Supporting Information

C–O Coupling of Hydrazones with Diacetyliminoxyl Radical Leading to Azo Oxime Ethers—Novel Antifungal Agents

Alexander S. Budnikov,[1,2] Igor B. Krylov,[1,2,3*] Mikhail I. Shevchenko,[1,3] O.O. Segida,[1,2] Andrey V. Lastovko,[1] Anna L. Alekseenko,[1,3] Alexey I. Ilovaisky,[1,2] Gennady I. Nikishin,[1] Alexander O. Terent'ev[1,2,3*]

E-mail: krylovigor@yandex.ru; terentev@ioc.ac.ru

[1] N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, 47 Leninsky Prospekt, 119991 Moscow, Russia

[2] All-Russian Research Institute for Phytopathology, B. Vyazyomy, 143050 Moscow, Russian

[3] Higher Chemical College of the Russian Academy of Sciences, D. I. Mendeleev University of Chemical Technology of Russia, 9 Miusskaya Square, 125047 Moscow, Russian

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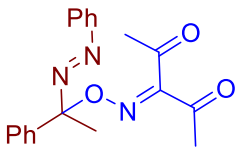
General

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.

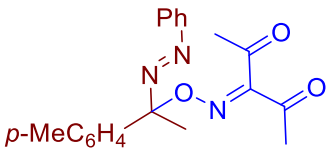
Phenylhydrazine 97%, *p*-tolylhydrazine hydrochloride 98%, 4-chlorophenylhydrazine hydrochloride 97%, 4-(trifluoromethyl)phenylhydrazine 96%, 2-hydrazinopyridine 98%, 2,4-dinitrophenylhydrazine 97%, methylhydrazine 98%, acetophenone 98%, 4-methylacetophenone 95%, 4-nitroacetophenone 98%, 4-methoxyacetophenone 98%, 4-bromoacetophenone 98%, 2-hydroxyacetophenone 98%, propiophenone 99%, benzophenone 99%, benzaldehyde 98%, 4-chlorobenzaldehyde 98%, 4-methoxybenzaldehyde 99%, 4-heptanone 98%, 6-undecanone 97%, 5-hexen-2-one 98%, cyclobutanone 98%, cyclopentanone 99%, cyclohexanone 99%, acetaldehyde 99.5%, propionaldehyde 98%, isobutyraldehyde 99+%, pivaldehyde 96%, hexanal 96%. Hydrazones **2** were synthesized by condensation with corresponding carbonyl compounds.[1–7] Ketones and corresponding hydrazones **2l–n** were synthesized according published procedures.[8–11] CH_2Cl_2 was distilled prior to use. Acetone was distilled over $KMnO_4$. Preparation of diacetyliminoxyl radical is described earlier.[12] 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.

Characterization data of synthesized products

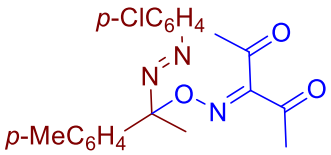


(*E*)-3-((1-phenyl-1-(phenyldiazenyl)ethoxy)imino)pentane-2,4-dione, **3aa** was synthesized as yellow oil (84%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300.13

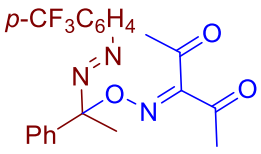
MHz, $CDCl_3$): δ = 7.81 – 7.69 (m, 2H), 7.56 – 7.43 (m, 5H), 7.43 – 7.28 (m, 3H), 2.48 (s, 3H), 2.27 (s, 3H), 2.05 (s, 3H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.8, 194.7, 156.6, 151.6, 139.4, 131.6, 129.2, 128.7, 128.6, 126.5, 122.9, 105.2, 30.5, 25.9, 23.8. **FT-IR** (thin layer): ν_{max} = 1725, 1690, 1363, 960, 695. **HR-MS** (ESI): *m/z* = 360.1313, calcd. for $C_{19}H_{19}N_3O_3$+Na^+: 360.1319.



(*E*)-3-((1-(phenyldiazenyl)-1-(p-tolyl)ethoxy)imino)pentane-2,4-dione, **3ab** was synthesized as yellow oil (96%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.81 – 7.71 (m, 2H), 7.54 – 7.44 (m, 3H), 7.41 (d, *J* = 8.2 Hz, 2H), 7.19 (d, *J* = 8.2 Hz, 2H), 2.49 (s, 3H), 2.35 (s, 3H), 2.29 (s, 3H), 2.06 (s, 3H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.7, 194.7, 156.5, 151.6, 138.6, 136.4, 131.4, 129.24, 129.18, 126.5, 122.8, 105.2, 30.5, 25.8, 23.5, 21.2. **FT-IR** (thin layer): ν_{max} = 1725, 1687, 1363, 1305, 968. **HR-MS** (ESI): *m/z* = 352.1654, calcd. for $C_{20}H_{21}N_3O_3$+H^+: 352.1656.

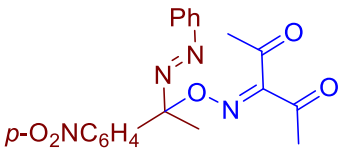


(*E*)-3-((1-((4-chlorophenyl)diazenyl)-1-(p-tolyl)ethoxy)imino)pentane-2,4-dione, **3ac** was synthesized as yellow oil (81%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.70 (d, *J* = 8.7 Hz, 2H), 7.44 (d, *J* = 8.7 Hz, 2H), 7.39 (d, *J* = 8.3 Hz, 2H), 7.19 (d, *J* = 8.3 Hz, 2H), 2.47 (s, 3H), 2.35 (s, 3H), 2.29 (s, 3H), 2.04 (s, 3H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.6, 194.6, 156.7, 149.9, 138.7, 137.5, 136.2, 129.4, 129.3, 126.4, 124.1, 105.3, 30.5, 25.8, 23.4, 21.2. **FT-IR** (thin layer): ν_{max} = 1726, 1690, 1362, 1300, 1088, 959. **HR-MS** (ESI): *m/z* = 386.1252, 388.1230, calcd. for $C_{20}H_{20}ClN_3O_3$+H^+: 386.1266, 388.1238.

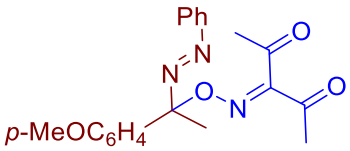


(*E*)-3-((1-phenyl-1-((4-(trifluoromethyl)phenyl)diazenyl)ethoxy)imino)pentane-2,4-dione, **3ad** was synthesized as yellow oil (95%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.85 (d, *J* = 8.4 Hz, 2H), 7.75 (d, *J* = 8.4 Hz, 2H), 7.58 – 7.49 (m, 2H), 7.47 – 7.32 (m, 3H), 2.49 (s, 3H), 2.29 (s, 3H), 2.10 (s, 3H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.5, 194.5, 156.7, 153.3, 138.8, 132.89 (q, *J* = 32.7 Hz), 128.9, 128.7, 126.42 (q, *J* = 3.6

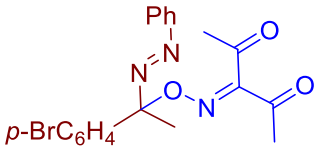
Hz), 123.84 (q, *J* = 272.5 Hz), 123.0, 105.5, 30.5, 25.7, 23.6. **FT-IR** (thin layer): ν_{max} = 1726, 1692, 1364, 1324, 1169, 1131, 1066, 959. **HR-MS** (ESI): *m/z* = 428.1198, calcd. for $C_{20}H_{18}F_3N_3O_3$+Na^+: 428.1192.



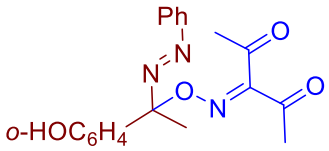
(*E*)-3-((1-(4-nitrophenyl)-1-(phenyldiazenyl)ethoxy)imino)pentane-2,4-dione, **3ae** was synthesized as yellow oil (98%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 8.25 (d, *J* = 8.9 Hz, 2H), 7.81 – 7.67 (m, 4H), 7.56 – 7.45 (m, 3H), 2.48 (s, 3H), 2.24 (s, 3H), 2.03 (s, 3H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.2, 194.3, 157.1, 151.3, 148.0, 146.6, 132.2, 129.4, 127.8, 123.8, 123.0, 104.1, 30.4, 25.9, 24.4. **FT-IR** (thin layer): ν_{max} = 1727, 1693, 1605, 1522, 1350, 1300, 1142, 1109, 1079, 1067, 958, 855, 769, 758, 693. **HR-MS** (ESI): *m/z* = 405.1161, calcd. for $C_{19}H_{18}N_4O_5$+Na^+: 405.1169.



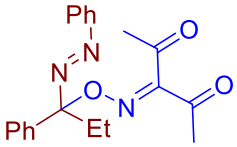
(*E*)-3-((1-(4-methoxyphenyl)-1-(phenyldiazenyl)ethoxy)imino)pentane-2,4-dione, **3af** was synthesized as yellow oil (75%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.80–7.67 (m, 2H), 7.55–7.38 (m, 5H), 6.95–6.82 (m, 2H), 3.80 (s, 3H), 2.47 (s, 3H), 2.28 (s, 3H), 2.04 (s, 3H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.8, 194.7, 159.9, 156.5, 151.6, 131.4, 129.2, 128.0, 122.8, 113.9, 105.1, 55.4, 30.5, 25.8, 23.3. **FT-IR** (thin layer): ν_{max} = 1725, 1690, 1608, 1514, 1363, 1303, 1253, 1185, 1109, 1030, 960, 834, 769. **HR-MS** (ESI): *m/z* = 390.1423, calcd. for $C_{20}H_{21}N_3O_4$+Na^+: 390.1424.



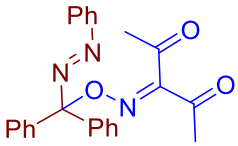
(*E*)-3-((1-(4-bromophenyl)-1-(phenyldiazenyl)ethoxy)imino)pentane-2,4-dione, **3ag** was synthesized as yellow crystals (82%, purified by column chromatography with DCM as eluent). Mp = 90–91 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.81 – 7.70 (m, 2H), 7.55 – 7.45 (m, 5H), 7.44–7.35 (m, 2H), 2.47 (s, 3H), 2.27 (s, 3H), 2.01 (s, 3H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.6, 194.6, 156.8, 151.4, 138.6, 131.8, 129.3, 128.4, 123.1, 122.9, 104.6, 102.8, 30.5, 25.9, 23.8. **FT-IR** (thin layer): ν_{max} = 1773, 1484, 1397, 1362, 1302, 1135, 1078, 1010, 966, 920, 828, 685, 550. **HR-MS** (ESI): *m/z* = 416.0608, 418.0592, calcd. for $C_{19}H_{18}BrN_3O_3$+H^+: 416.0604, 418.0585. Single crystal X-Ray analysis is available (see Fig. 1, page S15).



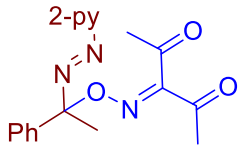
(*E*)-3-((1-(2-hydroxyphenyl)-1-(phenyldiazenyl)ethoxy)imino)pentane-2,4-dione, **3ah** was synthesized as pale yellow solid (74%, purified by column chromatography with DCM as eluent) Mp = 103–104 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 8.16 (s, 1H), 7.74–7.71 (m, 2H), 7.54–7.49 (m, 3H), 7.36–7.27 (m, 2H), 6.97–6.90 (m, 2H), 2.46 (s, 3H), 2.25 (s, 3H), 2.09 (s, 3H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.2, 194.4, 157.0, 155.4, 150.9, 132.5, 131.3, 129.6, 127.3, 124.0, 123.0, 120.3, 118.5, 106.9, 30.6, 25.9, 22.8. **FT-IR** (thin layer): ν_{max} = 1727, 1692, 1483, 1458, 1364, 1299, 1246, 1201, 1105, 957, 939, 76. **HR-MS** (ESI): *m/z* = 376.1260, cald. For $C_{19}H_{19}N_3O_4$+Na^+ = 376.1268.



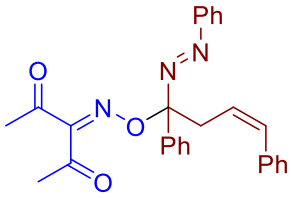
(*E*)-3-((1-phenyl-1-(phenyldiazenyl)propoxy)imino)pentane-2,4-dione, **3ai** was synthesized as yellow oil (87%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.85–7.69 (m, 2H), 7.57–7.53 (m, 2H), 7.51–7.47 (m, 3H), 7.44–7.30 (m, 3H), 2.52 (s, 3H), 2.60 – 2.35 (m, 2H), 2.23 (s, 3H), 0.88 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.8, 194.7, 156.7, 151.6, 138.2, 131.4, 129.2, 128.5, 128.3, 126.9, 122.8, 106.9, 31.1, 30.3, 25.8, 7.7. **FT-IR** (thin layer): ν_{max} =2979, 1726, 1691, 1450, 1363, 1296, 1138, 1070, 963, 763, 699, 691. **HR-MS** (ESI): *m/z* = 374.1472, calcd. for $C_{20}H_{21}N_3O_3$+Na^+: 374.1475.



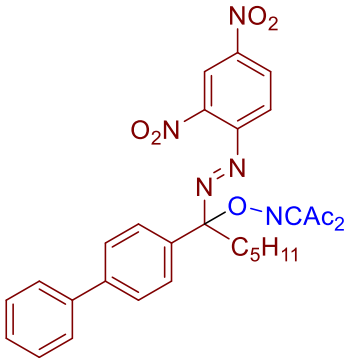
(*E*)-3-((diphenyl(phenyldiazenyl)methoxy)imino)pentane-2,4-dione, **3aj** was synthesized as slightly yellow solid (98%, purified by column chromatography with DCM as eluent). Mp = 103-104 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.86–7.75 (m, 2H), 7.58–7.45 (m, 7H), 7.43–7.30 (m, 6H), 2.56 (s, 3H), 2.05 (s, 3H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.7, 194.7, 156.3, 151.5, 139.9, 131.6, 129.3, 128.6, 128.4, 128.0, 123.0, 105.6, 30.1, 25.7. **FT-IR** (thin layer): ν_{max} = 1725, 1686, 1300, 1013, 976, 941, 762, 695. **HR-MS** (ESI): *m/z* = 422.1461, calcd. for $C_{24}H_{21}N_3O_3$+Na^+: 422.1475.



(*E*)-3-((1-phenyl-1-(pyridin-2-yldiazenyl)ethoxy)imino)pentane-2,4-dione, **3ak** was synthesized as yellow oil (89%, purified by column chromatography with PE/EtOAc = 2/5 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 8.70 (d, *J* = 4.2 Hz, 1H), 7.85 (td, *J* = 7.7, 1.8 Hz, 1H), 7.60 – 7.48 (m, 3H), 7.46 – 7.29 (m, 4H), 2.48 (s, 3H), 2.28 (s, 3H), 2.12 (s, 3H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.6, 194.6, 162.2, 156.8, 149.6, 138.6, 138.5, 129.0, 128.7, 126.5, 125.8, 114.3, 106.0, 30.6, 25.9, 23.5. **FT-IR** (thin layer): ν_{max} = 1725, 1690, 1583, 1455, 1425, 1363, 1299, 1261, 1194, 1145, 1119,1069, 955, 791, 770, 699. **HR-MS** (ESI): *m/z* = 339.1448, calcd. for $C_{18}H_{18}N_4O_3$+H^+: 339.1452.

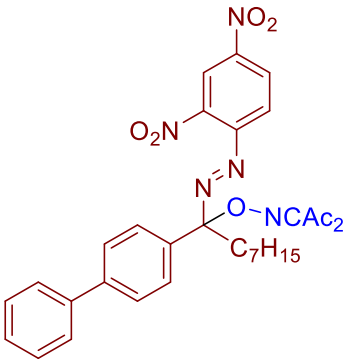


3-((((*Z*)-1,4-diphenyl-1-((*E*)-phenyldiazenyl)but-3-en-1-yl)oxy)imino)pentane-2,4-dione, **3al** was synthesized as slightly yellow viscous gum (87%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.79–7.70 (m, 2H), 7.58–7.45 (m, 5H), 7.45–7.17 (m, 8H), 6.54 (d, *J* = 11.8 Hz, 1H), 5.58 (dt, *J* = 11.8, 7.2 Hz, 1H), 3.57 (dd, *J* = 7.2, 1.8 Hz, 2H), 2.50 (s, 3H), 1.98 (s, 3H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.6, 194.7, 156.6, 151.5, 137.3, 137.2, 132.5, 131.6, 129.2, 128.74, 128.67, 128.61, 128.4, 127.0, 126.9, 124.9, 122.9, 106.3, 36.2, 30.3, 25.6. **FT-IR** (thin layer): ν_{max} = 1725, 1690, 1600, 1494, 1449, 1363, 1301, 1193, 1059, 1018, 1003, 950, 765, 699. **HR-MS** (ESI): *m/z* = 462.1781, calcd. for $C_{27}H_{25}N_3O_3$+Na^+: 462.1788.

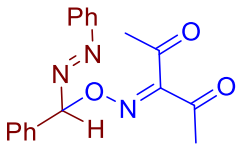


(*E*)-3-(((1-([1,1'-biphenyl]-4-yl)-1-((2,4-dinitrophenyl)diazenyl)hexyl)oxy)imino)pentane-2,4-dione, **3am** was synthesized as viscous orange gum (46%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 8.83 (d, *J* = 2.3 Hz, 1H),

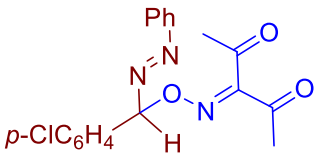
8.51 (dd, *J* = 8.7, 2.3 Hz, 1H), 7.73 – 7.56 (m, 6H), 7.52–7.41 (m, 3H), 7.41–7.32 (m, 1H), 2.60–2.47 (m, 2H), 2.44 (s, 3H), 2.33 (s, 3H), 1.42–1.20 (m, 6H), 0.94 – 0.77 (m, 3H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.5, 194.4, 157.1, 148.6, 148.1, 146.1, 141.7, 140.2, 135.6, 129.0, 128.4, 127.9, 127.5, 127.18, 127.15, 120.5, 120.3, 108.1, 37.3, 31.8, 30.2, 25.8, 22.6, 22.4, 14.0. **FT-IR** (thin layer): ν_{max} = 3103, 2957, 2931, 2869, 1726, 1692, 1608, 1536, 1487, 1346, 1298, 1147, 954, 836, 766, 744, 698. **HR-MS** (ESI): *m/z* = 582.1955, calcd. for $C_{29}H_{29}N_5O_7$+Na^+: 582.1959.



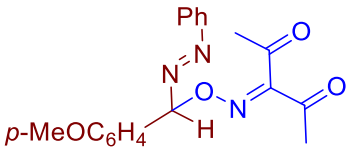
(*E*)-3-(((1-([1,1'-biphenyl]-4-yl)-1-((2,4-dinitrophenyl)diazenyl)octyl)oxy)imino)pentane-2,4-dione, **3an** was synthesized as viscous orange gum (42%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 8.82 (d, *J* = 2.3 Hz, 1H), 8.51 (dd, *J* = 8.7, 2.3 Hz, 1H), 7.78–7.55 (m, 6H), 7.54–7.40 (m, 3H), 7.39–7.29 (m, 1H), 2.66 – 2.49 (m, 2H), 2.45 (s, 3H), 2.34 (s, 3H), 1.55 – 1.09 (m, 10H), 0.86 (t, *J* = 6.5 Hz, 3H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.5, 194.4, 157.1, 148.6, 148.1, 146.1, 141.8, 140.2, 135.6, 129.0, 128.4, 127.9, 127.5, 127.2, 120.5, 120.3, 108.1, 37.4, 31.8, 30.3, 29.6, 29.1, 25.8, 23.0, 22.7, 14.2. **FT-IR** (thin layer): ν_{max} = 1724, 1691, 1607, 1545, 1541, 1346, 1297, 1194, 1146, 963, 835, 766, 747, 698. **HR-MS** (ESI): *m/z* = 605.2712, calcd. for $C_{31}H_{33}N_5O_7$+H^+: 605.2718.



(*E*)-3-((phenyl(phenyldiazenyl)methoxy)imino)pentane-2,4-dione, **3ba** was synthesized as yellow oil (79%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.79–7.76 (m, 2H), 7.55–7.51 (m, 2H), 7.50–7.47 (m, 3H), 7.44–7.39 (m, 3H), 6.50 (s, 1H), 2.46 (s, 3H), 2.35 (s, 3H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.9, 194.4, 157.2, 151.6, 134.4, 131.9, 130.7, 129.8, 129.3, 129.0, 127.9, 123.7, 107.3, 30.6, 25.9. **FT-IR** (thin layer): ν_{max} =1725, 1693, 1453, 1419, 1360, 1195, 1098, 1019, 952, 766, 695. **HR-MS** (ESI): *m/z* = 346.1162 cald. For $C_{18}H_{17}N_3O_3$+Na^+ = 346.1162.

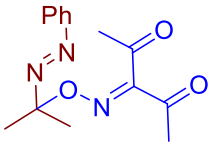


(*E*)-3-(((4-chlorophenyl)(phenyldiazenyl)methoxy)imino)pentane-2,4-dione, **3bb** was synthesized as yellow powder (58%, purified by column chromatography with DCM as eluent). Mp = 49–50 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.84–7.69 (m, 2H), 7.57–7.42 (m, 5H), 7.42–7.35 (m, 2H), 6.45 (s, 1H), 2.45 (s, 3H), 2.35 (s, 3H) **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 197.7, 194.3, 157.3, 151.4, 135.9, 132.9, 132.1, 129.3, 129.23, 129.19, 123.1, 106.5, 30.6, 26.0. **FT-IR** (thin layer): ν_{max} = 1725, 1697, 1488, 1413, 1363, 1296, 1091, 1049, 1019, 939, 821, 768, 691. **HR-MS** (ESI): *m/z* = 380.0770, cald. for $C_{18}H_{16}ClN_3O_3$+Na^+: 380.0772.

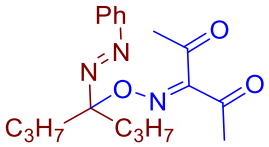


(*E*)-3-(((4-methoxyphenyl)(phenyldiazenyl)methoxy)imino)pentane-2,4-dione, **3bc** was synthesized as yellow solid (88%, purified by column chromatography with DCM as eluent). Mp = 69–70 °C **^{1}H NMR** (300 MHz, $CDCl_3$): δ = 7.81–7.69 (m, 2H), 7.51–7.38 (m, 5H), 6.98 – 6.89 (m, 2H), 6.44 (s, 1H), 3.81 (s, 3H), 2.45 (s, 3H), 2.35 (s, 3H). **^{13}C NMR** (76 MHz, CDCl3): δ = 198.0, 194.5, 160.8, 157.0, 151.5, 131.8, 129.3, 129.2, 126.6, 123.0, 114.4, 107.2, 55.4, 30.6, 25.9. **FT-IR** (thin layer): ν_{max} = 1725, 1692, 1515, 1360, 1300, 1253, 1027, 951. **HR-MS** (ESI): *m/z* = 376.1261 cald. For $C_{19}H_{19}N_3O_4$+Na^+ = 376.1268.

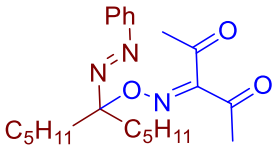
(*E*)-3-(((4-chlorophenyl)(methyldiazenyl)methoxy)imino)pentane-2,4-dione, **3bd** was synthesized as yellow oil (68%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300.13 MHz, DMSO-d_6): δ = 7.53 (d, *J* = 8.6 Hz, 2H), 7.47 (d, *J* = 8.6 Hz, 1H), 6.36 (s, 1H), 3.85 (s, 3H), 2.35 (s, 3H), 2.32 (s, 3H). **^{13}C NMR** (75.47 MHz, DMSO-d_6): δ = 198.2, 193.7, 156.9, 134.5, 133.1, 129.5, 128.9, 104.5, 57.0, 30.1, 25.6. **FT-IR** (thin layer): ν_{max} = 1727, 1693, 1493, 1363, 1298, 1090, 977, 950. **HR-MS** (ESI): *m/z* = 318.0611, cald. for $C_{13}H_{14}ClN_3O_3$+Na^+: 318.0616.



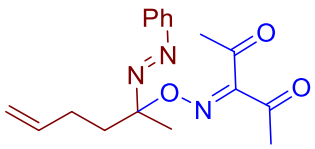
(*E*)-3-(((2-(phenyldiazenyl)propan-2-yl)oxy)imino)pentane-2,4-dione, **3ca** was synthesized as yellow oil (85%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.76–7.67 (m, 2H), 7.52 – 7.43 (m, 3H), 2.44 (s, 3H), 2.35 (s, 3H), 1.62 (s, 6H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.9, 194.8, 156.3, 151.6, 131.3, 129.2, 122.6, 104.7, 30.6, 25.8, 23.5. **FT-IR** (thin layer): ν_{max} =1726, 1690, 1384, 1303, 1196, 1173, 1145, 1070, 963, 767, 691. **HR-MS** (ESI): *m/z* = 298.1160, calcd. for $C_{14}H_{17}N_3O_3$+Na^+: 298.1162.



(*E*)-3-(((4-(phenyldiazenyl)heptan-4-yl)oxy)imino)pentane-2,4-dione, **3cb** was synthesized as yellow oil (73%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.75–7.63 (m, 2H), 7.54–7.41 (m, 3H), 2.44 (s, 3H), 2.34 (s, 3H), 2.15–1.91 (m, 4H), 1.55 – 1.19 (m, 4H), 0.90 (t, *J* = 7.3 Hz, 6H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 199.0, 194.8, 156.2, 151.6, 131.2, 129.2, 122.5, 107.5, 37.2, 30.4, 25.8, 16.3, 14.6. **FT-IR** (thin layer): ν_{max} = 2964, 2934, 2875, 1726, 1690, 1363, 1303, 960, 768, 691. **HR-MS** (ESI): *m/z* = 354.1782, calcd. for $C_{18}H_{25}N_3O_3$+Na^+: 354.1788.

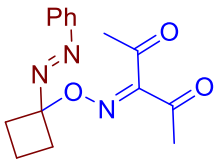


(*E*)-3-(((6-(phenyldiazenyl)undecan-6-yl)oxy)imino)pentane-2,4-dione, **3cc** was synthesized as yellow oil (70%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.73–7.64 (m, 2H), 7.53–7.42 (m, 3H), 2.44 (s, 3H), 2.34 (s, 3H), 2.13–1.93 (m, 4H), 1.49–1.18 (m, 12H), 0.86 (t, *J* = 6.8 Hz, 6H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.9, 194.8, 156.3, 151.7, 131.1, 129.2, 122.5, 107.6, 34.8, 32.2, 30.4, 25.8, 22.5, 22.4, 14.1. **FT-IR** (thin layer): ν_{max} = 2957, 2932, 2870, 1727, 1692, 1363, 1301, 960, 767. **HR-MS** (ESI): *m/z* = 410.2402, calcd. for $C_{22}H_{33}N_3O_3$+Na^+: 410.2414.

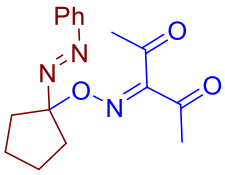


(E)-3-(((2-(phenyldiazenyl)hex-5-en-2-yl)oxy)imino)pentane-2,4-dione, **3cd** was synthesized as slightly yellow viscous gum (79%, purified by column chromatography with PE/EA

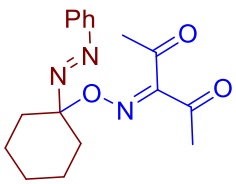
= 10/1 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.76–7.66 (m, 2H), 7.54–7.44 (m, 3H), 5.93–5.62 (m, 1H), 5.21–4.77 (m, 2H), 2.45 (s, 3H), 2.35 (s, 3H), 2.27 – 1.98 (m, 4H), 1.63 (s, 3H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.9, 194.8, 156.4, 151.6, 137.7, 131.4, 129.2, 122.6, 115.1, 106.0, 36.4, 30.5, 27.4, 25.9, 21.4. **FT-IR** (thin layer): ν_{max} = 1726, 1690, 1420, 1367, 1303, 982, 960, 826. **HR-MS** (ESI): *m/z* = 338.1475, calcd. for $C_{17}H_{21}N_3O_3$+Na^+: 338.1475.



(E)-3-((1-(phenyldiazenyl)cyclobutoxy)imino)pentane-2,4-dione, **3ce** was synthesized as slightly yellow viscous gum (89%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.81–7.70 (m, 2H), 7.56–7.42 (m, 3H), 2.69–2.50 (m, 4H), 2.46 (s, 3H), 2.35 (s, 3H), 2.09–1.84 (m, 2H).**^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.7, 194.7, 157.3, 151.7, 131.4, 129.2, 122.8, 105.2, 31.9, 30.7, 25.9, 12.0. **FT-IR** (thin layer): ν_{max} = 1727, 1690, 1364, 1304, 1251, 1143, 954, 768, 690. **HR-MS** (ESI): *m/z* = 310.1163, calcd. for $C_{15}H_{17}N_3O_3$+Na^+: 310.1162.

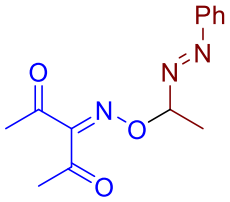


(E)-3-(((1-(phenyldiazenyl)cyclopentyl)oxy)imino)pentane-2,4-dione, **3cf** was synthesized as slightly yellow viscous gum (82%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.78–7.63 (m, 2H), 7.55–7.40 (m, 3H), 2.44 (s, 3H), 2.35 (s, 3H), 2.30–2.12 (m, 4H), 1.96–1.81 (m, 4H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.8, 194.8, 156.8, 151.7, 131.2, 129.2, 122.6, 115.6, 36.4, 30.5, 25.9, 24.8. **FT-IR** (thin layer): ν_{max} = 2959, 1725, 1685, 1363, 1302, 1188, 959, 766, 690. **HR-MS** (ESI): *m/z* = 340.1059, calcd. for $C_{16}H_{19}N_3O_3$+K^+: 340.1058.

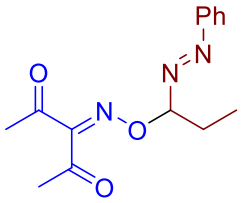


(E)-3-(((1-(phenyldiazenyl)cyclohexyl)oxy)imino)pentane-2,4-dione, **3cg** was synthesized as slightly yellow viscous gum (89%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.74–7.64 (m, 2H), 7.55–7.39 (m, 3H), 2.46 (s, 3H), 2.45 (s, 3H), 2.19–2.06 (m, 2H), 1.92–1.68 (m, 5H), 1.67–1.46 (m, 2H), 1.45–1.27 (m, 1H). **^{13}C NMR**

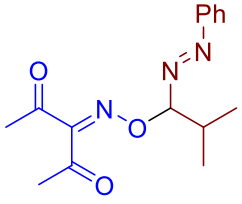
(75.47 MHz, $CDCl_3$): δ = 198.9, 194.8, 156.6, 151.7, 131.2, 129.2, 122.6, 105.2, 32.1, 30.6, 25.9, 25.0, 21.9. **FT-IR** (thin layer): ν_{max} = 2938, 2863, 1727, 1689, 1599, 1450, 1420, 1363, 1304, 1275, 1256, 1195, 1159, 1146, 1069, 1023, 983, 960, 928, 911, 766, 691. **HR-MS** (ESI): *m/z* = 316.1654, calcd. for $C_{17}H_{21}N_3O_3$+H^+: 316.1656.



(*E*)-3-((1-(phenyldiazenyl)ethoxy)imino)pentane-2,4-dione, **3da** was synthesized as pale brown gum (74%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300 MHz, $CDCl_3$): δ = 7.79–7.69 (m, 2H), 7.54–7.44 (m, 3H), 5.67 (q, *J* = 6.3 Hz, 1H), 2.45 (s, 3H), 2.34 (s, 3H), 1.59 (d, *J* = 6.3 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ = 198.2, 194.5, 156.8, 151.5, 131.7, 129.3, 122.8, 103.5, 30.6, 25.9, 17.5. **FT-IR** (thin layer): ν_{max} = 1727, 1691, 1365, 1299, 1107, 1088, 1060, 965, 770, 691. **HR-MS** (ESI): *m/z* = 300.0733, calcd. for $C_{13}H_{15}N_3O_3$+K^+: 300.0745.

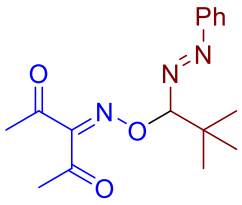


(*E*)-3-((1-(phenyldiazenyl)propoxy)imino)pentane-2,4-dione, **3db** was synthesized as pale yellow gum (59%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300 MHz, $CDCl_3$): δ = 7.83–7.64 (m, 2H), 7.60–7.39 (m, 3H), 5.55–5.41 (m, 1H), 2.45 (s, 3H), 2.33 (s, 3H), 2.15–1.88 (m, 2H), 1.05 (t, *J* = 7.5 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ = 198.2, 194.6, 156.9, 151.5, 131.6, 129.3, 122.8, 107.9, 30.6, 25.9, 25.3, 8.7. **FT-IR** (thin layer): ν_{max} = 1726, 1691, 1363, 1301, 1022, 988, 950, 769, 691. **HR-MS** (ESI): *m/z* = 298.1152, calcd. for $C_{14}H_{17}N_3O_3$+Na^+: 298.1162.

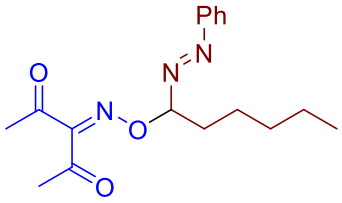


(*E*)-3-((2-methyl-1-(phenyldiazenyl)propoxy)imino)pentane-2,4-dione, **3dc** was synthesized as yellow gum (68%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300 MHz, DMSO-d_6): δ = 7.77–7.68 (m, 2H), 7.62–7.49 (m, 3H), 5.42 (d, *J* = 5.5 Hz, 1H), 2.40 (s, 3H), 2.39–2.28 (m, 1H), 2.26 (s, 3H), 0.99 (t, *J* = 7.5 Hz, 6H). **^{13}C NMR** (75 MHz, DMSO-

d_6): δ = 198.3, 193.7, 156.7, 150.9, 131.8, 129.4, 122.3, 109.1, 31.1, 30.0, 25.5, 17.5, 16.6. **FT-IR** (thin layer): ν_{max} = 2970, 1726, 1691, 1364, 1299, 1020, 998, 959, 769, 691. **HR-MS** (ESI): *m/z* = 290.1500, calcd. for $C_{15}H_{19}N_3O_3$+H^+: 290.1499.



(*E*)-3-((2,2-dimethyl-1-(phenyldiazenyl)propoxy)imino)pentane-2,4-dione, **3dd** was synthesized as pale yellow gum (21%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300 MHz, $CDCl_3$): δ = 7.80–7.69 (m, 2H), 7.53–7.44 (m, 3H), 5.27 (s, 1H), 2.44 (s, 3H), 2.29 (s, 3H), 1.08 (s, 9H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ = 198.1, 194.5, 156.8, 151.6, 131.6, 129.3, 122.9, 112.1, 36.0, 30.4, 25.7. **FT-IR** (thin layer): ν_{max} = 2973, 1727, 1693, 1365, 1300, 1021, 999, 959. **HR-MS** (ESI): *m/z* = 326.1474, calcd. for $C_{16}H_{21}N_3O_3$+Na^+: 326.1475.



(*E*)-3-(((1-(phenyldiazenyl)hexyl)oxy)imino)pentane-2,4-dione, **3de** was synthesized as yellow gum (70%, purified by column chromatography with DCM as eluent). **^{1}H NMR** (300 MHz, $CDCl_3$): δ = 7.80–7.67 (m, 2H), 7.55–7.42 (m, 3H), 5.55 (dd, *J* = 7.7, 5.1 Hz, 1H), 2.45 (s, 3H), 2.33 (s, 3H), 2.11–1.76 (m, 2H), 1.55–1.40 (m, 2H), 1.40–1.23 (m, 4H), 0.89 (t, *J* = 6.9 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ = 198.2, 194.6, 156.8, 151.5, 131.6, 129.2, 122.8, 107.0, 31.8, 31.6, 30.6, 25.9, 23.9, 22.5, 14.1. **FT-IR** (thin layer): ν_{max} = 2956, 2931, 1727, 1691, 1363, 1299, 964. **HR-MS** (ESI): *m/z* = 318.1810, calcd. for $C_{17}H_{23}N_3O_3$+H^+: 318.1812.

X-ray single-crystal diffraction: Structure determination of compound 3ag

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[13] and corrected for absorption and decay using SADABS.[14] The structure was solved by direct methods using SHELXT[15] and refined on F^2 using SHELXL-2018.[16] 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[13] was used for molecular graphics.

Table S1. Crystal data and structure refinement for **3ag**.

Empirical formula	$C_{19}H_{18}BrN_3O_3$	
Formula weight	416.27	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.5693(3) Å	α = 77.8358(8)°
	b = 8.6800(3) Å	β = 81.1246(9)°
	c = 13.7733(4) Å	γ = 69.2122(8)°
Volume	932.73(5) $Å^3$	
Z	2	
Density (calculated)	1.480 g/cm^3	
Absorption coefficient	2.227 mm^{-1}	
F(000)	424	
Crystal size	0.58 x 0.55 x 0.43 mm^3	
Theta range for data collection	2.546 to 37.807°.°	
Index ranges	-14<=h<=14, -14<=k<=14, -23<=l<=23	
Reflections collected	57161	
Independent reflections	9989 [R(int) = 0.0388]	
Observed reflections	8239	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.2763 and 0.1390	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9989 / 0 / 239	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2sigma(I)]	R1 = 0.0322, wR2 = 0.0812	
R indices (all data)	R1 = 0.0439, wR2 = 0.0861	
Largest diff. peak and hole	1.168 and -1.302 e.$Å^{-3}$	

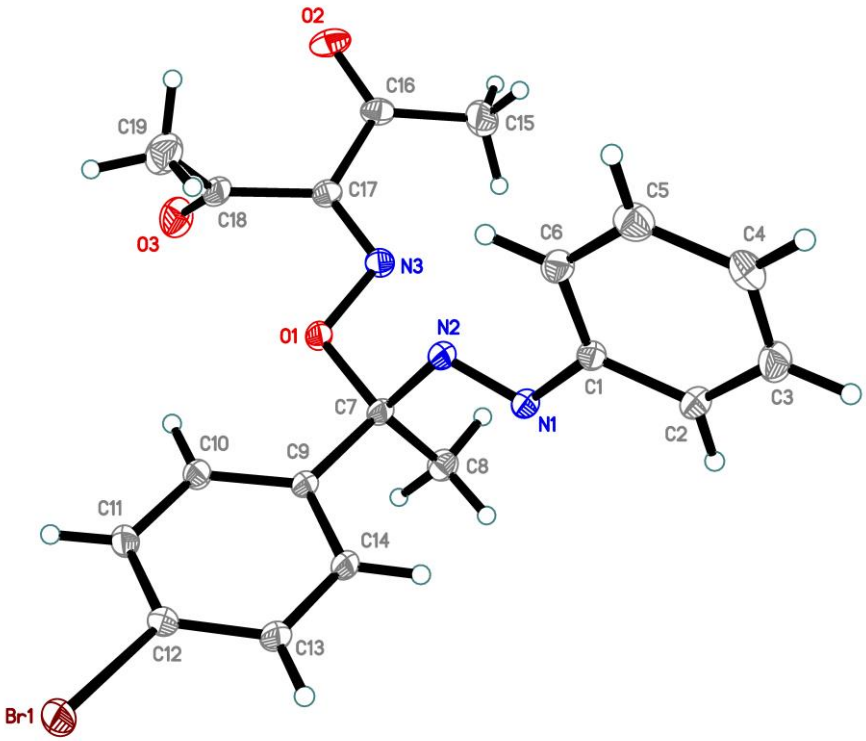


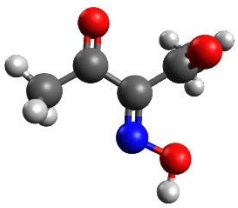
Figure S1. Crystal structure of compound **3ag**, showing the atomic numbering and 50% probability displacement ellipsoids

Compound **3ag** crystallizes in monoclinic space group P-1 (Fig. S1).

