Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Diacetyliminoxyl radical in oxidative functionalization of alkenes

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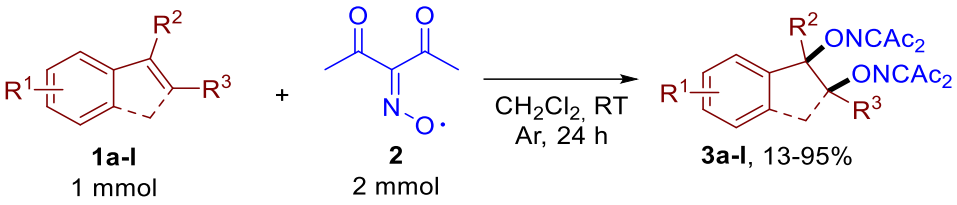
General

In all experiments RT stands for 22–25 °C. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AVANCE II 300 and Bruker Fourier 300HD (300.13 for ^{1}H and 75.47 MHz for ^{13}C, respectively) spectrometers in $CDCl_3$. Chemical shifts were reported in parts per million (ppm), and the residual solvent peak was used as an internal reference: ^{1}H ($CDCl_3$ δ = 7.26 ppm), ^{13}C ($CDCl_3$ δ = 77.16 ppm). Multiplicity was indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet). Coupling constants were reported in Hertz (Hz). FT-IR spectra were recorded on Bruker Alpha instrument. High resolution mass spectra (HR-MS) were measured on a Bruker maXis instrument using electrospray ionization (ESI). The measurements were performed in a positive ion mode (interface capillary voltage – 4500 V); mass range from m/z 50 to m/z 3000 Da; external calibration with Electrospray Calibrant Solution (Fluka). A syringe injection was used for all acetonitrile solutions (flow rate 3 μL/min). Nitrogen was applied as a dry gas; interface temperature was set at 180 °C. Gas chromatography-mass spectrometry (GC-MS) was performed on Chromatec crystal 5000 coupled with a quadrupole mass spectrometer (Chromatec MSD) with standard electron ionization (EI) at 70 eV (ion source temperature 200 °C, transfer line temperature, 250 °C) using a capillary low polarity column (5% phenyl / 95% dimethyl polysiloxane, length 30 m, inner diameter 0.25 mm, film thickness 0.25 μm). The inlet temperature was set at 250 °C, the helium flow rate was set at 1 mL/min. The initial column temperature was set at 70 °C; the heating rate was 25 °C/min to 250 °C.

Styrene 99.5%, 4-chlorostyrene 99%, 4-methoxystyrene 96%, α-methylstyrene 99%, β-methylstyrene 97%, 1,1-diphenylethylene 98%, *trans*-stilbene 96%, indene 90%, cyclopentene 95%, cyclohexene 99%, *cis*-cyclooctene 95%, 1,1,4,4-tetraphenyl-1,3-butadiene 99%, 2,5-dimethyl-2,4-hexadiene 96%, 2-methyl-1-pentene 99%, 2,4,4-trimethyl-1-pentene 96%, trifluoroacetic acid 99%, 4-dimethylaminopyridine 99%, 1,4-diazabicyclo[2.2.2]octane 97%, $Cu(hfac)_2 \cdot xH_2O$ 97% were used as is from commercial sources. CH_2Cl_2 was distilled prior to use. EtOAc were distilled over P_2O_5. [1-(Trifluoromethyl)vinyl]benzene and 2-methyl-1-phenyl-1-propene were synthesized according published procedures.[1,2] Anhydrous copper(II) hexafluoroacetylacetonate ($Cu(hfac)_2$) was prepared from corresponding hydrate by sublimation in vacuum at 120 ºC and subsequent storage over P_2O_5.[3] Preparation of diacetyliminoxyl radical is described earlier.[4] To a stirred solution of diacetyl oxime (258 mg, 2 mmol) in 4 mL of CH_2Cl_2 $Pb(OAc)_4$

(469 mg, 1.0 mmol) was added with vigorous stirring. Stirring was continued for 10 min, then the reaction mixture was chromatographed on silica gel using CH_2Cl_2 as eluent. The fraction corresponding to the dark-red spot was collected, so that the volume of the fraction was 50 mL. The solution of the diacetyliminoxyl radical **2** (2 mmol in 50 mL CH_2Cl_2) was rotary evaporated to 25 mL. Transfer of diacetyliminoxyl from CH_2Cl_2 to DMSO was achieved by the addition of 25 mL of DMSO to a solution of the diacetyliminoxyl in 25 mL of CH_2Cl_2 followed by water-jet vacuum evaporation of the latter. A MeCN solution of diacetyliminoxyl radical was prepared by threefold co-evaporation of the solution of diacetyliminoxyl radical in 25 mL of CH_2Cl_2 with acetonitrile (30 mL) to an approximate volume of 25 mL. For experiments under inert atmosphere, flasks with diacetyliminoxyl radical solutions were quickly evacuated (until the start of bubble formation) and then filled with argon three times using a three-way valve.

Reactions of diacetyliminoxyl radical 2 with vinylarenes 1a–l (experimental details for Tables 1–2)



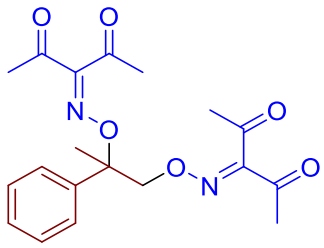
General procedure for Table 1: α-methylstyrene **1a** (1 mmol, 120 mg) in a solvent (2 mL), and an additive (1–2 mmol, 112–478 mg, except for additive-free experiments) were added under an argon atmosphere to the solution of diacetyliminoxyl **2** (2 mmol) in a solvent (25 mL). The resulting solution was stirred at 23–25 °C for 24 hours; then the reaction mixture was rotatory evaporated under a water-jet vacuum. In run 2 the reaction mixture was diluted with 20 mL of water and then extracted with CH_2Cl_2 (3x10 mL). The organic extracts were combined, washed with water (10 mL), and dried over Na_2SO_4 and rotatory evaporated under a water-jet vacuum. In run 6 the organic layer was separated and the aqueous layer was extracted with CH_2Cl_2 (2×10 mL), and all organic extracts were combined, dried over Na_2SO_4 and rotatory evaporated under a water-jet vacuum. The addition product **3a** was isolated by column chromatography on silica gel with CH_2Cl_2/EtOAc = 40/1 as eluent.

General procedure a for dioxyimination of vinylarenes 1a–l (experiments in Table 2 with note a): the solution of the diacetyliminoxyl radical **2** (2 mmol in 25 mL CH_2Cl_2) was

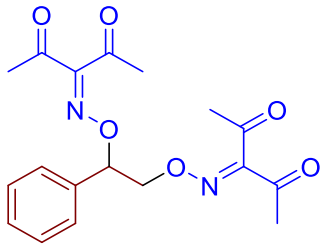
placed in a two-necked flask. Then vinylarenes **1a–l** (1 mmol, 104–358 mg) in CH_2Cl_2 (2 mL) were added. Reaction mixture was stirred for 24 hours at room temperature under an argon atmosphere, then rotary evaporated under a water-jet vacuum. Products **3a–l** were isolated by column chromatography on silica gel.

General procedure b (experiments in Table 2 with note b): The solution of the diacetyliminoxyl radical **2** (2 mmol in 25 mL CH_2Cl_2) was placed in a two-necked flask. Then β,β-dimethylstyrene **1f** (1 mmol, 132 mg) in CH_2Cl_2 (2 mL) was added. Reaction mixture was stirred for 3 hours at room temperature under an argon atmosphere, then diluted with solution of $Na_2S_2O_4$ (200 mg in 20 mL of water) and shaken. The organic layer was separated, dried over $MgSO_4$, and rotary evaporated under water-jet vacuum.

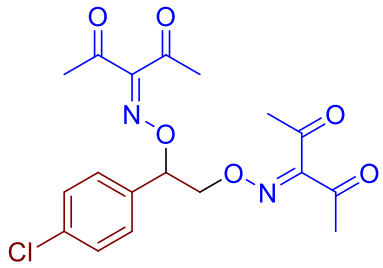
General procedure c (experiments in Table 2 with note c): The solution of the diacetyliminoxyl radical **2** (2 mmol in 25 mL CH_2Cl_2) was placed in a two-necked flask wrapped in foil to prevent light exposure. Then β,β-dimethylstyrene **1f** (1 mmol, 132 mg)) in CH_2Cl_2 (2 mL) was added. Reaction mixture was stirred for 3 hours at room temperature under an argon atmosphere, then diluted with solution of $Na_2S_2O_4$ (200 mg in 20 mL of water) and shaken. The organic layer was separated, dried over $MgSO_4$, and rotary evaporated under water-jet vacuum.



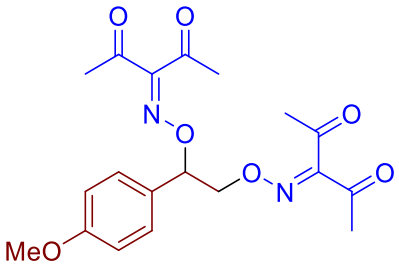
3,3'-(((2-Phenylpropane-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione) 3a, was isolated as yellow oil (33%, 125 mg, 0.333 mmol, purified by column chromatography with CH_2Cl_2/EtOAc = 40/1 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ 7.42–7.23 (m, 5H), 4.62 (s, 2H), 2.35 (s, 3H), 2.28 (s, 3H), 2.26 (s, 3H), 2.14 (s, 3H), 1.78 (s, 3H). **^{13}C{^{1}H} NMR** (75.47 MHz, $CDCl_3$): δ 198.5, 198.0, 194.3, 194.1, 156.6, 156.0, 140.6, 128.6, 128.2, 125.9, 86.5, 81.3, 30.6, 30.3, 25.7, 25.5, 22.3. **FTIR** (KBr): ν_{max} = 1727, 1689, 1597, 1420, 1364, 1302, 1196, 1033, 1007, 968, 734, 702. **HRMS** (ESI-TOF) *m/z*: [M+K$^+$] calcd. for $C_{19}H_{22}N_2O_6$+K$^+$ 413.1109; found 413.1101.



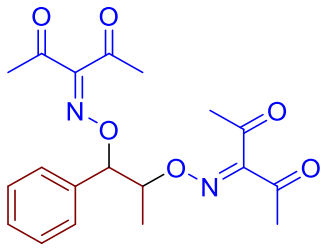
3,10-Diacetyl-6-phenyl-5,8-dioxa-4,9-diazadodeca-3,9-diene-2,11-dione 3b, was isolated as yellow solid (14%, 50 mg, 0.138 mmol, purified by column chromatography with CH_2Cl_2/EtOAc = 40/1 as eluent). Mp = 76–77 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ 7.43–7.35 (m, 3H), 7.32–7.27 (m, 2H), 5.57 (dd, *J* = 8.2, 3.9 Hz, 1H), 4.63 (dd, *J* = 12.4, 8.2 Hz, 1H), 4.53 (dd, *J* = 12.4, 3.9 Hz, 1H), 2.37 (s, 3H), 2.33 (s, 3H), 2.31 (s, 3H), 2.25 (s, 3H). **^{13}C{^{1}H} NMR** (75.47 MHz, $CDCl_3$): δ 198.03, 197.98, 194.20, 194.15, 156.8, 156.5, 136.0, 129.2, 129.0, 126.9, 86.1, 77.8, 30.7. 30.6, 25.8. **FTIR** (KBr): ν_{max} = 1728, 1685, 1595, 1364, 1299, 1039, 1020, 977, 764, 705, 548. **HRMS** (ESI-TOF) *m/z*: [M+NH_4^+] calcd. for $C_{18}H_{20}N_2O_6$+NH_4^+ 378.1660; found 378.1654.



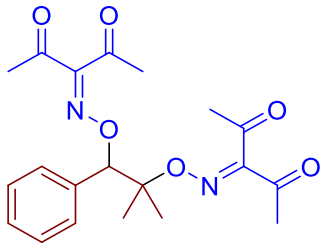
3,10-Diacetyl-6-(4-chlorophenyl)-5,8-dioxa-4,9-diazadodeca-3,9-diene-2,11-dione 3c, was isolated as white solid (13%, 51 mg, 0.129 mmol, purified by column chromatography with CH_2Cl_2/EtOAc = 40/1 as eluent). Mp = 105–106 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ 7.38 (d, *J* = 8.2 Hz, 2H), 7.23 (d, *J* = 8.2 Hz, 2H), 5.59–5.46 (m, 1H), 4.65–4.44 (m, 2H), 2.37 (s, 3H), 2.32 (s, 3H), 2.31 (s, 3H), 2.26 (s, 3H). **^{13}C{^{1}H} NMR** (75.47 MHz, $CDCl_3$): δ 197.72, 197.68, 194.0, 157.1, 156.7, 135.2, 134.6, 129.3, 128.4, 110.2, 85.3, 30.62, 30.58, 25.75, 25.74. **FTIR** (KBr): ν_{max} = 1729, 1685, 1597, 1367, 1298, 1197, 1088, 1041, 1022, 973, 838. **HRMS** (ESI-TOF) *m/z*: [M+Na^+] calcd. for $C_{18}H_{19}ClN_2O_6$+Na^+ 417.0824; found 417.0821.



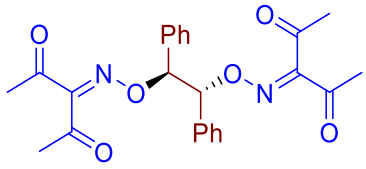
3,10-Diacetyl-6-(4-methoxyphenyl)-5,8-dioxa-4,9-diazadodeca-3,9-diene-2,11-dione 3d, was isolated as pale-yellow solid (32%, 125 mg, 0.32 mmol, purified by column chromatography with PE/EtOAc = 5/2 as eluent). Mp = 103–104 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ 7.22 (d, *J* = 8.5 Hz, 2H), 6.91 (d, *J* = 8.5 Hz, 2H), 5.50 (dd, *J* = 8.2, 3.8 Hz, 1H), 4.62 (dd, *J* = 12.3, 8.2 Hz, 1H), 4.50 (dd, *J* = 12.3, 3.8 Hz, 1H), 3.80 (s, 3H), 2.37 (s, 3H), 2.30 (s, 6H), 2.24 (s, 3H). **^{13}C{^{1}H} NMR** (75.47 MHz, $CDCl_3$): δ 198.0, 197.9, 194.2, 194.1, 160.3, 156.7, 156.5, 128.4, 128.0, 114.4, 85.7, 77.7, 55.4, 30.6, 30.5, 25.71, 25.70. **FTIR** (KBr): ν_{max} = 1729, 1684, 1612, 1599, 1517, 1367, 1300, 1249, 1037, 1018, 969, 624, 559. **HRMS** (ESI-TOF) *m/z*: [M+Na^+] calcd. for $C_{19}H_{22}N_2O_7$+Na^+ 413.1319; found 413.1309.



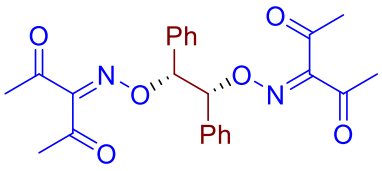
3,3'-(((1-Phenylpropane-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione) (mixture of diastereomers 1.7:1) 3e, was isolated as colorless oil (86%, 321 mg, 0.857 mmol, purified by column chromatography with PE/EtOAc = 5/2 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ 7.42–7.32 (m, 3H), 7.26–7.20 (m, 2H), 5.46 (d, *J* = 4.4 Hz, 0.63H), 5.32 (d, *J* = 7.6 Hz, 0.37H), 4.82–4.70 (m, 1H), 2.36 (s, 1.1H), 2.35 (s, 1.9H), 2.34 (s, 1.9H), 2.30 (s, 1.1H), 2.29 (s, 1.9H), 2.27 (s, 1.1H), 2.26 (s, 1.1H), 2.16 (s, 1.9H), 1.29 (d, *J* = 6.7 Hz, 1.9H), 1.18 (d, *J* = 6.7 Hz, 1.1H). **^{13}C{^{1}H} NMR** (75.47 MHz, $CDCl_3$): δ 198.4, 198.2, 198.1, 198.0, 194.28, 194.26, 194.22, 194.20, 156.8, 156.6, 156.2, 156.1, 136.50, 136.45, 136.3, 129.1, 128.9, 128.7, 127.5, 127.2, 90.0, 88.9, 83.9, 83.7, 30.61, 30.58, 30.5, 25.74, 25.72, 25.69, 16.40, 14.8. **FTIR** (KBr): ν_{max} = 1727, 1689, 1597, 1419, 1364, 1301, 1197, 1086, 1054, 1001, 703. **HRMS** (ESI-TOF) *m/z*: [M+NH_4^+] calcd. for $C_{19}H_{22}N_2O_6$+NH_4^+ 392.1816; found 392.1815.



3,3'-(((2-Methyl-1-phenylpropane-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione) 3f, was isolated as colorless oil (93%, 362 mg, 0.931 mmol, purified by column chromatography with CH_2Cl_2/EtOAc = 20/1 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ 7.40–7.31 (m, 3H), 7.26–7.19 (m, 2H), 5.44 (s, 1H), 2.40 (s, 3H), 2.36 (s, 3H), 2.25 (s, 3H), 2.22 (s, 3H), 1.40 (s, 3H), 1.33 (s, 3H). **^{13}C{^{1}H} NMR** (75.47 MHz, $CDCl_3$): δ 198.5, 198.0, 194.3, 194.1, 156.7, 156.0, 136.5, 128.7, 128.3, 128.0, 91.8, 85.9, 30.6, 25.8, 25.6, 23.1, 22.0. **FTIR** (KBr): ν_{max} = 1727, 1693, 1366, 1301, 1195, 979, 755, 704. **HRMS** (ESI-TOF) *m/z*: [M+NH_4^+] calcd. for $C_{20}H_{24}N_2O_6$+NH_4^+ 406.1973; found 406.1967.

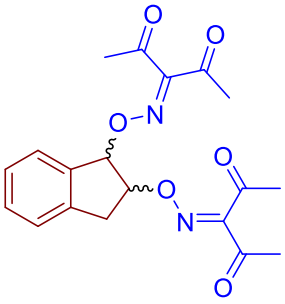


***anti*-3,10-Diacetyl-6,7-diphenyl-5,8-dioxa-4,9-diazadodeca-3,9-diene-2,11-dione 3g-*anti*,** pale-yellow solid (33%, 142 mg, 0.325 mmol, purified by column chromatography with CH_2Cl_2/EtOAc = 66/1 as eluent). Mp = 114–116 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ 7.37–7.28 (m, 6H), 7.16–7.05 (m, 4H), 5.59 (s, 2H), 2.24 (s, 6H), 2.19 (s, 6H). **^{13}C{^{1}H} NMR** (75.47 MHz, $CDCl_3$): δ 198.0, 194.2, 156.7, 135.7, 128.9, 128.5, 127.8, 89.1, 30.5, 25.7. **FTIR** (KBr): ν_{max} = 1722, 1692, 1301, 996, 739, 695. **HRMS** (ESI-TOF) *m/z*: [M+Na^+] calcd. for $C_{24}H_{24}N_2O_6$+Na^+ 459.1527; found 459.1525. Single crystal X-Ray analysis is available (see Fig. S1, page S18).

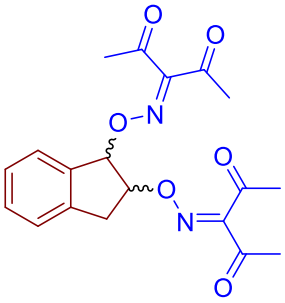


syn*-3,10-Diacetyl-6,7-diphenyl-5,8-dioxa-4,9-diazadodeca-3,9-diene-2,11-dione 3g-*syn, pale-yellow oil (32%, 140 mg, 0.32 mmol, purified by column chromatography with CH_2Cl_2/EtOAc = 66/1 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ 7.31–7.21 (m, 6H), 7.11–

6.98 (m, 4H), 5.64 (s, 2H), 2.34 (s, 6H), 2.31 (s, 6H). **$^{13}C\{^{1}H\}$ NMR** (75.47 MHz, $CDCl_3$): δ 198.1, 194.2, 156.5, 135.8, 128.8, 128.5, 127.6, 89.7, 30.6, 25.7. **FTIR** (KBr): ν_{max} = 1726, 1690, 1363, 1291, 1076, 998, 964, 736, 701. **HRMS** (ESI-TOF) *m/z*: [M+Na^+] calcd. for $C_{24}H_{24}N_2O_6$+Na^+ 459.1527; found 459.1525.

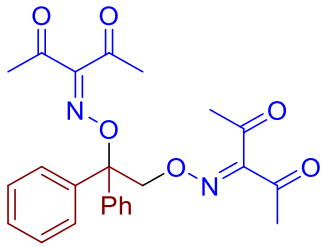


3,3'-(((2,3-Dihydro-1H-indene-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione)-1-*major* 3i-*major*, pale yellow oil (26%, 95 mg, 0.255 mmol, purified by column chromatography with $CHCl_3$/EtOAc = 40/1 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ 7.44–7.21 (m, 4H), 5.90 (d, *J* = 3.4 Hz, 1H), 5.26 (ddd, *J* = 7.4, 4.5, 3.4 Hz, 1H), 3.51 (dd, *J* = 16.9, 7.4 Hz, 1H), 3.12 (dd, *J* = 16.9, 4.5 Hz, 1H), 2.39 (s, 6H), 2.29 (s, 3H), 2.27 (s, 3H). **$^{13}C\{^{1}H\}$ NMR** (75.47 MHz, $CDCl_3$): δ 197.9, 194.1, 156.8, 140.7, 137.2, 130.3, 127.8, 125.7, 125.3, 92.0, 89.7, 36.2, 30.7, 25.8, 25.7. **FTIR** (KBr): ν_{max} = 2925, 1727, 1693, 1599, 1420, 1362, 1300, 1195, 1082, 1001, 962, 766, 733. **HRMS** (ESI-TOF) *m/z*: [M+NH_4^+] calcd. for $C_{19}H_{20}N_2O_6$+NH_4^+ 390.1660; found 390.1663.

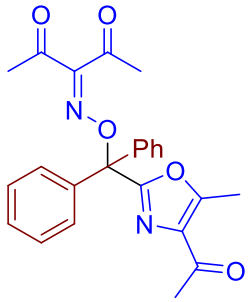


3,3'-(((2,3-Dihydro-1H-indene-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione)-2-*minor* 3i-*minor*, pale yellow oil (14%, 53 mg, 0.142 mmol, purified by column chromatography with $CHCl_3$/EtOAc = 40/1 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ 7.45–7.27 (m, 4H), 5.83 (d, *J* = 5.2 Hz, 1H), 5.34–5.19 (m, 1H), 3.38–3.14 (m, 2H), 2.38 (s, 3H), 2.36 (s, 3H), 2.21 (s, 6H). **$^{13}C\{^{1}H\}$ NMR** (75.47 MHz, $CDCl_3$): δ 197.9, 194.0, 156.5, 156.4, 140.2, 137.1, 130.5, 127.8, 126.2, 125.3, 87.1, 85.4, 35.6, 30.5, 25.63, 25.60. **FTIR** (KBr):

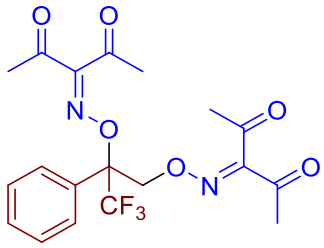
ν_{max} = 1723, 1689, 1359, 1306, 998, 977, 964, 745. **HRMS** (ESI-TOF) *m/z*: [M+Na^+] calcd. for $C_{19}H_{20}N_2O_6$+Na^+ 395.1214; found 395.1209.



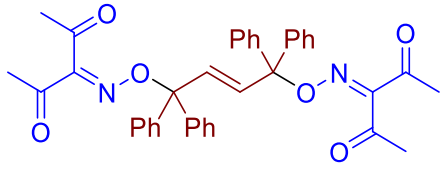
3,10-Diacetyl-6,6-diphenyl-5,8-dioxa-4,9-diazadodeca-3,9-diene-2,11-dione 3j, was isolated as yellow oil (56%, 244 mg, 0.559 mmol, purified by PTLC with PE/EtOAc = 5/2 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ 7.44–7.31 (m, 6H), 7.30–7.21 (m, 4H), 5.28 (s, 2H), 2.41, (s, 3H), 2.21 (s, 6H), 2.01 (s, 3H). **^{13}C{^{1}H} NMR** (75.47 MHz, $CDCl_3$): δ 198.3, 197.9, 194.1, 194.0, 156.8, 156.1, 140.4, 128.5, 128.4, 127.3, 89.1, 79.7, 30.6, 30.2, 25.7, 25.5. **FTIR** (KBr): ν_{max} = 1724, 1690, 1598, 1448, 1420, 1361, 1300, 1195, 1090, 1030, 963, 919, 738, 107, 622. **HRMS** (ESI-TOF) *m/z*: [M+Na^+] calcd. for $C_{24}H_{24}N_2O_6$+Na^+ 459.1527; found 459.1524.



3-(((4-Acetyl-5-methyloxazol-2-yl)diphenylmethoxy)imino)pentane-2,4-dione 3j', was isolated as white solid (17%, 71 mg, 0.169 mmol, purified by PTLC with PE/EtOAc = 5/2 as eluent). Mp = 127–129 ºC. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ 7.48–7.28 (m, 10H), 2.60 (s, 3H), 2.53 (s, 3H), 2.47 (s, 3H), 2.13 (s, 3H). **^{13}C{^{1}H} NMR** (75.47 MHz, $CDCl_3$): δ 198.1, 195.1, 194.2, 159.9, 156.7, 155.4, 139.8, 134.9, 128.8, 128.4, 128.0, 89.1, 30.5, 28.0, 25.8, 12.5. **FTIR** (KBr): ν_{max} = 1725, 1690, 1600, 1447, 1421, 1361, 1296, 1190, 1078, 1012, 958, 908, 755, 700, 636. **HRMS** (ESI-TOF) *m/z*: [M+NH_4^+] calcd. for $C_{24}H_{22}N_2O_5$+NH_4^+ 436.1867; found 436.1860. Single crystal X-Ray analysis is available (see Fig. S2, page S20).

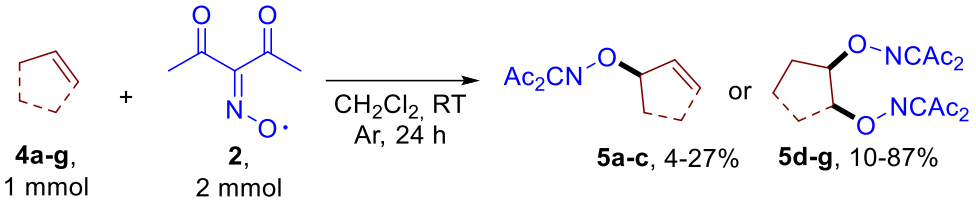


3,3'-(((3,3,3-Trifluoro-2-phenylpropane-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione 3k, was isolated as white gum (16%, 68 mg, 0.158 mmol, purified by PTLC with PE/EtOAc = 10/1 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ 7.46–7.36 (m, 5H), 5.21 (d, *J* = 12.8 Hz, 1H), 4.99 (d, *J* = 12.8 Hz, 1H), 2.41 (s, 3H), 2.32 (s, 3H), 2.29 (s, 3H), 2.04 (s, 3H). **^{13}C{^{1}H} NMR** (75.47 MHz, $CDCl_3$): δ 197.4, 197.2, 193.7, 193.6, 157.6, 156.6, 131.8, 129.9, 128.9, 126.9, 123.44 (q, *J* = 287.5 Hz), 86.57 (q, *J* = 27.9 Hz), 74.9, 30.5, 30.1, 25.9, 25.6. **FTIR** (KBr): ν_{max} = 1728, 1691, 1365, 1297, 1270, 1187, 1098, 1062, 1038, 952, 702. **HRMS** (ESI-TOF) *m/z*: [M+Na^{+}] calcd. for $C_{19}H_{19}F_3N_2O_6$+Na^{+} 451.1087; found 451.1072.

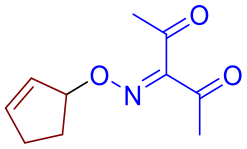


(E)-3,12-Diacetyl-6,6,9,9-tetraphenyl-5,10-dioxa-4,11-diazatetradeca-3,7,11-triene-2,13-dione 3l, was isolated as pale-yellow solid (92%, 565 mg, 0.919 mmol, purified by column chromatography with CH_2Cl_2/EtOAc = 40/1 as eluent). Mp = 157–159 ºC. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ 7.54–7.10 (m, 20H), 6.27 (s, 2H), 2.39 (s, 6H), 2.09 (s, 6H). **^{13}C{^{1}H} NMR** (75.47 MHz, $CDCl_3$): δ 198.5, 194.3, 156.4, 141.9, 137.1, 128.3, 128.2, 128.0, 91.5, 30.5, 25.6. **FTIR** (KBr): ν_{max} = 1723, 1689, 1360, 1301, 958, 911, 756, 702. **HRMS** (ESI-TOF) *m/z*: [M+Na^{+}] calcd. for $C_{38}H_{34}N_2O_6$+Na^{+}: 637.2309; found 637.2303. Single crystal X-Ray analysis is available (see Fig. S3, page S22).

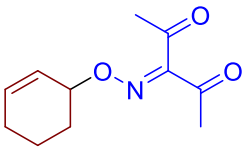
Reactions of diacetyliminoxyl radical with aliphatic alkenes 4a–g (experimental details for Table 3)



General procedure for dioxyimination of aliphatic alkenes 4a–g (experiment details for Table 2): the solution of the diacetyliminoxyl radical **2** (2 mmol in 25 mL CH_2Cl_2) was placed in a two-necked flask. Then alkenes **4a–g** (1 mmol, 68–118 mg) in 2 mL of CH_2Cl_2 were added. Reaction mixture was stirred for 24 hours at room temperature under an argon atmosphere, after that reaction mixture was rotary evaporated under a water-jet vacuum. The allylic hydrogen substitution or addition products **5a–g** were isolated by column chromatography on silica gel.

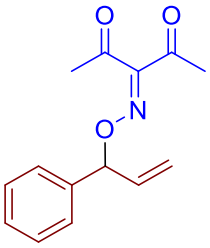


3-((Cyclopent-2-en-1-yloxy)imino)pentane-2,4-dione 5a, was isolated as a colorless liquid (18%, 35 mg, 0.179 mmol, purified by column chromatography with EtOAc/PE = 1/5 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ 6.23–6.10 (m, 1H), 5.94–5.81 (m, 1H), 5.50–5.35 (m, 1H), 2.61–2.44 (m, 1H), 2.37 (s, 3H), 2.33–2.28 (m, 2H), 2.28 (s, 3H), 2.01–1.89 (m, 1H). **^{13}C{^{1}H} NMR** (75.48 MHz, $CDCl_3$): δ 198.9, 194.7, 155.9, 139.3, 129.0, 92.1, 31.4, 30.7, 29.3, 25.6; **FTIR** (KBr): ν_{max} = 1725, 1688, 1592, 1421, 1363, 1302, 1195, 1030, 978, 737 cm^{-1}. **HRMS** (ESI-TOF) *m/z*: [M+Na^+] calcd. for $C_{10}H_{13}NO_3$+Na^+ 218.0788; found 218.0792.

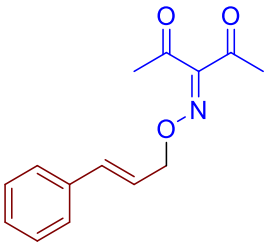


3-((Cyclohex-2-en-1-yloxy)imino)pentane-2,4-dione 5b, was isolated as a pale yellow oil (27%, 57 mg, 0.272 mmol, purified by column chromatography with CH_2Cl_2 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ 6.14–5.89 (m, 1H), 5.88–5.66 (m, 1H), 4.76 (s, 1H), 2.38 (s, 3H), 2.30 (s, 3H), 2.18–1.97 (m, 2H), 1.97–1.80 (m, 2H), 1.76–1.54 (m, 2H). **^{13}C{^{1}H}**

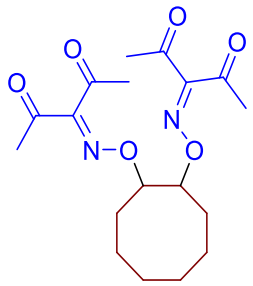
NMR (75.48 MHz, $CDCl_3$): δ 198.8, 194.6, 155.9, 133.9, 124.9, 79.7, 30.7, 28.1, 25.7, 25.1, 18.6. **FTIR** (KBr): ν_{max} = 1725, 1688, 1363, 1302, 982 cm^{-1}. **HRMS** (ESI-TOF) *m/z*: [M+Na^+] calcd. for $C_{11}H_{15}NO_3$+Na^+ 232.0944; found 232.0943.



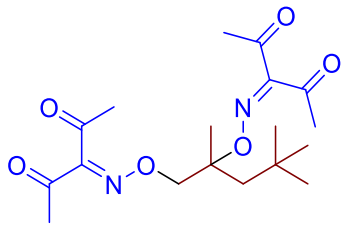
3-(((1-Phenylallyl)oxy)imino)pentane-2,4-dione 5c, was isolated as colorless oil (13%, 31 mg, 0.126 mmol, purified by PTLC with PE/EtOAc = 10/1 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ 7.40–7.28 (m, 5H), 6.10 (ddd, *J* = 17.0, 10.6, 6.3 Hz, 1H), 5.72 (d, *J* = 6.3 Hz, 1H), 5.34 (d, *J* = 10.6 Hz, 1H), 5.30 (d, *J* = 17.0 Hz, 1H), 2.34 (s, 3H), 2.33 (s, 3H). **^{13}C{^{1}H} NMR** (75.47 MHz, $CDCl_3$): δ 198.5, 194.5, 156.3, 138.6, 136.1, 128.8, 128.6, 127.4, 118.7, 88.9, 30.7, 25.8. **FTIR** (KBr): ν_{max} = 1726, 1688, 1363, 1300, 1195, 1108, 1072, 988, 701, 468. **HRMS** (ESI-TOF) *m/z*: [M+NH_4^+] calcd. for $C_{14}H_{15}NO_3$+NH_4^+ 263.1390; found 263.1391.



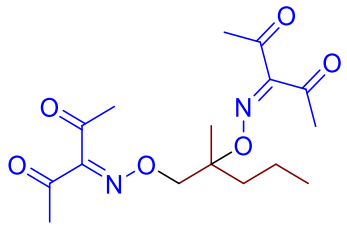
3-((Cinnamyloxy)imino)pentane-2,4-dione 5c', was isolated as colorless oil (4%, 9 mg, 0.037 mmol, purified by PTLC with PE/EtOAc = 10/1 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ 7.44–7.27 (m, 5H), 6.67 (d, *J* = 15.8 Hz, 1H), 6.33 (dt, *J* = 15.8, 6.5 Hz, 1H), 4.90 (d, J = 6.5 Hz, 2H), 2.40 (s, 3H), 2.34 (s, 3H). **^{13}C{^{1}H} NMR** (75.47 MHz, $CDCl_3$): δ 198.6, 194.5, 156.2, 136.1, 135.3, 128.8, 128.5, 126.9, 123.2, 77.6, 30.8, 25.8. **FTIR** (KBr): ν_{max} = 2923, 1726, 1685, 1364, 1299, 1195, 1094, 993, 967. **HRMS** (ESI-TOF) *m/z*: [M+Na^+] calcd. for $C_{14}H_{15}NO_3$+Na^+ 268.0944; found 268.0951.



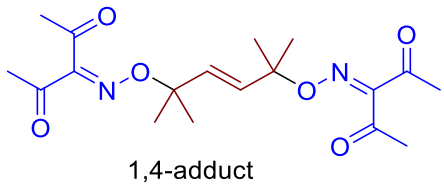
3,3'-((Cyclooctane-1,2-diylbis(oxy))bis(azanylylidene))bis(pentane-2,4-dione) 5d, was isolated as yellow oil (18%, 65 mg, 0.177 mmol, purified by column chromatography with PE/EtOAc = 4/1 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ 4.75–4.64 (m, 1H), 4.59–4.53 (m, 1H), 2.34 (s, 6H), 2.24 (s, 6H), 2.10–1.78 (m, 4H), 1.74–1.49 (m, 6H), 1.49–1.28 (m, 2H). **^{13}C{^{1}H} NMR** (75.47 MHz, $CDCl_3$): δ = 198.4, 198.3, 194.3, 156.04, 156.01, 88.3, 86.5, 30.5, 30.4, 28.8, 28.3, 26.2, 25.61, 25.58, 25.53, 24.5, 22.6. **FTIR** (KBr): ν_{max} = 2929, 1728, 1684, 1419, 1363, 1302, 985. **HRMS** (ESI-TOF) *m/z*: [M+NH_4^+] calcd. for $C_{18}H_{26}N_2O_6$+NH_4^+ 384.2129; found 384.2127.



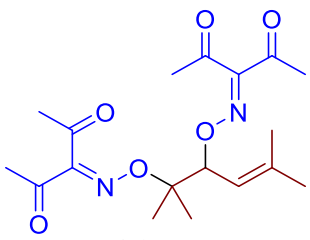
3,3'-(((2,4,4-Trimethylpentane-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione) 5e, was isolated as white gum (14%, 51 mg, 0.138 mmol, purified by PTLC with PE/EtOAc = 4/1 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ 4.42 (d, *J* = 11.7 Hz, 1H), 4.36 (d, *J* = 11.7 Hz, 1H), 2.39 (s, 3H), 2.34 (s, 3H), 2.30 (s, 3H), 2.26 (s, 3H), 1.81 (d, *J* = 15.2 Hz, 1H), 1.60 (d, *J* = 15.2 Hz, 1H), 1.45 (s, 3H), 0.99 (s, 9H). **^{13}C{^{1}H} NMR** (75.47 MHz, $CDCl_3$): δ 198.7, 198.1, 194.4, 194.2, 156.2, 155.7, 86.8, 81.3, 47.7, 31.6, 31.1, 30.60, 30.55, 25.7, 25.6, 21.9. **FTIR** (KBr): ν_{max} = 2955, 1727, 1688, 1365, 1302, 1196, 1082, 1033, 977. **HRMS** (ESI-TOF) *m/z*: [M+H^+] calcd. for $C_{18}H_{28}N_2O_6$+H^+ 369.2020; found 369.2017.



3,3'-(((2-Methylpentane-1,2-diyl)bis(oxy))bis(*azanylylidene*))bis(pentane-2,4-dione) 5f, was isolated as colorless oil (10%, 33 mg, 0.096 mmol, purified by PTLC with PE/EtOAc = 4/1 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ 4.45–4.32 (m, 2H), 2.39 (s, 3H), 2.35 (s, 3H), 2.29 (s, 3H), 2.27 (s, 3H), 1.68–1.59 (m, 2H), 1.42–1.29 (m, 5H), 0.93 (t, *J* = 7.3 Hz, 2H). **^{13}C{^{1}H} NMR** (75.47 MHz, $CDCl_3$): δ 198.5, 198.1, 194.3, 194.2, 156.2, 156.0, 85.6, 80.0, 38.0, 30.59, 30.57, 25.7, 25.60, 20.4, 16.6, 14.6. **FTIR** (KBr): ν_{max} = 2693, 1727, 1693, 1365, 1301, 1195, 1083, 1029, 967. **HRMS** (ESI-TOF) *m/z*: [M+K^+] calcd. for $C_{16}H_{24}N_2O_6$+K^+ 379.1266; found 379.1275.



1,4-adduct

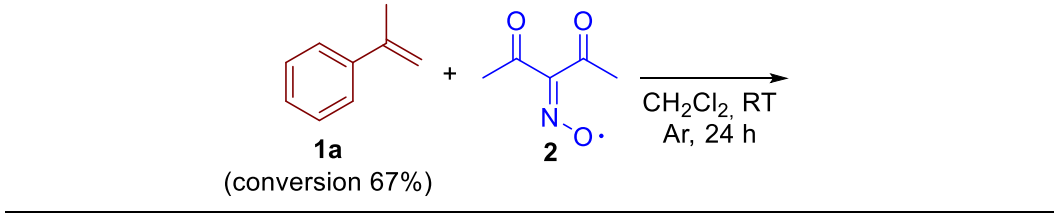


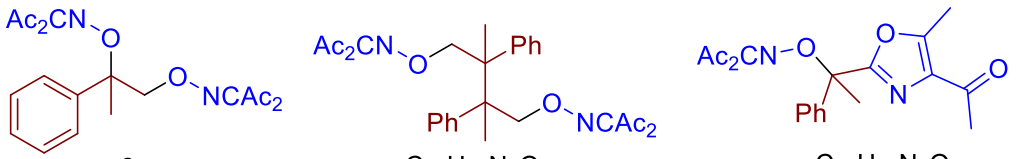
1,2-adduct

(E)-3,3'-(((2,5-Dimethylhex-3-ene-2,5-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione)-1-*major* and 3,3'-(((2,5-dimethylhex-4-ene-2,3-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione)-2-*minor* (mixture of regioisomers 1.75:1) 5g, was isolated as yellow oil (87%, 319 mg, 0.87 mmol, purified by column chromatography with CH_2Cl_2/EtOAc = 40/1 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): *major 1,4-isomer*: δ 5.77 (s, 2H), 2.34 (s, 6H), 2.28 (s, 6H), 1.44 (s, 12H); *minor 1,2-isomer*: δ 5.21 (d, *J* = 10.0 Hz, 1H), 5.14 (d, *J* = 10.0 Hz, 1H), 2.39 (s, 3H), 2.32 (s, 3H), 2.26 (s, 3H), 2.24 (s, 3H), 1.79 (s, 3H), 1.78 (s, 3H), 1.36 (s, 3H), 1.33 (s, 3H). **^{13}C{^{1}H} NMR** (75.47 MHz, $CDCl_3$): δ 198.7, 198.5, 198.3, 194.44, 194.29, 194.22, 155.82, 155.78, 141.1, 134.0, 119.1, 87.0, 86.0, 83.8, 30.62, 30.50, 30.49, 26.3, 26.0, 25.67, 25.57, 25.47, 22.8, 21.7, 18.9. **FTIR** (KBr): ν_{max} = 2986, 2937, 1726, 1688, 1297, 1192, 1070, 929, 550. **HRMS** (ESI-TOF) *m/z*: [M+NH_4^+] calcd. for $C_{18}H_{26}N_2O_6$+NH_4^+ 384.2129; found 384.2130.

Investigation of the reaction possible side products with α-methylstyrene 1a, styrene 1b and cyclopentene 4a

*Reaction with α-methylstyrene **1a**:* the solution of the diacetyliminoxyl radical **2** (2 mmol in 25 mL CH_2Cl_2) was placed in a two-necked flask. Then α-methylstyrene **1a** (1 mmol, 120 mg) in CH_2Cl_2 (2 mL) was added and the reaction mixture was stirred for 24 hours at room temperature under an argon atmosphere. 1,1,2,2-Tetrachloroathane was added as an internal standard, and then the crude reaction mixture was analyzed using ^{1}H NMR spectroscopy. The reaction mixture was rotary evaporated under a water-jet vacuum and analyzed employing HRMS and GC-MS.

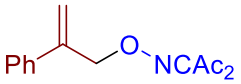




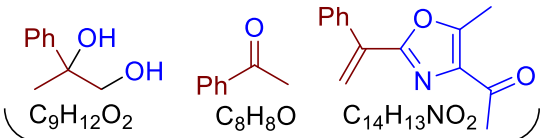
3a
isolated, 33%

$C_{28}H_{32}N_2O_6$
detected by HRMS*

$C_{19}H_{20}N_2O_5$
detected by HRMS*

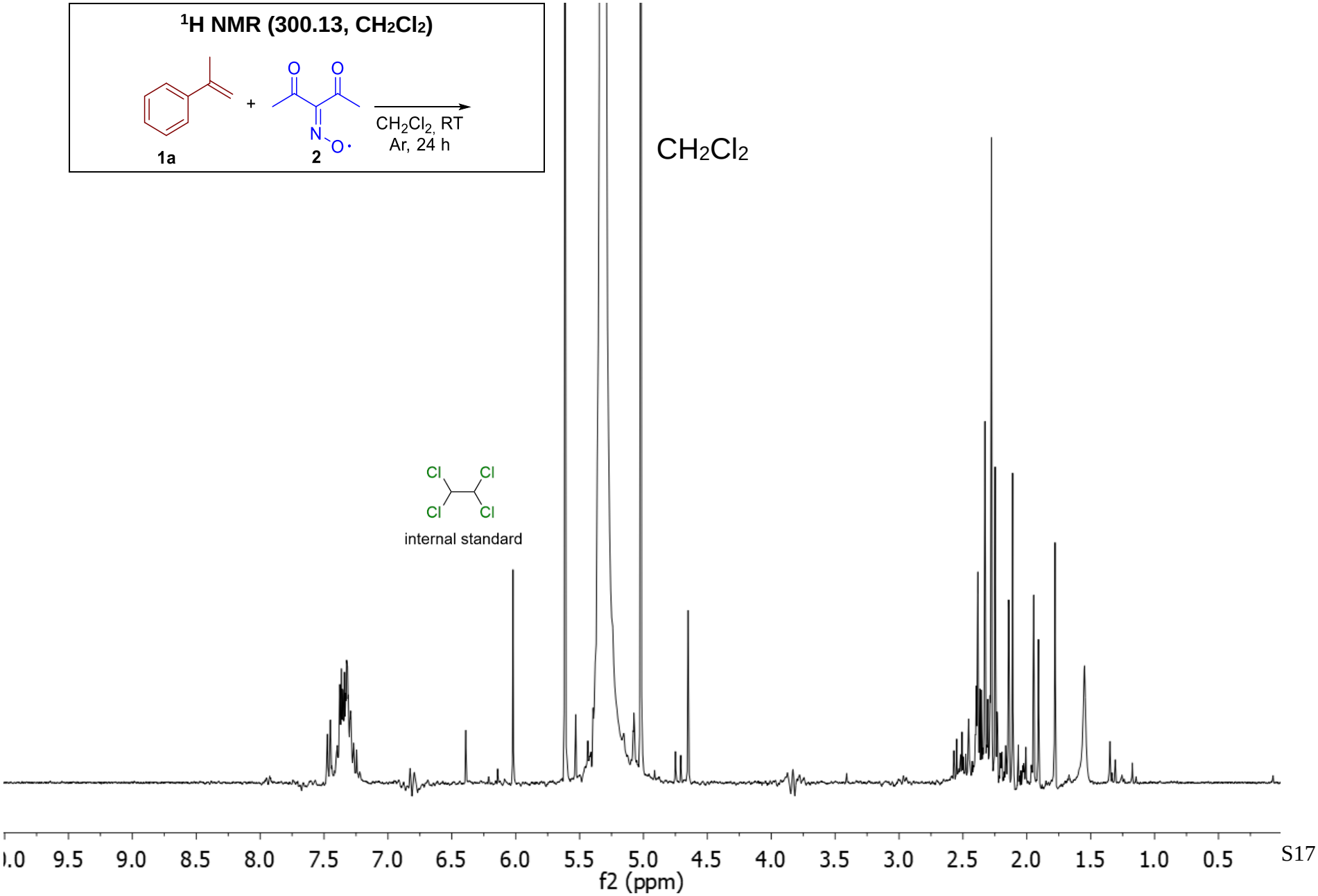


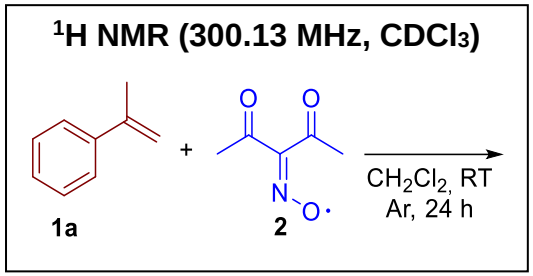
$C_{14}H_{15}NO_3$
detected by HRMS, GC-MS*
isolated, ~ 3%



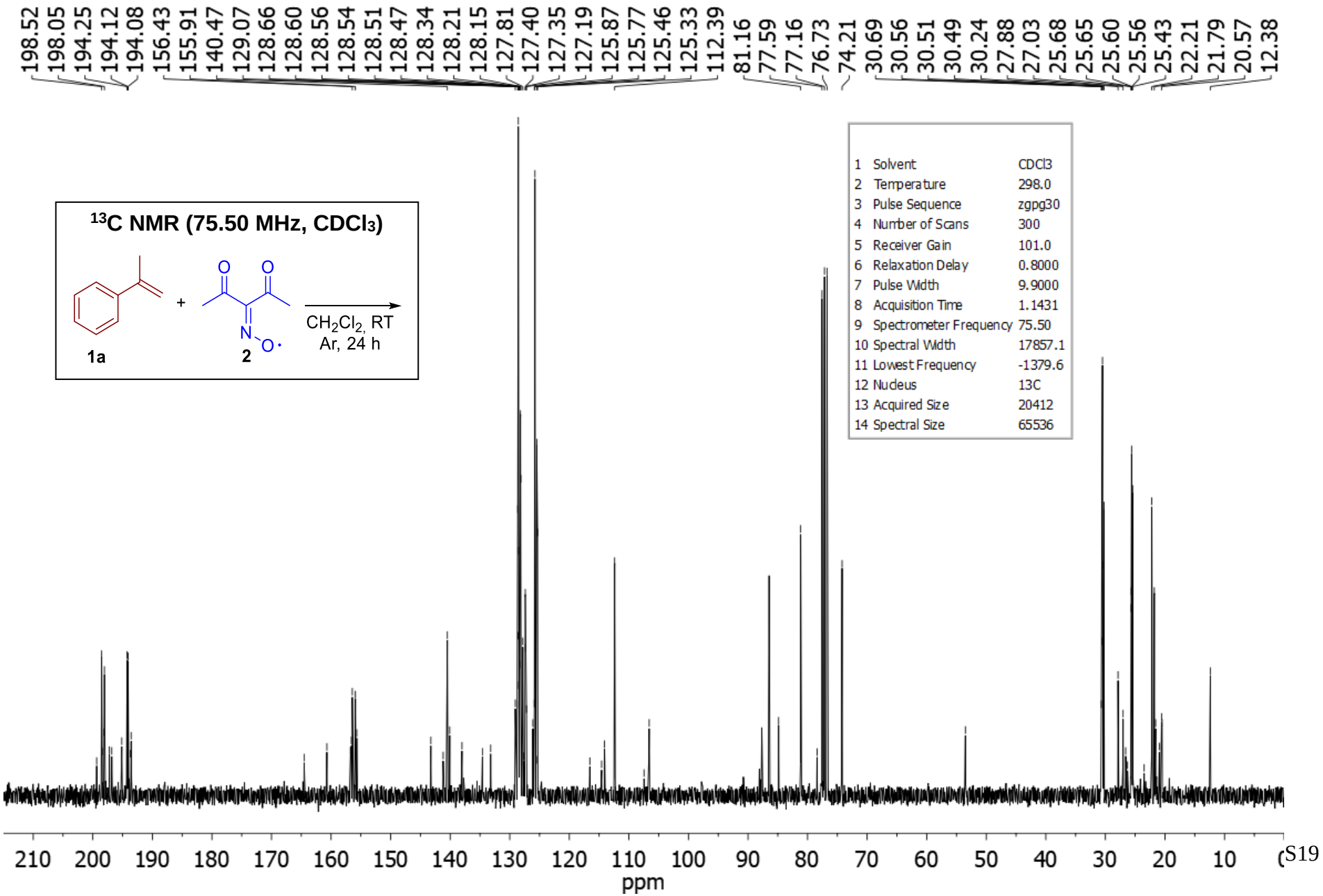
$C_9H_{12}O_2$ C_8H_8O $C_{14}H_{13}NO_2$
detected by GC-MS*

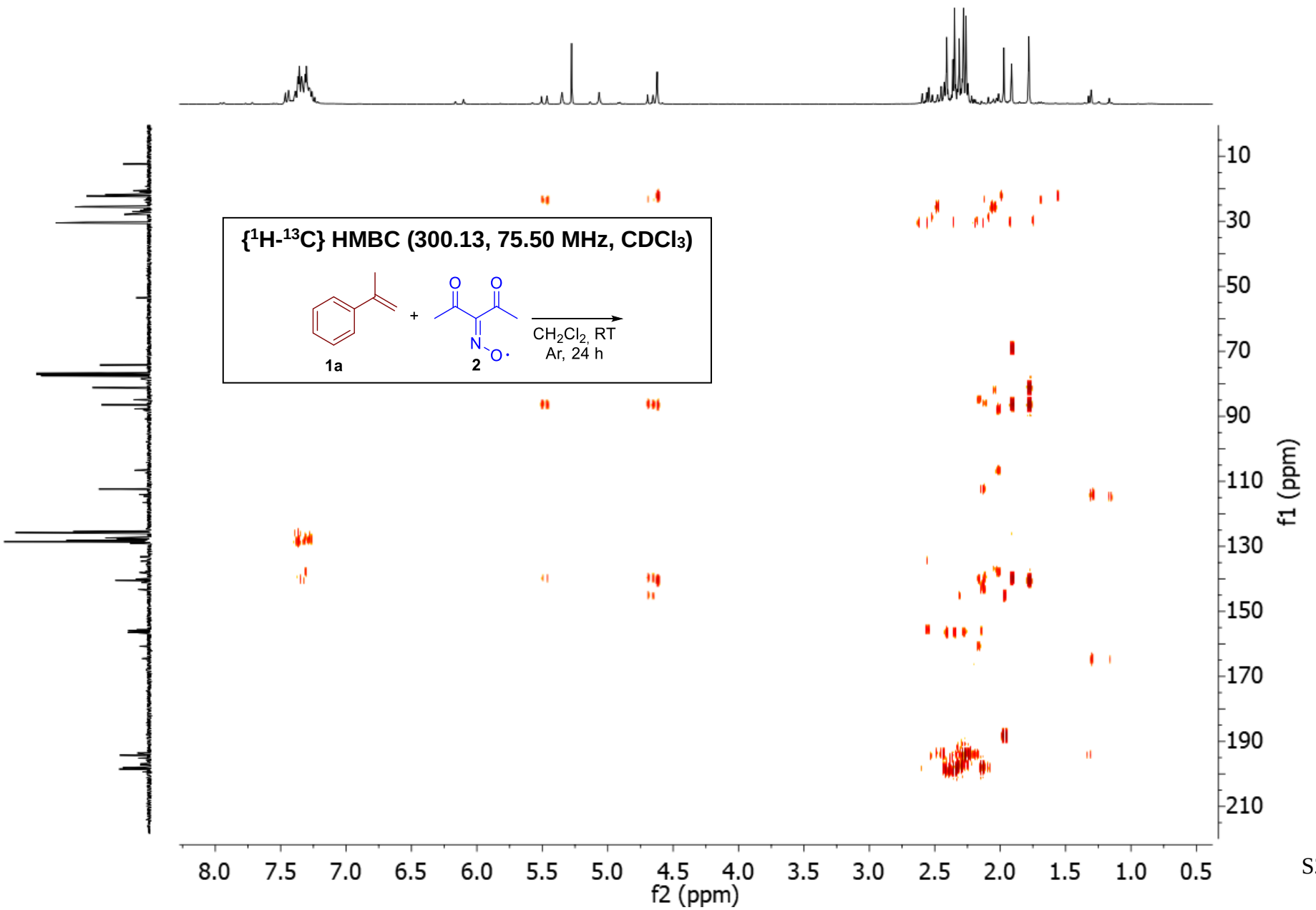
***Possible structures proposed based on HRMS and GC-MS data**

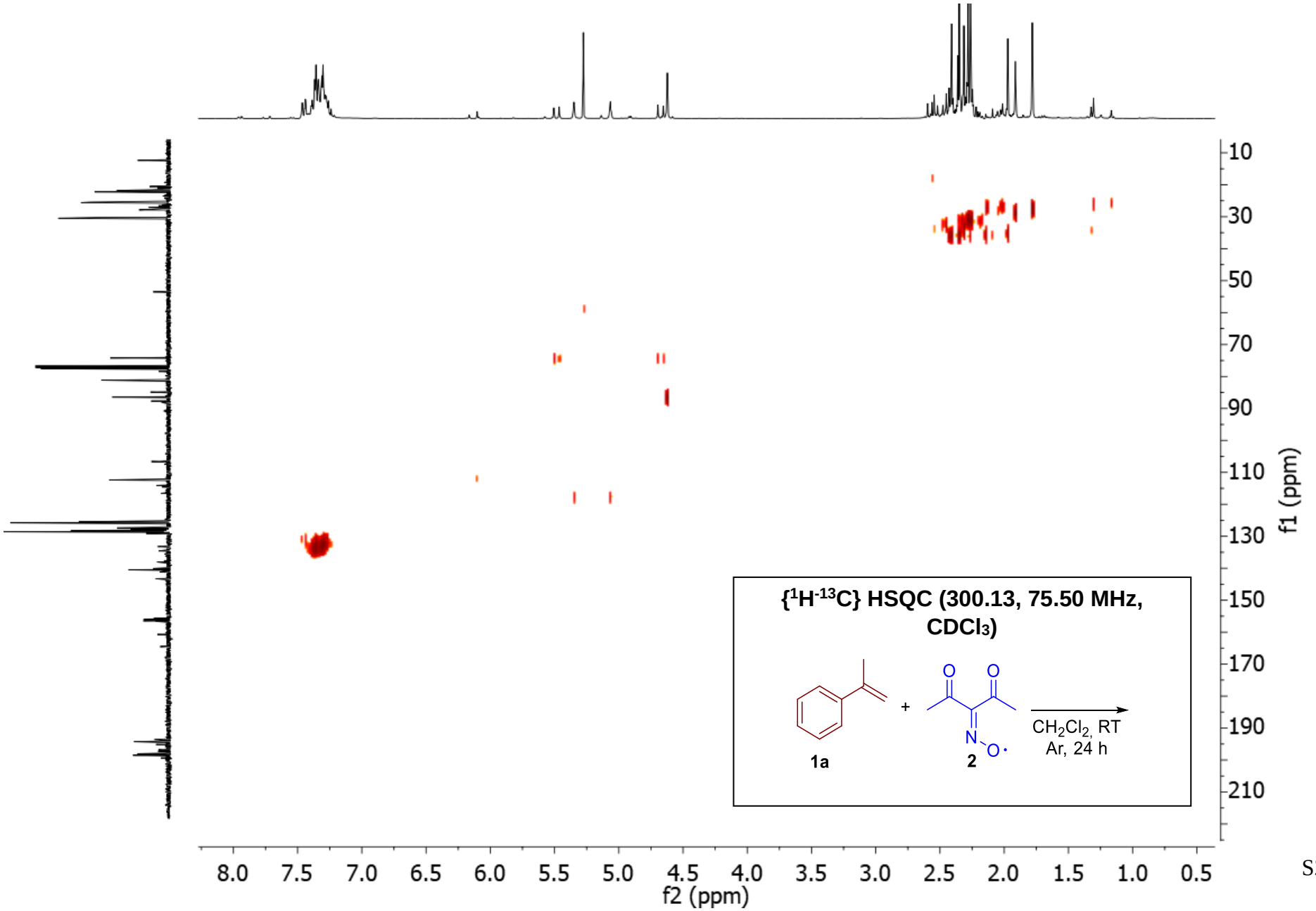

1H NMR (300.13, CH2Cl2)
1a
2
CH2Cl2, RT
Ar, 24 h
CH2Cl2
internal standard
f2 (ppm)

