

Electronic Supplementary Information

Novel bismuth compounds; Synthesis, characterization and biological activity against human adenocarcinoma cells

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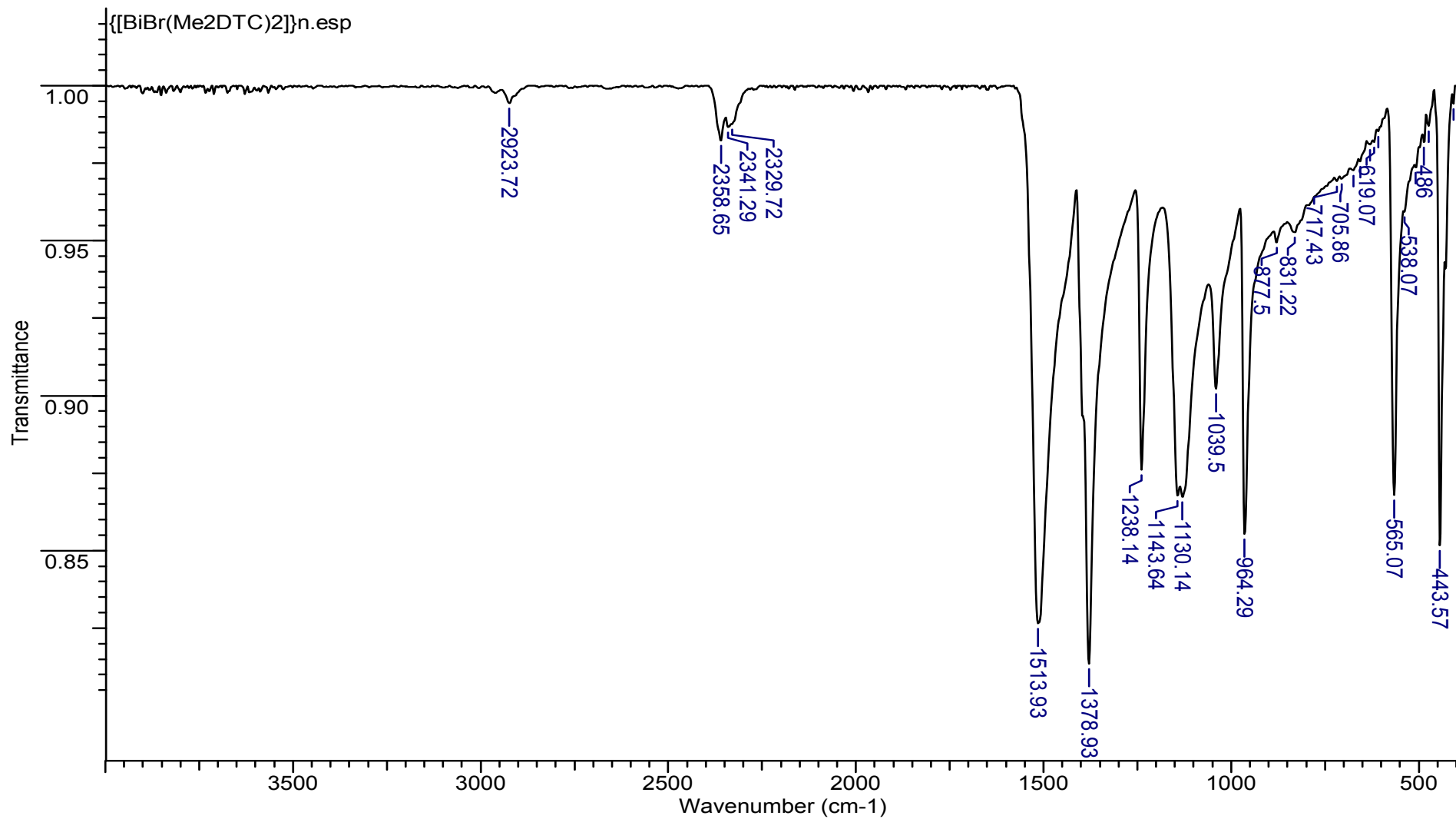


Figure S1. MID-IR spectrum of Complex 1 ($\{[\text{BiBr}(\text{Me}_2\text{DTC})_2]\}_n$)

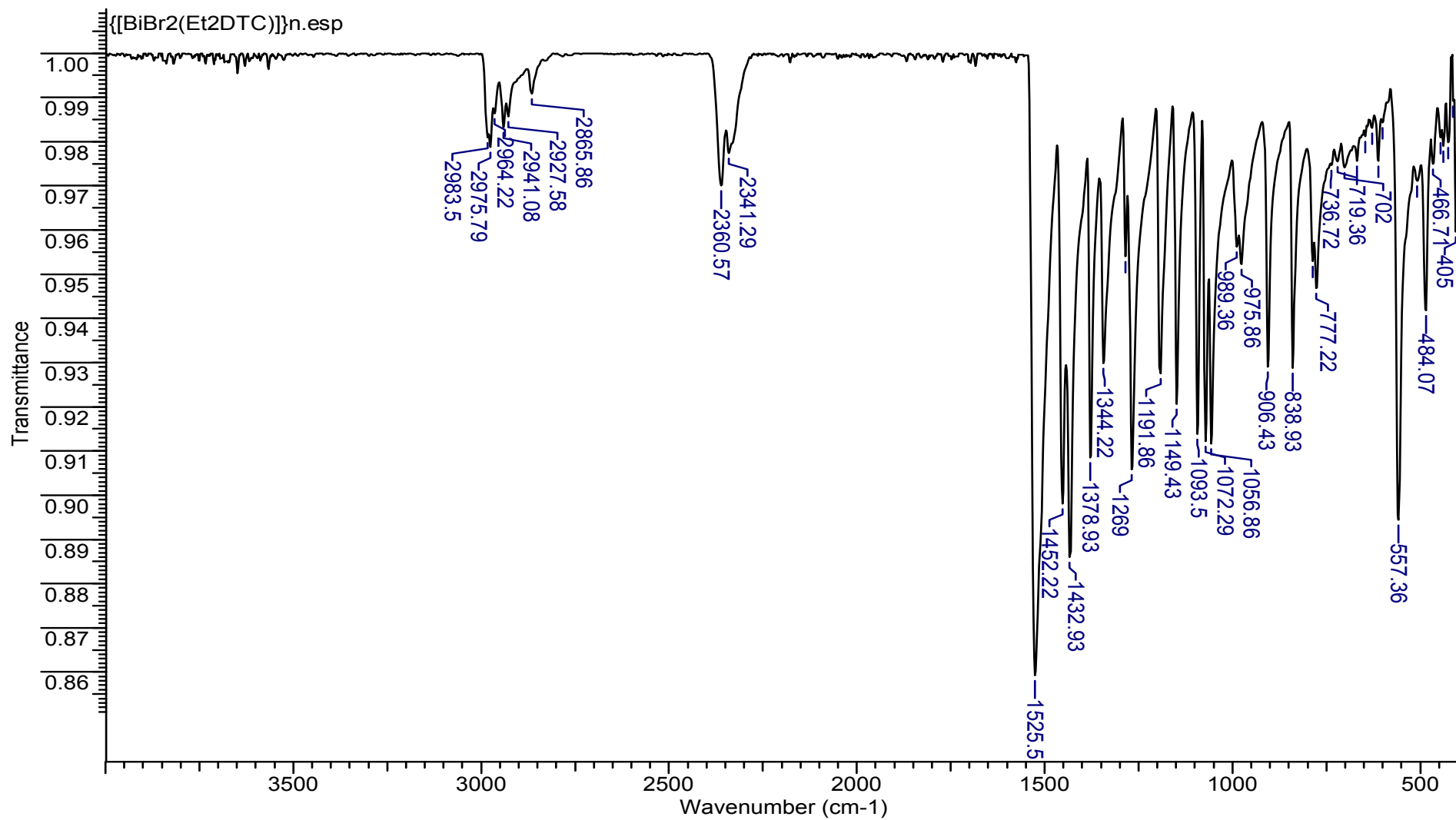


Figure S2. MID-IR spectrum of Complex 2 ($\{[BiBr_2(Et_2DTC)]\}_n$)

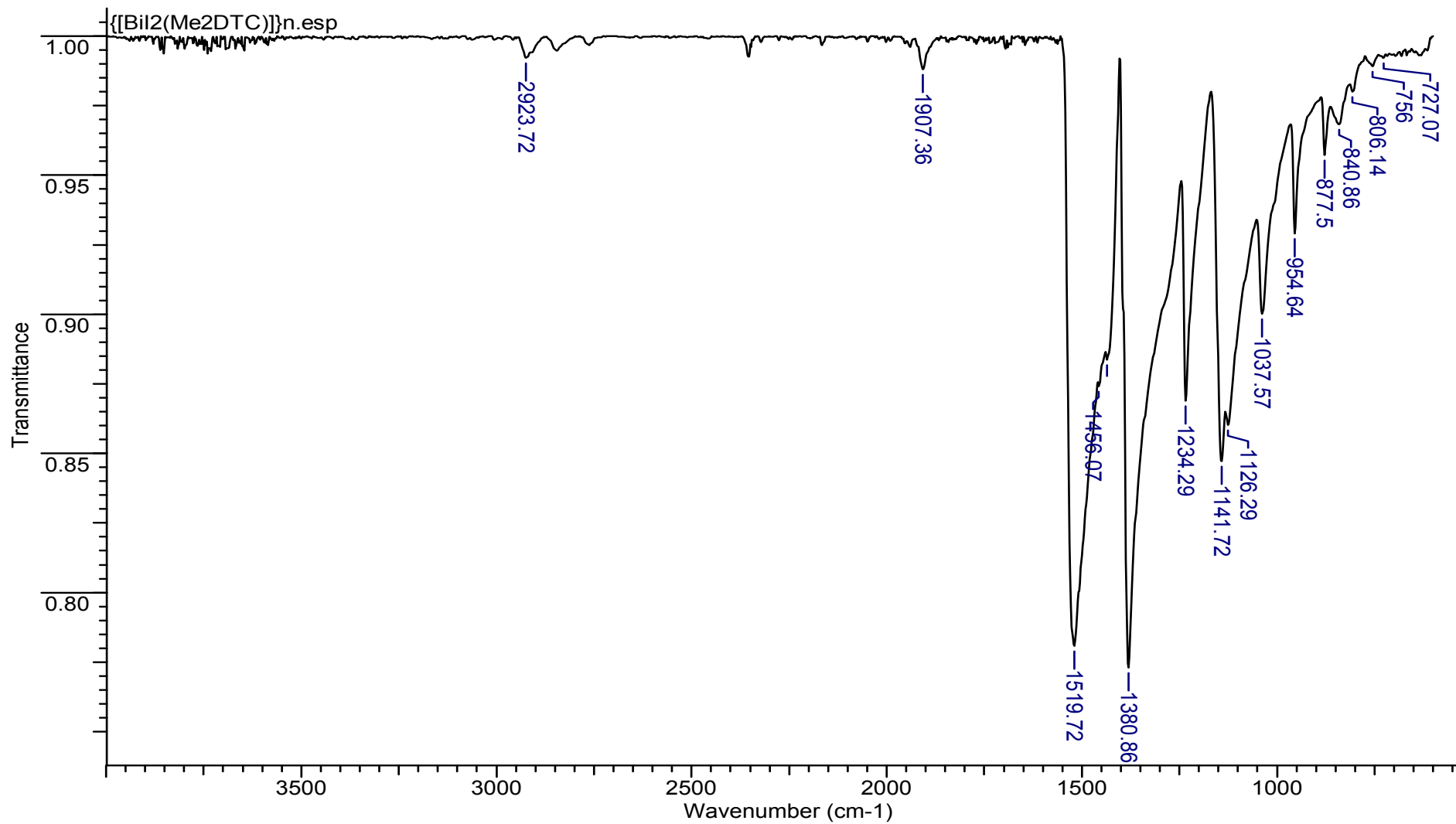


Figure S3. MID MID-IR spectrum of Complex 3 ($\{[\text{BiI}_2(\text{Me}_2\text{DTC})]_n\}$)

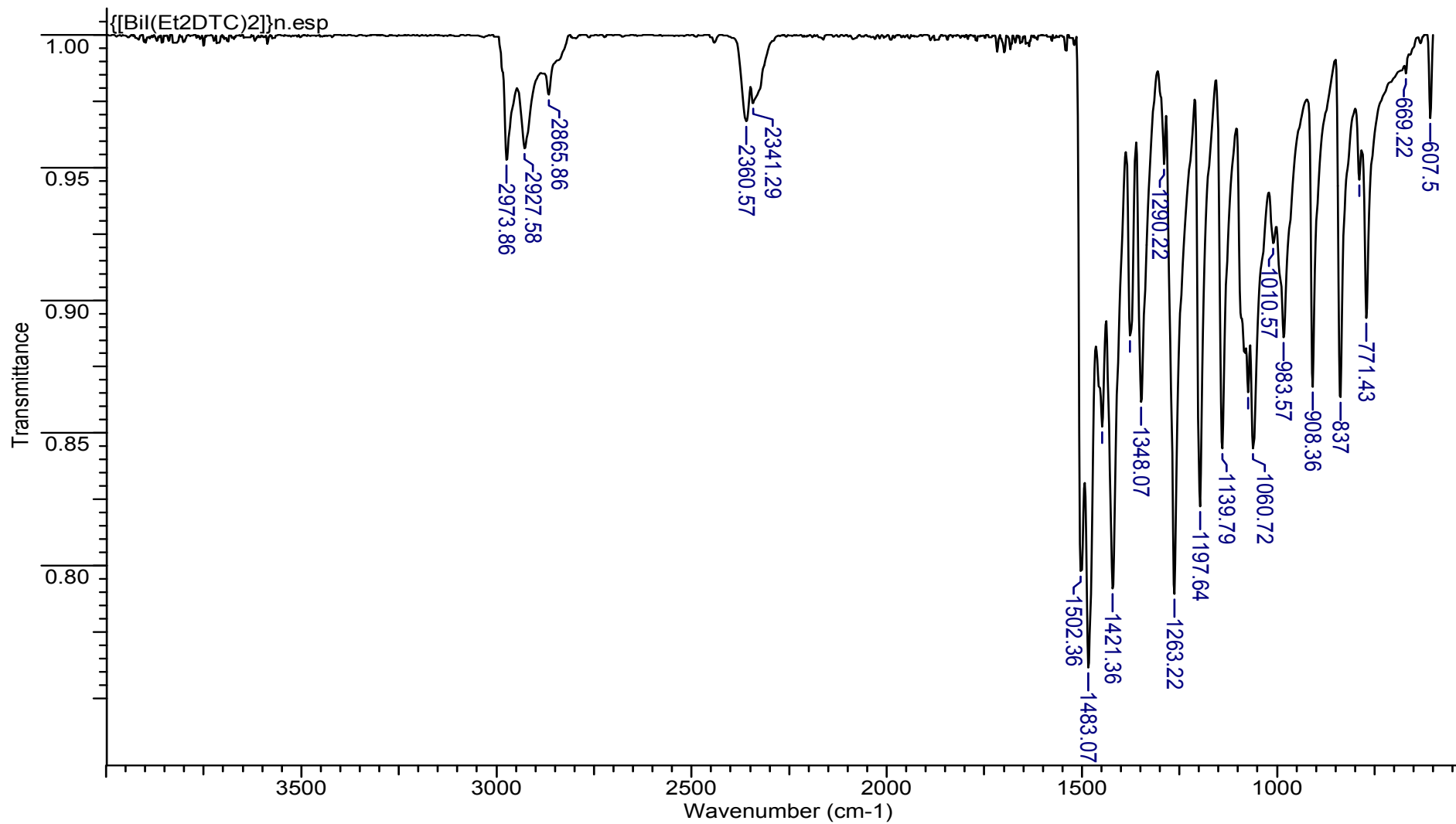


Figure S4. MID-IR spectrum of Complex 4 ($\{[\text{BiI}(\text{Et}_2\text{DTC})_2]\}_n$)

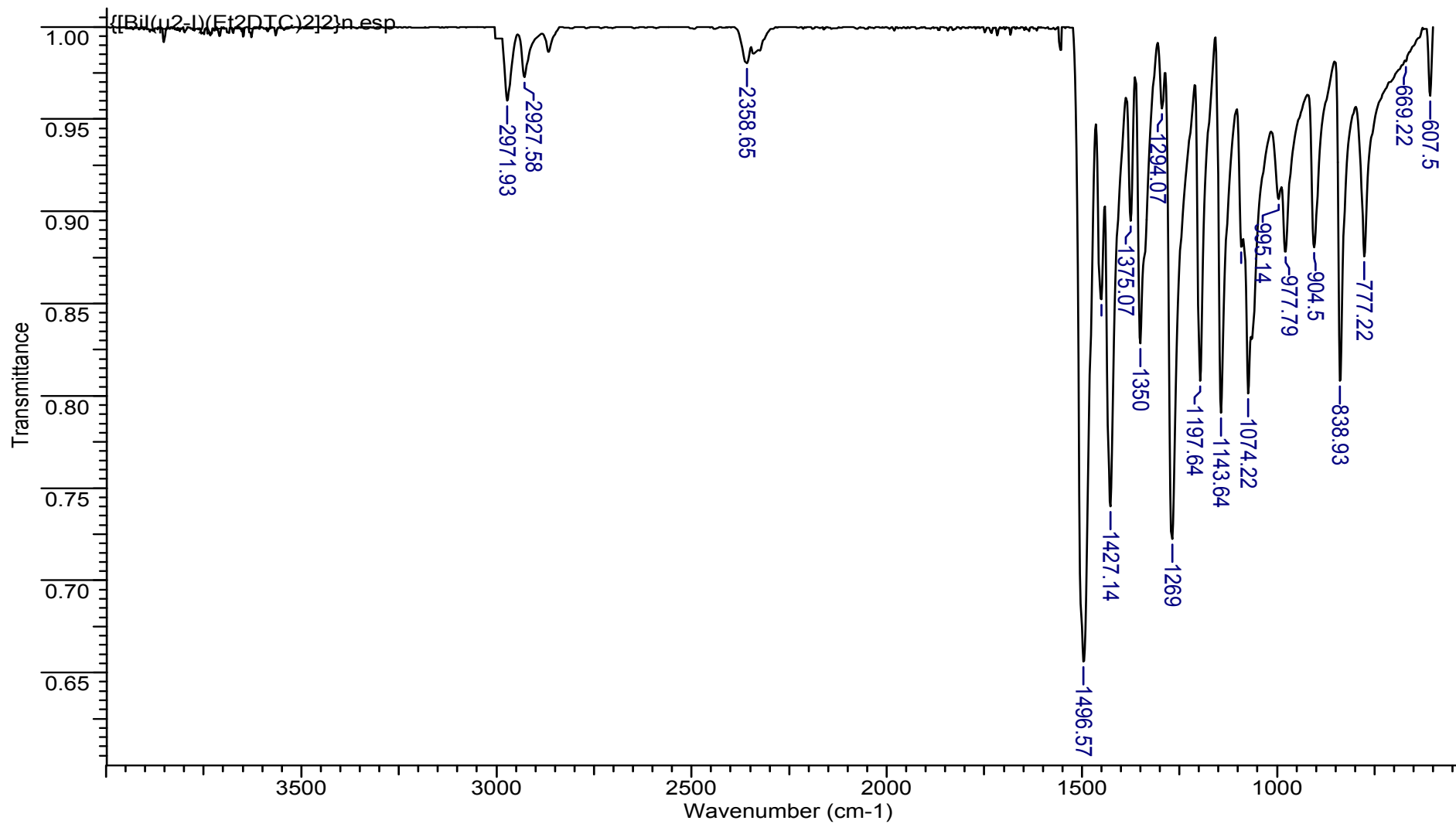


Figure S5. MID-IR spectrum of Complex 5 ($\{[\text{BiI}(\mu_2\text{-I})(\text{Et}_2\text{DTC})_2]_2\}_n$)