Computational details

DFT calculations were conducted by B97-3c composite method[17] including D3 dispersion correction[18,19] as implemented in Orca 5.0.4 program[20]. Main conformers of diacetyliminoxyl **1** and hydrazone **2ca** were considered in all calculations. Presented results correspond to 218.15 K and 1 atm. Cartesian coordinates and energy values of optimized structures of **1a**, **1**, **2ca**, **A**, **B**, and transition states for path I and path II are given below. Optimized geometries were visualized by Avogadro 1.2 program.[21]

Diacetyl oxime 1(a)



Unpaired electrons: 0

Imaginary frequencies: no

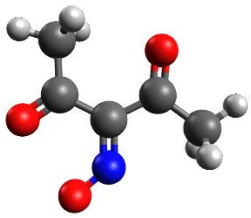
Final Gibbs free energy ... -474.83198681 Eh

Total Enthalpy ... -474.78529015 Eh

Electronic energy ... -474.91396710 Eh

N	0.06970225033778	1.54562566196768	0.00854359883869
C	0.08841033853849	0.26382198676505	0.07371521376140
C	-1.15107648533480	-0.59782234957868	0.22487853008821
C	1.40196017603439	-0.42333735426638	0.03322902618181
O	-1.54265829649431	-0.86755404828874	1.34410855371014
O	1.40954528713797	-1.64891879358009	0.06475775394007
O	-1.20870418302714	2.06009556558835	0.04595806704607
H	-1.07082430823139	3.01644889783864	-0.01859299086395
C	-1.79598390678403	-1.05316711770259	-1.03488608550523
H	-2.69013432158179	-1.63226785517786	-0.82657438779557
H	-2.03918075734542	-0.19077263723676	-1.65639698571686
H	-1.08467615232901	-1.65537516851252	-1.60210325386446
C	2.64933690106215	0.39673910326443	-0.03599672505283
H	2.61027263562725	1.09594619155812	-0.86862938540732
H	2.75198013657635	0.99236558635661	0.87075641067229
H	3.50731168581351	-0.25923066899526	-0.13816534003246

Diacetyliminoxyl radical (1)



Unpaired electrons: 1

Imaginary frequencies: no

Final Gibbs free energy ... -474.22068873 Eh

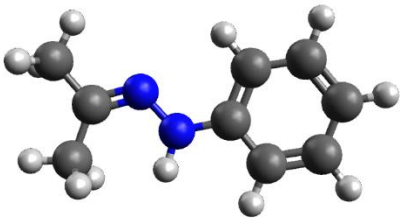
Total Enthalpy ... -474.17480563 Eh

Electronic energy ... -474.29128868 Eh

C	-1.33538414773864	-1.96184929957175	-0.00010017151065
C	-1.27946371058432	-0.46700782514113	-0.00040563769729
H	-2.37450916379125	-2.27239775783076	0.00049472164576

H	-0.81859334007738	-2.35823706627575	-0.87070509570917
H	-0.81768566092729	-2.35795354049976	0.87010043278926
C	0.04990145680954	0.22072226254471	-0.00041456707655
C	1.38326434561685	-0.42221970562381	-0.00060624263912
C	2.58086993574630	0.48363325680431	0.00010539993198
H	2.57346739547275	1.13127684194830	-0.87556596752056
H	3.48231145114325	-0.11952463580711	0.00046637524965
H	2.57262527054406	1.13105670448193	0.87593869695890
N	0.03632679688412	1.52809581527337	-0.00024512776745
O	-0.89676757675779	2.30058401146669	-0.00011685457034
O	-2.29609797732566	0.20998647163861	0.00059004640418
O	1.49821192498545	-1.64031853340783	-0.00010100848861

1-phenyl-2-(propan-2-ylidene)hydrazine (hydrazone 2ca)



Unpaired electrons: 0

Imaginary frequencies: no

Final Gibbs free energy ... -459.29164258 Eh

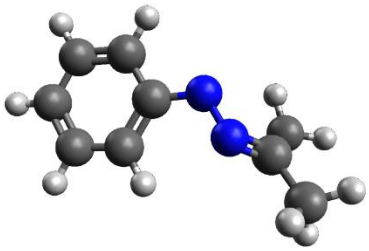
Total Enthalpy ... -459.24325792 Eh

Electronic energy ... -459.44600868 Eh

C	-2.68828473691068	-0.10798480311287	0.02771241309834
C	-3.15896750595697	1.31340080568908	0.00973857270202
H	-2.80479835013175	1.83964560149747	-0.87979305768191
H	-4.24298035489196	1.36556371948182	0.01771621721063
H	-2.79269322723717	1.86764647378725	0.87737274418745
C	0.84341944945057	0.20126289738187	0.00059373435521
C	1.76992448646290	1.25330467736635	0.01876207241468
C	1.31610657137754	-1.11631705582259	0.00025776409773
C	3.12821220921590	0.98988995939636	0.03525792802819
H	1.41403427492504	2.27641467402569	0.02005453646898

C	2.68041616682092	-1.36154042942581	0.01746875855271
H	0.61200986279974	-1.93365766507553	-0.01265148788478
C	3.59952948891468	-0.31905815019590	0.03475568779620
H	3.82503601980865	1.81786918352351	0.04967967676972
H	3.02738675709240	-2.38696238873642	0.01716708495444
H	4.66172093115328	-0.52102194782030	0.04805596986220
N	-1.44831891686306	-0.45898915543771	0.01231611269370
N	-0.50225727949582	0.50549952080282	-0.02496421741167
H	-0.76299821766264	1.48070371931762	0.01709855475445
C	-3.70944952532095	-1.19255080486344	0.06475426018305
H	-4.34260629361971	-1.09932941111583	0.94978551909342
H	-4.37462058201747	-1.12940871641359	-0.79929750923365
H	-3.23994122791342	-2.17221270424985	0.07306866498886

Hydrazyl radical (A)



Unpaired electrons: 1

Imaginary frequencies: no

Final Gibbs free energy ... -458.67006756 Eh

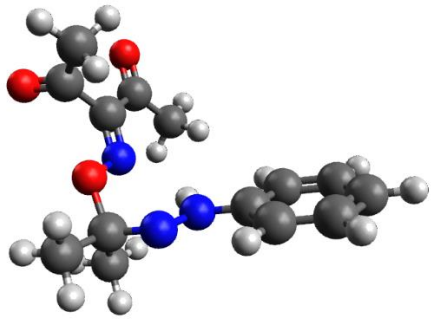
Total Enthalpy ... -458.62140860 Eh

Electronic energy ... -458.81114779 Eh

C	-1.72338616027636	2.71428469319100	0.22077940605414
C	-0.72622767139289	2.50766868189767	1.31216198697860
H	0.18104509298792	3.07704571522331	1.12605366397245
H	-1.13648232724174	2.84718908902932	2.26504759995647
H	-0.48897000170441	1.45108853103101	1.41968230462667
C	-3.75822670237235	0.18554628823212	1.02464620133219
C	-3.79792950046681	-1.16724211828324	1.42769582834566
C	-4.87414530822482	1.00703747685982	1.30363120159041

C	-4.89900688259140	-1.67020028425693	2.08858582276639
H	-2.94322464269852	-1.79360779123958	1.21106621686552
C	-5.96986247227073	0.48672231167988	1.96151612192368
H	-4.85948632092238	2.04162015133829	0.99353684068354
C	-5.99314213313639	-0.84951975888042	2.35983027948697
H	-4.91333287945769	-2.70781209614253	2.39425892196645
H	-6.82025745869417	1.12327433347172	2.16831933408262
H	-6.85684141493623	-1.24730204289183	2.87473683366425
N	-2.62294760358929	1.84380547466124	-0.07175586597223
N	-2.61585690500284	0.60863336080034	0.40834074110731
C	-1.70251713840699	3.99535279174785	-0.53550333929676
H	-1.78744327673710	4.84304979731567	0.14613016940992
H	-0.74953087045499	4.11028041889706	-1.05539058684360
H	-2.50974399140980	4.04016445531821	-1.26042722870066

Diacetyliminoxyl radical 1 adduct to hydrazone 2ca (B)



Unpaired electrons: 1

Imaginary frequencies: no

Final Gibbs free energy ... -933.48547166 Eh

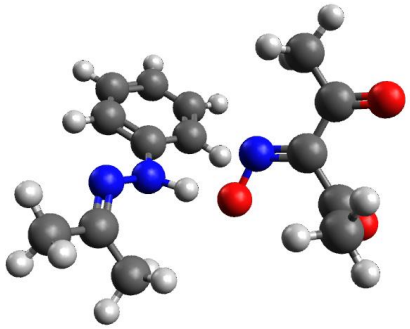
Total Enthalpy ... -933.41400148 Eh

Electronic energy ... -933.73578724 Eh

C	0.20208540057188	2.66697044318437	-1.44286809710738
H	-0.55294441937583	3.44936971465738	-1.44903454981695
H	1.13073696934283	3.07566803474246	-1.83307730219112
H	-0.12727525428895	1.87073852170414	-2.10292020364739
C	-2.45537056683475	0.00740354934420	0.38428907799657
C	-2.92719595691344	-1.08197545518958	-0.35908881243144

C	-3.14486128634428	0.41848900361807	1.53092881806197
C	-4.07128530401349	-1.74646687842773	0.04126119929755
H	-2.39309940117444	-1.39777631928556	-1.24581304649687
C	-4.28810438693986	-0.25959205196204	1.91642942925229
H	-2.77707133953158	1.25682765826169	2.10156177027238
C	-4.76099670377059	-1.34175827100304	1.18068594930122
H	-4.42721214666704	-2.58696353356826	-0.53898653117118
H	-4.81722357579462	0.06212412304624	2.80355867195593
H	-5.65533379714678	-1.86379029194511	1.49135821454483
N	-0.76376536018175	1.65658128708482	0.61878690122883
N	-1.31633689450645	0.65677545700822	-0.05201259323035
H	-0.83362752640751	0.25687190408940	-0.85244504024837
C	0.93388726634611	3.30464593773993	0.87419986002085
H	1.85760273274683	3.70950263374563	0.46981695888761
H	0.19756121201662	4.10191674506906	0.92944978109626
H	1.11444343105022	2.93045485208165	1.87884128955564
C	0.40533129577487	2.20034105891560	-0.01224958859179
O	1.52979315458969	1.19513271083804	0.03121839293010
N	1.32899146152188	0.15593448636255	-0.82560201624782
C	2.21033664143136	-0.77547762341932	-0.70491952953750
C	3.37523484582571	-0.69832815114747	0.26062970332883
C	2.08813309077490	-1.97170540927001	-1.55975140115902
C	3.13011641122726	-1.23771914571563	1.62487801780537
O	4.42594263980457	-0.21449578250983	-0.11632447000970
C	0.94892045439329	-2.05372011365357	-2.52685141339844
O	2.92280986455075	-2.86453552613147	-1.43722592606142
H	4.00023323554734	-1.10216977055046	2.25958505161548
H	2.26049408539129	-0.74627864659645	2.06245002308525
H	2.88449978798086	-2.29812335426272	1.54876371048518
H	-0.00164151365853	-2.00535008457258	-1.99772413117195
H	1.01205019185409	-2.98474881101989	-3.08011804610397
H	0.96922878080754	-1.21118930126280	-3.21599308209943

Transition state for hydrogen atom abstraction from hydrazone 2ca by diacetyliminoxyl radical 1 (Path I)



Unpaired electrons: 1

Imaginary frequencies: 1

Final Gibbs free energy ... -933.49075506 Eh

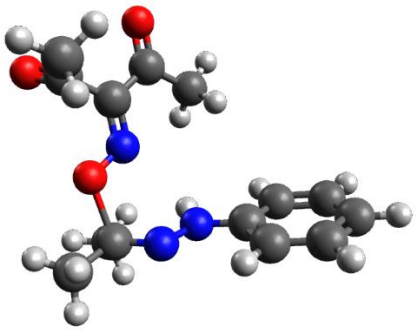
Total Enthalpy ... -933.41654700 Eh

Electronic energy ... -933.73278728 Eh

C	-2.67860679090951	-1.89648384316536	0.54948187300355
C	-2.21349691934370	-2.69406541384970	-0.61630877431048
H	-1.23401112093057	-3.12099090918240	-0.39076607843662
H	-2.88926453235783	-3.52519973779008	-0.79976550850007
H	-2.11596148367138	-2.09540955521574	-1.51662080451967
C	-1.84233979986778	1.35247254848249	-0.36616905182471
C	-0.89416093642782	1.99661365797425	-1.19094765247673
C	-2.89161455605118	2.09852871890858	0.20894655011364
C	-0.99581000643264	3.35085267846665	-1.42110394078054
H	-0.09703893464611	1.41927658179076	-1.63372013123499
C	-2.97551135014645	3.44992975529813	-0.03783327808182
H	-3.61056883023651	1.60290197412827	0.84180799133073
C	-2.03279527196658	4.08532682673897	-0.84930885363436
H	-0.26700398066986	3.84213868113130	-2.05000461453565
H	-3.77753397875648	4.02412622600595	0.40463997080790
H	-2.10784219008135	5.14799821418774	-1.03246808129819
N	-2.51251558185589	-0.61514819621273	0.69330444415441
N	-1.71422625673441	0.00685602376814	-0.19308017247196
C	-3.39967819943933	-2.60226185348514	1.63482633175767
H	-4.32654122283430	-3.03016502277996	1.24882676727505

H	-2.80094284232157	-3.44251639167538	1.98972906711072
H	-3.62541066195303	-1.94055397903985	2.46422746017884
O	0.58855737635927	-0.98181742929971	-0.52099404878882
N	1.36916130546165	-0.12792640383936	0.10693363272955
C	2.64715001430066	-0.38134769325150	0.08139044962258
C	3.20450362011337	-1.58447810306832	-0.64066550444963
C	3.56497584941896	0.51627341661213	0.76573881338546
C	3.25688354888892	-2.85107057610939	0.14497393136953
O	3.57379235165927	-1.49027918813163	-1.79889123430014
C	3.01965548097088	1.74449013515227	1.43872539190041
O	4.77311854177684	0.25397068444044	0.77841290055731
H	3.61323038951389	-3.67809719678589	-0.46202061043530
H	3.91563355439710	-2.70764394248505	1.00296149827240
H	2.26648439203522	-3.07242523129194	0.54353793737449
H	2.55714061488931	2.40509338235350	0.70664188127719
H	3.82883878371615	2.26756818221565	1.93872860745157
H	2.24721958844201	1.48357761405276	2.15911789502286
H	-0.70115596430925	-0.46753663504886	-0.42493705461618

Transition state for diacetyliminoxyl radical 1 addition to hydrazone 2ca (Path II)



Unpaired electrons: 1

Imaginary frequencies: 1

Final Gibbs free energy ... -933.48201377 Eh

Total Enthalpy ... -933.41053113 Eh

Electronic energy ... -933.73092950 Eh

C	0.27503802918850	2.72875138211409	-1.44429719853980

H	-0.57098327533227	3.37744680671123	-1.67204226740085
H	1.19138511223518	3.26243018180790	-1.67430515241035
H	0.22494528516479	1.86199991786022	-2.09922380573659
C	-2.54166763596767	0.12409290859729	0.14934655162066
C	-3.12931993714930	-0.73935017695603	-0.78484566037081
C	-3.05023429246225	0.19890325120213	1.45129888264606
C	-4.21048184080145	-1.51659297855103	-0.41644411877056
H	-2.73069905575516	-0.79247828402190	-1.78963826149161
C	-4.13408693506004	-0.58581782014549	1.80032681981692
H	-2.59115625534702	0.86303510570720	2.16640291152016
C	-4.72103089405013	-1.44584835997663	0.87645096392150
H	-4.65806166975304	-2.18193994437398	-1.14184954057883
H	-4.52559299716710	-0.52741319242802	2.80689424994056
H	-5.56732957675994	-2.05526102704758	1.16116868753842
N	-0.82406713412918	1.70951837542265	0.55579014107598
N	-1.46482702690720	0.88421082737468	-0.25713626351273
H	-1.11904272292404	0.72038374995890	-1.19574966621820
C	0.78132822972775	3.41551701216008	0.94455218615434
H	1.80070114046036	3.67702608800313	0.67433045712908
H	0.17182637684762	4.31589598019298	0.86732565355112
H	0.75461075718273	3.06825439477512	1.97324515170304
C	0.24090071758986	2.37393643751057	0.01637416488474

O	1.63957837305631	1.20190322979606	0.10492115377978
N	1.31501003832916	0.11026236533061	-0.54777222875358
C	2.19218147934141	-0.84525150624459	-0.55280665570219
C	3.54097590086083	-0.71526891607733	0.11831695631920
C	1.85935501177464	-2.09713378089655	-1.23225224973420
C	3.59664646490207	-1.10785944849598	1.55393815715428
O	4.49420838576509	-0.29789094283756	-0.51517947115887
C	0.51248646164902	-2.23678876185190	-1.87882440969830
O	2.68479419848239	-3.01233865993344	-1.23355081930947
H	4.58707516542079	-0.94498289679690	1.96776319468071
H	2.85418295042570	-0.53864429842055	2.11469010569789
H	3.31979105937952	-2.15901845532337	1.64789049440119
H	-0.26642593815953	-2.23632565090172	-1.11701009461966
H	0.47370575181046	-3.17054428653096	-2.43037770976349
H	0.30338499413126	-1.40136221871340	-2.54291145376550

References

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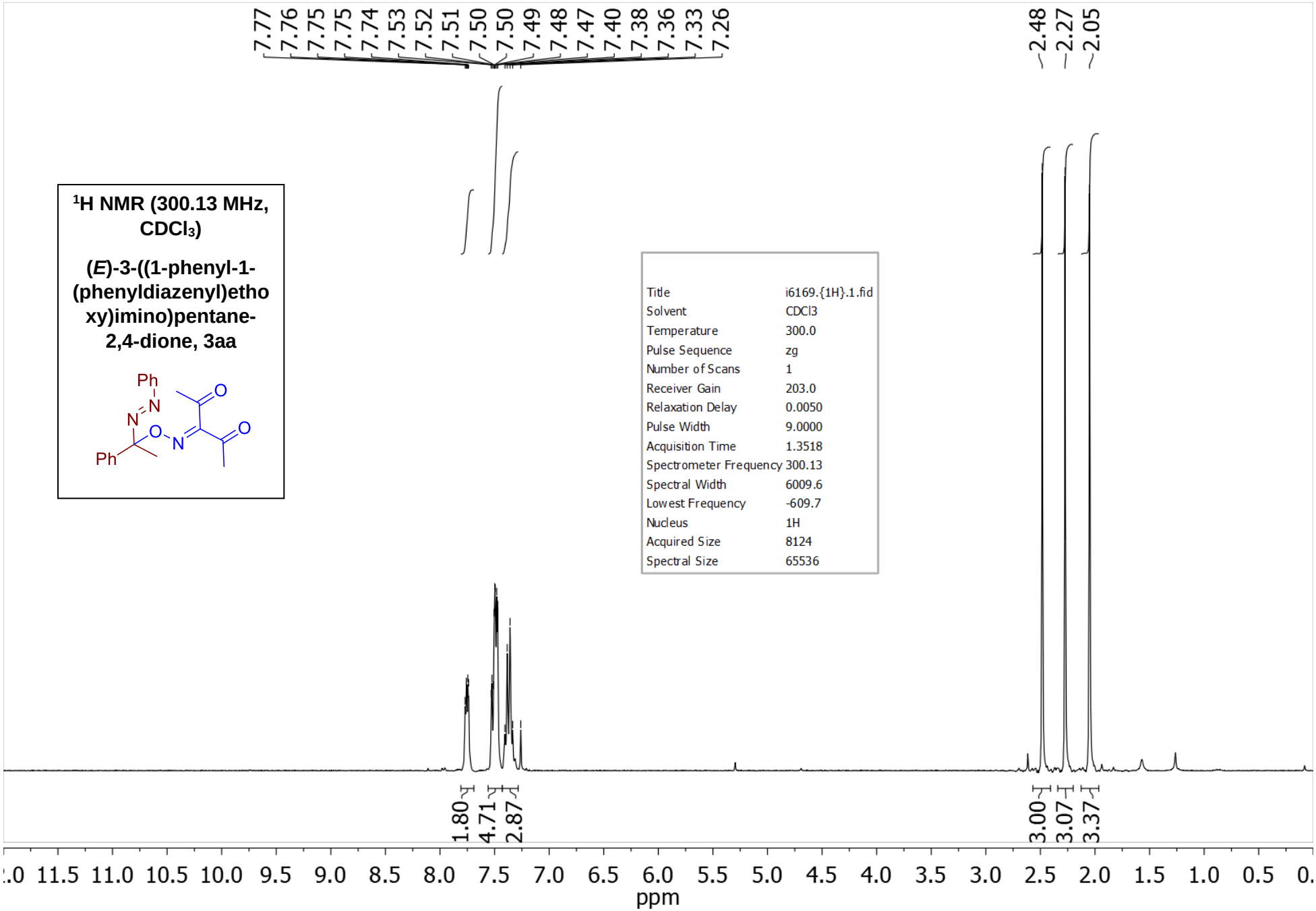
The ^{1}H and ^{13}C spectra of synthesized compounds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7.76
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7.51
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7.50
7.49
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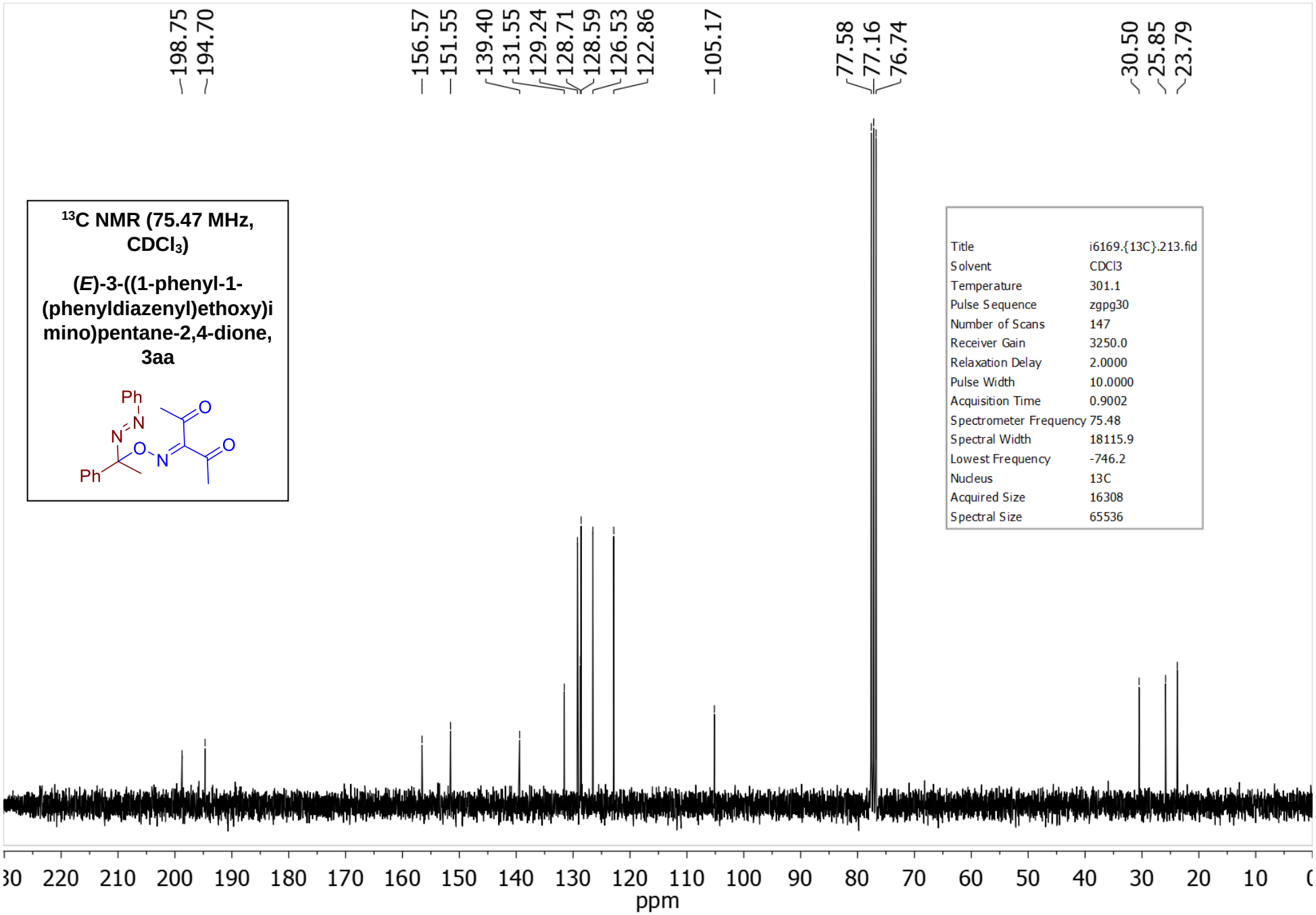
7.47
7.40
7.38
7.36
7.33
7.26
2.48
2.27
2.05
1H NMR (300.13 MHz, CDCl3)
(E)-3-((1-phenyl-1-(phenyldiazenyl)ethoxy)imino)pentane-2,4-dione, 3aa
Ph
N
N
O
O
N
O
O
Ph
Title i6169.{1H}.1.fid
Solvent CDCl3
Temperature 300.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 203.0
Relaxation Delay 0.0050
Pulse Width 9.0000
Acquisition Time 1.3518
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -609.7
Nucleus 1H
Acquired Size 8124
Spectral Size 65536
1.80
4.71
2.87
3.00
3.07
3.37
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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194.70
156.57
151.55
139.40
131.55
129.24
128.71
128.59
126.53
122.86
105.17
77.58
77.16
76.74
30.50
25.85
23.79
^{13}C NMR (75.47 MHz, $CDCl_3$)
(*E*)-3-((1-phenyl-1-(phenyldiazenyl)ethoxy)imino)pentane-2,4-dione, 3aa
Ph
N
N
O
N
O
O
Ph
Title i6169.{13C}.213.fid
Solvent CDCl3
Temperature 301.1
Pulse Sequence zgpg30
Number of Scans 147
Receiver Gain 3250.0
Relaxation Delay 2.0000
Pulse Width 10.0000
Acquisition Time 0.9002
Spectrometer Frequency 75.48
Spectral Width 18115.9
Lowest Frequency -746.2
Nucleus 13C
Acquired Size 16308
Spectral Size 65536
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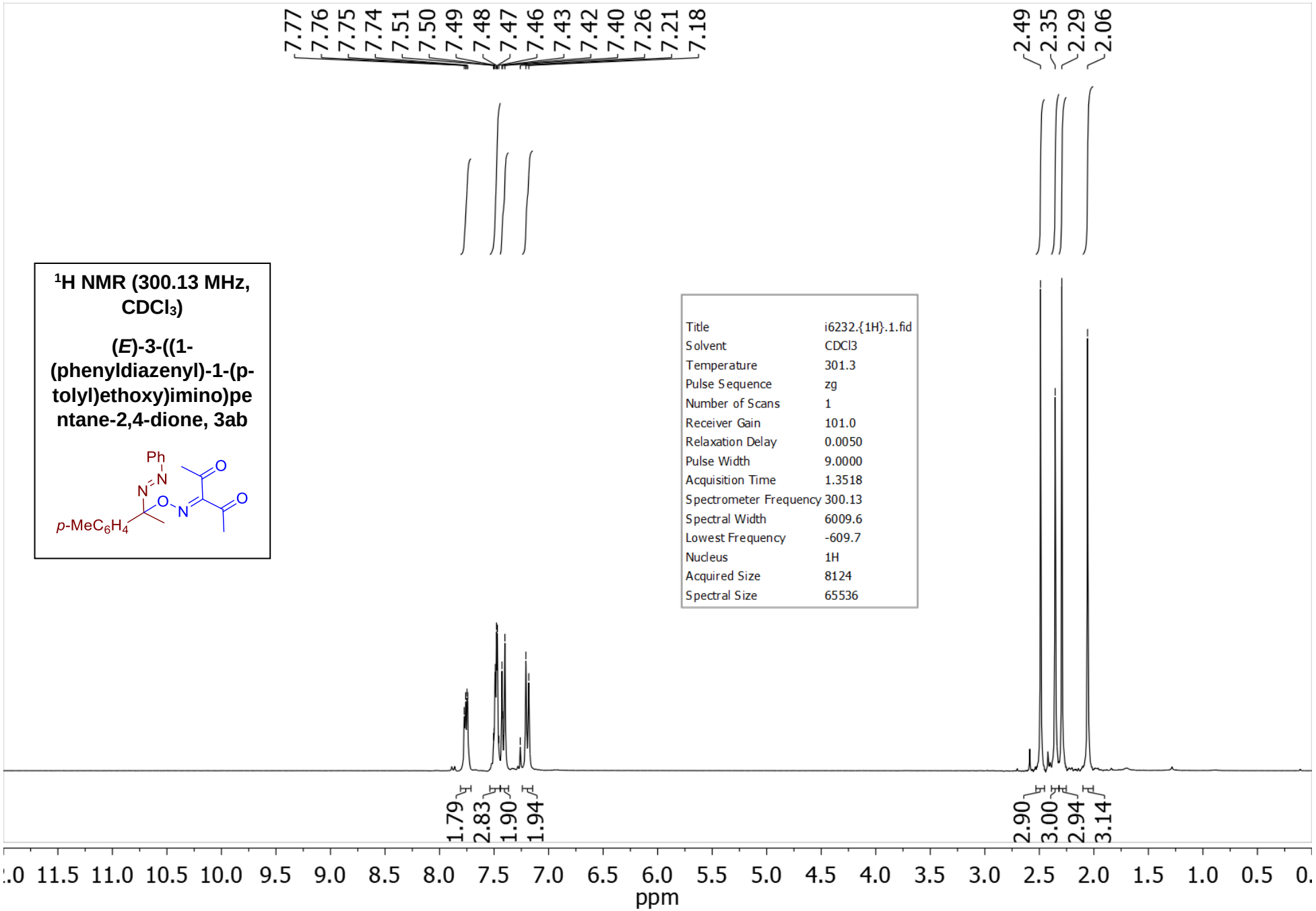
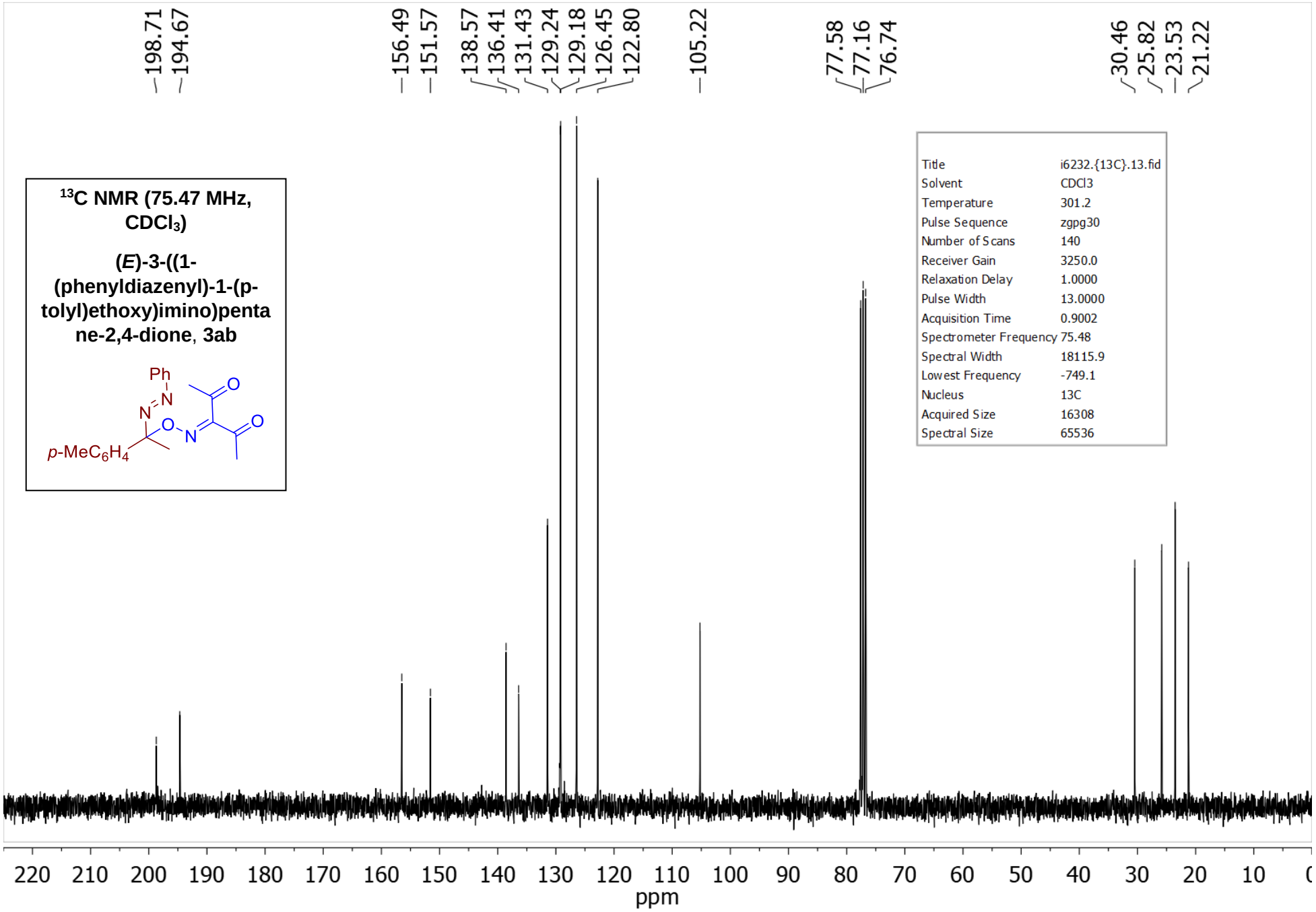
ppm



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

(*E*)-3-((1-(phenyldiazenyl)-1-(p-tolyl)ethoxy)imino)pentane-2,4-dione, 3ab

Title	i6232.{1H}.1.fid
Solvent	CDCl3
Temperature	301.3
Pulse Sequence	zg
Number of Scans	1
Receiver Gain	101.0
Relaxation Delay	0.0050
Pulse Width	9.0000
Acquisition Time	1.3518
Spectrometer Frequency	300.13
Spectral Width	6009.6
Lowest Frequency	-609.7
Nucleus	1H
Acquired Size	8124
Spectral Size	65536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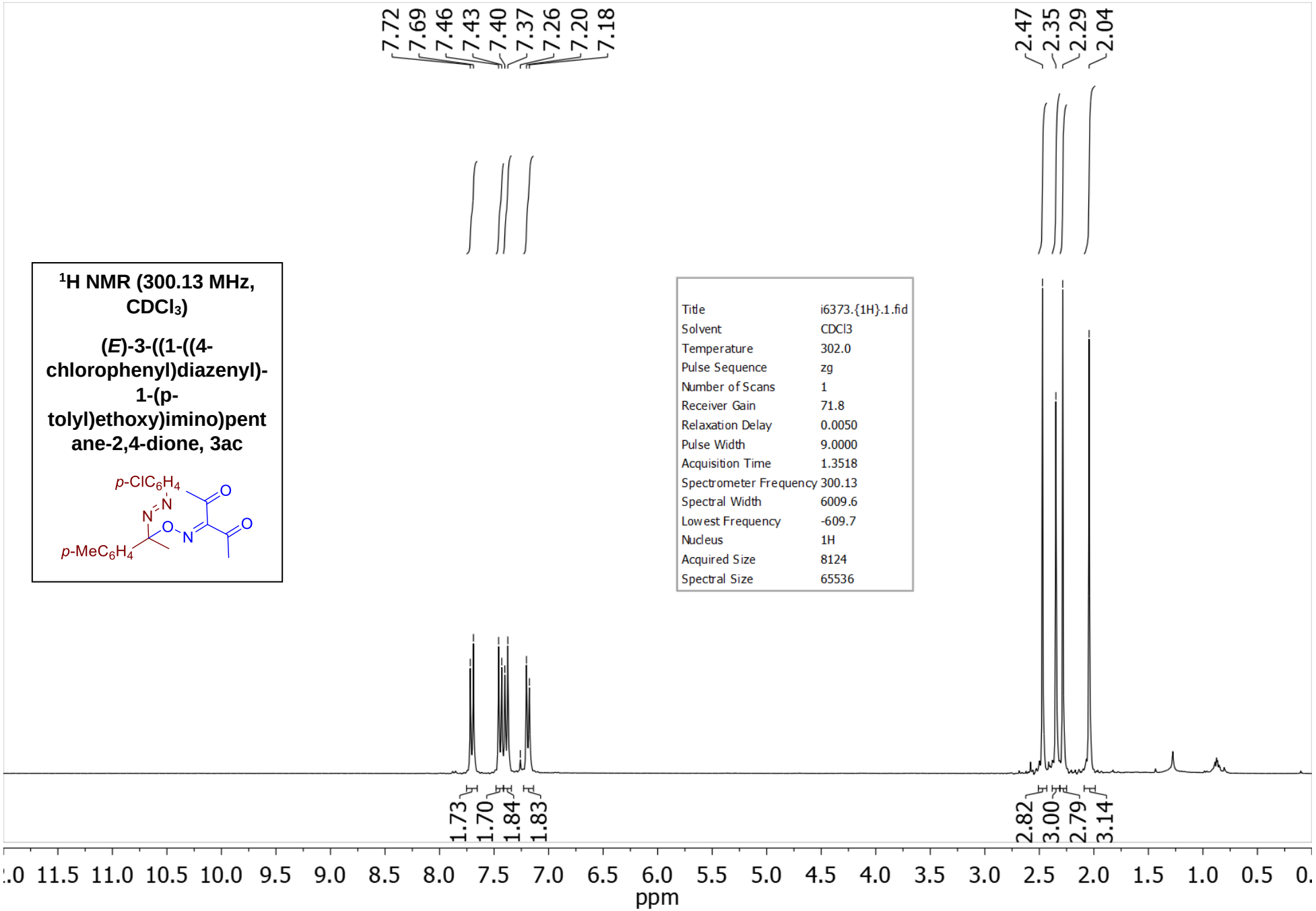
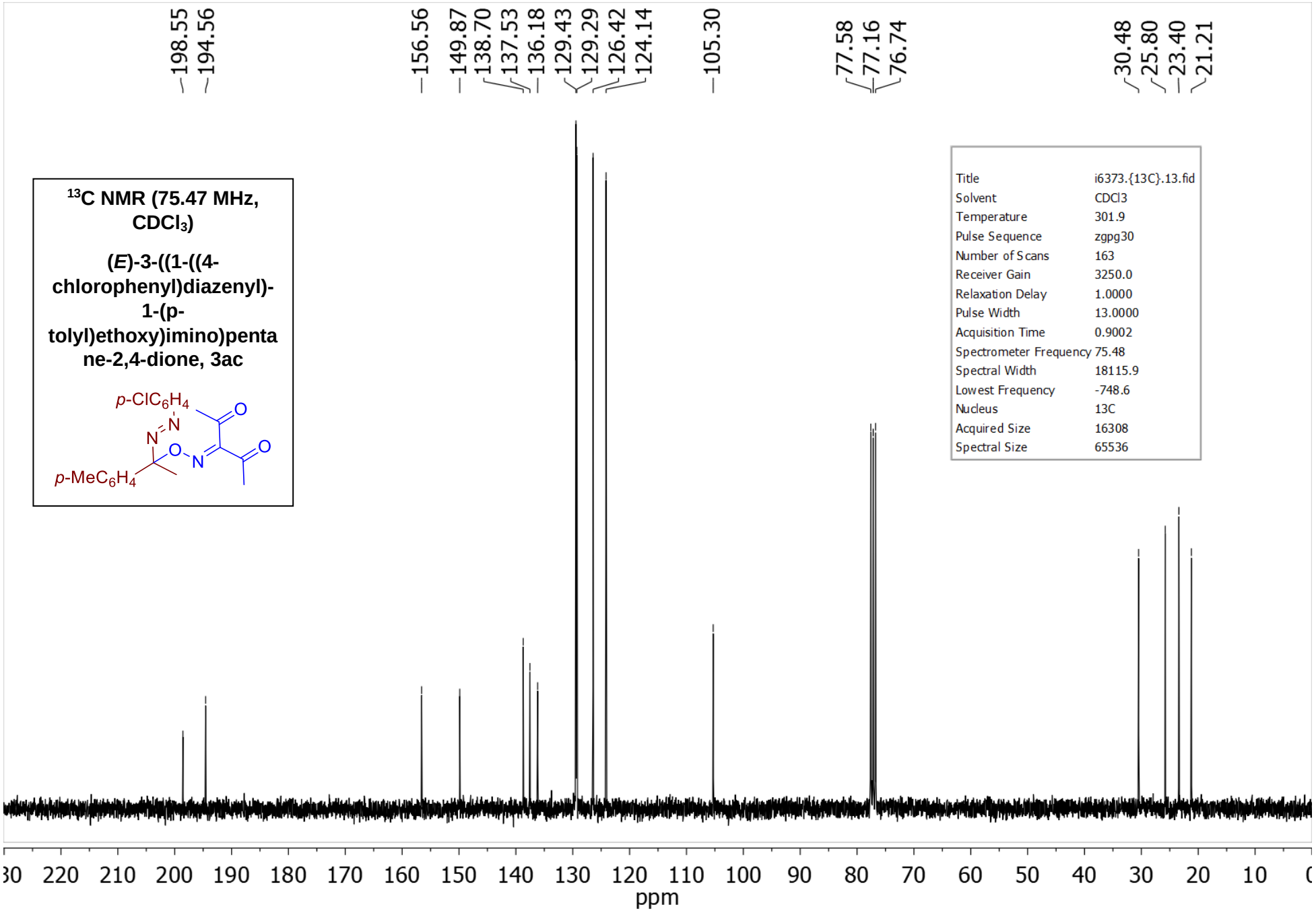
156.49
151.57
138.57
136.41
131.43
129.24
129.18
126.45
122.80
105.22
77.58
77.16
76.74
30.46
25.82
23.53
21.22
13C NMR (75.47 MHz, CDCl3)
(E)-3-((1-(phenyldiazenyl)-1-(p-tolyl)ethoxy)imino)pentane-2,4-dione, 3ab
Ph
N
N
O
N
O
O
p-MeC6H4
Title i6232.{13C}.13.fid
Solvent CDCl3
Temperature 301.2
Pulse Sequence zgpg30
Number of Scans 140
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 -749.1
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

