Design, Synthesis and Evaluation of Novel Dehydroabietic Acid-Dithiocarbamate Hybrids as Potential Multi-Targeted Compounds for Tumor Cytotoxicity

Supplementary Materials

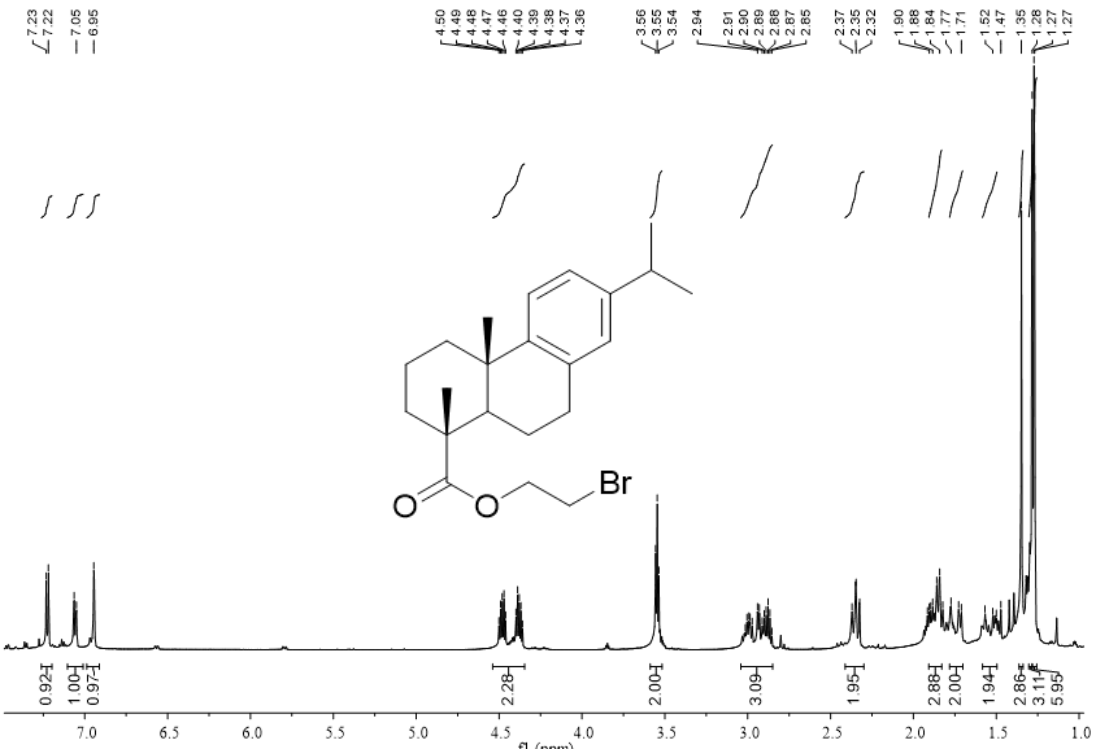

Figure S1. ^{1}H NMR spectrum of the target compound II.

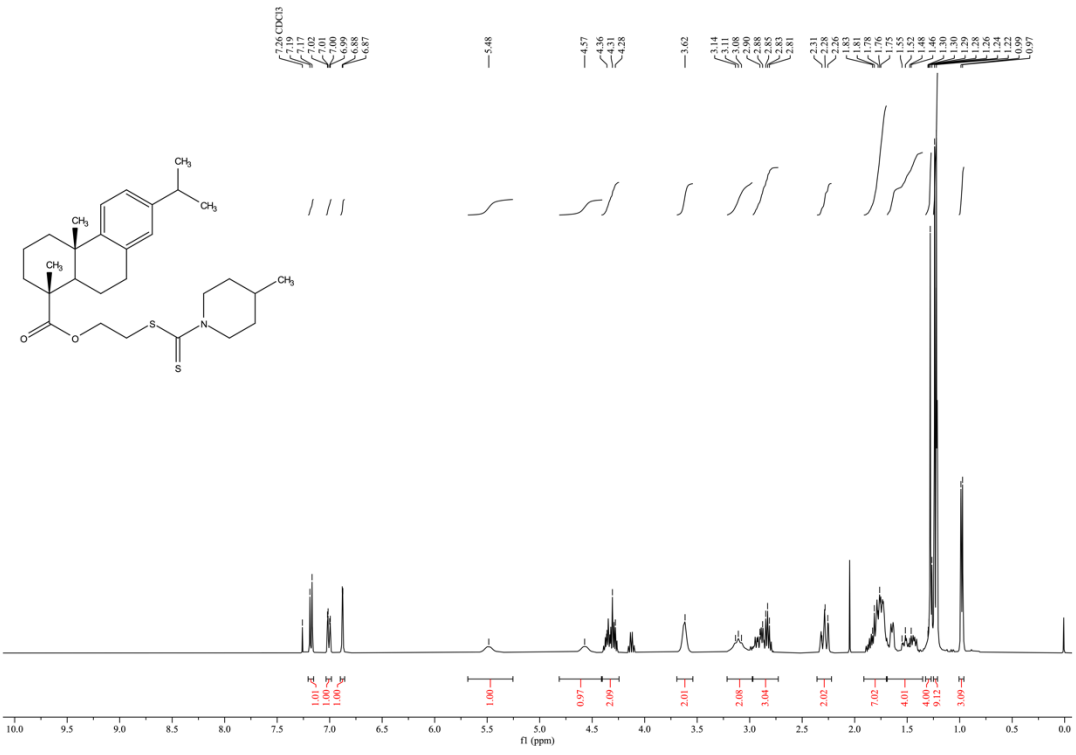

Figure S2. ^{1}H NMR spectrum of the target compound III-a.

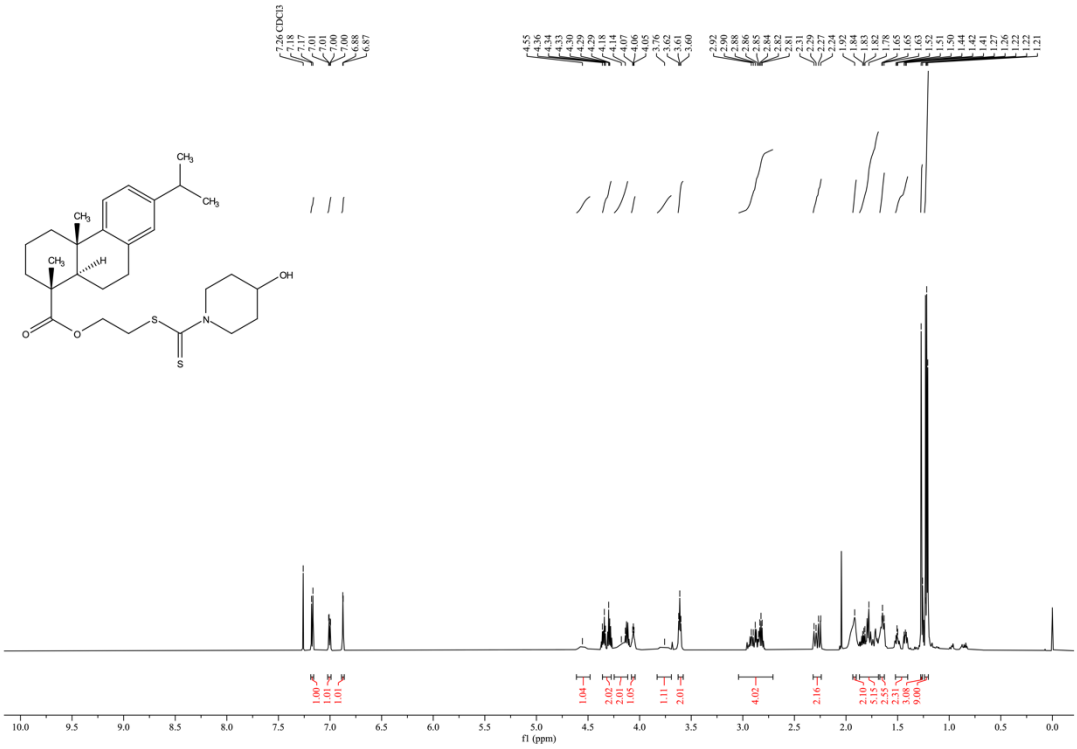

Figure S3. ^{1}H NMR spectrum of the target compound III-b.

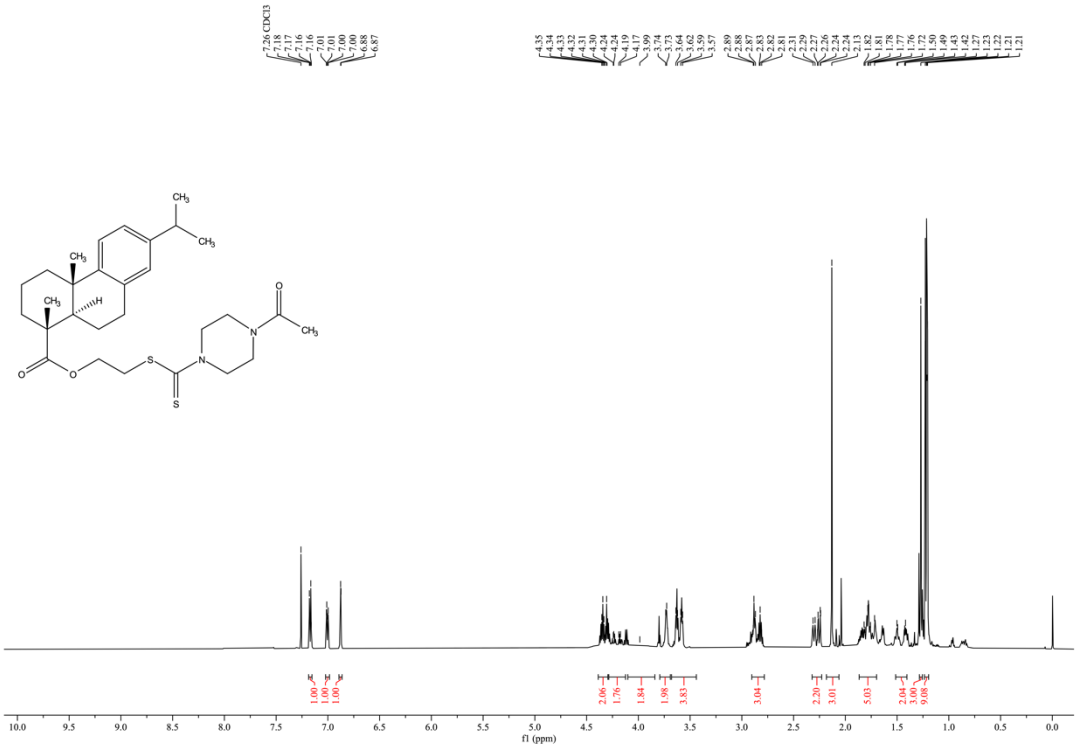

Figure S4. ^{1}H NMR spectrum of the target compound III-c.

Figure S5. ^{1}H NMR spectrum of the target compound III-d.

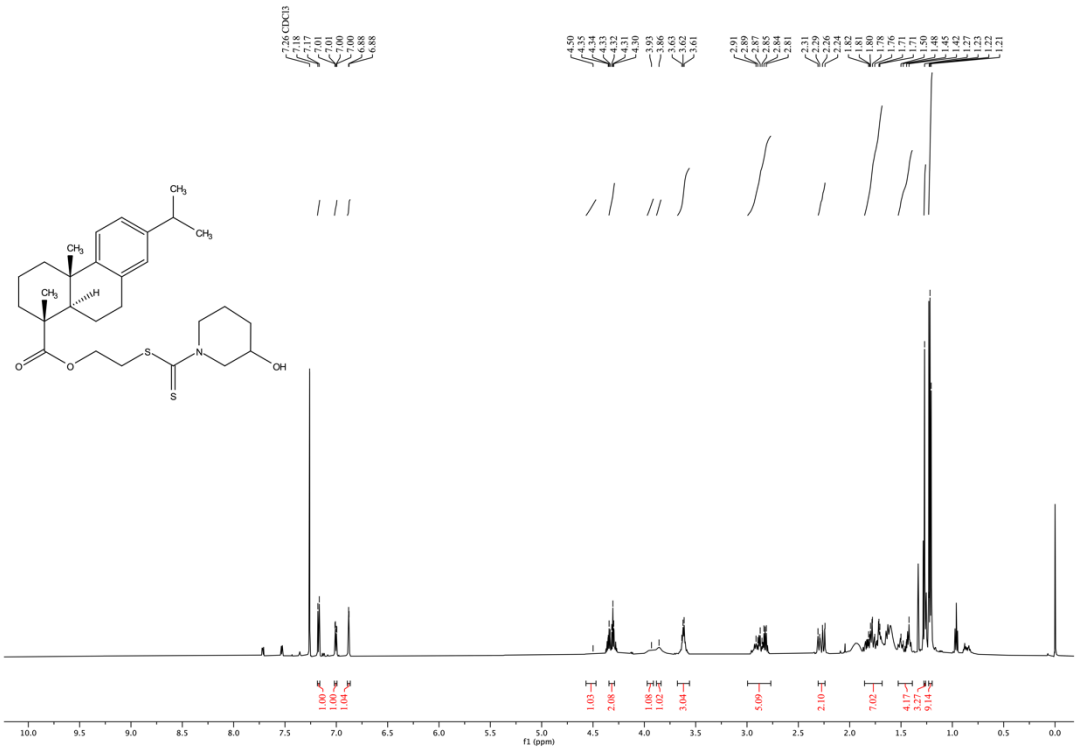

Figure S6. ^{1}H NMR spectrum of the target compound III-e.

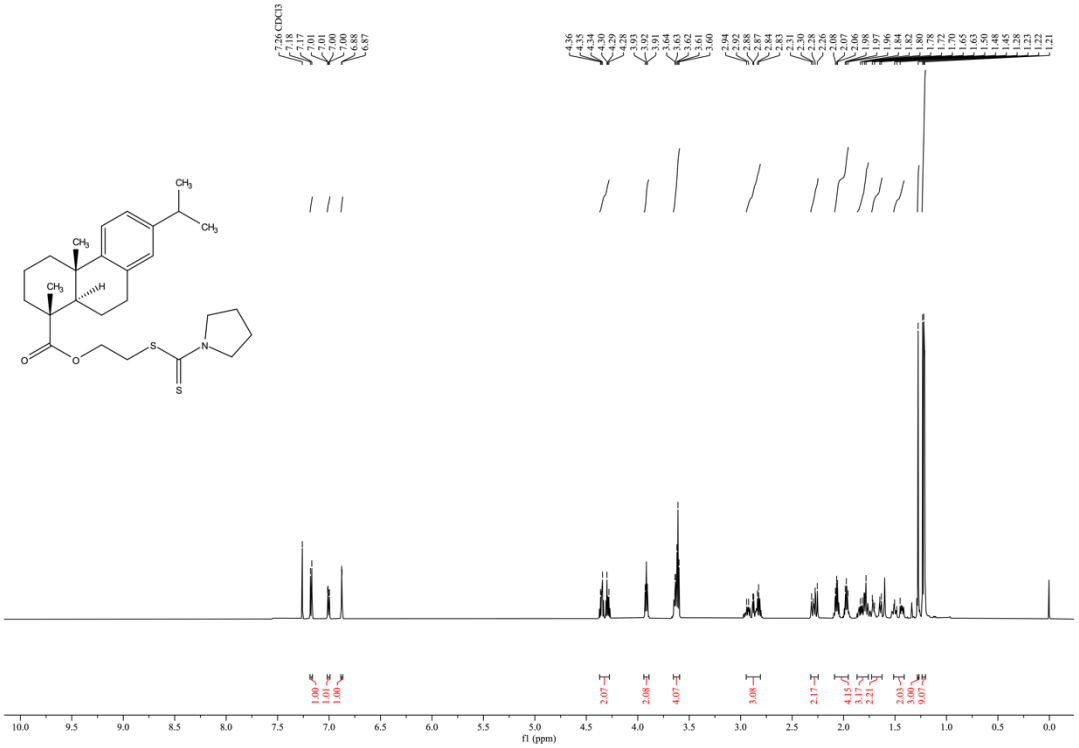

Figure S7. ^{1}H NMR spectrum of the target compound III-f.

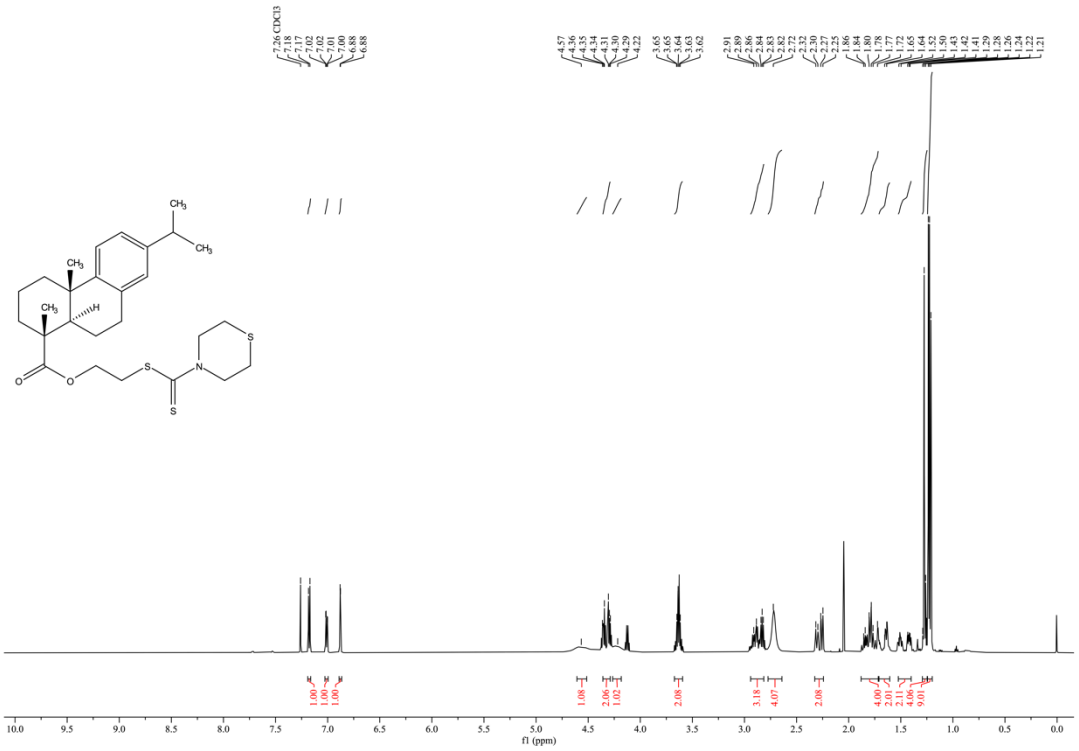

Figure S8. ^{1}H NMR spectrum of the target compound III-g.

