

Supplementary Information

**Design, synthesis, and evaluation of novel
coumarin-dithiocarbamate derivatives (IDs) as
anti-colorectal cancer agents**

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Corresponding authors:

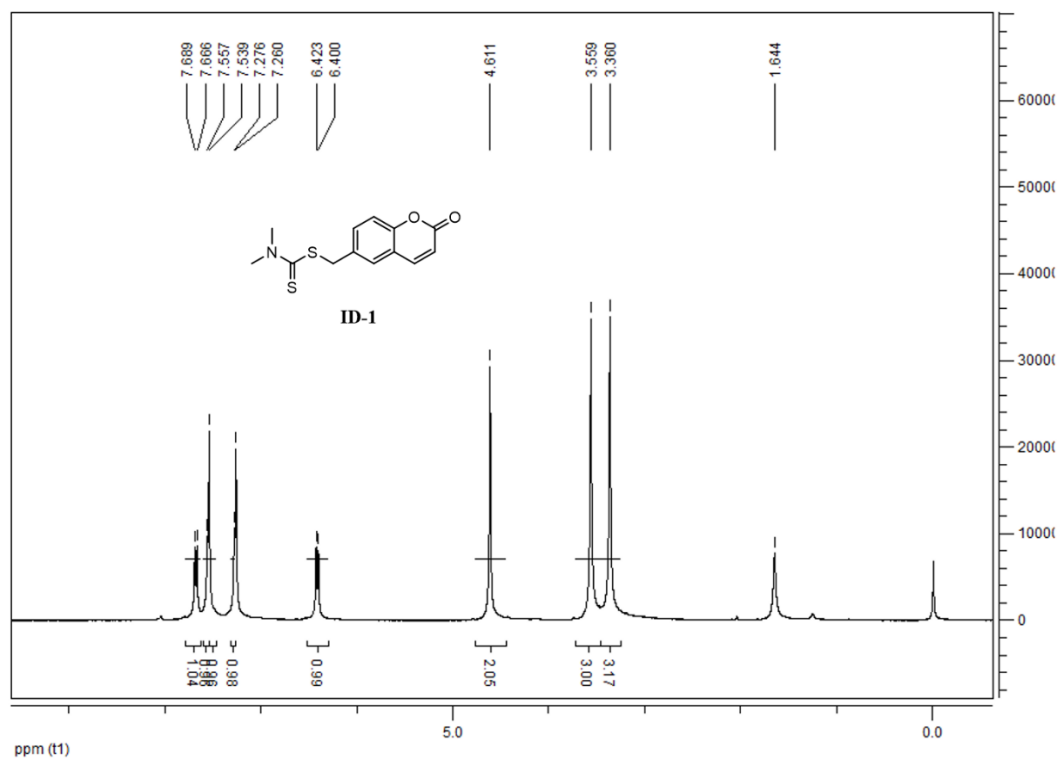
E-mail address: panyuanjiang@zju.edu.cn (YJ. Pan)

E-mail address: jinhc@zju.edu.cn (HC. Jin)

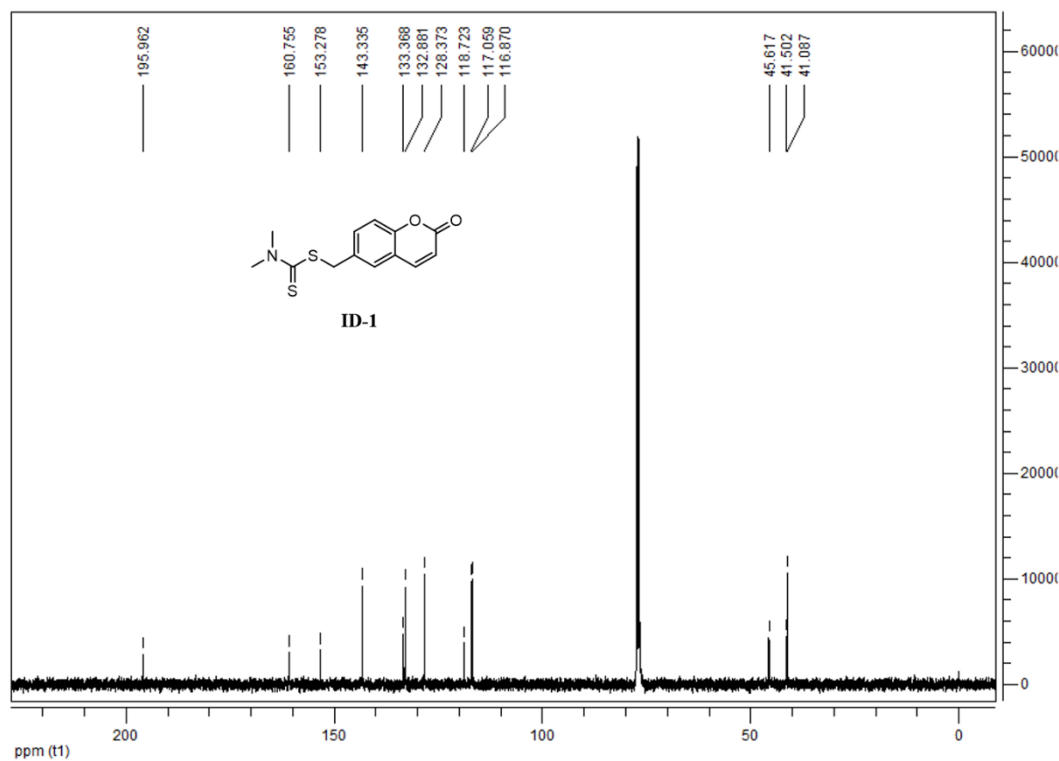
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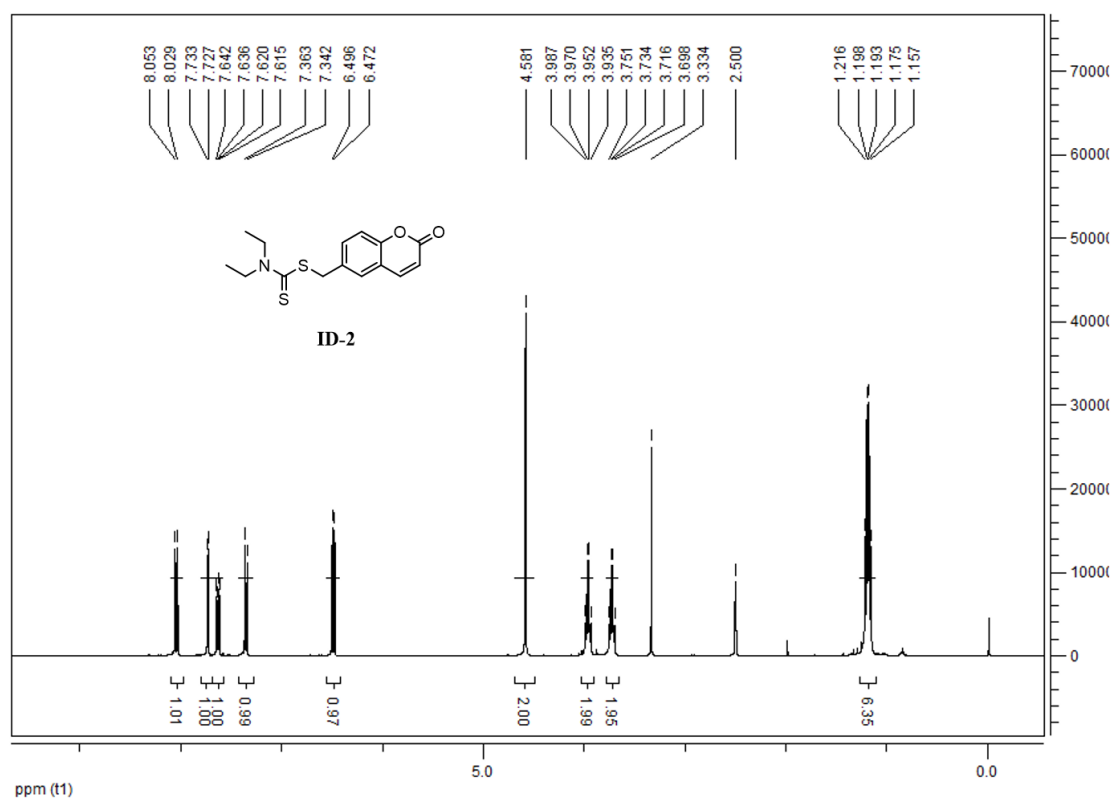
¹H NMR, CDCl₃ (Bruker AVANCE III 400) (ID-1)



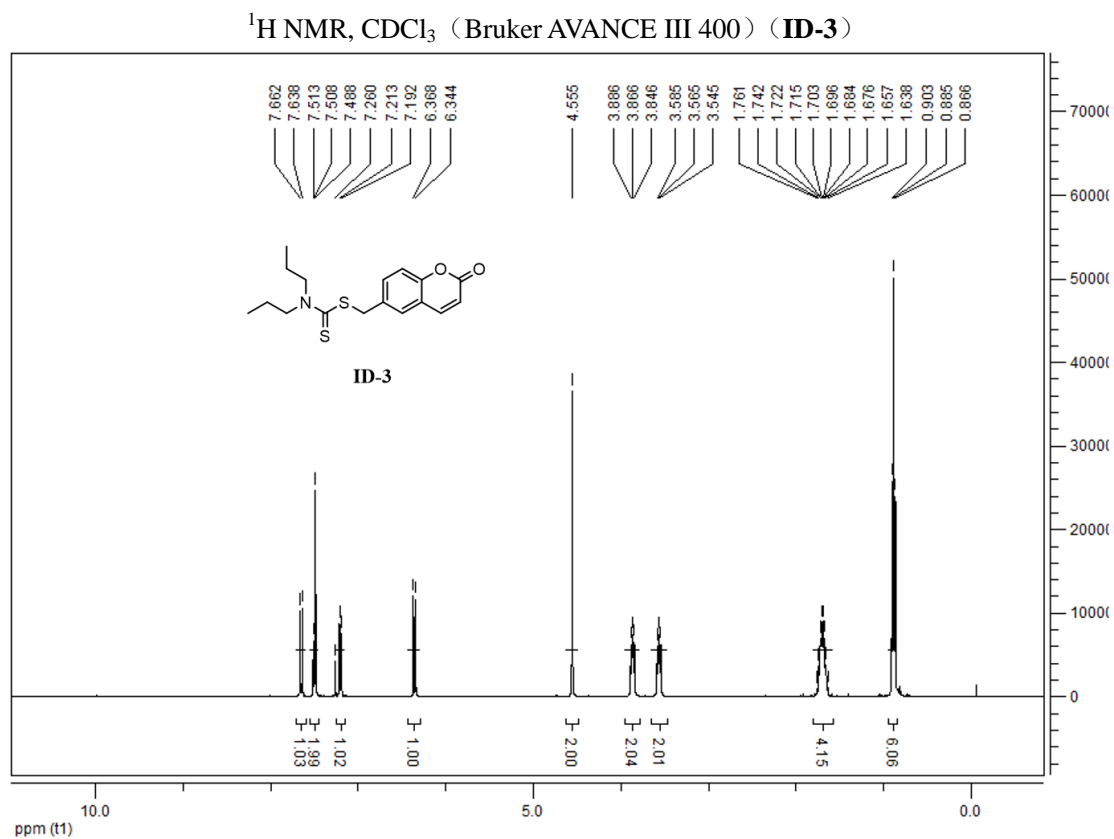
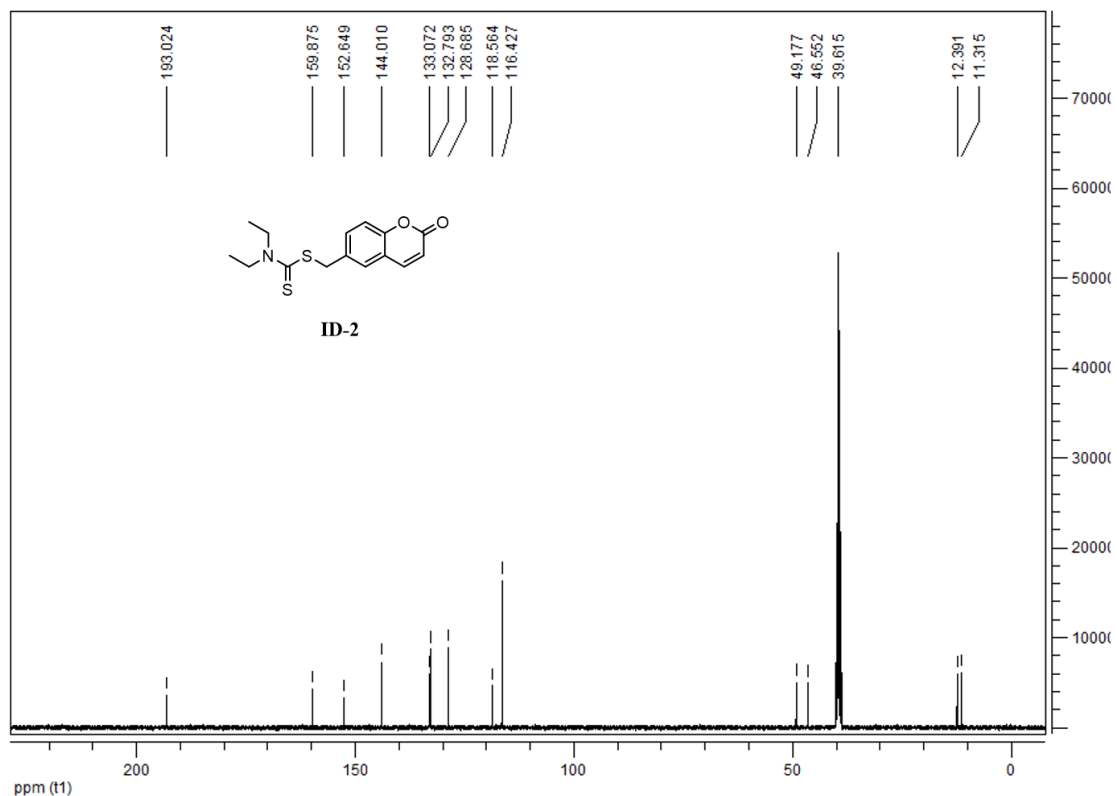
¹³C NMR, CDCl₃ (Bruker AVANCE III 400) (ID-1)



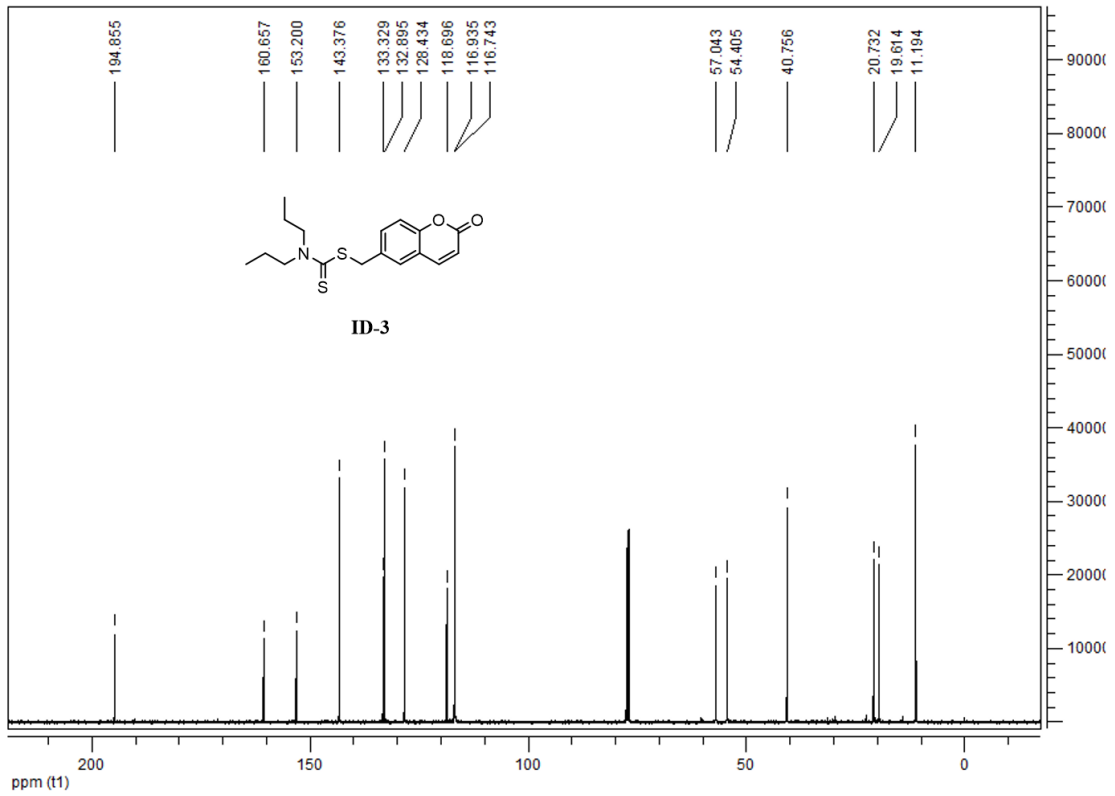
^1H NMR, DMSO- d_6 (Bruker AVANCE III 400) (**ID-2**)



