

Synthesis and biological activity of thia-Michael-type adducts between naphthoquinones and *N*-acetyl-*L*-cysteine

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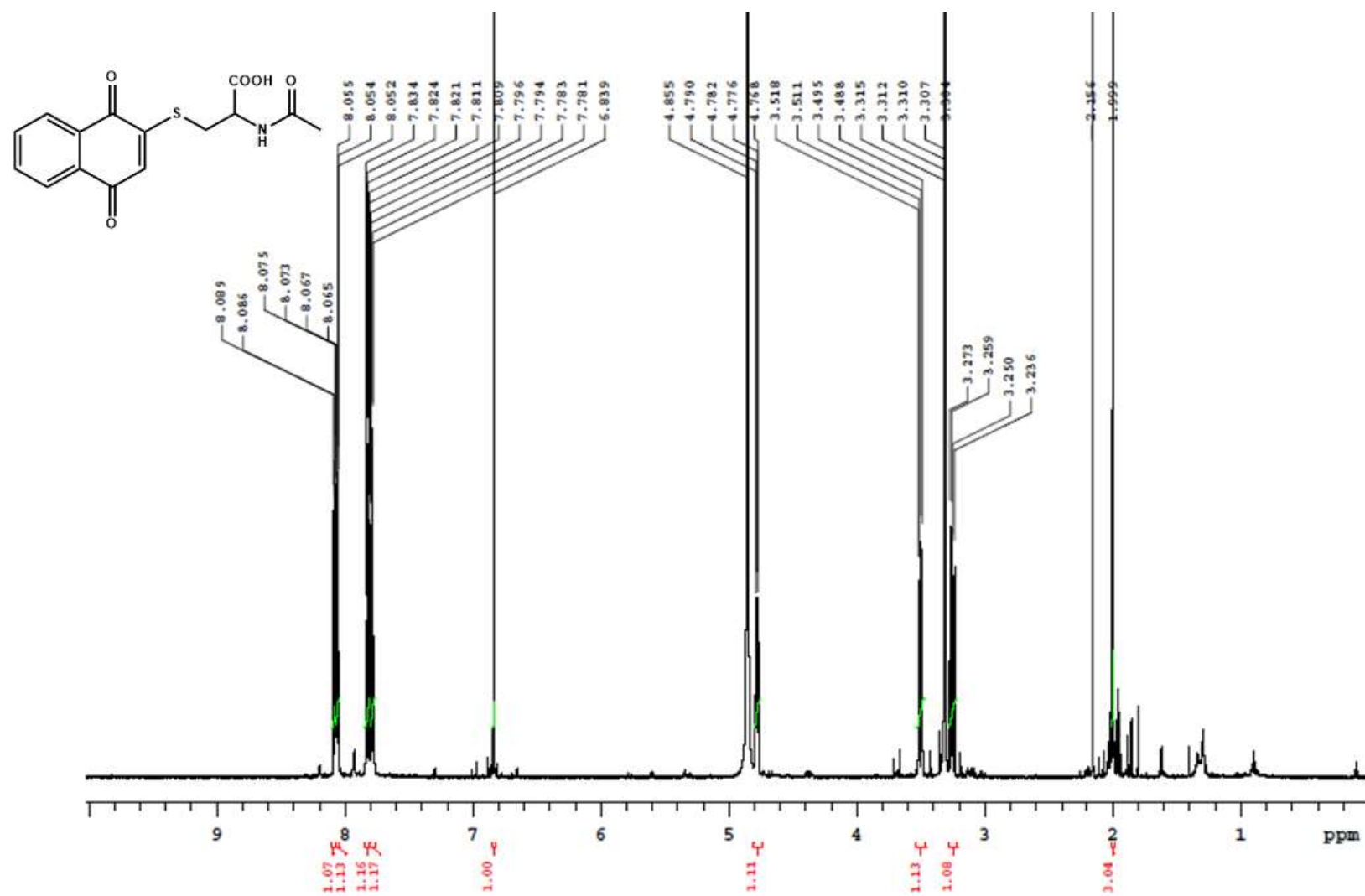


Figure S1. ¹H NMR spectrum in CD₃OD of compound 8.

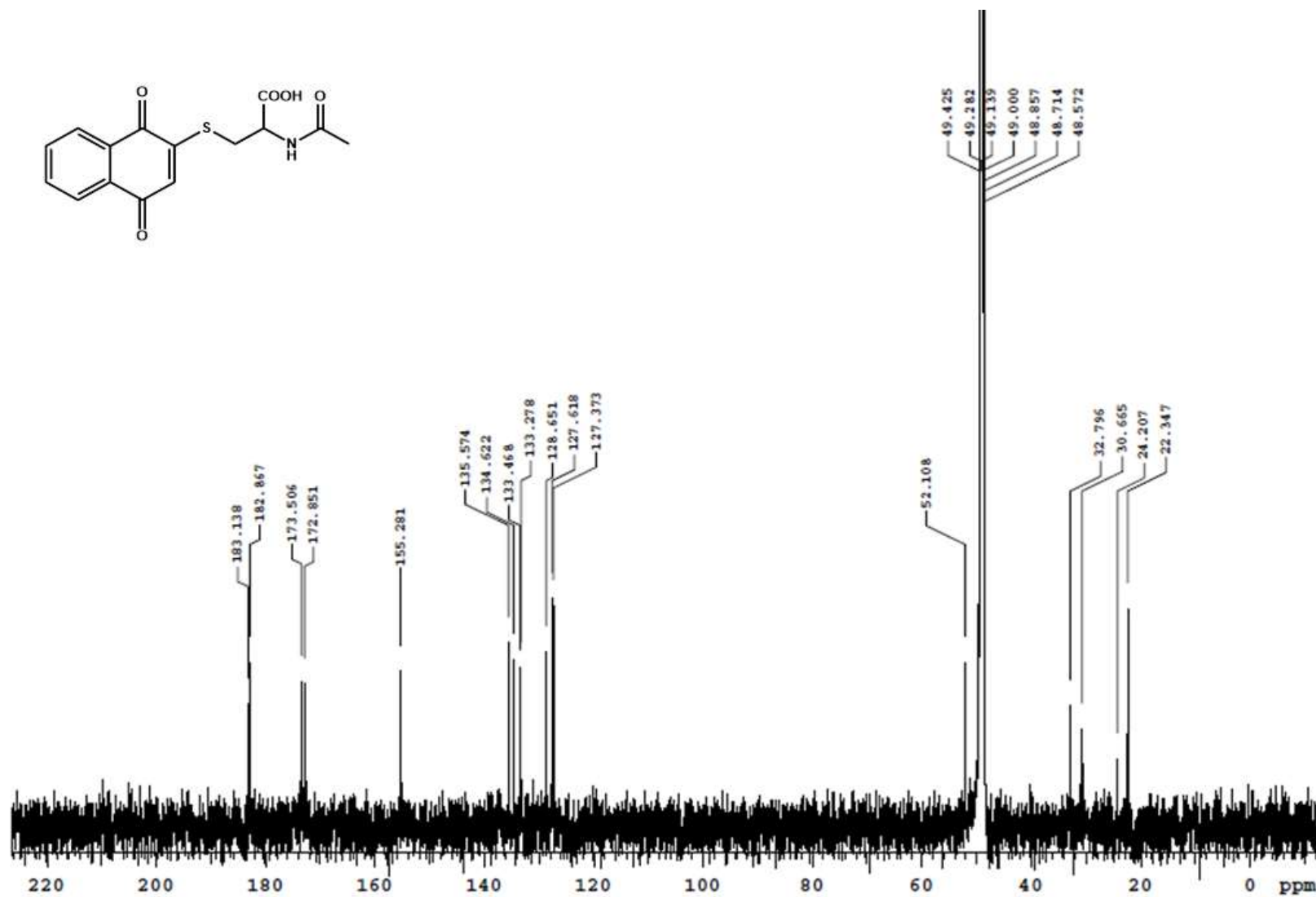


Figure S2. ¹³C NMR spectrum in CD₃OD of compound 8.

