

Synthesis, Characterisation and Reactivity studies of Chiral β -Diketimate Supported Aluminum Lewis Acid Complexes Towards Difficult Diels Alder Cycloadditions

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Supporting Information

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NMR Spectrum of Ligands and Complexes
(oxa = oxazoline)

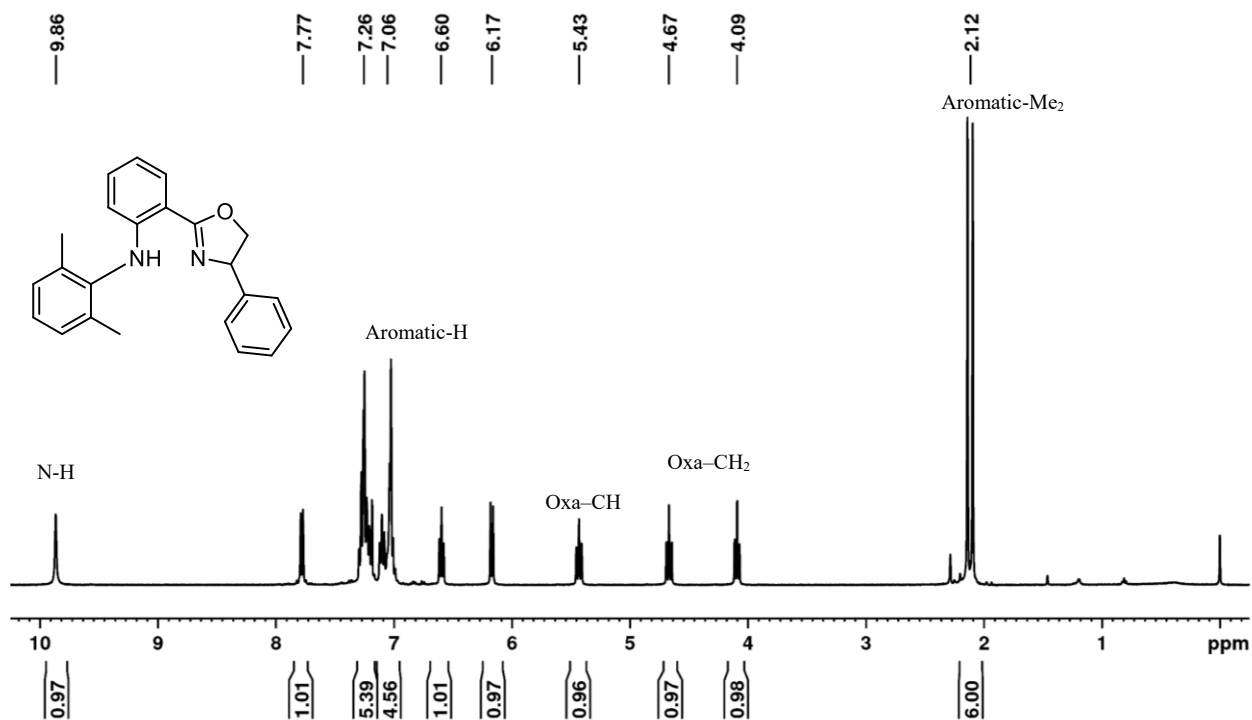


Figure S1. ¹H NMR spectrum of **3H**

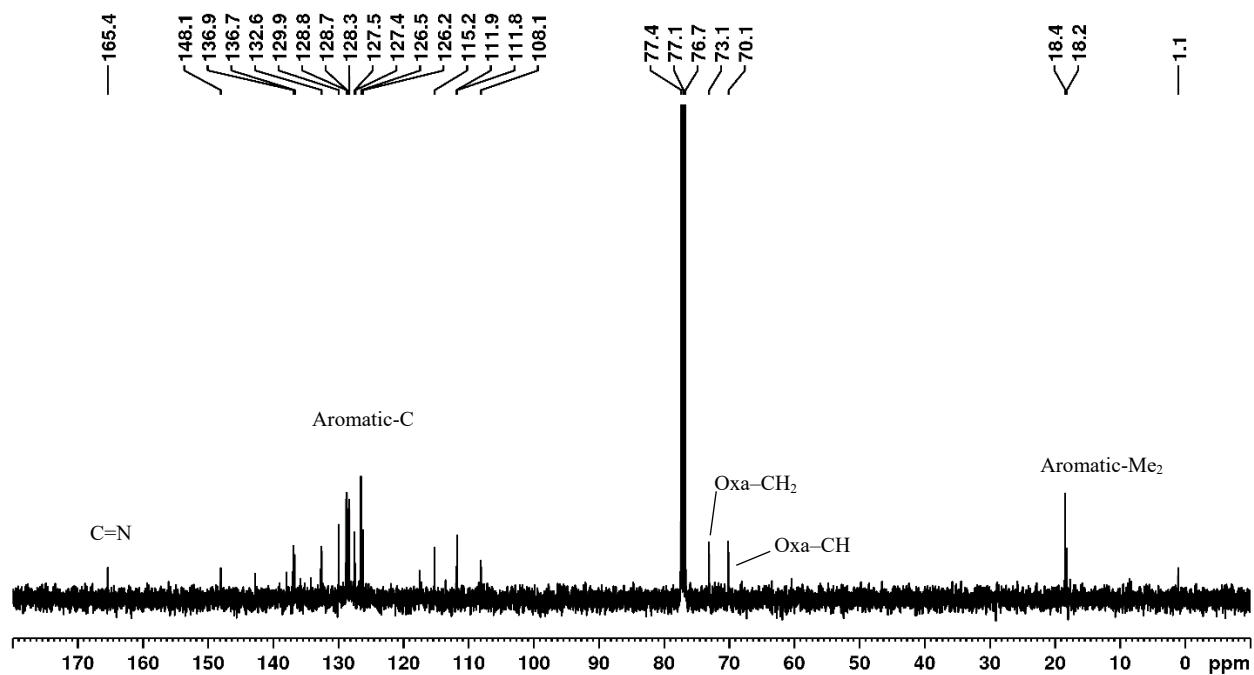


Figure S2. ¹³C NMR spectrum of **3H**

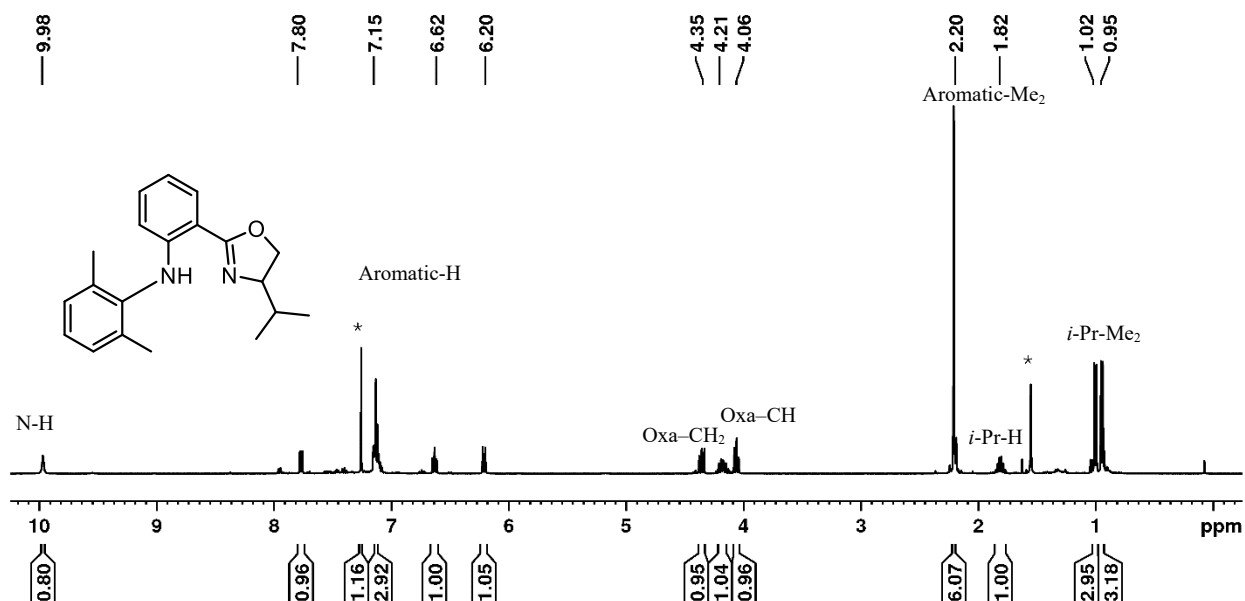


Figure S3. ¹H NMR spectrum of **4aH**. Note: solvent impurities are indicated by *

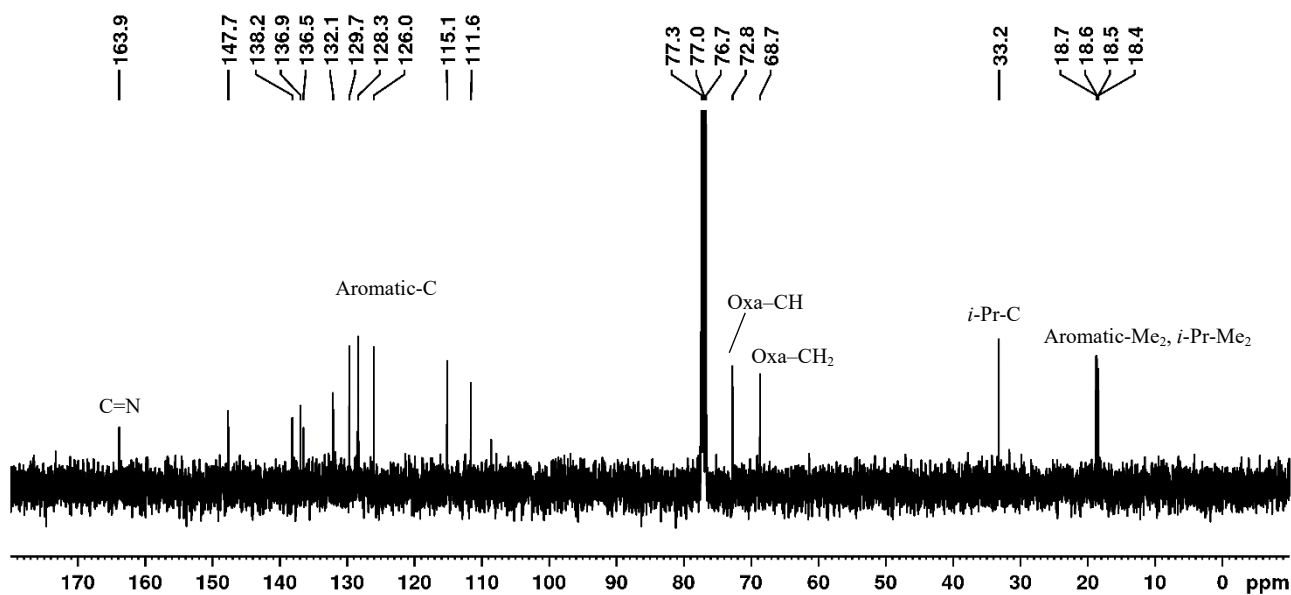


Figure S4. ¹³C NMR spectrum of **4aH**

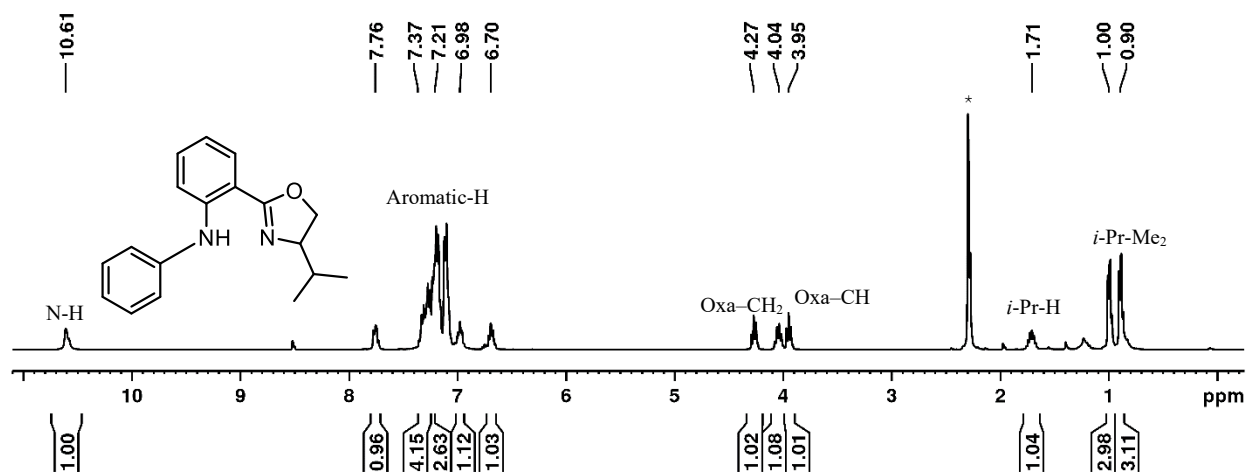


Figure S5. ¹H NMR spectrum of **4bH**. Note: solvent impurities are indicated by *

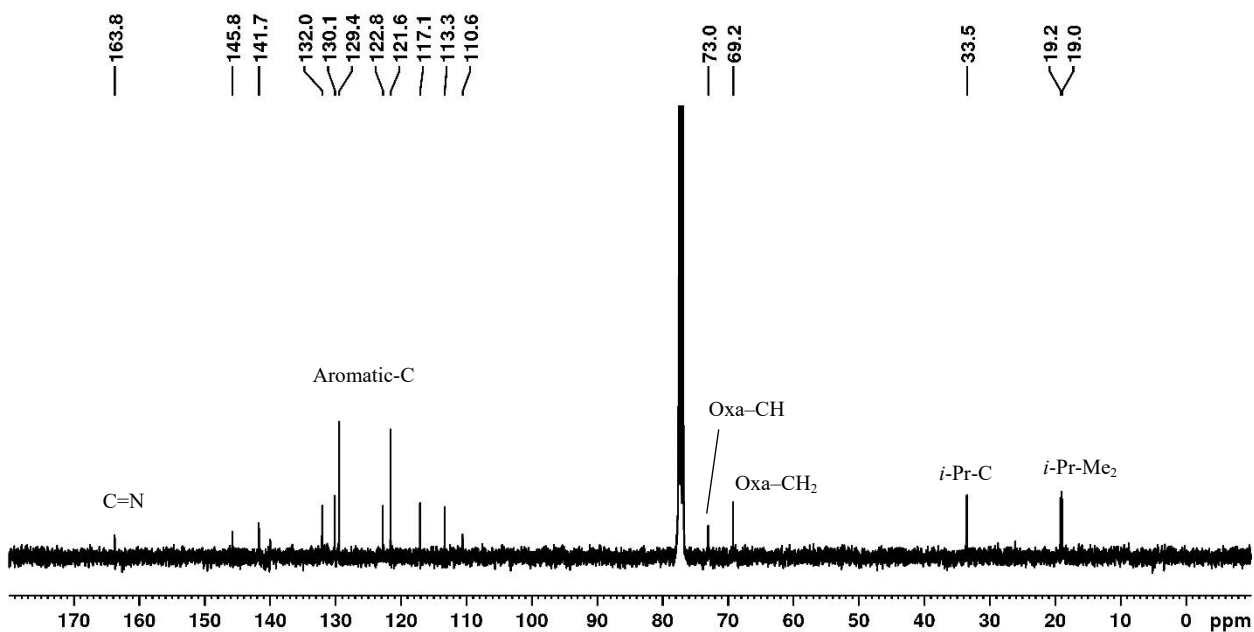


Figure S6. ¹³C NMR spectrum of **4bH**.

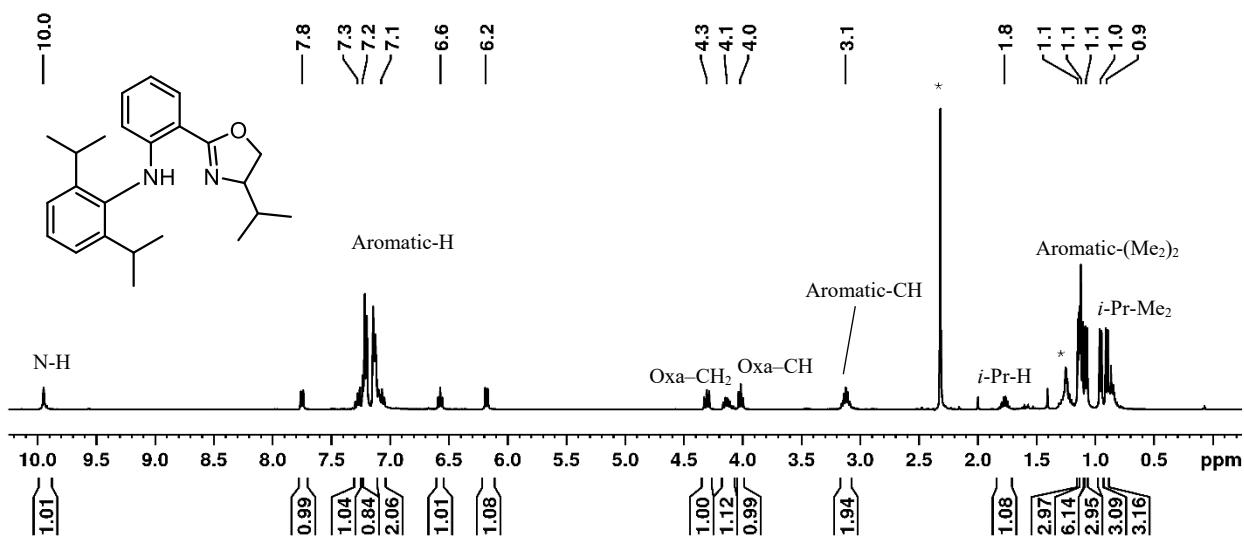


Figure S7. ^1H NMR spectrum of **4cH**. Note: solvent impurities are indicated by *

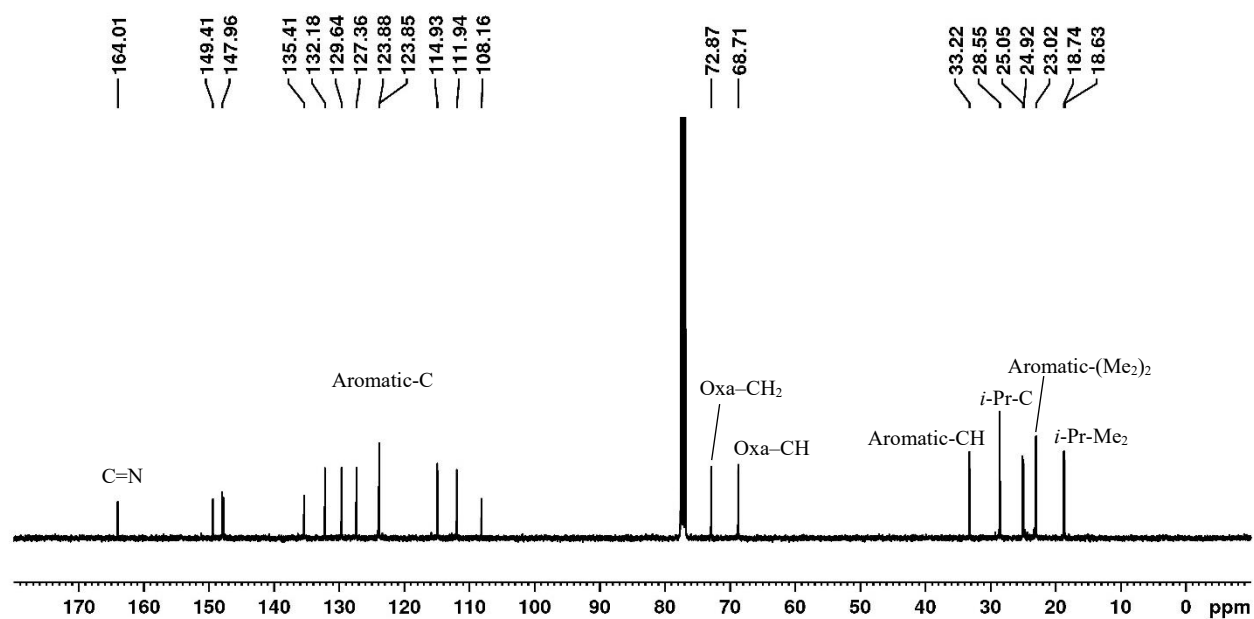


Figure S8. ^{13}C NMR spectrum of **4cH**.

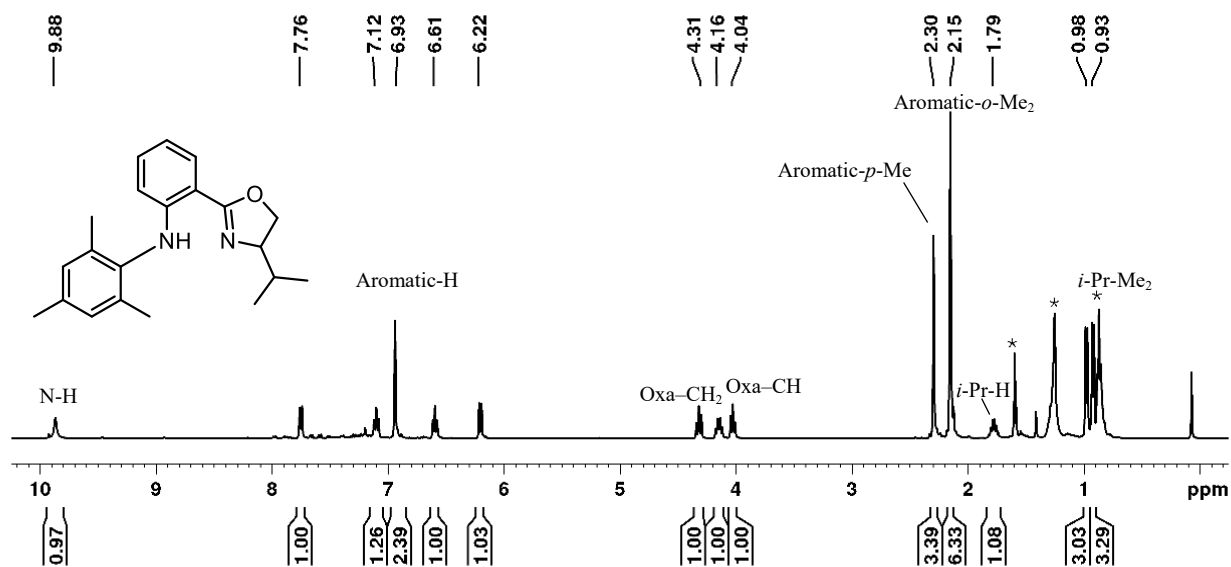


Figure S9. ^1H NMR spectrum of **4dH**. Note: solvent impurities are indicated by *

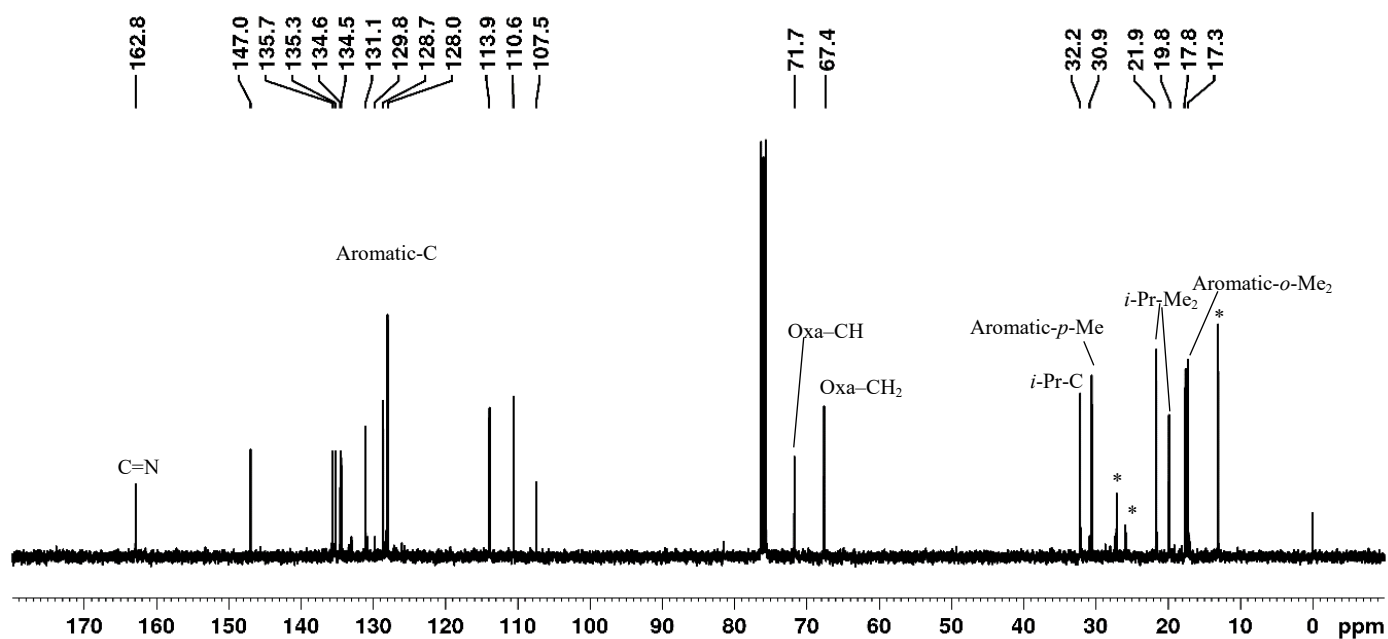


Figure S10. ^{13}C NMR spectrum of **4dH**. solvent impurities are indicated by *

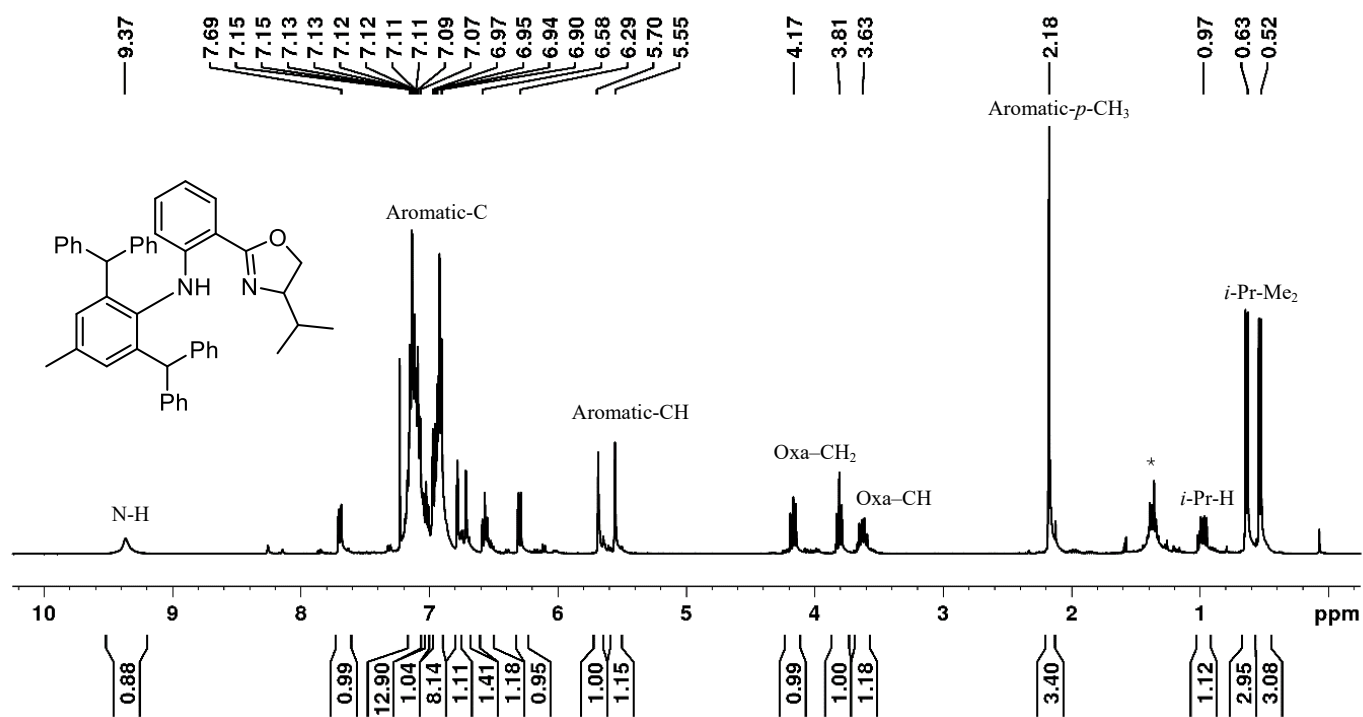


Figure S11. ^1H NMR spectrum of **4eH**. Note: solvent impurities are indicated by *

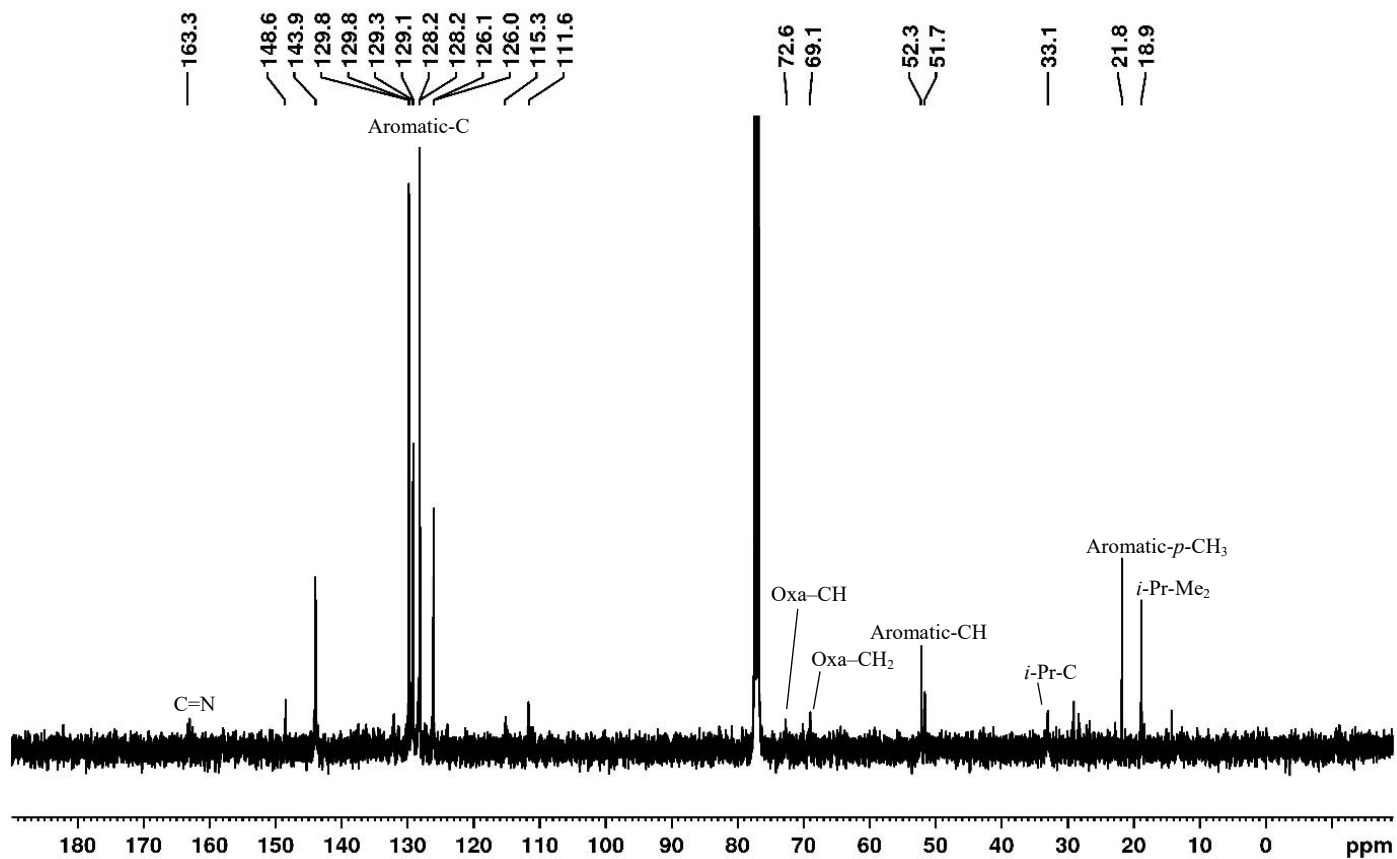


Figure S12. ^{13}C NMR spectrum of **4eH**

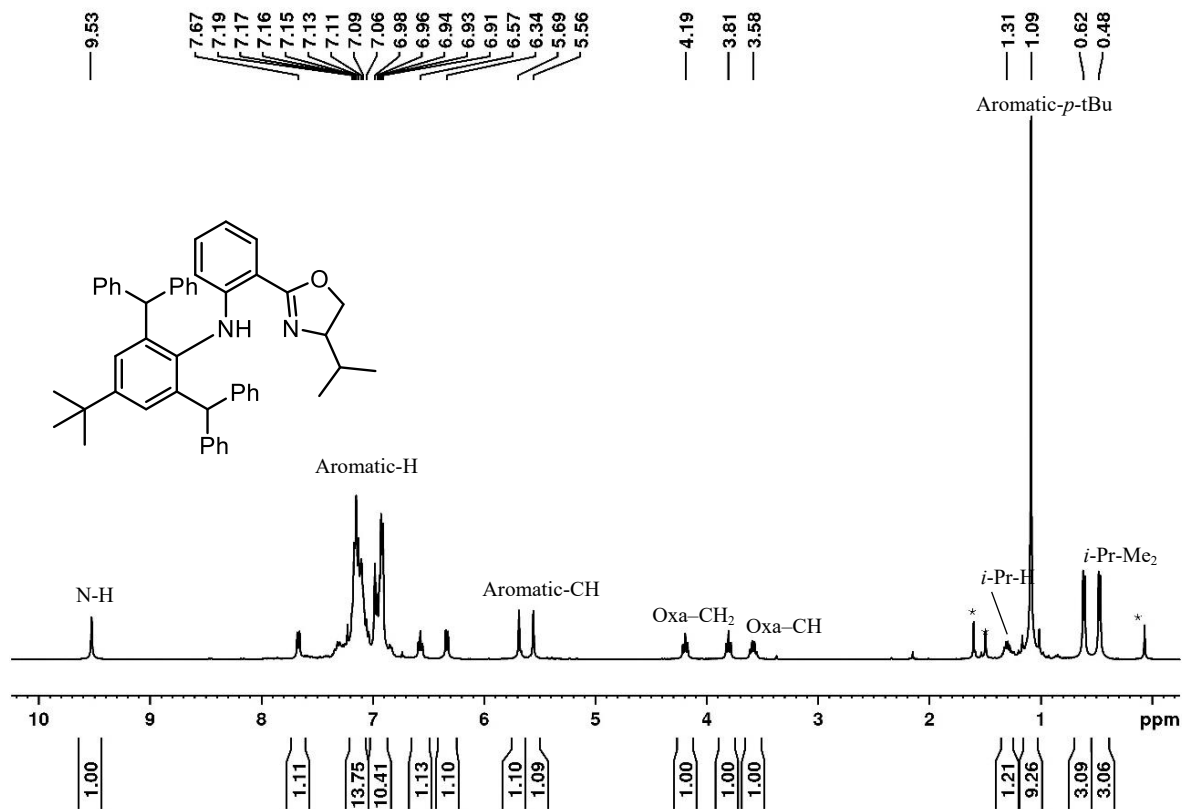


Figure S13. ¹H NMR spectrum of **4fH**. Note: solvent impurities are indicated by *

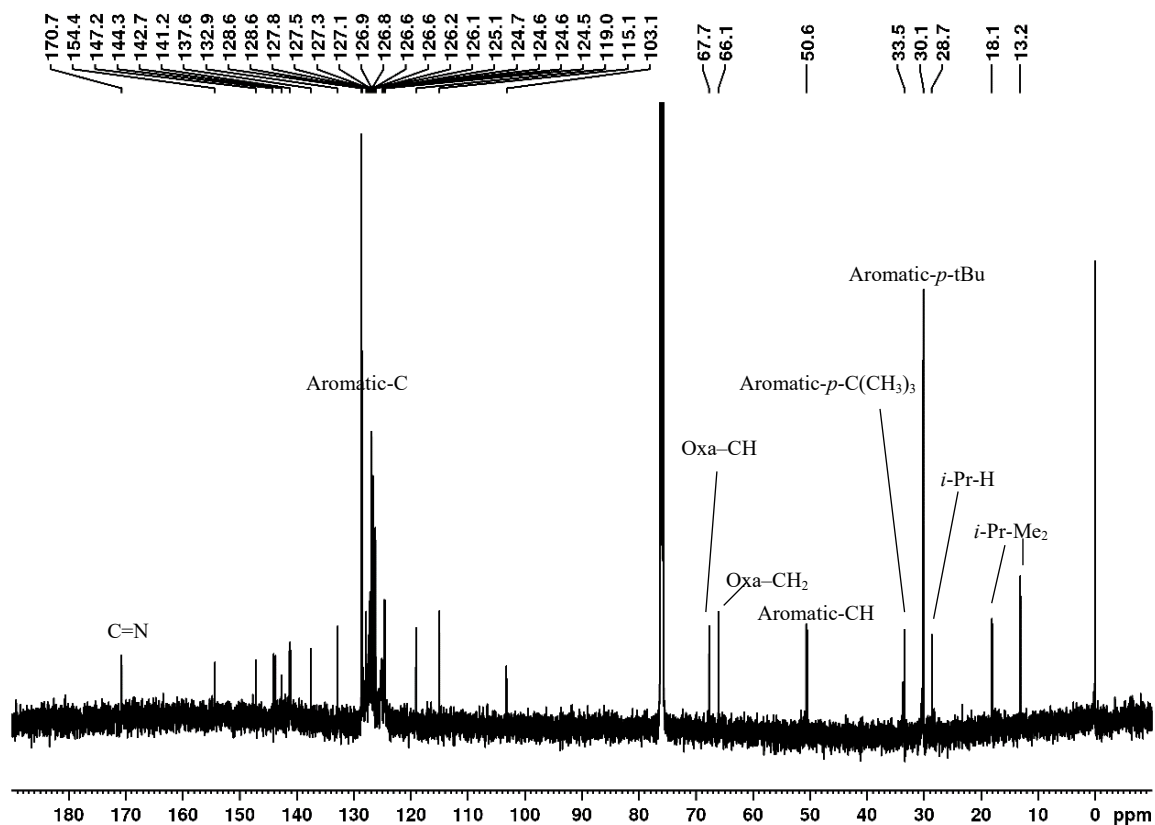


Figure S14. ¹³C NMR spectrum of **4fH**.

