Synthesis, ^{123}I-radiolabeling optimization, and initial preclinical evaluation of novel urea-based PSMA inhibitors with a tributylstannyl prosthetic group in their structures

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Supplementary Materials

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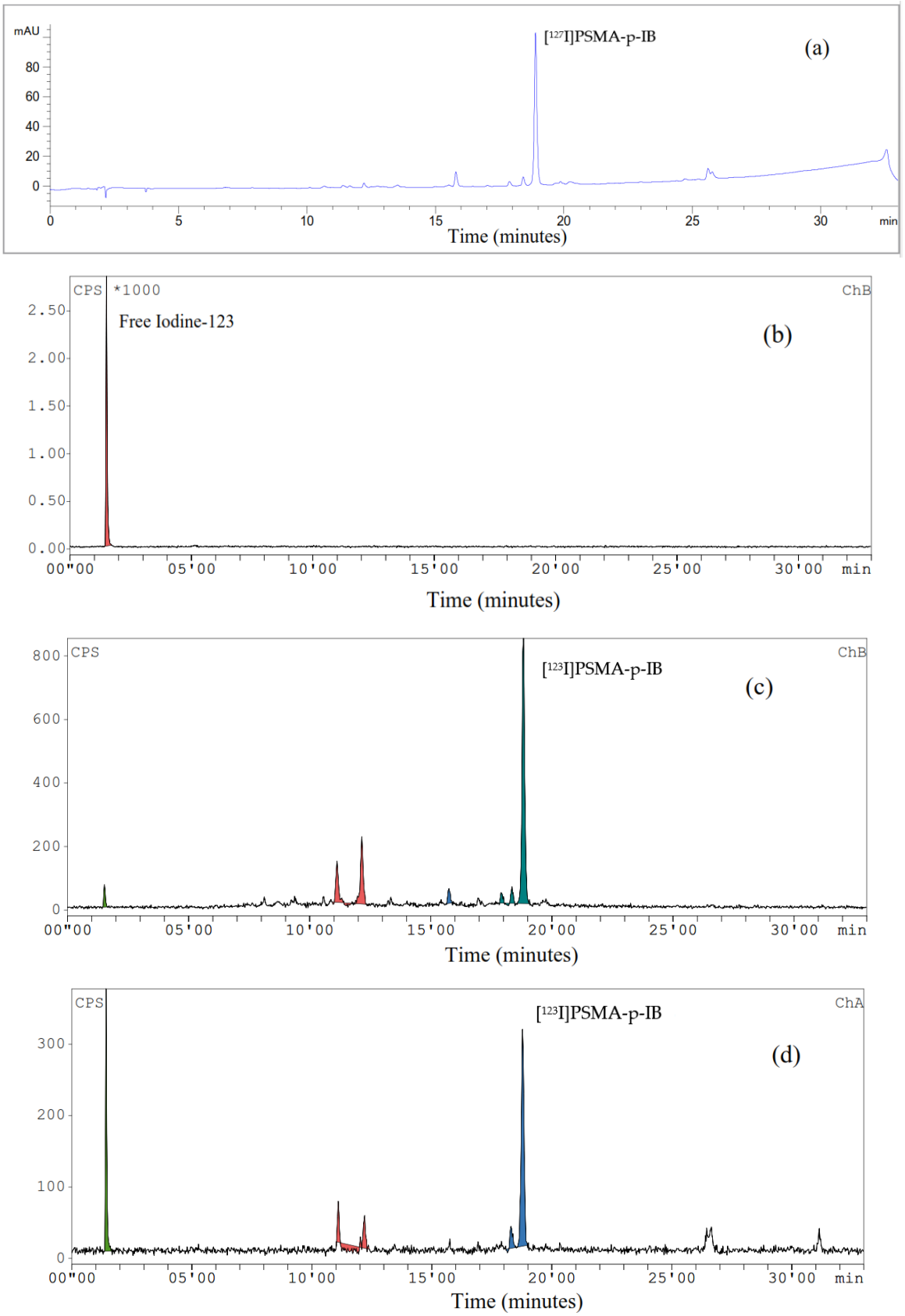

Figure S1. Radio-HPLC chromatograms of (a) [^{127}I]PSMA-p-IB reference sample, (b) blank solution, (c) radiolabeling yield with [^{123}I]PSMA-p-IB yield of 69.99%, and (d) radiolabeling yield with [^{123}I]PSMA-p-IB yield of 65.73%.

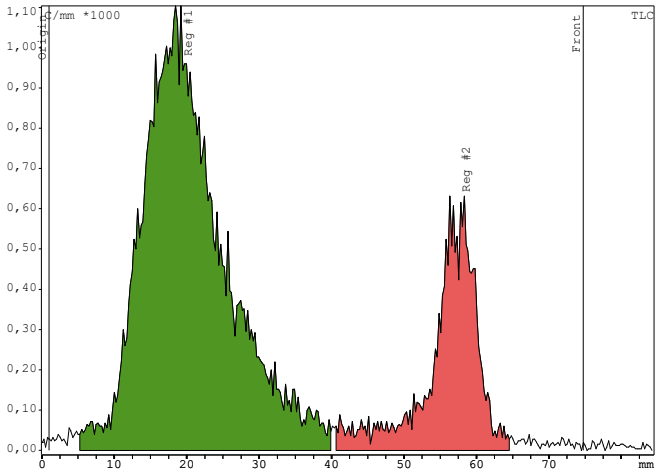

Figure S2. Radio-iTLC chromatogram of [^{123}I]PSMA-p-IB based on the results of radiolabeling optimization (the left peak: [^{123}I]PSMA-p-IB, the right peak: free Iodine-123). The chromatography was performed using iTLC-SG glass fiber sheet with a developing solution of CH_3CN/H_2O, 95/5 (v/v).

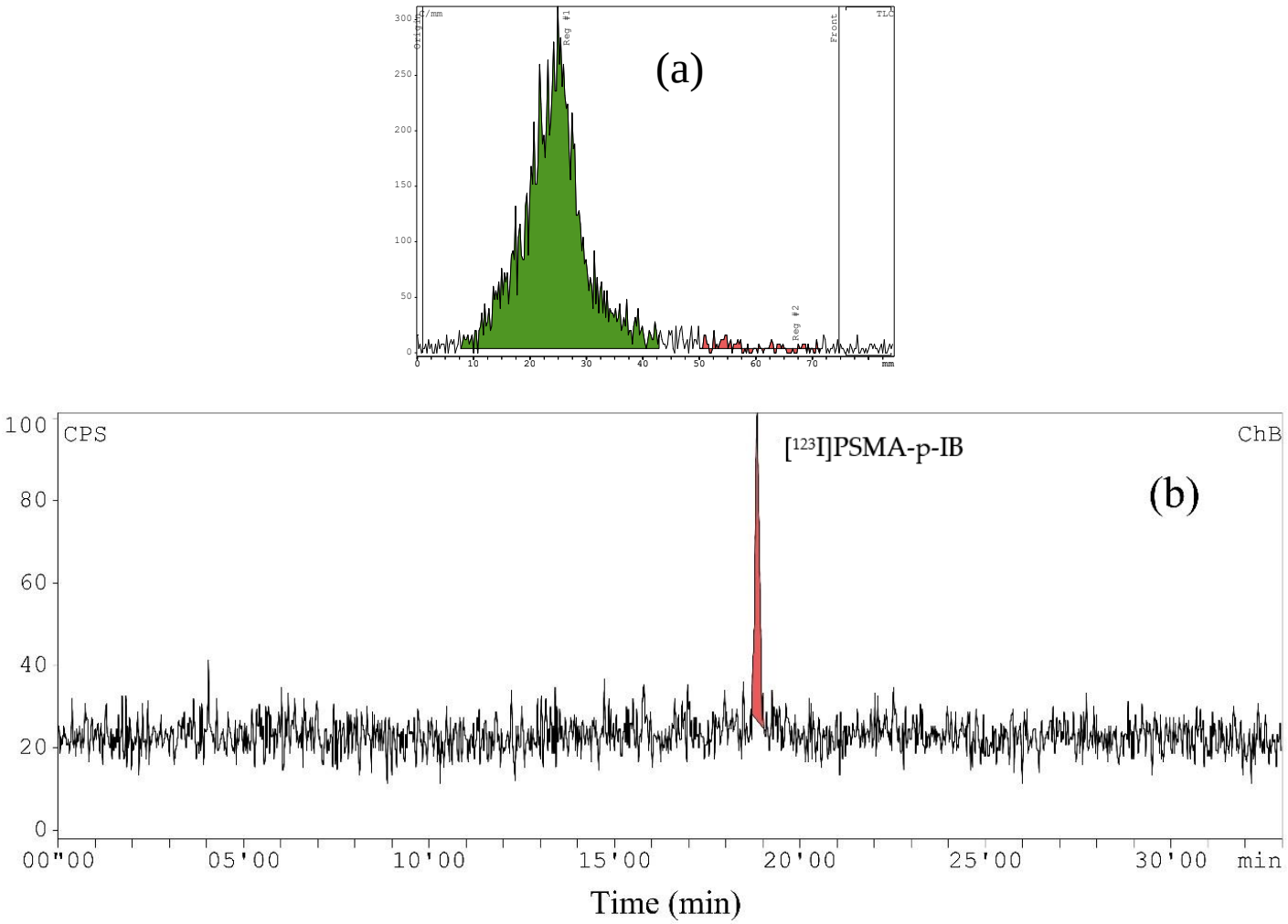

Figure S3. Chromatograms of [^{123}I]PSMA-p-IB after purification analyzed by (a) Radio-TLC-SG 60 F254 and (b) Radio-HPLC

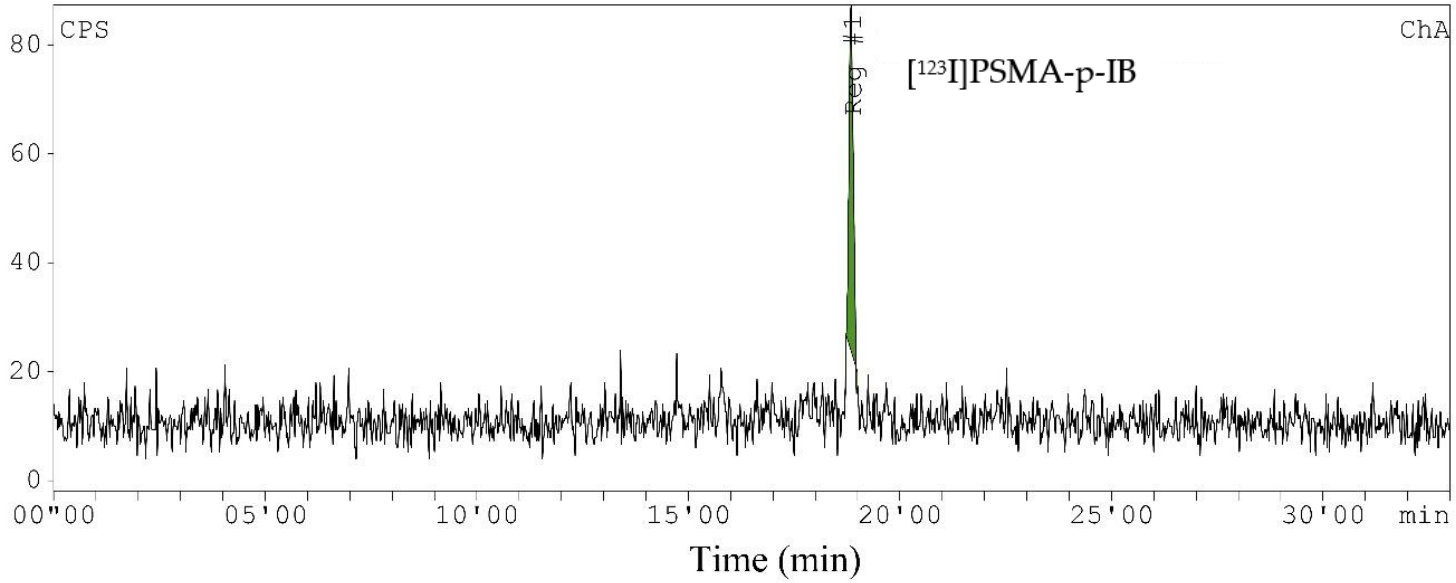

Figure S4. Radio-HPLC chromatogram of [^{123}I]PSMA-p-IB after 3 days storage period

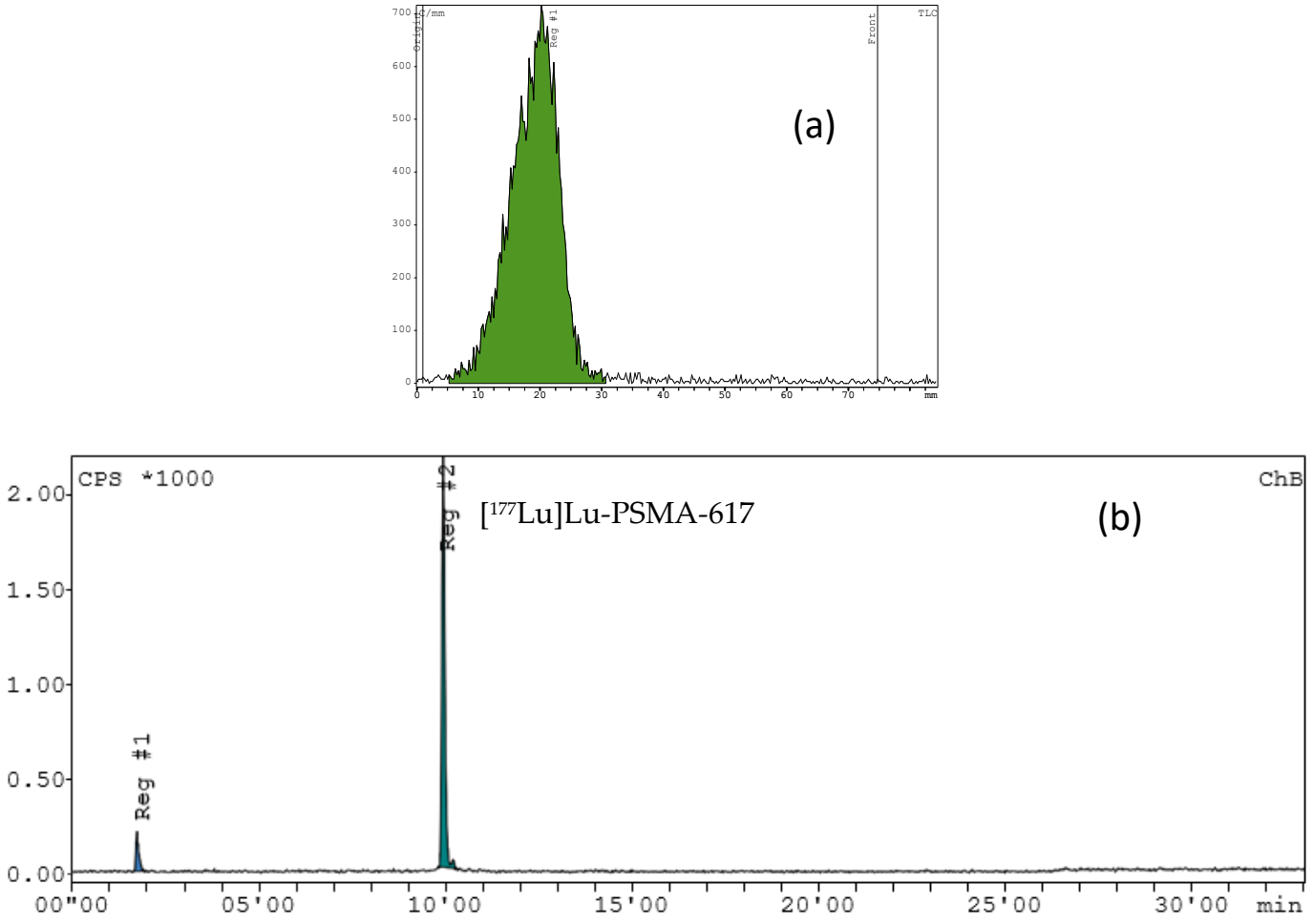

Figure S5. Chromatograms of [^{177}Lu]Lu-PSMA-617 by (a) Radio-iTLC and (b) Radio-HPLC

Compound 6

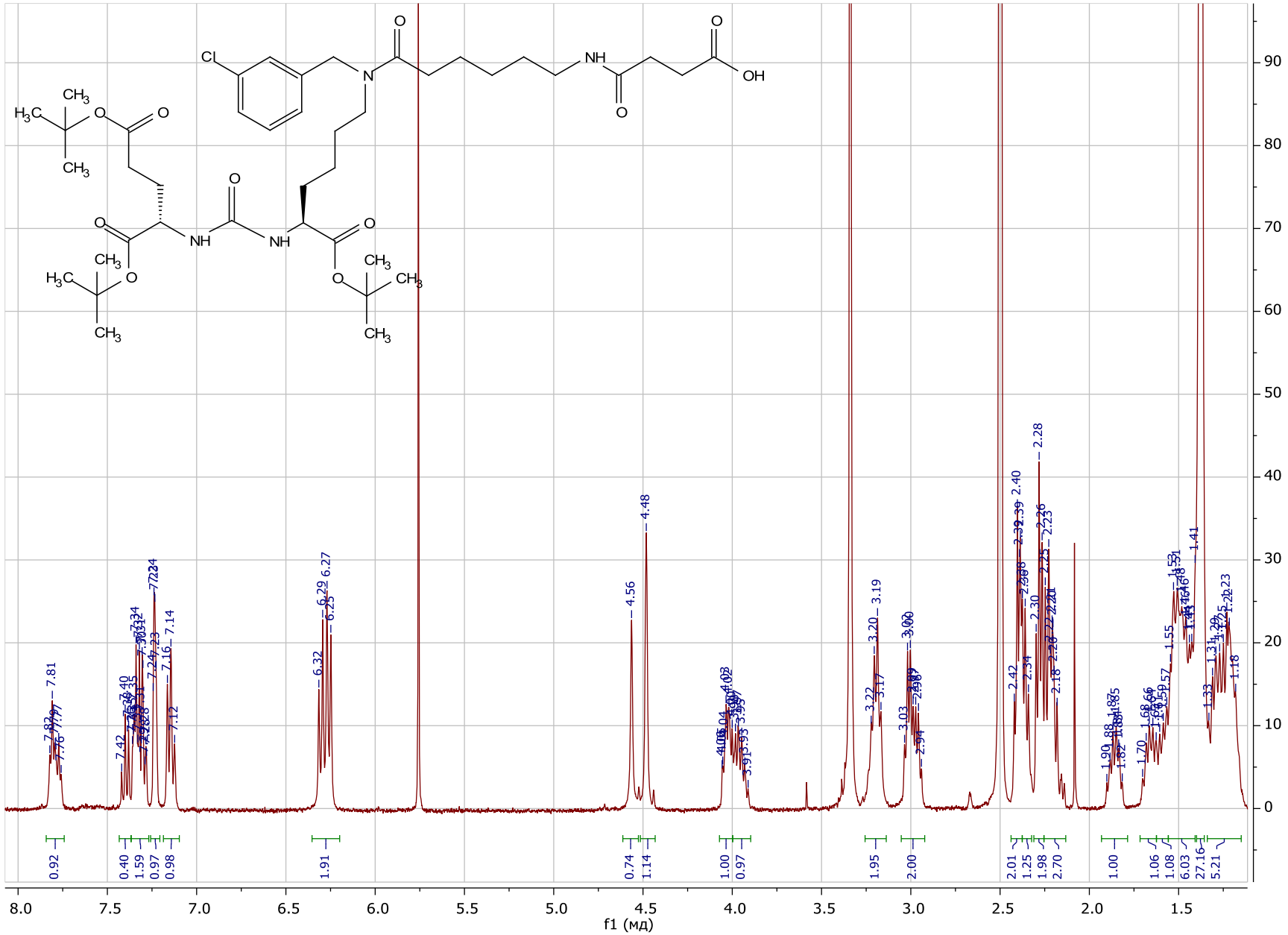

Figure S6. ^{1}H NMR spectrum of compound № **6** in DMSO-*d*$_6$.

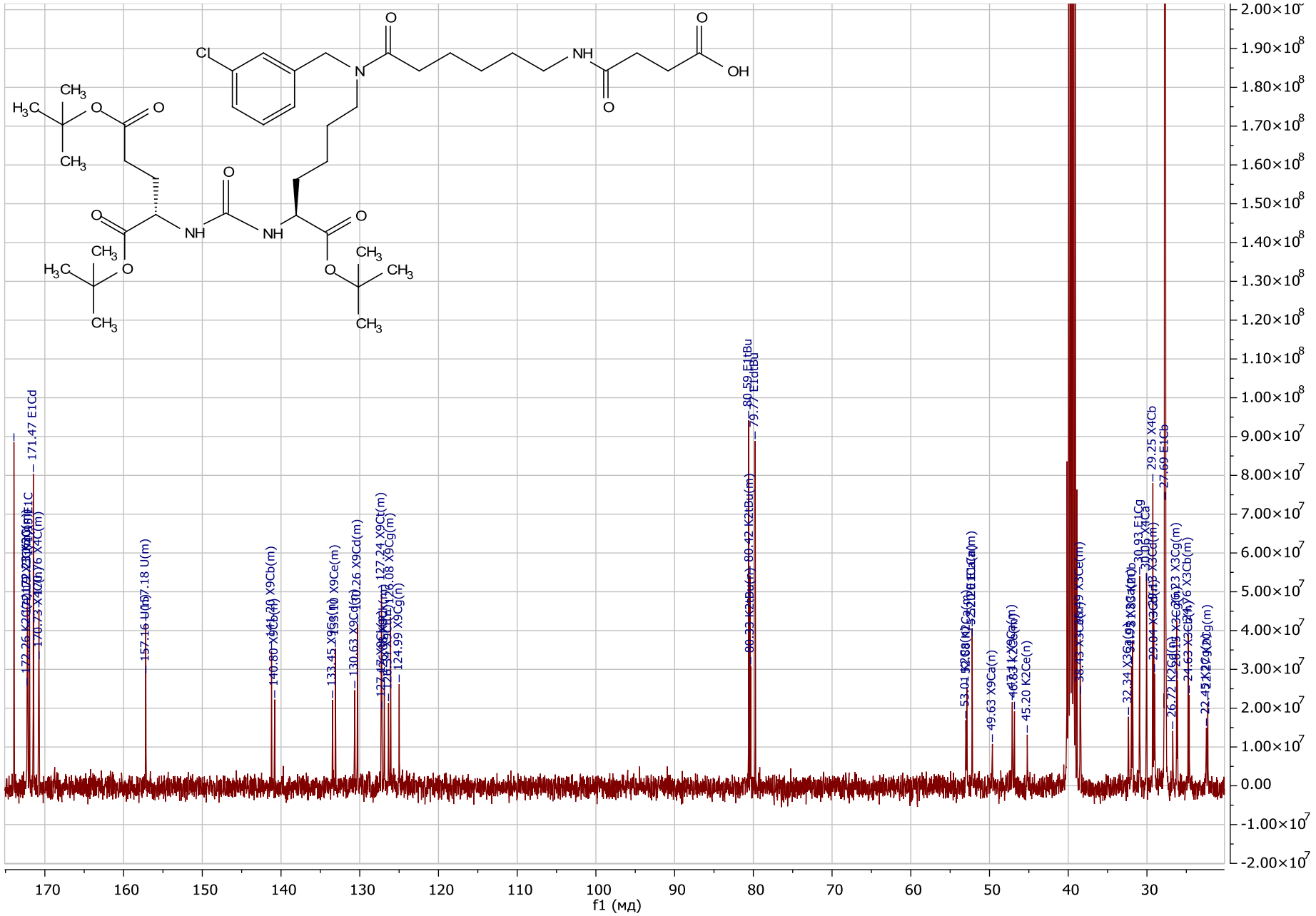

Figure S7. ^{13}C NMR spectrum of compound № **6** in DMSO-d_6.

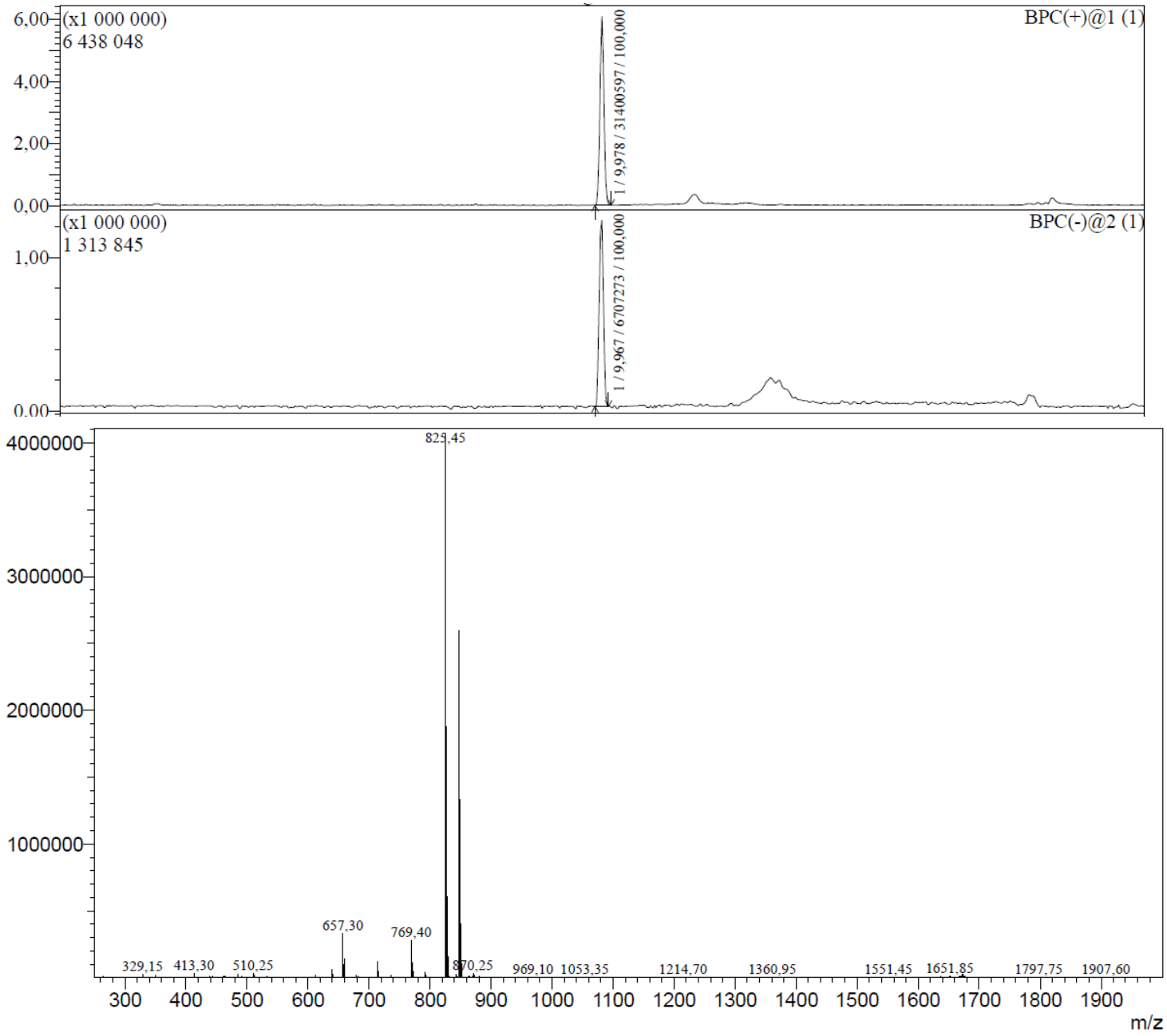

Figure S8. ESI-MS of compound № **6**

Compound 9

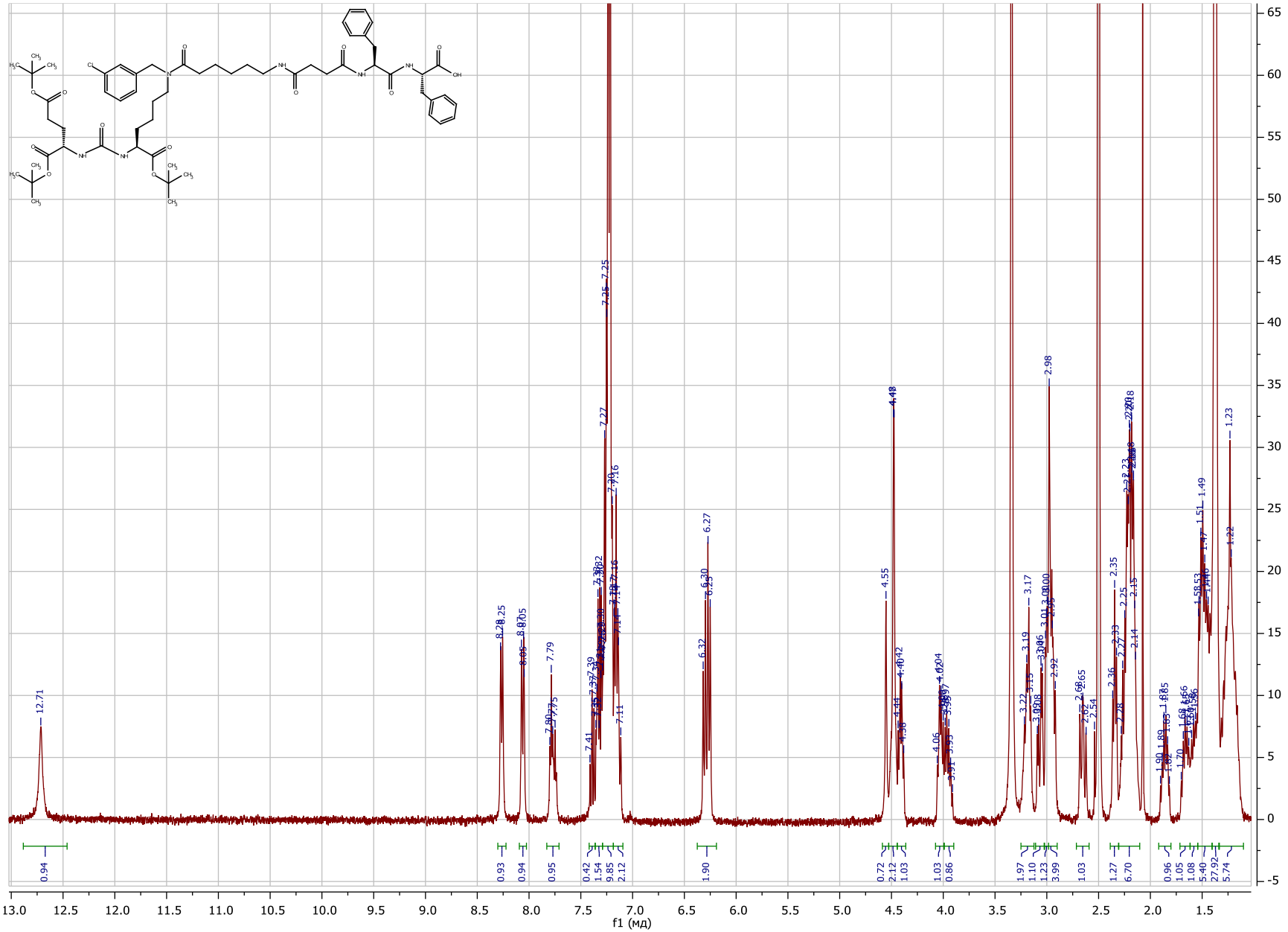

Figure S9. ^{1}H NMR spectrum of compound № **9** in DMSO-d_6.

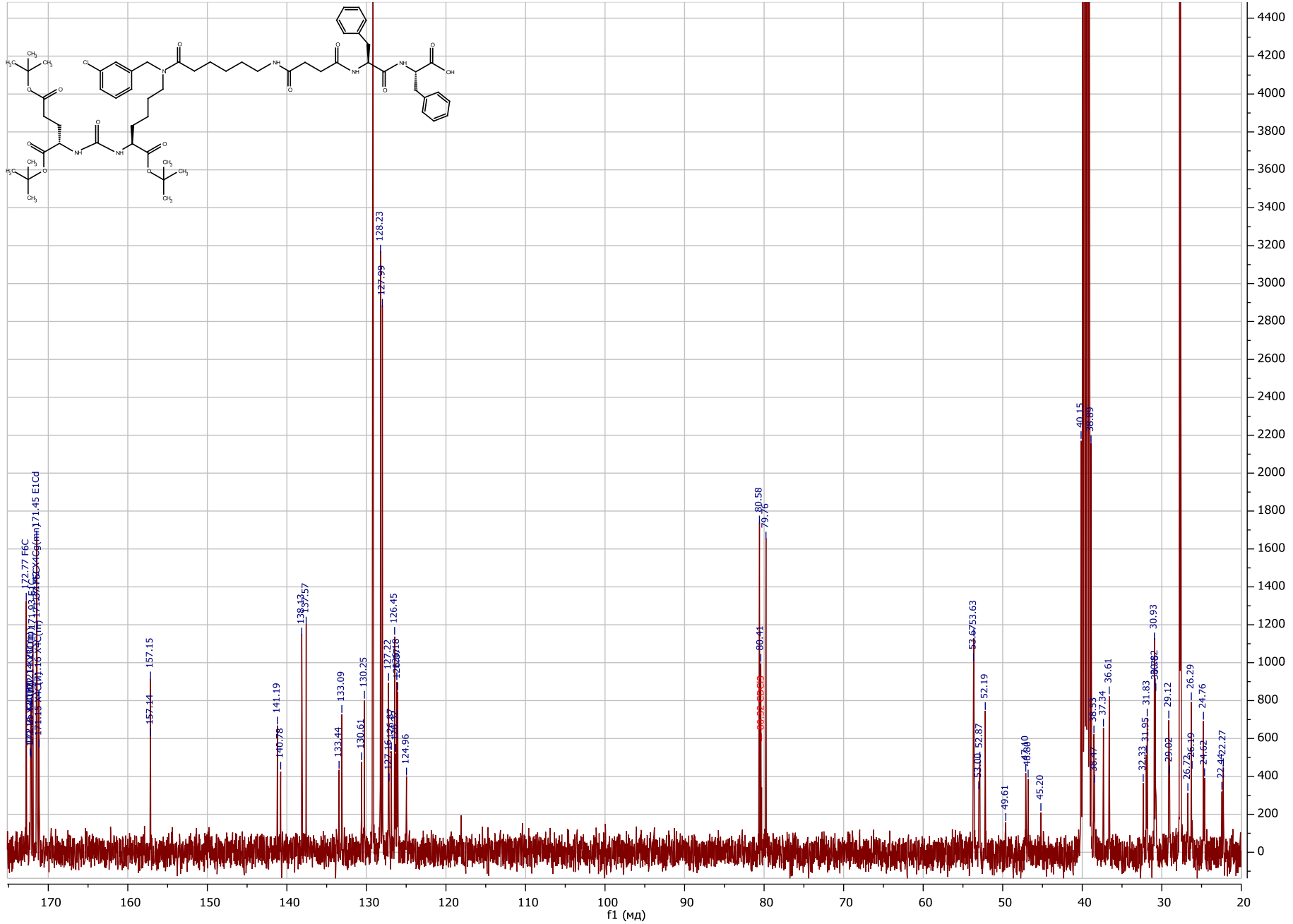

Figure S10. ^{13}C NMR spectrum of compound № **9** in DMSO-d_6.

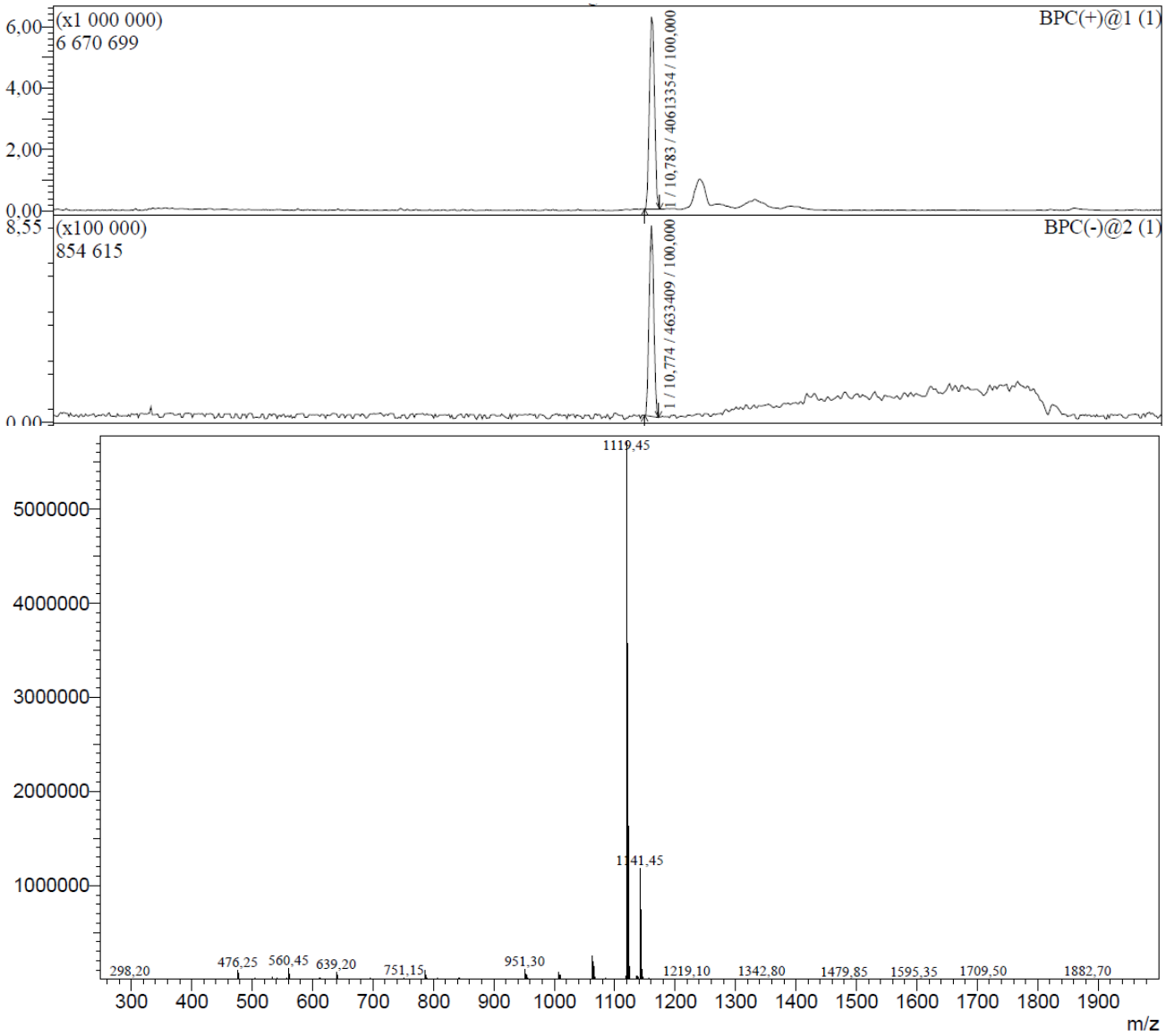

Figure S11. ESI-MS of compound № **9**

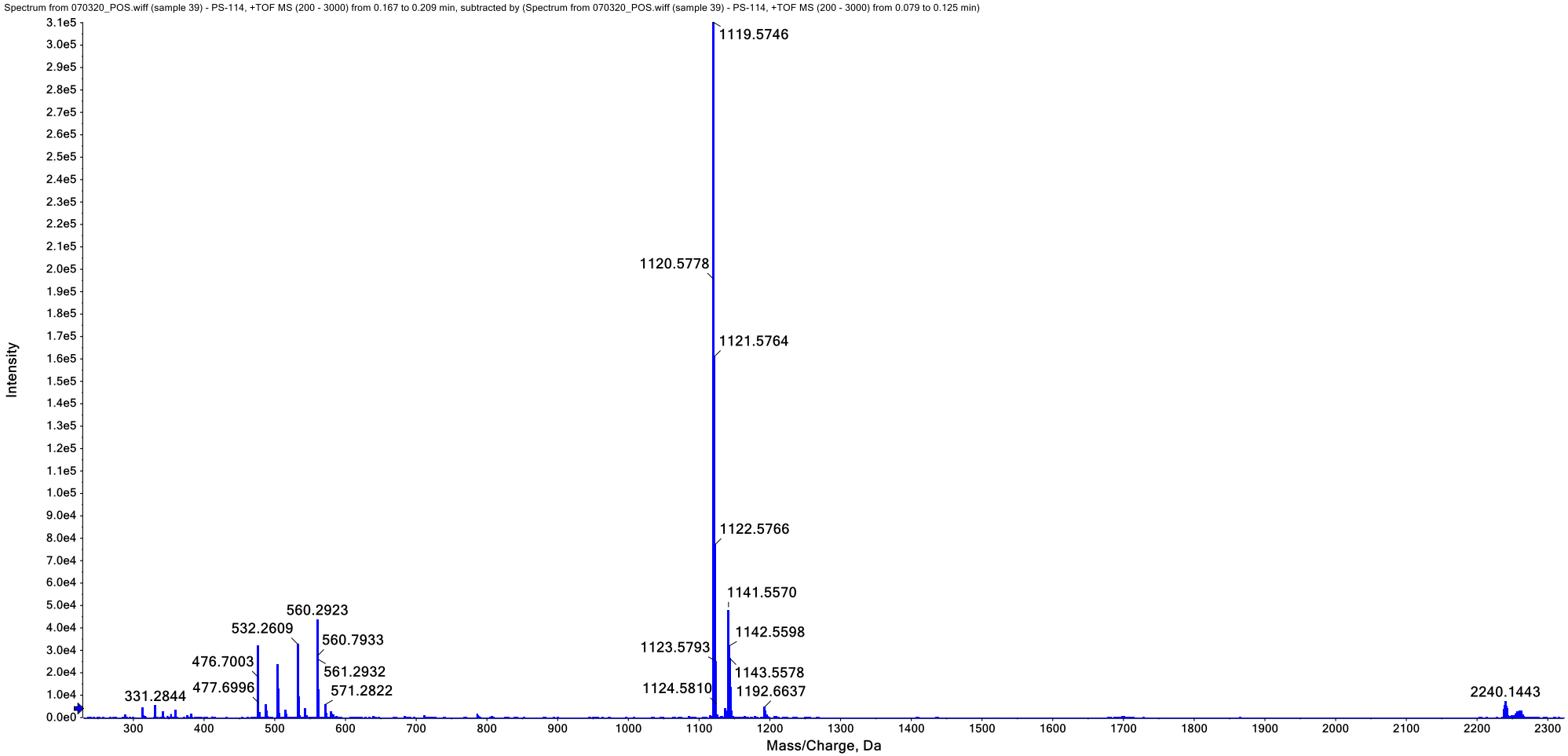

Figure S12. HRMS (m/z, ESI) of compound № **9**

Compound 10

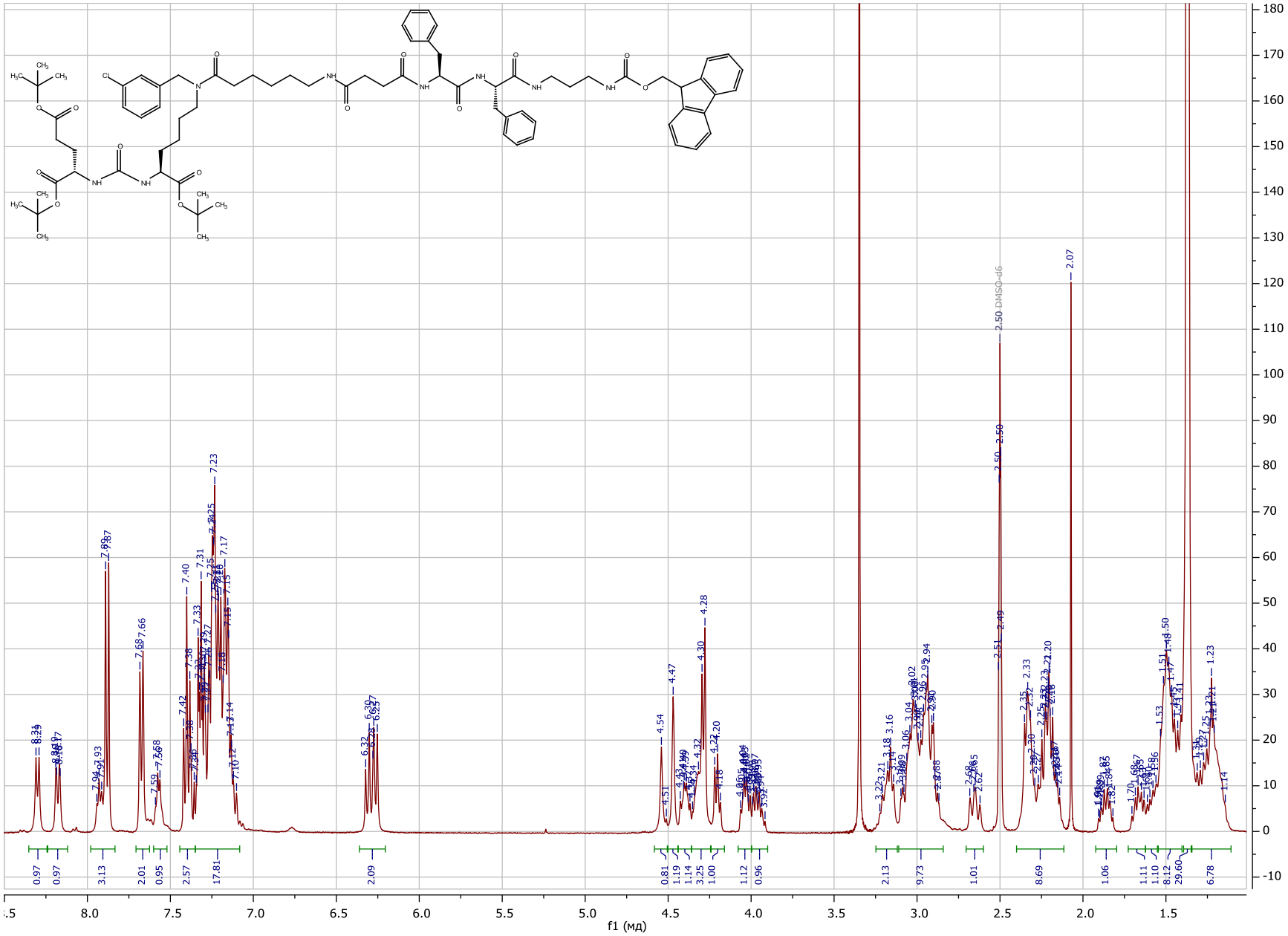

Figure S13. ^{1}H NMR spectrum of compound № **10** in DMSO-d_6.