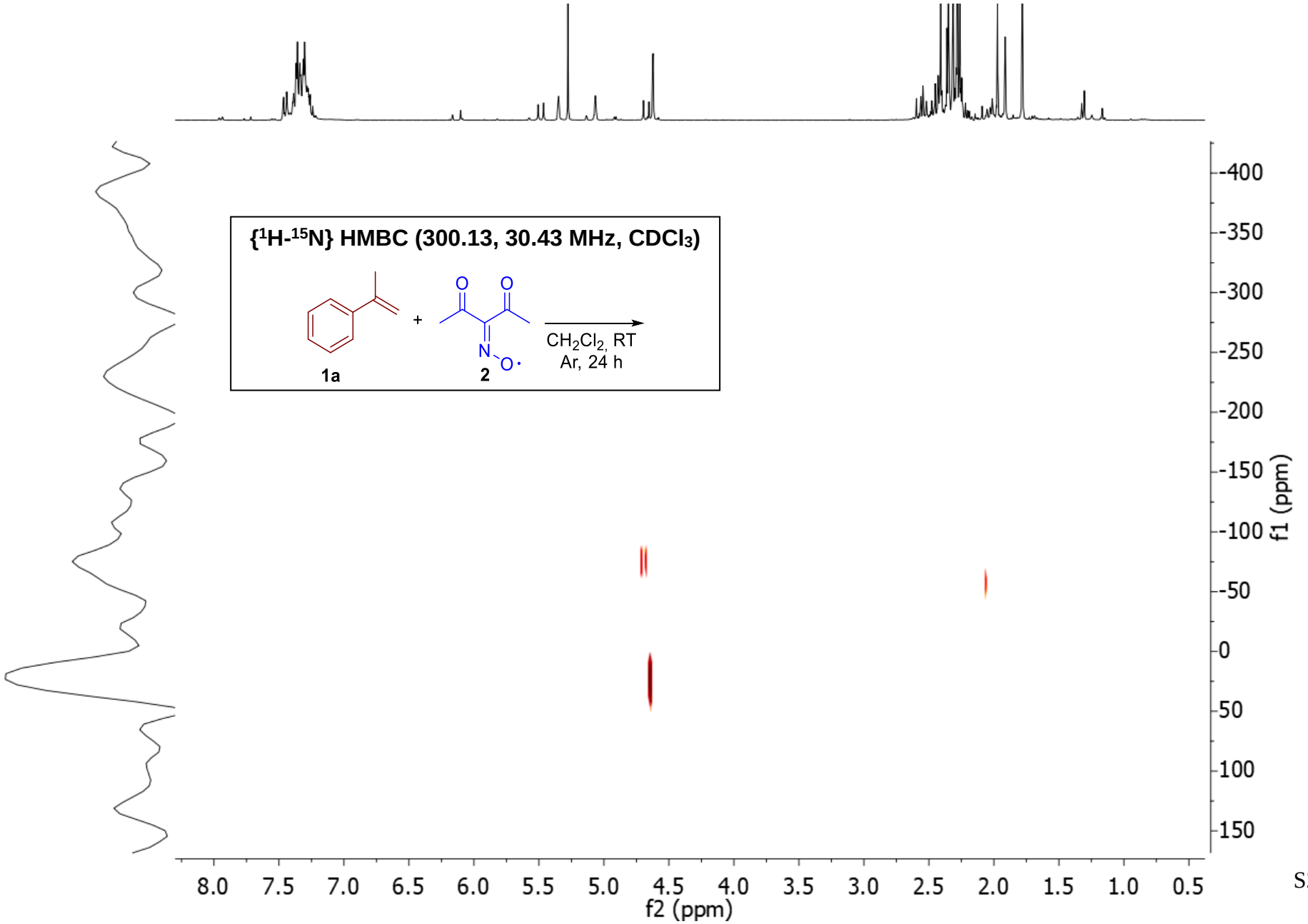


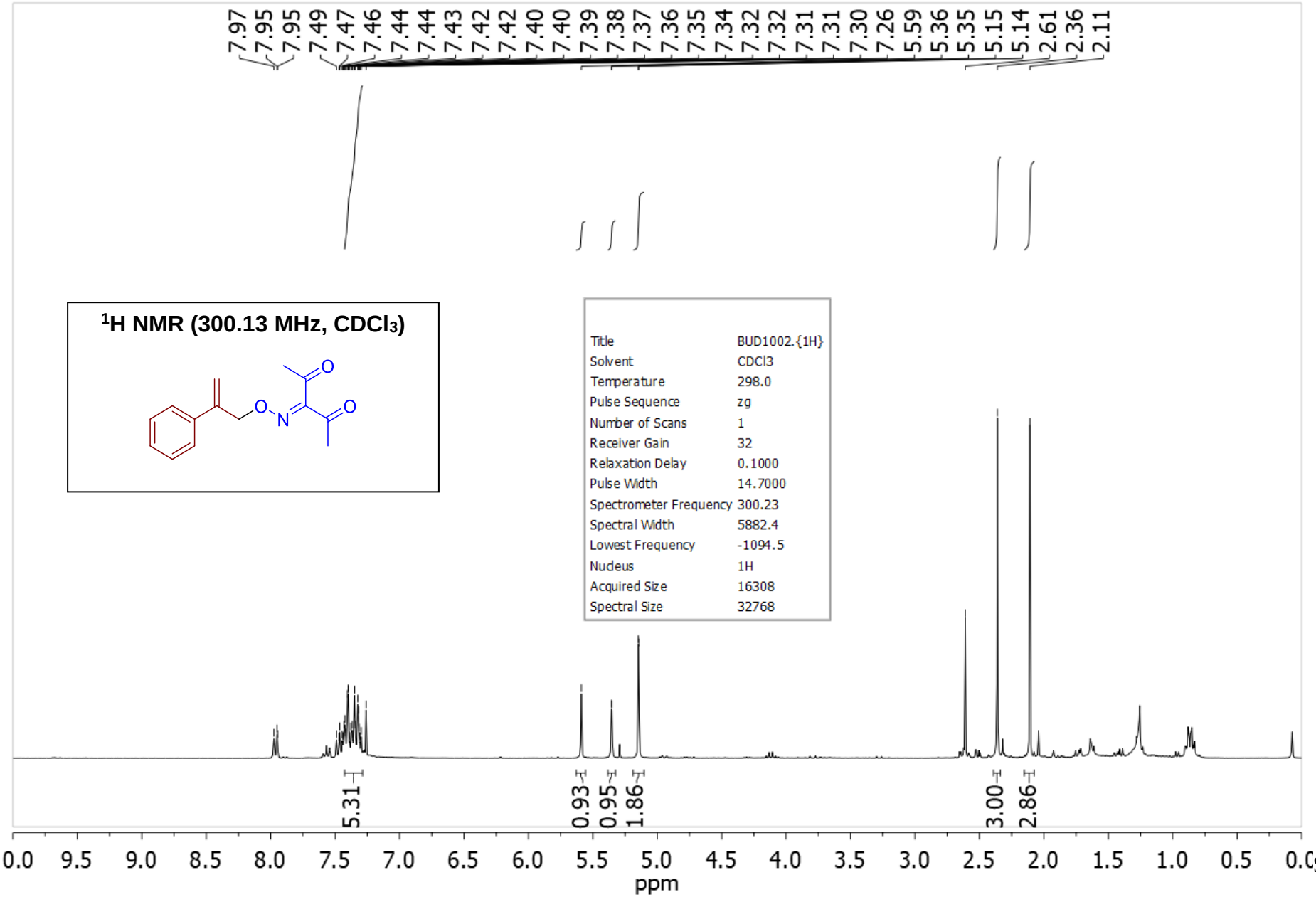
1	Title	BUD987.{1H}.2.fid
2	Solvent	CDCl3
3	Temperature	298.0
4	Pulse Sequence	zgpr30
5	Number of Scans	16
6	Receiver Gain	101.0
7	Relaxation Delay	2.0000
8	Pulse Width	14.7000
9	Acquisition Time	2.4869
10	Spectrometer Frequency	300.23
11	Spectral Width	5882.4
12	Lowest Frequency	-2297.6
13	Nucleus	1H
14	Acquired Size	14629
15	Spectral Size	65536

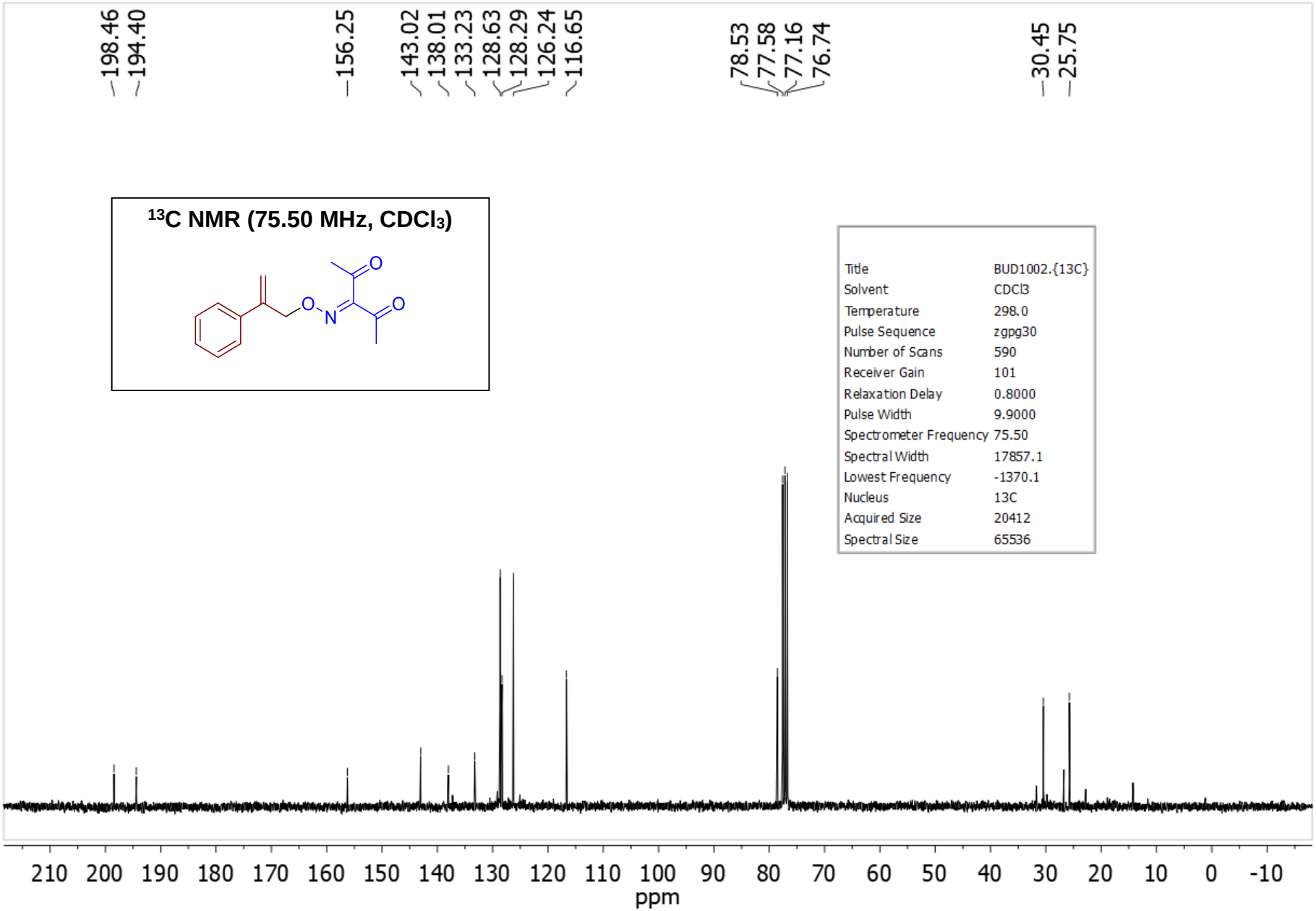

198.52
198.05
194.25
194.12
194.08
156.43
155.91
140.47
129.07
128.66
128.60
128.56
128.54
128.51
128.47
128.34
128.21
128.15
127.81
127.40
127.35
127.19
125.87
125.77
125.46
125.33
112.39
81.16
77.59
77.16
76.73
74.21
30.69
30.56
30.51
30.49
30.24
27.88
27.03
25.68
25.65
25.60
25.56
25.43
22.21
21.79
20.57
12.38
13C NMR (75.50 MHz, CDCl3)
1a
2
CH2Cl2, RT
Ar, 24 h
1 Solvent CDCl3
2 Temperature 298.0
3 Pulse Sequence zgpg30
4 Number of Scans 300
5 Receiver Gain 101.0
6 Relaxation Delay 0.8000
7 Pulse Width 9.9000
8 Acquisition Time 1.1431
9 Spectrometer Frequency 75.50
10 Spectral Width 17857.1
11 Lowest Frequency -1379.6
12 Nucleus 13C
13 Acquired Size 20412
14 Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


{1H-13C} HMBC (300.13, 75.50 MHz, CDCl3)
1a
2
CH2Cl2, RT
Ar, 24 h
f2 (ppm)
f1 (ppm)

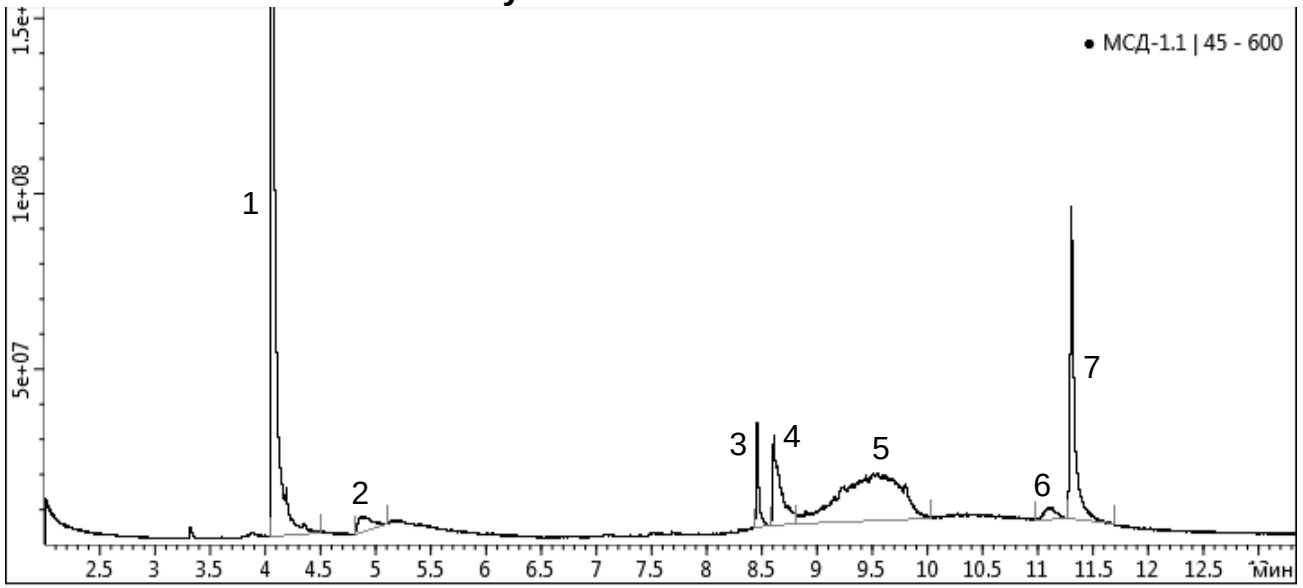

{1H-13C} HSQC (300.13, 75.50 MHz, CDCl3)
1a
2
CH2Cl2, RT
Ar, 24 h
f2 (ppm)
f1 (ppm)

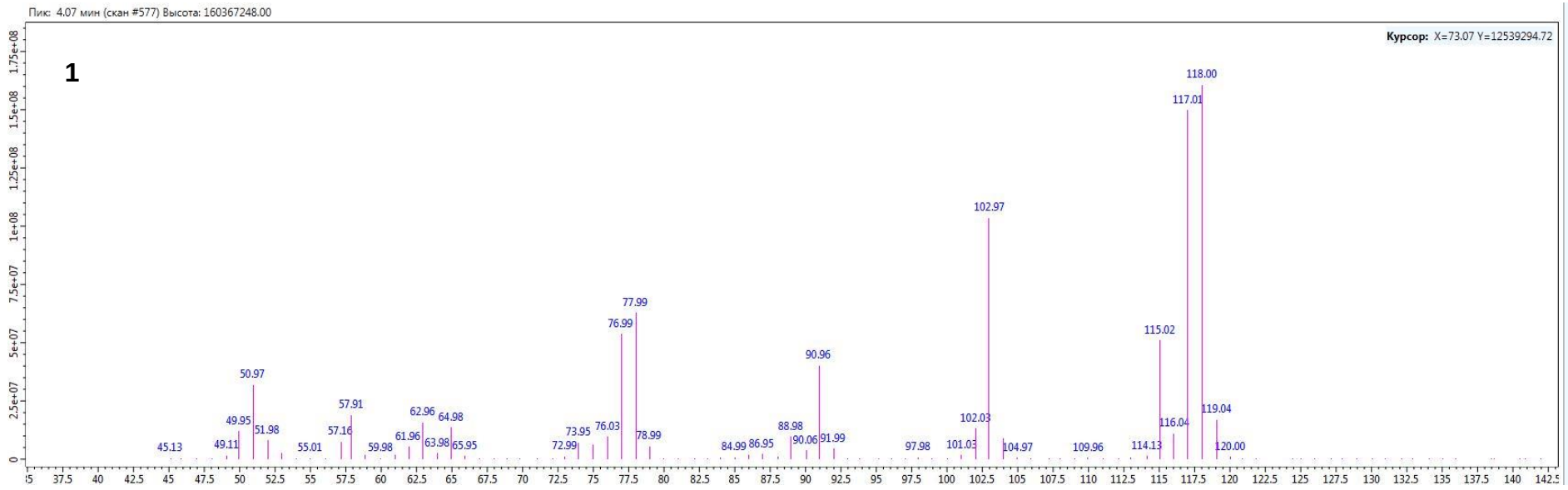

{1H-15N} HMBC (300.13, 30.43 MHz, CDCl3)
1a
2
CH2Cl2, RT
Ar, 24 h
f1 (ppm)
f2 (ppm)

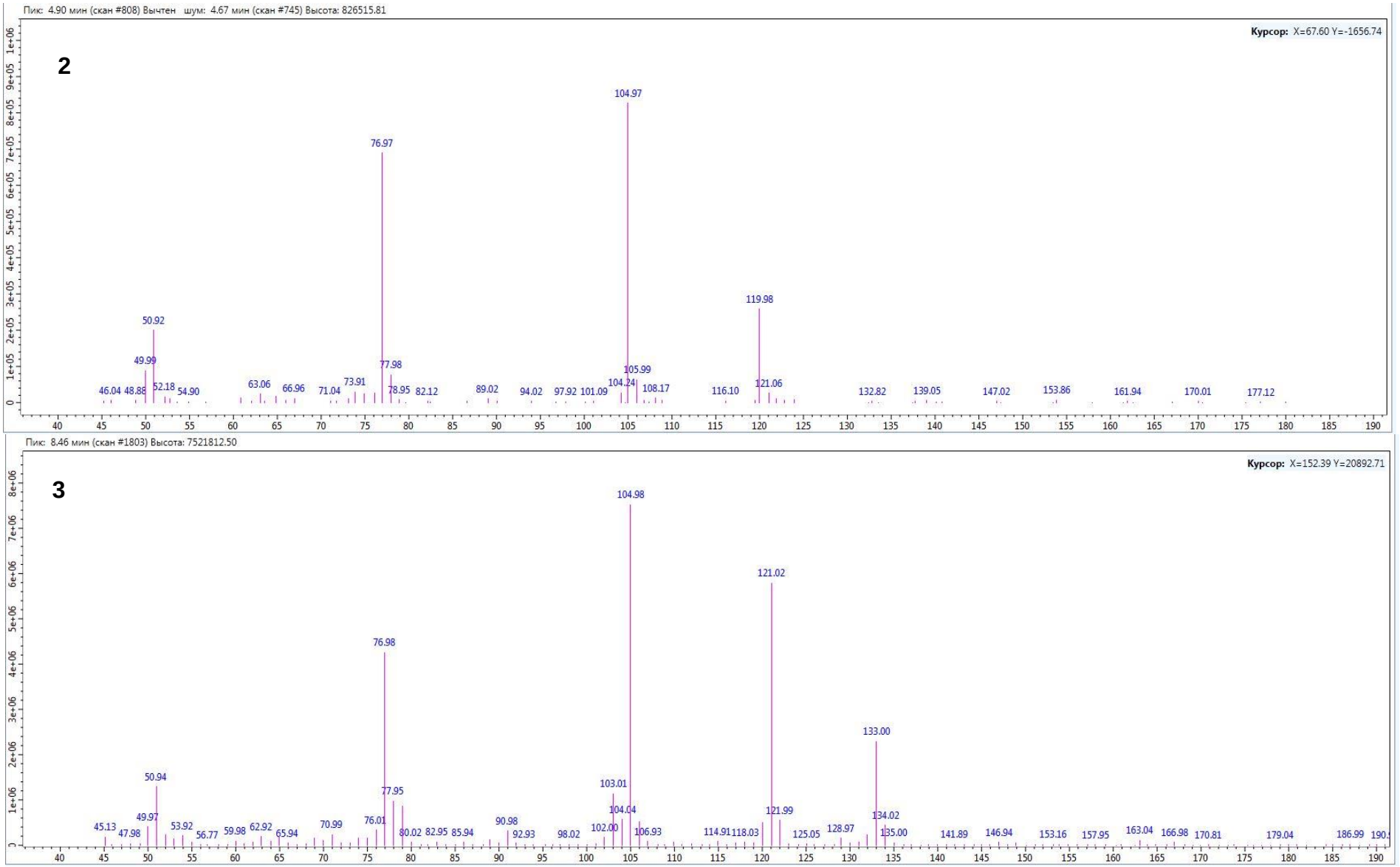

7.97
7.95
7.95
7.49
7.47
7.46
7.44
7.44
7.43
7.42
7.42
7.40
7.40
7.39
7.38
7.37
7.36
7.35
7.34
7.32
7.32
7.31
7.31
7.30
7.26
5.59
5.36
5.35
5.15
5.14
2.61
2.36
2.11
^{1}H NMR (300.13 MHz, CDCl$_3$)
Title BUD1002.{1H}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32
Relaxation Delay 0.1000
Pulse Width 14.7000
Spectrometer Frequency 300.23
Spectral Width 5882.4
Lowest Frequency -1094.5
Nucleus 1H
Acquired Size 16308
Spectral Size 32768
5.31
0.93
0.95
1.86
3.00
2.86
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

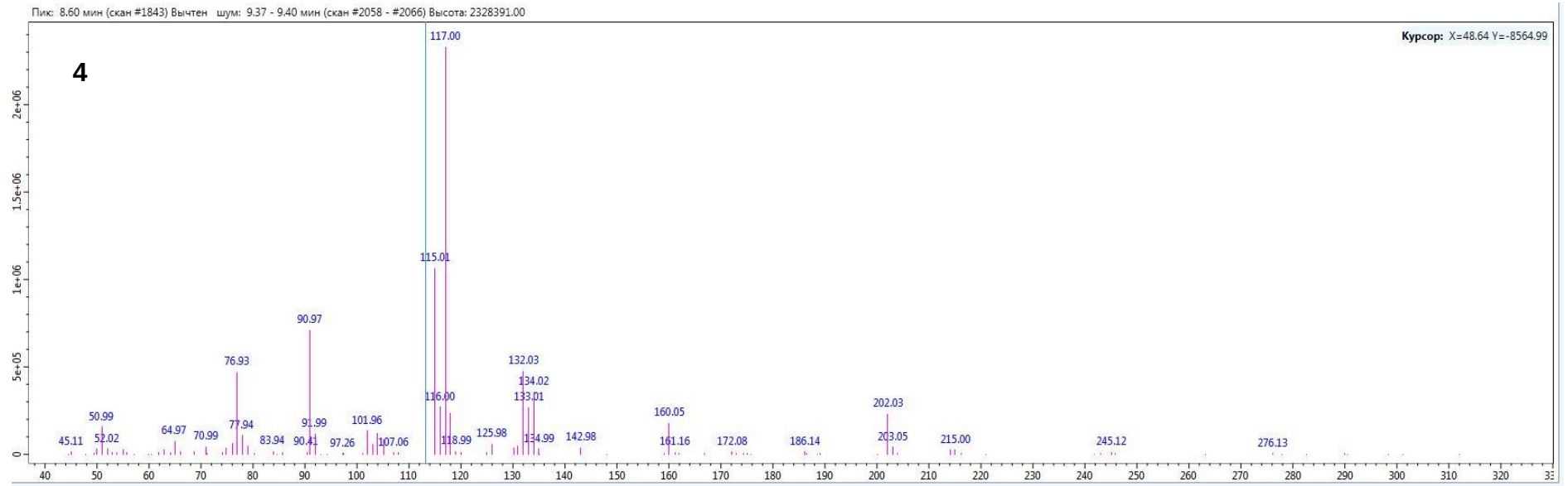

198.46
194.40
156.25
143.02
138.01
133.23
128.63
128.29
126.24
116.65
78.53
77.58
77.16
76.74
30.45
25.75
13C NMR (75.50 MHz, CDCl3)
Title BUD1002.{13C}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 590
Receiver Gain 101
Relaxation Delay 0.8000
Pulse Width 9.9000
Spectrometer Frequency 75.50
Spectral Width 17857.1
Lowest Frequency -1370.1
Nucleus 13C
Acquired Size 20412
Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
ppm

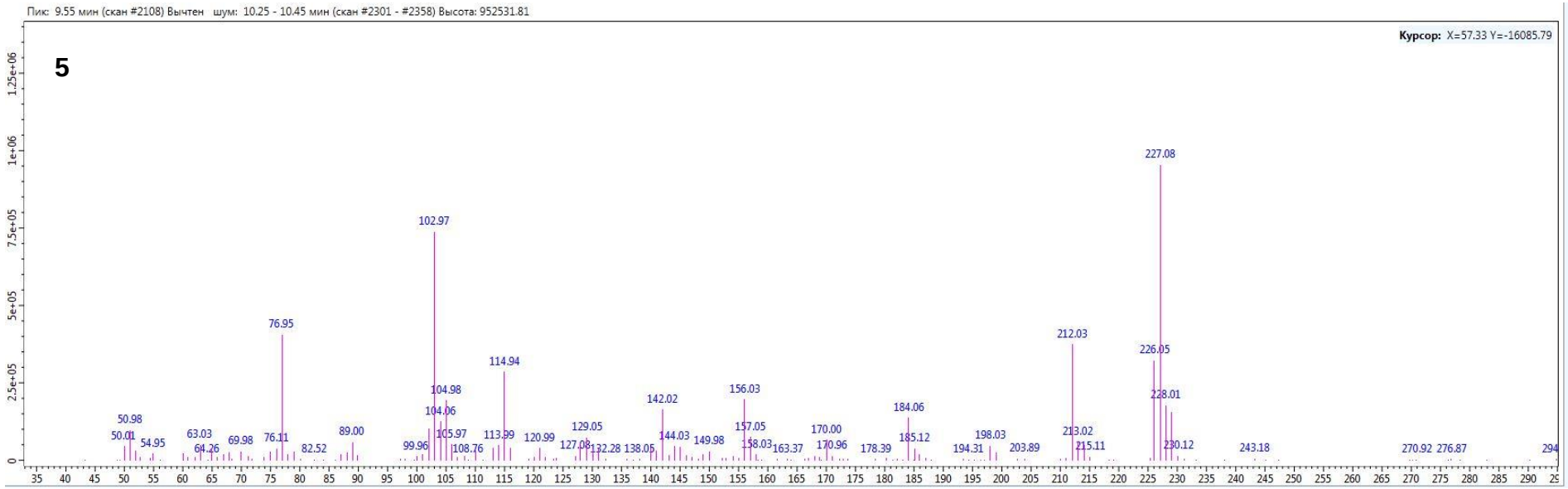
GC-MS analysis of the crude reaction mixture

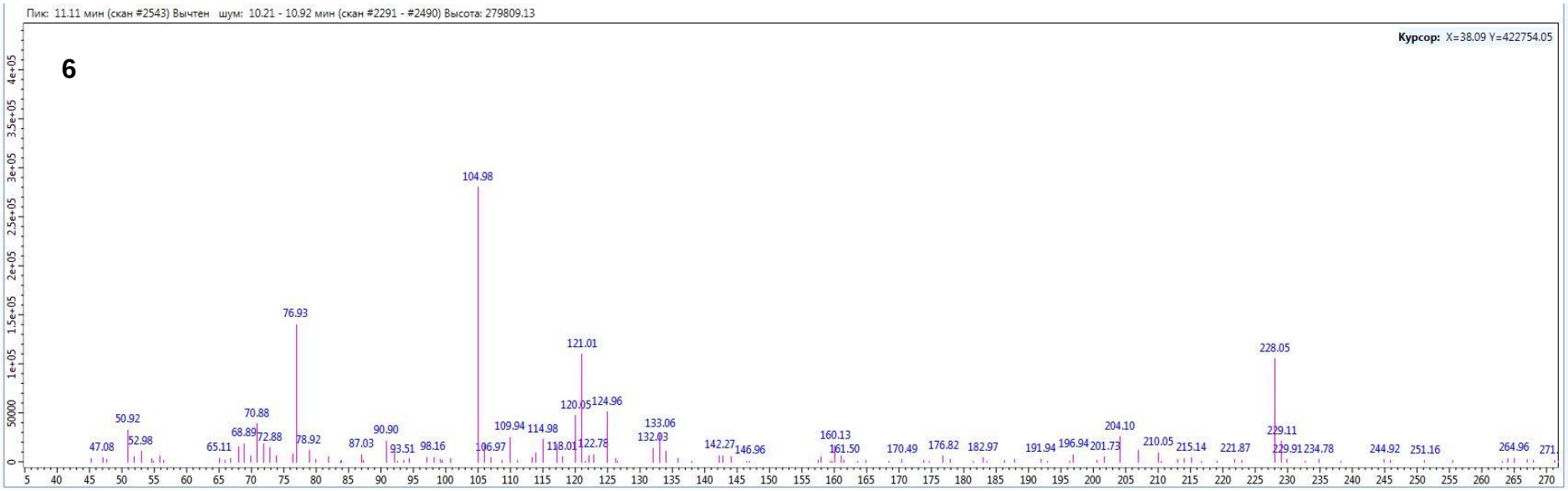


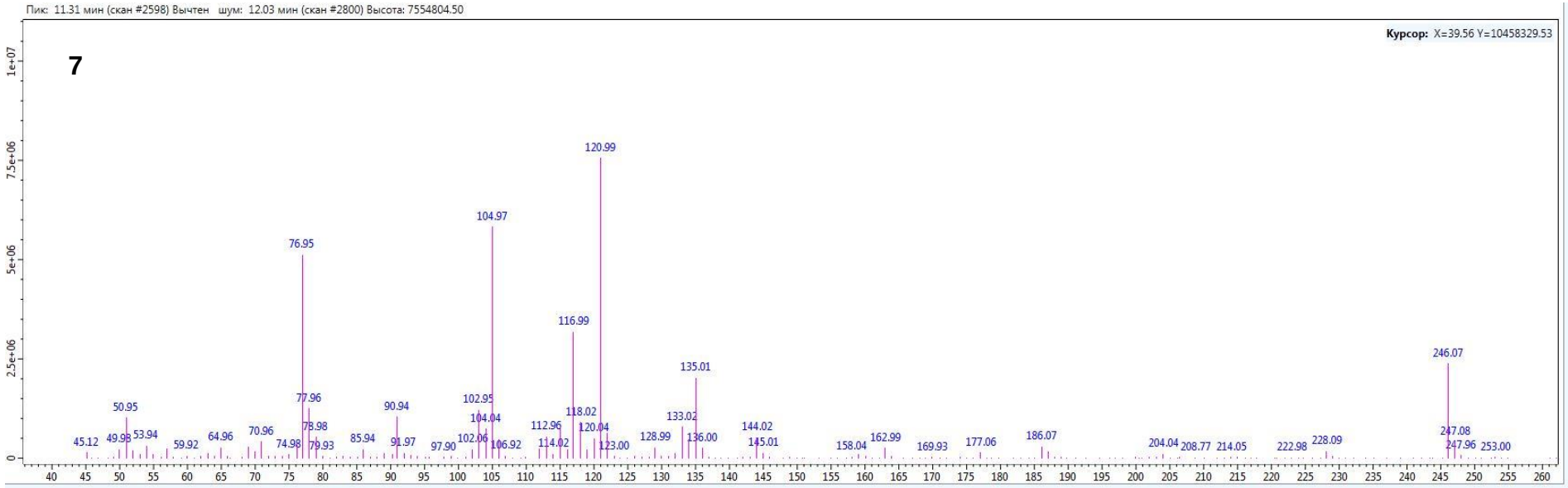



Пик: 4.90 мин (скан #808) Вычтен шум: 4.67 мин (скан #745) Высота: 826515.81
Курсор: X=67.60 Y=-1656.74
2
104.97
76.97
119.98
50.92
49.99
77.98
105.99
46.04 48.88 52.18 54.90 63.06 66.96 71.04 73.91 78.95 82.12 89.02 94.02 97.92 101.09 104.24 108.17 116.10 121.06 132.82 139.05 147.02 153.86 161.94 170.01 177.12
Пик: 8.46 мин (скан #1803) Высота: 7521812.50
Курсор: X=152.39 Y=20892.71
3
104.98
121.02
76.98
133.00
50.94
103.01
77.95
104.04
121.99
134.02
45.13 47.98 49.97 53.92 56.77 59.98 62.92 65.94 70.99 76.01 80.02 82.95 85.94 90.98 92.93 98.02 102.00 106.93 114.91 118.03 125.05 128.97 135.00 141.89 146.94 153.16 157.95 163.04 166.98 170.81 179.04 186.99


Пик: 8.60 мин (скан #1843) Вычтен шум: 9.37 - 9.40 мин (скан #2058 - #2066) Высота: 2328391.00
Курсор: X=48.64 Y=-8564.99
4
117.00
115.01
90.97
76.93
132.03
134.02
133.01
116.00
202.03
160.05
50.99
52.02
64.97
70.99
77.94
83.94
90.41
91.99
97.26
101.96
107.06
118.99
125.98
134.99
142.98
161.16
172.08
186.14
203.05
215.00
245.12
276.13
45.11


Пик: 9.55 мин (скан #2108) Вычтен шум: 10.25 - 10.45 мин (скан #2301 - #2358) Высота: 952531.81
Курсор: X=57.33 Y=-16085.79
5
227.08
102.97
76.95
114.94
212.03
226.05
104.98
104.06
142.02
156.03
228.01
50.98
50.01
54.95
63.03
64.26
69.98
76.11
82.52
89.00
99.96
105.97
108.76
113.99
120.99
127.08
129.05
132.28
138.05
144.03
149.98
157.05
158.03
163.37
170.00
170.96
178.39
184.06
185.12
194.31
198.03
203.89
213.02
215.11
230.12
243.18
270.92
276.87


Пик: 11.11 мин (скан #2543) Вычтен шум: 10.21 - 10.92 мин (скан #2291 - #2490) Высота: 279809.13
Курсор: X=38.09 Y=422754.05
6
104.98
76.93
121.01
228.05
120.05
124.96
50.92
70.88
68.89
72.88
78.92
90.90
109.94
114.98
133.06
132.03
204.10
229.11
47.08
52.98
65.11
87.03
93.51
98.16
106.97
118.01
122.78
142.27
146.96
160.13
161.50
170.49
176.82
182.97
191.94
196.94
201.73
210.05
215.14
221.87
229.91
234.78
244.92
251.16
264.96
271


Пик: 11.31 мин (скан #2598) Вычтен шум: 12.03 мин (скан #2800) Высота: 7554804.50
Курсор: X=39.56 Y=10458329.53
7
120.99
104.97
76.95
116.99
246.07
135.01
50.95
77.96
90.94
102.95
104.04
118.02
133.02
144.02
45.12
49.98
53.94
59.92
64.96
70.96
74.98
78.98
79.93
85.94
91.97
97.90
102.06
106.92
112.96
114.02
120.04
123.00
128.99
136.00
145.01
158.04
162.99
169.93
177.06
186.07
204.04
208.77
214.05
222.98
228.09
247.08
247.96
253.00

HRMS analysis of crude reaction mixture

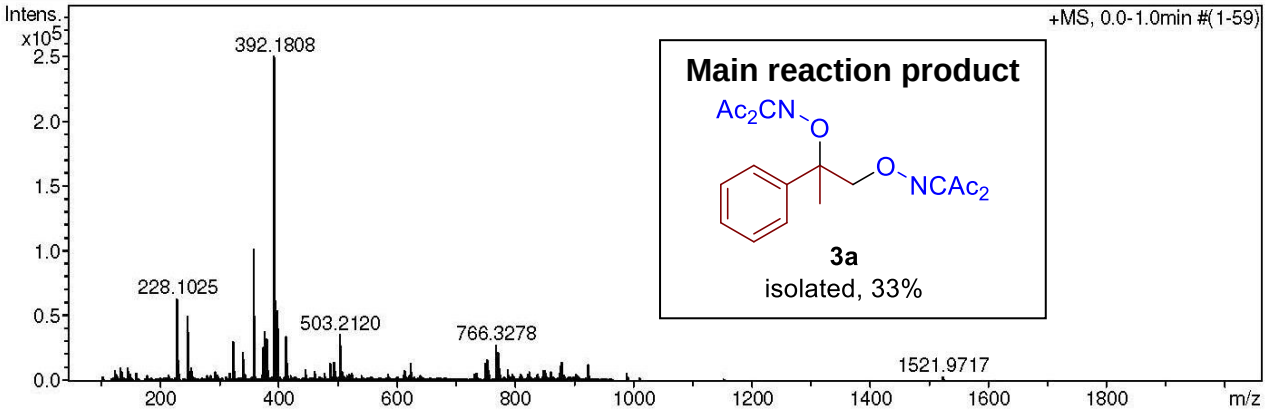
Display Report

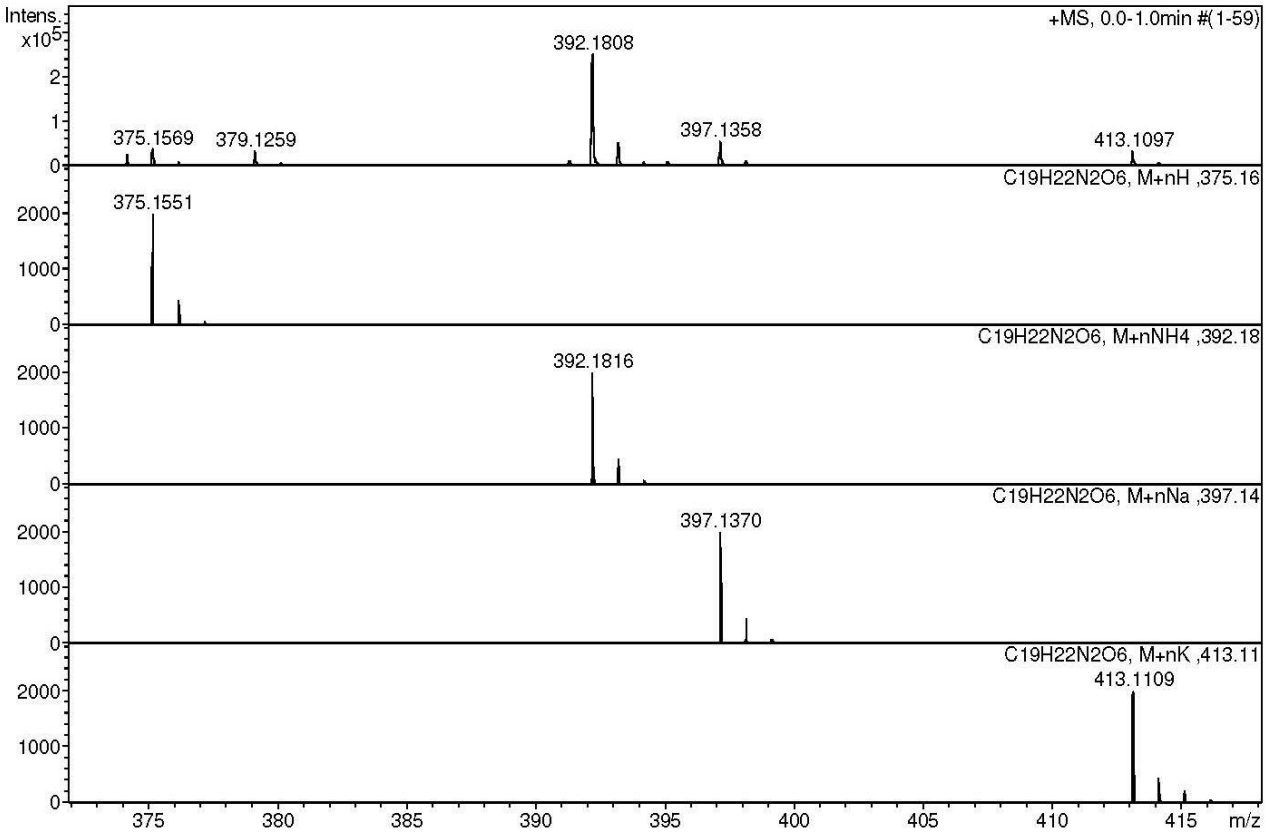
Analysis Info

Analysis Name	D:\Data\Chizhov\Terentiev\Budnikov\sm-171_&clblow.d	Acquisition Date	24.07.2023 12:04:53
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SM-171	Instrument / Ser#	micrOTOF 10248
Comment	CH3CN 100 %, dil. 2000, calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





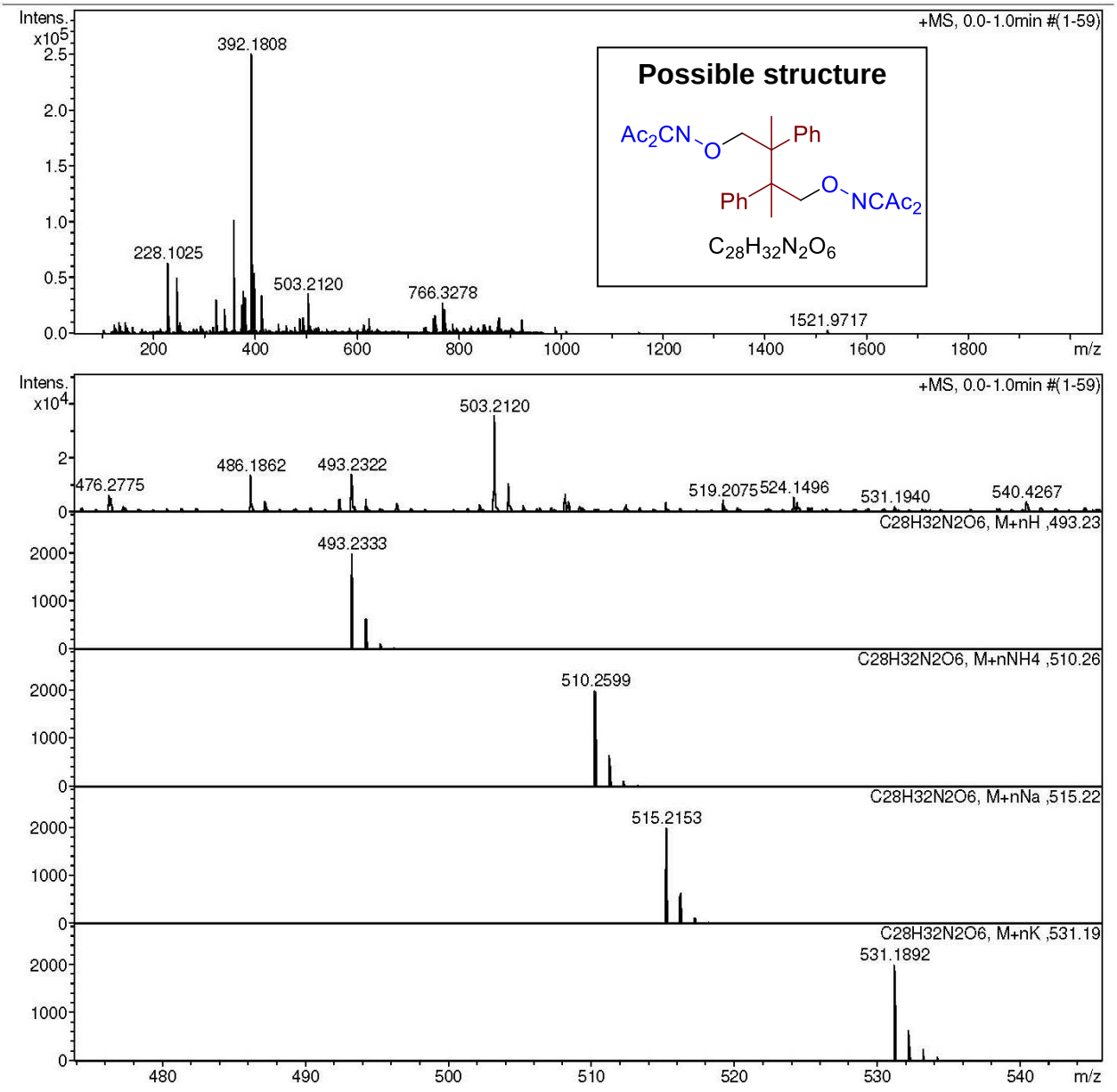
Display Report

Analysis Info

Analysis Name	D:\Data\Chizhov\Terentiev\Budnikov\sm-171_&clblow.d	Acquisition Date	24.07.2023 12:04:53
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SM-171	Instrument / Ser#	micrOTOF 10248
Comment	CH3CN 100 %, dil. 2000, calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



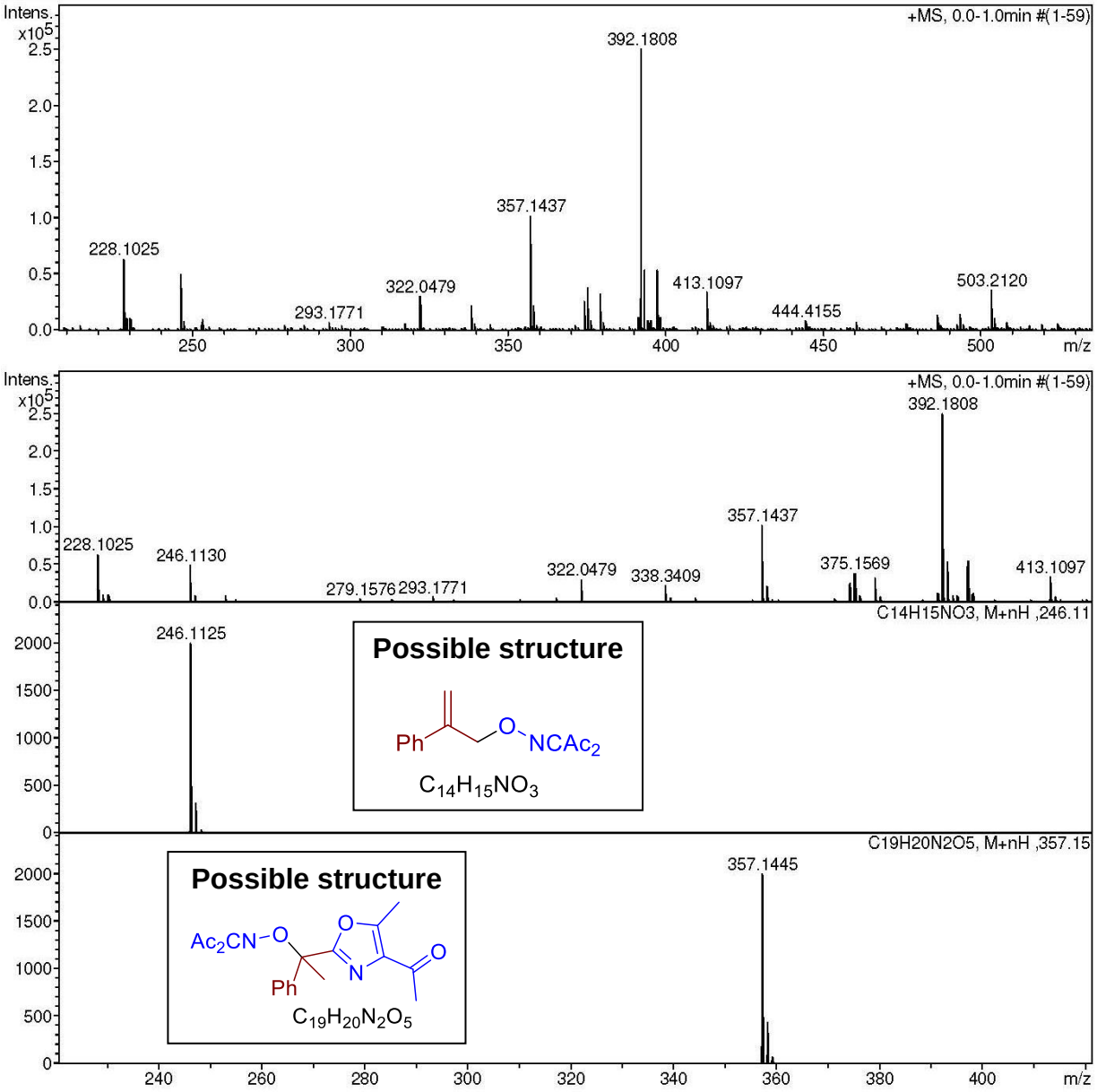
Display Report

Analysis Info

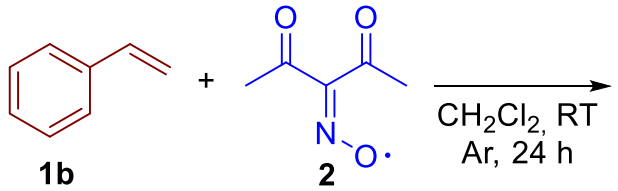
Analysis Name	D:\Data\Chizhov\Terentiev\Budnikov\sm-171_&clblow.d	Acquisition Date	24.07.2023 12:04:53
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SM-171	Instrument / Ser#	micrOTOF 10248
Comment	CH3CN 100 %, dil. 2000, calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

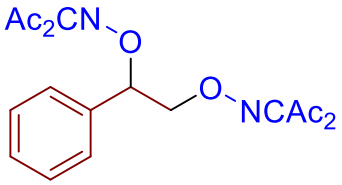


*Reaction with styrene **1b**:* the solution of the diacetyliminoxyl radical **2** (10 mmol in 125 mL CH_2Cl_2) was placed in a two-necked flask. Then styrene **1a** (5 mmol, 520 mg) in CH_2Cl_2 (2 mL) was added and the reaction mixture was stirred for 24 hours at room temperature under an argon atmosphere. 1,1,2,2-Tetrachloroathane was added as an internal standard, and then the crude reaction mixture was analyzed using ^1H NMR spectroscopy. The reaction mixture was rotary evaporated under a water-jet vacuum and analyzed employing HRMS and GC-MS.

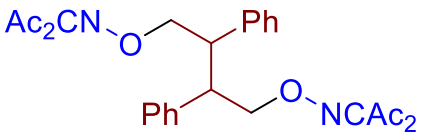


1b
(conversion 50%)

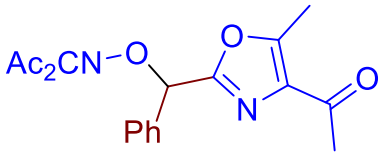
2



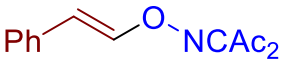
3b
isolated, 14%



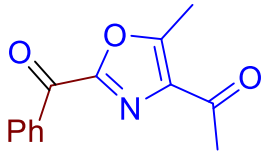
$C_{26}H_{28}N_2O_6$
detected by HRMS*



$C_{18}H_{18}N_2O_5$
detected by HRMS*

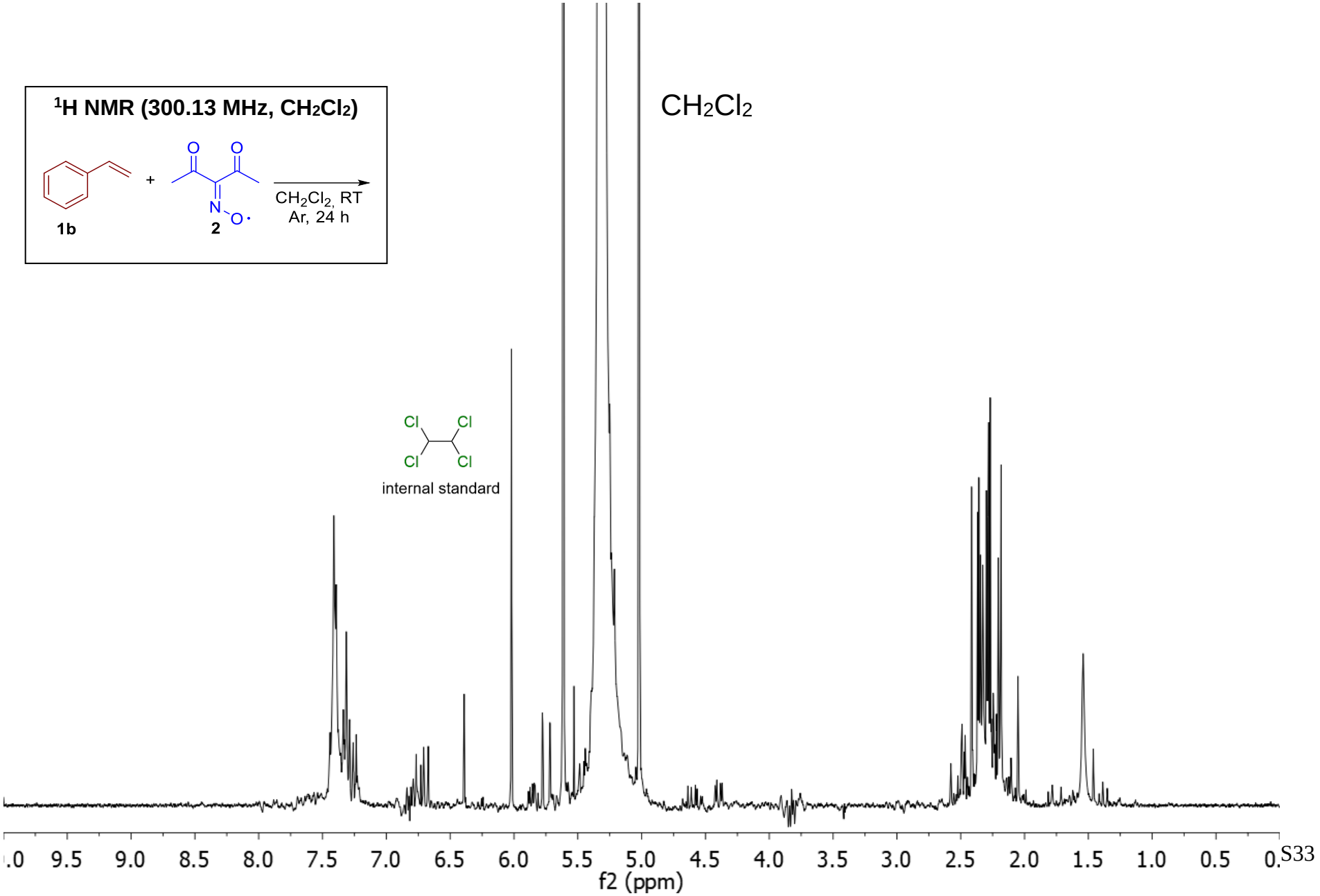


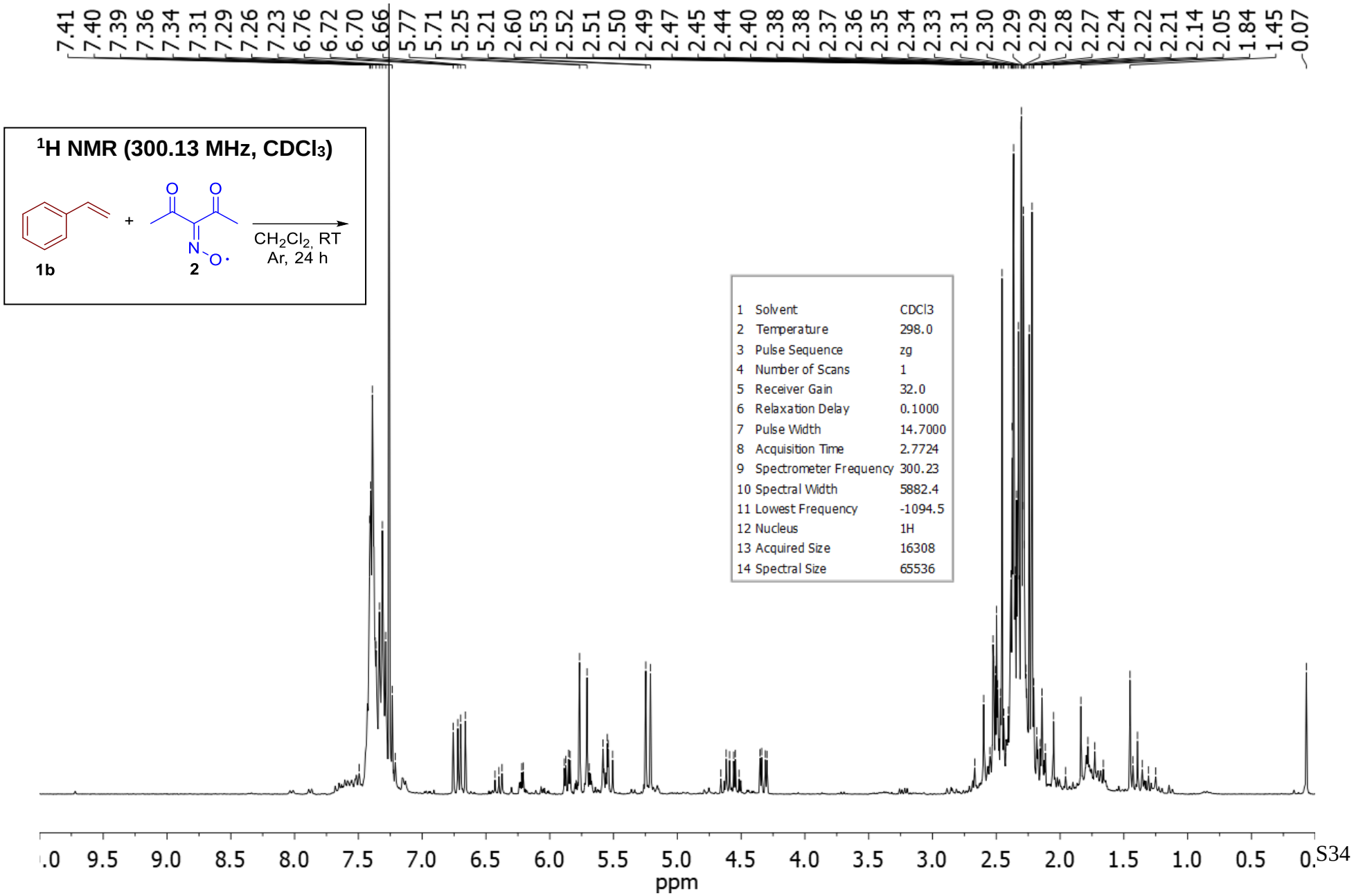
$C_{13}H_{13}NO_3$
detected by HRMS, GC-MS*

