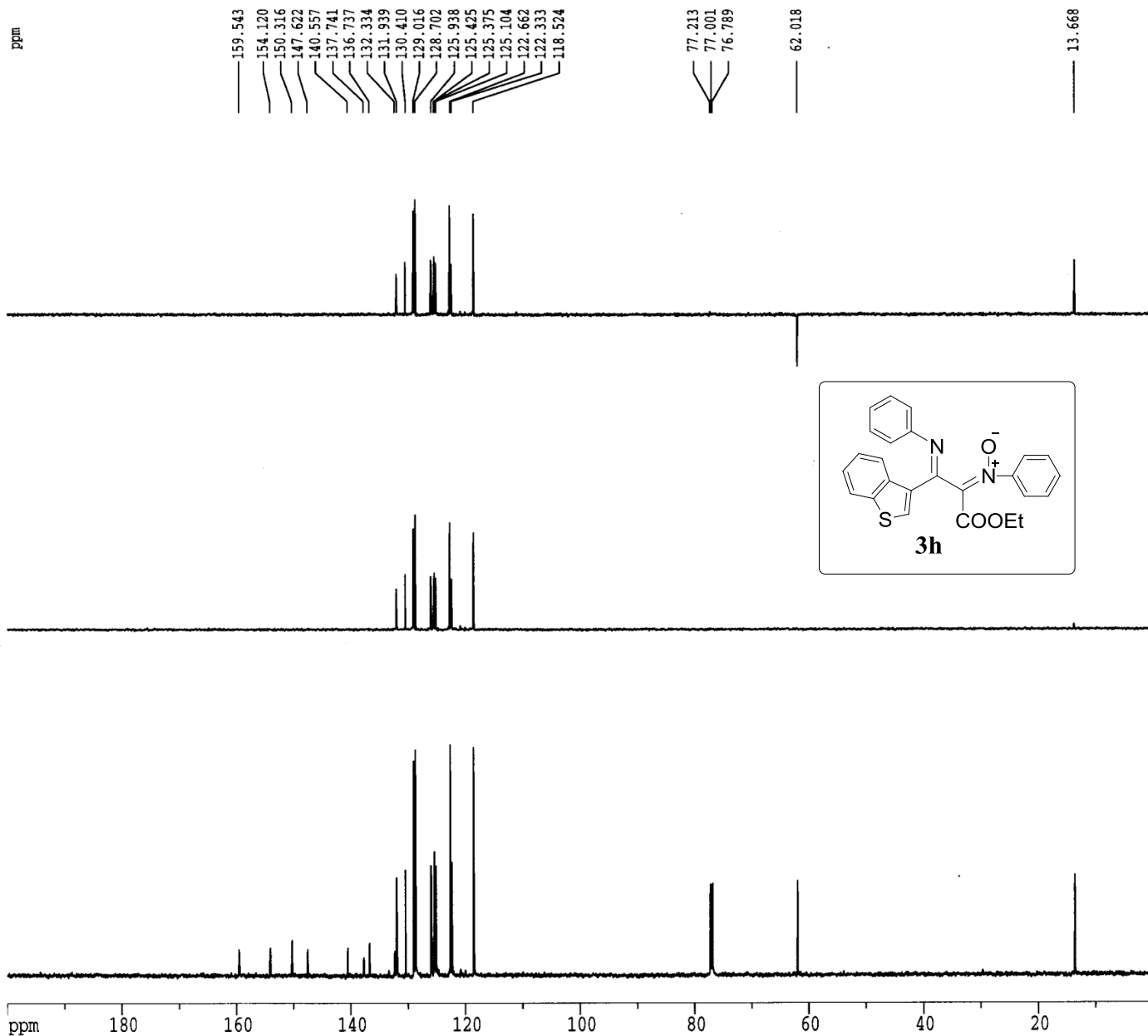
F2 - Acquisition Parameters
 Date_ 20130730
 Time_ 20.55
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg
 TD 32768
 SOLVENT CDC13
 NS 133
 DS 0
 SWH 45045.047 Hz
 FIDRES 1.374666 Hz
 AQ 0.3637748 sec
 RG 2048
 DW 11.100 usec
 DE 6.50 usec
 TE 302.3 K
 D1 3.5000000 sec
 d11 0.0300000 sec
 DELTA 3.4000010 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 4.80 usec
 PL1 0.00 dB
 SFO1 150.5849425 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 92.00 usec
 PL2 120.00 dB
 PL12 9.00 dB
 PL13 14.00 dB
 SFO2 598.8029940 MHz

F2 - Processing parameters
 SI 65536
 SF 150.5683883 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 0.50

1D NMR plot parameters
 CX 20.00 cm
 CY 4.00 cm
 F1P 200.000 ppm
 F1 30113.68 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 10.0000 ppm/cm
 HZCM 1505.68384 Hz/cm



Current Data Parameters
 NAME RKS-1-165
 EXPNO 1
 PROCNO 1

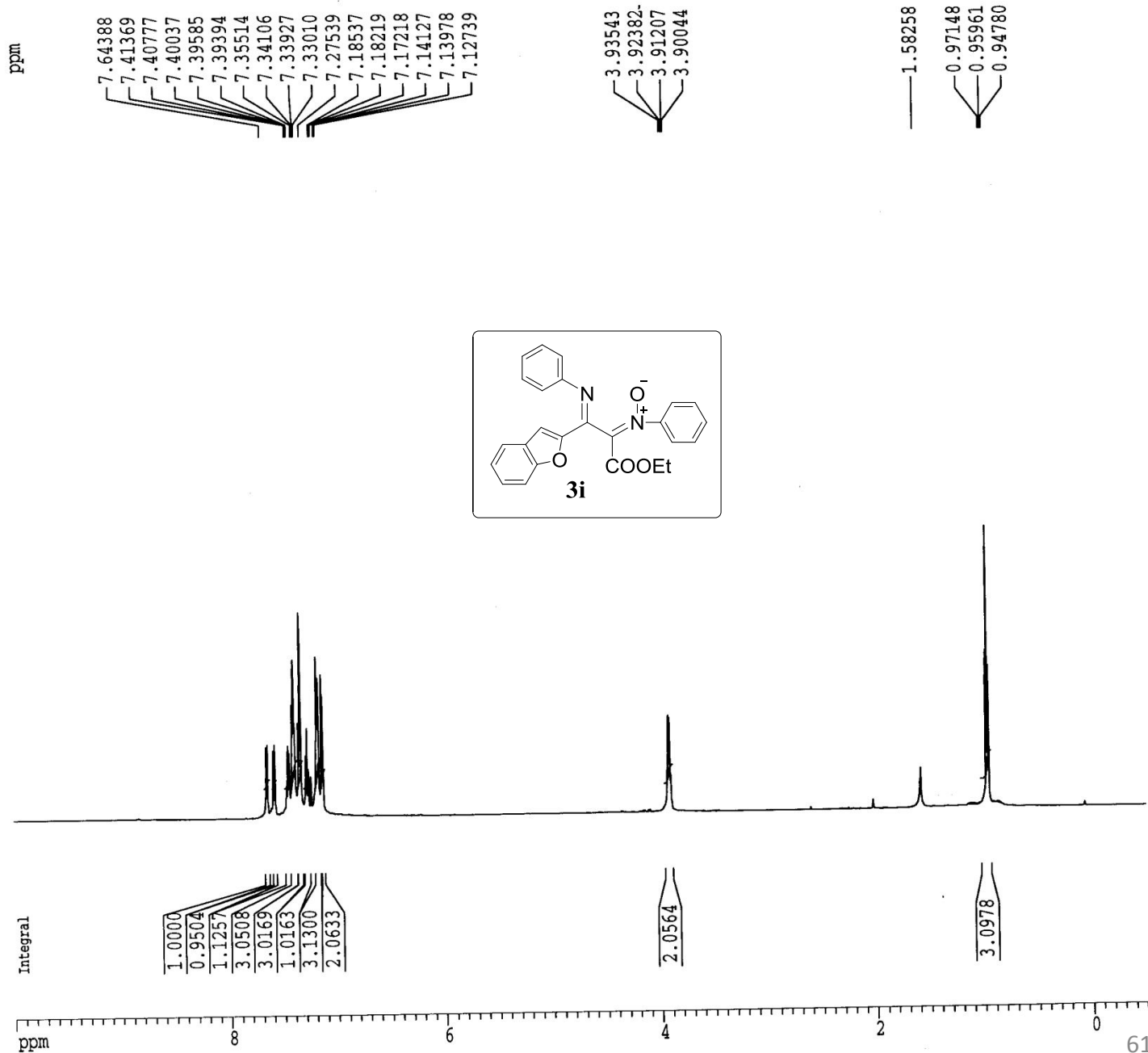
F2 - Acquisition Parameters

Date_ 20130811
 Time 20.45
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8382.229 Hz
 FIDRES 0.255805 Hz
 AQ 1.9546613 sec
 RG 256
 DW 59.650 usec
 DE 6.50 usec
 TE 303.8 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 3.00 dB
 SFO1 598.8035928 MHz

F2 - Processing parameters
 SI 32768
 SF 598.8000285 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 5.00 cm
 F1P 10.000 ppm
 F1 5988.00 Hz
 F2P -0.500 ppm
 F2 -299.40 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 314.37003 Hz/cm



Current Data Parameters
NAME RKS-1-165
EXPNO 2
PROCNO 1

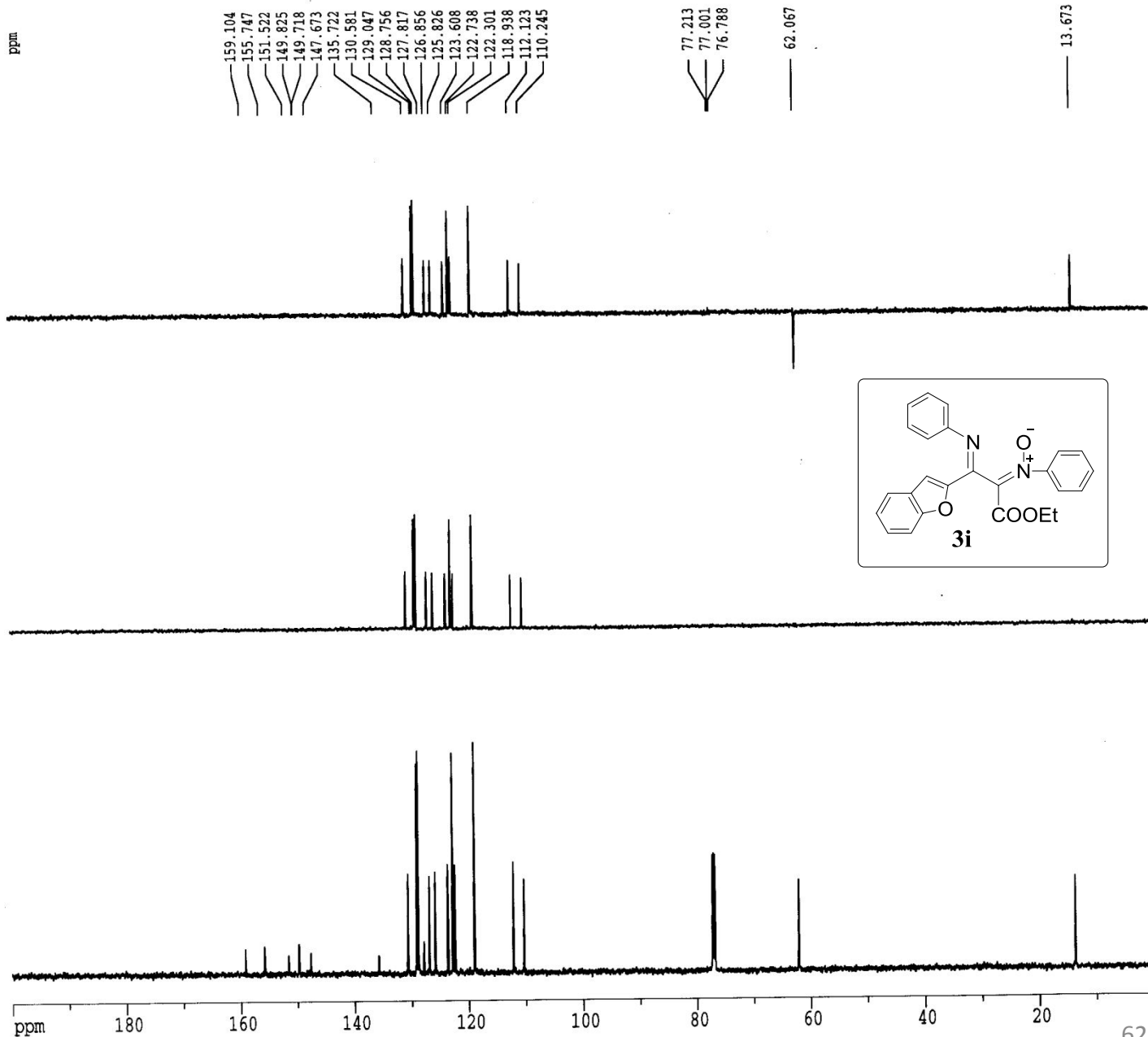
F2 - Acquisition Parameters
Date_ 20130811
Time 20.28
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 148
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 304.6 K
D1 3.5000000 sec
d11 0.0300000 sec
DELTA 3.4000010 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

