
Supplementary Materials

‘Click Chemistry’ Synthesis of Novel Natural Product-Like Caged Xanthones Bearing a 1,2,3-Triazole Moiety with Improved Druglike Properties as Orally Active Antitumor Agents

Xiang Li ^{1,2}, Yue Wu ^{1,3}, Yanyan Wang ^{1,3}, Qidong You ^{1,3,*} and Xiaojin Zhang ^{1,4,*}

¹ Jiangsu Key Laboratory of Drug Design and Optimization, State Key Laboratory of Natural Medicines, China Pharmaceutical University, Nanjing 210009, China

² Department of Pharmaceutical Engineering, China Pharmaceutical University, Nanjing 211198, China

³ Department of Medicinal Chemistry, China Pharmaceutical University, Nanjing 21009, China

⁴ Department of Organic Chemistry, China Pharmaceutical University, Nanjing 211198, China

*Corresponding author

E-mail addresses: youqd@163.com (Q. You)

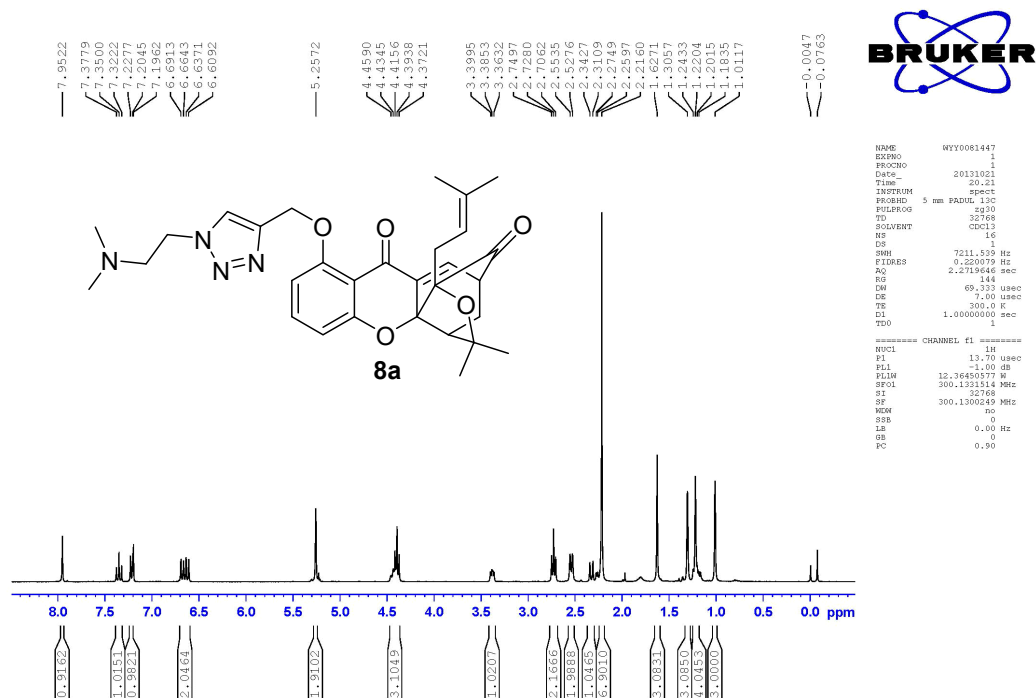
E-mail addresses: zxj@cpu.edu.cn (X. Zhang)

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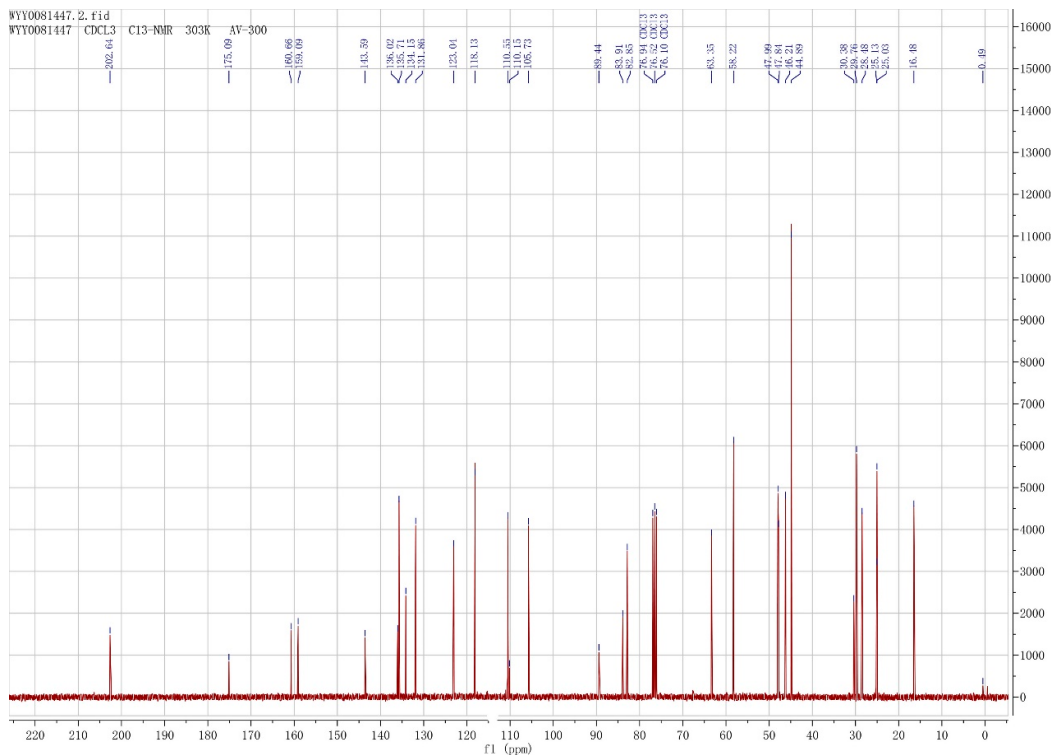
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1. Spectra for target compounds

