

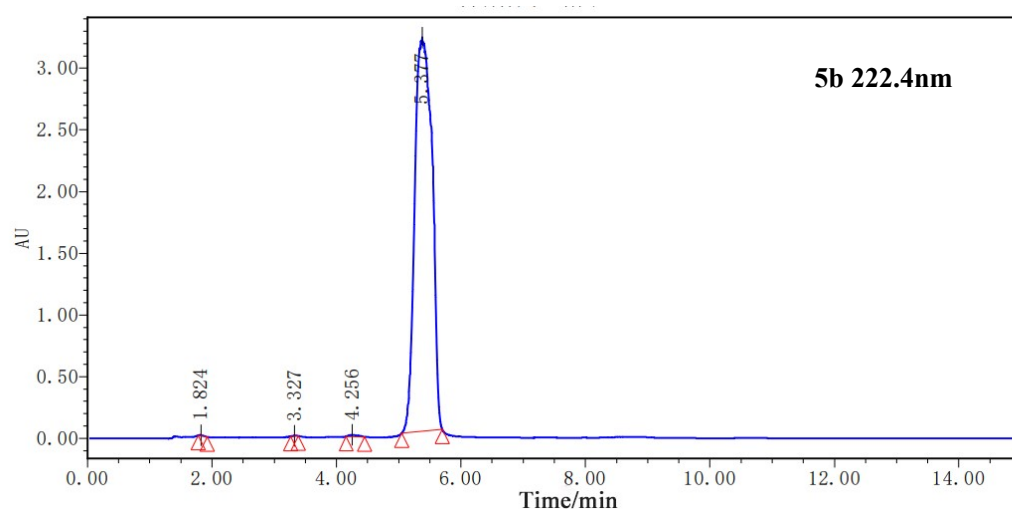
Supporting information

Synthesis and anti-proliferative activity of dehydroabietinol derivatives bearing a triazole moiety

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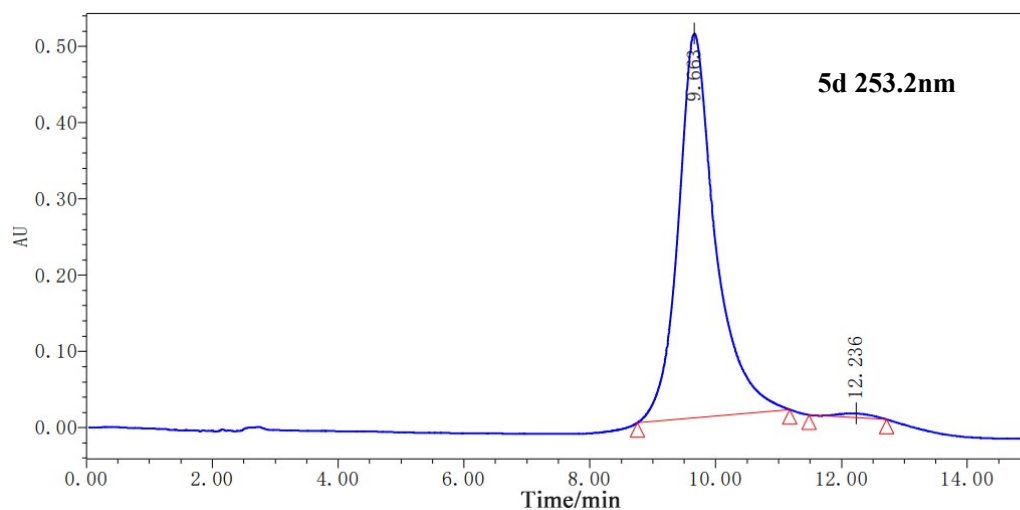
Guangxi Key Laboratory of Drug Discovery and Optimization, Guangxi Engineering Research Center for Pharmaceutical Molecular Screening and Druggability Evaluation, School of Pharmacy, Guilin Medical University, Guilin 541199, PR China.

Key Laboratory of Chemistry and Engineering of Forest Products, State Ethnic Affairs Commission, Guangxi Key Laboratory of Chemistry and Engineering of Forest Products, Guangxi Minzu University, Nanning 530006, China.



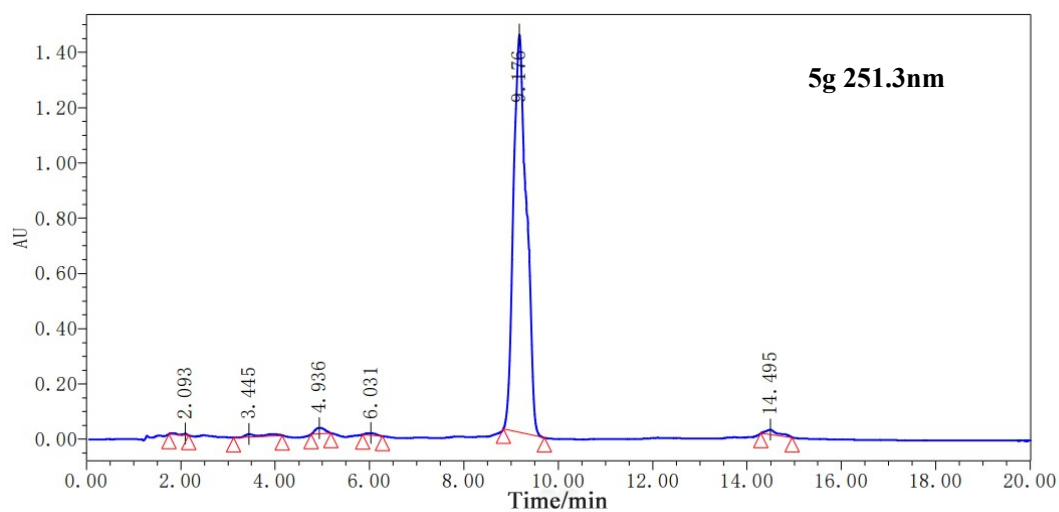
	RT (min)	Area (mV/s)	High(mV)	%Area
1	1.824	26511	5650	0.04
2	3.327	18032	3615	0.03
3	4.256	134472	13259	0.22
4	5.377	61413608	3189525	99.71

Fig. S1 Purity of **5b** analyzed by Waters Acquity UPLC. Column: reversed-phase C18 column (SHIMADZU Shim-pack GIST-HP C18 2.1 μ m 100mm). Column temperature: 35°C. Mobile phase: Acetonitrile/ H₂O with 0.1% triethylamine (90:10). Flow rate: 0.15 ml/min. Injection volume: 5 μ L.



