SUPPORTING INFORMATION FOR

The potential of achiral sponge-derived and synthetic bromoindoles as selective cytotoxins against PANC-1 tumor cells

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Figure S1. ^{1}H NMR spectrum (600 MHz) of 6-Br-8-keto-conicamin A (**2**) in DMSO-d6.

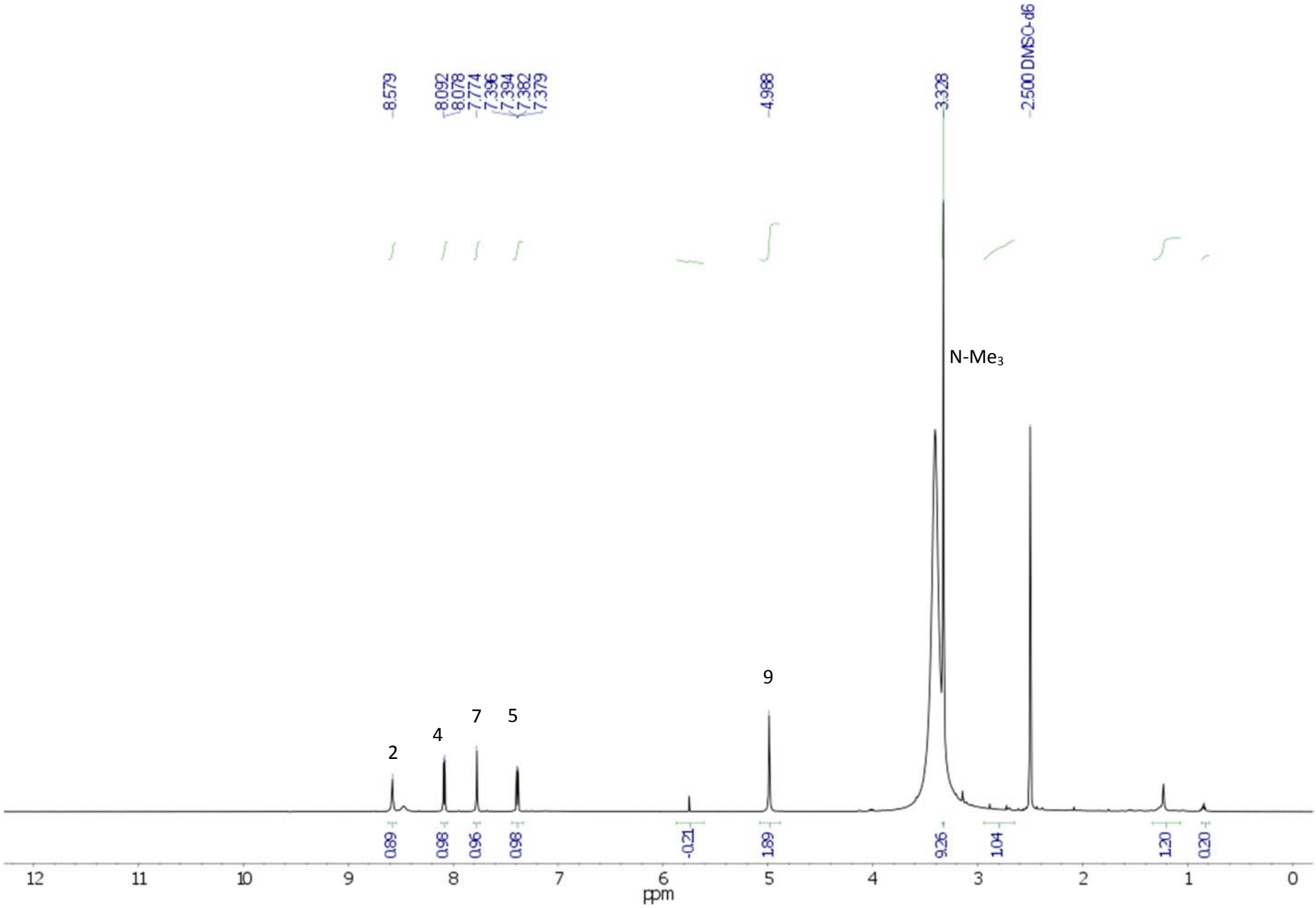

Figure S2. ^{13}C NMR spectrum (150 MHz) of in DMSO-d6.

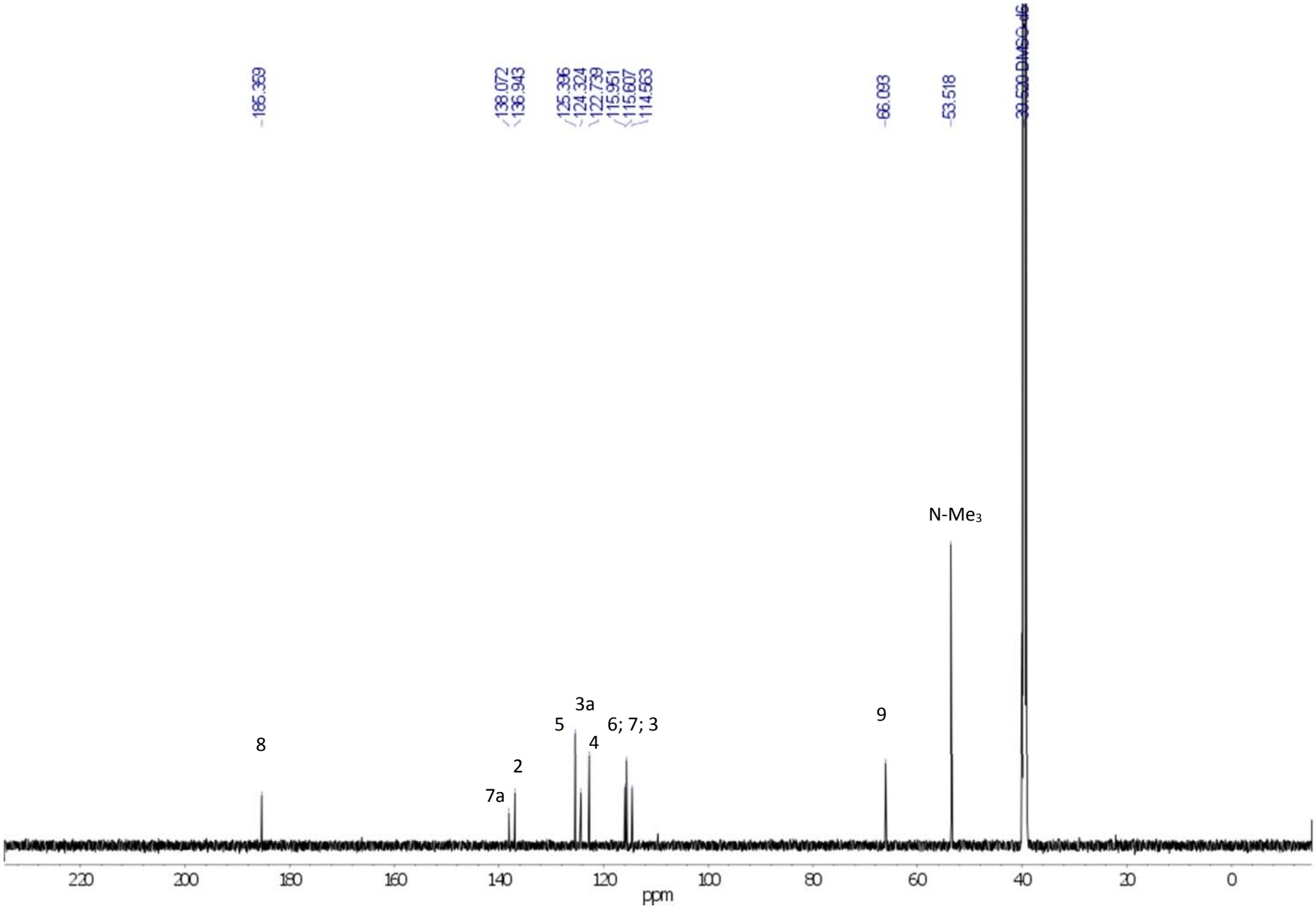

Figure S3. gHSQCAD spectrum (600MHz) of 6-Br-8-keto-conicamin A (**2**) in DMSO-d6.

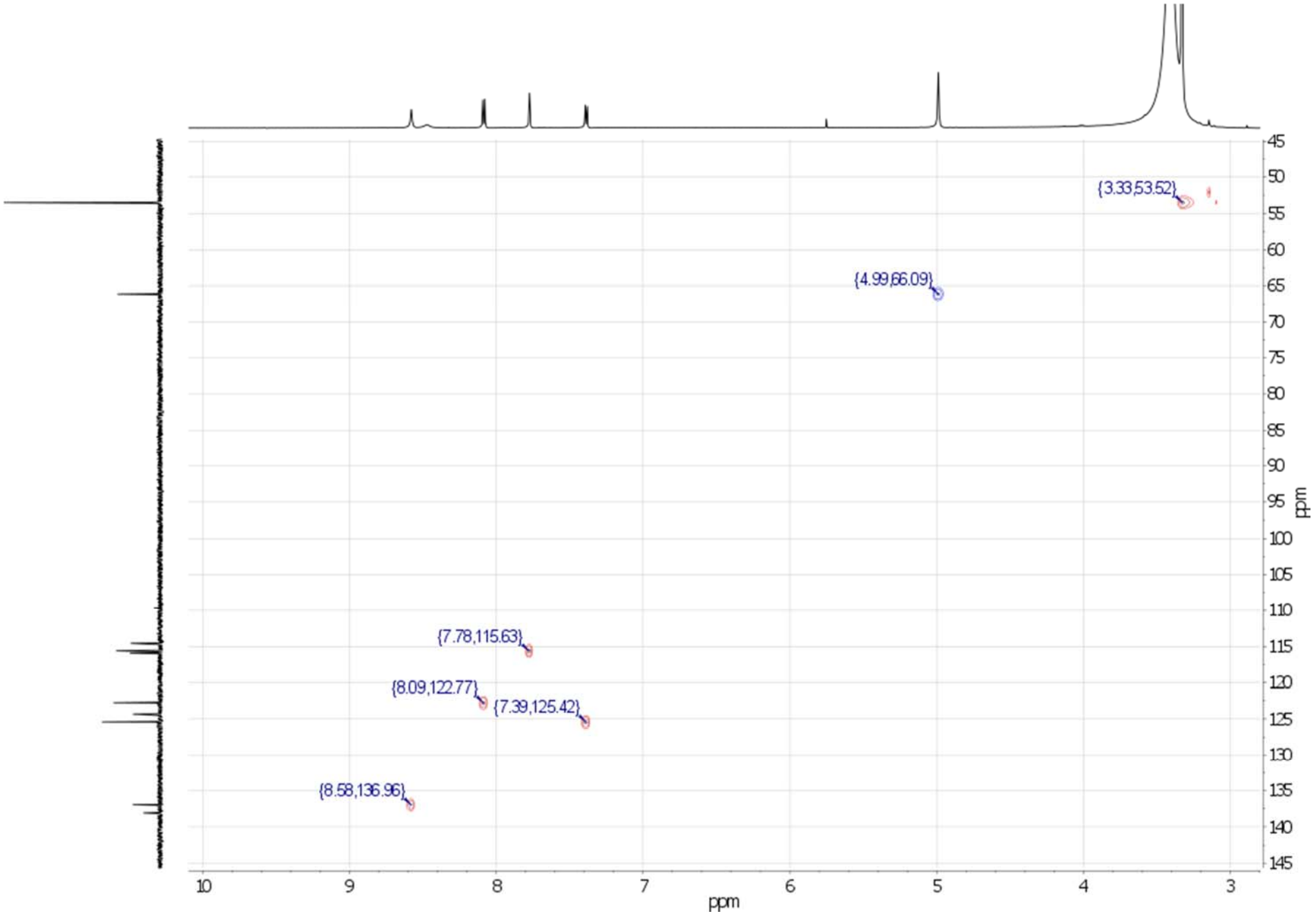

Figure S4. gHMBCAD spectrum (600MHz) of 6-Br-8-keto-conicamin A (**2**) in DMSO-d6.

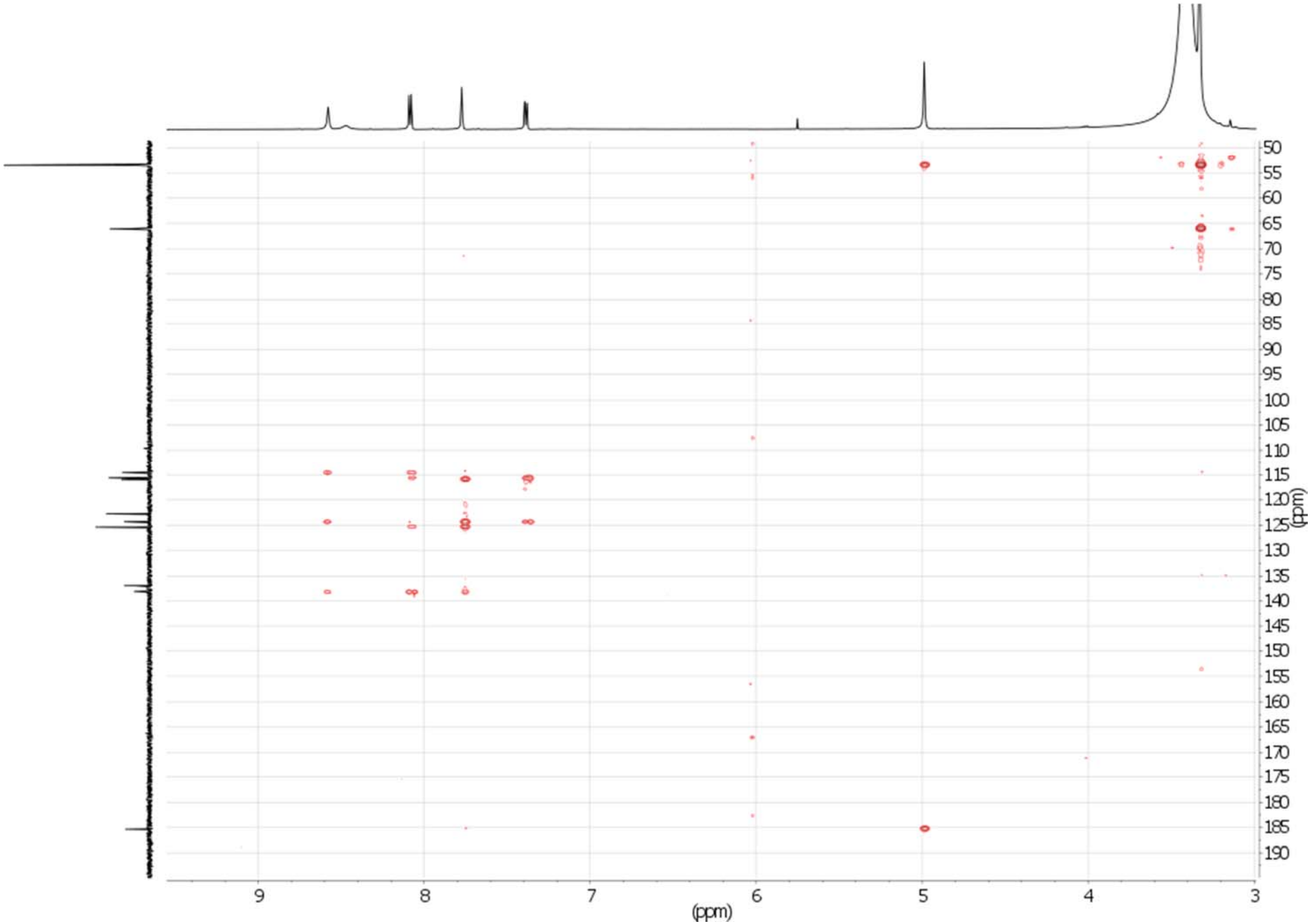

Figure S5. [1]H spectrum (600 MHz) of 6-bromo-β-oxo-*N,N,N*-trimethyl-tryptamine (formate salt) in DMSO-d6.

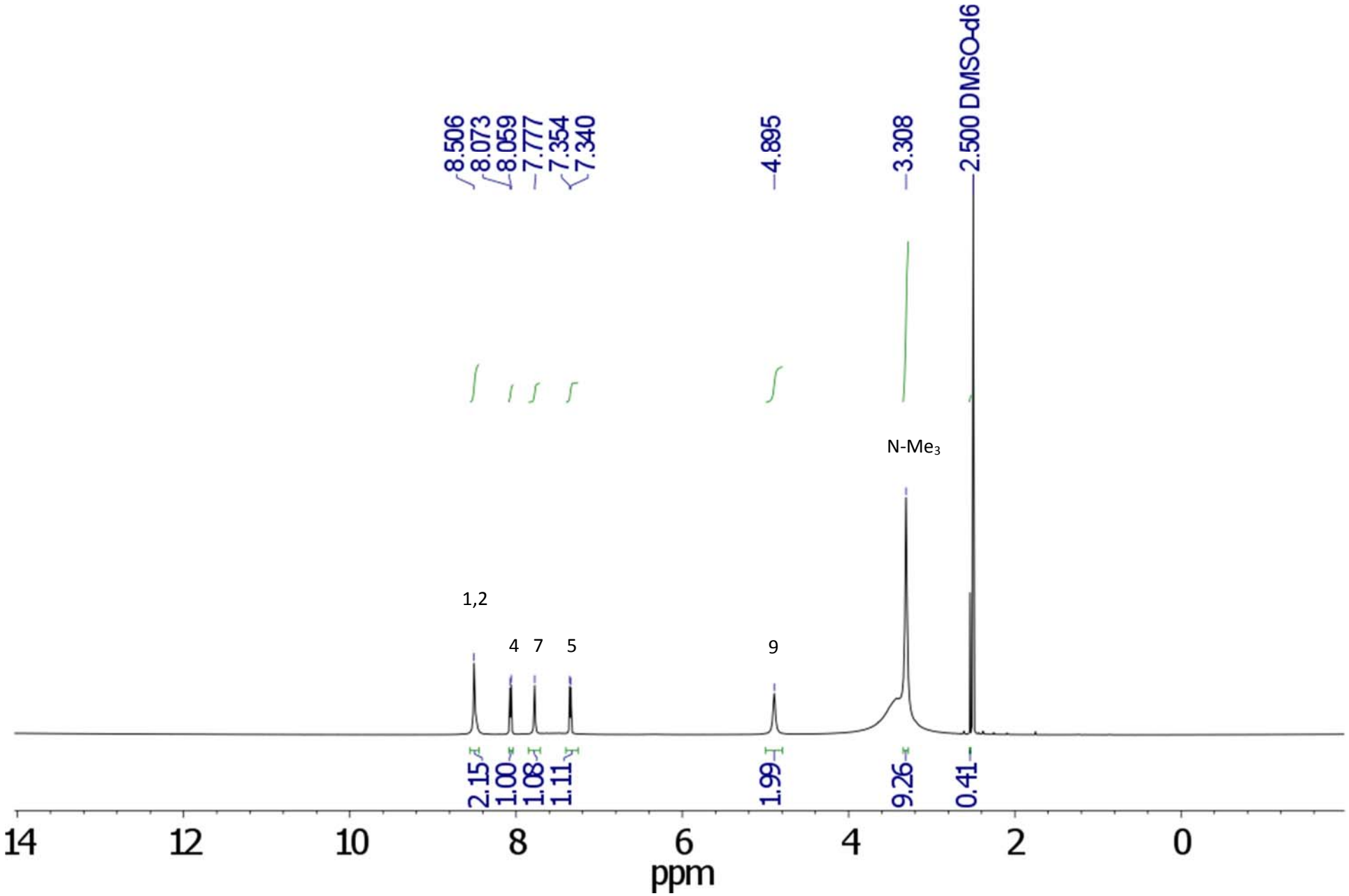

Figure S6. ^{13}C spectrum (150 MHz) of 6-bromo-8-keto-*N,N,N*-trimethyl-tryptamine (**2s**) (formate salt) in DMSO-d6.

