pharmaceuticals

MDPI

Article

Synthetic Inhibitors of Snake Venom Enzymes: Thioesters Derived From 2-Sulfenyl Ethylacetate

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SUPPLEMENTARY MATERIAL

Figure S1. ^{1}H NMR Spectrum Ethyl 2-((4-chlorobenzoyl)thio)acetate (I)

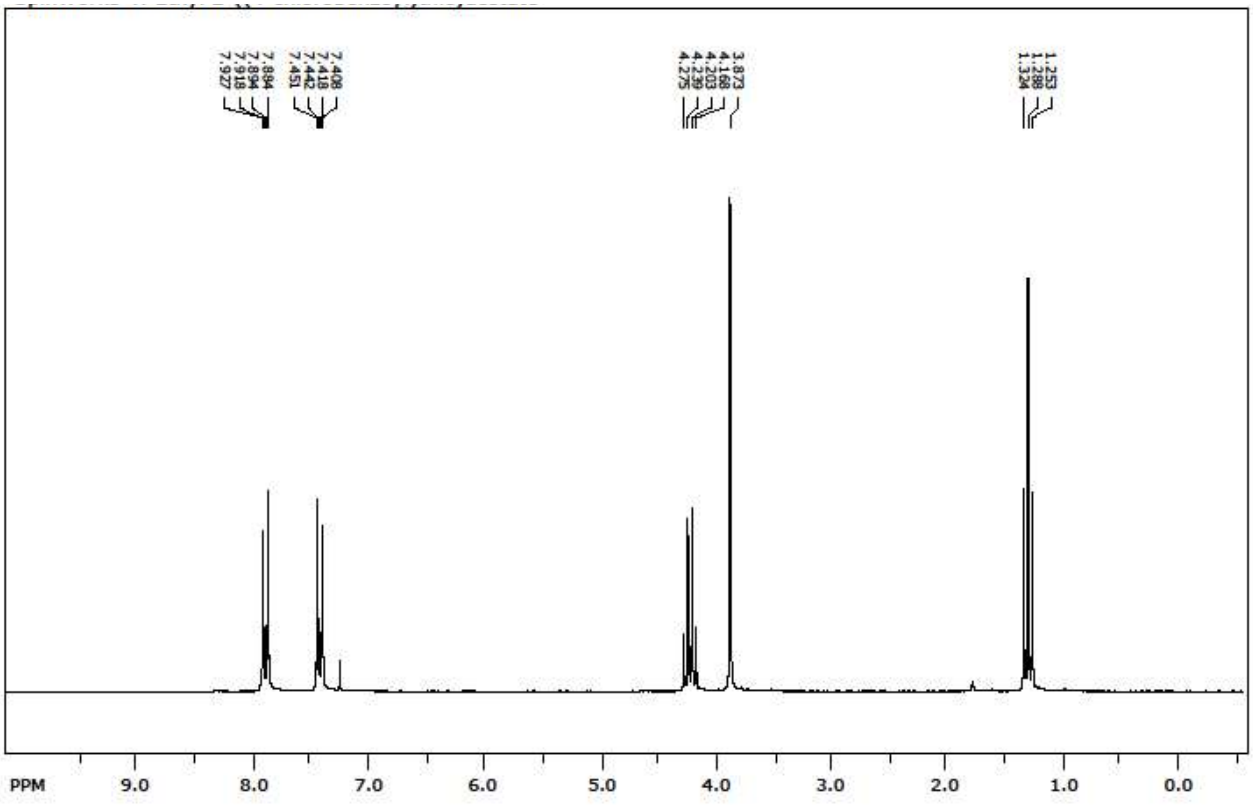


Figure S2. ^{13}C NMR Spectrum Ethyl 2-((4-chlorobenzoyl)thio)acetate (I)