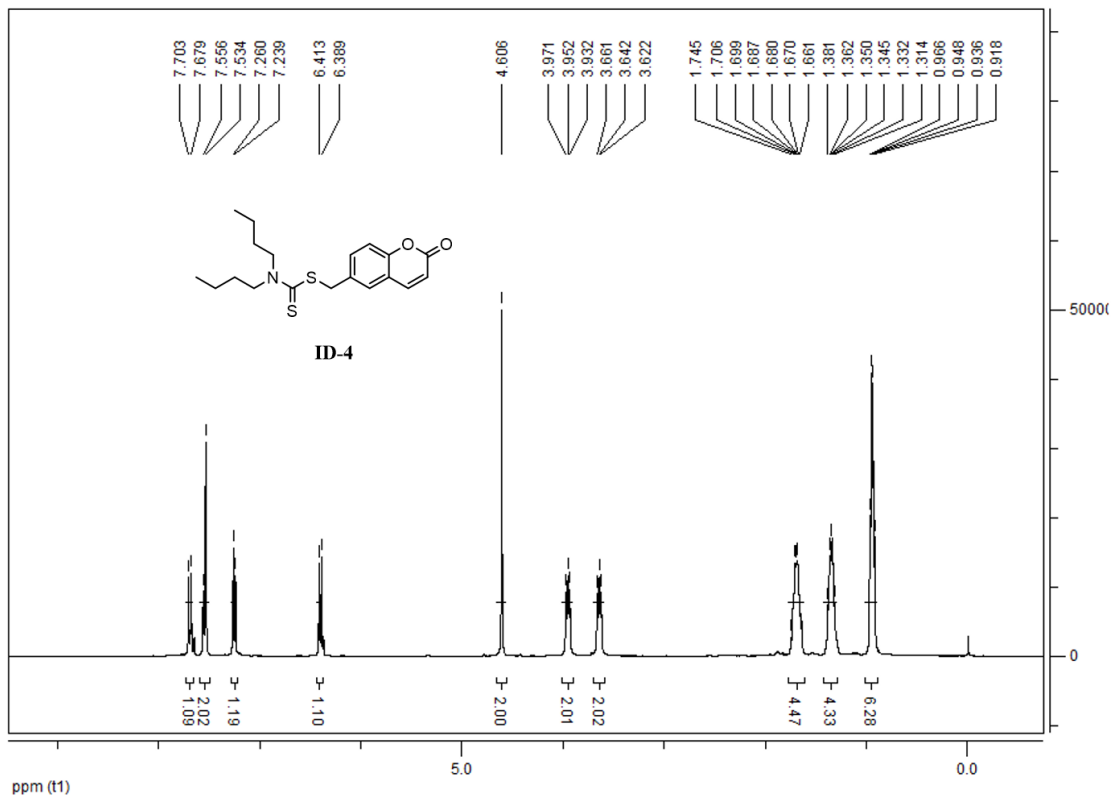
^{13}C NMR, DMSO- d_6 (Bruker AVANCE III 400) (**ID-2**)



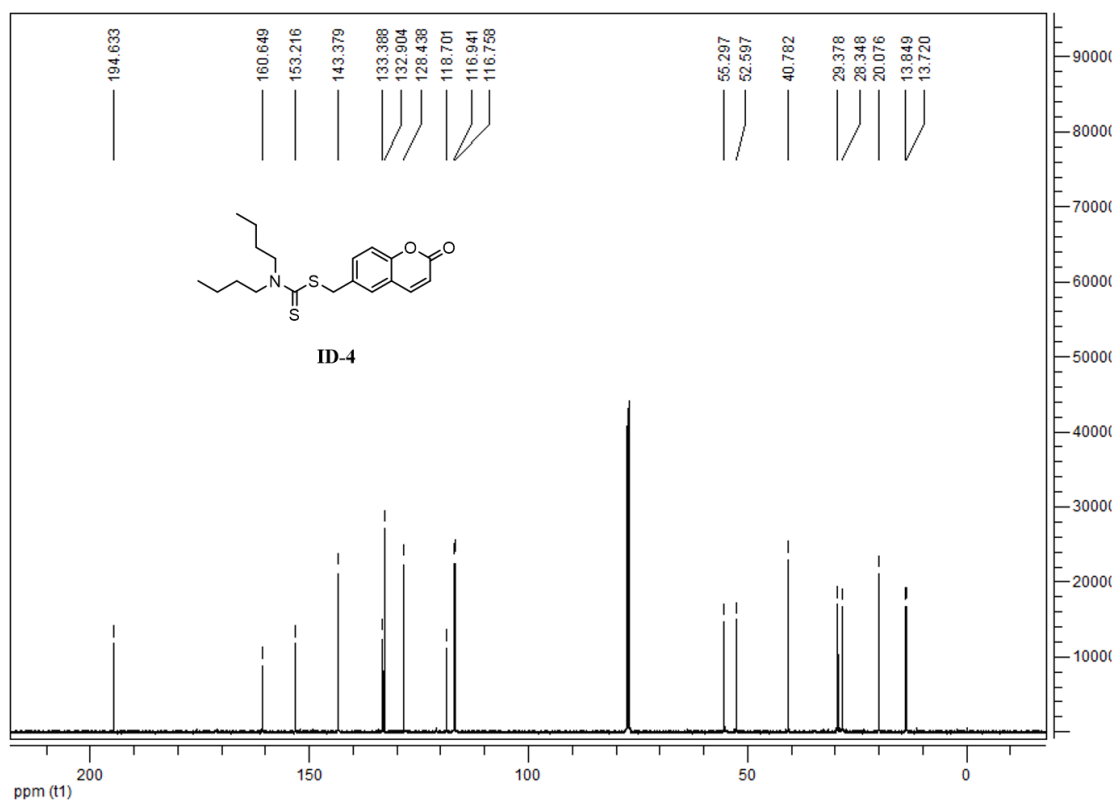
13C NMR, CDCl₃ (Bruker AVANCE III 400) (ID-3)



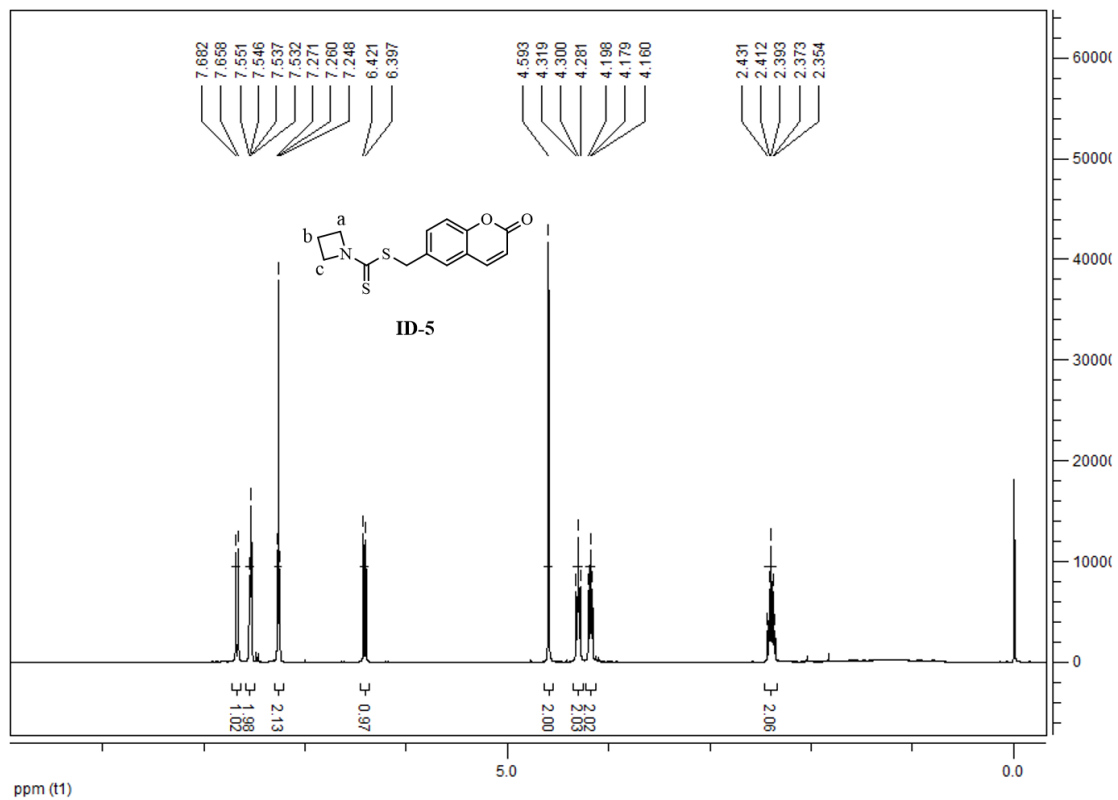
¹H NMR, CDCl₃ (Bruker AVANCE III 400) (**ID-4**)



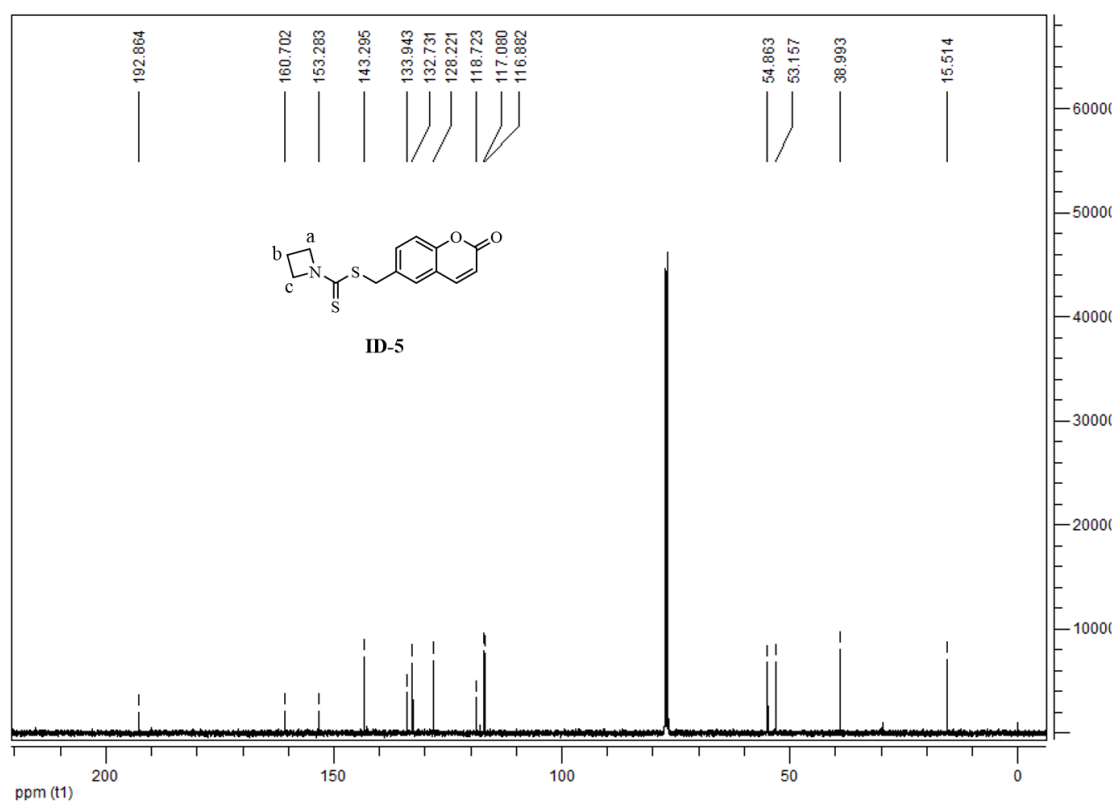
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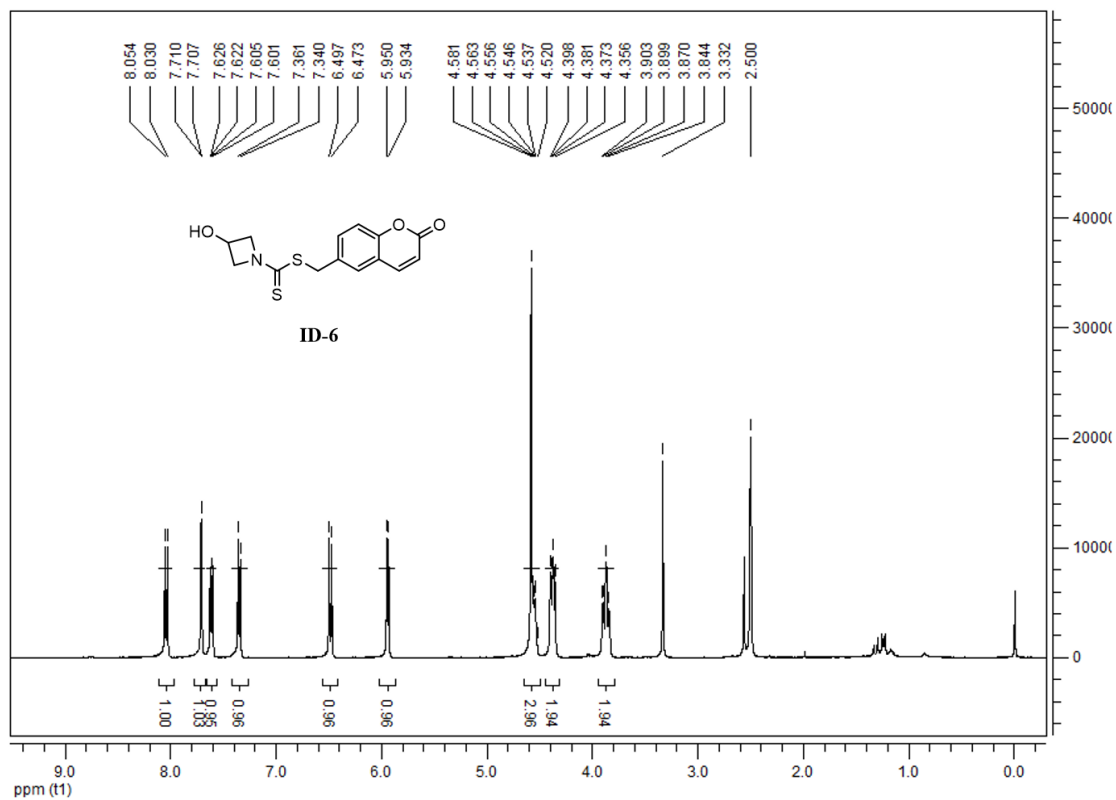
¹H NMR, CDCl₃ (Bruker AVANCE III 400) (ID-5)



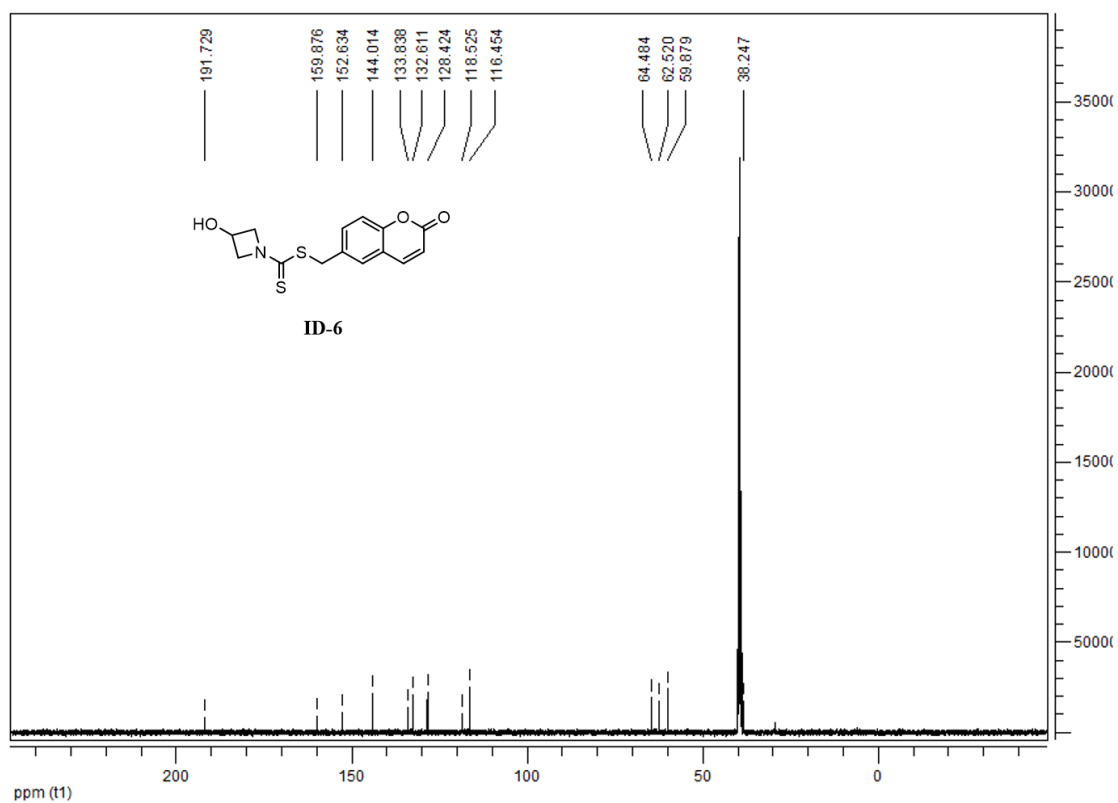
^{13}C NMR, CDCl_3 (Bruker AVANCE III 400) (**ID-5**)