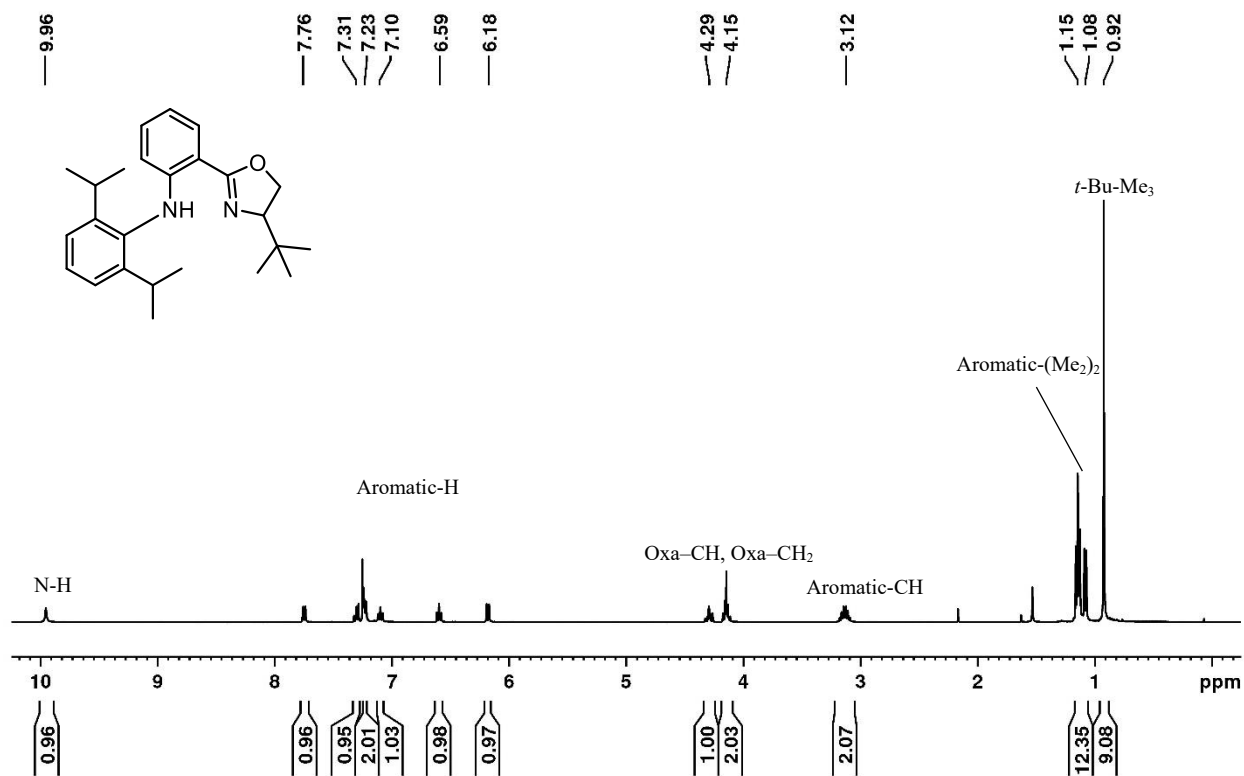


Figure S15. ¹H NMR spectrum of **5cH**.

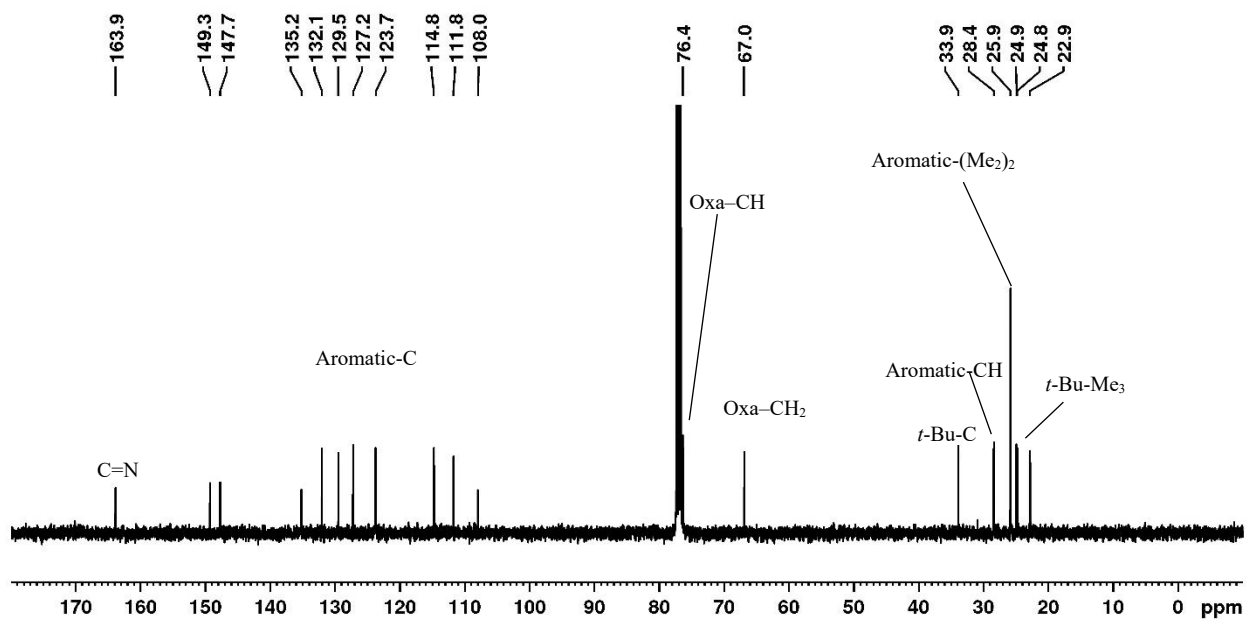


Figure S16. ¹³C NMR spectrum of **5cH**.

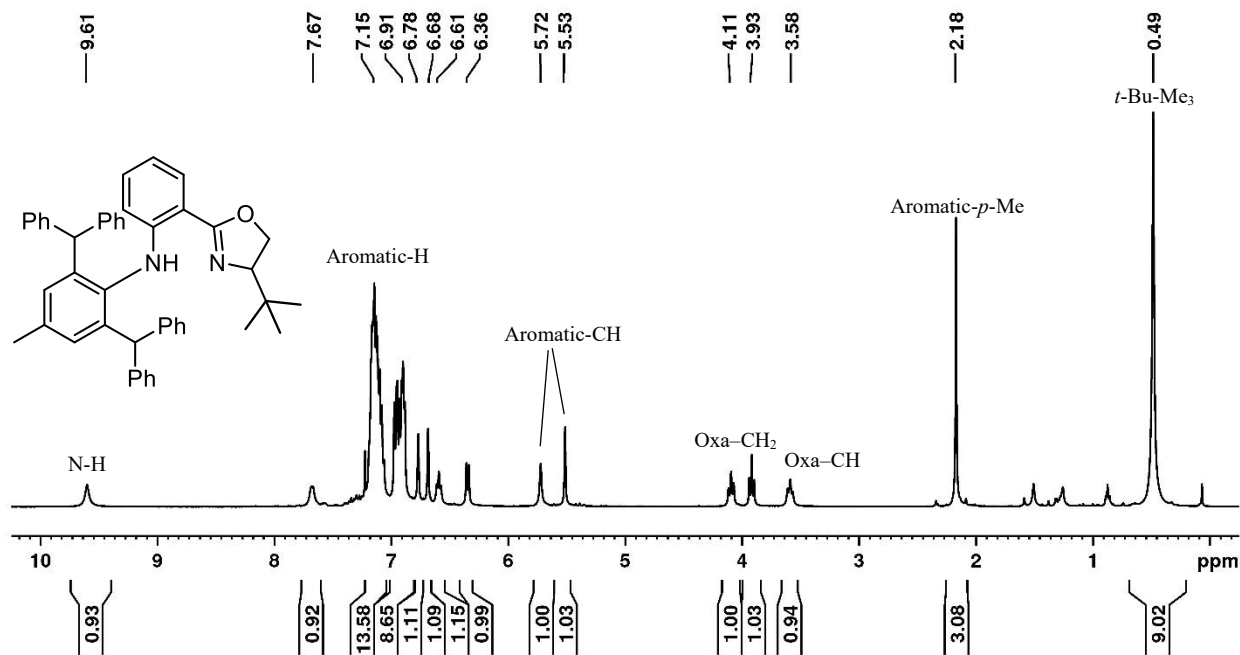


Figure S17. ^1H NMR spectrum of **5eH**.

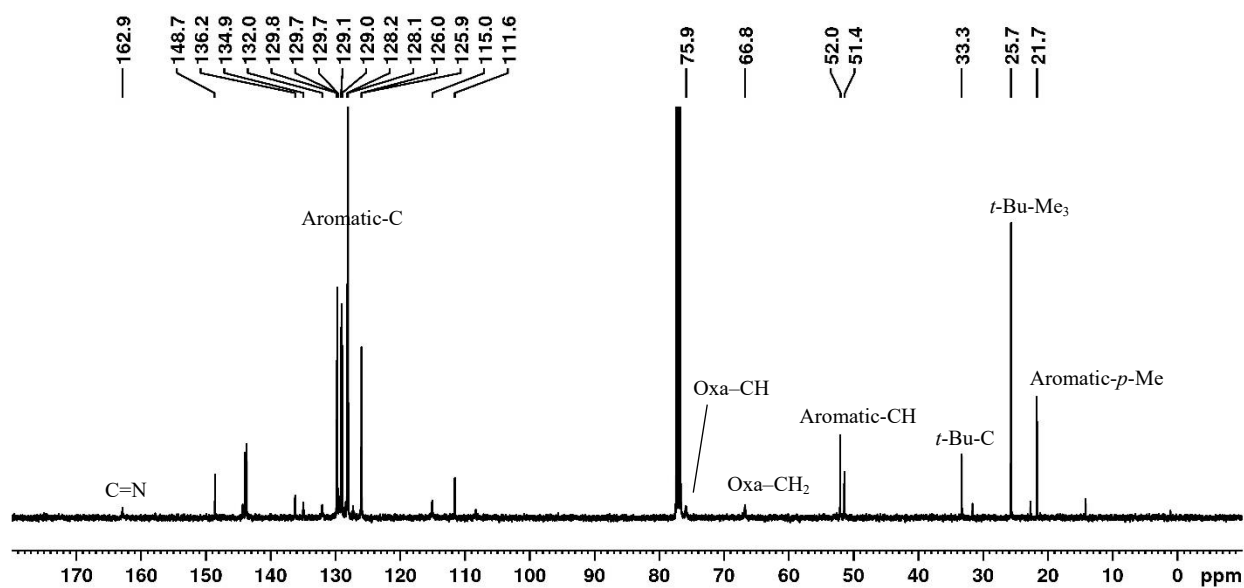


Figure S18. ^{13}C NMR spectrum of **5eH**.

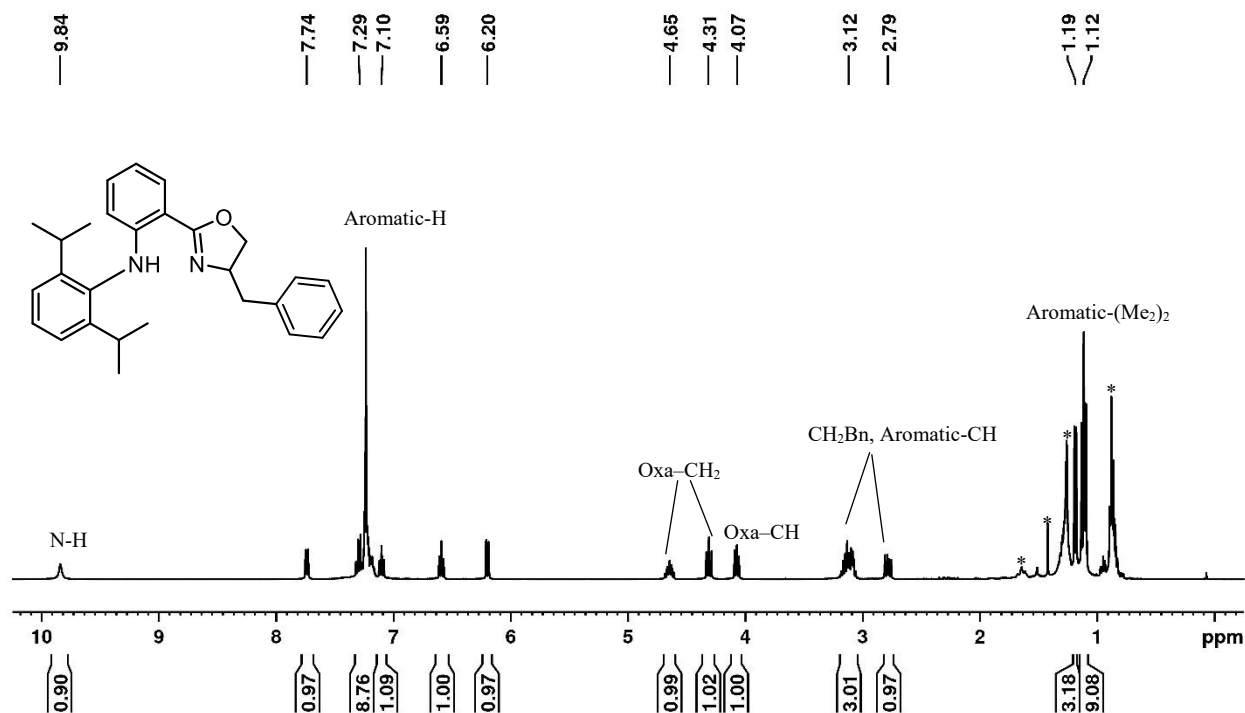


Figure S19. ¹H NMR spectrum of **6cH**. solvent impurities are indicated by *

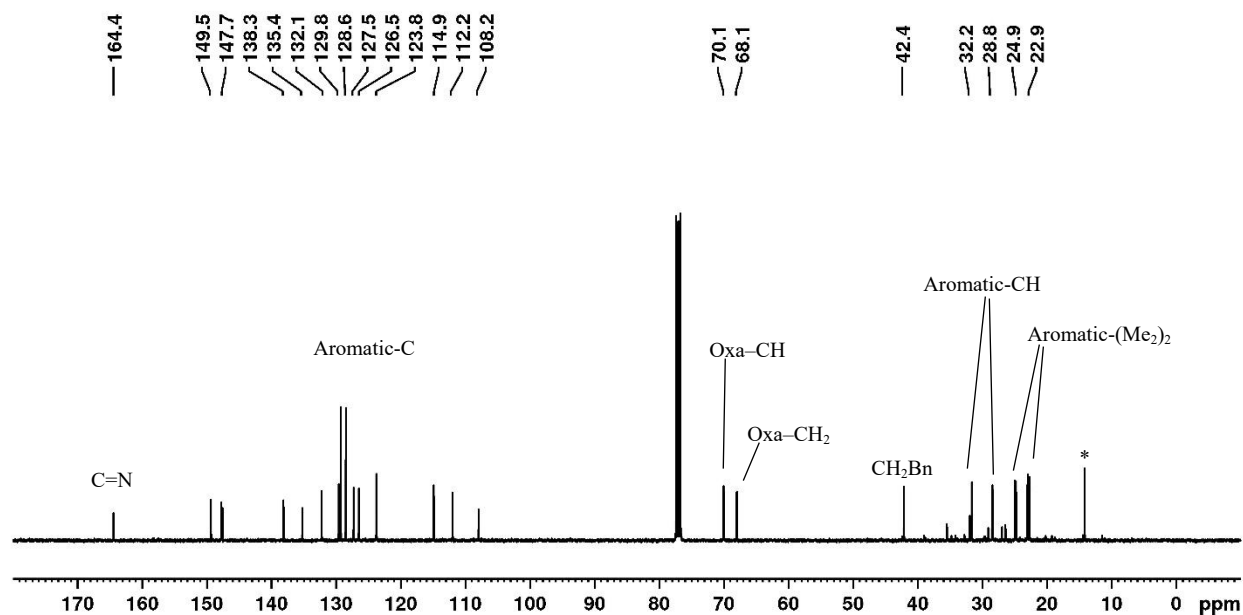


Figure S20. ¹³C NMR spectrum of **6cH**. solvent impurities are indicated by *

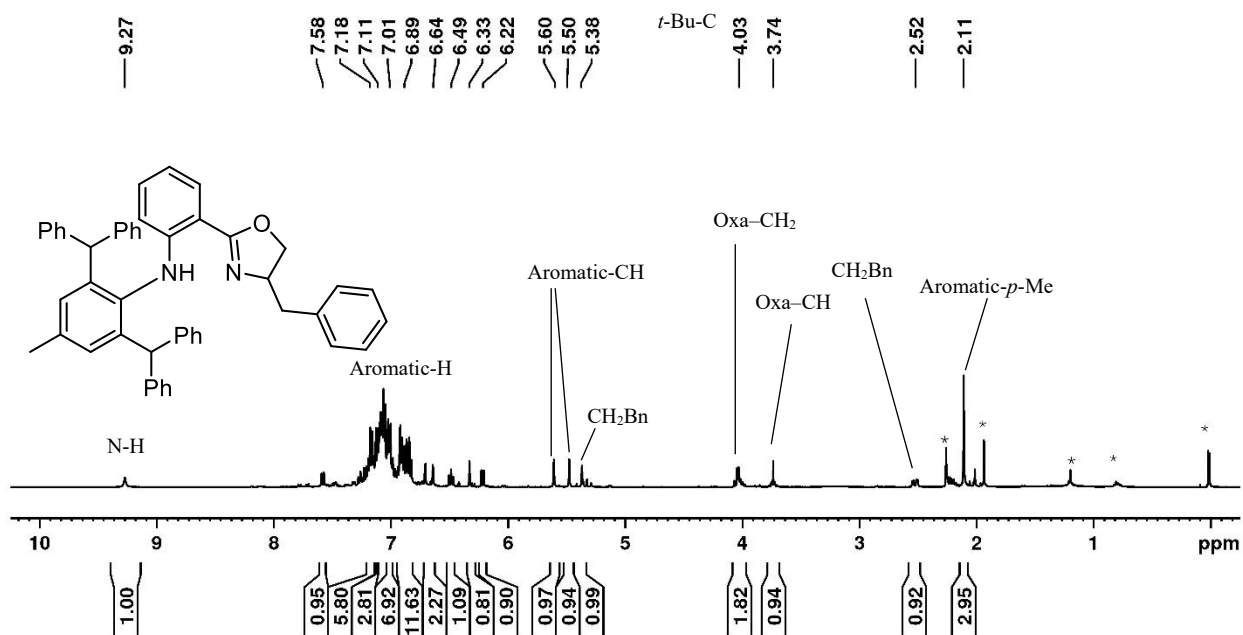


Figure S21. ^1H NMR spectrum of **6eH**. solvent impurities are indicated by *

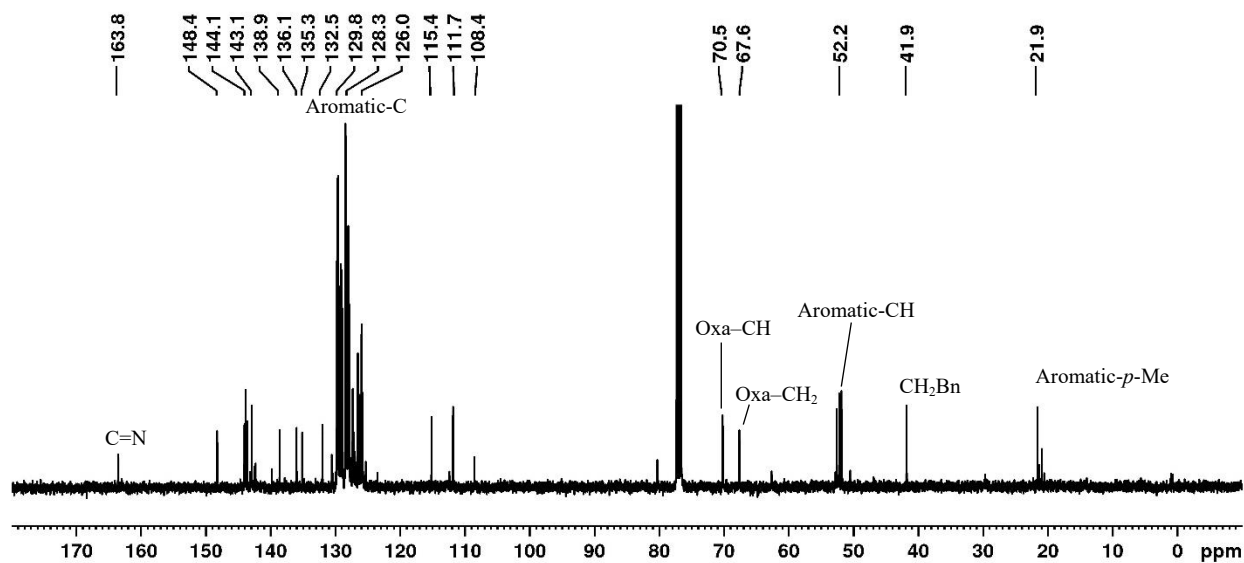


Figure S22. ^{13}C NMR spectrum of **6eH**.

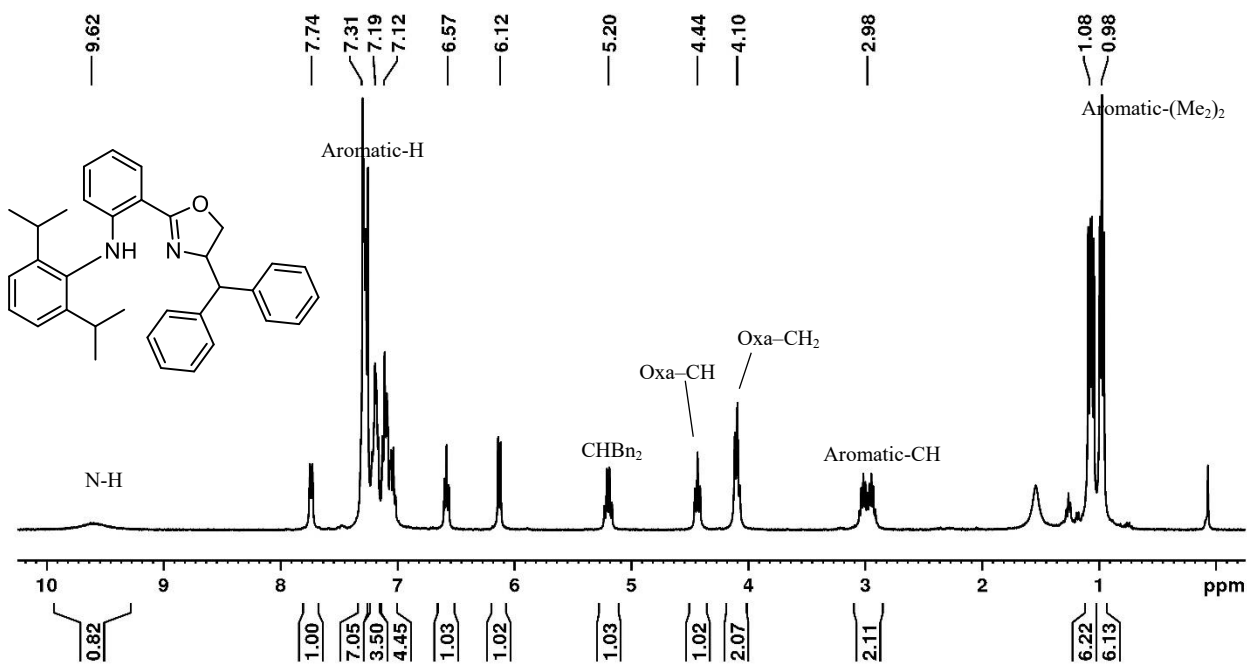


Figure S23. ^1H NMR spectrum of **7cH**.

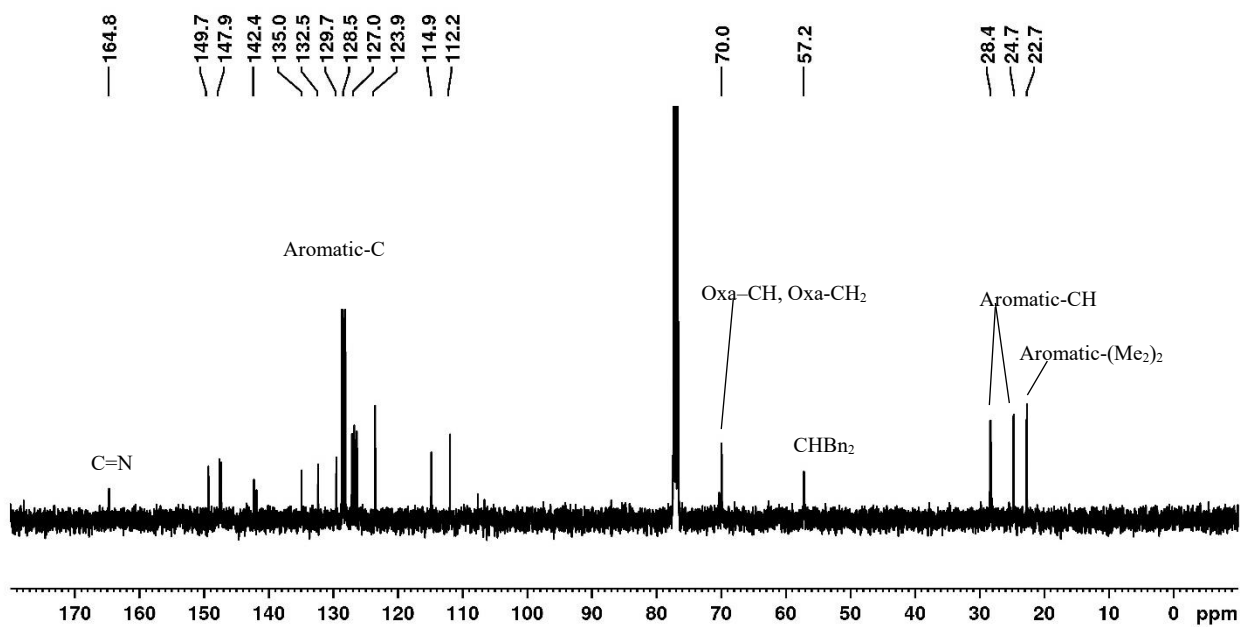


Figure S24. ^{13}C NMR spectrum of **7cH**.

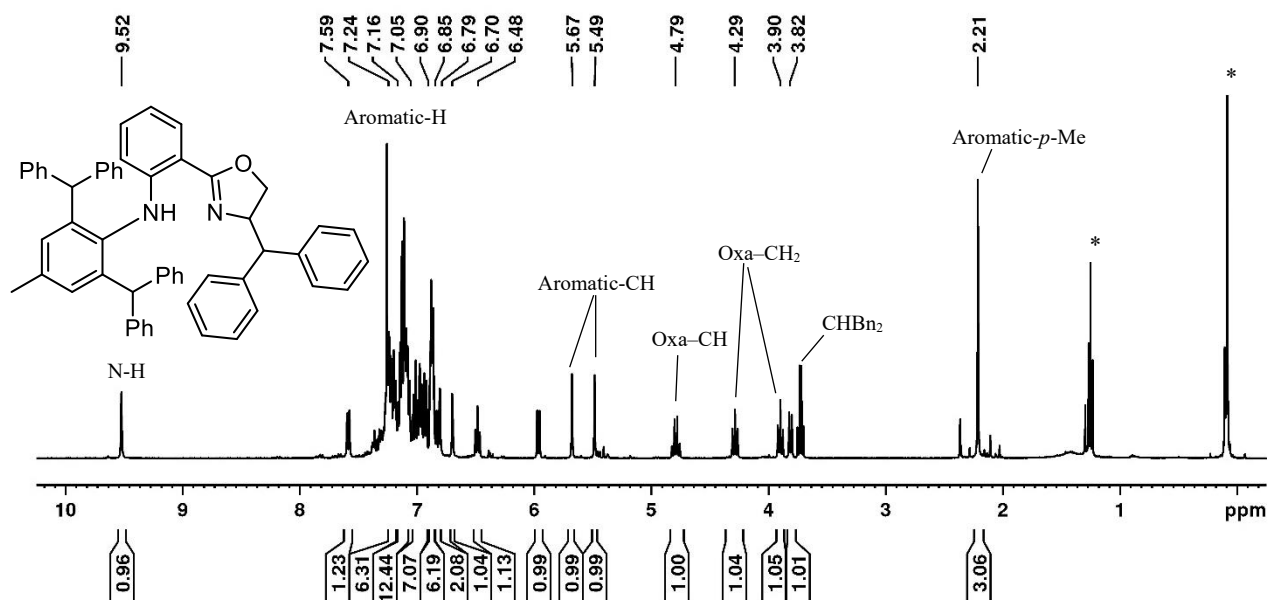


Figure S25. ¹H NMR spectrum of **7eH**. solvent impurities are indicated by *

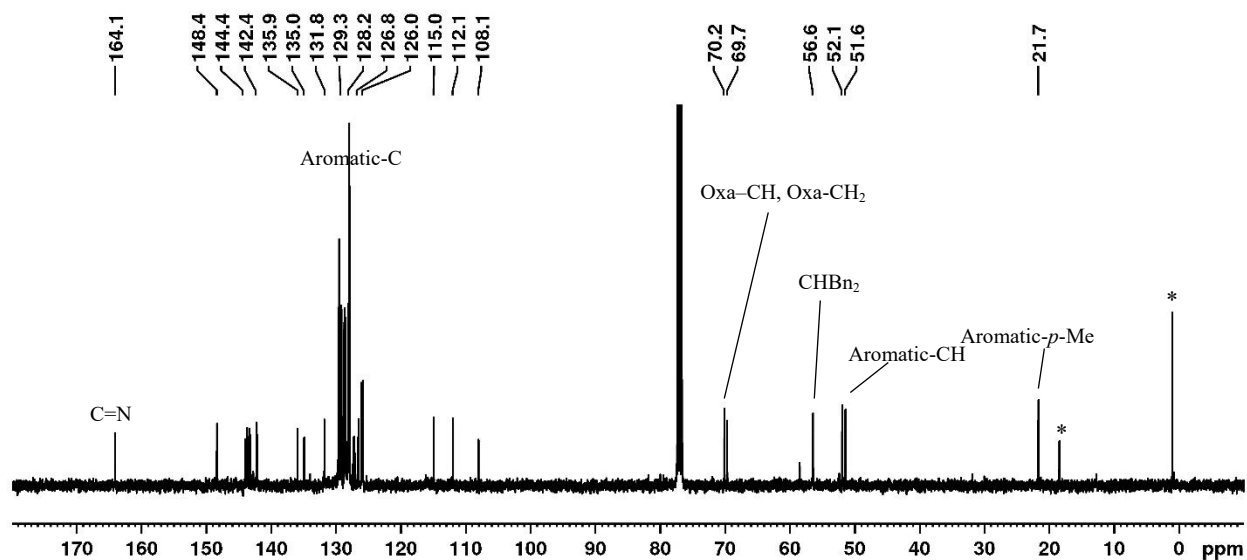


Figure S26. ¹³C NMR spectrum of **7eH**.

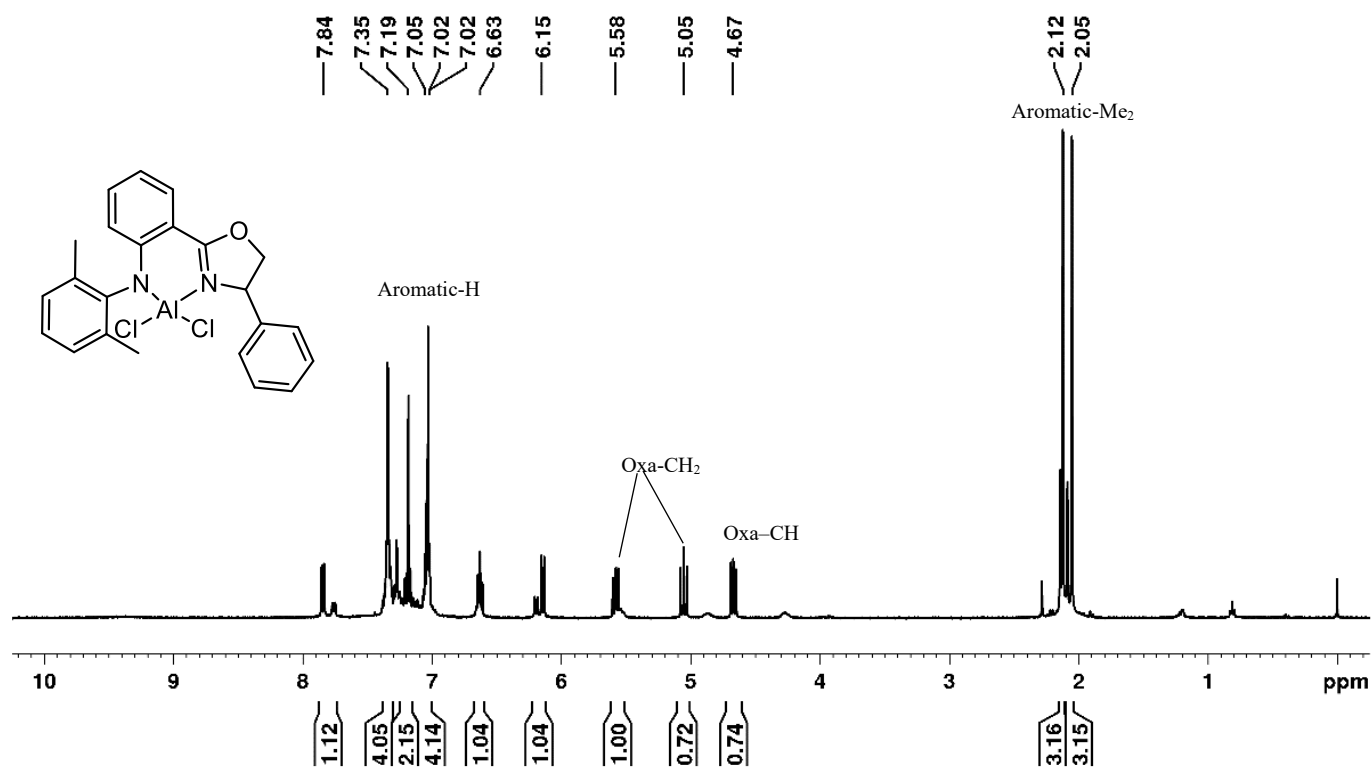


Figure S27. ^1H NMR spectrum of 3AlCl_2 .

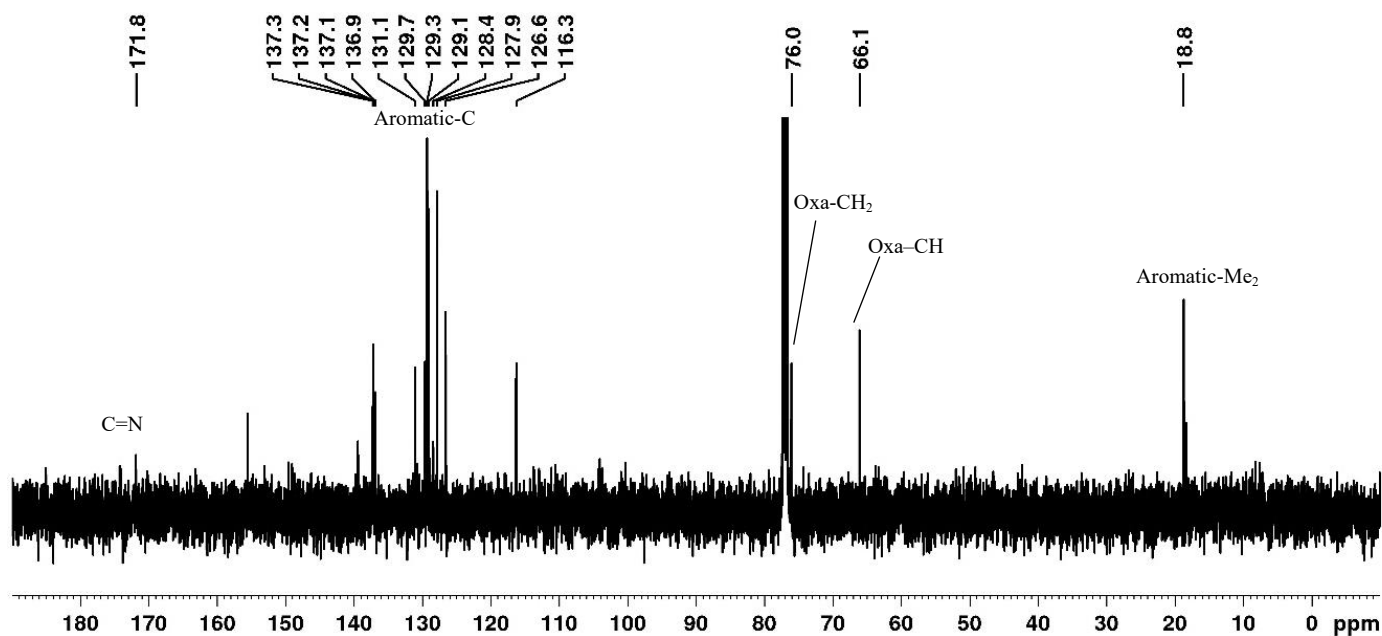


Figure S28. ^{13}C NMR of 3AlCl_2 .

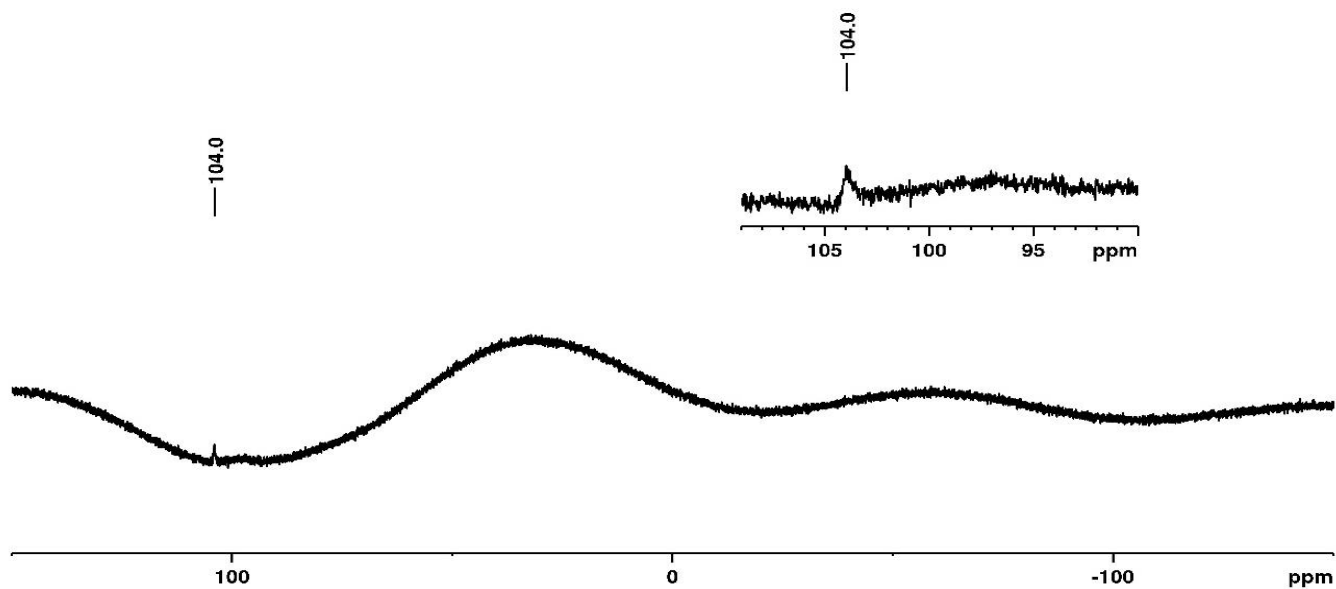


Figure S29. ^{27}Al NMR spectrum of 3AlCl_2 .