=====
CHANNEL f1
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5849425 MHz

=====
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.8029940 MHz

F2 - Processing parameters
SI 65536
SF 150.5683855 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30113.68 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.68384 Hz/cm



Current Data Parameters
 NAME RKS-1-146
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20130728
 Time 15.59
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8382.229 Hz
 FIDRES 0.255805 Hz
 AQ 1.9546613 sec
 RG 128
 DW 59.650 usec
 DE 6.50 usec
 TE 300.7 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====

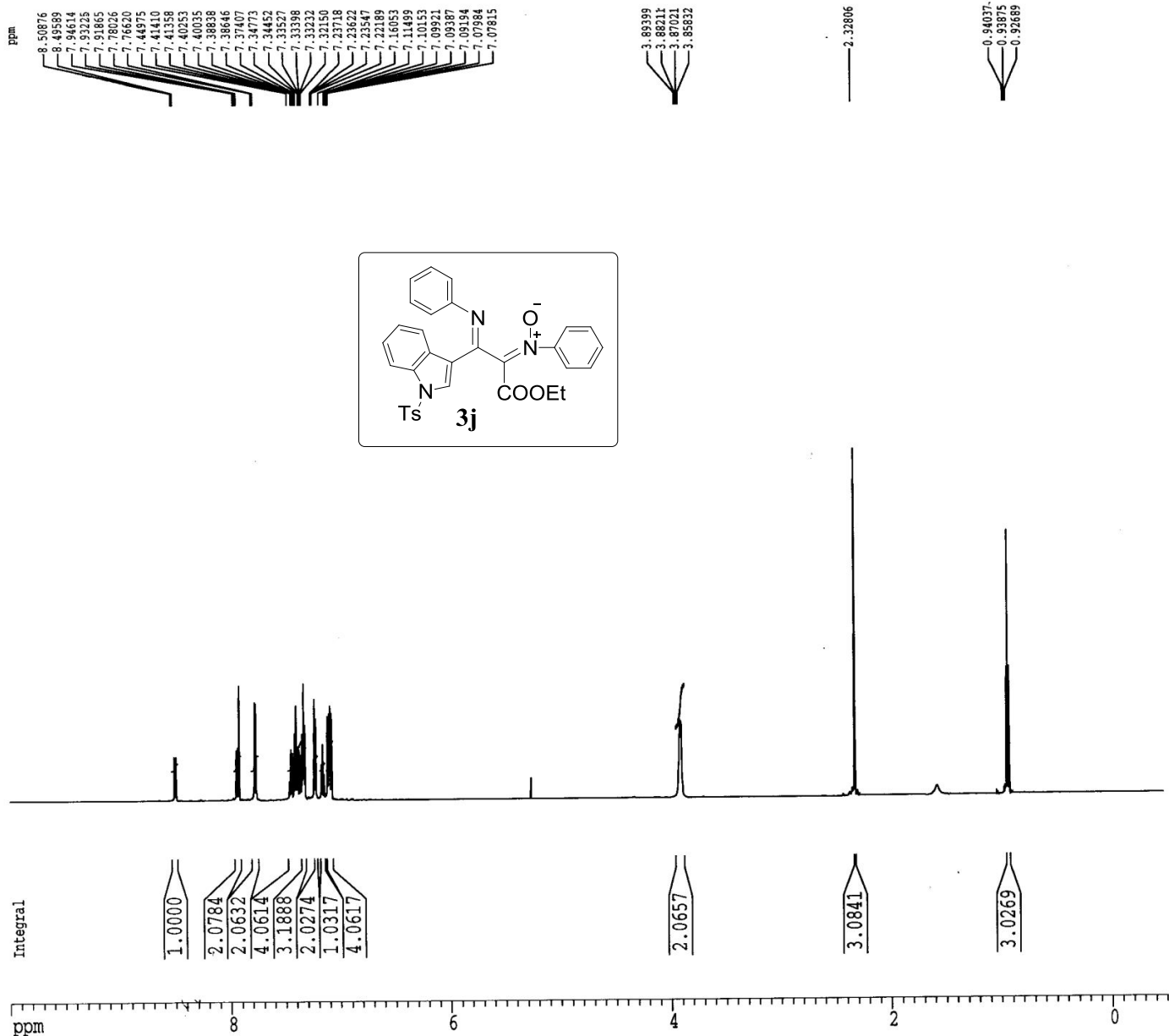
NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 598.8029940 MHz

F2 - Processing parameters

SI 32768
 SF 598.8000301 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters

CX 20.00 cm
 CY 6.00 cm
 F1P 10.000 ppm
 F1 5988.00 Hz
 F2P -0.500 ppm
 F2 -299.40 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 314.37003 Hz/cm



Current Data Parameters
 NAME RKS-1-146
 EXPNO 2
 PROCNO 1

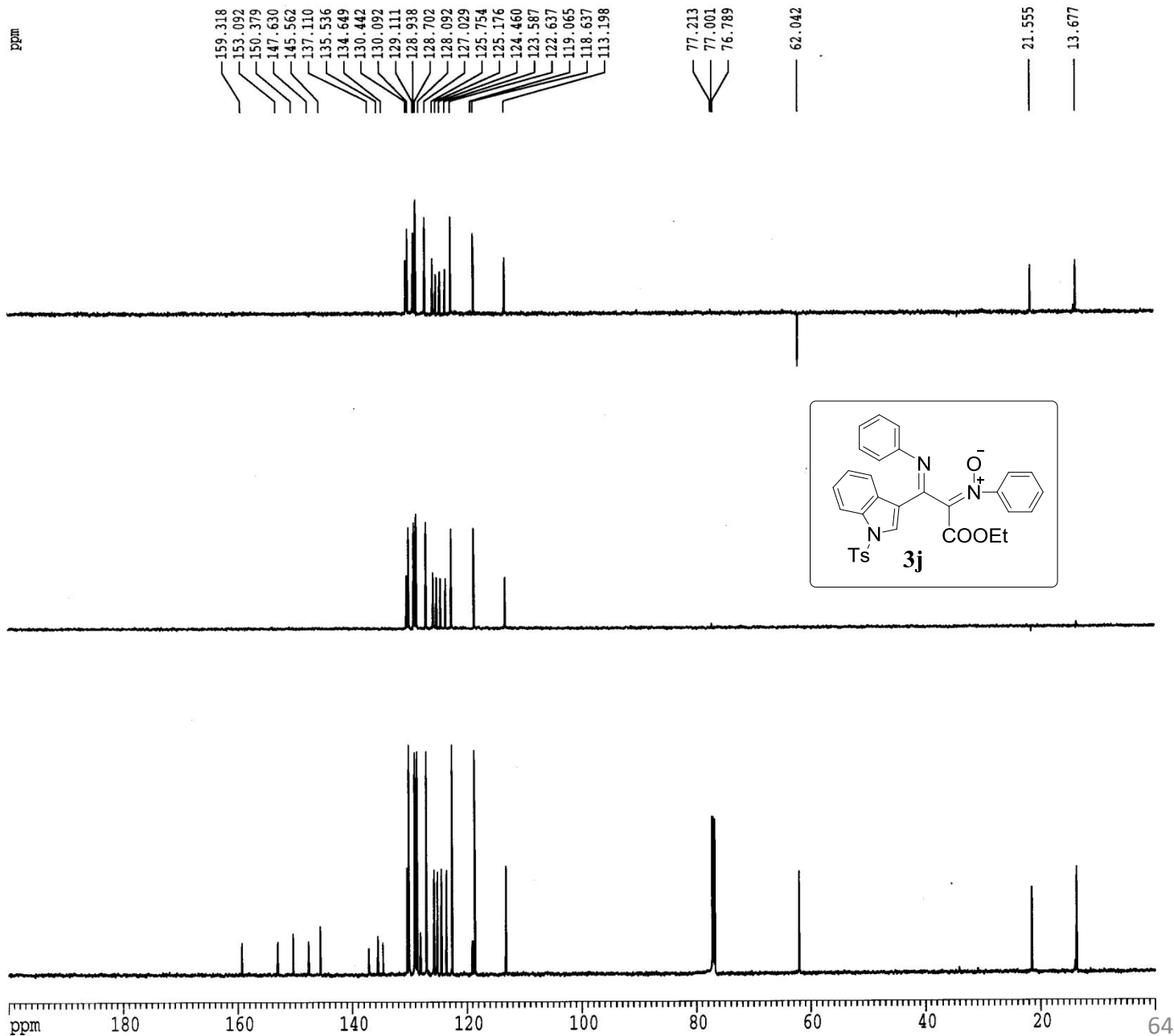
F2 - Acquisition Parameters
 Date_ 20130728
 Time 16.19
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg
 TD 32768
 SOLVENT CDCl3
 NS 300
 DS 0
 SWH 45045.047 Hz
 FIDRES 1.374666 Hz
 AQ 0.3637748 sec
 RG 2048
 DW 11.100 usec
 DE 6.500 usec
 TE 301.5 K
 D1 3.50000000 sec
 d11 0.03000000 sec
 DELTA 3.40000010 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 4.80 usec
 PL1 0.00 dB
 SFO1 150.5849425 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 92.00 usec
 PL2 120.00 dB
 PL12 9.00 dB
 PL13 14.00 dB
 SFO2 598.8029940 MHz

F2 - Processing parameters
 SI 65536
 SF 150.5683876 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 0.50

1D NMR plot parameters
 CX 20.00 cm
 CY 4.00 cm
 F1P 200.000 ppm
 F1 30113.68 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 10.00000 ppm/cm
 HZCM 1505.68384 Hz/cm