^1H NMR(300 MHz) of **8a** in CDCl_3



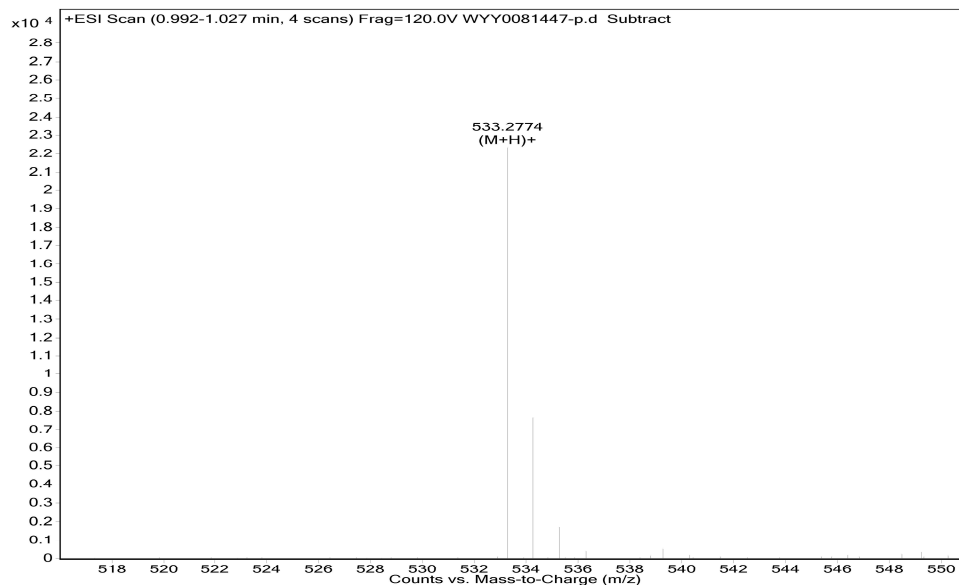
^{13}C NMR(75 MHz) of **8a** in CDCl_3



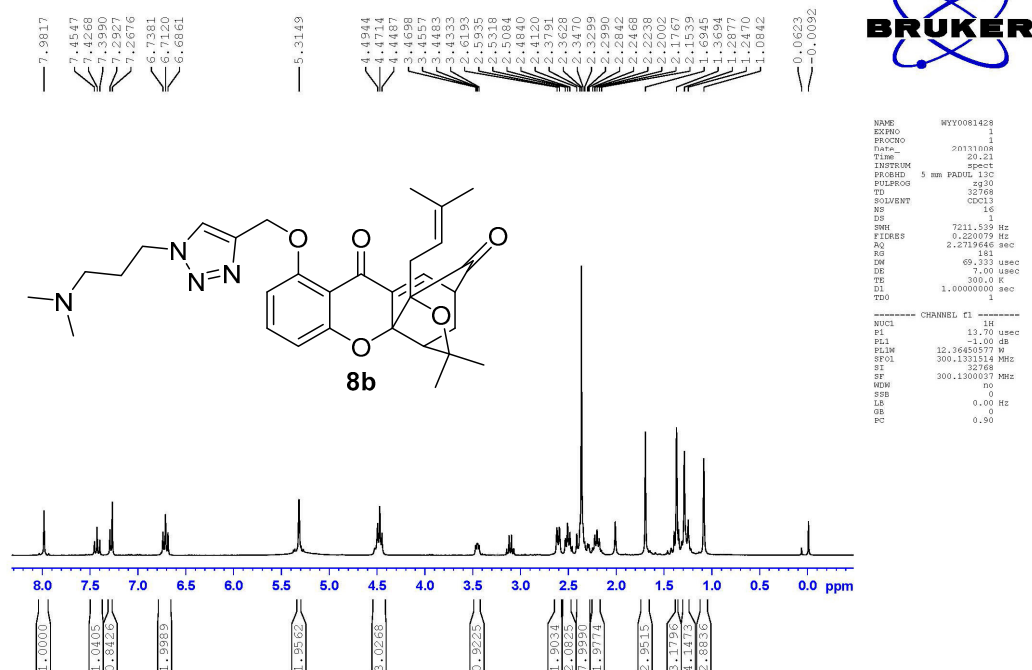
HRMS of 8a

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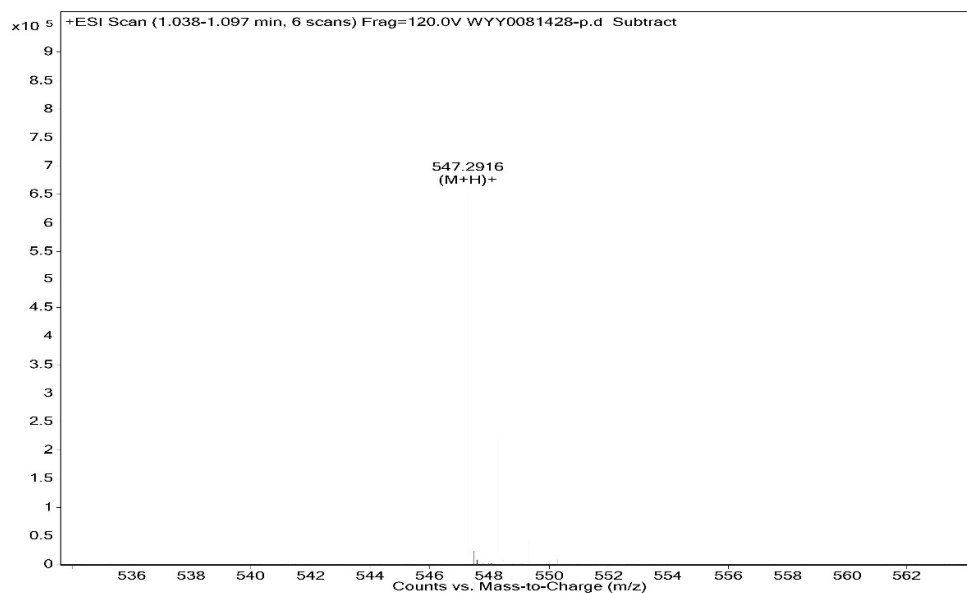
¹H NMR(300 MHz) of 8b in CDCl₃



