

Phenolato Ti(IV) Hexacoordinate Complexes as Anticancer Chemotherapy: Enhancement of Solubility, Hydrolytic Stability, and Cytotoxicity

Mohammad Taha and Edit Y. Tshuva*

Institute of Chemistry, Edmond J Safra Campus, The Hebrew University of Jerusalem, Jerusalem 9190401, Israel. Edit.tshuva@mail.huji.ac.il

Supplementary Information

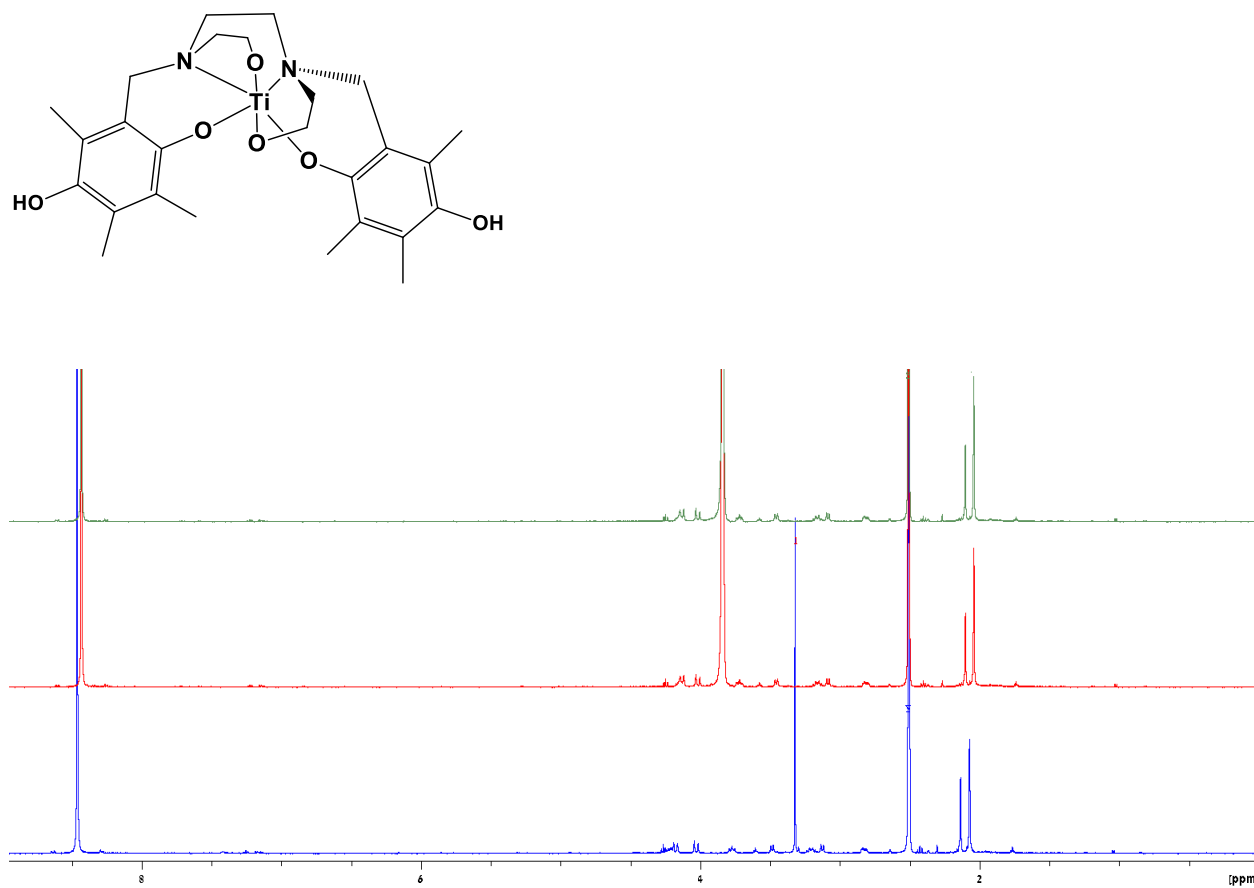


Figure S1. ¹H NMR spectra of L²Ti in DMSO-*d*⁶ before (bottom), immediately after (middle), and 8 days after (top) the addition of 10% D₂O.

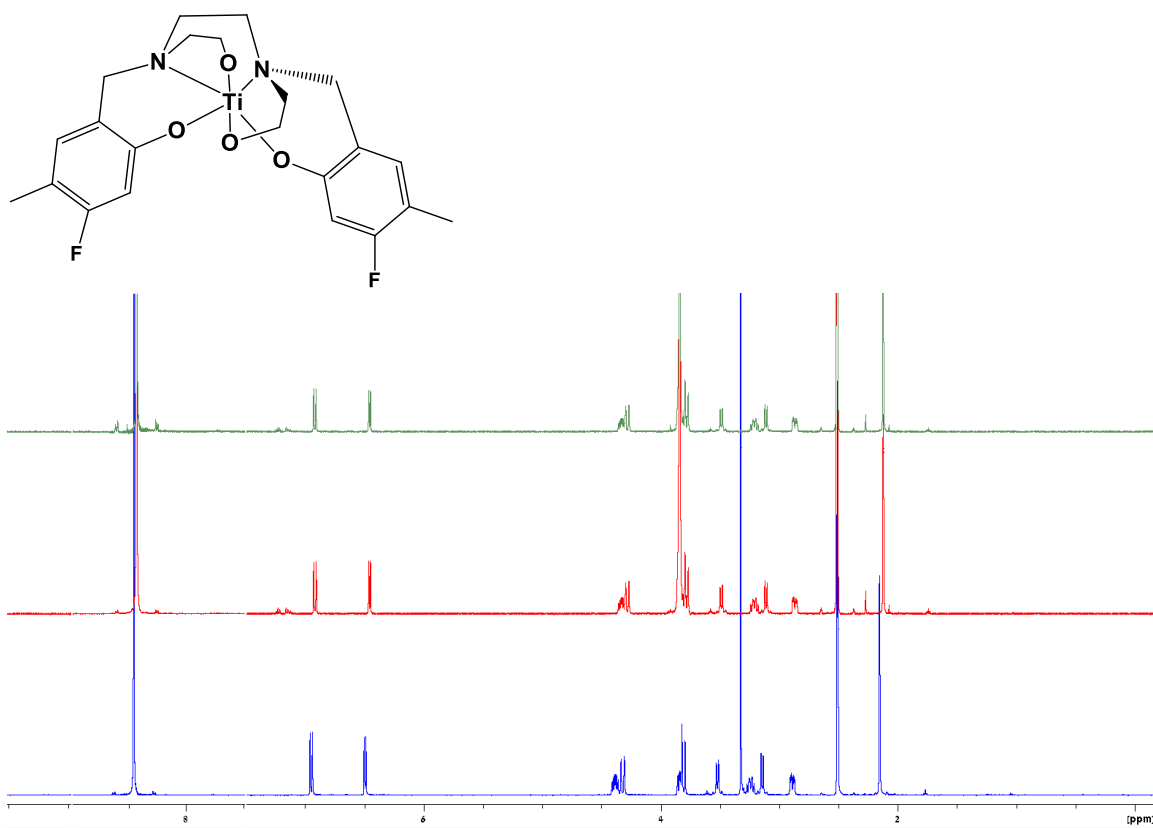


Figure S2. ¹H NMR spectra of L³Ti in DMSO-*d*⁶ before (bottom), immediately after (middle), and 8 days after (top) the addition of 10% D₂O.

