

Supporting Information

Cytotoxic impact of fluorinated ligands in equatorial position of *trans*-configured diam(m)inetetracarboxylato-platinum(IV) complexes

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1. NMR spectra of platinum(II) complexes

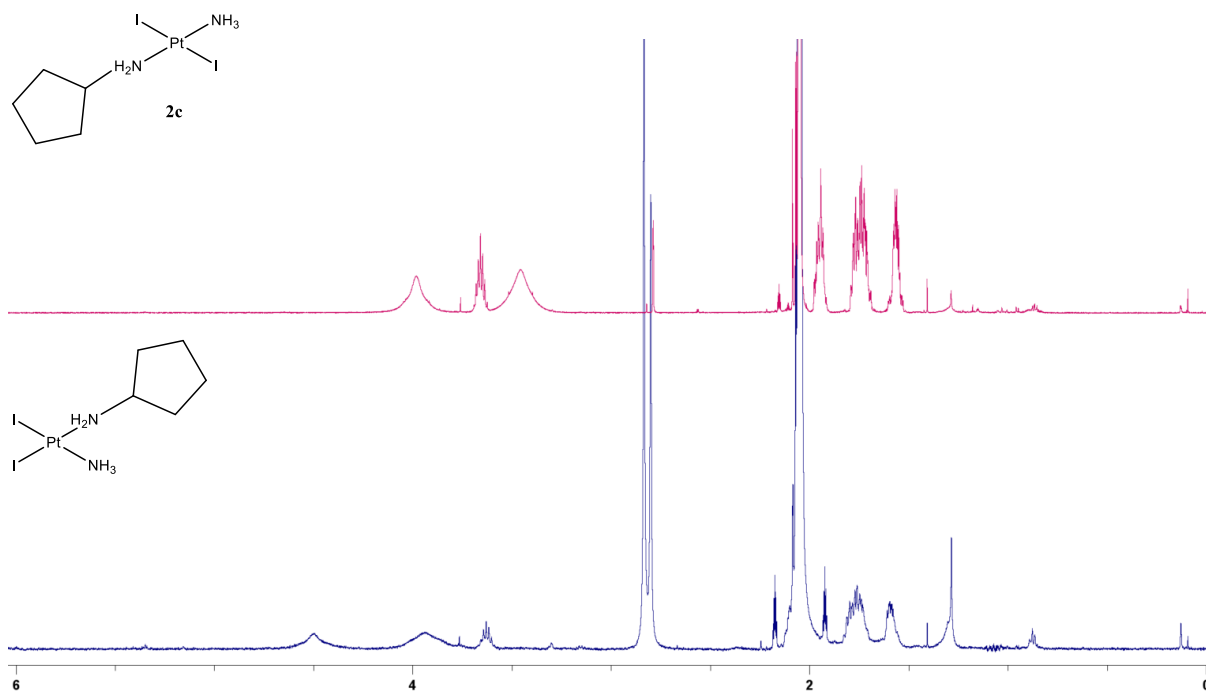


Figure S1. ¹H NMR spectra of *cis*-(SP-4-2)-amminecyclopentylaminediiodoplatinum(II) (bottom) and *trans*-(SP-4-1)-amminecyclopentylaminediiodoplatinum(II) **2c** (top) in d₆-acetone.

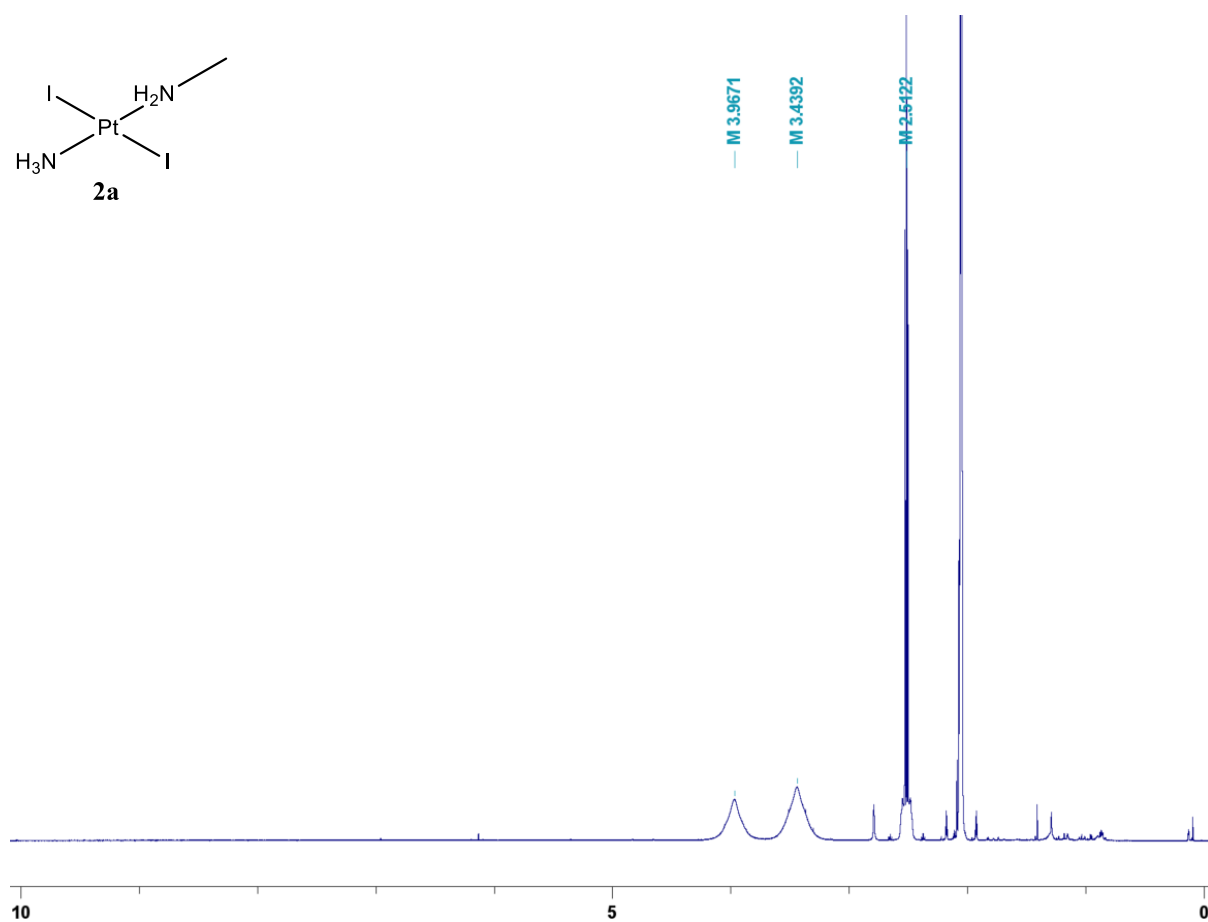
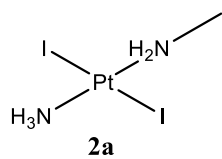


Figure S2. ^1H NMR spectrum of **2a** in d_6 -acetone.

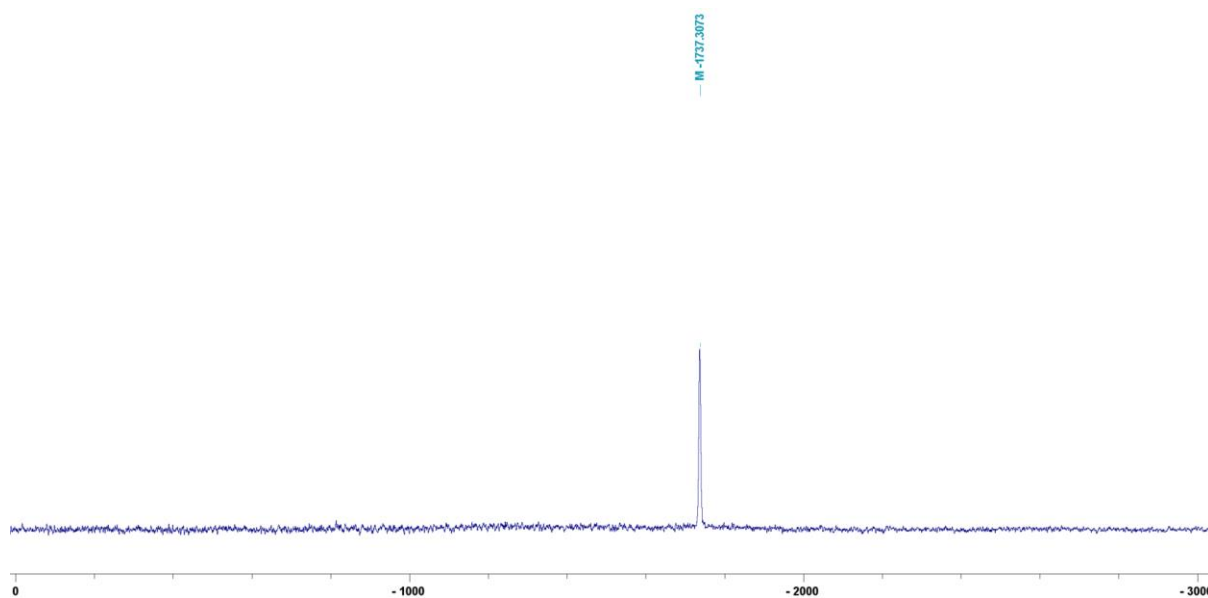


Figure S3. ^{195}Pt NMR spectrum of **2a** in d_6 -acetone.

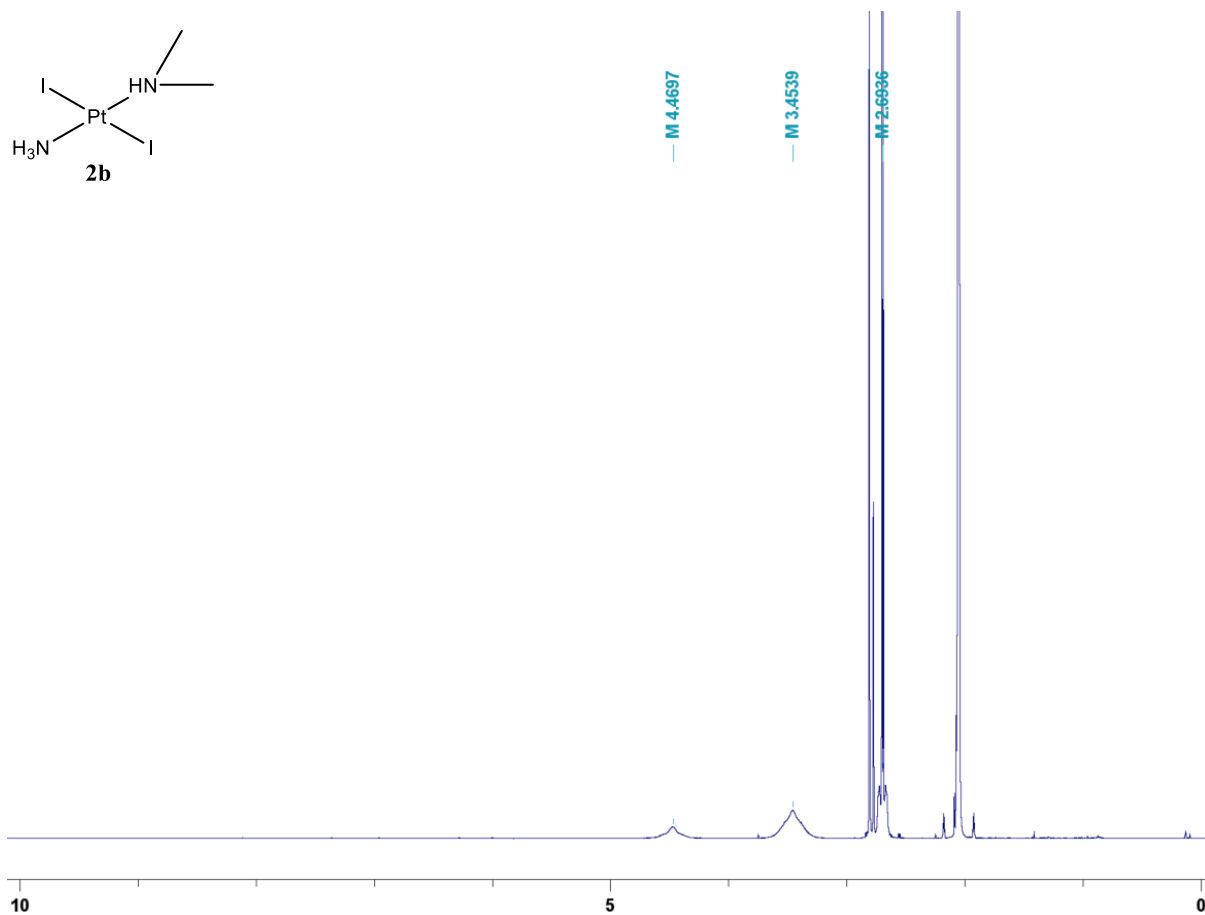


Figure S4. ¹H NMR spectrum of **2b** in d₆-acetone.

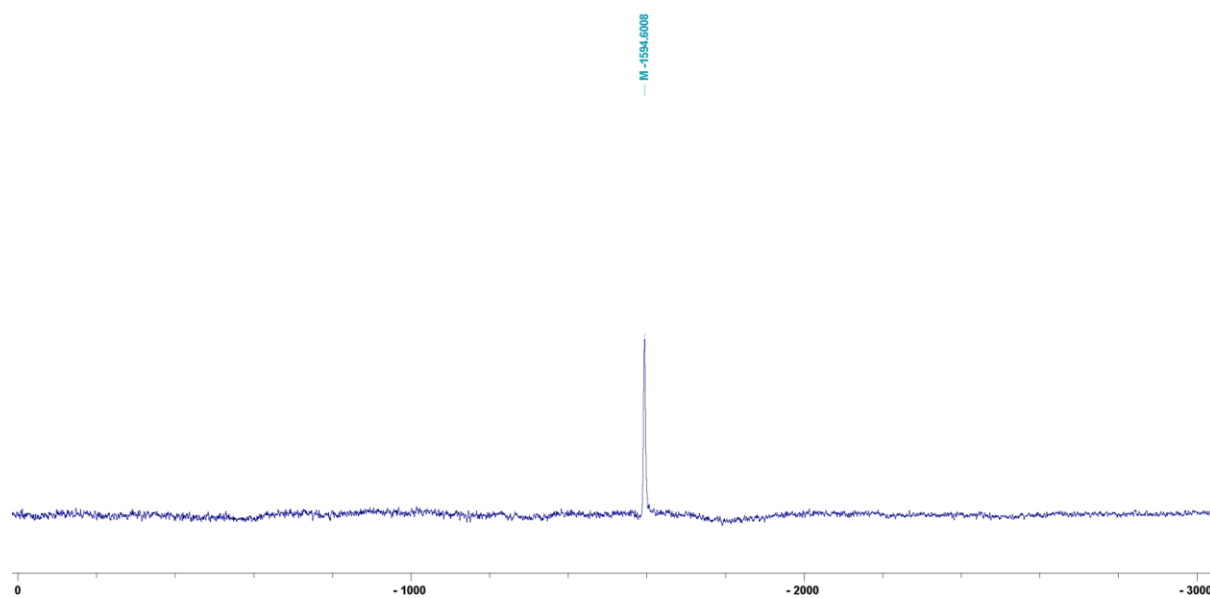


Figure S5. ¹⁹⁵Pt NMR spectrum of **2b** in d₆-acetone.

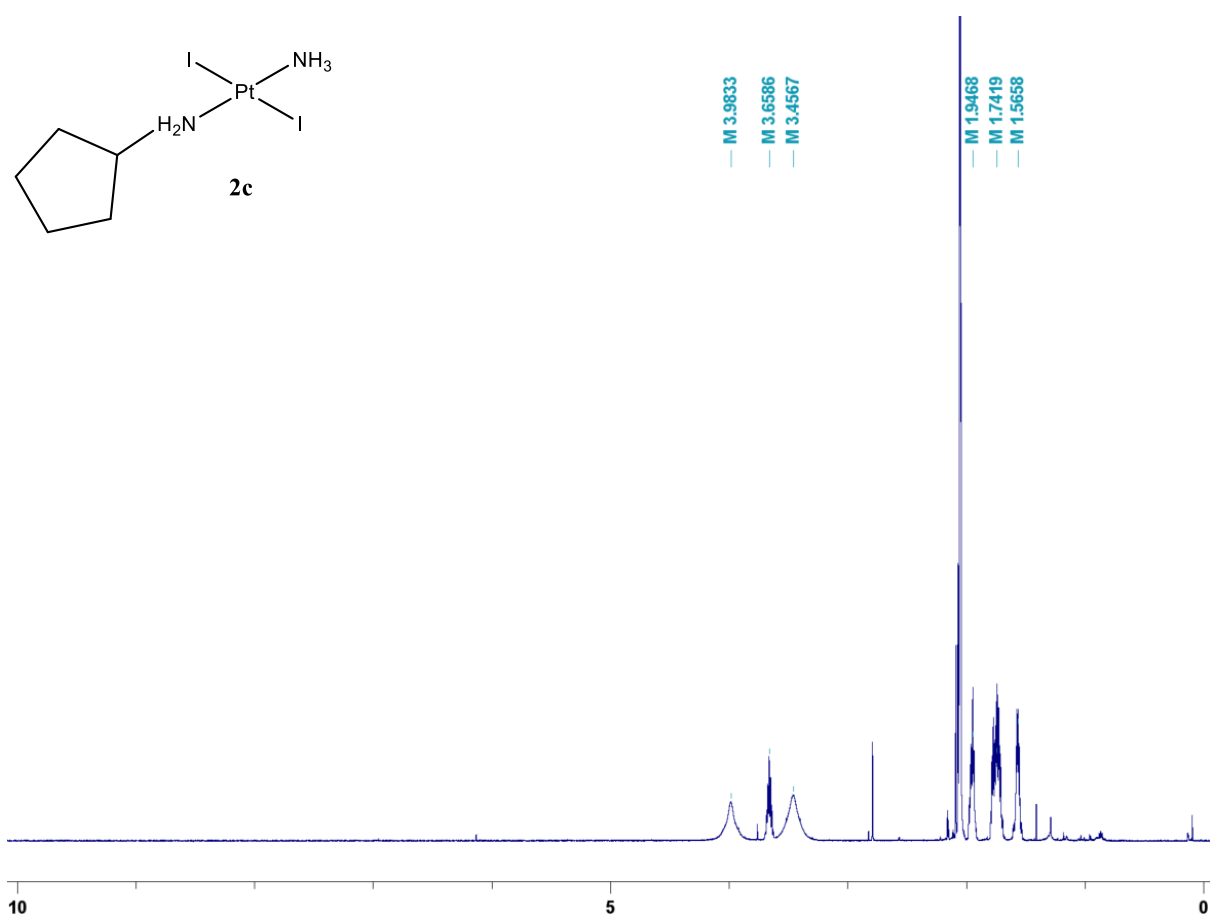


Figure S6. ^1H NMR spectrum of **2c** in d_6 -acetone.

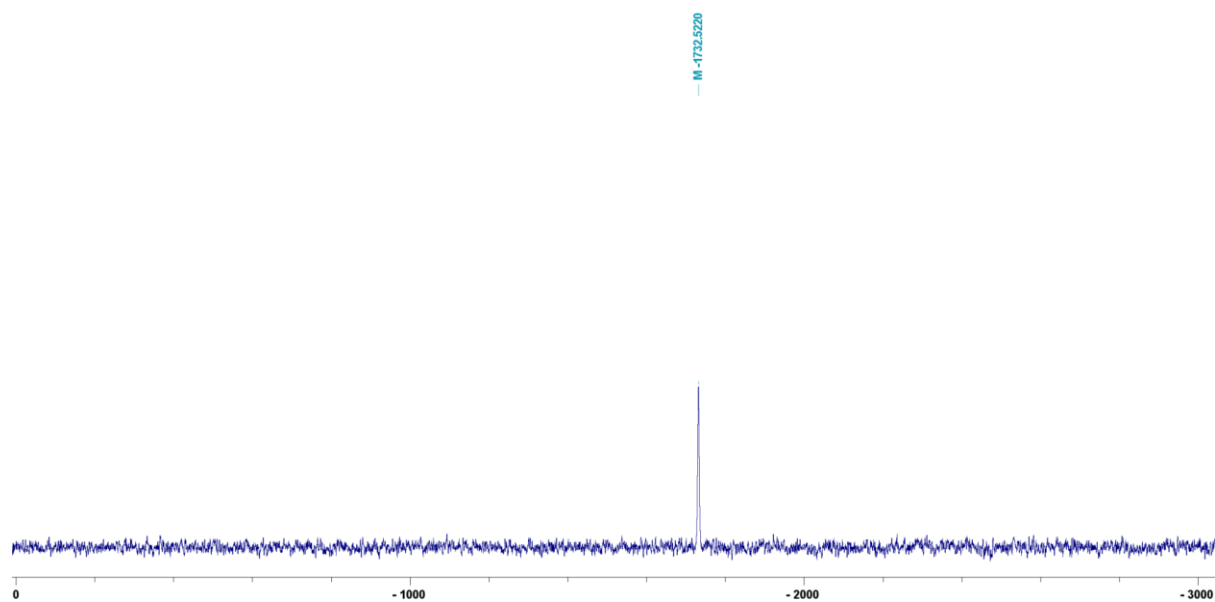


Figure S7. ^{195}Pt NMR spectrum of **2c** in d_6 -acetone.

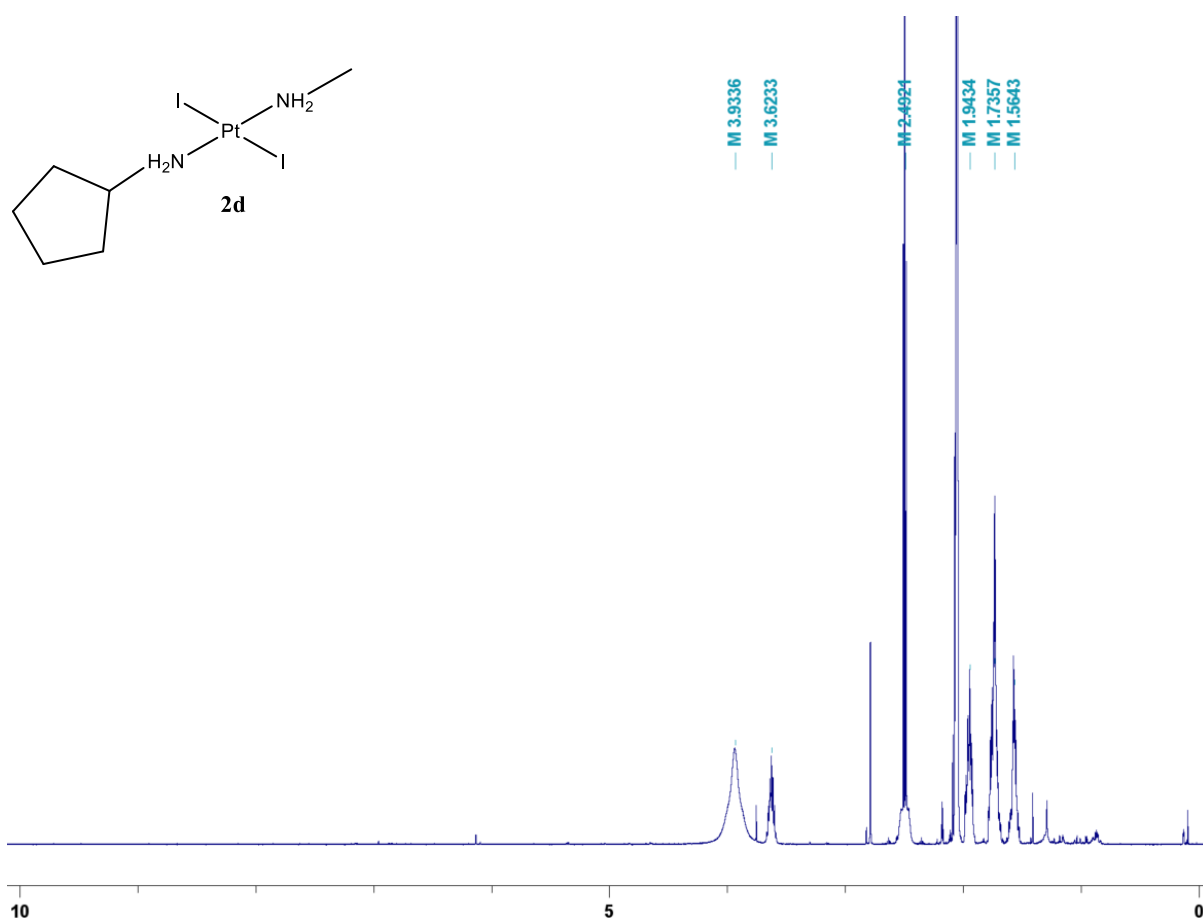


Figure S8. ¹H NMR spectrum of **2d** in d₆-acetone.

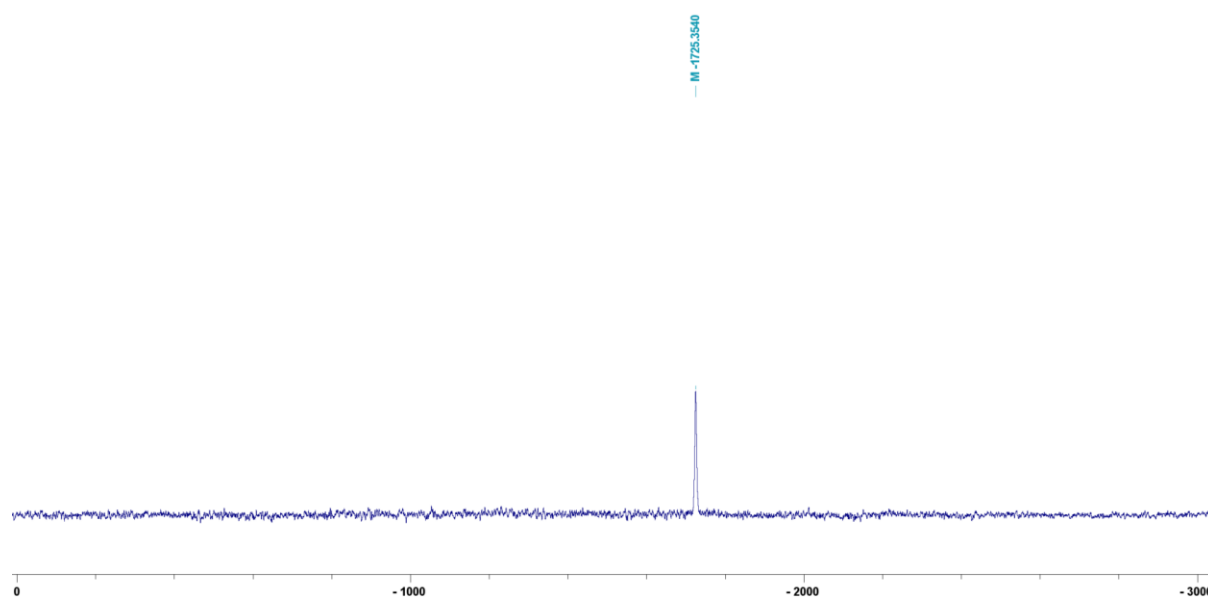


Figure S9. ¹⁹⁵Pt NMR spectrum of **2d** in d₆-acetone.

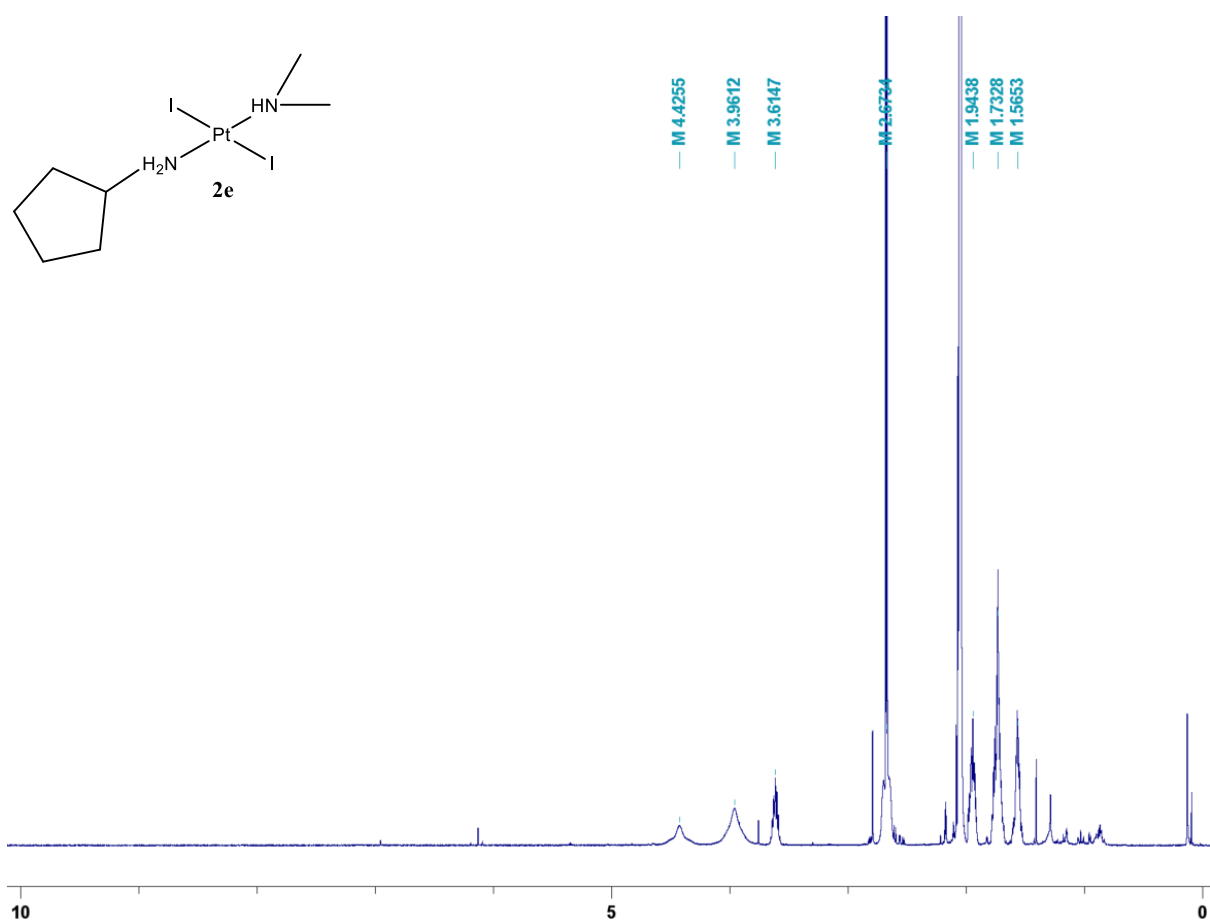


Figure S10. ¹H NMR spectrum of **2e** in d₆-acetone.

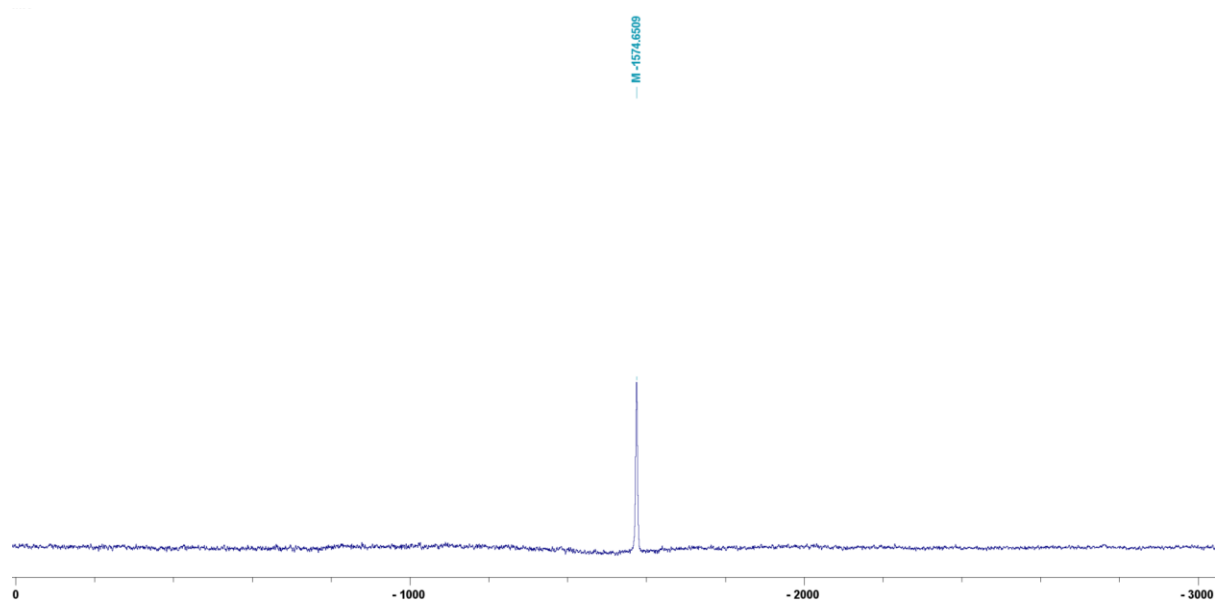


Figure S11. ¹⁹⁵Pt NMR spectrum of **2e** in d₆-acetone.

2. NMR spectra of platinum(IV) complexes

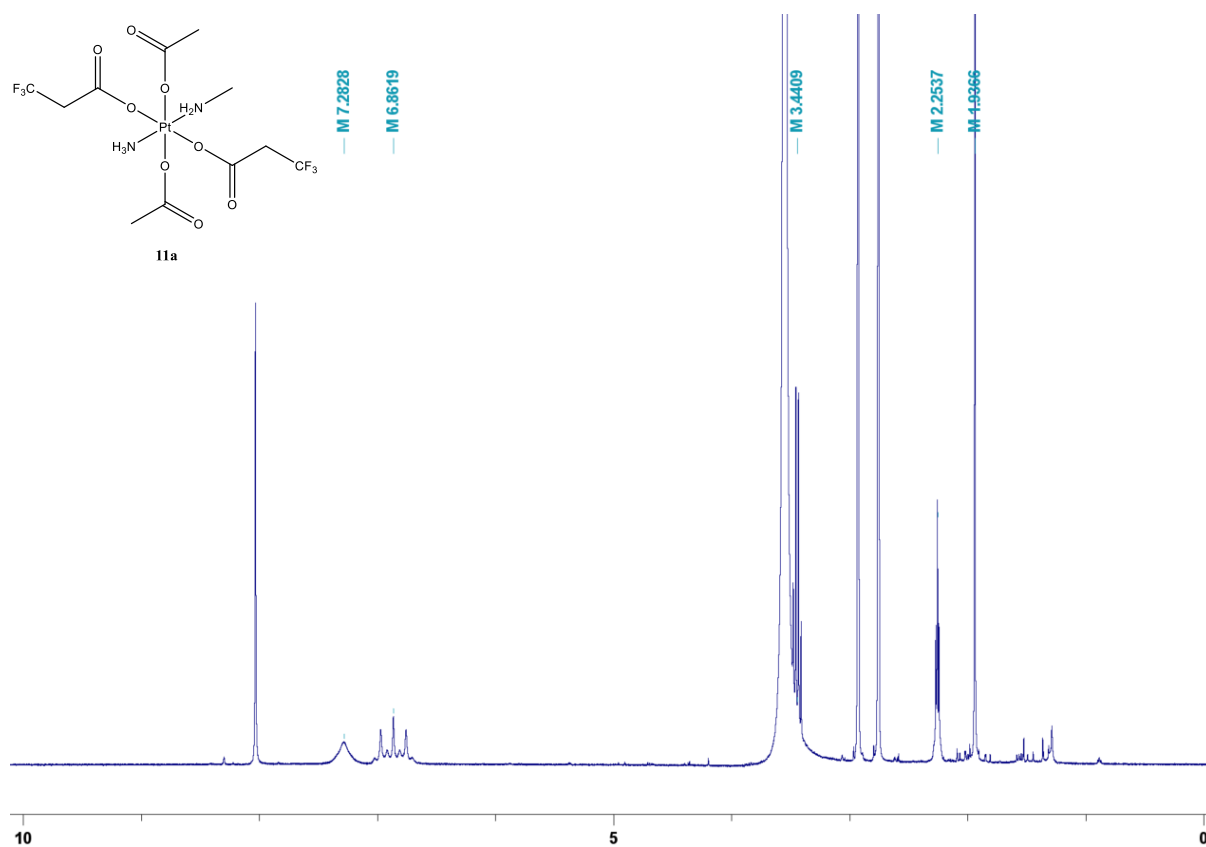


Figure S12. ¹H NMR spectrum of **11a** in d₇-DMF.

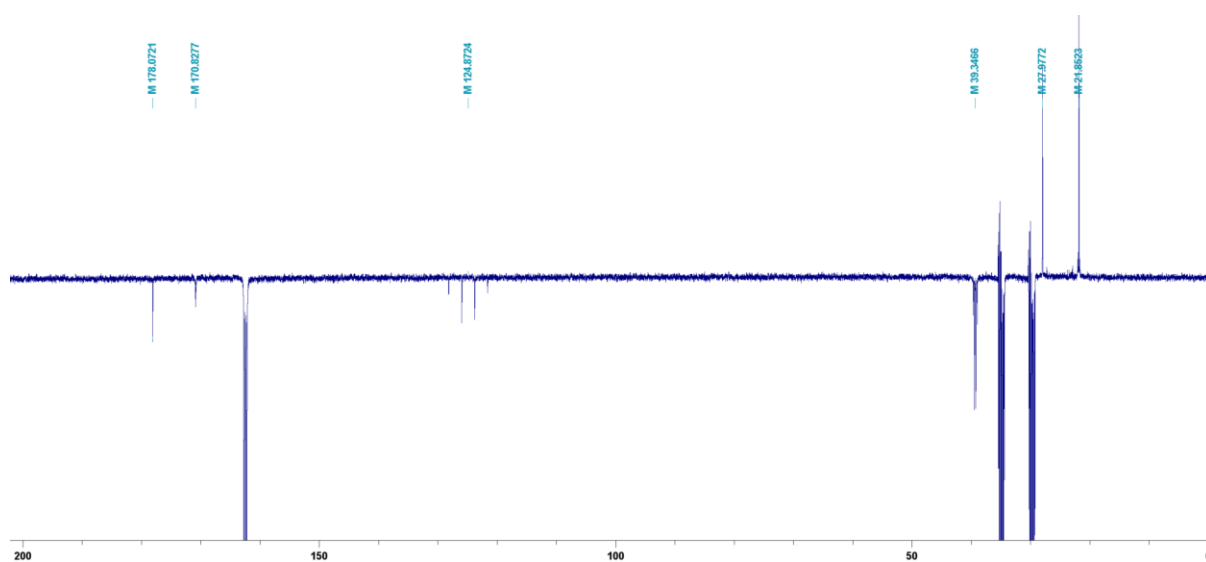


Figure S13. ¹³C NMR spectrum of **11a** in d₇-DMF.

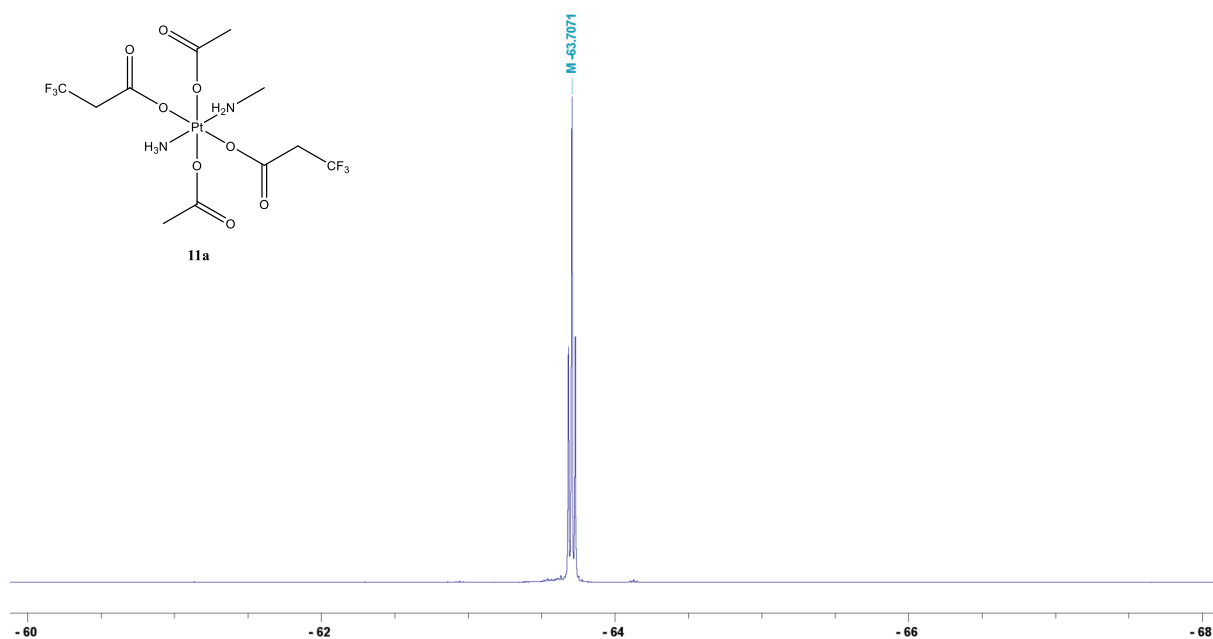


Figure S14. ¹⁹F NMR spectrum of **11a** in d₇-DMF.

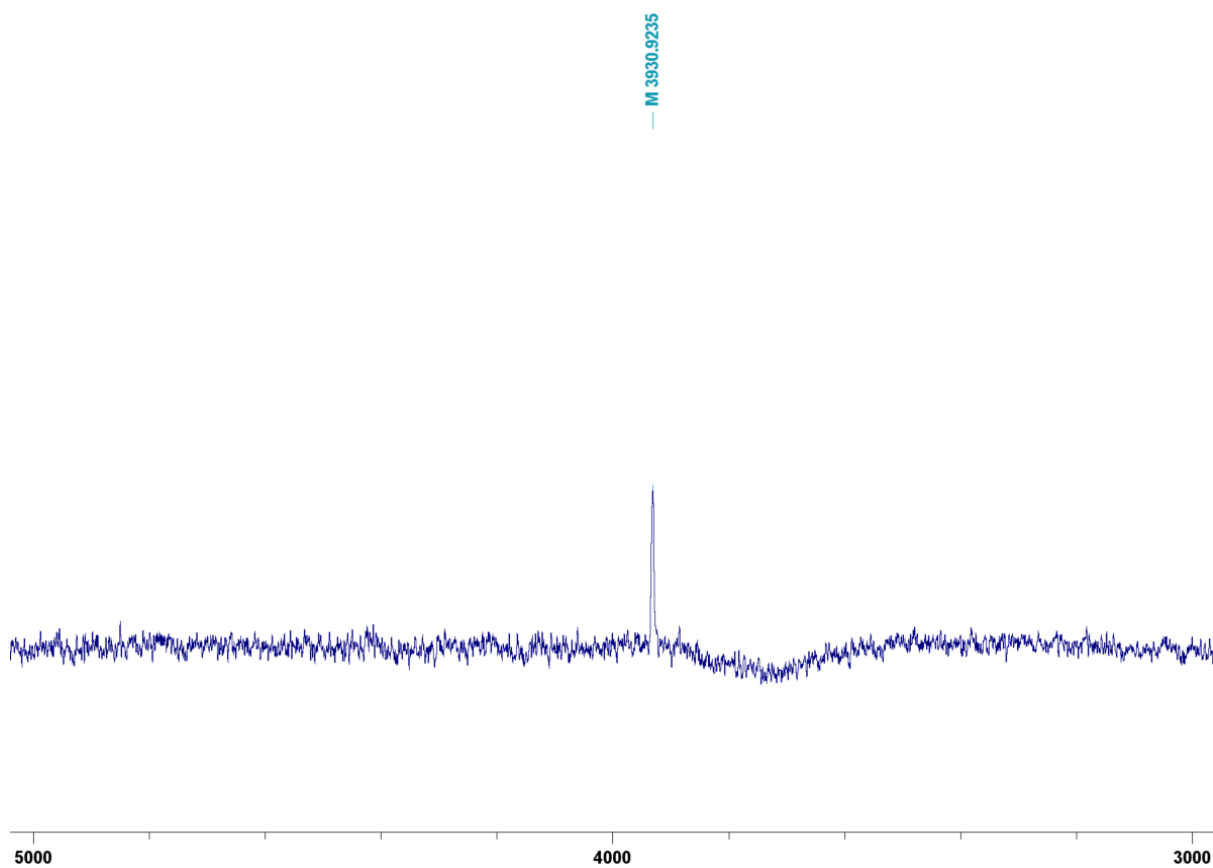


Figure S15. ¹⁹⁵Pt NMR spectrum of **11a** in d₇-DMF.

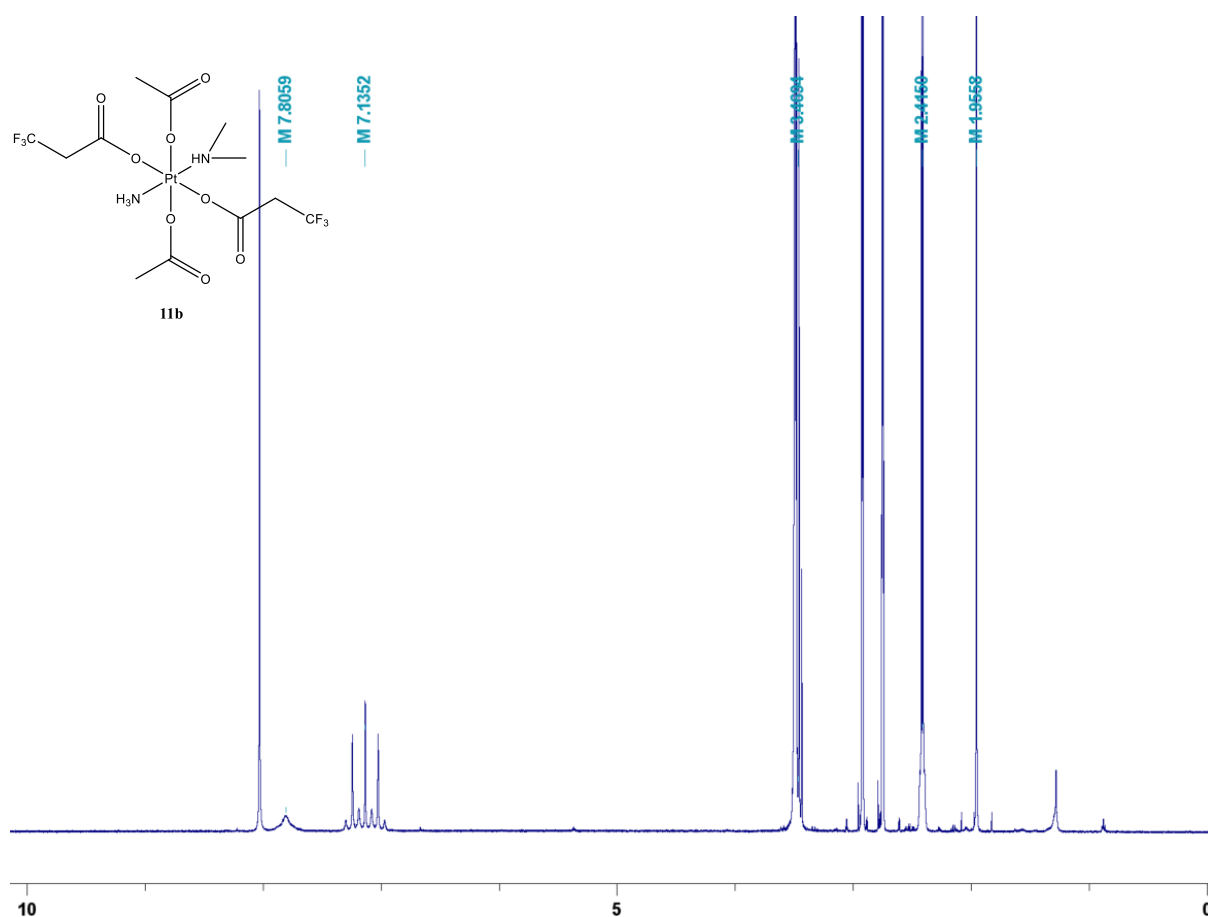


Figure S16. ¹H NMR spectrum of **11b** in d₇-DMF.

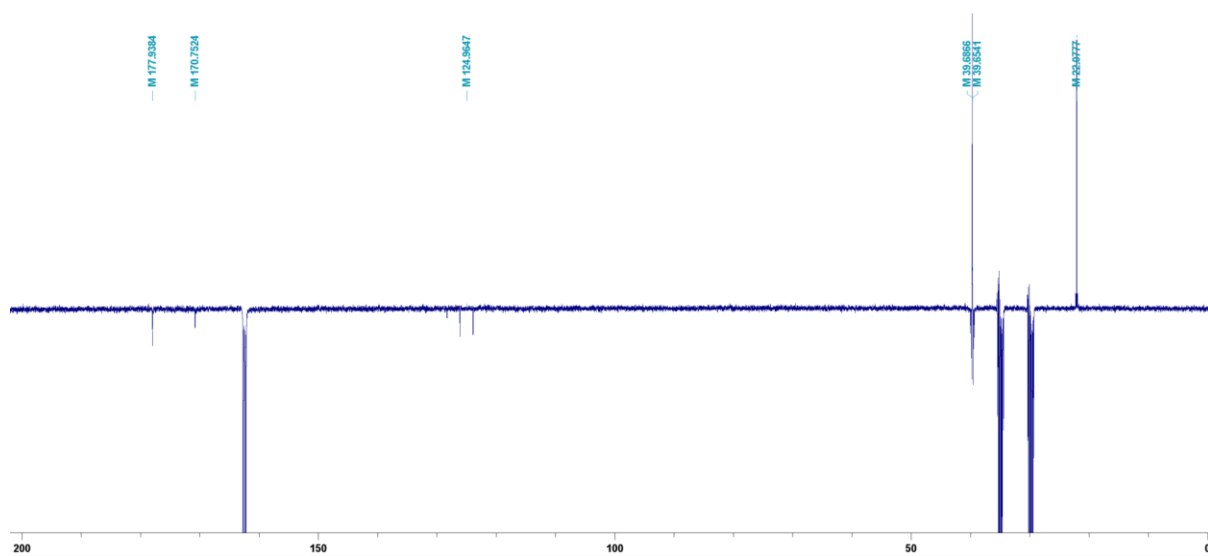


Figure S17. ¹³C NMR spectrum of **11b** in d₇-DMF.

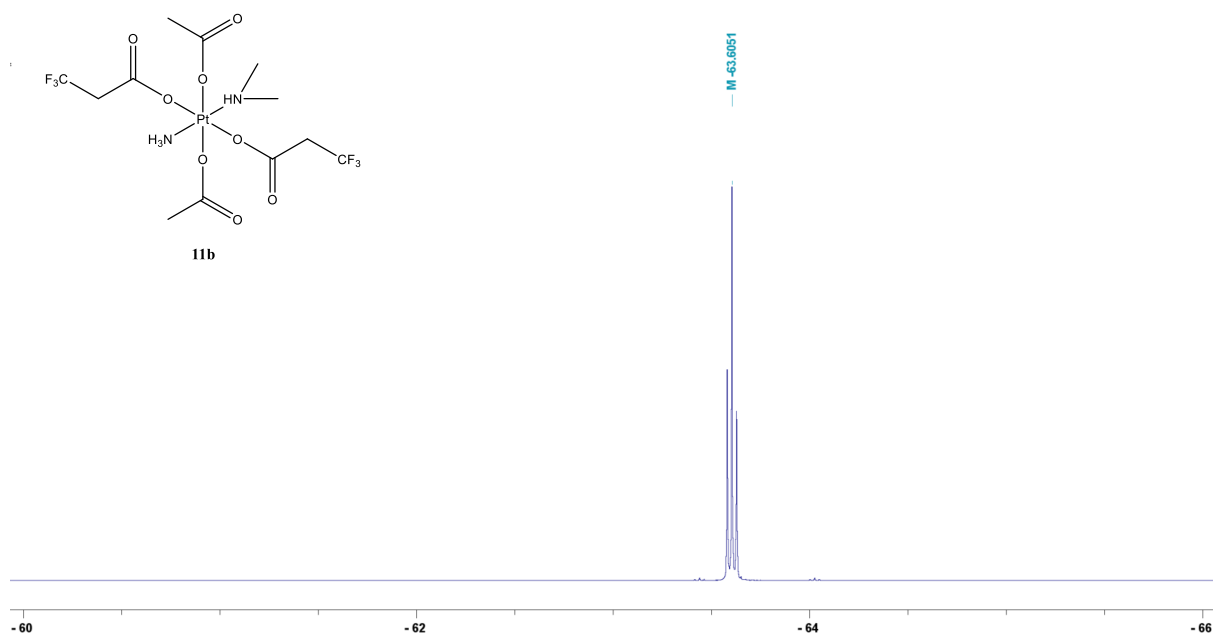


Figure S18. ^{19}F NMR spectrum of **11b** in d_7 -DMF.

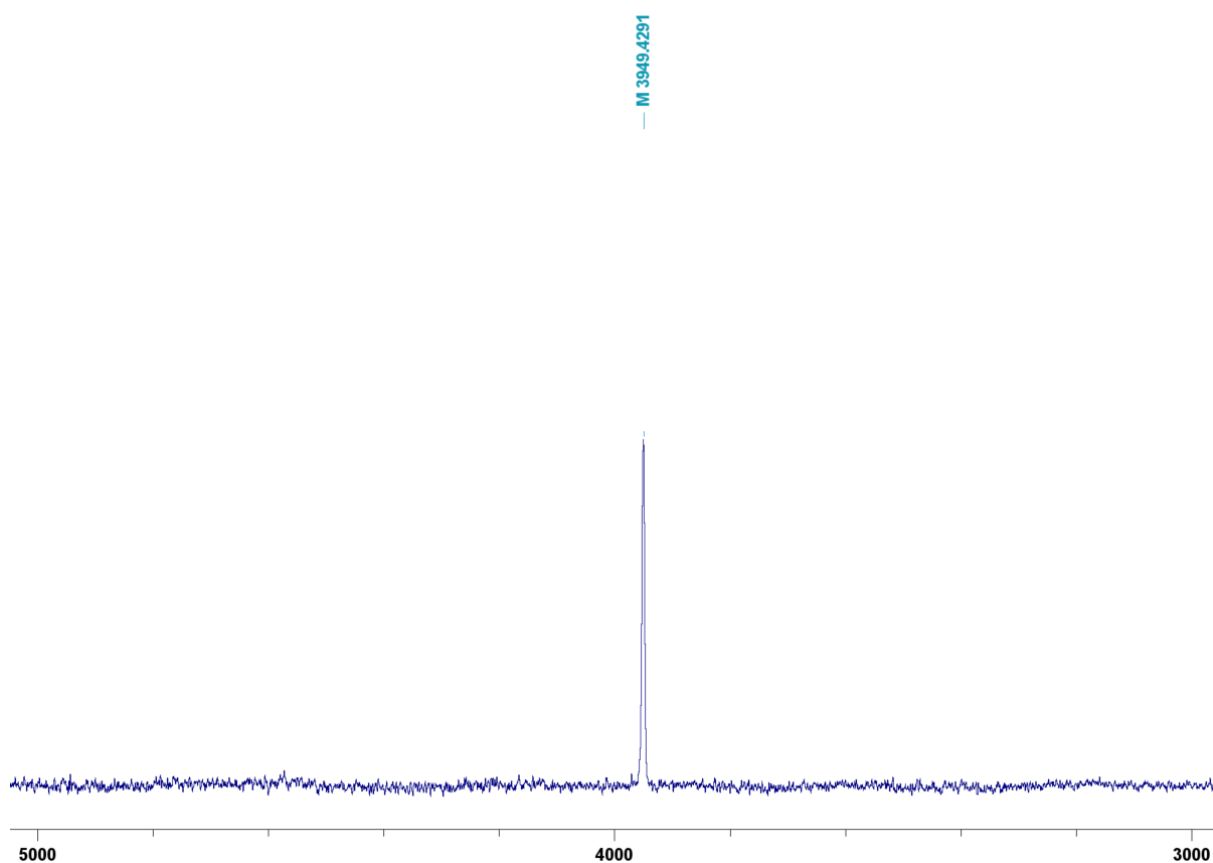


Figure S19. ^{195}Pt NMR spectrum of **11b** in d_7 -DMF.

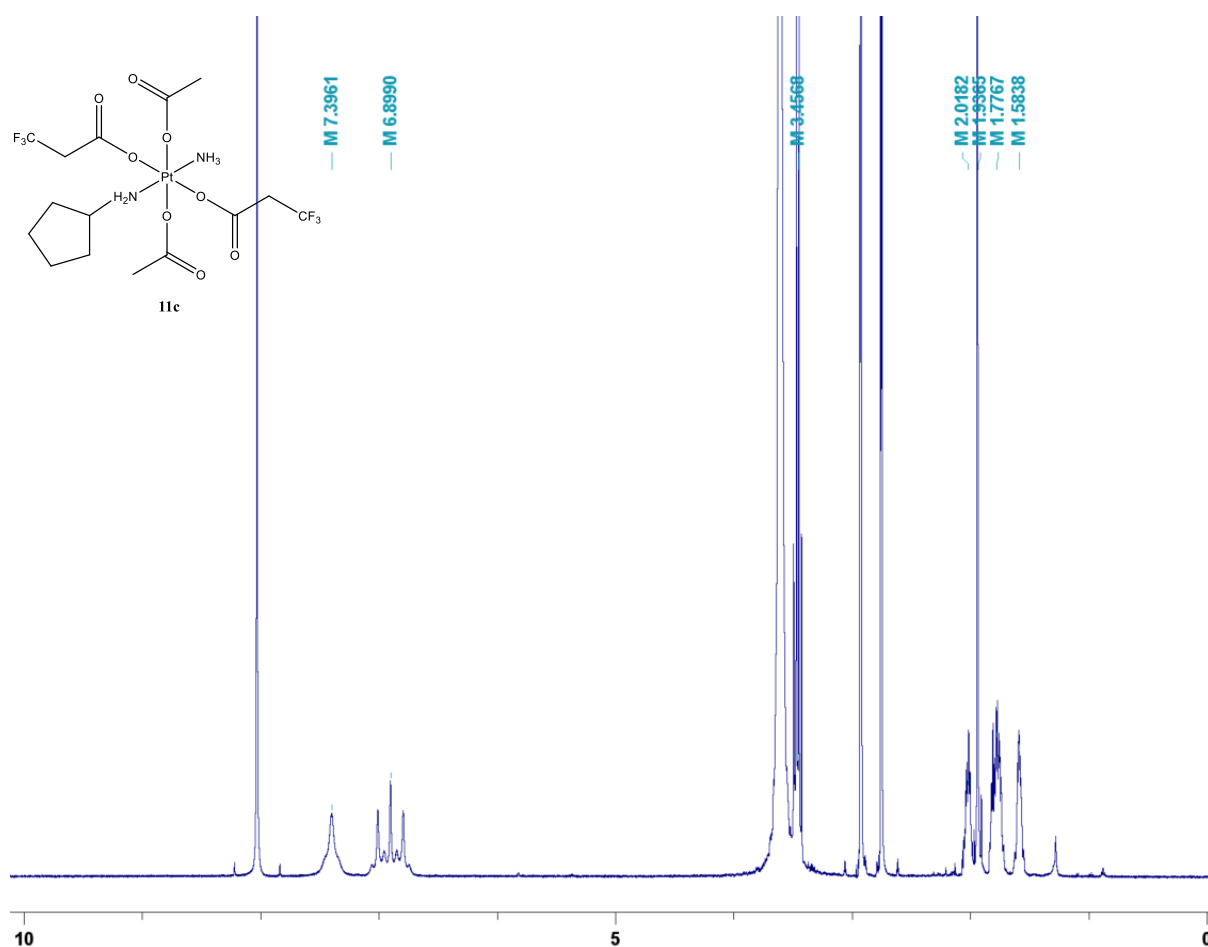


Figure S20. ¹H NMR spectrum of **11c** in d₇-DMF.