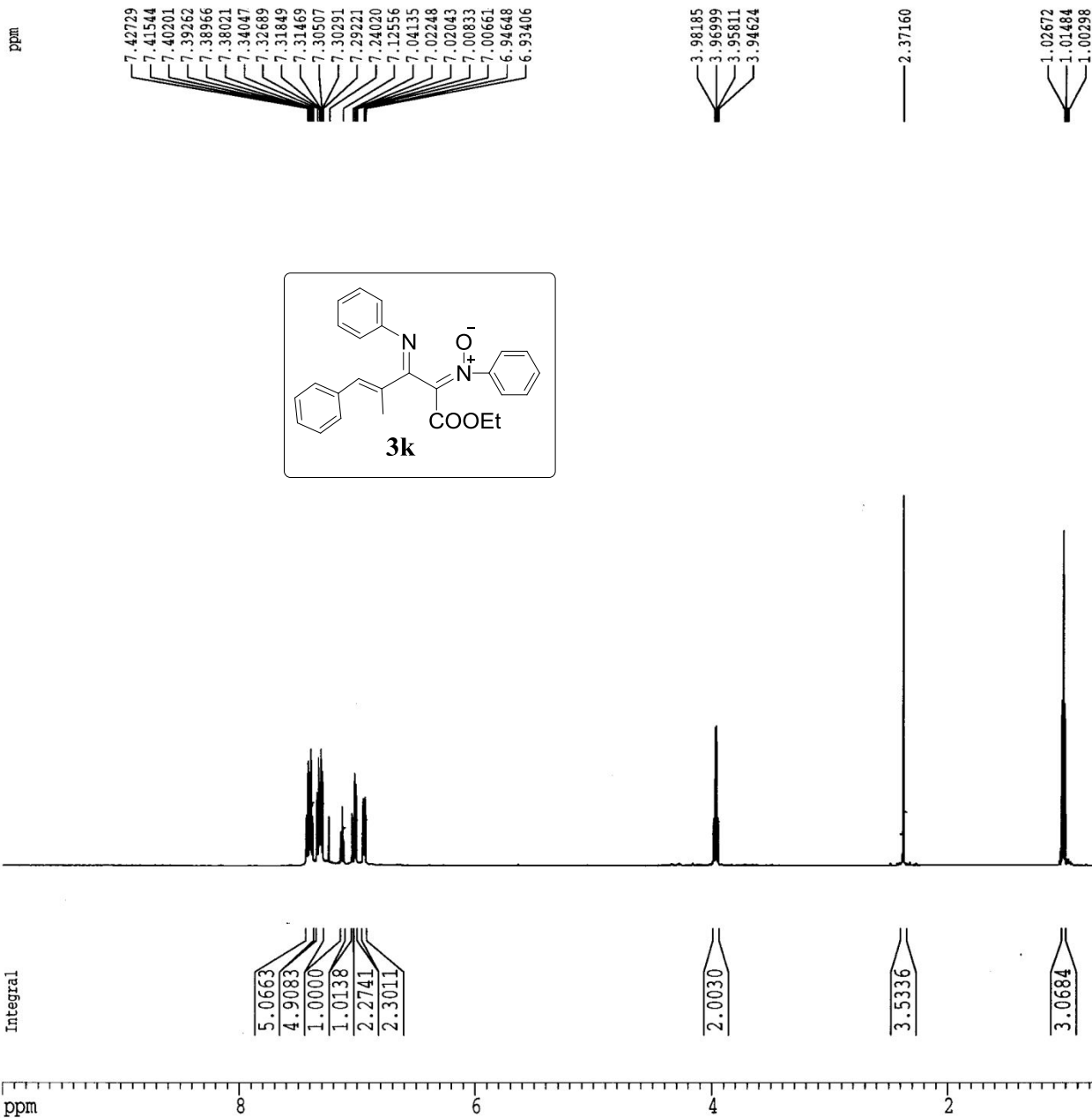
Current Data Parameters
 NAME RKS-1-1-108
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130610
 Time 20.19
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8382.229 Hz
 FIDRES 0.255805 Hz
 AQ 1.9546613 sec
 RG 128
 DW 59.650 usec
 DE 6.50 usec
 TE 299.6 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SF01 598.8026946 MHz

F2 - Processing parameters
 SI 32768
 SF 598.8000269 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 6.00 cm
 F1P 10.000 ppm
 F1 5988.00 Hz
 F2P -0.500 ppm
 F2 -299.40 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 314.37003 Hz/cm



Current Data Parameters
NAME RKS-1-1-108
EXPNO 2
PROCNO 1

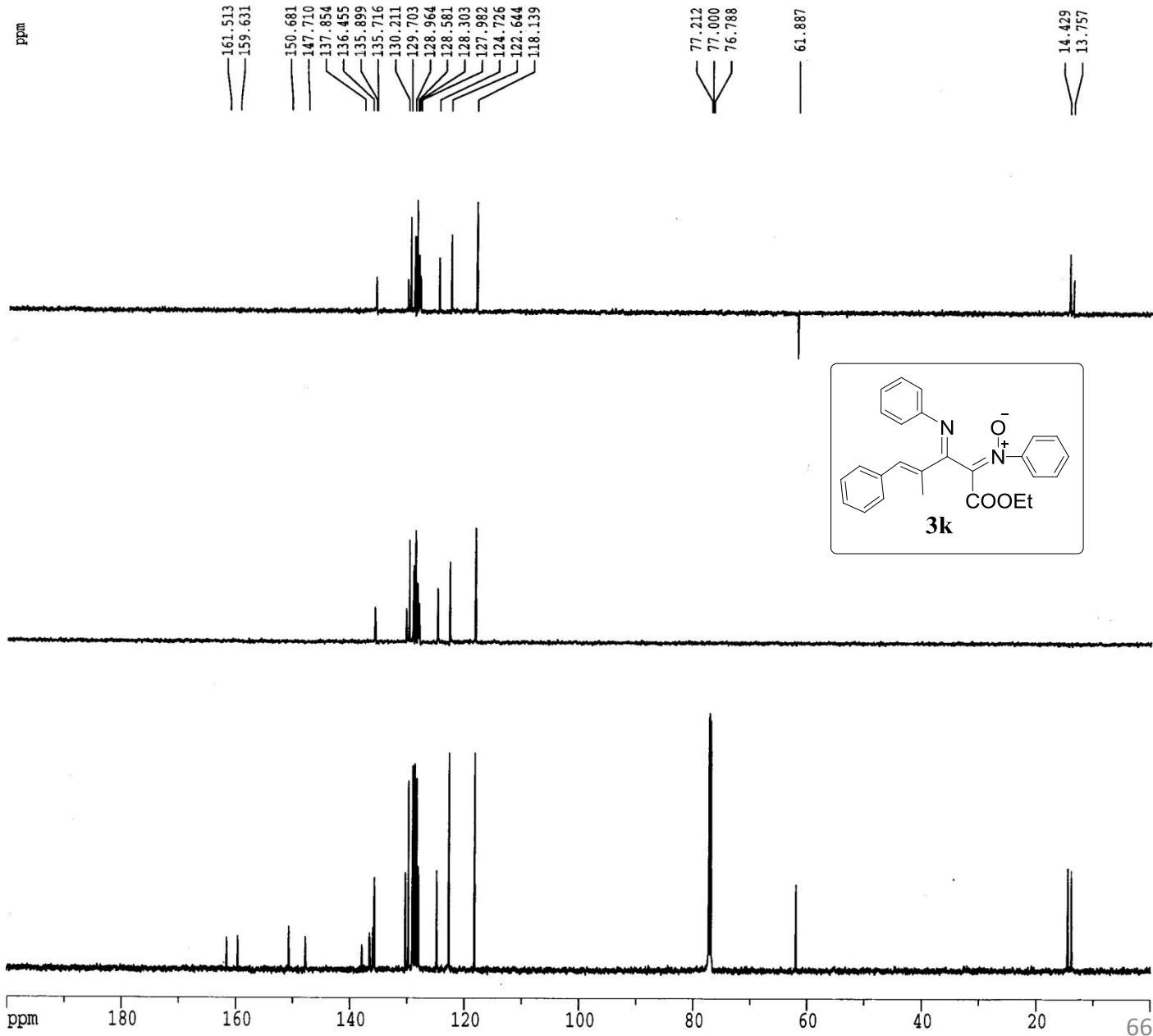
F2 - Acquisition Parameters
Date_ 20130610
Time 20.38
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 300
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 300.9 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5849425 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.8029940 MHz

F2 - Processing parameters
SI 65536
SF 150.5683841 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 4.50 cm
F1P 200.000 ppm
F1 30113.68 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.68384 Hz/cm



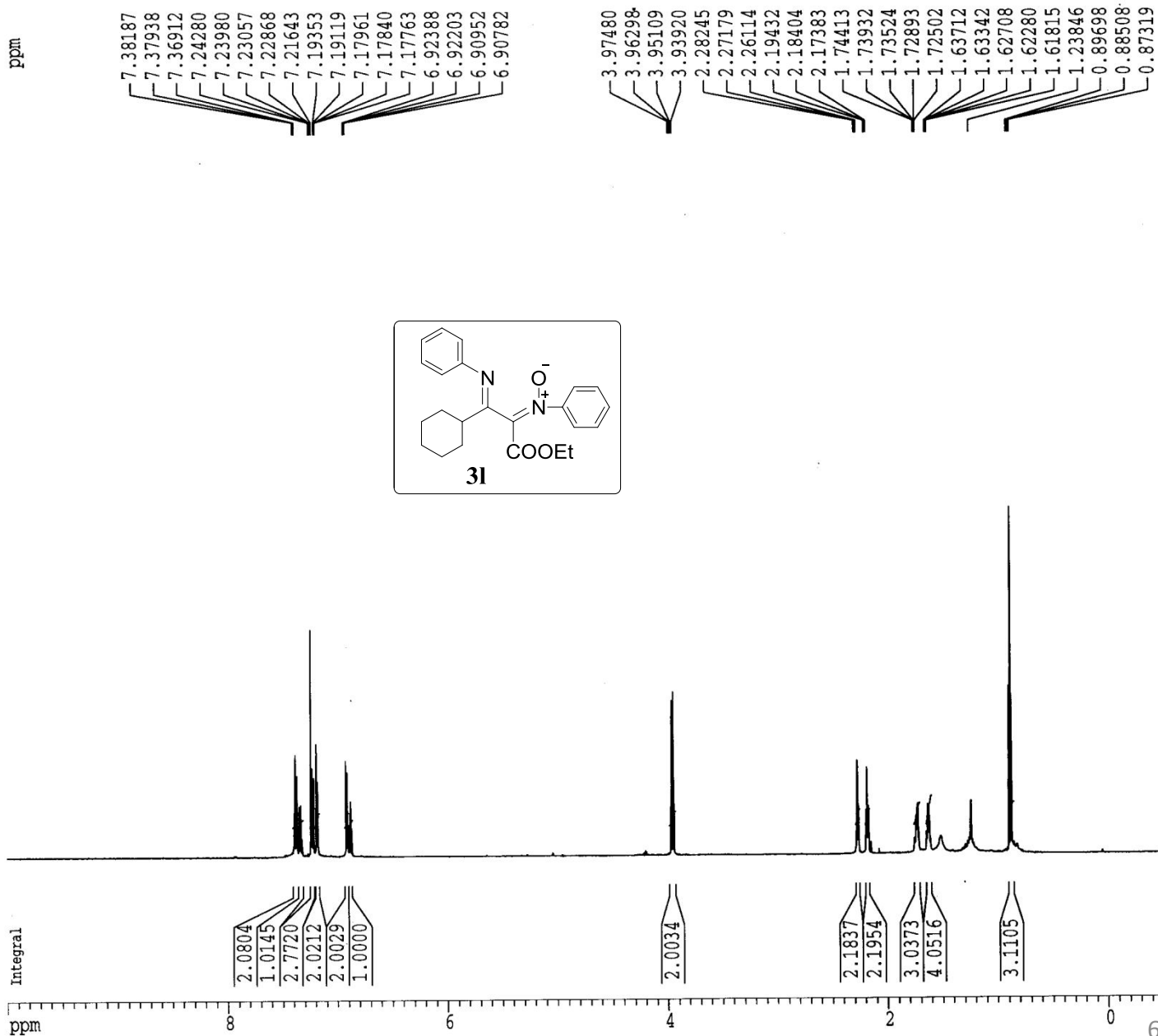
Current Data Parameters
 NAME RKS-1-157-F
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140828
 Time 22.26
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 33556
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8389.262 Hz
 FIDRES 0.250008 Hz
 AQ 1.9999876 sec
 RG 512
 DW 59.600 usec
 DE 6.50 usec
 TE 303.8 K
 DL 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 598.7029935 MHz