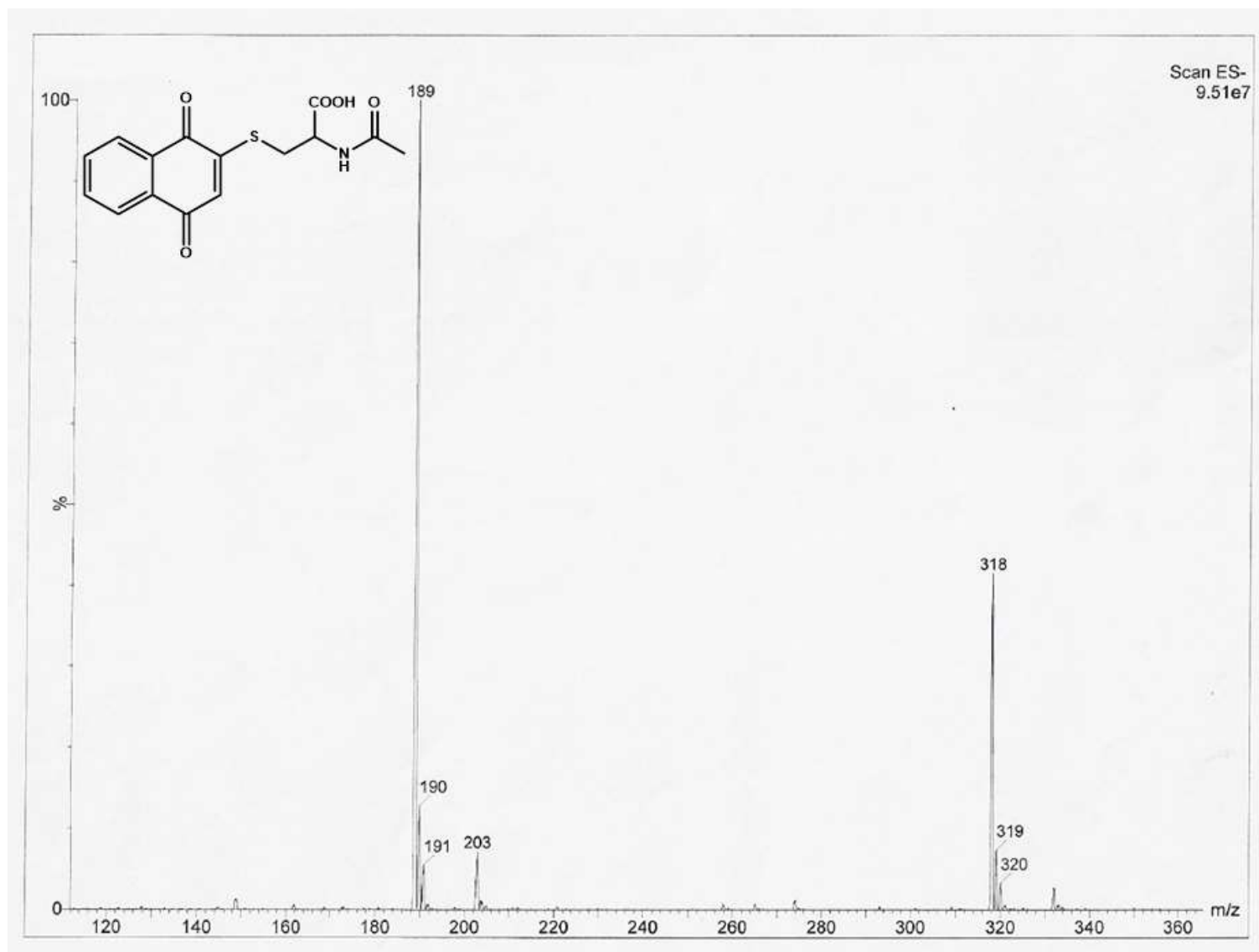


Figure S3. ESI-MS⁻ spectrum of compound 8.

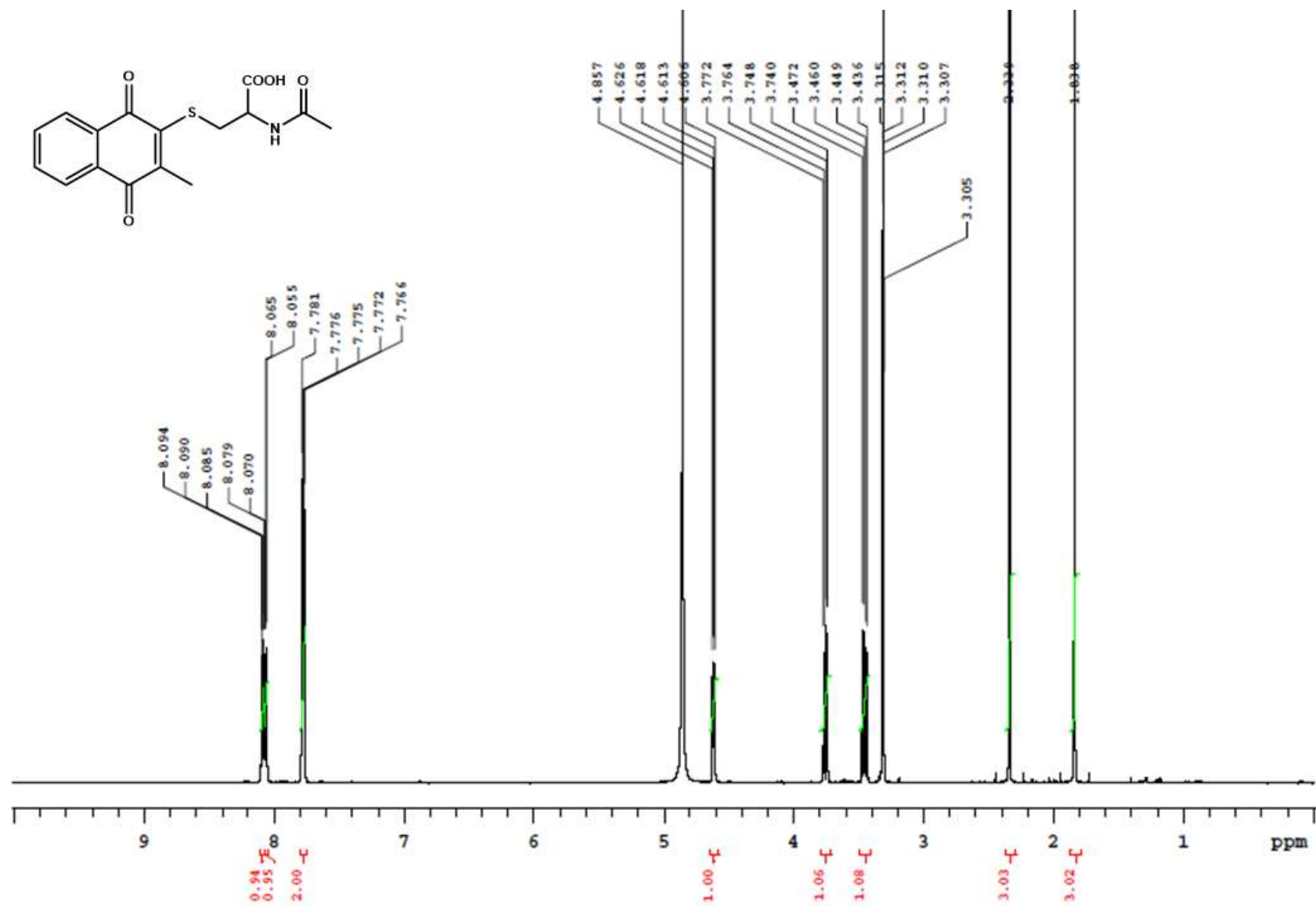


Figure S4. ¹H NMR spectrum in CD₃OD of compound 9.