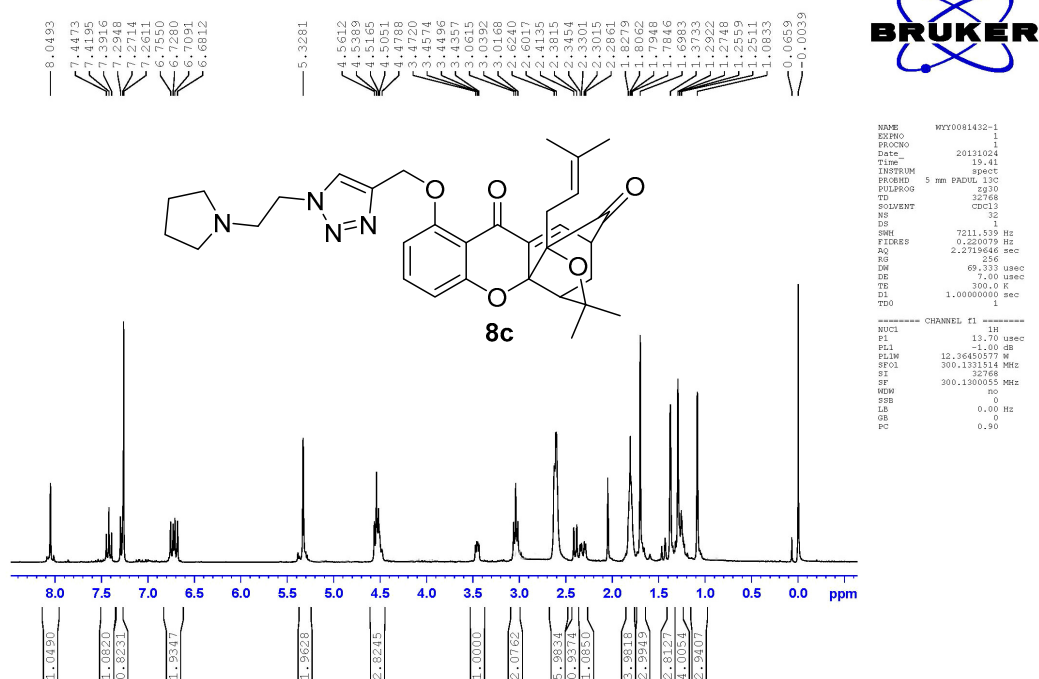
HRMS of 8b

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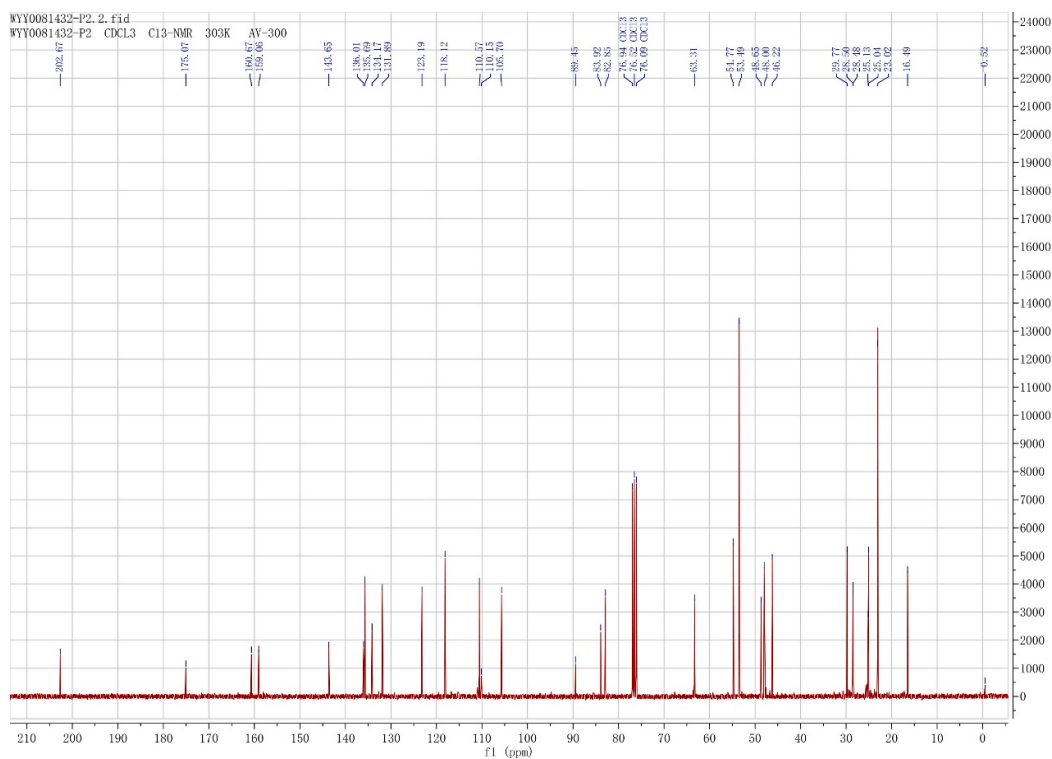
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¹H NMR(300 MHz) of 8c in CDCl₃