F2 - Processing parameters
 SI 32768
 SF 598.7000263 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 6.00 cm
 FIP 10.000 ppm
 F1 5987.00 Hz
 F2P -0.500 ppm
 F2 -299.35 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 314.31750 Hz/cm



Current Data Parameters
 NAME RKS-1-157-F
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20140829
 Time 5.09
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg
 TD 32768
 SOLVENT CDCl3
 NS 6144
 DS 0
 SWH 45045.047 Hz
 FIDRES 1.374666 Hz
 AQ 0.3637748 sec
 RG 2048
 DW 11.100 usec
 DE 6.50 usec
 TE 305.2 K
 D1 3.5000000 sec
 d11 0.03000000 sec
 DELTA 3.40000010 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

ppm

161.762

143.989

139.821

137.275

128.788

128.411

127.796

127.336

120.452

118.329

111.611

77.212

77.000

76.788

58.974

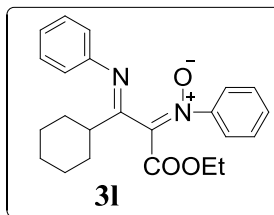
23.321

23.246

23.132

22.759

13.837

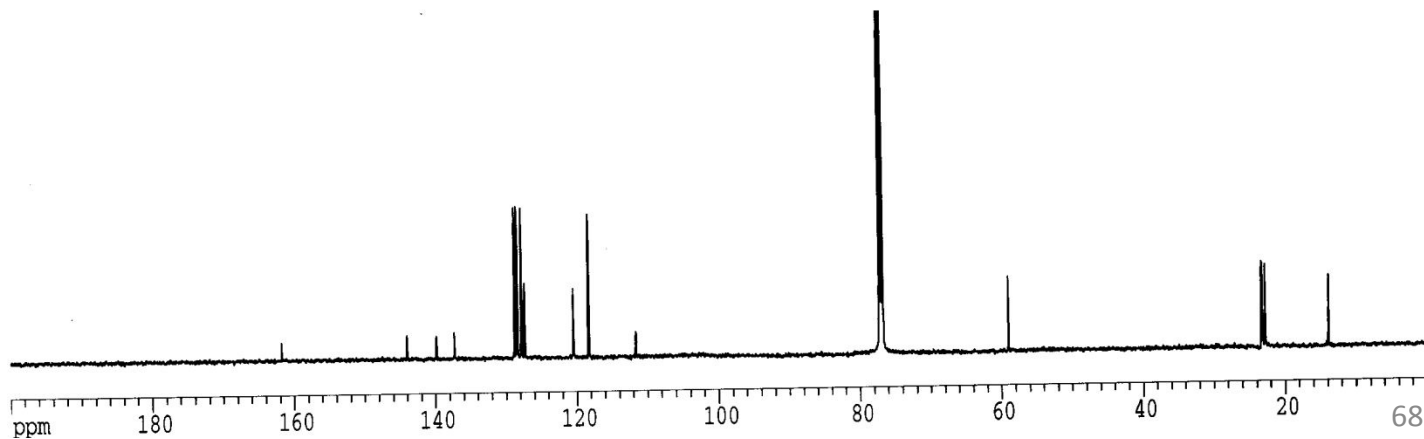


===== CHANNEL f1 =====
 NUC1 13C
 P1 4.80 usec
 PL1 0.00 dB
 SFO1 150.5597948 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 92.00 usec
 PL2 120.00 dB
 PL12 9.00 dB
 PL13 14.00 dB
 SFO2 598.7029935 MHz

F2 - Processing parameters
 SI 65536
 SF 150.5432335 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 FLP 200.000 ppm
 F1 30108.65 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 10.00000 ppm/cm



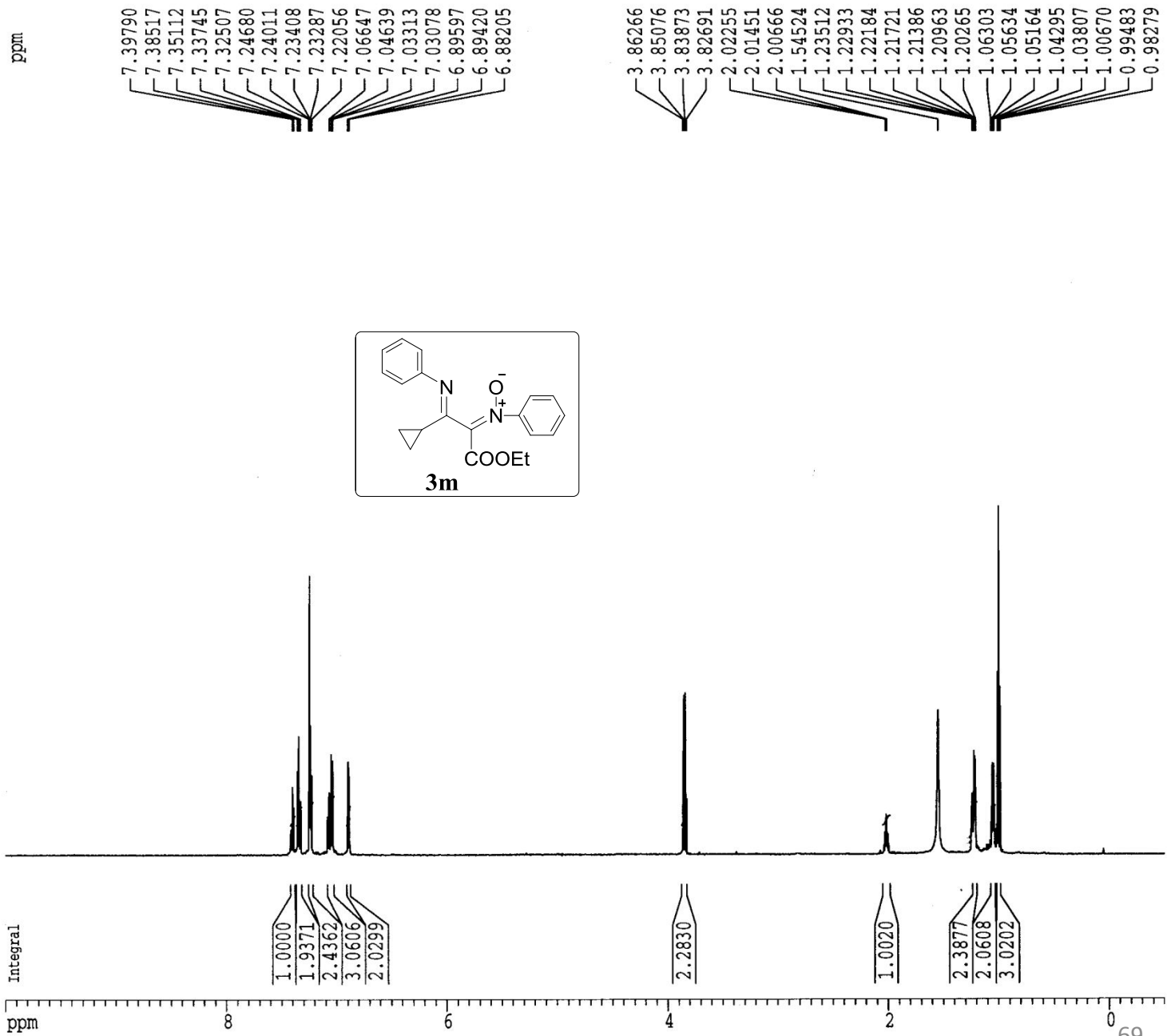
Current Data Parameters
 NAME RKS-1-166-P
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140801
 Time 12.19
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 33556
 SOLVENT CDCl3
 NS 16
 DS 0
 SMH 9615.385 Hz
 FIDRES 0.236547 Hz
 AQ 1.7449620 sec
 RG 512
 DW 52.000 usec
 DE 6.50 usec
 TE 301.8 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 598.7029935 MHz

F2 - Processing parameters
 SI 32768
 SF 598.7000260 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 6.00 cm
 F1P 10.000 ppm
 F1 5987.00 Hz
 F2P -0.500 ppm
 F2 -299.35 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 314.31750 Hz/cm



Current Data Parameters
NAME RKS-1-166-P
EXPNO 2
PROCNO 1

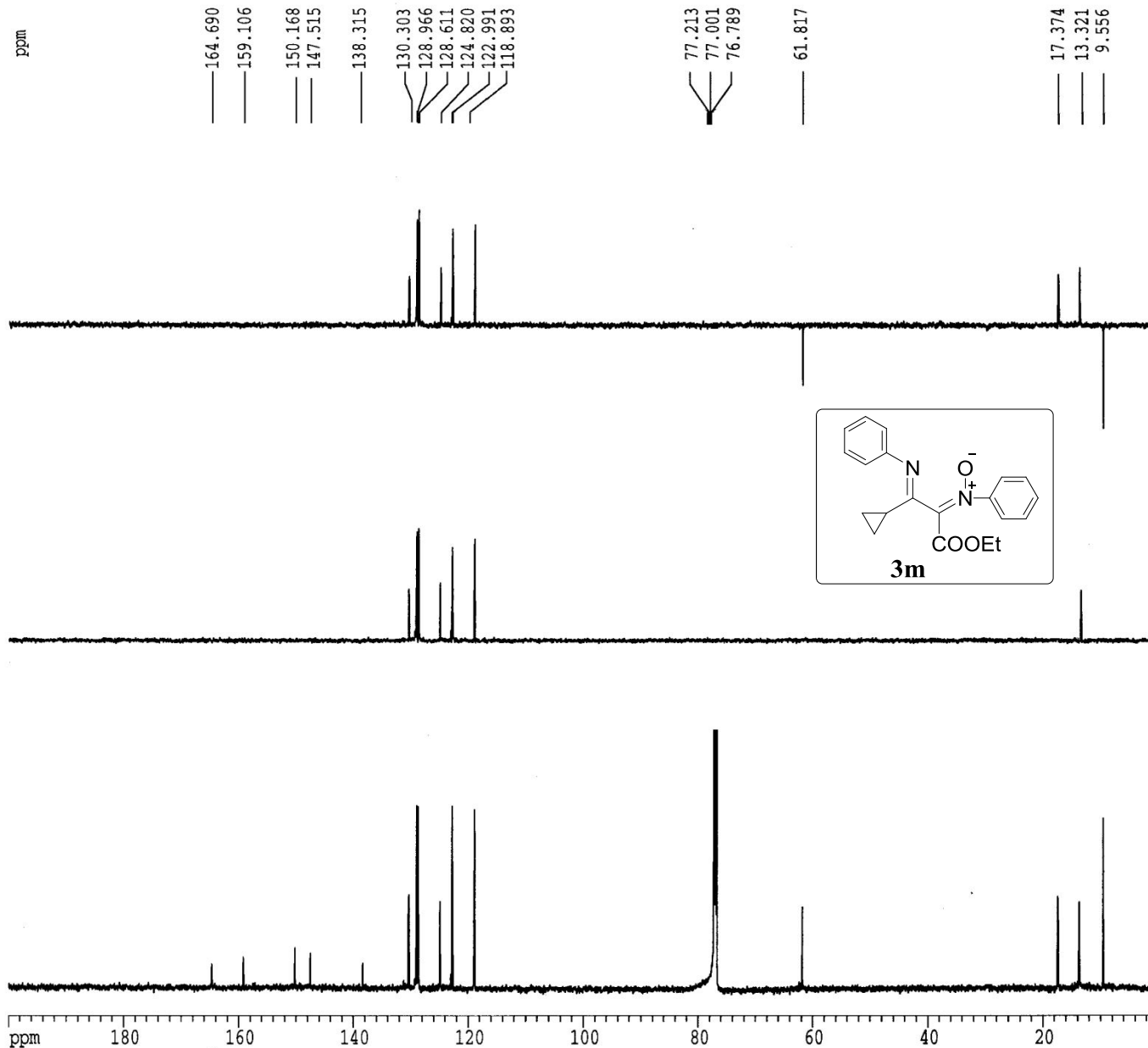
F2 - Acquisition Parameters
Date_ 20140801
Time 12.21
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 8192
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
EW 11.100 usec
DE 6.50 usec
TE 301.8 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