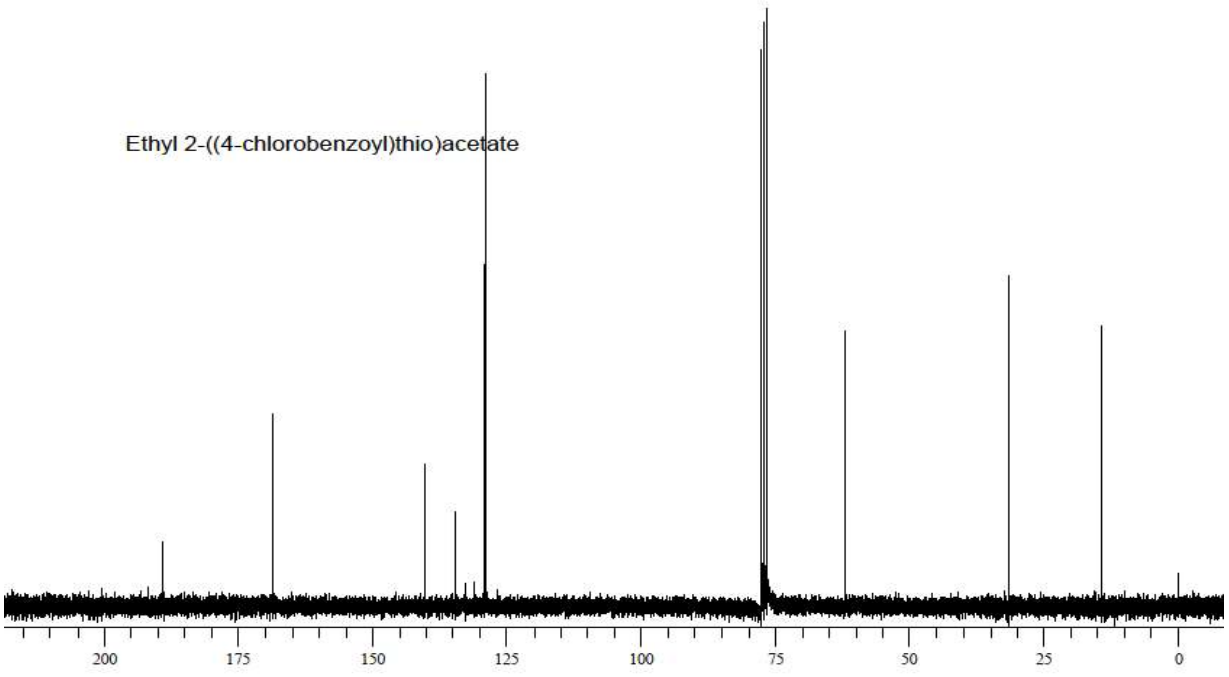


Figure S3. ^{1}H NMR Spectrum Ethyl 2-((3-nitrobenzoyl)thio)acetate (II)