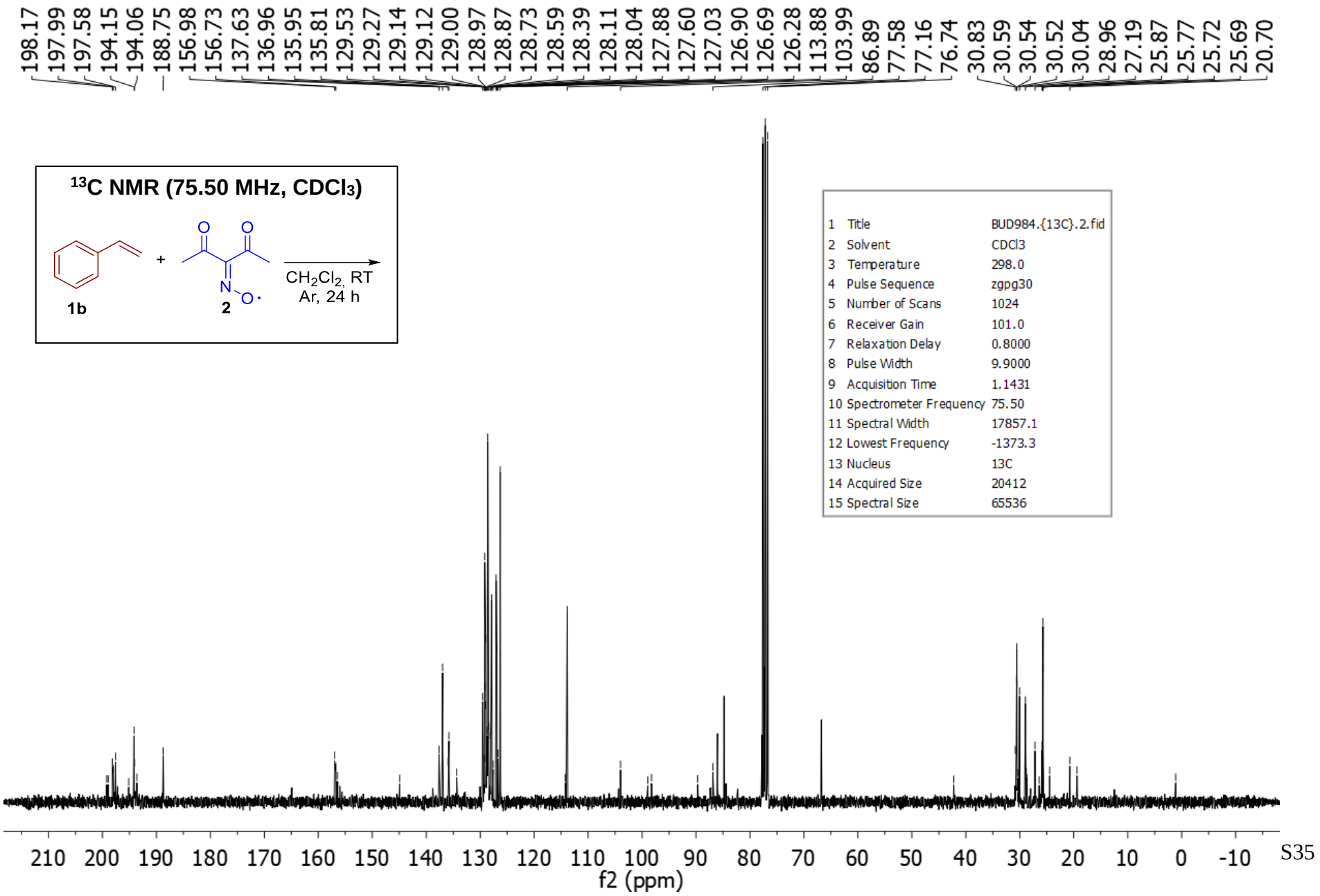


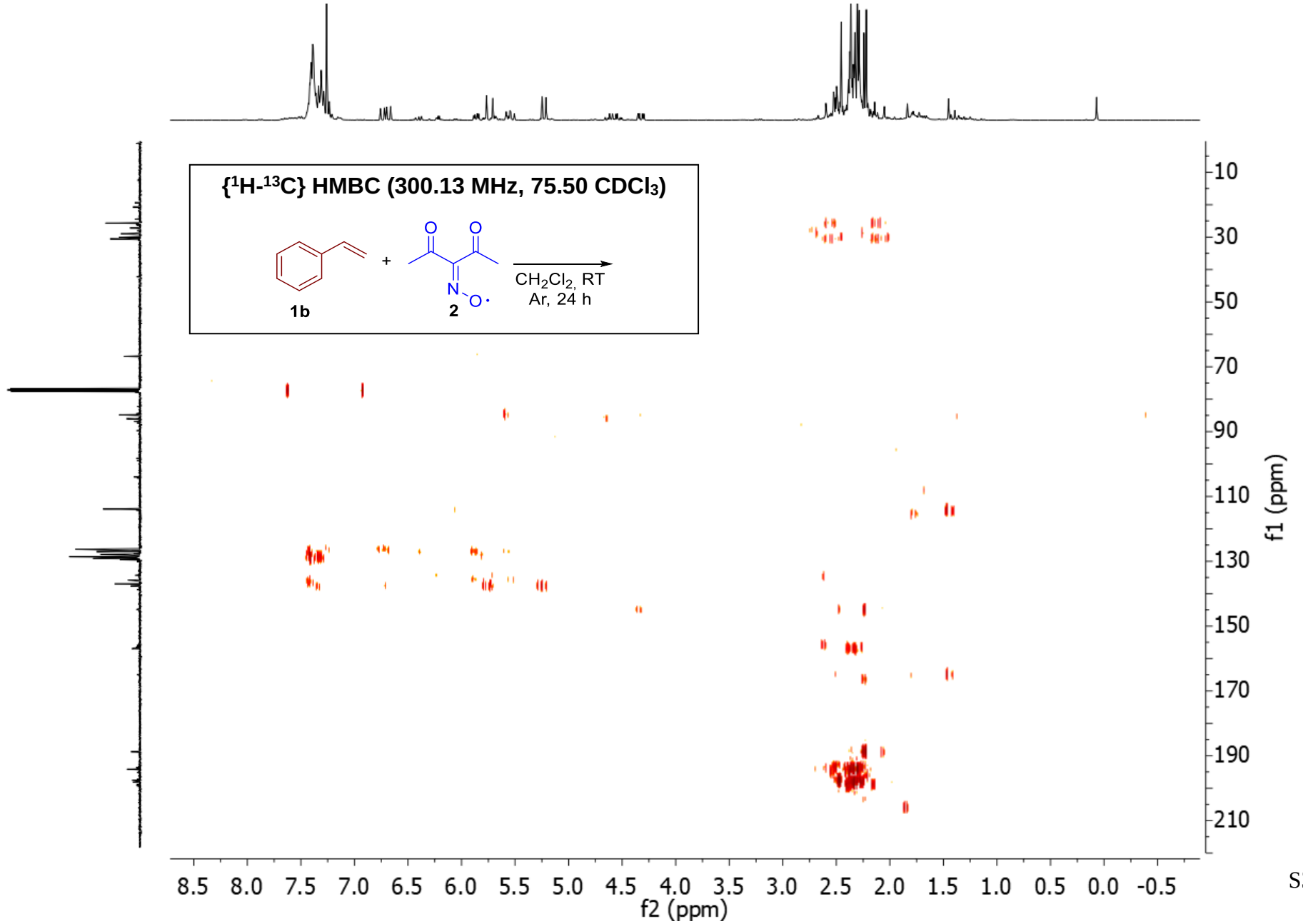
$C_{13}H_{11}NO_3$
detected by GC-MS*

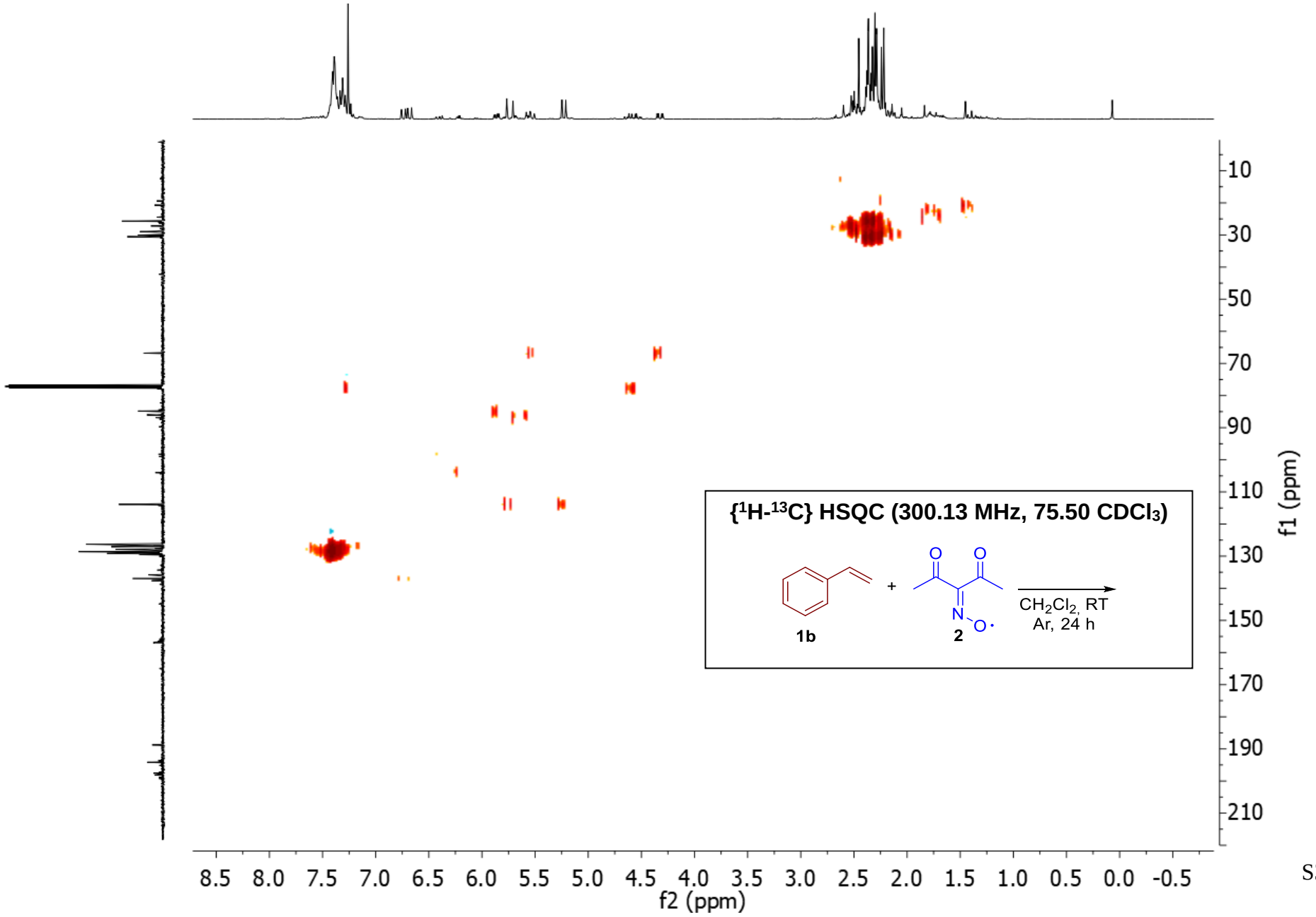
***Possible structures proposed based on HRMS and GC-MS data**

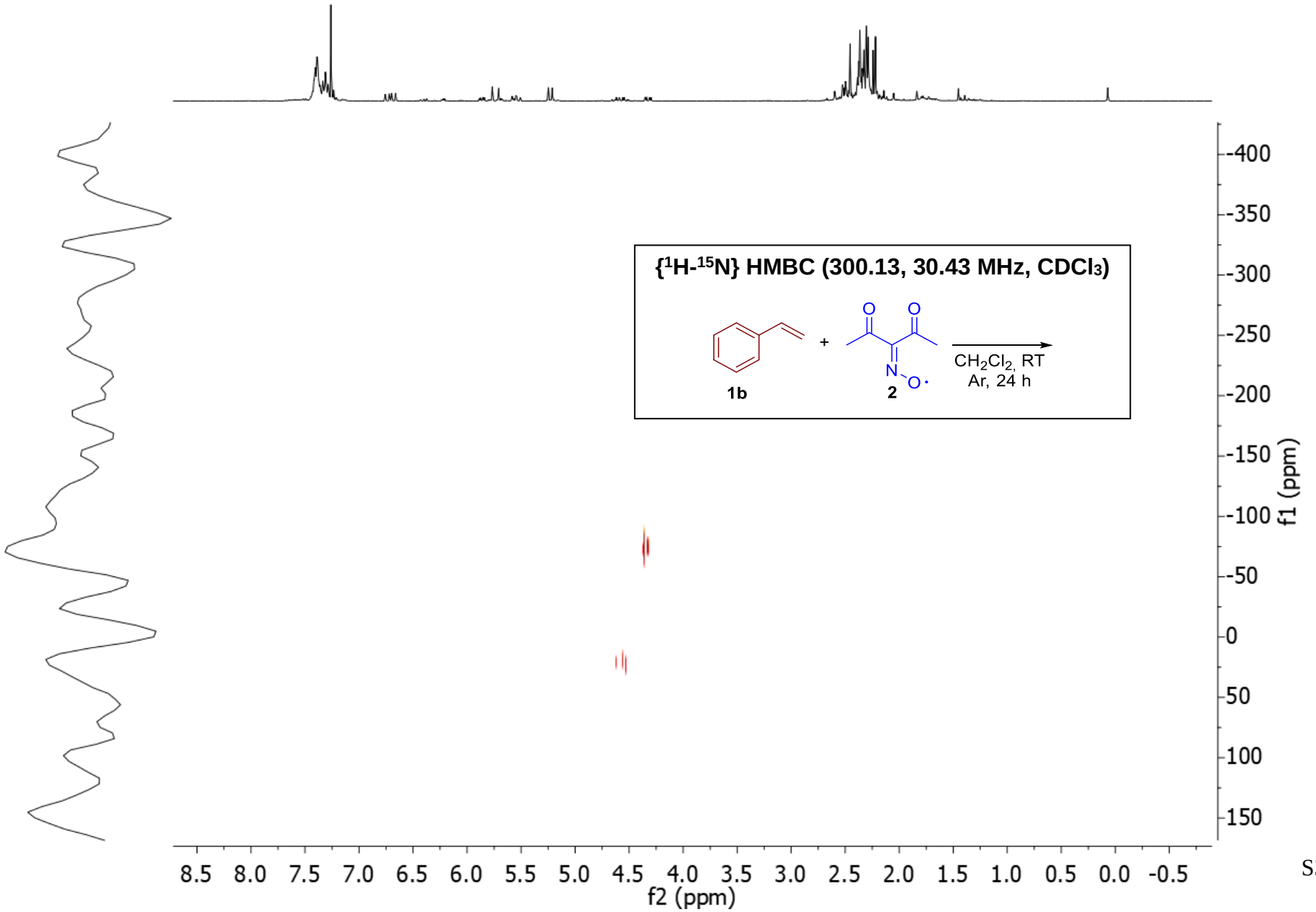

1H NMR (300.13 MHz, CH2Cl2)
1b
2
CH2Cl2, RT
Ar, 24 h
CH2Cl2
internal standard
f2 (ppm)


7.41 7.40 7.39 7.36 7.34 7.31 7.29 7.26 7.23 6.76 6.72 6.70 6.66 5.77 5.71 5.25 5.21 2.60 2.53 2.52 2.51 2.50 2.49 2.47 2.45 2.44 2.40 2.38 2.38 2.37 2.36 2.35 2.34 2.33 2.31 2.30 2.29 2.29 2.28 2.27 2.24 2.22 2.21 2.14 2.05 1.84 1.45 0.07
1H NMR (300.13 MHz, CDCl3)
1b
2
CH2Cl2, RT
Ar, 24 h
1 Solvent CDCl3
2 Temperature 298.0
3 Pulse Sequence zg
4 Number of Scans 1
5 Receiver Gain 32.0
6 Relaxation Delay 0.1000
7 Pulse Width 14.7000
8 Acquisition Time 2.7724
9 Spectrometer Frequency 300.23
10 Spectral Width 5882.4
11 Lowest Frequency -1094.5
12 Nucleus 1H
13 Acquired Size 16308
14 Spectral Size 65536
ppm

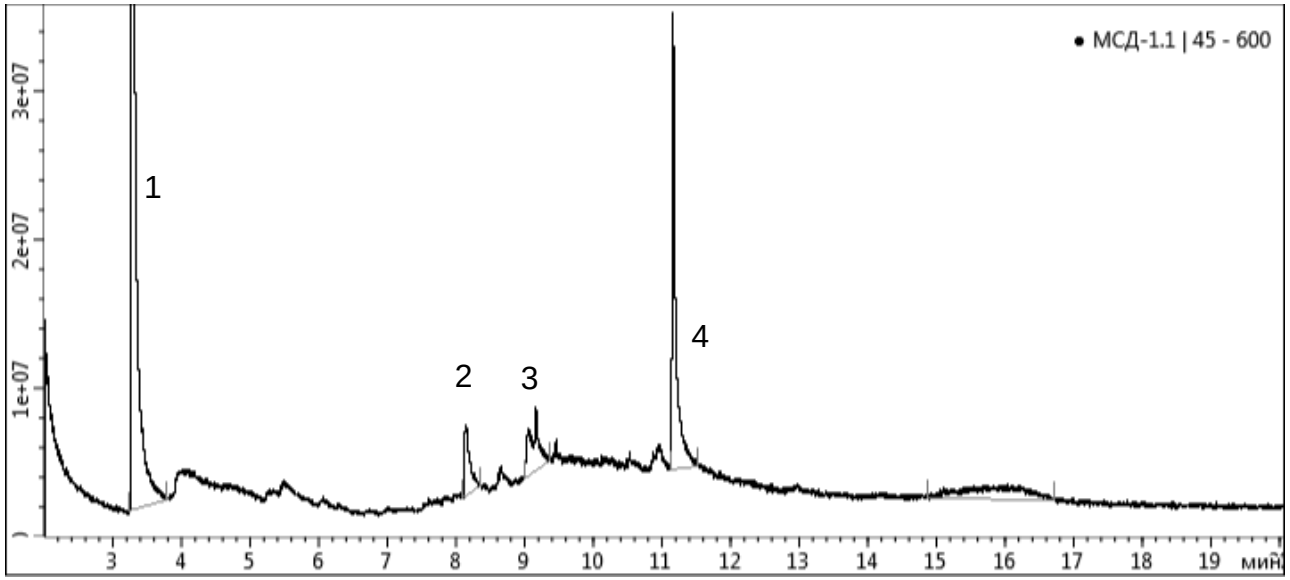

198.17
197.99
197.58
194.15
194.06
188.75
156.98
156.73
137.63
136.96
135.95
135.81
129.53
129.27
129.14
129.12
129.00
128.97
128.87
128.73
128.59
128.39
128.11
128.04
127.88
127.60
127.03
126.90
126.69
126.28
113.88
103.99
86.89
77.58
77.16
76.74
30.83
30.59
30.54
30.52
30.04
28.96
27.19
25.87
25.77
25.72
25.69
20.70
13C NMR (75.50 MHz, CDCl3)
1b
2
CH2Cl2, RT
Ar, 24 h
1 Title BUD984.{13C}.2.fid
2 Solvent CDCl3
3 Temperature 298.0
4 Pulse Sequence zgpg30
5 Number of Scans 1024
6 Receiver Gain 101.0
7 Relaxation Delay 0.8000
8 Pulse Width 9.9000
9 Acquisition Time 1.1431
10 Spectrometer Frequency 75.50
11 Spectral Width 17857.1
12 Lowest Frequency -1373.3
13 Nucleus 13C
14 Acquired Size 20412
15 Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f2 (ppm)

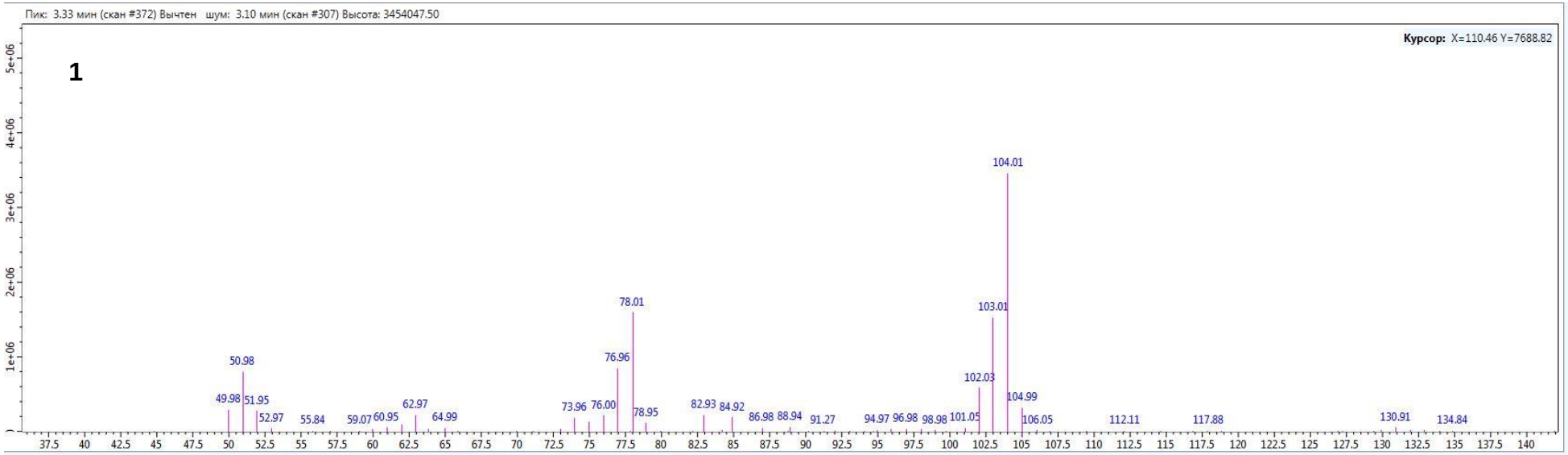

{1H-13C} HMBC (300.13 MHz, 75.50 CDCl3)
1b
2
CH2Cl2, RT
Ar, 24 h
f1 (ppm)
f2 (ppm)

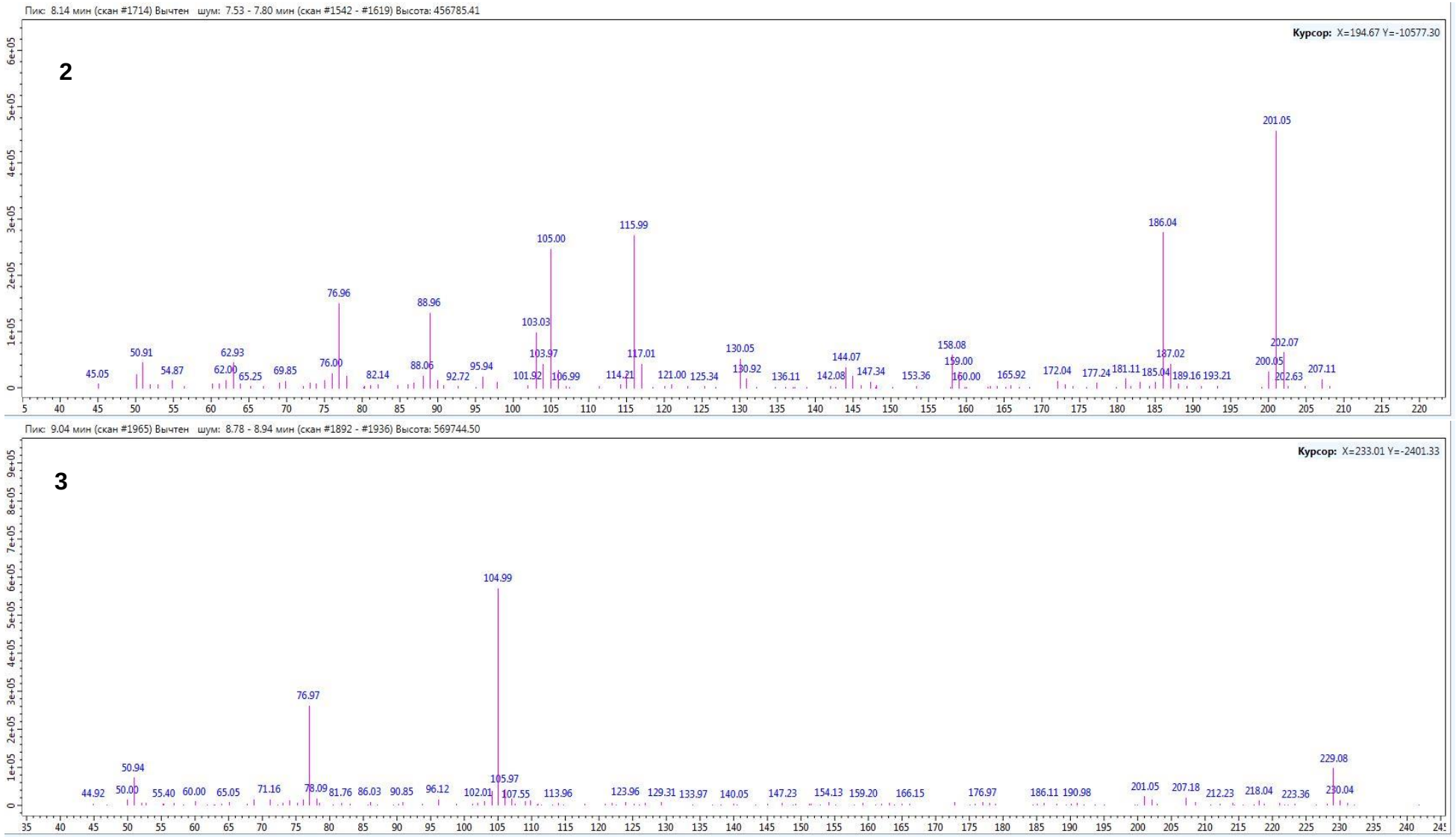

{1H-13C} HSQC (300.13 MHz, 75.50 CDCl3)
1b
2
CH2Cl2, RT
Ar, 24 h
f2 (ppm)
f1 (ppm)

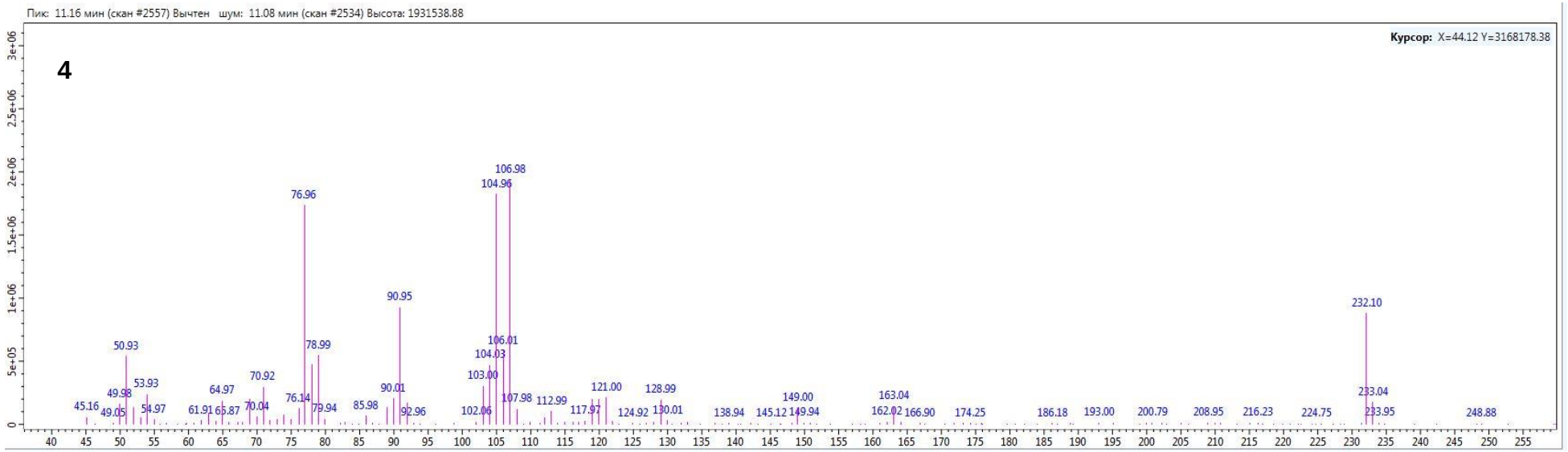

{1H-15N} HMBC (300.13, 30.43 MHz, CDCl3)
1b
2
CH2Cl2, RT
Ar, 24 h
f1 (ppm)
f2 (ppm)

GC-MS analysis of crude reaction mixture






Пик: 8.14 мин (скан #1714) Вычтен шум: 7.53 - 7.80 мин (скан #1542 - #1619) Высота: 456785.41
Курсор: X=194.67 Y=-10577.30
2
201.05
186.04
115.99
105.00
76.96
88.96
103.03
50.91
62.93
103.97
117.01
130.05
158.08
144.07
202.07
187.02
45.05
54.87
62.00
65.25
69.85
76.00
82.14
88.06
92.72
95.94
101.92
106.99
114.21
121.00
125.34
130.92
136.11
142.08
147.34
153.36
159.00
160.00
165.92
172.04
177.24
181.11
185.04
189.16
193.21
200.05
202.63
207.11
Пик: 9.04 мин (скан #1965) Вычтен шум: 8.78 - 8.94 мин (скан #1892 - #1936) Высота: 569744.50
Курсор: X=233.01 Y=-2401.33
3
104.99
76.97
50.94
229.08
105.97
44.92
50.00
55.40
60.00
65.05
71.16
78.09
81.76
86.03
90.85
96.12
102.01
107.55
113.96
123.96
129.31
133.97
140.05
147.23
154.13
159.20
166.15
176.97
186.11
190.98
201.05
207.18
212.23
218.04
223.36
230.04


Пик: 11.16 мин (скан #2557) Вычтен шум: 11.08 мин (скан #2534) Высота: 1931538.88
Курсор: X=44.12 Y=3168178.38
4
3e+06
2.5e+06
2e+06
1.5e+06
1e+06
5e+05
0
106.98
104.96
76.96
90.95
232.10
50.93
78.99
106.01
104.03
103.00
70.92
53.93
64.97
90.01
121.00
128.99
233.04
149.00
163.04
49.98
76.14
107.98
112.99
45.16
49.05
54.97
61.91
65.87
70.04
79.94
85.98
92.96
102.06
117.97
124.92
130.01
138.94
145.12
149.94
162.02
166.90
174.25
186.18
193.00
200.79
208.95
216.23
224.75
233.95
248.88
40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 150 155 160 165 170 175 180 185 190 195 200 205 210 215 220 225 230 235 240 245 250 255

HRMS analysis of crude reaction mixture

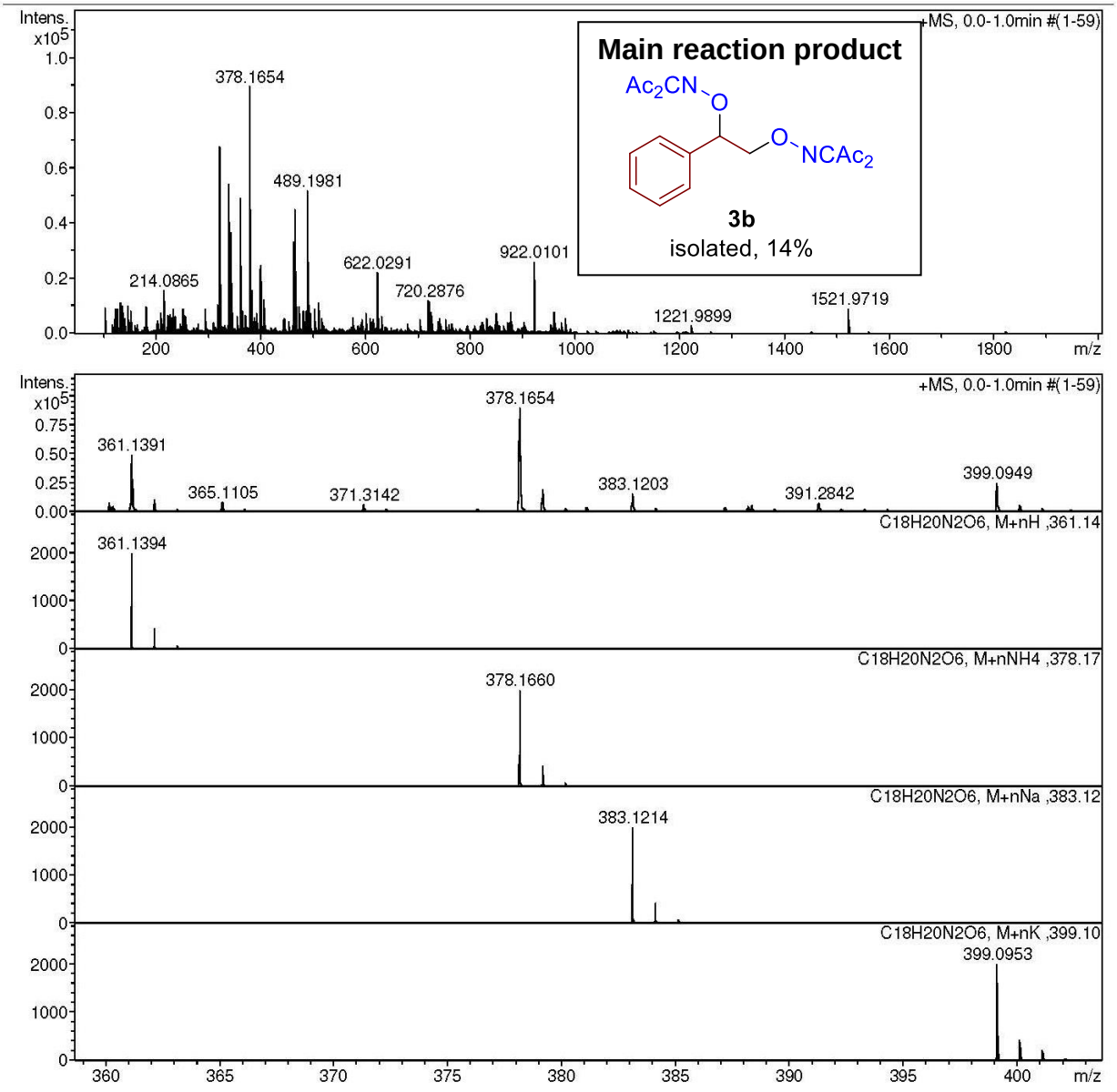
Display Report

Analysis Info

Analysis Name	D:\Data\Chizhov\Terentiev\Budnikov\sm-169_&clblow.d	Acquisition Date	20.07.2023 12:41:45
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SM-169	Instrument / Ser#	micrOTOF 10248
Comment	CH3CN 100 %, dil. 200, calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



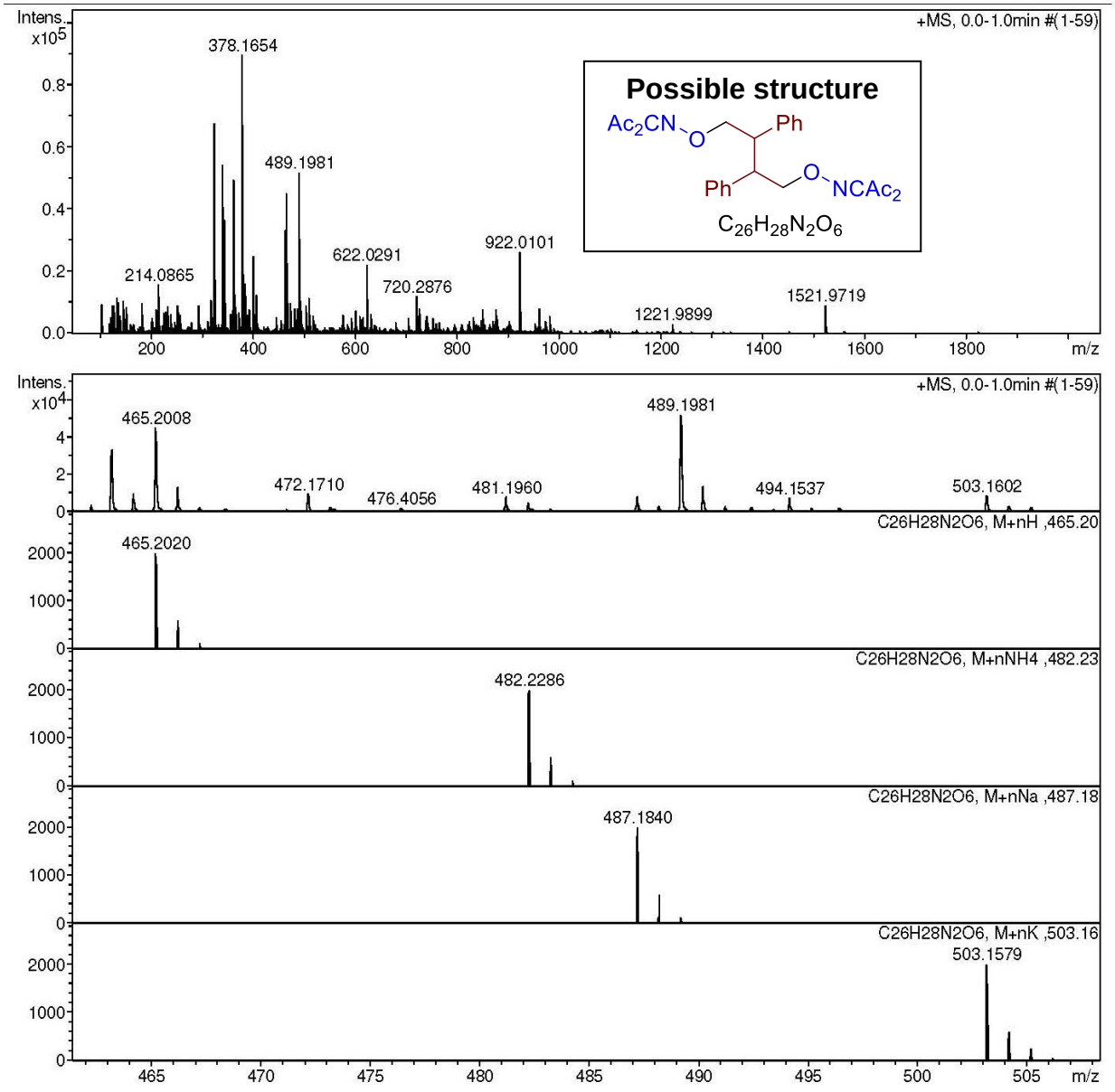
Display Report

Analysis Info

Analysis Name	D:\Data\Chizhov\Terentiev\Budnikov\sm-169_&clblow.d	Acquisition Date	20.07.2023 12:41:45
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SM-169	Instrument / Ser#	micrOTOF 10248
Comment	CH3CN 100 %, dil. 200, calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



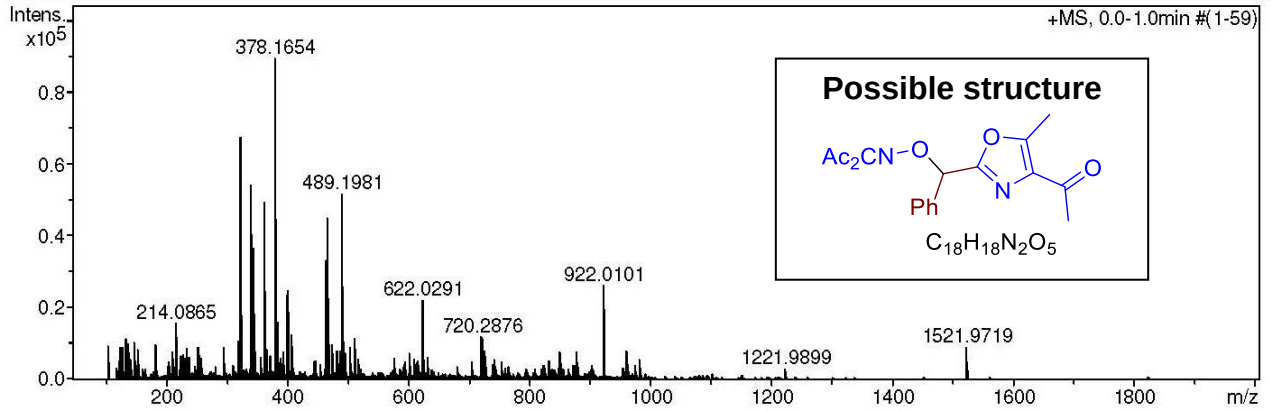
Display Report

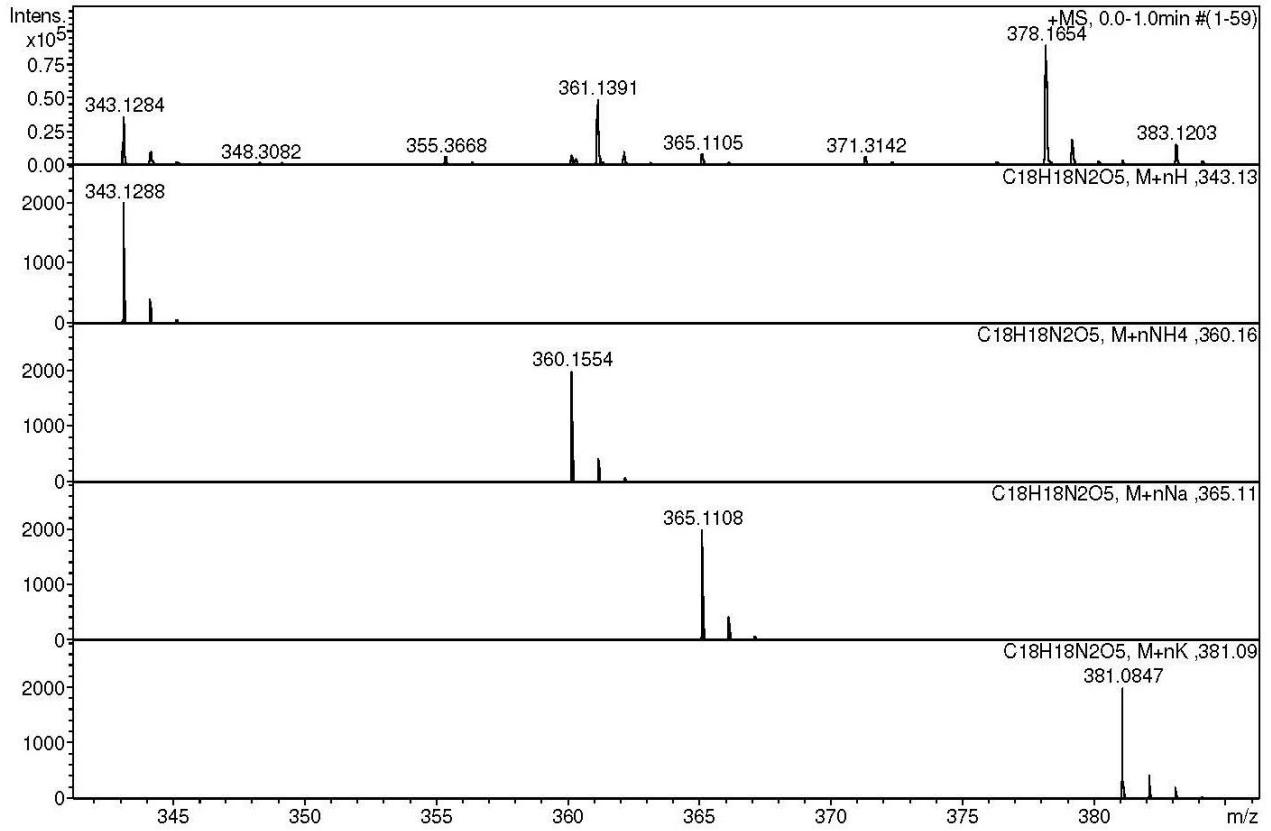
Analysis Info

Analysis Name	D:\Data\Chizhov\Terentiev\Budnikov\sm-169_&clblow.d	Acquisition Date	20.07.2023 12:41:45
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SM-169	Instrument / Ser#	micrOTOF 10248
Comment	CH3CN 100 %, dil. 200, calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





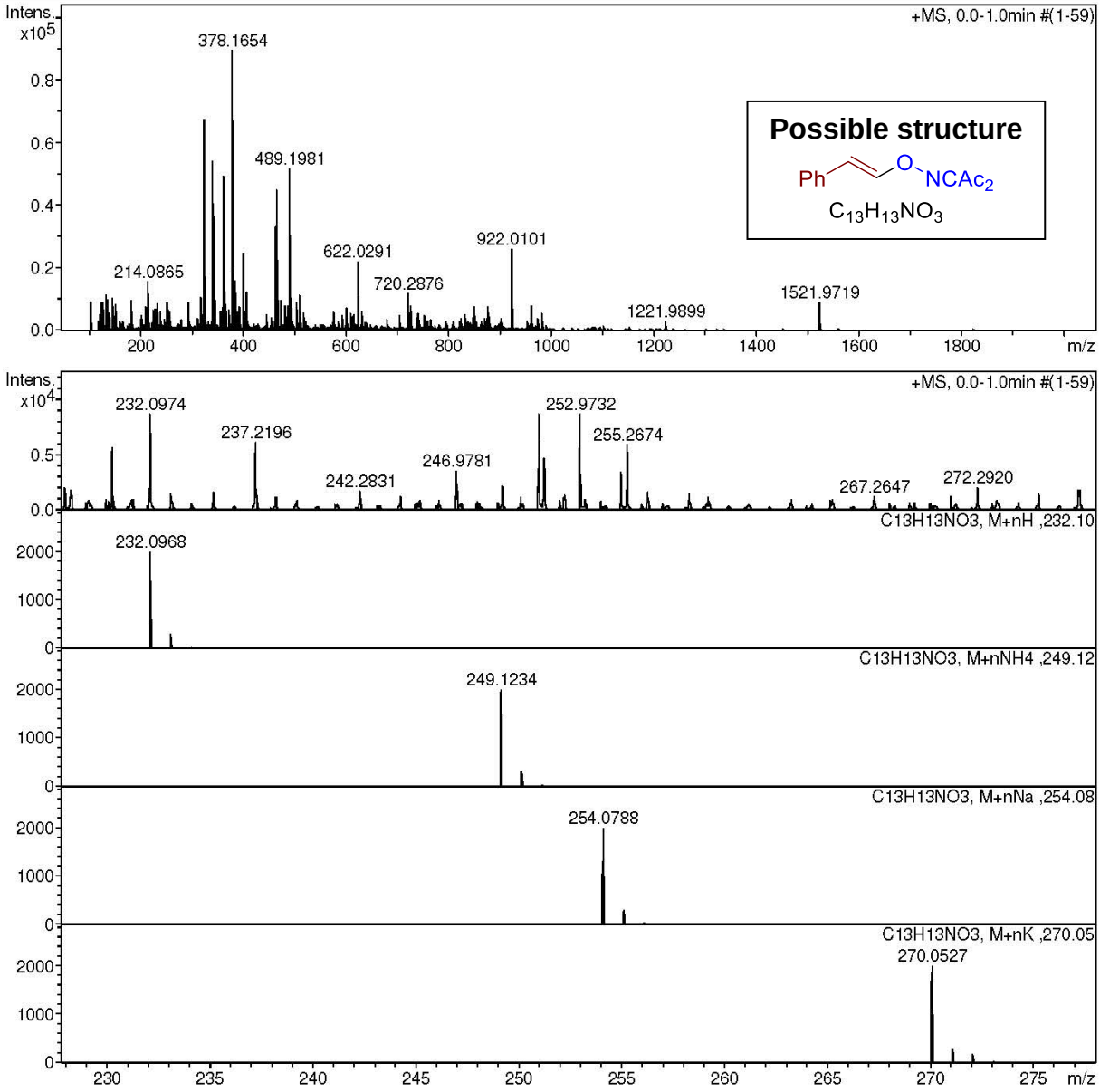
Display Report

Analysis Info

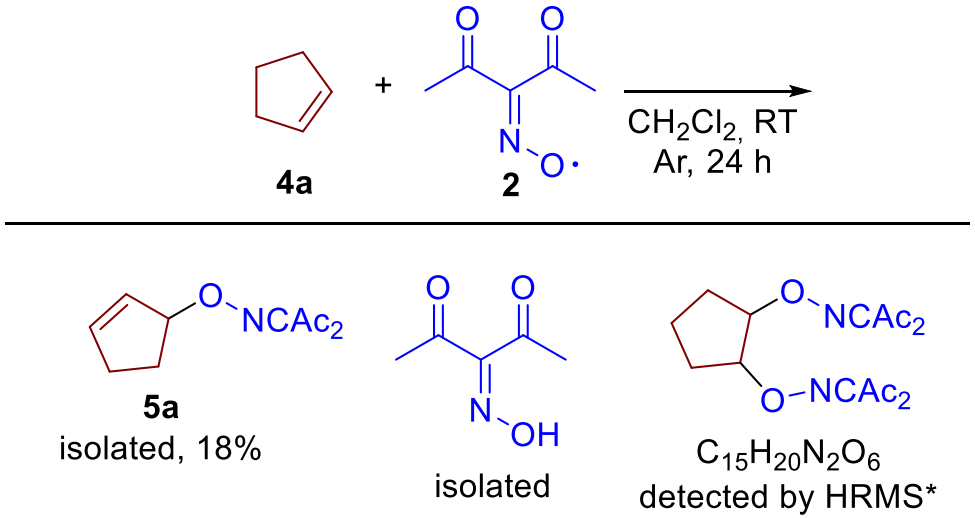
Analysis Name	D:\Data\Chizhov\Terentiev\Budnikov\sm-169_&clblow.d	Acquisition Date	20.07.2023 12:41:45
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SM-169	Instrument / Ser#	micrOTOF 10248
Comment	CH3CN 100 %, dil. 200, calibrant added		

Acquisition Parameter

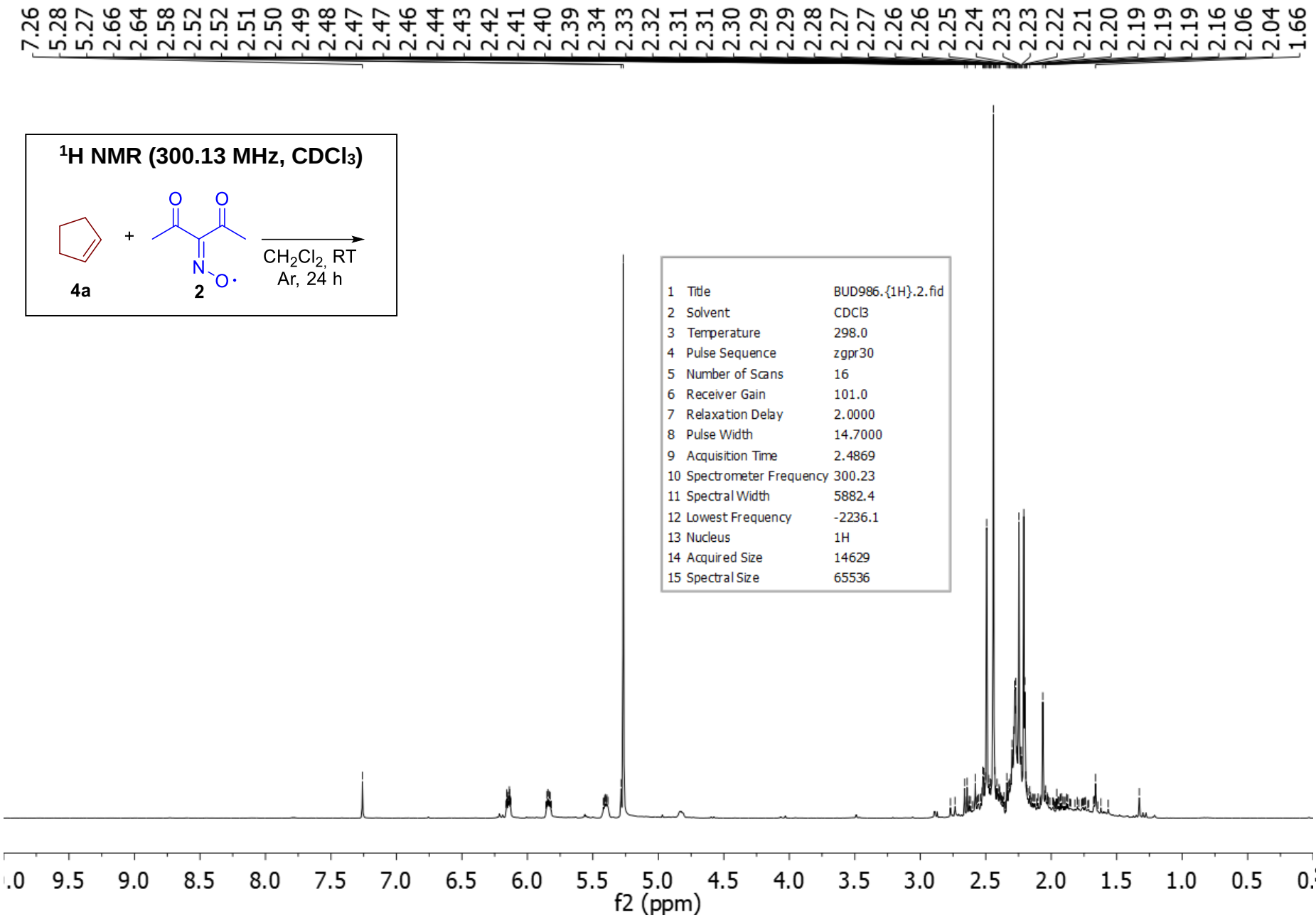
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

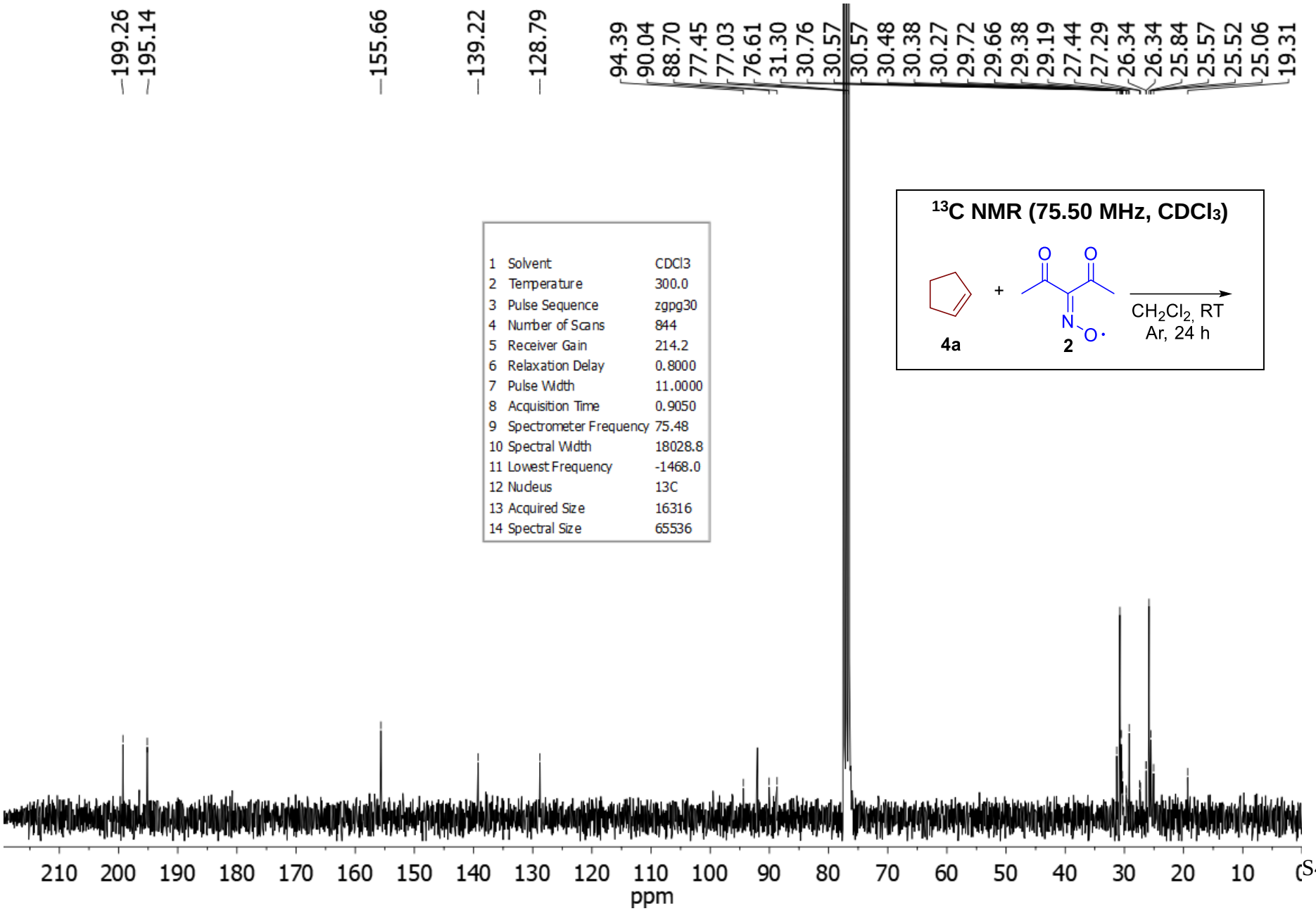


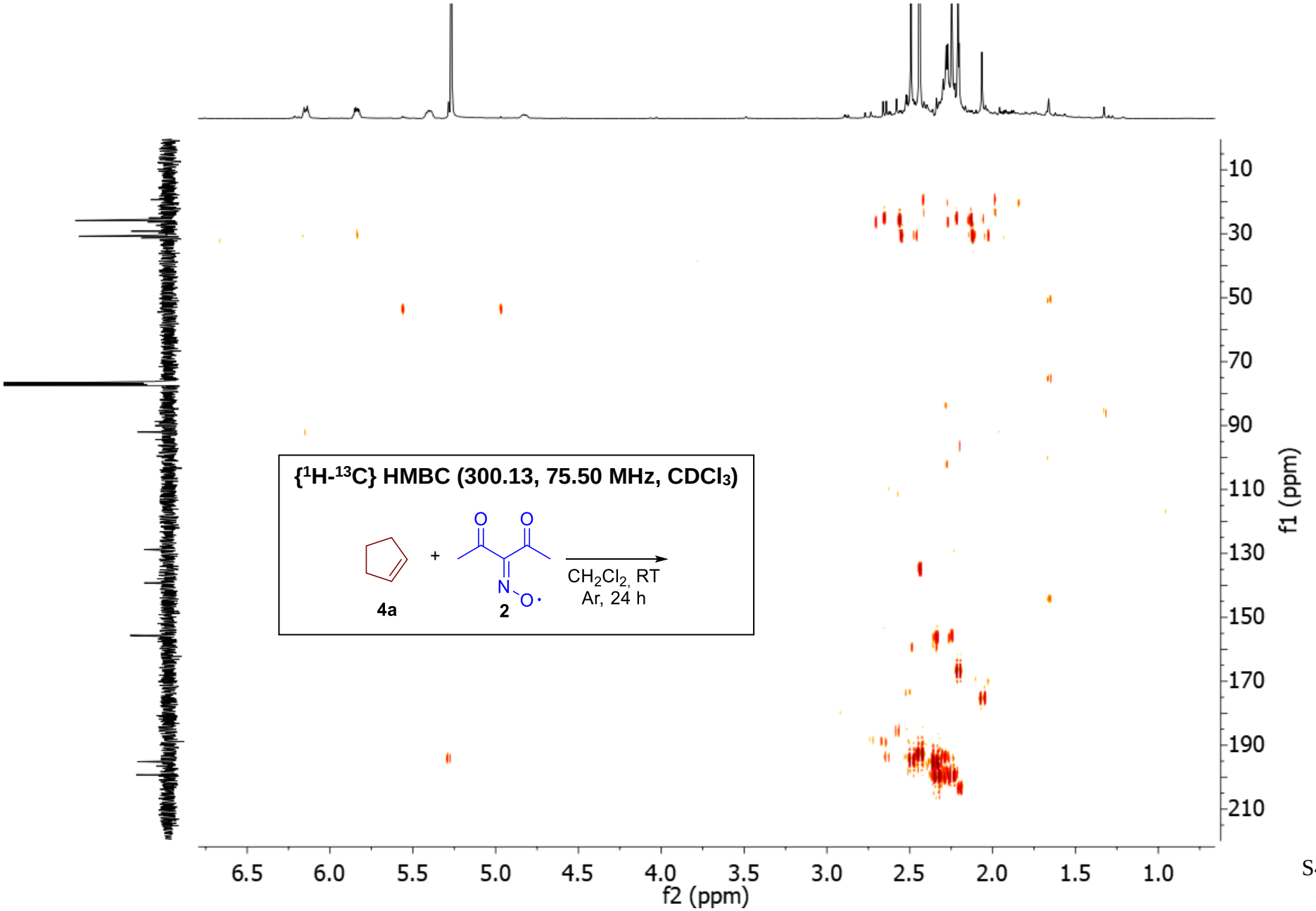
*Reaction with cyclopentene **4a**:* the solution of the diacetyliminoxyl radical **2** (10 mmol in 125 mL CH_2Cl_2) was placed in a two-necked flask. Then cyclopentene **4a** (5 mmol, 340 mg) in CH_2Cl_2 (2 mL) was added and the reaction mixture was stirred for 24 hours at room temperature under an argon atmosphere. 1,1,2,2-Tetrachloroathane was added as an internal standard, and then the crude reaction mixture was analyzed using ^{1}H NMR spectroscopy. The reaction mixture was rotary evaporated under a water-jet vacuum and analyzed employing HRMS and GC-MS.