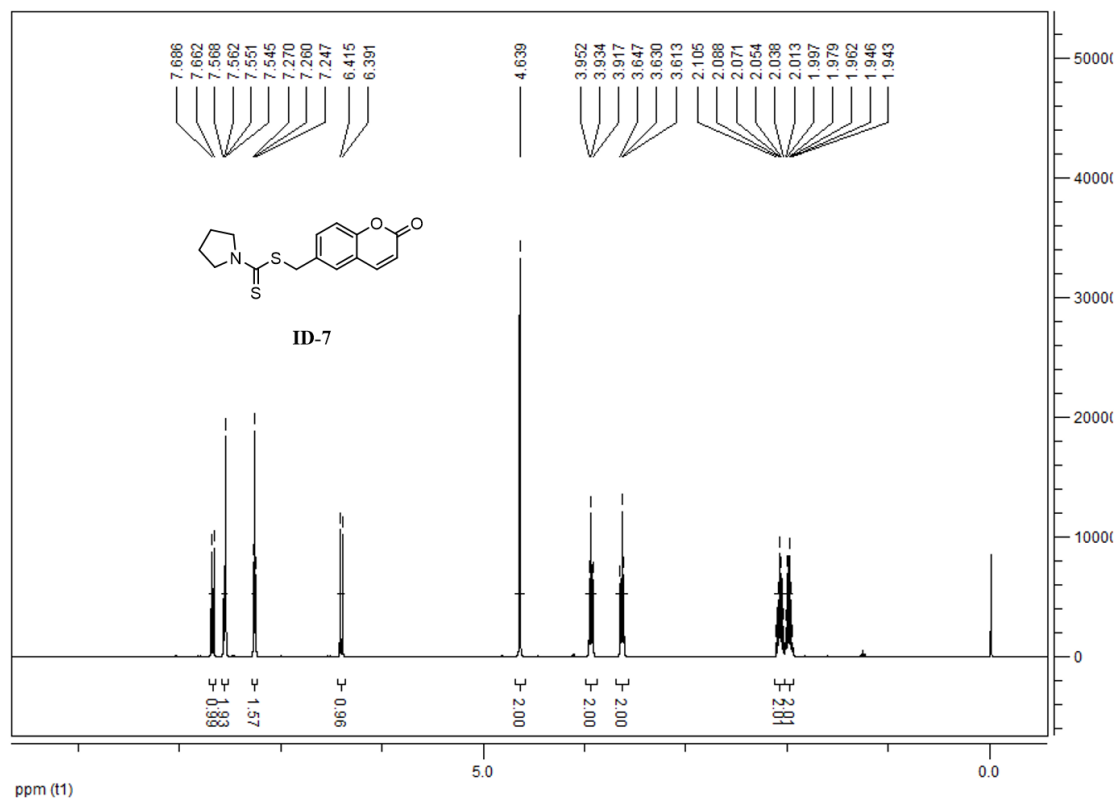
^1H NMR, $\text{DMSO}-d_6$ (Bruker AVANCE III 400) (**ID-6**)



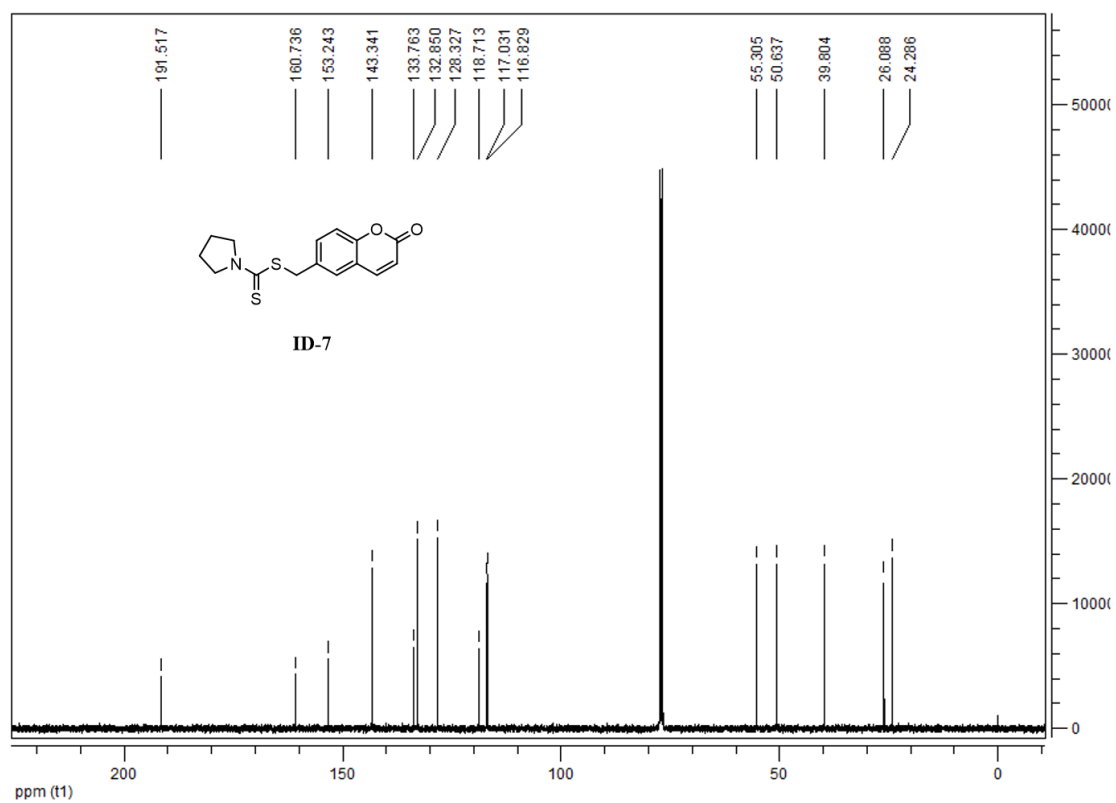
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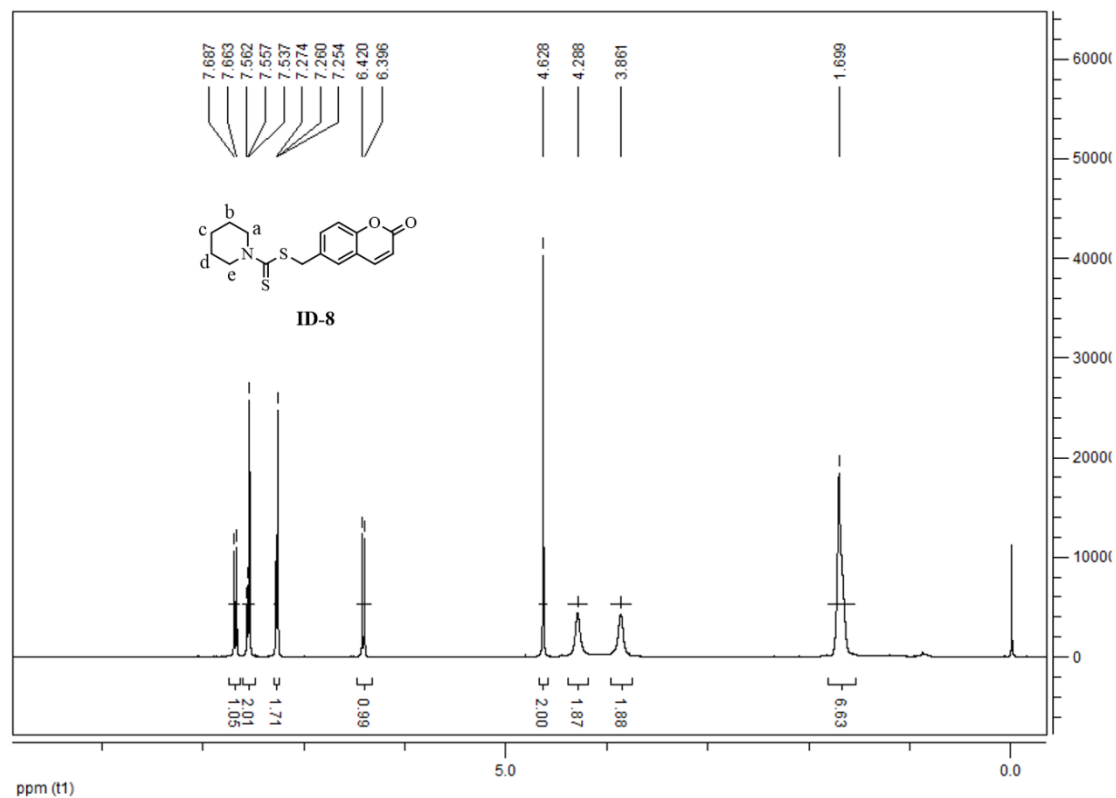
^1H NMR, CDCl_3 (Bruker AVANCE III 400) (**ID-7**)