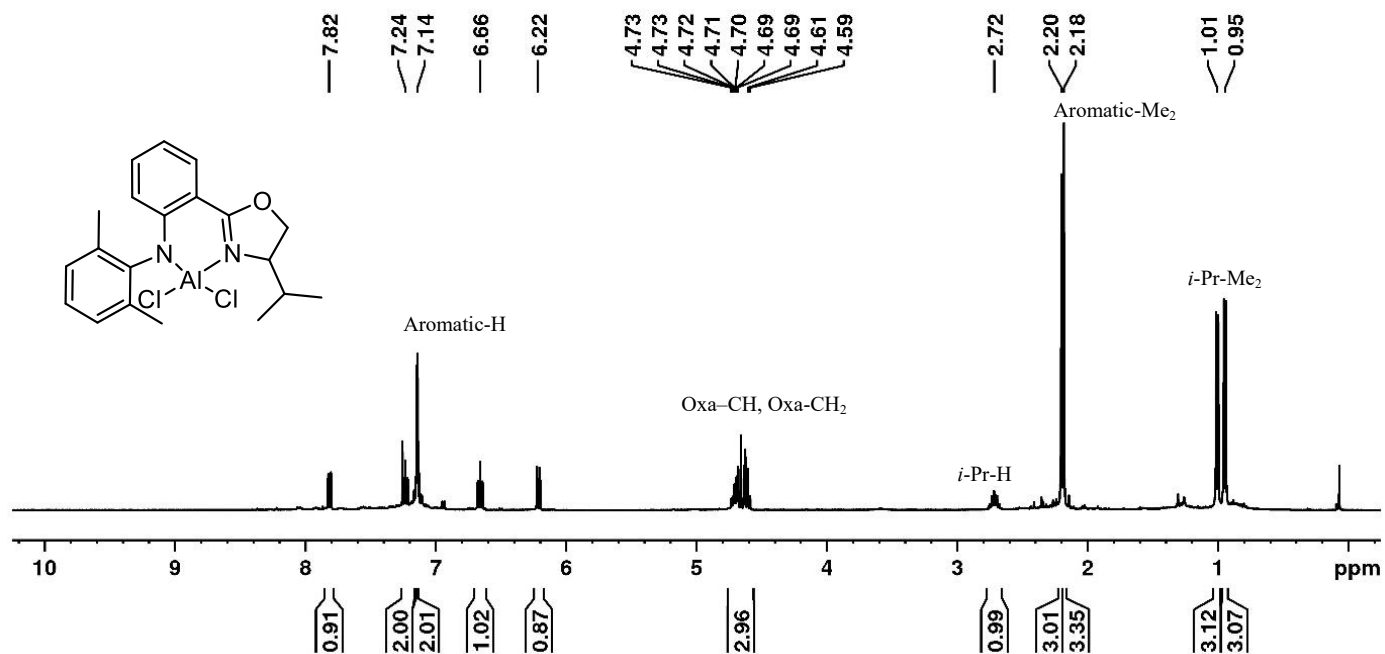


Figure S30. ^1H NMR spectrum of 4aAlCl_2 .

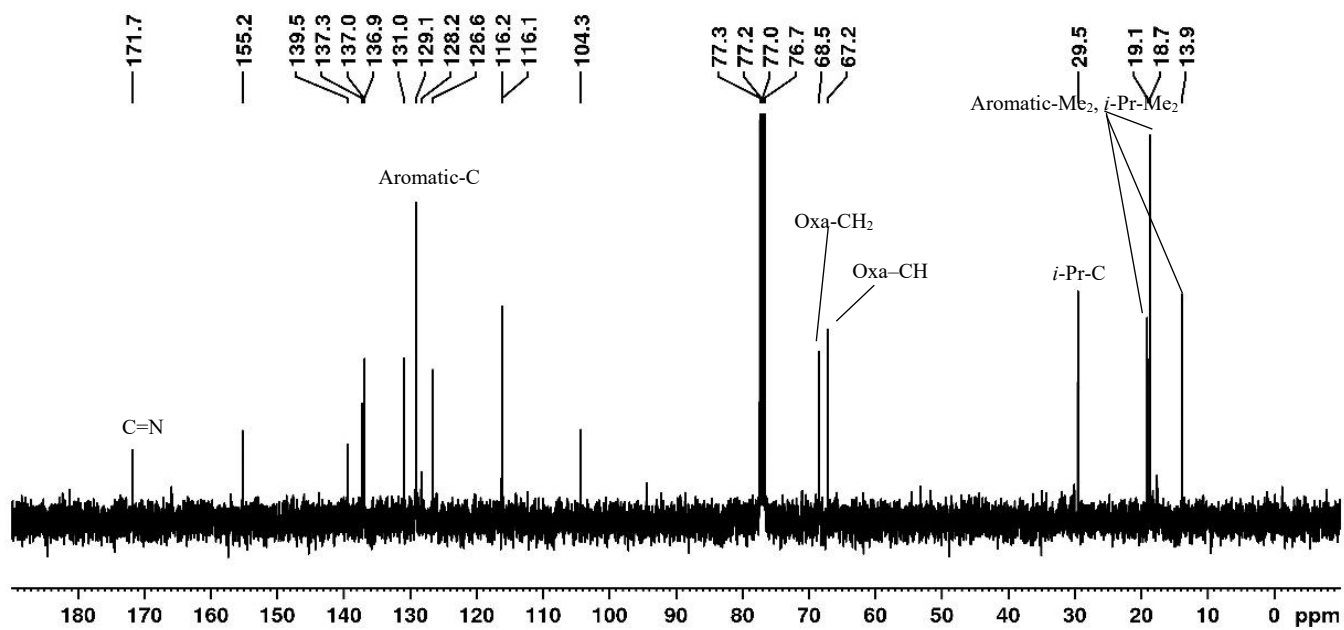


Figure S31. ^{13}C NMR spectrum of **4aAlCl₂**.

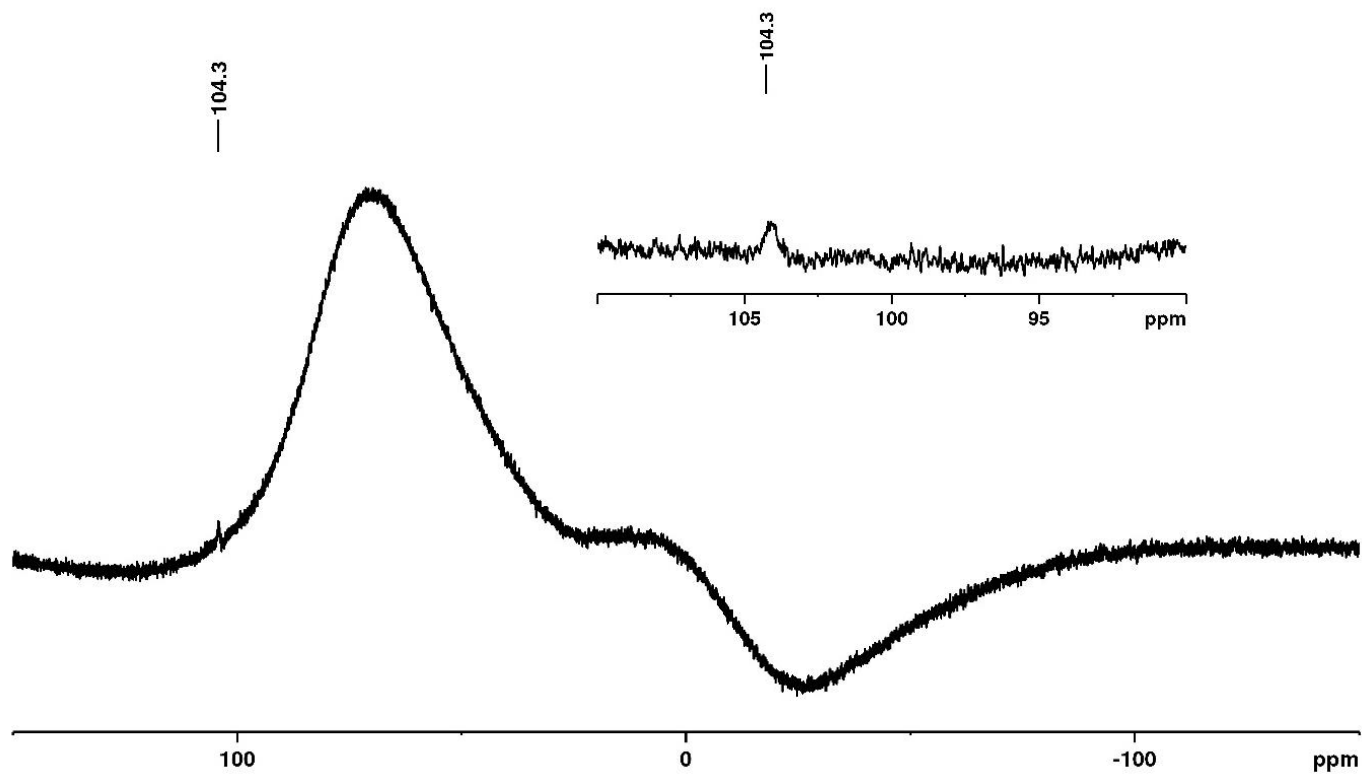


Figure S32. ^{27}Al NMR spectrum of **4aAlCl₂**.

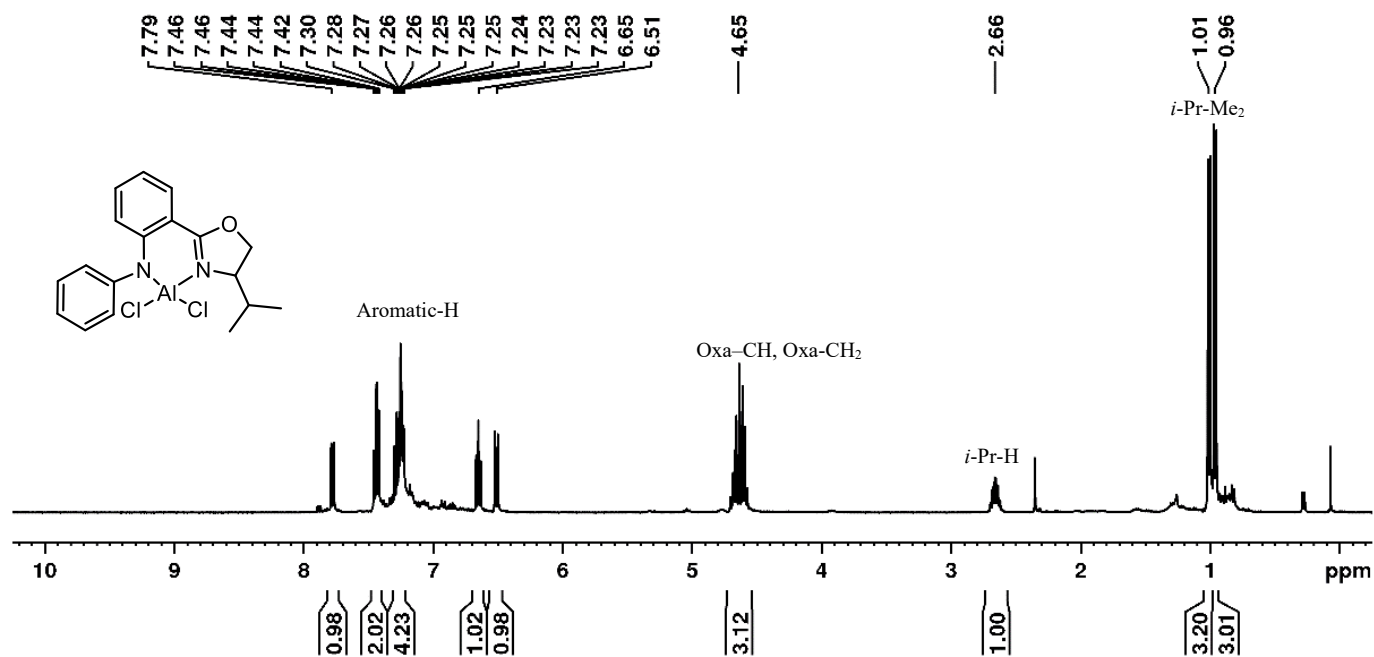


Figure S33. ¹H NMR spectrum of **4bAlCl₂**.

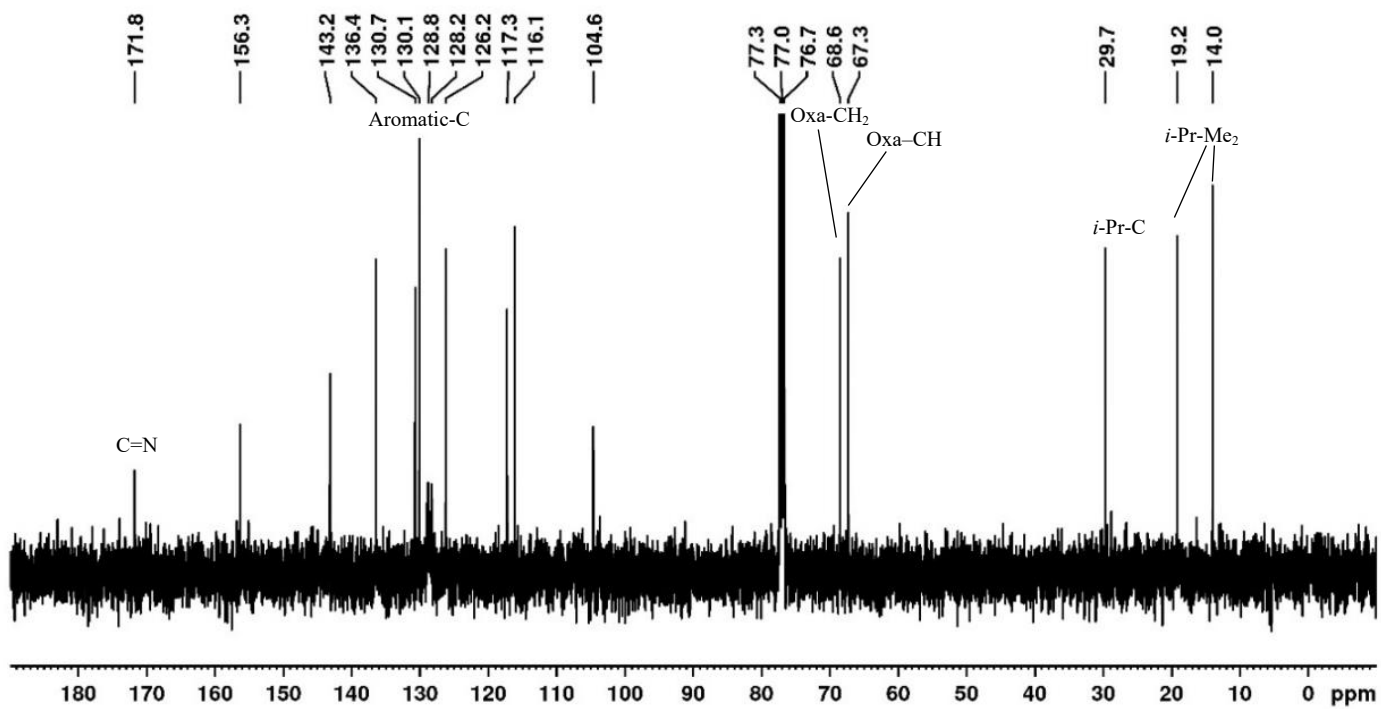


Figure S34. ¹³C NMR spectrum of **4bAlCl₂**.

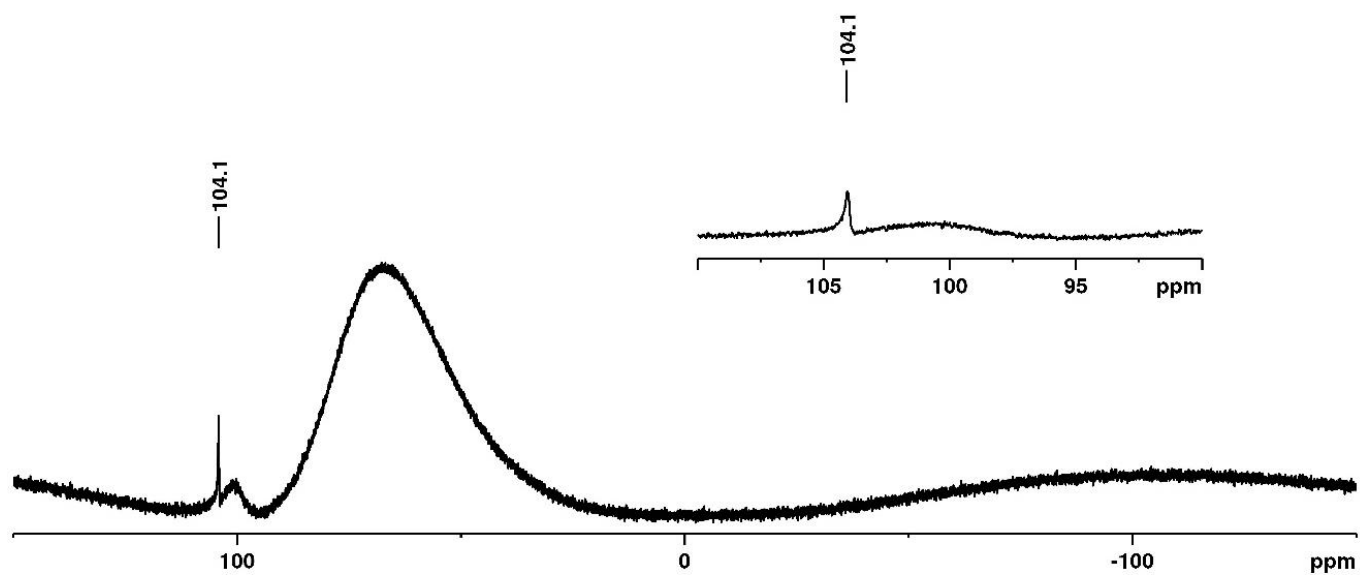


Figure S35. ^{27}Al NMR spectrum of 4bAlCl_2 .

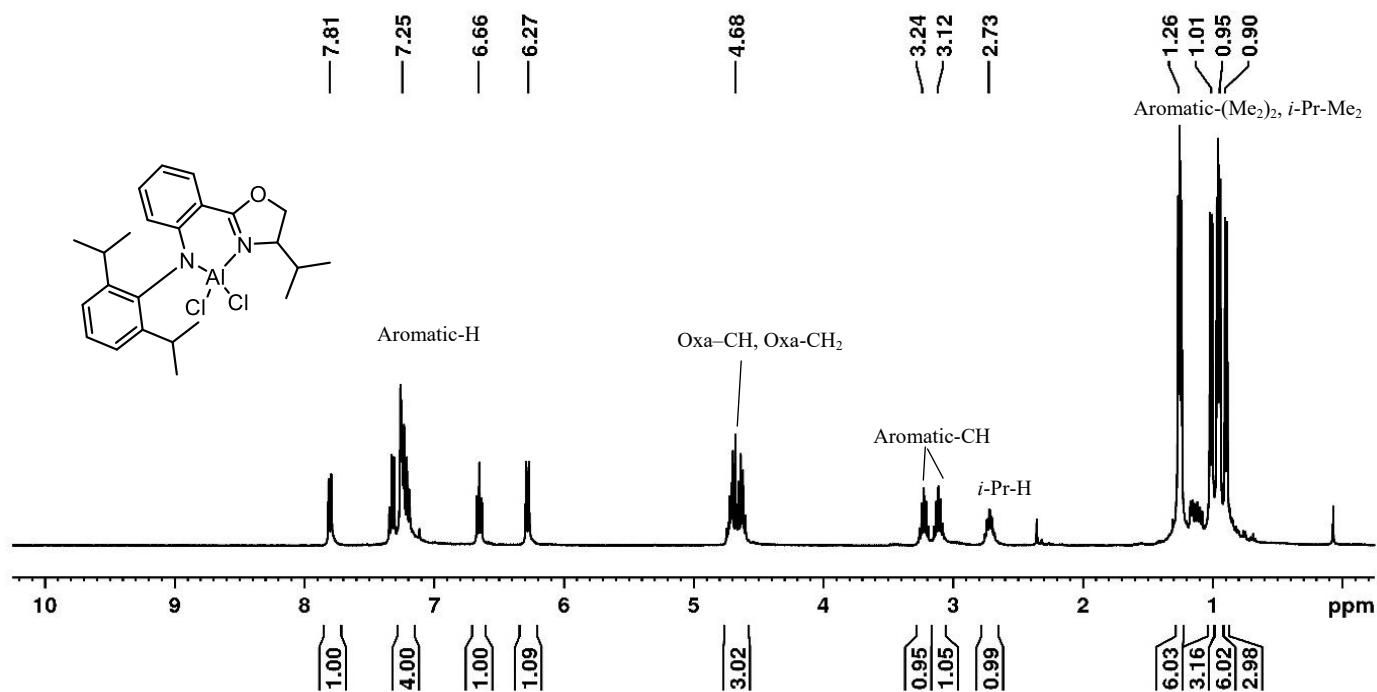


Figure S36. ^1H NMR spectrum of 4cAlCl_2 .

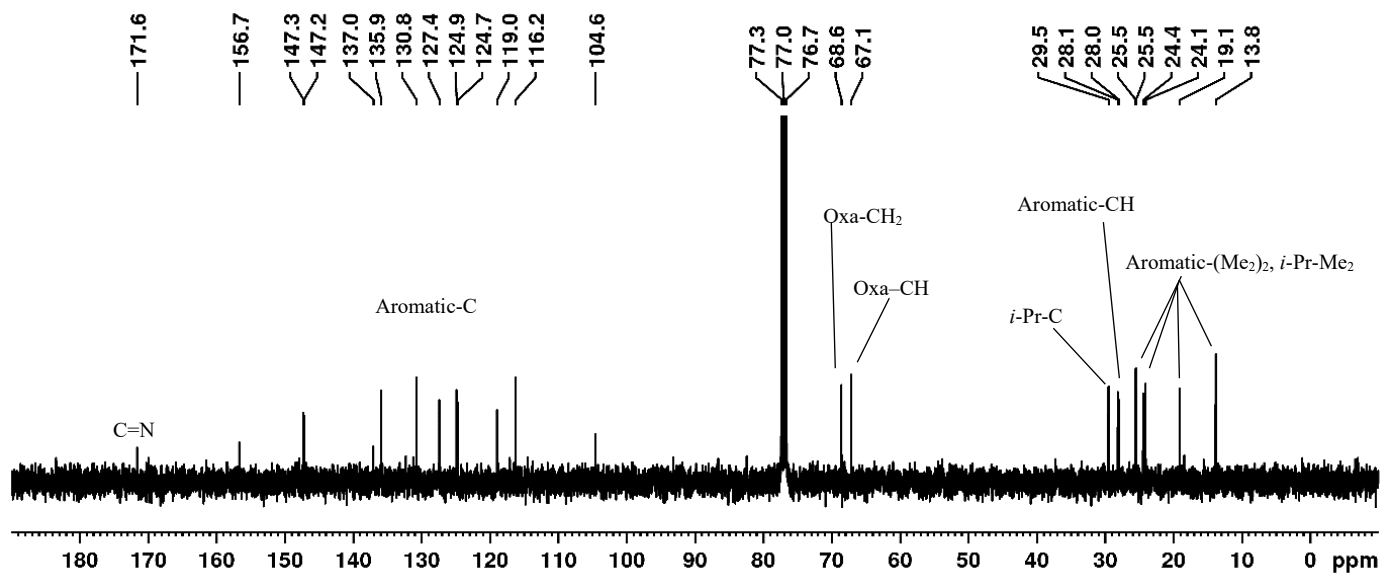


Figure S37. ¹³C NMR spectrum of **4cAlCl₂**.

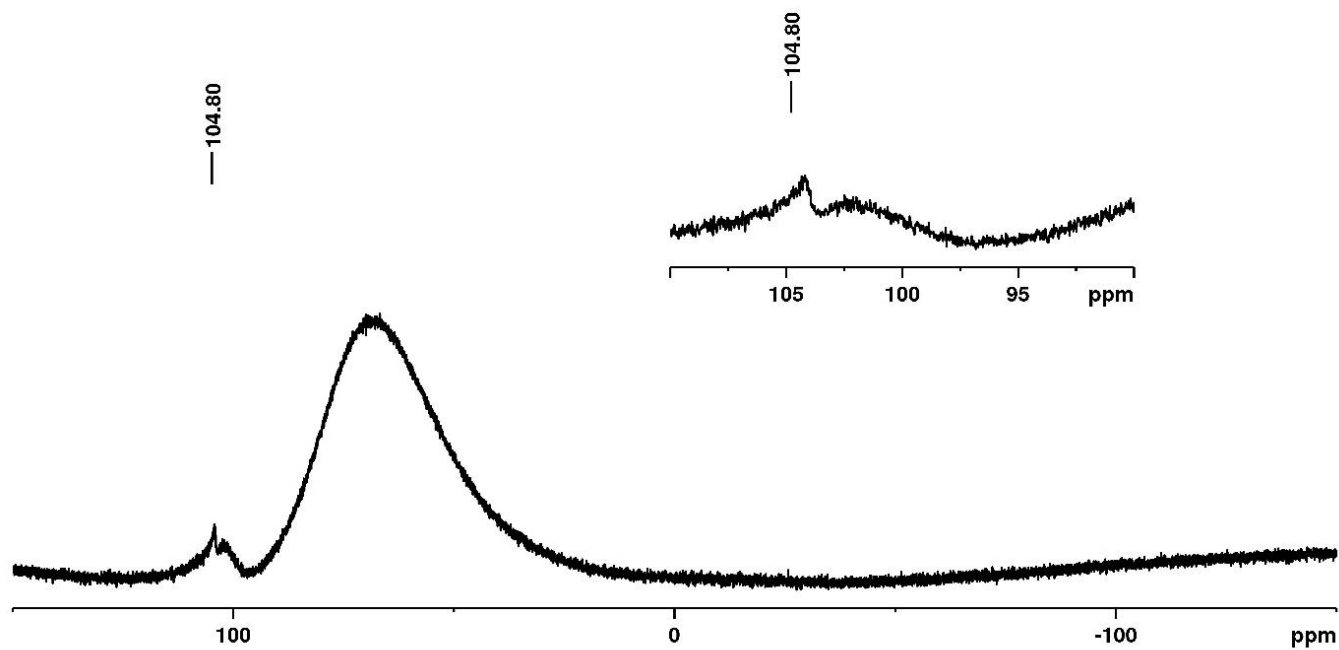


Figure S38. ²⁷Al NMR spectrum of **4cAlCl₂**.

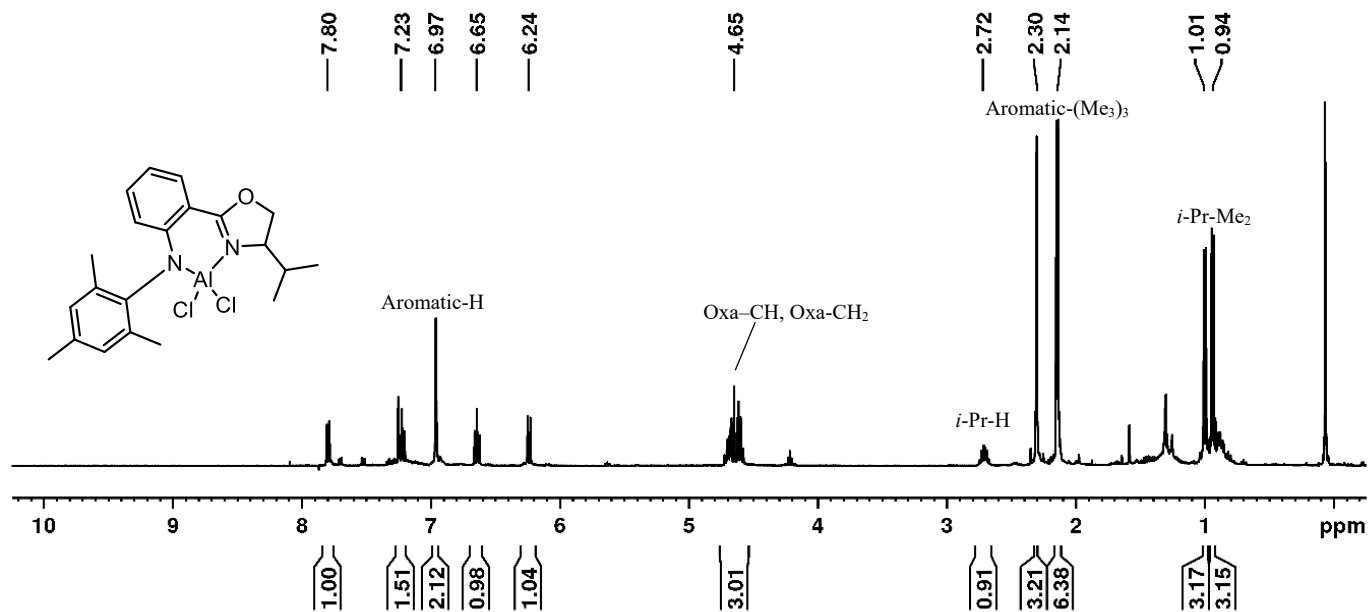


Figure S39. ¹H NMR spectrum of 4dAlCl₂.

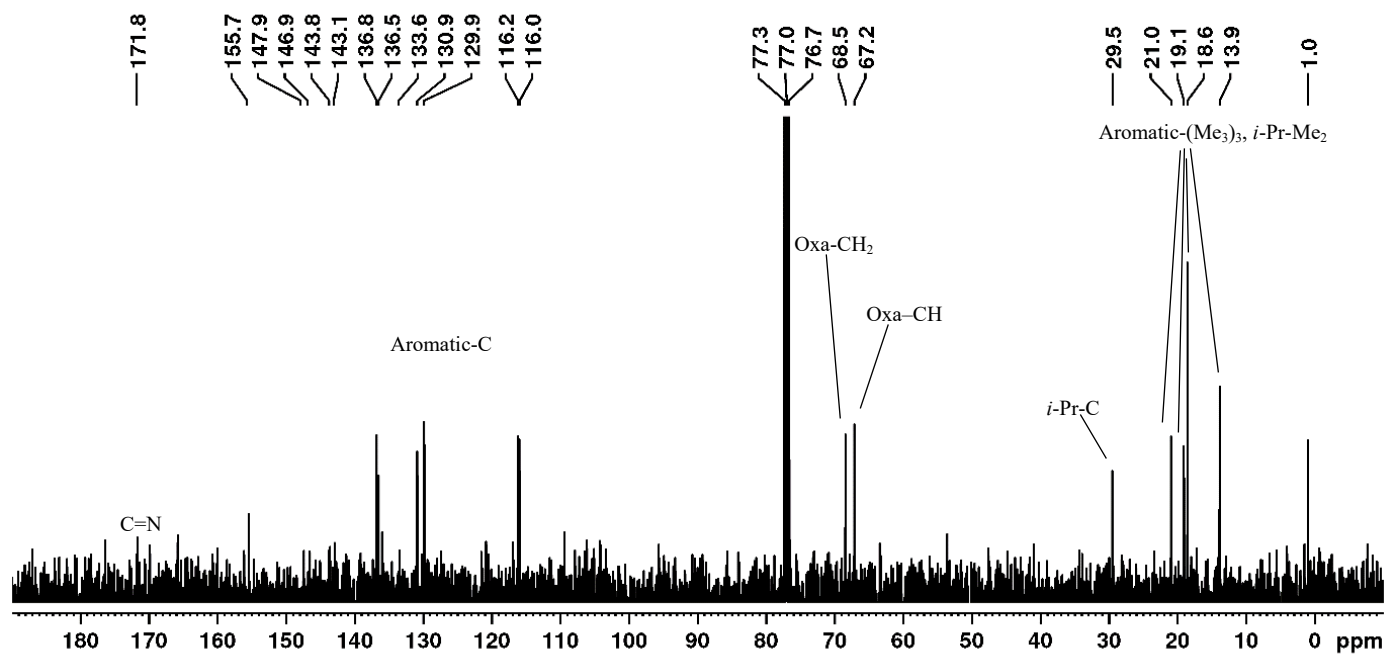


Figure S40. ¹³C NMR spectrum of 4dAlCl₂.

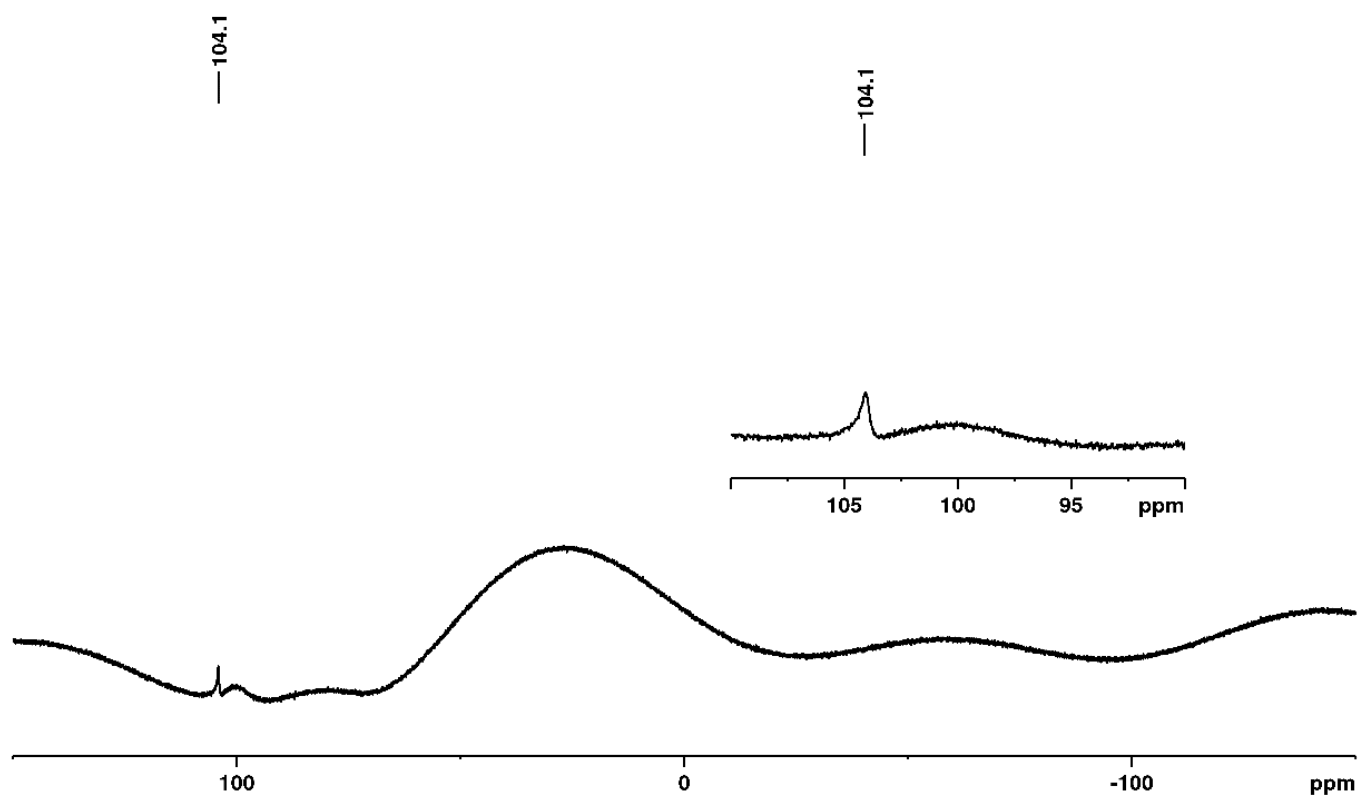


Figure S41. ^{27}Al NMR spectrum of 4dAlCl_2 .

