

Electronic Supplementary Information for

**Detection and disaggregation of amyloid fibrils by luminescent
amphiphilic platinum(II) complexes**

*Zhuoheng Li,^a Akalanka B. Ekanayake,^a Anna E. Bartman,^b Jonathan A. Doorn,^b
Alexei V. Tivanski,^a and F. Christopher Pigge^{*a}*

^aDepartment of Chemistry, University of Iowa, Iowa City, Iowa, USA 52242

^bDepartment of Pharmaceutical Sciences and Experimental Therapeutics, University of Iowa,
Iowa City, Iowa, USA 52242

Corresponding author: chris-pigge@uiowa.edu

Table of Contents

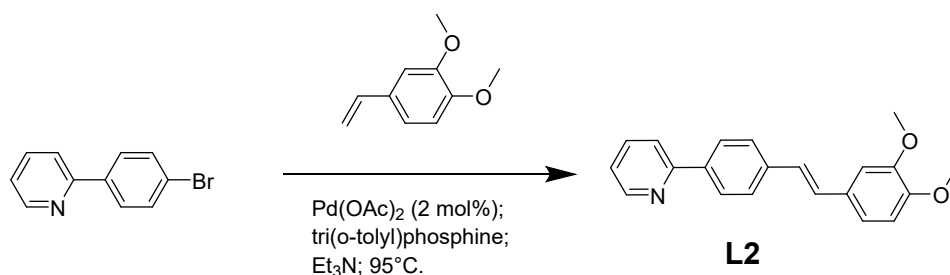
Materials and general methods.....	S2
Synthesis of ligands L2-L4 , L6-L8	S2-S5
Synthesis of Pt(II) complexes 6-14	S6-S12
Figs. S1-S9: UV-Visible absorption spectra of Pt(II) complexes 6-14	S12-S16
Fig. S10-S16: Emission spectra of Pt(II) complexes 6-7 , 9-12 , and 14	S17-S20
Fig. S17: ThT Fluorescence assay of HEWL fibrillization.....	S20
Fig. S18: Plot of emission enhancement of complexes 13 and 14 as a function of HEWL aggregation.....	S21
Figs. S19-S20: Plots of saturation binding isotherms for binding of 8 and 13 to HEWL fibrils.....	S21-S22
Fig. S21: Luminescence of 13 in the presence of other biomolecules.....	S22
Preparation of HEWL and A β ₄₂ fibrils.....	S22-S23
Procedures for luminescence assays.....	S23
Determination of K _d for binding of 8 and 13 to HEWL fibrils.....	S24
Procedures for AFM imaging experiments.....	S24-S25
Procedures for MTT cell viability assays.....	S25
Procedures for obtaining X-ray crystal structures and crystallographic data for 7-9	S25-S31
References.....	S32
¹ H- and ¹³ C-NMR spectra of all new compounds.....	S33-S57

Materials and general methods

All reactions were carried out under Ar unless specifically noted. All commercially available materials, reagents and solvents were used as supplied unless otherwise noted. K_2PtCl_4 was purchased from Strem Chemicals, Inc., hen egg-white lysozyme (HEWL, lyophilized powder) was purchased from Sigma-Aldrich, and beta amyloid 1-42 ($A\beta_{42}$, HFIP-treated) was purchased from rPeptide. SH-SY5Y neuroblastoma cells were obtained from ATCC. Reported chemical yields are isolated yields. Proton (1H) and carbon (^{13}C) NMR were collected on Bruker NMR spectrometers at 600, 500, or 400 MHz for 1H and 150, 125, or 100 MHz for ^{13}C . Chemical shifts (δ) are reported in parts per million (ppm) referenced to undeuterated residual solvent. High resolution mass spectra were collected on a Thermo Q-Exactive (Orbitrap) mass spectrometer. Absorption spectra were obtained using an Agilent Cary 100 UV-Vis spectrophotometer. Emission spectra were obtained using either an Agilent Cary Eclipse fluorescence spectrometer or a FluoroMax Plus fluorimeter (HORIBA Scientific, Ltd.). All luminescence spectrophotometry was performed on samples open to air. Dynamic light scattering (DLS) experiments were performed using a Malvern Zetasizer Nano ZS instrument.

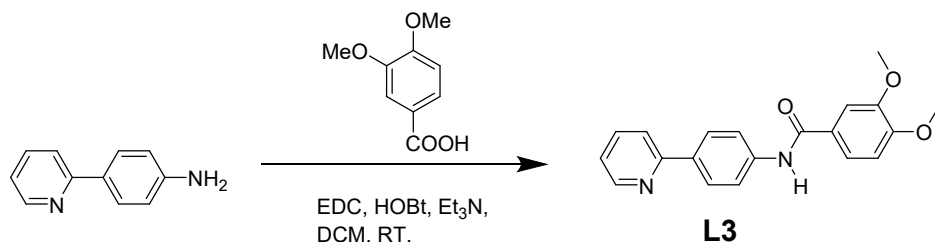
Synthesis of Ligands (L2, L3, L4, L6-L8)

Synthesis of L2



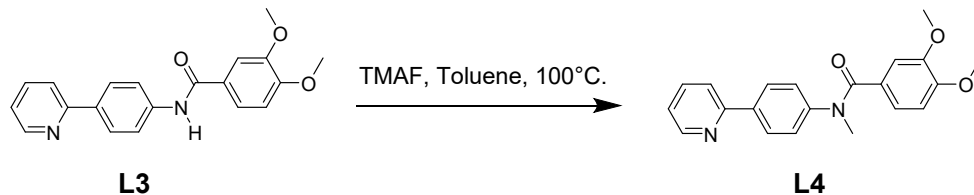
3,4-Dimethoxystyrene was prepared according to literature reports.¹ 2-(4-Bromophenyl)pyridine (0.56 g, 2.37 mmol) was dissolved in 3.3 mL Et_3N and the solution was stirred and purged with Ar for 15 mins. 3,4-Dimethoxystyrene (0.43 g, 2.62 mmol), $Pd(OAc)_2$ (0.011 g, 0.047 mmol) and tri(o-tolyl)phosphine (0.043 g, 0.14 mmol) were added. The reaction mixture was stirred at $95^\circ C$ for 24 hours. The resulting mixture was allowed to cool to room temperature. Brine was added and the reaction mixture was extracted with DCM. The combined extracts were dried over Na_2SO_4 , filtered, and concentrated under vacuum. The crude product was further purified by silica gel column chromatography, eluting with 30% EtOAc/70% hexane, to give L2 in 88% yield (0.67 g, 2.09 mmol). 1H NMR (500 MHz, $CDCl_3$) δ 8.67 (dt, $J = 4.7, 1.3$ Hz, 1H), 7.99-7.97 (m, 2H), 7.70-7.65 (m, 2H), 7.58-7.56 (m, 2H), 7.18-7.15 (m, 1H), 7.10 (d, $J = 16.3$ Hz, 1H), 7.07-7.02 (m, 2H), 6.99 (d, $J = 16.3$ Hz, 1H), 6.82 (d, $J = 8.3$ Hz, 1H), 3.91 (s, 3H), 3.86 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.0, 149.8, 149.3, 149.2, 138.3, 138.2, 136.8, 130.5, 129.2, 127.2, 126.8, 126.4, 122.1, 120.4, 120.2, 111.4, 109.0, 56.0, 56.0; HRMS (ESI) calcd for $C_{21}H_{20}O_2N$ $[M+H]^+$ 318.1489, found 318.1483.

Synthesis of **L3**



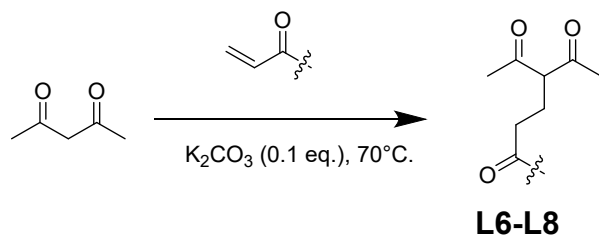
3,4-Dimethoxybenzoic acid (2.01 g, 10.97 mmol) was dissolved in 40 mL DCM. 4-(2-Pyridinyl)benzenamine (2.02 g, 12.07 mmol), EDC (hydrochloride, 3.15 g, 16.46 mmol), HOBT (monohydrate, 2.52 g, 16.46 mmol), and Et₃N (1.66 g, 16.46 mmol) were added. The reaction mixture was stirred at room temperature for 24 h. The solvent was removed under vacuum. Ethanol (200 mL) was added to the crude sample and the resulting mixture was stirred at 78 °C for 10 mins. Insoluble **L3** was collected by vacuum filtration and dried under vacuum. NMR indicated this material was of sufficient purity for use in subsequent reactions. Yield – 1.45 g (4.33 mmol), 40%. ¹H NMR (600 MHz, CDCl₃) δ 8.61-8.60 (m, 1H), 7.96-7.94 (m, 2H) 7.90 (br s, 1H), 7.70-7.65 (m, 4H), 7.45 (d, J = 2.0 Hz, 1H), 7.35 (dd, J = 8.4, 2.1 Hz, 1H), 7.15-7.13 (m, 1H), 6.84-6.83 (m, 1H), 3.88 (s, 3H), 3.87 (s, 3H); ¹³C NMR (150 MHz, CDCl₃) δ 165.2, 156.7, 152.1, 149.6, 149.2, 138.9, 136.8, 135.2, 127.6, 127.4, 121.9, 120.1, 120.0, 119.4, 110.7, 110.3, 56.0; HRMS (ESI) calcd for C₂₀H₁₉O₃N₂ [M+H]⁺ 335.1390, found 335.1385.

Synthesis of **L4**

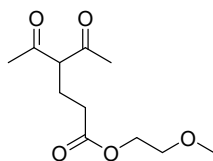


L4 was prepared using a method reported in the literature.² **L3** (0.21 g, 0.59 mmol) was dissolved in 6 mL toluene and tetramethylammonium fluoride (TMAF, 0.14 g, 1.43 mmol) was added. The reaction mixture was allowed to stir at 100 °C for 16 hours. The mixture was allowed to cool to room temperature and the solvent was removed under vacuum. The crude product was purified by silica gel column chromatography, eluting with hexane with increasing amount of EtOAc from 50% hexane/50% EtOAc to 30% hexane/70%EtOAc, to give **L4** in 72% yield (0.15 g, 0.43mmol). ¹H NMR (400 MHz, CDCl₃) δ 8.65 (dt, J = 4.7, 0.8 Hz, 1H), 7.91-7.88 (m, 2H), 7.72 (td, J = 7.6 Hz, 1.7Hz, 1H), 7.65 (d, J = 7.9Hz, 1H), 7.23-7.20 (m, 1H), 7.16-7.14 (m, 2H), 6.96-6.91 (m, 2H), 6.61 (d, J = 8.3 Hz, 1H), 3.78 (s, 3H), 3.67 (s, 3H), 3.53 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 171.0, 170.0, 156.1, 150.2, 149.6, 148.0, 146.1, 137.1, 136.8, 127.7, 127.6, 126.8, 122.7, 122.3, 120.2, 112.3, 109.9, 55.7, 55.6, 38.4, 14.1; HRMS (ESI) calcd for C₂₁H₂₁O₃N₂ [M+H]⁺ 349.1547, found 349.1539.

Synthesis of L6-L8

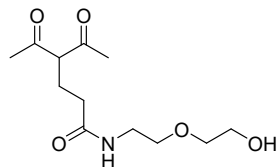


L6-L8 were prepared using modifications of a previously reported procedure.³ In general, K_2CO_3 (0.1 equivalent) was added to acetylacetone (acac, neat, 5 equivalents) and stirred at room temperature. The appropriate acrylate (1 equivalent) was then added and the reaction mixture was heated to $70^\circ C$ and maintained with stirring for 24 h. Insoluble material from the reaction mixture was removed by vacuum filtration and washed with DCM and MeOH. The filtrate was then concentrated under vacuum to give crude product. The acrylates were prepared using previously reported methods.^{4,5}



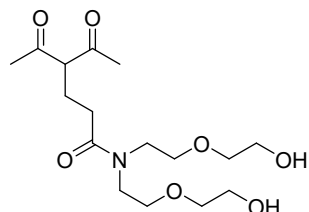
L6

L6 was prepared according to the general procedure from acac and 2-methoxyethyl acrylate (0.78 g, 5.99 mmol). Crude **L6** obtained from the reaction (93%, 1.28 g, 5.55 mmol) was used directly in subsequent reactions. 1H NMR (600 MHz, $CDCl_3$), mixture of tautomers: δ 4.27-4.25 (m, 2H), 3.8 (t, $J = 7.0$ Hz, 0.6H), 3.63-3.61 (m, 2H), 3.41-3.40 (m, 3H), 2.65-2.62 (m, 0.6H), 2.50-2.47 (m, 0.6H), 2.39-2.38 (t, $J = 7.2$ Hz, 1.4H), 2.23 (s, 4H), 2.19-2.14 (m, 3H); ^{13}C NMR (150 MHz, $CDCl_3$), mixture of tautomers δ 203.6, 191.2, 172.3, 172.3, 108.5, 70.2, 70.1, 66.6, 63.4, 63.4, 58.7, 58.7, 34.4, 31.3, 29.2, 22.7, 22.7, 22.6; HRMS (ESI) calcd for $C_{11}H_{19}O_5$ $[M+H]^+$ 231.1227, found 231.1225.



L7

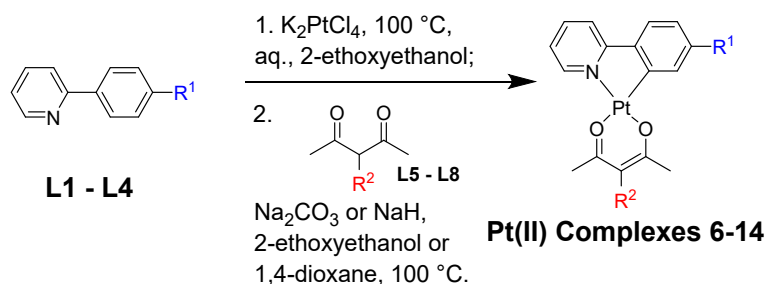
L7 was prepared according to the general procedure from acac and N-(2-(2-hydroxyethoxy)ethyl)acrylamide (1.75 g, 10.99 mmol). The crude product obtained directly from the reaction mixture was further purified by silica gel column chromatography, eluting with DCM with increasing amount of MeOH from 99% DCM/1% MeOH to 94% DCM/6% MeOH, to give **L7** in 17% yield (0.50 g, 1.94 mmol). ¹H NMR (400 MHz, CDCl₃), mixture of tautomers: δ 3.79-3.75 (m, 2H), 3.61-3.54 (m, 4H), 3.48-3.43 (m, 4H), 2.65-2.61 (m, 0.5H), 2.29-2.25 (m, 0.5H), 2.21 (s, 4H), 2.17-2.15 (m, 4H); ¹³C NMR (100 MHz, CDCl₃), mixture of tautomers δ 204.6, 191.6, 172.2, 172.0, 170.8, 146.2, 117.5, 109.1, 72.5, 72.2, 69.7, 69.6, 69.3, 66.8, 61.5, 41.3, 39.3, 39.2, 36.9, 33.3, 31.2, 29.8, 29.4, 23.5, 23.4, 22.9, 22.1, 16.3; HRMS (ESI) calcd for C₁₂H₂₂O₅N [M+H]⁺ 260.1492, found 260.1491.



L8

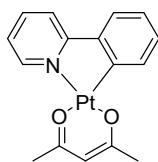
L8 was prepared according to the general procedure from acac and N,N-bis[2-(2-hydroxyethoxy)ethyl]-2-propenamide (0.53 g, 2.16 mmol). The crude product was further purified by silica gel column chromatography, eluting with DCM with increasing amount of MeOH from 95% DCM/5% MeOH to 92% DCM/ 8% MeOH, to give **L8** in 54% yield (0.40 g, 1.16 mmol). ¹H NMR (400 MHz, CDCl₃), mixture of tautomers: δ 3.81 (t, J = 6.8 Hz, 1H), 3.72-3.53 (m, 21H), 2.62-2.58 (m, 0.5H), 2.50-2.46 (m, 0.5H), 2.43 (t, J = 7.1 Hz, 2H), 2.22 (s, 5H), 2.18-2.11 (m, 3.5H); ¹³C NMR (100 MHz, CDCl₃), mixture of tautomers: δ 205.0, 191.3, 172.7, 172.6, 128.1, 127.8, 109.1, 72.9, 72.8, 72.4, 72.3, 69.2, 69.1, 69.1, 69.0, 66.8, 61.6, 61.5, 61.5, 48.8, 48.7, 46.6, 46.4, 33.6, 30.2, 29.4, 23.0, 23.0, 22.9; HRMS (ESI) calcd for C₁₆H₃₀O₇N [M+H]⁺ 348.2017, found 348.2020.

Synthesis of Pt(II) Complexes 6-14



Complexes **7-14** were prepared via modifications to the two-step method previously reported for the preparation of **6**.⁶ In general, K_2PtCl_4 (1 equivalent) was suspended in a mixture of H_2O /2-ethoxyethanol (~1:3 – 1:4, v/v) and the 2-phenylpyridine ligand (ppy, 1.0 – 3.5 equivalents, **L1-L4**) was added. The reaction mixture was heated with stirring to 100 °C for 48 h. The reaction was allowed to cool to room temperature and H_2O added until precipitation of the intermediate chloride-bridged Pt dimer was complete. The precipitate was collected by vacuum filtration, washed with H_2O , and dried under vacuum. These materials were used directly in the next step without further purification.

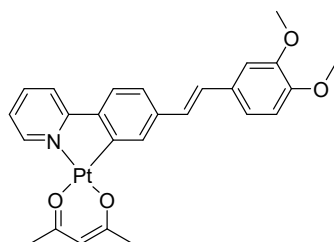
For the second step, the chloride-bridged dimer obtained in the first step (1 equivalent) was suspended in 2-ethoxyethanol or 1,4-dioxane. The acetylacetonate (acac) ligand **L5-L8** (3 equivalents) and base (3 – 10 equivalents of Na_2CO_3 or NaH) were added. The reaction mixture was heated to 100 °C for 24 h. The reaction mixture was then allowed to cool to room temperature and MeOH was added. The solvent was then removed under vacuum to give the crude product. Overall yields were calculated based on amount of K_2PtCl_4 used.



Complex 6

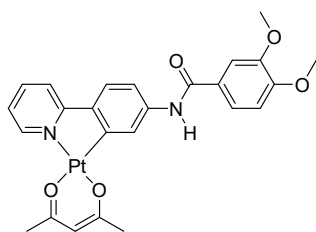
Complex **6** was prepared according to the general procedure using **L1** (0.11 g, 0.96 mmol) and K_2PtCl_4 (0.30 g, 0.96 mmol) in 10 mL H_2O /2-ethoxyethanol (1:4, v/v) for the first step. The chloride-bridged dimer obtained from this reaction (0.22 g, 0.28 mmol) was suspended in 6 mL 1,4-dioxane and combined with **L5** (0.087 g, 0.87 mmol) and Na_2CO_3 (0.30 g, 2.90 mmol). The crude product obtained from the reaction was further purified by silica gel column chromatography, eluting with 20% EtOAc/80% hexane, to give **6** in 37% overall yield (0.12 g, 0.27 mmol). ^1H NMR (400 MHz, CDCl_3) δ 9.02-8.93 (m, 1H), 7.77 (td, $J = 7.8, 1.5$ Hz, 1H), 7.62-7.58 (m, 2H), 7.42 (dd, $J = 7.8, 1.0$ Hz, 1H), 7.19 (td, $J = 7.49, 1.3$ Hz, 1H), 7.10-7.06 (m, 2H), 5.46 (s, 1H), 1.99 (s, 3H), 1.99(s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 185.7, 184.1, 168.3,

147.3, 144.6, 138.9, 138.1, 130.5, 129.2, 123.5, 123.0, 121.1, 118.3, 102.5, 28.3, 27.1; HRMS (ESI) calcd for $C_{16}H_{16}O_2NPt$ $[M+H]^+$ 449.0823, found 449.0820.



Complex 7

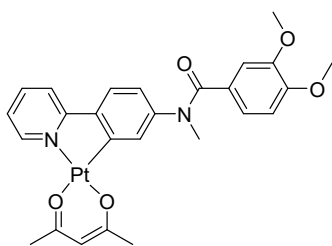
Complex **7** was prepared according to the general procedure except that all operations were performed in the dark (aluminum foil-wrapped glassware) to prevent light-induced isomerization of the stilbene alkene. Ligand **L2** (3.5 equivalents, 0.57 g, 1.81 mmol) and K_2PtCl_4 (0.21 g, 0.51 mmol) were combined in 12 mL $H_2O/2$ -ethoxyethanol (1:3, v/v) for the first step. Platinum dimer obtained from this reaction (0.40 g, 0.36 mmol) was suspended in 3 mL 2-ethoxyethanol. Acetylacetonone (**L5**, 0.11 g, 1.12 mmol) and Na_2CO_3 (0.39 g, 3.74 mmol) were added and the reaction performed as described in the general procedure. The crude product was further purified by silica gel column chromatography, eluting with 20% hexane/80% DCM, to give **7** in 51% overall yield (0.12 g, 0.27 mmol). X-ray quality single crystals of **7** were grown from $CH_2Cl_2/MeOH$ solution. 1H NMR (600 MHz, $CDCl_3$) δ 9.03-8.93 (m, 1H), 7.78 (td, $J = 7.7, 1.5$ Hz, 1H), 7.70 (d, $J = 1.6$ Hz, 1H), 7.61-7.57 (m, 1H), 7.42 (d, $J = 8.0$ Hz, 1H), 7.28 (dd, $J = 8.0, 1.6$ Hz, 1H), 7.15 (d, $J = 16.1$ Hz, 1H), 7.12-7.06 (m, 3H), 7.04 (d, $J = 16.1$ Hz, 1H), 6.86 (d, $J = 8.2$ Hz, 1H), 5.49 (s, 1H), 3.96 (s, 3H), 3.91 (s, 3H), 2.06 (s, 3H), 2.01 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 185.8, 184.1, 167.8, 149.0, 148.9, 147.3, 143.8, 138.7, 138.2, 138.0, 130.8, 129.0, 128.4, 127.6, 123.2, 121.6, 120.8, 120.1, 118.3, 111.1, 108.8, 102.5, 55.9, 55.9, 28.2, 27.2; HRMS (ESI) calcd for $C_{26}H_{26}O_4NPt$ $[M+H]^+$ 611.1504, found 611.1499.



