Thielavins W–Z_7, New Antifouling Thielavins from the Marine-Derived Fungus *Thielavia* sp. UST030930-004

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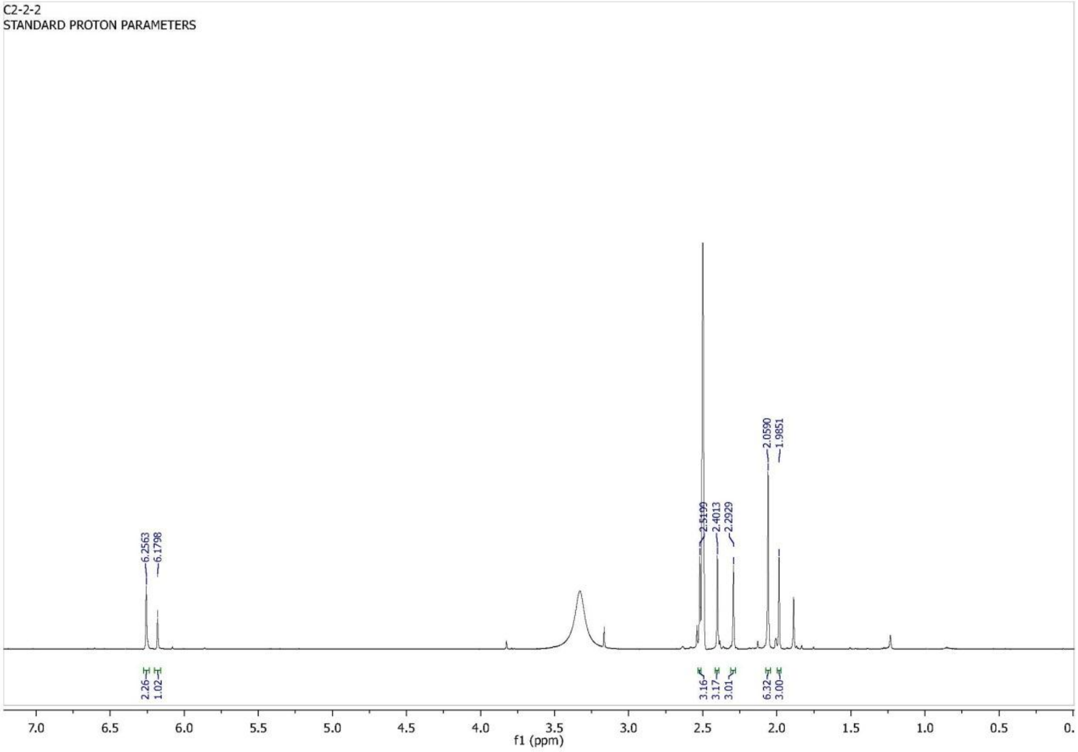

Figure S1 ^{1}H NMR spectrum of **1** in DMSO-*d₆* (500 MHz)

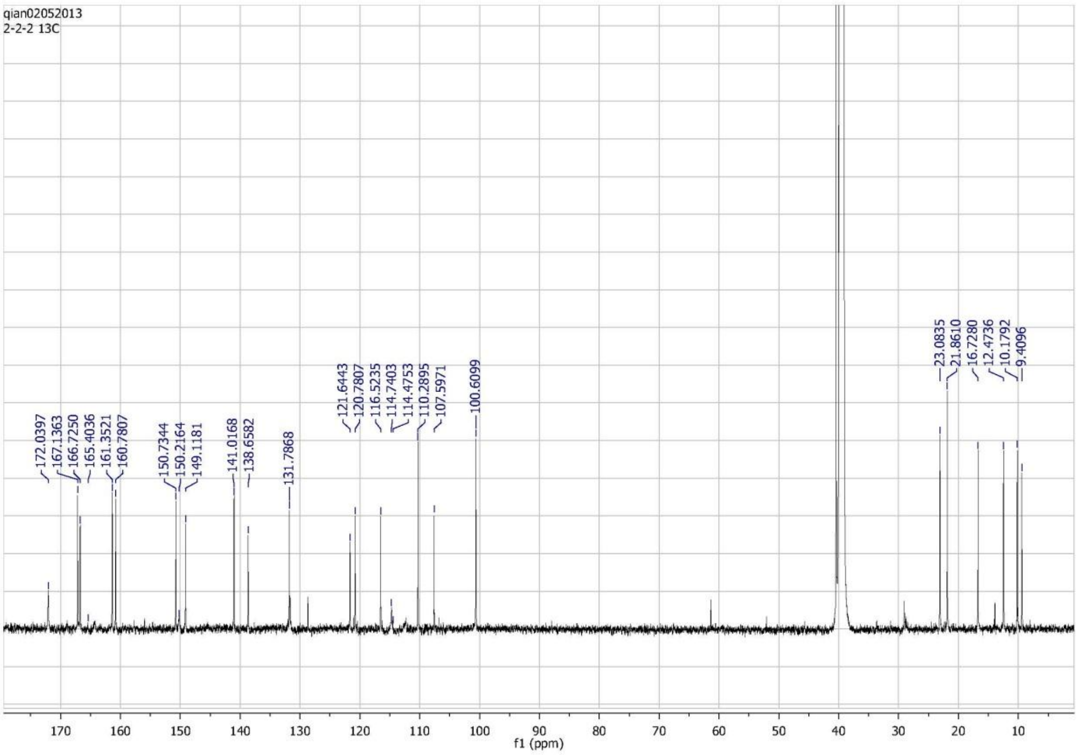

Figure S2 ^{13}C NMR spectrum of **1** in DMSO-*d₆* (125 MHz)

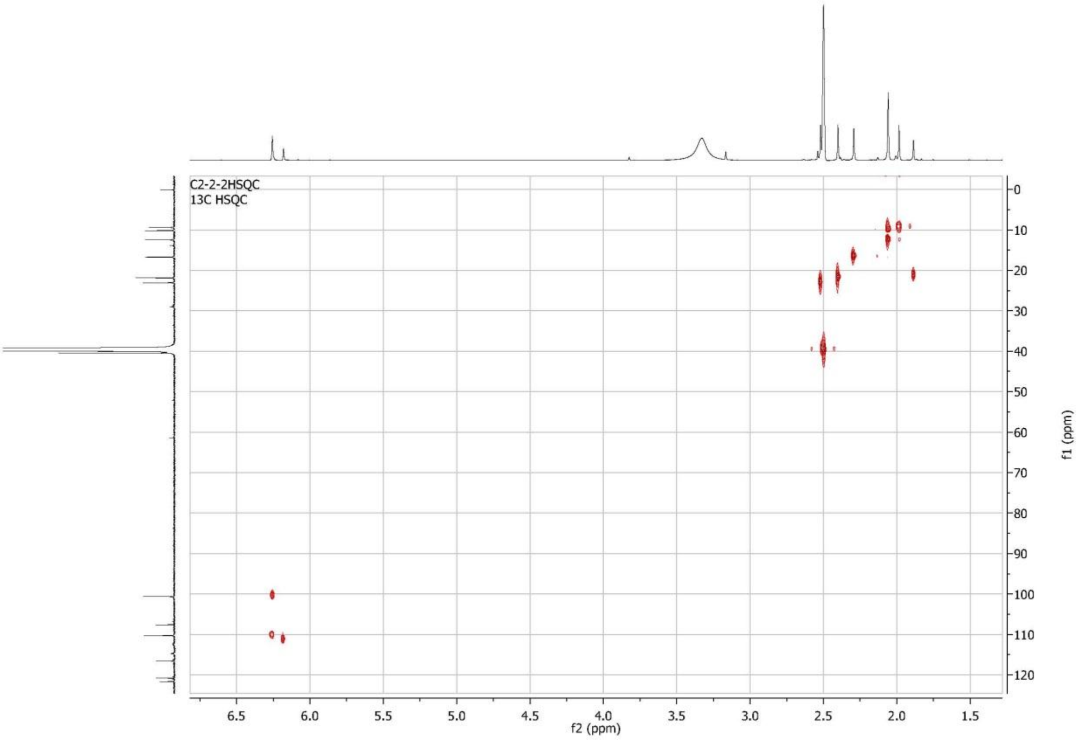

Figure S3 HMQC spectrum of **1** in DMSO-d_6

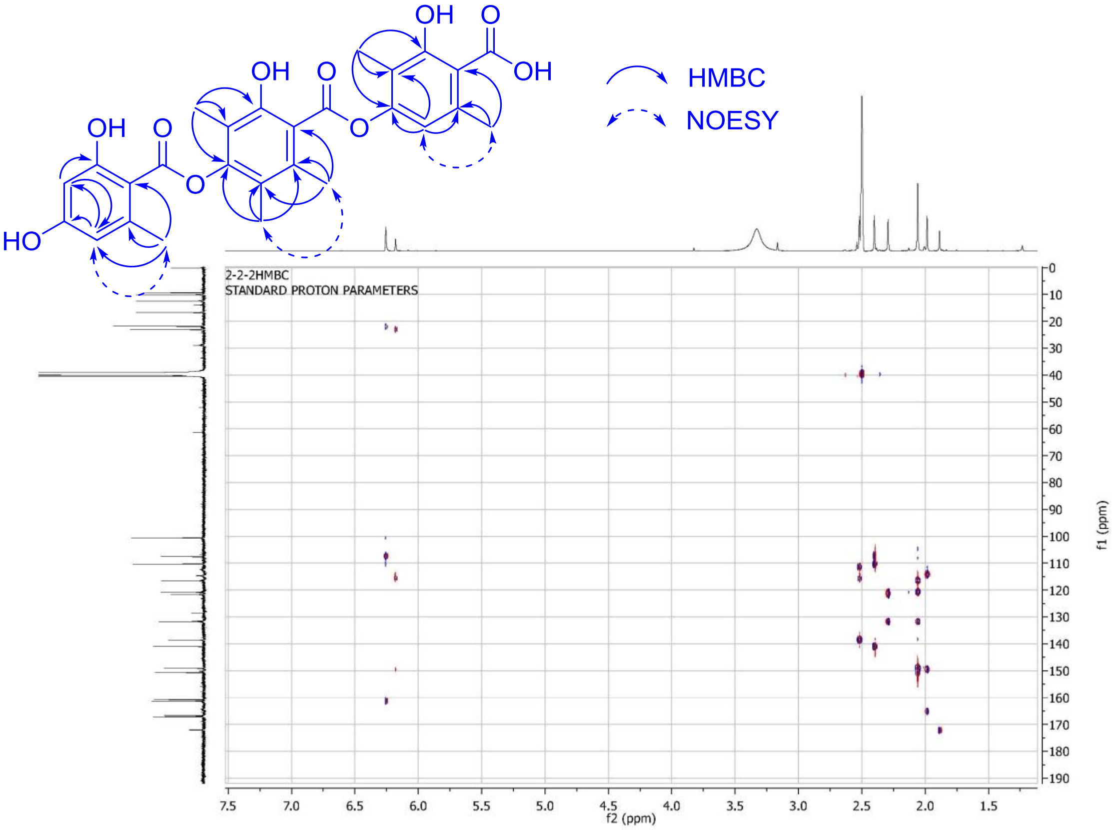

Figure S4 HMBC spectrum of **1** in DMSO-d_6

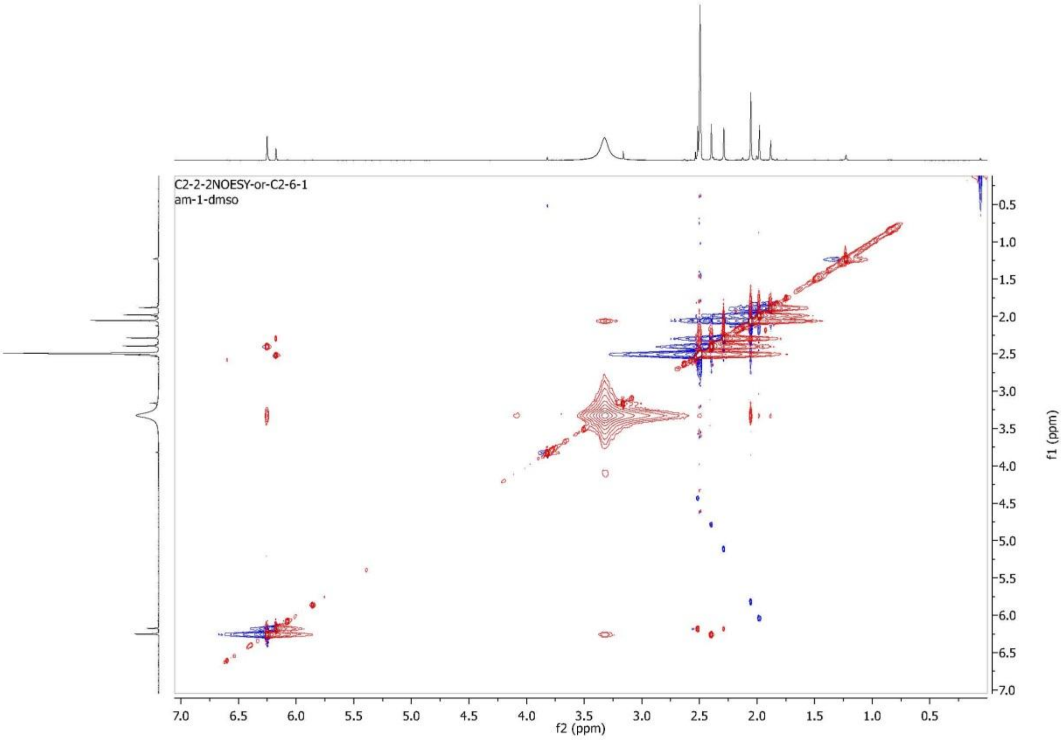

Figure S5 NOESY spectrum of **1** in DMSO-d_6

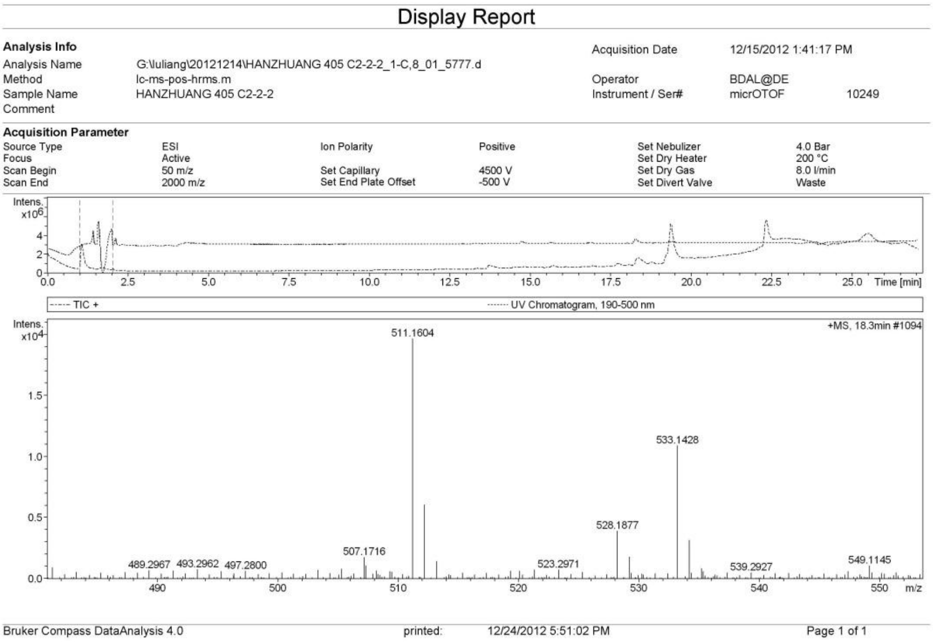

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Figure S6 HRESIMS spectrum of **1**

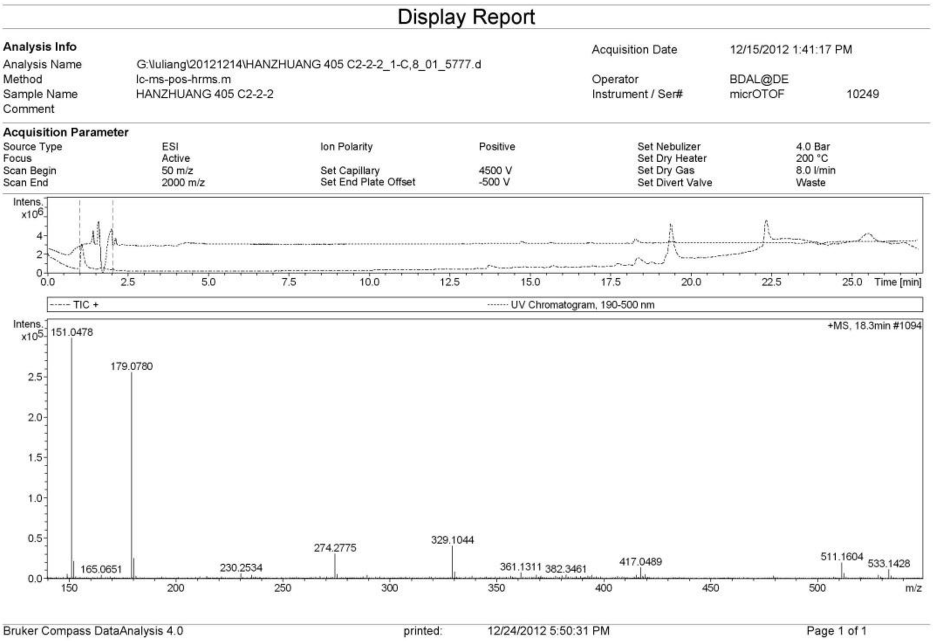

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Figure S7 ISCID spectrum of **1**

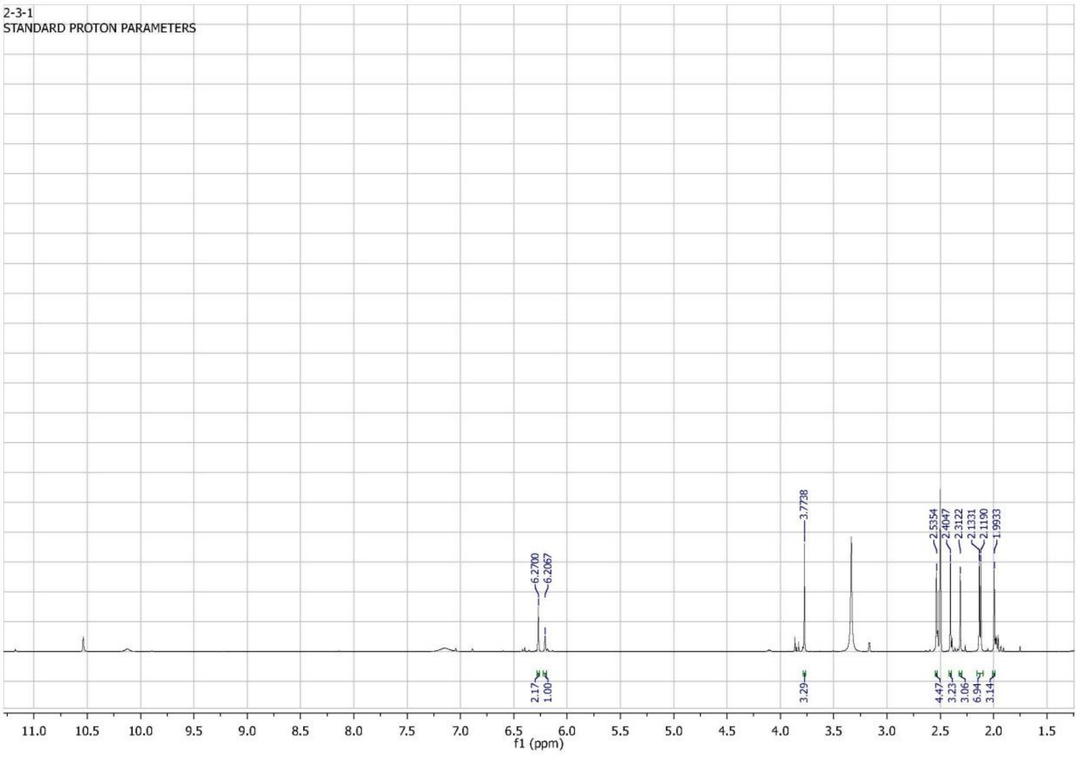

Figure S8 ^{1}H NMR spectrum of **2** in DMSO-d_6 (500 MHz)

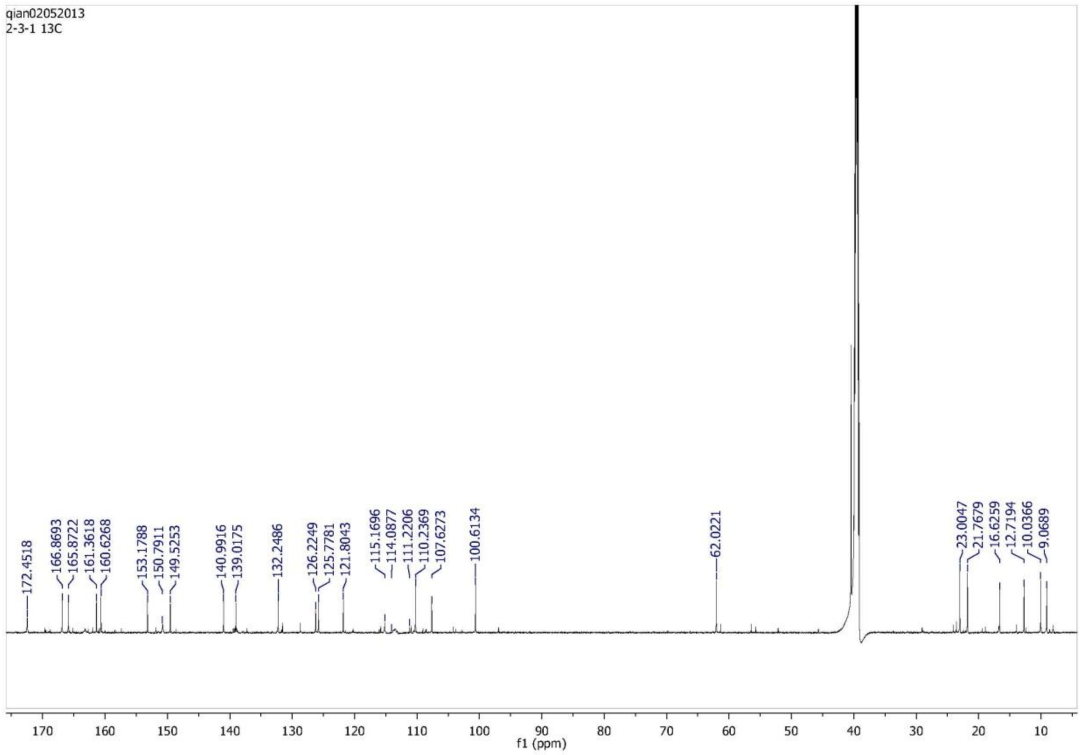

Figure S9 ^{13}C NMR spectrum of **2** in DMSO-d_6 (125 MHz)