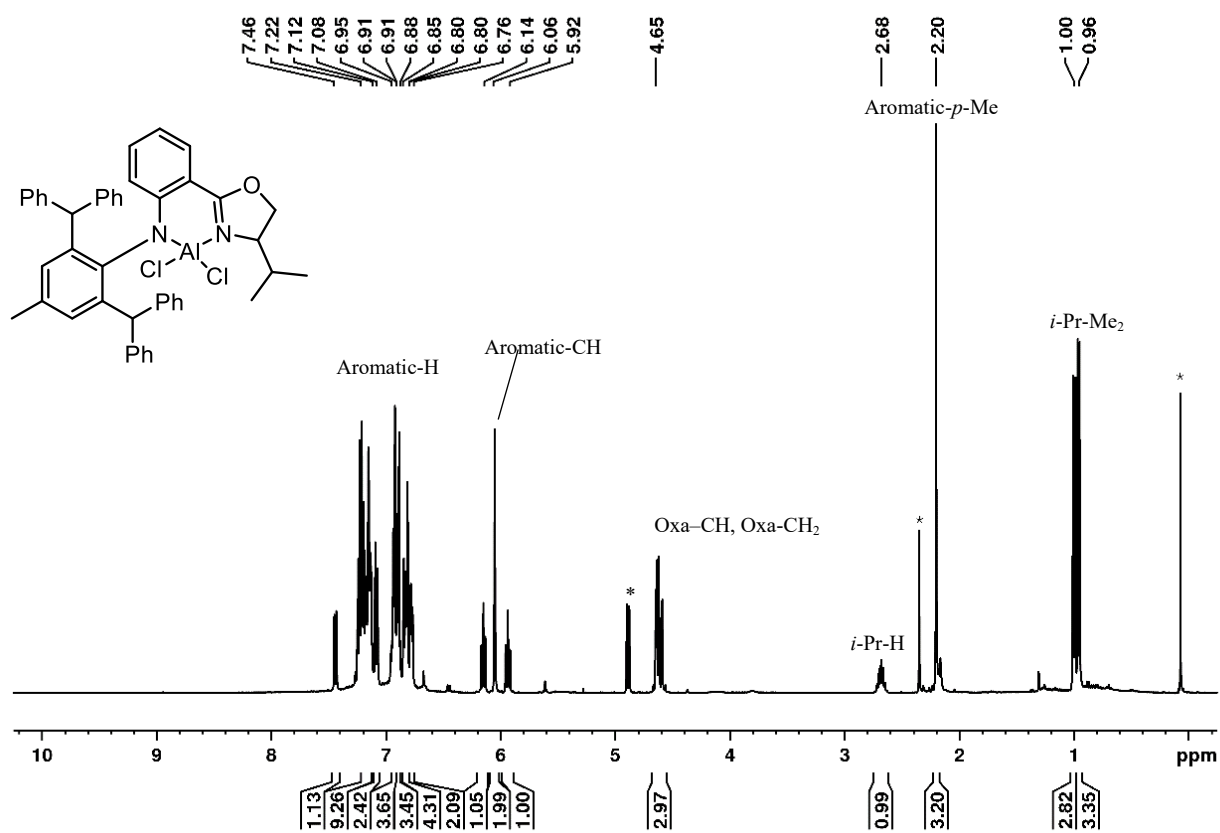


Figure S42. ^1H NMR spectrum of 4eAlCl_2 . Note: solvent impurities are indicated by *

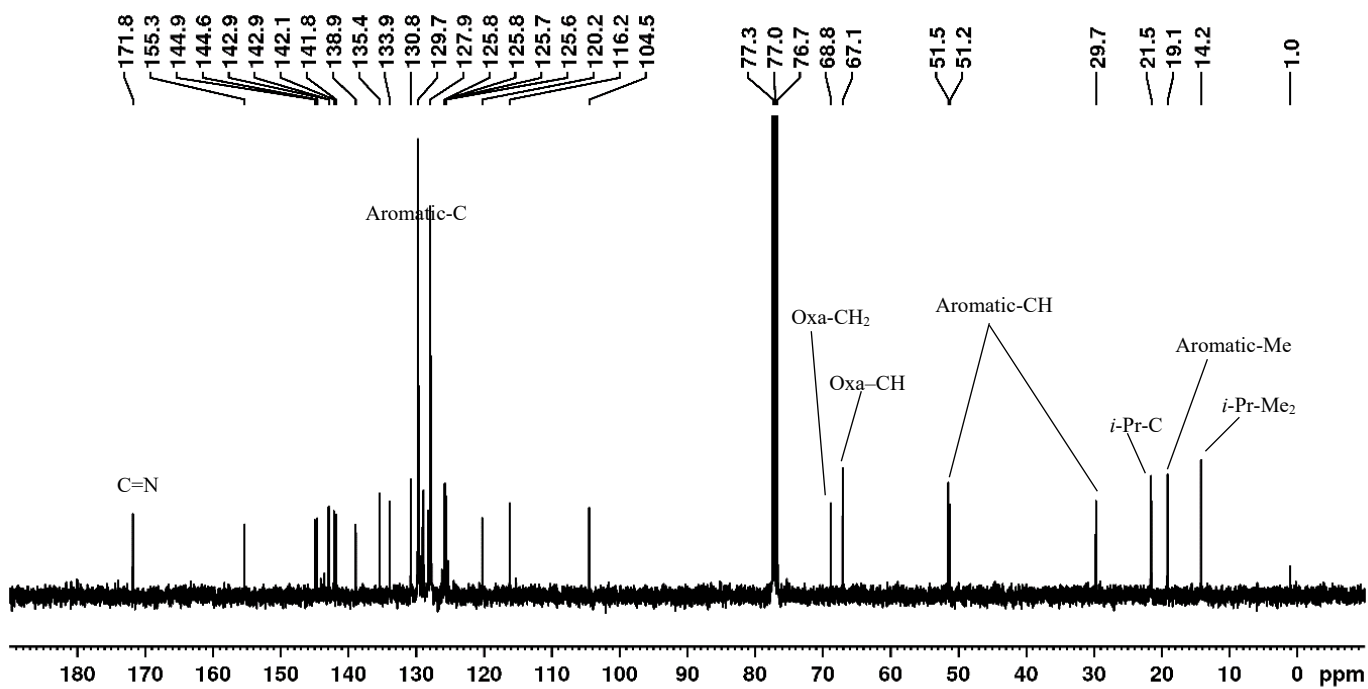


Figure S43. ¹³C NMR spectrum of **4eAlCl₂**.

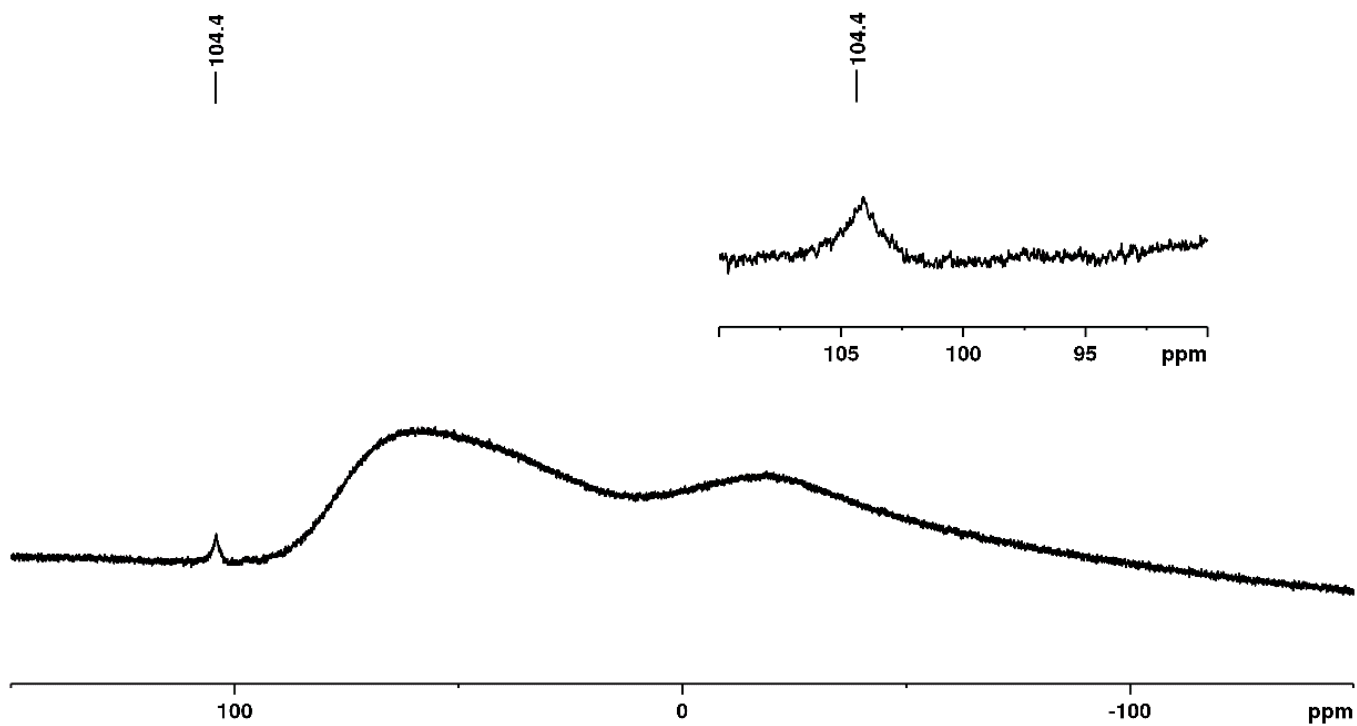


Figure S44. ²⁷Al NMR spectrum of **4eAlCl₂**.

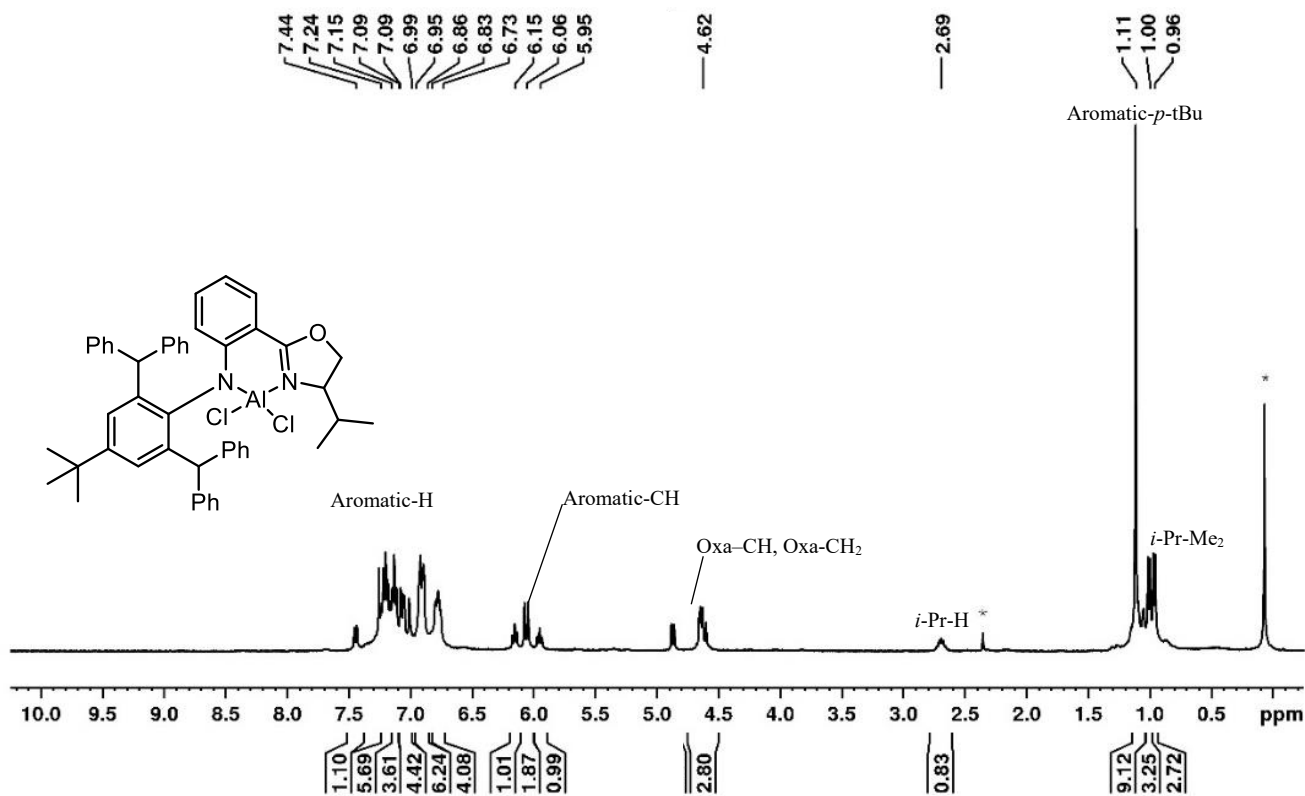
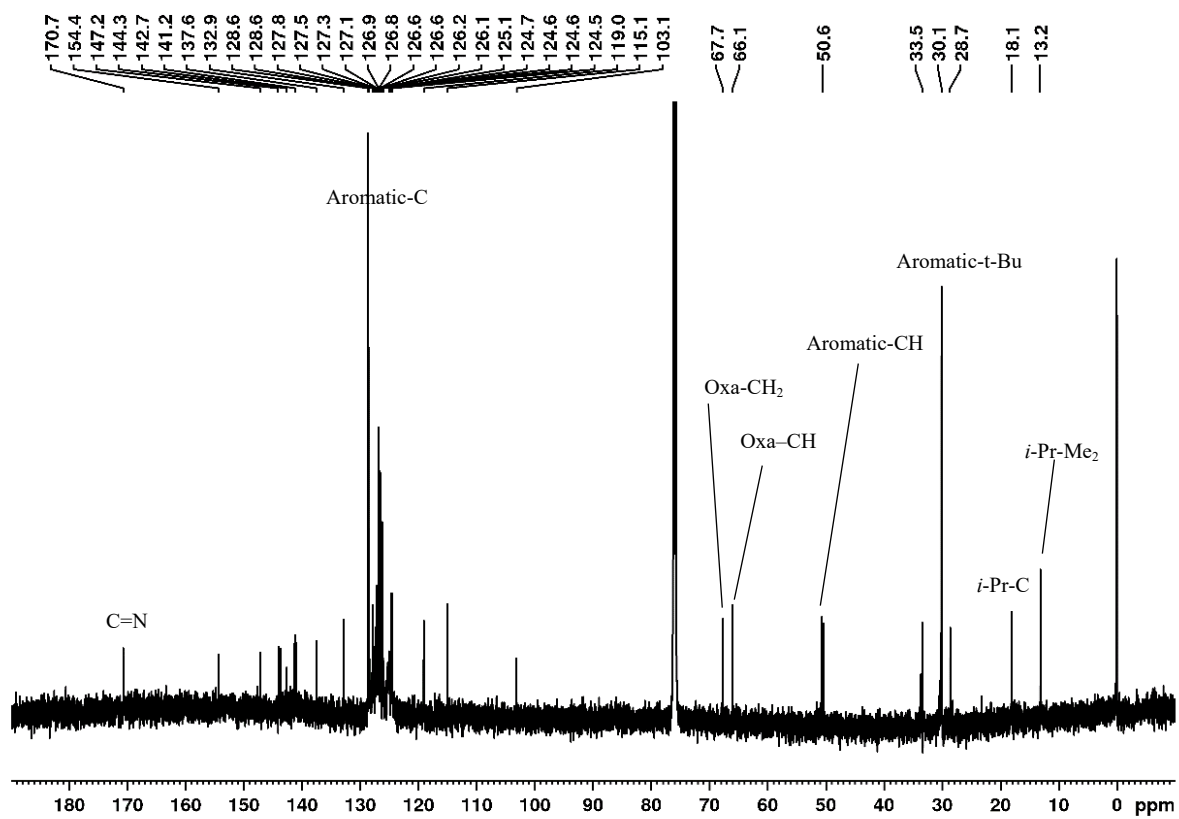


Figure S45. ¹H NMR spectrum of **4fAlCl₂**. Note: solvent impurities are indicated by *



S46. ¹³C NMR spectrum of **4fAlCl₂**.

Figure

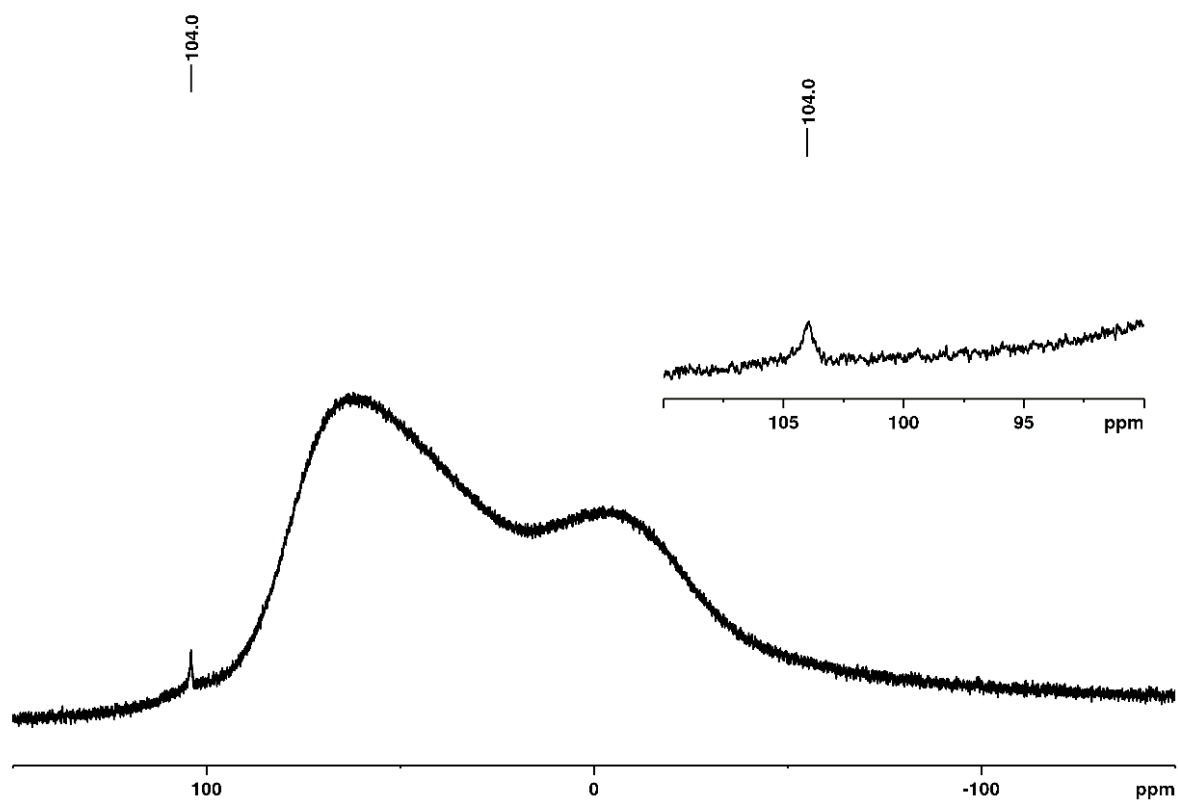


Figure S47. ^{27}Al NMR spectrum of 4fAlCl_2 .

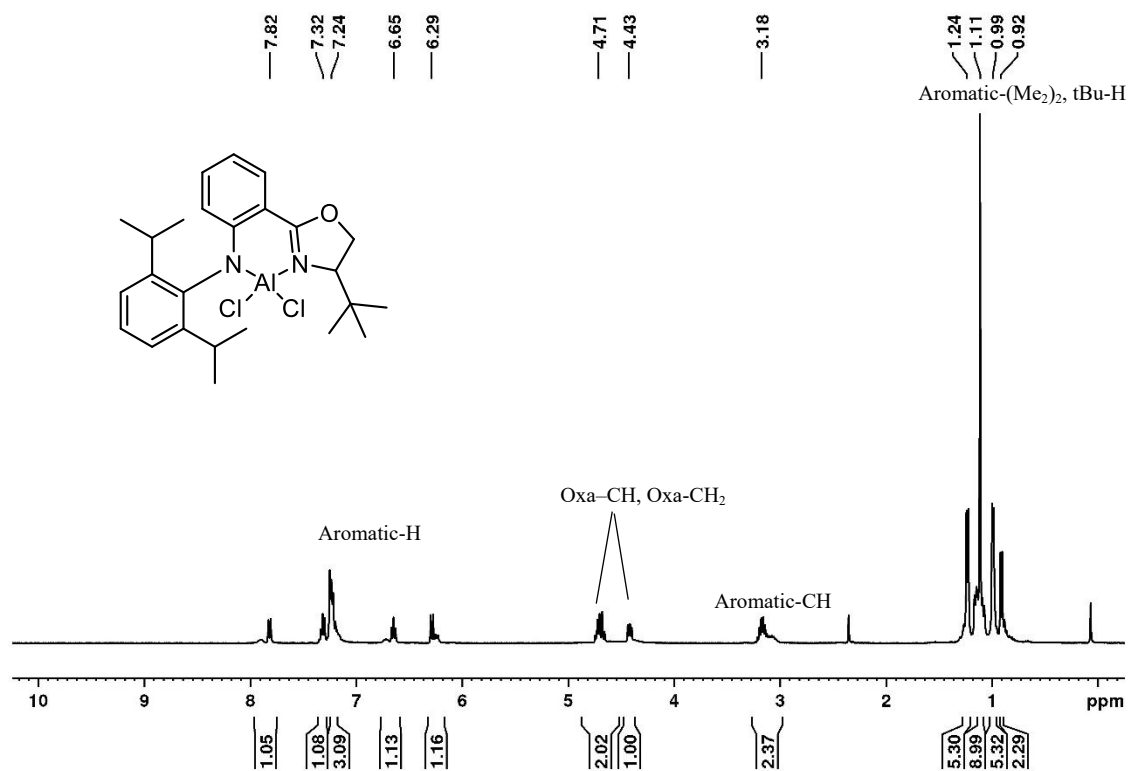


Figure S48. ^1H NMR spectrum of 5cAlCl_2 .

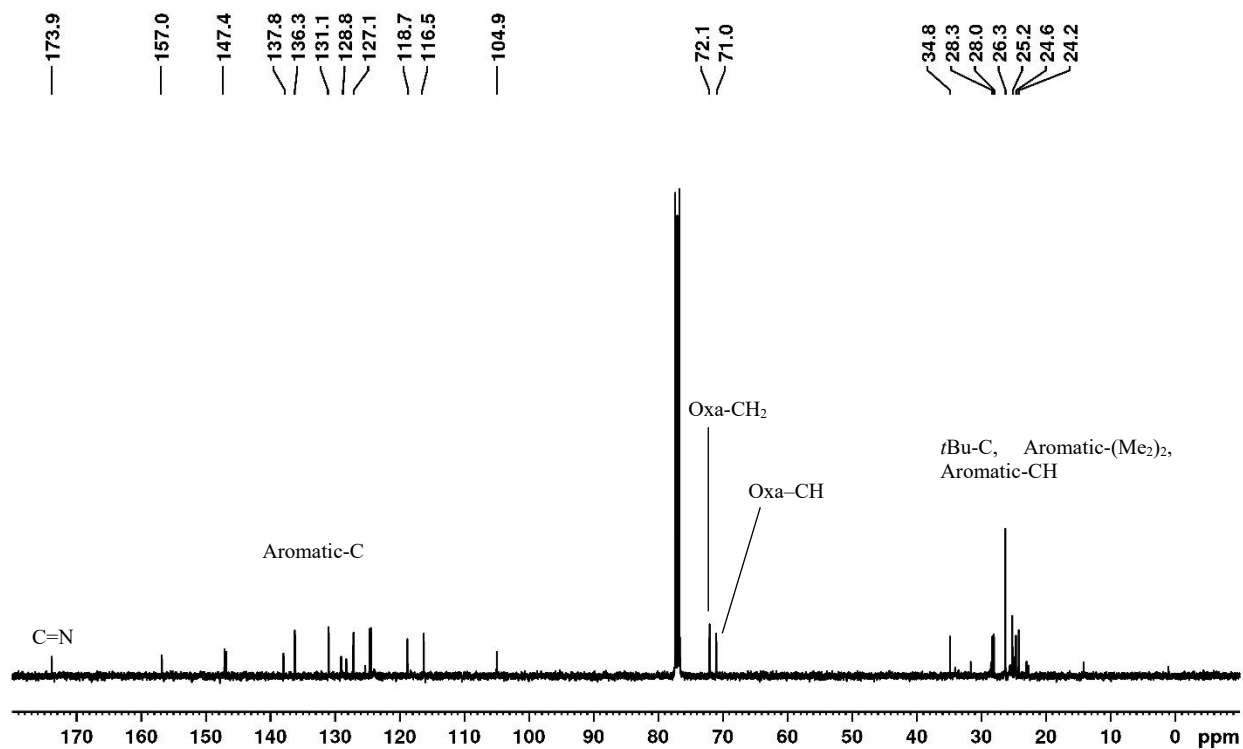


Figure S49. ^{13}C NMR spectrum of **5cAlCl₂**.

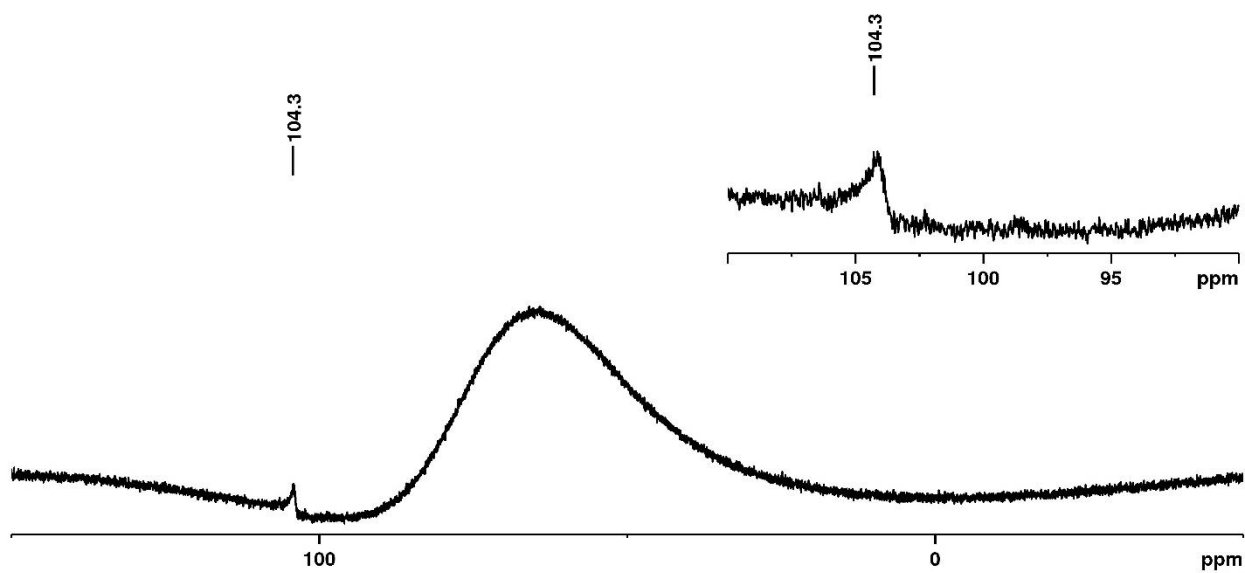


Figure S50. ^{27}Al NMR spectrum of **5cAlCl₂**.

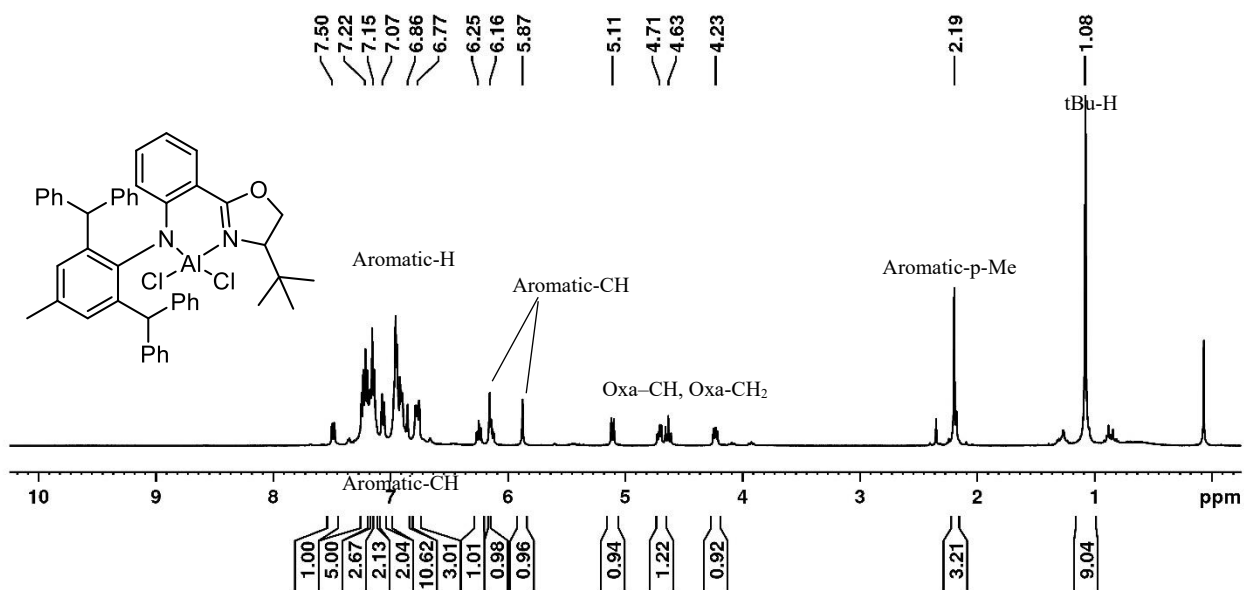


Figure S51. ^1H NMR spectrum of **5eAlCl₂**.

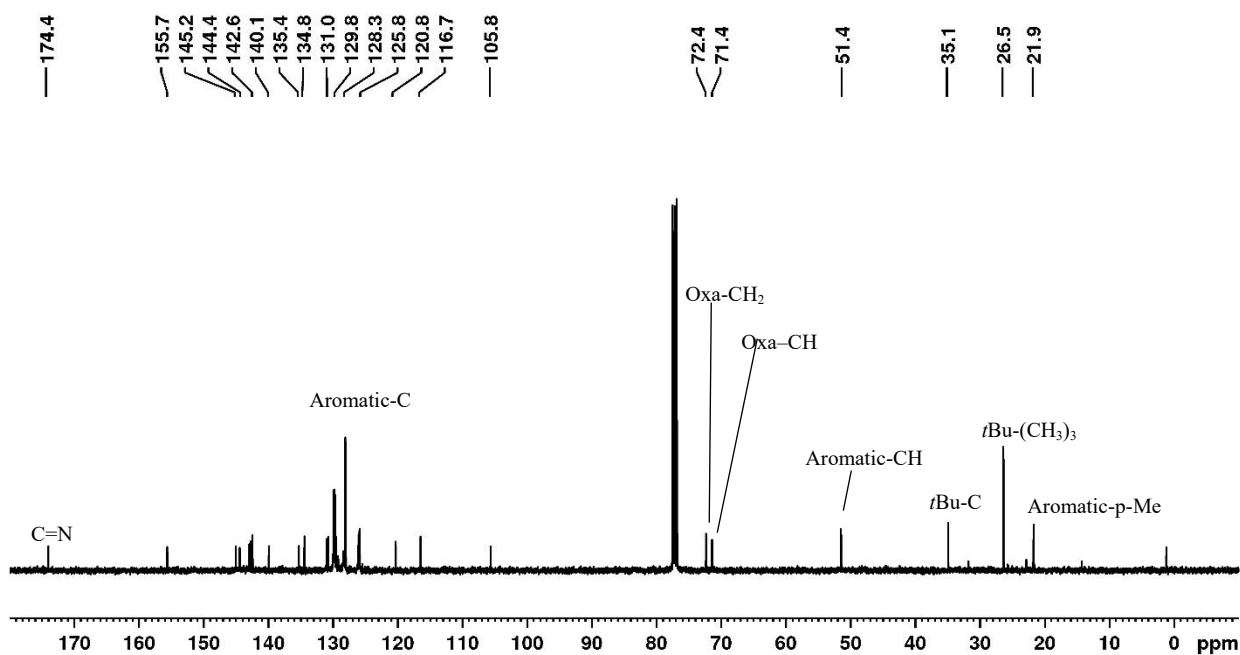


Figure S52. ^{13}C NMR spectrum of **5eAlCl₂**.

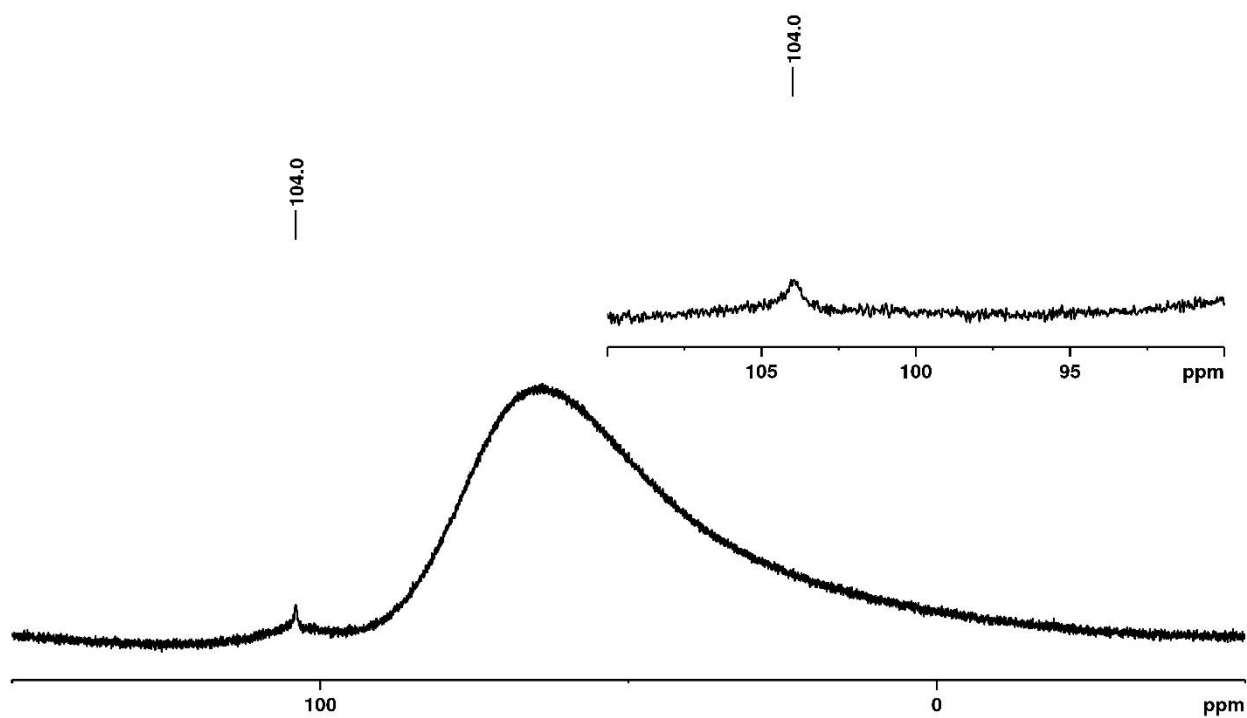


Figure S53. ^{27}Al NMR spectrum of $5e\text{AlCl}_2$.

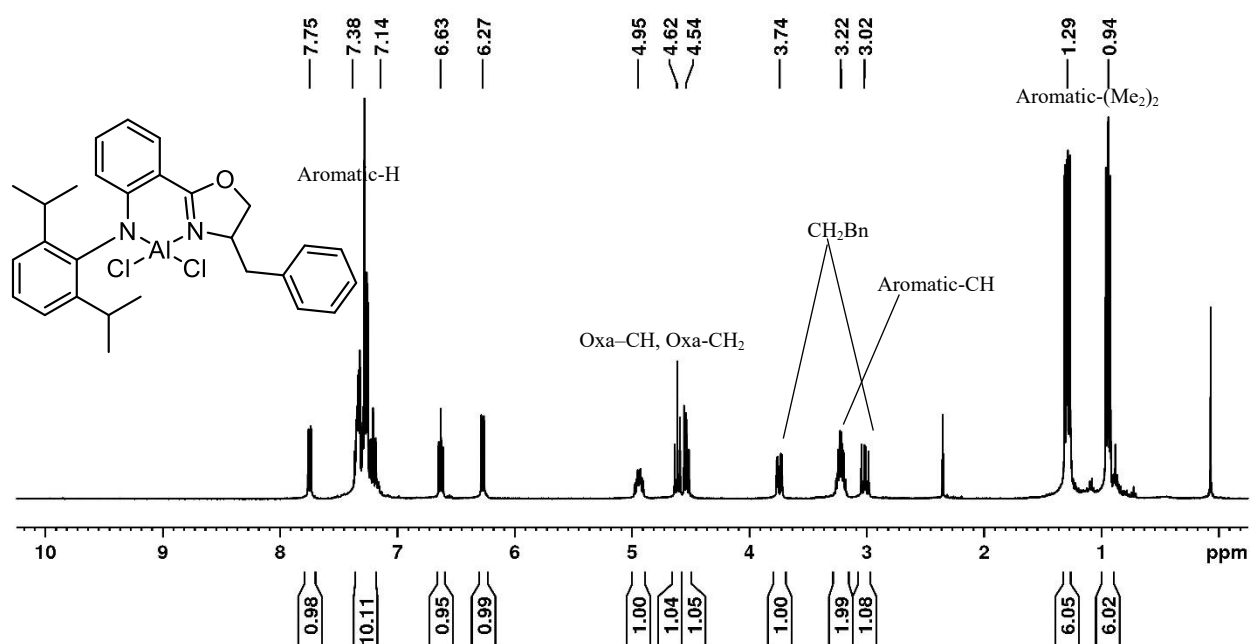


Figure S54. ^1H NMR spectrum of $6c\text{AlCl}_2$.

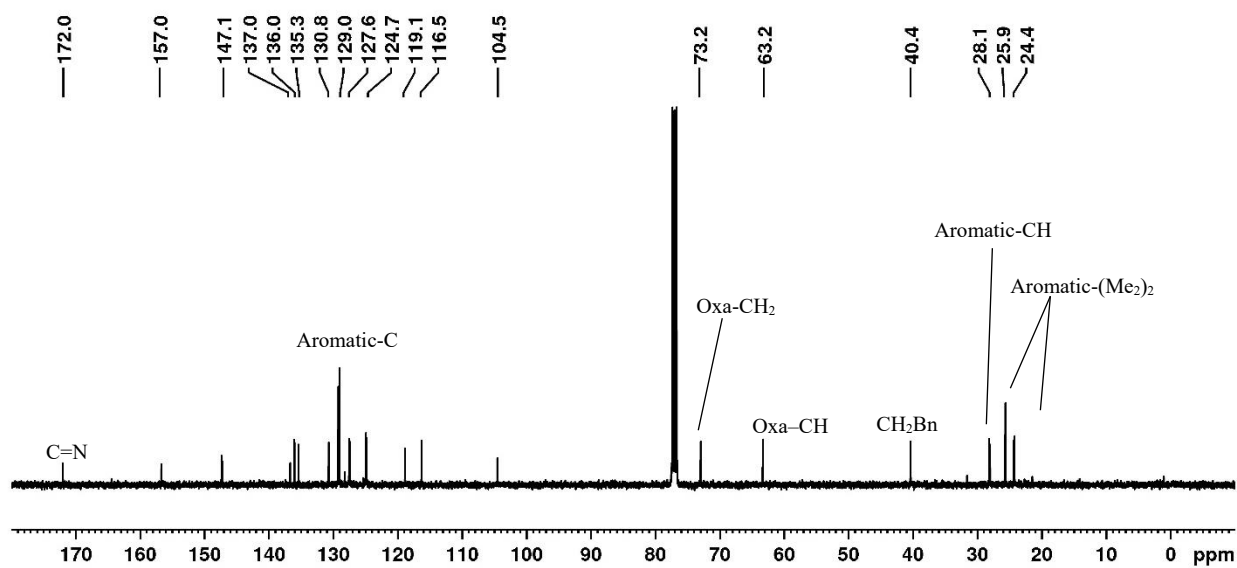


Figure S55. ^{13}C NMR spectrum of **6cAlCl₂**.