Complex 8

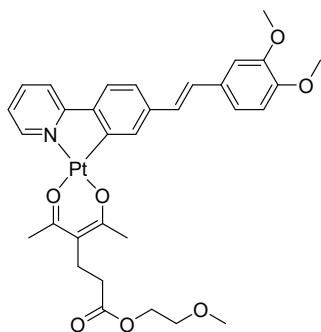
Complex **8** was prepared according to the general procedure using **L3** (0.30 g, 0.91 mmol) and K_2PtCl_4 (0.37 g, 0.91 mmol) in 10 mL $H_2O/2$ -ethoxyethanol (1:4, v/v) for the first step. The resulting chloride-bridged dimer (0.45 g, 0.40 mmol) was suspended into 10 mL 1,4-dioxane, and combined with **L5** (0.12 g, 1.20 mmol) and Na_2CO_3 (0.42 g, 4.01 mmol). The crude product was further purified by silica gel column chromatography, eluting with 4% MeOH/96% DCM, to

give **8** in 26% overall yield (0.15g, 0.24 mmol). X-ray quality single crystals of **8** were grown from CH₂Cl₂/MeOH solution. ¹H NMR (500 MHz, CDCl₃) δ 9.02-8.88 (m, 1H), 8.02 (dd, J = 8.3, 1.7 Hz, 1H), 7.87 (s, 1H), 7.79-7.76 (m, 1H), 7.57 (d, J = 7.8 Hz, 1H), 7.53-7.501 (m, 1H), 7.48 (d, J = 8.3 Hz, 1H), 7.42 (dd, J = 8.1, 1.8 Hz, 1H), 7.27-7.26 (m, 1H), 7.08-7.06 (m, 1H), 6.92 (d, J = 8.3 Hz, 1H), 5.48 (s, 1H), 3.96 (s, 3H), 3.94 (s, 3H), 2.03 (s, 3H), 2.01 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 186.1, 184.1, 167.9, 165.3, 152.1, 149.3, 147.2, 141.1, 139.5, 138.7, 138.3, 128.2, 124.3, 120.7, 120.4, 119.5, 118.3, 115.4, 111.0, 110.5, 102.8, 56.2, 56.2, 28.3, 27.3; HRMS (ESI) calcd for C₂₅H₂₅O₅N₂Pt [M+H]⁺ 628.1411, found 628.1408.



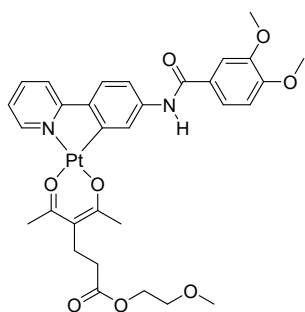
Complex 9

Complex **9** was prepared according to the general procedure using **L4** (0.22 g, 0.64 mmol) and K₂PtCl₄ (0.26 g, 0.64 mmol) in 10 mL H₂O/2-ethoxyethanol (1:4, v/v) for the first step. The resulting chloride-bridged dimer (0.13 g, 0.11 mmol) was suspended in 7 mL 1,4-dioxane and combined with **L5** (0.034 g, 0.34 mmol) and Na₂CO₃ (0.12 g, 1.13 mmol). The crude sample was further purified by silica gel column chromatography, eluting with hexane with increasing amount of EtOAc from 50% hexane/50% EtOAc to 30% hexane/70% EtOAc, to give **9** in 23% overall yield (0.092 g, 0.14 mmol). X-ray quality single crystals of **9** were grown from CH₂Cl₂/MeOH solution. ¹H NMR (400 MHz, CDCl₃) δ 9.00-8.92 (m, 1H), 7.80-7.75 (m, 1H), 7.48 (d, J = 8.0 Hz, 1H), 7.43 (d, J = 2.1 Hz, 1H), 7.20 (d, J = 8.2 Hz, 1H), 7.12-7.09 (m, 1H), 7.05-7.00 (m, 2H), 6.62-6.57 (m, 2H), 5.48 (s, 1H), 3.78 (s, 3H), 3.69 (s, 3H), 3.55 (s, 3H), 2.01 (s, 6H); ¹³C NMR (100 MHz, CDCl₃) δ 185.9, 184.2, 170.0, 167.1, 150.0, 147.8, 147.3, 145.6, 142.7, 140.2, 138.3, 128.2, 127.5, 123.3, 122.8, 122.7, 121.3, 118.5, 112.5, 109.7, 102.6, 55.7, 55.7, 38.5, 28.2, 21.1; HRMS (ESI) calcd for C₂₆H₂₇O₅N₂Pt [M+H]⁺ 642.1562, found 642.1559.



Complex 10

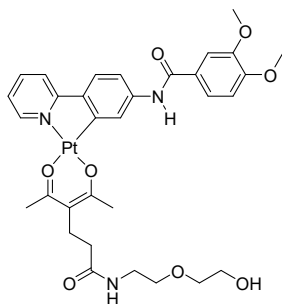
Complex **10** was prepared according to the general procedure except that all operations were performed in the dark (aluminum foil-wrapped glassware) to prevent light-induced isomerization of the stilbene alkene. Two equivalents **L2** (0.88 g, 2.79 mmol) and K_2PtCl_4 (0.56 g, 1.38 mmol) were reacted in 100 mL $H_2O/2$ -ethoxyethanol (1:3, v/v) for the first step. The crude dimer intermediate (0.83 g, 0.76 mmol) was suspended in 50 mL 1,4-dioxane and combined with **L6** (0.53 g, 2.29 mmol) and NaH (60% wt, 0.092 g, 2.29 mmol). The crude product was further purified by silica gel column chromatography, eluting with 60% hexane/40% EtOAc, to give **10** in 29% overall yield (0.29g, 0.34 mmol). 1H NMR (600 MHz, $CDCl_3$) δ 8.95-8.89 (m, 1H), 7.79-7.76 (m, 1H), 7.68 (d, $J = 1.6$ Hz, 1H), 7.58 (d, $J = 8.1$ Hz, 1H), 7.41 (d, $J = 8.0$ Hz, 1H), 7.28-7.26 (m, 1H), 7.15 (d, $J = 16.1$ Hz, 1H), 7.11-7.06 (m, 3H), 7.03 (d, $J = 16.1$ Hz, 1H), 6.87 (d, $J = 8.2$ Hz, 1H), 4.28-4.25 (m, 2H), 3.96 (s, 3H), 3.91 (s, 3H), 3.63-3.61 (m, 2H), 3.40 (s, 3H), 2.77-2.74 (m, 2H), 2.52-2.49 (m, 2H), 2.21 (s, 3H), 2.17 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 184.8, 182.7, 173.0, 168.0, 149.0, 148.9, 147.1, 143.9, 139.4, 138.2, 138.0, 130.7, 129.0, 128.5, 127.6, 123.2, 121.6, 120.8, 120.1, 118.3, 111.1, 110.0, 108.8, 70.4, 63.6, 59.0, 55.9, 55.9, 35.2, 27.8, 27.1, 26.4; HRMS (ESI) calcd for $C_{32}H_{36}O_7NPt$ $[M+H]^+$ 741.2134, found 741.2130.



Complex 11

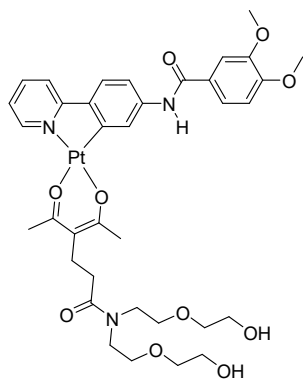
Complex **11** was prepared according to the general procedure using 2 equivalents of **L3** (1.27 g, 3.81 mmol) and K_2PtCl_4 (0.79 g, 1.90 mmol) in 100 mL $H_2O/2$ -ethoxyethanol (1:3, v/v) for the first step. The dimer intermediate (1.05 g, 0.93 mmol) was suspended in 50 mL 1,4-dioxane and combined with **L6** (0.65 g, 2.82 mmol) and NaH (60% wt, 0.11 g, 2.82 mmol). The crude

product was further purified by silica gel column chromatography, eluting with 40% hexane/60% EtOAc, to give **11** in 32% overall yield (0.47 g, 0.62 mmol). ¹H NMR (500 MHz, CDCl₃) δ 8.87 (d, J = 5.5 Hz, 1H), 7.97-7.93 (m, 2H), 7.79-7.72 (m, 1H), 7.56-7.46 (m, 3H), 7.41 (dd, J = 8.4, 2.0 Hz, 1H), 7.32-7.29 (m, 1H), 7.05 (t, J = 6.6 Hz, 1H), 6.91-6.89 (m, 1H), 4.26-4.24 (m, 2H), 3.95 (s, 3H), 3.93 (s, 3H), 3.62-6.60 (m, 2H), 3.39 (s, 3H), 2.75-2.71 (m, 2H), 2.50-2.46 (m, 2H), 2.16 (s, 6H); ¹³C NMR (125 MHz, CDCl₃) δ 185.0, 182.7, 173.1, 167.9, 165.3, 152.0, 149.2, 147.0, 141.1, 140.2, 138.7, 138.2, 128.0, 124.2, 120.6, 120.6, 119.5, 118.3, 115.3, 110.9, 110.4, 110.2, 70.5, 63.7, 59.1, 56.2, 56.1, 35.3, 27.9, 27.1, 26.5; HRMS (ESI) calcd for C₃₁H₃₅O₈N₂Pt [M+H]⁺ 758.2036, found 758.2036.



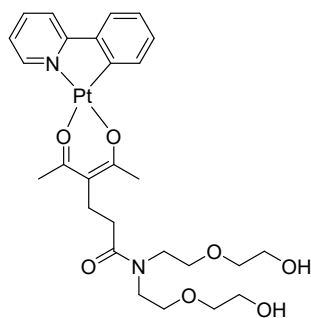
Complex 12

Complex **12** was prepared according to the general procedure using **L3** (0.24 g, 0.72 mmol) and K₂PtCl₄ (0.30 g, 0.72 mmol) in 10 mL H₂O/2-ethoxyethanol (1:4, v/v) for the first step. The resulting chloride-bridged dimer (0.35 g, 0.31 mmol) was suspended in 15 mL 1,4-dioxane and combined with **L7** (0.24 g, 0.93 mmol) and NaH (60% wt, 0.075 g, 1.87 mmol). The crude sample was further purified by silica gel column chromatography, eluting with DCM with increasing amount of MeOH from 98% DCM/2% MeOH to 95% DCM/5% MeOH, to give **12** in 17% overall yield (0.078 g, 0.099 mmol). ¹H NMR (400 MHz, CDCl₃) δ 7.78 (d, J = 5.5 Hz, 1H), 8.58 (s, 1H), 7.81-7.73 (m, 1H), 7.65 (t, J = 7.6 Hz, 1H), 7.52-7.44 (m, 4H), 7.38 (d, J = 8.5 Hz, 1H), 7.02-6.94 (m, 1H), 6.93-6.88 (m, 1H), 6.79 (d, J = 8.3 Hz, 1H), 3.86 (s, 3H), 3.85 (s, 3H), 3.67-3.59 (m, 2H), 3.51-3.43 (m, 4H), 3.38-3.31 (m, 2H), 2.66-2.55 (m, 2H), 2.24-2.15 (m, 2H), 2.02 (s, 3H), 1.98 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 184.9, 182.5, 173.0, 167.6, 165.8, 151.9, 148.9, 146.7, 141.0, 140.6, 138.6, 138.1, 127.6, 124.0, 121.3, 120.6, 120.2, 118.3, 115.8, 110.9, 110.5, 110.3, 72.3, 69.8, 61.5, 56.0, 56.0, 39.3, 37.2, 27.9, 27.0, 26.8; HRMS (ESI) calcd for C₃₂H₃₈O₈N₃Pt [M+H]⁺ 787.2301, found 787.2296.



Complex 13

Complex **13** was prepared according to the general procedure using **L3** (0.15 g, 0.45 mmol) and K_2PtCl_4 (0.18 g, 0.45 mmol) in 5 mL $H_2O/2$ -ethoxyethanol (1:4, v/v) for the first step. The crude dimer intermediate (0.089 g, 0.08 mmol) was suspended in 8 mL 1,4-dioxane and combined with **L8** (0.083 g, 0.24 mmol) and NaH (60% wt, 0.028 g, 0.71 mmol). The crude sample was further purified by silica gel column chromatography, eluting with DCM with increasing amount of MeOH from 99% DCM/1% MeOH to 96% DCM/4% MeOH, to give **13** in 45% overall yield (0.17 g, 0.19 mmol). 1H NMR (400 MHz, $CDCl_3$) δ 8.88-8.86 (m, 1H), 8.03 (s, 1H), 7.94-7.89 (m, 1H), 7.80-7.73 (m, 1H), 7.55 (d, $J = 8.1$ Hz, 1H), 7.51 (d, $J = 1.7$ Hz, 1H), 7.48-7.41 (m, 2H), 7.39-7.31 (m, 1H), 7.09-7.02 (m, 1H), 6.90 (d, $J = 8.3$ Hz, 1H), 3.94 (s, 3H), 3.93 (s, 3H), 3.75-3.49 (m, 16H), 2.79-2.68 (m, 2H), 2.56-2.47 (m, 2H), 2.16 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.1, 182.7, 173.3, 167.9, 165.4, 152.1, 149.2, 147.0, 141.1, 140.3, 138.7, 138.2, 128.0, 124.2, 120.7, 120.7, 119.6, 118.3, 115.4, 110.9, 110.6, 110.4, 72.9, 72.4, 69.5, 69.2, 61.8, 61.7, 56.2, 56.1, 49.0, 46.9, 34.4, 28.0, 27.2, 26.6; HRMS (ESI) calcd for $C_{36}H_{46}O_{10}N_3Pt$ $[M+H]^+$ 875.2825, found 875.2815.



Complex 14

Complex **14** was prepared according to the general procedure using **L1** (0.11g, 0.72 mmol) and K_2PtCl_4 (0.30 g, 0.72 mmol) in 5 mL $H_2O/2$ -ethoxyethanol (1:4, v/v) for the first step. The dimer intermediate (0.18 g, 0.23 mmol) was suspended in 6 mL 1,4-dioxane and combined with **L8** (0.21 g, 0.61 mmol) and NaH (60% wt, 0.088 g, 2.22 mmol). The crude sample was further purified by silica gel column chromatography, eluting with DCM with increasing amount of MeOH from 98% DCM/2% MeOH to 94% DCM/6% MeOH, to give **14** in 33% overall yield

(0.16 g, 0.23 mmol). ^1H NMR (400 MHz, CDCl_3) δ 8.99-8.86 (m, 1H), 7.81-7.74 (m, 1H), 7.66-7.54 (m, 2H), 7.43 (dd, $J = 7.8, 1.0$ Hz, 1H) 7.19 (td, $J = 7.4, 1.3$ Hz, 1H), 7.12-7.05 (m, 2H), 3.71-3.54 (m, 16H), 2.78-2.72 (m, 2H), 2.54-2.48 (m, 2H), 2.16 (s, 3H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 185.0, 182.8, 173.3, 168.5, 147.2, 144.8, 139.8, 138.2, 130.7, 129.3, 123.6, 123.1, 121.2, 118.4, 110.5, 72.9, 72.4, 69.5, 69.3, 61.8, 61.7, 49.0, 46.9, 34.4, 28.0, 27.1, 26.6 ; HRMS (ESI) calcd for $\text{C}_{27}\text{H}_{37}\text{O}_7\text{N}_2\text{Pt}$ $[\text{M}+\text{H}]^+$ 696.2243, found 696.2236.

Absorption and Emission Spectra

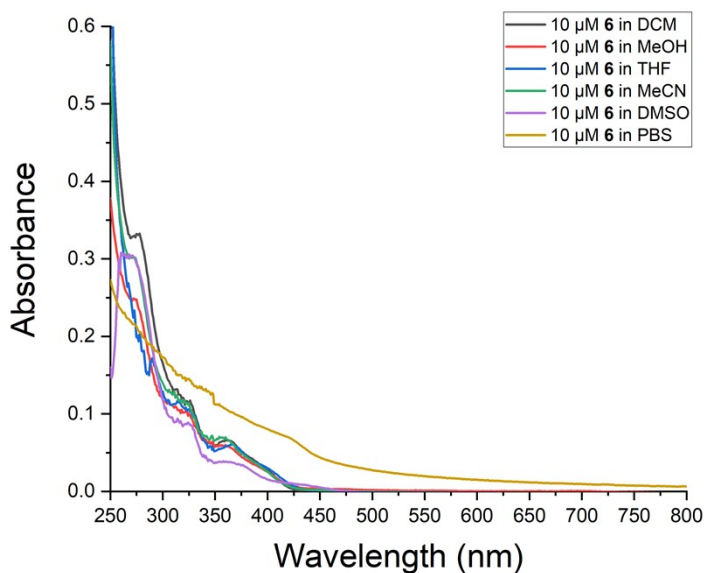


Fig. S1. Absorption spectra of **6** in various solvents. $[\mathbf{6}] = 10 \mu\text{M}$ with 0.5% (v/v) DMSO in the indicated solvents.

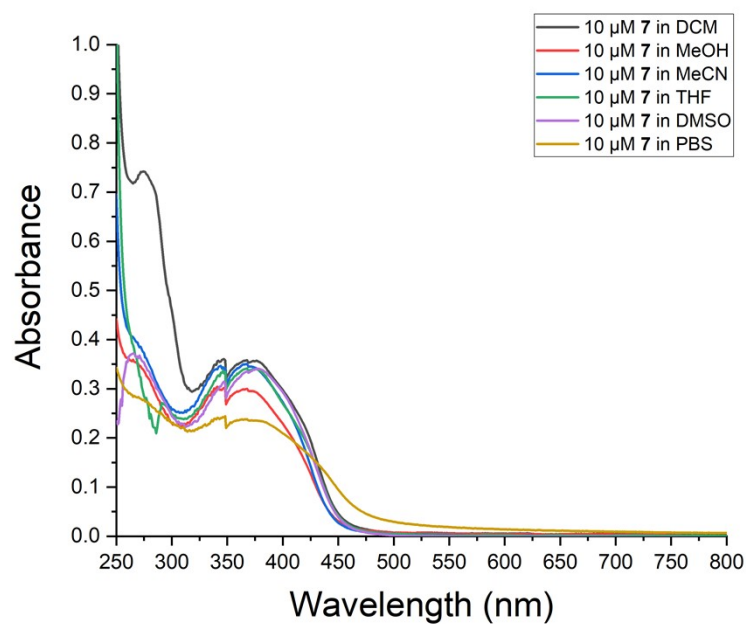


Fig. S2. Absorption spectra of **7** in various solvents. [**7**] = 10 μM with 0.5% (v/v) DMSO in the indicated solvents.

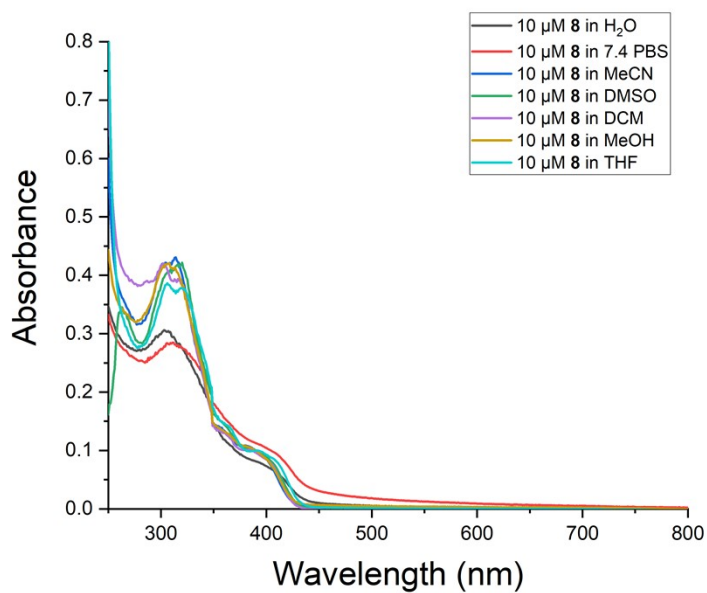


Fig. S3. Absorption spectra of **8** in various solvents. [**8**] = 10 μM with 0.5% (v/v) DMSO in the indicated solvents.

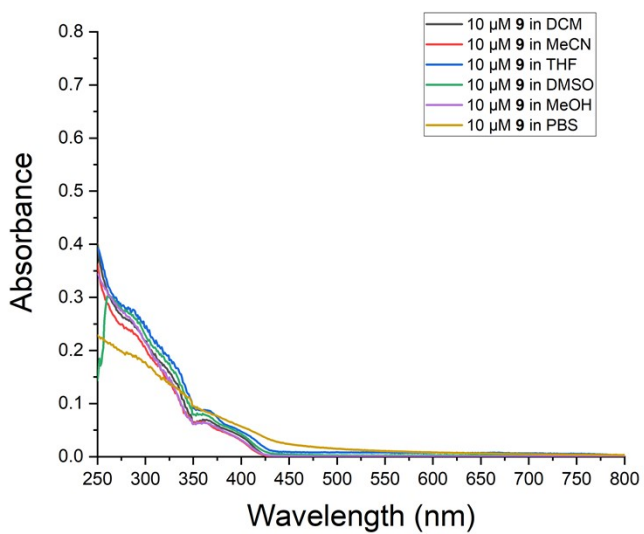


Fig. S4. Absorption spectra of **9** in various solvents. [**9**] = 10 μ M with 0.5% (v/v) DMSO in the indicated solvents.

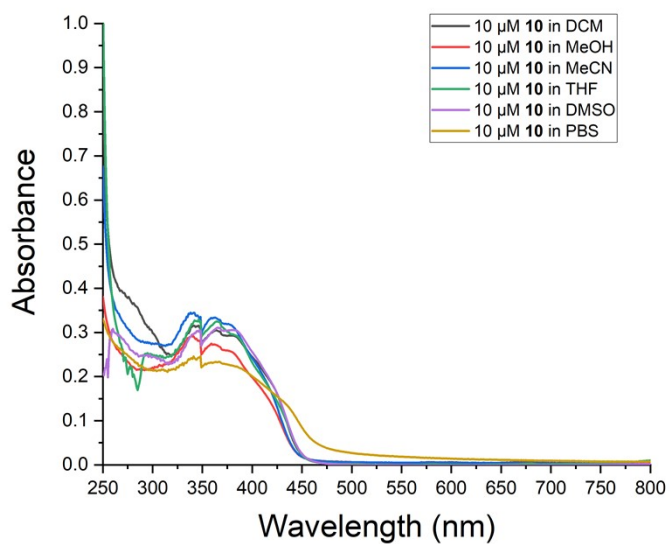


Fig. S5. Absorption spectra of **10** in various solvents. [**10**] = 10 μ M with 0.5% (v/v) DMSO in the indicated solvents.

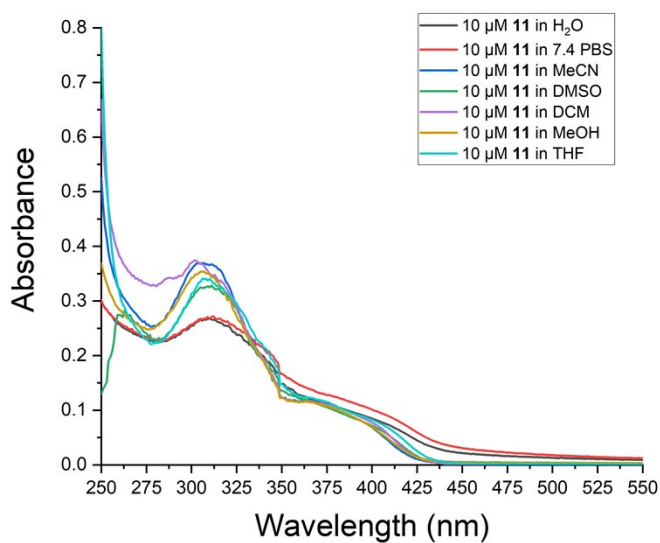


Fig. S6. Absorption spectra of **11** in various solvents. [**11**] = 10 μ M with 0.5% (v/v) DMSO in the indicated solvents.