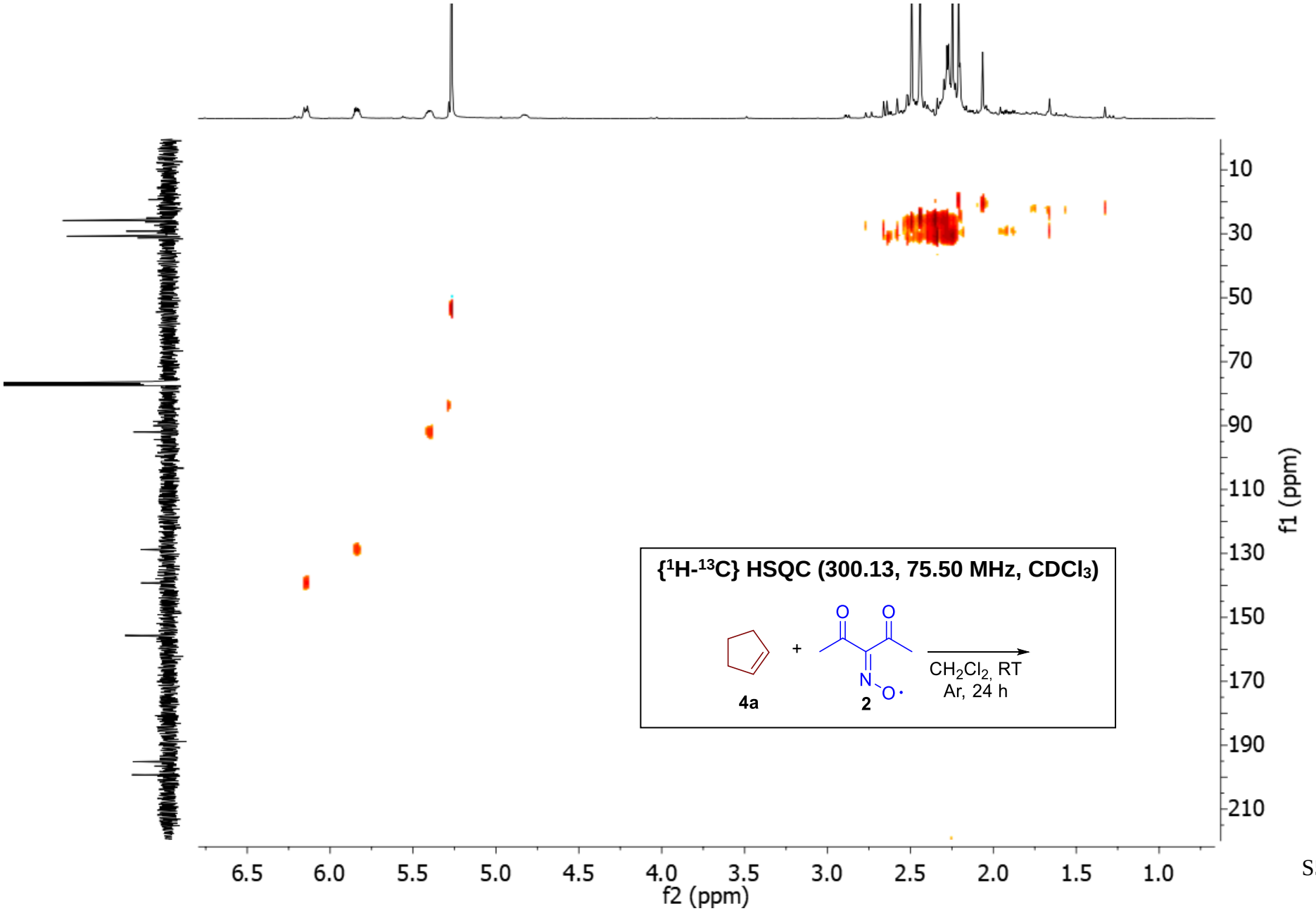


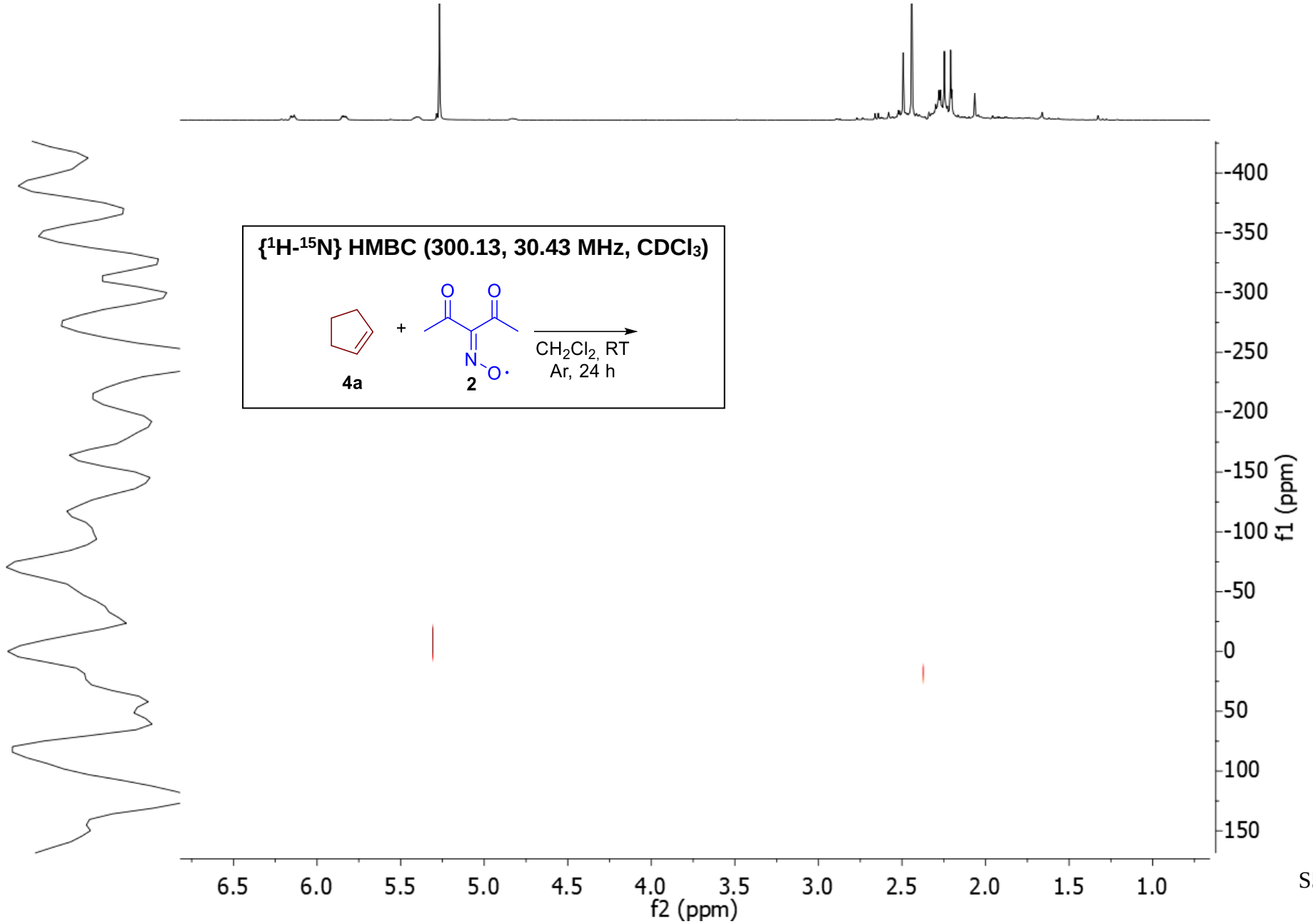
***Possible structure proposed based on HRMS and GC-MS data**


7.26 5.28 5.27 2.66 2.64 2.58 2.52 2.52 2.51 2.50 2.49 2.48 2.47 2.47 2.46 2.44 2.43 2.42 2.41 2.40 2.39 2.34 2.33 2.32 2.31 2.31 2.30 2.29 2.29 2.28 2.27 2.27 2.26 2.26 2.25 2.24 2.23 2.23 2.22 2.21 2.20 2.19 2.19 2.19 2.16 2.06 2.04 1.66
1H NMR (300.13 MHz, CDCl3)
4a
2
CH2Cl2, RT
Ar, 24 h
1 Title BUD986.{1H}.2.fid
2 Solvent CDCl3
3 Temperature 298.0
4 Pulse Sequence zgpr30
5 Number of Scans 16
6 Receiver Gain 101.0
7 Relaxation Delay 2.0000
8 Pulse Width 14.7000
9 Acquisition Time 2.4869
10 Spectrometer Frequency 300.23
11 Spectral Width 5882.4
12 Lowest Frequency -2236.1
13 Nucleus 1H
14 Acquired Size 14629
15 Spectral Size 65536
f2 (ppm)

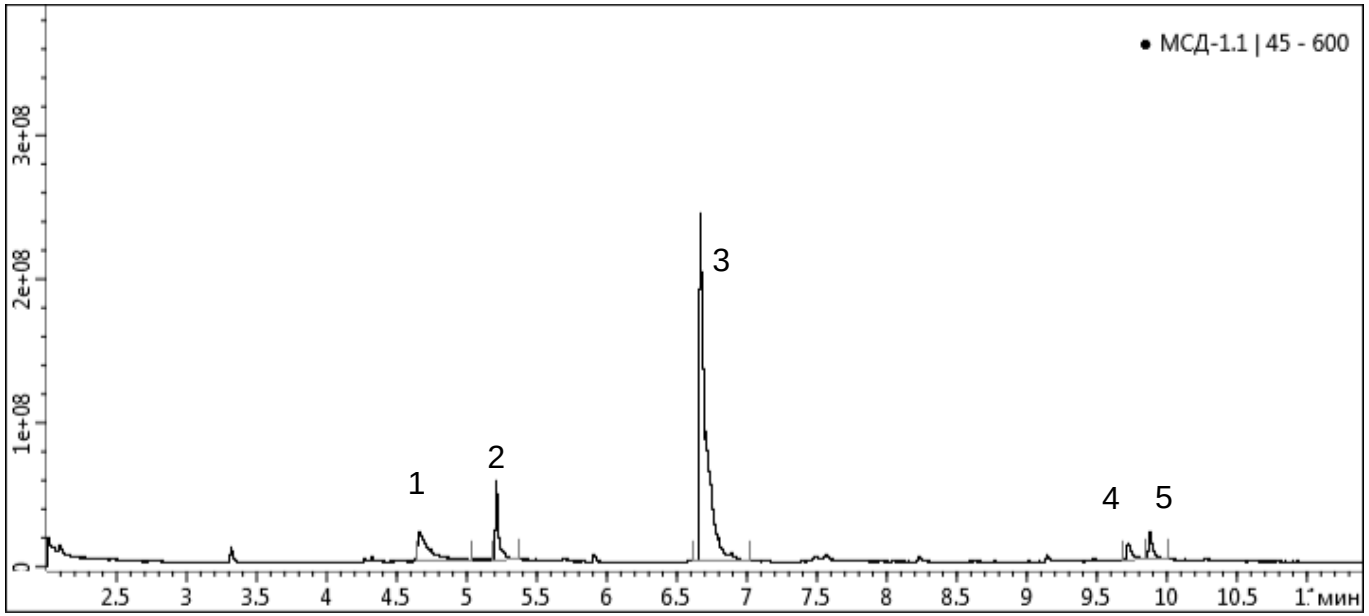

199.26
195.14
155.66
139.22
128.79
94.39
90.04
88.70
77.45
77.03
76.61
31.30
30.76
30.57
30.57
30.48
30.38
30.27
29.72
29.66
29.38
29.19
27.44
27.29
26.34
26.34
25.84
25.57
25.52
25.06
19.31
1 Solvent CDCl3
2 Temperature 300.0
3 Pulse Sequence zgpg30
4 Number of Scans 844
5 Receiver Gain 214.2
6 Relaxation Delay 0.8000
7 Pulse Width 11.0000
8 Acquisition Time 0.9050
9 Spectrometer Frequency 75.48
10 Spectral Width 18028.8
11 Lowest Frequency -1468.0
12 Nucleus 13C
13 Acquired Size 16316
14 Spectral Size 65536
13C NMR (75.50 MHz, CDCl3)
4a
2
CH2Cl2, RT
Ar, 24 h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

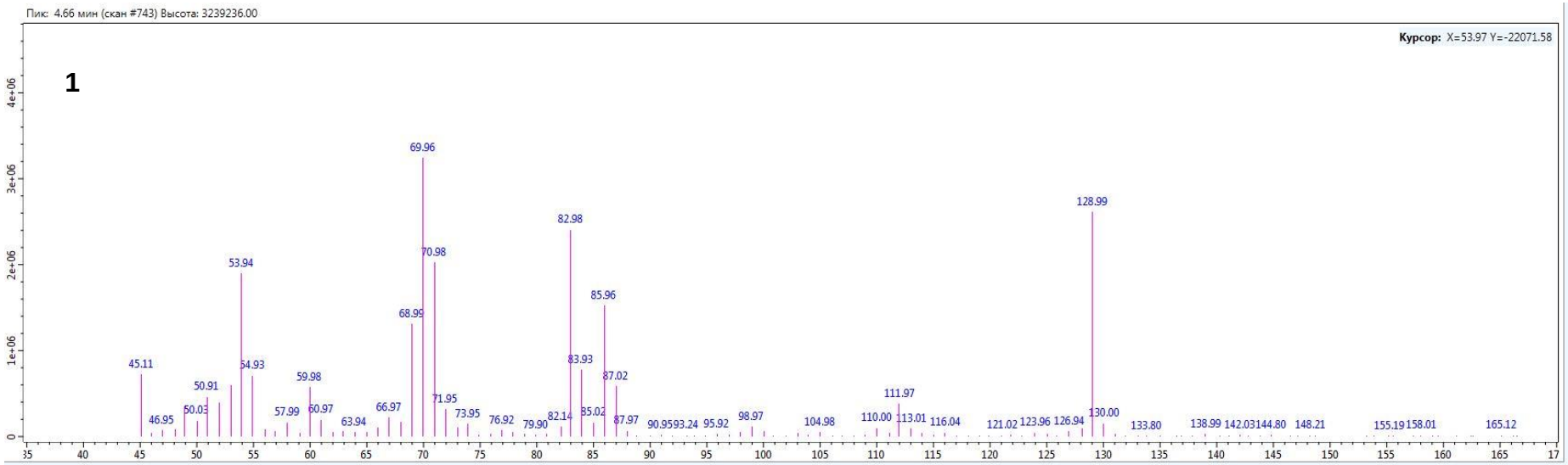

{1H-13C} HMBC (300.13, 75.50 MHz, CDCl3)
4a
2
CH2Cl2, RT
Ar, 24 h
f2 (ppm)
f1 (ppm)

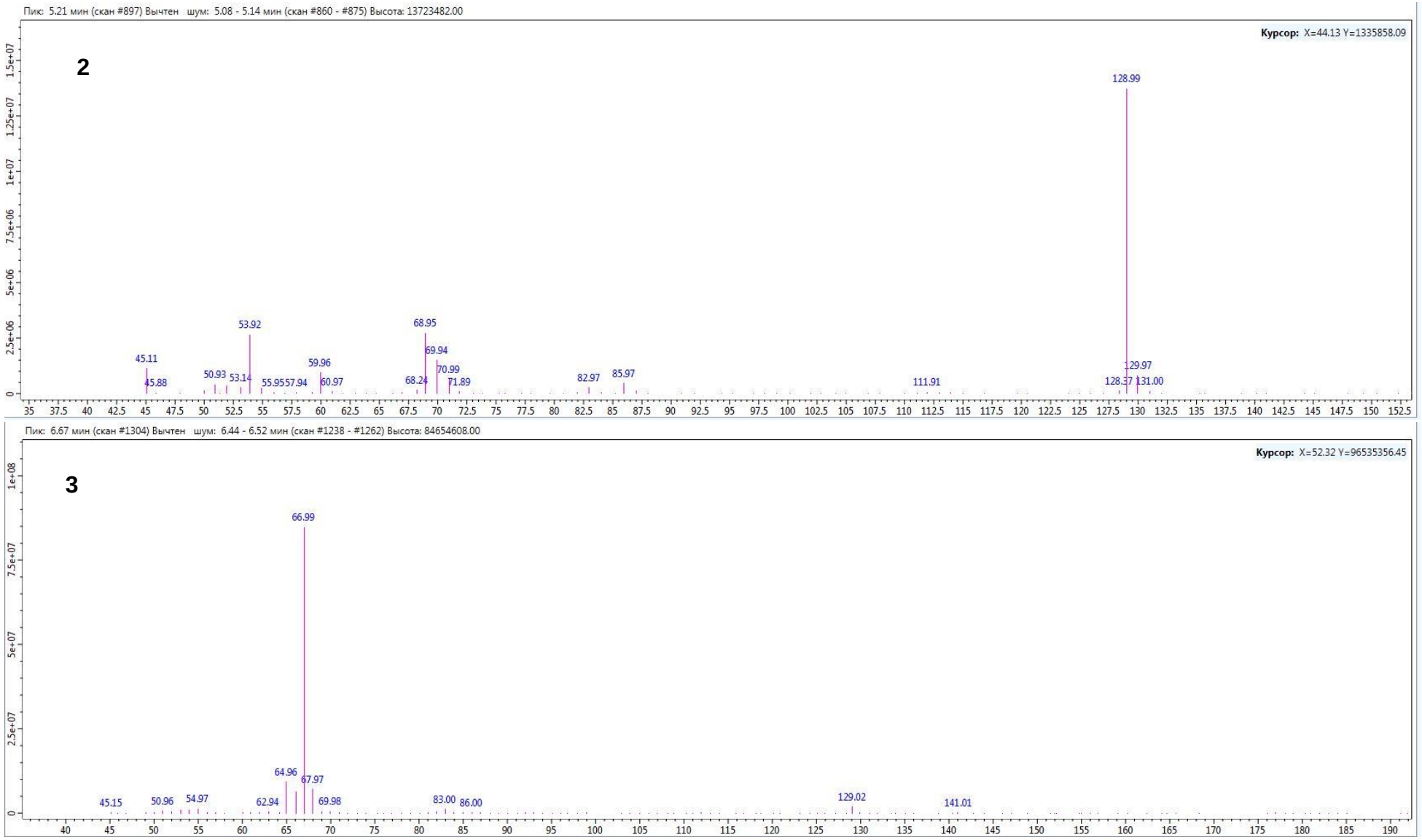

{1H-13C} HSQC (300.13, 75.50 MHz, CDCl3)
4a
2
CH2Cl2, RT
Ar, 24 h
f2 (ppm)
f1 (ppm)


{1H-15N} HMBC (300.13, 30.43 MHz, CDCl3)
4a
2
CH2Cl2, RT
Ar, 24 h
f1 (ppm)
f2 (ppm)

GC-MS analysis of crude reaction mixture






Пик: 5.21 мин (скан #897) Вычтен шум: 5.08 - 5.14 мин (скан #860 - #875) Высота: 13723482.00
Курсор: X=44.13 Y=1335858.09
2
128.99
53.92
68.95
69.94
45.11
59.96
70.99
50.93
53.14
45.88
55.95
57.94
60.97
68.24
71.89
82.97
85.97
111.91
129.97
128.37
131.00
Пик: 6.67 мин (скан #1304) Вычтен шум: 6.44 - 6.52 мин (скан #1238 - #1262) Высота: 84654608.00
Курсор: X=52.32 Y=96535356.45
3
66.99
64.96
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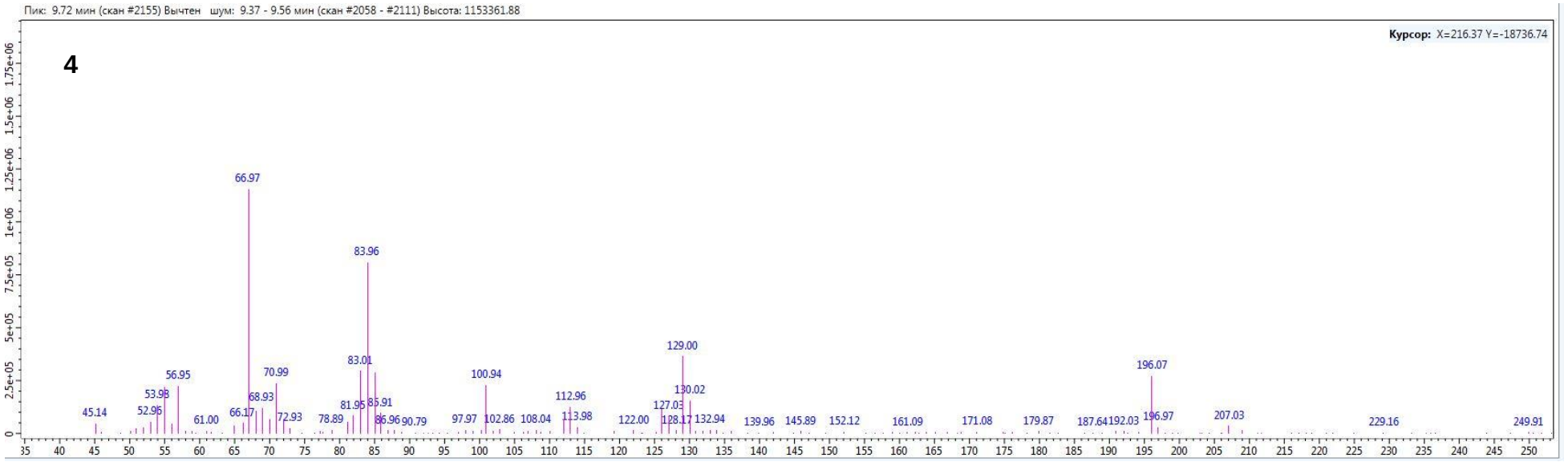
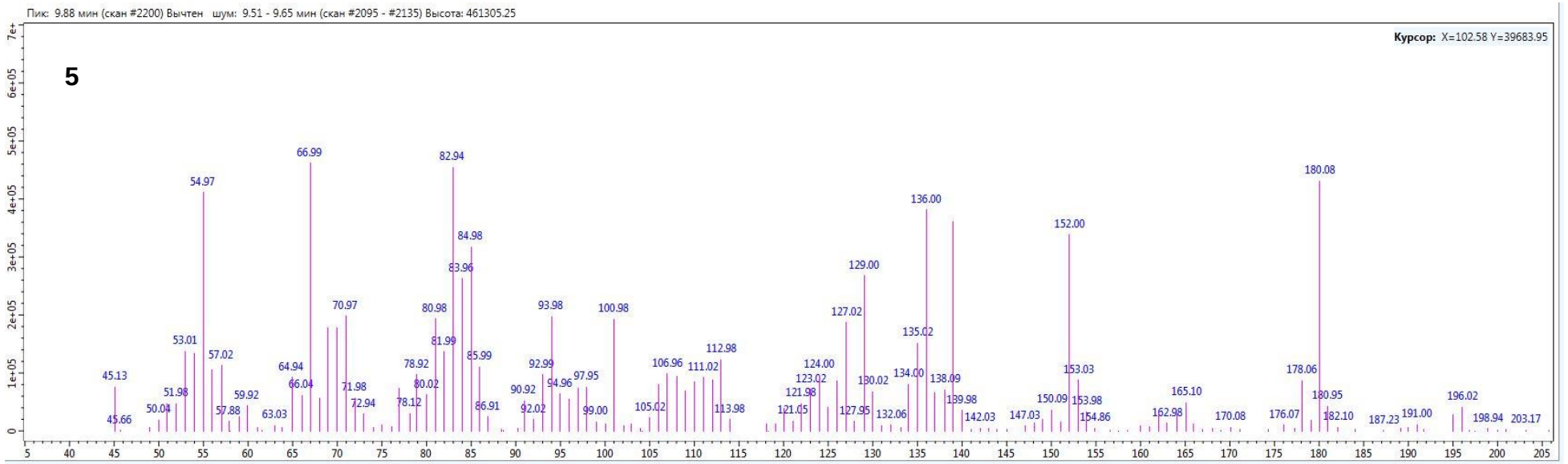
54.97
62.94
69.98
83.00
86.00
129.02
141.01


Пик: 9.72 мин (скан #2155) Вычтен шум: 9.37 - 9.56 мин (скан #2058 - #2111) Высота: 1153361.88
Курсор: X=216.37 Y=-18736.74
4
66.97
83.96
129.00
83.01
56.95
100.94
196.07
70.99
130.02
53.98
68.93
112.96
52.96
45.14
66.17
72.93
78.89
81.95
85.91
86.96
90.79
97.97
102.86
108.04
113.98
122.00
127.03
128.17
132.94
139.96
145.89
152.12
161.09
171.08
179.87
187.64
192.03
196.97
207.03
229.16
249.91


Пик: 9.88 мин (скан #2200) Вычтен шум: 9.51 - 9.65 мин (скан #2095 - #2135) Высота: 461305.25
Курсор: X=102.58 Y=39683.95
5
66.99
82.94
180.08
54.97
136.00
152.00
84.98
83.96
129.00
70.97
80.98
93.98
100.98
127.02
53.01
57.02
81.99
85.99
112.98
135.02
64.94
78.92
92.99
106.96
111.02
124.00
45.13
66.04
71.98
80.02
94.96
97.95
123.02
134.00
138.09
153.03
178.06
51.98
59.92
72.94
78.12
90.92
99.00
121.98
130.02
139.98
150.09
153.98
180.95
165.10
196.02
50.04
57.88
63.03
86.91
92.02
105.02
113.98
121.05
127.95
132.06
142.03
147.03
154.86
162.98
170.08
176.07
182.10
187.23
191.00
198.94
203.17
45.66

HRMS analysis of crude reaction mixture

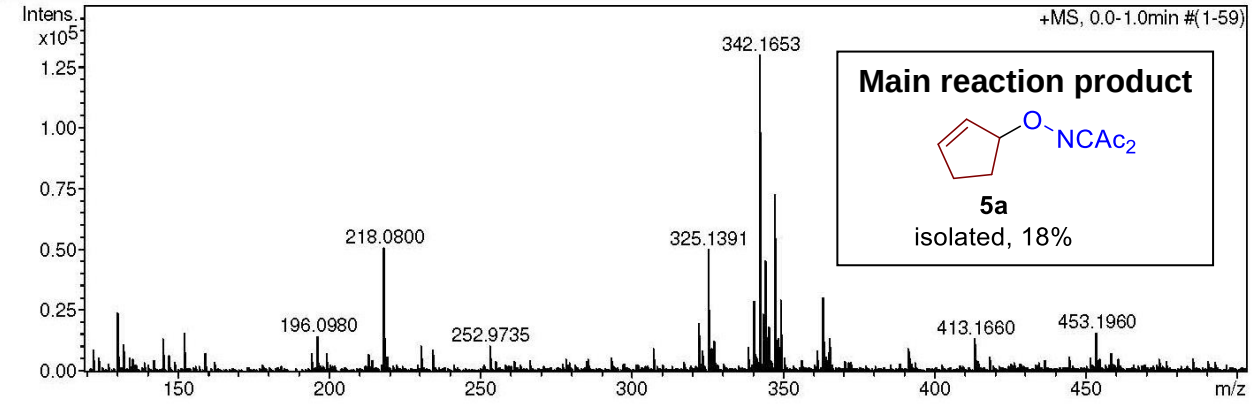
Display Report

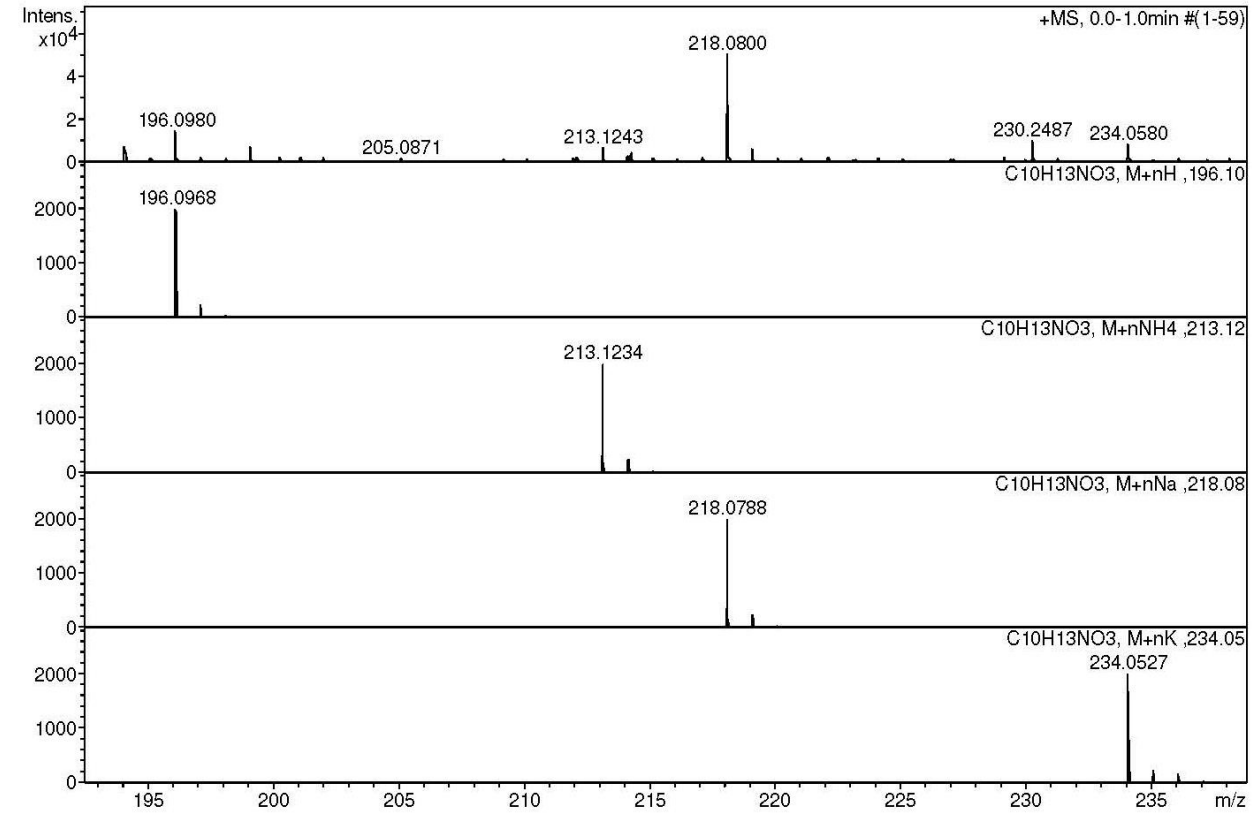
Analysis Info

Analysis Name	D:\Data\Chizhov\Terentiev\Budnikov\sm-170_&clblow.d	Acquisition Date	24.07.2023 11:58:31
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SM-170	Instrument / Ser#	micrOTOF 10248
Comment	CH3CN 100 %, dil 200, calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





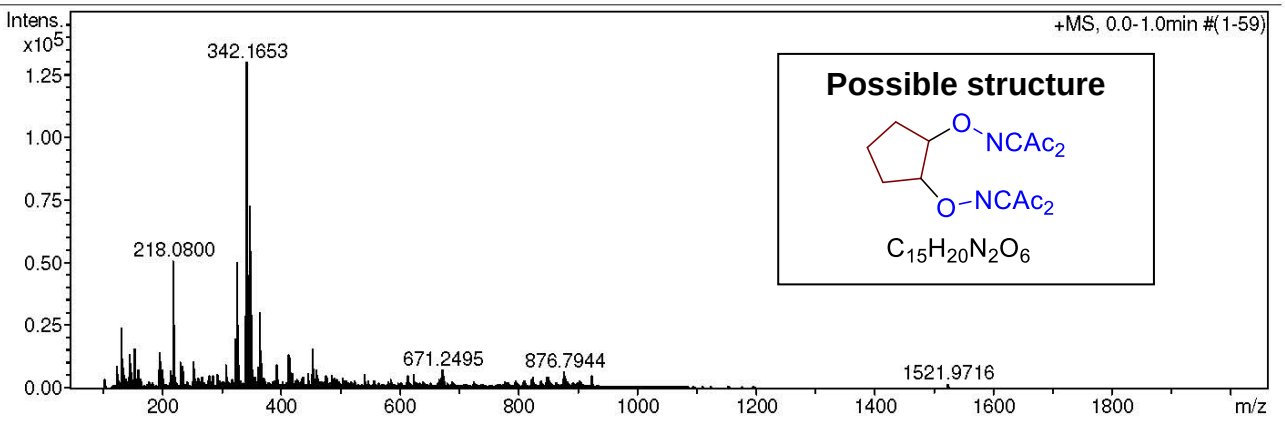
Display Report

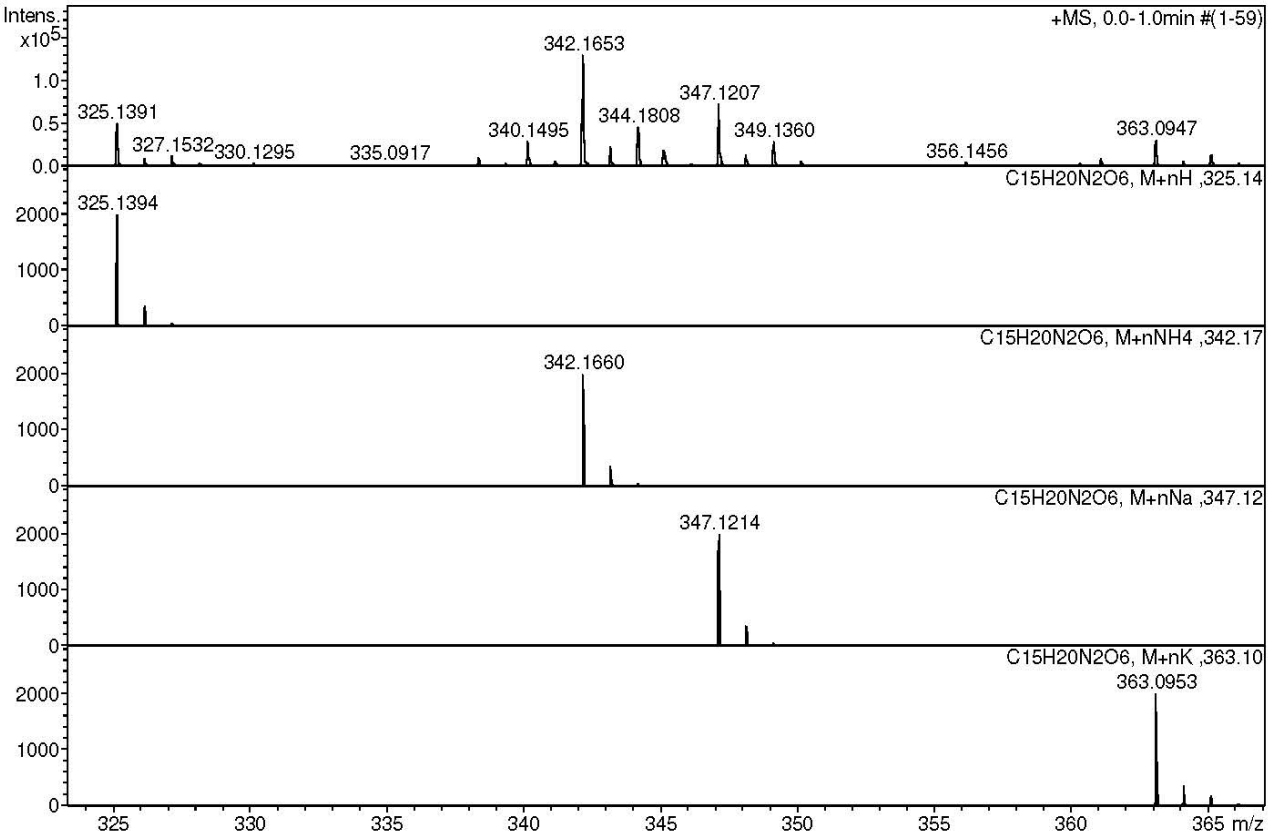
Analysis Info

Analysis Name	D:\Data\Chizhov\Terentiev\Budnikov\sm-170_&clblow.d	Acquisition Date	24.07.2023 11:58:31
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN SM-170	Instrument / Ser#	micrOTOF 10248
Comment	CH3CN 100 %, dil 200, calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





X-ray single-crystal diffraction: Structure determination of compounds *anti*-3g, 3j' and 3l

X-ray diffraction data were collected at 100K on a Bruker Quest D8 diffractometer equipped with a Photon-III area-detector (graphite monochromator, shutterless φ- and ω-scan technique), using Mo K_α-radiation (0.71073 Å). The intensity data were integrated by the SAINT program[5] and corrected for absorption and decay using SADABS.[6] The structure was solved by direct methods using SHELXT[7] and refined on F^2 using SHELXL-2018.[8] All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were placed in ideal calculated positions and refined as riding atoms with relative isotropic displacement parameters. The SHELXTL program suite[5] was used for molecular graphics. Crystal data and structure refinement for ***anti*-3g**, **3j'** and **3l** are summarized in Table S1–S3.

Compound ***anti*-3g** crystallizes in monoclinic space group $P2_1/c$ (Figure S1).

Table S1. Crystal data and structure refinement for ***anti*-3g.**

Identification code	B.699-1	
Empirical formula	$C_{24}H_{24}N_2O_6$	
Formula weight	436.45	
Temperature	100.0(1) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 11.2566(2) Å	α = 90°.
	b = 5.41860(10) Å	β = 92.9970(10)°.
	c = 18.4668(3) Å	γ = 90°.
Volume	1124.84(3) $Å^3$	
Z	4	
Density (calculated)	1.289 g/cm^3	
Absorption coefficient	0.772 mm^{-1}	
F(000)	460	
Crystal size	0.16 x 0.04 x 0.02 mm^3	

Theta range for data collection	3.932 to 79.466°.	
Index ranges	-14<=h<=14, -6<=k<=4, -23<=l<=23	
Reflections collected	12674	
Independent reflections	2420 [R(int) = 0.0356]	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.75658	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2420 / 0 / 148	
Goodness-of-fit on F^2	1.100	
Final R indices [I>2sigma(I)]	R1 = 0.0441, wR2 = 0.1203	
R indices (all data)	R1 = 0.0466, wR2 = 0.1223	
Extinction coefficient	0.0045(8)	

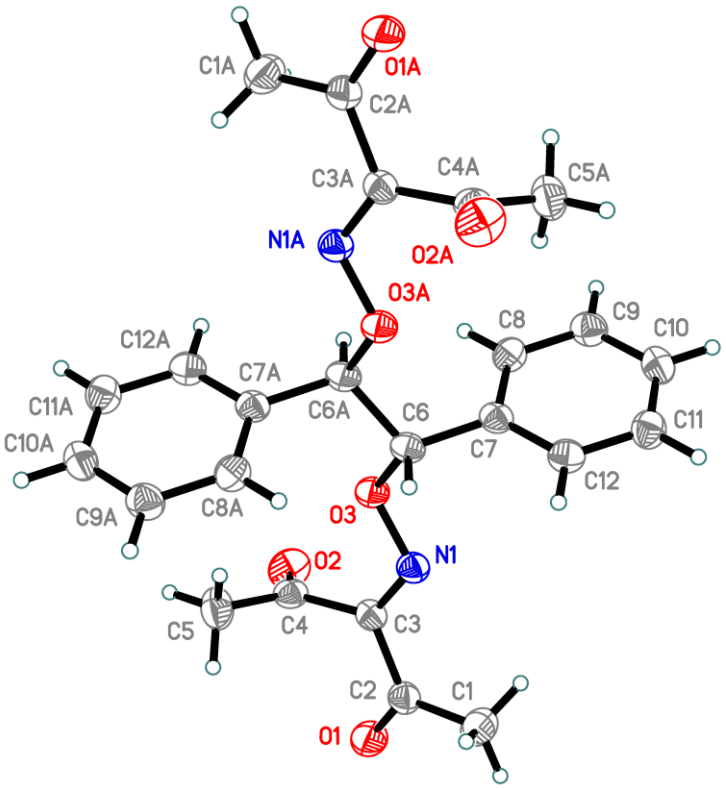


Figure S1. Crystal structure of compound ***anti*-3g**, showing the atomic numbering and 50% probability displacement ellipsoids

Crystal data and structure refinement for **3j'** are summarized in Table S2. Compound **3j'** crystallizes in monoclinic space group P 2_1/n (Figure S3).

Table S2. Crystal data and structure refinement for **3j'**.

Identification code	LA-293	
Empirical formula	$C_{24}H_{22}N_2O_5$	
Formula weight	418.43	
Temperature	99.9(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P 2_1/n	
Unit cell dimensions	a = 11.6766(3) Å	α = 90°.
	b = 15.1780(4) Å	β = 104.950(2)°.
	c = 12.1389(3) Å	γ = 90°.
Volume	2078.53(9) $Å^3$	
Z	4	

Density (calculated)	1.337 g/cm^3	
Absorption coefficient	0.777 mm^{-1}	
F(000)	880	
Crystal size	0.12 x 0.06 x 0.02 mm^3	
Theta range for data collection	4.686 to 77.826°.	
Index ranges	-12<=h<=14, -19<=k<=17, -15<=l<=15	
Reflections collected	25662	
Independent reflections	4433 [R(int) = 0.1019]	
Observed reflections	3958	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.13417	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4433 / 23 / 333	
Goodness-of-fit on F^2	1.044	
Final R indices [I>2sigma(I)]	R1 = 0.0655, wR2 = 0.1740	
R indices (all data)	R1 = 0.0707, wR2 = 0.1776	
Largest diff. peak and hole	0.343 and -0.330 e.Å^{-3}	

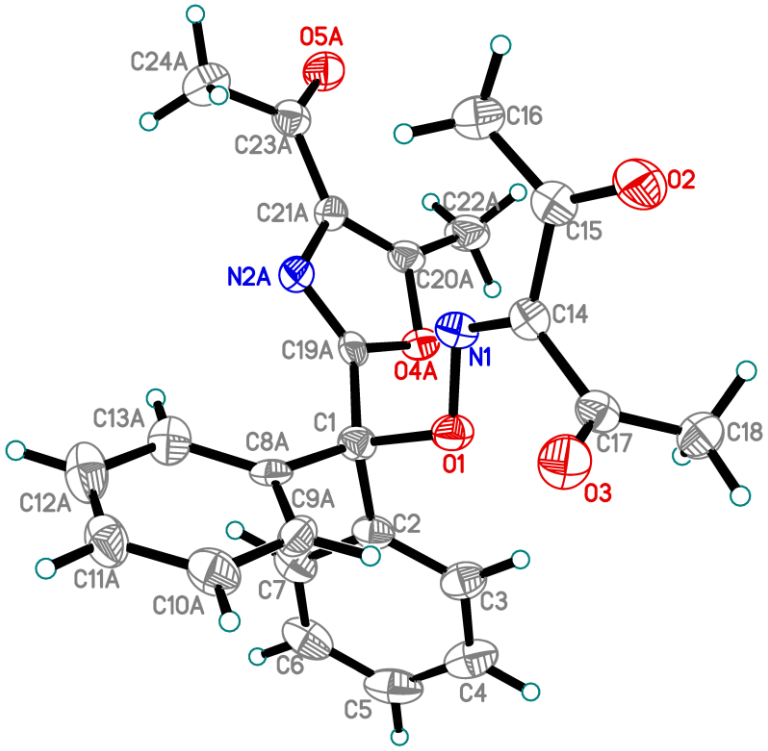


Figure S2. Crystal structure of compound **3j'**, showing two independent molecules, atomic numbering and 50% probability displacement ellipsoids.

Crystal data and structure refinement for **3l** are summarized in Table S3. Compound **3l** crystallizes in orthorombic space group P-1 (Figure S3).

Table S3. Crystal data and structure refinement for **3l.**

Identification code	LA88	
Empirical formula	$C_{44}H_{46}N_2O_8$	
Formula weight	730.83	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.9695(4) Å	α = 62.1699(10)°.
	b = 10.9993(5) Å	β = 79.6611(10)°.
	c = 11.5562(5) Å	γ = 79.0306(10)°.

Volume	984.41(8) $Å^3$	
Z	1	
Density (calculated)	1.233 Mg/m^3	
Absorption coefficient	0.085 mm^{-1}	
F(000)	388	
Crystal size	0.48 x 0.42 x 0.38 mm^3	
Theta range for data collection	2.813 to 29.996°.	
Index ranges	-12<=h<=12, -15<=k<=15, -16<=l<=16	
Reflections collected	24408	
Independent reflections	5739 [R(int) = 0.0450]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8751 and 0.8335	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5739 / 7 / 260	
Goodness-of-fit on F^2	1.052	
Final R indices [I>2sigma(I)]	R1 = 0.0474, wR2 = 0.1074	
R indices (all data)	R1 = 0.0653, wR2 = 0.1208	
Extinction coefficient	n/a	

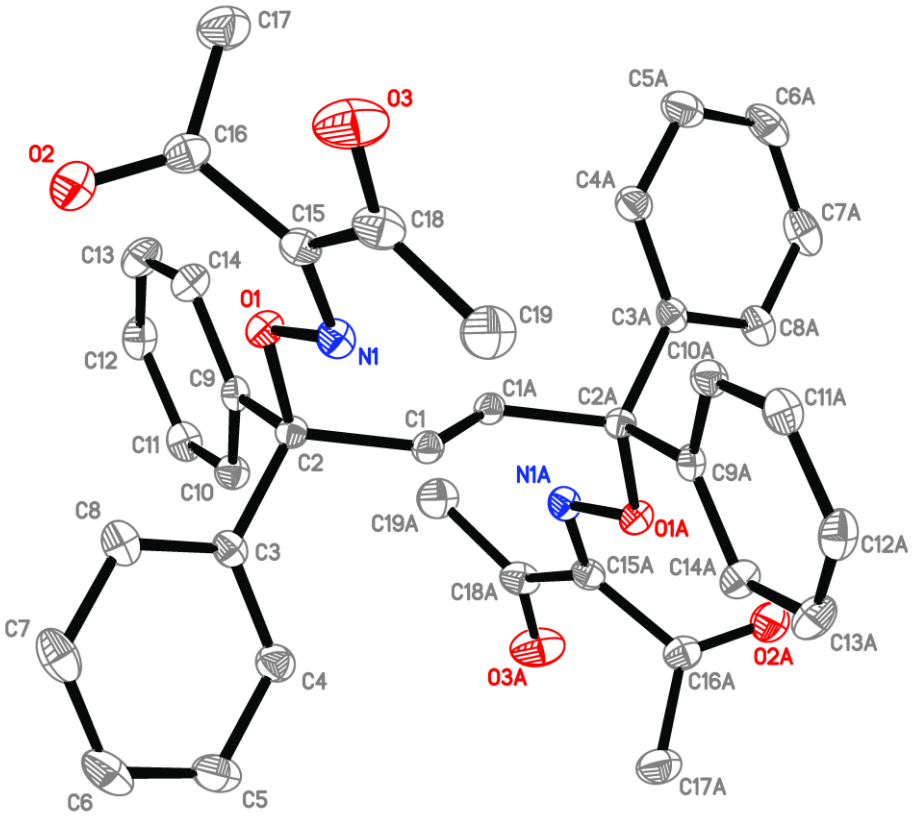
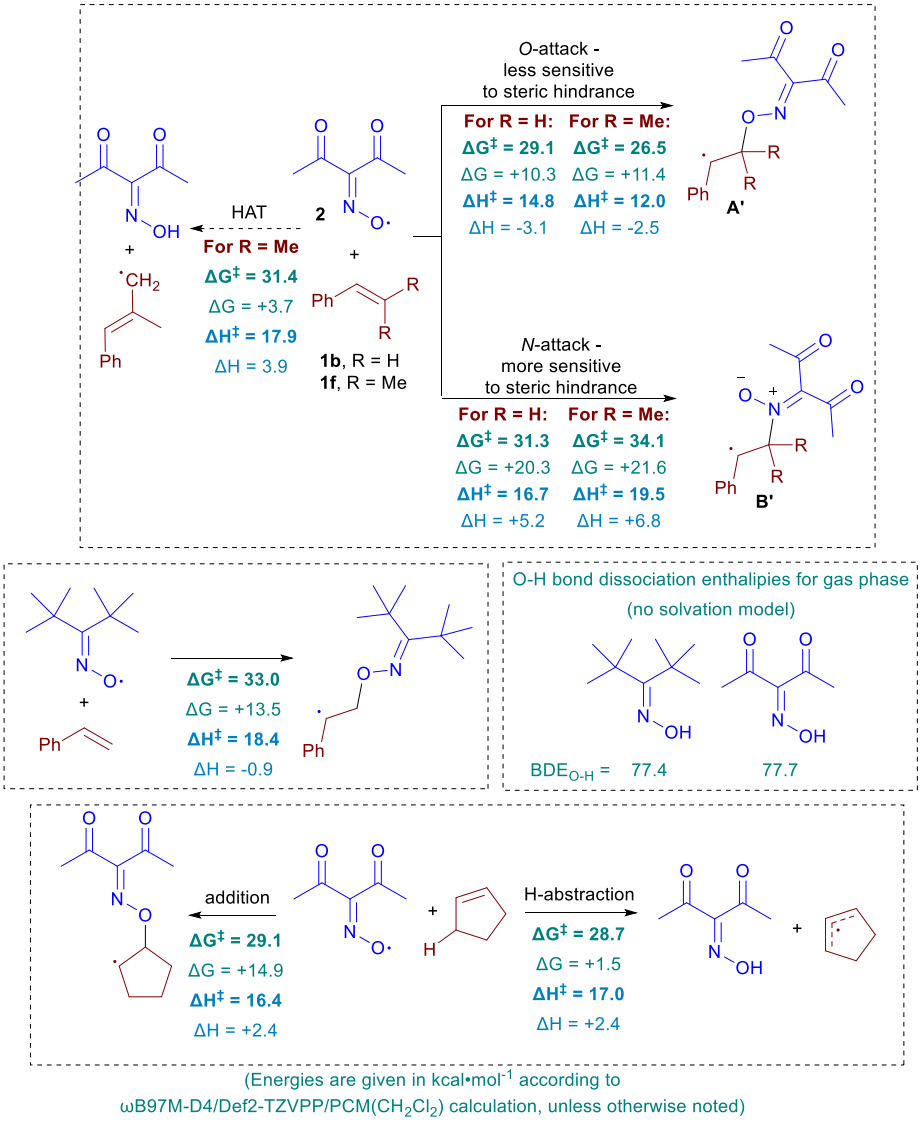


Figure S3. Crystal structure of compound **3l**, showing two independent molecules, atomic numbering and 50% probability displacement ellipsoids.

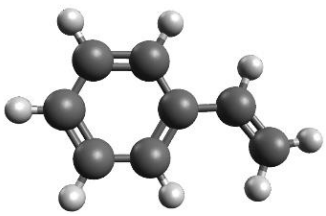
Computational details

All calculations were performed using Orca 5.04 software[9] for 218.15 K and 1 atm. pressure. DFT calculations were performed at ωB97M-D4[10–14]/Def2-TZVPP[15,16]/ CPCM(CH_2Cl_2) level. The resultant geometries were visualized by Avogadro[17] 1.2 program. Default integration grids were used for all DFT calculations. Schematic calculation summary and optimized geometries are given below.