=====
CHANNEL f1
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5597948 MHz

=====
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.7029935 MHz

F2 - Processing parameters
SI 65536
SF 150.5432356 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 20.00 cm
CY 20.00 cm
F1P 200.000 ppm
F1 30108.65 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.43225 Hz/cm



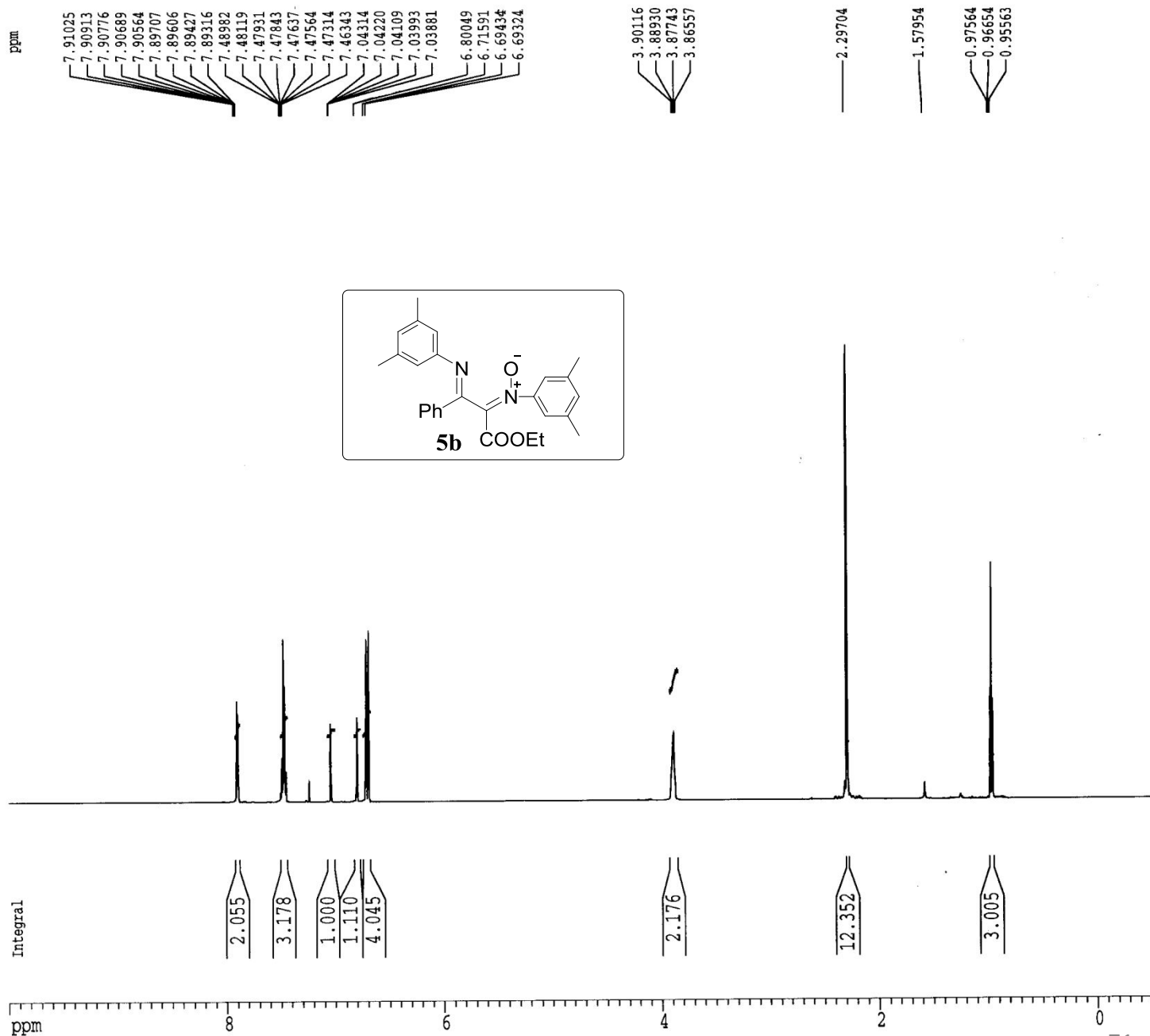
Current Data Parameters
 NAME RKS-1-203
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131006
 Time 20.26
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8389.262 Hz
 FIDRES 0.256020 Hz
 AQ 1.9530228 sec
 RG 256
 DW 59.600 usec
 DE 6.50 usec
 TE 304.9 K
 D1 2.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 598.8029940 MHz

F2 - Processing parameters
 SI 32768
 SF 598.8000287 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 8.00 cm
 F1P 10.000 ppm
 F1 5988.00 Hz
 F2P -0.500 ppm
 F2 -299.40 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 314.37003 Hz/cm



Current Data Parameters
 NAME RKS-1-204
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20131010
 Time 12.45
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8389.262 Hz
 FIDRES 0.256020 Hz
 AQ 1.9530228 sec
 RG 256
 DW 59.600 usec
 DE 6.50 usec
 TE 297.5 K
 D1 2.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

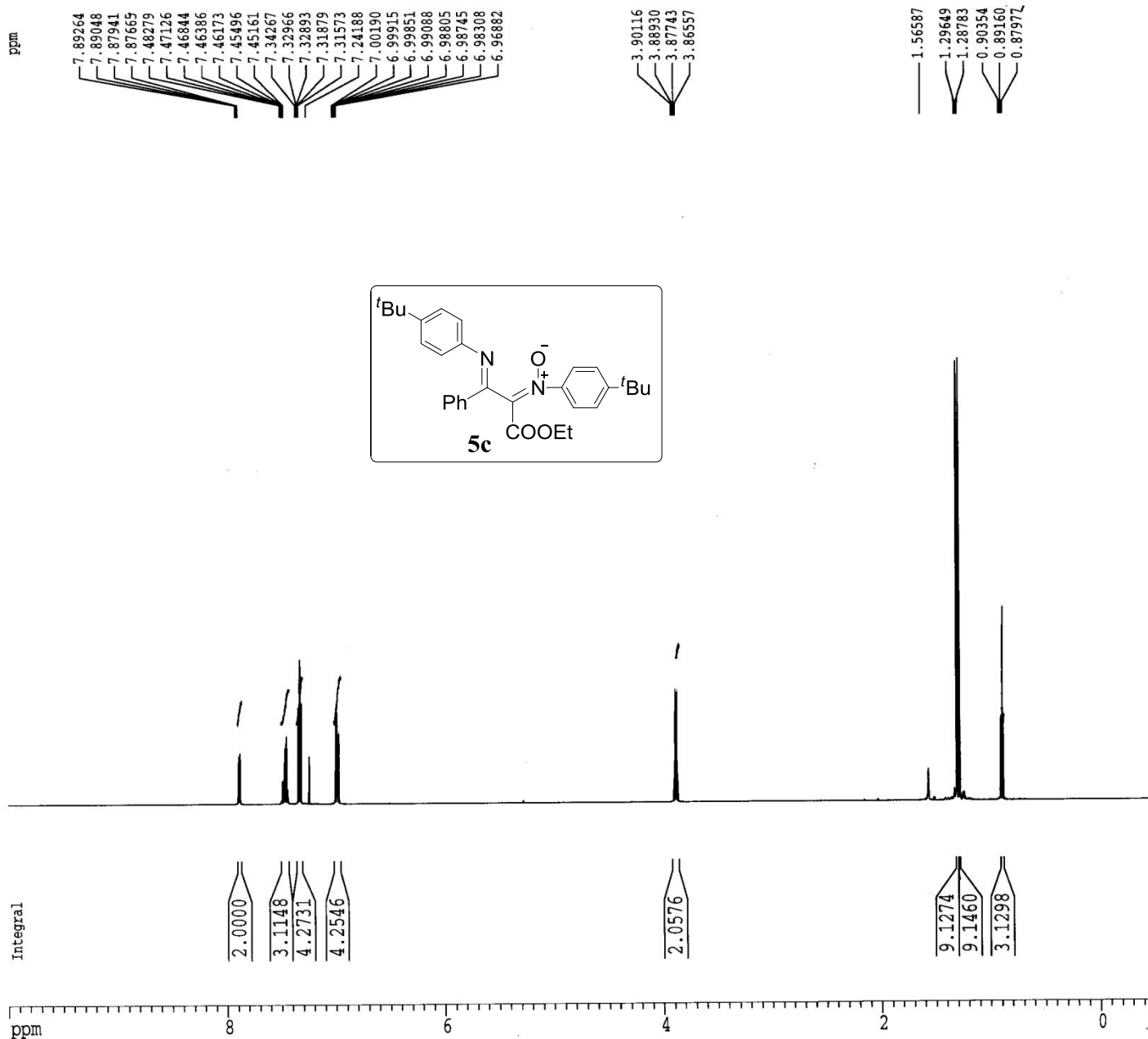
===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 598.7029935 MHz

F2 - Processing parameters

SI 32768
 SF 598.7000250 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters

CX 20.00 cm
 CY 8.00 cm
 F1P 10.000 ppm
 F1 5987.00 Hz
 F2P -0.500 ppm
 F2 -299.35 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 314.31750 Hz/cm