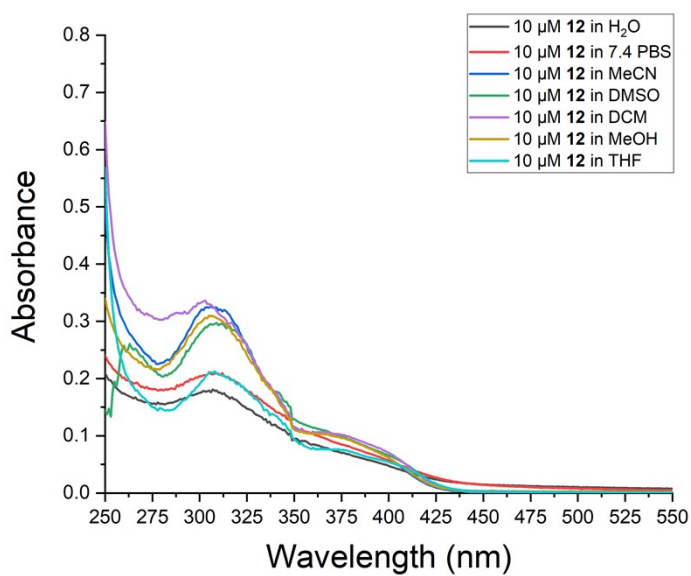


Fig. S7. Absorption spectra of **12** in various solvents. [**12**] = 10 μ M with 0.5% (v/v) DMSO in the indicated solvents.

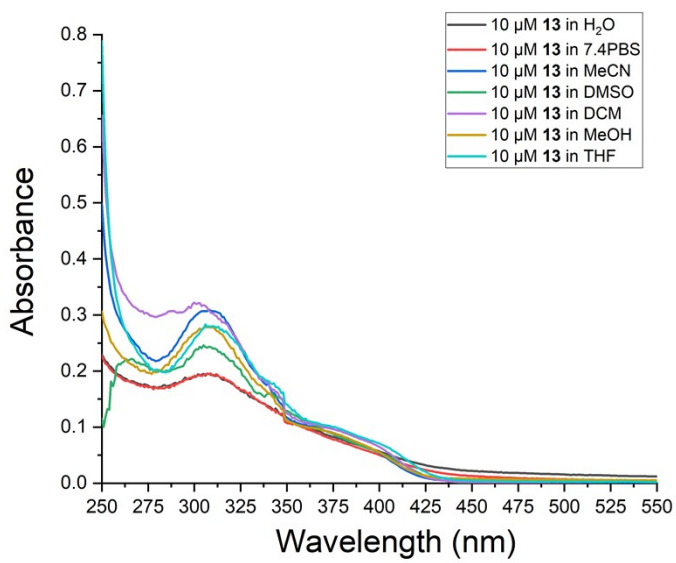


Fig. S8. Absorption spectra of **13** in various solvents. [**13**] = 10 μM with 0.5% (v/v) DMSO in the indicated solvents.

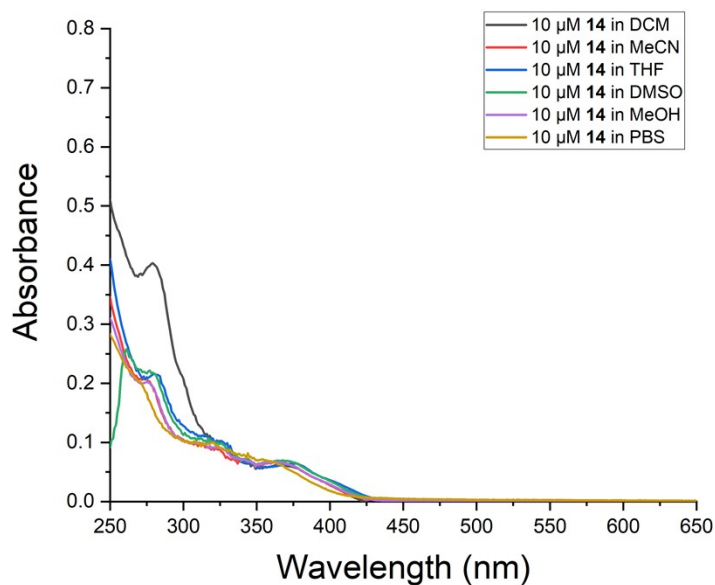


Fig. S9. Absorption spectra of **14** in various solvents. [**14**] = 10 μM with 0.5% (v/v) DMSO in the indicated solvents.

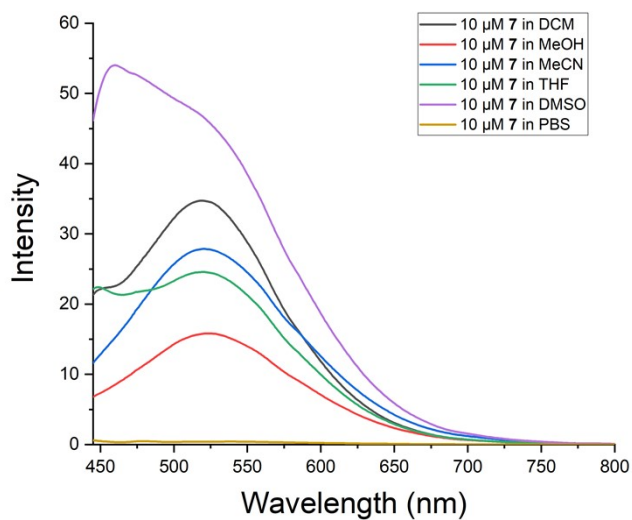


Fig. S10. Emission spectra of **7** in different solvents (containing 0.5% (v/v) DMSO); [**7**] = 10 μM ; λ_{ex} = 410 nm.

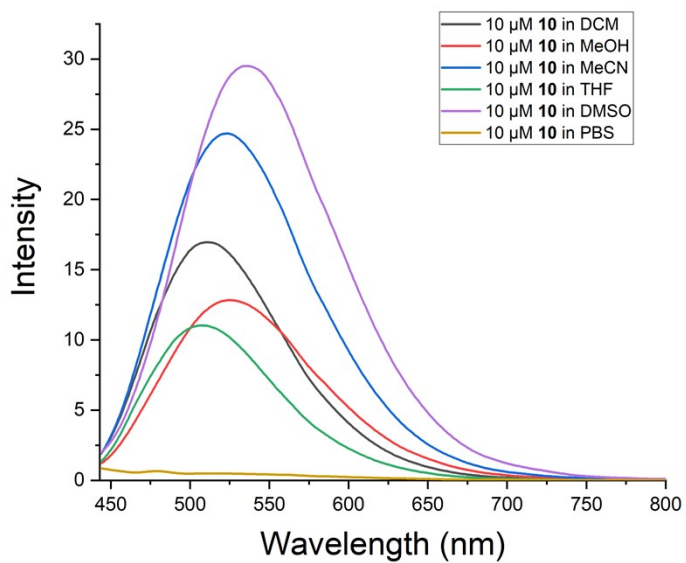


Fig. S11. Emission spectra of **10** in different solvents containing 0.5% (v/v) DMSO; [**10**] = 10 μM ; λ_{ex} = 410 nm.

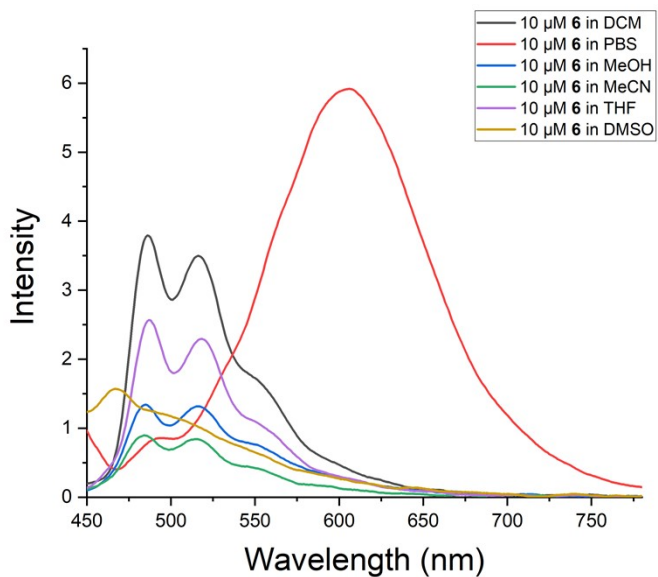


Fig. S12. Emission spectra of **6** in different solvents containing 0.5% (v/v) DMSO; [**6**] = 10 μM ; λ_{ex} = 410 nm.

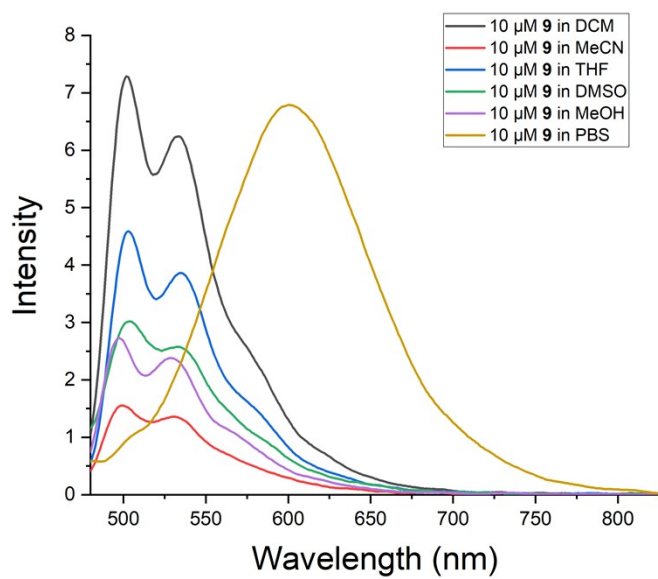


Fig. S13. Emission spectra of **9** in different solvents containing 0.5% (v/v) DMSO; [**9**] = 10 μM ; λ_{ex} = 410 nm.

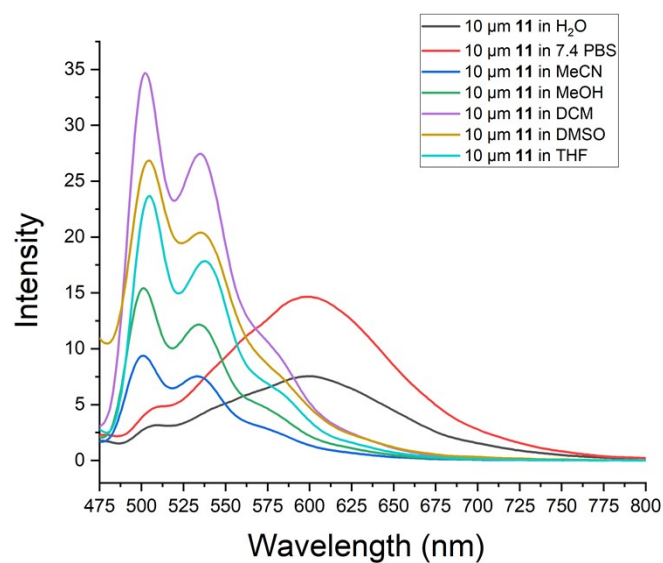


Fig. S14. Emission spectra of **11** in different solvents containing 0.5% (v/v) DMSO; [**11**] = 10 μM ; λ_{ex} = 410 nm.

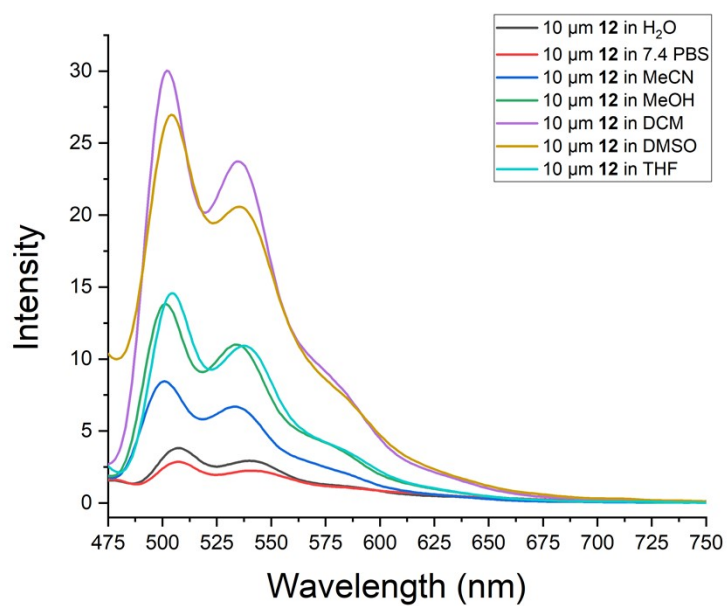


Fig. S15. Emission spectra of **12** in different solvents containing 0.5% (v/v) DMSO; [**12**] = 10 μM ; λ_{ex} = 410 nm.

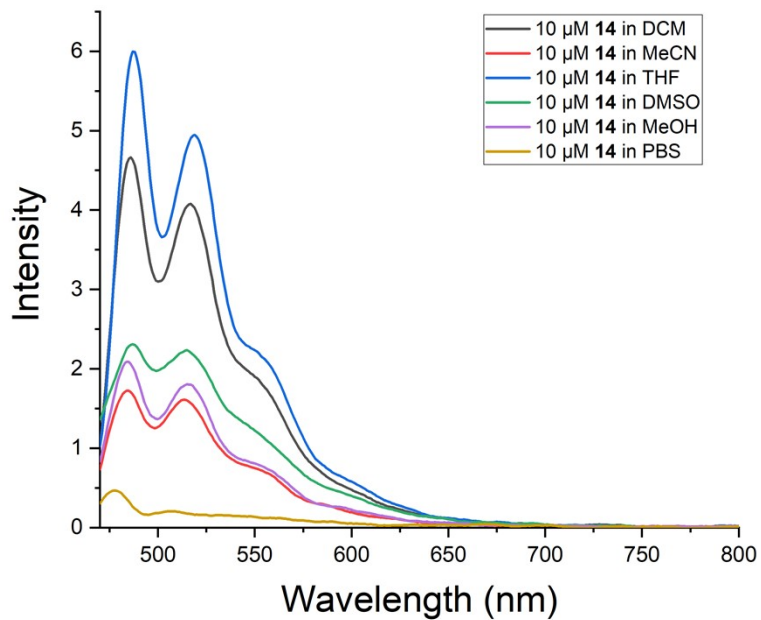


Fig. S16. Emission spectra of **14** in different solvents containing 0.5% (v/v) DMSO; [**14**] = 10 μM ; λ_{ex} = 410 nm.

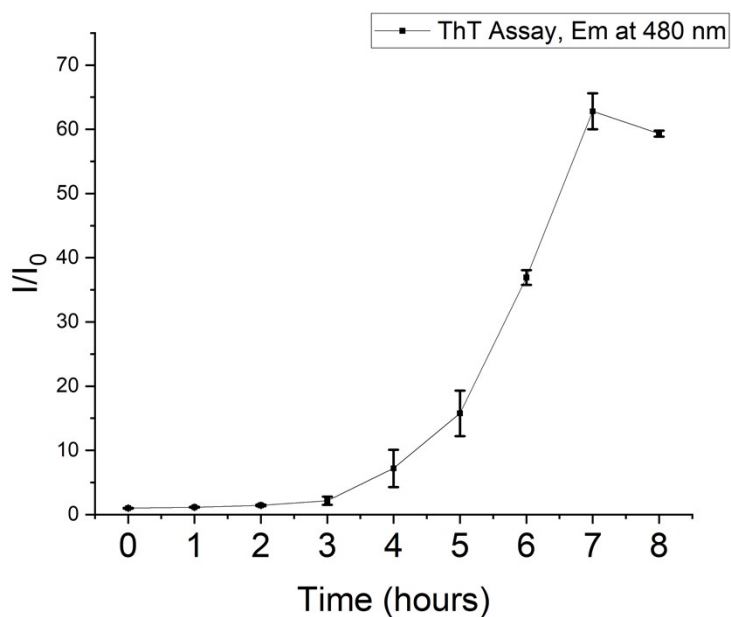


Fig. S17. ThT fluorescence assay of HEWL fibrillization. λ_{ex} = 440 nm, λ_{em} = 480 nm, error bar $n = 3$, I_0 = ThT emission at $T = 0$.

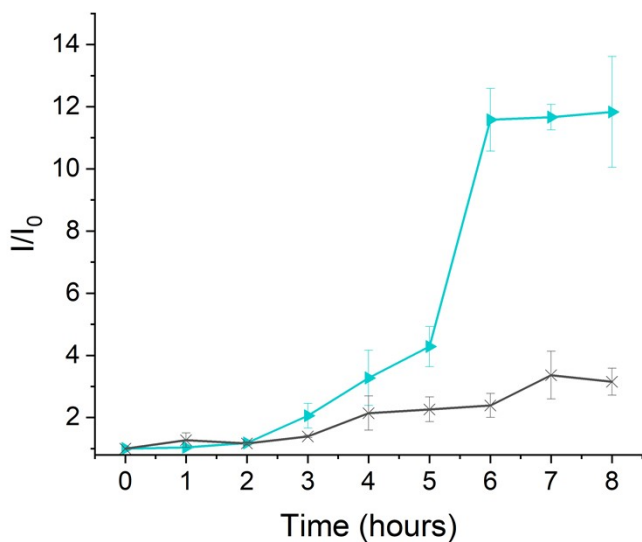
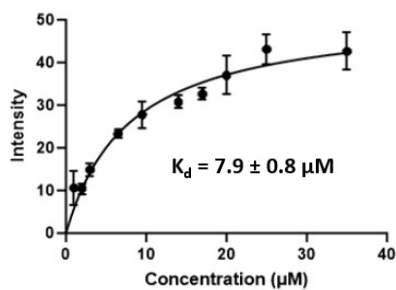


Fig. S18. Plot of emission enhancement (I/I_0) for complex **13** (cyan line) and **14** (black line) as a function of HEWL aggregation. $\lambda_{ex} = 410$ nm for both complexes, $\lambda_{em} = 490$ nm for **14** and 510 nm for **13**, error bar $n = 3$.



One site - Specific binding	
Best-fit values	
Bmax	51.85
Kd	7.908
95% CI (profile likelihood)	
Bmax	46.38 to 58.99
Kd	5.613 to 11.23
Goodness of Fit	
Degrees of Freedom	28
R squared	0.9227
Sum of Squares	328.1
Sy.x	3.423
Number of points	
# of X values	30
# Y values analyzed	30

Fig. S19. Saturation binding isotherm generated by plotting maximum emission of **8** at 510 nm in the presence of 5 µM HEWL fibrils versus [**8**] (0-35 µM). Data analysis performed using GraphPad Prism, error bars reflect results of 3 trials.

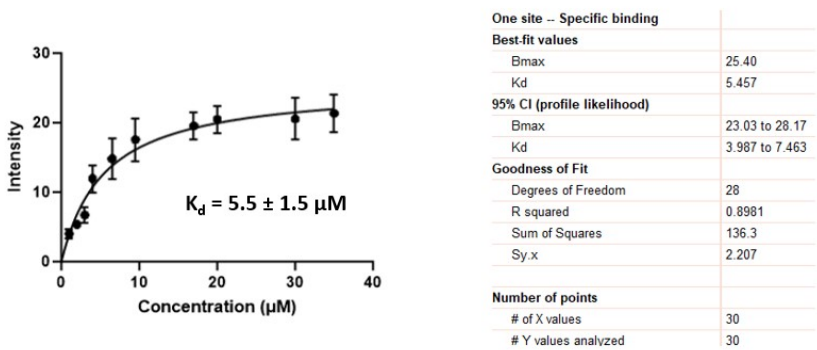


Fig. S20. Saturation binding isotherm generated by plotting maximum emission of **13** at 510 nm in the presence of 5 µM HEWL fibrils versus [**13**] (0-35 µM). Data analysis performed using GraphPad Prism, error bars reflect results of 3 trials.

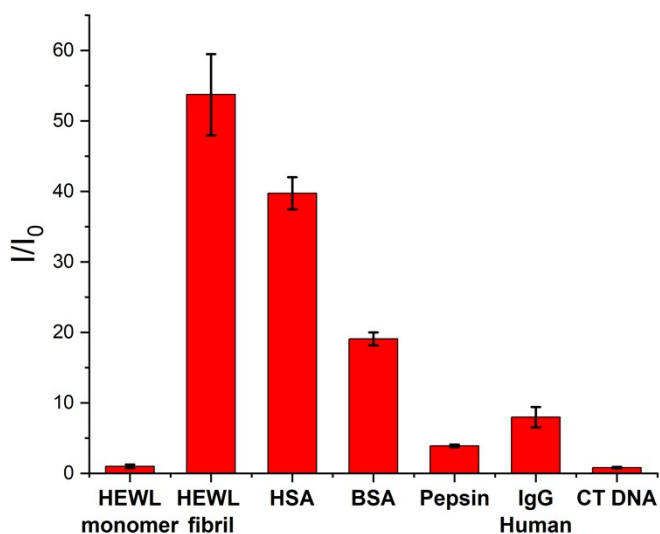


Fig. S21. Relative luminescence response (I/I_0) of **13** (20 µM) at 505 nm in the presence of select biomolecules (10 µM) in PBS (0.5% DMSO); I_0 = emission intensity in presence of HEWL monomer; $\lambda_{\text{ex}} = 410 \text{ nm}$, error bar $n = 3$.

Preparation of HEWL oligomers/fibrils

HEWL oligomers/fibrils were prepared according to literature procedures.^{7, 8} Specifically, lyophilized HEWL was dissolved at 5 mg/mL (350 µM) in 10 mM pH 3 sodium citrate buffer with 0.1 M NaCl. The solution was sonicated for 1 minute and then incubated in a 70 °C oil bath and magnetically stirred at 80 rpm for 8 hours. During this time aliquots were withdrawn at different time intervals and immediately diluted with pH 7.4 PBS (phosphate buffer saline) to stop further fibrillization. Samples were then refrigerated

until use in spectroscopic experiments. Fibrillization was complete after 8 h of incubation according to ThT fluorescence assay (see Fig. S17) and AFM imaging.

Preparation of A β ₄₂ fibrils

A β ₄₂ fibrils were prepared according to literature methods.⁹ Specifically, HFIP-treated A β ₄₂ (0.5 mg) was solubilized in 22 μ L dry DMSO (5 mM) and sonicated for 2 minutes. The A β ₄₂ solution was then diluted to 100 μ M with 1085 μ L 7.4 PBS buffer. The solution was incubated at 37 °C for 21 hours, after which time fibrillization was complete as determined by ThT fluorescence assay and AFM imaging.