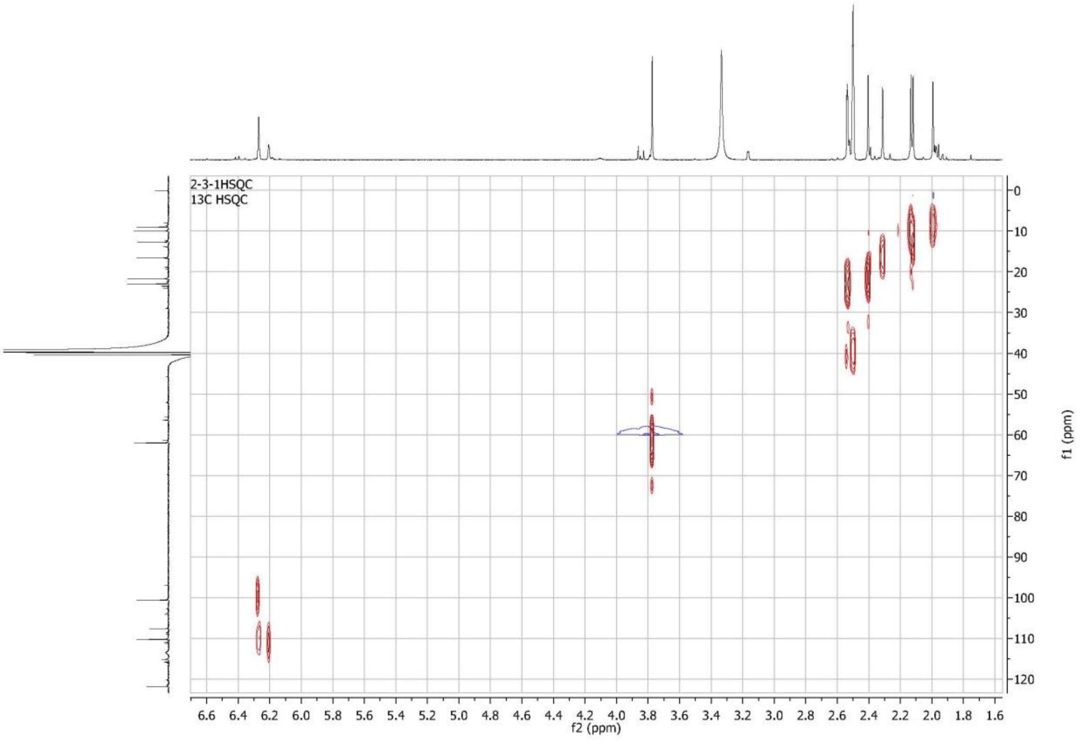

Figure S10 HMQC spectrum of **2** in DMSO-d_6

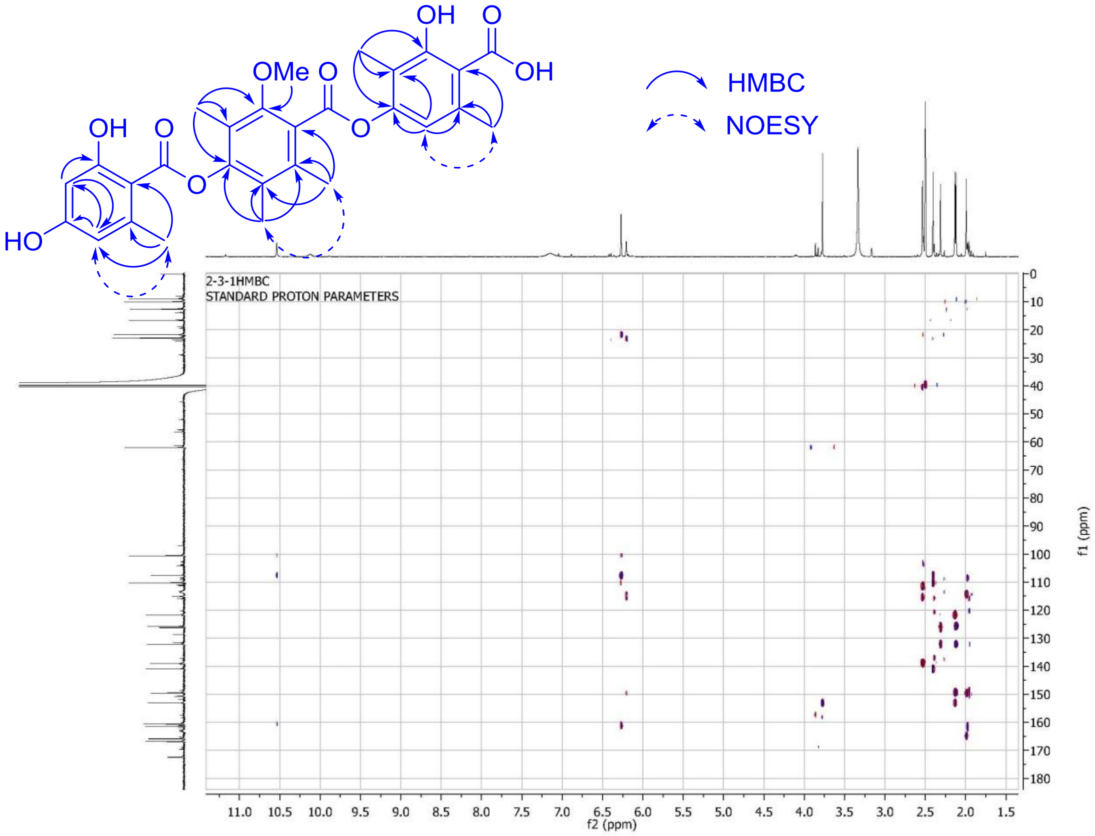

Figure S11 HMBC spectrum of **2** in DMSO-d_6

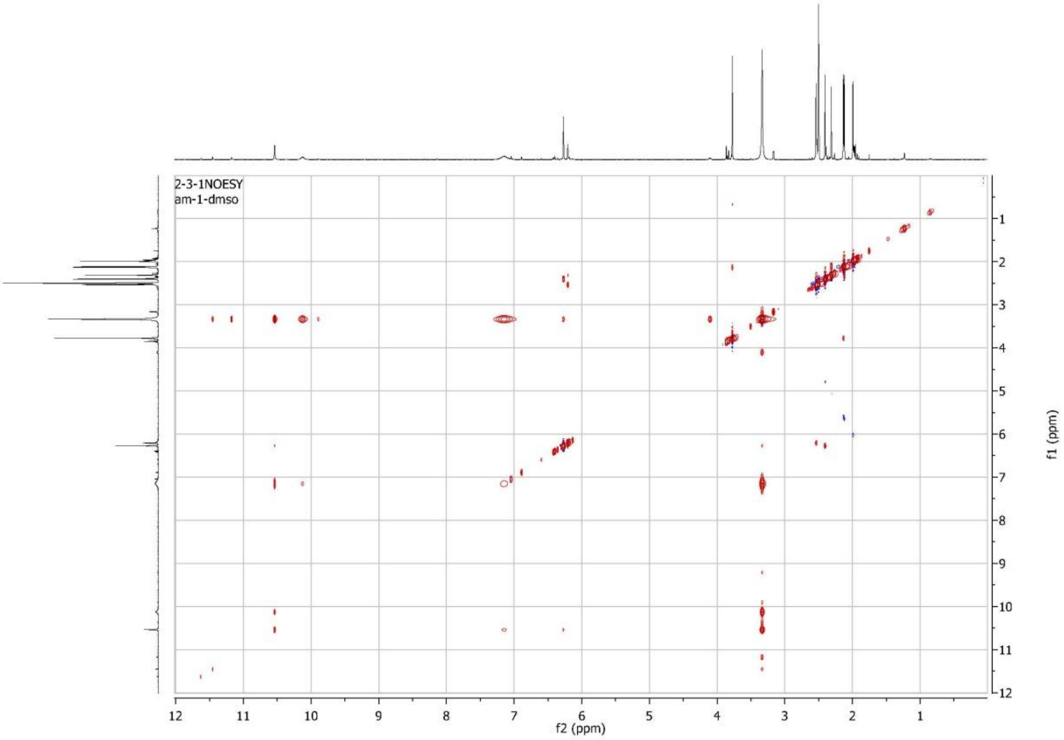

Figure S12 NOESY spectrum of **2** in DMSO-d_6

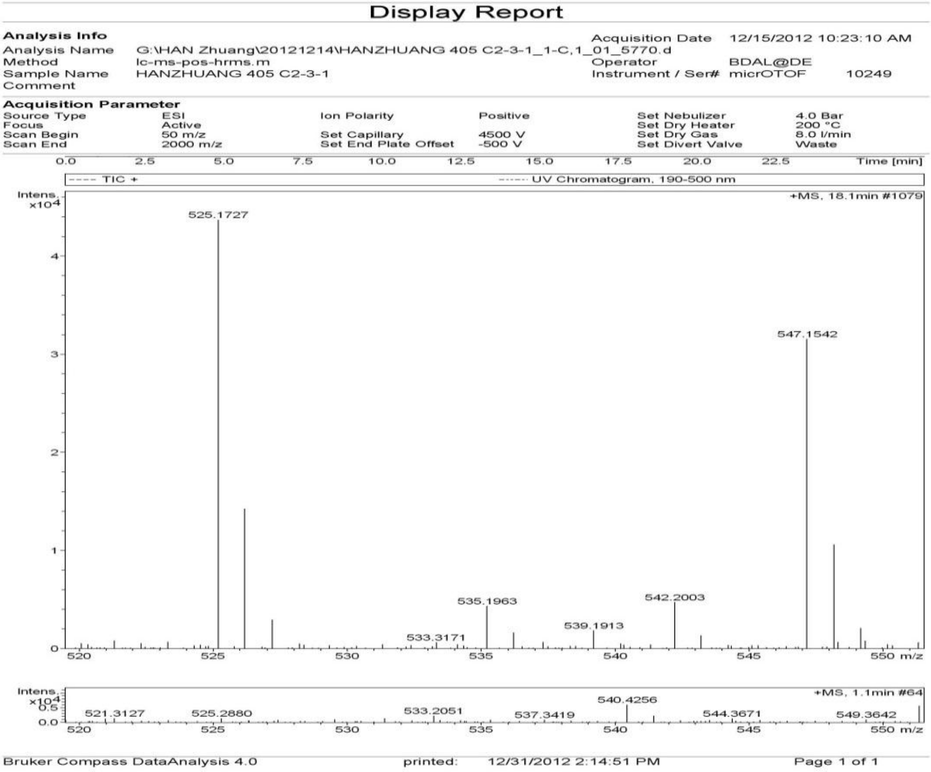

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Figure S13 HRESIMS spectrum of **2**

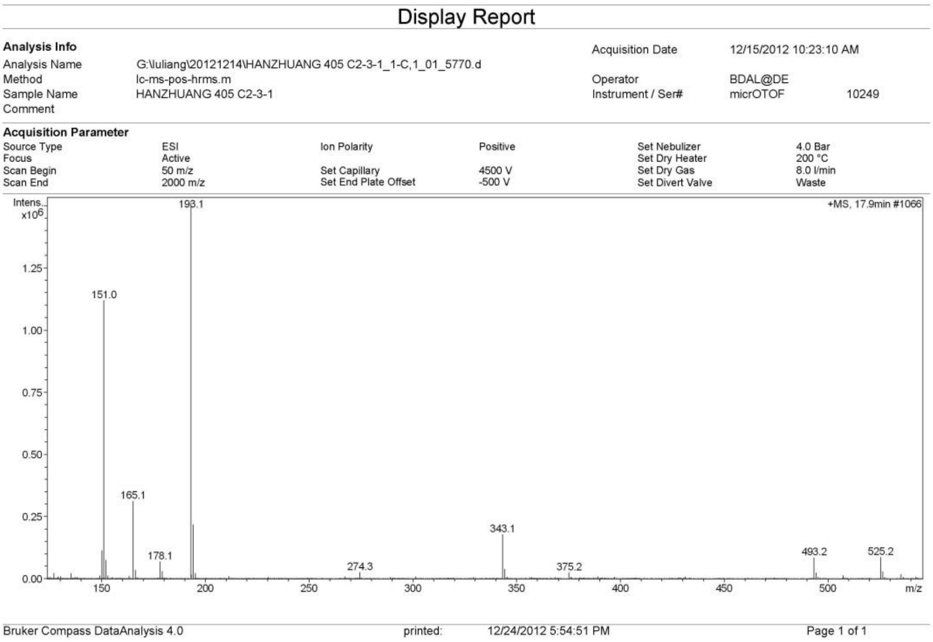

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Figure S14 ISCID spectrum of **2**

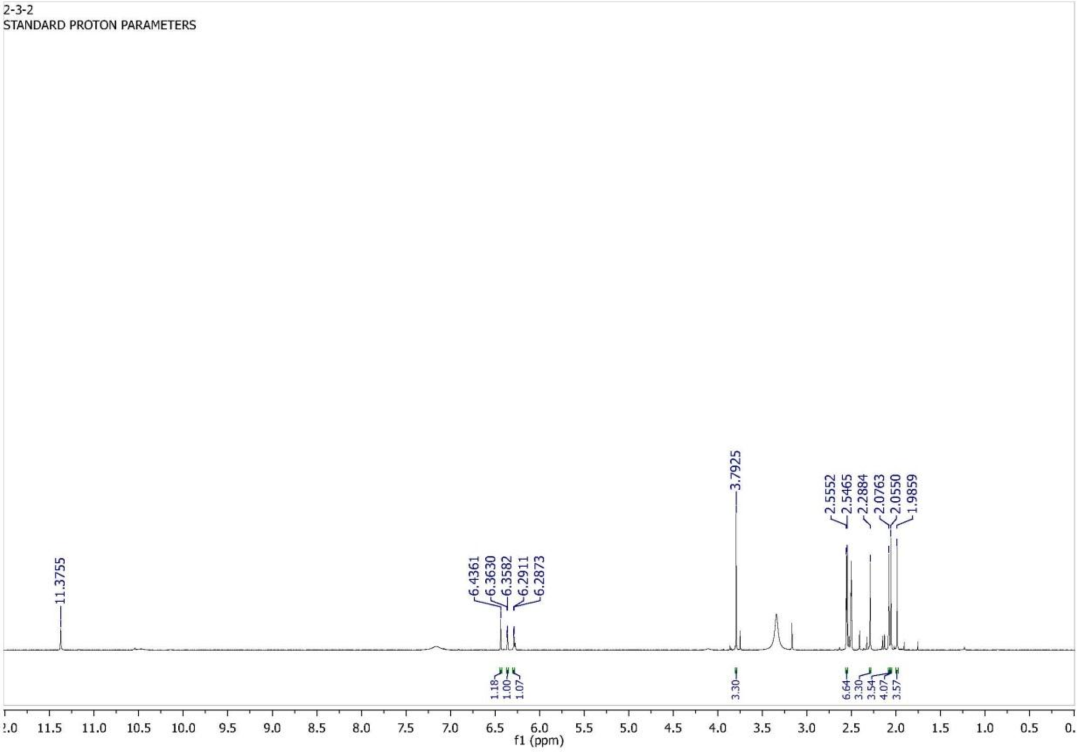

Figure S15 ^{1}H NMR spectrum of **3** in DMSO-d_6 (500 MHz)

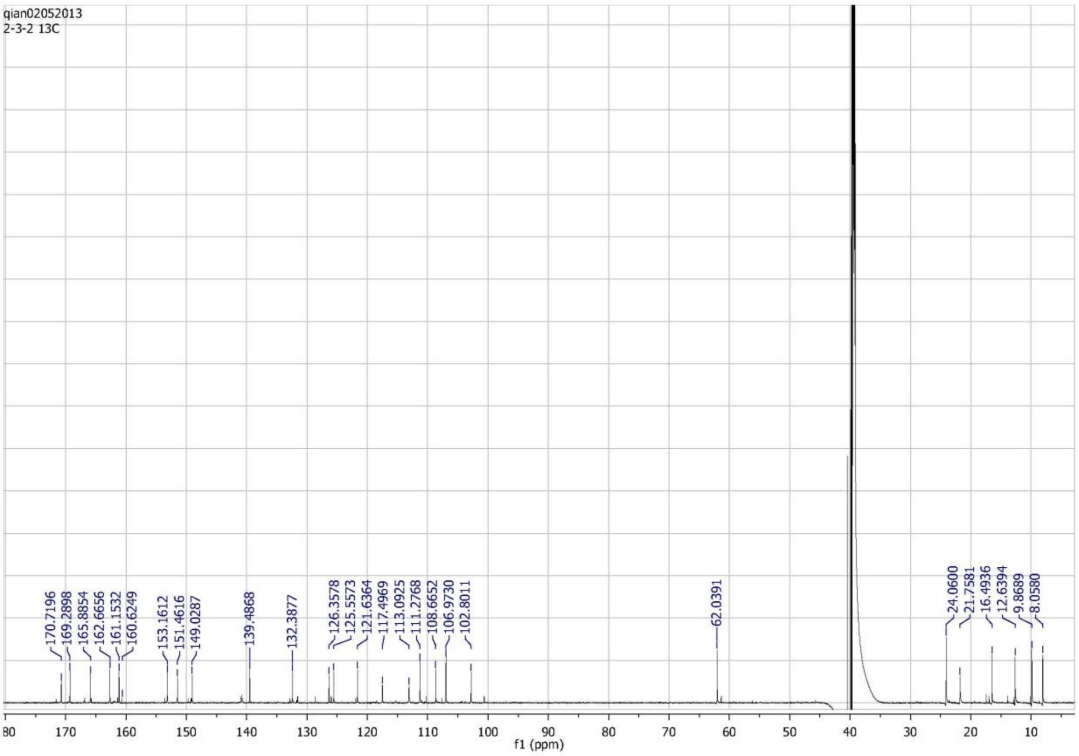

Figure S16 ^{13}C NMR spectrum of **3** in DMSO-d_6 (125 MHz)

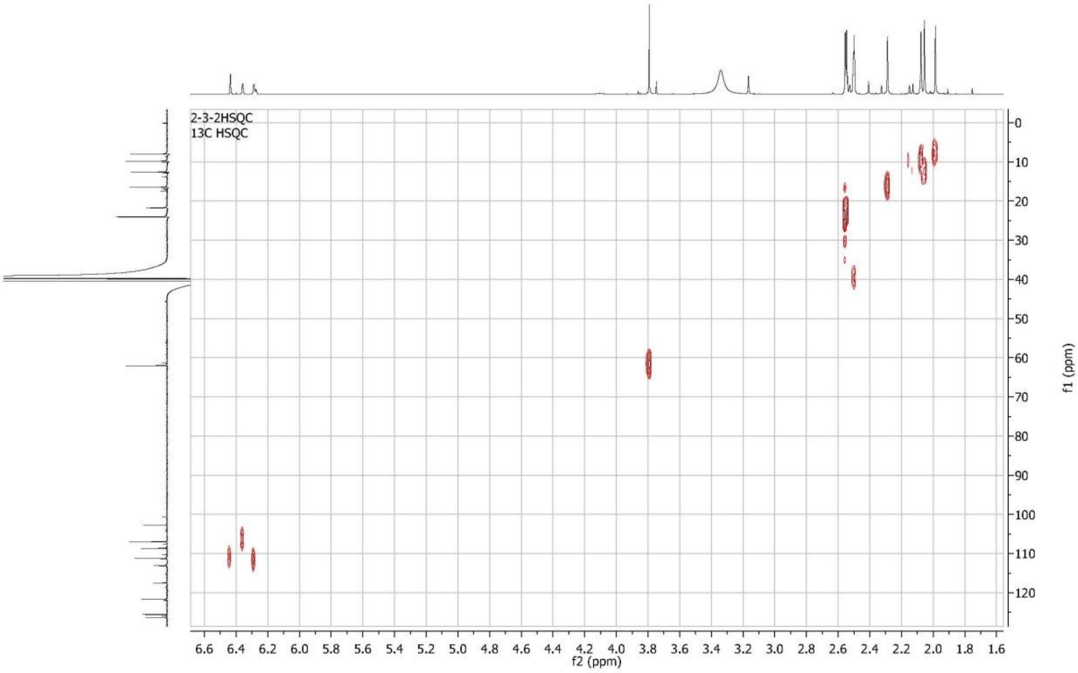

Figure S17 HMQC spectrum of **3** in DMSO-d_6

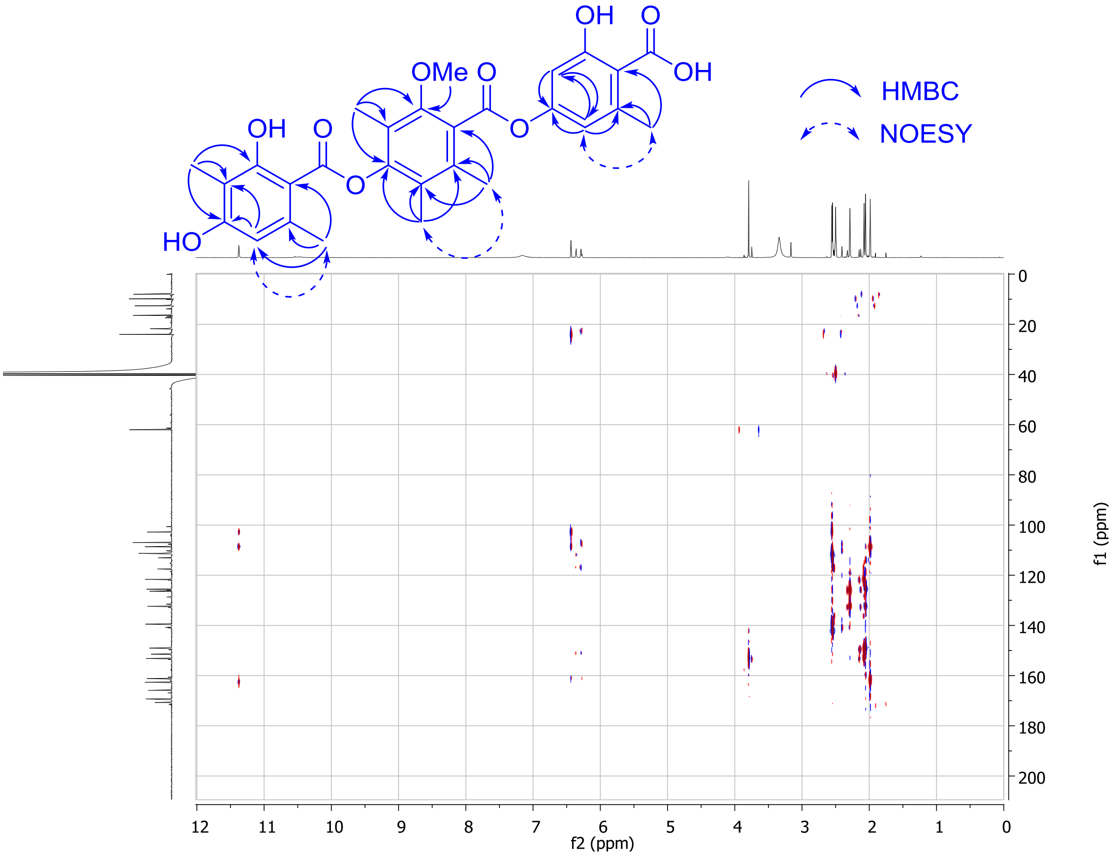

Figure S18 HMBC spectrum of **3** in DMSO-d_6

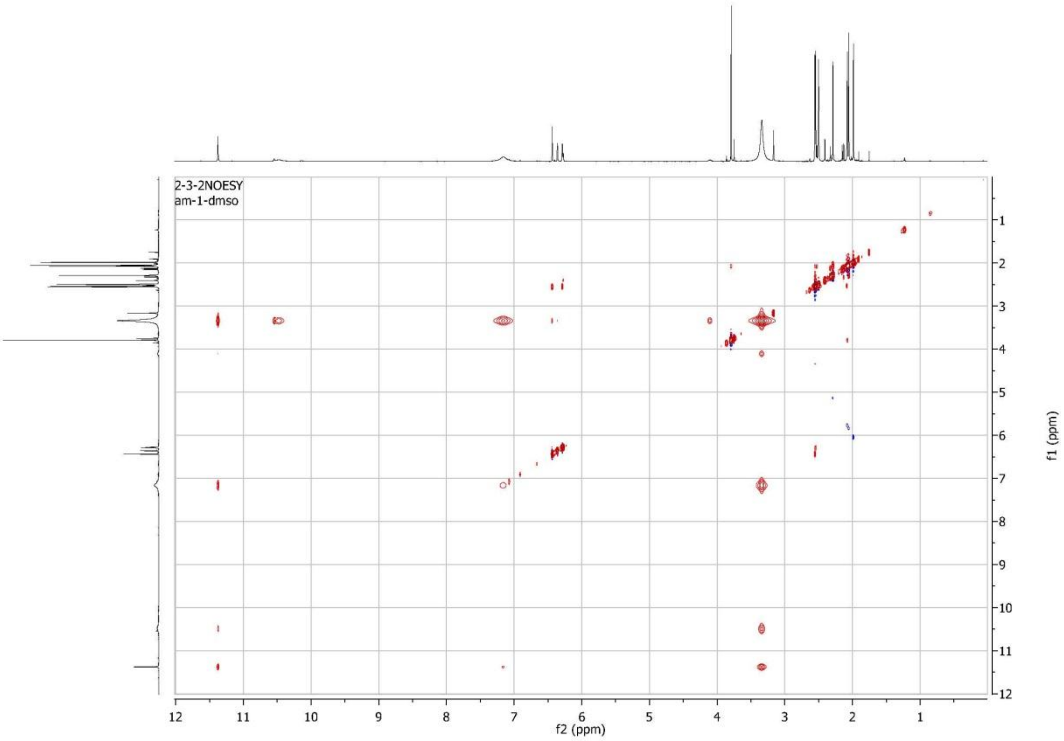

Figure S19 NOESY spectrum of **3** in DMSO-*d₆*

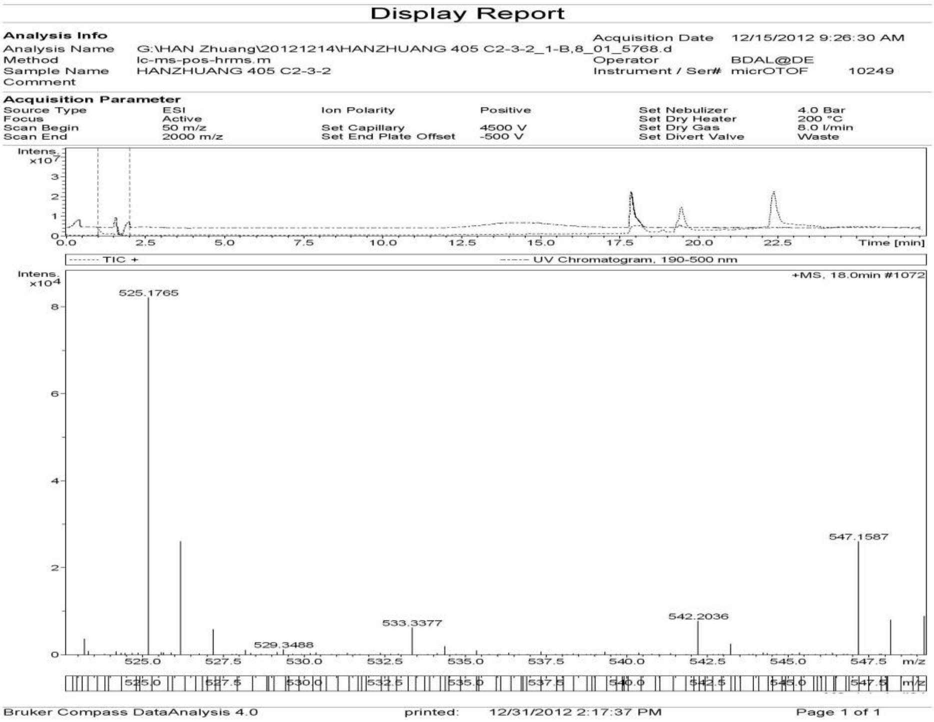

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Figure S20 HRESIMS spectrum of **3**