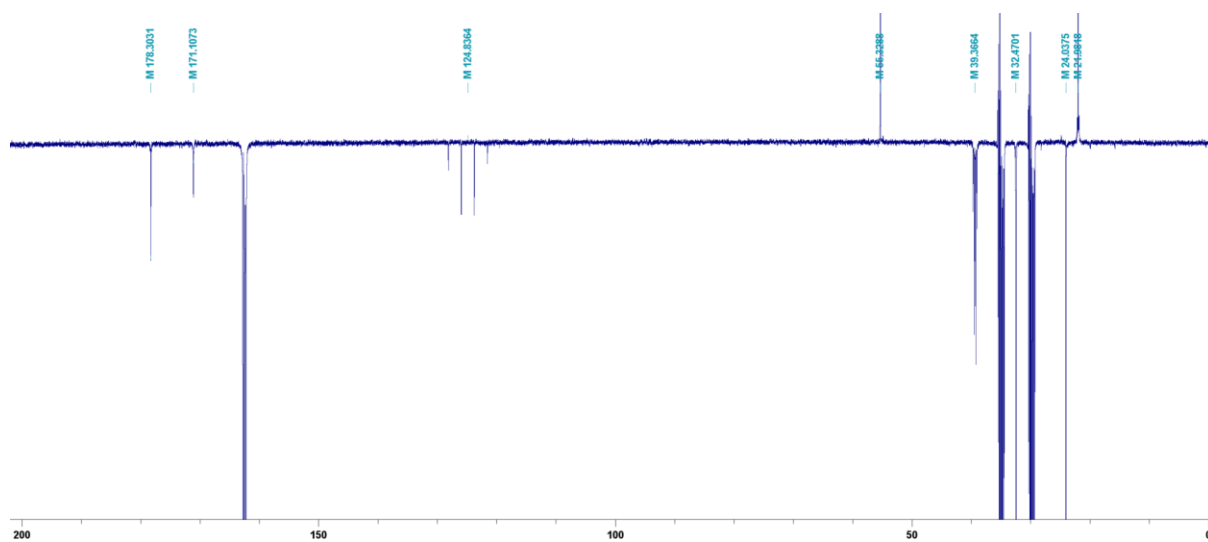


Figure S21. ¹³C NMR spectrum of **11c** in d₇-DMF.

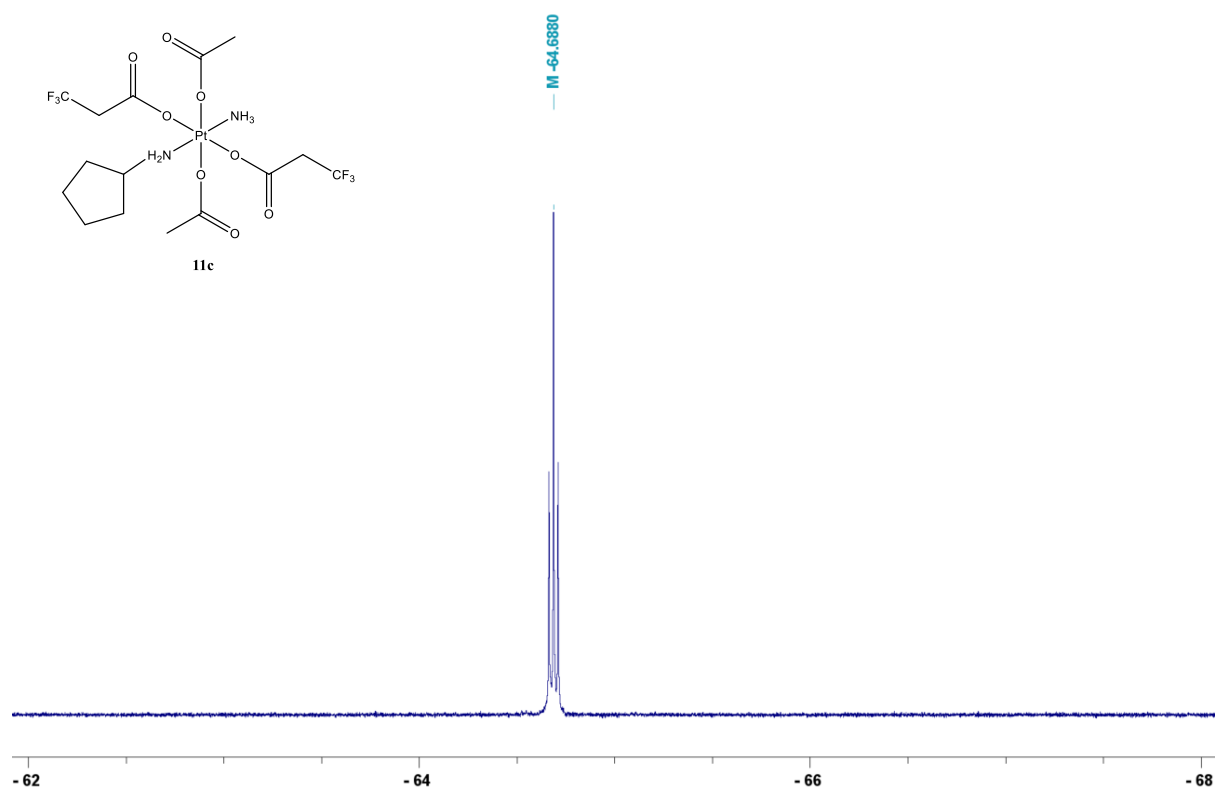


Figure S22. ^{19}F NMR spectrum of **11c** in d_7 -DMF.

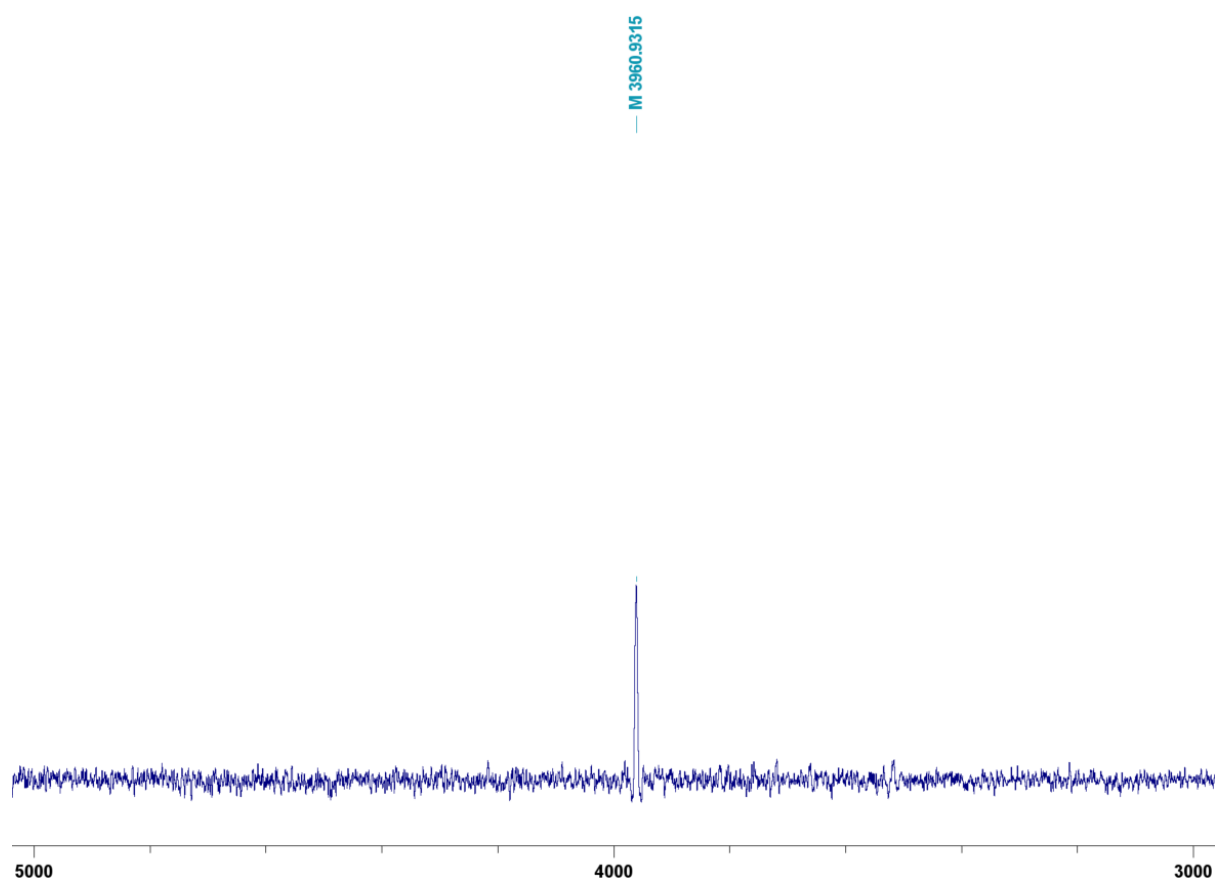


Figure S23. ^{195}Pt NMR spectrum of **11c** in d_7 -DMF.

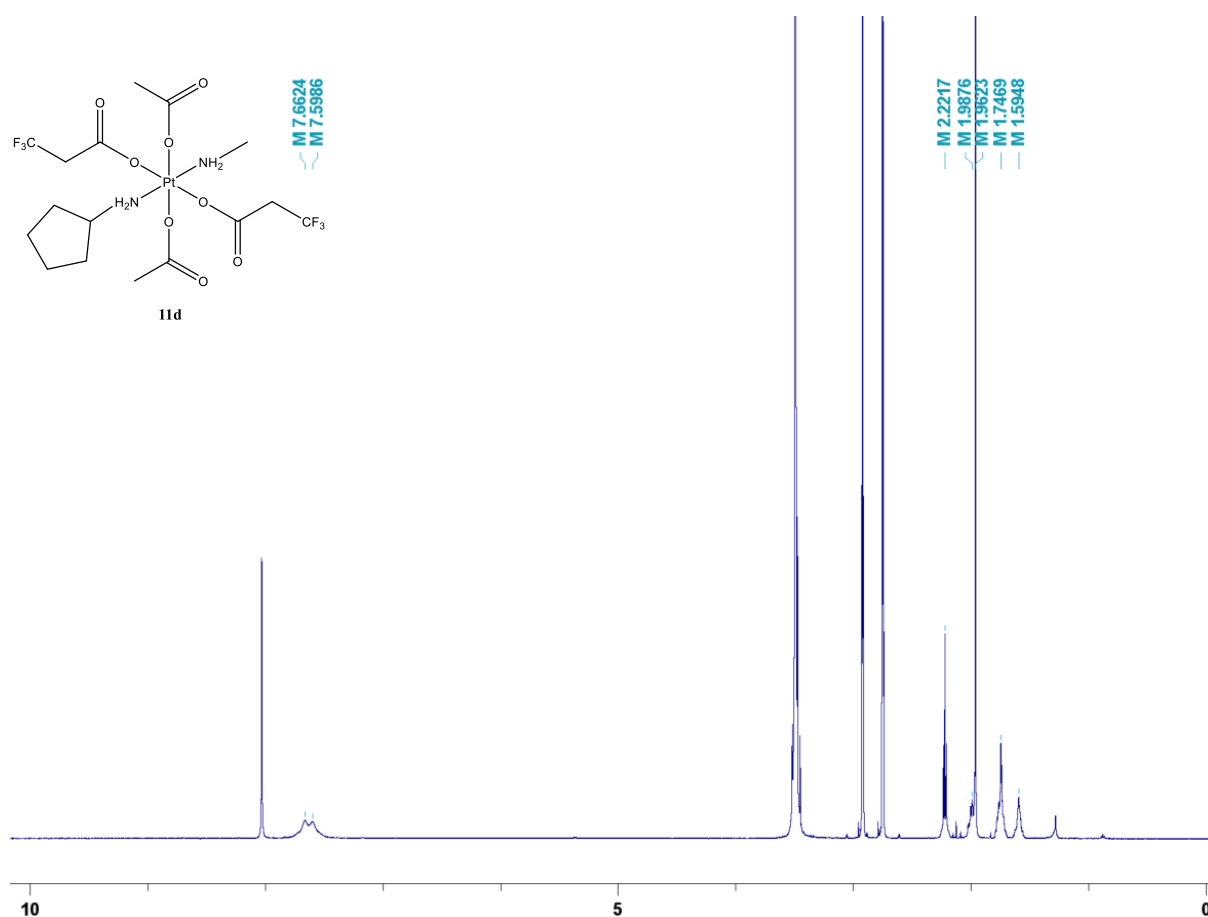


Figure S24. ¹H NMR spectrum of **11d** in d₇-DMF.

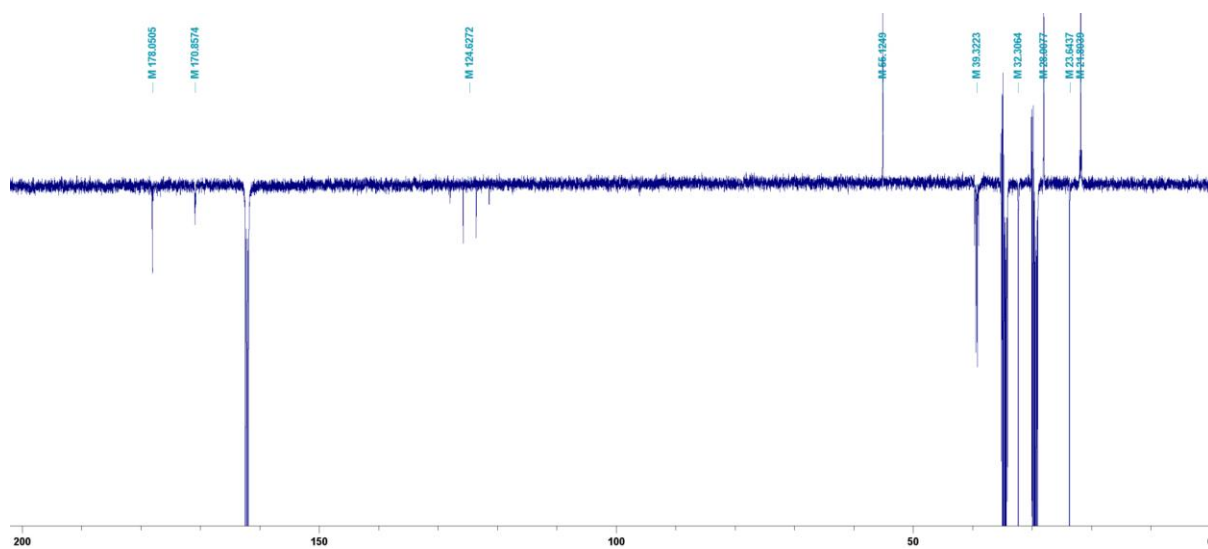


Figure S25. ¹³C NMR spectrum of **11d** in d₇-DMF.

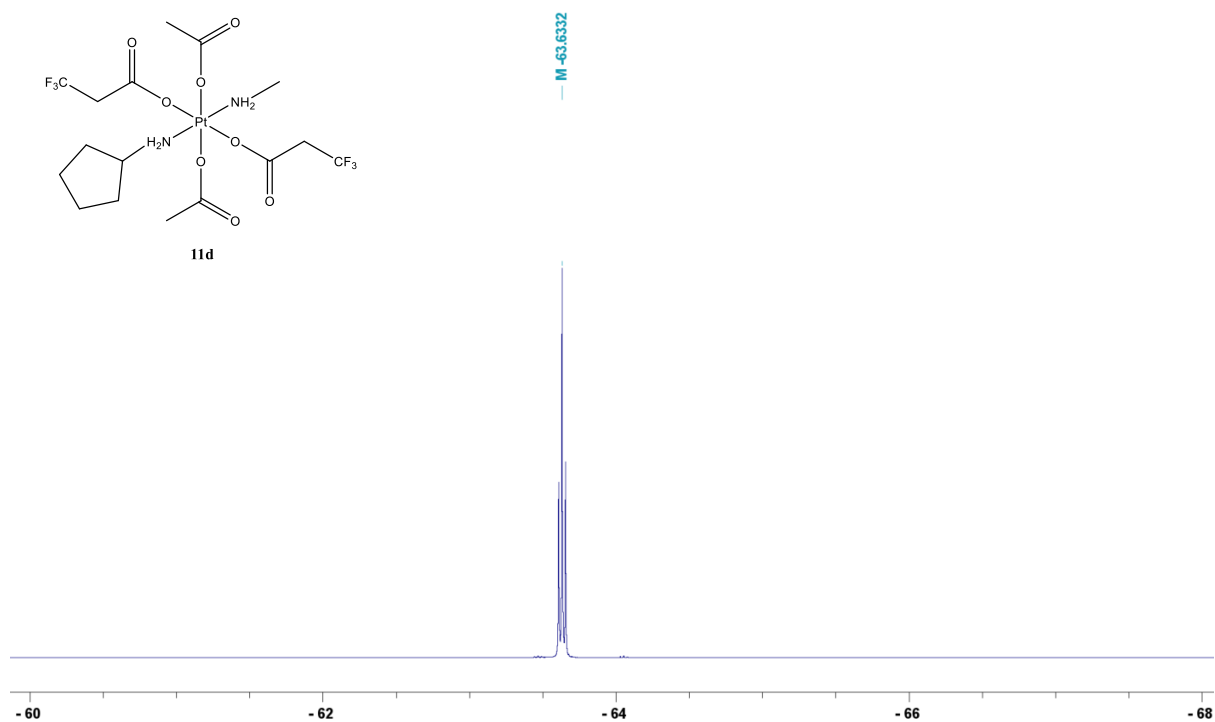


Figure S26. ^{19}F NMR spectrum of **11d** in $\text{d}_7\text{-DMF}$.

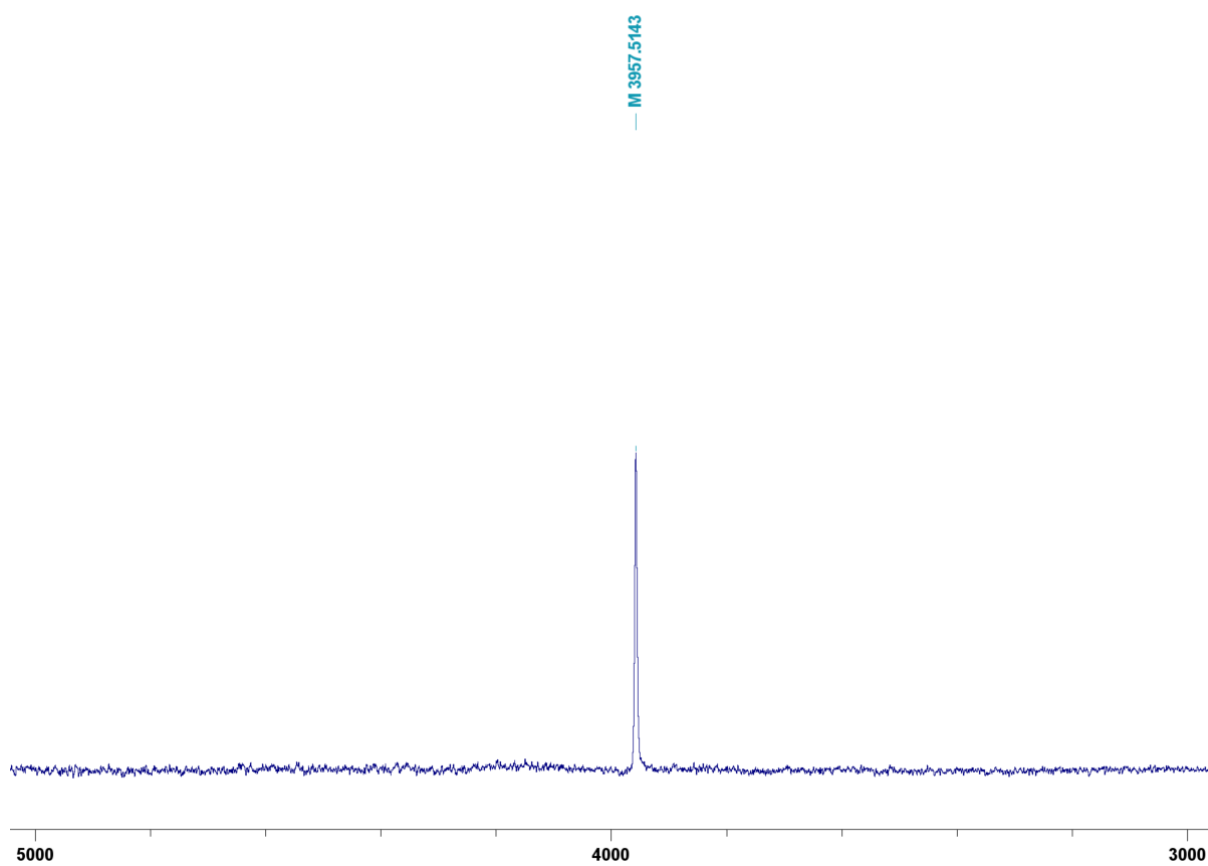


Figure S27. ^{195}Pt NMR spectrum of **11d** in $\text{d}_7\text{-DMF}$.

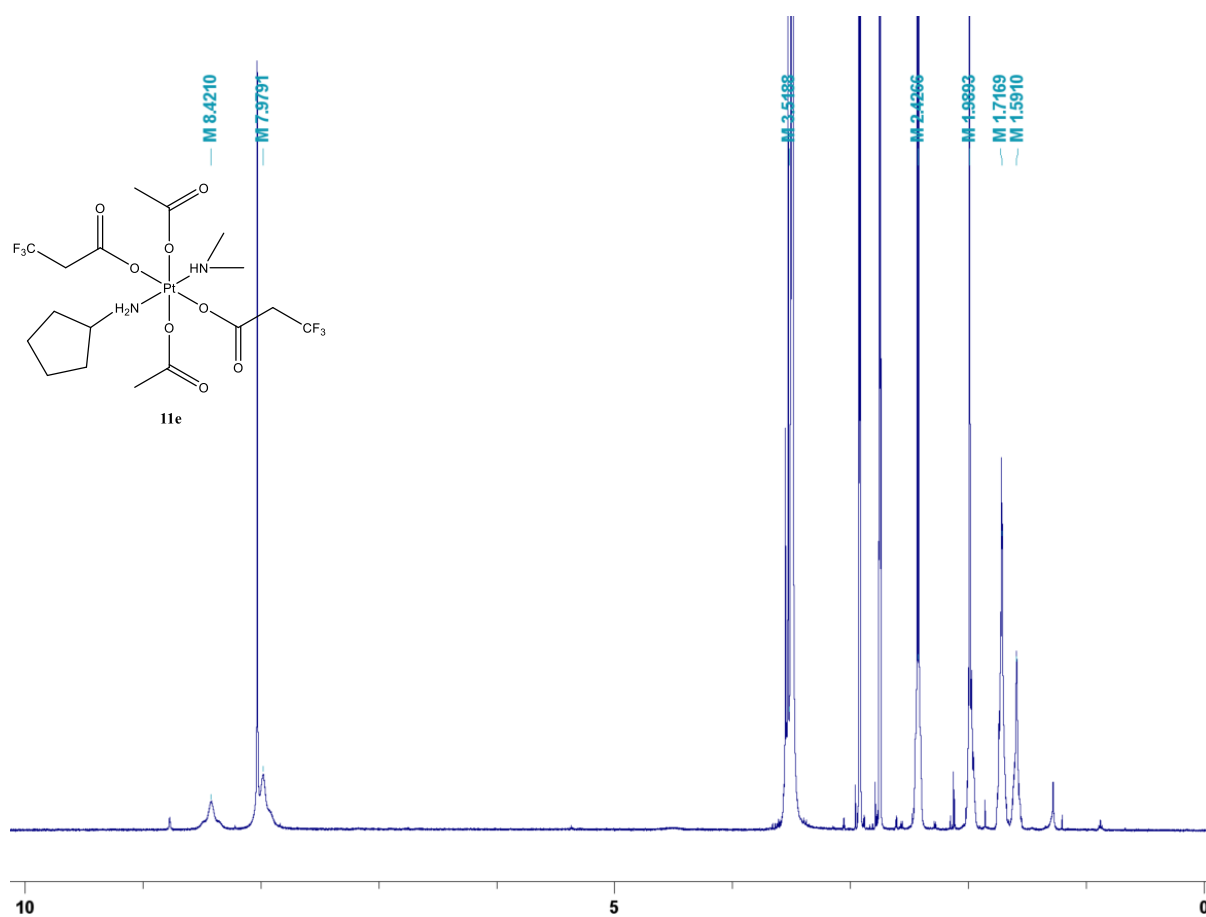


Figure S28. ^1H NMR spectrum of **11e** in d_7 -DMF.

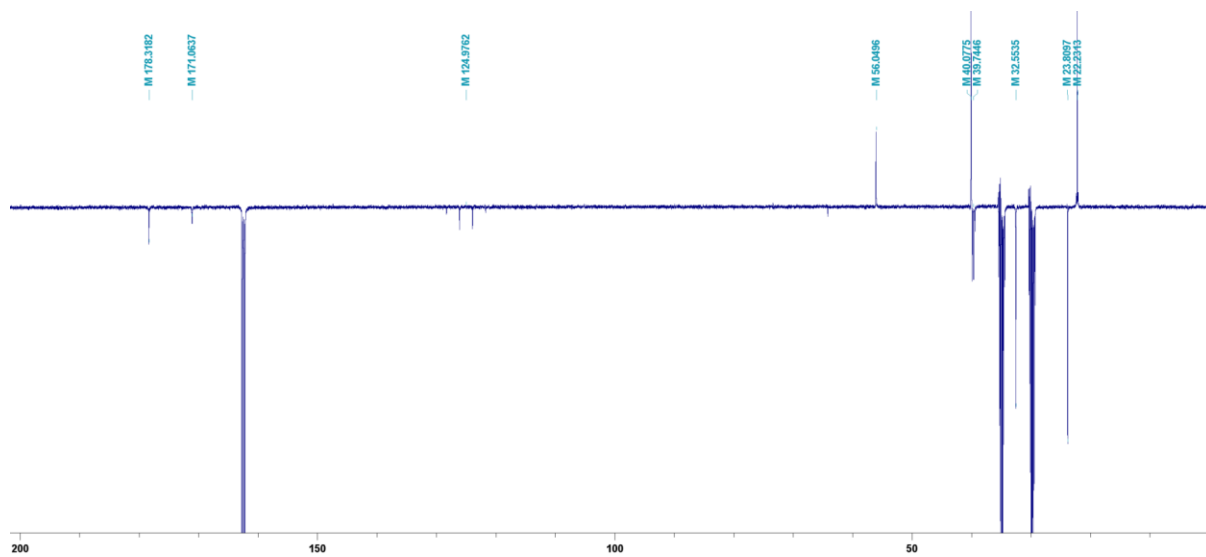


Figure S29. ^{13}C NMR spectrum of **11e** in d_7 -DMF.

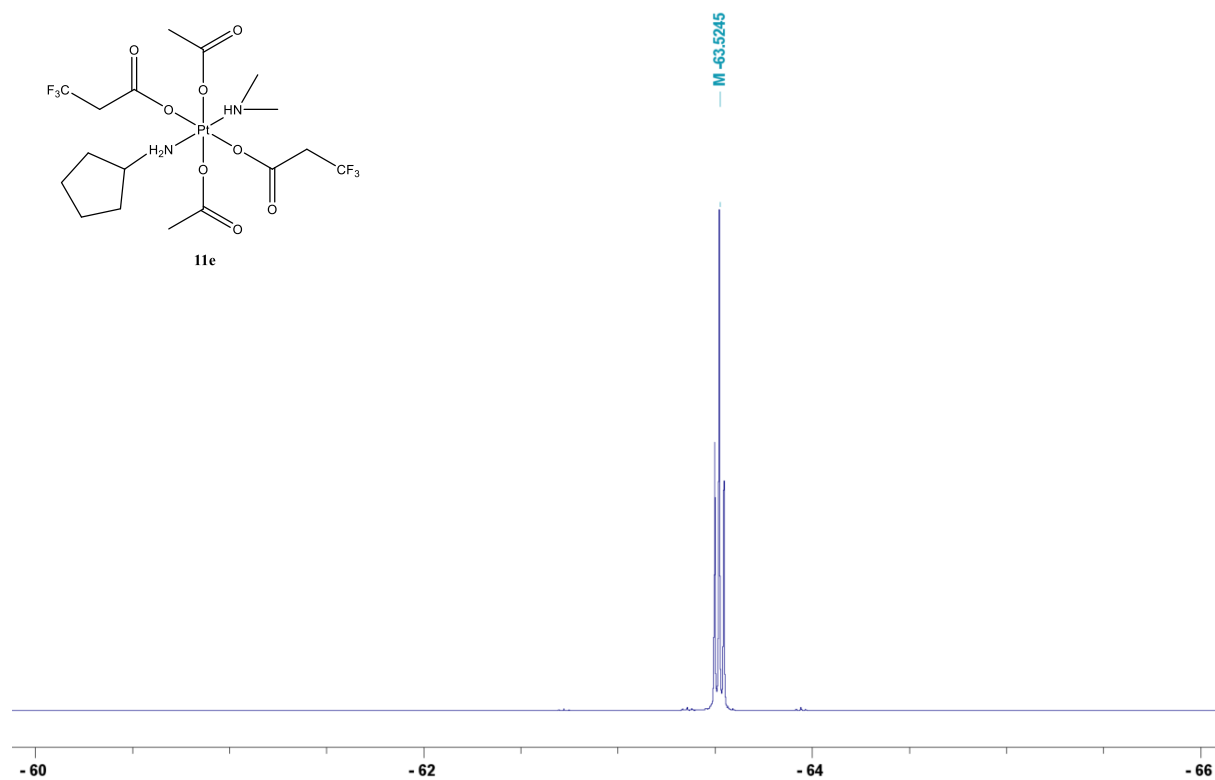


Figure S30. ^{19}F NMR spectrum of **11e** in $\text{d}_7\text{-DMF}$.

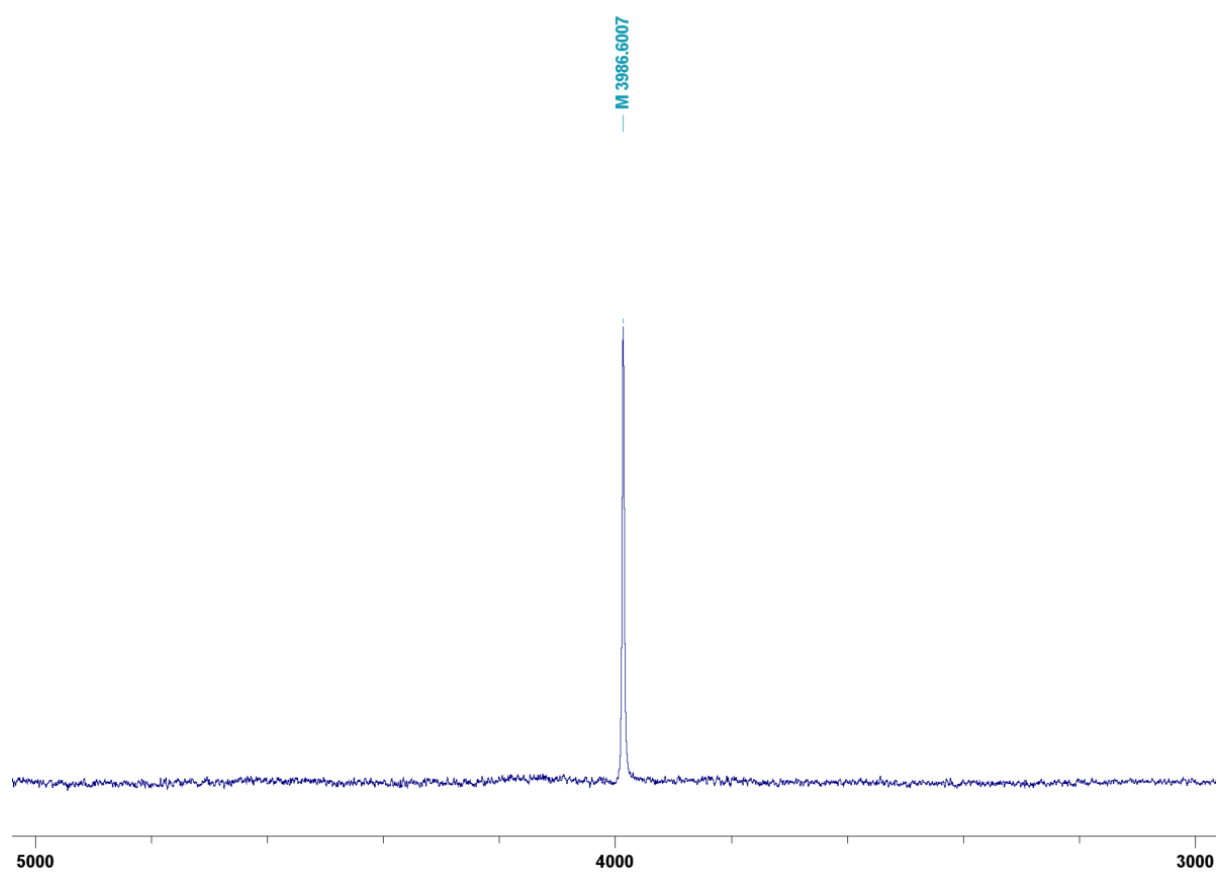


Figure S31. ^{195}Pt NMR spectrum of **11e** in $\text{d}_7\text{-DMF}$.

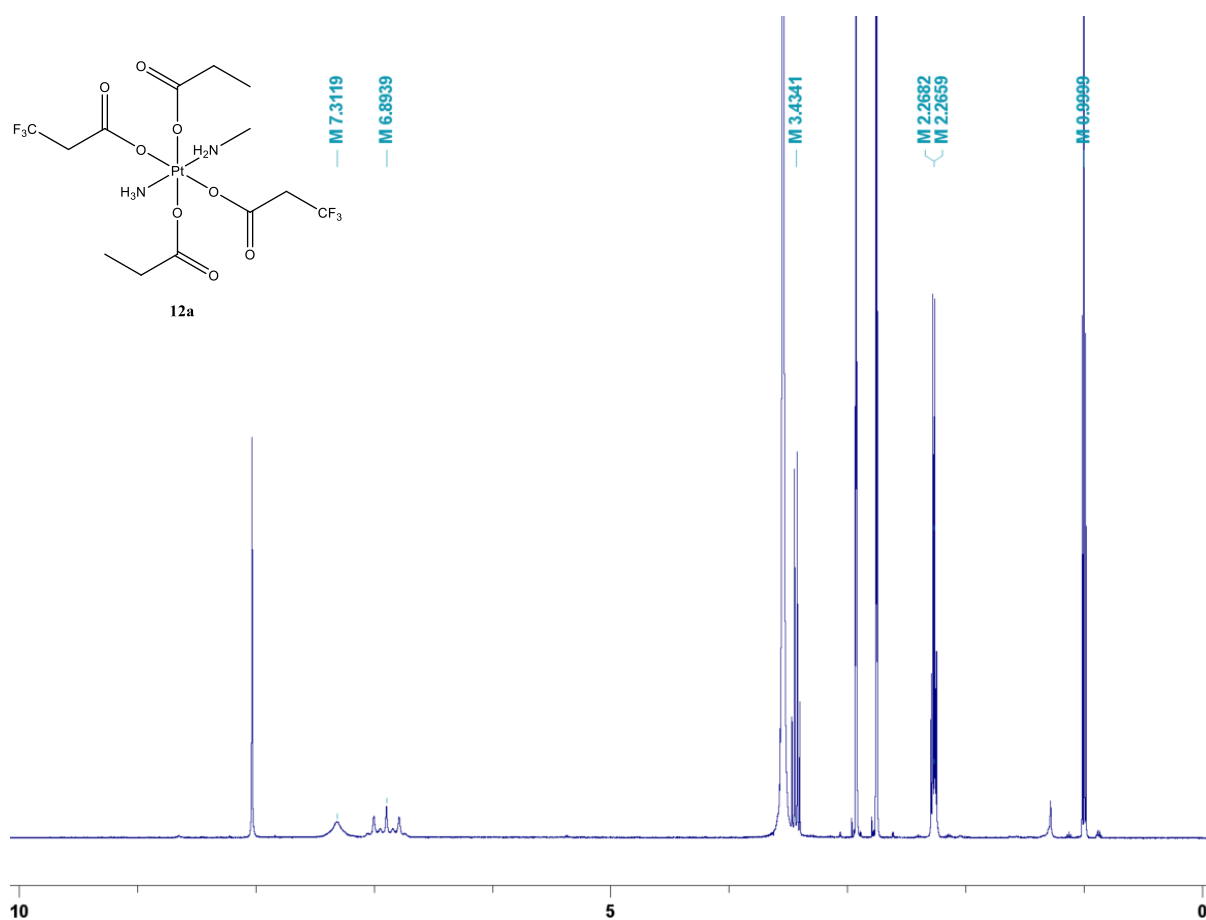


Figure S32. ^1H NMR spectrum of **12a** in d_7 -DMF.

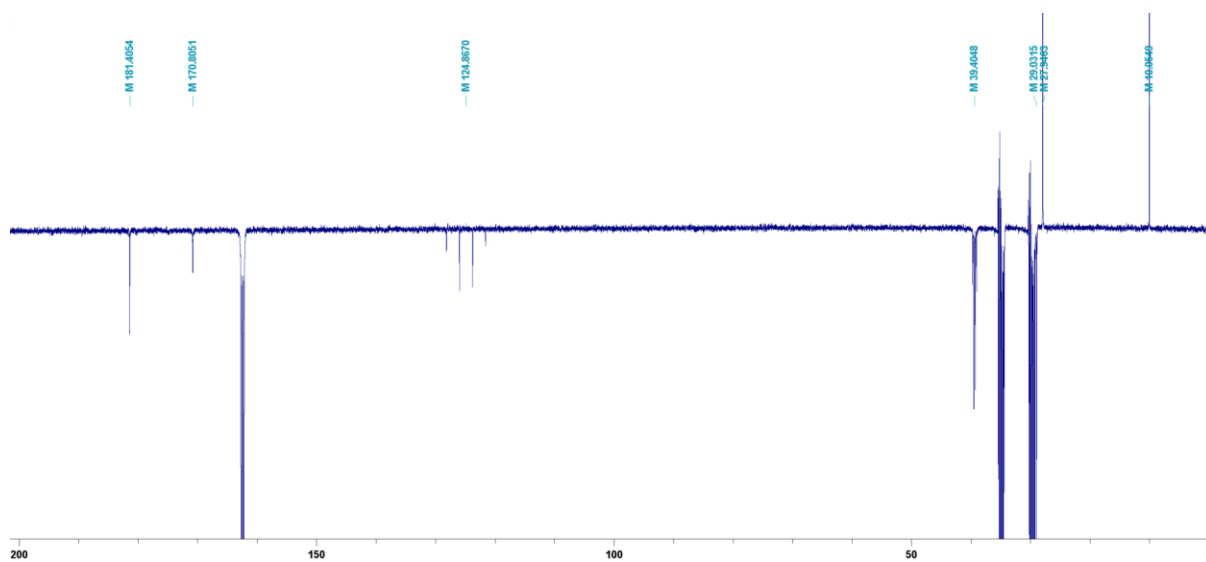


Figure S33. ^{13}C NMR spectrum of **12a** in d_7 -DMF.

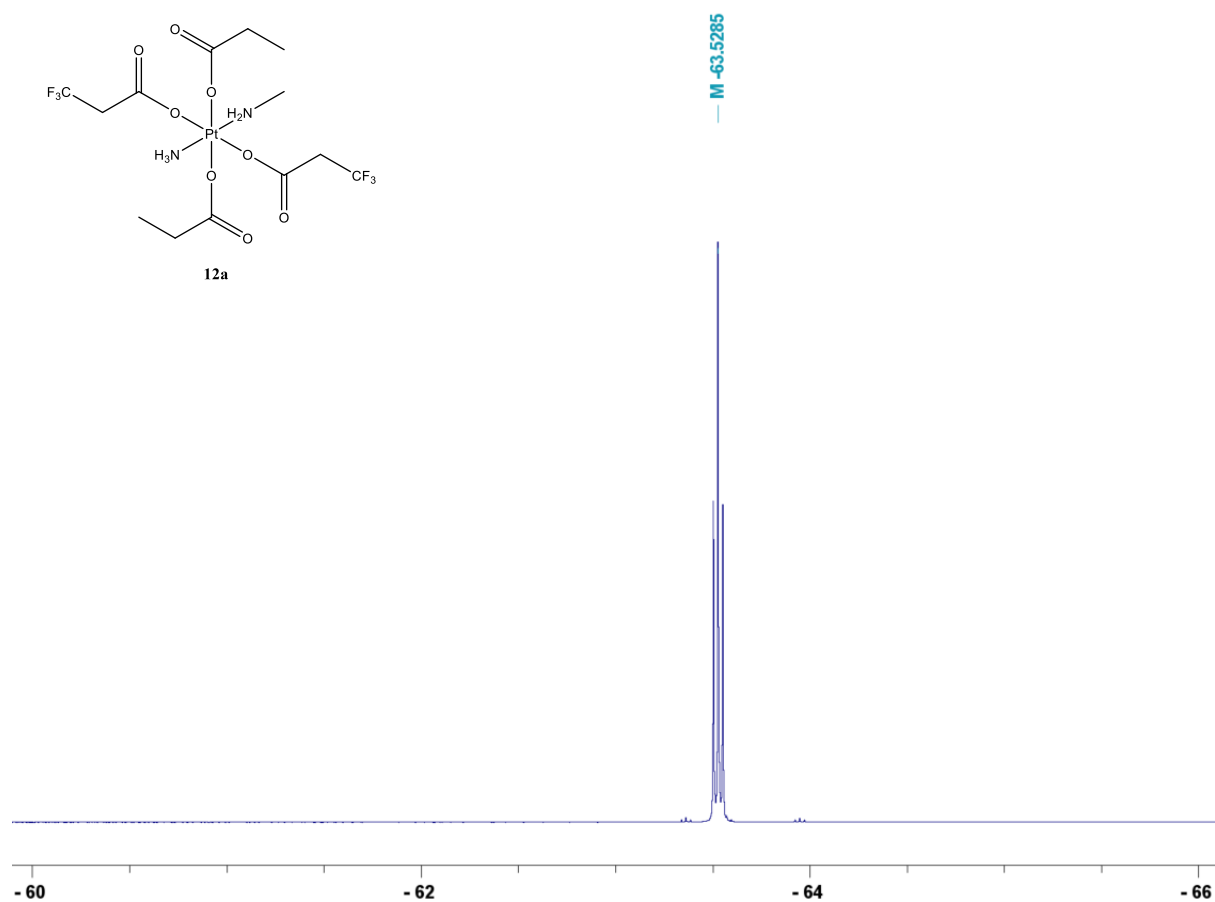


Figure S34. ¹⁹F NMR spectrum of **12a** in d₇-DMF.

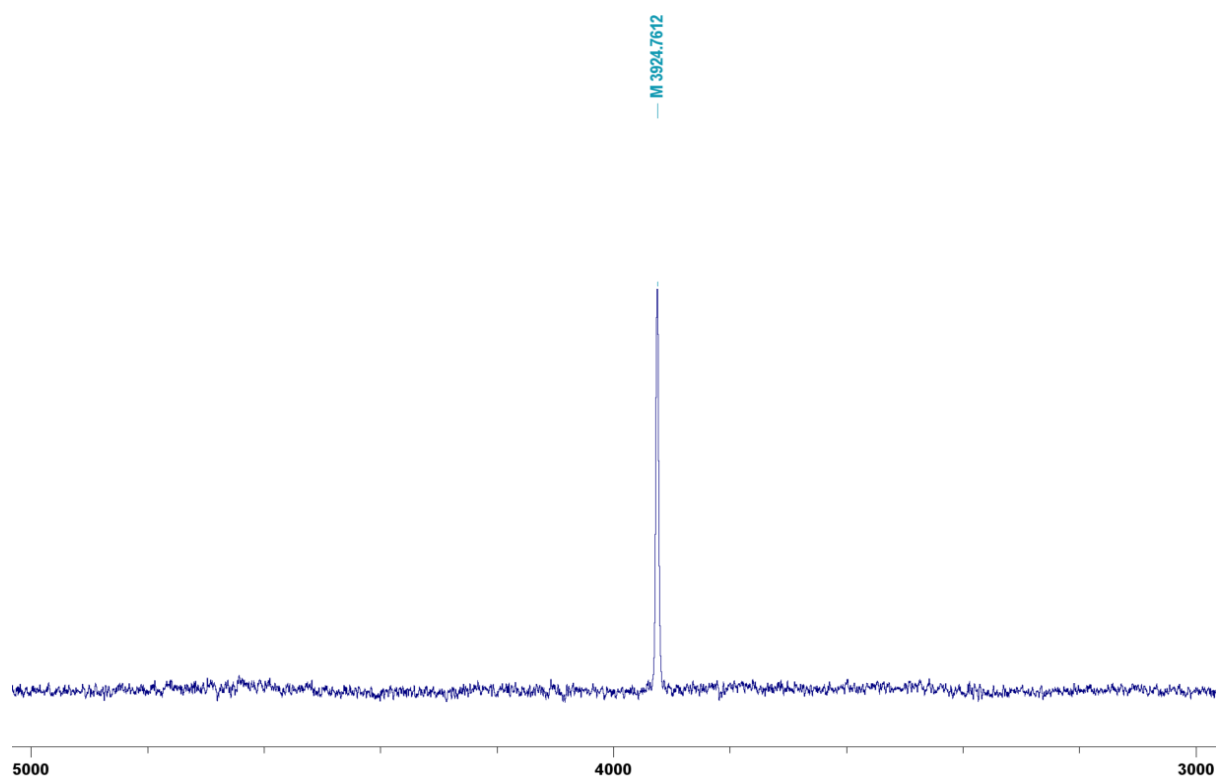


Figure S35. ¹⁹⁵Pt NMR spectrum of **12a** in d₇-DMF.

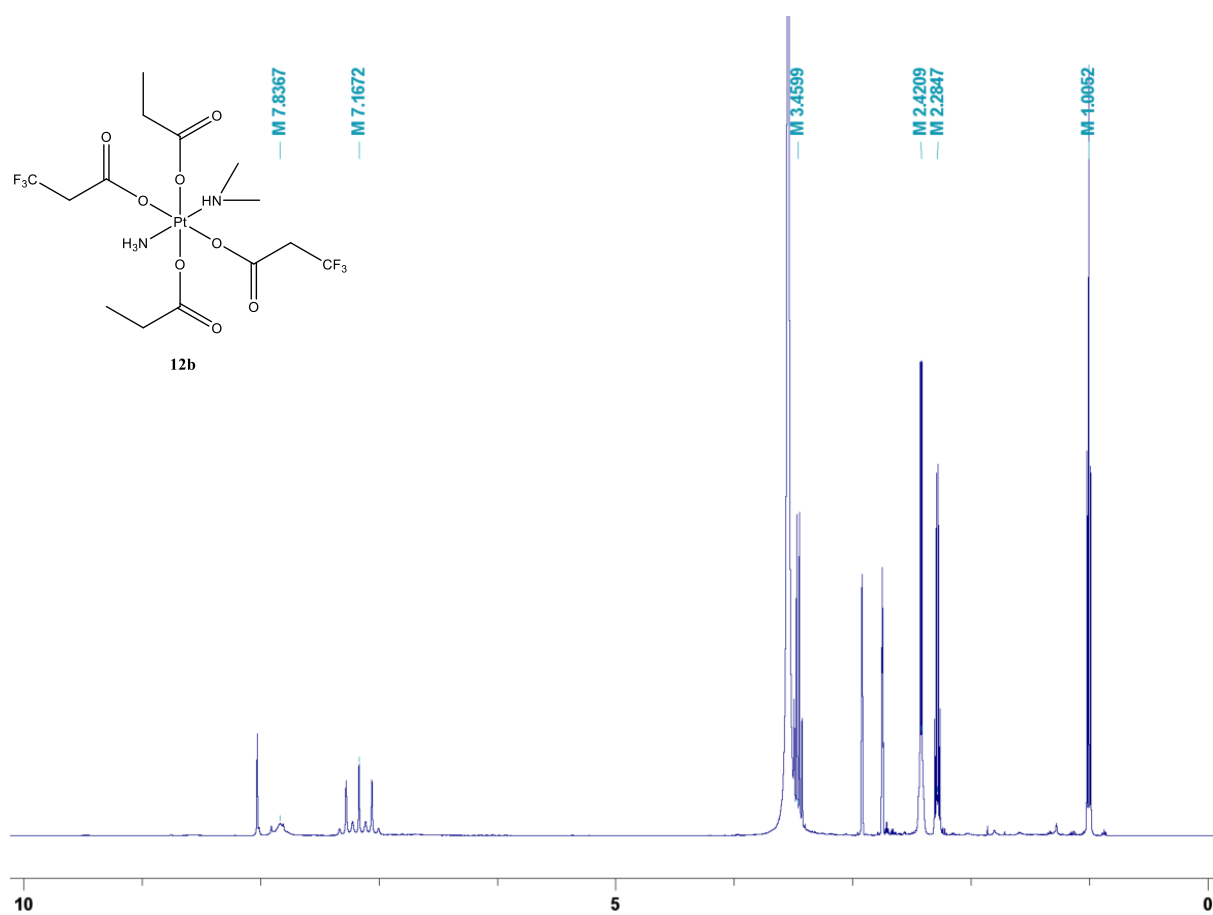


Figure S36. ^1H NMR spectrum of **12b** in $\text{d}_7\text{-DMF}$.

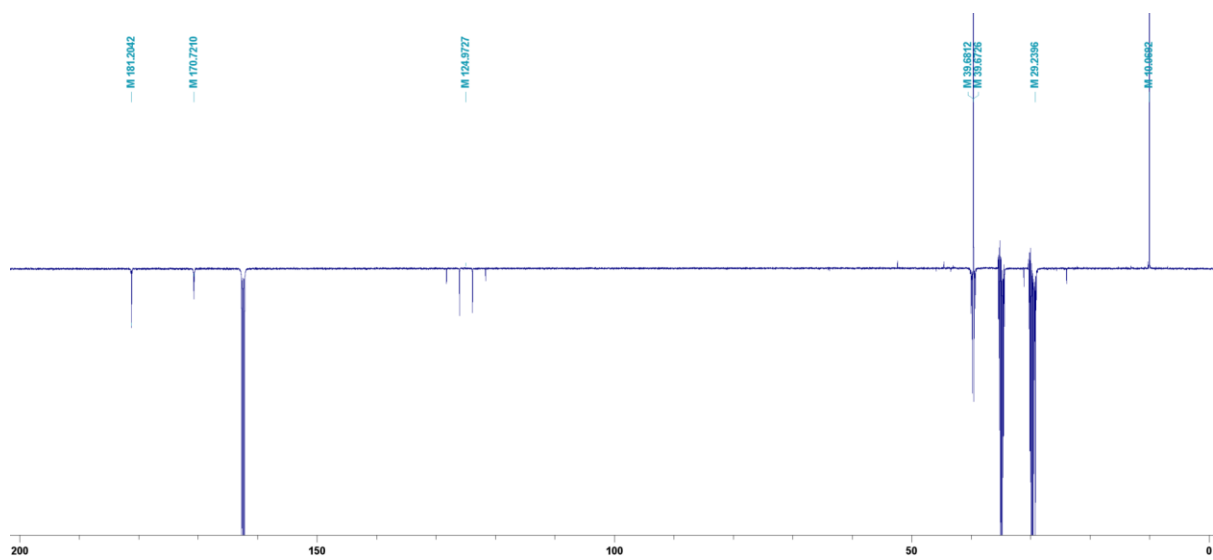


Figure S37. ^{13}C NMR spectrum of **12b** in $\text{d}_7\text{-DMF}$.

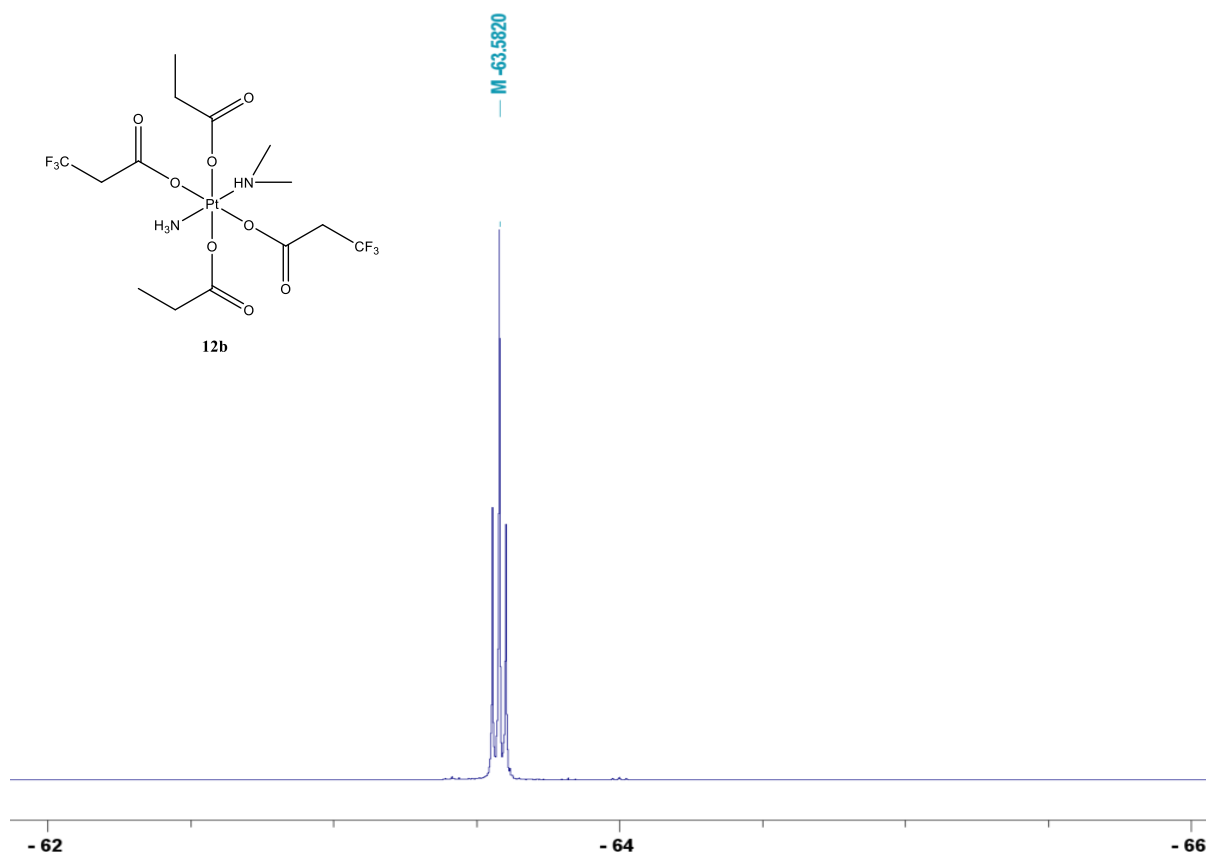


Figure S38. ^{19}F NMR spectrum of **12b** in d_7 -DMF.

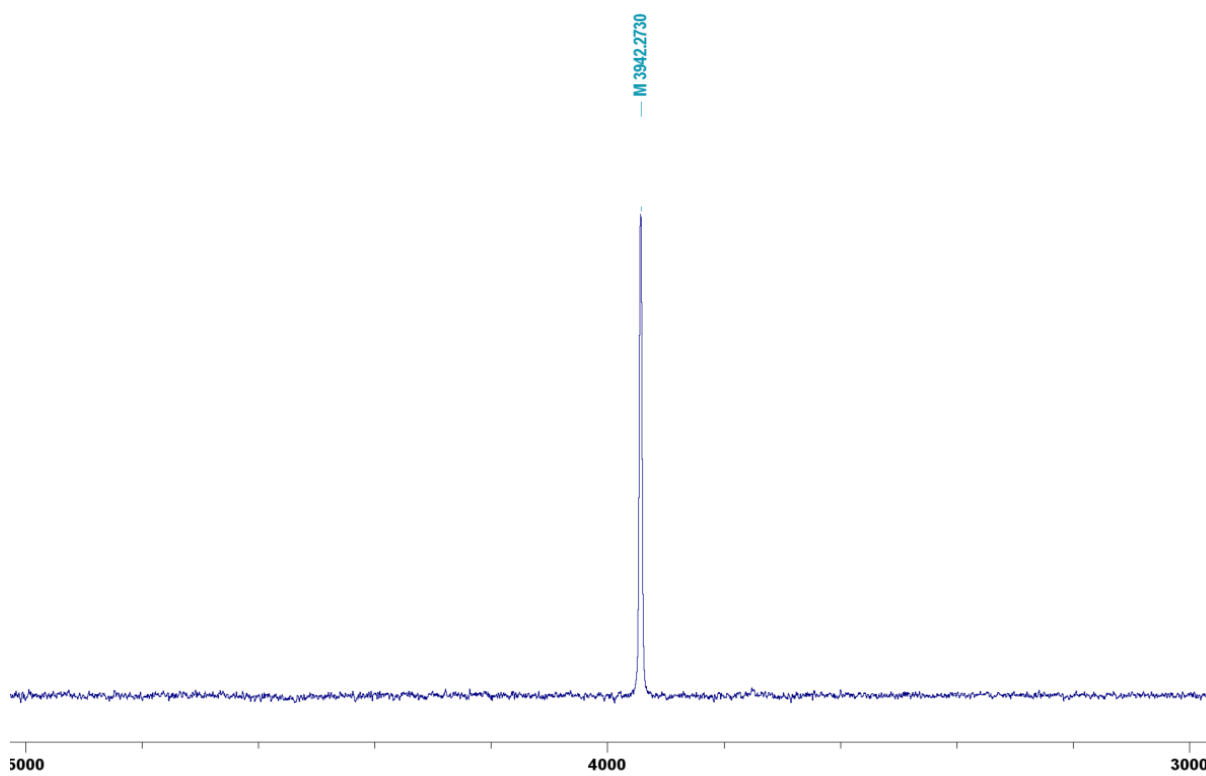


Figure S39. ^{195}Pt NMR spectrum of **12b** in d_7 -DMF.

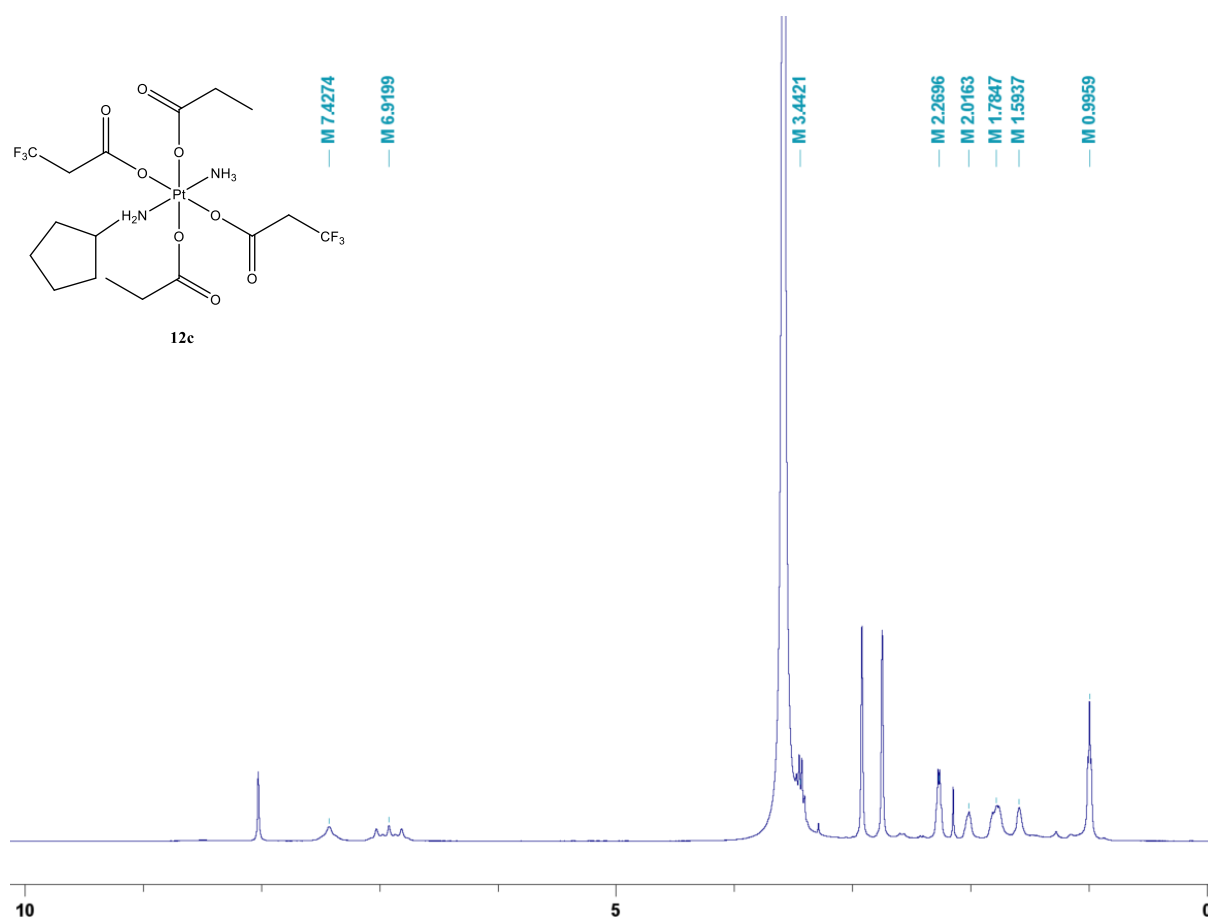


Figure S40. ^1H NMR spectrum of **12c** in $\text{d}_7\text{-DMF}$.