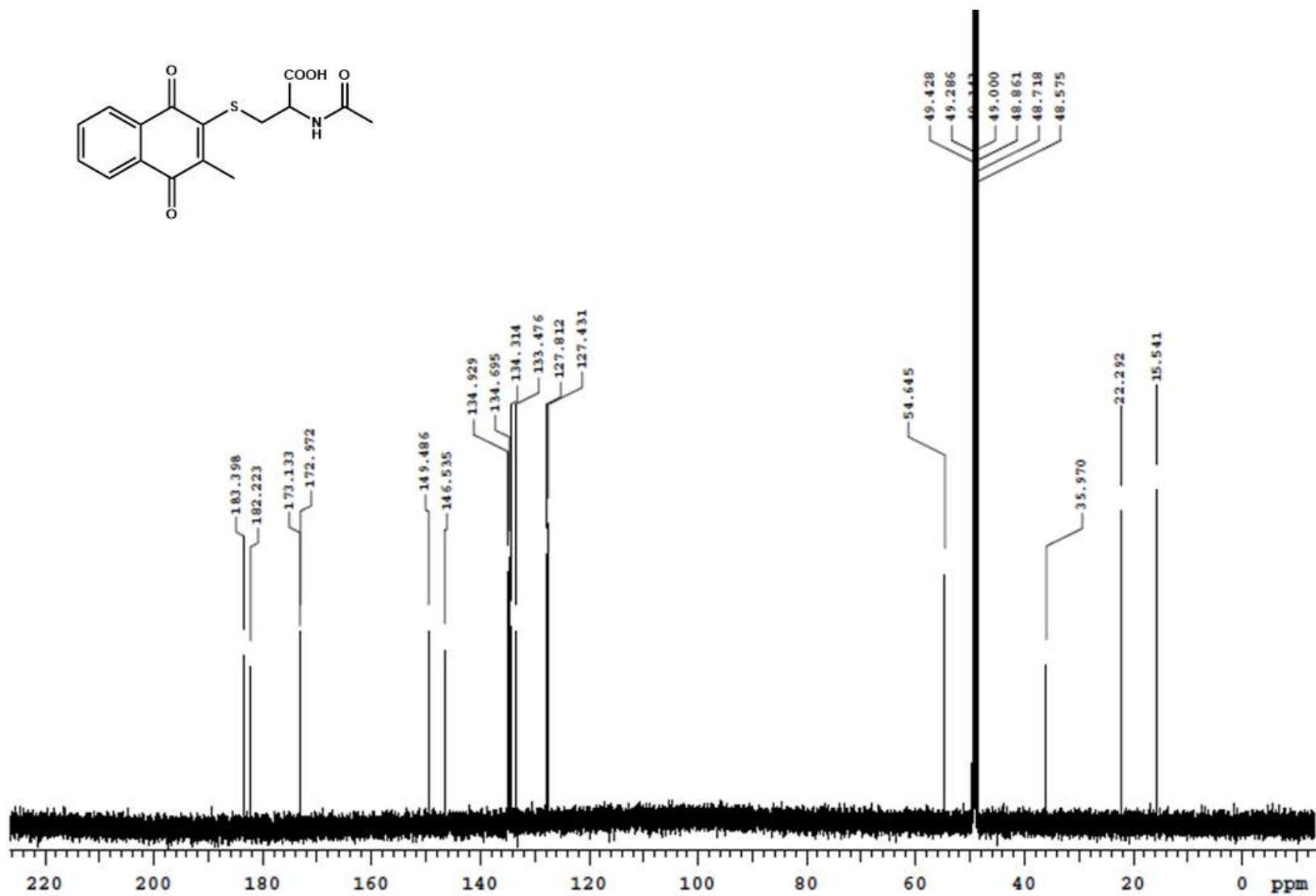


Figure S5. ¹³C NMR spectrum in CD₃OD of compound 9.

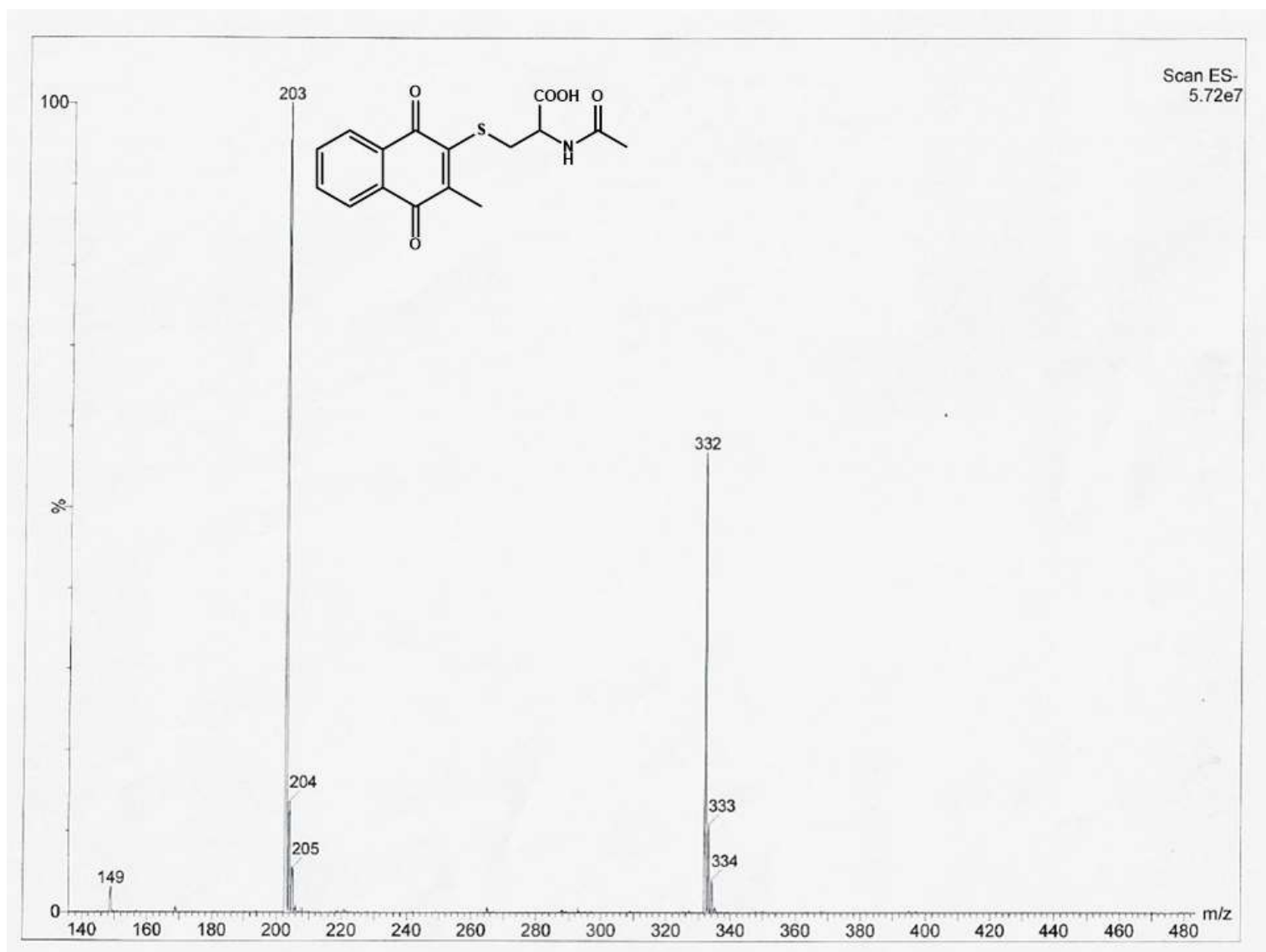


Figure S6. ESI-MS⁻ spectrum of compound 9.

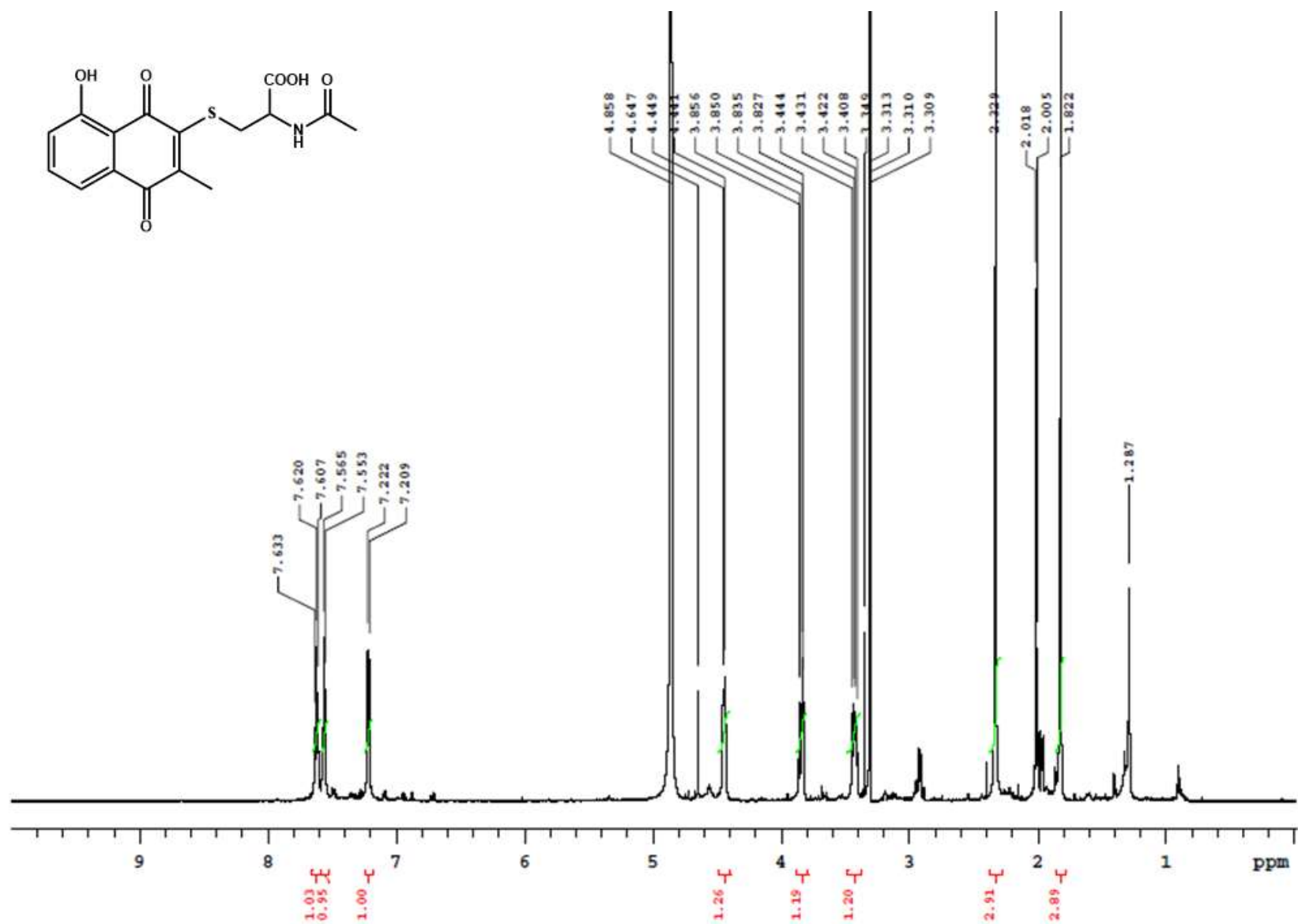


Figure S7. ¹H NMR spectrum in CD₃OD of compound 10.

