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

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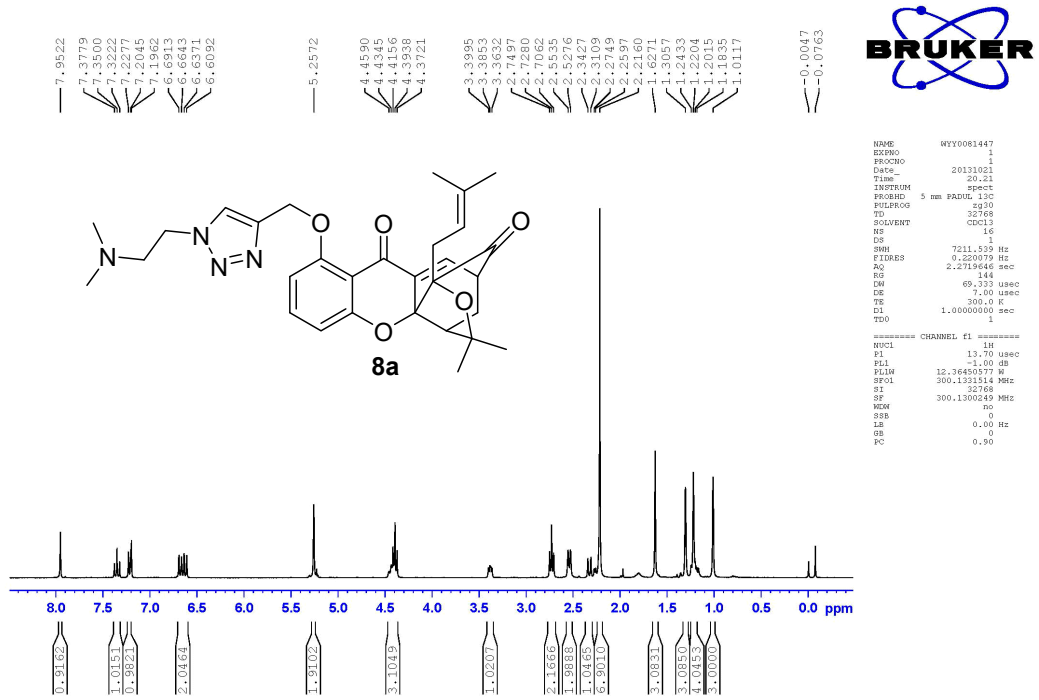
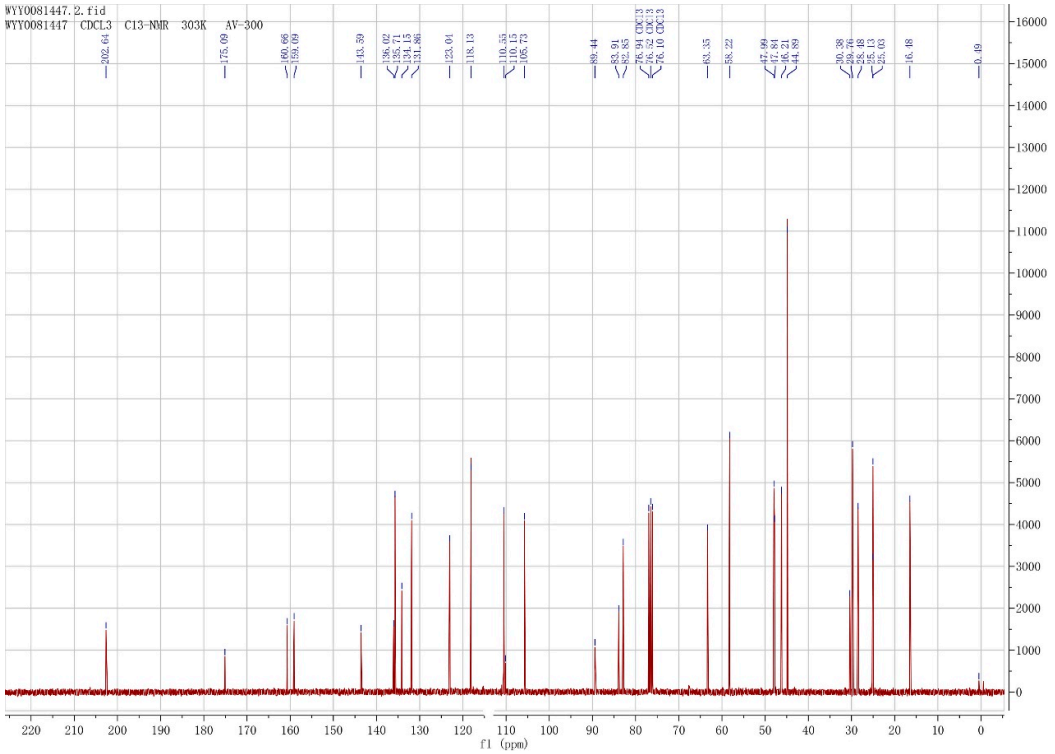
1. Spectra for target compounds

^{1}H 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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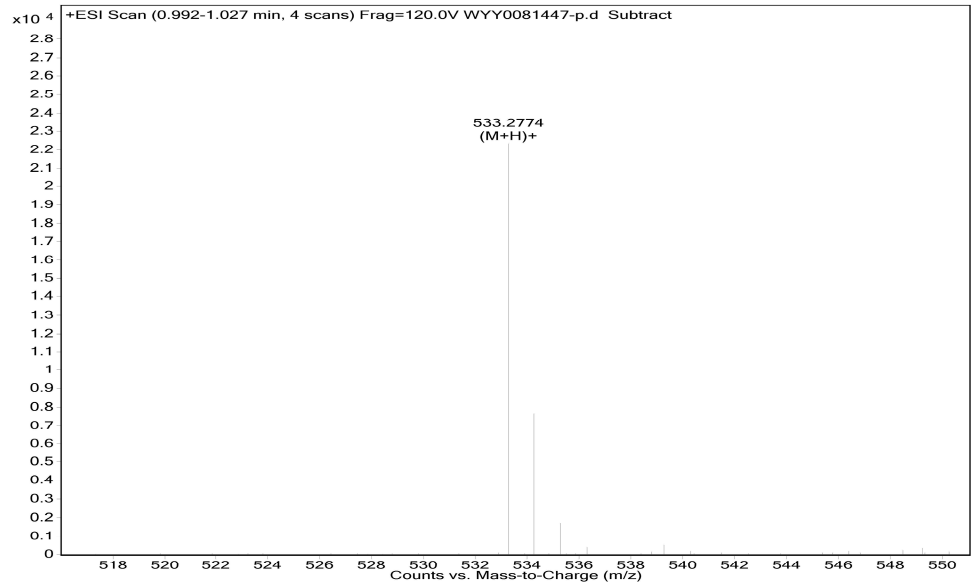
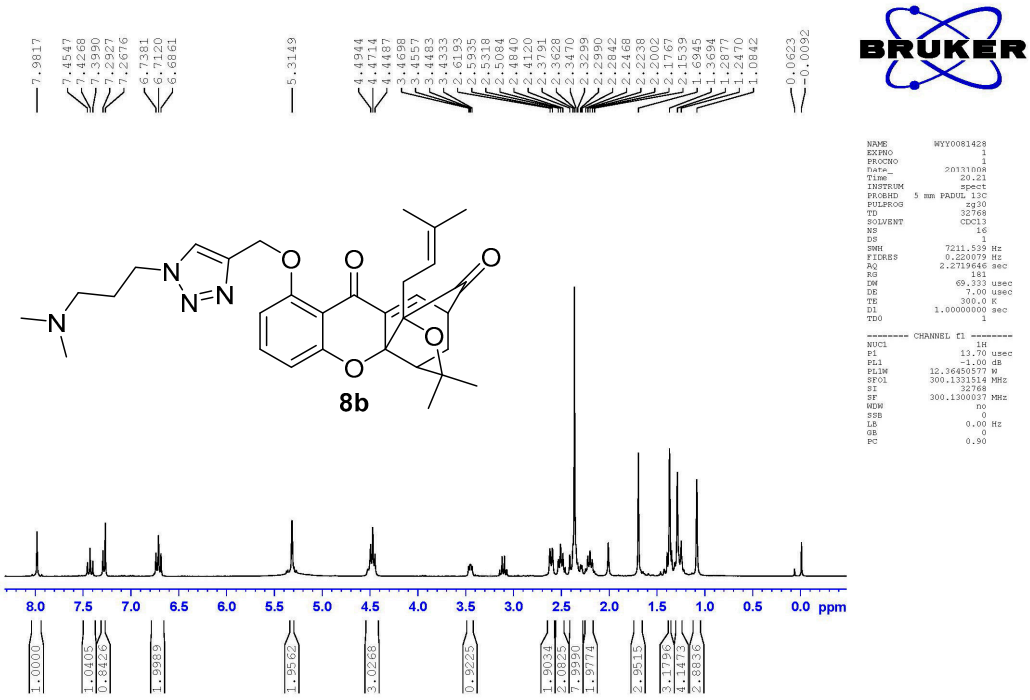