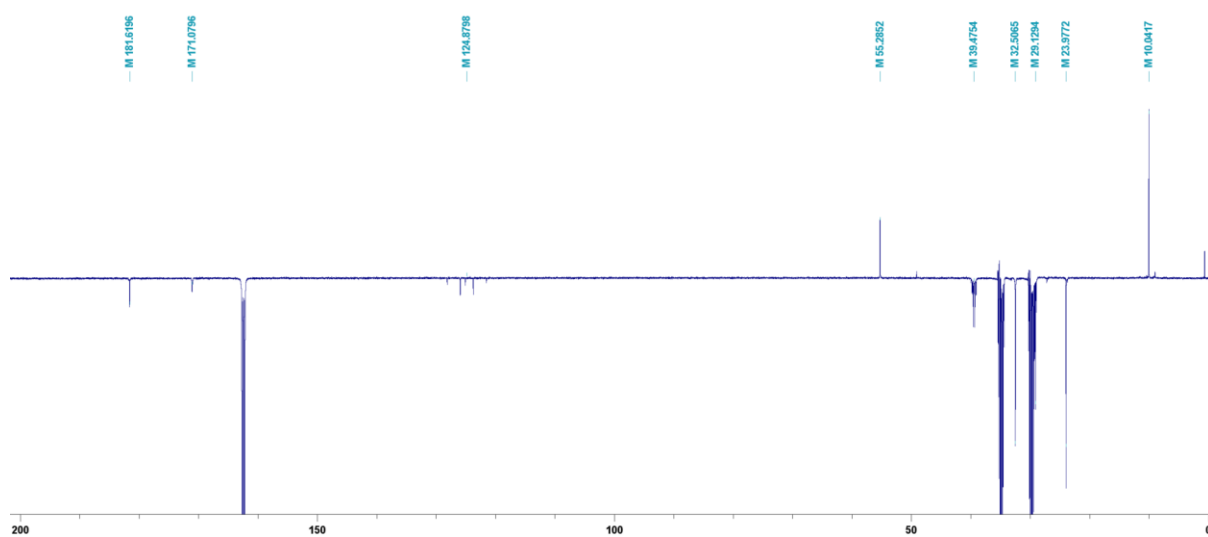


Figure S41. ^{13}C NMR spectrum of **12c** in $\text{d}_7\text{-DMF}$.

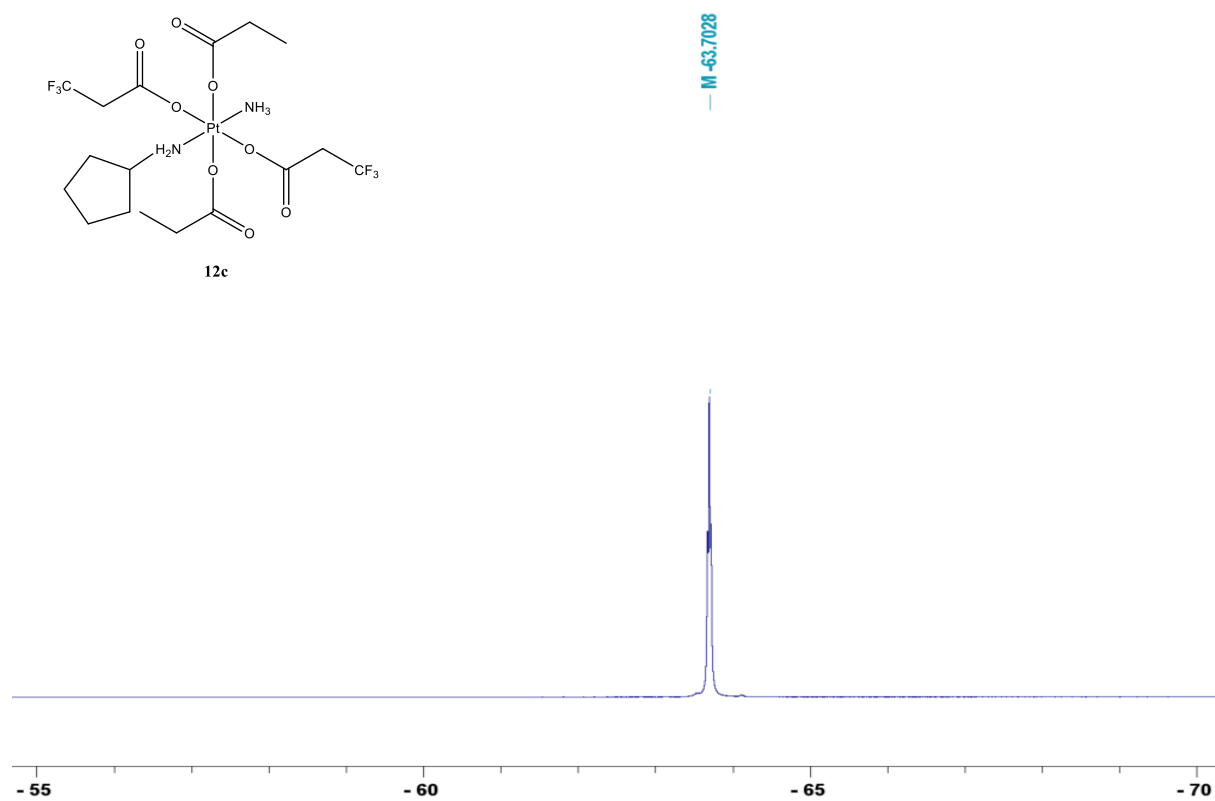


Figure S42. ^{19}F NMR spectrum of **12c** in d_7 -DMF.

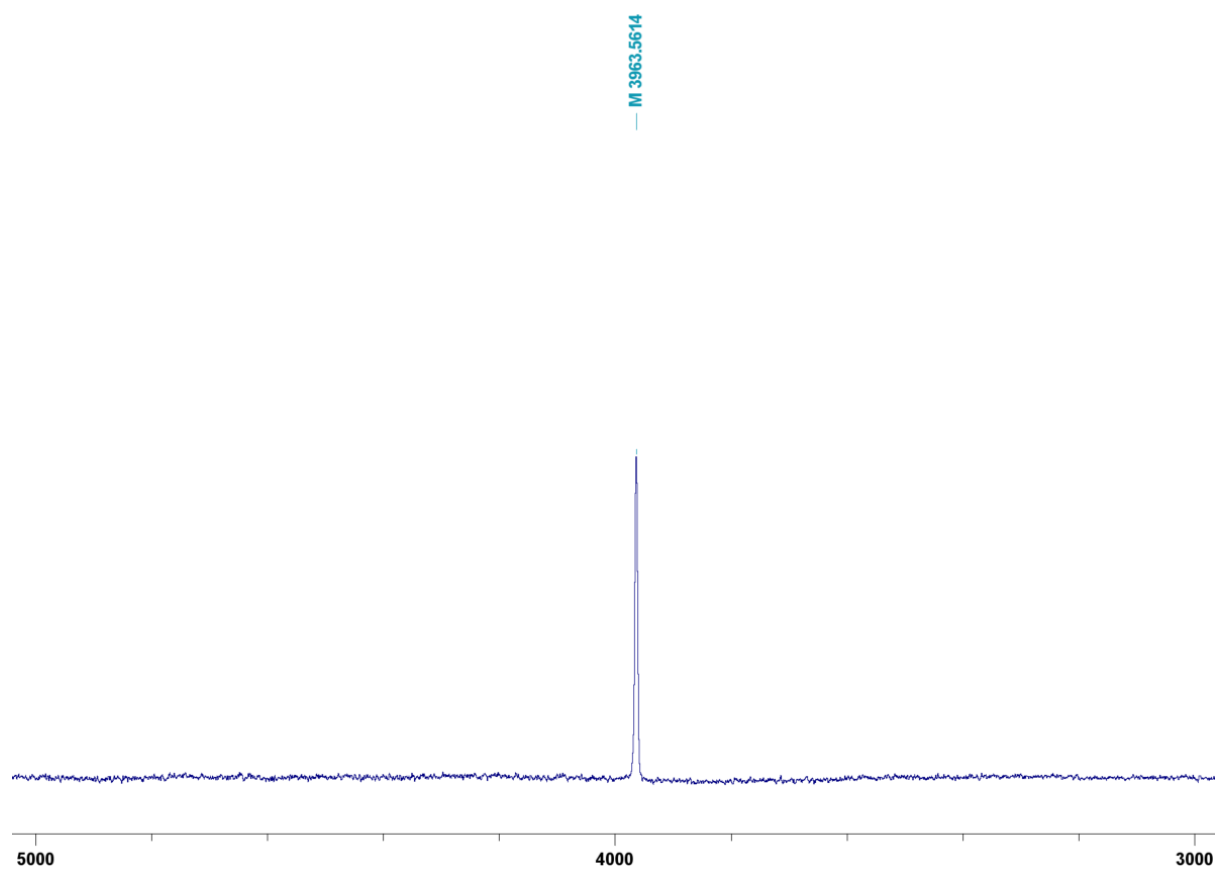


Figure S43. ^{195}Pt NMR spectrum of **12c** in d_7 -DMF.

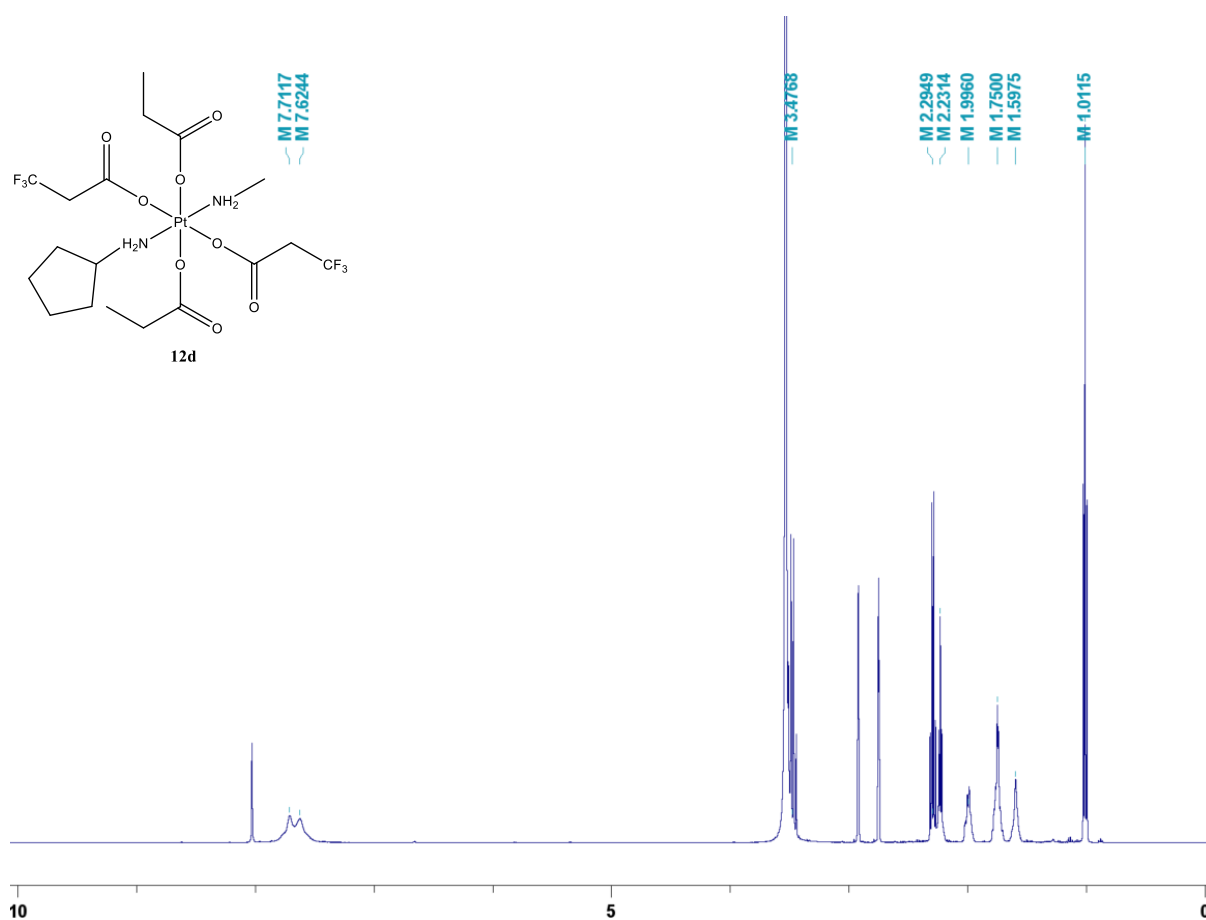


Figure S44. ¹H NMR spectrum of **12d** in d₇-DMF.

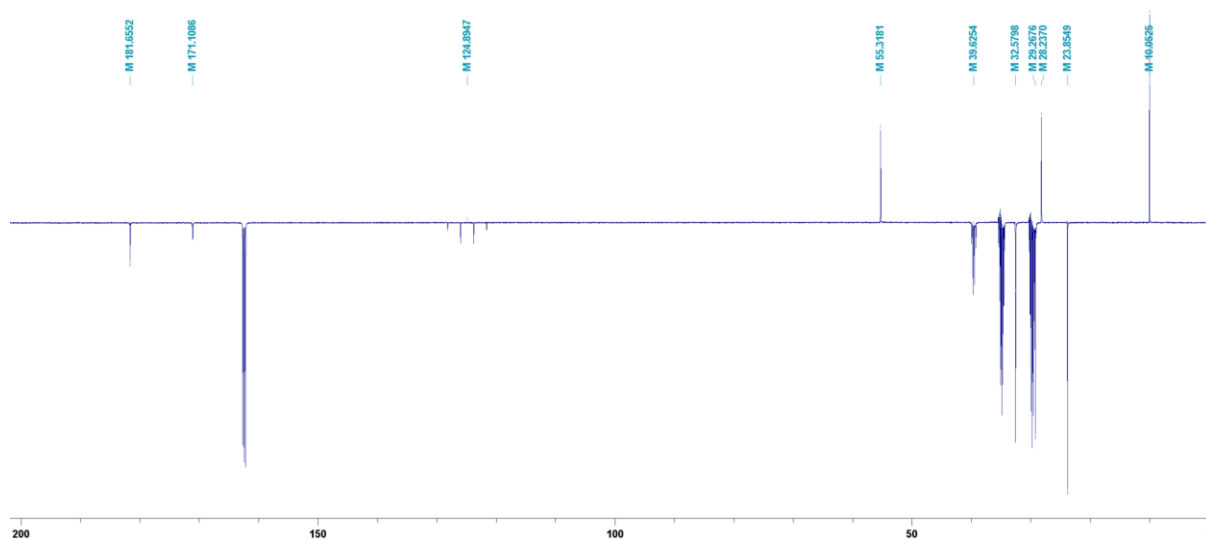


Figure S45. ¹³C NMR spectrum of **12d** in d₇-DMF.

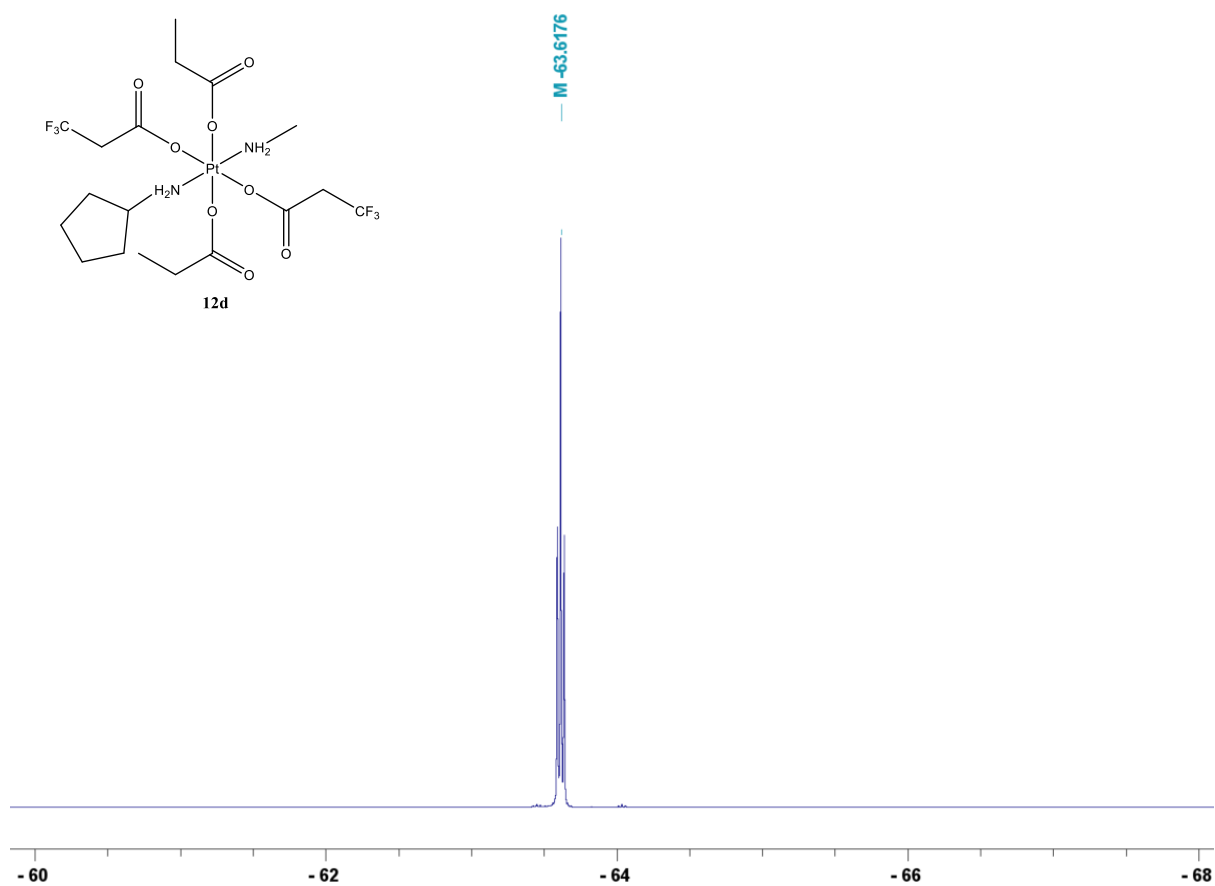


Figure S46. ^{19}F NMR spectrum of **12d** in d_7 -DMF.

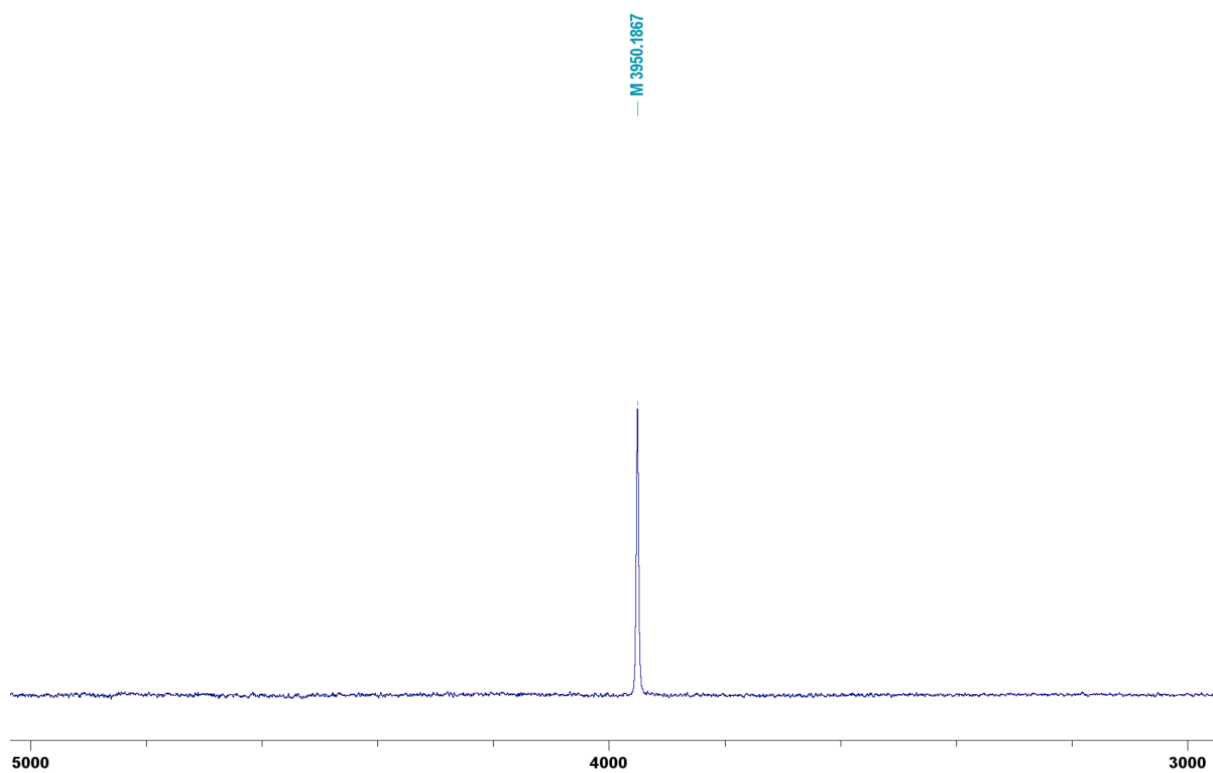


Figure S47. ^{195}Pt NMR spectrum of **12d** in d_7 -DMF.

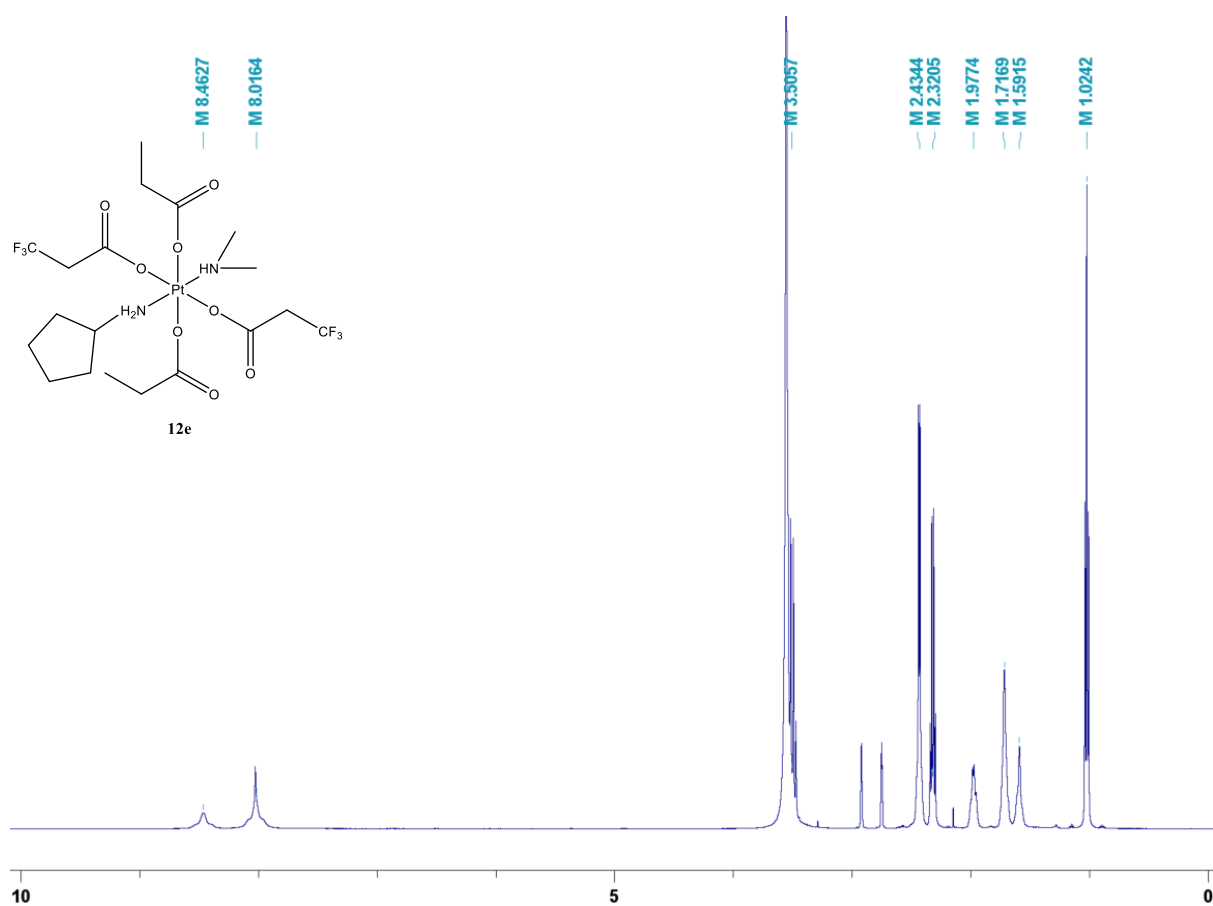


Figure S48. ^1H NMR spectrum of **12e** in $\text{d}_7\text{-DMF}$.

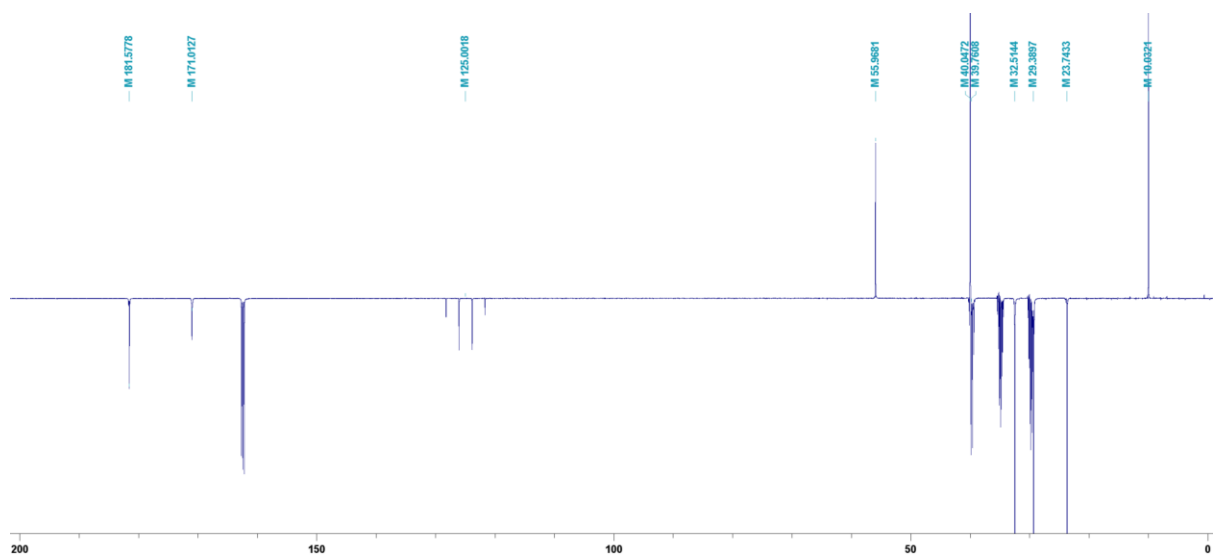
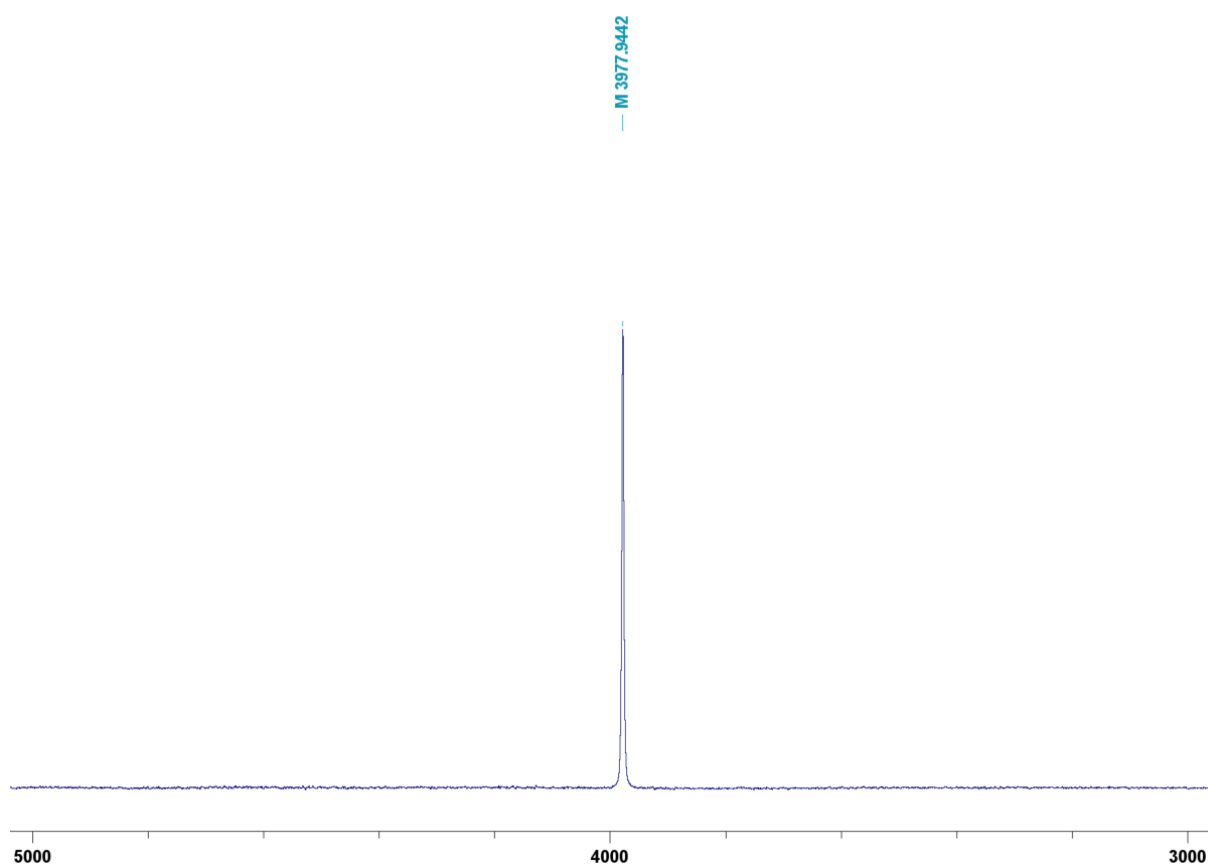
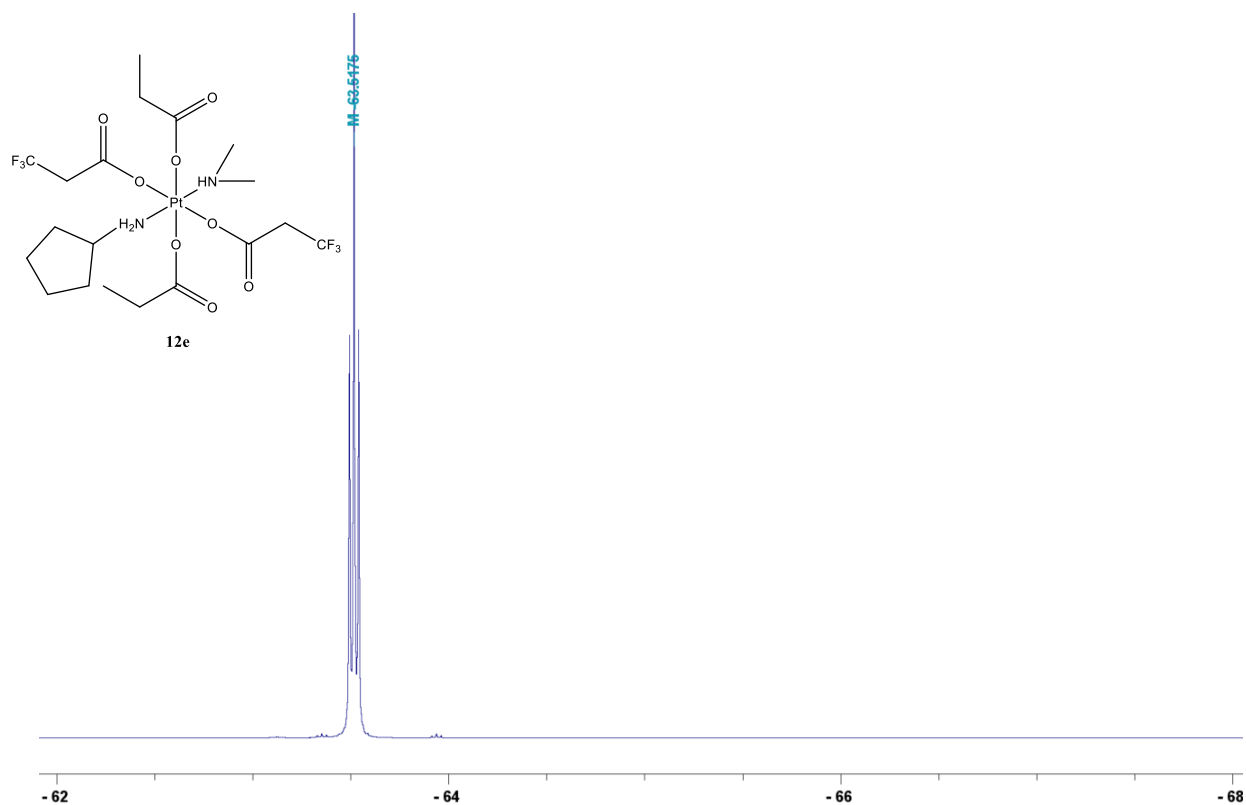


Figure S49. ^{13}C NMR spectrum of **12e** in $\text{d}_7\text{-DMF}$.



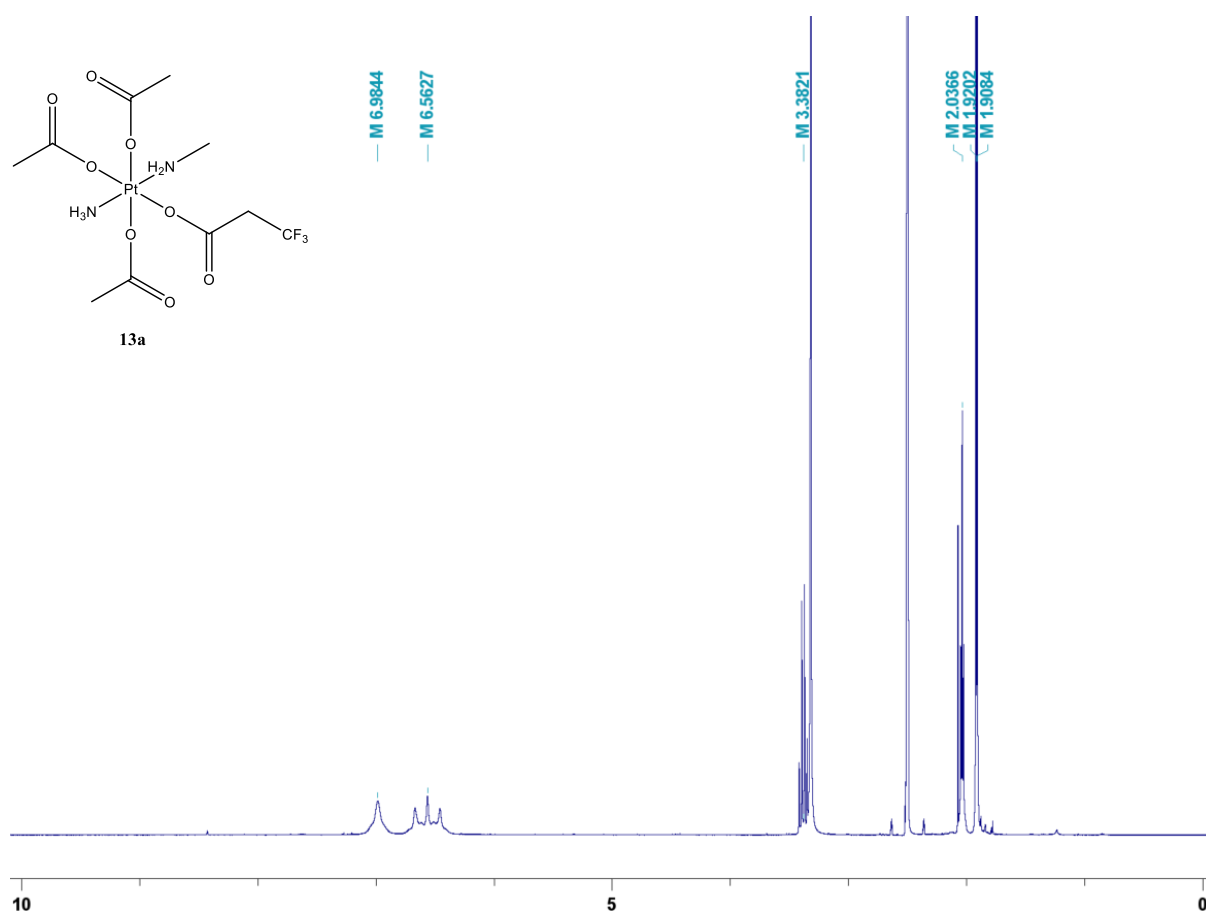


Figure S52. ¹H NMR spectrum of **13a** in d₆-DMSO.

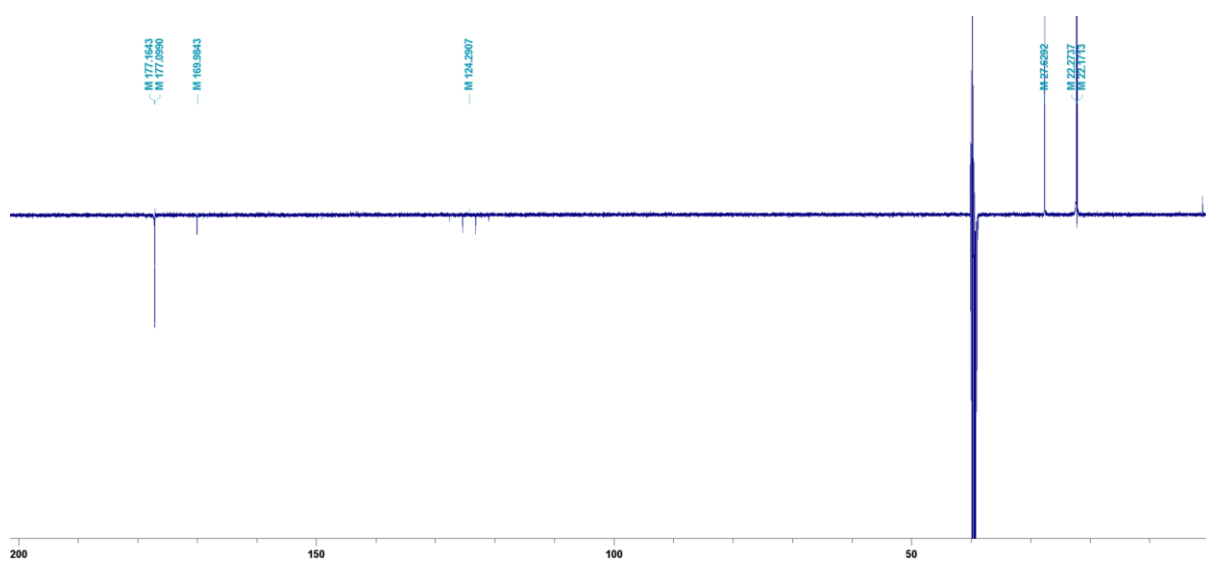


Figure S53. ¹³C NMR spectrum of **13a** in d₆-DMSO.

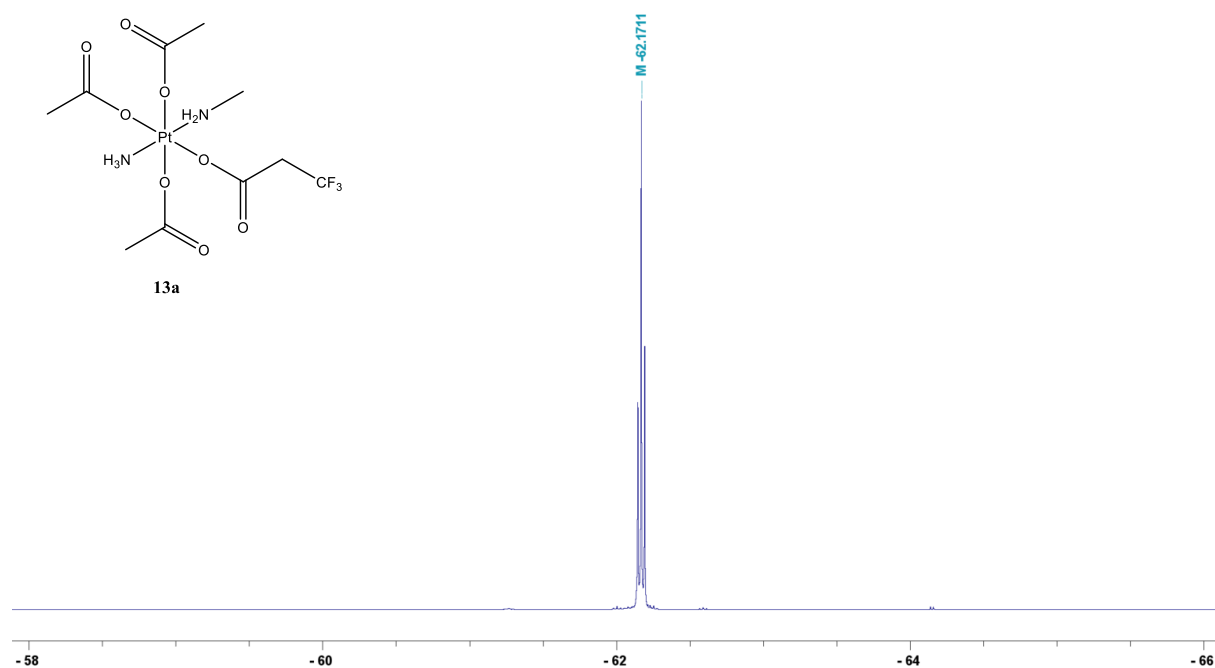


Figure S54. ^{19}F NMR spectrum of **13a** in d_6 -DMSO.

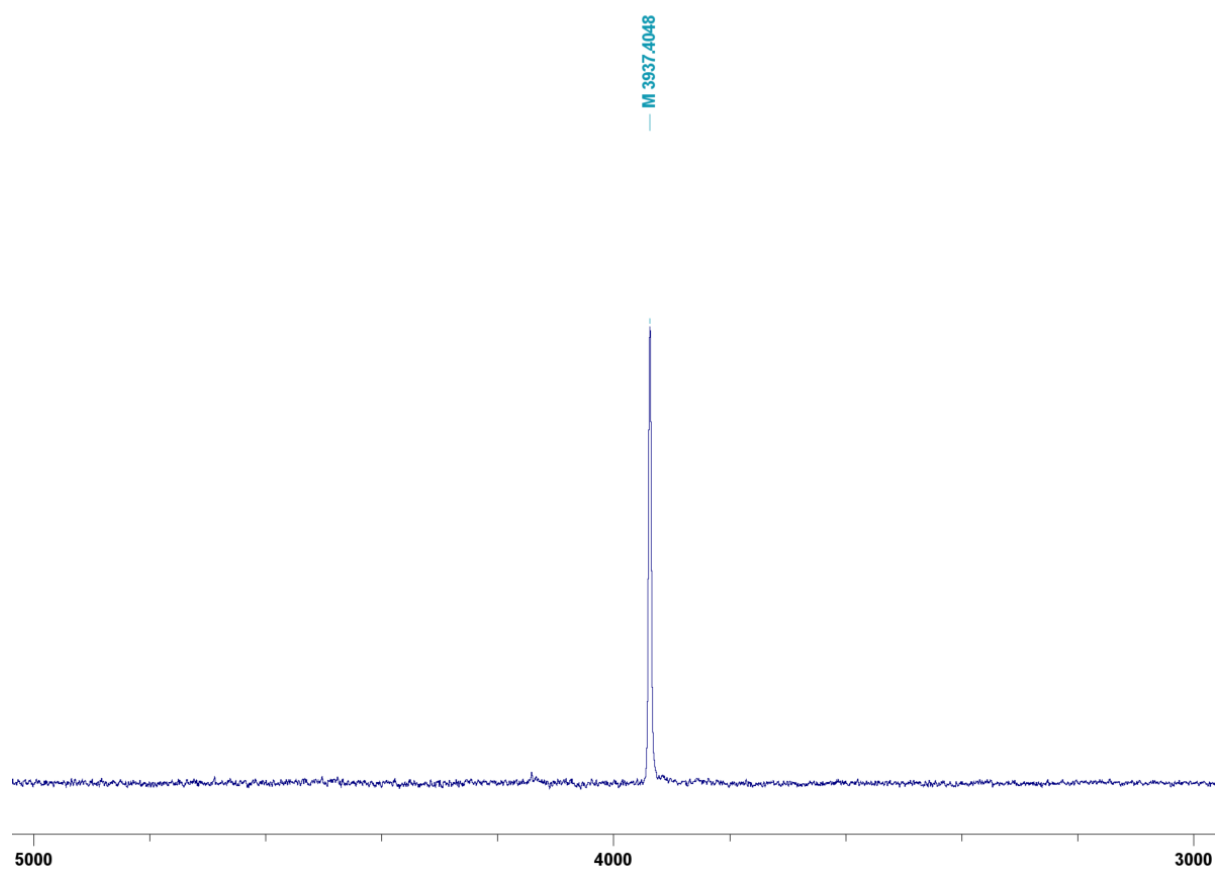


Figure S55. ^{195}Pt NMR spectrum of **13a** in d_6 -DMSO.

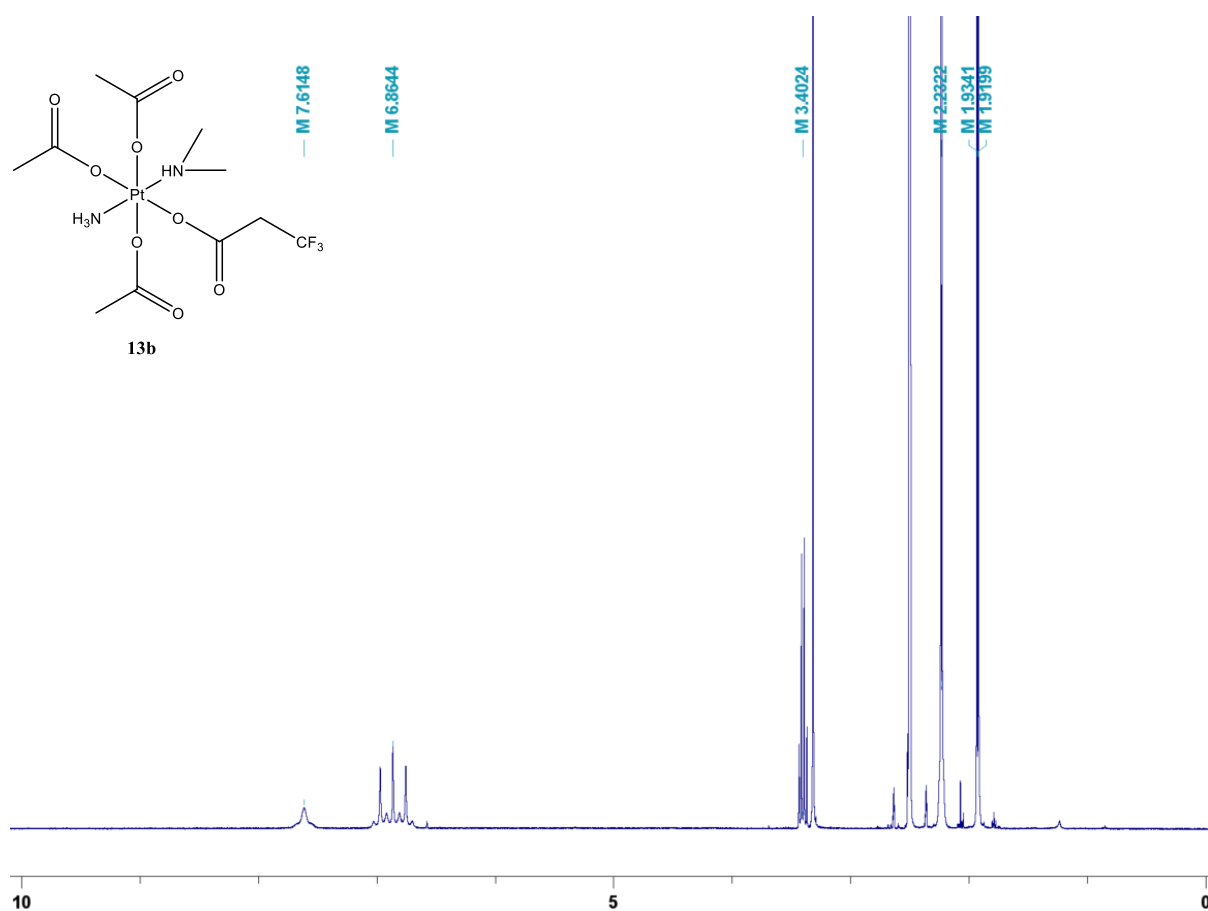


Figure S56. ^1H NMR spectrum of **13b** in d_6 -DMSO.

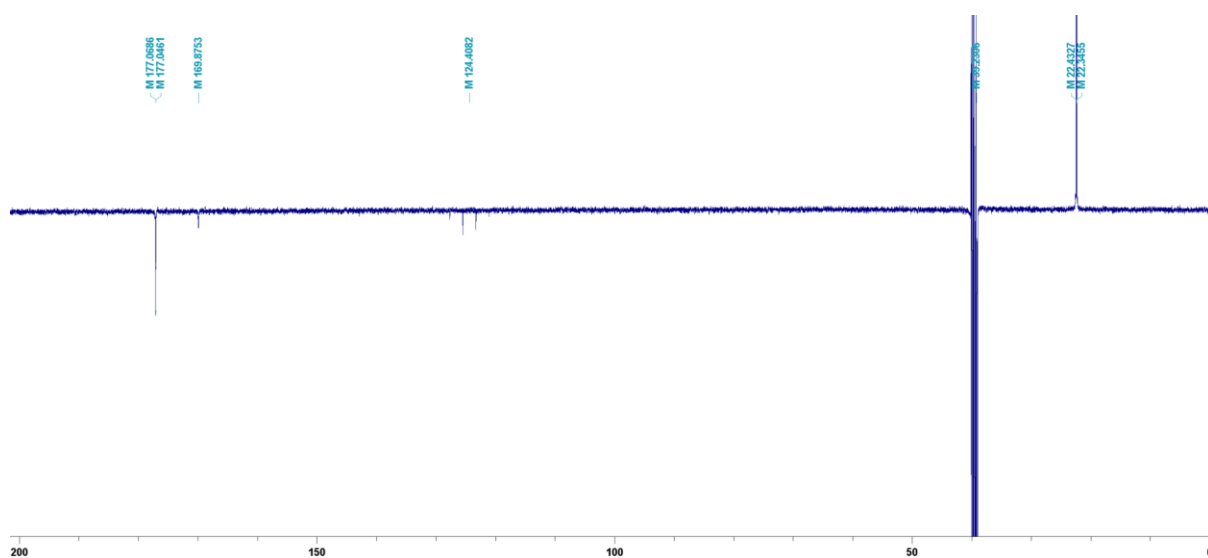


Figure S57. ^{13}C NMR spectrum of **13b** in d_6 -DMSO.

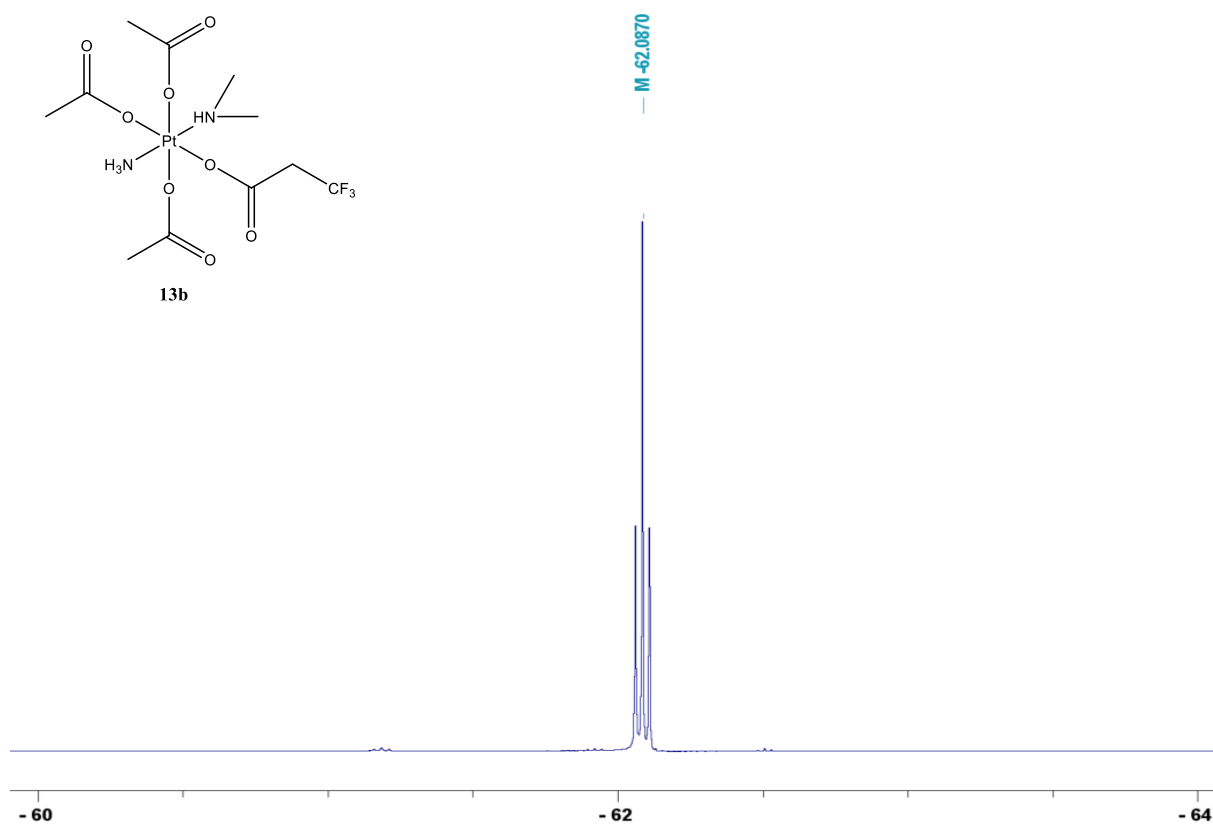


Figure S58. ^{19}F NMR spectrum of **13b** in d_6 -DMSO.

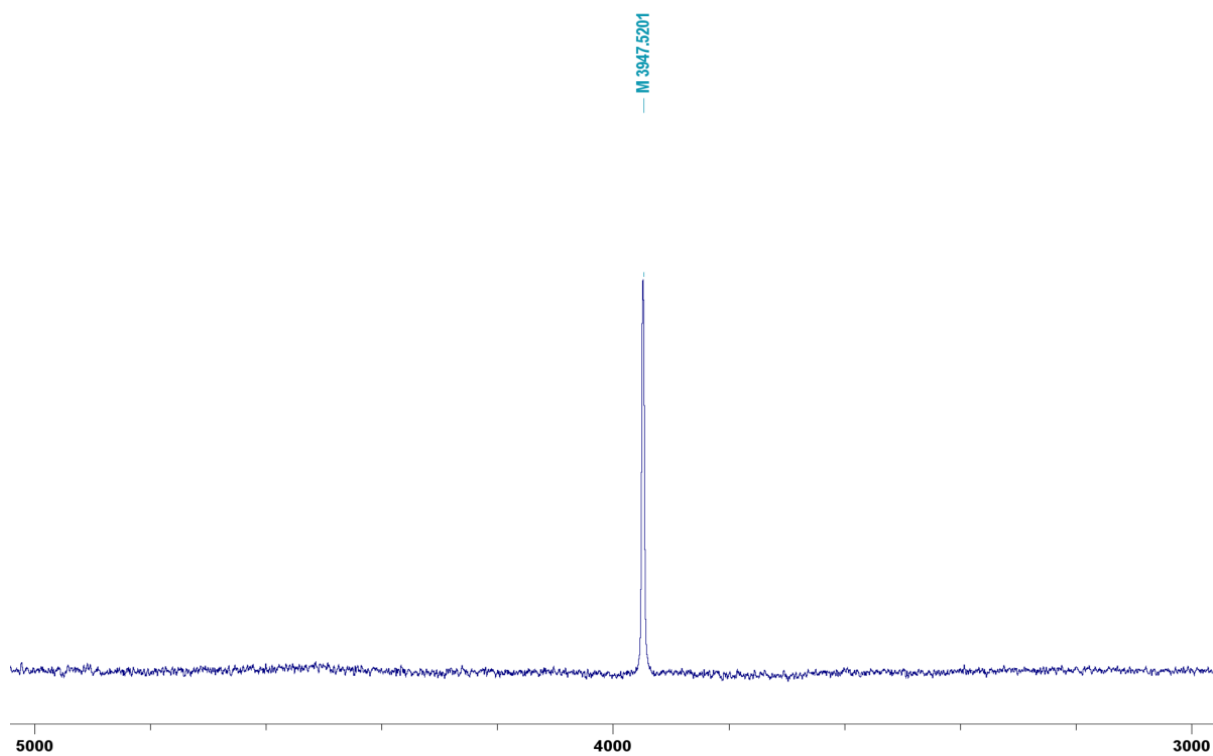


Figure S59. ^{195}Pt NMR spectrum of **13b** in d_6 -DMSO.

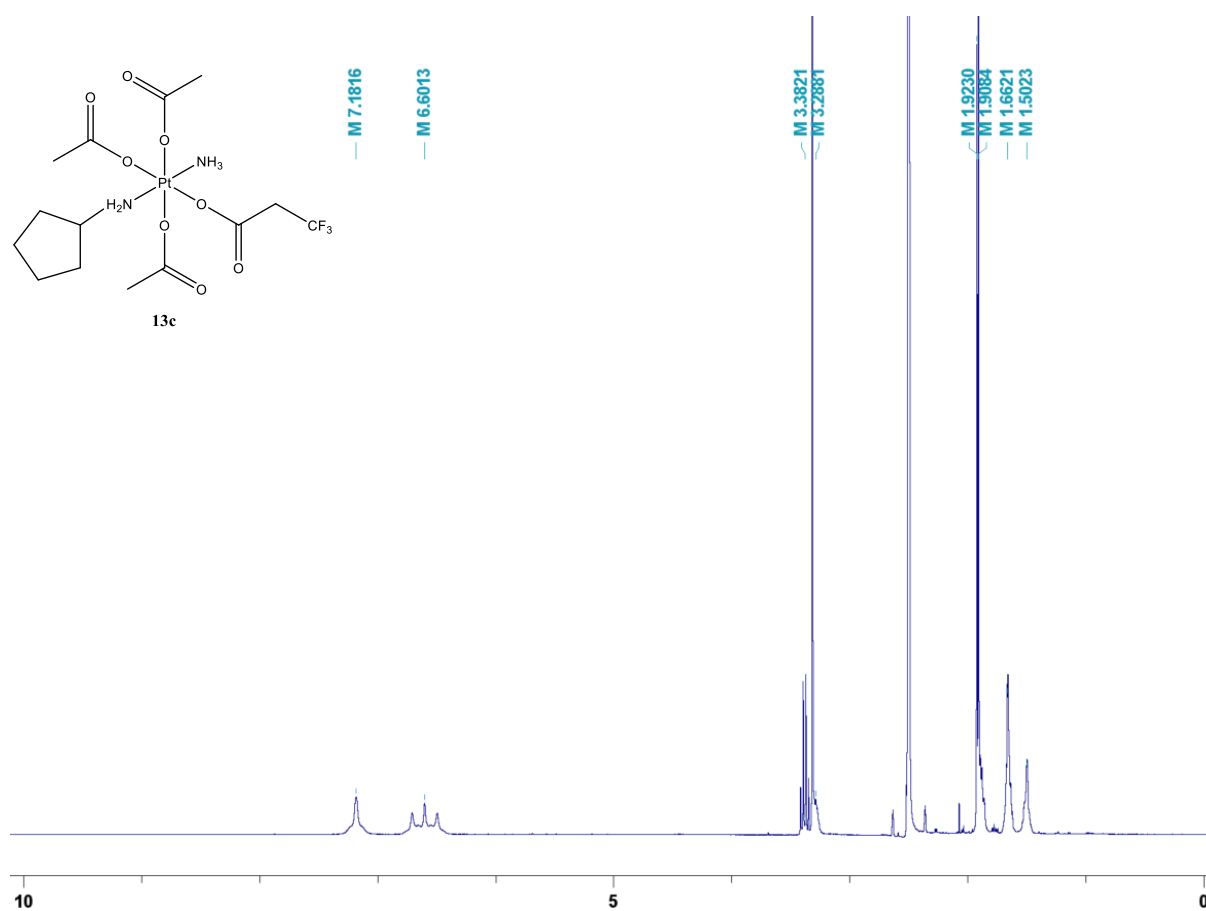


Figure S60. ¹H NMR spectrum of **13c** in d₆-DMSO.