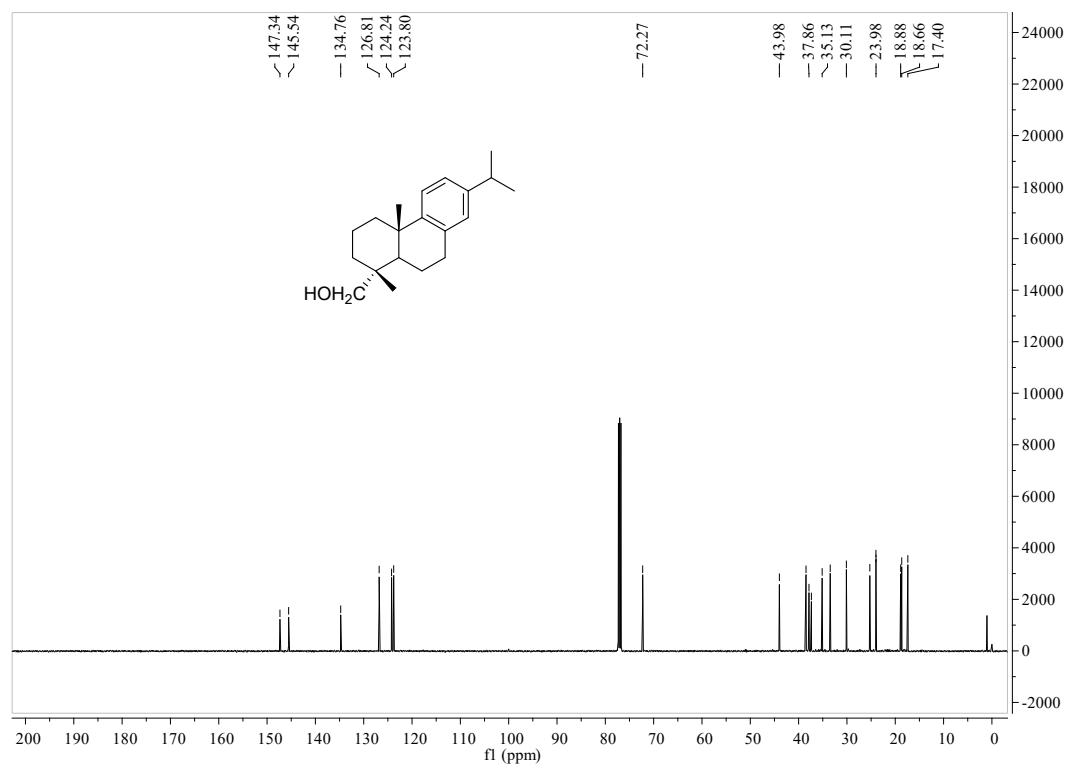
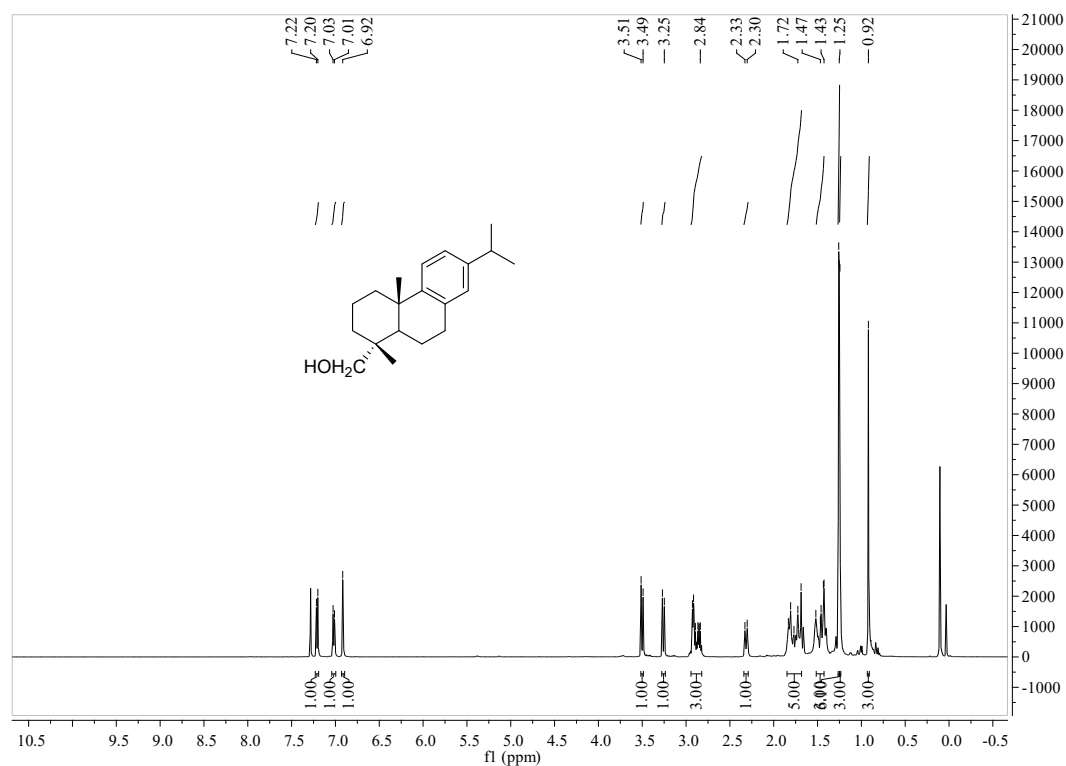
	RT (min)	Area (mV/s)	High(mV)	%Area
1	9.663	20721085	503873	99.02
2	12.236	204544	5476	0.98

Fig. S2 Purity of **5d** analyzed by Waters Acquity UPLC. Column: reversed-phase C18 column (SHIMADZU Shim-pack GIST-HP C18 2.1 $\times$ 100mm). Column temperature: 35°C. Mobile phase: Acetonitrile/ H₂O (70:30). Flow rate: 0.10 ml/min. Injection volume: 5 μ L.



	RT (min)	Area (mV/s)	High(mV)	%Area
1	2.093	61241	5433	0.21
2	3.445	252429	9789	0.88
3	4.936	300578	21243	1.05
4	6.031	120511	8142	0.42
5	9.176	27452124	1438462	96.20
6	14.495	350938	18010	1.23

Fig. S3 Purity of **5g** analyzed by Waters Acquity UPLC. Column: reversed-phase C18 column (SHIMADZU Shim-pack GIST-HP C18 2.1 $\times$ 100mm). Column temperature: 35°C. Mobile phase: Acetonitrile/ H₂O with 0.1% triethylamine (70:30). Flow rate: 0.15 ml/min. Injection volume: 5 μ L.