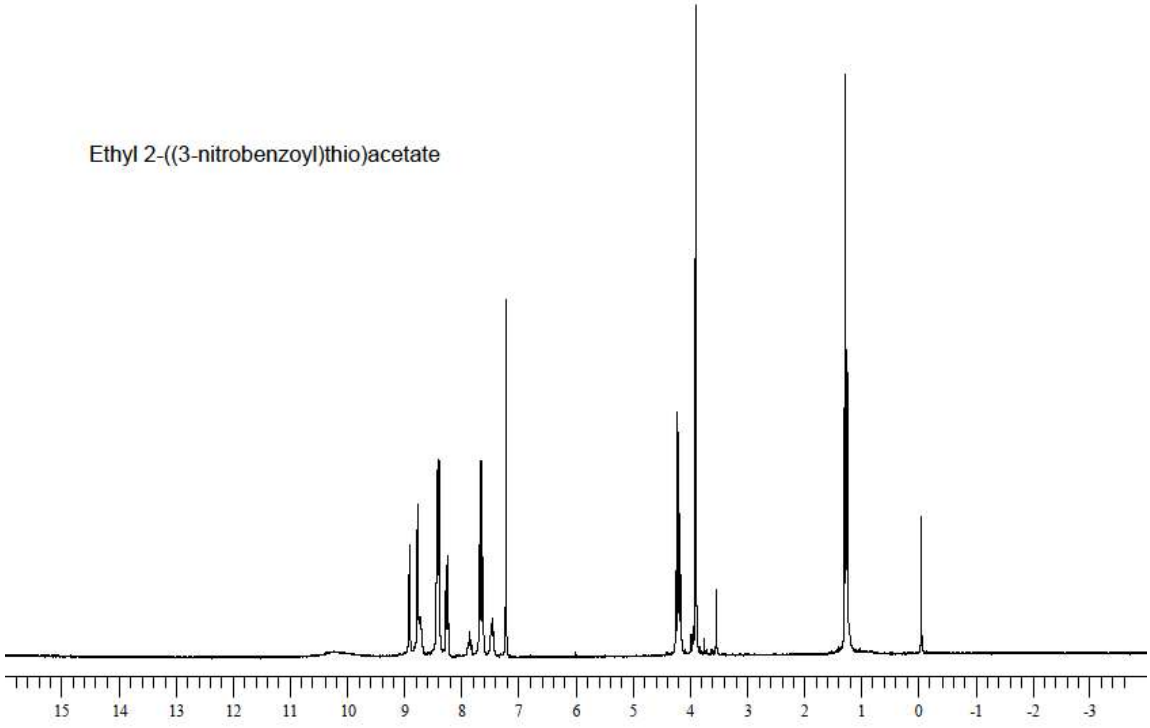


Figure S4. ^{13}C NMR Spectrum Ethyl 2-((3-nitrobenzoyl)thio)acetate (II)

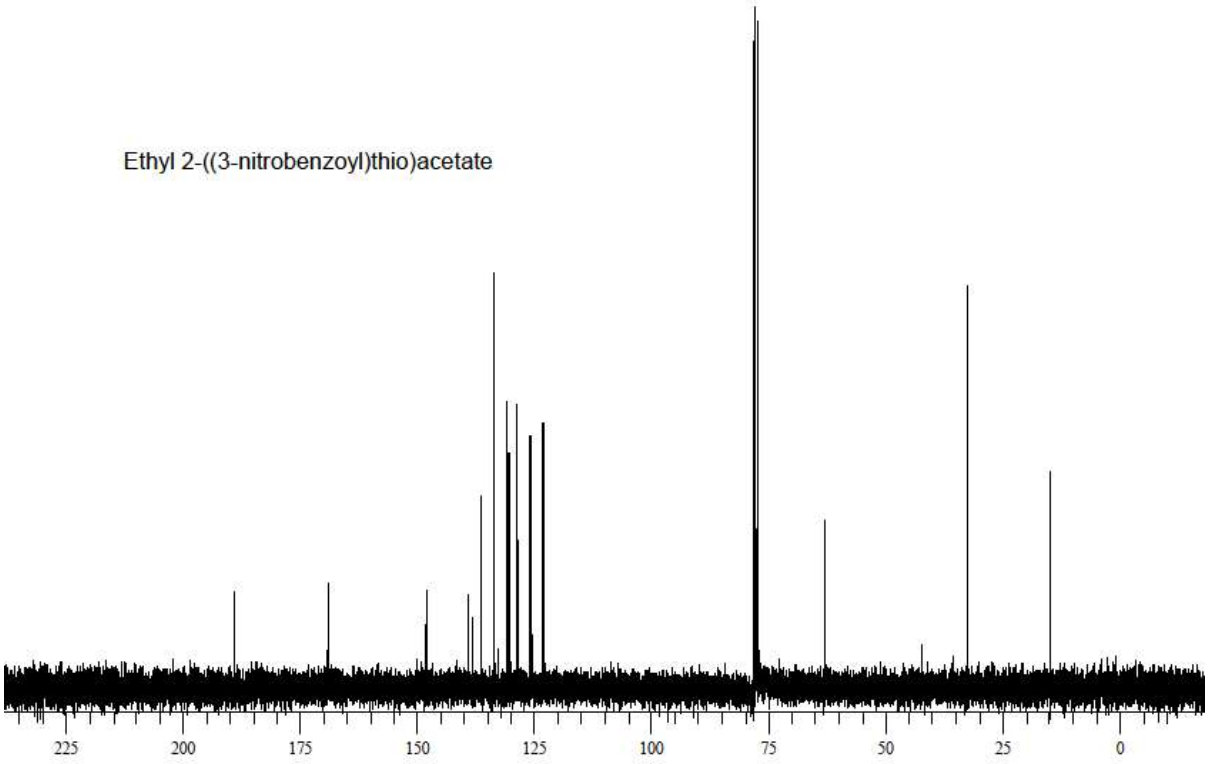


Figure S5. ^{1}H NMR Spectrum Ethyl 2-((4-nitrobenzoyl)thio)acetate (III)