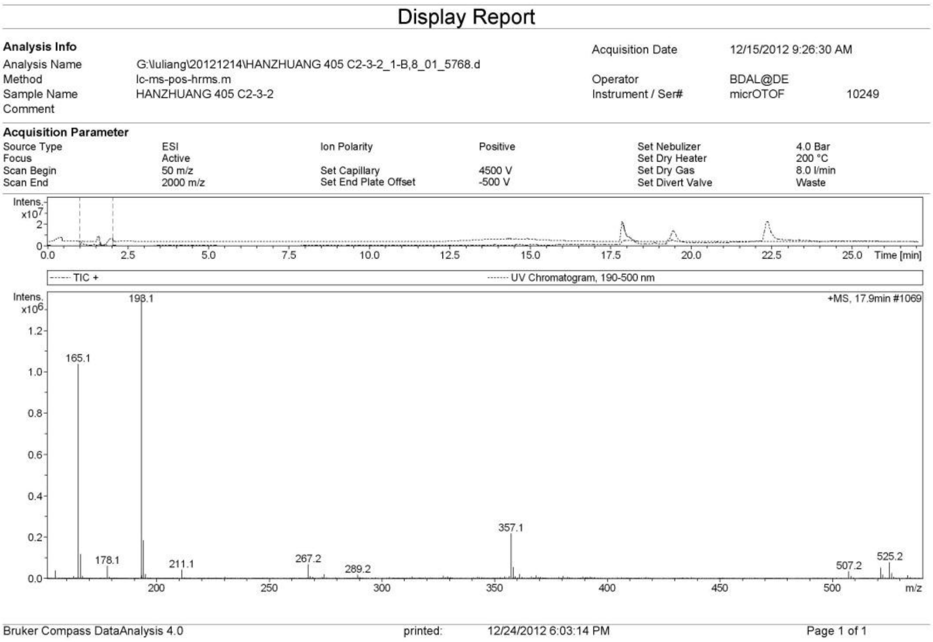

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Figure S21 ISCID spectrum of **3**

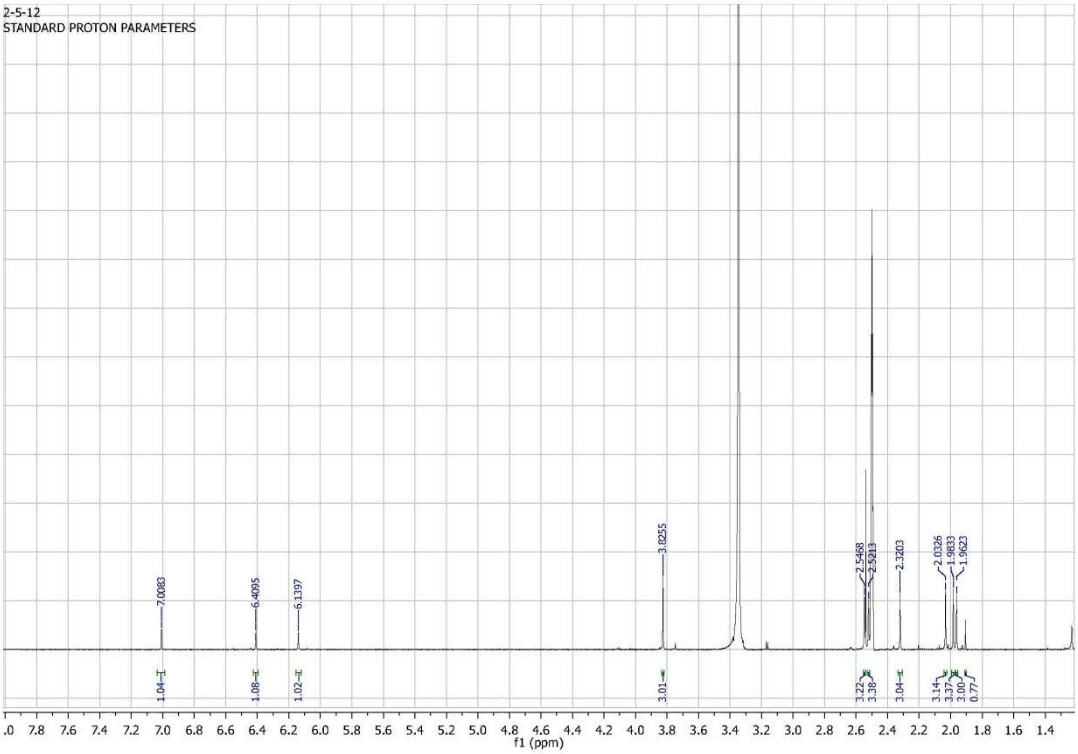

Figure S22 ^{1}H NMR spectrum of **4** in DMSO-d_6 (500 MHz)

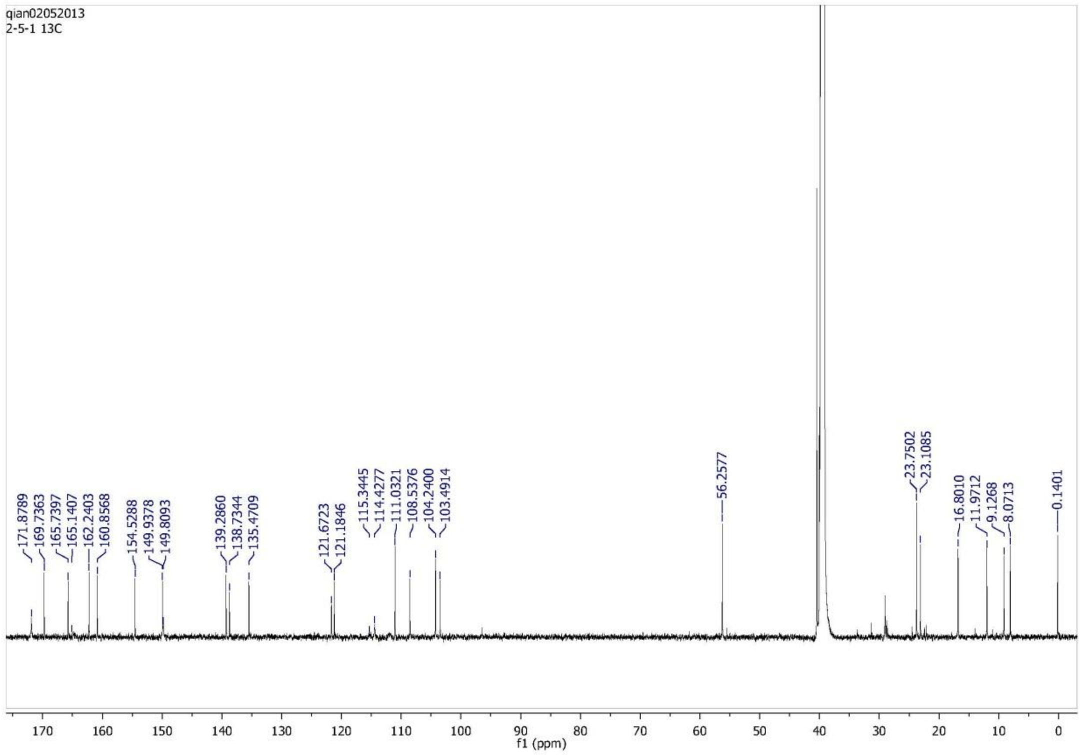

Figure S23 ^{13}C NMR spectrum of **4** in DMSO-*d*$_6$ (125 MHz)

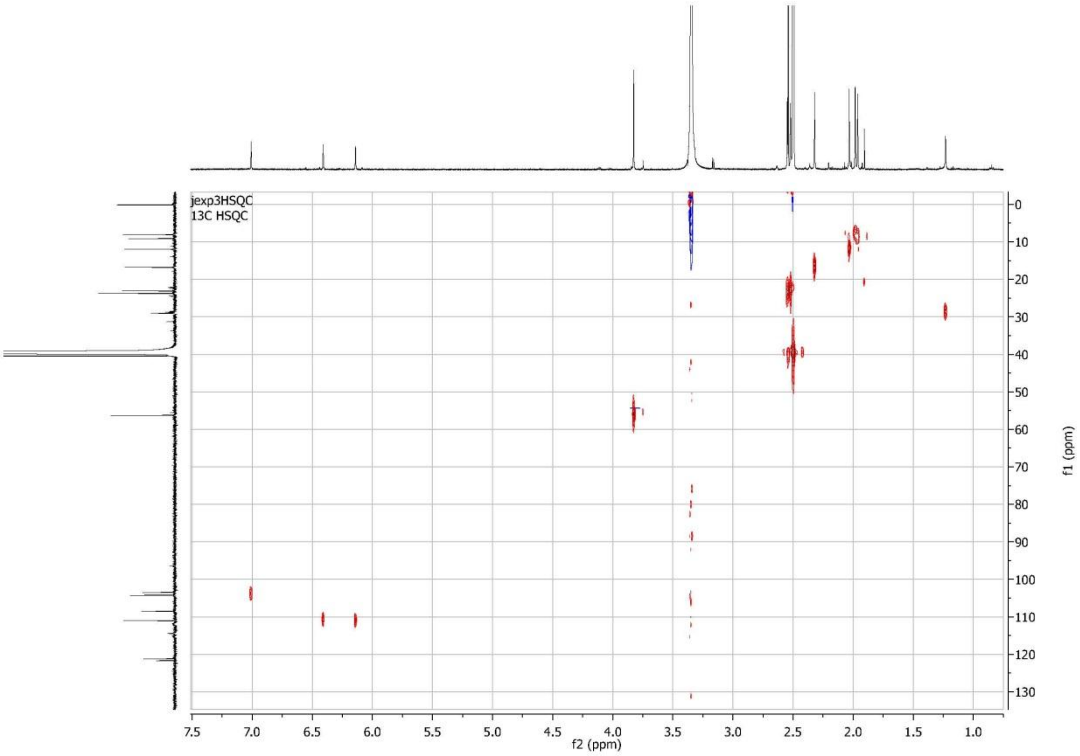

Figure S24 HMQC spectrum of **4** in DMSO-*d*$_6$

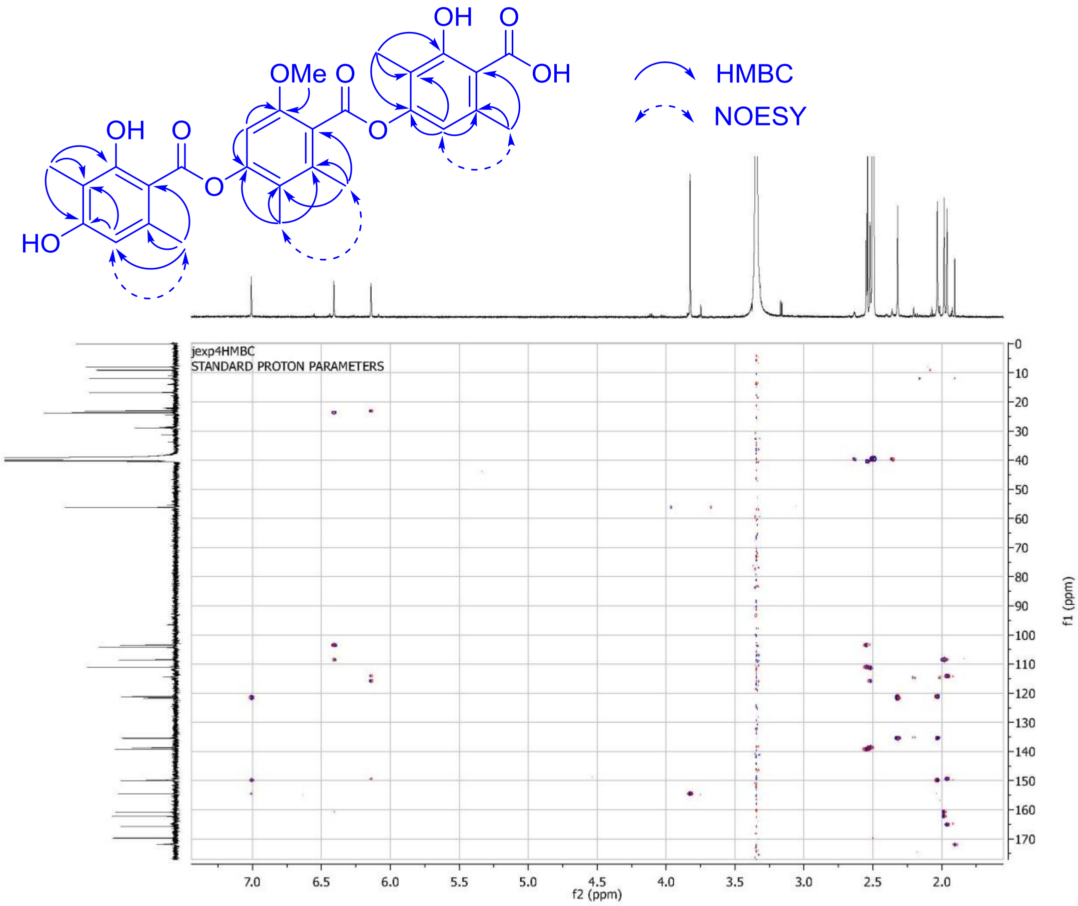

Figure S25 HMBC spectrum of **4** in DMSO-d_6

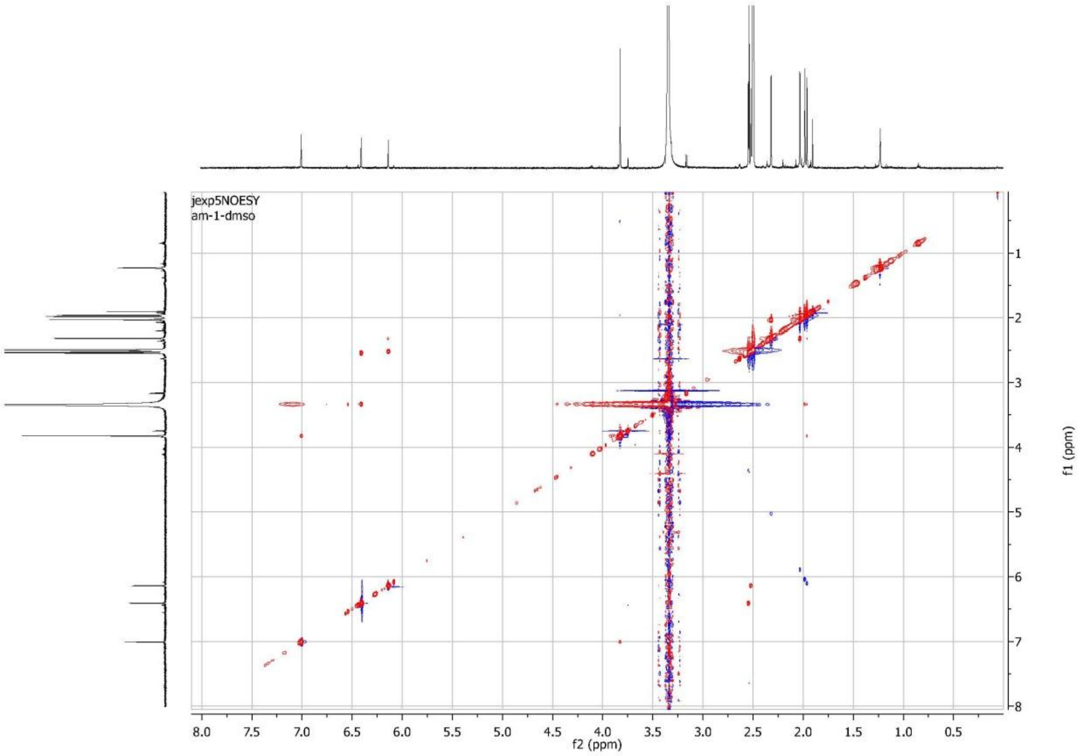

Figure S26 NOESY spectrum of **4** in DMSO-d_6

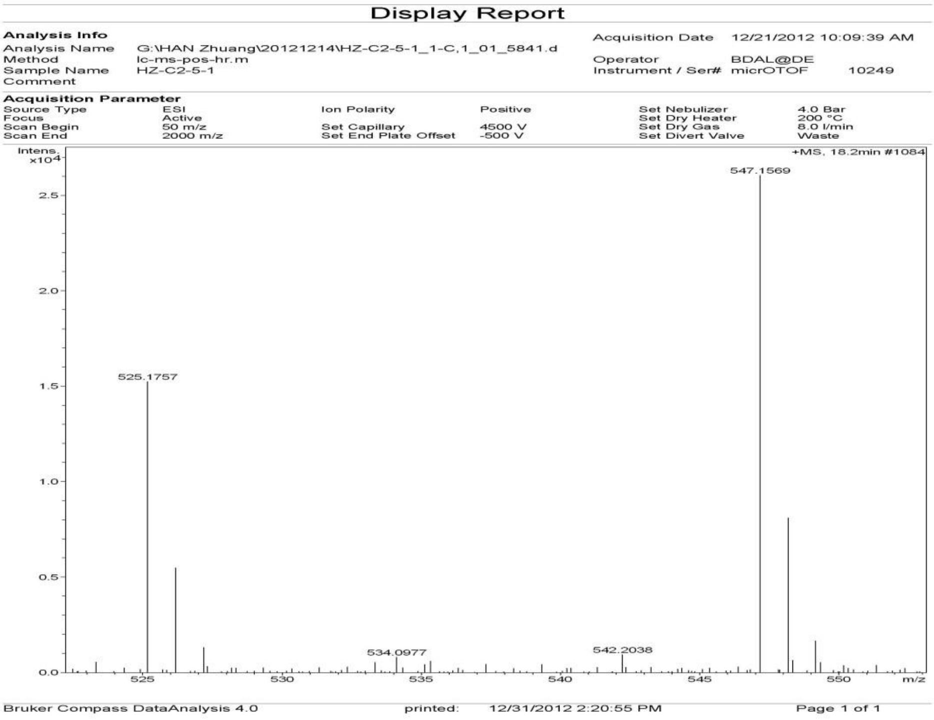

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Figure S27 HRESIMS spectrum of **4**

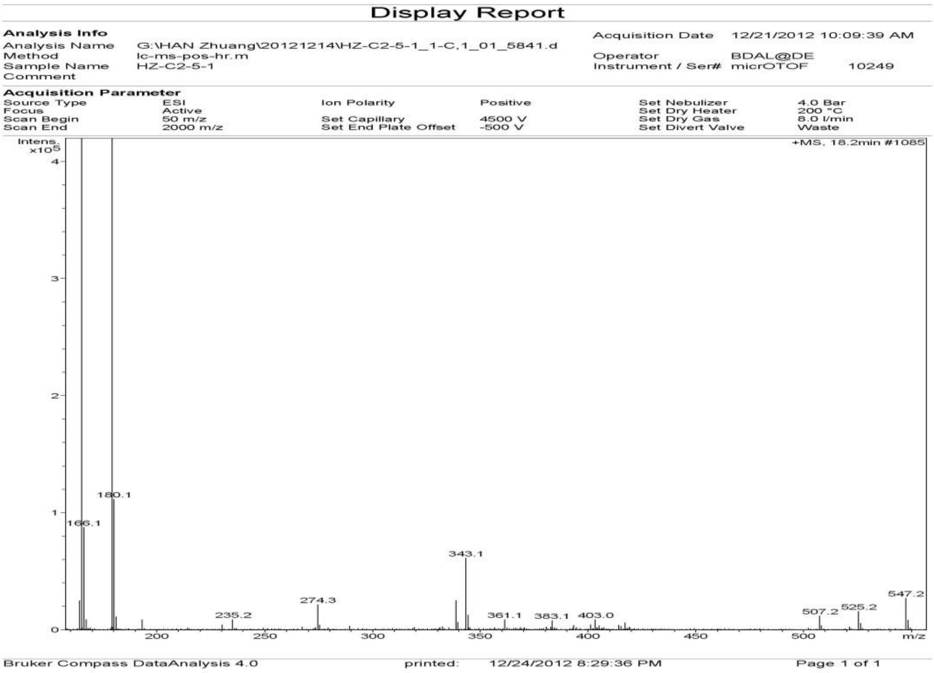

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Figure S28 ISCID spectrum of **4**

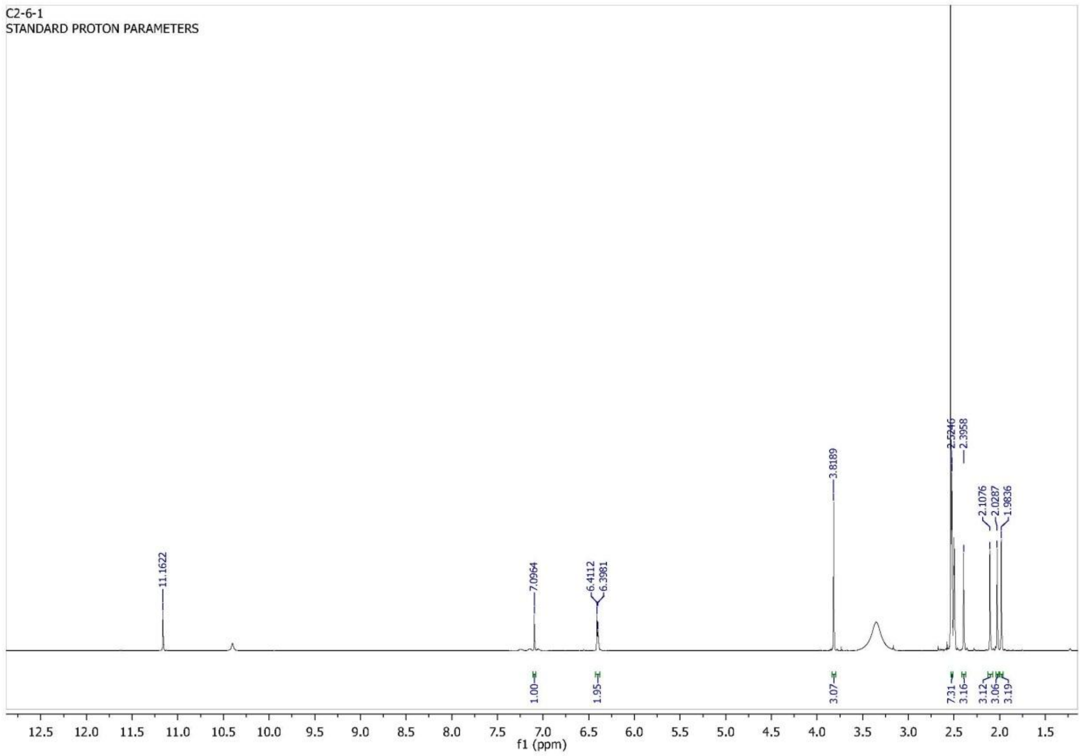

Figure S29 ^{1}H NMR spectrum of **5** in DMSO-d_6 (500 MHz)