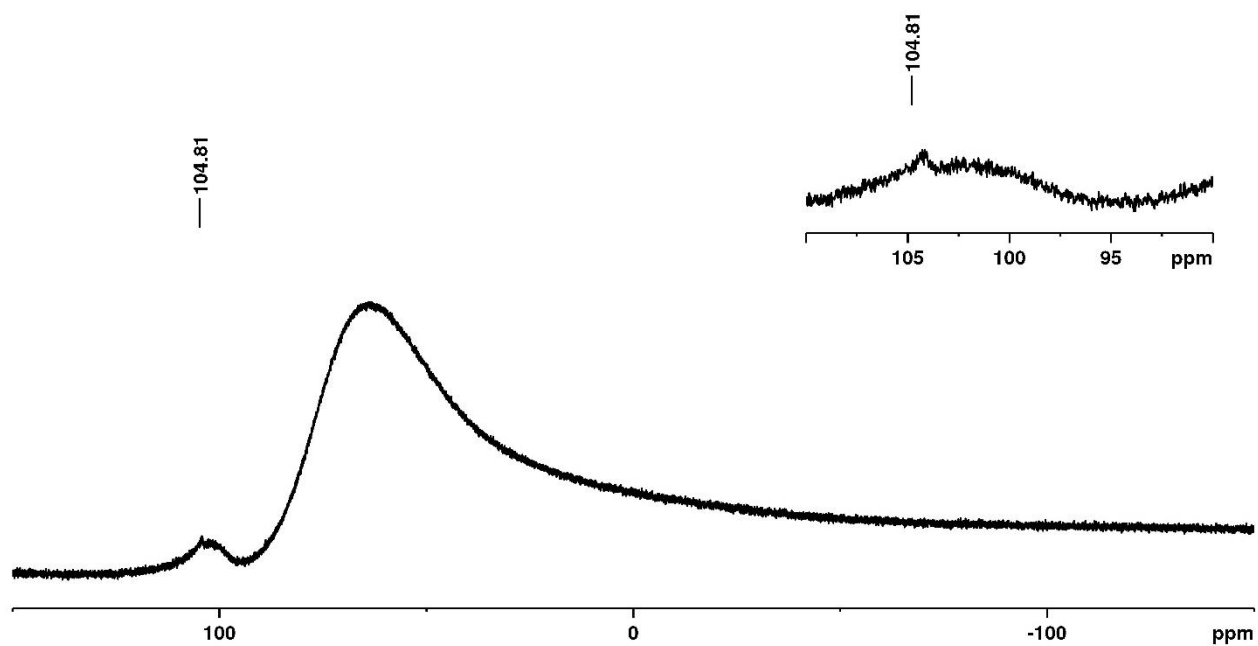


Figure S56. ^{27}Al NMR spectrum of **6cAlCl₂**.

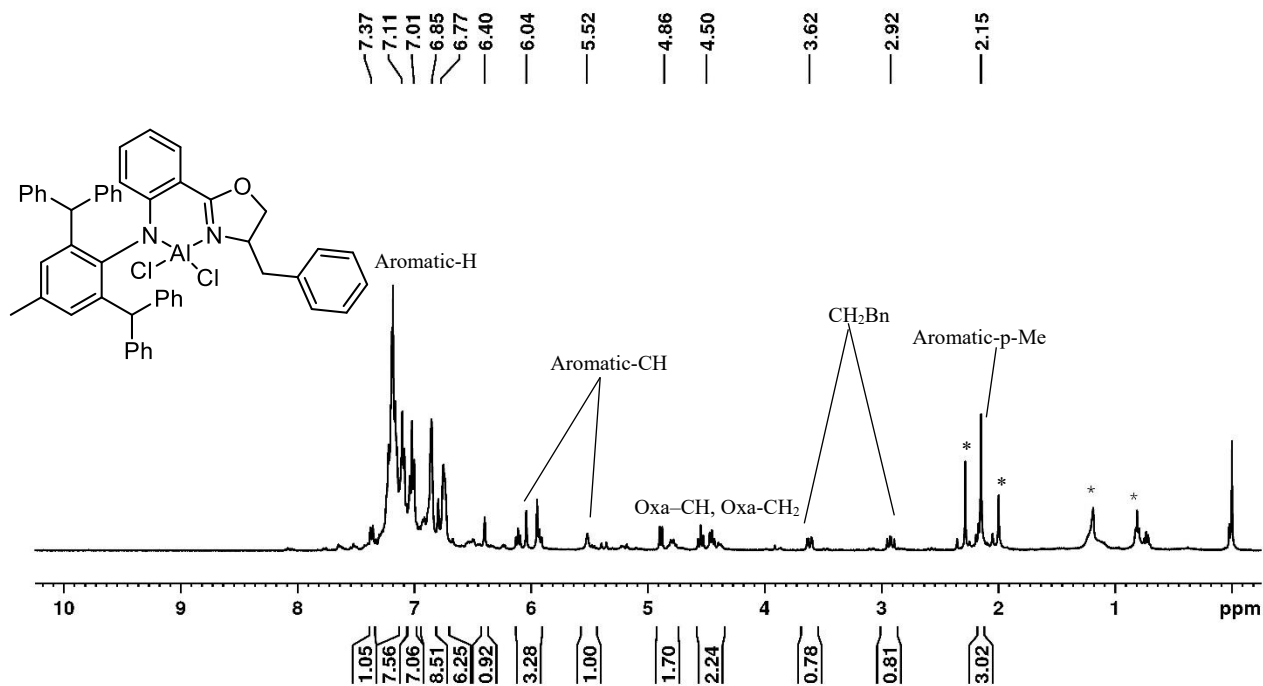


Figure S57. ¹H NMR spectrum of **6eAlCl₂**. solvent impurities are indicated by *

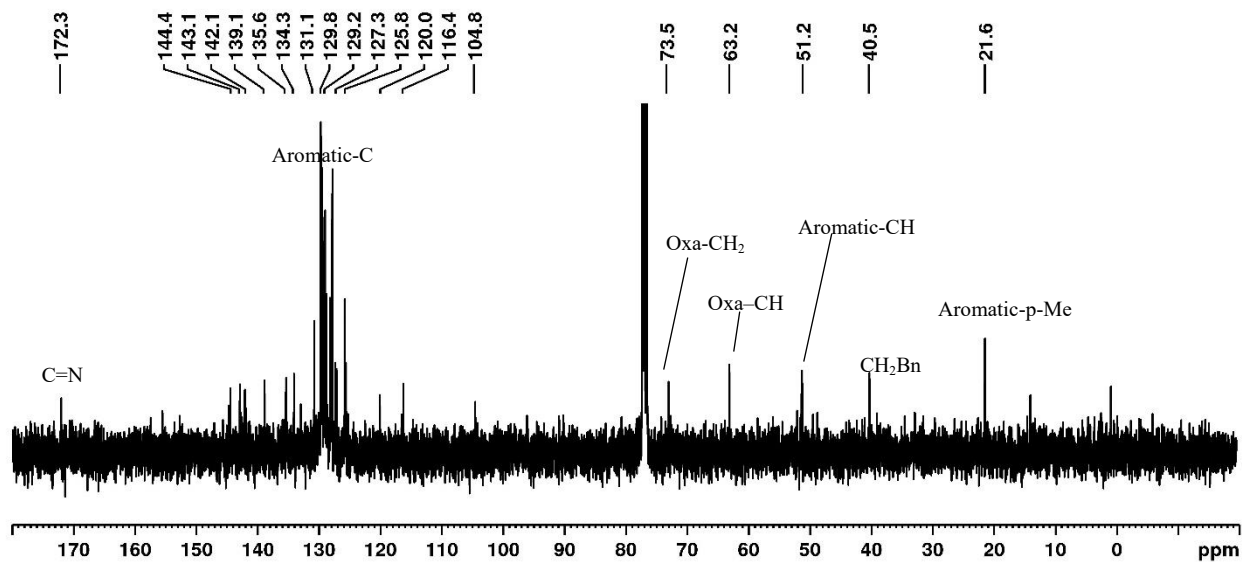


Figure S58. ¹³C NMR spectrum of **6eAlCl₂**.

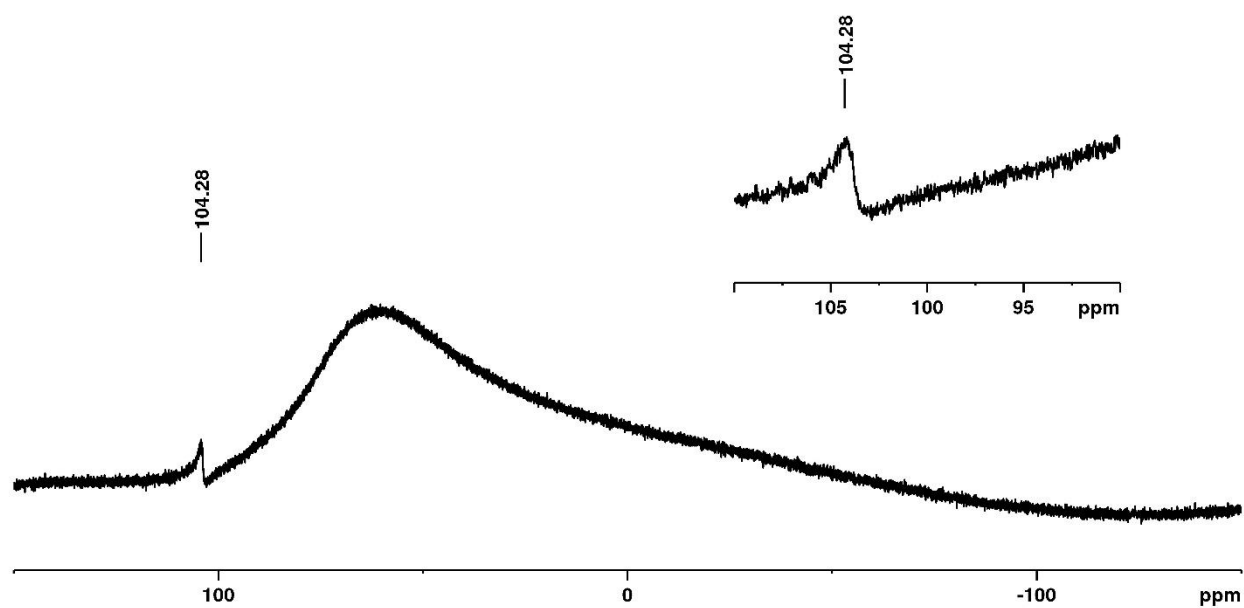


Figure S59. ^{27}Al NMR spectrum of 6eAlCl_2 .

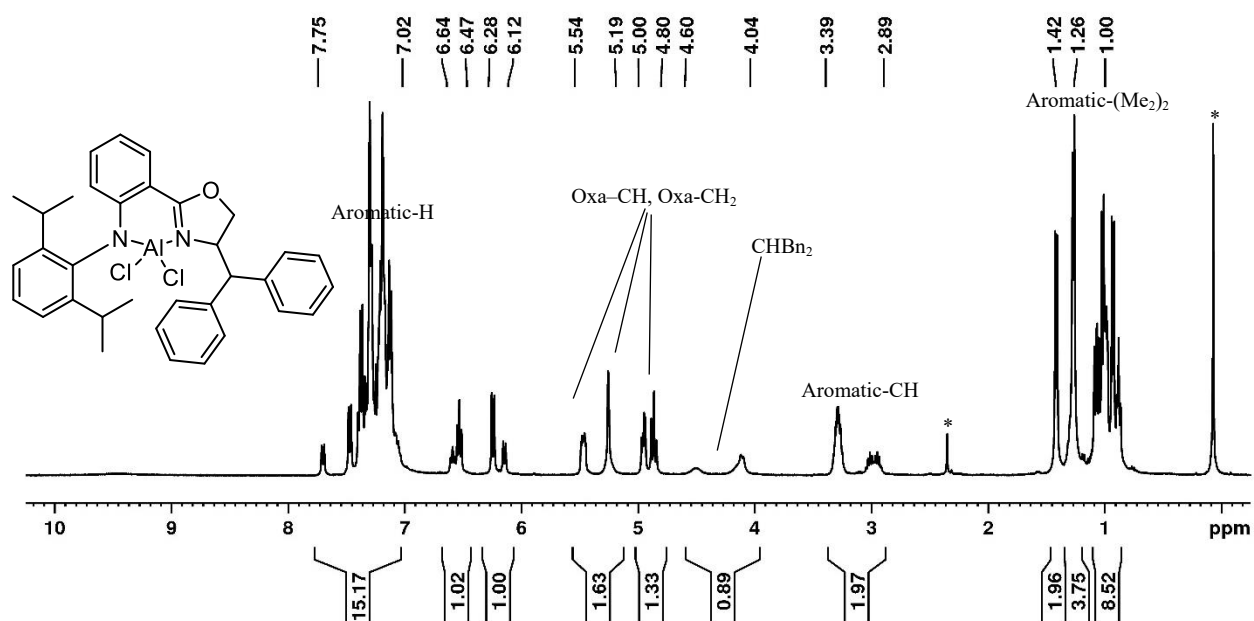


Figure S60. ^1H NMR spectrum of 7cAlCl_2 . solvent impurities are indicated by *

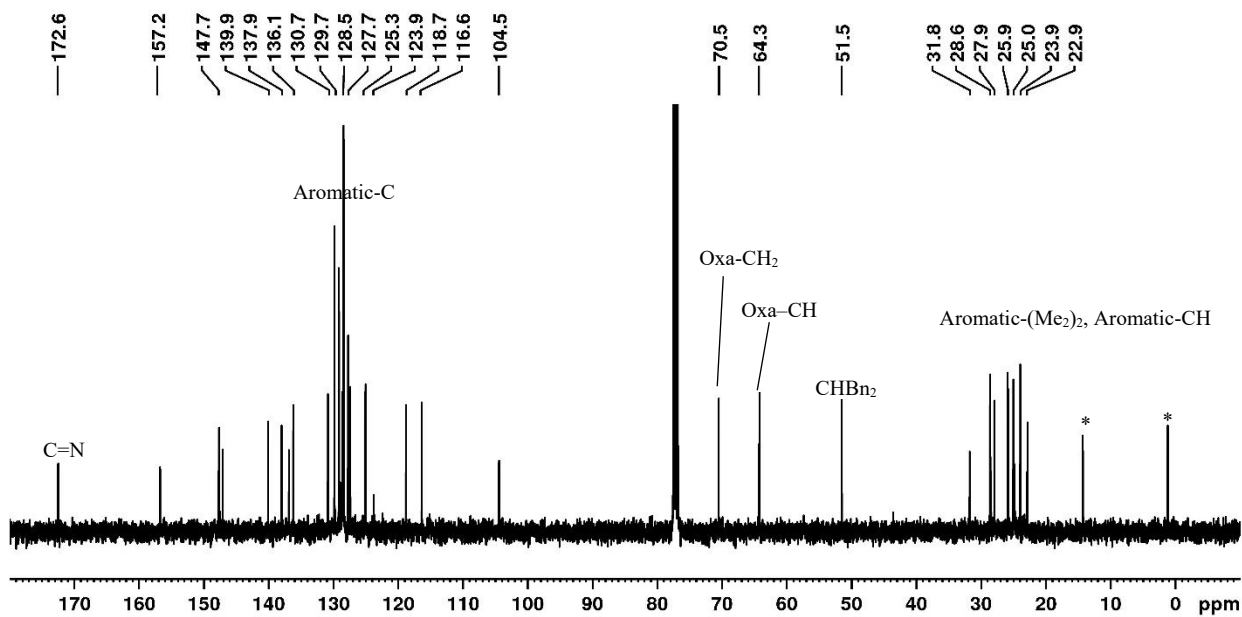


Figure S61. ^{13}C NMR spectrum of 7cAlCl_2 , solvent impurities are indicated by *

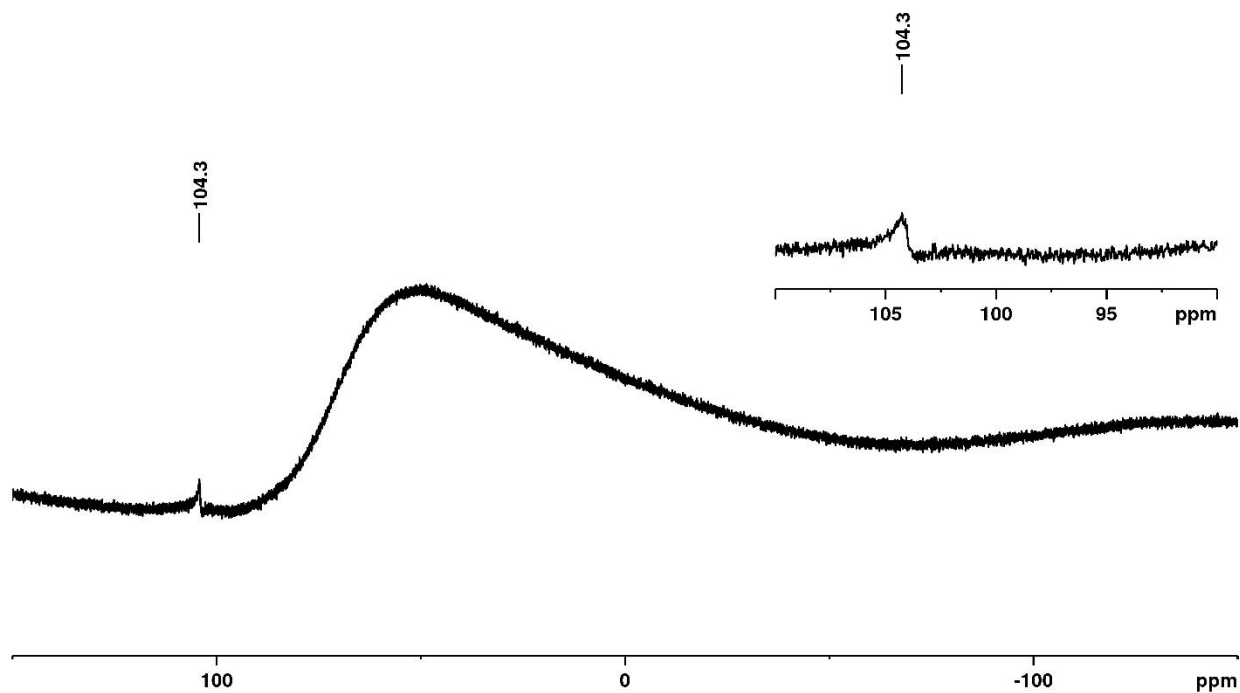


Figure S62. ^{27}Al NMR spectrum of 7cAlCl_2 .

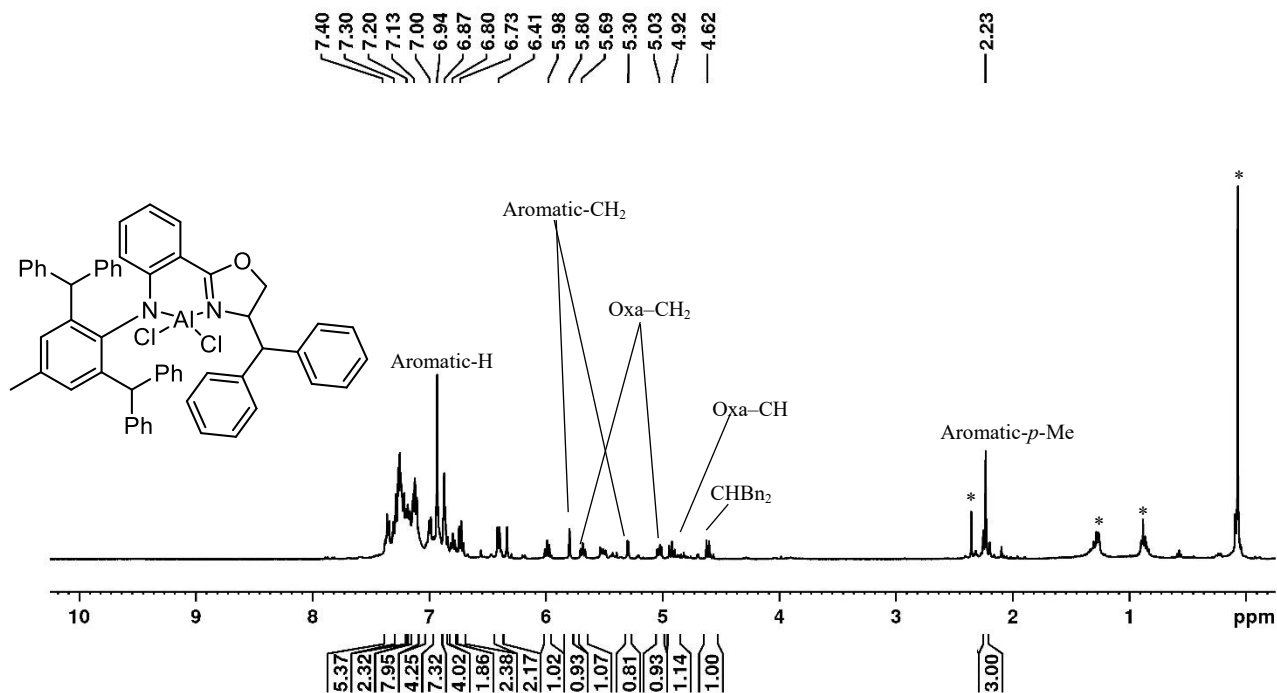


Figure S63. 1H NMR spectrum of $7eAlCl_2$. solvent impurities are indicated by *

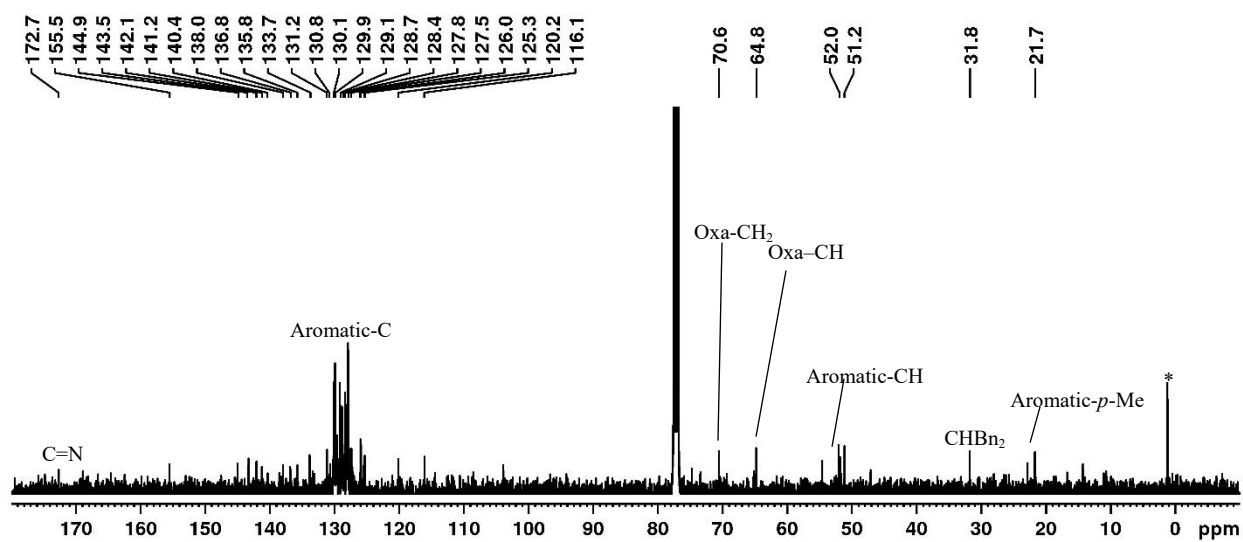


Figure S64. ^{13}C NMR spectrum of $7eAlCl_2$.

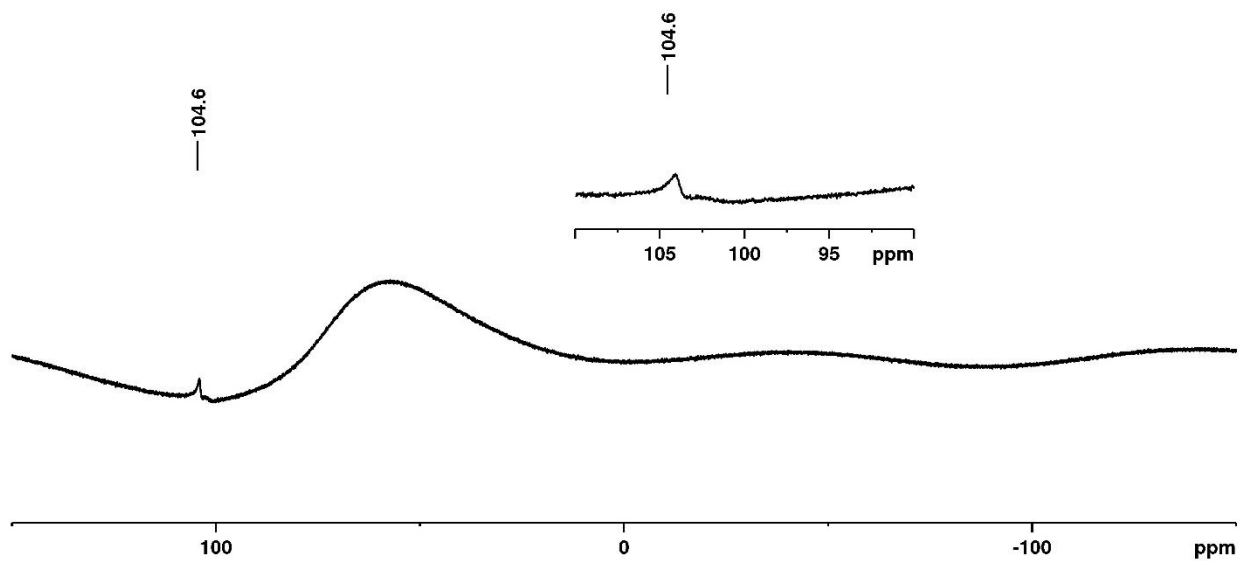


Figure S65. ^{27}Al NMR spectrum of 7eAlCl_2 .

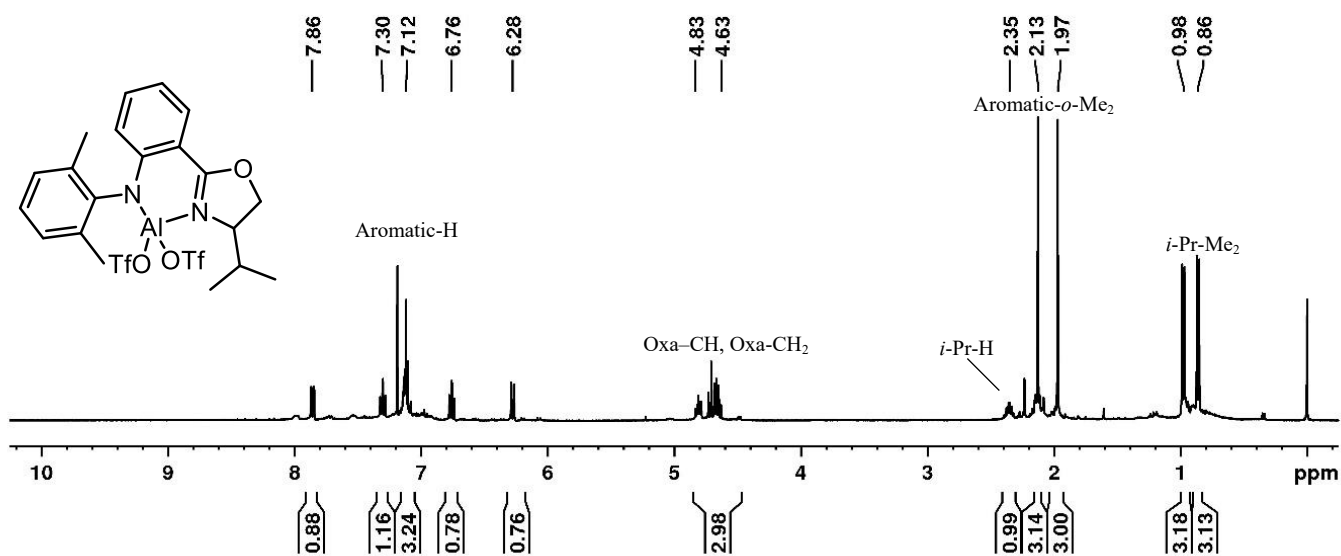


Figure S66. ^1H NMR spectrum of $4\text{aAl}(\text{OTf})_2$.

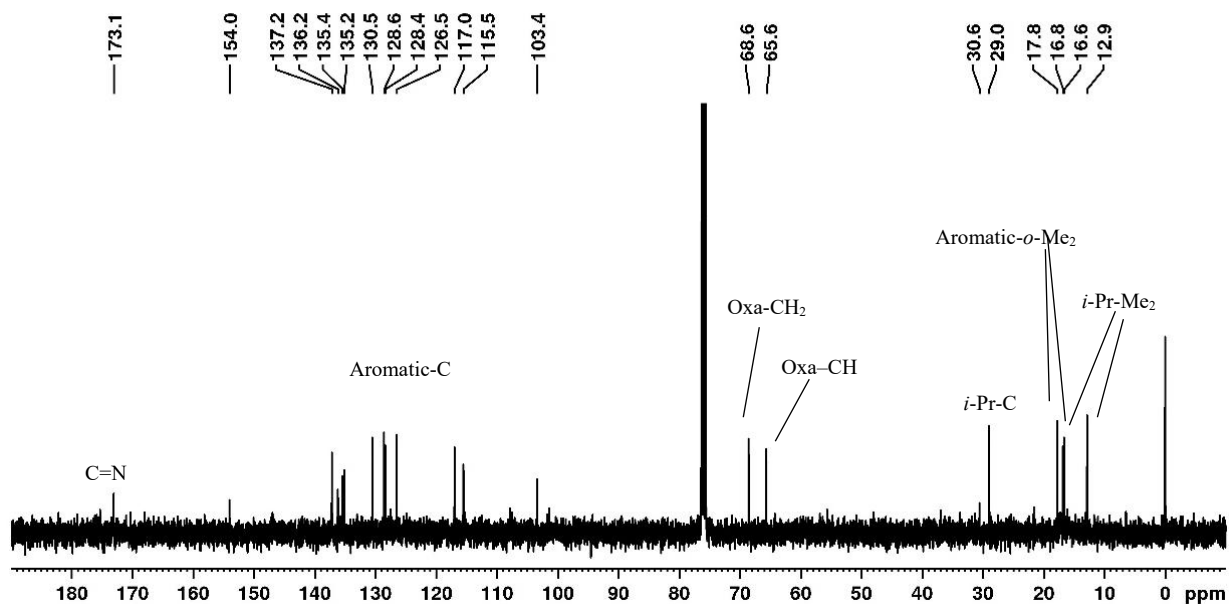


Figure S67. ^{13}C NMR spectrum of **4aAl(OTf)₂**.

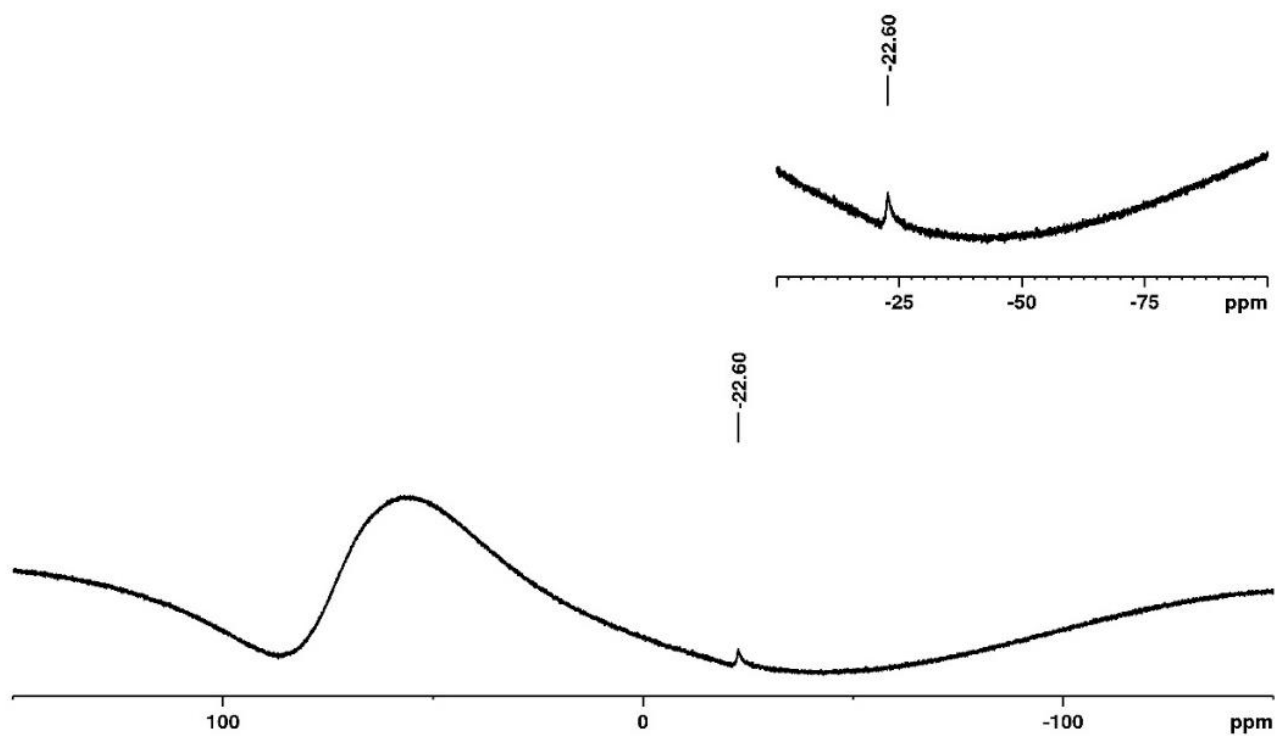


Figure S68. ^{27}Al NMR spectrum of **4aAl(OTf)₂**.

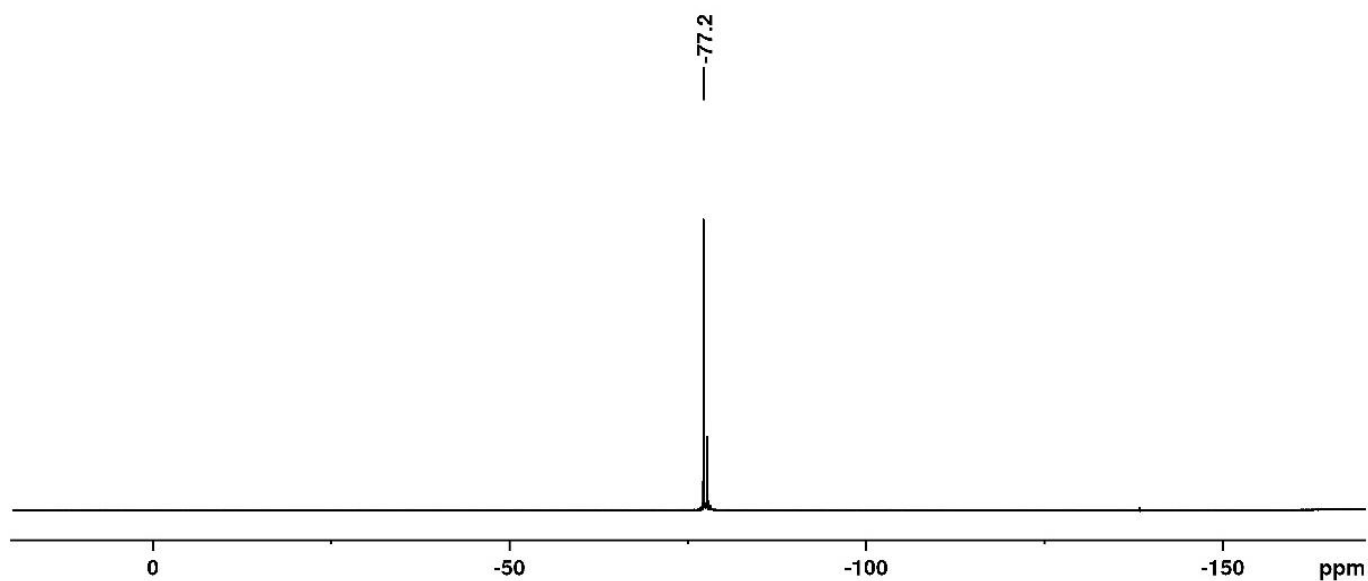


Figure S68. ^{19}F NMR spectrum of $4\text{aAl}(\text{OTf})_2$.

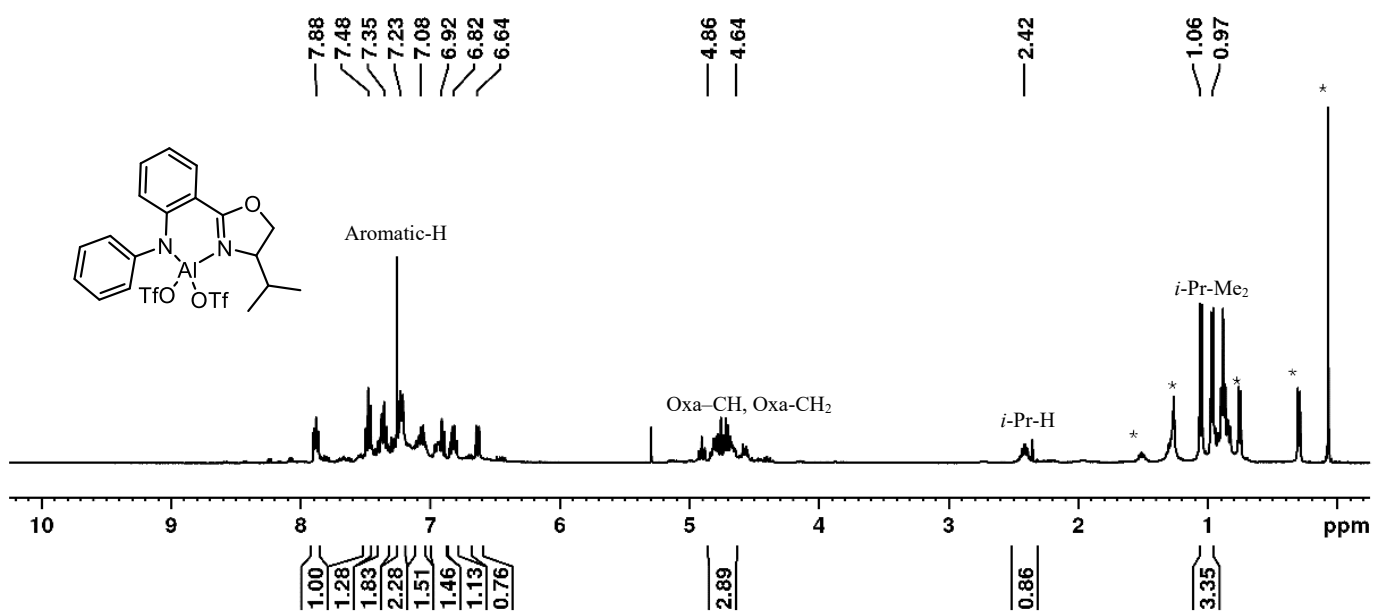


Figure S69. ^1H NMR spectrum of $4\text{bAl}(\text{OTf})_2$. Note: solvent impurities are indicated by *

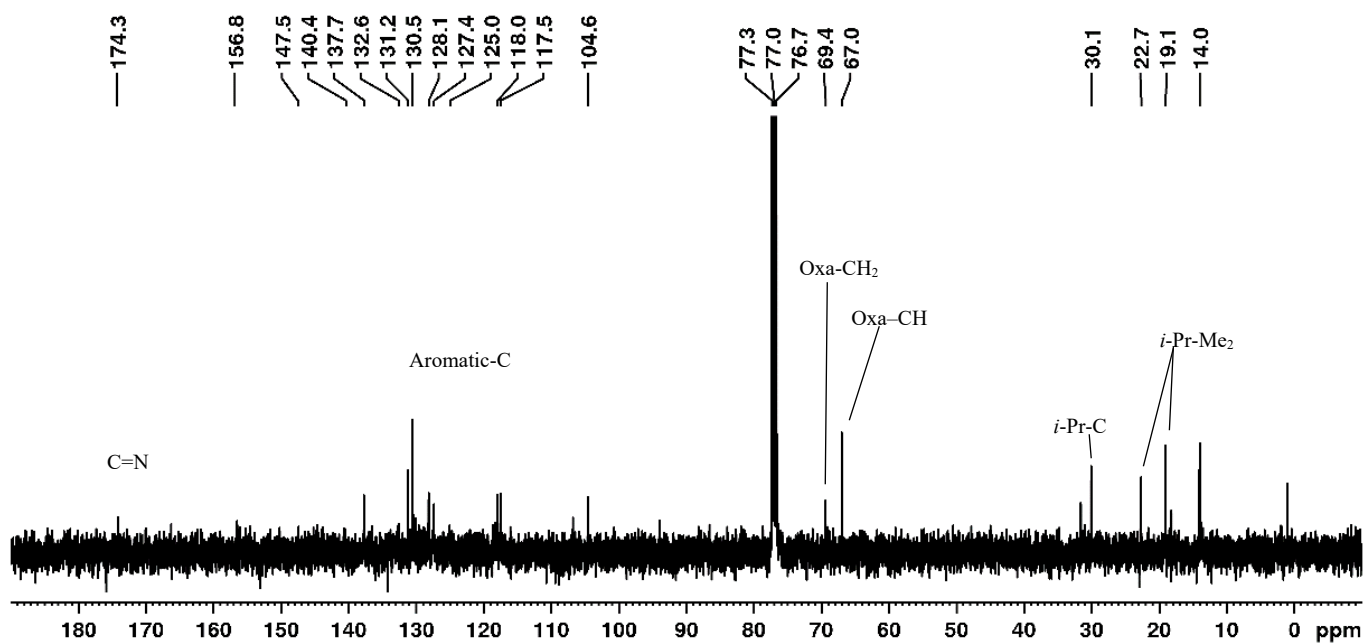


Figure S70. ^{13}C NMR spectrum of **4bAl(OTf)₂**.