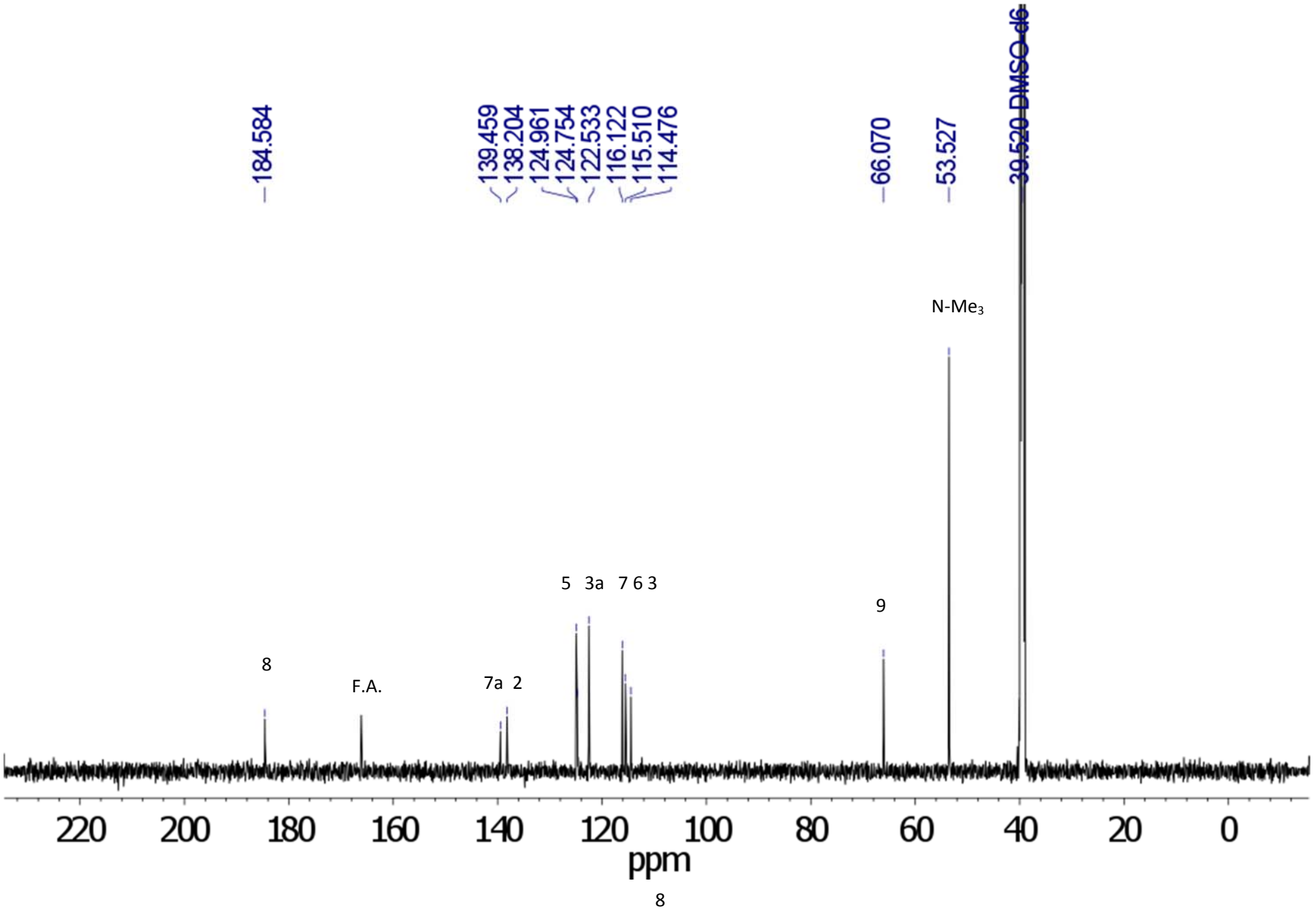

Figure S7. [1]H spectrum (600 MHz) of 5-bromo-8-keto-*N,N,N*-trimethyl-tryptamine (**3**) (formate salt) in DMSO-d6.

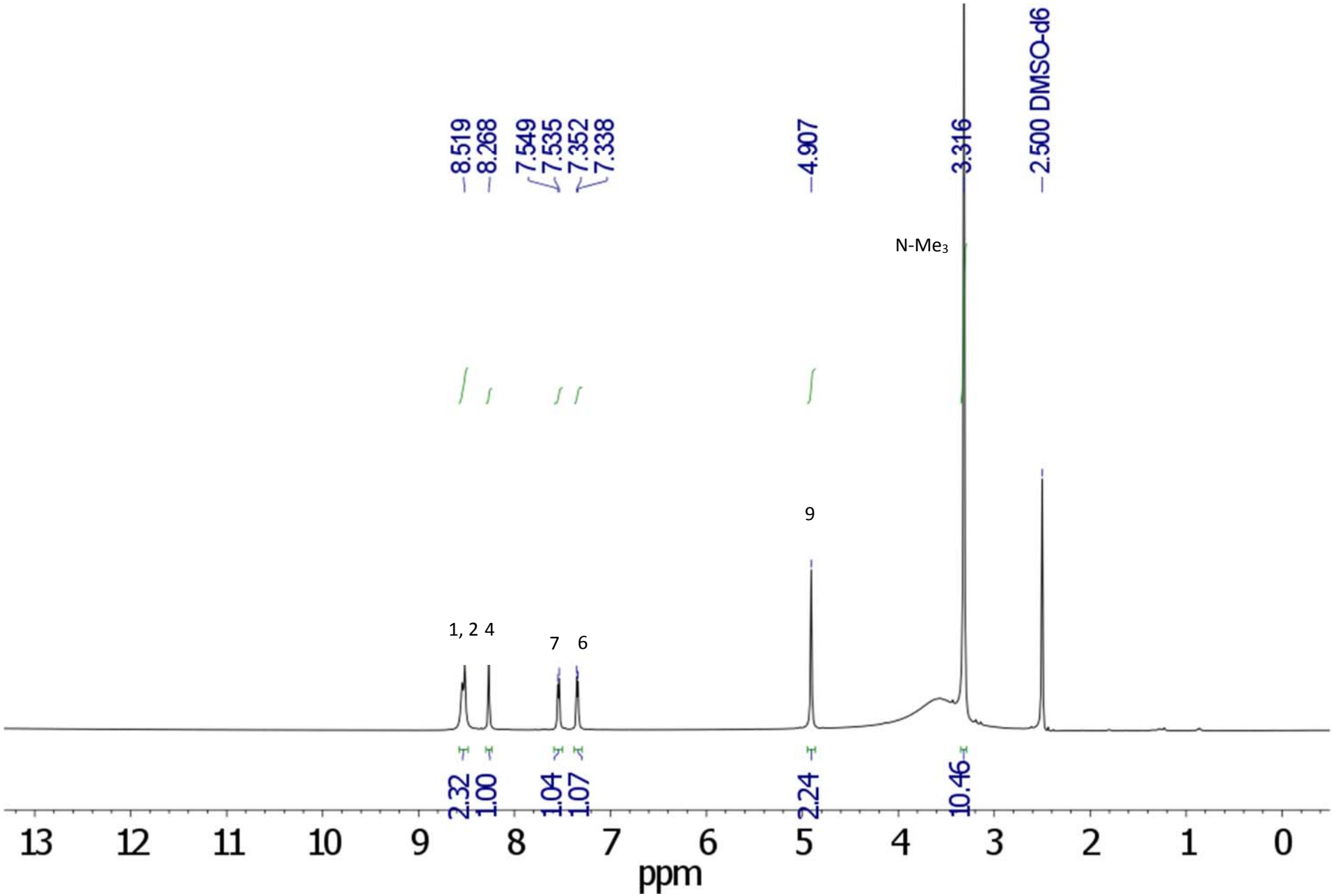

Figure S8. ^{13}C spectrum (150 MHz) of 5-bromo-8-keto-*N,N,N*-trimethyl-tryptamine (**3**) (formate salt) in DMSO-d6.

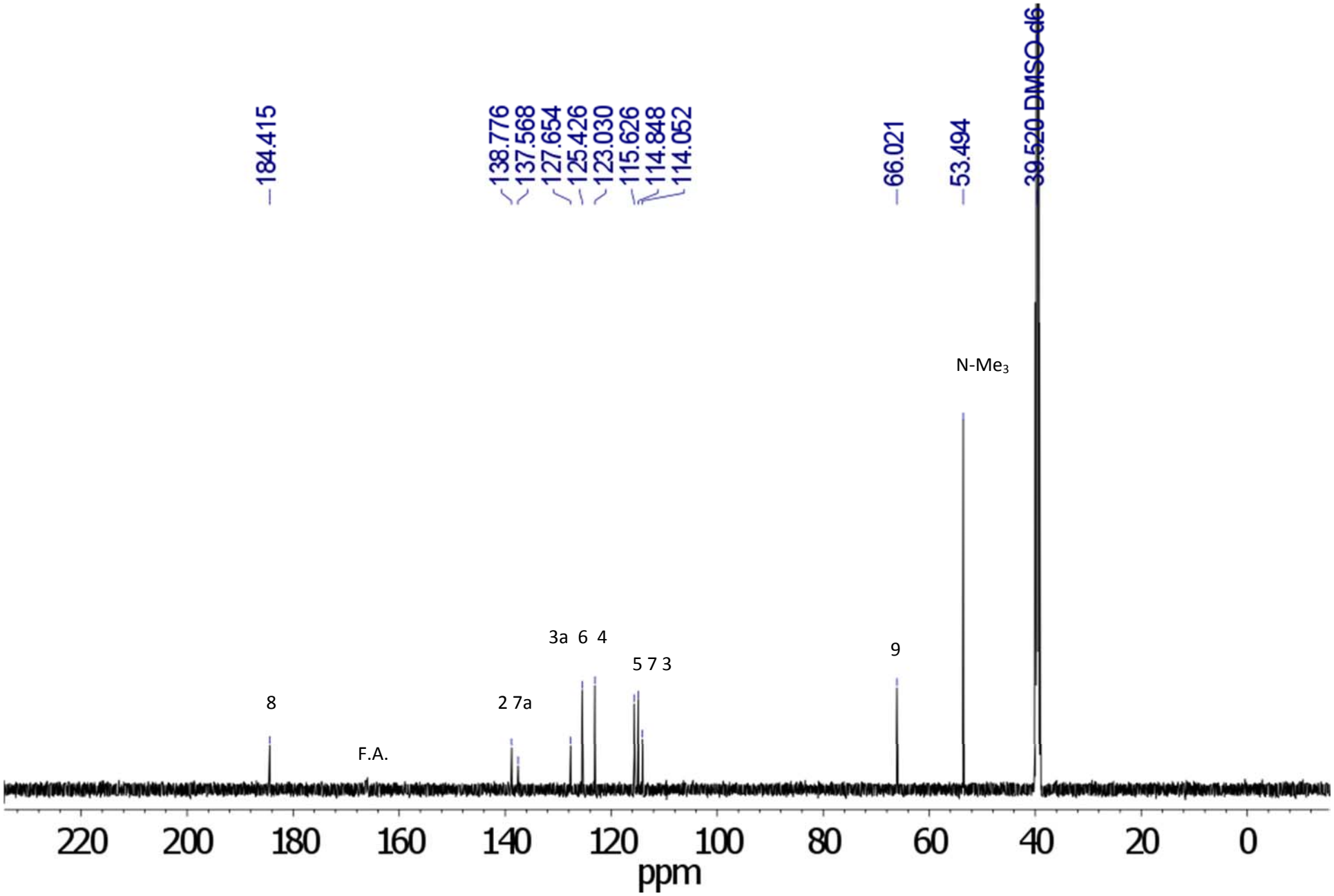

Figure S9. Stacked ^{13}C NMR spectra of the natural product and 5- and 6-bromo isomers of beta-keto-N,N,N-trimethyl-tryptamine (150MHz, DMSO-d6)

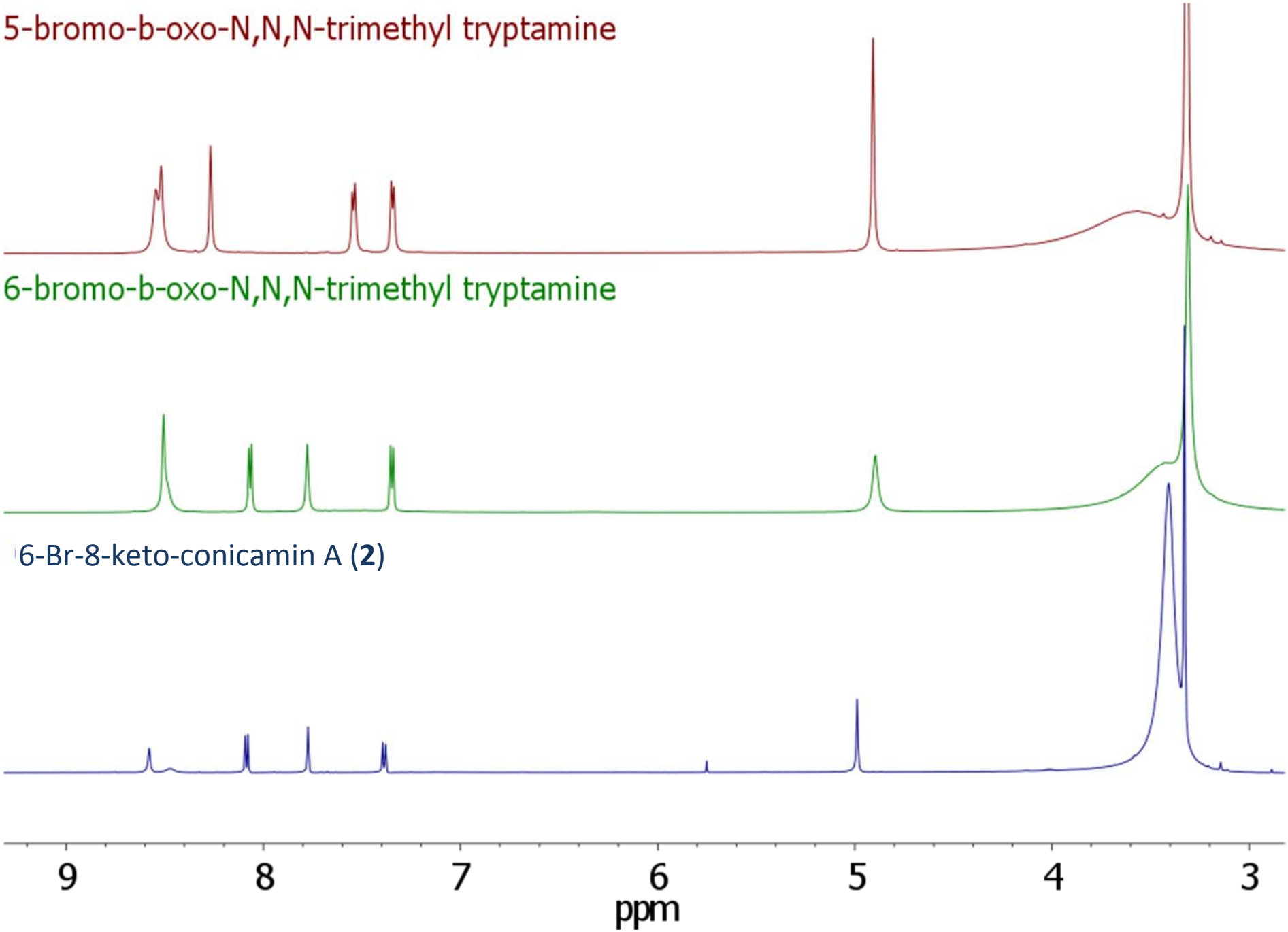

Figure S10. Stacked ^{13}C NMR spectra of the natural product and 5- and 6-bromo isomers of beta-oxo-tryptamine (150MHz, DMSO-d6)