General methods for luminescence assays

All luminescence assays involving ThT and Pt(II) complexes **6-14** in the presence of HEWL or A β ₄₂ aggregates were performed in 96-well plates using a SpectraMax® M3 plate reader (Molecular Device). Emission spectra of Pt complexes were obtained using $\lambda_{\text{ex}} = 410$ nm and monitoring emission wavelength from 440-800 nm. ThT assays were performed using $\lambda_{\text{ex}} = 440$ nm and monitoring emission at 480 nm.

Luminescence spectra of Pt(II) complexes in the presence of HEWL aggregates and fibrils

A 350 μ M HEWL solution in pH 3 sodium citrate buffer was prepared as described above and aliquots were withdrawn and diluted to 10 μ M in pH 7.4 PBS at 1 h time intervals throughout the fibrillization reaction (0 to 8 hours). Stock solutions of each Pt(II) complex (2 mM in DMSO) were prepared and aliquots from stock solutions were added to 10 μ M HEWL solutions in pH 7.4 PBS to give final Pt(II) complex concentrations of 20 μ M. The HEWL-Pt(II) complex solutions were allowed to stand at room temperature for 2 min and then the emission spectra were recorded.

Luminescence measurements of Pt(II) complexes 12 and 13 in the presence of A β ₄₂ fibrils

Aliquots from a 100 μ M solution of A β ₄₂ fibrils (prepared as described above) were diluted to 10 μ M in pH 7.4 PBS. Aliquots from stock solutions of platinum(II) complexes **12** and **13** (0.4 mM in DMSO) were added to 10 μ M A β ₄₂ fibril solutions to give a final Pt complex concentration of 20 μ M. The A β ₄₂-Pt(II) complex solutions were allowed to stand at room temperature for 2 min, and then the emission spectra were recorded.

ThT fluorescence assays

ThT fluorescence assays were performed by adding aliquots of a ThT stock solution (2 mM in DMSO for HEWL experiments and 0.4 mM in DMSO for A β ₄₂ experiments) to 10 μ M amyloid solutions in pH 7.4 PBS to achieve a final ThT concentration of 20 μ M. The respective ThT-amyloid mixtures were allowed to stand at room temperature for 2 min and then emission spectra were recorded.

Determination of K_d for binding of **8** and **13** to HEWL fibrils

Equilibrium dissociation constants (K_d) for binding of Pt complexes **8** and **13** to HEWL fibrils:

$$K_d = [\text{Pt(II) probe}][\text{HEWL fibrils}]/[\text{Pt(II) probe-HEWL complex}]$$

were determined using luminescence titration experiments. Specifically, different concentrations of **8** and **13** (1-35 μM) were titrated against a fixed concentration of HEWL fibrils (5 μM) in 7.4 PBS. Emission spectra of Pt complexes were recorded with excitation at 410 nm and emission at 510 nm after incubation with HEWL fibrils for 2 mins at room temperature.

Changes in emission intensity were plotted versus probe concentration to yield binding isotherms (Figs. S19-S20). Experiments were performed in triplicate and results are given as the mean \pm SD. The corresponding isotherms were analyzed by GraphPad Prism (GraphPad Software, Inc., San Diego, CA, USA) by non-linear regression using one-site-binding equation. The K_d values were calculated using following equation:¹⁰

$$Y = B_{\text{max}} * X / (K_d + X)$$

where X is concentration of Pt(II) complex, Y is change in emission intensity, B_{max} is the maximum specific binding, which refers to the total number of receptors, and K_d is the equilibrium binding constant. It should be noted that while the presence of multiple binding sites in amyloid fibrils is possible,¹¹ application of a one-site binding model greatly simplifies data analysis.

AFM imaging experiments – general materials and methods

AFM height imaging was carried at room temperature and ambient pressure using a Molecular Force Probe 3D AFM system (Asylum Research, Santa Barbara, CA). Si_3N_4 AFM probes (MikroMasch, San Jose, CA) were used for all AFM experiments with a nominal spring constant of 0.4 N/m and a typical tip radius of curvature of 8 nm. AFM height images were acquired in intermittent contact mode (AC mode) at a typical scan rate of 1 Hz.

Preparation of Pt(II) complex – HEWL fibril samples for AFM imaging

HEWL fibrils were prepared by incubation of HEWL (350 μM) in pH 3 sodium citrate buffer for 8 hours as described above. Aliquots were removed from the incubation solution and diluted to 10 μM in pH 7.4 PBS. Aliquots from 2 mM DMSO stock solutions of platinum(II) complexes (**8**, **13**, and **14**) were added to diluted fibril solutions to give final Pt(II) complex concentrations of 20 μM . The HEWL fibril/Pt complex mixtures were allowed to stand at room temperature for 24 h. After this time, 70 μL aliquots from each solution were transferred onto freshly cleaved mica and placed in a room temperature dust-free environment for 20 min to allow physisorption to occur. The mica substrates were then washed with 70 μL of HPLC-grade H_2O three times and air-dried in a dust-free environment overnight prior to AFM imaging. A control sample of

HEWL fibrils was prepared as described above by mixing diluted HEWL fibril solutions with an equivalent amount of DMSO instead of Pt(II) complex stock solution.

Preparation of A β ₄₂ fibril samples for AFM imaging

A solution of A β ₄₂ fibrils (100 μ M) was prepared as described above. A 10 μ L aliquot of this solution was withdrawn and transferred directly onto freshly cleaved mica. The sample was placed in a room temperature dust-free environment for 20 min. for physisorption to occur and then washed with 20 μ L HPLC-grade H₂O three times followed by air-drying overnight in a dust-free environment prior to AFM imaging.

MTT assays

SH-SY5Y cells (purchased from ATCC) were treated with Pt(II) complexes **8** and **11-13** at concentrations ranging from 1 μ M to 100 μ M for 24 h. Cells were also treated with the cytotoxic agent Rotenone (1 μ M, 5 μ M and/or 10 μ M) as a negative control. Cell viability was assessed using the colorimetric reagent, 3-[4,5-dimethylthiazol-2-yl]-2,5-diphenyl tetrazolium bromide (MTT) (Sigma Aldrich). Cultures were incubated in HBSS/glucose with 2 mg/mL MTT for 2 h at 37 °C. Following incubation, 0.4 mL DMSO was added to each well to solubilize the formazan product. Reduced MTT was measured on a microplate reader (Molecular Devices Spectra Max 190) at 570 nm with a reference of 650 nm.

X-Ray crystallography

General data collection

Data were collected on a Bruker D8 VENTURE DUO diffractometer equipped with a I μ S 3.0 microfocus source operated at 75 W (50kV, 1.5 mA) to generate Mo K α radiation ($\lambda = 0.71073$ Å) and a PHOTON III detector. Crystals were transferred from the vial and placed on a glass slide in type NVH immersion oil by Cargille. A Zeiss Stemi 305 microscope was used to identify a suitable specimen for X-ray diffraction from a representative sample of the material. The crystal and a small amount of the oil were collected on a MiTeGen 100 micron MicroLoop and transferred to the instrument where it was placed under a cold nitrogen stream (Oxford 800 series) maintained at 100K throughout the duration of each experiment. Samples were optically centered with the aid of a video camera to ensure that no translations were observed as crystals were rotated through all positions. A unit cell collection was then carried out. After it was determined that the unit cell was not present in the CCDC database a data collection strategy was calculated by *APEX4*.¹² The crystal was measured for size, morphology, and color.

Refinement details

After data collection, the unit cell was re-determined using a subset of the full data collection. Intensity data were corrected for Lorentz, polarization, and background effects using the *APEX4*.¹² A numerical absorption correction was applied based on a Gaussian

integration over a multifaceted crystal and followed by a semi-empirical correction for adsorption applied using *SADABS*.¹² The program *SHELXT*¹³ was used for the initial structure solution and *SHELXL*¹⁴ was used for the refinement of the structure. Both programs were utilized within the OLEX2 software.¹⁵ Hydrogen atoms bound to carbon atoms were located in the difference Fourier map and were geometrically constrained using the appropriate AFIX commands.

Table S1. Crystallographic data for 7.

CCDC number	2322597
Empirical formula	C ₂₆ H ₂₅ NO ₄ Pt
Formula weight	610.56
Temperature/K	150.15
Crystal system	monoclinic
Space group	C/c
a/Å	15.5673(16)
b/Å	21.225(2)
c/Å	6.6731(7)
α/°	90
β/°	95.563(5)
γ/°	90
Volume/Å ³	2194.5(4)
Z	4
ρ _{calc} /g/cm ³	1.848
μ/mm ⁻¹	6.428
F(000)	1192.0
Crystal size/mm ³	0.220 × 0.220 × 0.145
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	5.258 to 54.010
Index ranges	-19 ≤ h ≤ 19, -27 ≤ k ≤ 27, -8 ≤ l ≤ 8
Reflections collected	12942
Independent reflections	4529 [R _{int} = 0.0199, R _{sigma} = 0.0379]
Data/restraints/parameters	4529/2/293
Goodness-of-fit on F ²	0.609
Final R indexes [I >= 2σ (I)]	R ₁ = 0.0181, wR ₂ = 0.0518
Final R indexes [all data]	R ₁ = 0.0212, wR ₂ = 0.0715
Largest diff. peak/hole / e Å ⁻³	1.225/-0.519

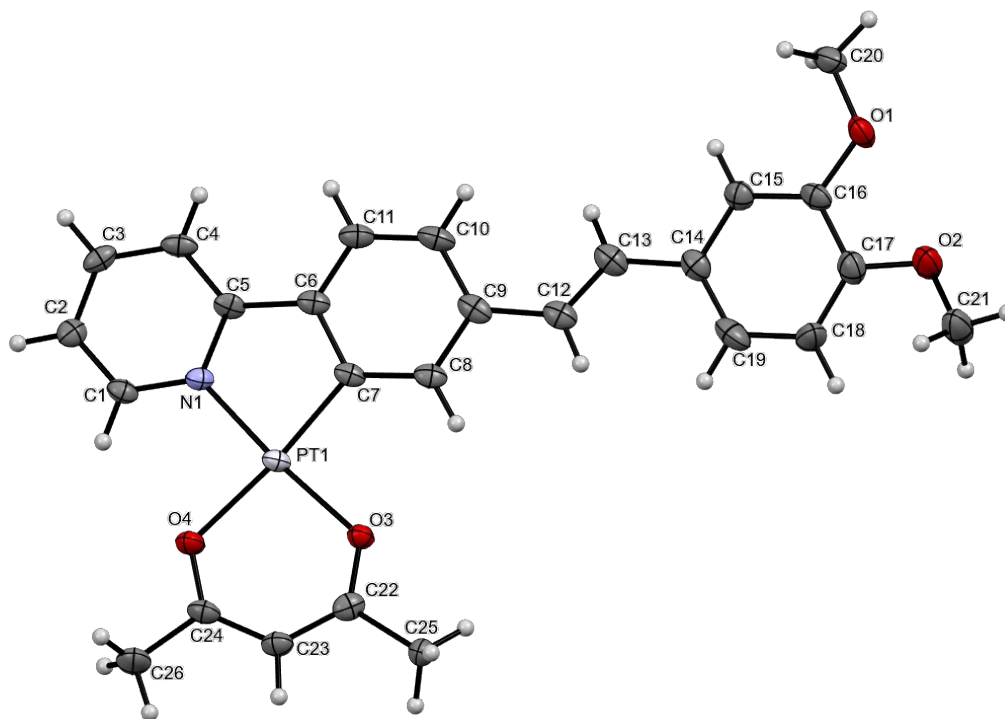


Fig. S22. ORTEP plot of Pt(II) complex **7** with thermal ellipsoids represented at 50% probability. Carbon, nitrogen, oxygen, and platinum atoms are represented by gray, blue, red, and light blue ellipsoids, respectively. Platinum(II) bond distances and angles are typical for a cyclometallated square-planar Pt(II) acac complex. Pt1 \cdots N1 1.996 Å; Pt1 \cdots C7 1.978 Å; Pt1 \cdots O3 2.011 Å; Pt1 \cdots O4 2.087 Å; N1-Pt1-C7 81.61°; C7-Pt1-O3 93.58°; O3-Pt1-O4 91.98°; O4-Pt1-N1 92.81°; N1-Pt1-O3 175.19°; C7-Pt1-O4 174.12°. $\tau_4 = 0.08$.¹⁶

Table S2. Crystallographic data for **8**·CH₃OH.

CCDC number	2322598
Empirical formula	C ₂₆ H ₂₈ N ₂ O ₆ Pt
Formula weight	659.59
Temperature/K	100.00
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	11.5142(6)
b/Å	12.2748(6)
c/Å	17.2202(10)
α/°	90
β/°	96.978(2)
γ/°	90
Volume/Å ³	2415.8(2)
Z	4
ρ _{calc} /cm ³	1.814
μ/mm ⁻¹	5.853
F(000)	1296.0
Crystal size/mm ³	0.238 × 0.139 × 0.118
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.766 to 72.734
Index ranges	-19 ≤ h ≤ 18, -20 ≤ k ≤ 17, -28 ≤ l ≤ 28
Reflections collected	99722
Independent reflections	11747 [R _{int} = 0.0769, R _{sigma} = 0.0463]
Data/restraints/parameters	11747/0/323
Goodness-of-fit on F ²	1.032
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0340, wR ₂ = 0.0668
Final R indexes [all data]	R ₁ = 0.0505, wR ₂ = 0.0726
Largest diff. peak/hole / e Å ⁻³	2.17/-1.57

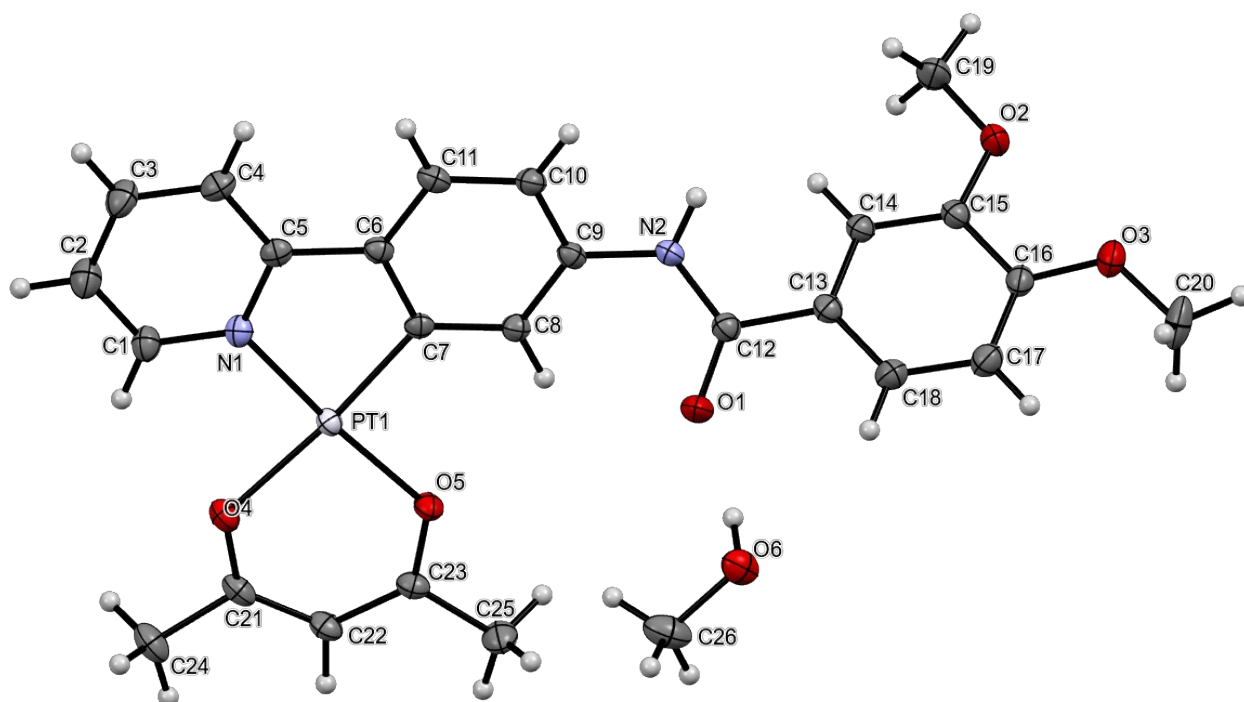


Fig. S23. ORTEP plot of Pt(II) complex **8**·CH₃OH with thermal ellipsoids represented at 50% probability. Carbon, nitrogen, oxygen, and platinum atoms are represented by gray, blue, red, and light blue ellipsoids, respectively. Platinum(II) bond distances and angles are typical for a cyclometallated square-planar Pt(II) acac complex. Pt1···N1 1.991 Å; Pt1···C7 1.971 Å; Pt1···O5 2.003 Å; Pt1···O4 2.081 Å; N1-Pt1-C7 81.66°; C7-Pt1-O5 93.69°; O5-Pt1-O4 91.79°; O4-Pt1-N1 92.85°; N1-Pt1-O5 175.34°; C7-Pt1-O4 174.51°. $\tau_4 = 0.07$.¹⁶

Table S3. Crystallographic data for **9**.

CCDC number	2322599
Empirical formula	C ₂₆ H ₂₆ N ₂ O ₅ Pt
Formula weight	641.58
Temperature/K	100.00
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	14.1430(6)
b/Å	12.3571(7)
c/Å	14.0848(8)
α/°	90
β/°	107.375(2)
γ/°	90
Volume/Å ³	2349.2(2)
Z	4
ρ _{calc} /cm ³	1.814
μ/mm ⁻¹	6.013
F(000)	1256.0
Crystal size/mm ³	0.16 × 0.137 × 0.132
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.468 to 61.04
Index ranges	-18 ≤ h ≤ 20, -17 ≤ k ≤ 17, -20 ≤ l ≤ 20
Reflections collected	52908
Independent reflections	7167 [R _{int} = 0.0685, R _{sigma} = 0.0431]
Data/restraints/parameters	7167/0/313
Goodness-of-fit on F ²	1.041
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0278, wR ₂ = 0.0530
Final R indexes [all data]	R ₁ = 0.0379, wR ₂ = 0.0564
Largest diff. peak/hole / e Å ⁻³	1.22/-1.12

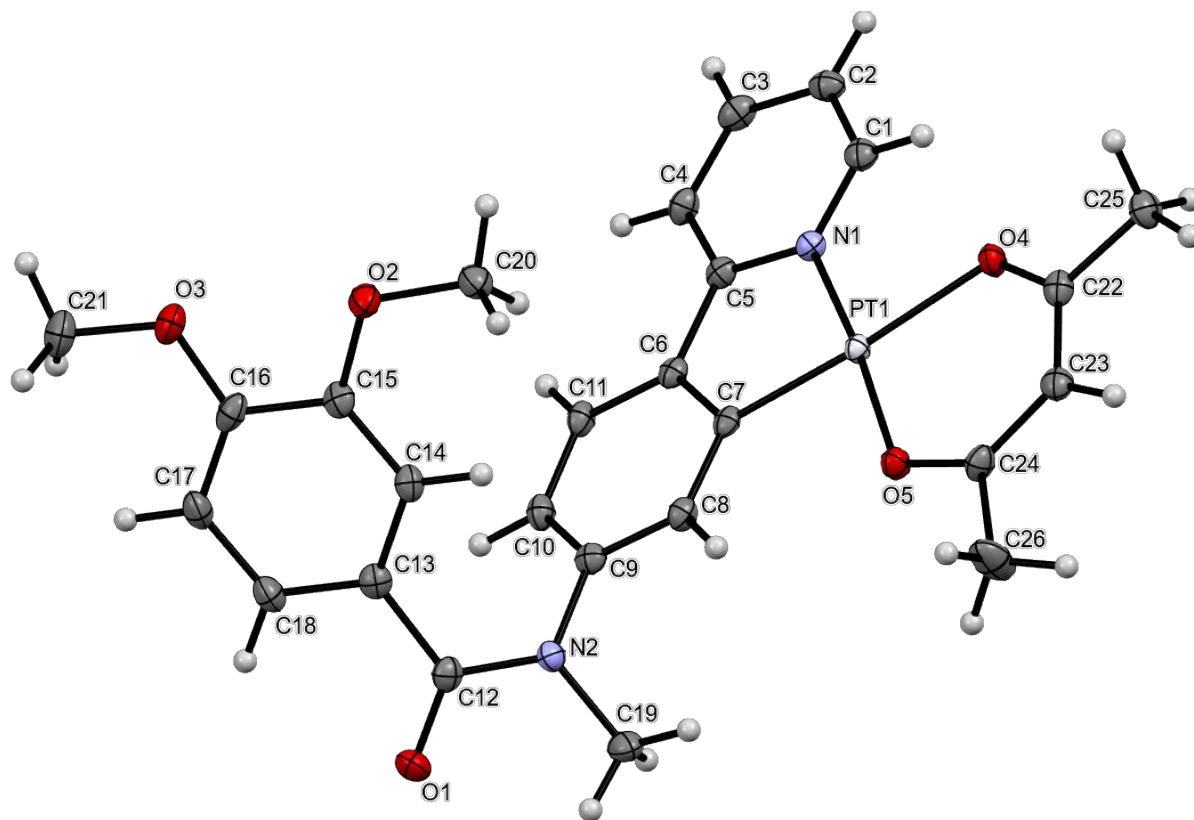
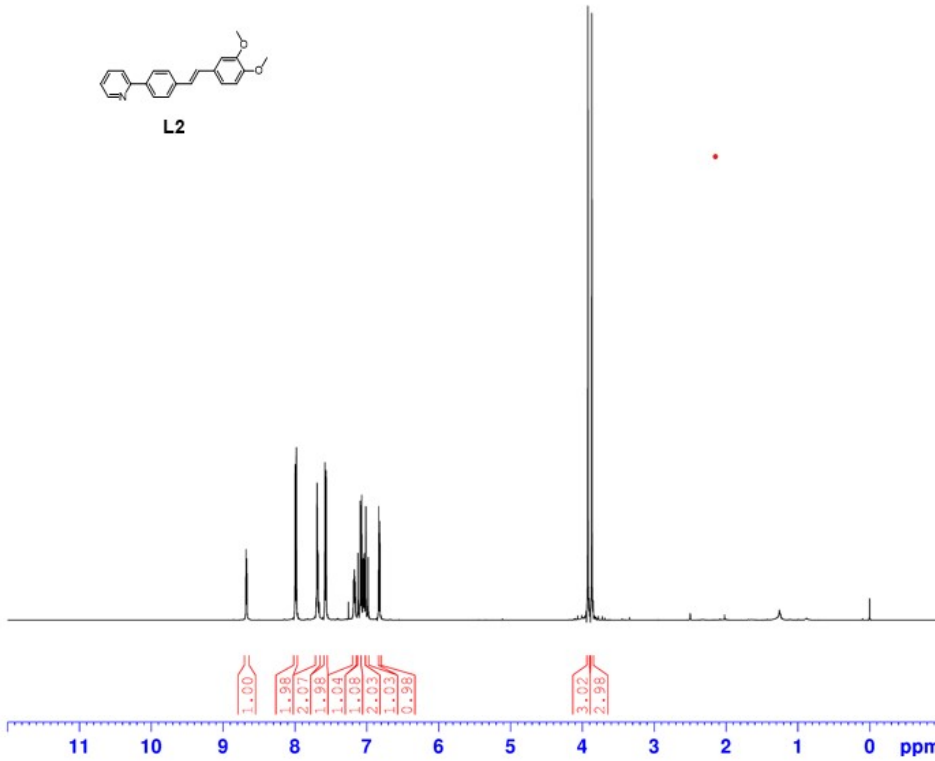
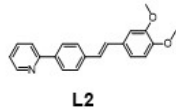