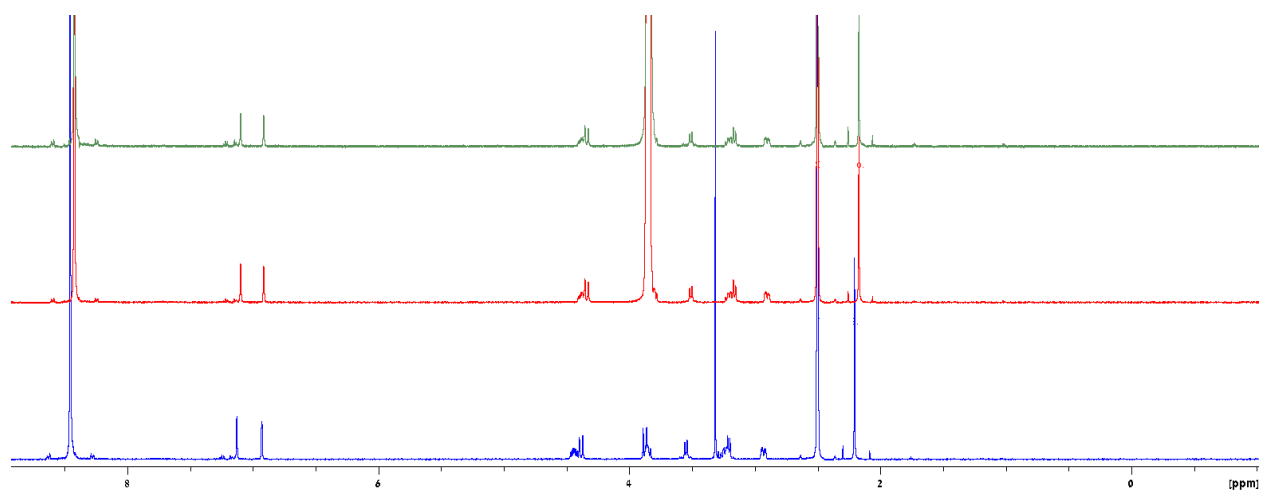
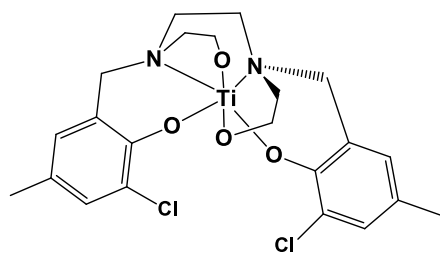


Figure S3. ^1H NMR spectra of L^4Ti in $\text{DMSO-}d^6$ before (bottom), immediately after (middle), and 8 days after (top) the addition of standard and 10% D_2O .