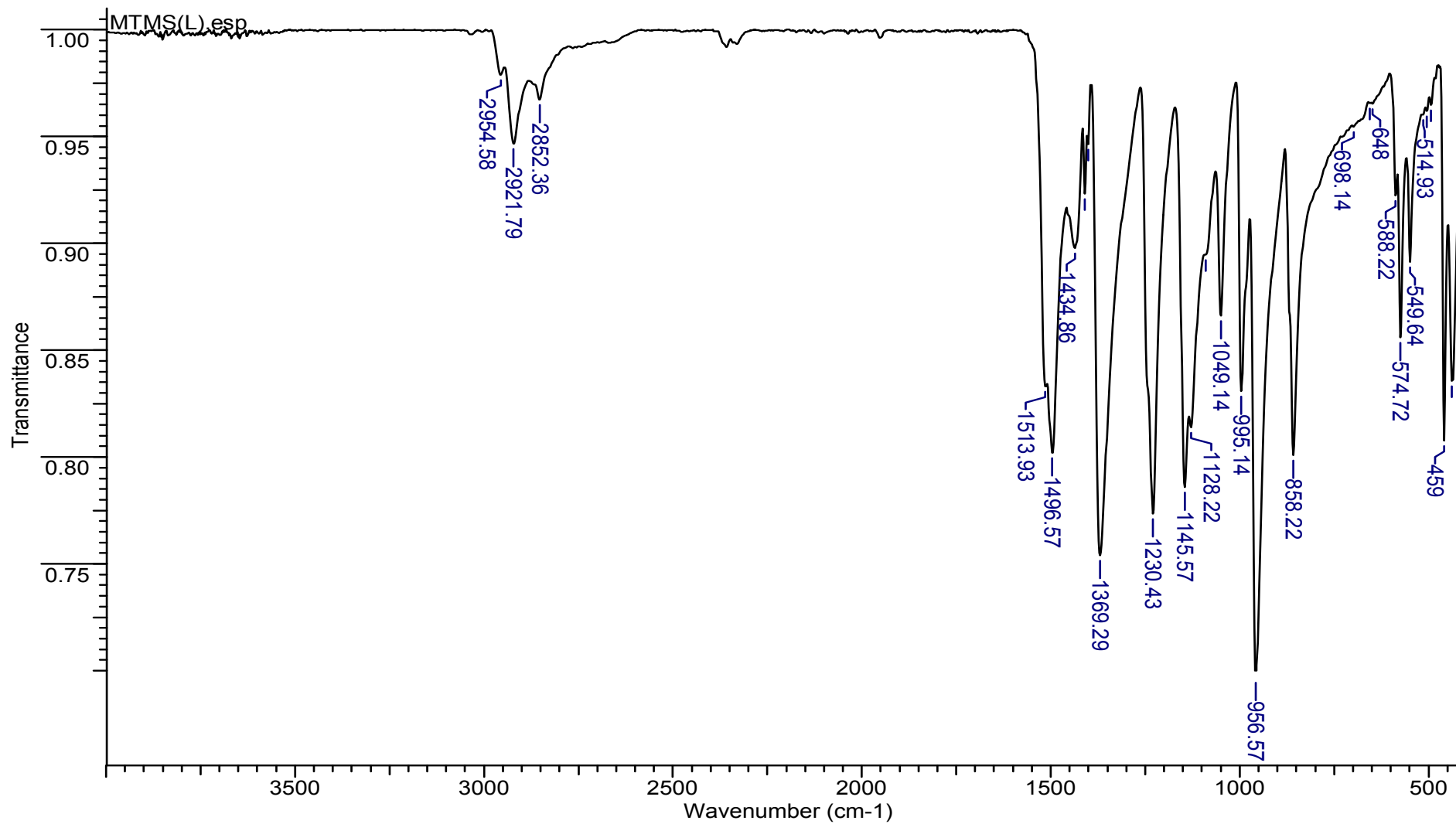


Figure S6. MID-IR spectrum of Tetramethylthiuram monosulfide (MTMS)

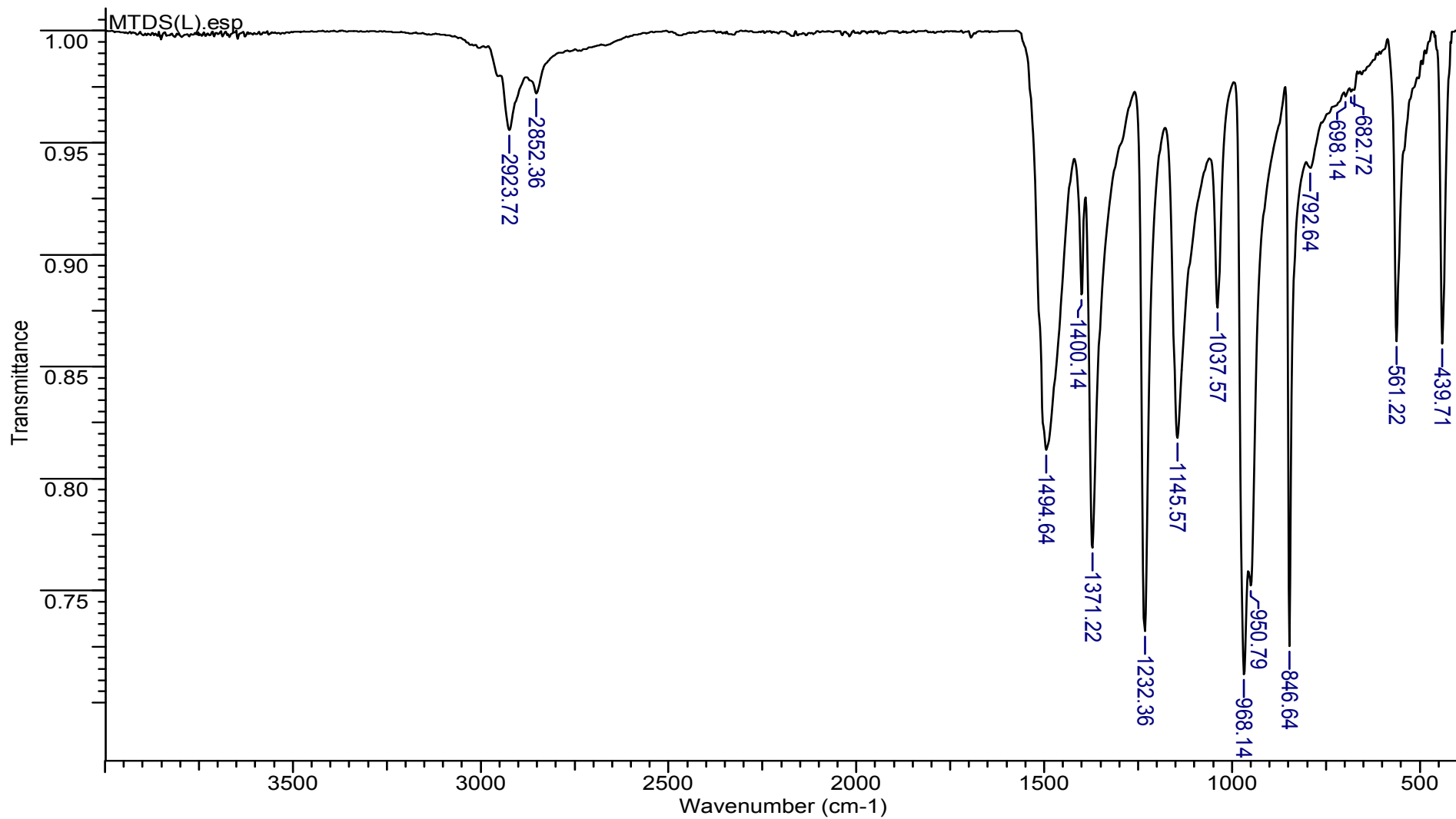


Figure S7. MID-IR spectrum of Tetramethylthiuram disulfide (MTDS)

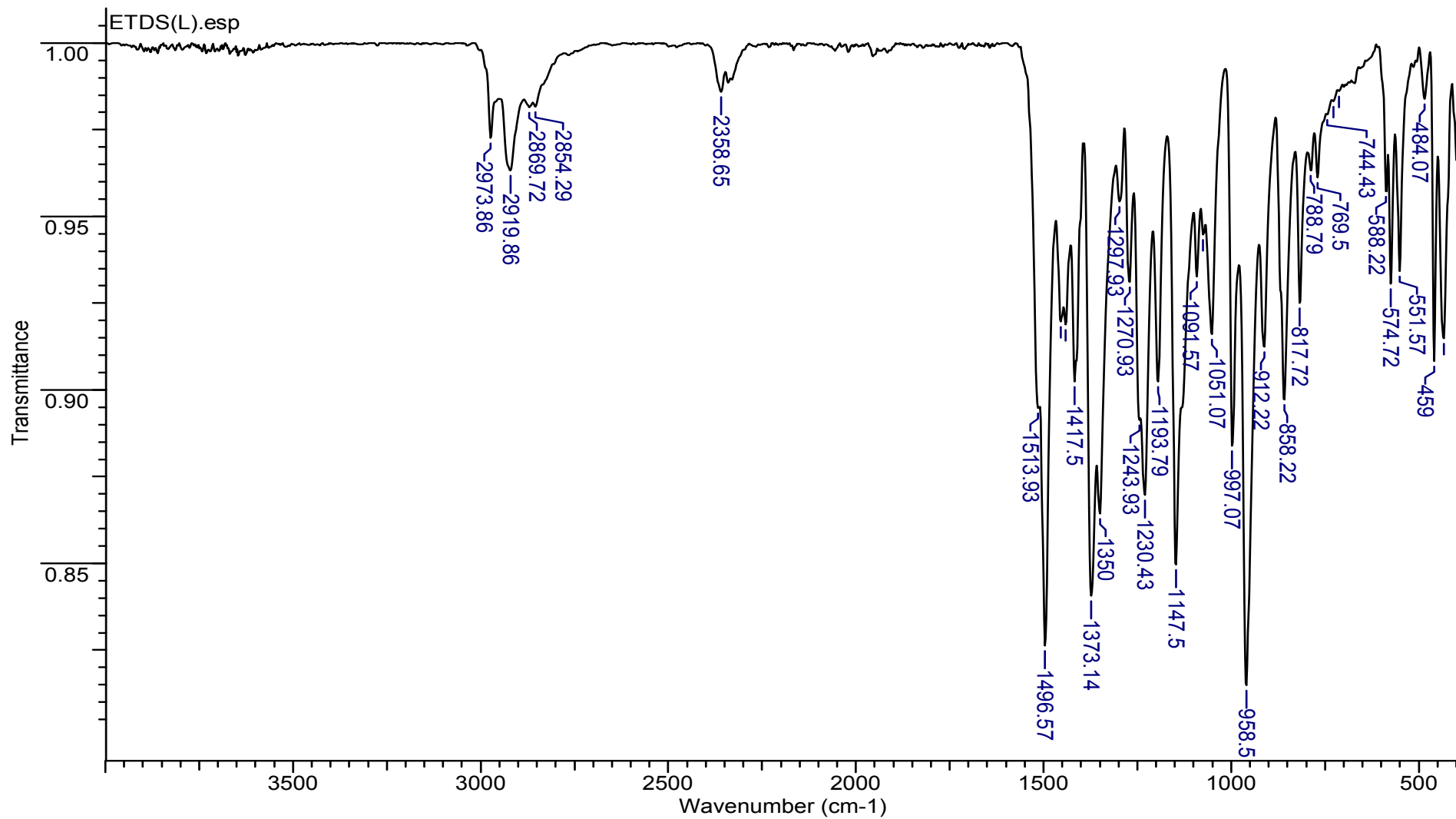


Figure S8. MID-IR spectrum of Tetraethylthiuram disulfide (ETDS)

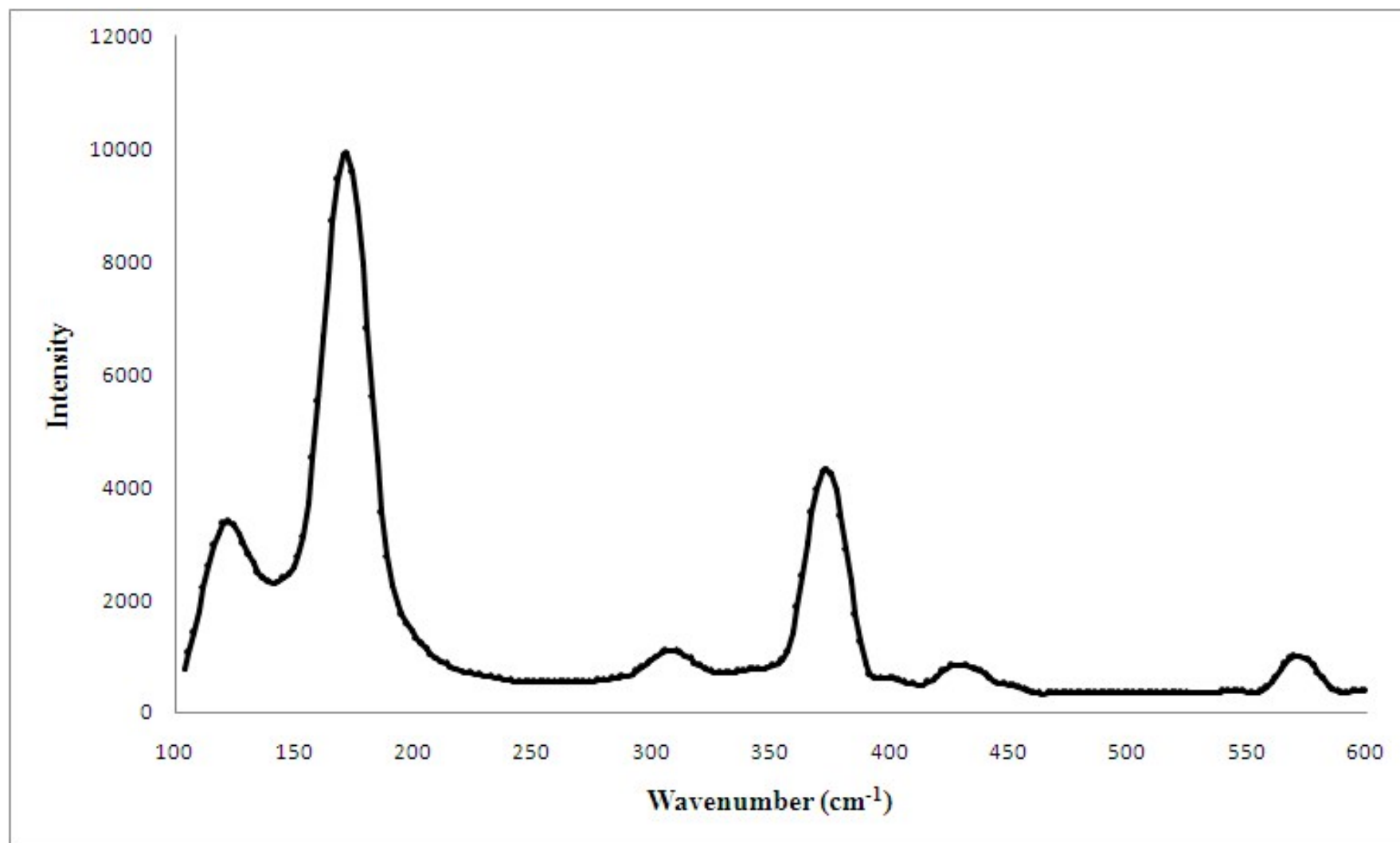


Figure S9. Raman spectrum of Complex 1 ($\{[\text{BiBr}(\text{Me}_2\text{DTC})_2]\}_n$)