Fig. S24. ORTEP plot of Pt(II) complex **9** with thermal ellipsoids represented at 50% probability. Carbon, nitrogen, oxygen, and platinum atoms are represented by gray, blue, red, and light blue ellipsoids, respectively. Platinum(II) bond distances and angles are typical for a cyclometallated square-planar Pt(II) acac complex. Pt1···N1 1.991 Å; Pt1···C7 1.967 Å; Pt1···O5 2.008 Å; Pt1···O4 2.087 Å; N1-Pt1-C7 81.67°; C7-Pt1-O5 92.81°; O5-Pt1-O4 91.81°; O4-Pt1-N1 93.74°; N1-Pt1-O5 174.10°; C7-Pt1-O4 175.32°. $\tau_4 = 0.08$.¹⁶

References

1. E. K. Aratikatla, T. R. Valkute, S. K. Puri, K. Srivastava and A. K. Bhattacharya, *Eur. J. Med. Chem.*, 2017, **138**, 1089-1105.
2. H.-G. Cheng, M. Pu, G. Kundu and F. Schoenebeck, *Org. Lett.*, 2019, **22**, 331-334.
3. J. Suttill, J. Kucharyson, I. Escalante-Garcia, P. Cabrera, B. James, R. Savinell, M. Sanford and L. Thompson, *J. Mater. Chem. A*, 2015, **3**, 7929-7938.
4. M. Fu, L. Chen, Y. Jiang, Z.-X. Jiang and Z. Yang, *Org. Lett.*, 2016, **18**, 348-351.
5. L. J. O'Driscoll, D. J. Welsh, S. W. Bailey, D. Visontai, H. Frampton, M. R. Bryce and C. J. Lambert, *Chem-Eur. J.*, 2015, **21**, 3891-3894.
6. J. Brooks, Y. Babayan, S. Lamansky, P. I. Djurovich, I. Tsyba, R. Bau and M. E. Thompson, *Inorg. Chem.*, 2002, **41**, 3055-3066.
7. P. L. Donabedian, T. K. Pham, D. G. Whitten and E. Y. Chi, *ACS Chem. Neurosci.*, 2015, **6**, 1526-1535.
8. M. Mulaj, J. Foley and M. Muschol, *J. Am. Chem. Soc.*, 2014, **136**, 8947-8956.
9. L. Sun, H.-J. Cho, S. Sen, A. S. Arango, T. T. Huynh, Y. Huang, N. Bandara, B. E. Rogers, E. Tajkhorshid and L. M. Mirica, *J. Am. Chem. Soc.*, 2021, **143**, 10462-10476.
10. S. Dhein, F. W. Mohr and M. Delmar, *Practical methods in cardiovascular research*, Springer, 2005.
11. B. Jiang, U. Umezaki, A. Augustine, V. M. Jayasinghe-Arachchige, L. F. Serafim, Z. M. S. He, K. M. Wyss, R. Prabhakar and A. A. Martí, *Chemical Science*, 2023, **14**, 1072-1081.
12. Bruker (2021). APEX4, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
13. G. M. Sheldrick, *Acta Crystallogr.*, 2015, **A71**, 3-8.
14. G. M. Sheldrick, *Acta Crystallogr.*, 2015, **C71**, 3-8.
15. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, and H. Puschmann, *J. Appl. Cryst.*, 2009, **42**, 339-341.
16. L. Yang, D. R. Powell, and R. P. Houser, *Dalton Trans.* 2007, 955-964.

8.67
7.99
7.98
7.70
7.70
7.69
7.69
7.68
7.68
7.66
7.66
7.58
7.56
7.18
7.18
7.17
7.17
7.17
7.17
7.16
7.16
7.12
7.09
7.07
7.07
7.05
7.04
7.03
7.03
7.01
6.98
6.83
6.82
3.92
3.86

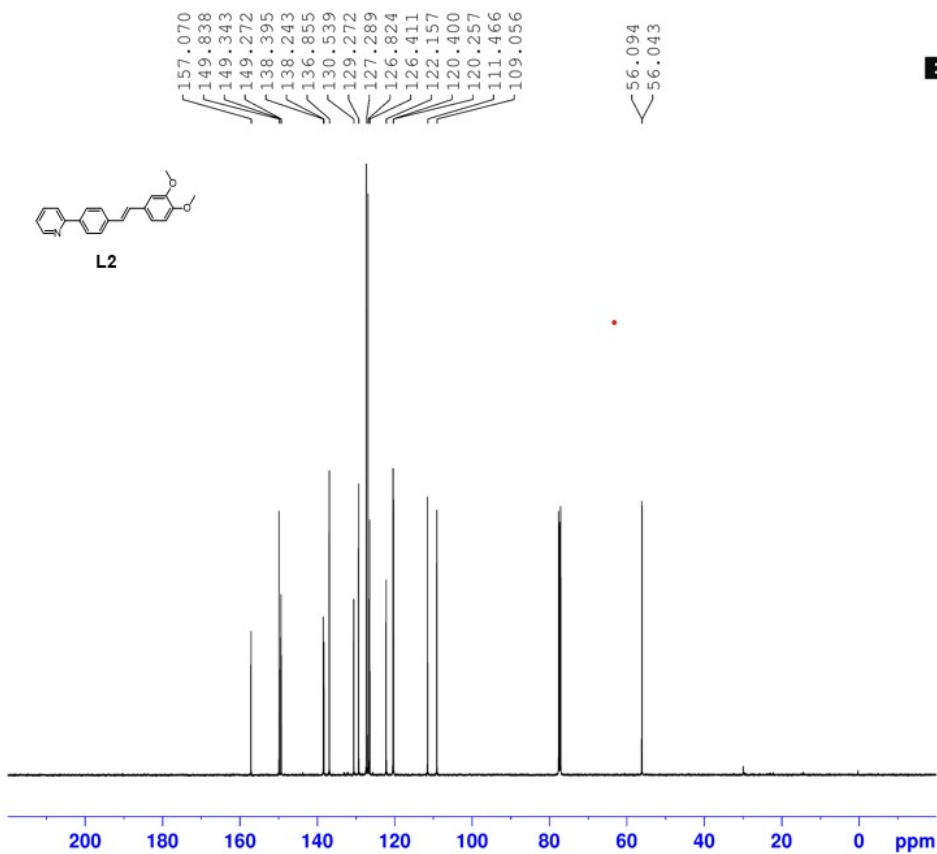


Current Data Parameters
NAME pig_Li_4_104-15_End-1F
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210105
Time 13.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 28.5
DW 50.000 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 1H
P1 12.00 usec
PL1 -1.10 dB
PL1W 19.41561890 W
SFO1 500.3020014 MHz

F2 - Processing parameters
SI 65536
SF 500.3000160 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME pig_Li_4_104-15_End-13C
 EXPNO 1
 PROCNO 1

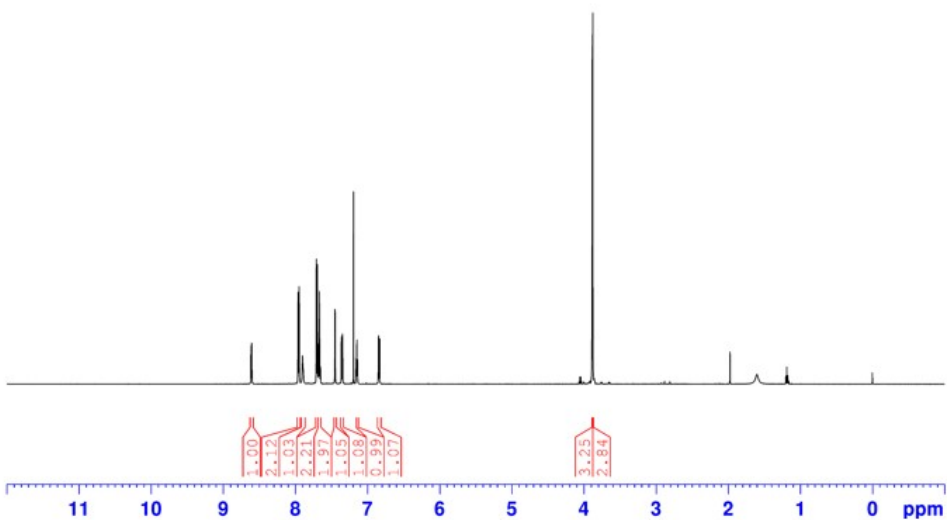
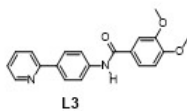
F2 - Acquisition Parameters
 Date_ 20210105
 Time 14.38
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 2
 SWH 31446.541 Hz
 FIDRES 0.479836 Hz
 AQ 1.0420223 sec
 RG 20642.5
 DW 15.900 usec
 DE 6.50 usec
 TE 300.2 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 -1.70 dB
 PL1W 148.61408997 W
 SFO1 125.8131150 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 FCPD2 80.00 usec
 PL2 -1.10 dB
 PL12 15.40 dB
 PL13 17.40 dB
 PL2W 19.41561890 W
 PL12W 0.43466163 W
 PL13W 0.27425295 W
 SFO2 500.3020014 MHz

F2 - Processing parameters
 SI 32768
 SF 125.8005161 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

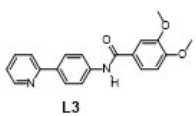
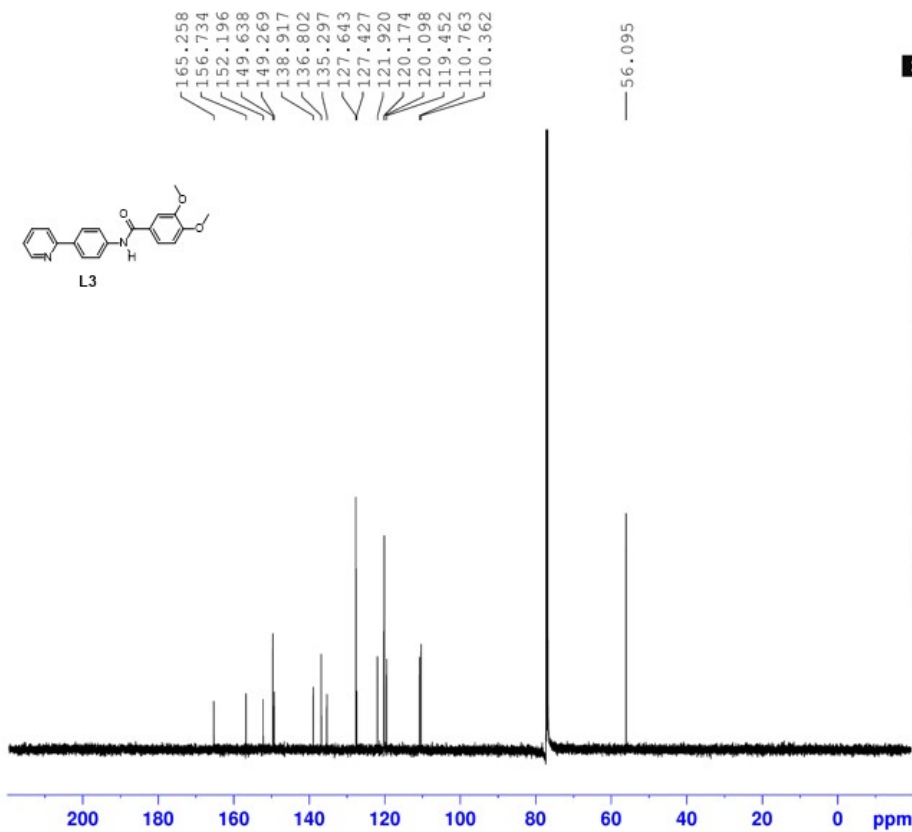
8.61
8.61
8.61
8.60
7.96
7.95
7.90
7.71
7.69
7.68
7.68
7.67
7.67
7.65
7.65
7.45
7.45
7.45
7.36
7.36
7.35
7.34
7.16
7.15
7.15
7.14
7.14
7.14
6.84
6.83
3.88



Current Data Parameters
NAME 1H-2L-3-56-hotfiltrate-110823
EXNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231108
Time 13.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262376 sec
RG 512
DW 41.600 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 11.80 usec
PLM1 26.91500092 W
SFO1 600.2124008 MHz
F2 - Processing parameters
SI 65536
SF 600.2100540 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME 13C-EL-3-56-hotfiltrate-110823
 EXPNO 1
 PROCNO 1

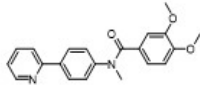
F2 - Acquisition Parameters
 Date_ 20231108
 Time 14.06
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 871
 DS 4
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087059 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 300.3 K
 D1 2.0000000 sec
 D11 0.0300000 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 10.00 usec
 PLW1 60.25600002 W
 SFO1 150.5380173 MHz

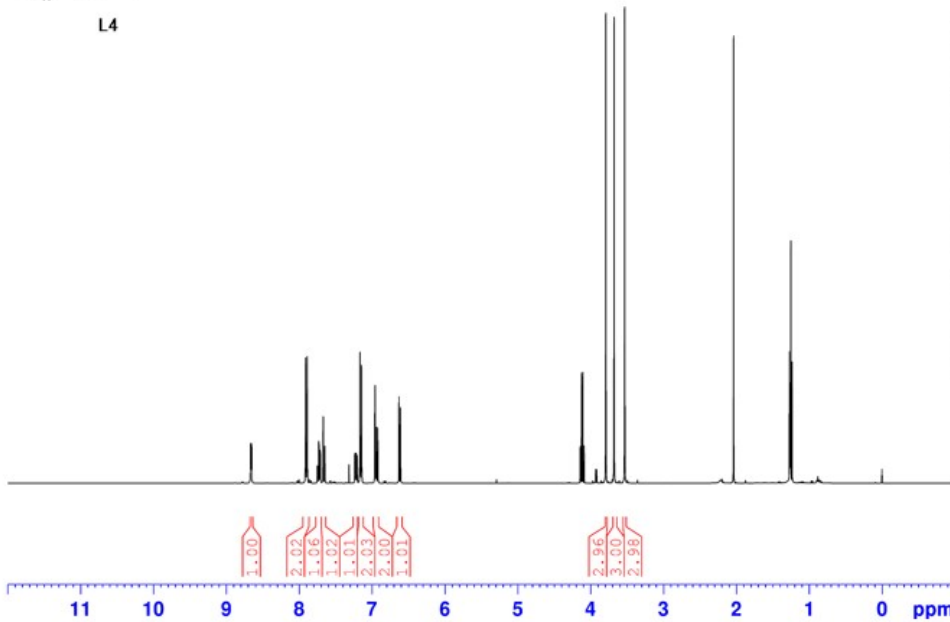
----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUCC 18
 PCPD2 70.00 usec
 PLW2 26.91500092 W
 PLW22 0.7507998 W
 PLW13 0.38758001 W
 SFO2 600.2124008 MHz

F2 - Processing parameters
 SI 65536
 SF 150.5229050 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

8.65
8.65
7.91
7.91
7.89
7.89
7.75
7.74
7.73
7.73
7.71
7.71
7.67
7.65
7.23
7.22
7.22
7.22
7.20
7.20
7.16
7.16
7.15
7.14
6.96
6.96
6.94
6.94
6.92
6.92
6.63
6.61
3.79
3.68
3.53



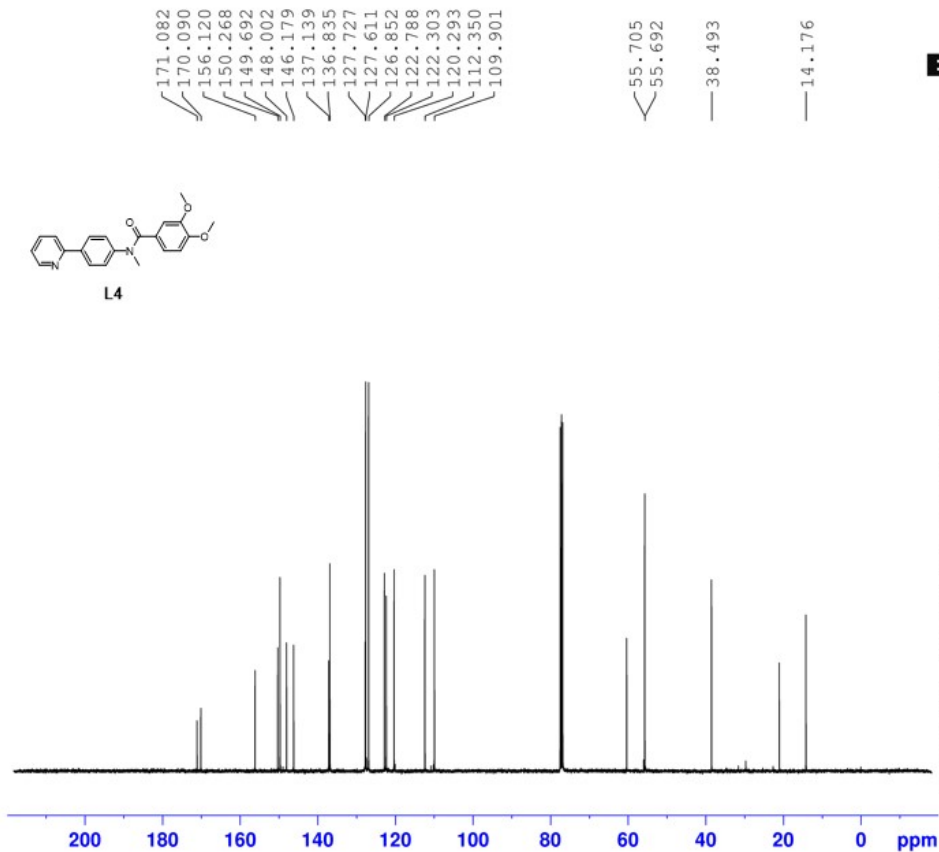
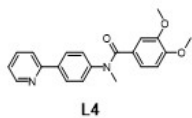
L4



Current Data Parameters
NAME 1H-ZL-5-114-17-37
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230103
Time 15.32 h
INSTRUM Avance
PROBHD Z167430_0032 (4
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 55.3025
DW 61.000 usec
DE 13.20 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.3024719 MHz
NUC1 1H
P0 4.00 usec
P1 12.00 usec
PLW1 8.80000019 W

F2 - Processing parameters
SI 65536
SF 400.2999878 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



171.082
170.090
156.120
150.268
149.692
148.002
146.179
137.139
136.835
127.727
127.611
126.852
122.788
122.303
120.293
112.350
109.901

55.705
55.692

38.493

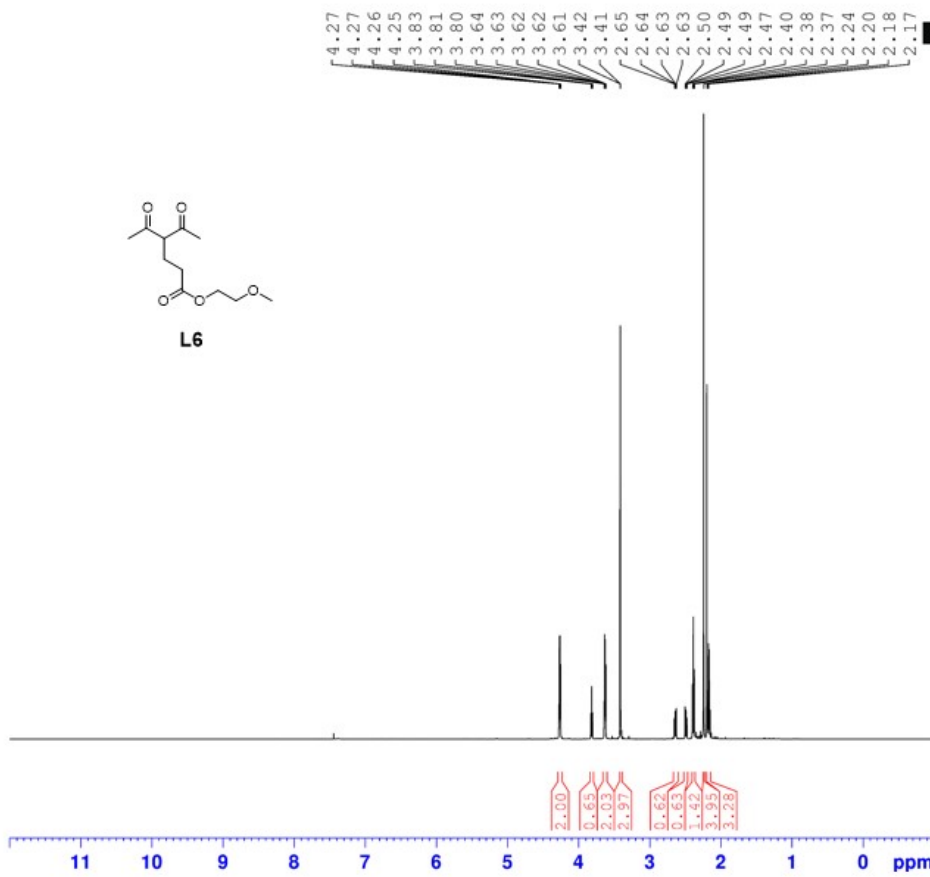
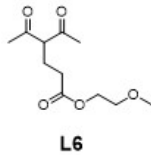
14.176



Current Data Parameters
NAME 13C-ZL-5-114-17-37
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230103
Time 15.55 h
INSTRUM Avance
PROBHD z167430_0032 (zpgg30)
PULPROG zpgg30
TD 65536
SOLVENT CDCl3
NS 77
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 3.25
DW 21.000 usec
DE 19.29 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1
SFO1 100.6655806 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 39.31399918 W
SFO2 400.3016012 MHz
NUC2 1H
CPDPRG2 waltz64
PCPD2 80.00 usec
PLW2 8.80000019 W
PLW12 0.20176961 W
PLW13 0.10112690 W

F2 - Processing parameters
SI 131072
SF 100.6555149 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