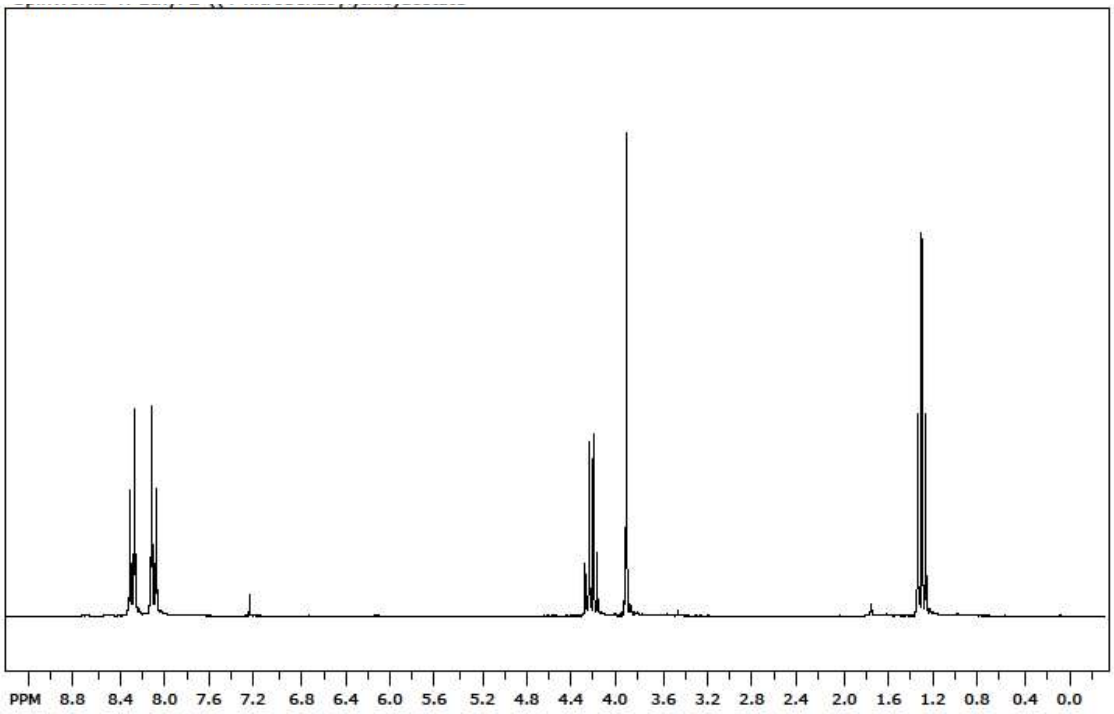


Figure S6. ^{13}C NMR Spectrum Ethyl 2-((4-nitrobenzoyl)thio)acetate (III)

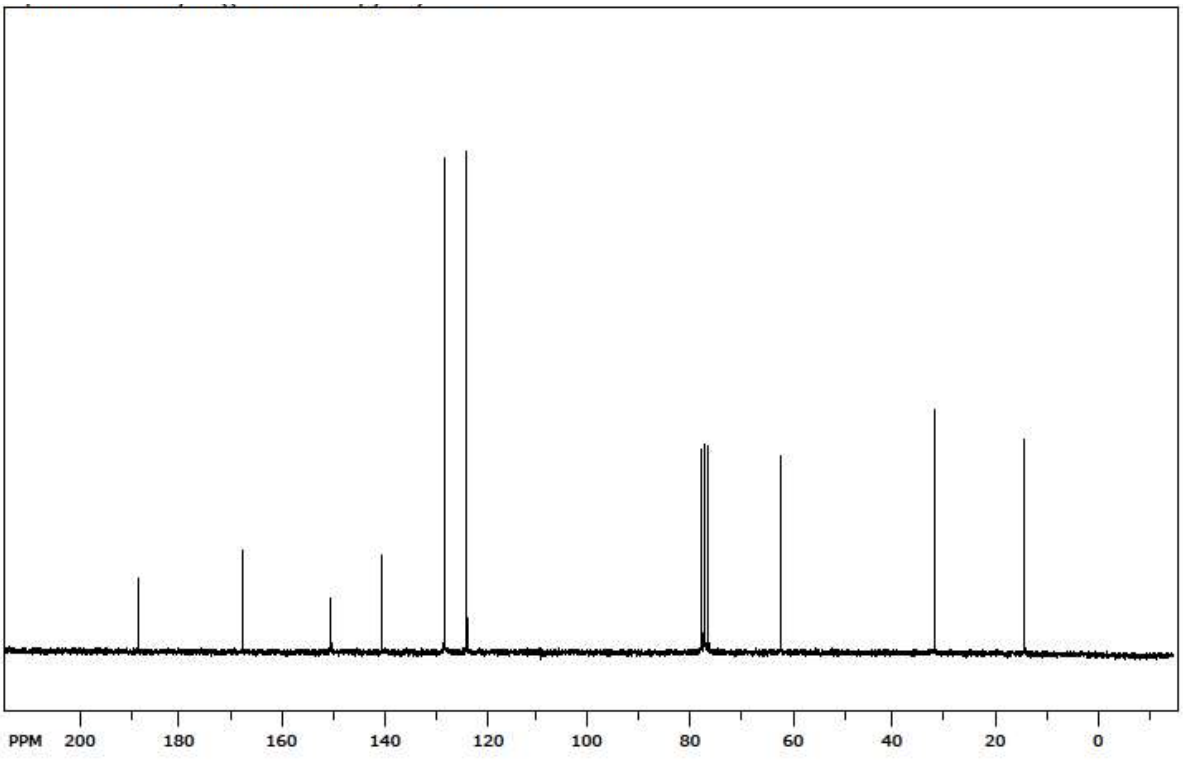
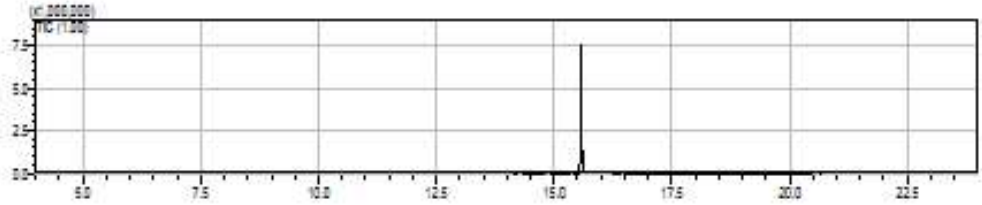
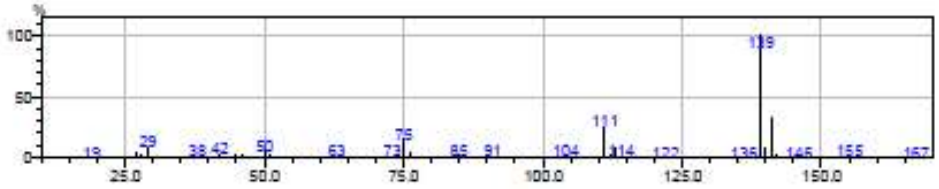


Figure S7. GC-MS Ethyl 2-((4-chlorobenzoyl)thio)acetate (I)

Ethyl 2-((4-chlorobenzoyl)thio)acetate





Method

[Comment]

——— Analytical Line 1 ———

[GC-2010]

Column Oven Temp.	:100.0 °C
Injection Temp.	:200.00 °C
Injection Mode	:Split
Flow Control Mode	:Pressure
Pressure	:100.0 kPa
Total Flow	:31.0 mL/min
Column Flow	:1.33 mL/min
Linear Velocity	:43.0 cm/sec
Purge Flow	:3.0 mL/min
Split Ratio	:20.0
High Pressure Injection	:OFF
Carrier Gas Saver	:OFF
Splitter Hold	:OFF

Oven Temp. Program

Rate	Temperature(°C)	Hold Time(min)
-	100.0	3.00
10.00	250.0	0.00
10.00	300.0	1.00

< Ready Check Heat Unit >

Column Oven	: Yes
SPL1	: Yes
MS	: Yes

< Ready Check Detector(FTD/BID) >
< Ready Check Baseline Drift >
< Ready Check Injection Flow >

SPL1 Carrier	: Yes
SPL1 Purge	: Yes

< Ready Check APC Flow >
< Ready Check Detector APC Flow >

External Wait	:No
Equilibrium Time	:0.0 min

[GC Program]

[GCMS-QP2010]

IonSourceTemp	:200.00 °C
Interface Temp.	:250.00 °C
Solvent Cut Time	:3.50 min
Detector Gain Mode	:Relative to the Tuning Result
Detector Gain	:1.08 kV +0.00 kV
Threshold	:50

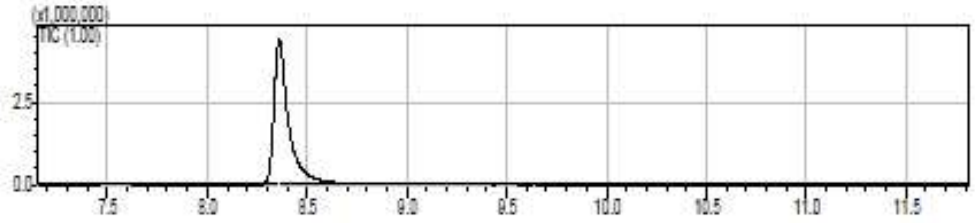
[MS Table]

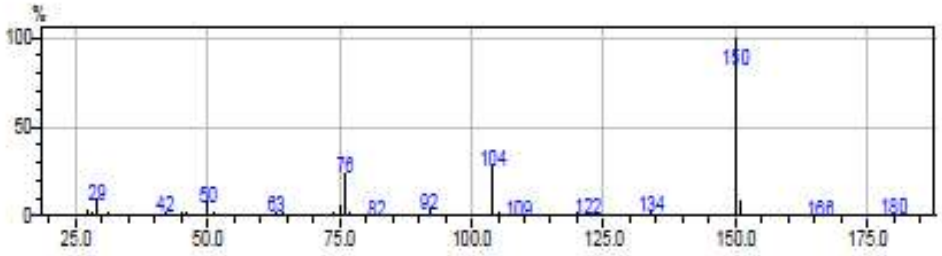
--Group 1 - Event 1--

Start Time	:4.00min

Figure S8. GC-MS Ethyl 2-((3-nitrobenzoyl)thio)acetate (II)

Ethyl 2-((3-nitrobenzoyl)thio)acetate (II)





Method

[Comment]

——— Analytical Line 1 ———

[GC-2010]

Column Oven Temp.	:200.0 °C
Injection Temp.	:200.00 °C
Injection Mode	:Split
Flow Control Mode	:Pressure
Pressure	:100.0 kPa
Total Flow	:21.8 mL/min
Column Flow	:0.90 mL/min
Linear Velocity	:36.6 cm/sec
Purge Flow	:3.0 mL/min
Split Ratio	:20.0
High Pressure Injection	:OFF
Carrier Gas Saver	:OFF
Splitter Hold	:OFF

Oven Temp. Program

Rate	Temperature(°C)	Hold Time(min)
-	200.0	2.00
5.00	300.0	2.00

< Ready Check Heat Unit >

Column Oven	: Yes
SPL1	: Yes
MS	: Yes

< Ready Check Detector(FTD/BID) >

< Ready Check Baseline Drift >

< Ready Check Injection Flow >

SPL1 Carrier	: Yes
SPL1 Purge	: Yes

< Ready Check APC Flow >

< Ready Check Detector APC Flow >

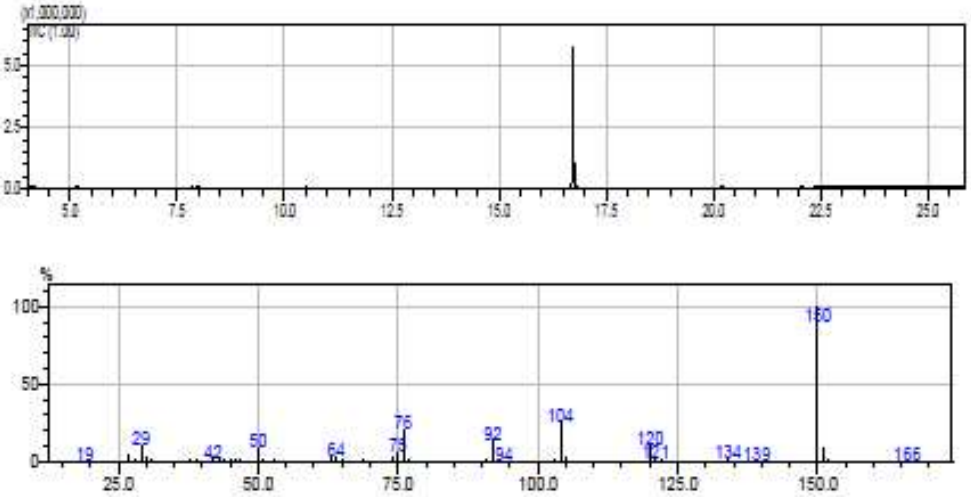
External Wait	:No
Equilibrium Time	:0.0 min

[GC Program]

[GCMS-QP2010]

Figure S9. GC-MS Ethyl 2-((4-nitrobenzoyl)thio)acetate (III)

Ethyl 2-((4-nitrobenzoyl)thio)acetate



Method

[Comment]

Analytical Line 1

[GC-2010]

Column Oven Temp.	:100.0 °C
Injection Temp.	:200.00 °C
Injection Mode	:Split
Flow Control Mode	:Pressure
Pressure	:100.0 kPa
Total Flow	:31.0 mL/min
Column Flow	:1.33 mL/min
Linear Velocity	:43.0 cm/sec
Purge Flow	:3.0 mL/min
Split Ratio	:20.0
High Pressure Injection	:OFF
Carrier Gas Saver	:OFF
Splitter Hold	:OFF

Oven Temp. Program

Rate	Temperature(°C)	Hold Time(min)
-	100.0	2.00
10.00	250.0	0.00
10.00	300.0	7.00

< Ready Check Heat Unit >

Column Oven	: Yes
SPL1	: Yes
MS	: Yes

< Ready Check Detector(FTD/BID) >
< Ready Check Baseline Drift >
< Ready Check Injection Flow >

SPL1 Carrier	: Yes
SPL1 Purge	: Yes

< Ready Check APC Flow >
< Ready Check Detector APC Flow >

External Wait	:No
Equilibrium Time	:0.0 min

[GC Program]

[GCMS-QP2010]

IonSourceTemp	:200.00 °C
Interface Temp.	:250.00 °C
Solvent Cut Time	:3.50 min
Detector Gain Mode	:Relative to the Tuning Result
Detector Gain	:1.08 kV +0.00 kV
Threshold	:50

[MS Table]

Figure S10. IR Ethyl 2-((4-clorobenzoyl)thio)acetate (I)

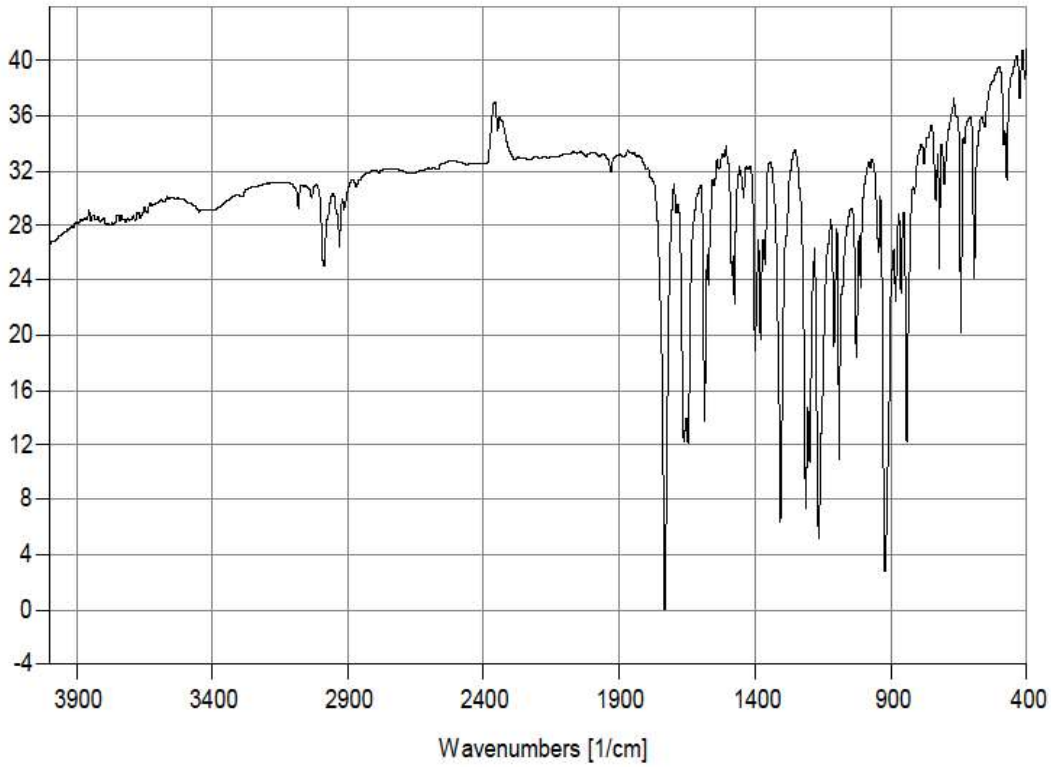


Figure S11. IR Ethyl 2-((3-nitrobenzoyl)thio)acetate (II)

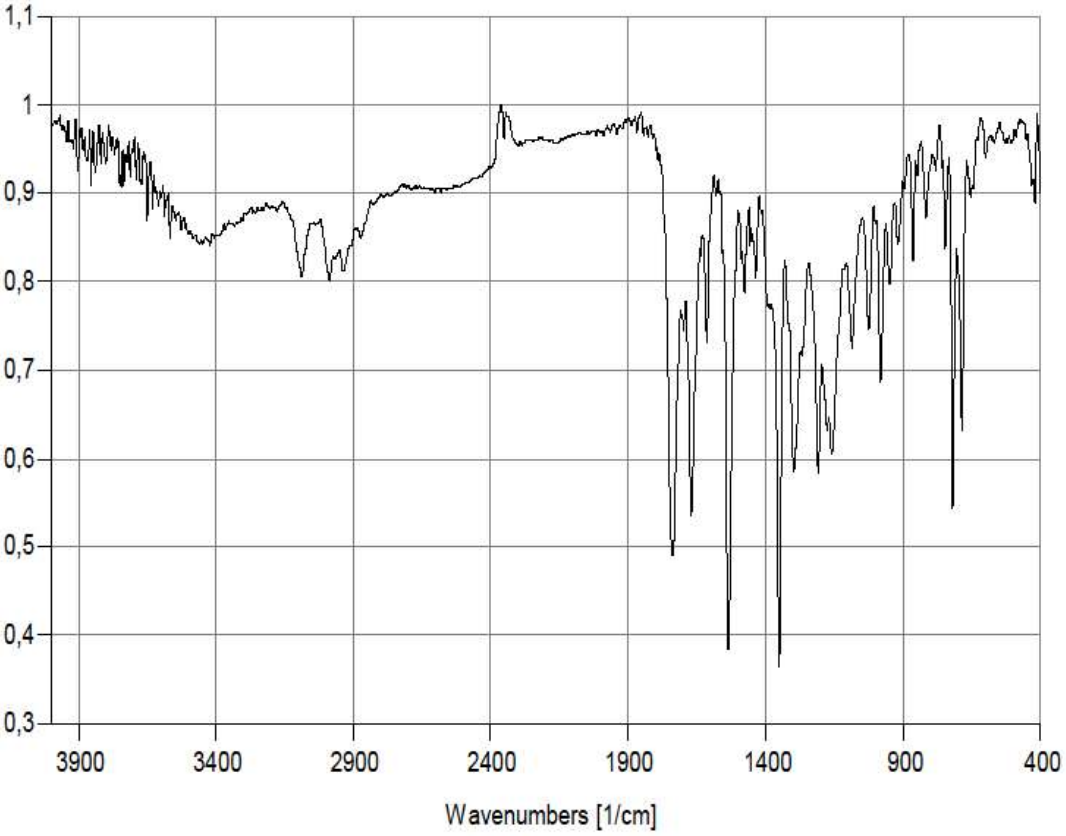


Figure S12. IR Ethyl 2-((4-nitrobenzoyl)thio)acetate (III)