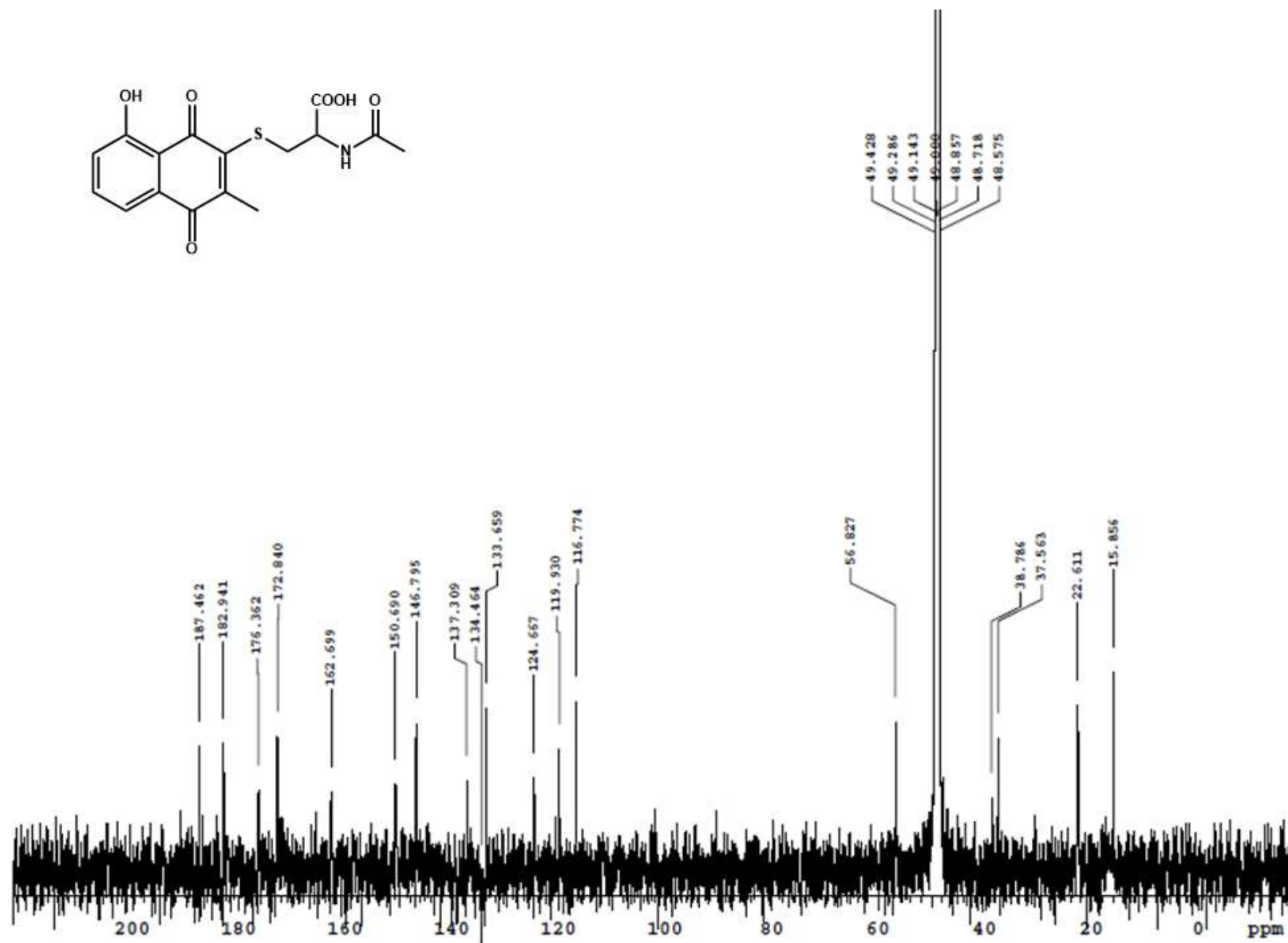


Figure S8. ¹³C NMR spectrum in CD₃OD of compound 10.

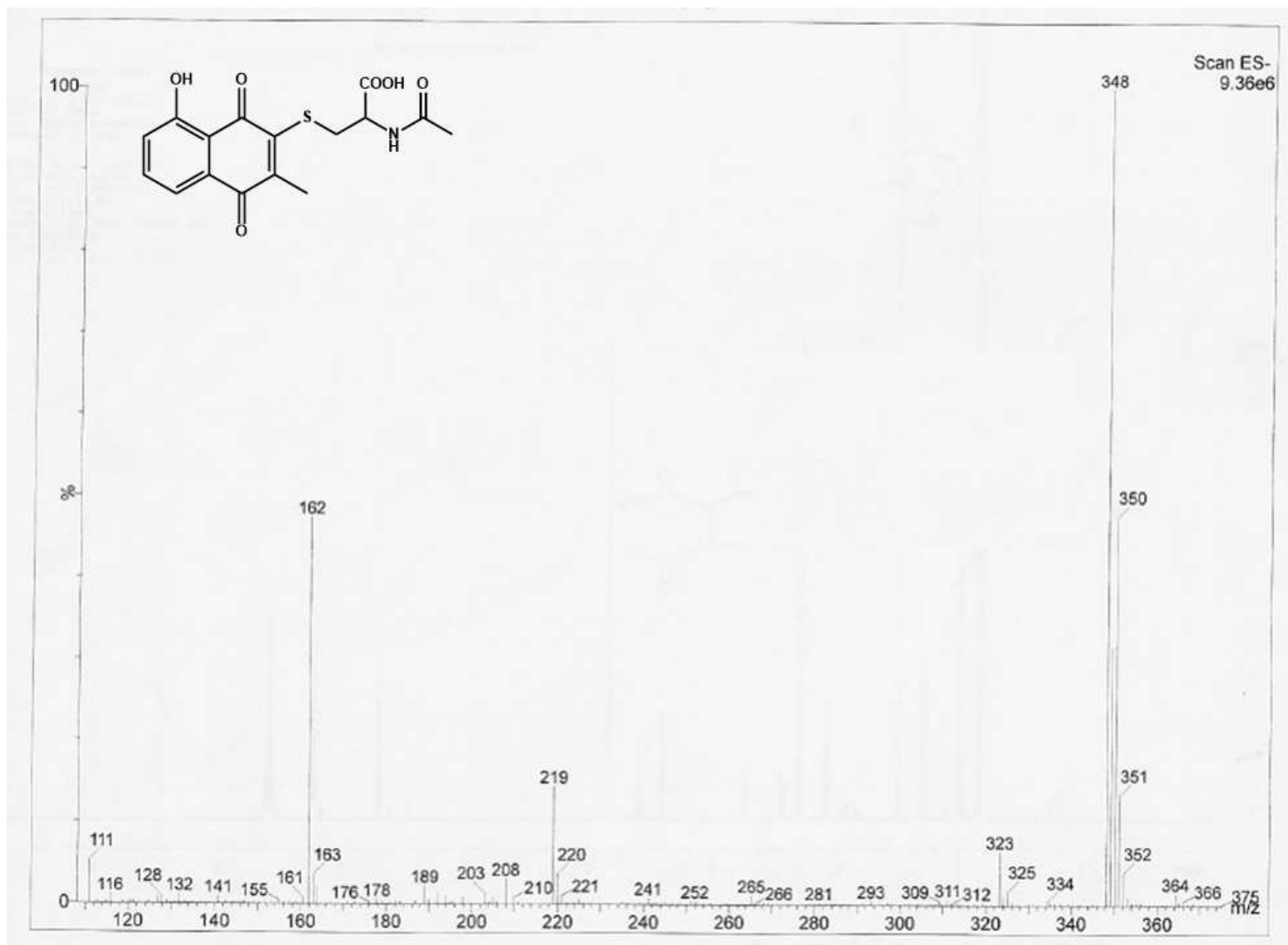


Figure S9. ESI-MS⁻ spectrum of compound 10.