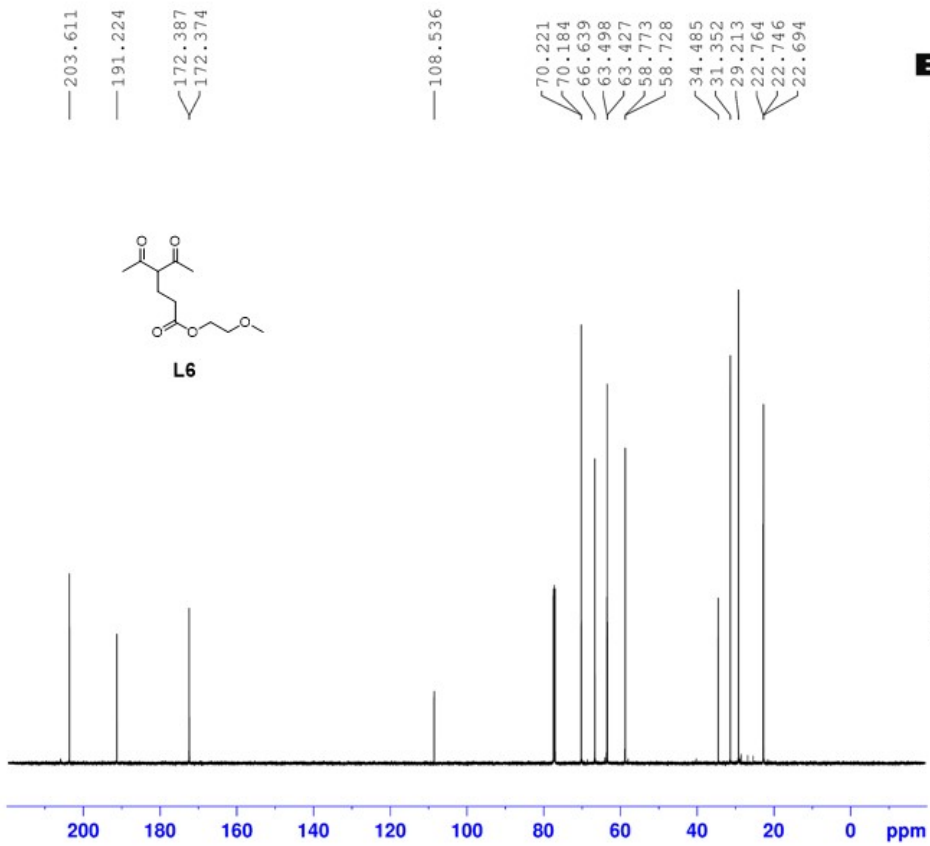


Current Data Parameters
 NAME 1H-ZL-4-232-filtrate-110823
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20231108
 Time 14.13
 INSTRUM spect
 PROBRD 5 mm PABCO B5-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWE 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 20.2
 DW 41.600 usec
 DE 6.50 usec
 TE 299.6 K
 D1 1.00000000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 11.80 usec
 PLW1 26.91500092 W
 SFO1 600.2124008 MHz