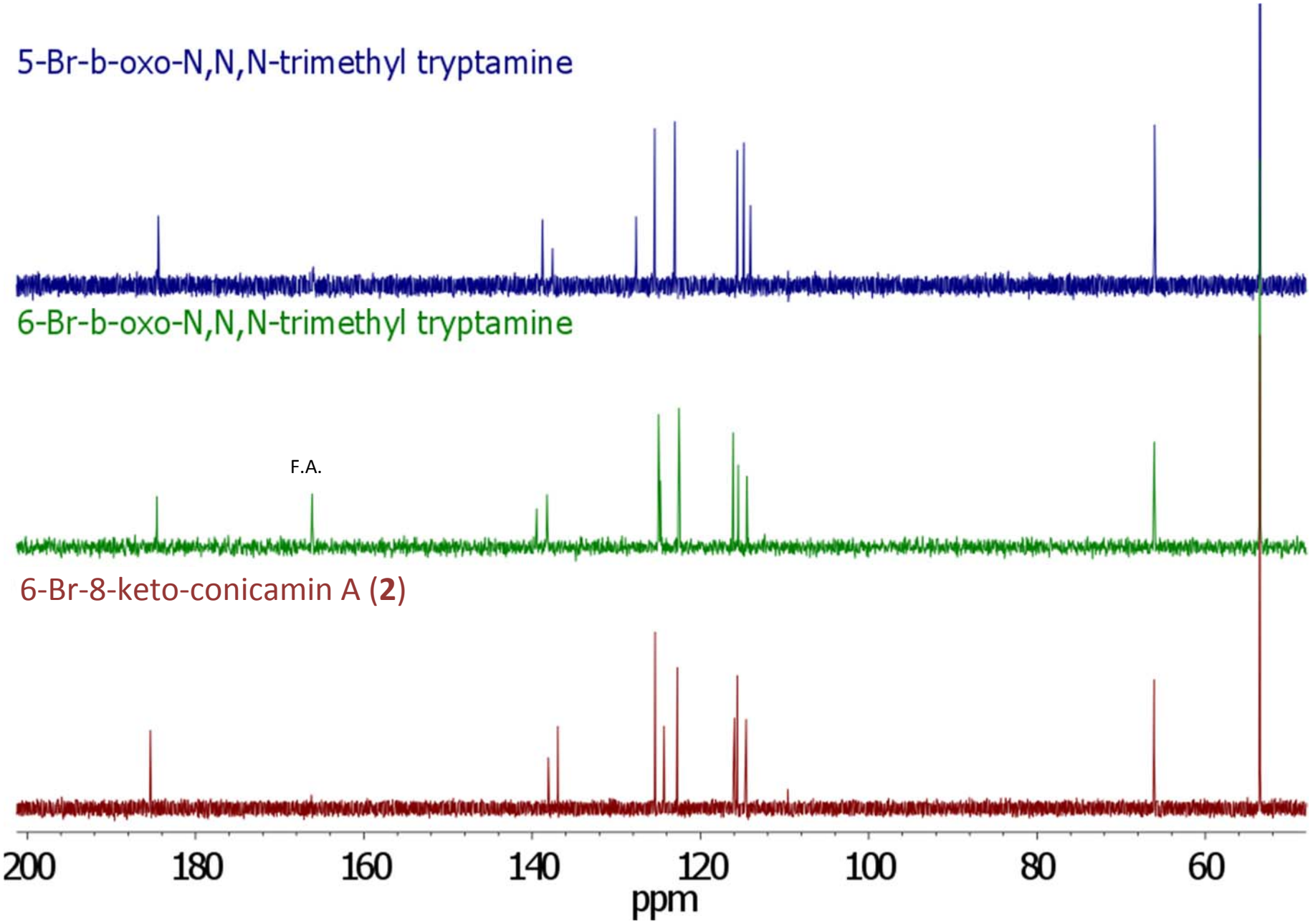

Figure S11. ^{1}H spectrum (600 MHz) of 5uL formic acid in DMSO-d6. Note that chemical shift varies with presence of other compounds.

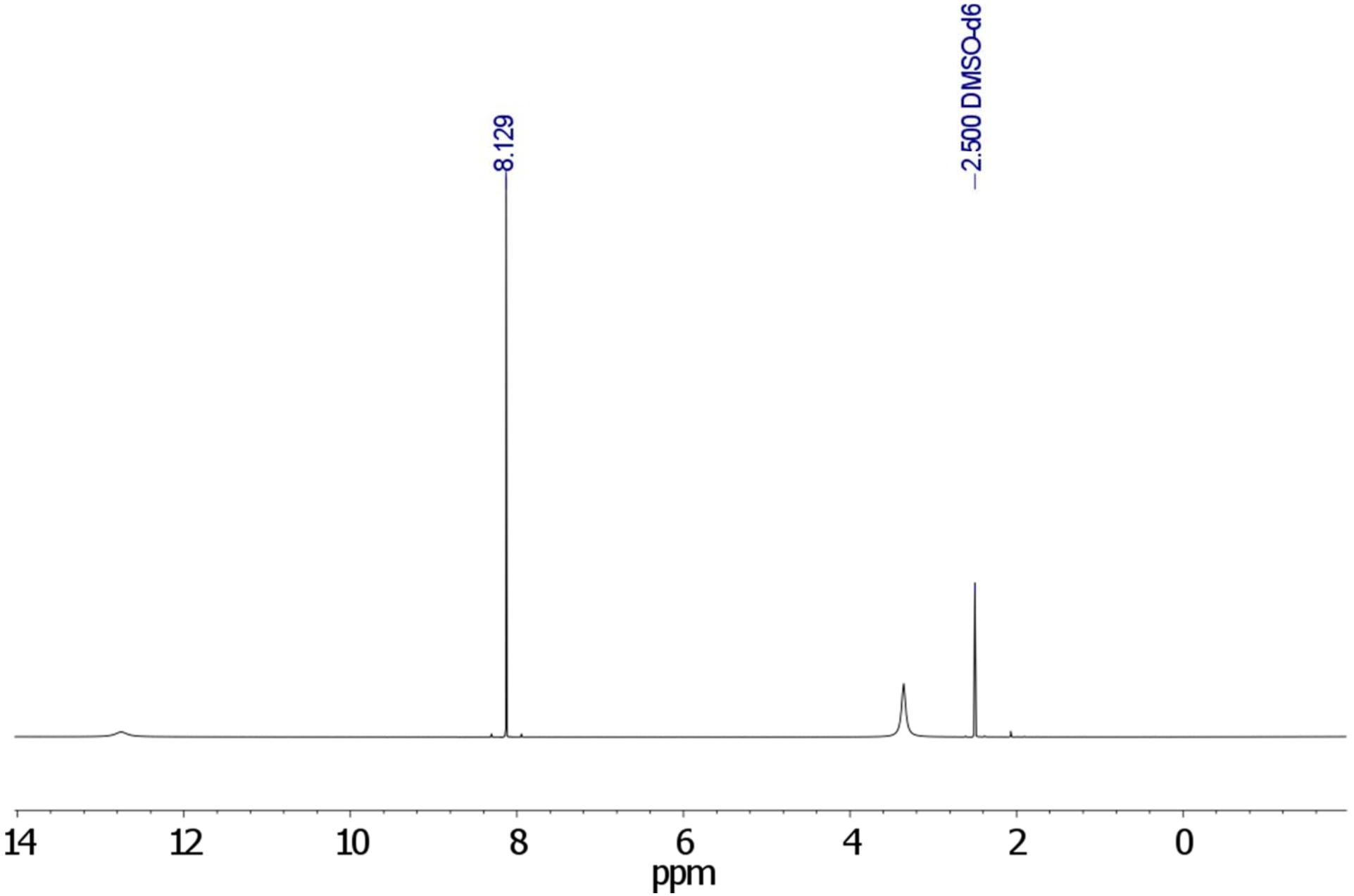

Figure S12. ^{13}C spectrum (150 MHz) of 5uL formic acid in DMSO-d6. Note that chemical shift varies with presence of other compounds.

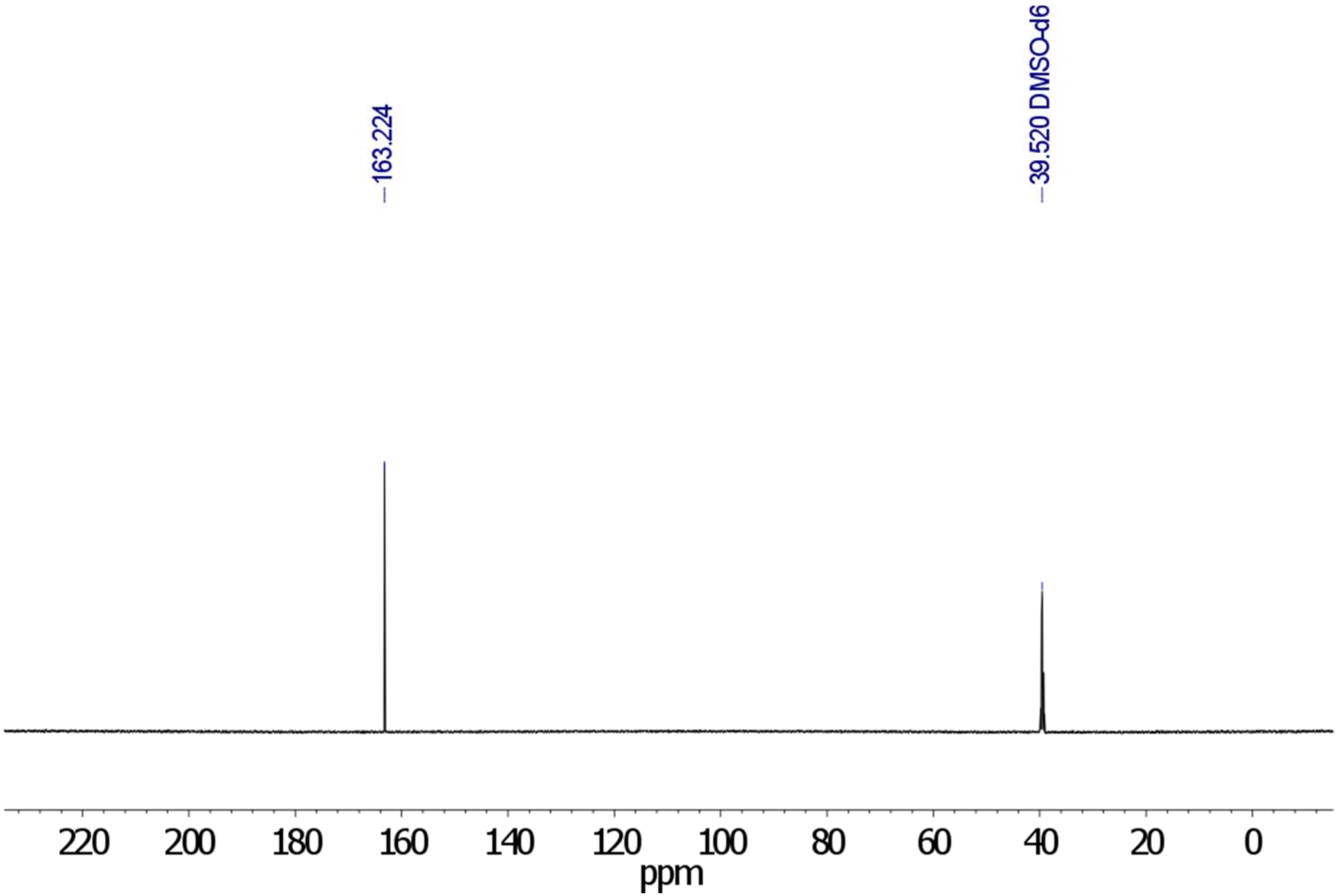

Figure S13. [1]H spectrum (600 MHz) of 2-(6-Bromo-1H-indol-3yl)-2-(trimethylsiloxy)acetonitrile (**7**) in DMSO-d6.

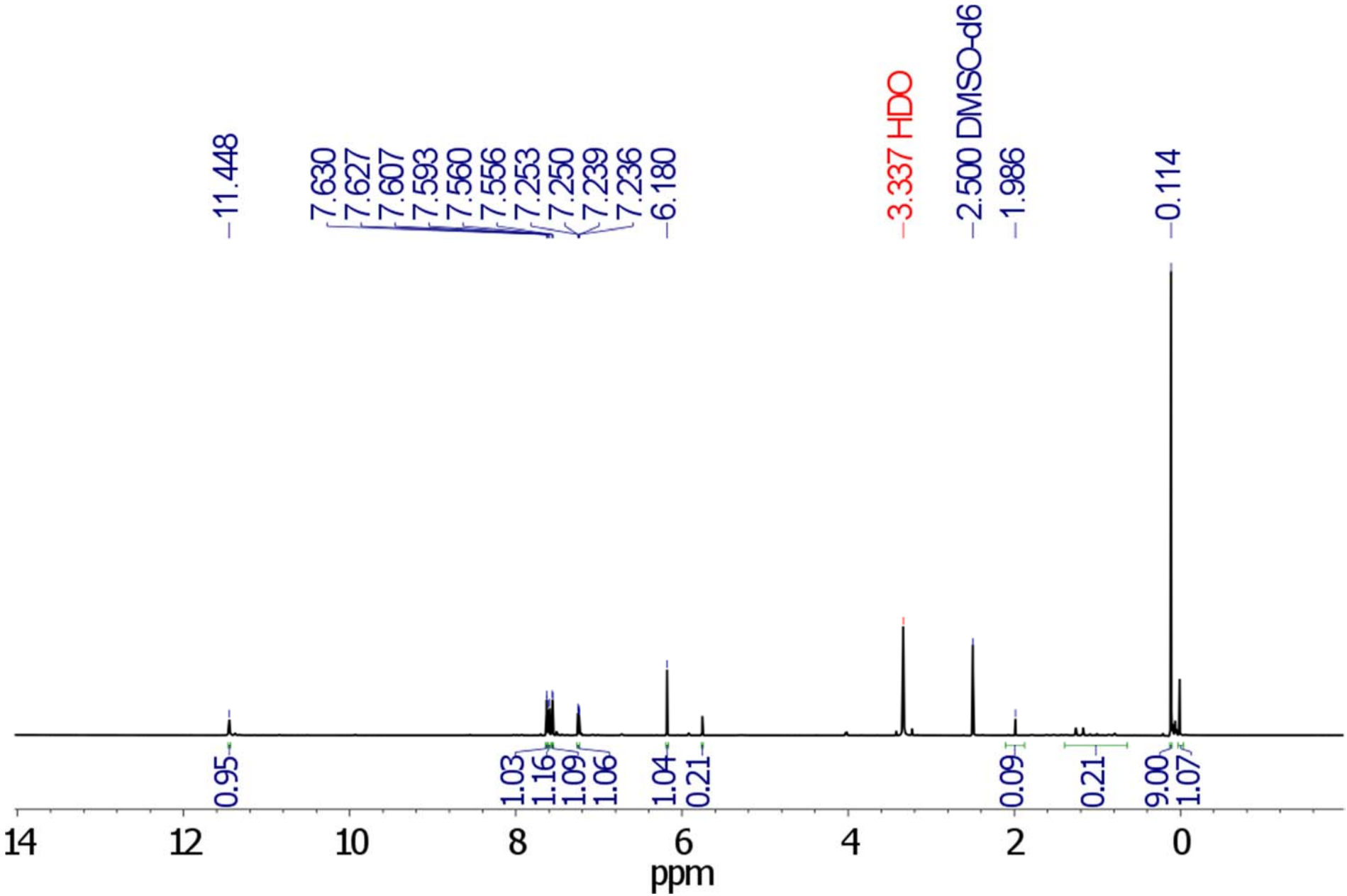

Figure S14. ^{13}C spectrum (150 MHz) of (6-Bromo-1H-indol-3yl)-(trimethylsiloxy)acetonitrile (**7**) in DMSO-d6.

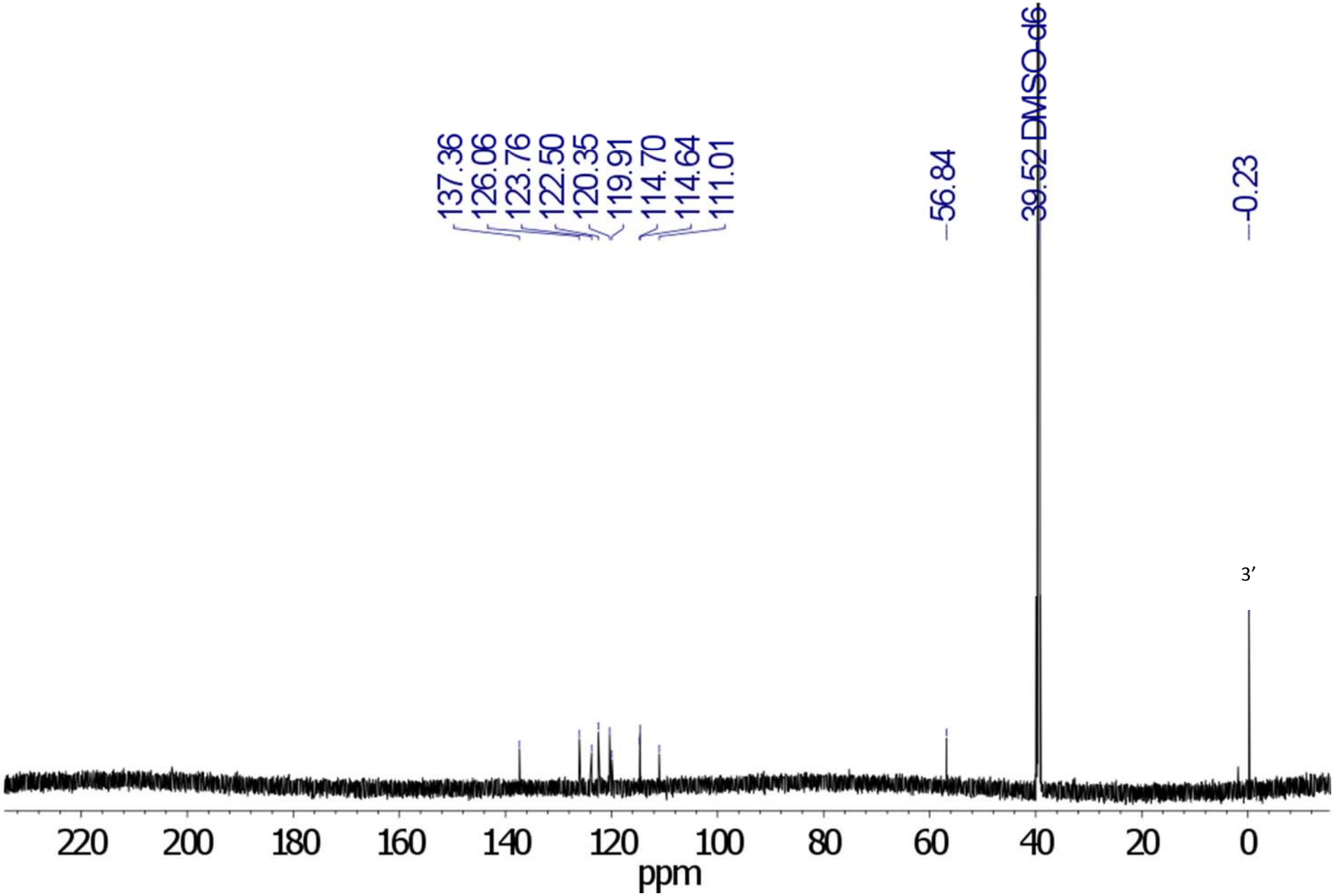

Figure S15. ^{1}H spectrum (600 MHz) of 6-bromo-1H-indol-3-carbonyl cyanide (**9**) in DMSO-d6.