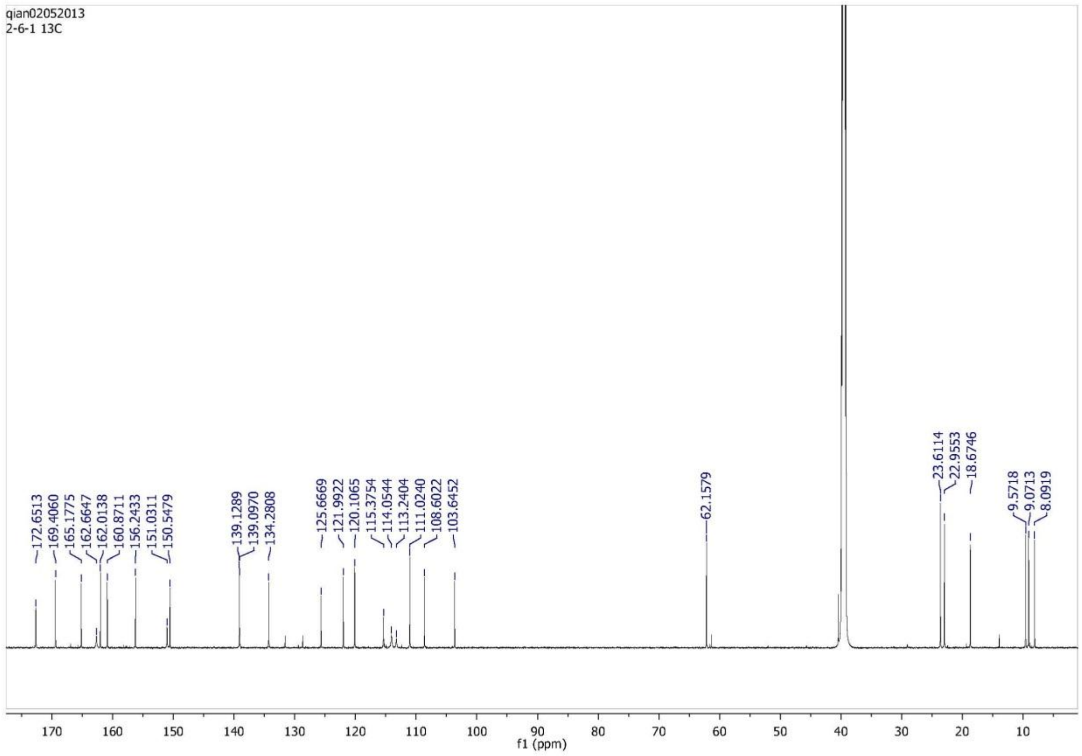

Figure S30 ^{13}C NMR spectrum of **5** in DMSO-d_6 (125 MHz)

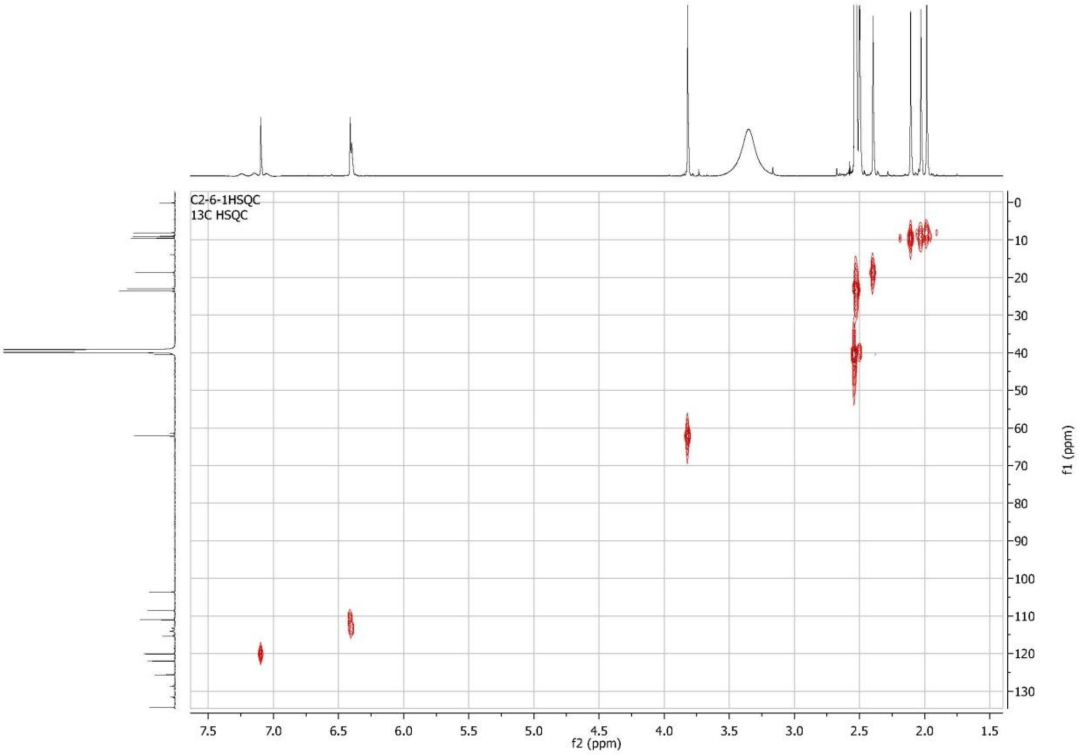

Figure S31 HMQC spectrum of **5** in DMSO-d_6

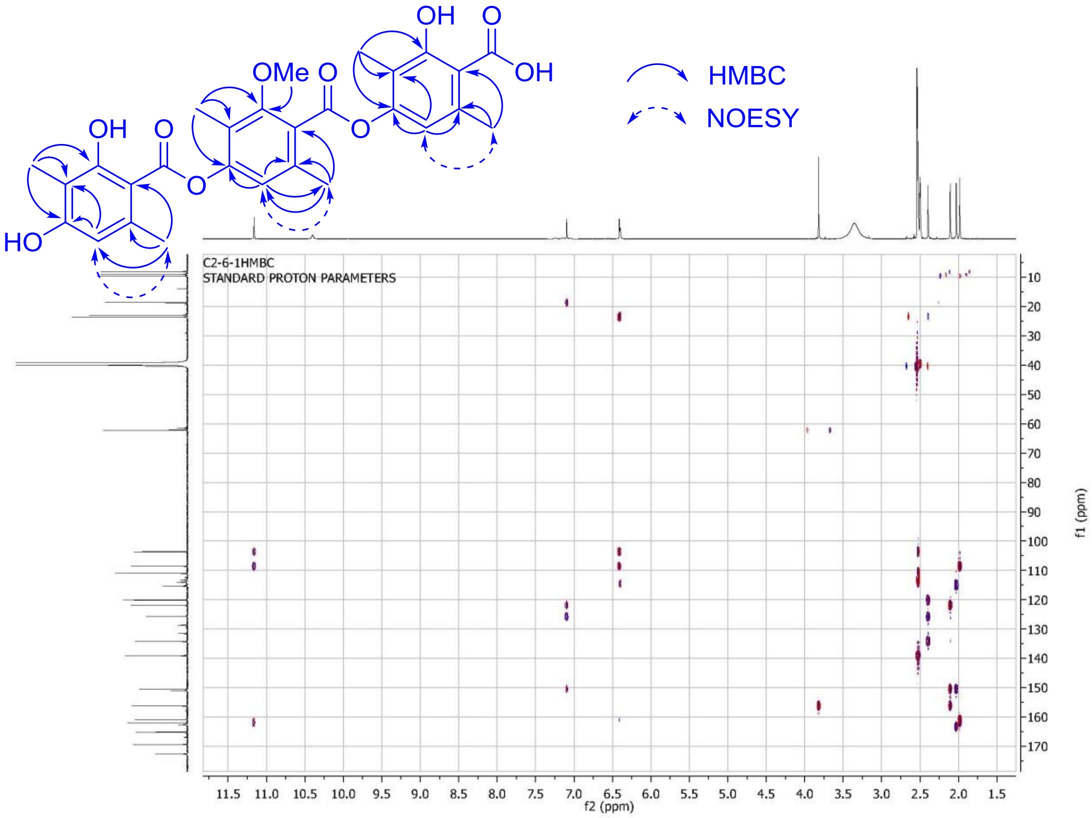

Figure S32 HMBC spectrum of **5** in DMSO-d_6

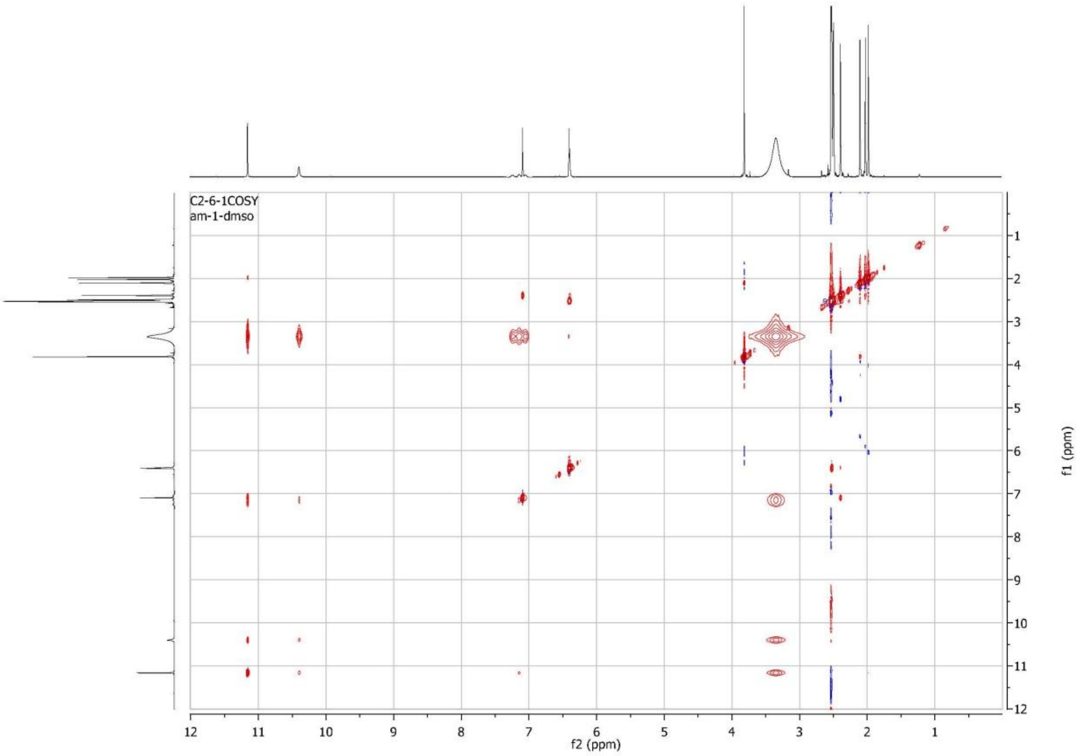

Figure S33 NOESY spectrum of **5** in DMSO-d_6

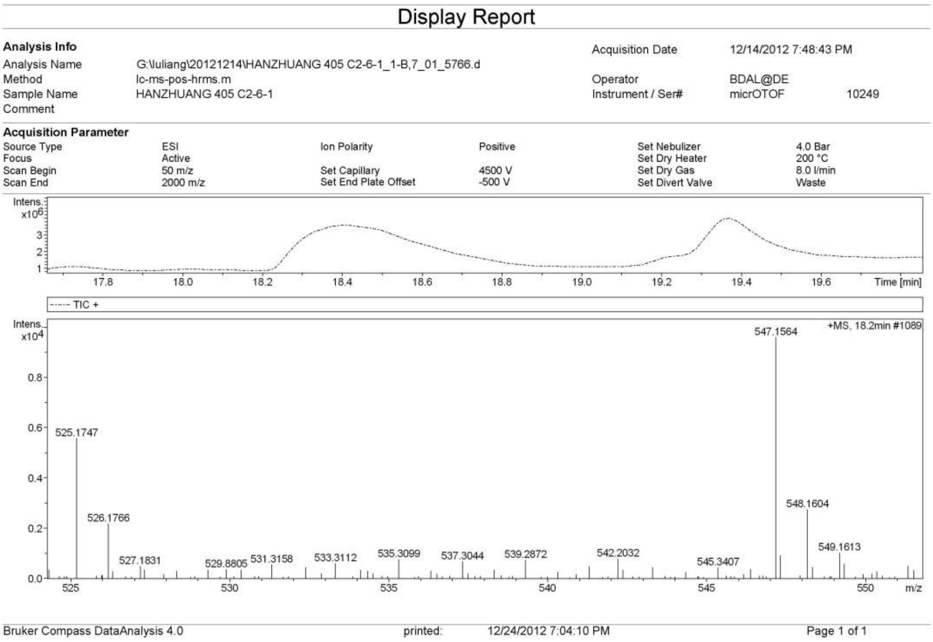

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Figure S34 HRESIMS spectrum of **5**

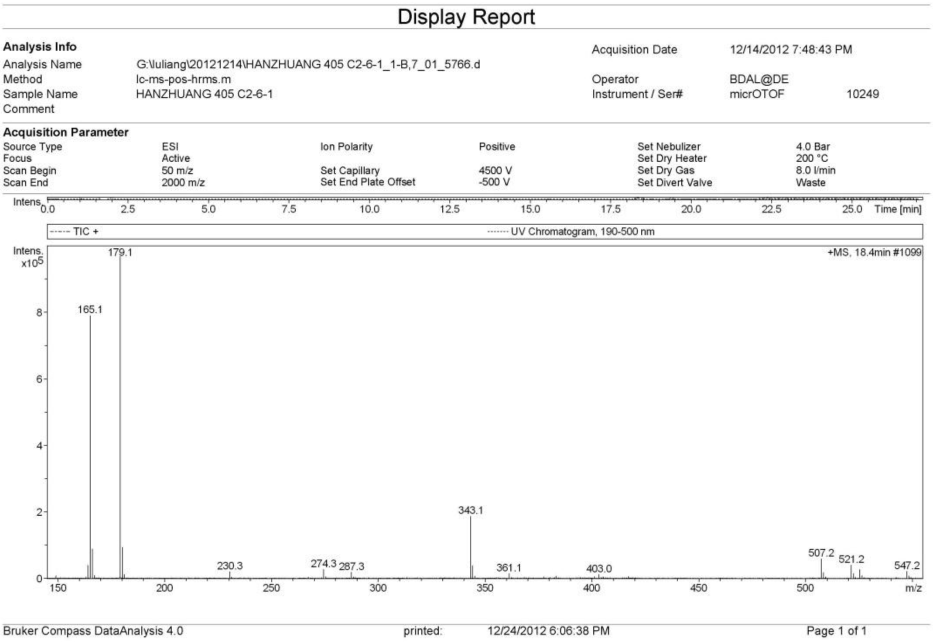

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Figure S35 ISCID spectrum of **5**

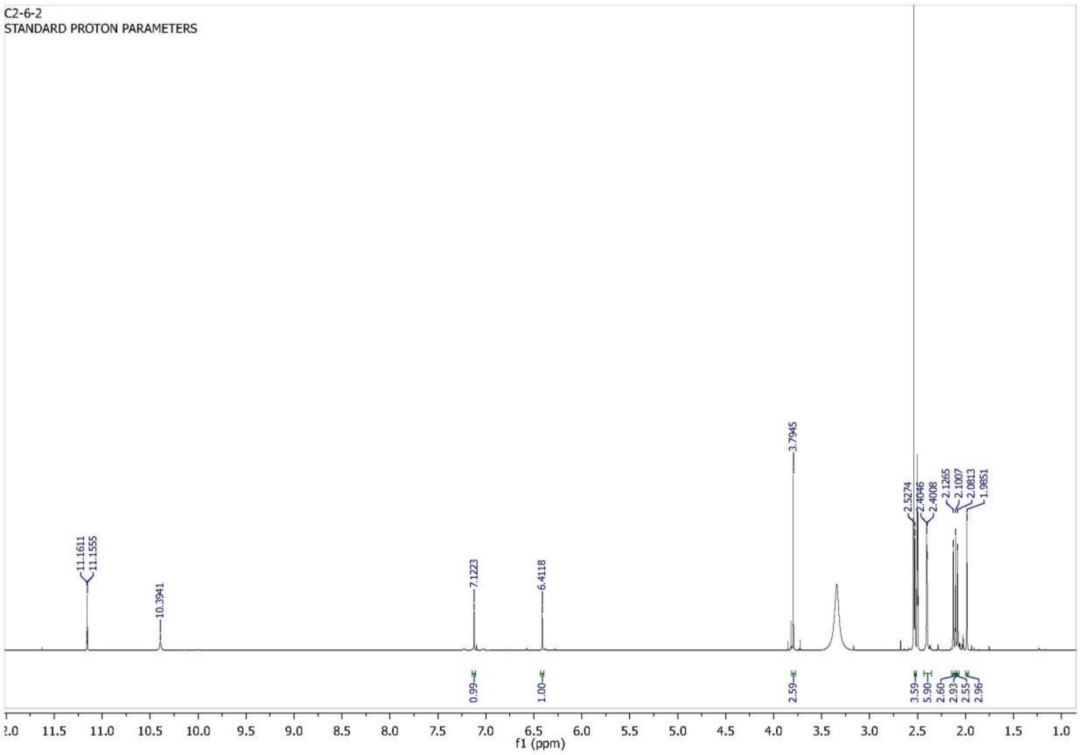


Figure S36 ^{1}H NMR spectrum of **6** in DMSO-d_6 (500 MHz)

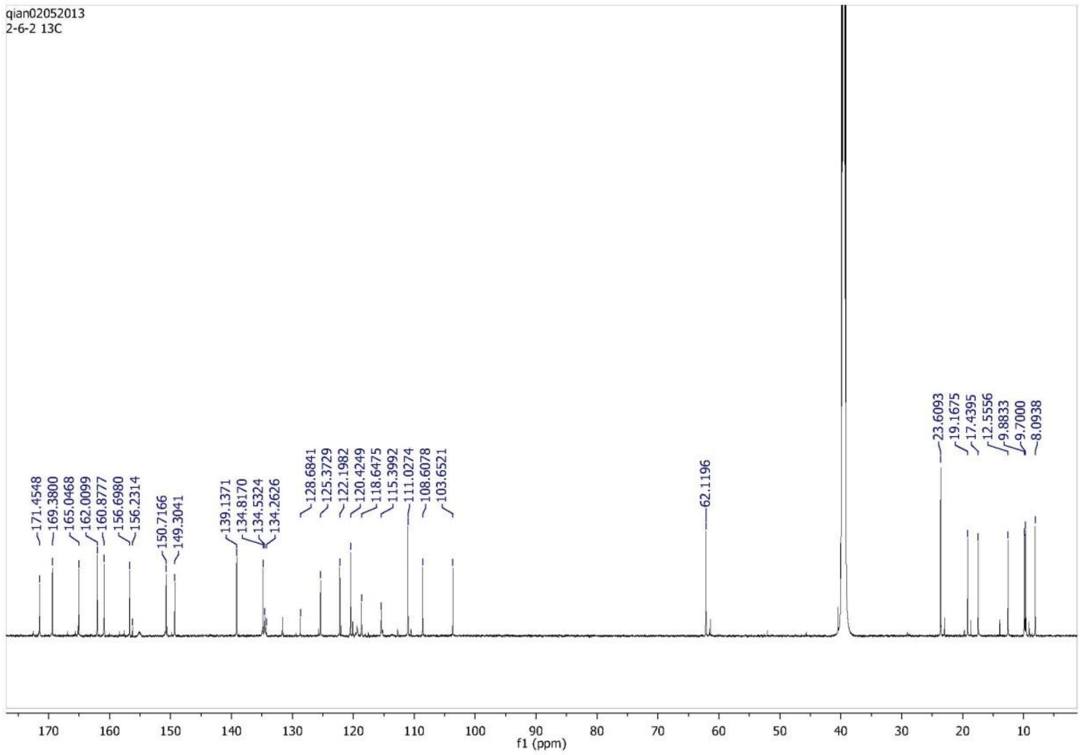


Figure S37 ^{13}C NMR spectrum of **6** in DMSO-d_6 (125 MHz)

