

Supplementary Information

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compound **4**

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The 18S rDNA Gene Sequences Data of *Penicillium* sp. J-54

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3'.

Figure S1. The ^1H NMR (500 MHz, $\text{DMSO}-d_6$) spectrum of compound **1**

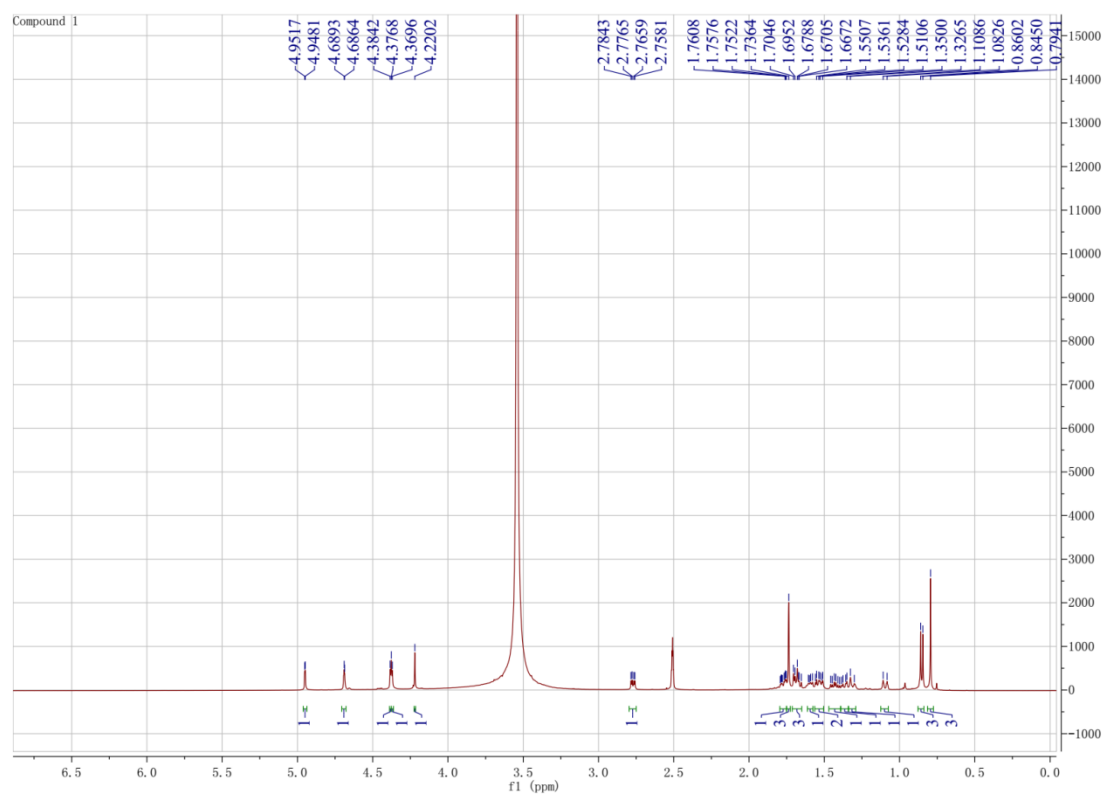


Figure S2. The ^{13}C NMR and DEPT135 (125 MHz, $\text{DMSO-}d_6$) spectrum of compound **1**

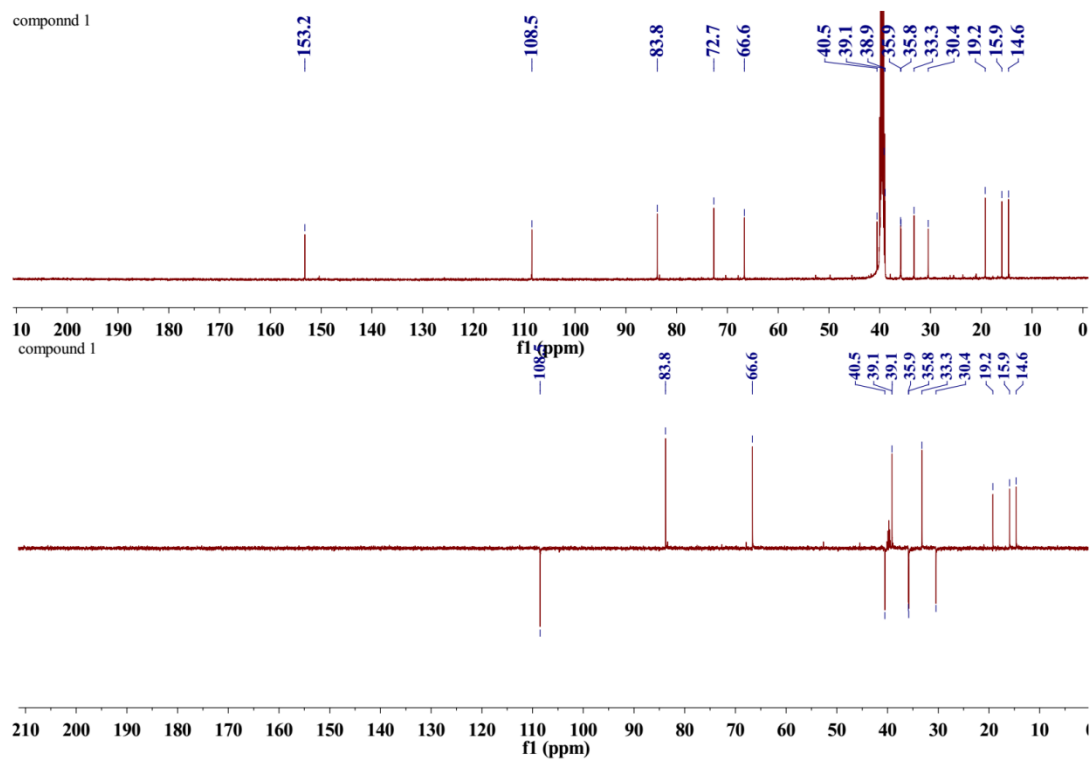


Figure S3. The ^1H - ^1H COSY (500 MHz, $\text{DMSO-}d_6$) spectrum of compound **1**