F2 - Processing parameters
 SI 65536
 SF 600.2099034 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



```

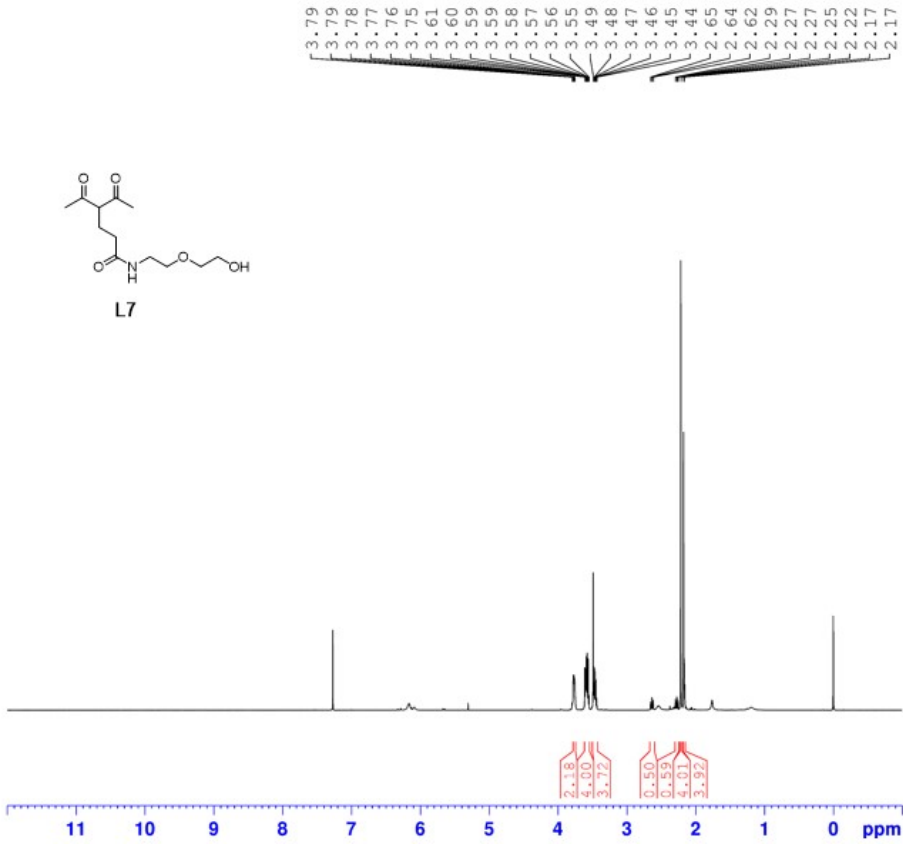
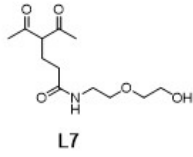
Current Data Parameters
NAME      13C-ZL-4-232-filtrate-110823
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20231108
Time     14.24
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD       65536
SOLVENT  cdcl3
NS       127
DS       4
SWH      36057.691 Hz
FIDRES   0.550197 Hz
AQ       0.9087659 sec
RG       2050
DW       13.867 usec
DE       6.50 usec
TE       300.4 K
D1       2.0000000 sec
D11      0.0300000 sec

===== CHANNEL f1 =====
NUC1     13C
P1       10.00 usec
PLM1     60.25600052 W
SFO1     150.9380173 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2    70.00 usec
PLM2     26.91500092 W
PLM12    0.79097998 W
PLM13    0.38758001 W
SFO2     600.2124008 MHz

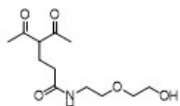
F2 - Processing parameters
SI       65536
SF       150.9229250 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```

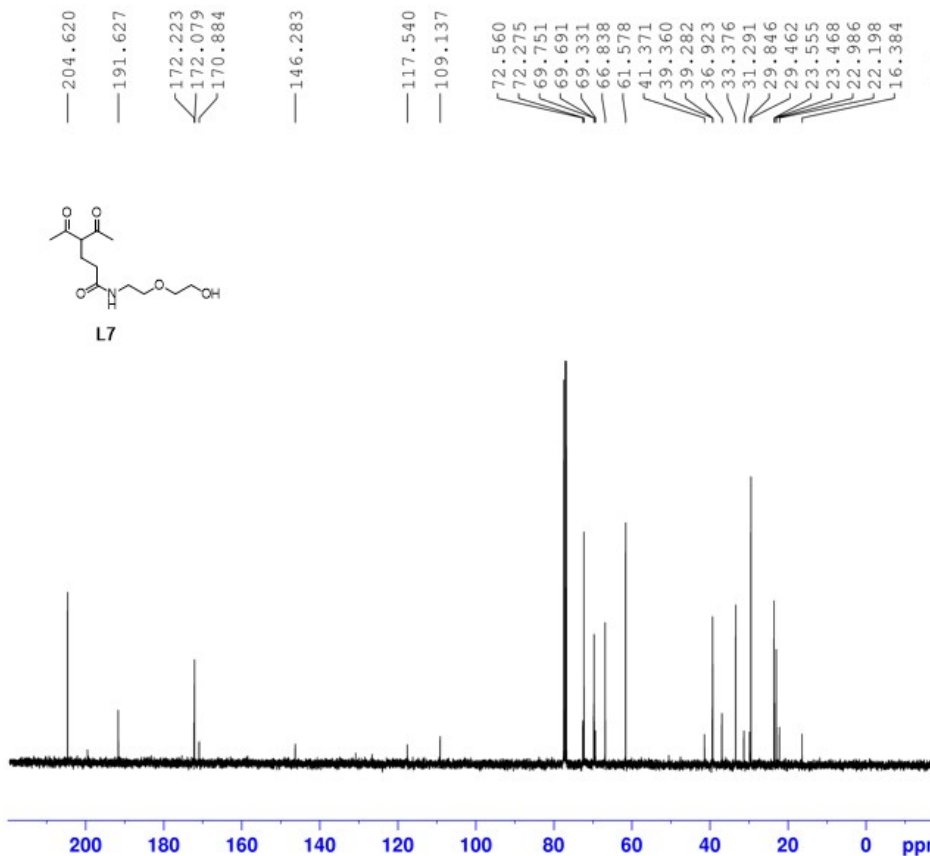
Current Data Parameters
 NAME 1H-2L-3-118-2nd-11-922
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210922
 Time 10.18 h
 INSTRUM spect
 PROBHD Z104450_0192 f
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 256
 DM 62.400 usec
 DE 16.92 usec
 TE 295.4 K
 D1 1.00000000 sec
 TDO 1
 SFO1 400.1324706 MHz
 NUC1 1H
 P0 5.00 usec
 P1 15.00 usec
 PLW1 8.47000027 W

F2 - Processing parameters
 SI 65536
 SF 400.1300061 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



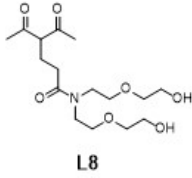
L7



Current Data Parameters
 NAME 13C-ZL-3-118-2nd-11-13c
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210922
 Time 18.27 h
 INSTRUM spect
 PROBHD Z104450_0192 (4
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 108
 DS 2
 SMH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 1.3631488 sec
 RG 203
 DM 20.800 usec
 DE 6.50 usec
 TE 296.1 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1
 SF01 100.6228298 MHz
 NUC1 13C
 F0 3.28 usec
 P1 9.85 usec
 PLW1 28.6399939 W
 SF02 400.1316005 MHz
 NUC2 1H
 CPDPRG2 waltz65
 PCPD2 90.00 usec
 PLW2 8.4700027 W
 PLW12 0.23528001 W
 PLW13 0.11834000 W

F2 - Processing parameters
 SI 32768
 SF 100.6127685 MHz
 WDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



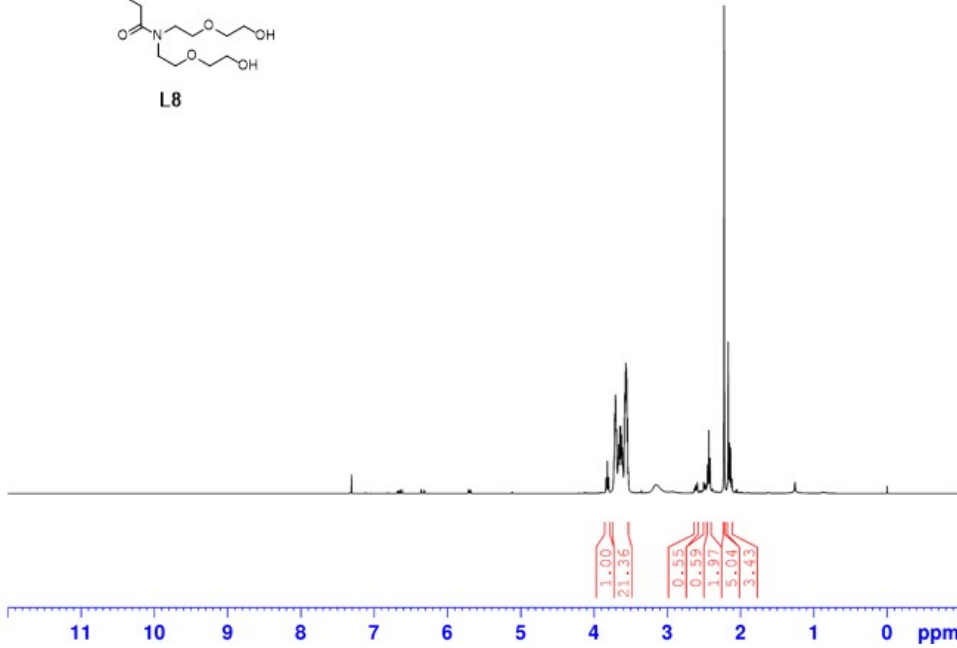
3.83
3.82
3.80
3.73
3.71
3.69
3.66
3.65
3.63
3.62
3.61
3.58
3.58
3.57
3.57
3.56
3.54
3.53
2.63
2.61
2.60
2.59
2.50
2.49
2.48
2.46
2.45
2.43
2.42
2.22



Current Data Parameters
NAME 1H-ZL-3-70-45-55
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210727
Time 10.29 h
INSTRUM Avance
PROBHD z167430_0032 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 54.9115
DW 61.000 usec
DE 13.20 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1
SFO1 400.3024719 MHz
NUC1 1H
PO 4.00 usec
P1 12.00 usec
PLW1 8.80000019 W

F2 - Processing parameters
SI 65536
SF 400.2999882 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



— 205.000
 — 191.350
 < 172.762
 < 172.631

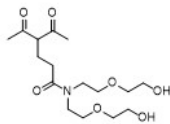
< 128.162
 < 127.863
 < 109.198
 < 72.914
 < 72.804
 < 72.426
 < 72.396
 < 69.251
 < 69.156
 < 69.104
 < 69.016
 < 66.810
 < 61.618
 < 61.583
 < 61.530
 < 48.815
 < 48.723
 < 46.609
 < 46.497
 < 33.601
 < 30.297
 < 29.462
 < 23.091
 < 23.026
 < 22.938



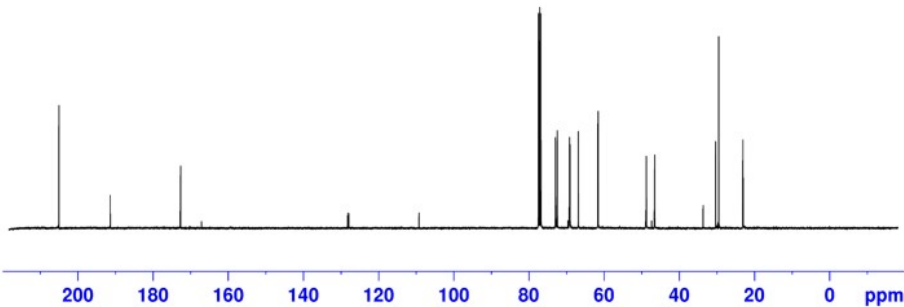
Current Data Parameters
 NAME 13C-ZL-3-70-45-55
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210727
 Time 10.48 h
 INSTRUM Avance
 PROBHD Z167430_0032 (
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 200
 DS 4
 SWH 23809.523 Hz
 FIDRES 0.726609 Hz
 AQ 1.3762560 sec
 RG 3.25
 DW 21.000 usec
 DE 19.29 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1
 SFO1 100.6655806 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 39.31399918 W
 SFO2 400.3016012 MHz
 NUC2 1H
 CPDPRG[2] waltz64
 PCPD2 80.00 usec
 PLW2 8.80000019 W
 PLW12 0.20176961 W
 PLW13 0.10112690 W

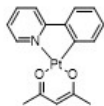
F2 - Processing parameters
 SI 131072
 SF 100.6555151 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



L8



9.03
8.99
8.99
8.97
8.97
8.93
7.79
7.79
7.77
7.77
7.75
7.75
7.63
7.63
7.61
7.58
7.44
7.44
7.42
7.42
7.22
7.22
7.20
7.20
7.18
7.18
7.11
7.10
7.09
7.08
7.07
7.07
5.47
2.00
2.00

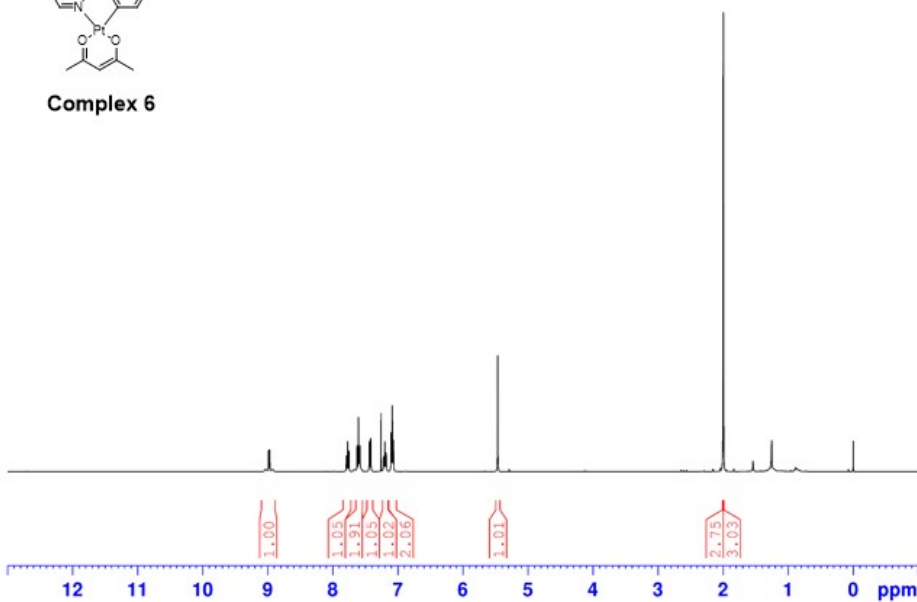


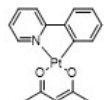
Complex 6

Current Data Parameters
 NAME 1H-2L-3-194-4-26
 EXPNO 1
 PROCNO 1

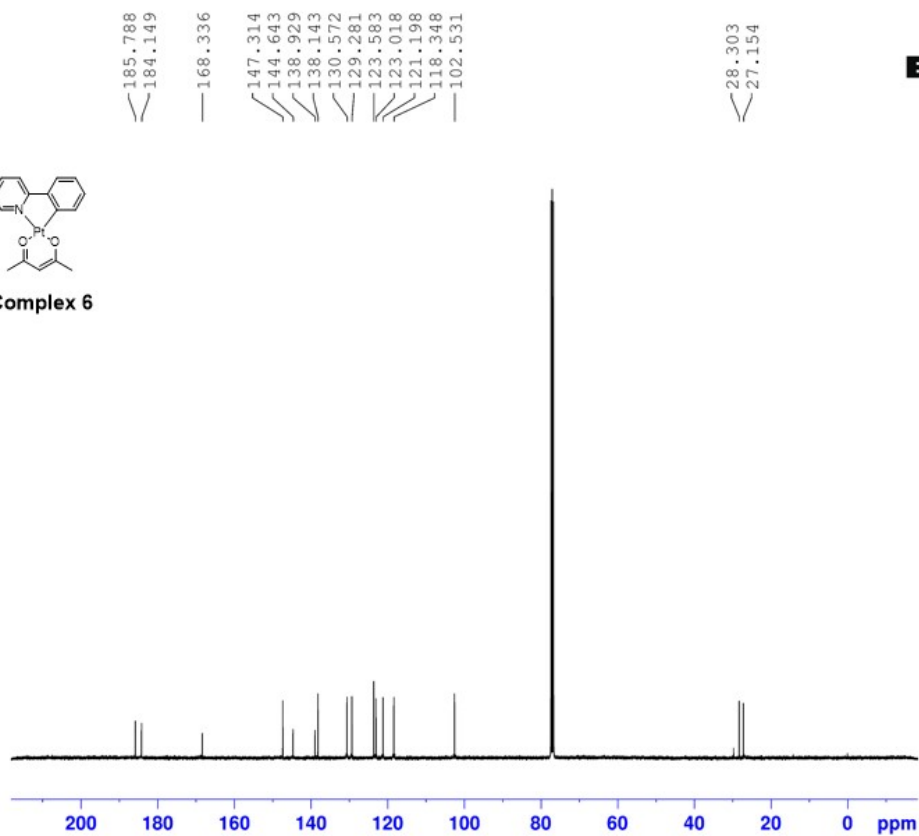
F2 - Acquisition Parameters
 Date_ 20220321
 Time 17.20 h
 INSTRUM Avance
 PROBHD Z167430_0032 ()
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8196.722 Hz
 FIDRES 0.250144 Hz
 AQ 3.9976959 sec
 RG 101
 DW 61.000 usec
 DE 13.20 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.3024719 MHz
 NUC1 1H
 P0 4.00 usec
 P1 12.00 usec
 PLW1 8.80000019 W

F2 - Processing parameters
 SI 65536
 SF 400.3000107 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





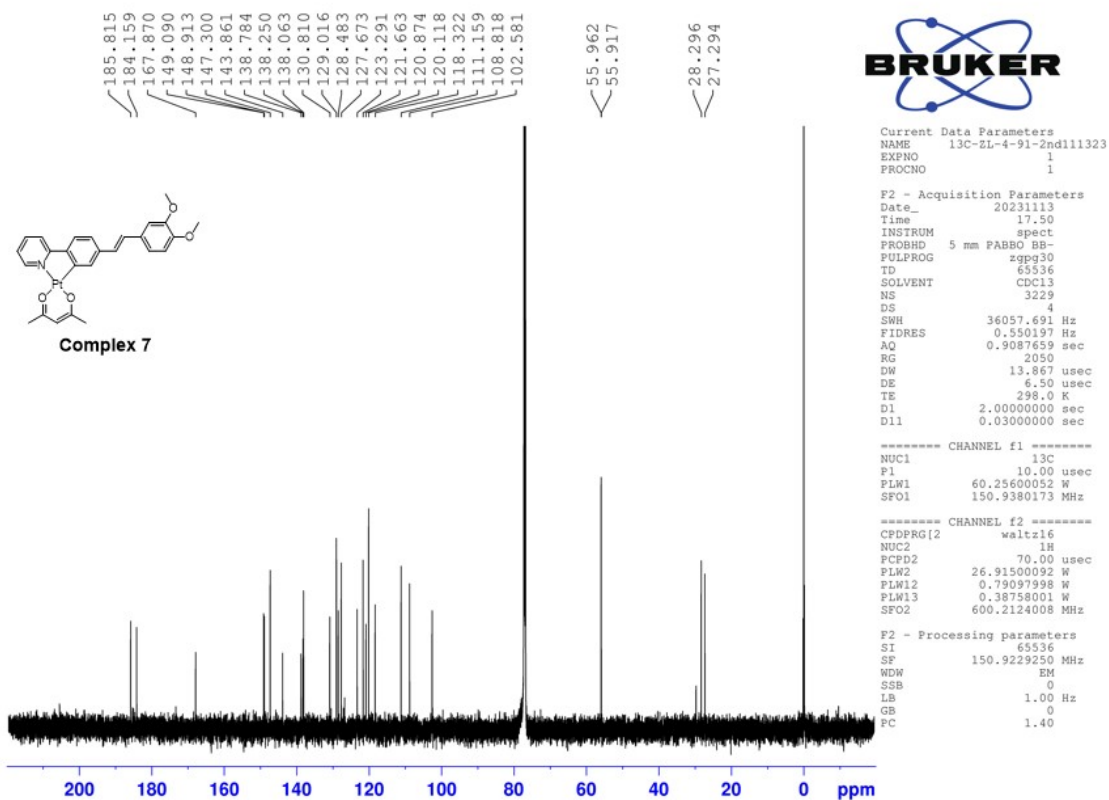
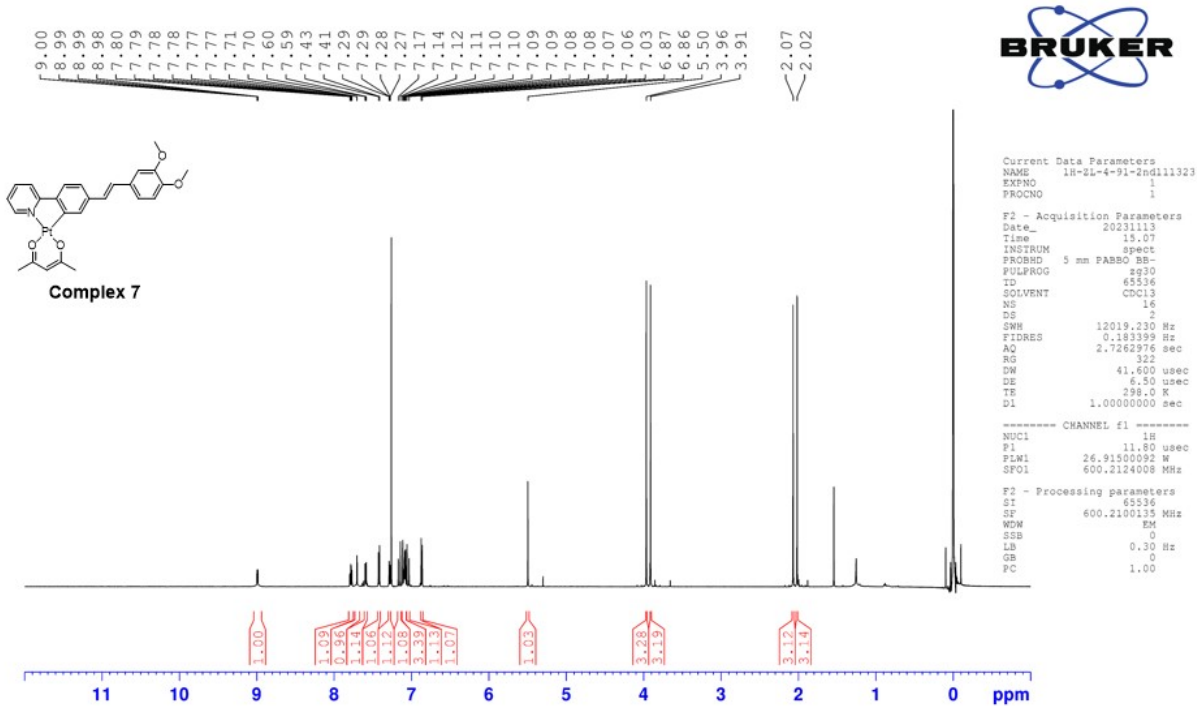
Complex 6

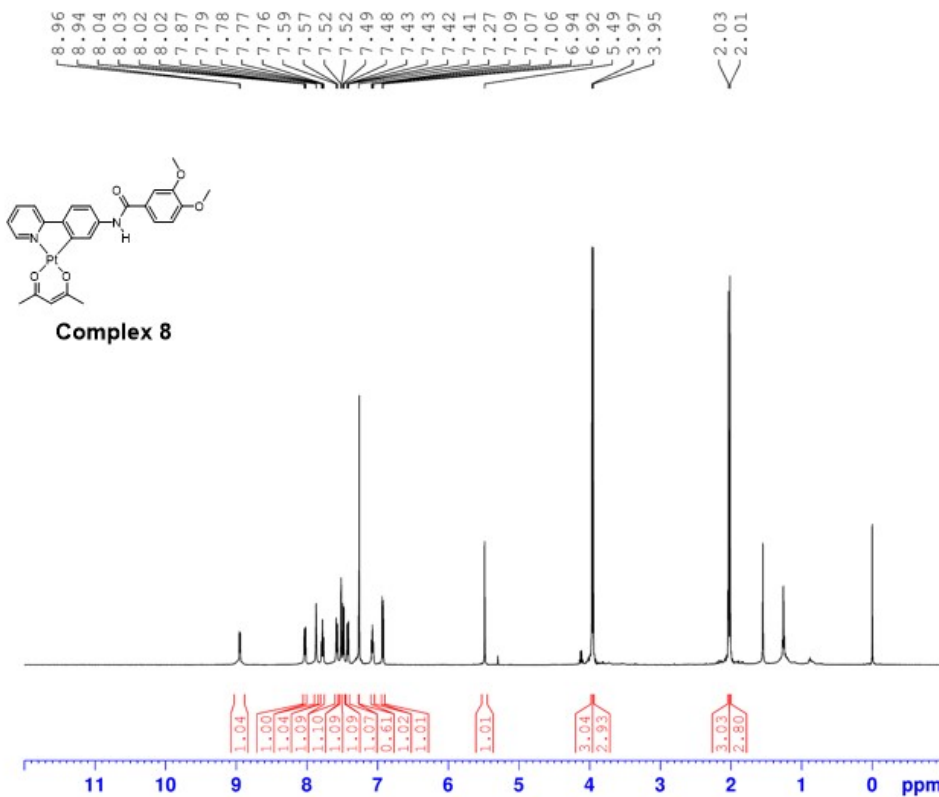


Current Data Parameters
 NAME 13C-ZL-3-194-4-26
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220321
 Time 17.32 h
 INSTRUM Avance
 PROBHD Z167430_0032 (65536
 PULPROG zgpg30
 TD 4
 SOLVENT CDCl3
 NS 144
 DS 4
 SWH 23809.523 Hz
 FIDRES 0.726609 Hz
 AQ 1.3762560 sec
 RG 3.25
 DW 21.000 usec
 DE 19.29 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1
 SFO1 100.6655806 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 39.31399918 W
 SFO2 400.3016012 MHz
 NUC2 1H
 CPDPRG[2] waltz64
 PCPD2 80.00 usec
 PLW2 8.80000019 W
 PLW12 0.20176961 W
 PLW13 0.10112690 W

F2 - Processing parameters
 SI 131072
 SF 100.6555151 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



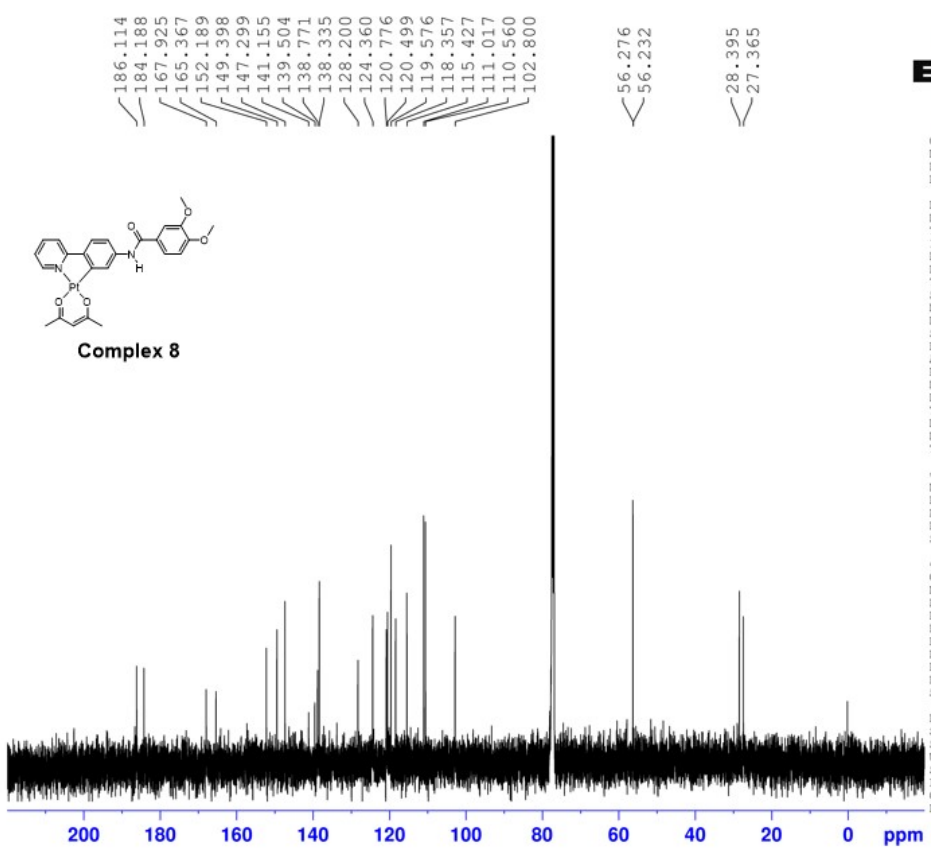


Current Data Parameters
 NAME pig_Li-4-118_17_20_1H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210125
 Time 11:35
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 228.1
 DW 50.000 usec
 DE 6.50 usec
 TE 300.2 K
 D1 2.00000000 sec
 TDO 1

----- CHANNEL f1 -----
 NUC1 1H
 P1 12.00 usec
 PL1 -1.10 dB
 PL1W 19.41561890 W
 SFO1 500.3020014 MHz

F2 - Processing parameters
 SI 65536
 SF 500.3000126 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



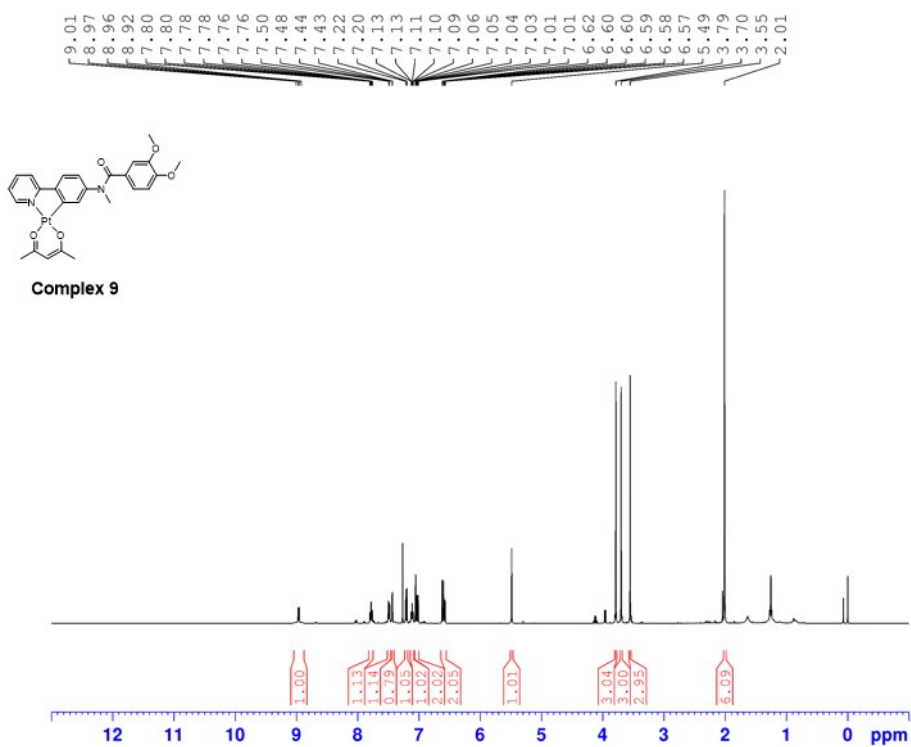
Current Data Parameters
 NAME pig_Li-4-118_17_20_13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210125
 Time 12:28
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 2
 SWH 31446.541 Hz
 FIDRES 0.479836 Hz
 AQ 1.0420223 sec
 RG 20642.5
 DW 15.900 usec
 DE 6.50 usec
 TE 300.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

----- CHANNEL f1 -----
 NUC1 13C
 P1 10.00 usec
 PL1 -1.70 dB
 PL1W 148.61408997 W
 SFO1 125.8131150 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 FCPD2 80.00 usec
 PL2 -1.10 dB
 PL12 15.40 dB
 PL13 17.40 dB
 PL2W 19.41561890 W
 PL12W 0.43466163 W
 PL13W 0.27425295 W
 SFO2 500.3020014 MHz

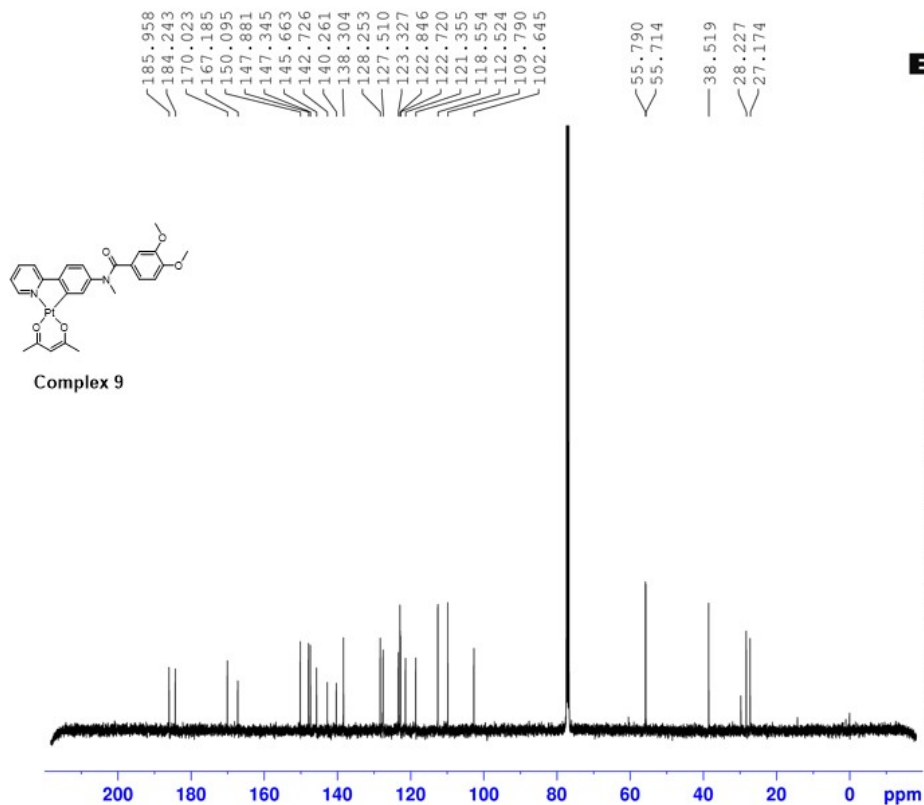
F2 - Processing parameters
 SI 32768
 SF 125.8005161 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME 1H-ZL-3-130-33-57
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230109
 Time 17.43 h
 INSTRUM Avance
 PROBHD z167430_0032 (zpg30)
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8196.722 Hz
 FIDRES 0.250144 Hz
 AQ 3.9976959 sec
 RG 101
 DW 61.000 usec
 DE 13.20 usec
 TE 298.0 K
 D1 1.0000000 sec
 TDO 1
 SFO1 400.3024719 MHz
 NUC1 1H
 P0 4.00 usec
 P1 12.00 usec
 PLW1 8.80000019 W

F2 - Processing parameters
 SI 65536
 SF 400.3000073 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

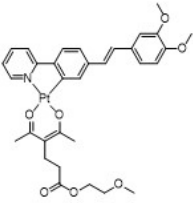


Current Data Parameters
 NAME 13C-ZL-5-130-33-57
 EXPNO 1
 PROCNO 1

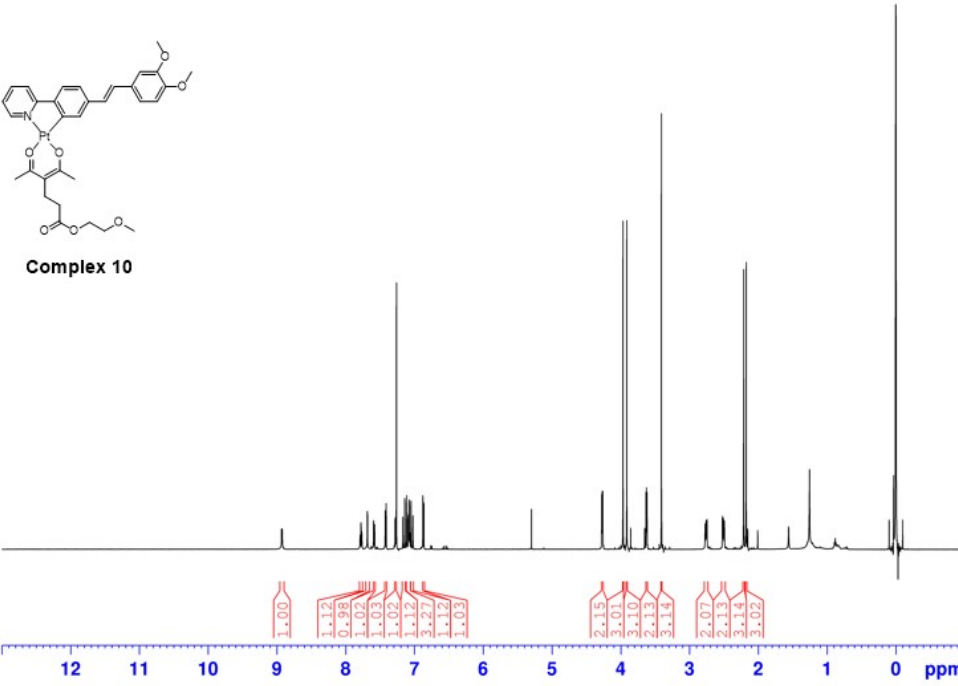
F2 - Acquisition Parameters
 Date_ 20230109
 Time 17.59 h
 INSTRUM Avance
 PROBHD z167430_0032 (zpgg30)
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 203
 DS 4
 SWH 23809.523 Hz
 FIDRES 0.726609 Hz
 AQ 1.3762560 sec
 RG 3.25
 DW 21.000 usec
 DE 19.29 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TDO 1
 SFO1 100.6655806 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 39.31399918 W
 SFO2 400.3016012 MHz
 NUC2 1H
 CPDPRG2 waltz64
 PCPD2 80.00 usec
 PLW2 8.80000019 W
 PLW12 0.20176961 W
 PLW13 0.10112690 W

F2 - Processing parameters
 SI 131072
 SF 100.6555151 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

8.93
8.92
7.78
7.69
7.68
7.59
7.58
7.42
7.41
7.28
7.28
7.27
7.17
7.14
7.11
7.11
7.09
7.09
7.08
7.08
7.05
7.02
6.88
6.86
4.28
4.27
4.27
4.26
3.97
3.91
3.63
3.63
3.63
3.62
3.62
3.41
2.77
2.76
2.76
2.75
2.75
2.52
2.51
2.51
2.50
2.49
2.21
2.18



Complex 10



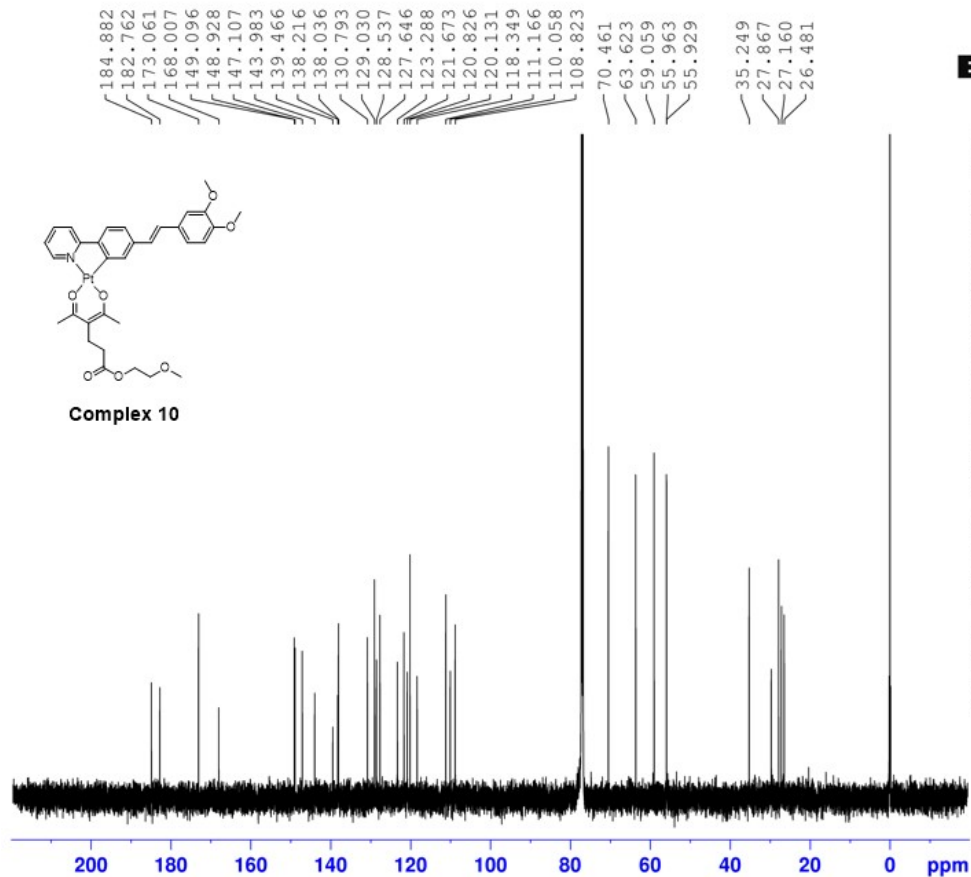
```

Current Data Parameters
NAME      1H-ZL-4-238-41-92-111423
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20231114
Time      13.41
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        12019.230 Hz
FIDRES     0.183399 Hz
AQ         2.7262976 sec
RG         256
DW         41.600 usec
DE         6.50 usec
TE         298.0 K
D1         1.00000000 sec

===== CHANNEL f1 =====
NUC1       1H
P1         11.80 usec
PLW1       26.91500092 W
SFO1       600.2124008 MHz