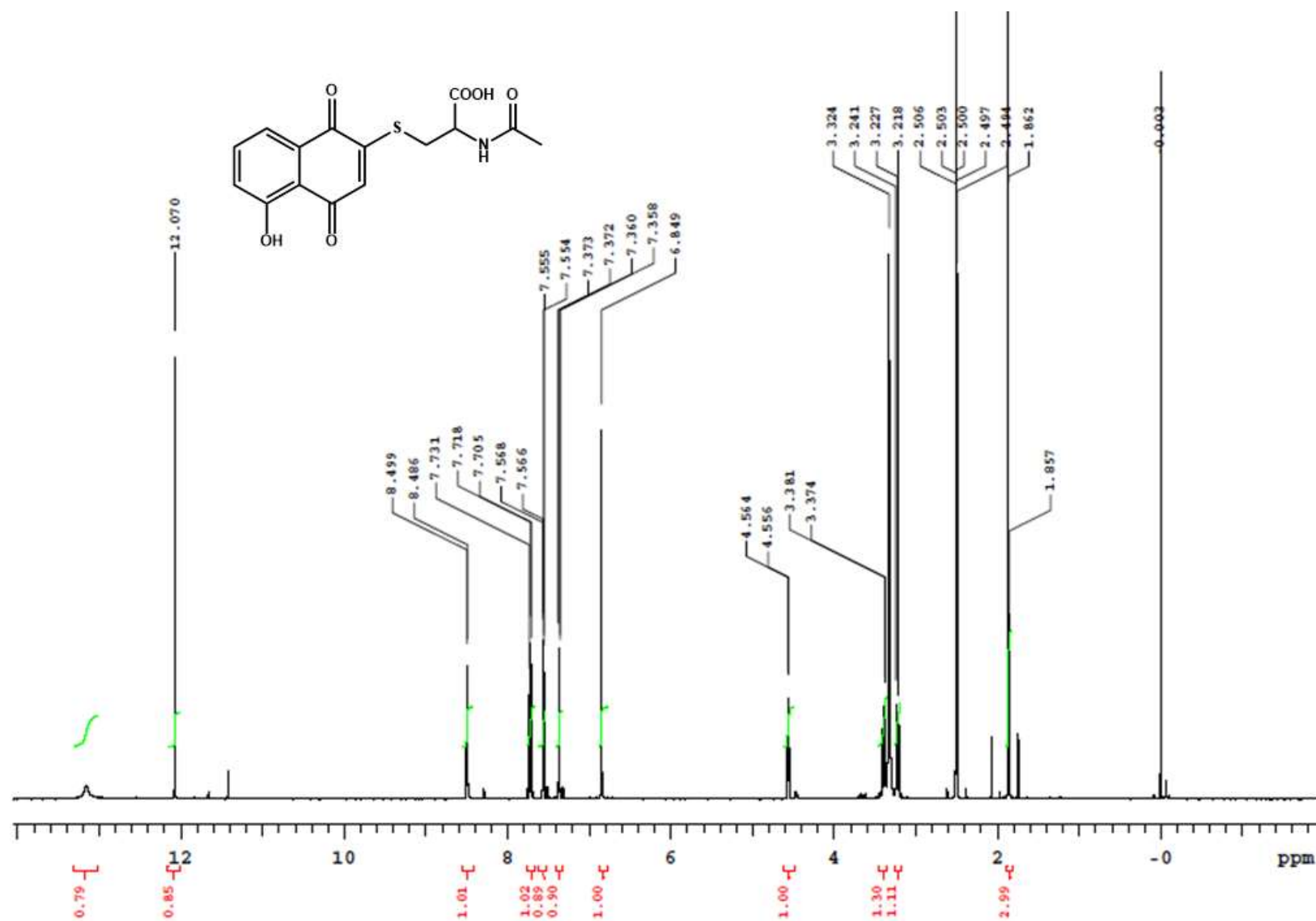


Figure S10. ¹H NMR spectrum in DMSO-d₆ of compound 11.

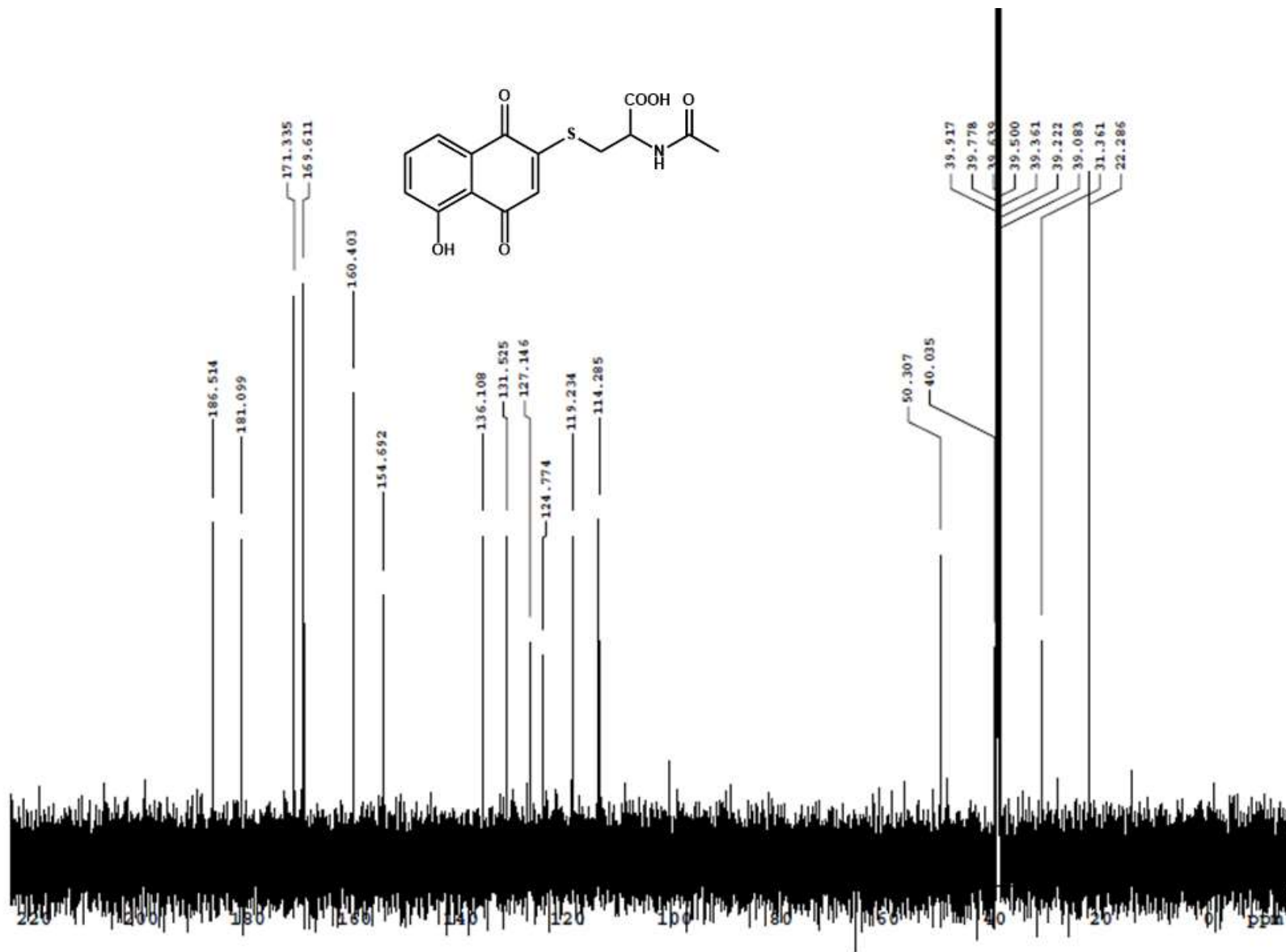


Figure S11 ¹³C NMR spectrum in DMSO-d₆ of compound 11.