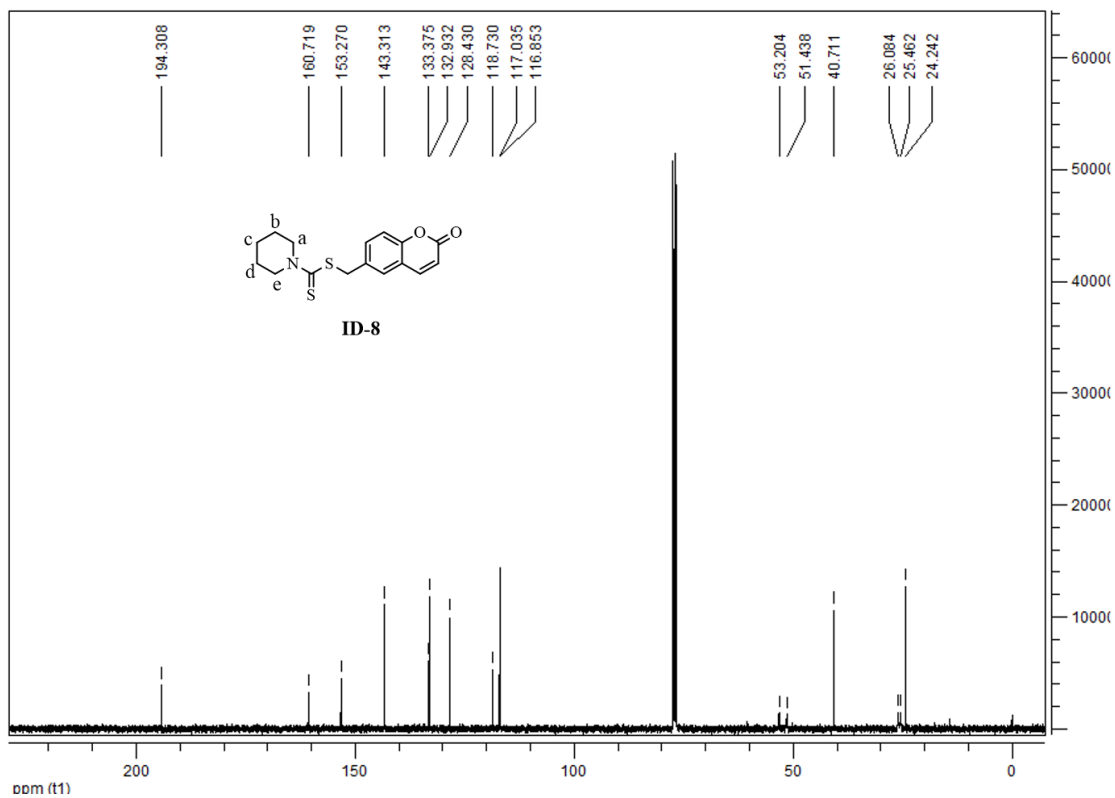
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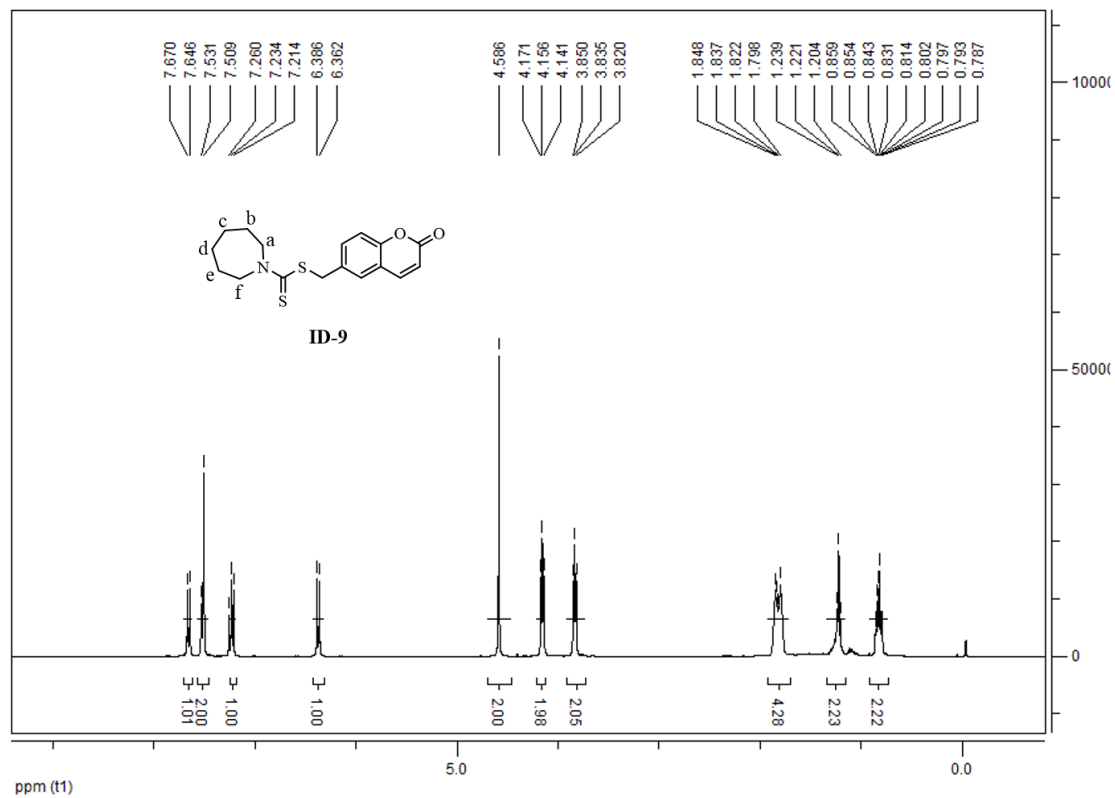
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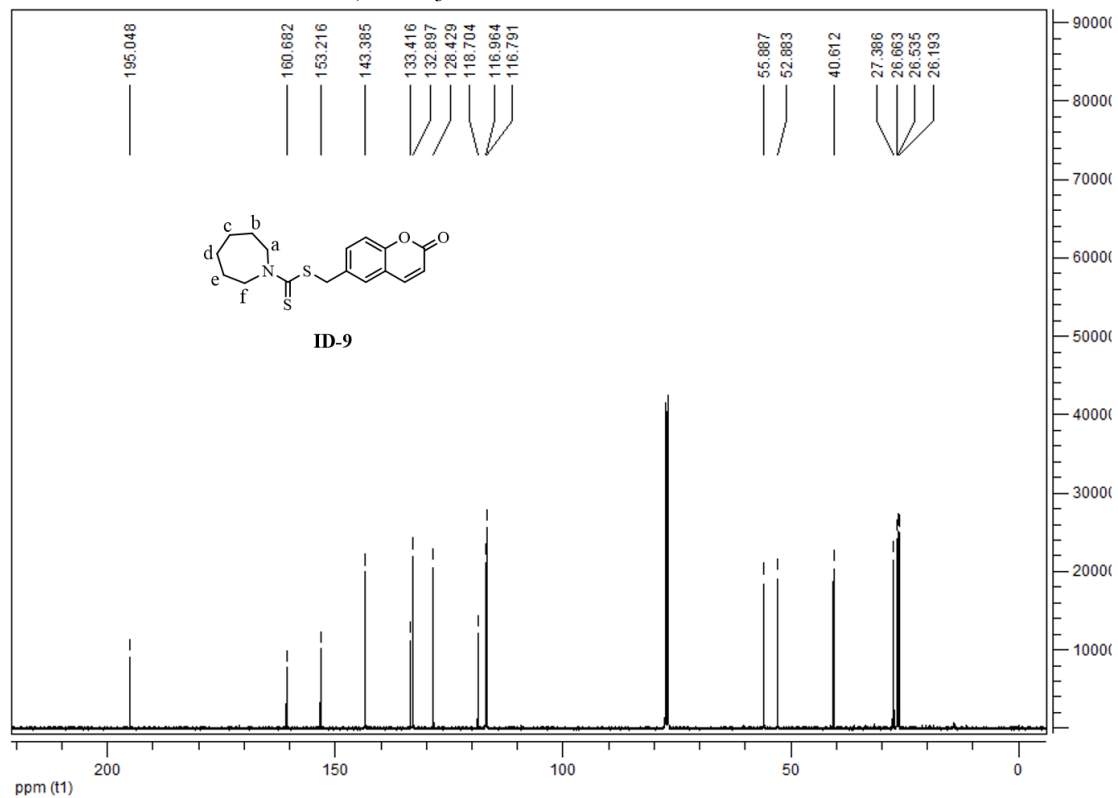
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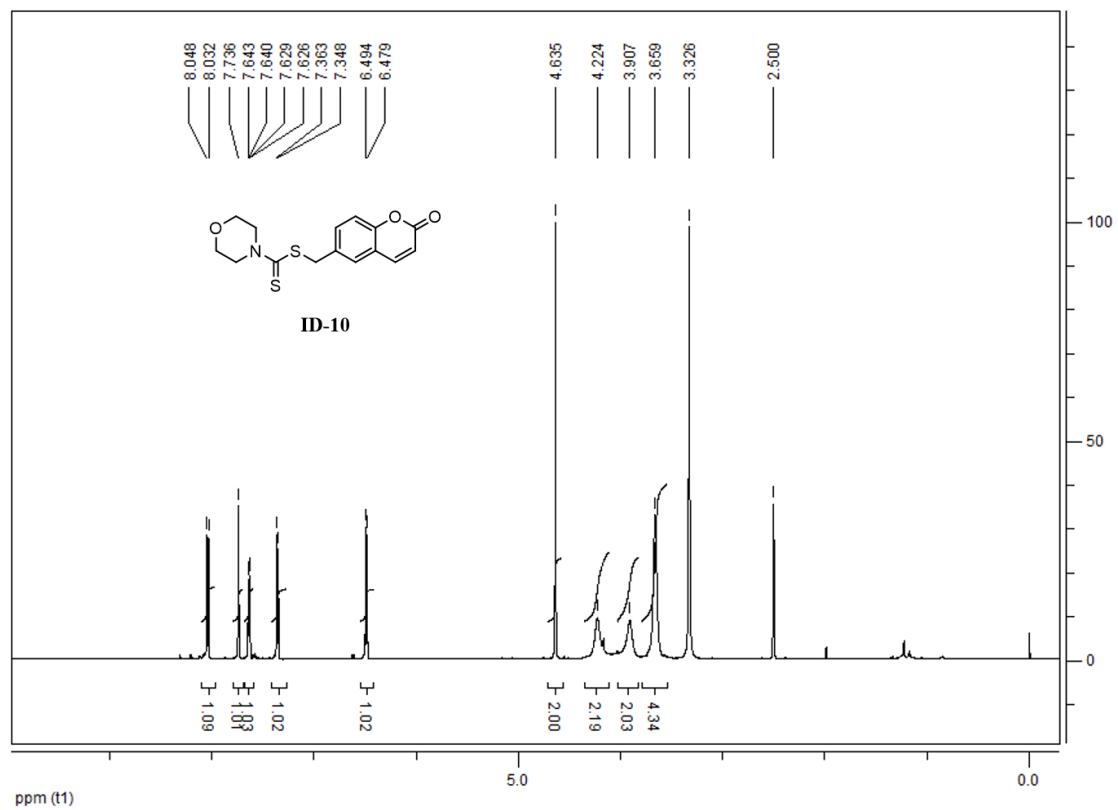
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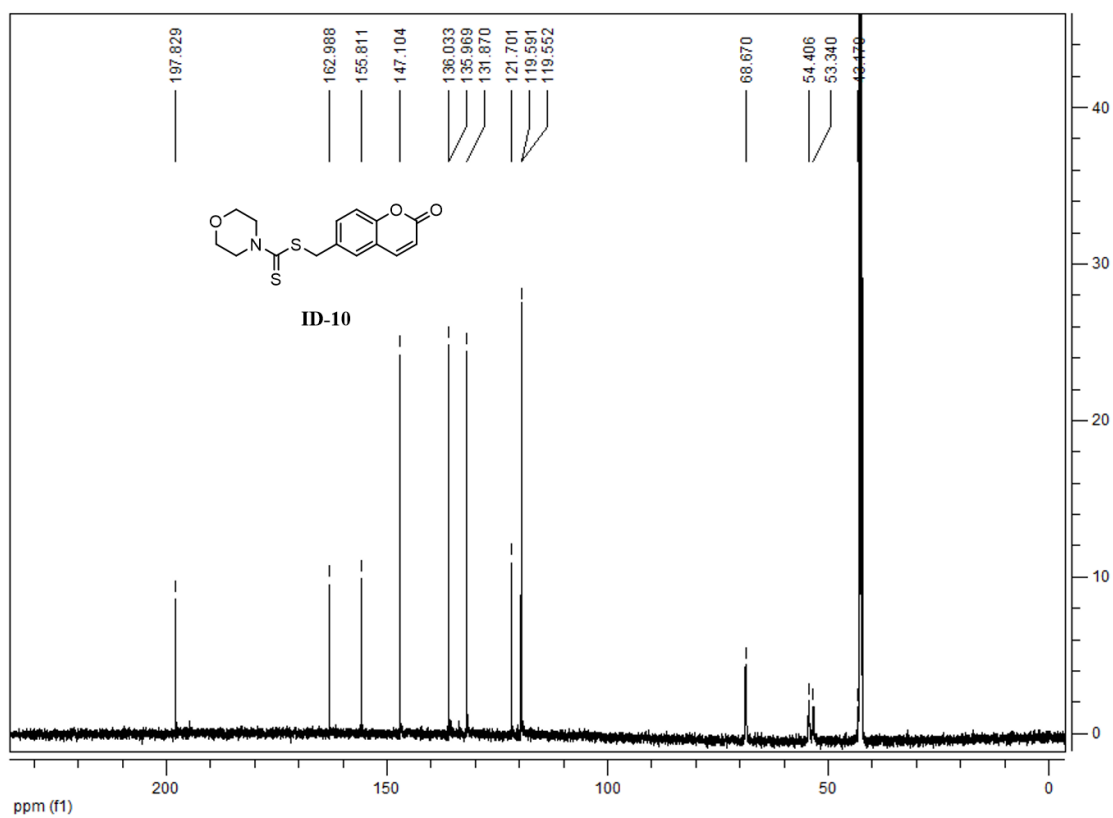
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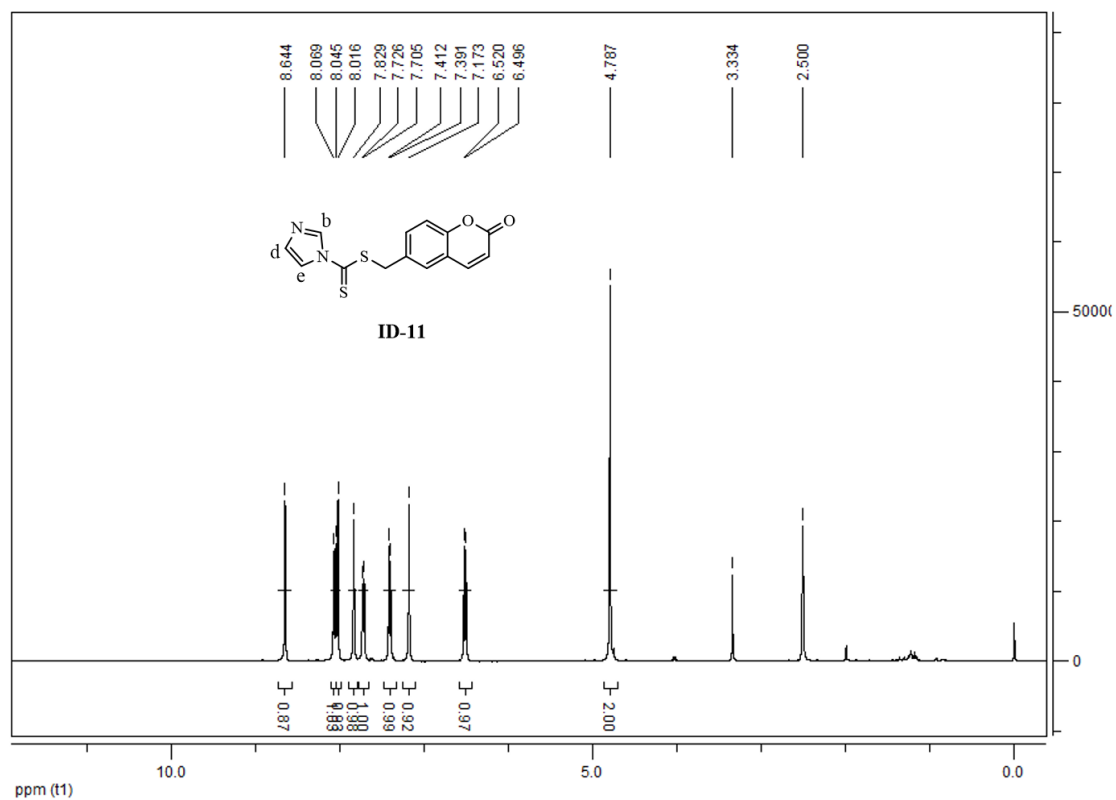
¹H NMR, DMSO-d₆ (Bruker AVANCE III 600) (ID-10)



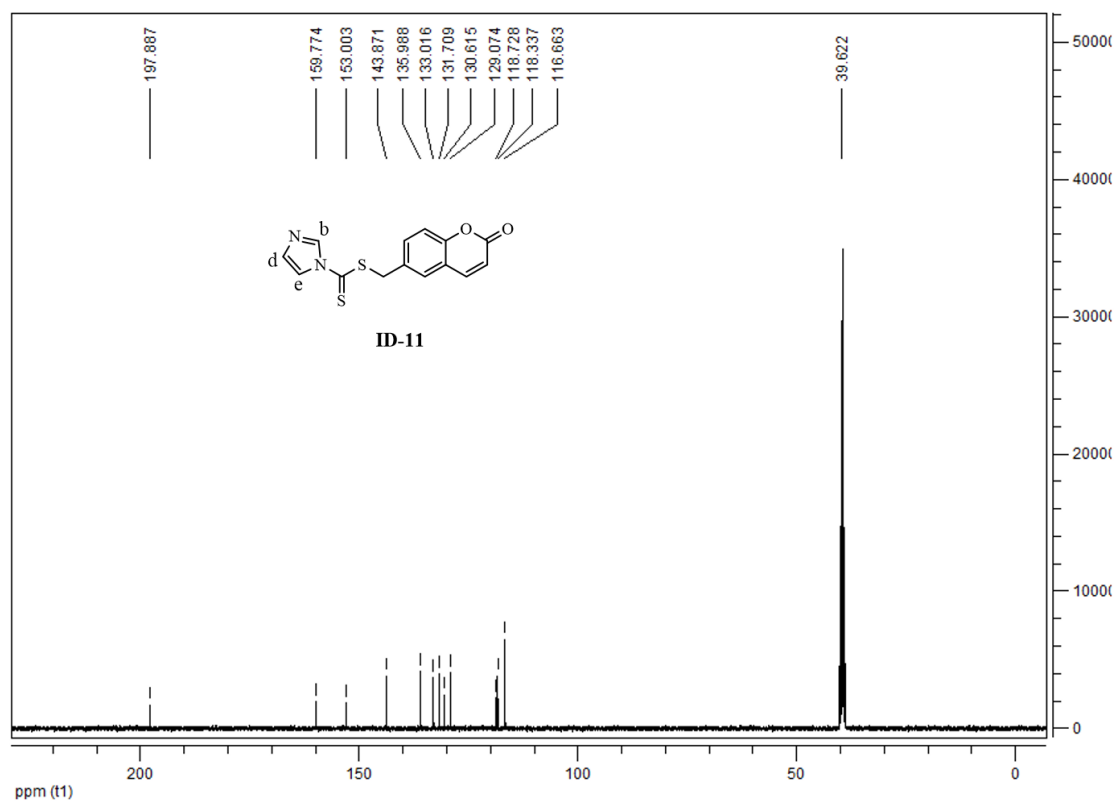
^{13}C NMR, DMSO- d_6 (Bruker AVANCE III 600) (ID-10)



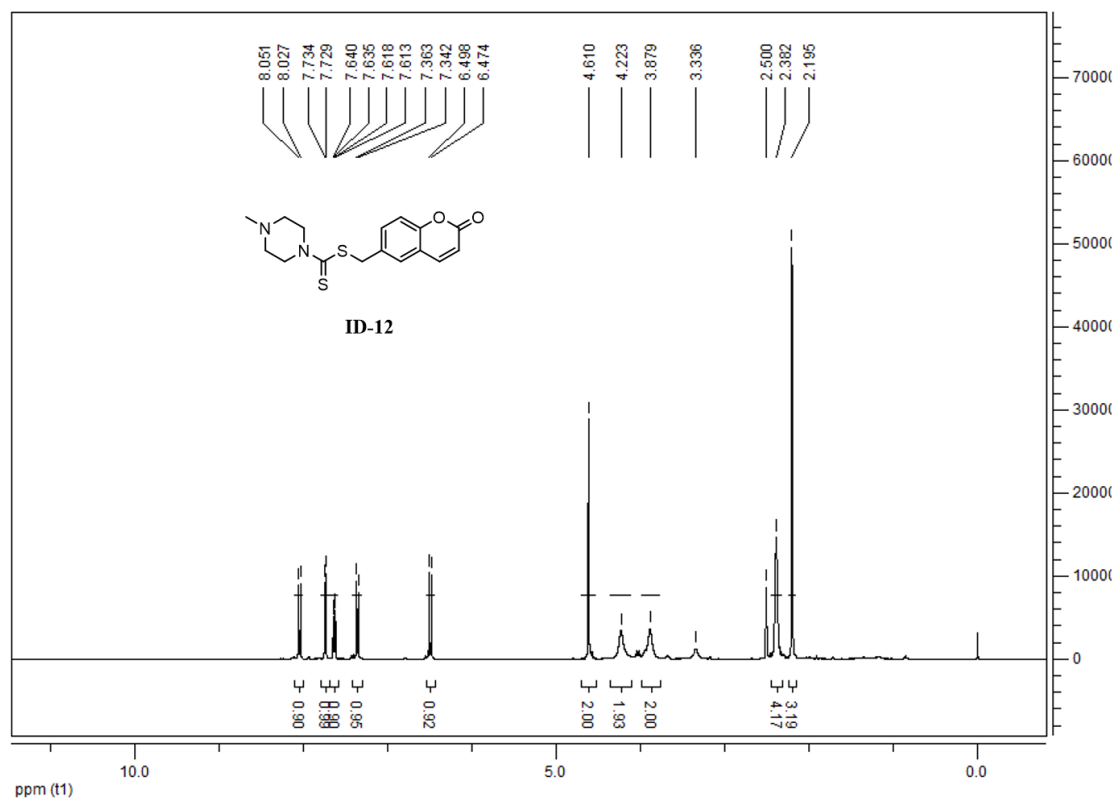
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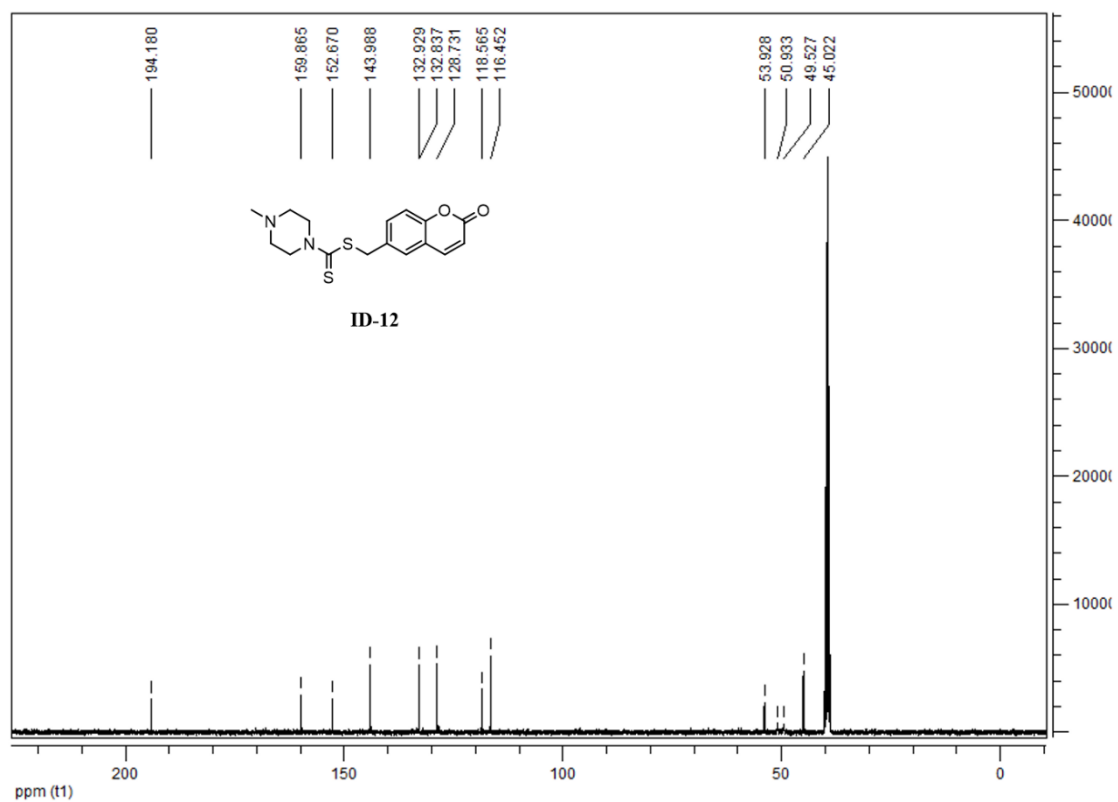
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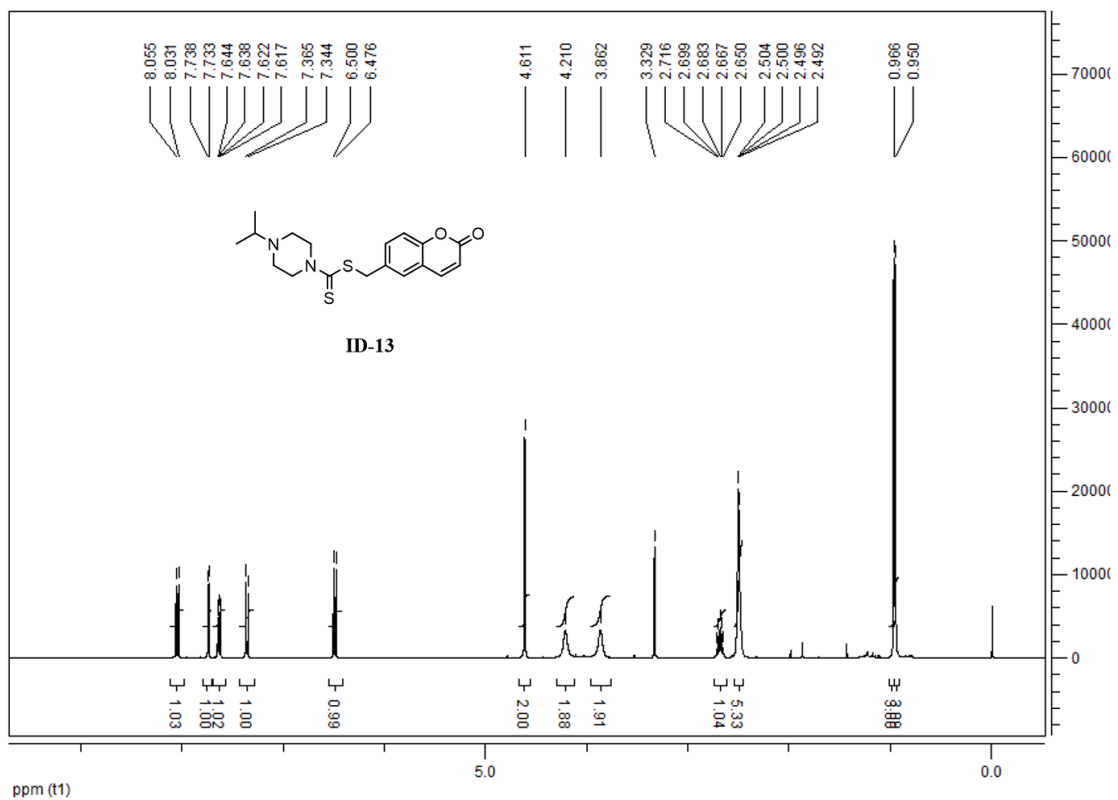
^1H NMR, DMSO- d_6 (Bruker AVANCE III 400) (ID-12)