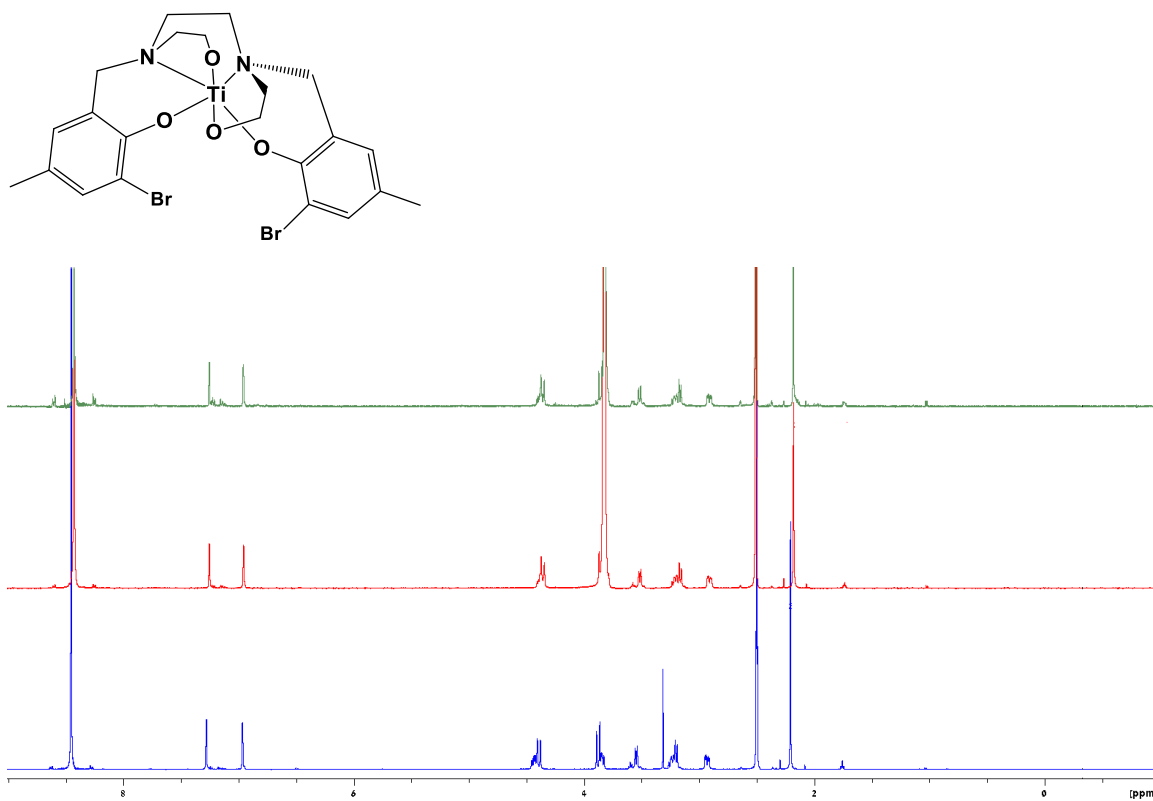
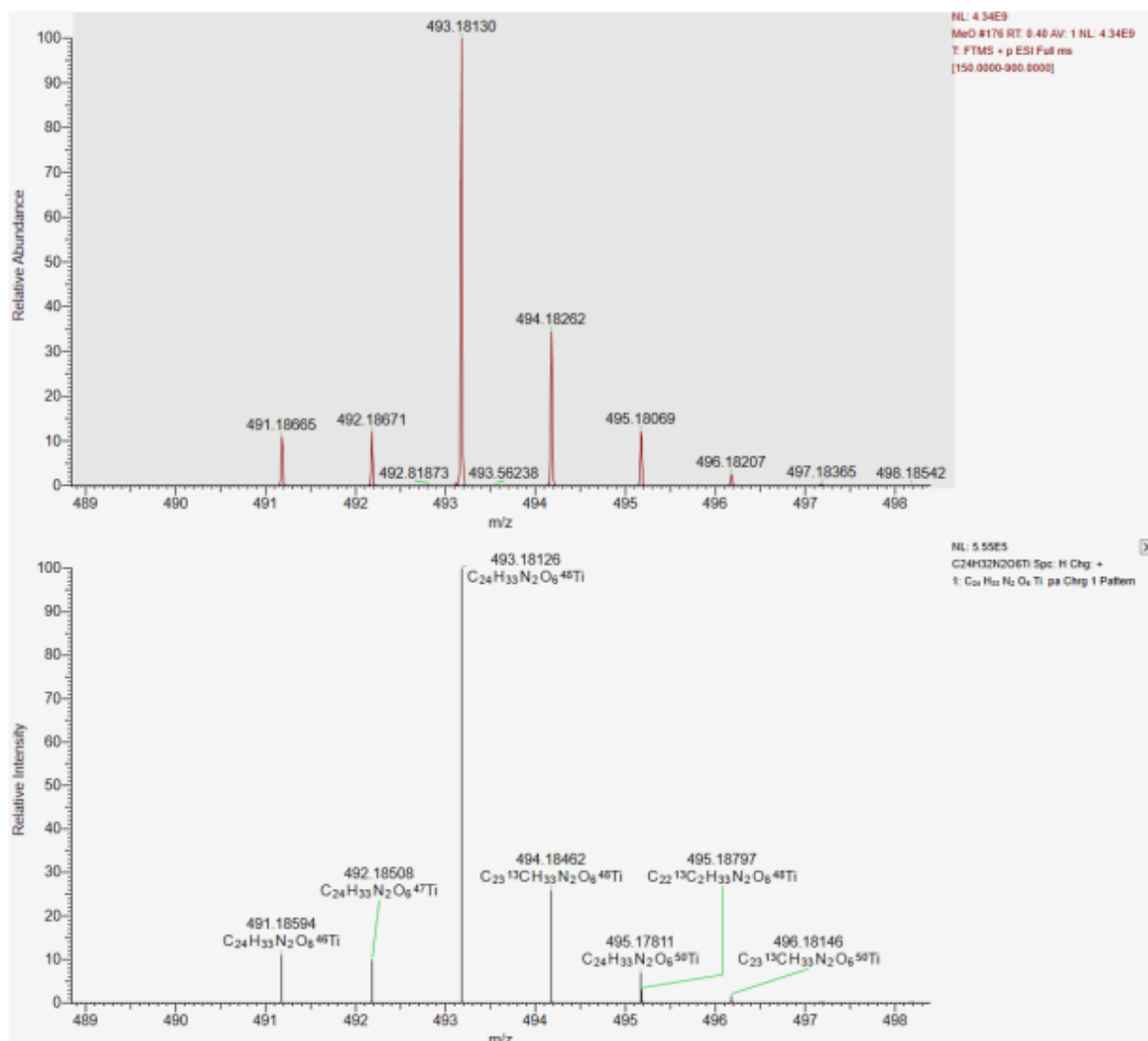
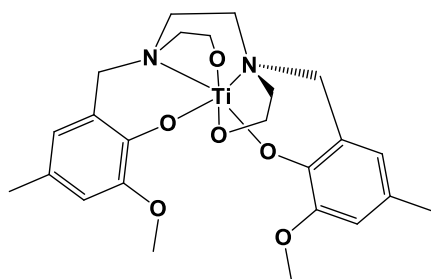


Figure S4. ¹H NMR spectra of L⁵Ti in DMSO-*d*⁶ before (bottom), immediately after (middle), and 8 days after (top) the addition of standard and 10% D₂O.



Above -Experimental Spectrum
 Bottom -Calculated Spectrum

Figure S5. HR-MS of L^1Ti 8 days following its insertion to an aqueous (10% H_2O , 90% CH_3CN) solution.

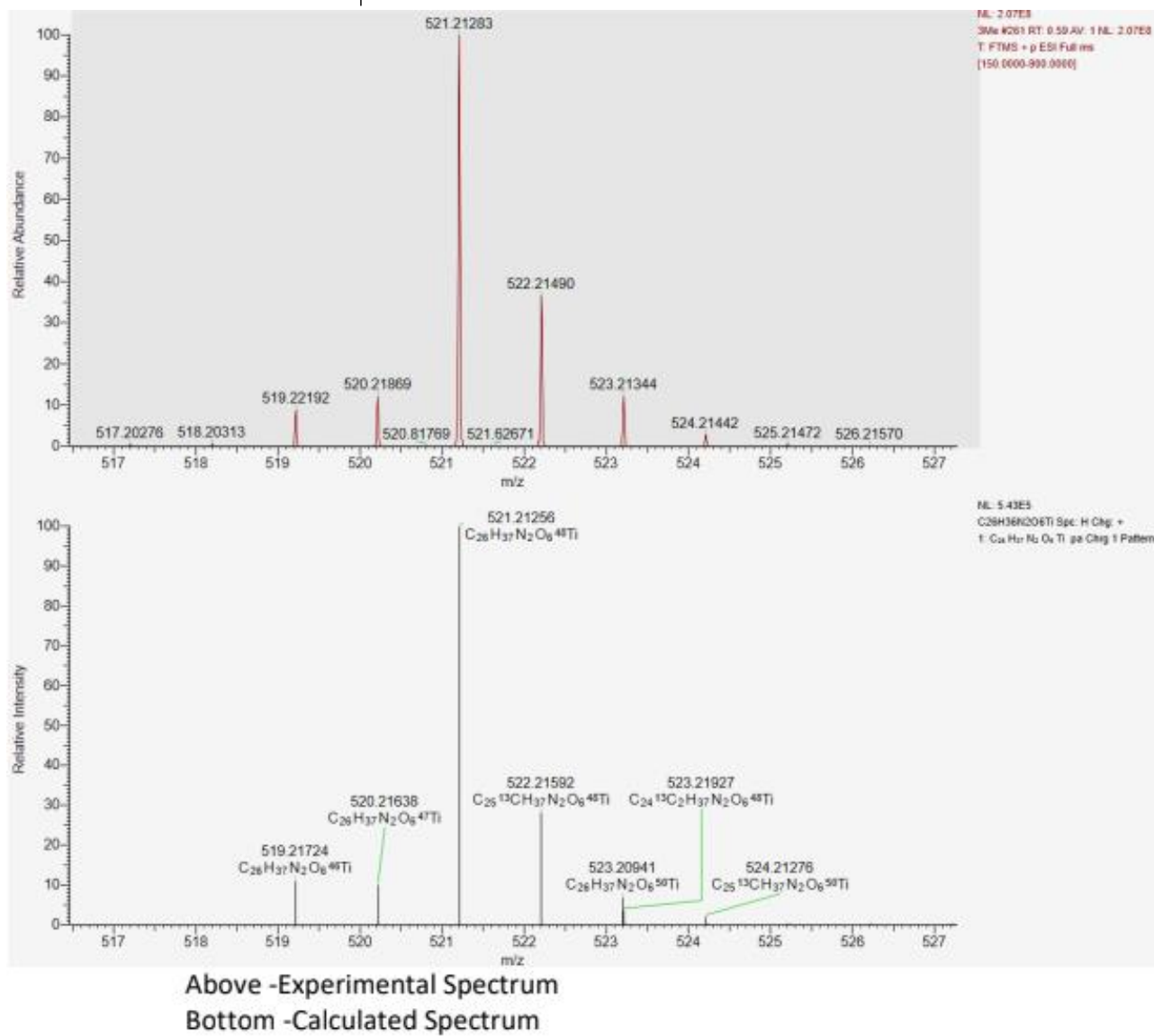
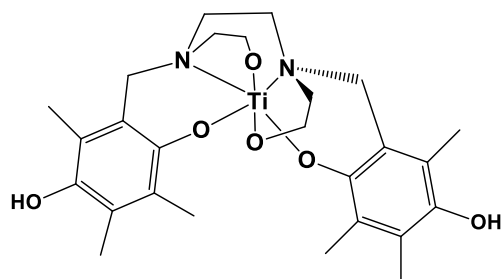