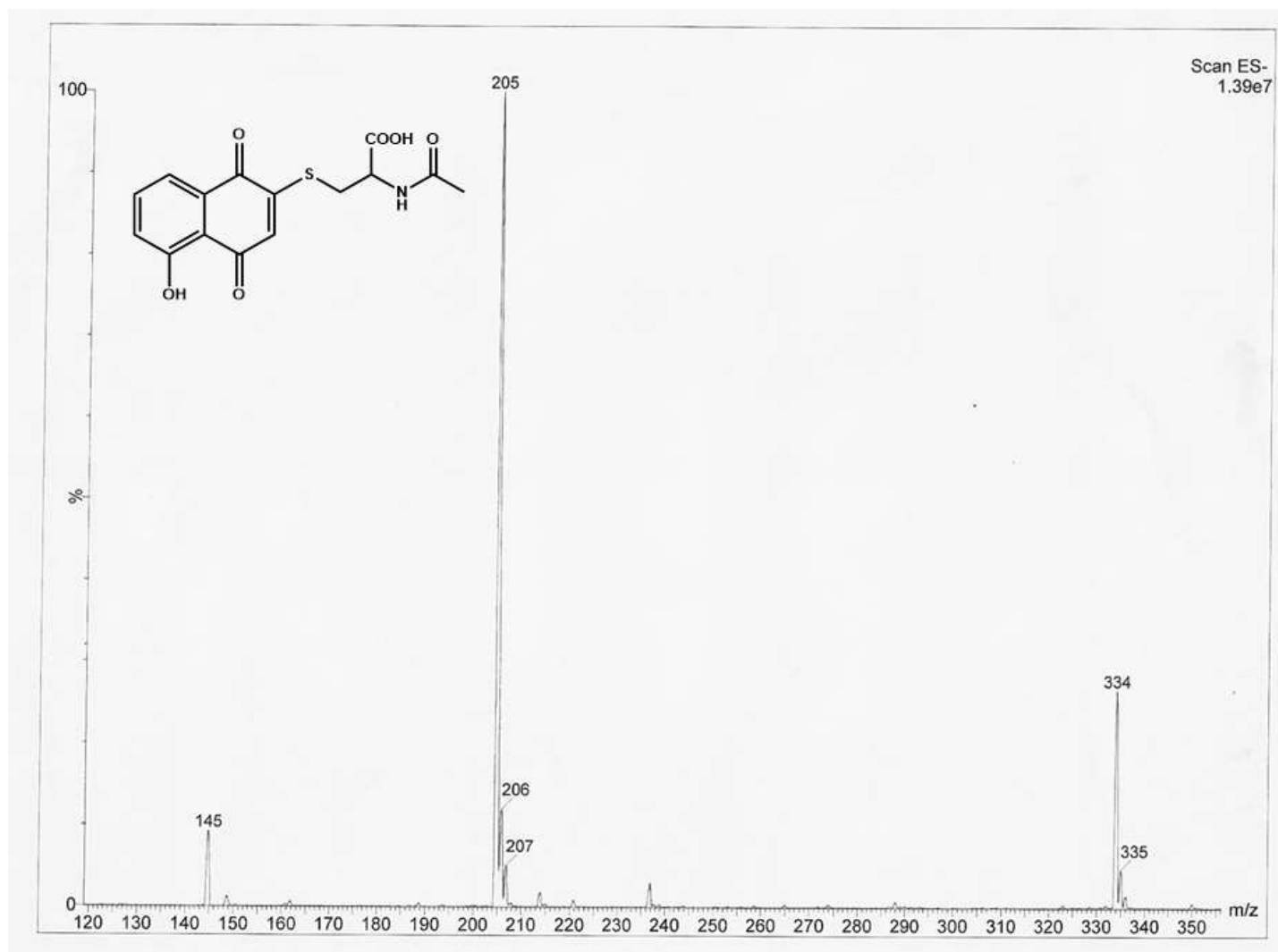


Figure S12. ESI-MS⁻ spectrum of compound 11.

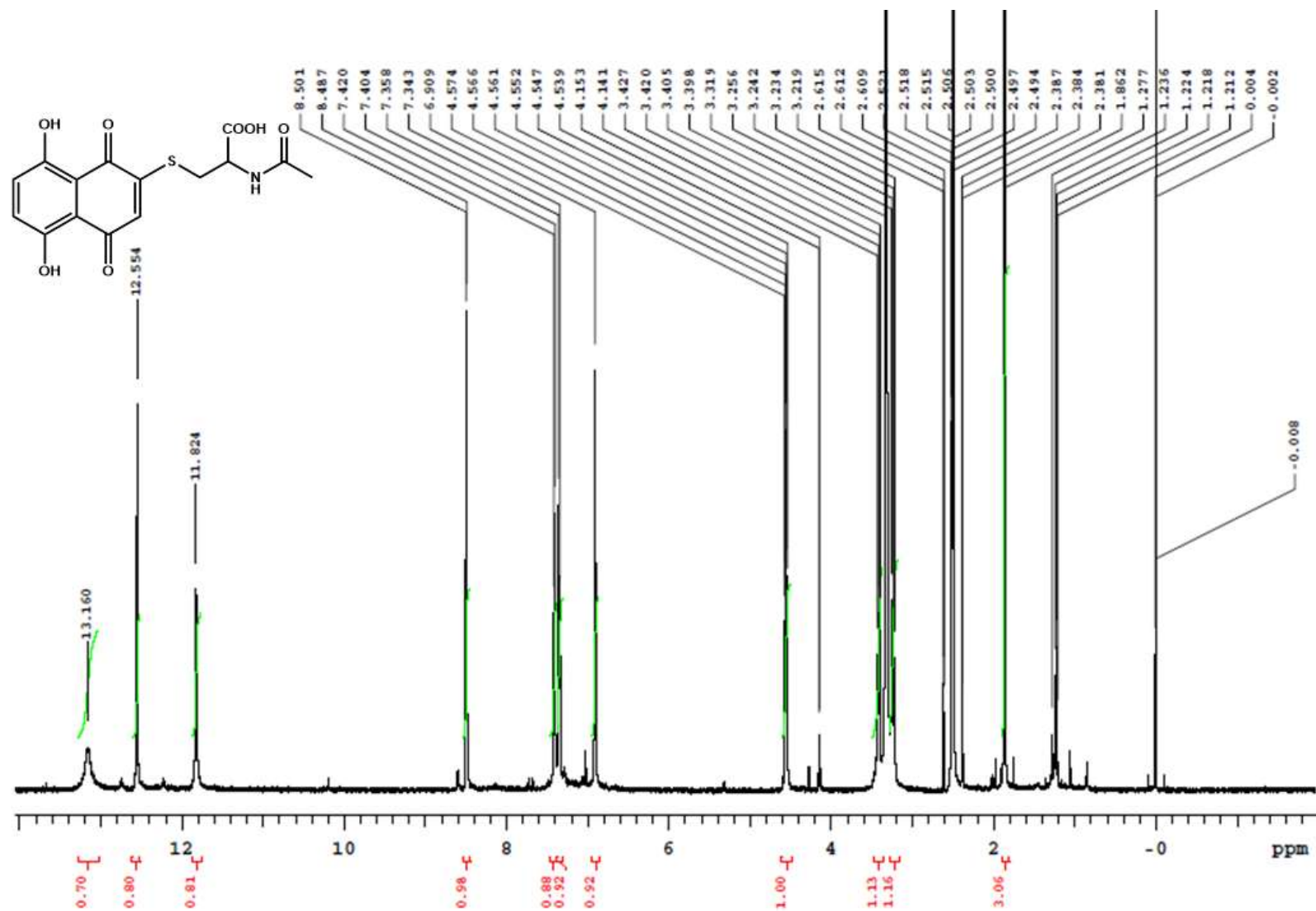


Figure S13. ¹H NMR spectrum in DMSO-d₆ of compound 12.

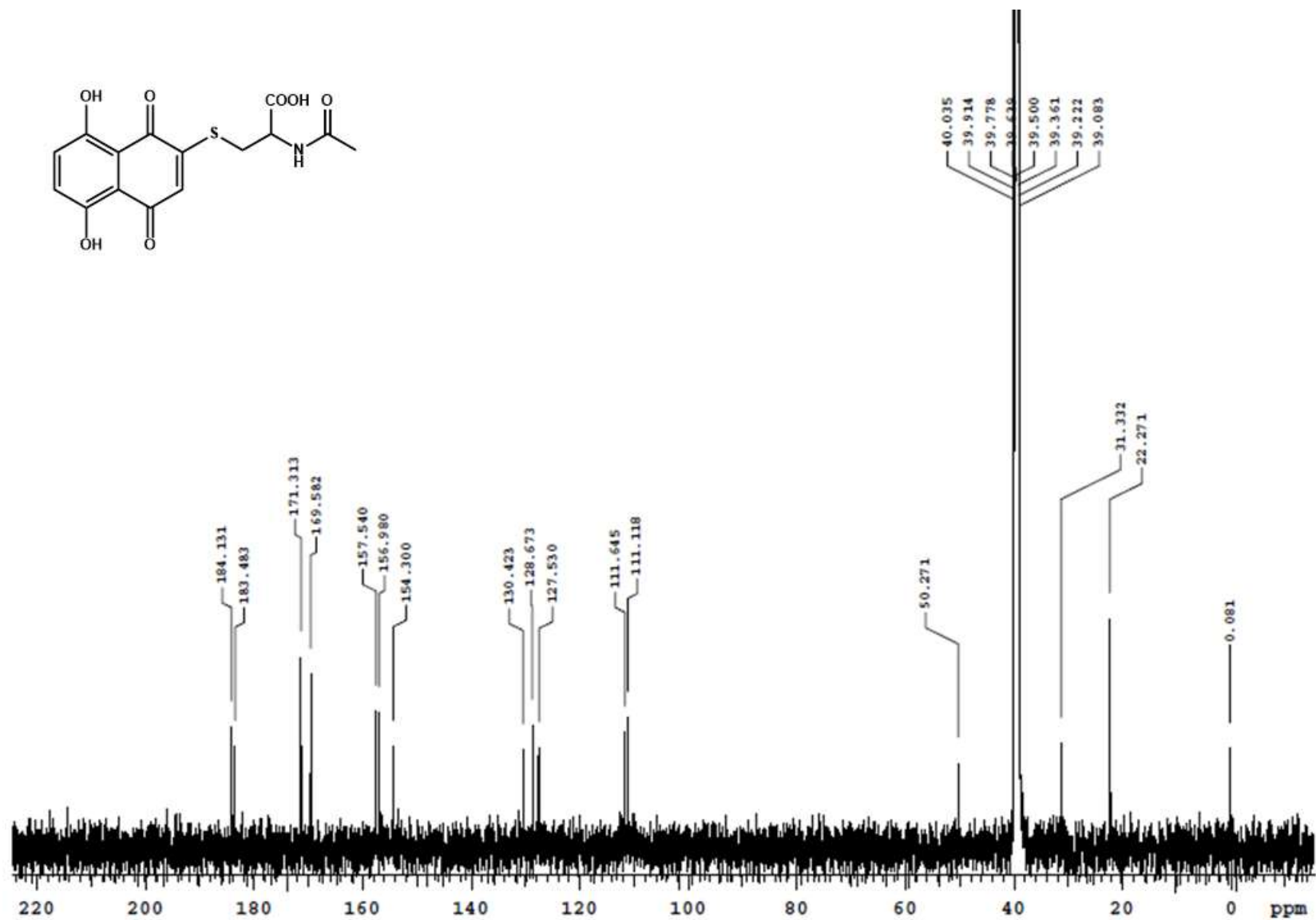


Figure S14. ¹³C NMR spectrum in DMSO-d₆ of compound 12.