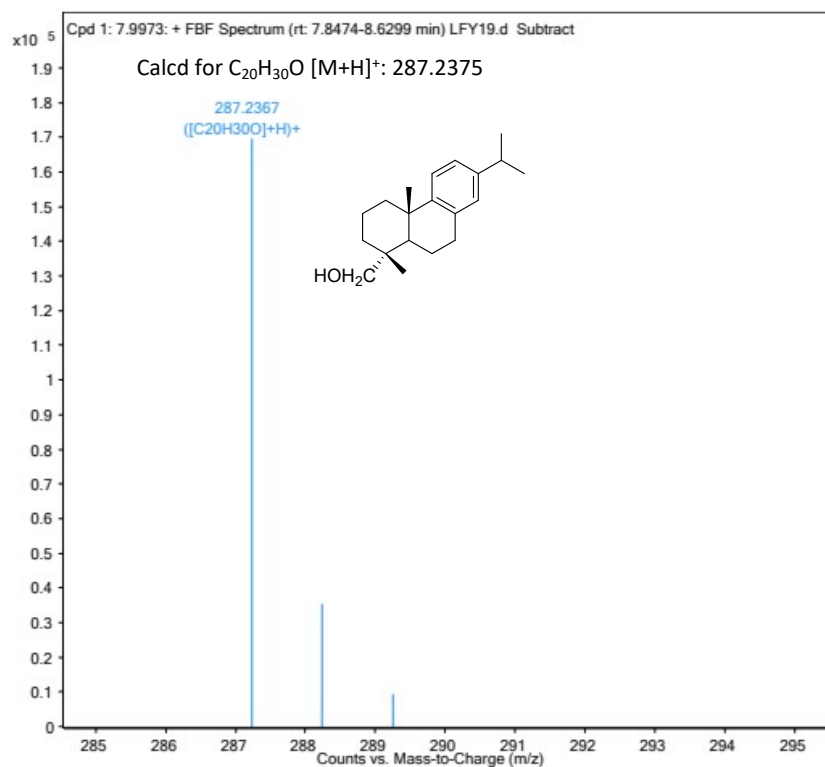


Figure S6 HRMS-ESI spectrum of the intermediate **2**

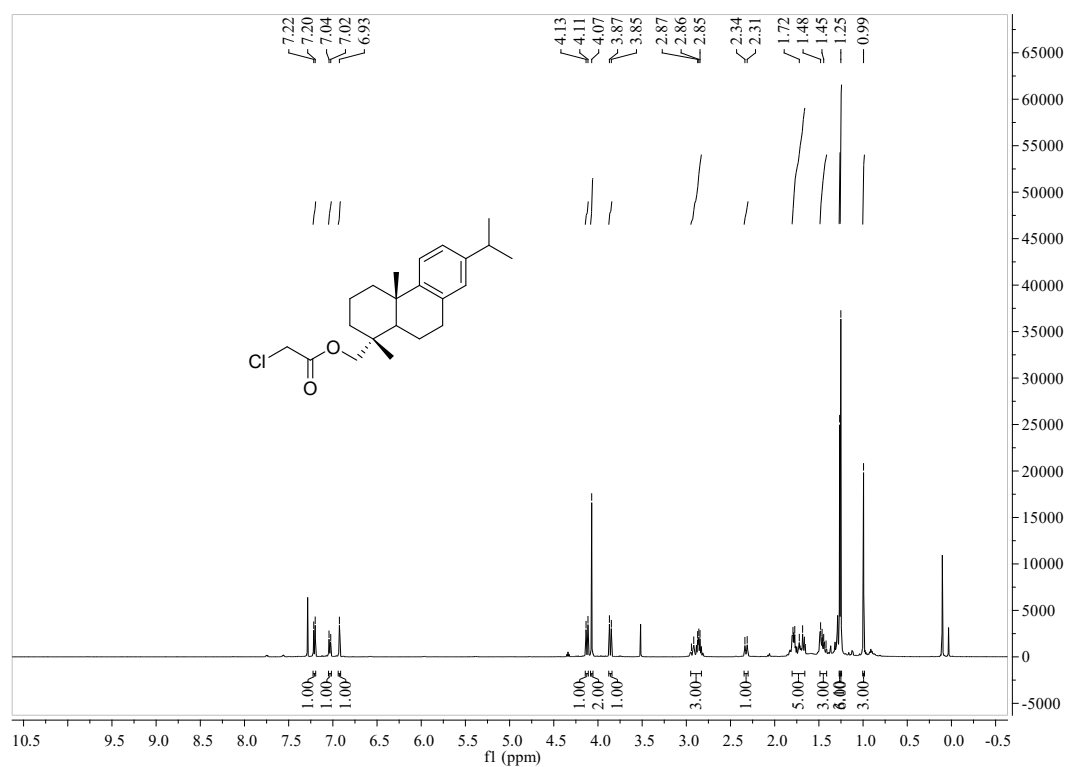


Figure S7 1H -NMR spectrum of the intermediate **3** in $CDCl_3$

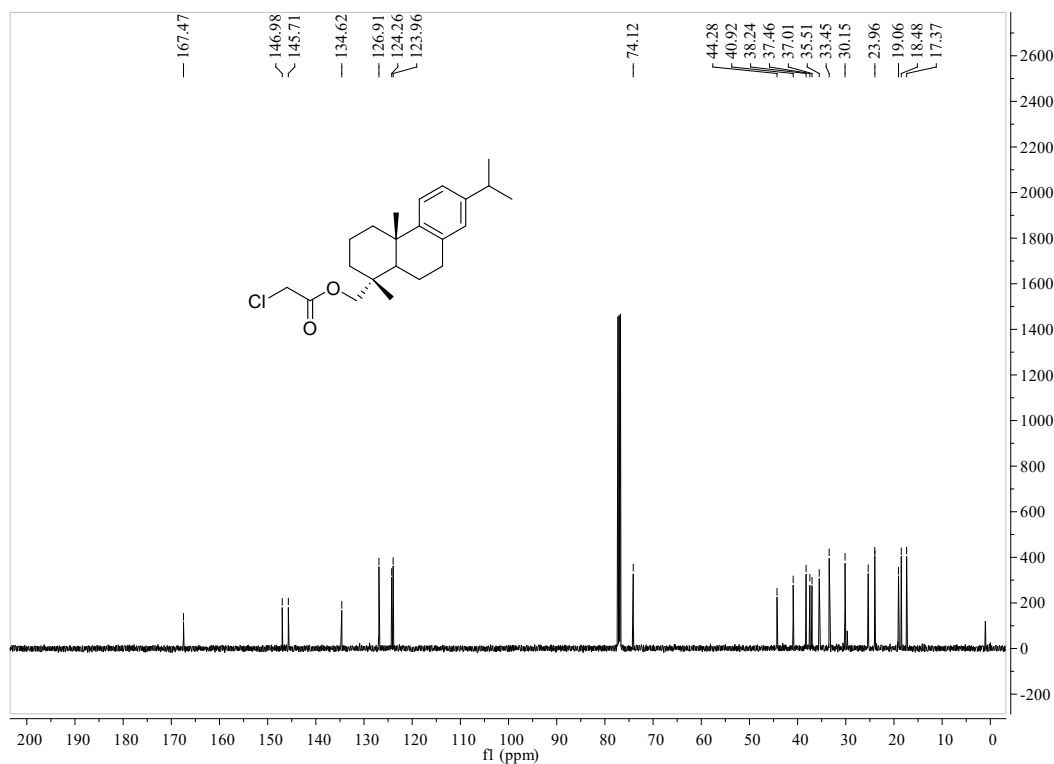


Figure S8 ¹³C-NMR spectrum of the intermediate **3** in CDCl₃