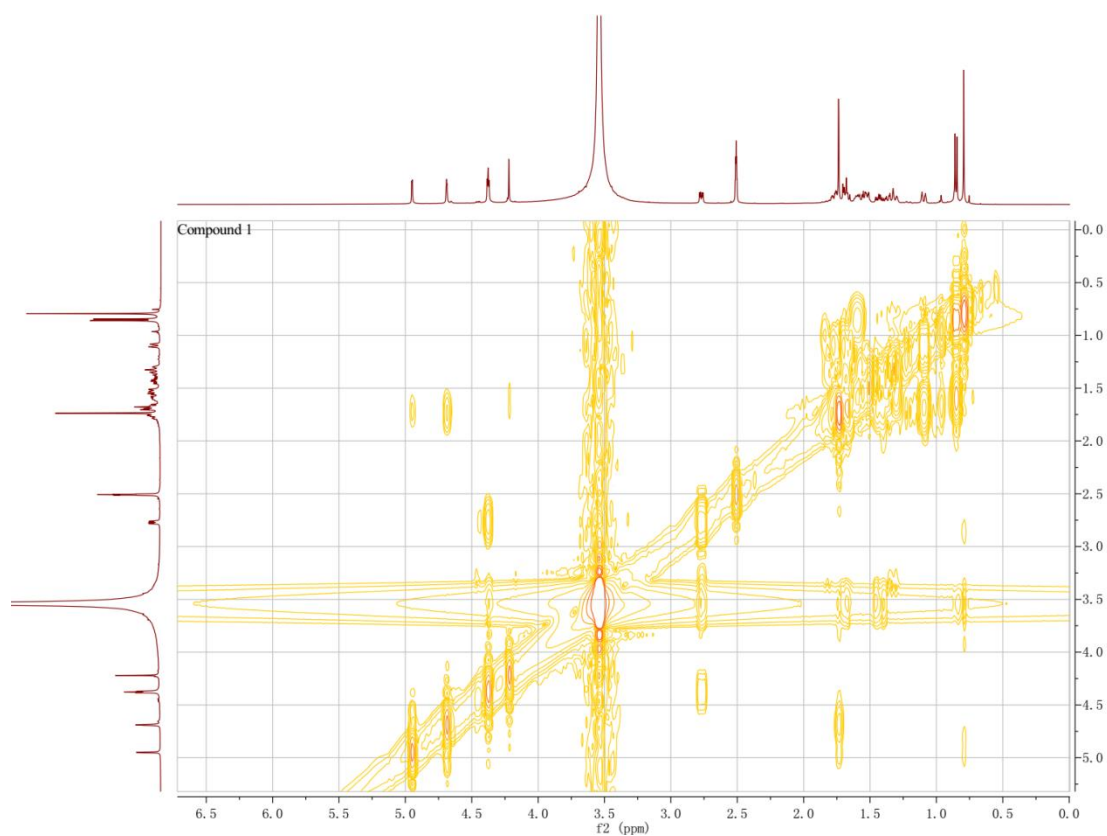


Figure S4. The HSQC (500 MHz, $\text{DMSO-}d_6$) spectrum of compound **1**

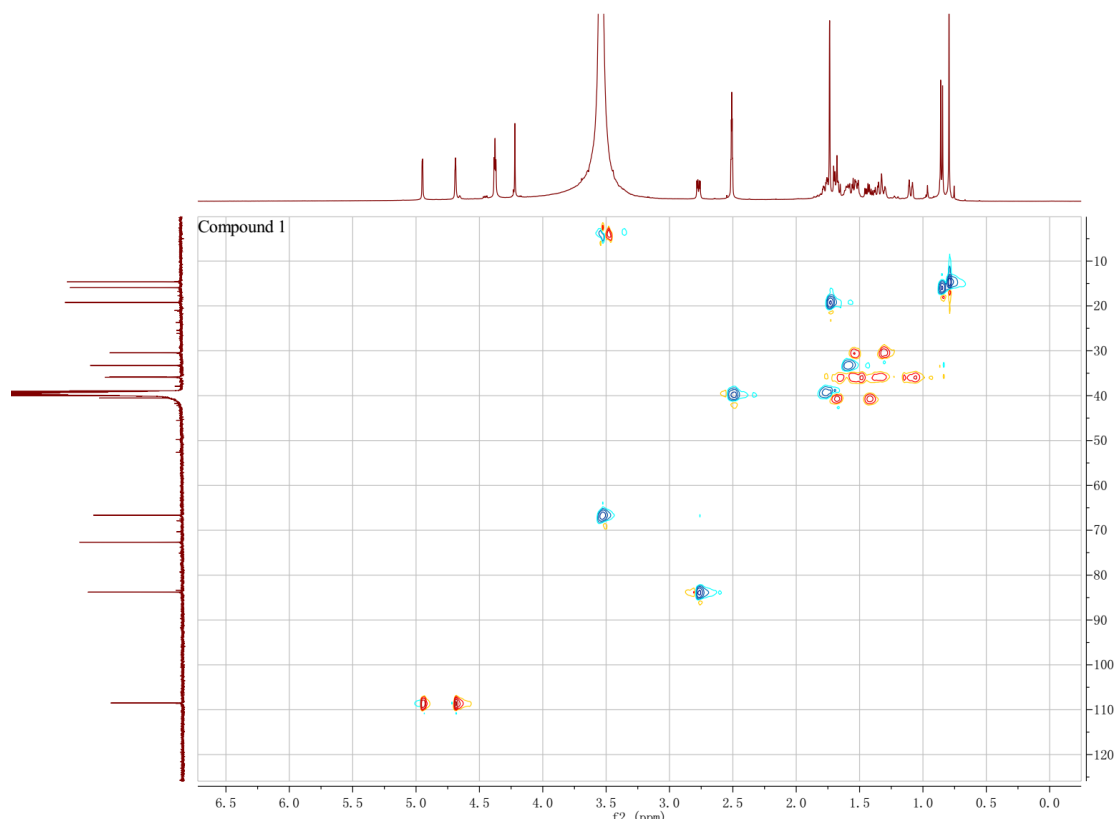


Figure S5. The HMBC (500 MHz, DMSO- d_6) spectrum of compound **1**

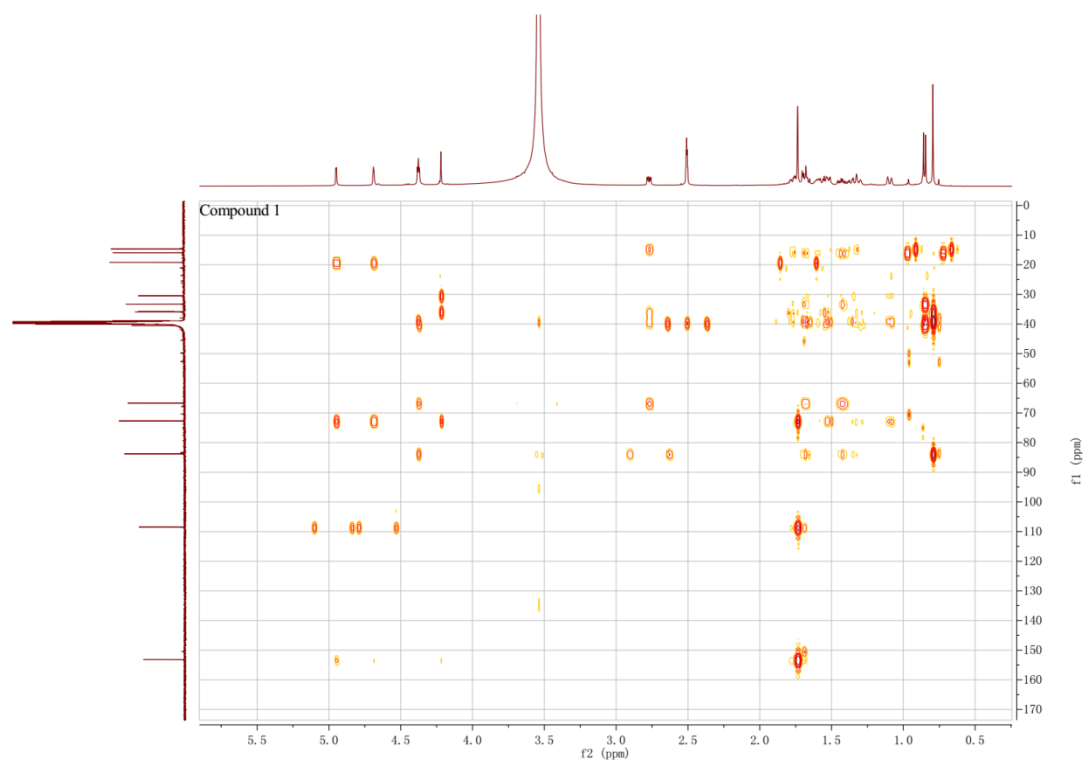
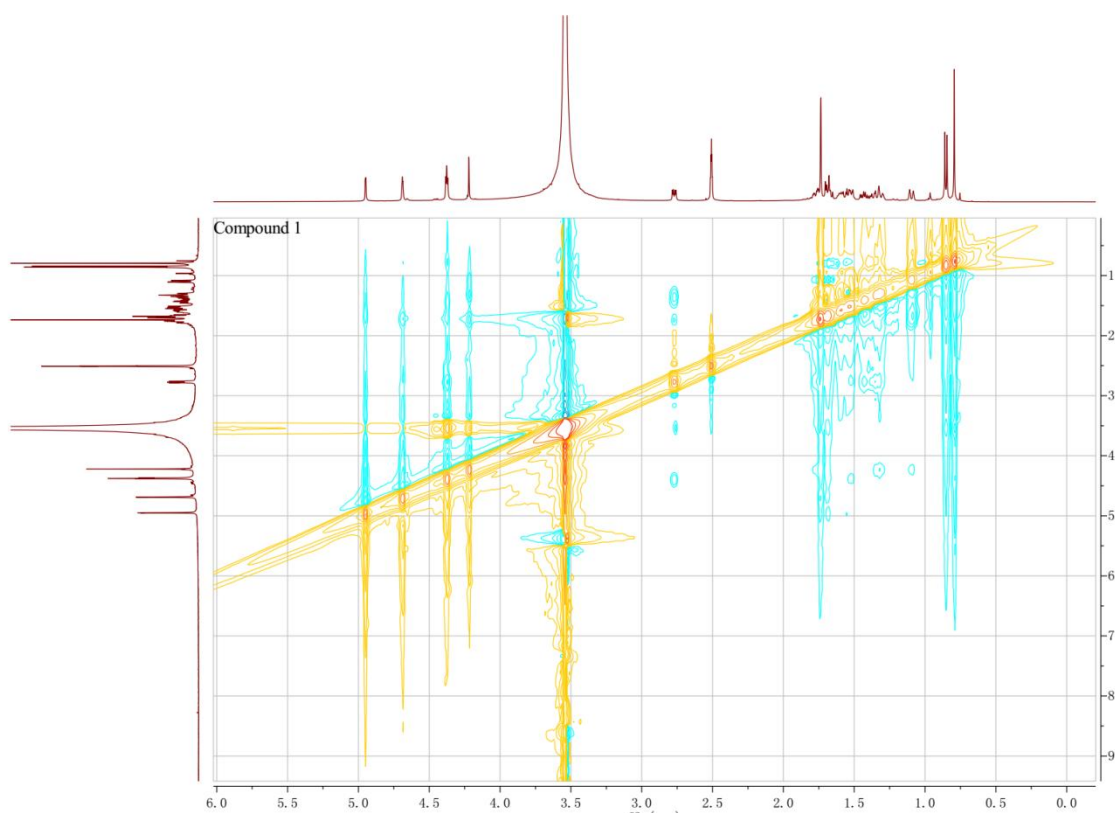


Figure S6. The ROESY (500 MHz, DMSO- d_6) spectrum of compound **1**



Elemental Composition Report

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
14 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:
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LM-2
13:12:37 18-Jun-2014
Voltage E1+

Autospec Premier
P776
162

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
254.1878	254.1882	-0.4	-1.6	3.0	8546087.0	C15 H26 O3

[illegible]

Figure S9. The ^{13}C NMR and DEPT135 (125 MHz, $\text{DMSO-}d_6$) spectrum of compound **2**

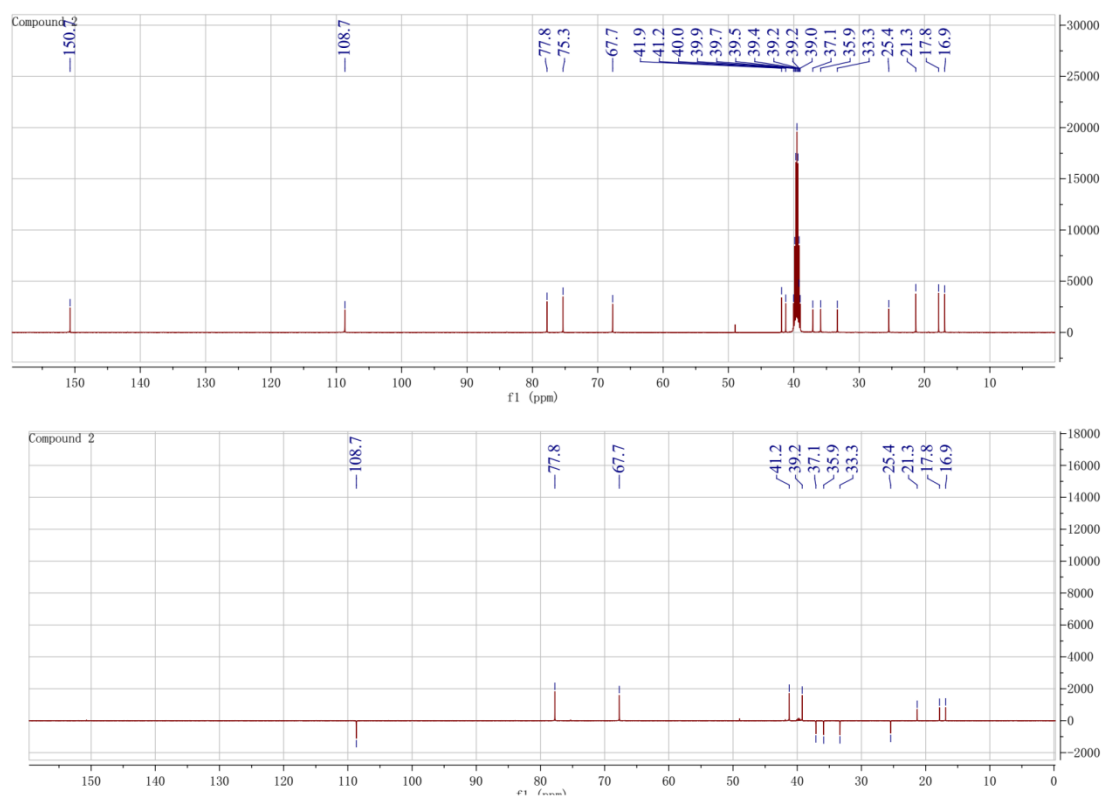


Figure S10. The ^1H - ^1H COSY (500 MHz, $\text{DMSO-}d_6$) spectrum of compound **2**

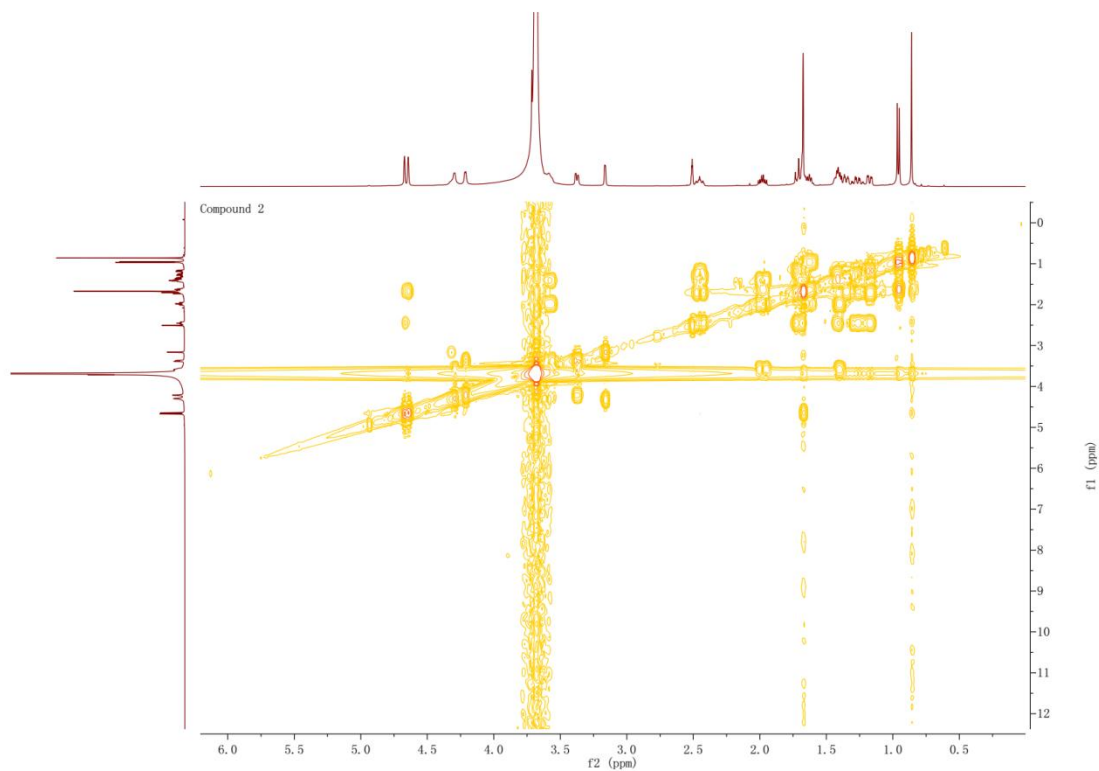


Figure S11. The HSQC (500 MHz, DMSO- d_6) spectrum of compound **2**

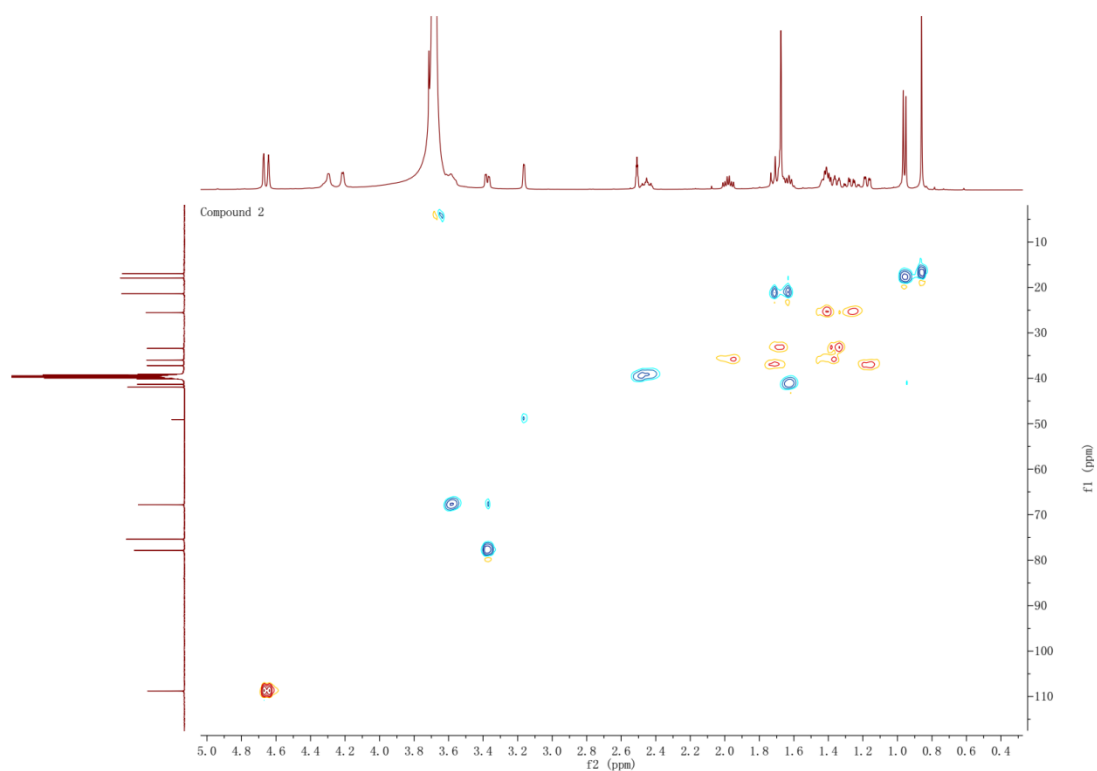


Figure S12. The HMBC (500 MHz, DMSO- d_6) spectrum of compound **2**

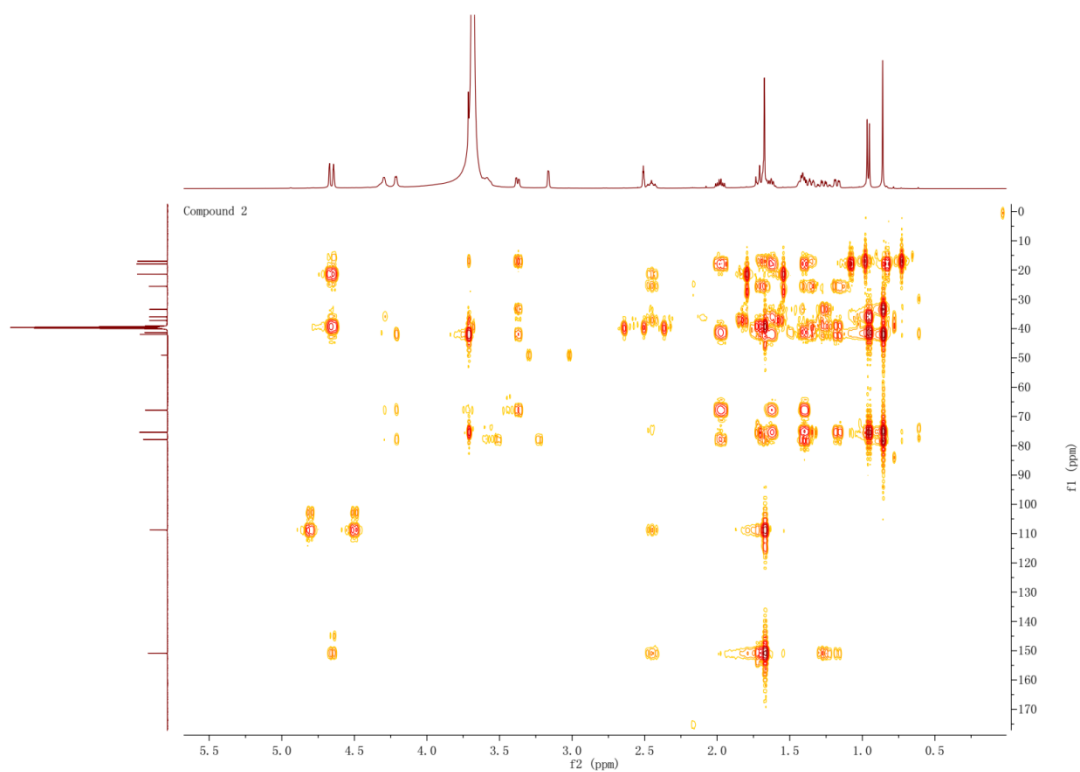


Figure S13. The ROESY (500 MHz, DMSO-*d*₆) spectrum of compound **2**

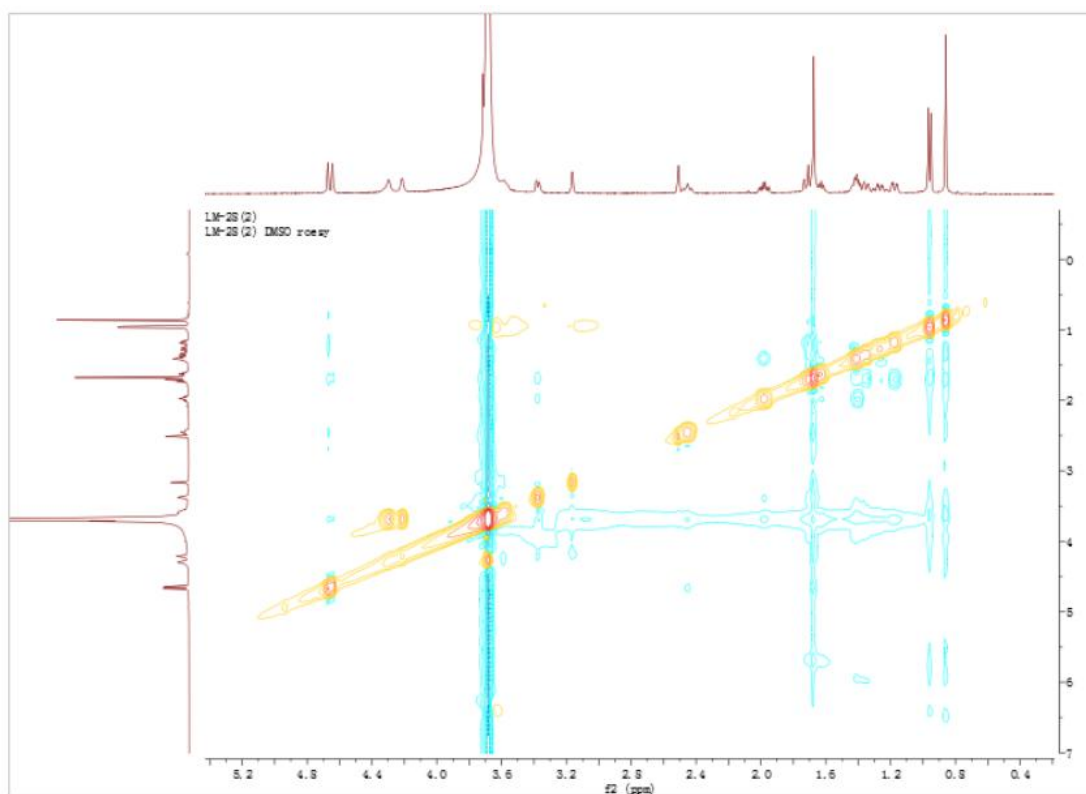


Figure S14. The HRESI spectrum of compound **2**

Elemental Composition Report

Single Mass Analysis

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Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

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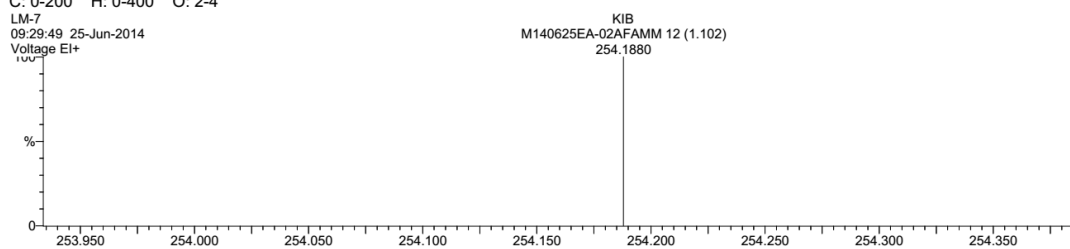
Elements Used:

C: 0-200 H: 0-400 O: 2-4

LM-7

09:29:49 25-Jun-2014

Voltage EI+



Minimum: 22.0 10.0 -10.0

Maximum: 22.0 10.0 120.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
254.1880	254.1882	-0.2	-0.8	3.0	5546025.5	C15 H26 O3

Figure S15. The ^1H NMR (500 MHz, $\text{DMSO-}d_6$) spectrum of compound **3**

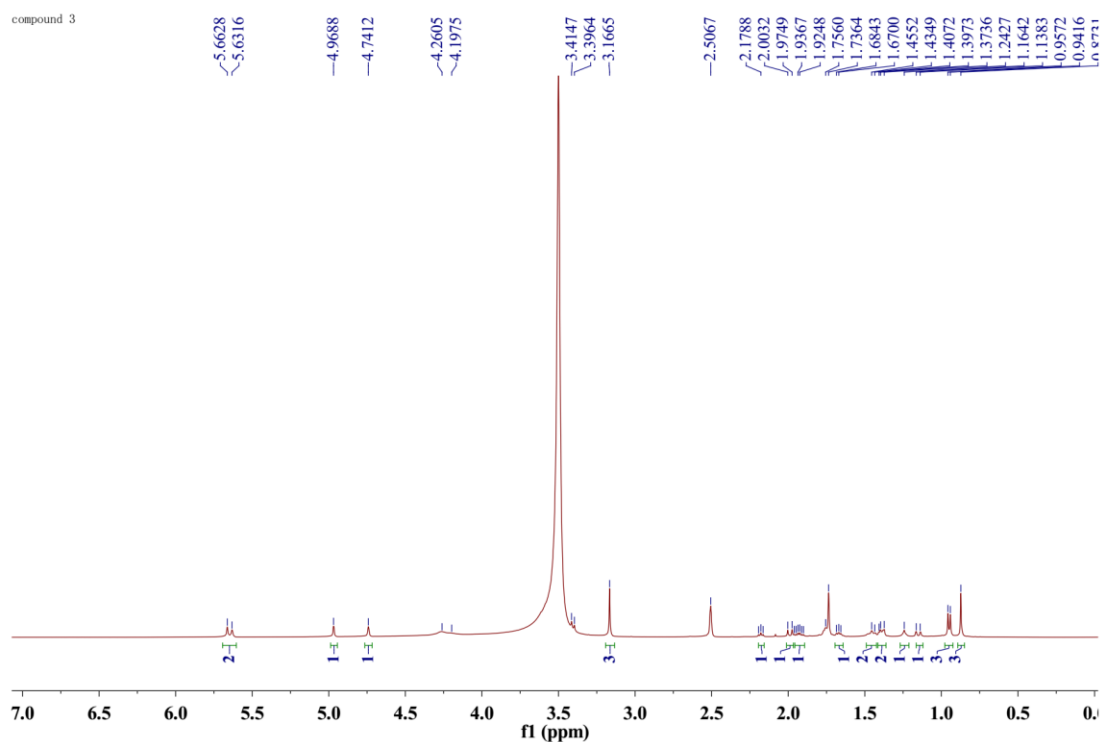


Figure S16. The ^{13}C NMR and DEPT135 (125 MHz, $\text{DMSO-}d_6$) spectrum of compound **3**