(Energies are given in kcal•mol^{-1} according to ωB97M-D4/Def2-TZVPP/PCM(CH_2Cl_2) calculation, unless otherwise noted)

Styrene (1b)



imaginary frequencies: no

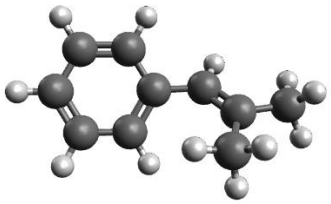
Electronic energy ... -309.86030125 Eh

Enthalpy ... -309.71856849 Eh

Gibbs free energy ... -309.75773404 Eh

C	1.35064444930595	1.32285636676826	-0.00909465416026
C	-0.01326930397236	1.08374238149484	-0.03007820802393
C	-0.50829409550763	-0.22214852839123	-0.02198155917194
C	0.40425079540716	-1.27598422148730	-0.00032551208730
C	1.77180128034358	-1.03898147069135	0.02094581599019
C	2.25020140184891	0.26265496750450	0.01786466846375
H	1.71550398358938	2.34049877744947	-0.01614900906108
H	-0.69550832202782	1.92137185176208	-0.05709328124003
H	0.03435394727448	-2.29294776030456	0.00176818458279
H	2.46115827350658	-1.87144076880670	0.03926810186412
H	3.31405482787927	0.45276626417100	0.03350131357436
C	-1.95152197062312	-0.53222148720687	-0.03422886674933
H	-2.18753571247781	-1.58800650333930	-0.10957671804308
C	-2.95224479048337	0.33771703879056	0.04647441775945
H	-2.79262052715321	1.40390586193978	0.13277573851620
H	-3.97773623690999	-0.00228576965317	0.03005356778609

(2-methylprop-1-en-1-yl)benzene (β,β-dimethylstyrene) 1f



imaginary frequencies: no

Electronic energy ... -388.54403884 Eh

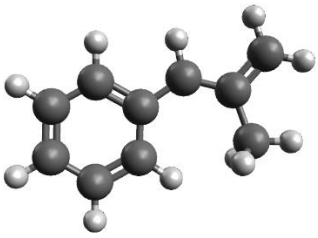
Total Enthalpy ... -388.34336482 Eh

Final Gibbs free energy ... -388.38816500 Eh

C	-2.15704560281568	1.24974497311216	0.33875332042756
C	-0.81331857634033	0.93233715876228	0.48282909654364

C	-0.34526334642931	-0.34873644332281	0.18792661639243
C	-1.27146243308766	-1.31021748960175	-0.22320470387375
C	-2.61339105472013	-0.99542318644190	-0.37024679548621
C	-3.06157924735317	0.29035982376467	-0.09454970034026
H	-2.49848299932525	2.24846362578972	0.57347409556190
H	-0.12441108637013	1.68125942334572	0.84551471074623
H	-0.92873697008276	-2.31503879894638	-0.43318677026536
H	-3.31054534749651	-1.75436950406402	-0.69739352464516
H	-4.10773515202765	0.53828181618724	-0.20604943458653
C	1.07321867236141	-0.73469679128677	0.33715415685108
H	1.23406930746848	-1.71893493559219	0.76472661021493
C	2.15337551855281	-0.03639158490855	-0.02010114657689
C	2.12749900776848	1.29983218540747	-0.70699723012818
H	1.15116076561144	1.54396978071722	-1.11441994577269
H	2.41692729613681	2.09480536661592	-0.01727879567552
H	2.85566481300382	1.30700508796618	-1.51892323622867
C	3.53037939904781	-0.58467220452443	0.23037986423919
H	4.07085453676758	-0.70671078065830	-0.71008902346508
H	4.11172833808878	0.11136039509930	0.83825757679864
H	3.49643616124116	-1.54437091742078	0.74120425926872

2-Methyl-1-phenylprop-1-en-3-yl radical



imaginary frequencies: no

Electronic energy ... -387.89990072 Eh

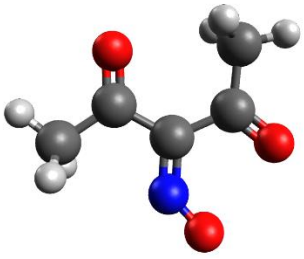
Total Enthalpy ... -387.71227132 Eh

Final Gibbs free energy ... -387.75663674 Eh

C	-3.96031606002087	-0.93019108439408	-0.96677533863619
C	-3.05660130685274	0.10610114840669	-0.80456237859033

C	-2.44897075031993	0.34961143018948	0.44352081809416
C	-2.81038560999974	-0.50470890672764	1.50813301473507
C	-3.70993977947637	-1.53843195678433	1.33930257403297
C	-4.29421973198797	-1.76064733673339	0.09624539015213
H	-4.41121270365126	-1.08957412766283	-1.93651953352189
H	-2.83454844653251	0.72764292691957	-1.65351159085377
H	-2.36229167201403	-0.33987214064692	2.47896509278320
H	-3.95900454291653	-2.17404145681755	2.17761271469372
H	-5.00053425746656	-2.56691668333561	-0.04055915480963
C	-1.50025367739266	1.38854935841779	0.73864533022498
H	-1.20899204829062	1.42910013874898	1.78151565705924
C	-0.86141462539453	2.35125474681098	-0.07943525847286
C	0.01466818898108	3.21558822592768	0.51179221747604
H	0.53748497429643	3.96388175691154	-0.06585374377525
H	0.20917039623609	3.17178157284158	1.57441650921053
C	-1.09085623075870	2.46049157202426	-1.56562916299703
H	-0.87144850545836	1.52162341667105	-2.07207772720940
H	-2.12390565397140	2.72302899909343	-1.78972205986267
H	-0.44939195700880	3.23079740013933	-1.98600136973302

Diacetyliminoxyl radical (2)



imaginary frequencies: no

Data for CH_2Cl_2 solution (CPCM(CH_2Cl_2)):

Electronic energy ... -474.79857777 Eh

Enthalpy ... -474.68017033 Eh

Gibbs free energy ... -474.72589061 Eh

C	-1.34391360268917	-1.97489389616281	-0.00005508129894
C	-1.29677176677711	-0.47756232467834	-0.00009543238447

H	-2.38322784105653	-2.28665930100941	-0.00021990196048
H	-0.82517510300463	-2.36461085576818	-0.87290544328720
H	-0.82546969950591	-2.36455281244627	0.87299536447581
C	0.04154194160710	0.21507142047776	0.00001427702651
C	1.38966042617646	-0.42147987116027	0.00009814188540
C	2.58263817947926	0.49500607097513	-0.00005264118030
H	2.56416614070916	1.13845972353522	-0.87821958817116
H	3.48502730169563	-0.10697632165089	-0.00017051530053
H	2.56438424013185	1.13844121096024	0.87813158923802
N	0.03481973270437	1.50895276970314	0.00015508023160
O	-0.83385838676950	2.33124860472034	0.00016743220168
O	-2.29782998789552	0.20371349514827	-0.00036257502337
O	1.50248542519456	-1.62831091264392	-0.00004570645257

Data for gas phase (no solvation model):

Electronic energy ... -474.78841609 Eh

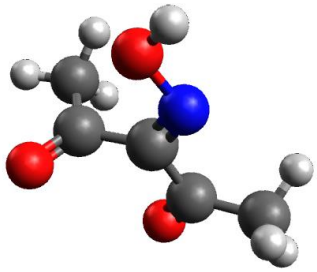
Total Enthalpy ... -474.66962929 Eh

Final Gibbs free energy ... -474.71520932 Eh

C	-1.34140521527958	-1.97497917431078	-0.00006898190978
C	-1.30009685803088	-0.47344664682899	0.00003582030632
H	-2.38112157417478	-2.28481331571107	-0.00023764645348
H	-0.81958013166151	-2.36818143761489	-0.86923887197598
H	-0.81982855812343	-2.36828624207888	0.86920050151119
C	0.03964953081903	0.22197756909311	0.00005825624254
C	1.38382950166388	-0.41891134061871	0.00008269222782
C	2.58669678869240	0.49279531190972	-0.00004607428814
H	2.57874464641103	1.13806076658519	-0.87674362076284
H	3.48095650495777	-0.12084335186668	-0.00014204149497
H	2.57892882532954	1.13804891115957	0.87666144233512
N	0.02863839009441	1.51829825812232	0.00006197468771

O	-0.85402233003329	2.32544483874120	0.00005348506205
O	-2.29858871541537	0.20363937064273	-0.00024825399379
O	1.49567619475078	-1.62295651722384	0.00000631850623

Diacetyl oxime



imaginary frequencies: no

Data for CH_2Cl_2 solution (CPCM(CH_2Cl_2)):

Electronic energy ... -475.43603163 Eh

Total Enthalpy ... -475.30507158 Eh

Final Gibbs free energy ... -475.35153736 Eh

N	0.07089856643062	1.52642995515225	-0.00351077400450
C	0.09391872015488	0.25994541679991	0.08295747963054
C	-1.14880453602613	-0.60169367959328	0.23302511795449
C	1.42095344832879	-0.43176562240576	0.03938659293772
O	-1.52376143229452	-0.90537804735630	1.33914707485547
O	1.42808377307751	-1.64462235134335	0.06185830751165
O	-1.20828387321412	2.02501270283204	0.03685887663770
H	-1.09579506008548	2.97690770658330	-0.05630439506377
C	-1.81159149778430	-1.02781361077846	-1.03574877159937
H	-2.70240724415936	-1.60972223480520	-0.82113584508559
H	-2.06125774375224	-0.14702992639916	-1.62696189882794
H	-1.10457114967474	-1.61984872279287	-1.61819578312573
C	2.66344389280294	0.40118639869039	-0.02793145442179
H	2.62153047039046	1.07158117488709	-0.88381899167265
H	2.73586931615177	1.02101682870923	0.86468435827721

H	3.52705534965393	-0.25160898817983	-0.09970789400344

Data for gas phase (no solvation model):

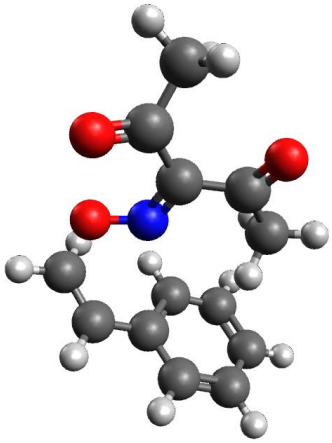
Electronic energy ... -475.42109299 Eh

Total Enthalpy ... -475.28970514 Eh

Final Gibbs free energy ... -475.33616994 Eh

N	0.08075203245620	1.53933963430191	-0.06160082723126
C	0.09389766677403	0.27545302367987	0.04711312552590
C	-1.14626634858892	-0.58462682288332	0.24538917077548
C	1.41772643337483	-0.42472984377246	-0.03932661092301
O	-1.50267667676238	-0.84739159007333	1.36177456844722
O	1.41781117779620	-1.62709348078861	-0.15970698118199
O	-1.20338466868230	2.04676356682059	-0.02077028221388
H	-1.07399025653585	2.99408446643658	-0.10682832376416
C	-1.82538948018700	-1.05845821642233	-1.00316687940917
H	-2.70988692735234	-1.63361734974042	-0.74836681886310
H	-2.09288636310239	-0.20104876478177	-1.62033319114934
H	-1.12615192871671	-1.67437870327486	-1.56891138519947
C	2.66956862615221	0.40216382045639	0.02293038630222
H	2.64778041415619	1.18187510629507	-0.73513530848706
H	2.73046952158723	0.90032259829666	0.98940325991114
H	3.52790777763101	-0.24606044454996	-0.11786190253953

Transition state for C–O bond formation between 1b and 2 (TS 1b+2 to A')



imaginary frequencies: 1

Electronic energy ... -784.63566730 Eh

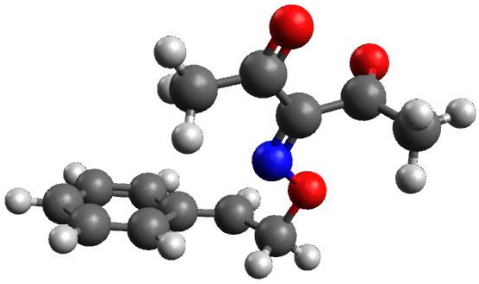
Enthalpy ... -784.37508299 Eh

Gibbs free energy ... -784.43728515 Eh

C	3.08584849141190	-0.88367859667221	1.29886834836609
C	2.40934625915239	0.30736917727047	1.12214314116860
C	2.33059337514589	0.90342022219311	-0.14740237885170
C	2.95944973622774	0.25987105710713	-1.22561185874273
C	3.62783253926060	-0.93709409469049	-1.04662300860070
C	3.69381691688695	-1.51330849855844	0.21712898233504
H	3.13902425091451	-1.32925046497454	2.28194516186280
H	1.94613754068418	0.78301766951673	1.97344085564036
H	2.90644330961534	0.71157787166706	-2.20691676796653
H	4.09899385141955	-1.42295846535473	-1.88902162288454
H	4.21851931420111	-2.44727169659257	0.35952805030743
C	1.62692995931962	2.13673416949112	-0.38919808430383
H	1.71626137367679	2.55501826057280	-1.38358639773012
C	0.75210883791492	2.73039738325204	0.48758646060574
H	0.72092823790530	2.44366924196827	1.52678609863258
H	0.34632805296204	3.70156669138716	0.25283915792117
O	-0.98399940039963	1.84318263426478	0.09417613343292
N	-0.84781884885466	0.58246099084676	0.06241204516530
C	-1.87332542241840	-0.20103333902281	-0.05620384766176

C	-1.54991436438170	-1.65014814671292	-0.14502475015873
C	-3.28583211707872	0.30960619128066	-0.12407509032288
C	-0.13349827129797	-2.08504115347306	0.11001371754488
H	0.55958120587937	-1.55634626879067	-0.53974383895801
H	0.15058081804980	-1.84464212242468	1.13261508563110
H	-0.06454173180117	-3.15559637325521	-0.05421792701341
C	-4.39075281255046	-0.53883664227565	0.44146030838633
H	-4.71302690394220	-1.25240706769849	-0.31436560088629
H	-4.05624320594898	-1.10823563616230	1.30468197128654
H	-5.22242404168774	0.10900742605747	0.70383821809889
O	-2.41812190413774	-2.45211200795641	-0.43598334898364
O	-3.51079004612864	1.40641758773965	-0.59191421332092

Adduct of 2 to 1b with C–O bond formed (A’ from styrene)



imaginary frequencies: no

Electronic energy ... -784.66639181 Eh

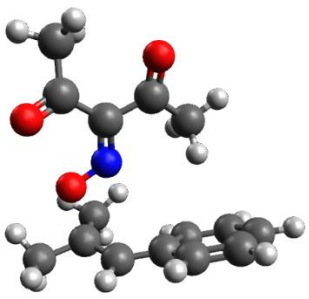
Enthalpy ... -784.40361552 Eh

Gibbs free energy ... -784.46714027 Eh

C	3.45485807864087	-1.07804865628327	0.94634657923005
C	2.46979526817143	-0.11229218498602	0.94835570758927
C	2.39583168392104	0.85129258846341	-0.08729195349574
C	3.36593333747242	0.77492702572442	-1.11819966945453
C	4.34496719109904	-0.19520364964789	-1.11001399967898
C	4.39932521128666	-1.12925212205297	-0.07696908033344
H	3.48989017022490	-1.80449055605057	1.74624927837756
H	1.74116757762369	-0.10414989499804	1.74405951815395

H	3.32685589206828	1.49973690619866	-1.92019479222810
H	5.07300663426471	-0.23015165962238	-1.90831558260321
H	5.16687374956912	-1.88964952937965	-0.07054525200316
C	1.41737480498965	1.86524678490168	-0.13899761987566
H	1.42136224984509	2.52268272029587	-0.99818817098404
C	0.34673812902697	2.08365373753722	0.86364113311919
H	0.56586695915944	1.63987958126929	1.83062191414855
H	0.14785901811627	3.14354772313955	0.99905340477489
O	-0.93889099817663	1.56751612097666	0.41192765003731
N	-0.90391846126033	0.20222001157758	0.39716406661969
C	-1.99650601632124	-0.30691156123648	-0.00352195172390
C	-2.10370368870626	-1.79765918134904	-0.04696535414300
C	-3.20053020705655	0.50683066728265	-0.44237506749624
C	-0.89048159406791	-2.60944668681262	0.28963266380572
H	-0.07564587737072	-2.35471373553140	-0.38594812851056
H	-0.55488664874261	-2.37524487264381	1.29825536882625
H	-1.13276859589794	-3.66392541709739	0.20825666862751
C	-4.12649679461616	0.95043123150643	0.64282535627261
H	-4.53497249364549	0.06652200748521	1.13463687990031
H	-3.56449756870776	1.50789309874629	1.39150083005565
H	-4.92826324735581	1.55791668981137	0.23485310671395
O	-3.17281607505023	-2.28370275954414	-0.35228053546858
O	-3.35807968850393	0.73791957231938	-1.61680496825332

Transition state for C–O bond formation between 1f and 2 (TS 1f+2 to A')



imaginary frequencies: 1

Electronic energy ... -863.32381023 Eh

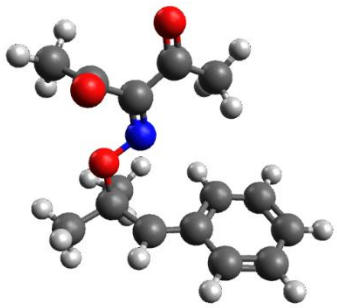
Total Enthalpy ... -863.00442015 Eh

Final Gibbs free energy ... -863.07187058 Eh

C	3.35426385286969	-1.31317136837829	0.92067772876835
C	2.74393480043490	-0.07544968420893	0.82288267621426
C	2.25944651637591	0.38886324166243	-0.41170763674149
C	2.44735831183254	-0.42923459250633	-1.54133409832436
C	3.04429037404458	-1.67102625997059	-1.43640658227090
C	3.49689560762894	-2.12132492166469	-0.20099547047961
H	3.72416498691537	-1.65005393859019	1.87861611893013
H	2.67352158626139	0.54074208204584	1.70278011379745
H	2.09871218890057	-0.07695571087902	-2.50257887650929
H	3.16297049653397	-2.28792644883096	-2.31573830135551
H	3.96759468466587	-3.09028762333221	-0.11521486285370
C	1.59742165364171	1.65135222294678	-0.61959637289532
H	1.57476434083429	1.98546583244846	-1.64950242357751
C	0.80914599636017	2.39579285107307	0.25690904447028
O	-0.92585627394664	1.49420695106451	-0.23693110249807
N	-0.87317819271409	0.26466030069869	0.06608912435796
C	-1.91372482348866	-0.50702866025597	-0.01963009236343
C	-1.64552584867499	-1.92757805060533	0.32640000788387
C	-3.26785073132575	-0.01790931446791	-0.44114208747959
C	-0.30570264495443	-2.27355111547551	0.92055455766062
H	0.49506700803621	-2.01460062130421	0.23116348893910
H	-0.13373728643992	-1.70334085489662	1.83107614143888
H	-0.28550953998785	-3.33773280559312	1.13336913895459
C	-4.49042519930015	-0.73354668987128	0.06511157425320
H	-4.68830495045390	-1.59496440932908	-0.56986840296093
H	-4.34910860458484	-1.10345168779675	1.07713194646001

H	-5.33275771073682	-0.04904099829850	0.01659112075877
O	-2.48171761920209	-2.78669464458180	0.11263358054244
O	-3.36831094208529	0.96408983295143	-1.14889452924609
C	0.36694753559619	3.75549667151238	-0.19069459664862
H	0.38402781623367	3.84954147466522	-1.27321709255390
H	-0.63619988224718	3.96363874647017	0.17594209404424
H	1.03516313952809	4.50572093303769	0.23480385384415
C	0.73857968980592	2.15609219712488	1.73231802519858
H	0.61711884801357	1.10145296204344	1.96315984120919
H	1.65345562957026	2.50826560337013	2.21028165192799
H	-0.09670681394120	2.70942649772217	2.15444369910424

Adduct of 2 to 1f with C–O bond formed (A' from β,β-dimethylstyrene 1f)



imaginary frequencies: no

Electronic energy ... -863.34852118 Eh

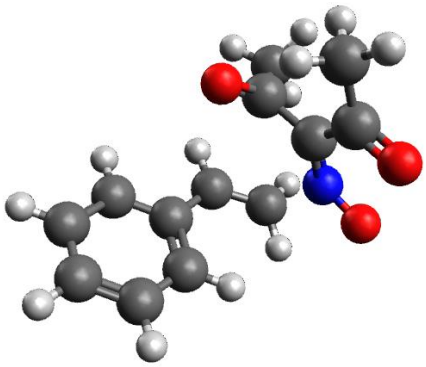
Total Enthalpy ... -863.02749899 Eh

Final Gibbs free energy ... -863.09595492 Eh

C	3.24164359481398	-1.53169612885499	0.67602244655307
C	2.29970024633643	-0.52573284255949	0.59142530898164
C	2.24272274021828	0.32704465107479	-0.53732288012151
C	3.18902672309597	0.08755681618147	-1.56888340413370
C	4.12518500582934	-0.91926605377139	-1.47461351584750
C	4.16170751979095	-1.73887204055666	-0.34820032708125
H	3.25538167927546	-2.17132866959455	1.54767575328183

H	1.58292603623969	-0.41748467920214	1.38448224648261
H	3.16571240636119	0.71983469092943	-2.44627211549323
H	4.83099828203416	-1.07244431928099	-2.27892106755170
H	4.89293834108958	-2.53070142646588	-0.27275578219713
C	1.32631138394726	1.38444072964373	-0.73697525526388
H	1.39350772477993	1.86820480198696	-1.70325388686356
C	0.25368049467399	1.95354427239683	0.14695744533535
O	-1.00410816284124	1.19911214741199	-0.05503571834968
N	-0.87515007854549	-0.09571012782188	0.33630901299276
C	-1.93147984824182	-0.77363011472348	0.13724379255290
C	-1.92453622801600	-2.21277484772447	0.53669142609376
C	-3.19022450240304	-0.20913656639609	-0.49525093815590
C	-0.65472522349693	-2.79400941818180	1.07905006384214
H	0.14664929253796	-2.67925571576808	0.35163252376729
H	-0.35088088199245	-2.25350632114535	1.97374948658671
H	-0.81211819132218	-3.84274356863498	1.30852662683053
C	-4.15308149035830	0.46223180672067	0.42902279343270
H	-4.51476647948555	-0.27391888946012	1.14839590379881
H	-3.63507156310341	1.23870681918452	0.99111888369748
H	-4.98516351706191	0.88176272506864	-0.12783670649854
O	-2.94927206656036	-2.85041333033415	0.40676379689641
O	-3.35959177536593	-0.33738045034933	-1.68399161517256
C	-0.12342019664898	3.33620186567867	-0.36579147704069
H	-0.39328091145161	3.29315943802641	-1.41912512810696
H	-0.96284100109900	3.73077582463118	0.20242114911917
H	0.72401536580736	4.00875377049827	-0.24981668173582
C	0.55964876153287	2.01855500331399	1.63733439584182
H	0.54619291055328	1.04134505035320	2.10496263307524
H	1.54003904593006	2.46406653207331	1.79257948430339
H	-0.18667443685359	2.63950756565175	2.12951532614798

Transition state for C–N bond formation between 1b and 2 (TS 1b+2 to B')



imaginary frequencies: 1

Electronic energy ... -784.63301352 Eh

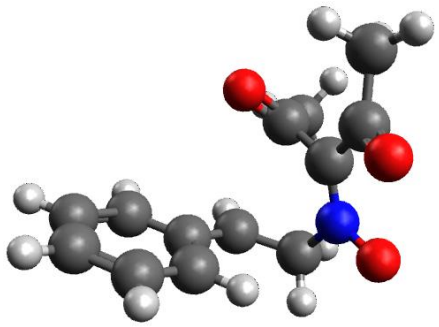
Enthalpy ... -784.37211312 Eh

Gibbs free energy ... -784.43369526 Eh

C	3.08400687008365	1.69761945582824	0.37725008051594
C	2.13602392359473	1.12014742153377	-0.44753384162212
C	2.02100190385288	-0.27622582341806	-0.53081101447020
C	2.87849166586955	-1.06479751113955	0.25080486753097
C	3.82907604334246	-0.48370853983361	1.07016473279872
C	3.93582048177733	0.90091633250570	1.13580906274347
H	3.15942015262534	2.77419392377328	0.43470486997464
H	1.47510673059805	1.75552760109072	-1.01914370348627
H	2.78639161144443	-2.14153424059389	0.20349618871608
H	4.48448917554306	-1.10683774922626	1.66179451493199
H	4.67482143424224	1.35830991441118	1.77819560308415
C	1.04042359309724	-0.93061783390170	-1.36237881469429
H	0.96650071128108	-2.00446077833433	-1.25494940300074
C	0.16071868694001	-0.28642032647819	-2.21616785324152
H	0.38784701842974	0.70759879554312	-2.56830803134107
H	-0.43756950589834	-0.88179158848594	-2.88979779180396
O	-1.67775693746769	1.59242003080400	-1.75765787595800
N	-1.36758720348070	0.54589179990861	-1.22002364490820

C	-1.76573059798202	0.05866899995332	-0.08122567098693
C	-2.70502249301229	0.82335737386964	0.78979832832441
C	-1.25644225785006	-1.29009682837618	0.35670510311315
C	-3.16245178009492	0.14658564224839	2.05523137068089
H	-3.48937928249532	-0.87333705446400	1.85852684653449
H	-2.33680752767164	0.09362599535219	2.76233476769118
H	-3.97604714886872	0.72335710676318	2.48238544183884
C	-1.65725372681985	-2.48149332539909	-0.46145299474174
H	-1.60956380663427	-2.28223631462533	-1.52775058356700
H	-1.05276881912123	-3.34330565114471	-0.19631728429862
H	-2.70334914563389	-2.68856250755678	-0.22319635373655
O	-3.08782589203043	1.93451155867480	0.48992441971568
O	-0.65589887766041	-1.39183787928251	1.40328766366259

Adduct of 2 to 1b with C–N bond formed (B')



imaginary frequencies: no

Electronic energy ... -784.65390944 Eh

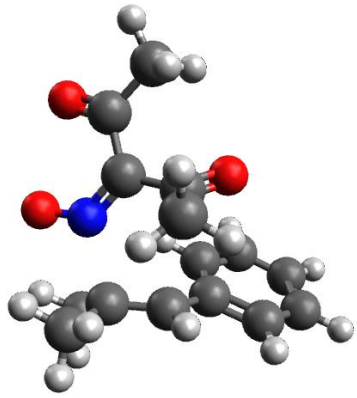
Enthalpy ... -784.39053023 Eh

Gibbs free energy ... -784.45124714 Eh

C	2.81322777262960	1.69980972606475	0.51224249991749
C	1.90123607113960	1.11293731897811	-0.34187104634758
C	1.89501053475322	-0.28768510211069	-0.53406331484526
C	2.84492390134527	-1.05845466295303	0.17445933625122
C	3.75059440485679	-0.46168393289354	1.02523497558822
C	3.74035452984214	0.92122377750789	1.20037432203010

H	2.80532043167048	2.77211690651479	0.64705506590969
H	1.19260160032096	1.73832377937669	-0.86589427789898
H	2.84636904332258	-2.13176406892923	0.04112414594591
H	4.46841815447681	-1.06824971071731	1.55899151599137
H	4.44940746110708	1.38868929712836	1.86837878182208
C	0.96130890039903	-0.93659736302640	-1.36991503885430
H	1.03701485374241	-2.00649055685169	-1.49026505201737
C	-0.08934692135983	-0.21960449455816	-2.12962213971706
H	0.31397998529881	0.58617859203872	-2.73814258375244
H	-0.65542084714042	-0.87956782996650	-2.77946531312186
O	-1.49787101252906	1.59070069216713	-1.78779188479341
N	-1.10802282284189	0.51599861240787	-1.27965250973608
C	-1.50138836164008	0.04809872495689	-0.11949097112425
C	-2.35170778112070	0.87496589251313	0.79425812266969
C	-1.07208830939341	-1.30817497285739	0.37973929453085
C	-3.12557057192678	0.13796377213089	1.85676519517416
H	-3.48702035357648	-0.82643686212836	1.50585520228601
H	-2.47861557039810	-0.03922180514407	2.71434185266865
H	-3.95960695476020	0.75996789984758	2.16631548976976
C	-1.49400901103457	-2.53450192434904	-0.37998008307862
H	-1.54015850398696	-2.38522175561520	-1.45345519820204
H	-0.84206760697213	-3.36669991056252	-0.13242811731622
H	-2.50562155893365	-2.77124046677113	-0.04174206900068
O	-2.40277491151112	2.08180704223792	0.70659373470107
O	-0.55756585377939	-1.38168747043644	1.47524515654991

Transition state for C–N bond formation between 1f and 2 (TS 1f+2 to B')



imaginary frequencies: 1

Electronic energy ... -863.31194929 Eh

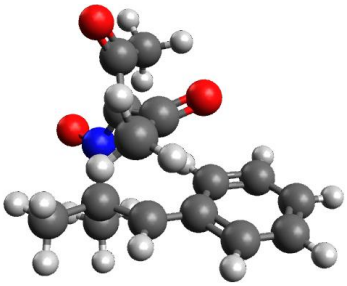
Total Enthalpy ... -862.99243932 Eh

Final Gibbs free energy ... -863.05968954 Eh

C	-2.72549641274618	-1.17476707103012	-1.62946489426982
C	-1.79051750944056	-0.27614667823057	-1.14998301689542
C	-1.96143579274090	0.33351813753386	0.10313483998491
C	-3.08792118877225	-0.02375306080851	0.86269181800071
C	-4.02803614313370	-0.91163632480058	0.37425199095043
C	-3.85260316626794	-1.48881050192250	-0.87795783057813
H	-2.56939354659383	-1.64448922801725	-2.59024304043964
H	-0.90186523484453	-0.08683073448082	-1.73100997376580
H	-3.21661779917429	0.41473898129106	1.84312242054140
H	-4.89336708449493	-1.16175985432355	0.97147566365153
H	-4.58062831779144	-2.19056673762253	-1.25915229869287
C	-1.01854742416445	1.24721197322869	0.69737643855559
H	-1.09165463885504	1.33973345969275	1.77366835409910
C	-0.05146837222086	2.05929760024101	0.07199924695003
O	2.21624342646036	1.40102027051495	-1.24971000857407
N	1.52597227872372	0.85384648110938	-0.39920471399649
C	1.68154151671096	-0.36461507448446	0.04754221961773
C	2.71934925139925	-1.26845426843662	-0.52820886682551
C	0.83526243857577	-0.88777870300729	1.17870708247519
C	2.90345462210205	-2.61039284590278	0.13586551334814
H	2.96756070997178	-2.51317743320305	1.21848195530940

H	2.05203743965186	-3.25152524832252	-0.08383884261902
H	3.81082772491286	-3.06299796883616	-0.25020279307422
C	1.04735761304707	-0.29554658961281	2.54186151150678
H	1.28754679876005	0.76066889627443	2.50510076849733
H	0.18606692487545	-0.48348117702737	3.17609816587932
H	1.91457937587179	-0.80760541656011	2.96708220768704
O	3.39231357905509	-0.95147160794505	-1.48783381694434
O	0.14203940541993	-1.86664021563233	1.00836418977928
C	-0.28590022609151	2.59948102090779	-1.31198944092448
H	-0.79922528827897	1.91742802569584	-1.97610802269815
H	-0.89970458192658	3.49399152130551	-1.20003009667429
H	0.65775397229622	2.90057789160637	-1.75912833240966
C	0.66640073797469	3.05323425930222	0.94886118231878
H	1.64327973669416	3.29133838453821	0.53212570918119
H	0.08823362288341	3.97746584803853	0.97298343416790
H	0.78271455215152	2.70223598892637	1.96955127688013

Adduct of 2 to 1f with C–N bond formed (B')



imaginary frequencies: no

Electronic energy ... -863.33439995 Eh

Total Enthalpy ... -863.01271931 Eh

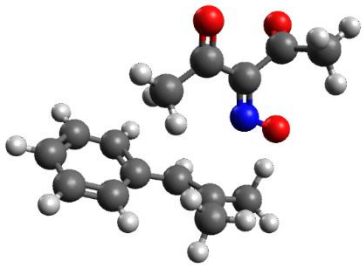
Final Gibbs free energy ... -863.07963942 Eh

C	-2.85232195671178	-1.15606381995109	-1.59352824037309
C	-1.83681798042441	-0.33791783372696	-1.14523924770319
C	-1.95850774381469	0.36496386602414	0.07707711585190
C	-3.15318451315521	0.18568859318877	0.81612556247175

C	-4.16273292496921	-0.63298288554942	0.35814313764992
C	-4.02068273134867	-1.31068734937432	-0.85102210565286
H	-2.73424775273519	-1.68701188379741	-2.52755812743194
H	-0.93474342560663	-0.26035088942703	-1.73115952694908
H	-3.26231999856142	0.70832243445902	1.75678440364416
H	-5.06548290047732	-0.74932877883060	0.94101590356329
H	-4.81002990843424	-1.95574737698389	-1.20904654661551
C	-0.95241643358739	1.18742728093473	0.62848654413462
H	-1.16750959786621	1.63894710762008	1.58677537346015
C	0.30987486630425	1.64943742637660	-0.03123374785993
O	2.11684024183932	0.72812567290092	-1.26125533443873
N	1.24083161859134	0.48385046626126	-0.36519493512491
C	1.20098017134601	-0.68103310551751	0.19533019121566
C	2.15269892106115	-1.71081798620808	-0.37666827774611
C	0.32314933844236	-1.19354926242479	1.30576540901163
C	1.84419469072628	-2.21912195212504	-1.75073558884474
H	1.10158213961640	-3.01148724261317	-1.63628607837040
H	1.42172289071562	-1.43878978123962	-2.37590753231142
H	2.73910318929015	-2.63498755549364	-2.20452446019443
C	0.42996191487733	-0.62148520179414	2.68674881638709
H	0.69714884185575	0.42693898551449	2.69988359730785
H	-0.49911697594527	-0.78938176540100	3.22397793856861
H	1.22799180460983	-1.17623089743123	3.18603332671253
O	3.04465916425961	-2.13975788884405	0.31658637152726
O	-0.30396829977476	-2.20568053019097	1.07791192051840
C	0.00174647554277	2.39474600524764	-1.33570951135504
H	-0.46831925650915	1.75894871665683	-2.07749596174730
H	-0.68593443477462	3.20096142765163	-1.08985073277463
H	0.90792639863678	2.81898898930078	-1.75389414235769
C	1.11025402487768	2.57979113189377	0.88036578234021

H	2.03360413021662	2.87132809889777	0.38728242094036
H	0.51950063830640	3.47246586382641	1.07230068391252
H	1.35119308358052	2.11447407016913	1.83168070863307

TS for allylic hydrogen atom abstraction by diacetyliminoxyl from β,β-dimethylstyrene 1f



imaginary frequencies: 1

Electronic energy ... -863.31025191 Eh

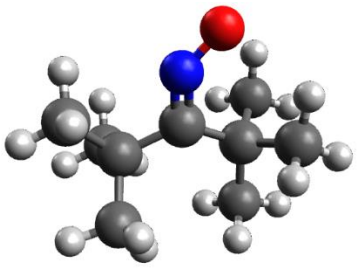
Total Enthalpy ... -862.99507143 Eh

Final Gibbs free energy ... -863.06399519 Eh

C	-4.07436247169920	-0.80801724029081	-0.92601776397643
C	-3.20838171520678	0.25551414726664	-0.73374525197334
C	-2.49744651616364	0.38672362973655	0.46695257330288
C	-2.72235949229083	-0.56395652231521	1.47500072907147
C	-3.57999098253216	-1.63011567082950	1.27681221806100
C	-4.25602915855193	-1.75967560505502	0.06966694314078
H	-4.61590061755576	-0.89190843157275	-1.85749571113684
H	-3.10908235751523	0.99312266767980	-1.51188926742643
H	-2.19688630212899	-0.46269263481410	2.41493381867146
H	-3.72495669949284	-2.35825742788338	2.06203065096669
H	-4.92959563301325	-2.58961161569069	-0.08971473809839
C	-1.54143014771227	1.43856248976972	0.75951260110328
H	-1.30791062913522	1.53979150399849	1.81294475148573
C	-0.85982042903180	2.28946188334346	-0.07690966900932
O	2.12477636126409	1.64482205195100	0.51034825593388

N	1.50253604450603	0.60273099350276	0.06912900492626
C	2.16667760526282	-0.49057479782500	-0.03677340693009
C	1.51183707908368	-1.70426500801009	-0.57326423871448
C	3.62665831442284	-0.57552083008047	0.36256680603121
C	0.04640640967792	-1.66451609961236	-0.88550687943861
H	-0.51922132724569	-1.55321618032312	0.03792767062142
H	-0.19141633332997	-0.80737224494397	-1.50955207136429
H	-0.23827965591571	-2.58655082114397	-1.38193867257312
C	4.61864745178278	-0.09291154993270	-0.64760951086446
H	4.53704047958243	-0.71575400310833	-1.53952276593675
H	4.36848779803075	0.92647423000841	-0.94024355917162
H	5.62711428906872	-0.13845139517018	-0.24827504419283
O	2.19164879692409	-2.70085433679154	-0.74333142885373
O	3.92734096554248	-1.01646106353533	1.44727307190987
C	0.05136100863172	3.23029073797634	0.51991207339726
H	1.10079330945446	2.59368336412730	0.53175263047253
H	0.29615668079195	4.09962719719961	-0.08321683626909
H	-0.11815263151224	3.45682931327099	1.56804288913757
C	-0.93452095491202	2.27010229285762	-1.57448281540361
H	-1.02884158369703	1.26324957334487	-1.96965238681740
H	-1.79319836269727	2.84860105130593	-1.91951947046476
H	-0.04161459268690	2.72742835158904	-1.99366519961768

Di-*tert*-butyliminoxyl



imaginary frequencies: no

Data for CH_2Cl_2 solution (CPCM(CH_2Cl_2)):

Electronic energy ... -484.00852848 Eh

Total Enthalpy ... -483.73536868 Eh

Final Gibbs free energy ... -483.78750995 Eh

C	1.48505611190356	-0.10821599106567	-0.00526578777287
C	0.02776470797310	0.36120739939316	-0.08446857663970
C	-1.25097818689600	-0.50354138410602	-0.01853493319373
N	-0.12248407212637	1.62647860912031	-0.10602531630711
O	-1.07028617972230	2.41549718968185	-0.09402982002960
C	-1.02231263496831	-2.00603639866905	-0.20744342153225
H	-0.32280186603530	-2.42957007611189	0.50620069267879
H	-1.98051280363957	-2.50376770609761	-0.06173130146380
H	-0.68327476897607	-2.23702526738784	-1.21361217173865
C	-1.88807189864805	-0.27350918643794	1.36081462709572
H	-1.23197757915507	-0.62909760627916	2.15407511700184
H	-2.09797557152118	0.78091904031373	1.52994902780533
H	-2.82815148962782	-0.82108043250422	1.42404872982644
C	1.83511482990698	-1.11323018999704	-1.11357203599846
H	1.50056094020875	-0.75411145124894	-2.08639897839901
H	2.91784238121134	-1.22862360738898	-1.15195750542407
H	1.40922802057120	-2.09475567497683	-0.94092261842955
C	2.42586826472033	1.09243888254863	-0.16694773204811
H	3.45424439892022	0.74313996102165	-0.08576309442322
H	2.30168348776757	1.56560242197384	-1.14001963664158
H	2.25949183495558	1.84233642795977	0.60384179088991
C	-2.22722273965304	-0.07134835993333	-1.12242030065597
H	-2.53554429752678	0.96499855665411	-1.02375089809539
H	-1.77942960773110	-0.21019441686403	-2.10595521502344
H	-3.11931523863041	-0.69428704389816	-1.06543982586241
C	1.75251348544203	-0.72207942159150	1.37819169775556

H	1.58913376403134	0.01869035707343	2.16028618574364
H	1.12068478160598	-1.58053387458416	1.58677911002330
H	2.79040392563936	-1.05092875659810	1.43059519085838

Data for gas phase (no solvation model):

Electronic energy ... -484.00313355 Eh

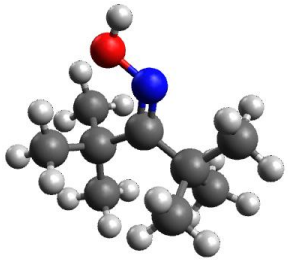
Total Enthalpy ... -483.72937146 Eh

Final Gibbs free energy ... -483.78144111 Eh

C	1.48538621296869	-0.10840043900506	-0.00608410998947
C	0.02795126487502	0.36044351618773	-0.07835235777090
C	-1.25054290067749	-0.50404505808203	-0.01686496152727
N	-0.12537629895293	1.62744751538659	-0.08445335069458
O	-1.07948081528923	2.39893915524152	-0.06094979908692
C	-1.02498483416919	-2.00781174581831	-0.19895326078497
H	-0.32925333804643	-2.43182894124587	0.51850292375425
H	-1.98272113198804	-2.50710538658429	-0.05546865187740
H	-0.68301975025723	-2.24610547667715	-1.20246523532601
C	-1.89870479794306	-0.26879641237661	1.35654959169185
H	-1.25093468620568	-0.62477840234797	2.15673733546299
H	-2.10350208720132	0.78677982208298	1.52128800994531
H	-2.84250161402676	-0.81052323722490	1.41798742581205
C	1.83512944322935	-1.11114577455228	-1.11648161512189
H	1.50118260877837	-0.74956812137058	-2.08849756927146
H	2.91732202777045	-1.23017660033863	-1.15978770739592
H	1.40925999928689	-2.09358200466919	-0.94818013395103
C	2.42296311216440	1.09441394519065	-0.17038408190299
H	3.45398132927534	0.75097659675900	-0.09495458102886
H	2.29151485469673	1.57035974950028	-1.14057567984759
H	2.25695979406230	1.84478659540454	0.59916859894409
C	-2.21850952673110	-0.07251067208297	-1.12854419717196

H	-2.50853544340310	0.97009829426108	-1.04554764200971
H	-1.77095468797593	-0.22947633096028	-2.10943635912392
H	-3.12176595803095	-0.67947155448472	-1.06981500848280
C	1.76283816471021	-0.72461929720096	1.37443579896695
H	1.60064477118177	0.01326925725378	2.15912973438625
H	1.13402112221329	-1.58488222630099	1.58596547912678
H	2.80088516568562	-1.05331476594534	1.42655440427512

Di-*tert*-butyl oxime



imaginary frequencies: no

Data for CH_2Cl_2 solution (CPCM(CH_2Cl_2)):

Electronic energy ... -484.64242241 Eh

Total Enthalpy ... -484.35641949 Eh

Final Gibbs free energy ... -484.40821716 Eh

C	-2.63100117462698	-0.76780137877159	1.76589585788899
C	-1.54738687273796	-0.07366322042404	0.91306764506208
C	-1.54861809121093	1.42502292585447	0.53882462614114
N	-0.59564197500111	-0.87156490311250	0.62196548224139
O	0.48575838289180	-0.31696180710315	-0.07425135988392
C	-2.84035444132422	2.19315559112385	0.85570064974351
H	-3.15341692419693	2.11875500997400	1.89130288253904
H	-2.64639647878828	3.24553636807633	0.65012533129625
H	-3.66242507814269	1.88571416563458	0.21576576122852
C	-0.41579449769076	2.11270646640038	1.32316632131868
H	-0.61796060139844	2.07510380037535	2.39351049150196

H	0.54786916452197	1.65210726493923	1.13479546667906
H	-0.36273197324273	3.16109702731269	1.02869466677277
C	-4.04934559279504	-0.58047802617793	1.19820028032610
H	-4.06433541880445	-0.72934869386561	0.11854563721636
H	-4.70515320482382	-1.32611024929916	1.64599759676686
H	-4.47102013671868	0.39236816363115	1.41817404399531
C	-2.38780718973971	-2.28261459737975	1.83798176279238
H	-3.16301573018978	-2.72098796042580	2.46602833521585
H	-2.44307674298726	-2.74251867949739	0.85291079214349
H	-1.42004999100856	-2.52081432535933	2.26905736425178
C	-1.34761572601645	1.60389857231581	-0.97916206674174
H	-0.37482125888292	1.27697584130394	-1.32083832444450
H	-2.11221901419154	1.05363034374059	-1.52790377403831
H	-1.46187832924276	2.66078237415395	-1.22079586829582
C	-2.55159547385236	-0.23870152678295	3.20765272175839
H	-1.57430703315706	-0.45945183449616	3.63606054396076
H	-2.71824171631252	0.83145563757533	3.28114148436294
H	-3.30838460530222	-0.73580841754332	3.81480385595113
H	1.06943639397241	-1.07242281417297	-0.17787453175047

Data for gas phase (no solvation model):

Electronic energy ... -484.63578452 Eh

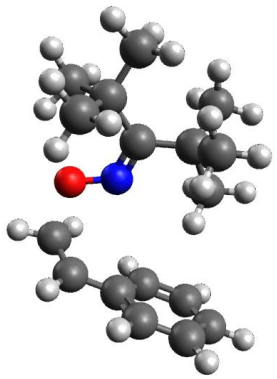
Total Enthalpy ... -484.34901212 Eh

Final Gibbs free energy ... -484.40074377 Eh

C	-2.63385893714907	-0.76747576764489	1.76572015386315
C	-1.55064088148861	-0.07042041312441	0.91506580344054
C	-1.54837203052908	1.42771666322387	0.54028678854116
N	-0.60086735628602	-0.86908360540321	0.62655961856964
O	0.48029349564300	-0.31358230401036	-0.06678940780731
C	-2.83761283434894	2.19848658367092	0.85942147687698

H	-3.14905356248942	2.12533374028414	1.89582408481829
H	-2.64554010862452	3.25135479241573	0.65487614709052
H	-3.66298600682254	1.89435690127586	0.22210397795593
C	-0.41097919611635	2.11185415204172	1.32046368771698
H	-0.60861359093796	2.07700833821858	2.39176479388015
H	0.54889465541557	1.64527103320530	1.12971161325609
H	-0.35129805040804	3.15990617902581	1.02586750832789
C	-4.05171198126964	-0.58439820412589	1.19689010895488
H	-4.06688237256675	-0.74261149858335	0.11867787662603
H	-4.70973330186737	-1.32655510723615	1.64709273632836
H	-4.47575395502405	0.38948958745876	1.40855112932135
C	-2.38160954614782	-2.28098812180410	1.83296248171404
H	-3.15259827454991	-2.72955052297928	2.45947957608053
H	-2.42980279942530	-2.73585803966516	0.84589774996464
H	-1.41043255780378	-2.51304329858494	2.25822118886125
C	-1.34761320685732	1.60254372400797	-0.97783466738736
H	-0.37965316360998	1.26210720802252	-1.31886670968879
H	-2.11730756192673	1.05966643318358	-1.52650715105267
H	-1.44978926789099	2.65976660340636	-1.22391813545752
C	-2.55898106238807	-0.24073607739843	3.20811583256095
H	-1.58000134540916	-0.45390820263910	3.63540977723563
H	-2.73396023834739	0.82814612049952	3.28450585195761
H	-3.31043518148200	-0.74254084586172	3.81792410948487
H	1.05536888970824	-1.07319493287966	-0.16893432603380

TS for di-*tert*-butyliminoxyl addition to styrene



imaginary frequencies: 1

Electronic energy ... -793.83980804 Eh

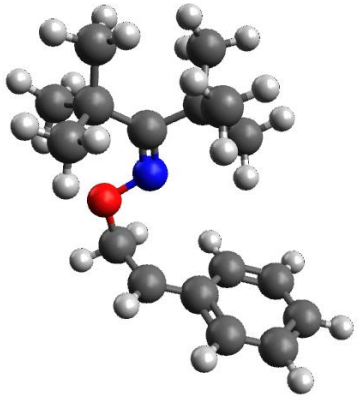
Total Enthalpy ... -793.42459572 Eh

Final Gibbs free energy ... -793.49269612 Eh

C	-3.66271600407402	-0.84998066099842	-1.04488687102718
C	-2.98588050753169	0.35553066457654	-1.04682176657616
C	-2.67810491628565	1.00570290416357	0.15682056622625
C	-3.08458356345800	0.40614131158547	1.35738465508223
C	-3.74870840193772	-0.80826109159506	1.35778871593744
C	-4.04179564388259	-1.44119991319364	0.15563229204840
H	-3.89477417744447	-1.33550646324719	-1.98230975634805
H	-2.70130610137363	0.80265233621936	-1.98792805347662
H	-2.85763301075128	0.90047512792803	2.29258833985503
H	-4.04170595156100	-1.26145713885040	2.29433857952276
H	-4.56613274020837	-2.38628226276593	0.15329102610570
C	-1.95554422482956	2.25778580956688	0.20602155316329
H	-1.96830059500705	2.78445499456496	1.15193611253124
C	-1.12694785915131	2.72146378448635	-0.78535127700739
H	-1.15732087185735	2.29323666877000	-1.77507316700949
H	-0.72894271878325	3.72184121068316	-0.71676824781950
O	0.59392757500429	1.93351643523456	-0.33361937685401
N	0.50824930668371	0.62085607115011	-0.40990716988521
C	1.52549458781993	-0.12124378549756	-0.17395740575078

C	2.89303722664485	0.48479818573644	0.20881277383320
C	1.20161139240387	-1.62611832686628	-0.19578772448551
C	2.12887589808107	-2.42472589836081	-1.12737415702611
H	3.11977833256992	-2.57956918973875	-0.71811622643315
H	1.69152251158600	-3.40813962559807	-1.29839033103586
H	2.22797940413417	-1.93121276071632	-2.09436862439525
C	1.26761093825511	-2.18314191094539	1.23639167869502
H	0.54220770229042	-1.67335239258908	1.87035017218713
H	1.01845947371219	-3.24467732660521	1.22371967419518
H	2.24721821487629	-2.07876347741726	1.69283811821550
C	-0.22896542999335	-1.86437723943237	-0.69277422403003
H	-0.36584326240437	-1.50012995193322	-1.70937705486737
H	-0.42253964685366	-2.93714158091116	-0.68339023805263
H	-0.96543556410384	-1.37443834358191	-0.06384553813901
C	4.06662906532778	-0.50016060017225	0.29113243882647
H	3.88921398464810	-1.34001512712182	0.95412285619839
H	4.34316749583973	-0.88039370139208	-0.68881133588982
H	4.92450723128873	0.04669161635182	0.68224579177114
C	2.74439342146681	1.13945795939543	1.59373496832632
H	3.66876387286958	1.65693734359277	1.85196075007395
H	1.93110443972018	1.85972889397008	1.61078185837787
H	2.55712911454725	0.38401840110817	2.35600739717701
C	3.32166517905645	1.53678643683315	-0.83075004155027
H	2.65480916249512	2.39047235496369	-0.86438380692774
H	4.32082785821874	1.89265912224981	-0.57851472611152
H	3.36571280195185	1.09284713639984	-1.82544219765090

Adduct of di-*tert*-butyliminoxyl to styrene



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Electronic energy ... -793.87312573 Eh

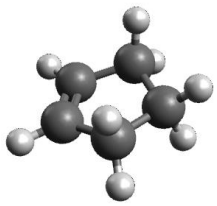
Total Enthalpy ... -793.45538211 Eh

Final Gibbs free energy ... -793.52372926 Eh

C	-4.00843628285750	-0.76270898194489	-0.93066117141551
C	-3.00779823294097	0.18548701964832	-0.87337483505520
C	-2.76326580864179	0.91605391886993	0.31527953735155
C	-3.58813166361845	0.62973418326335	1.43259116238923
C	-4.58374004409966	-0.32157883683570	1.36475251855712
C	-4.80377701762618	-1.02690509703730	0.18272596502758
H	-4.17128011267596	-1.30989545699215	-1.84891436303592
H	-2.39322456227871	0.35659333850403	-1.74359696986913
H	-3.42095895898938	1.17398544206753	2.35252001789745
H	-5.19523610632177	-0.52139968299137	2.23370221822860
H	-5.58315981530219	-1.77346885728888	0.13052890836321
C	-1.74965500637694	1.88860488110926	0.43648930982972
H	-1.62343353883893	2.35745377810460	1.40424726365604
C	-0.78916179819391	2.29106479494611	-0.62487373914419
H	-1.09366570750470	1.95609756921725	-1.61378447096007
H	-0.67790837672744	3.37435029244241	-0.64742386105666
O	0.54591064526445	1.81884125268262	-0.36188717788244
N	0.53356659646752	0.43012772122026	-0.47311140254184
C	1.62919688663852	-0.17595028302356	-0.22960115277743

C	2.93650389002088	0.54346598385991	0.16756607161500
C	1.44878026635471	-1.70847366114426	-0.27805225953554
C	2.47295304321236	-2.40413440864187	-1.19089454418651
H	3.45297274825422	-2.50076221907496	-0.74033319925372
H	2.11750195240933	-3.41010909754450	-1.41106795382262
H	2.57811218723804	-1.87369952346531	-2.13737094750573
C	1.52943581866575	-2.26432141230429	1.15356744612675
H	0.74190726982934	-1.82999582738749	1.76888071082970
H	1.38278814298972	-3.34435963794008	1.12883168529187
H	2.48216874051044	-2.06977030115545	1.63645318856438
C	0.05926155553922	-2.08306362519839	-0.81603086646738
H	-0.08188449018309	-1.73205331776557	-1.83684991813595
H	-0.02403856470925	-3.16977276372069	-0.81173813497263
H	-0.74091981631962	-1.67266291788931	-0.20757523981889
C	4.18618322935414	-0.34471683300955	0.26278193269242
H	4.06967184820786	-1.19843289476309	0.92127262249070
H	4.50963313329674	-0.69506076903059	-0.71364330064119
H	4.98794454588342	0.27129041816082	0.66917239964950
C	2.73104381596141	1.17886110423666	1.55480137530974
H	3.61280968087119	1.76572135614451	1.81304899868247
H	1.86333311209247	1.82989654910505	1.57780021101534
H	2.60967847333720	0.40613307552613	2.31333558921515
C	3.29536759924758	1.62190725940811	-0.87381095653141
H	2.59272352742216	2.44447843807623	-0.88782837917755
H	4.28472292762136	2.01403586510432	-0.63815666232698
H	3.33970103151641	1.18526266845185	-1.87176647566903

Cyclopentene



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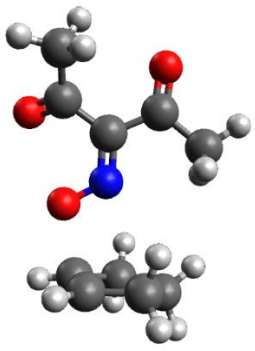
Electronic energy ... -195.45534040 Eh

Total Enthalpy ... -195.33276800 Eh

Final Gibbs free energy ... -195.36569652 Eh

H	-0.10059251039296	0.36278871643851	-0.01771234973230
C	-0.06603036851488	0.14985137861258	1.05054143204981
C	0.95842185709363	0.98200064979877	1.77989327688274
C	0.47405116603016	1.49117210141289	2.90577724813819
C	-0.96240425581040	1.09270093124594	3.13351269116512
C	-1.38254540444644	0.51352327129654	1.76715376951645
H	0.17185926636185	-0.91274768051049	1.15014132859199
H	1.97499743432533	1.10177238396492	1.43120624909763
H	1.03786447004863	2.08686182404278	3.61038548471295
H	-1.58956980645485	1.92874546435003	3.44228275578921
H	-1.02415881835795	0.34533198231130	3.92917858687129
H	-1.90044484981350	1.28300048498679	1.19571291629704
H	-2.05680318006861	-0.33471250795056	1.86106261061986

TS for addition of diacetyliminoxyl to cyclopentene



imaginary frequencies: 1

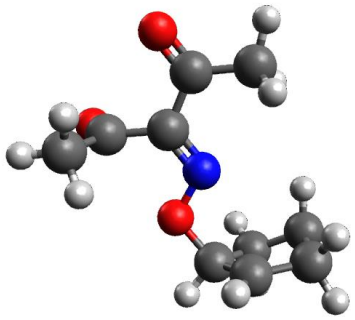
Electronic energy ... -670.22775512 Eh

Total Enthalpy ... -669.98677397 Eh

Final Gibbs free energy ... -670.04525127 Eh

O	0.43026215375998	-1.34978254293341	-0.18082620049352
N	-0.01333978734951	-0.14890555789693	-0.16457624017508
C	-1.28687497913156	0.07417952638345	-0.13680389154223
C	-1.68084791290992	1.50534705139803	-0.15298552095676
C	-2.32053495580141	-1.02036253613068	-0.10234994773467
C	-0.59841488348303	2.54593414206579	-0.05541211066837
H	-0.02536865879545	2.41168628442962	0.85983275941107
H	0.09707360667600	2.44524697401639	-0.88608993227134
H	-1.05735870371900	3.52926080278817	-0.07172995876548
C	-3.51858892881544	-0.84206028618265	0.78798954731264
H	-3.28094647783659	-0.24749668218735	1.66659561140599
H	-4.29238296325510	-0.31441220761623	0.23329306024834
H	-3.88905419659866	-1.82255929614770	1.07439654339829
O	-2.85381100252981	1.81305947944111	-0.26386400064408
O	-2.16097990930798	-2.02871556392489	-0.75627080539720
C	2.66162643049187	-0.95599656771408	1.04740385056028
C	2.85962421419071	0.51047343335713	1.18912789590453
C	2.39931356735224	-1.30434747811453	-0.26405027834384
H	2.62193567486059	-1.64484719048897	1.87759862050540
C	3.11793248903660	1.00485958248823	-0.24896183011005
H	3.66374509805995	0.75572282783788	1.88324186729469
H	1.94807217043172	0.95256079855105	1.60878537287039
C	2.69857609732847	-0.15434677164288	-1.18162112736708
H	2.39575469577086	-2.32532226108206	-0.61173288221793
H	2.56396506825217	1.91371576117841	-0.46551340347710
H	4.17473869396790	1.22718161096163	-0.37915486860235
H	1.82434311847075	0.09445313139231	-1.78208157173705
H	3.48981828088363	-0.43320446422684	-1.87671955840749

Adduct of diacetyliminoxyl to cyclopentene



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Electronic energy ... -670.25181360 Eh

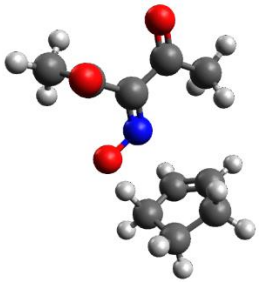
Total Enthalpy ... -670.00908299 Eh

Final Gibbs free energy ... -670.06790452 Eh

O	0.30505106875483	-1.07695687309565	-0.15293233480835
N	-0.05353672445357	0.23515298595179	-0.08001260536161
C	-1.29912149239869	0.40761422556938	-0.26557938006827
C	-1.83947461664696	1.79788457263608	-0.19688177140217
C	-2.27168256745938	-0.72322098892859	-0.54548480040212
C	-0.88328540708311	2.92750744267057	0.03665148223021
H	-0.36863962993635	2.78545304158576	0.98541072518060
H	-0.12311178661044	2.93960076019313	-0.74237366884549
H	-1.43173065071602	3.86364824573614	0.04445737891111
C	-2.83980715969526	-1.41303864177002	0.65214405608588
H	-2.02465594091971	-1.78339134997676	1.27342120496183
H	-3.39548457784167	-0.68508459845189	1.24464360801434
H	-3.49070729547719	-2.22729065343632	0.34943808591363
O	-3.03657167572237	1.95336177339258	-0.32495166097962
O	-2.54515439188327	-1.00000187198886	-1.68847686740450
C	2.19089009668850	-0.60298252866219	1.34948786697248
C	3.12232100808119	0.53033218382249	1.10347373744308
C	1.74710188697013	-1.24045727210601	0.08743143673648
H	1.86925281741833	-0.93602435169010	2.32408396707491
C	3.04786428688792	0.76508479198686	-0.41673446337621
H	4.14217276605618	0.26323714838540	1.40802284909285

H	2.86085600704812	1.41872726733716	1.68256011745861
C	2.61038404096099	-0.58853444879296	-0.99475729902433
H	1.82395933529898	-2.32641817974271	0.09048258475606
H	2.29917778028559	1.52324911354466	-0.63385515245591
H	3.99492150118268	1.10116175155564	-0.83262888136279
H	2.07714668003263	-0.50934322762284	-1.93965561646702
H	3.47998564117796	-1.22554231810277	-1.15771559887368

TS for allylic hydrogen atom abstraction from cyclopentene by diacetyliminoxyl



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Electronic energy ... -670.22219104 Eh

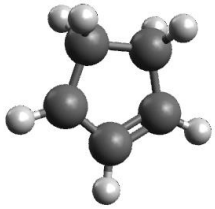
Total Enthalpy ... -669.98583360 Eh

Final Gibbs free energy ... -670.04579697 Eh

O	0.19051881492244	-1.49503530895391	-0.23064878040731
N	-0.12422618271396	-0.23982552606205	-0.23134043198410
C	-1.34344460379876	0.07733006762132	-0.00000773252514
C	-1.72140893821343	1.51099178173488	-0.01001812176930
C	-2.41570321133336	-0.95681980074297	0.27884769552624
C	-0.64204677100795	2.53778042942807	-0.19037384432065
H	0.07339441432169	2.46828975666087	0.62748854595558
H	-0.09332209243923	2.35117209301401	-1.11099127115483
H	-1.09153740049613	3.52527620162976	-0.21152460638753
C	-2.99296592038148	-1.64710990130313	-0.91595648740010
H	-3.50714524876821	-0.90325723883271	-1.52672400112261
H	-2.18889277221078	-2.06318436957989	-1.52202370245762

H	-3.68614811994500	-2.42525909918482	-0.61188500159294
O	-2.89447817713779	1.80402889970416	0.12593806343990
O	-2.75841657063619	-1.17195470245061	1.41760065167061
H	1.54162126206581	-1.45626437293429	-0.49706851120203
C	2.73259886374039	-1.15886490904818	-0.59729748069884
C	3.23657643120121	-0.96028801648239	0.82894657302239
C	2.68688017578407	0.16253467706024	-1.19867908548144
H	3.12679953877619	-1.98868870458799	-1.17803333933043
C	3.00432584356873	0.53779718652383	1.10636916784849
H	4.30164067110315	-1.19124720701894	0.87128118707080
H	2.73510007007128	-1.60689334092925	1.54527606732295
C	2.81207608305344	1.12204610477072	-0.25907285467445
H	2.51311425615092	0.34392790934115	-2.24886564887505
H	2.10719320975814	0.70482331772007	1.70822046681015
H	3.82967792870860	1.00488513811318	1.64316221660045
H	2.76654444585620	2.18411993478885	-0.45060973388322

Cyclopent-2-en-1-yl radical



imaginary frequencies: no

Electronic energy ... -194.81246607 Eh

Total Enthalpy ... -194.70402738 Eh

Final Gibbs free energy ... -194.73770623 Eh

C	3.01249392922390	-1.08834925416119	-0.65799288234626
C	3.25657331490488	-0.95470829580557	0.81865805773622
C	2.73291946300559	0.14733873557959	-1.21243386268792
H	3.06101814195659	-2.02264614596484	-1.19521939732767

C	3.05204039048020	0.55501986292088	1.09964062991537
H	4.26354236720548	-1.28301527632976	1.08616621675526
H	2.57144897913222	-1.57541707632556	1.39943141389304
C	2.74734851319064	1.14048593837548	-0.25039777667894
H	2.52931891610873	0.31519242227681	-2.26050230541433
H	2.23398762387593	0.72814828358292	1.80253215378918
H	3.93705789031097	1.01185966602138	1.54688826793722
H	2.55939847060486	2.18837413982988	-0.42517851557117

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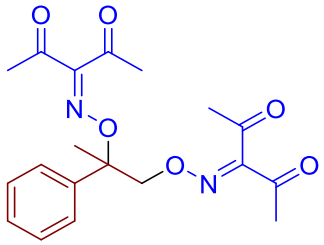
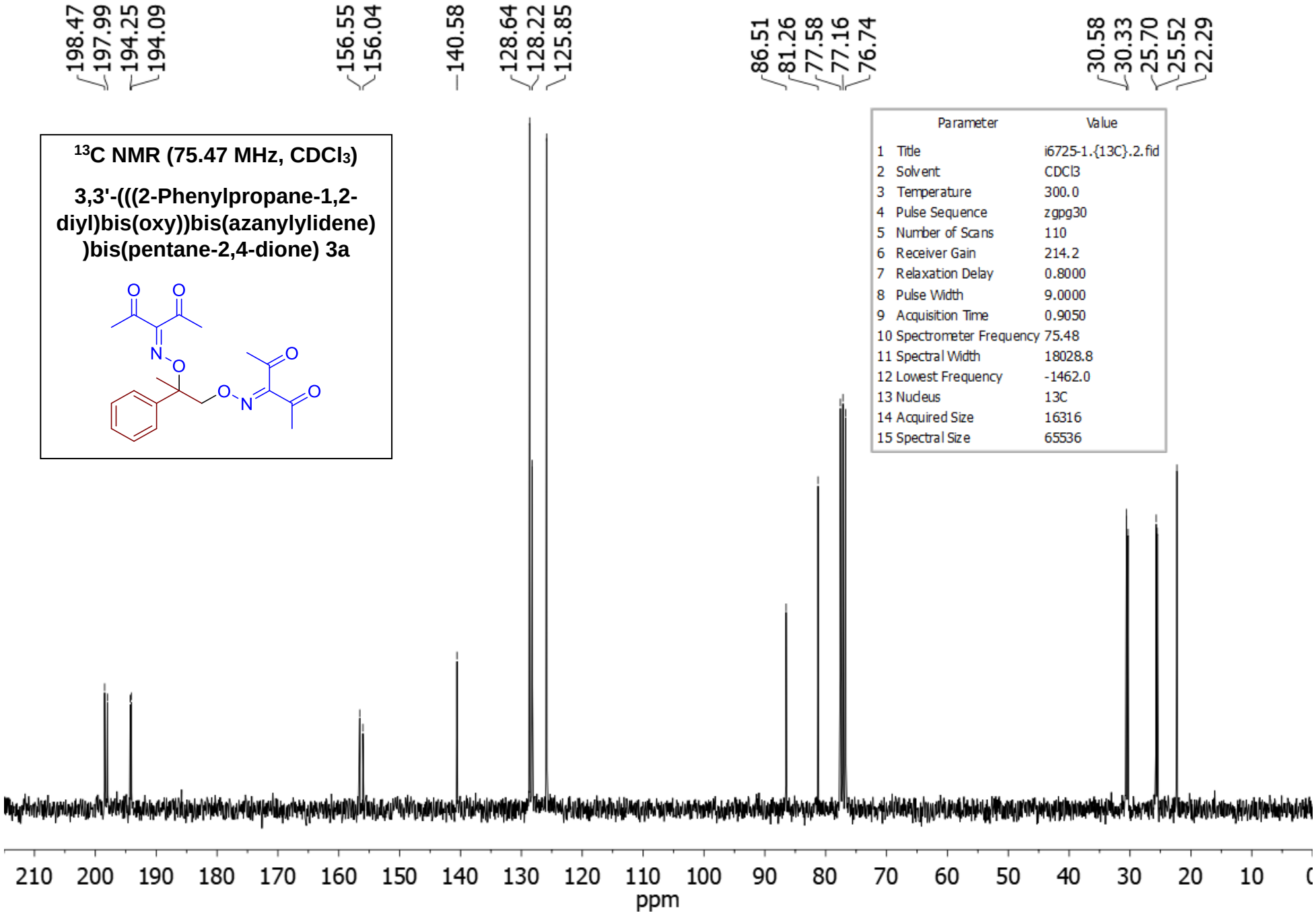
The ^{1}H and ^{13}C spectra of synthesized compounds