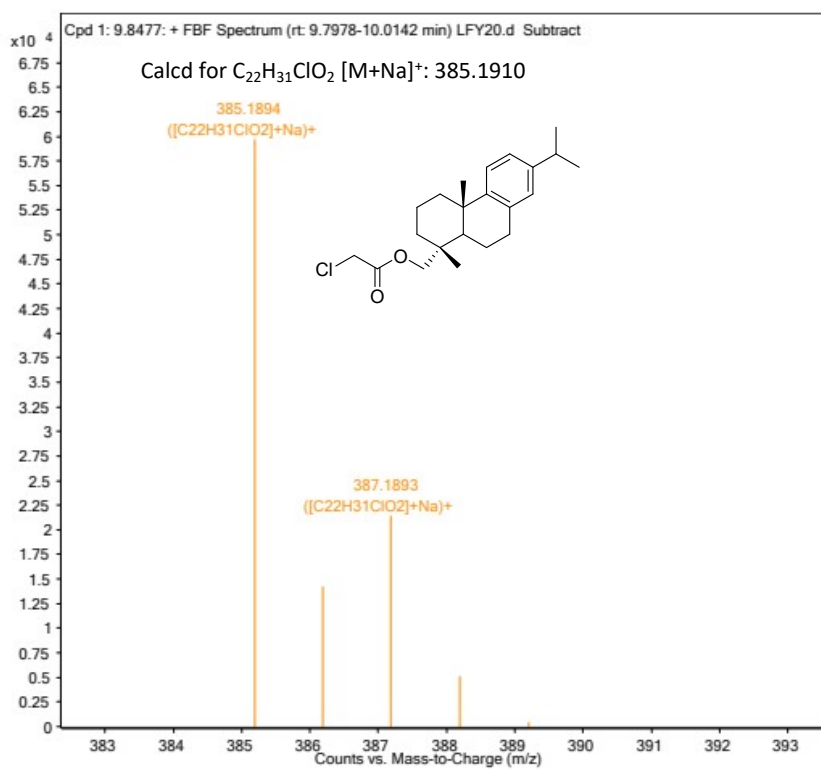


Figure S9 HRMS-ESI spectrum of intermediate **3**

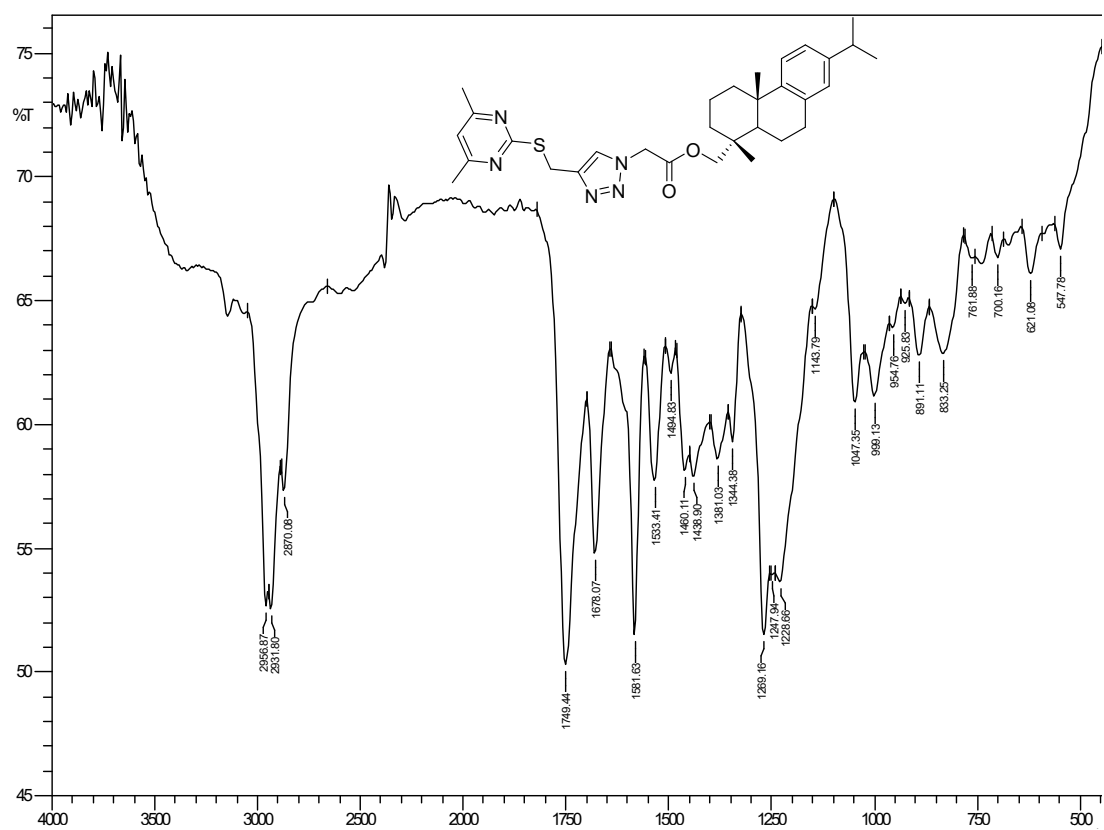


Figure S10 FTIR spectrum of the target compound **5a**

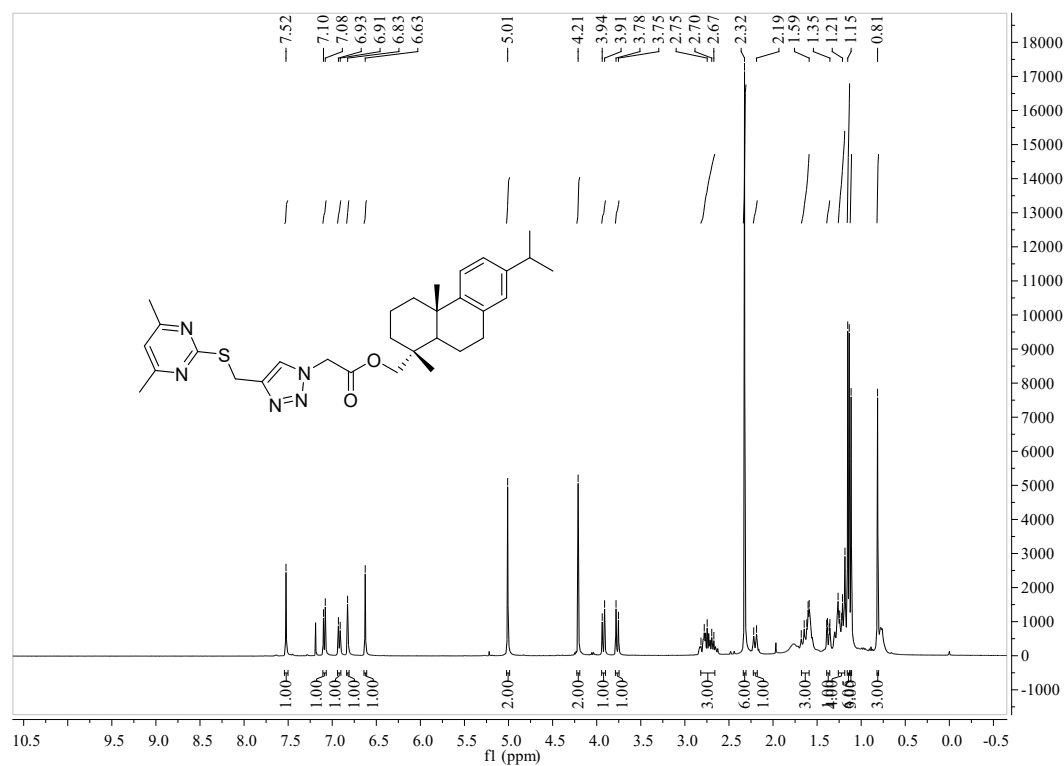