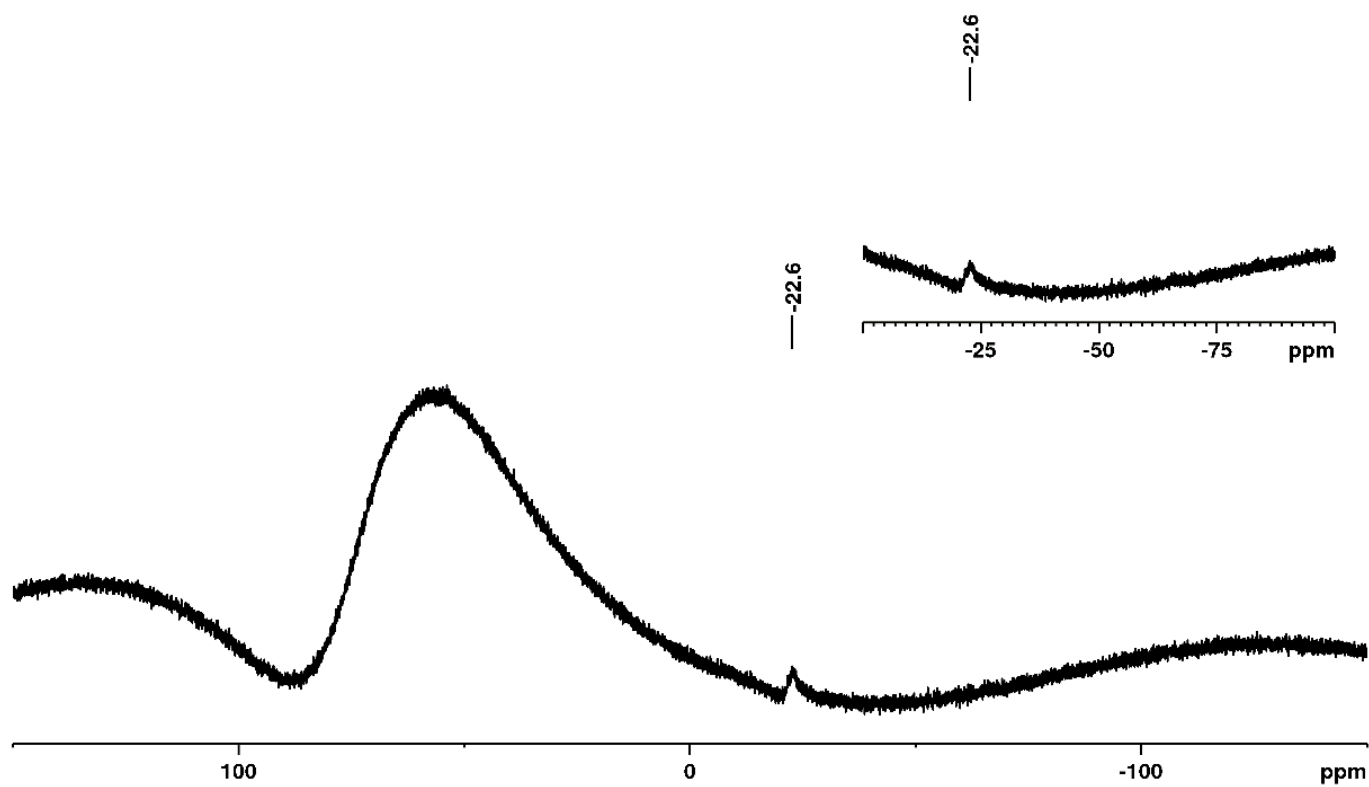


Figure S71. ^{27}Al NMR spectrum of **4bAl(OTf)₂**.

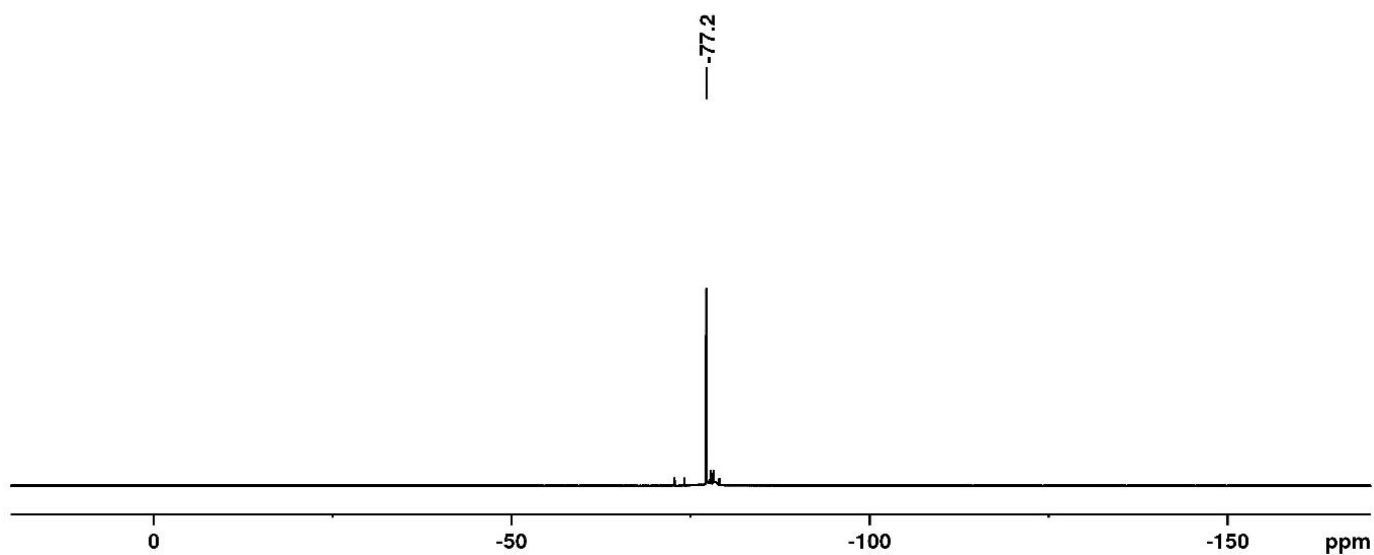


Figure S72. ^{19}F NMR spectrum of $4\text{bAl}(\text{OTf})_2$.

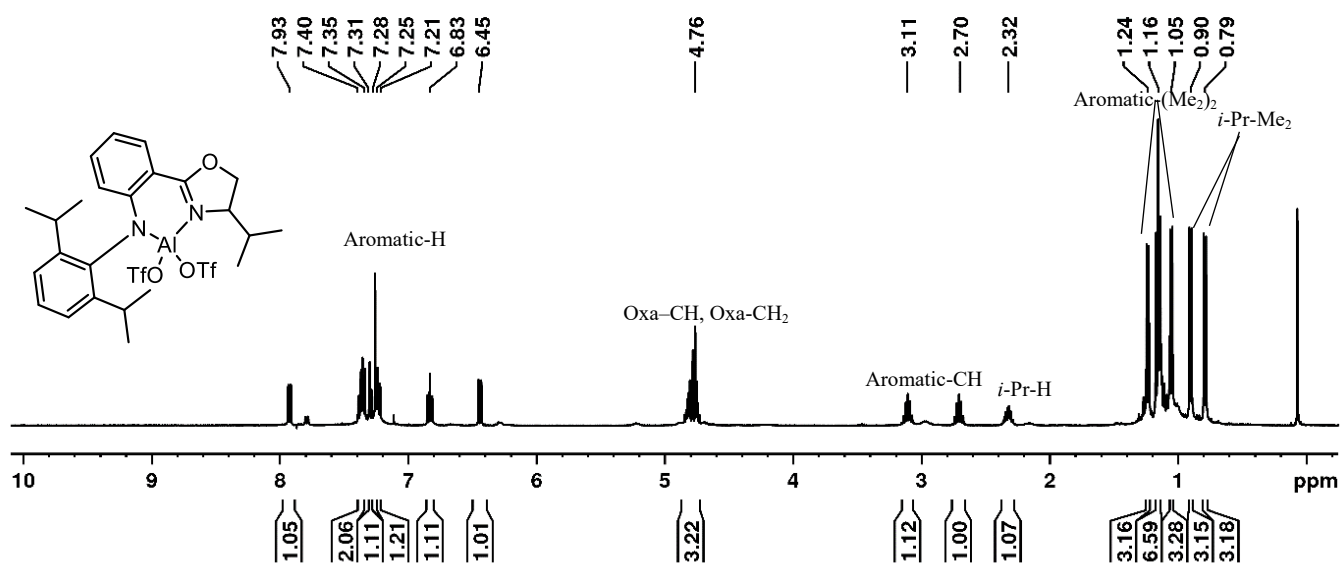


Figure S73. ^1H NMR spectrum of $4\text{cAl}(\text{OTf})_2$.

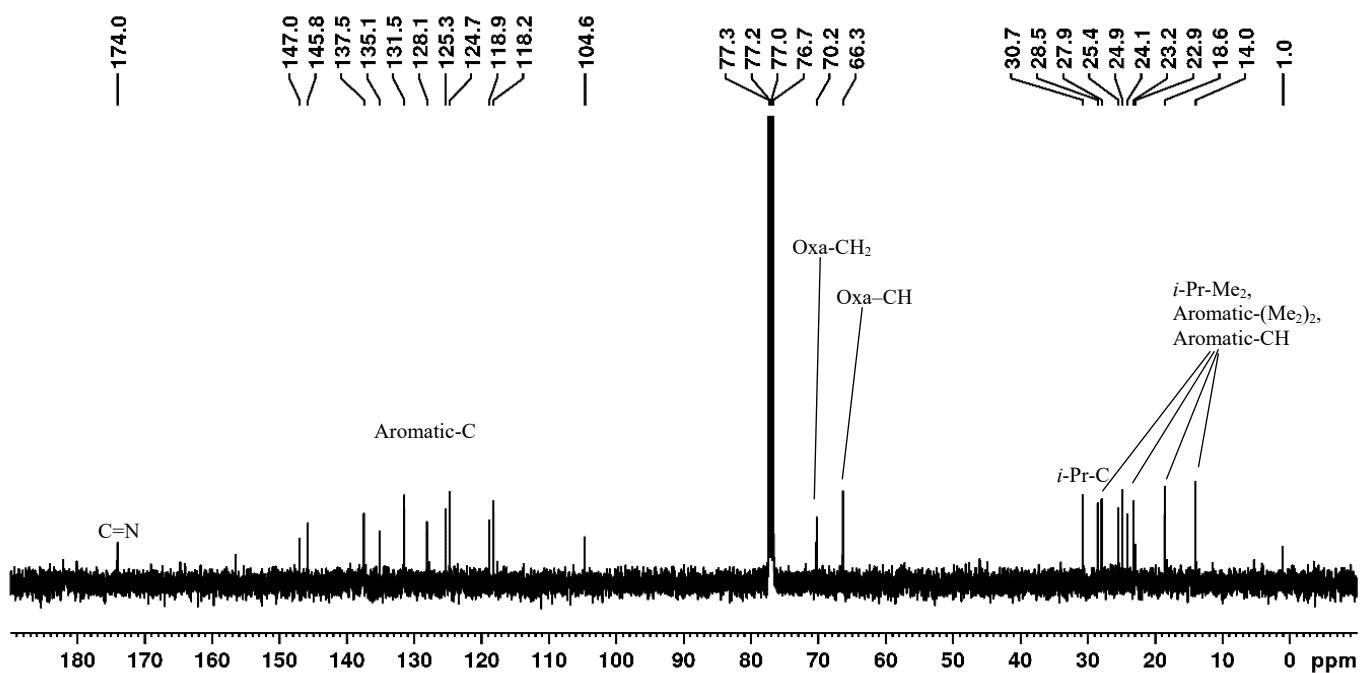


Figure S74. ^{13}C NMR spectrum of $4\text{cAl}(\text{OTf})_2$.

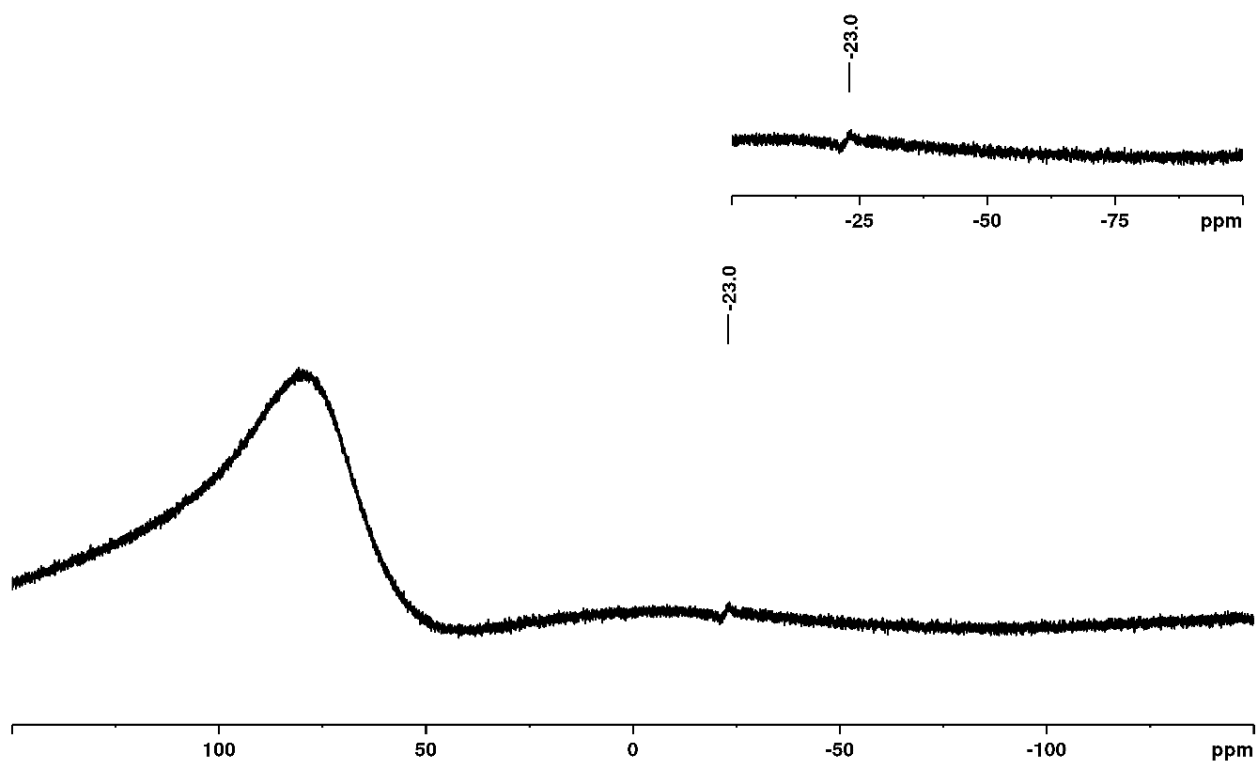


Figure S75. ^{27}Al NMR spectrum of $4\text{cAl}(\text{OTf})_2$.

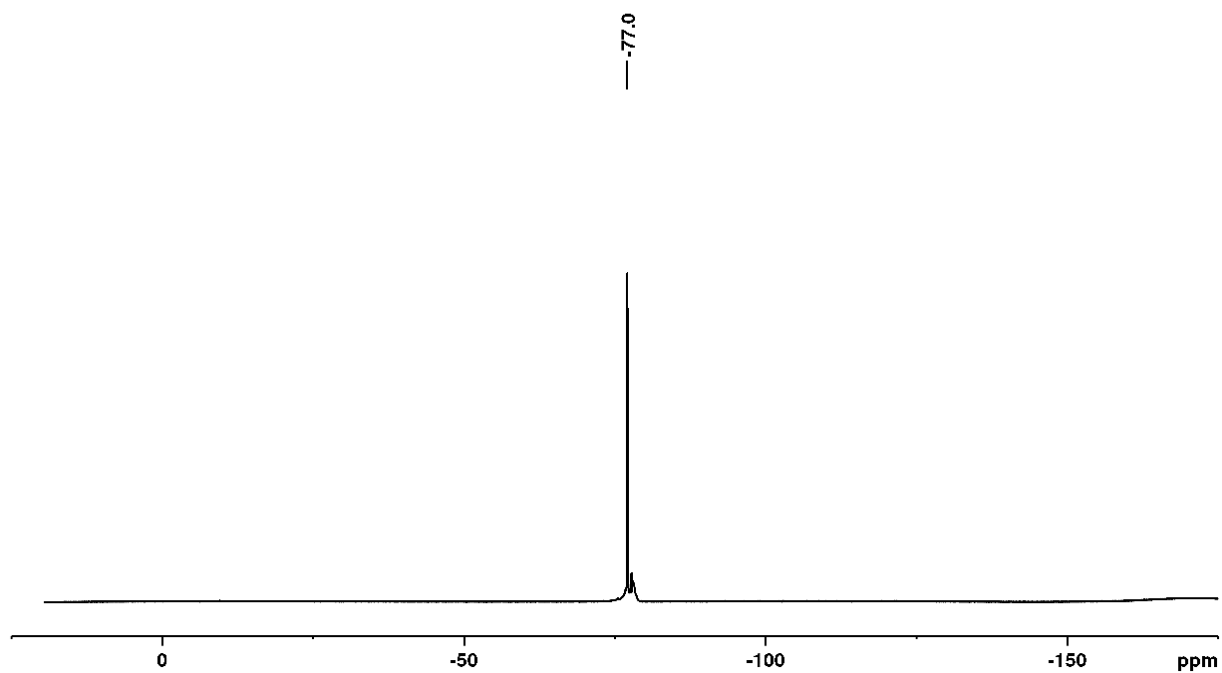


Figure S76. ^{19}F NMR spectrum of $4\text{cAl}(\text{OTf})_2$.

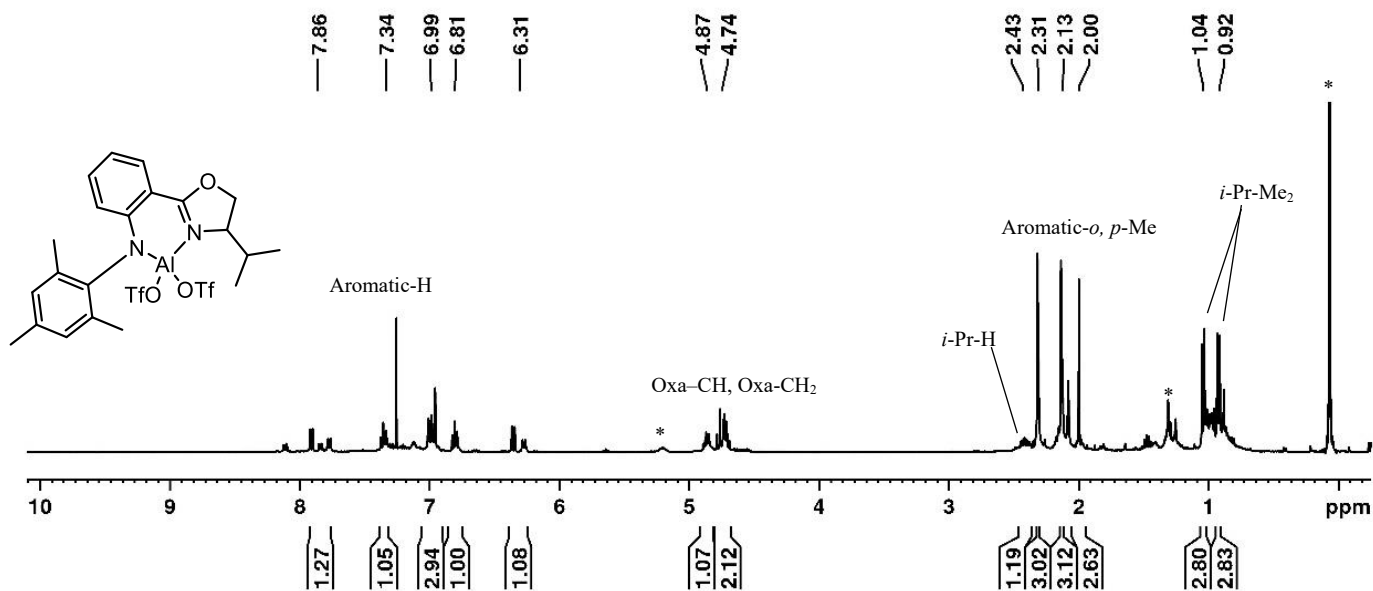


Figure S 77. ^1H NMR spectrum of $4\text{dAl}(\text{OTf})_2$. Note: solvent impurities are indicated by *

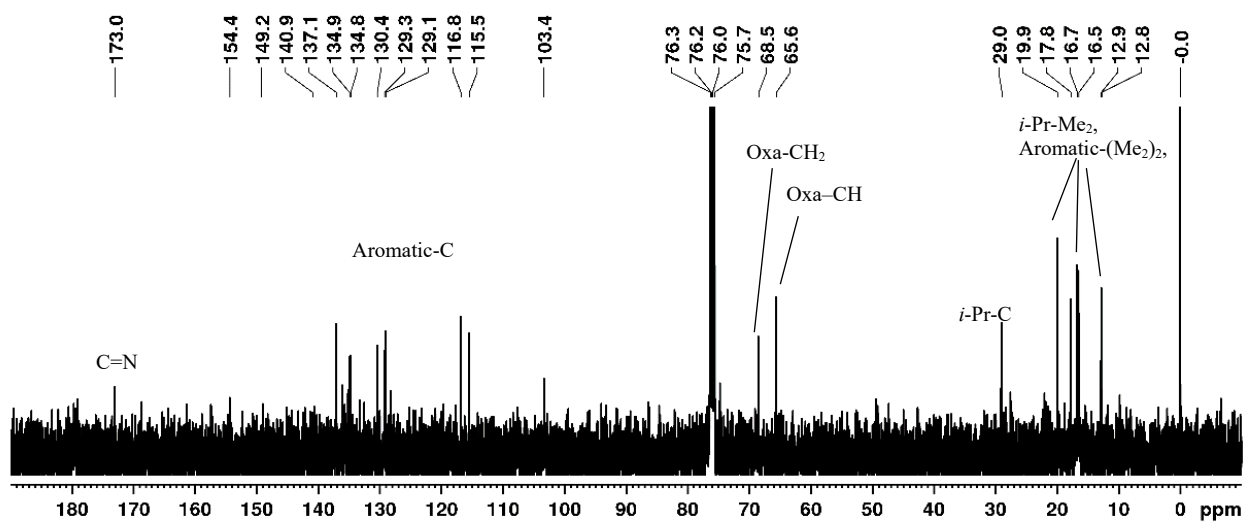


Figure S78. ¹³C NMR spectrum of **4dAl(OTf)₂**.

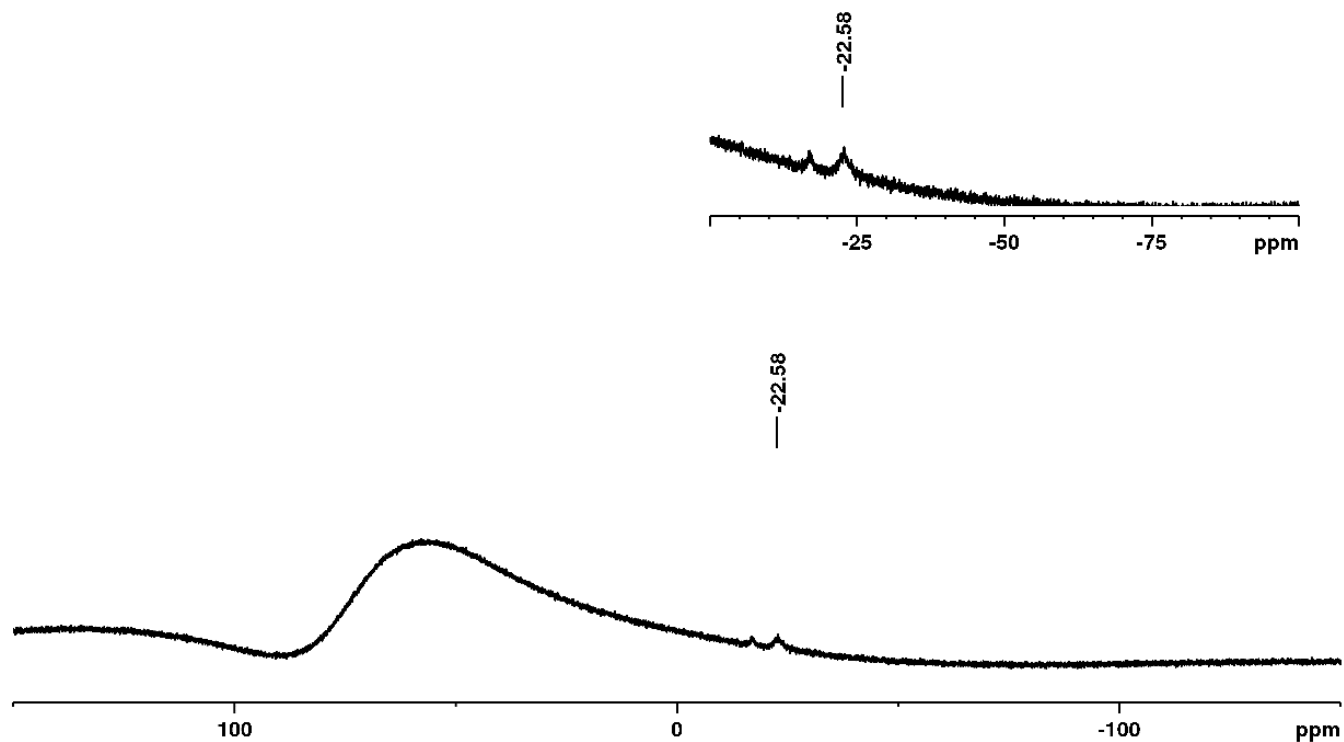


Figure S79. ²⁷Al NMR spectrum of **4dAl(OTf)₂**.

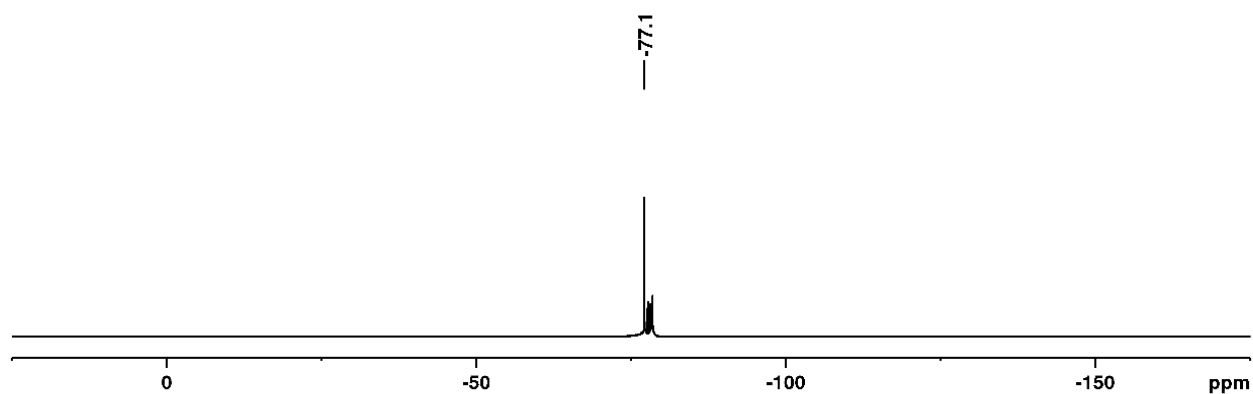


Figure S80. ^{19}F NMR spectrum of $4\text{dAl}(\text{OTf})_2$.

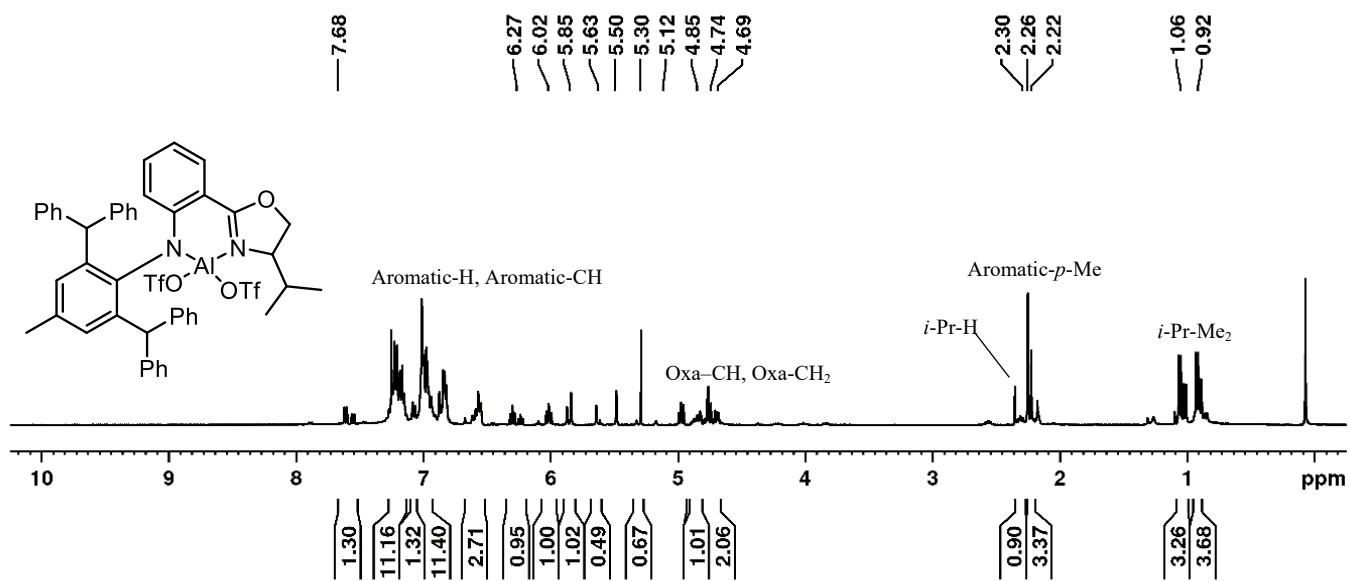


Figure S81. ^1H NMR spectrum spectrum of $4\text{eAl}(\text{OTf})_2$.

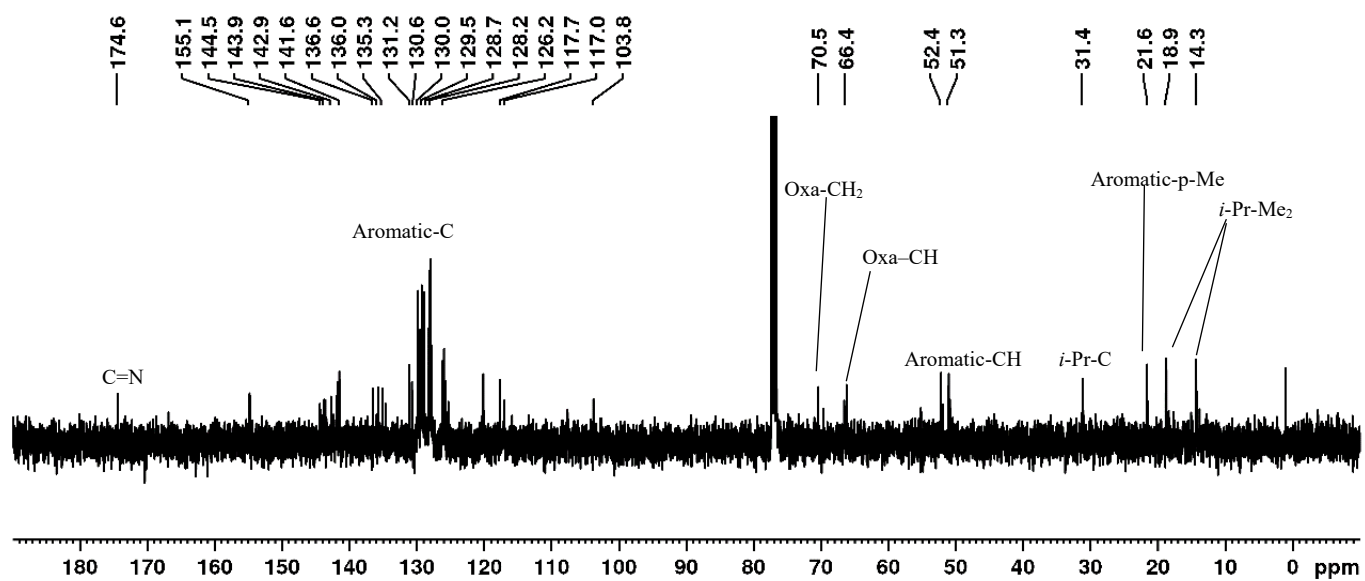


Figure S82. ^{13}C NMR spectrum of $4\text{eAl}(\text{OTf})_2$.

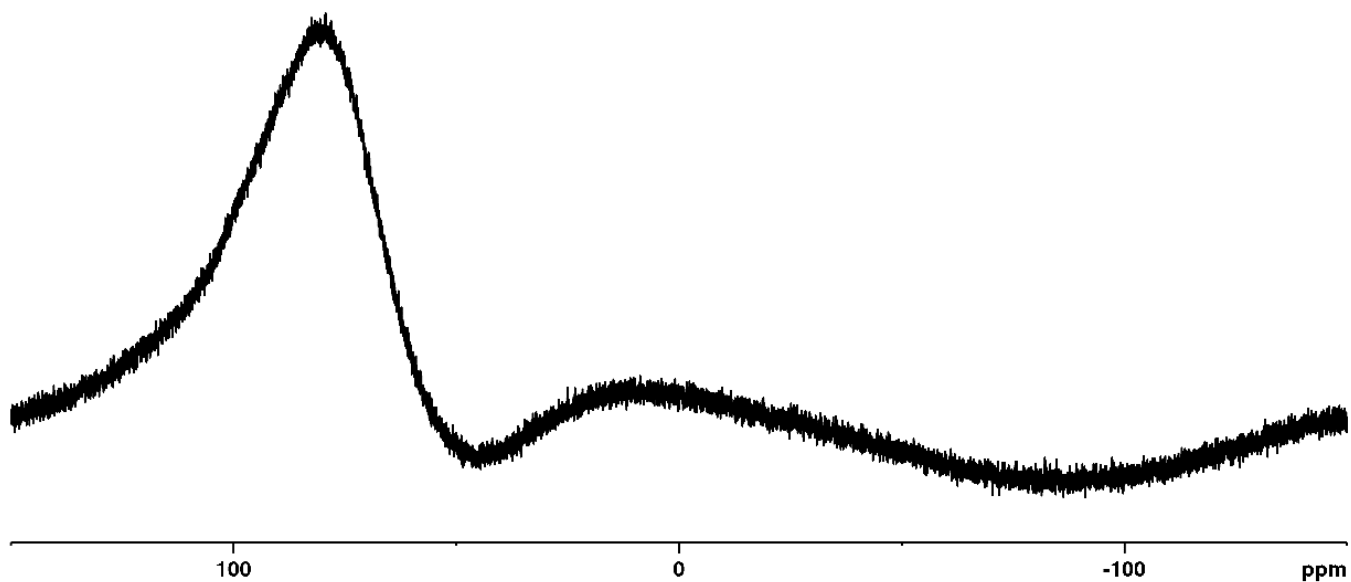


Figure S83. ^{27}Al NMR spectrum of $4\text{eAl}(\text{OTf})_2$.