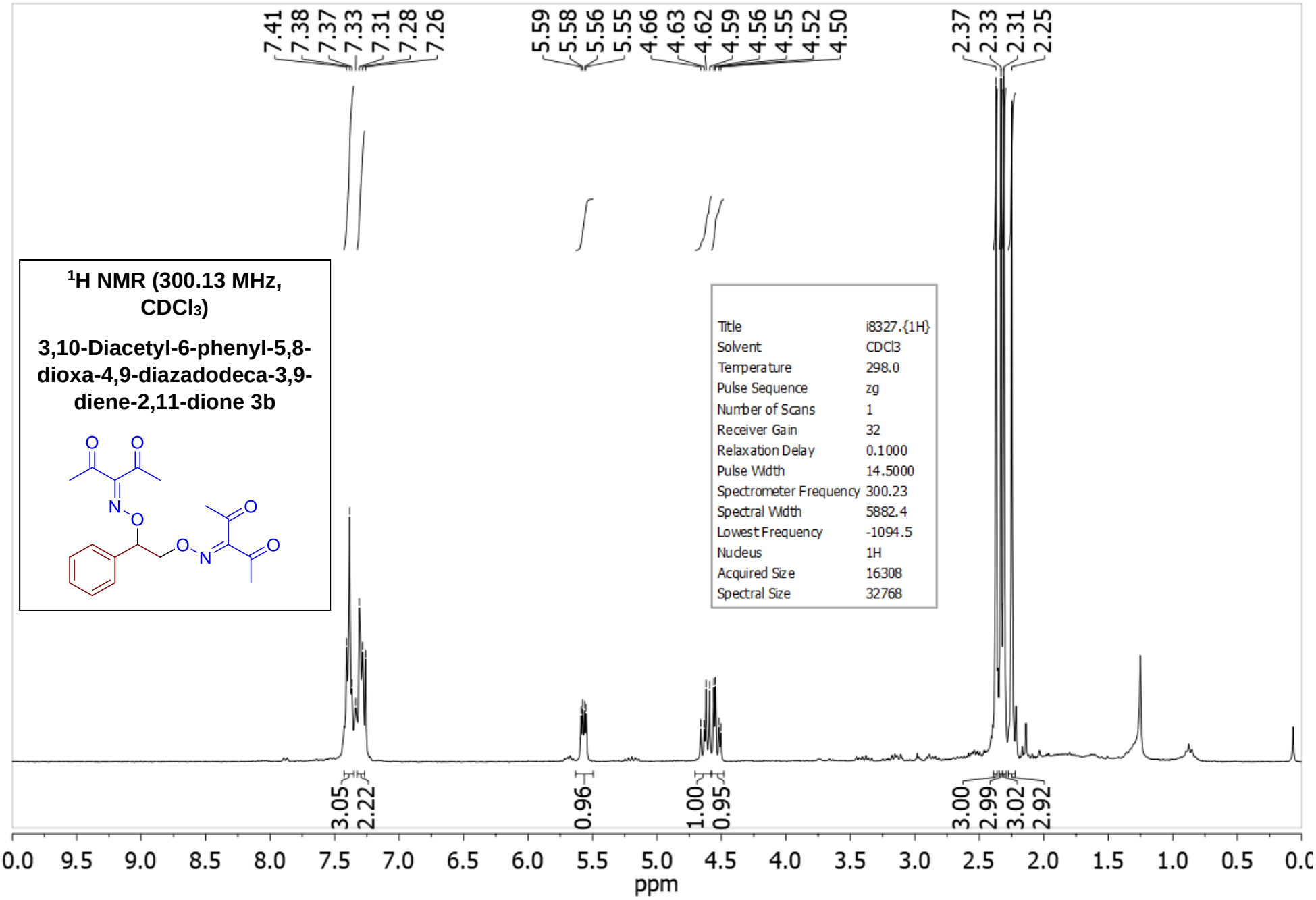
^{1}H NMR (300.13 MHz, $CDCl_3$)

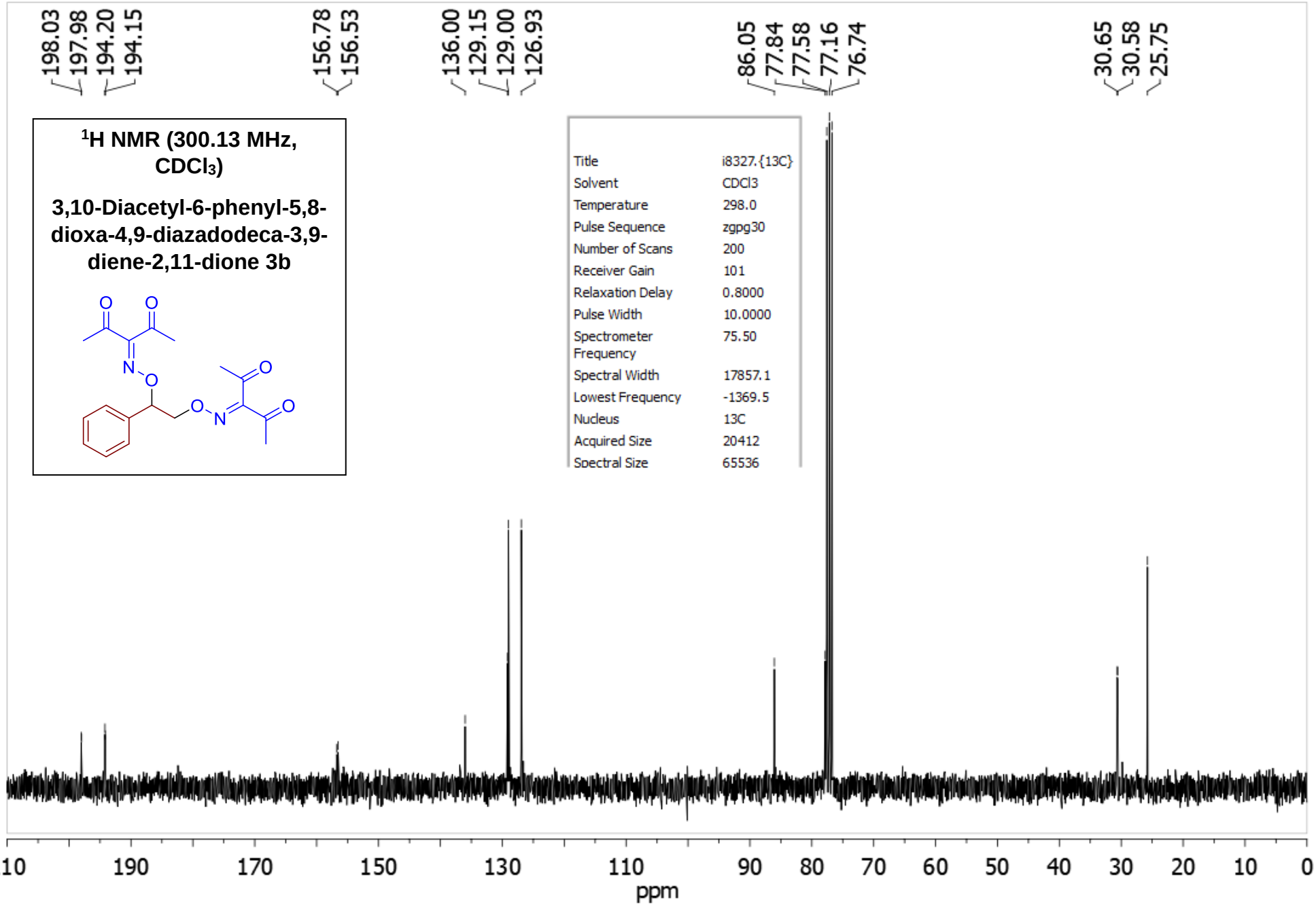
3,3'-(((2-Phenylpropane-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione) 3a

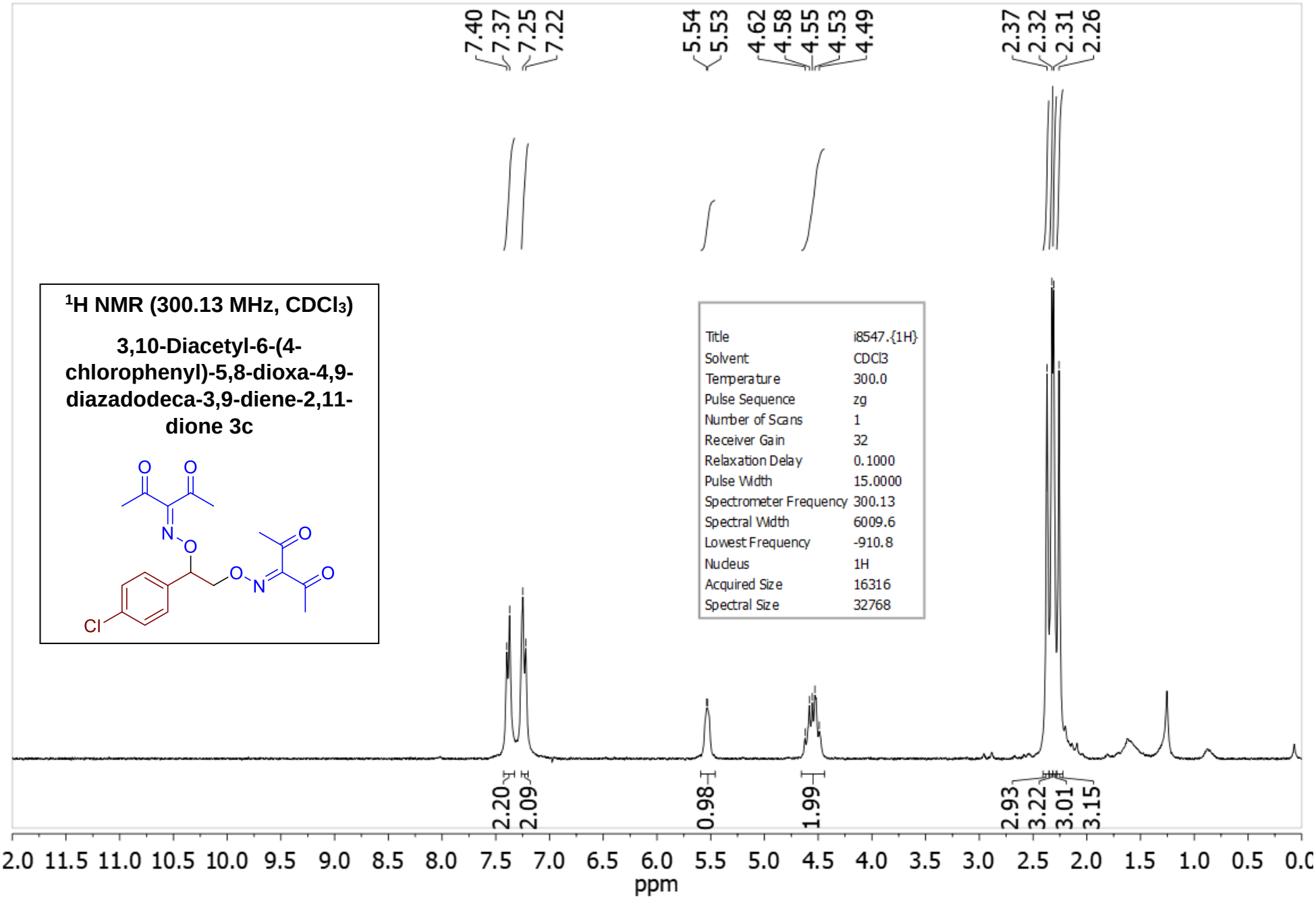


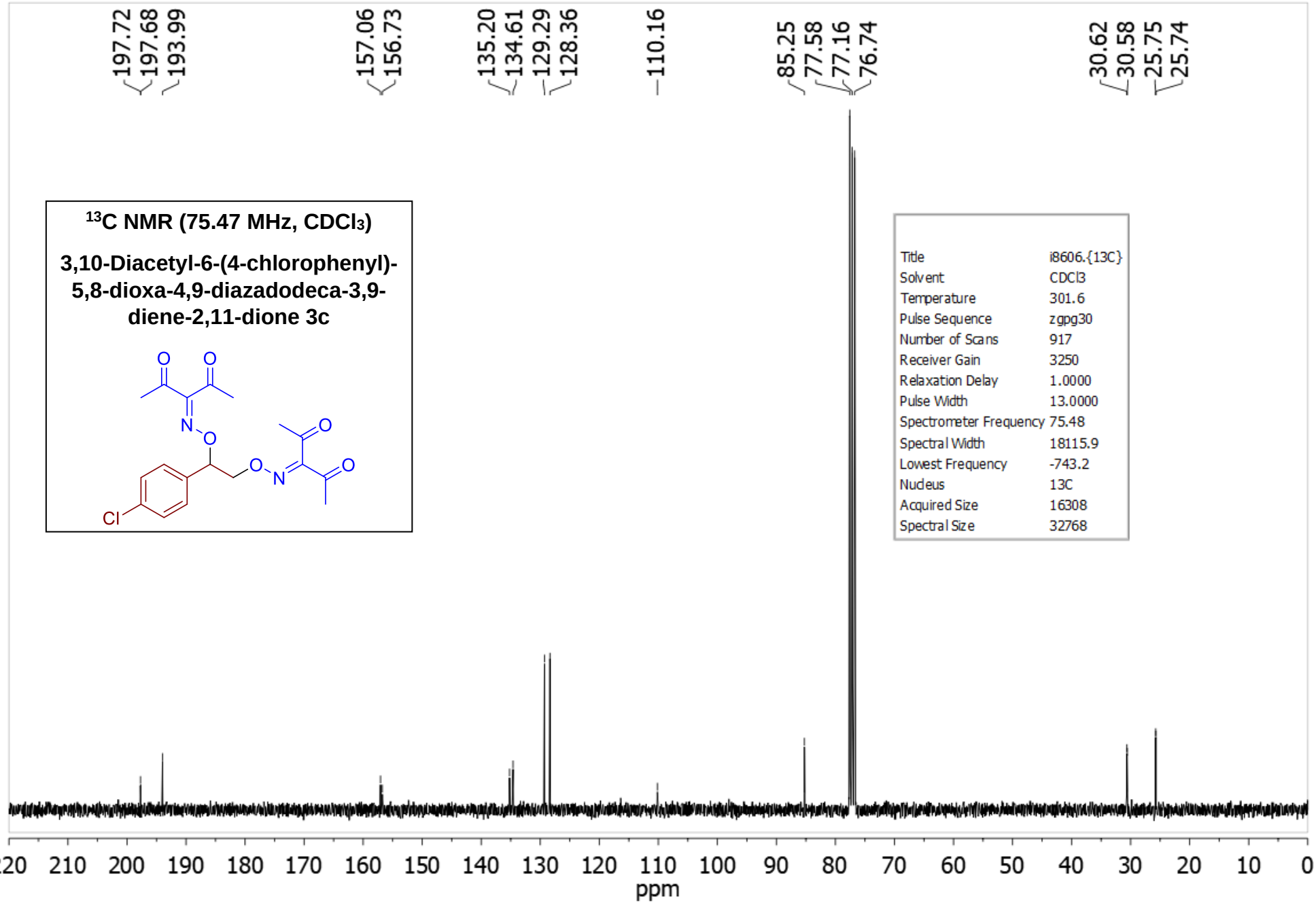
	Parameter	Value
1	Title	i6725-1.{1H}.1.fid
2	Solvent	CDCl3
3	Temperature	300.0
4	Pulse Sequence	zg
5	Number of Scans	1
6	Receiver Gain	32.1
7	Relaxation Delay	0.1000
8	Pulse Width	15.0000
9	Acquisition Time	2.7150
10	Spectrometer Frequency	300.13
11	Spectral Width	6009.6
12	Lowest Frequency	-911.1
13	Nucleus	1H
14	Acquired Size	16316
15	Spectral Size	65536

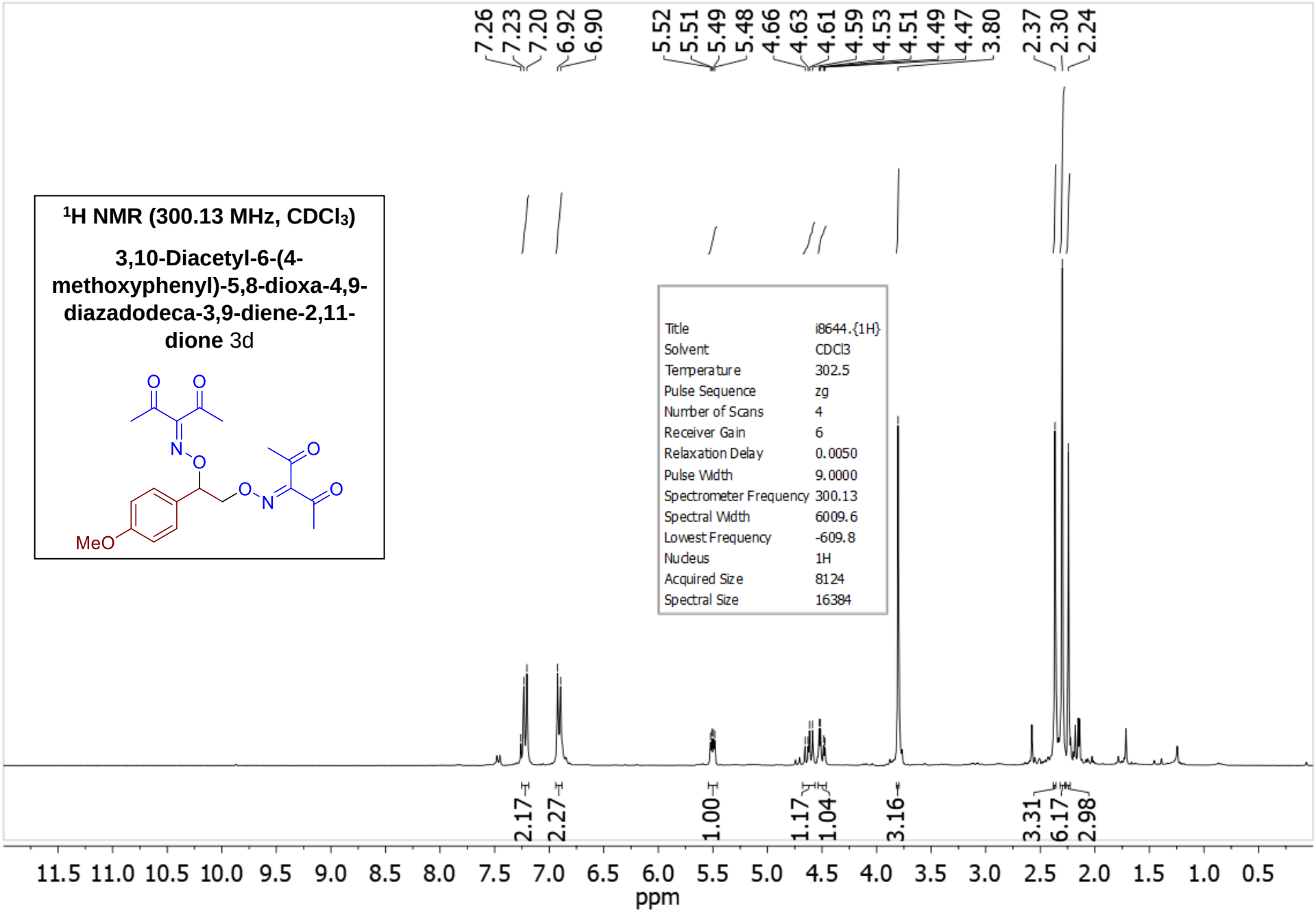

198.47
197.99
194.25
194.09
156.55
156.04
140.58
128.64
128.22
125.85
86.51
81.26
77.58
77.16
76.74
30.58
30.33
25.70
25.52
22.29
^{13}C NMR (75.47 MHz, CDCl$_3$)
3,3'-(((2-Phenylpropane-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione) 3a
Parameter Value
1 Title i6725-1.{13C}.2.fid
2 Solvent CDCl3
3 Temperature 300.0
4 Pulse Sequence zgpg30
5 Number of Scans 110
6 Receiver Gain 214.2
7 Relaxation Delay 0.8000
8 Pulse Width 9.0000
9 Acquisition Time 0.9050
10 Spectrometer Frequency 75.48
11 Spectral Width 18028.8
12 Lowest Frequency -1462.0
13 Nucleus 13C
14 Acquired Size 16316
15 Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm

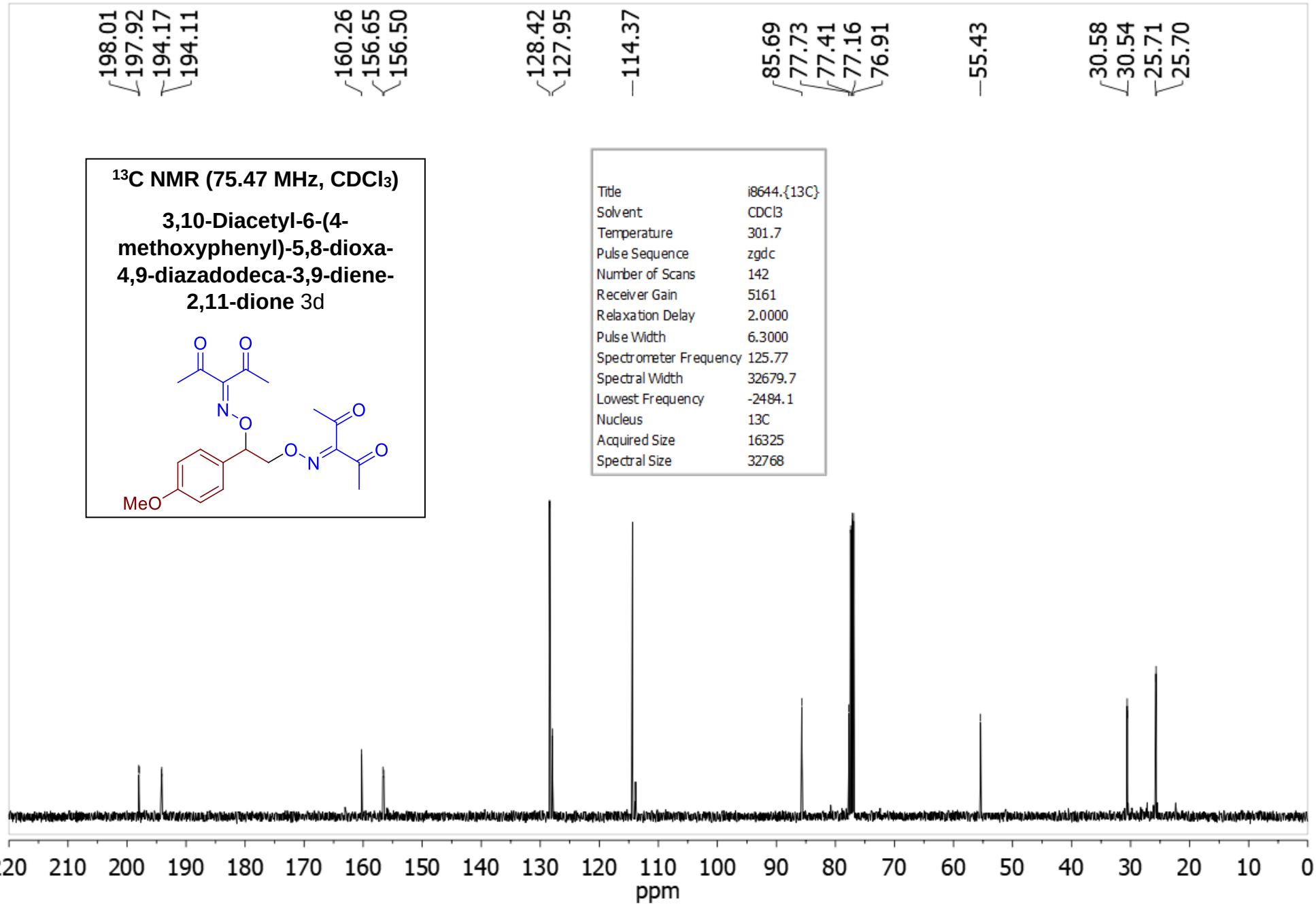

7.41
7.38
7.37
7.33
7.31
7.28
7.26
5.59
5.58
5.56
5.55
4.66
4.63
4.62
4.59
4.56
4.55
4.52
4.50
2.37
2.33
2.31
2.25
^{1}H NMR (300.13 MHz, CDCl$_3$)
3,10-Diacetyl-6-phenyl-5,8-dioxa-4,9-diazadodeca-3,9-diene-2,11-dione 3b
Title i8327.{1H}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32
Relaxation Delay 0.1000
Pulse Width 14.5000
Spectrometer Frequency 300.23
Spectral Width 5882.4
Lowest Frequency -1094.5
Nucleus 1H
Acquired Size 16308
Spectral Size 32768
3.05
2.22
0.96
1.00
0.95
3.00
2.99
3.02
2.92
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm


198.03
197.98
194.20
194.15
156.78
156.53
136.00
129.15
129.00
126.93
86.05
77.84
77.58
77.16
76.74
30.65
30.58
25.75
^{1}H NMR (300.13 MHz, $CDCl_3$)
3,10-Diacetyl-6-phenyl-5,8-dioxa-4,9-diazadodeca-3,9-diene-2,11-dione 3b
Title i8327.{13C}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 200
Receiver Gain 101
Relaxation Delay 0.8000
Pulse Width 10.0000
Spectrometer Frequency 75.50
Spectral Width 17857.1
Lowest Frequency -1369.5
Nucleus 13C
Acquired Size 20412
Spectral Size 65536
ppm


7.40
7.37
7.25
7.22
5.54
5.53
4.62
4.58
4.55
4.53
4.49
2.37
2.32
2.31
2.26
^{1}H NMR (300.13 MHz, CDCl$_3$)
3,10-Diacetyl-6-(4-chlorophenyl)-5,8-dioxa-4,9-diazadodeca-3,9-diene-2,11-dione 3c
Title i8547.{1H}
Solvent CDCl3
Temperature 300.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32
Relaxation Delay 0.1000
Pulse Width 15.0000
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -910.8
Nucleus 1H
Acquired Size 16316
Spectral Size 32768
2.20
2.09
0.98
1.99
2.93
3.22
3.01
3.15
2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm


197.72
197.68
193.99
157.06
156.73
135.20
134.61
129.29
128.36
110.16
85.25
77.58
77.16
76.74
30.62
30.58
25.75
25.74
^{13}C NMR (75.47 MHz, CDCl$_3$)
3,10-Diacetyl-6-(4-chlorophenyl)-5,8-dioxa-4,9-diazadodeca-3,9-diene-2,11-dione 3c
Cl
Title i8606.{13C}
Solvent CDCl3
Temperature 301.6
Pulse Sequence zgpg30
Number of Scans 917
Receiver Gain 3250
Relaxation Delay 1.0000
Pulse Width 13.0000
Spectrometer Frequency 75.48
Spectral Width 18115.9
Lowest Frequency -743.2
Nucleus 13C
Acquired Size 16308
Spectral Size 32768
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


7.26
7.23
7.20
6.92
6.90
5.52
5.51
5.49
5.48
4.66
4.63
4.61
4.59
4.53
4.51
4.49
4.47
3.80
2.37
2.30
2.24
^{1}H NMR (300.13 MHz, CDCl$_3$)
3,10-Diacetyl-6-(4-methoxyphenyl)-5,8-dioxa-4,9-diazadodeca-3,9-diene-2,11-dione 3d
MeO
Title i8644.{1H}
Solvent CDCl3
Temperature 302.5
Pulse Sequence zg
Number of Scans 4
Receiver Gain 6
Relaxation Delay 0.0050
Pulse Width 9.0000
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -609.8
Nucleus 1H
Acquired Size 8124
Spectral Size 16384
2.17
2.27
1.00
1.17
1.04
3.16
3.31
6.17
2.98
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
ppm


198.01
197.92
194.17
194.11
160.26
156.65
156.50
128.42
127.95
114.37
85.69
77.73
77.41
77.16
76.91
55.43
30.58
30.54
25.71
25.70
^{13}C NMR (75.47 MHz, CDCl$_3$)
3,10-Diacetyl-6-(4-methoxyphenyl)-5,8-dioxa-4,9-diazadodeca-3,9-diene-2,11-dione 3d
MeO
Title i8644.{13C}
Solvent CDCl3
Temperature 301.7
Pulse Sequence zgdc
Number of Scans 142
Receiver Gain 5161
Relaxation Delay 2.0000
Pulse Width 6.3000
Spectrometer Frequency 125.77
Spectral Width 32679.7
Lowest Frequency -2484.1
Nucleus 13C
Acquired Size 16325
Spectral Size 32768
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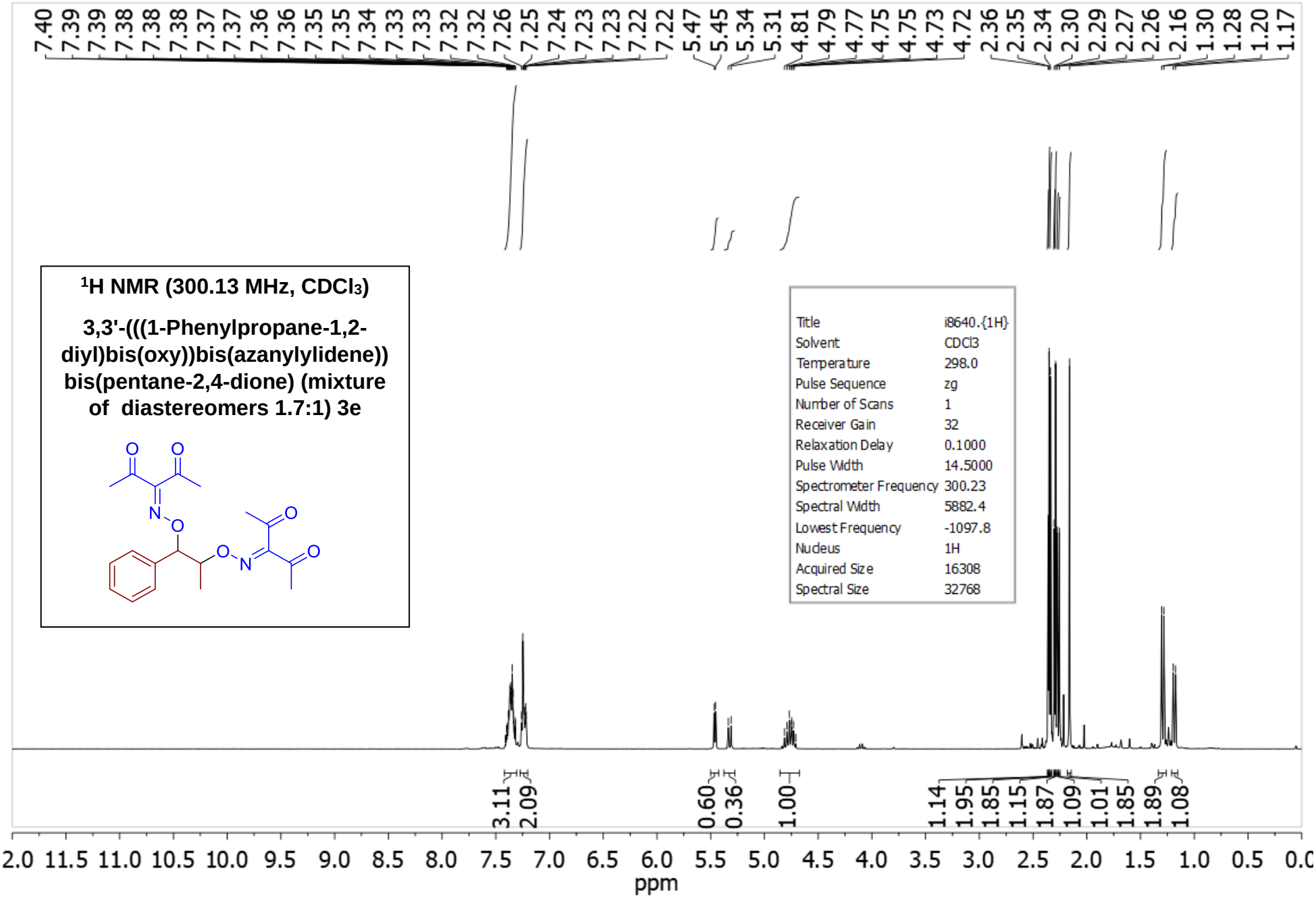
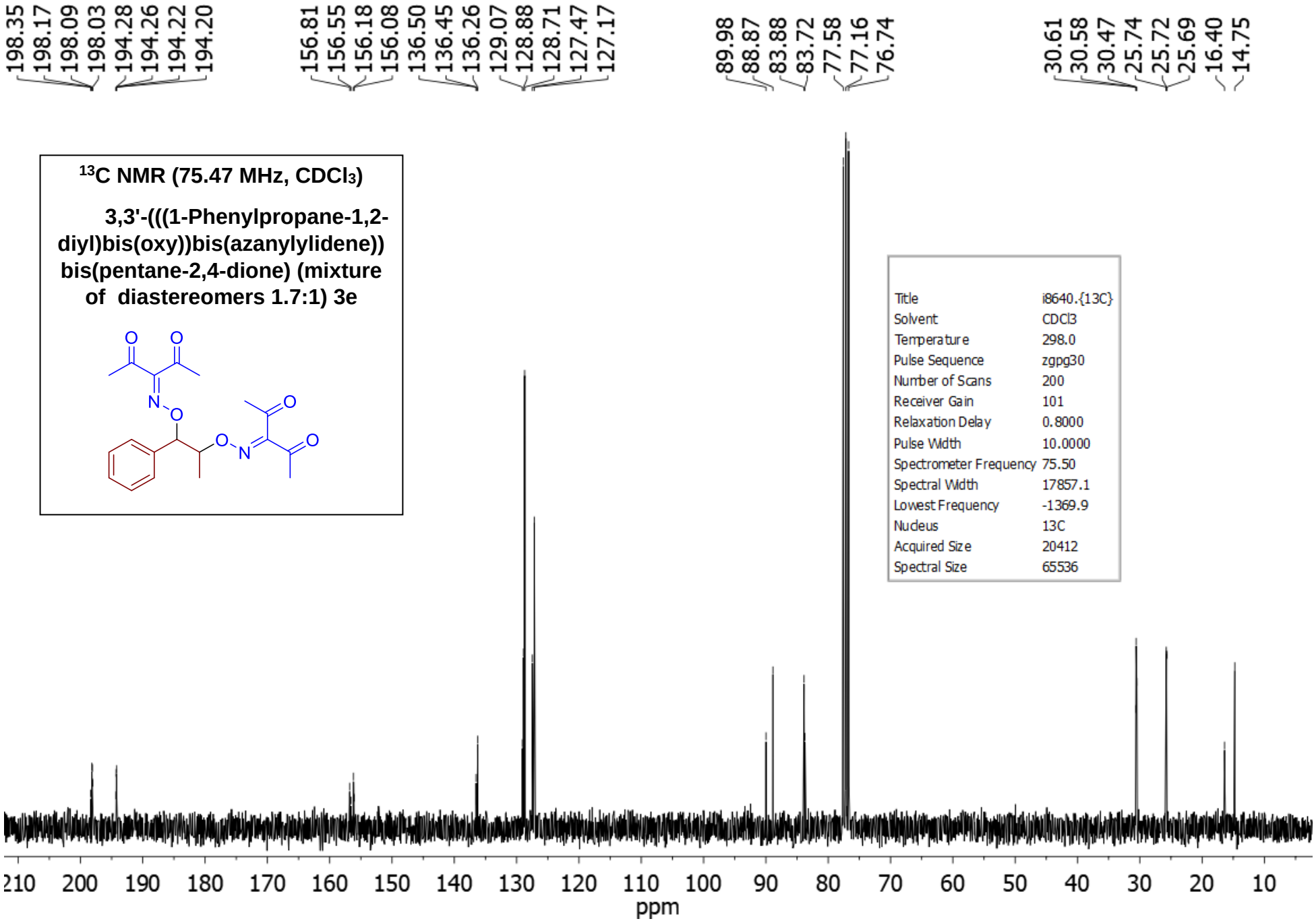
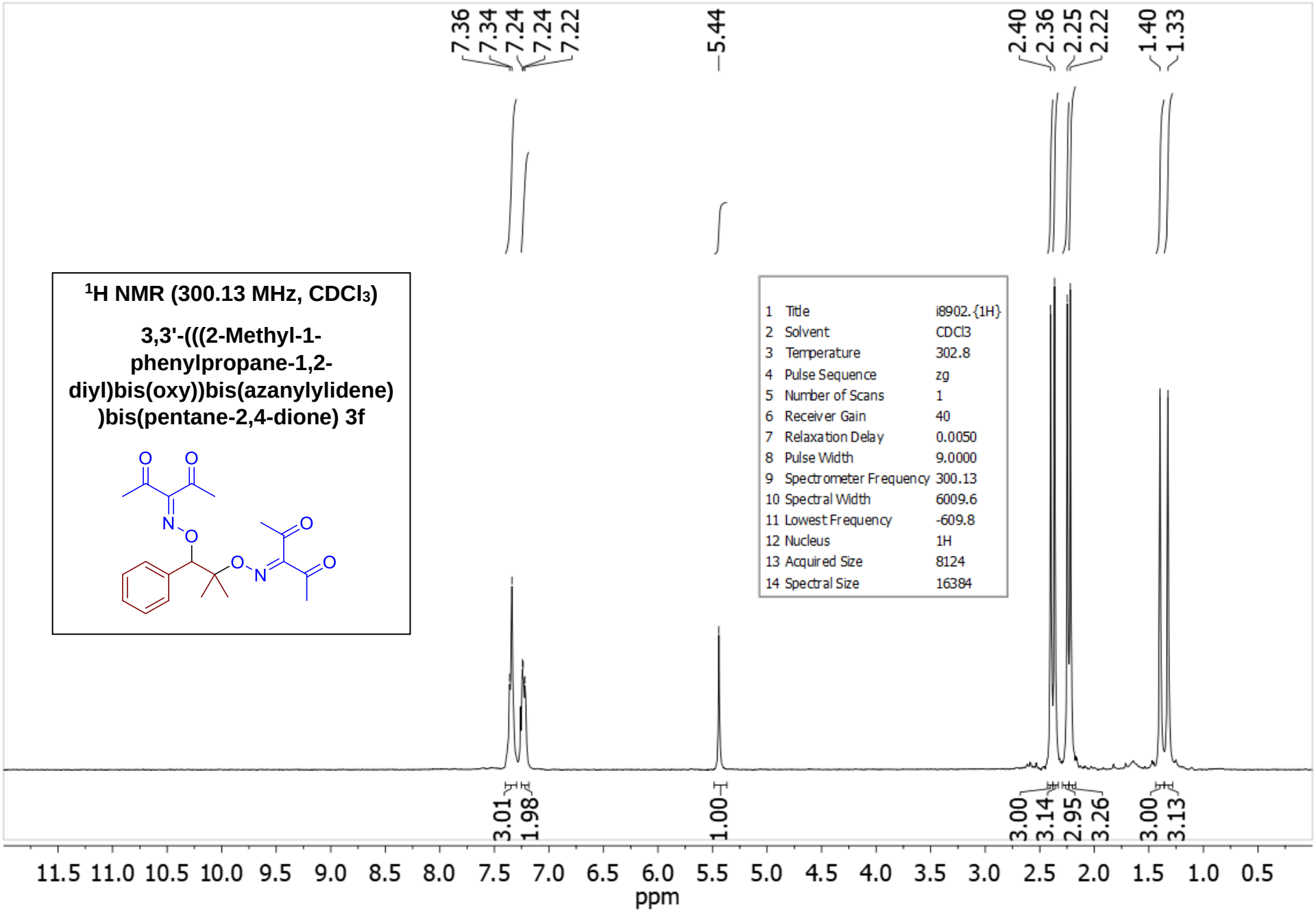
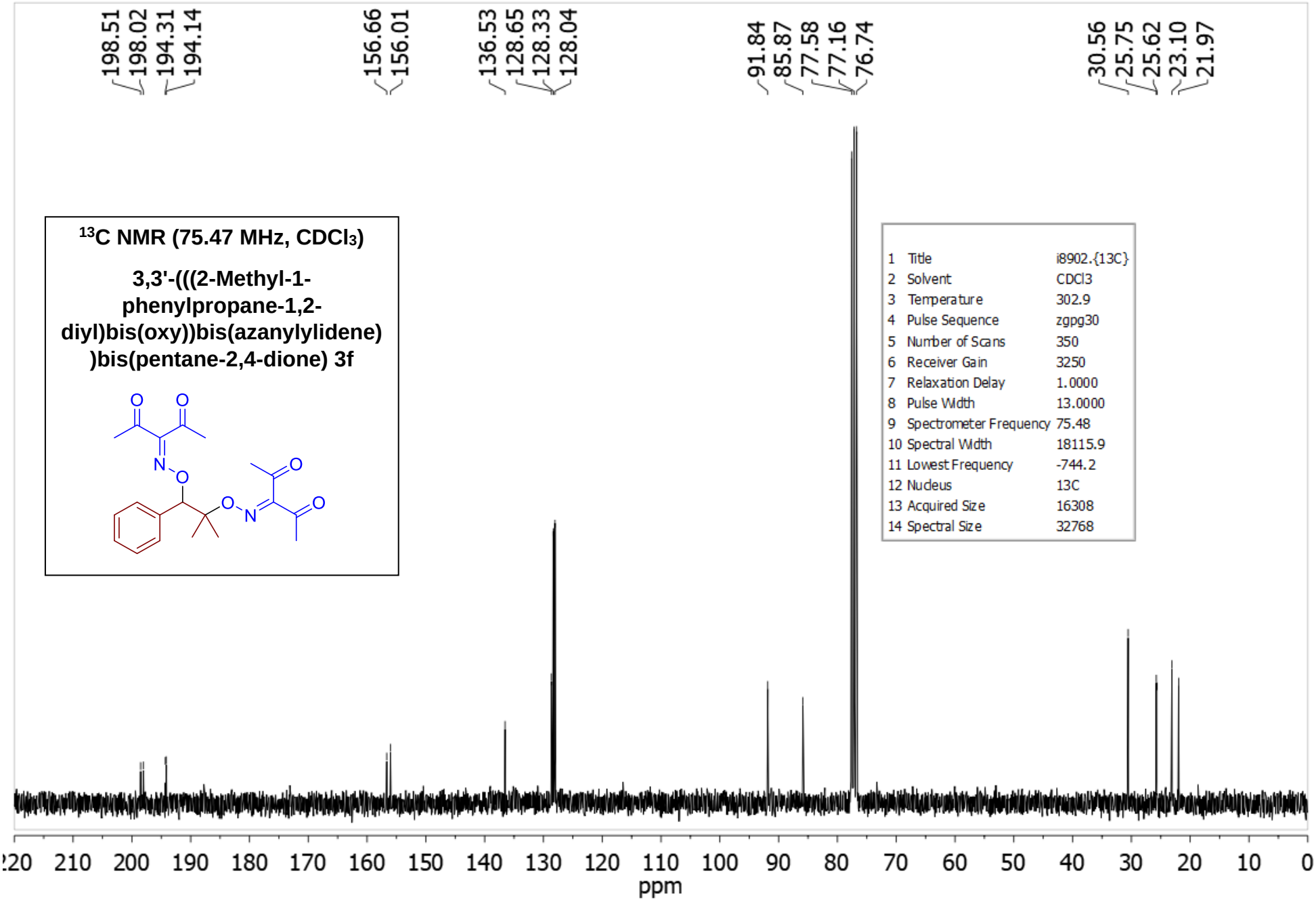
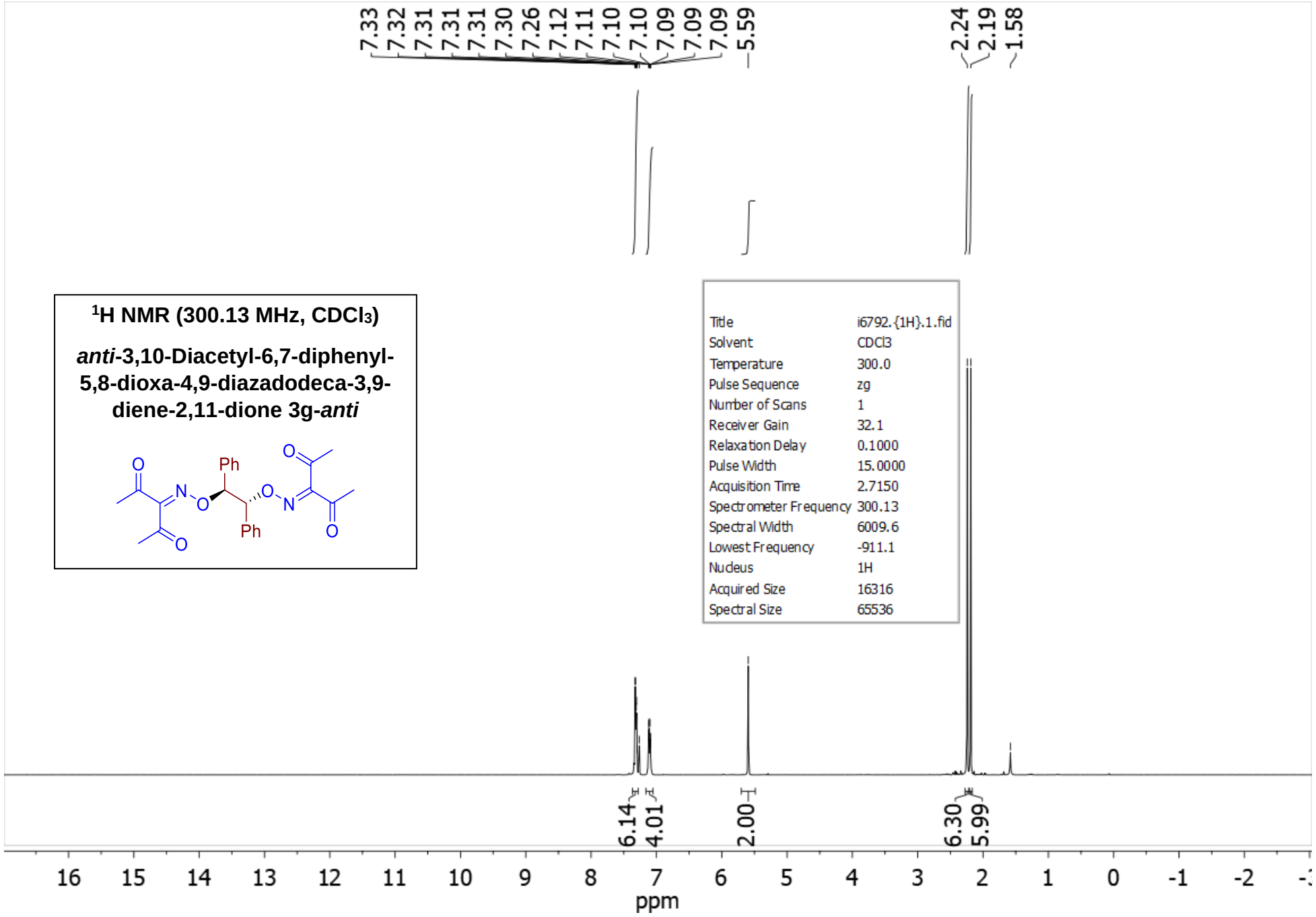
ppm

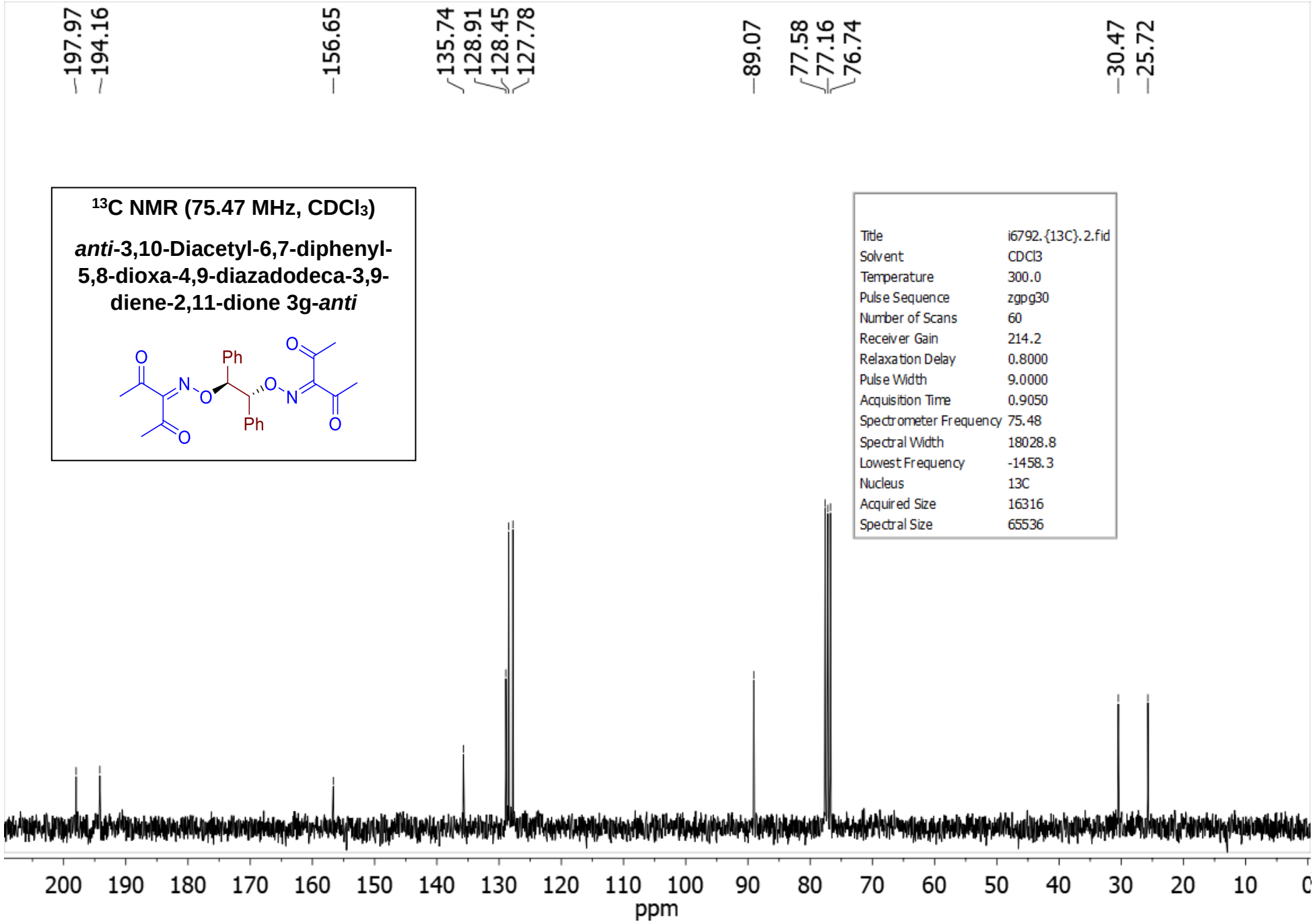

7.40 7.39 7.39 7.38 7.38 7.38 7.37 7.37 7.36 7.36 7.35 7.35 7.34 7.33 7.33 7.32 7.32 7.26 7.25 7.24 7.23 7.23 7.22 7.22
5.47 5.45 5.34 5.31
4.81 4.79 4.77 4.75 4.75 4.73 4.72
2.36 2.35 2.34 2.30 2.29 2.27 2.26 2.16 1.30 1.28 1.20 1.17
^{1}H NMR (300.13 MHz, CDCl$_3$)
3,3'-(((1-Phenylpropane-1,2-diyl)bis(oxy))bis(azanylylidene)) bis(pentane-2,4-dione) (mixture of diastereomers 1.7:1) 3e
Title i8640.{1H}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32
Relaxation Delay 0.1000
Pulse Width 14.5000
Spectrometer Frequency 300.23
Spectral Width 5882.4
Lowest Frequency -1097.8
Nucleus 1H
Acquired Size 16308
Spectral Size 32768
3.11 2.09 0.60 0.36 1.00 1.14 1.95 1.85 1.15 1.87 1.09 1.01 1.85 1.89 1.08
2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm


198.35
198.17
198.09
198.03
194.28
194.26
194.22
194.20
156.81
156.55
156.18
156.08
136.50
136.45
136.26
129.07
128.88
128.71
127.47
127.17
89.98
88.87
83.88
83.72
77.58
77.16
76.74
30.61
30.58
30.47
25.74
25.72
25.69
16.40
14.75
^{13}C NMR (75.47 MHz, CDCl$_3$)
3,3'-(((1-Phenylpropane-1,2-diyl)bis(oxy))bis(azanylylidene)) bis(pentane-2,4-dione) (mixture of diastereomers 1.7:1) 3e
Title i8640.{13C}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 200
Receiver Gain 101
Relaxation Delay 0.8000
Pulse Width 10.0000
Spectrometer Frequency 75.50
Spectral Width 17857.1
Lowest Frequency -1369.9
Nucleus 13C
Acquired Size 20412
Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm


7.36
7.34
7.24
7.24
7.22
5.44
2.40
2.36
2.25
2.22
1.40
1.33
^{1}H NMR (300.13 MHz, CDCl$_3$)
3,3'-(((2-Methyl-1-phenylpropane-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione) 3f
1 Title i8902.{1H}
2 Solvent CDCl3
3 Temperature 302.8
4 Pulse Sequence zg
5 Number of Scans 1
6 Receiver Gain 40
7 Relaxation Delay 0.0050
8 Pulse Width 9.0000
9 Spectrometer Frequency 300.13
10 Spectral Width 6009.6
11 Lowest Frequency -609.8
12 Nucleus 1H
13 Acquired Size 8124
14 Spectral Size 16384
3.01
1.98
1.00
3.00
3.14
2.95
3.26
3.00
3.13
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
ppm

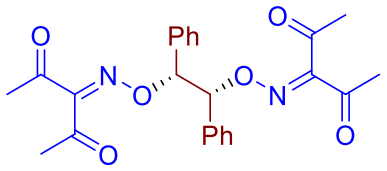

198.51
198.02
194.31
194.14
156.66
156.01
136.53
128.65
128.33
128.04
91.84
85.87
77.58
77.16
76.74
30.56
25.75
25.62
23.10
21.97
^{13}C NMR (75.47 MHz, CDCl$_3$)
3,3'-(((2-Methyl-1-phenylpropane-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione) 3f
1 Title i8902.{13C}
2 Solvent CDCl3
3 Temperature 302.9
4 Pulse Sequence zgpg30
5 Number of Scans 350
6 Receiver Gain 3250
7 Relaxation Delay 1.0000
8 Pulse Width 13.0000
9 Spectrometer Frequency 75.48
10 Spectral Width 18115.9
11 Lowest Frequency -744.2
12 Nucleus 13C
13 Acquired Size 16308
14 Spectral Size 32768
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

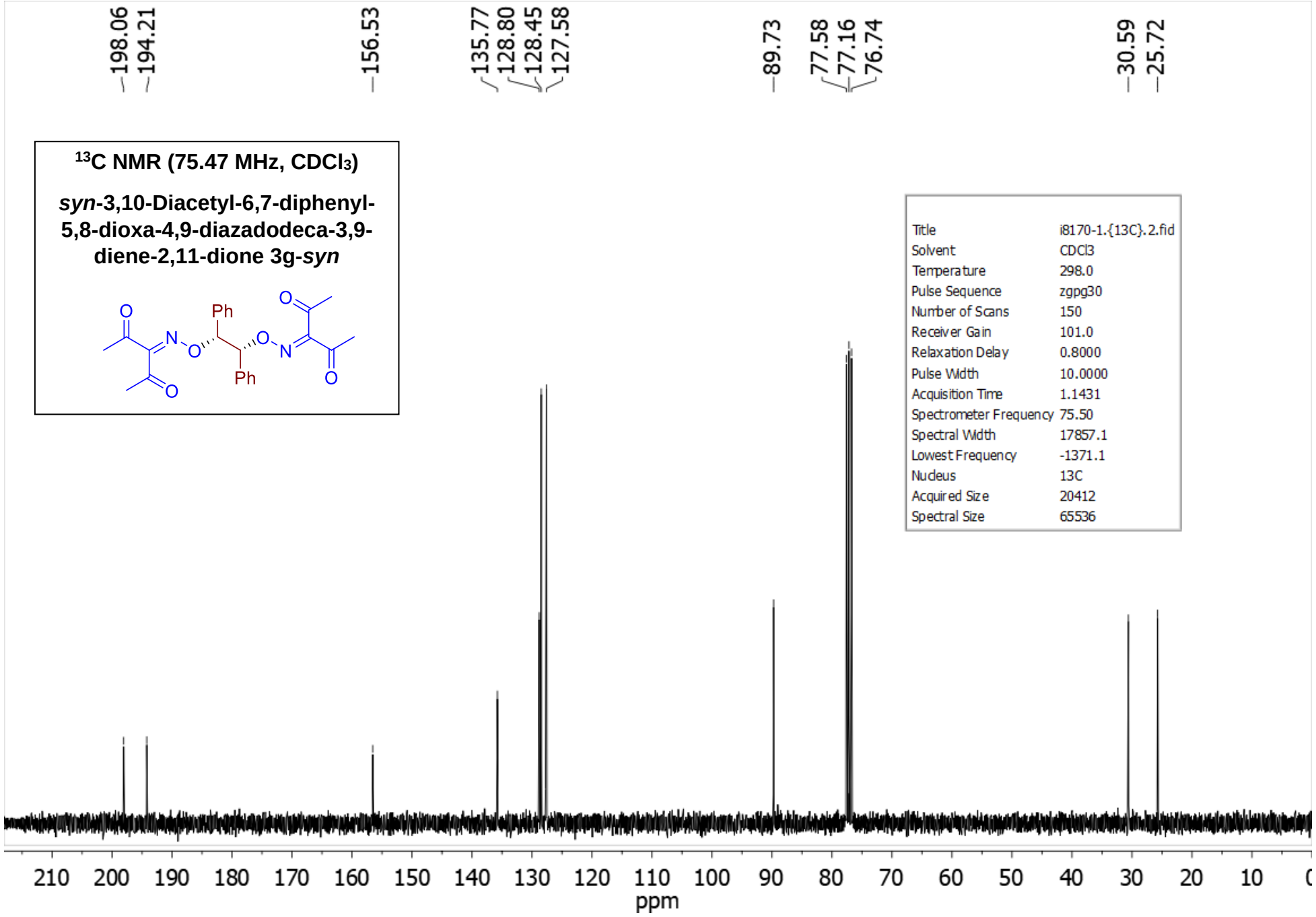

7.33
7.32
7.31
7.31
7.31
7.30
7.26
7.12
7.11
7.10
7.10
7.09
7.09
7.09
5.59
2.24
2.19
1.58
¹H NMR (300.13 MHz, CDCl₃)
anti-3,10-Diacetyl-6,7-diphenyl-5,8-dioxa-4,9-diazadodeca-3,9-diene-2,11-dione 3g-anti
Ph
Ph
Title i6792.{1H}.1.fid
Solvent CDCl3
Temperature 300.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32.1
Relaxation Delay 0.1000
Pulse Width 15.0000
Acquisition Time 2.7150
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -911.1
Nucleus 1H
Acquired Size 16316
Spectral Size 65536
6.14
4.01
2.00
6.30
5.99
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
ppm


197.97
194.16
156.65
135.74
128.91
128.45
127.78
89.07
77.58
77.16
76.74
30.47
25.72
13C NMR (75.47 MHz, CDCl3)
anti-3,10-Diacetyl-6,7-diphenyl-5,8-dioxa-4,9-diazadodeca-3,9-diene-2,11-dione 3g-anti
Ph
Ph
Title i6792.{13C}.2.fid
Solvent CDCl3
Temperature 300.0
Pulse Sequence zgpg30
Number of Scans 60
Receiver Gain 214.2
Relaxation Delay 0.8000
Pulse Width 9.0000
Acquisition Time 0.9050
Spectrometer Frequency 75.48
Spectral Width 18028.8
Lowest Frequency -1458.3
Nucleus 13C
Acquired Size 16316
Spectral Size 65536
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

^{1}H NMR (300.13 MHz, $CDCl_3$)