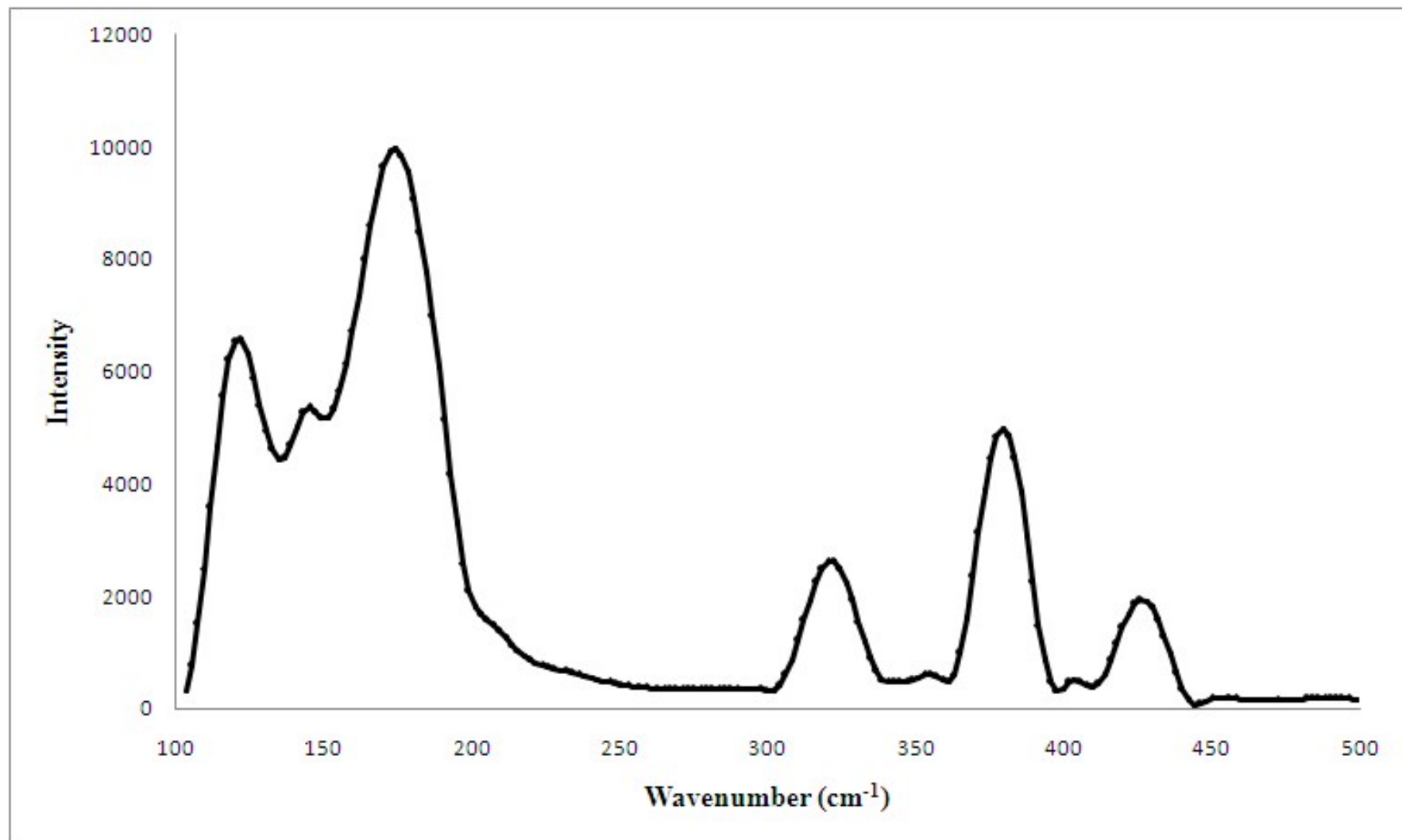


Figure S10. Raman spectrum of Complex 2 ($\{[\text{BiBr}_2(\text{Et}_2\text{DTC})]\}_n$)

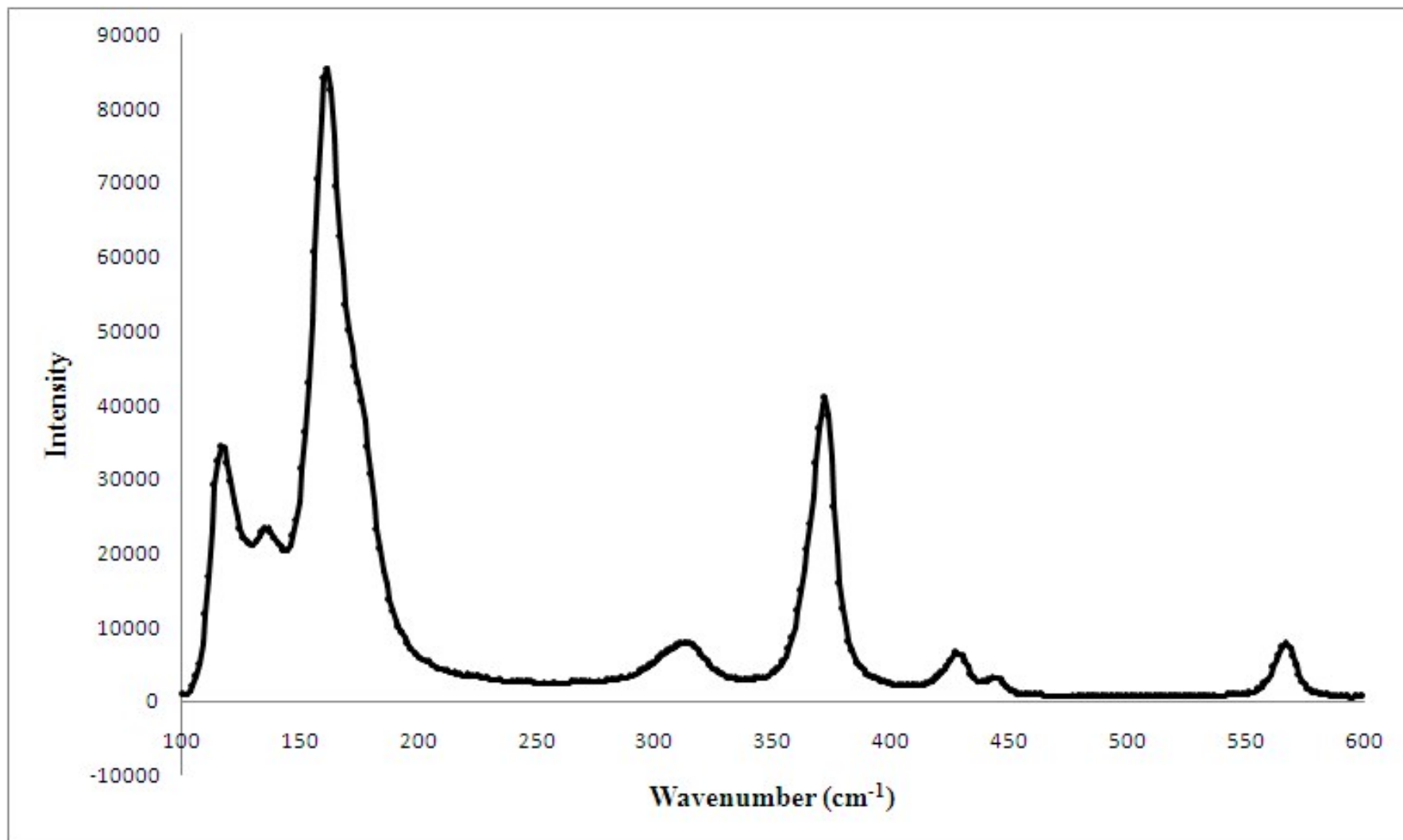


Figure S11. Raman spectrum of Complex 3 ($\{[\text{BiI}_2(\text{Me}_2\text{DTC})]\}_n$)

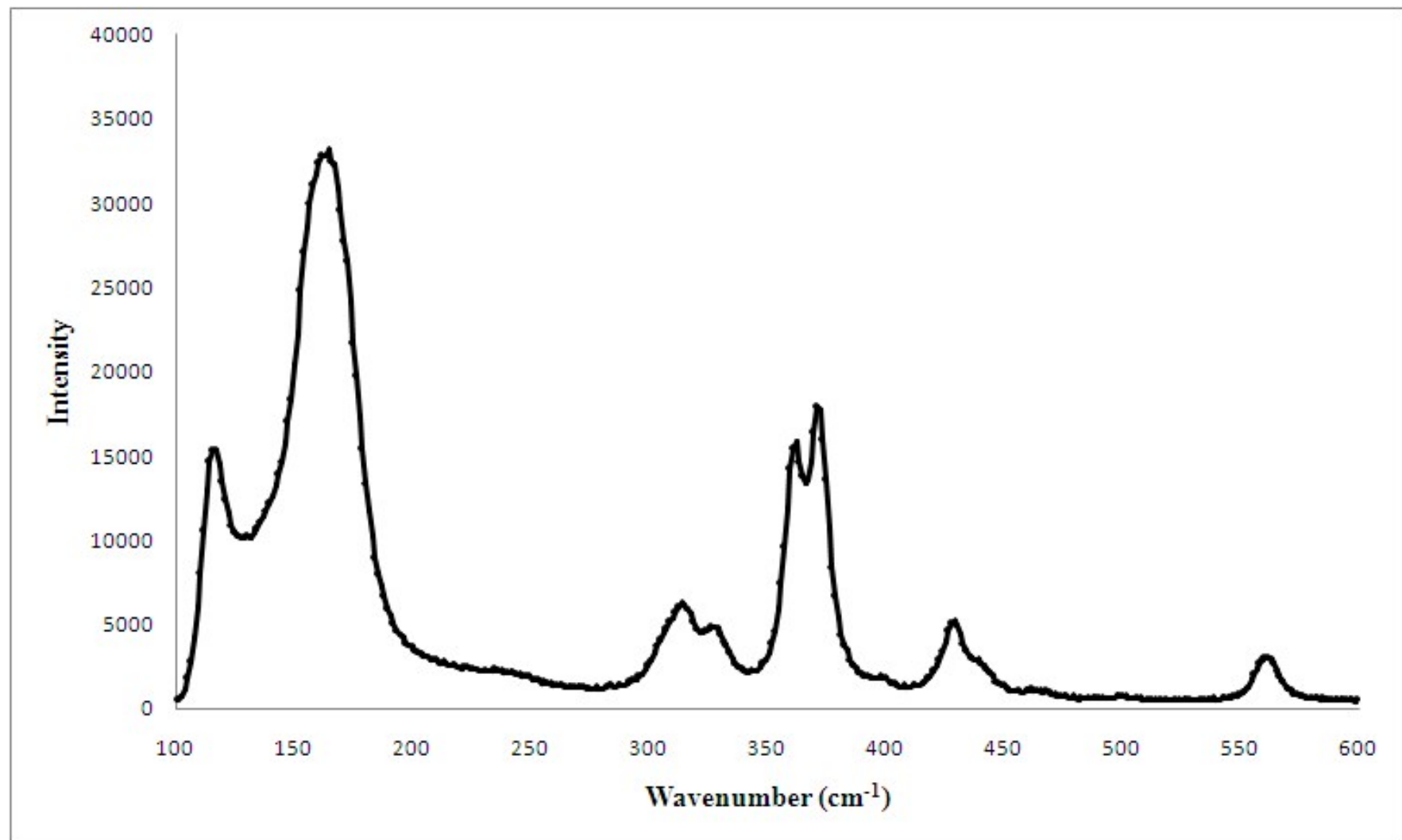


Figure S12. Raman spectrum of Complex 4 ($\{[\text{BiI}(\text{Et}_2\text{DTC})_2]\}_n$)

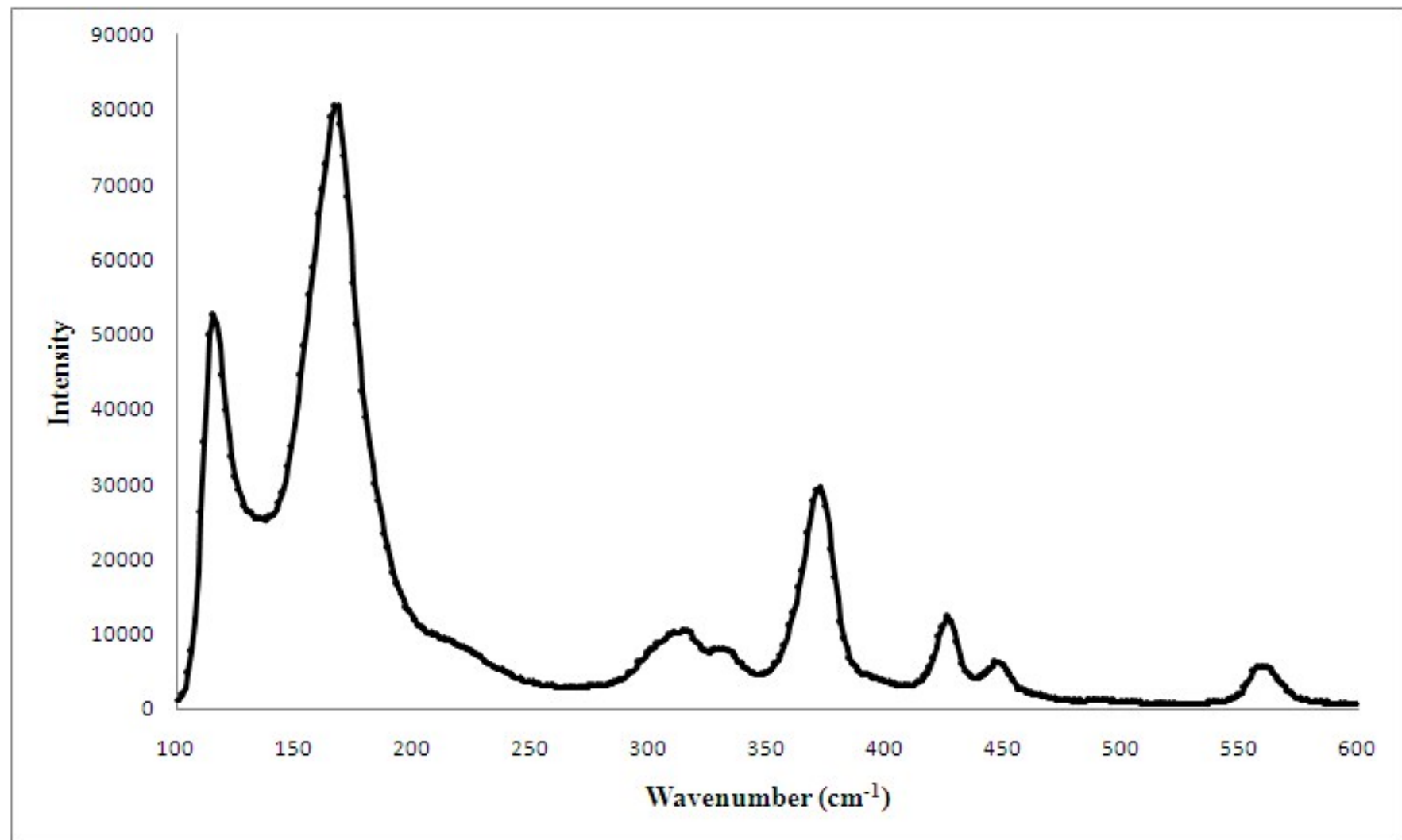


Figure S13. Raman spectrum of Complex 5 ($\{[\text{BiI}(\mu_2\text{-I})(\text{Et}_2\text{DTC})_2]_2\}_n$)

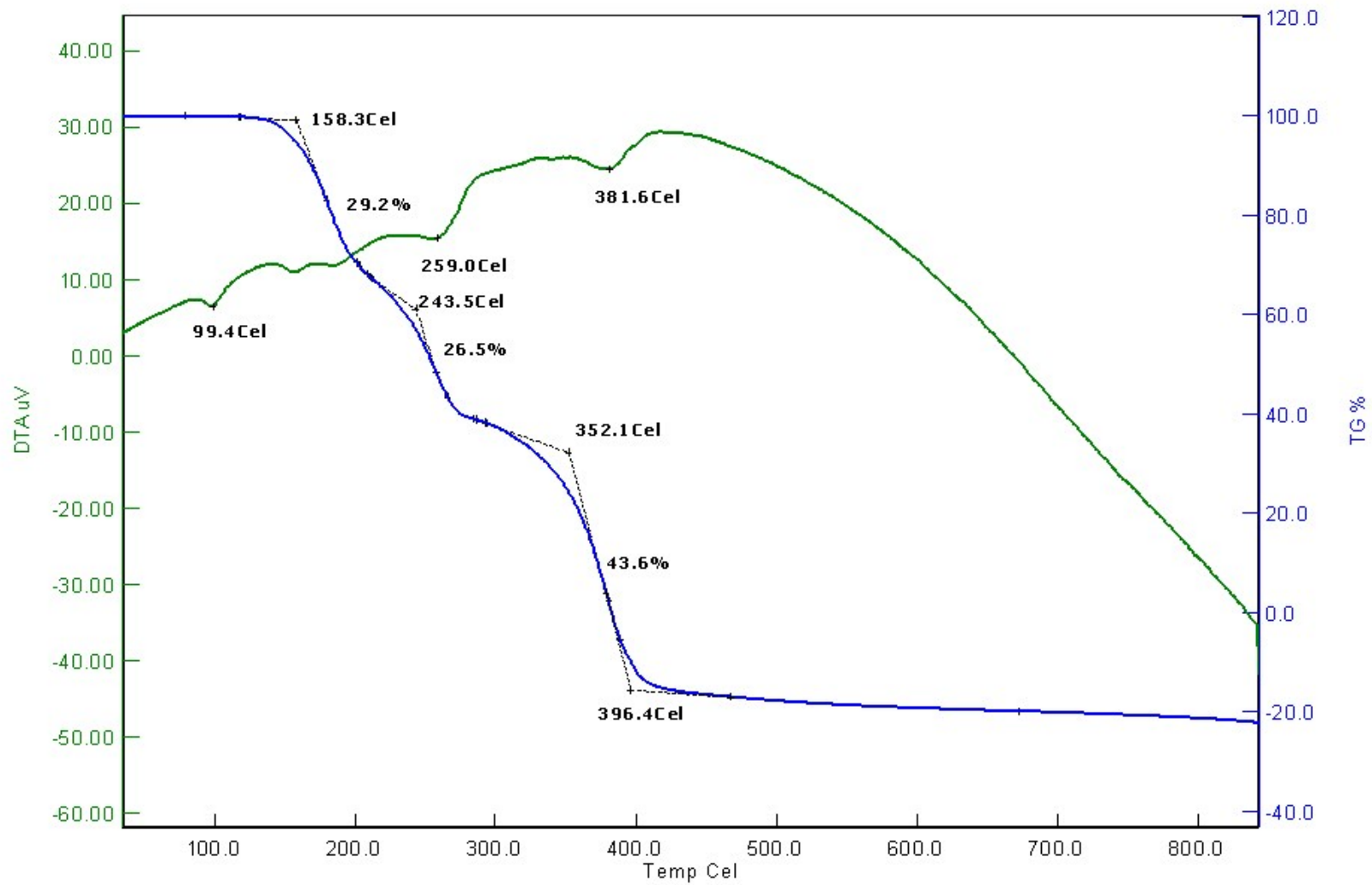


Figure S14. TG-DTA analysis of Complex 1 ($\{[\text{BiBr}(\text{Me}_2\text{DTC})_2]\}_n$)