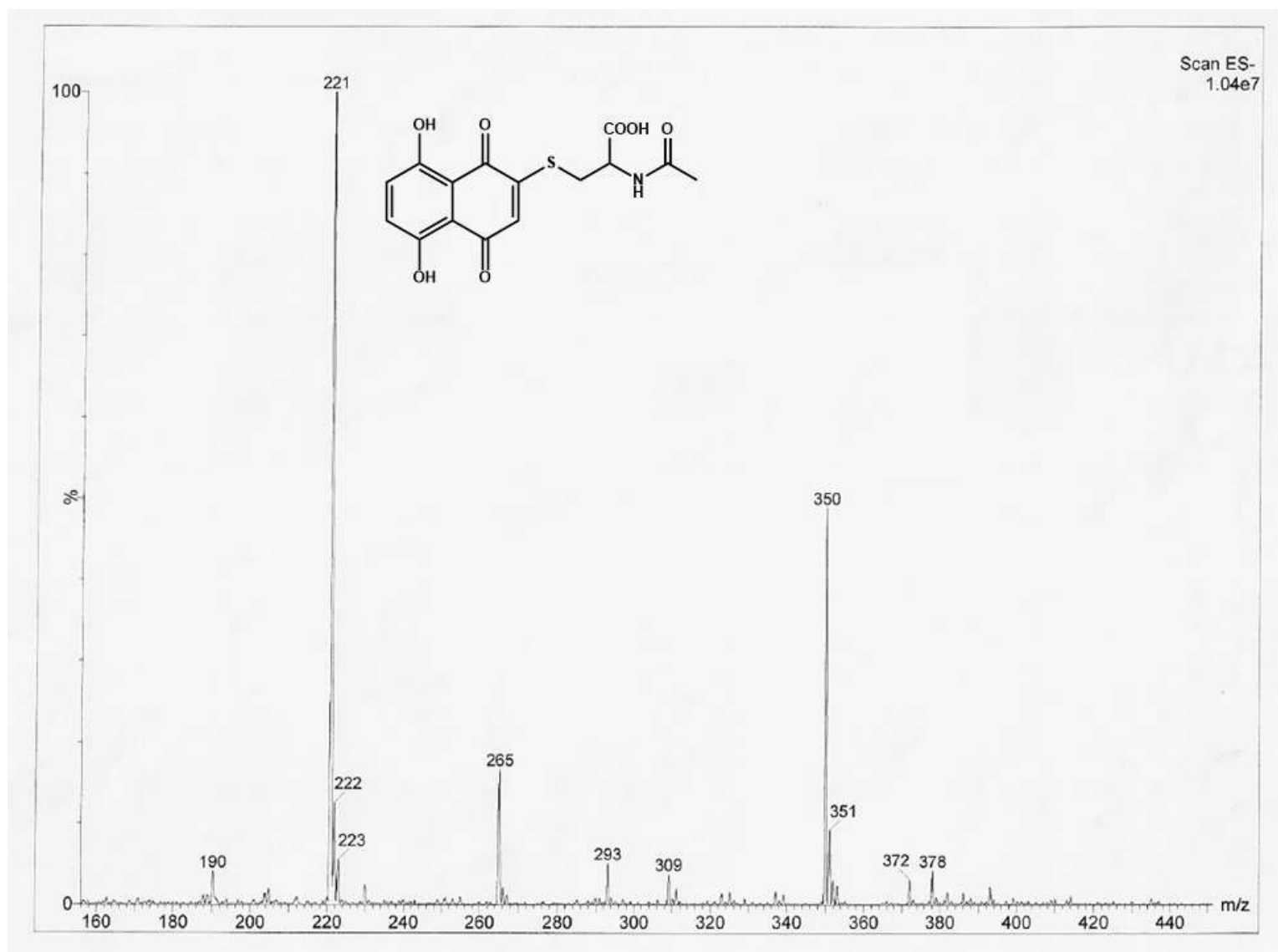


Figure S15. ESI-MS⁻ spectrum of compound 12.

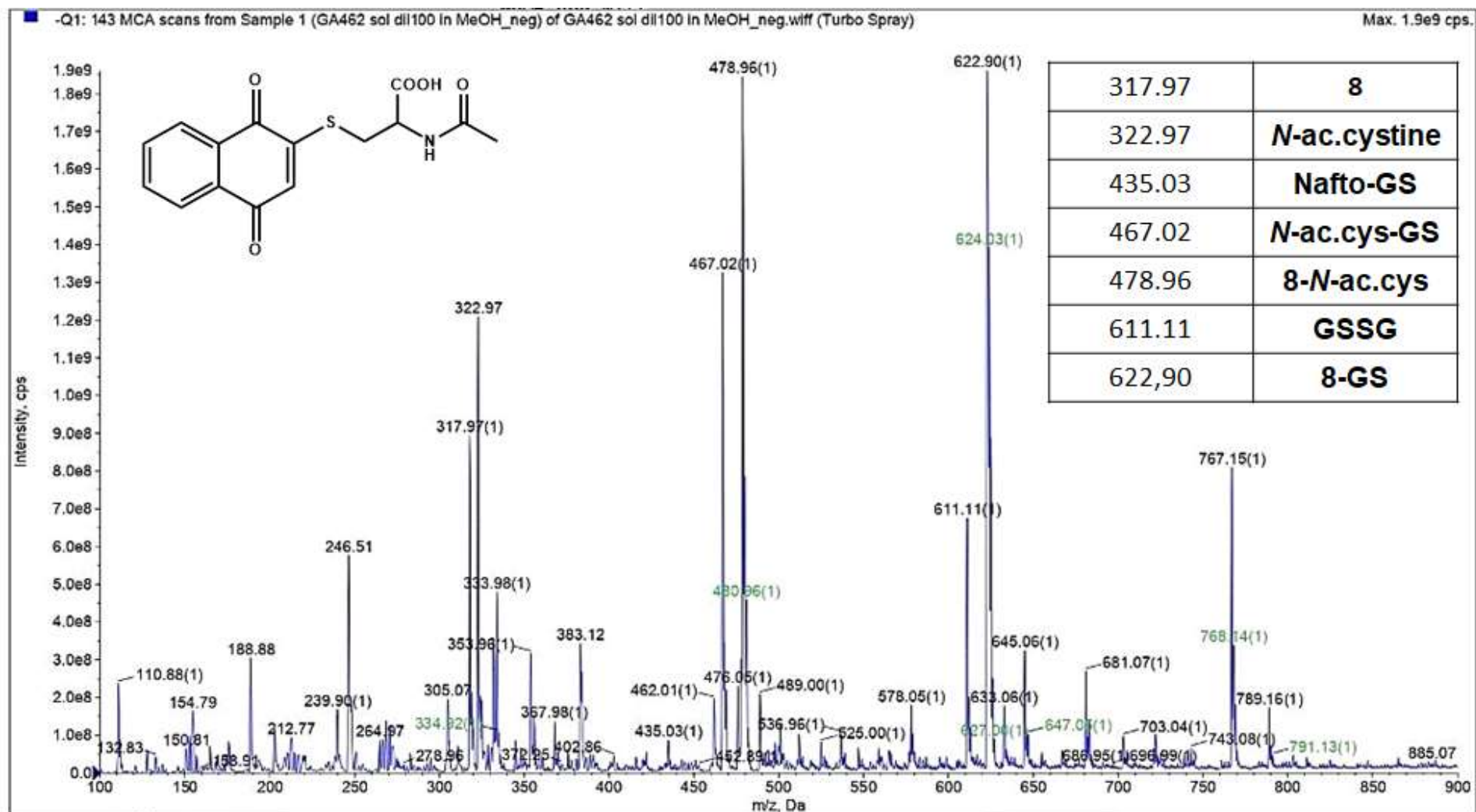


Figure S16. Direct infusion mass spectra of the reaction mixtures with GSH of compound **8**. All the detected ions are in the deprotonated form $[M-H]^-$. Abbreviations: 8-GS is the adduct of **8** with glutathione, 8-*N*-ac.cys is the adduct of **8** with *N*-acetyl-*L*-cysteine, Nafto-GS is the adduct of naphthoquinone (**1**) and glutathione, GSSG: glutathione dimer; *N*-ac.cystine is the *N*-acetyl-*L*-cysteine dimer; *N*-ac.cys-GS is the *N*-acetyl-*L*-cysteine – glutathione heterodimer.