Figure S11 ¹H-NMR spectrum of the target compound **5a** in CDCl₃

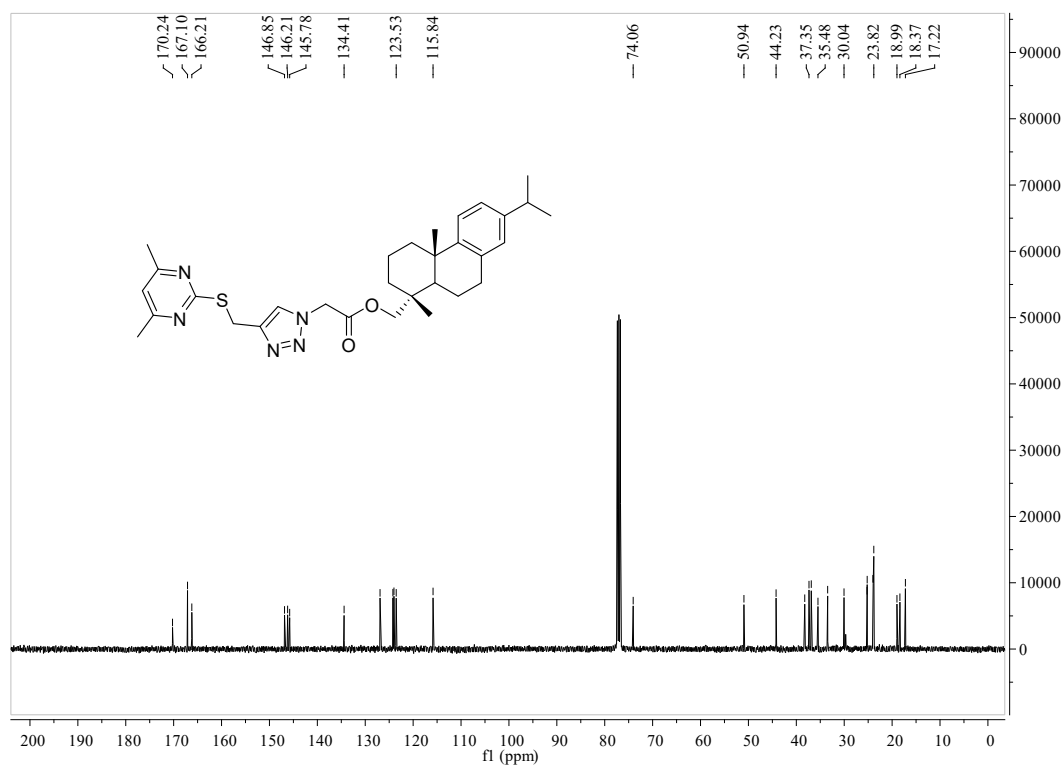


Figure S12 ^{13}C -NMR spectrum of the target compound **5a** in CDCl_3

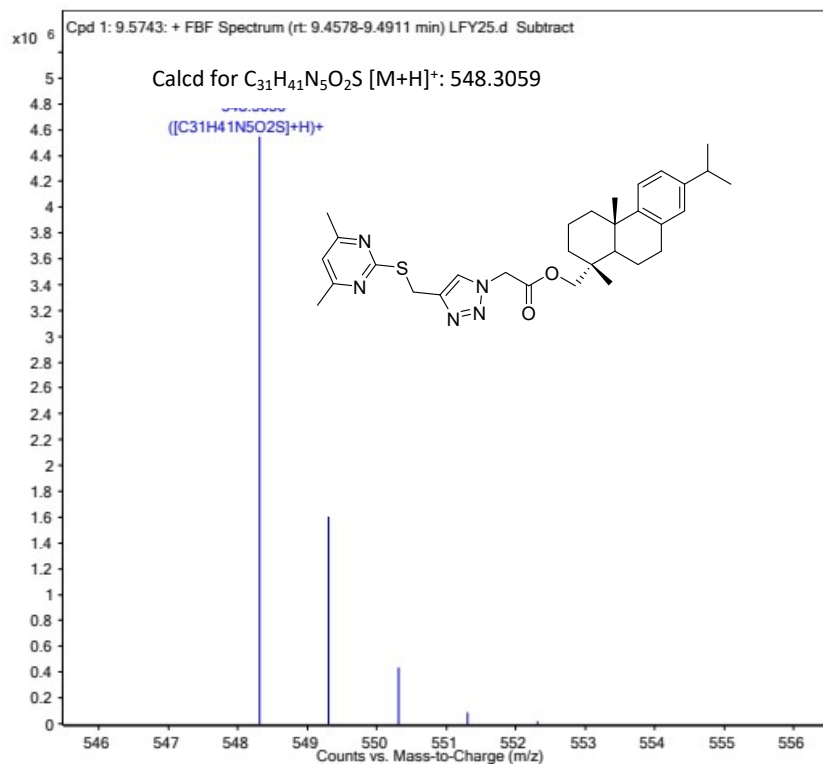
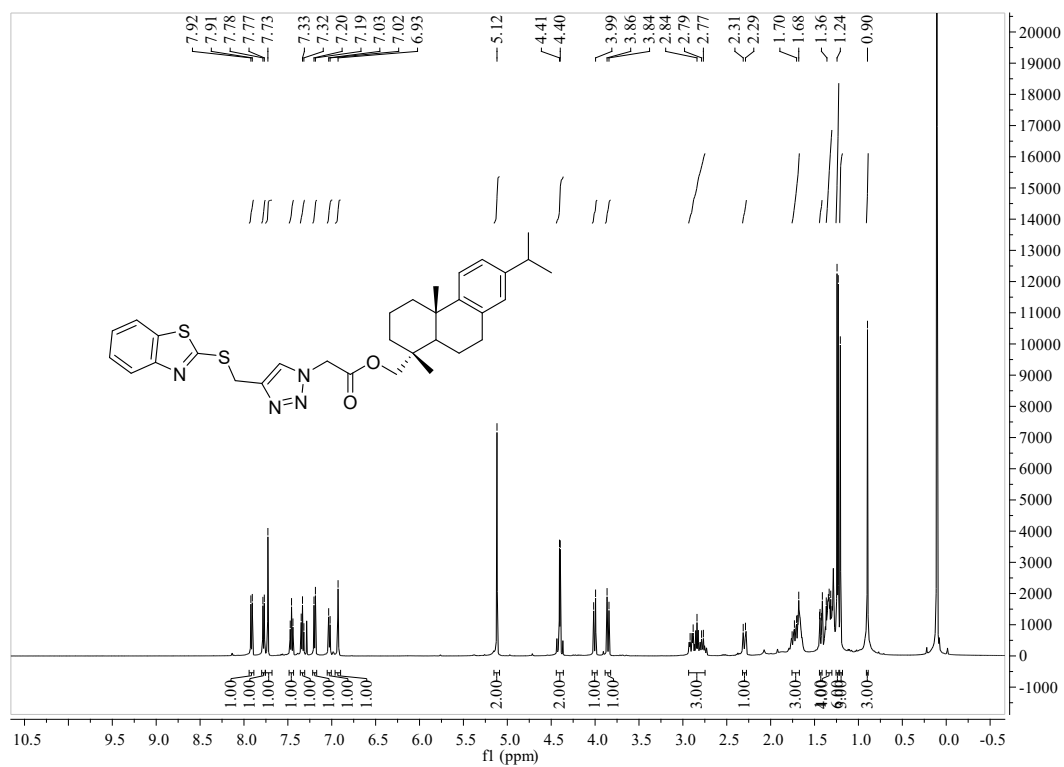
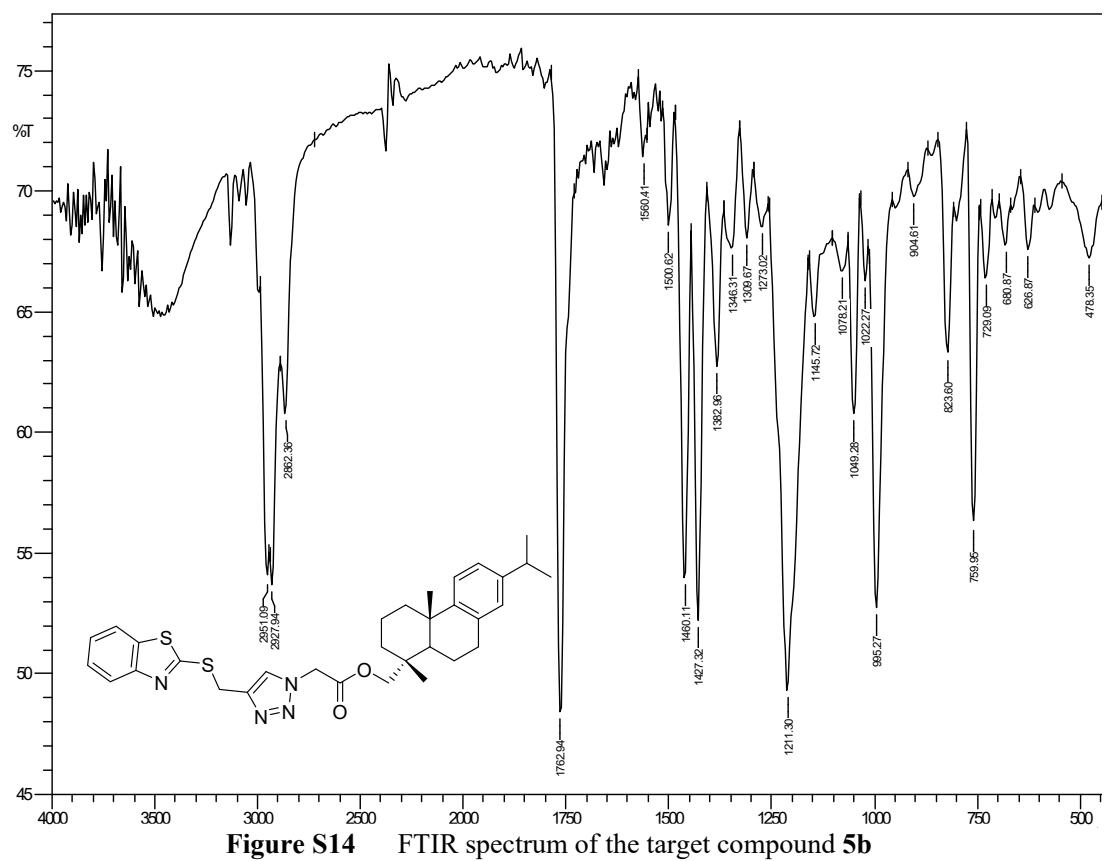