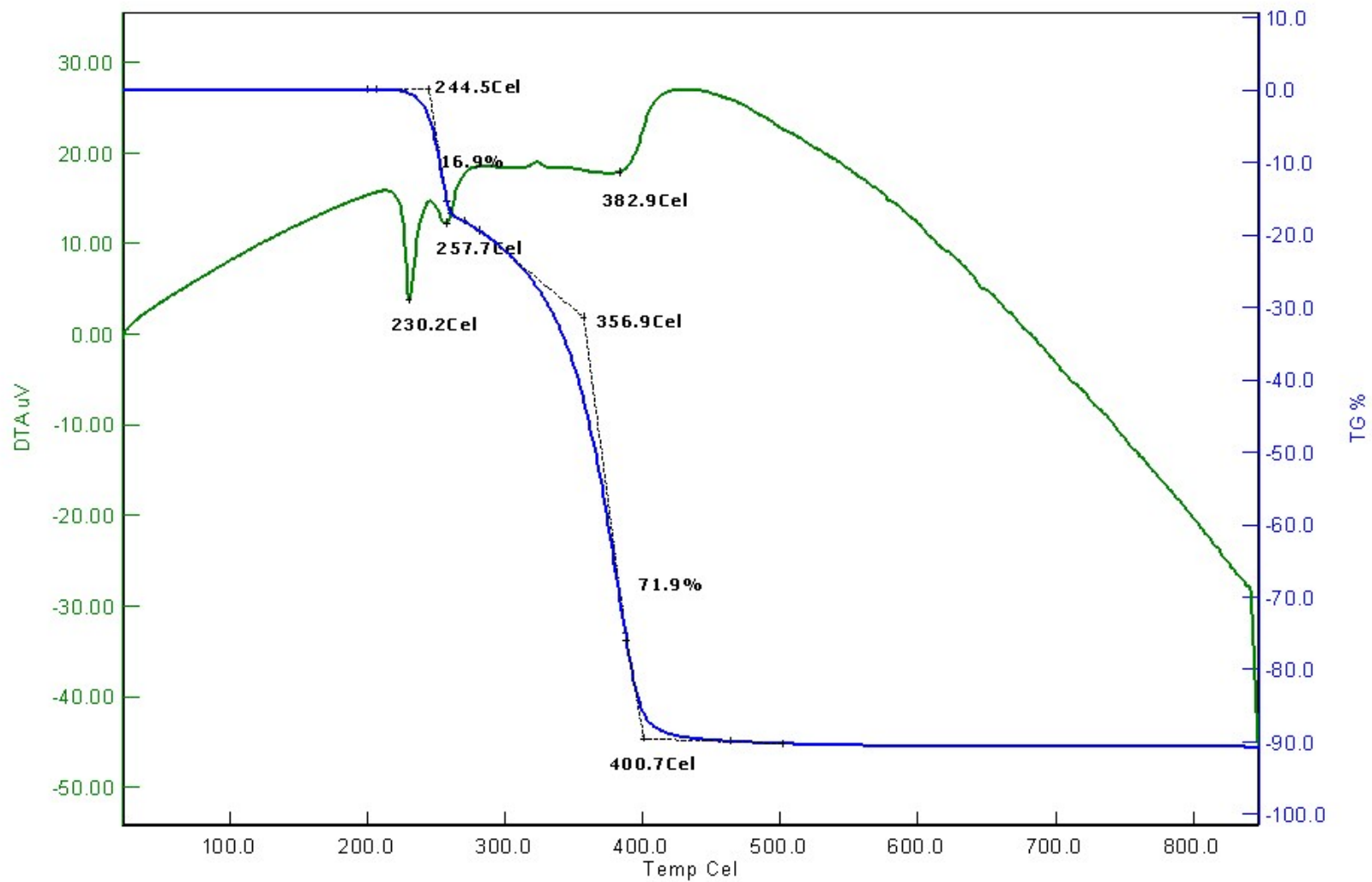


Figure S15. TG-DTA analysis of Complex 2 ($\{[\text{BiBr}_2(\text{Et}_2\text{DTC})]\}_n$)

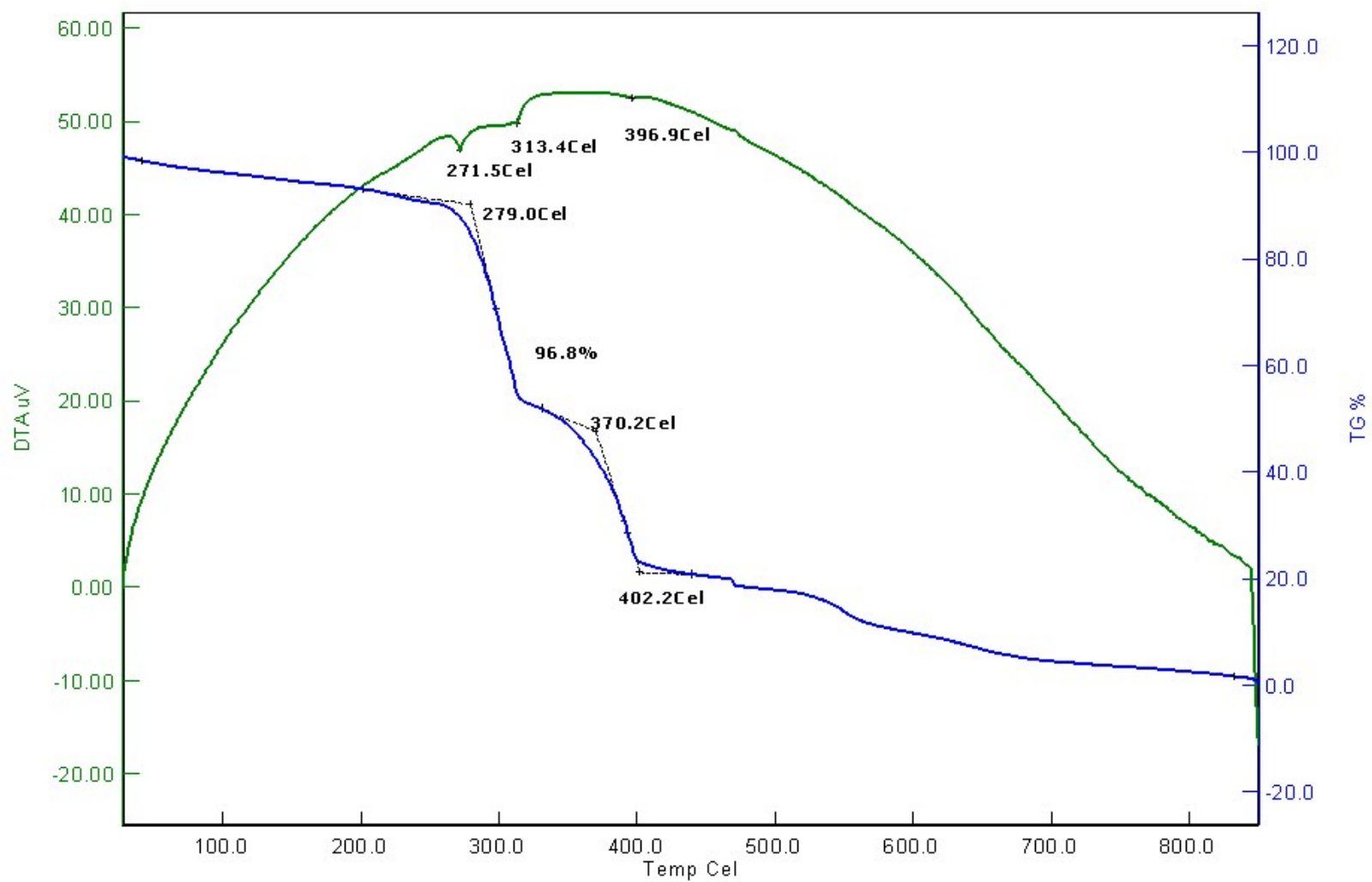


Figure S16. TG-DTA analysis of Complex 3 ($\{[\text{BiI}_2(\text{Me}_2\text{DTC})]\}_n$)

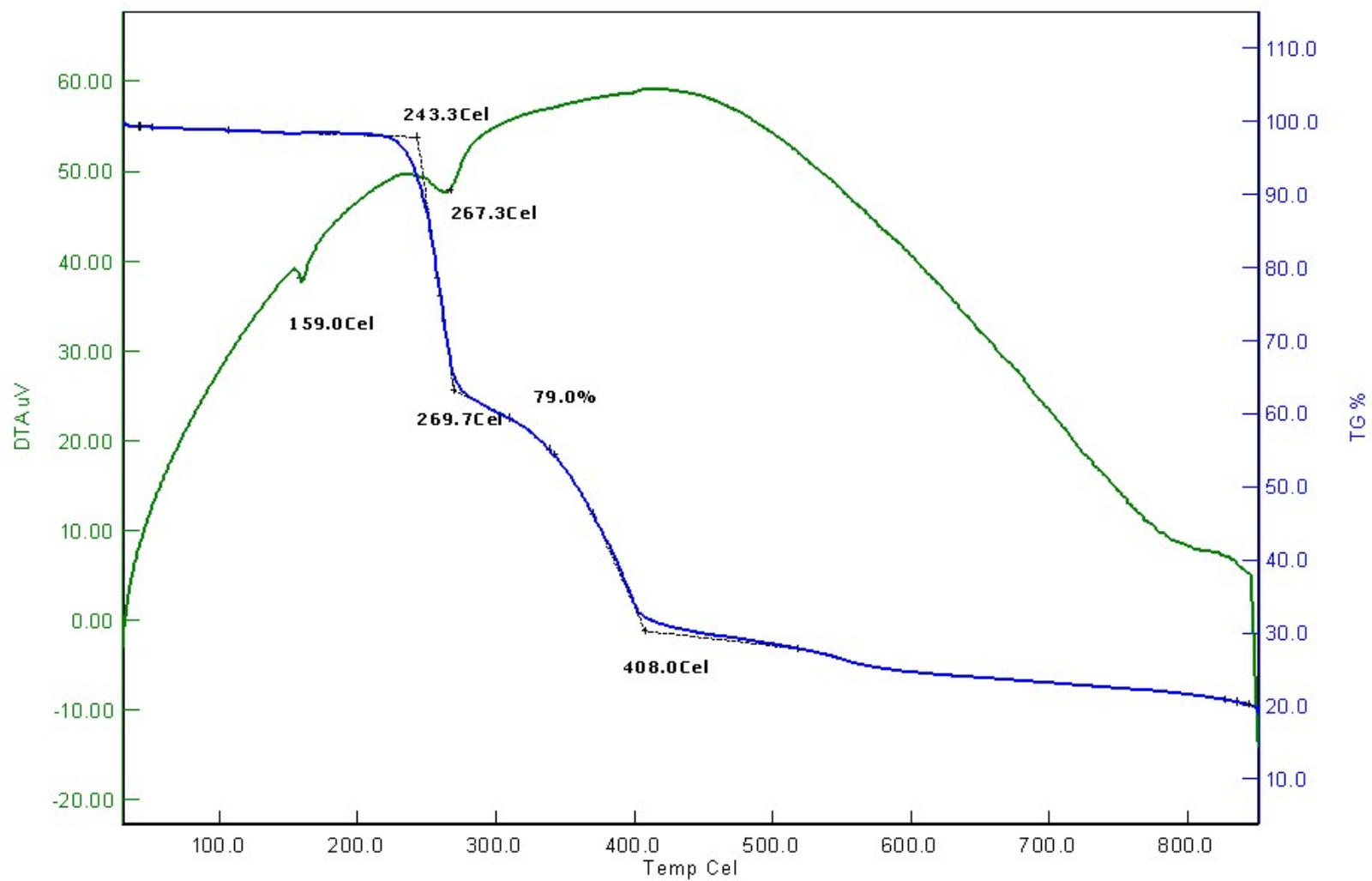


Figure S17. TG-DTA analysis of Complex 4 ($\{[\text{BiI}(\text{Et}_2\text{DTC})_2]\}_n$)

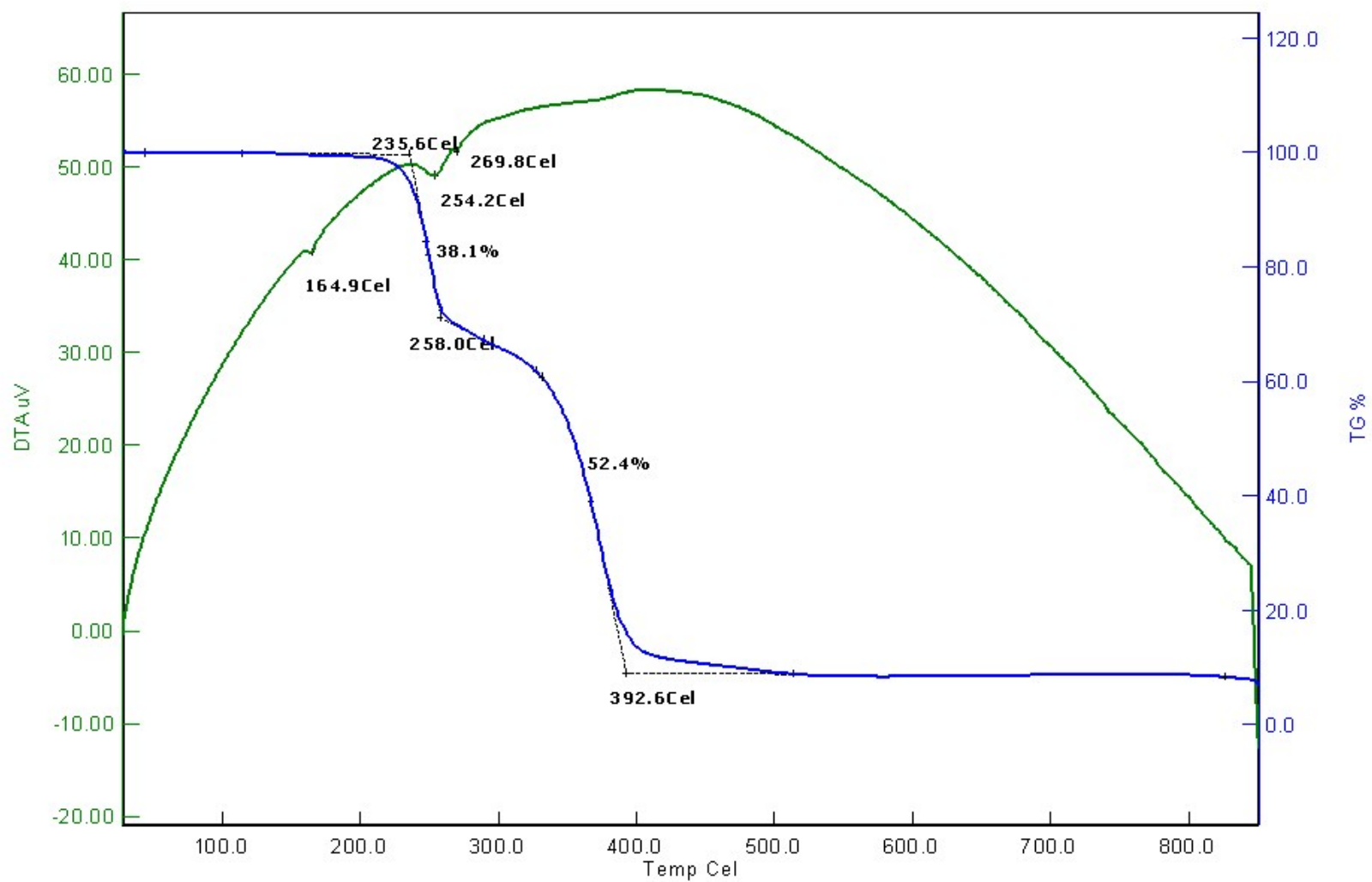


Figure S18. TG-DTA analysis of Complex 5 ($\{[\text{BiI}(\mu_2\text{-I})(\text{Et}_2\text{DTC})_2]_2\}_n$)