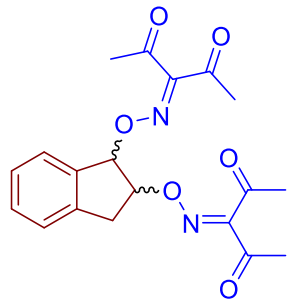
syn*-3,10-Diacetyl-6,7-diphenyl-5,8-dioxa-4,9-diazadodeca-3,9-diene-2,11-dione 3g-*syn



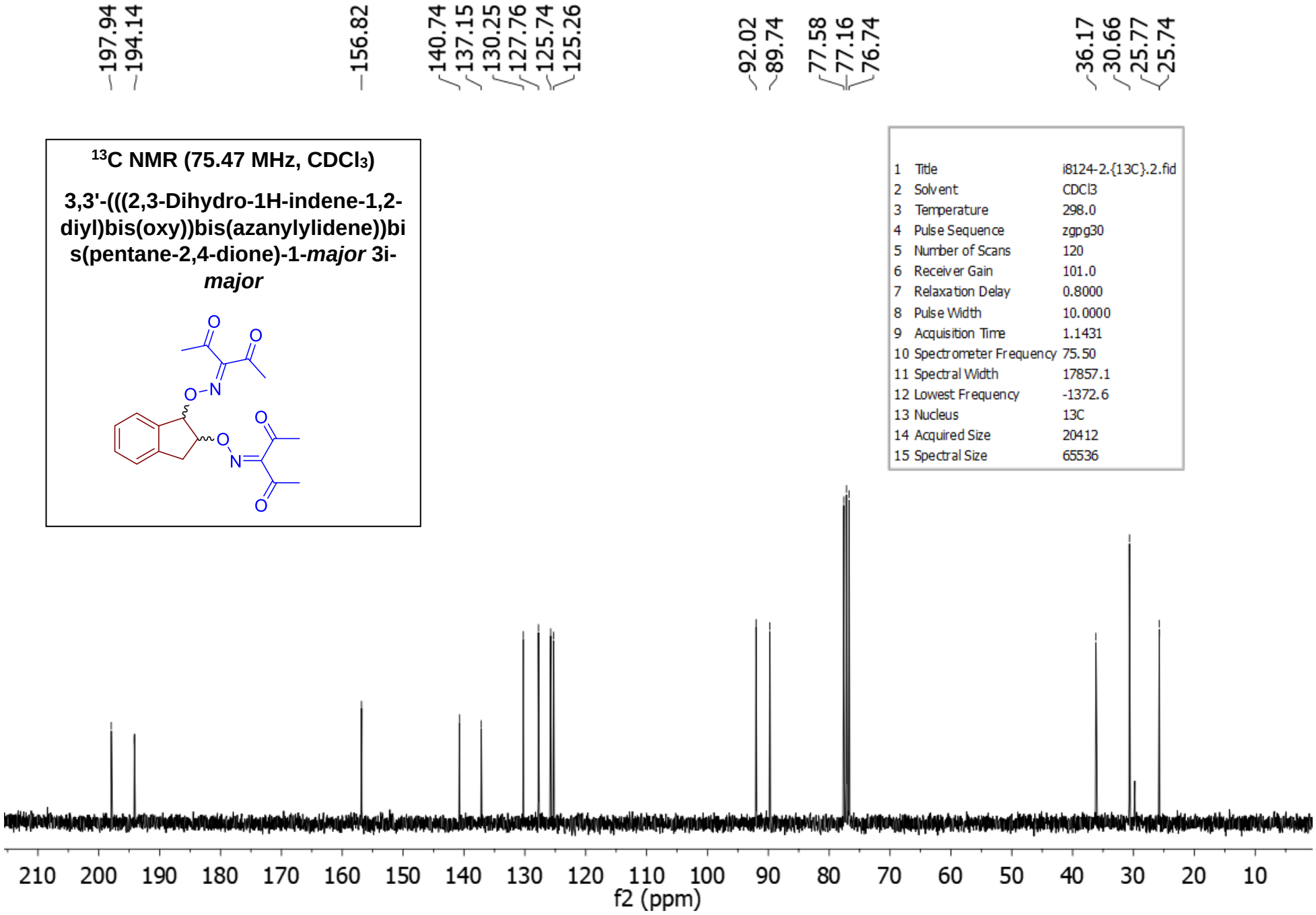

198.06
194.21
156.53
135.77
128.80
128.45
127.58
89.73
77.58
77.16
76.74
30.59
25.72
13C NMR (75.47 MHz, CDCl3)
syn-3,10-Diacetyl-6,7-diphenyl-5,8-dioxa-4,9-diazadodeca-3,9-diene-2,11-dione 3g-syn
Ph
Ph
Title i8170-1.{13C}.2.fid
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 150
Receiver Gain 101.0
Relaxation Delay 0.8000
Pulse Width 10.0000
Acquisition Time 1.1431
Spectrometer Frequency 75.50
Spectral Width 17857.1
Lowest Frequency -1371.1
Nucleus 13C
Acquired Size 20412
Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm

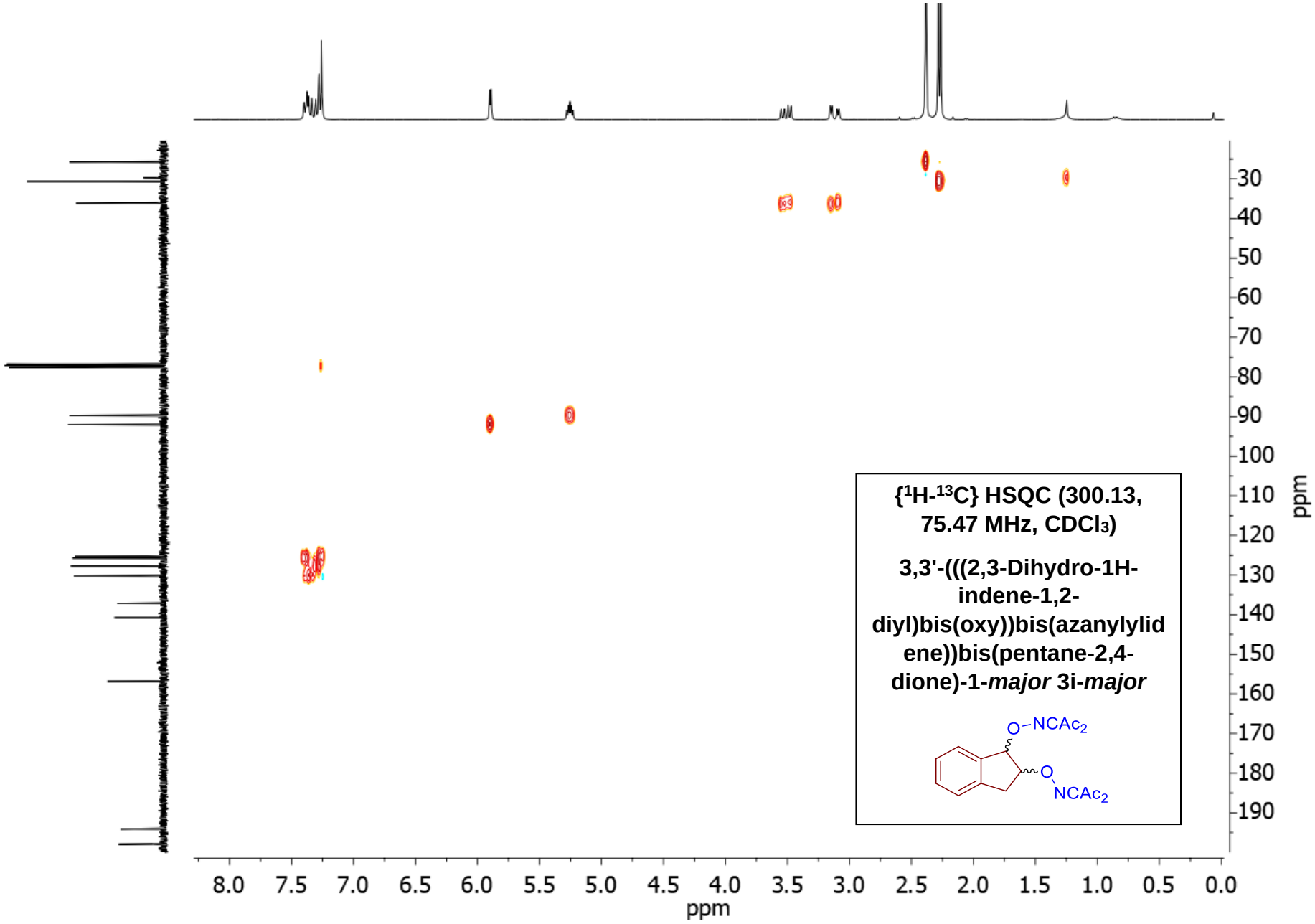
^{1}H NMR (300.13 MHz, $CDCl_3$)

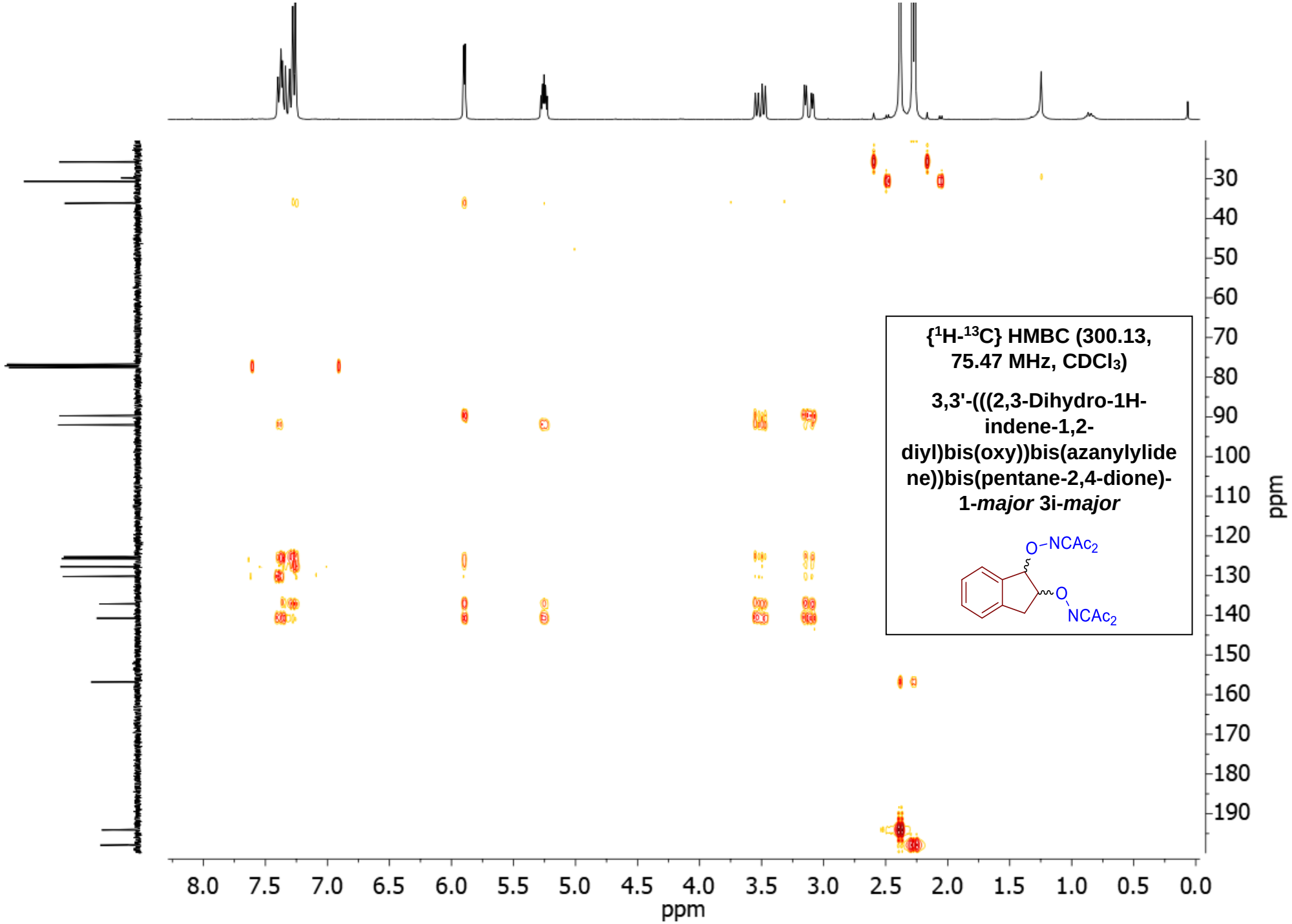
3,3'-(((2,3-Dihydro-1H-indene-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione)-1-*major* 3i-*major*



1	Title	i8124-2.{1H}.1.fid
2	Solvent	CDCl3
3	Temperature	298.0
4	Pulse Sequence	zg
5	Number of Scans	1
6	Receiver Gain	32.0
7	Relaxation Delay	0.1000
8	Pulse Width	14.5000
9	Acquisition Time	2.7724
10	Spectrometer Frequency	300.23
11	Spectral Width	5882.4
12	Lowest Frequency	-1094.2
13	Nucleus	1H
14	Acquired Size	16308
15	Spectral Size	65536

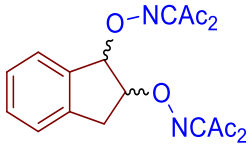

197.94
194.14
156.82
140.74
137.15
130.25
127.76
125.74
125.26
92.02
89.74
77.58
77.16
76.74
36.17
30.66
25.77
25.74
^{13}C NMR (75.47 MHz, CDCl$_3$)
3,3'-(((2,3-Dihydro-1H-indene-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione)-1-*major* 3i-*major*
1 Title i8124-2.{13C}.2.fid
2 Solvent CDCl3
3 Temperature 298.0
4 Pulse Sequence zgpg30
5 Number of Scans 120
6 Receiver Gain 101.0
7 Relaxation Delay 0.8000
8 Pulse Width 10.0000
9 Acquisition Time 1.1431
10 Spectrometer Frequency 75.50
11 Spectral Width 17857.1
12 Lowest Frequency -1372.6
13 Nucleus 13C
14 Acquired Size 20412
15 Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f2 (ppm)


{^{1}H-^{13}C} HSQC (300.13, 75.47 MHz, $CDCl_3$)
3,3'-(((2,3-Dihydro-1H-indene-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione)-1-*major* 3i-*major*
O–NCAc2
O
NCAc2
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm
30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190
ppm


{1H-13C} HMBC (300.13, 75.47 MHz, CDCl3)
3,3'-(((2,3-Dihydro-1H-indene-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione)-1-major 3i-major
O–NCAc2
O
NCAc2
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm
30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190
ppm

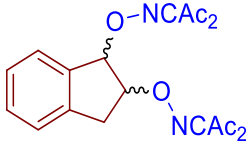
NOESY (300.13 MHz, $CDCl_3$)

3,3'-(((2,3-Dihydro-1H-indene-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione)-1-*major* 3i-*major*



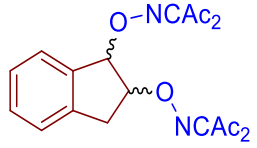
NOESY (300.13 MHz, $CDCl_3$)

3,3'-(((2,3-Dihydro-1H-indene-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione)-1-*major* 3i-*major*



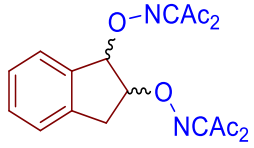
NOESY (300.13 MHz, $CDCl_3$)

3,3'-(((2,3-Dihydro-1H-indene-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione)-1-*major* 3i-*major*



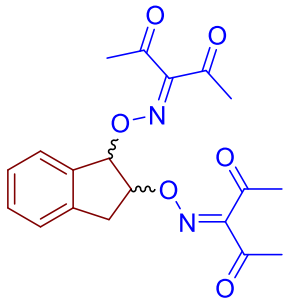
NOESY (300.13 MHz, $CDCl_3$)

3,3'-(((2,3-Dihydro-1H-indene-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione)-1-*major* 3i-*major*



^{1}H NMR (300.13 MHz, $CDCl_3$)

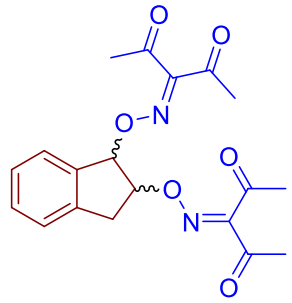
3,3'-(((2,3-Dihydro-1H-indene-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione)-2-*minor* 3i-*minor*



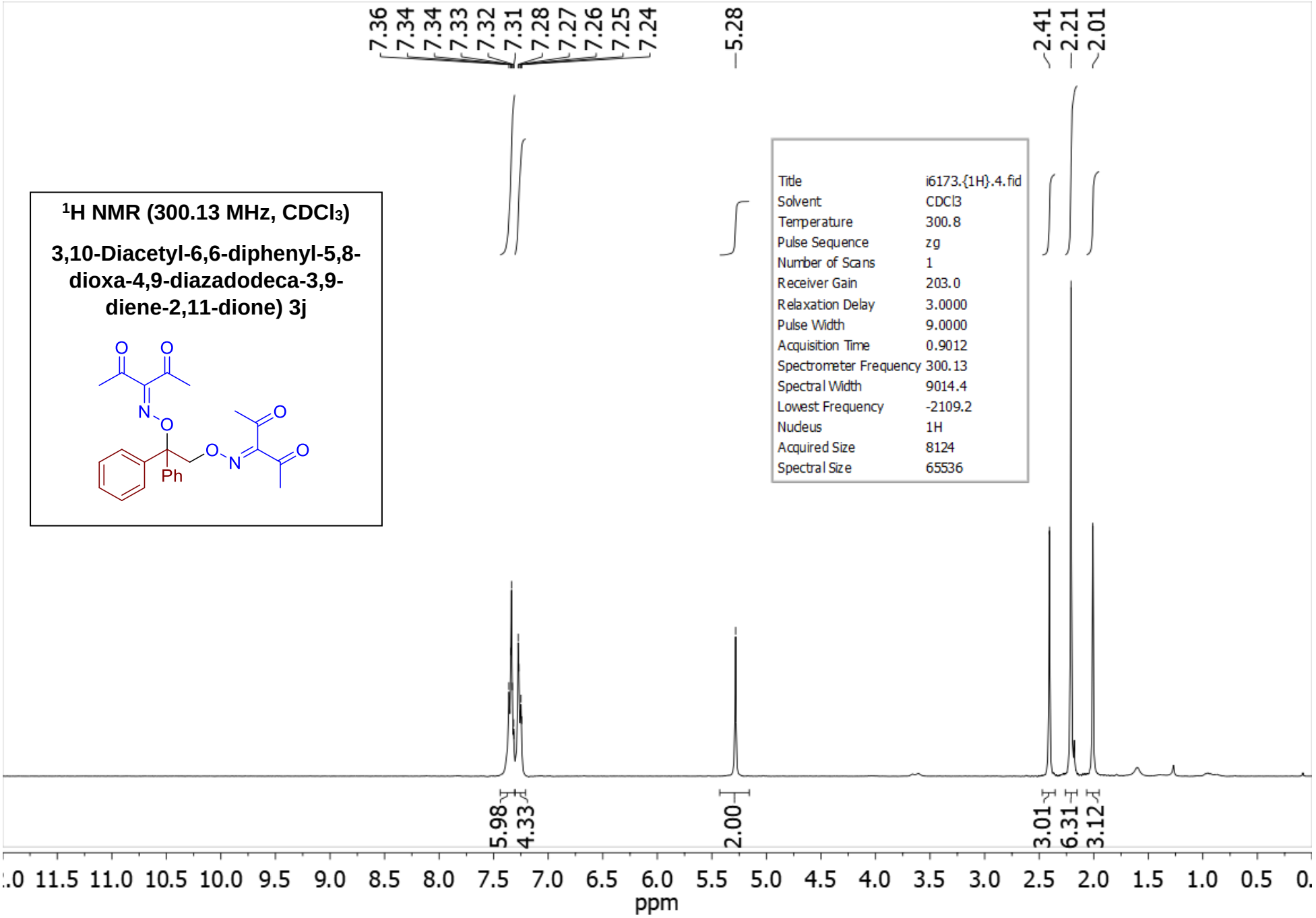
1	Title	i8125.{1H}.1.fid
2	Solvent	CDCl3
3	Temperature	301.0
4	Pulse Sequence	zg
5	Number of Scans	4
6	Receiver Gain	14.2
7	Relaxation Delay	0.0050
8	Pulse Width	9.0000
9	Acquisition Time	1.3518
10	Spectrometer Frequency	300.13
11	Spectral Width	6009.6
12	Lowest Frequency	-610.8
13	Nucleus	1H
14	Acquired Size	8124
15	Spectral Size	65536

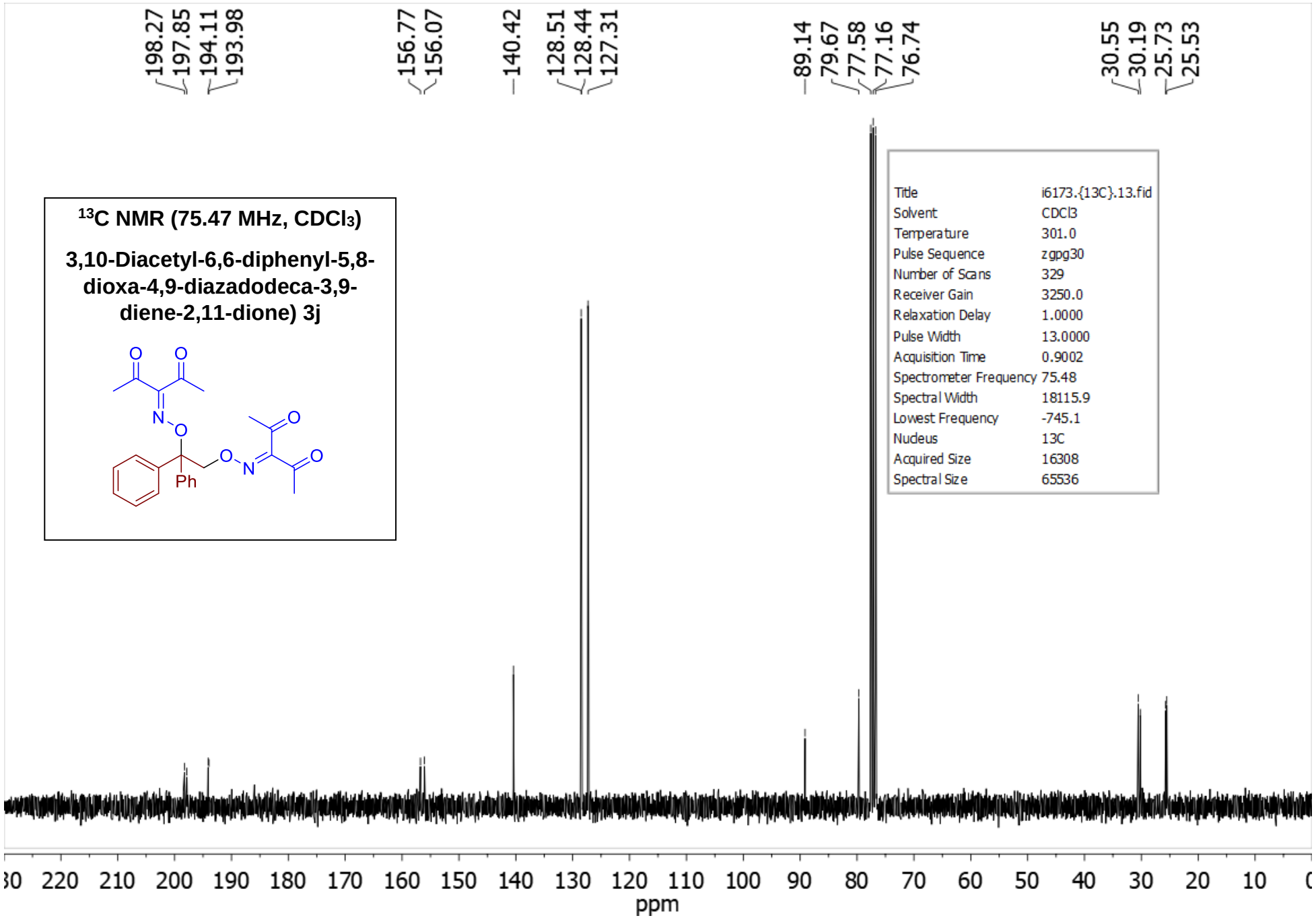
^{13}C NMR (75.47 MHz, $CDCl_3$)

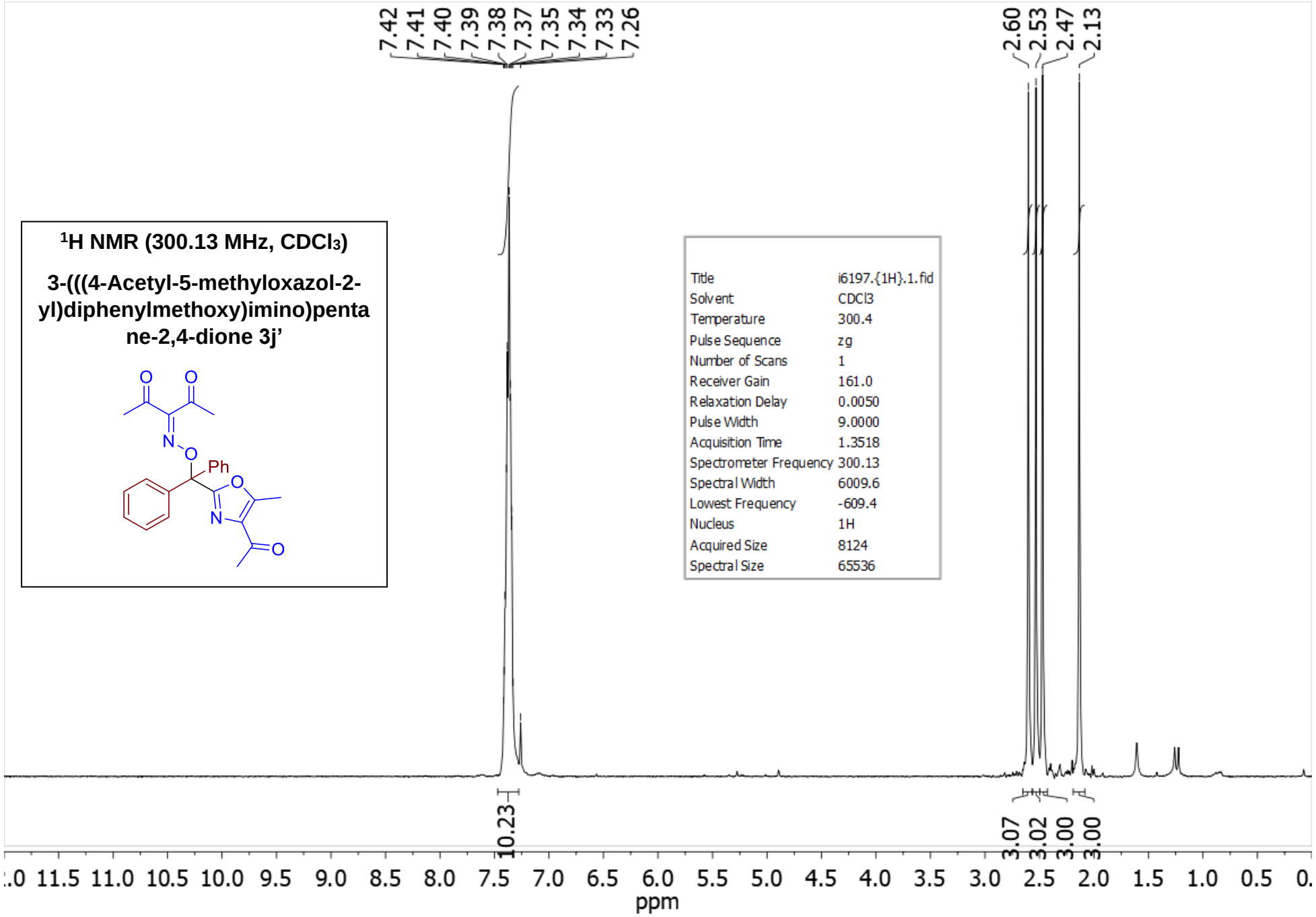
3,3'-(((2,3-Dihydro-1H-indene-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione)-2-*minor* 3i-*minor*

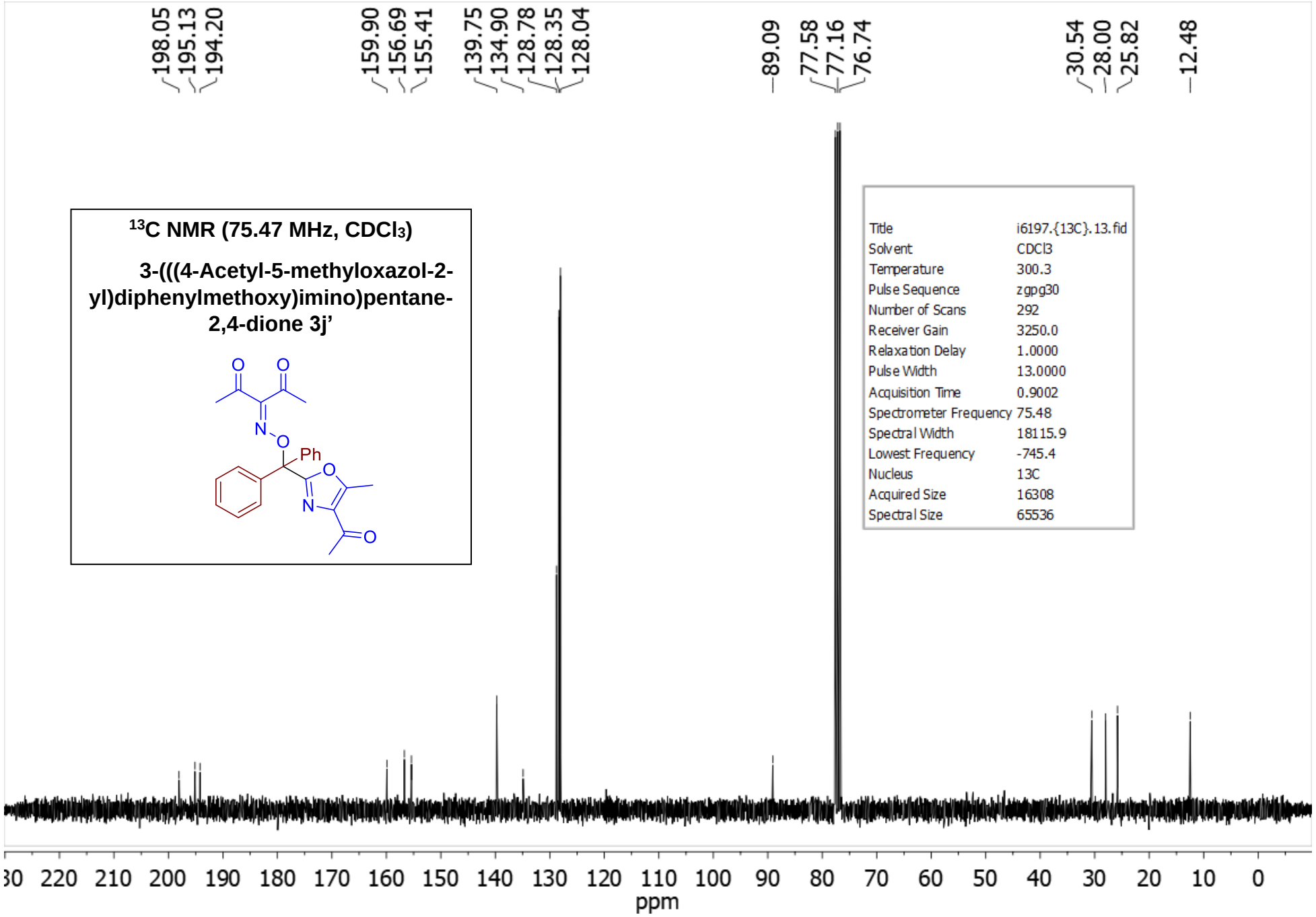


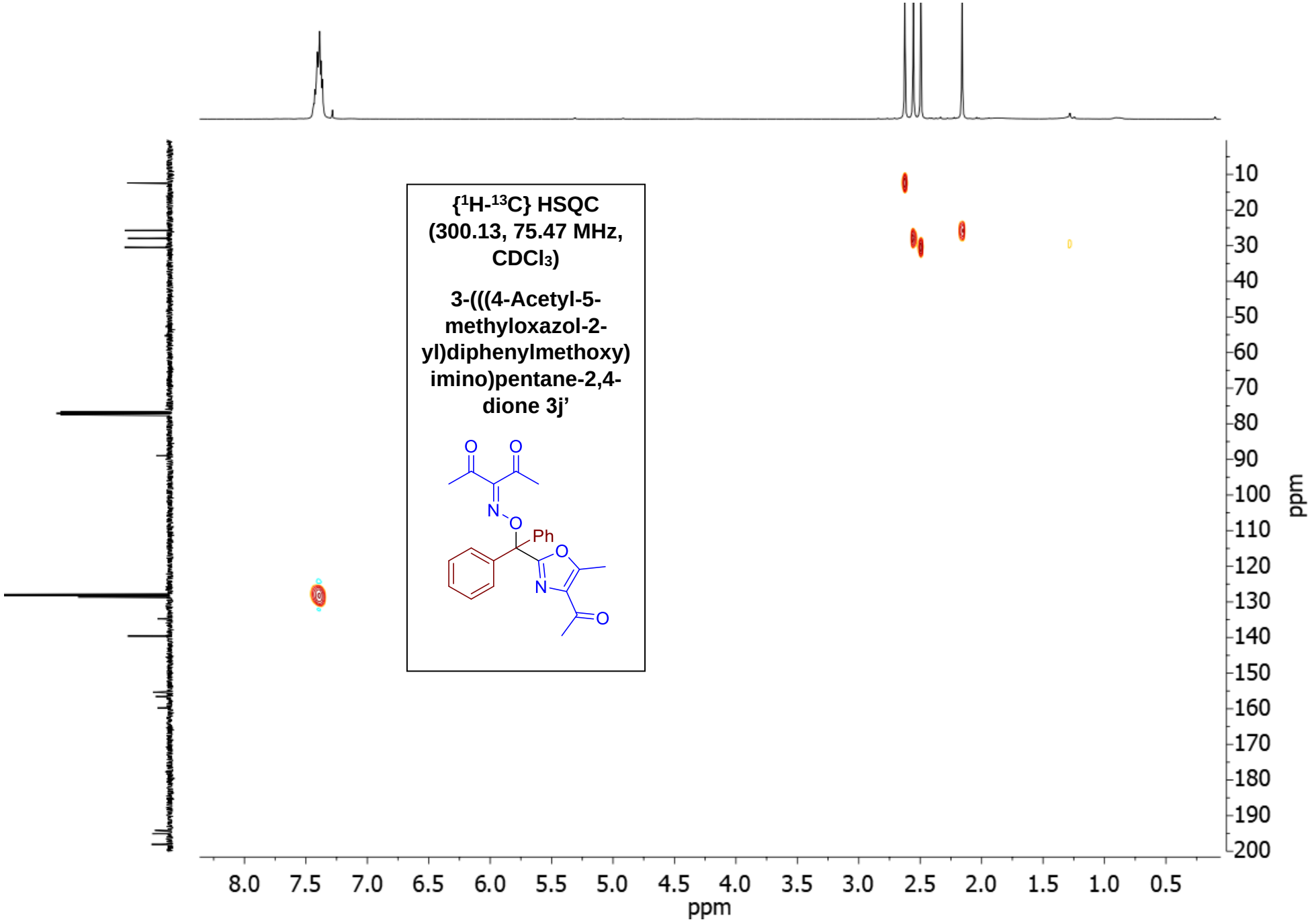
1	Title	i8604.{13C}.13.fid
2	Solvent	CDCl3
3	Temperature	301.9
4	Pulse Sequence	zgpg30
5	Number of Scans	919
6	Receiver Gain	3250.0
7	Relaxation Delay	1.0000
8	Pulse Width	13.0000
9	Acquisition Time	0.9002
10	Spectrometer Frequency	75.48
11	Spectral Width	18115.9
12	Lowest Frequency	-745.9
13	Nucleus	13C
14	Acquired Size	16308
15	Spectral Size	65536

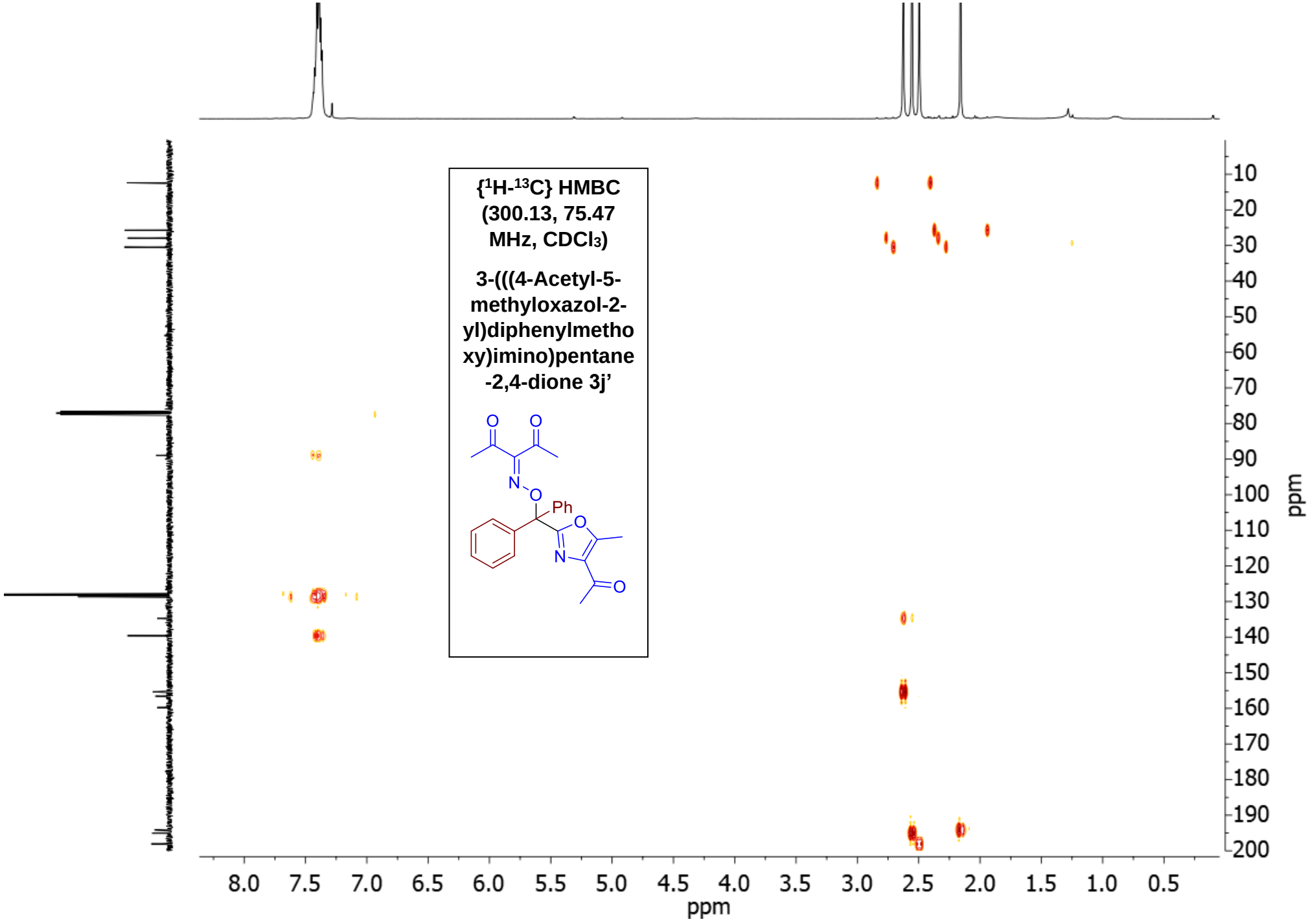

7.36
7.34
7.34
7.33
7.32
7.31
7.28
7.27
7.26
7.25
7.24
5.28
2.41
2.21
2.01
^{1}H NMR (300.13 MHz, CDCl$_3$)
3,10-Diacetyl-6,6-diphenyl-5,8-dioxa-4,9-diazadodeca-3,9-diene-2,11-dione) 3j
Title i6173.{1H}.4.fid
Solvent CDCl3
Temperature 300.8
Pulse Sequence zg
Number of Scans 1
Receiver Gain 203.0
Relaxation Delay 3.0000
Pulse Width 9.0000
Acquisition Time 0.9012
Spectrometer Frequency 300.13
Spectral Width 9014.4
Lowest Frequency -2109.2
Nucleus 1H
Acquired Size 8124
Spectral Size 65536
5.98
4.33
2.00
3.01
6.31
3.12
ppm


198.27
197.85
194.11
193.98
156.77
156.07
140.42
128.51
128.44
127.31
89.14
79.67
77.58
77.16
76.74
30.55
30.19
25.73
25.53
^{13}C NMR (75.47 MHz, CDCl$_3$)
3,10-Diacetyl-6,6-diphenyl-5,8-dioxa-4,9-diazadodeca-3,9-diene-2,11-dione) 3j
Ph
Title i6173.{13C}.13.fid
Solvent CDCl3
Temperature 301.0
Pulse Sequence zgpg30
Number of Scans 329
Receiver Gain 3250.0
Relaxation Delay 1.0000
Pulse Width 13.0000
Acquisition Time 0.9002
Spectrometer Frequency 75.48
Spectral Width 18115.9
Lowest Frequency -745.1
Nucleus 13C
Acquired Size 16308
Spectral Size 65536
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm


7.42
7.41
7.40
7.39
7.38
7.37
7.35
7.34
7.33
7.26
2.60
2.53
2.47
2.13
^{1}H NMR (300.13 MHz, CDCl$_3$)
3-(((4-Acetyl-5-methyloxazol-2-yl)diphenylmethoxy)imino)pentane-2,4-dione 3j'
Ph
Title i6197.{1H}.1.fid
Solvent CDCl3
Temperature 300.4
Pulse Sequence zg
Number of Scans 1
Receiver Gain 161.0
Relaxation Delay 0.0050
Pulse Width 9.0000
Acquisition Time 1.3518
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -609.4
Nucleus 1H
Acquired Size 8124
Spectral Size 65536
10.23
3.07
3.02
3.00
3.00
ppm

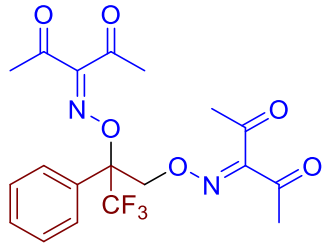

198.05
195.13
194.20
159.90
156.69
155.41
139.75
134.90
128.78
128.35
128.04
89.09
77.58
77.16
76.74
30.54
28.00
25.82
12.48
^{13}C NMR (75.47 MHz, CDCl$_3$)
3-(((4-Acetyl-5-methyloxazol-2-yl)diphenylmethoxy)imino)pentane-2,4-dione 3j'
Ph
Title i6197.{13C}.13.fid
Solvent CDCl3
Temperature 300.3
Pulse Sequence zgpg30
Number of Scans 292
Receiver Gain 3250.0
Relaxation Delay 1.0000
Pulse Width 13.0000
Acquisition Time 0.9002
Spectrometer Frequency 75.48
Spectral Width 18115.9
Lowest Frequency -745.4
Nucleus 13C
Acquired Size 16308
Spectral Size 65536
ppm

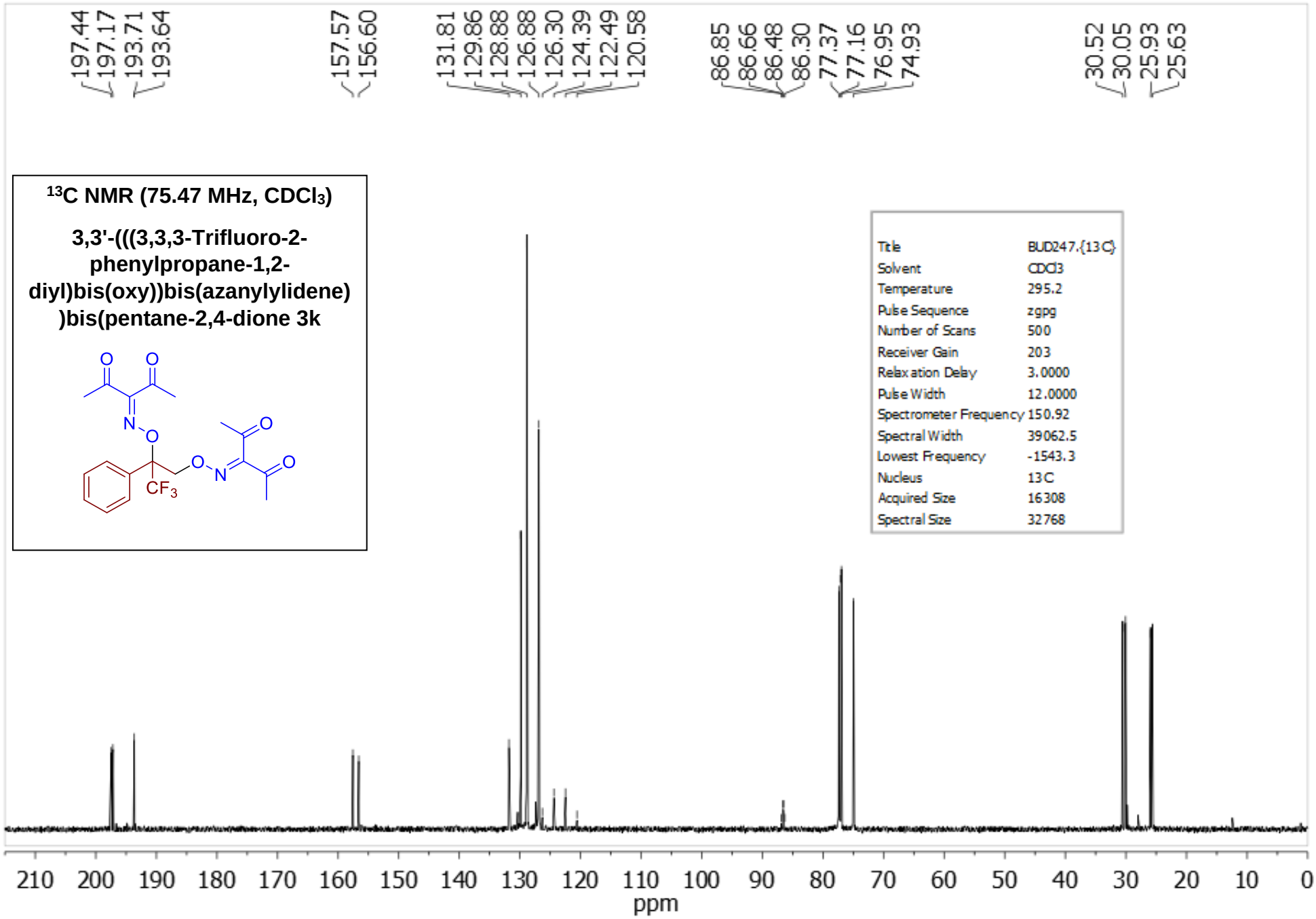

{1H-13C} HSQC
(300.13, 75.47 MHz,
CDCl3)
3-(((4-Acetyl-5-
methyloxazol-2-
yl)diphenylmethoxy)
imino)pentane-2,4-
dione 3j'
O
O
N
O
Ph
O
N
O
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
ppm

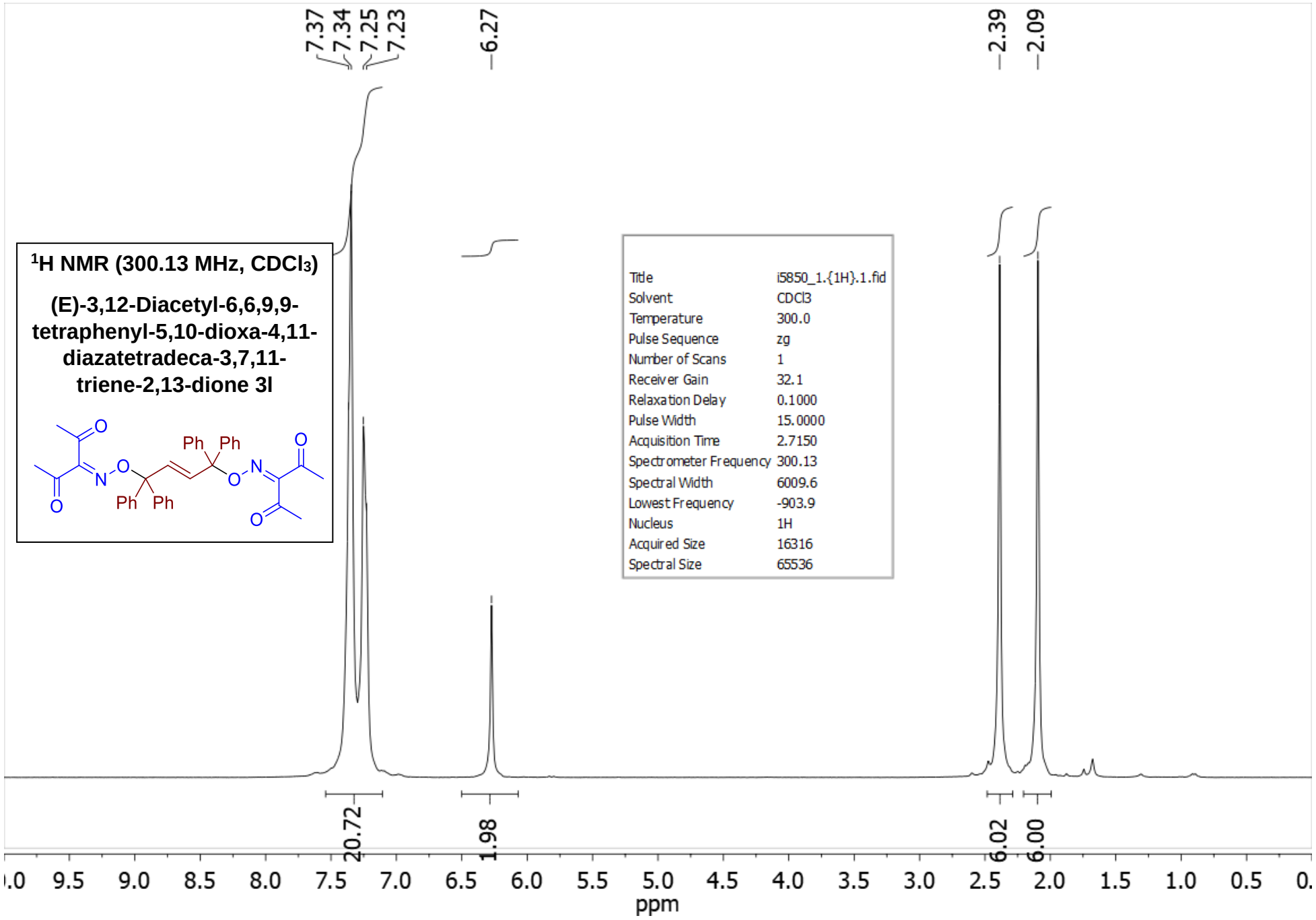

{1H-13C} HMBC (300.13, 75.47 MHz, CDCl3)
3-(((4-Acetyl-5-methyloxazol-2-yl)diphenylmethoxy)imino)pentane-2,4-dione 3j'
O
O
N
O
Ph
O
N
O
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
ppm

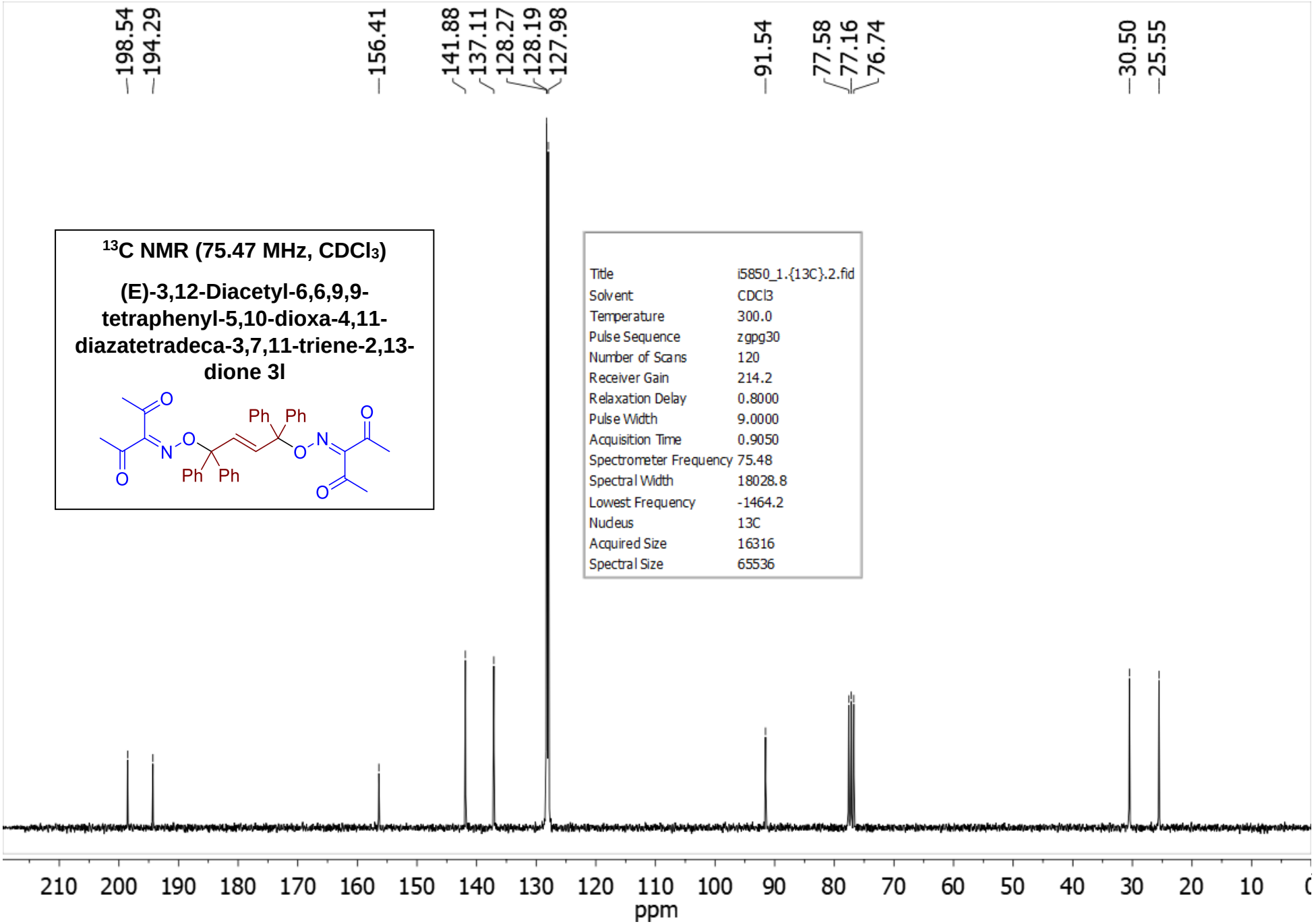
^{1}H NMR (300.13 MHz, $CDCl_3$)

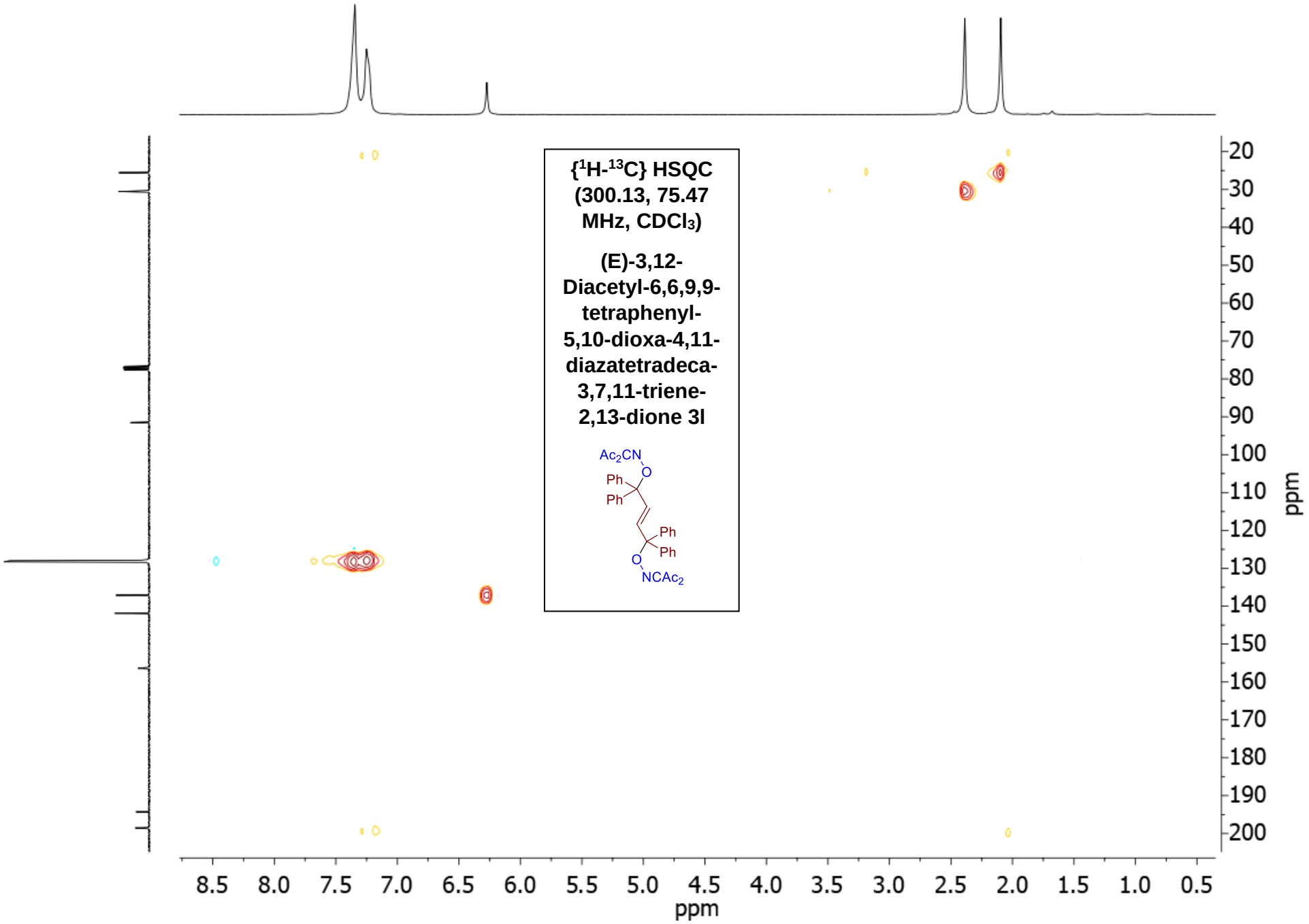
3,3'-(((3,3,3-Trifluoro-2-phenylpropane-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione 3k