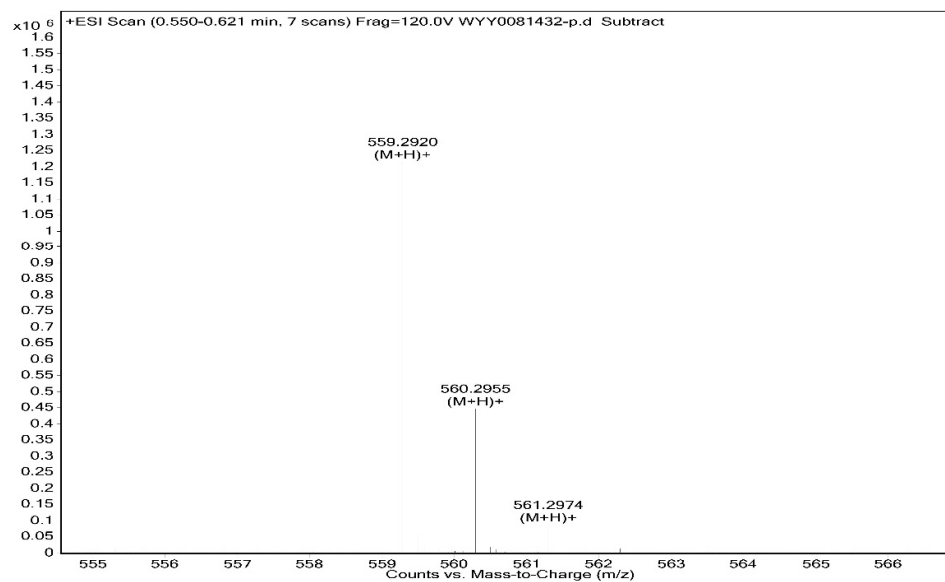


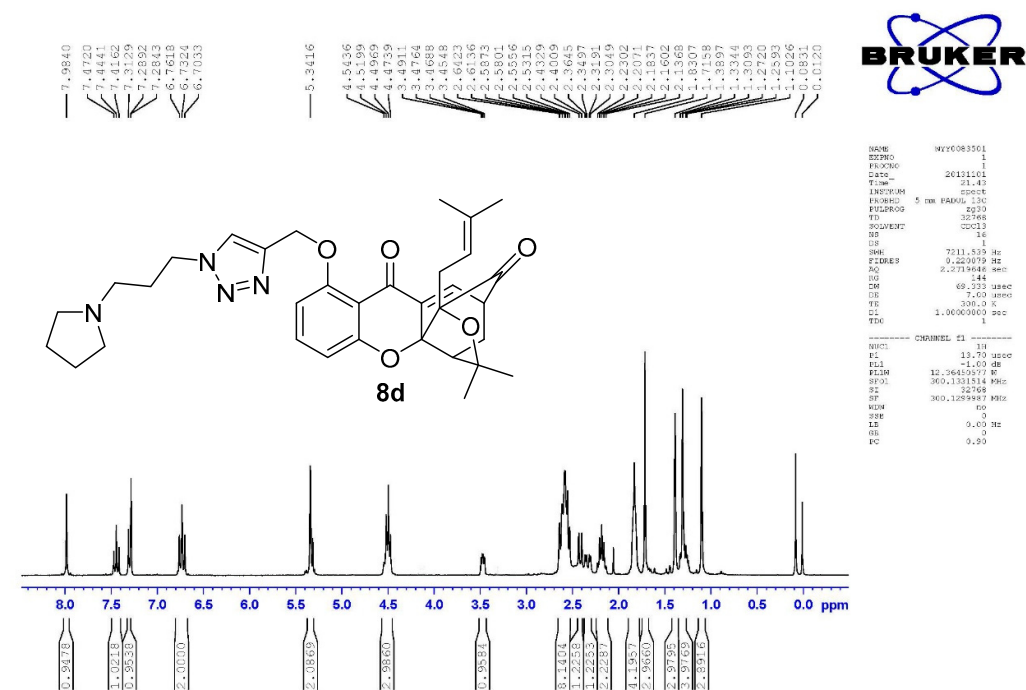
^{13}C NMR(75 MHz) of **8c** in CDCl_3



HRMS of **8c**

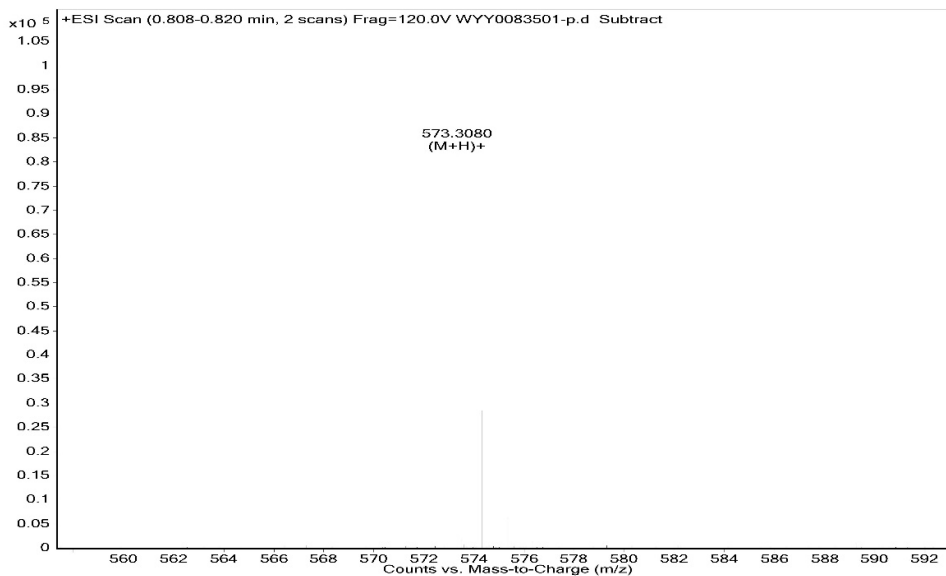
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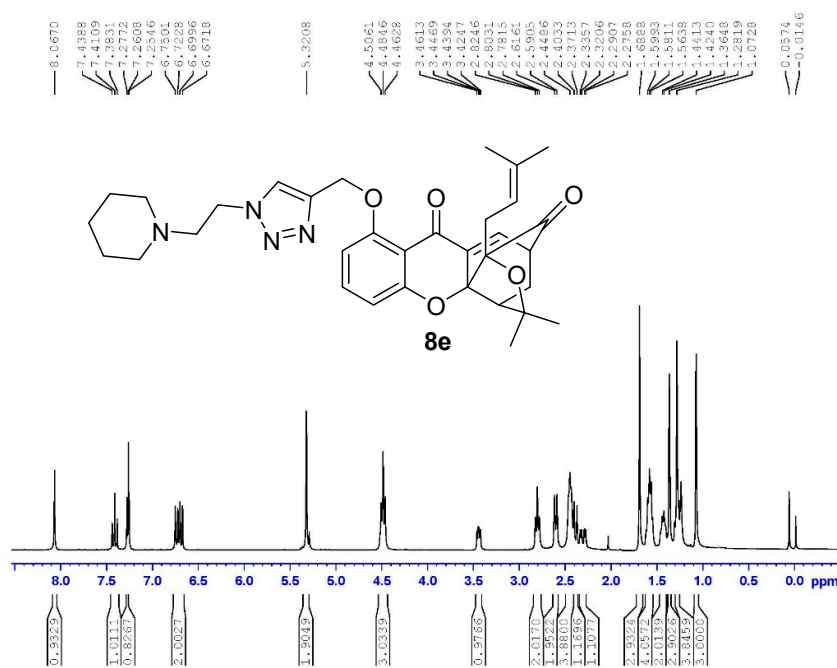


HRMS of **8d**

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¹H NMR(300 MHz) of **8e** in CDCl₃

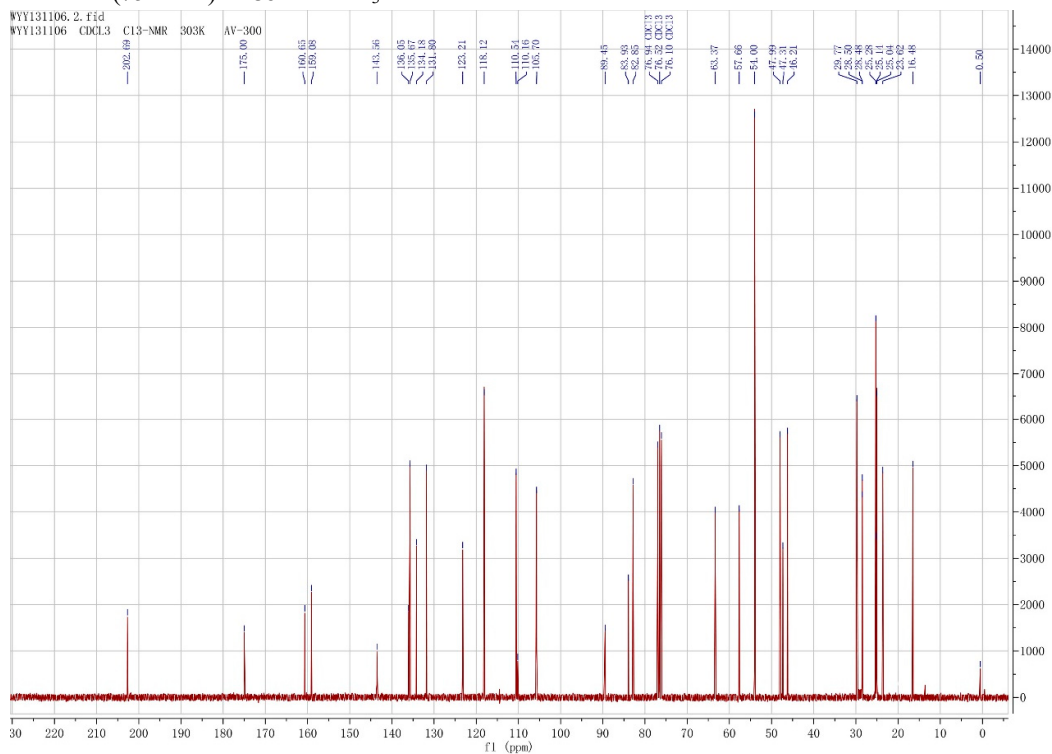


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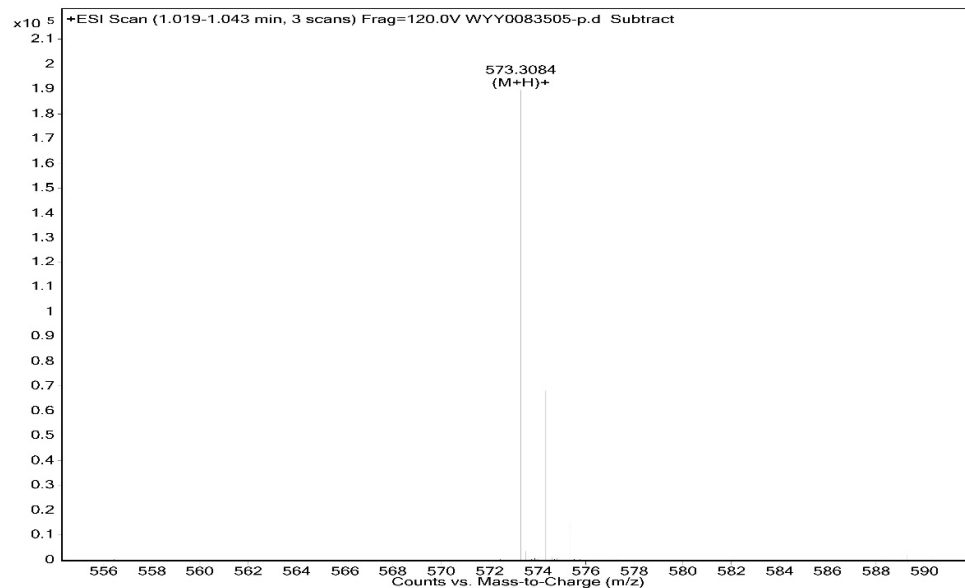
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¹³C NMR(75 MHz) of **8e** in CDCl₃