Current Data Parameters
 NAME RKS-1-204
 EXPNO 2
 PROCNO 1

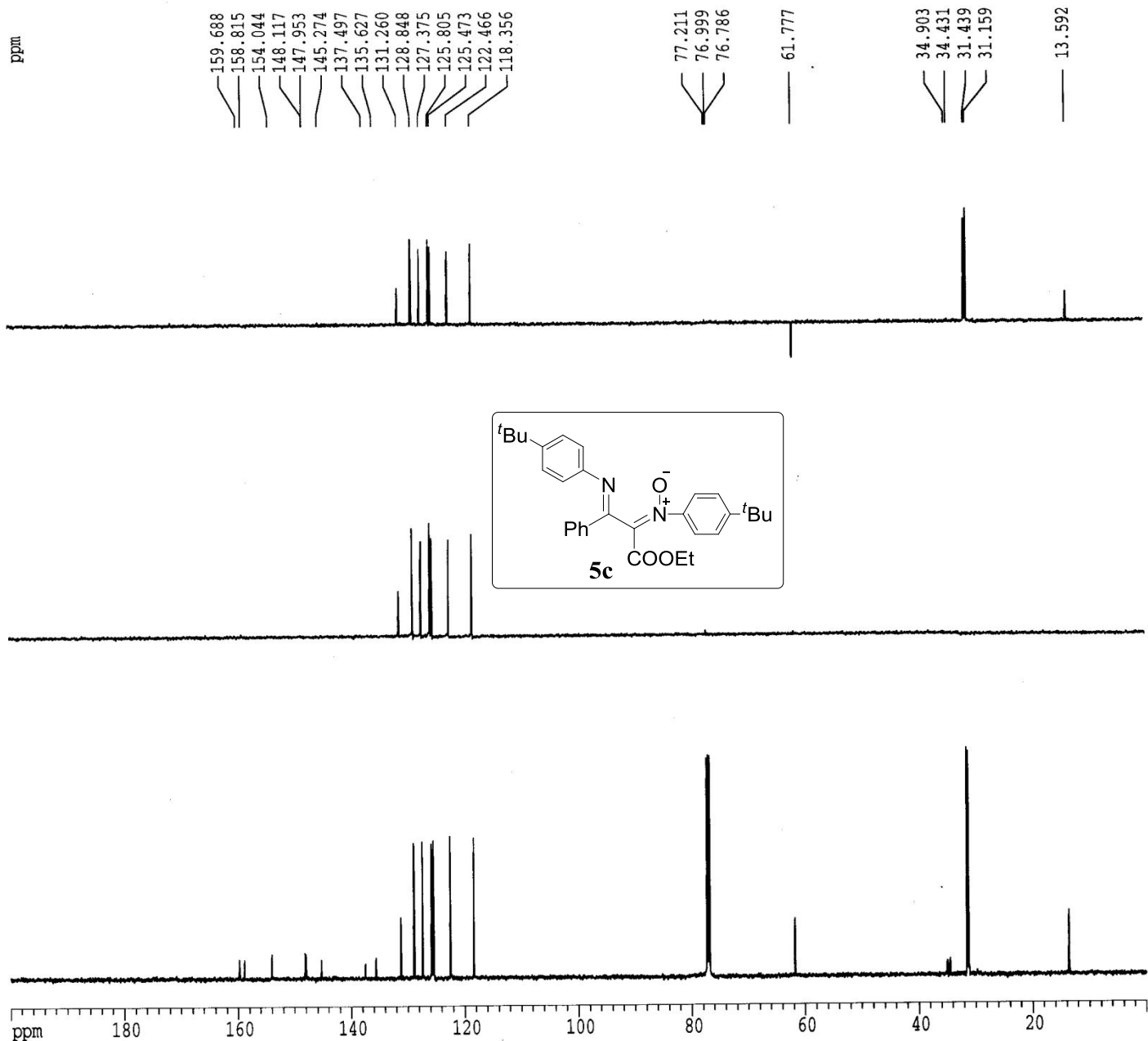
F2 - Acquisition Parameters
 Date_ 20131010
 Time 12.46
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg
 TD 32768
 SOLVENT CDCl3
 NS 518
 DS 0
 SWH 45045.047 Hz
 FIDRES 1.374666 Hz
 AQ 0.3637748 sec
 RG 2048
 DW 11.100 usec
 DE 6.50 usec
 TE 297.7 K
 D1 3.50000000 sec
 d11 0.03000000 sec
 DELTA 3.40000010 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 4.80 usec
 PL1 0.00 dB
 SFO1 150.5597948 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 92.00 usec
 PL2 120.00 dB
 PL12 9.00 dB
 PL13 14.00 dB
 SFO2 598.7029935 MHz

F2 - Processing parameters
 SI 65536
 SF 150.5432383 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 0.50

1D NMR plot parameters
 CK 20.00 cm
 CY 4.00 cm
 F1P 200.000 ppm
 F1 30108.65 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 10.00000 ppm/cm
 HZCM 1505.43237 Hz/cm



Current Data Parameters
 NAME 20140429
 EXPNO 2
 PROCNO 1

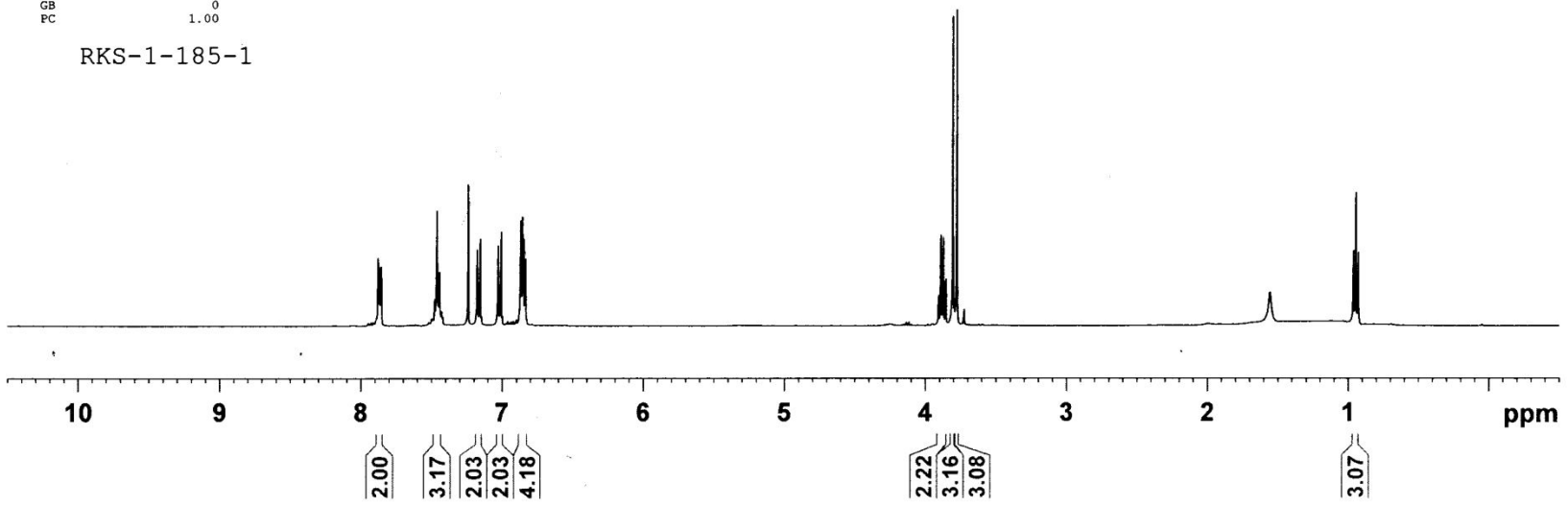
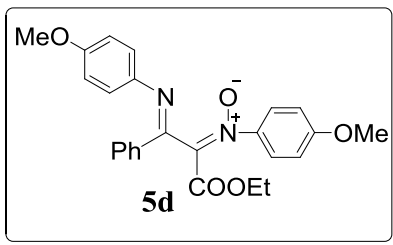
F2 - Acquisition Parameters
 Date_ 20140429
 Time 0.16
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 39
 DS 0
 SWH 6410.256 Hz
 FIDRES 0.195625 Hz
 AQ 2.5559540 sec
 RG 456
 DW 78.000 usec
 DE 6.00 usec
 TE 300.0 K
 DI 2.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 -2.40 dB
 SFO1 400.1528010 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1500168 MHz
 WDW EM
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

RKS-1-185-1

7.8799
7.8767
7.8619
7.8566
7.4650
7.4626
7.4577
7.4447
7.2426
7.2403
7.1782
7.1610
7.1582
7.1558
7.0303
7.0134
7.0105
7.0081
6.8719
6.8664
6.8607
6.8585
6.8523
6.8495
6.8412
6.8384
6.8366
3.9083
3.8906
3.8728
3.8539
3.8057
3.7763
1.5573
0.9641
0.9485
0.9460



Current Data Parameters
 NAME 20140429
 EXPNO 3
 PROCNO 1

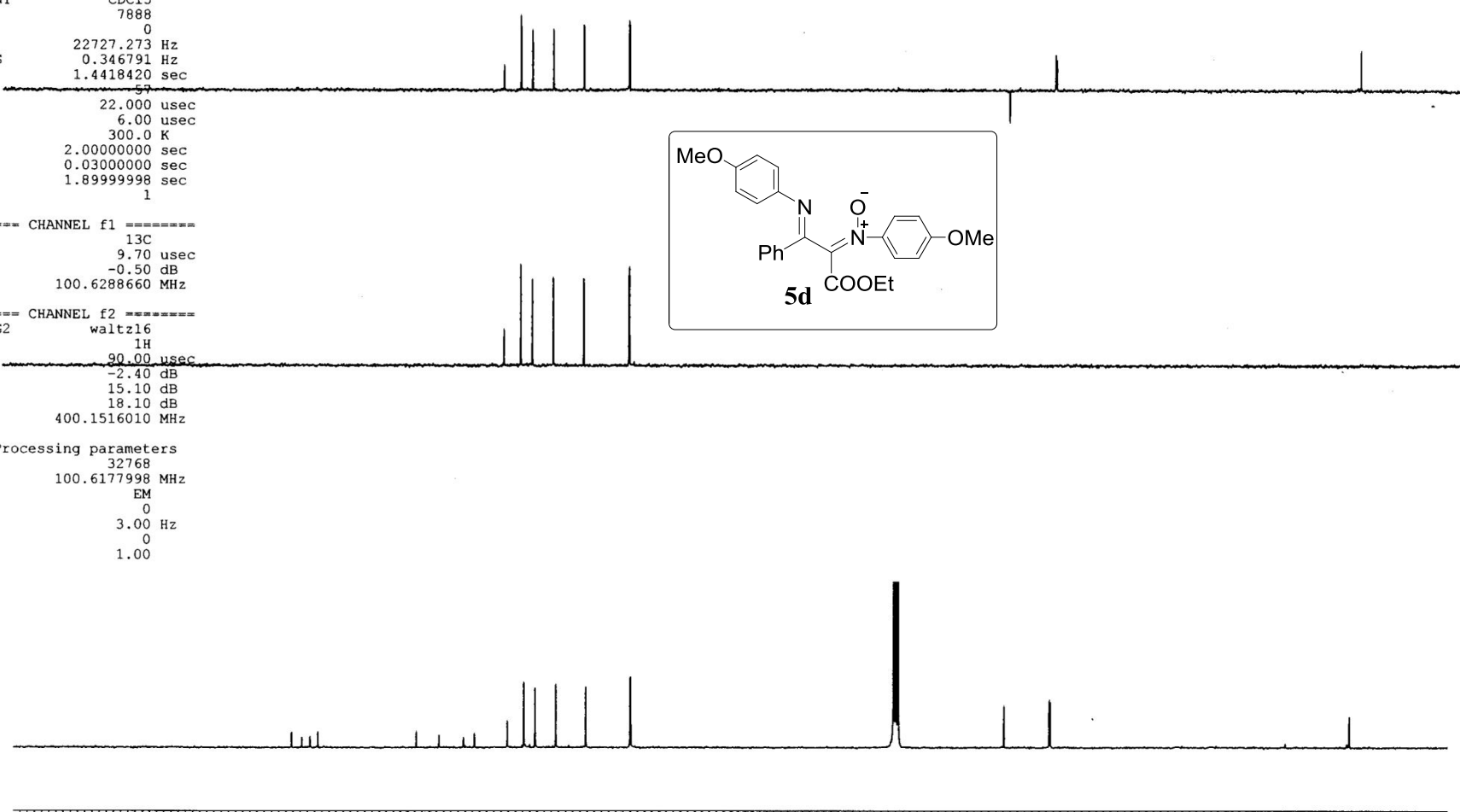
F2 - Acquisition Parameters
 Date_ 20140429
 Time_ 0.22
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 7888
 DS 0
 SWH 22727.273 Hz
 FIDRES 0.346791 Hz
 AQ 1.4418420 sec
 RG 59
 DW 22.000 usec
 DE 6.000 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 9.70 usec
 PL1 -0.50 dB
 SFO1 100.6288660 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -2.40 dB
 PL12 15.10 dB
 PL13 18.10 dB
 SFO2 400.1516010 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6177998 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.00