^{1}H NMR(300 MHz) of **8b** in $CDCl_3$



HRMS of **8b**

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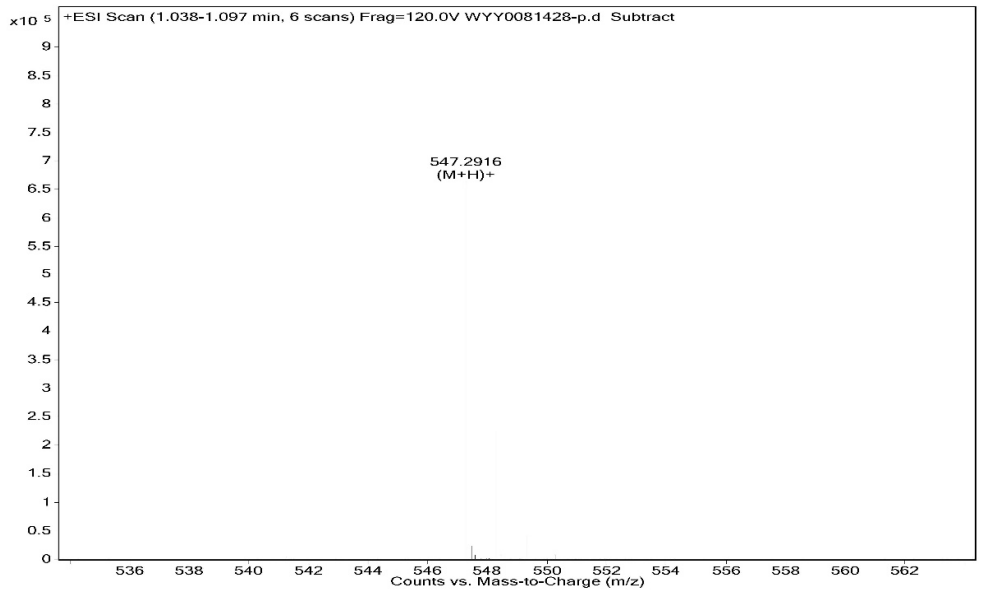
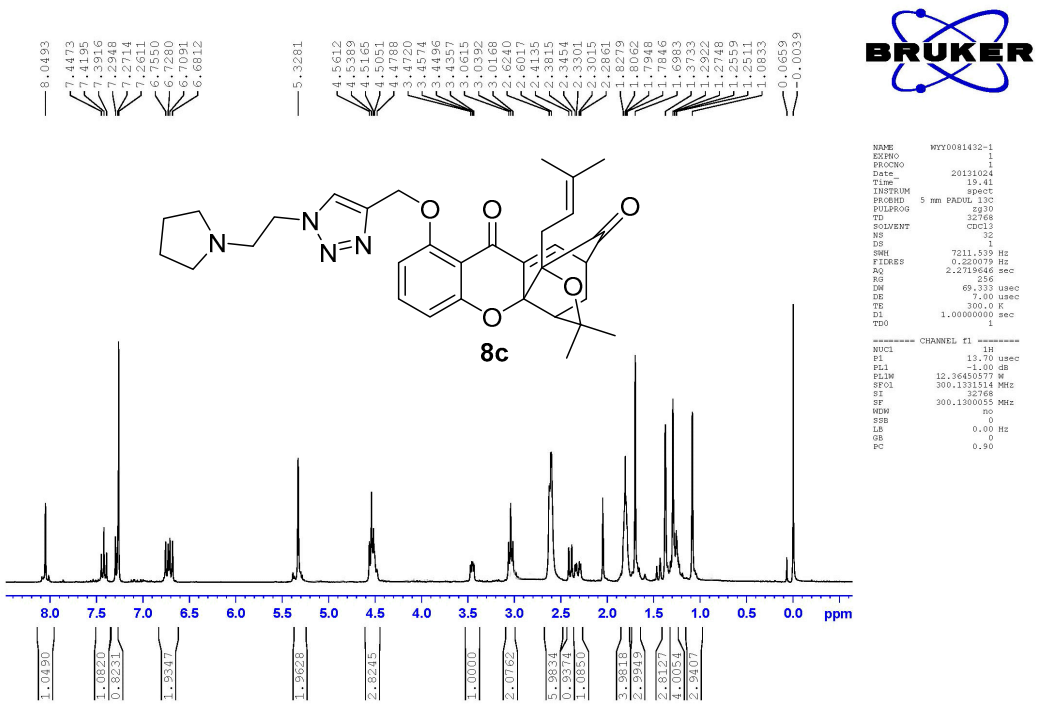
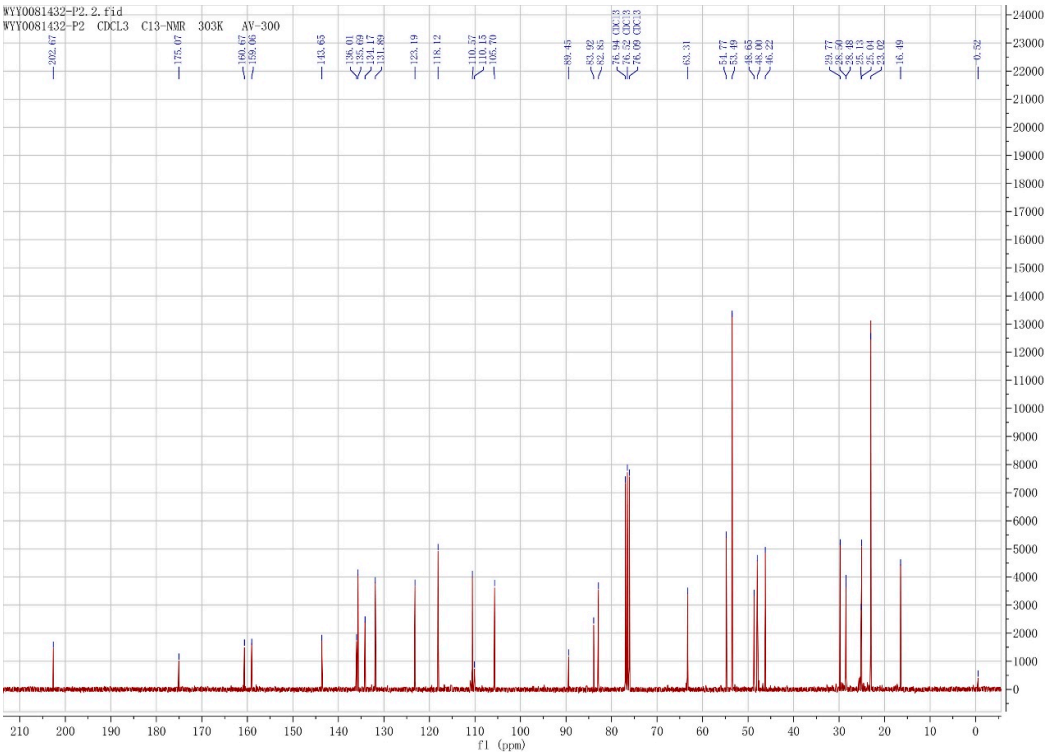