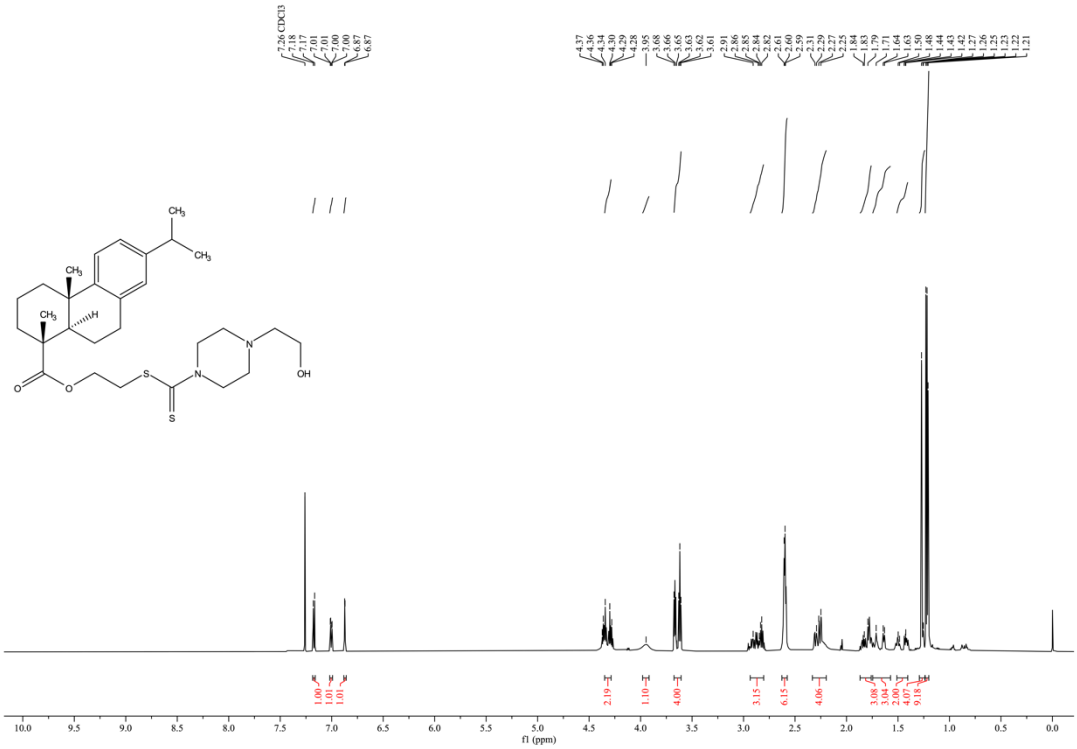

Figure S9. ^{1}H NMR spectrum of the target compound III-h.

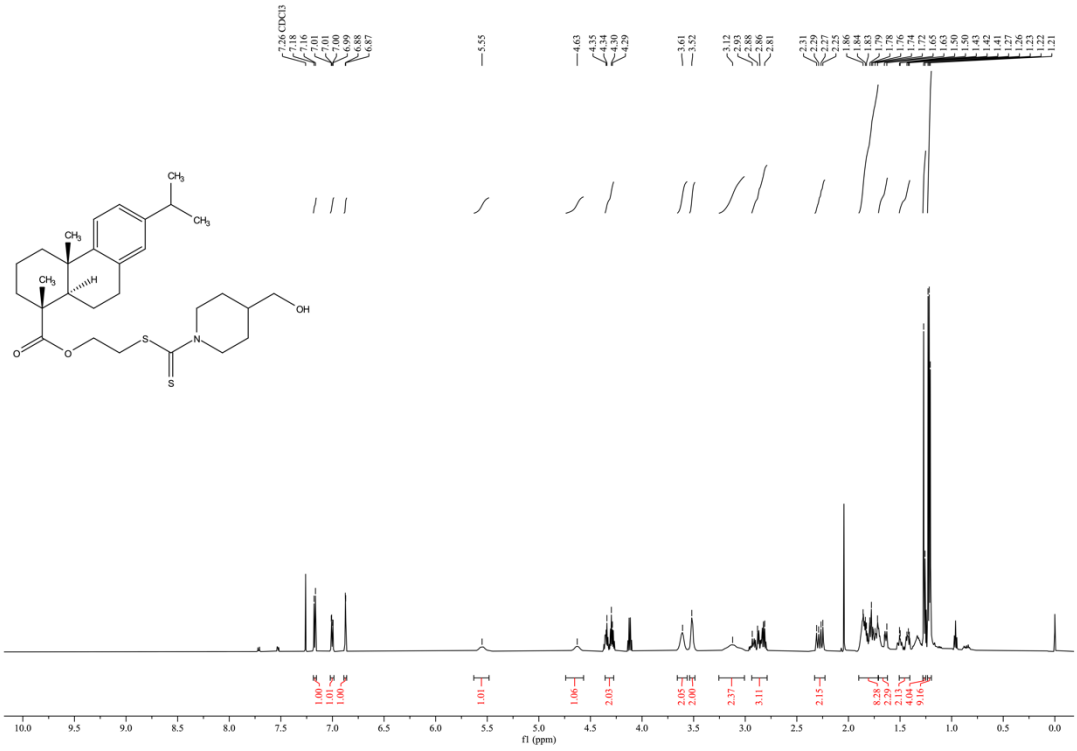

Figure S10. ^{1}H NMR spectrum of the target compound III-i.

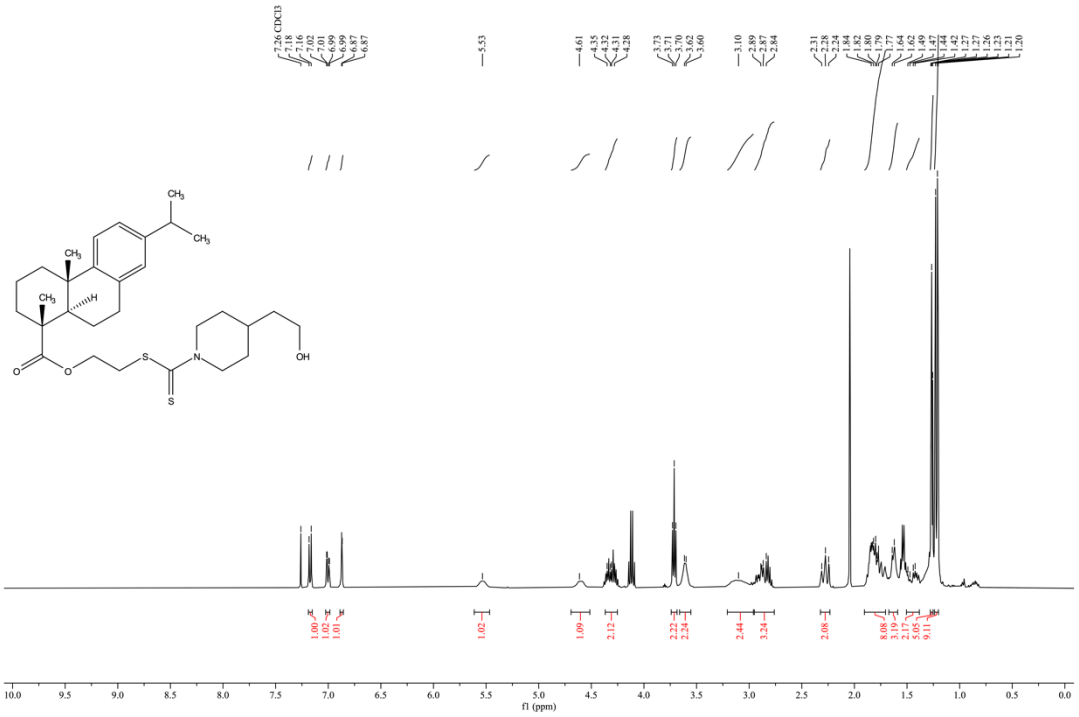

Figure S11. ^{1}H NMR spectrum of the target compound III-j.

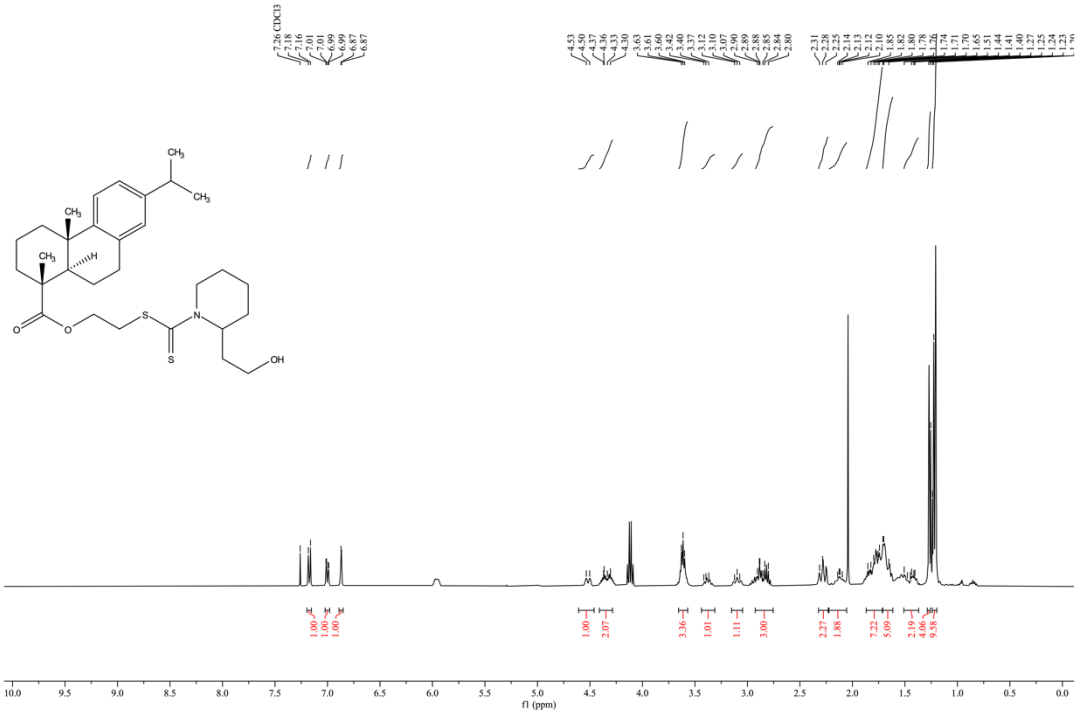

Figure S12. ^{1}H NMR spectrum of the target compound III-k.

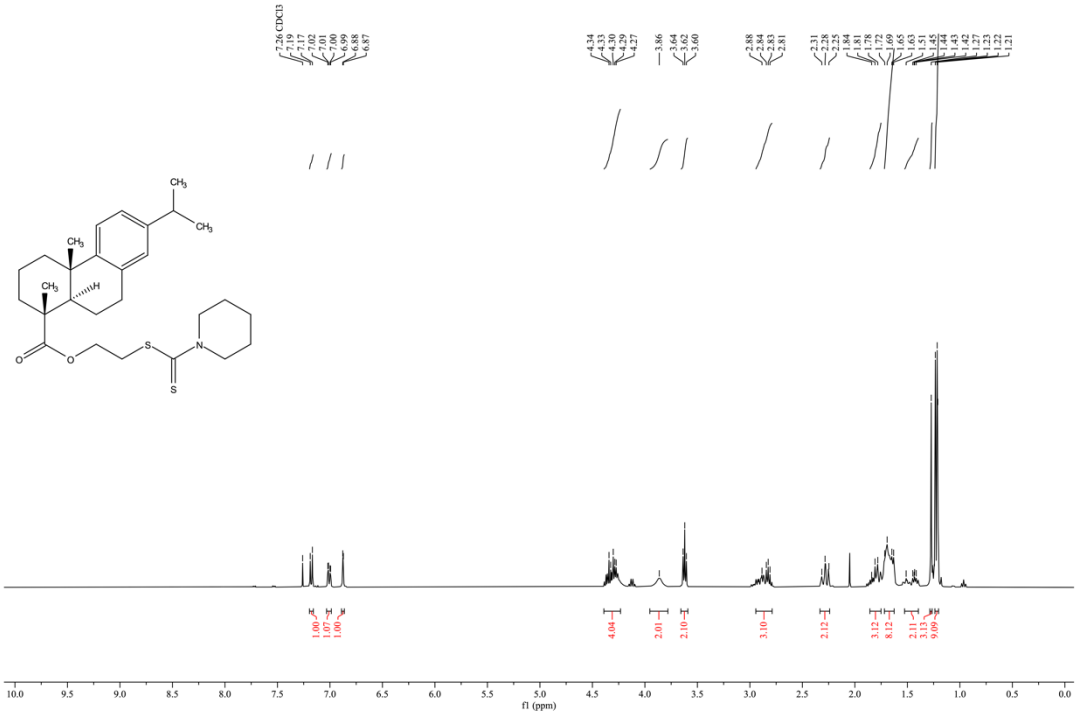

Figure S13. ^{1}H NMR spectrum of the target compound III-l.

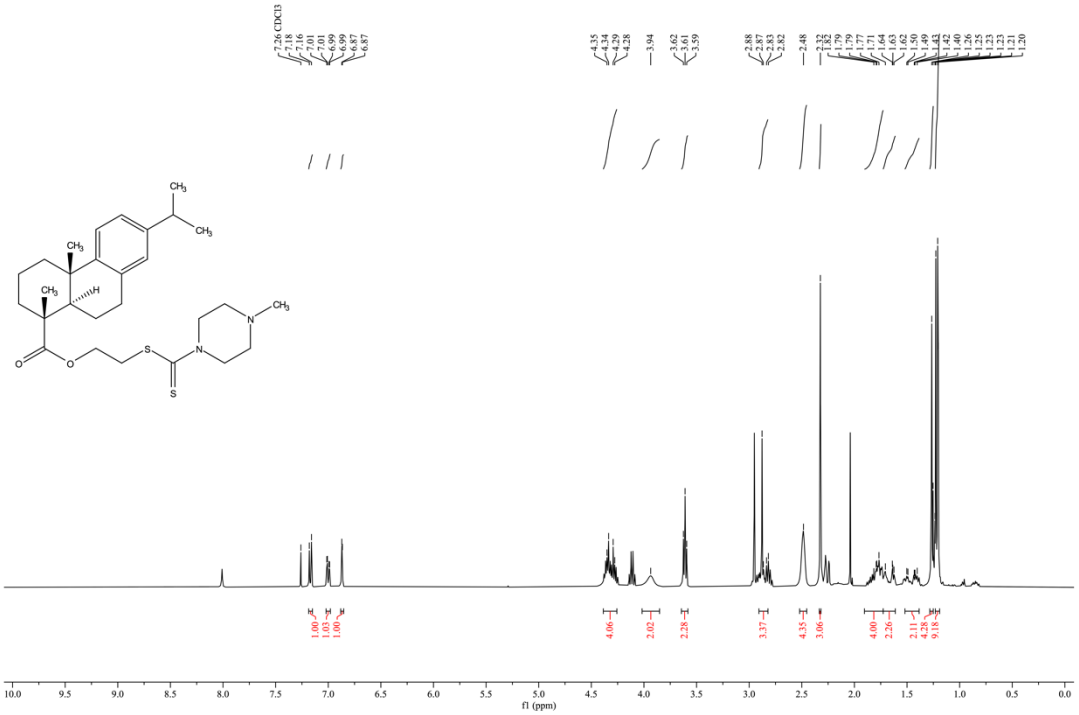

Figure S14. ^{1}H NMR spectrum of the target compound III-m.

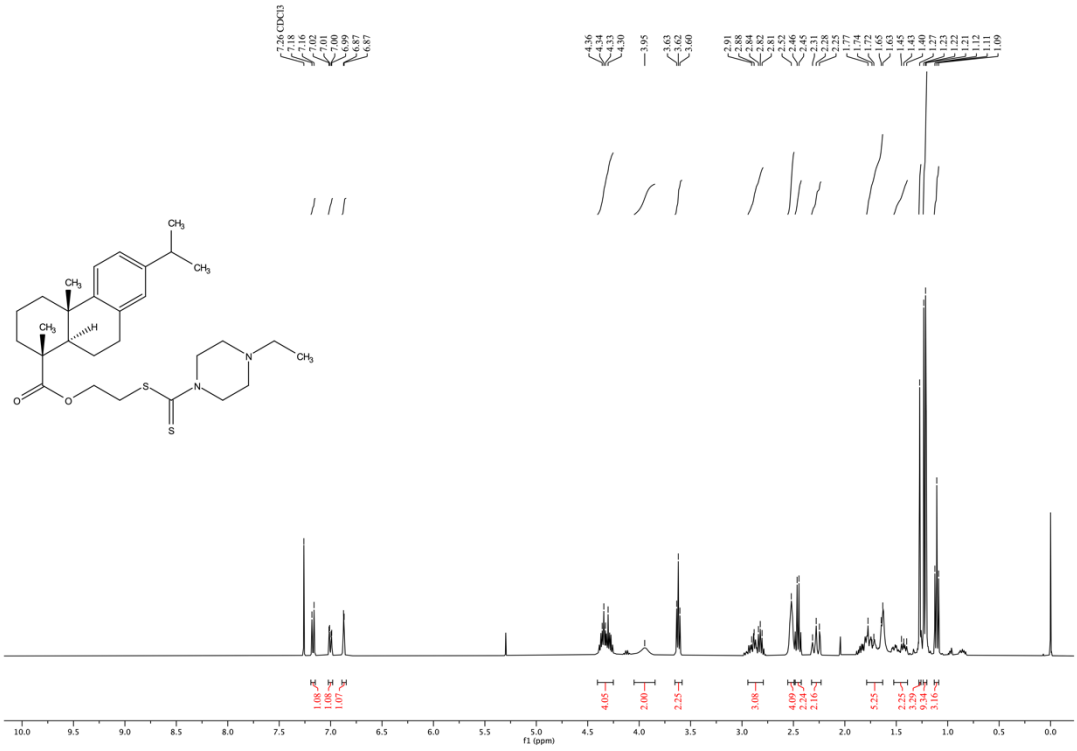

Figure S15. ^{1}H NMR spectrum of the target compound III-n.

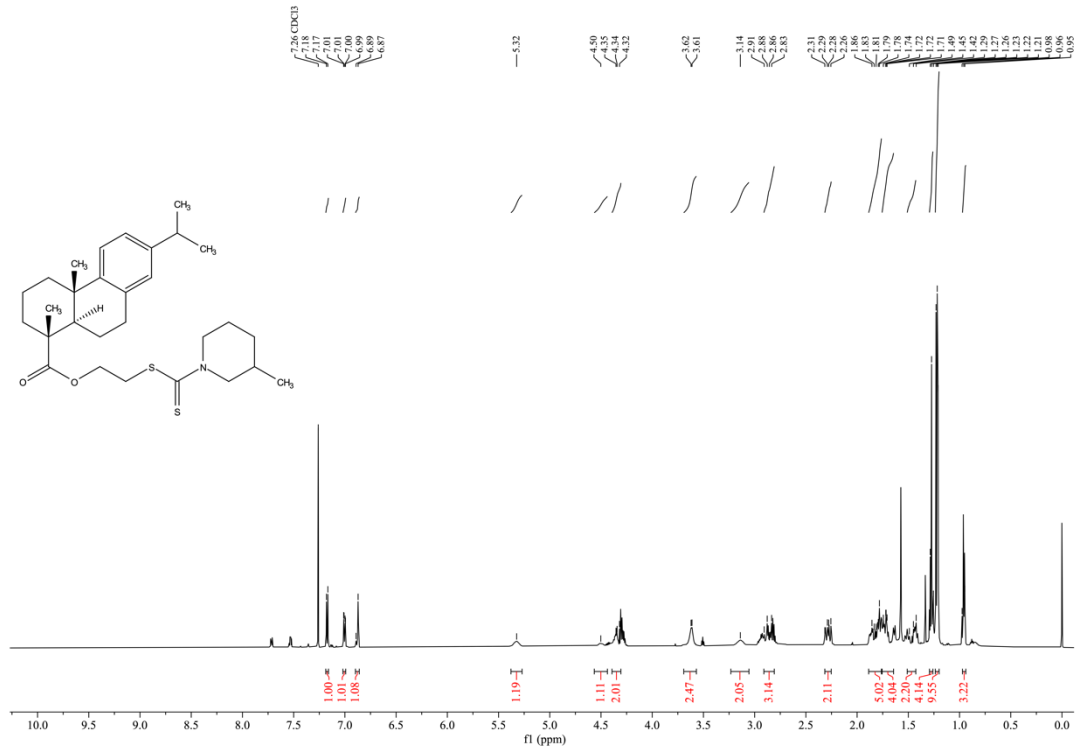

Figure S16. ^{1}H NMR spectrum of the target compound III-o.

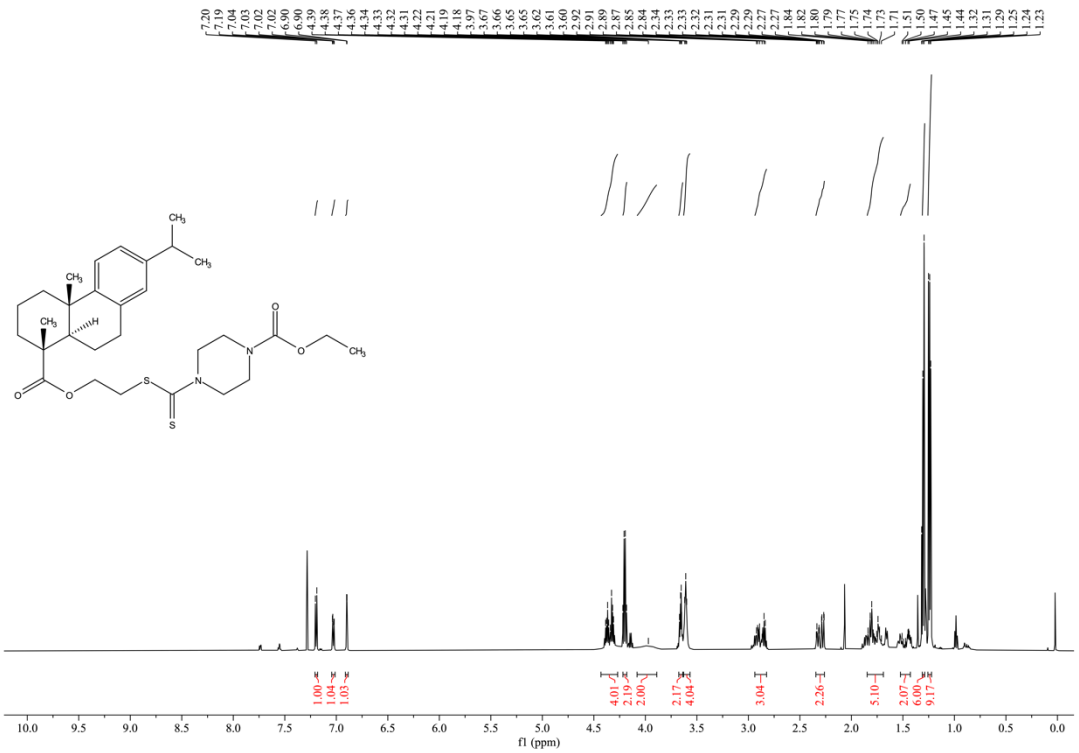

Figure S17. ^{1}H NMR spectrum of the target compound III-p.

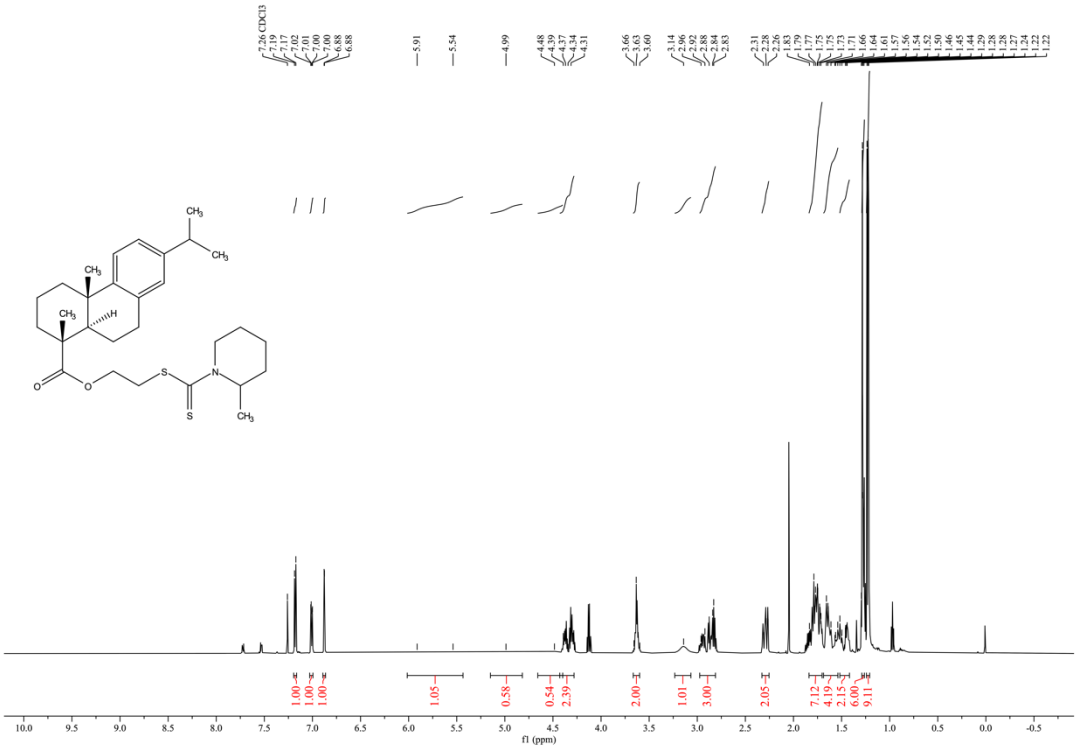

Figure S18. ^{1}H NMR spectrum of the target compound III-q.

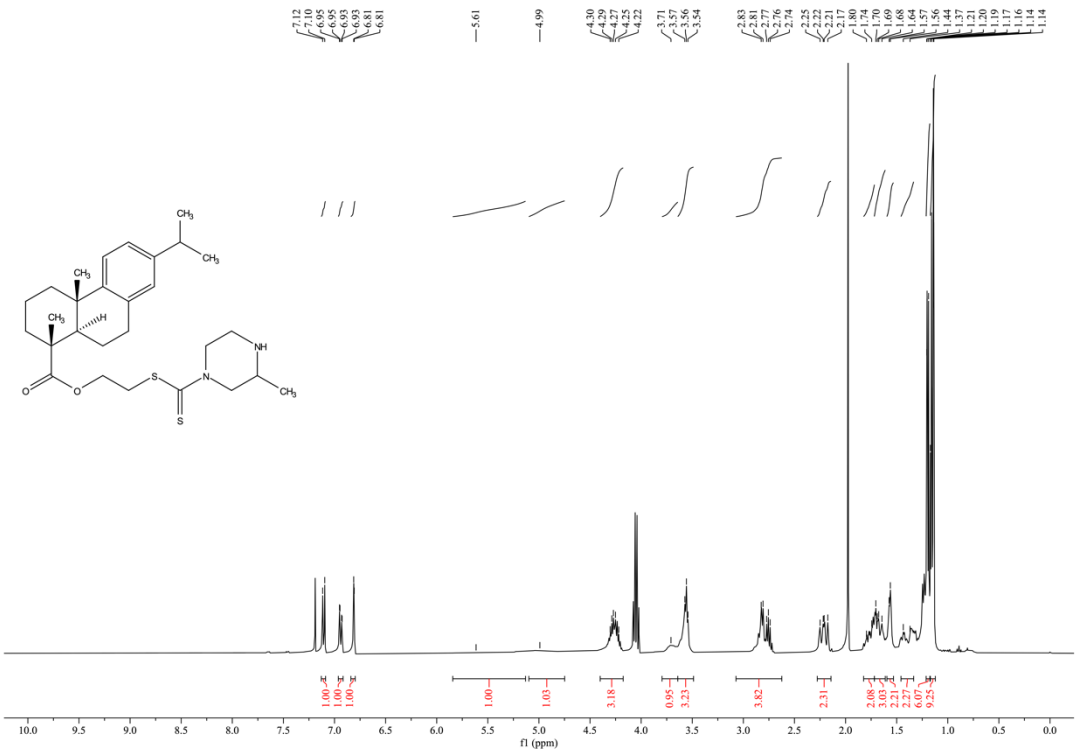

Figure S19. ^{1}H NMR spectrum of the target compound III-r.

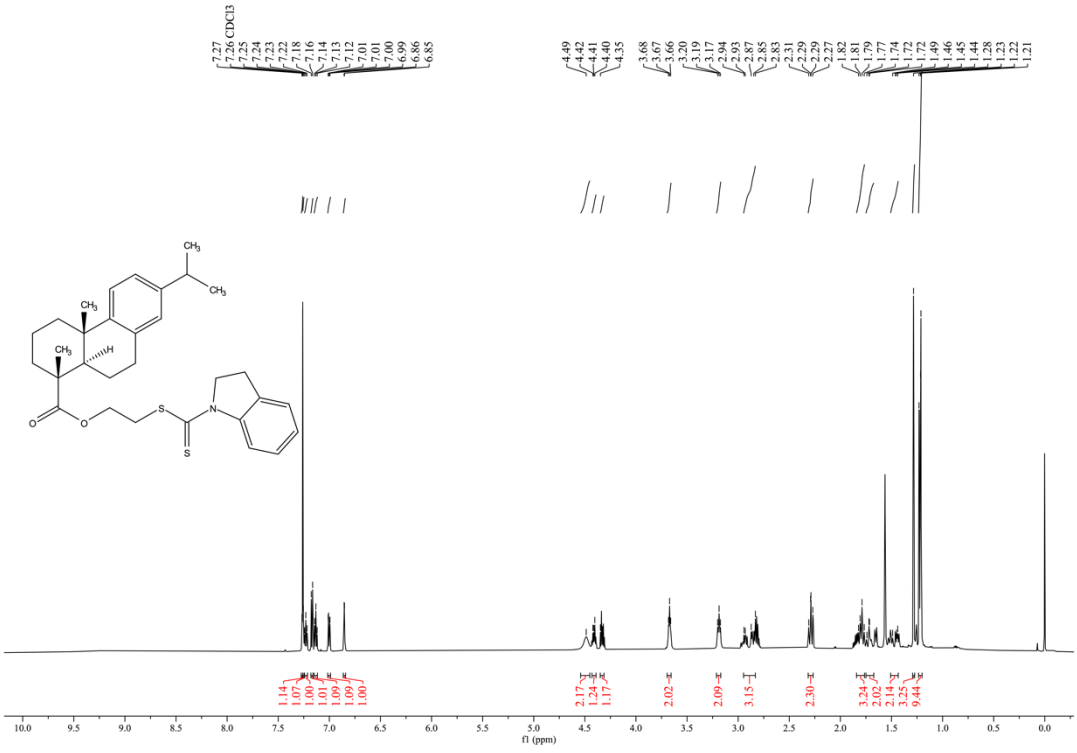

Figure S20. ^{1}H NMR spectrum of the target compound III-s.

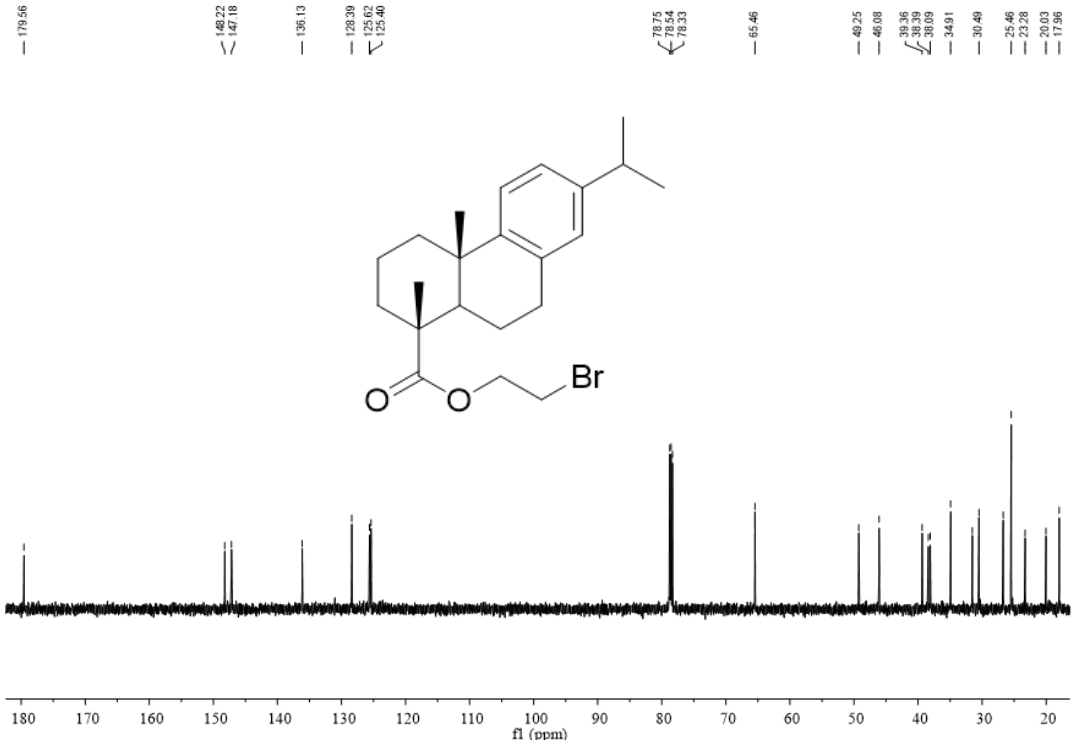

Figure S21. ^{13}C NMR spectrum of the target compound II.

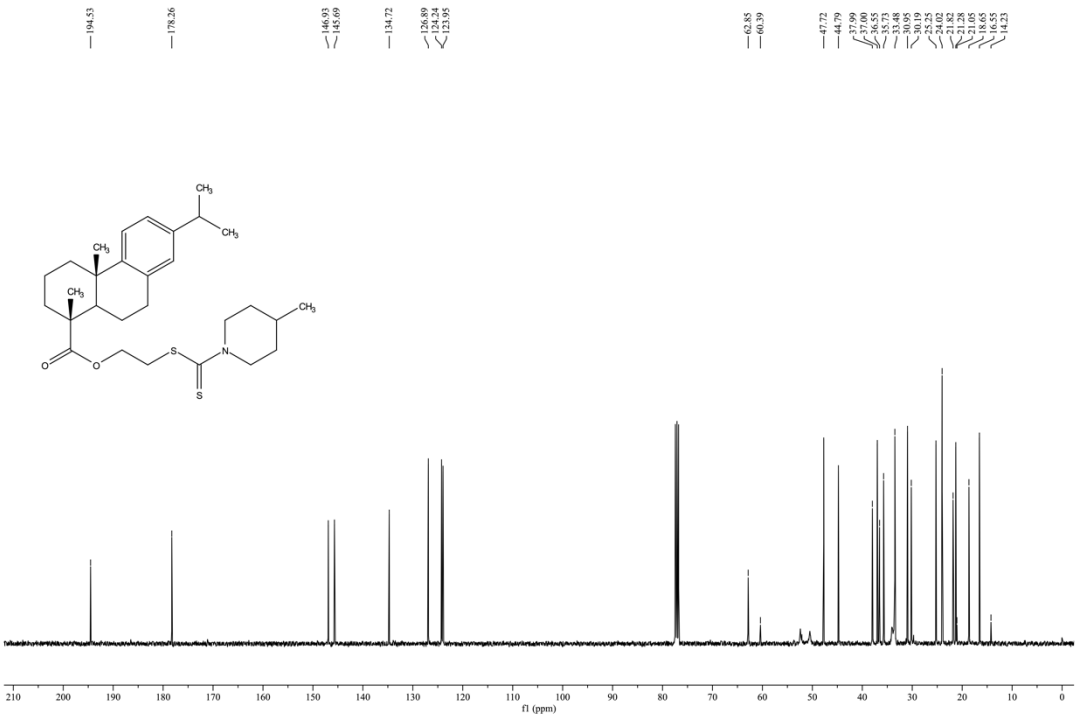

Figure S22. ^{13}C NMR spectrum of the target compound III-a.

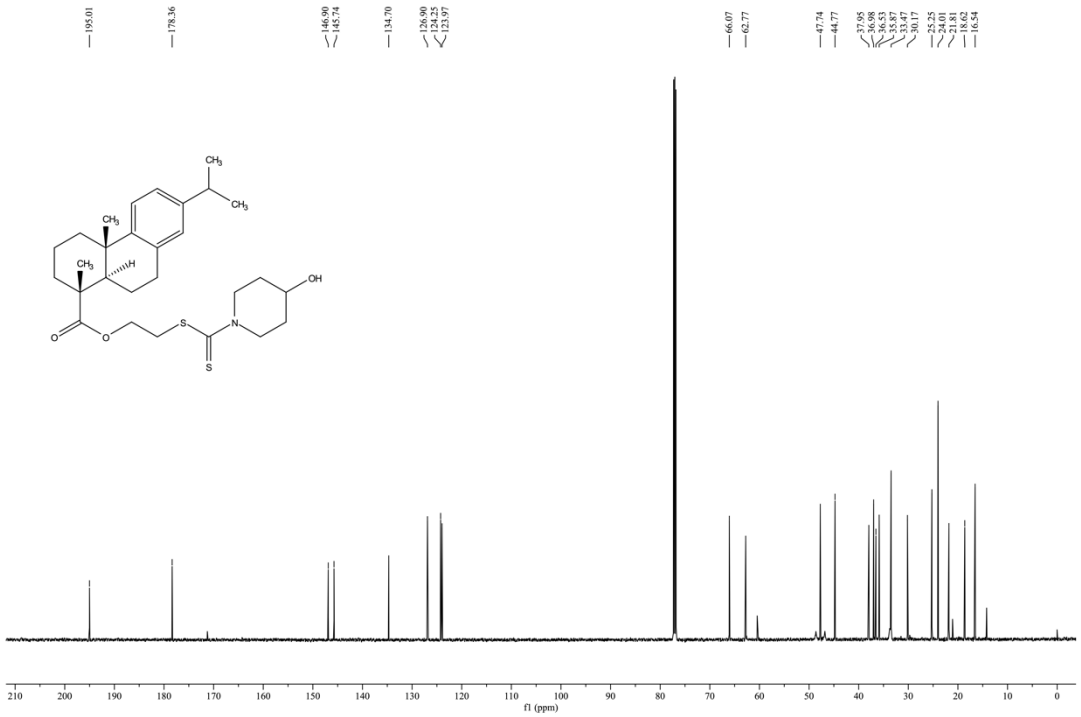

Figure S23. ^{13}C NMR spectrum of the target compound III-b.

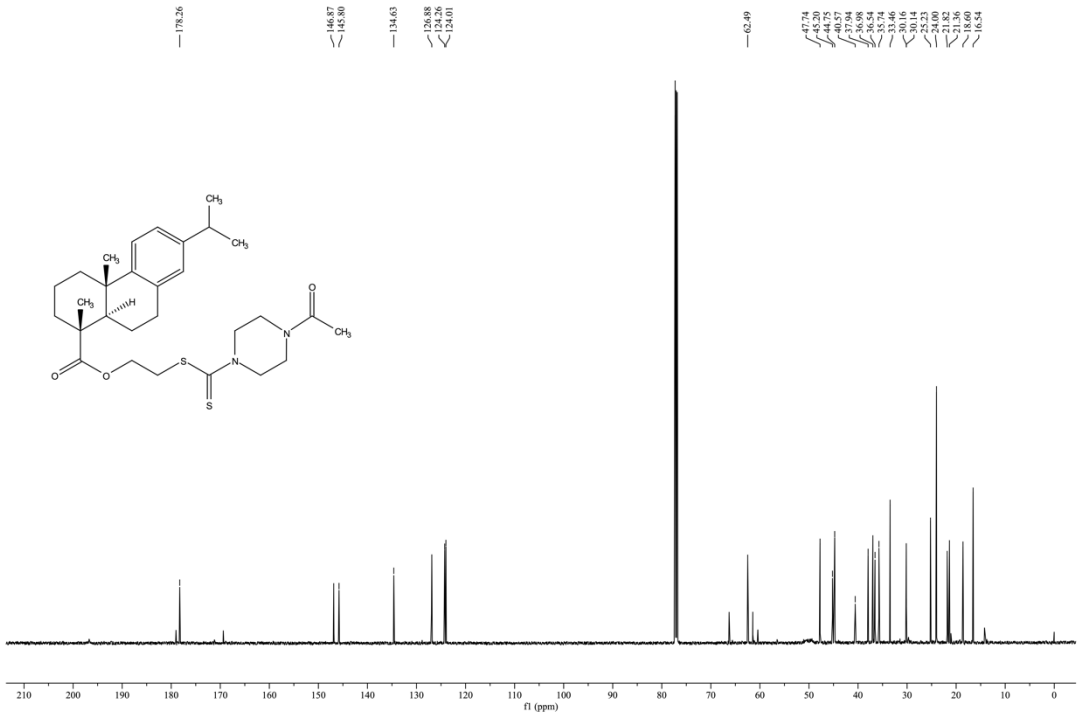

Figure S24. ^{13}C NMR spectrum of the target compound III-c.