161.228
 159.796
 158.673
 157.587
 143.848
 140.699
 137.283
 135.768
 131.169
 128.856
 127.286
 124.413
 120.247
 114.041
 113.974
 77.319
 77.001
 76.684
 61.892
 55.596
 55.456
 13.738



190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

Current Data Parameters
 NAME RKS-1-187
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20130912
 Time 14.16
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 47890
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 7183.908 Hz
 FIDRES 0.150009 Hz
 AQ 3.3331940 sec
 RG 128
 DW 69.600 usec
 DE 6.50 usec
 TE 302.4 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====

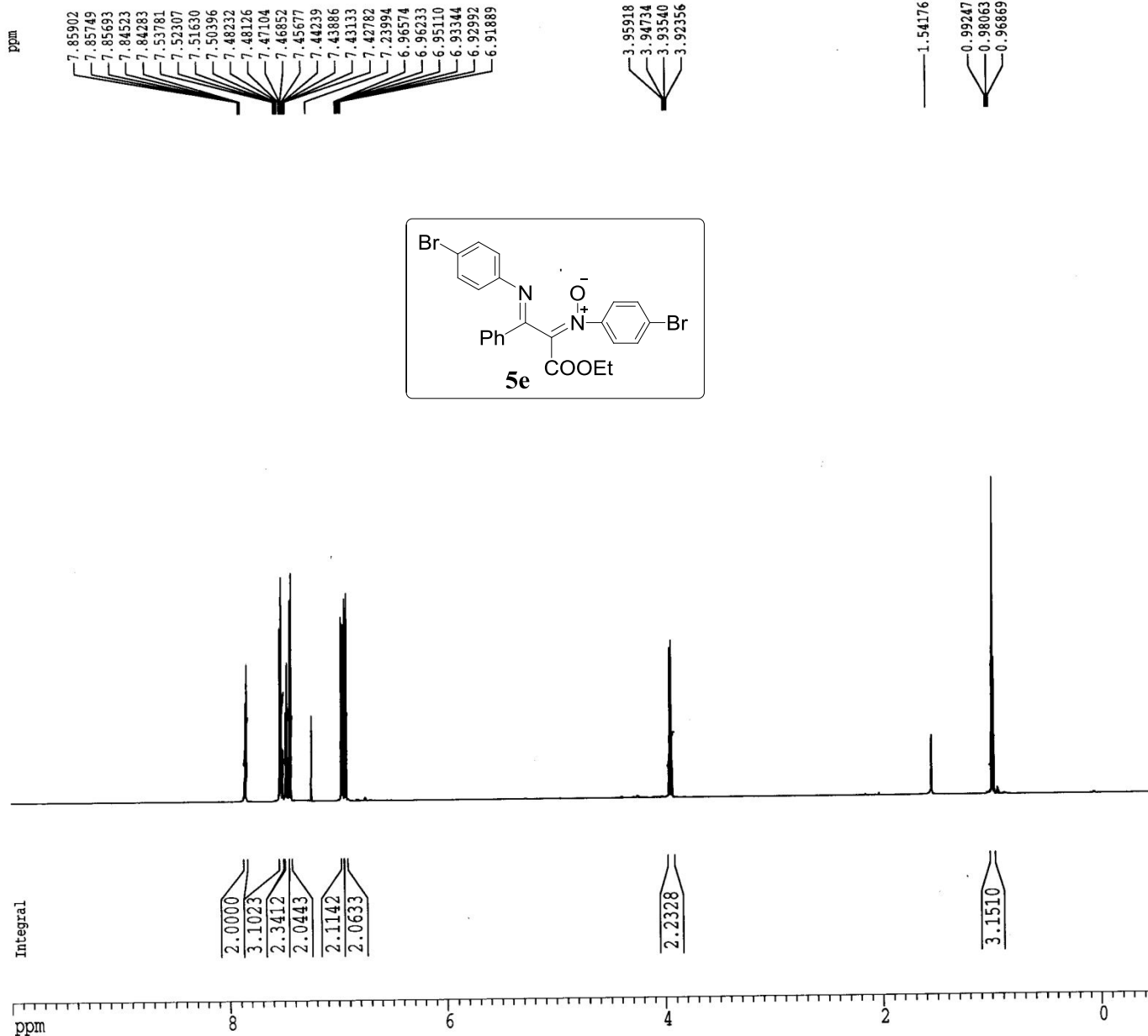
NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 598.8029940 MHz

F2 - Processing parameters

SI 32768
 SF 598.8000289 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters

CX 20.00 cm
 CY 4.00 cm
 F1P 10.000 ppm
 F1 5988.00 Hz
 F2P -0.500 ppm
 F2 -299.40 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 314.37003 Hz/cm



Current Data Parameters
 NAME RKS-1-187
 EXPNO 2
 PROCNO 1

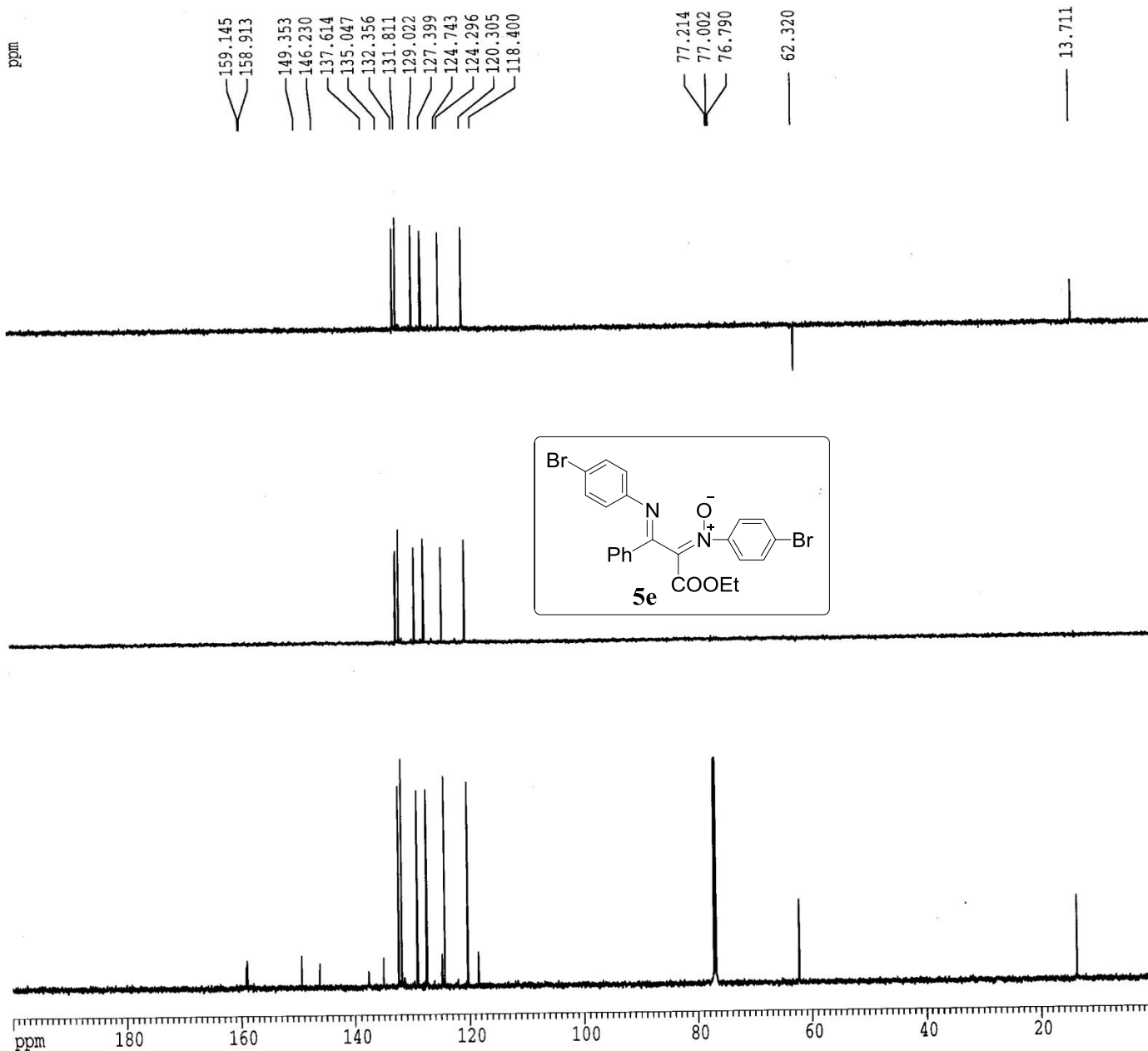
F2 - Acquisition Parameters
 Date_ 20130912
 Time 14.19
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg
 TD 32768
 SOLVENT CDCl3
 NS 324
 DS 0
 SWH 45045.047 Hz
 FIDRES 1.374666 Hz
 AQ 0.3637748 sec
 RG 2048
 DW 11.100 usec
 DE 6.50 usec
 TE 302.9 K
 D1 3.5000000 sec
 d11 0.0300000 sec
 DELTA 3.4000010 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

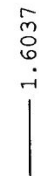
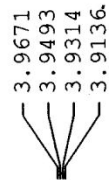
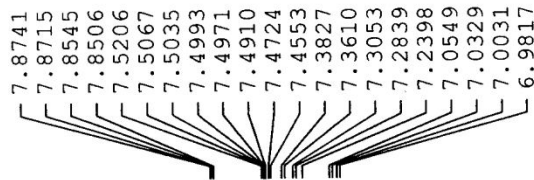
==== CHANNEL f1 =====
 NUC1 13C
 P1 4.80 usec
 PL1 0.00 dB
 SFO1 150.5849425 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 92.00 usec
 PL2 120.00 dB
 PL12 9.00 dB
 PL13 14.00 dB
 SFO2 598.8029940 MHz

F2 - Processing parameters
 SI 65536
 SF 150.5683821 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 0.50

1D NMR plot parameters
 CX 20.00 cm
 CY 4.00 cm
 F1P 200.000 ppm
 F1 30113.68 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 10.00000 ppm/cm
 HZCM 1505.68372 Hz/cm



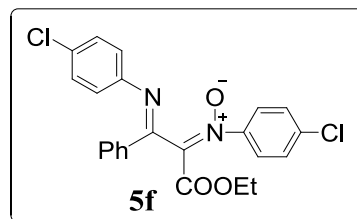


Current Data Parameters
NAME 20140425
EXPNO 5
PROCNO 1

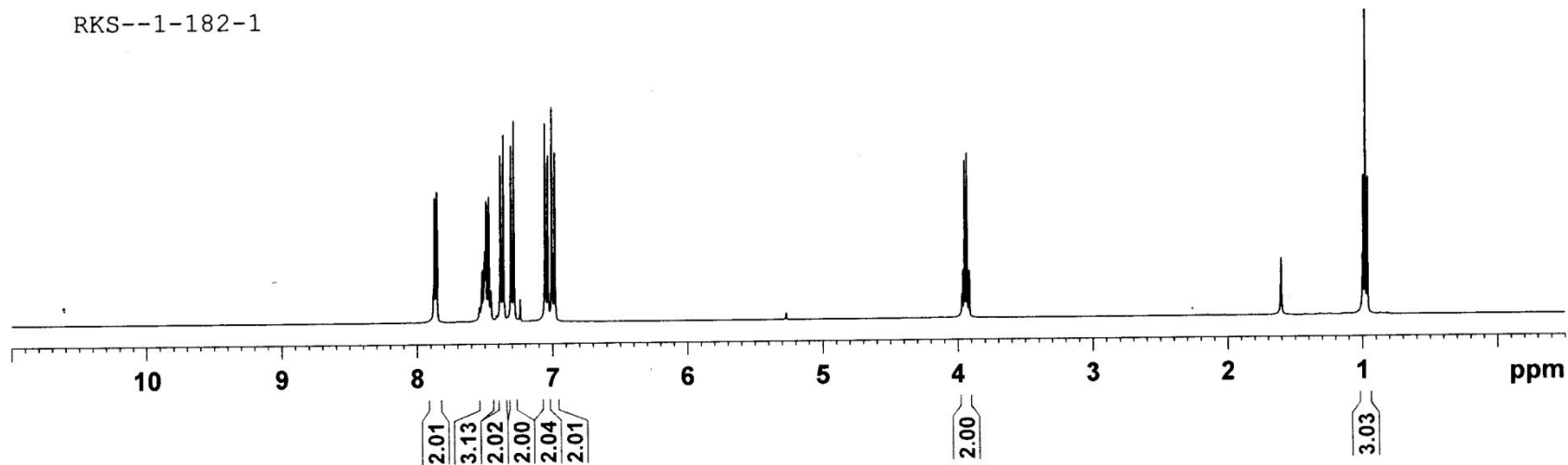
F2 - Acquisition Parameters
Date_ 20140425
Time 23.21
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 30
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 128
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SF01 400.1528010 MHz