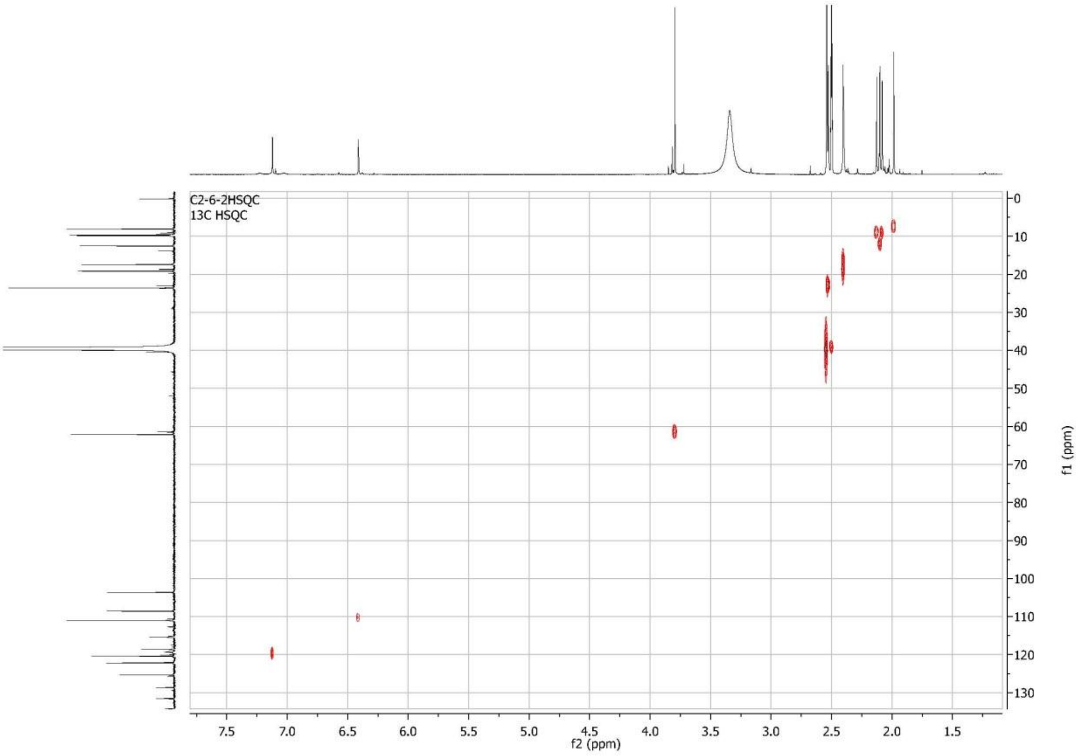


Figure S38 HMQC spectrum of **6** in DMSO-d_6

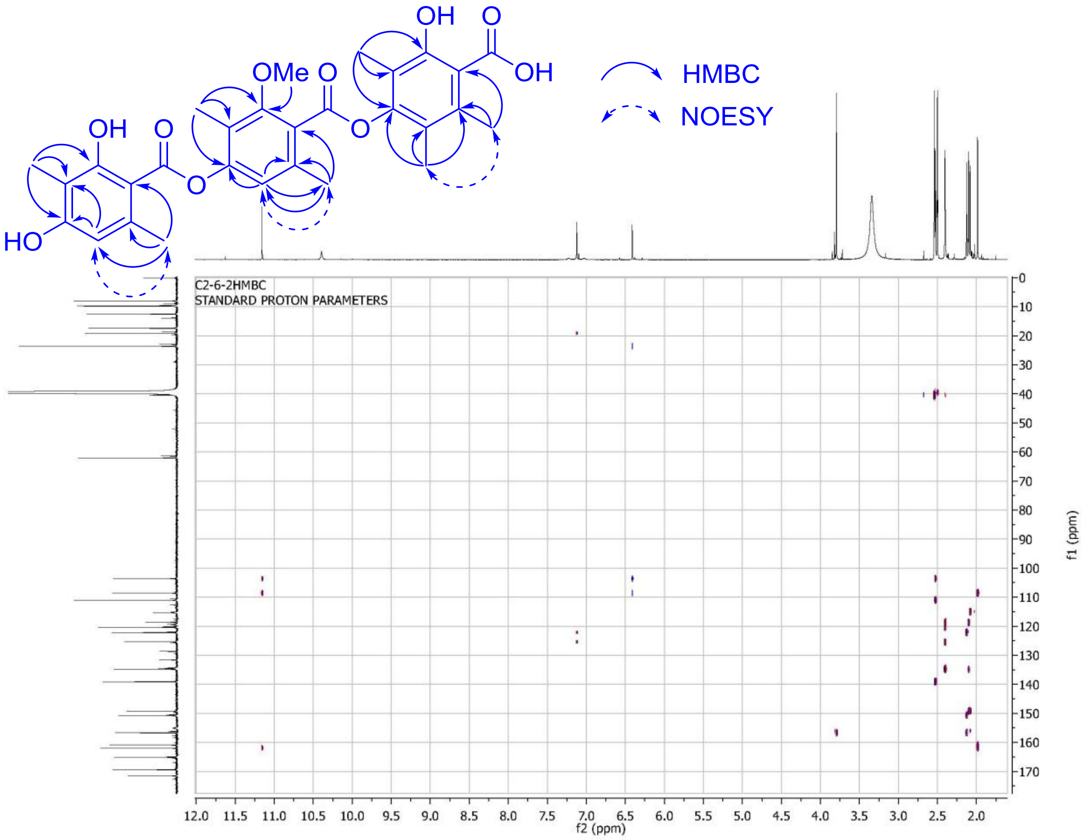


Figure S39 HMBC spectrum of **6** in DMSO-d_6

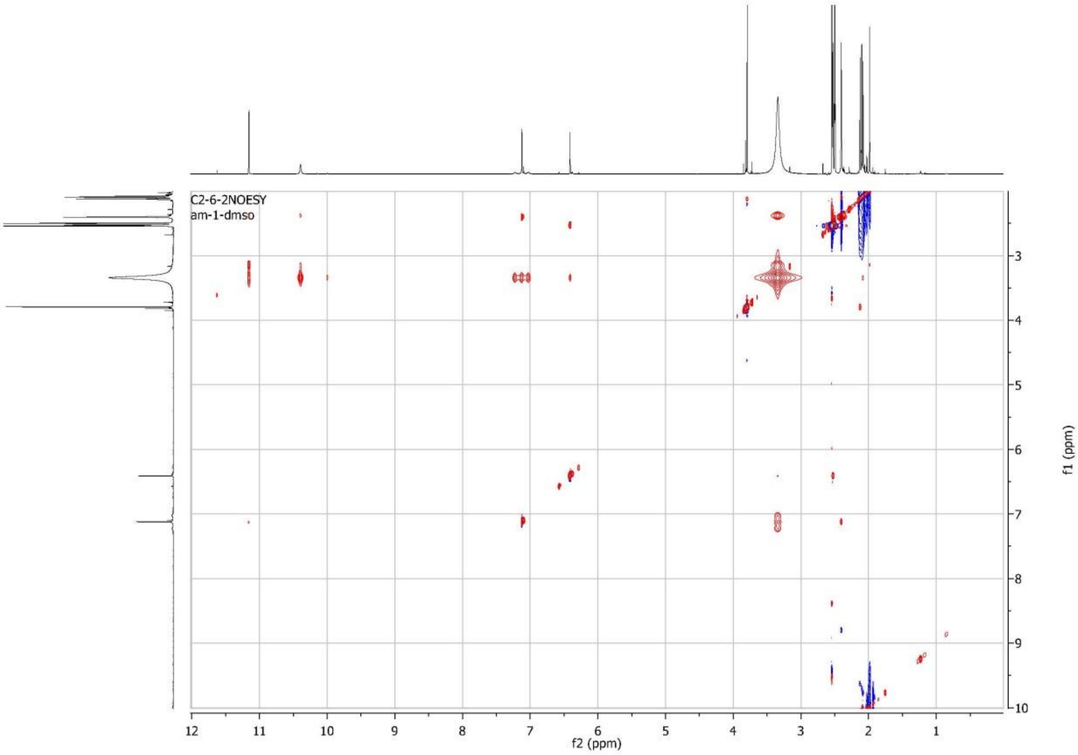
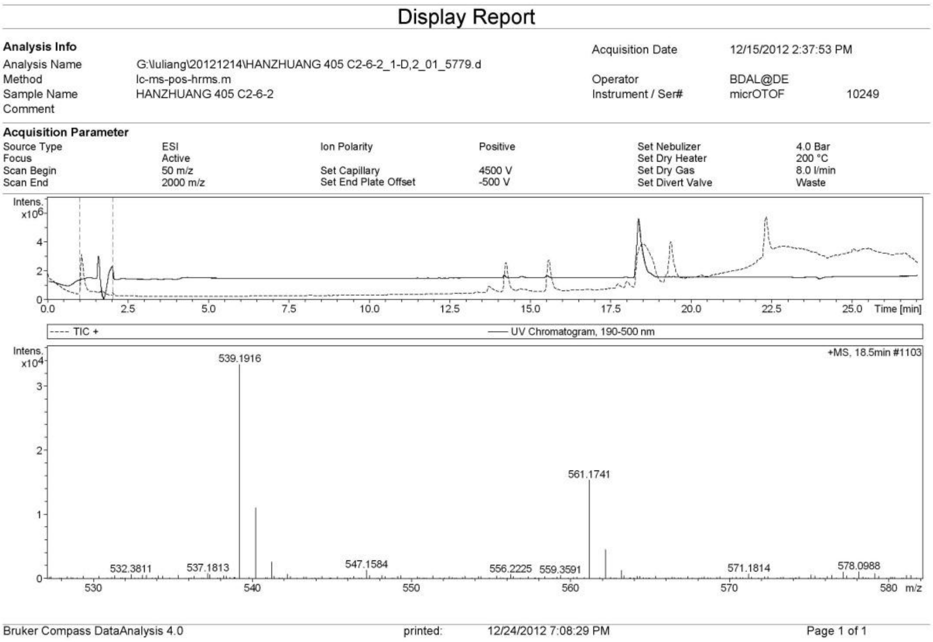


Figure S40 NOESY spectrum of **6** in DMSO-d_6



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Sample Name HANZHUANG 405 C2-6-2
Comment

Acquisition Date 12/15/2012 2:37:53 PM
Operator BDAL@DE
Instrument / Ser# micrOTOF 10249

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

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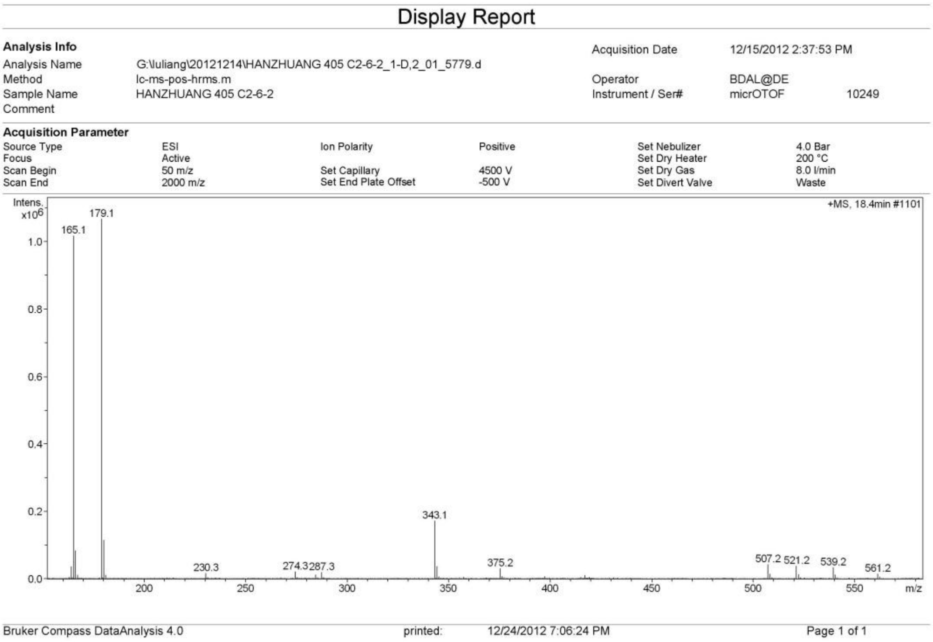
Figure S41 HRESIMS spectrum of **6**



Display Report

Analysis Info

Analysis Name G:\luliang\20121214\HANZHUANG 405 C2-6-2_1-D,2_01_5779.d
Method lc-ms-pos-hrms.m
Sample Name HANZHUANG 405 C2-6-2
Comment

Acquisition Date 12/15/2012 2:37:53 PM
Operator BDAL@DE
Instrument / Ser# micrOTOF 10249

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

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Figure S42 ISCID spectrum of **6**

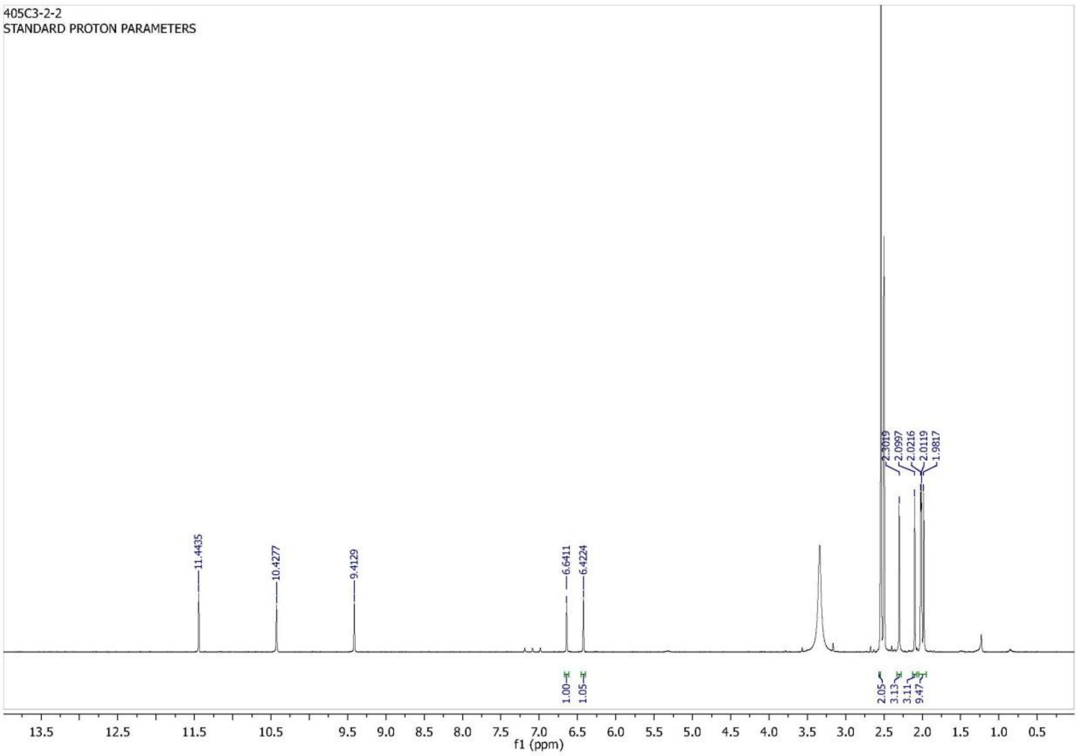


Figure S43 ^{1}H NMR spectrum of **7** in DMSO-*d6* (500 MHz)

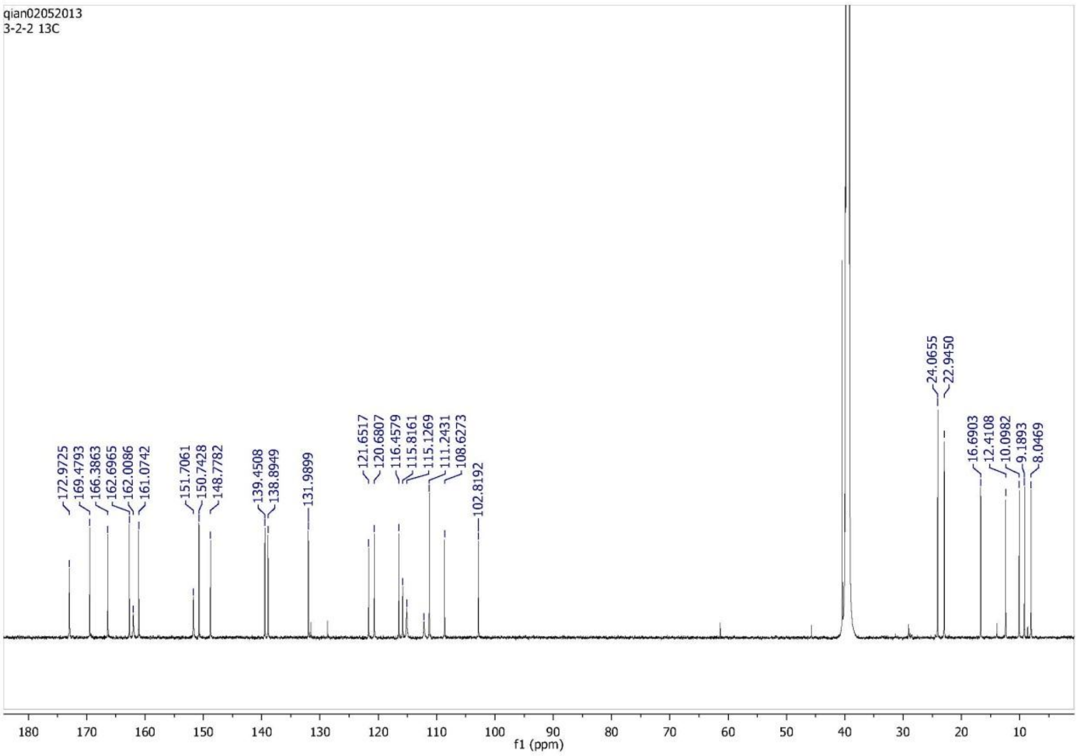


Figure S44 ^{13}C NMR spectrum of **7** in DMSO-*d6* (125 MHz)

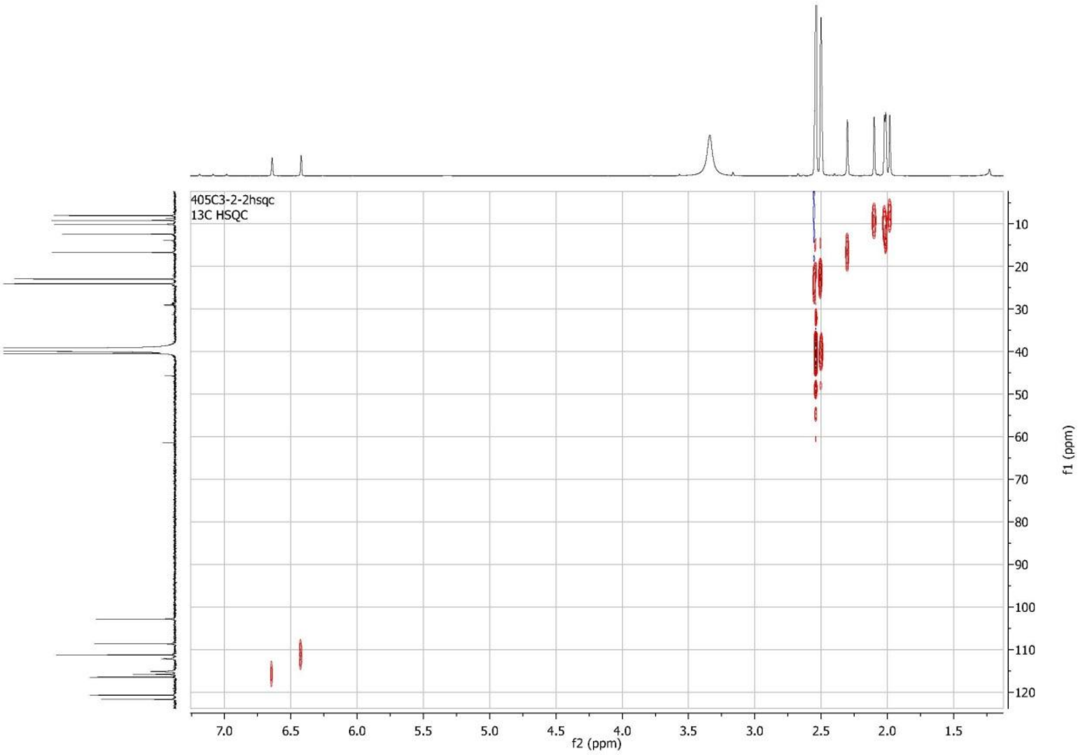


Figure S45 HMQC spectrum of **7** in DMSO-*d*6

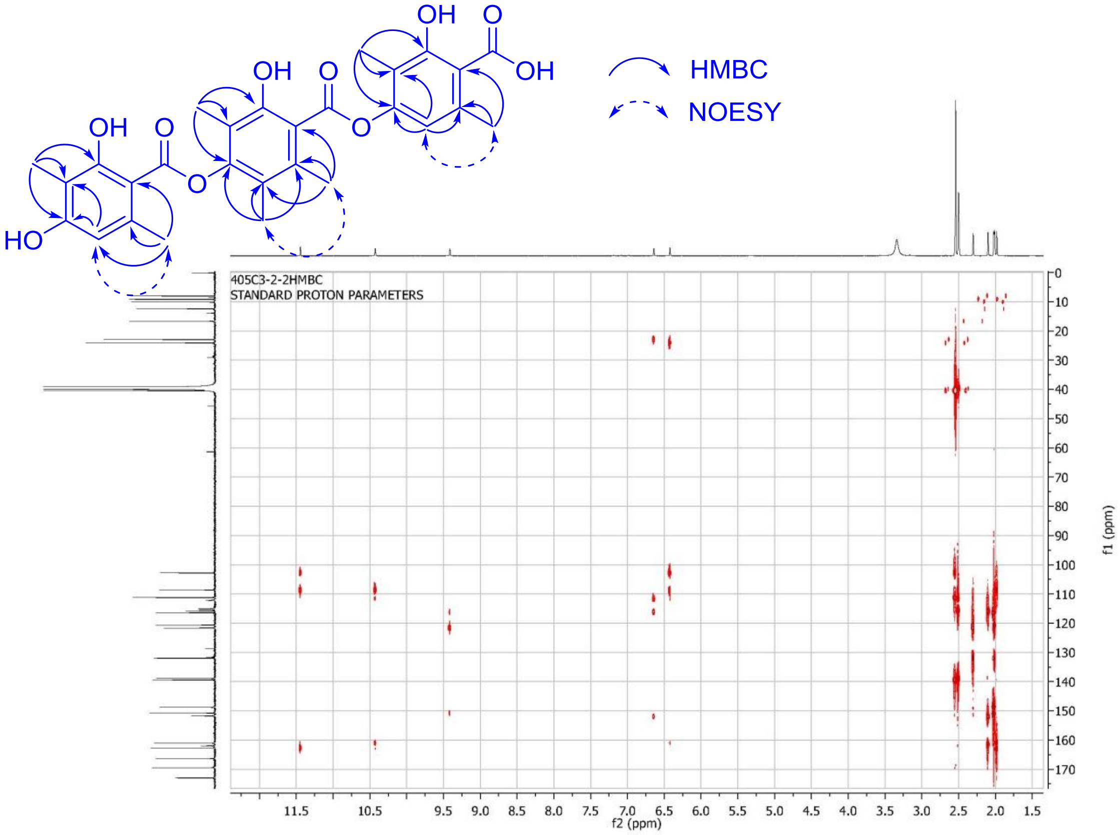


Figure S46 HMBC spectrum of **7** in DMSO-*d*6

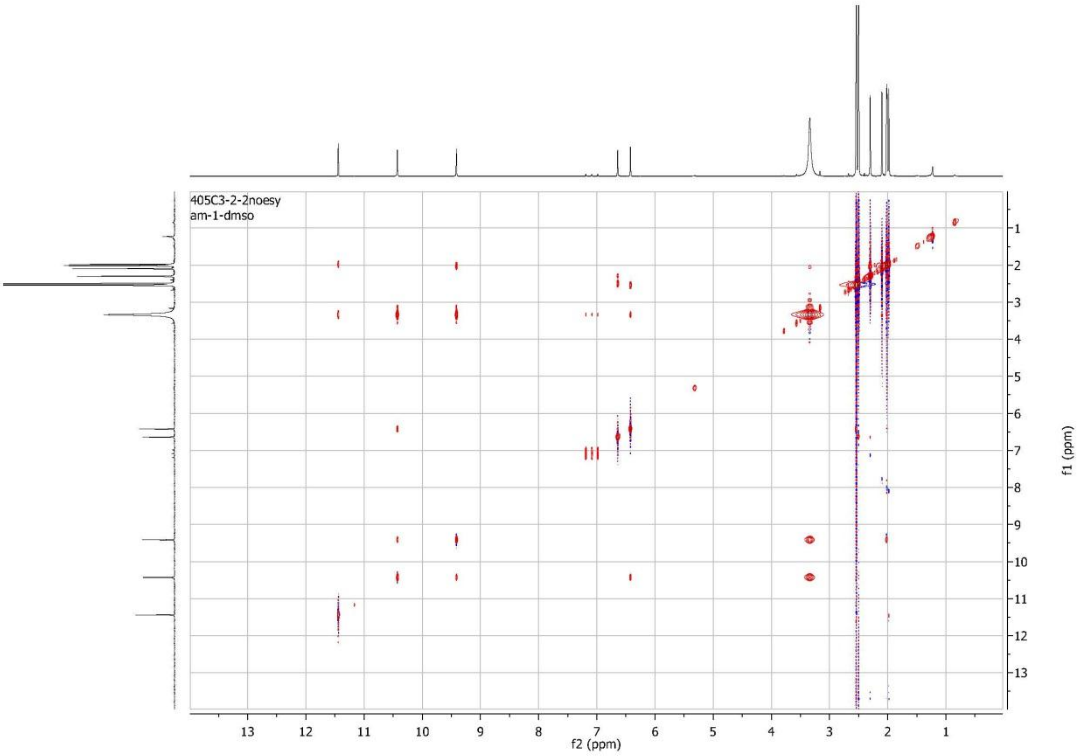
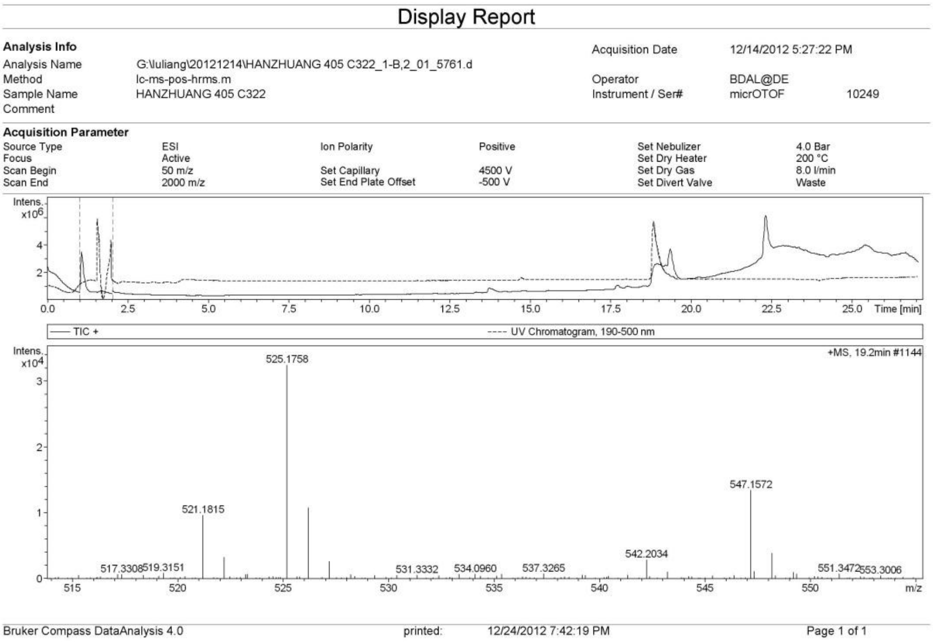


Figure S47 NOESY spectrum of **7** in DMSO-d_6



Display Report

Analysis Info

Analysis Name	G:\luliang\20121214\HANZHUANG 405 C322_1-B,2_01_5761.d	Acquisition Date	12/14/2012 5:27:22 PM	
Method	lc-ms-pos-hrms.m	Operator	BDAL@DE	
Sample Name	HANZHUANG 405 C322	Instrument / Ser#	micrOTOF	10249
Comment				

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

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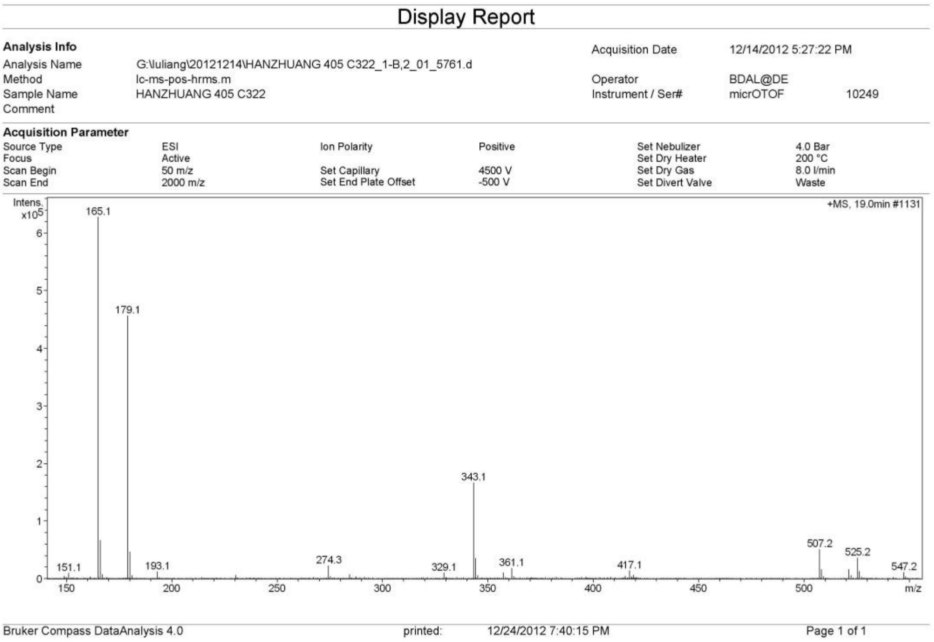
Figure S48 HRESIMS spectrum of **7**



Display Report

Analysis Info

Analysis Name G:\luliang\20121214\HANZHUANG 405 C322_1-B,2_01_5761.d
Method lc-ms-pos-hrms.m
Sample Name HANZHUANG 405 C322
Comment

Acquisition Date 12/14/2012 5:27:22 PM
Operator BDAL@DE
Instrument / Ser# micrOTOF 10249

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

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Figure S49 ISCID spectrum of **7**

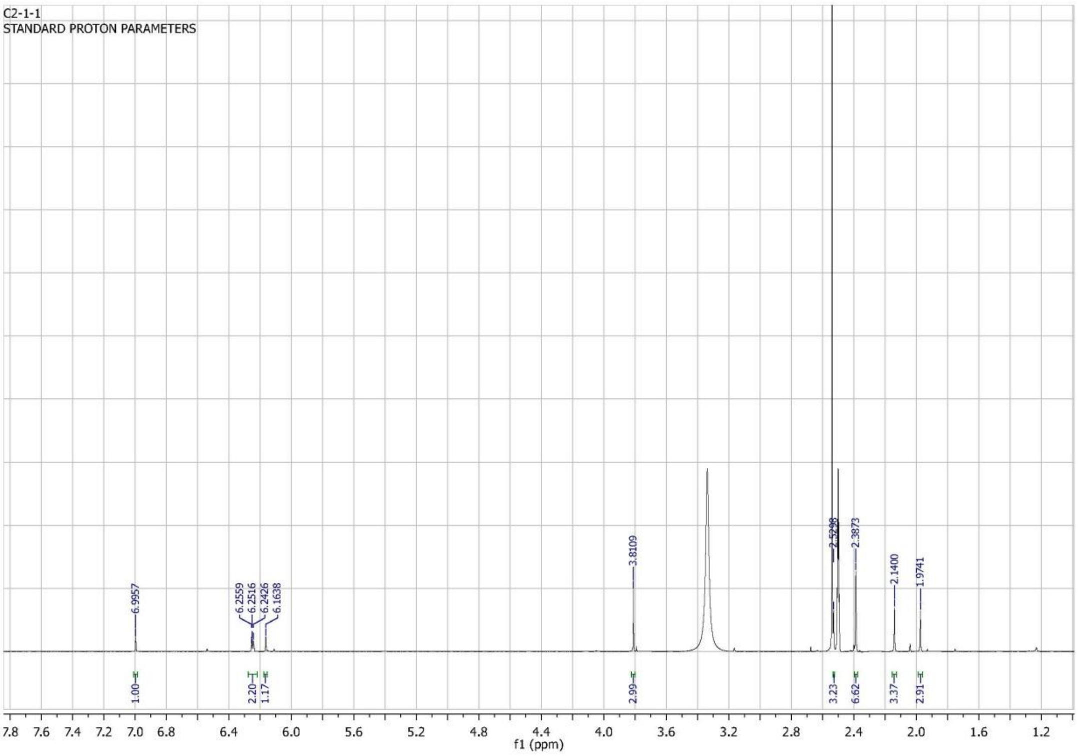


Figure S50 ^{1}H NMR spectrum of **8** in DMSO-d_6 (500 MHz)

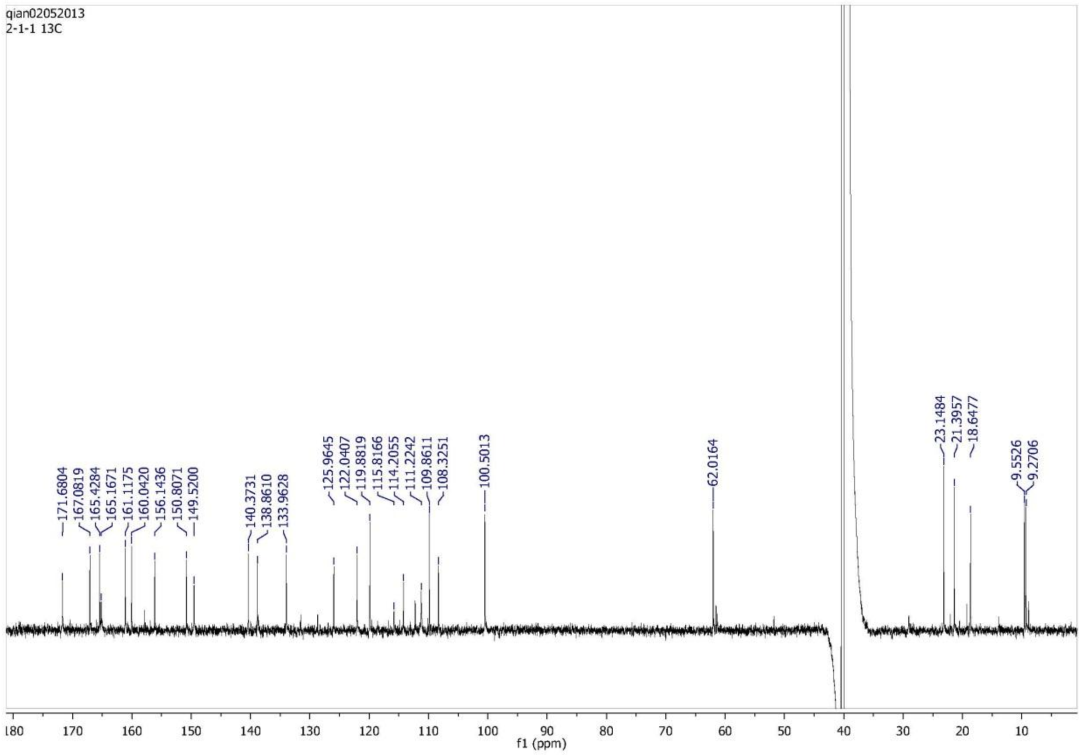


Figure S51 ^{13}C NMR spectrum of **8** in DMSO-d_6 (125 MHz)

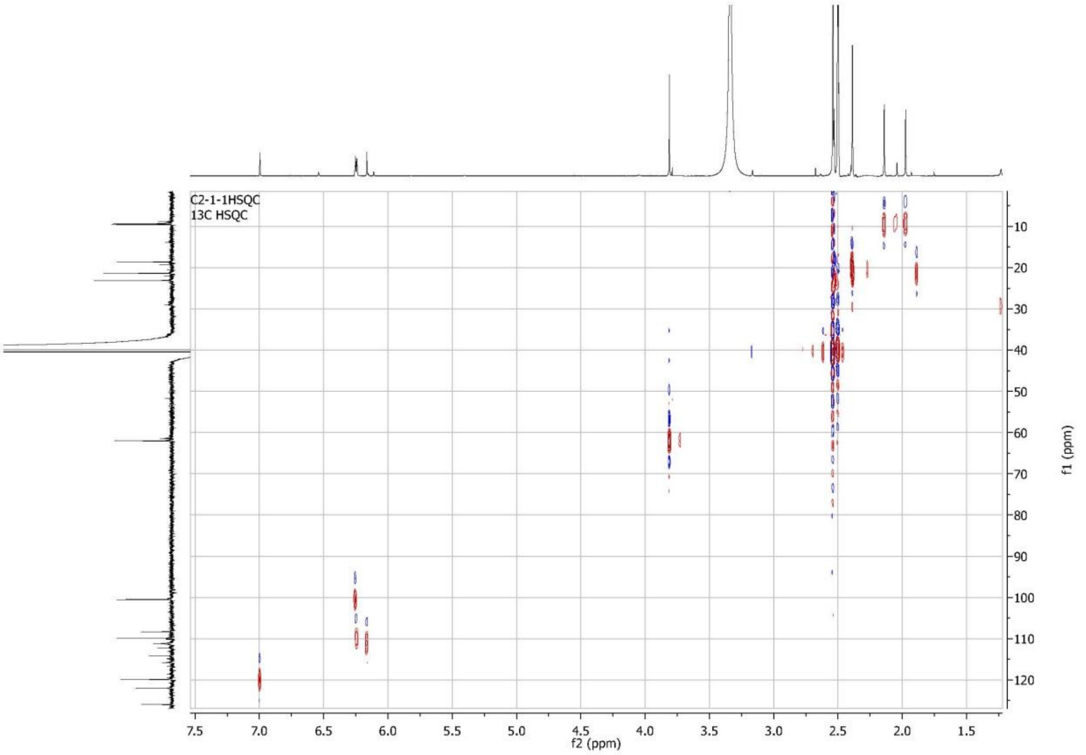


Figure S52 HMQC spectrum of **8** in DMSO-d_6

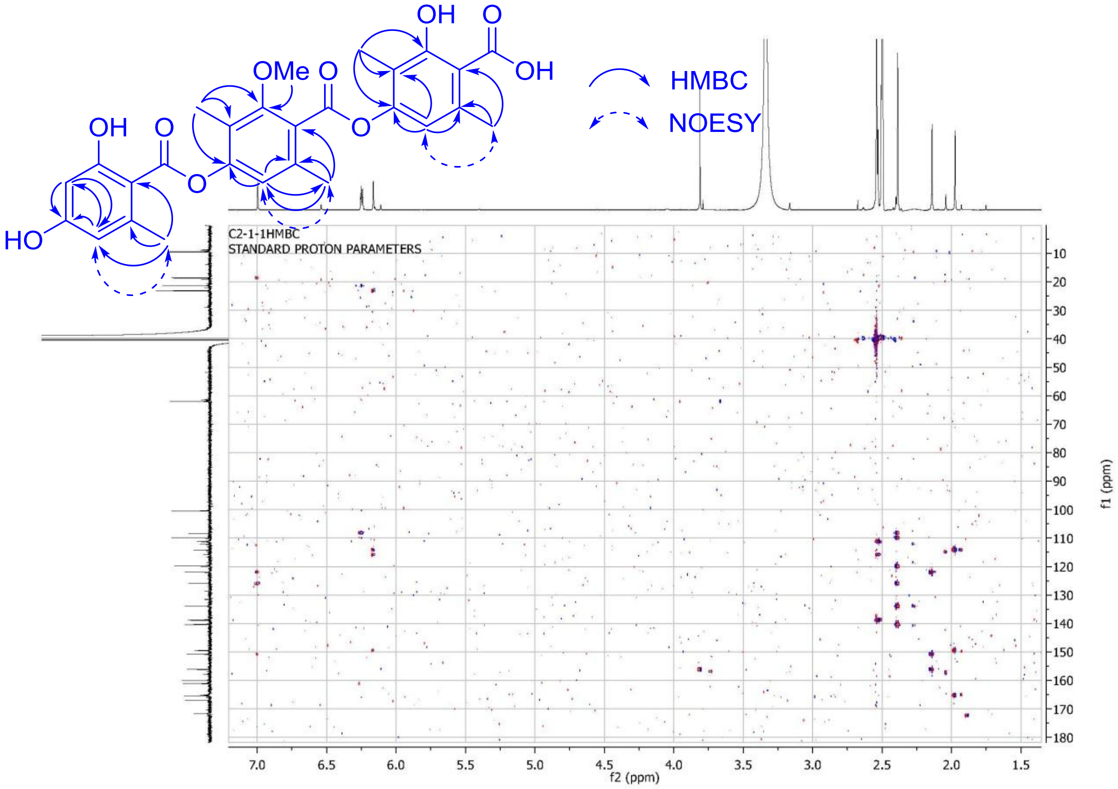


Figure S53 HMBC spectrum of **8** in DMSO-d_6

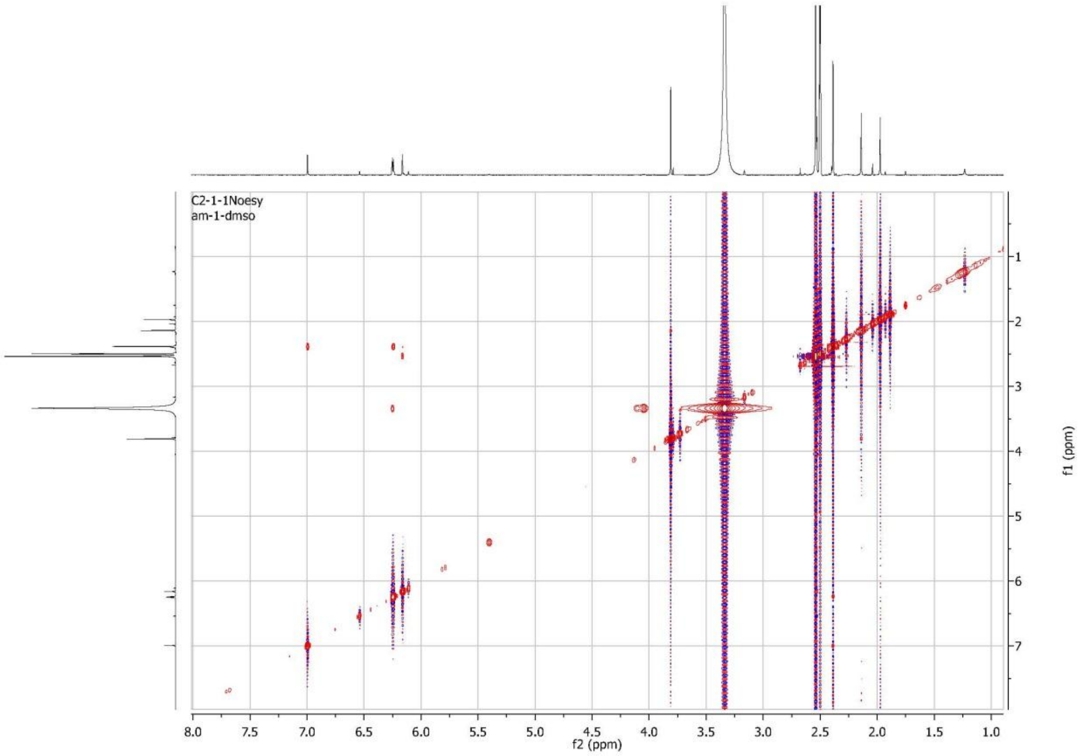
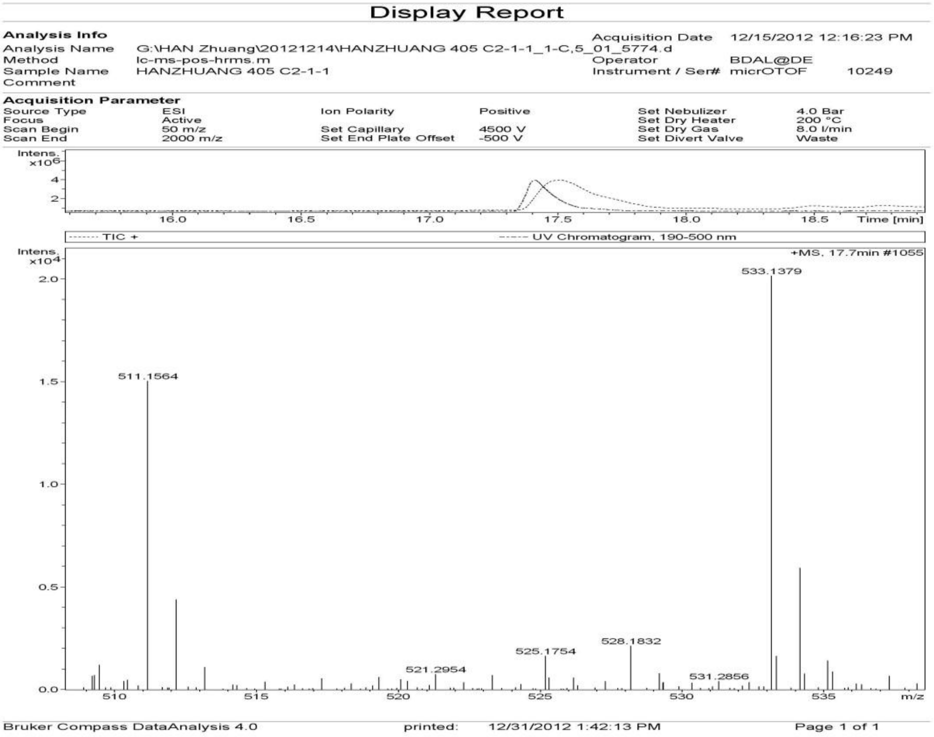


Figure S54 NOESY spectrum of **8** in DMSO-d_6



Display Report

Analysis Info

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Method	lc-ms-pos-hrms.m	Operator	BDAL@DE
Sample Name	HANZHUANG 405 C2-1-1	Instrument / Ser#	micrOTOF 10249
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

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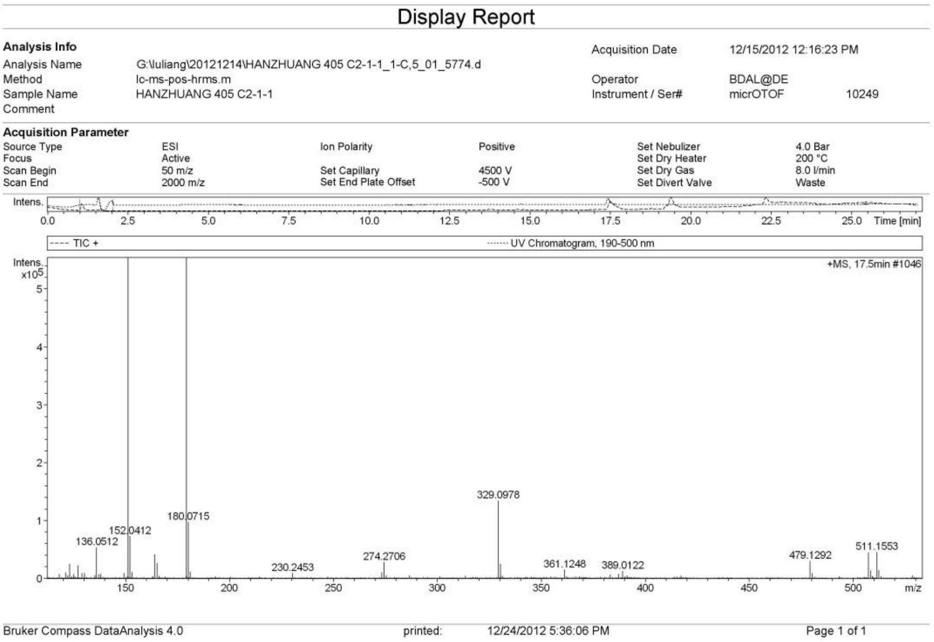
Figure S55 HRESIMS spectrum of **8**



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Analysis Info

Analysis Name	G:\luliang\20121214\HANZHUANG 405 C2-1-1_1-C,5_01_5774.d	Acquisition Date	12/15/2012 12:16:23 PM
Method	lc-ms-pos-hrms.m	Operator	BDAL@DE
Sample Name	HANZHUANG 405 C2-1-1	Instrument / Ser#	micrOTOF 10249
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

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Figure S56 ISCID spectrum of **8**

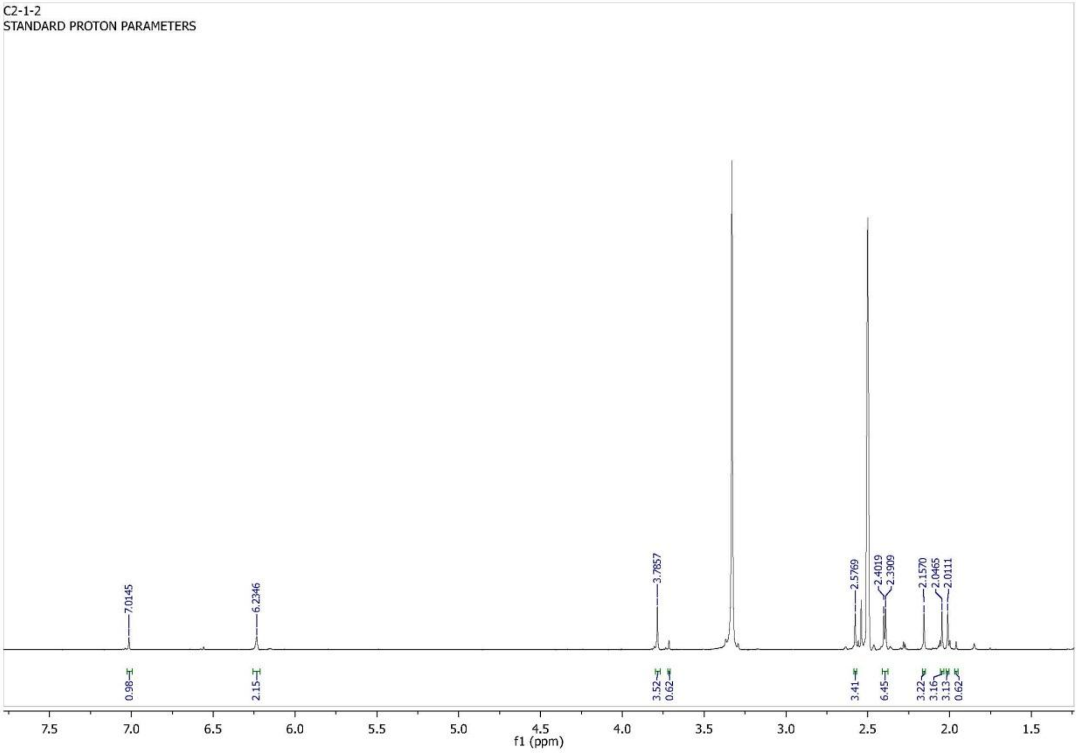


Figure S57 ^{1}H NMR spectrum of **9** in DMSO-*d₆* (500 MHz)