^{1}H NMR(300 MHz) of **8c** in $CDCl_3$



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



HRMS of **8c**

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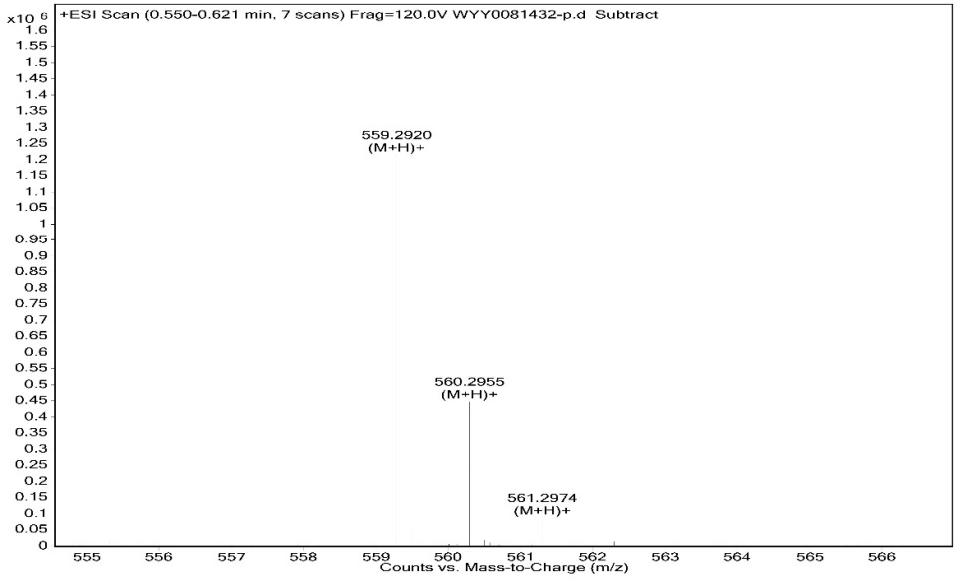
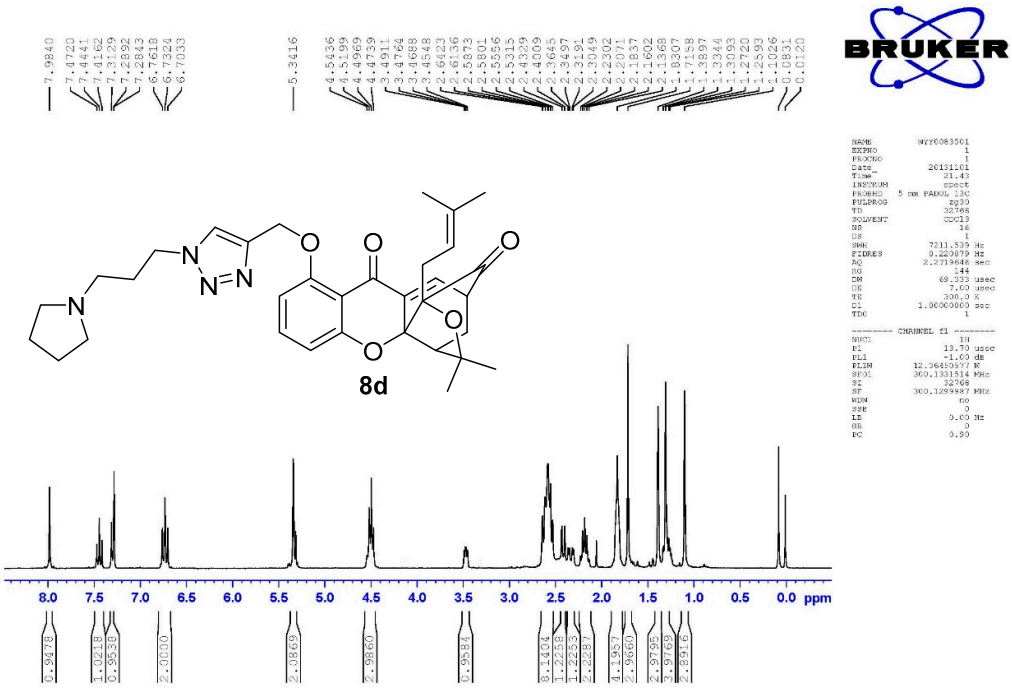