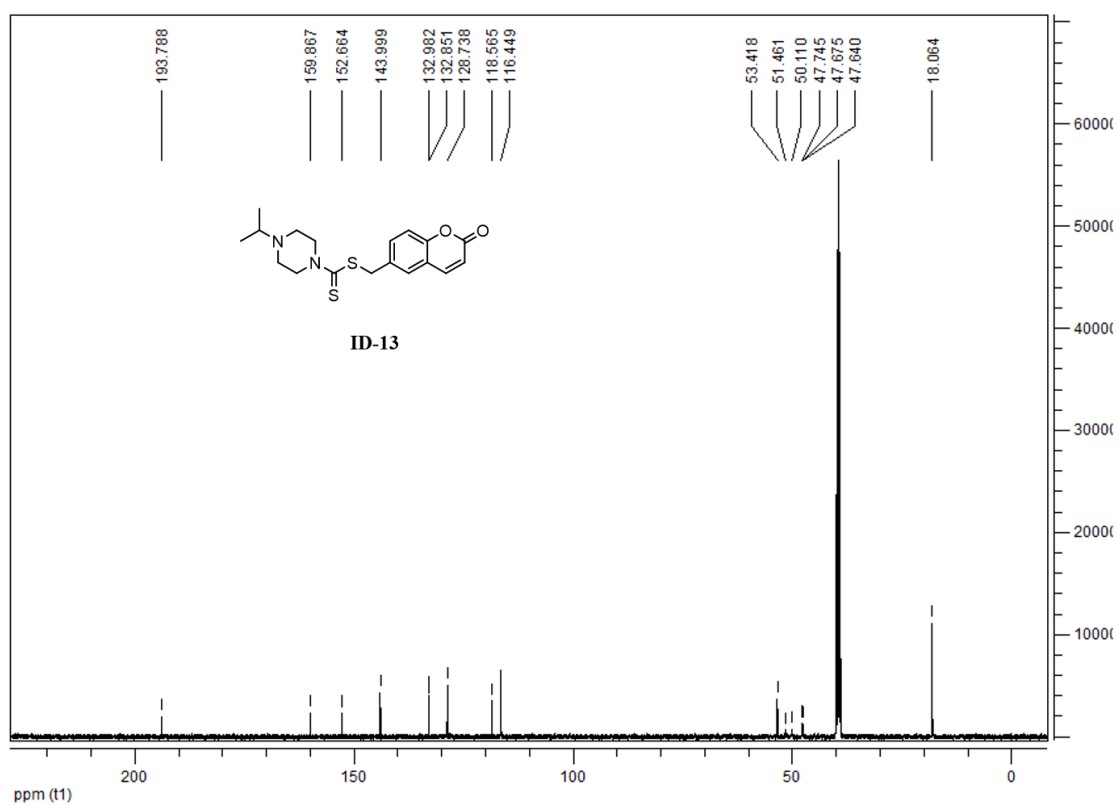
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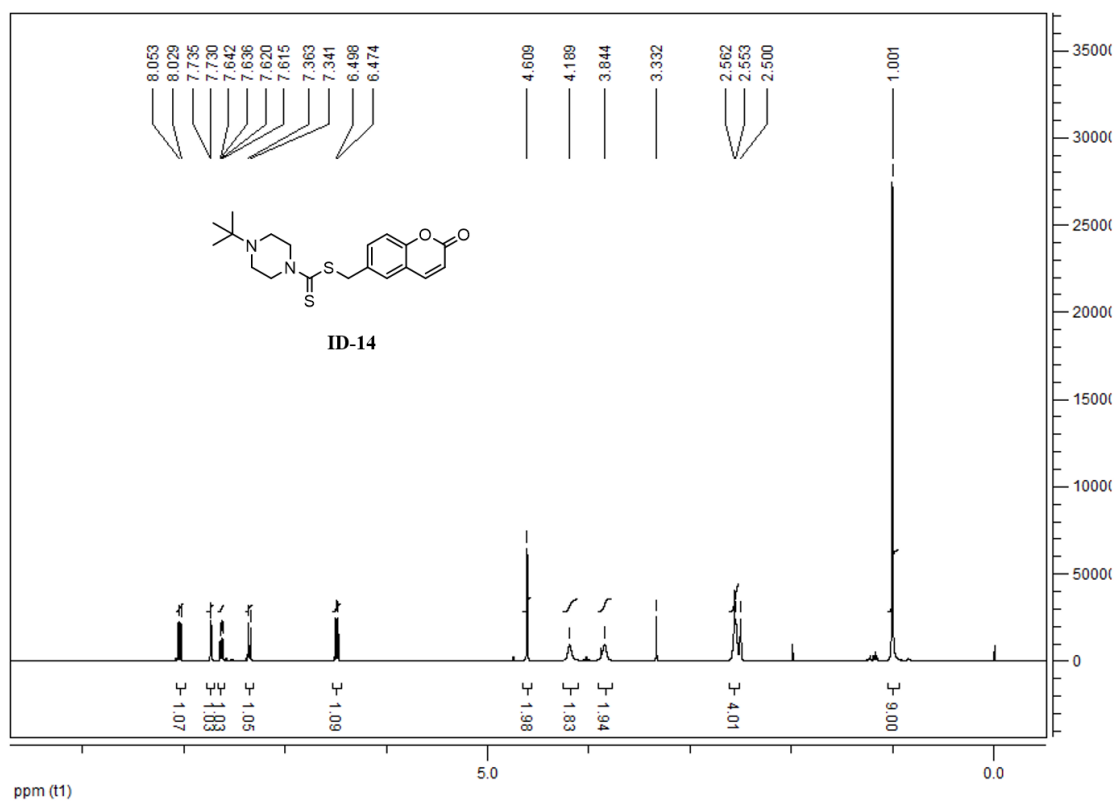
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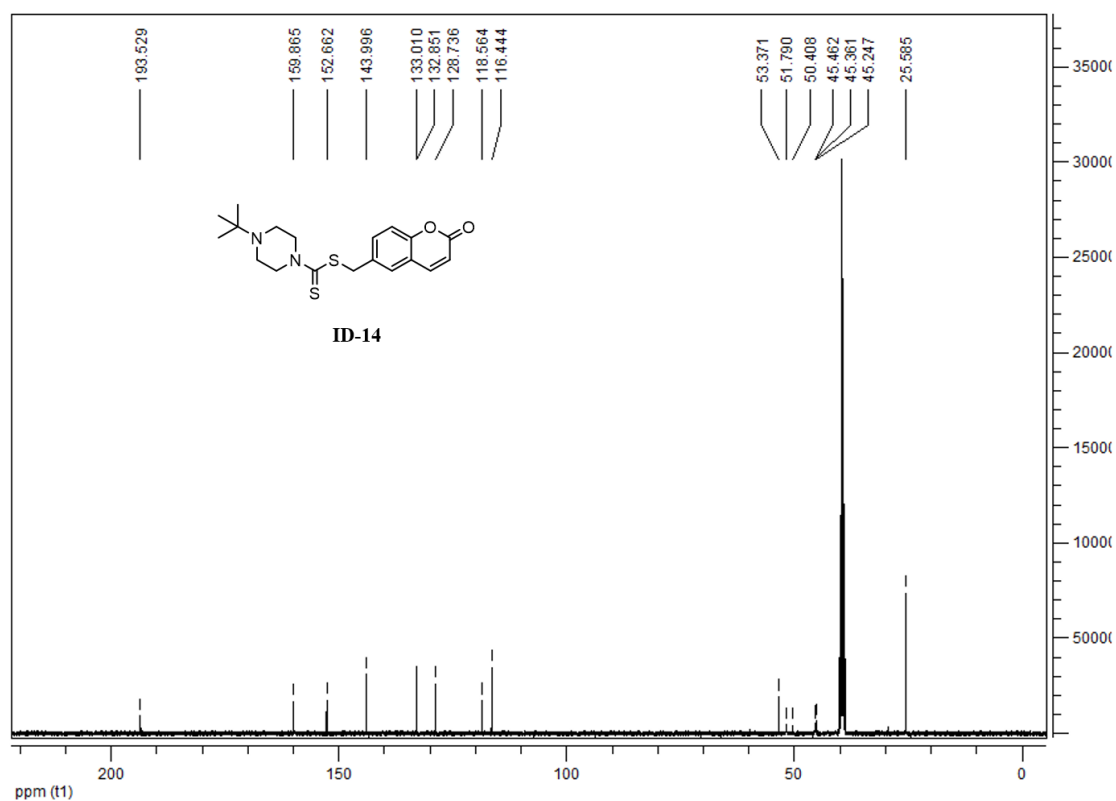
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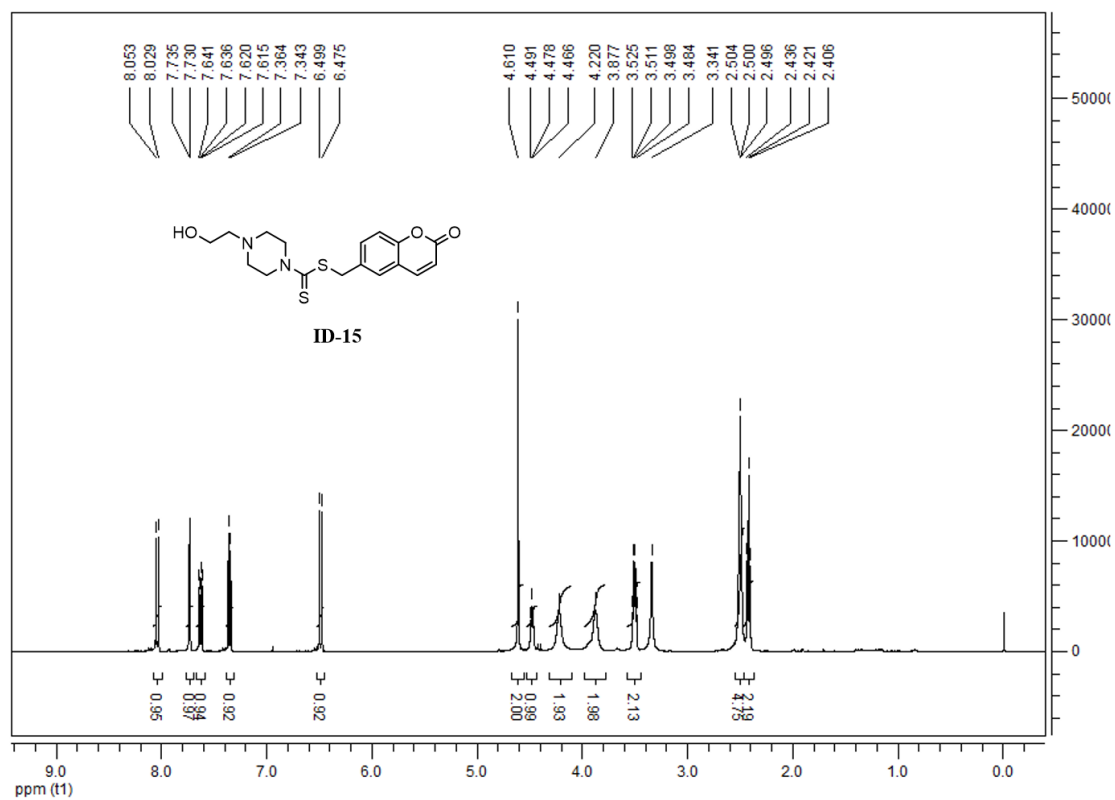
¹H NMR, DMSO-d₆ (Bruker AVANCE III 400) (ID-14)



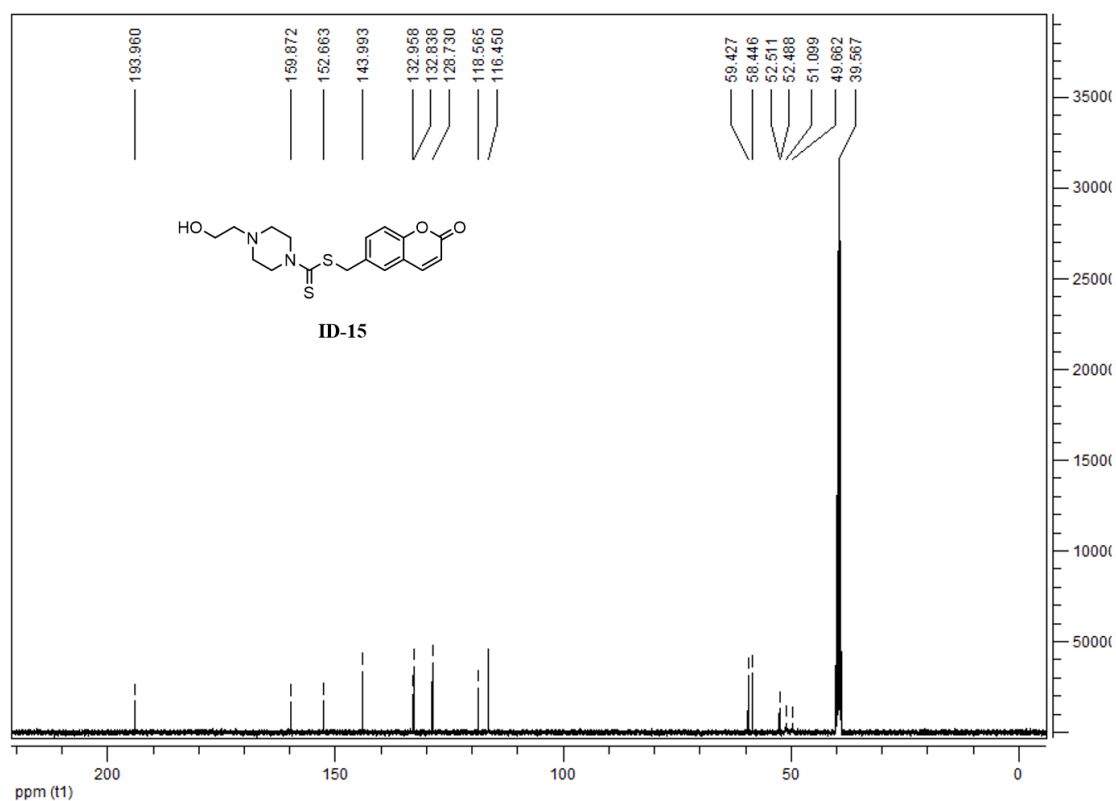
¹³C NMR, DMSO-*d*₆ (Bruker AVANCE III 400) (ID-14)



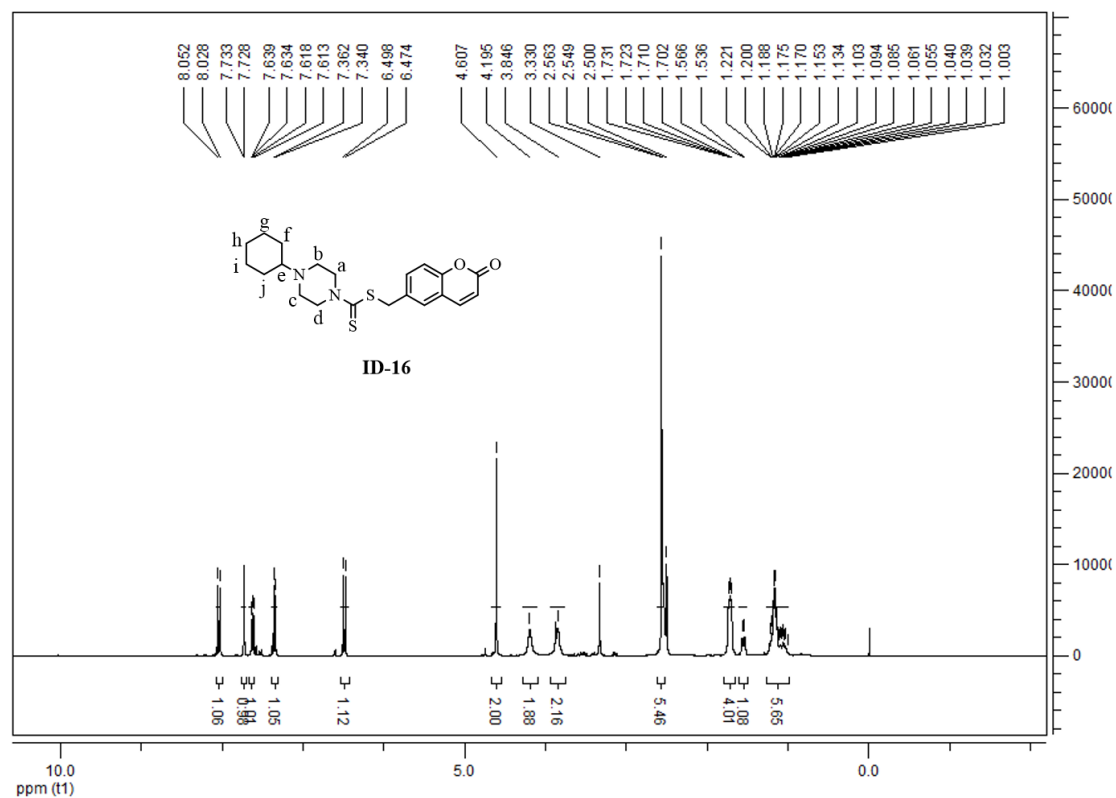
¹H NMR, DMSO-*d*₆ (Bruker AVANCE III 400) (ID-15)



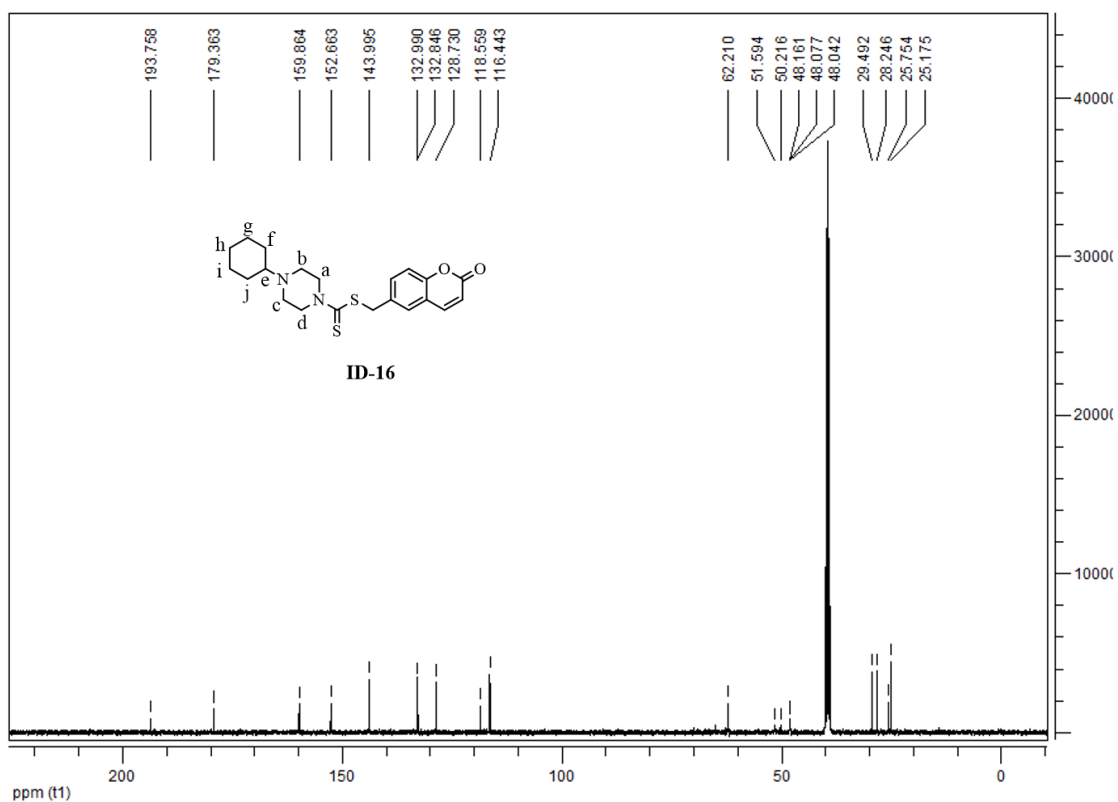
¹³C NMR, DMSO-d₆ (Bruker AVANCE III 400) (ID-15)



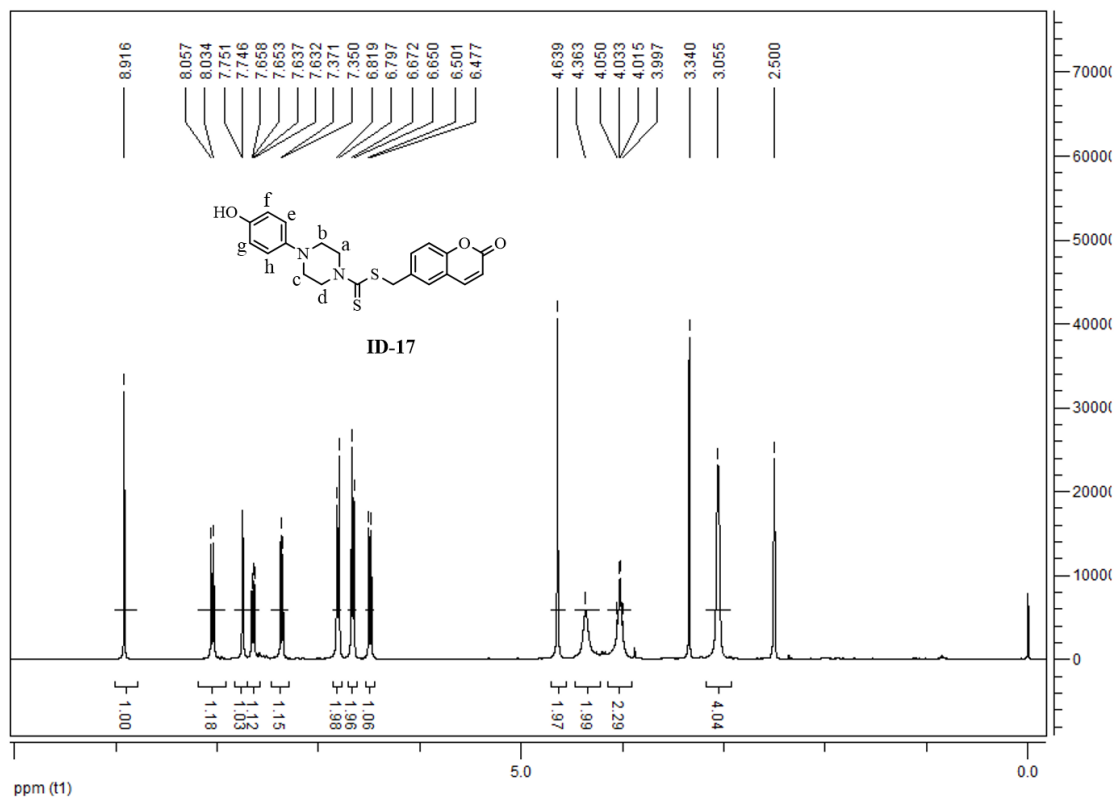
¹H NMR, DMSO-d₆ (Bruker AVANCE III 400) (ID-16)



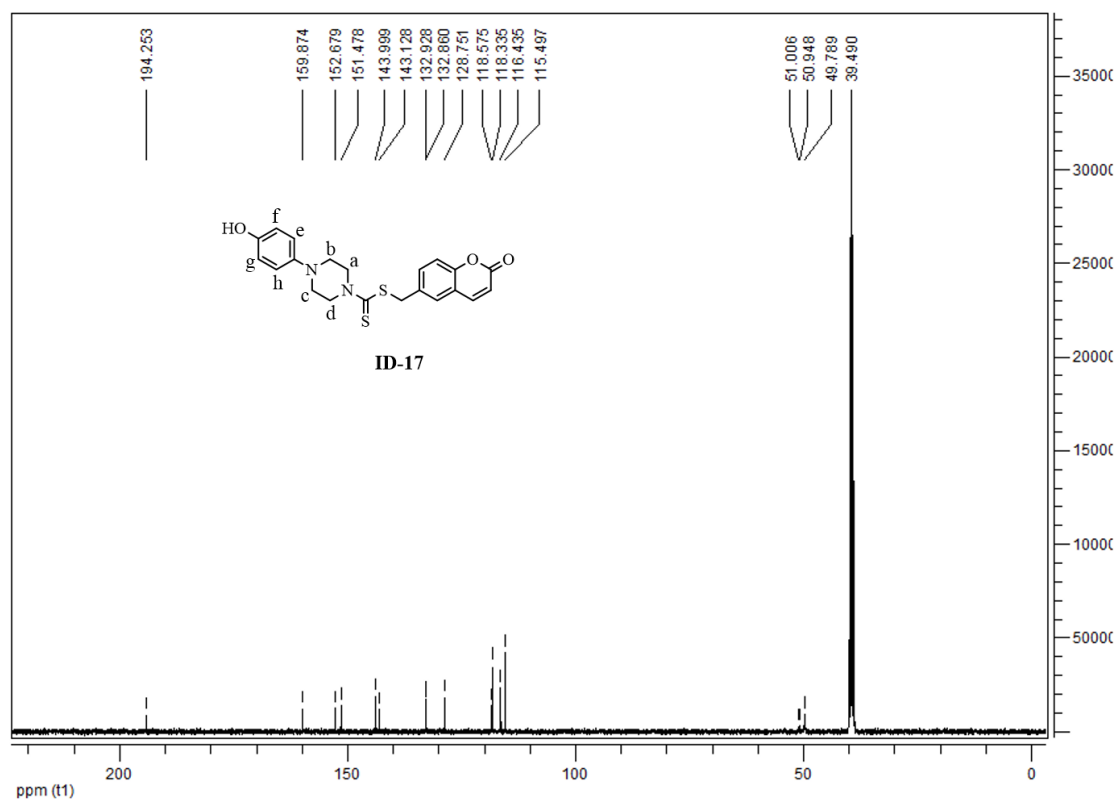
^{13}C NMR, DMSO- d_6 (Bruker AVANCE III 400) (ID-16)



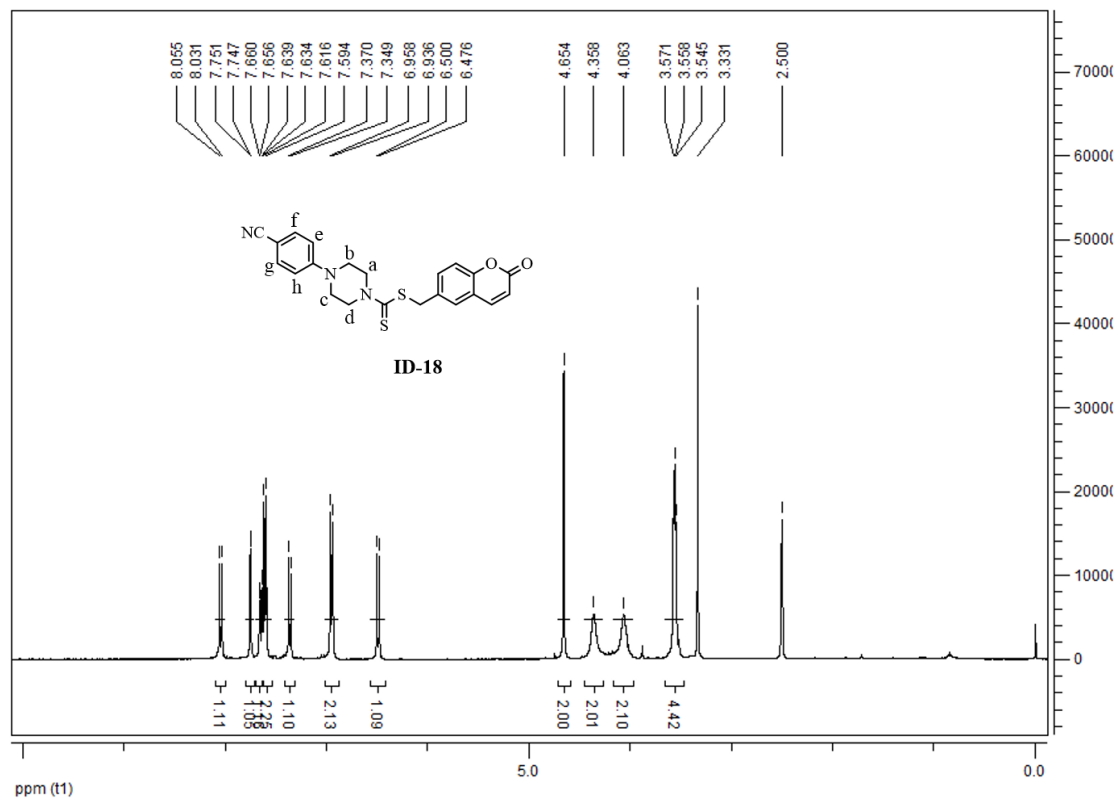
^1H NMR, DMSO- d_6 (Bruker AVANCE III 400) (ID-17)