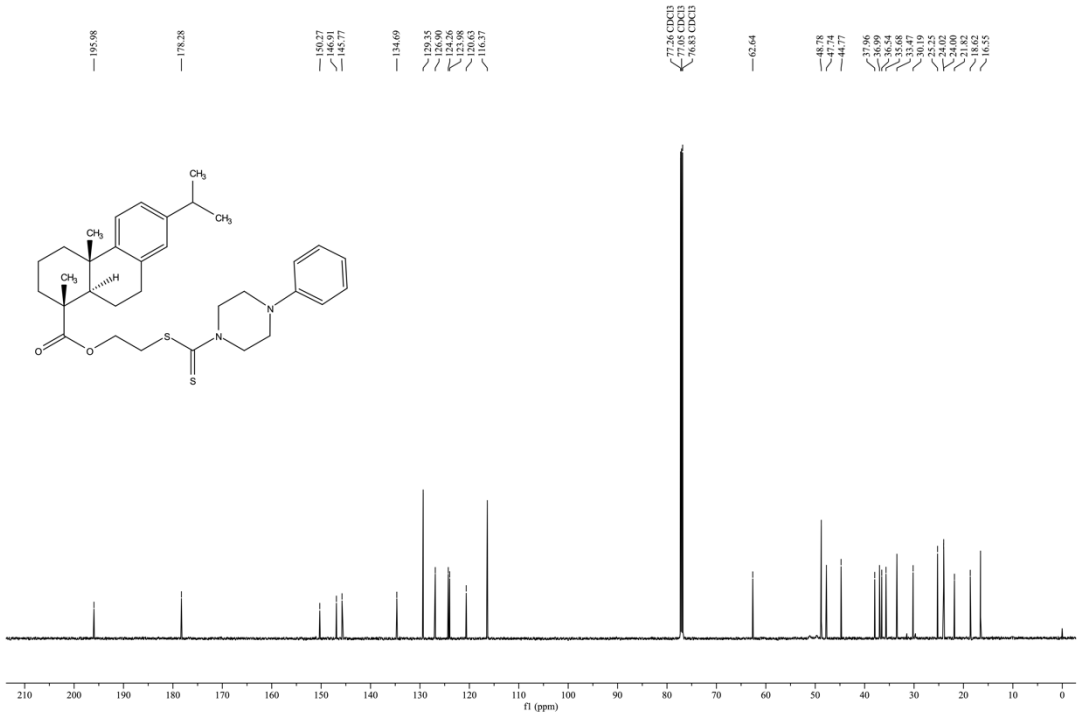

Figure S25. ^{13}C NMR spectrum of the target compound III-d.

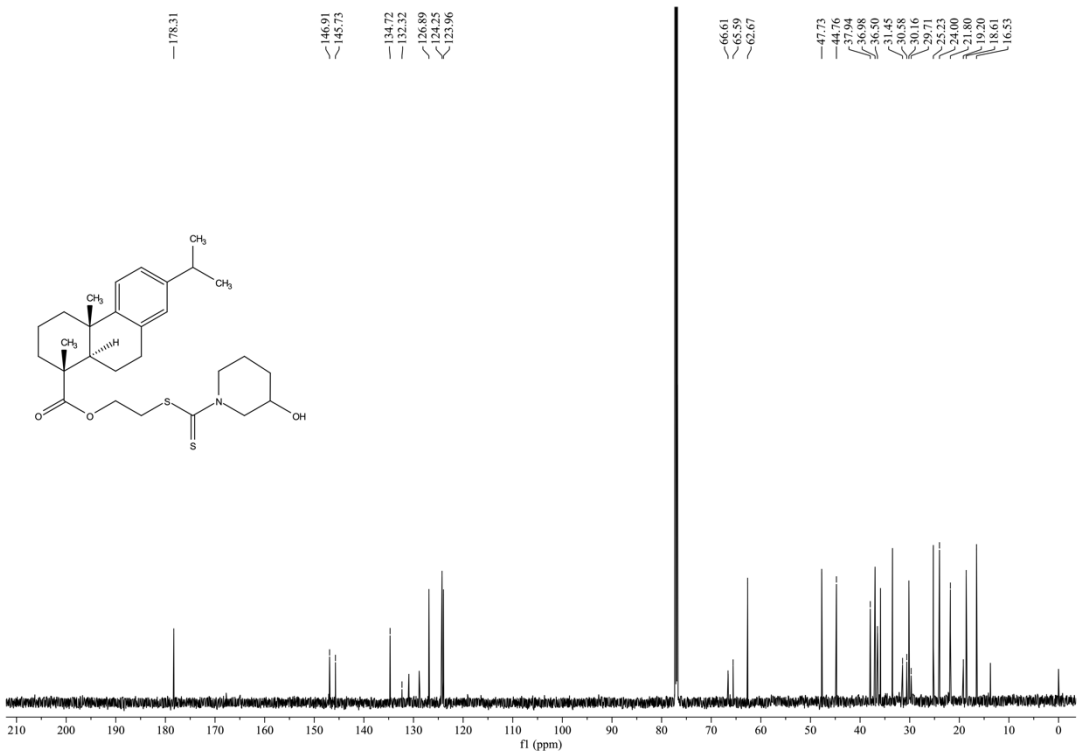

Figure S26. ^{13}C NMR spectrum of the target compound III-e.

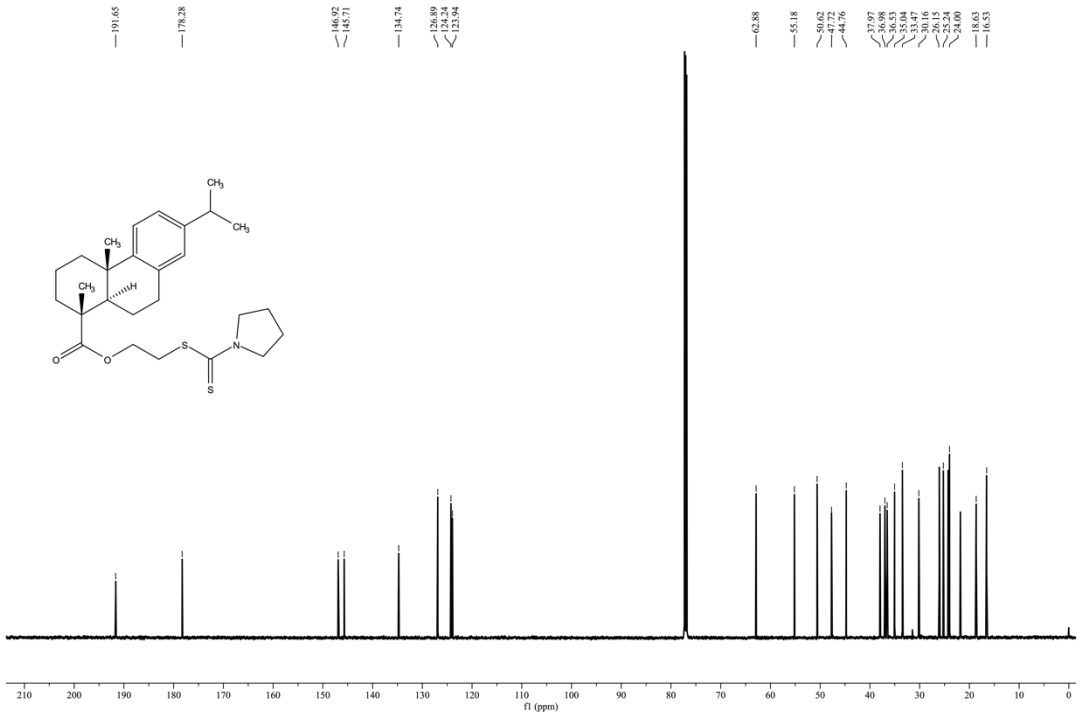

Figure S27. ^{13}C NMR spectrum of the target compound III-f.

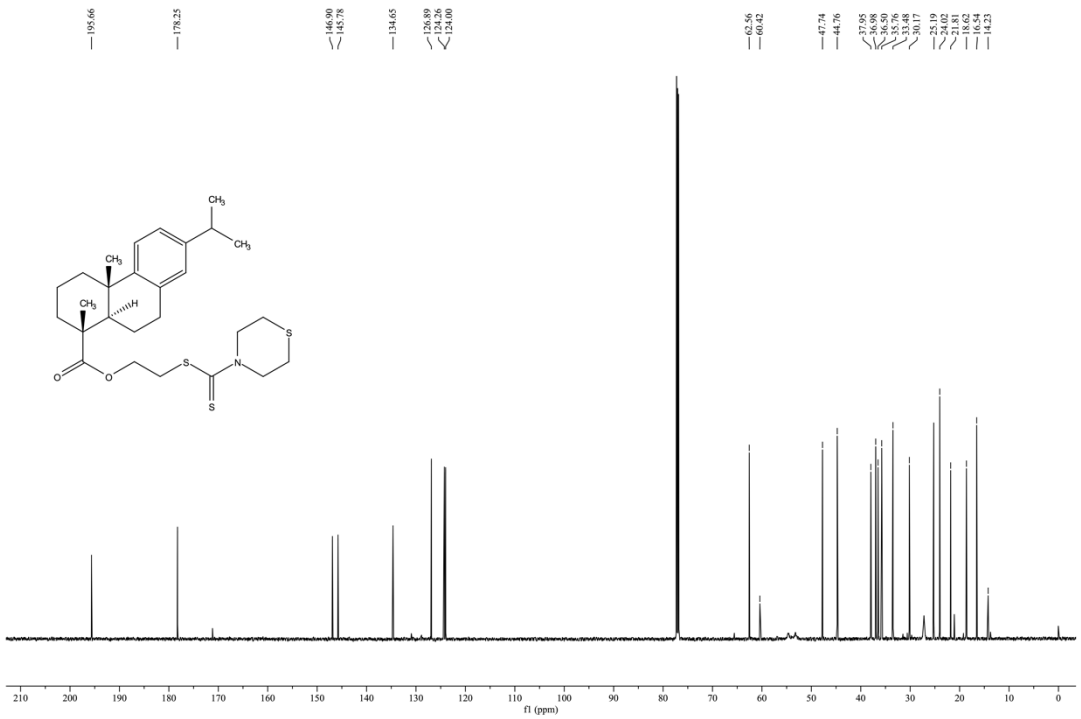

Figure S28. ^{13}C NMR spectrum of the target compound III-g.

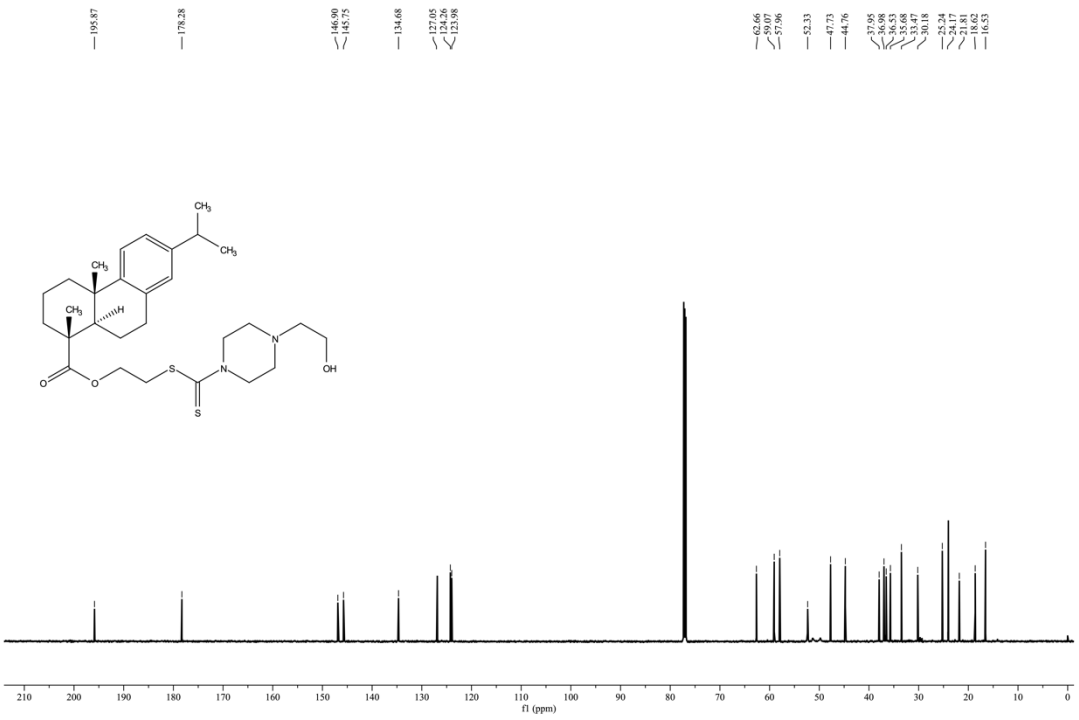

Figure S29. ^{13}C NMR spectrum of the target compound III-h.

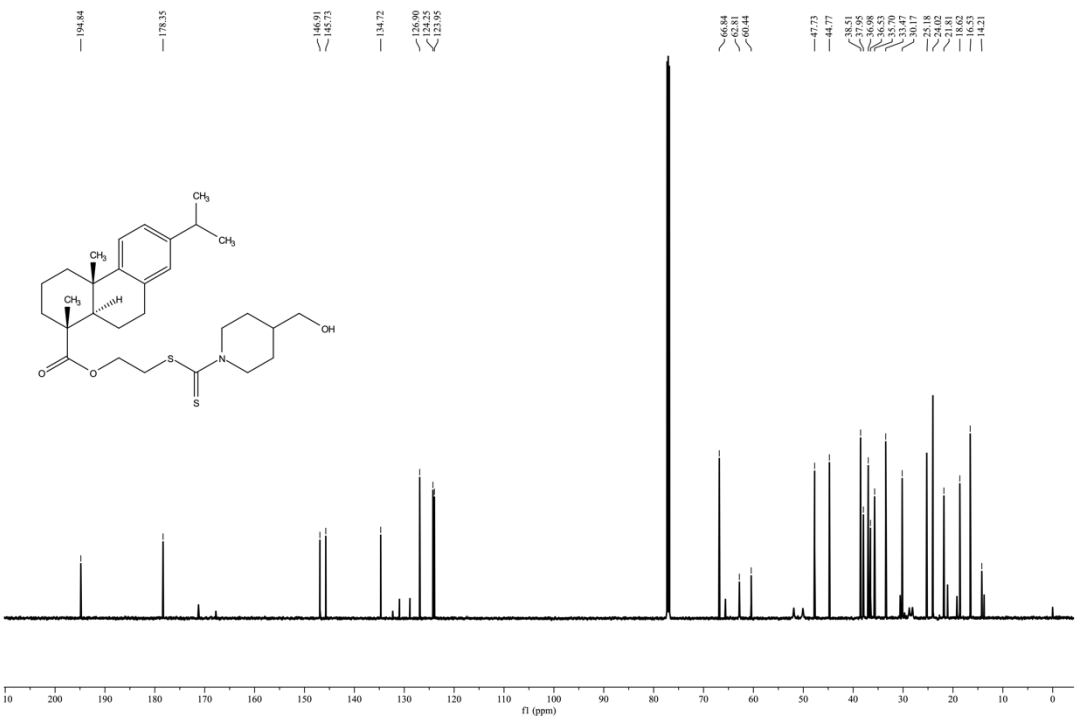

Figure S30. ^{13}C NMR spectrum of the target compound III-i.

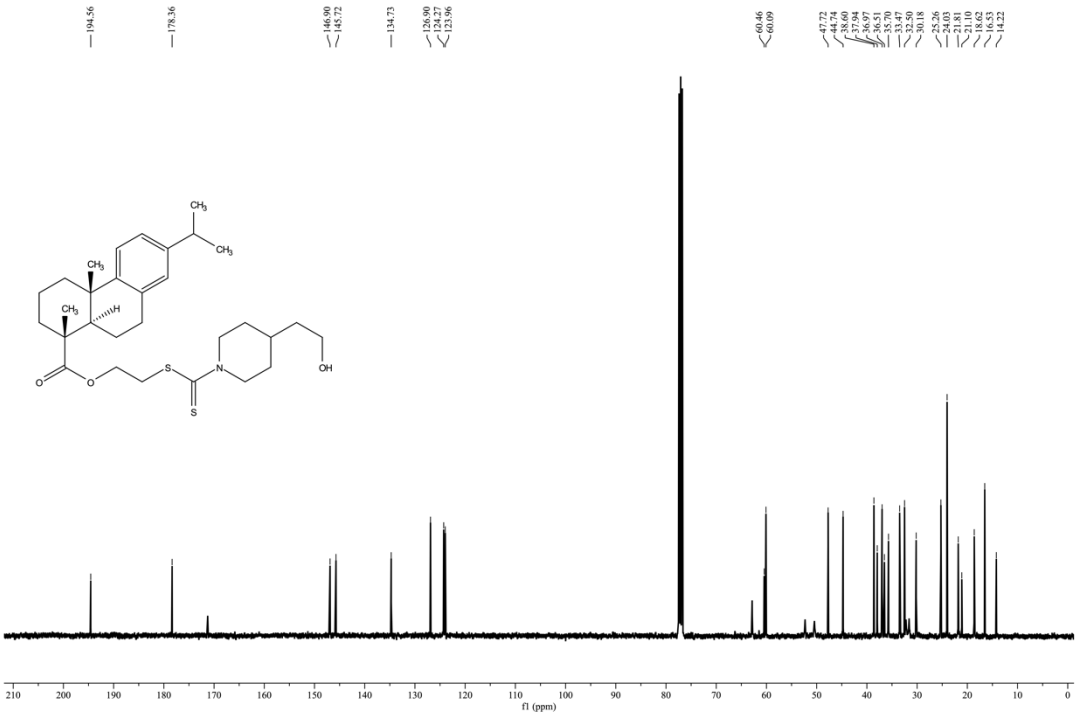

Figure S31. ^{13}C NMR spectrum of the target compound III-j.