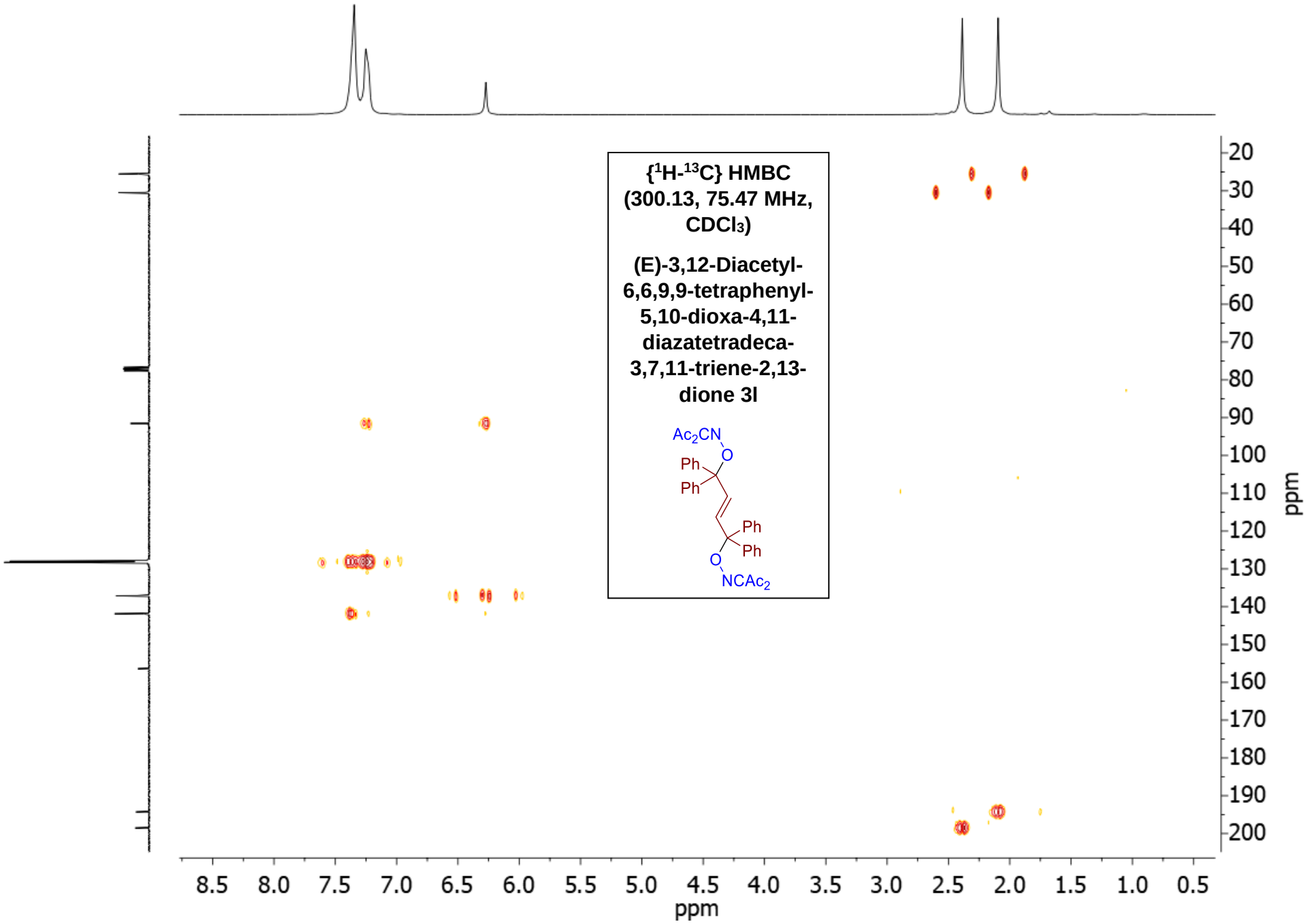


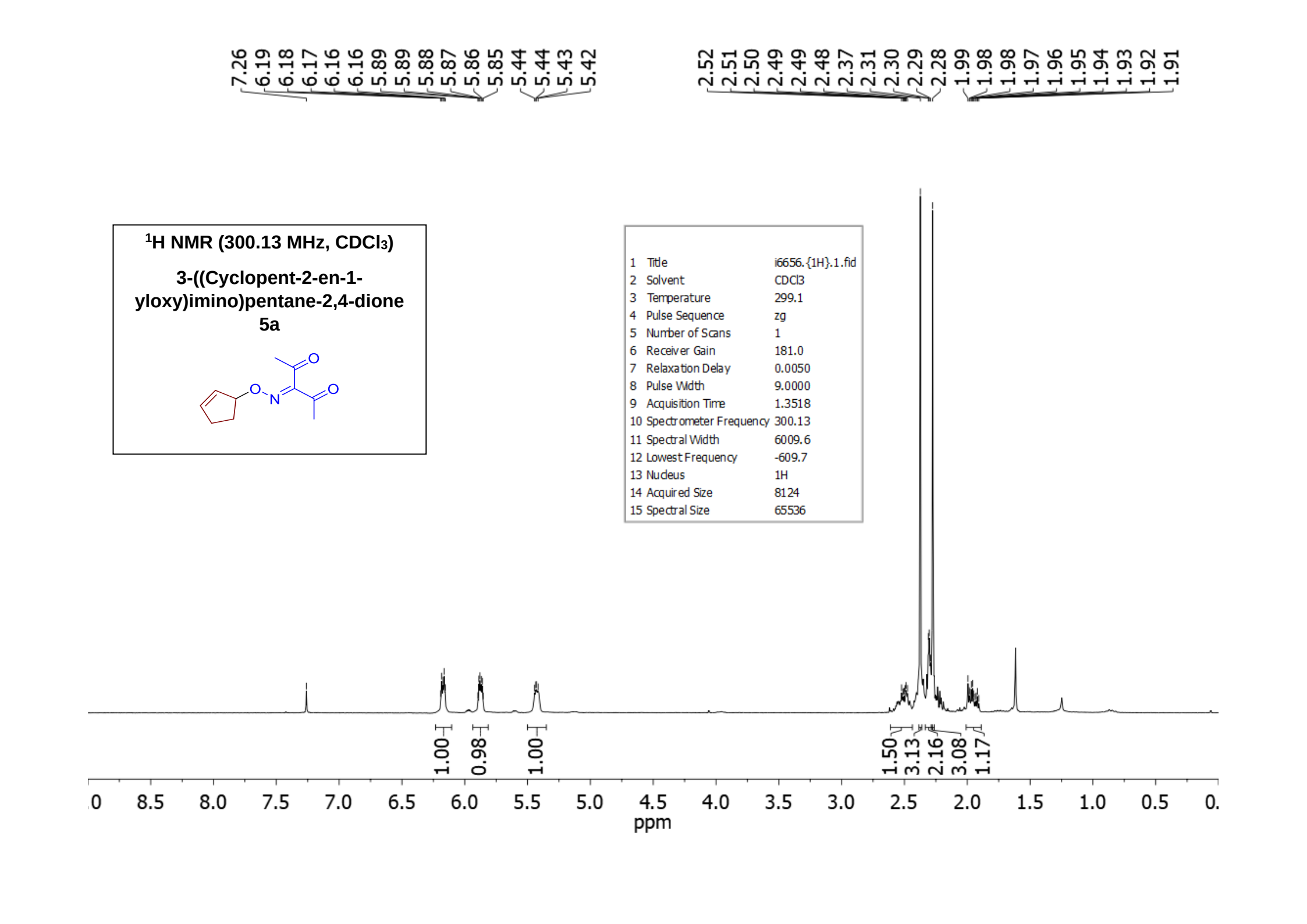

197.44
197.17
193.71
193.64
157.57
156.60
131.81
129.86
128.88
126.88
126.30
124.39
122.49
120.58
86.85
86.66
86.48
86.30
77.37
77.16
76.95
74.93
30.52
30.05
25.93
25.63
^{13}C NMR (75.47 MHz, CDCl$_3$)
3,3'-(((3,3,3-Trifluoro-2-phenylpropane-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione 3k
Title BUD247.{13C}
Solvent CDCl3
Temperature 295.2
Pulse Sequence zgpg
Number of Scans 500
Receiver Gain 203
Relaxation Delay 3.0000
Pulse Width 12.0000
Spectrometer Frequency 150.92
Spectral Width 39062.5
Lowest Frequency -1543.3
Nucleus 13C
Acquired Size 16308
Spectral Size 32768
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


7.37
7.34
7.25
7.23
6.27
2.39
2.09
^{1}H NMR (300.13 MHz, CDCl$_3$)
(E)-3,12-Diacetyl-6,6,9,9-tetraphenyl-5,10-dioxa-4,11-diazatetradeca-3,7,11-triene-2,13-dione 3l
Ph Ph
Ph Ph
O
N
O
N
O
O
O
O
Title i5850_1.{1H}.1.fid
Solvent CDCl3
Temperature 300.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32.1
Relaxation Delay 0.1000
Pulse Width 15.0000
Acquisition Time 2.7150
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -903.9
Nucleus 1H
Acquired Size 16316
Spectral Size 65536
20.72
1.98
6.02
6.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
ppm


198.54
194.29
156.41
141.88
137.11
128.27
128.19
127.98
91.54
77.58
77.16
76.74
30.50
25.55
13C NMR (75.47 MHz, CDCl3)
(E)-3,12-Diacetyl-6,6,9,9-tetraphenyl-5,10-dioxa-4,11-diazatetradeca-3,7,11-triene-2,13-dione 3l
Ph Ph
Ph Ph
O
N
O
Title i5850_1.{13C}.2.fid
Solvent CDCl3
Temperature 300.0
Pulse Sequence zgpg30
Number of Scans 120
Receiver Gain 214.2
Relaxation Delay 0.8000
Pulse Width 9.0000
Acquisition Time 0.9050
Spectrometer Frequency 75.48
Spectral Width 18028.8
Lowest Frequency -1464.2
Nucleus 13C
Acquired Size 16316
Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm


{^{1}H-^{13}C} HSQC (300.13, 75.47 MHz, $CDCl_3$)
(E)-3,12-Diacetyl-6,6,9,9-tetraphenyl-5,10-dioxa-4,11-diazatetradeca-3,7,11-triene-2,13-dione 3l
Ac_2CN
O
Ph
Ph
Ph
Ph
O
$NCAc_2$
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
ppm
20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200
ppm

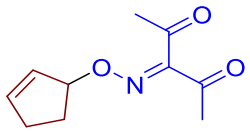

{1H-13C} HMBC (300.13, 75.47 MHz, CDCl3)
(E)-3,12-Diacetyl-6,6,9,9-tetraphenyl-5,10-dioxa-4,11-diazatetradeca-3,7,11-triene-2,13-dione 3l
Ac2CN
O
Ph
Ph
Ph
Ph
O
NCAc2
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
ppm
20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200
ppm


7.26
6.19
6.18
6.17
6.16
6.16
5.89
5.89
5.88
5.87
5.86
5.85
5.44
5.44
5.43
5.42
2.52
2.51
2.50
2.49
2.49
2.48
2.37
2.31
2.30
2.29
2.28
1.99
1.98
1.98
1.97
1.96
1.95
1.94
1.93
1.92
1.91
1H NMR (300.13 MHz, CDCl3)
3-((Cyclopent-2-en-1-yloxy)imino)pentane-2,4-dione
5a
O
O
O
N
1 Title i6656.{1H}.1.fid
2 Solvent CDCl3
3 Temperature 299.1
4 Pulse Sequence zg
5 Number of Scans 1
6 Receiver Gain 181.0
7 Relaxation Delay 0.0050
8 Pulse Width 9.0000
9 Acquisition Time 1.3518
10 Spectrometer Frequency 300.13
11 Spectral Width 6009.6
12 Lowest Frequency -609.7
13 Nucleus 1H
14 Acquired Size 8124
15 Spectral Size 65536
1.00
0.98
1.00
1.50
3.13
2.16
3.08
1.17
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
ppm

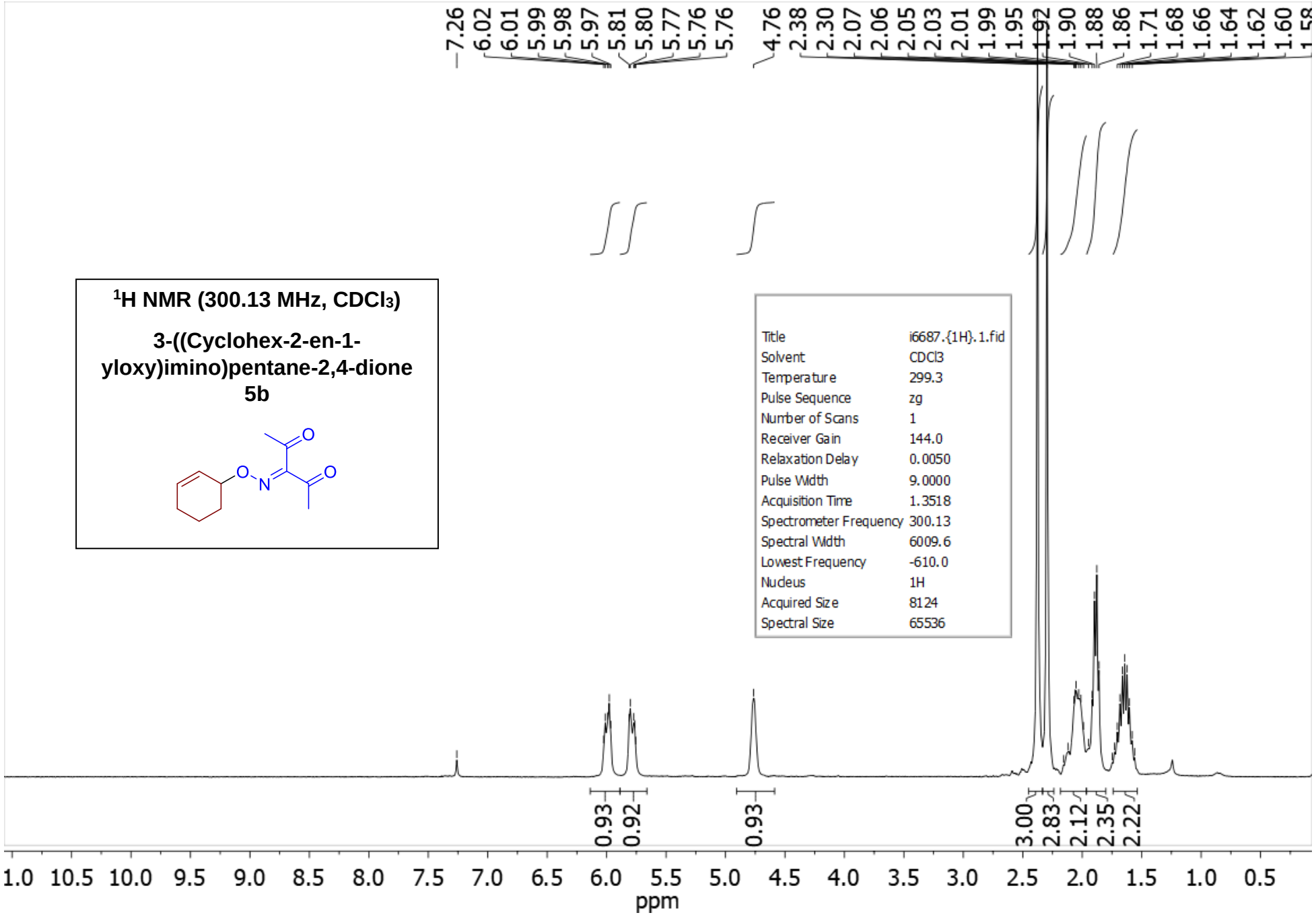
^{13}C NMR (75.47 MHz, $CDCl_3$)

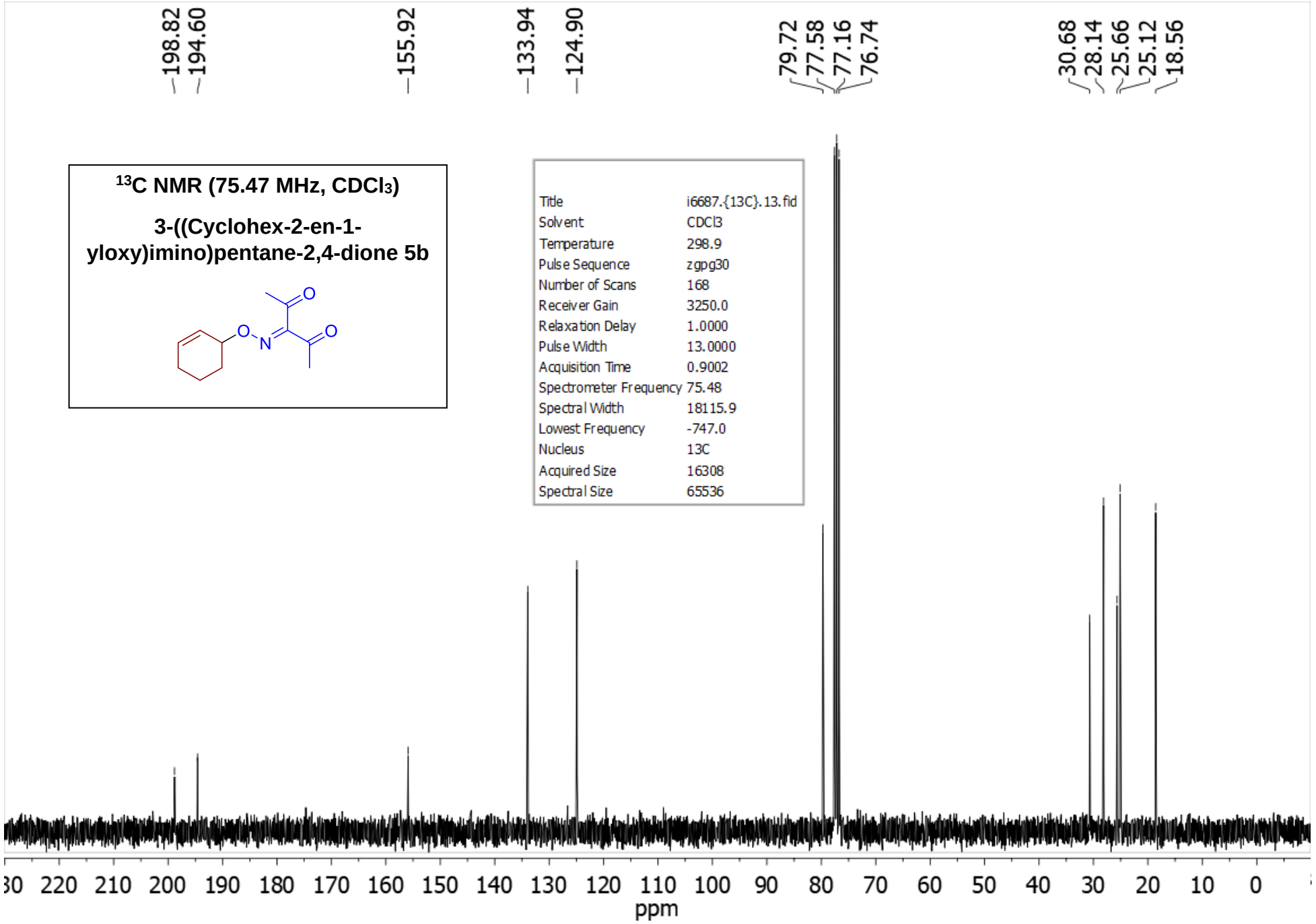
3-((Cyclopent-2-en-1-yloxy)imino)pentane-2,4-dione

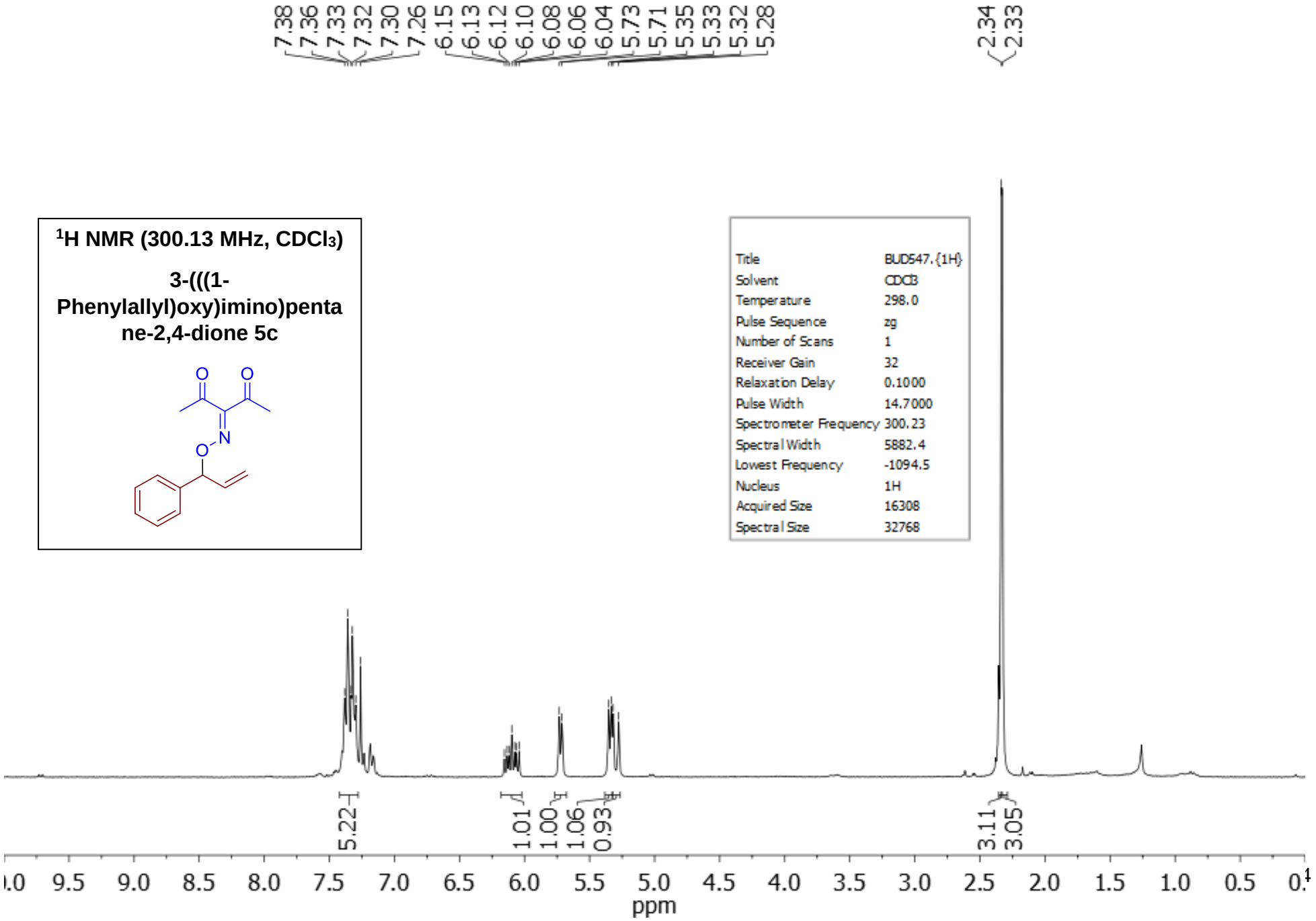
5a



1	Title	i6656.{13C}.13.fid
2	Solvent	CDCl3
3	Temperature	299.6
4	Pulse Sequence	zgpg30
5	Number of Scans	136
6	Receiver Gain	3250.0
7	Relaxation Delay	1.0000
8	Pulse Width	13.0000
9	Acquisition Time	0.9002
10	Spectrometer Frequency	75.48
11	Spectral Width	18115.9
12	Lowest Frequency	-746.0
13	Nucleus	13C
14	Acquired Size	16308
15	Spectral Size	65536


7.26
6.02
6.01
5.99
5.98
5.97
5.81
5.80
5.77
5.76
5.76
4.76
2.38
2.30
2.07
2.06
2.05
2.03
2.01
1.99
1.95
1.92
1.90
1.88
1.86
1.71
1.68
1.66
1.64
1.62
1.60
1H NMR (300.13 MHz, CDCl3)
3-((Cyclohex-2-en-1-yloxy)imino)pentane-2,4-dione
5b
O
O
O
N
Title i6687.{1H}.1.fid
Solvent CDCl3
Temperature 299.3
Pulse Sequence zg
Number of Scans 1
Receiver Gain 144.0
Relaxation Delay 0.0050
Pulse Width 9.0000
Acquisition Time 1.3518
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -610.0
Nucleus 1H
Acquired Size 8124
Spectral Size 65536
0.93
0.92
0.93
3.00
2.83
2.12
2.35
2.22
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
ppm

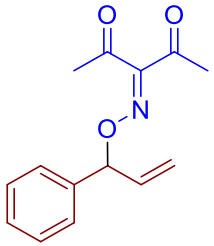

198.82
194.60
155.92
133.94
124.90
79.72
77.58
77.16
76.74
30.68
28.14
25.66
25.12
18.56
^{13}C NMR (75.47 MHz, CDCl$_3$)
3-((Cyclohex-2-en-1-yloxy)imino)pentane-2,4-dione 5b
Title i6687.{13C}.13.fid
Solvent CDCl3
Temperature 298.9
Pulse Sequence zgpg30
Number of Scans 168
Receiver Gain 3250.0
Relaxation Delay 1.0000
Pulse Width 13.0000
Acquisition Time 0.9002
Spectrometer Frequency 75.48
Spectral Width 18115.9
Lowest Frequency -747.0
Nucleus 13C
Acquired Size 16308
Spectral Size 65536
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


7.38
7.36
7.33
7.32
7.30
7.26
6.15
6.13
6.12
6.10
6.08
6.06
6.04
5.73
5.71
5.35
5.33
5.32
5.28
2.34
2.33
^{1}H NMR (300.13 MHz, CDCl$_3$)
3-(((1-Phenylallyl)oxy)imino)pentane-2,4-dione 5c
Title BUD547.{1H}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32
Relaxation Delay 0.1000
Pulse Width 14.7000
Spectrometer Frequency 300.23
Spectral Width 5882.4
Lowest Frequency -1094.5
Nucleus 1H
Acquired Size 16308
Spectral Size 32768
5.22
1.01
1.00
1.06
0.93
3.11
3.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

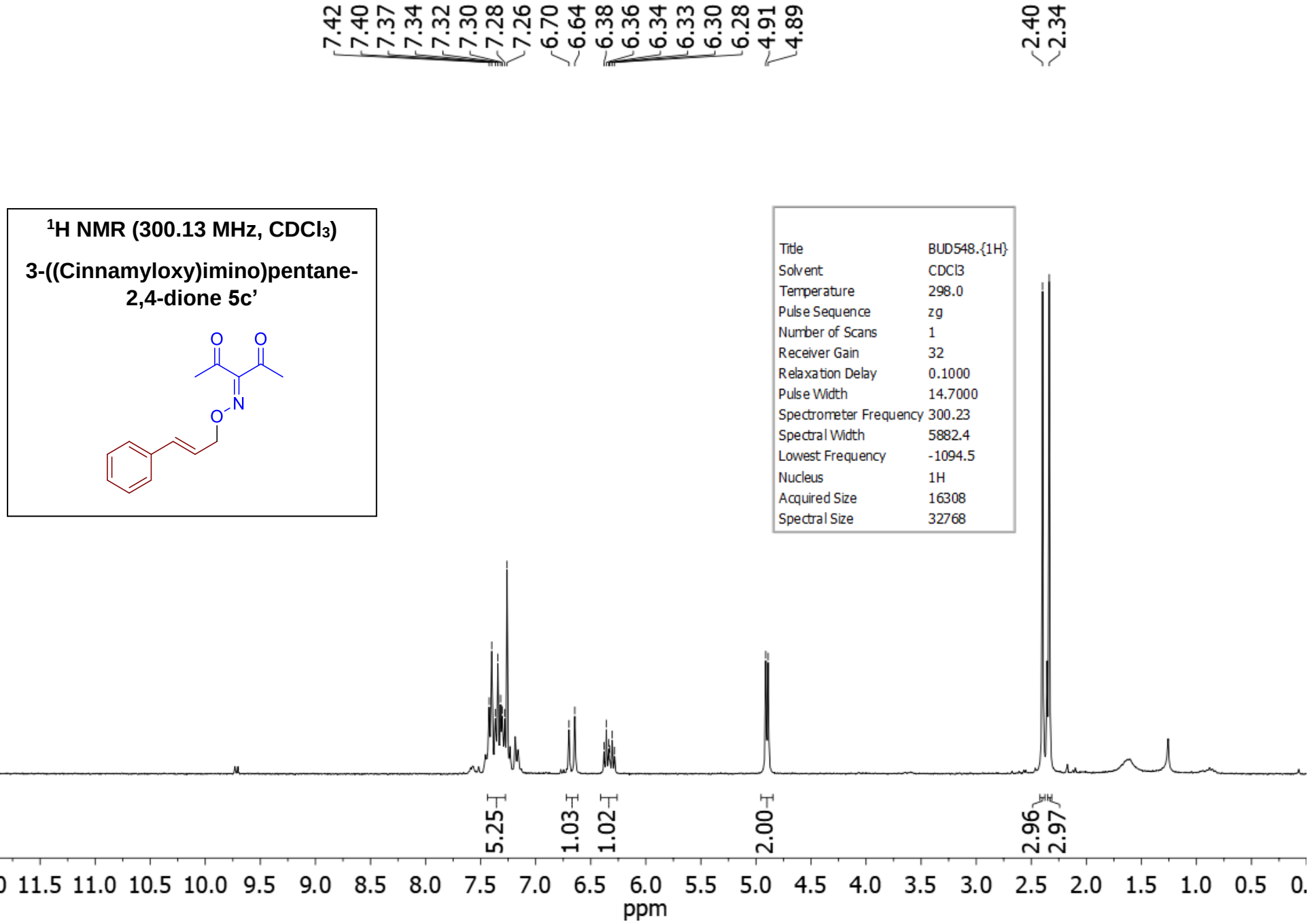
198.49
194.54
156.28
138.55
136.05
128.76
128.60
127.36
118.67
88.94
77.58
77.16
76.74
30.68
25.77

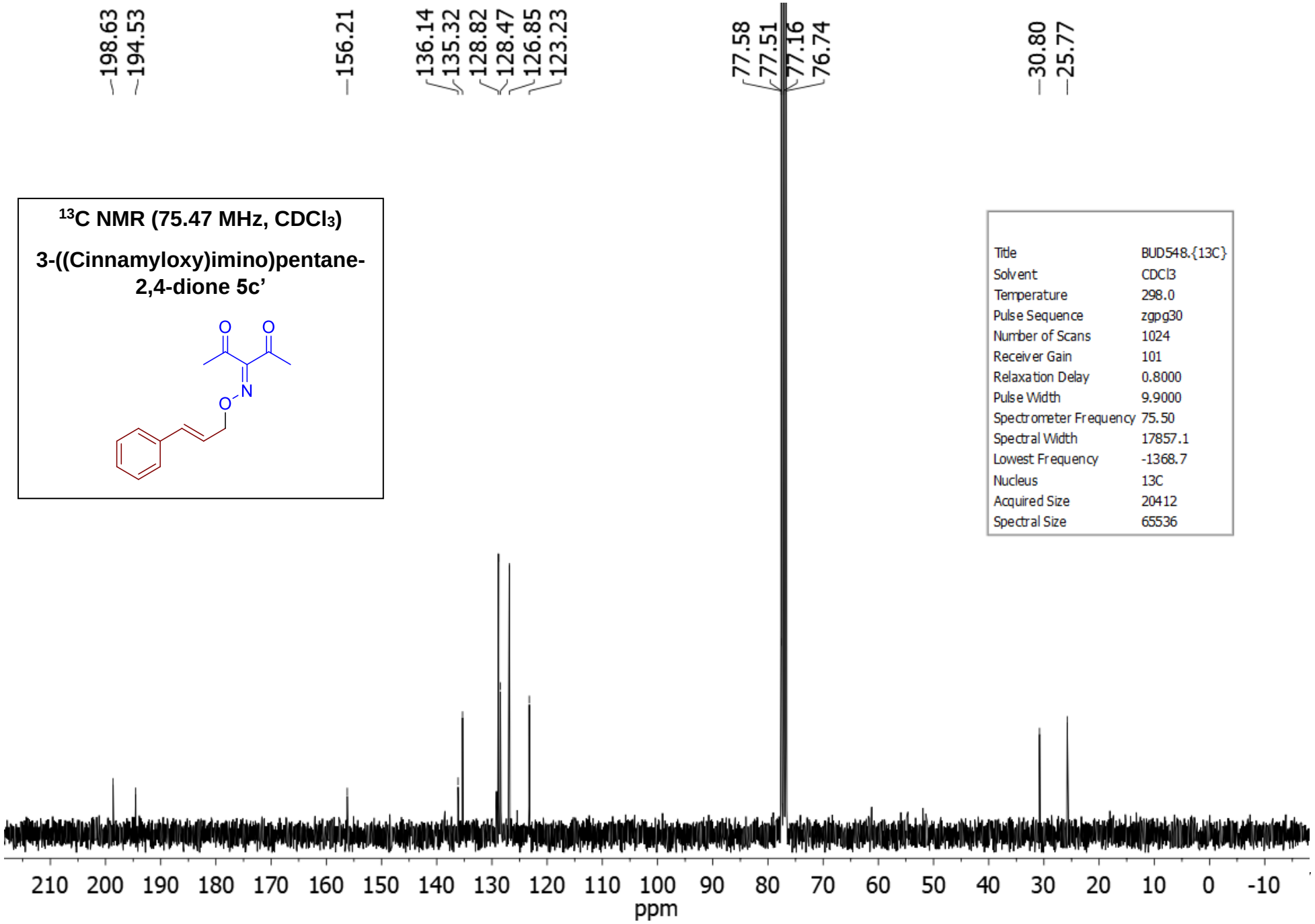
^{13}C NMR (75.47 MHz, $CDCl_3$)

3-(((1-Phenylallyl)oxy)imino)pentane-2,4-dione 5c



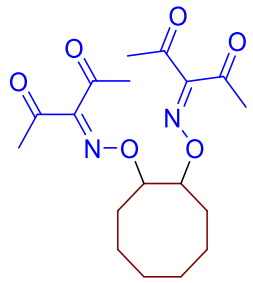
Title	BUD547.{13C}
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Number of Scans	580
Receiver Gain	101
Relaxation Delay	0.8000
Pulse Width	9.9000
Spectrometer Frequency	75.50
Spectral Width	17857.1
Lowest Frequency	-1369.2
Nucleus	13C
Acquired Size	20412
Spectral Size	65536


7.42
7.40
7.37
7.34
7.32
7.30
7.28
7.26
6.70
6.64
6.38
6.36
6.34
6.33
6.30
6.28
4.91
4.89
2.40
2.34
1H NMR (300.13 MHz, CDCl3)
3-((Cinnamyloxy)imino)pentane-2,4-dione 5c'
O
O
N
O
Title BUD548.{1H}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32
Relaxation Delay 0.1000
Pulse Width 14.7000
Spectrometer Frequency 300.23
Spectral Width 5882.4
Lowest Frequency -1094.5
Nucleus 1H
Acquired Size 16308
Spectral Size 32768
5.25
1.03
1.02
2.00
2.96
2.97
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
ppm


198.63
194.53
156.21
136.14
135.32
128.82
128.47
126.85
123.23
77.58
77.51
77.16
76.74
30.80
25.77
^{13}C NMR (75.47 MHz, CDCl$_3$)
3-((Cinnamyloxy)imino)pentane-2,4-dione 5c'
O
O
N
O
Title BUD548.{13C}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 1024
Receiver Gain 101
Relaxation Delay 0.8000
Pulse Width 9.9000
Spectrometer Frequency 75.50
Spectral Width 17857.1
Lowest Frequency -1368.7
Nucleus 13C
Acquired Size 20412
Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
ppm

^{1}H NMR (300.13 MHz, $CDCl_3$)

3,3'-((Cyclooctane-1,2-diylbis(oxy))bis(azanylylidene))bis(pentane-2,4-dione)
5d



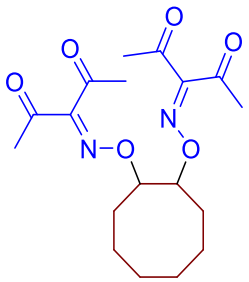
1	Title	i8884.{1H}.1.fid
2	Solvent	CDCl3
3	Temperature	300.0
4	Pulse Sequence	zg
5	Number of Scans	1
6	Receiver Gain	32.1
7	Relaxation Delay	0.1000
8	Pulse Width	14.1000
9	Acquisition Time	2.7150
10	Spectrometer Frequency	300.13
11	Spectral Width	6009.6
12	Lowest Frequency	-911.1
13	Nucleus	1H
14	Acquired Size	16316
15	Spectral Size	65536

198.41
198.31
194.26
156.04
156.01
88.29
86.47
77.58
77.16
76.74
30.49
30.42
28.84
28.25
26.16
25.61
25.58
25.53
24.48
22.64

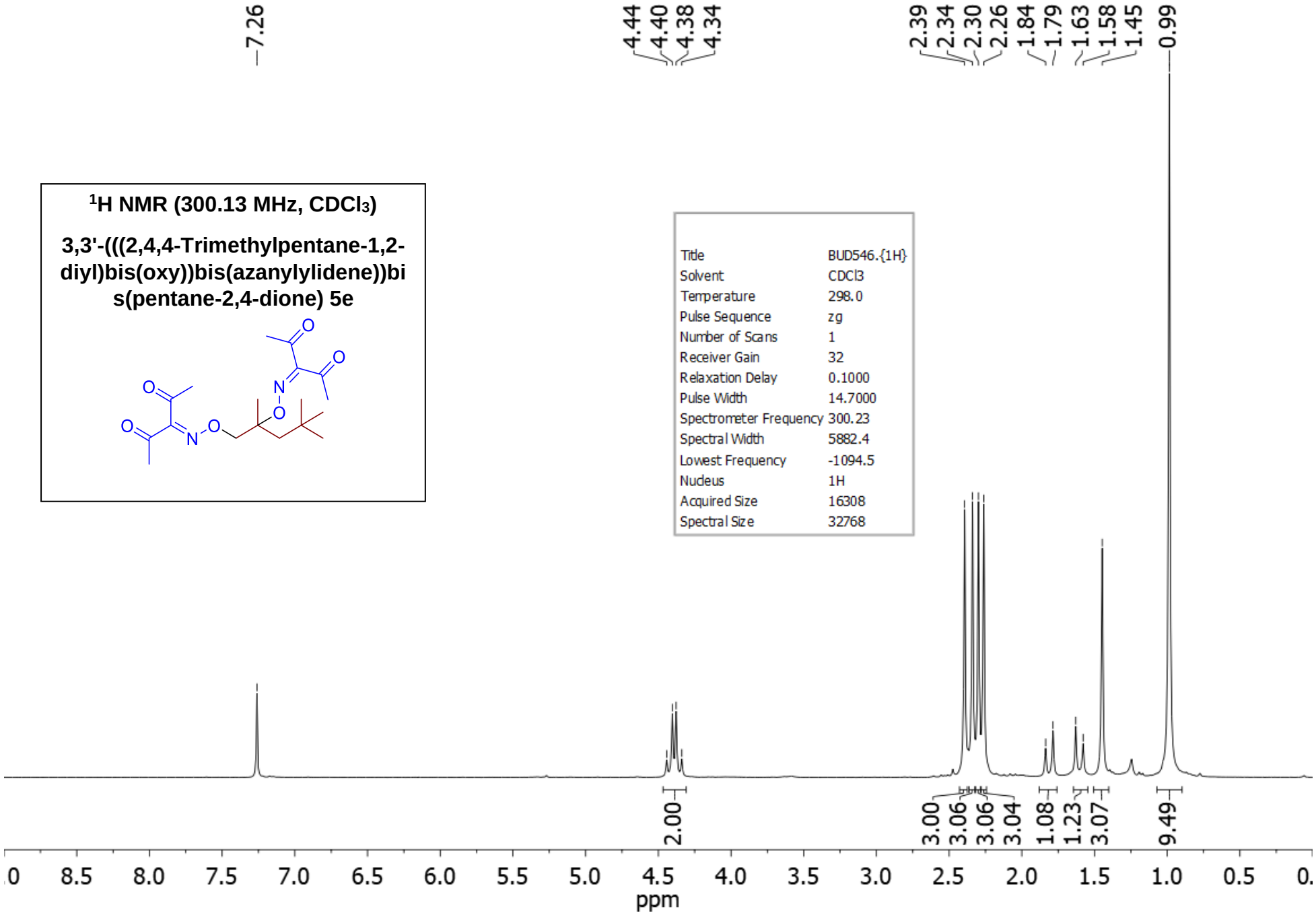
^{13}C NMR (75.47 MHz, $CDCl_3$)

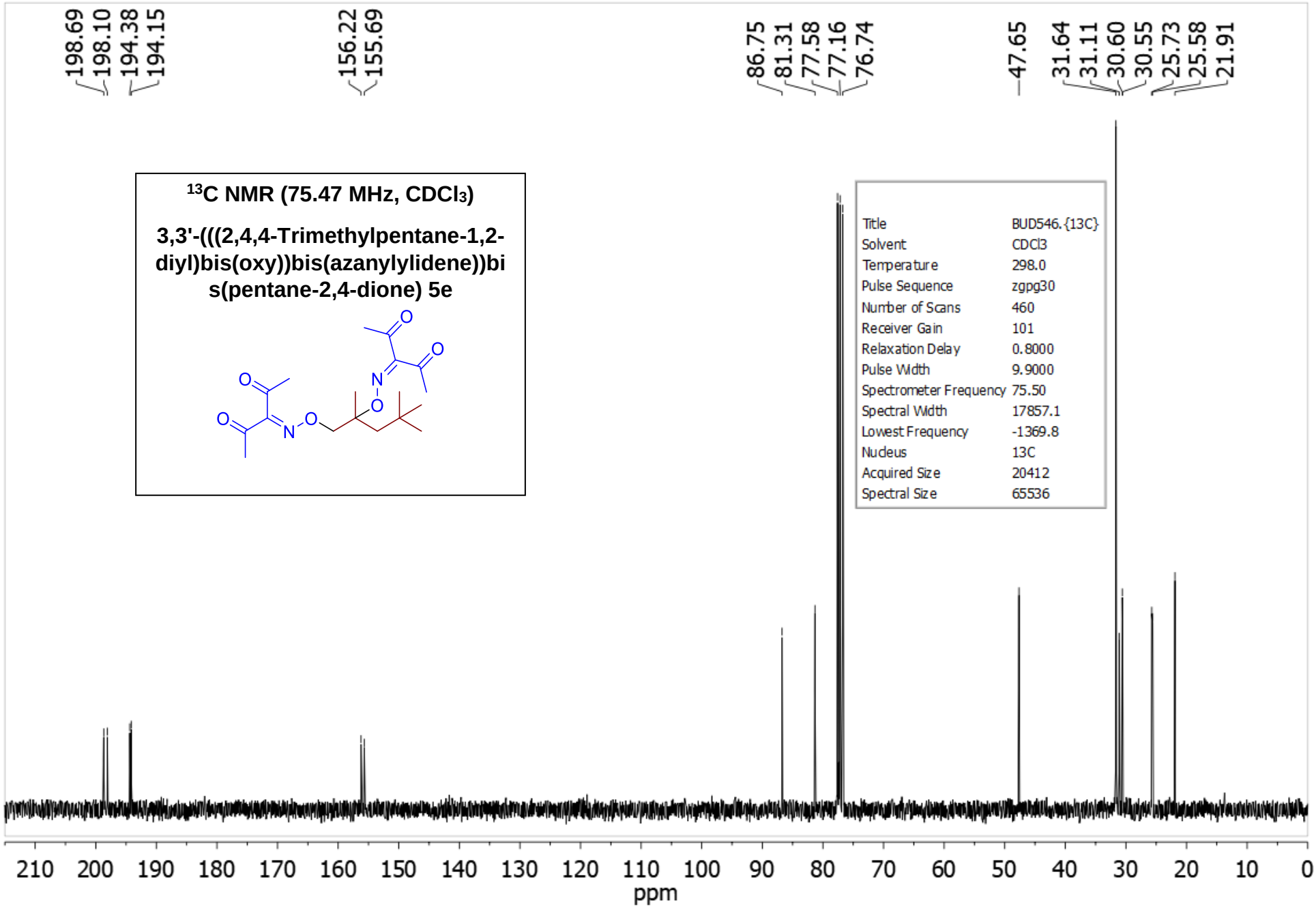
3,3'-((Cyclooctane-1,2-diylbis(oxy))bis(azanylylidene))bis(pentane-2,4-dione)

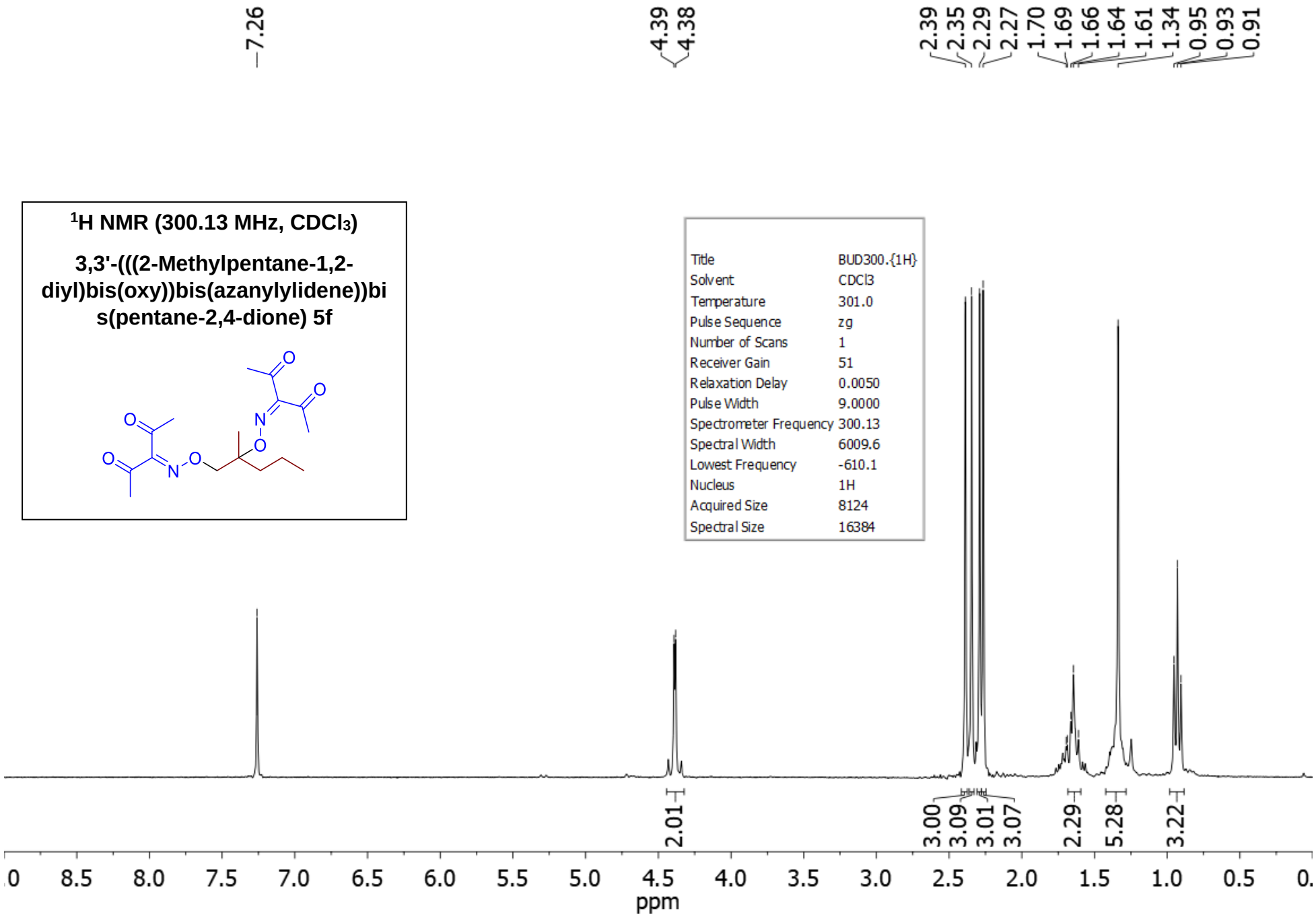
5d



1	Title	i8884.{13C}.1.fid
2	Solvent	CDCl3
3	Temperature	298.0
4	Pulse Sequence	zgpg30
5	Number of Scans	128
6	Receiver Gain	101.0
7	Relaxation Delay	0.8000
8	Pulse Width	9.9000
9	Acquisition Time	1.1431
10	Spectrometer Frequency	75.50
11	Spectral Width	17857.1
12	Lowest Frequency	-1374.6
13	Nucleus	13C
14	Acquired Size	20412
15	Spectral Size	65536


7.26
4.44
4.40
4.38
4.34
2.39
2.34
2.30
2.26
1.84
1.79
1.63
1.58
1.45
0.99
1H NMR (300.13 MHz, CDCl3)
3,3'-(((2,4,4-Trimethylpentane-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione) 5e
Title BUD546.{1H}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32
Relaxation Delay 0.1000
Pulse Width 14.7000
Spectrometer Frequency 300.23
Spectral Width 5882.4
Lowest Frequency -1094.5
Nucleus 1H
Acquired Size 16308
Spectral Size 32768
2.00
3.00
3.06
3.06
3.04
1.08
1.23
3.07
9.49
ppm

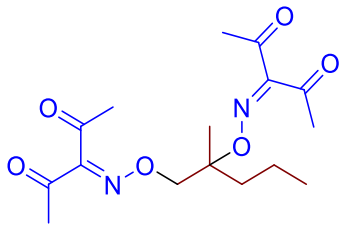

198.69
198.10
194.38
194.15
156.22
155.69
86.75
81.31
77.58
77.16
76.74
47.65
31.64
31.11
30.60
30.55
25.73
25.58
21.91
13C NMR (75.47 MHz, CDCl3)
3,3'-(((2,4,4-Trimethylpentane-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione) 5e
Title BUD546.{13C}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 460
Receiver Gain 101
Relaxation Delay 0.8000
Pulse Width 9.9000
Spectrometer Frequency 75.50
Spectral Width 17857.1
Lowest Frequency -1369.8
Nucleus 13C
Acquired Size 20412
Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


7.26
4.39
4.38
2.39
2.35
2.29
2.27
1.70
1.69
1.66
1.64
1.61
1.34
0.95
0.93
0.91
^{1}H NMR (300.13 MHz, CDCl$_3$)
3,3'-(((2-Methylpentane-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione) 5f
Title BUD300.{1H}
Solvent CDCl3
Temperature 301.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 51
Relaxation Delay 0.0050
Pulse Width 9.0000
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -610.1
Nucleus 1H
Acquired Size 8124
Spectral Size 16384
2.01
3.00
3.09
3.01
3.07
2.29
5.28
3.22
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

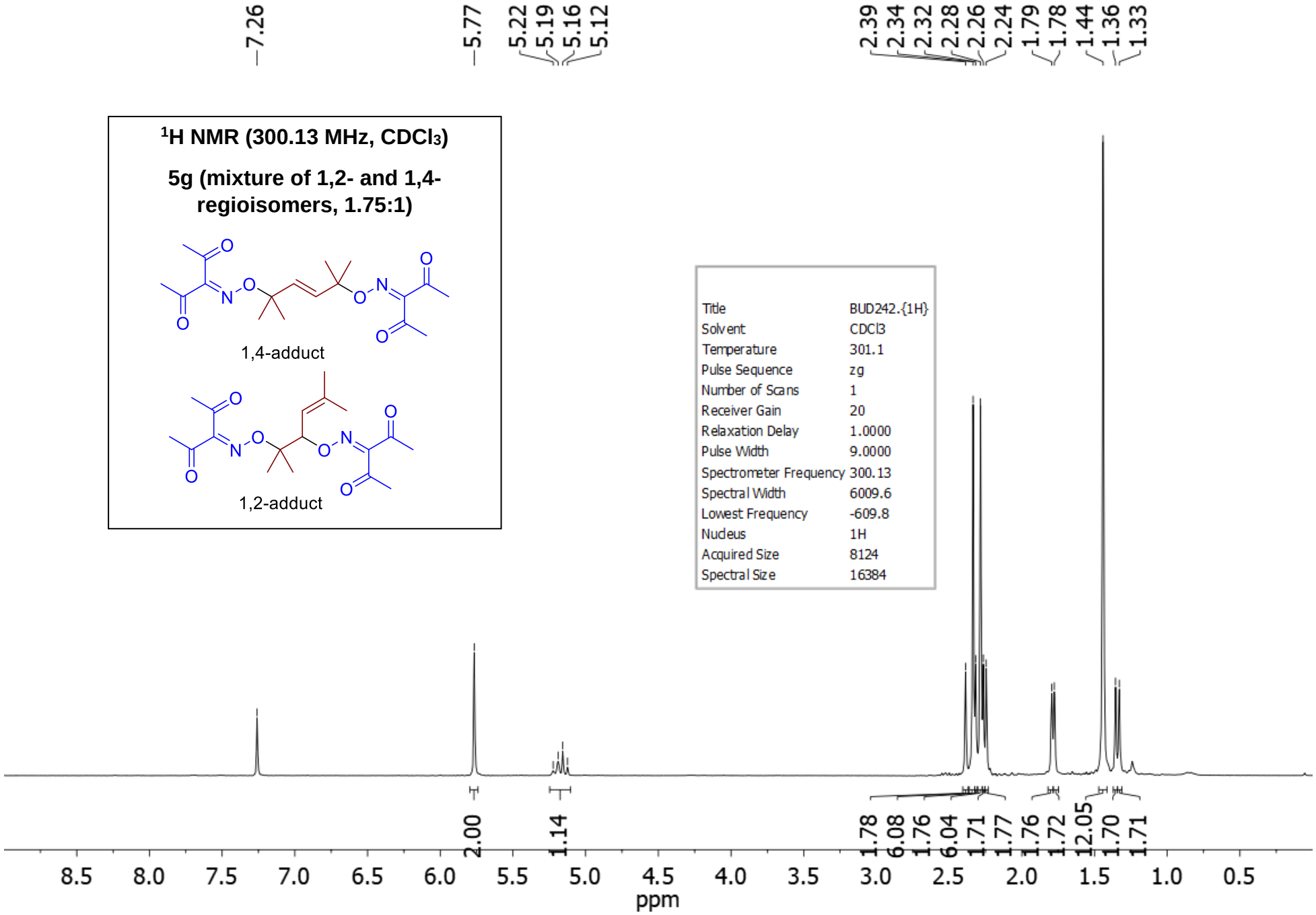
198.54
198.07
194.34
194.18
156.22
156.01
85.60
79.99
77.58
77.16
76.74
38.01
30.59
30.57
25.74
25.60
20.39
16.64
14.64

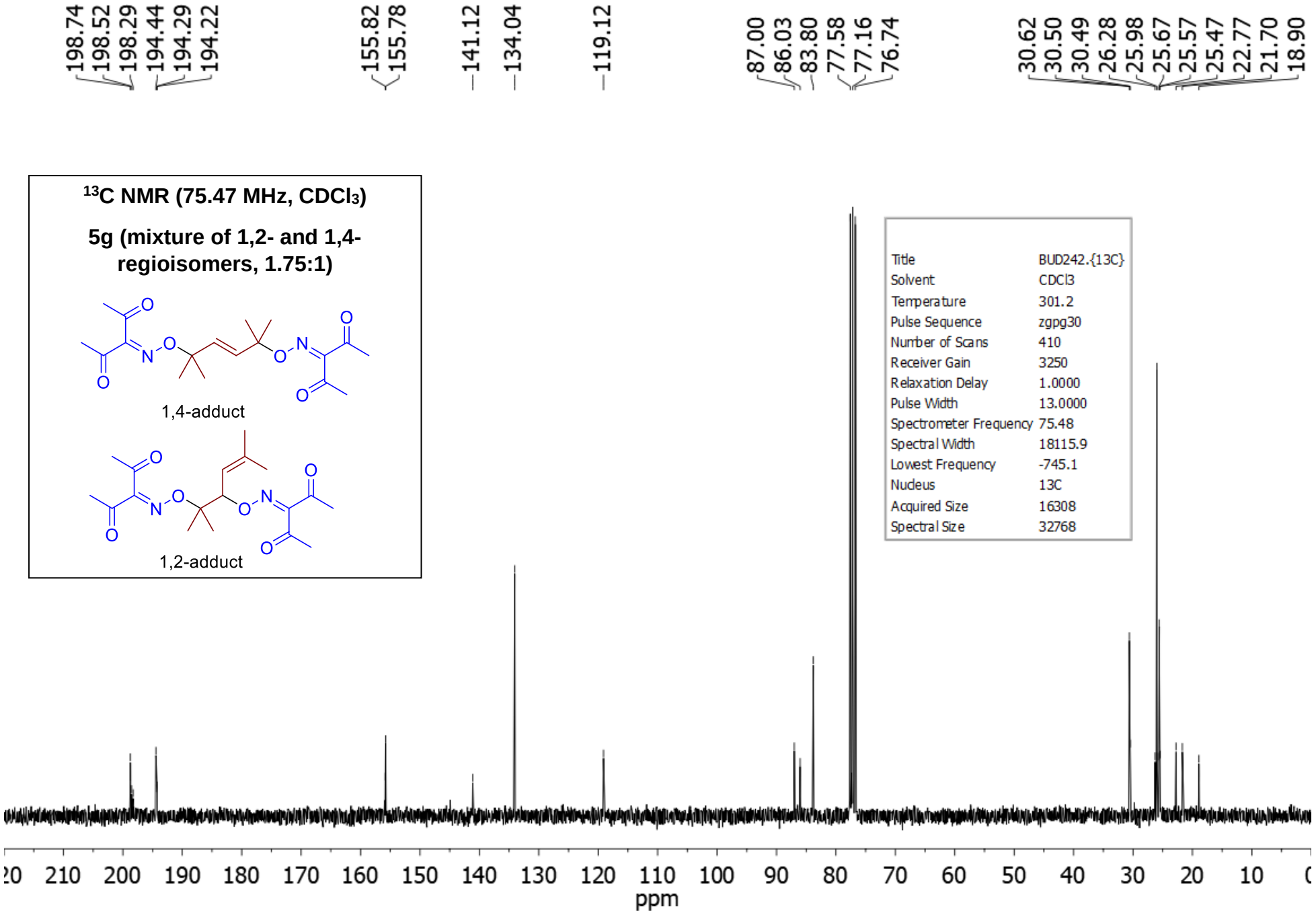
^{13}C NMR (75.47 MHz, $CDCl_3$)

3,3'-(((2-Methylpentane-1,2-diyl)bis(oxy))bis(azanylylidene))bis(pentane-2,4-dione) 5f



Title	BUD300.{13C}
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgpg30
Number of Scans	200
Receiver Gain	101
Relaxation Delay	0.8000
Pulse Width	9.9000
Spectrometer Frequency	75.50
Spectral Width	17857.1
Lowest Frequency	-1369.5
Nucleus	13C
Acquired Size	20412
Spectral Size	65536


7.26
5.77
5.22
5.19
5.16
5.12
2.39
2.34
2.32
2.28
2.26
2.24
1.79
1.78
1.44
1.36
1.33
¹H NMR (300.13 MHz, CDCl₃)
5g (mixture of 1,2- and 1,4-regioisomers, 1.75:1)
1,4-adduct
1,2-adduct
Title BUD242.{1H}
Solvent CDCl3
Temperature 301.1
Pulse Sequence zg
Number of Scans 1
Receiver Gain 20
Relaxation Delay 1.0000
Pulse Width 9.0000
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -609.8
Nucleus 1H
Acquired Size 8124
Spectral Size 16384
2.00
1.14
1.78
6.08
1.76
6.04
1.71
1.77
1.76
1.72
12.05
1.70
1.71
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm


198.74
198.52
198.29
194.44
194.29
194.22
155.82
155.78
141.12
134.04
119.12
87.00
86.03
83.80
77.58
77.16
76.74
30.62
30.50
30.49
26.28
25.98
25.67
25.57
25.47
22.77
21.70
18.90
13C NMR (75.47 MHz, CDCl3)
5g (mixture of 1,2- and 1,4-regioisomers, 1.75:1)
1,4-adduct
1,2-adduct
Title BUD242.{13C}
Solvent CDCl3
Temperature 301.2
Pulse Sequence zgpg30
Number of Scans 410
Receiver Gain 3250
Relaxation Delay 1.0000
Pulse Width 13.0000
Spectrometer Frequency 75.48
Spectral Width 18115.9
Lowest Frequency -745.1
Nucleus 13C
Acquired Size 16308
Spectral Size 32768
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm