BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

Convenient alternative synthesis of the *Malassezia*-derived virulence factor malassezione and related compounds

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Copies of NMR and MS spectra of synthesized compounds

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Figure S1. ^{1}H NMR spectrum of *tert*-butyl 3-(2-methoxy-2-oxoethyl)-1*H*-indole-1-carboxylate (**21**) in $CDCl_3$

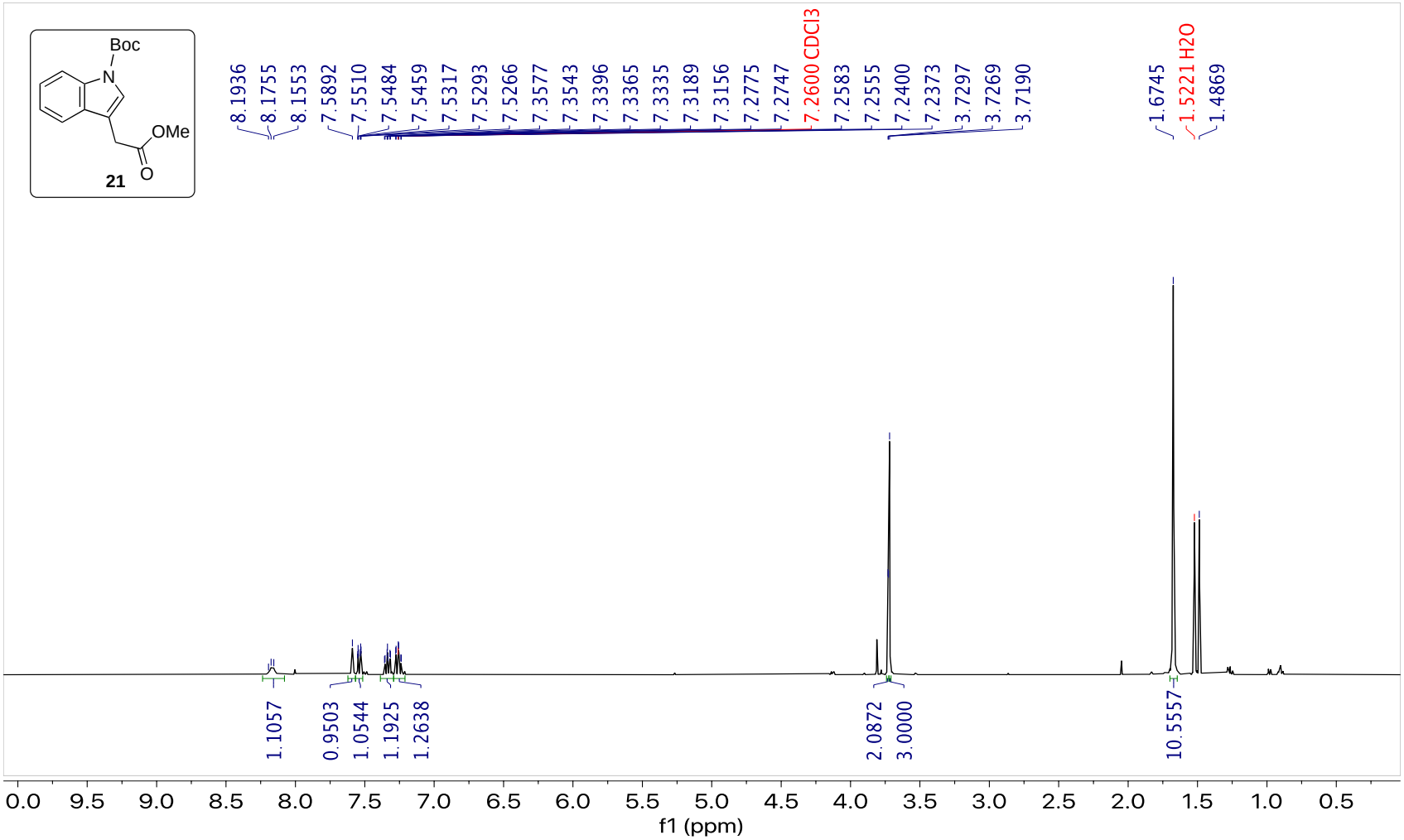

Figure S2. ^{13}C NMR spectrum of *tert*-butyl 3-(2-methoxy-2-oxoethyl)-1*H*-indole-1-carboxylate (**21**) in $CDCl_3$

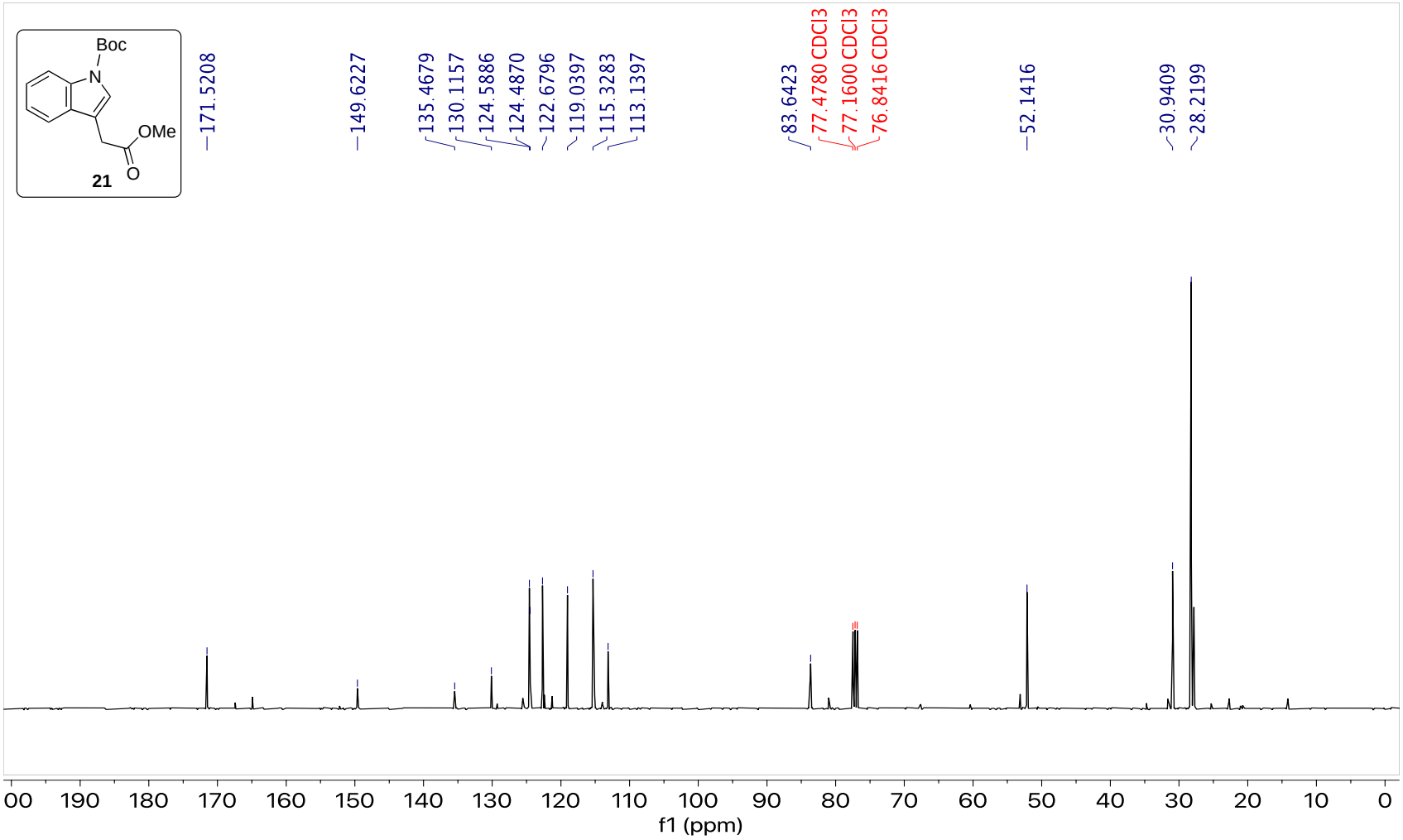

Figure S3. ^{1}H NMR spectrum of 2-(1-(*tert*-butoxycarbonyl)-1*H*-indol-3-yl)acetic acid (**22**) in $CDCl_3$

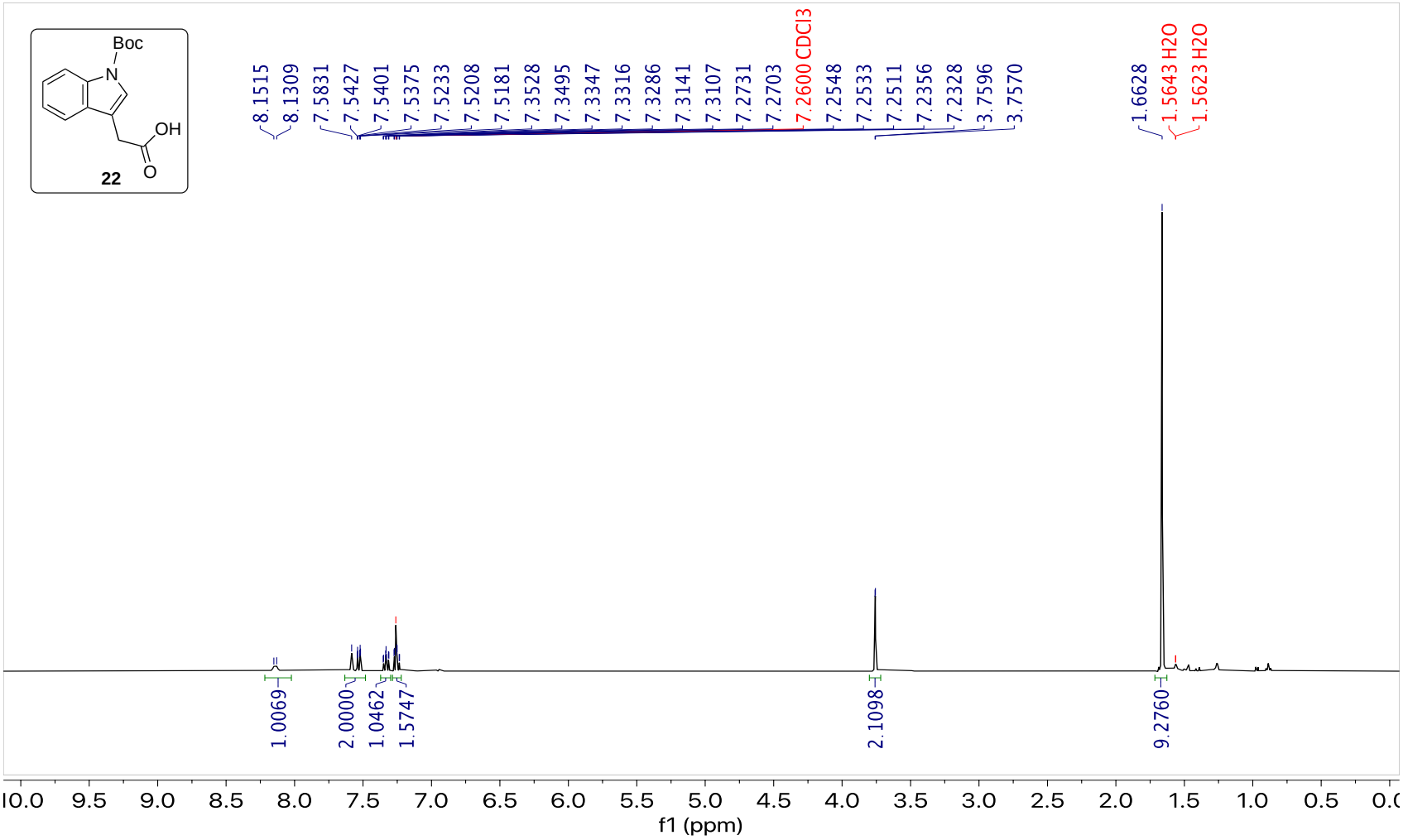

Figure S4. ^{13}C NMR spectrum of 2-(1-(*tert*-butoxycarbonyl)-1*H*-indol-3-yl)acetic acid (**22**) in $CDCl_3$