Figure S6. HR-MS of L²Ti 8 days following its insertion to an aqueous (10% H₂O, 90% CH₃CN) solution.

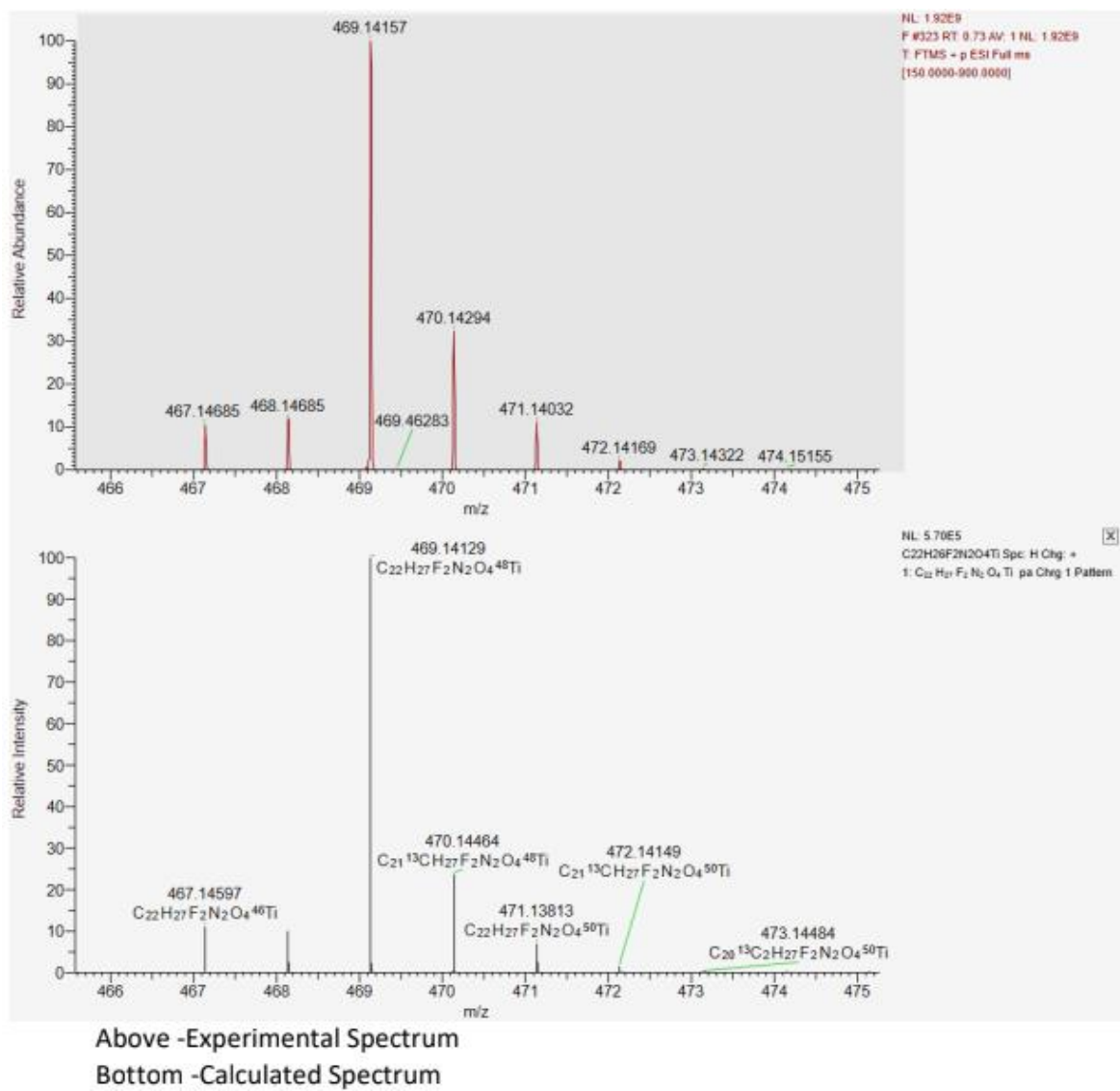
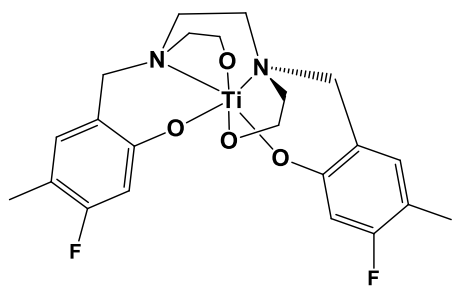