Figure S13 HRMS-ESI spectrum of the target compound **5a**



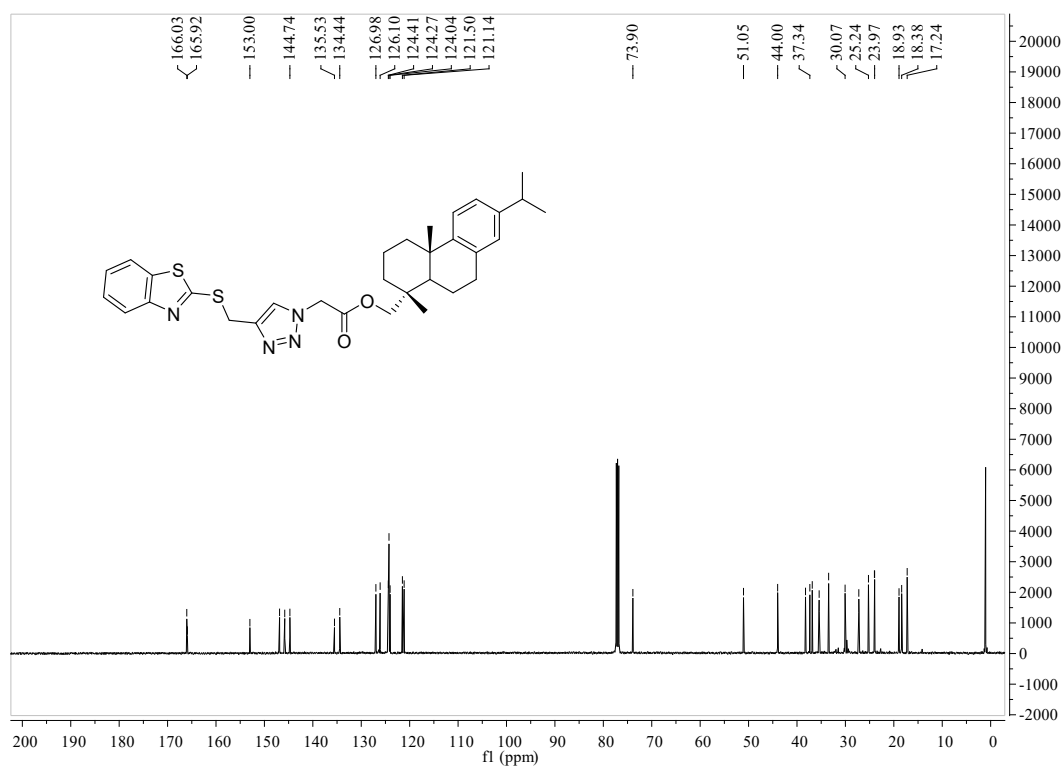


Figure S16 ^{13}C -NMR spectrum of the target compound **5b** in CDCl_3

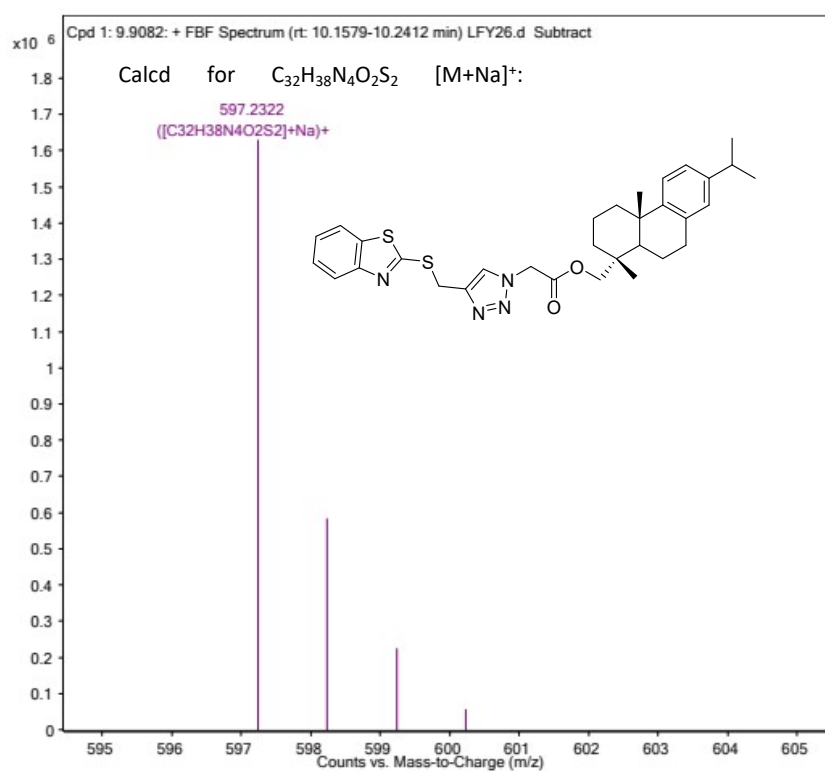


Figure S17 HRMS-ESI spectrum of the target compound **5b**