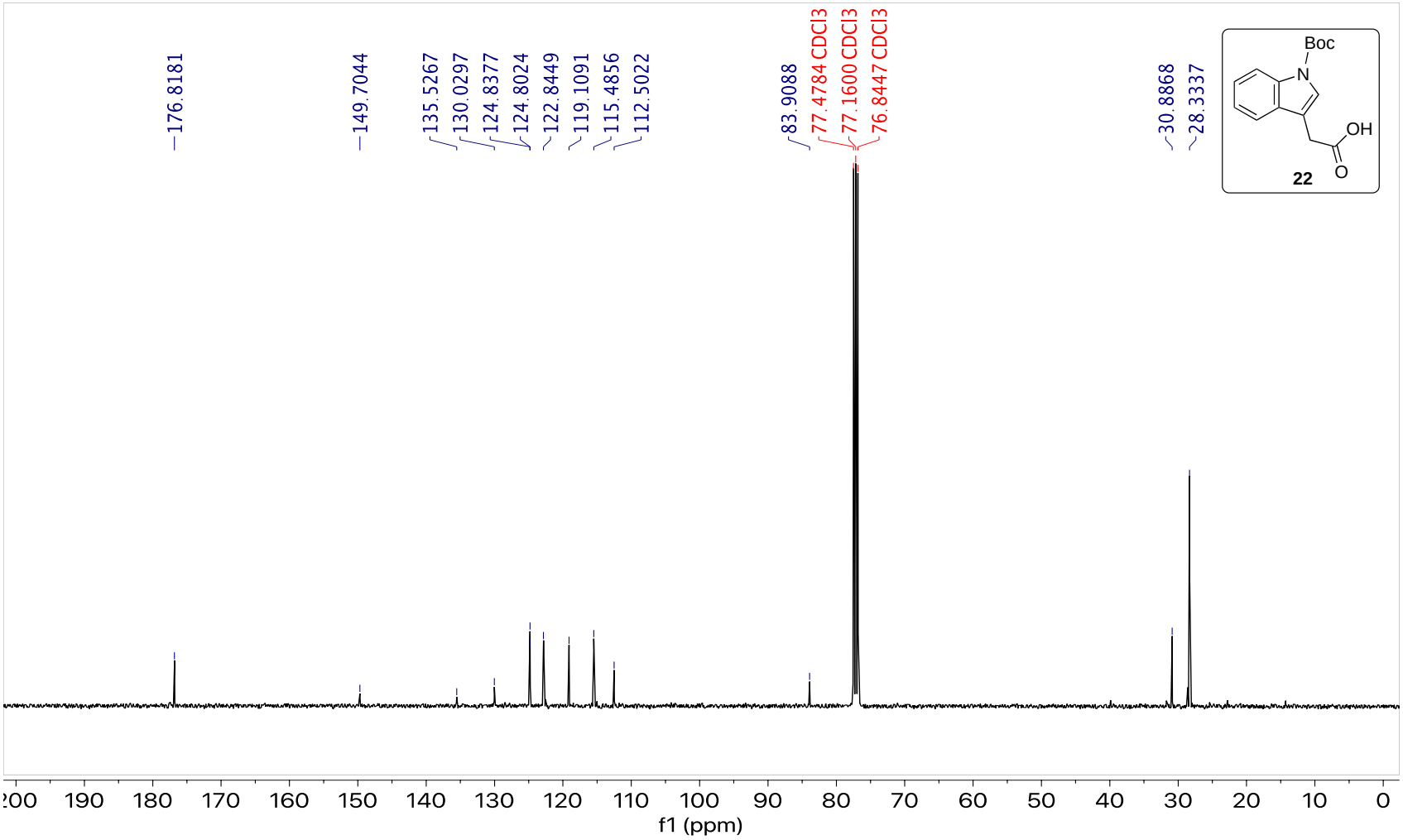

Figure S5. ^{1}H NMR spectrum of di-*tert*-butyl 3,3'-(2-oxopropane-1,3-diyl)bis(1*H*-indole-1-carboxylate) (**23**) in $CDCl_3$

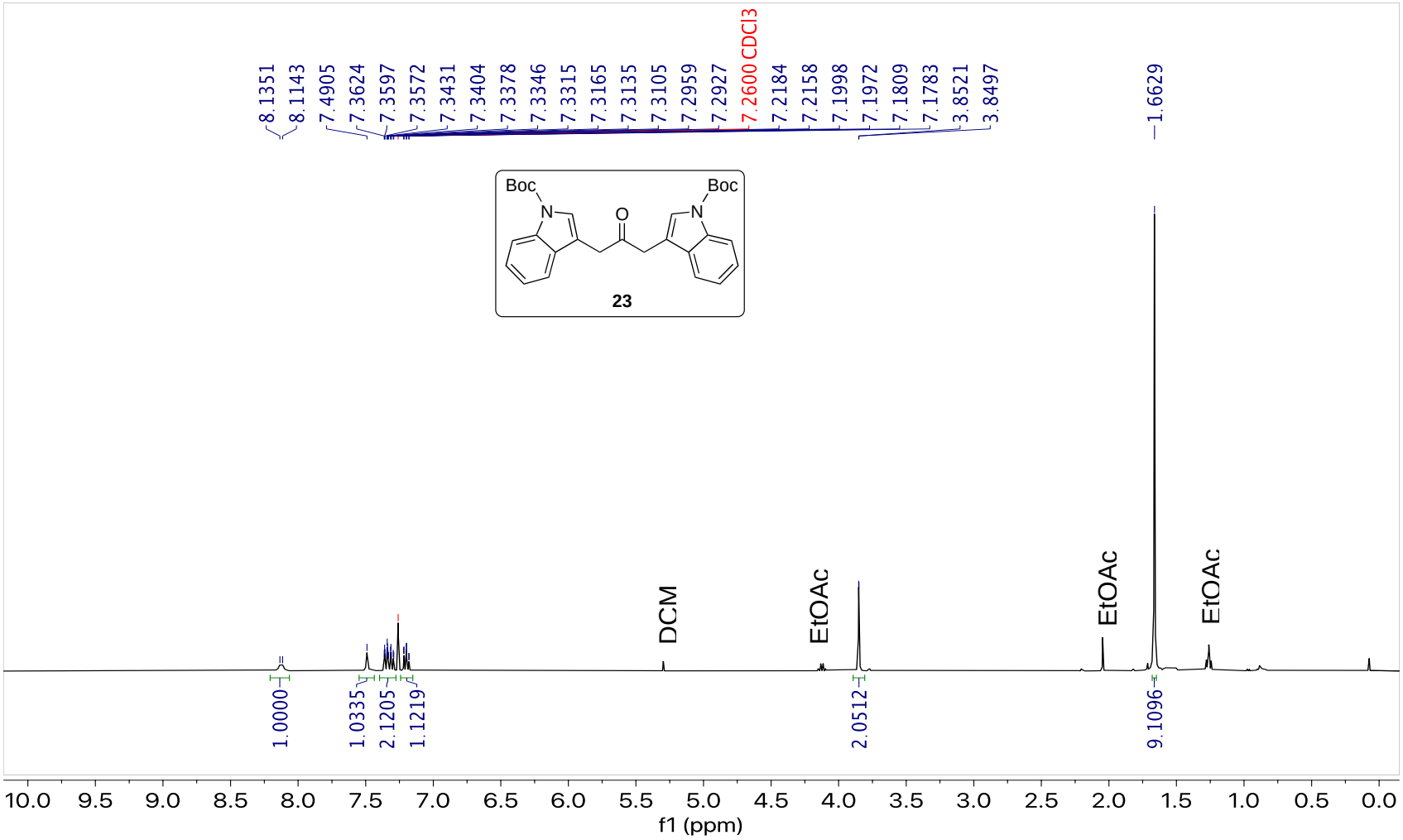

Figure S6. ^{13}C NMR spectrum of di-*tert*-butyl 3,3'-(2-oxopropane-1,3-diyl)bis(1*H*-indole-1-carboxylate) (**23**) in $CDCl_3$

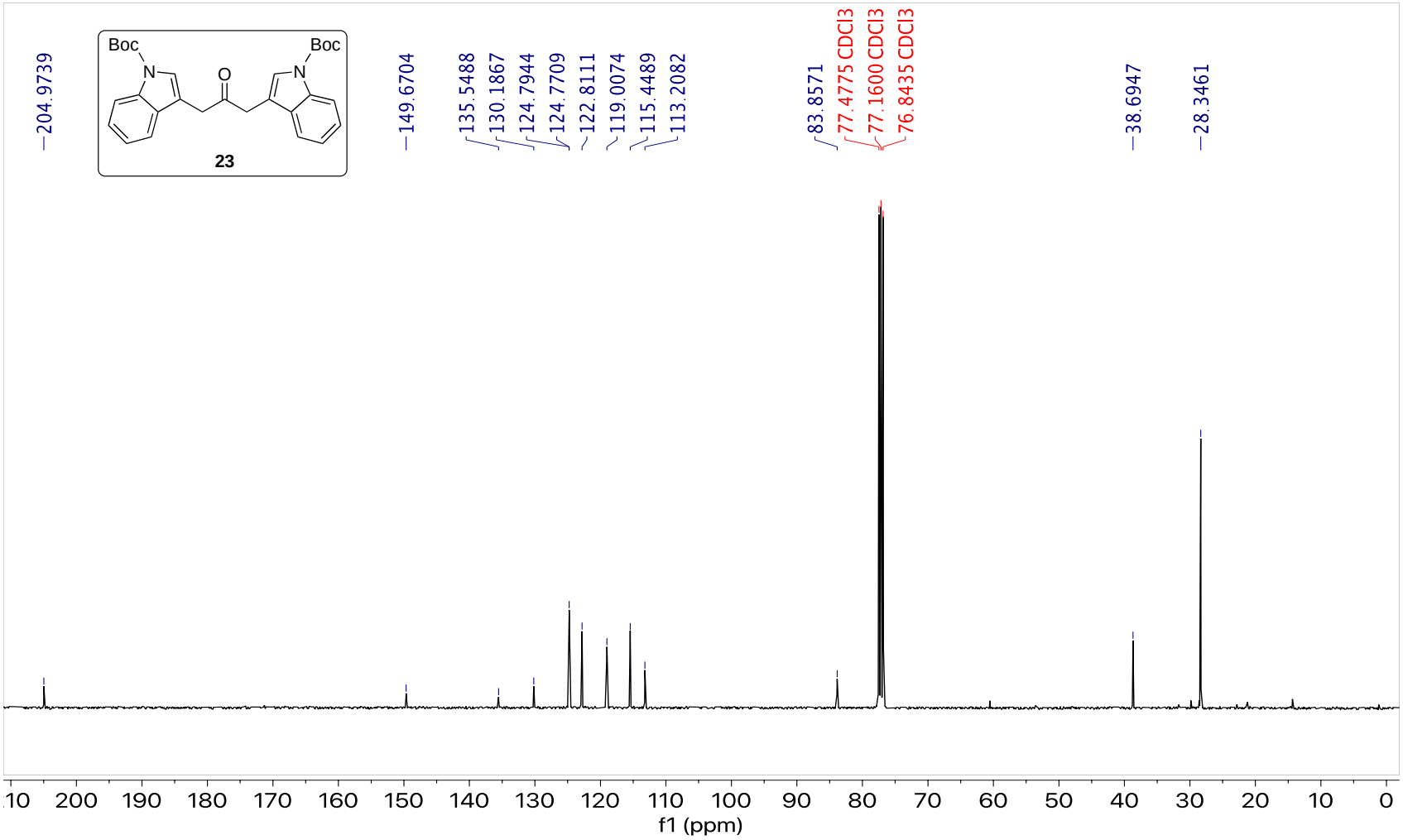

Figure S7. ^{1}H NMR spectrum of 1,3-di(1*H*-indol-3-yl)propan-2-one (**1**) in $CDCl_3$