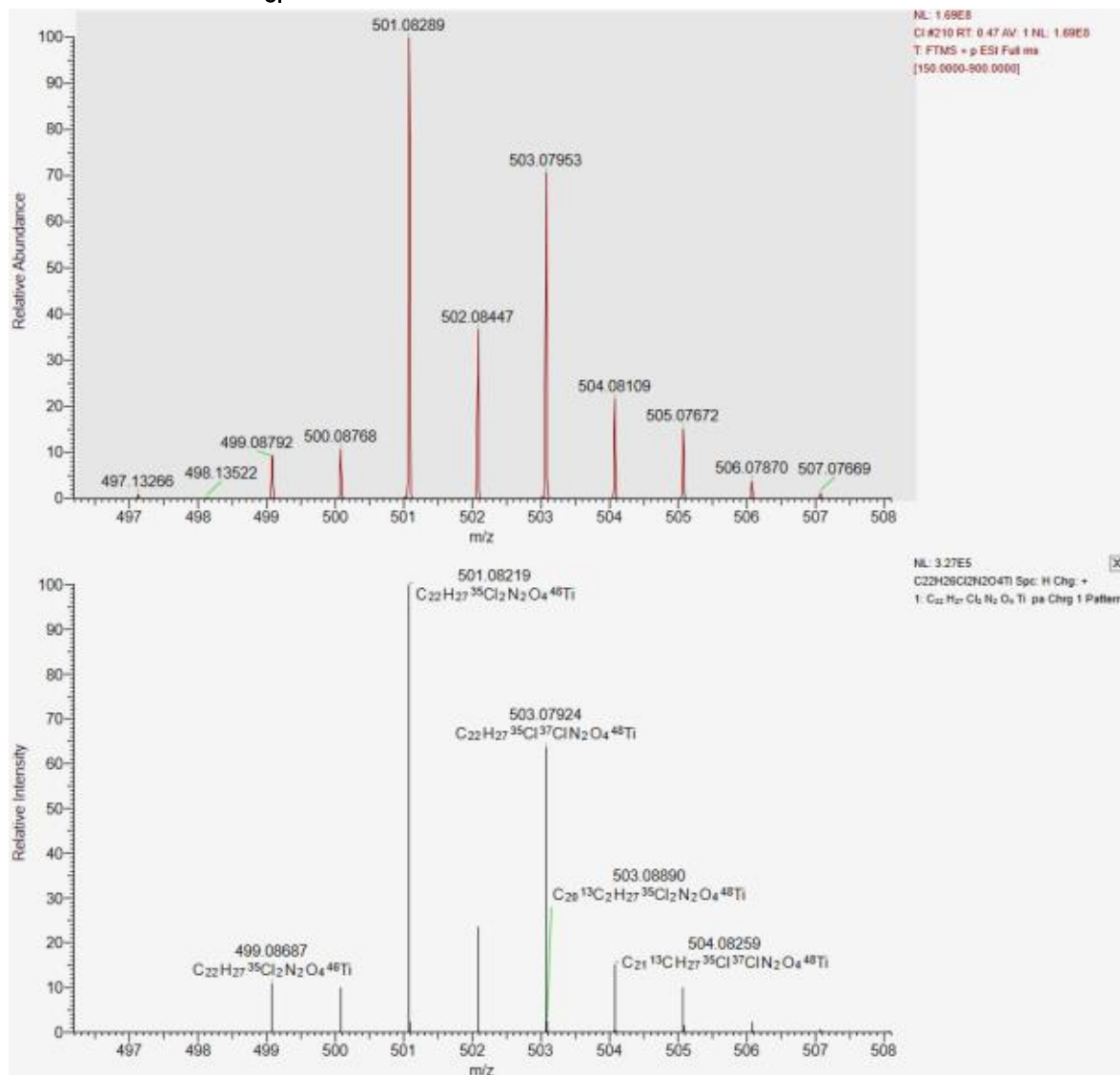
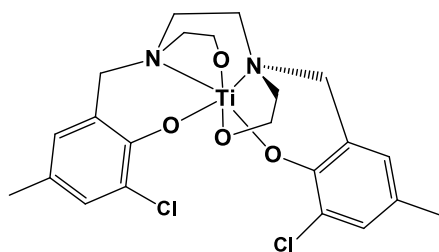
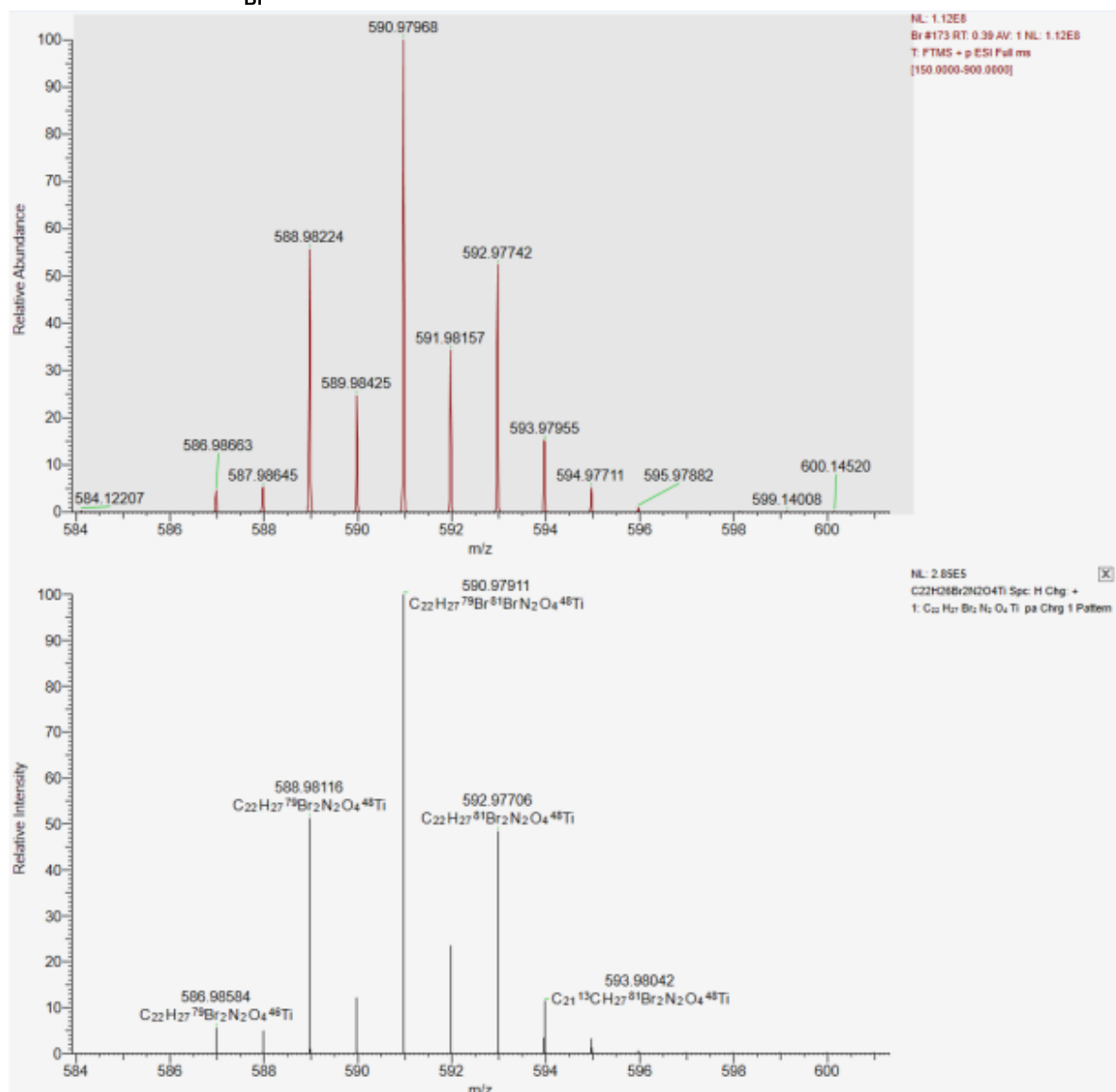
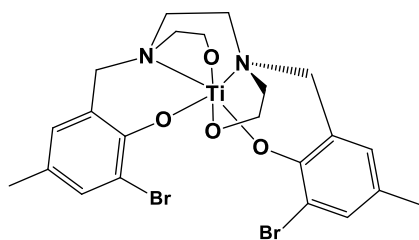