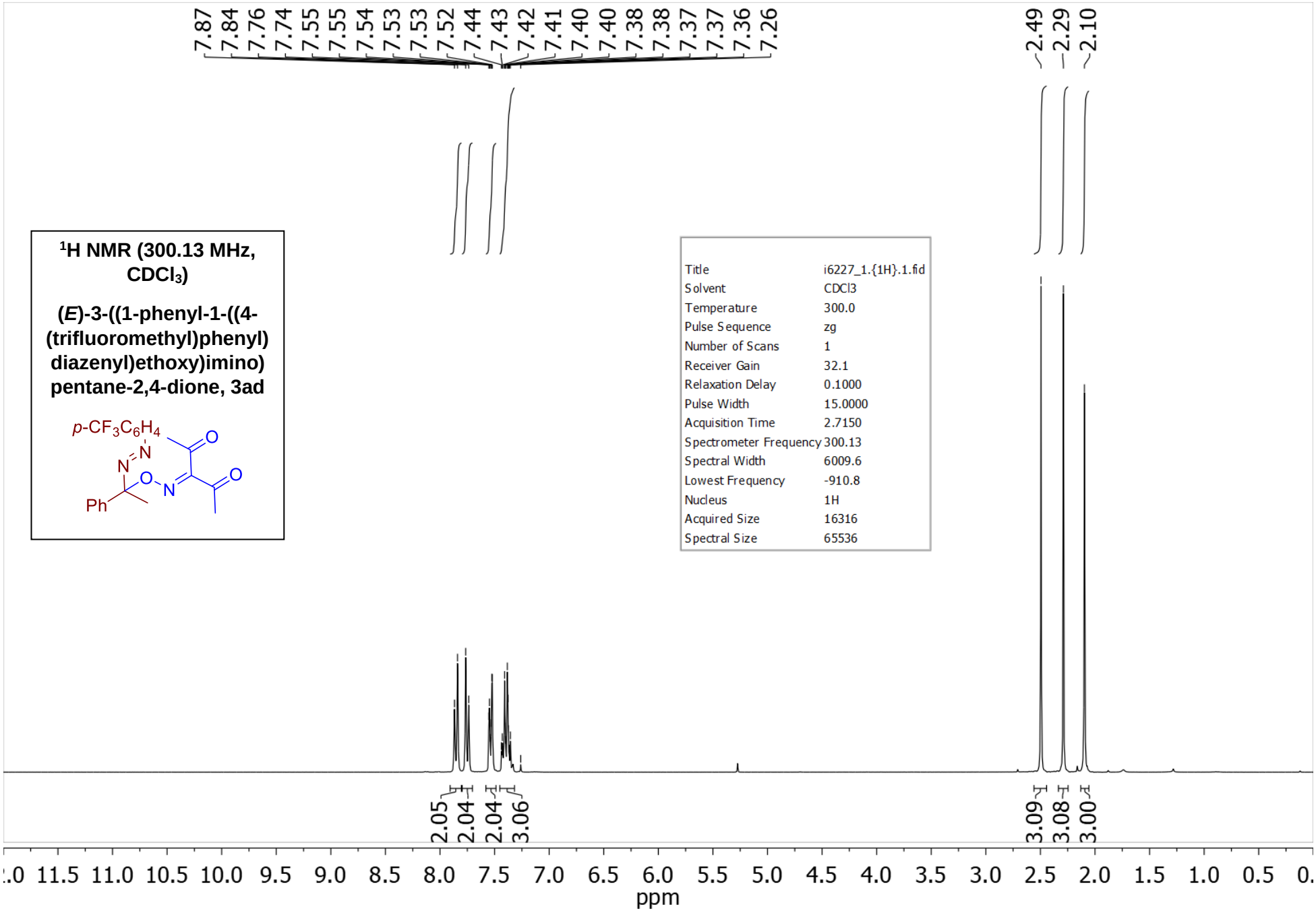


^{1}H NMR (300.13 MHz, $CDCl_3$)

(*E*)-3-((1-((4-chlorophenyl)diazenyl)-1-(p-tolyl)ethoxy)imino)pentane-2,4-dione, 3ac

Title	i6373.{1H}.1.fid
Solvent	CDCl3
Temperature	302.0
Pulse Sequence	zg
Number of Scans	1
Receiver Gain	71.8
Relaxation Delay	0.0050
Pulse Width	9.0000
Acquisition Time	1.3518
Spectrometer Frequency	300.13
Spectral Width	6009.6
Lowest Frequency	-609.7
Nucleus	1H
Acquired Size	8124
Spectral Size	65536

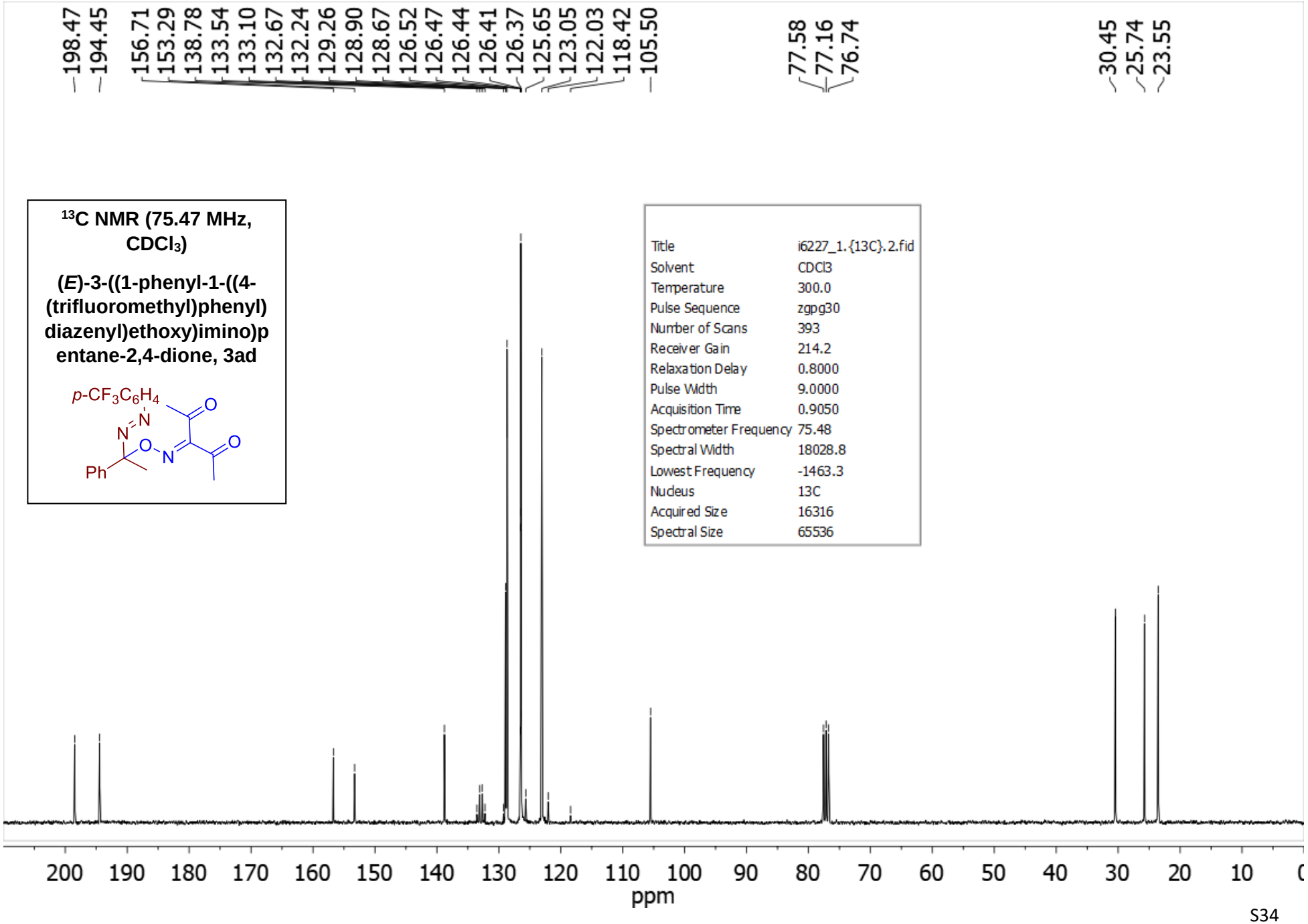

198.55
194.56
156.56
149.87
138.70
137.53
136.18
129.43
129.29
126.42
124.14
105.30
77.58
77.16
76.74
30.48
25.80
23.40
21.21
13C NMR (75.47 MHz, CDCl3)
(E)-3-((1-((4-chlorophenyl)diazenyl)-1-(p-tolyl)ethoxy)imino)pentane-2,4-dione, 3ac
p-ClC6H4
p-MeC6H4
Title i6373.{13C}.13.fid
Solvent CDCl3
Temperature 301.9
Pulse Sequence zgpg30
Number of Scans 163
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 -748.6
Nucleus 13C
Acquired Size 16308
Spectral Size 65536
ppm



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

(*E*)-3-((1-phenyl-1-((4-(trifluoromethyl)phenyl)diazenyl)ethoxy)imino)pentane-2,4-dione, 3ad

Title	i6227_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	-910.8
Nucleus	1H
Acquired Size	16316
Spectral Size	65536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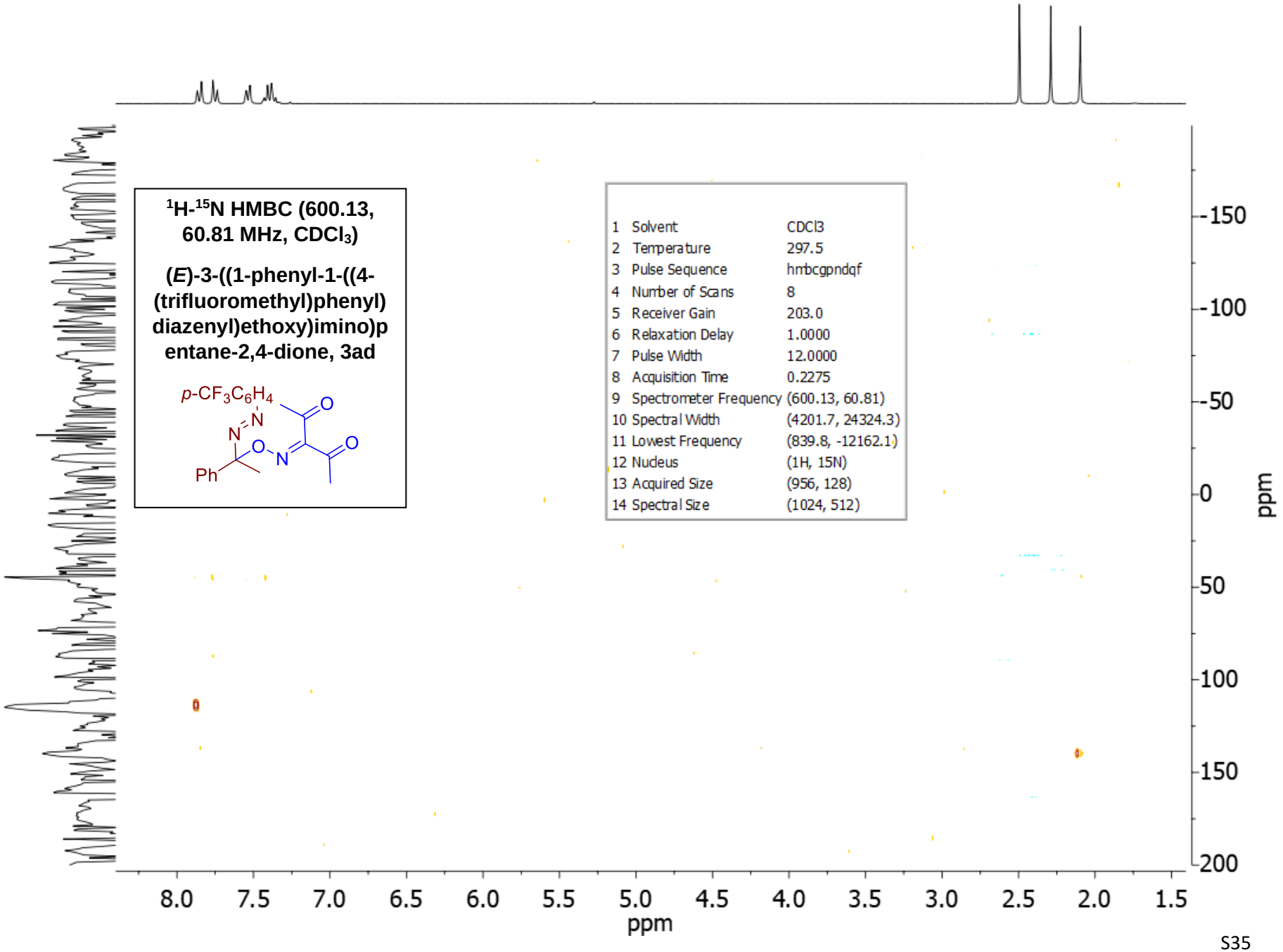
126.52
126.47
126.44
126.41
126.37
125.65
123.05
122.03
118.42
105.50
77.58
77.16
76.74
30.45
25.74
23.55
13C NMR (75.47 MHz, CDCl3)
(E)-3-((1-phenyl-1-((4-(trifluoromethyl)phenyl)diazenyl)ethoxy)imino)pentane-2,4-dione, 3ad
p-CF3C6H4
Ph
Title i6227_1.{13C}.2.fid
Solvent CDCl3
Temperature 300.0
Pulse Sequence zgpg30
Number of Scans 393
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 -1463.3
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
ppm


^{1}H-^{15}N HMBC (600.13, 60.81 MHz, $CDCl_3$)
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p-CF3C6H4
N
N
O
N
O
O
Ph
1 Solvent CDCl3
2 Temperature 297.5
3 Pulse Sequence hmbcgpndqf
4 Number of Scans 8
5 Receiver Gain 203.0
6 Relaxation Delay 1.0000
7 Pulse Width 12.0000
8 Acquisition Time 0.2275
9 Spectrometer Frequency (600.13, 60.81)
10 Spectral Width (4201.7, 24324.3)
11 Lowest Frequency (839.8, -12162.1)
12 Nucleus (1H, 15N)
13 Acquired Size (956, 128)
14 Spectral Size (1024, 512)
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7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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2.5
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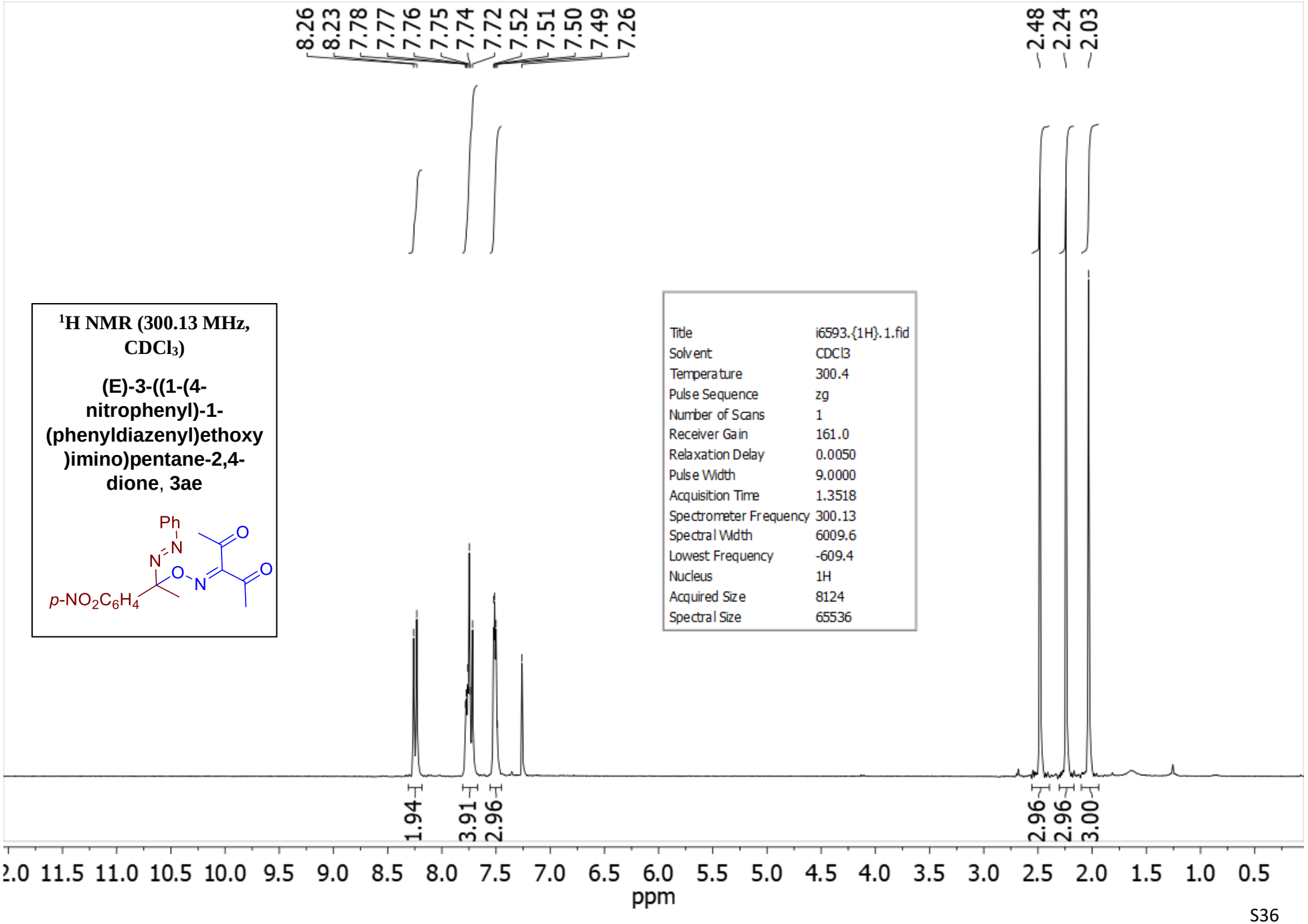
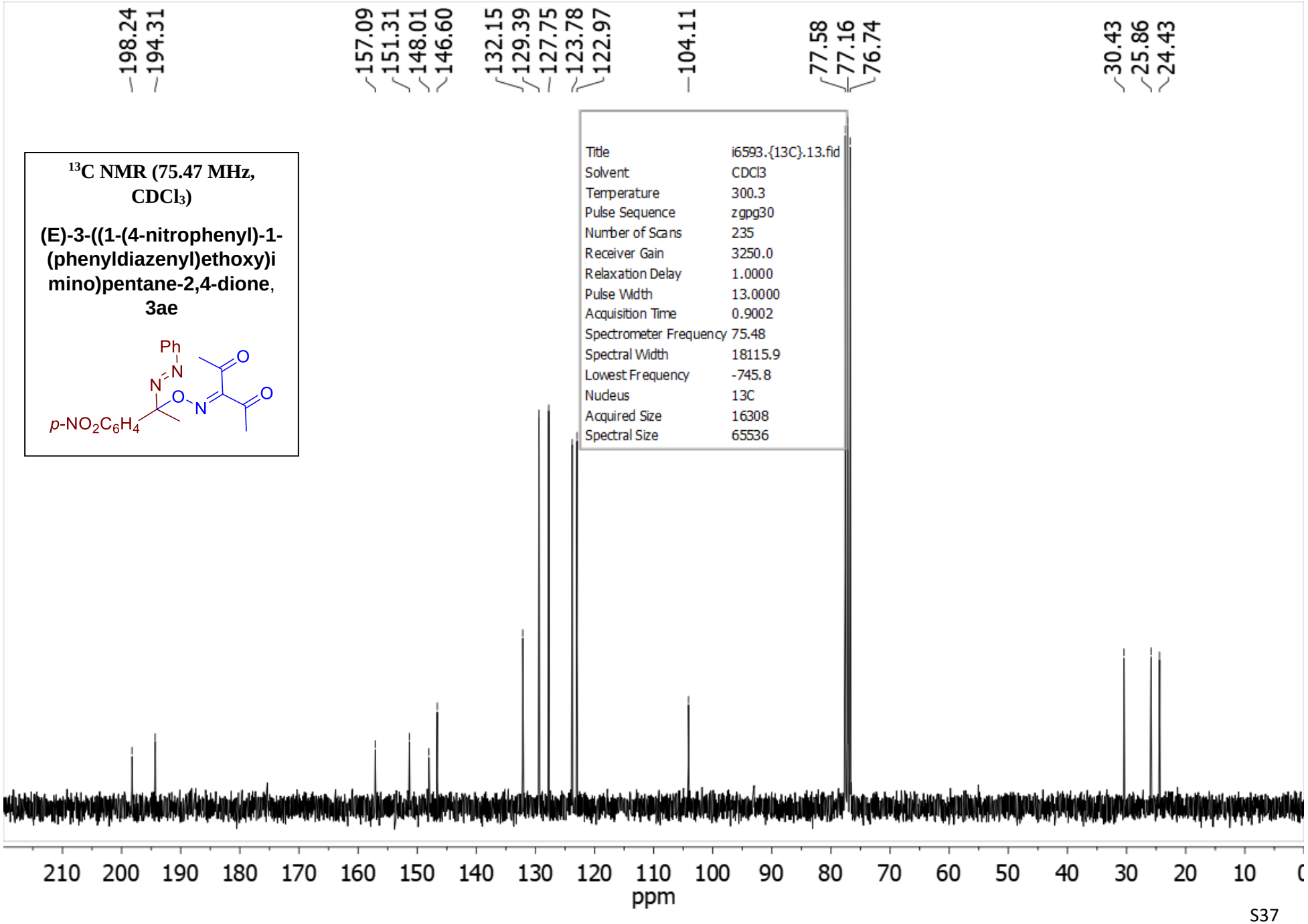
-100
-50
0
50
100
150
200
ppm



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

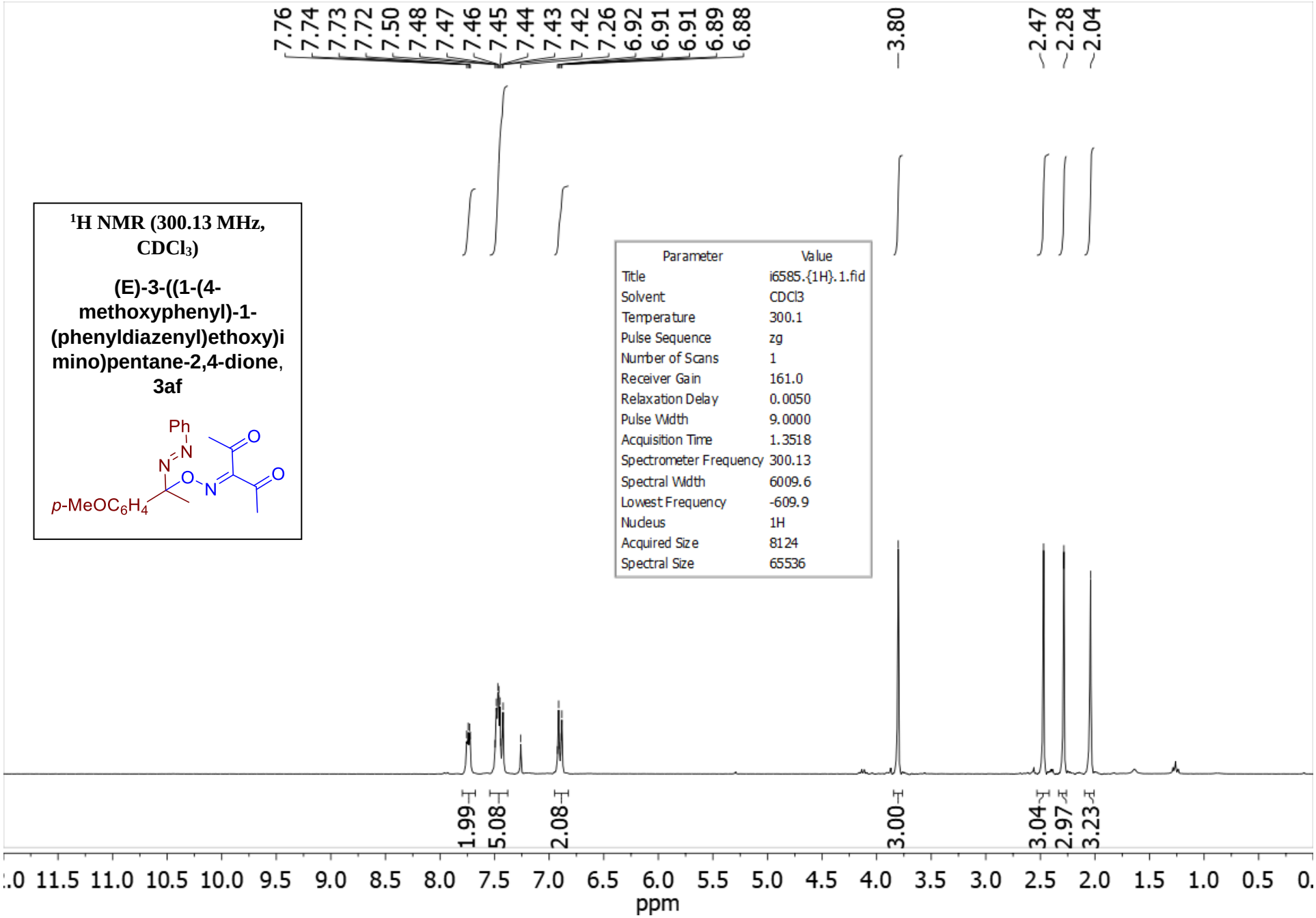
(E)-3-((1-(4-nitrophenyl)-1-(phenyldiazenyl)ethoxy)imino)pentane-2,4-dione, 3ae

Title	i6593.{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



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

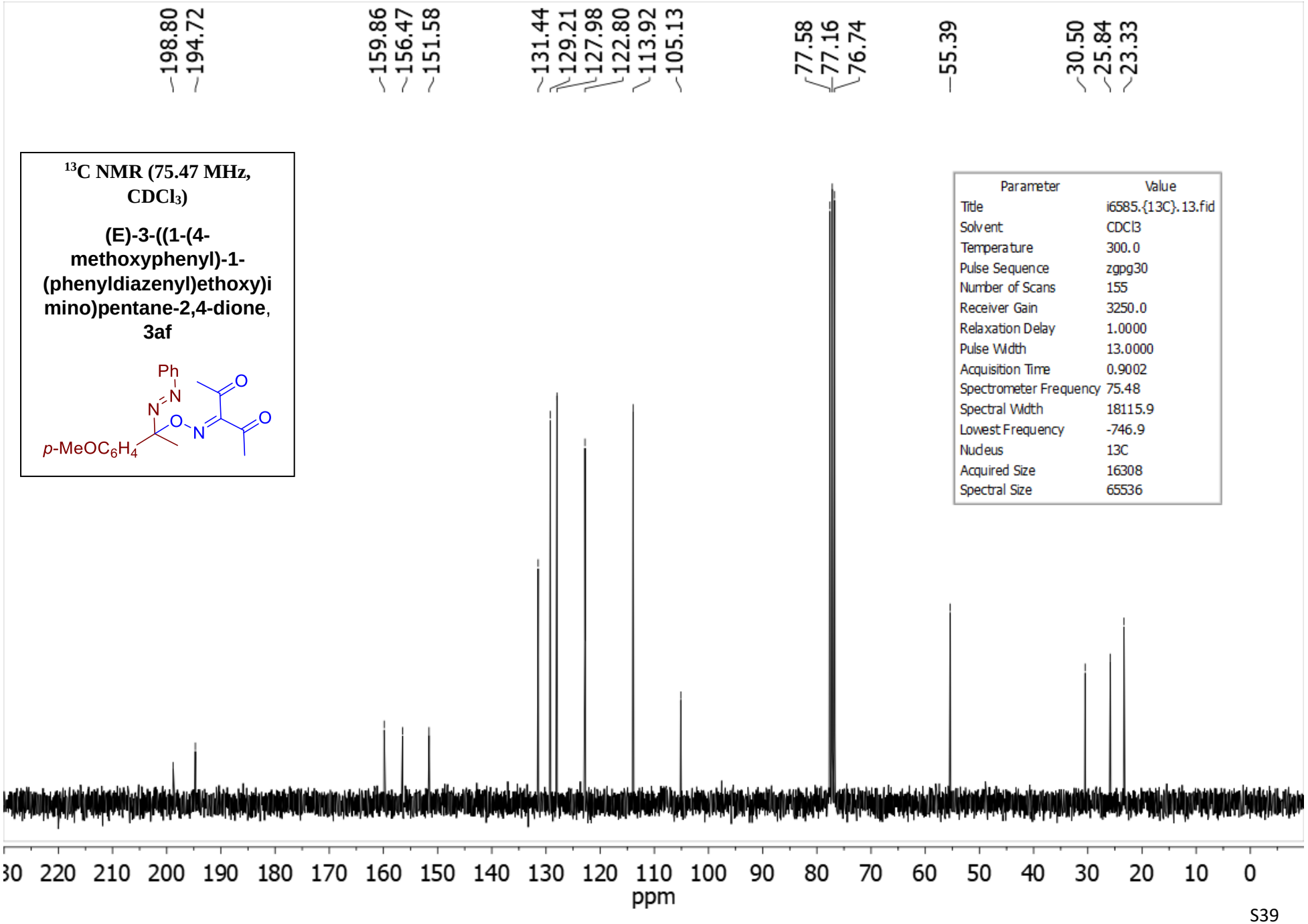
(E)-3-((1-(4-nitrophenyl)-1-(phenyldiazenyl)ethoxy)imino)pentane-2,4-dione, 3ae



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

(E)-3-((1-(4-methoxyphenyl)-1-(phenyldiazenyl)ethoxy)imino)pentane-2,4-dione, 3af

Parameter	Value
Title	i6585.{1H}.1.fid
Solvent	CDCl3
Temperature	300.1
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	-609.9
Nucleus	1H
Acquired Size	8124
Spectral Size	65536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194.72
159.86
156.47
151.58
131.44
129.21
127.98
122.80
113.92
105.13
77.58
77.16
76.74
55.39
30.50
25.84
23.33
^{13}C NMR (75.47 MHz, CDCl$_3$)
(E)-3-((1-(4-methoxyphenyl)-1-(phenyldiazenyl)ethoxy)imino)pentane-2,4-dione, 3af
Ph
N
N
O
N
O
O
p-MeOC$_6$H$_4$
Parameter Value
Title i6585.{13C}.13.fid
Solvent CDCl3
Temperature 300.0
Pulse Sequence zgpg30
Number of Scans 155
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Relaxation Delay 1.0000
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Spectrometer Frequency 75.48
Spectral Width 18115.9
Lowest Frequency -746.9
Nucleus 13C
Acquired Size 16308
Spectral Size 65536
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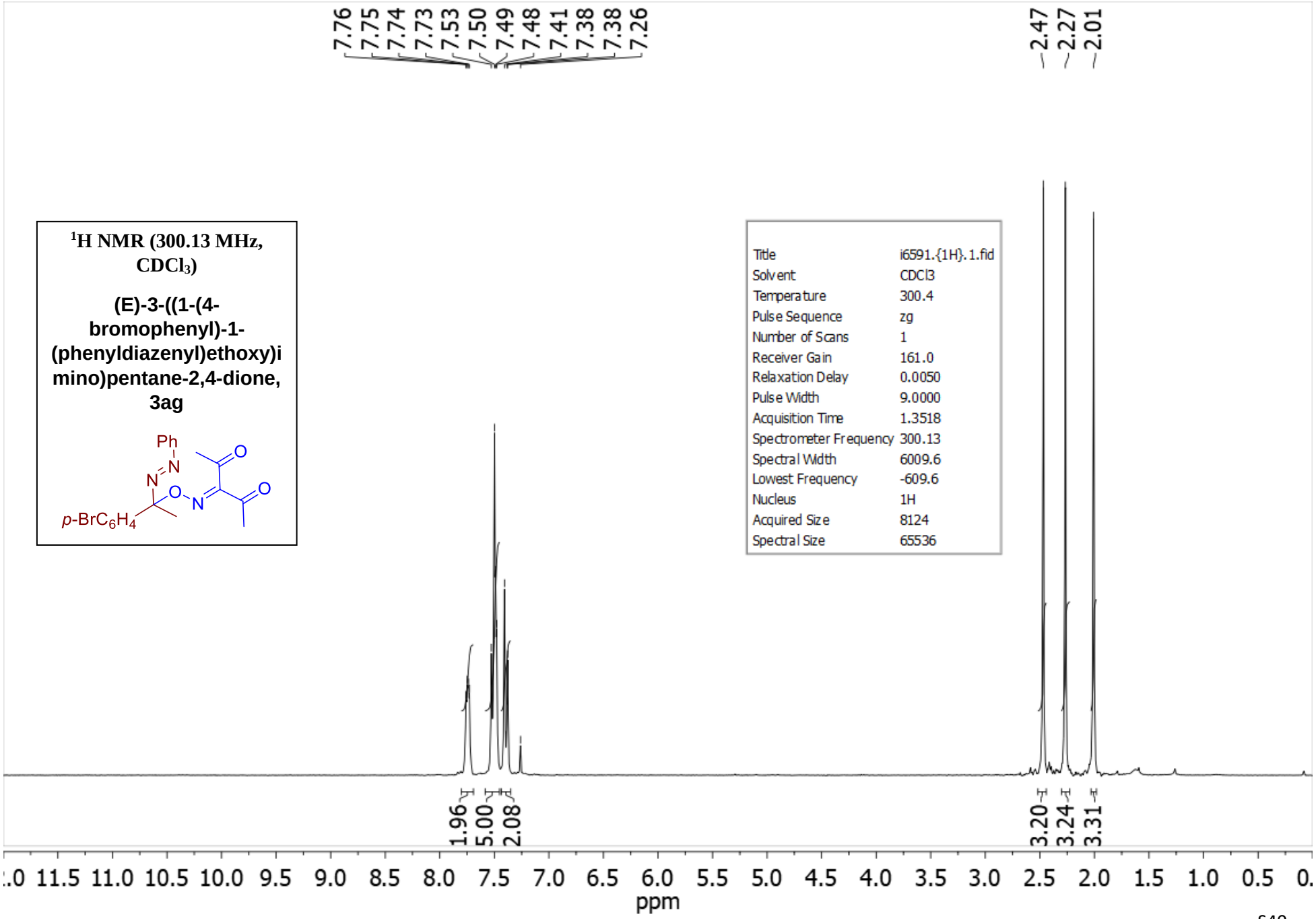
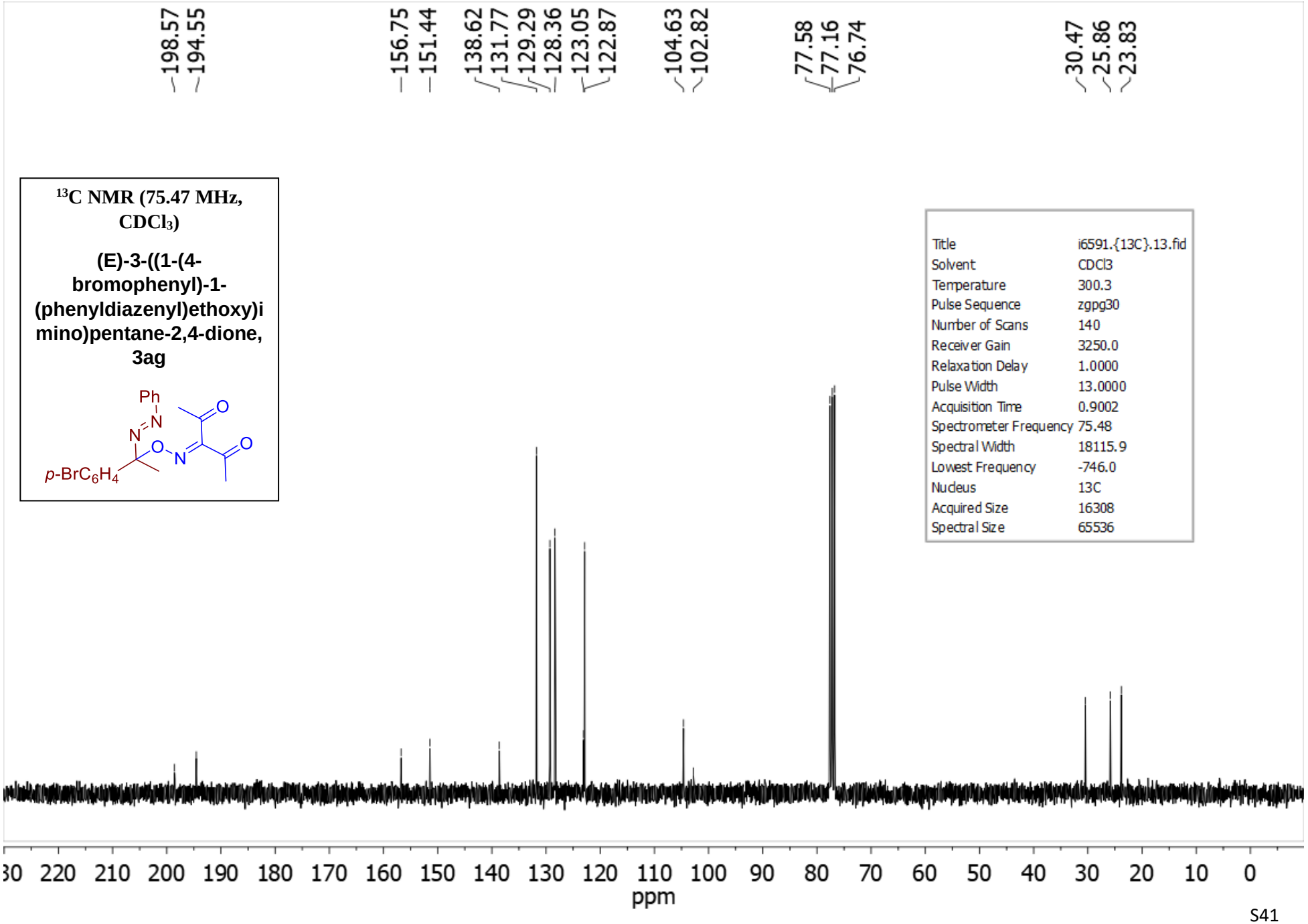
ppm