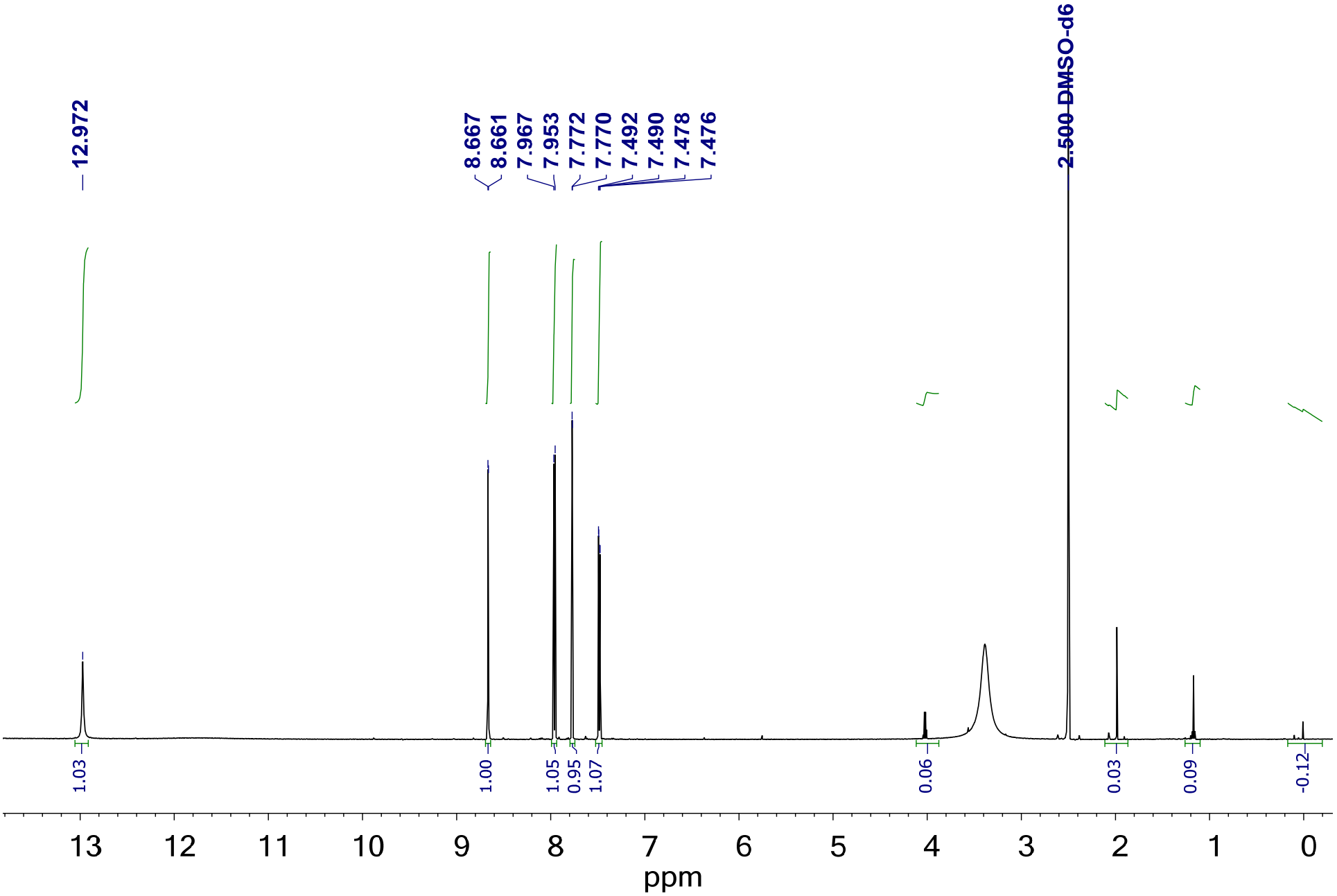

Figure S16. ^{13}C spectrum (150 MHz) of 6-bromo-1H-indol-3-carbonyl cyanide (**9**) in DMSO-d6. Unmarked peaks are putatively of reduced DDQ (predicted 13C NMR: 151.5, 129.0, 113.5, 102.8 via nmrdb.org) or other aprotic contaminants as there are no associated proton signals (see above). However rigorous assignment was not done at this stage.

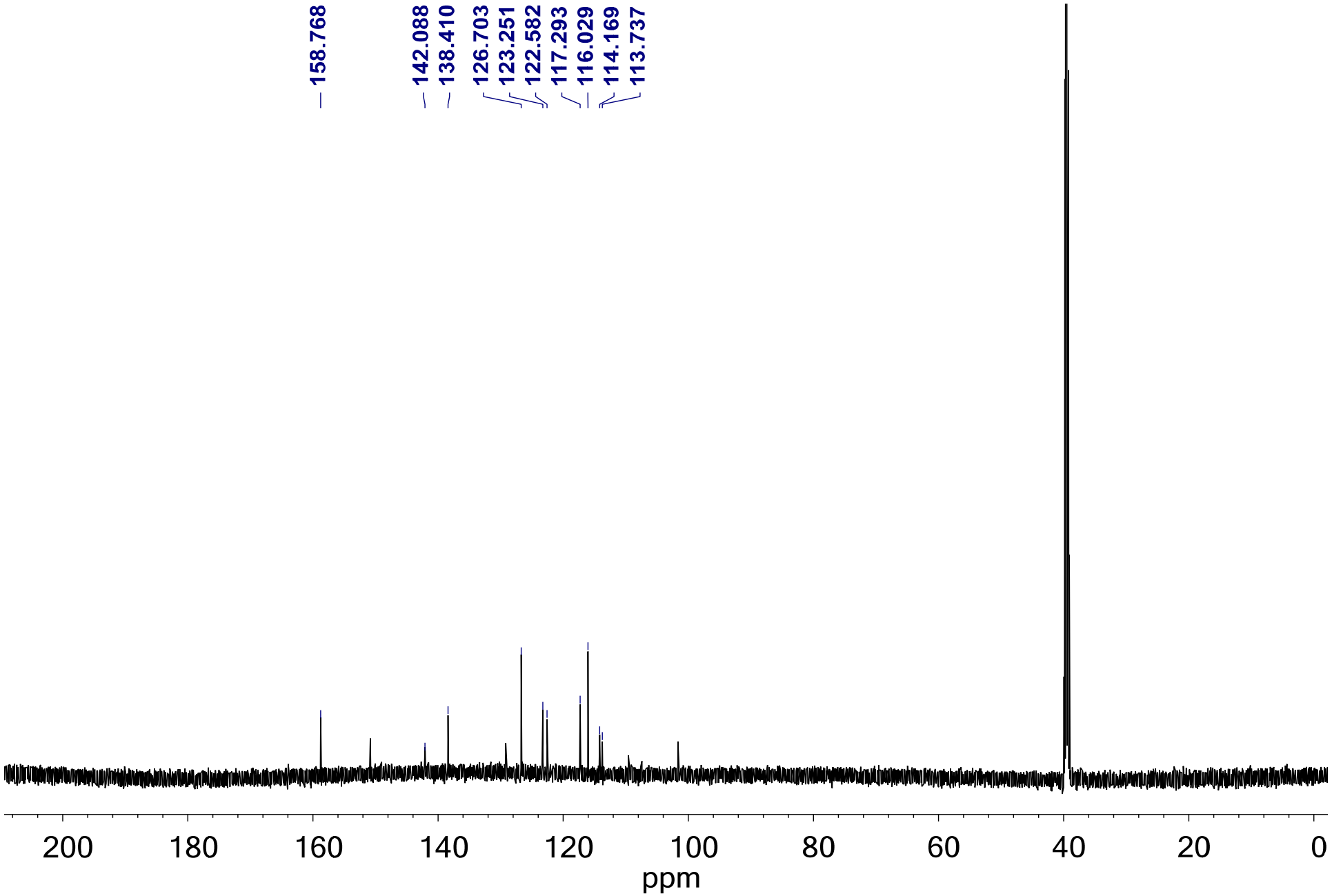

Figure S17. ^{1}H spectrum (600 MHz) of 8-keto-tryptamine (**10**) in DMSO-d6.

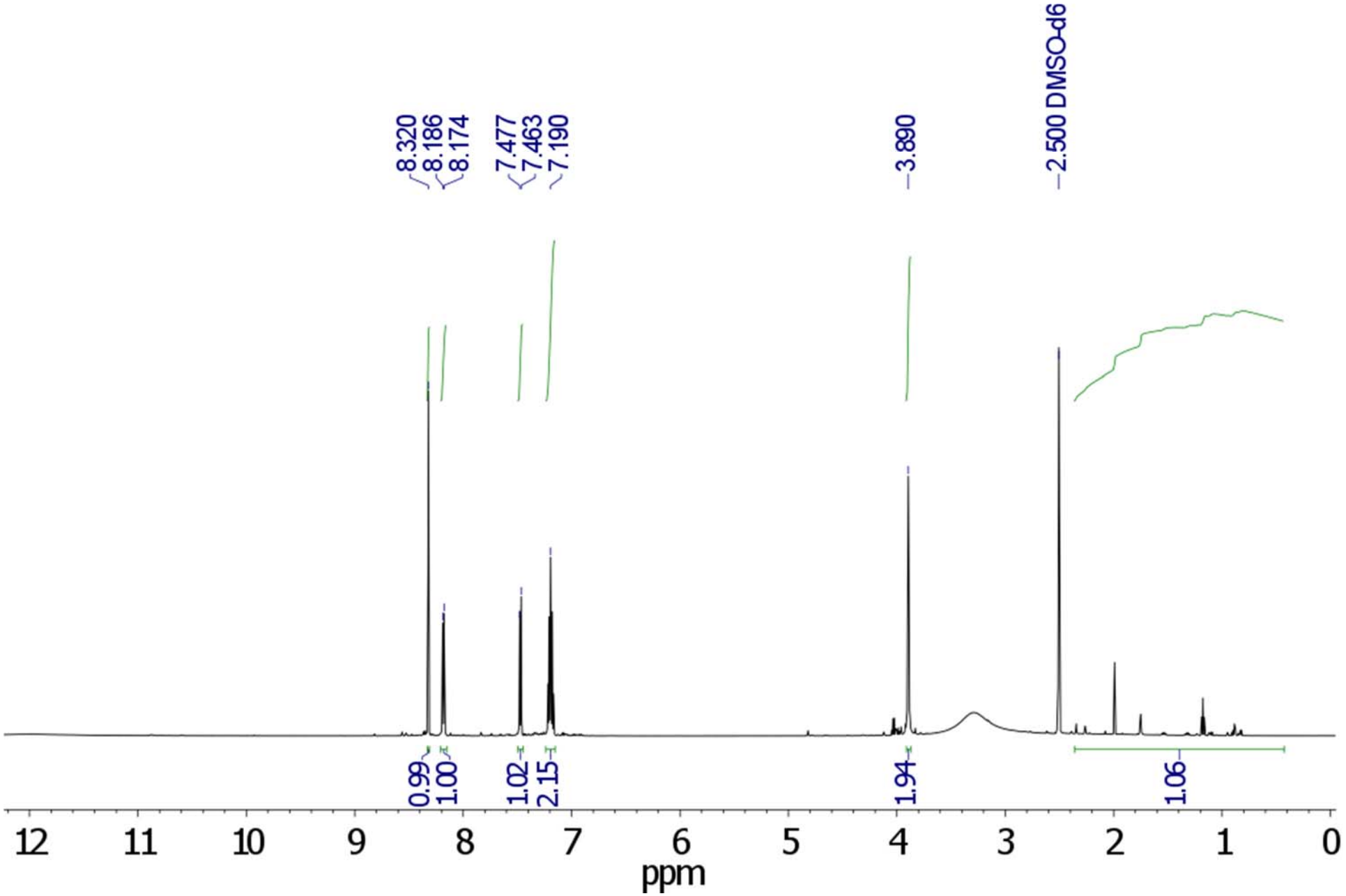

Figure S18. ^{13}C spectrum (150 MHz) of 8-keto-tryptamine (**10**) in DMSO-d6.

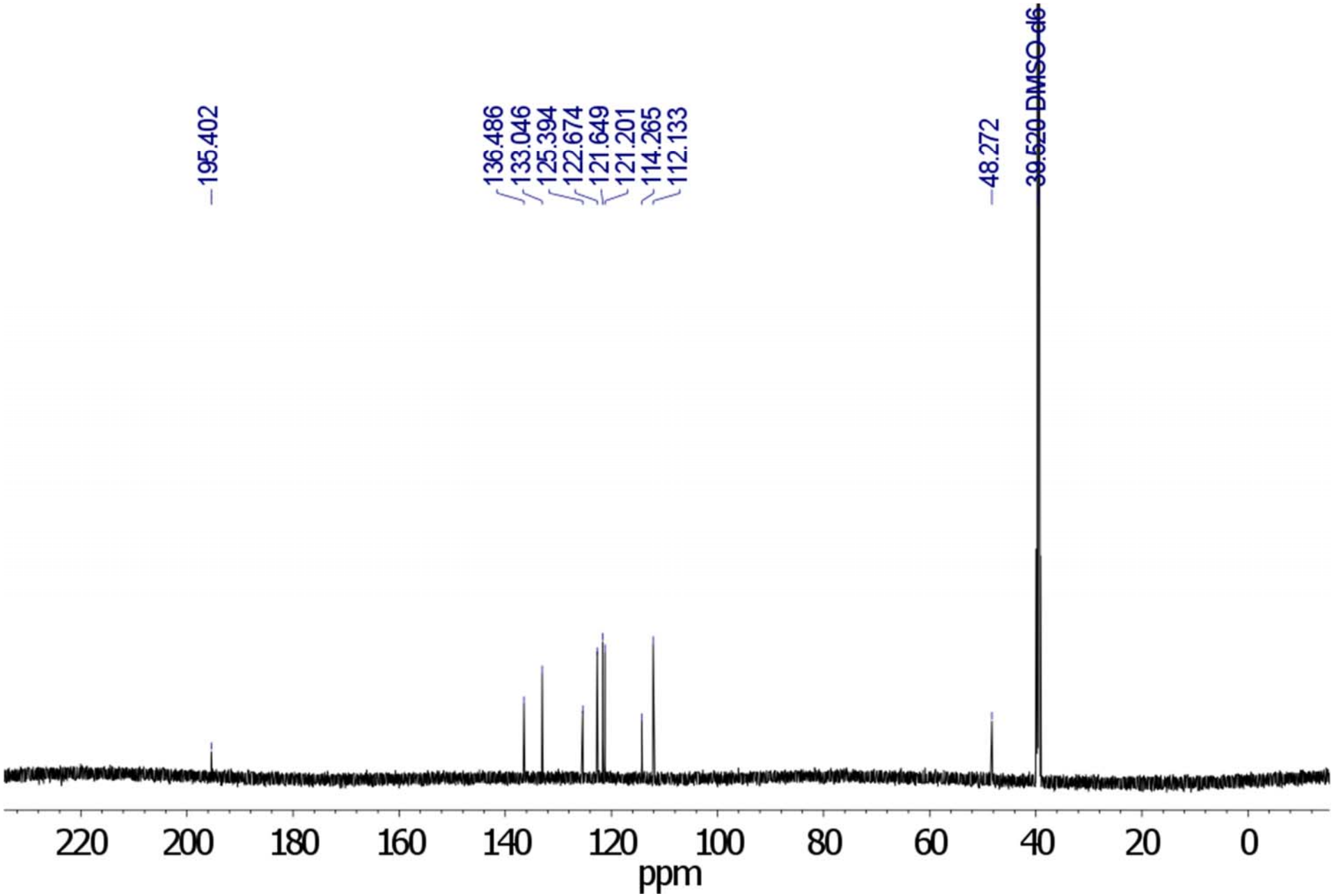

Figure S**19**. [1]H spectrum (500 MHz) of 6-Br-8-keto-tryptamine (**11**) (formate salt) in DMSO-d6.