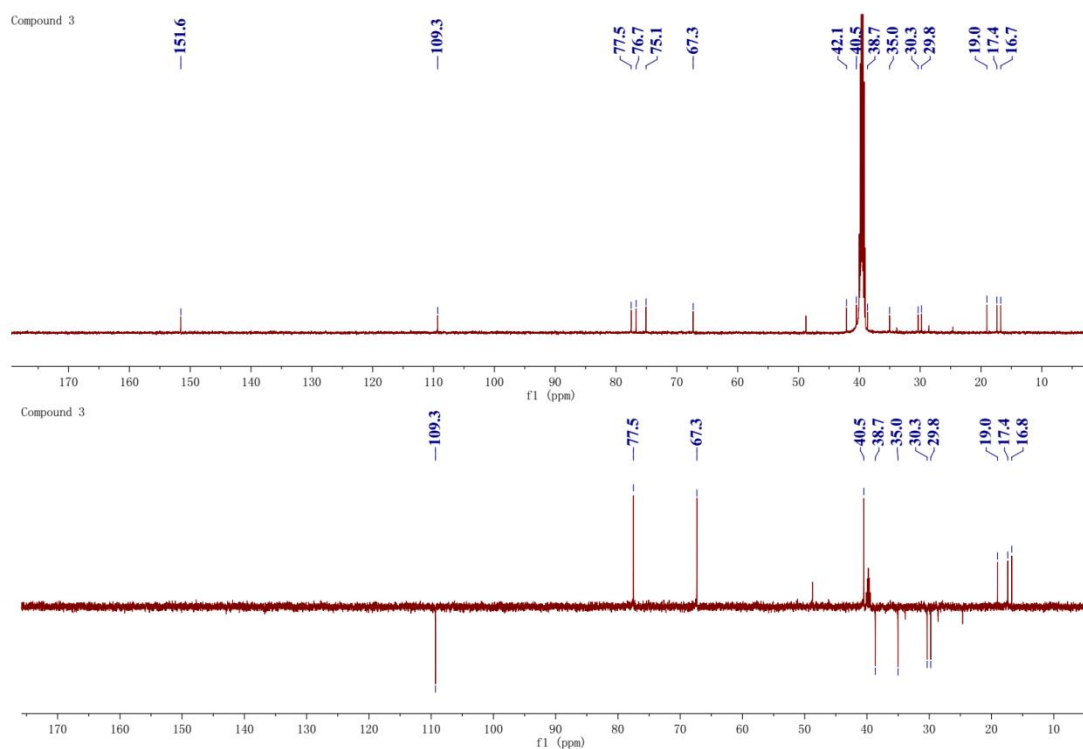


Figure S17. The ^1H - ^1H COSY (500 MHz, $\text{DMSO-}d_6$) spectrum of compound **3**