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

(E)-3-((1-(4-bromophenyl)-1-(phenyldiazenyl)ethoxy)imino)pentane-2,4-dione, 3ag

Title	i6591.{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	-609.6
Nucleus	1H
Acquired Size	8124
Spectral Size	65536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194.55
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151.44
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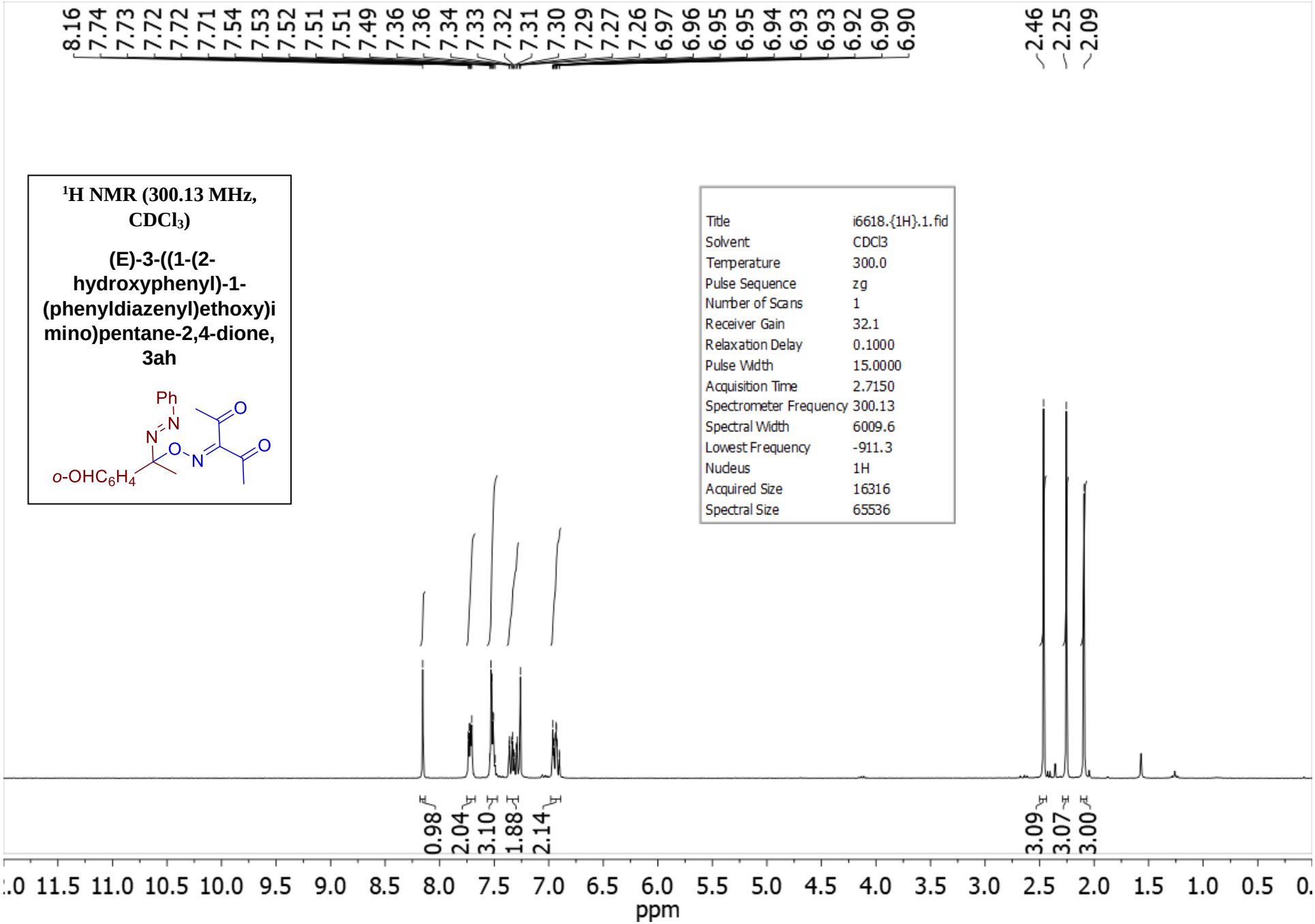
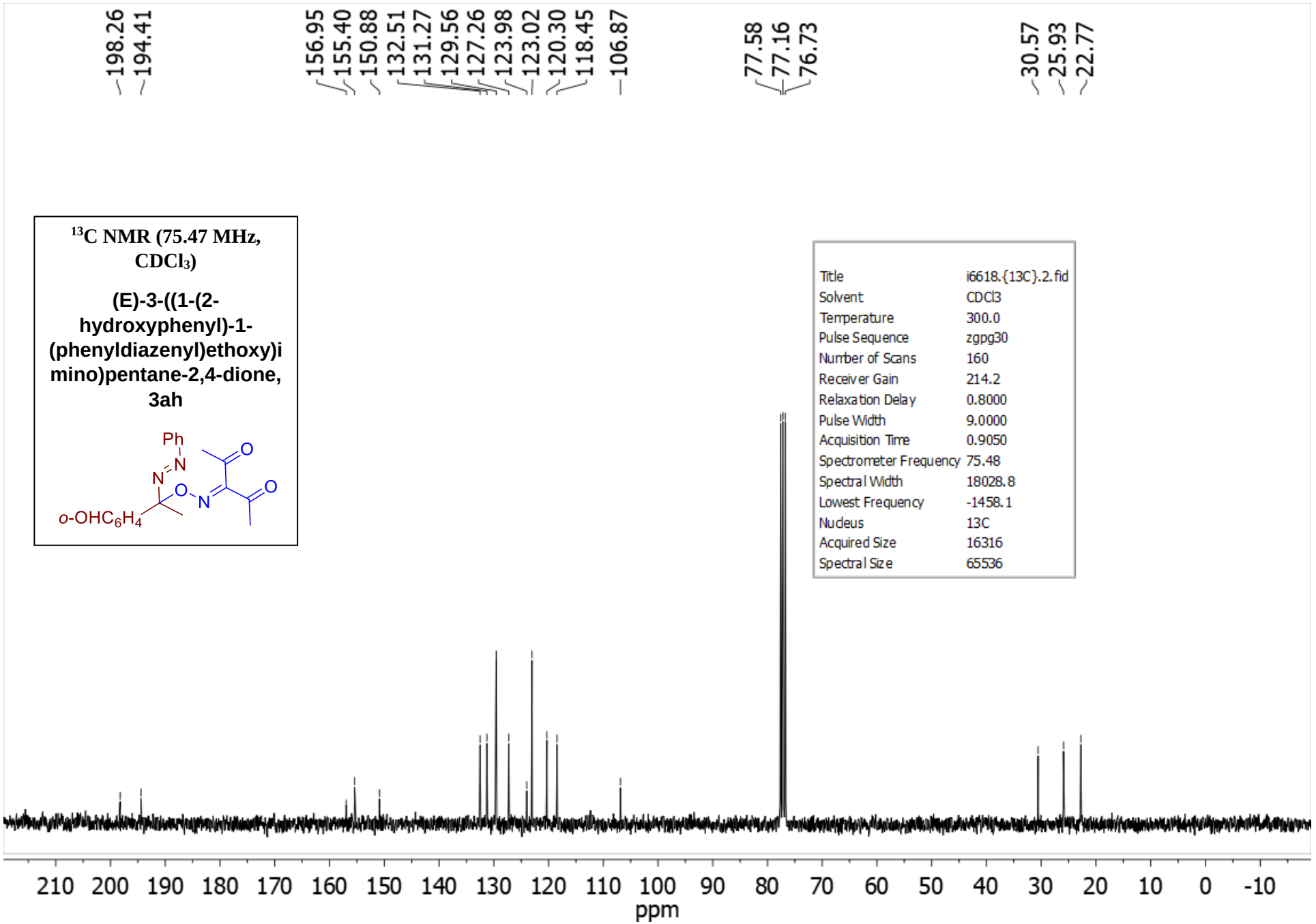
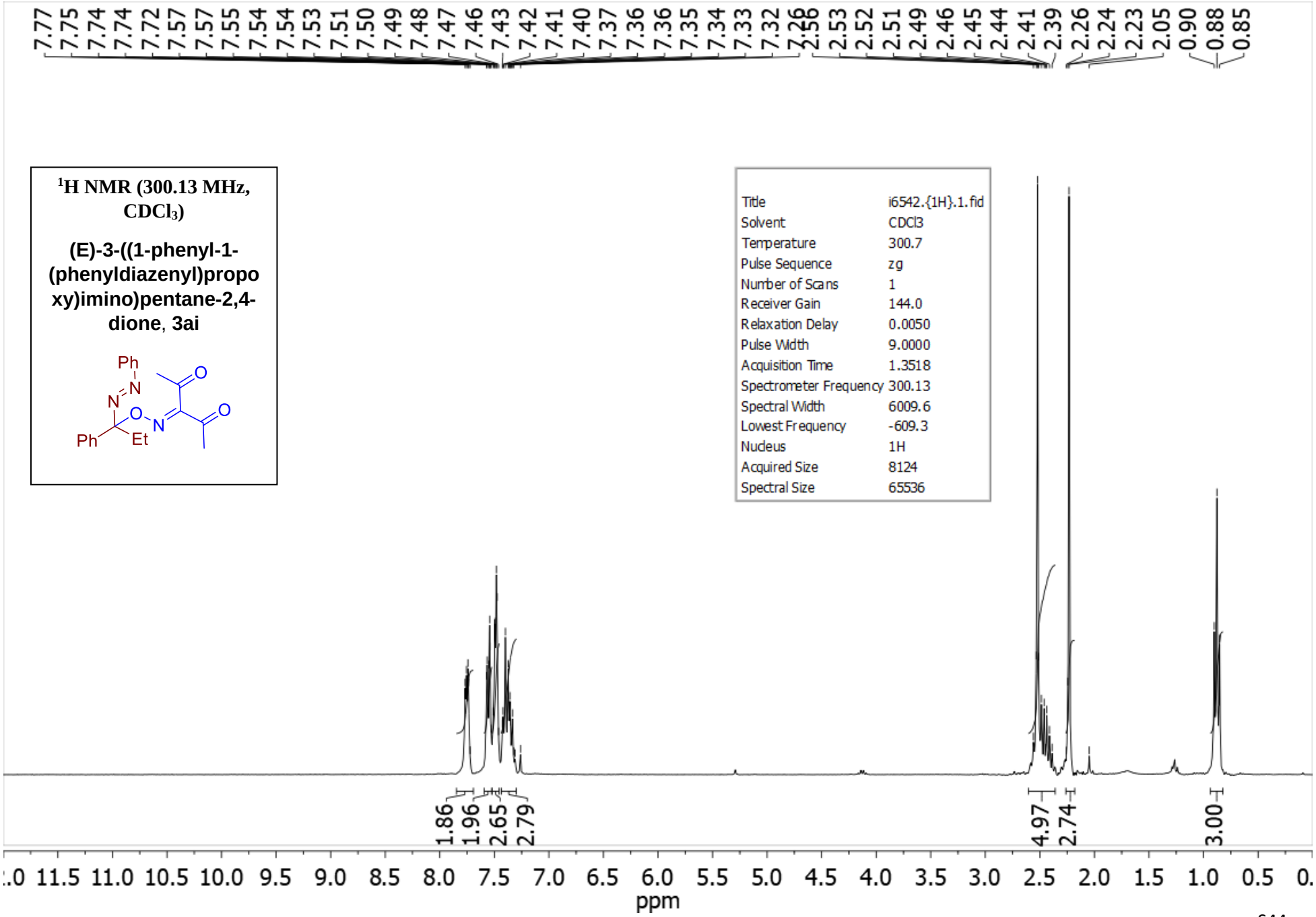
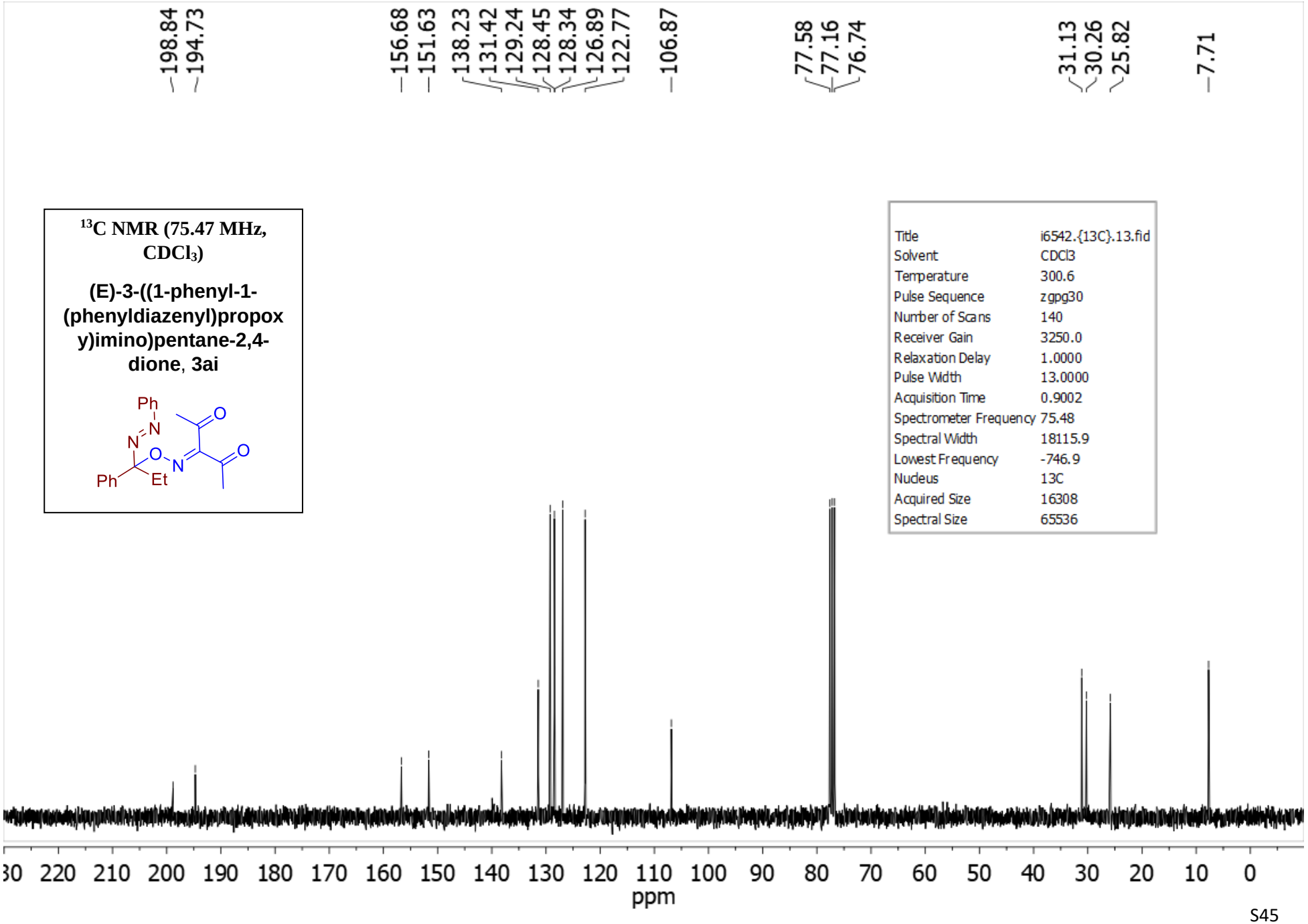
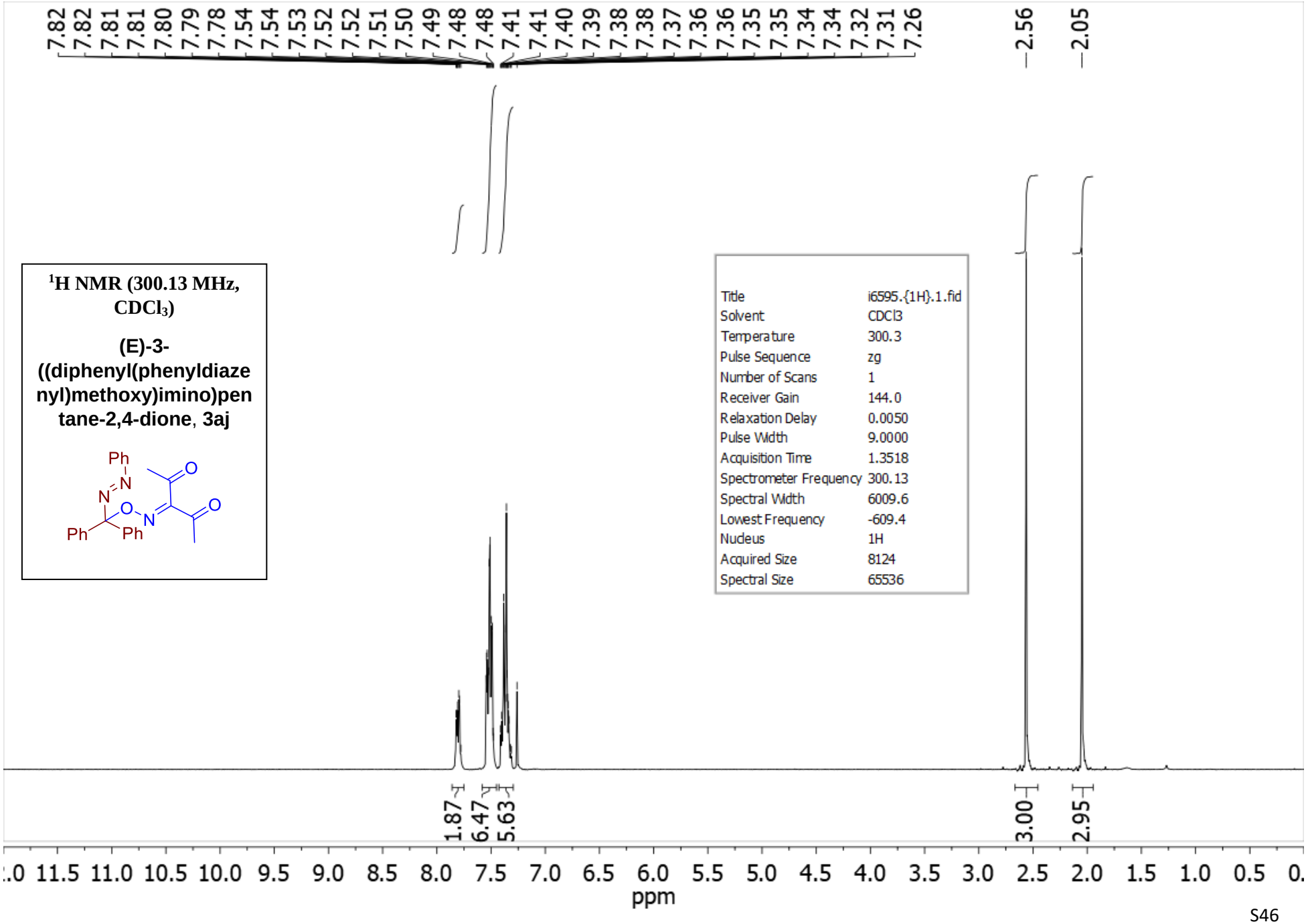
128.36
123.05
122.87
104.63
102.82
77.58
77.16
76.74
30.47
25.86
23.83
^{13}C NMR (75.47 MHz, $CDCl_3$)
(E)-3-((1-(4-bromophenyl)-1-(phenyldiazenyl)ethoxy)imino)pentane-2,4-dione, 3ag
Ph
N
N
O
N
O
O
p-BrC6H4
Title i6591.{13C}.13.fid
Solvent CDCl3
Temperature 300.3
Pulse Sequence zgpg30
Number of Scans 140
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 -746.0
Nucleus 13C
Acquired Size 16308
Spectral Size 65536
30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

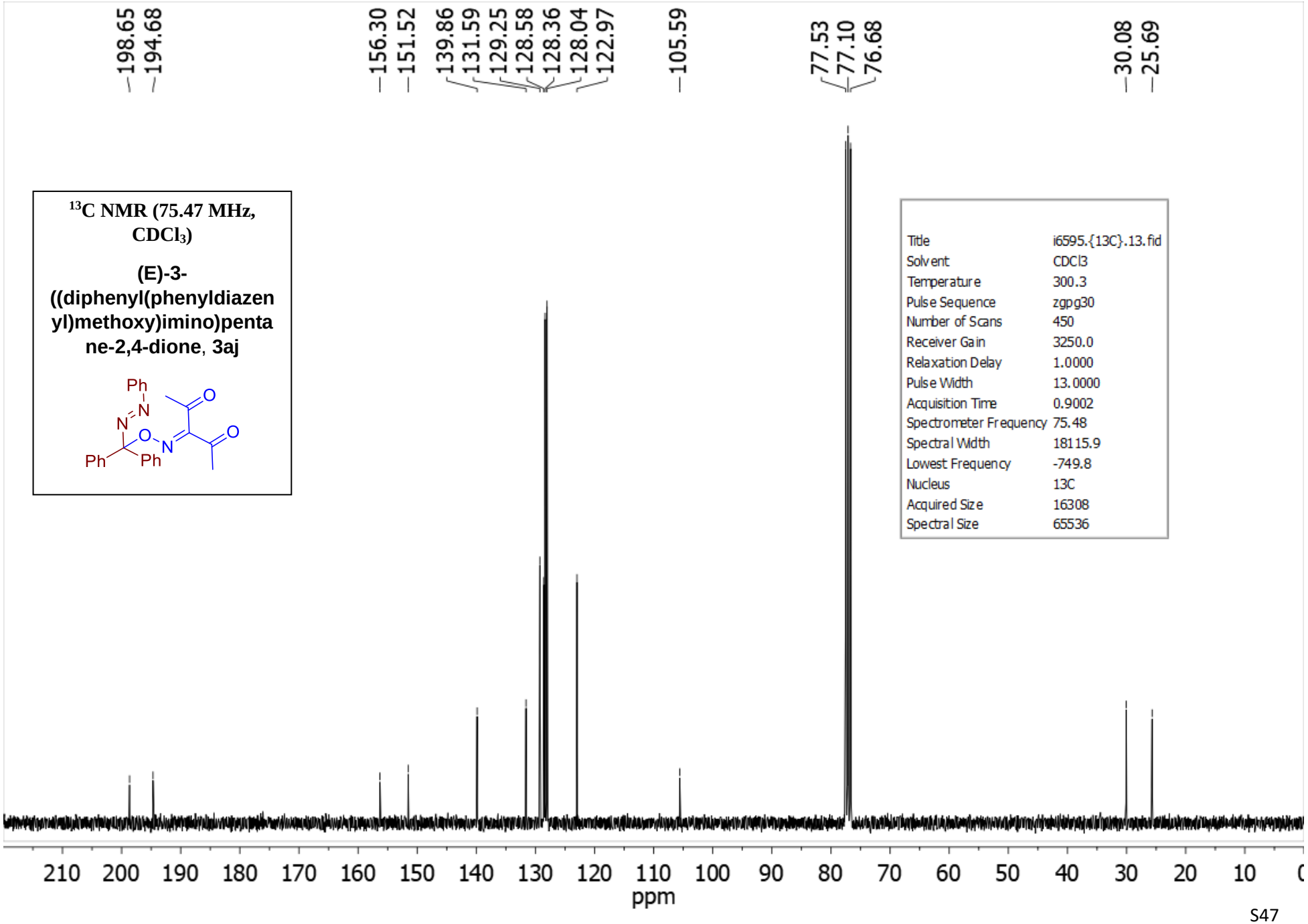

8.16
7.74
7.73
7.72
7.72
7.71
7.54
7.53
7.52
7.51
7.51
7.49
7.36
7.36
7.34
7.33
7.32
7.31
7.30
7.29
7.27
7.26
6.97
6.96
6.95
6.95
6.94
6.93
6.93
6.92
6.90
6.90
2.46
2.25
2.09
¹H NMR (300.13 MHz, CDCl₃)
(E)-3-((1-(2-hydroxyphenyl)-1-(phenyldiazenyl)ethoxy)imino)pentane-2,4-dione, 3ah
Ph
N
N
O
N
O
O
o-OHC6H4
Title i6618.{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 -911.3
Nucleus 1H
Acquired Size 16316
Spectral Size 65536
0.98
2.04
3.10
1.88
2.14
3.09
3.07
3.00
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

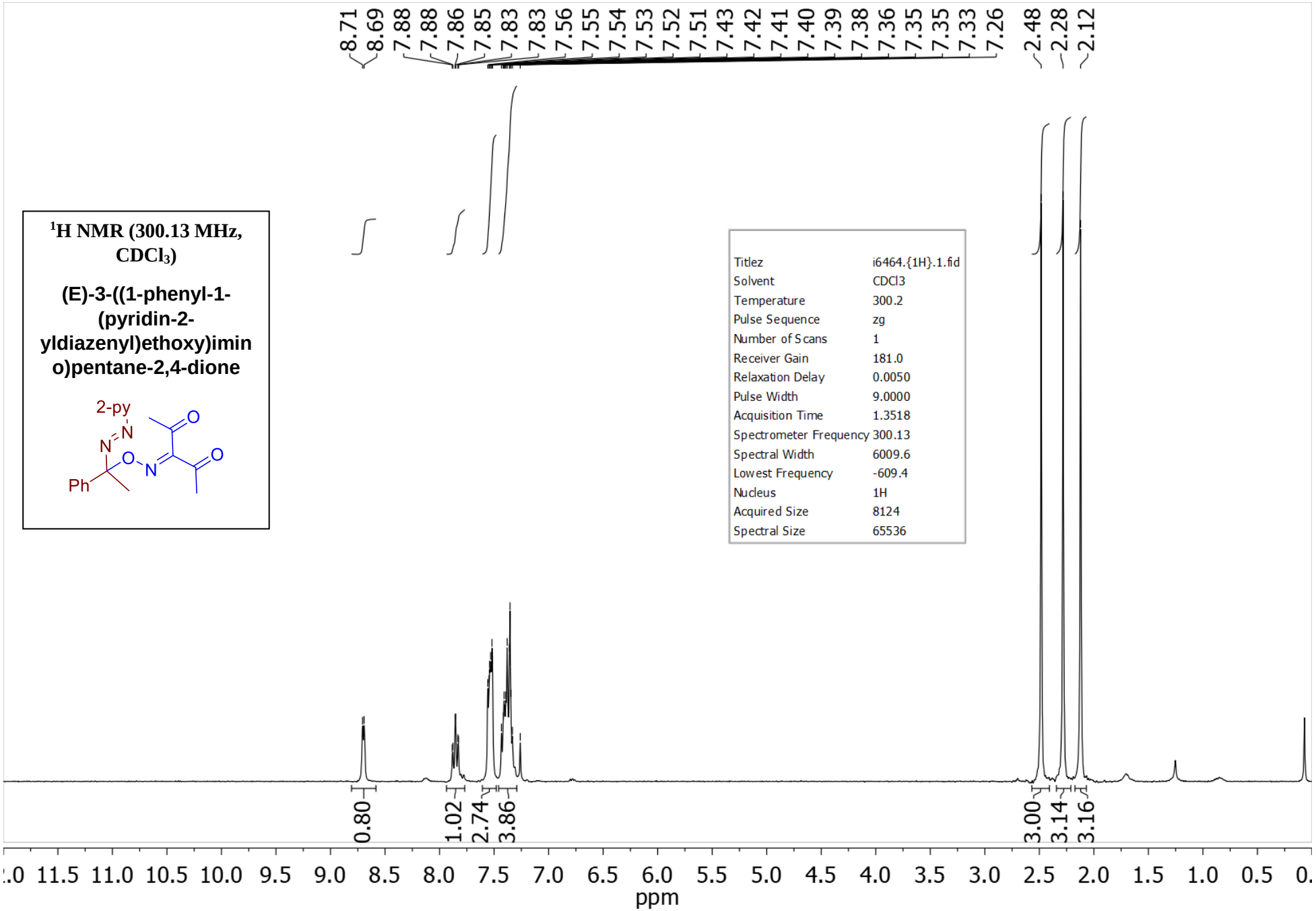

198.26
194.41
156.95
155.40
150.88
132.51
131.27
129.56
127.26
123.98
123.02
120.30
118.45
106.87
77.58
77.16
76.73
30.57
25.93
22.77
13C NMR (75.47 MHz, CDCl3)
(E)-3-((1-(2-hydroxyphenyl)-1-(phenyldiazenyl)ethoxy)imino)pentane-2,4-dione, 3ah
Ph
N
N
O
N
O
O
o-OHC6H4
Title i6618.{13C}.2.fid
Solvent CDCl3
Temperature 300.0
Pulse Sequence zgpg30
Number of Scans 160
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 -1458.1
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 0 -10
ppm


7.77 7.75 7.74 7.74 7.72 7.57 7.57 7.55 7.54 7.54 7.53 7.51 7.50 7.49 7.48 7.47 7.46 7.43 7.42 7.41 7.40 7.37 7.36 7.36 7.35 7.34 7.33 7.32 7.26 2.58 2.53 2.52 2.51 2.49 2.46 2.45 2.44 2.41 2.39 2.26 2.24 2.23 2.05 0.90 0.88 0.85
1H NMR (300.13 MHz, CDCl3)
(E)-3-((1-phenyl-1-(phenyldiazenyl)propoxy)imino)pentane-2,4-dione, 3ai
Ph
N
N
O
N
O
O
Ph
Et
Title i6542.{1H}.1.fid
Solvent CDCl3
Temperature 300.7
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 -609.3
Nucleus 1H
Acquired Size 8124
Spectral Size 65536
1.86 1.96 2.65 2.79 4.97 2.74 3.00
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


198.84
194.73
156.68
151.63
138.23
131.42
129.24
128.45
128.34
126.89
122.77
106.87
77.58
77.16
76.74
31.13
30.26
25.82
7.71
^{13}C NMR (75.47 MHz, $CDCl_3$)
(E)-3-((1-phenyl-1-(phenyldiazenyl)propoxy)imino)pentane-2,4-dione, 3ai
Ph
N
N
O
N
O
O
Ph
Et
Title i6542.{13C}.13.fid
Solvent CDCl3
Temperature 300.6
Pulse Sequence zgpg30
Number of Scans 140
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 -746.9
Nucleus 13C
Acquired Size 16308
Spectral Size 65536
30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


7.82 7.82 7.81 7.81 7.80 7.79 7.78 7.54 7.54 7.53 7.52 7.52 7.51 7.50 7.49 7.48 7.48 7.41 7.41 7.40 7.39 7.38 7.38 7.37 7.36 7.36 7.35 7.35 7.34 7.34 7.32 7.31 7.26
2.56
2.05
1H NMR (300.13 MHz, CDCl3)
(E)-3-((diphenyl(phenyldiazenyl)methoxy)imino)pentane-2,4-dione, 3aj
Ph
N
N
O
N
O
O
Ph
Ph
Title i6595.{1H}.1.fid
Solvent CDCl3
Temperature 300.3
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 -609.4
Nucleus 1H
Acquired Size 8124
Spectral Size 65536
1.87
6.47
5.63
3.00
2.95
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

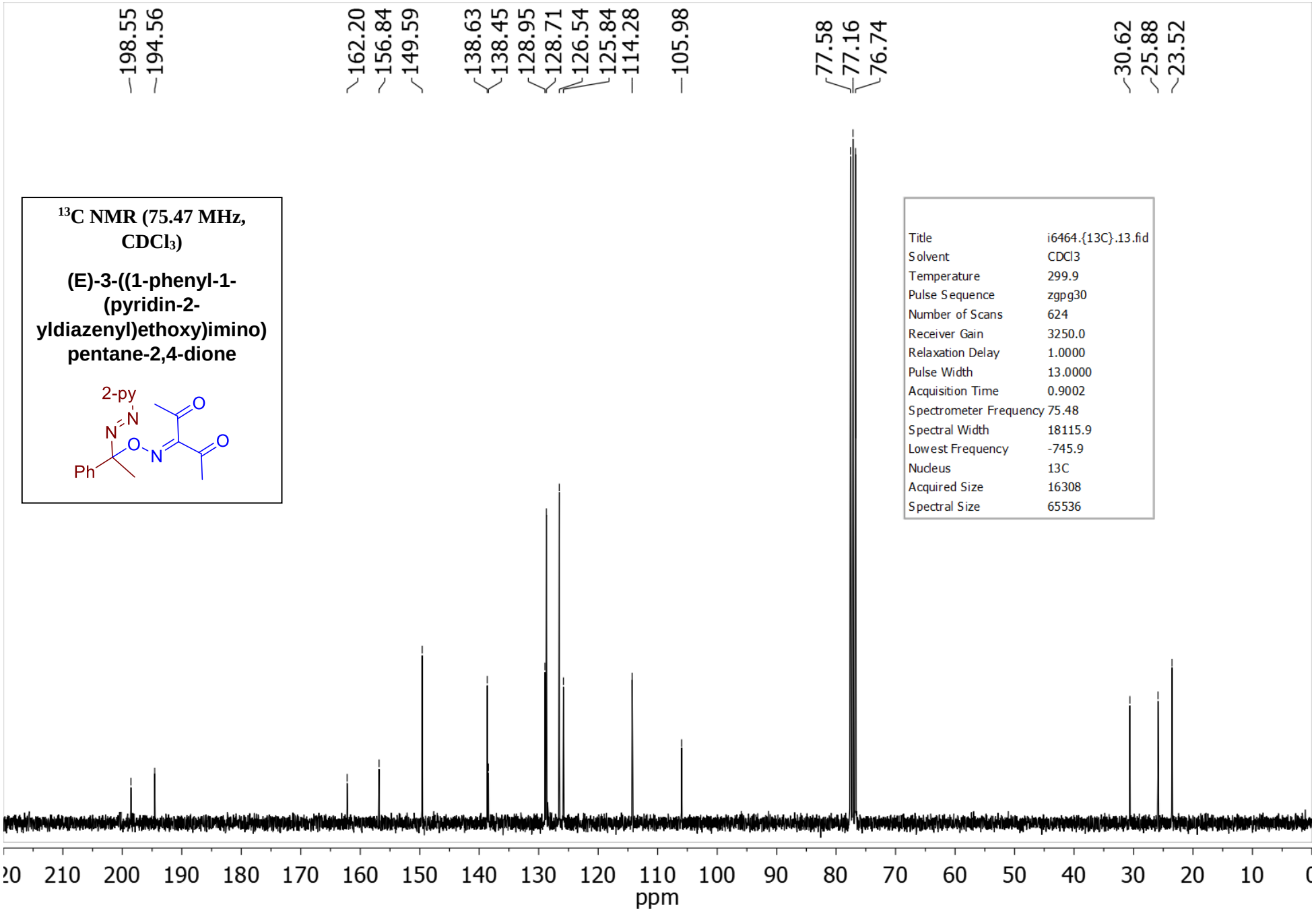

198.65
194.68
156.30
151.52
139.86
131.59
129.25
128.58
128.36
128.04
122.97
105.59
77.53
77.10
76.68
30.08
25.69
13C NMR (75.47 MHz, CDCl3)
(E)-3-((diphenyl(phenyldiazenyl)methoxy)imino)pentane-2,4-dione, 3aj
Ph
N
N
O
N
O
O
Ph
Ph
Title i6595.{13C}.13.fid
Solvent CDCl3
Temperature 300.3
Pulse Sequence zgpg30
Number of Scans 450
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 -749.8
Nucleus 13C
Acquired Size 16308
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

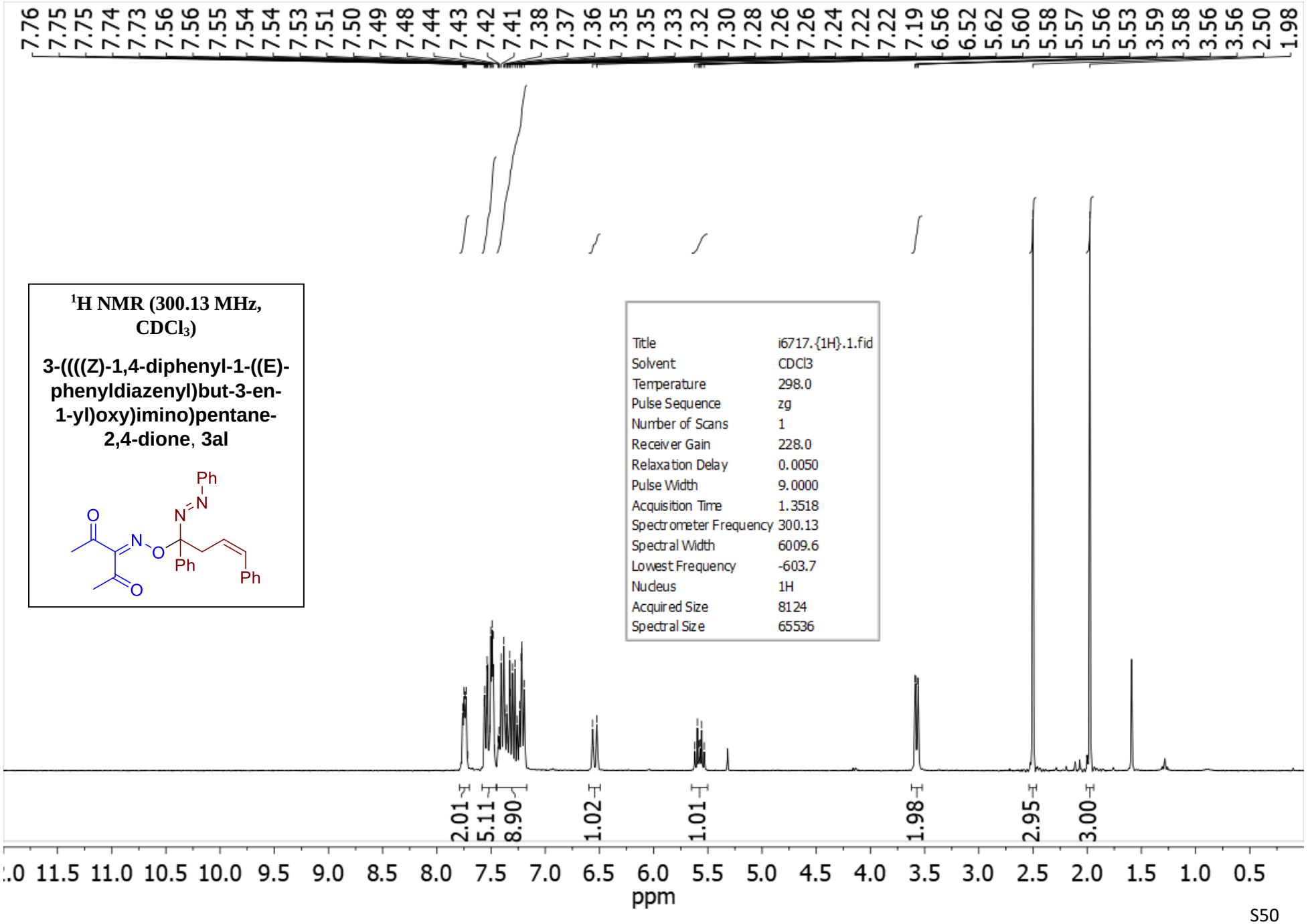


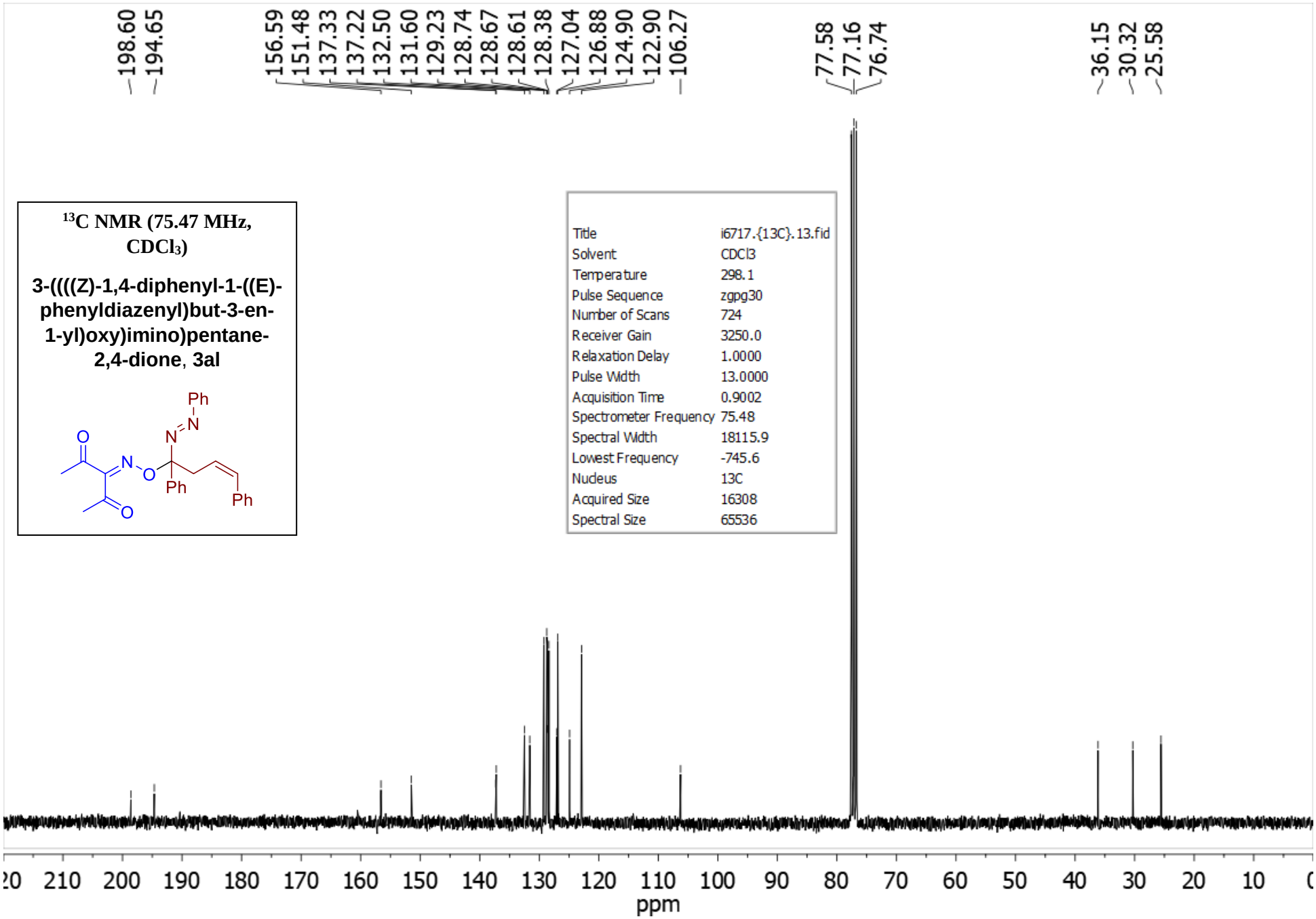
^{1}H NMR (300.13 MHz, $CDCl_3$)