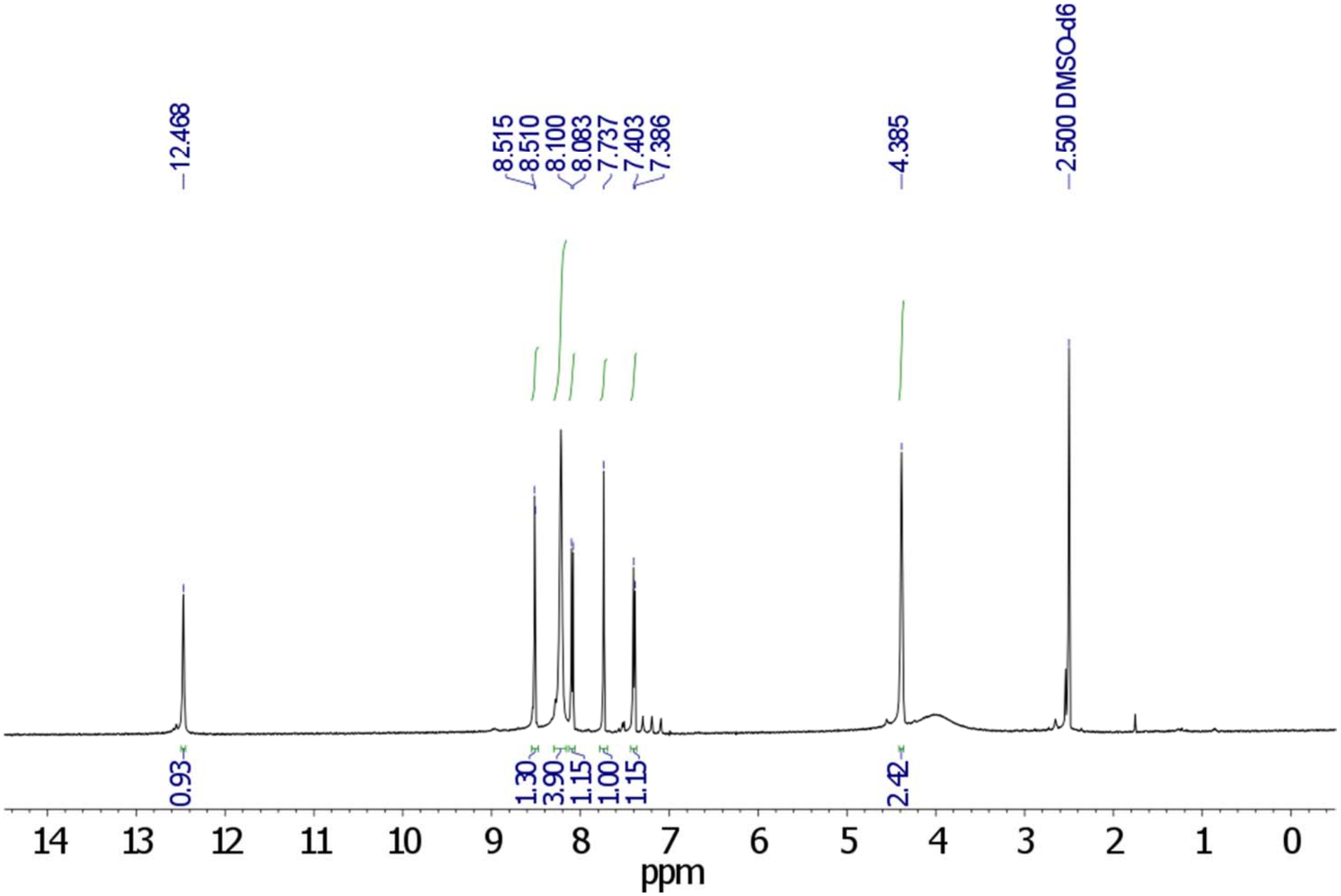

Figure S20. ^{13}C spectrum (125 MHz) of 6-Br-8-keto-tryptamine (**11**) in DMSO-d6.

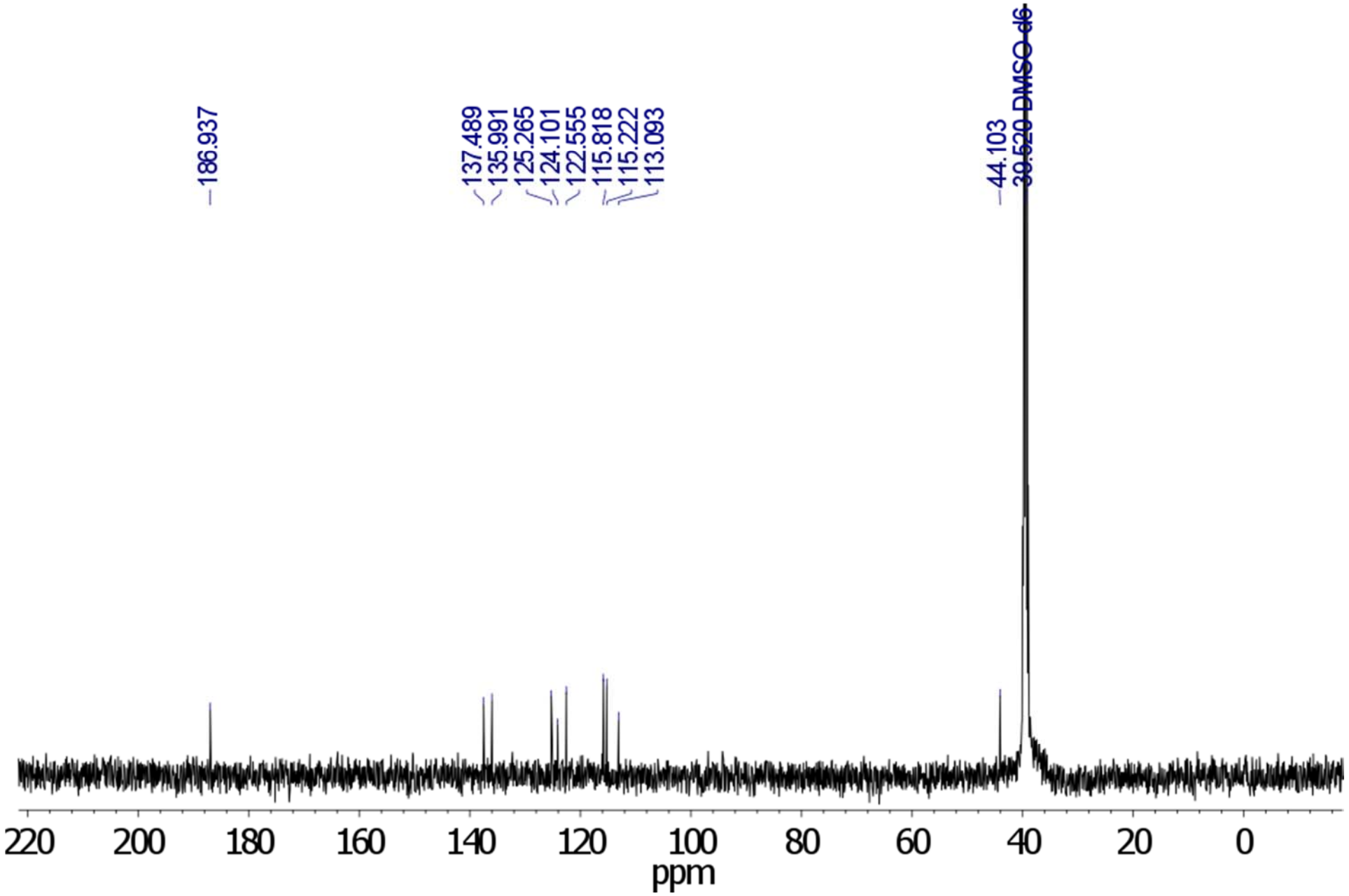

Figure S21. ^{1}H spectrum (500 MHz) of 5-Br-8-keto-tryptamine (**12**) (formate salt) in DMSO-d6.

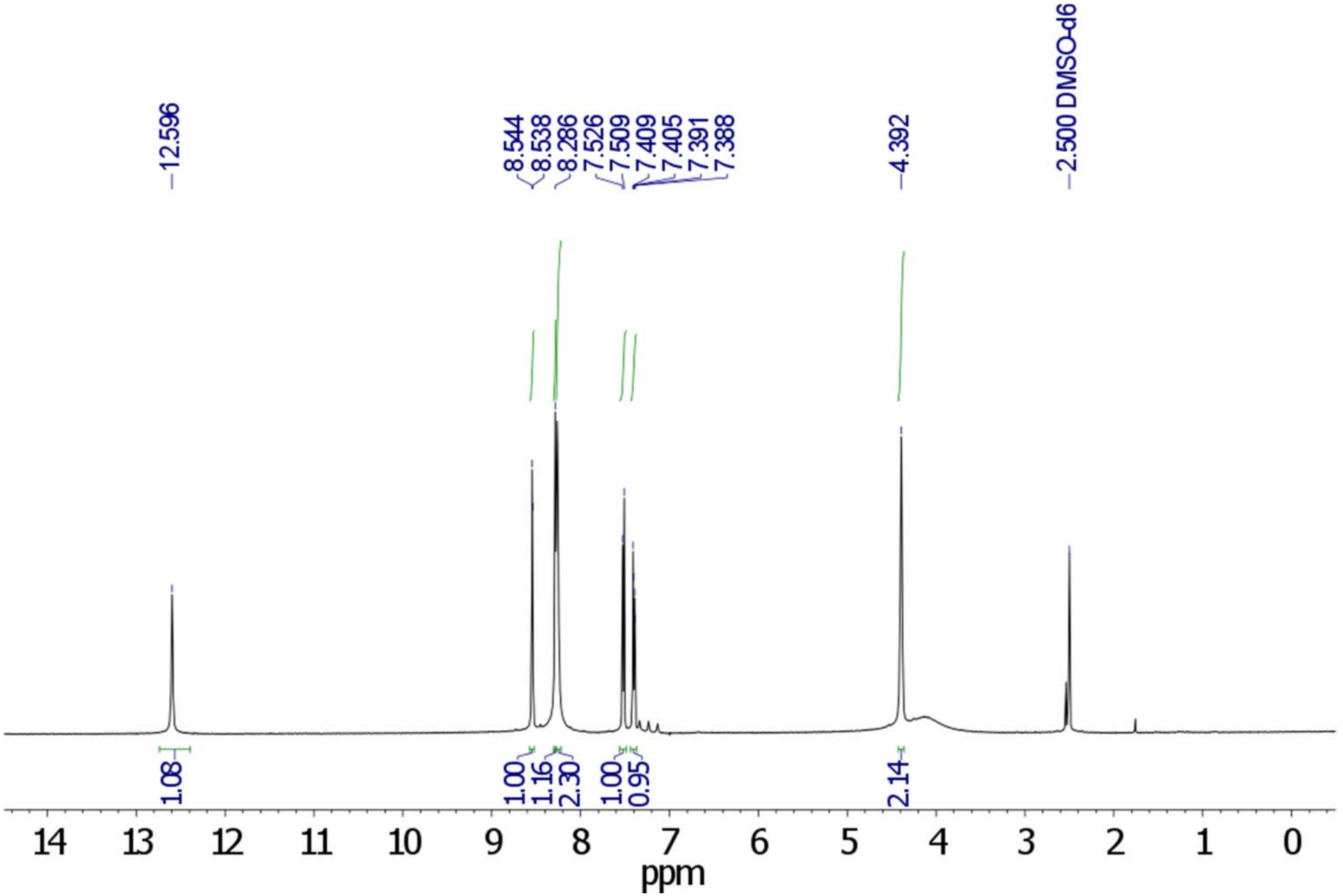

Figure S22. ^{13}C spectrum (125 MHz) of 5-Br-8-keto-tryptamine (**12**) in DMSO-d6.

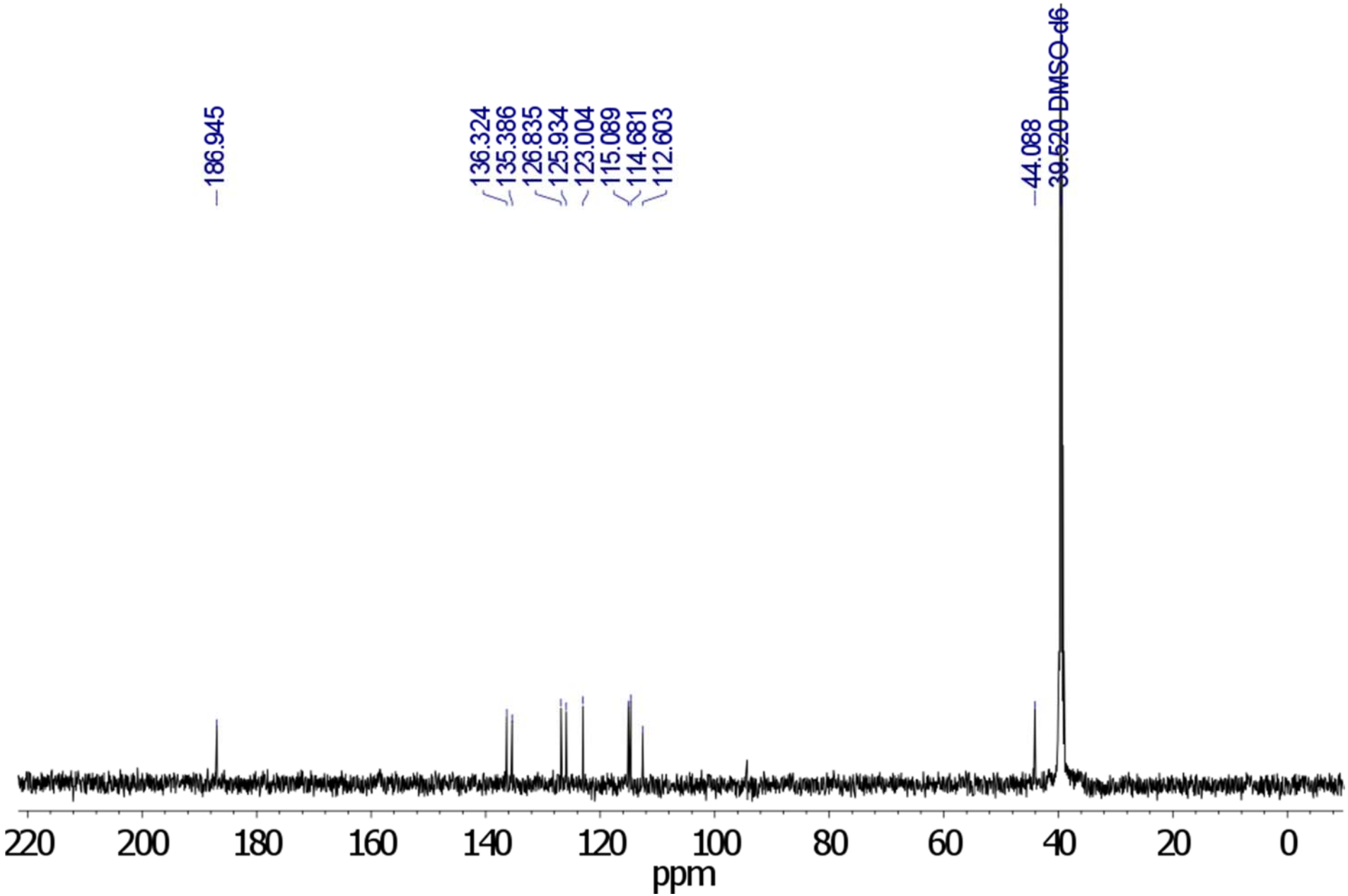

Figure S23. ^{1}H spectrum (600 MHz) of 8-keto-N,N,N-trimethyl-tryptamine (**13**) (formate salt) in DMSO-d6.

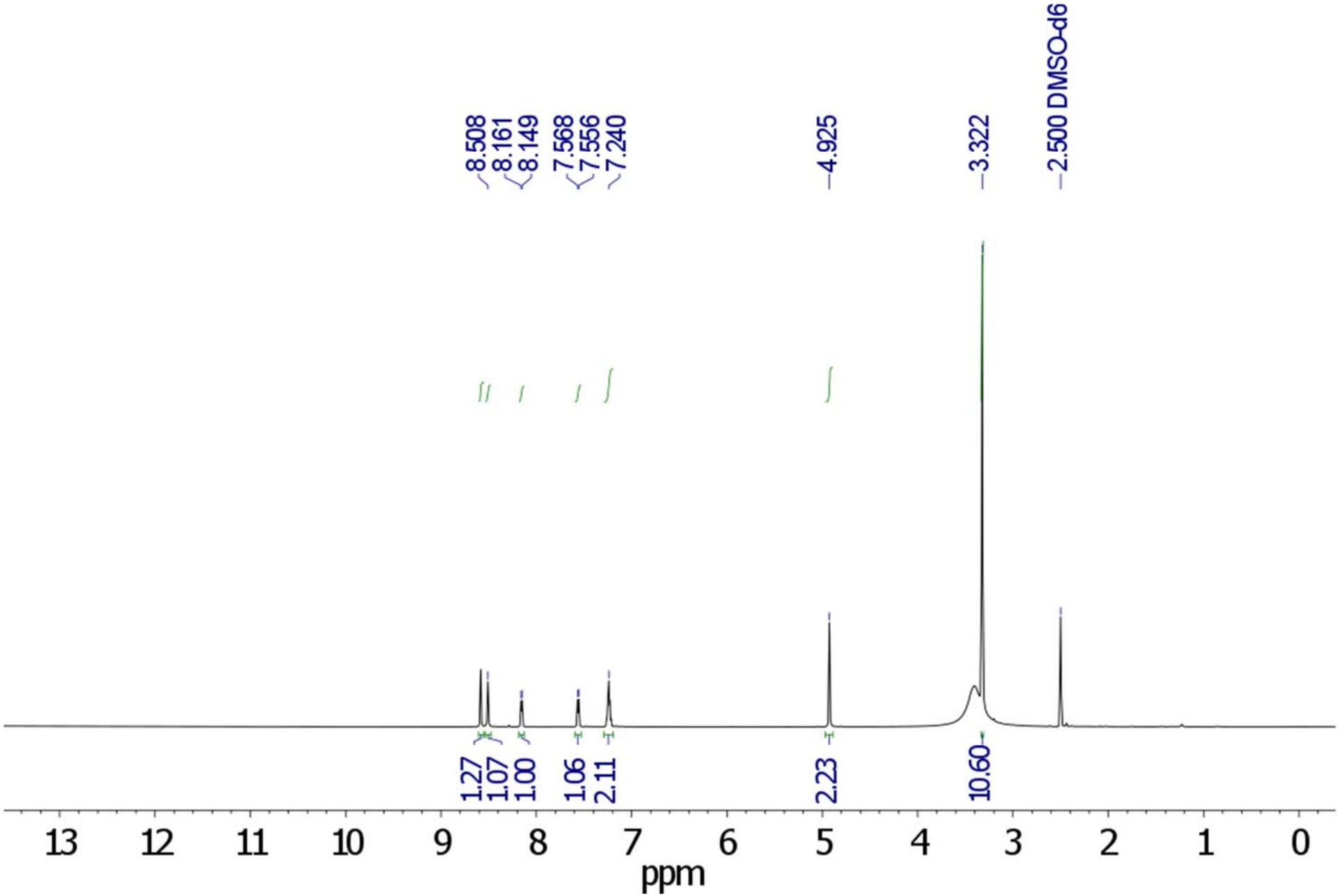

Figure S24. ^{13}C spectrum (150 MHz) of β-oxo-*N,N,N*-trimethyl-tryptamine (**13**) (formate salt) in DMSO-d6.

