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Supplementary Material

Synthesis and characterization of indium(III) bis-thiosemicarbazone complexes: ¹⁸F incorporation for PET imaging

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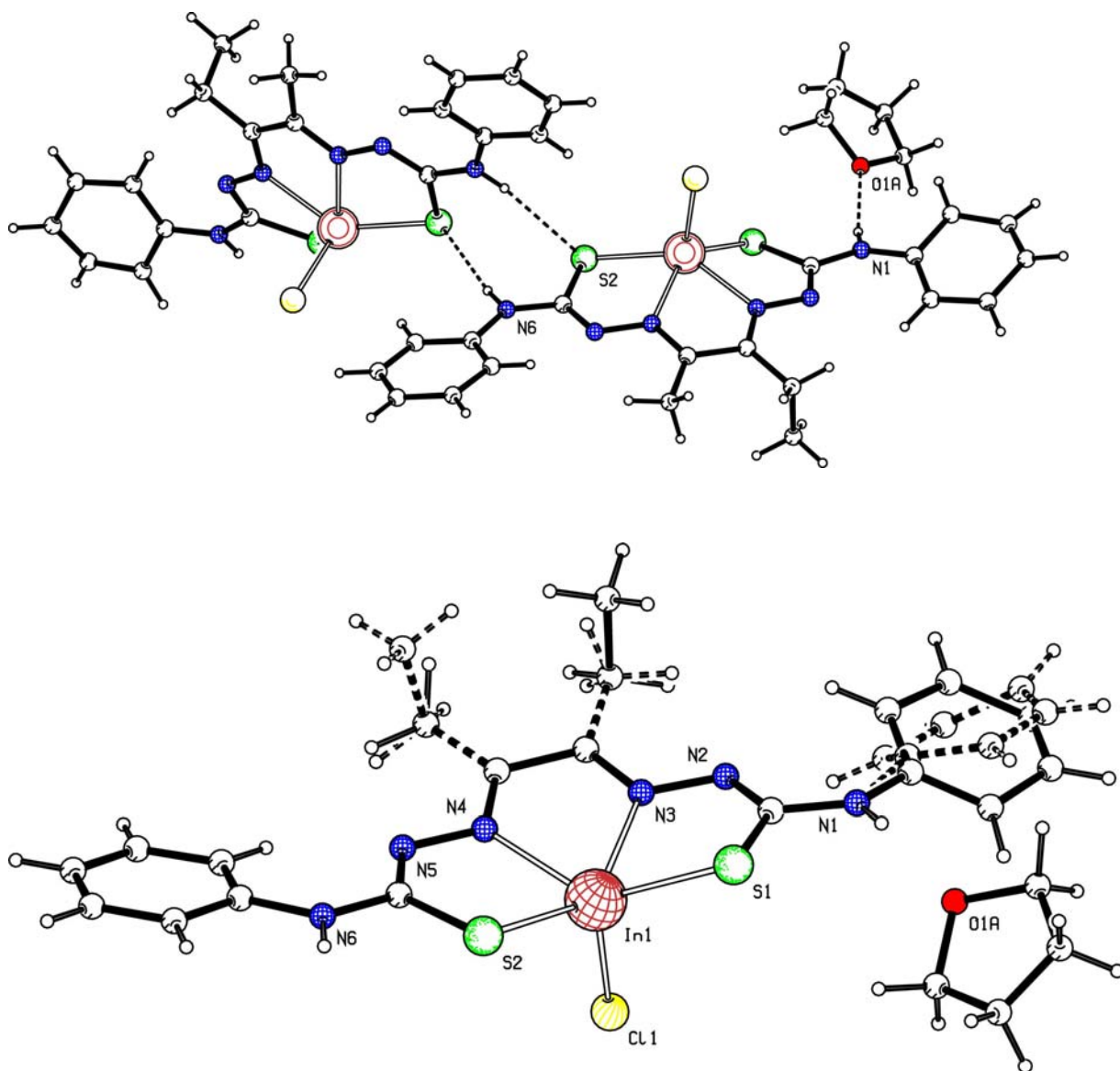


Fig. S1. (top) H-bonding in compound 1.THF and (bottom) disorder in the methyl/ethyl and phenyl groups.

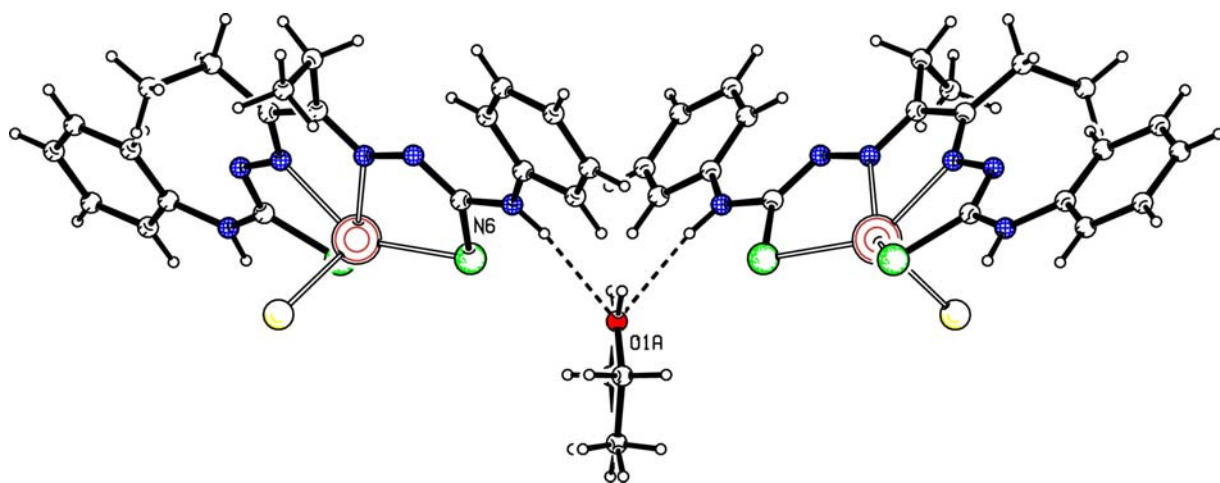


Fig. S2. H-bonding in the structure of compound 2.5 EtOH.

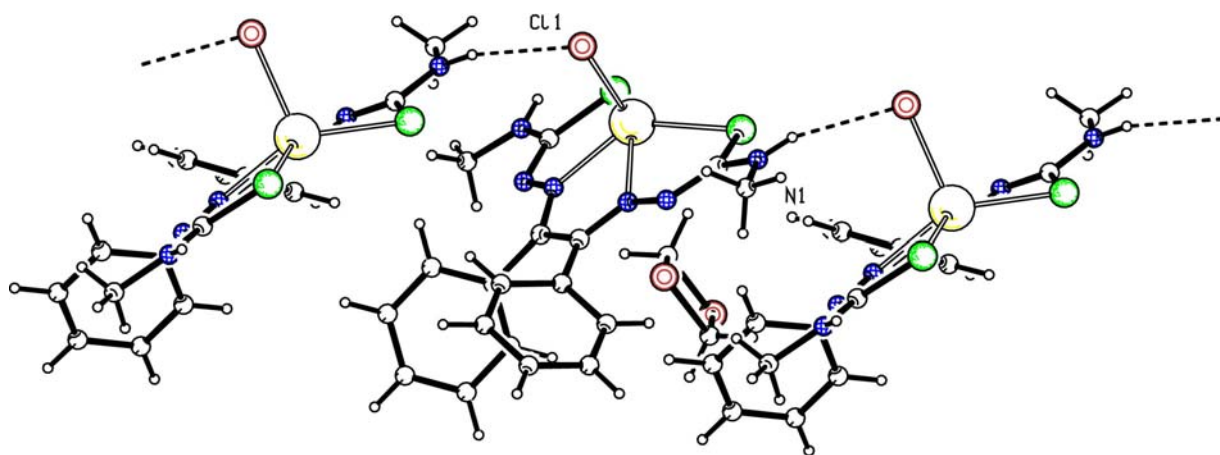


Fig. S3. H-bonding in the structure of compound **3**. $\frac{1}{2}$ CH₂Cl₂.

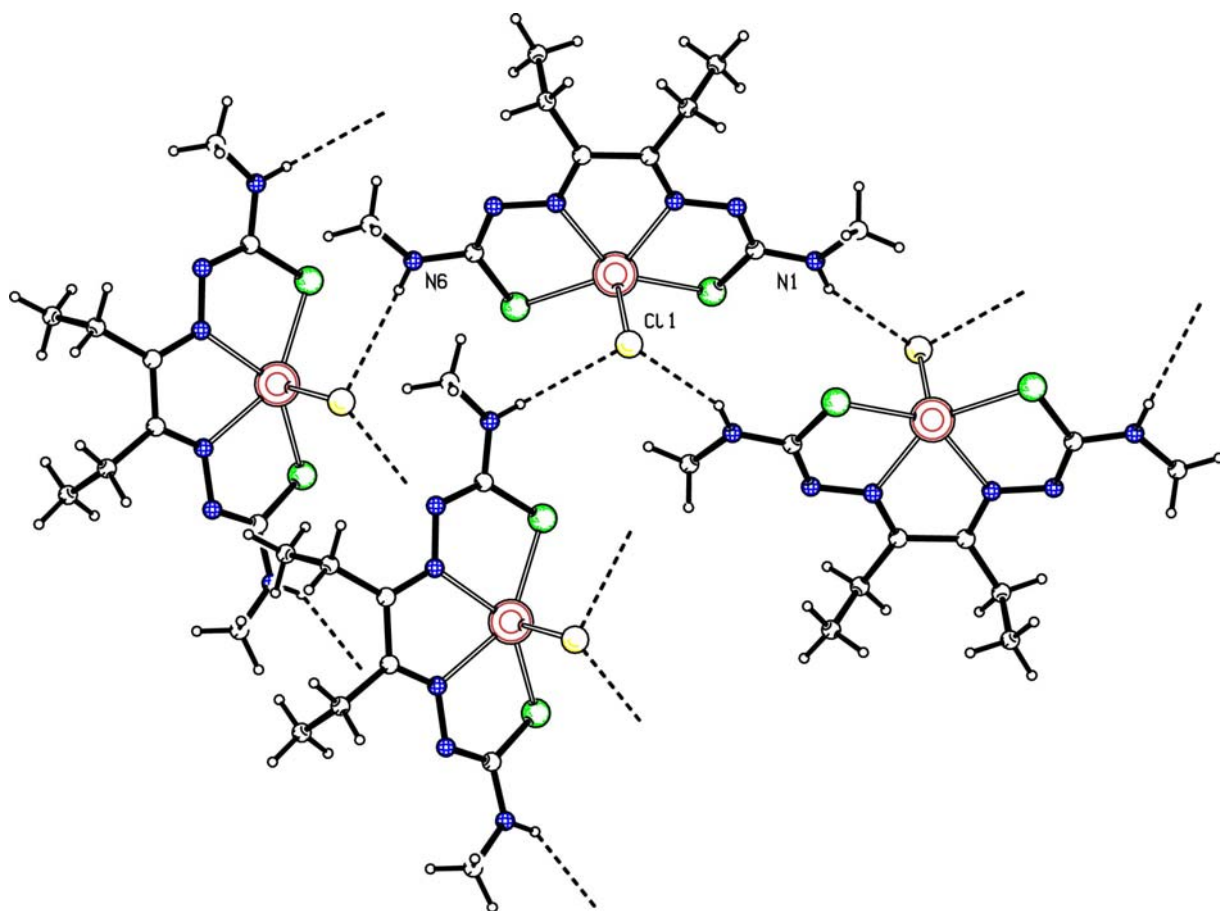


Fig. S4. H-bonding in the structure of compound 5.

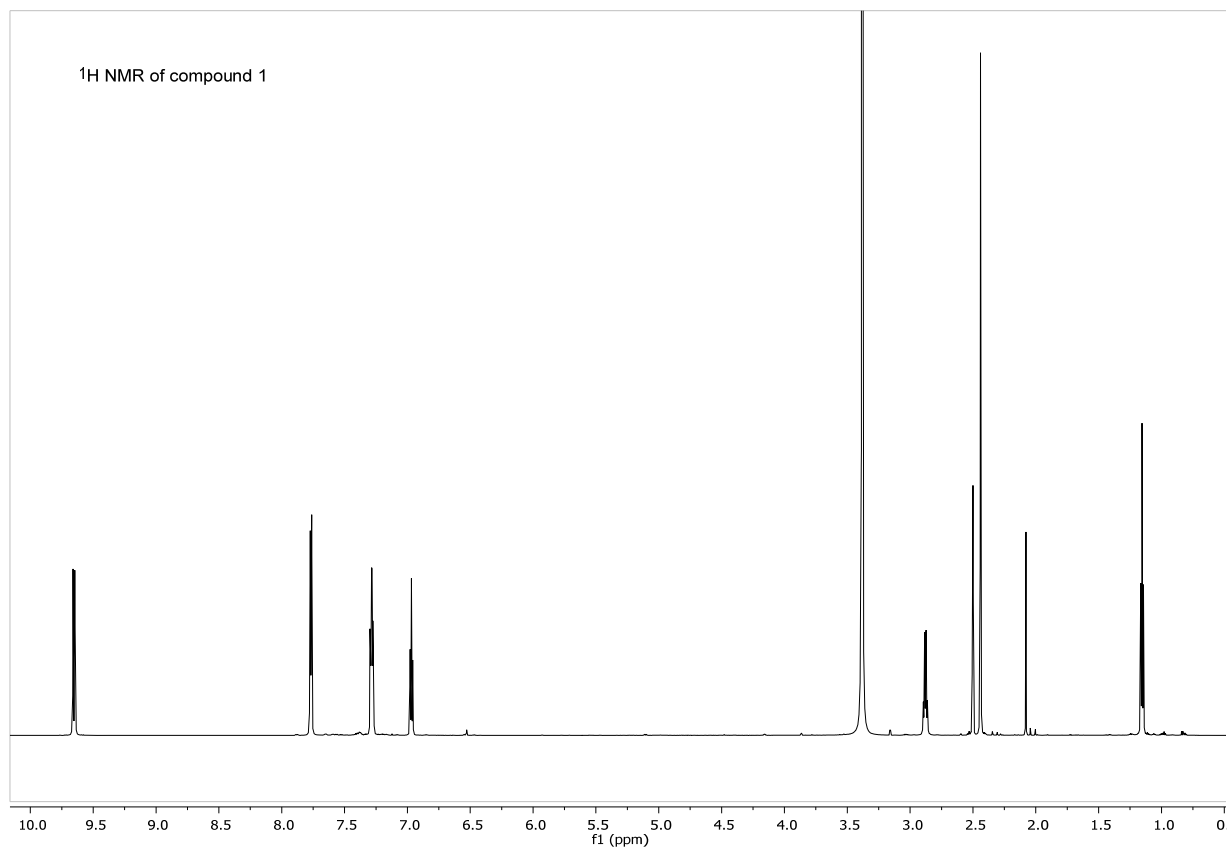


Fig. S5. ¹H NMR of compound 1 (d₆-DMSO)

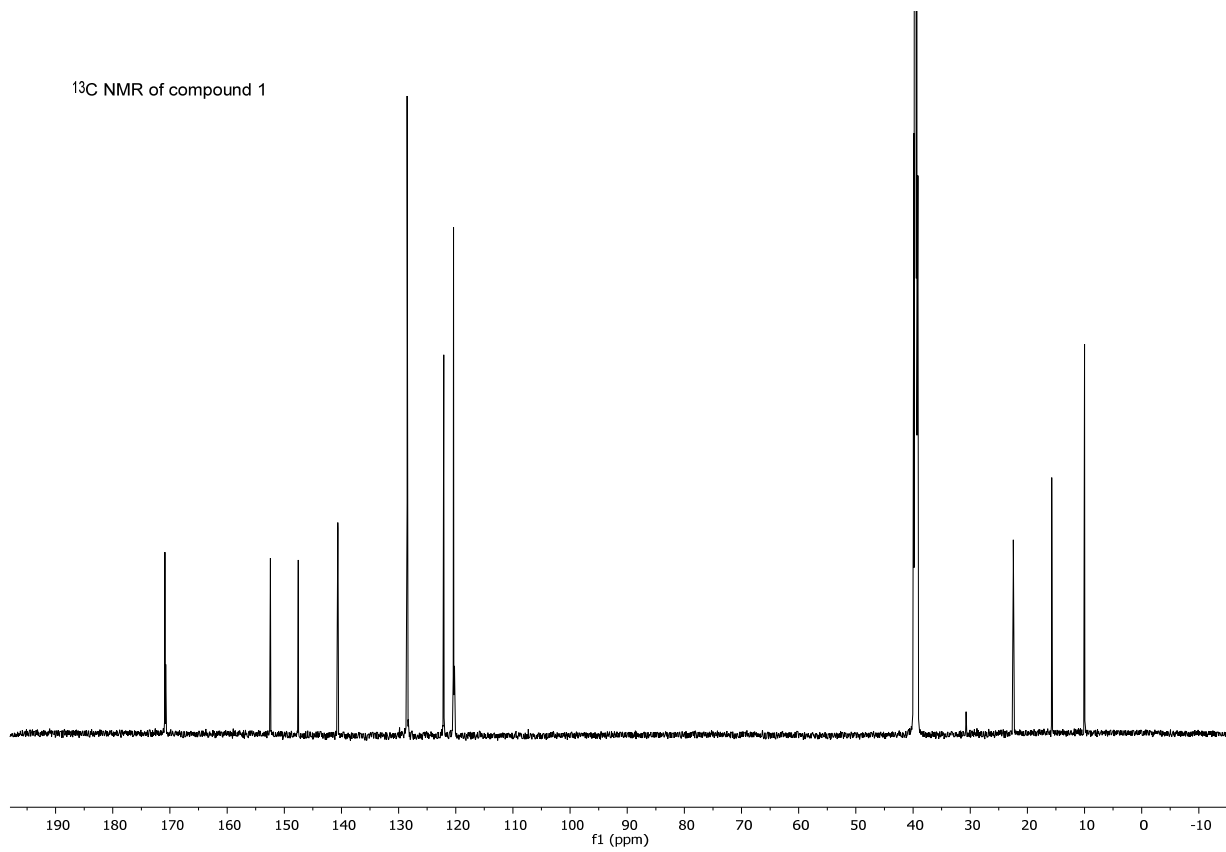


Fig. S6. ¹³C NMR of compound 1 (d₆-DMSO)