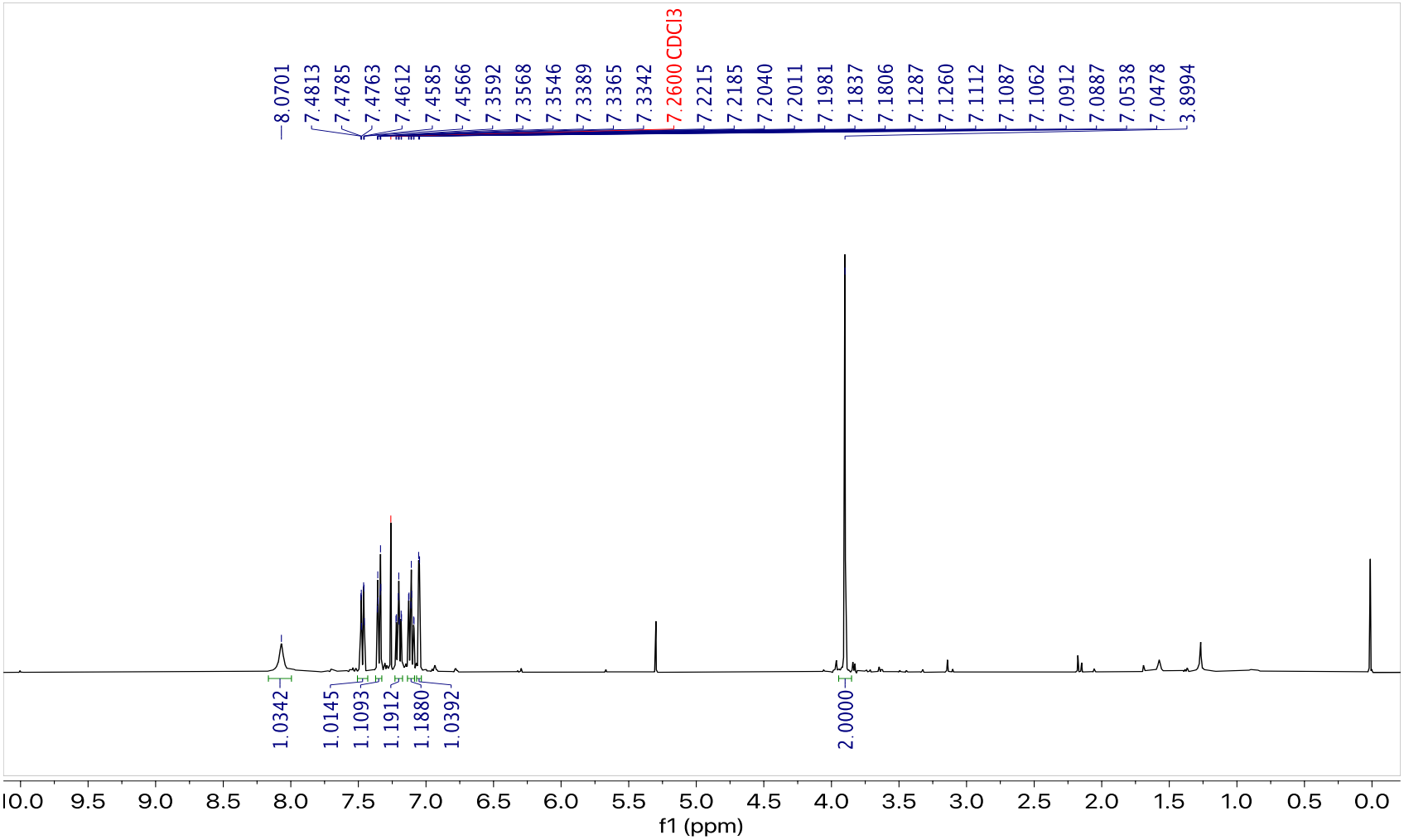

Figure S8. ^{13}C NMR spectrum of 1,3-di(1*H*-indol-3-yl)propan-2-one (**1**) in $CDCl_3$

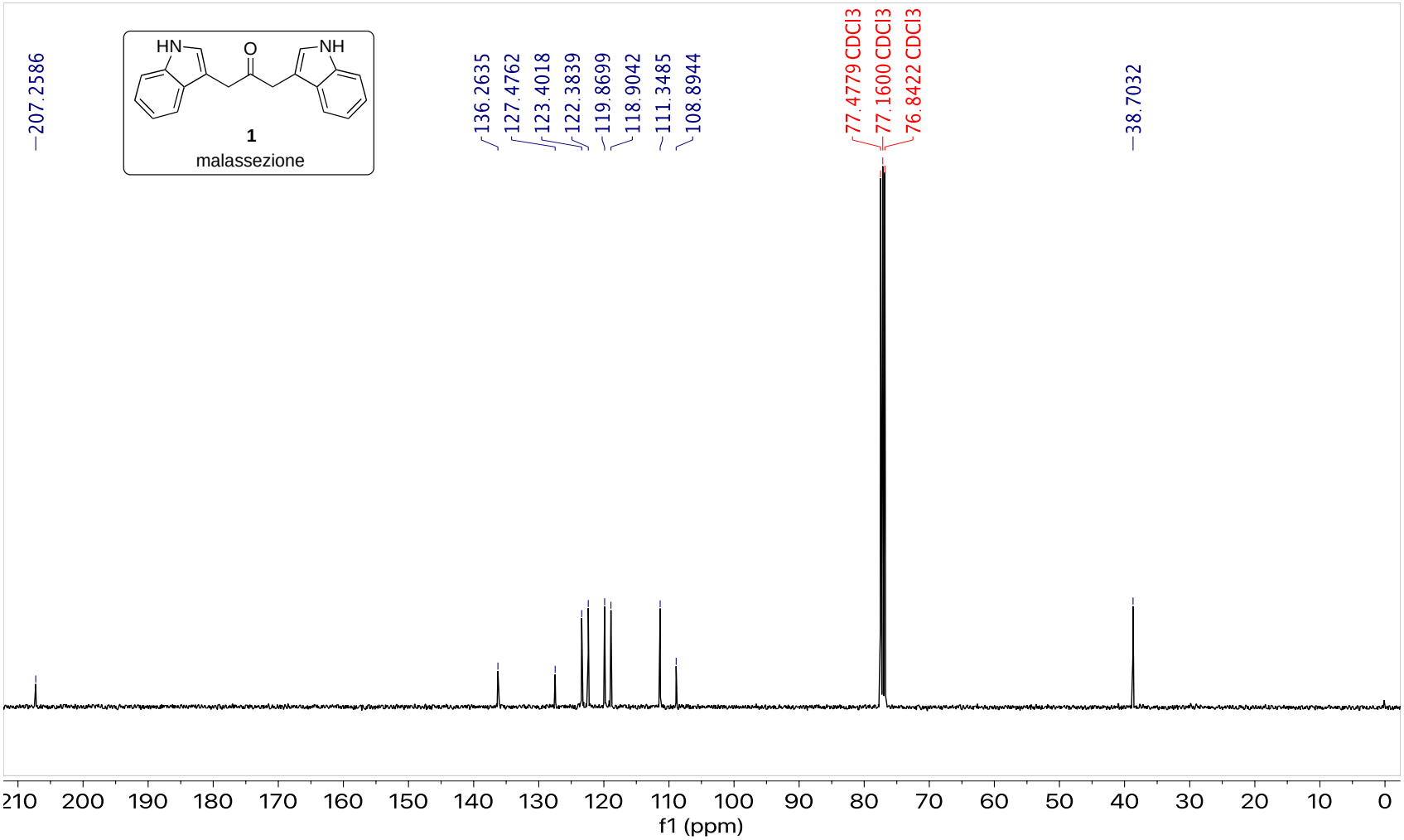

Figure S9. ^{1}H-^{1}H-COSY NMR spectrum of 1,3-di(1*H*-indol-3-yl)propan-2-one **(1)** in $CDCl_3$

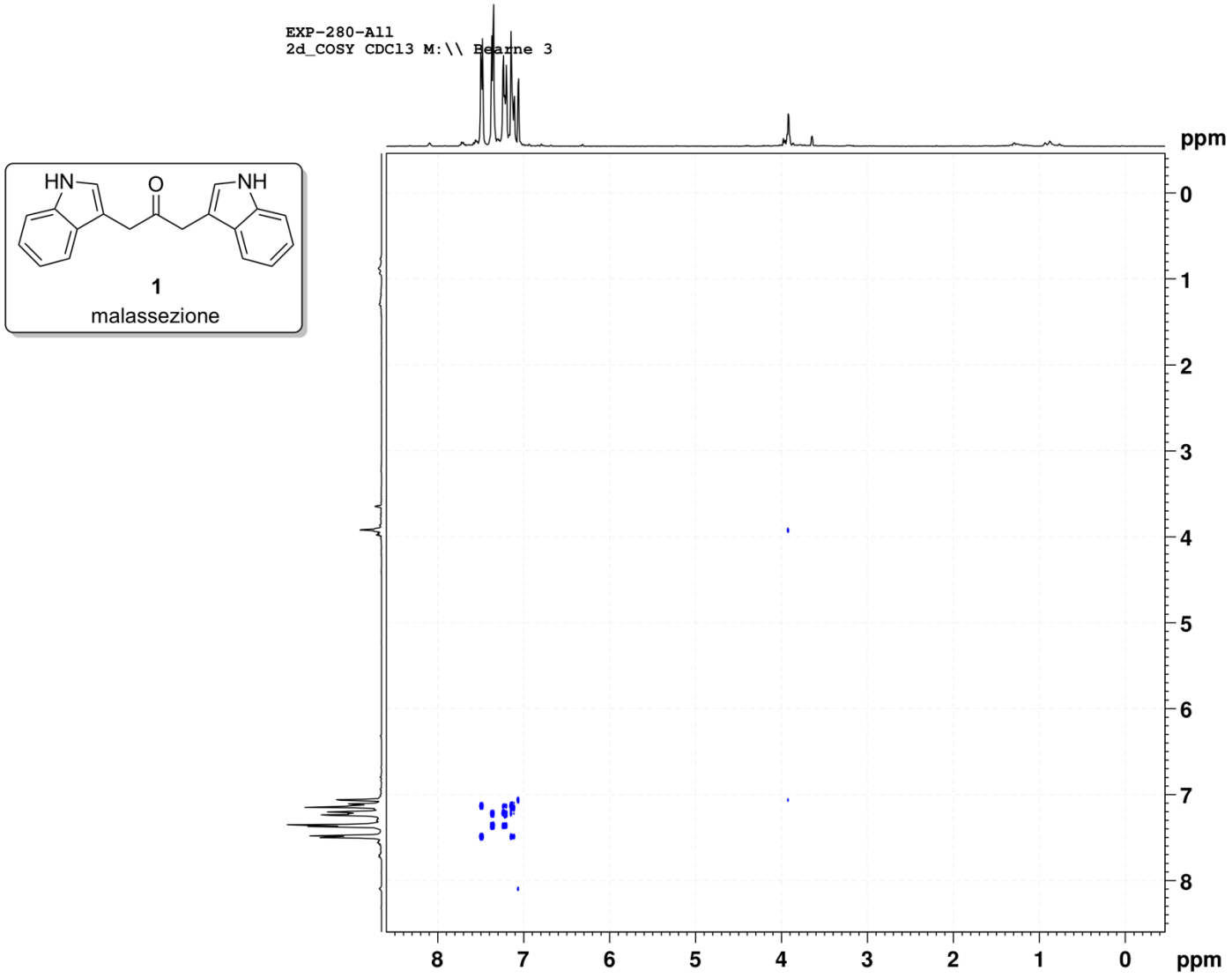


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Figure S10. Expanded ^{1}H-^{1}H-COSY NMR spectrum of 1,3-di(1*H*-indol-3-yl)propan-2-one (**1**)

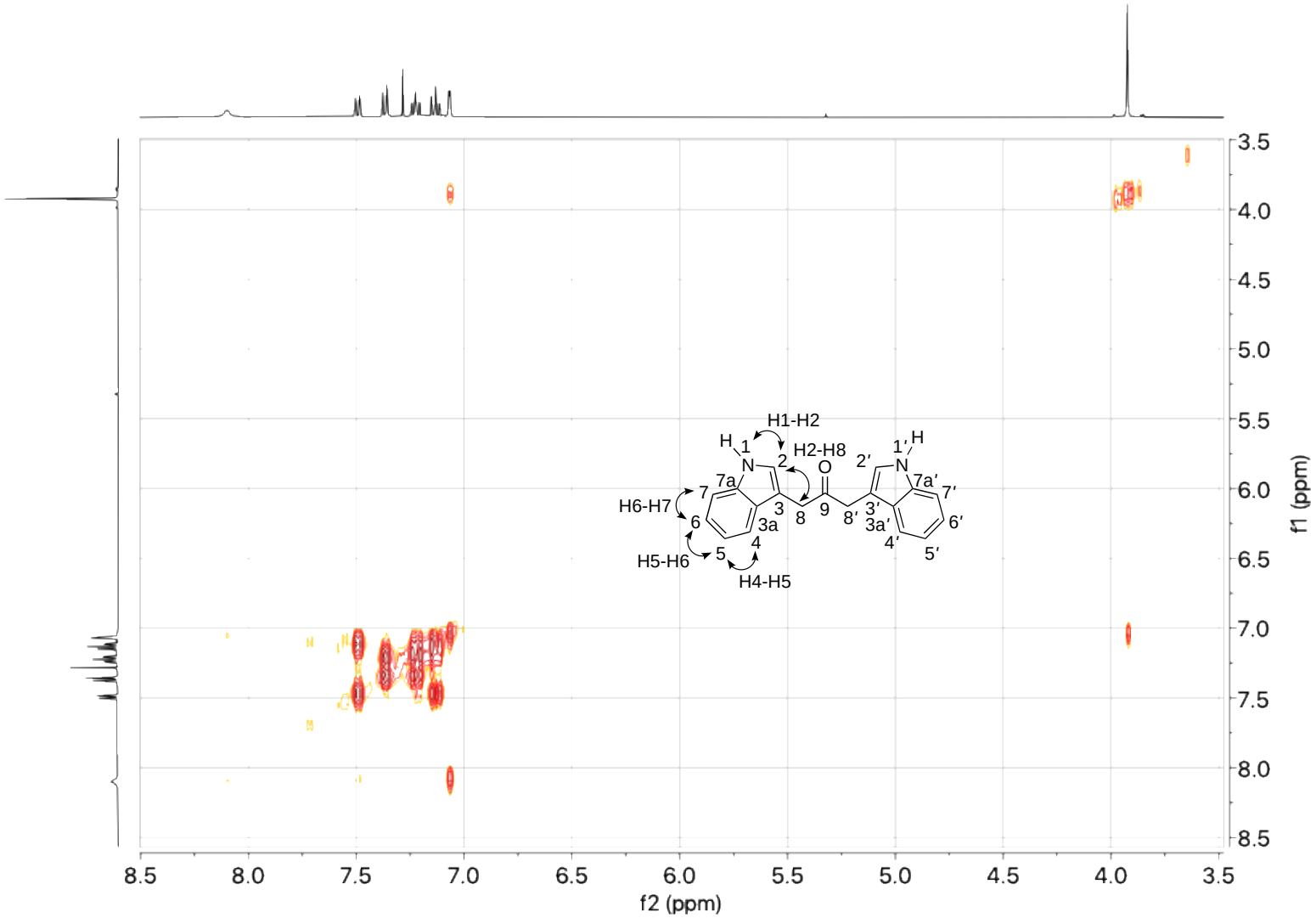

Figure S11. Expanded aromatic region of the ^{1}H-^{1}H-COSY NMR spectrum of 1,3-di(1*H*-indol-3-yl)propan-2-one (**1**)