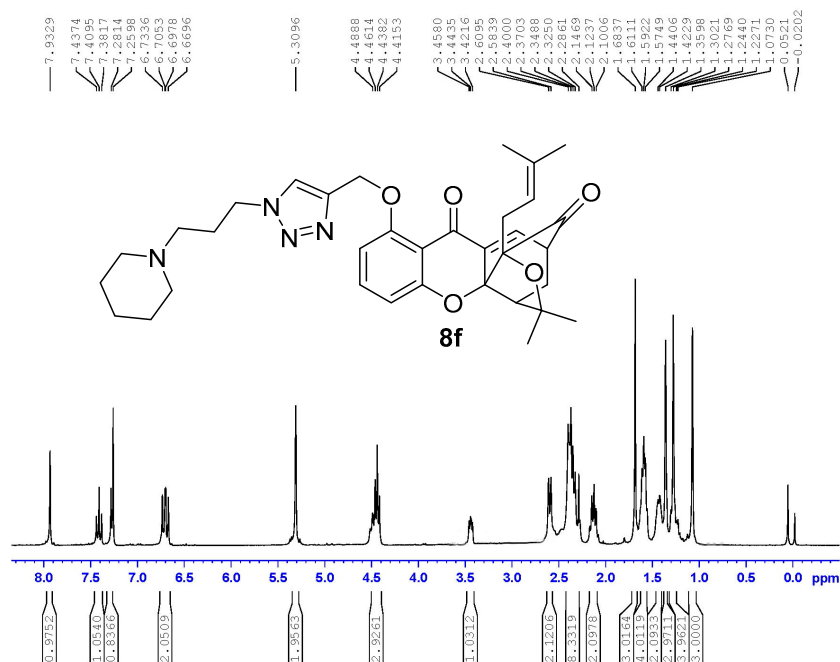


HRMS of 8e

Sample Name		Position	P2-B1	Instrument Name	Instrument 1	User Name	
Inj Vol	0.5	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	WYY0083505-p.d	ACQ Method		Comment		Acquired Time	11/13/2013 2:46:29 PM