^{1}H NMR(300 MHz) of **8d** in $CDCl_3$



HRMS of **8d**

Sample Name		**Position**	P1-C6	**Instrument Name**	Instrument 1	**User Name**	
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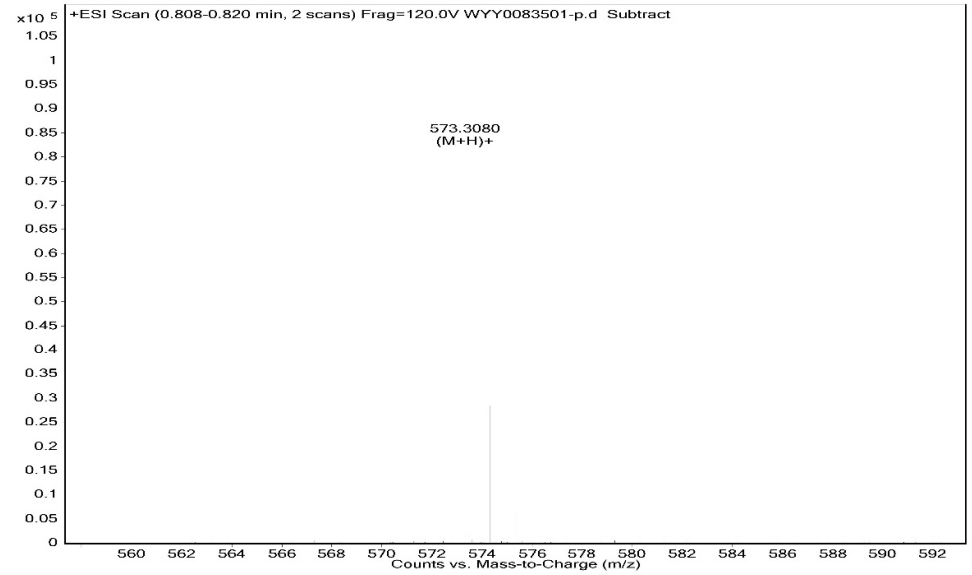
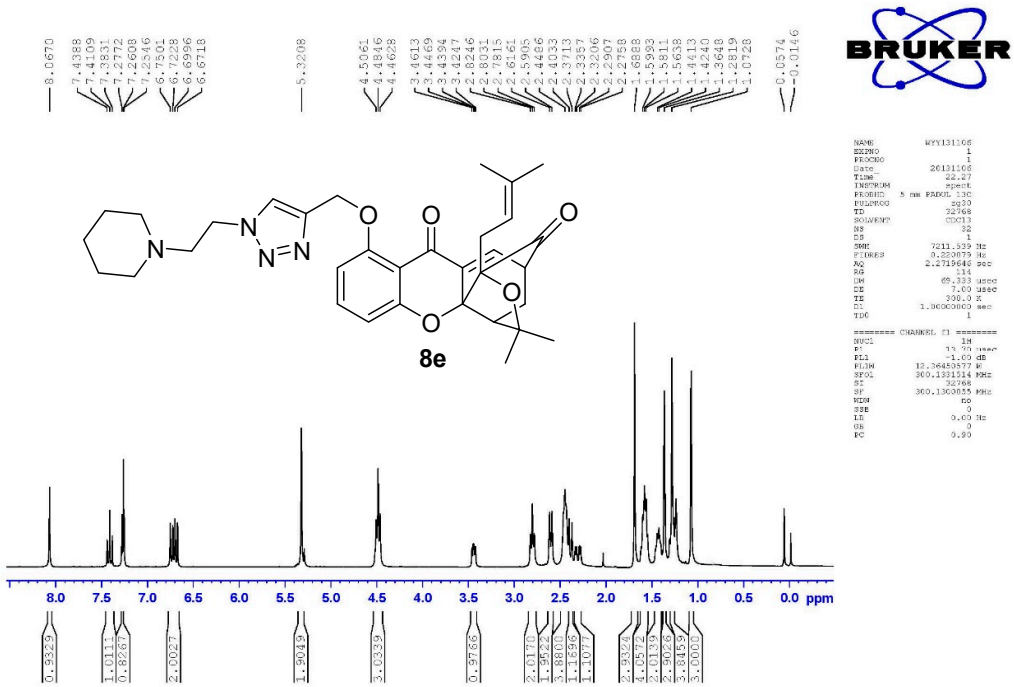
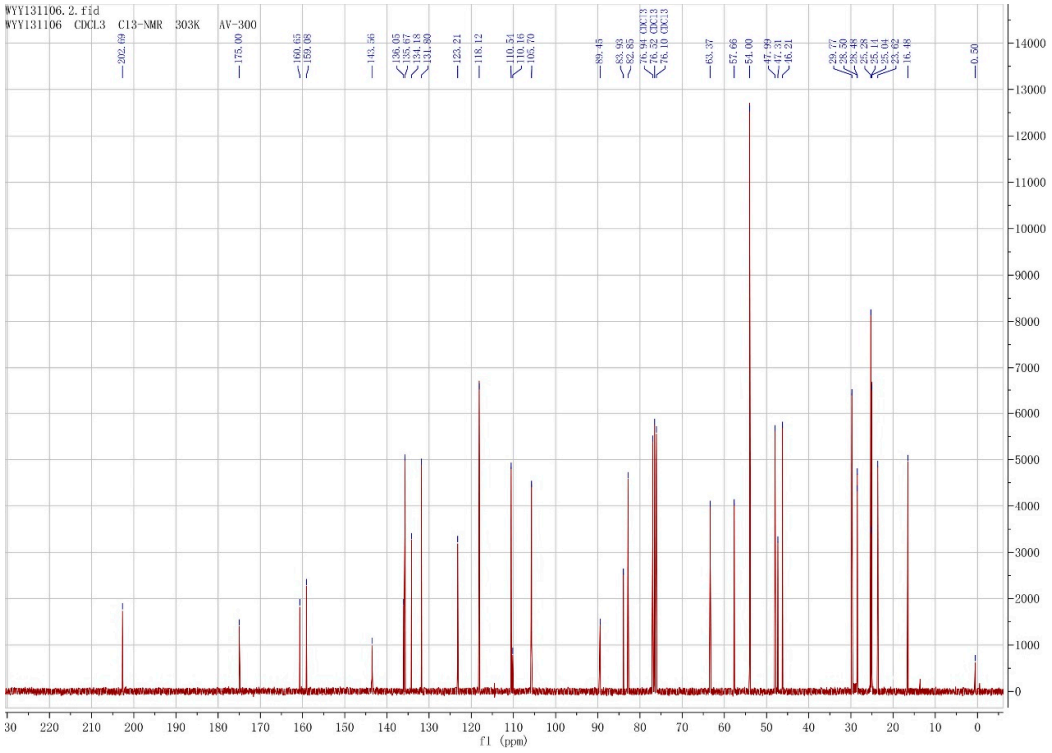