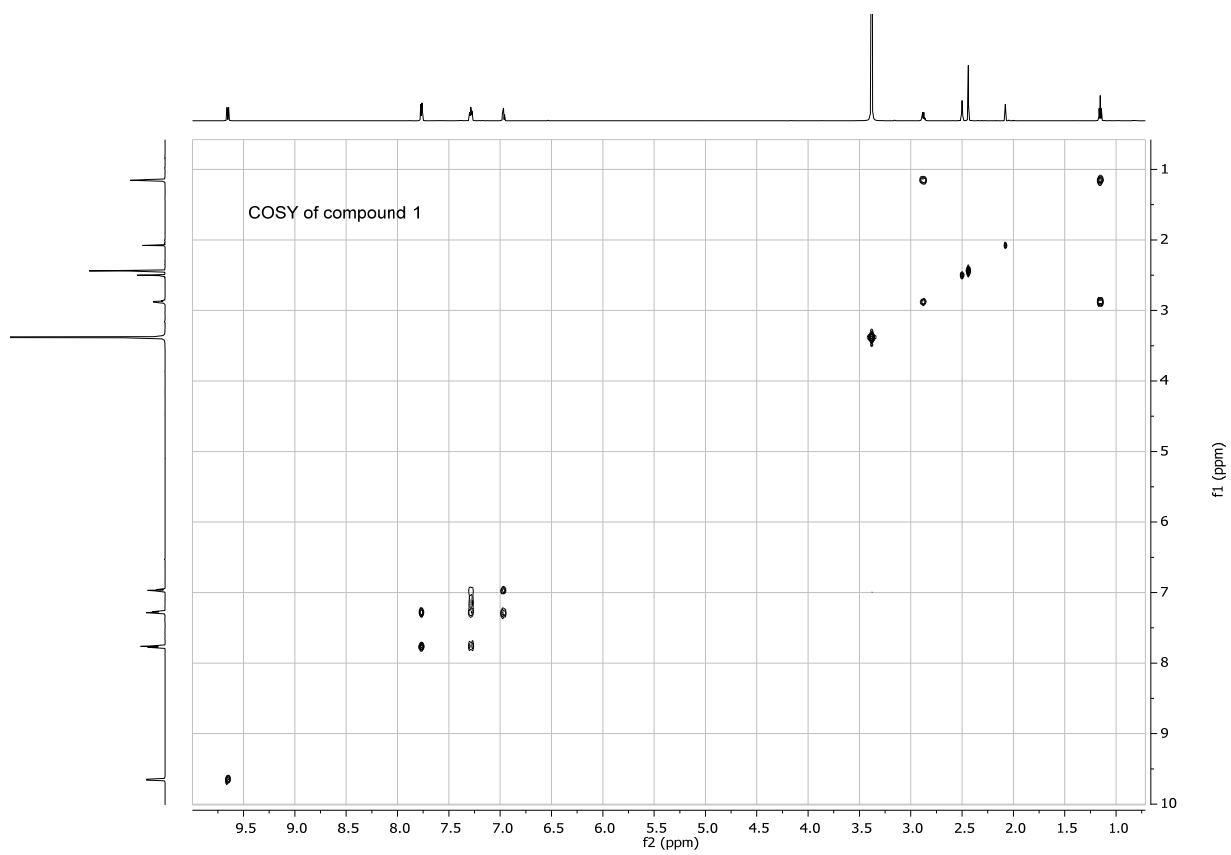


Fig. S7. COSY NMR of compound **1** (d_6 -DMSO)

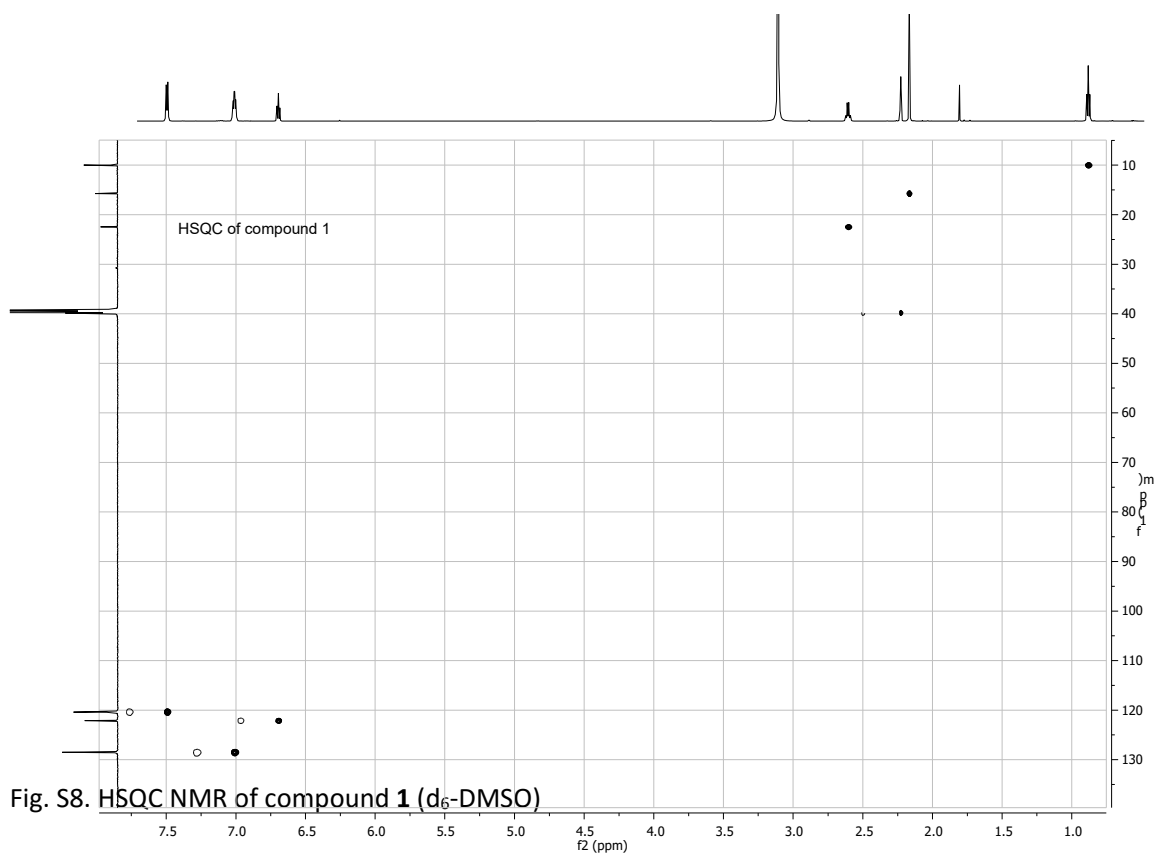


Fig. S8. HSQC NMR of compound 1 (d₆-DMSO)

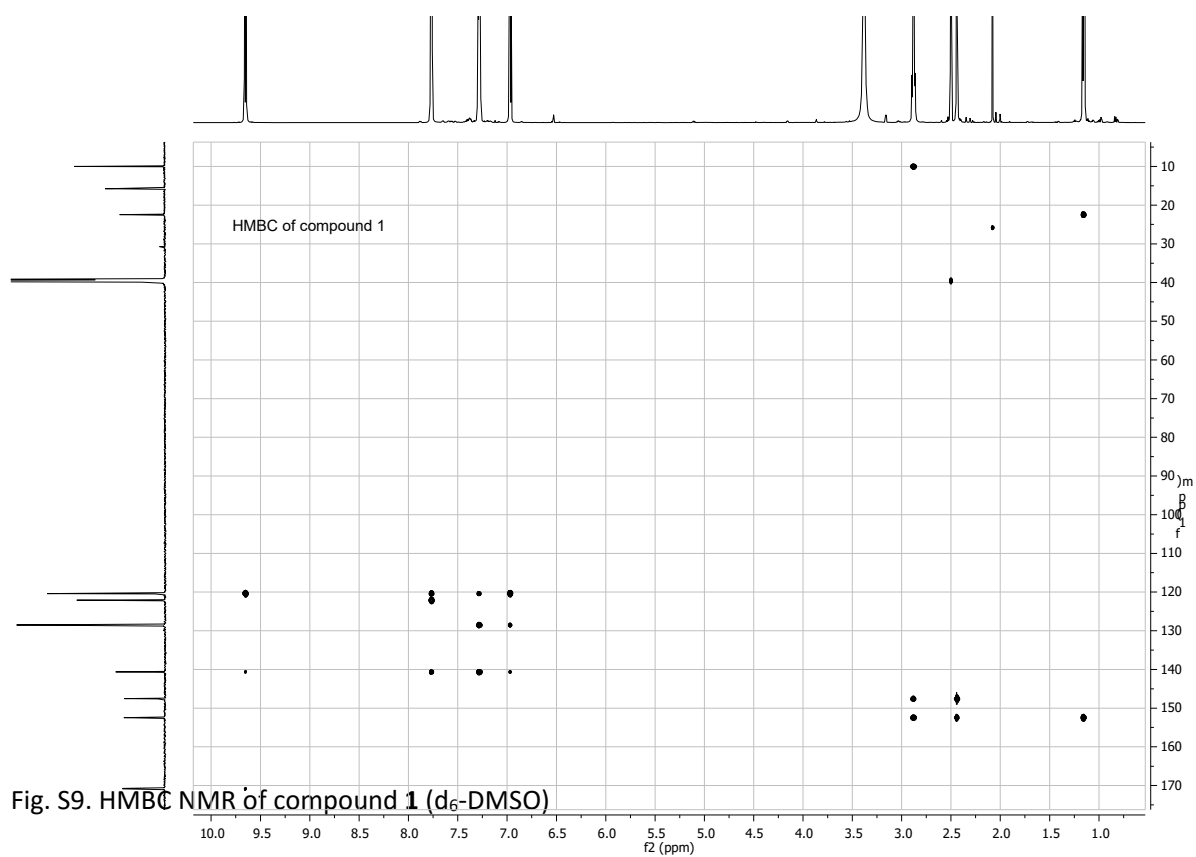


Fig. S9. HMBC NMR of compound **1** (d_6 -DMSO)

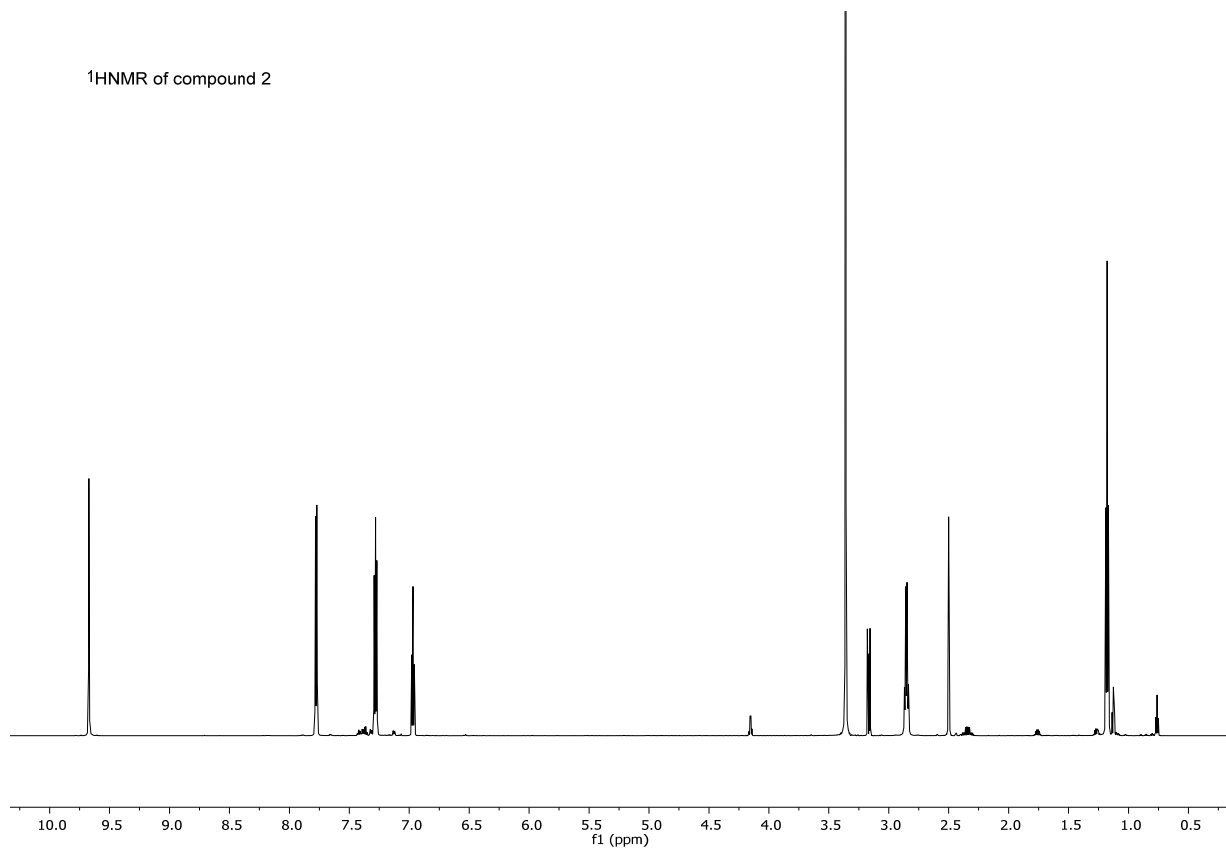


Fig. S10. ¹H NMR of compound 2 (d₆-DMSO)

¹³C NMR of compound 2

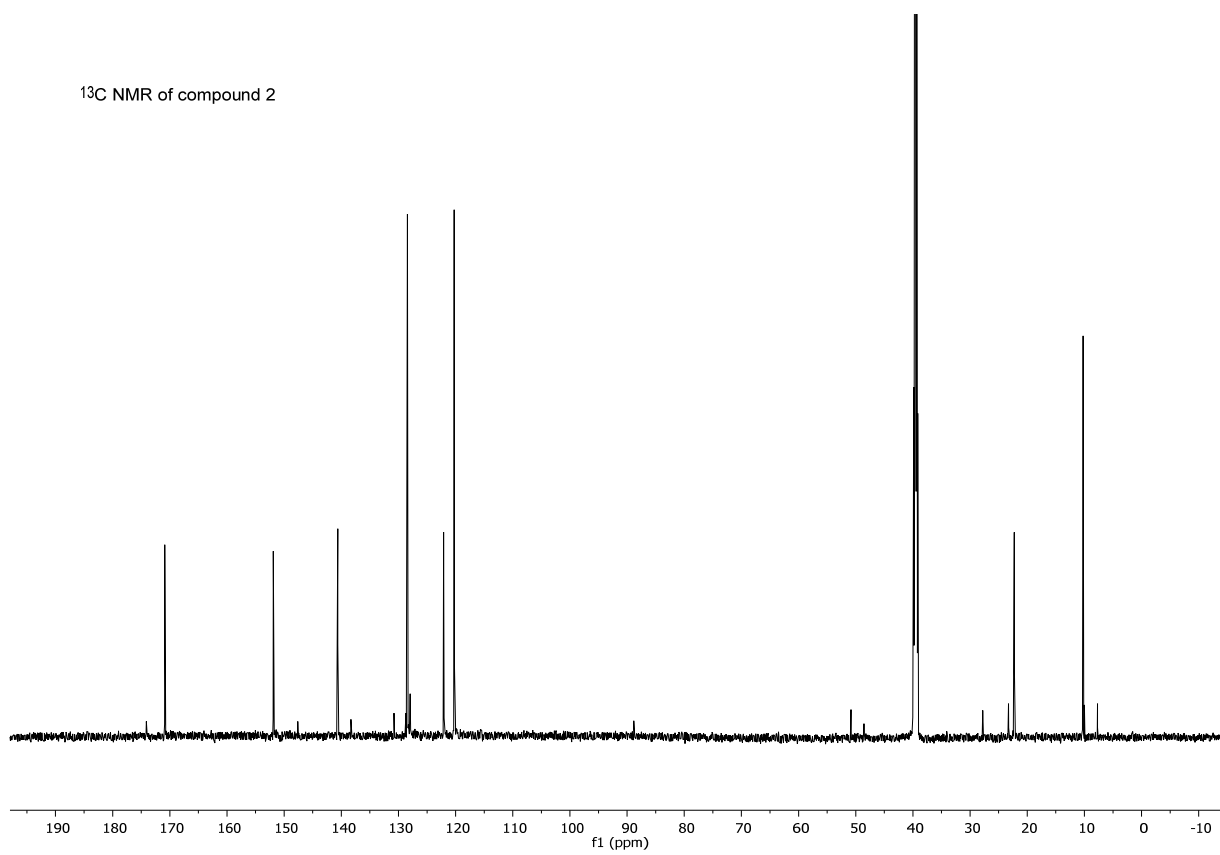


Fig. S11. ¹³C NMR of compound 2 (d₆-DMSO)