F2 - Processing parameters
SI         65536
SF         600.2100127 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



```

Current Data Parameters
NAME      13C-ZL-4-238-cdcl3-111423
EXPNO    1
PROCNO   1

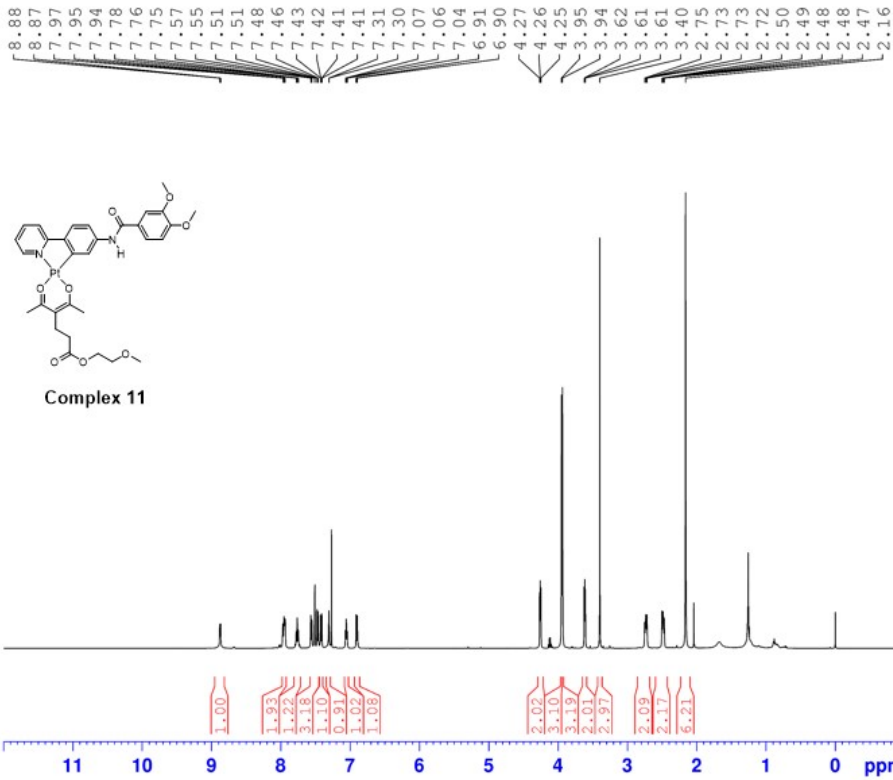
F2 - Acquisition Parameters
Date_    20231114
Time     15.44
INSTRUM spect
PROBHD   5 mm PABBO BB-
PULPROG zgpg30
TD       65536
SOLVENT  CDCl3
NS       2411
DS       4
SWH      36057.691 Hz
FIDRES   0.550197 Hz
AQ       0.9087659 sec
RG       2050
DW       13.867 usec
DE       6.50 usec
TE       298.0 K
D1       2.00000000 sec
D11      0.03000000 sec

----- CHANNEL f1 -----
NUC1     13C
P1       10.00 usec
PLM1     60.25600052 W
SFO1     150.9380173 MHz

----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2     1H
PCPD2    70.00 usec
PLM2     26.91500092 W
PLM12    0.79097998 W
PLM13    0.38758001 W
SFO2     600.2124008 MHz

F2 - Processing parameters
SI       65536
SF       150.9229250 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

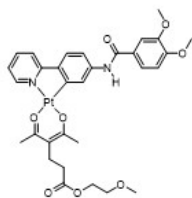
```



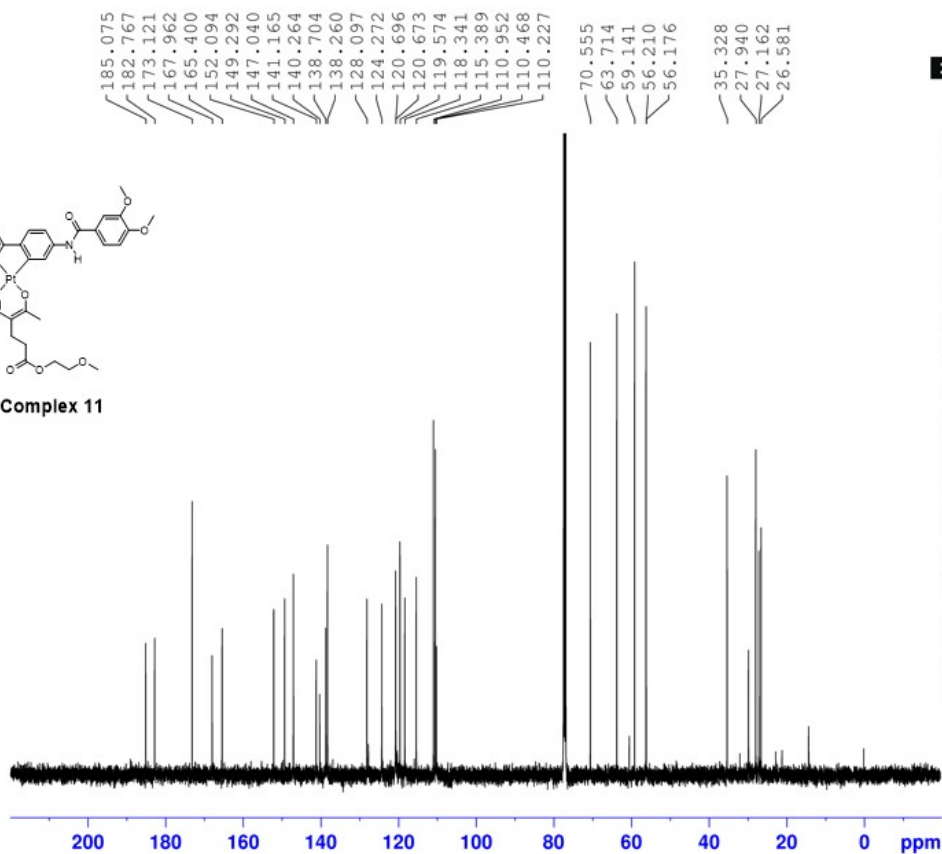
Current Data Parameters
 NAME pig-11-4-236-59-end-1F
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210503
 Time 12.25 h
 INSTRUM Avance NEO 500
 PROBHD Z113652_0071 ()
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 101
 DW 50.000 usec
 DE 10.45 usec
 TE 298.0 K
 DI 1.00000000 sec
 TDO 1
 SFO1 500.3030894 MHz
 NUC1 1H
 P0 4.00 usec
 P1 12.00 usec
 PLW1 13.35999966 W

F2 - Processing parameters
 SI 65536
 SF 500.3000074 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Complex 11



```

Current Data Parameters
NAME      pig-11-4-236-59-end-11
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20210503
Time     13.35 h
INSTRUM  Avance NEO 500
PROBHD   Z113652_0071 (
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       1024
DS       4
SWH      30120.482 Hz
FIDRES   0.919204 Hz
AQ       1.0878977 sec
RG       101
DW       16.600 usec
DE       10.00 usec
TE       298.0 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1
SFO1     125.8131151 MHz
NUC1     13C
P0       3.33 usec
P1       10.00 usec
PLM1     103.61000061 W
SFG2     500.3020012 MHz
NUC2     1H
CPDPRG2  waltz65
PCPD2    80.00 usec
PLM2     13.35999966 W
PLM12    0.30400079 W
PLM13    0.15236519 W

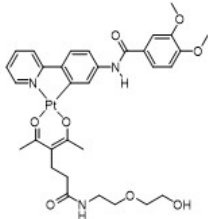
F2 - Processing parameters
SI       32768
SF       125.8005207 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```



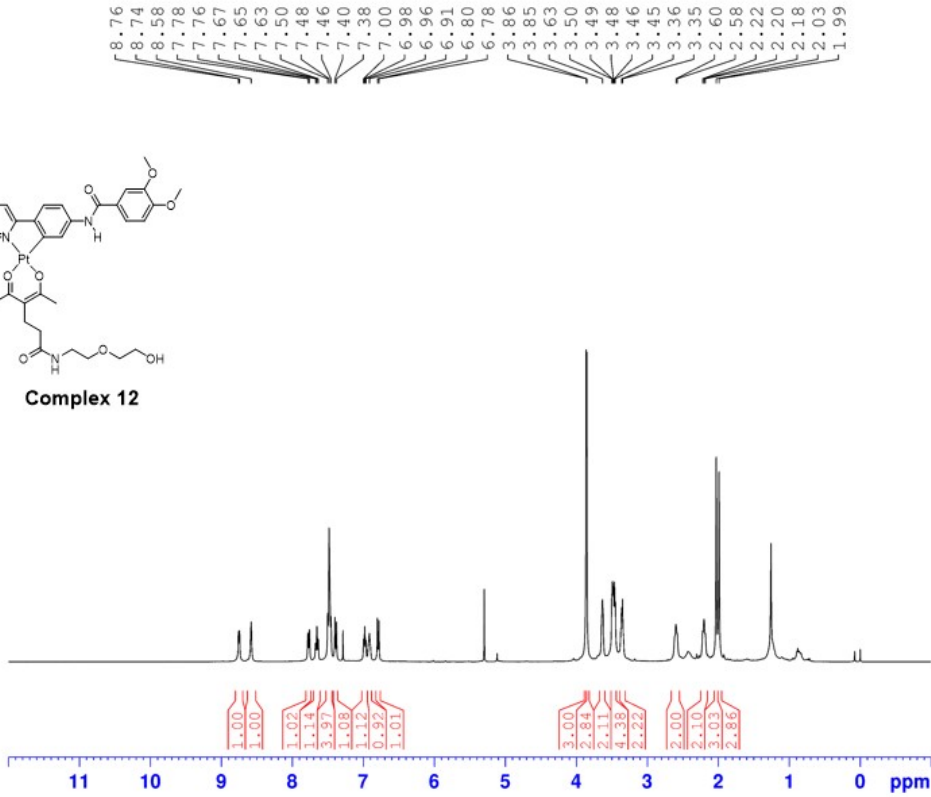
Current Data Parameters
NAME 1H-ZL-3-130-38-75
EXPNO 1
PROCNO 1

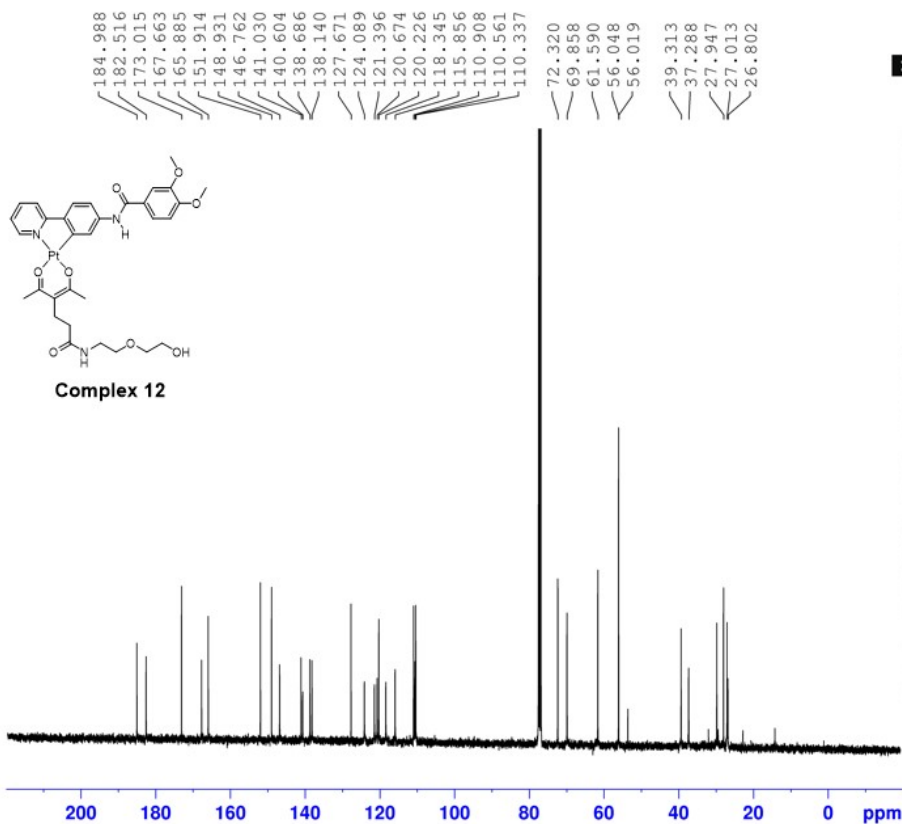
F2 - Acquisition Parameters
Date_ 20211012
Time 16.02 h
INSTRUM spect
PROBHD Z104450_0192 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 64
DW 62.400 usec
DE 16.92 usec
TE 294.1 K
D1 1.00000000 sec
TDO 1
SF01 400.1324708 MHz
NUC1 1H
PO 5.00 usec
P1 15.00 usec
PLW1 8.47000027 W

F2 - Processing parameters
SI 65536
SF 400.1299987 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Complex 12

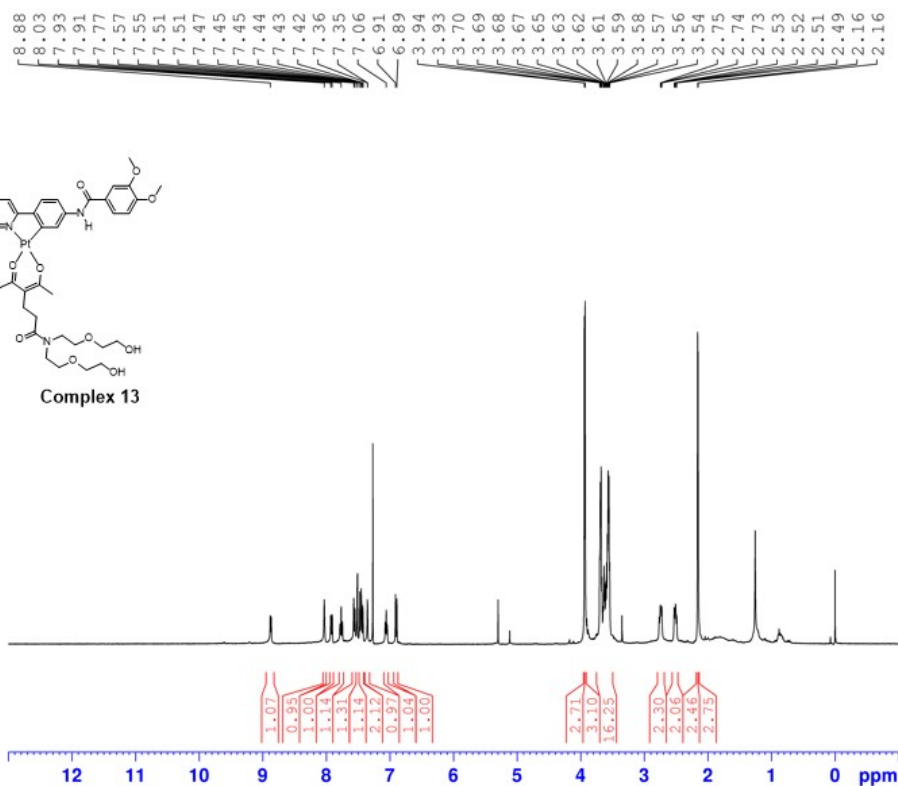




Current Data Parameters
 NAME 13C-2L-3-130-38-75-13C
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211012
 Time 17.36 h
 INSTRUM spect
 PROBHD z104450_0192 (
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1521
 DS 2
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 1.3631488 sec
 RG 287
 DW 20.800 usec
 DE 6.50 usec
 TE 294.9 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1
 SFO1 100.6228298 MHz
 NUC1 13C
 P0 3.28 usec
 P1 9.85 usec
 PLW1 28.63999939 W
 SFO2 400.1316005 MHz
 NUC2 1H
 CDPFRG12 waltz65
 PCPD2 90.00 usec
 PLW2 8.47000027 W
 PLW12 0.23528001 W
 PLW13 0.11834000 W

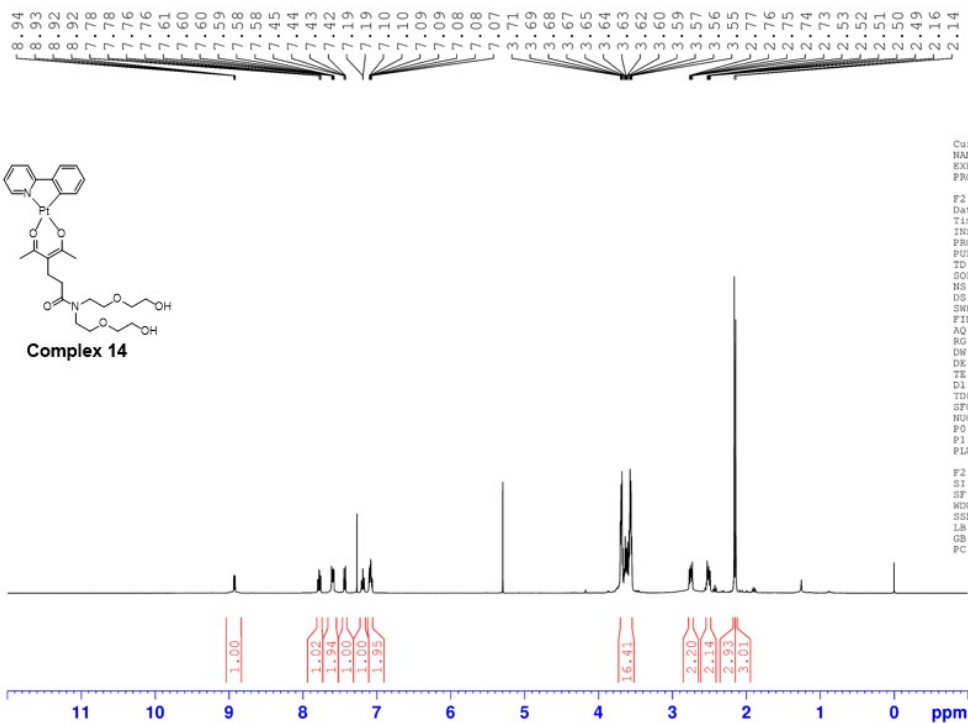
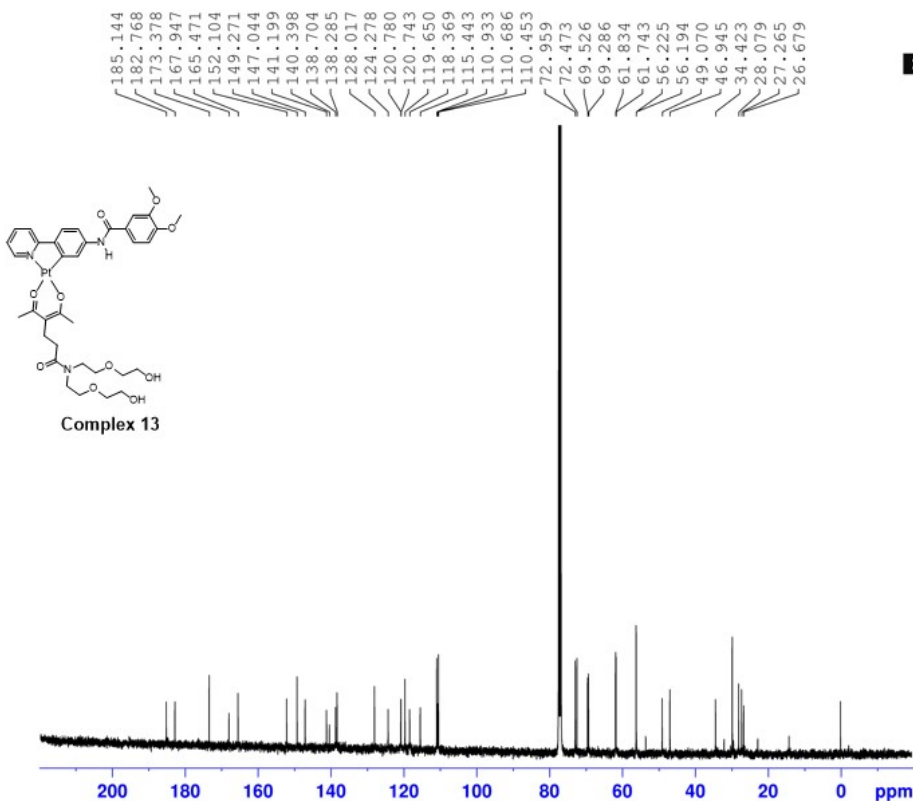
F2 - Processing parameters
 SI 32768
 SF 100.6127623 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

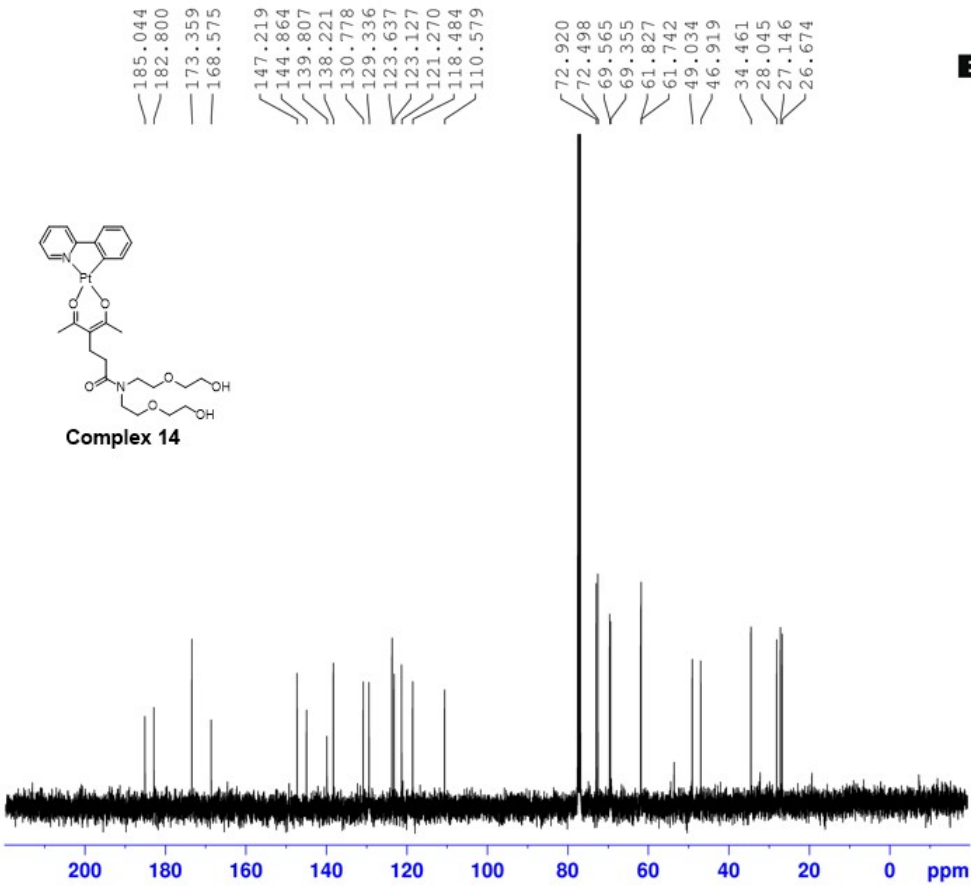


Current Data Parameters
 NAME 1H-2L-3-74-12-28
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210802
 Time 17.32 h
 INSTRUM spect
 PROBHD z104450_0192 (
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 2050
 DW 62.400 usec
 DE 16.92 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1
 SFO1 400.1324708 MHz
 NUC1 1H
 P0 5.00 usec
 P1 15.00 usec
 PLW1 8.47000027 W

F2 - Processing parameters
 SI 65536
 SF 400.1300060 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





Current Data Parameters
NAME 13C-ZL-5-156-33-43
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230222
Time 16.18 h
INSTRUM spect
PROBHD Z104450_0192 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 209
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 114
DW 20.800 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.28 usec
P1 9.85 usec
PLW1 28.63999939 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz65
PCPD2 90.00 usec
PLW2 8.47000027 W
PLW12 0.23528001 W
PLW13 0.11834000 W

F2 - Processing parameters
SI 32768
SF 100.6127571 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40