F2 - Processing parameters
SI 16384
SF 400.1500175 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



RKS--1-182-1



Current Data Parameters
 NAME 20140425
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140425
 Time_ 22.15
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 723
 DS 0
 SWH 22727.273 Hz
 FIDRES 0.346791 Hz
 AQ 1.4418420 sec
 RG
 DW 22.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.70 usec
 PL1 -0.50 dB
 SFO1 100.6288660 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -2.40 dB
 PL12 15.10 dB
 PL13 18.10 dB
 SFO2 400.1516010 MHz

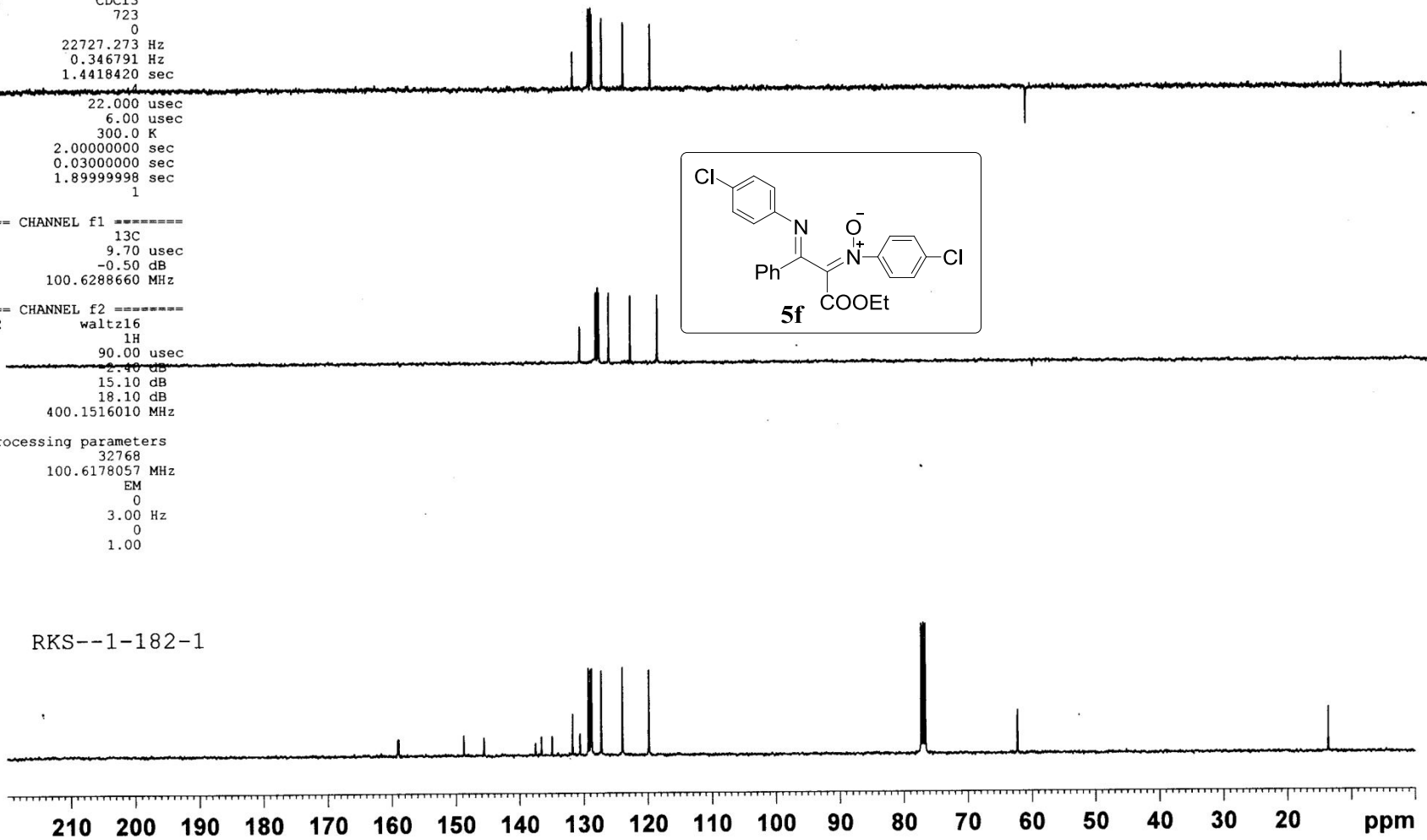
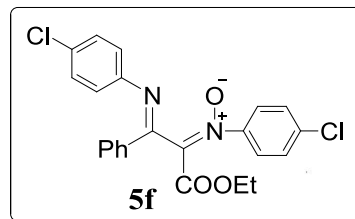
F2 - Processing parameters
 SI 32768
 SF 100.6178057 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.00

159.095
 158.953
 148.807
 145.638
 137.574
 136.626
 134.958
 131.790
 130.650
 129.327
 128.986
 128.830
 127.329
 124.036
 119.883

77.306
 76.988
 76.670

62.276

13.668



RKS--1-182-1

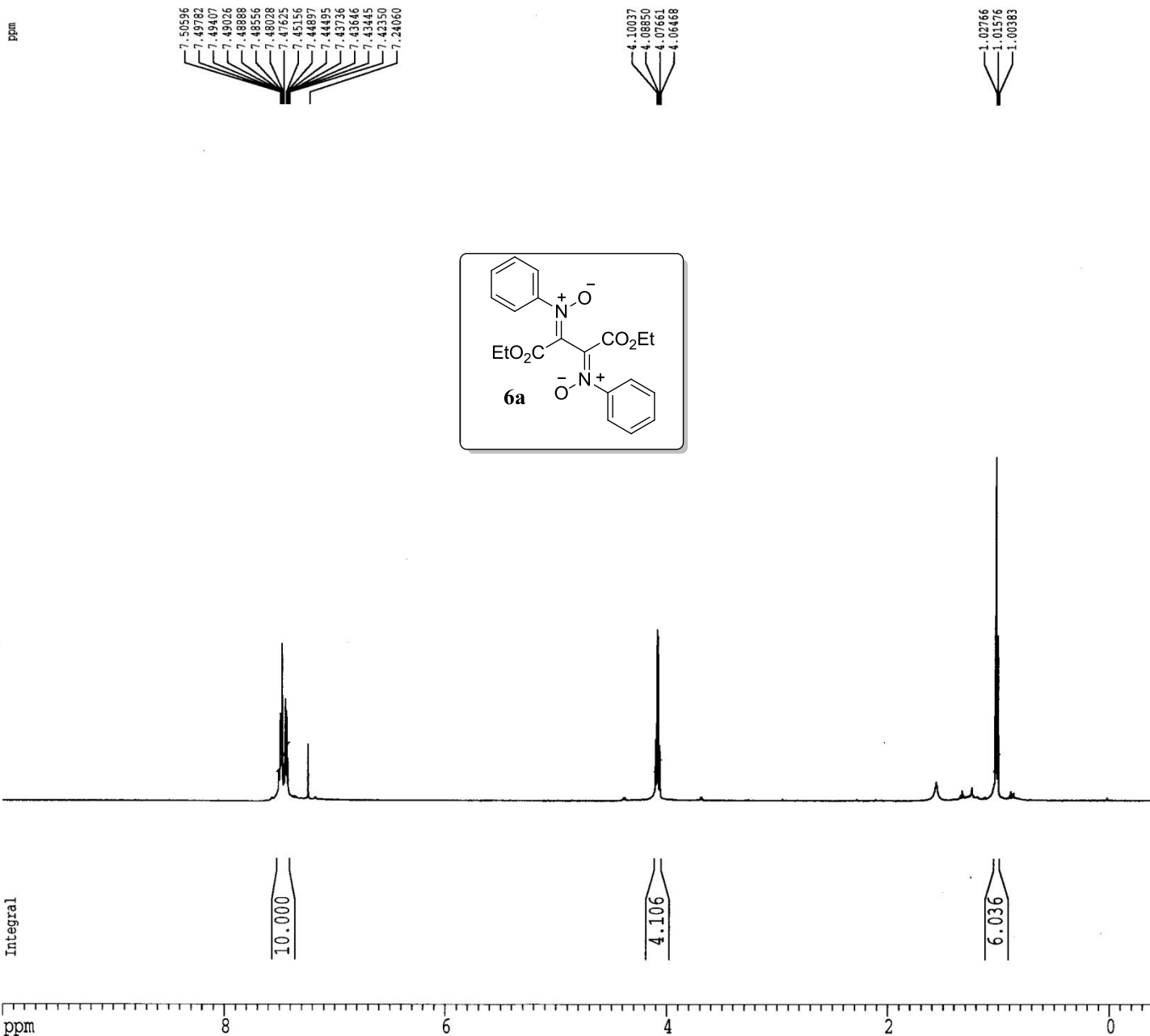
Current Data Parameters
 NAME RKS-2-143
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140814
 Time 19.54
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 9615.385 Hz
 FIDRES 0.293438 Hz
 AQ 1.7039860 sec
 RG 128
 DW 52.000 usec
 DE 6.50 usec
 TE 302.5 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 3.00 dB
 SFO1 598.7029935 MHz

F2 - Processing parameters
 SI 32768
 SF 598.7000255 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 6.00 cm
 FIP 10.000 ppm
 F1 5987.00 Hz
 F2P -0.500 ppm
 F2 -299.35 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 314.31750 Hz/cm



Current Data Parameters
 NAME RKS-2-143
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140814
 Time 19.54
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg
 TD 32768
 SOLVENT CDC13
 NS 331
 DS 0
 SWH 45045.047 Hz
 FIDRES 1.374666 Hz
 AQ 0.3637748 sec
 RG 2048
 DW 11.100 usec
 DE 6.50 usec
 TE 302.5 K
 D1 3.5000000 sec
 d11 0.0300000 sec
 DELTA 3.4000010 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 4.80 usec
 PL1 0.00 dB
 SFO1 150.5597948 MHz

===== CHANNEL f2' =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 92.00 usec
 PL2 120.00 dB
 PL12 9.00 dB
 PL13 14.00 dB
 SFO2 598.7029935 MHz

F2 - Processing parameters
 SI 65536
 SF 150.5432369 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 0.50

1D NMR plot parameters
 CX 20.00 cm
 CY 4.00 cm
 F1P 200.000 ppm
 F1 30108.65 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 10.00000 ppm/cm
 HZCM 1505.43237 Hz/cm