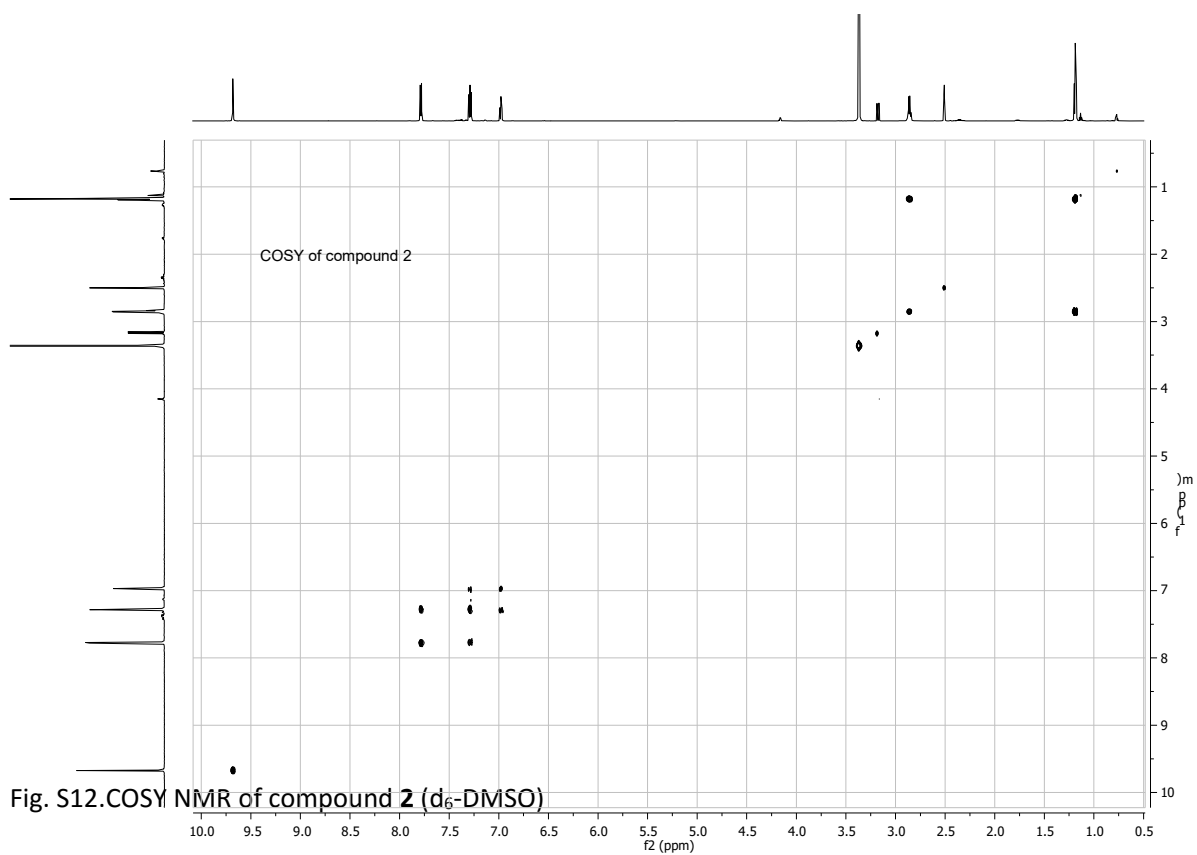


Fig. S12. COSY NMR of compound 2 (d₆-DMSO)

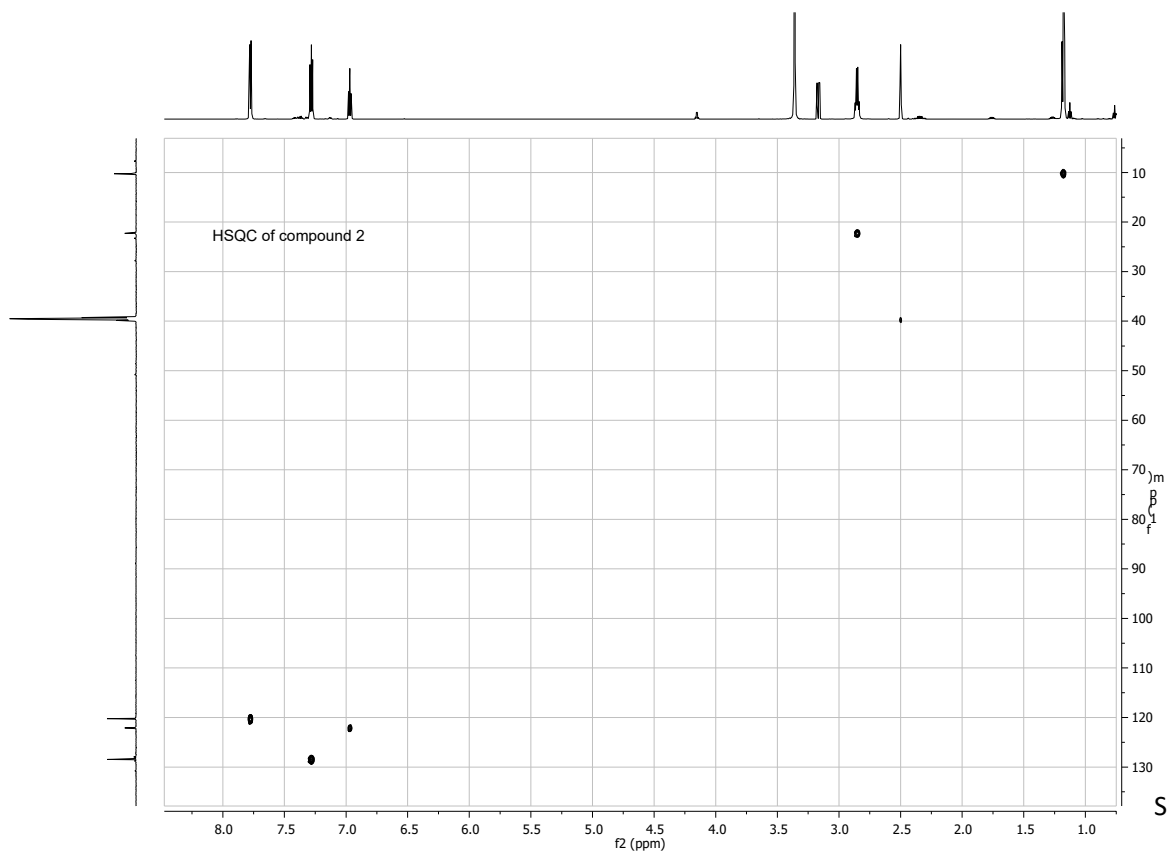


Fig. S13. HSQC NMR of compound 2 (d₆-DMSO)

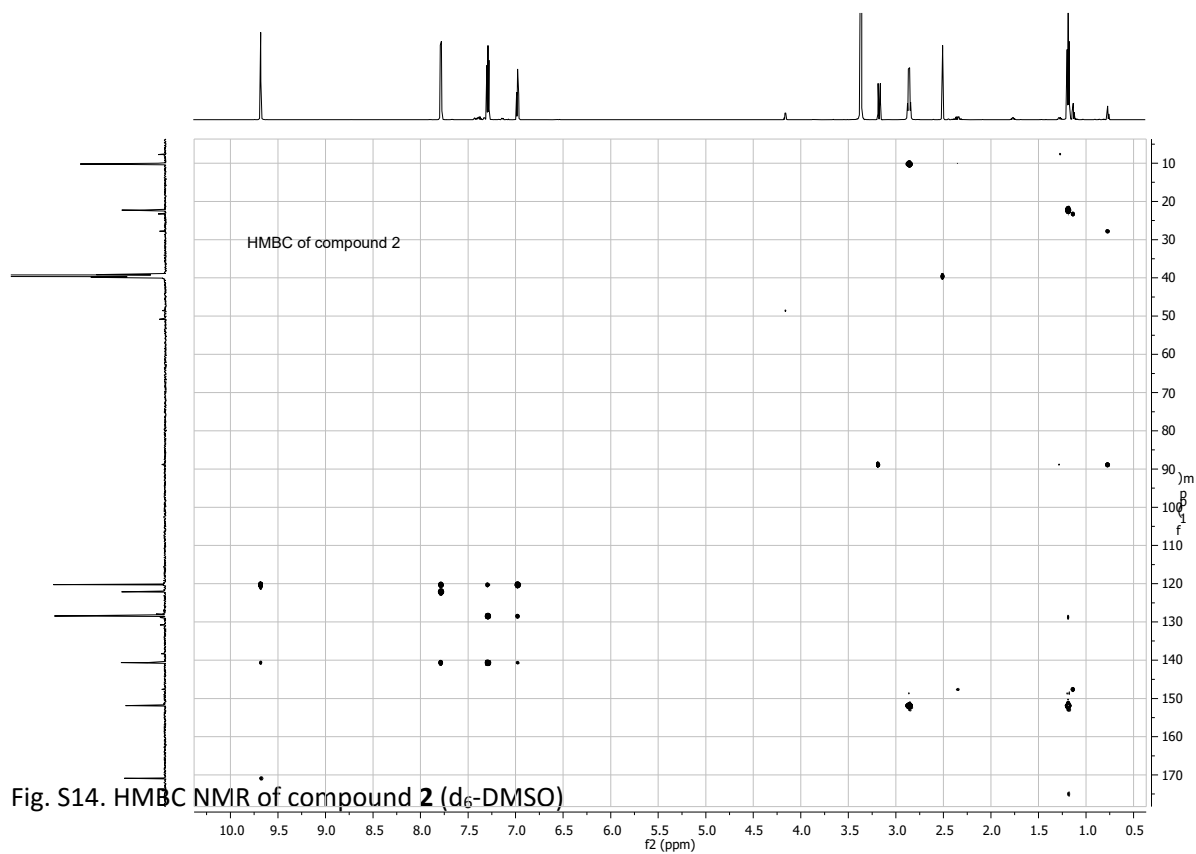


Fig. S14. HMBC NMR of compound 2 (d₆-DMSO)

diphenylaminomethyldithiosemicarindiumchloride_dmsol_20170703.1.1.1r
diphenylaminomethyldithiosemicarindiumchloride_dmsol_20170703

^1H NMR compd 3

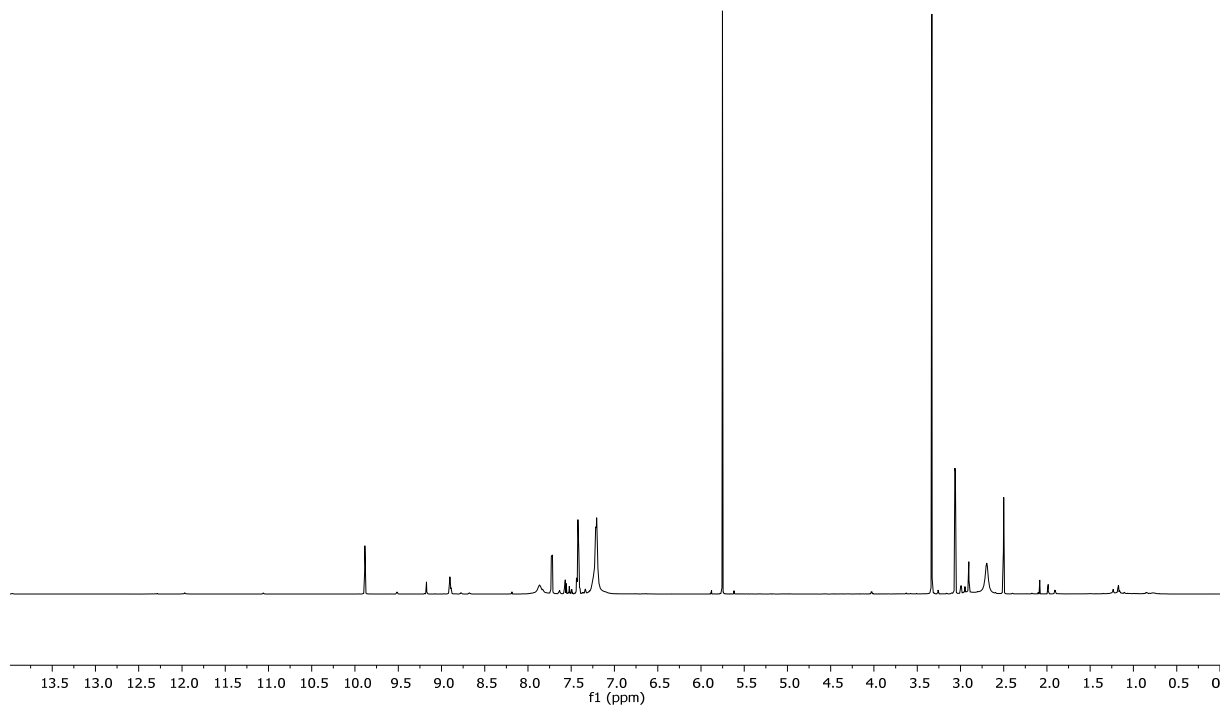


Fig. S15. ^1H NMR of compound **3** ($\text{d}_6\text{-DMSO}$)

diphenylaminomethyldithiosemicarindiumchloride_dmsol_20170703.2.1.1r
diphenylaminomethyldithiosemicarindiumchloride_dmsol_20170703

^{13}C NMRcompd 3

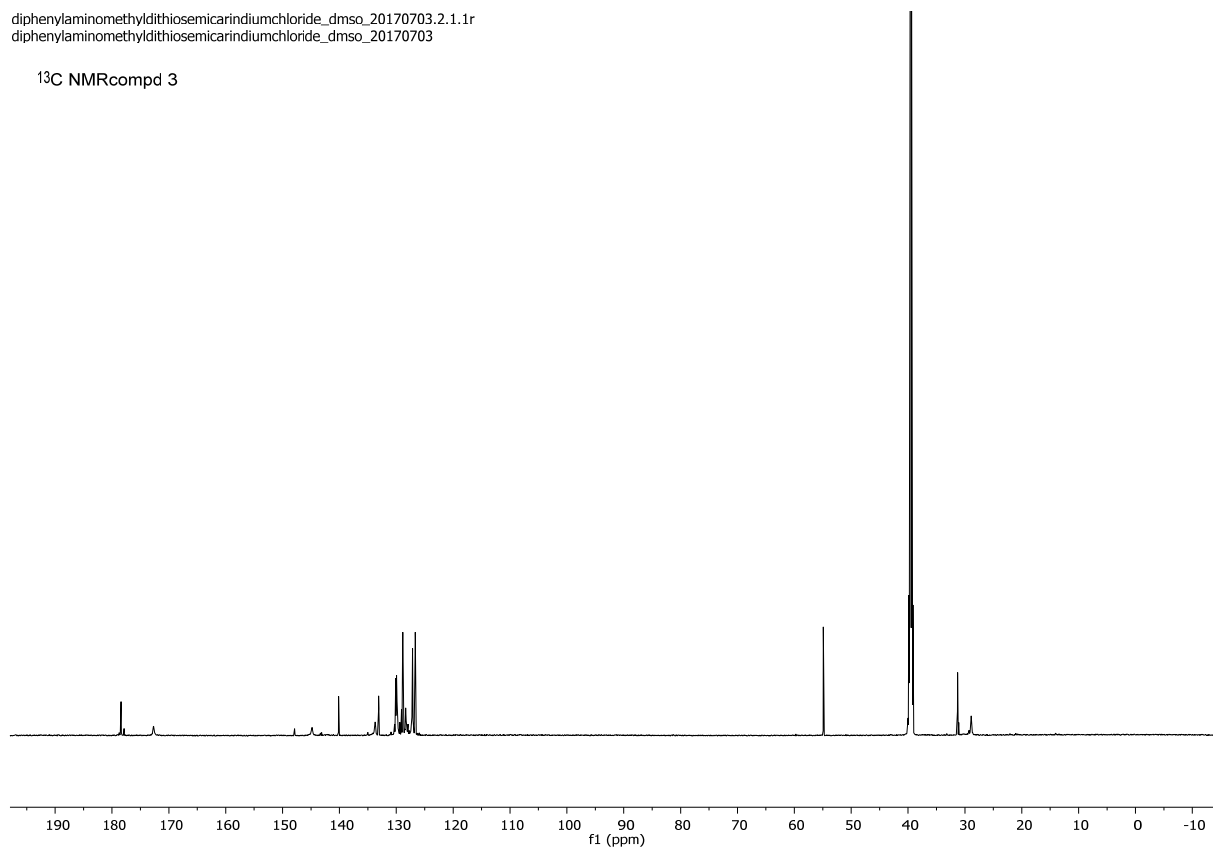


Fig. S16. ^{13}C NMR of compound **3** (d_6 -DMSO)