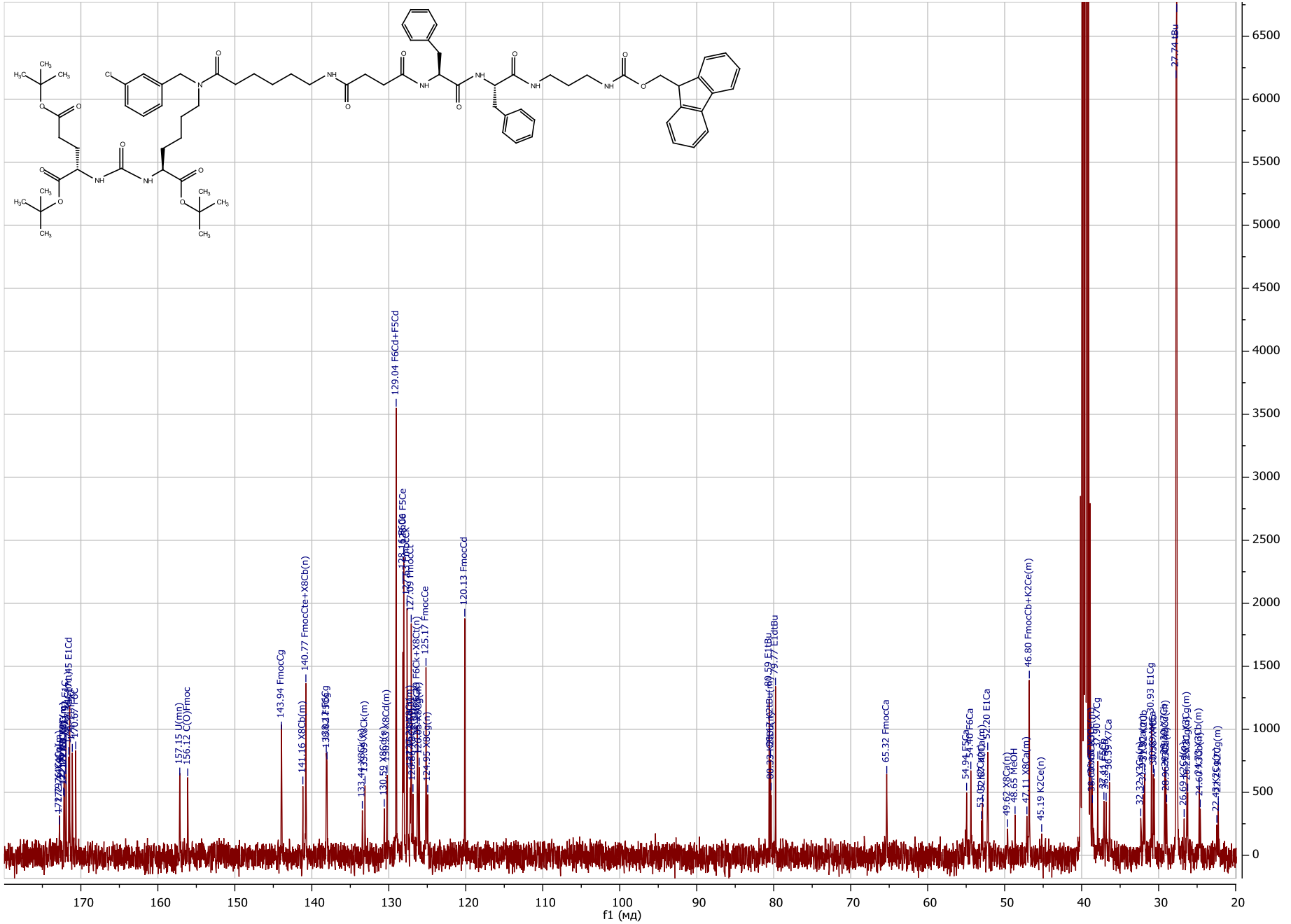

Figure S14. ^{13}C NMR spectrum of compound № **10** in DMSO-*d*$_6$.

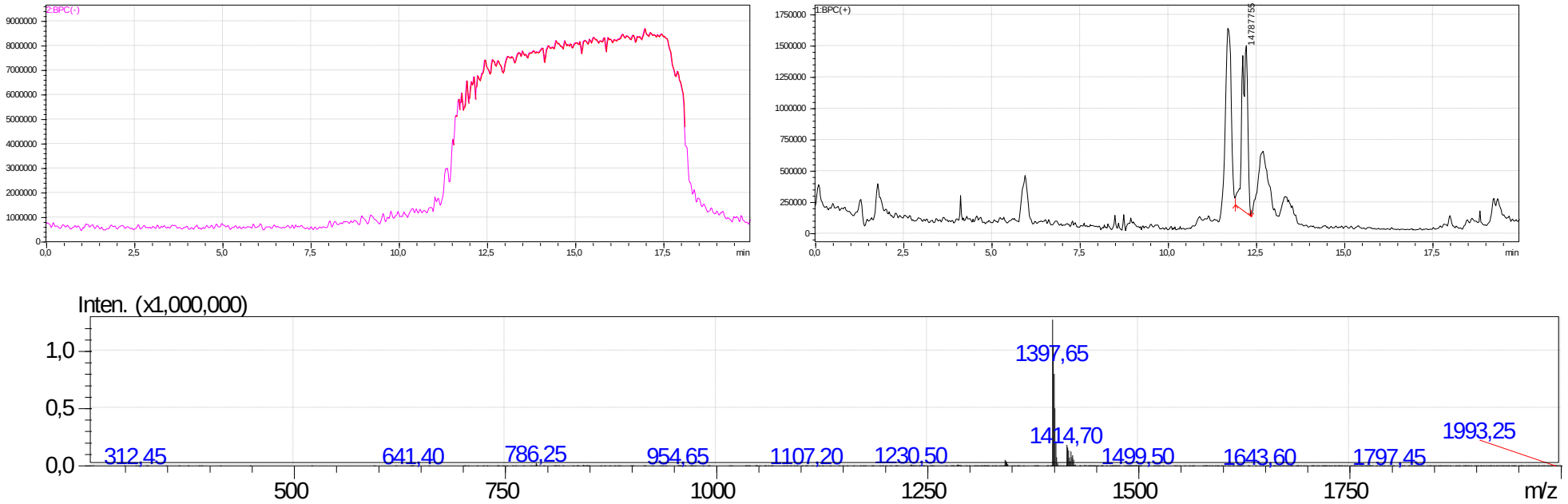

Figure S15. ESI-MS of compound № **10**

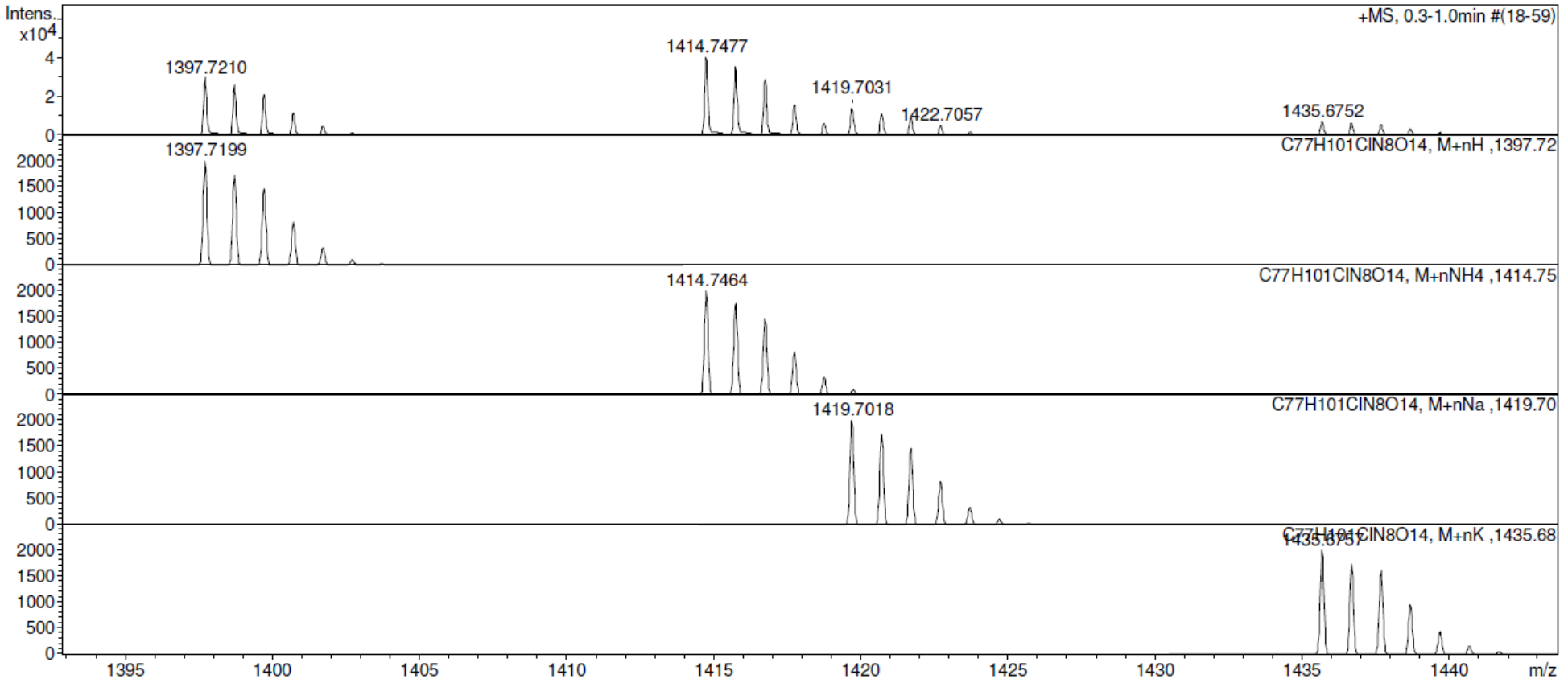

Figure S16. HRMS (m/z, ESI) of compound № **10**

Compound 11

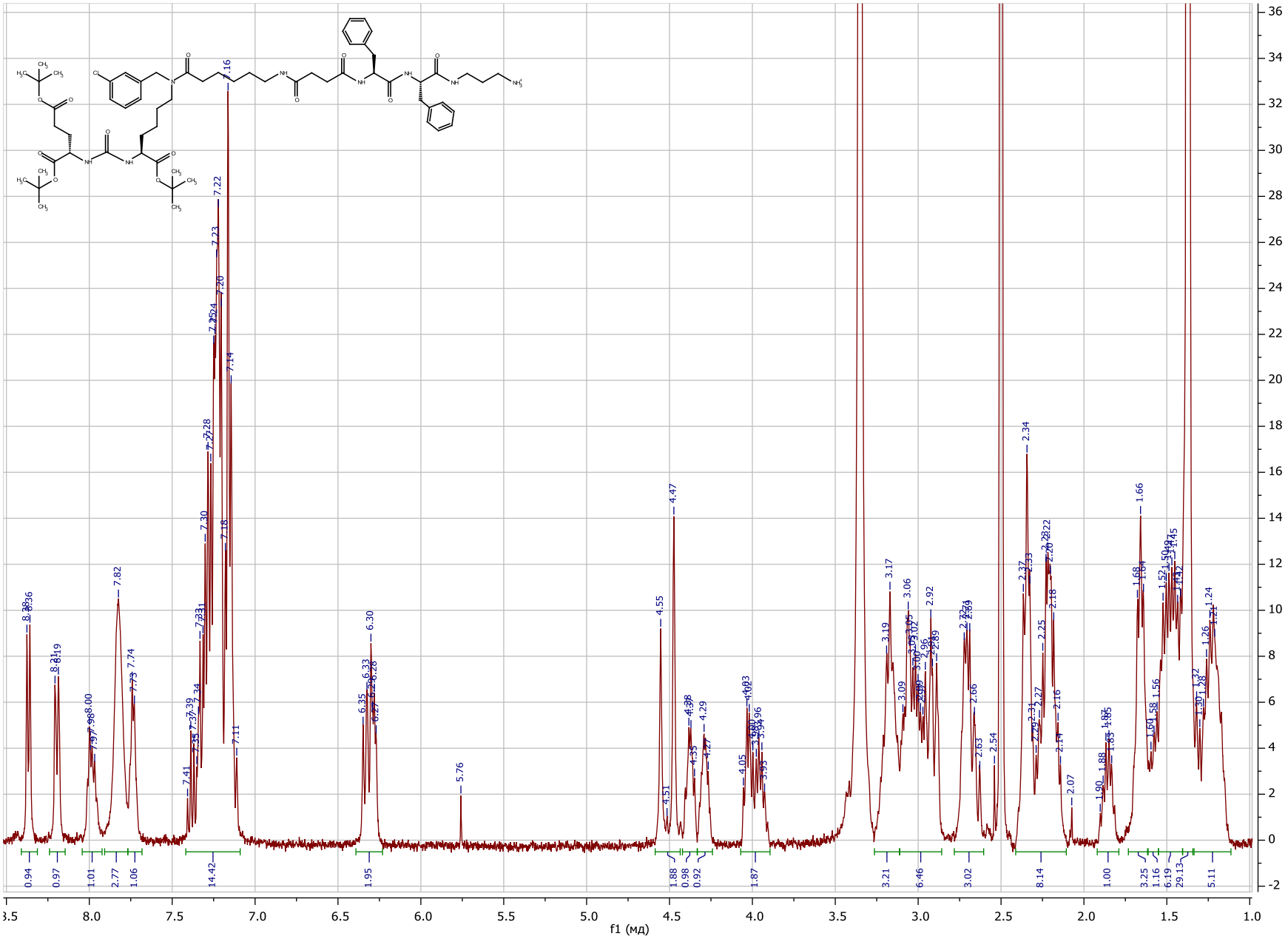

Figure S17. ^{1}H NMR spectrum of compound № **11** in DMSO-d_6.

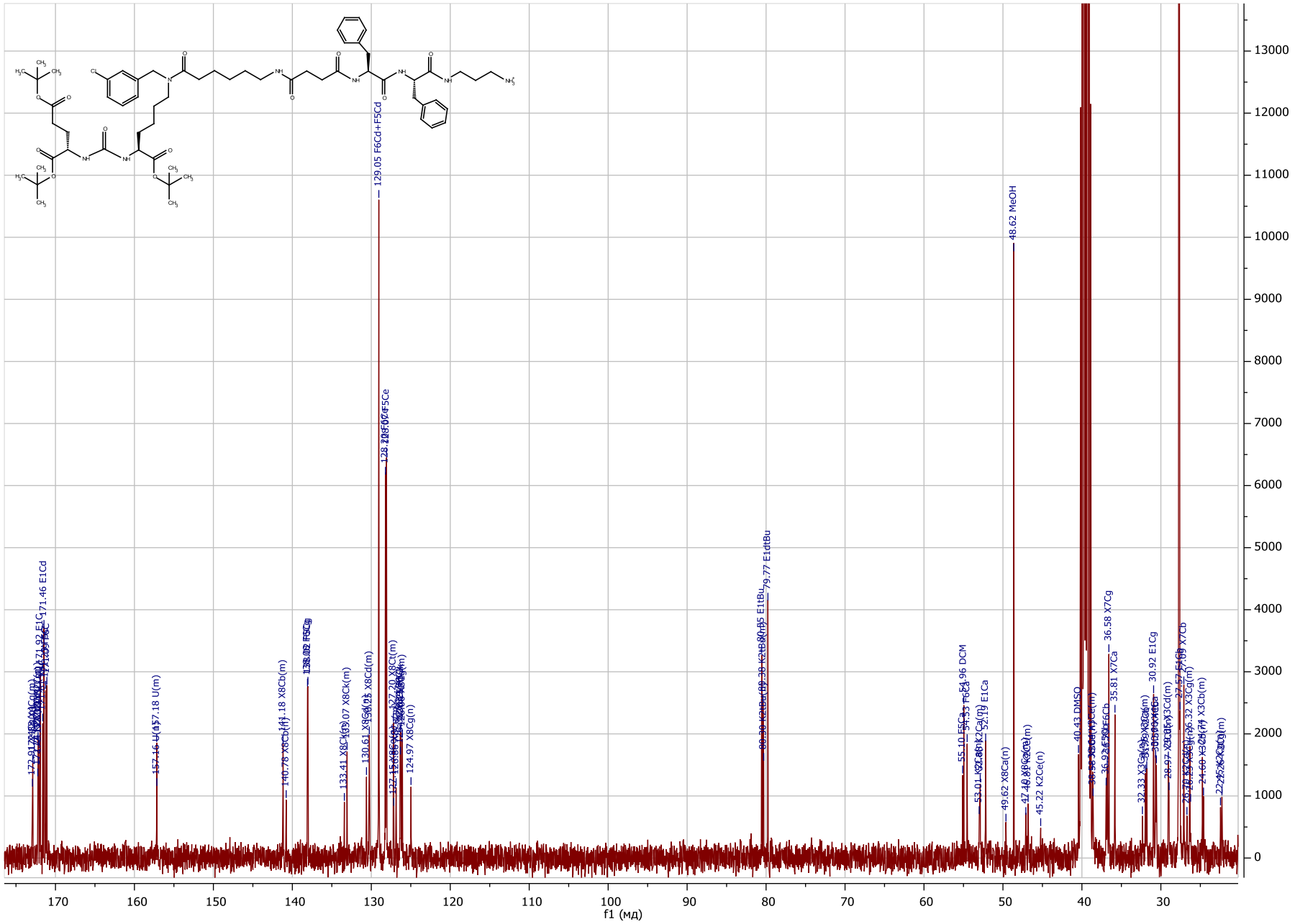

Figure S18. ^{13}C NMR spectrum of compound № **11** in DMSO-*d*$_6$.