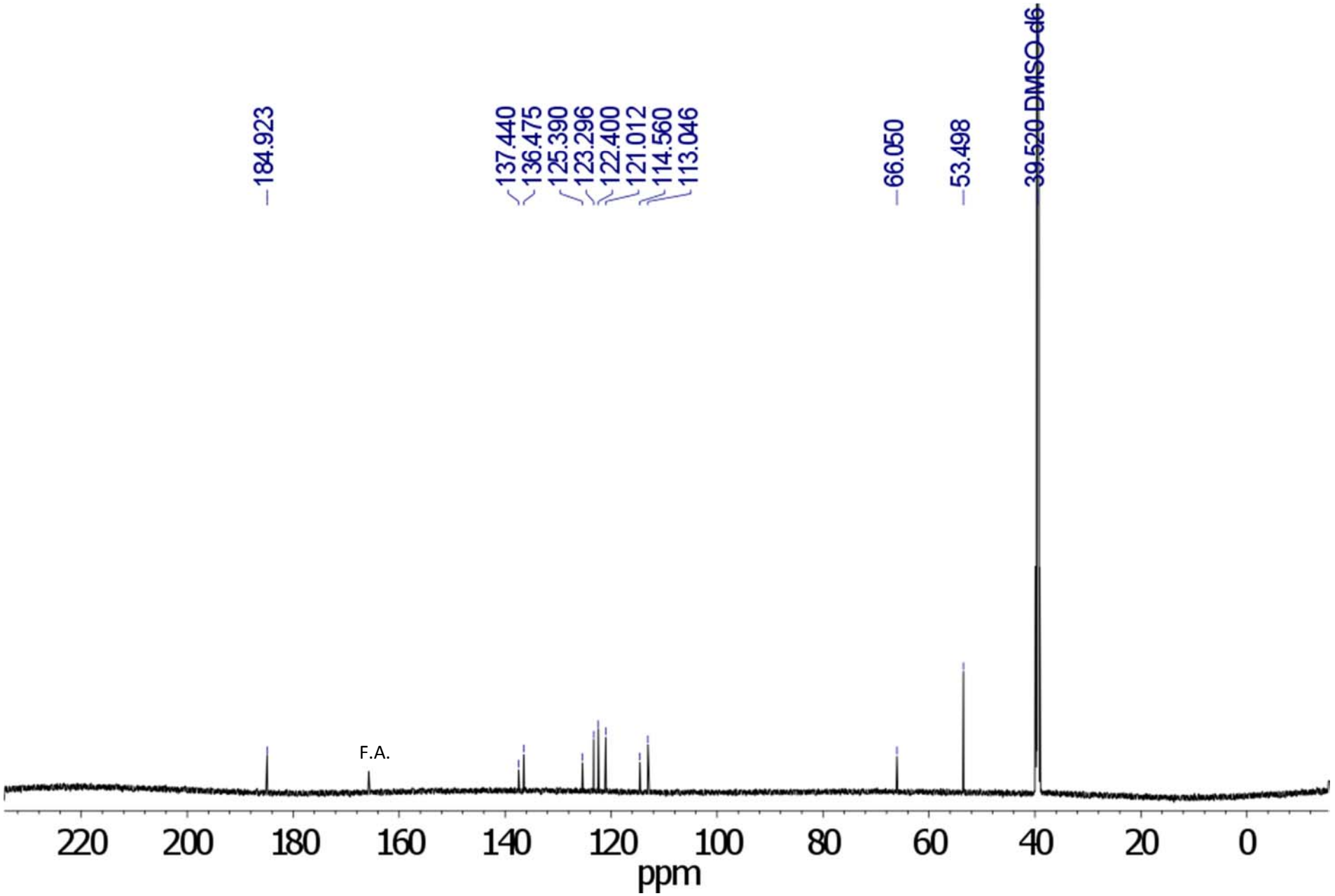

Figure S25. ^{1}H spectrum (600 MHz) of 6-Br-8-keto-*N,N*-dimethyl-tryptamine (**14**) in DMSO-d6.

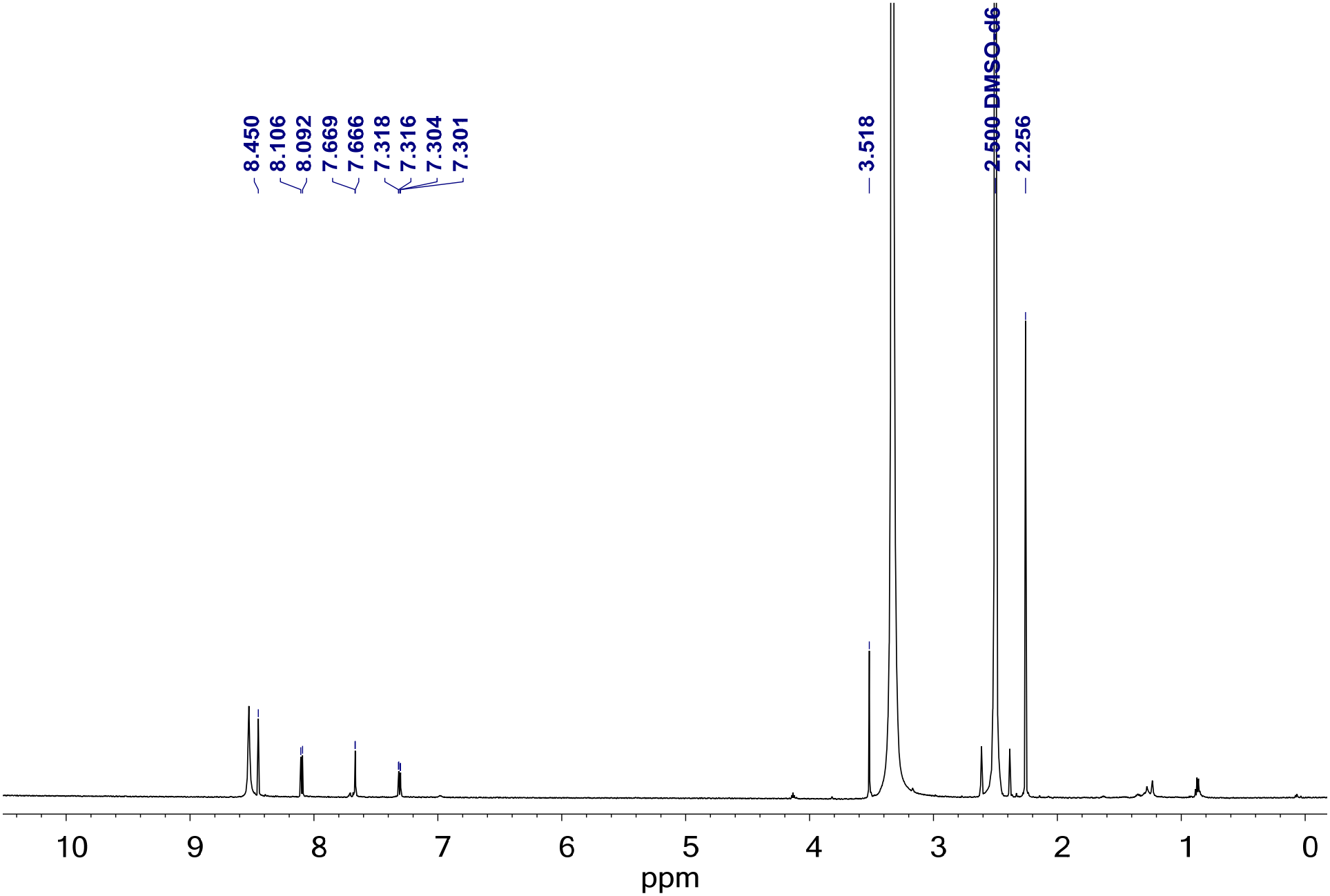

Figure S26. gHMBCAD spectrum (600 MHz) of 6-Br-8-keto-*N,N*-dimethyl-tryptamine (**14**) in DMSO-d6.

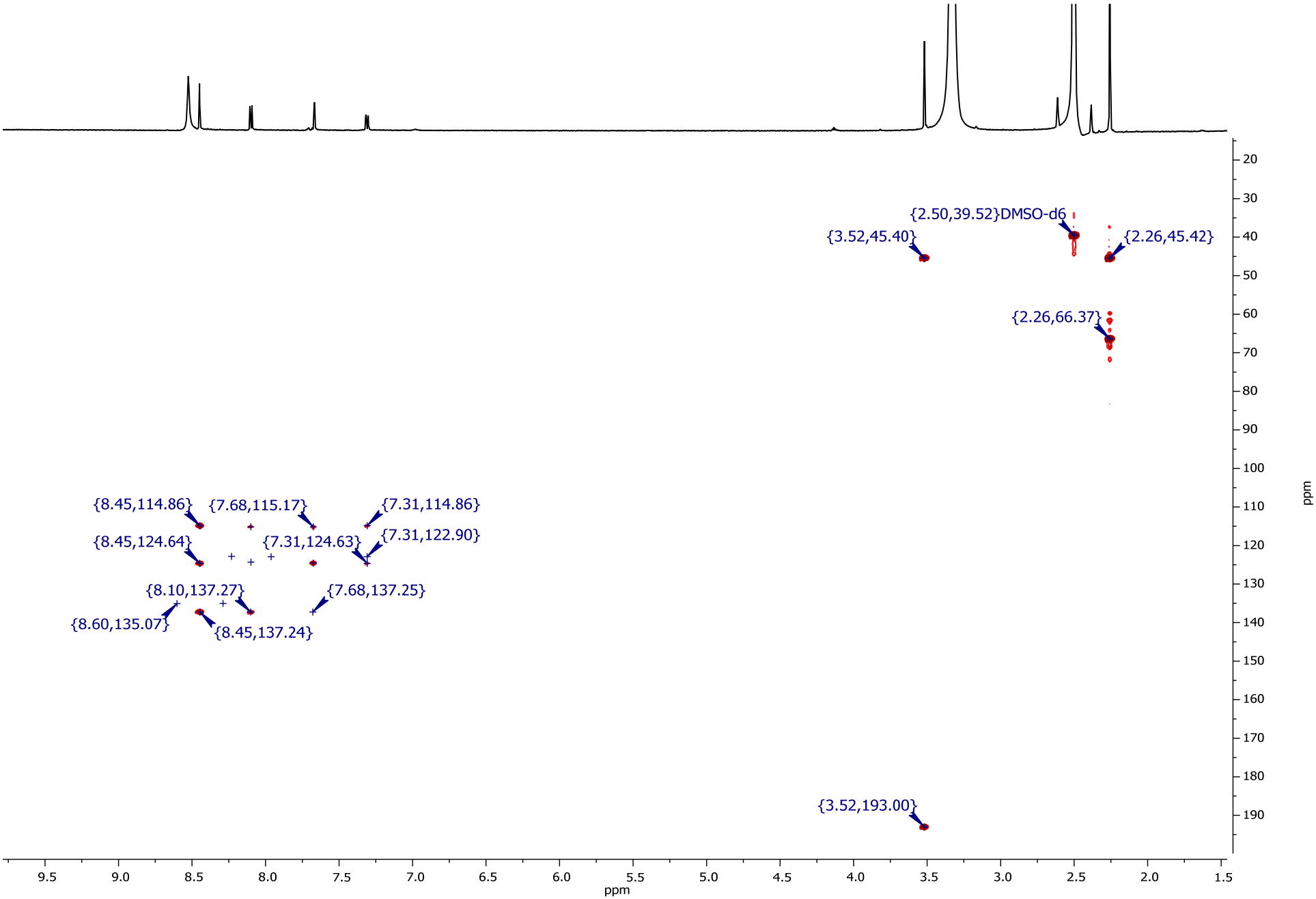

Figure S27. gHMBCAD spectrum (600 MHz) expansion of 6-Br-8-keto-*N,N*-dimethyl-tryptamine (**14**) in DMSO-d6.

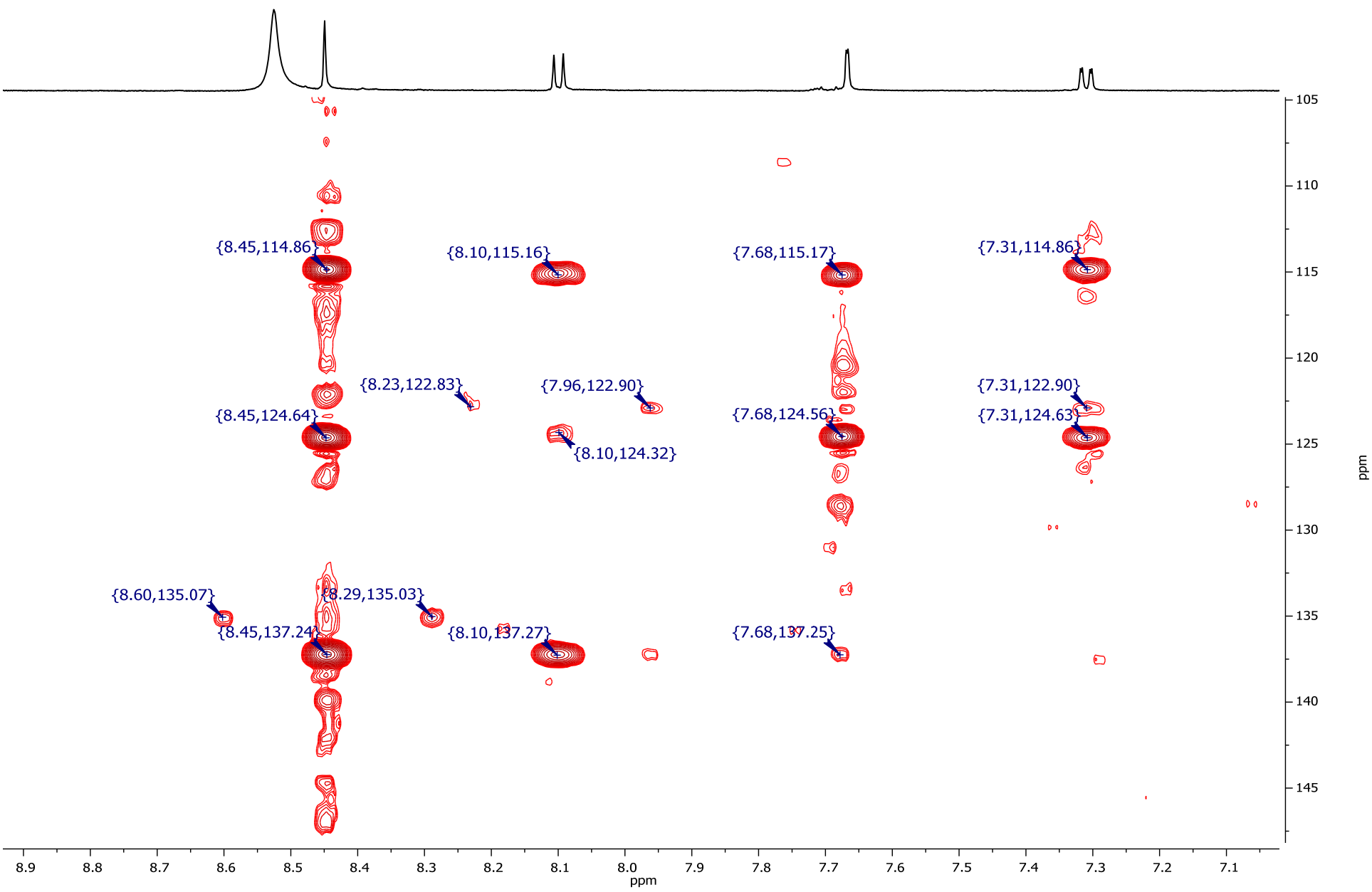

Figure S28. ^{1}H spectrum (600 MHz) of 5-Br-8-keto-*N,N*-dimethyl-tryptamine (**15**) in DMSO-d6.

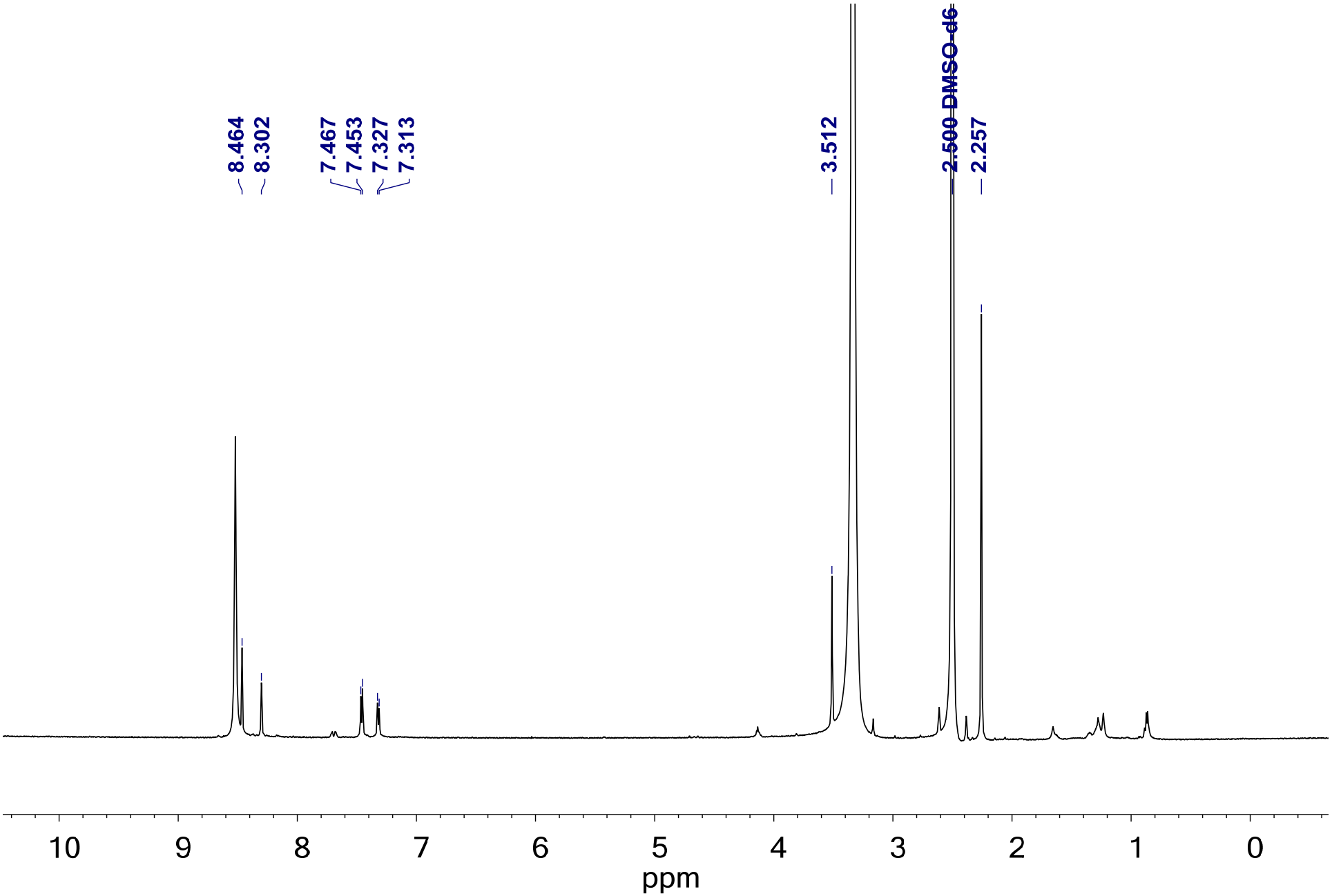

Figure S29. gHMBCAD spectrum (600 MHz) of 5-Br-8-keto-*N,N*-dimethyl-tryptamine (**15**) in DMSO-d6.