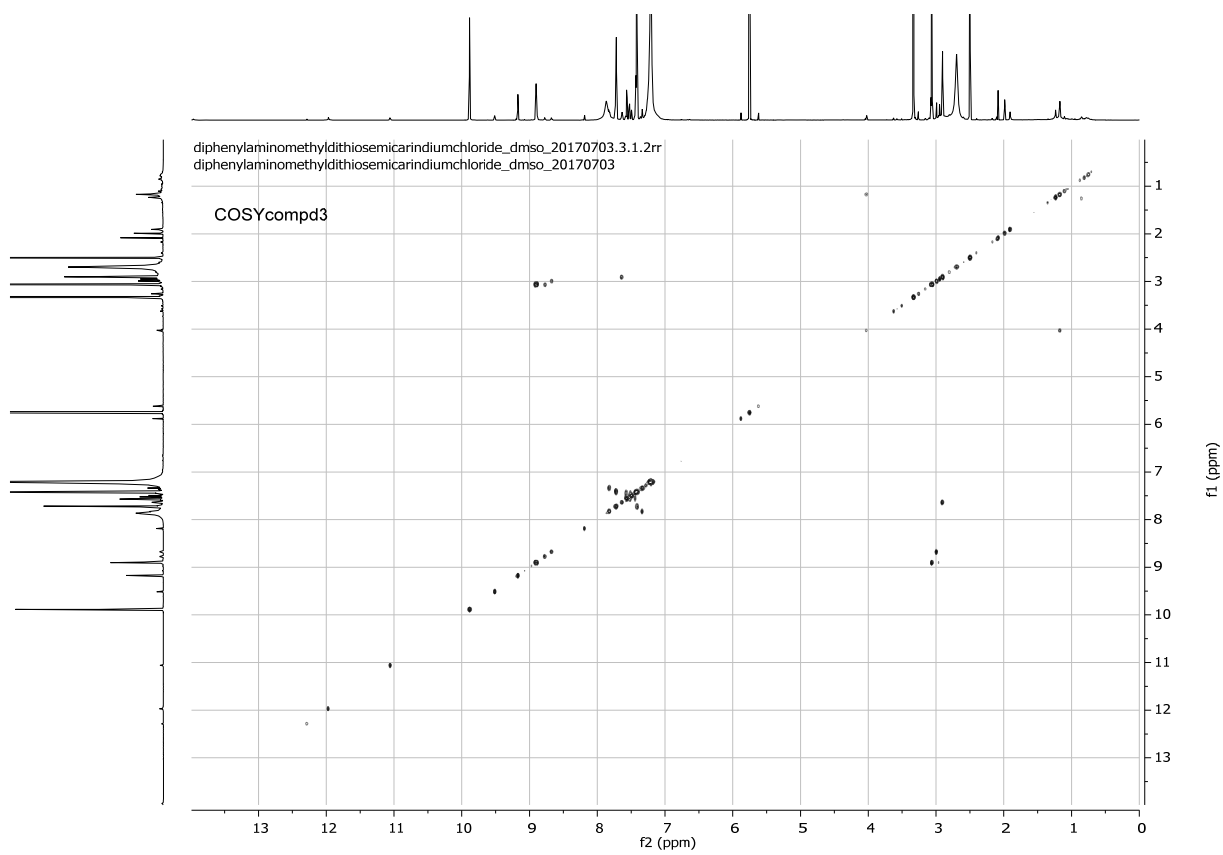


Fig. S17. COSY NMR of compound **3** (d_6 -DMSO)

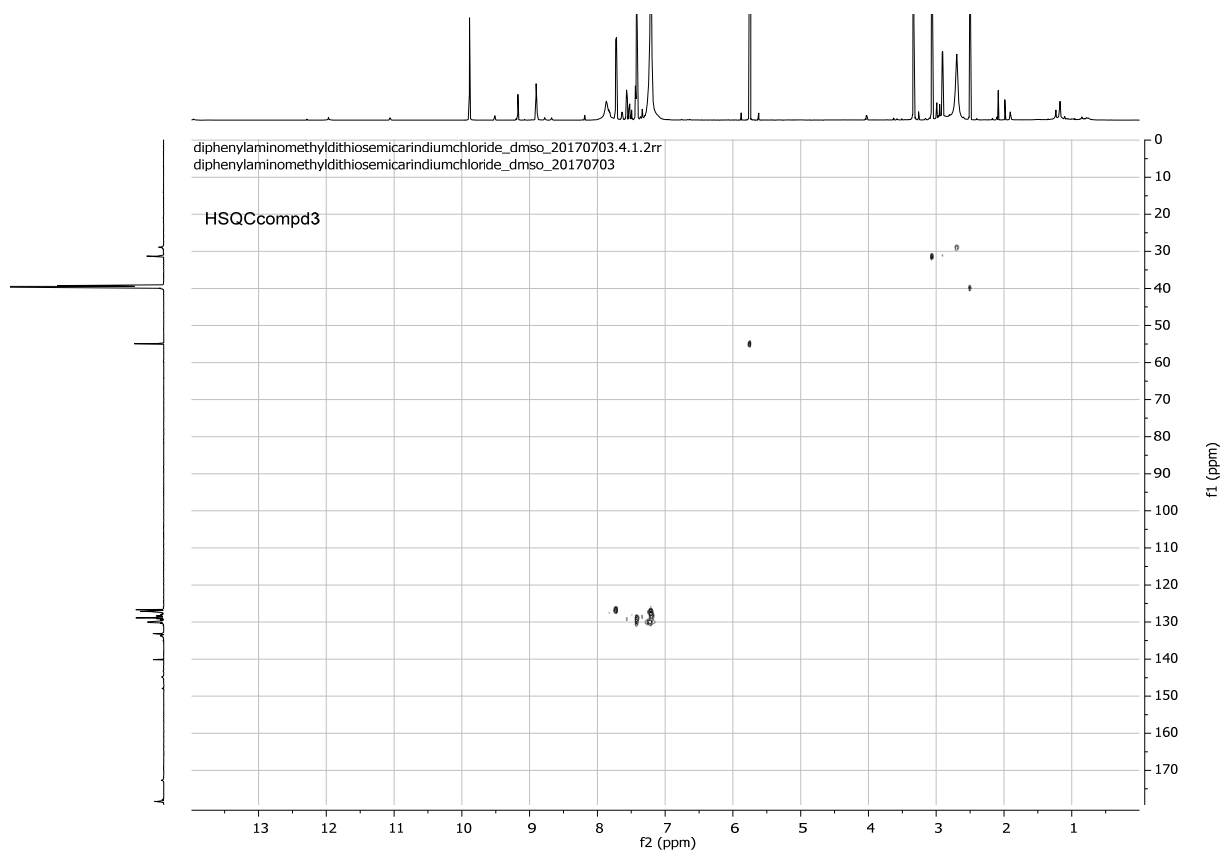


Fig. S18. HSQC NMR of compound **3** (d₆-DMSO)

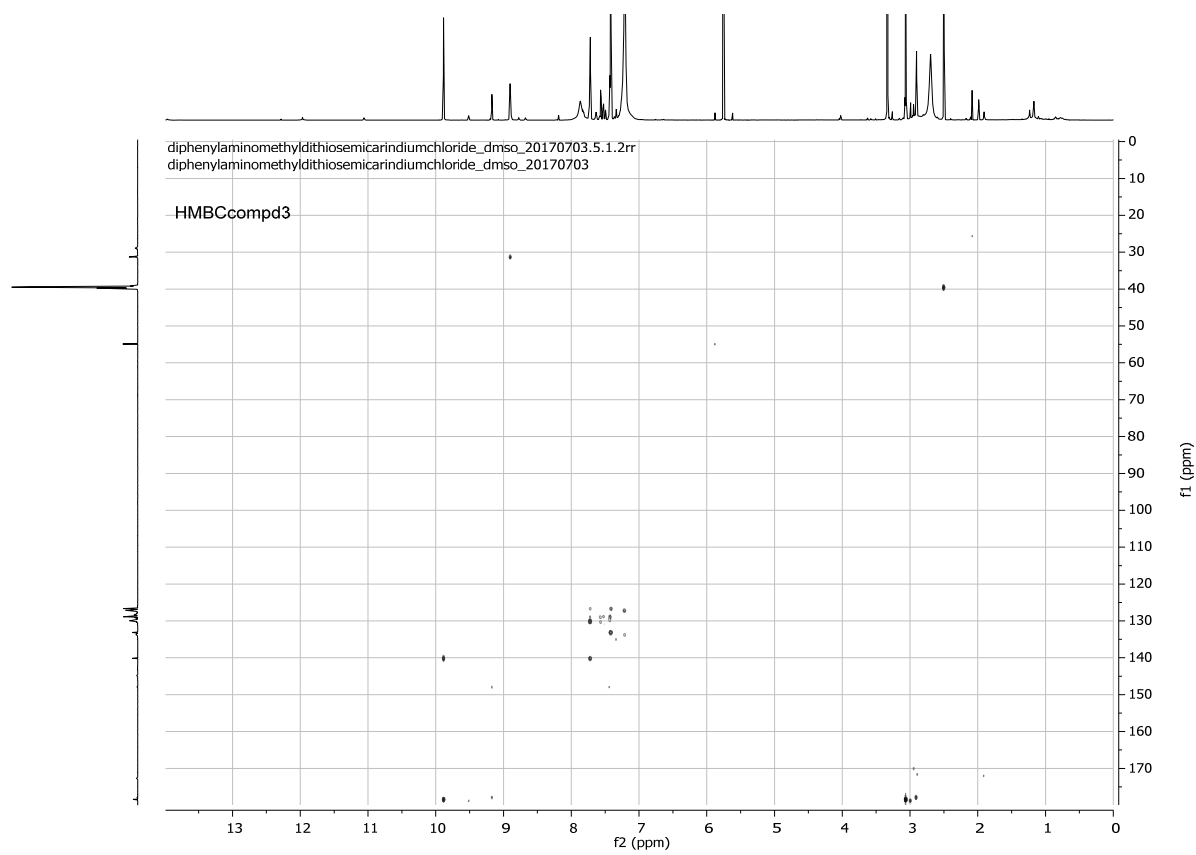


Fig. S19. HMBC NMR of compound **3** (d_6 -DMSO)

¹H NMR of compound 4

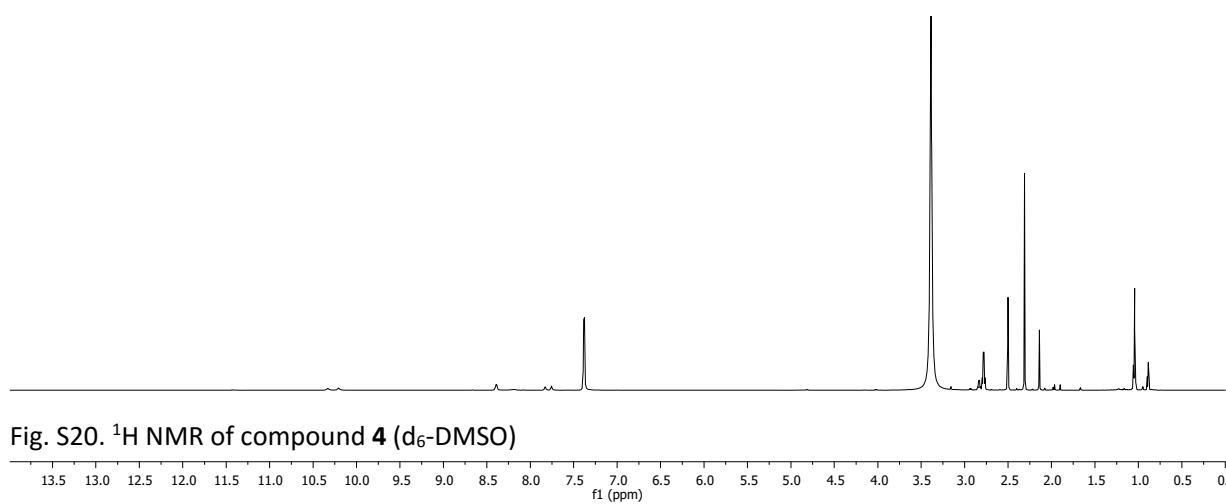


Fig. S20. ¹H NMR of compound 4 (d₆-DMSO)

^{13}C NMR of compound 4

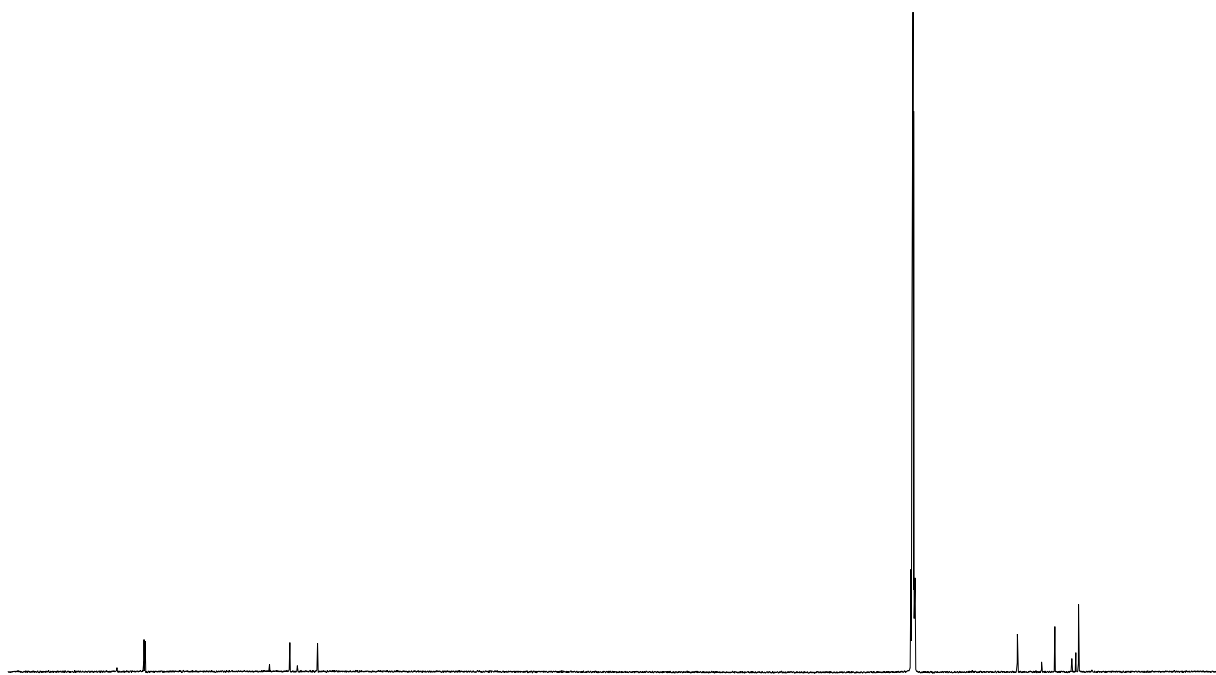
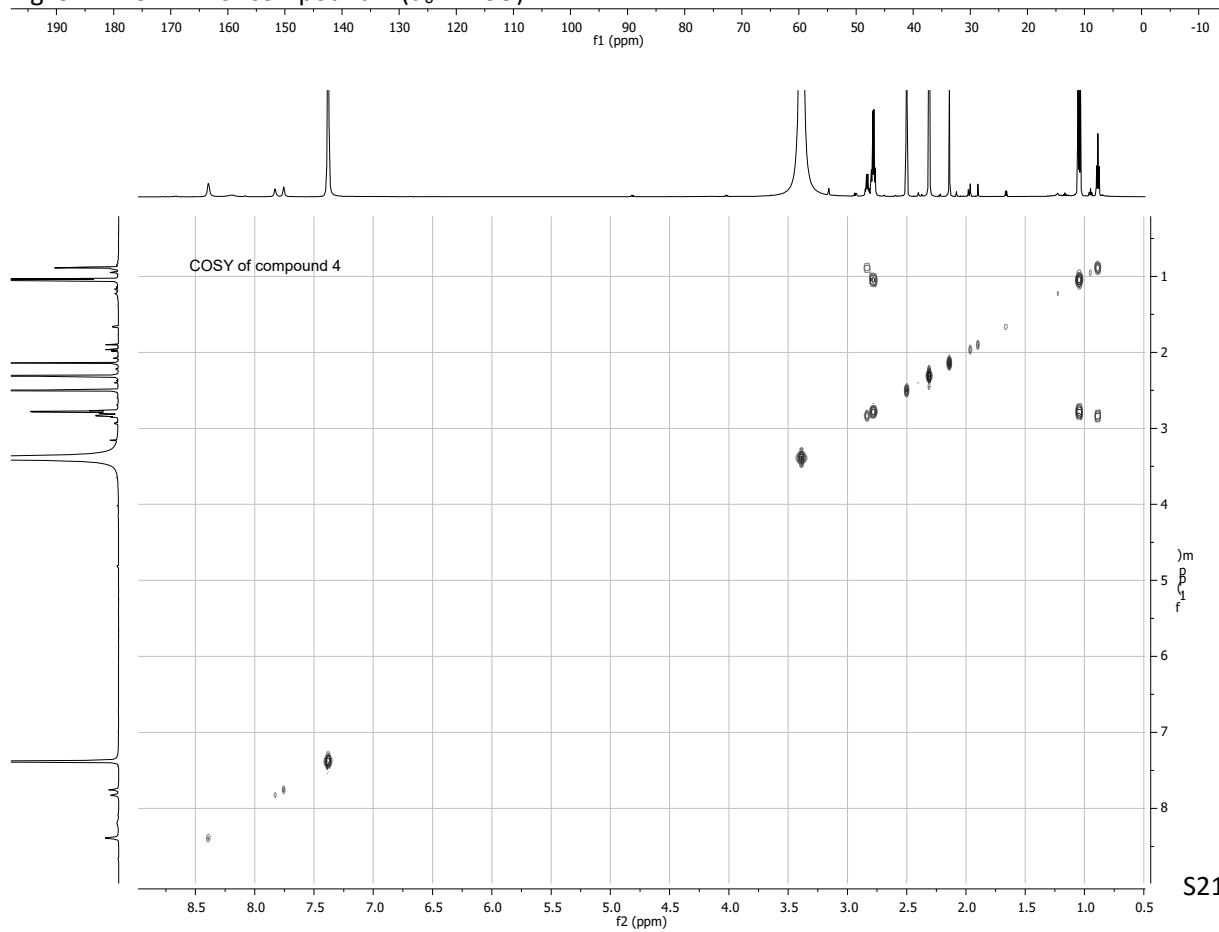