^{1}H NMR(300 MHz) of **8e** in $CDCl_3$



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



HRMS of **8e**

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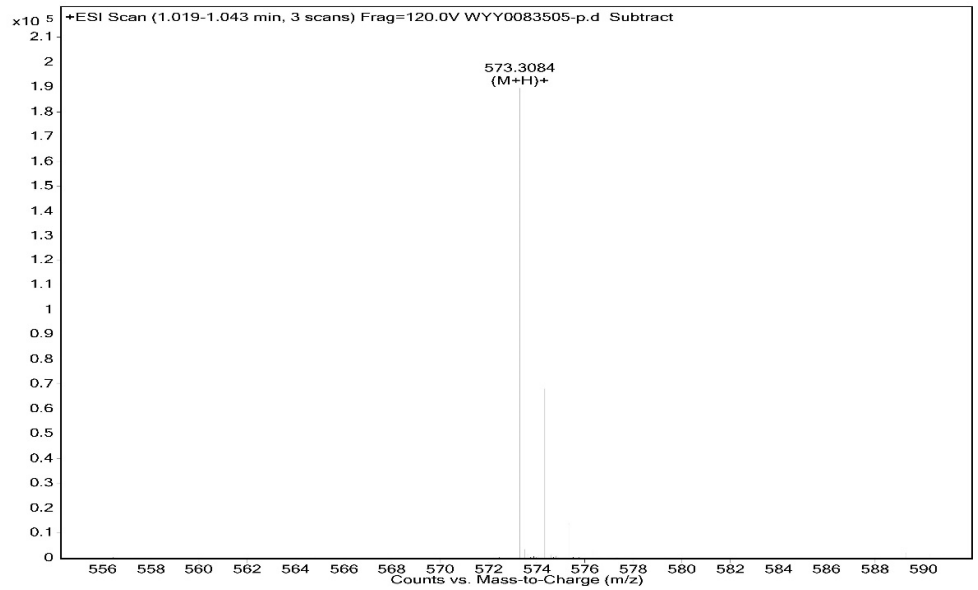
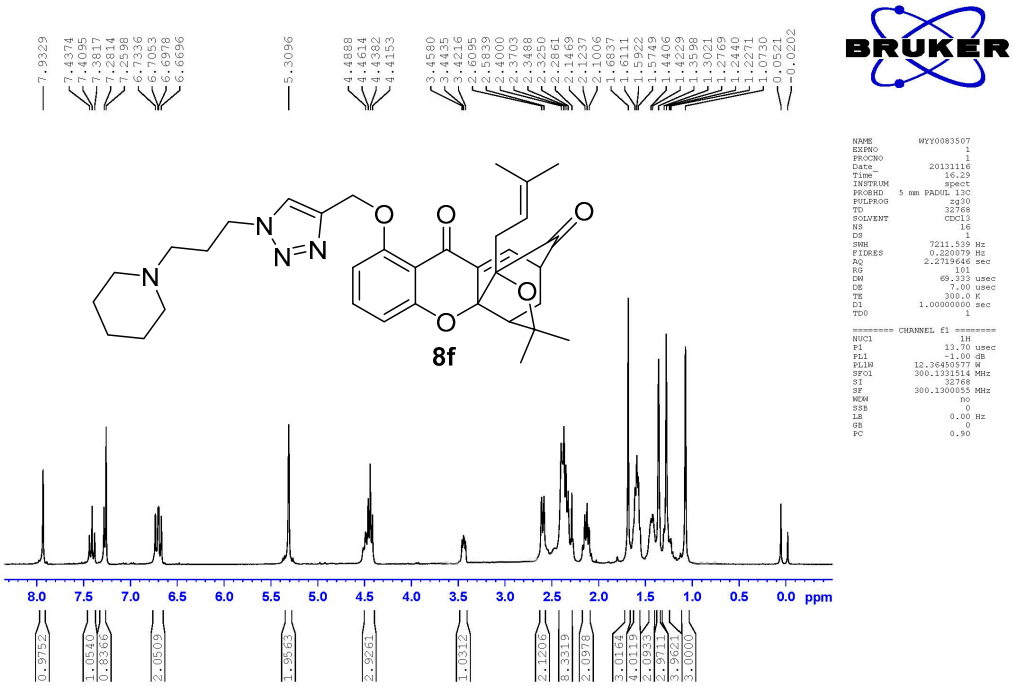


^{1}H NMR(300 MHz) of **8f** in $CDCl_3$



HRMS of **8f**

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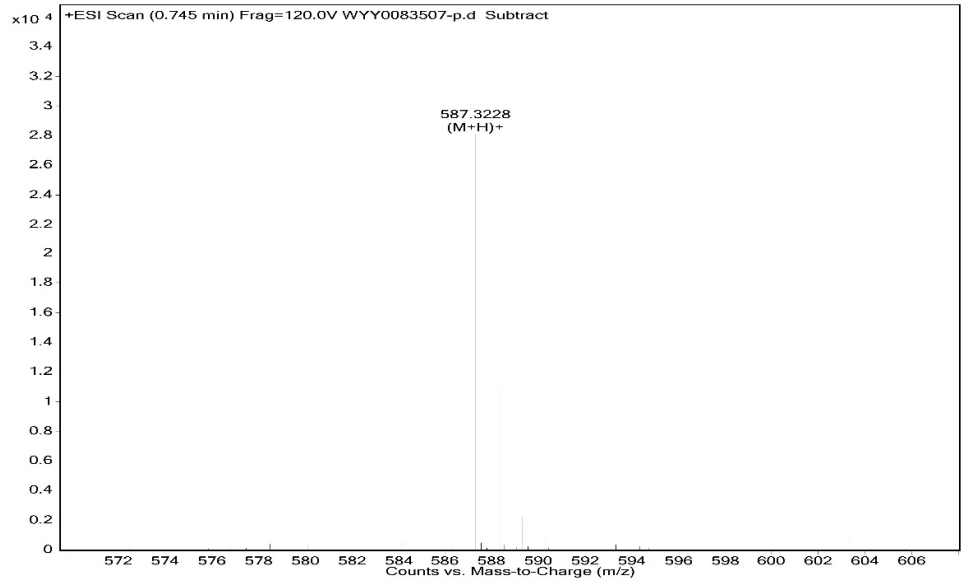
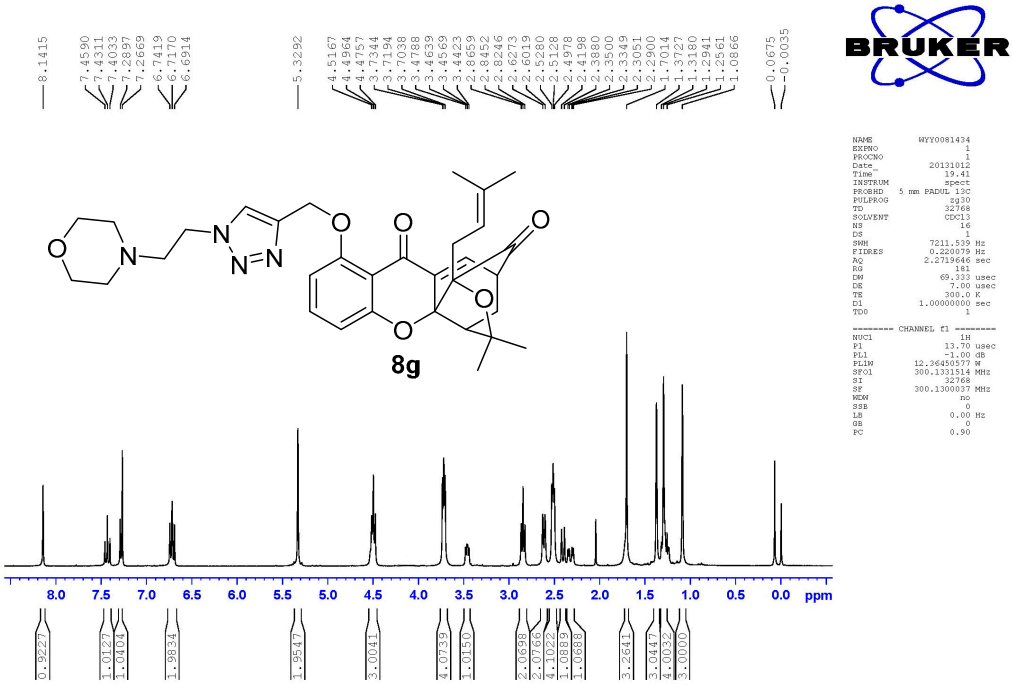
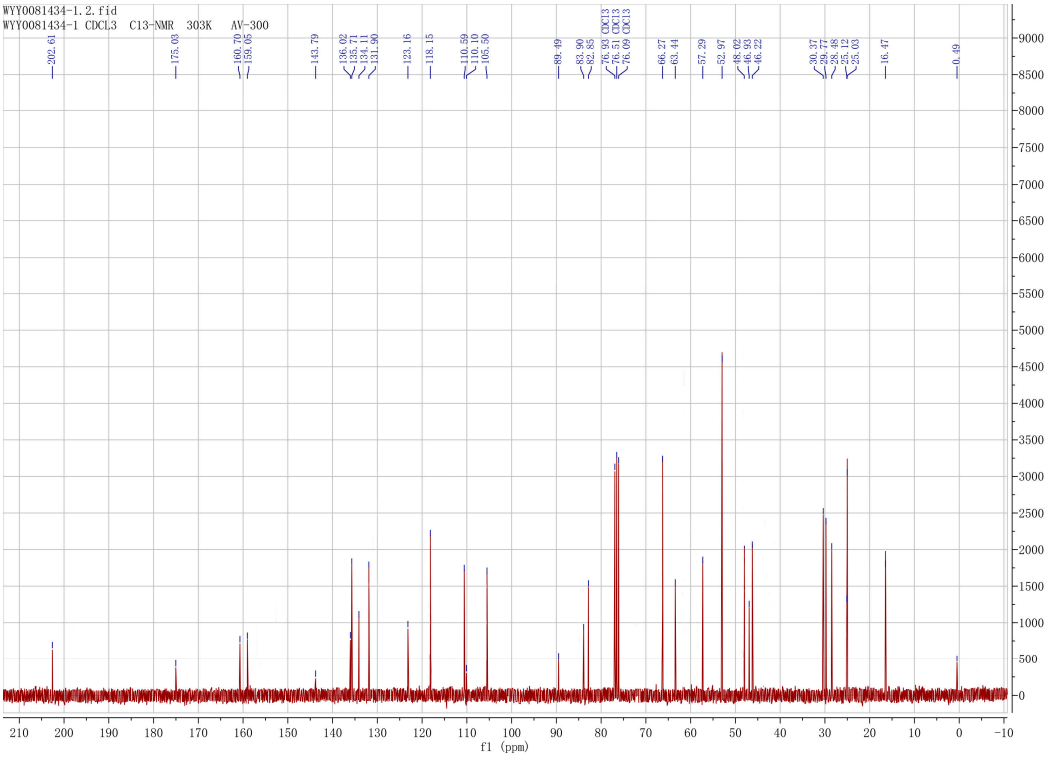