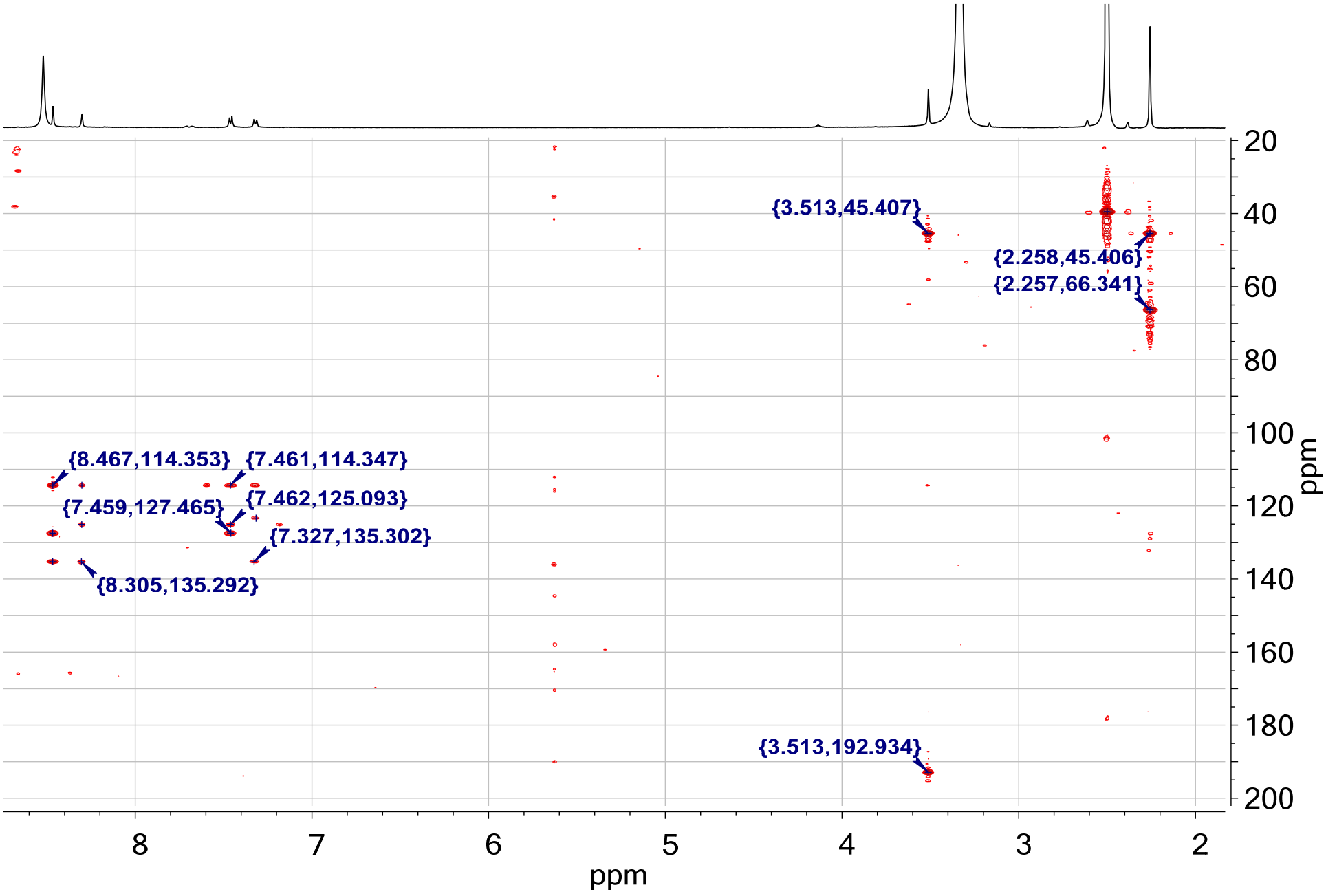

Figure S30. gHMBCAD spectrum (600 MHz) expansion of 5-Br-8-keto-*N,N*-dimethyl-tryptamine (**15**) in DMSO-d6.

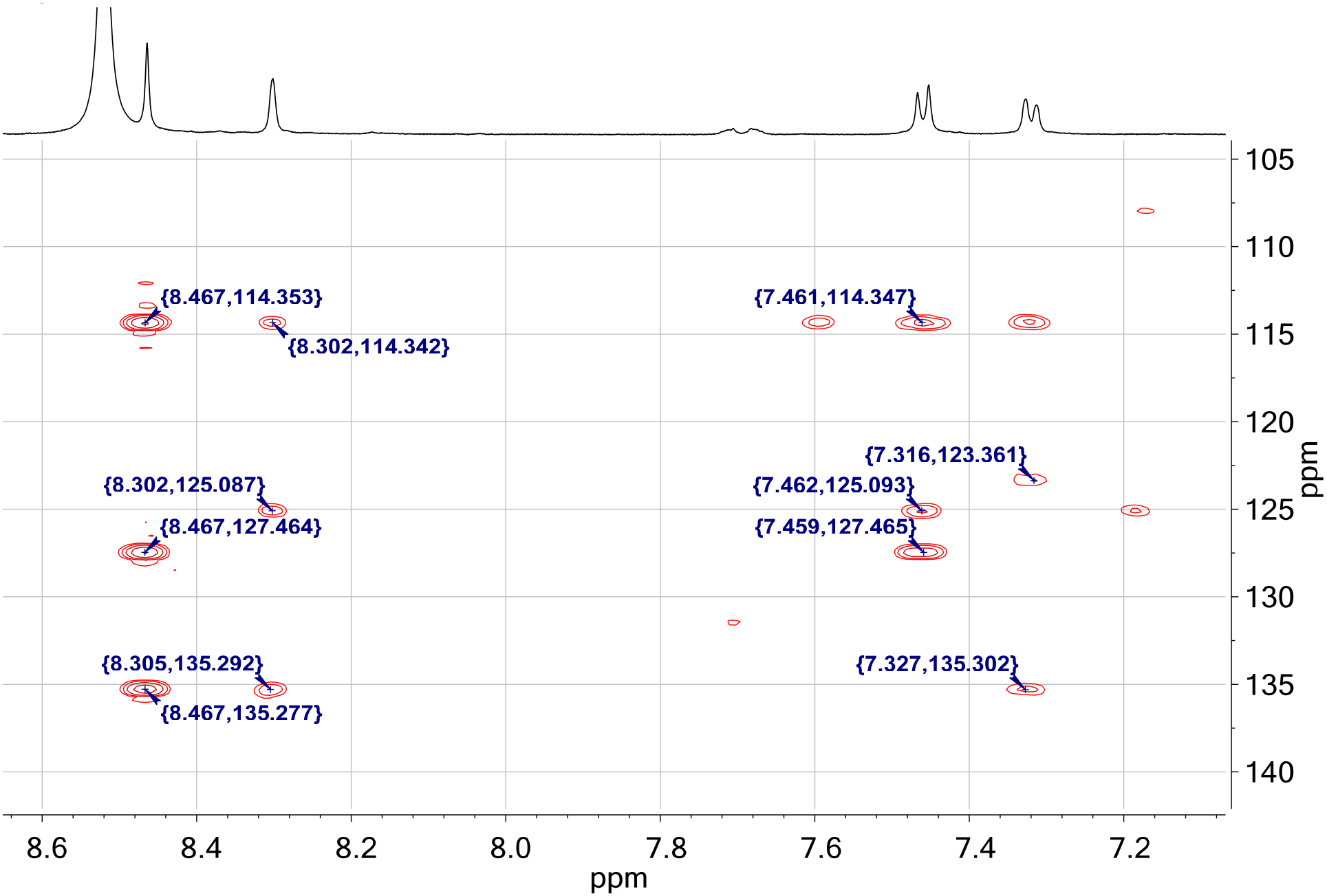

Figure S31. [1]H spectrum (600 MHz) of 8-keto-*N,N*-dimethyl-tryptamine (**16**) in DMSO-d6.

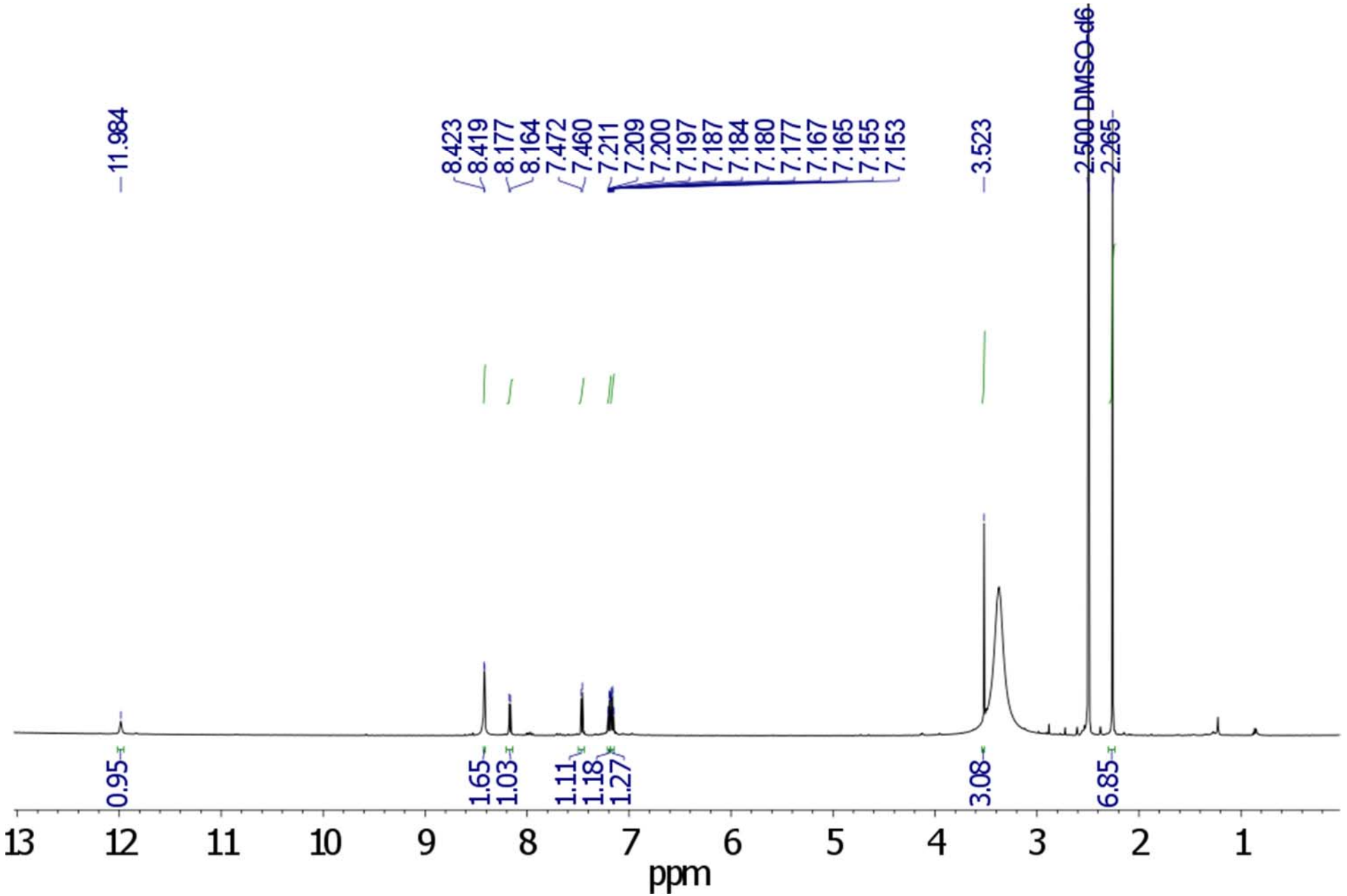

Figure S32. gHMBCAD spectrum (600 MHz) of 8-keto-*N,N*-dimethyl-tryptamine (**16**) in DMSO-d6.

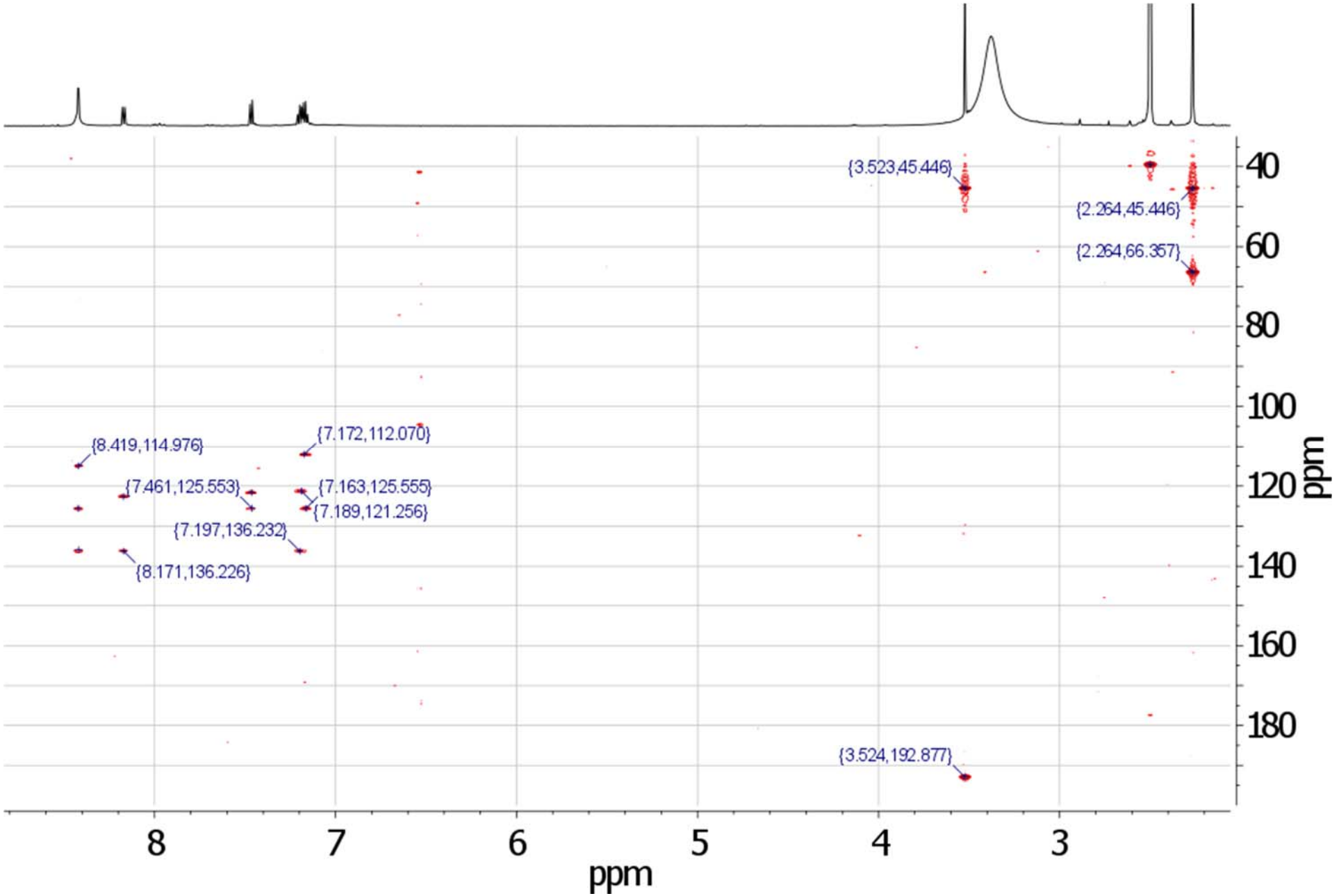

Figure S33. gHMBCAD spectrum expansion (600 MHz) of 8-keto-*N,N*-dimethyl-tryptamine (**16**) in DMSO-d6.