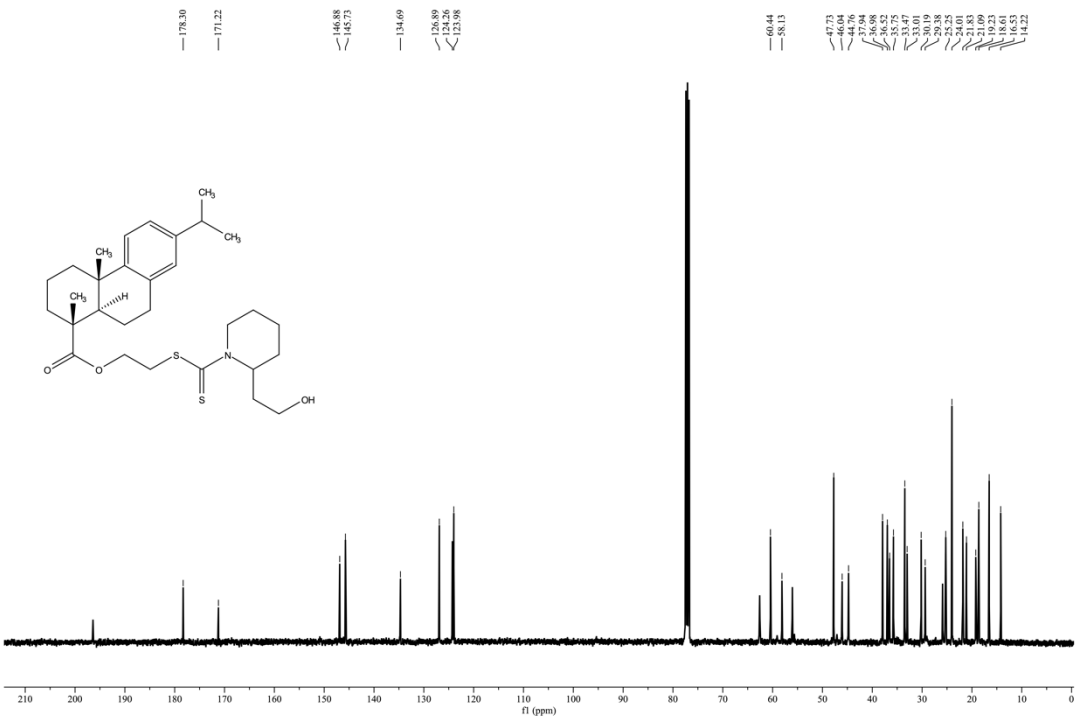

Figure S32. ^{13}C NMR spectrum of the target compound III-k.

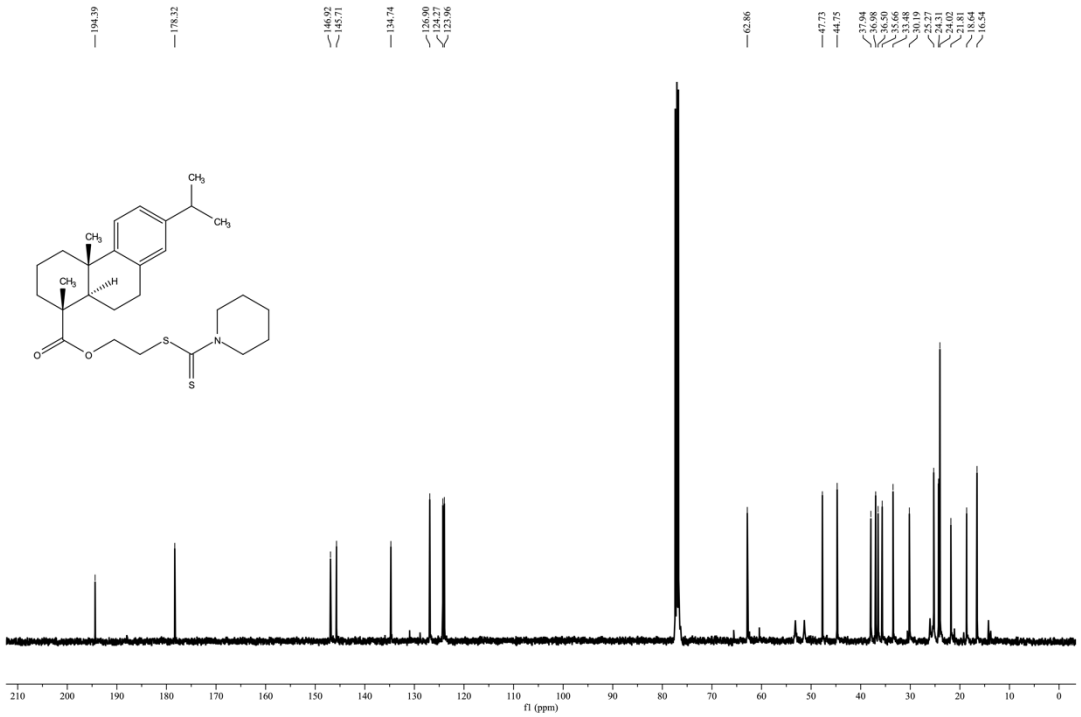

Figure S33. ^{13}C NMR spectrum of the target compound III-l.

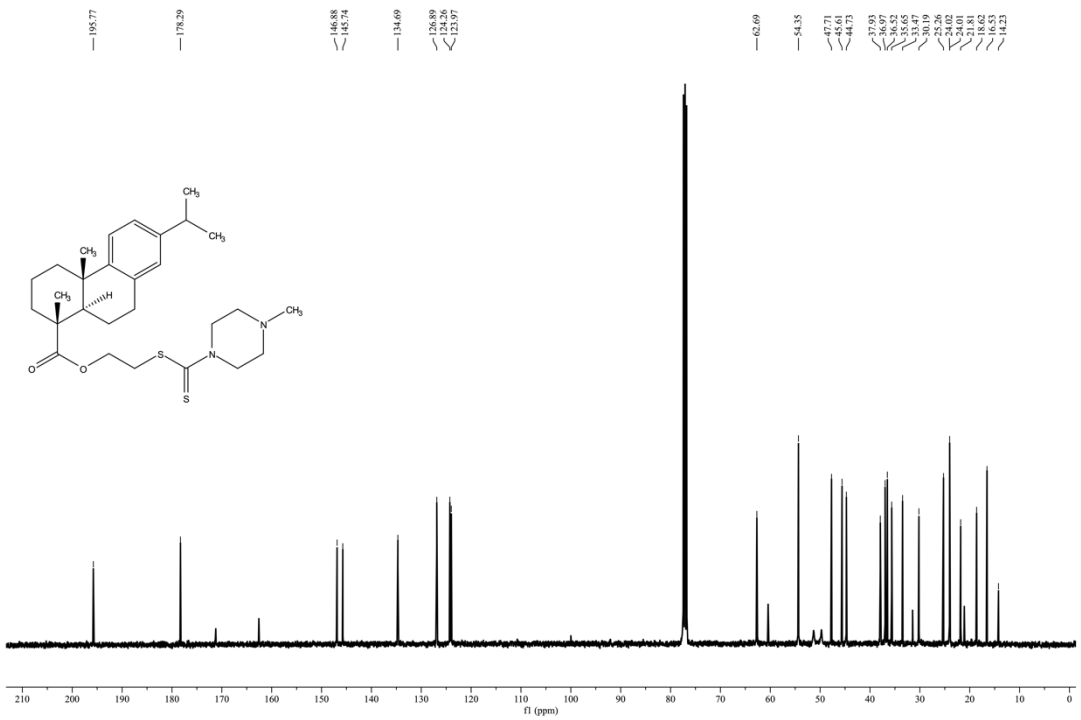

Figure S34. ^{13}C NMR spectrum of the target compound III-m.

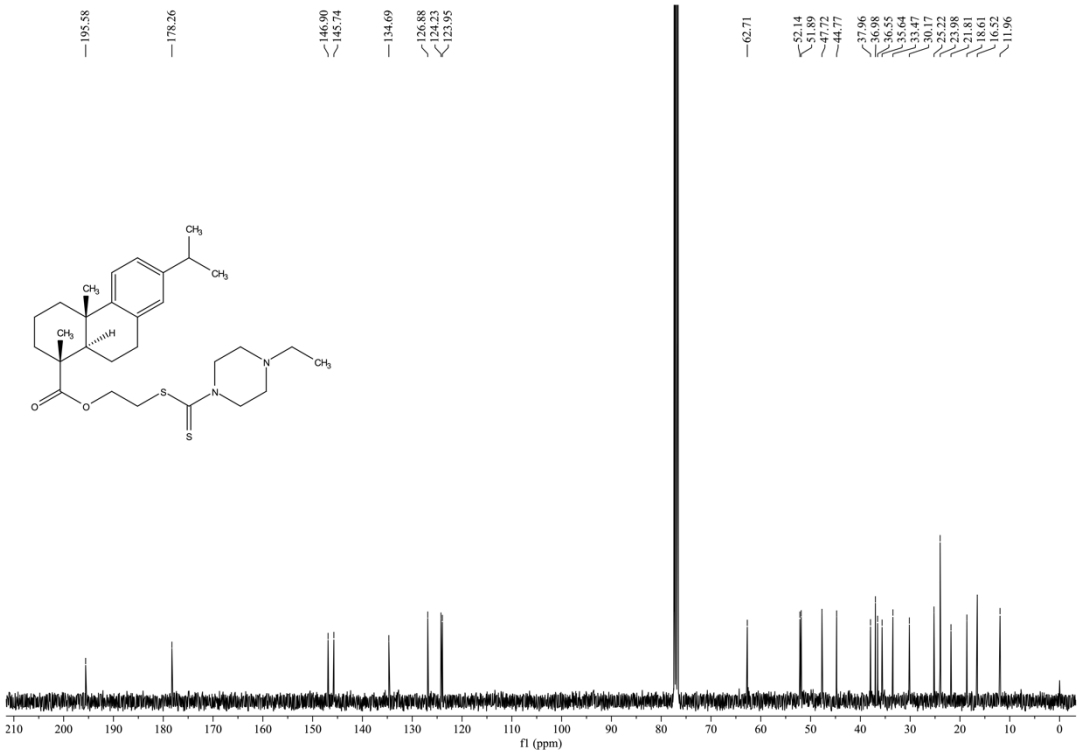

Figure S35. ^{13}C NMR spectrum of the target compound III-n.

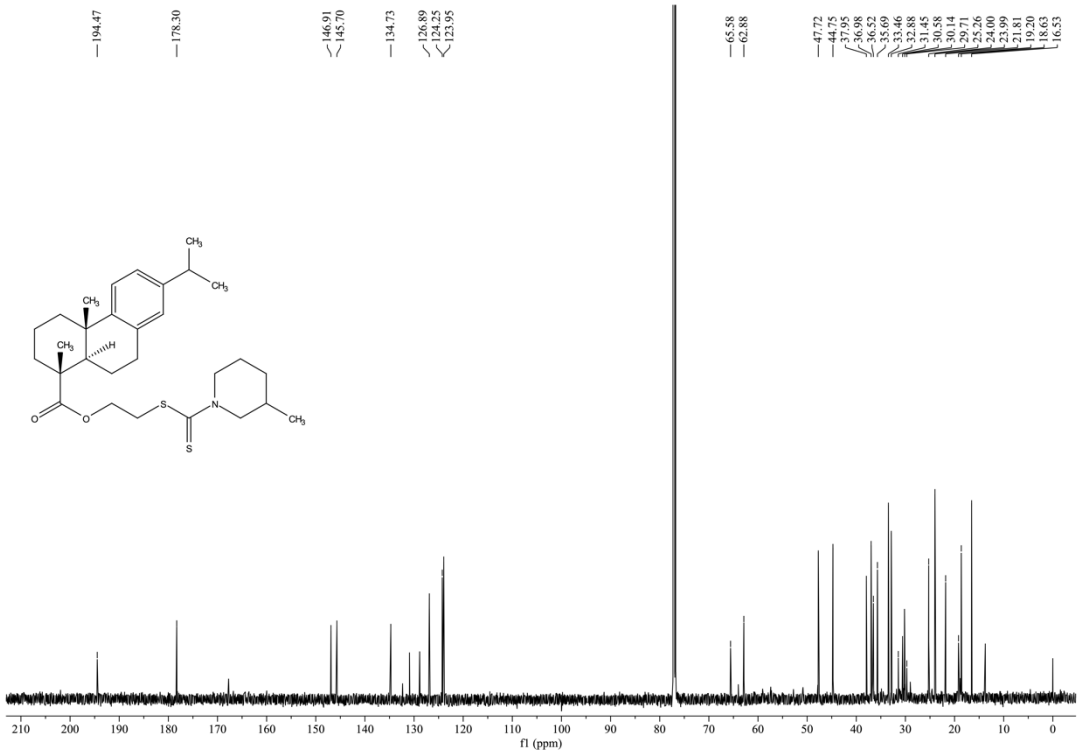

Figure S36. ^{13}C NMR spectrum of the target compound III-o.

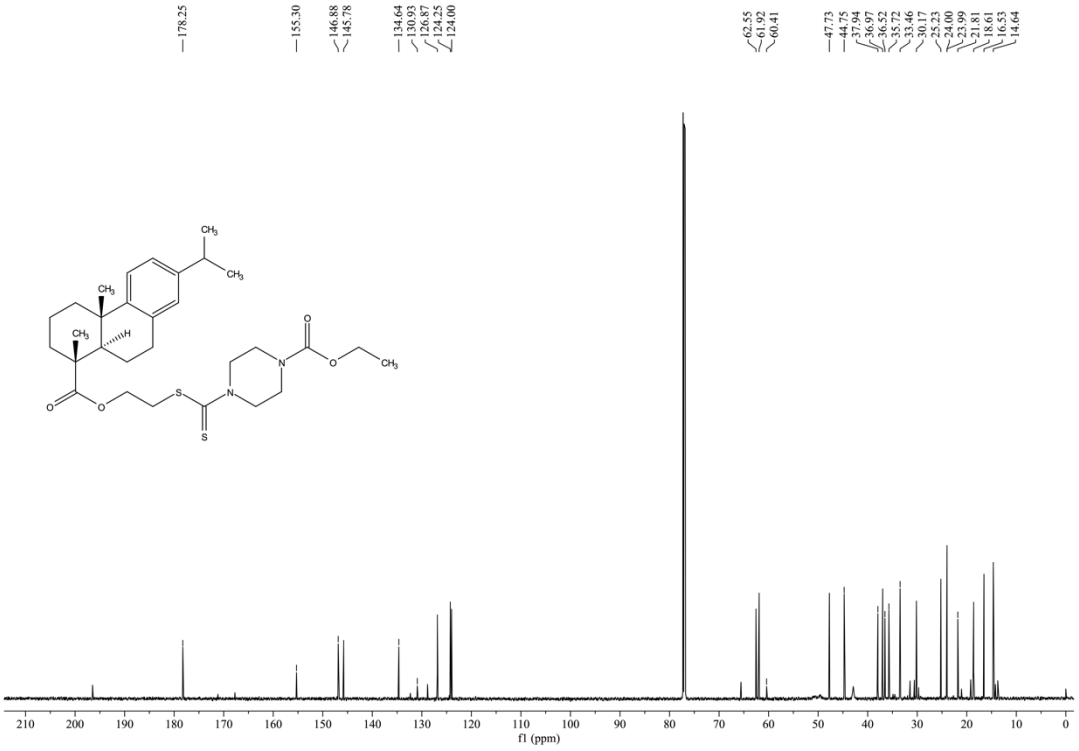

Figure S37. ^{13}C NMR spectrum of the target compound III-p.

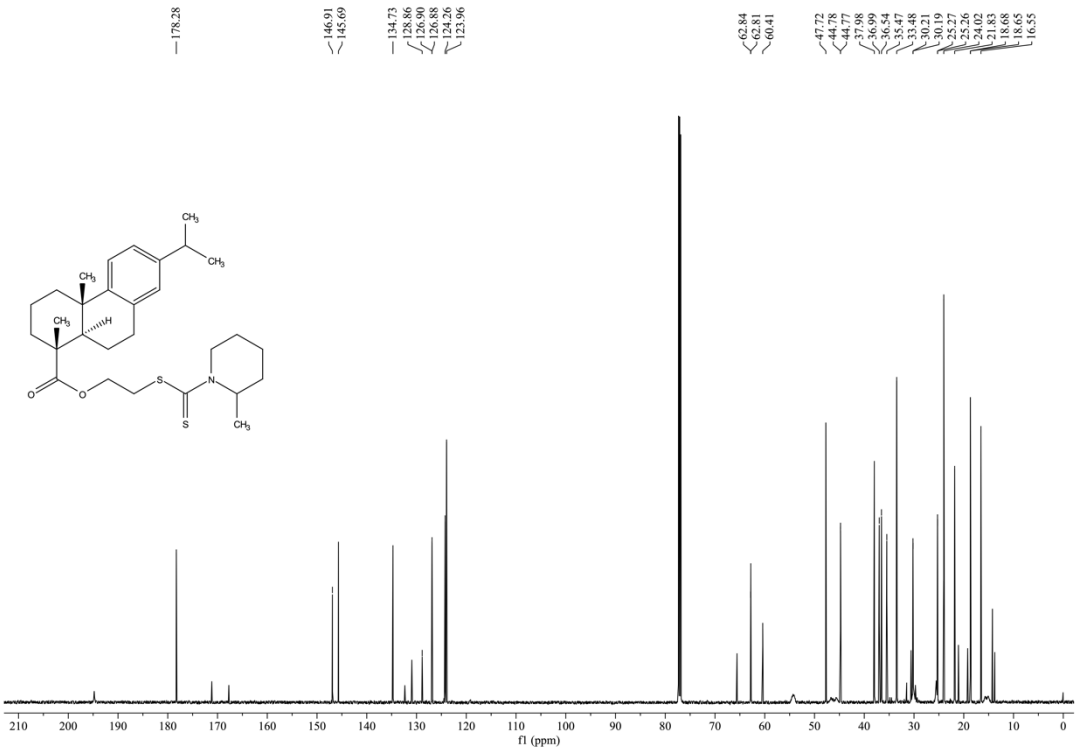

Figure S38. ^{13}C NMR spectrum of the target compound III-q.

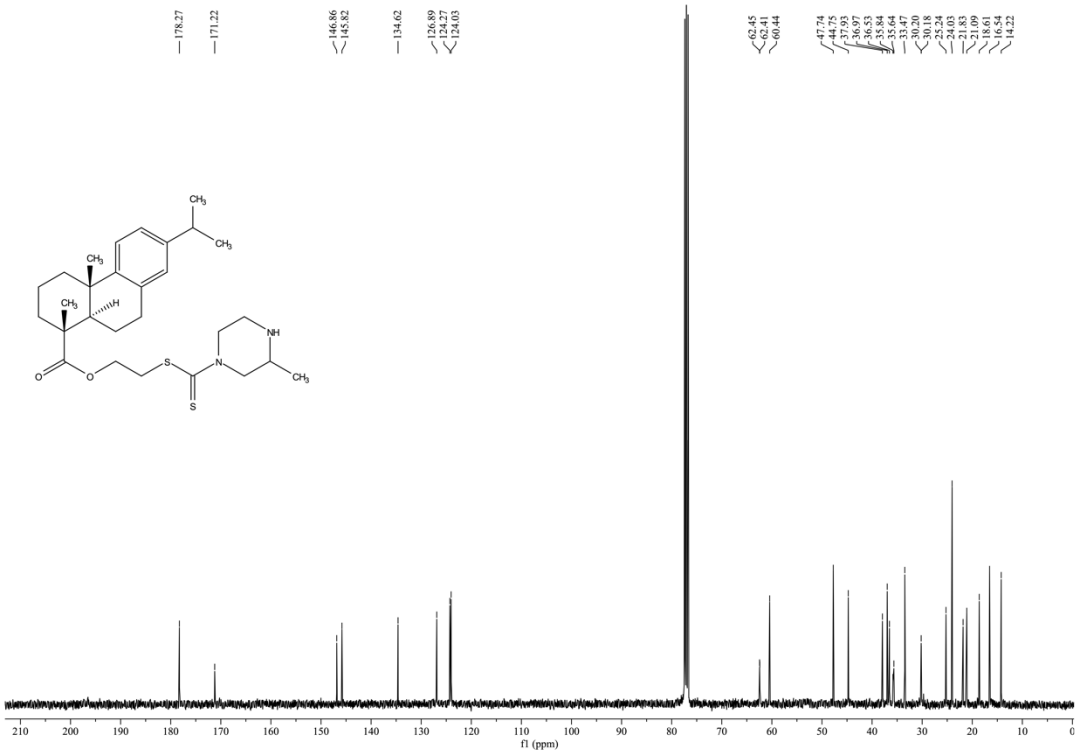

Figure S39. ^{13}C NMR spectrum of the target compound III-r.