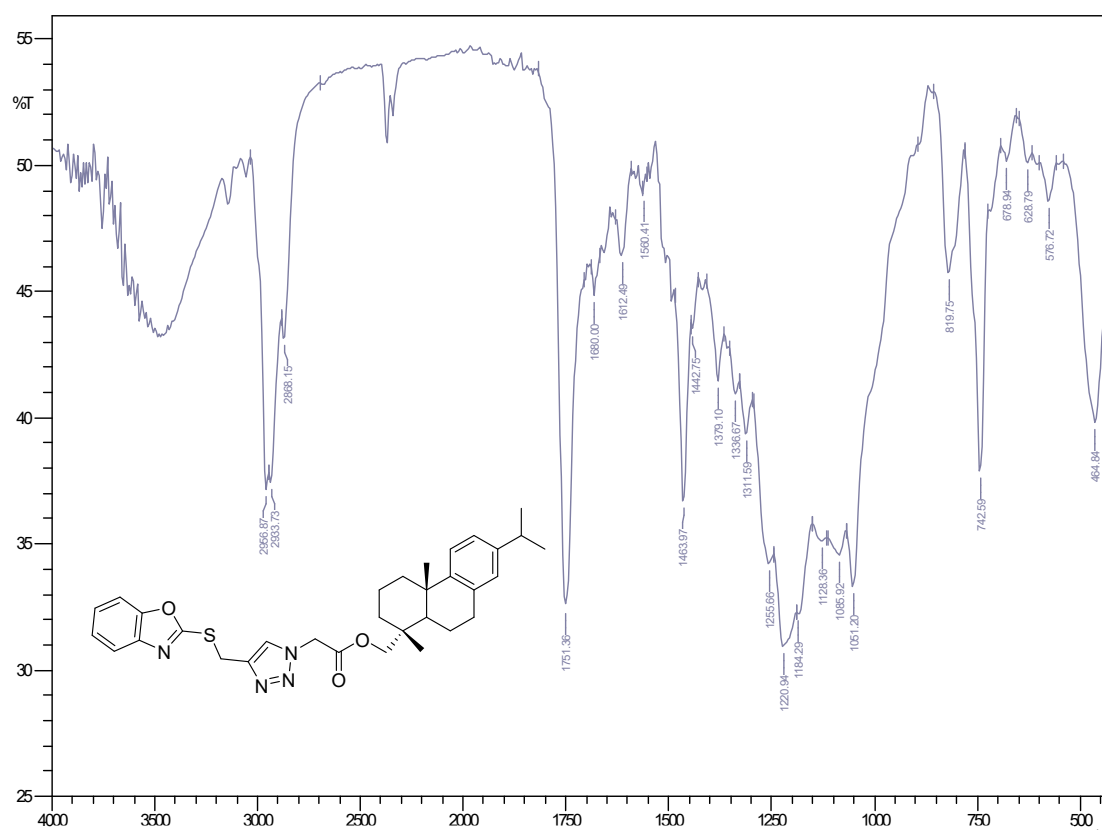


Figure S18 FTIR spectrum of the target compound **5c**

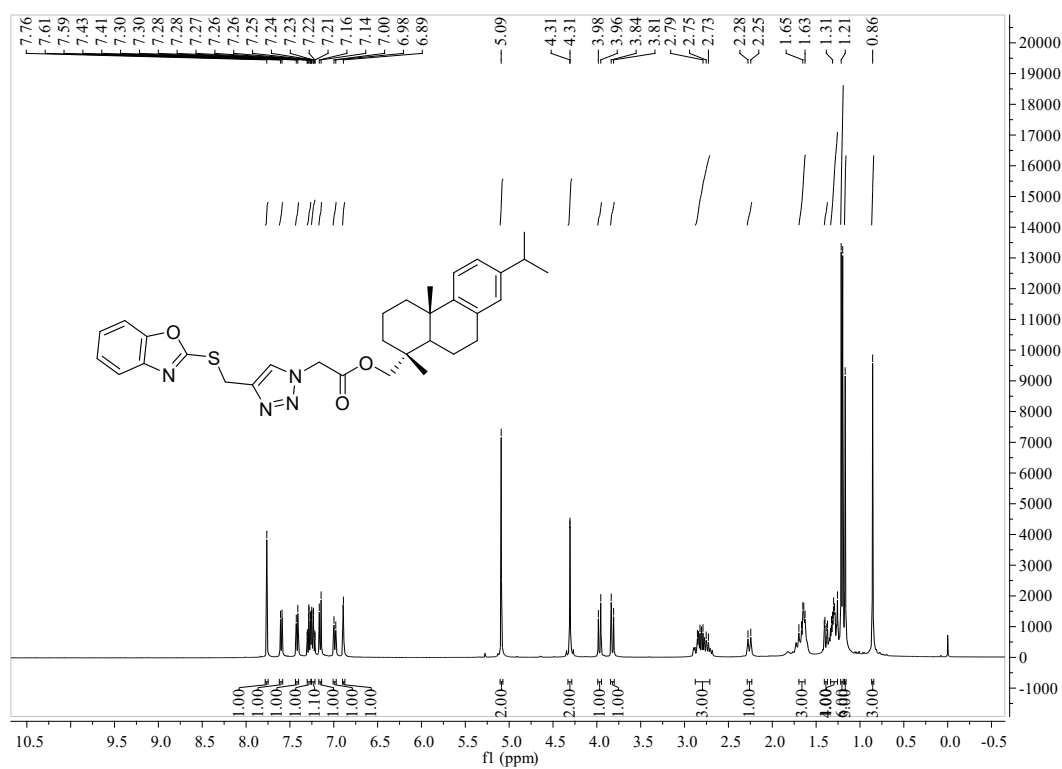


Figure S19 ¹H-NMR spectrum of the target compound **5c** in CDCl₃

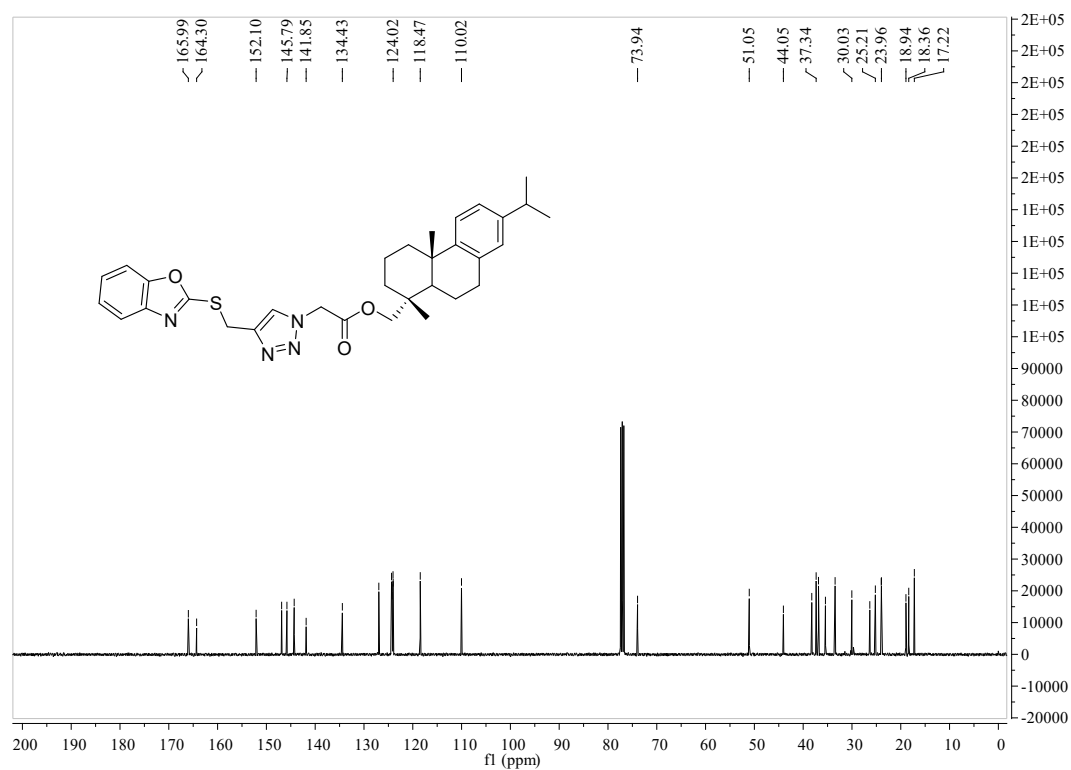


Figure S20 ¹³C-NMR spectrum of the target compound **5c** in CDCl₃