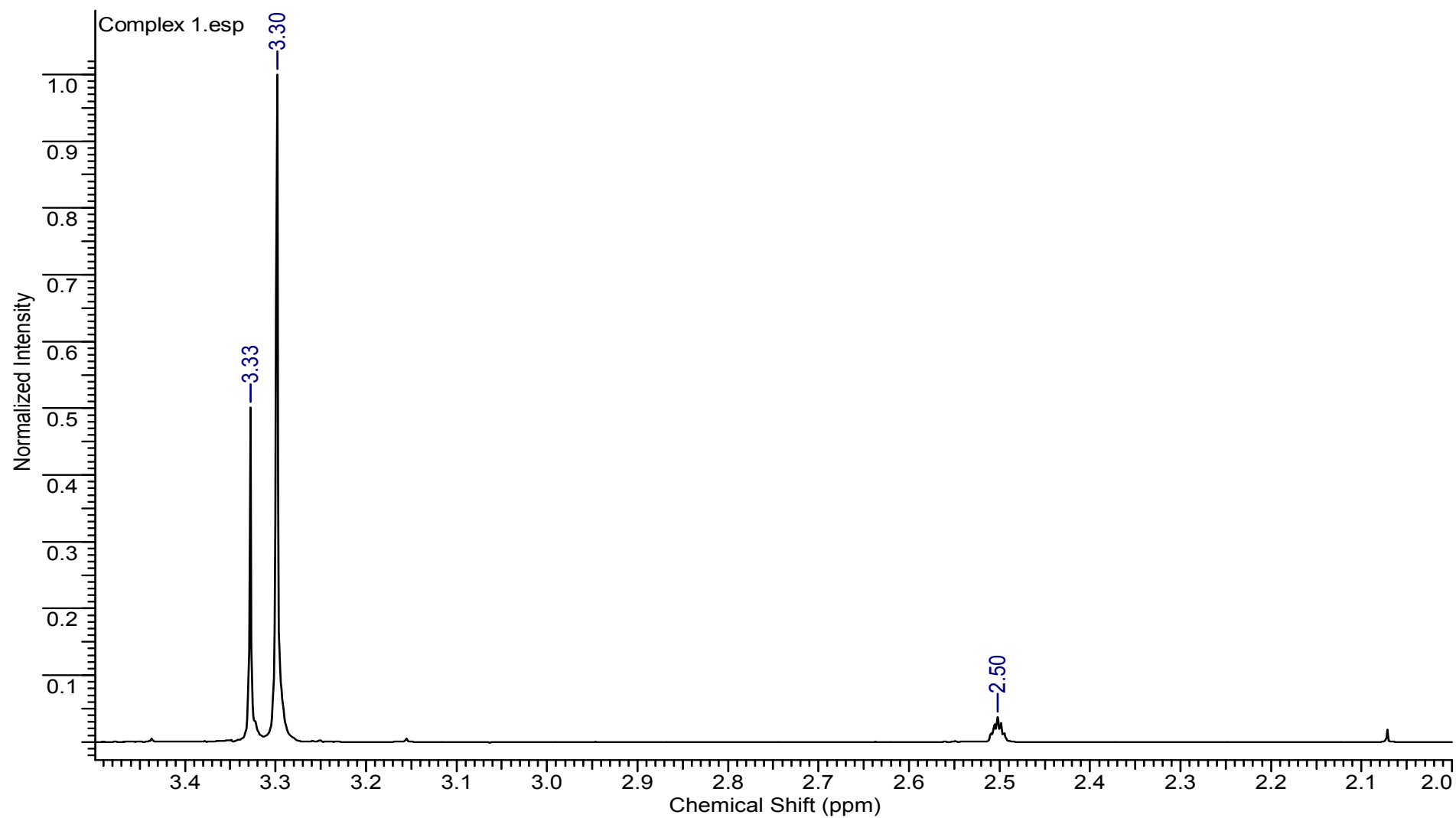


Figure S19. $^1\text{H-NMR}$ spectrum of Complex 1 ($\{[\text{BiBr}(\text{Me}_2\text{DTC})_2]\}_n$)

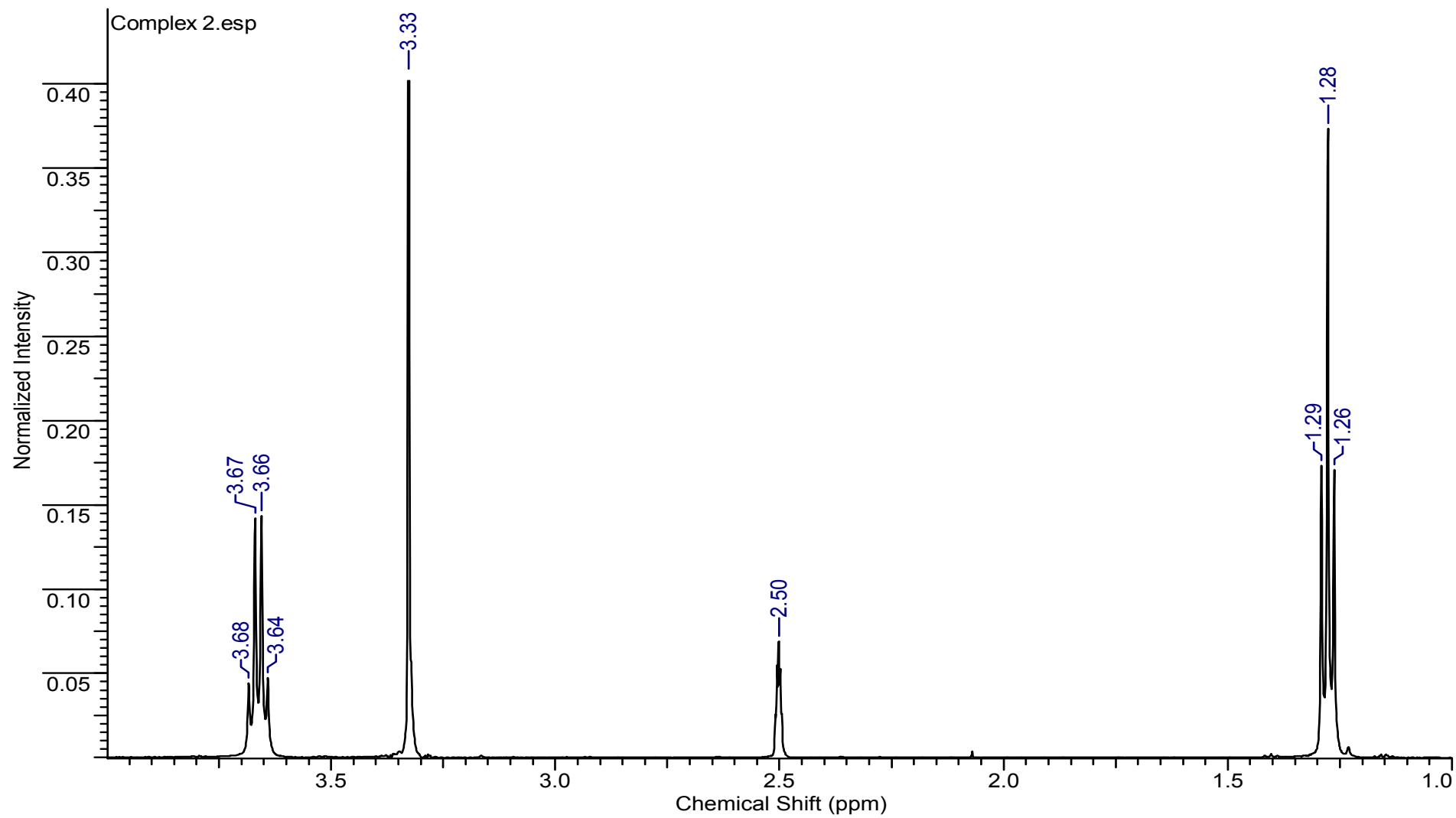


Figure S20. ¹H-NMR spectrum of Complex 2 ($\{[\text{BiBr}_2(\text{Et}_2\text{DTC})]\}_n$)

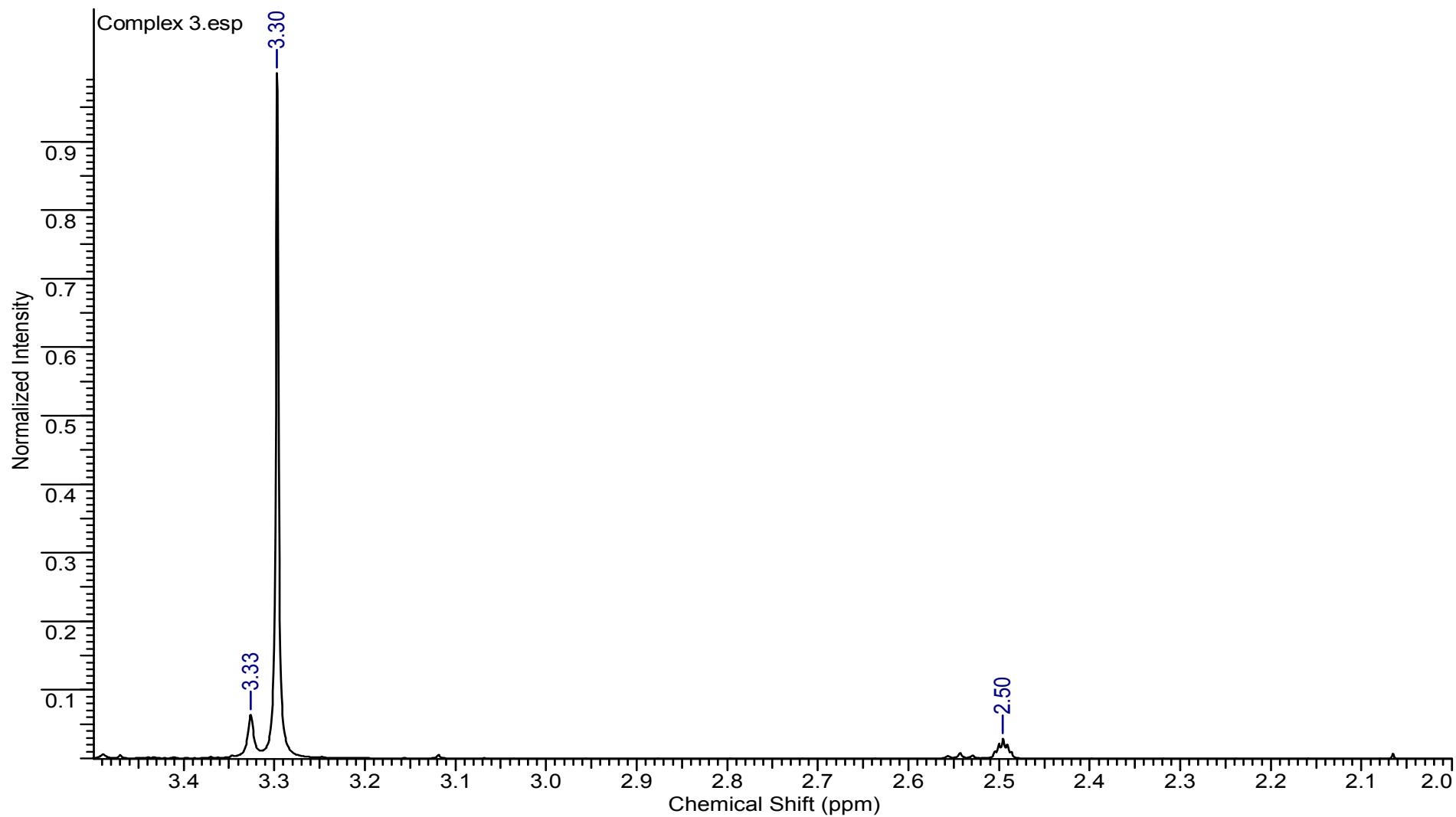


Figure S21. ¹H-NMR spectrum of Complex 3 ($\{[\text{BiI}_2(\text{Me}_2\text{DTC})]\}_n$)

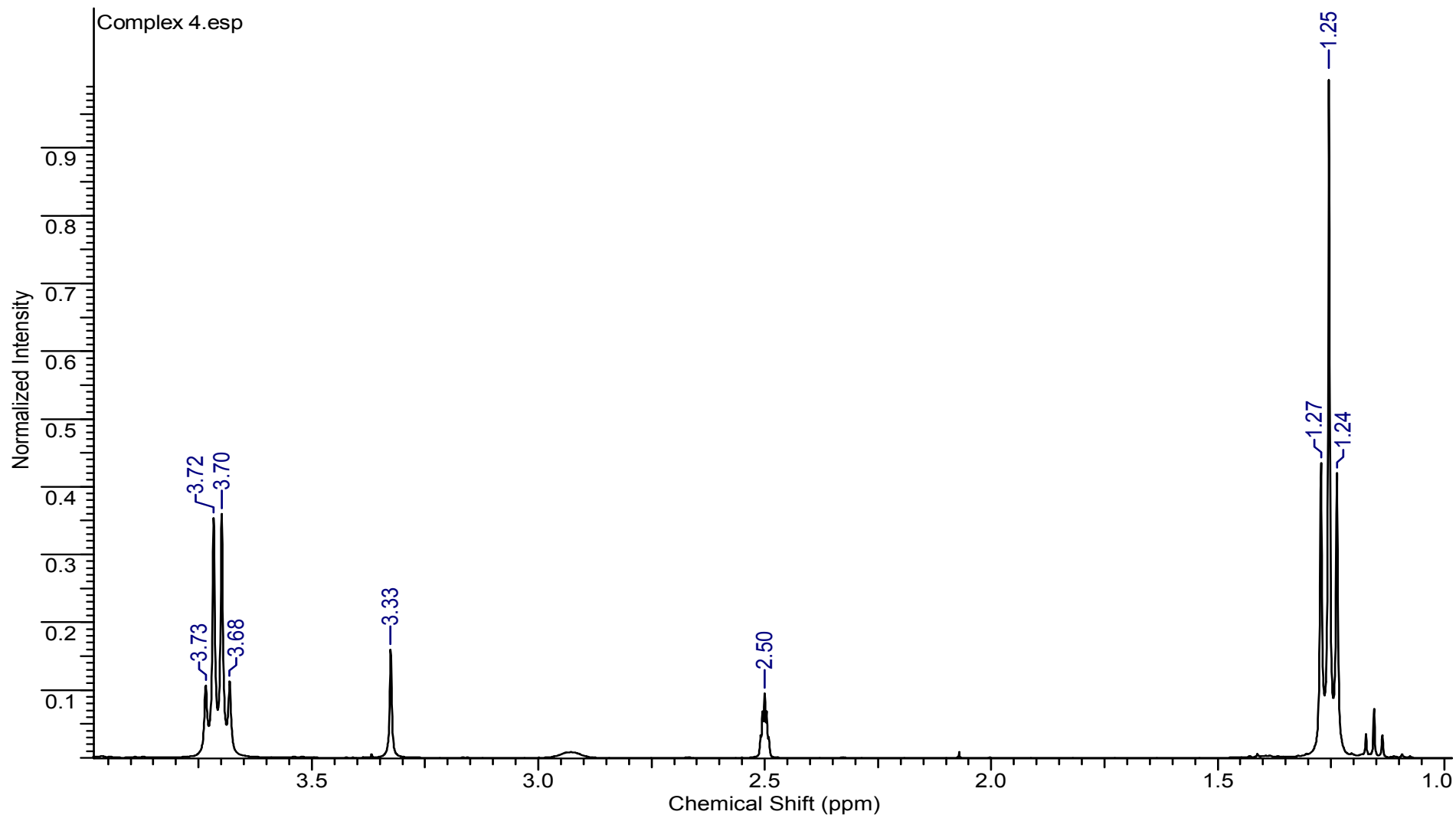


Figure S22. ^1H -NMR spectrum of Complex 4 ($\{[\text{Bi}(\text{Et}_2\text{DTC})_2]\}_n$)

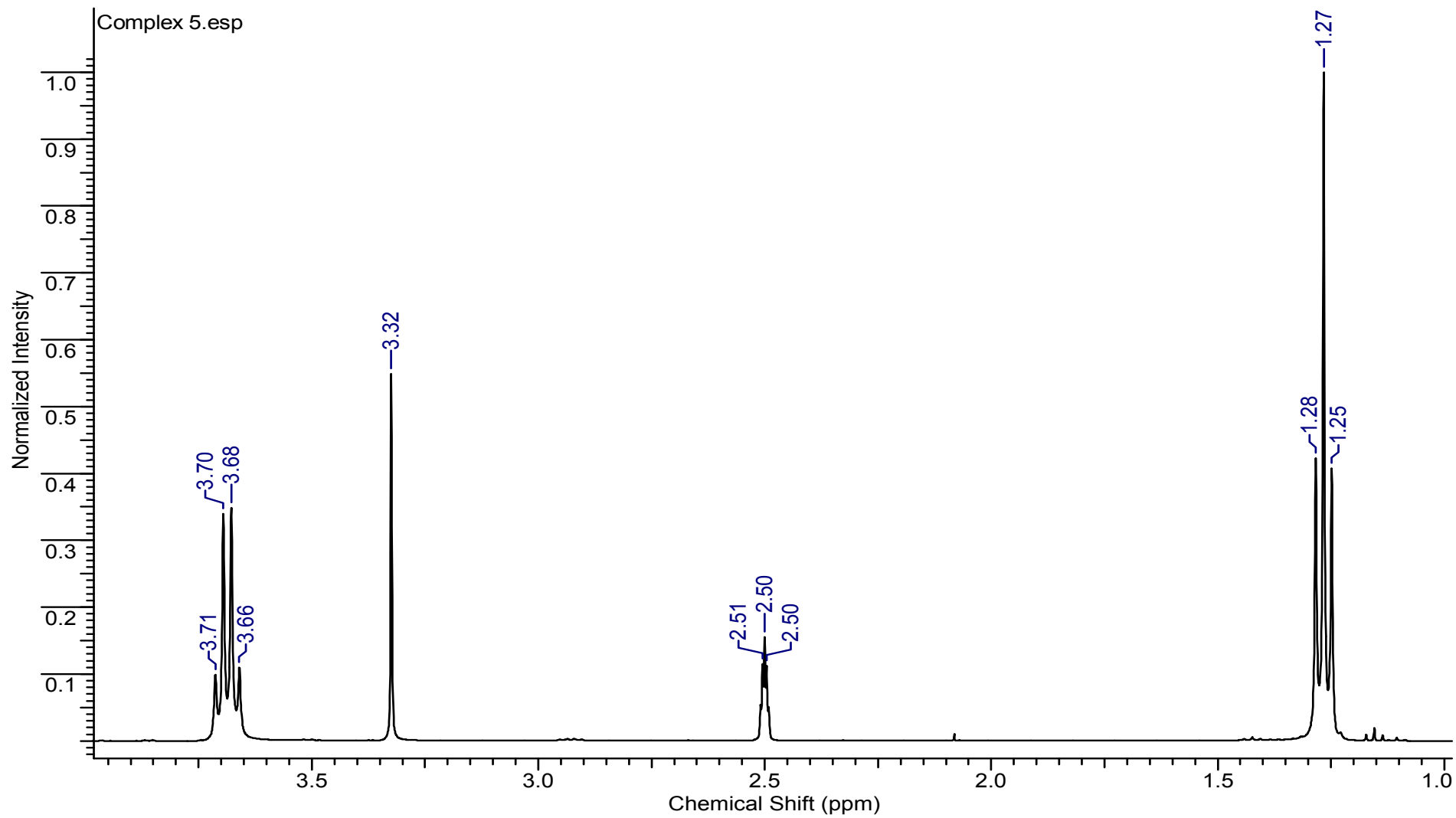


Figure S23. ^1H -NMR spectrum of Complex **5** ($\{[\text{BiI}(\mu_2\text{-I})(\text{Et}_2\text{DTC})_2]_2\}_n$)