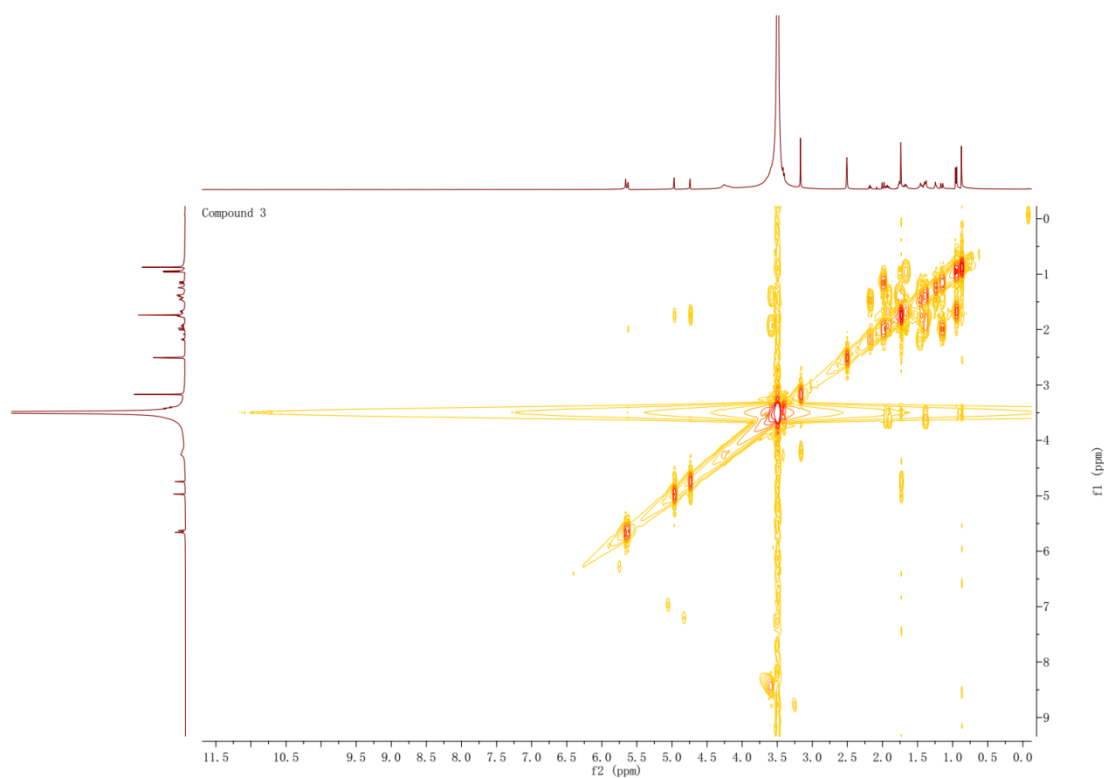


Figure S18. The HSQC (500 MHz, DMSO-*d*₆) spectrum of compound **3**

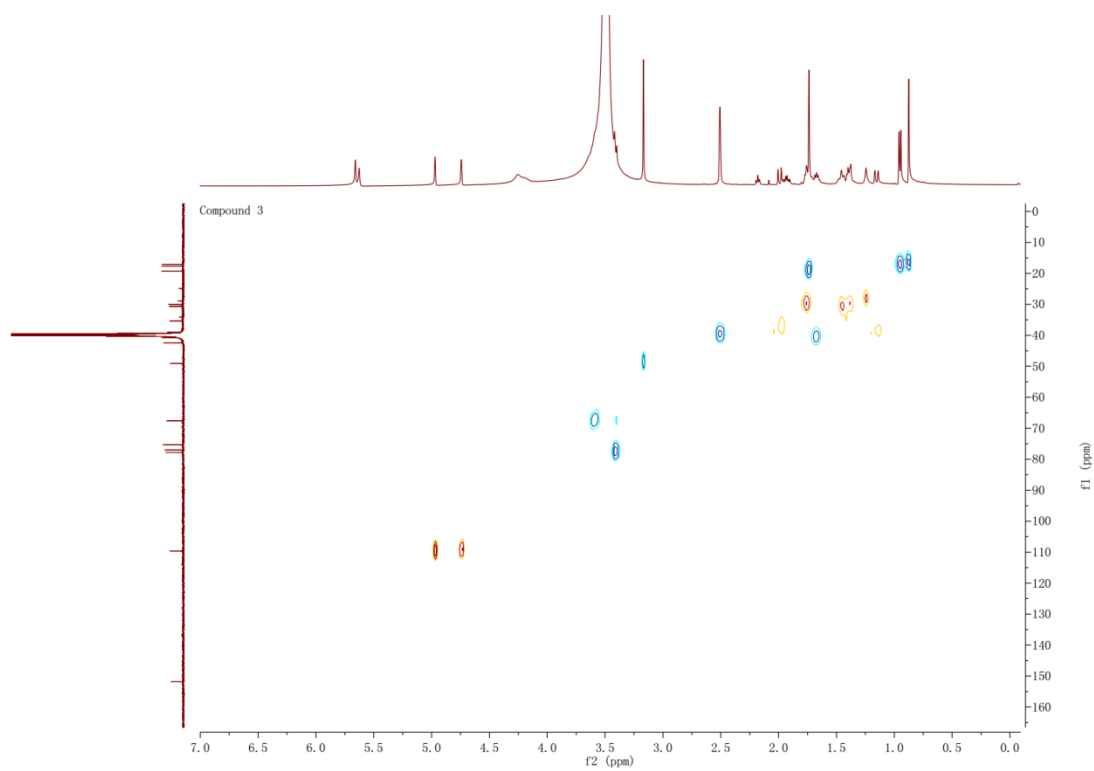


Figure S19. The HMBC (500 MHz, DMSO-*d*₆) spectrum of compound **3**

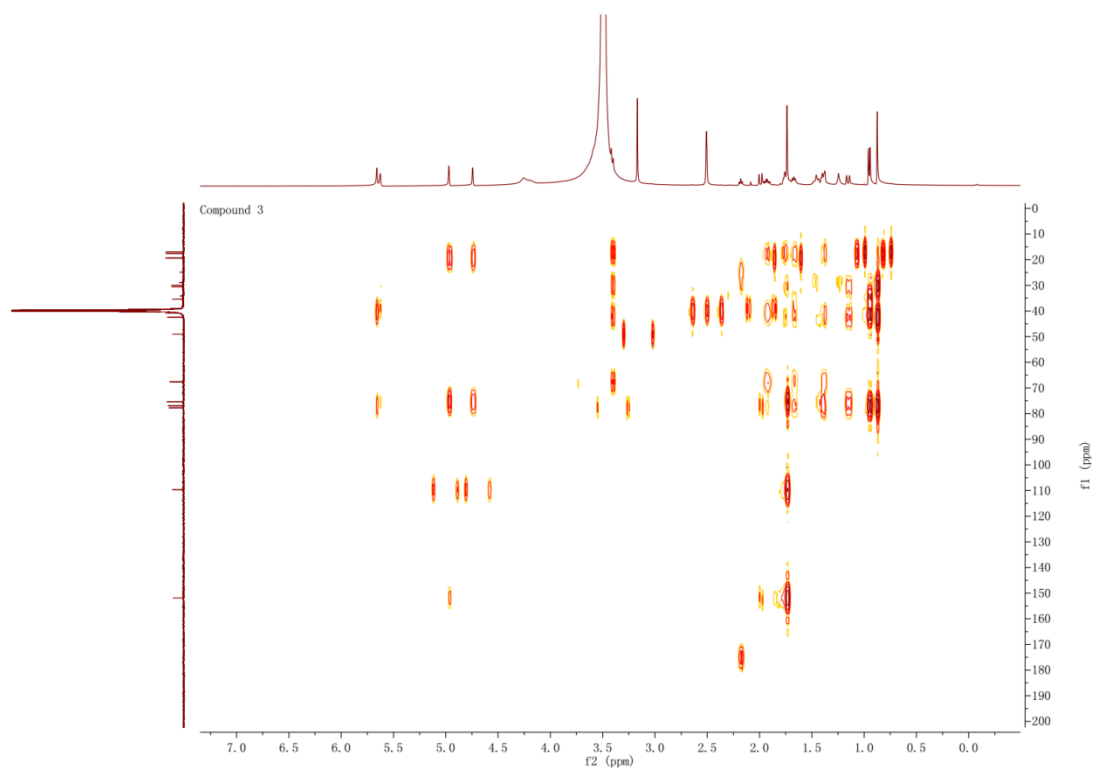


Figure S20. The ^1H - ^1H ROESY (500 MHz, $\text{DMSO}-d_6$) spectrum of compound **3**

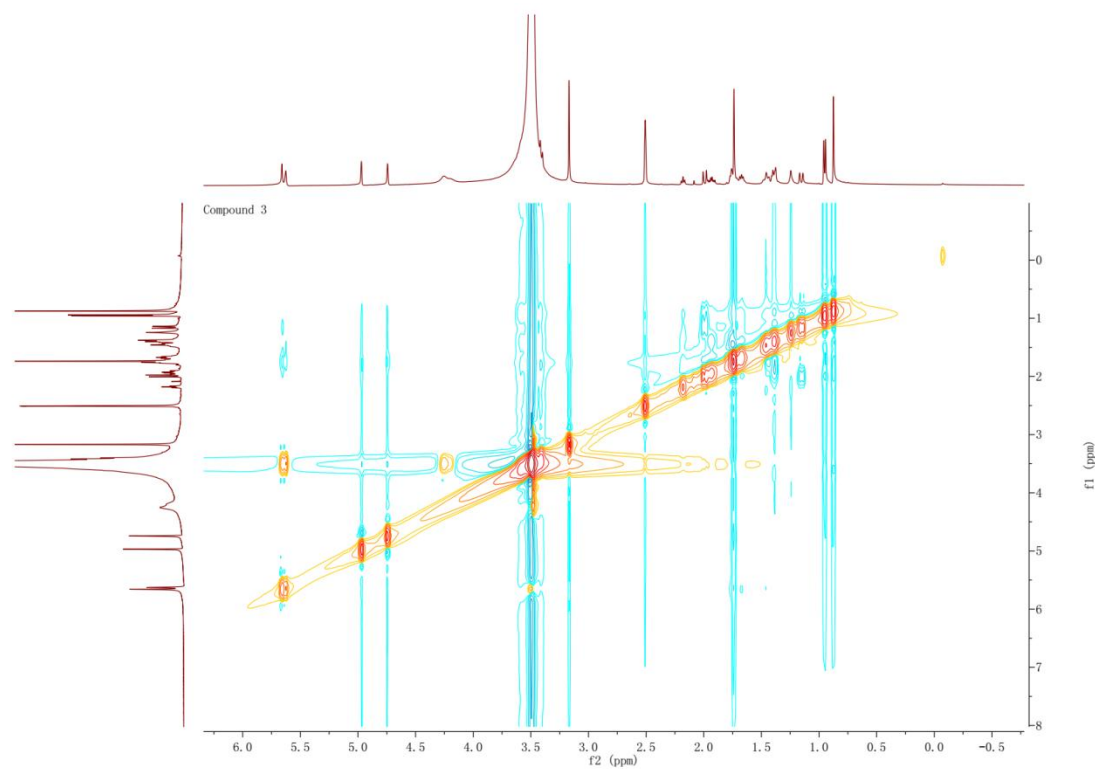


Figure S21. The HRESI spectrum of compound **3**

Single Mass Analysis

Tolerance = 22.0 mDa / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

14 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

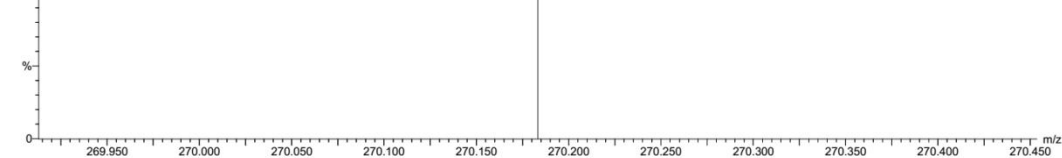
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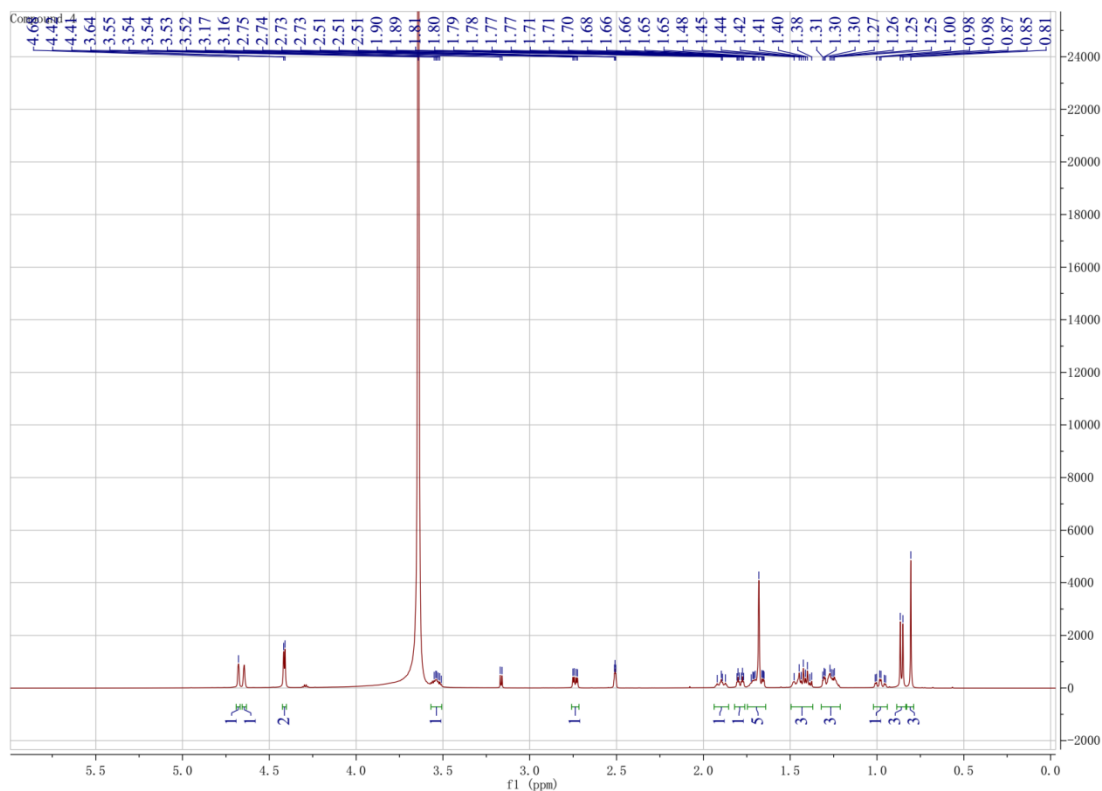
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09:48:02 25-Jun-2014

Voltage EI+

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270.1833Autospec Premier
P776
4.89

Minimum:	22.0	10.0	-10.0			
Maximum:			120.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
270.1833	270.1831	0.2	0.7	3.0	5546025.5	C15 H26 O4

Figure S22 The ^1H NMR (500 MHz, DMSO- d_6) spectrum of compound **4****Figure S23.** The ^{13}C NMR (125 MHz, DMSO- d_6) spectrum of compound **4**