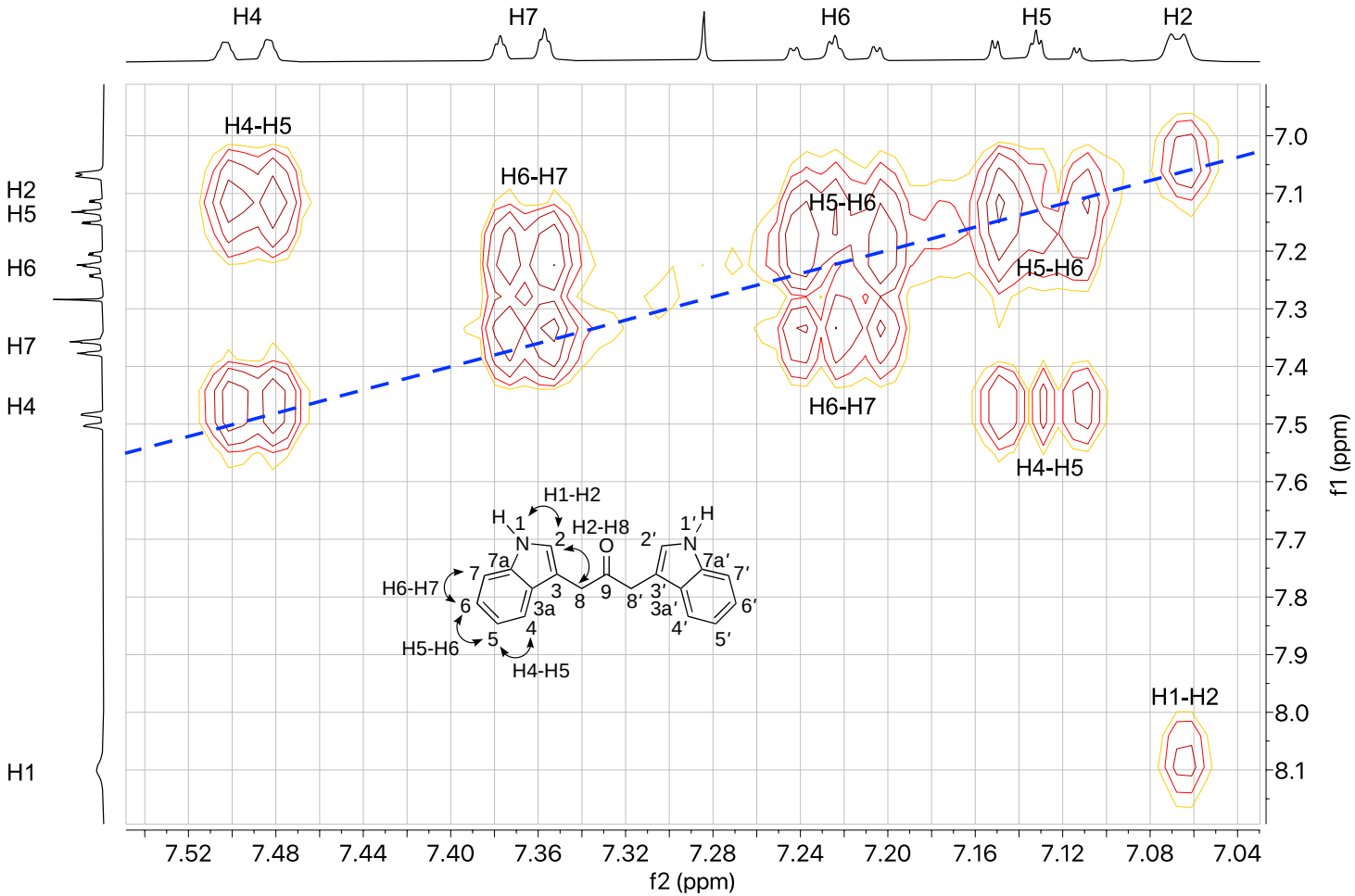

Figure S12. ^{1}H-^{13}C-HMBC NMR spectrum of 1,3-di(1*H*-indol-3-yl)propan-2-one (**1**) in $CDCl_3$

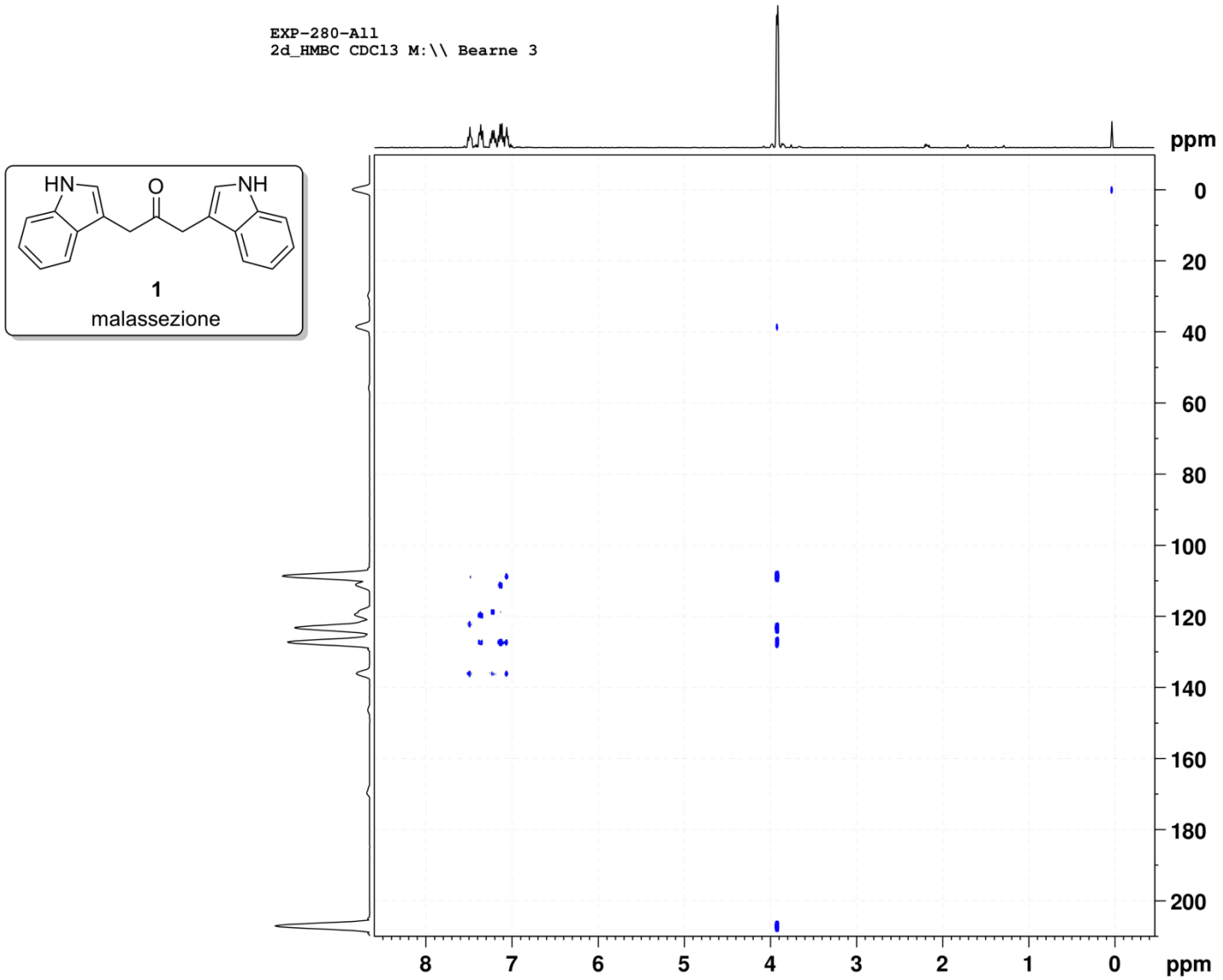


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Figure S13. Expanded ^{1}H-^{13}C-HMBC NMR spectrum of 1,3-di(1*H*-indol-3-yl)propan-2-one (**1**)