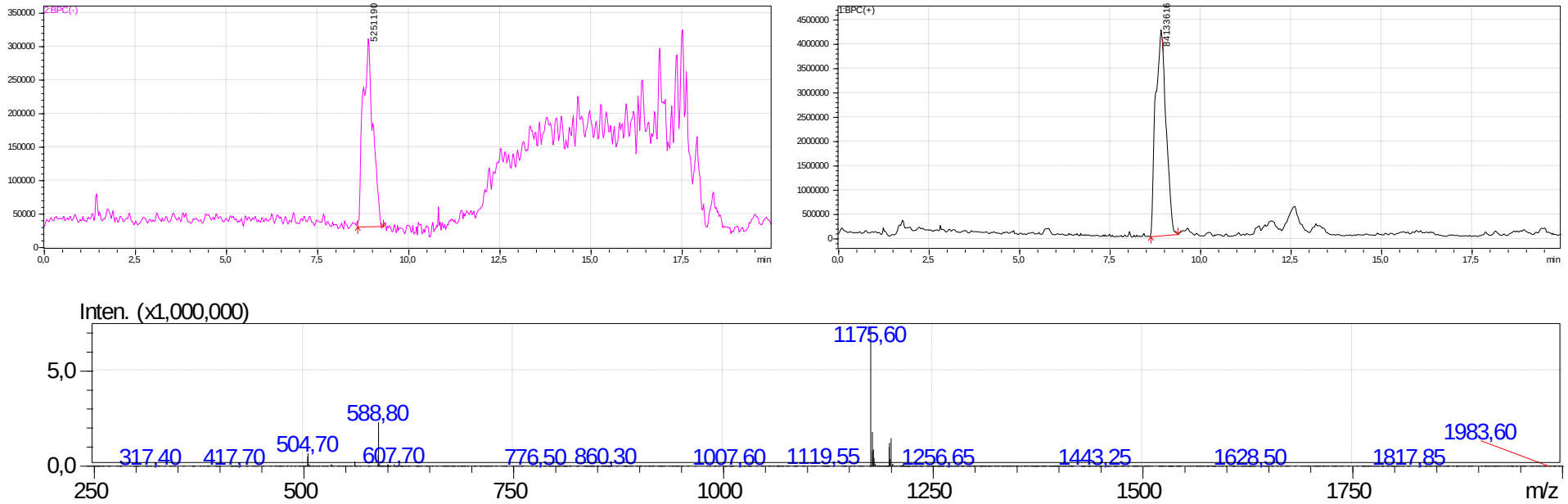

Figure S19. ESI-MS of compound № **11**

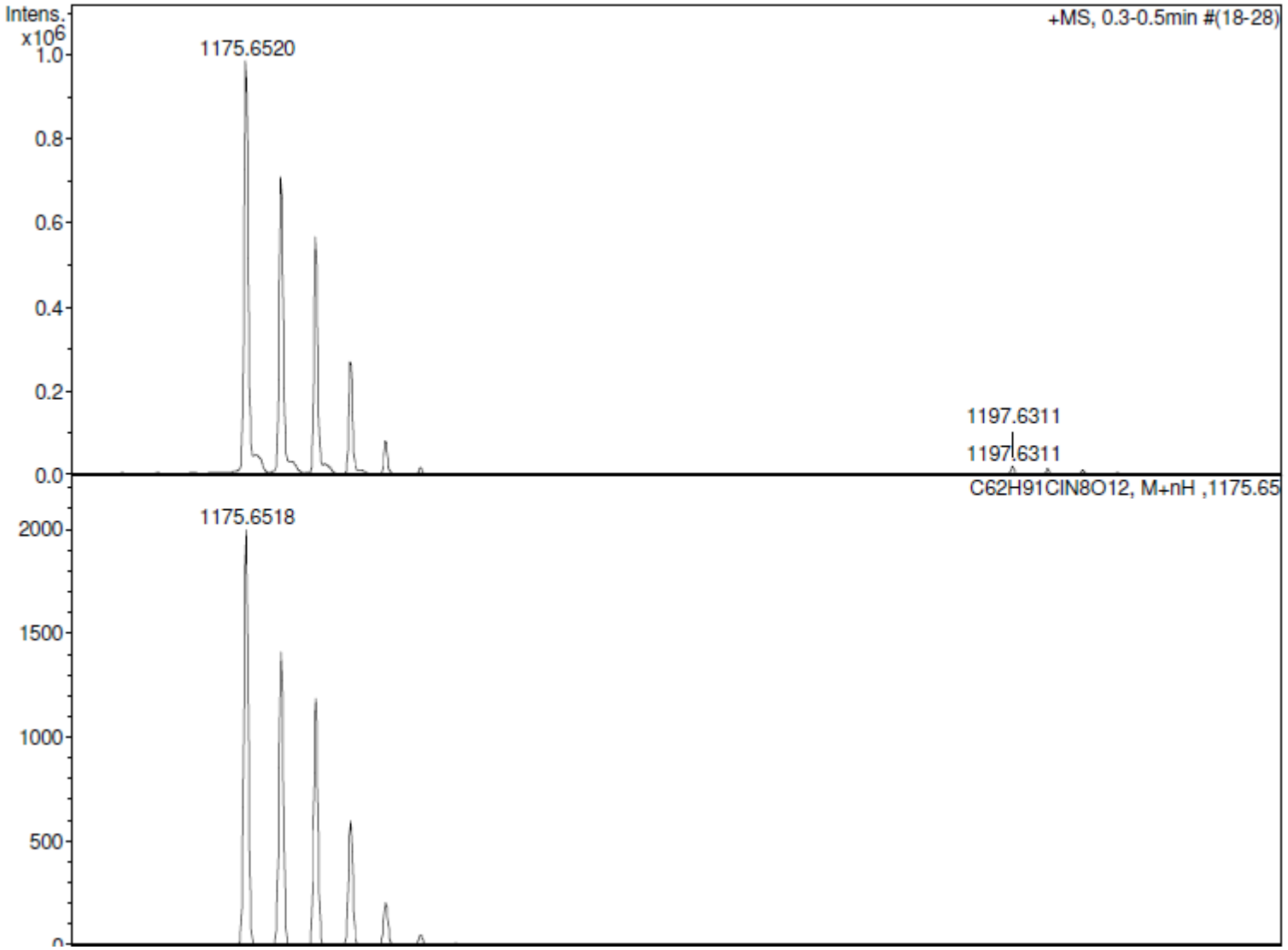

Figure S20. HRMS (m/z, ESI) of compound № **11**

Compound 13

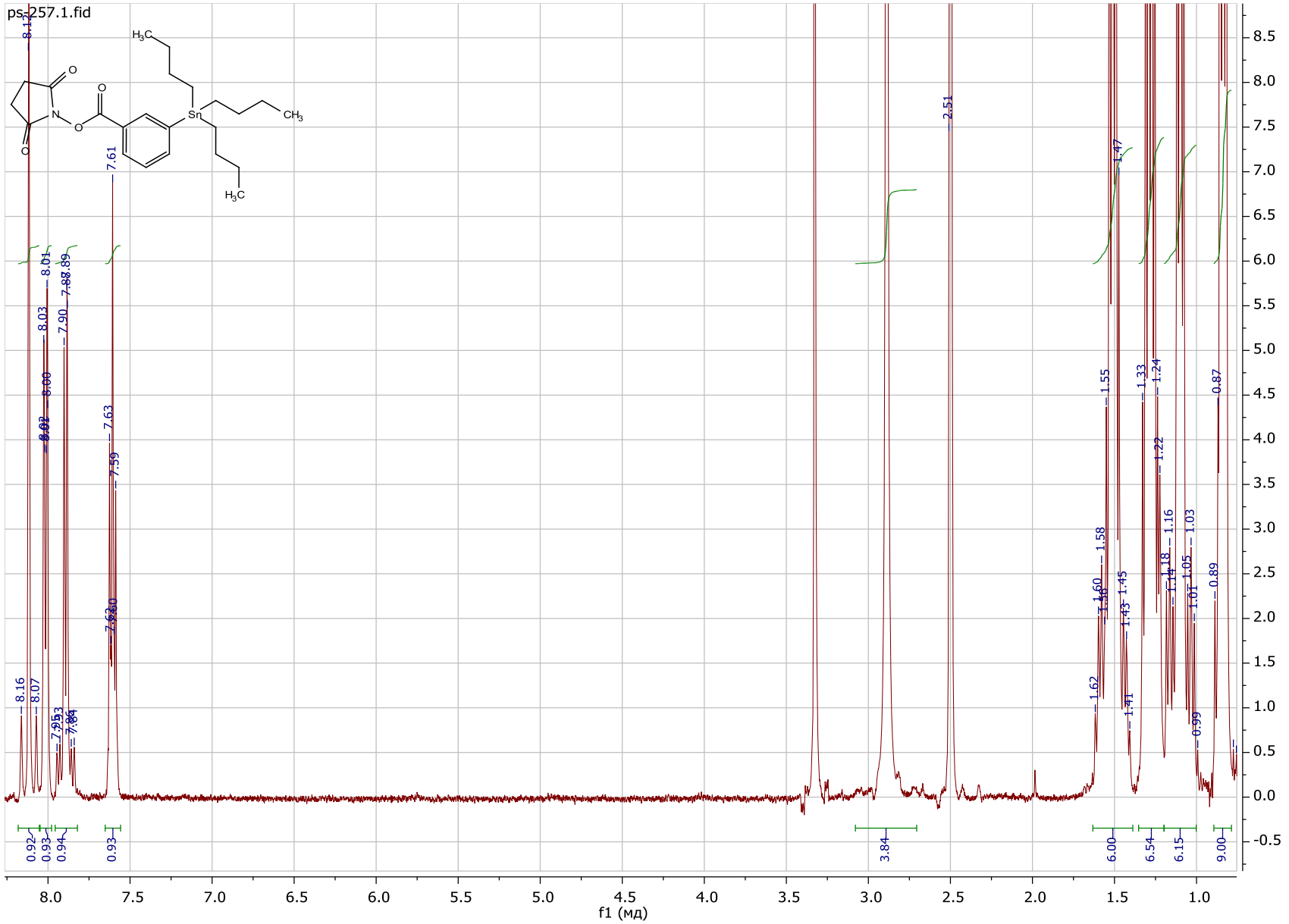

Figure S21. ^{1}H NMR spectrum of compound № **13** in DMSO-*d*$_6$.

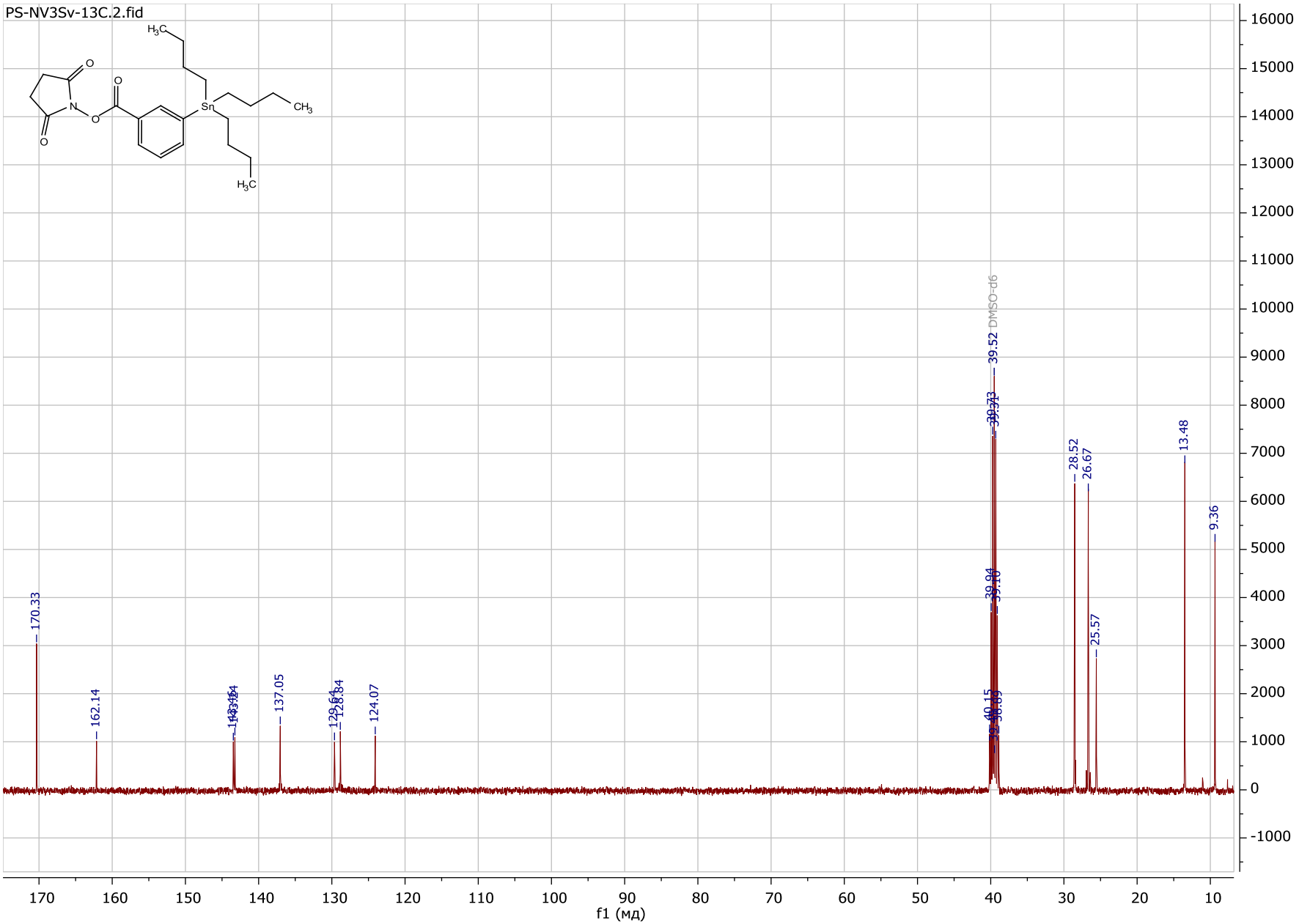

Figure S22. ^{13}C NMR spectrum of compound № **13** in DMSO-*d*$_6$.

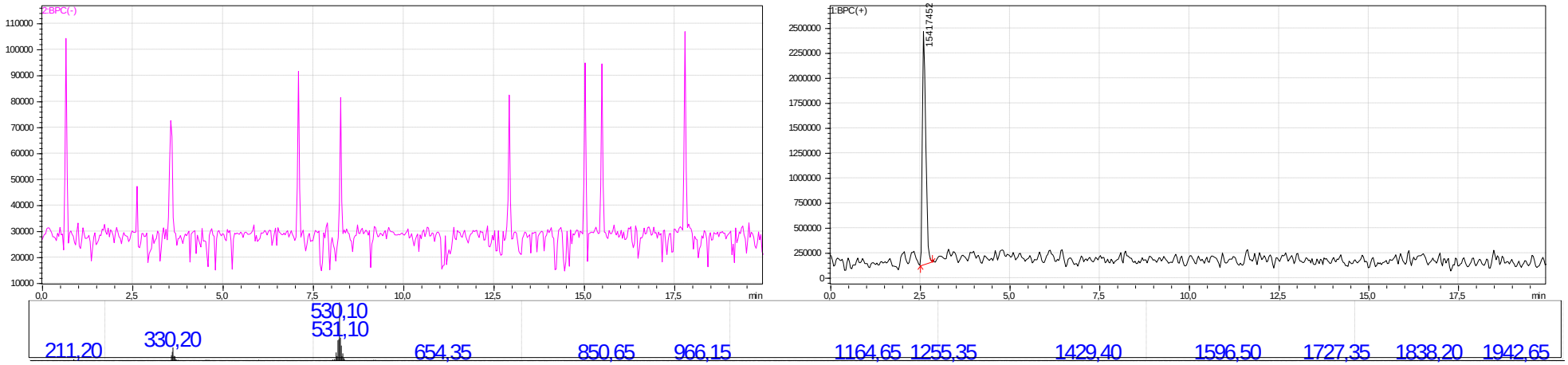

Figure S23. ESI-MS of compound № **13**

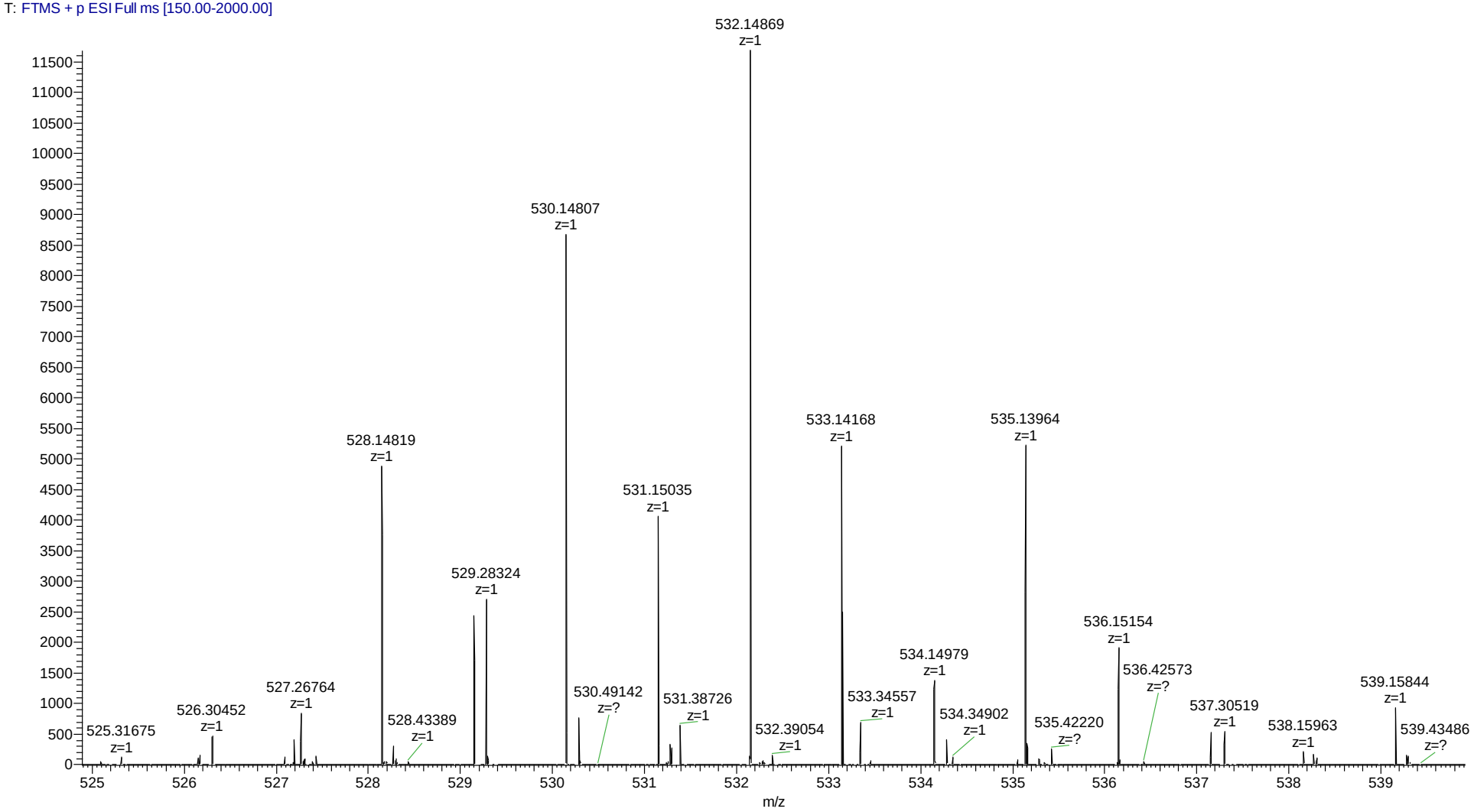

Figure S24. HRMS (m/z, ESI) of compound № **13**

Compound 14

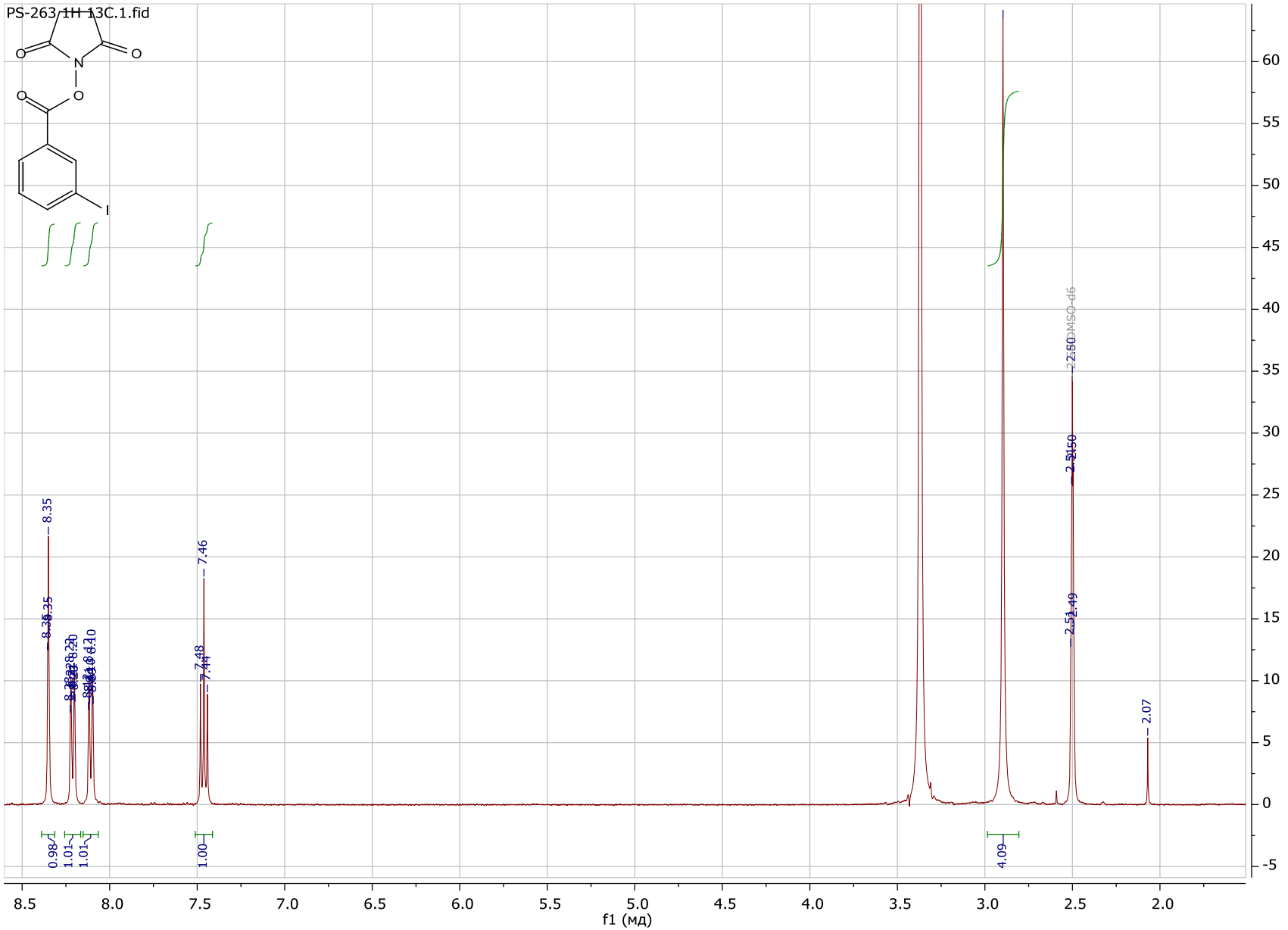

Figure S25. ^{1}H NMR spectrum of compound № **14** in DMSO-*d*$_6$.