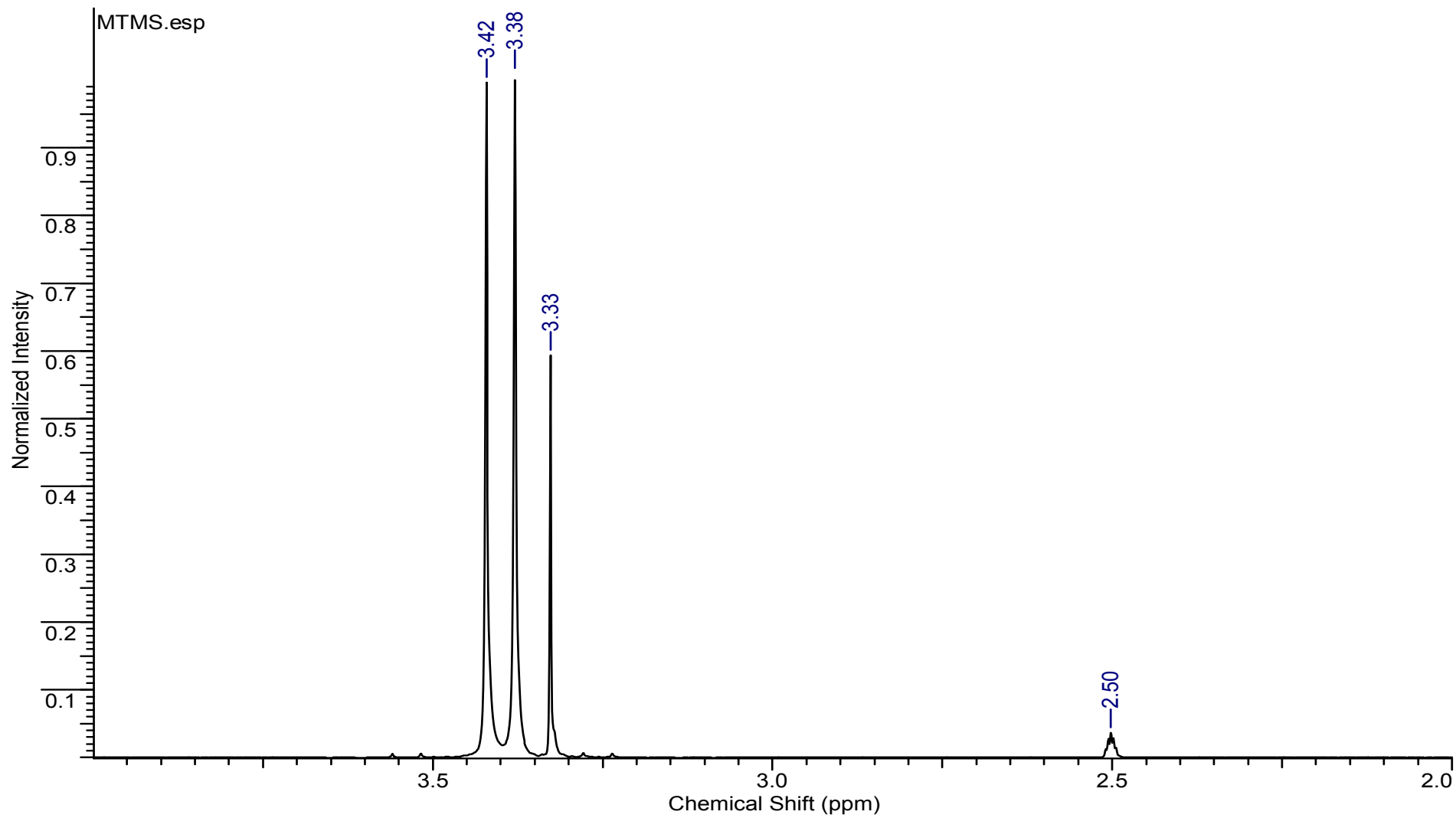


Figure S24. $^1\text{H-NMR}$ spectrum of *Tetramethylthiuram monosulfide* (MTMS)

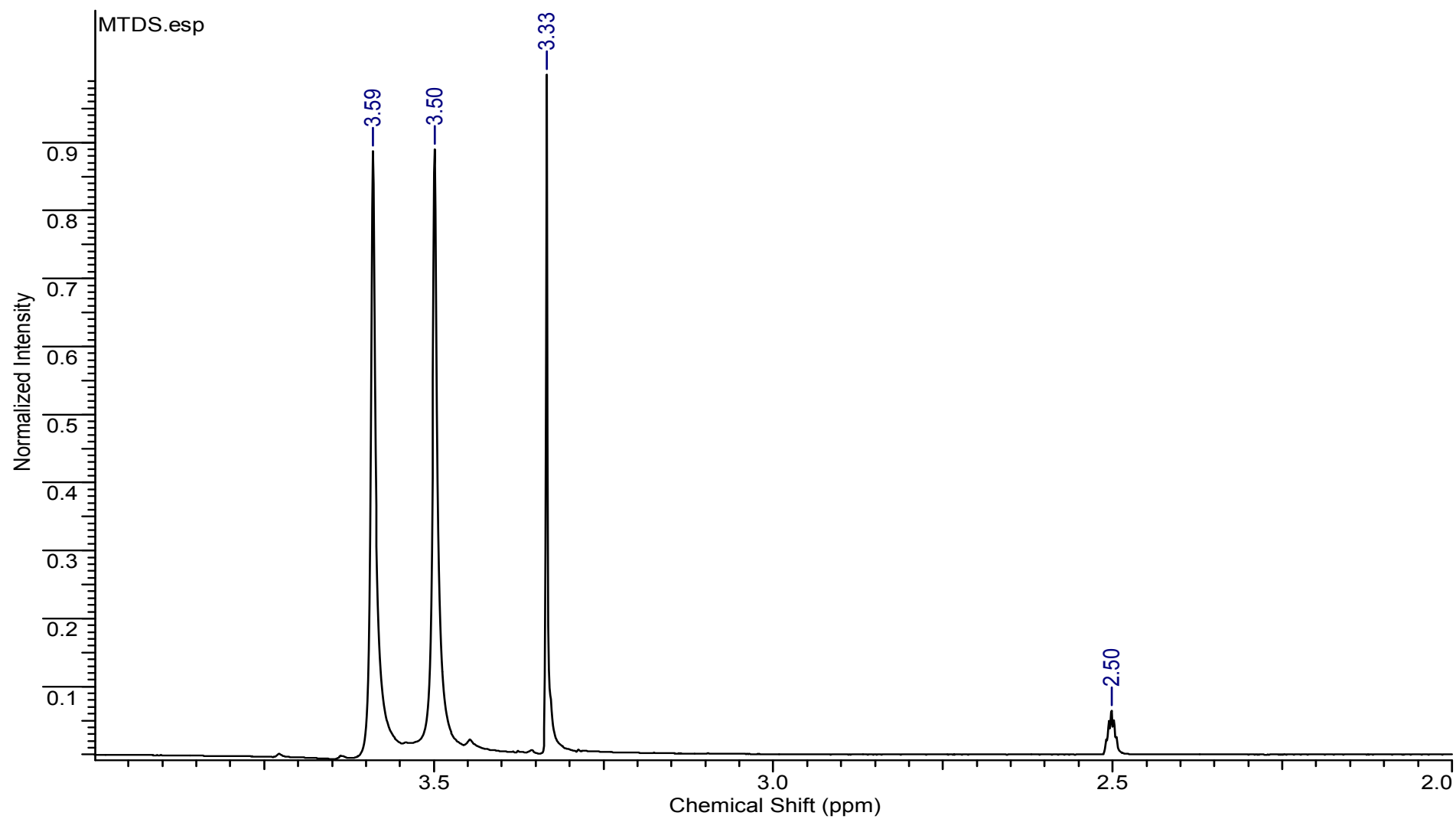


Figure S25. ¹H-NMR spectrum of *Tetramethylthiuram disulfide* (MTDS)

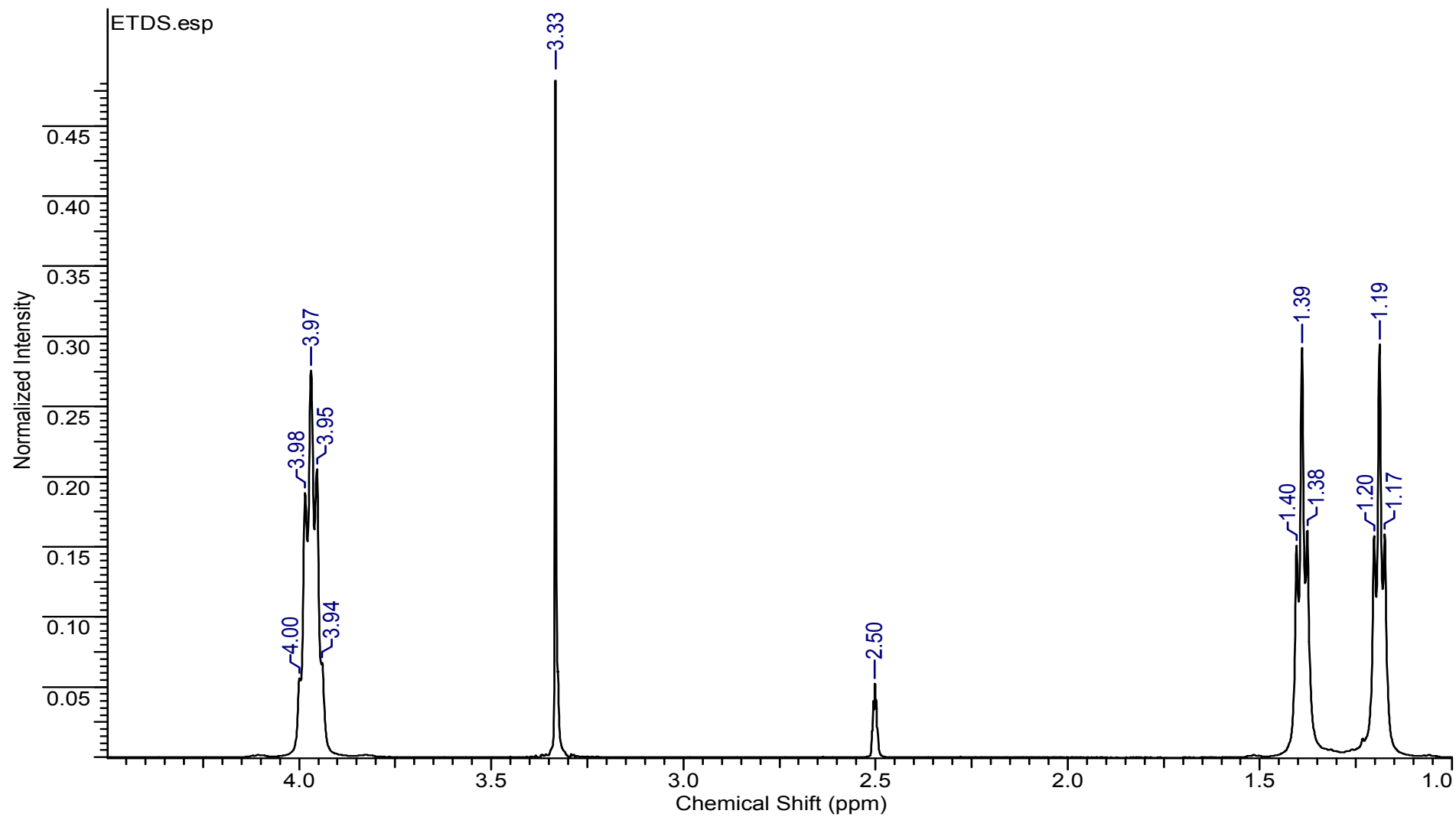


Figure S26. ¹H-NMR spectrum of Tetraethylthiuram disulfide (ETDS)

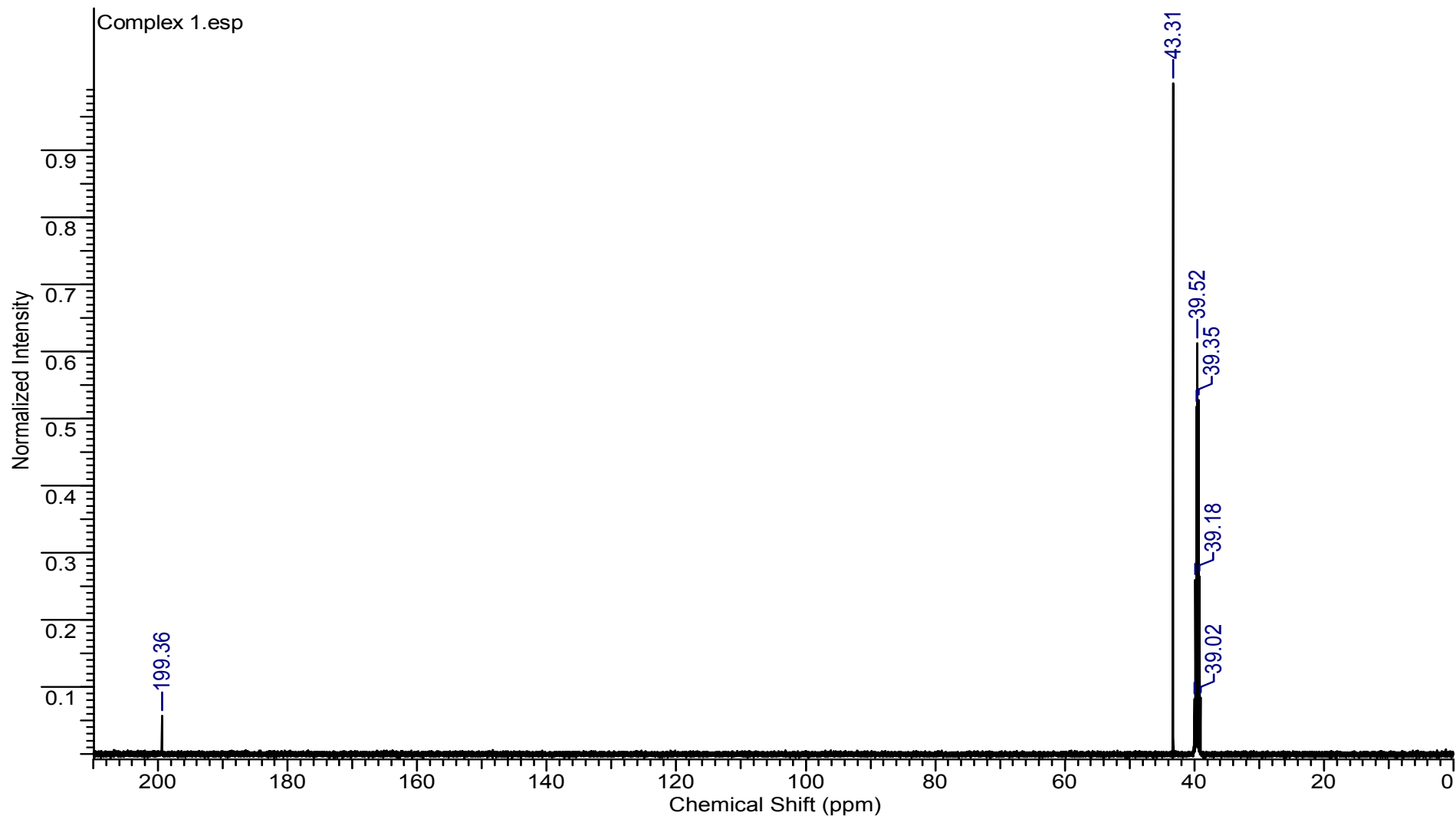


Figure S27. ^{13}C -NMR spectrum of Complex 1 ($\{\{\text{BiBr}(\text{Me}_2\text{DTC})_2\}\}_n$)