¹H NMR(300 MHz) of 8f in CDCl₃



```

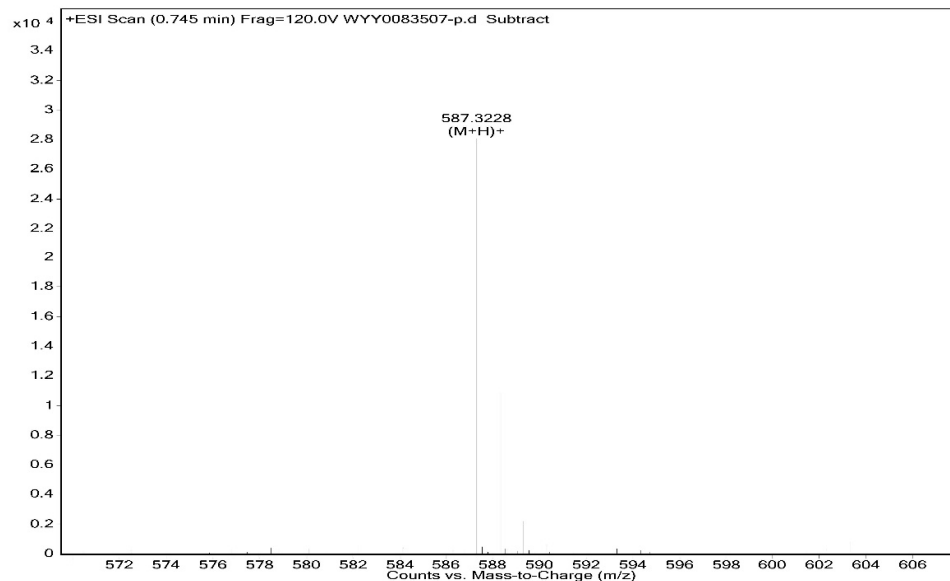
NAME      WYY0083507
EXPNO     1
PROCNO    1
Date_     20131116
Time      16:29
INSTRUM   spect
PROBHD    5 mm PABUL-13C
PULPROG   zg30
TD        32768
SOLVENT   CDCl3
NS         16
DS         1
SWH        7211.559 Hz
FIDRES     0.220979 Hz
AQ         2.2719446 sec
RG         101
DM         69.123 usec
DE         7.00 usec
TE         300.0 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13
P1         13.70 usec
PL1        -1.00 dB
PL12       12.36450577 W
SFO1       300.1351114 MHz
SI         32768
SF         300.1350055 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         0.90
  
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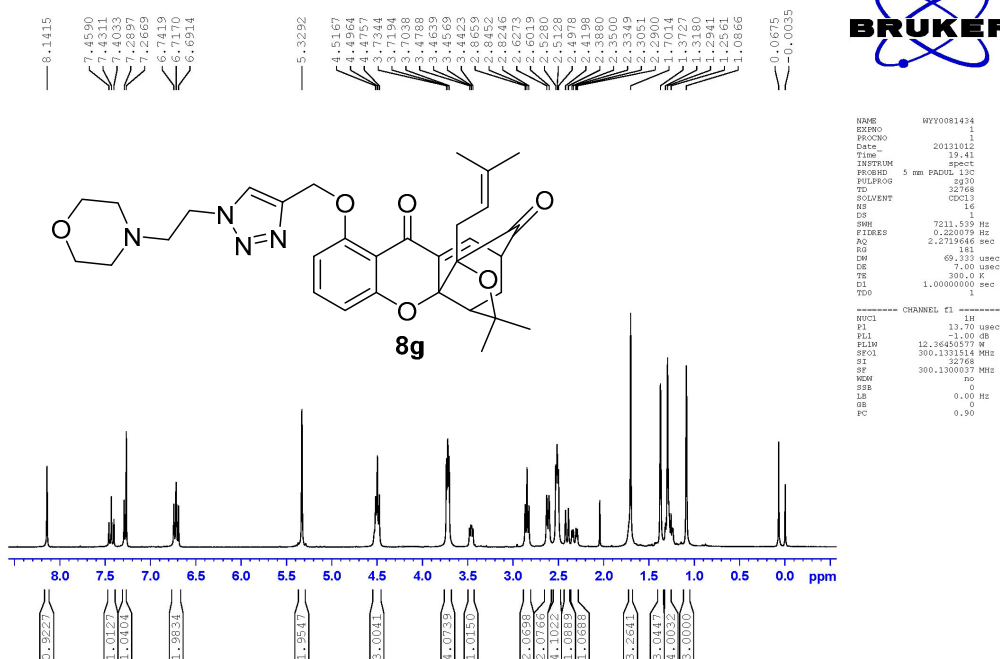
HRMS of 8f

Sample Name	Position	P1-D8	Instrument Name	Instrument 1	User Name
Inj Vol	0.5	InjPosition	SampleType	Sample	IRM Calibration Status
Data Filename	WYY0083507-p.d	ACQ Method	Comment		Acquired Time

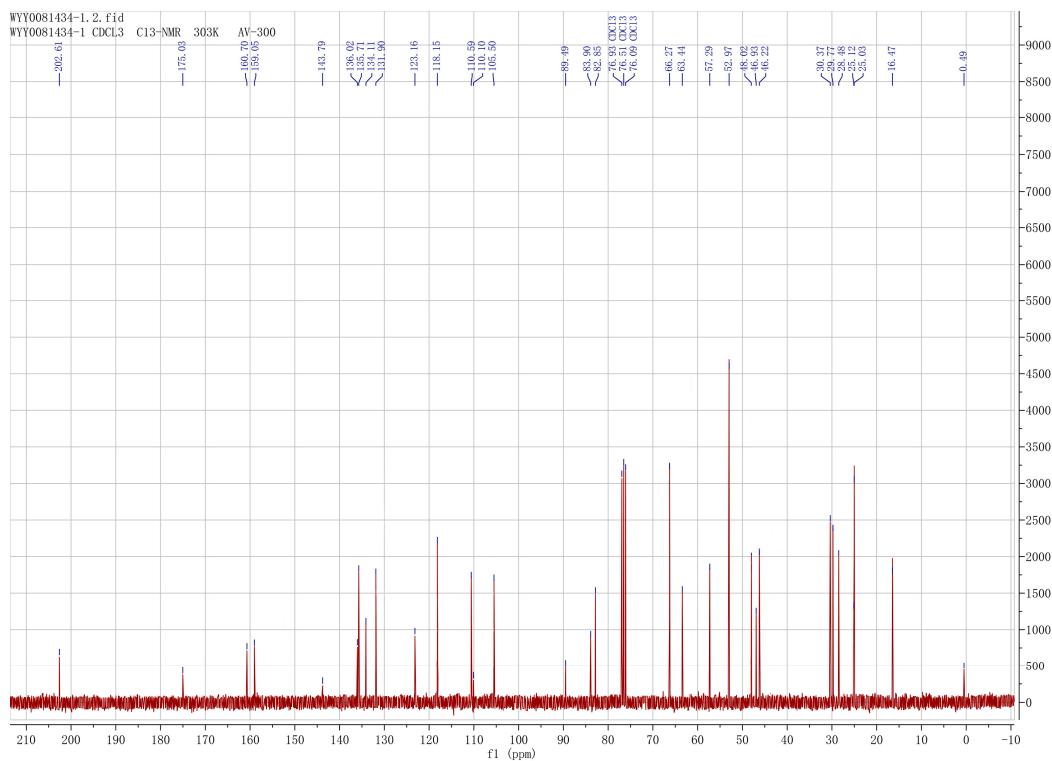
Success
11/19/2013 4:17:43 PM



¹H NMR(300 MHz) of 8g in CDCl₃

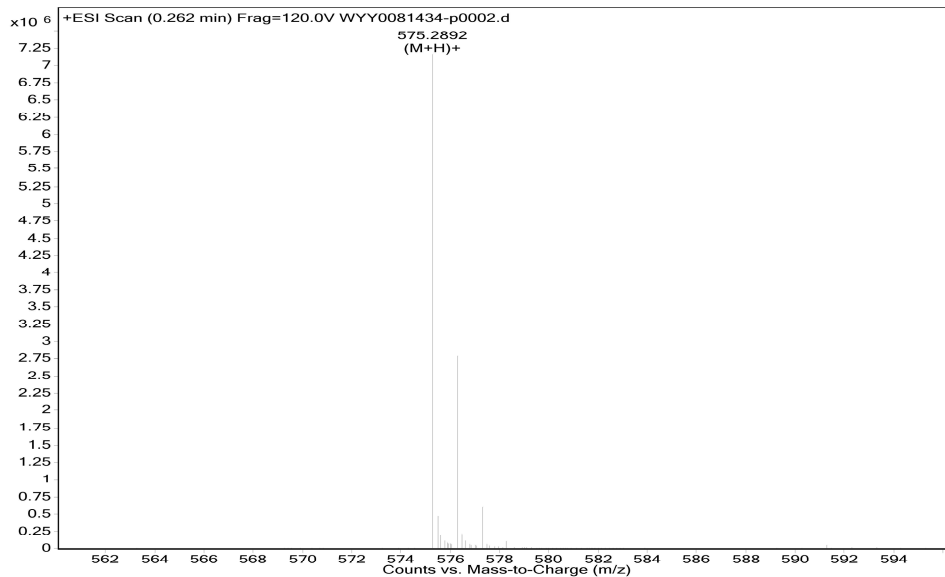


¹³C NMR(75 MHz) of **8g** in CDCl₃

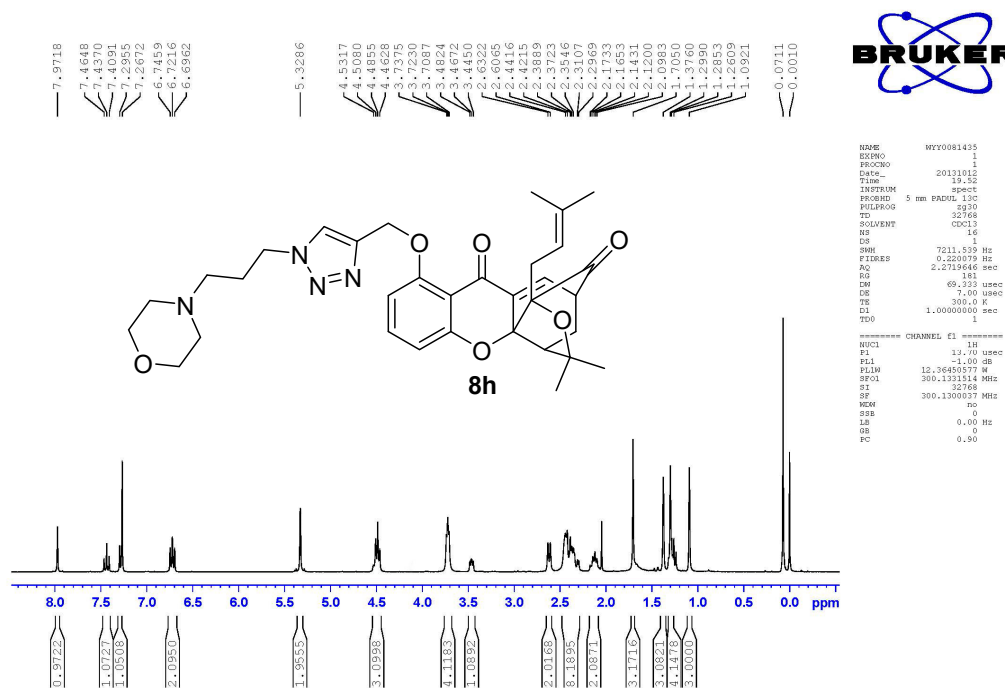


HRMS of **8g**

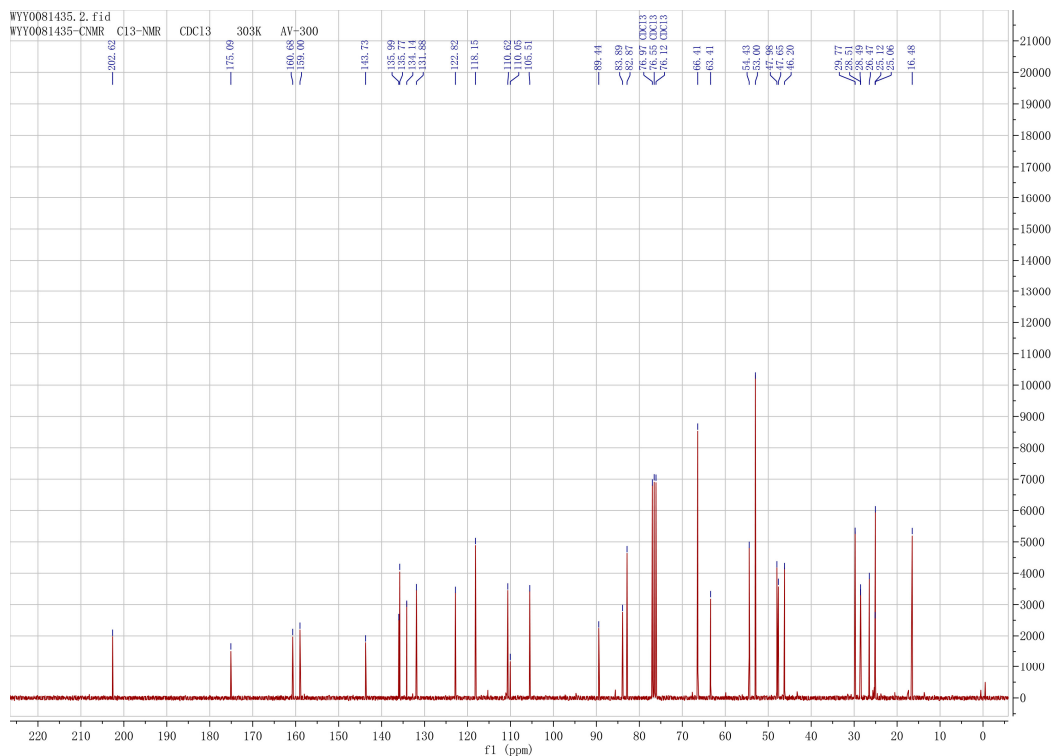
Sample Name	Position	PZ-E8	Instrument Name	Instrument 1	User Name	IRM Calibration Status	Success