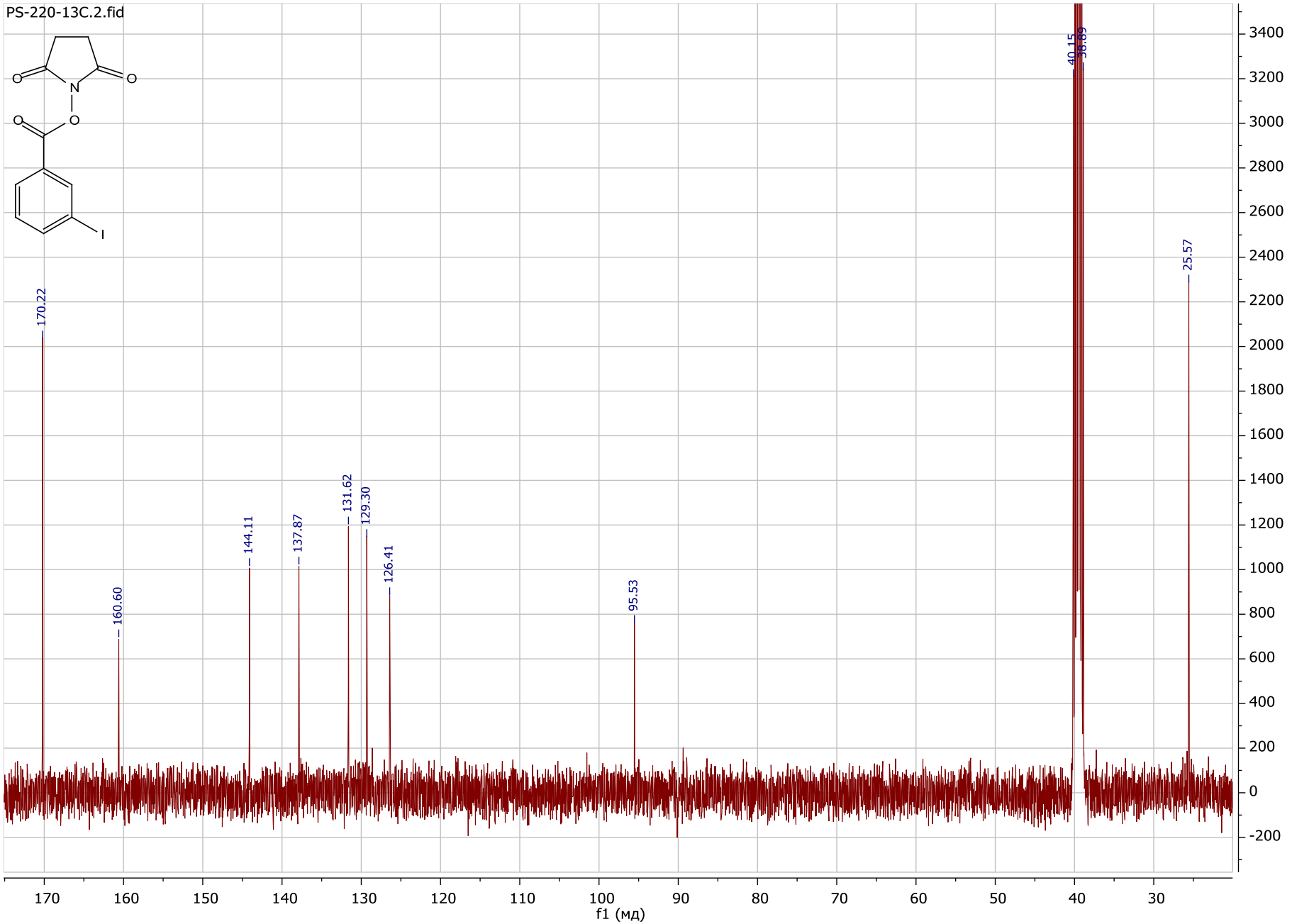

Figure S26. ^{13}C NMR spectrum of compound № **14** in DMSO-*d*$_6$.

Compound 16

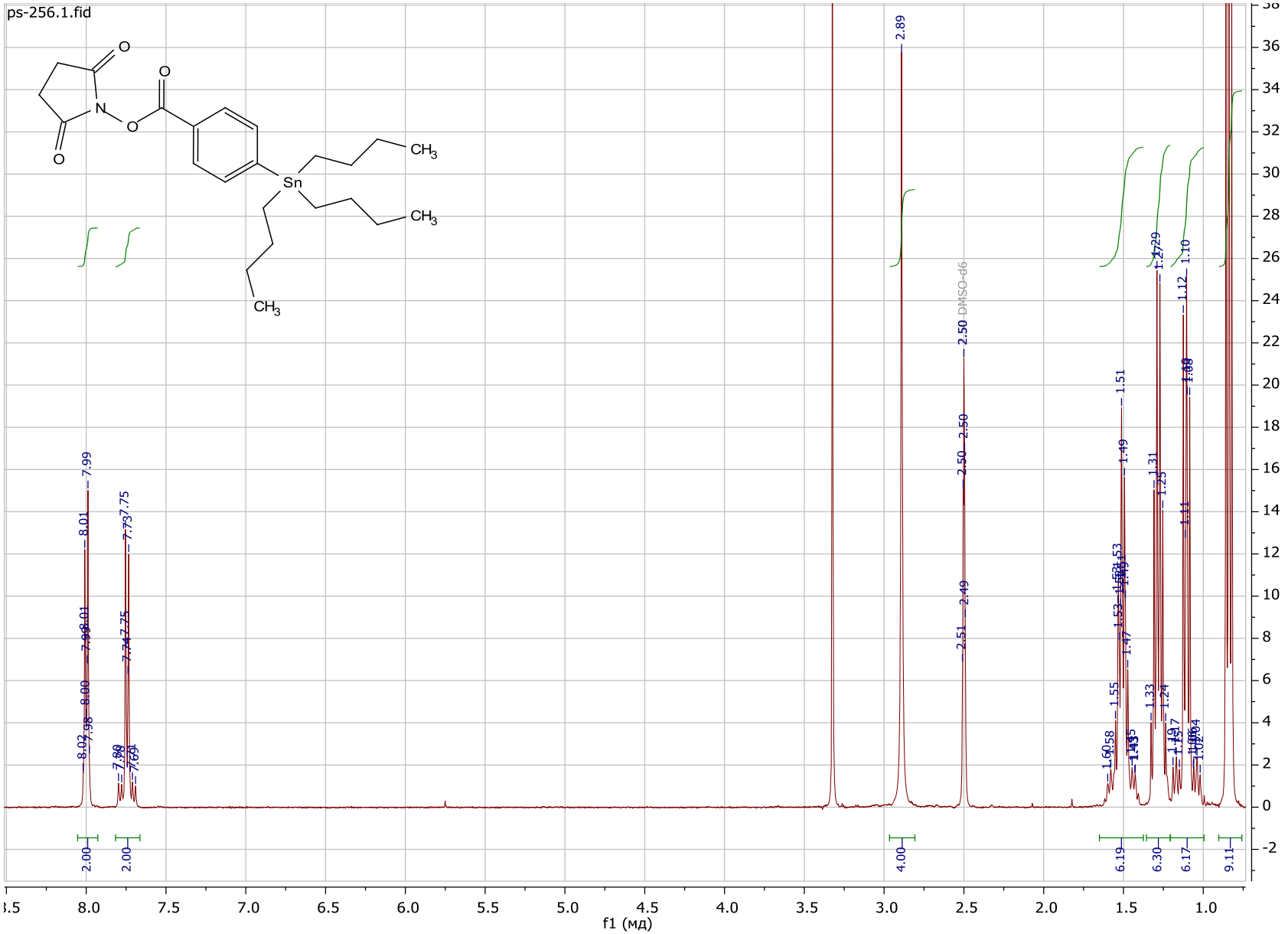

Figure S27. ^{1}H NMR spectrum of compound № **16** in DMSO-*d*$_6$.

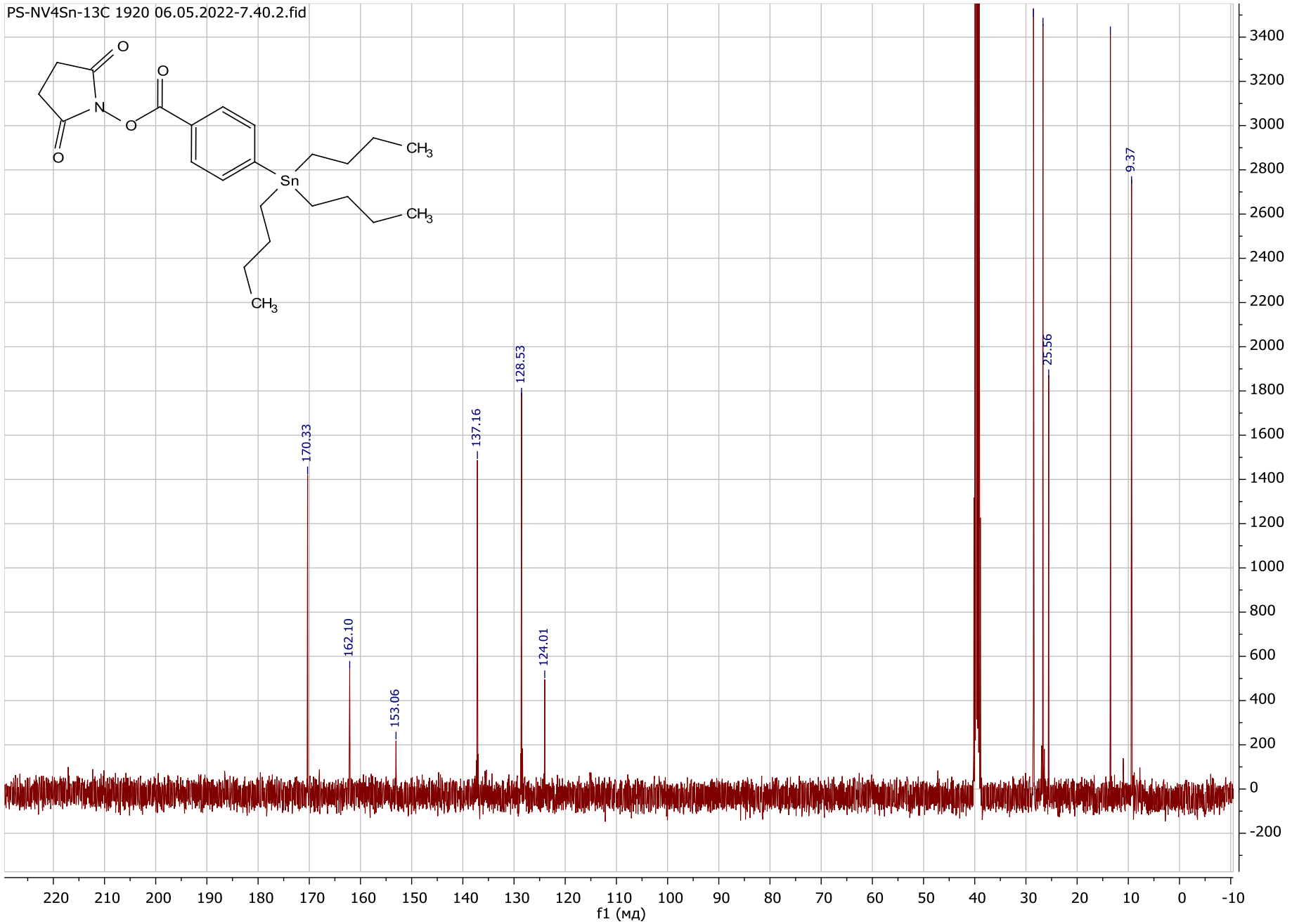

Figure S28. ^{13}C NMR spectrum of compound № **16** in DMSO-*d*$_6$.

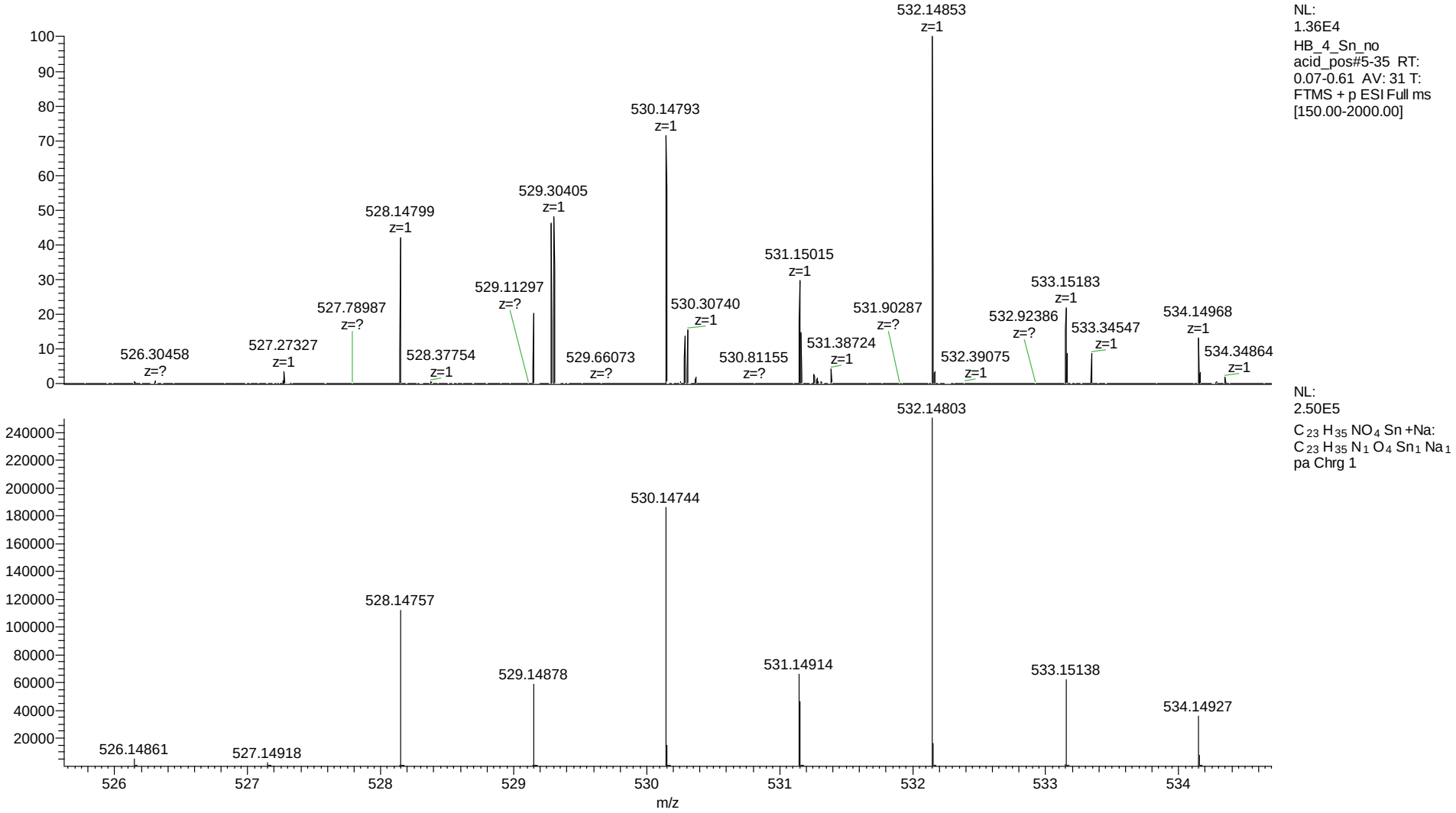

Figure S29. HRMS (m/z, ESI) of compound № **16**

Compound 17

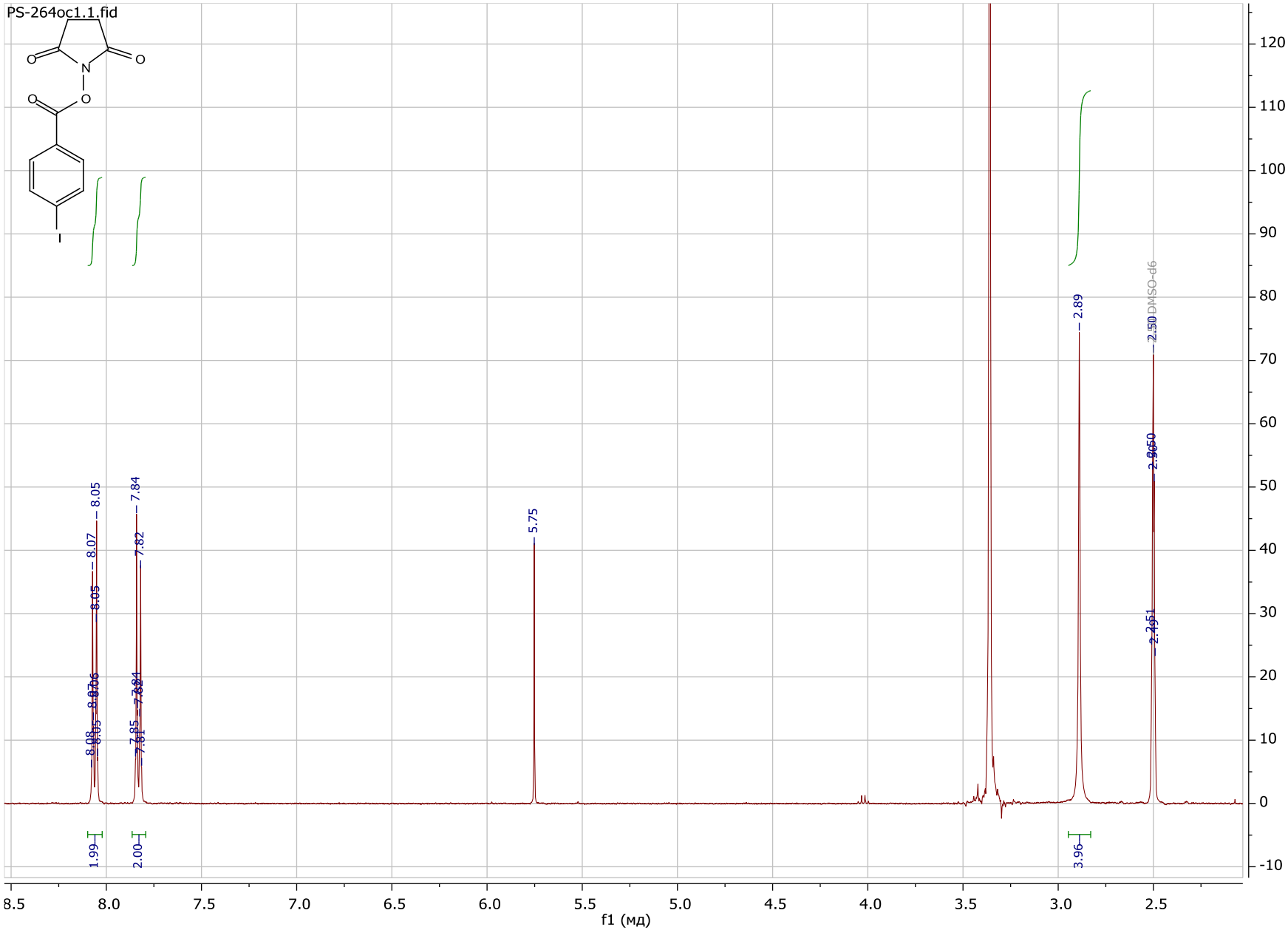

Figure S30. ^{1}H NMR spectrum of compound № **17** in DMSO-d_6.

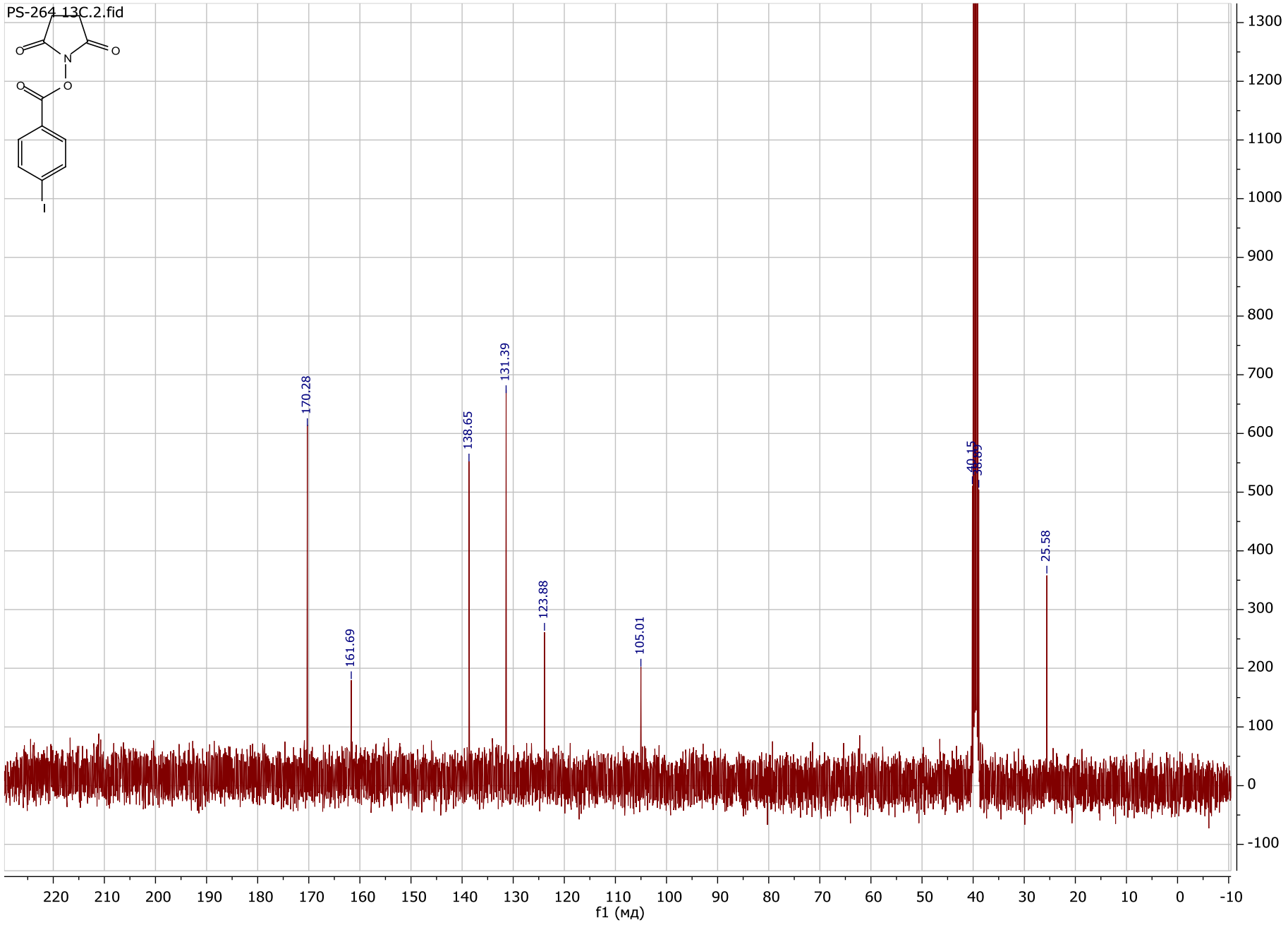

Figure S31. ^{13}C NMR spectrum of compound № **17** in DMSO-*d*$_6$.