^{1}H NMR(300 MHz) of **8g** in $CDCl_3$



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



HRMS of **8g**

Sample Name		**Position**	P2-E8	**Instrument Name**	Instrument 1	**User Name**	
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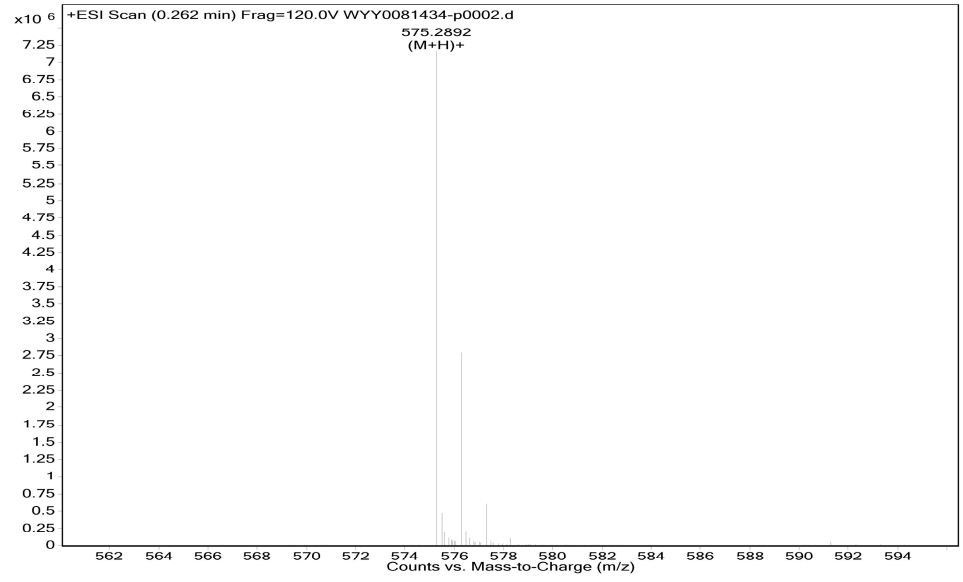
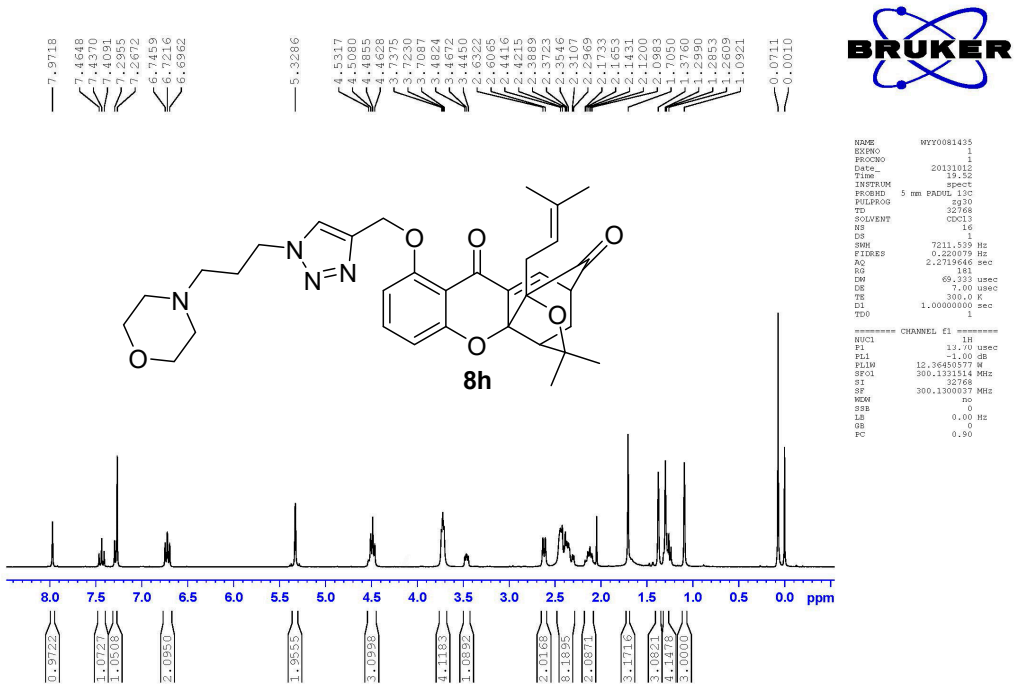
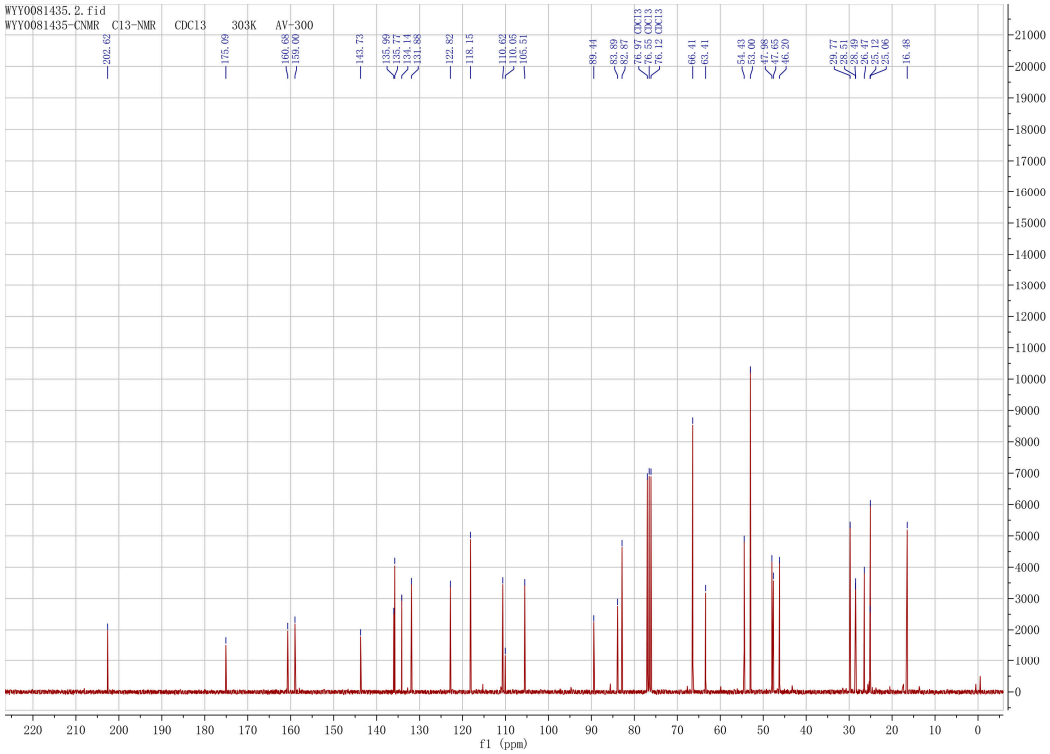