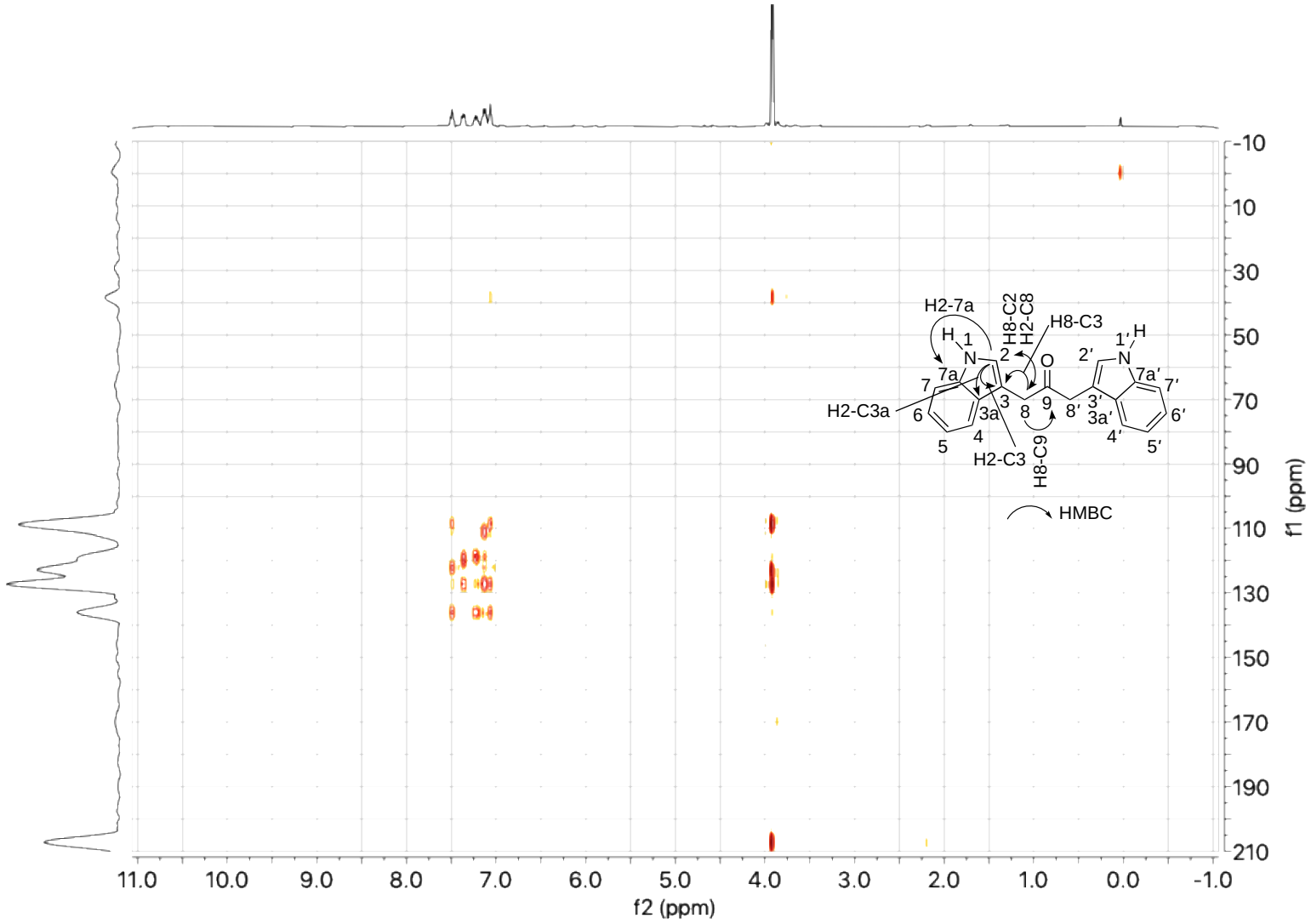

Figure S14. ^{1}H NMR spectrum of 1,3-diphenylpropan-2-one (**25a**) in $CDCl_3$

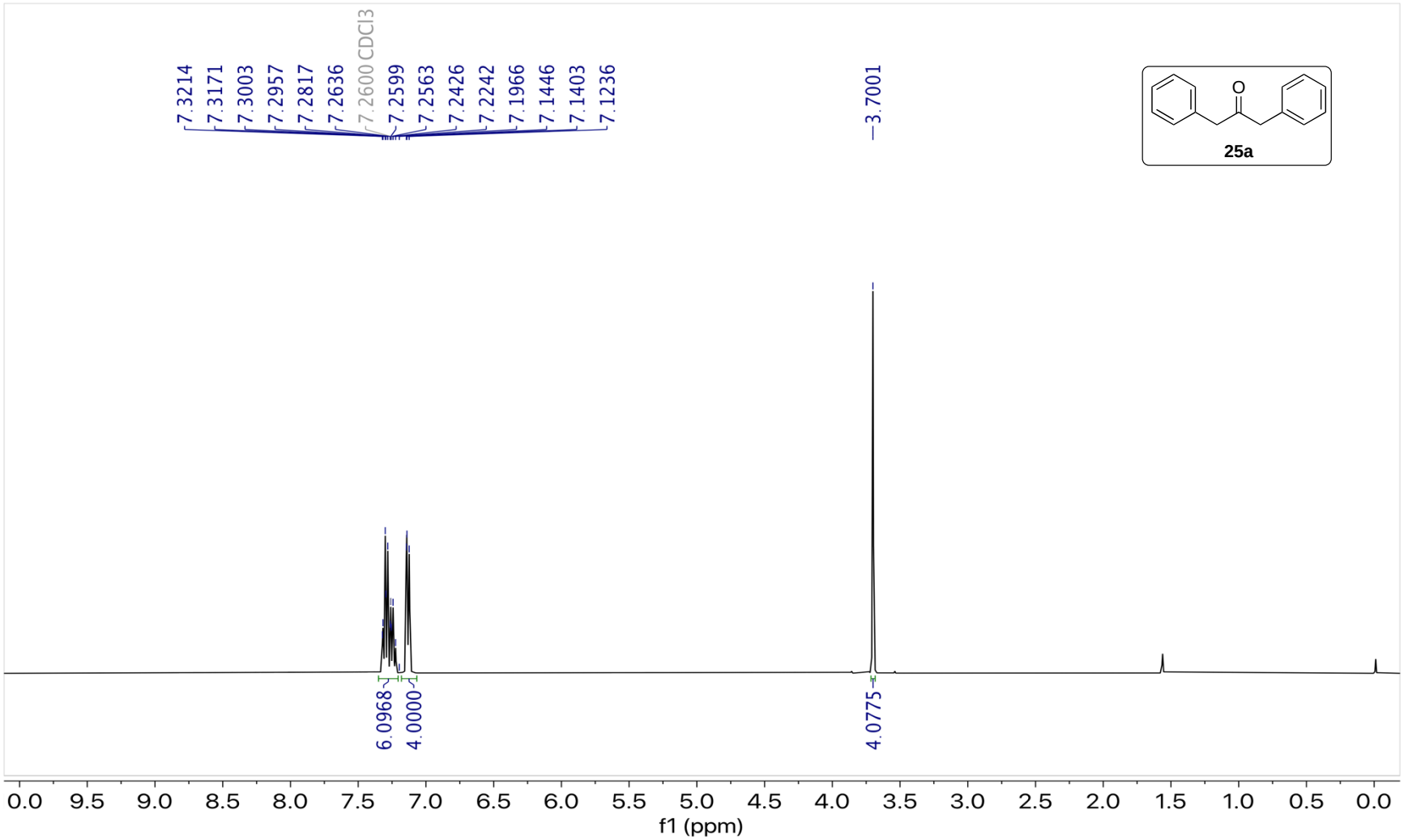

Figure S15. ^{13}C NMR spectrum of 1,3-diphenylpropan-2-one (**25a**) in $CDCl_3$

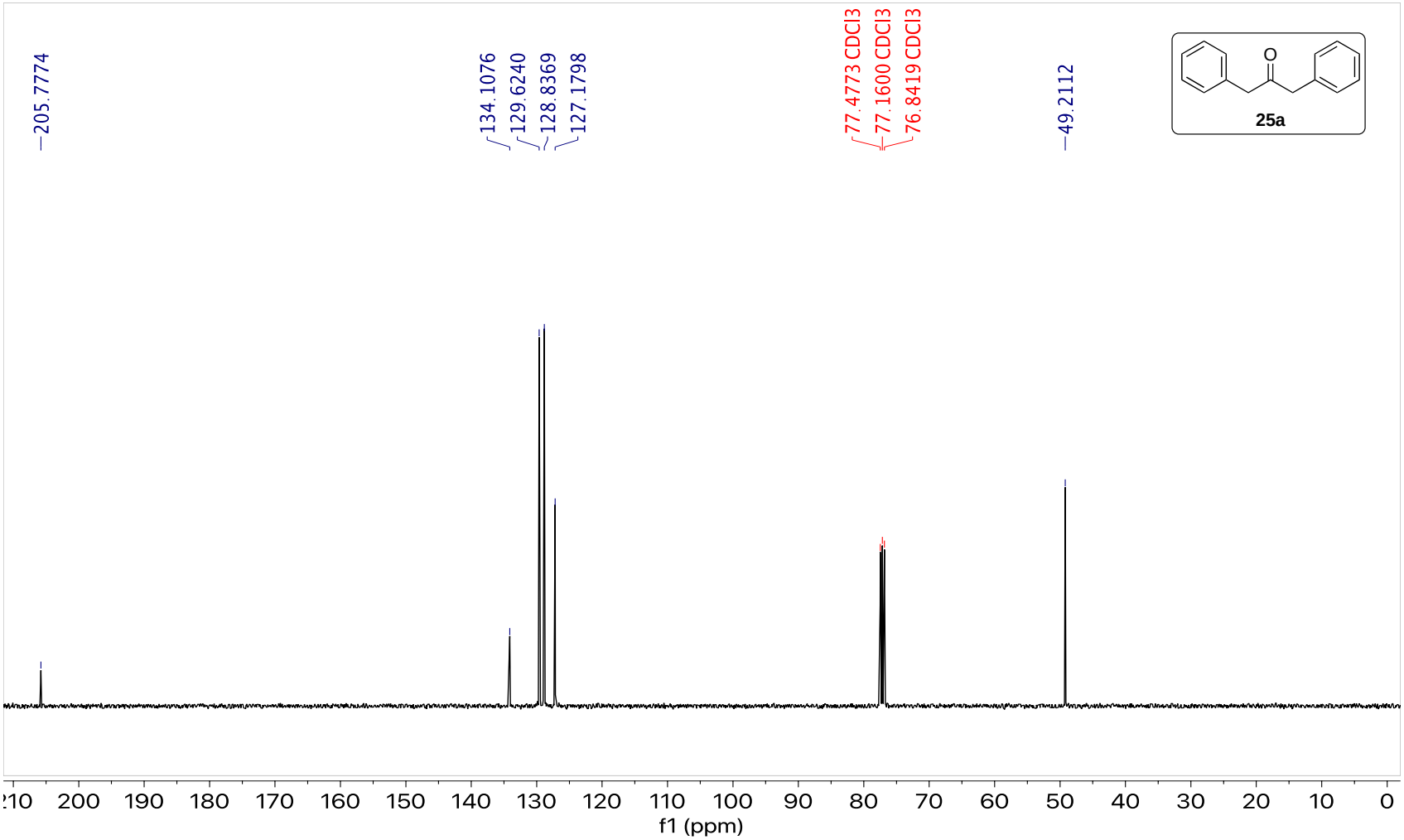

Figure S16. ^{1}H NMR spectrum of 1,3-bis(4-(benzyloxy)phenyl)propan-2-one (**25b**) in $CDCl_3$

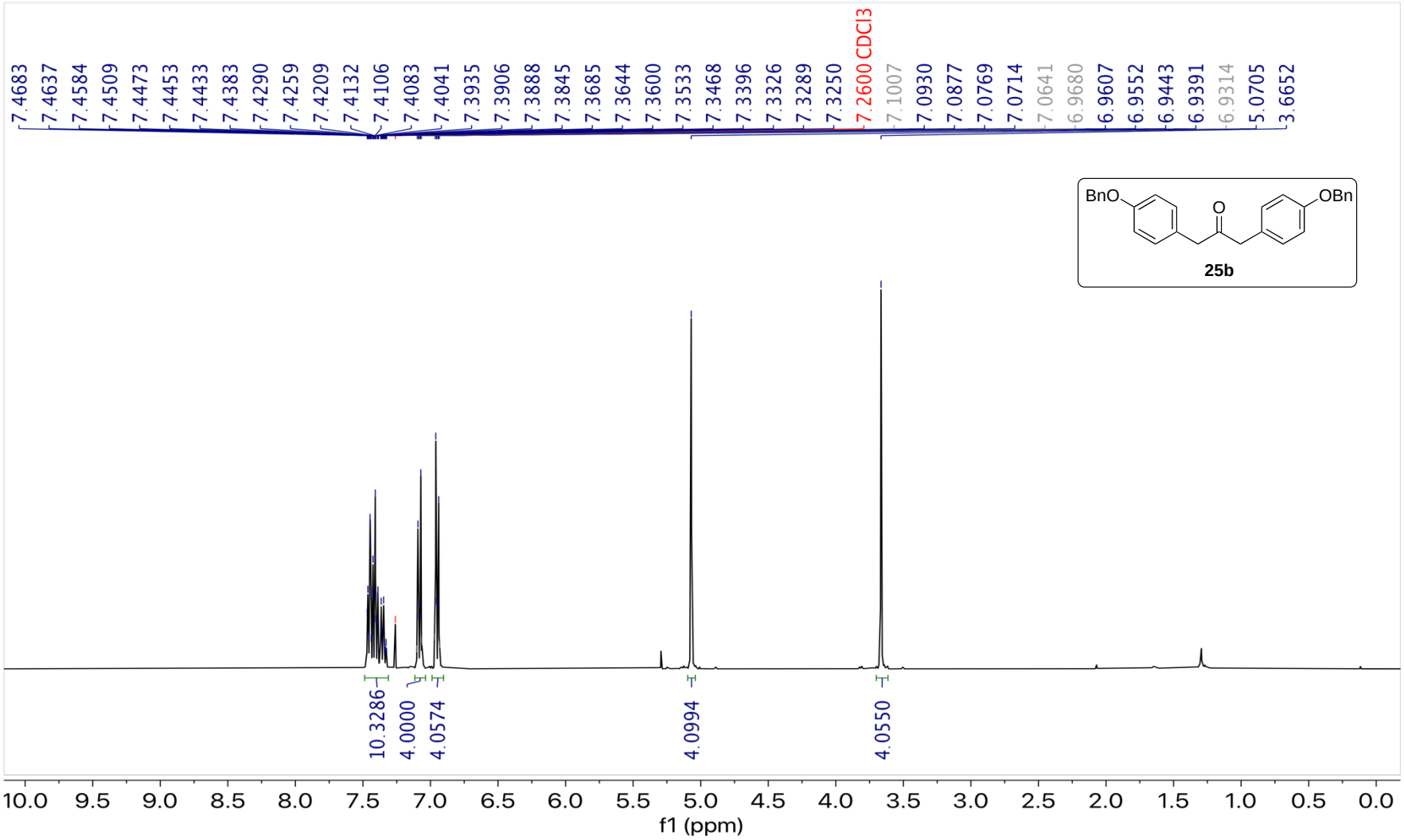

Figure S17. ^{13}C NMR spectrum of 1,3-bis(4-(benzyloxy)phenyl)propan-2-one (**25b**) in $CDCl_3$