Compound 18

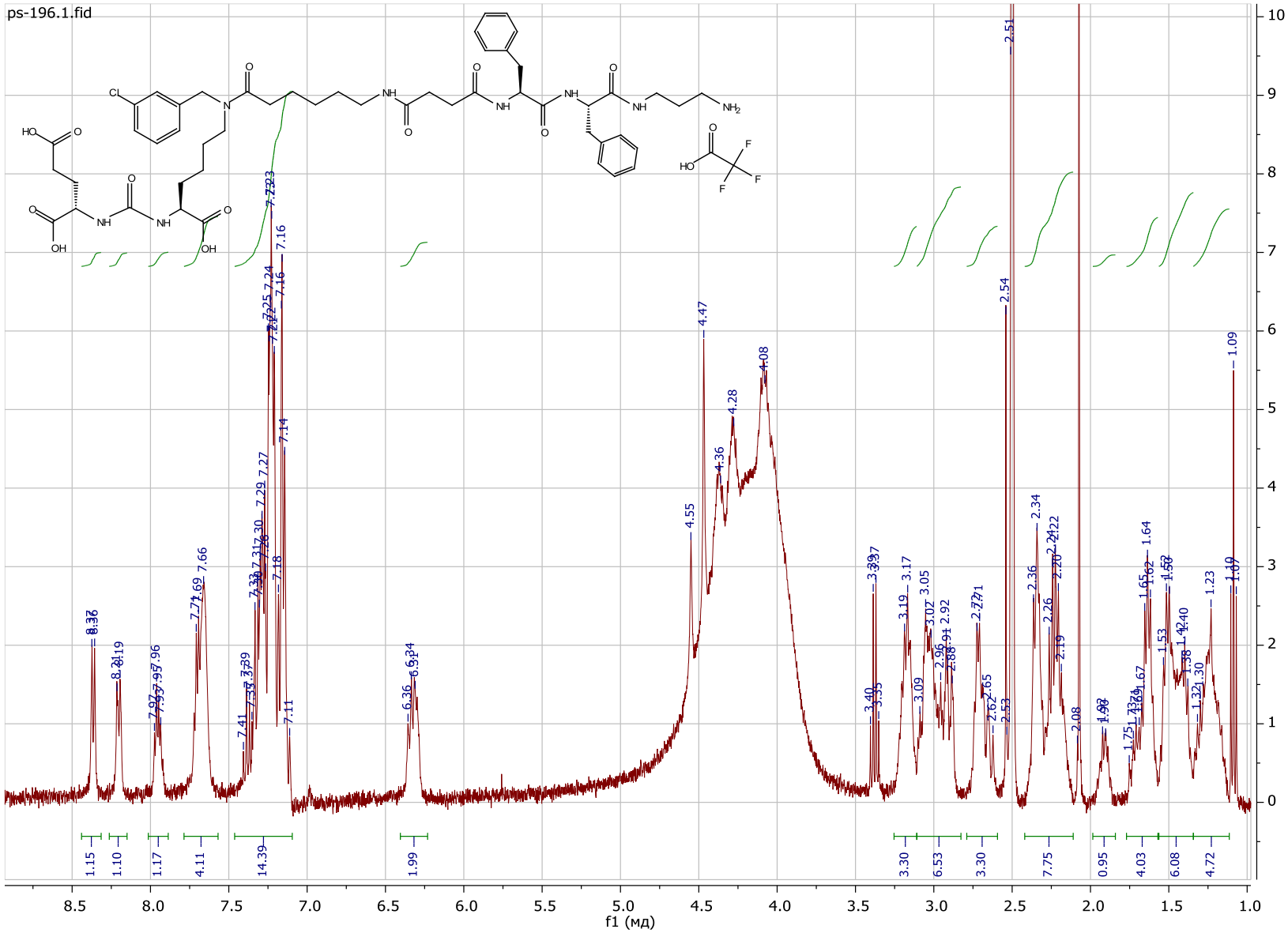

Figure S32. ^{1}H NMR spectrum of compound № **18** in DMSO-*d*$_6$.

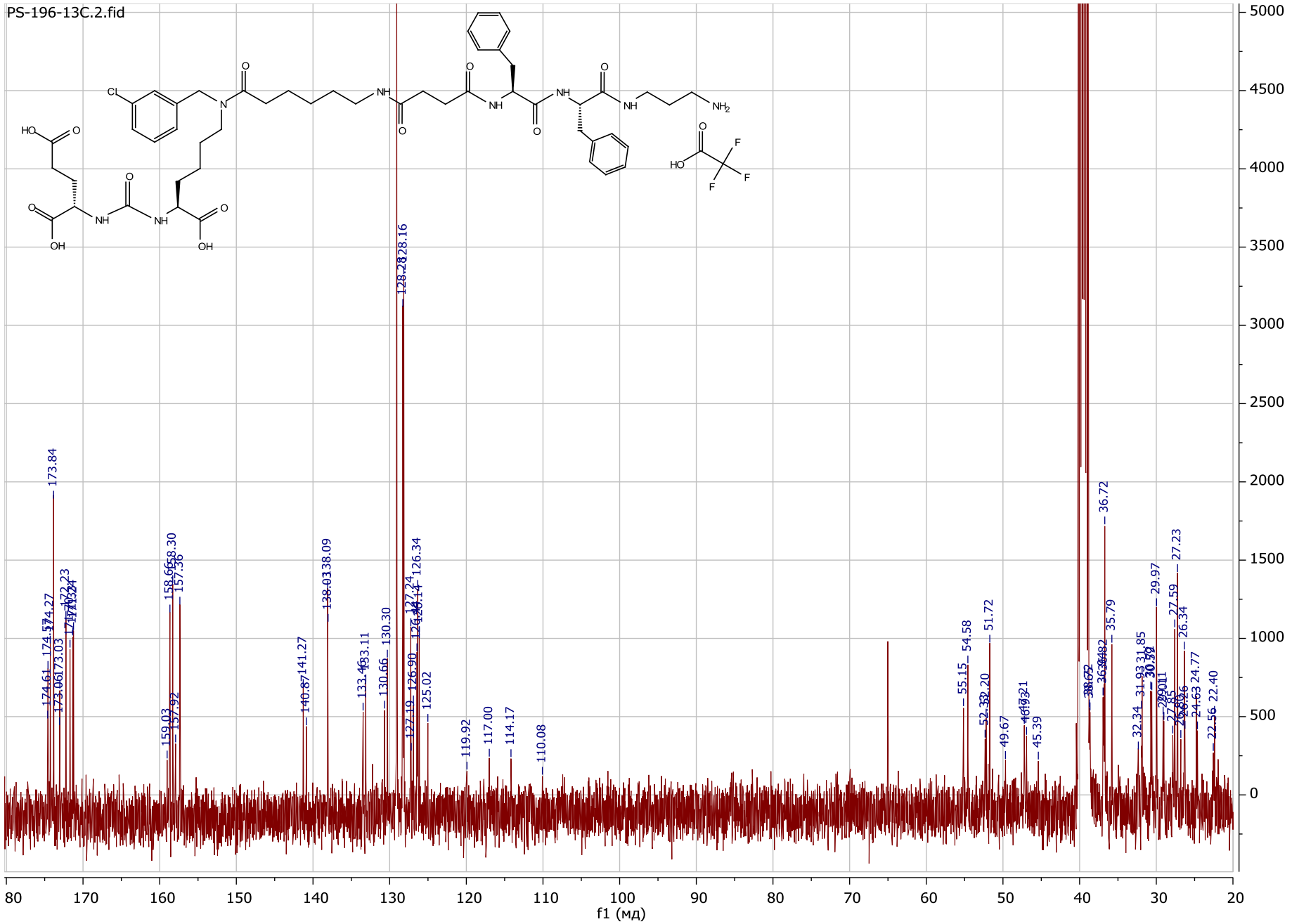

Figure S33. ^{13}C NMR spectrum of compound № **18** in DMSO-*d*$_6$.

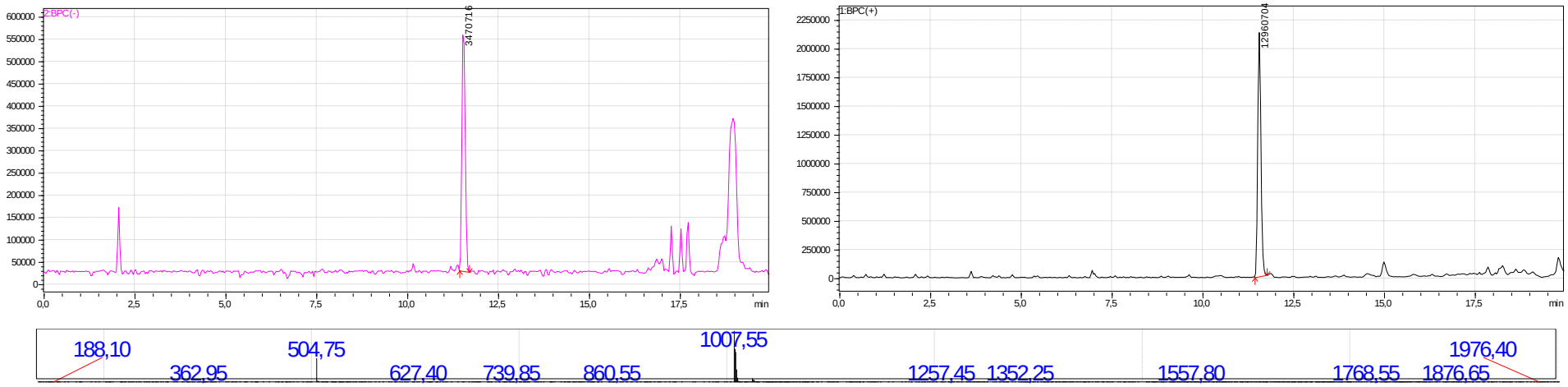

Figure S34. ESI-MS of compound № **18**

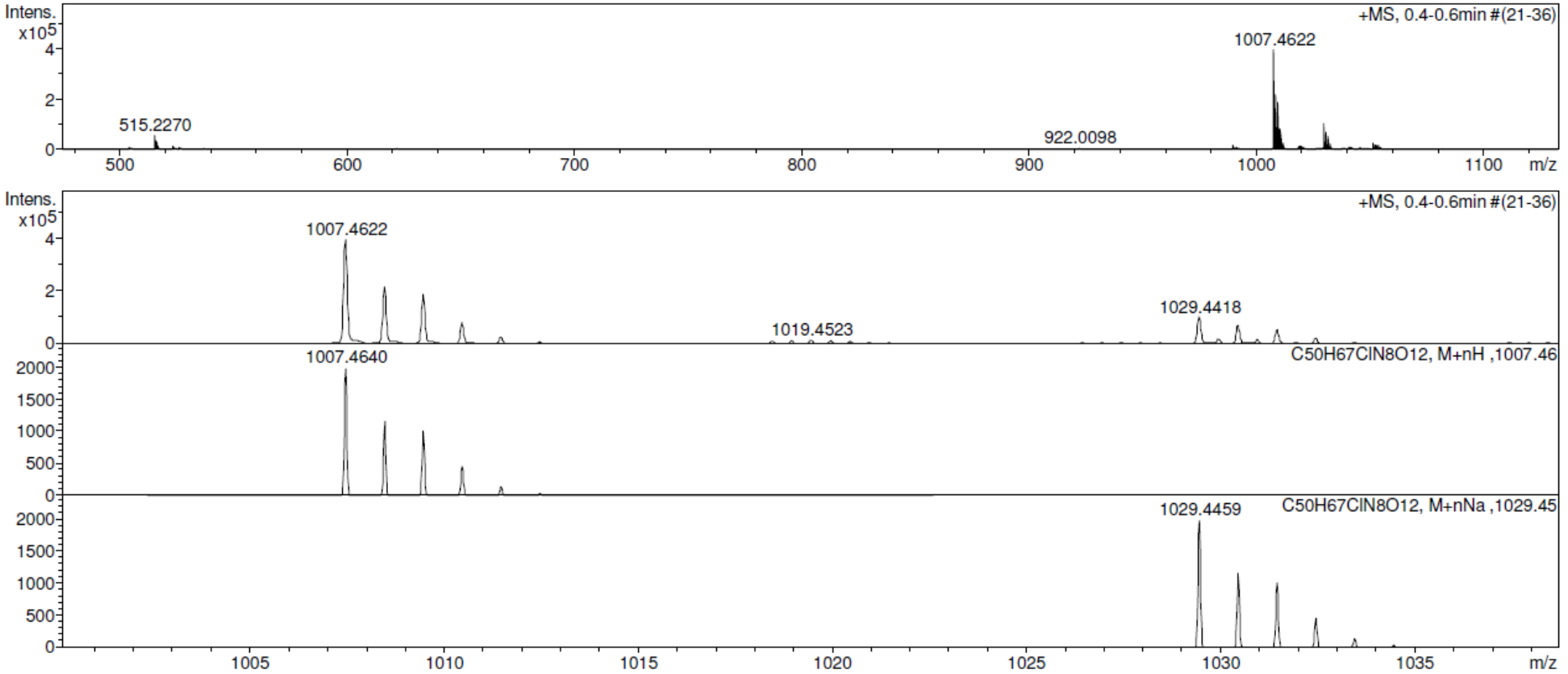

Figure S35. HRMS (m/z, ESI) of compound № **18**

Compound 19

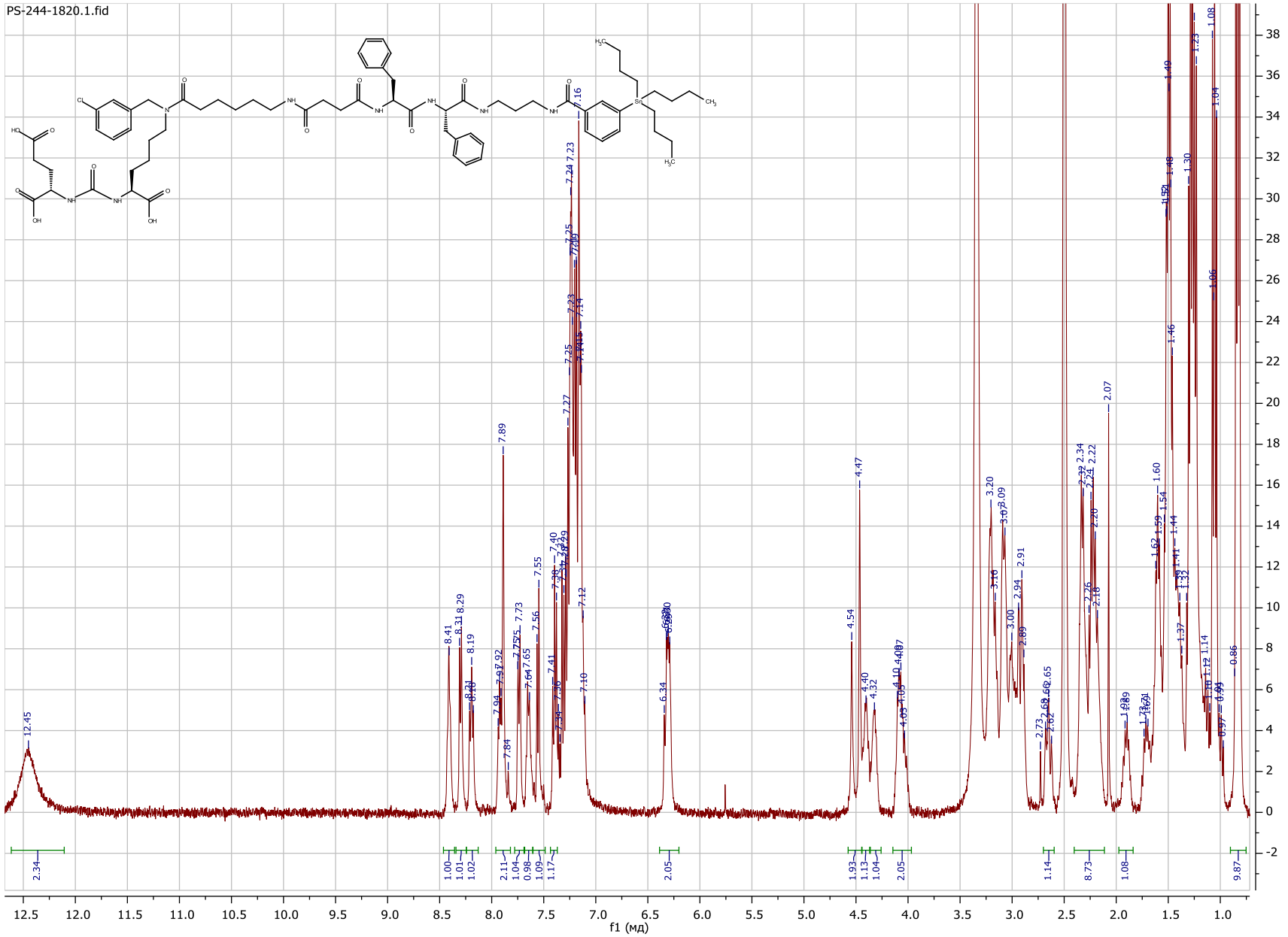

Figure S36. ^{1}H NMR spectrum of compound № **19** in DMSO-*d*$_6$.

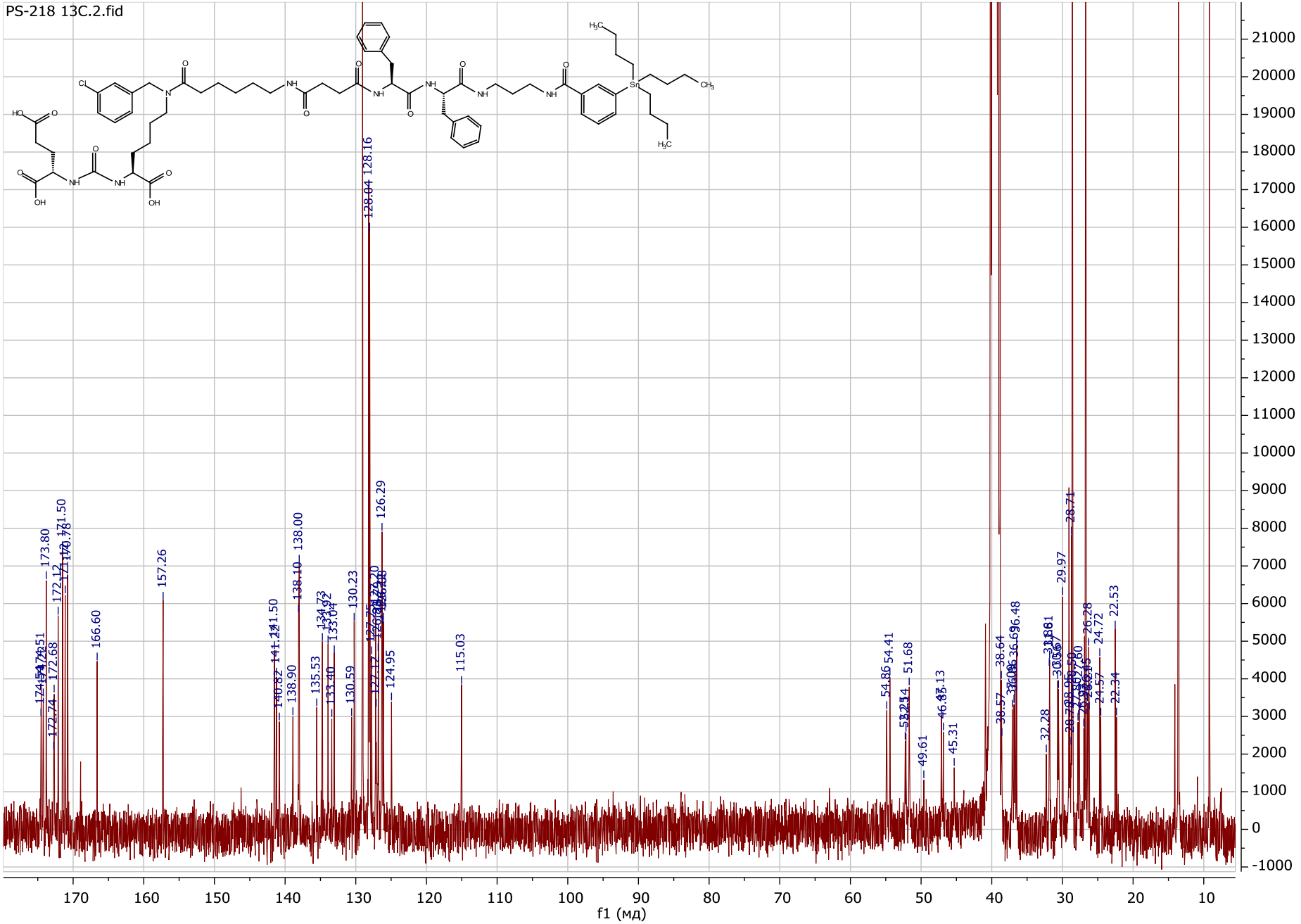

Figure S37. ^{13}C NMR spectrum of compound № **19** in DMSO-*d*$_6$.