Figure S7. HR-MS of L^3Ti 8 days following its insertion to an aqueous (10% H_2O , 90% CH_3CN) solution.



Above -Experimental Spectrum
 Bottom -Calculated Spectrum

Figure S8. HR-MS of L⁴Ti 8 days following its insertion to an aqueous (10% H₂O, 90% CH₃CN) solution.



Above -Experimental Spectrum
 Bottom -Calculated Spectrum

Figure S9. HR-MS of L⁵Ti 8 days following its insertion to an aqueous (10% H₂O, 90% CH₃CN) solution.

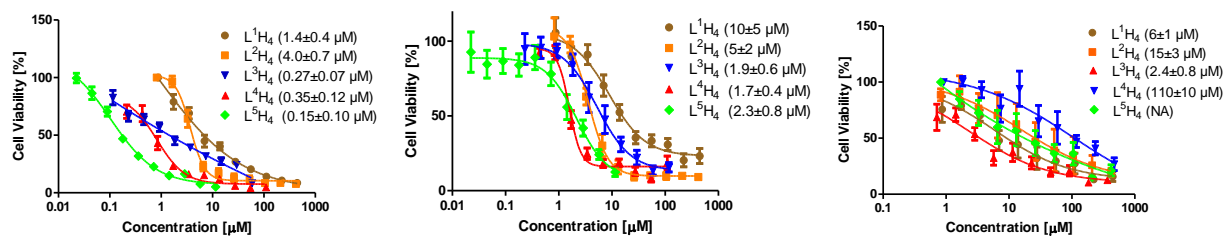


Figure S10. Dependence of human ovarian A2780 (left), colon HT-29 (middle), and cervical HeLa (right) cancer cell viability on different concentrations of H_4L^{1-5} following a three-day incubation period as analyzed by the MTT assay.

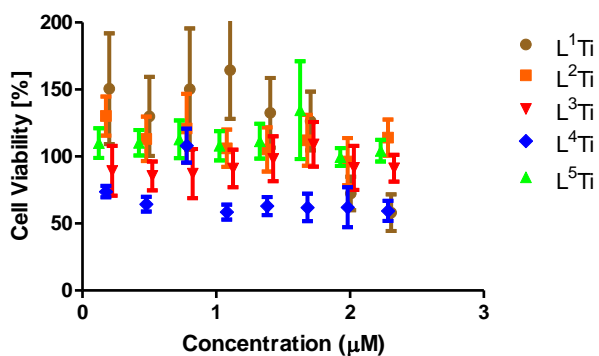


Figure S11. Dependence of human fibroblast lung MRC-5 cell viability on different concentrations of $L^{1-5}Ti$ following a three-day incubation period as analyzed by the MTT assay.