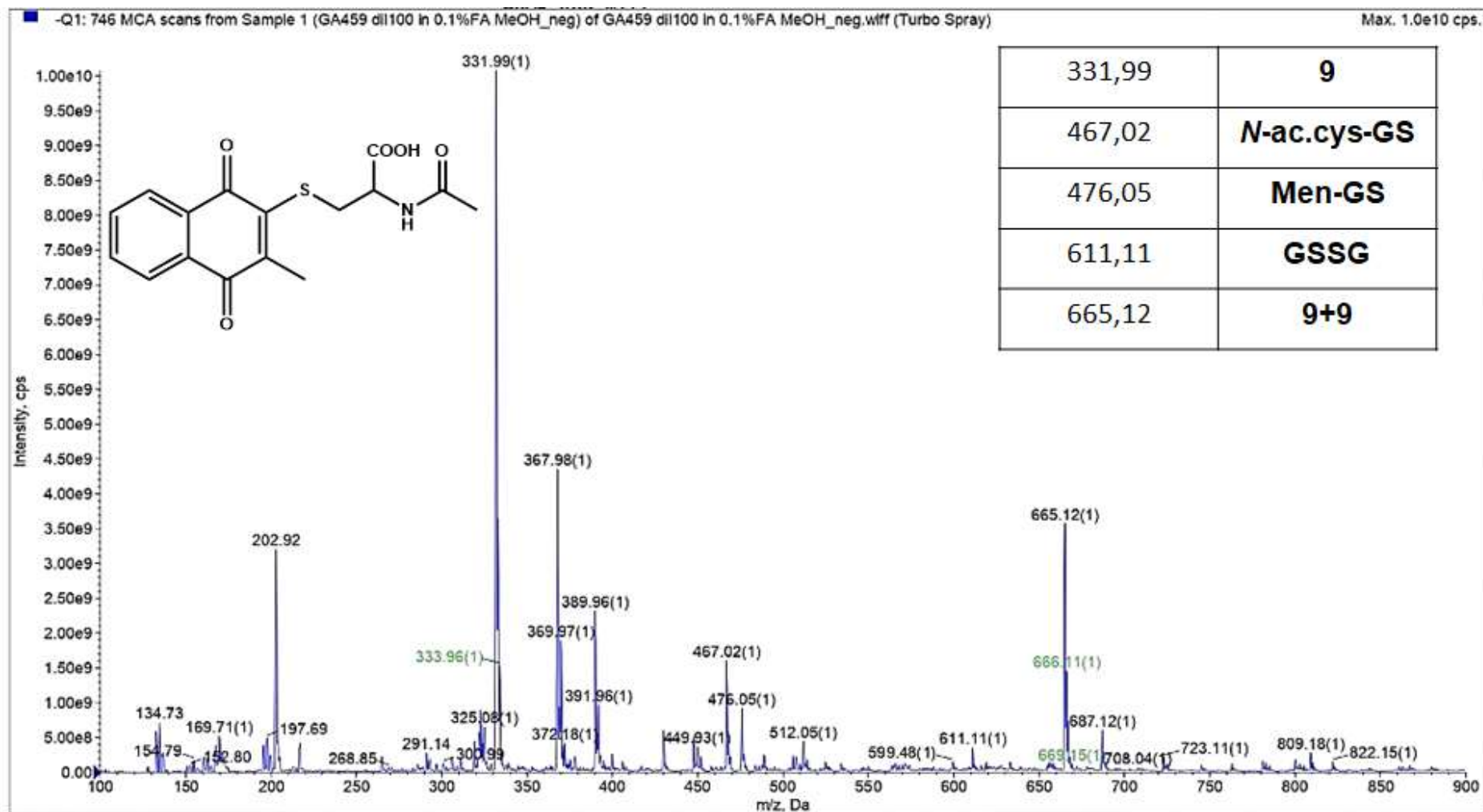


Figure S17. Direct infusion mass spectra of the reaction mixtures with GSH of compound **9**. All the detected ions are in the deprotonated form [M-H]⁻. Abbreviations: Men-GS is the adduct of Menadione (**2**) and glutathione, GSSG: glutathione dimer, *N*-ac.cys-GS is the *N*-acetyl-*L*-cysteine – glutathione heterodimer. 9+9 is the cluster of compound **9**.

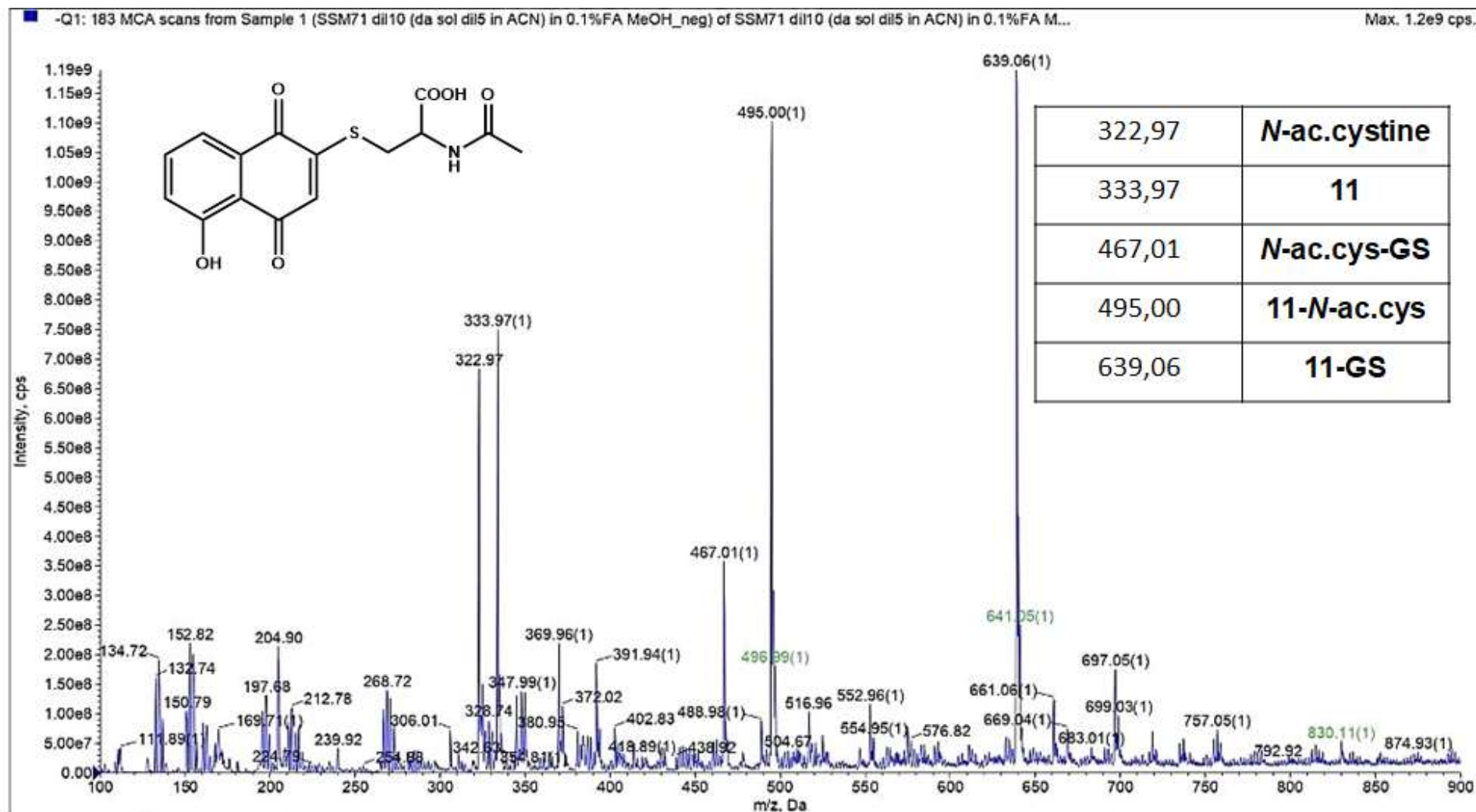


Figure S18. Direct infusion mass spectra of the reaction mixtures with GSH of compound **11**. All the detected ions are in the deprotonated form $[M-H]^-$. Abbreviations: 11-GS is the adduct of **11** with glutathione, 11-N-ac.cys is the adduct of **11** with *N*-acetyl-*L*-cysteine, *N*-ac.cystine is the *N*-acetyl-*L*-cysteine dimer; *N*-ac.cys-GS is the *N*-acetyl-*L*-cysteine – glutathione heterodimer.