Fig. S21. ^{13}C NMR of compound 4 (d₆-DMSO)



S21

Fig. S22. COSY NMR of compound 4 (d₆-DMSO)

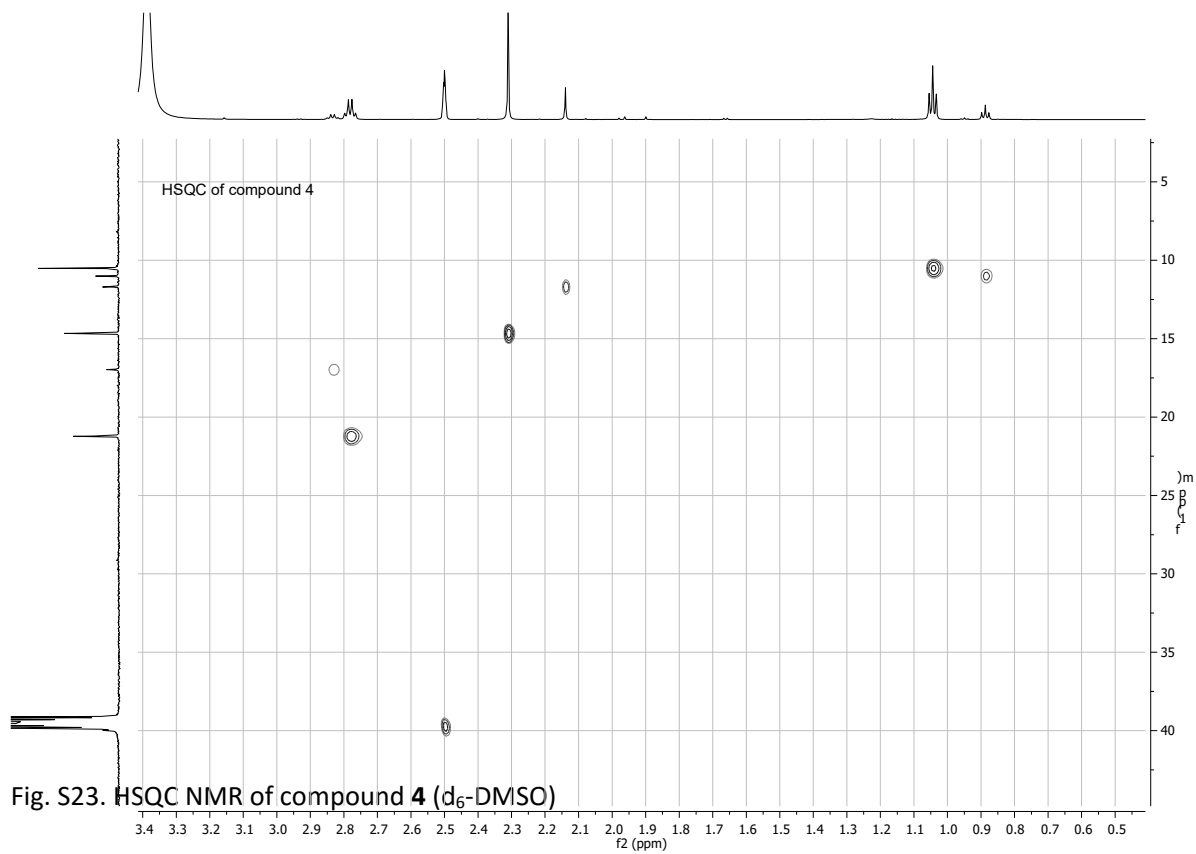


Fig. S23. HSQC NMR of compound 4 (d₆-DMSO)

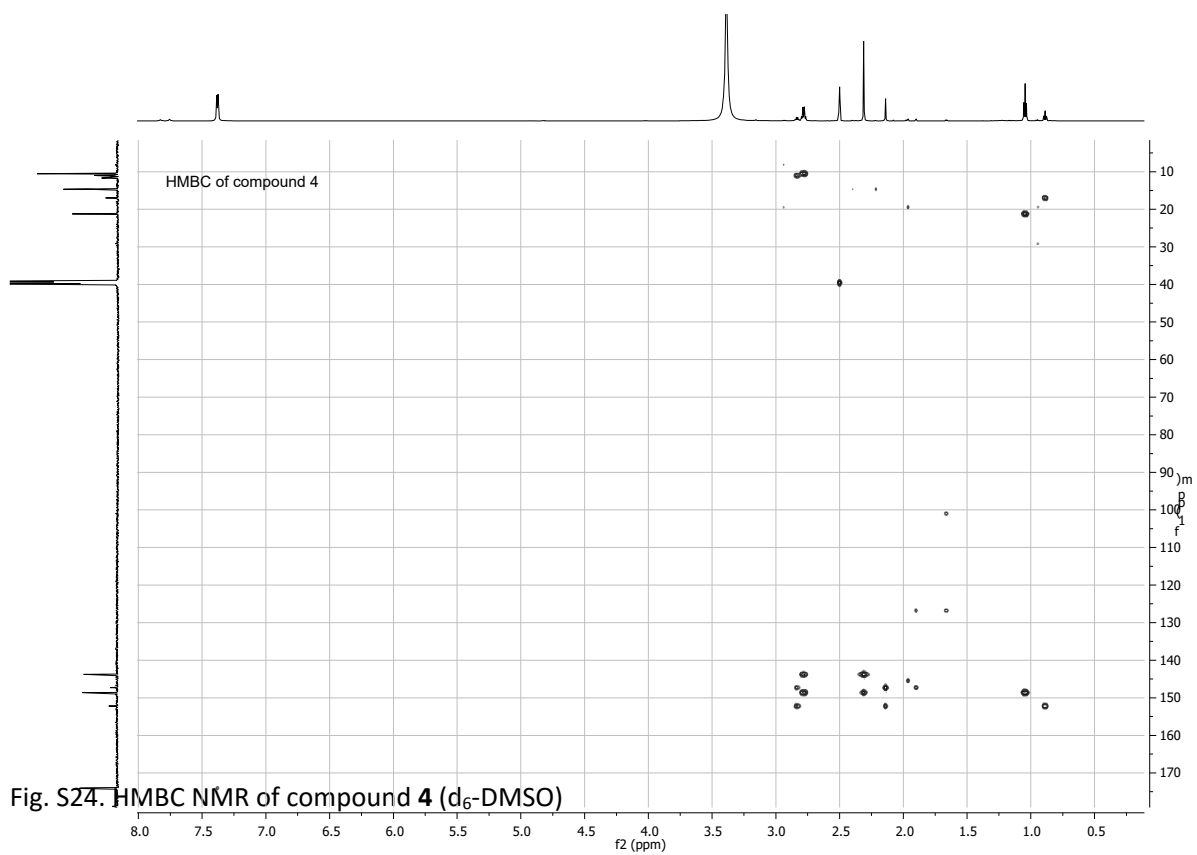


Fig. S24. HMBC NMR of compound 4 (d₆-DMSO)

symmetricaldiethyldimethylindiumchloride_DMSO_20170705.1.1.1r
symmetricaldiethyldimethylindiumchloride_DMSO_20170705

¹H NMR compd 5

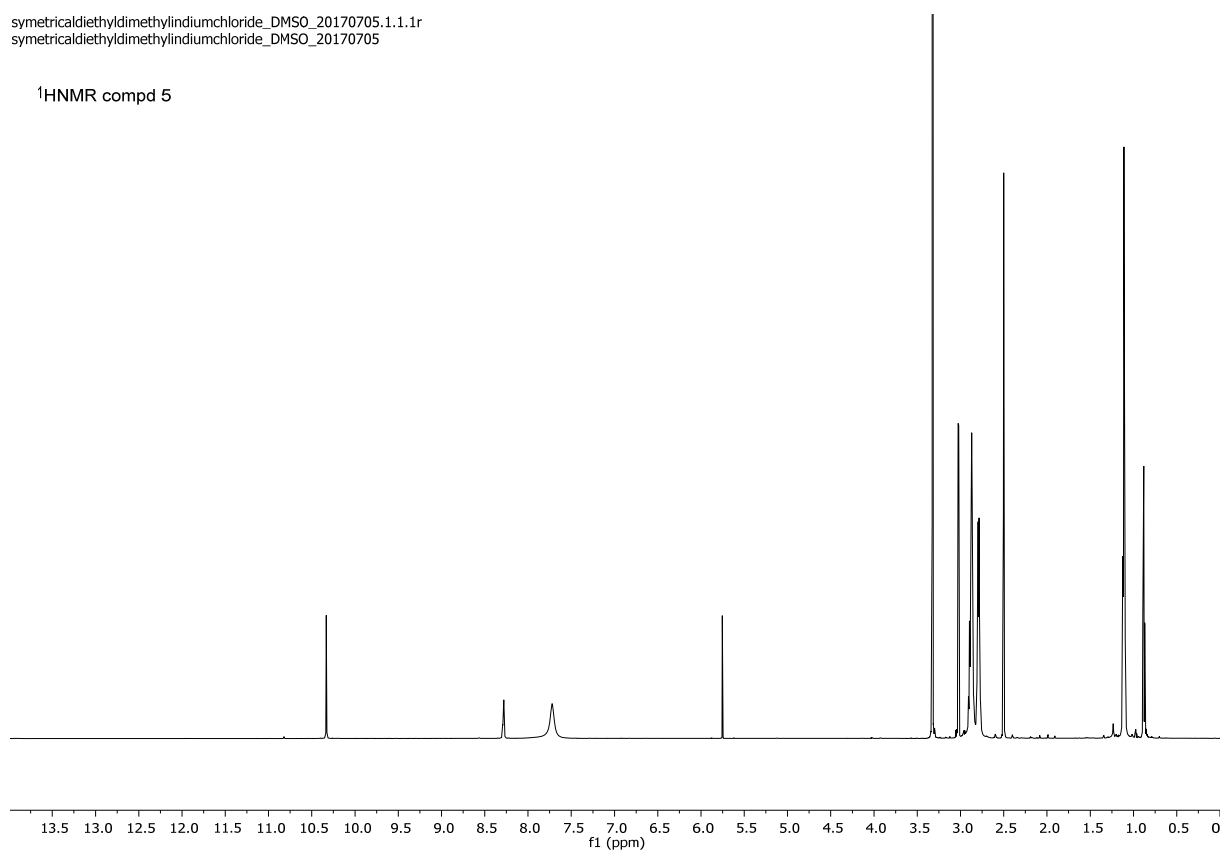


Fig. S25. ¹H NMR of compound 5 (d₆-DMSO)

symetricaldiethylidimethylindiumchloride_DMSO_20170705.2.1.1r
symetricaldiethylidimethylindiumchloride_DMSO_20170705

^{13}C NMR compd 5

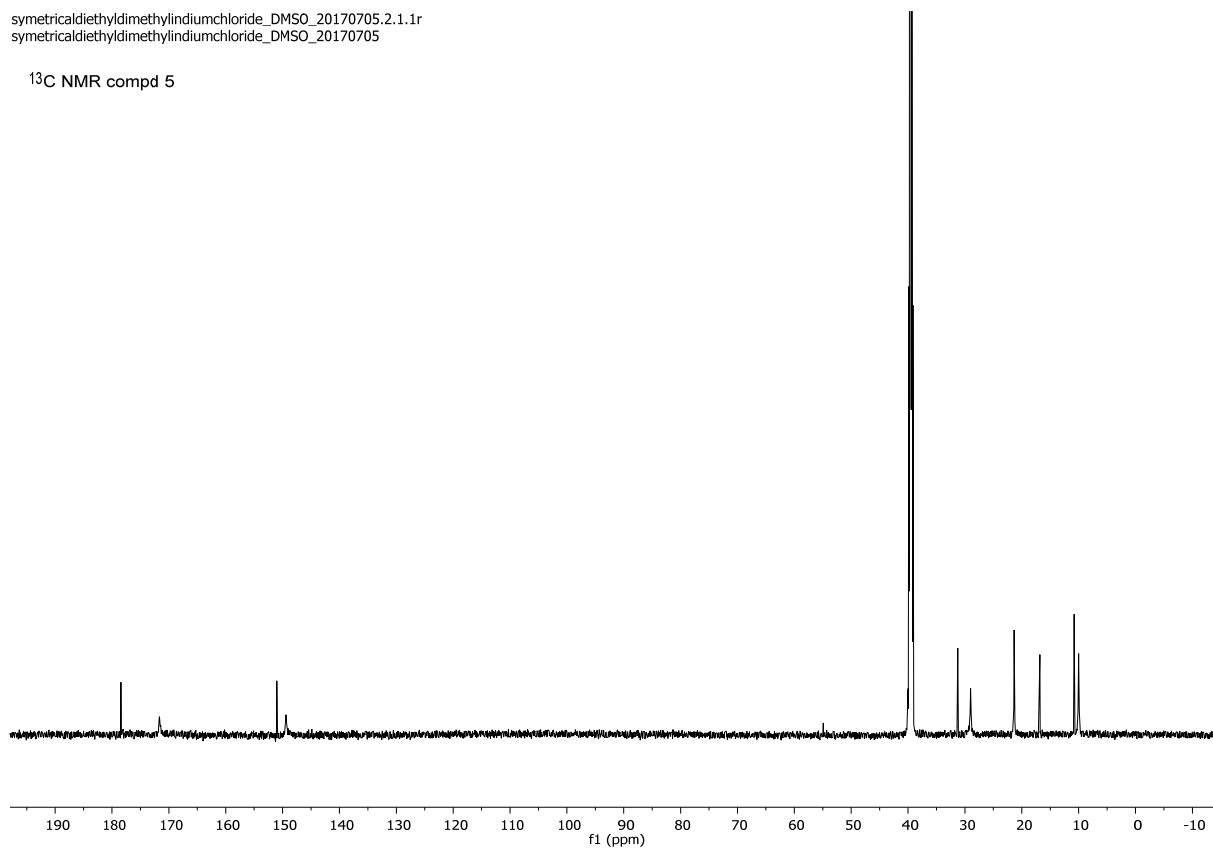


Fig. S26. ^{13}C NMR of compound 5 (d_6 -DMSO)