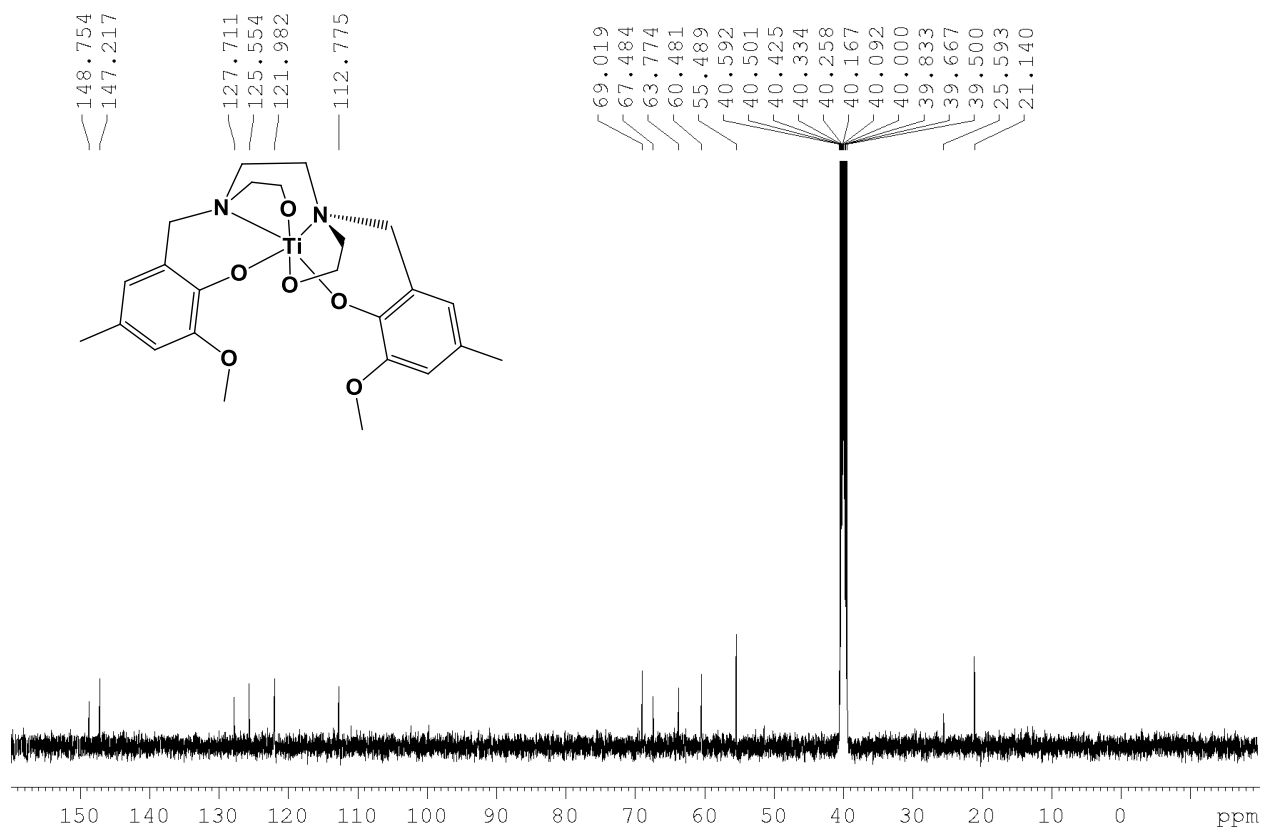


Figure S12. ^{13}C NMR spectrum of L^1Ti in $\text{DMSO-}d^6$.

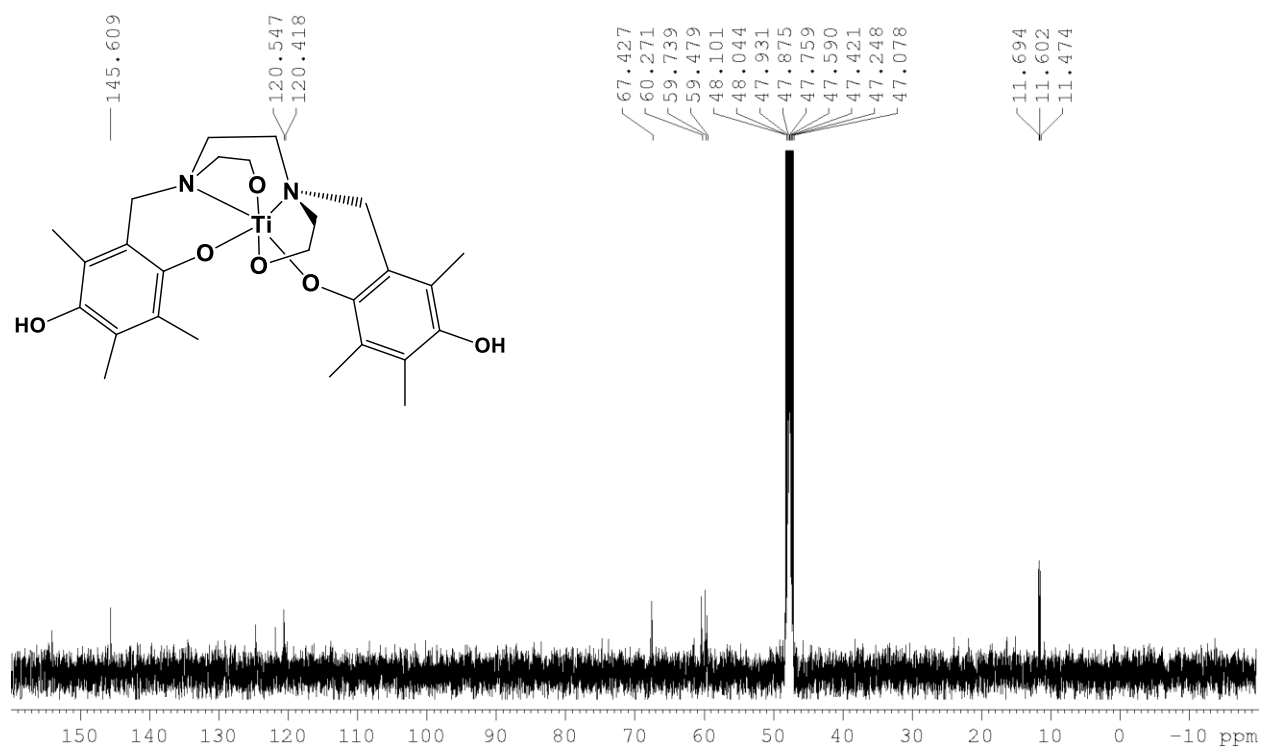


Figure S13. ¹³C NMR spectrum of L²Ti in DMSO-d⁶.

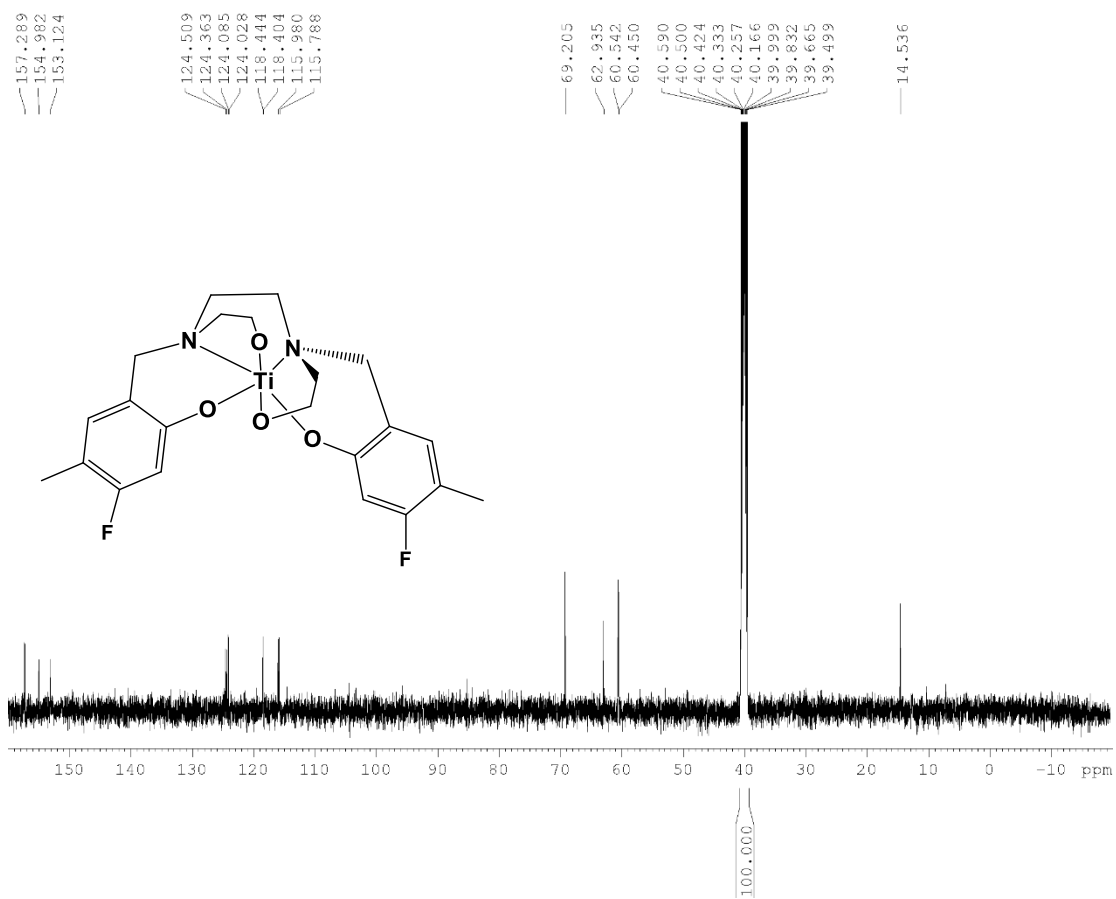


Figure S14. ^{13}C NMR spectrum of L^3Ti in $DMSO-d_6$.