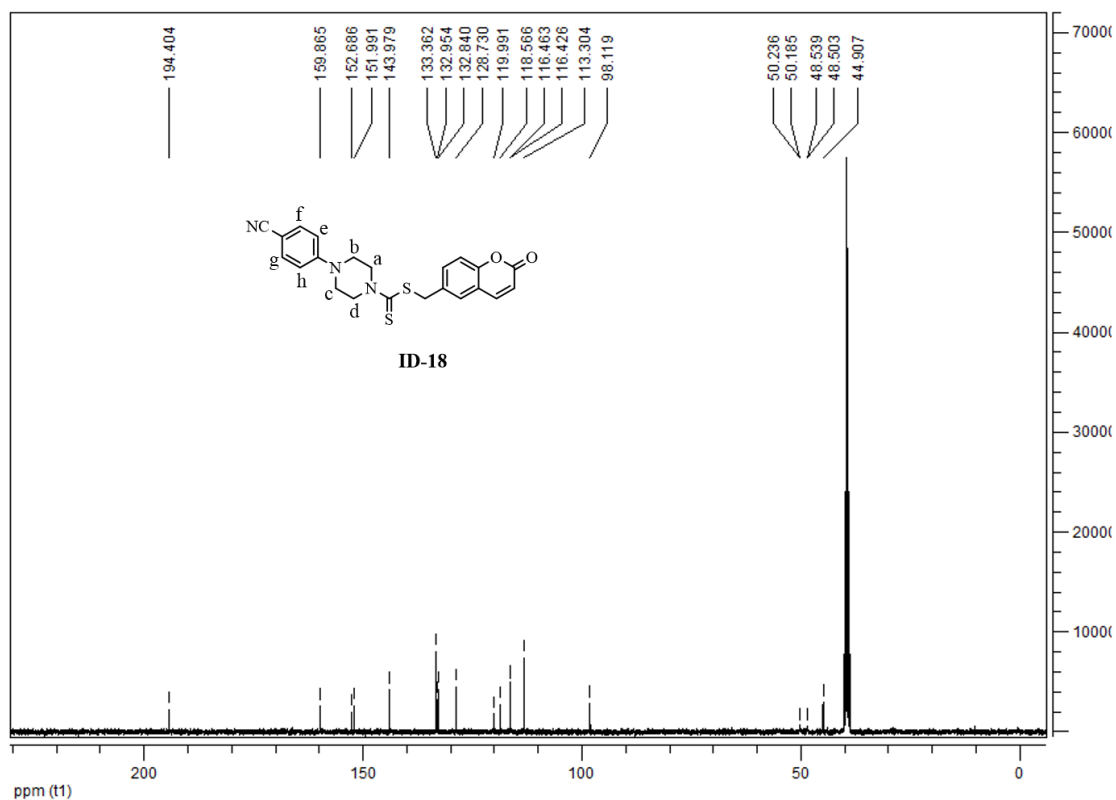
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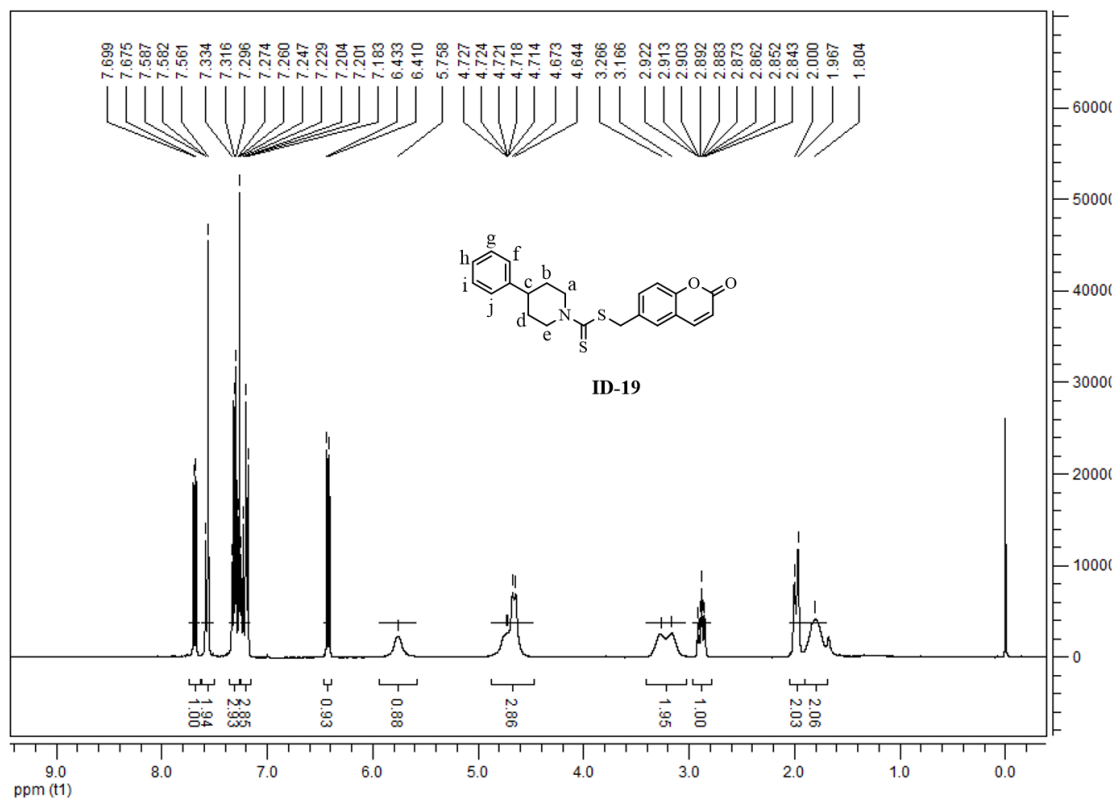
^1H NMR, DMSO- d_6 (Bruker AVANCE III 400) (ID-18)



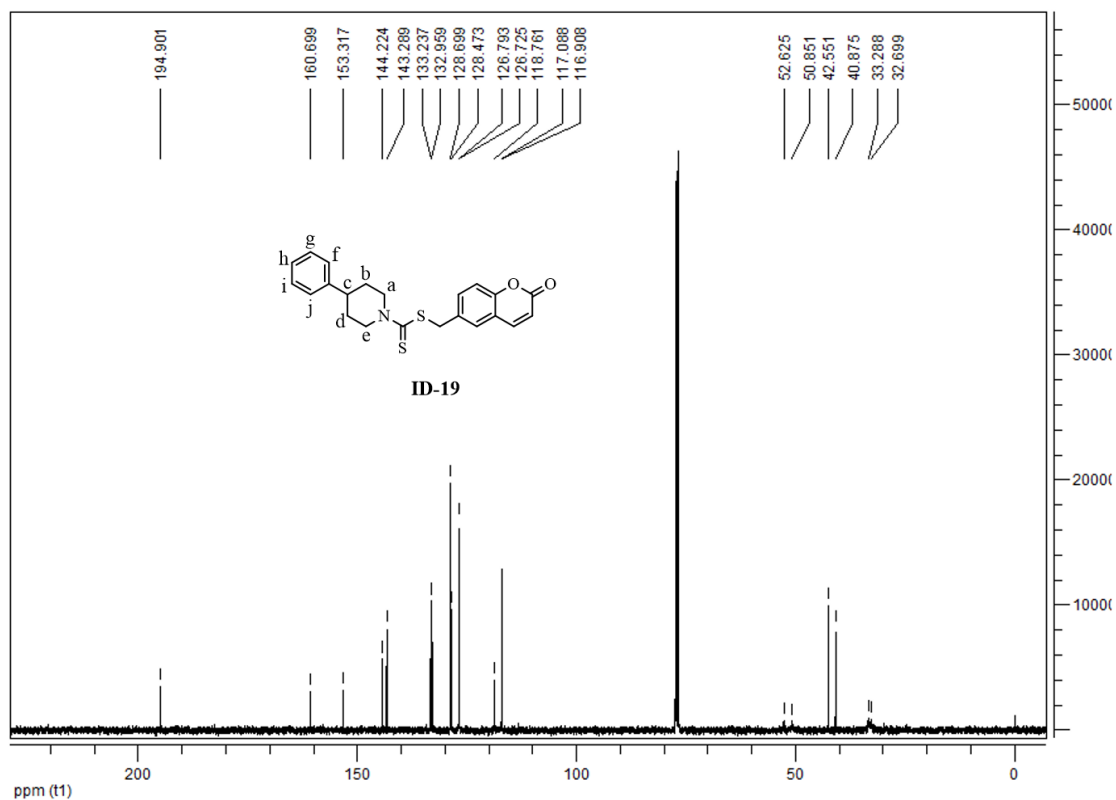
^{13}C NMR, $\text{DMSO}-d_6$ (Bruker AVANCE III 400) (ID-18)



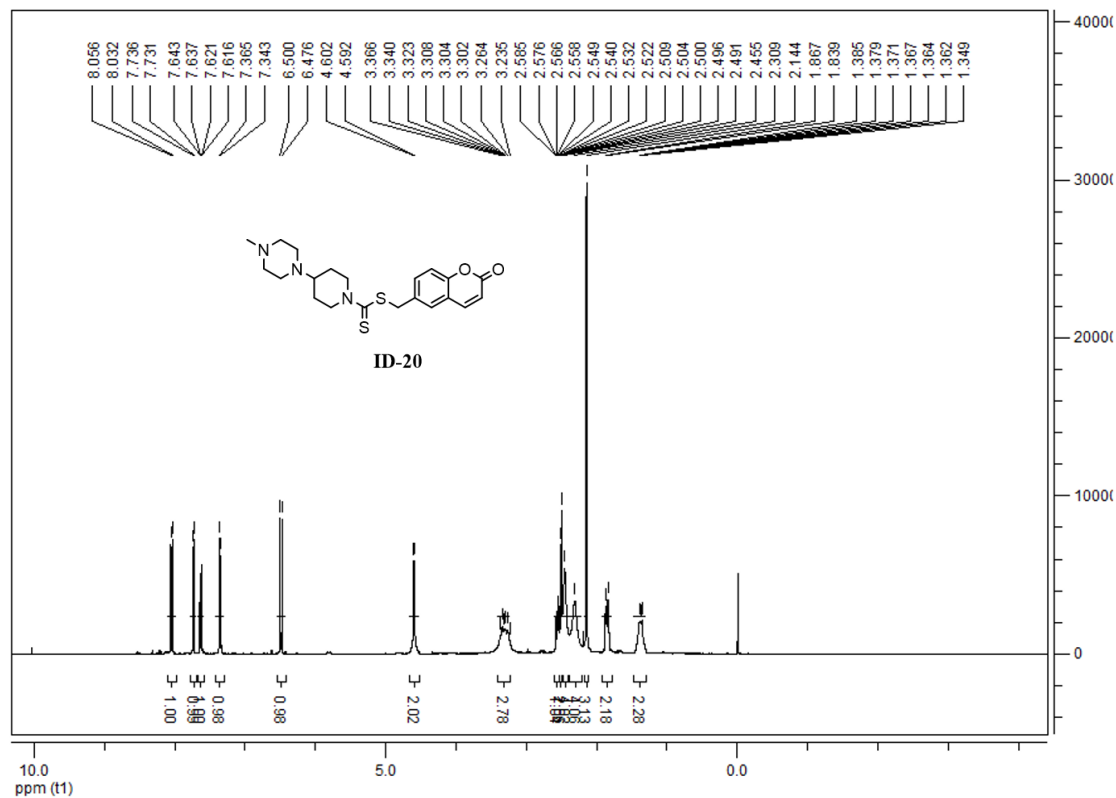
^1H NMR, CDCl_3 (Bruker AVANCE III 400) (ID-19)



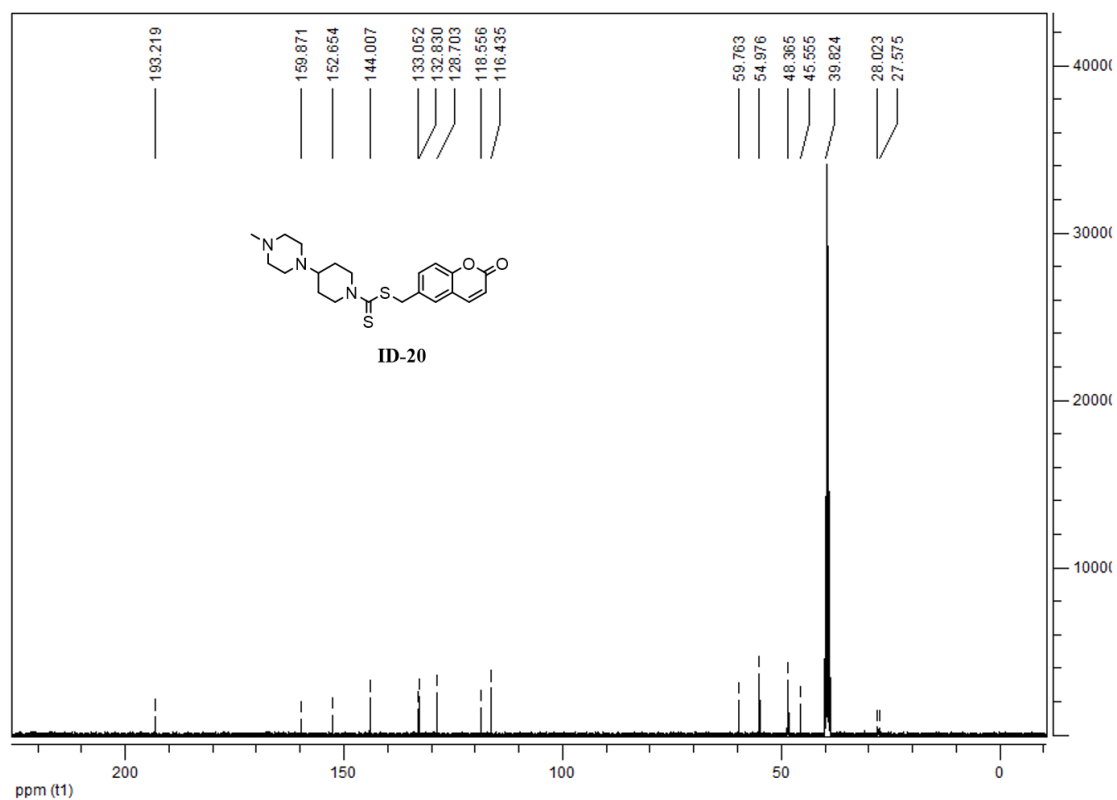
¹³C NMR, CDCl₃ (Bruker AVANCE III 400) (ID-19)



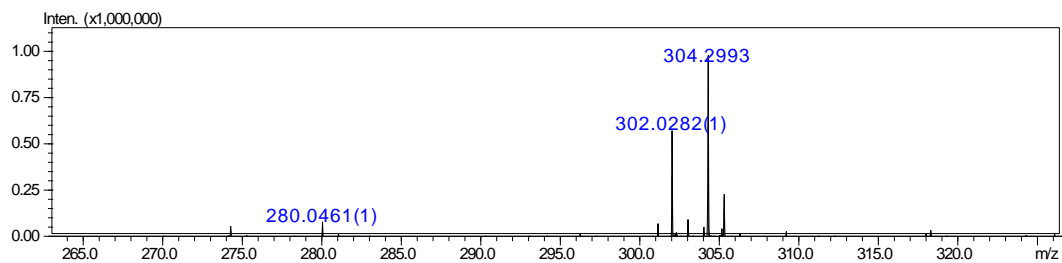
¹H NMR, DMSO-d₆ (Bruker AVANCE III 400) (ID-20)



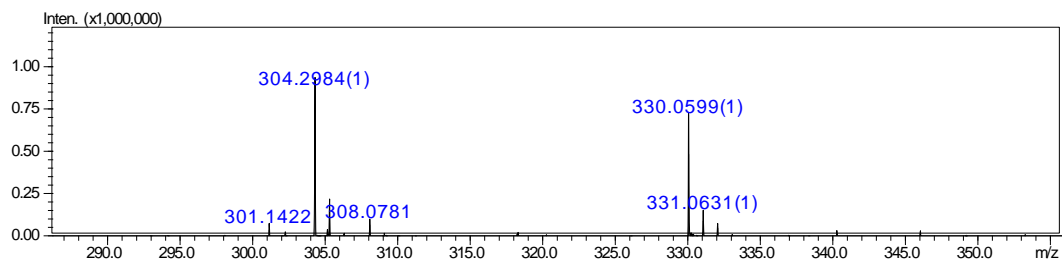
^{13}C NMR, DMSO- d_6 (Bruker AVANCE III 400) (**ID-20**)



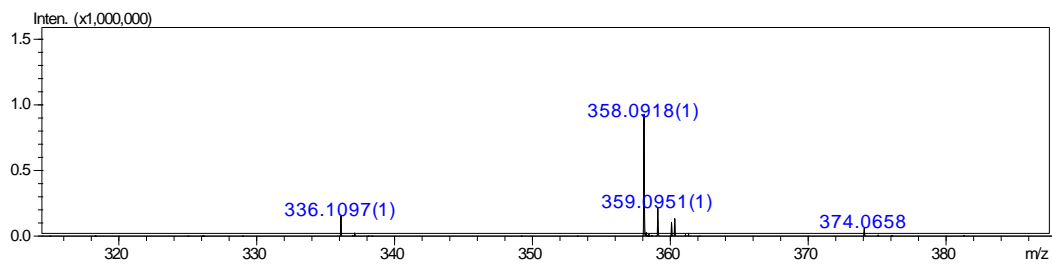
(ID-1): HRMS (ESI, m/z) calcd. for $\text{C}_{13}\text{H}_{13}\text{NO}_2\text{S}_2$ ($\text{M}+\text{Na}$) $^+$ 302.0280, found 302.0282.



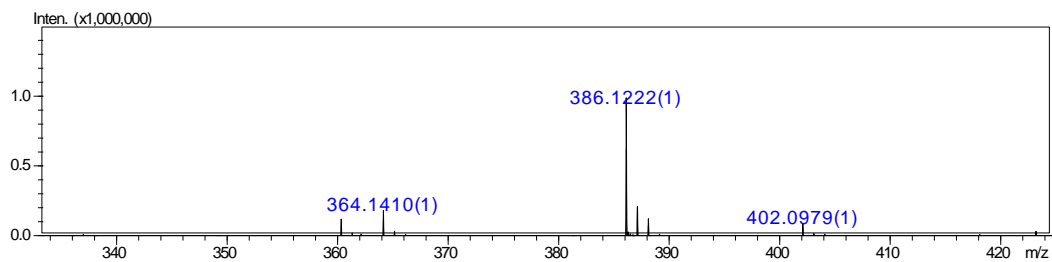
(ID-2): HRMS (ESI, m/z) calcd. for $\text{C}_{15}\text{H}_{17}\text{NO}_2\text{S}_2$ ($\text{M}+\text{Na}$) $^+$ 330.0593, found 330.0599.