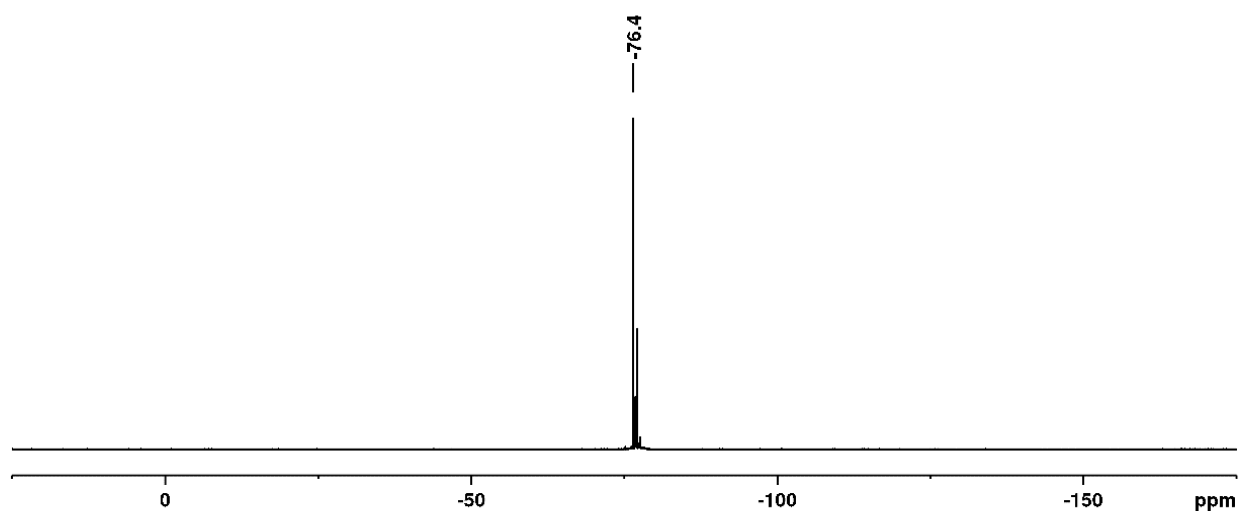


Figure S84. ^{19}F NMR spectrum of $4\text{eAl}(\text{OTf})_2$.

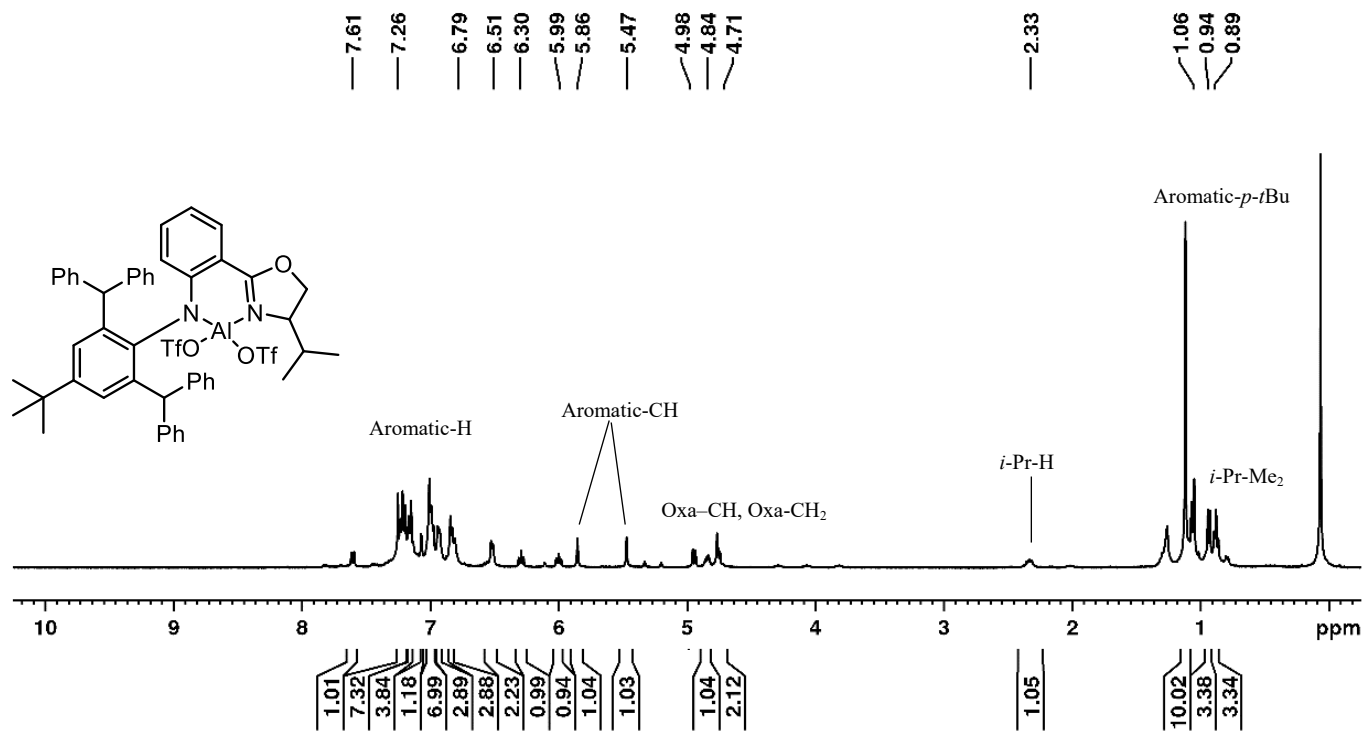


Figure S85. ^1H NMR spectrum of $4\text{fAl}(\text{OTf})_2$.

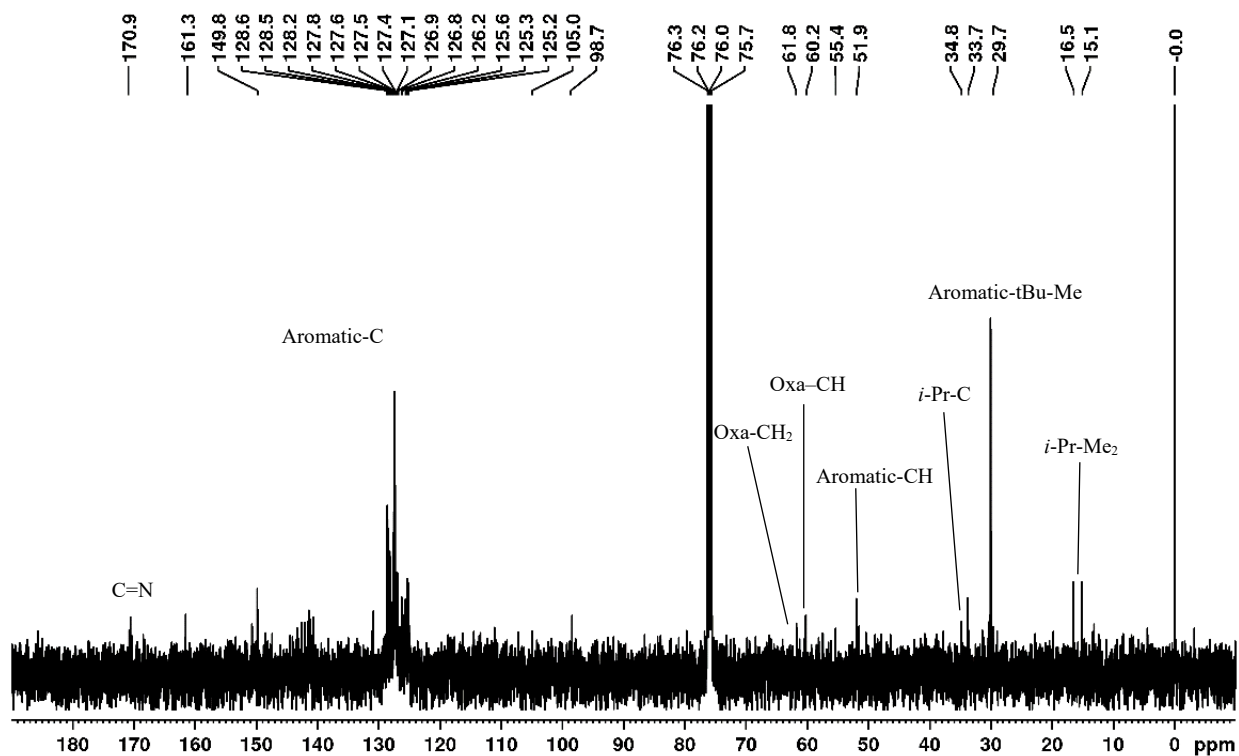


Figure S86. ^{13}C NMR spectrum of $4\text{fAl}(\text{OTf})_2$.

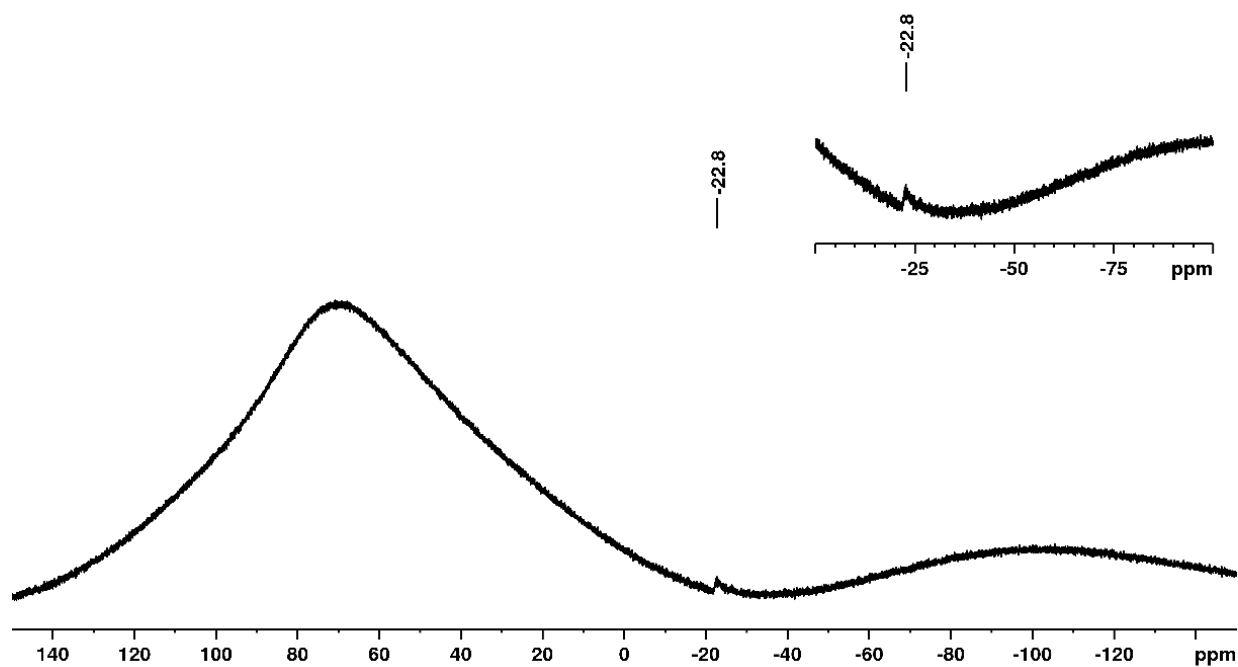


Figure S87. ^{27}Al NMR spectrum of $4\text{fAl}(\text{OTf})_2$.

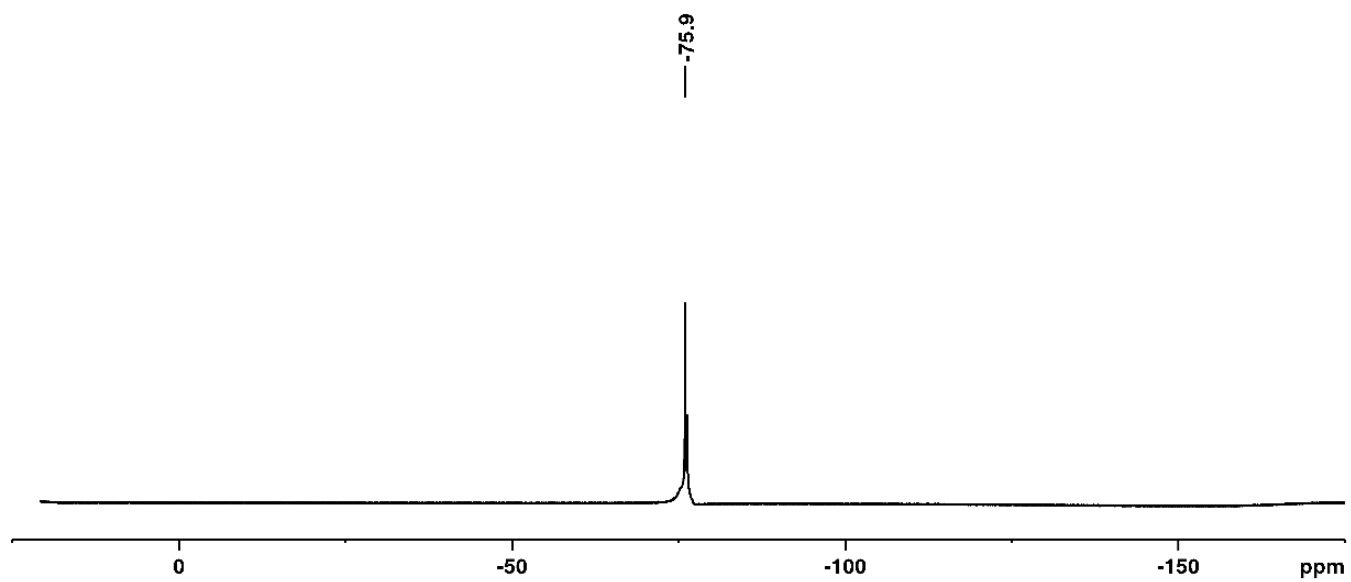


Figure S88. ^{19}F NMR spectrum of $4\text{fAl}(\text{OTf})_2$.

NMR Spectrum of DA Adducts

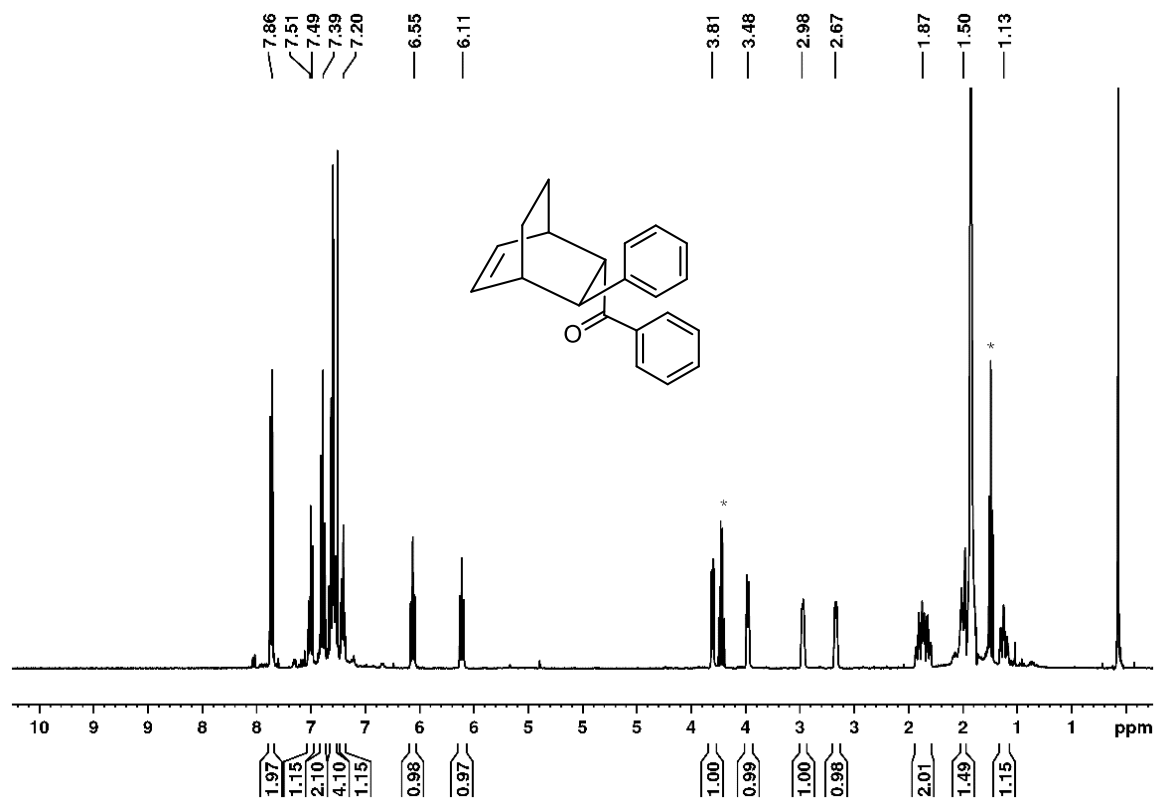


Figure S89. ¹H NMR spectrum of **P1**. Note: solvent impurities are indicated by *

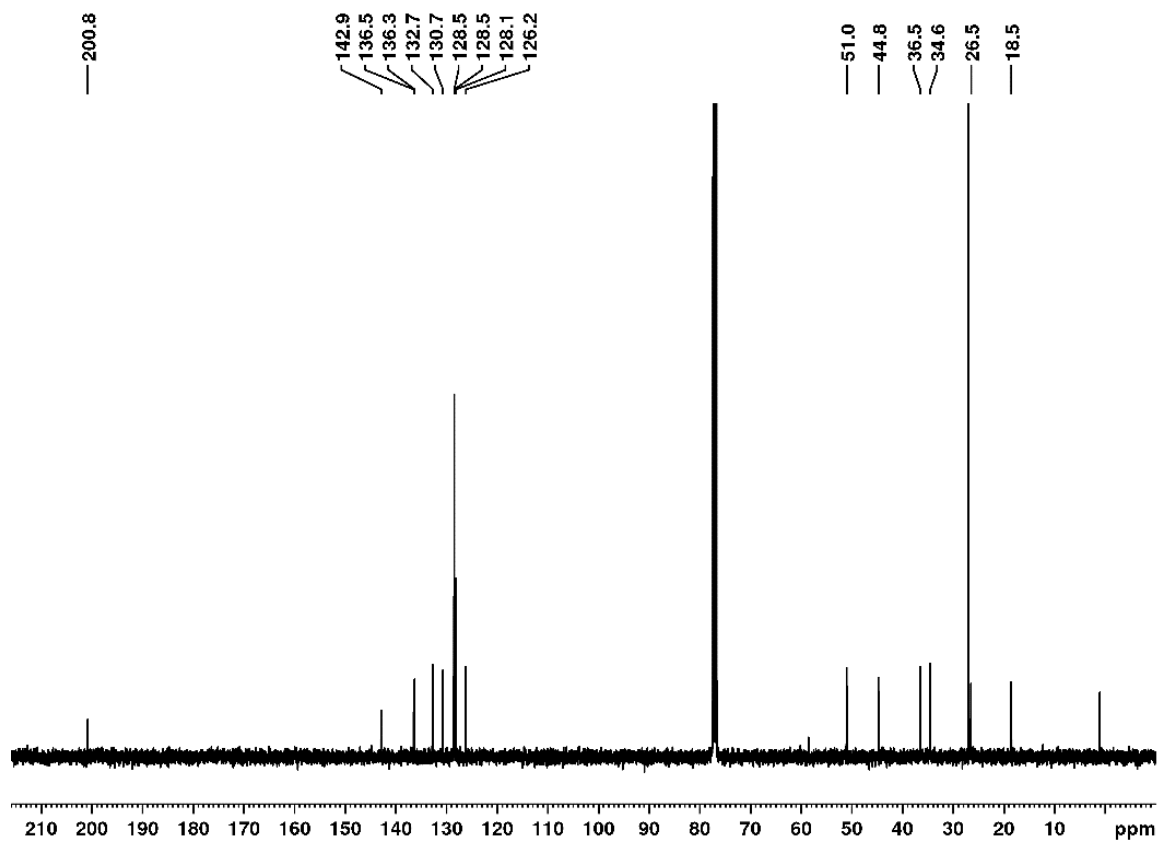


Figure S90. ¹³C NMR spectrum of **P1**.

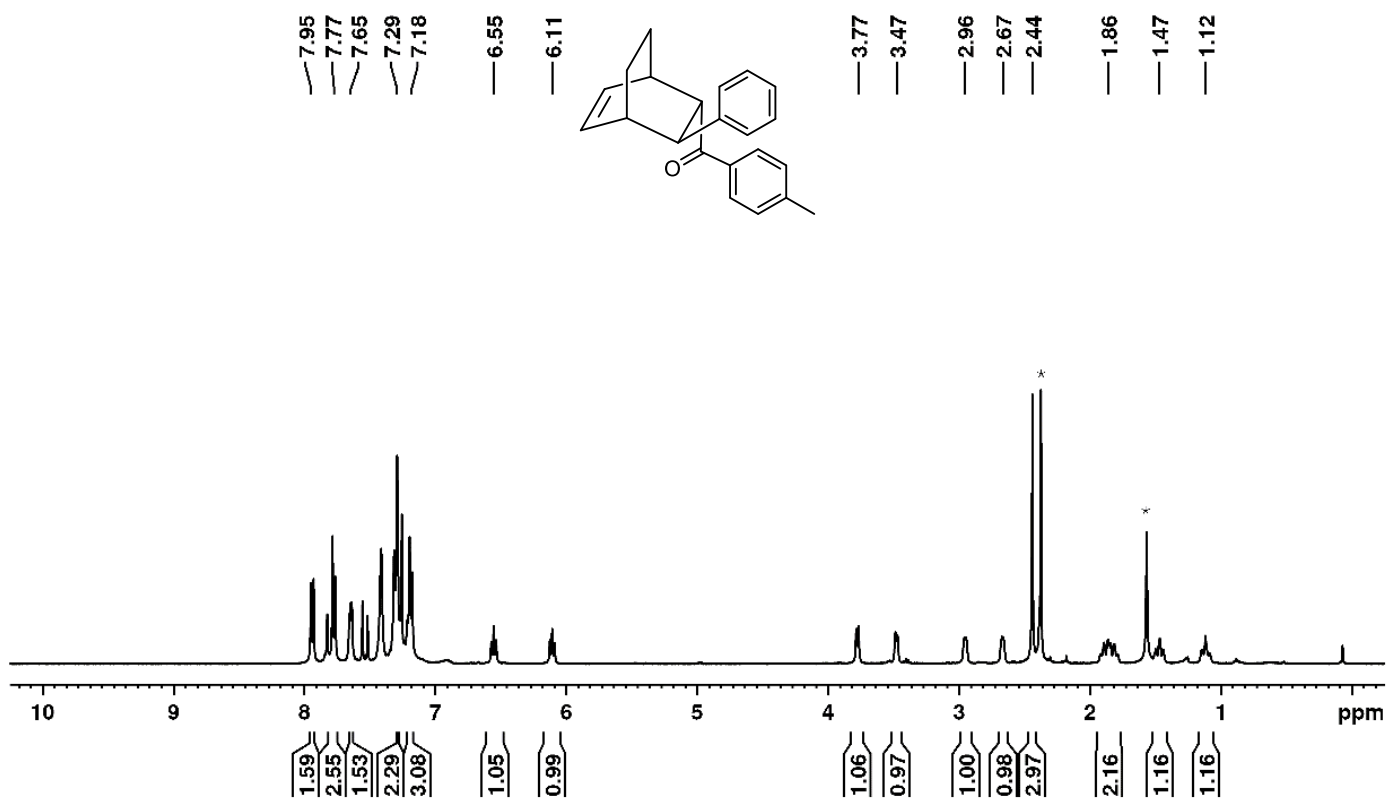


Figure S91. ¹H NMR spectrum of **P2**. Note: solvent impurities are indicated by *

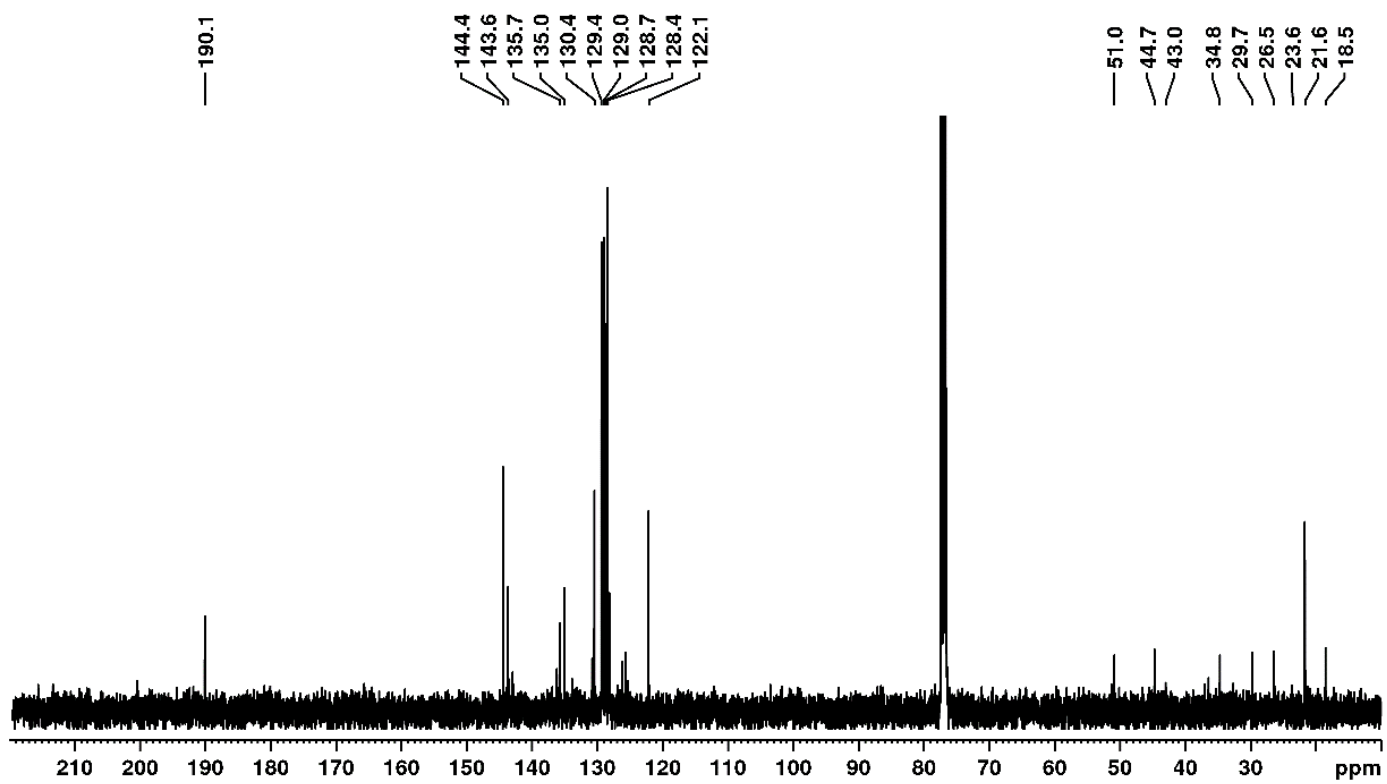


Figure S92. ¹³C NMR spectrum of **P2**.

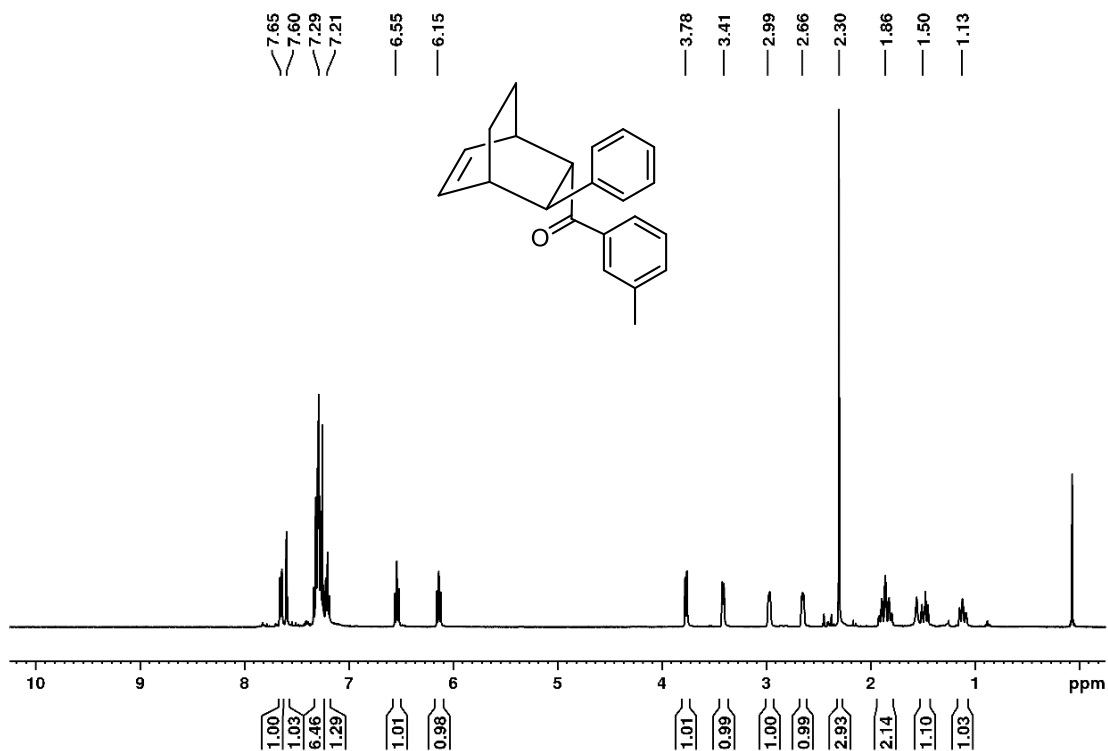


Figure S93. ¹H NMR spectrum of **P3**.

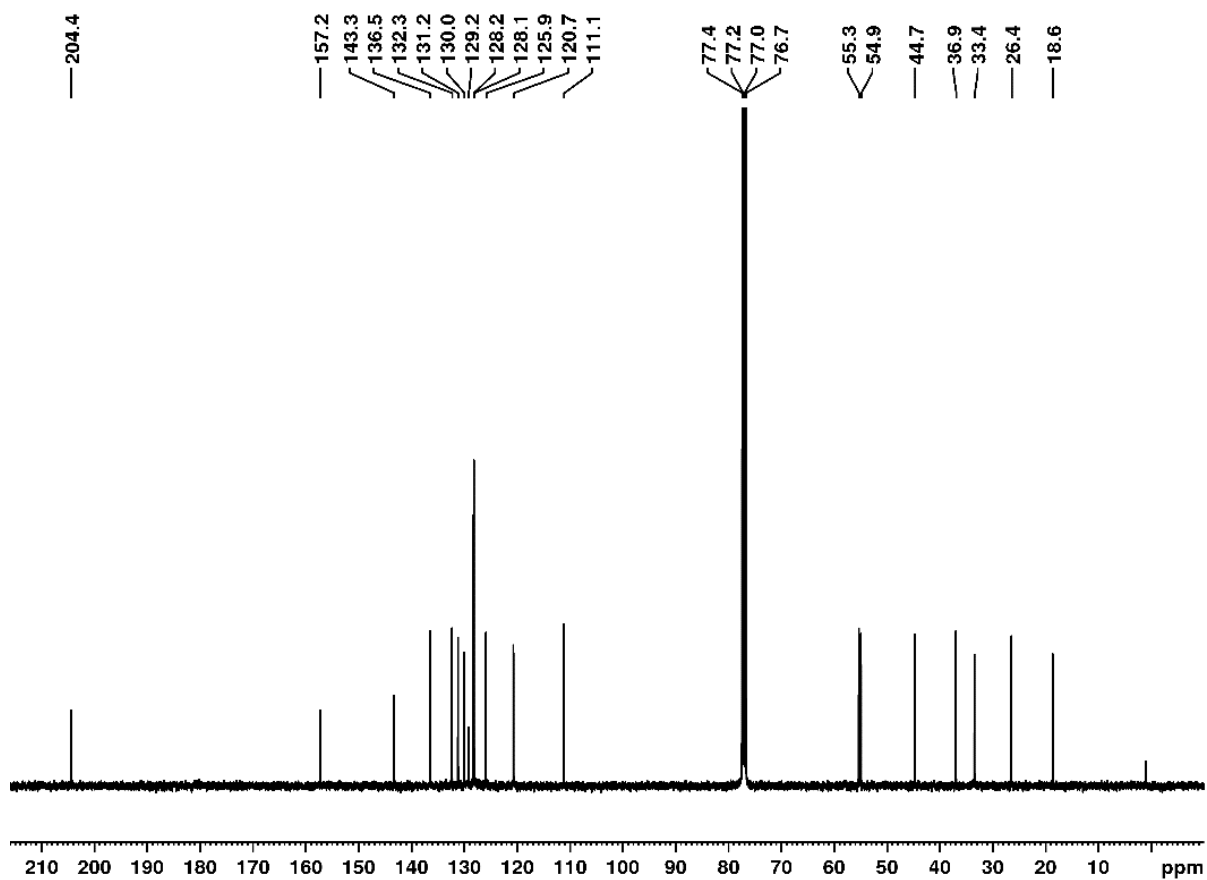


Figure S94. ¹³C NMR spectrum of **P3**.

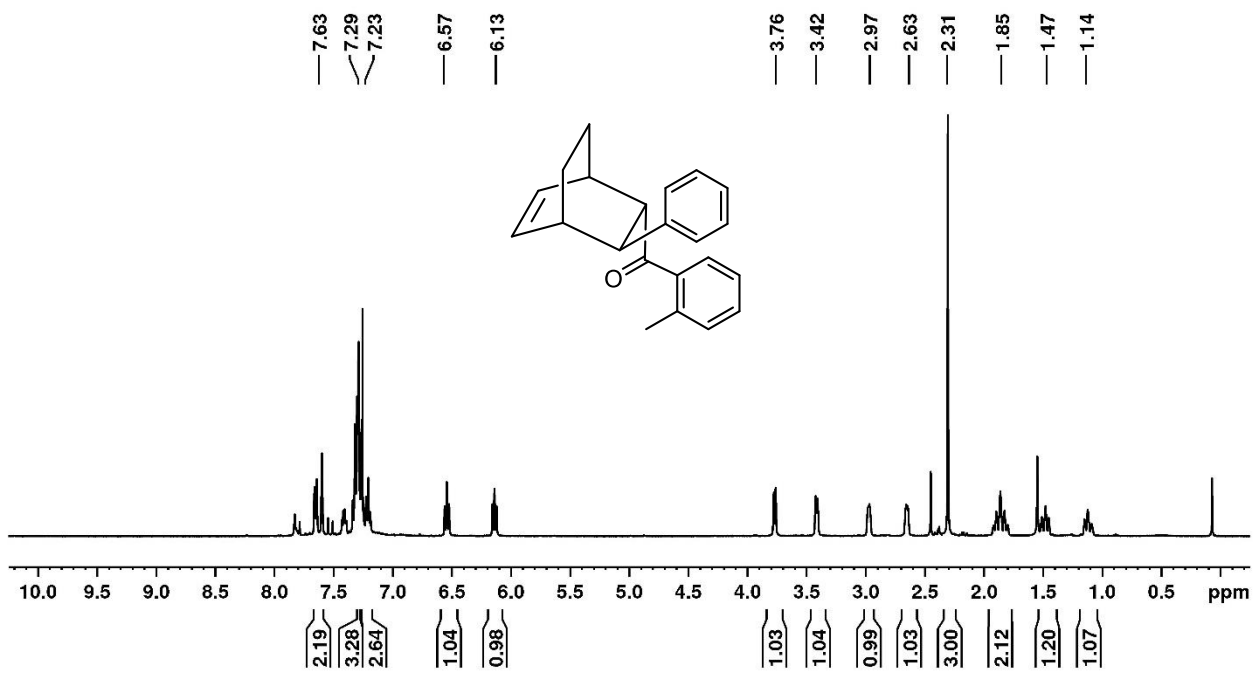


Figure S95. ^1H NMR spectrum of **P4**.

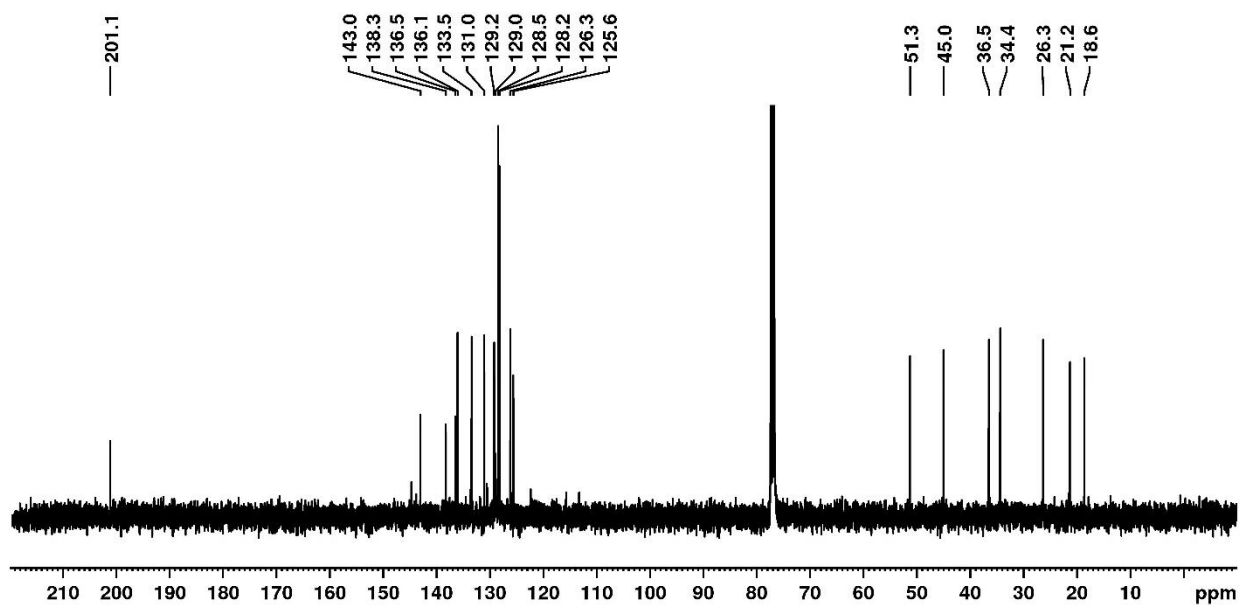


Figure S96. ^{13}C NMR spectrum of **P4**.