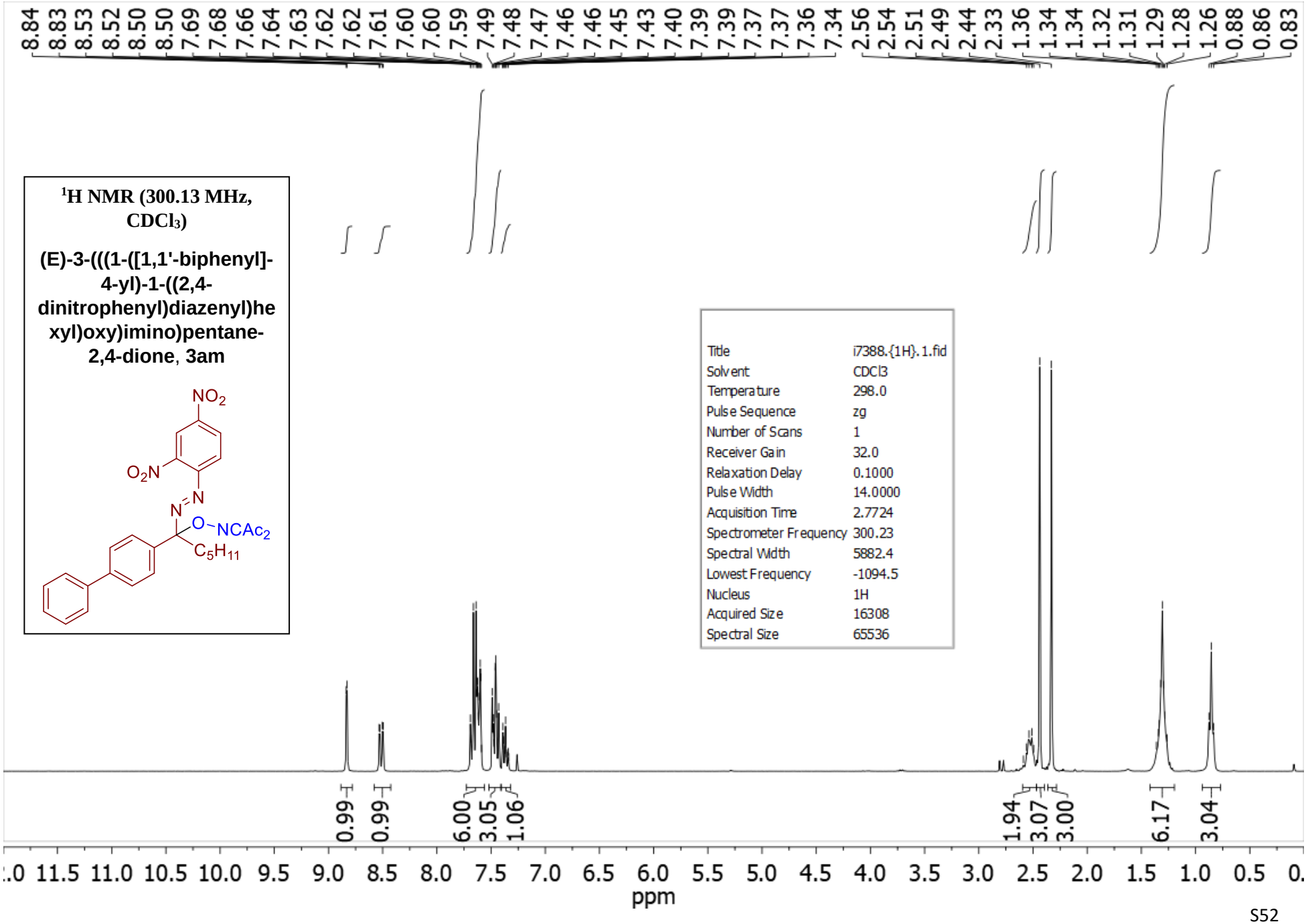
(E)-3-((1-phenyl-1-(pyridin-2-yldiazenyl)ethoxy)imino)pentane-2,4-dione

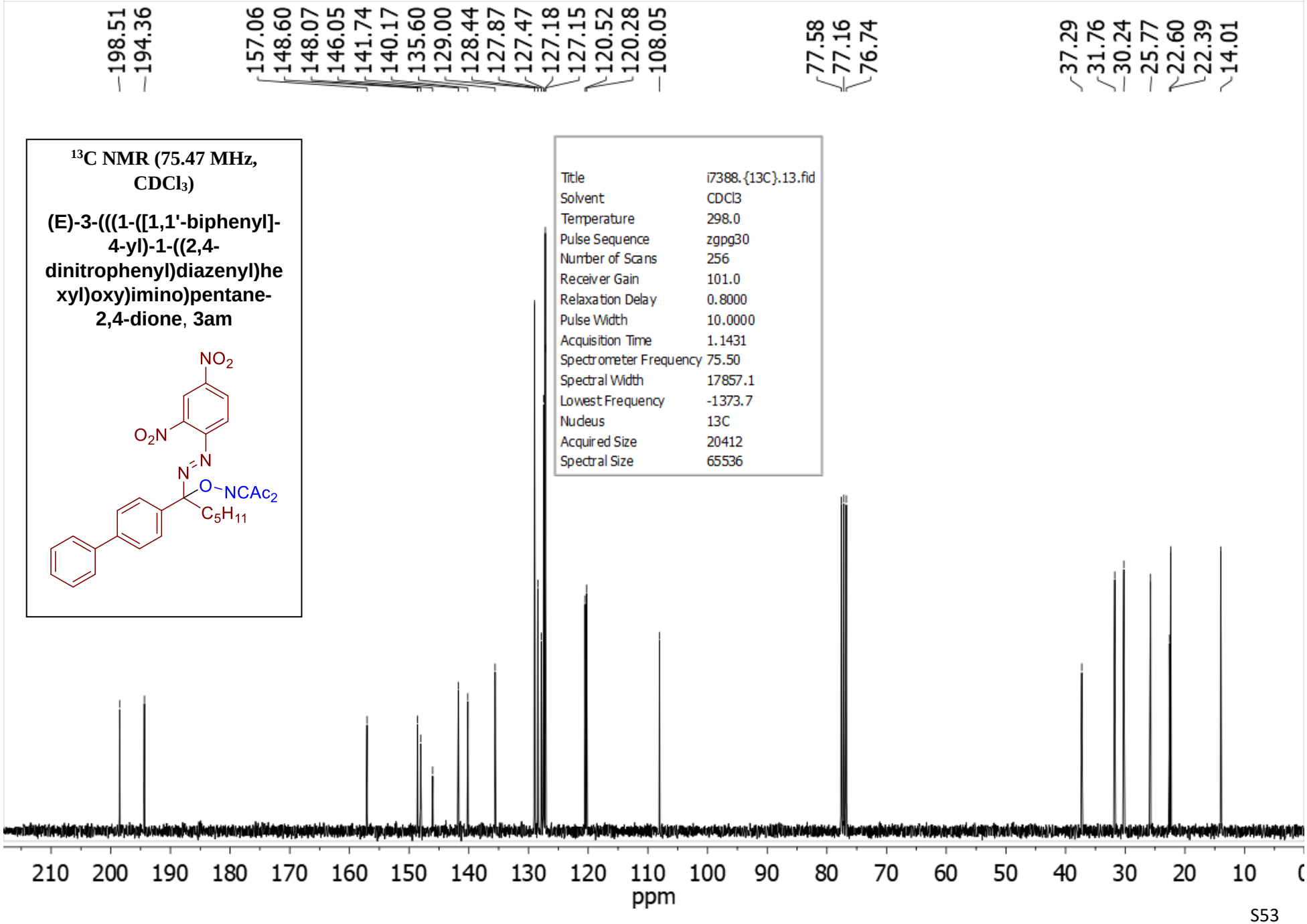
Titlez	i6464.{1H}.1.fid
Solvent	CDCl3
Temperature	300.2
Pulse Sequence	zg
Number of Scans	1
Receiver Gain	181.0
Relaxation Delay	0.0050
Pulse Width	9.0000
Acquisition Time	1.3518
Spectrometer Frequency	300.13
Spectral Width	6009.6
Lowest Frequency	-609.4
Nucleus	1H
Acquired Size	8124
Spectral Size	65536


198.55
194.56
162.20
156.84
149.59
138.63
138.45
128.95
128.71
126.54
125.84
114.28
105.98
77.58
77.16
76.74
30.62
25.88
23.52
^{13}C NMR (75.47 MHz, $CDCl_3$)
(E)-3-((1-phenyl-1-(pyridin-2-yldiazenyl)ethoxy)imino)pentane-2,4-dione
2-py
N
N
O
N
O
O
Ph
Title i6464.{13C}.13.fid
Solvent CDCl3
Temperature 299.9
Pulse Sequence zgpg30
Number of Scans 624
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 -745.9
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


7.76 7.75 7.75 7.74 7.73 7.56 7.56 7.55 7.54 7.54 7.53 7.51 7.50 7.49 7.48 7.44 7.43 7.42 7.41 7.38 7.37 7.36 7.35 7.35 7.33 7.32 7.30 7.28 7.26 7.26 7.24 7.22 7.22 7.19 6.56 6.52 5.62 5.60 5.58 5.57 5.56 5.53 3.59 3.58 3.56 3.56 2.50 1.98
1H NMR (300.13 MHz, CDCl3)
3-((((Z)-1,4-diphenyl-1-((E)-phenyldiazenyl)but-3-en-1-yl)oxy)imino)pentane-2,4-dione, 3al
Ph
N
N
O
N
O
O
Ph
Ph
Title i6717.{1H}.1.fid
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 228.0
Relaxation Delay 0.0050
Pulse Width 9.0000
Acquisition Time 1.3518
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -603.7
Nucleus 1H
Acquired Size 8124
Spectral Size 65536
2.01
5.11
8.90
1.02
1.01
1.98
2.95
3.00
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

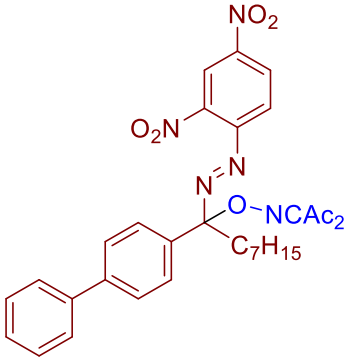

198.60
194.65
156.59
151.48
137.33
137.22
132.50
131.60
129.23
128.74
128.67
128.61
128.38
127.04
126.88
124.90
122.90
106.27
77.58
77.16
76.74
36.15
30.32
25.58
^{13}C NMR (75.47 MHz, CDCl$_3$)
3-((((Z)-1,4-diphenyl-1-((E)-phenyldiazenyl)but-3-en-1-yl)oxy)imino)pentane-2,4-dione, 3al
Ph
N
N
O
N
O
Ph
Ph
O
Title i6717.{13C}.13.fid
Solvent CDCl3
Temperature 298.1
Pulse Sequence zgpg30
Number of Scans 724
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 -745.6
Nucleus 13C
Acquired Size 16308
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

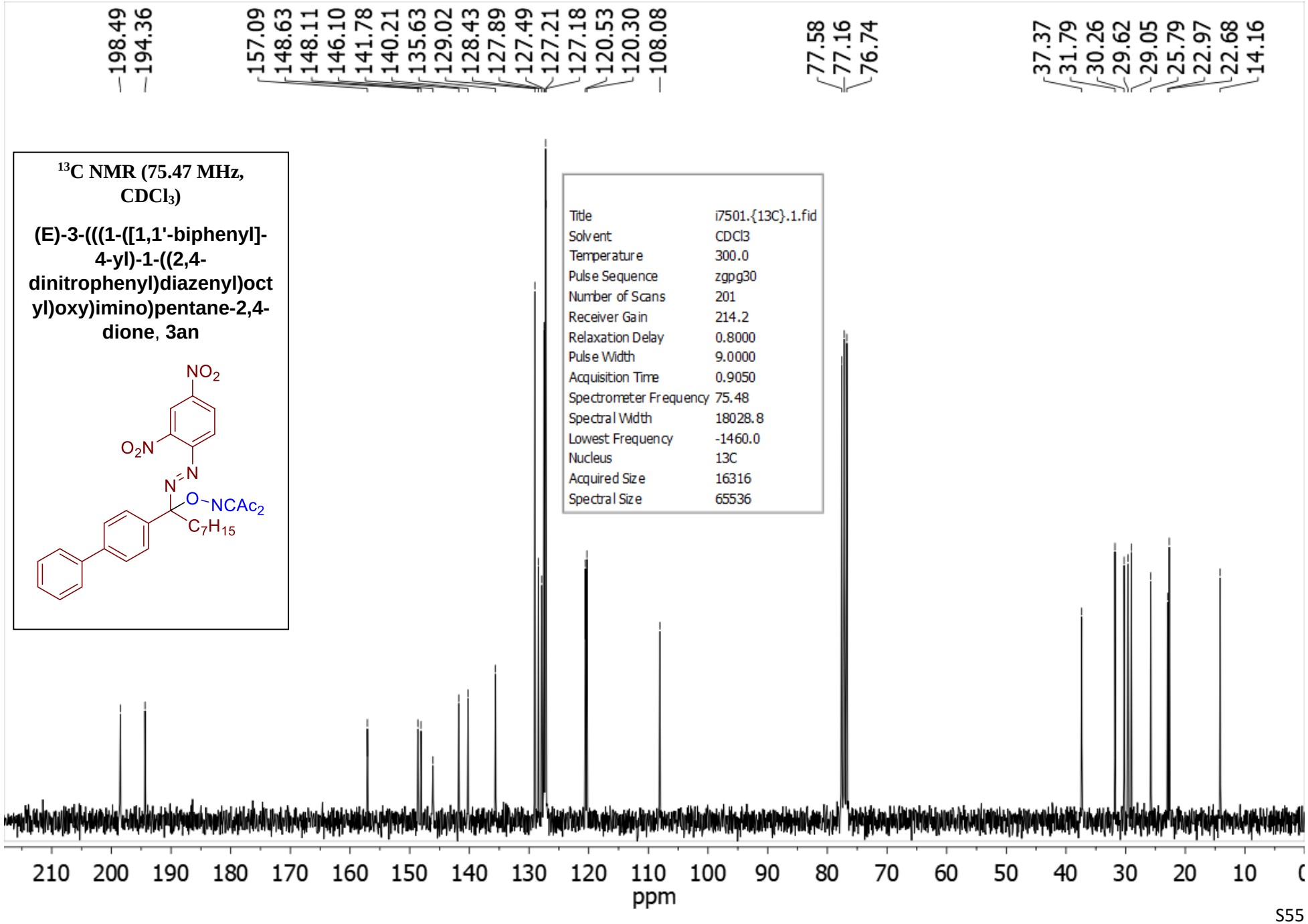

8.84 8.83 8.53 8.52 8.50 8.50 7.69 7.68 7.66 7.64 7.63 7.62 7.62 7.61 7.60 7.60 7.59 7.49 7.48 7.47 7.46 7.46 7.45 7.43 7.40 7.39 7.39 7.37 7.37 7.36 7.34
2.56 2.54 2.51 2.49 2.44 2.33 1.36 1.34 1.34 1.32 1.31 1.29 1.28 1.26 0.88 0.86 0.83
¹H NMR (300.13 MHz, CDCl₃)
(E)-3-(((1-([1,1'-biphenyl]-4-yl)-1-((2,4-dinitrophenyl)diazenyl)hexyl)oxy)imino)pentane-2,4-dione, 3am
NO2
O2N
N
N
O
NCAc2
C5H11
Title i7388.{1H}.1.fid
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32.0
Relaxation Delay 0.1000
Pulse Width 14.0000
Acquisition Time 2.7724
Spectrometer Frequency 300.23
Spectral Width 5882.4
Lowest Frequency -1094.5
Nucleus 1H
Acquired Size 16308
Spectral Size 65536
0.99 0.99 6.00 3.05 1.06 1.94 3.07 3.00 6.17 3.04
ppm

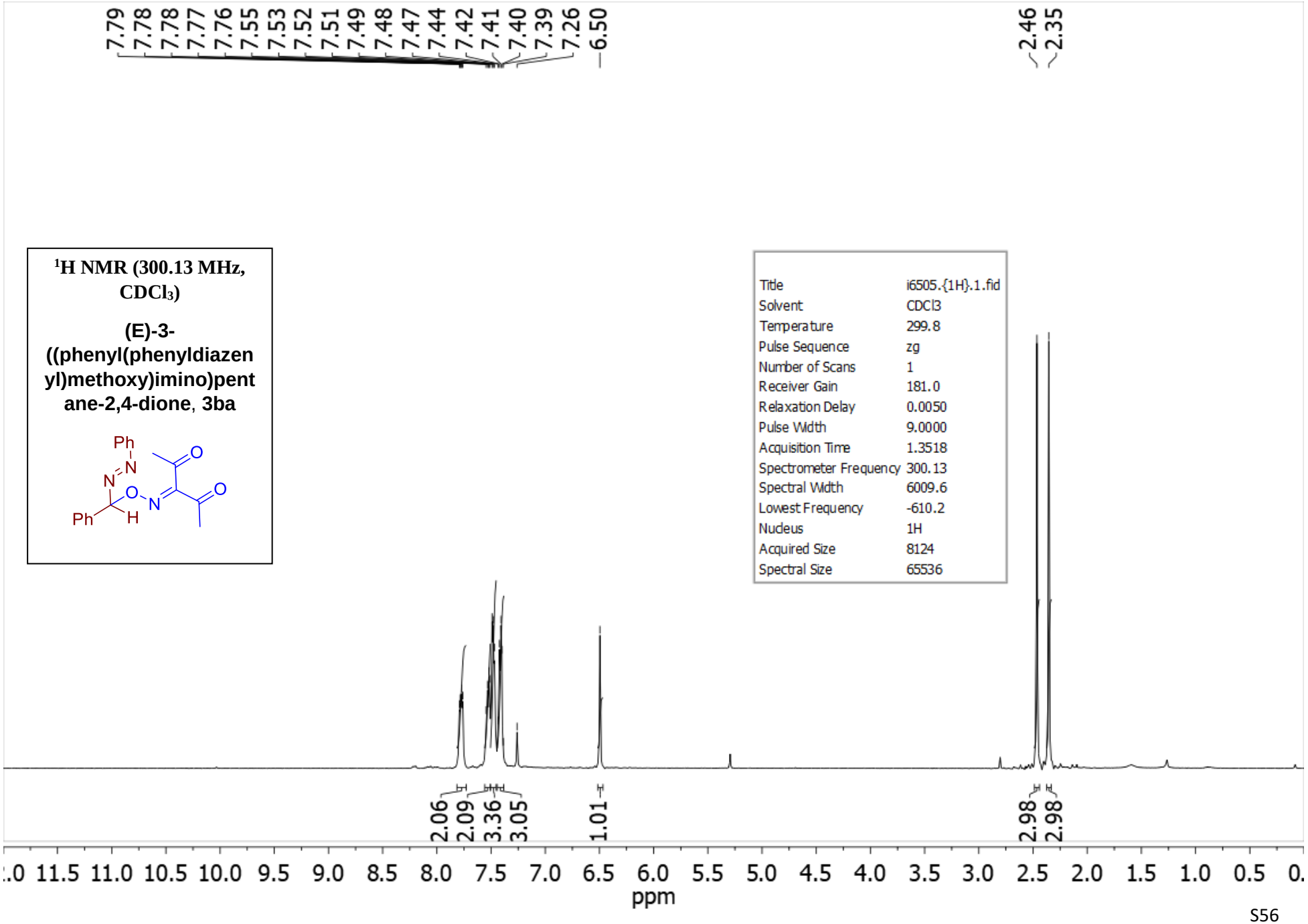

198.51
194.36
157.06
148.60
148.07
146.05
141.74
140.17
135.60
129.00
128.44
127.87
127.47
127.18
127.15
120.52
120.28
108.05
77.58
77.16
76.74
37.29
31.76
30.24
25.77
22.60
22.39
14.01
^{13}C NMR (75.47 MHz, $CDCl_3$)
(E)-3-(((1-([1,1'-biphenyl]-4-yl)-1-((2,4-dinitrophenyl)diazenyl)hexyl)oxy)imino)pentane-2,4-dione, 3am
NO_2
O_2N
N
N
O
$NCAc_2$
C_5H_{11}
Title i7388.{13C}.13.fid
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 256
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 -1373.7
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
ppm

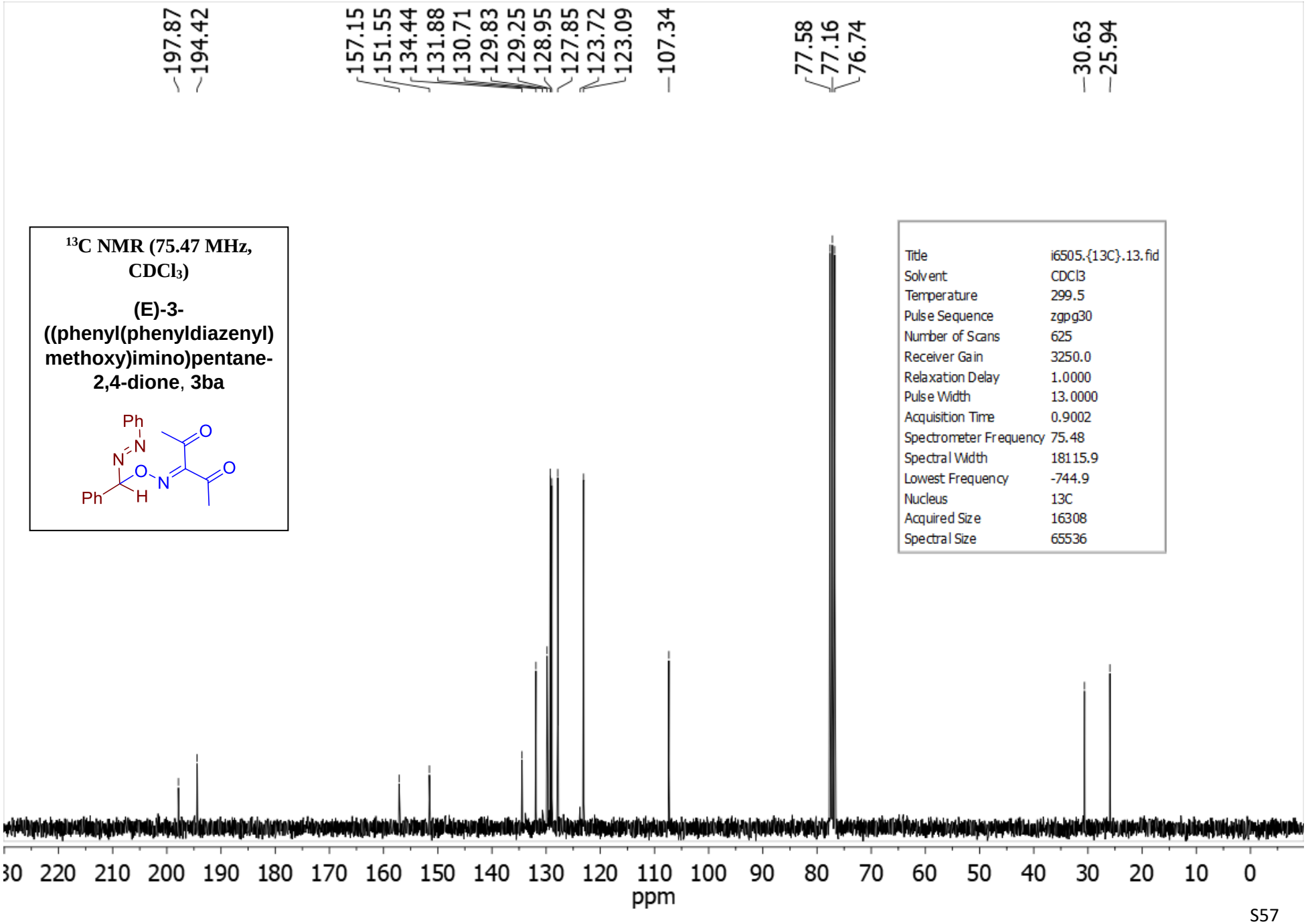
^{1}H NMR (300.13 MHz, $CDCl_3$)

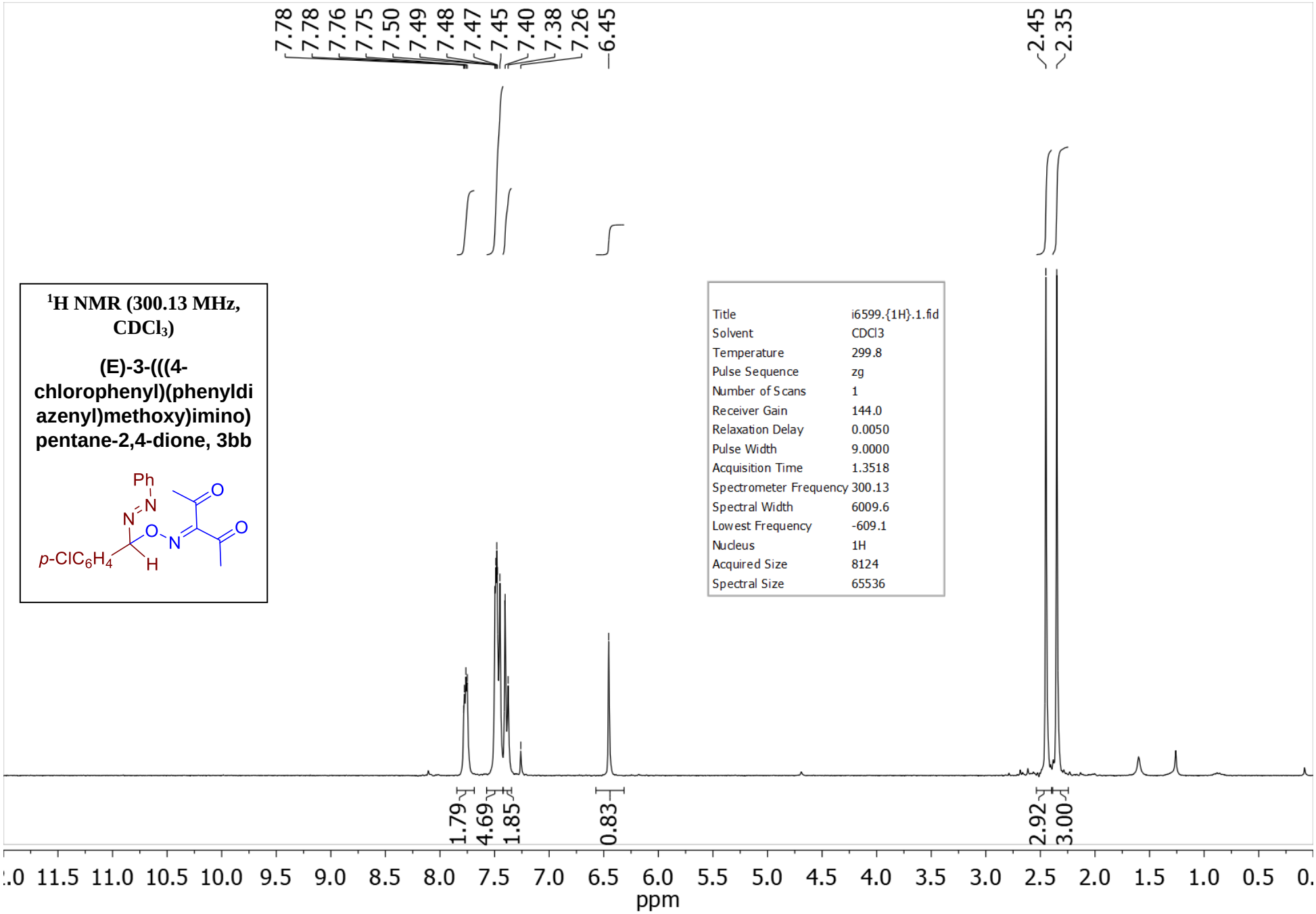
(E)-3-(((1-([1,1'-biphenyl]-4-yl)-1-((2,4-dinitrophenyl)diazenyl)octyl)oxy)imino)pentane-2,4-dione, 3an

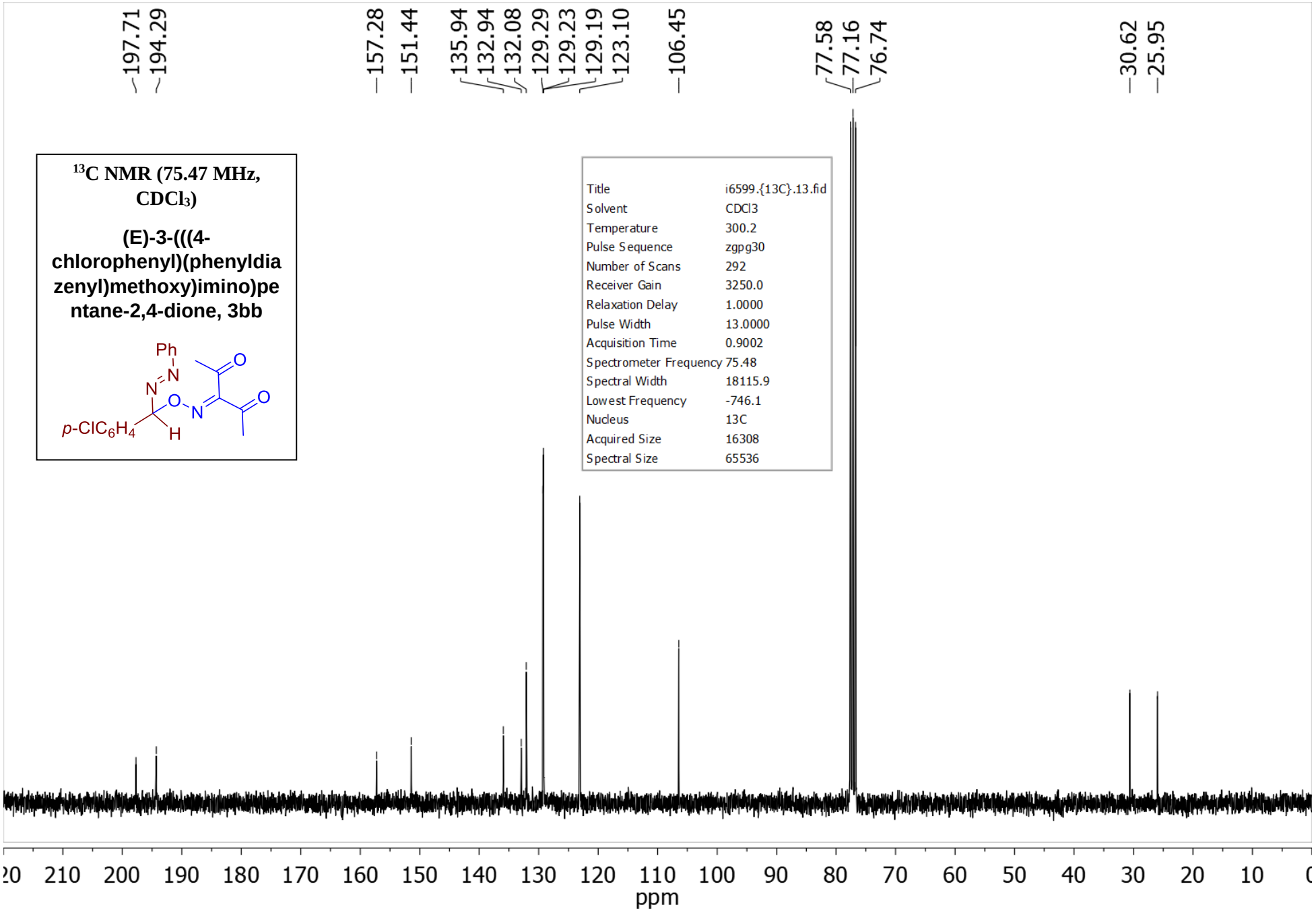


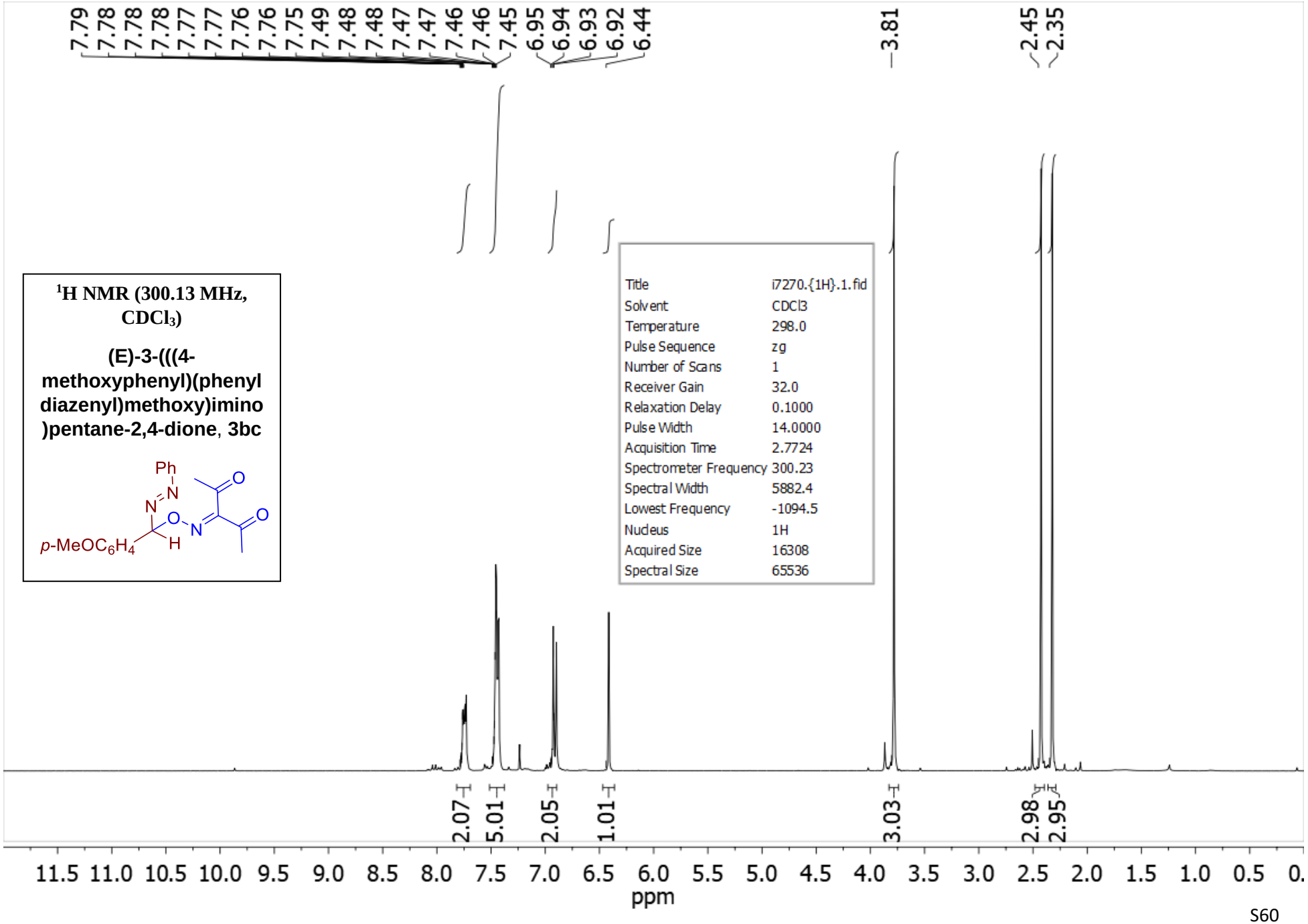

198.49
194.36
157.09
148.63
148.11
146.10
141.78
140.21
135.63
129.02
128.43
127.89
127.49
127.21
127.18
120.53
120.30
108.08
77.58
77.16
76.74
37.37
31.79
30.26
29.62
29.05
25.79
22.97
22.68
14.16
^{13}C NMR (75.47 MHz, $CDCl_3$)
(E)-3-(((1-([1,1'-biphenyl]-4-yl)-1-((2,4-dinitrophenyl)diazenyl)octyl)oxy)imino)pentane-2,4-dione, 3an
NO_2
O_2N
N
N
O
$NCAc_2$
C_7H_{15}
Title i7501.{13C}.1.fid
Solvent CDCl3
Temperature 300.0
Pulse Sequence zgpg30
Number of Scans 201
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 -1460.0
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