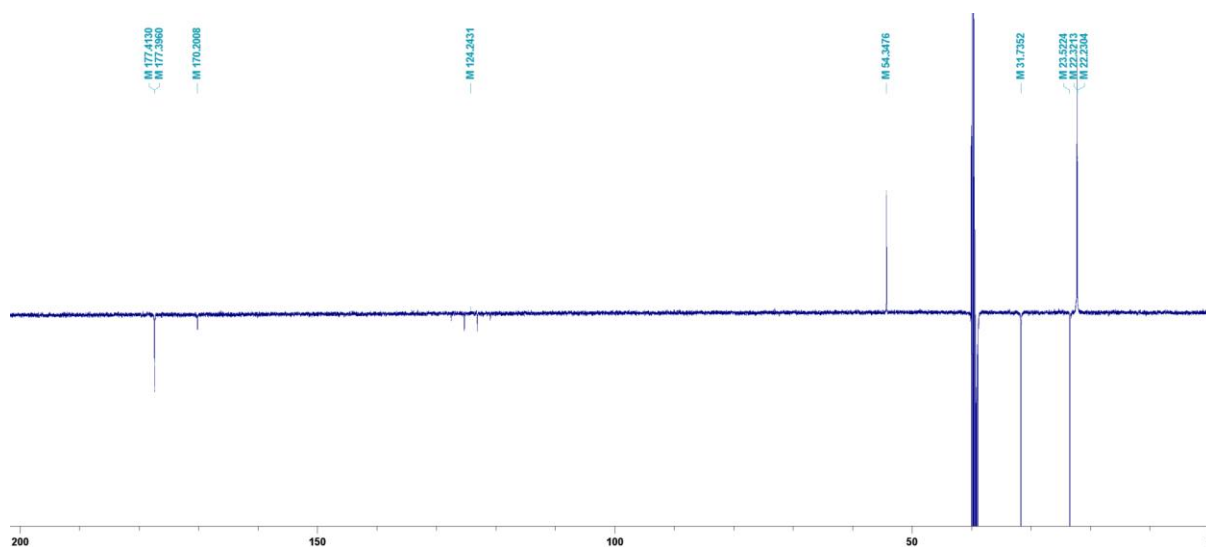


Figure S61. ¹³C NMR spectrum of **13c** in d₆-DMSO.

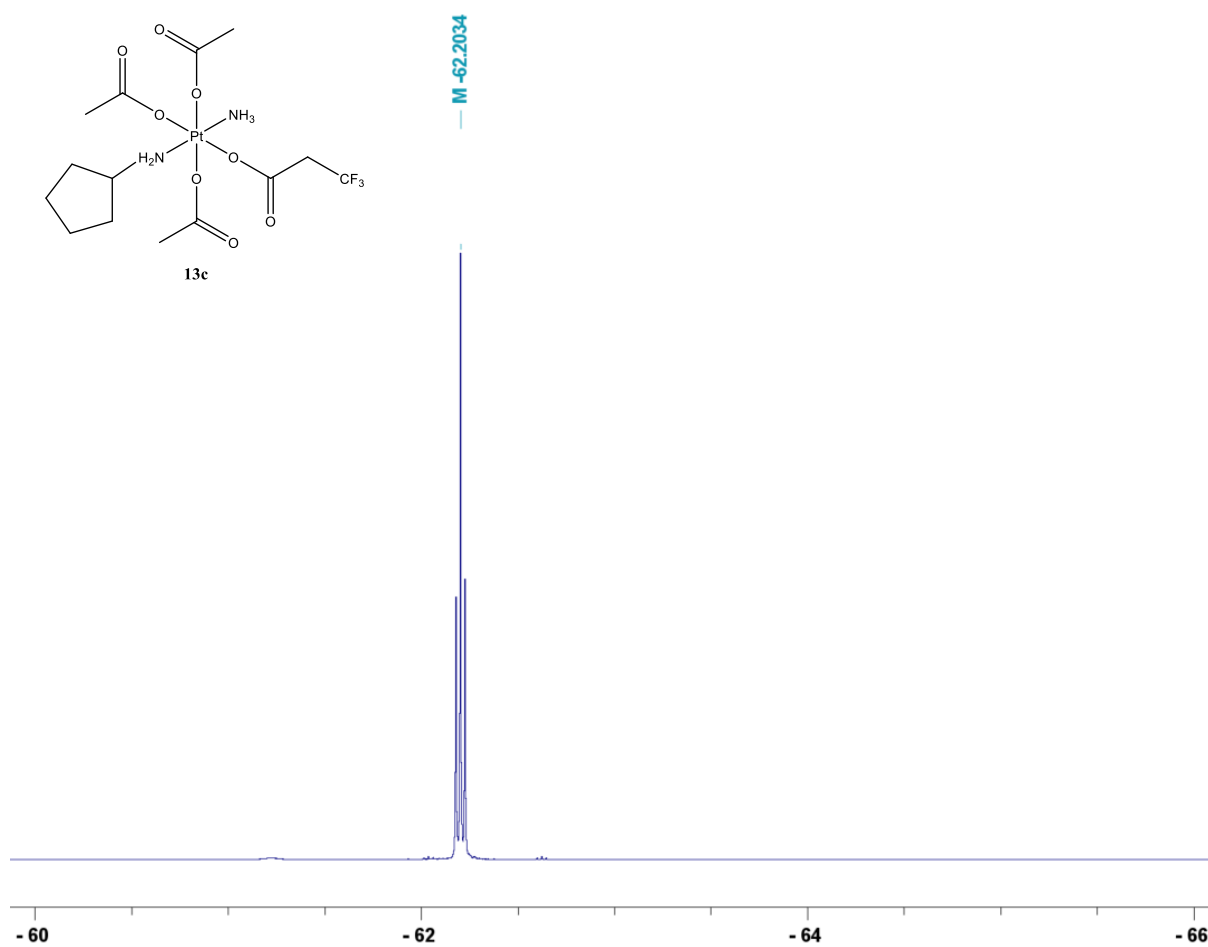


Figure S62. ¹⁹F NMR spectrum of **13c** in d₆-DMSO.

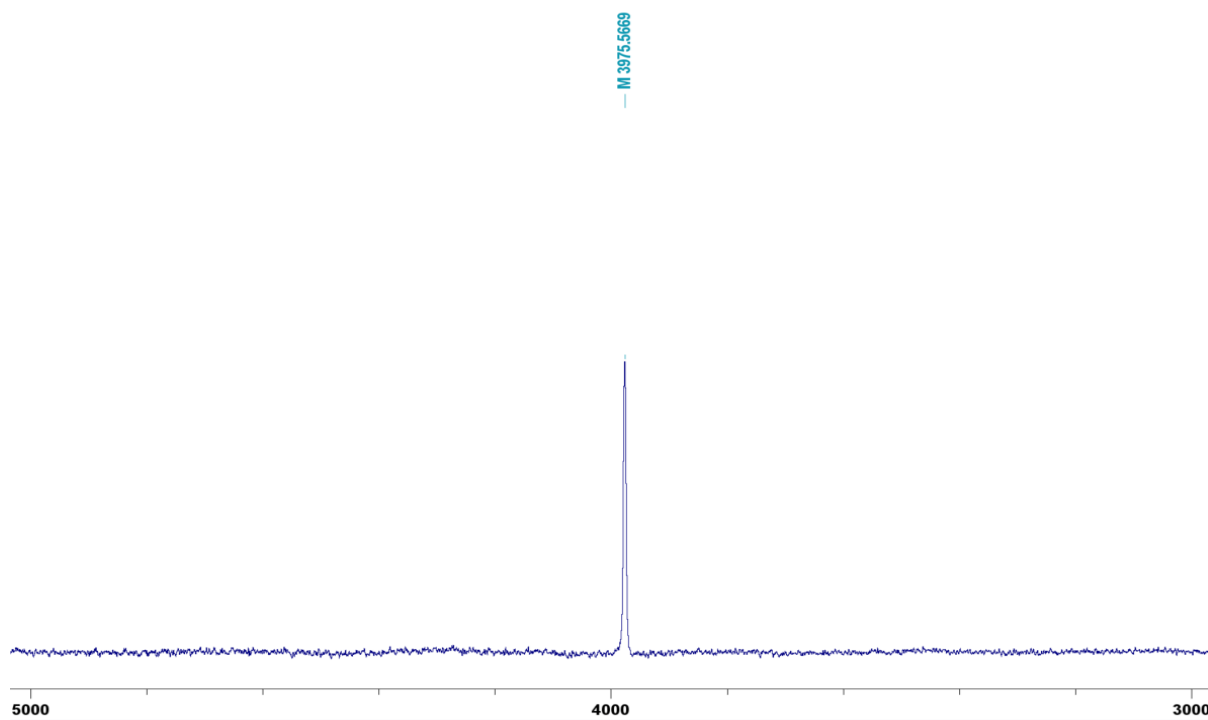


Figure S63. ¹⁹⁵Pt NMR spectrum of **13c** in d₆-DMSO.

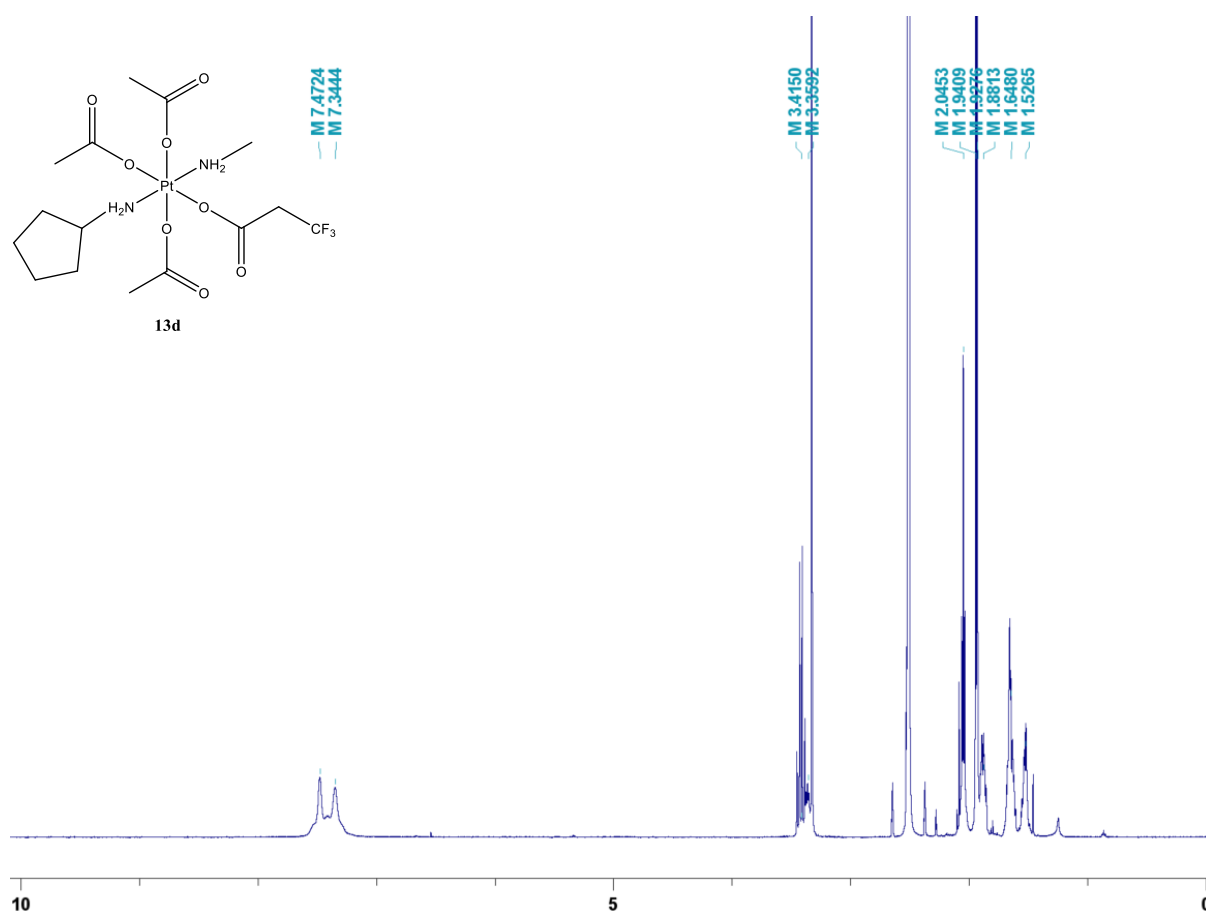


Figure S64. ^1H NMR spectrum of **13d** in d_6 -DMSO.

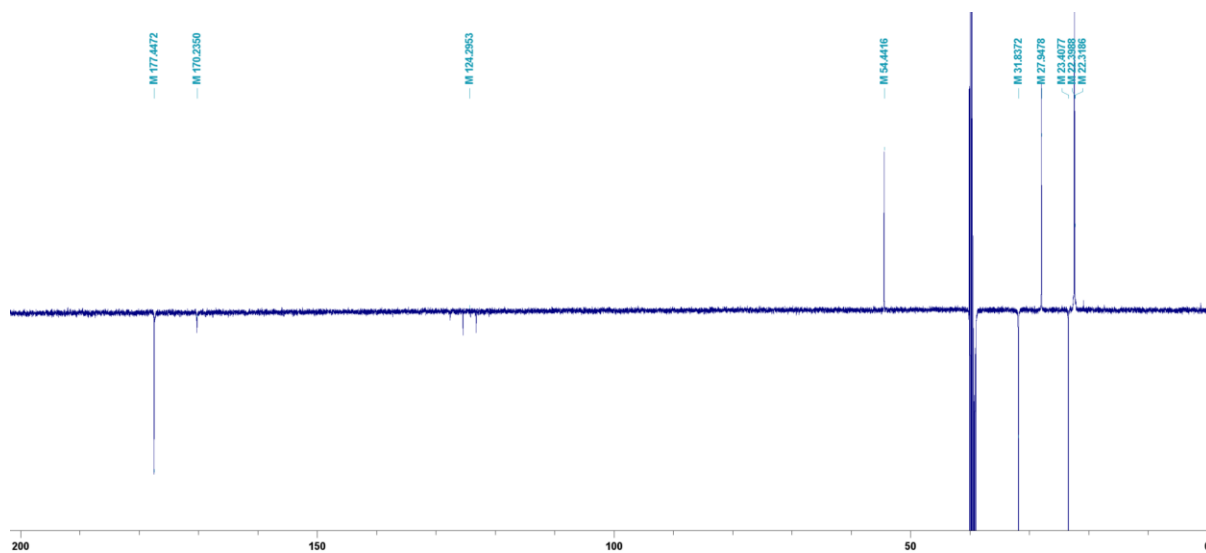


Figure S65. ^{13}C NMR spectrum of **13d** in d_6 -DMSO.

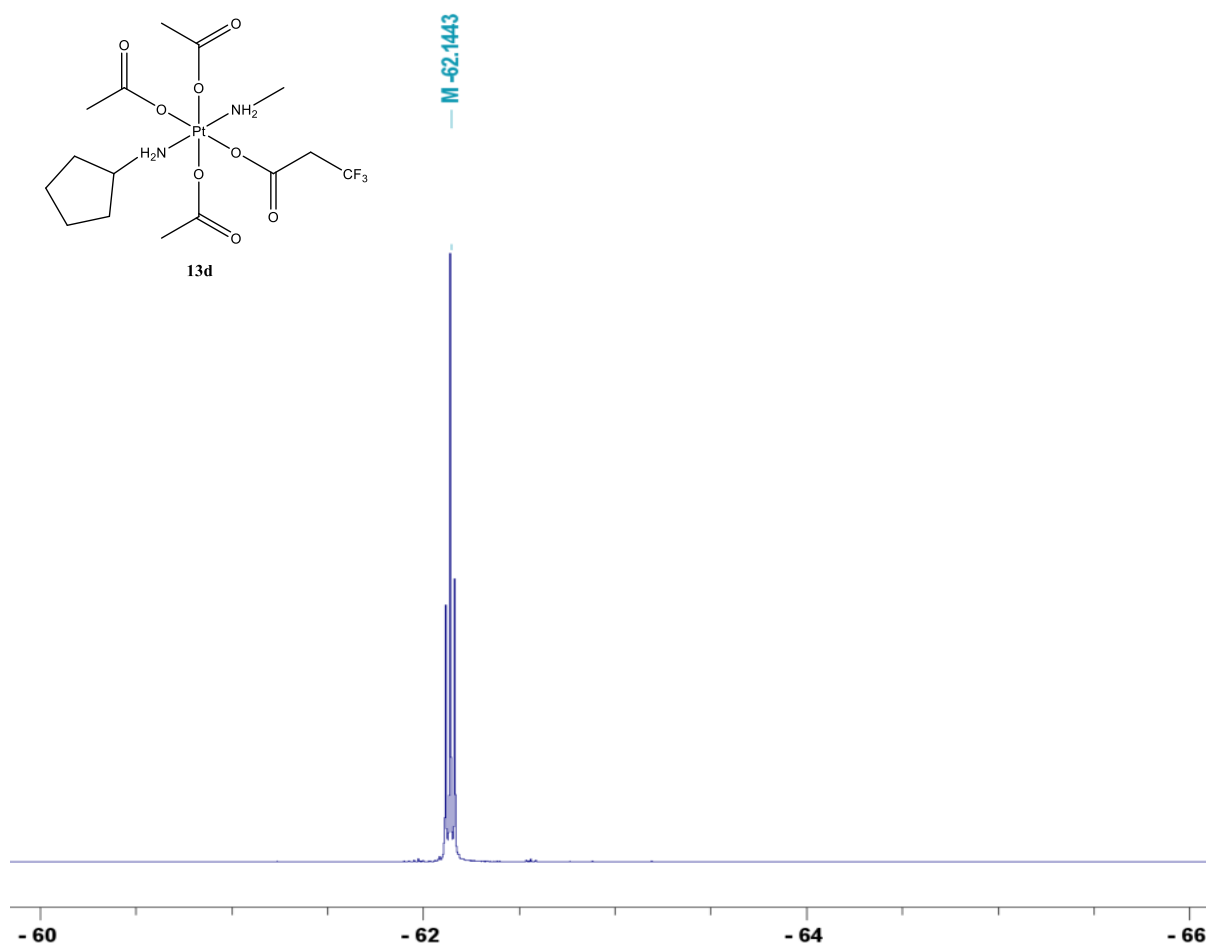


Figure S66. ^{19}F NMR spectrum of **13d** in d_6 -DMSO.

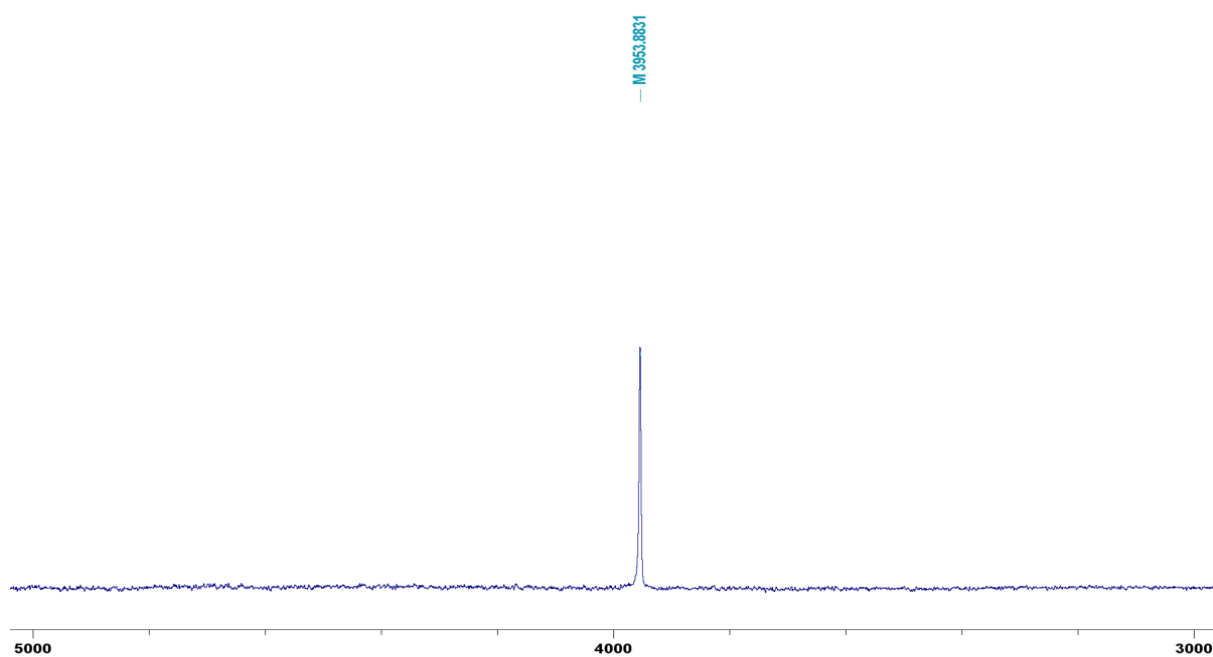


Figure S67. ^{195}Pt NMR spectrum of **13d** in d_6 -DMSO.

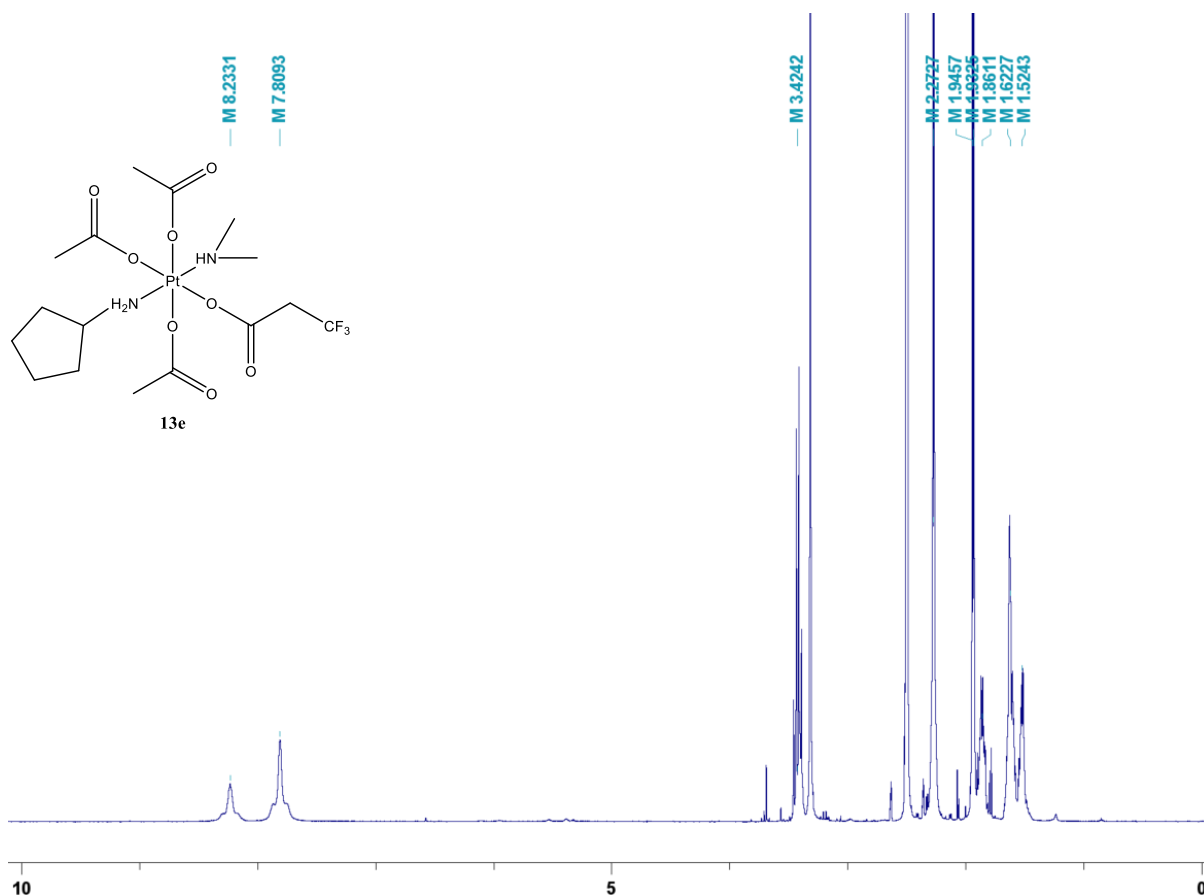


Figure S68. ¹H NMR spectrum of **13e** in d₆-DMSO.

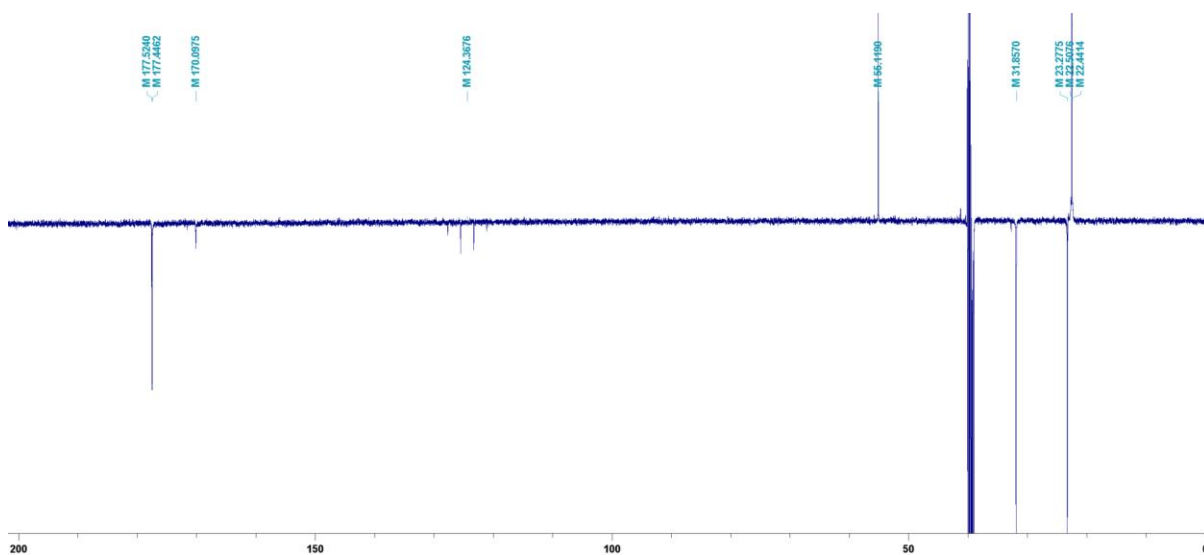


Figure S69. ¹³C NMR spectrum of **13e** in d₆-DMSO.

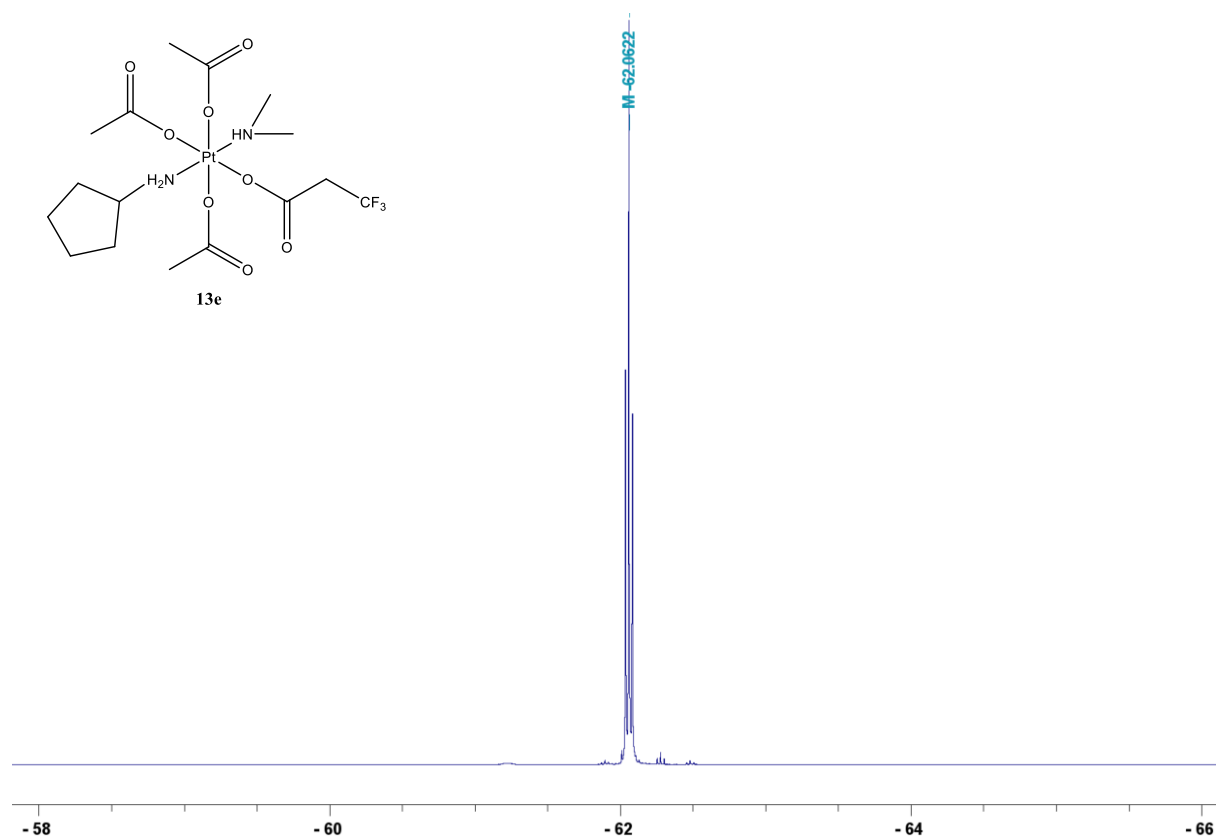


Figure S70. ^{19}F NMR spectrum of **13e** in d_6 -DMSO.

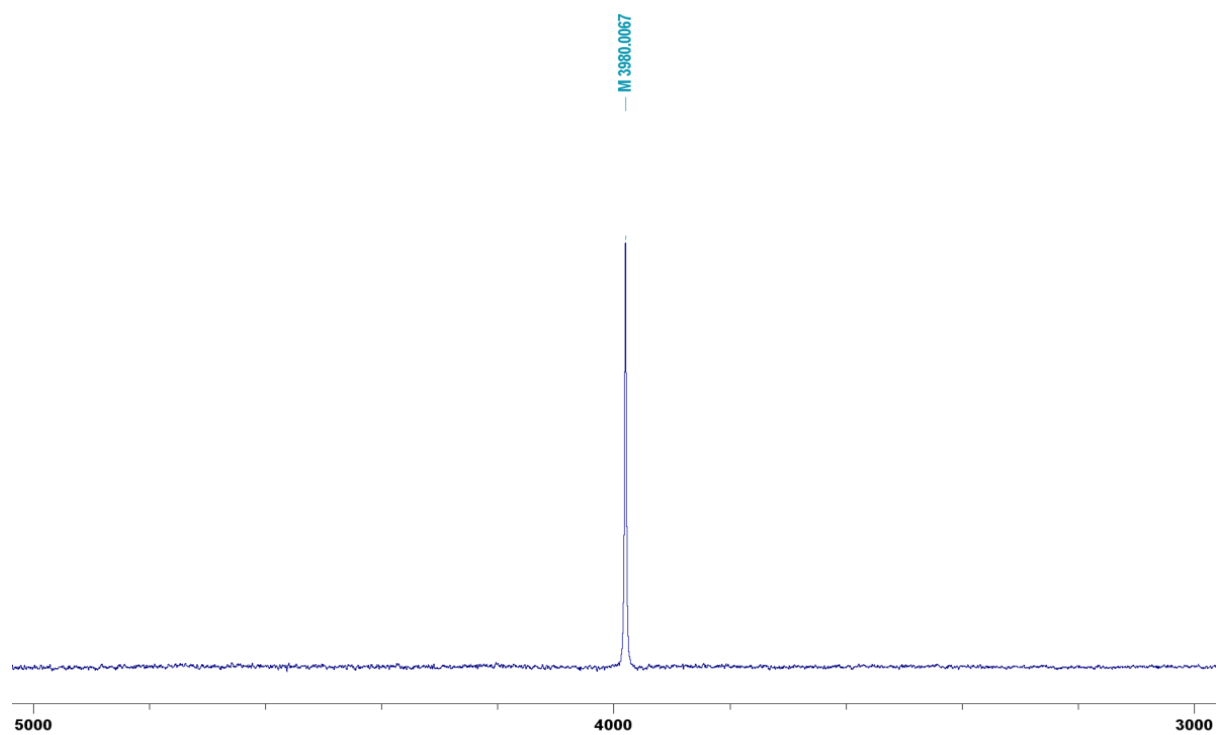


Figure S71. ^{195}Pt NMR spectrum of **13e** in d_6 -DMSO.

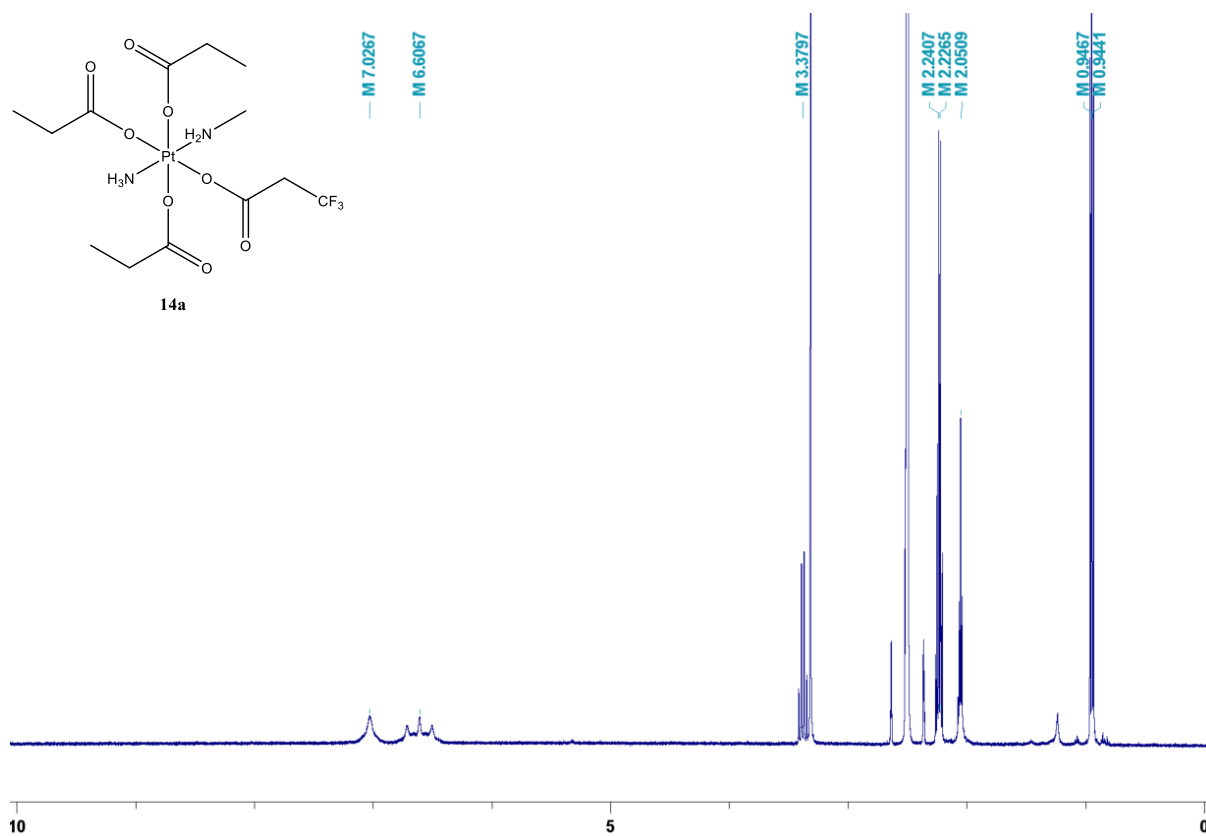


Figure S72. ¹H NMR spectrum of **14a** in d₆-DMSO.

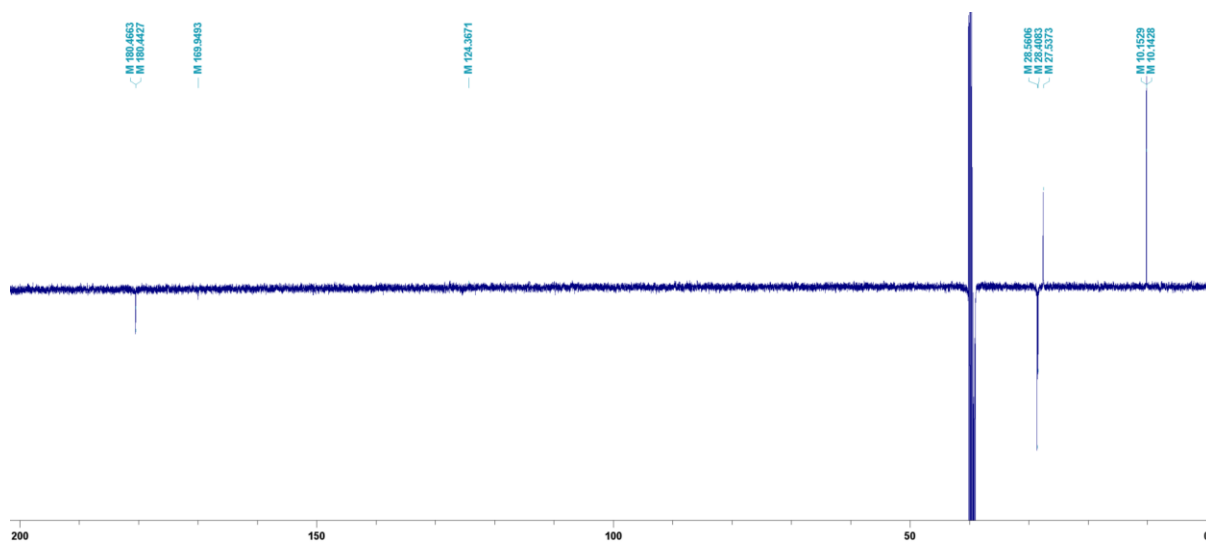


Figure S73. ¹³C NMR spectrum of **14a** in d₆-DMSO.

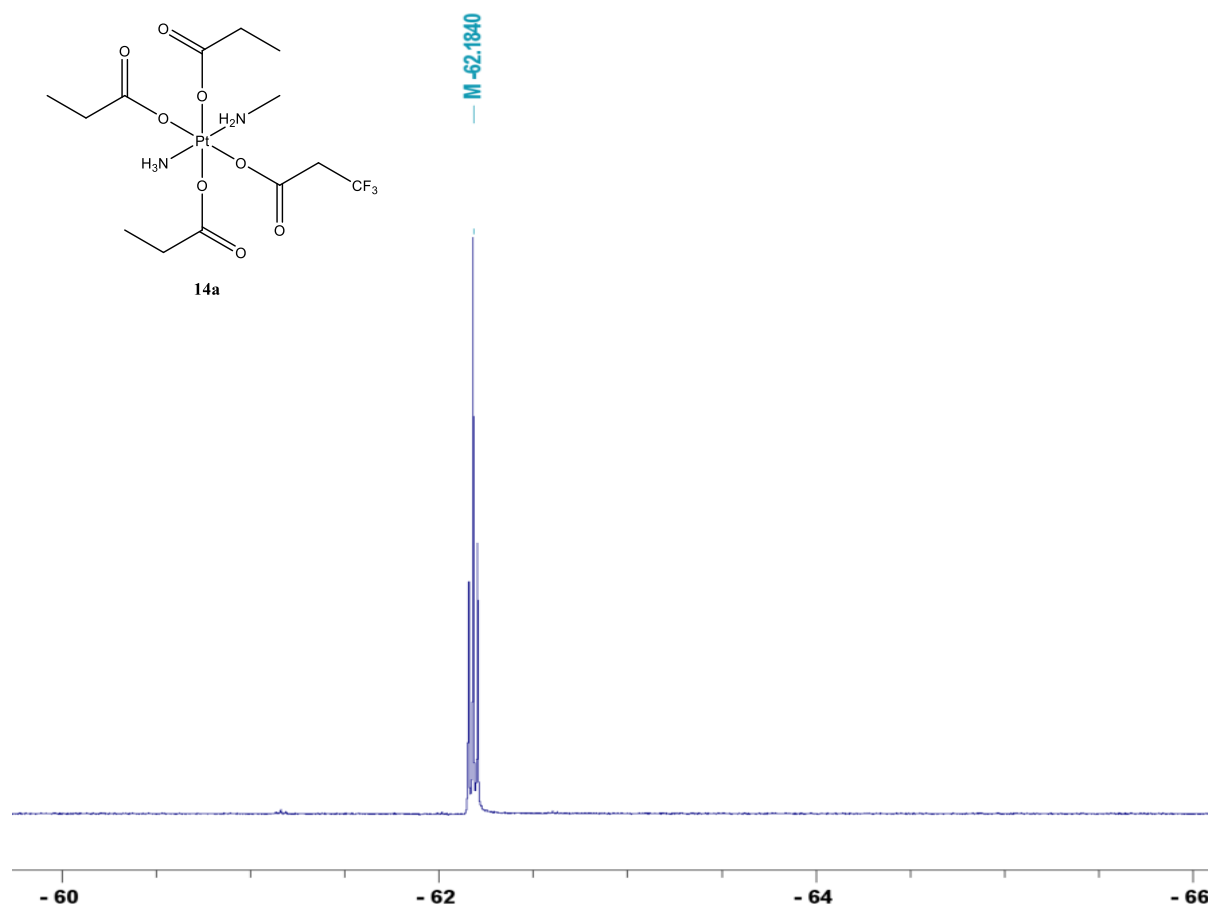


Figure S74. ¹⁹F NMR spectrum of **14a** in d₆-DMSO.

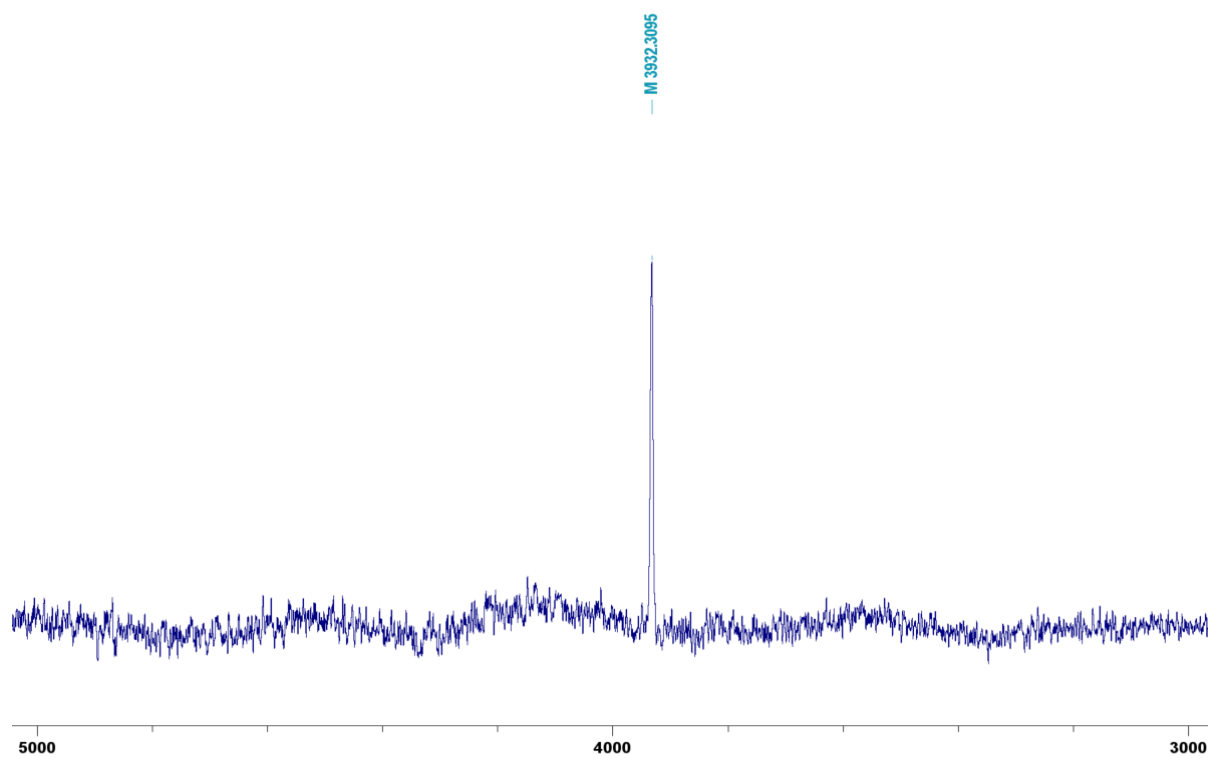


Figure S75. ¹⁹⁵Pt NMR spectrum of **14a** in d₆-DMSO.

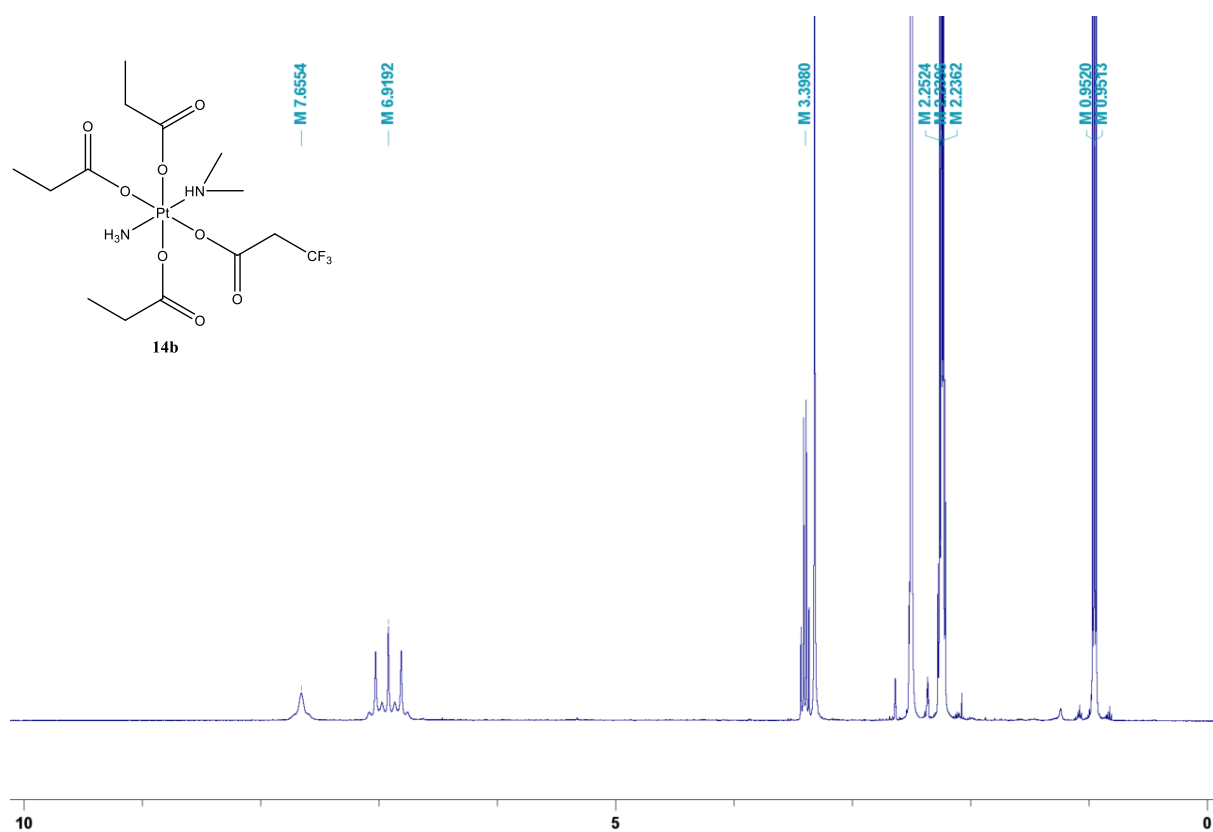


Figure S76. ¹H NMR spectrum of **14b** in d₆-DMSO.

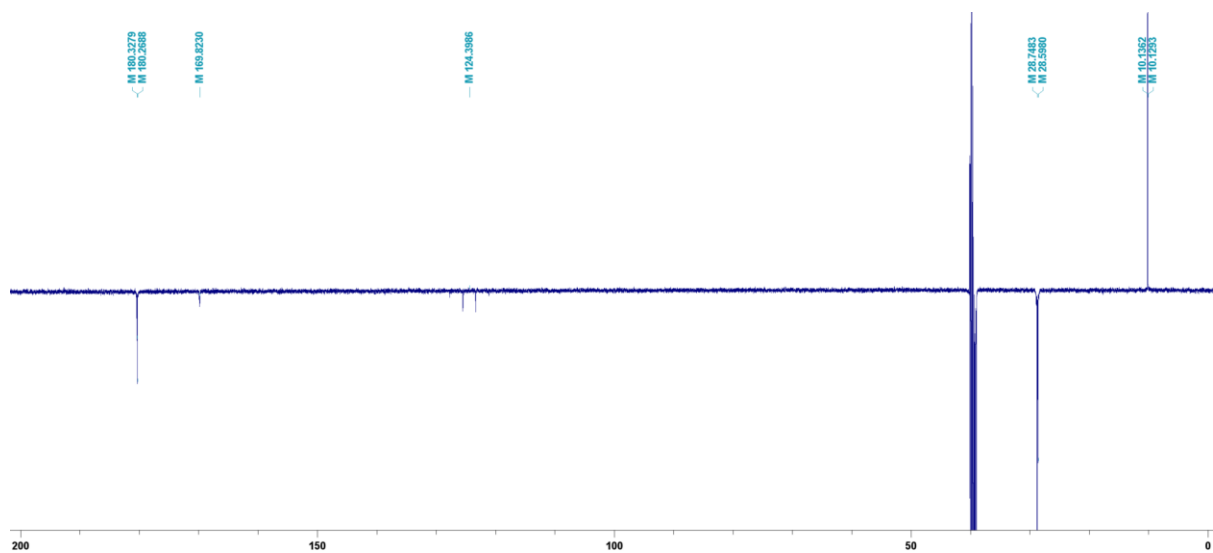


Figure S77. ¹³C NMR spectrum of **14b** in d₆-DMSO.

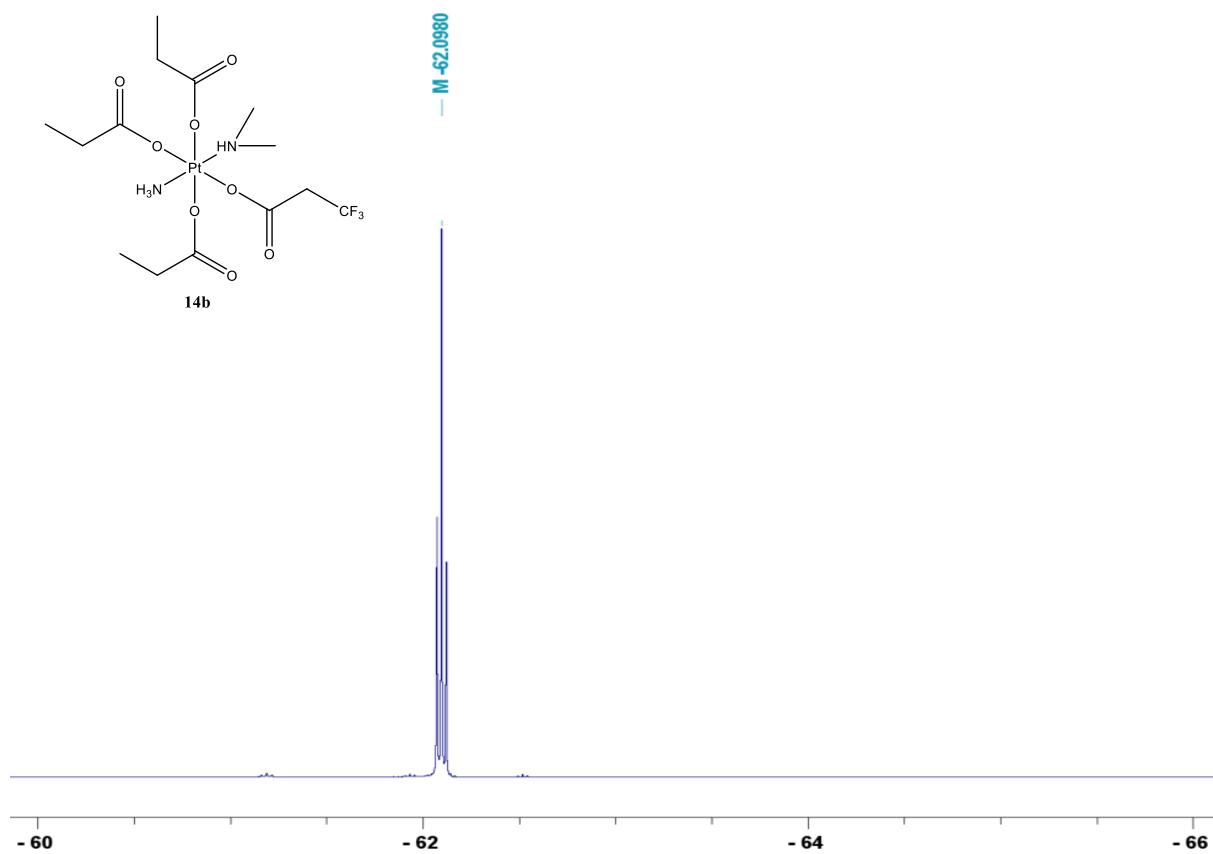


Figure S78. ¹⁹F NMR spectrum of **14b** in d₆-DMSO.

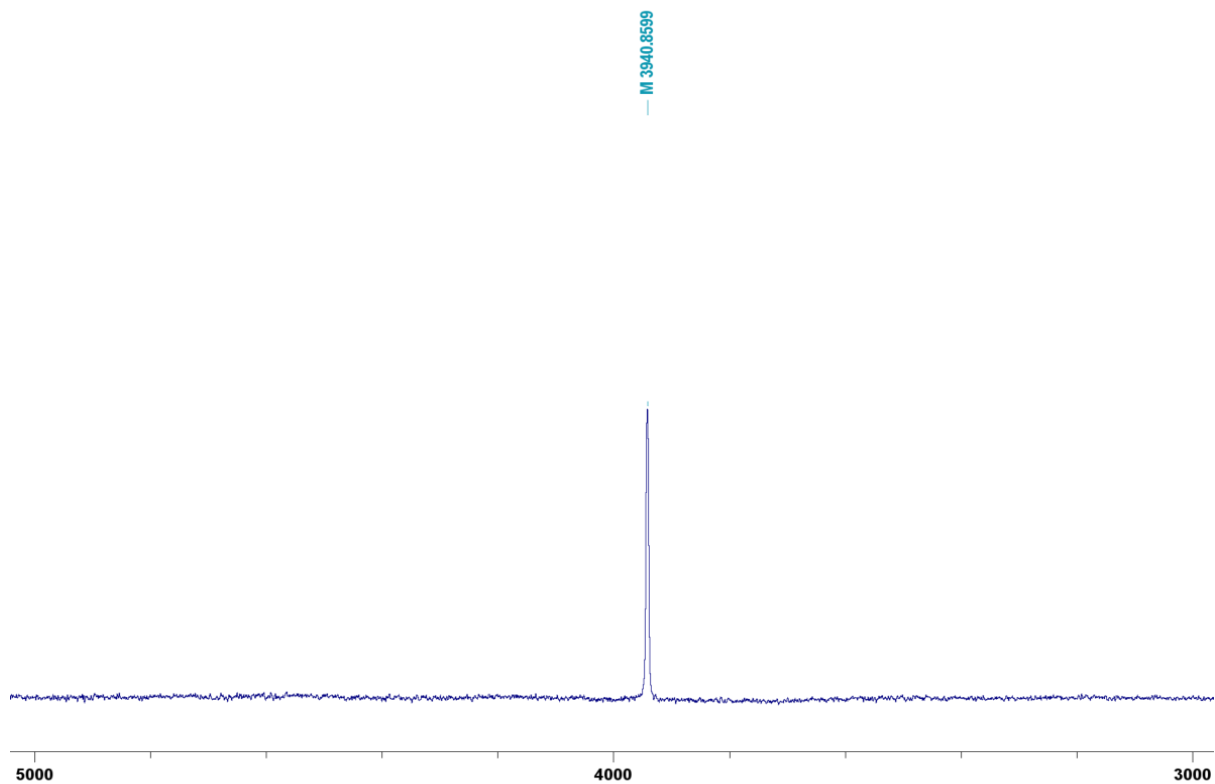


Figure S79. ¹⁹⁵Pt NMR spectrum of **14b** in d₆-DMSO.

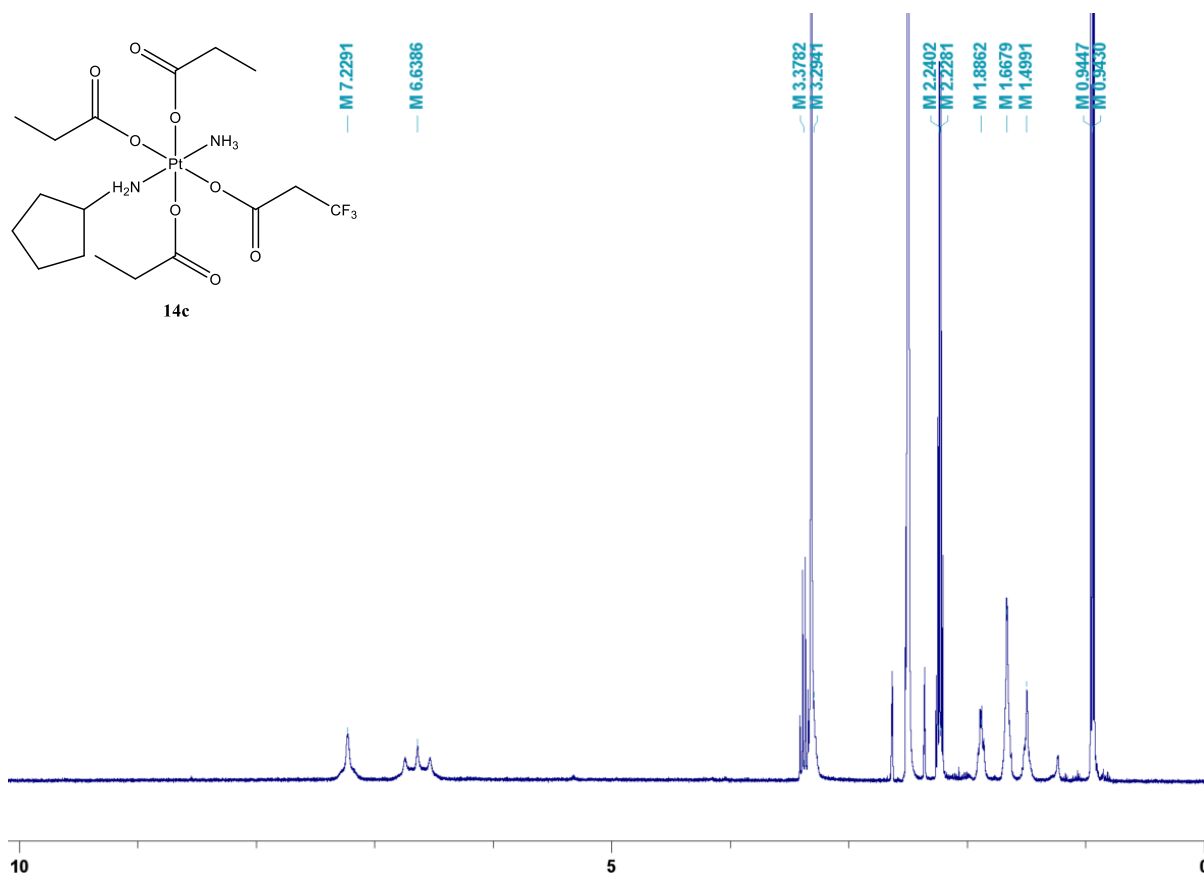


Figure S80. ¹H NMR spectrum of **14c** in d₆-DMSO.

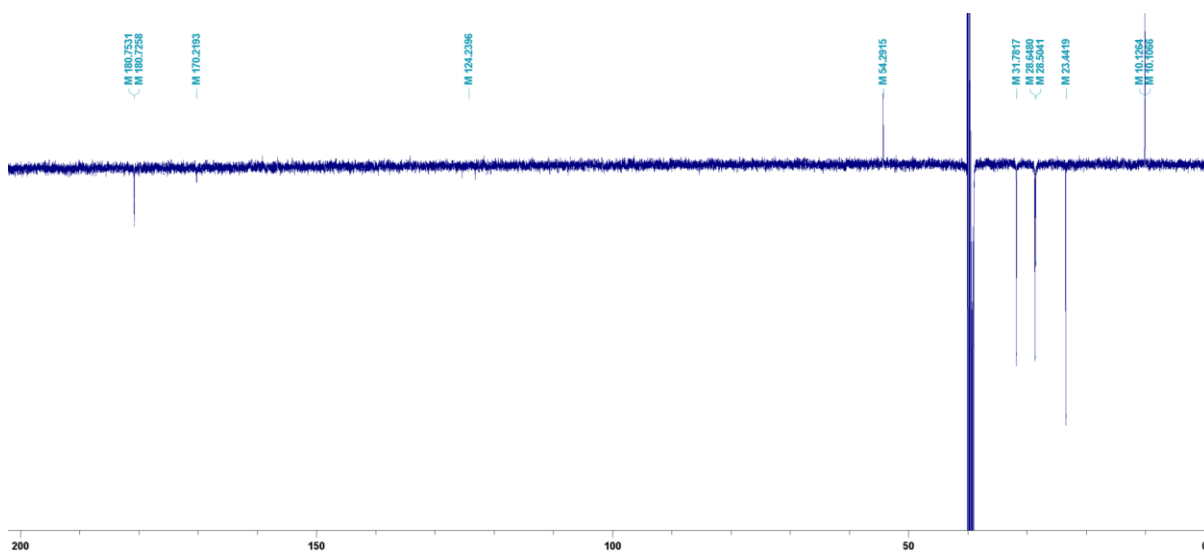


Figure S81. ¹³C NMR spectrum of **14c** in d₆-DMSO.