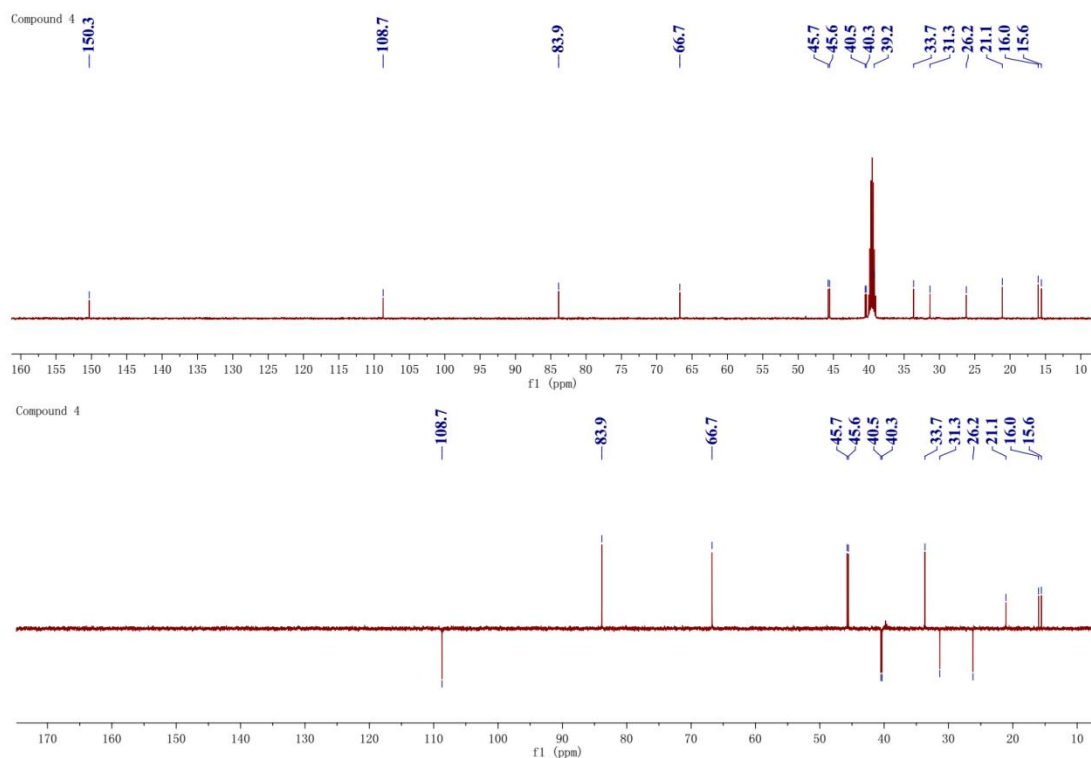


Figure S24. The ^1H - ^1H COSY (500 MHz, $\text{DMSO-}d_6$) spectrum of compound **4**