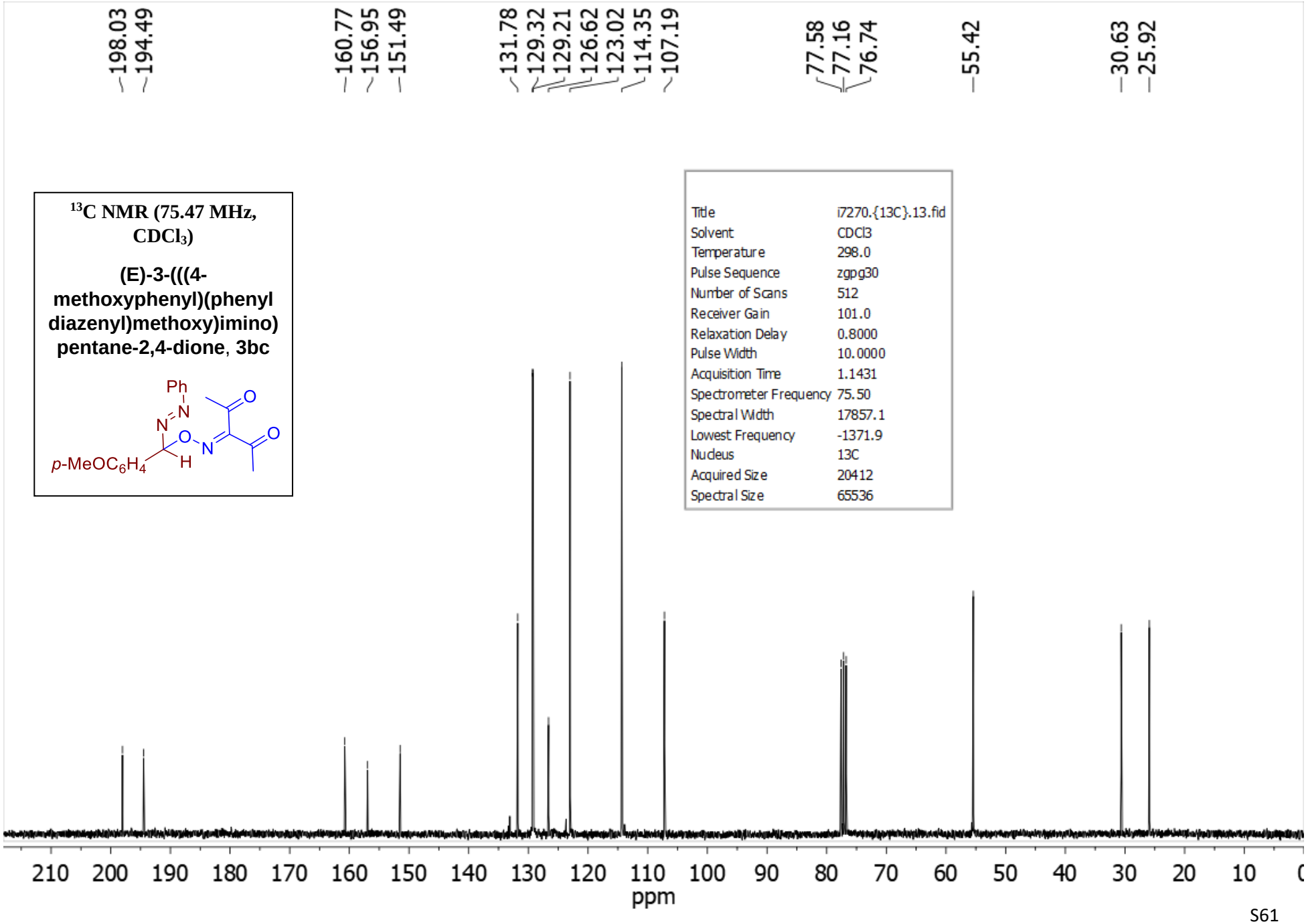

7.79
7.78
7.78
7.77
7.76
7.55
7.53
7.52
7.51
7.49
7.48
7.47
7.44
7.42
7.41
7.40
7.39
7.26
6.50
2.46
2.35
¹H NMR (300.13 MHz, CDCl₃)
(E)-3-((phenyl(phenyldiazenyl)methoxy)imino)pentane-2,4-dione, 3ba
Ph
N
N
O
N
O
O
Ph
H
Title i6505.{1H}.1.fid
Solvent CDCl3
Temperature 299.8
Pulse Sequence zg
Number of Scans 1
Receiver Gain 181.0
Relaxation Delay 0.0050
Pulse Width 9.0000
Acquisition Time 1.3518
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -610.2
Nucleus 1H
Acquired Size 8124
Spectral Size 65536
2.06
2.09
3.36
3.05
1.01
2.98
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

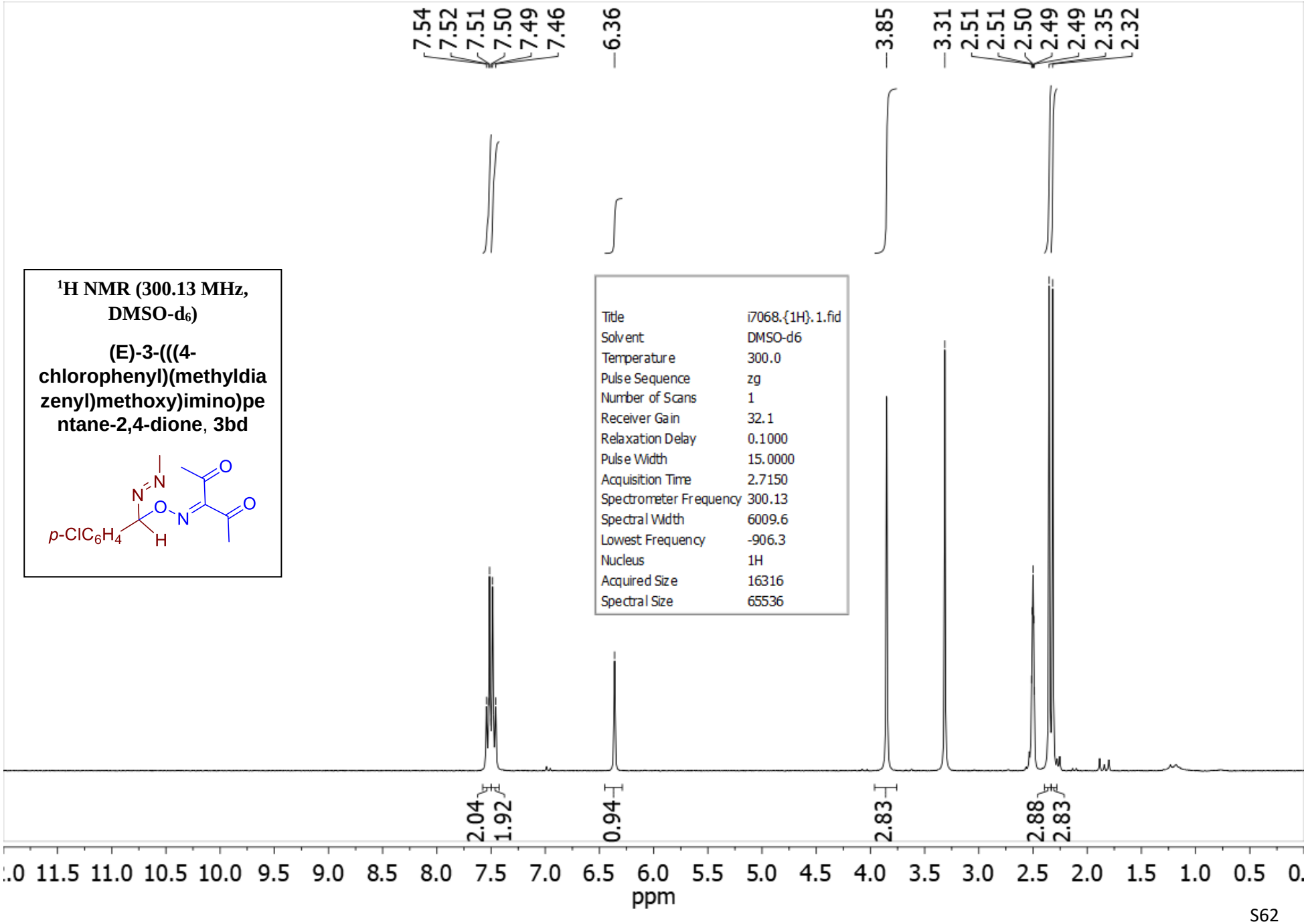

197.87
194.42
157.15
151.55
134.44
131.88
130.71
129.83
129.25
128.95
127.85
123.72
123.09
107.34
77.58
77.16
76.74
30.63
25.94
13C NMR (75.47 MHz, CDCl3)
(E)-3-((phenyl(phenyldiazenyl)methoxy)imino)pentane-2,4-dione, 3ba
Ph
N
N
O
N
O
O
Ph
H
Title i6505.{13C}.13.fid
Solvent CDCl3
Temperature 299.5
Pulse Sequence zgpg30
Number of Scans 625
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 -744.9
Nucleus 13C
Acquired Size 16308
Spectral Size 65536
30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


7.78
7.78
7.76
7.75
7.50
7.49
7.48
7.47
7.45
7.40
7.38
7.26
6.45
2.45
2.35
1.79
4.69
1.85
0.83
2.92
3.00
ppm
¹H NMR (300.13 MHz, CDCl₃)
(E)-3-(((4-chlorophenyl)(phenyldiazenyl)methoxy)imino)pentane-2,4-dione, 3bb
Ph
N
N
O
N
O
O
p-ClC6H4
H
Title i6599.{1H}.1.fid
Solvent CDCl3
Temperature 299.8
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 -609.1
Nucleus 1H
Acquired Size 8124
Spectral Size 65536


197.71
194.29
157.28
151.44
135.94
132.94
132.08
129.29
129.23
129.19
123.10
106.45
77.58
77.16
76.74
30.62
25.95
13C NMR (75.47 MHz, CDCl3)
(E)-3-(((4-chlorophenyl)(phenyldiazenyl)methoxy)imino)pentane-2,4-dione, 3bb
Ph
N
N
O
N
O
O
p-ClC6H4
H
Title i6599.{13C}.13.fid
Solvent CDCl3
Temperature 300.2
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 -746.1
Nucleus 13C
Acquired Size 16308
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


7.79
7.78
7.78
7.78
7.77
7.77
7.76
7.76
7.75
7.49
7.48
7.48
7.47
7.47
7.46
7.46
7.45
6.95
6.94
6.93
6.92
6.44
3.81
2.45
2.35
¹H NMR (300.13 MHz, CDCl₃)
(E)-3-(((4-methoxyphenyl)(phenyldiazenyl)methoxy)imino)pentane-2,4-dione, 3bc
Ph
N
N
O
N
O
O
H
p-MeOC6H4
Title i7270.{1H}.1.fid
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32.0
Relaxation Delay 0.1000
Pulse Width 14.0000
Acquisition Time 2.7724
Spectrometer Frequency 300.23
Spectral Width 5882.4
Lowest Frequency -1094.5
Nucleus 1H
Acquired Size 16308
Spectral Size 65536
2.07
5.01
2.05
1.01
3.03
2.98
2.95
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.
ppm

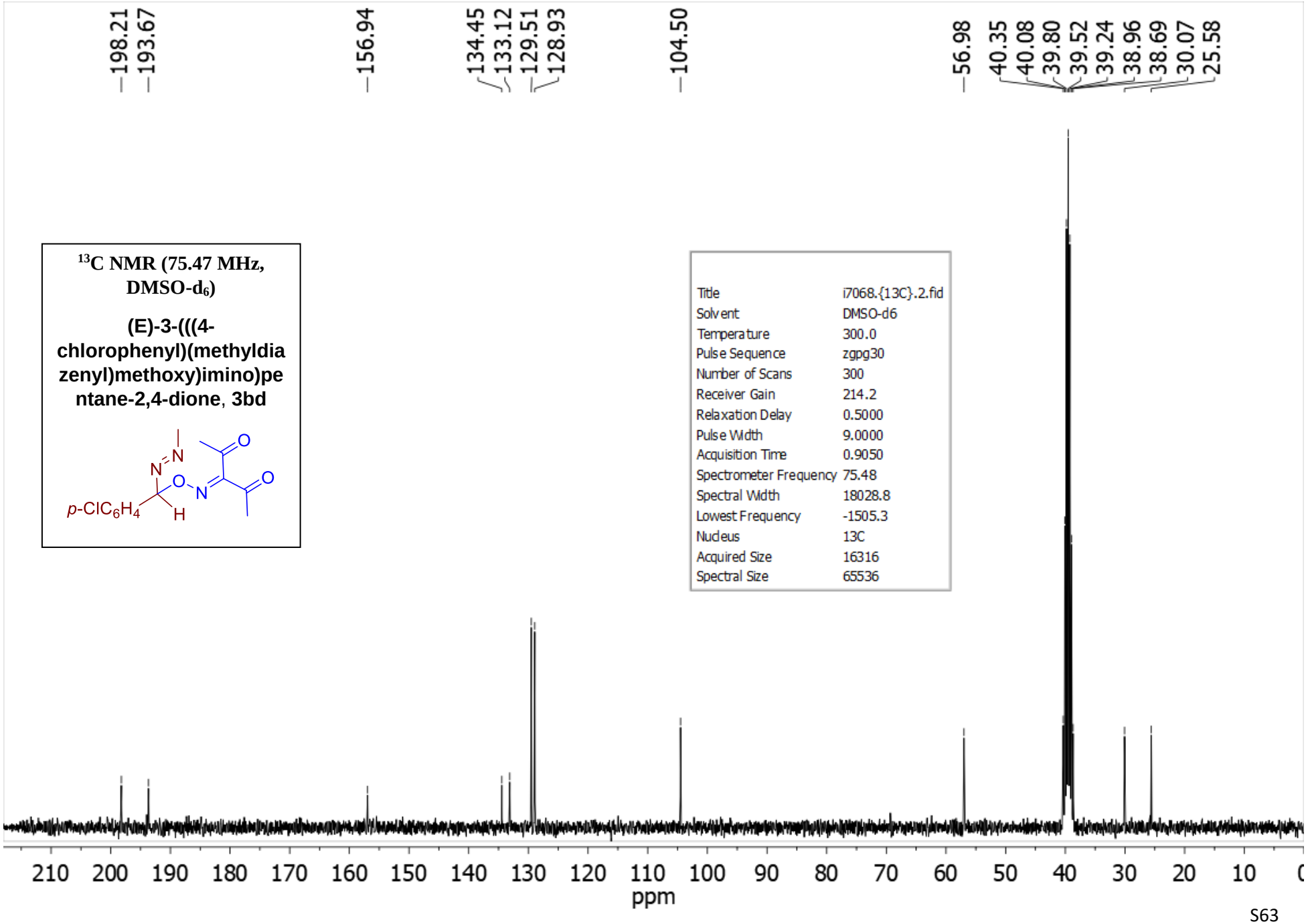

198.03
194.49
160.77
156.95
151.49
131.78
129.32
129.21
126.62
123.02
114.35
107.19
77.58
77.16
76.74
55.42
30.63
25.92
^{13}C NMR (75.47 MHz, $CDCl_3$)
(E)-3-(((4-methoxyphenyl)(phenyldiazenyl)methoxy)imino)pentane-2,4-dione, 3bc
Ph
N
N
O
N
O
O
H
p-MeOC6H4
Title i7270.{13C}.13.fid
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 512
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 -1371.9
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

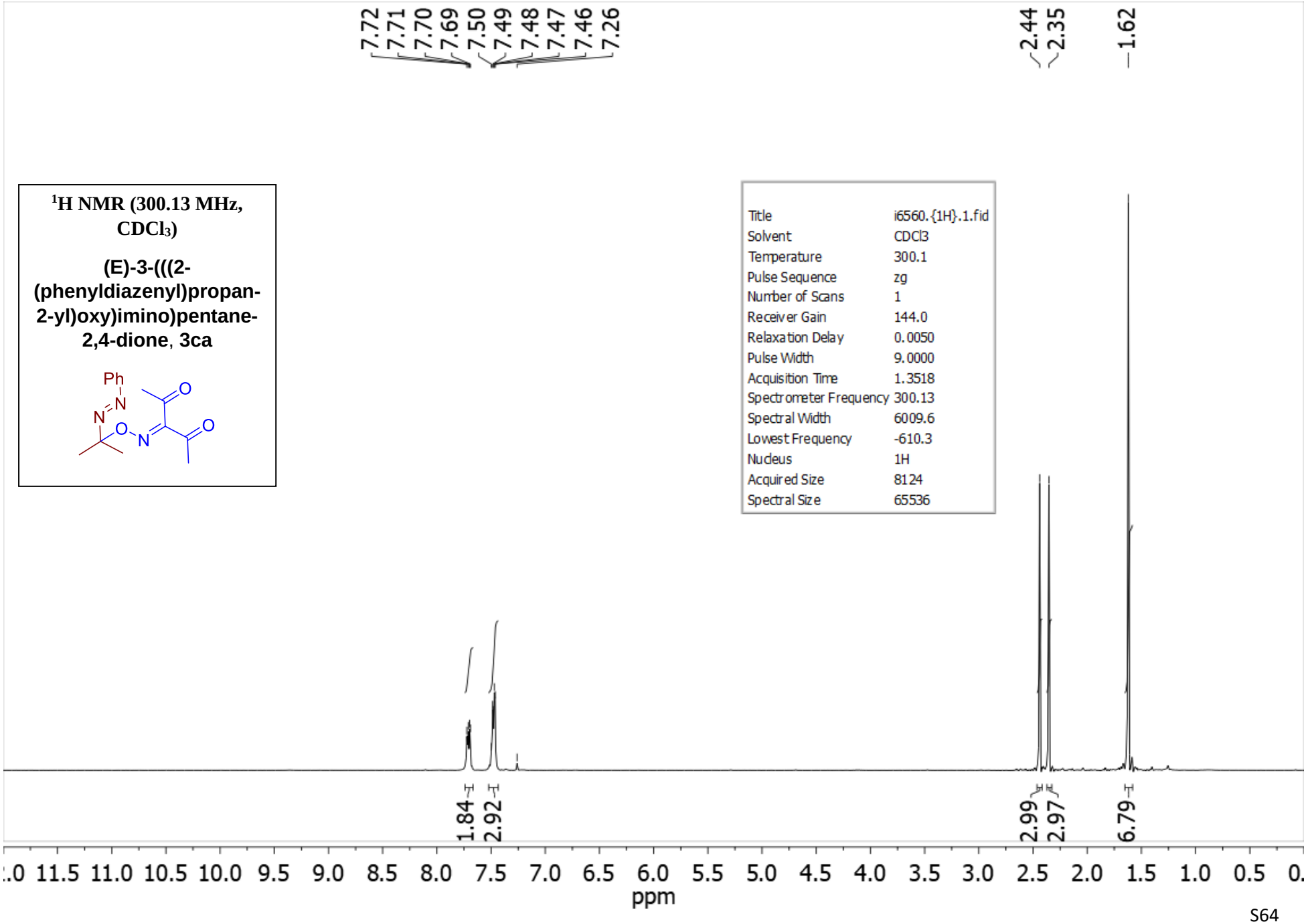


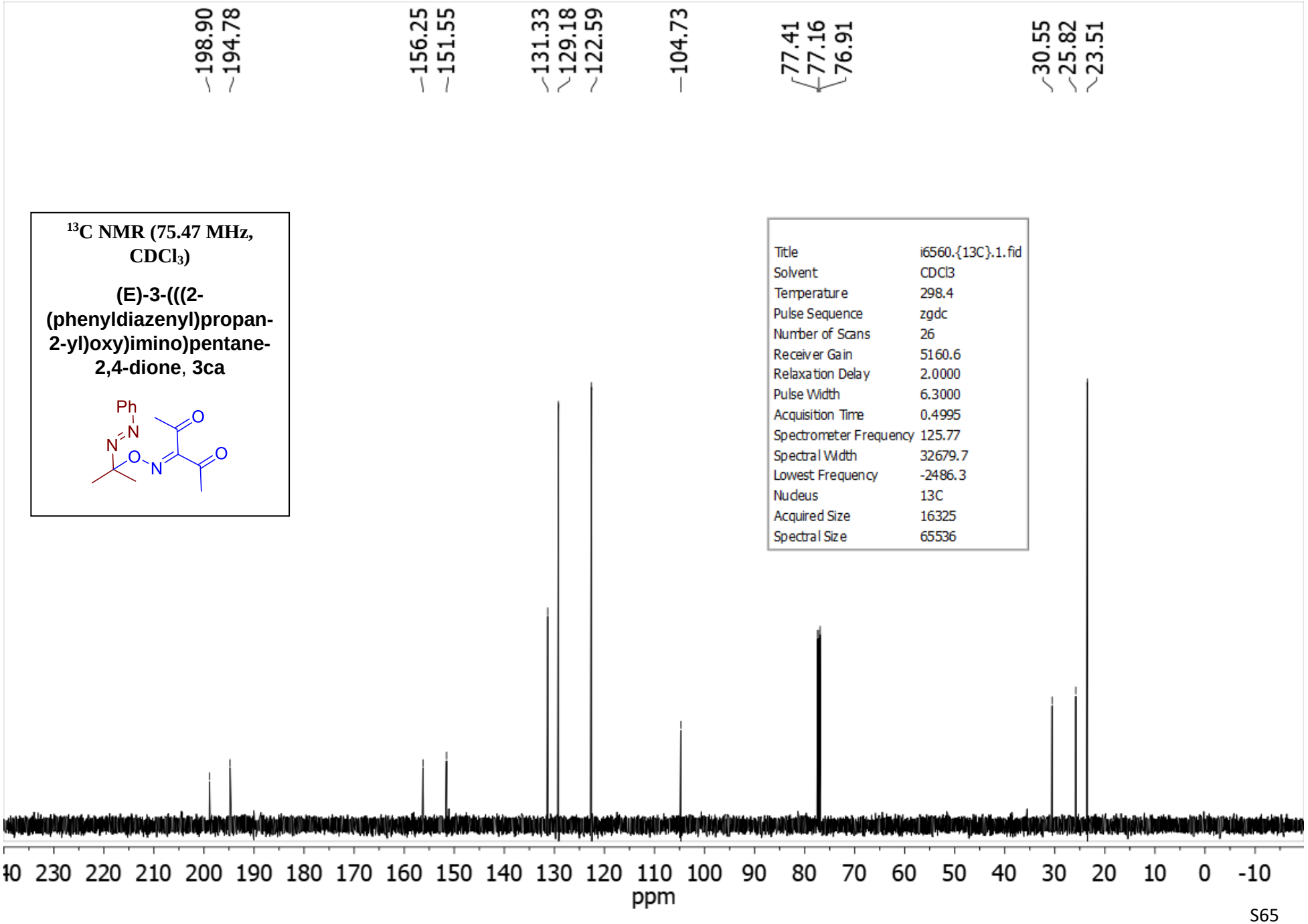
^{1}H NMR (300.13 MHz, DMSO-d_6)

(E)-3-(((4-chlorophenyl)(methyldiazenyl)methoxy)imino)pentane-2,4-dione, 3bd

Title	i7068.{1H}.1.fid
Solvent	DMSO-d6
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	-906.3
Nucleus	1H
Acquired Size	16316
Spectral Size	65536

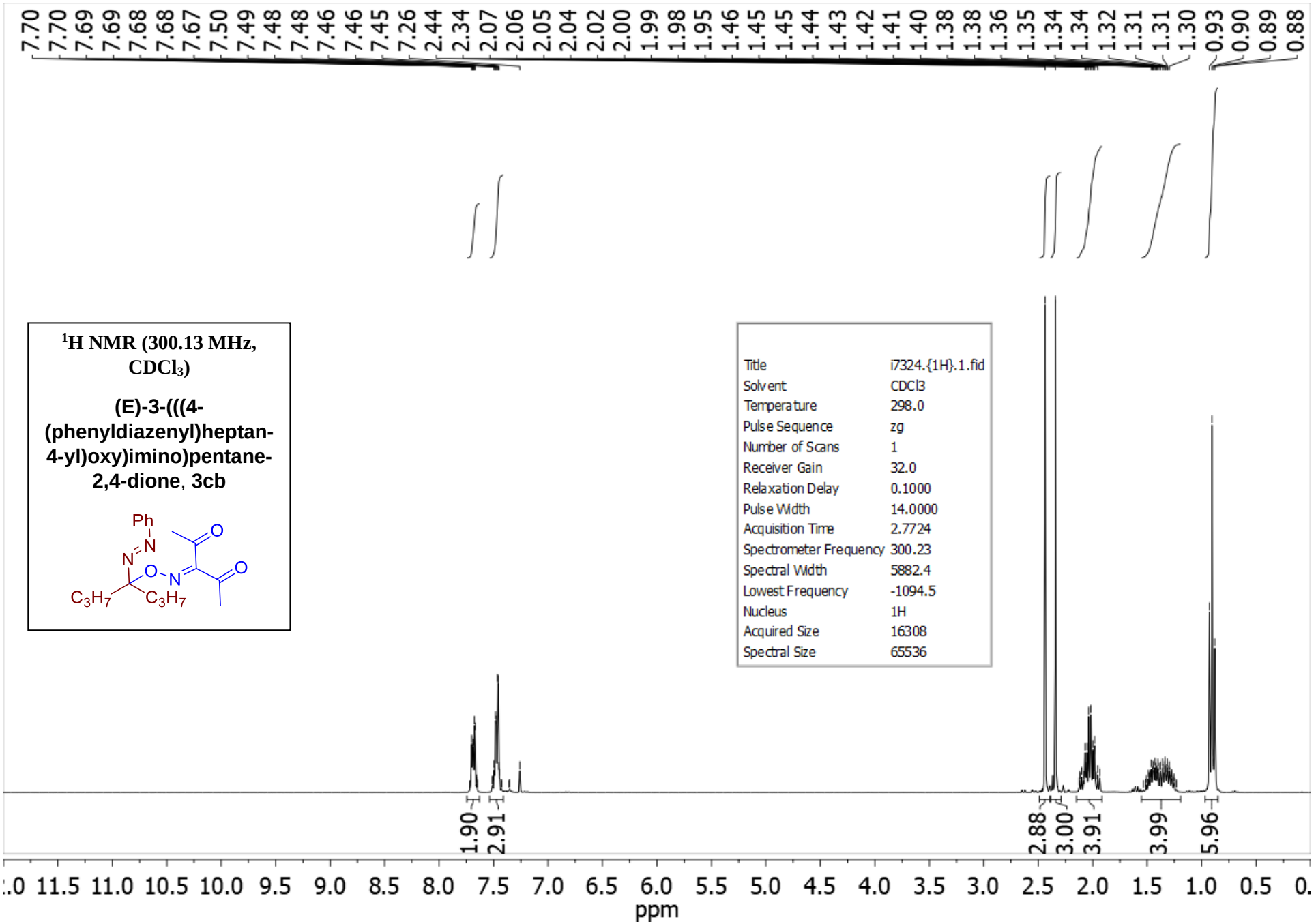

198.21
193.67
156.94
134.45
133.12
129.51
128.93
104.50
56.98
40.35
40.08
39.80
39.52
39.24
38.96
38.69
30.07
25.58
^{13}C NMR (75.47 MHz, DMSO-d$_6$)
(E)-3-(((4-chlorophenyl)(methyldiazenyl)methoxy)imino)pentane-2,4-dione, 3bd
p-ClC$_6$H$_4$
Title i7068.{13C}.2.fid
Solvent DMSO-d6
Temperature 300.0
Pulse Sequence zgpg30
Number of Scans 300
Receiver Gain 214.2
Relaxation Delay 0.5000
Pulse Width 9.0000
Acquisition Time 0.9050
Spectrometer Frequency 75.48
Spectral Width 18028.8
Lowest Frequency -1505.3
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

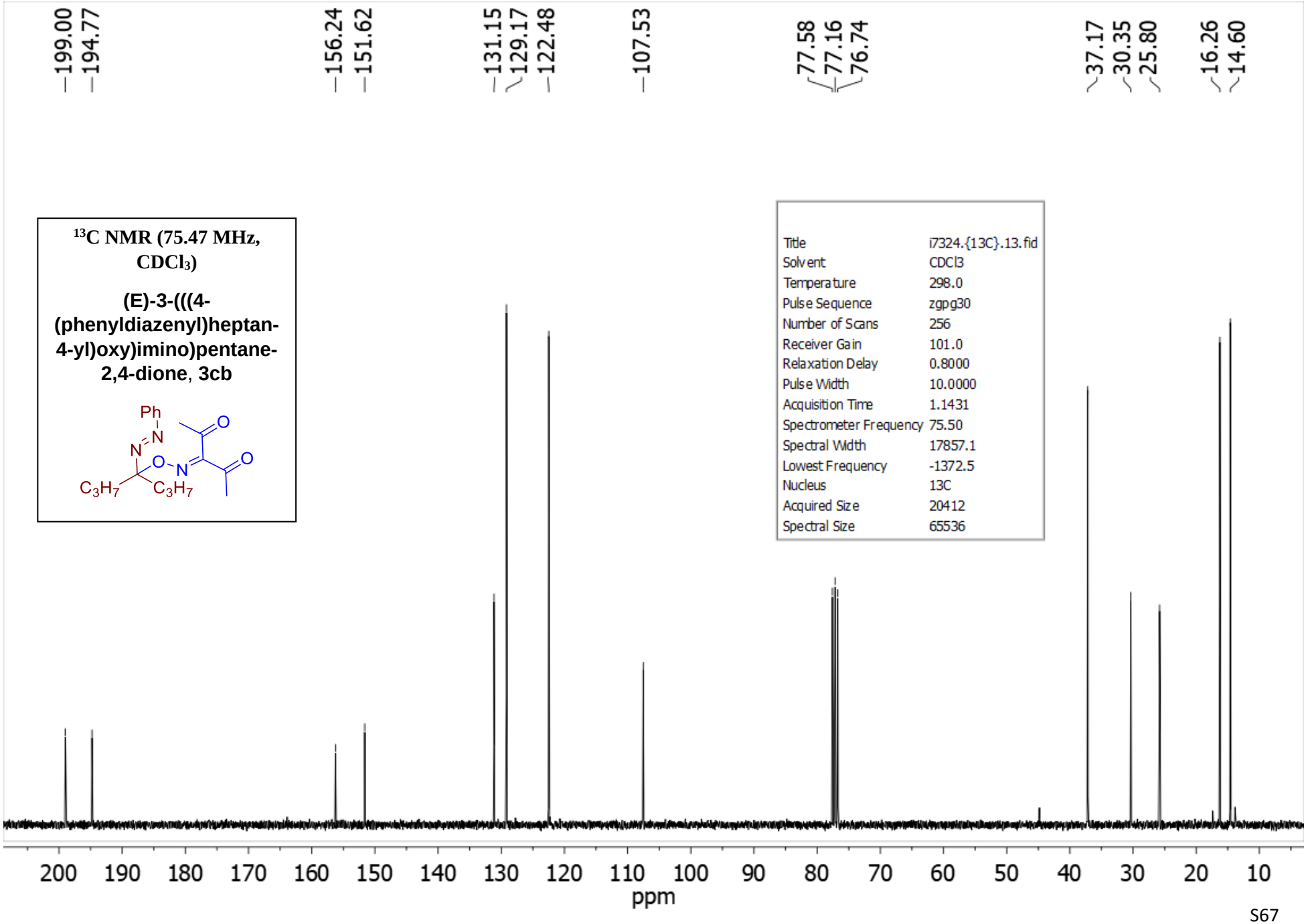

7.72
7.71
7.70
7.69
7.50
7.49
7.48
7.47
7.46
7.26
2.44
2.35
1.62
1H NMR (300.13 MHz, CDCl3)
(E)-3-(((2-(phenyldiazenyl)propan-2-yl)oxy)imino)pentane-2,4-dione, 3ca
Ph
N
N
O
N
O
O
Title i6560.{1H}.1.fid
Solvent CDCl3
Temperature 300.1
Pulse Sequence zg
Number of Scans 1
Receiver Gain 144.0
Relaxation Delay 0.0050
Pulse Width 9.0000
Acquisition Time 1.3518
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -610.3
Nucleus 1H
Acquired Size 8124
Spectral Size 65536
1.84
2.92
2.99
2.97
6.79
ppm

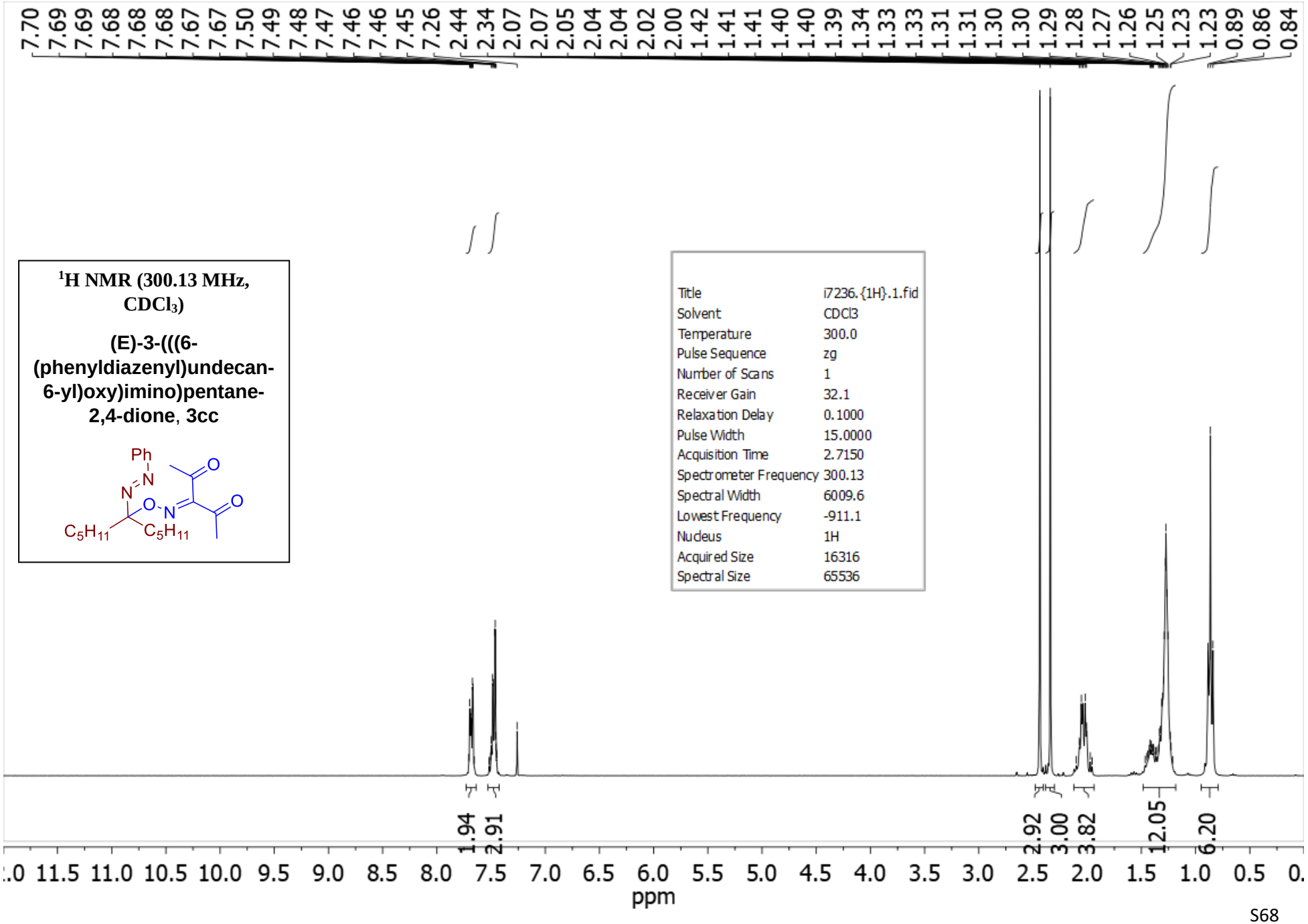


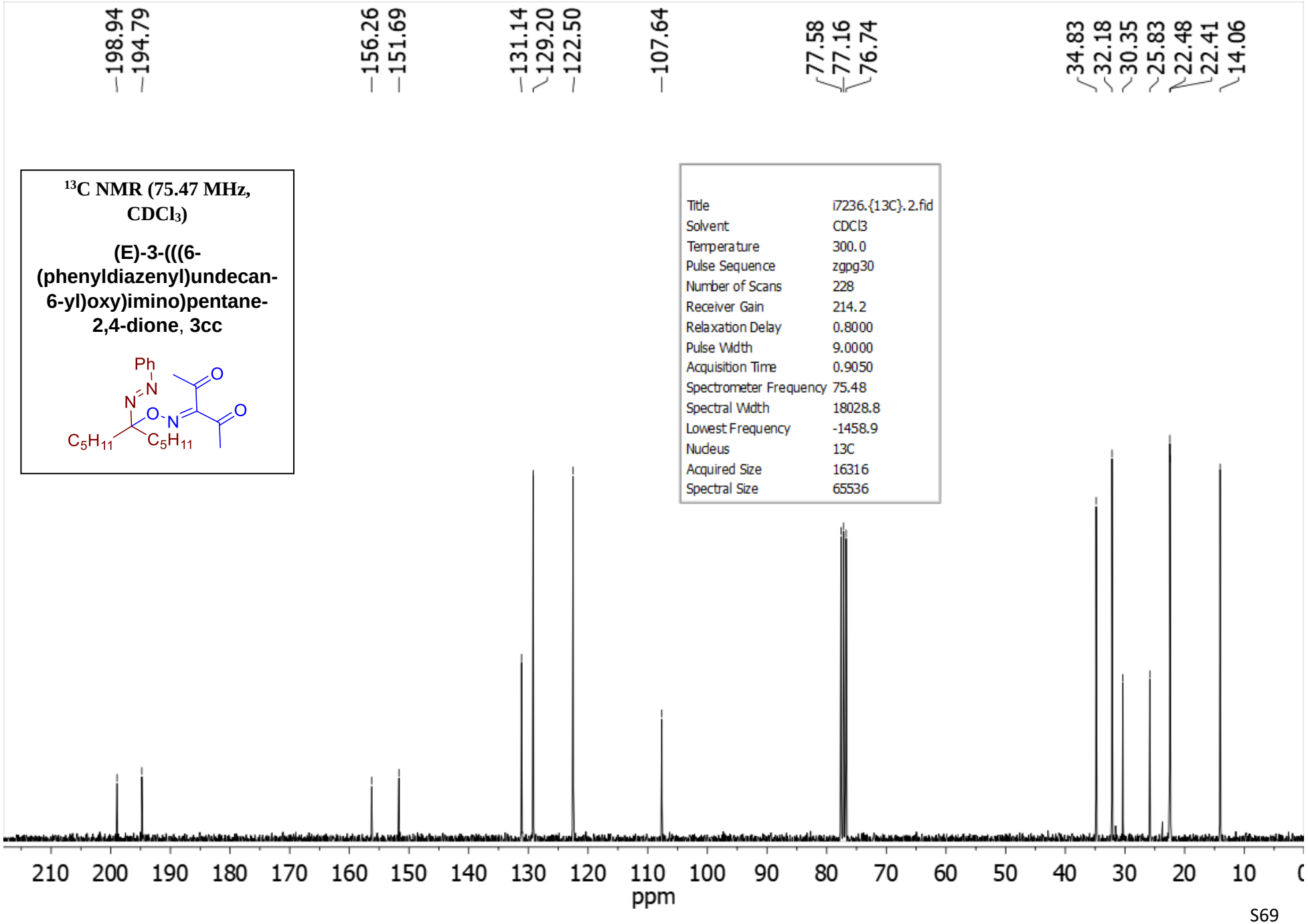
^{13}C NMR (75.47 MHz, $CDCl_3$)

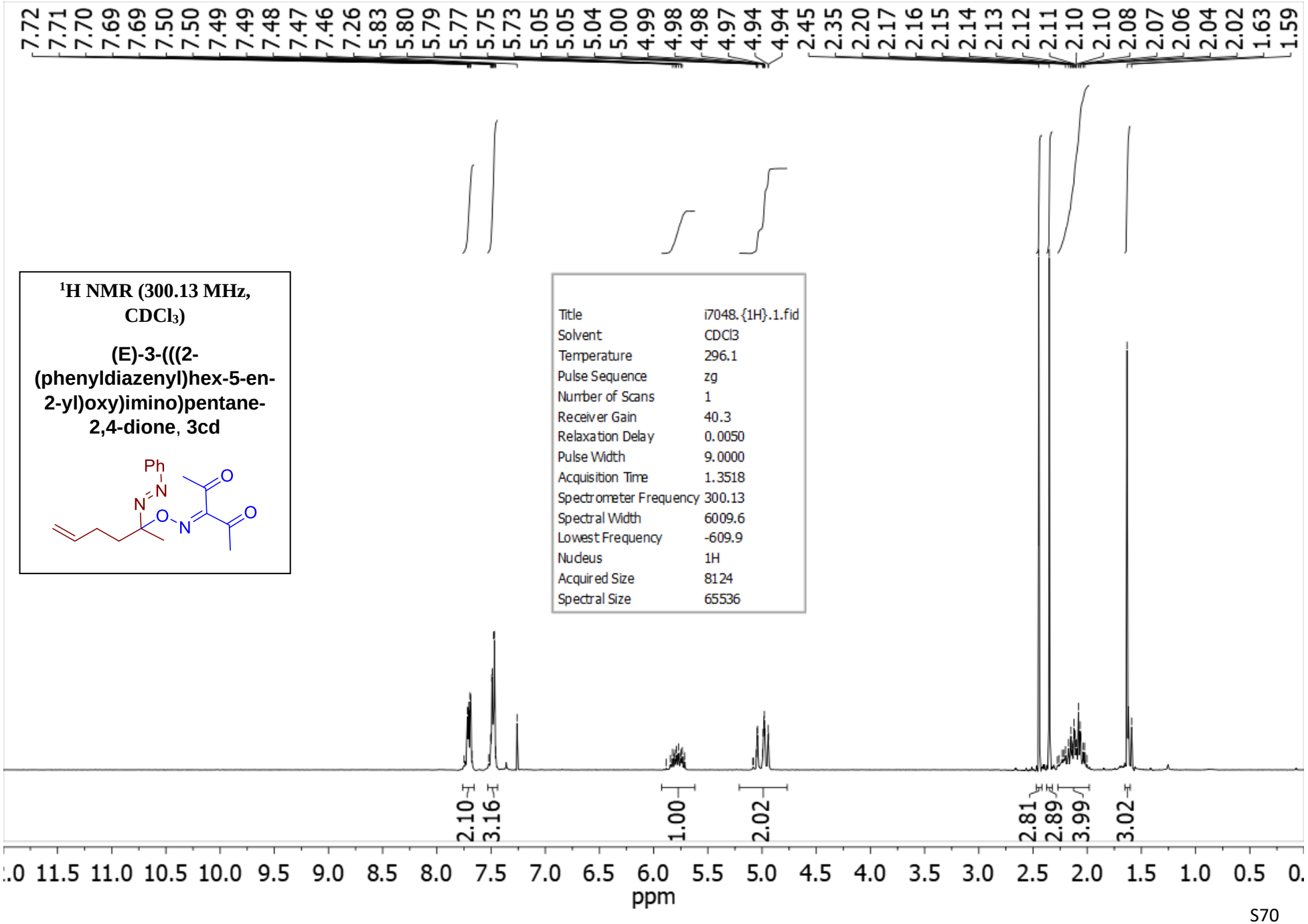
(E)-3-(((2-(phenyldiazenyl)propan-2-yl)oxy)imino)pentane-2,4-dione, 3ca