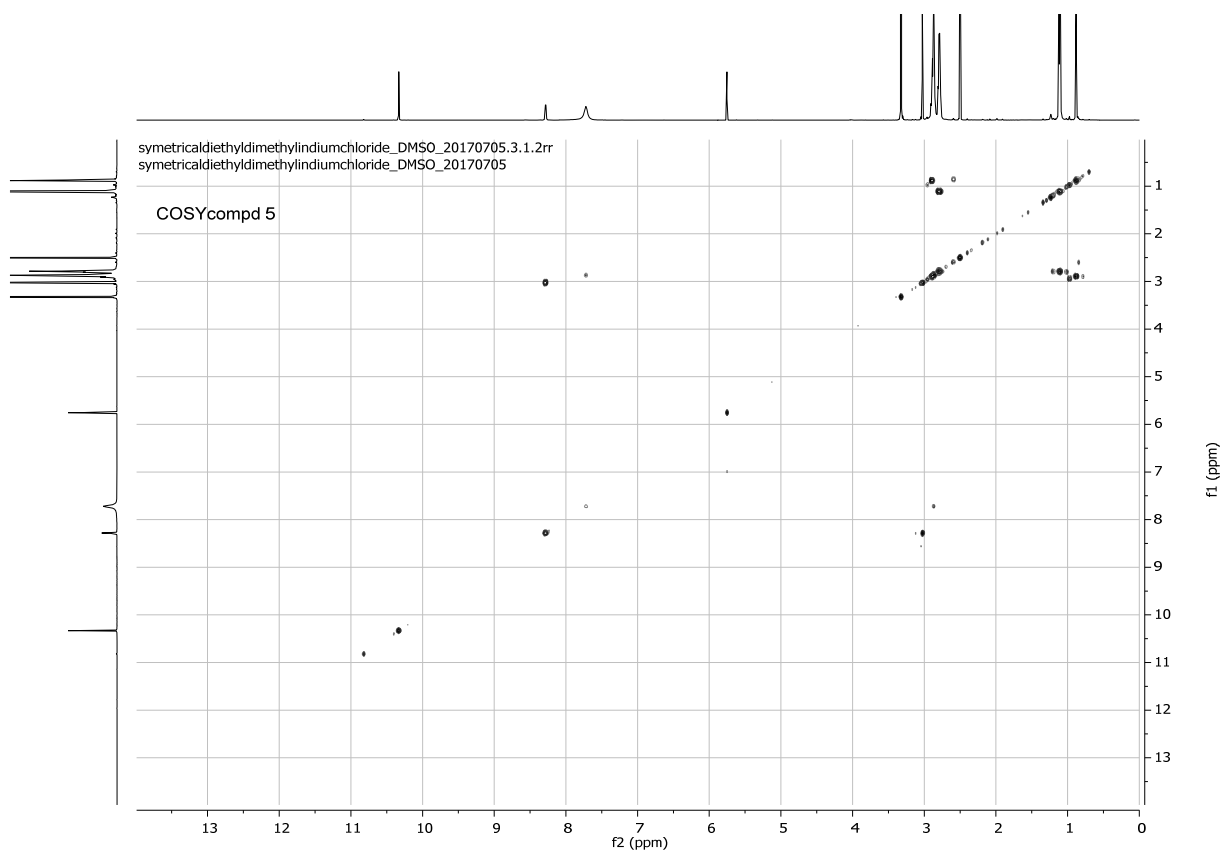


Fig. S27. COSY NMR of compound **5** (d_6 -DMSO)

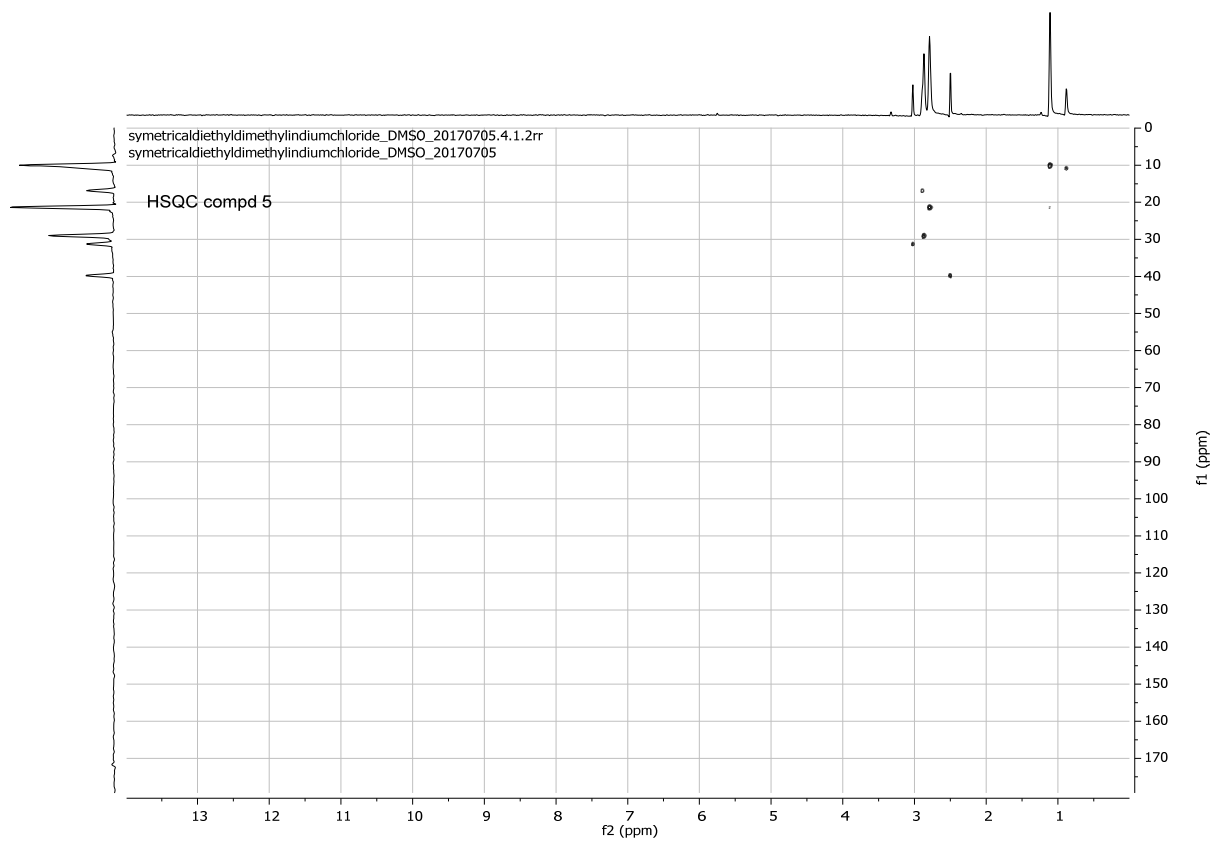


Fig. S28. HSQC NMR of compound 5 (d_6 -DMSO)

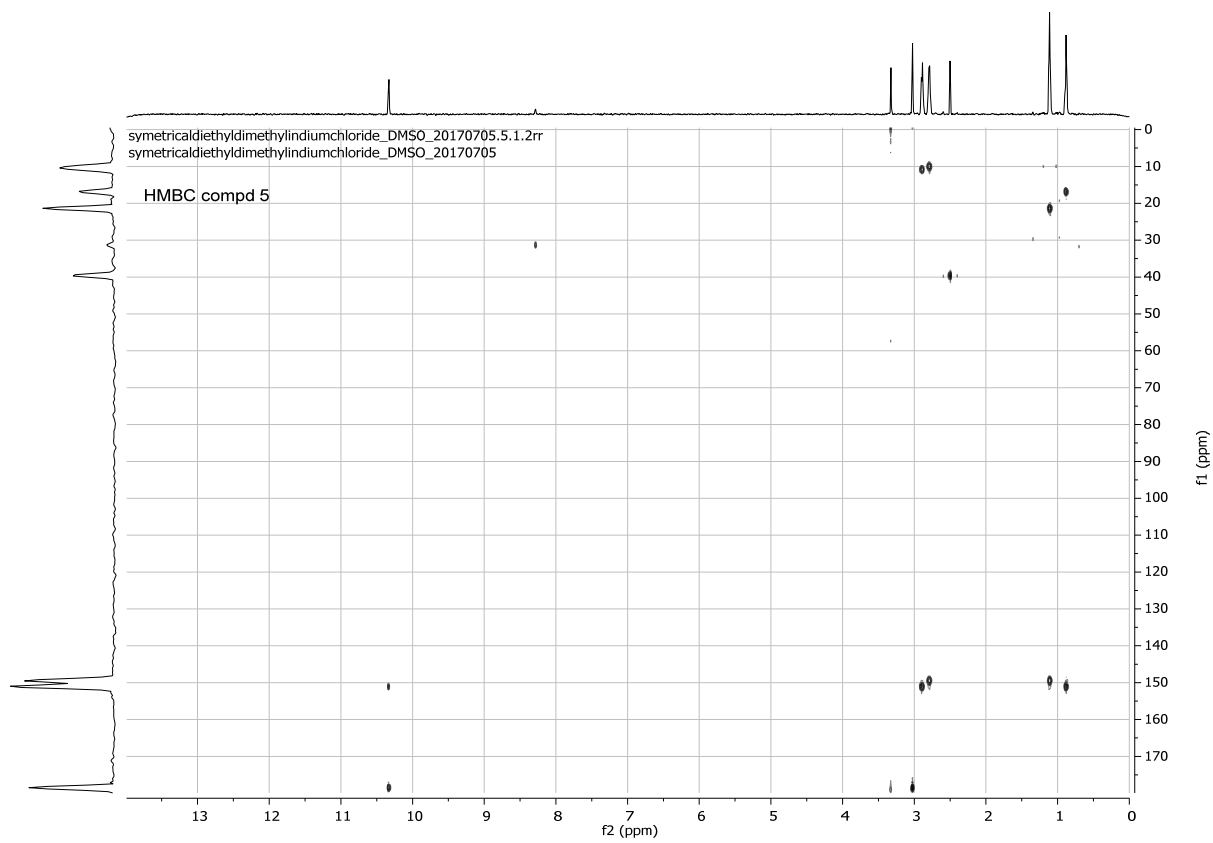


Fig. S29. HMBC NMR of compound 5 (d_6 -DMSO)

methylethylindiumchloridethiosemicarbazone_DMSO_20170427.1.1.1r
methylethylindiumchloridethiosemicarbazone_DMSO_20170427

¹HNMRcompd6

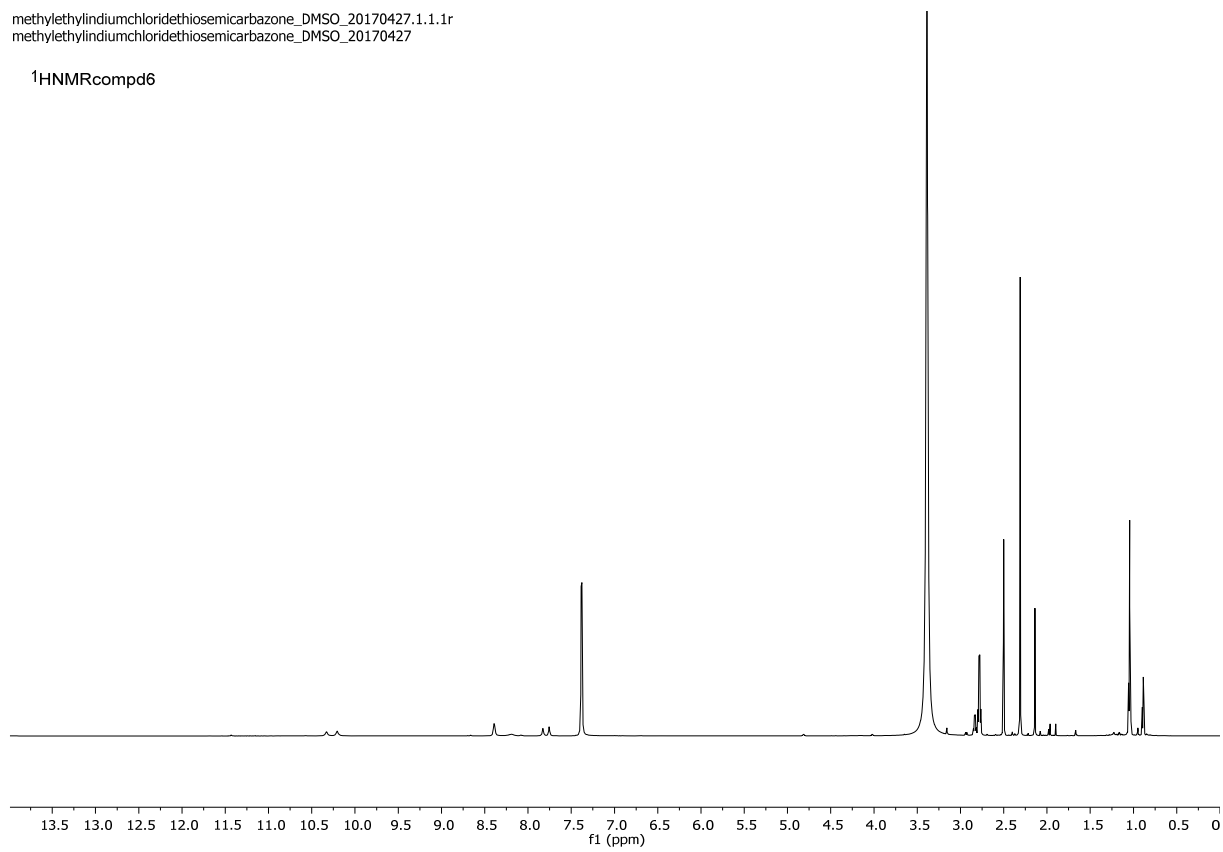


Fig. S30. ¹H NMR of compound **6** (d₆-DMSO)

methylethylindiumchloridethiosemicarbazone_DMSO_20170427.2.1.1r
methylethylindiumchloridethiosemicarbazone_DMSO_20170427

^{13}C NMRcompd 6

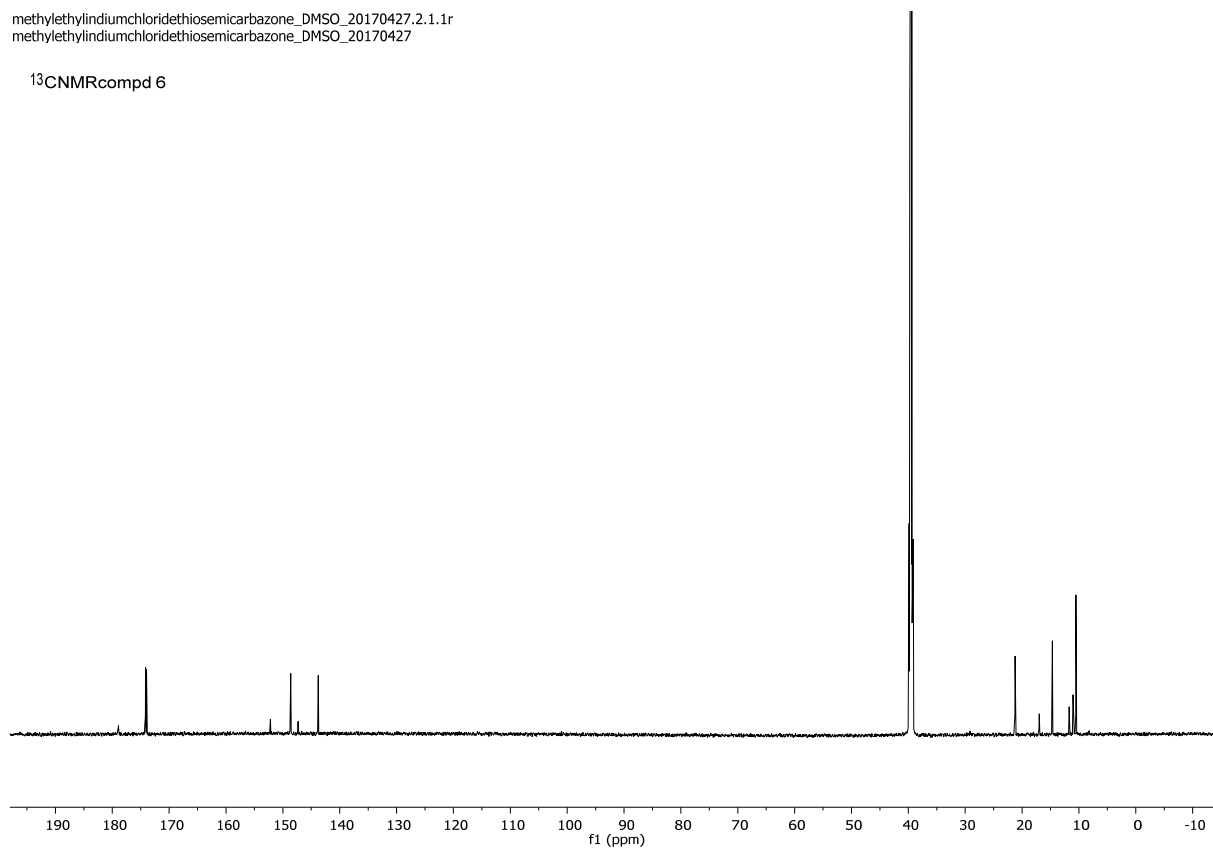


Fig. S31. ^{13}C NMR of compound 6 (d_6 -DMSO)