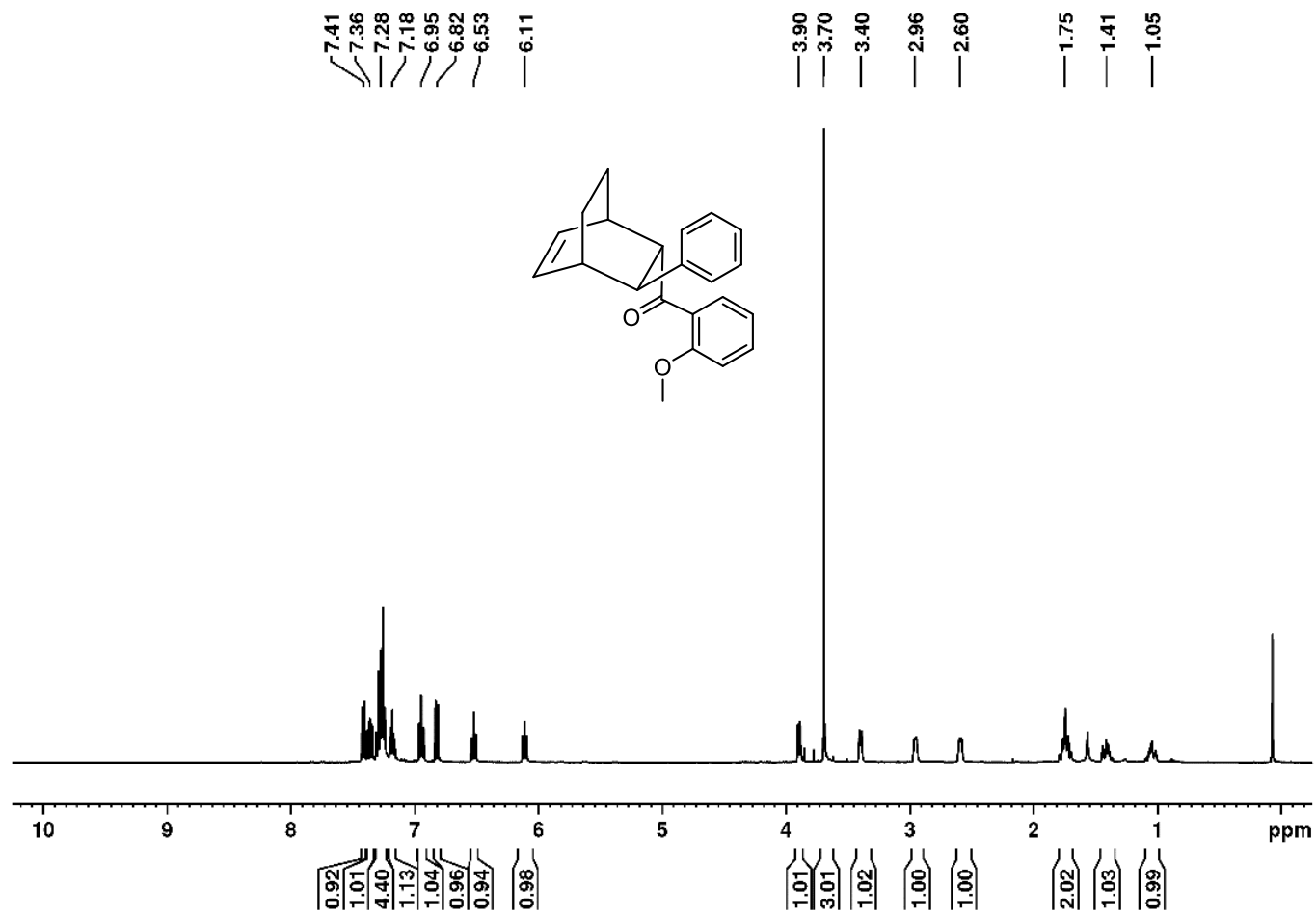


Figure S97. ¹H NMR spectrum of P5.

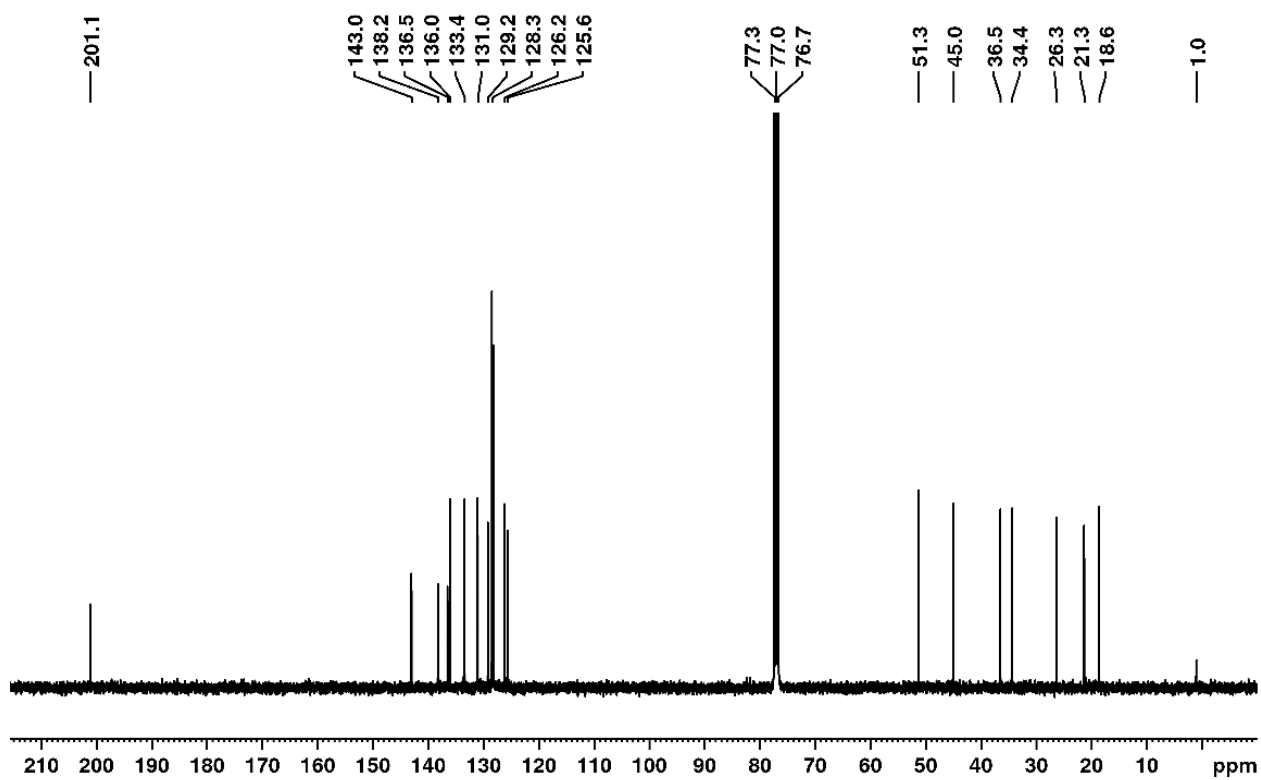


Figure S98. ¹³C NMR spectrum of P5.

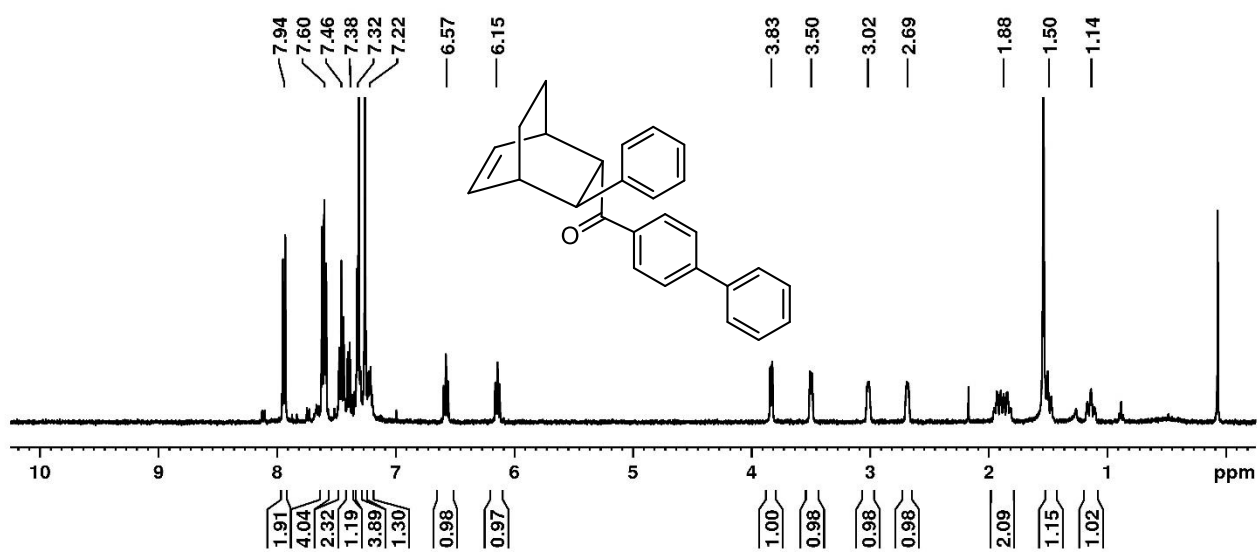


Figure S99. ^1H NMR spectrum of **P6**.

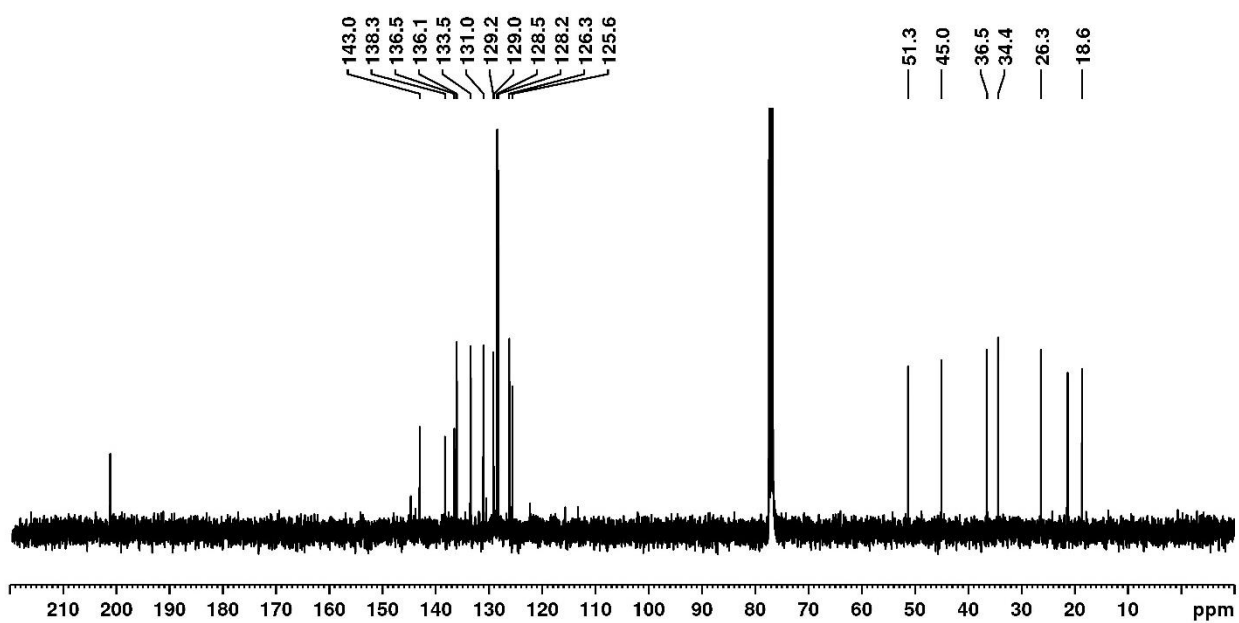


Figure S100. ^{13}C NMR spectrum of **P**.

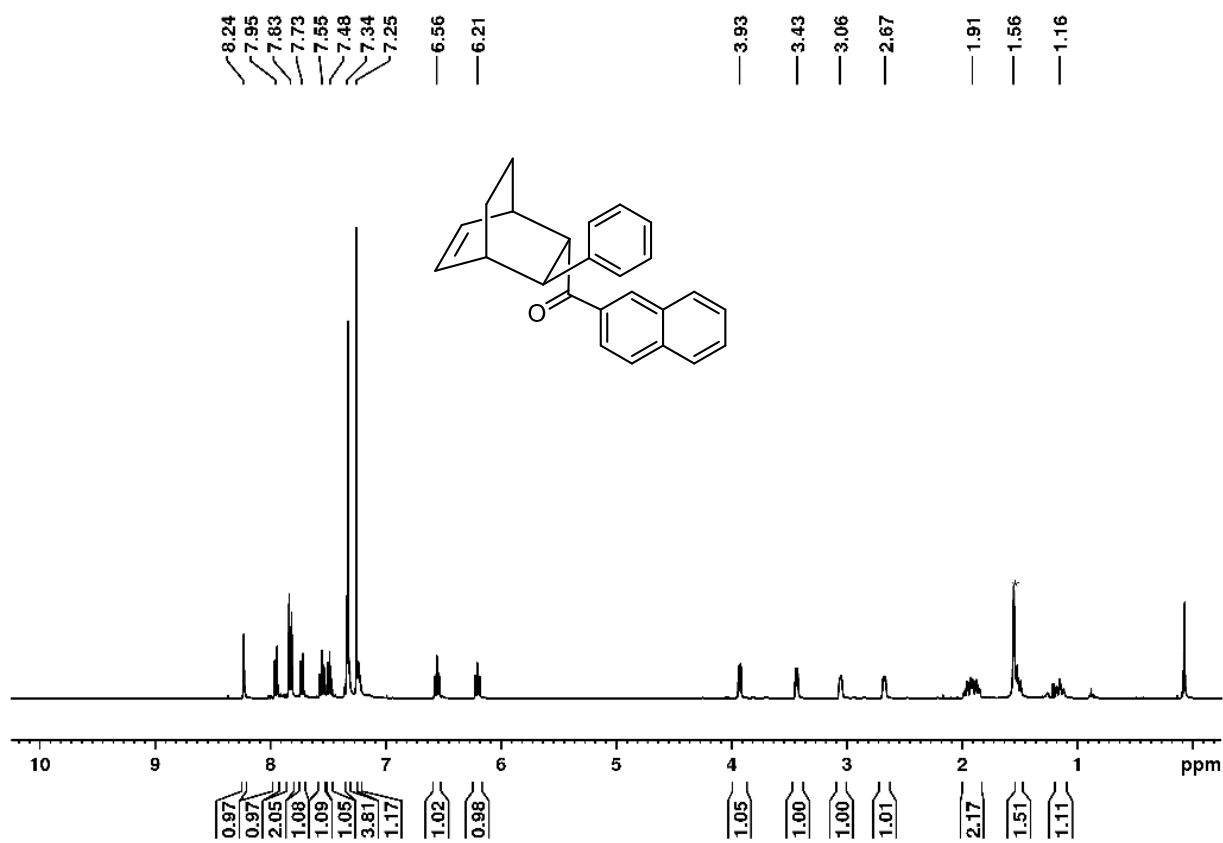


Figure S101. ¹H NMR spectrum of **P5**. Note: solvent impurities are indicated by *

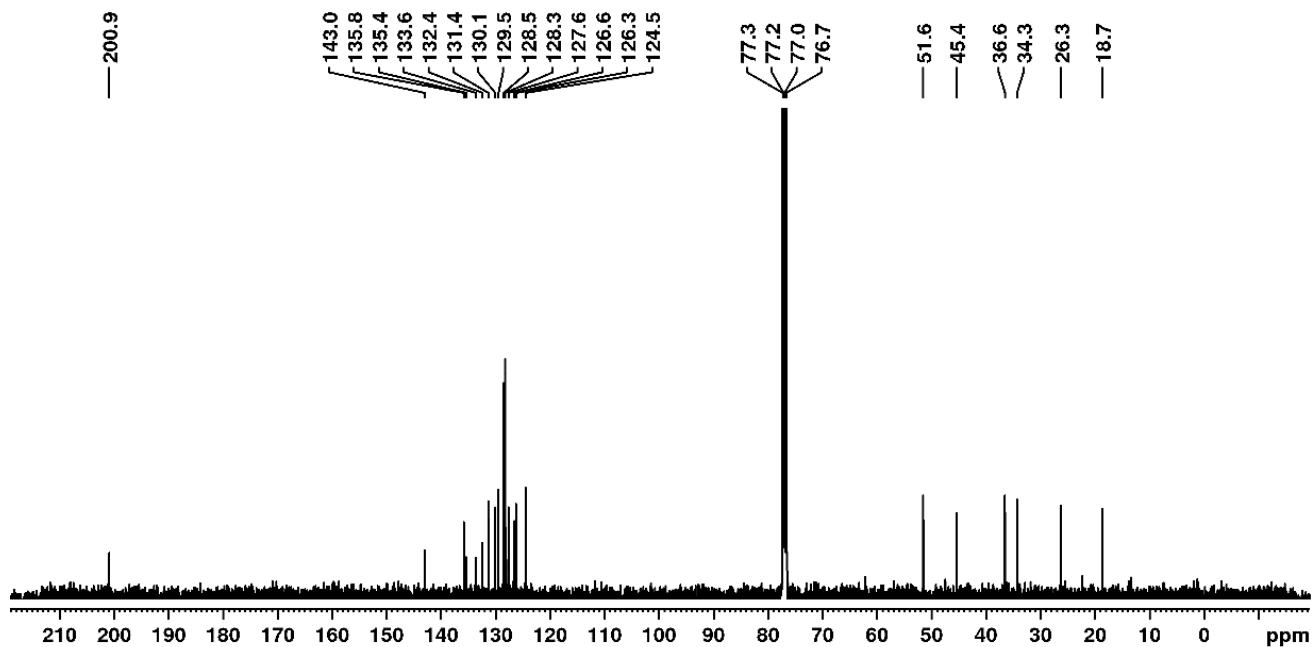
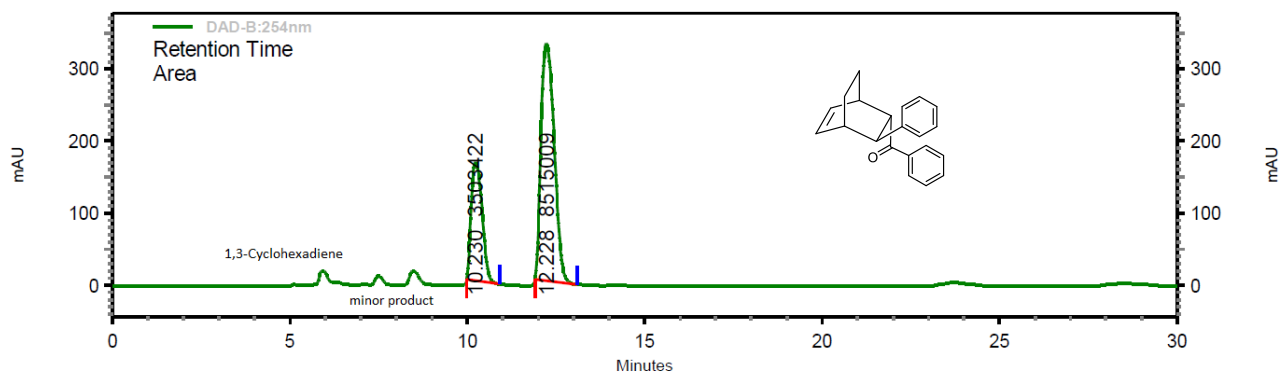
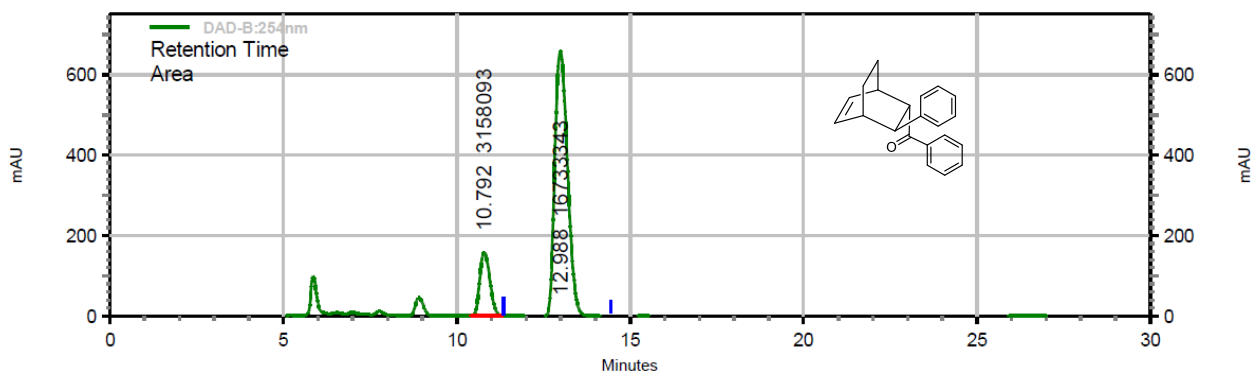


Figure S102. ¹³C NMR spectrum of **P5**.

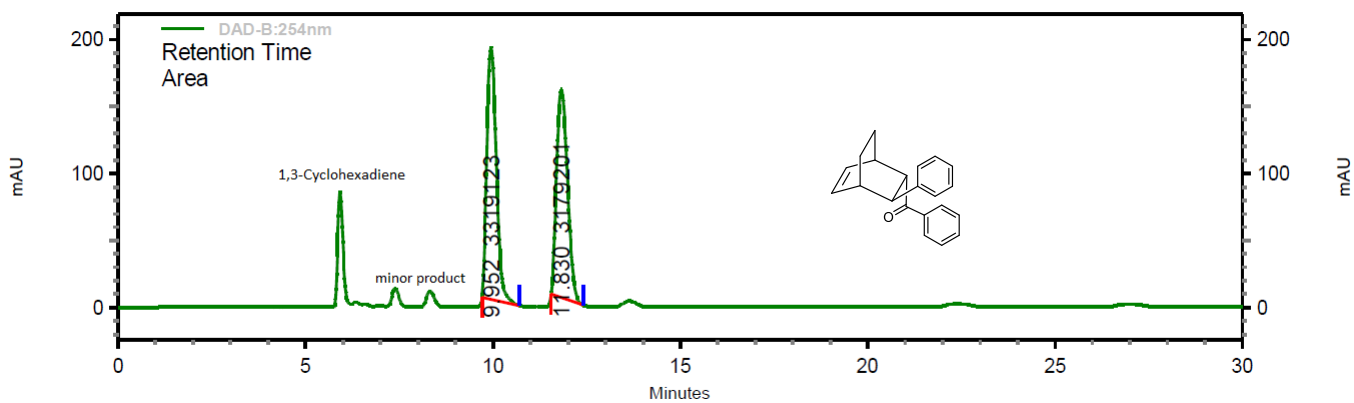
HPLC studies of enantiomers



Retention time	Area	Area %
10.230	3503422	29.15
12.228	8515009	70.85

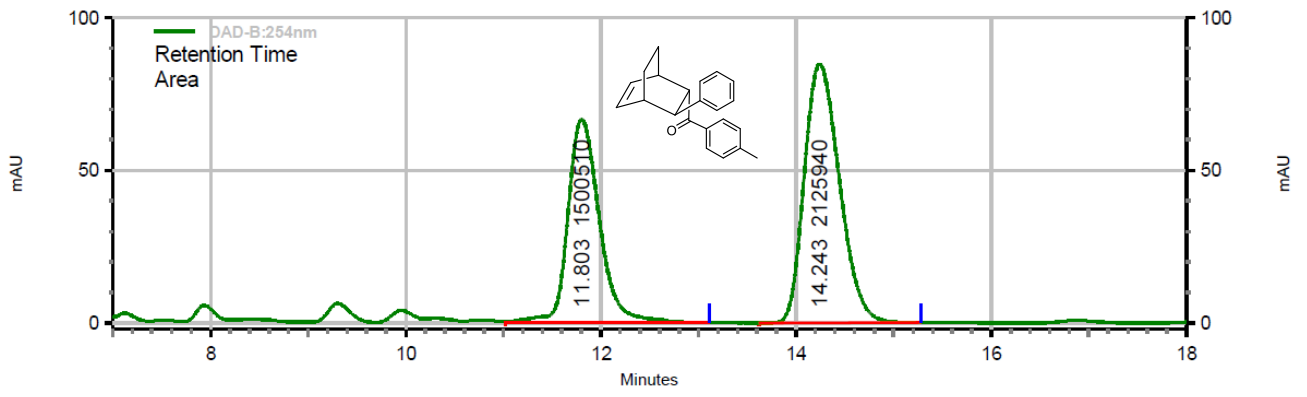


Retention time	Area	Area %
10.792	3158093	15.88
12.988	16733343	84.12

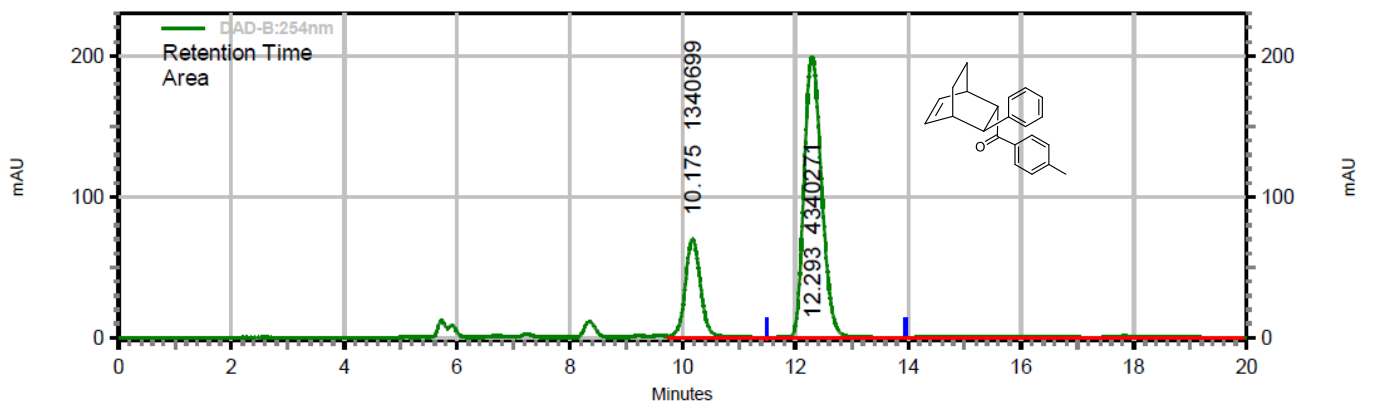


Racemic mixture

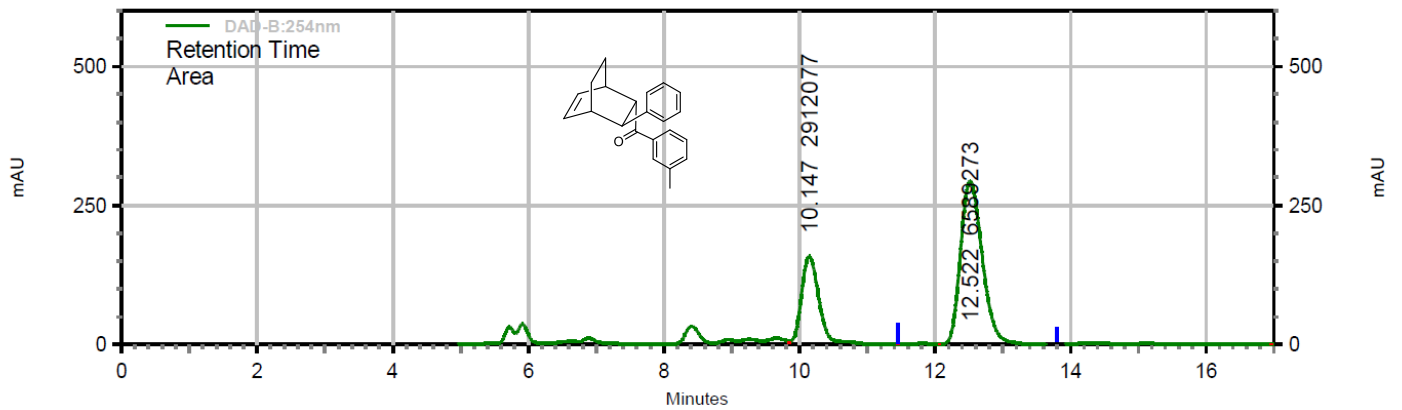
Retention time	Area	Area %
9.952	3319123	51.09
11.830	3179201	48.91



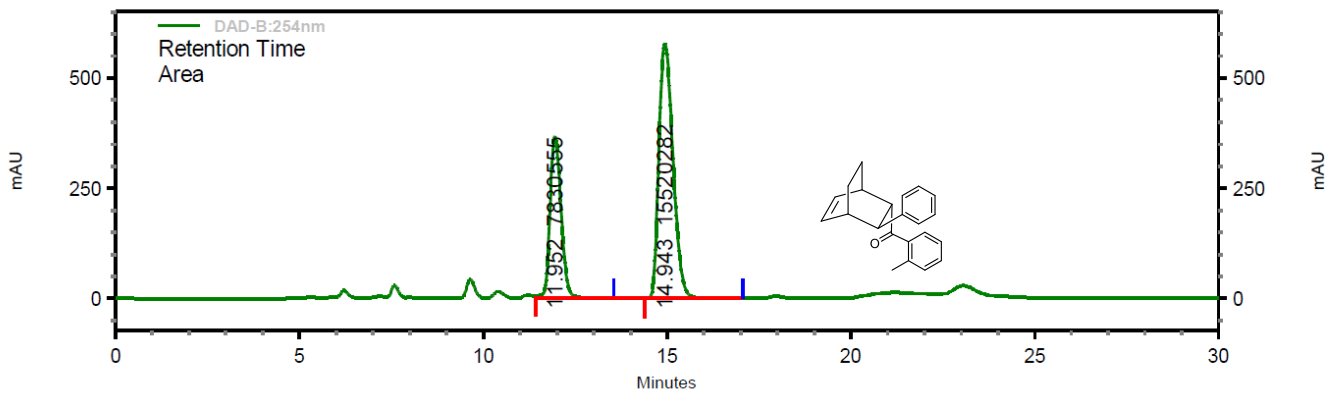
Retention time	Area	Area %
11.803	1500510	41.37
14.243	2125940	58.63



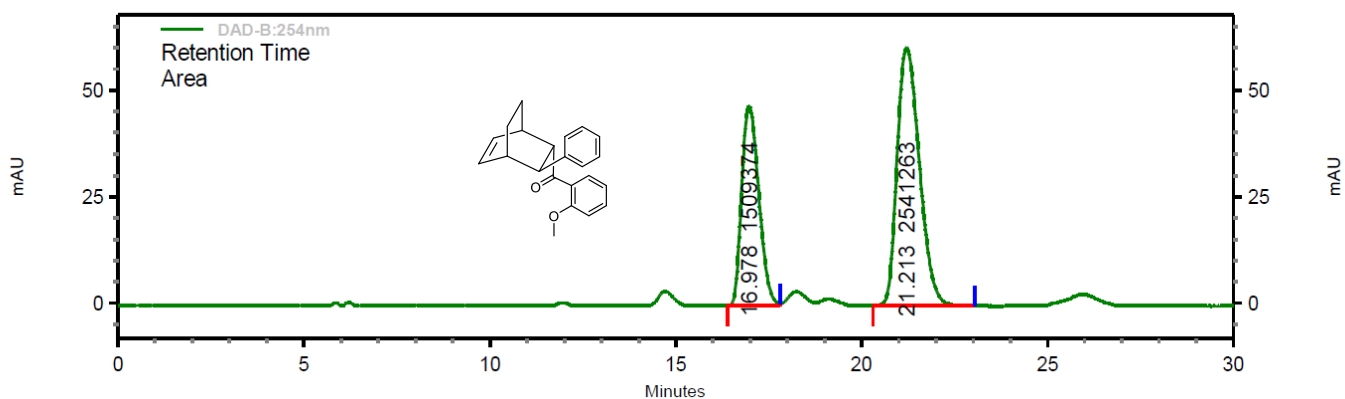
Retention time	Area	Area %
10.175	1340699	23.60
12.293	4340271	76.40



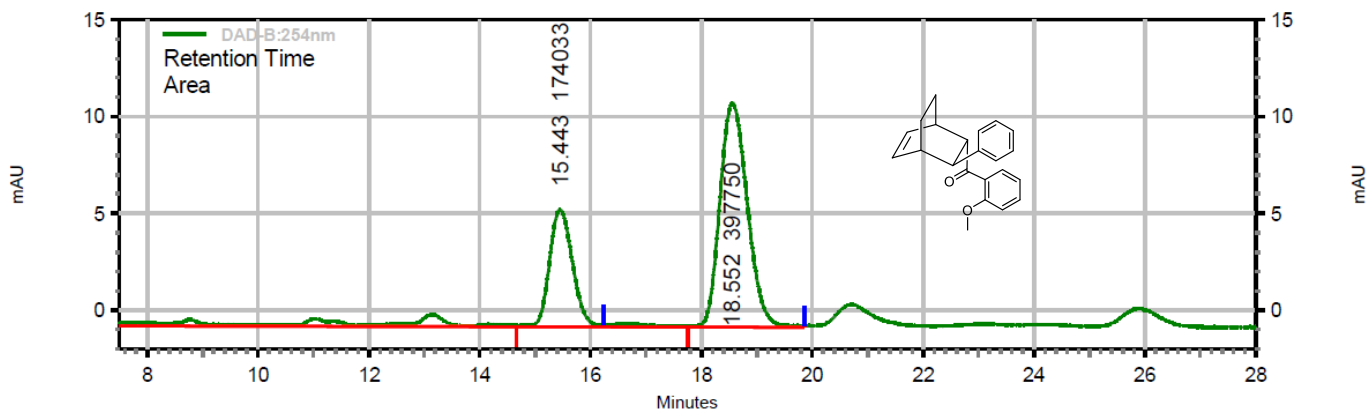
Retention time	Area	Area %
10.147	2912077	30.65
12.522	6589273	69.35



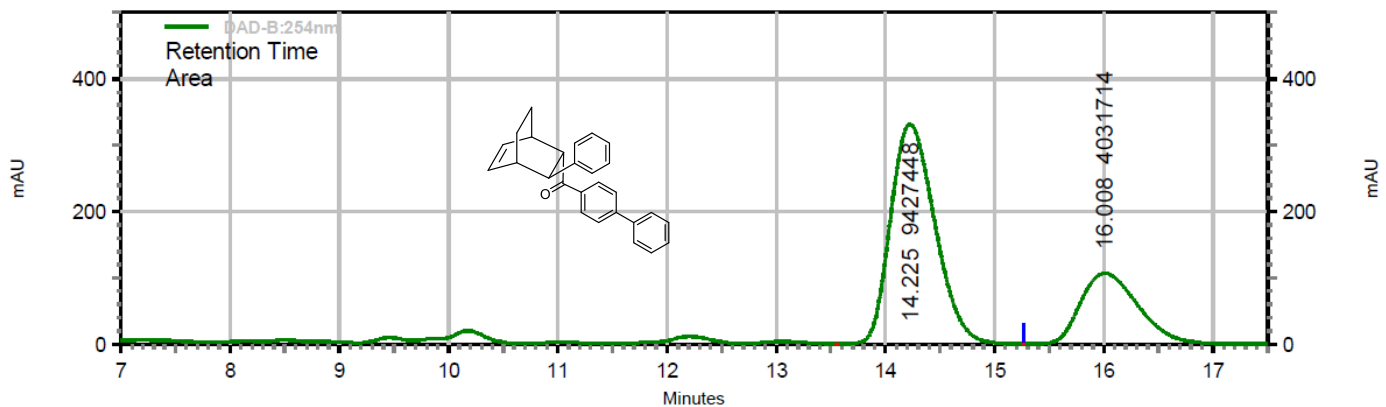
Retention time	Area	Area %
11.952	7830555	33.53
14.943	15520282	66.47



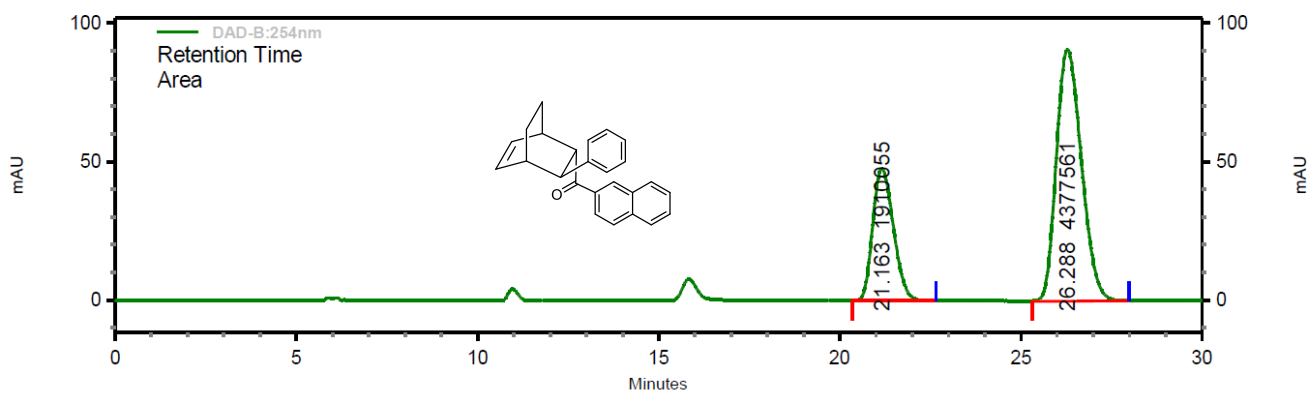
Retention time	Area	Area %
16.978	1509374	37.26
21.213	2541263	62.74



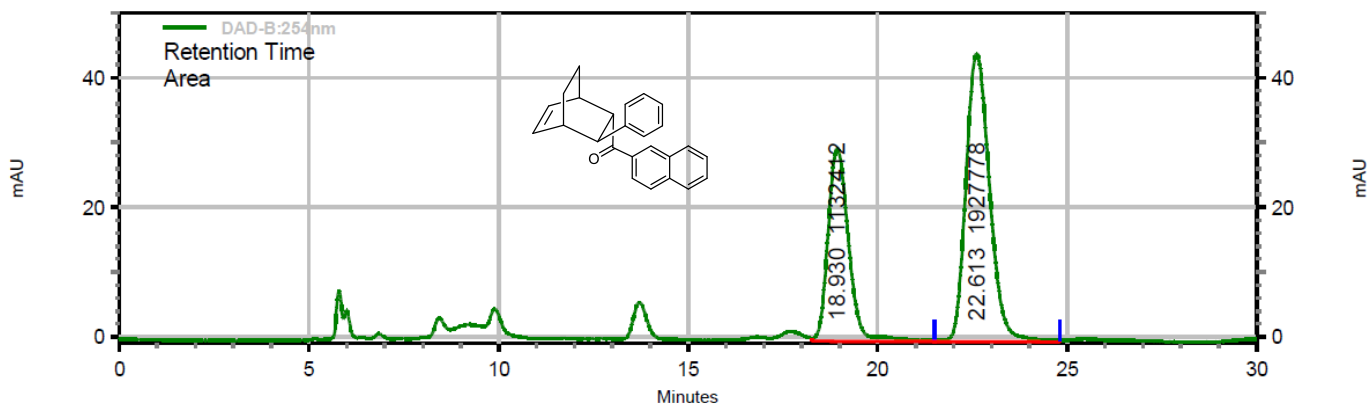
Retention time	Area	Area %
15.443	174033	30.43
18.552	397750	69.56



Retention time	Area	Area %
14.225	9427448	70.04
16.008	4031714	29.96



Retention time	Area	Area %
21.163	1910055	30.38
26.288	4377561	69.62



Retention time	Area	Area %
18.930	1132412	37.00
22.613	1927778	63.00