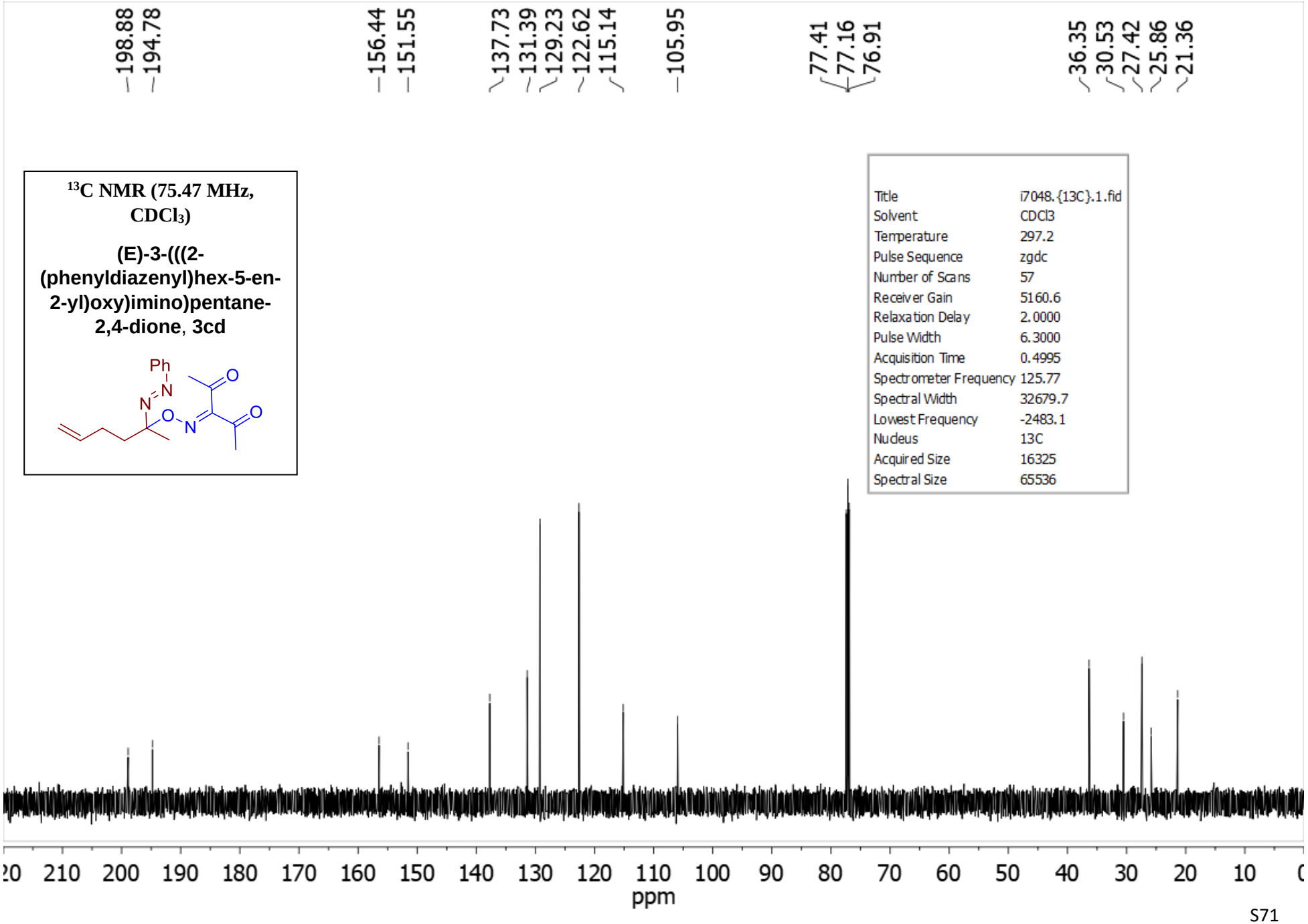

7.70 7.70 7.69 7.69 7.68 7.68 7.67 7.50 7.49 7.48 7.48 7.46 7.46 7.45 7.26 2.44 2.34 2.07 2.06 2.05 2.04 2.02 2.00 1.99 1.98 1.95 1.46 1.45 1.45 1.44 1.43 1.42 1.41 1.40 1.38 1.38 1.36 1.35 1.34 1.34 1.32 1.31 1.31 1.30 0.93 0.90 0.89 0.88
1H NMR (300.13 MHz, CDCl3)
(E)-3-(((4-(phenyldiazenyl)heptan-4-yl)oxy)imino)pentane-2,4-dione, 3cb
Ph
N
N
O
N
O
O
C3H7
C3H7
Title i7324.{1H}.1.fid
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32.0
Relaxation Delay 0.1000
Pulse Width 14.0000
Acquisition Time 2.7724
Spectrometer Frequency 300.23
Spectral Width 5882.4
Lowest Frequency -1094.5
Nucleus 1H
Acquired Size 16308
Spectral Size 65536
1.90
2.91
2.88
3.00
3.91
3.99
5.96
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

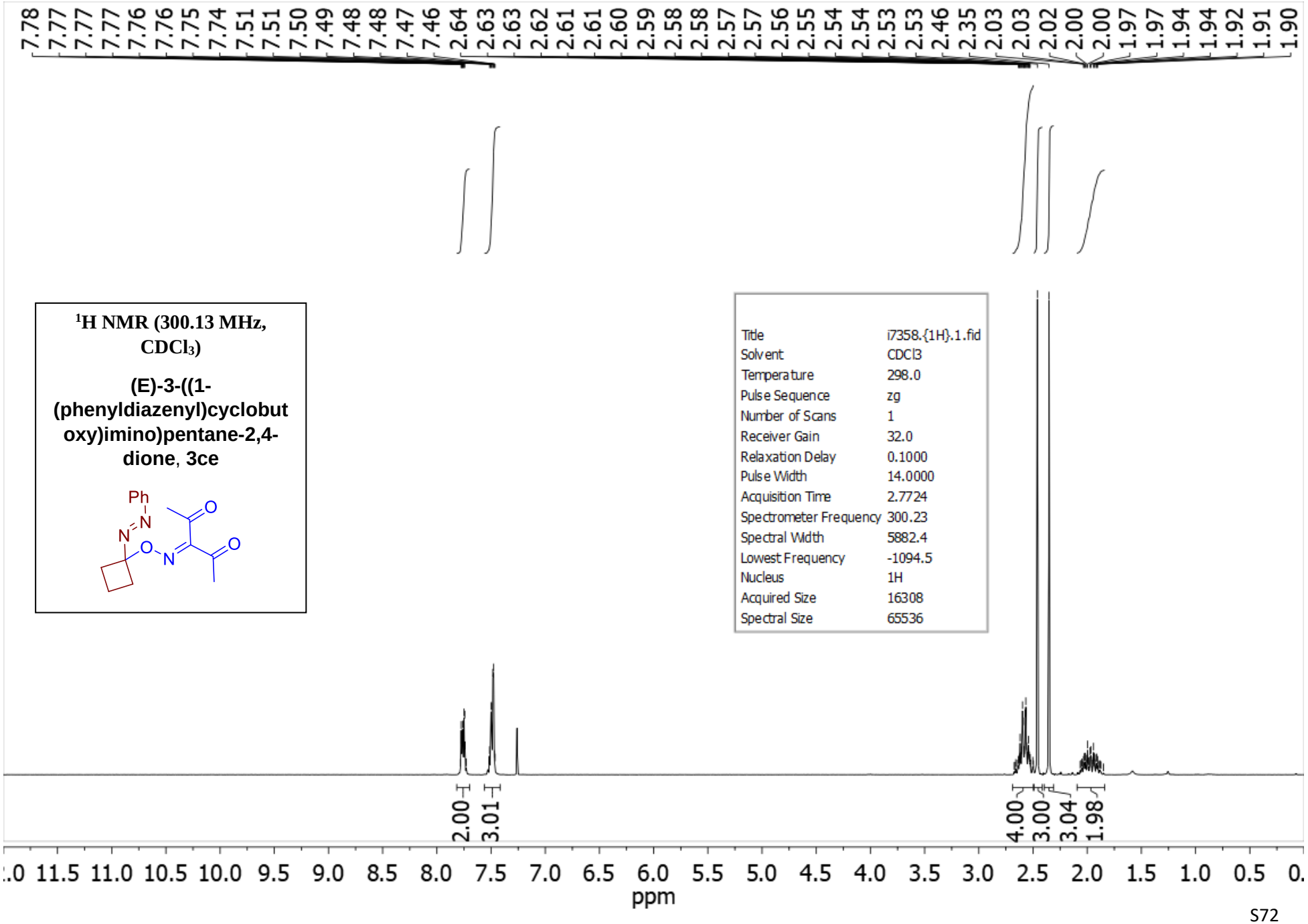

199.00
194.77
156.24
151.62
131.15
129.17
122.48
107.53
77.58
77.16
76.74
37.17
30.35
25.80
16.26
14.60
^{13}C NMR (75.47 MHz, $CDCl_3$)
(E)-3-(((4-(phenyldiazenyl)heptan-4-yl)oxy)imino)pentane-2,4-dione, 3cb
Ph
N
N
O
N
O
O
C_3H_7
C_3H_7
Title i7324.{13C}.13.fid
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 256
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 -1372.5
Nucleus 13C
Acquired Size 20412
Spectral Size 65536
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm

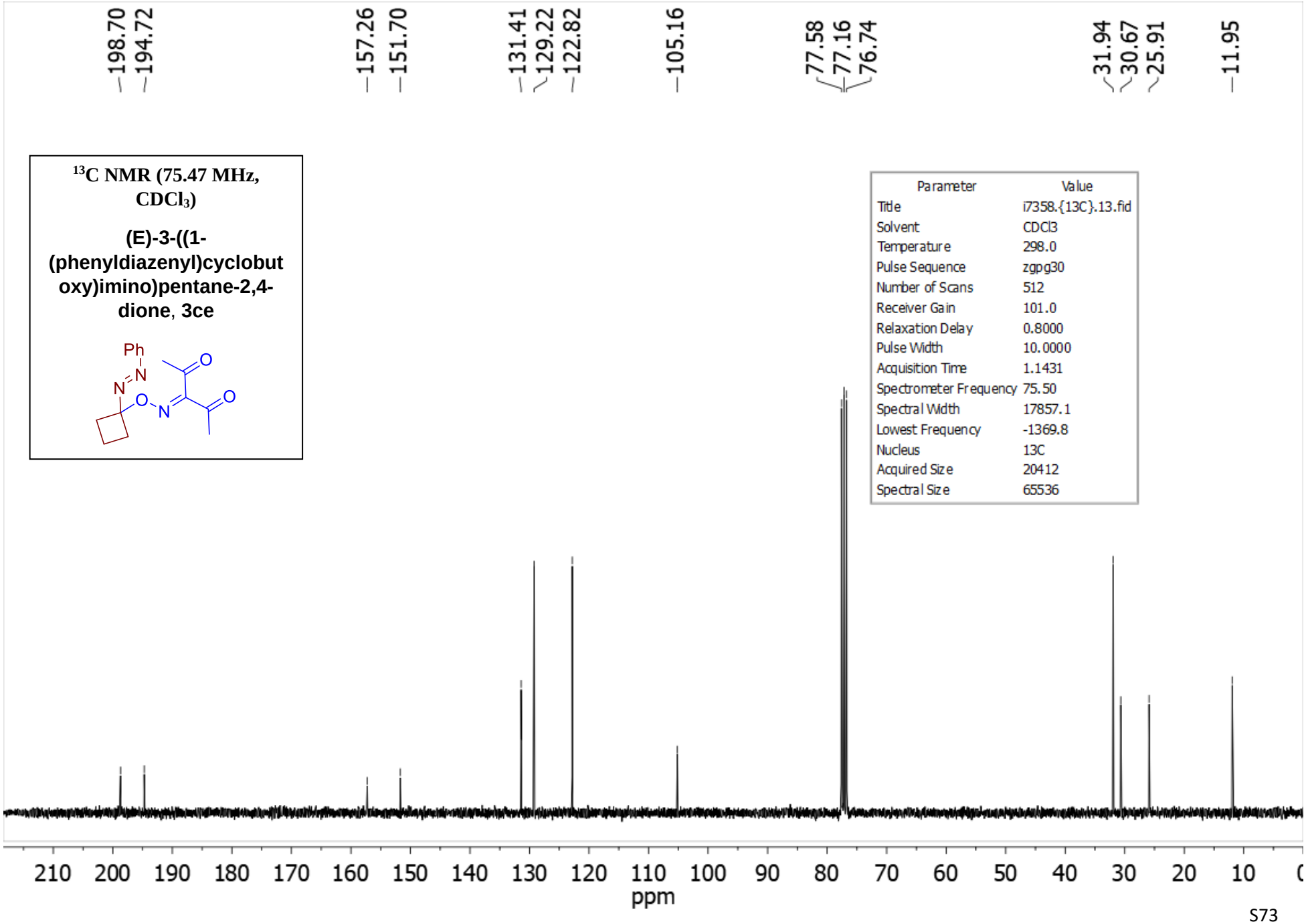

7.70 7.69 7.69 7.68 7.68 7.68 7.67 7.67 7.50 7.49 7.48 7.47 7.46 7.46 7.45 7.26 2.44 2.34 2.07 2.07 2.05 2.04 2.04 2.02 2.00 1.42 1.41 1.41 1.40 1.40 1.39 1.34 1.33 1.33 1.31 1.31 1.30 1.30 1.29 1.28 1.27 1.26 1.25 1.23 1.23 0.89 0.86 0.84
1H NMR (300.13 MHz, CDCl3)
(E)-3-(((6-(phenyldiazenyl)undecan-6-yl)oxy)imino)pentane-2,4-dione, 3cc
Ph
N
N
O
N
O
O
C5H11
C5H11
Title i7236.{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
1.94
2.91
2.92
3.00
3.82
12.05
6.20
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

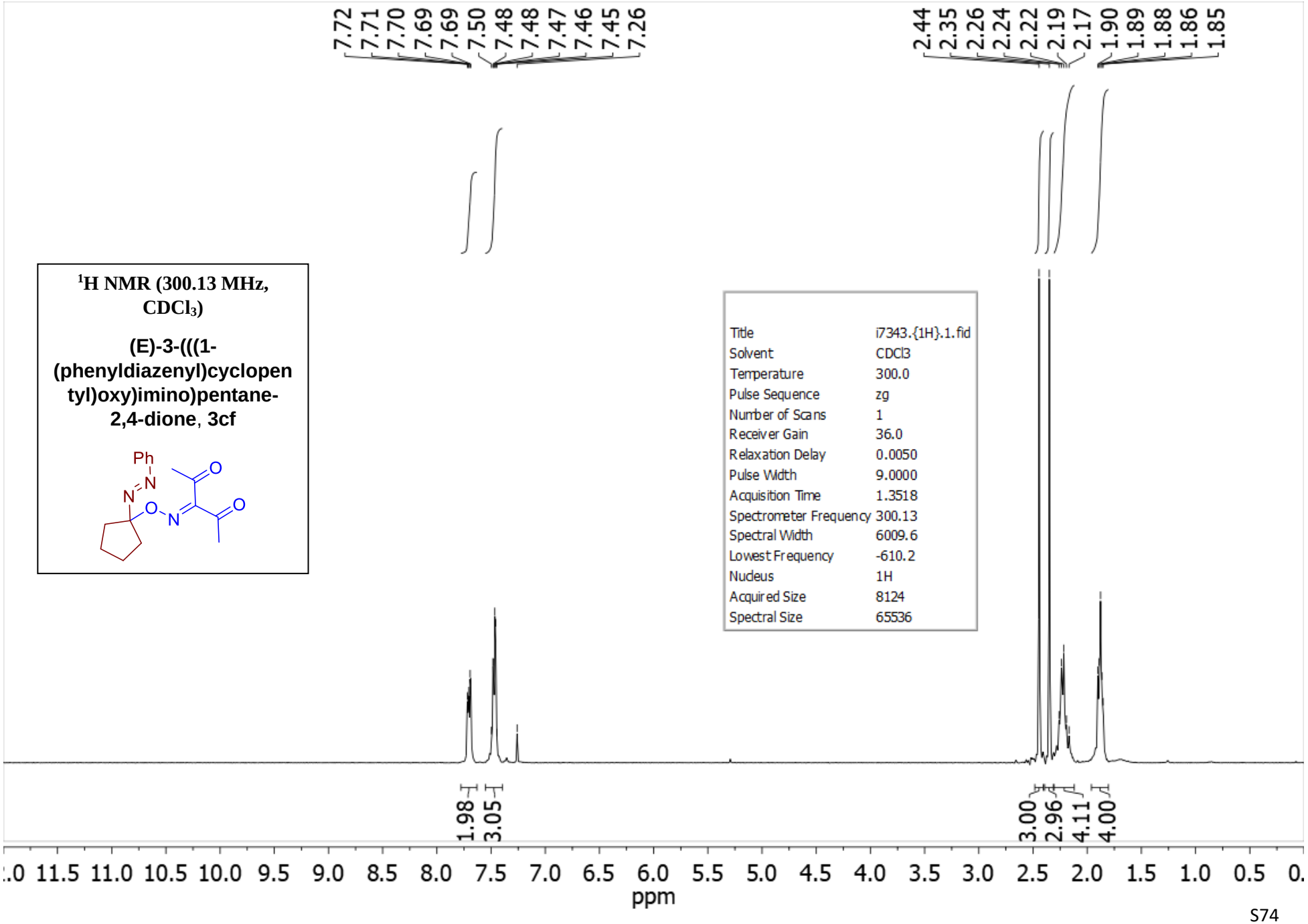

198.94
194.79
156.26
151.69
131.14
129.20
122.50
107.64
77.58
77.16
76.74
34.83
32.18
30.35
25.83
22.48
22.41
14.06
^{13}C NMR (75.47 MHz, $CDCl_3$)
(E)-3-(((6-(phenyldiazenyl)undecan-6-yl)oxy)imino)pentane-2,4-dione, 3cc
Ph
N
N
O
N
O
O
C_5H_{11}
C_5H_{11}
Title i7236.{13C}.2.fid
Solvent CDCl3
Temperature 300.0
Pulse Sequence zgpg30
Number of Scans 228
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 -1458.9
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

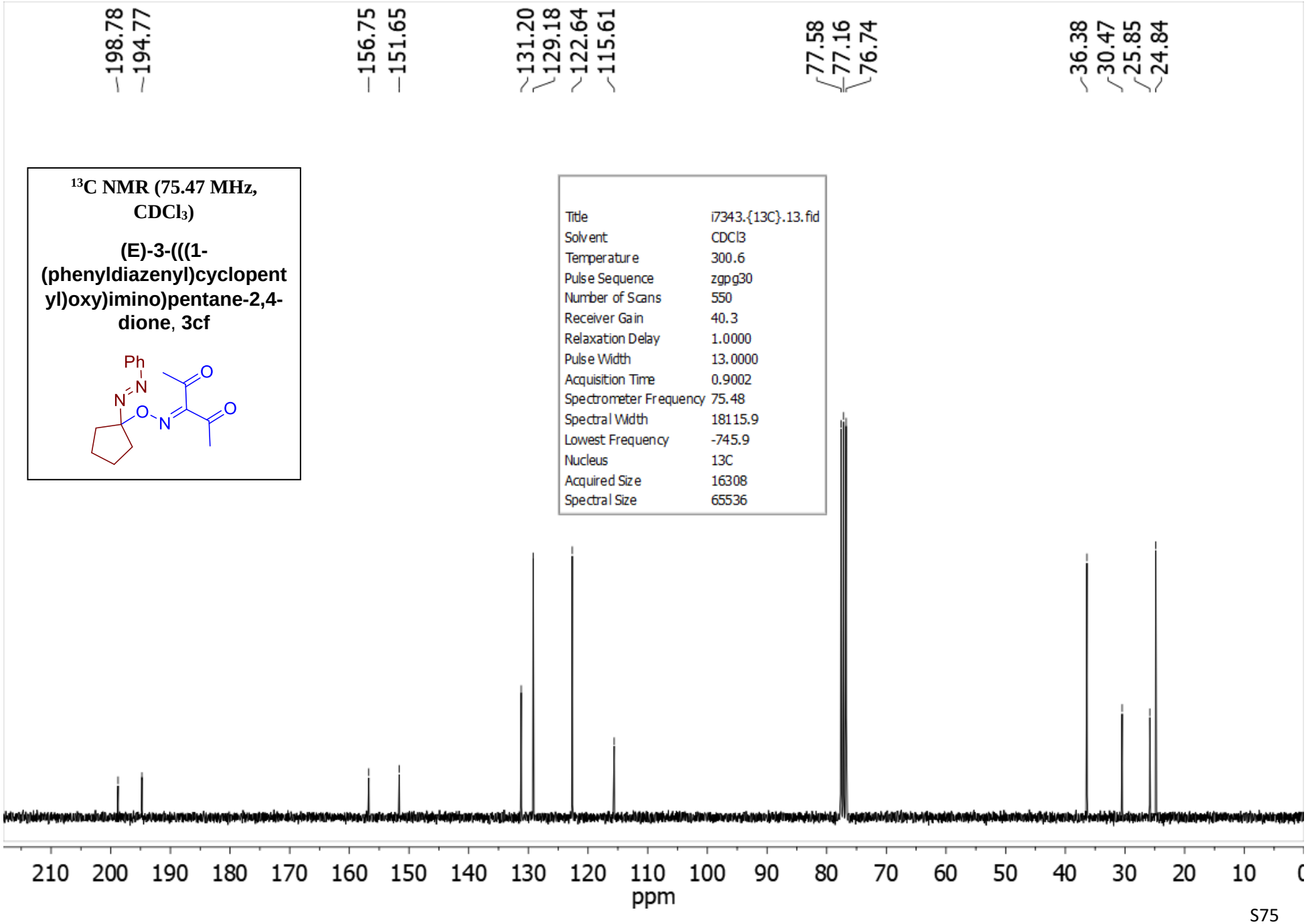

7.72 7.71 7.70 7.69 7.69 7.50 7.50 7.49 7.49 7.48 7.47 7.46 7.26 5.83 5.80 5.79 5.77 5.75 5.73 5.05 5.05 5.04 5.00 4.99 4.98 4.98 4.97 4.94 4.94 2.45 2.35 2.20 2.17 2.16 2.15 2.14 2.13 2.12 2.11 2.10 2.10 2.08 2.07 2.06 2.04 2.02 1.63 1.59
¹H NMR (300.13 MHz, CDCl₃)
(E)-3-(((2-(phenyldiazenyl)hex-5-en-2-yl)oxy)imino)pentane-2,4-dione, 3cd
Ph
N
N
O
N
O
O
Title i7048.{1H}.1.fid
Solvent CDCl3
Temperature 296.1
Pulse Sequence zg
Number of Scans 1
Receiver Gain 40.3
Relaxation Delay 0.0050
Pulse Width 9.0000
Acquisition Time 1.3518
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -609.9
Nucleus 1H
Acquired Size 8124
Spectral Size 65536
2.10
3.16
1.00
2.02
2.81
2.89
3.99
3.02
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

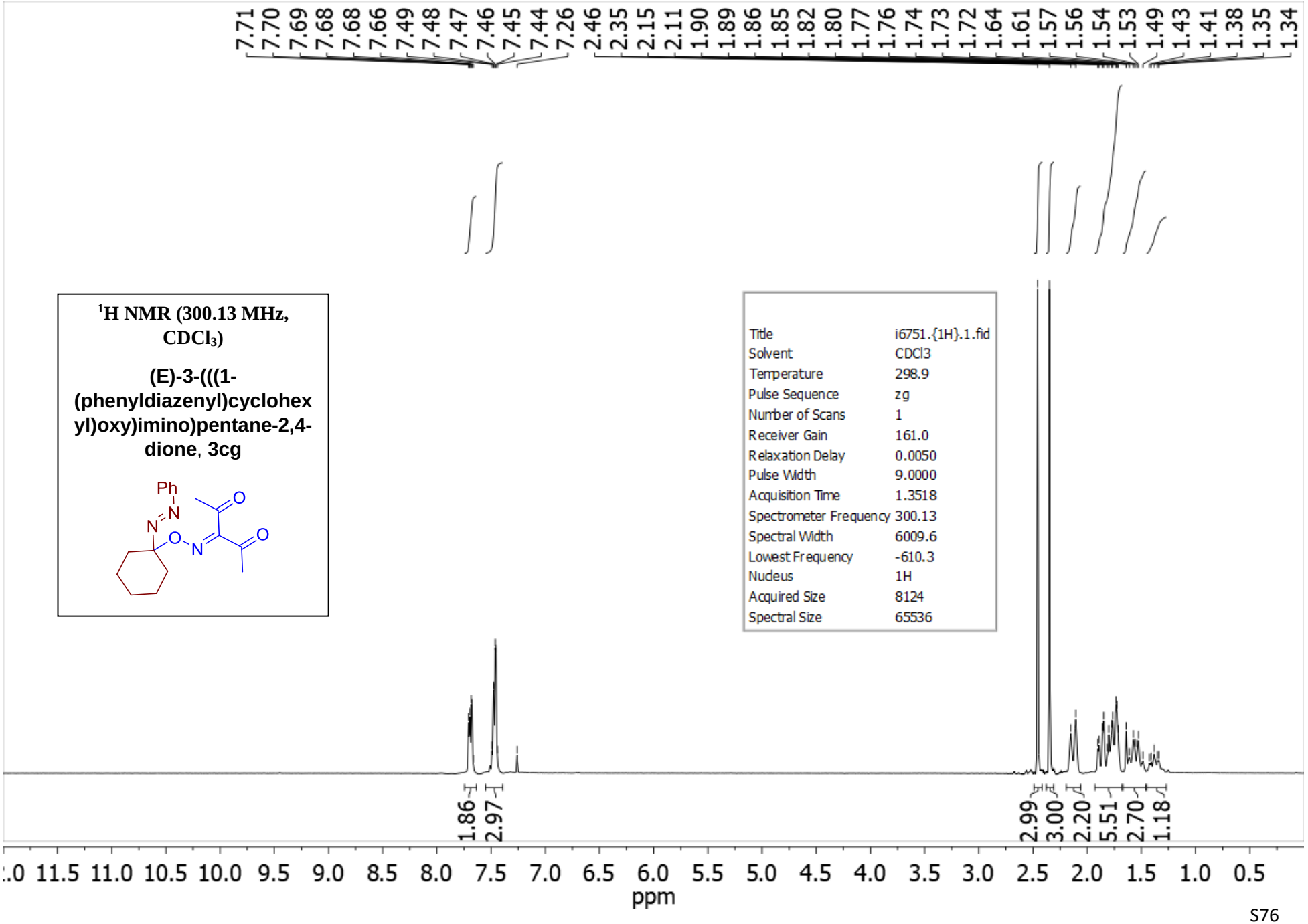

198.88
194.78
156.44
151.55
137.73
131.39
129.23
122.62
115.14
105.95
77.41
77.16
76.91
36.35
30.53
27.42
25.86
21.36
^{13}C NMR (75.47 MHz, $CDCl_3$)
(E)-3-(((2-(phenyldiazenyl)hex-5-en-2-yl)oxy)imino)pentane-2,4-dione, 3cd
Ph
N
N
O
N
O
O
Title i7048.{13C}.1.fid
Solvent CDCl3
Temperature 297.2
Pulse Sequence zgdc
Number of Scans 57
Receiver Gain 5160.6
Relaxation Delay 2.0000
Pulse Width 6.3000
Acquisition Time 0.4995
Spectrometer Frequency 125.77
Spectral Width 32679.7
Lowest Frequency -2483.1
Nucleus 13C
Acquired Size 16325
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

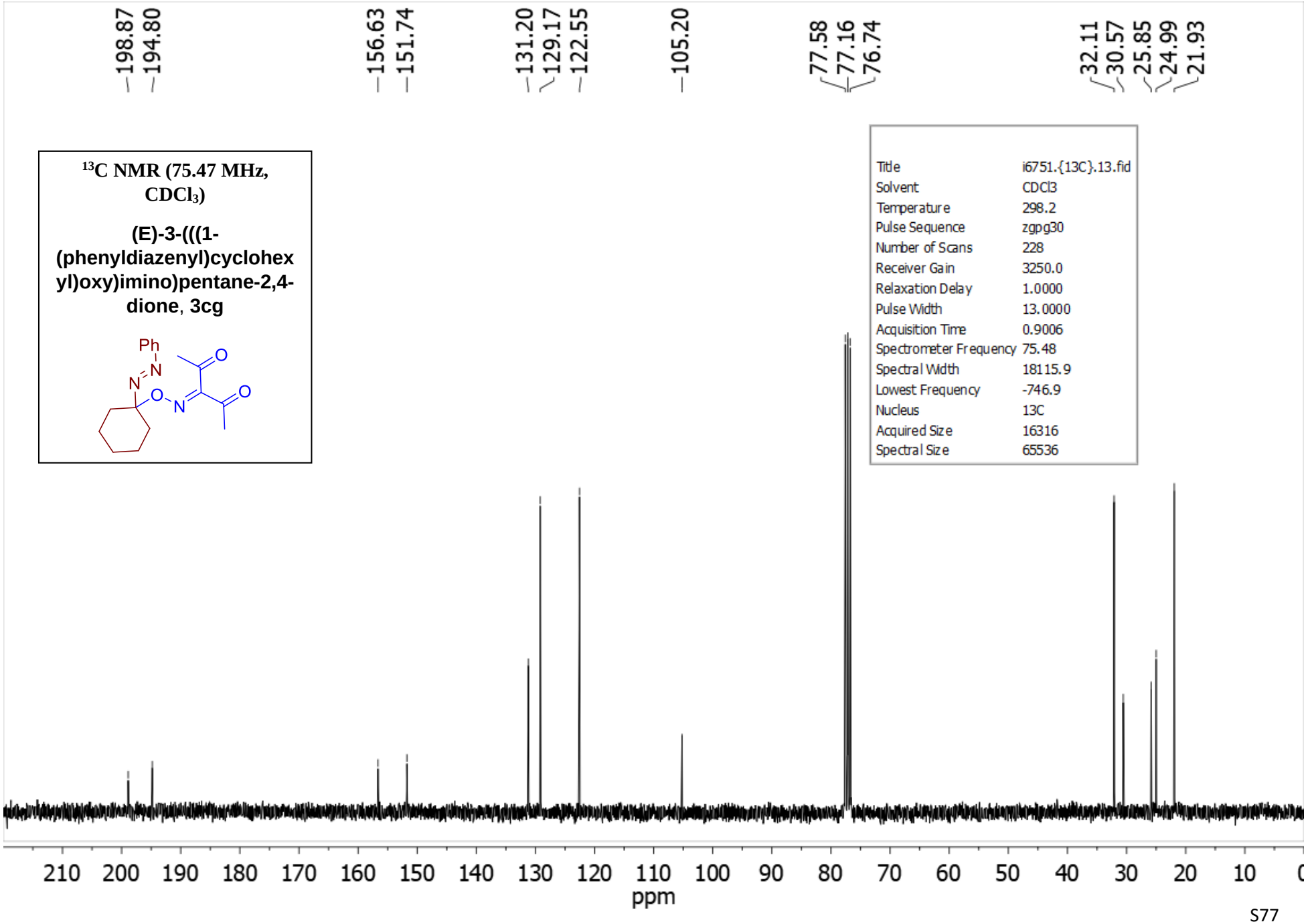

7.78 7.77 7.77 7.77 7.76 7.76 7.75 7.74 7.51 7.51 7.50 7.49 7.48 7.48 7.47 7.46 2.64 2.63 2.63 2.62 2.61 2.61 2.60 2.59 2.58 2.58 2.57 2.57 2.56 2.55 2.54 2.54 2.53 2.53 2.46 2.35 2.03 2.03 2.02 2.00 2.00 1.97 1.97 1.94 1.94 1.92 1.91 1.90
¹H NMR (300.13 MHz, CDCl₃)
(E)-3-((1-(phenyldiazenyl)cyclobutoxy)imino)pentane-2,4-dione, 3ce
Ph
N
N
O
N
O
O
Title i7358.{1H}.1.fid
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32.0
Relaxation Delay 0.1000
Pulse Width 14.0000
Acquisition Time 2.7724
Spectrometer Frequency 300.23
Spectral Width 5882.4
Lowest Frequency -1094.5
Nucleus 1H
Acquired Size 16308
Spectral Size 65536
2.00
3.01
4.00
3.00
3.04
1.98
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

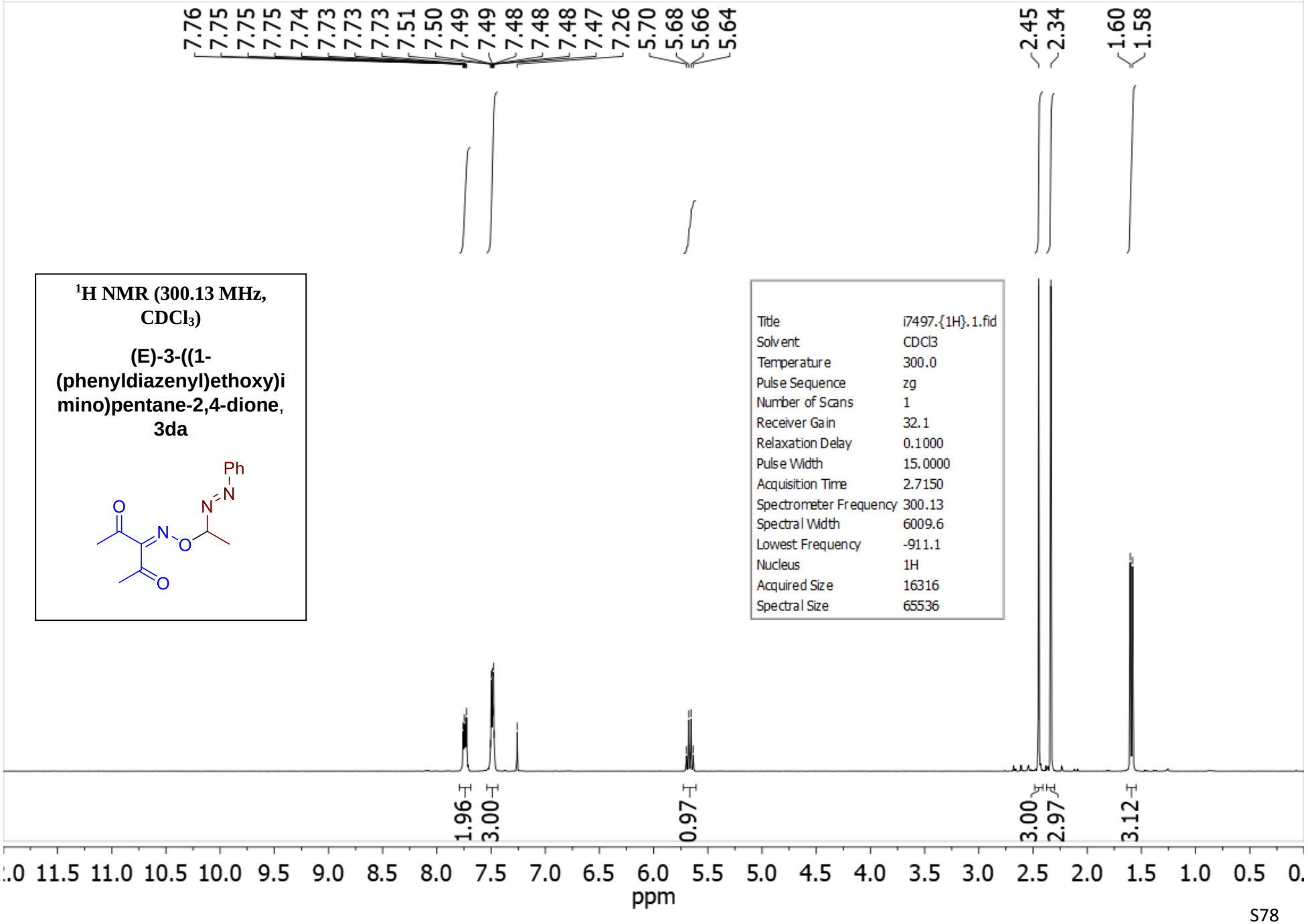

198.70
194.72
157.26
151.70
131.41
129.22
122.82
105.16
77.58
77.16
76.74
31.94
30.67
25.91
11.95
^{13}C NMR (75.47 MHz, $CDCl_3$)
(E)-3-((1-(phenyldiazenyl)cyclobutoxy)imino)pentane-2,4-dione, 3ce
Ph
N
N
O
N
O
O
Parameter Value
Title i7358.{13C}.13.fid
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 512
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 -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
ppm

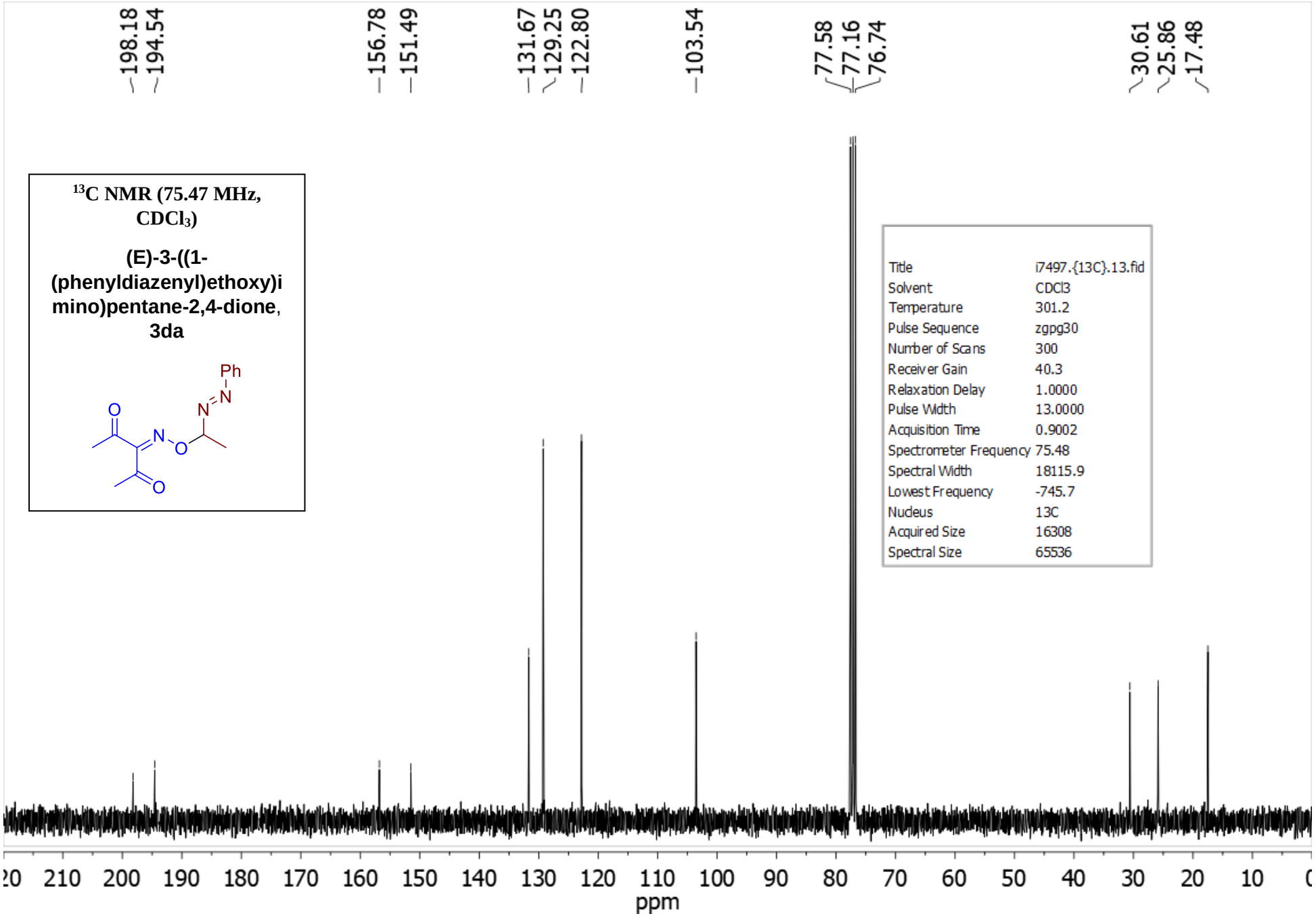

7.72
7.71
7.70
7.69
7.69
7.50
7.48
7.48
7.47
7.46
7.45
7.26
2.44
2.35
2.26
2.24
2.22
2.19
2.17
1.90
1.89
1.88
1.86
1.85
1H NMR (300.13 MHz, CDCl3)
(E)-3-(((1-(phenyldiazenyl)cyclopentyl)oxy)imino)pentane-2,4-dione, 3cf
Ph
N
N
O
N
O
O
Title i7343.{1H}.1.fid
Solvent CDCl3
Temperature 300.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 36.0
Relaxation Delay 0.0050
Pulse Width 9.0000
Acquisition Time 1.3518
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -610.2
Nucleus 1H
Acquired Size 8124
Spectral Size 65536
1.98
3.05
3.00
2.96
4.11
4.00
ppm