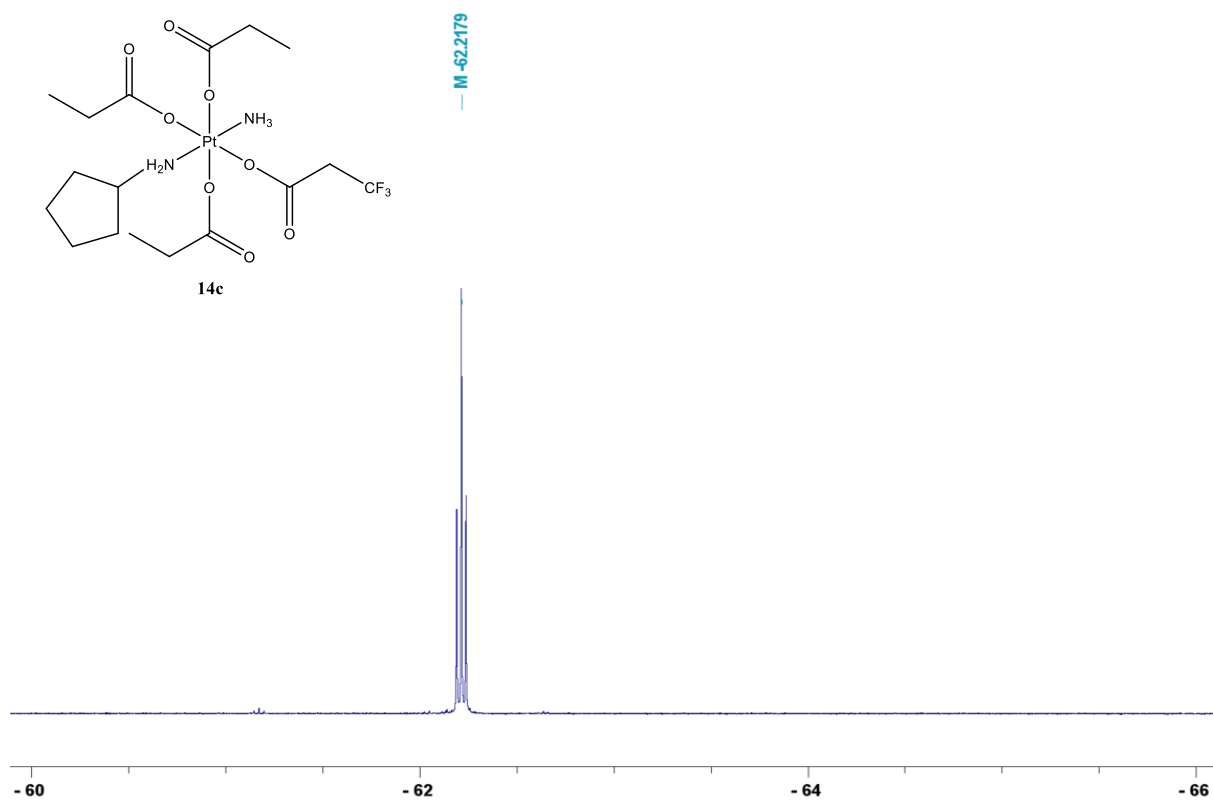


Figure S82. ¹⁹F NMR spectrum of **14c** in d₆-DMSO.

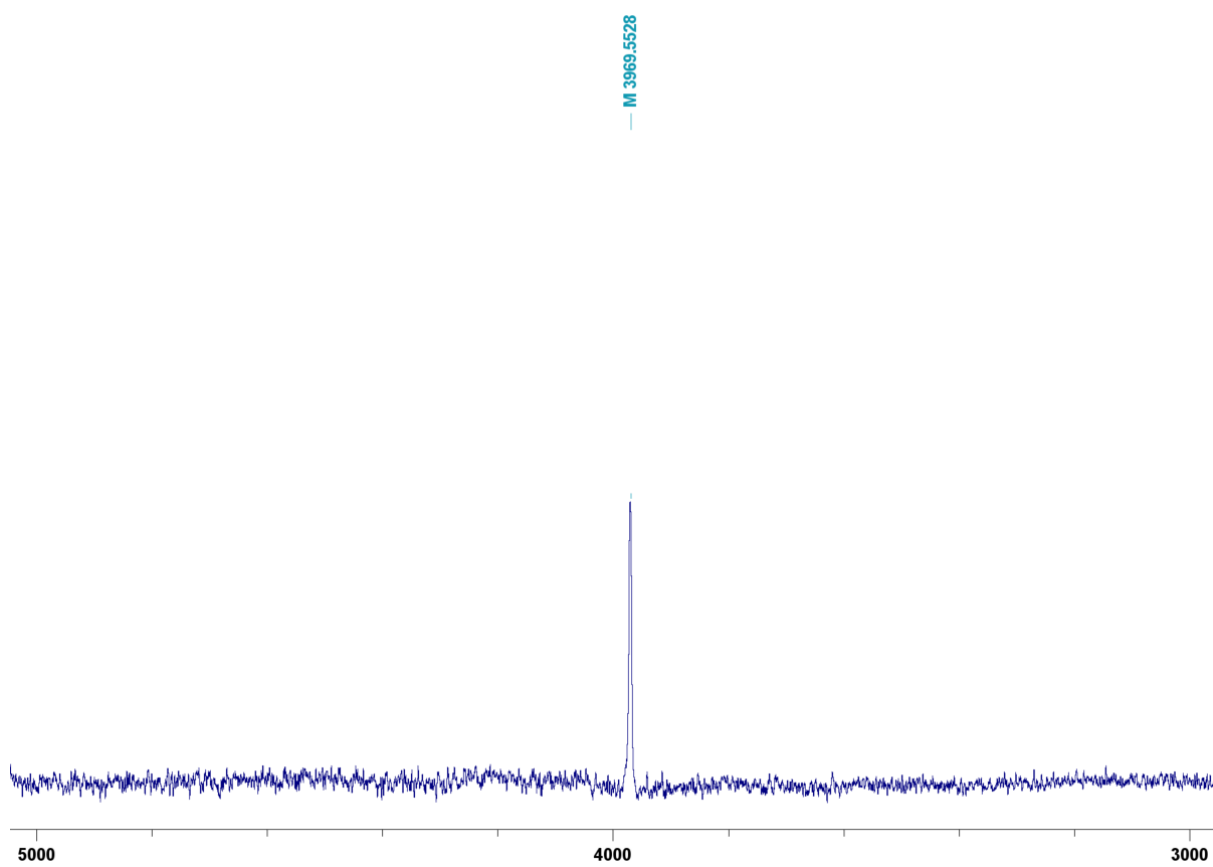


Figure S83. ¹⁹⁵Pt NMR spectrum of **14c** in d₆-DMSO.

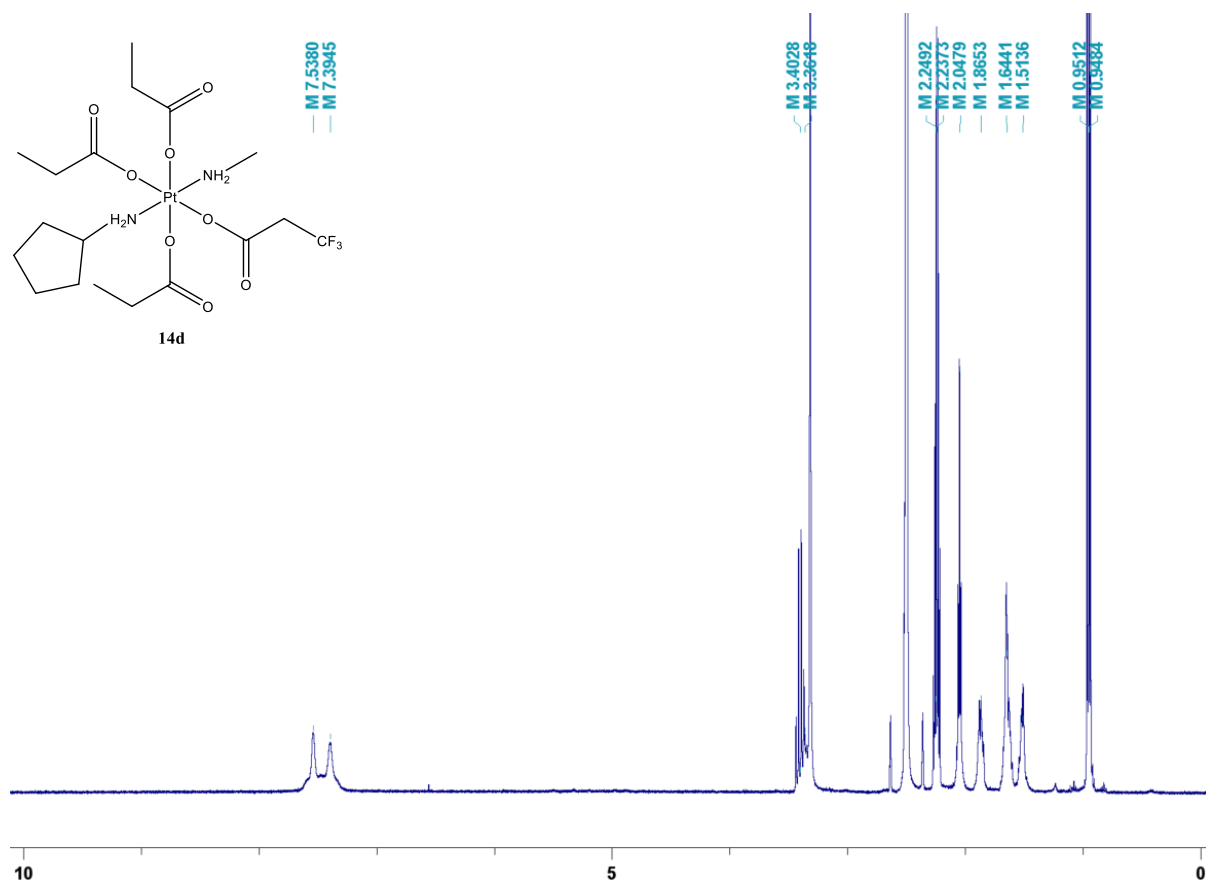


Figure S84. ¹H NMR spectrum of **14d** in d₆-DMSO.

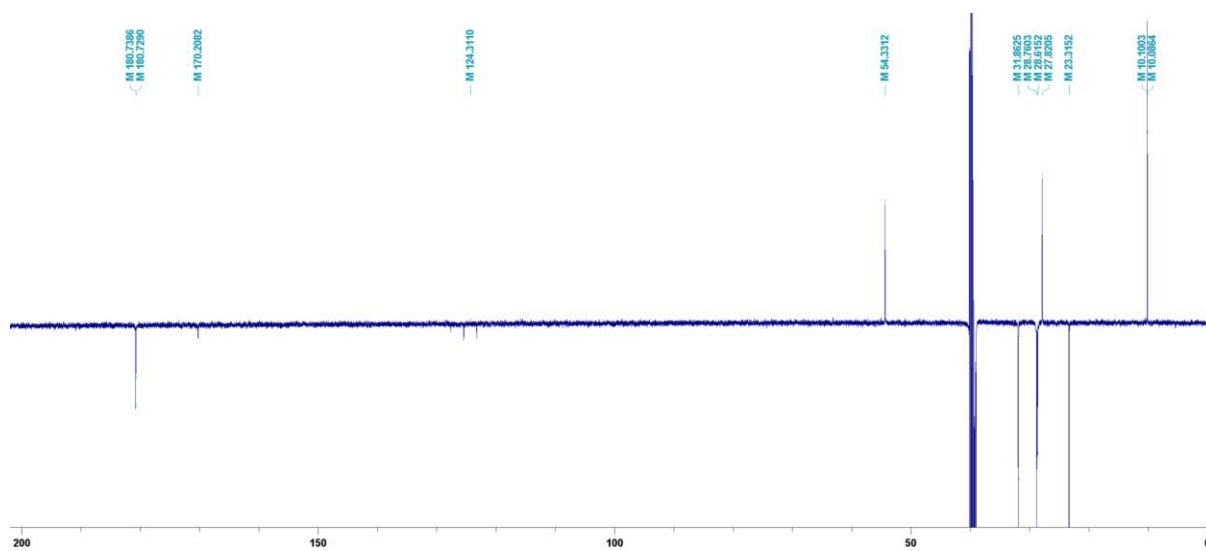


Figure S85. ¹³C NMR spectrum of **14d** in d₆-DMSO.

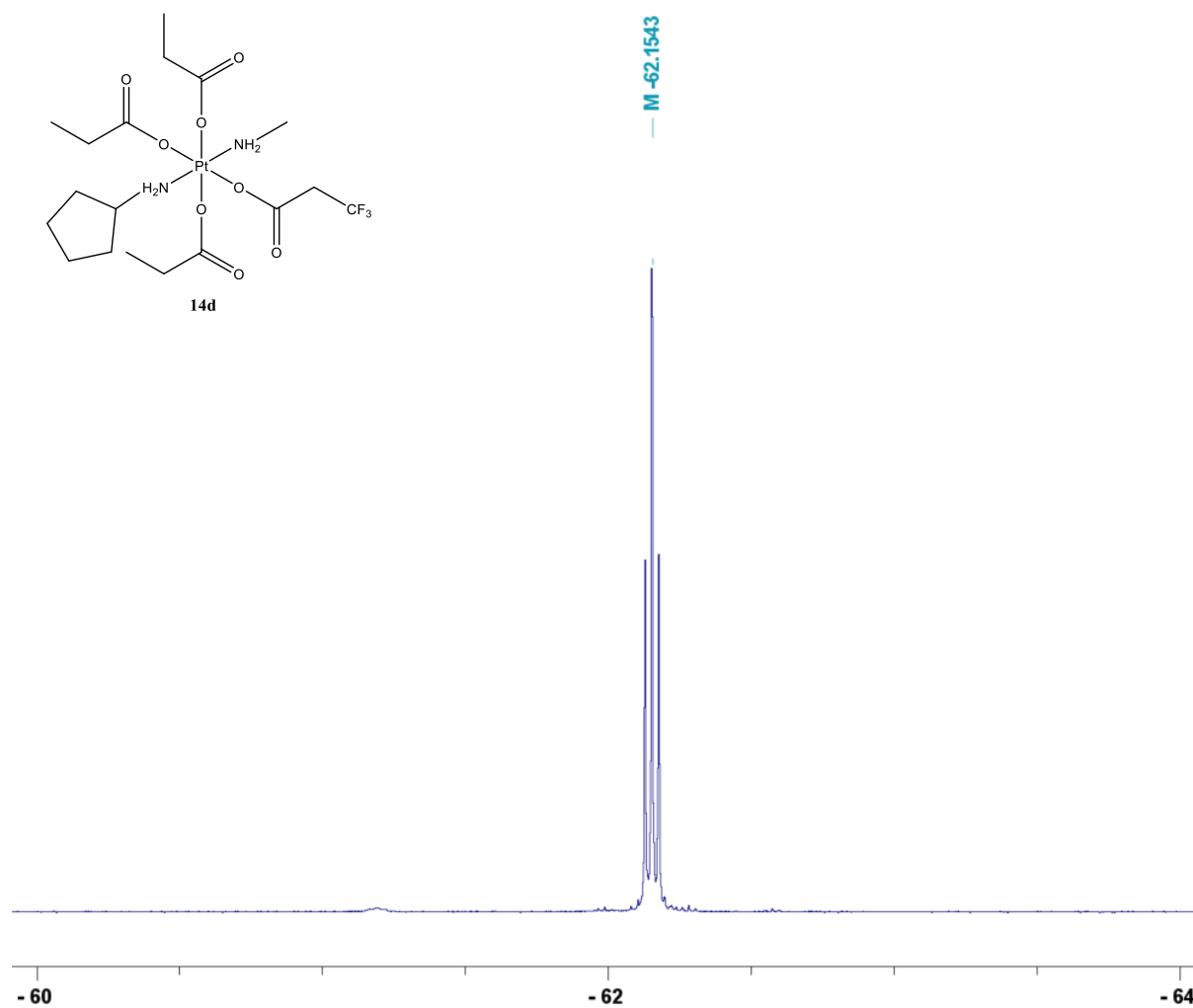


Figure S86. ^{19}F NMR spectrum of **14d** in d_6 -DMSO.

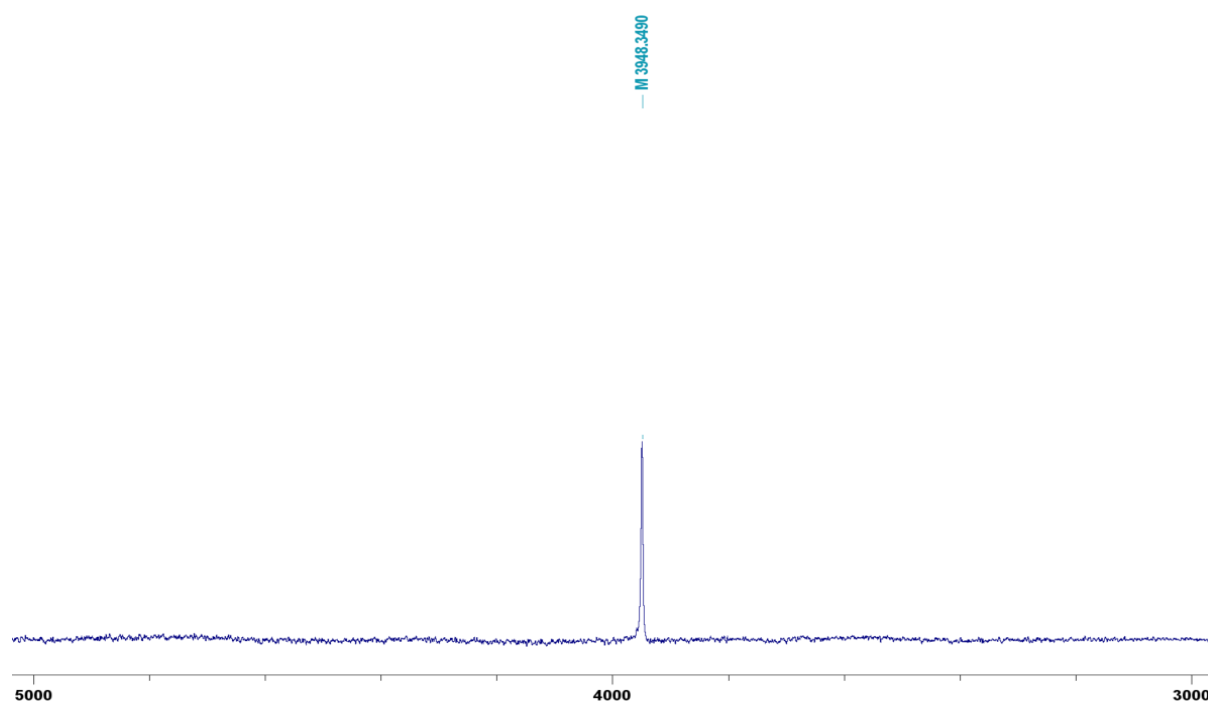


Figure S87. ^{195}Pt NMR spectrum of **14d** in d_6 -DMSO.

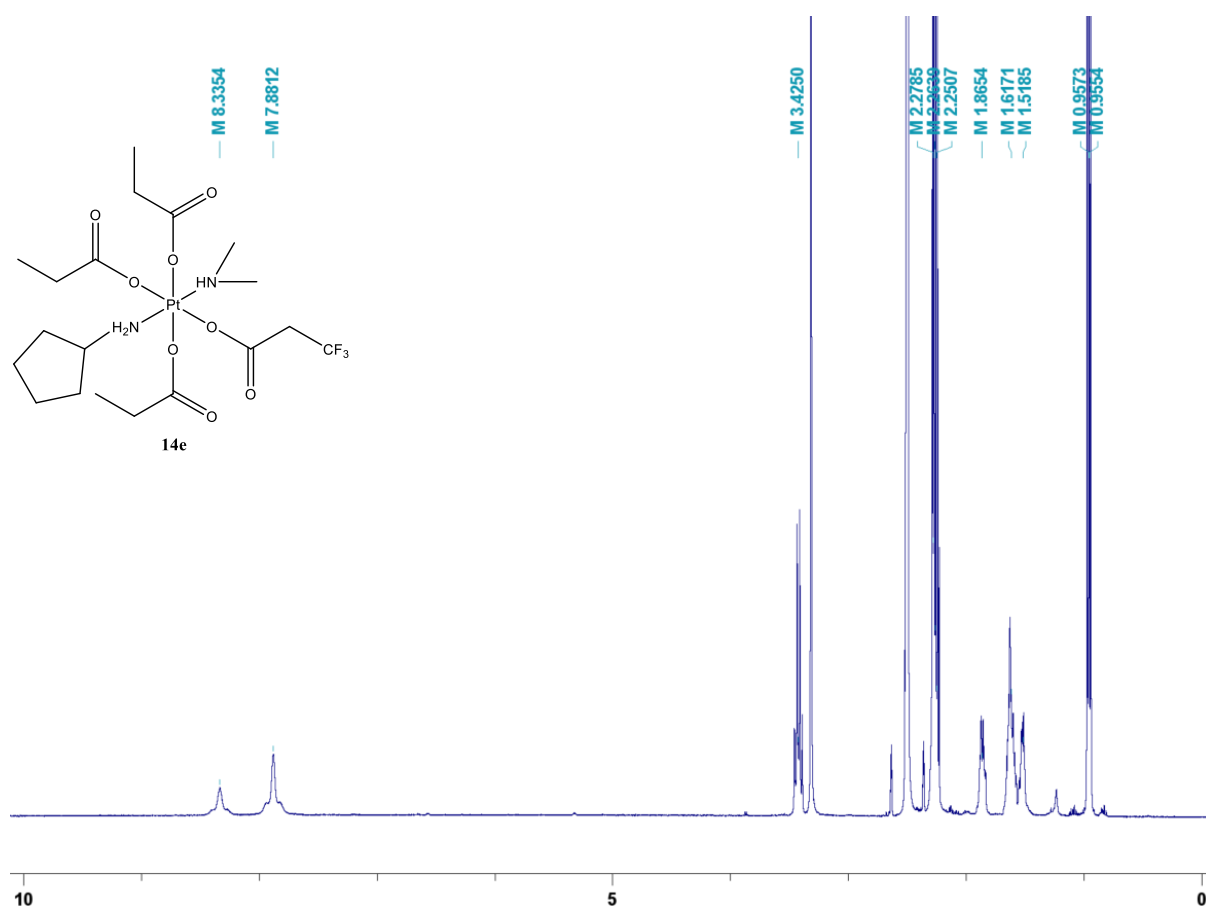


Figure S88. ^1H NMR spectrum of **14e** in d_6 -DMSO.

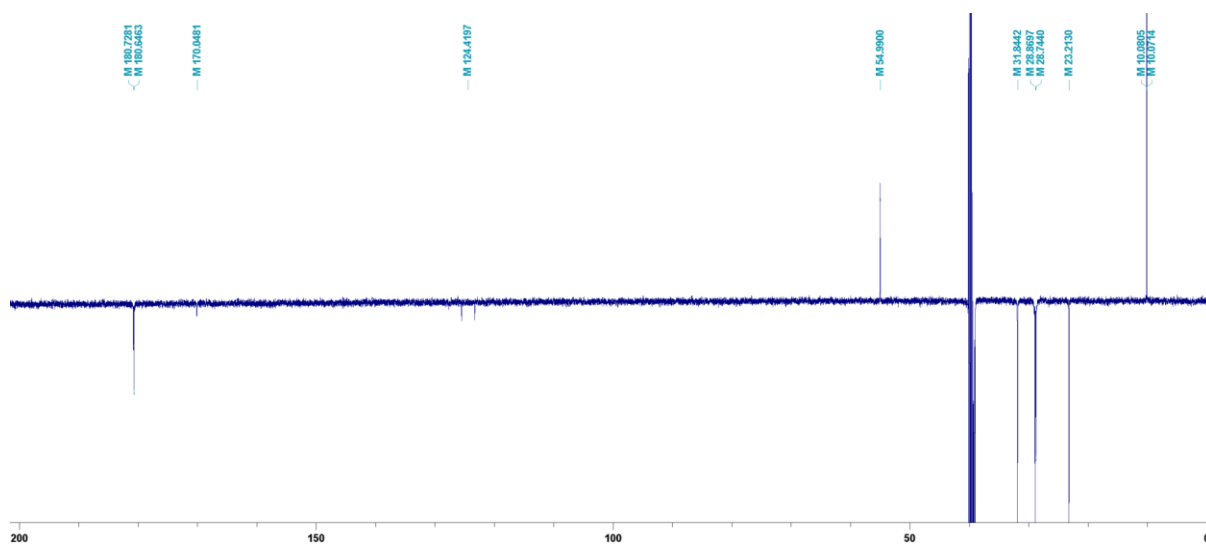


Figure S89. ^{13}C NMR spectrum of **14e** in d_6 -DMSO.

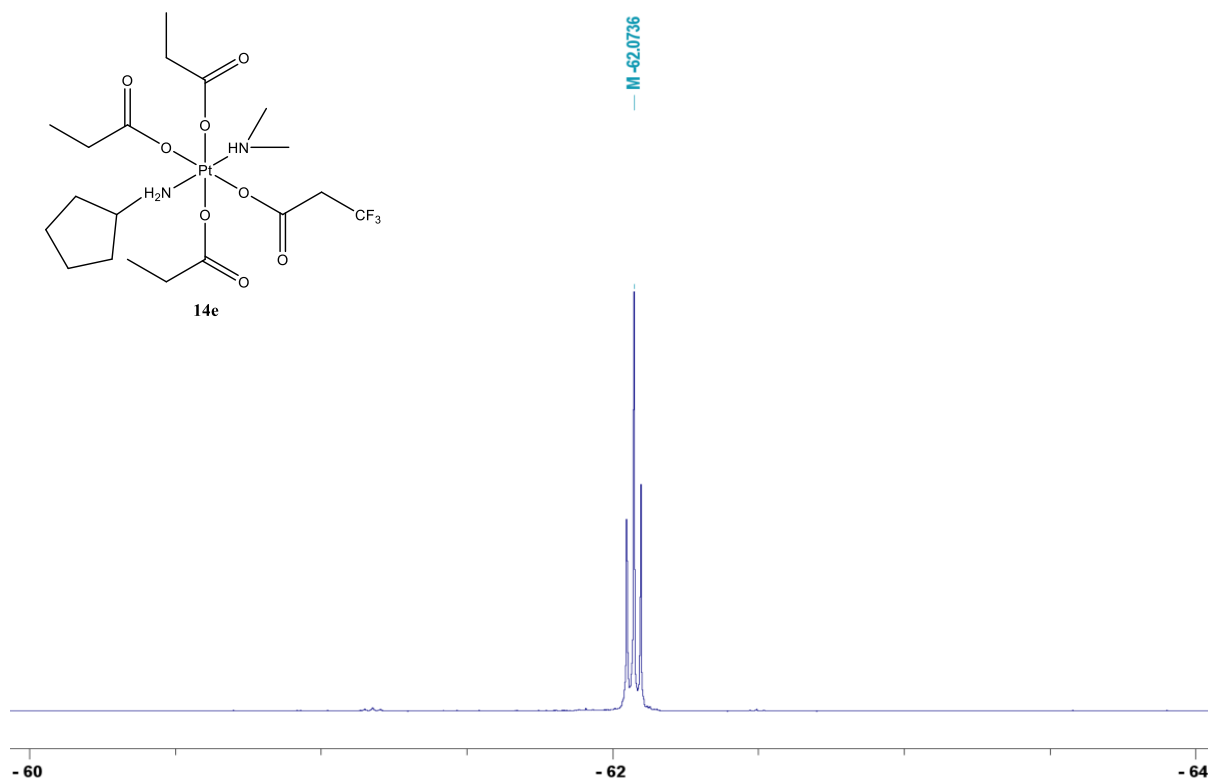


Figure S90. ^{19}F NMR spectrum of **14e** in d_6 -DMSO.

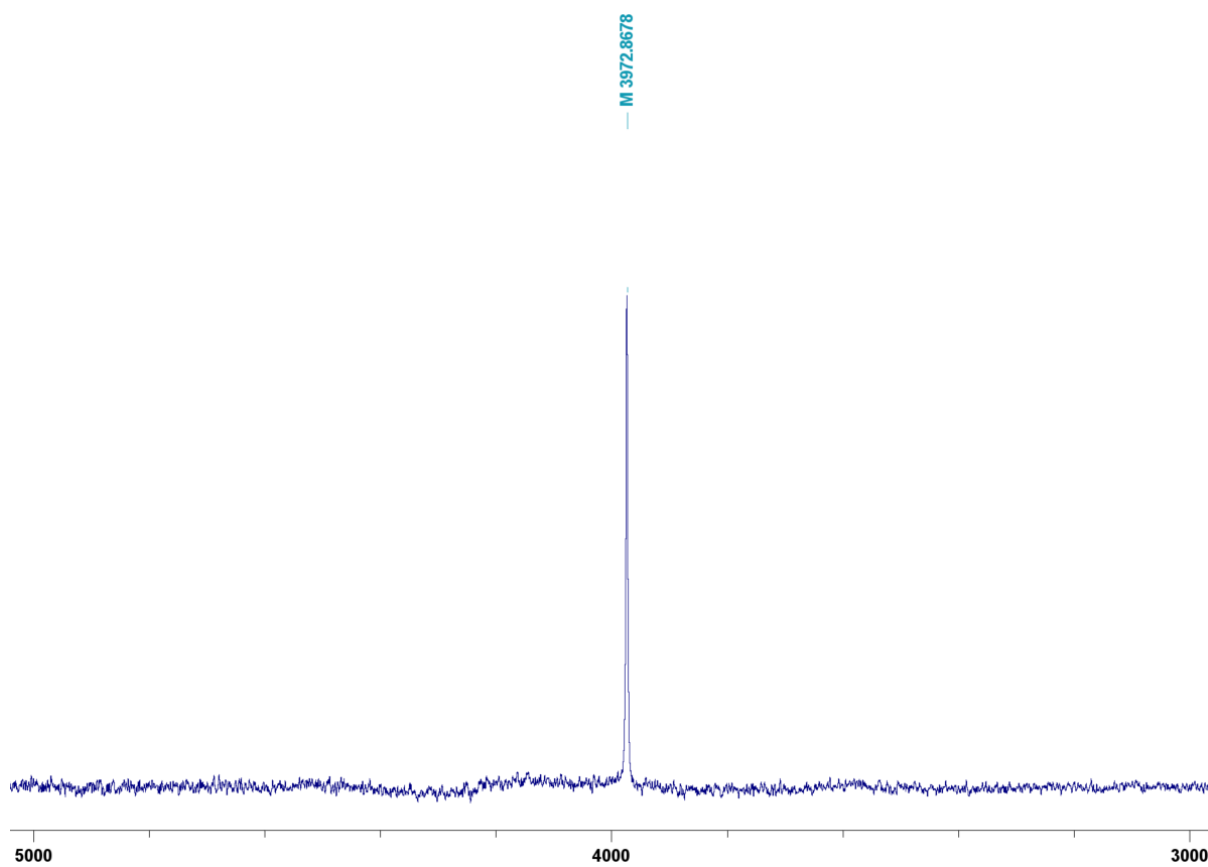


Figure S91. ^{195}Pt NMR spectrum of **14e** in d_6 -DMSO.

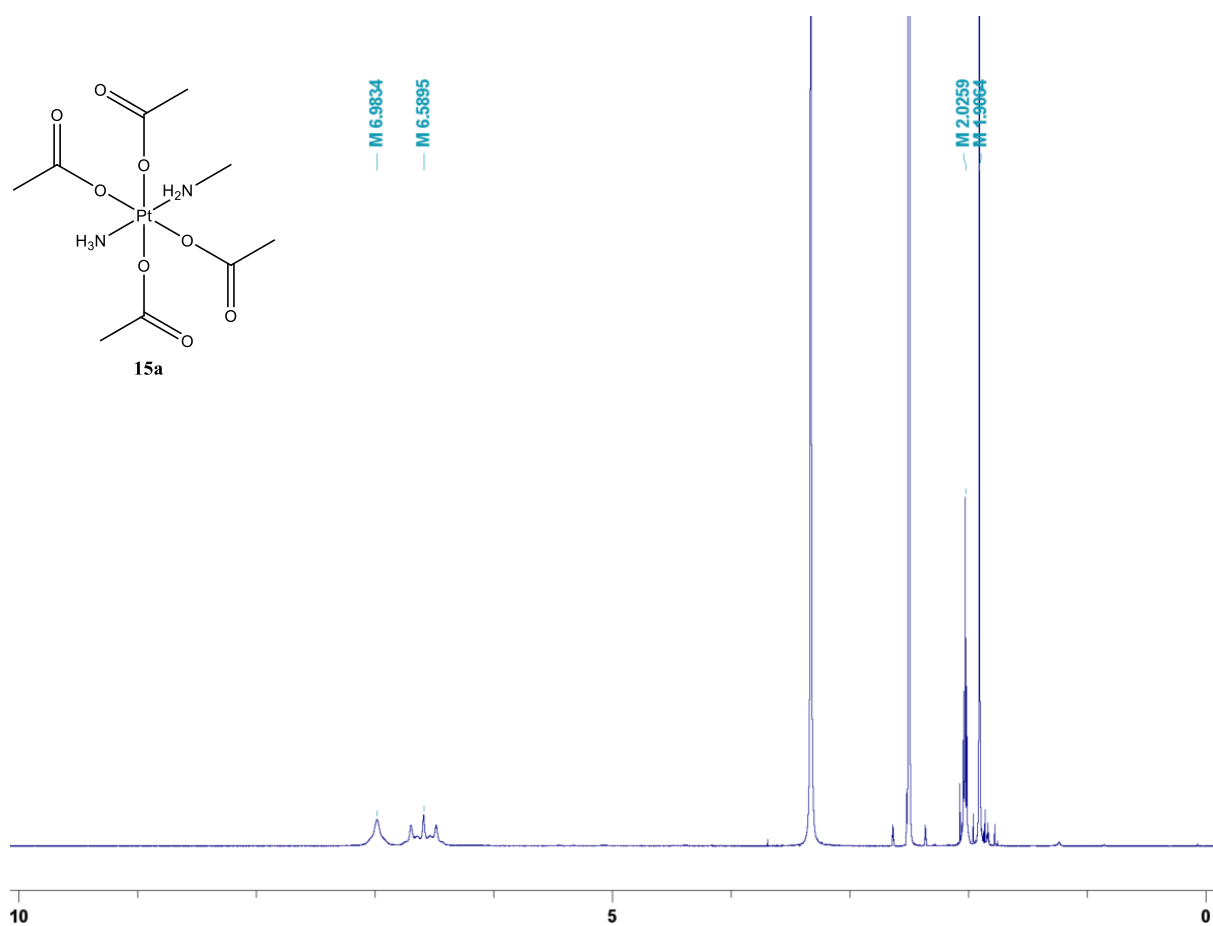


Figure S92. ¹H NMR spectrum of **15a** in d₆-DMSO.

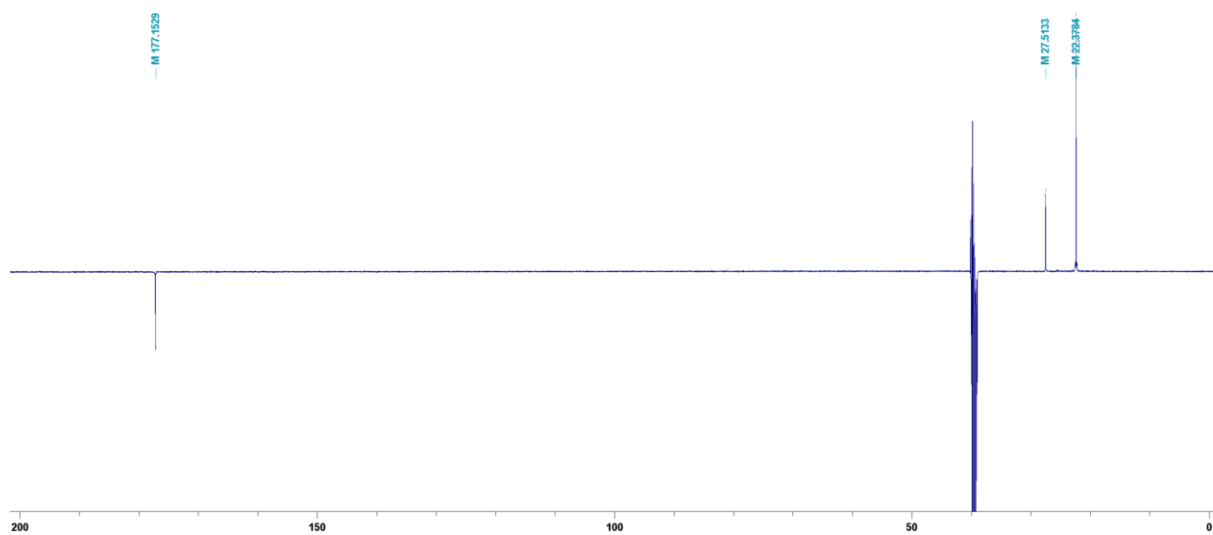


Figure S93. ¹³C NMR spectrum of **15a** in d₆-DMSO.

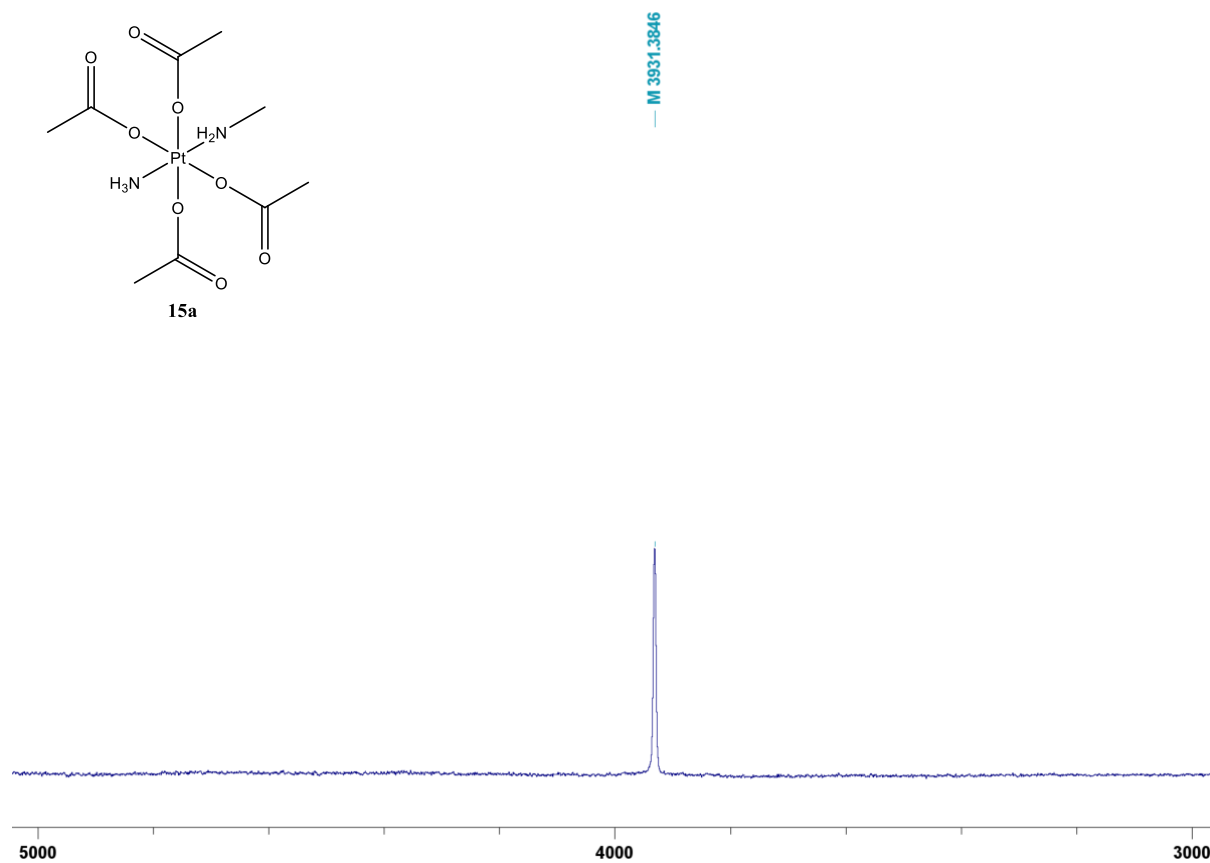


Figure S94. ¹⁹⁵Pt NMR spectrum of **15a** in d₆-DMSO.

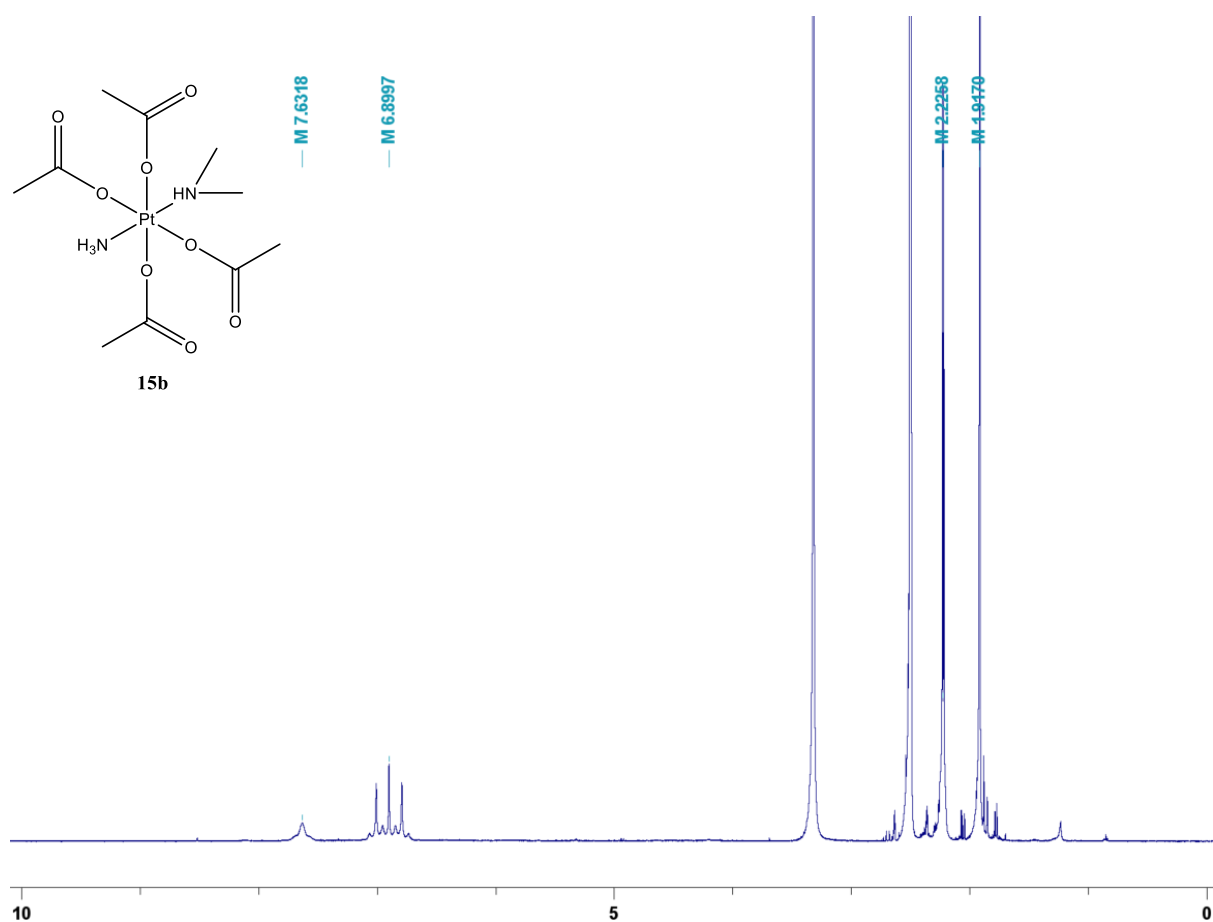


Figure S95. ¹H NMR spectrum of **15b** in d₆-DMSO.

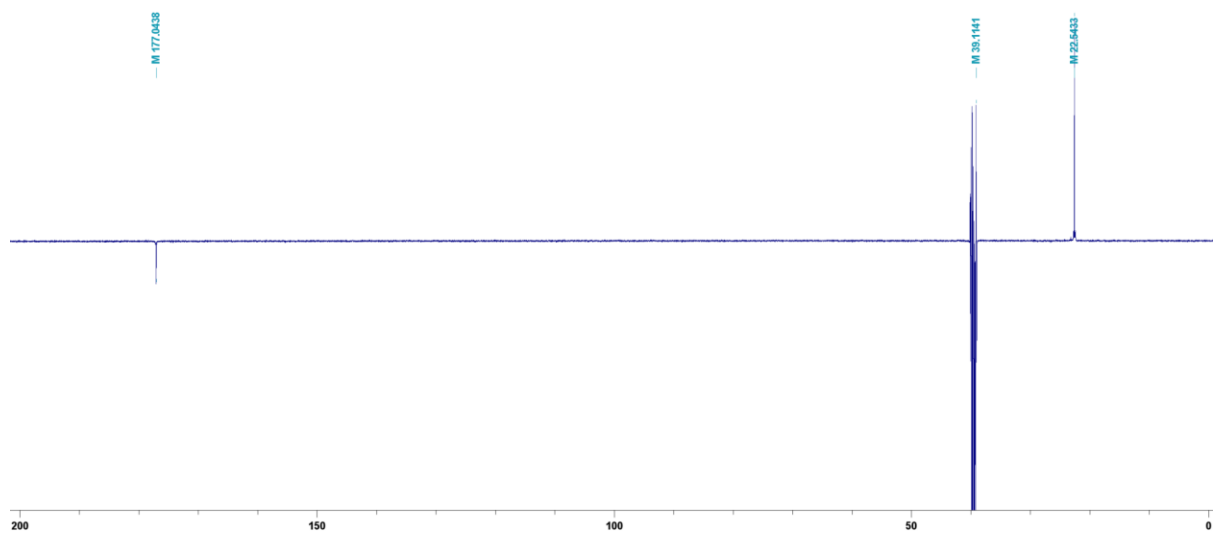


Figure S96. ¹³C NMR spectrum of **15b** in d₆-DMSO.

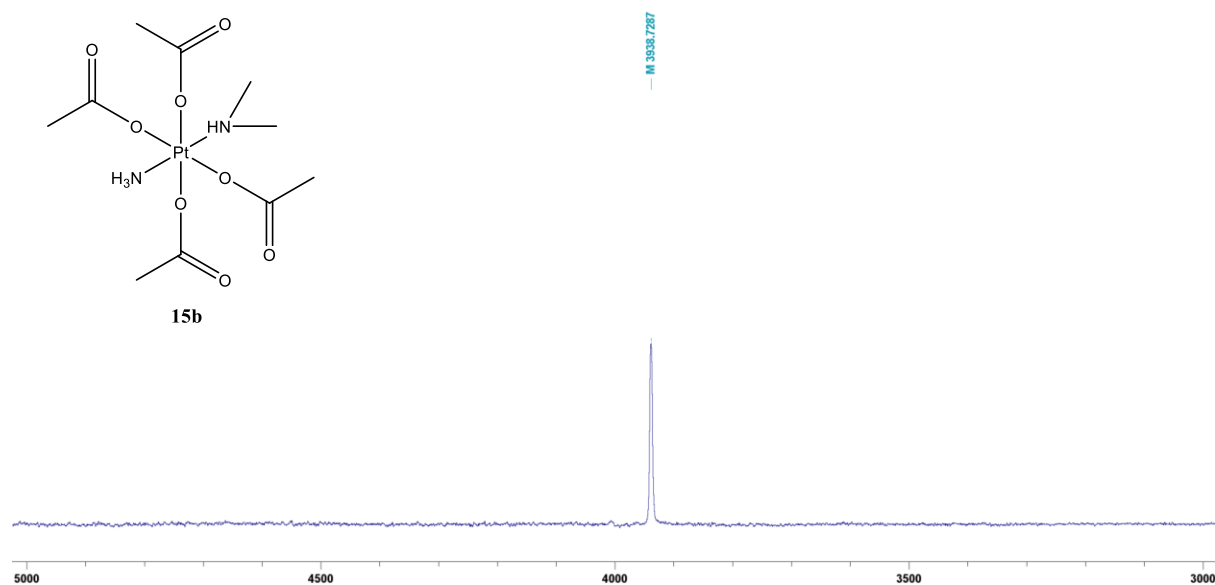


Figure S97. ^{195}Pt NMR spectrum of **15b** in d_6 -DMSO.

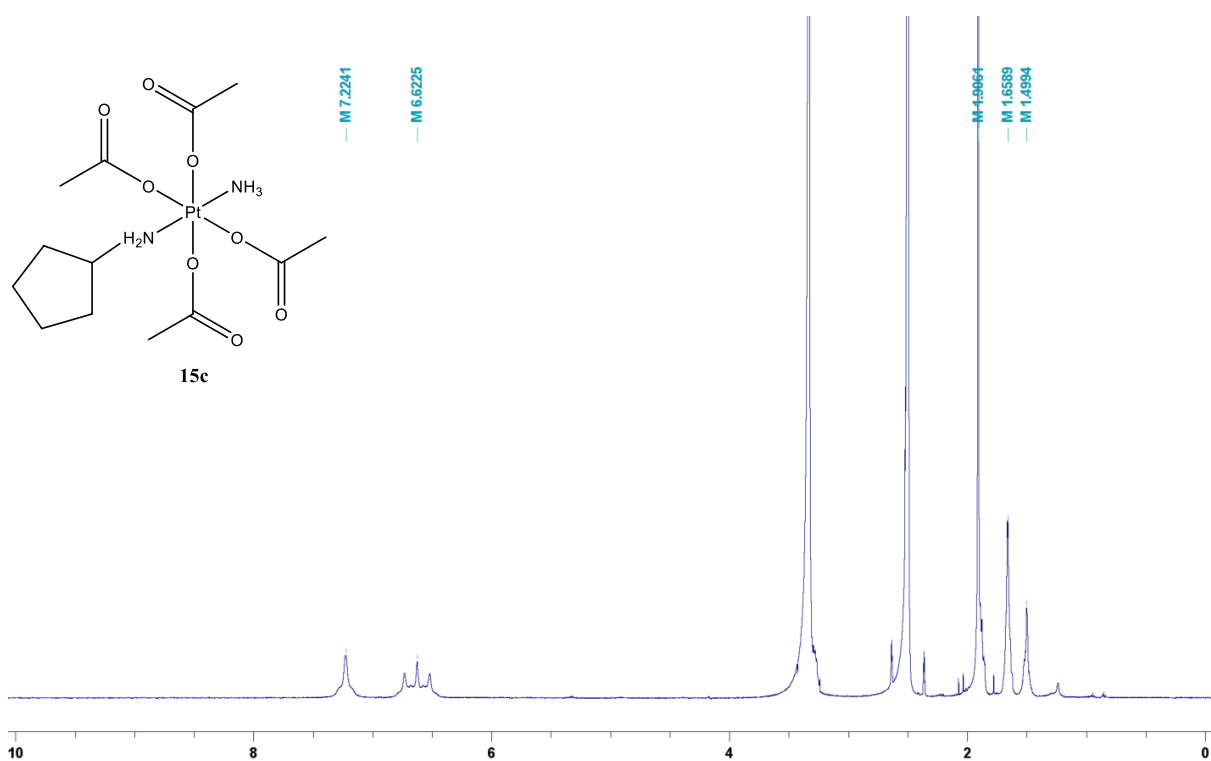


Figure S98. ^1H NMR spectrum of **15c** in d_6 -DMSO.

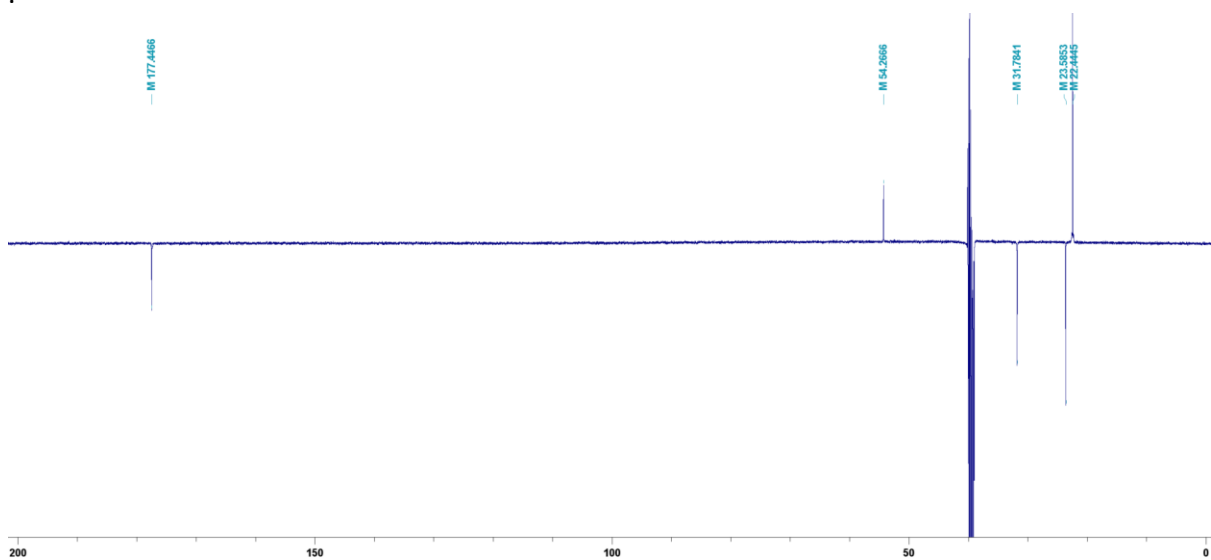


Figure S99. ^{13}C NMR spectrum of **15c** in d_6 -DMSO.

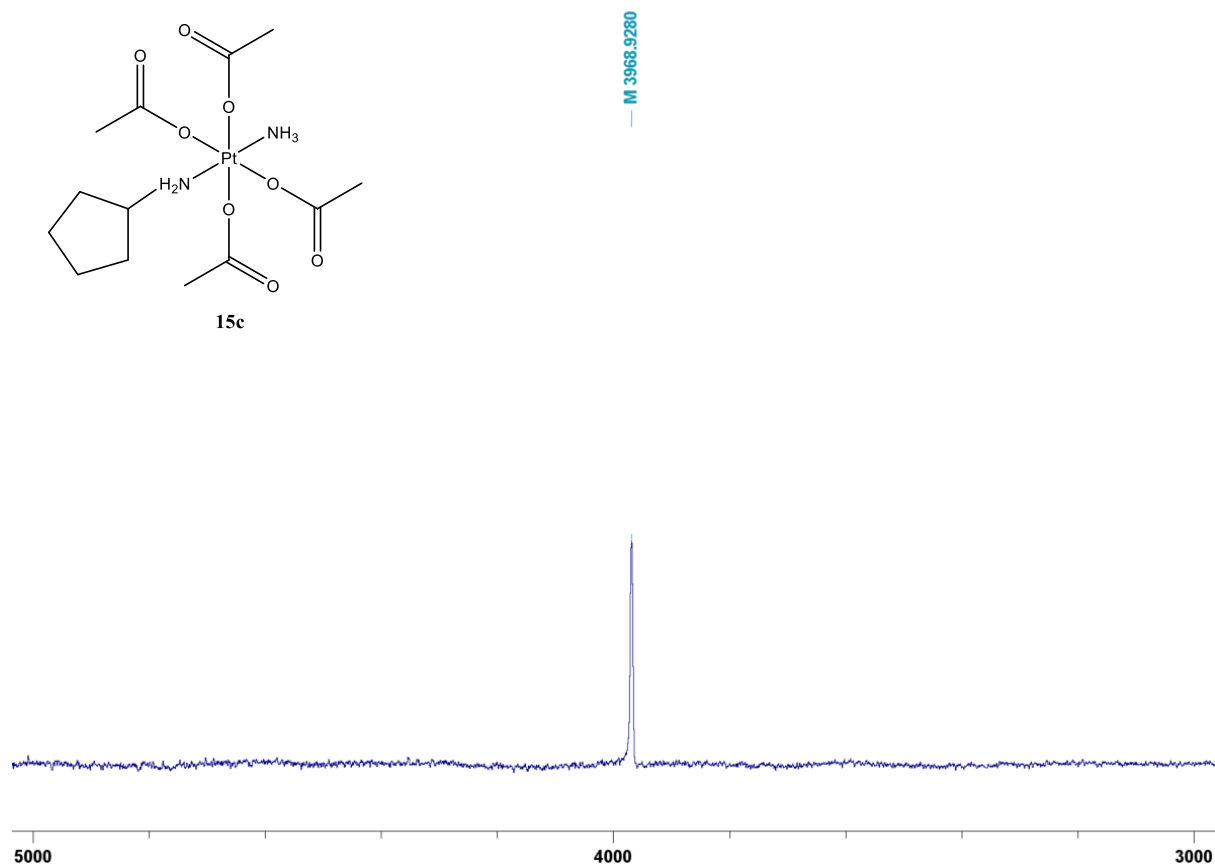


Figure S100. ¹⁹⁵Pt NMR spectrum of **15c** in d₆-DMSO.

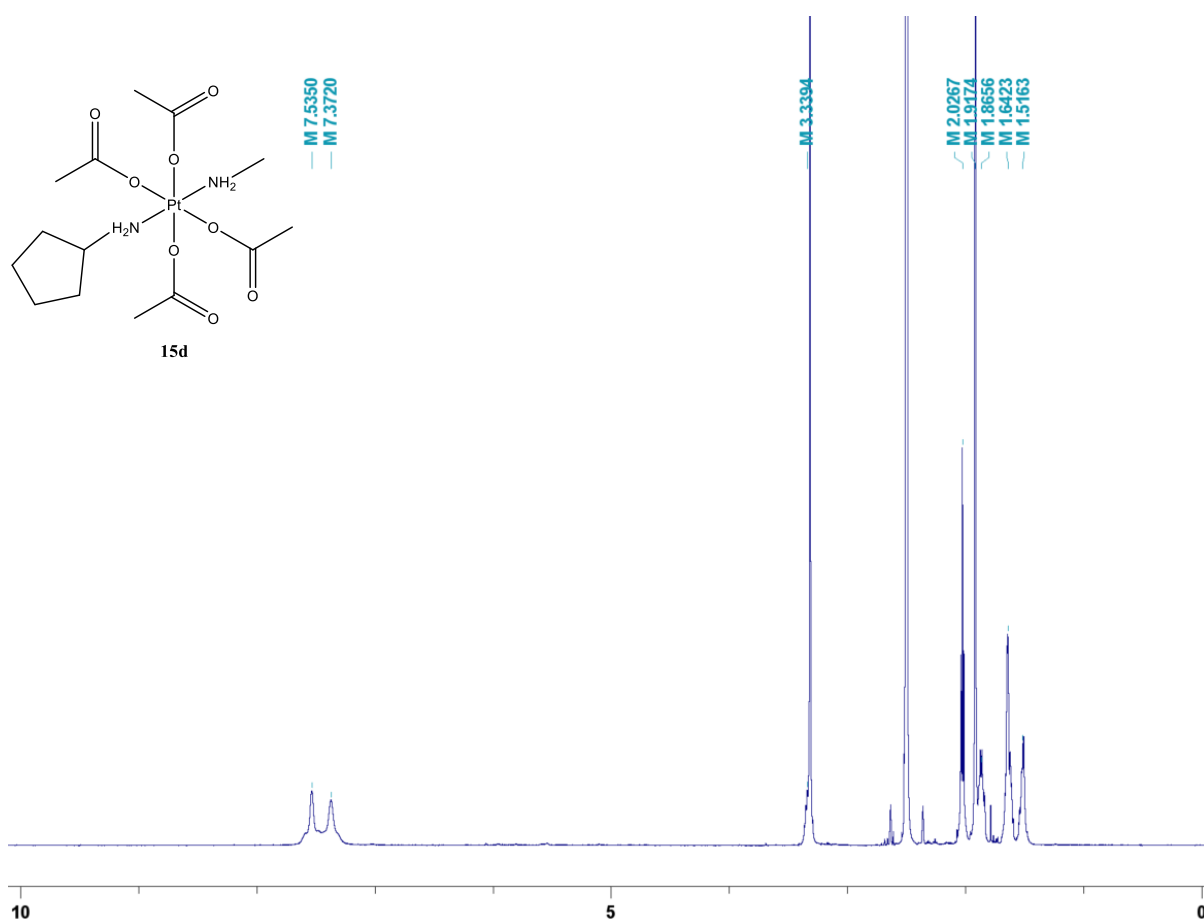


Figure S101. ¹H NMR spectrum of **15d** in d₆-DMSO.