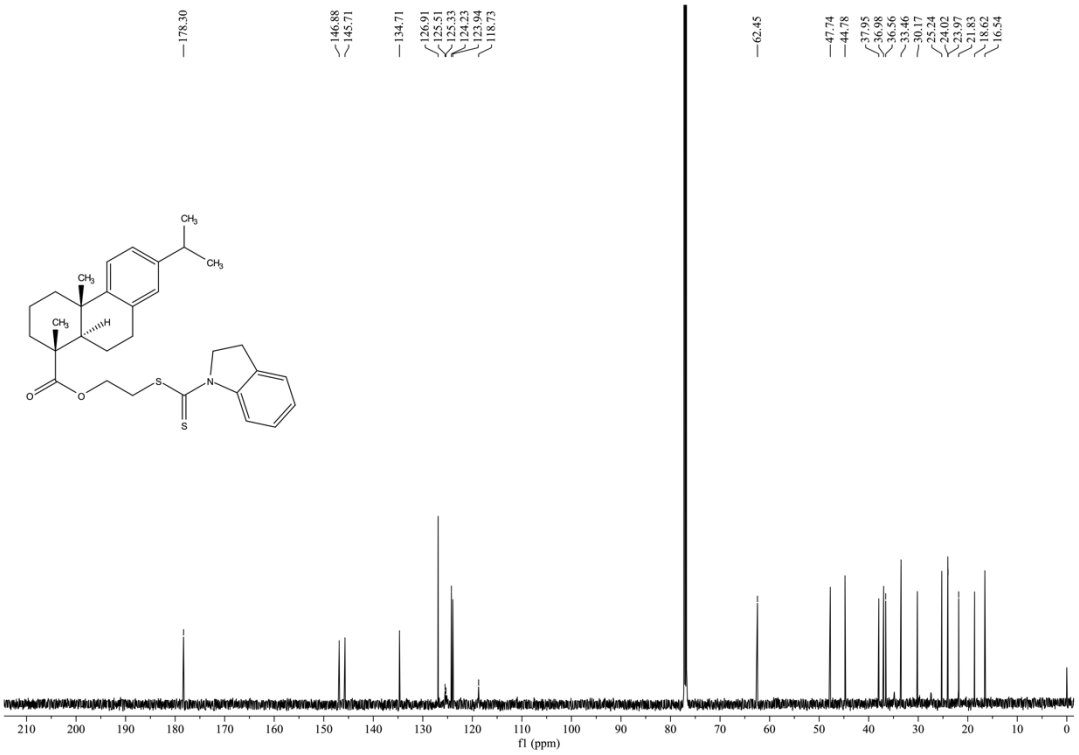

Figure S40. ^{13}C NMR spectrum of the target compound III-s.

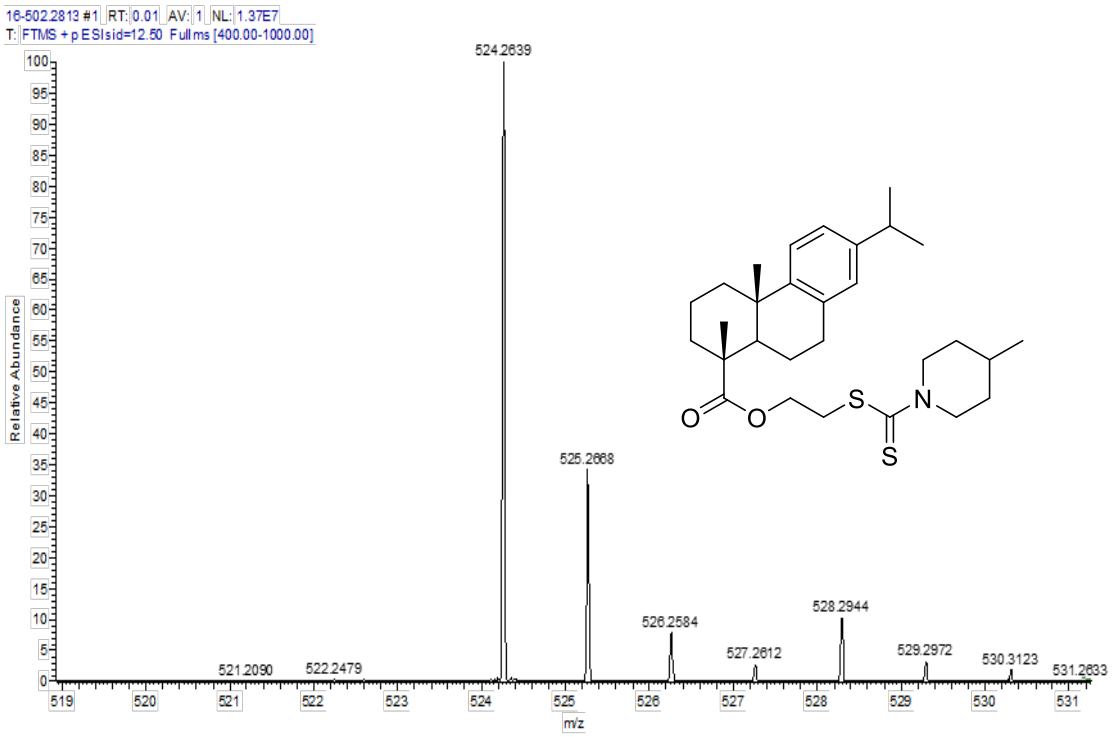

Figure S41. HR-MS spectrum of the target compound III-a.

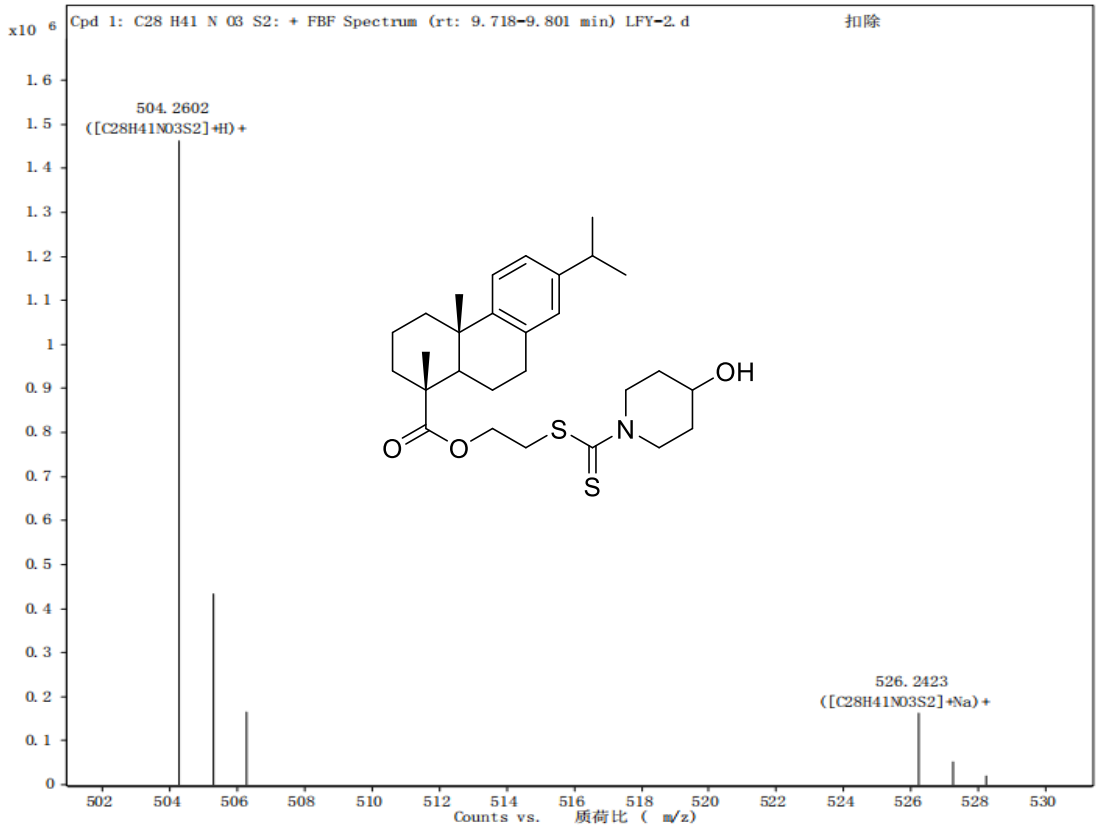

Figure S42. HR-MS spectrum of the target compound III-b.

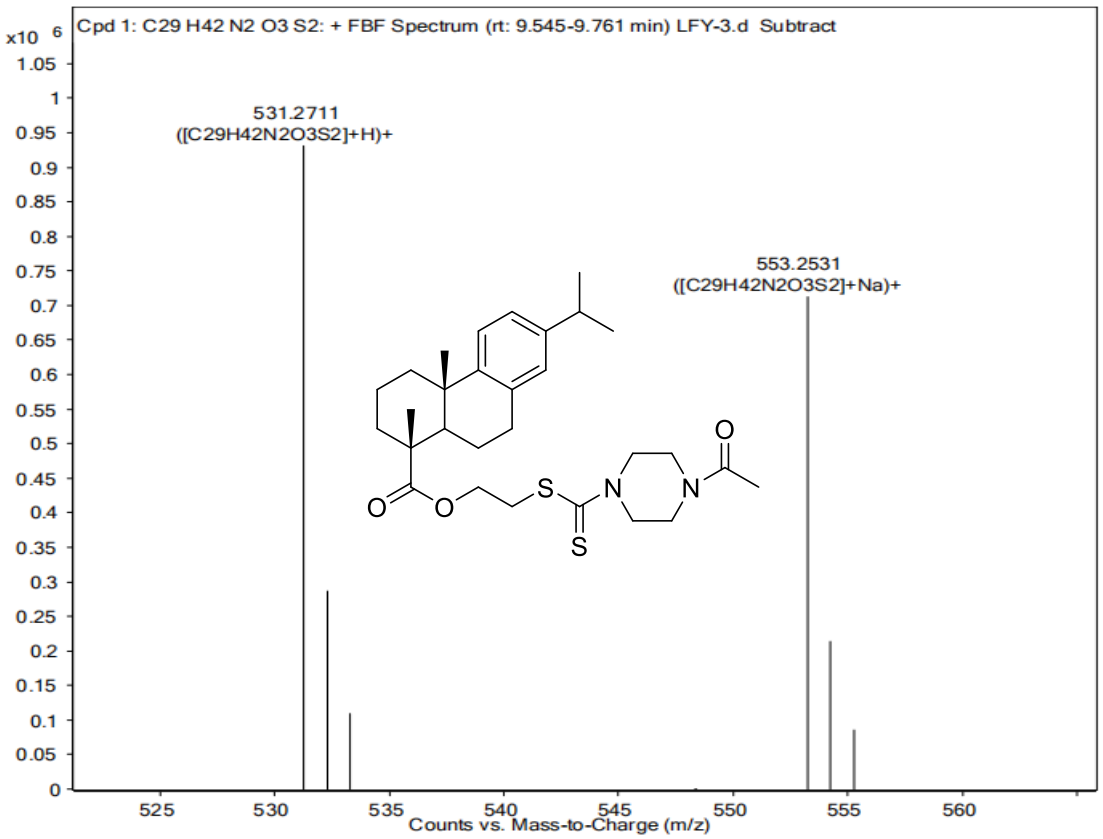

Figure S43. HR-MS spectrum of the target compound III-c.

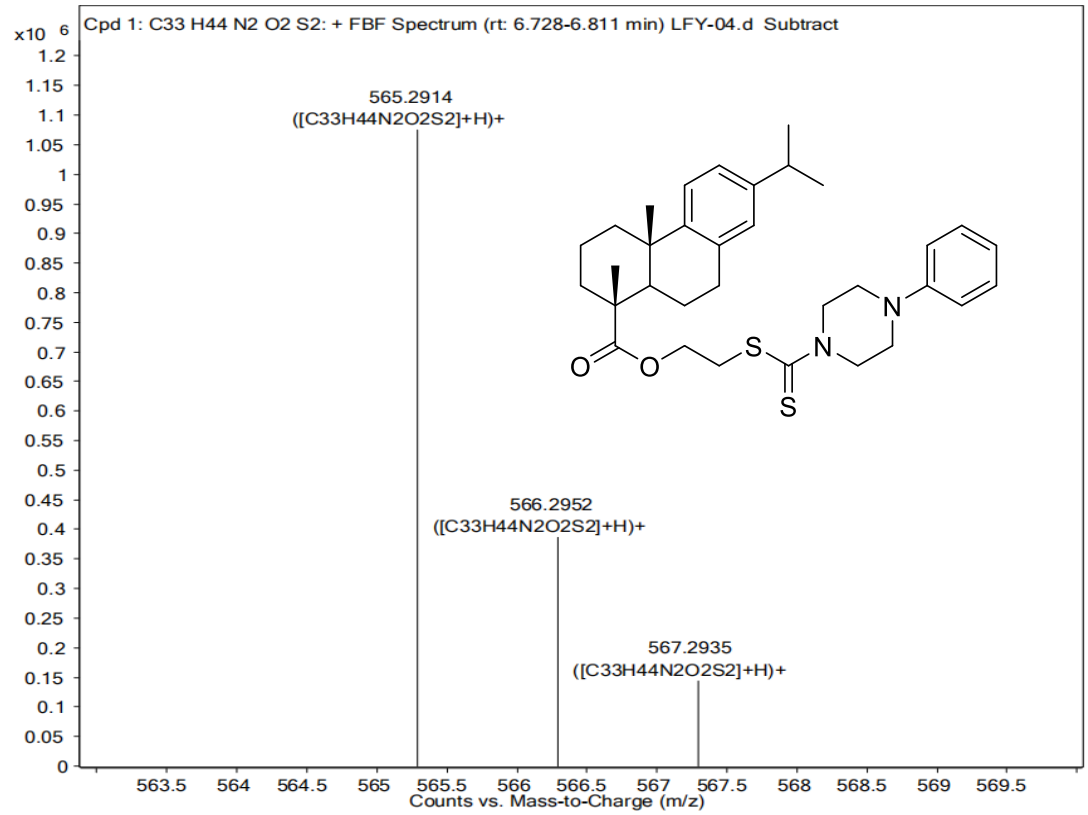

Figure S44. HR-MS spectrum of the target compound III-d.

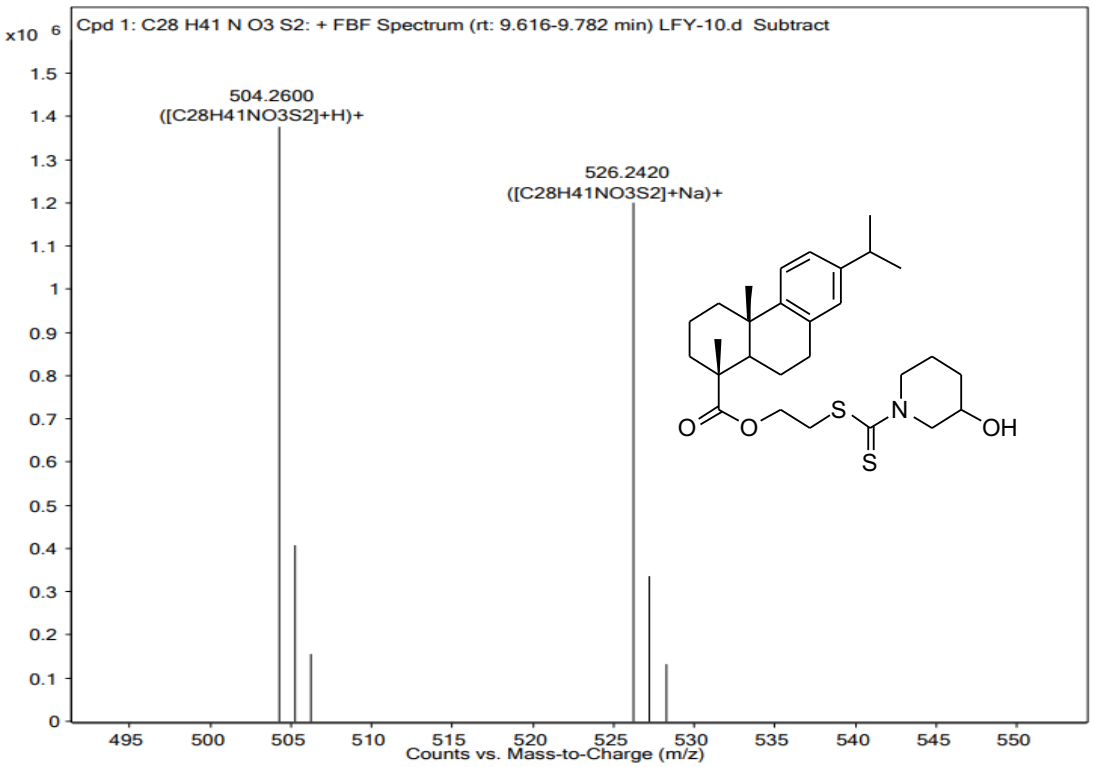

Figure S45. HR-MS spectrum of the target compound III-e.

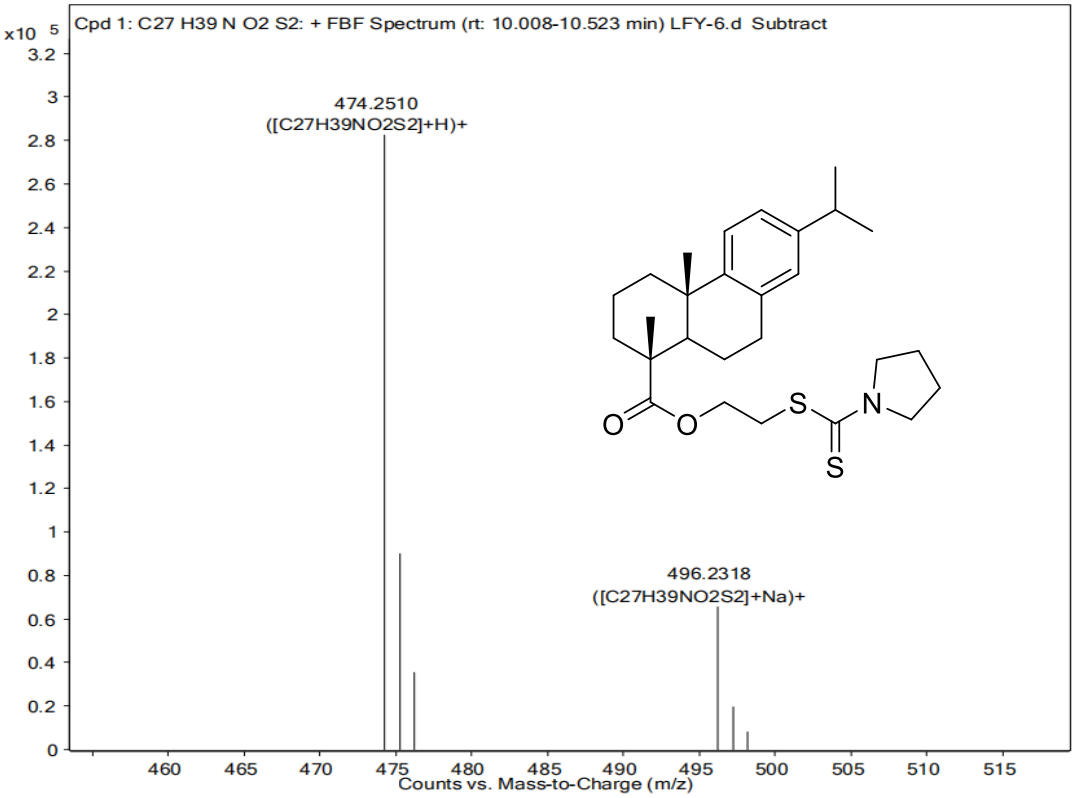

Figure S46. HR-MS spectrum of the target compound III-f.