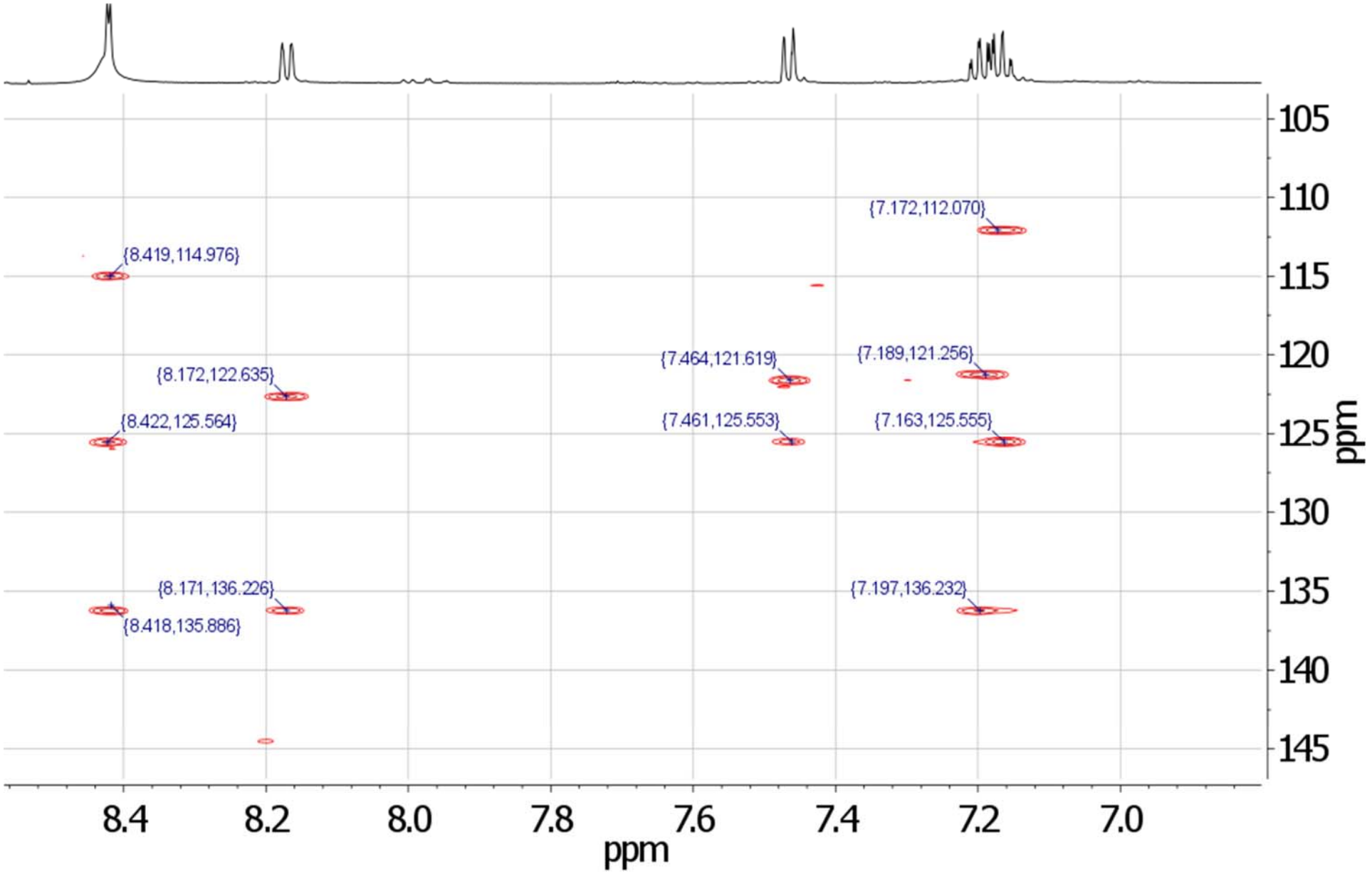

Figure S34. ^{1}H spectrum (600 MHz) of 6-bromo-1H-indol-3-yl-carboxaldehyde (Tokyo Chemical Industry, Tokyo, Japan) (**5**) in DMSO-d6.

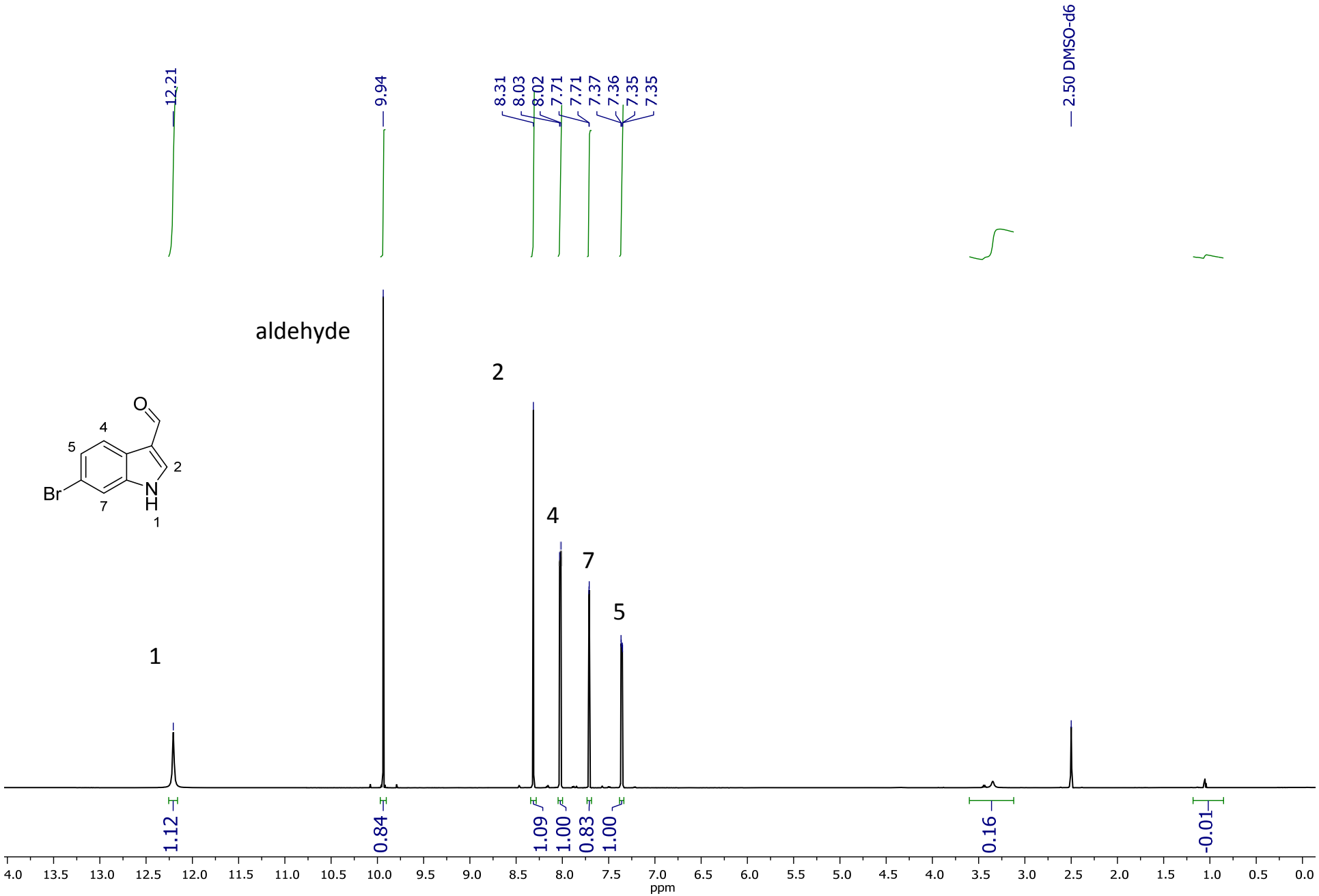

Figure S35. ^{1}H spectrum expansion (600 MHz) of 6-bromo-1H-indol-3-yl-carboxaldehyde (Tokyo Chemical Industry, Tokyo, Japan) (**5**) in DMSO-d6.

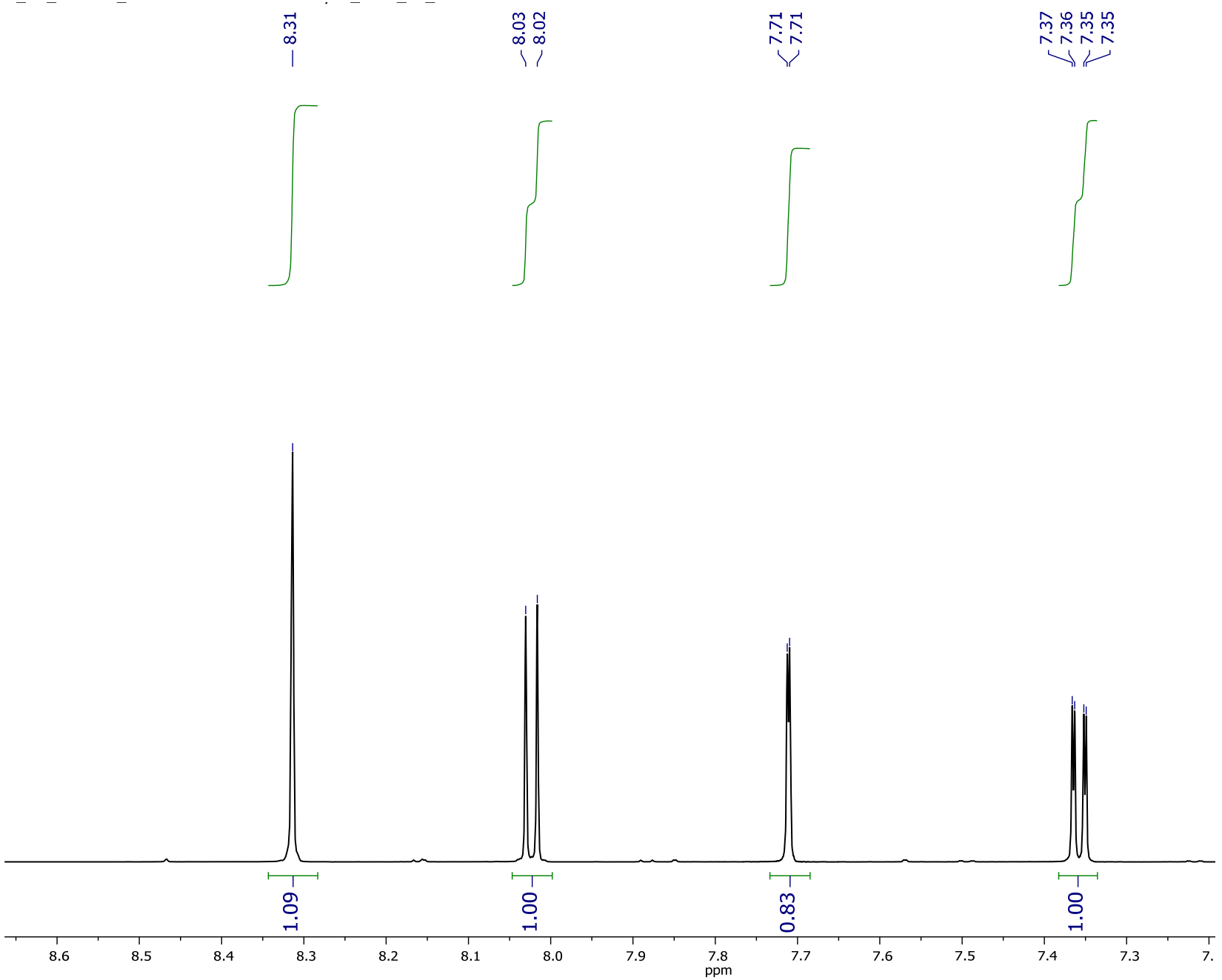

Figure S36. ^{13}C spectrum (150 MHz) of 6-bromo-1H-indol-3-yl-carboxaldehyde (Tokyo Chemical Industry, Tokyo, Japan) (**5**) in DMSO-d6.

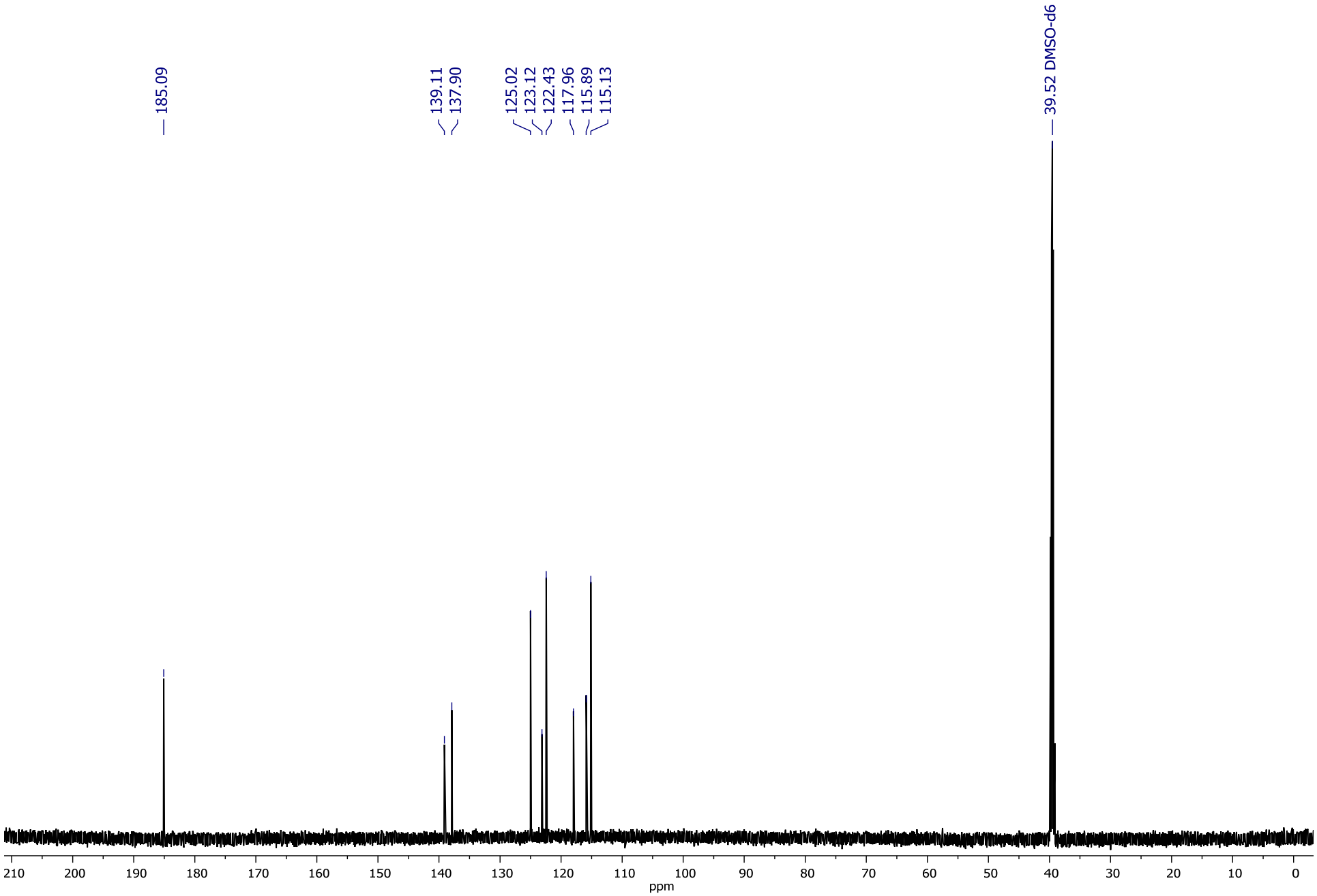

Figure S37. gHSQCAD spectrum (600 MHz) of 6-bromo-1H-indol-3-yl-carboxaldehyde (Tokyo Chemical Industry, Tokyo, Japan) (**5**) in DMSO-d6.

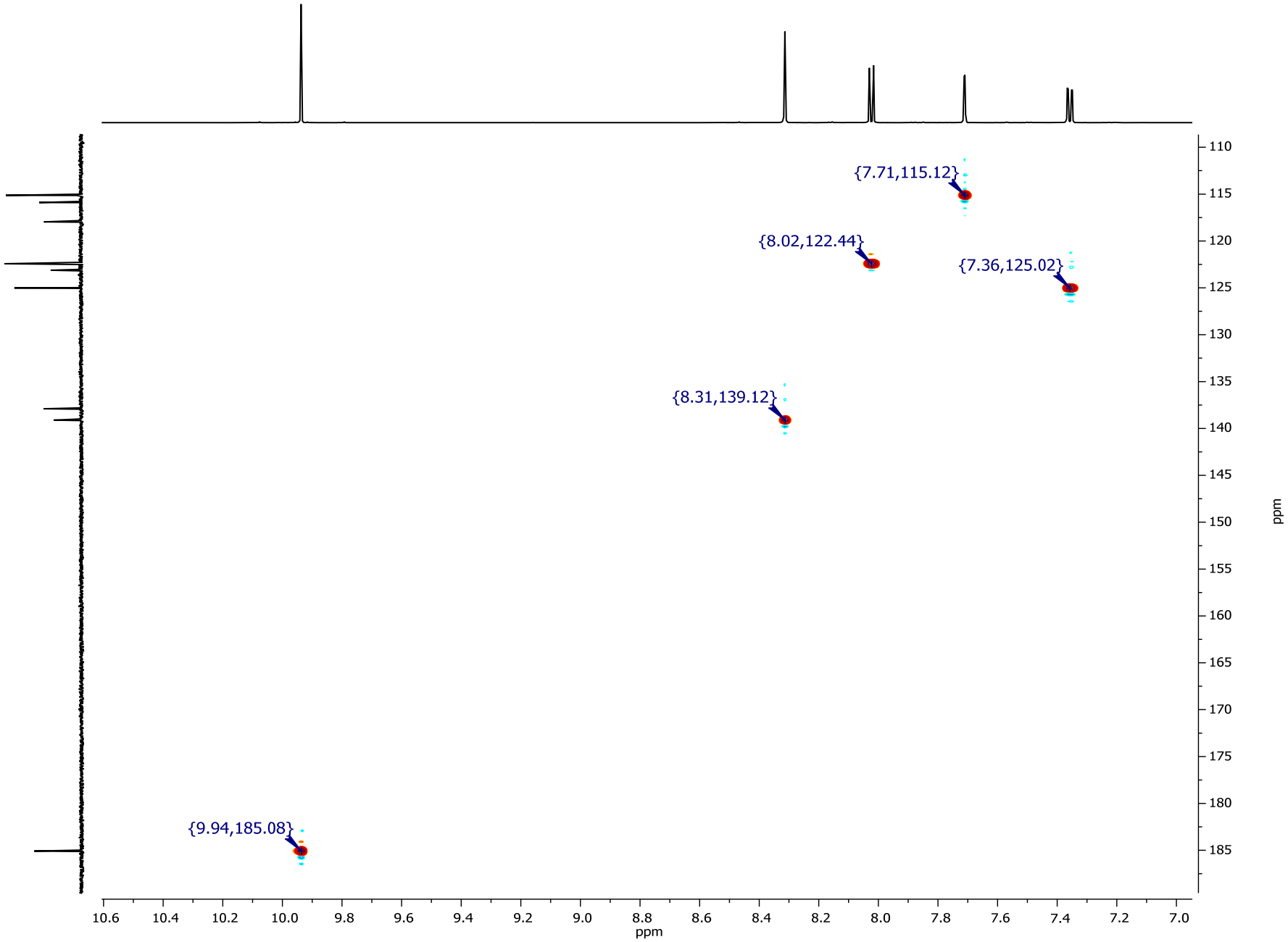

Figure S38. NOESY spectrum (600 MHz, 600ms mixing time) of 6-bromo-1H-indol-3-yl-carboxaldehyde (Tokyo Chemical Industry, Tokyo, Japan) (**5**) in DMSO-d6.