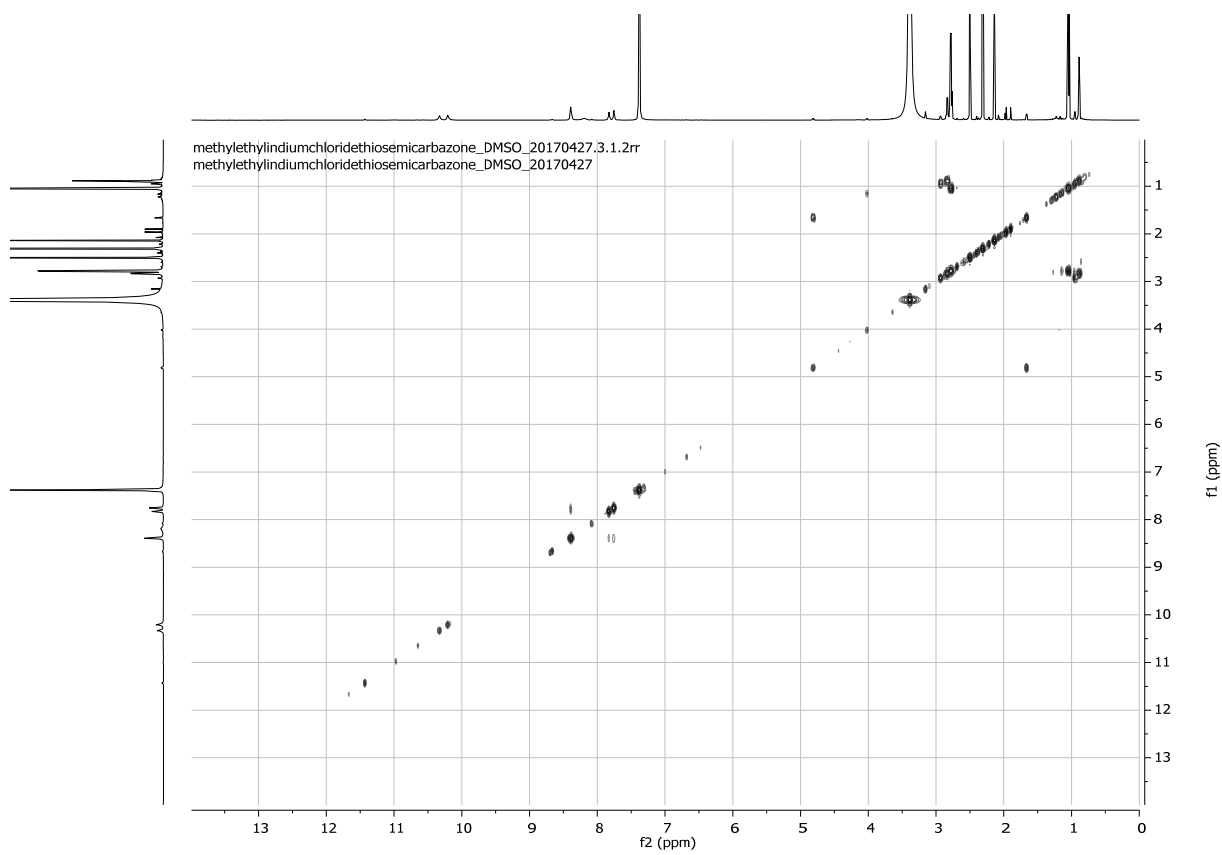


Fig. S32. COSY NMR of compound **6** (d_6 -DMSO)

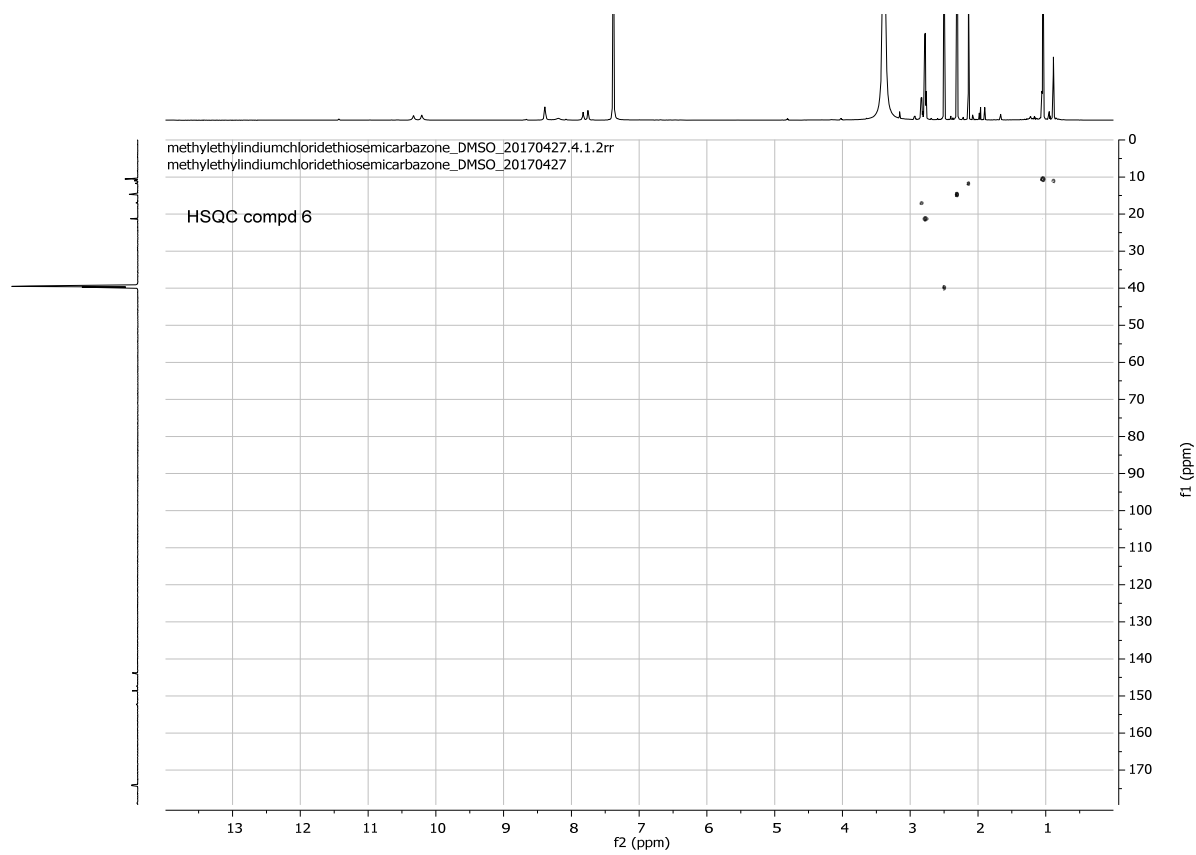


Fig. S33. HSQC NMR of compound **6** (d_6 -DMSO)

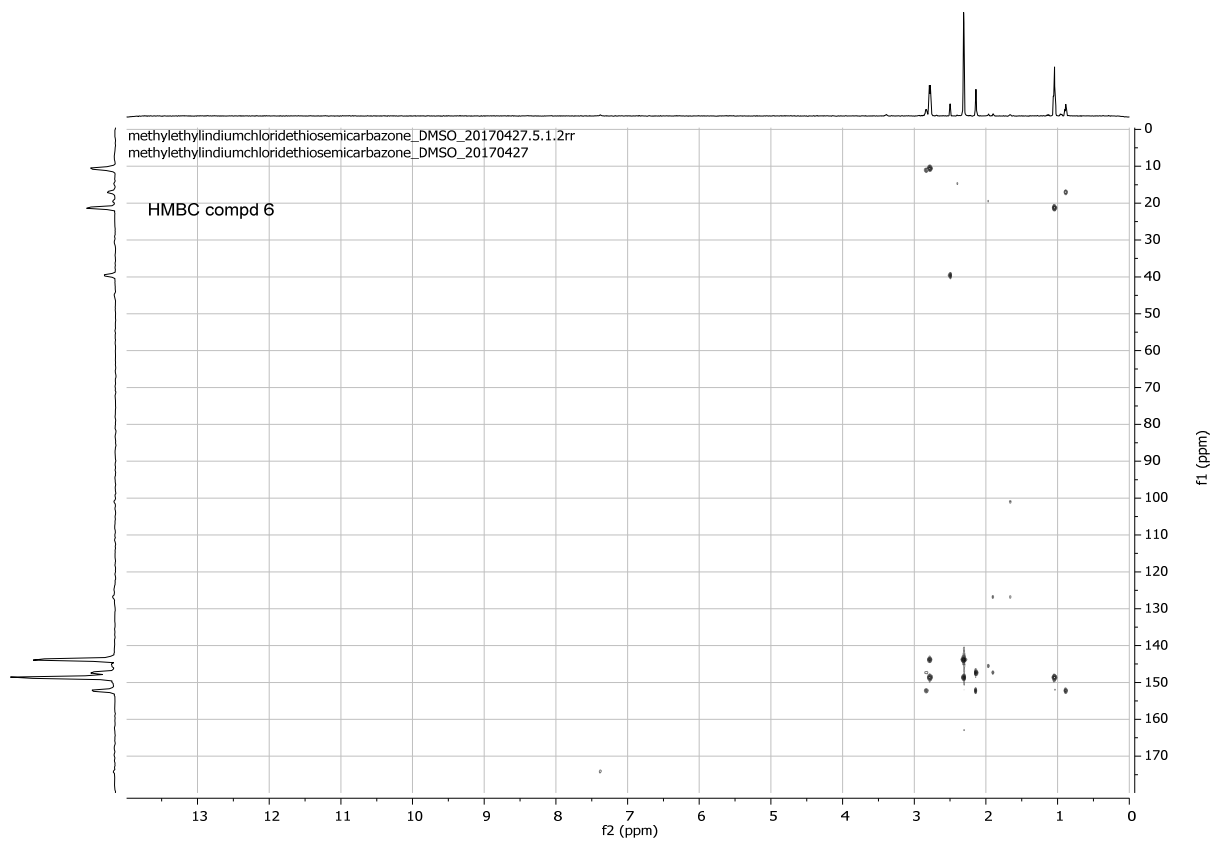


Fig. S34. HMBC NMR of compound **6** (d_6 -DMSO)

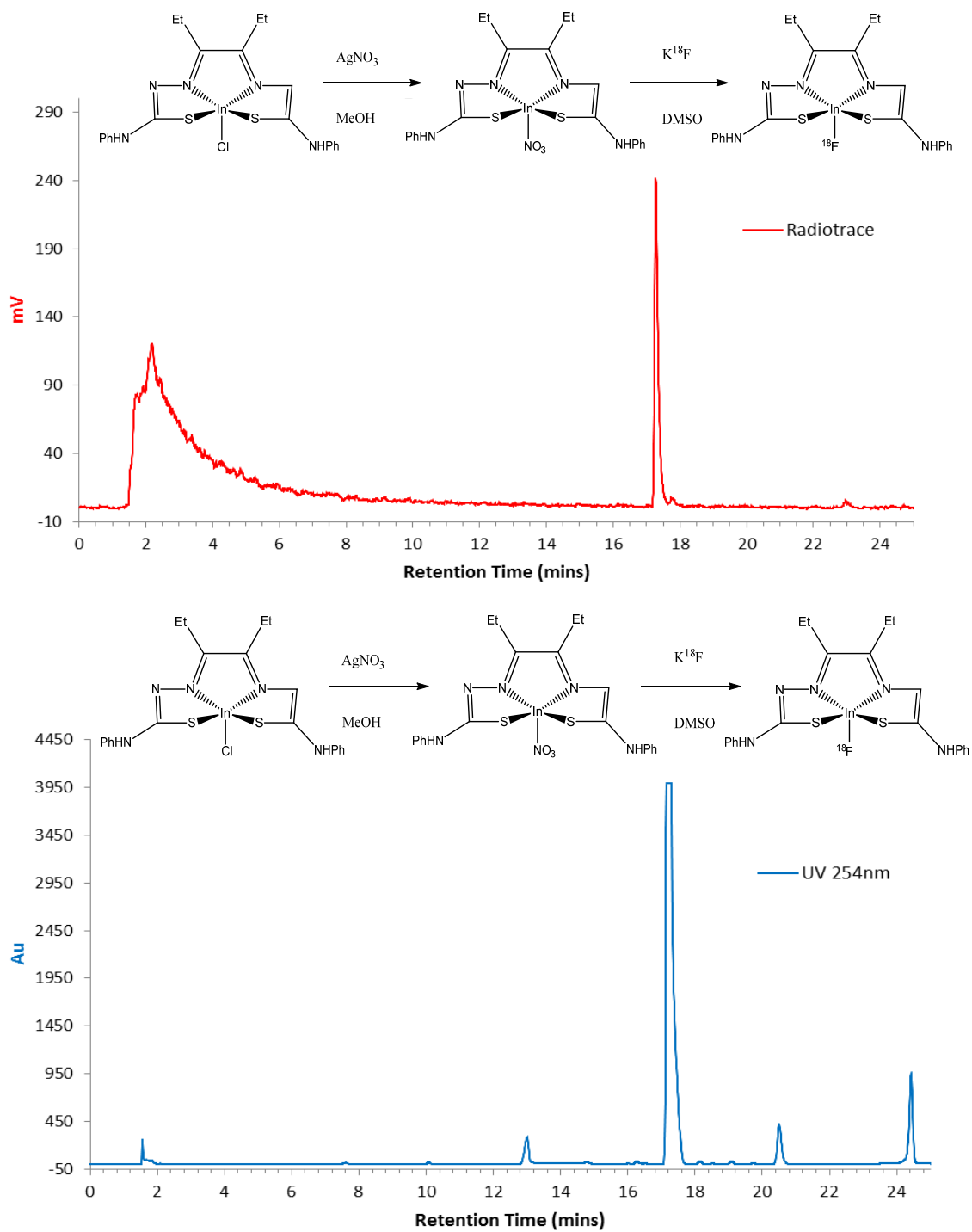


Fig. S35 HPLC chromatograms of ^{18}F -radiolabeled compound **2** (note: the ^{19}F UV peak is buried under the starting material peak)