Inj Vol	0.5	InjPosition	SampleType	Sample	Acquired Time	10/13/2013 6:00:40 PM	
Data Filename	WYY0081434-p0002.d	ACQ Method	Comment				



^1H NMR(300 MHz) of **8h** in CDCl_3

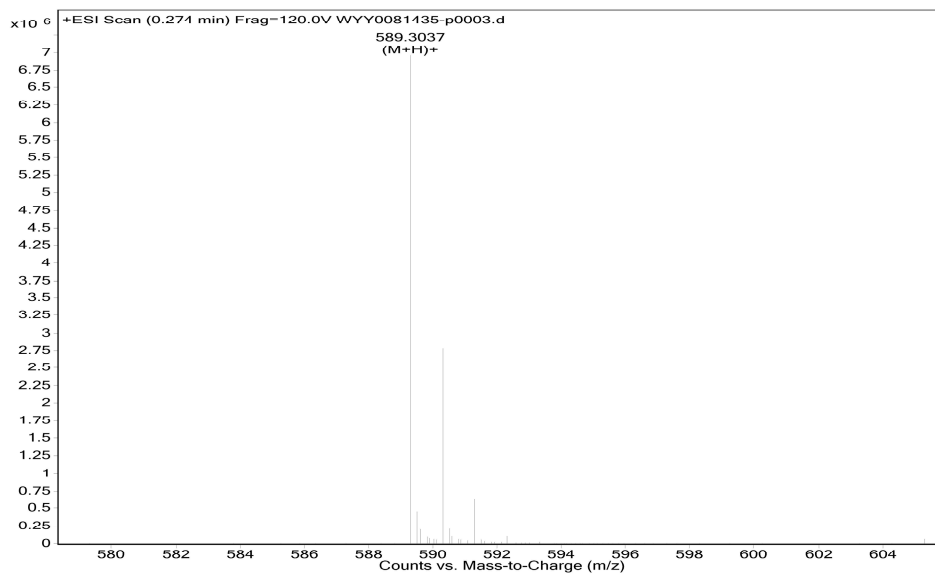


^{13}C NMR(75 MHz) of **8h** in CDCl_3

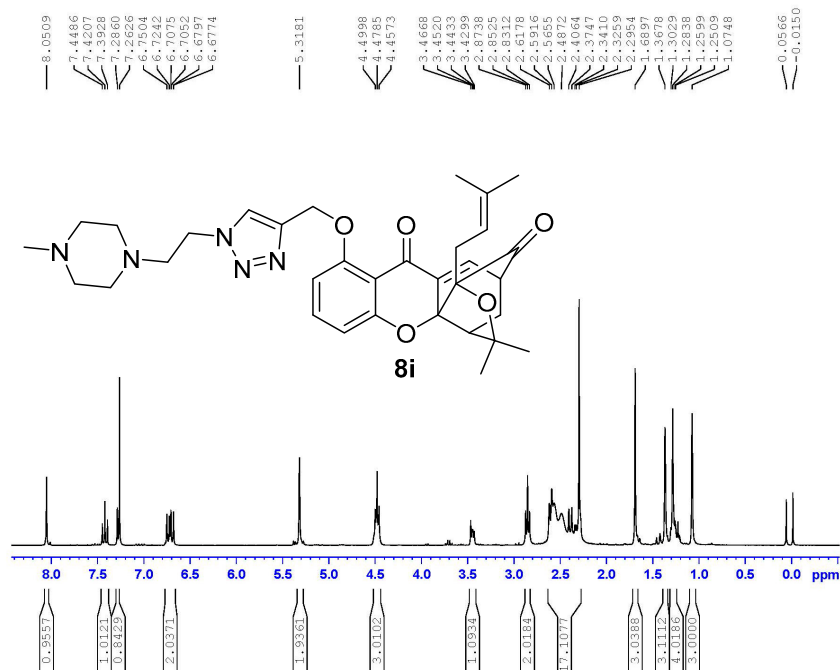


HRMS of 8h

Sample Name	Position	P2-E9	Instrument Name	Instrument 1	User Name	
Inj Vol	2	InjPosition	SampleType	Sample	IRM Calibration Status	Success
Data Filename	WYY0081435 p0003.d	ACQ Method	Comment		Acquired Time	10/13/2013 6:03:48 PM



¹H NMR(300 MHz) of 8i in CDCl₃



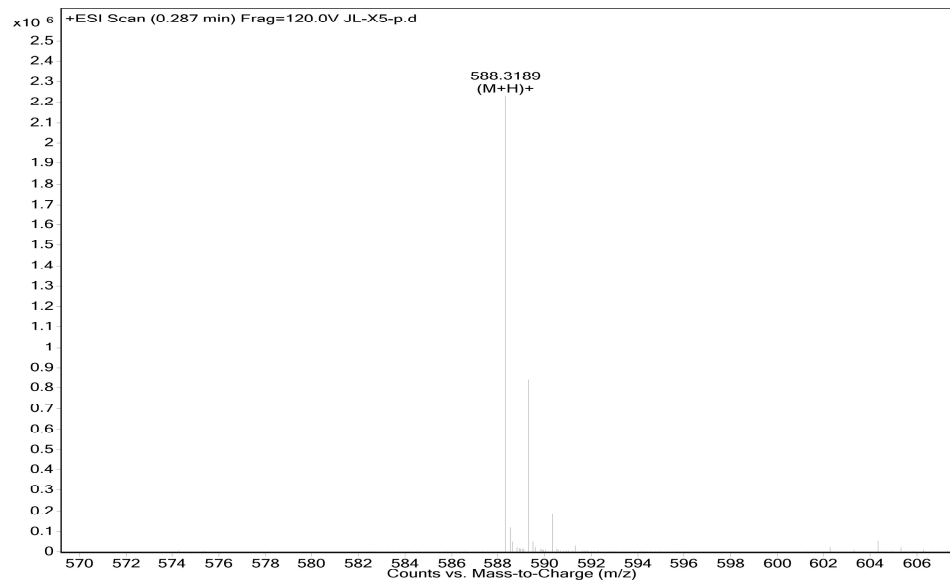
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NAME      WYY0083512
EXPNO     1
PROCNO    1
Date_     20131205
Time      21.32
INSTRUM    spect
PROBHD     5 mm PADUL 13C
PULPROG    zg30
TD          32768
SOLVENT    CDCl3
NS          16
DS          1
SWH         6188.119 Hz
FIDRES     0.188846 Hz
AQ          2.6477044 sec
RG          128
DS          80.400 usec
DE          7.00 usec
TE          300.0 K
D1          1.00000000 sec
TD0         1

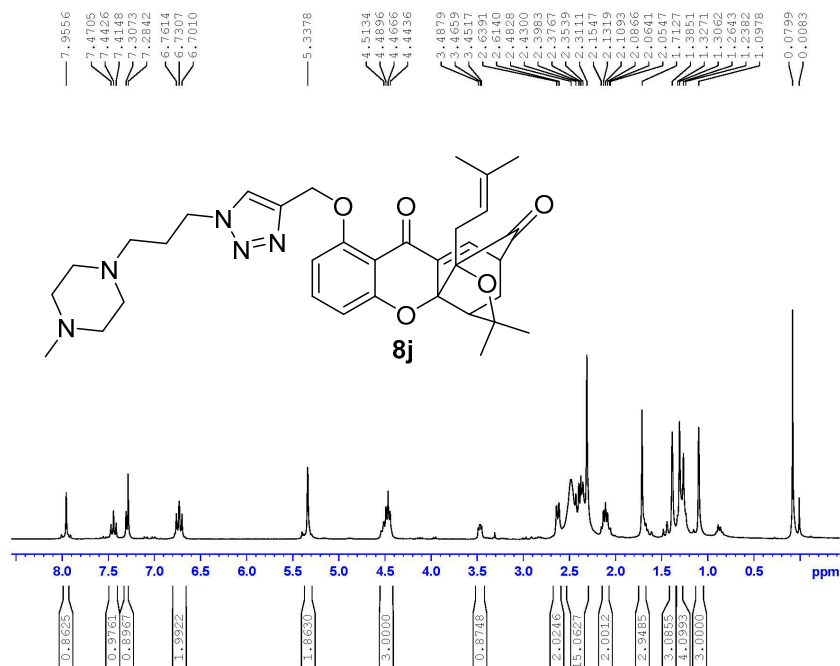
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NUC1       1H
P1          13.70 usec
PL1        -1.50 dB
PL12       12.36450577 dB
SFO1       300.1318534 MHz
SI          32768
SF          300.1300051 MHz
WDW         no
SSB         0
LB          0.00 Hz
GB          0
PC          1.00
  