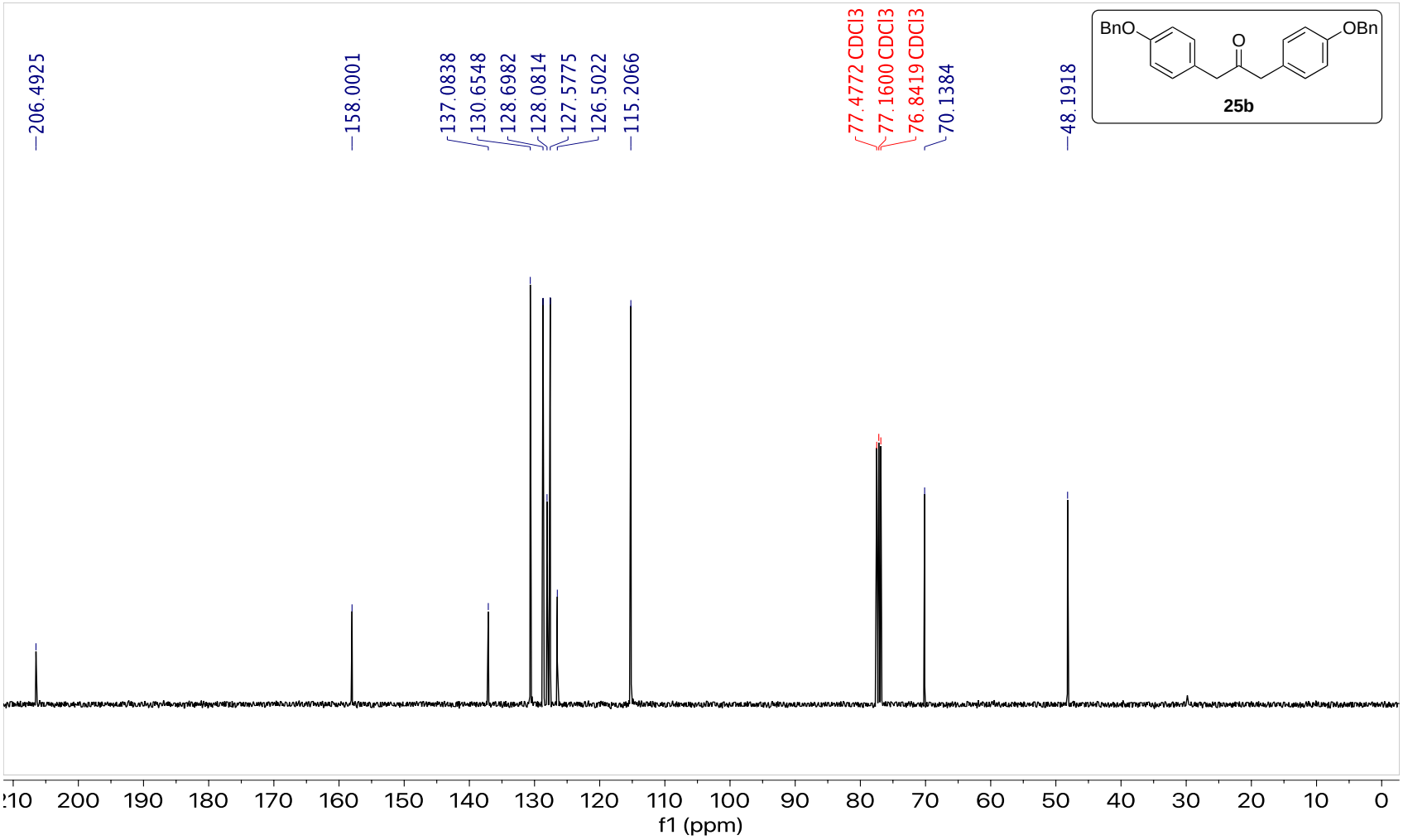

Figure S18. ^{1}H NMR spectrum of 1,3-bis(4-hydroxyphenyl)propan-2-one (**25c**) in methanol-d_4

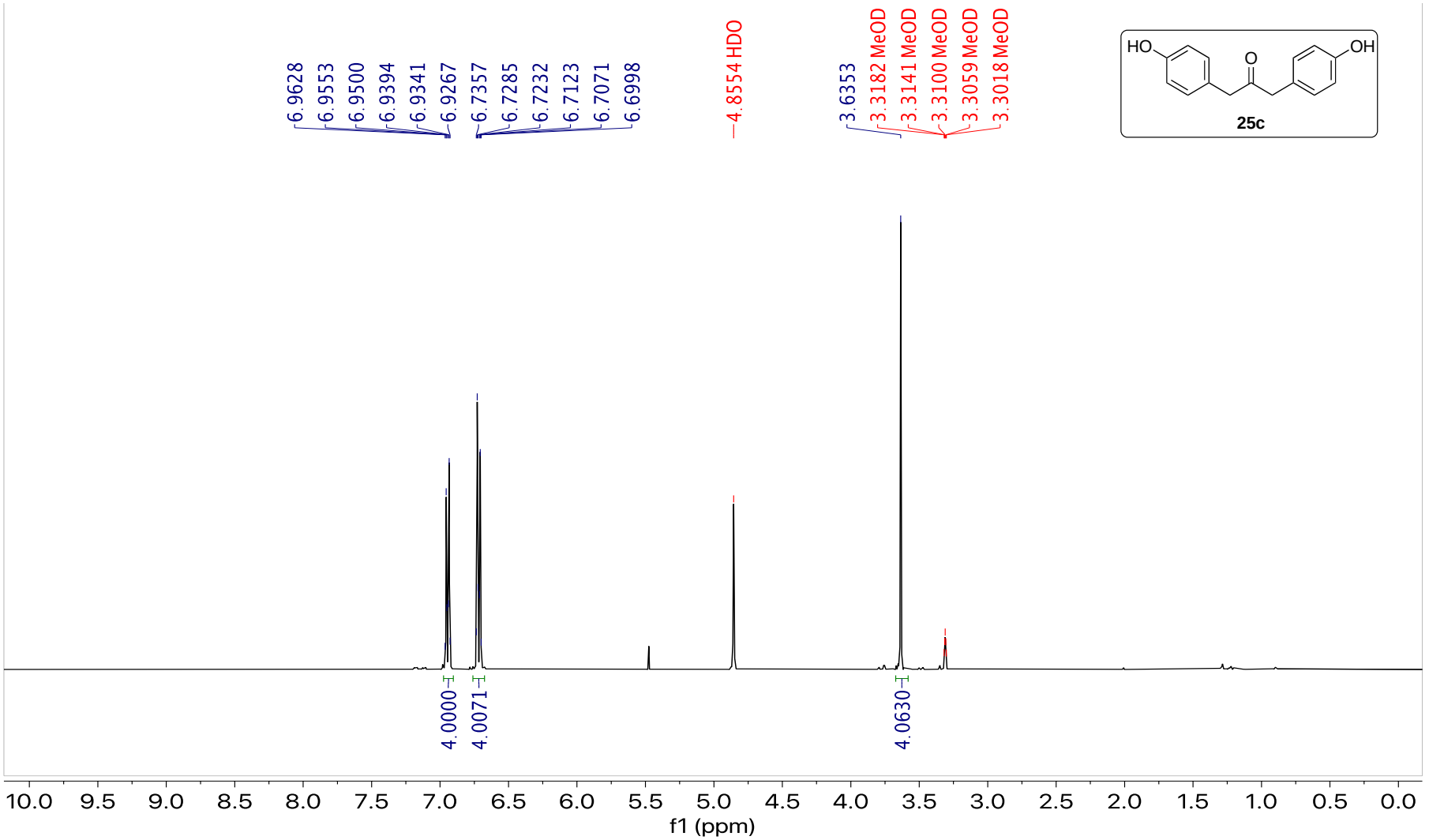

Figure S19. ^{13}C NMR spectrum of 1,3-bis(4-hydroxyphenyl)propan-2-one (**25c**) in methanol-d_4

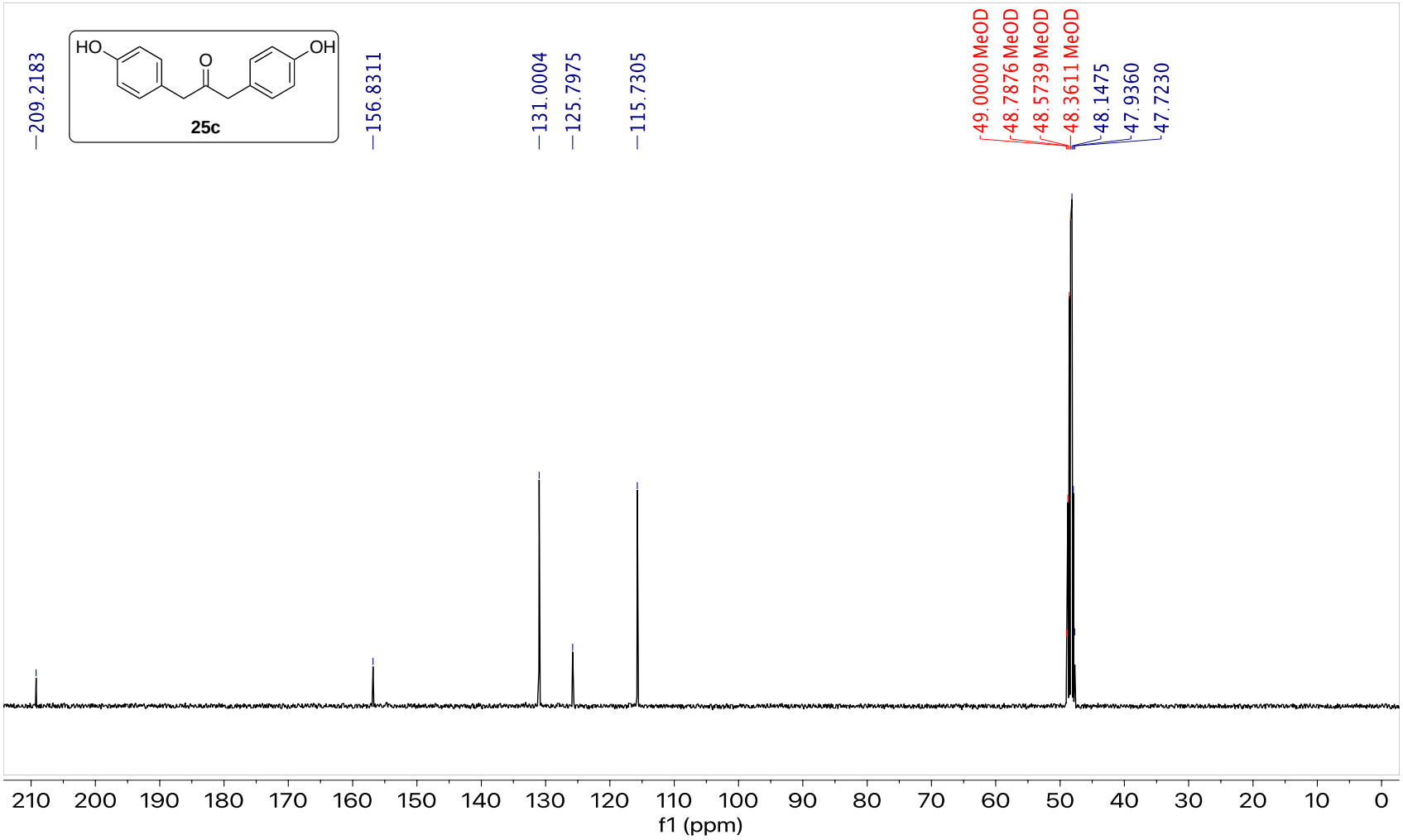

Figure S20. ^{1}H NMR spectrum of 1,3-bis(1-benzyl-1*H*-indol-3-yl)propan-2-one (**25d**) in $CDCl_3$