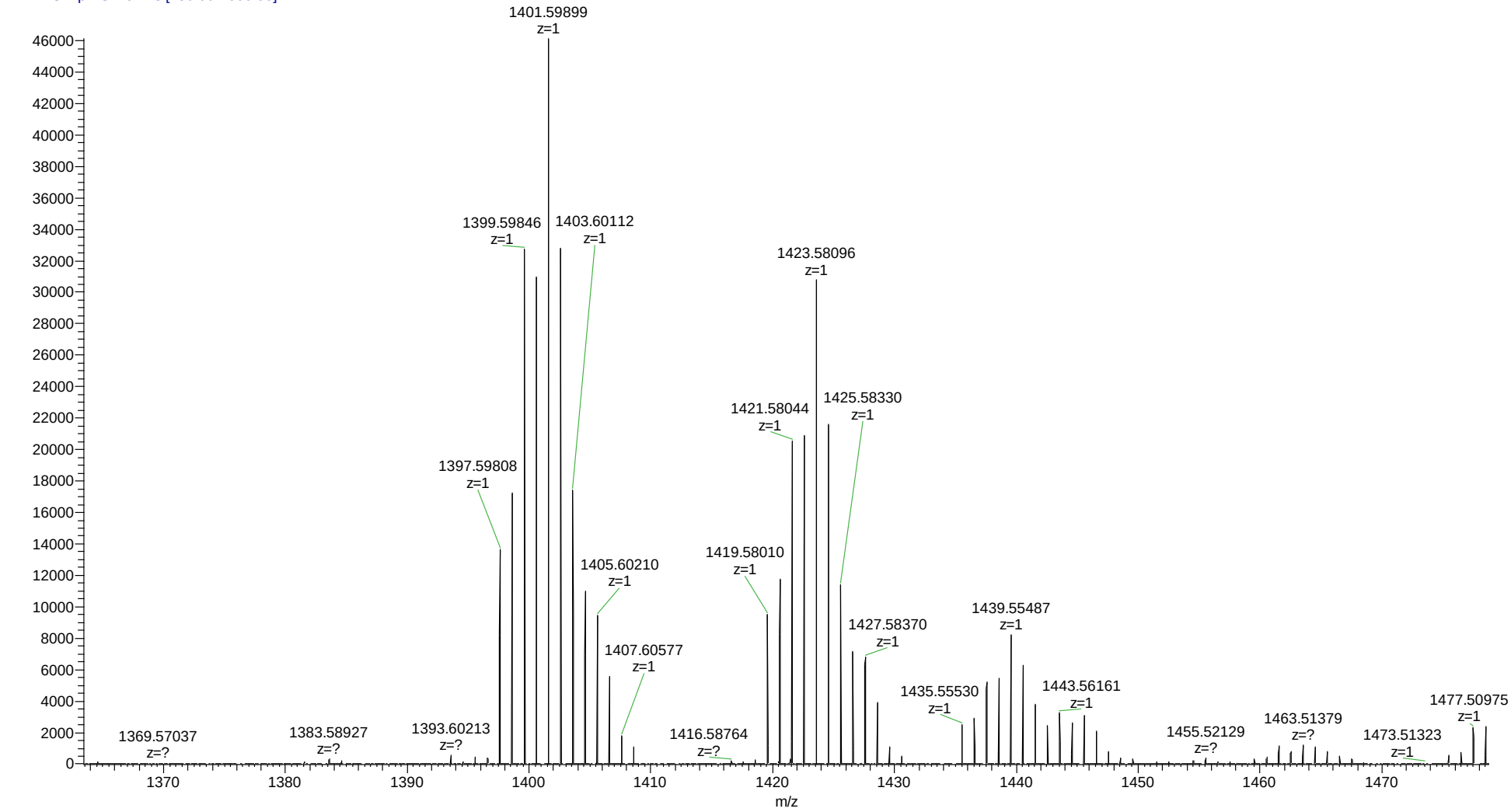

Figure S38. HRMS (m/z, ESI) of compound № **19**

Compound 20

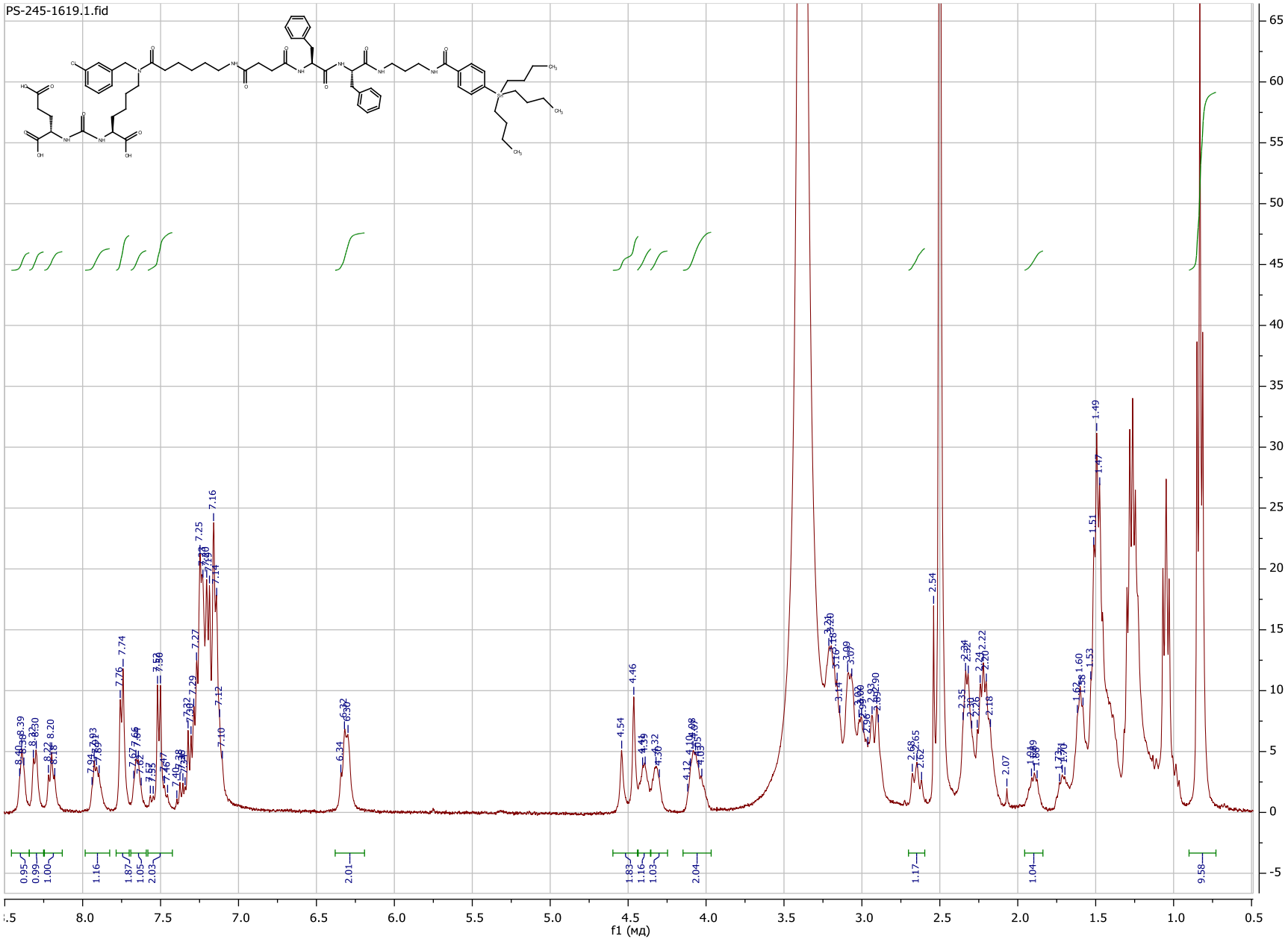

Figure S39. ^{1}H NMR spectrum of compound № **20** in DMSO-d_6.

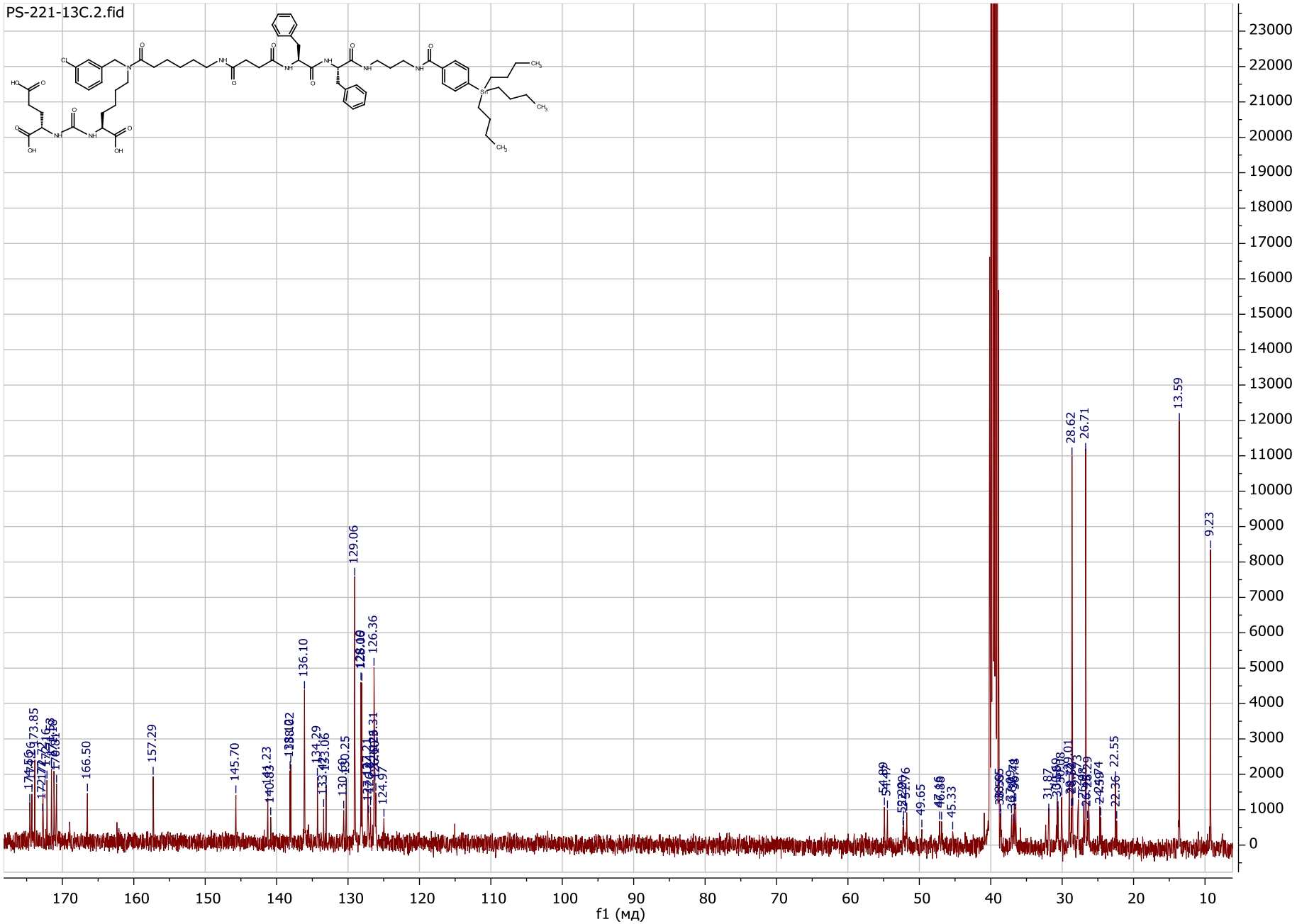

Figure S40. ^{13}C NMR spectrum of compound № **20** in DMSO-*d*$_6$.

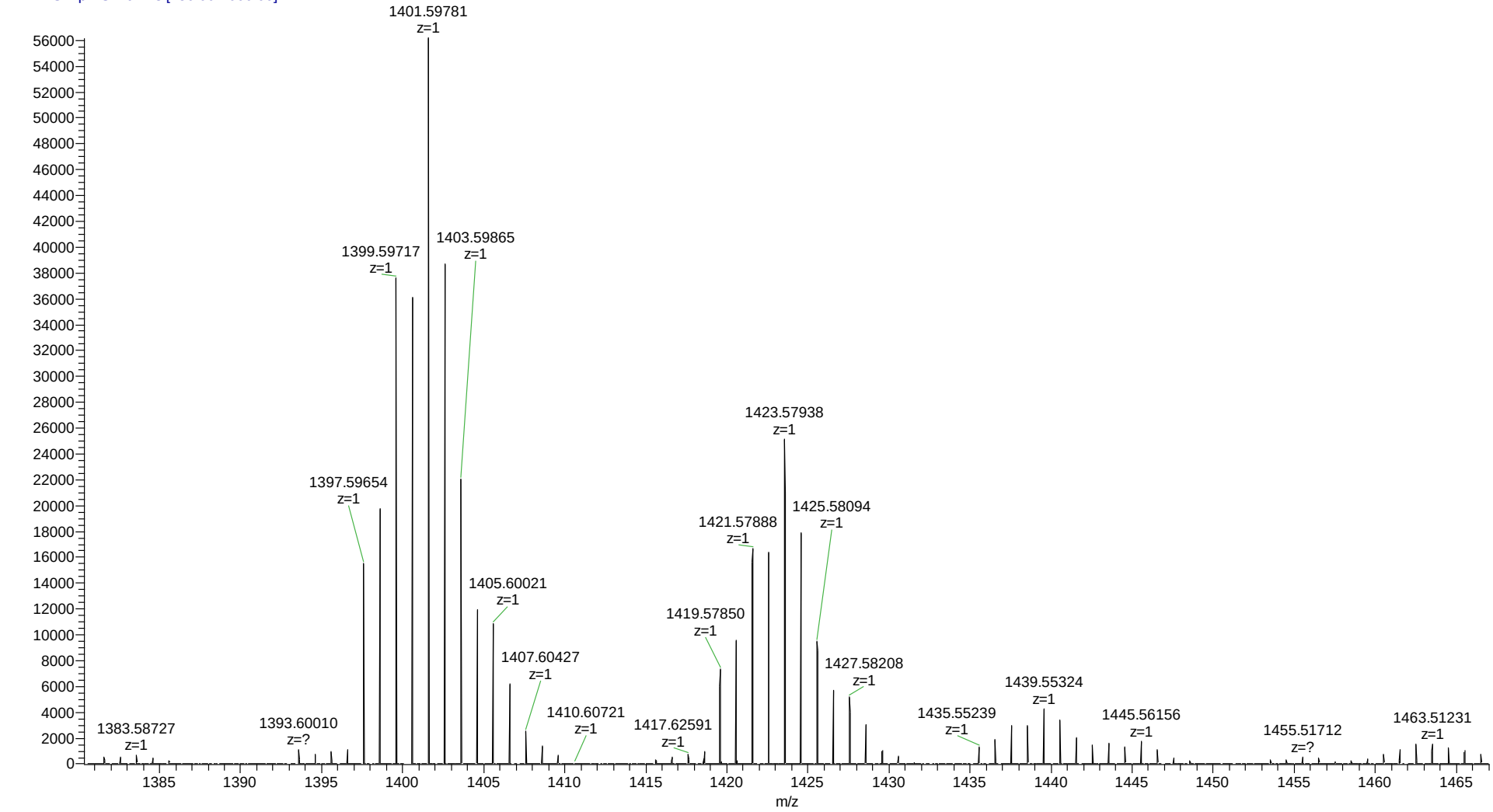

Figure S41. HRMS (m/z, ESI) of compound № **20**

Compound 21

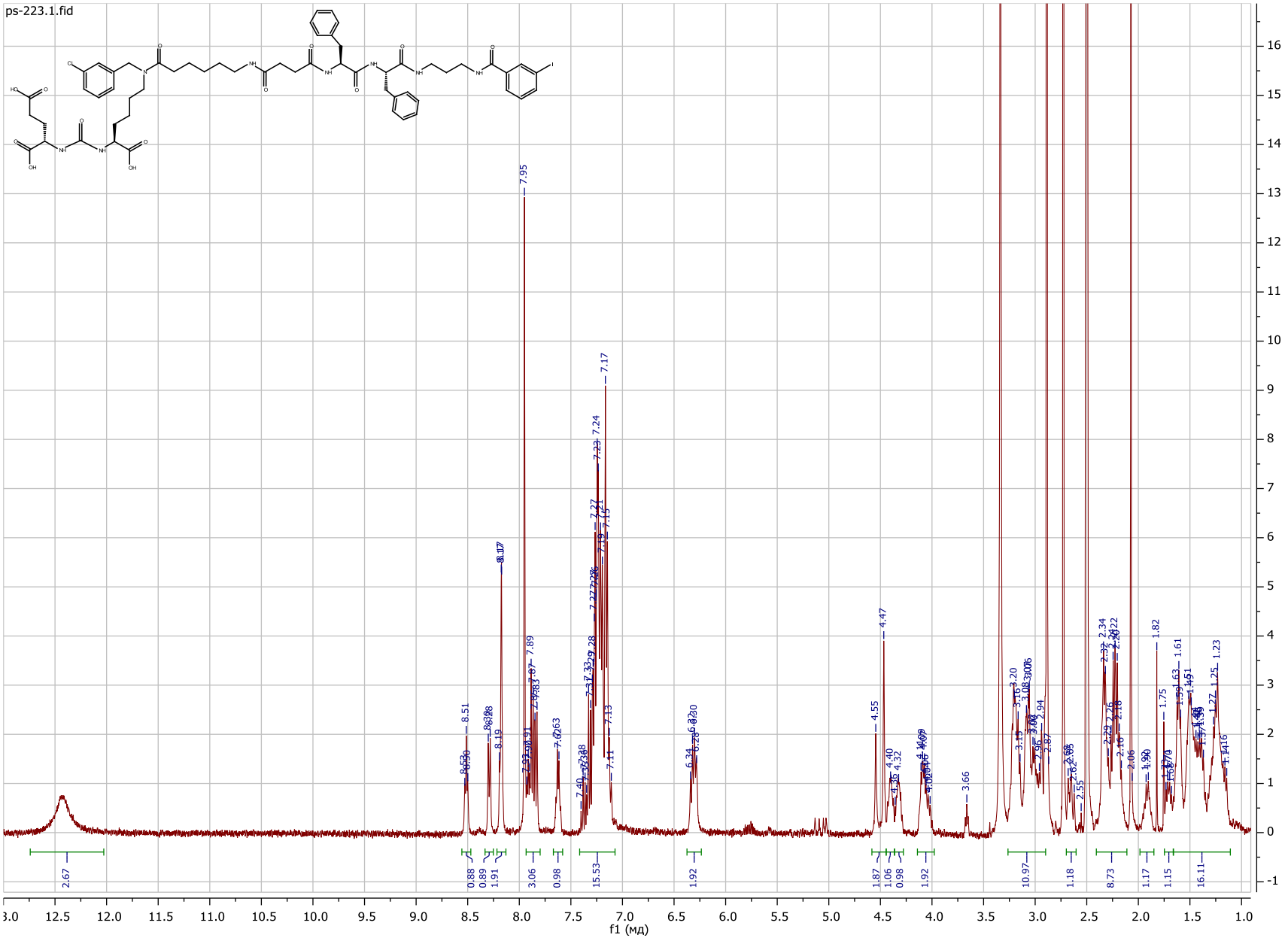

Figure S42. ^{1}H NMR spectrum of compound № **21** in DMSO-*d*$_6$.

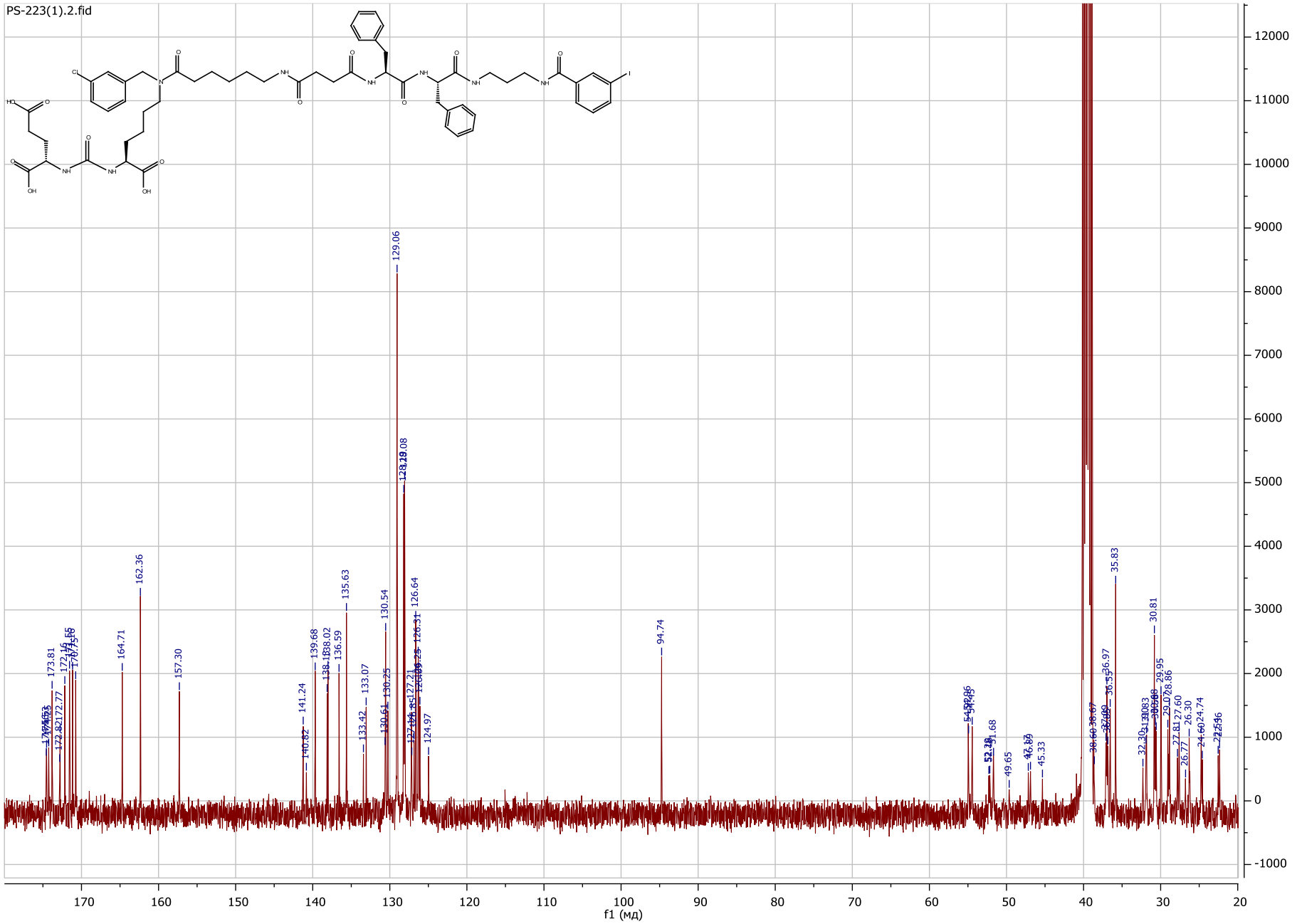

Figure S43. ^{13}C NMR spectrum of compound № **21** in DMSO-*d*$_6$.