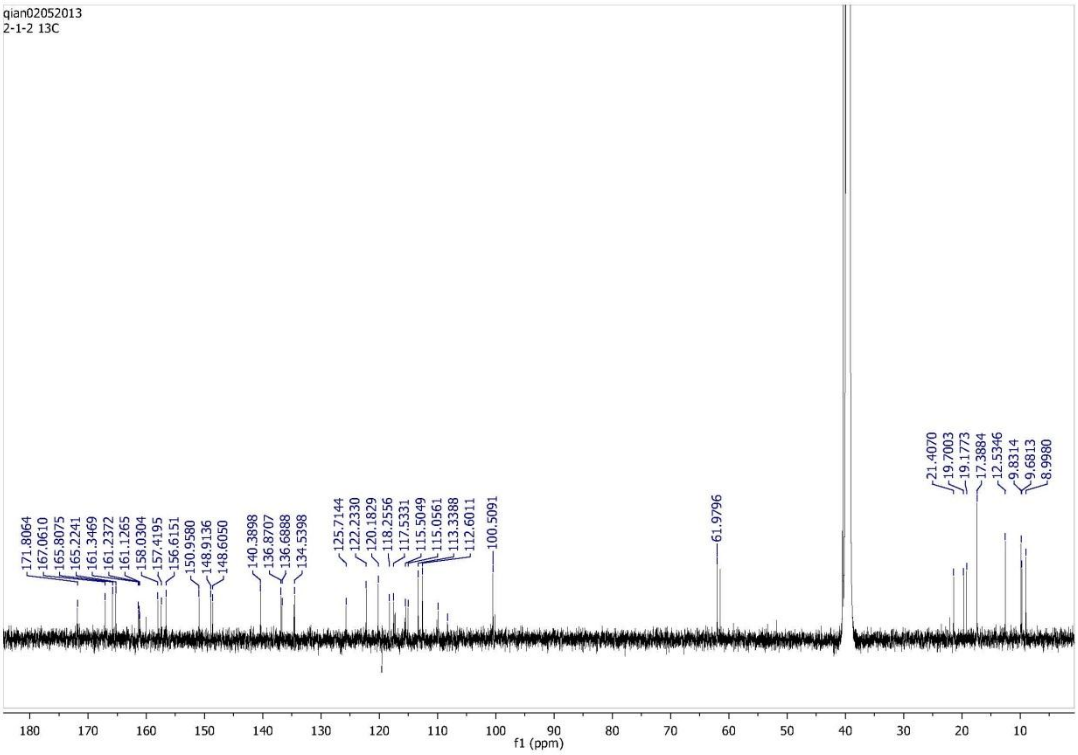


Figure S58 ^{13}C NMR spectrum of **9** in DMSO-*d₆* (125 MHz)

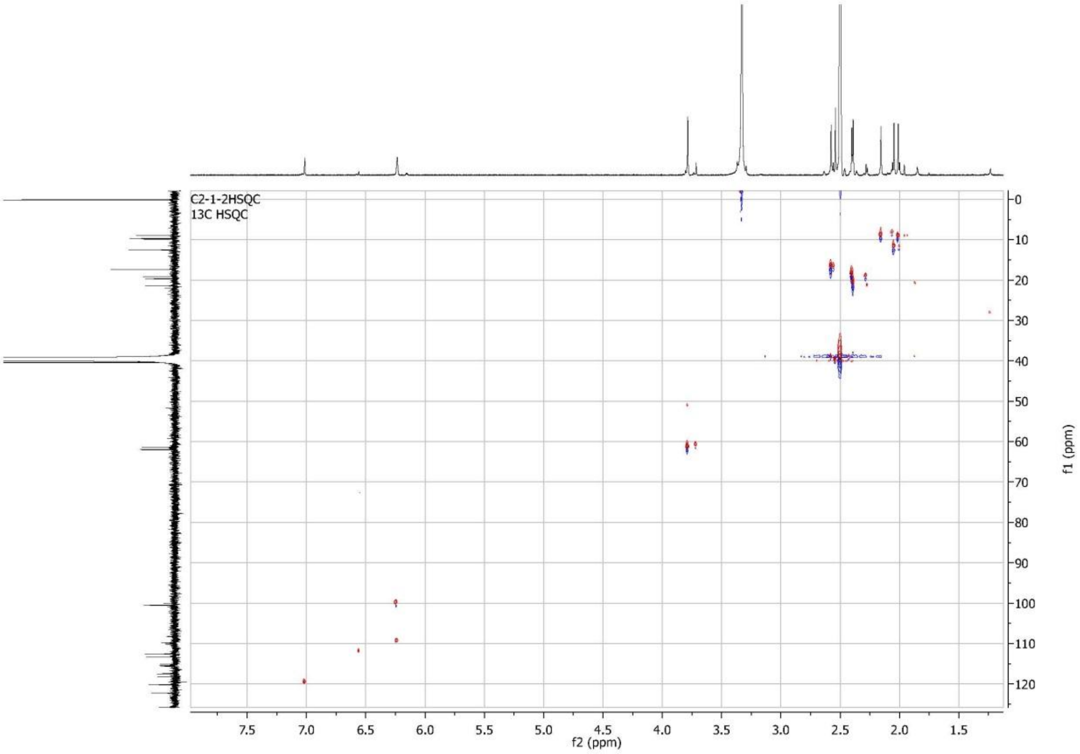


Figure S59 HMQC spectrum of **9** in DMSO-*d*$_6$

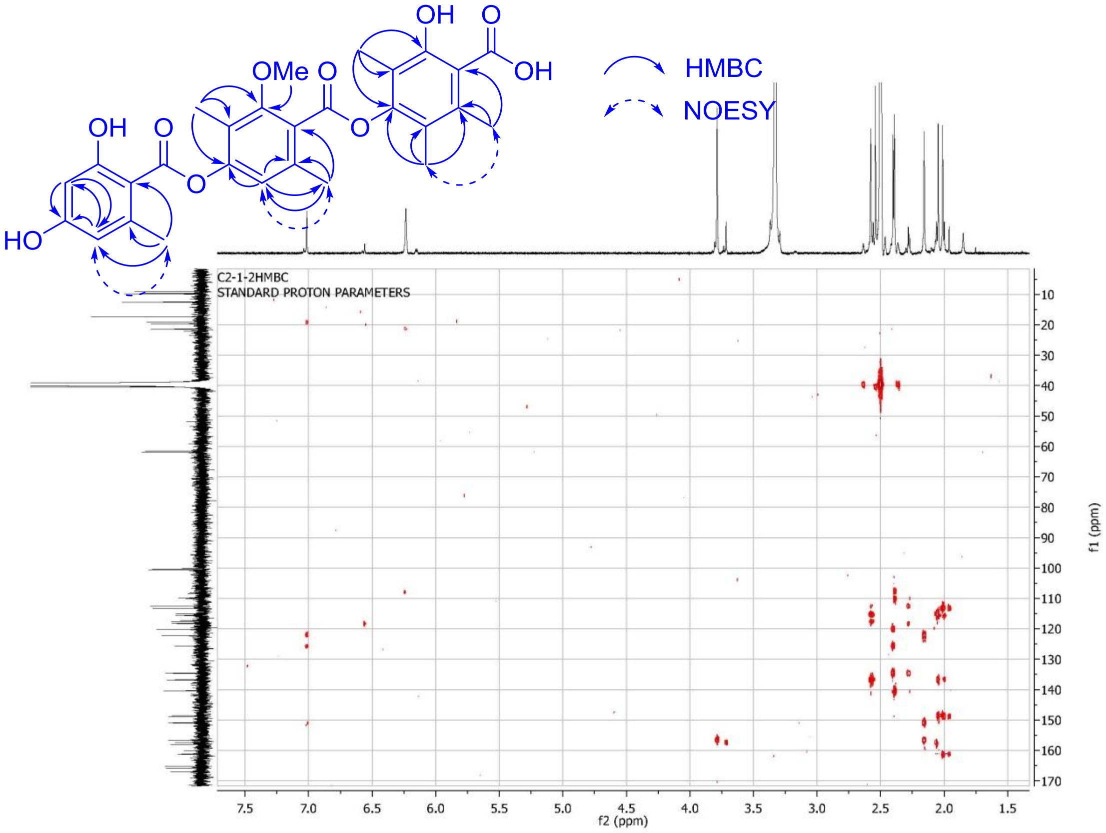


Figure S60 HMBC spectrum of **9** in DMSO-*d*$_6$

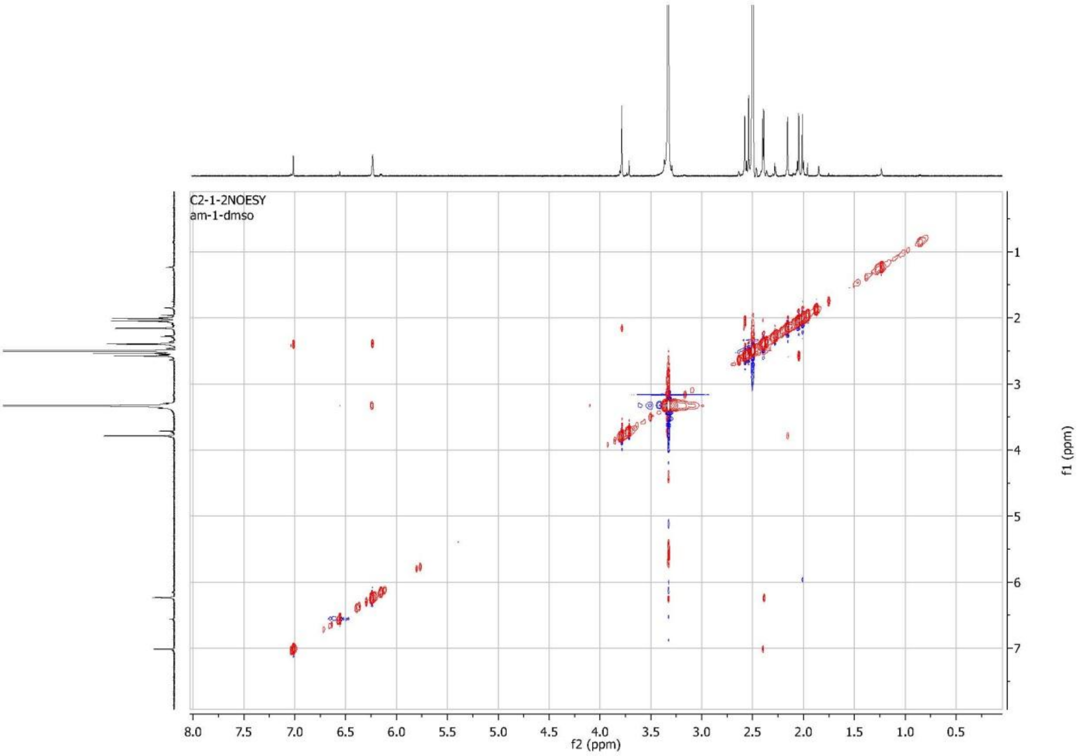
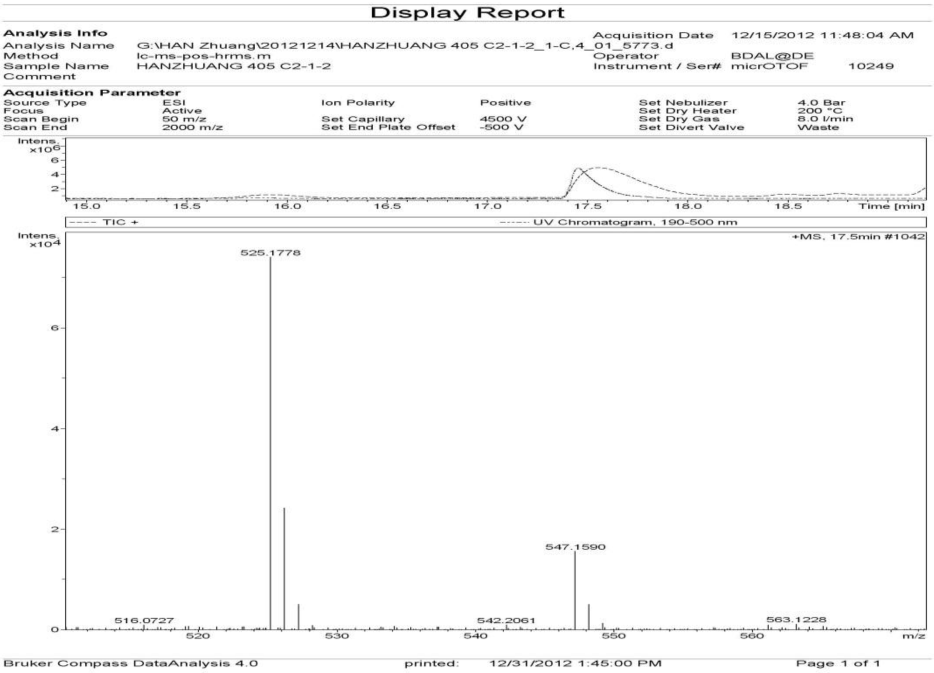


Figure S61 NOESY spectrum of **9** in DMSO-d_6



Display Report

Analysis Info
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Method lc-ms-pos-hrms.m
Sample Name HANZHUANG 405 C2-1-2
Comment
Acquisition Date 12/15/2012 11:48:04 AM
Operator BDAL@DE
Instrument / Ser# micrOTOF 10249

Acquisition Parameter
Source Type ESI
Focus Active
Scan Begin 50 m/z
Scan End 2000 m/z
Ion Polarity Positive
Set Capillary 4500 V
Set End Plate Offset -500 V
Set Nebulizer 4.0 Bar
Set Dry Heater 200 °C
Set Dry Gas 8.0 l/min
Set Divert Valve Waste

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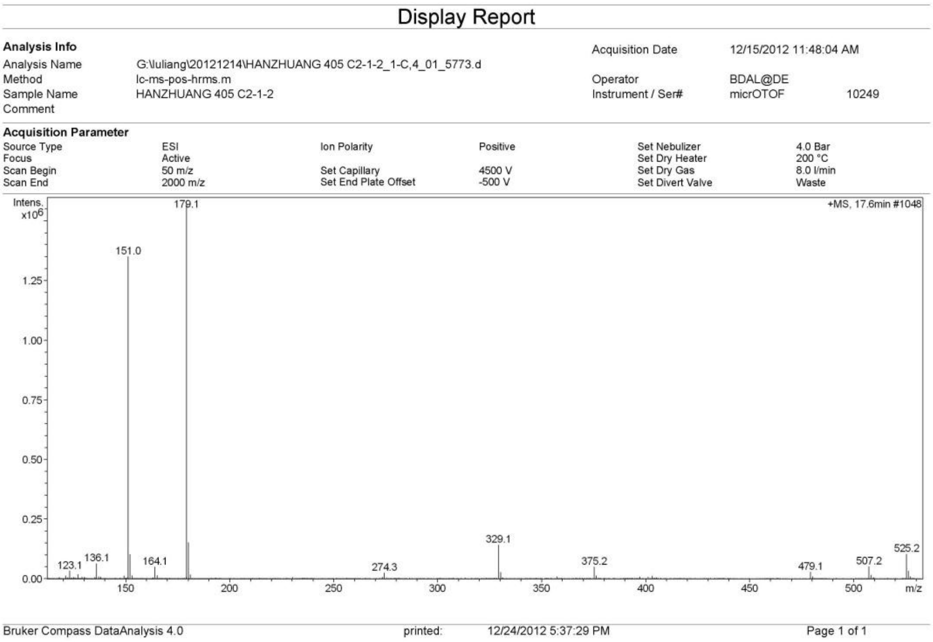
Figure S62 HRESIMS spectrum of **9**



Display Report

Analysis Info
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Method lc-ms-pos-hrms.m
Sample Name HANZHUANG 405 C2-1-2
Comment
Acquisition Date 12/15/2012 11:48:04 AM
Operator BDAL@DE
Instrument / Ser# micrOTOF 10249

Acquisition Parameter
Source Type ESI
Focus Active
Scan Begin 50 m/z
Scan End 2000 m/z
Ion Polarity Positive
Set Capillary 4500 V
Set End Plate Offset -500 V
Set Nebulizer 4.0 Bar
Set Dry Heater 200 °C
Set Dry Gas 8.0 l/min
Set Divert Valve Waste

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Figure S63 ISCID spectrum of **9**

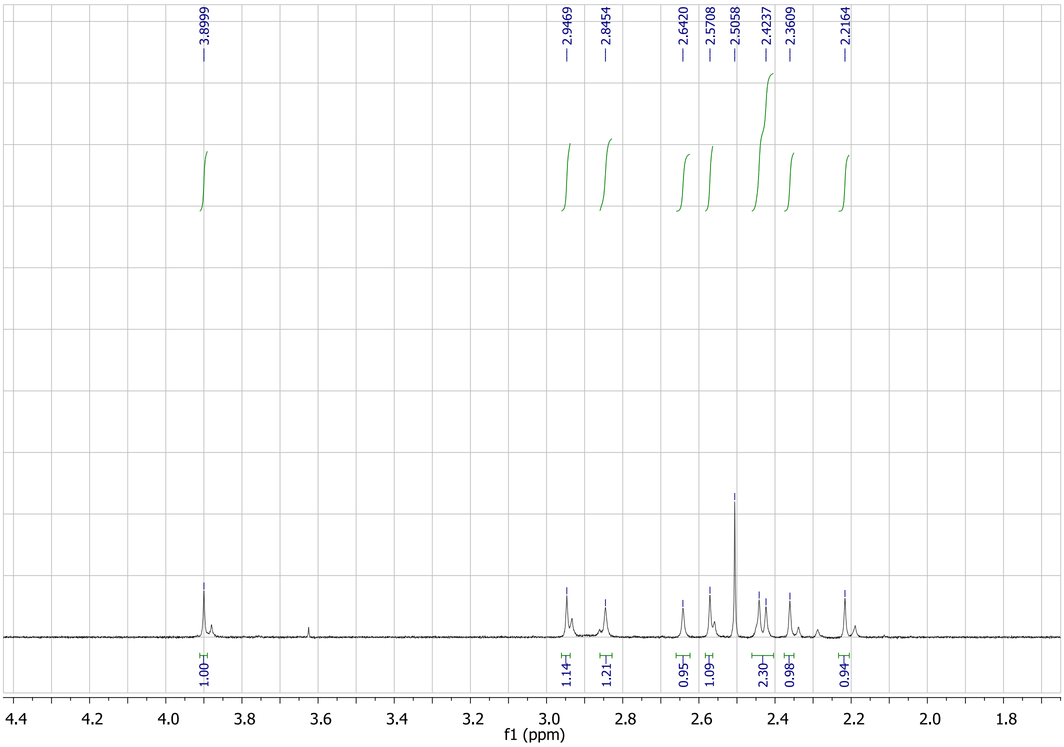


Figure S64 ^{1}H NMR spectrum of **10** in DMSO-d_6 (500 MHz)

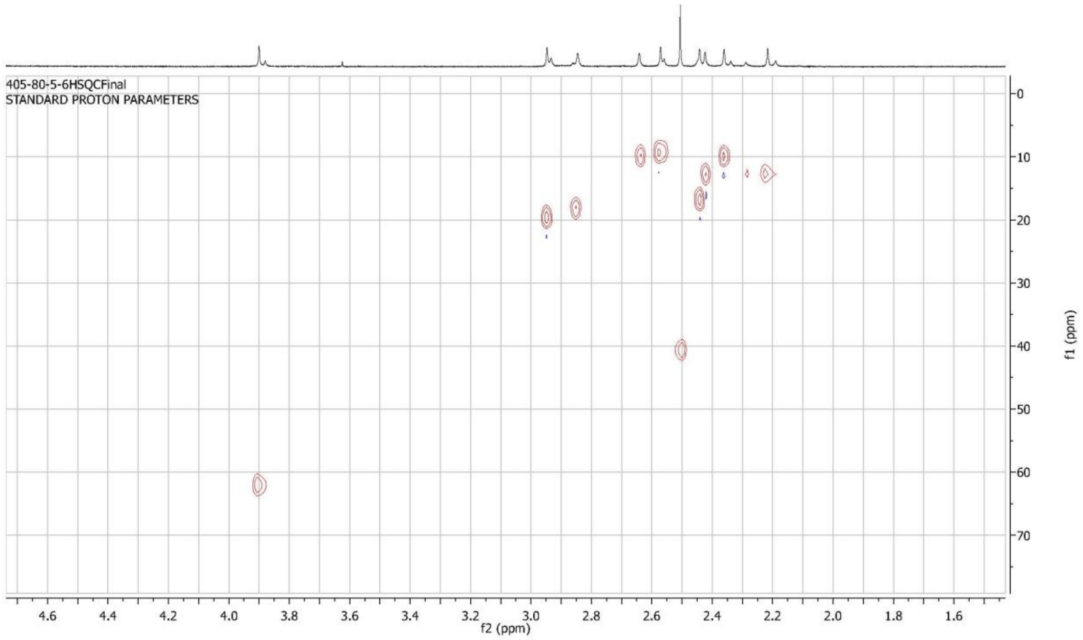


Figure S65 HMQC spectrum of **10** in DMSO-d_6

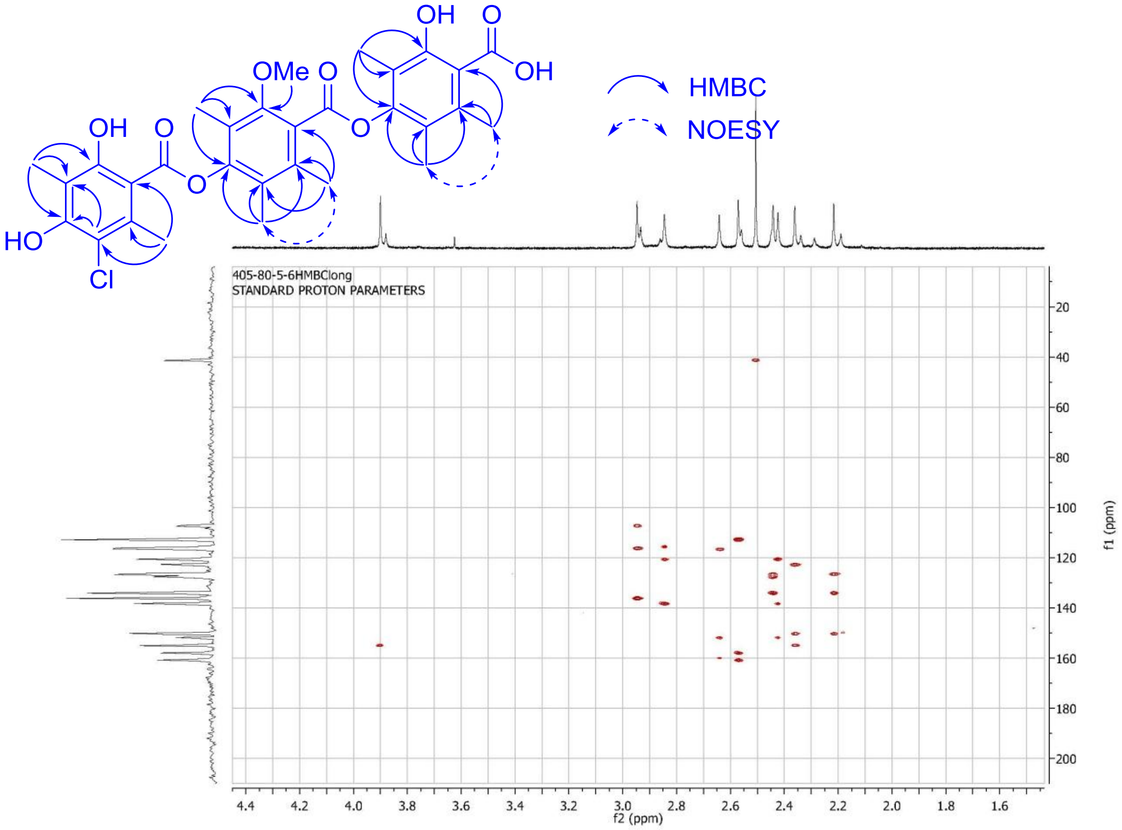


Figure S66 HMBC spectrum of **10** in DMSO-d_6

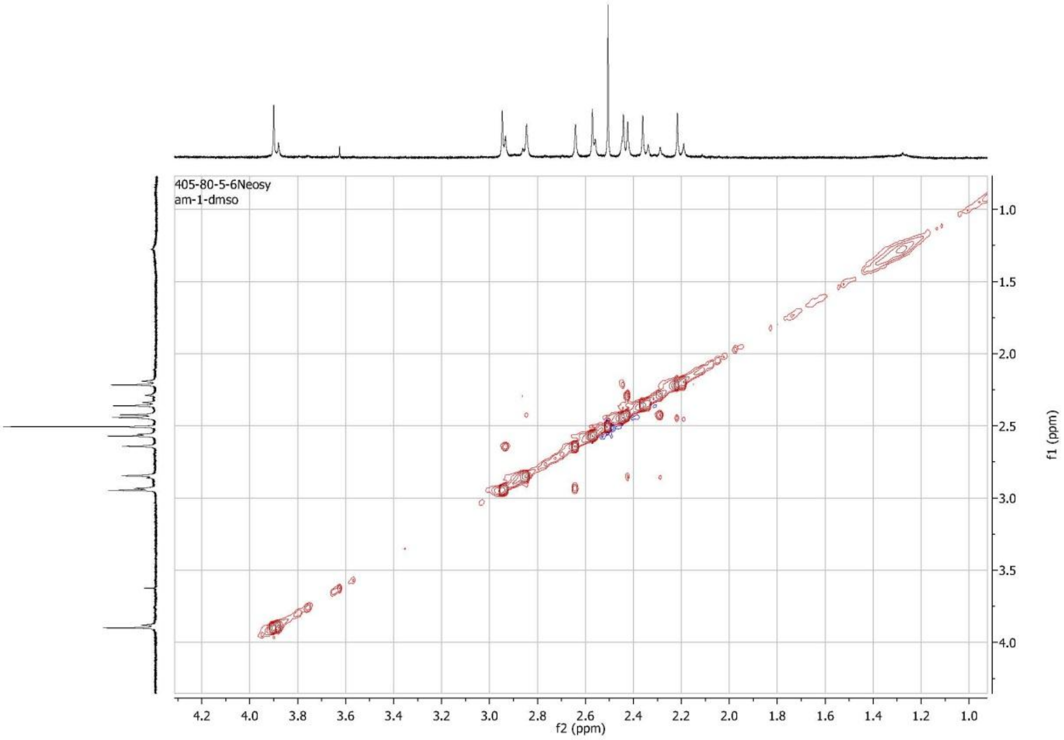
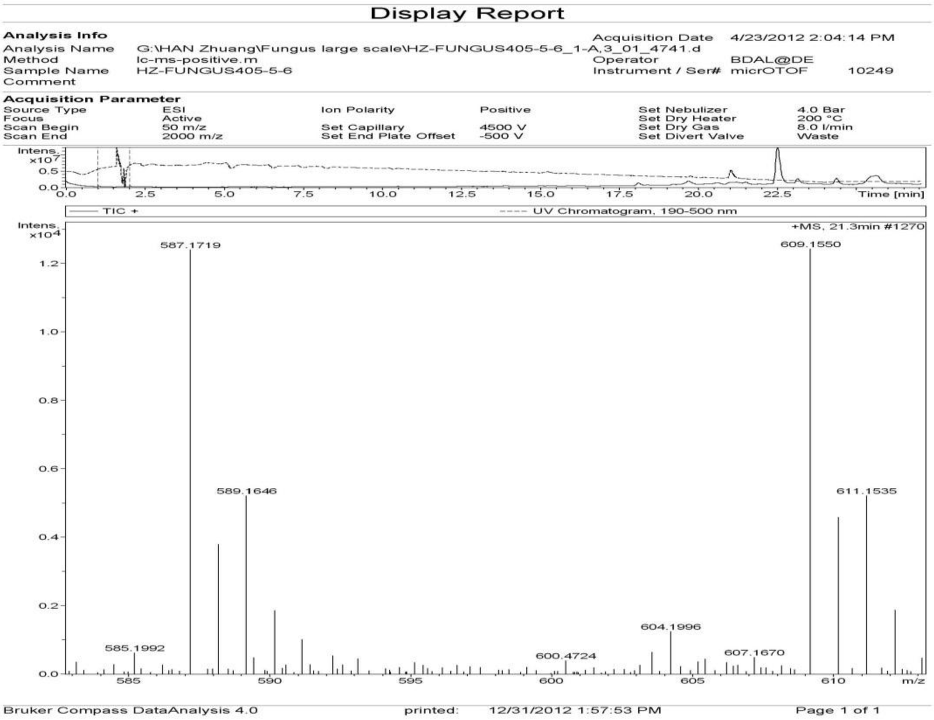