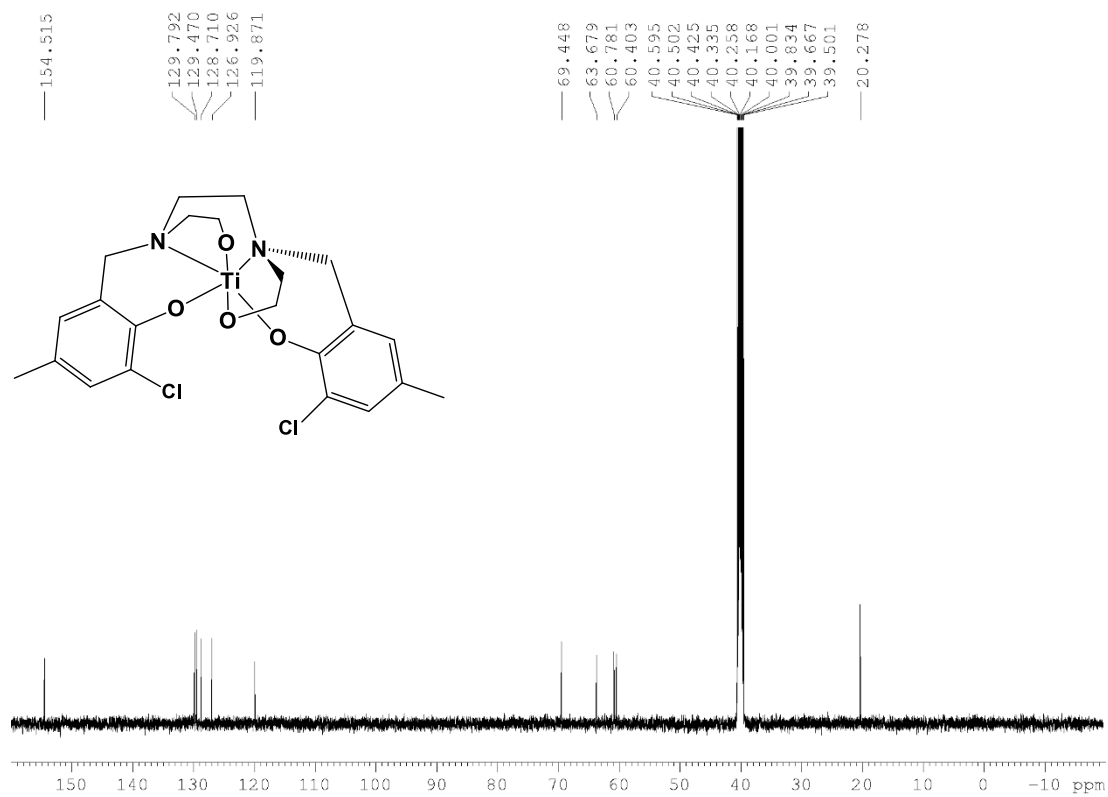


Figure S15. ^{13}C NMR spectrum of L^4Ti in $DMSO-d_6$.

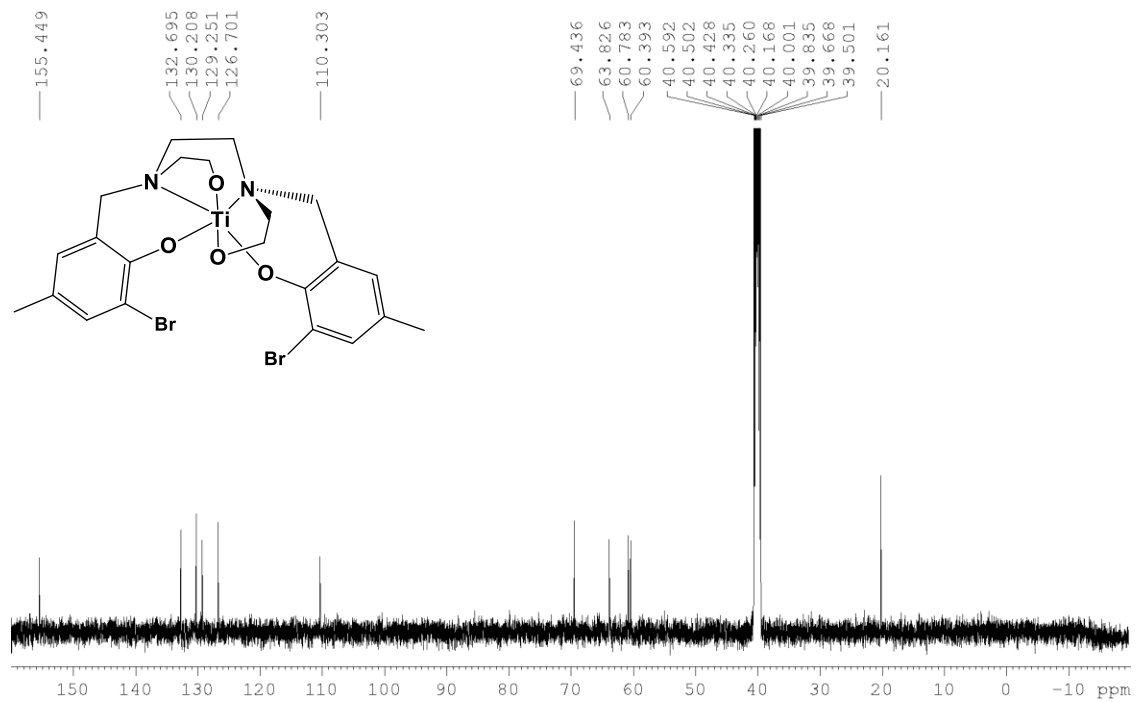


Figure S16. ^{13}C NMR spectrum of L^5Ti in DMSO-d_6