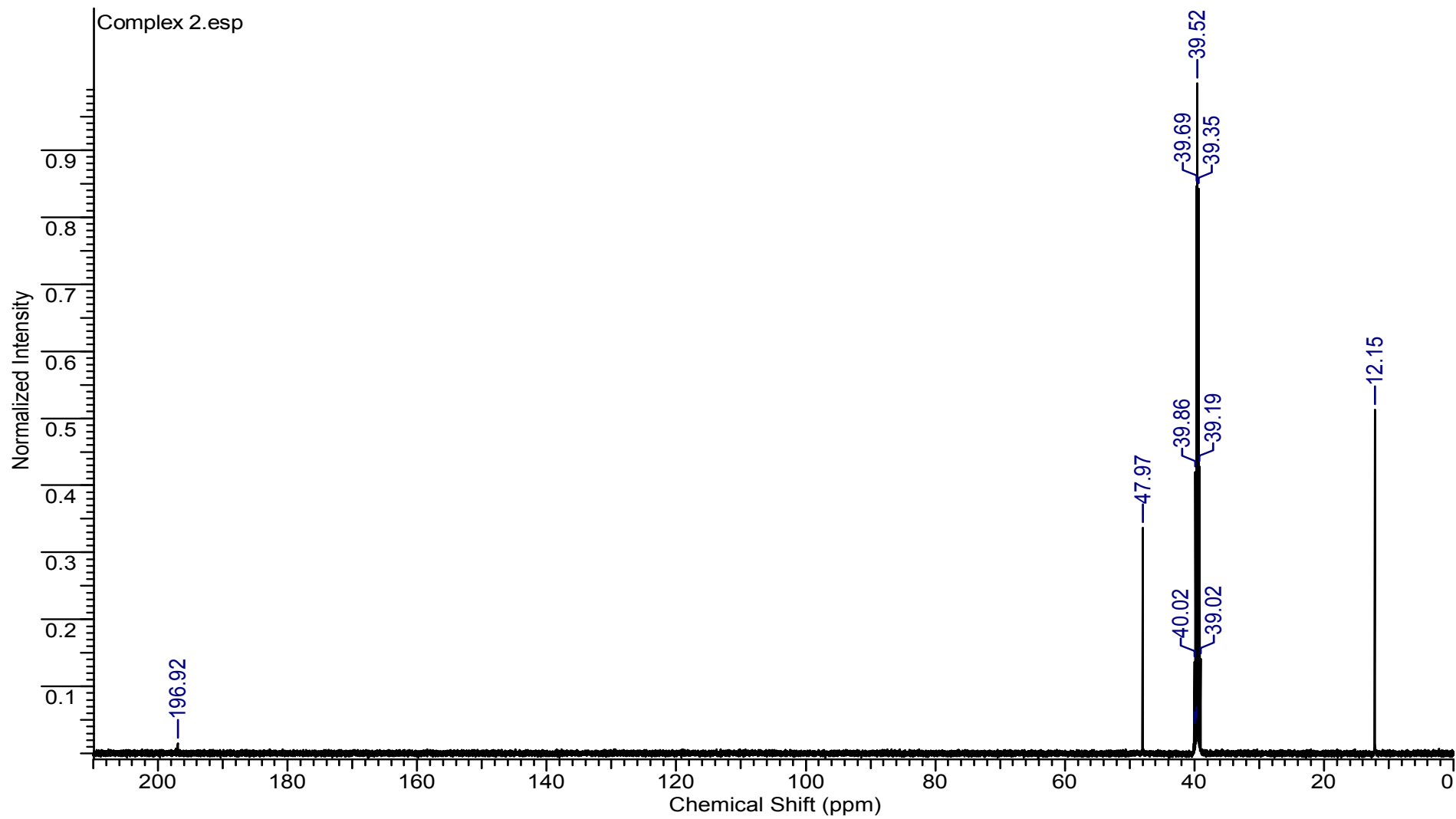


Figure S28. ^{13}C -NMR spectrum of Complex 2 ($\{[\text{BiBr}_2(\text{Et}_2\text{DTC})]\}_n$)

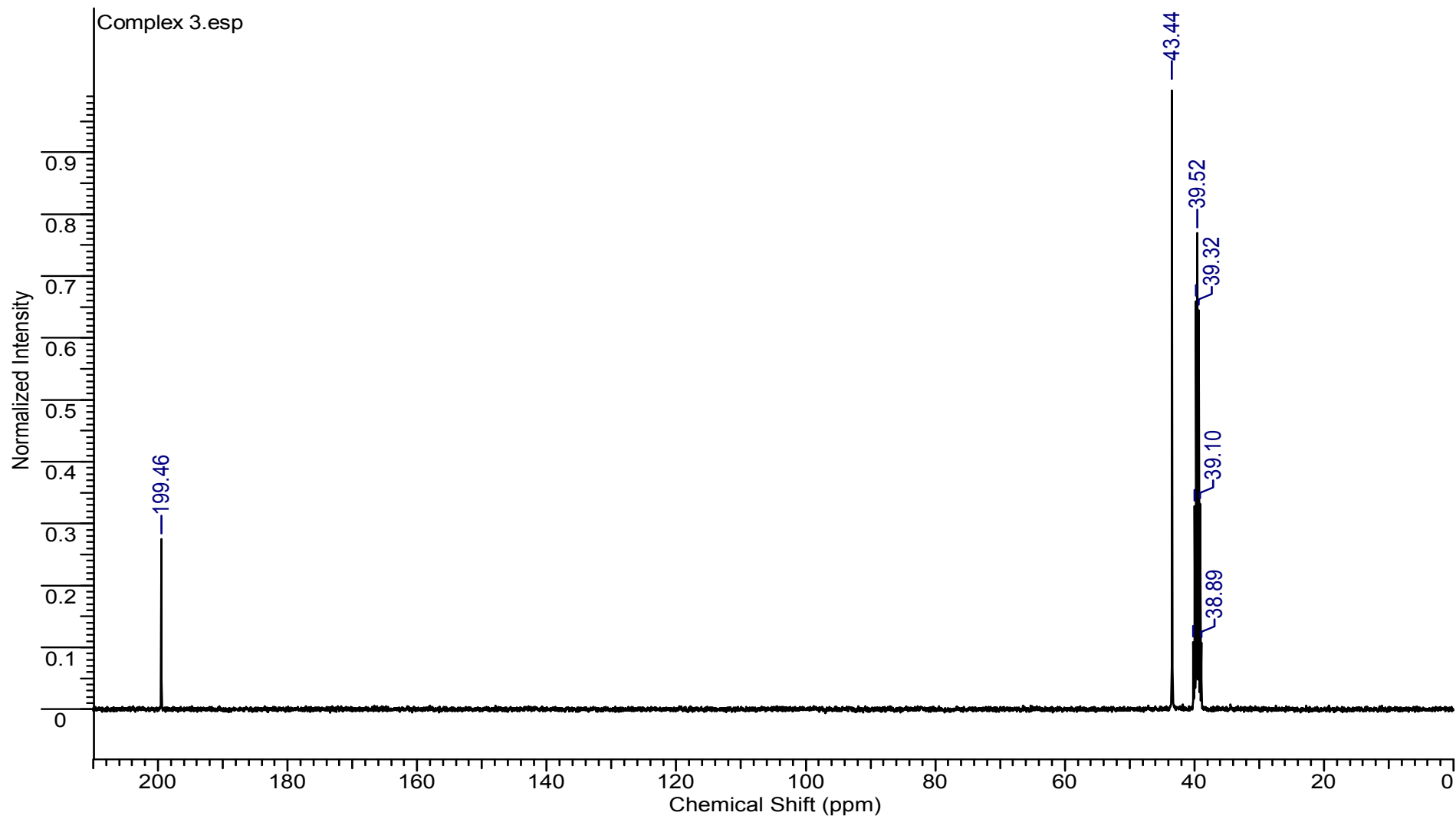


Figure S29. ^{13}C -NMR spectrum of Complex 3 ($\{\{\text{BiI}_2(\text{Me}_2\text{DTC})\}_n\}$)

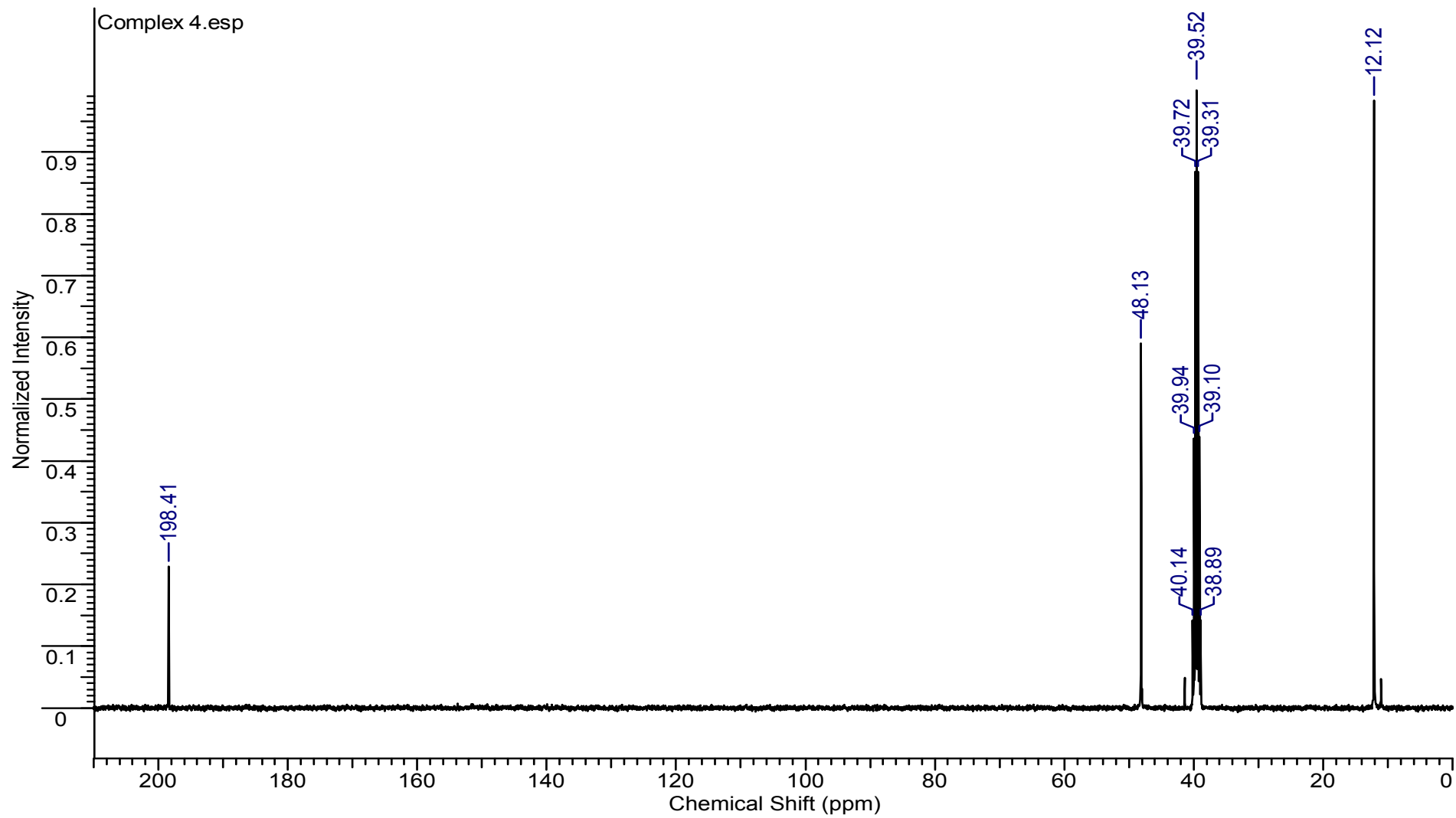


Figure S30. ^1H -NMR spectrum of Complex 4 ($\{[\text{Bi}(\text{Et}_2\text{DTC})_2]\}_n$)

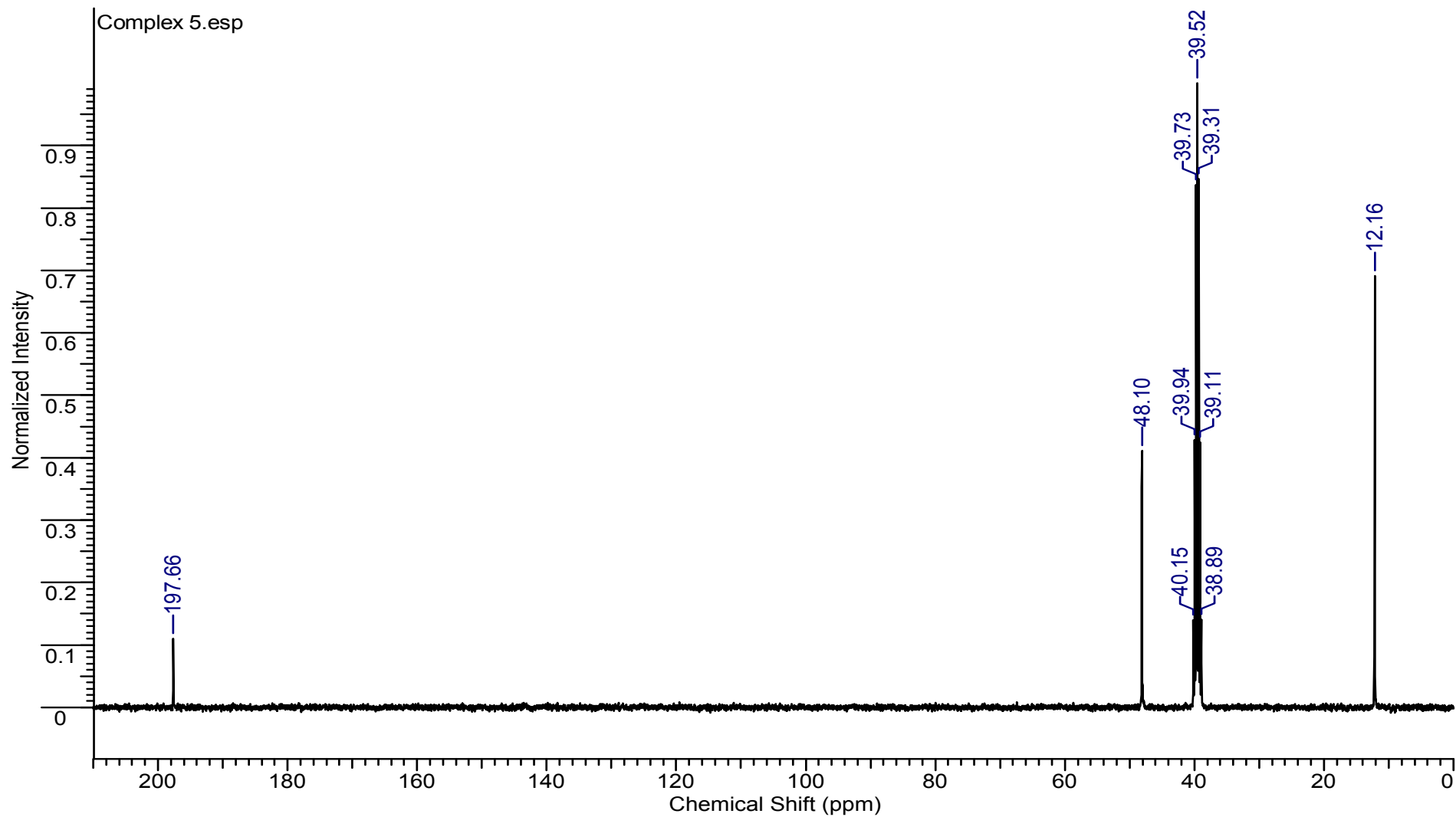


Figure S31. ^{13}C -NMR spectrum of Complex 5 ($\{[\text{BiI}(\mu_2\text{-I})(\text{Et}_2\text{DTC})_2]_2\}_n$)

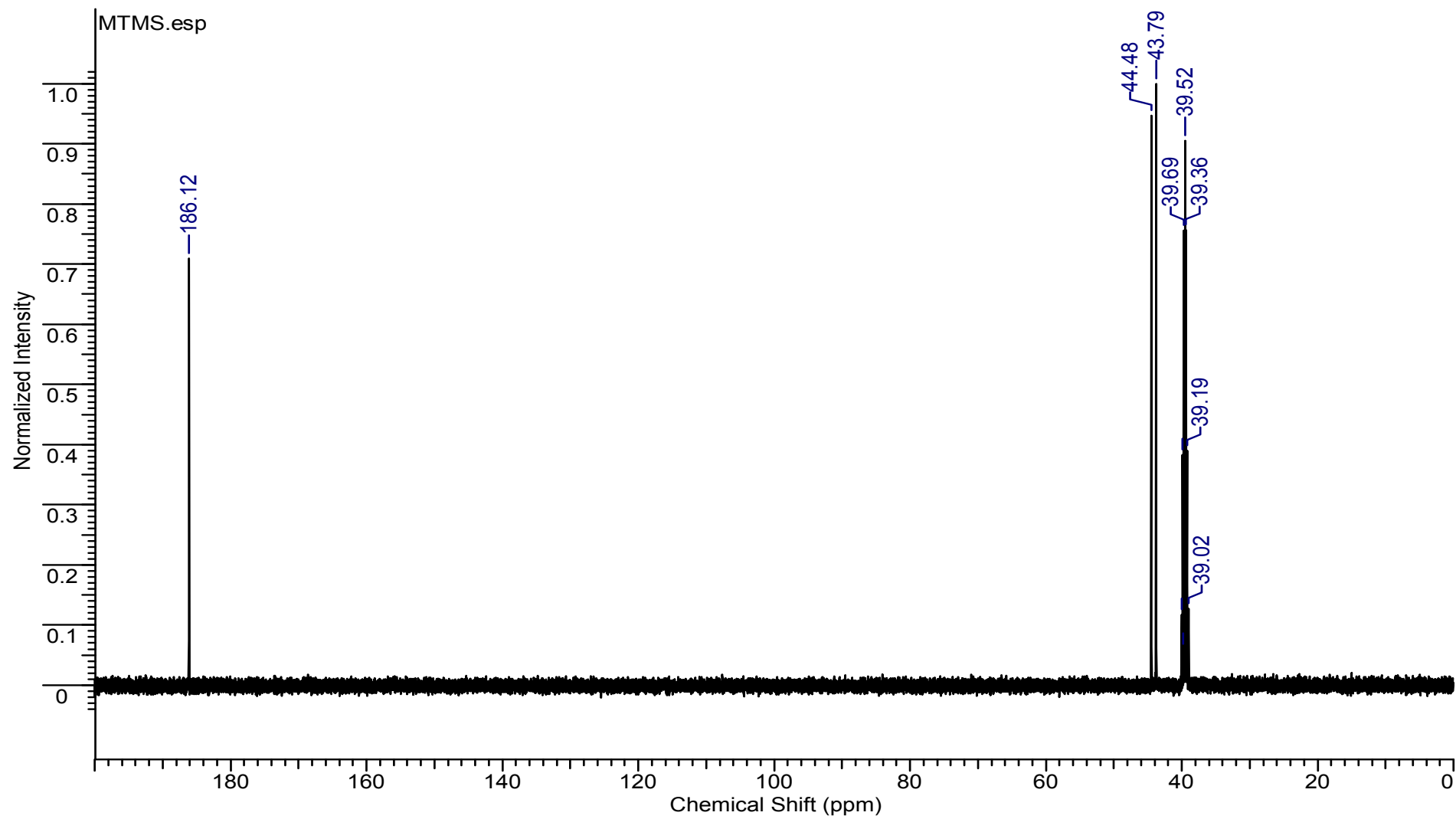


Figure S32. ^{13}C -NMR spectrum of *Tetramethylthiuram monosulfide* (MTMS)