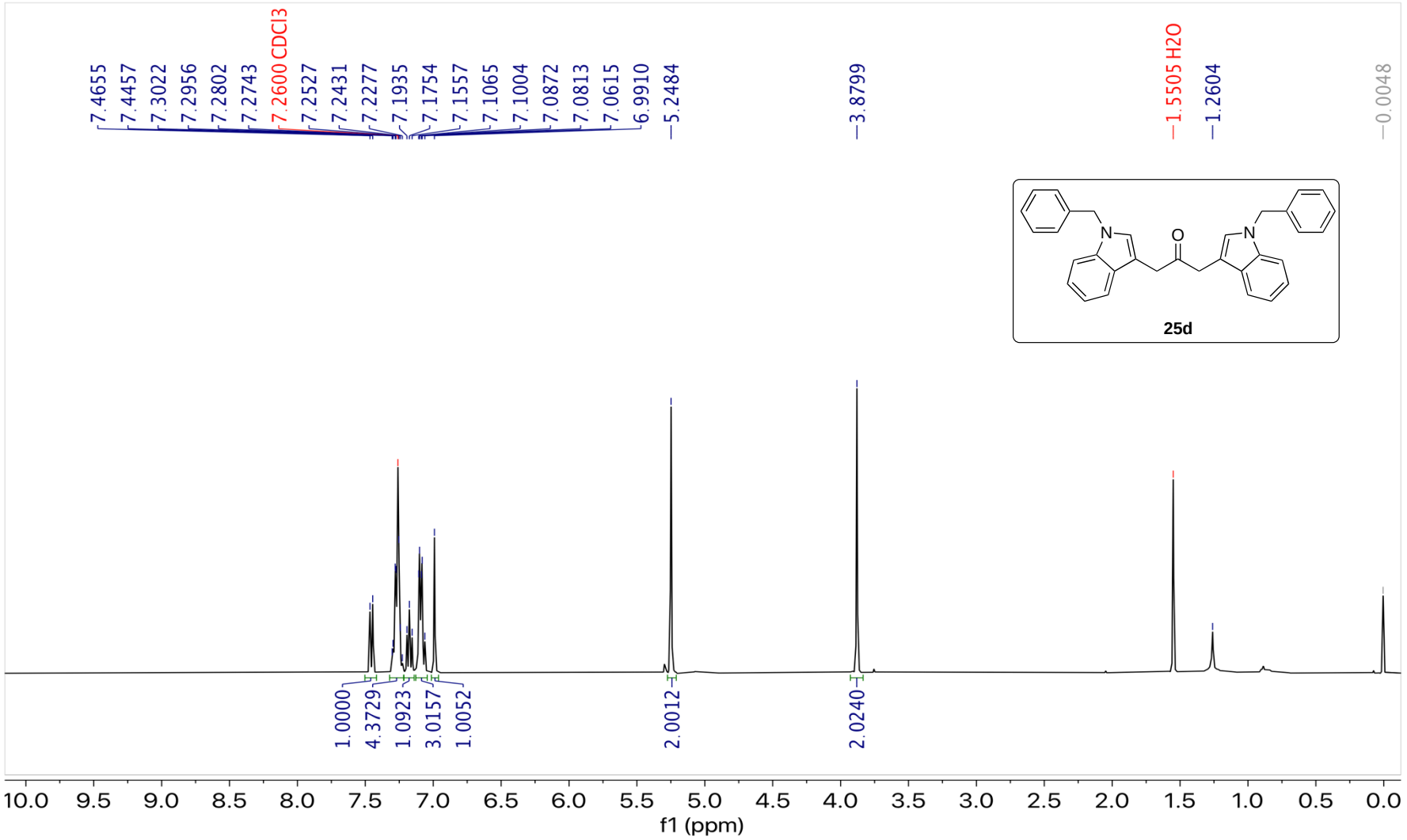

Figure S21. ^{13}C NMR spectrum of 1,3-bis(1-benzyl-1*H*-indol-3-yl)propan-2-one (**25d**) in $CDCl_3$

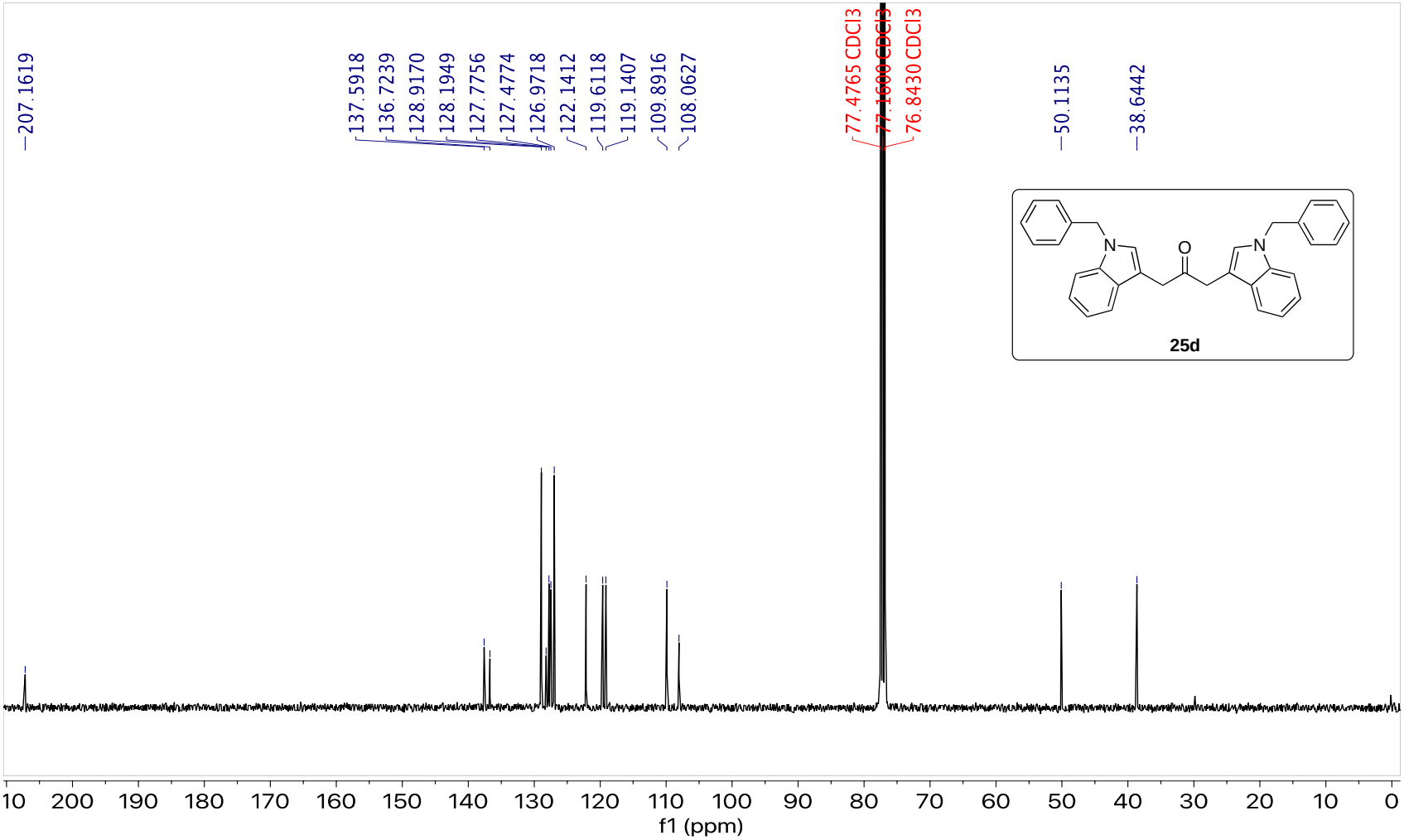

Figure S22. High-resolution mass spectrum of 2-(1-(*tert*-butoxycarbonyl)-1*H*-indol-3-yl)acetic acid (**22**)

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Comment		Instrument	compact 8255754.20059

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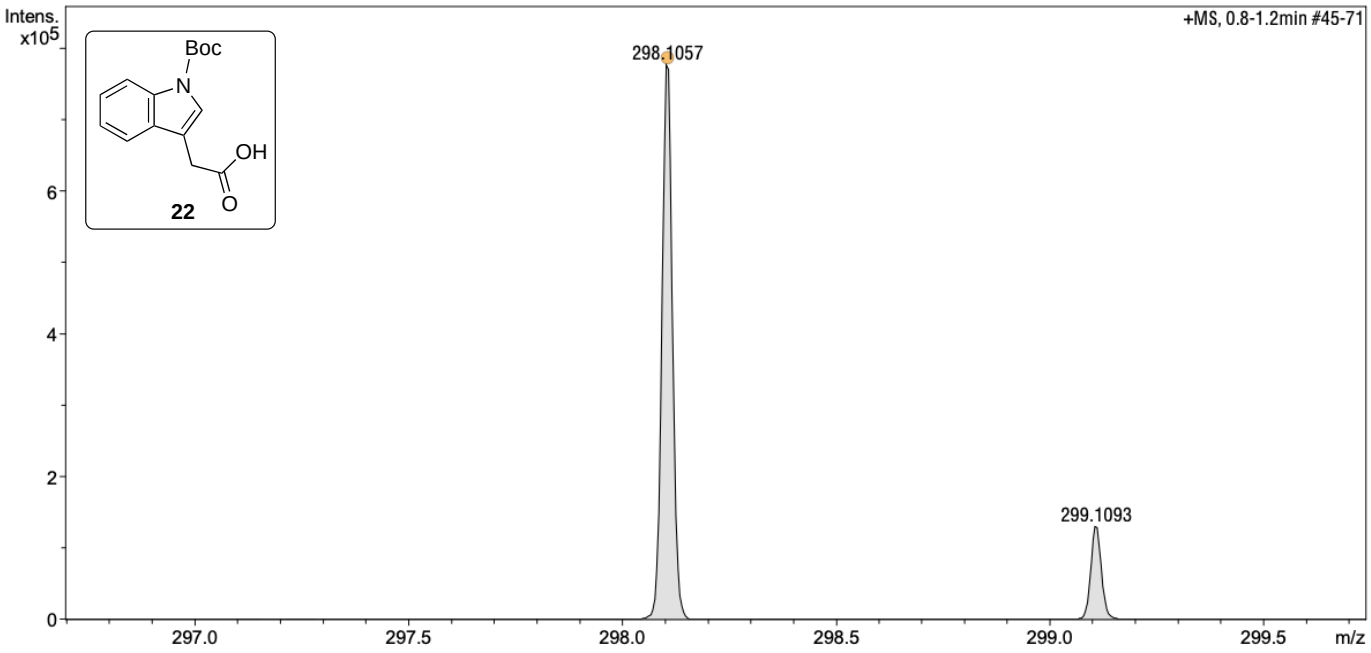

Nov 20 2024000009.d

Bruker Compass DataAnalysis 4.3 printed: 2024-11-20 11:38:29 AM by: x Page 1 of 1

Figure S23. High-resolution mass spectrum of di-*tert*-butyl 3,3'-(2-oxopropane-1,3-diyl)bis(1*H*-indole-1-carboxylate) (**23**)

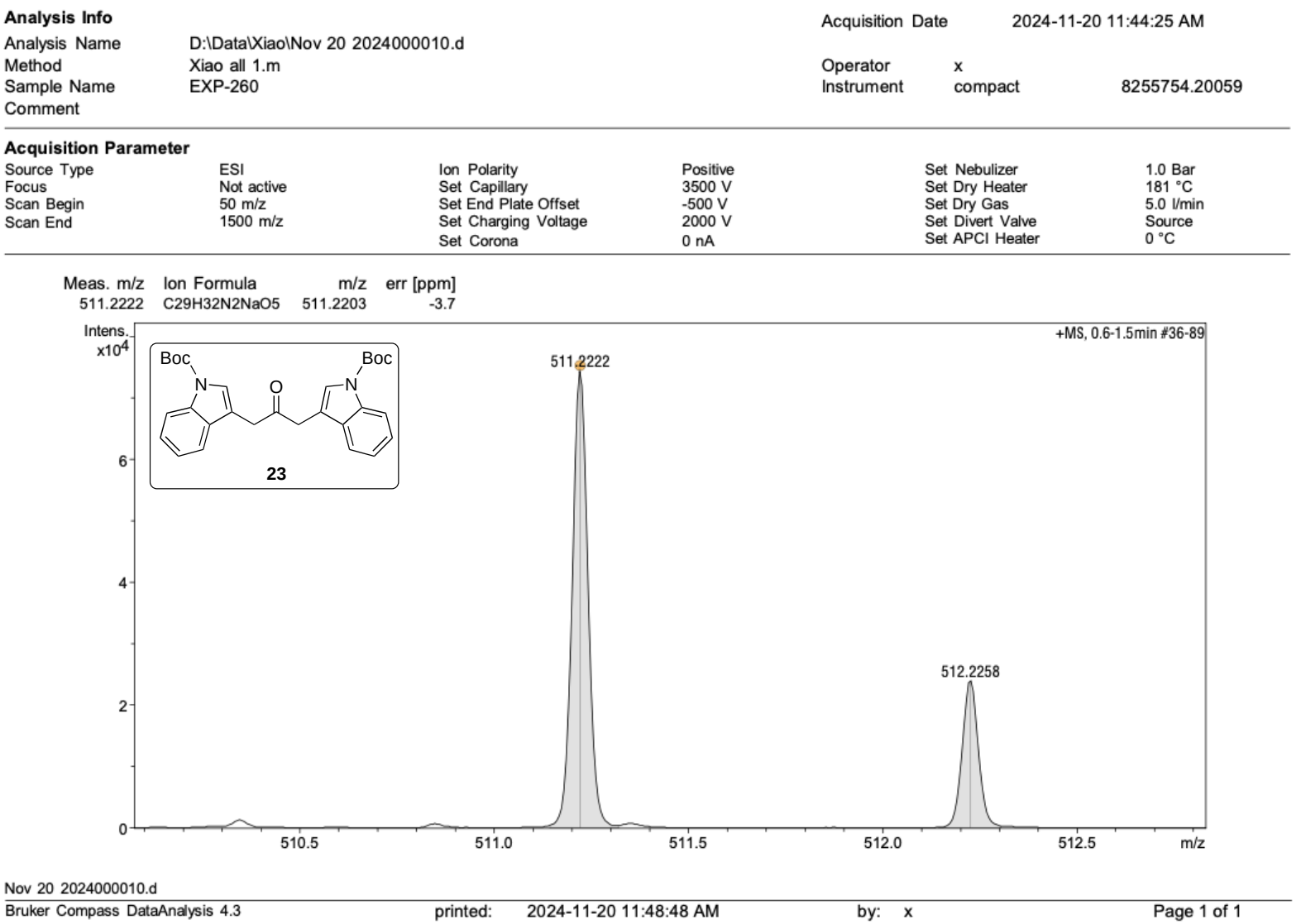

Figure S24. High resolution mass spectrum of 1,3-di(1*H*-indol-3-yl)propan-2-one (**1**)