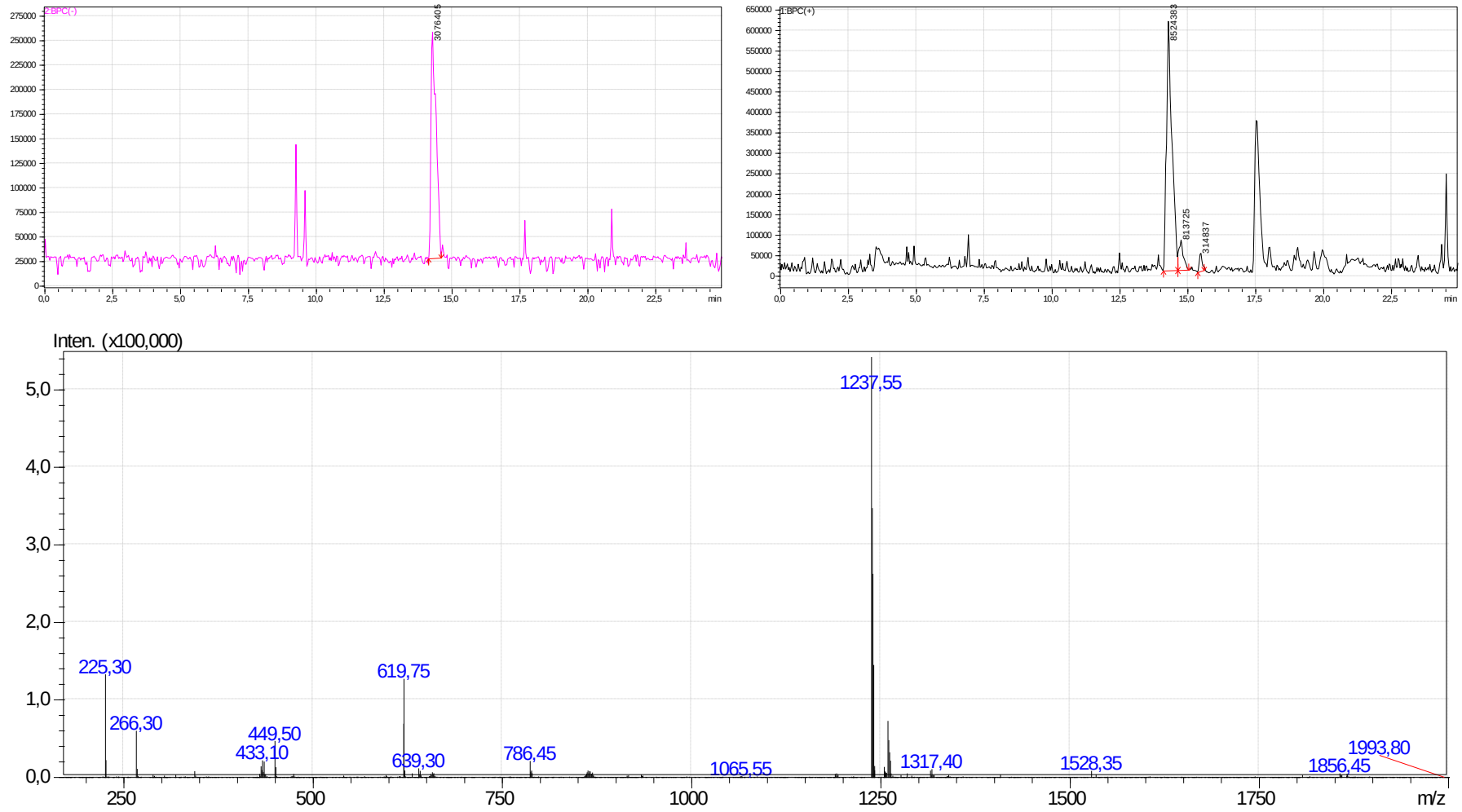

Figure S44. ESI-MS of compound № **21**

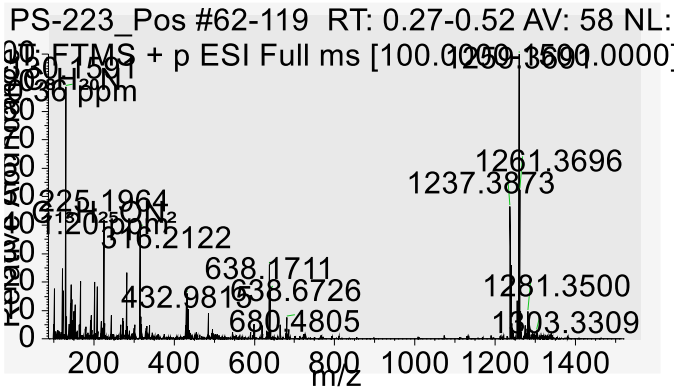

Figure S45. HRMS (m/z, ESI) of compound № **21**

Compound 22

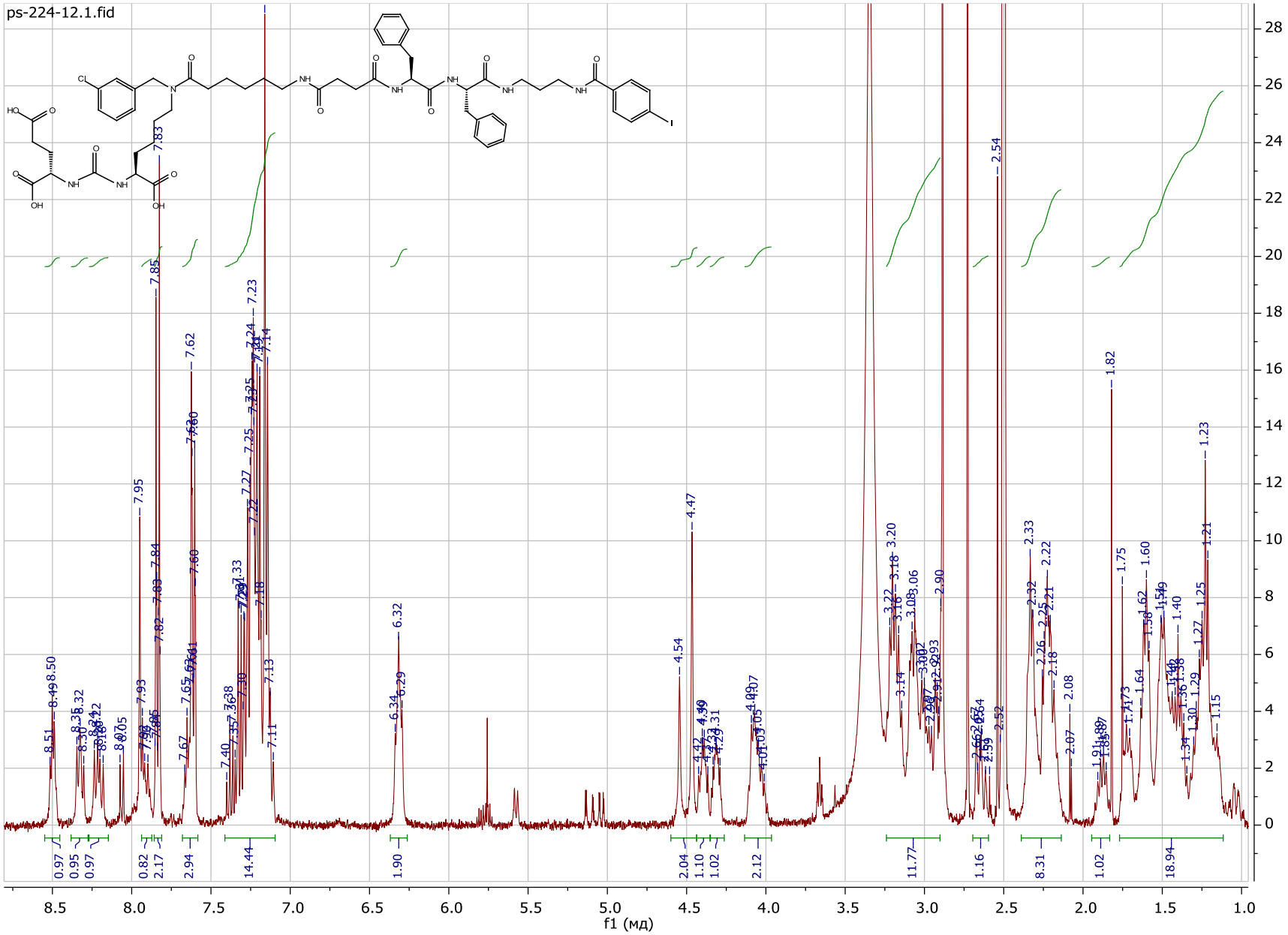

Figure S46. ^{1}H NMR spectrum of compound № **22** in DMSO-*d*$_6$.

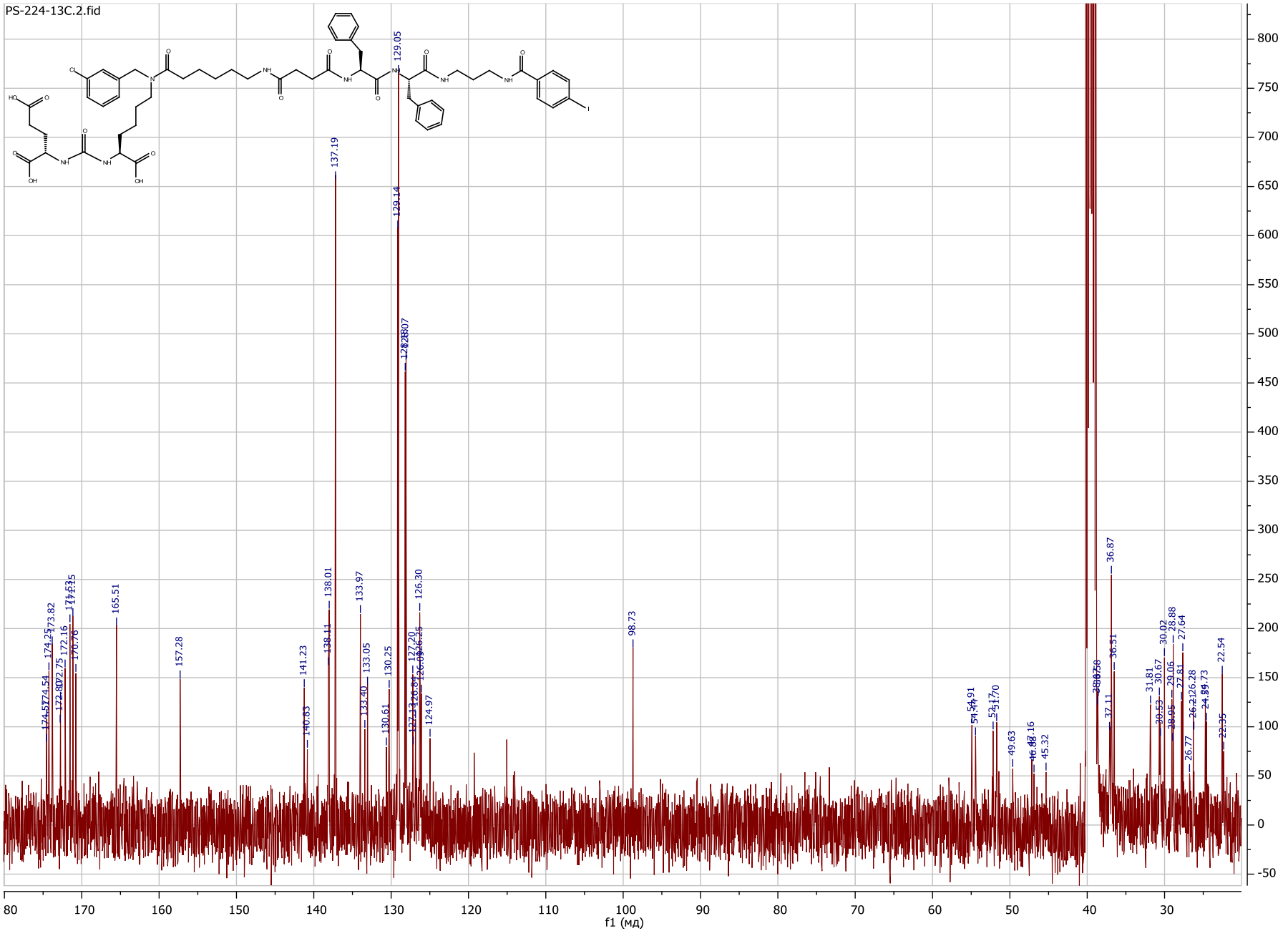

Figure S47. ^{13}C NMR spectrum of compound № **22** in DMSO-*d*$_6$.

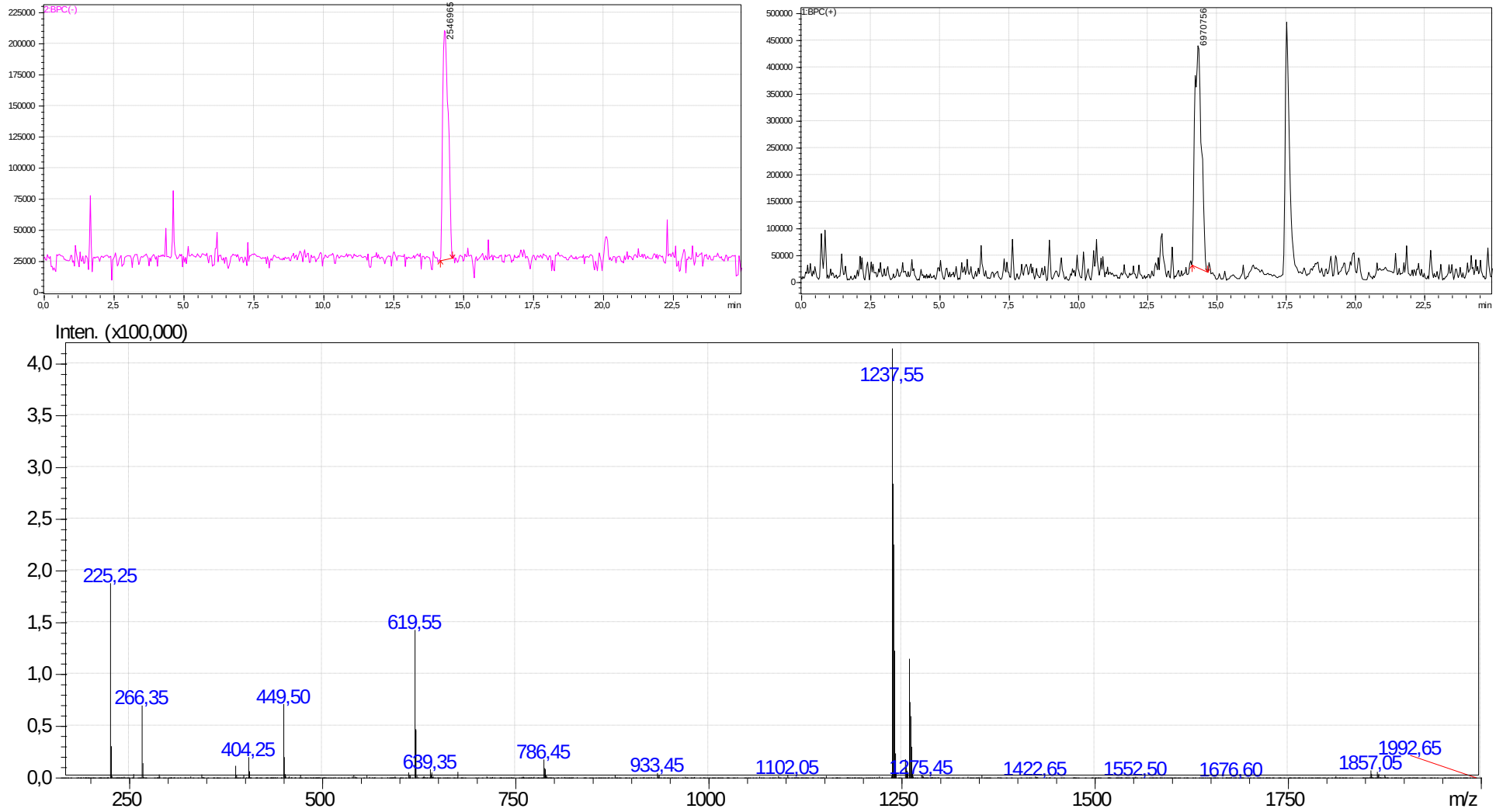

Figure S48. ESI-MS of compound № **22**

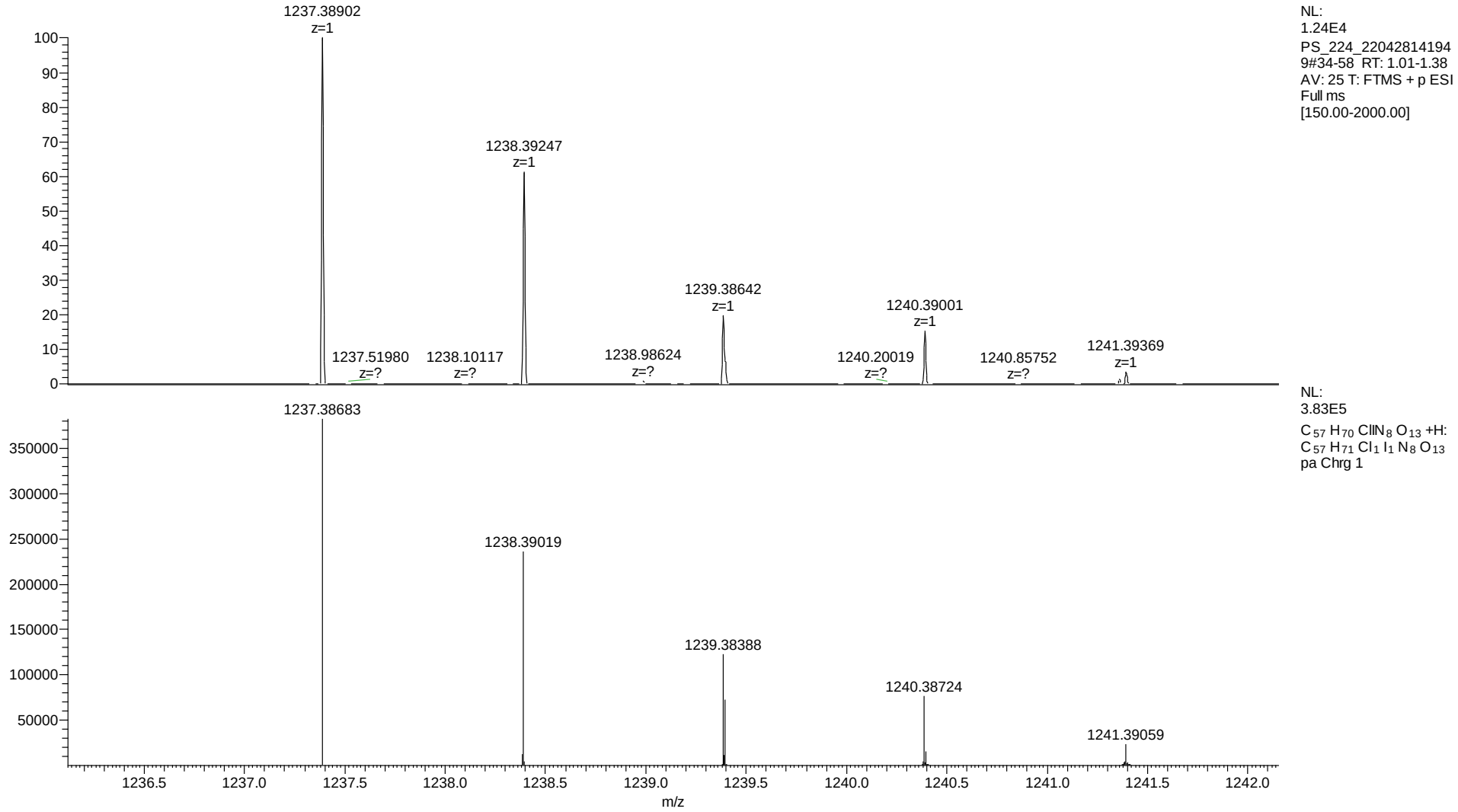

Figure S49. HRMS (m/z, ESI) of compound № **22**