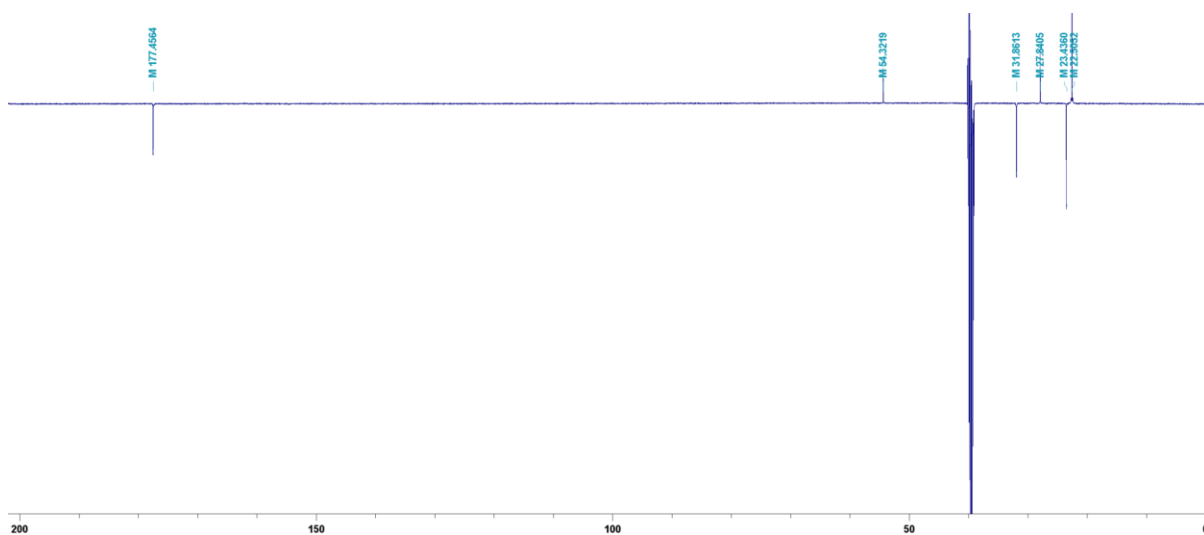


Figure S102. ¹³C NMR spectrum of **15d** in d₆-DMSO.

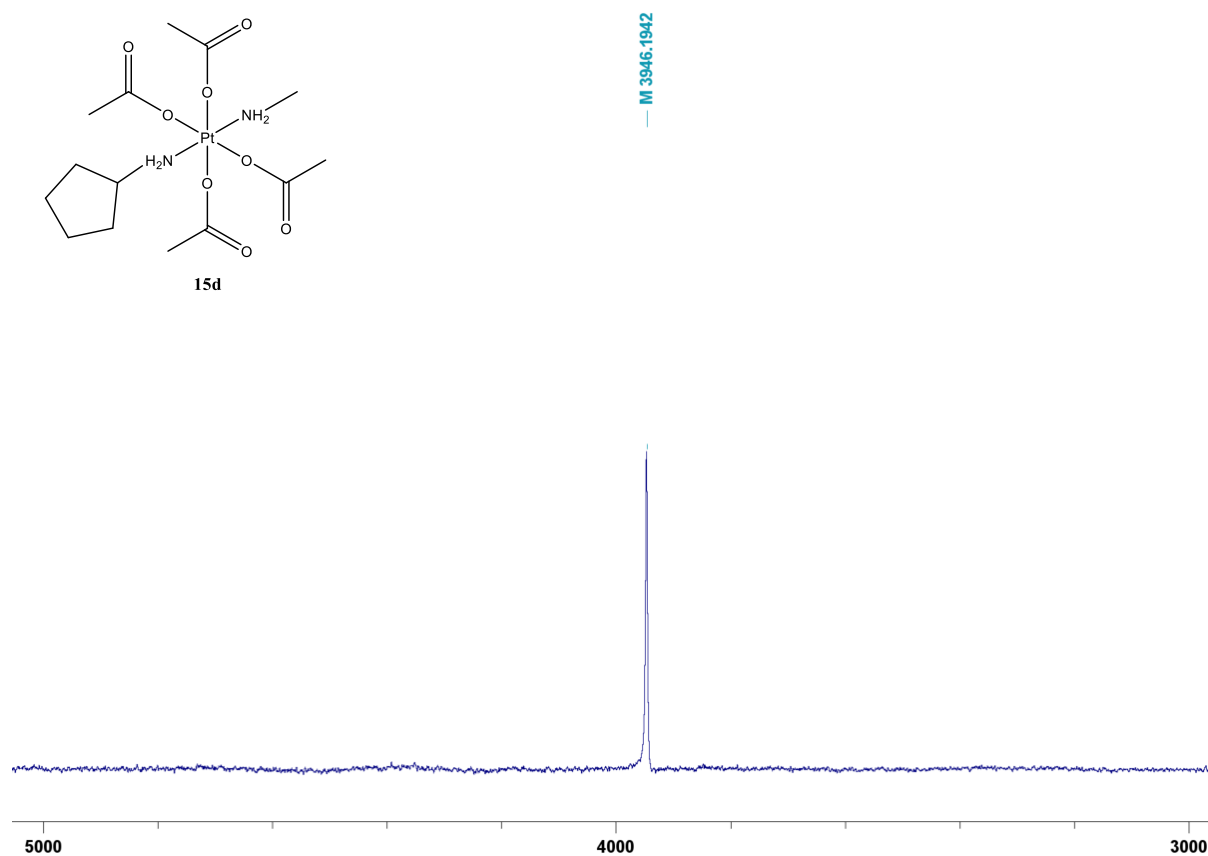


Figure S103. ¹⁹⁵Pt NMR spectrum of **15d** in d₆-DMSO.

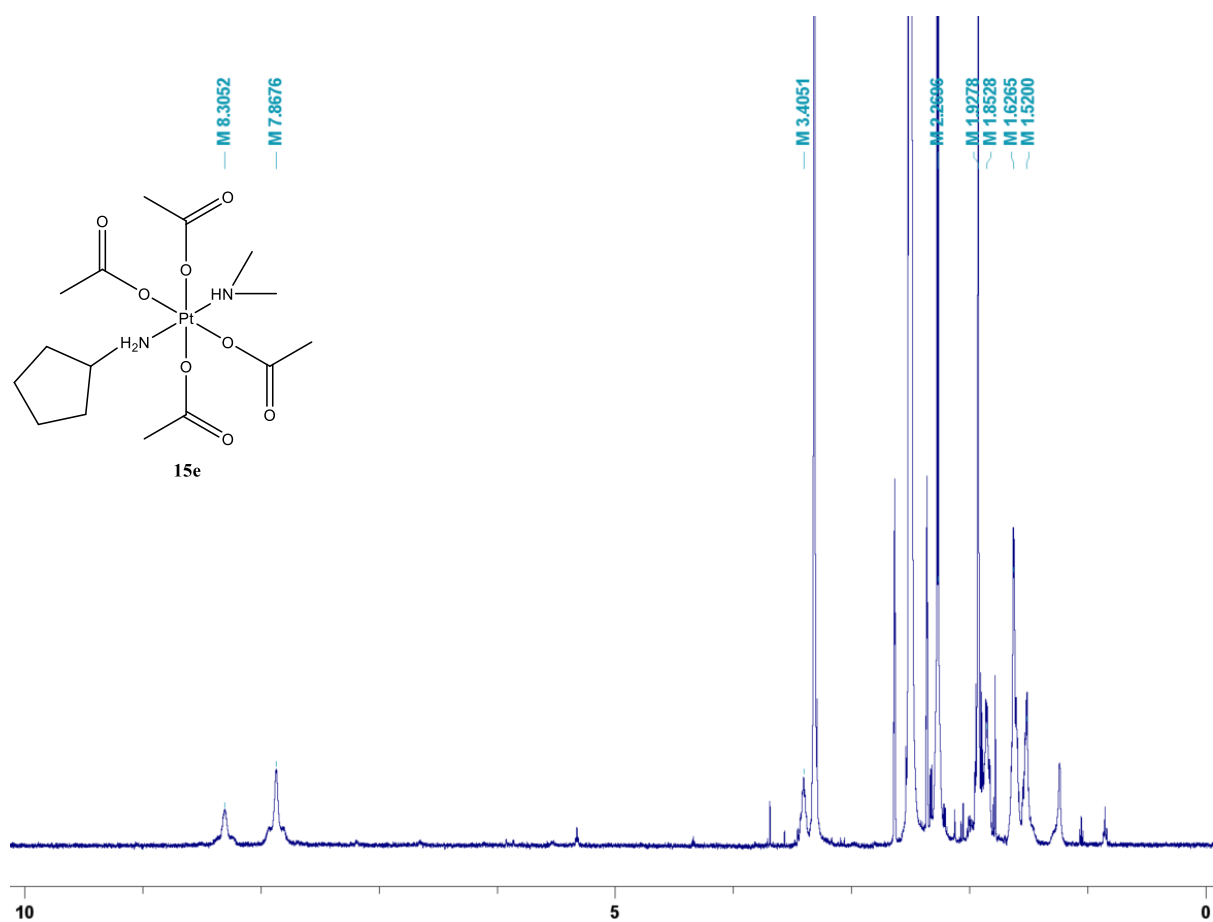


Figure S104. ¹H NMR spectrum of **15e** in d₆-DMSO.

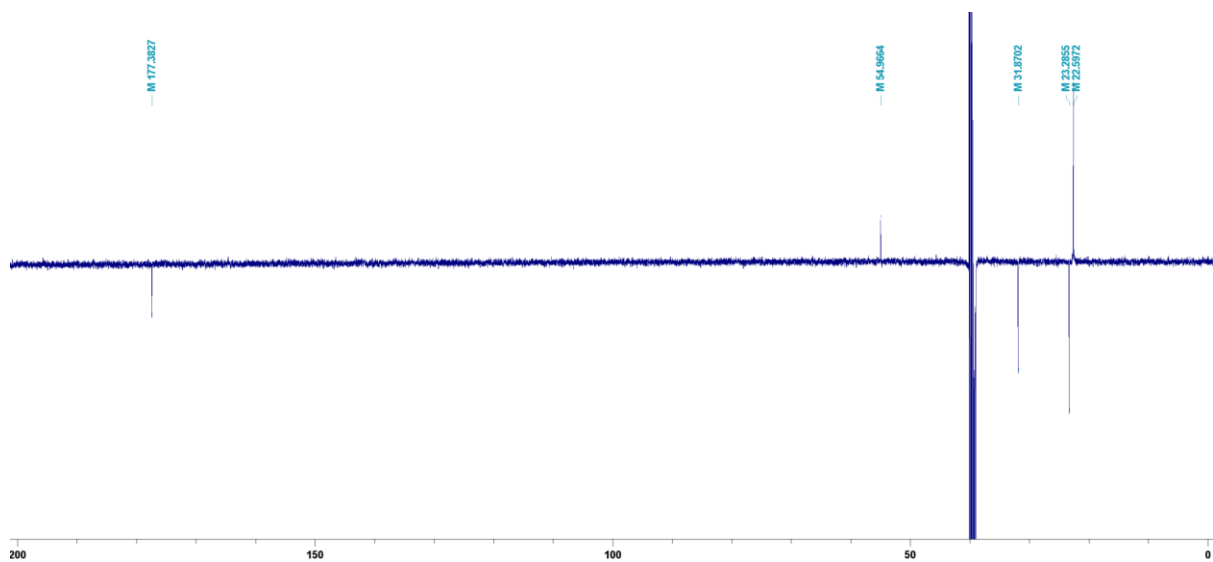


Figure S105. ¹³C NMR spectrum of **15e** in d₆-DMSO.

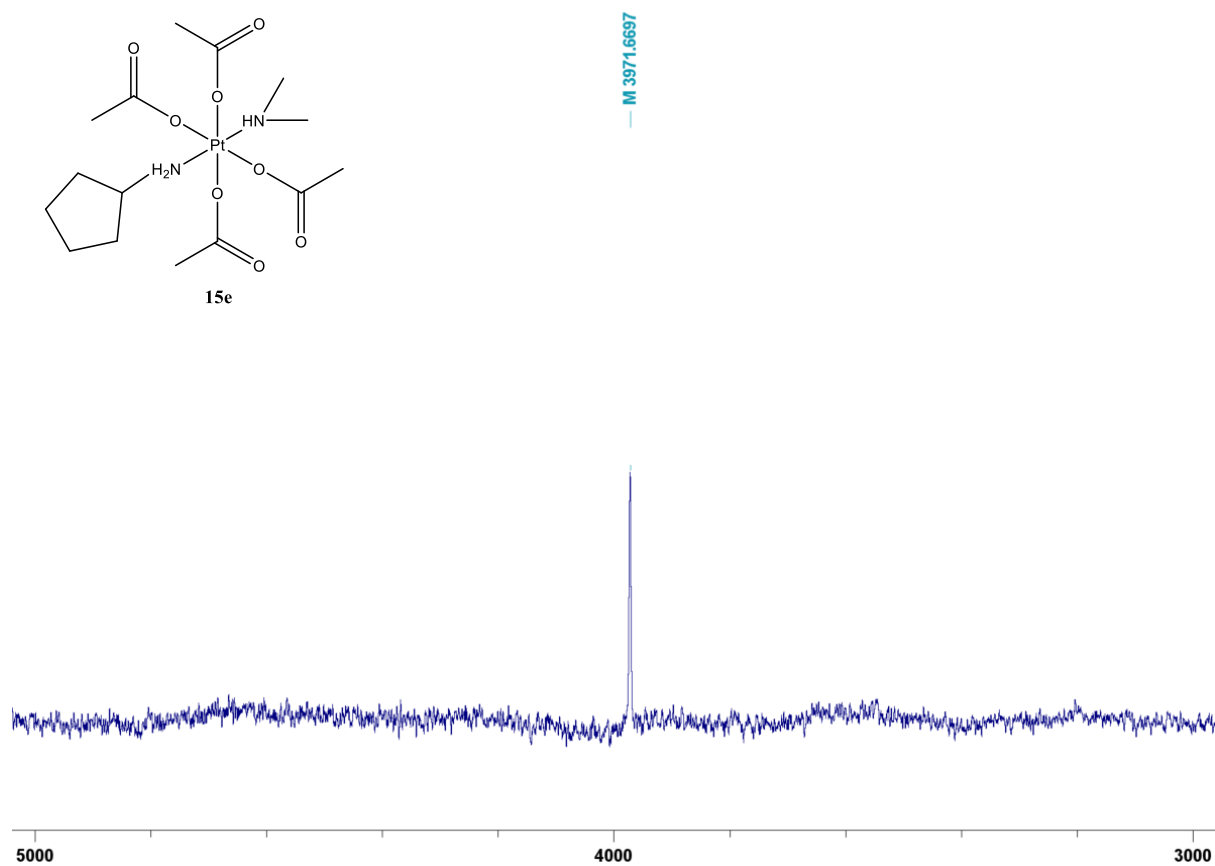


Figure S106. ^{195}Pt NMR spectrum of **15e** in d_6 -DMSO.

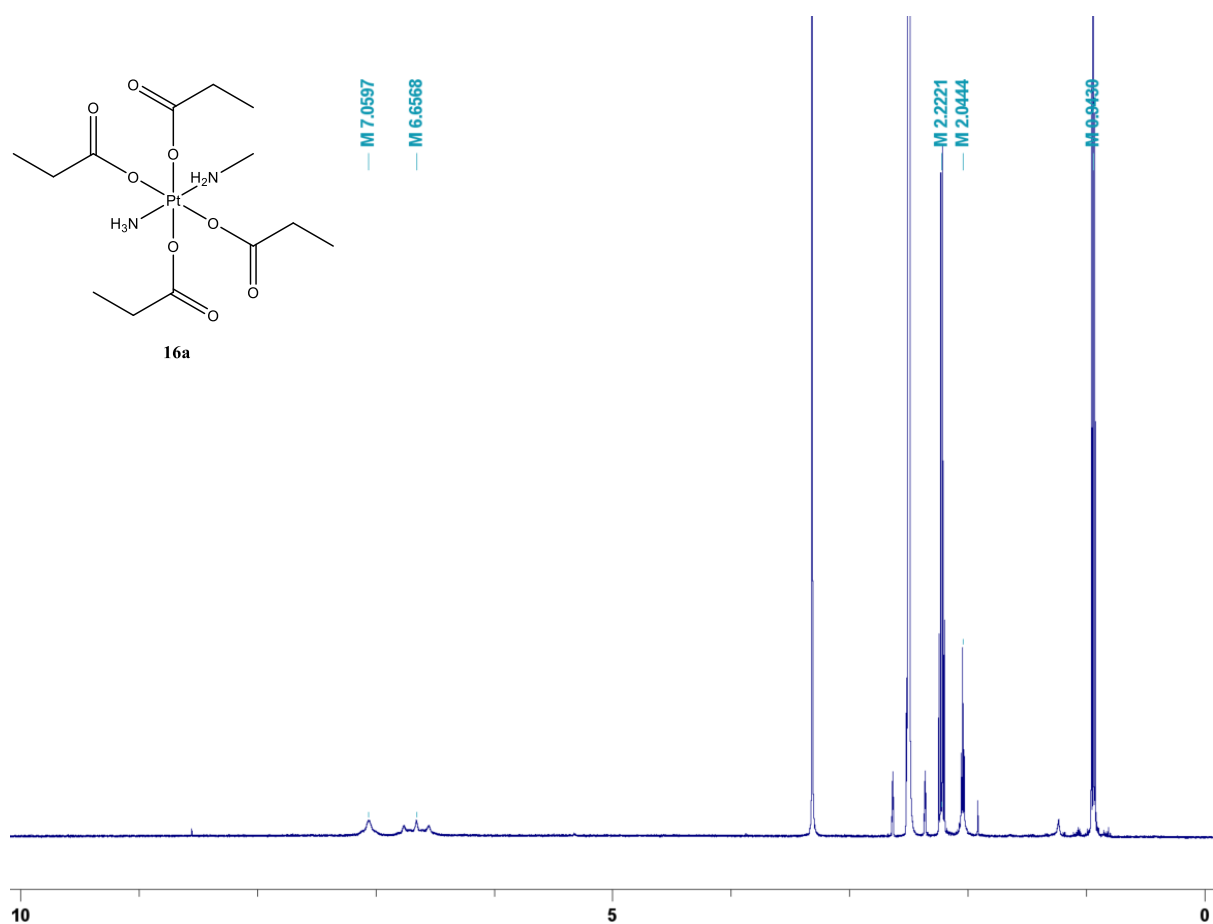


Figure S107. ¹H NMR spectrum of **16a** in d₆-DMSO.

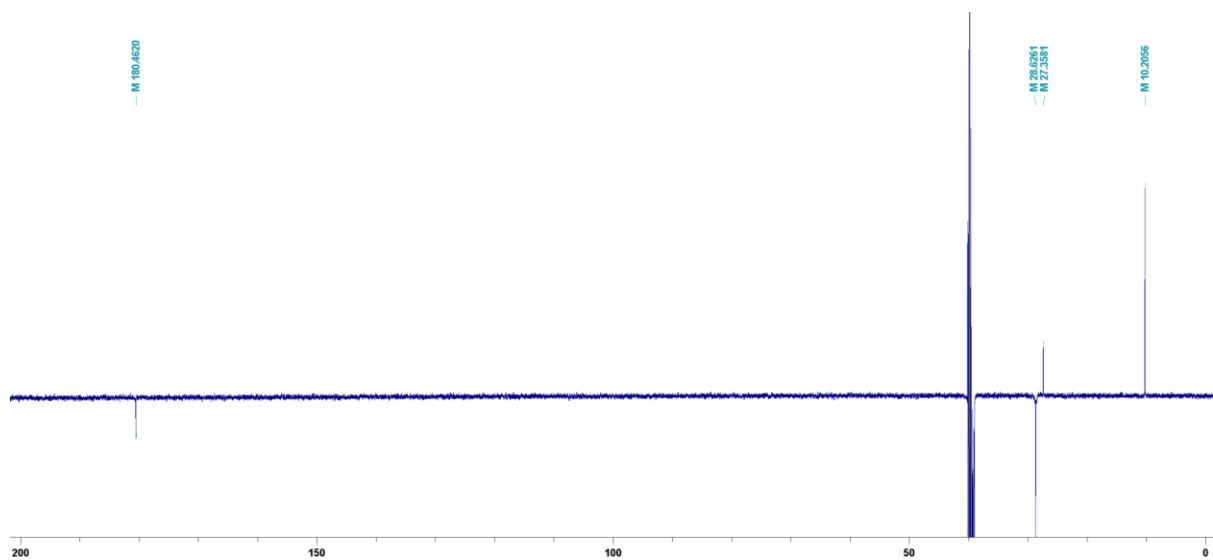


Figure S108. ¹³C NMR spectrum of **16a** in d₆-DMSO.

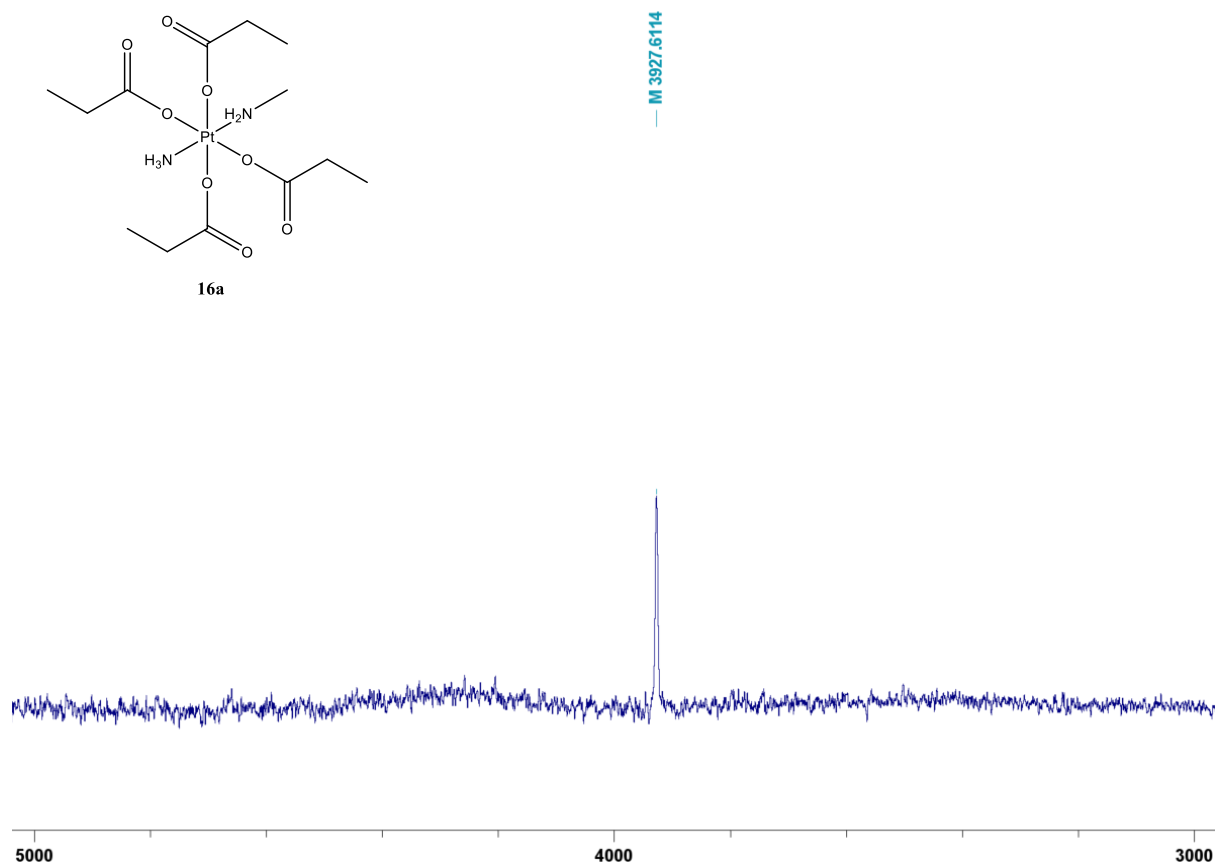


Figure S109. ^{195}Pt NMR spectrum of **16a** in d_6 -DMSO.

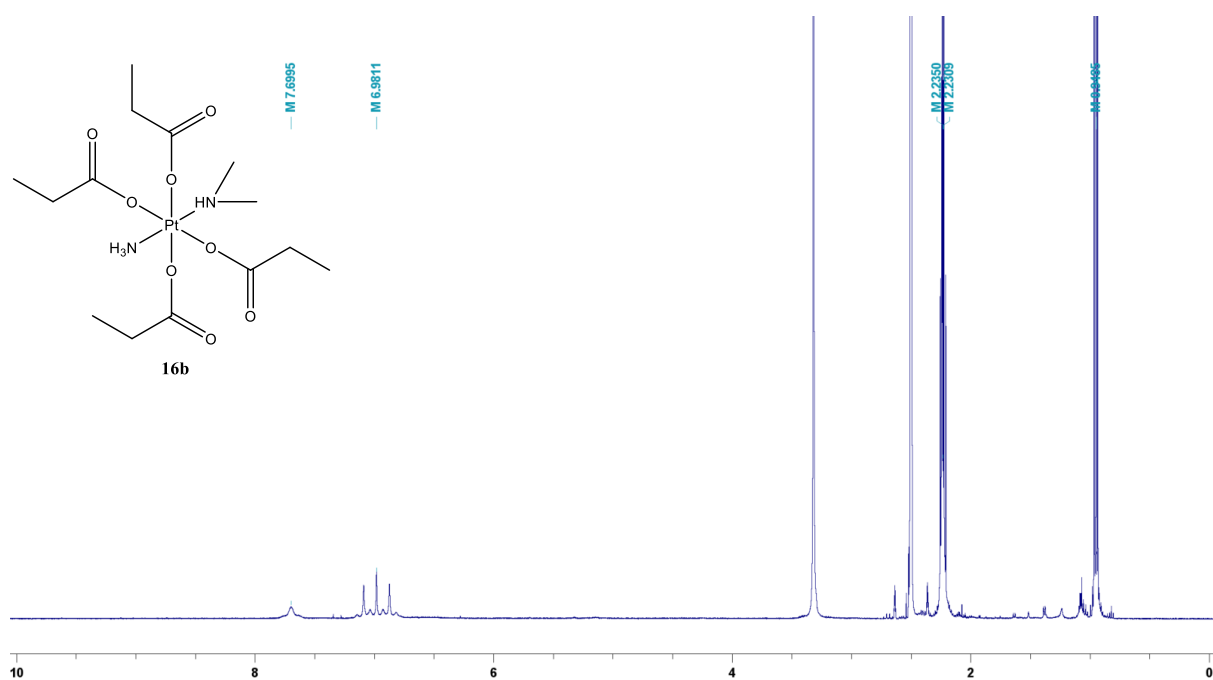


Figure S110. ^1H NMR spectrum of **16b** in d_6 -DMSO.

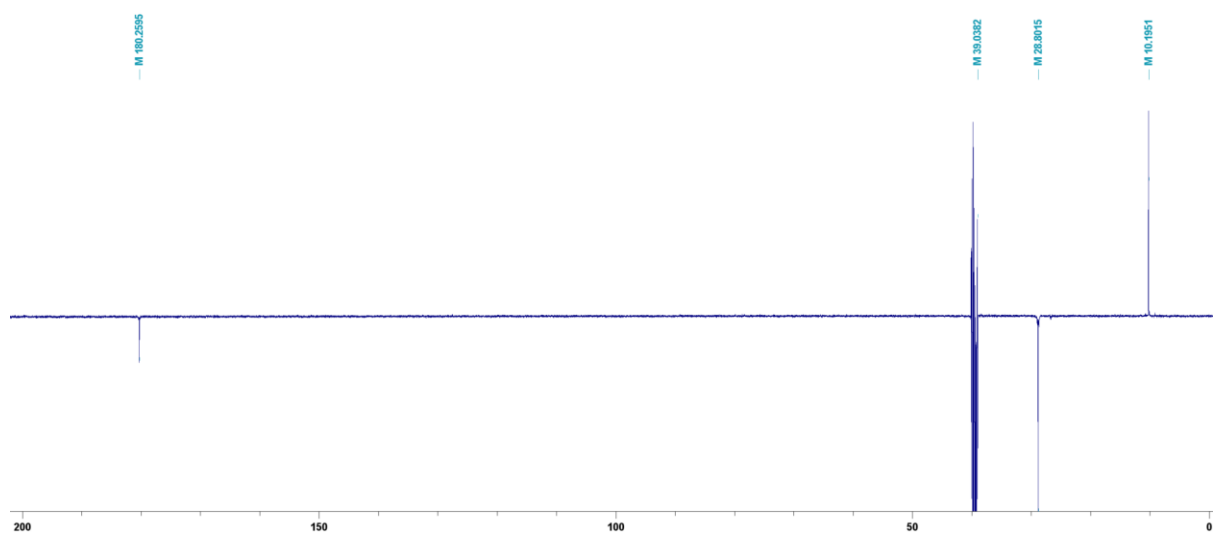


Figure S111. ^{13}C NMR spectrum of **16b** in d_6 -DMSO.

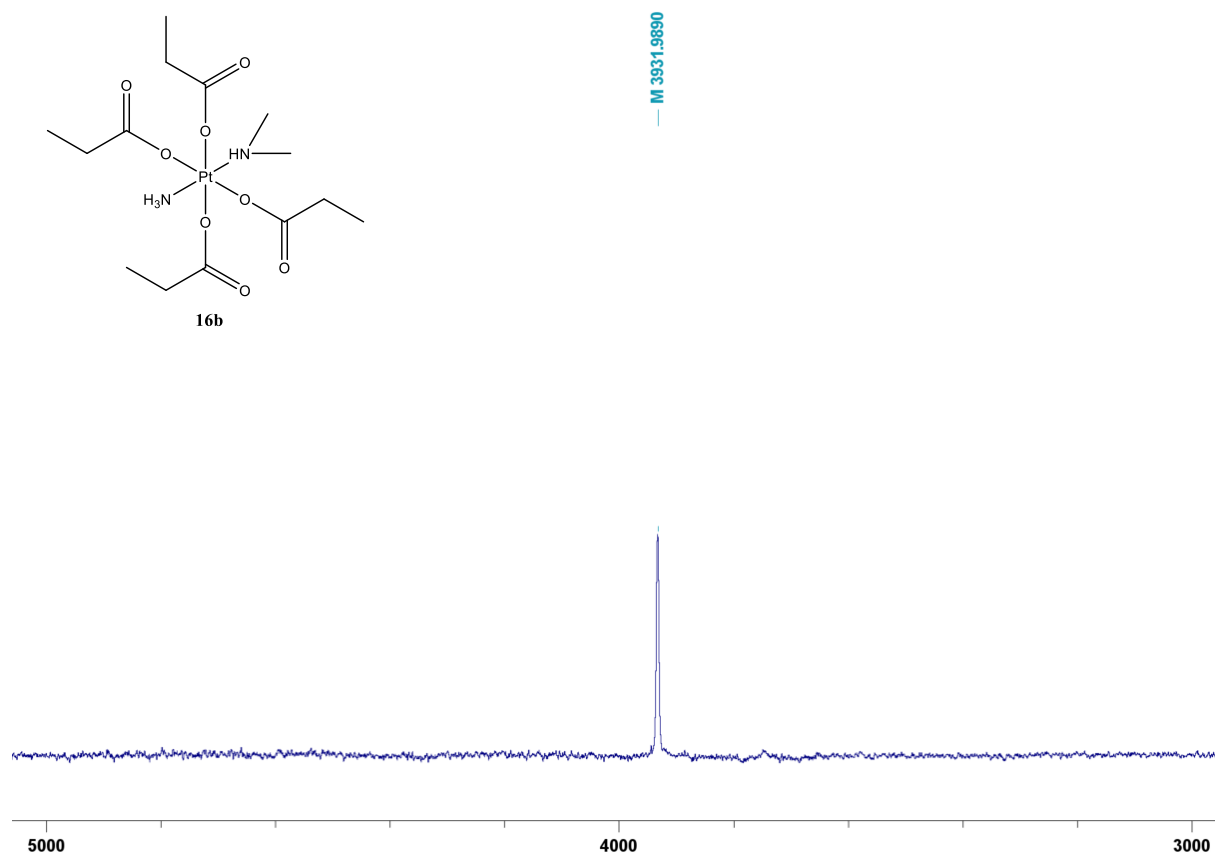


Figure S112. ¹⁹⁵Pt NMR spectrum of **16b** in d₆-DMSO.

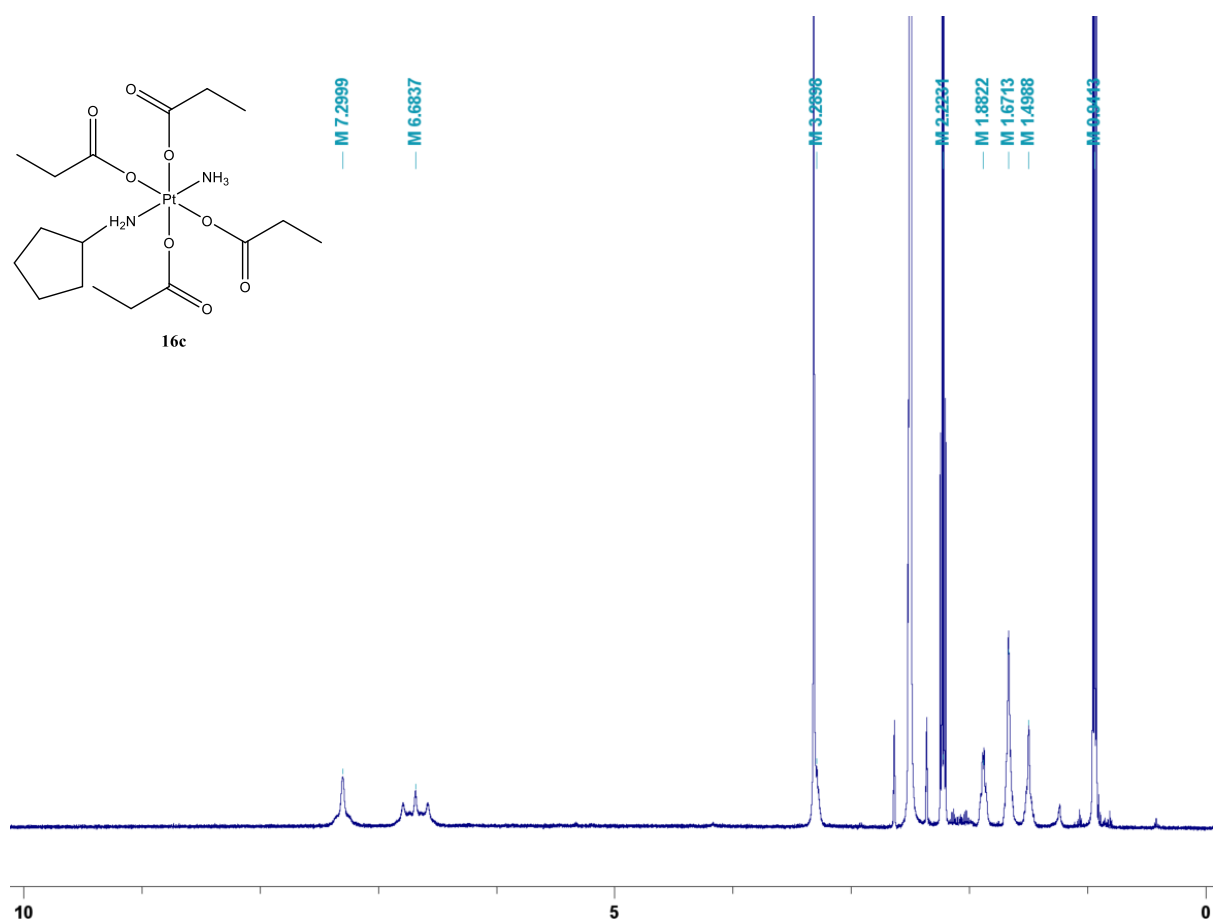


Figure S113. ^1H NMR spectrum of **16c** in $\text{d}_6\text{-DMSO}$.

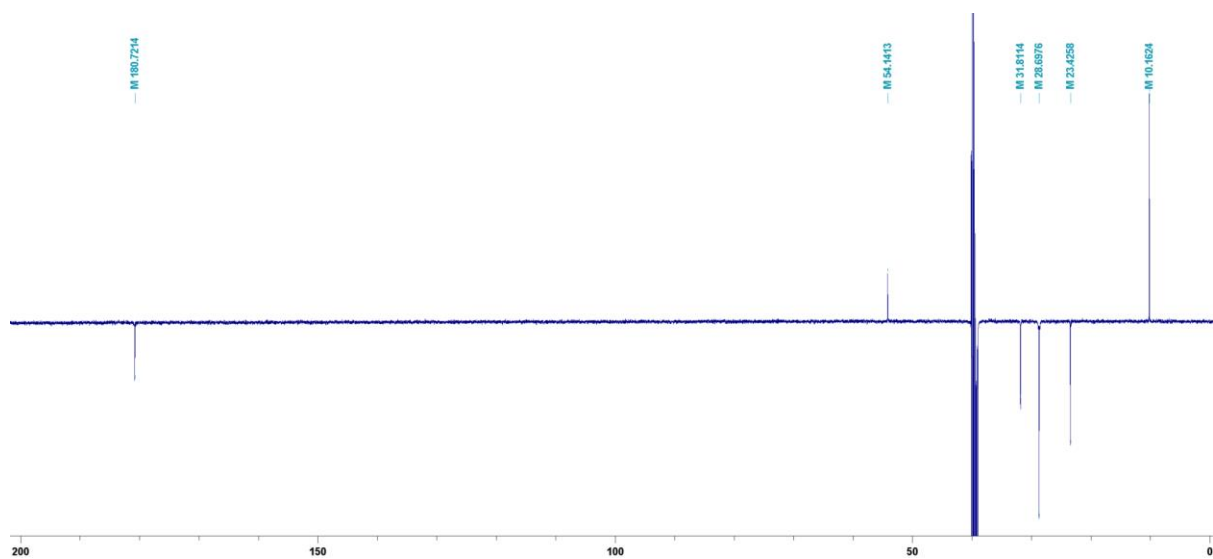


Figure S114. ^{13}C NMR spectrum of **16c** in $\text{d}_6\text{-DMSO}$.

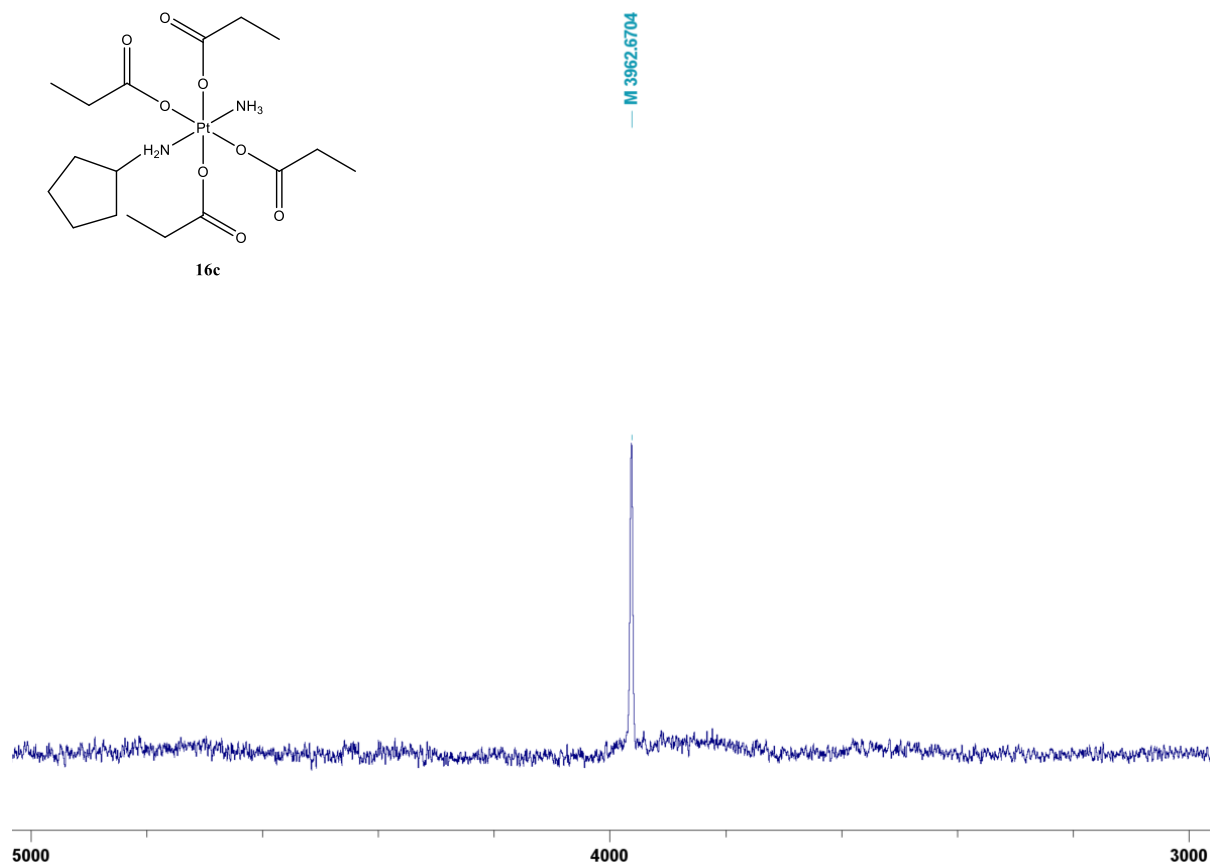


Figure S115. ^{195}Pt NMR spectrum of **16c** in d_6 -DMSO.

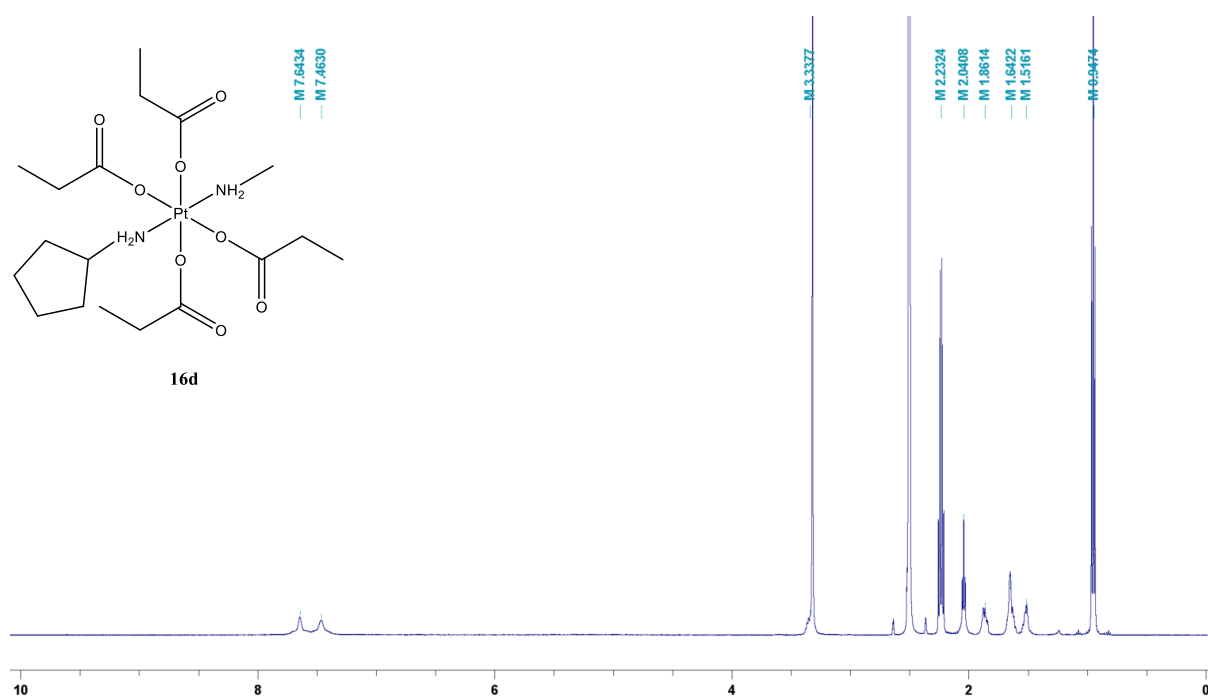


Figure S116. ^1H NMR spectrum of **16d** in d_6 -DMSO.

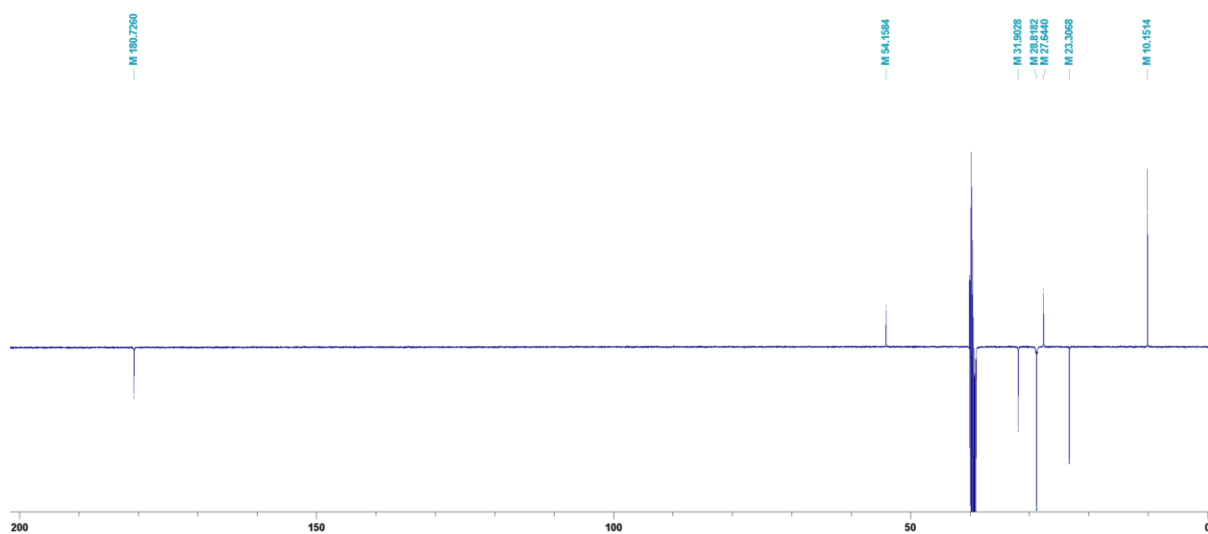


Figure S117. ^{13}C NMR spectrum of **16d** in d_6 -DMSO.

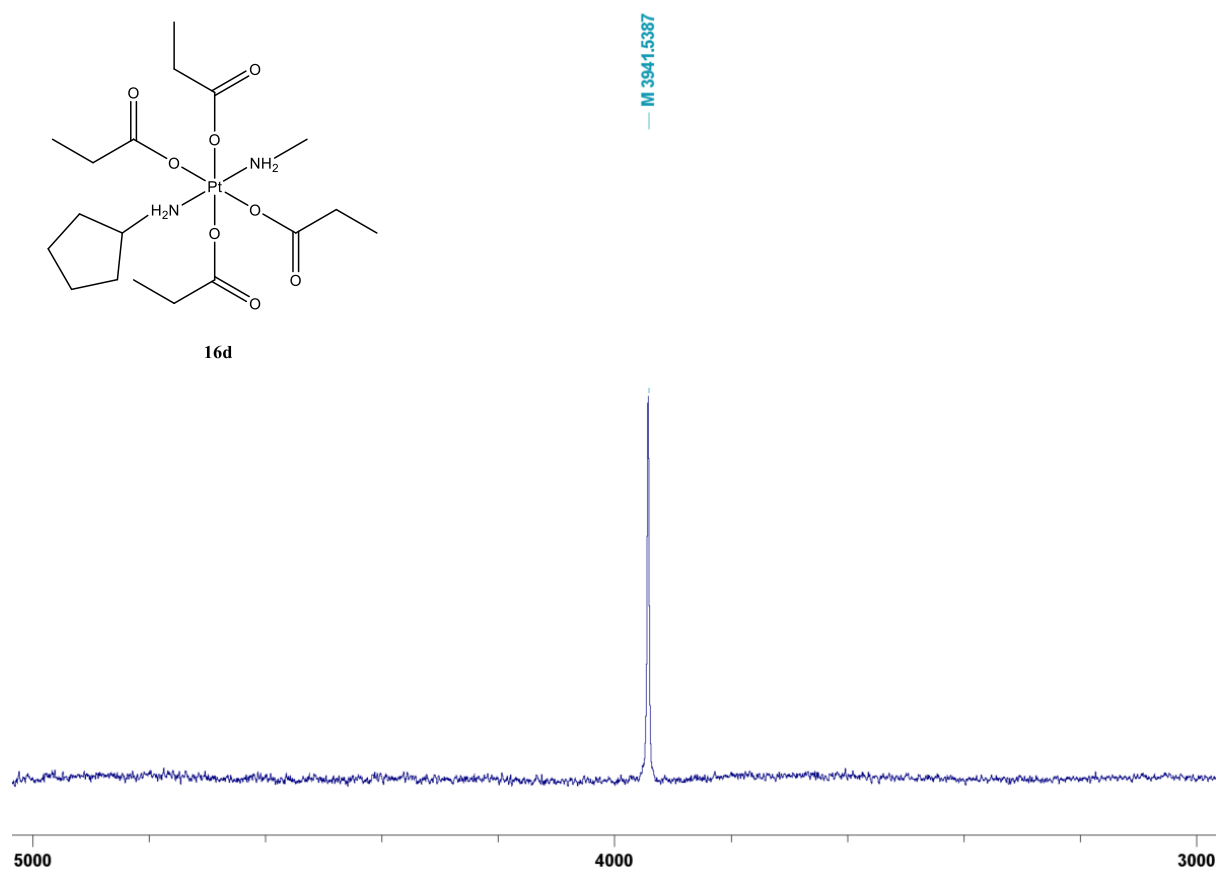


Figure S118. ^{195}Pt NMR spectrum of **16d** in $\text{d}_6\text{-DMSO}$.

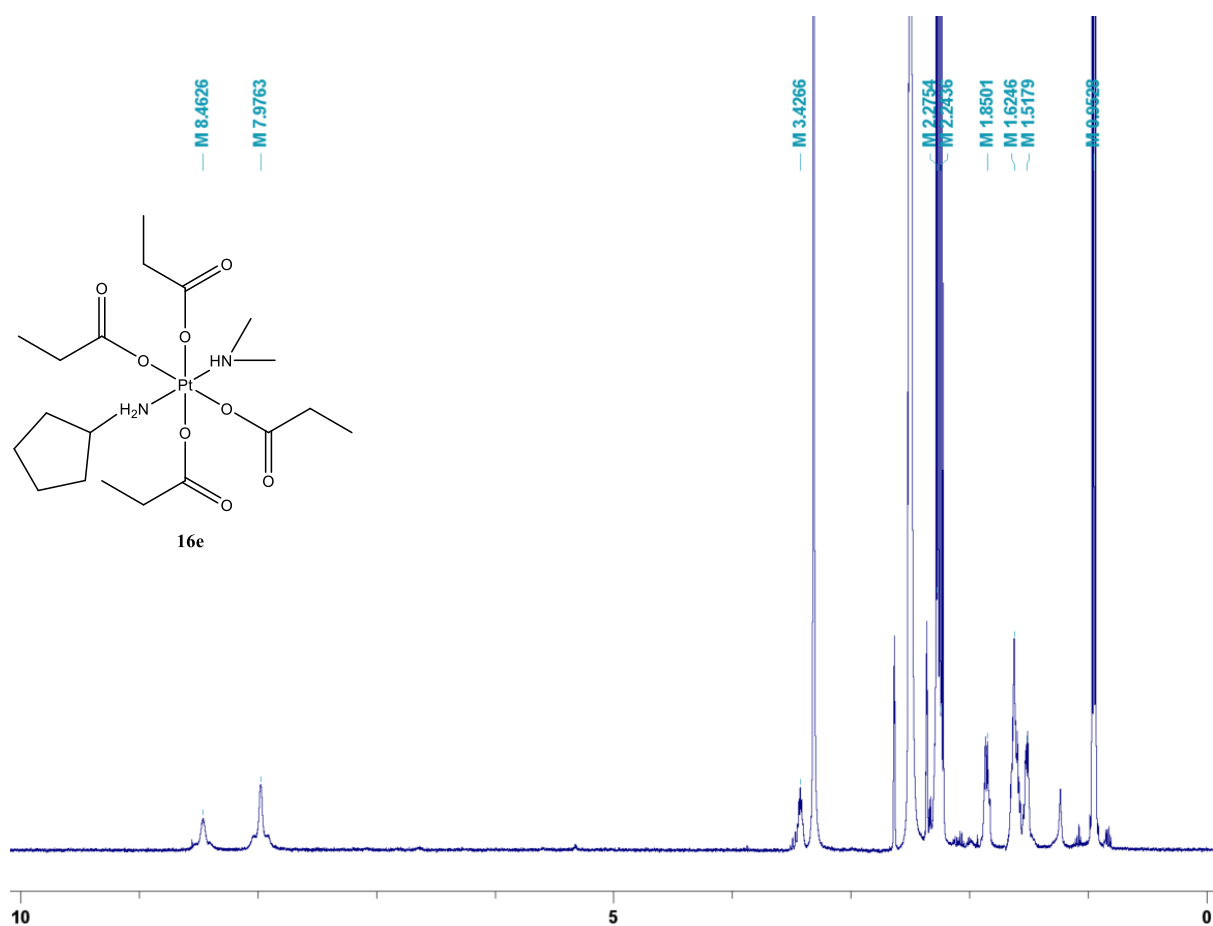


Figure S119. ¹H NMR spectrum of **16e** in d₆-DMSO.

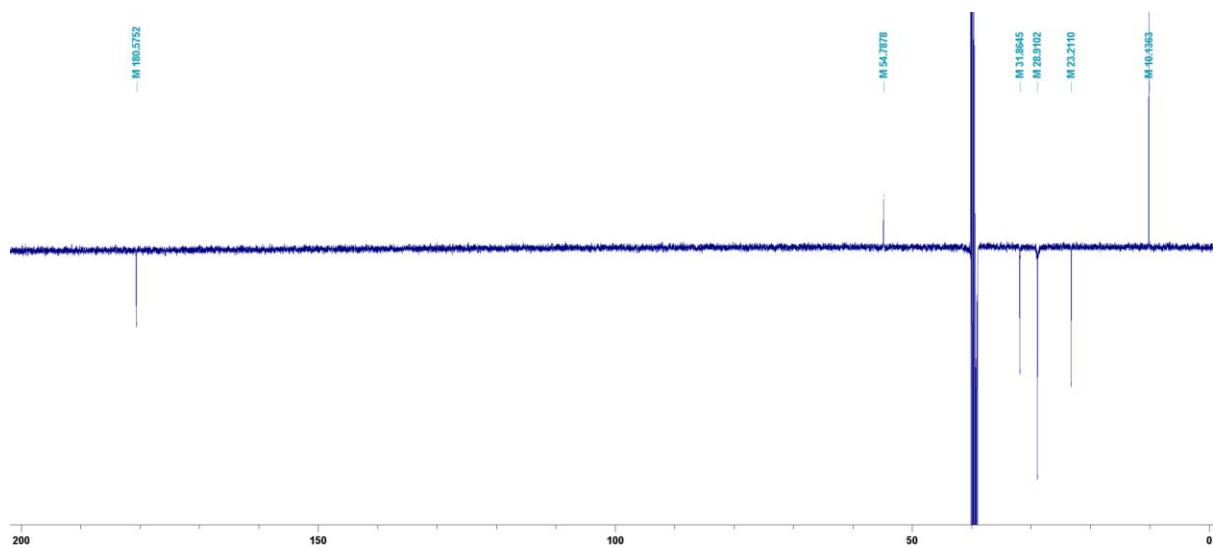


Figure S120. ¹³C NMR spectrum of **16e** in d₆-DMSO.

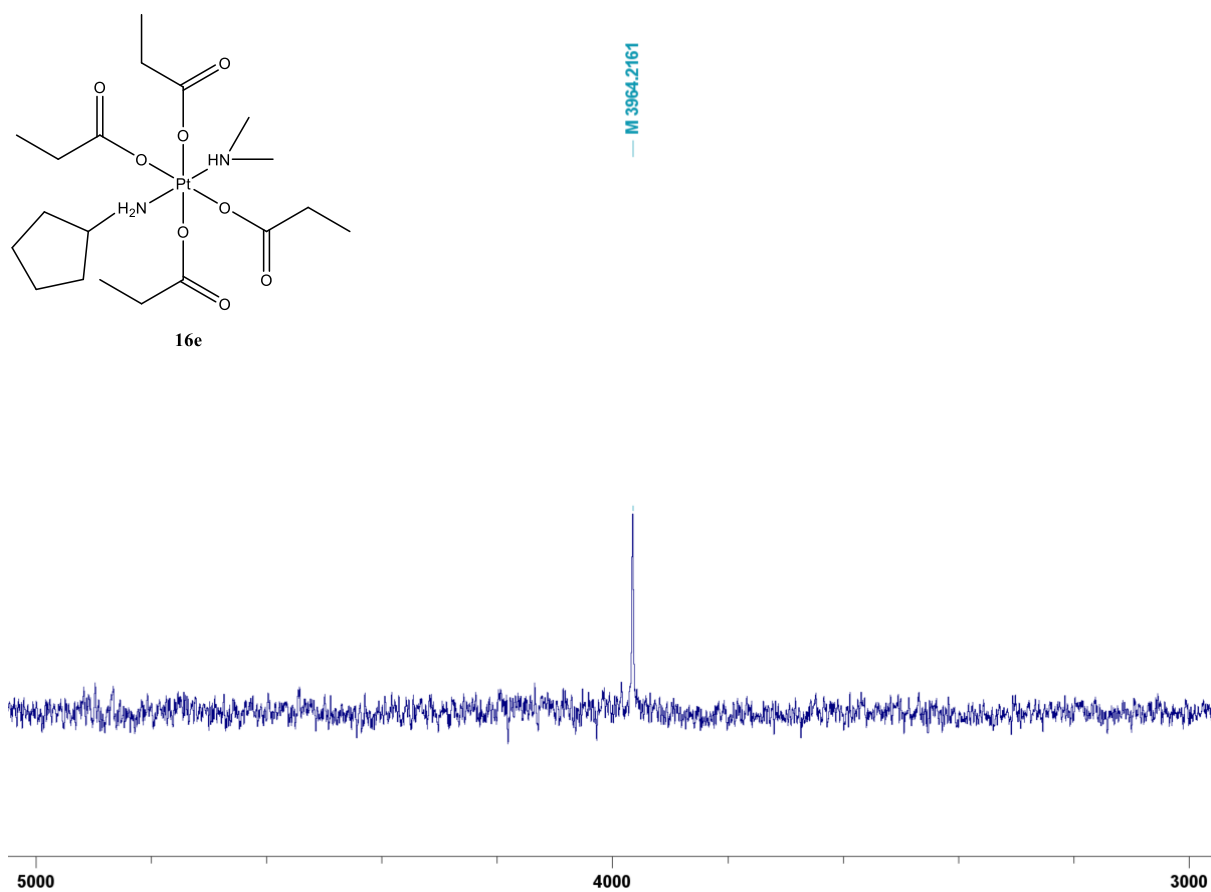


Figure S121. ^{195}Pt NMR spectrum of **16e** in d_6 -DMSO.

3. X-Ray Diffraction Analysis

X-ray intensity data was measured on Bruker D8 Venture diffractometer equipped with multilayer monochromator, Mo K/ α INCOATEC micro focus sealed tube and Oxford cooling system. The structure was solved by Direct Methods. Non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were inserted at calculated positions and refined with riding model. The following software was used: Bruker SAINT software package [1] using a narrow-frame algorithm for frame integration, SADABS [2] for absorption correction, OLEX2 [3] for structure solution, refinement, molecular diagrams and graphical user-interface, ShelXle [4] for refinement and graphical userinterface SHELXS-2015 [5] for structure solution, SHELXL-2015 [6] for refinement, Platon [7] for symmetry check. Crystallographic data have been deposited with the Cambridge Crystallographic Data Center with No. CSD 2252956 (**2a**), 2252957 (**2c**), 2252958 (**1e**), 2252959 (**12e**), 2252960 (**1d**), 2252961 (**2e**), 2252962 (**1a**), 2252963 (**13c**) and 2252964 (**15e**). Copies of data can be obtained free of charge (available online: <https://www.ccdc.cam.ac.uk/structures/>).