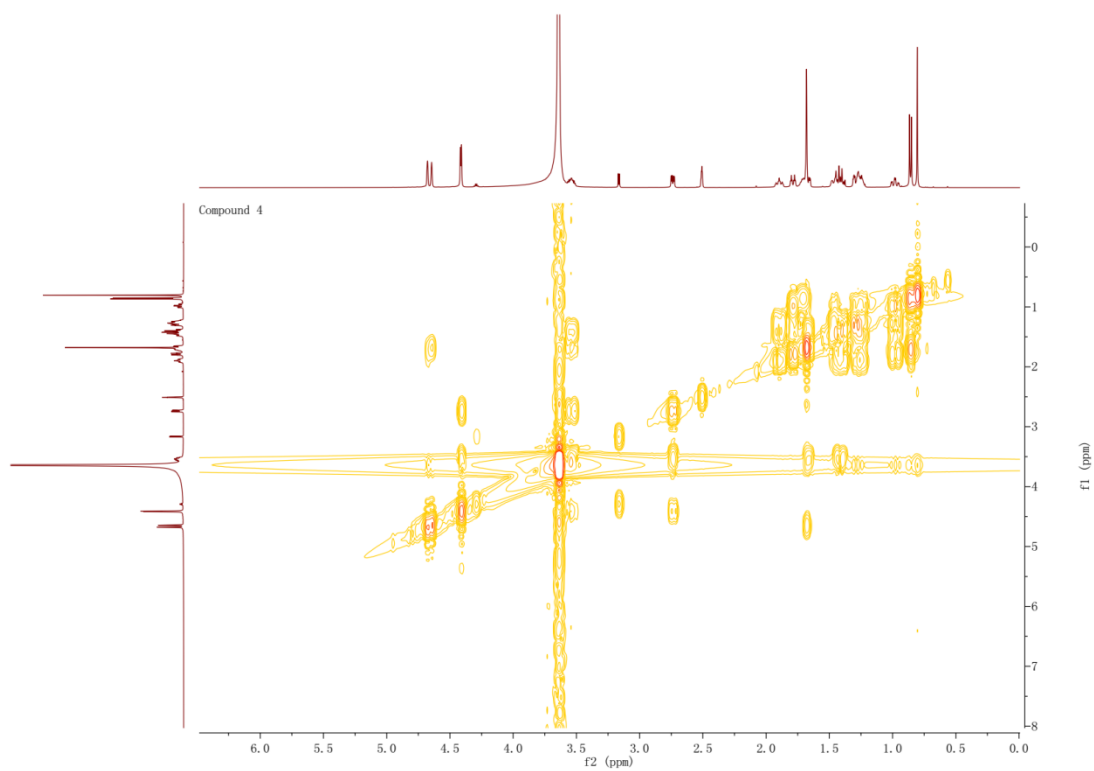


Figure S25. The HSQC (500 MHz, DMSO- d_6) spectrum of compound **4**

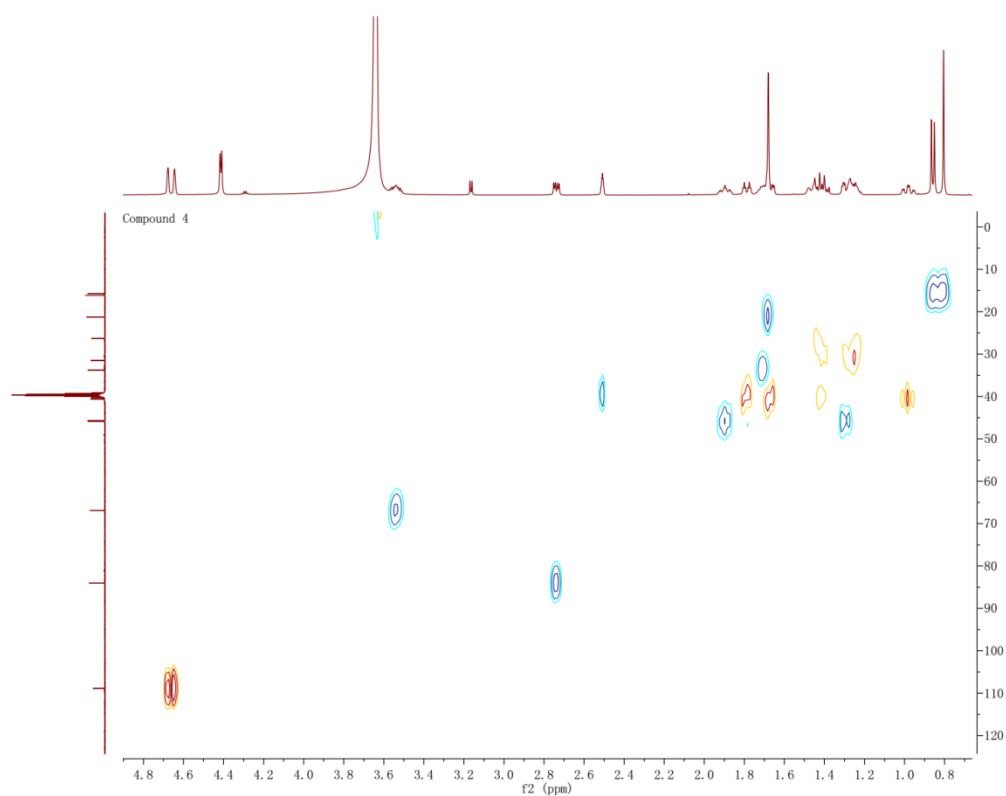


Figure S26. The HMBC (500 MHz, DMSO- d_6) spectrum of compound **4**

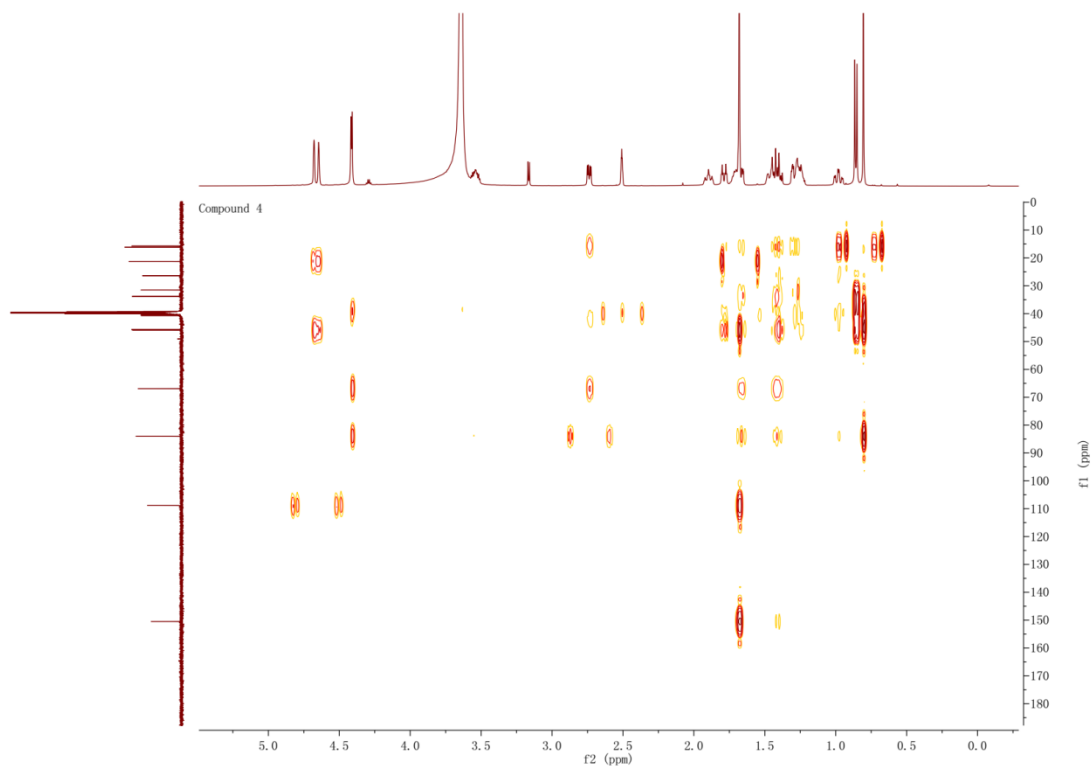


Figure S27. The ^1H - ^1H ROESY (500 MHz, DMSO- d_6) spectrum of compound **4**

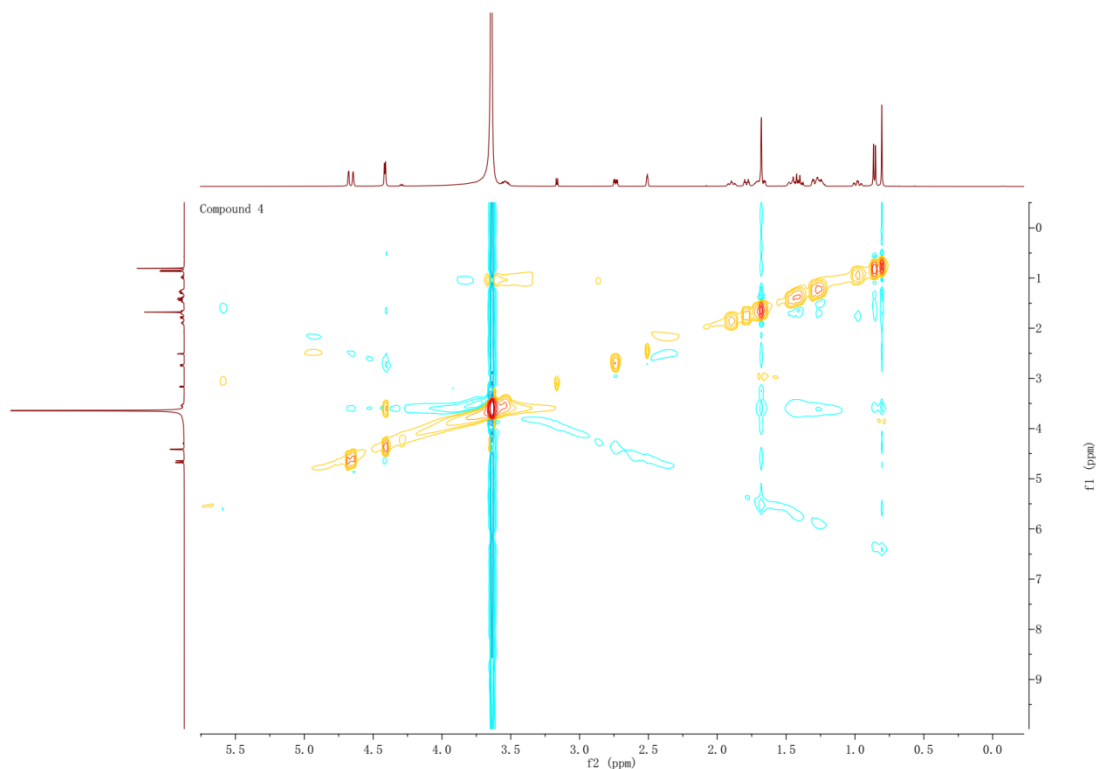


Figure S28. The HRESI spectrum of compound **4**

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 22.0 mDa / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

14 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

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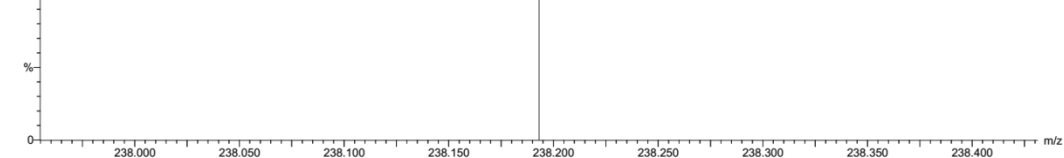
LM-6

09:24:18 25-Jun-2014

Voltage E1+

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238.1931

Autospec Premier
P776
12.4



Minimum:				-10.0		
Maximum:	22.0	10.0		120.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
238.1931	238.1933	-0.2	-0.8	3.0	5546026.0	C15 H26 O2

Figure S29. The ^1H NMR (500 MHz, $\text{CD}_3\text{OD}-d_4$) spectrum of *S*-MTPA ester **1a** and

¹H NMR spectrum of compound 10a in CDCl₃. The x-axis represents chemical shift (ppm) from 0.0 to 8.5. The y-axis represents intensity from 0.0E+00 to 1.2E+08. The spectrum shows a complex set of peaks in the aromatic region (6.5-7.5 ppm) and aliphatic region (1.0-3.5 ppm). Integration values are provided below the baseline for various peak groups.

Chemical Shift (ppm)	Integration
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7.504	1.00
7.496	1.00
7.3367	1.00
7.3296	1.00
7.3241	1.00
7.3173	1.00
7.3154	1.00
7.3112	1.00
7.3083	1.00
5.2458	1.00
5.2319	1.00
5.2257	1.00
5.2119	1.00
4.9340	1.00
4.6994	1.00
3.5198	1.00
3.2136	1.00
3.2105	1.00
3.2074	1.00
3.1709	1.00
3.1510	1.00
1.8427	1.00
1.8394	1.00
1.8297	1.00
1.8173	1.00
1.8135	1.00
1.8085	1.00
1.7969	1.00
1.7240	1.00
1.6849	1.00
1.6658	1.00
1.6575	1.00
1.6305	1.00
1.5936	1.00
1.5888	1.00
1.5803	1.00
1.5680	1.00
1.5620	1.00
1.5279	1.00
1.5164	1.00
1.5034	1.00
1.4921	1.00
1.4790	1.00
1.4580	1.00
1.4508	1.00
1.4319	1.00
1.4243	1.00
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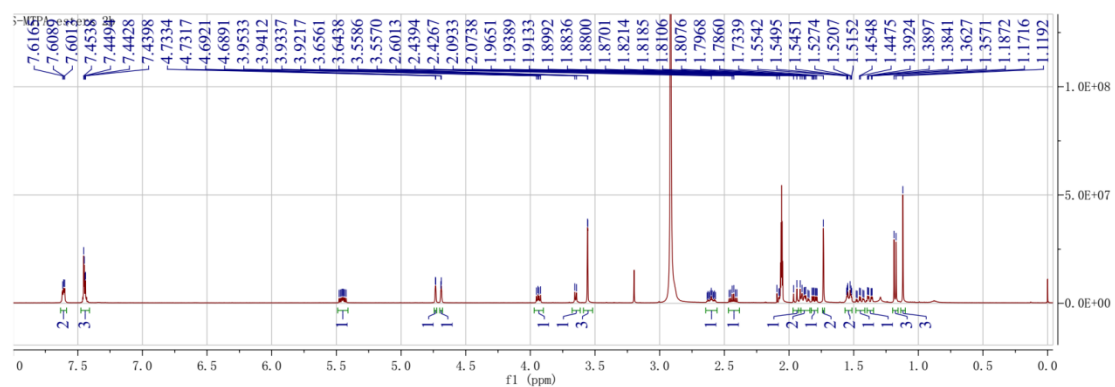
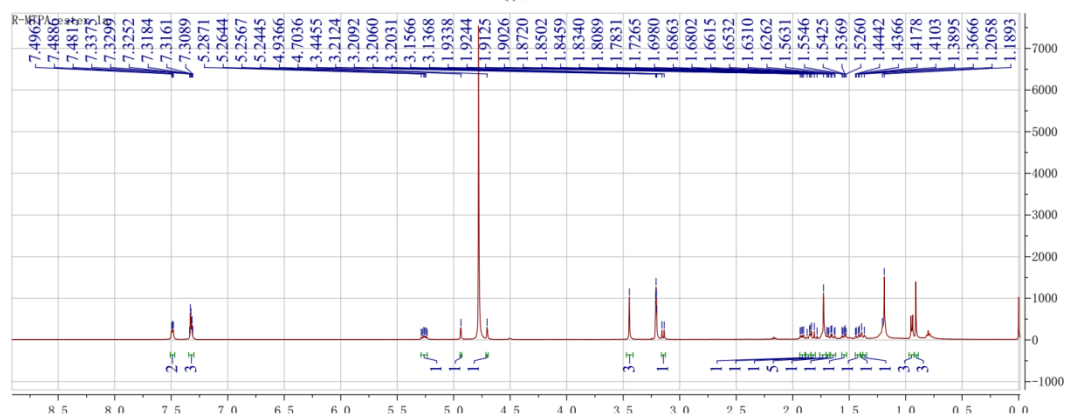


Figure S31. The ^1H NMR (500 MHz, $\text{CD}_3\text{OD}-d_4$) spectrum of *S*-MTPA ester **3a** and

R-MTPA ester**3b**