```

HRMS of **8i**

Sample Name	Position	P1-C9	Instrument Name	Instrument 1	User Name	
Inj Vol	0.6	InjPosition	SampleType	Sample	IRM Calibration Status	Success
Data Filename	JL-X5-p.d	ACQ Method	Comment		Acquired Time	12/12/2013 12:59:57 PM



¹H NMR(300 MHz) of **8j** in CDCl₃

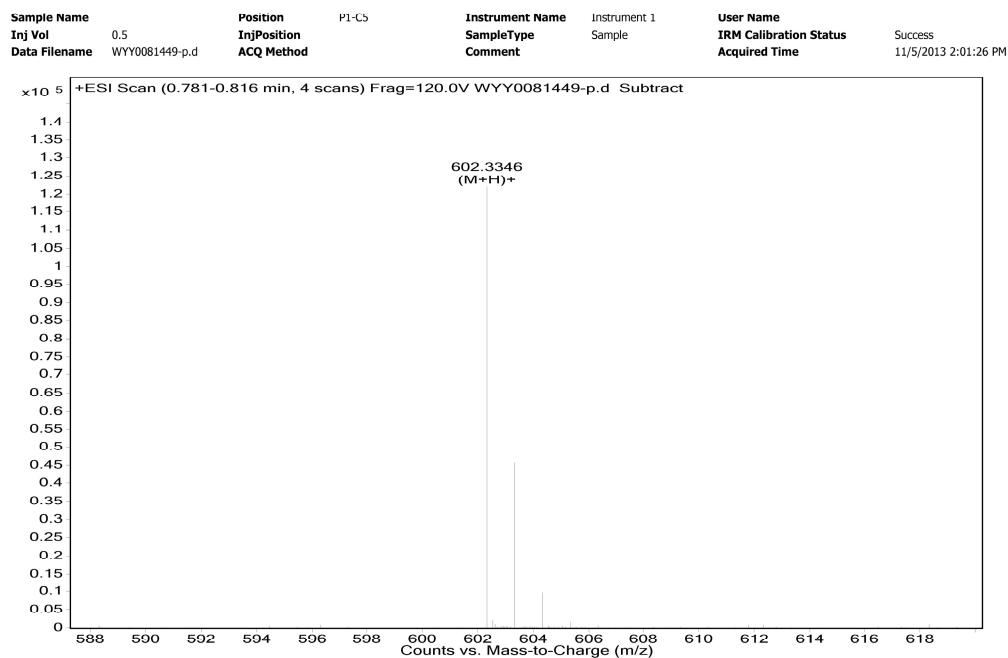


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NAME      MYV0081449
EXPNO     1
PROCNO    1
Date_     20121101
Time      22.05
INSTRUM    spect
PROBHD     5 mm PABUL 13C
PULPROG    zg30
TD         65536
SOLVENT    CDCl3
NS         16
DS         1
SWH         7211.539 Hz
FIDRES     0.220079 Hz
AQ         2.2719646 sec
RG         144
DM         69.333 usec
DE         7.00 usec
TE         300.0 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         13.70 usec
PL1        -1.00 dB
ELN        12.36450577 Hz
SF01       300.1331514 MHz
ST         32768
SF         300.1299967 MHz
WDW         Hanning
SSB         0
LB         0.00 Hz
GB         0
PC         0.90
  
```

HRMS of 8j



2. Data for Figure 3.

Table S1. Data of membrane permeability for Figure 3

Cpd	$P_e (10^{-6} \text{ cm/s})^a$		
	pH=5.0	pH=6.2	pH=7.4
8a	27.9±3.3	58.8±2.1	91.4±9.8
8b	16.3±1.2	41.7±3.2	76.1±6.4
8c	42.3±1.5	75.4±6.9	91.9±6.0
8d	15.4±2.1	52.8±1.6	66.4±8.4
8e	47.8±4.7	57.2±1.4	78.2±8.8
8f	34.9±3.6	55.1±0.8	68.7±5.3
8g	51.3±4.8	63.1±5.6	74.4±6.8
8h	40.0±0.1	58.0±6.1	72.6±0.1
8i	11.3±0.6	41.5±1.3	67.5±4.2
8j	9.7±0.5	43.2±0.7	64.9±5.4
DDO-6101	23.6±5.5	25.8±1.1	18.0±3.9
GA	0.9±0.5	1.8±0.2	2.3±0.3
Ketoprofen ^a	—	—	1.8±0.3
Propranolol ^a	—	—	127.5±15.8

^a Ketoprofen and propranolol are internal standards in permeability determinations. Data are expressed as the mean P_e from three independent experiments.