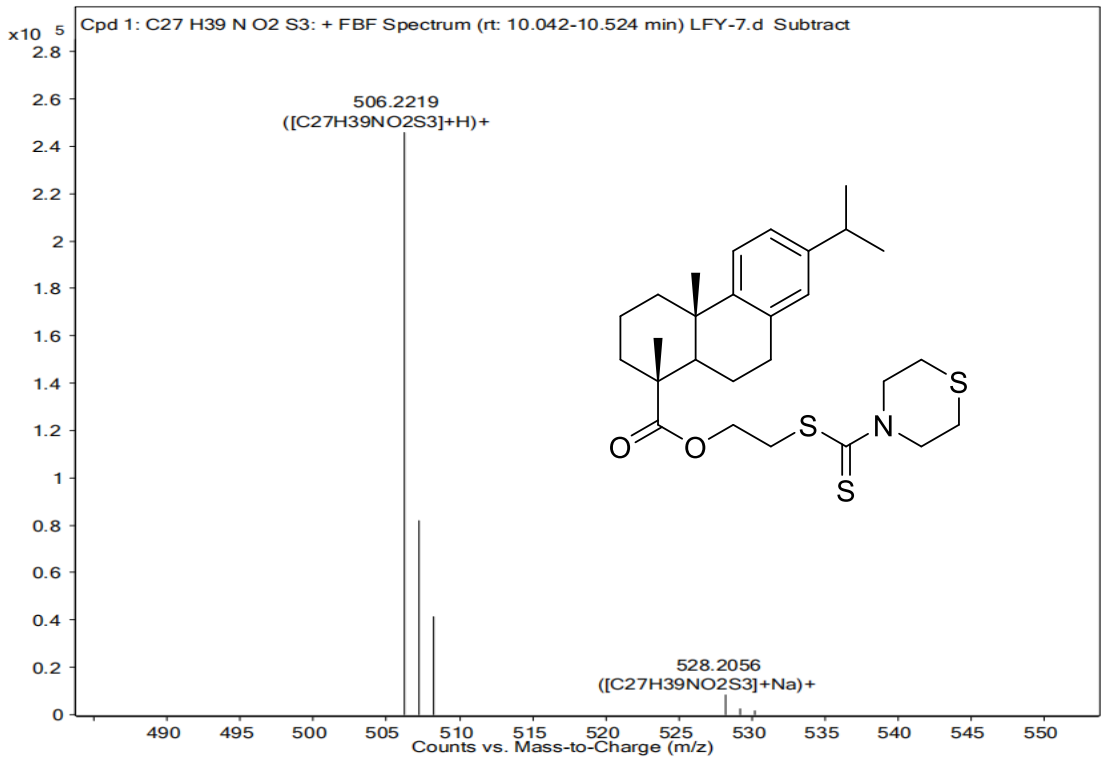

Figure S47. HR-MS spectrum of the target compound III-g.

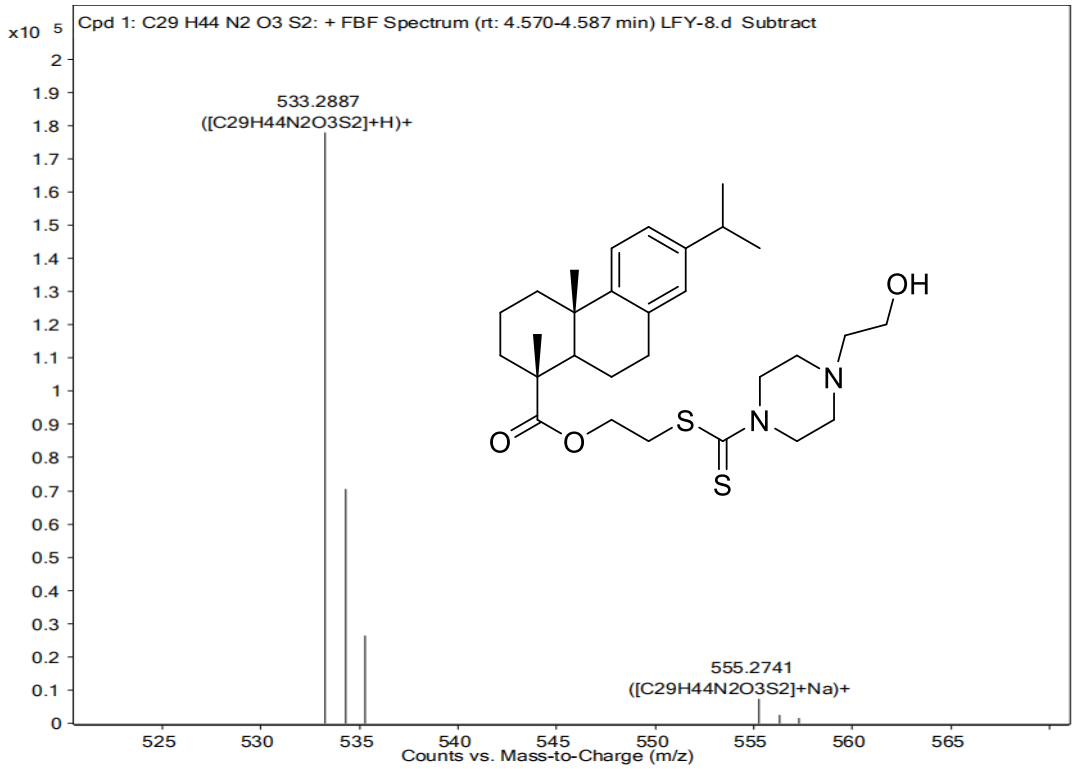

Figure S48. HR-MS spectrum of the target compound III-h.

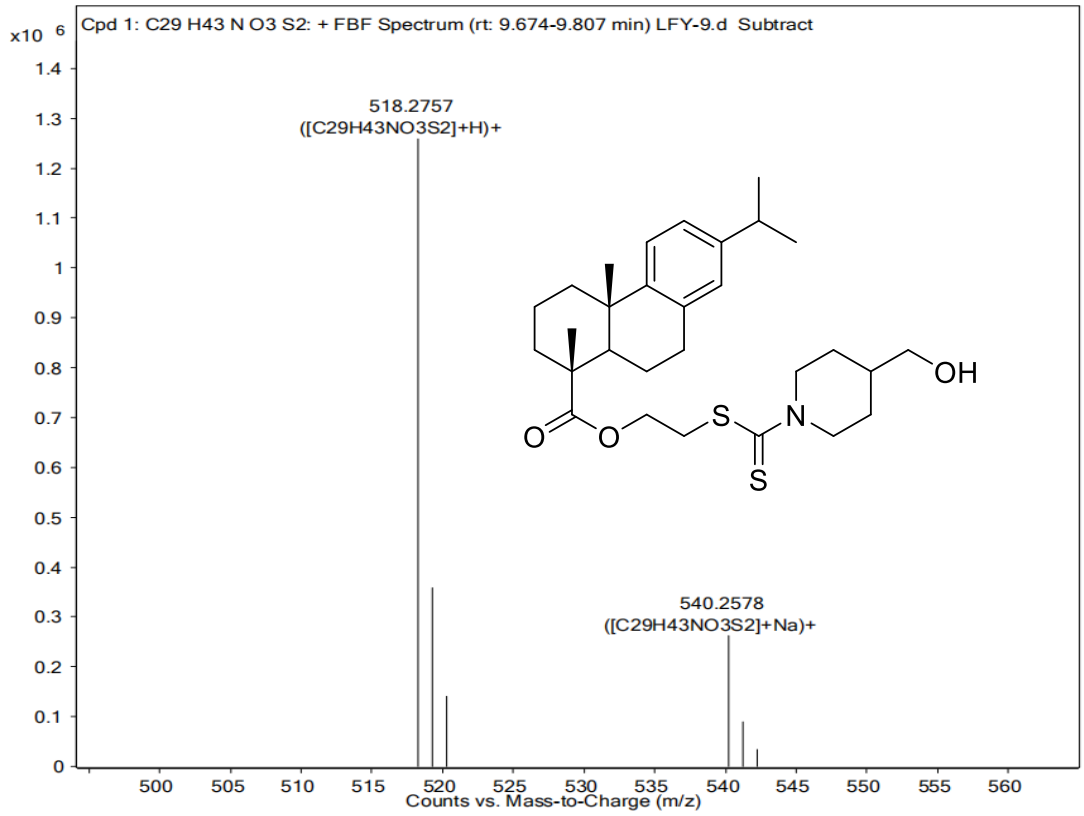

Figure S49. HR-MS spectrum of the target compound III-i.

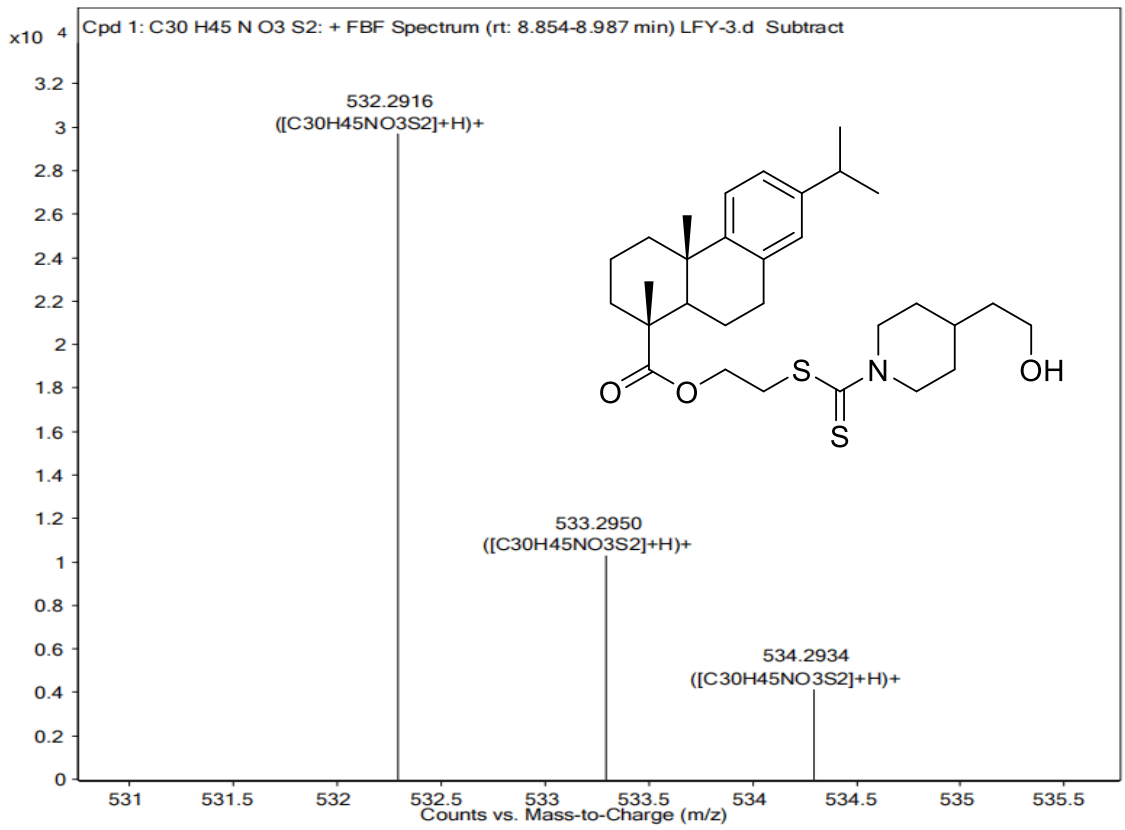

Figure S50. HR-MS spectrum of the target compound III-j.

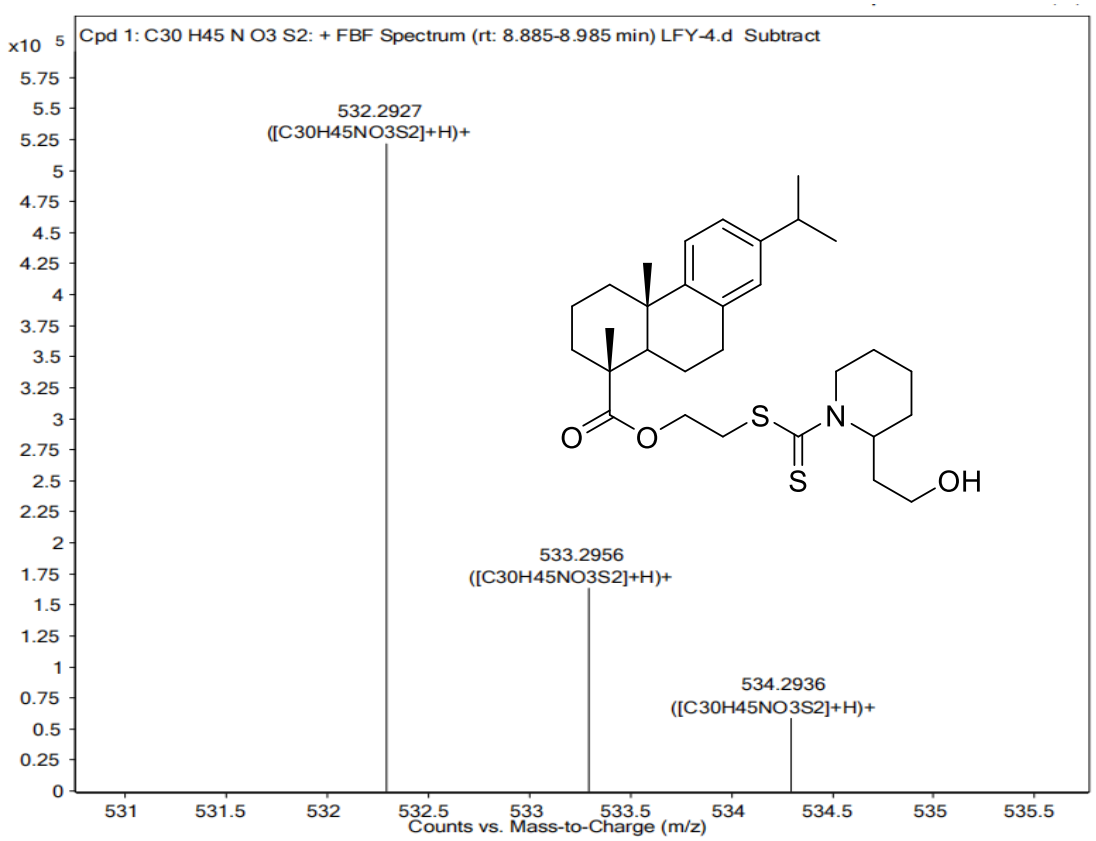

Figure S51. HR-MS spectrum of the target compound III-k.

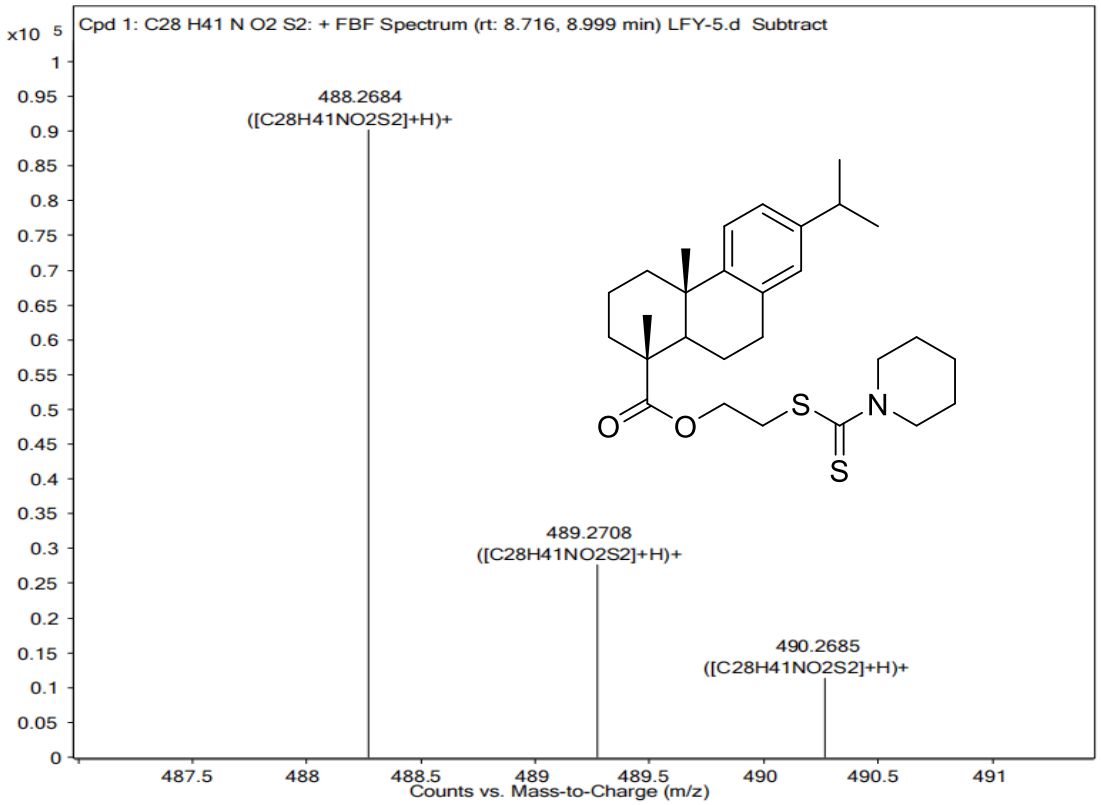

Figure S52. HR-MS spectrum of the target compound III-l.

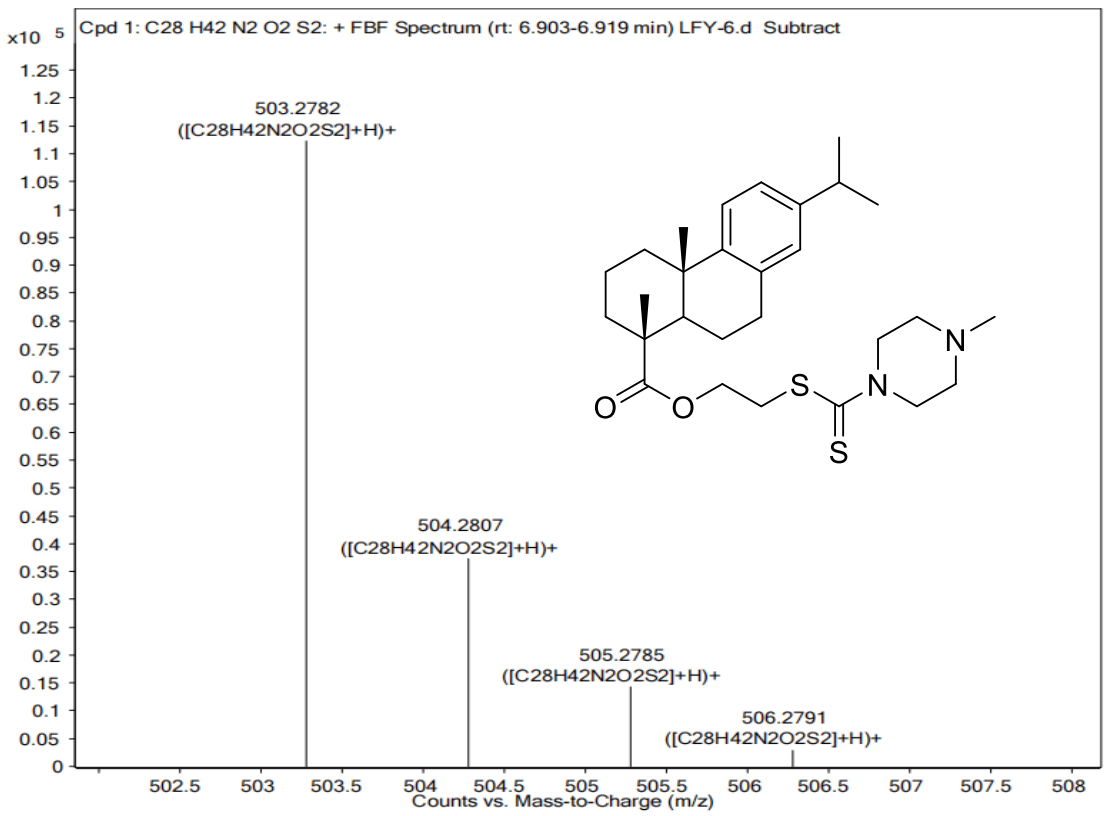

Figure S53. HR-MS spectrum of the target compound III-m.