^{1}H NMR(300 MHz) of **8h** in $CDCl_3$



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



HRMS of **8h**

Sample Name		**Position**	P2-E9	**Instrument Name**	Instrument 1	**User Name**	
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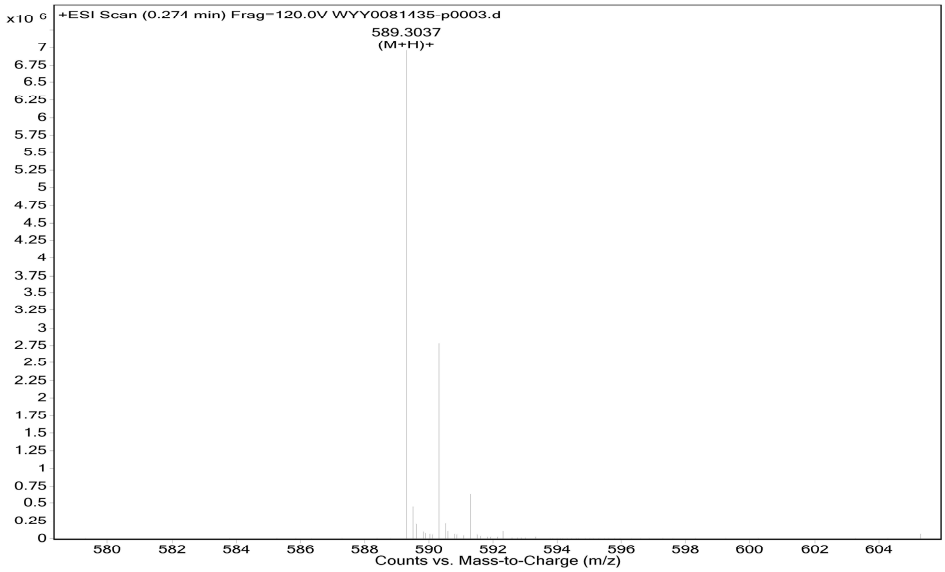
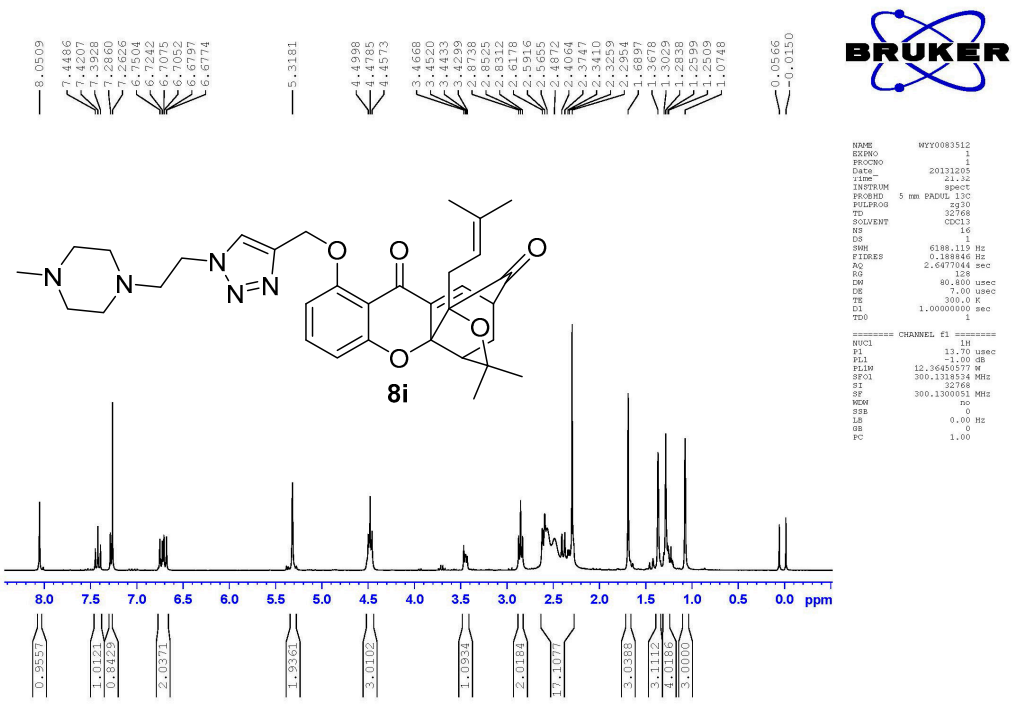