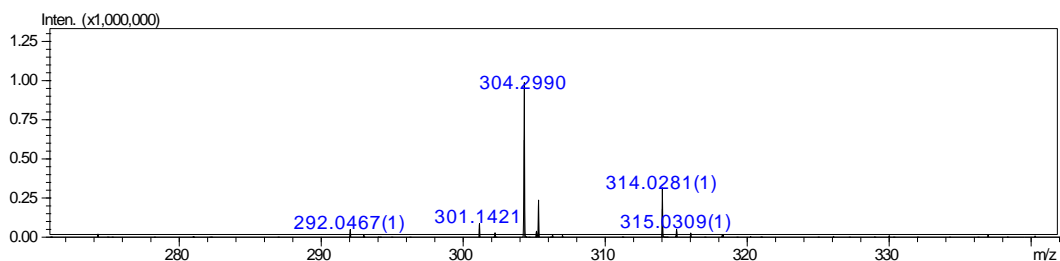
(ID-3): HRMS (ESI, m/z) calcd. for $\text{C}_{17}\text{H}_{21}\text{NO}_2\text{S}_2$ ($\text{M}+\text{Na}$) $^+$ 358.0906, found 358.0918.



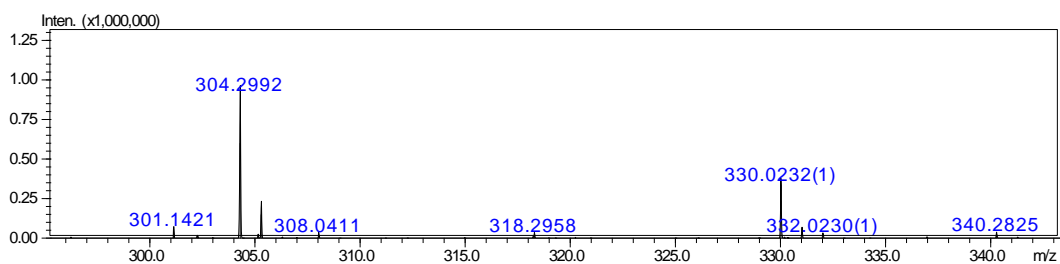
(ID-4): HRMS (ESI, m/z) calcd. for $C_{19}H_{25}NO_2S_2$ ($M+Na$)⁺ 386.1219, found 386.1222.



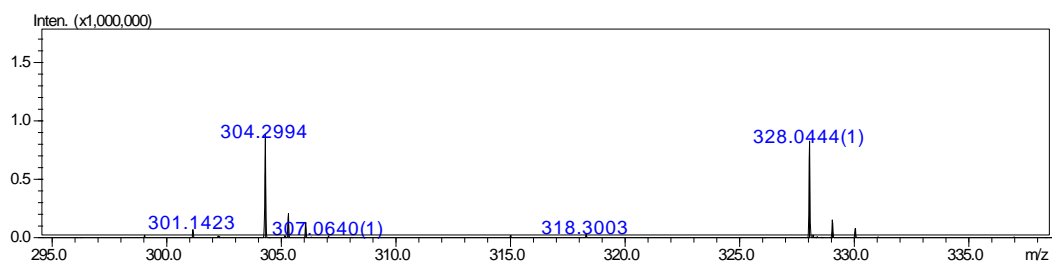
(ID-5): HRMS (ESI, m/z) calcd. for $C_{14}H_{13}NO_2S_2$ ($M+Na$)⁺ 314.0280, found 314.0281.



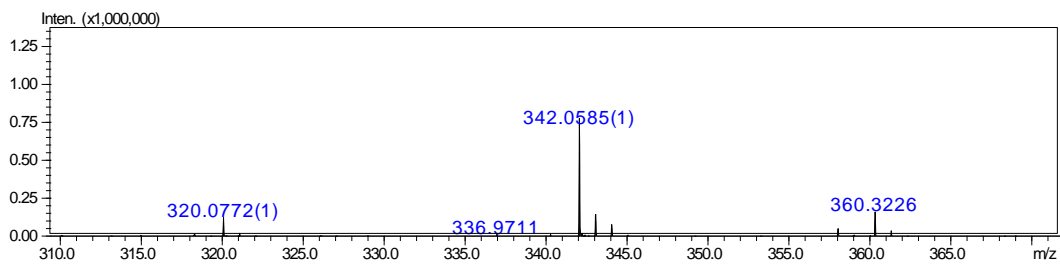
(ID-6): HRMS (ESI, m/z) calcd. for $C_{14}H_{13}NO_3S_2$ ($M+Na$)⁺ 330.0229, found 330.0232.



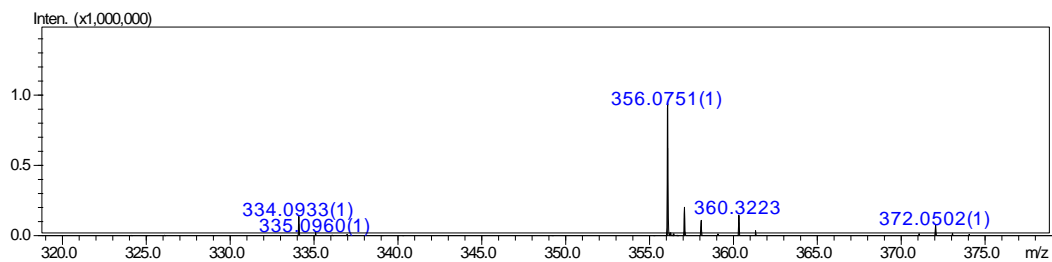
(ID-7): HRMS (ESI, m/z) calcd. for $C_{15}H_{15}NO_2S_2$ ($M+Na$)⁺ 328.0436, found 328.0444.



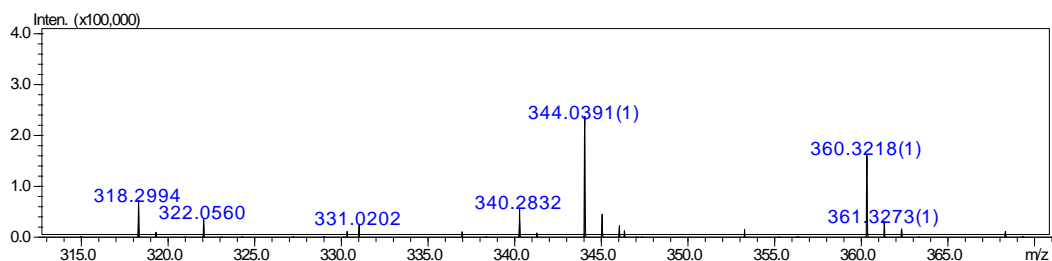
(ID-8): HRMS (ESI, m/z) calcd. for $C_{16}H_{17}NO_2S_2$ ($M+Na$)⁺ 342.0593, found 342.0585.



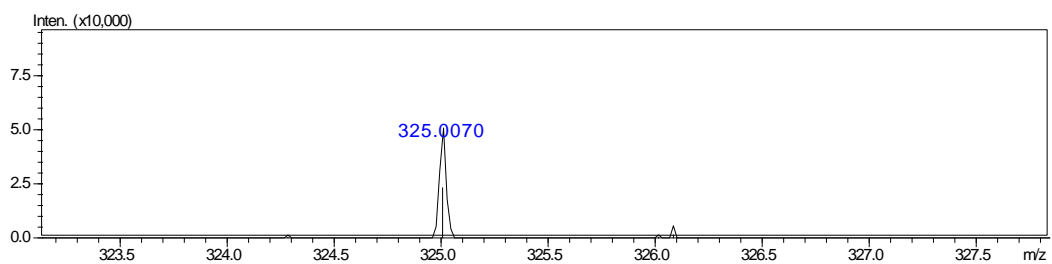
(ID-9): HRMS (ESI, m/z) calcd. for $C_{17}H_{19}NO_2S_2$ ($M+Na$)⁺ 356.0749, found 356.0751.



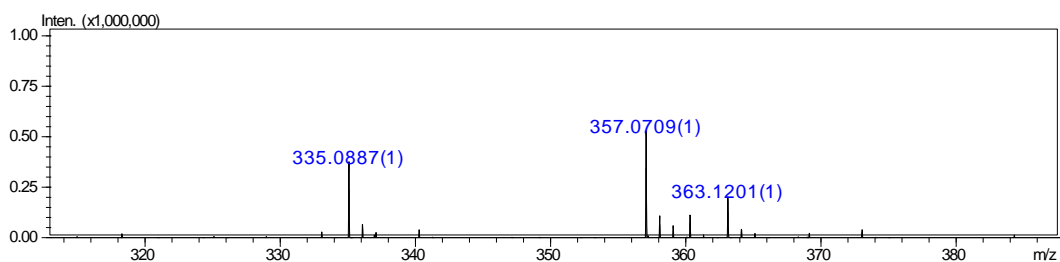
(ID-10): HRMS (ESI, m/z) calcd. for $C_{15}H_{15}NO_3S_2$ ($M+Na$)⁺ 344.0386, found 344.0391.



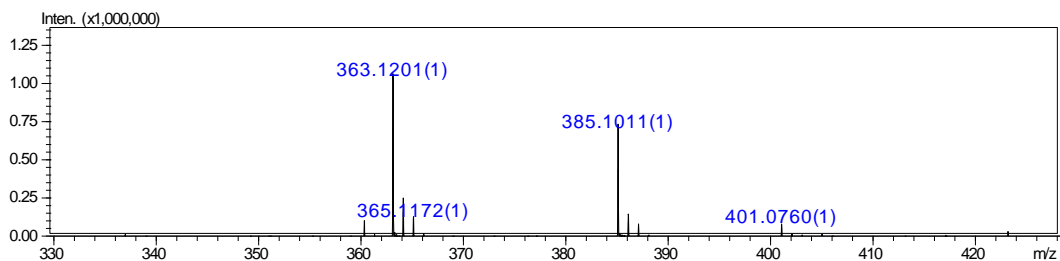
(ID-11): HRMS (ESI, m/z) calcd. for $C_{14}H_{10}N_2O_2S_2$ ($M+Na$)⁺ 325.0076, found 325.0070.



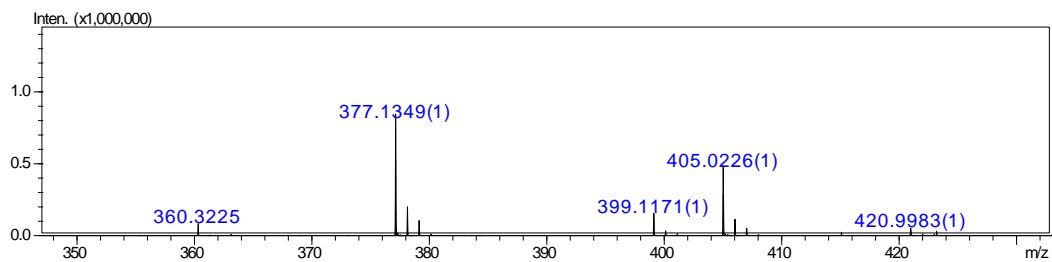
(ID-12): HRMS (ESI, m/z) calcd. for $C_{16}H_{18}N_2O_2S_2$ ($M+Na$)⁺ 357.0702, found 357.0709.



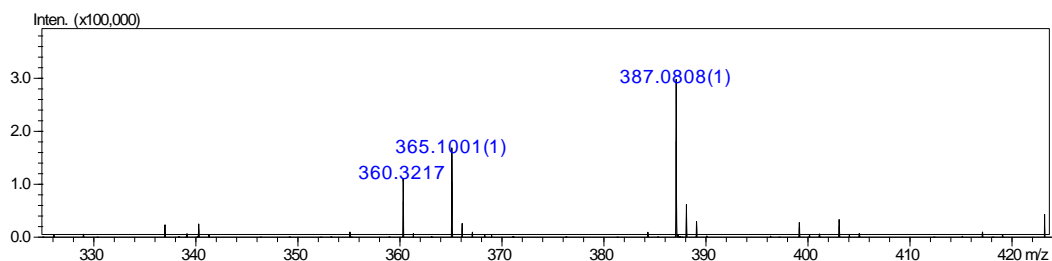
(ID-13): HRMS (ESI, m/z) calcd. for $C_{18}H_{22}N_2O_2S_2$ ($M+H$)⁺ 363.1195, found 363.1201.



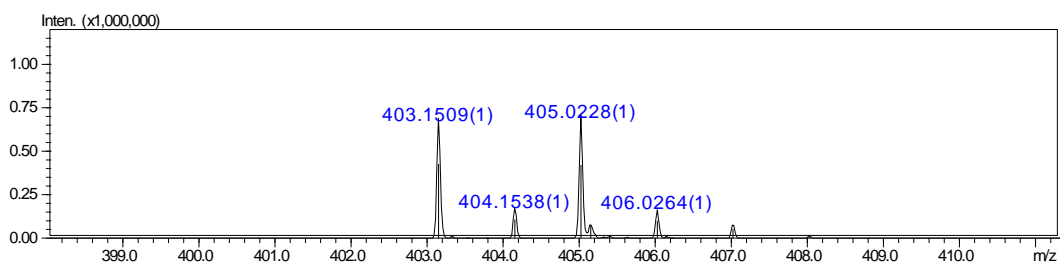
(ID-14): HRMS (ESI, m/z) calcd. for $C_{19}H_{24}N_2O_2S_2$ ($M+H$)⁺ 377.1352, found 377.1349.



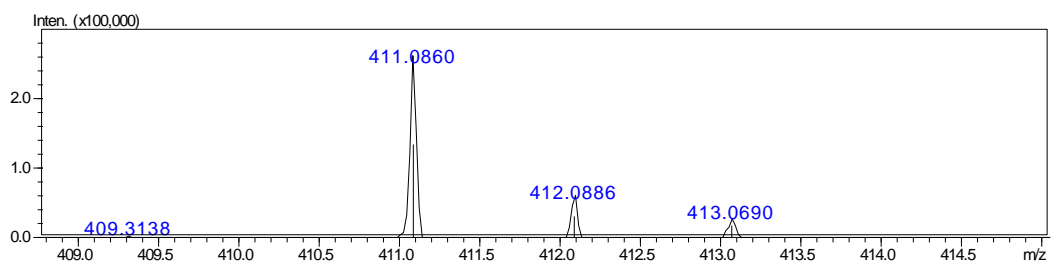
(ID-15): HRMS (ESI, m/z) calcd. for $C_{17}H_{20}N_2O_3S_2$ ($M+Na$)⁺ 387.0808, found 387.0808.



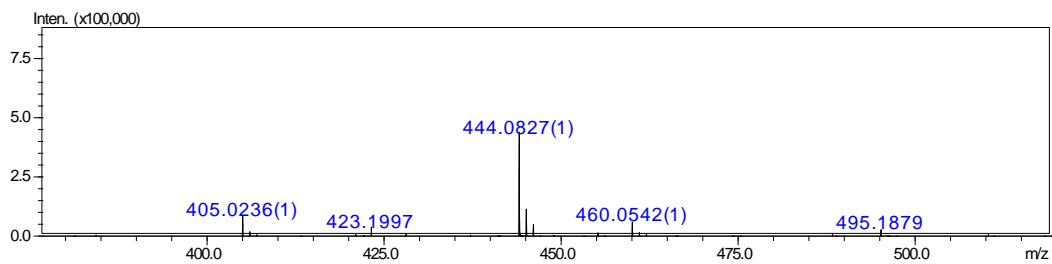
(ID-16): HRMS (ESI, m/z) calcd. for $C_{21}H_{26}N_2O_2S_2$ ($M+H$)⁺ 403.1508, found 403.1509.



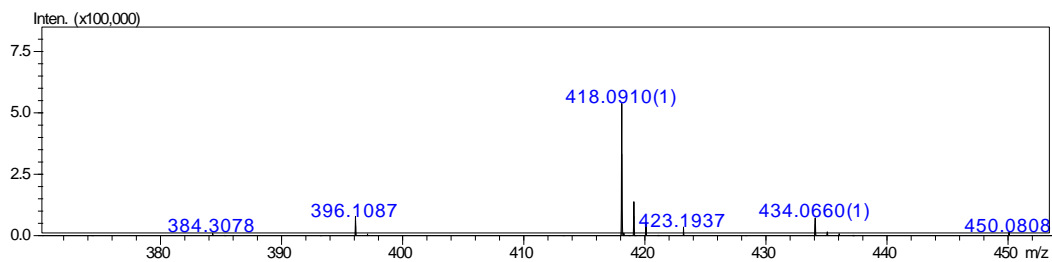
(ID-17): HRMS (ESI, m/z) calcd. for $C_{21}H_{20}N_2O_3S_2$ ($M-H$)⁻ 411.0843, found 411.0860.



(ID-18): HRMS (ESI, m/z) calcd. for $C_{22}H_{19}N_3O_2S_2$ ($M+Na$)⁺ 444.0811, found 444.0827.



(ID-19): HRMS (ESI, m/z) calcd. for $C_{22}H_{21}NO_2S_2$ ($M+Na$)⁺ 418.0906, found 418.0910.



(ID-20): HRMS (ESI, m/z) calcd. for $C_{21}H_{27}N_3O_2S_2$ ($M+H$)⁺ 418.1617, found 418.1630.