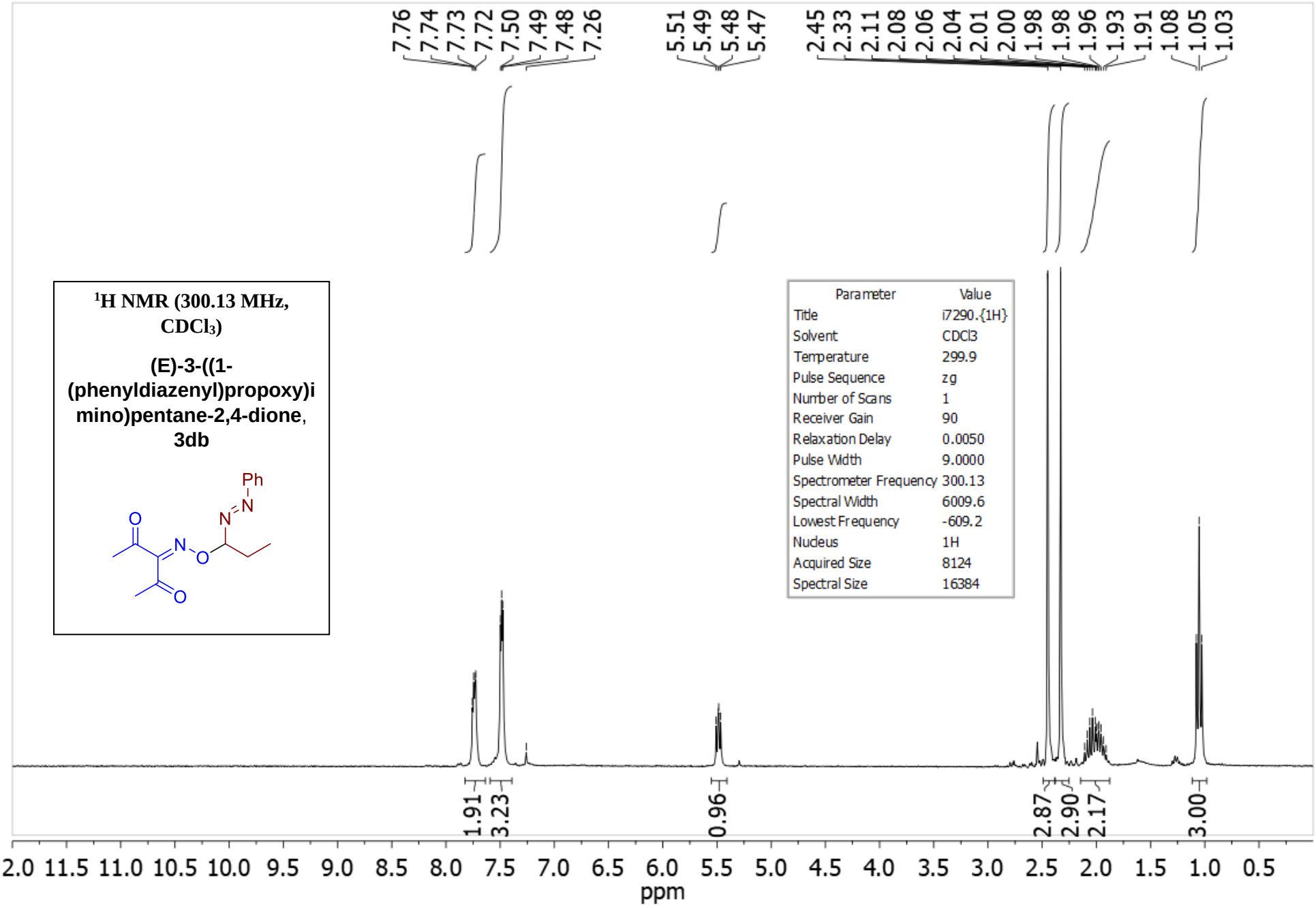

198.78
194.77
156.75
151.65
131.20
129.18
122.64
115.61
77.58
77.16
76.74
36.38
30.47
25.85
24.84
^{13}C NMR (75.47 MHz, $CDCl_3$)
(E)-3-(((1-(phenyldiazenyl)cyclopentyl)oxy)imino)pentane-2,4-dione, 3cf
Ph
N
N
O
N
O
O
Title i7343.{13C}.13.fid
Solvent CDCl3
Temperature 300.6
Pulse Sequence zgpg30
Number of Scans 550
Receiver Gain 40.3
Relaxation Delay 1.0000
Pulse Width 13.0000
Acquisition Time 0.9002
Spectrometer Frequency 75.48
Spectral Width 18115.9
Lowest Frequency -745.9
Nucleus 13C
Acquired Size 16308
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

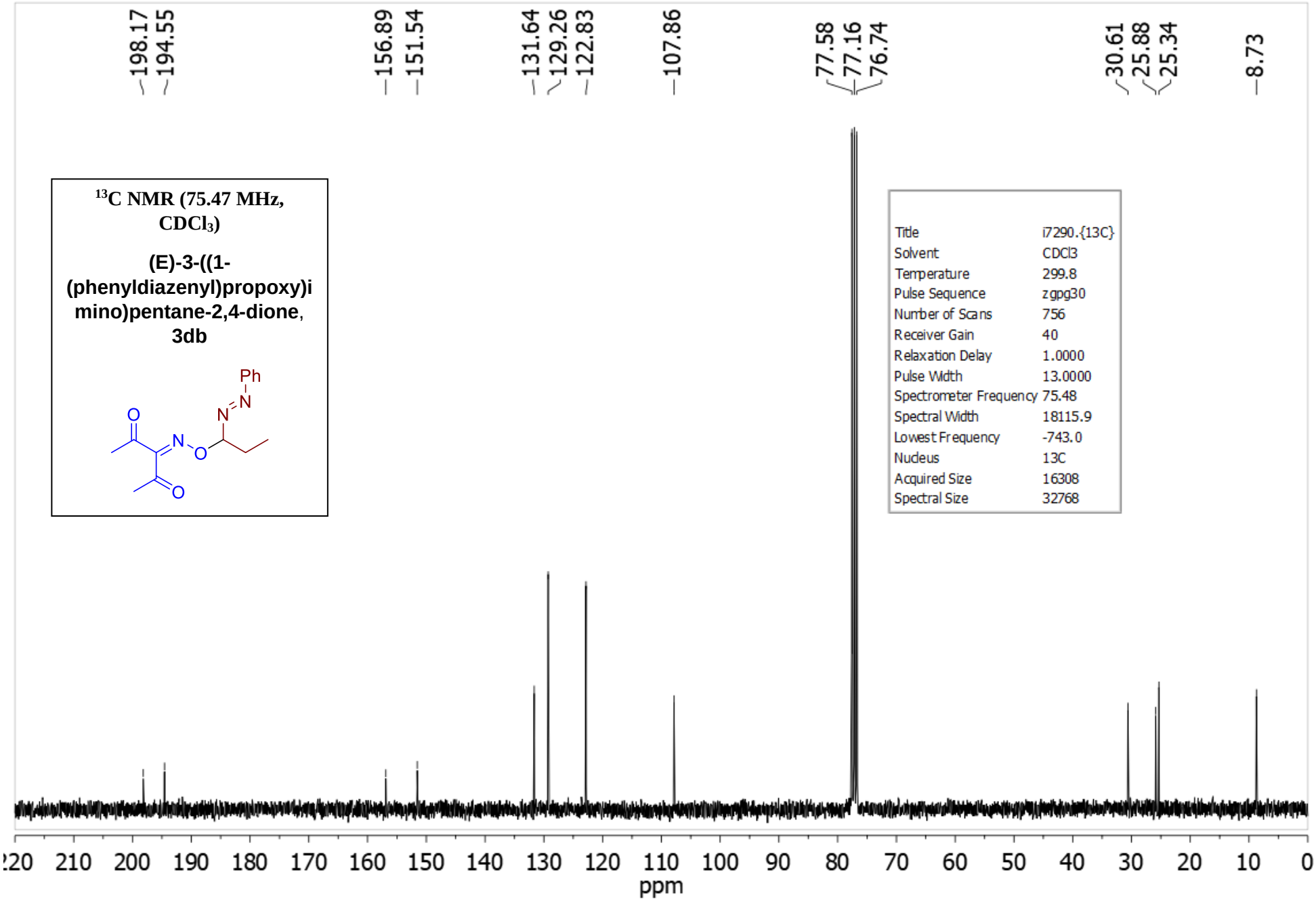

7.71 7.70 7.69 7.68 7.68 7.66 7.49 7.48 7.47 7.46 7.45 7.44 7.26
2.46 2.35 2.15 2.11 1.90 1.89 1.86 1.85 1.82 1.80 1.77 1.76 1.74 1.73 1.72 1.64 1.61 1.57 1.56 1.54 1.53 1.49 1.43 1.41 1.38 1.35 1.34
^{1}H NMR (300.13 MHz, $CDCl_3$)
(E)-3-(((1-(phenyldiazenyl)cyclohexyl)oxy)imino)pentane-2,4-dione, 3cg
Ph
N
N
O
N
O
O
Title i6751.{1H}.1.fid
Solvent CDCl3
Temperature 298.9
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 -610.3
Nucleus 1H
Acquired Size 8124
Spectral Size 65536
1.86 2.97 2.99 3.00 2.20 5.51 2.70 1.18
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

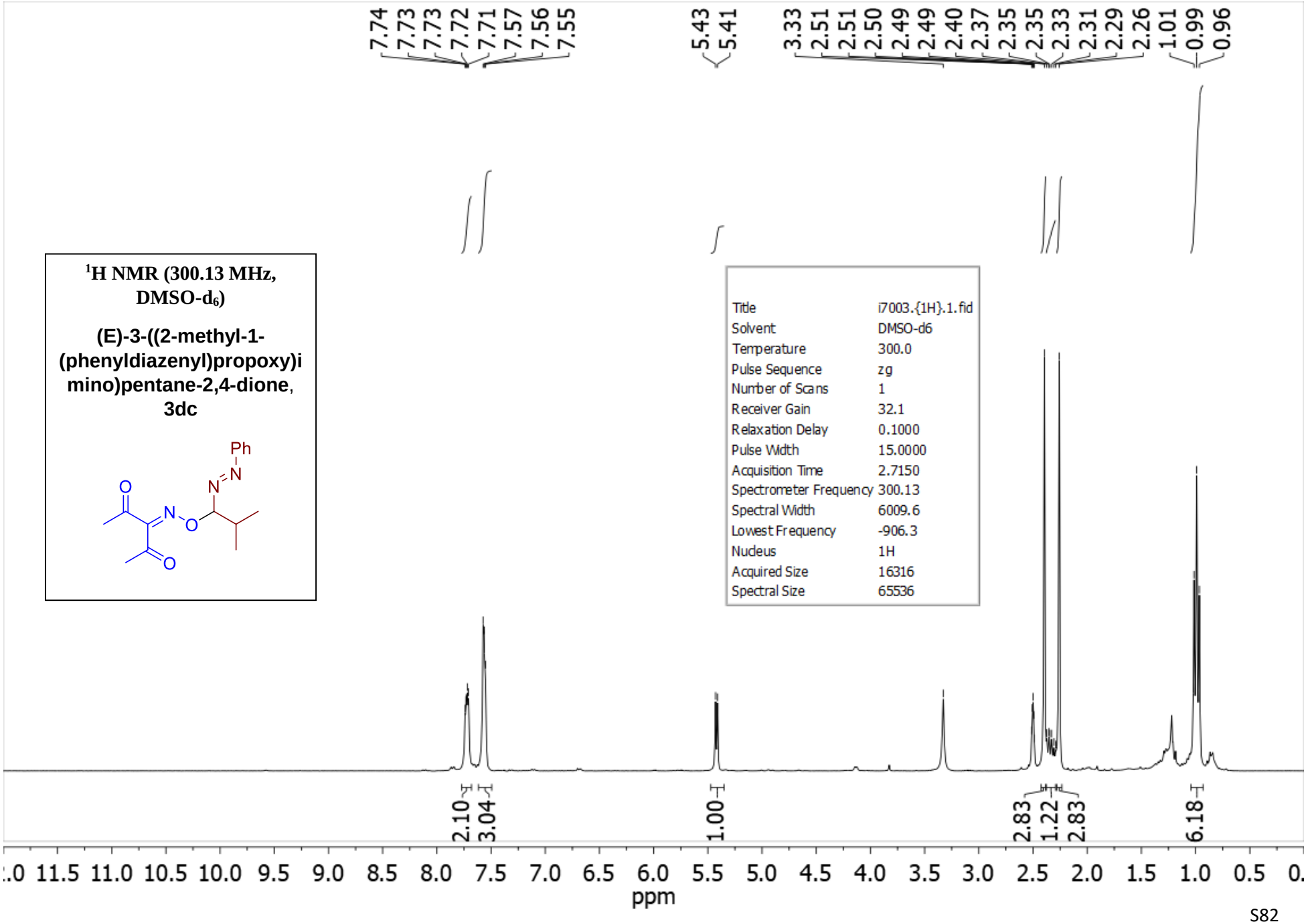

198.87
194.80
156.63
151.74
131.20
129.17
122.55
105.20
77.58
77.16
76.74
32.11
30.57
25.85
24.99
21.93
^{13}C NMR (75.47 MHz, $CDCl_3$)
(E)-3-(((1-(phenyldiazenyl)cyclohexyl)oxy)imino)pentane-2,4-dione, 3cg
Ph
N
N
O
N
O
O
Title i6751.{13C}.13.fid
Solvent CDCl3
Temperature 298.2
Pulse Sequence zgpg30
Number of Scans 228
Receiver Gain 3250.0
Relaxation Delay 1.0000
Pulse Width 13.0000
Acquisition Time 0.9006
Spectrometer Frequency 75.48
Spectral Width 18115.9
Lowest Frequency -746.9
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

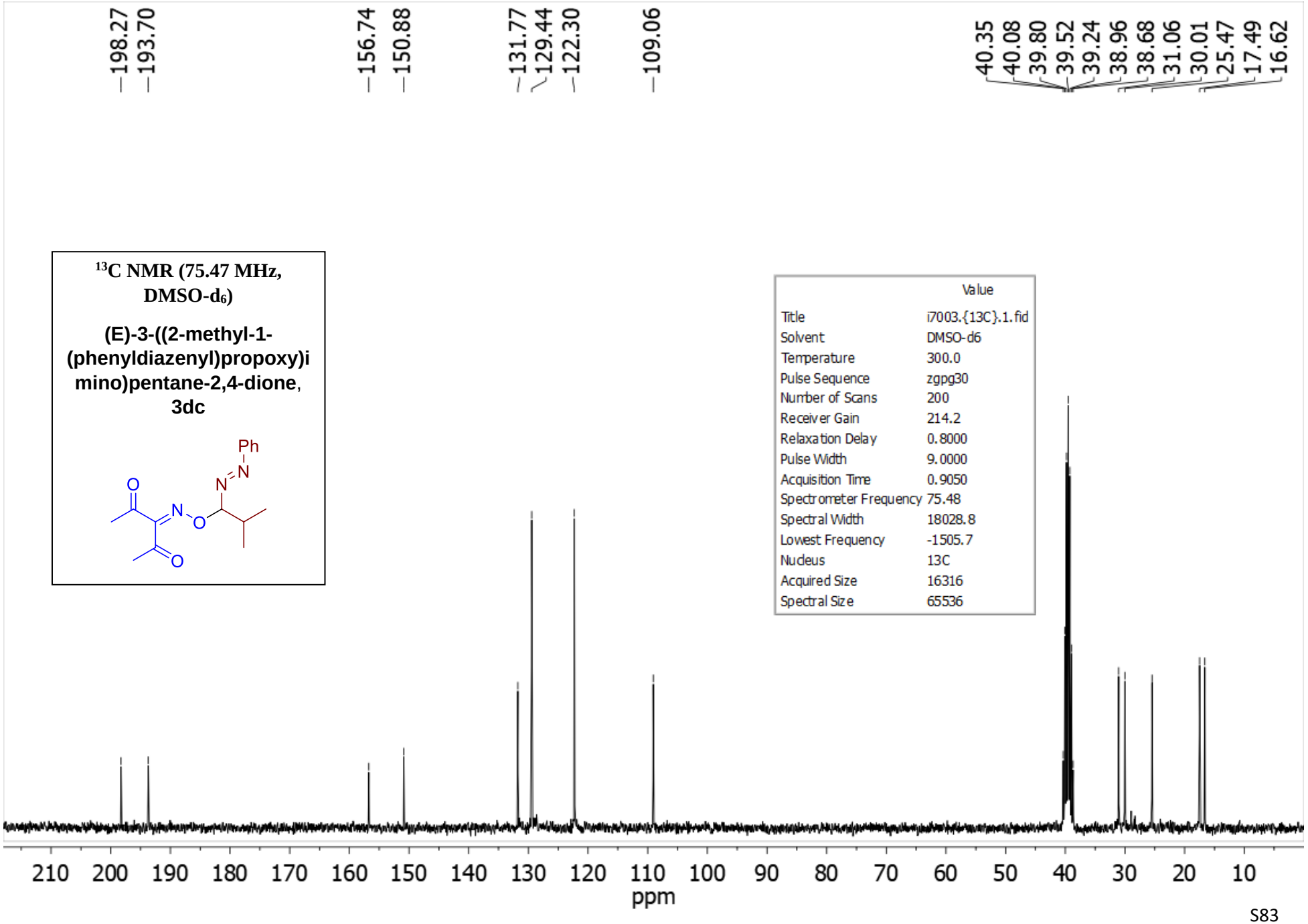

7.76
7.75
7.75
7.75
7.74
7.73
7.73
7.73
7.51
7.50
7.49
7.49
7.48
7.48
7.48
7.47
7.26
5.70
5.68
5.66
5.64
2.45
2.34
1.60
1.58
^{1}H NMR (300.13 MHz, $CDCl_3$)
(E)-3-((1-(phenyldiazenyl)ethoxy)imino)pentane-2,4-dione, 3da
Ph
N
N
O
N
O
O
O
Title i7497.{1H}.1.fid
Solvent CDCl3
Temperature 300.0
Pulse Sequence 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
1.96
3.00
0.97
3.00
2.97
3.12
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

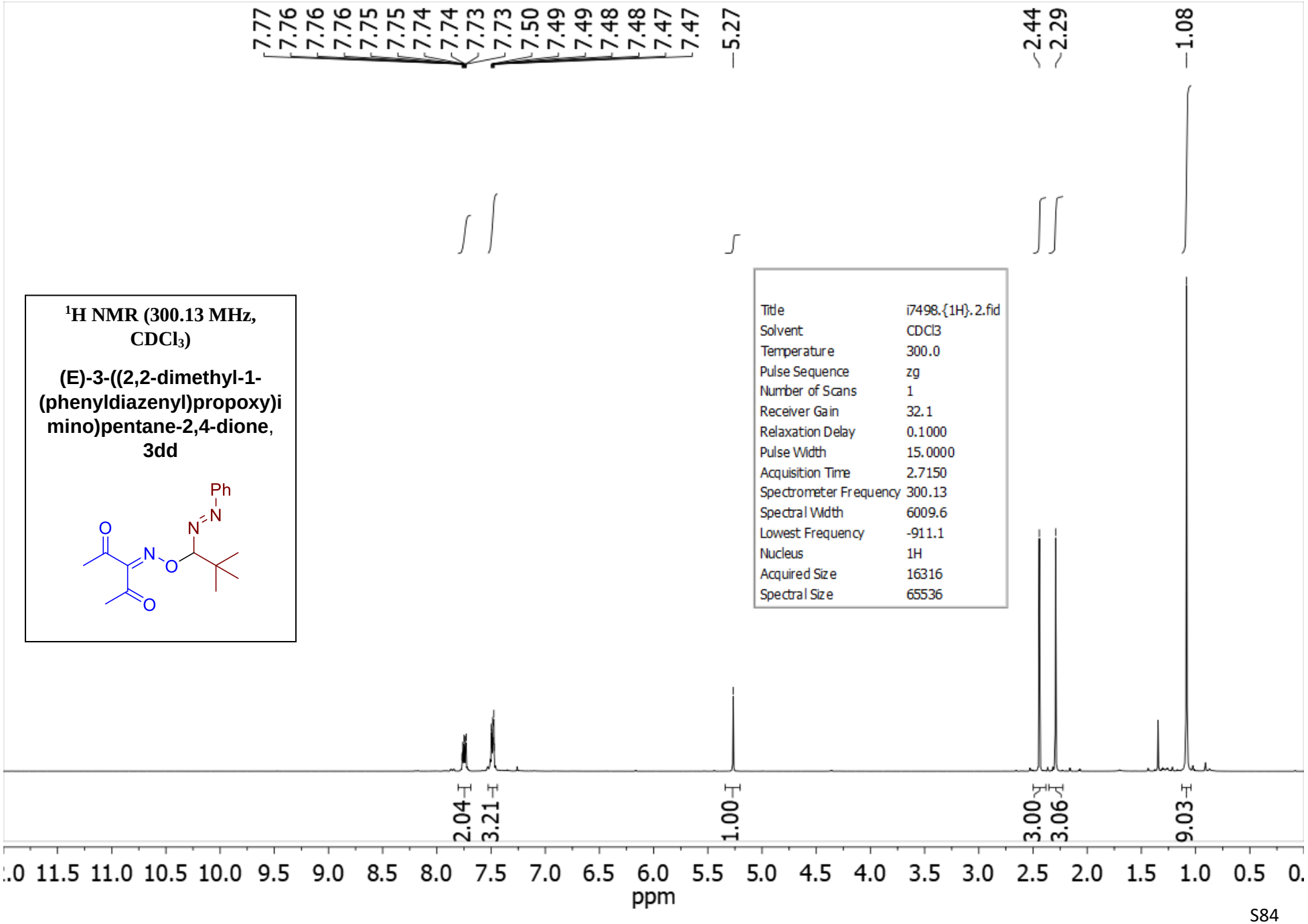

198.18
194.54
156.78
151.49
131.67
129.25
122.80
103.54
77.58
77.16
76.74
30.61
25.86
17.48
13C NMR (75.47 MHz, CDCl3)
(E)-3-((1-(phenyldiazenyl)ethoxy)imino)pentane-2,4-dione, 3da
Ph
N
N
O
N
O
O
Title i7497.{13C}.13.fid
Solvent CDCl3
Temperature 301.2
Pulse Sequence zgpg30
Number of Scans 300
Receiver Gain 40.3
Relaxation Delay 1.0000
Pulse Width 13.0000
Acquisition Time 0.9002
Spectrometer Frequency 75.48
Spectral Width 18115.9
Lowest Frequency -745.7
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

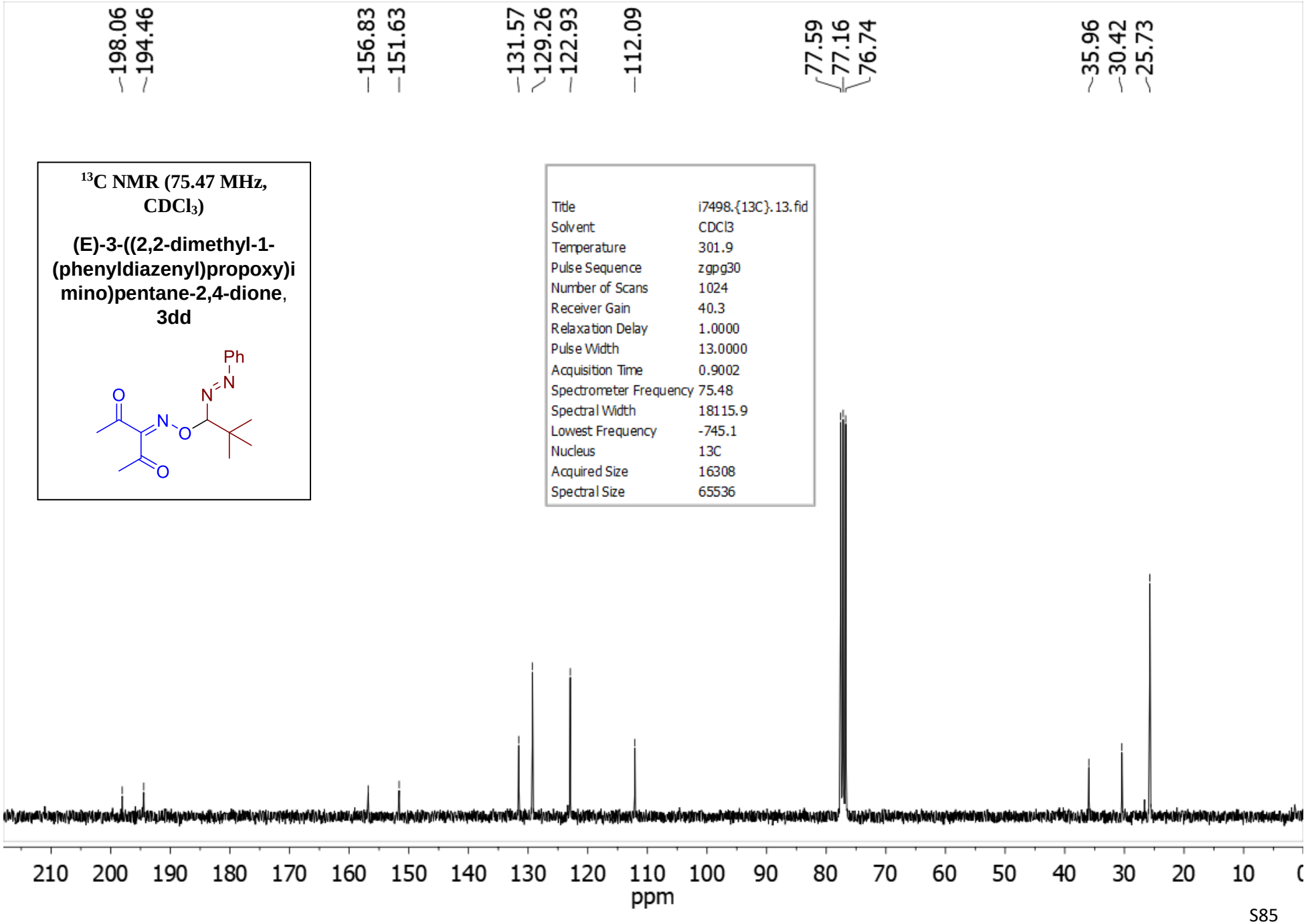

7.76 7.74 7.73 7.72 7.50 7.49 7.48 7.26
5.51 5.49 5.48 5.47
2.45 2.33 2.11 2.08 2.06 2.04 2.01 2.00 1.98 1.98 1.96 1.93 1.91 1.08 1.05 1.03
1H NMR (300.13 MHz, CDCl3)
(E)-3-((1-(phenyldiazenyl)propoxy)imino)pentane-2,4-dione, 3db
Ph
N
N
O
N
O
O
Parameter Value
Title i7290.{1H}
Solvent CDCl3
Temperature 299.9
Pulse Sequence zg
Number of Scans 1
Receiver Gain 90
Relaxation Delay 0.0050
Pulse Width 9.0000
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -609.2
Nucleus 1H
Acquired Size 8124
Spectral Size 16384
1.91
3.23
0.96
2.87
2.90
2.17
3.00
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
ppm

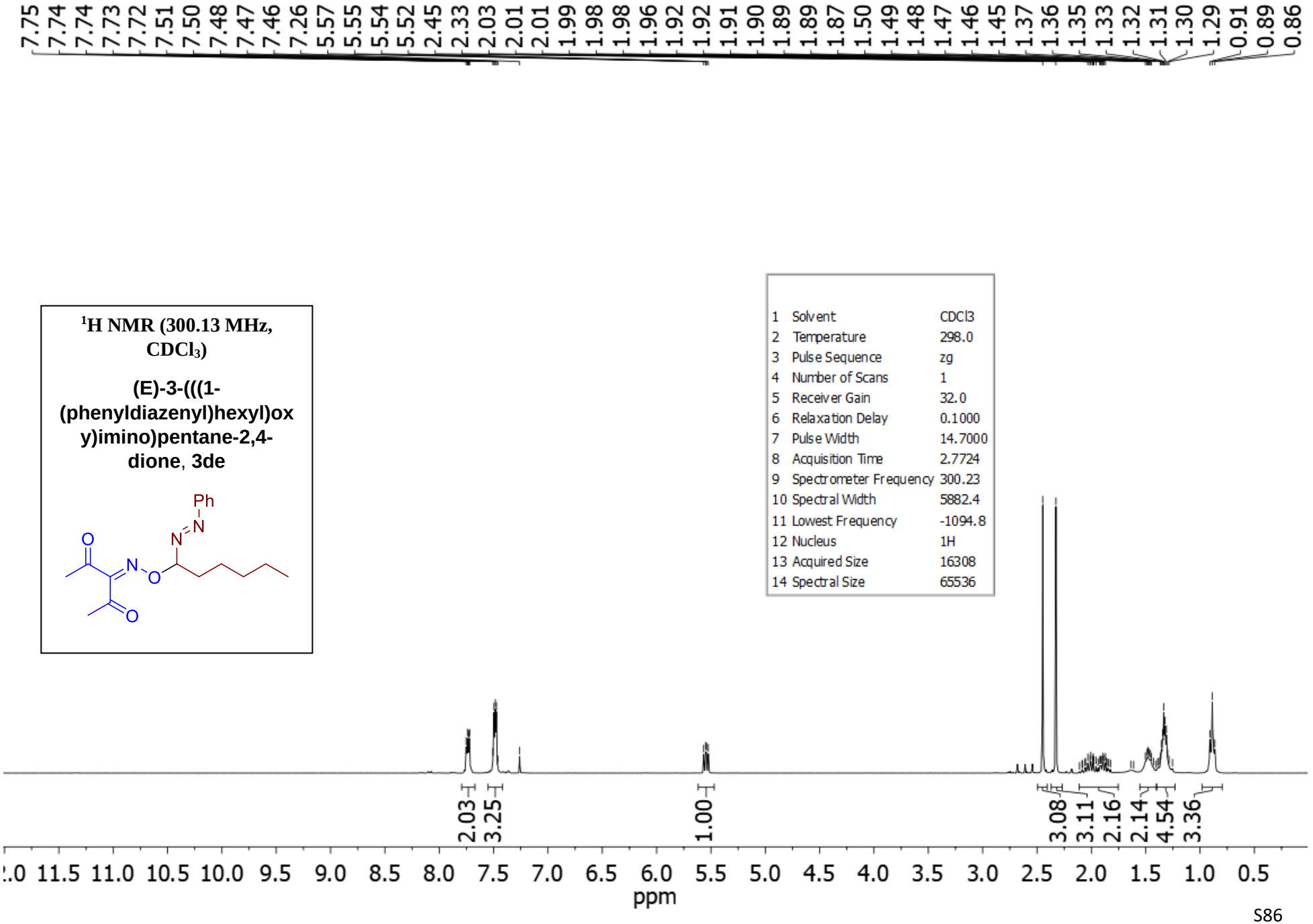

198.17
194.55
156.89
151.54
131.64
129.26
122.83
107.86
77.58
77.16
76.74
30.61
25.88
25.34
8.73
^{13}C NMR (75.47 MHz, $CDCl_3$)
(E)-3-((1-(phenyldiazenyl)propoxy)imino)pentane-2,4-dione, 3db
Ph
N
N
O
N
O
O
Title i7290.{13C}
Solvent CDCl3
Temperature 299.8
Pulse Sequence zgpg30
Number of Scans 756
Receiver Gain 40
Relaxation Delay 1.0000
Pulse Width 13.0000
Spectrometer Frequency 75.48
Spectral Width 18115.9
Lowest Frequency -743.0
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

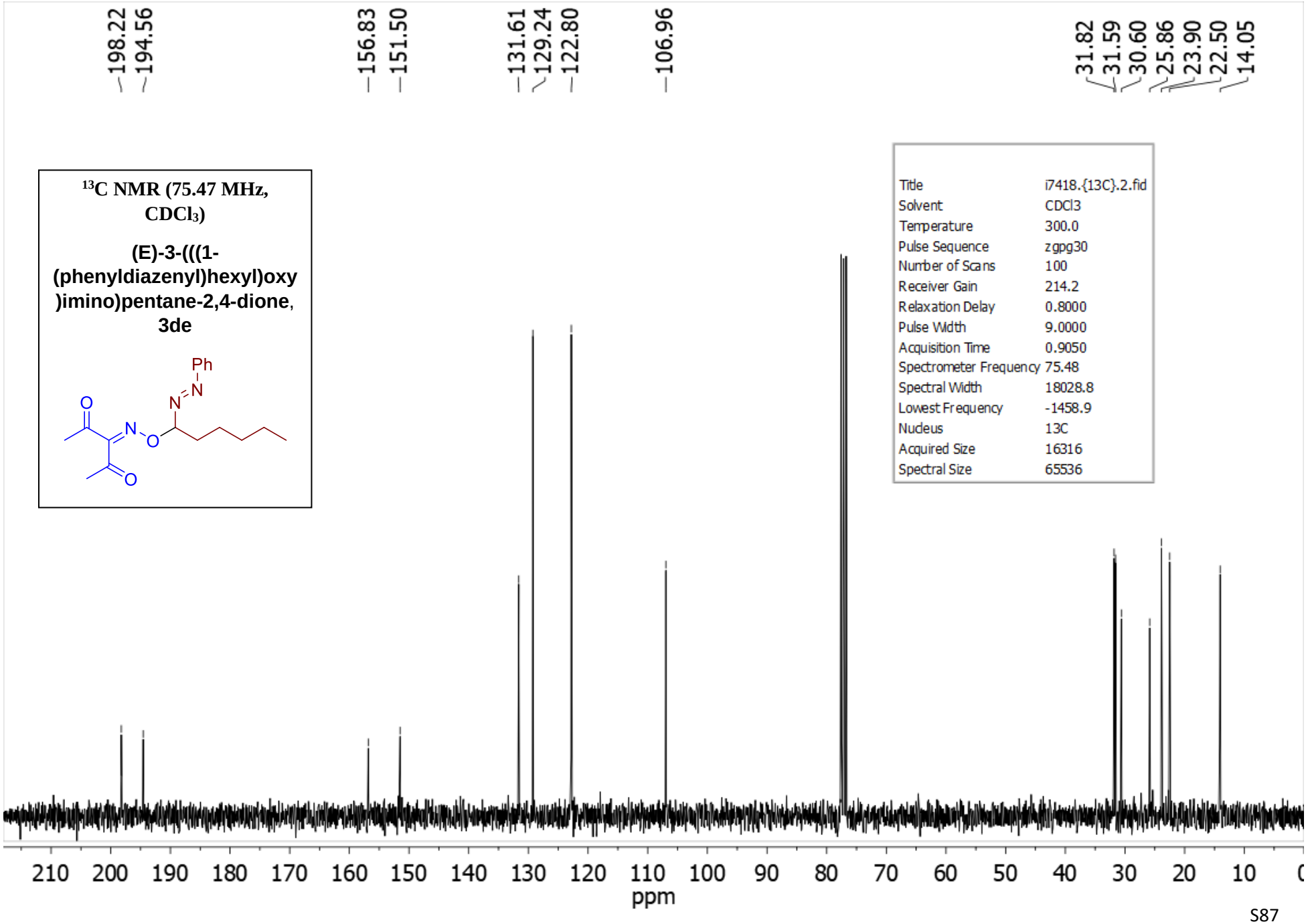

7.74
7.73
7.73
7.72
7.71
7.57
7.56
7.55
5.43
5.41
3.33
2.51
2.51
2.50
2.49
2.49
2.40
2.37
2.35
2.35
2.33
2.31
2.29
2.26
1.01
0.99
0.96
¹H NMR (300.13 MHz, DMSO-d6)
(E)-3-((2-methyl-1-(phenyldiazenyl)propoxy)imino)pentane-2,4-dione, 3dc
Ph
N
N
O
N
O
O
Title i7003.{1H}.1.fid
Solvent DMSO-d6
Temperature 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 -906.3
Nucleus 1H
Acquired Size 16316
Spectral Size 65536
2.10
3.04
1.00
2.83
1.22
2.83
6.18
.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.
ppm


198.27
193.70
156.74
150.88
131.77
129.44
122.30
109.06
40.35
40.08
39.80
39.52
39.24
38.96
38.68
31.06
30.01
25.47
17.49
16.62
13C NMR (75.47 MHz, DMSO-d6)
(E)-3-((2-methyl-1-(phenyldiazenyl)propoxy)imino)pentane-2,4-dione, 3dc
Ph
N
N
O
N
O
O
Value
Title i7003.{13C}.1.fid
Solvent DMSO-d6
Temperature 300.0
Pulse Sequence zgpg30
Number of Scans 200
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 -1505.7
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


7.77
7.76
7.76
7.76
7.75
7.75
7.74
7.74
7.73
7.73
7.50
7.49
7.49
7.48
7.48
7.47
7.47
5.27
2.44
2.29
1.08
^{1}H NMR (300.13 MHz, $CDCl_3$)
(E)-3-((2,2-dimethyl-1-(phenyldiazenyl)propoxy)imino)pentane-2,4-dione, 3dd
Ph
N
N
O
N
O
O
Title i7498.{1H}.2.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
2.04
3.21
1.00
3.00
3.06
9.03
ppm


198.06
194.46
156.83
151.63
131.57
129.26
122.93
112.09
77.59
77.16
76.74
35.96
30.42
25.73
^{13}C NMR (75.47 MHz, $CDCl_3$)
(E)-3-((2,2-dimethyl-1-(phenyldiazenyl)propoxy)imino)pentane-2,4-dione, 3dd
Ph
N
N
O
N
O
O
Title i7498.{13C}.13.fid
Solvent CDCl3
Temperature 301.9
Pulse Sequence zgpg30
Number of Scans 1024
Receiver Gain 40.3
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
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm


7.75 7.74 7.74 7.73 7.72 7.51 7.50 7.48 7.47 7.46 7.26 5.57 5.55 5.54 5.52 2.45 2.33 2.03 2.01 2.01 1.99 1.98 1.98 1.96 1.92 1.92 1.91 1.90 1.89 1.89 1.87 1.50 1.49 1.48 1.47 1.46 1.45 1.37 1.36 1.35 1.33 1.32 1.31 1.30 1.29 0.91 0.89 0.86
1H NMR (300.13 MHz, CDCl3)
(E)-3-(((1-(phenyldiazenyl)hexyl)oxy)imino)pentane-2,4-dione, 3de
Ph
N
N
O
N
O
O
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 -1094.8
12 Nucleus 1H
13 Acquired Size 16308
14 Spectral Size 65536
2.03
3.25
1.00
3.08
3.11
2.16
2.14
4.54
3.36
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


198.22
194.56
156.83
151.50
131.61
129.24
122.80
106.96
31.82
31.59
30.60
25.86
23.90
22.50
14.05
^{13}C NMR (75.47 MHz, $CDCl_3$)
(E)-3-(((1-(phenyldiazenyl)hexyl)oxy)imino)pentane-2,4-dione, 3de
Ph
N
N
O
N
O
O
Title i7418.{13C}.2.fid
Solvent CDCl3
Temperature 300.0
Pulse Sequence zgpg30
Number of Scans 100
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 -1458.9
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