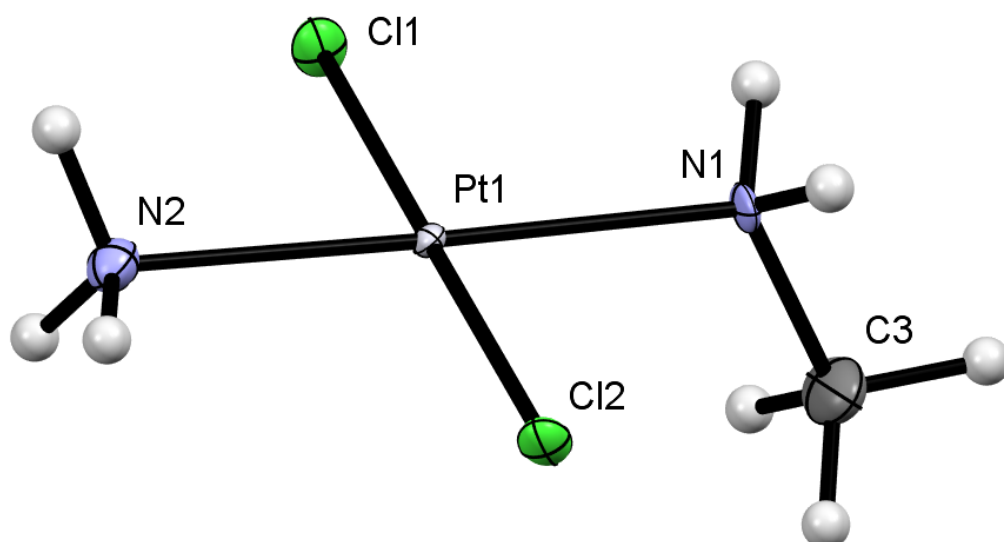


Figure S122. ORTEP view of complex **1a** drawn with 50% displacement ellipsoids.

Table S1. Overview of the sample and crystal data, data collection and structure refinement of complex **1a**.

Identification code	kryv770_a
Empirical formula	CH ₈ Cl ₂ N ₂ Pt
Formula weight	314.08
Temperature	100 K
Wavelength	1.54186 Å
Crystal system	Monoclinic
Space group	P 1 2 ₁ /c 1
Unit cell dimensions	a = 5.6990(11) Å b = 5.9525(12) Å c = 18.890(4) Å $\alpha = 90^\circ$ $\beta = 96.19(3)^\circ$ $\gamma = 90^\circ$
Volume	637.09(11) Å ³
Z	4
Density (calculated)	3.275 Mg/m ³
Absorption coefficient	47.919 mm ⁻¹
F(000)	560
Crystal size	0.090 x 0.070 x 0.060 mm ³
Theta range for data collection	4.709 to 68.070°
Index ranges	-6 ≤ h ≤ 6, -7 ≤ k ≤ 6, -8 ≤ l ≤ 22
Reflections collected	9699
Independent reflections	1147 [R(int) = 0.0300]
Completeness to theta = 67.679°	99.2%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.4959 and 0.3492
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1147 / 0 / 55
Goodness-of-fit on F ²	1.265
Final R indices [I>2sigma(I)]	R ₁ = 0.0260, wR ₂ = 0.0667
R indices (all data)	R ₁ = 0.0263, wR ₂ = 0.0669
Extinction coefficient	n/a
Largest diff. peak and hole	1.176 and -2.454 e·Å ⁻³

Table S2. Overview of bond lengths of complex **1a**.

Atoms	Length [Å]	Atoms	Length [Å]
Pt(1)-Cl(1)	2.2913(16)	C(3)-H(3A)	0.98
Pt(1)-Cl(2)	2.2975(15)	C(3)-H(3B)	0.98
Pt(1)-N(1)	2.046(5)	C(3)-H(3C)	0.98
Pt(1)-N(2)	2.038(6)	N(2)-H(2A)	0.91
N(1)-H(1A)	0.91	N(2)-H(2B)	0.91
N(1)-H(1B)	0.91	N(2)-H(2C)	0.91
N(1)-C(3)	1.476(9)		

Table S3. Overview of angles of complex **1a**.

Atoms	Angle [°]	Atoms	Angle [°]
Cl(1)-Pt(1)-Cl(2)	178.24(5)	N(1)-C(3)-H(3A)	109.5
N(1)-Pt(1)-Cl(1)	89.38(17)	N(1)-C(3)-H(3B)	109.5
N(1)-Pt(1)-Cl(2)	89.56(17)	N(1)-C(3)-H(3C)	109.5
N(2)-Pt(1)-Cl(1)	89.83(17)	H(3A)-C(3)-H(3B)	109.5
N(2)-Pt(1)-Cl(2)	91.25(17)	H(3A)-C(3)-H(3C)	109.5
N(2)-Pt(1)-N(1)	178.7(2)	H(3B)-C(3)-H(3C)	109.5
Pt(1)-N(1)-H(1A)	108.3	Pt(1)-N(2)-H(2A)	109.5
Pt(1)-N(1)-H(1B)	108.3	Pt(1)-N(2)-H(2B)	109.5
H(1A)-N(1)-H(1B)	107.4	Pt(1)-N(2)-H(2C)	109.5
C(3)-N(1)-Pt(1)	115.8(4)	H(2A)-N(2)-H(2B)	109.5
C(3)-N(1)-H(1A)	108.3	H(2A)-N(2)-H(2C)	109.5
C(3)-N(1)-H(1B)	108.3	H(2B)-N(2)-H(2C)	109.5

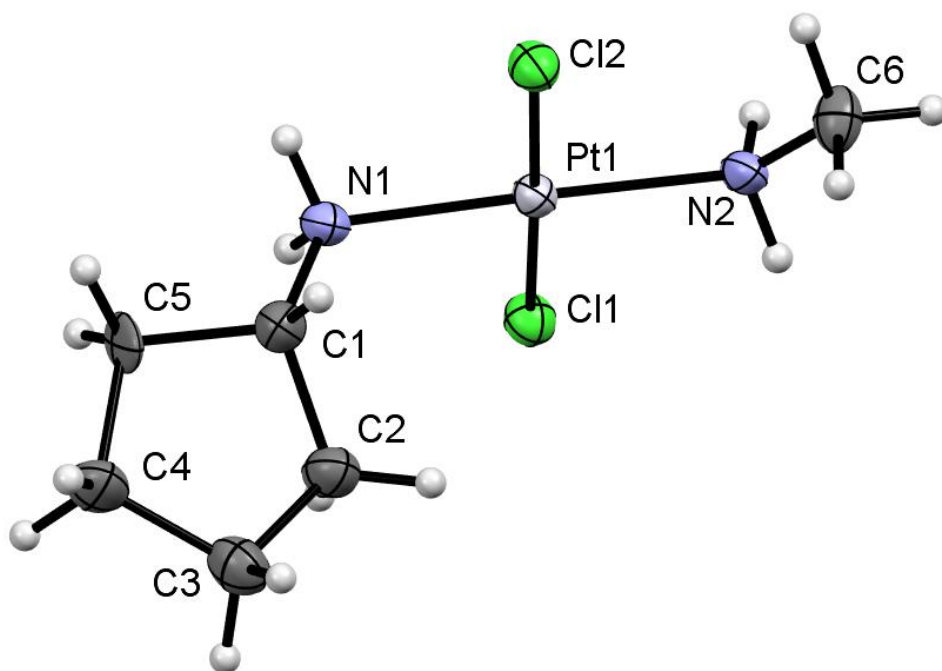


Figure S123. ORTEP view of complex **1d** drawn with 50% displacement ellipsoids.

Table S4. Overview of the sample and crystal data, data collection and structure refinement of complex **1d**.

Identification code	KRYV682_a
Empirical formula	C ₆ H ₁₆ Cl ₂ N ₂ Pt
Formula weight	382.19
Temperature	100 K
Wavelength	1.54186 Å
Crystal system	Monoclinic
Space group	P2 ₁ /n
Unit cell dimensions	a = 11.6303(5) Å b = 6.2055(3) Å c = 14.8908(7) Å α = 90° β = 104.791(4)° γ = 90°
Volume	1039.09(8) Å ³
Z	4
Density (calculated)	2.443 Mg/m ³
Absorption coefficient	29.555 mm ⁻¹
F(000)	712
Crystal size	0.160 x 0.028 x 0.015 mm ³
Theta range for data collection	4.327 to 69.989°
Index ranges	-12 ≤ h ≤ 14, -7 ≤ k ≤ 6, -11 ≤ l ≤ 18
Reflections collected	10602
Independent reflections	1949 [R(int) = 0.0596]
Completeness to theta = 67.679°	99.6%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.1923 and 0.1104
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1949 / 0 / 101
Goodness-of-fit on F ²	1.040
Final R indices [I>2σ(I)]	R ₁ = 0.0665, wR ₂ = 0.1770
R indices (all data)	R ₁ = 0.0685, wR ₂ = 0.1797
Extinction coefficient	n/a
Largest diff. peak and hole	6.419 and -3.428 e·Å ⁻³

Table S5. Overview of bond lengths of complex **1d**.

Atoms	Length [Å]	Atoms	Length [Å]
Pt1-N1	2.044(8)	C1-C2	1.510(15)
Pt1-N2	2.046(8)	C1-C5	1.518(14)
Pt1-Cl1	2.295(2)	C2-C3	1.544(16)
Pt1-Cl2	2.299(2)	C3-C4	1.550(18)
N1-C1	1.467(14)	C4-C5	1.519(15)
N2-C6	1.474(13)		

Table S6. Overview of angles of complex **1d**.

Atoms	Angle [°]	Atoms	Angle [°]
N1-Pt1-N2	177.5(3)	N1-C1-C2	113.7(10)
N1-Pt1-Cl1	90.5(3)	N1-C1-C5	114.5(9)
N2-Pt1-Cl1	87.0(3)	C2-C1-C5	104.0(9)
N1-Pt1-Cl2	88.4(3)	C1-C2-C3	103.9(10)
N2-Pt1-Cl2	94.1(3)	C2-C3-C4	104.9(10)
Cl1-Pt1-Cl2	177.95(8)	C5-C4-C3	106.2(9)
C1-N1-Pt1	117.0(7)	C1-C5-C4	106.5(10)
C6-N2-Pt1	122.0(7)		

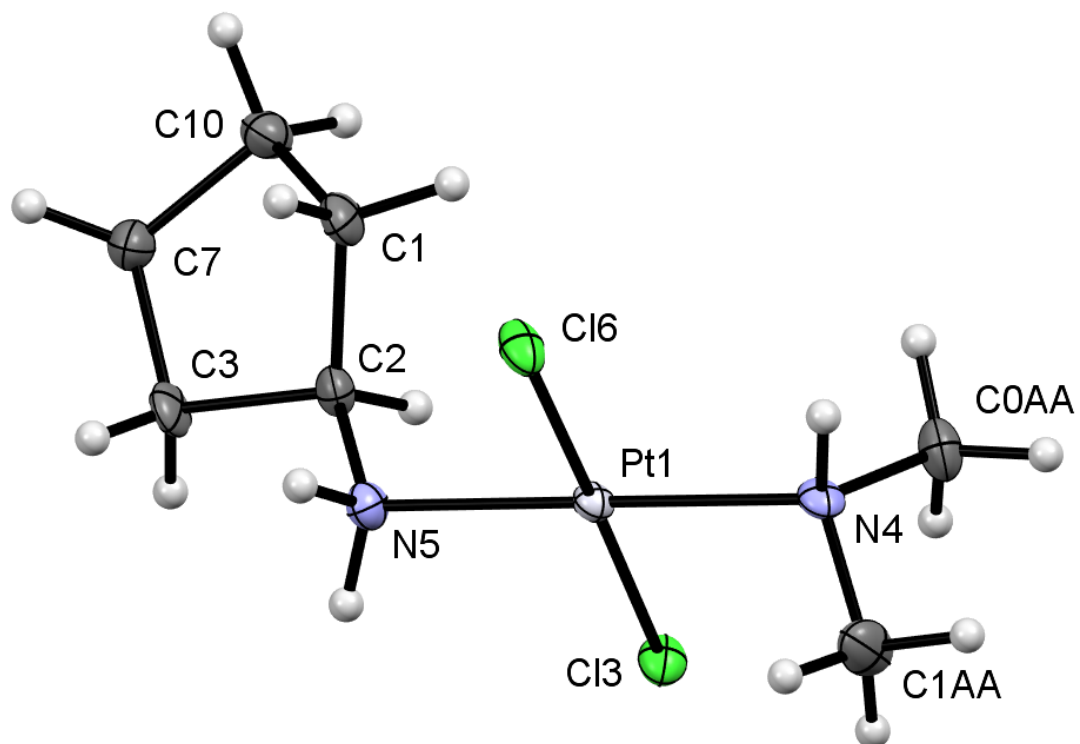


Figure S124. ORTEP view of complex **1e** drawn with 50% displacement ellipsoids.

Table S7. Overview of the sample and crystal data, data collection and structure refinement of complex **1e**.

Identification code	mo_kryv483_p21
Empirical formula	C ₇ H ₁₈ Cl ₂ N ₂ Pt
Formula weight	396.22
Temperature	100 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 1 2 ₁ 1
Unit cell dimensions	a = 9.5407(9) Å b = 6.2601(6) Å c = 9.6833(9) Å α = 90° β = 90.942(4)° γ = 90°
Volume	578.26(9) Å ³
Z	2
Density (calculated)	2.276 Mg/ m ³
Absorption coefficient	12.550 mm ⁻¹
F(000)	372
Crystal size	0.061 x 0.032 x 0.009 mm ³
Theta range for data collection	2.103 to 30.072°
Index ranges	-13 ≤ h ≤ 13, -8 ≤ k ≤ 8, -13 ≤ l ≤ 13
Reflections collected	17378
Independent reflections	3383 [R(int) = 0.0636]
Completeness to theta = 25.242°	99.9%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.6477 and 0.5479
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3383 / 1 / 111
Goodness-of-fit on F ²	1.043
Final R indices [I>2sigma(I)]	R ₁ = 0.0248, wR ₂ = 0.0498
R indices (all data)	R ₁ = 0.0285, wR ₂ = 0.0519
Absolute structure parameter	-0.014(9)
Extinction coefficient	n/a
Largest diff. peak and hole	0.911 and -1.030 e·Å ⁻³

Table S8. Overview of bond lengths of complex **1e**.

Atoms	Length [Å]	Atoms	Length [Å]
Pt1-Cl3	2.2969(17)	N5-C2	1.490(8)
Pt1-Cl6	2.3045(18)	C1-C2	1.523(13)
Pt1-N4	2.067(6)	C1-C10	1.545(10)
Pt1-N5	2.053(6)	C2-C3	1.538(10)
N4-COAA	1.491(9)	C3-C7	1.557(10)
N4-C1AA	1.466(9)	C7-C10	1.548(10)

Table S9. Overview of angles of complex **1e**.

Atoms	Angle [°]	Atoms	Angle [°]
Cl3-Pt1-Cl6	178.71(6)	C2-N5-Pt1	114.8(4)
N4-Pt1-Cl3	92.31(17)	C2-C1-C10	101.8(7)
N4-Pt1-Cl6	88.07(17)	N5-C2-C1	114.1(6)
N5-Pt1-Cl3	87.62(18)	N5-C2-C3	113.2(5)
N5-Pt1-N4	179.9(3)	C1-C2-C3	104.2(6)
N5-Pt1-Cl6	92.00(18)	C2-C3-C7	105.0(6)
COAA-N4-Pt1	113.6(4)	C10-C7-C3	105.7(6)
C1AA-N4-Pt1	112.4(5)	C1-C10-C7	104.8(6)
C1AA-N4-COAA	111.4(6)		

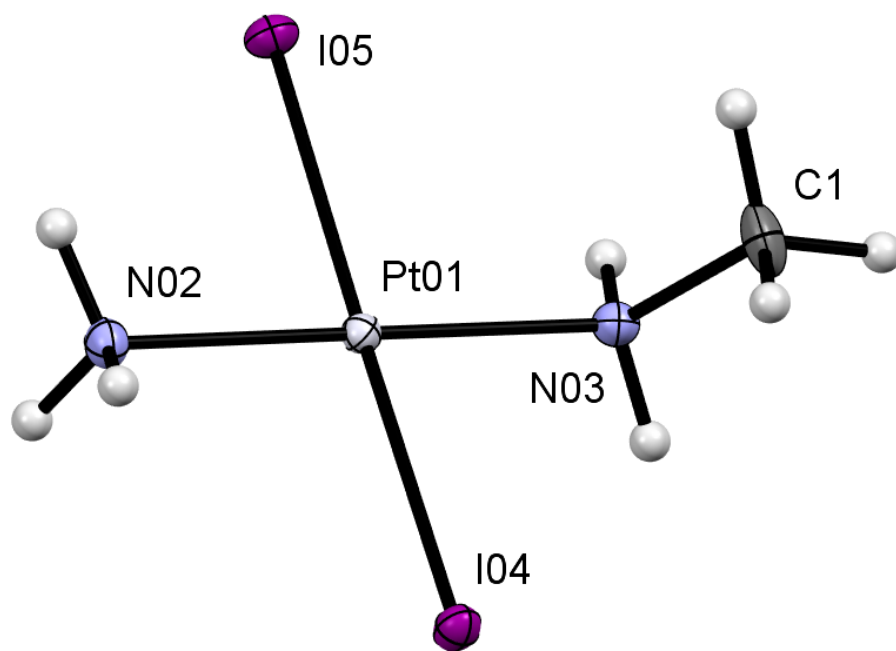


Figure S125. ORTEP view of complex **2a** drawn with 50% displacement ellipsoids.

Table S10. Overview of the sample and crystal data, data collection and structure refinement of complex **2a**.

Identification code	kryv465_1_p21c
Empirical formula	C ₂ H ₁₆ I ₄ N ₄ Pt ₂
Formula weight	993.97
Temperature	100.0 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 1 2 ₁ /c 1
Unit cell dimensions	a = 10.2120(2) Å b = 13.0130(2) Å c = 5.96810(10) Å α = 90° β = 96.6227(11)° γ = 90°
Volume	787.80(2) Å ³
Z	2
Density (calculated)	4.190 Mg/m ³
Absorption coefficient	25.547 mm ⁻¹
F(000)	848
Crystal size	0.07 x 0.07 x 0.03 mm ³
Theta range for data collection	2.008 to 33.149°
Index ranges	-12 ≤ h ≤ 15, -20 ≤ k ≤ 19, -9 ≤ l ≤ 8
Reflections collected	15787
Independent reflections	2887 [R(int) = 0.0442]
Completeness to theta = 25.242°	99.6%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.3840 and 0.2829
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2887 / 0 / 57
Goodness-of-fit on F ²	1.050
Final R indices [I>2sigma(I)]	R ₁ = 0.0231, wR ₂ = 0.0486
R indices (all data)	R ₁ = 0.0341, wR ₂ = 0.0523
Extinction coefficient	n/a
Largest diff. peak and hole	2.377 and -3.196 e·Å ⁻³

Table S11. Overview of bond lengths of complex **2a**.

Atoms	Length [Å]	Atoms	Length [Å]
Pt01-N02	2.052(3)	N03-H03A	0.91
Pt01-N03	2.052(3)	N03-H03B	0.91
Pt01-I04	2.6074(2)	N03-C1	1.483(5)
Pt01-I05	2.5908(3)	C1-H1A	0.98
N02-H02A	0.91	C1-H1B	0.98
N02-H02B	0.91	C1-H1C	0.98
N02-H02C	0.91		

Table S12. Overview of angles of complex **2a**.

Atoms	Angle [°]	Atoms	Angle [°]
N02-Pt01-I04	89.53(9)	Pt01-N03-H03A	108.5
N02-Pt01-I05	90.89(9)	Pt01-N03-H03B	108.5
N03-Pt01-N02	179.66(11)	H03A-N03-H03B	107.5
N03-Pt01-I04	90.50(8)	C1-N03-Pt01	114.9(2)
N03-Pt01-I05	89.09(8)	C1-N03-H03A	108.5
I05-Pt01-I04	178.749(8)	C1-N03-H03B	108.5
Pt01-N02-H02A	109.5	N03-C1-H1A	109.5
Pt01-N02-H02B	109.5	N03-C1-H1B	109.5
Pt01-N02-H02C	109.5	N03-C1-H1C	109.5
H02A-N02-H02B	109.5	H1A-C1-H1B	109.5
H02A-N02-H02C	109.5	H1A-C1-H1C	109.5
H02B-N02-H02C	109.5	H1B-C1-H1C	109.5

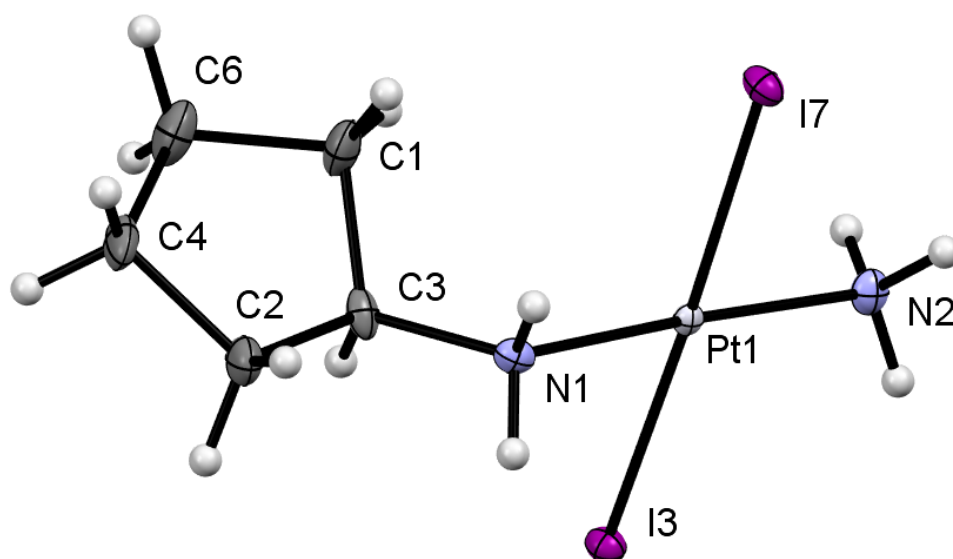


Figure S126. ORTEP view of complex **2c**. One of the two molecules in the asymmetric unit of complex **2c** is drawn with 50% displacement ellipsoids.

Table S13. Overview of the sample and crystal data, data collection and structure refinement of complex **2c**.

Identification code	kryv469_3_p-1
Empirical formula	C ₅ H ₁₄ I ₂ N ₂ Pt
Formula weight	550.58
Temperature	100.0 K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 9.2544(2) Å b = 10.3452(3) Å c = 13.7550(3) Å α = 69.6378(12)° β = 89.8550(15)° γ = 63.5008(9)°
Volume	1086.43(5) Å ³
Z	4
Density (calculated)	3.366 Mg/m ³
Absorption coefficient	18.511 mm ⁻¹
F(000)	967
Crystal size	0.208 x 0.194 x 0.101 mm ³
Theta range for data collection	2.386 to 25.734°
Index ranges	-11 ≤ h ≤ 11, -12 ≤ k ≤ 12, -16 ≤ l ≤ 16
Reflections collected	36297
Independent reflections	4151 [R(int) = 0.0623]
Completeness to theta = 25.242°	99.9%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.5621 and 0.2987
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4151 / 0 / 186
Goodness-of-fit on F ²	1.185
Final R indices [I>2sigma(I)]	R ₁ = 0.0227, wR ₂ = 0.0572
R indices (all data)	R ₁ = 0.0233, wR ₂ = 0.0575
Extinction coefficient	0.00267(10)
Largest diff. peak and hole	1.648 and -1.581 e.Å ⁻³

Table S14. Overview of bond lengths of complex **2c**.

Atoms	Length [Å]	Atoms	Length [Å]
Pt1-I3	2.6034(3)	C14-H14B	0.9900
Pt1-I7	2.6007(3)	C14-C16	1.550(7)
Pt1-N1	2.050(4)	C16-H16A	0.9900
Pt1-N2	2.055(4)	C16-H16B	0.9900
Pt2-I4	2.5973(3)	N1-H1A	0.9100
Pt2-I5	2.5907(4)	N1-H1B	0.9100
Pt2-N3	2.052(4)	N1-C3	1.493(6)
Pt2-N6	2.056(4)	N2-H2A	0.9100
N3-H3A	0.9100	N2-H2B	0.9100
N3-H3B	0.9100	N2-H2C	0.9100
N3-C5	1.497(6)	C3-H3	1.0000
C5-H5	1.0000	C3-C1	1.517(7)
C5-C8	1.540(7)	C3-C2	1.548(7)
C5-C10	1.537(7)	C1-H1C	0.9900
N6-H6C	0.9100	C1-H1D	0.9900
N6-H6D	0.9100	C1-C6	1.530(7)
N6-H6E	0.9100	C2-H2D	0.9900
C8-H8A	0.9900	C2-H2E	0.9900
C8-H8B	0.9900	C2-C4	1.550(7)
C8-C14	1.534(7)	C4-H4A	0.9900
C10-H10A	0.9900	C4-H4B	0.9900
C10-H10B	0.9900	C4-C6	1.524(8)
C10-C16	1.530(7)	C6-H6A	0.9900
C14-H14A	0.9900	C6-H6B	0.9900

Table S15. Overview of angles of complex **2c**.

Atoms	Angle [°]	Atoms	Angle [°]
I7-Pt1-I3	177.248(12)	C10-C16-C14	104.3(4)
N1-Pt1-I3	89.57(11)	C10-C16-H16A	110.9
N1-Pt1-I7	90.60(11)	C10-C16-H16B	110.9
N1-Pt1-N2	176.63(16)	C14-C16-H16A	110.9
N2-Pt1-I3	90.15(12)	C14-C16-H16B	110.9
N2-Pt1-I7	89.85(12)	H16A-C16-H16B	108.9
I5-Pt2-I4	178.125(12)	Pt1-N1-H1A	107.5
N3-Pt2-I4	89.58(11)	Pt1-N1-H1B	107.5
N3-Pt2-I5	90.31(11)	H1A-N1-H1B	107
N3-Pt2-N6	178.94(16)	C3-N1-Pt1	119.3(3)
N6-Pt2-I4	90.49(12)	C3-N1-H1A	107.5
N6-Pt2-I5	89.66(12)	C3-N1-H1B	107.5
Pt2-N3-H3A	108	Pt1-N2-H2A	109.5
Pt2-N3-H3B	108	Pt1-N2-H2B	109.5
H3A-N3-H3B	107.2	Pt1-N2-H2C	109.5
C5-N3-Pt2	117.3(3)	H2A-N2-H2B	109.5
C5-N3-H3A	108	H2A-N2-H2C	109.5
C5-N3-H3B	108	H2B-N2-H2C	109.5
N3-C5-H5	108.7	N1-C3-H3	109
N3-C5-C8	112.7(4)	N1-C3-C1	113.1(4)
N3-C5-C10	113.7(4)	N1-C3-C2	112.1(4)
C8-C5-H5	108.7	C1-C3-H3	109
C10-C5-H5	108.7	C1-C3-C2	104.5(4)
C10-C5-C8	104.3(4)	C2-C3-H3	109
Pt2-N6-H6C	109.5	C3-C1-H1C	111.4
Pt2-N6-H6D	109.5	C3-C1-H1D	111.4
Pt2-N6-H6E	109.5	C3-C1-C6	102.0(4)
H6C-N6-H6D	109.5	H1C-C1-H1D	109.2
H6C-N6-H6E	109.5	C6-C1-H1C	111.4
H6D-N6-H6E	109.5	C6-C1-H1D	111.4
C5-C8-H8A	110.5	C3-C2-H2D	110.8
C5-C8-H8B	110.5	C3-C2-H2E	110.8
H8A-C8-H8B	108.7	C3-C2-C4	104.9(4)
C14-C8-C5	106.3(4)	H2D-C2-H2E	108.8

Atoms	Angle [°]	Atoms	Angle [°]
C14-C8-H8A	110.5	C4-C2-H2D	110.8
C14-C8-H8B	110.5	C4-C2-H2E	110.8
C5-C10-H10A	111.6	C2-C4-H4A	110.5
C5-C10-H10B	111.6	C2-C4-H4B	110.5
H10A-C10-H10B	109.4	H4A-C4-H4B	108.7
C16-C10-C5	100.9(4)	C6-C4-C2	106.0(4)
C16-C10-H10A	111.6	C6-C4-H4A	110.5
C16-C10-H10B	111.6	C6-C4-H4B	110.5
C8-C14-H14A	110.8	C1-C6-H6A	110.8
C8-C14-H14B	110.8	C1-C6-H6B	110.8
C8-C14-C16	104.9(4)	C4-C6-C1	104.8(4)
H14A-C14-H14B	108.8	C4-C6-H6A	110.8
C16-C14-H14A	110.8	C4-C6-H6B	110.8
C16-C14-H14B	110.8	H6A-C6-H6B	108.9

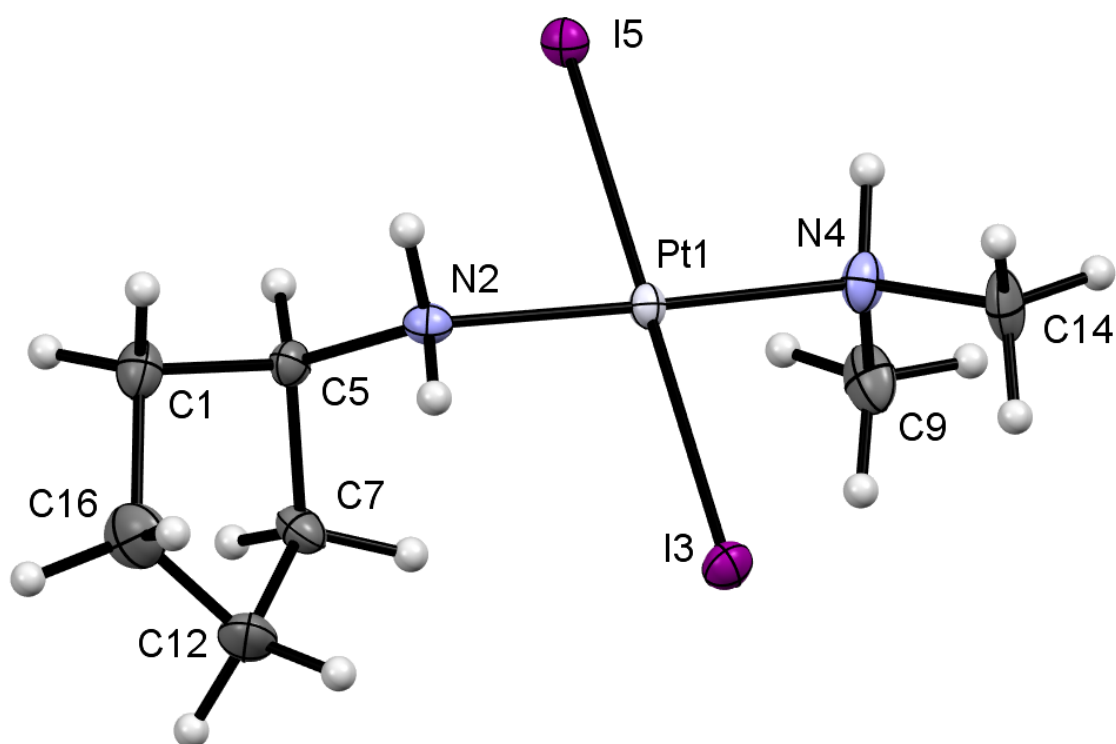


Figure S127. ORTEP view of complex **2e**. One of the two molecules in the asymmetric unit of complex **2e** is drawn with 50% displacement ellipsoids.

Table S16. Overview of the sample and crystal data, data collection and structure refinement of complex **2e**.

Identification code	kryv687_p21c
Empirical formula	C ₇ H ₁₈ I ₂ N ₂ Pt
Formula weight	579.12
Temperature	100.0 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 1 2 ₁ /c 1
Unit cell dimensions	a = 15.1132(5) Å b = 10.8253(3) Å c = 16.0145(5) Å α = 90° β = 93.2005(14)° γ = 90°
Volume	2615.96(14) Å ³
Z	8
Density (calculated)	2.941 Mg/m ³
Absorption coefficient	15.410 mm ⁻¹
F(000)	2064
Crystal size	0.176 x 0.148 x 0.118 mm ³
Theta range for data collection	2.272 to 25.715°
Index ranges	-18 ≤ h ≤ 18, -12 ≤ k ≤ 13, -18 ≤ l ≤ 19
Reflections collected	26249
Independent reflections	4988 [R(int) = 0.0508]
Completeness to theta = 25.242°	99.9%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.5621 and 0.3668
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4988 / 0 / 222
Goodness-of-fit on F ²	1.052
Final R indices [I>2σ(I)]	R ₁ = 0.0193, wR ₂ = 0.0430
R indices (all data)	R ₁ = 0.0217, wR ₂ = 0.0437
Extinction coefficient	0.00048(2)
Largest diff. peak and hole	1.530 and -1.140 e·Å ⁻³

Table S17. Overview of bond lengths of complex **2e**.

Atoms	Length [Å]	Atoms	Length [Å]
Pt1-I3	2.6075(3)	C8-H8A	0.98
Pt1-I5	2.6020(3)	C8-H8B	0.98
Pt1-N2	2.060(3)	C8-H8C	0.98
Pt1-N4	2.070(3)	C9-H9A	0.98
Pt2-I4	2.6002(3)	C9-H9B	0.98
Pt2-I6	2.6091(3)	C9-H9C	0.98
Pt2-N1	2.062(3)	C10-H10A	0.98
Pt2-N3	2.069(3)	C10-H10B	0.98
N1-H1C	0.91	C10-H10C	0.98
N1-H1D	0.91	C12-H12A	0.99
N1-C17	1.476(5)	C12-H12B	0.99
N2-H2A	0.91	C12-C16	1.543(6)
N2-H2B	0.91	C13-H13A	0.99
N2-C5	1.491(5)	C13-H13B	0.99
N3-H3	1	C13-C15	1.524(6)
N3-C8	1.478(5)	C14-H14A	0.98
N3-C10	1.480(5)	C14-H14B	0.98
N4-H4	1	C14-H14C	0.98
N4-C9	1.474(5)	C15-H15A	0.99
N4-C14	1.468(5)	C15-H15B	0.99
C5-H5	1	C15-C17	1.514(6)
C5-C7	1.518(5)	C16-H16A	0.99
C5-C1	1.536(5)	C16-H16B	0.99
C6-H6A	0.99	C16-C1	1.532(7)
C6-H6B	0.99	C17-H17	1
C6-C13	1.526(6)	C17-C18	1.541(6)
C6-C18	1.527(6)	C18-H18A	0.99
C7-H7A	0.99	C18-H18B	0.99
C7-H7B	0.99	C1-H1A	0.99
C7-C12	1.532(6)	C1-H1B	0.99

Table S18. Overview of angles of complex **2e**.

Atoms	Angle [°]	Atoms	Angle [°]
I5-Pt1-I3	177.795(10)	N4-C9-H9A	109.5
N2-Pt1-I3	88.75(10)	N4-C9-H9B	109.5
N2-Pt1-I5	90.07(10)	N4-C9-H9C	109.5
N2-Pt1-N4	177.29(14)	H9A-C9-H9B	109.5
N4-Pt1-I3	93.67(10)	H9A-C9-H9C	109.5
N4-Pt1-I5	87.55(10)	H9B-C9-H9C	109.5
I4-Pt2-I6	178.322(10)	N3-C10-H10A	109.5
N1-Pt2-I4	90.12(10)	N3-C10-H10B	109.5
N1-Pt2-I6	88.29(10)	N3-C10-H10C	109.5
N1-Pt2-N3	176.81(14)	H10A-C10-H10B	109.5
N3-Pt2-I4	87.44(10)	H10A-C10-H10C	109.5
N3-Pt2-I6	94.13(10)	H10B-C10-H10C	109.5
Pt2-N1-H1C	107.8	C7-C12-H12A	110.6
Pt2-N1-H1D	107.8	C7-C12-H12B	110.6
H1C-N1-H1D	107.1	C7-C12-C16	105.5(4)
C17-N1-Pt2	118.0(2)	H12A-C12-H12B	108.8
C17-N1-H1C	107.8	C16-C12-H12A	110.6
C17-N1-H1D	107.8	C16-C12-H12B	110.6
Pt1-N2-H2A	107.5	C6-C13-H13A	111
Pt1-N2-H2B	107.5	C6-C13-H13B	111
H2A-N2-H2B	107	H13A-C13-H13B	109
C5-N2-Pt1	119.2(2)	C15-C13-C6	103.6(4)
C5-N2-H2A	107.5	C15-C13-H13A	111
C5-N2-H2B	107.5	C15-C13-H13B	111
Pt2-N3-H3	105.6	N4-C14-H14A	109.5
C8-N3-Pt2	117.9(3)	N4-C14-H14B	109.5
C8-N3-H3	105.6	N4-C14-H14C	109.5
C8-N3-C10	110.4(3)	H14A-C14-H14B	109.5
C10-N3-Pt2	110.8(3)	H14A-C14-H14C	109.5
C10-N3-H3	105.6	H14B-C14-H14C	109.5
Pt1-N4-H4	105.6	C13-C15-H15A	111
C9-N4-Pt1	111.0(3)	C13-C15-H15B	111
C9-N4-H4	105.6	H15A-C15-H15B	109
C14-N4-Pt1	117.9(3)	C17-C15-C13	103.6(4)

Atoms	Angle [°]	Atoms	Angle [°]
C14-N4-H4	105.6	C17-C15-H15A	111
C14-N4-C9	110.3(3)	C17-C15-H15B	111
N2-C5-H5	110.6	C12-C16-H16A	110.5
N2-C5-C7	111.8(3)	C12-C16-H16B	110.5
N2-C5-C1	110.2(3)	H16A-C16-H16B	108.6
C7-C5-H5	110.6	C1-C16-C12	106.4(4)
C7-C5-C1	102.8(3)	C1-C16-H16A	110.5
C1-C5-H5	110.6	C1-C16-H16B	110.5
H6A-C6-H6B	108.8	N1-C17-C15	113.4(4)
C13-C6-H6A	110.7	N1-C17-H17	108.7
C13-C6-H6B	110.7	N1-C17-C18	112.5(4)
C13-C6-C18	105.3(3)	C15-C17-H17	108.7
C18-C6-H6A	110.7	C15-C17-C18	104.9(4)
C18-C6-H6B	110.7	C18-C17-H17	108.7
C5-C7-H7A	110.7	C6-C18-C17	106.7(4)
C5-C7-H7B	110.7	C6-C18-H18A	110.4
C5-C7-C12	105.3(4)	C6-C18-H18B	110.4
H7A-C7-H7B	108.8	C17-C18-H18A	110.4
C12-C7-H7A	110.7	C17-C18-H18B	110.4
C12-C7-H7B	110.7	H18A-C18-H18B	108.6
N3-C8-H8A	109.5	C5-C1-H1A	110.7
N3-C8-H8B	109.5	C5-C1-H1B	110.7
N3-C8-H8C	109.5	C16-C1-C5	105.4(3)
H8A-C8-H8B	109.5	C16-C1-H1A	110.7
H8A-C8-H8C	109.5	C16-C1-H1B	110.7
H8B-C8-H8C	109.5	H1A-C1-H1B	108.8

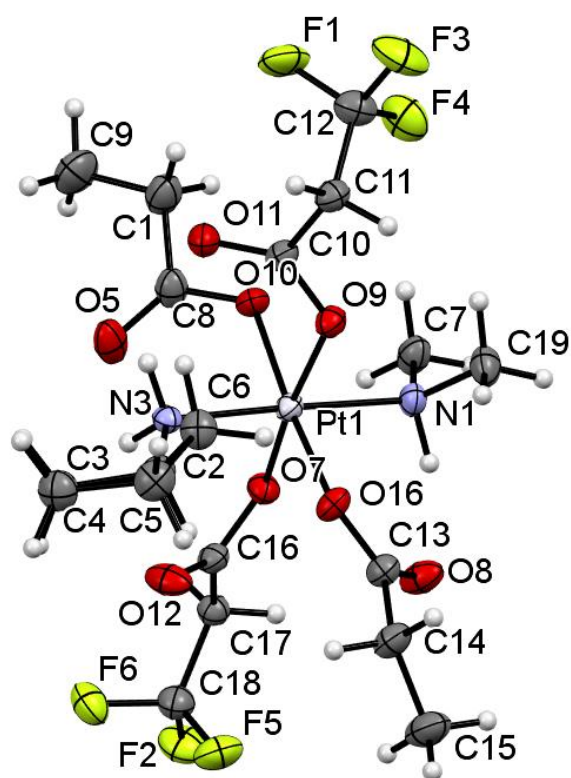


Figure S128. ORTEP view of complex **12e**. One of the two molecules in the asymmetric unit of complex **12e** is drawn with 50% displacement ellipsoids.

Table S19. Overview of the sample and crystal data, data collection and structure refinement of complex **12e**.

Identification code	kryv668_b
Empirical formula	C ₁₉ H ₃₁ F ₆ N ₂ O ₈ Pt
Formula weight	724.55
Temperature	100 K
Wavelength	1.54186 Å
Crystal system	Monoclinic
Space group	P 1 2 ₁ /n 1
Unit cell dimensions	a = 23.408(5) Å b = 9.4904(19) Å c = 23.714(5) Å α = 90° β = 99.87(3)° γ = 90°
Volume	5190.3(19) Å ³
Z	8
Density (calculated)	1.854 Mg/m ³
Absorption coefficient	10.927 mm ⁻¹
F(000)	2840
Crystal size	0.180 x 0.110 x 0.050 mm ³
Theta range for data collection	2.45 to 72.25°
Index ranges	-26 ≤ h ≤ 28, -10 ≤ k ≤ 11, -27 ≤ l ≤ 5
Reflections collected	41577
Independent reflections	9605 [R(int) = 0.0524]
Completeness to theta = 67.679°	95.4%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9366 and 0.8772
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	9605 / 1057 / 694
Goodness-of-fit on F ²	1.033
Final R indices [I>2sigma(I)]	R ₁ = 0.0524, wR ₂ = 0.1448
R indices (all data)	R ₁ = 0.0576, wR ₂ = 0.1511
Extinction coefficient	n/a
Largest diff. peak and hole	4.649 and -2.377 e·Å ⁻³

Table S20. Overview of bond lengths of complex **12e**.

Atoms	Length [Å]	Atoms	Length [Å]
Pt1-O7	2.010(4)	C7-H7C	0.98
Pt1-O9	2.002(4)	C9-H9A	0.98
Pt1-O10	1.993(4)	C9-H9B	0.98
Pt1-O16	1.999(5)	C9-H9C	0.98
Pt1-N1	2.084(5)	C10-C11	1.523(9)
Pt1-N3	2.071(5)	C11-H11A	0.99
Pt2-O1	2.020(5)	C11-H11B	0.99
Pt2-O2	2.009(5)	C11-C12	1.500(10)
Pt2-O3	1.994(5)	C13-C14	1.511(10)
Pt2-O6	1.998(5)	C14-H14A	0.99
Pt2-N2	2.052(6)	C14-H14B	0.99
Pt2-N5	2.082(7)	C14-C15	1.518(11)
F1-C12	1.336(10)	C15-H15A	0.98
F2-C18	1.333(9)	C15-H15B	0.98
F3-C12	1.331(9)	C15-H15C	0.98
F4-C12	1.329(9)	C16-C17	1.519(9)
F5-C18	1.337(9)	C17-H17A	0.99
F6-C18	1.341(9)	C17-H17B	0.99
F8-C37	1.305(12)	C17-C18	1.497(9)
F11-C37	1.341(11)	C19-H19A	0.98
F12-C37	1.340(13)	C19-H19B	0.98
O1-C35	1.275(9)	C19-H19C	0.98
O2-C32	1.290(10)	C20-H20	1
O3-C29	1.312(9)	C20-C21	1.521(13)
O4-C35	1.236(9)	C20-C24	1.512(12)
O5-C8	1.219(8)	C21-H21A	0.99
O6-C26	1.270(9)	C21-H21B	0.99
O7-C16	1.293(8)	C21-C22	1.509(16)
O8-C13	1.225(9)	C22-H22A	0.99
O9-C10	1.298(8)	C22-H22B	0.99
O10-C8	1.302(8)	C22-C23	1.502(19)
O11-C10	1.225(8)	C23-H23A	0.99
O12-C16	1.210(8)	C23-H23B	0.99
O13-C26	1.239(9)	C23-C24	1.514(15)

Atoms	Length [Å]	Atoms	Length [Å]
O14-C29	1.208(10)	C24-H24A	0.99
O15-C32	1.239(10)	C24-H24B	0.99
O16-C13	1.294(8)	C25-H25A	0.98
N1-H1	1	C25-H25B	0.98
N1-C7	1.454(9)	C25-H25C	0.98
N1-C19	1.484(9)	C26-C27	1.533(10)
N2-H2A	0.91	C27-C28	1.489(13)
N2-H2B	0.91	C27-C1A	1.41(6)
N2-C20	1.477(9)	C28-F7	1.346(10)
N3-H3A	0.91	C28-F9	1.351(9)
N3-H3B	0.91	C28-F10	1.339(10)
N3-C2	1.488(8)	C1A-F13	1.58(8)
N5-H5	1	C1A-F14	1.23(7)
N5-C25	1.433(10)	C1A-F15	1.39(7)
N5-C38	1.425(11)	C29-C30	1.505(12)
C1-H1A	0.99	C30-H30A	0.99
C1-H1B	0.99	C30-H30B	0.99
C1-C8	1.506(10)	C30-C31	1.518(14)
C1-C9	1.477(11)	C31-H31A	0.98
C2-H2	1	C31-H31B	0.98
C2-C3	1.529(9)	C31-H31C	0.98
C2-C6	1.506(9)	C32-C33	1.528(11)
C3-H3C	0.99	C33-H33A	0.99
C3-H3D	0.99	C33-H33B	0.99
C3-C4	1.539(10)	C33-C34	1.456(14)
C4-H4A	0.99	C34-H34A	0.98
C4-H4B	0.99	C34-H34B	0.98
C4-C5	1.525(10)	C34-H34C	0.98
C5-H5A	0.99	C35-C36	1.495(10)
C5-H5B	0.99	C36-H36A	0.99
C5-C6	1.514(10)	C36-H36B	0.99
C6-H6A	0.99	C36-C37	1.485(11)
C6-H6B	0.99	C38-H38A	0.98
C7-H7A	0.98	C38-H38B	0.98
C7-H7B	0.98	C38-H38C	0.98

Table S21. Overview of angles of complex **12e**.

Atoms	Angle [°]	Atoms	Angle [°]
O7-Pt1-N1	81.6(2)	H14A-C14-H14B	107.6
O7-Pt1-N3	97.32(19)	C15-C14-H14A	108.7
O9-Pt1-O7	171.98(18)	C15-C14-H14B	108.7
O9-Pt1-N1	90.5(2)	C14-C15-H15A	109.5
O9-Pt1-N3	90.60(19)	C14-C15-H15B	109.5
O10-Pt1-O7	90.27(19)	C14-C15-H15C	109.5
O10-Pt1-O9	87.88(19)	H15A-C15-H15B	109.5
O10-Pt1-O16	174.32(19)	H15A-C15-H15C	109.5
O10-Pt1-N1	87.4(2)	H15B-C15-H15C	109.5
O10-Pt1-N3	94.1(2)	O7-C16-C17	110.0(5)
O16-Pt1-O7	94.95(19)	O12-C16-O7	126.7(6)
O16-Pt1-O9	86.64(19)	O12-C16-C17	123.2(6)
O16-Pt1-N1	91.2(2)	C16-C17-H17A	108.6
O16-Pt1-N3	87.5(2)	C16-C17-H17B	108.6
N3-Pt1-N1	178.2(2)	H17A-C17-H17B	107.6
O1-Pt2-N2	94.9(2)	C18-C17-C16	114.7(6)
O1-Pt2-N5	88.7(3)	C18-C17-H17A	108.6
O2-Pt2-O1	82.3(2)	C18-C17-H17B	108.6
O2-Pt2-N2	85.2(2)	F2-C18-F5	107.0(6)
O2-Pt2-N5	92.6(3)	F2-C18-F6	107.0(6)
O3-Pt2-O1	97.2(2)	F2-C18-C17	110.9(6)
O3-Pt2-O2	171.7(2)	F5-C18-F6	105.9(6)
O3-Pt2-O6	83.9(2)	F5-C18-C17	112.6(6)
O3-Pt2-N2	86.6(2)	F6-C18-C17	113.1(6)
O3-Pt2-N5	95.7(3)	N1-C19-H19A	109.5
O6-Pt2-O1	173.5(2)	N1-C19-H19B	109.5
O6-Pt2-O2	97.5(2)	N1-C19-H19C	109.5
O6-Pt2-N2	91.5(2)	H19A-C19-H19B	109.5
O6-Pt2-N5	84.8(3)	H19A-C19-H19C	109.5
N2-Pt2-N5	175.4(3)	H19B-C19-H19C	109.5
C35-O1-Pt2	124.9(5)	N2-C20-H20	107.3
C32-O2-Pt2	124.4(5)	N2-C20-C21	114.9(8)
C29-O3-Pt2	123.6(5)	N2-C20-C24	113.9(7)
C26-O6-Pt2	124.5(4)	C21-C20-H20	107.3
C16-O7-Pt1	122.8(4)	C24-C20-H20	107.3

Atoms	Angle [°]	Atoms	Angle [°]
C10-O9-Pt1	122.3(4)	C24-C20-C21	105.8(8)
C8-O10-Pt1	124.2(4)	C20-C21-H21A	110.4
C13-O16-Pt1	125.3(4)	C20-C21-H21B	110.4
Pt1-N1-H1	104.9	H21A-C21-H21B	108.6
C7-N1-Pt1	116.0(4)	C22-C21-C20	106.6(10)
C7-N1-H1	104.9	C22-C21-H21A	110.4
C7-N1-C19	110.9(5)	C22-C21-H21B	110.4
C19-N1-Pt1	113.8(4)	C21-C22-H22A	111.1
C19-N1-H1	104.9	C21-C22-H22B	111.1
Pt2-N2-H2A	107.5	H22A-C22-H22B	109.1
Pt2-N2-H2B	107.5	C23-C22-C21	103.1(10)
H2A-N2-H2B	107	C23-C22-H22A	111.1
C20-N2-Pt2	119.5(5)	C23-C22-H22B	111.1
C20-N2-H2A	107.5	C22-C23-H23A	111.1
C20-N2-H2B	107.5	C22-C23-H23B	111.1
Pt1-N3-H3A	107.2	C22-C23-C24	103.4(9)
Pt1-N3-H3B	107.2	H23A-C23-H23B	109
H3A-N3-H3B	106.8	C24-C23-H23A	111.1
C2-N3-Pt1	120.5(4)	C24-C23-H23B	111.1
C2-N3-H3A	107.2	C20-C24-C23	101.7(8)
C2-N3-H3B	107.2	C20-C24-H24A	111.4
Pt2-N5-H5	98.4	C20-C24-H24B	111.4
C25-N5-Pt2	116.9(5)	C23-C24-H24A	111.4
C25-N5-H5	98.4	C23-C24-H24B	111.4
C38-N5-Pt2	117.9(5)	H24A-C24-H24B	109.3
C38-N5-H5	98.4	N5-C25-H25A	109.5
C38-N5-C25	119.0(7)	N5-C25-H25B	109.5
H1A-C1-H1B	107.5	N5-C25-H25C	109.5
C8-C1-H1A	108.6	H25A-C25-H25B	109.5
C8-C1-H1B	108.6	H25A-C25-H25C	109.5
C9-C1-H1A	108.6	H25B-C25-H25C	109.5
C9-C1-H1B	108.6	O6-C26-C27	113.7(6)
C9-C1-C8	114.9(7)	O13-C26-O6	126.7(7)
N3-C2-H2	108.5	O13-C26-C27	119.5(7)
N3-C2-C3	111.4(5)	C28-C27-C26	111.5(7)

Atoms	Angle [°]	Atoms	Angle [°]
N3-C2-C6	114.6(5)	C1A-C27-C26	130(3)
C3-C2-H2	108.5	F7-C28-C27	114.8(8)
C6-C2-H2	108.5	F7-C28-F9	104.7(7)
C6-C2-C3	105.1(6)	F9-C28-C27	110.5(8)
C2-C3-H3C	110.7	F10-C28-C27	113.4(7)
C2-C3-H3D	110.7	F10-C28-F7	106.5(8)
C2-C3-C4	105.3(6)	F10-C28-F9	106.2(8)
H3C-C3-H3D	108.8	C27-C1A-F13	104(4)
C4-C3-H3C	110.7	F14-C1A-C27	125(6)
C4-C3-H3D	110.7	F14-C1A-F13	106(5)
C3-C4-H4A	110.6	F14-C1A-F15	117(5)
C3-C4-H4B	110.6	F15-C1A-C27	107(4)
H4A-C4-H4B	108.8	F15-C1A-F13	92(5)
C5-C4-C3	105.5(6)	O3-C29-C30	113.2(8)
C5-C4-H4A	110.6	O14-C29-O3	124.8(7)
C5-C4-H4B	110.6	O14-C29-C30	122.1(7)
C4-C5-H5A	110.9	C29-C30-H30A	109.5
C4-C5-H5B	110.9	C29-C30-H30B	109.5
H5A-C5-H5B	108.9	C29-C30-C31	110.8(8)
C6-C5-C4	104.4(6)	H30A-C30-H30B	108.1
C6-C5-H5A	110.9	C31-C30-H30A	109.5
C6-C5-H5B	110.9	C31-C30-H30B	109.5
C2-C6-C5	102.1(6)	C30-C31-H31A	109.5
C2-C6-H6A	111.3	C30-C31-H31B	109.5
C2-C6-H6B	111.3	C30-C31-H31C	109.5
C5-C6-H6A	111.3	H31A-C31-H31B	109.5
C5-C6-H6B	111.3	H31A-C31-H31C	109.5
H6A-C6-H6B	109.2	H31B-C31-H31C	109.5
N1-C7-H7A	109.5	O2-C32-C33	112.8(7)
N1-C7-H7B	109.5	O15-C32-O2	124.6(7)
N1-C7-H7C	109.5	O15-C32-C33	122.5(7)
H7A-C7-H7B	109.5	C32-C33-H33A	108.4
H7A-C7-H7C	109.5	C32-C33-H33B	108.4
H7B-C7-H7C	109.5	H33A-C33-H33B	107.5
O5-C8-O10	125.0(7)	C34-C33-C32	115.4(8)

Atoms	Angle [°]	Atoms	Angle [°]
O5-C8-C1	125.1(6)	C34-C33-H33A	108.4
O10-C8-C1	109.8(6)	C34-C33-H33B	108.4
C1-C9-H9A	109.5	C33-C34-H34A	109.5
C1-C9-H9B	109.5	C33-C34-H34B	109.5
C1-C9-H9C	109.5	C33-C34-H34C	109.5
H9A-C9-H9B	109.5	H34A-C34-H34B	109.5
H9A-C9-H9C	109.5	H34A-C34-H34C	109.5
H9B-C9-H9C	109.5	H34B-C34-H34C	109.5
O9-C10-C11	111.6(6)	O1-C35-C36	113.3(7)
O11-C10-O9	127.9(6)	O4-C35-O1	125.5(7)
O11-C10-C11	120.5(6)	O4-C35-C36	121.2(7)
C10-C11-H11A	109.4	C35-C36-H36A	109
C10-C11-H11B	109.4	C35-C36-H36B	109
H11A-C11-H11B	108	H36A-C36-H36B	107.8
C12-C11-C10	111.2(6)	C37-C36-C35	112.8(7)
C12-C11-H11A	109.4	C37-C36-H36A	109
C12-C11-H11B	109.4	C37-C36-H36B	109
F1-C12-C11	113.2(7)	F8-C37-F11	107.7(9)
F3-C12-F1	105.1(6)	F8-C37-F12	106.6(9)
F3-C12-C11	111.8(7)	F8-C37-C36	113.6(8)
F4-C12-F1	106.5(7)	F11-C37-C36	111.7(7)
F4-C12-F3	107.7(7)	F12-C37-F11	106.1(8)
F4-C12-C11	112.1(6)	F12-C37-C36	110.7(9)
O8-C13-O16	125.9(6)	N5-C38-H38A	109.5
O8-C13-C14	121.5(6)	N5-C38-H38B	109.5
O16-C13-C14	112.6(6)	N5-C38-H38C	109.5
C13-C14-H14A	108.7	H38A-C38-H38B	109.5
C13-C14-H14B	108.7	H38A-C38-H38C	109.5
C13-C14-C15	114.1(7)	H38B-C38-H38C	109.5

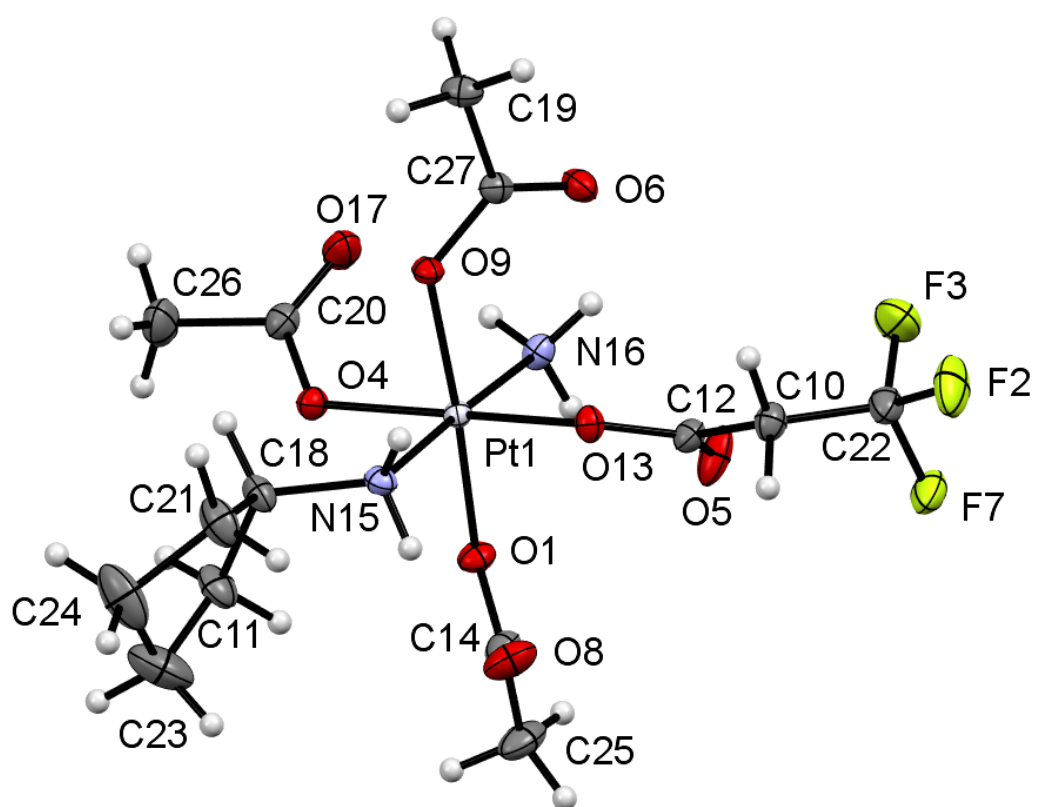


Figure S129. ORTEP view of complex **13c** drawn with 50% displacement ellipsoids.

Table S22. Overview of the sample and crystal data, data collection and structure refinement of complex **13c**.

Identification code	mo_kryv976_p21n
Empirical formula	C ₁₄ H ₂₅ F ₃ N ₂ O ₈ Pt
Formula weight	601.45
Temperature	100.0 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 1 2 ₁ /n 1
Unit cell dimensions	a = 13.0409(8) Å b = 9.6876(12) Å c = 17.1451(12) Å α = 90° β = 111.571(4)° γ = 90°
Volume	2014.3(3) Å ³
Z	4
Density (calculated)	1.983 Mg/m ³
Absorption coefficient	7.036 mm ⁻¹
F(000)	1168
Crystal size	0.12 x 0.05 x 0.01 mm ³
Theta range for data collection	2.456 to 30.030°
Index ranges	-18 ≤ h ≤ 18, -9 ≤ k ≤ 12, -24 ≤ l ≤ 24
Reflections collected	55642
Independent reflections	5679 [R(int) = 0.0406]
Completeness to theta = 25.242°	97.0%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.6056 and 0.5306
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5679 / 0 / 257
Goodness-of-fit on F ²	1.067
Final R indices [I>2sigma(I)]	R ₁ = 0.0208, wR ₂ = 0.0415
R indices (all data)	R ₁ = 0.0260, wR ₂ = 0.0438
Extinction coefficient	n/a
Largest diff. peak and hole	1.179 and -0.732 e·Å ⁻³

Table S23. Overview of bond lengths of complex **13c**.