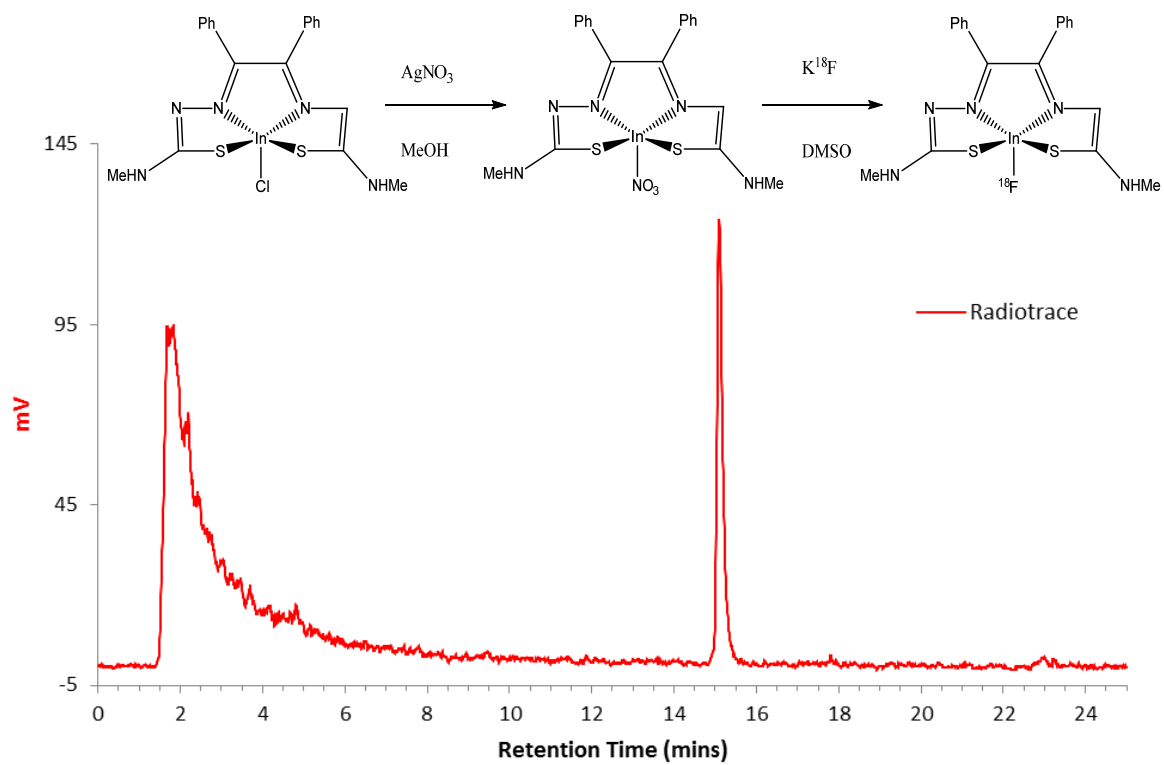


Fig. S36. HPLC chromatograms of ^{18}F -radiolabeled compound **3**

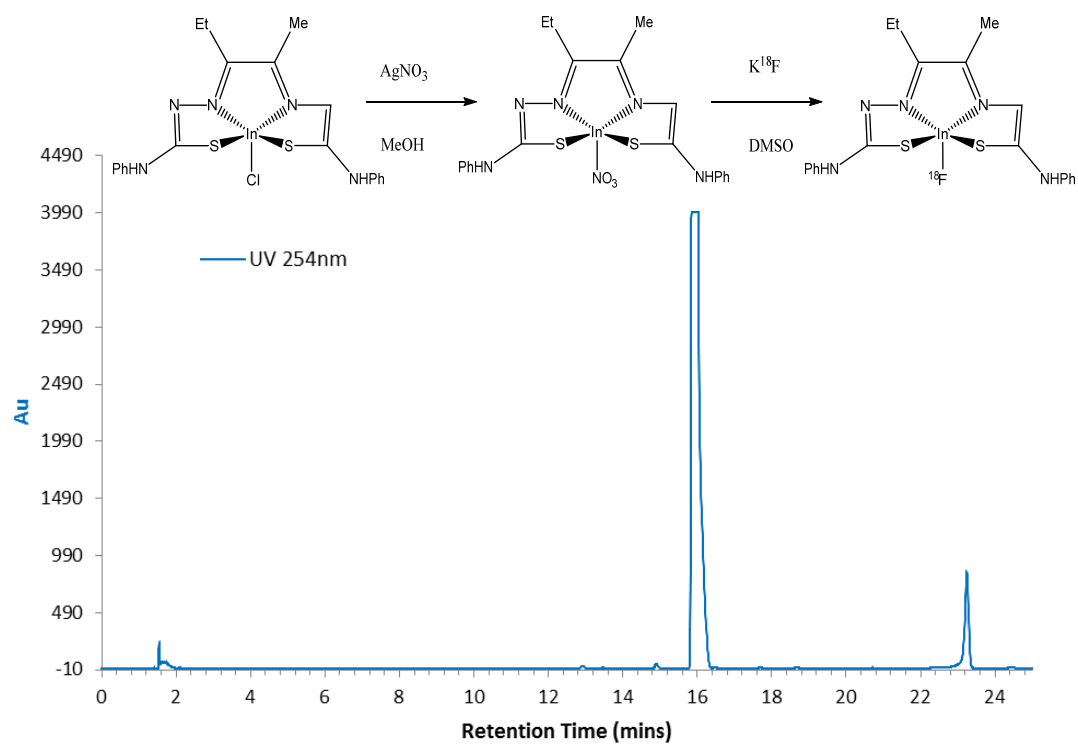
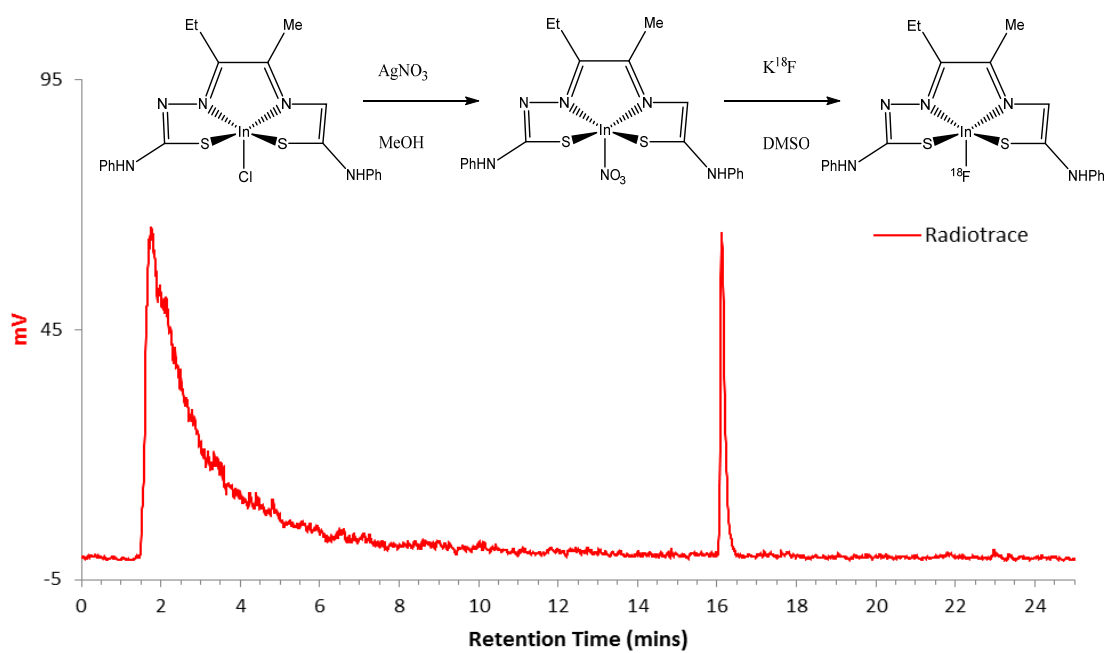


Fig. S37. HPLC chromatograms of ^{18}F -radiolabeled compound **1** (note: the ^{19}F UV peak is buried under the starting material peak)

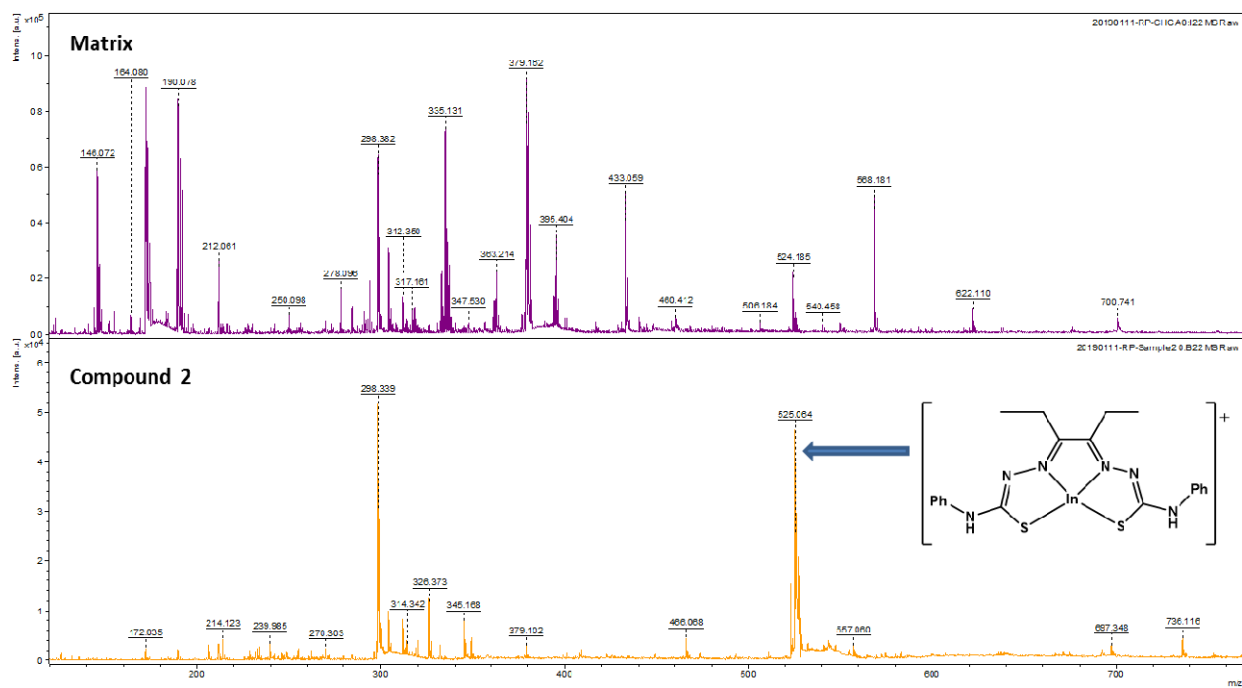


Fig. S38. Mass spectrum of compound 2

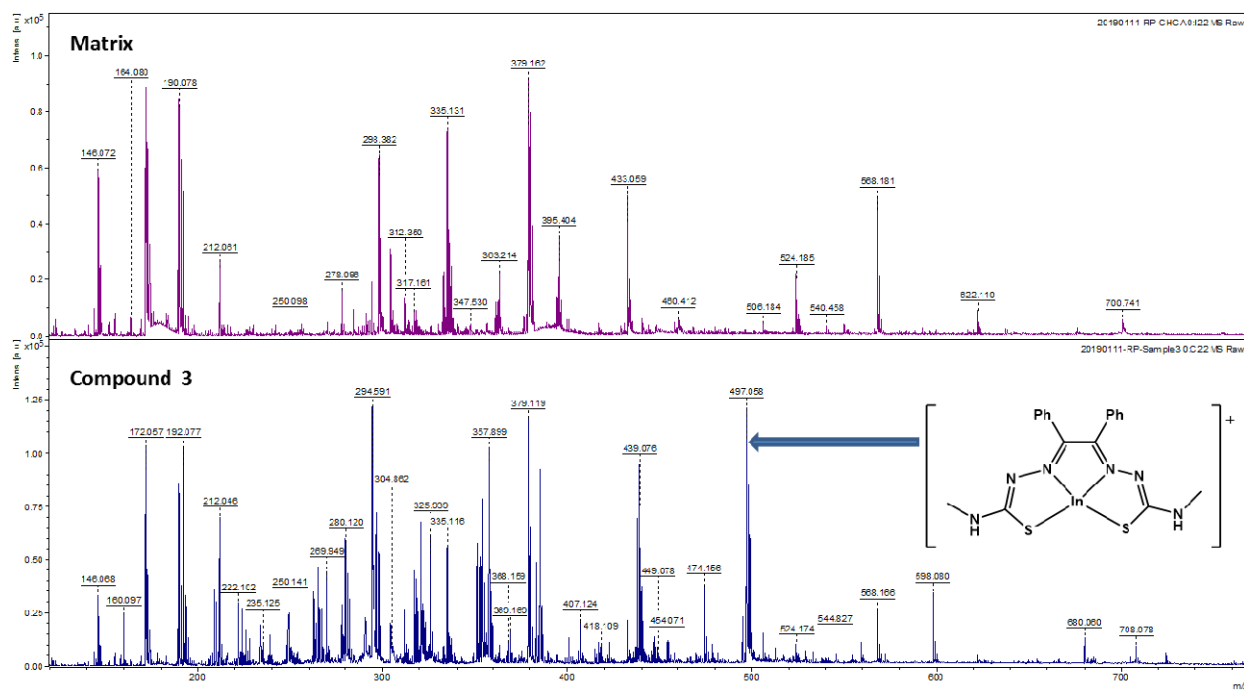


Fig. S39. Mass spectrum of compound **3**

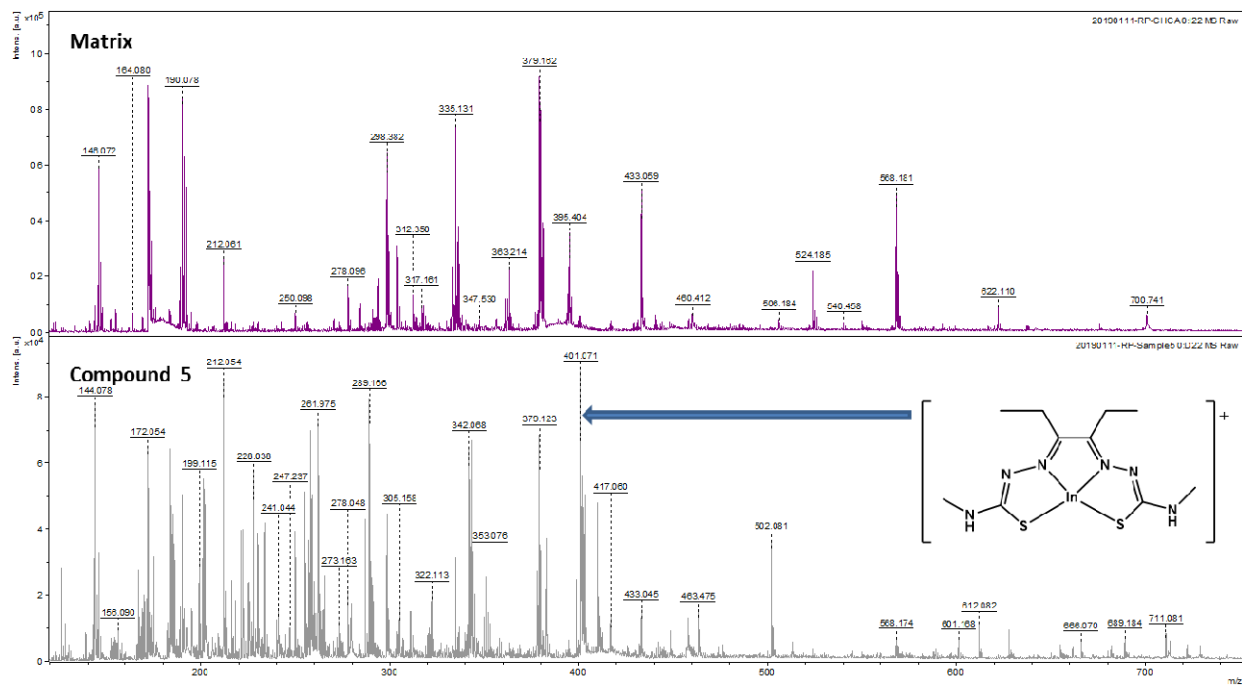


Fig. S40. Mass spectrum of compound 5

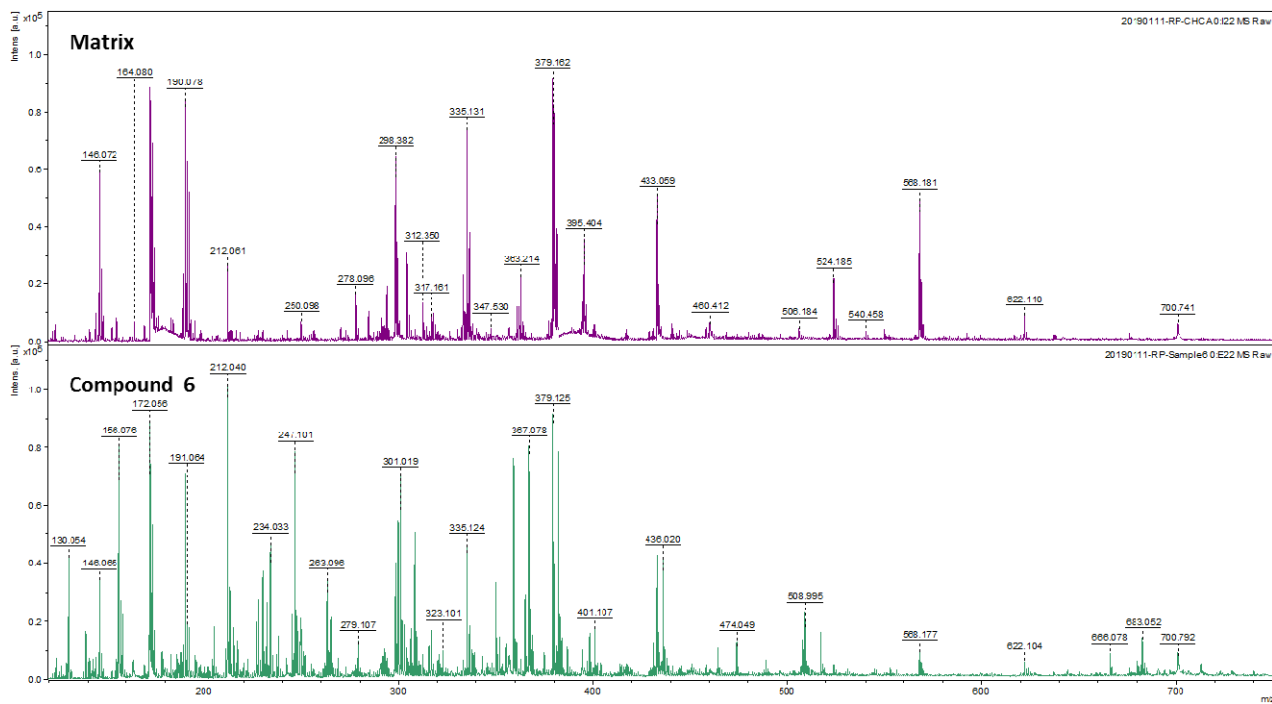


Fig. S41(a). Mass spectrum of compound 6 (zoomed, together with simulation)

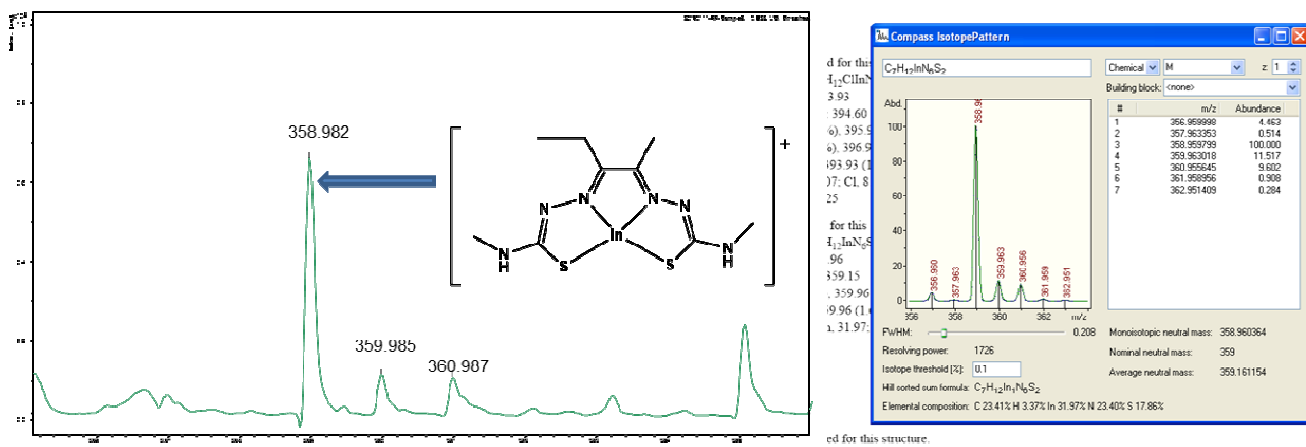


Fig. S41(b). Mass spectrum of compound 6 (zoomed, together with simulation)