Figure S67 NOESY spectrum of **10** in DMSO-*d*6



Display Report

Analysis Info

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Method	lc-ms-positive.m	Operator	BDAL@DE
Sample Name	HZ-FUNGUS405-5-6	Instrument / Ser#	micrOTOF 10249
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

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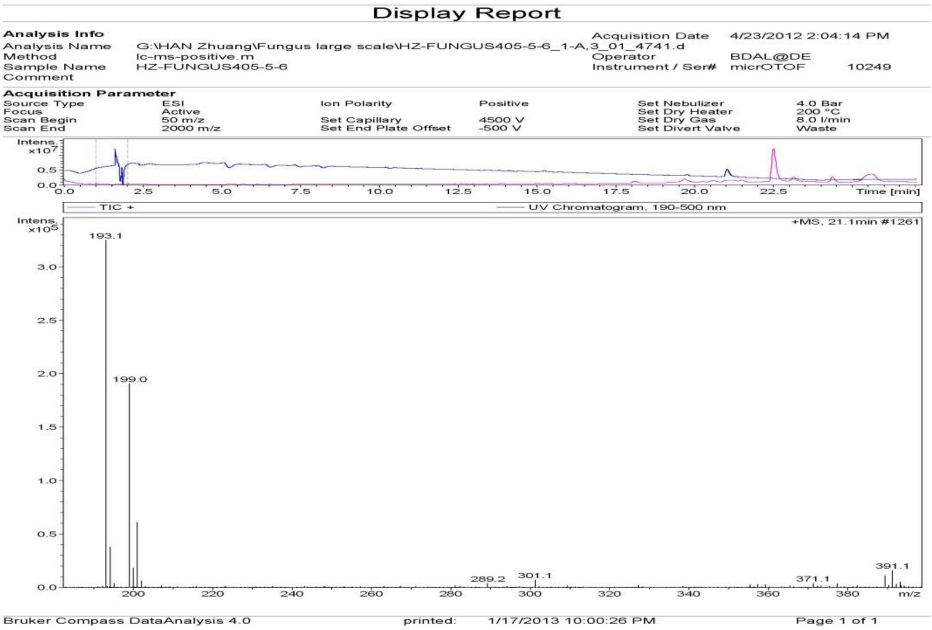
Figure S68 HRESIMS spectrum of **10**



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Method	lc-ms-positive.m	Operator	BDAL@DE
Sample Name	HZ-FUNGUS405-5-6	Instrument / Ser#	micrOTOF 10249
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Active			Set Dry Heater	200 °C
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Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

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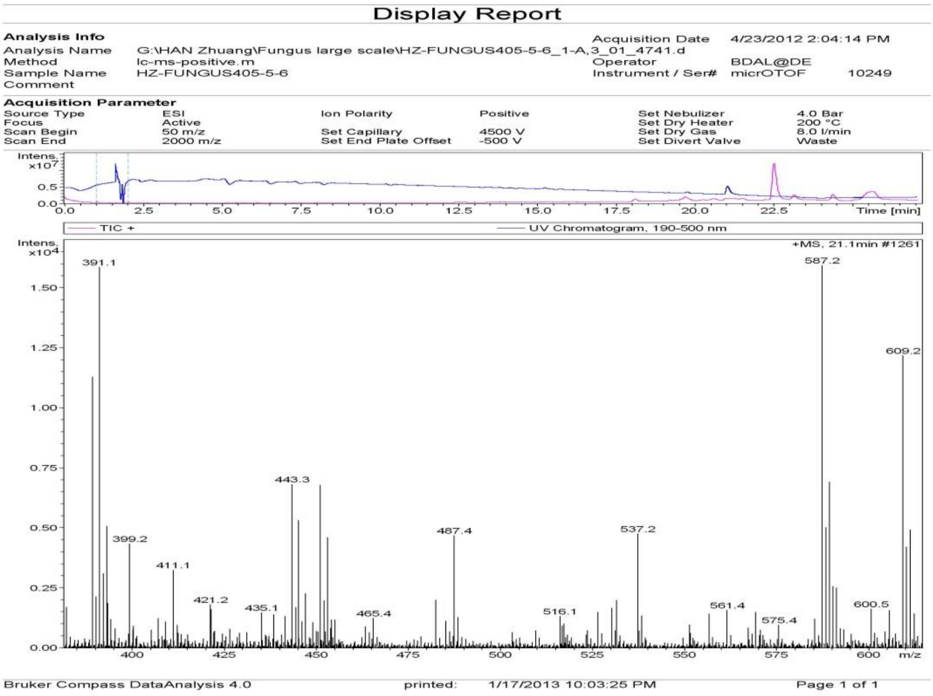
Figure S69A ISCID spectra of **10**



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Method	lc-ms-positive.m	Operator	BDAL@DE
Sample Name	HZ-FUNGUS405-5-6	Instrument / Ser#	micrOTOF 10249
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

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Figure S69B ISCID spectra of **10**

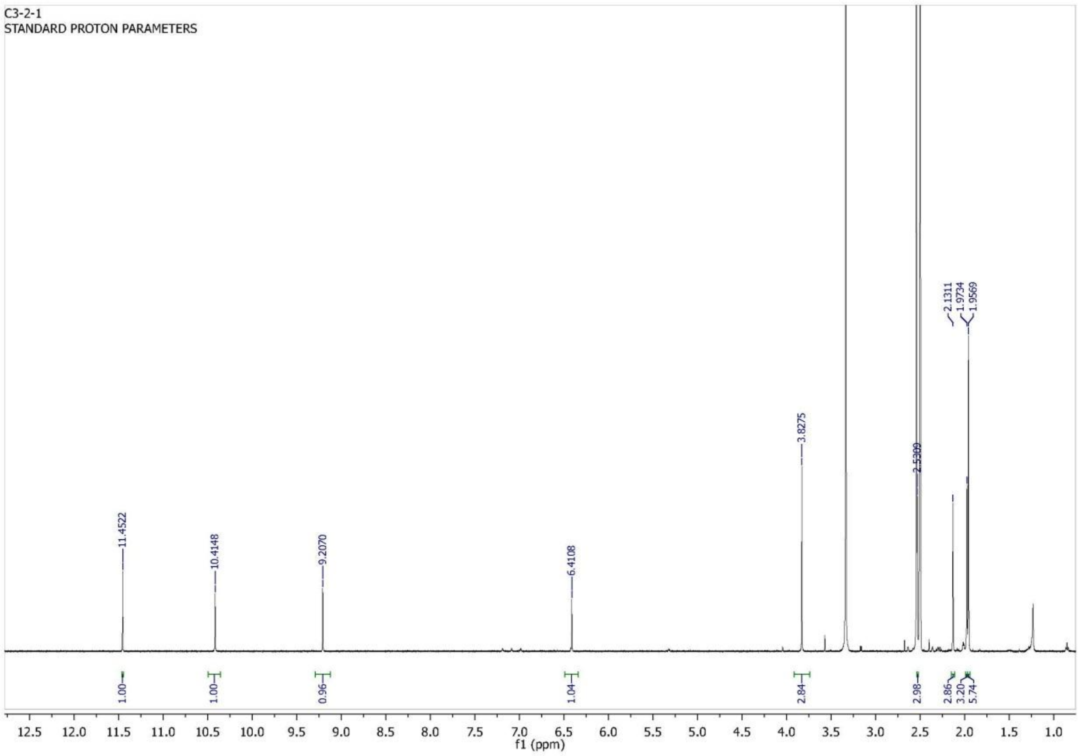


Figure S70 ^{1}H NMR spectrum of **11** in DMSO-d_6 (500 MHz)

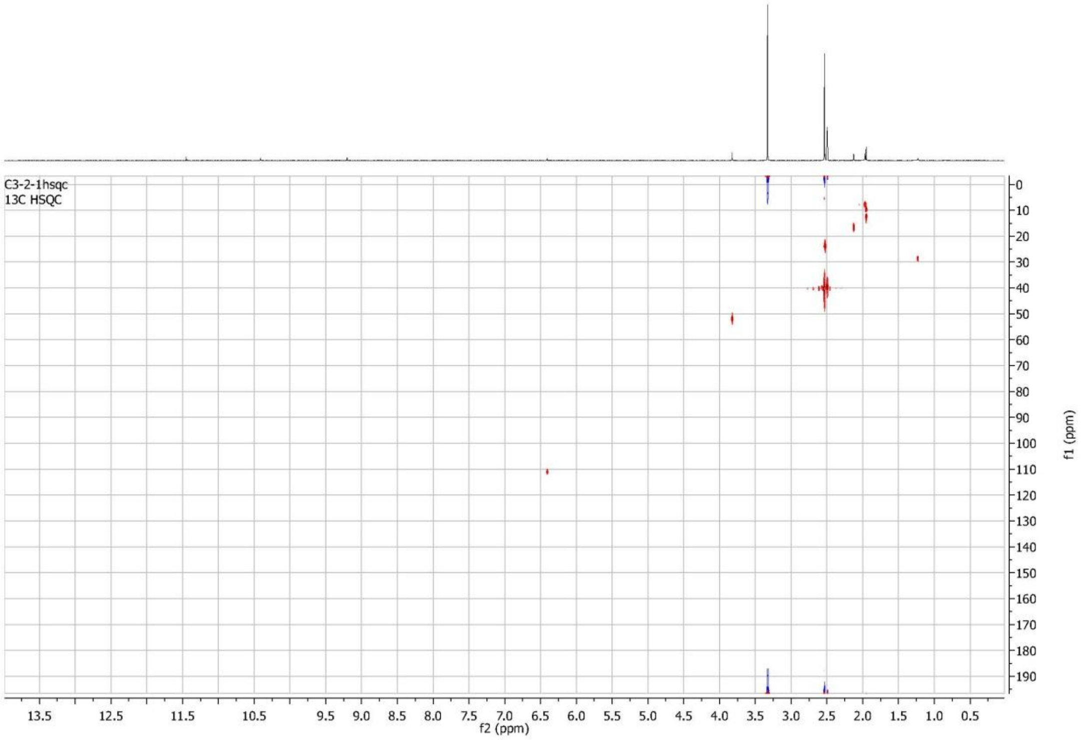


Figure S71 HMQC spectrum of **11** in DMSO-d_6

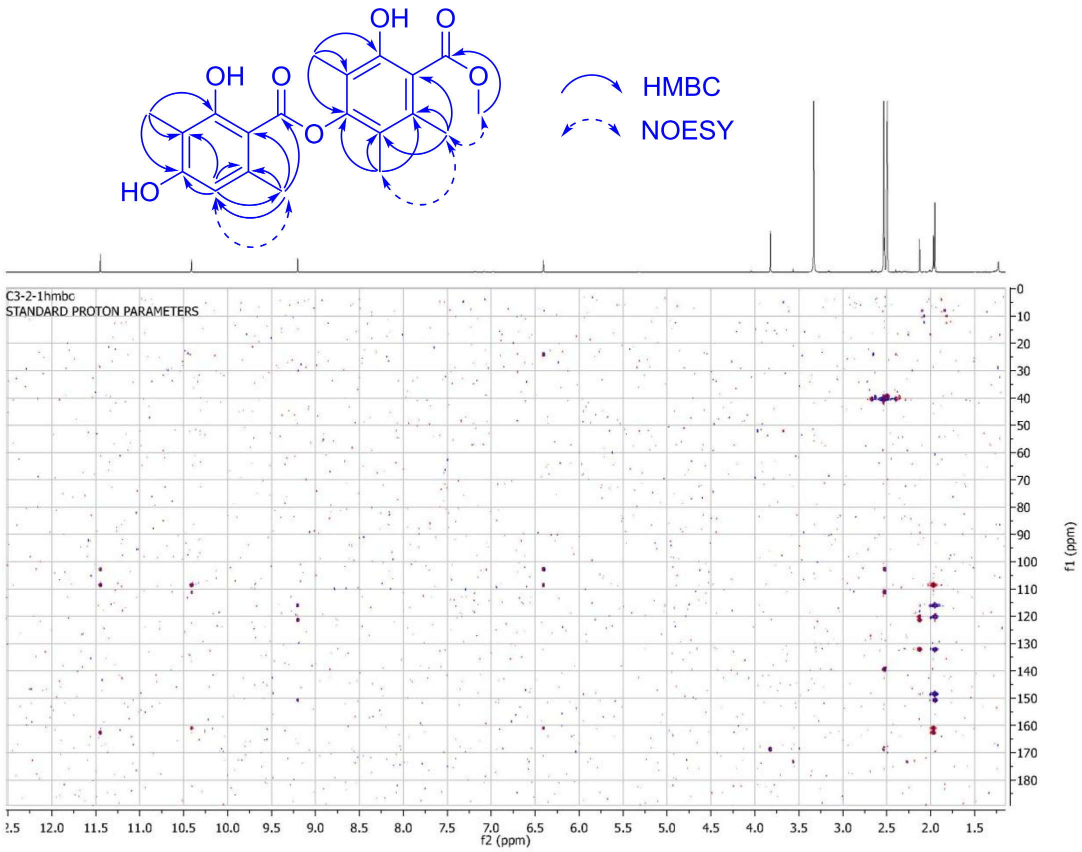


Figure S72 HMBC spectrum of **11** in DMSO-d_6

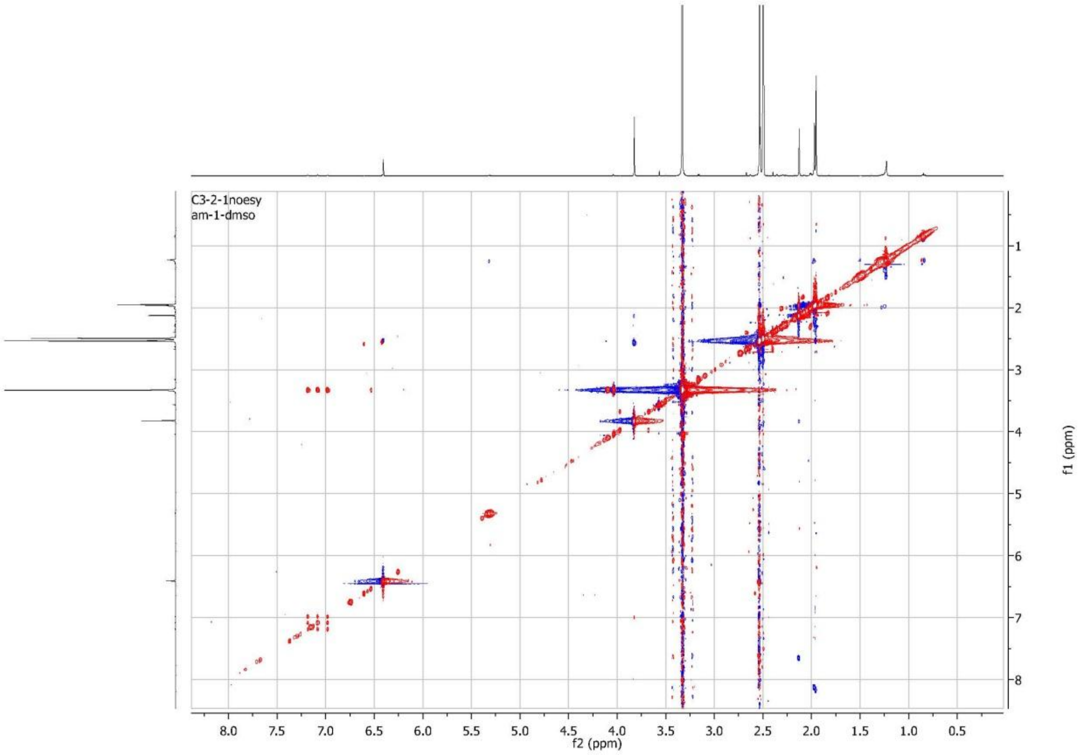
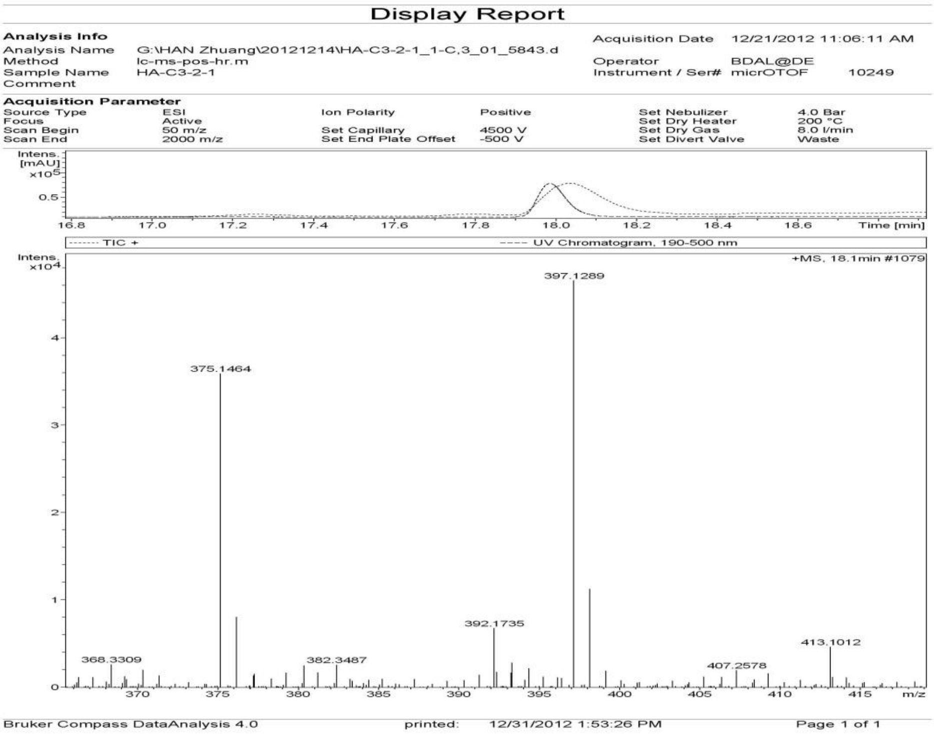


Figure S73 NOESY spectrum of **11** in DMSO-d_6



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Method lc-ms-pos-hr.m
Sample Name HA-C3-2-1
Comment
Acquisition Date 12/21/2012 11:06:11 AM
Operator BDAL@DE
Instrument / Ser# micrOTOF 10249

Acquisition Parameter
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Set Capillary 4500 V
Set End Plate Offset -500 V
Set Nebulizer 4.0 Bar
Set Dry Heater 200 °C
Set Dry Gas 8.0 l/min
Set Divert Valve Waste

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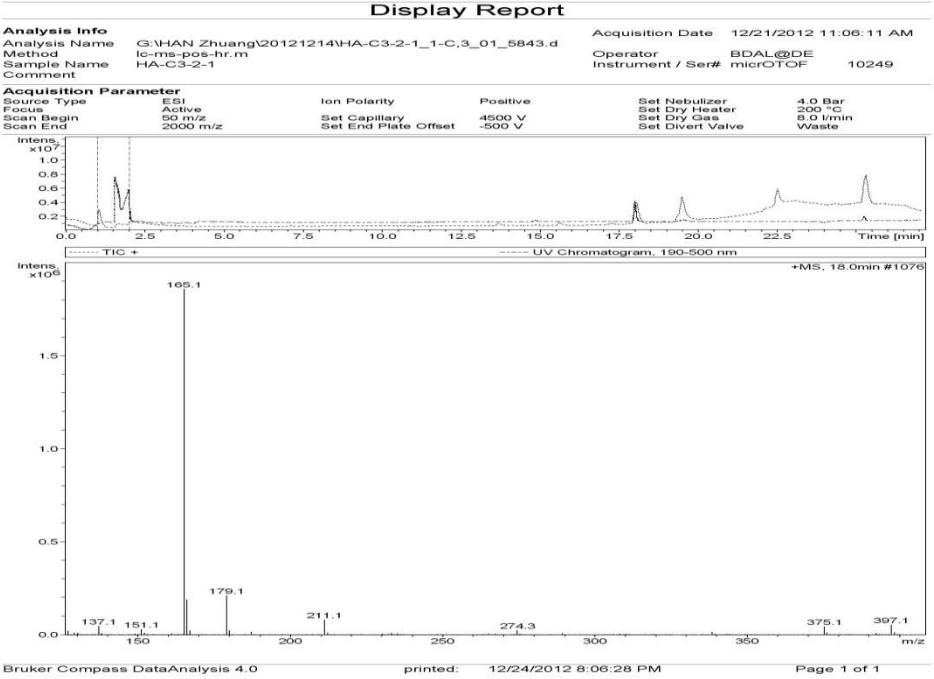
Figure S74 HRESIMS spectrum of **11**



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Analysis Info
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Sample Name HA-C3-2-1
Comment
Acquisition Date 12/21/2012 11:06:11 AM
Operator BDAL@DE
Instrument / Ser# micrOTOF 10249

Acquisition Parameter
Source Type ESI
Focus Active
Scan Begin 50 m/z
Scan End 2000 m/z
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Set Capillary 4500 V
Set End Plate Offset -500 V
Set Nebulizer 4.0 Bar
Set Dry Heater 200 °C
Set Dry Gas 8.0 l/min
Set Divert Valve Waste

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Figure S75 ISCID spectrum of **11**