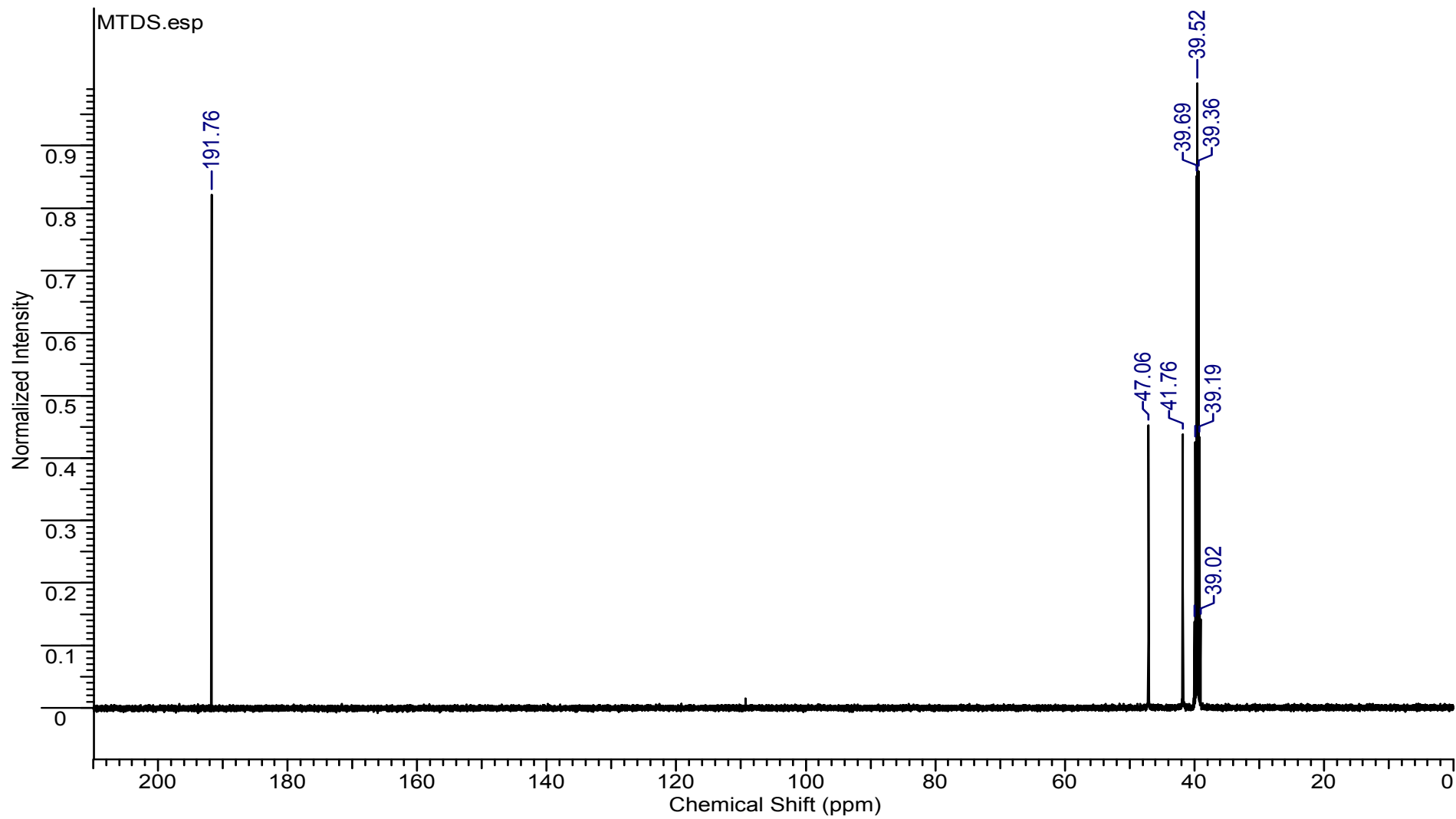


Figure S33. ^{13}C -NMR spectrum of *Tetramethylthiuram disulfide* (MTDS)

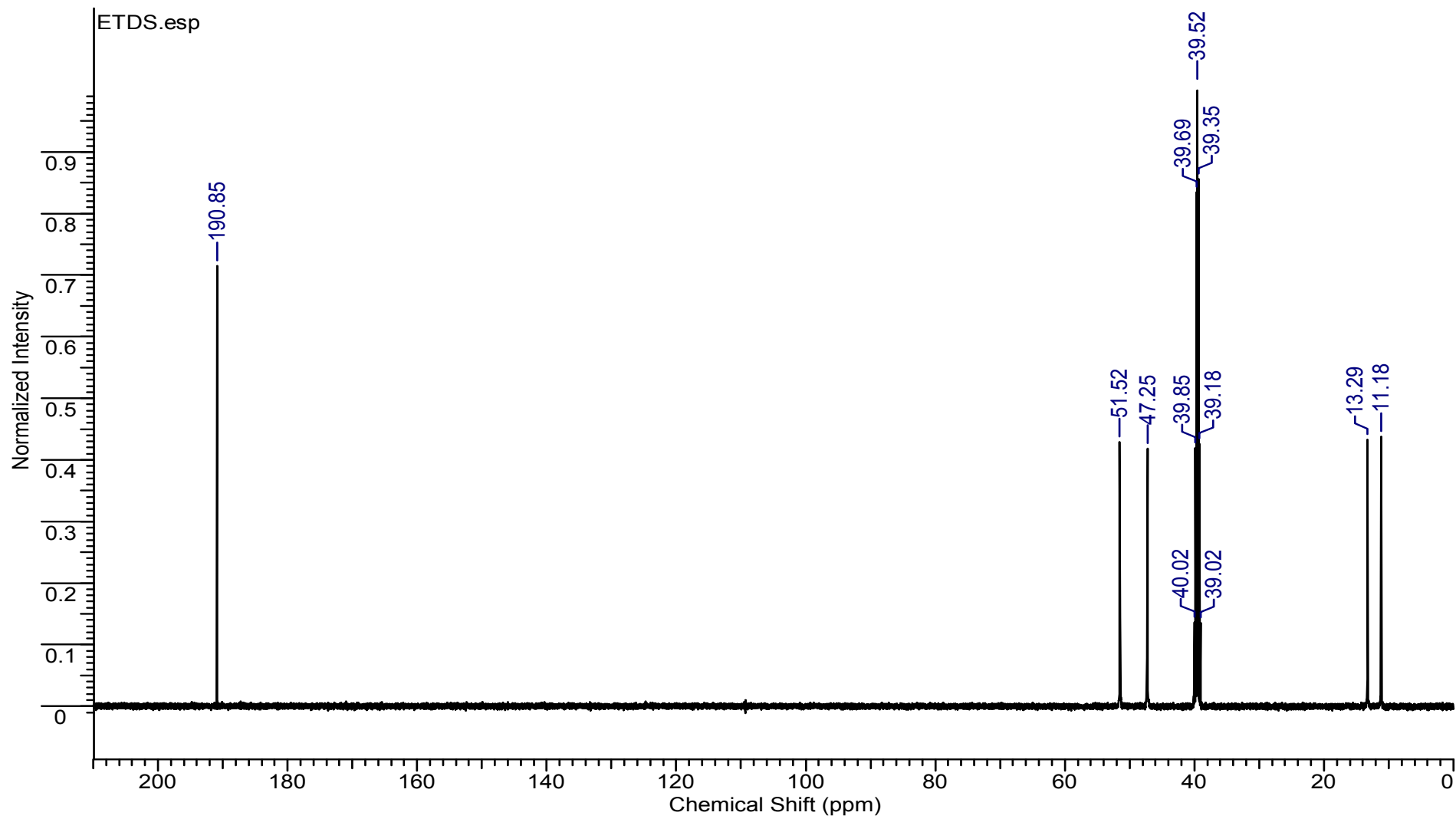
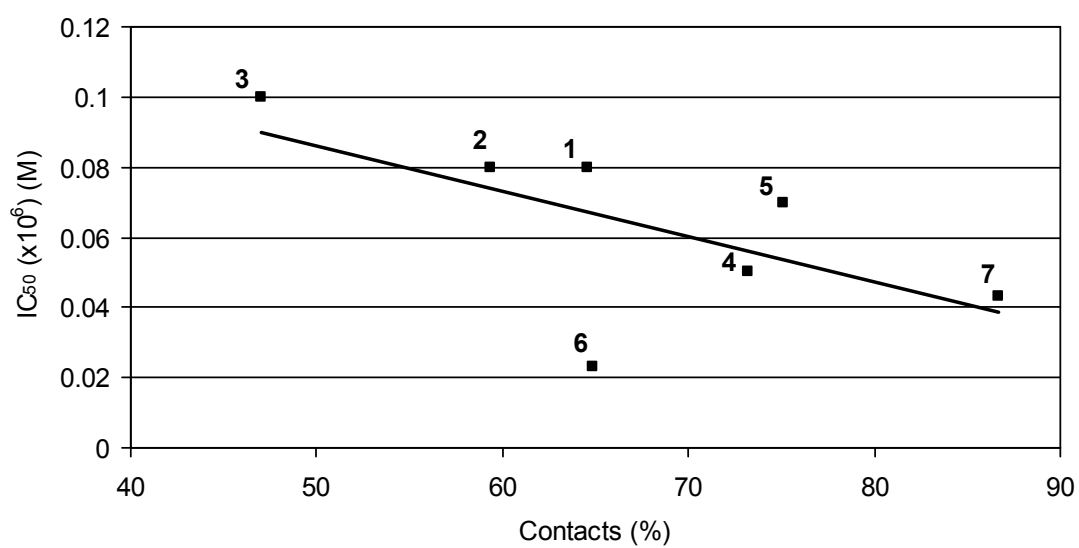
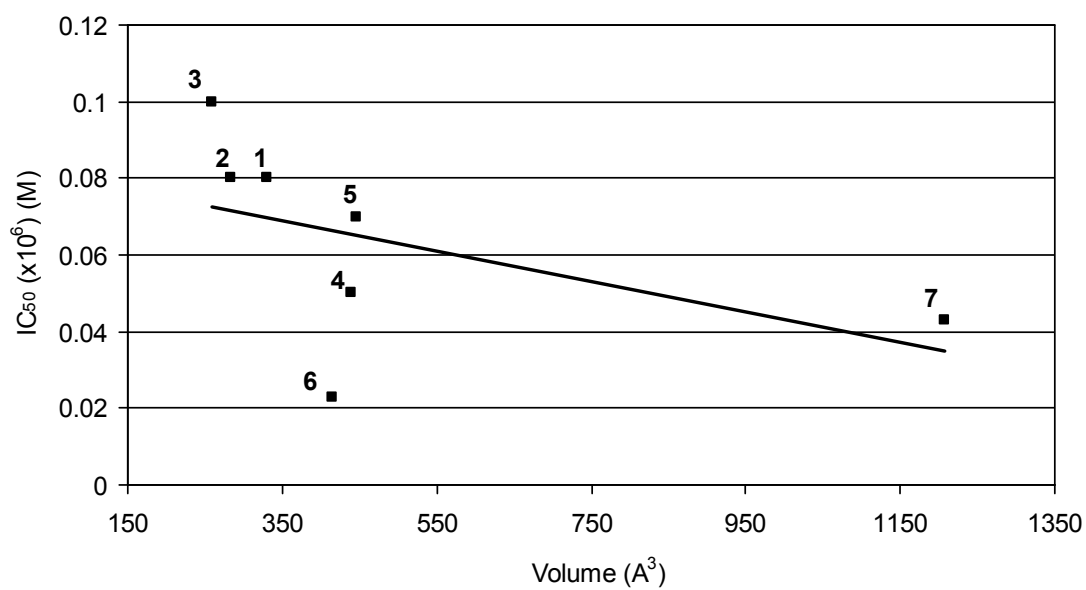


Figure S34. ^{13}C -NMR spectrum of *Tetraethylthiuram disulfide* (ETDS)

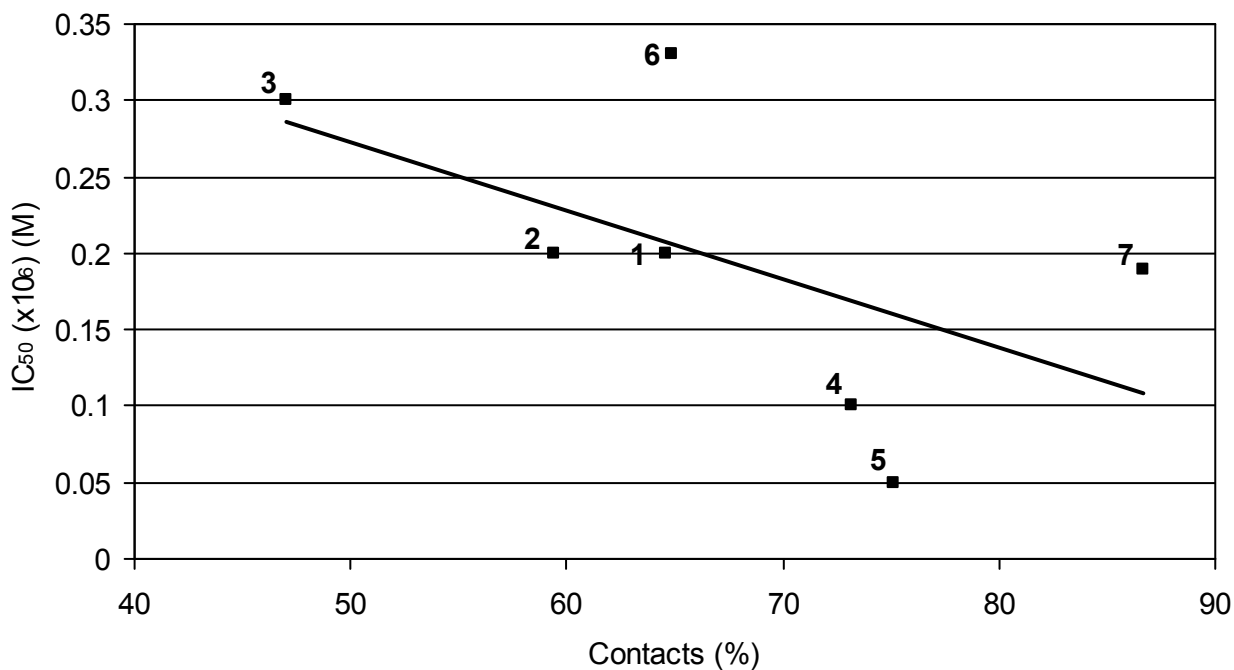


(A)

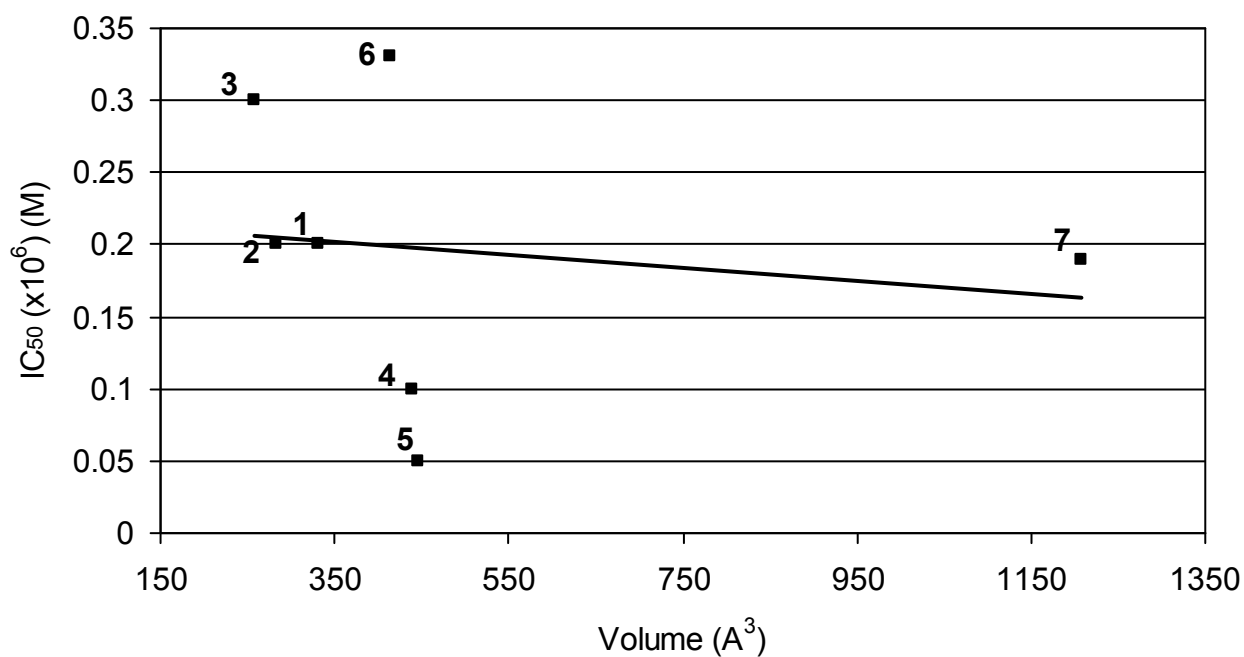


(B)

Figure S35. (A) IC₅₀ of the complexes against MCF-7 cells versus the close contacts (%) of all elements inside the area with the outer hydrogen atoms (B) IC₅₀ of the complexes against MCF-7 cells versus the volumes (Å³).



(A)



(B)

Figure S36. (A) IC₅₀ of the complexes against HeLa cells versus the volumes (Å³). (B) IC₅₀ of the complexes against HeLa cells versus the close contacts (%) of all elements inside the area with the outer hydrogen atoms