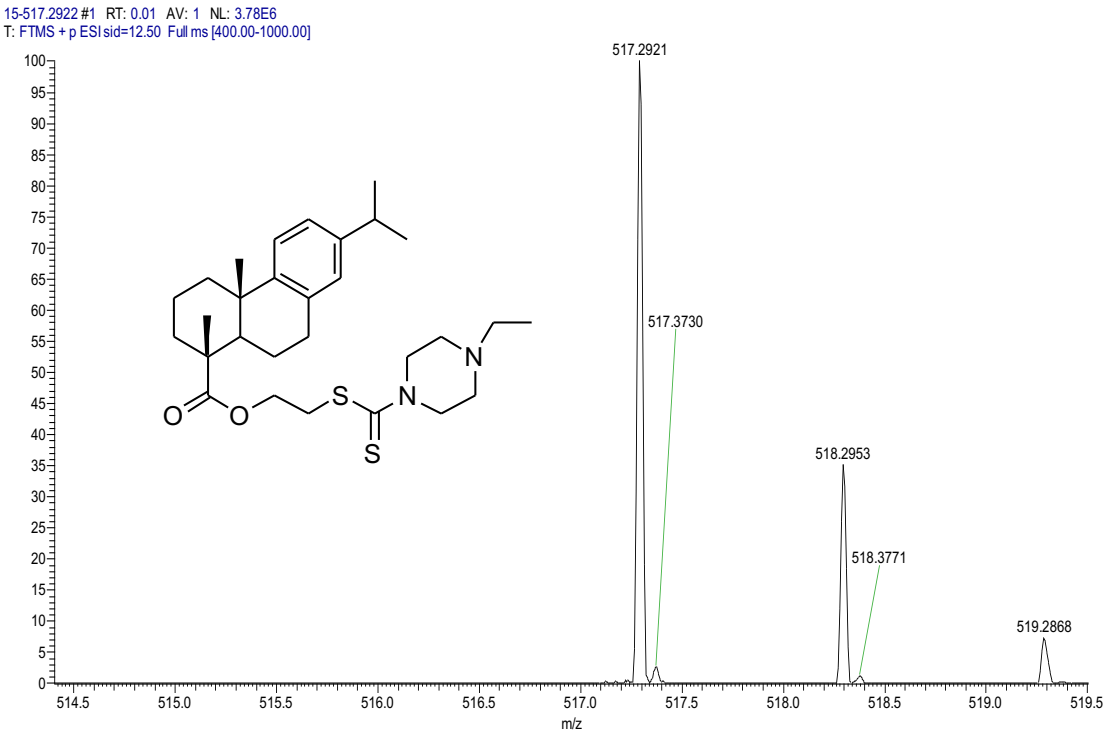

Figure S54. HR-MS spectrum of the target compound III-n.

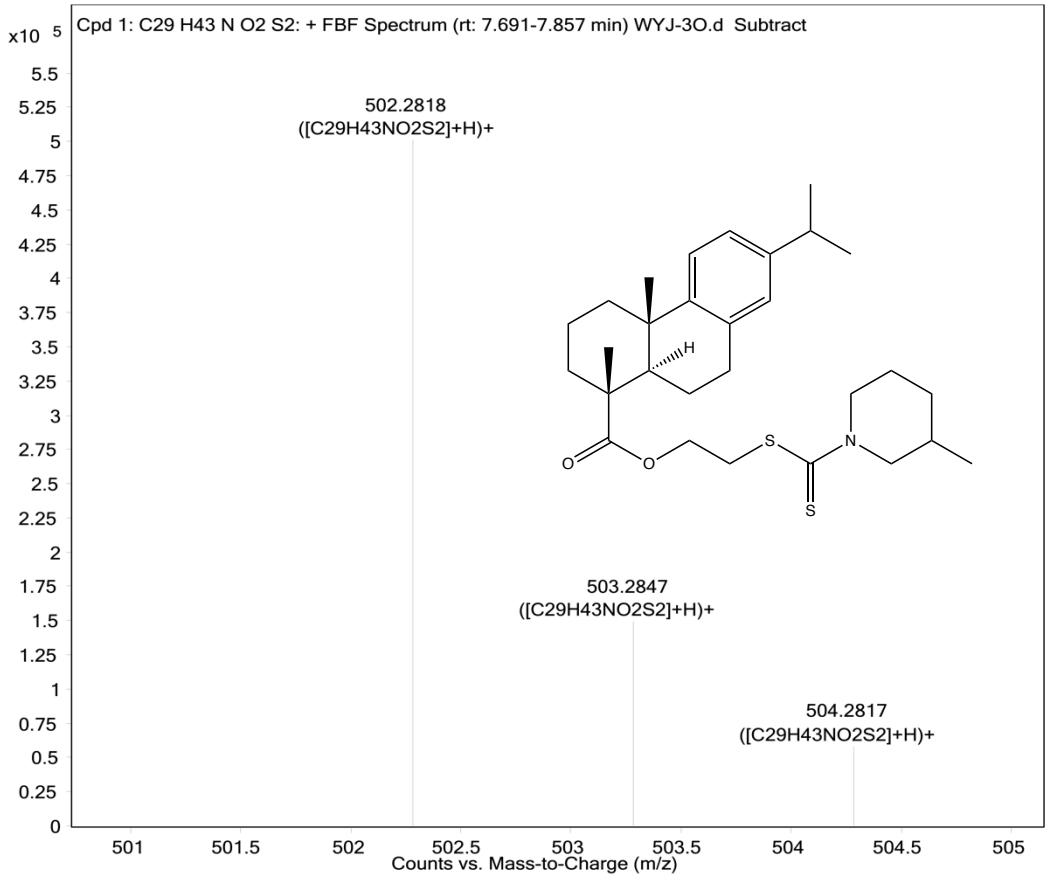

Figure S55. HR-MS spectrum of the target compound III-o.

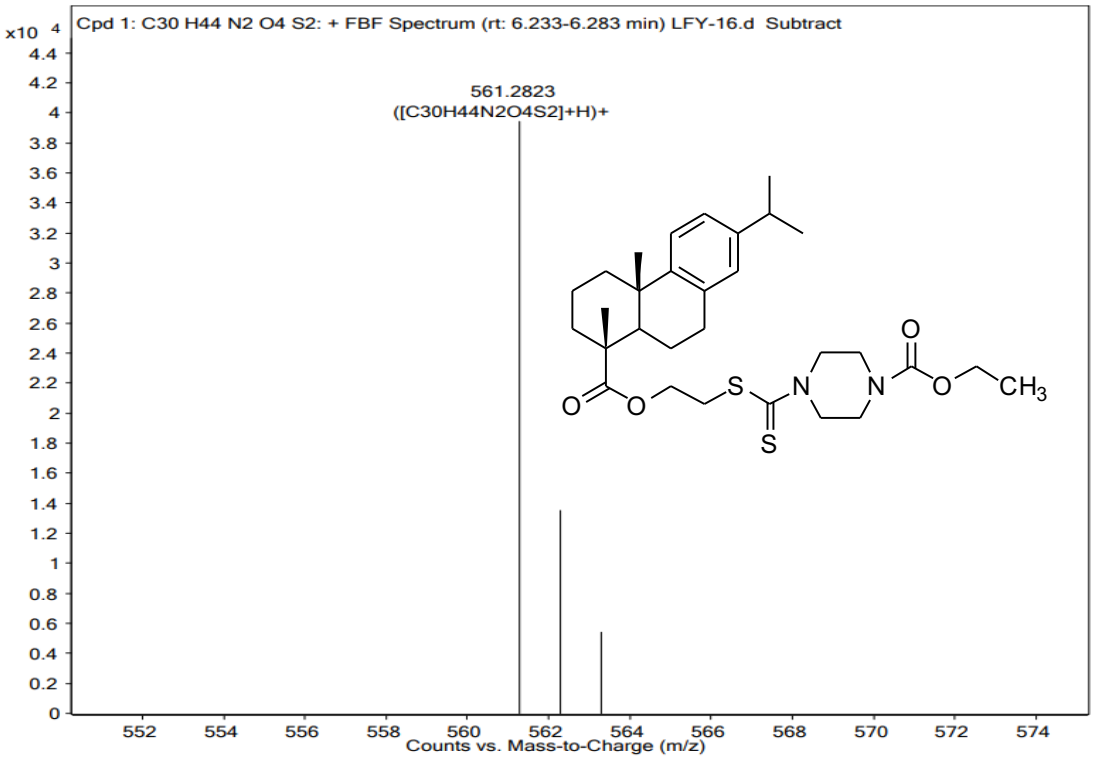

Figure S56. HR-MS spectrum of the target compound III-p.

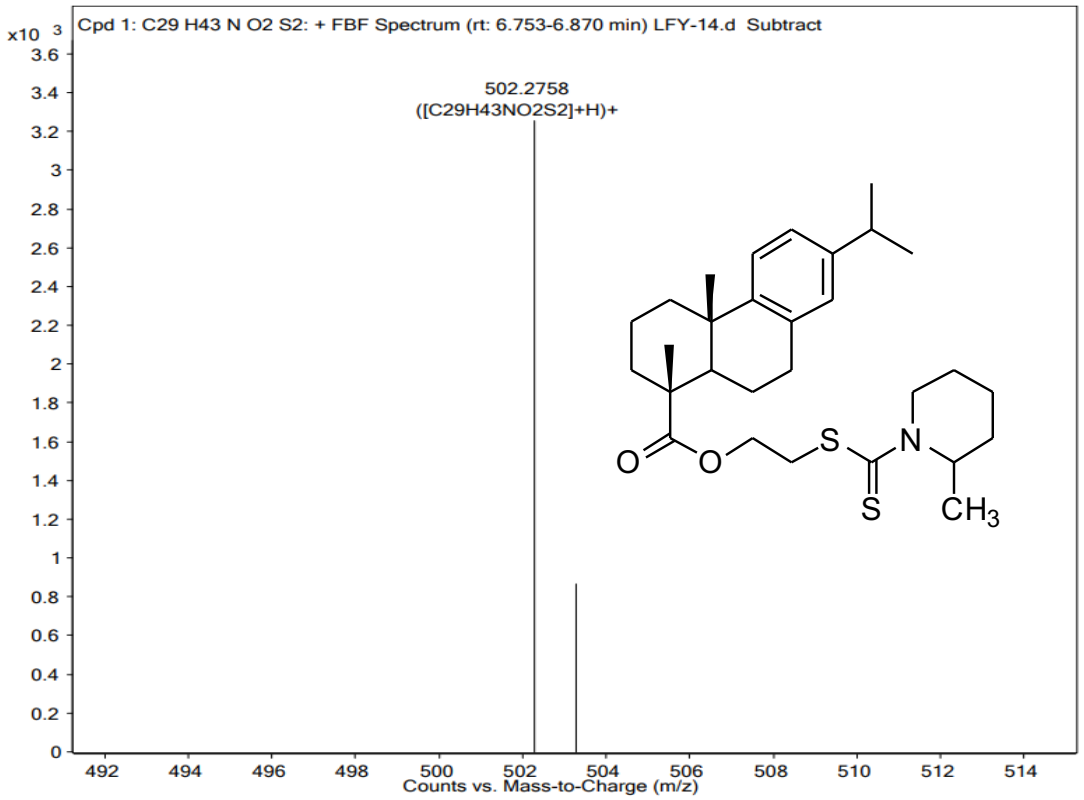

Figure S57. HR-MS spectrum of the target compound III-q.

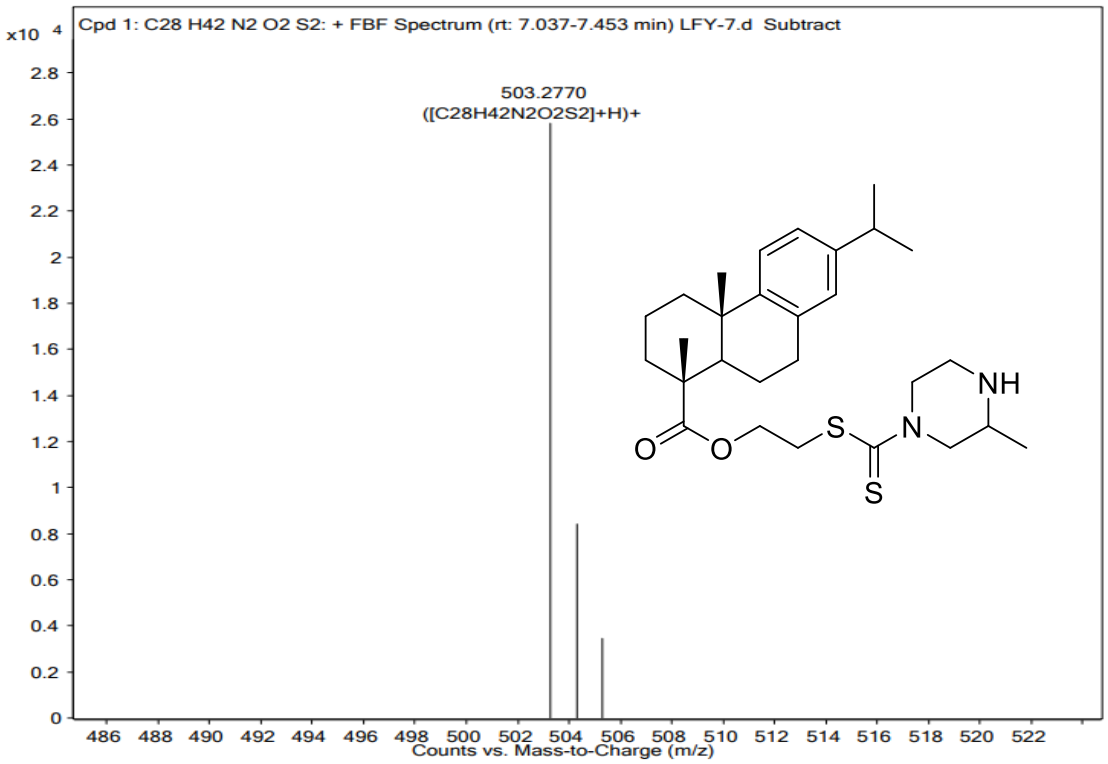

Figure S58. HR-MS spectrum of the target compound III-r.

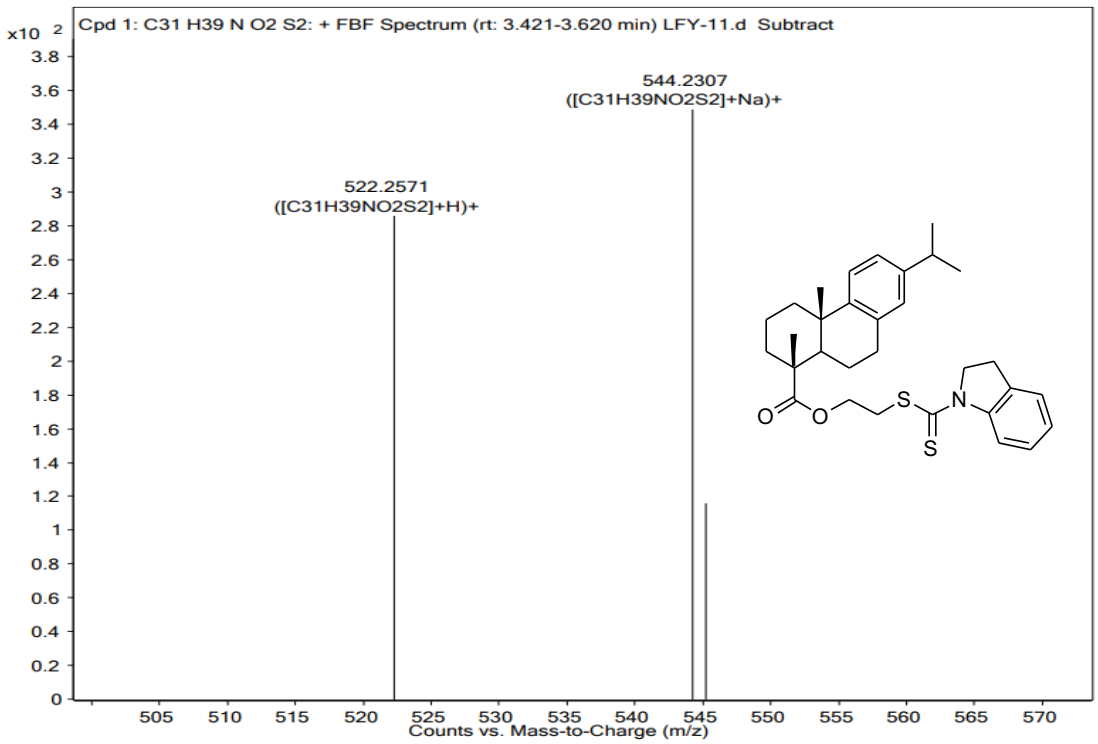

Figure S59. HR-MS spectrum of the target compound III-s.

Compound	Canonical SMILES	Formula	Molecular Weight（≤500）	Rotatable Bonds（≤10）	H-bond acceptors（≤10）	H-bond donors（≤5）	TPSA（A^2）（≤140）	iLOGP（≤5）	ABS
III-a	CC(C)C1=CC=C2C(CCC3C(C)(CCCC23C)C(=O)OCCSC(=S)N2CCC(C)CC2)=C1	$C_{29}H_{43}NO_2S_2$	501.79	8	2	1	86.93	4.53	0.17
III-b	OC1CCN(CC1)C(=S)SCCOC(=O)C1(C)CCCC2(C1CCc1c2ccc(c1)C(C)C)C	$C_{28}H_{41}NO_3S_2$	503.76	8	3	1	107.16	4.77	0.55
III-c	S=C(N1CCN(CC1)C(=O)C)SCCOC(=O)C1(C)CCCC2(C1CCc1c2ccc(c1)C(C)C)C	$C_{29}H_{42}N_2O_3S_2$	530.79	9	3	0	107.24	4.73	0.17
III-e	OC1CCCN(C1)C(=S)SCCOC(=O)C1(C)CCCC2(C1CCc1c2ccc(c1)C(C)C)C	$C_{28}H_{41}NO_3S_2$	503.76	8	3	1	107.16	4.94	0.17

III-h	OCCN1CCN(CC1)C(=S)SCCOC(=O)C1(C)CCCC2(C1CCc1c2ccc(c1)C(C)C)C	$C_{29}H_{44}N_2O_3S_2$	532.80	10	4	1	110.40	5.29	0.55
III-i	OCC1CCN(CC1)C(=S)SCCOC(=O)C1(C)CCCC2(C1CCc1c2ccc(c1)C(C)C)C	$C_{29}H_{43}NO_3S_2$	517.79	9	3	1	107.16	4.98	0.17
III-j	OCCC1CCN(CC1)C(=S)SCCOC(=O)C1(C)CCCC2(C1CCc1c2ccc(c1)C(C)C)C	$C_{30}H_{45}NO_3S_2$	531.81	10	3	1	107.16	4.98	0.17
III-k	OCCC1CCCCN1C(=S)SCCOC(=O)C1(C)CCCC2(C1CCc1c2ccc(c1)C(C)C)C	$C_{30}H_{45}NO_3S_2$	531.81	10	3	1	107.16	4.75	0.17

Table S1. Evaluation data of drug properties of target compounds.