^{1}H NMR(300 MHz) of **8i** in $CDCl_3$



HRMS of **8i**

Sample Name		**Position**	P1-C9	**Instrument Name**	Instrument 1	**User Name**	
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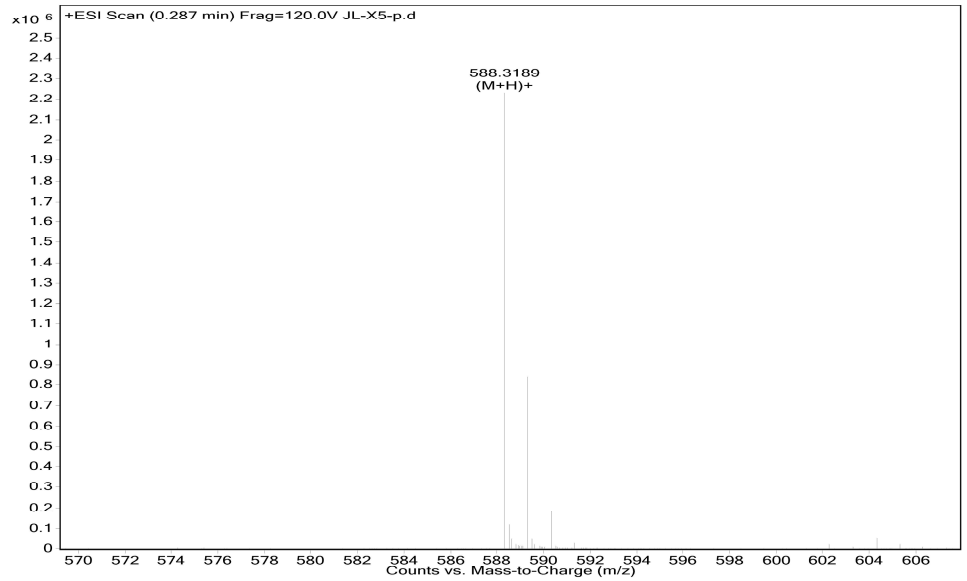
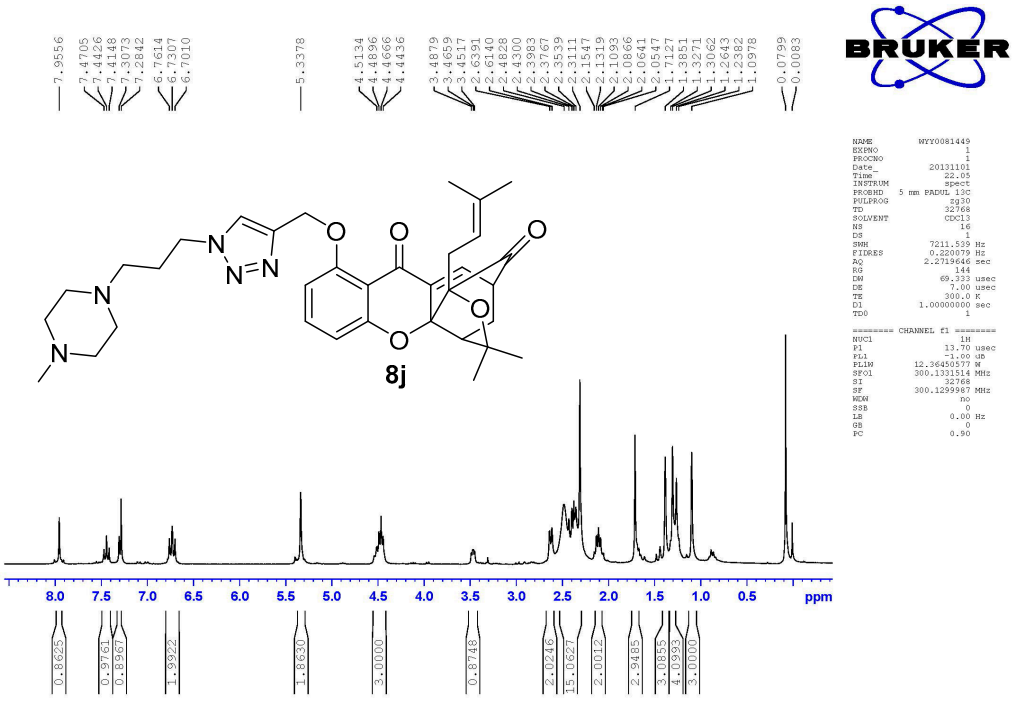
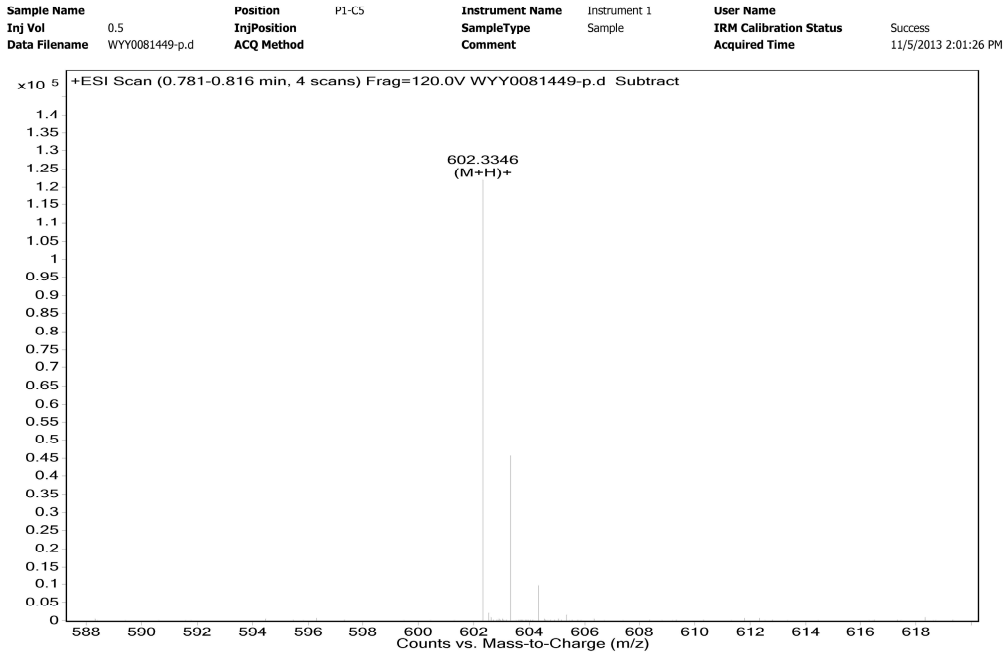


^{1}H NMR(300 MHz) of **8j** in $CDCl_3$



HRMS of **8j**



2. Data for Figure 3.

Table S1. Data of membrane permeability for Figure 3

Cpd	P_e (10^{-6} 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.