Atoms	Length [Å]	Atoms	Length [Å]
Pt1-O1	2.0050(17)	N15-C18	1.492(3)
Pt1-O4	2.0013(17)	N16-H16A	0.91
Pt1-O9	2.0091(16)	N16-H16B	0.91
Pt1-O13	2.0095(18)	N16-H16C	0.91
Pt1-N15	2.059(2)	O17-C20	1.222(4)
Pt1-N16	2.041(2)	C18-H18	1
O1-C14	1.307(3)	C18-C21	1.532(4)
F2-C22	1.347(3)	C19-H19A	0.98
F3-C22	1.334(4)	C19-H19B	0.98
O4-C20	1.310(3)	C19-H19C	0.98
O5-C12	1.207(3)	C19-C27	1.511(3)
O6-C27	1.226(3)	C20-C26	1.514(4)
F7-C22	1.342(3)	C21-H21A	0.99
O8-C14	1.218(4)	C21-H21B	0.99
O9-C27	1.313(3)	C21-C24	1.512(4)
C10-H10A	0.99	C26-H26A	0.98
C10-H10B	0.99	C26-H26B	0.98
C10-C12	1.517(4)	C26-H26C	0.98
C10-C22	1.497(4)	C24-H24A	0.99
C11-H11A	0.99	C24-H24B	0.99
C11-H11B	0.99	C24-C23	1.520(5)
C11-C18	1.543(4)	C25-H25A	0.98
C11-C23	1.514(5)	C25-H25B	0.98
C12-O13	1.308(3)	C25-H25C	0.98
C14-C25	1.511(4)	C23-H23A	0.99
N15-H15A	0.91	C23-H23B	0.99
N15-H15B	0.91		

Table S24. Overview of angles of complex **13c**.

Atoms	Angle [°]	Atoms	Angle [°]
O1-Pt1-O9	176.03(7)	N15-C18-C21	111.0(2)
O1-Pt1-O13	97.87(7)	C21-C18-C11	105.7(2)
O1-Pt1-N15	95.09(8)	C21-C18-H18	108.9
O1-Pt1-N16	83.73(8)	H19A-C19-H19B	109.5
O4-Pt1-O1	86.67(7)	H19A-C19-H19C	109.5
O4-Pt1-O9	89.38(7)	H19B-C19-H19C	109.5
O4-Pt1-O13	170.89(8)	C27-C19-H19A	109.5
O4-Pt1-N15	89.13(8)	C27-C19-H19B	109.5
O4-Pt1-N16	92.63(8)	C27-C19-H19C	109.5
O9-Pt1-O13	85.98(7)	O4-C20-C26	111.6(2)
O9-Pt1-N15	84.44(8)	O17-C20-O4	126.4(2)
O9-Pt1-N16	96.86(8)	O17-C20-C26	122.0(3)
O13-Pt1-N15	82.63(8)	C18-C21-H21A	110.9
O13-Pt1-N16	95.70(8)	C18-C21-H21B	110.9
N16-Pt1-N15	177.82(8)	H21A-C21-H21B	109
C14-O1-Pt1	123.15(18)	C24-C21-C18	104.1(3)
C20-O4-Pt1	124.31(16)	C24-C21-H21A	110.9
C27-O9-Pt1	121.97(15)	C24-C21-H21B	110.9
H10A-C10-H10B	107.7	F2-C22-C10	110.4(3)
C12-C10-H10A	108.8	F3-C22-F2	106.5(2)
C12-C10-H10B	108.8	F3-C22-F7	106.4(3)
C22-C10-H10A	108.8	F3-C22-C10	113.3(2)
C22-C10-H10B	108.8	F7-C22-F2	105.8(2)
C22-C10-C12	113.9(2)	F7-C22-C10	113.9(2)
H11A-C11-H11B	108.7	C20-C26-H26A	109.5
C18-C11-H11A	110.6	C20-C26-H26B	109.5
C18-C11-H11B	110.6	C20-C26-H26C	109.5
C23-C11-H11A	110.6	H26A-C26-H26B	109.5
C23-C11-H11B	110.6	H26A-C26-H26C	109.5
C23-C11-C18	105.9(3)	H26B-C26-H26C	109.5
O5-C12-C10	123.8(2)	O6-C27-O9	125.7(2)
O5-C12-O13	126.0(2)	O6-C27-C19	121.1(2)
O13-C12-C10	110.2(2)	O9-C27-C19	113.2(2)
C12-O13-Pt1	123.69(18)	C21-C24-H24A	111.2

Atoms	Angle [°]	Atoms	Angle [°]
O1-C14-C25	111.9(3)	C21-C24-H24B	111.2
O8-C14-O1	125.7(2)	C21-C24-C23	102.9(3)
O8-C14-C25	122.3(3)	H24A-C24-H24B	109.1
Pt1-N15-H15A	107.2	C23-C24-H24A	111.2
Pt1-N15-H15B	107.2	C23-C24-H24B	111.2
H15A-N15-H15B	106.8	C14-C25-H25A	109.5
C18-N15-Pt1	120.70(18)	C14-C25-H25B	109.5
C18-N15-H15A	107.2	C14-C25-H25C	109.5
C18-N15-H15B	107.2	H25A-C25-H25B	109.5
Pt1-N16-H16A	109.5	H25A-C25-H25C	109.5
Pt1-N16-H16B	109.5	H25B-C25-H25C	109.5
Pt1-N16-H16C	109.5	C11-C23-C24	103.9(3)
H16A-N16-H16B	109.5	C11-C23-H23A	111
H16A-N16-H16C	109.5	C11-C23-H23B	111
H16B-N16-H16C	109.5	C24-C23-H23A	111
C11-C18-H18	108.9	C24-C23-H23B	111
N15-C18-C11	113.3(2)	H23A-C23-H23B	109
N15-C18-H18	108.9		

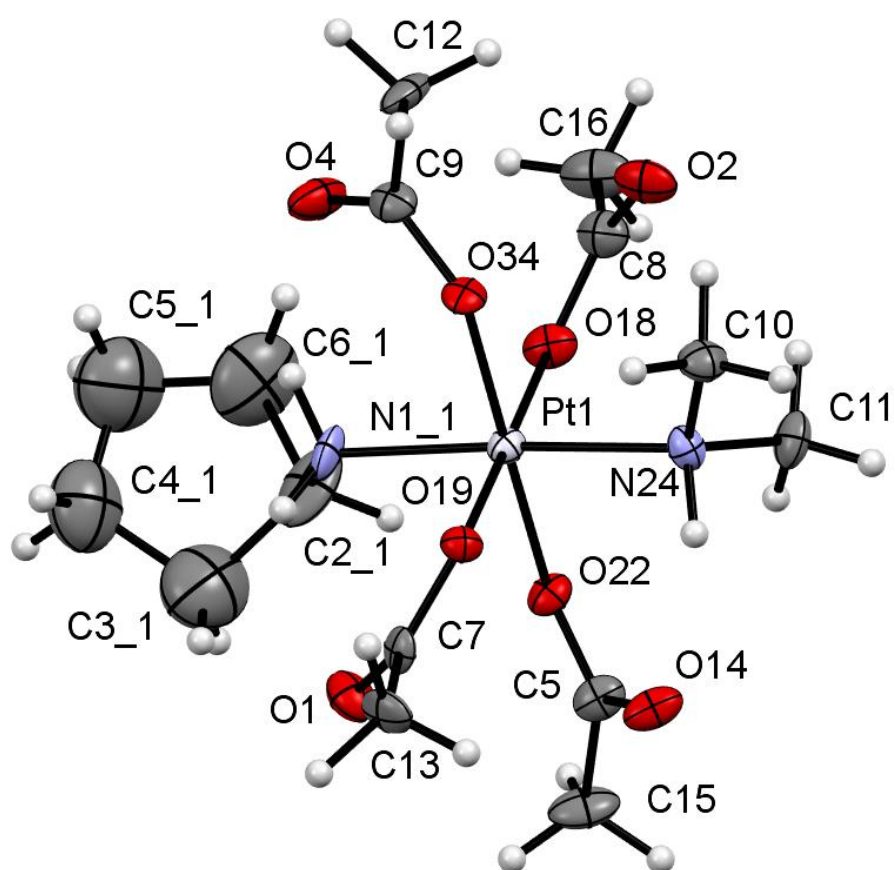


Figure S130. ORTEP view of complex **15e** drawn with 50% displacement ellipsoids.

Table S25. Overview of the sample and crystal data, data collection and structure refinement of complex **15e**.

Identification code	KRYV901
Empirical formula	C ₁₅ H ₃₀ N ₂ O ₈ Pt
Formula weight	561.50
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Tetragonal
Space group	P4 ₁ 2 ₁ 2
Unit cell dimensions	a = 15.7587(4) Å b = 15.7587(4) Å c = 16.1203(7) Å $\alpha = 90^\circ$ $\beta = 90^\circ$ $\gamma = 90^\circ$
Volume	4003.3(3) Å ³
Z	8
Density (calculated)	1.863 Mg/m ³
Absorption coefficient	7.052 mm ⁻¹
F(000)	2208
Crystal size	0.072 x 0.07 x 0.013 mm ³
Theta range for data collection	1.807 to 30.101°
Index ranges	-20 ≤ h ≤ 22, -22 ≤ k ≤ 14, -19 ≤ l ≤ 22
Reflections collected	37973
Independent reflections	5876 [R(int) = 0.0664]
Completeness to theta = 25.242°	99.9%
Absorption correction	None
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5876 / 324 / 241
Goodness-of-fit on F ²	1.366
Final R indices [I>2sigma(I)]	R ¹ = 0.0477, wR ² = 0.1498
R indices (all data)	R ¹ = 0.0563, wR ² = 0.1626
Absolute structure parameter	-0.001(13)
Extinction coefficient	n/a
Largest diff. peak and hole	2.332 and -2.097 e·Å ⁻³

Table S26. Overview of bond lengths of complex **15e**.

Atoms	Length [Å]	Atoms	Length [Å]
Pt1-O18	2.008(9)	C12-H12B	0.98
Pt1-O34	2.013(8)	C12-H12C	0.98
Pt1-O19	2.014(8)	C16-H16A	0.98
Pt1-O22	2.014(8)	C16-H16B	0.98
Pt1-N11	2.064(9)	C16-H16C	0.98
Pt1-N24	2.103(10)	C15-H15A	0.98
O34-C9	1.290(15)	C15-H15B	0.98
O18-C8	1.321(16)	C15-H15C	0.98
O19-C7	1.300(14)	C13-H13A	0.98
O22-C5	1.313(16)	C13-H13B	0.98
N24-C10	1.463(16)	C13-H13C	0.98
N24-C11	1.502(16)	N11-C21	1.494(12)
N24-H24	1	N11-H1A1	0.91
O1-C7	1.244(15)	N11-H1B1	0.91
O2-C8	1.221(17)	C21-C61	1.526(14)
O4-C9	1.257(16)	C21-C31	1.546(15)
C5-O14	1.221(14)	C21-H21	1
C5-C15	1.498(18)	C31-C41	1.54(2)
C7-C13	1.512(16)	C31-H3A1	0.99
C8-C16	1.493(19)	C31-H3B1	0.99
C9-C12	1.518(17)	C41-C51	1.43(3)
C10-H10A	0.98	C41-H4A1	0.99
C10-H10B	0.98	C41-H4B1	0.99
C10-H10C	0.98	C51-C61	1.45(3)
C11-H11A	0.98	C51-H5A1	0.99
C11-H11B	0.98	C51-H5B1	0.99
C11-H11C	0.98	C61-H6A1	0.99
C12-H12A	0.98	C61-H6B1	0.99

Table S27. Overview of angles of complex **15e**.

Atoms	Angle [°]	Atoms	Angle [°]
O18-Pt1-O34	95.8(3)	C8-C16-H16A	109.5
O18-Pt1-O19	179.4(3)	C8-C16-H16B	109.5
O34-Pt1-O19	83.6(3)	H16A-C16-H16B	109.5
O18-Pt1-O22	83.5(4)	C8-C16-H16C	109.5
O34-Pt1-O22	179.2(4)	H16A-C16-H16C	109.5
O19-Pt1-O22	97.2(3)	H16B-C16-H16C	109.5
O18-Pt1-N11	85.0(4)	C5-C15-H15A	109.5
O34-Pt1-N11	92.8(4)	C5-C15-H15B	109.5
O19-Pt1-N11	94.8(4)	H15A-C15-H15B	109.5
O22-Pt1-N11	87.4(4)	C5-C15-H15C	109.5
O18-Pt1-N24	97.8(4)	H15A-C15-H15C	109.5
O34-Pt1-N24	88.4(4)	H15B-C15-H15C	109.5
O19-Pt1-N24	82.3(3)	C7-C13-H13A	109.5
O22-Pt1-N24	91.4(4)	C7-C13-H13B	109.5
N11-Pt1-N24	176.8(4)	H13A-C13-H13B	109.5
C9-O34-Pt1	126.3(8)	C7-C13-H13C	109.5
C8-O18-Pt1	125.2(8)	H13A-C13-H13C	109.5
C7-O19-Pt1	122.2(7)	H13B-C13-H13C	109.5
C5-O22-Pt1	122.1(8)	C21-N11-Pt1	120.3(8)
C10-N24-C11	112.3(10)	C21-N11-H1A1	107.3
C10-N24-Pt1	115.0(8)	Pt1-N11-H1A1	107.3
C11-N24-Pt1	113.9(7)	C21-N11-H1B1	107.3
C10-N24-H24	104.8	Pt1-N11-H1B1	107.3
C11-N24-H24	104.8	H1A1-N11-H1B1	106.9
Pt1-N24-H24	104.8	N11-C21-C61	113.0(13)
O14-C5-O22	126.2(12)	N11-C21-C31	109.4(14)
O14-C5-C15	121.8(12)	C61-C21-C31	101.3(15)
O22-C5-C15	112.0(11)	N11-C21-H21	110.9
O1-C7-O19	125.7(10)	C61-C21-H21	110.9
O1-C7-C13	121.9(11)	C31-C21-H21	110.9
O19-C7-C13	112.3(10)	C41-C31-C21	102.8(15)
O2-C8-O18	124.6(12)	C41-C31-H3A1	111.2
O2-C8-C16	123.7(13)	C21-C31-H3A1	111.2
O18-C8-C16	111.5(12)	C41-C31-H3B1	111.2

Atoms	Angle [°]	Atoms	Angle [°]
O4-C9-O34	126.4(11)	C21-C31-H3B1	111.2
O4-C9-C12	122.0(11)	H3A1-C31-H3B1	109.1
O34-C9-C12	111.6(11)	C51-C41-C31	109.1(19)
N24-C10-H10A	109.5	C51-C41-H4A1	109.9
N24-C10-H10B	109.5	C31-C41-H4A1	109.9
H10A-C10-H10B	109.5	C51-C41-H4B1	109.9
N24-C10-H10C	109.5	C31-C41-H4B1	109.9
H10A-C10-H10C	109.5	H4A1-C41-H4B1	108.3
H10B-C10-H10C	109.5	C41-C51-C61	108(2)
N24-C11-H11A	109.5	C41-C51-H5A1	110.2
N24-C11-H11B	109.5	C61-C51-H5A1	110.2
H11A-C11-H11B	109.5	C41-C51-H5B1	110.2
N24-C11-H11C	109.5	C61-C51-H5B1	110.2
H11A-C11-H11C	109.5	H5A1-C51-H5B1	108.5
H11B-C11-H11C	109.5	C51-C61-C21	108.9(17)
C9-C12-H12A	109.5	C51-C61-H6A1	109.9
C9-C12-H12B	109.5	C21-C61-H6A1	109.9
H12A-C12-H12B	109.5	C51-C61-H6B1	109.9
C9-C12-H12C	109.5	C21-C61-H6B1	109.9
H12A-C12-H12C	109.5	H6A1-C61-H6B1	108.3
H12B-C12-H12C	109.5		

4. Concentration-effect curves

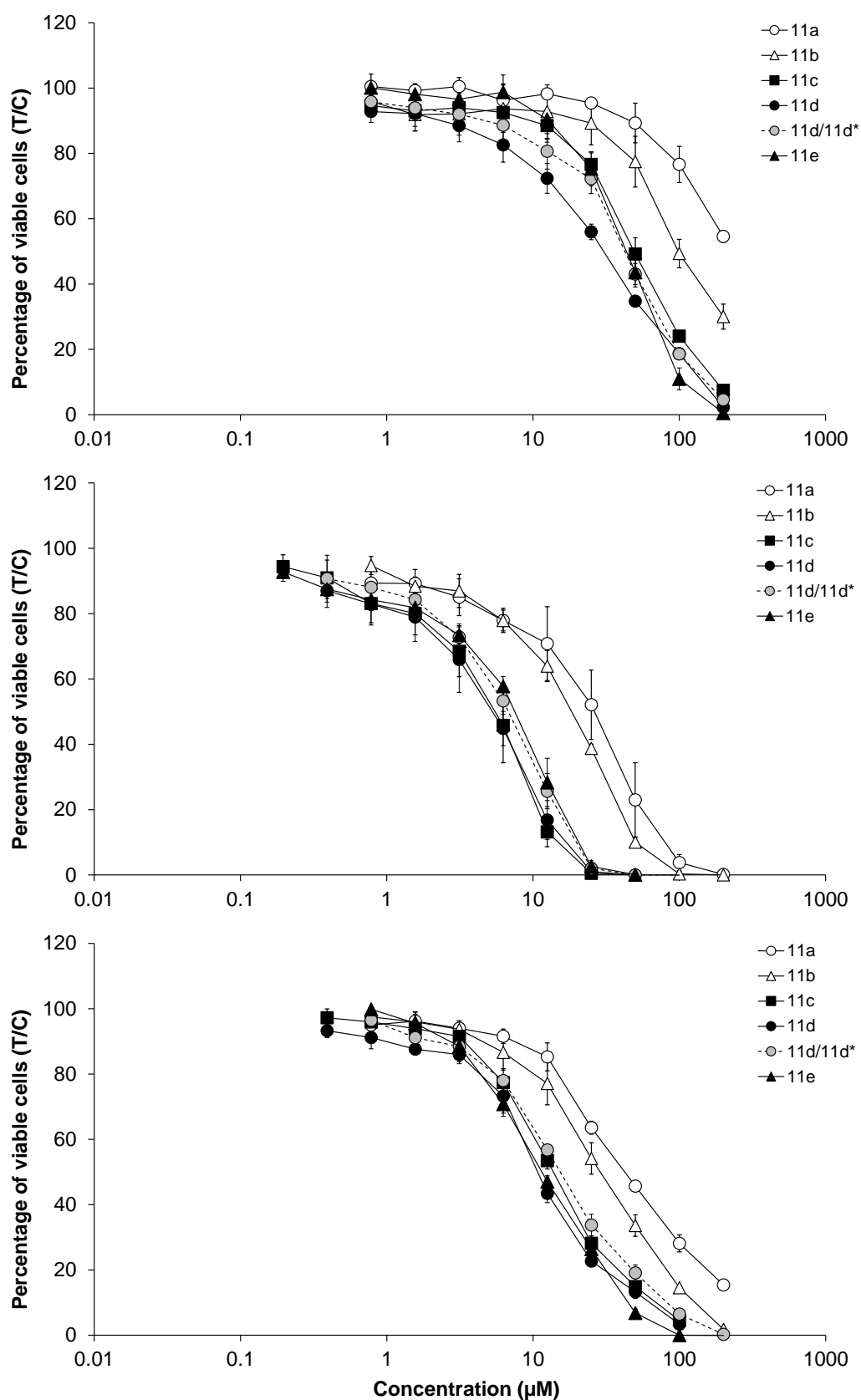


Figure S131. Concentration-effect curves of **11a–11e** in A549 (top), CH1/PA-1 (middle) and SW480 (bottom) cells, obtained by MTT assays with 96 h exposure time. Values are means \pm standard deviations from at least three independent experiments.

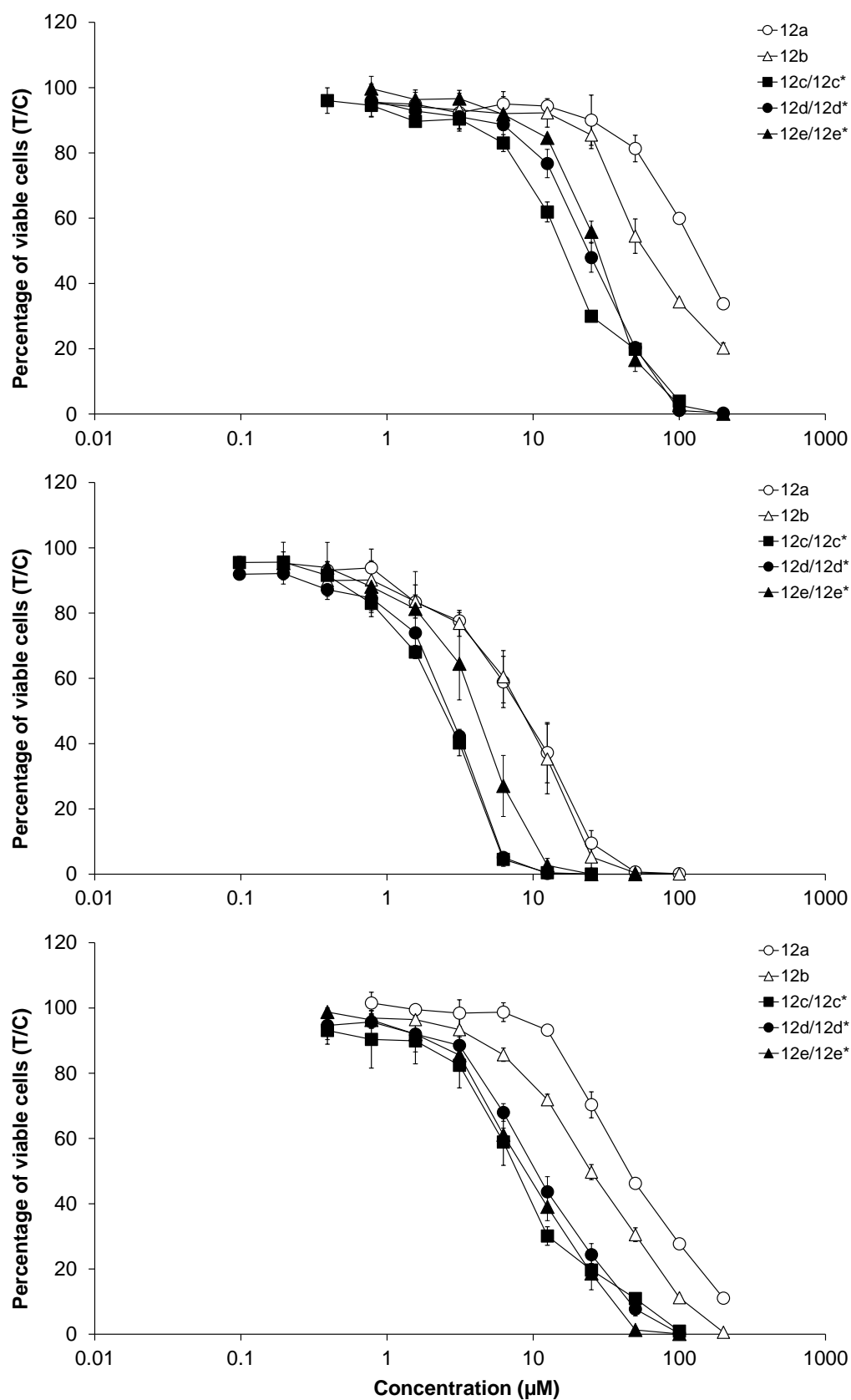


Figure S132. Concentration-effect curves of **12a–12e** in A549 (top), CH1/PA-1 (middle) and SW480 (bottom) cells, obtained by MTT assays with 96 h exposure time. Values are means \pm standard deviations from at least three independent experiments.

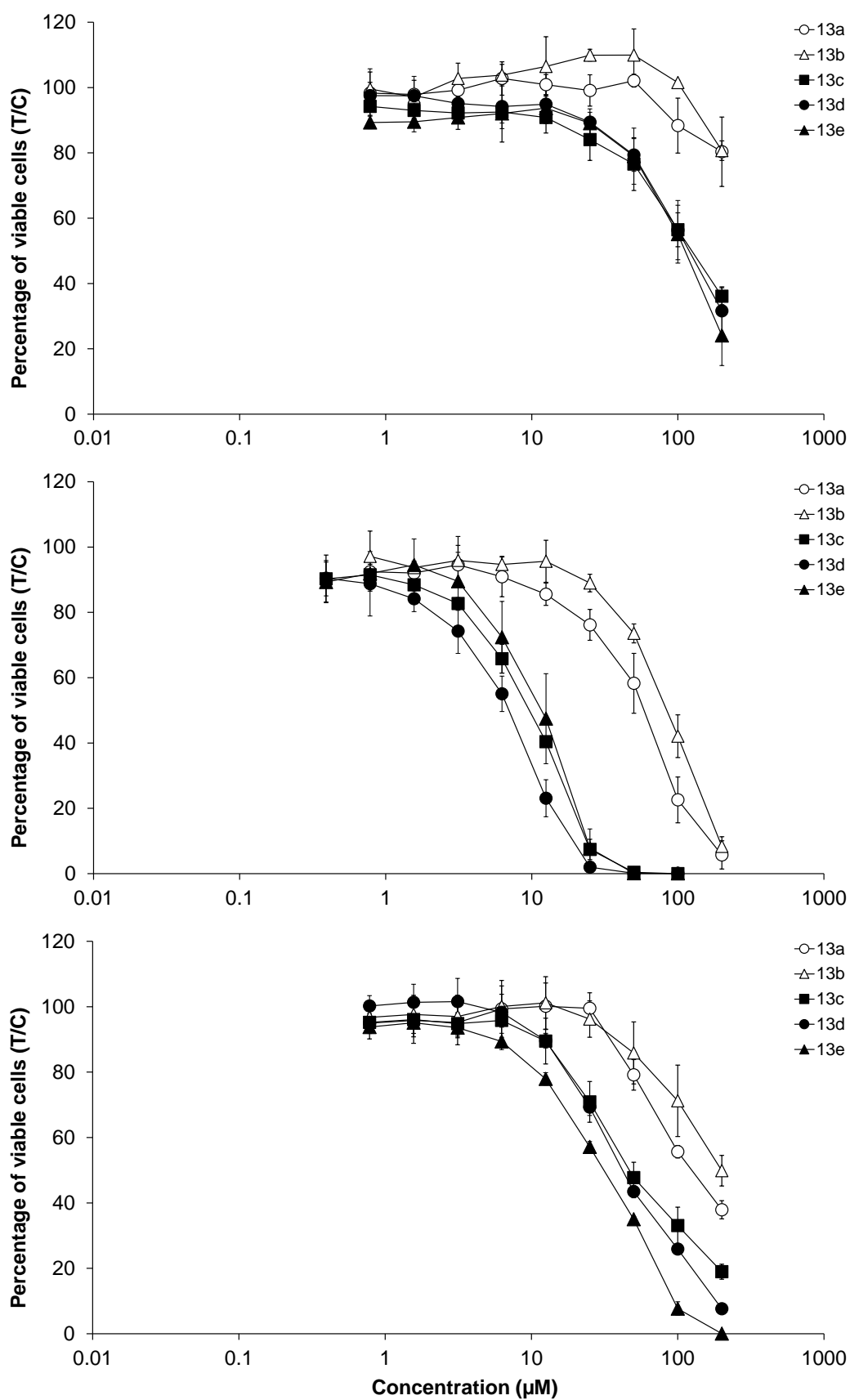


Figure S133. Concentration-effect curves of **13a–13e** in A549 (top), CH1/PA-1 (middle) and SW480 (bottom) cells, obtained by MTT assays with 96 h exposure time. Values are means \pm standard deviations from at least three independent experiments.

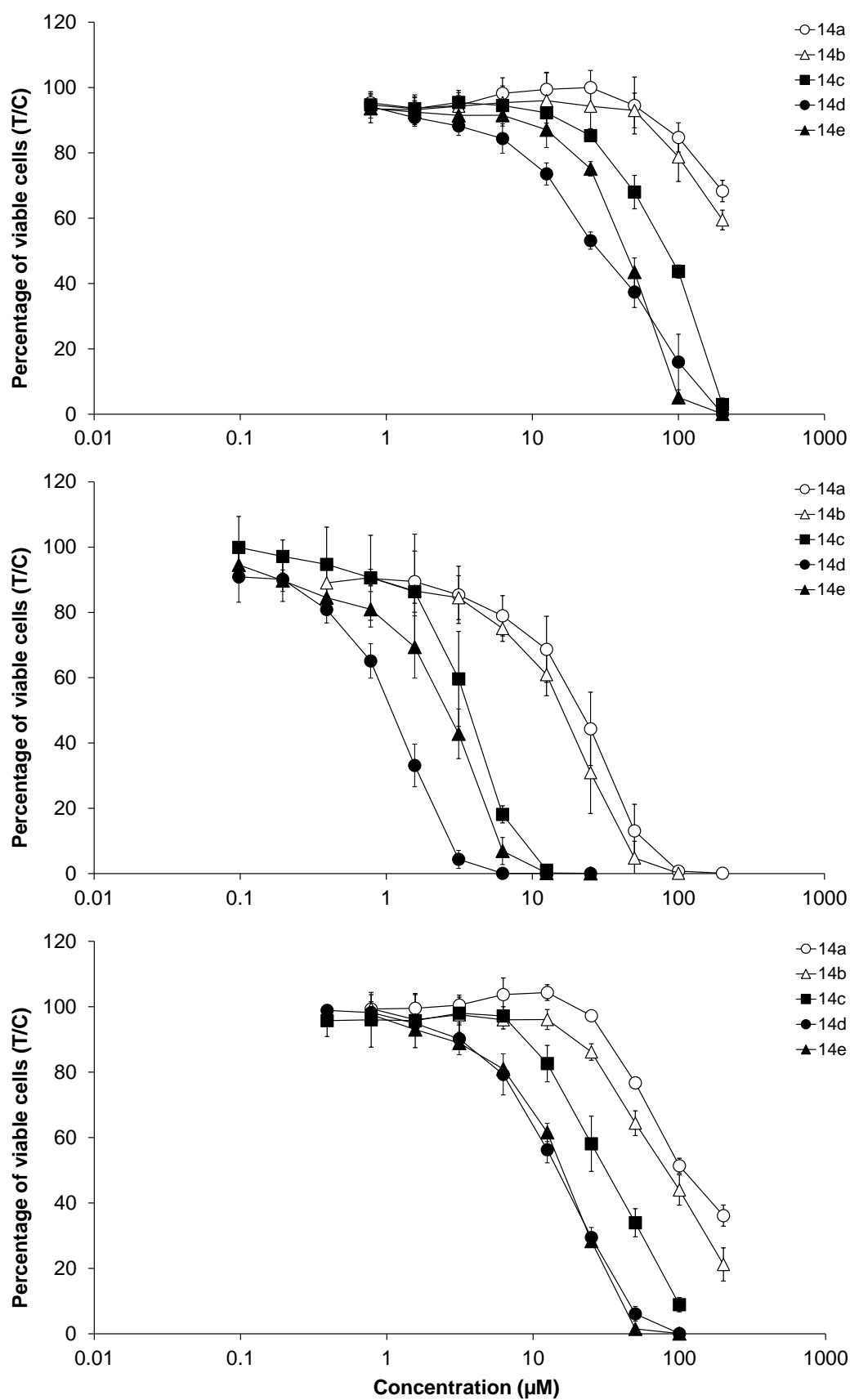


Figure S134. Concentration-effect curves of **14a–14e** in A549 (top), CH1/PA-1 (middle) and SW480 (bottom) cells, obtained by MTT assays with 96 h exposure time. Values are means \pm standard deviations from at least three independent experiments.

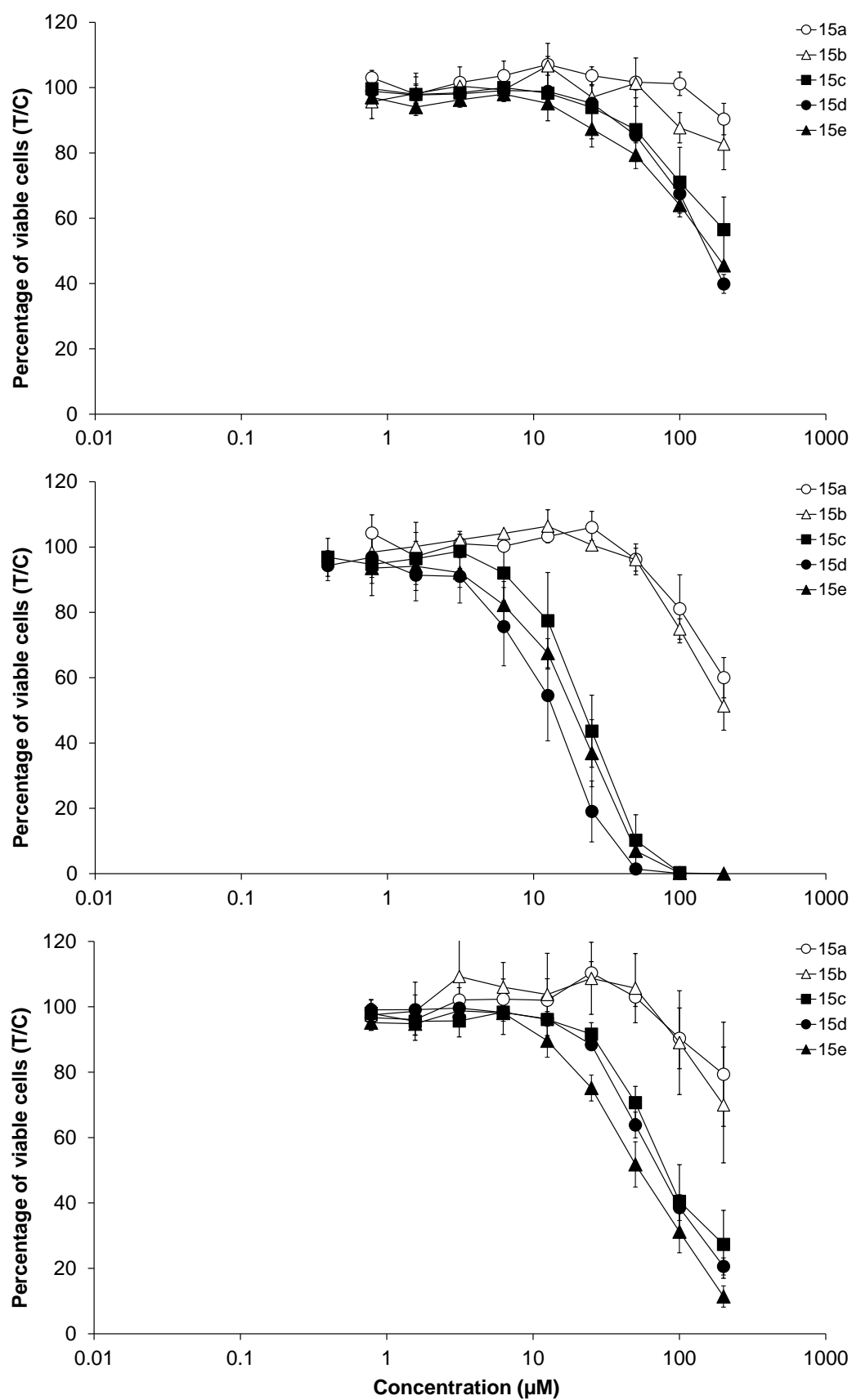


Figure S135. Concentration-effect curves of **15a–15e** in A549 (top), CH1/PA-1 (middle) and SW480 (bottom) cells, obtained by MTT assays with 96 h exposure time. Values are means \pm standard deviations from at least three independent experiments.

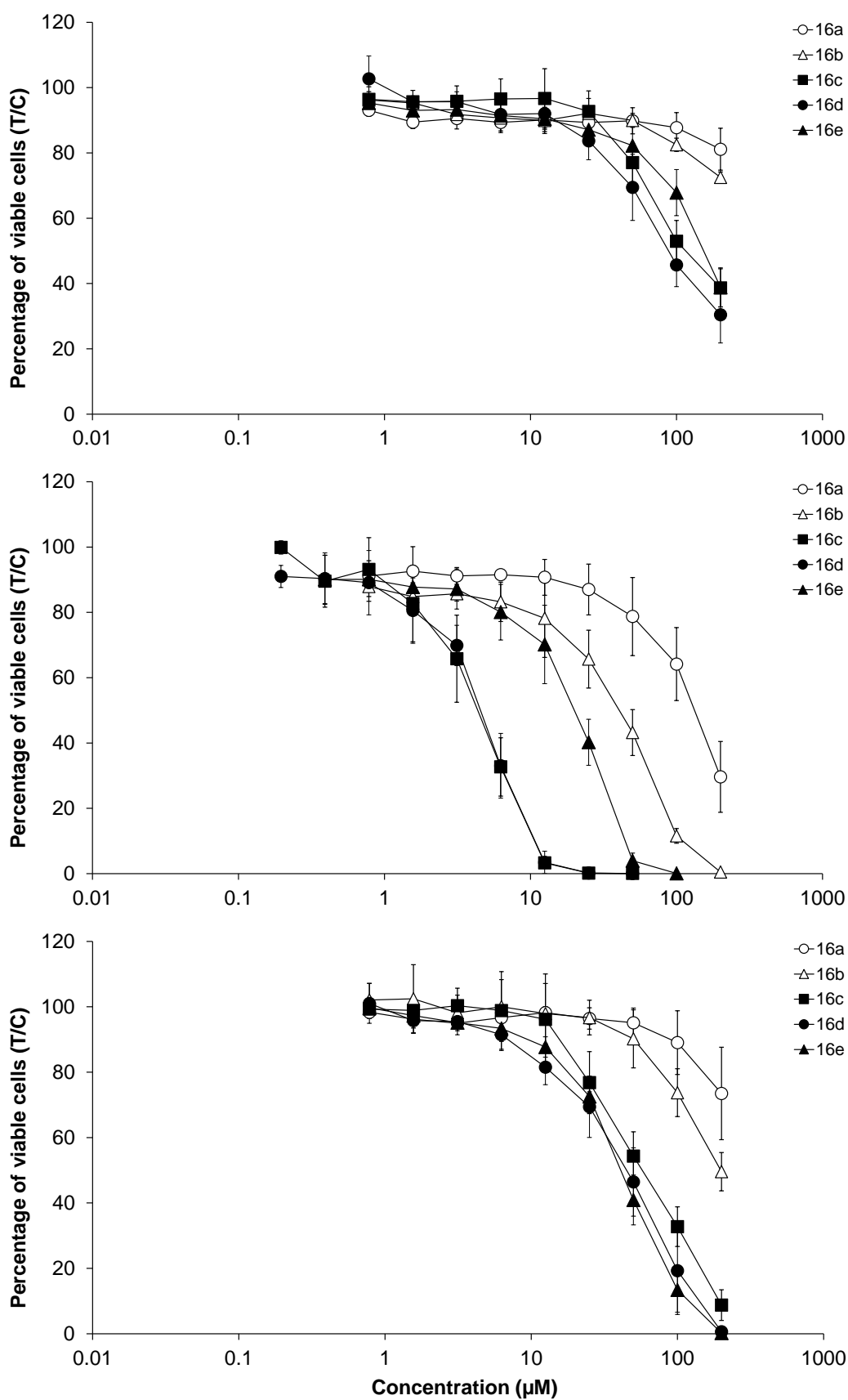


Figure S136. Concentration-effect curves of **16a–16e** in A549 (top), CH1/PA-1 (middle) and SW480 (bottom) cells, obtained by MTT assays with 96 h exposure time. Values are means \pm standard deviations from at least three independent experiments.

5. Flow-cytometric analysis

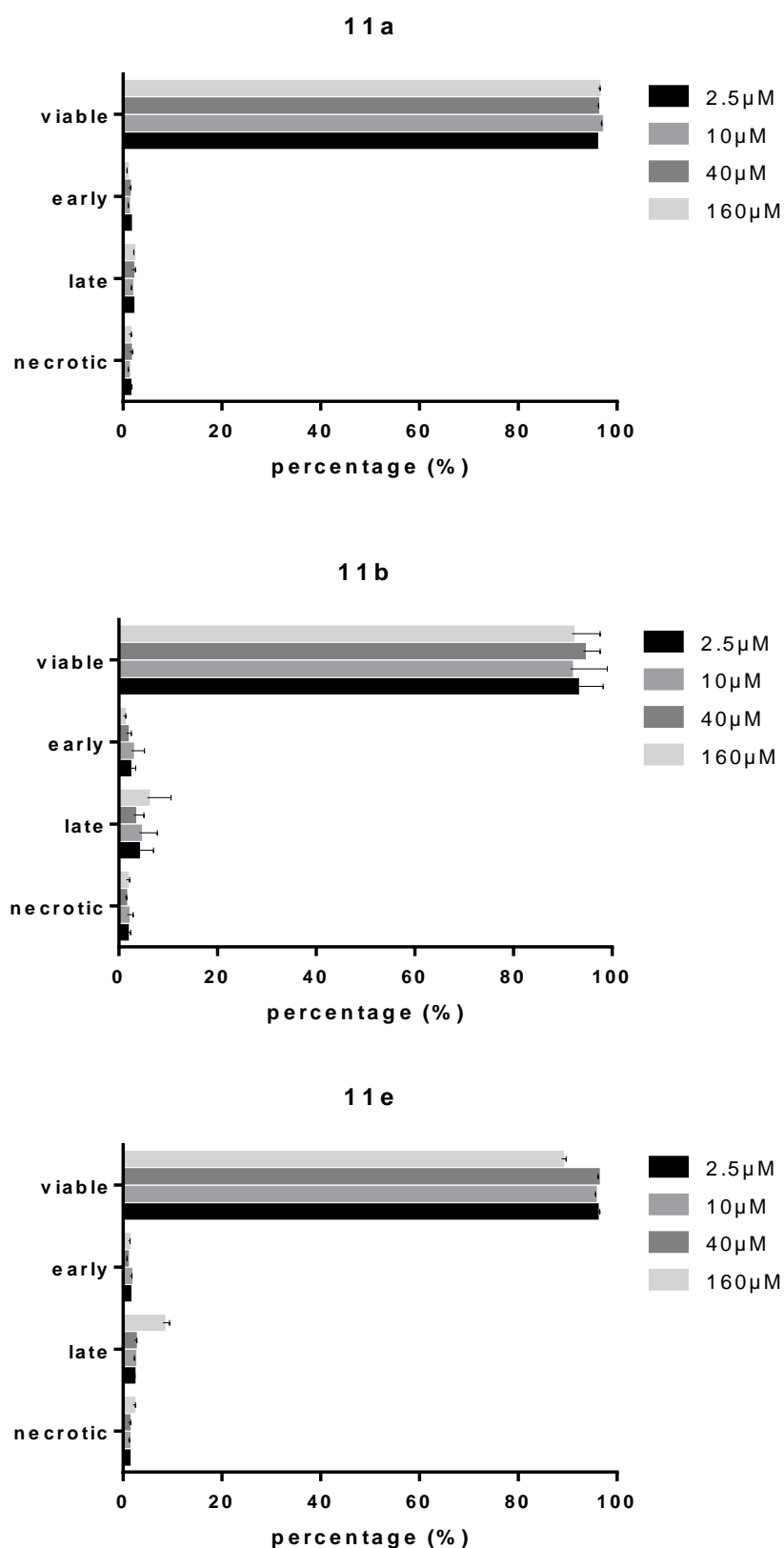


Figure S137. Flow-cytometric analysis of induction of early and late apoptosis as well as necrosis in SW480 after 24 h incubation with different concentrations of platinum(IV) complexes **11a**, **11b** and **11e**. The results are means with standard deviations from at least three independent experiments.

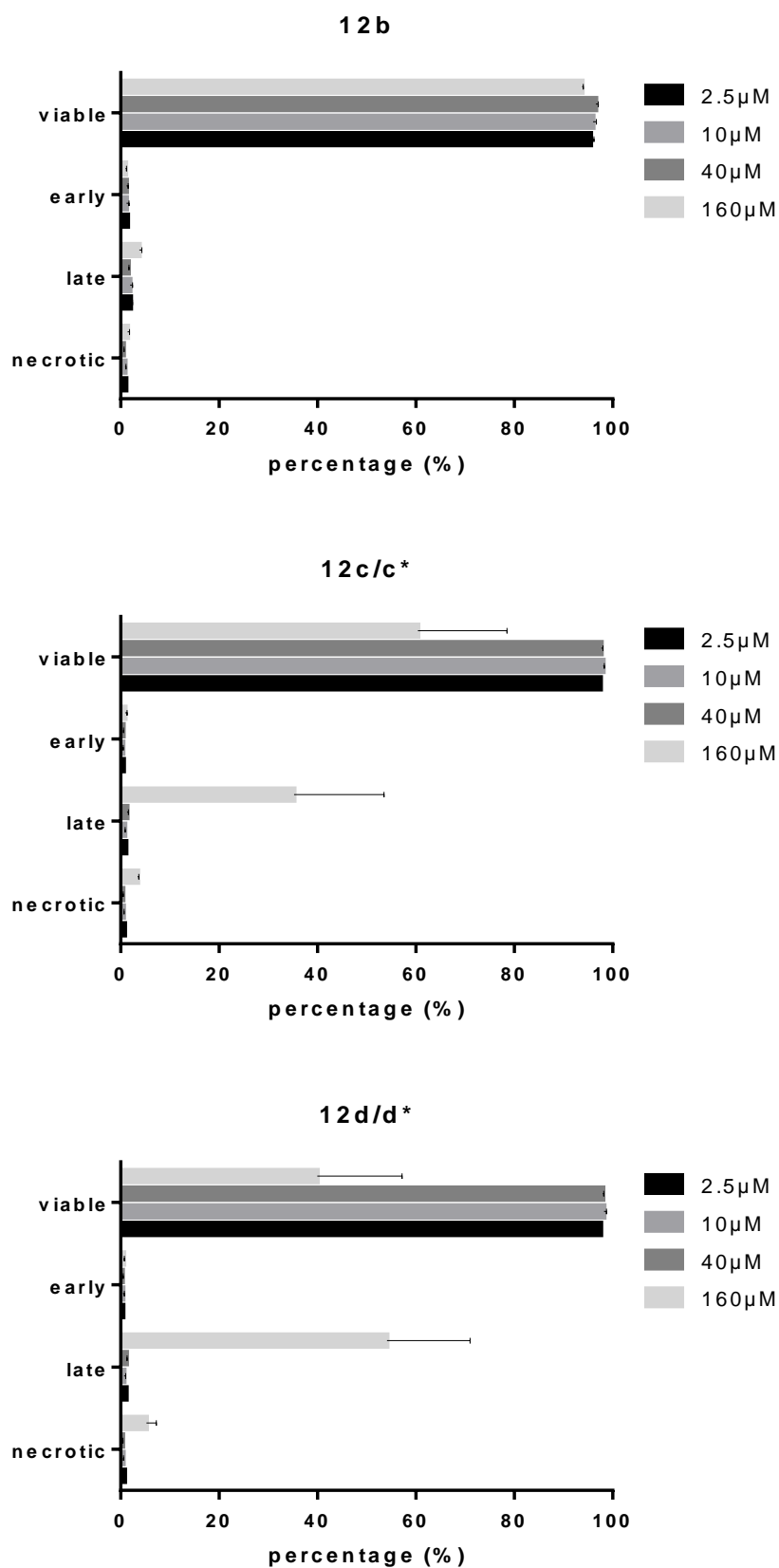


Figure S138. Flow-cytometric analysis of induction of early and late apoptosis as well as necrosis in SW480 after 24 h incubation with different concentrations of platinum(IV) complexes **12b**, **12c/12c*** and **12d/12d***. The results are means with standard deviations from at least three independent experiments.

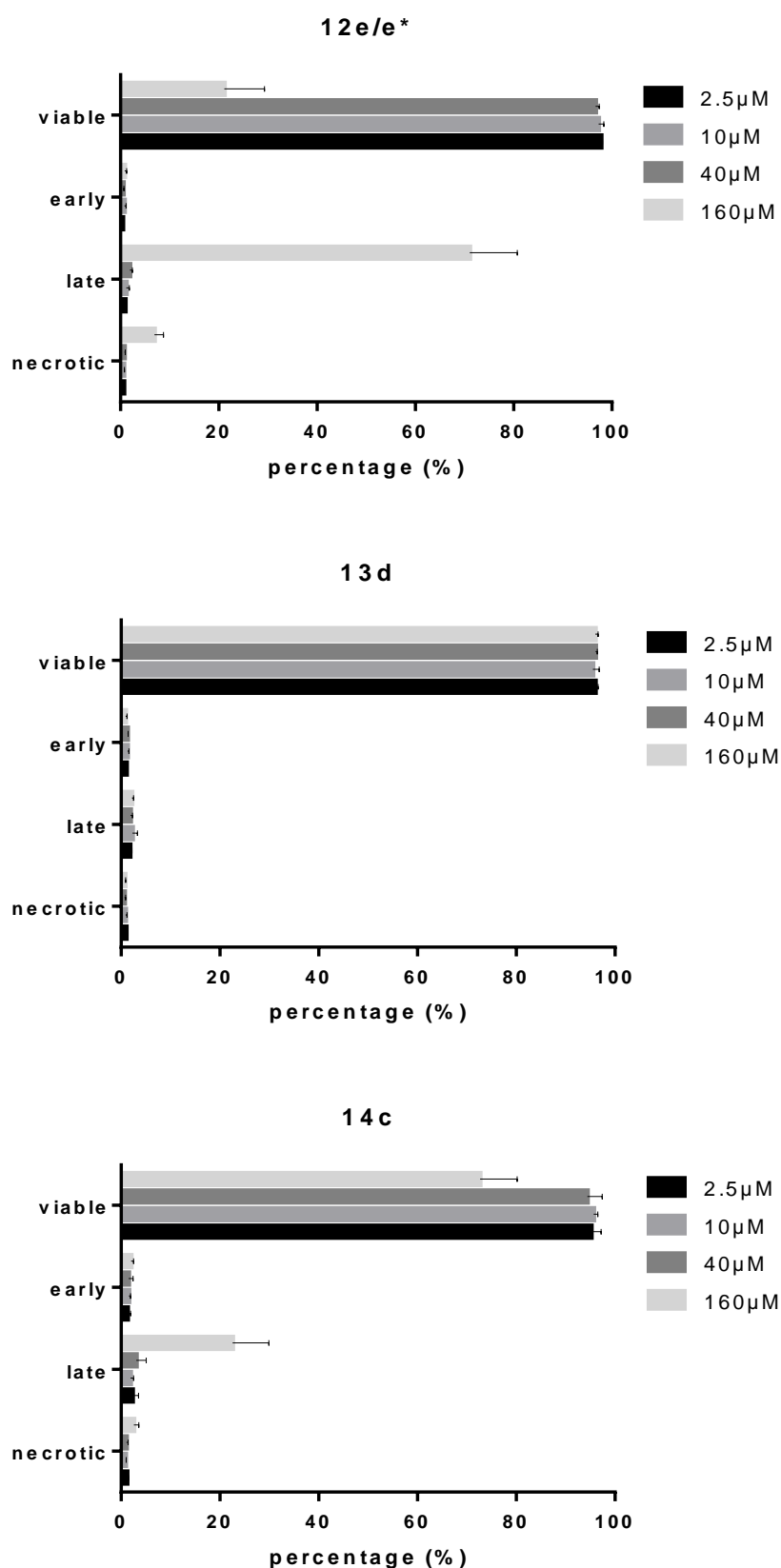


Figure S139. Flow-cytometric analysis of induction of early and late apoptosis as well as necrosis in SW480 after 24 h incubation with different concentrations of platinum(IV) complexes **12e/12e***, **13d** and **14c**. The results are means with standard deviations from at least three independent experiments.

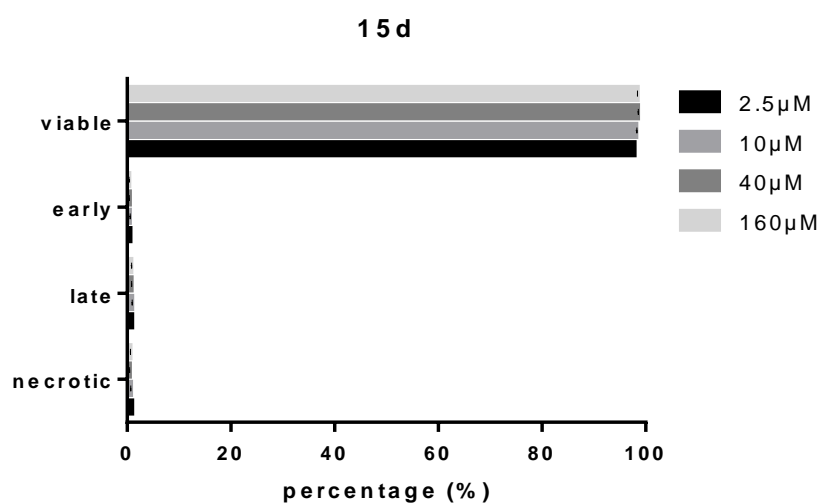
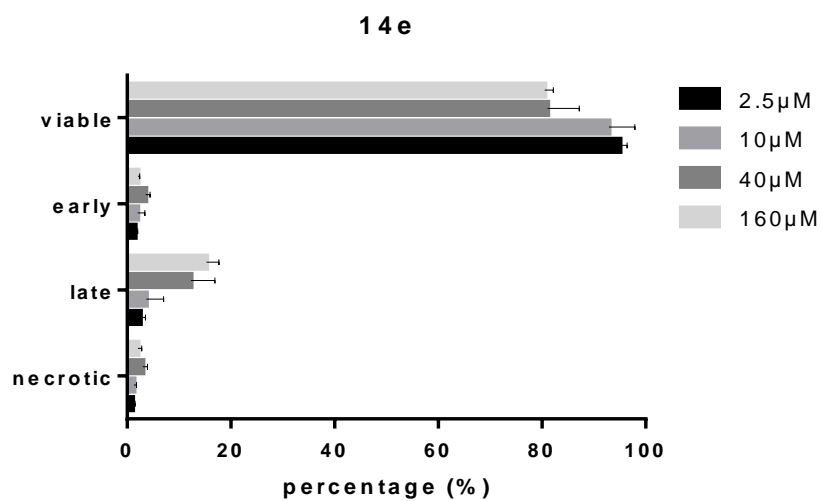
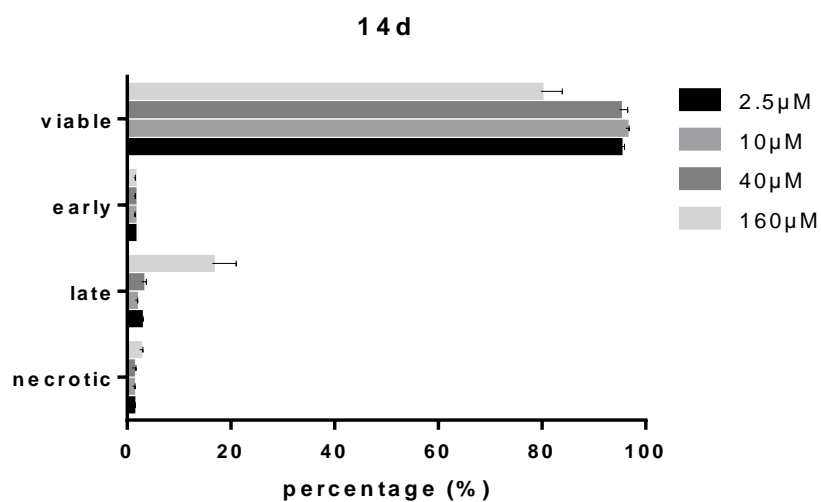


Figure S140. Flow-cytometric analysis of induction of early and late apoptosis as well as necrosis in SW480 after 24 h incubation with different concentrations of platinum(IV) complexes **14d**, **14e** and **15d**. The results are means with standard deviations from at least three independent experiments.

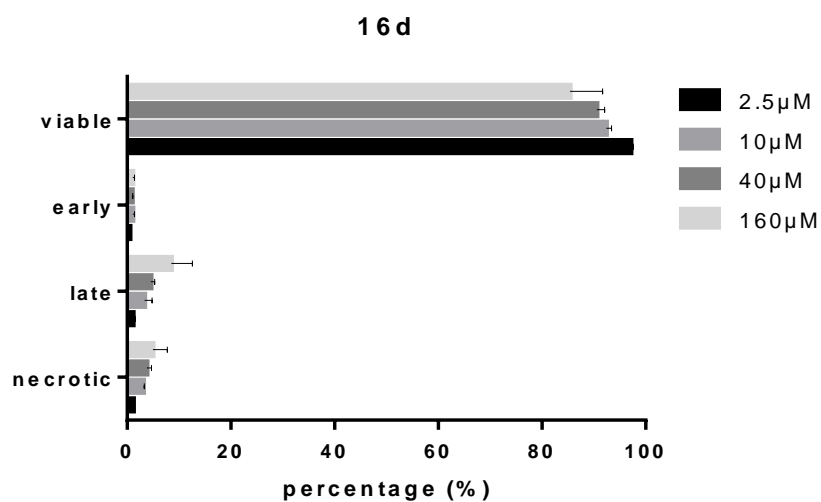


Figure S141. Flow-cytometric analysis of induction of early and late apoptosis as well as necrosis in SW480 after 24 h incubation with different concentrations of platinum(IV) complexes **16d**. The results are means with standard deviations from at least three independent experiments.

Table S28. Determination of apoptosis and necrosis induction by means of flow-cytometric annexin V/PI assays in SW480 colon cancer cells of selected platinum(IV) complexes.

Sample	Concentration [μ M]	Viable cells [%]	Early apoptotic cells [%]	Late apoptotic cells [%]	Necrotic cells [%]
11a	2.5	95.7 \pm 0.4	1.3 \pm 0.0	1.8 \pm 0.2	1.2 \pm 0.6
	10	96.7 \pm 0.2	0.9 \pm 0.2	1.6 \pm 0.1	0.9 \pm 0.2
11b	2.5	92.8 \pm 5.4	2.0 \pm 1.4	3.8 \pm 3.2	1.5 \pm 0.9
	10	91.6 \pm 7.4	2.6 \pm 2.6	4.2 \pm 3.6	1.7 \pm 1.2
11e	2.5	95.8 \pm 0.7	1.2 \pm 0.3	2.0 \pm 0.4	1.0 \pm 0.2
	10	95.4 \pm 0.3	1.4 \pm 0.4	2.2 \pm 0.1	1.0 \pm 0.3
12b	2.5	95.5 \pm 0.7	1.4 \pm 0.3	2.0 \pm 0.4	1.1 \pm 0.1
	10	96.0 \pm 0.7	1.2 \pm 0.5	1.9 \pm 0.5	0.9 \pm 0.2
12c/12c*	2.5	97.5 \pm 0.2	0.6 \pm 0.1	1.1 \pm 0.1	0.8 \pm 0.1
	10	98.1 \pm 0.3	0.5 \pm 0.1	0.9 \pm 0.1	0.6 \pm 0.1
12d/12d*	2.5	97.6 \pm 0.2	0.5 \pm 0.1	1.1 \pm 0.2	0.8 \pm 0.2
	10	98.3 \pm 0.5	0.5 \pm 0.3	0.7 \pm 0.3	0.6 \pm 0.1
12e/12e*	2.5	97.8 \pm 0.3	0.5 \pm 0.1	1.0 \pm 0.2	0.7 \pm 0.1
	10	97.3 \pm 1.1	0.8 \pm 0.4	1.2 \pm 0.6	0.7 \pm 0.1
13d	2.5	96.0 \pm 0.6	1.1 \pm 0.2	1.8 \pm 0.4	1.0 \pm 0.4
	10	95.5 \pm 1.3	1.3 \pm 0.3	2.3 \pm 1.0	0.9 \pm 0.3
14c	2.5	95.2 \pm 2.0	1.3 \pm 0.6	2.3 \pm 1.2	1.2 \pm 0.3
	10	95.7 \pm 0.8	1.6 \pm 0.3	1.9 \pm 0.6	0.9 \pm 0.1
14d	2.5	95.0 \pm 0.9	1.3 \pm 0.3	2.5 \pm 0.6	1.1 \pm 0.5
	10	96.2 \pm 0.6	1.3 \pm 0.2	1.6 \pm 0.4	1.0 \pm 0.5
14e	2.5	95.0 \pm 1.4	1.5 \pm 0.5	2.5 \pm 1.0	1.0 \pm 0.5
	10	92.9 \pm 5.0	2.0 \pm 1.4	3.7 \pm 3.3	1.3 \pm 0.5
15d	2.5	97.3 \pm 0.2	0.5 \pm 0.1	0.9 \pm 0.2	0.9 \pm 0.2
	10	98.1 \pm 0.2	0.4 \pm 0.2	0.9 \pm 0.1	0.6 \pm 0.1
16d	2.5	97.1 \pm 0.5	0.5 \pm 0.1	1.2 \pm 0.4	1.2 \pm 0.1
	10	92.4 \pm 1.0	1.1 \pm 0.4	3.4 \pm 1.5	3.2 \pm 0.1

6. References

1. Bruker SAINT v8.38B Copyright © 2005-2019 Bruker AXS.
2. Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
3. Dolomanov, O. V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H. OLEX2: A Complete Structure Solution, Refinement and Analysis Program. *J Appl Crystallogr* **2009**, *42*, 339–341, doi:10.1107/S0021889808042726.
4. Hübschle, C.B.; Sheldrick, G.M.; Dittrich, B. ShelXle: A Qt Graphical User Interface for SHELXL. *J Appl Crystallogr* **2011**, *44*, 1281–1284, doi:10.1107/S0021889811043202.
5. Sheldrick, G. M. (2015). SHELXS v 2016/4 University of Göttingen, Germany.
6. Sheldrick, G. M. (2015). SHELXL v 2016/4 University of Göttingen, Germany.
7. Spek, A.L. Structure Validation in Chemical Crystallography. *Acta Crystallogr D Biol Crystallogr* **2009**, *65*, 148–155, doi:10.1107/S090744490804362X.