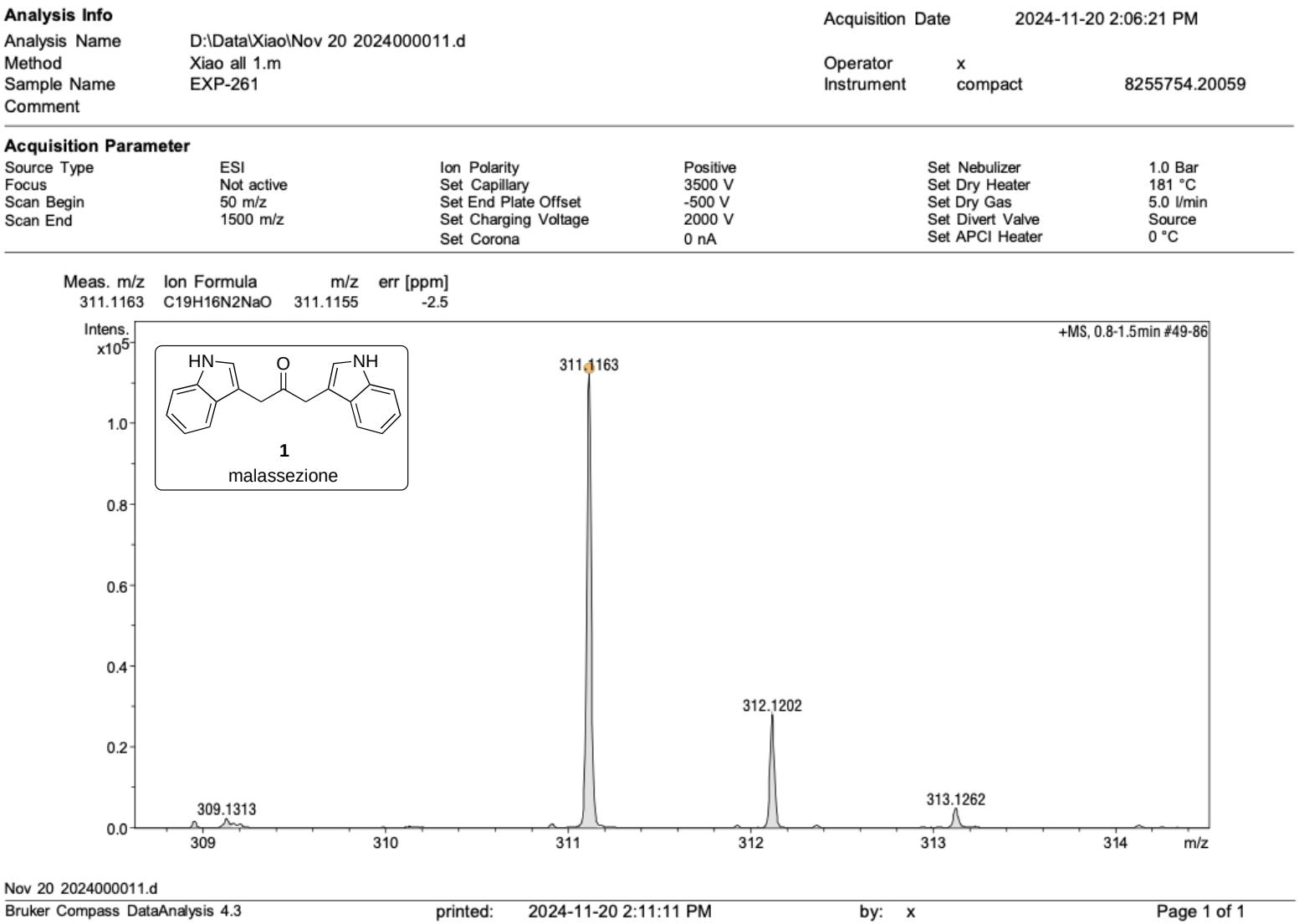

Figure S25. High resolution mass spectrum of 1,3-bis(4-(benzyloxy)phenyl)propan-2-one (**25b**)

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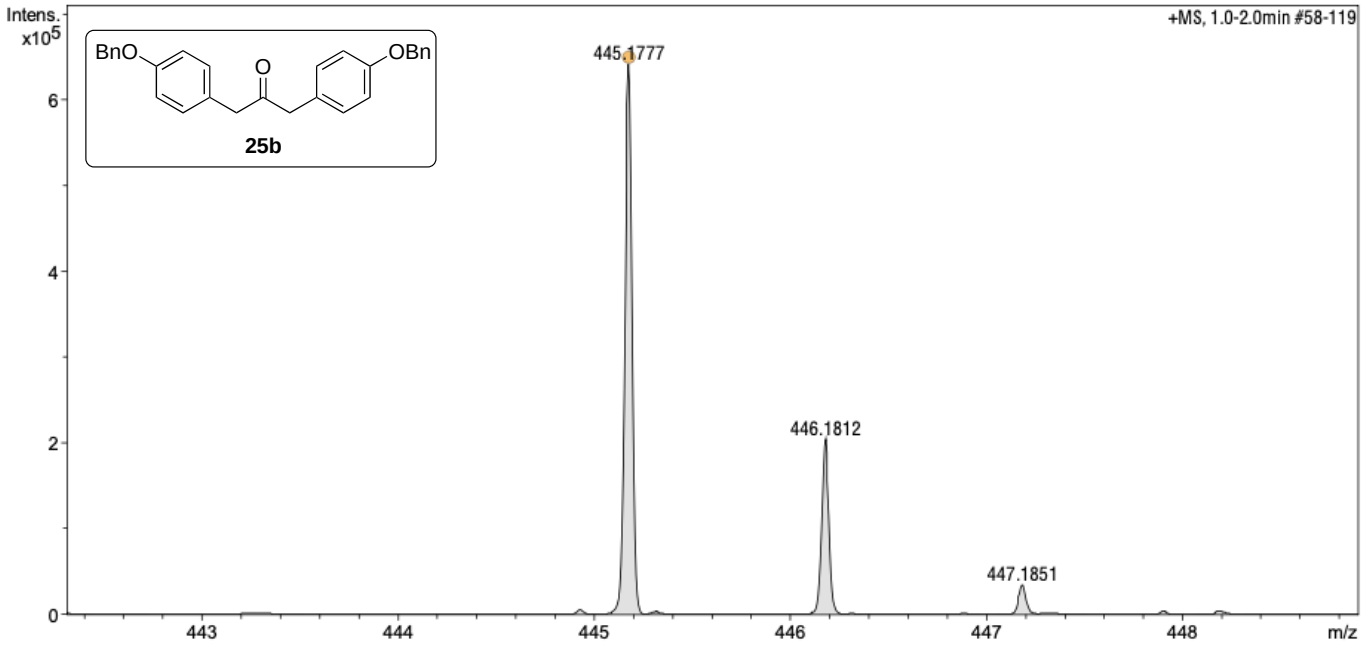

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Figure S26. High resolution mass spectrum of 1,3-bis(4-hydroxyphenyl)propan-2-one (**25c**)

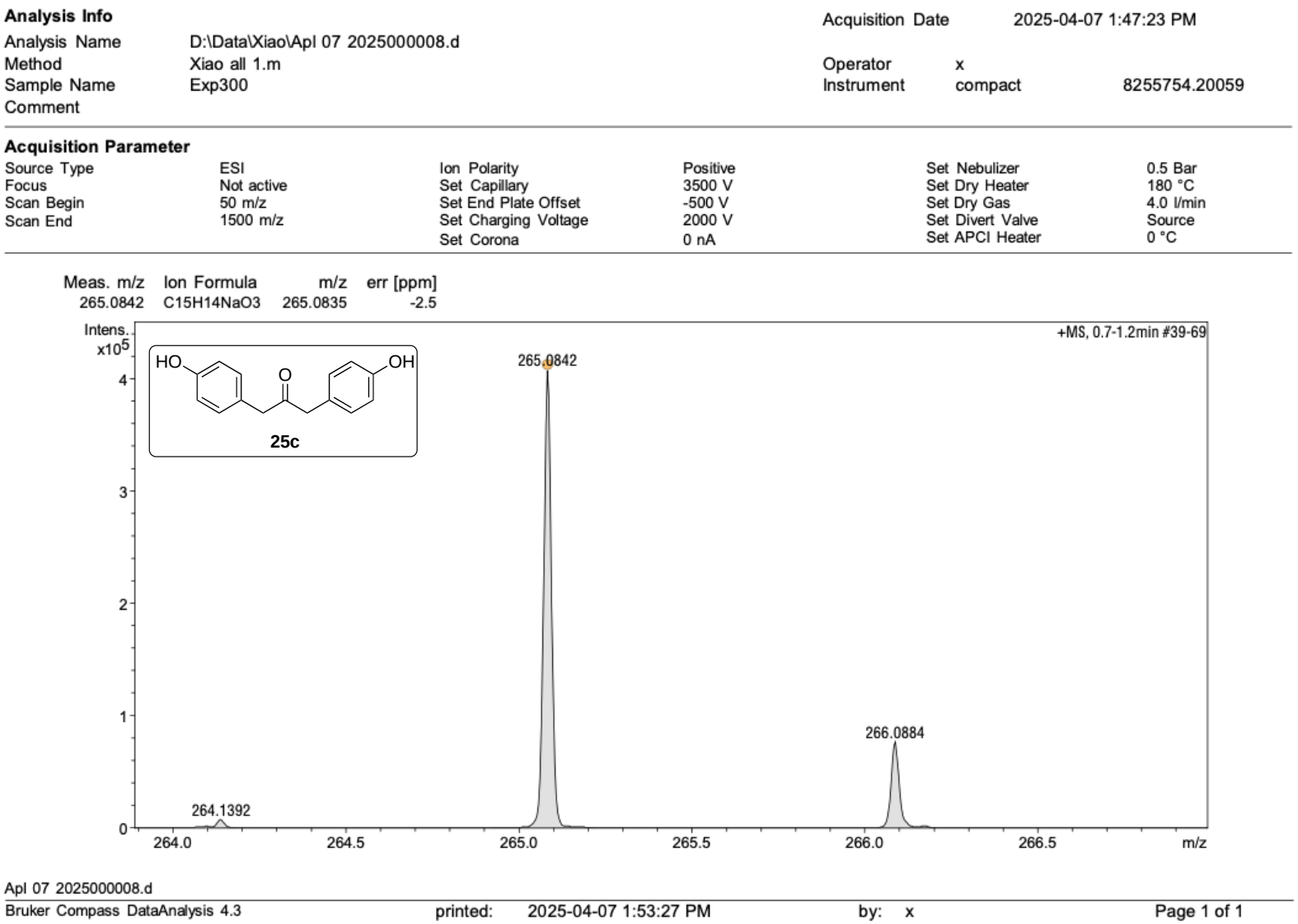

Figure S27. High-resolution mass spectrum of 1,3-bis(1-benzyl-1*H*-indol-2-yl)propan-2-one (**25d**)