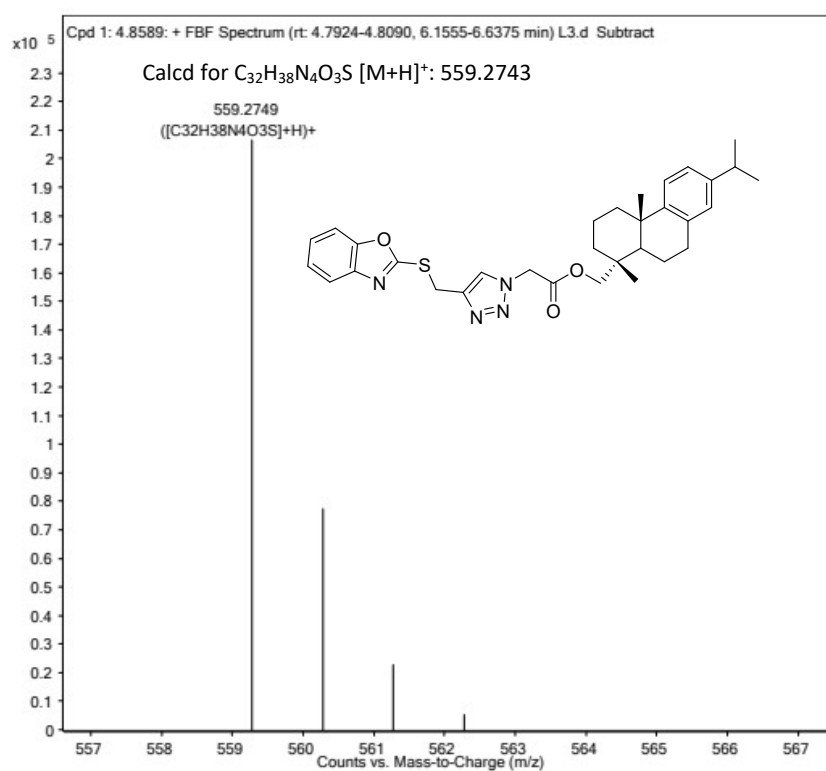
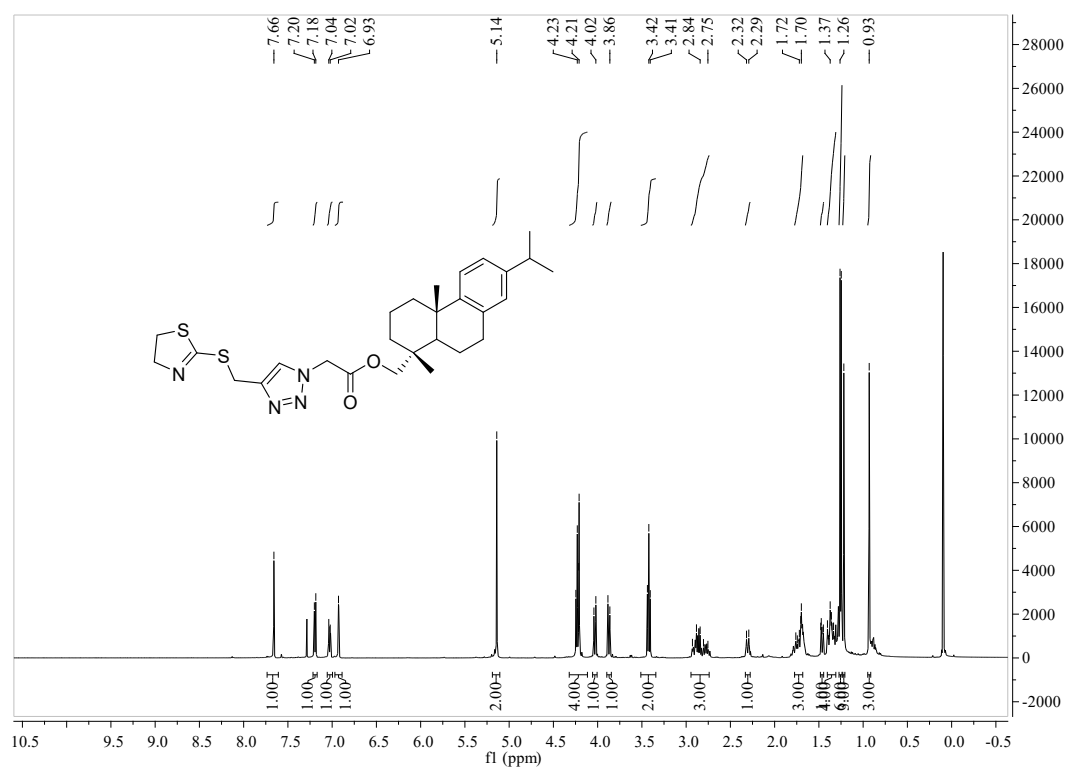
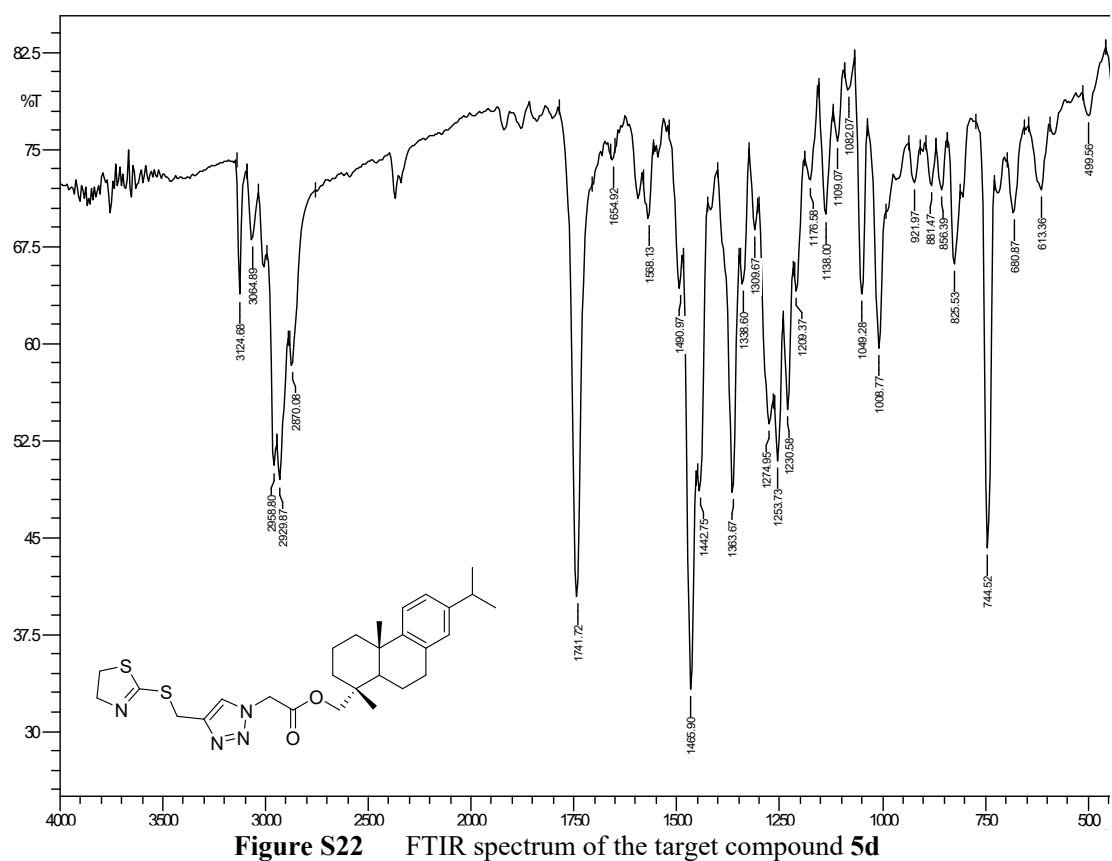


Figure S21 HRMS-ESI spectrum of the target compound **5c**



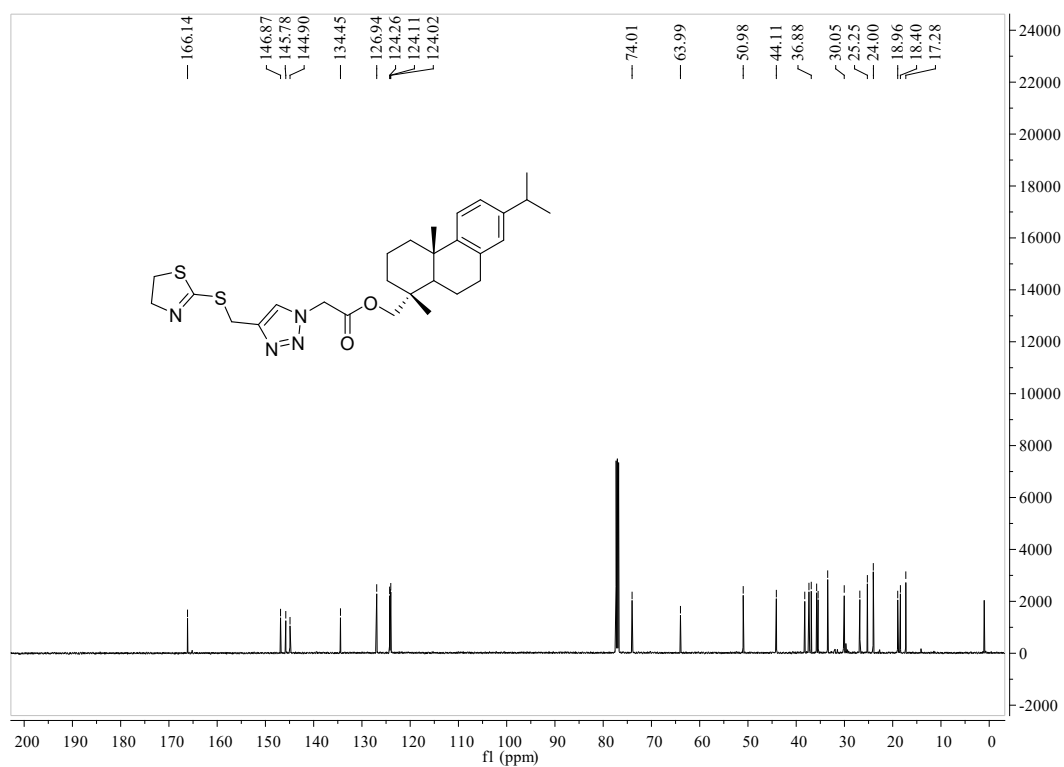


Figure S24 ¹³C-NMR spectrum of the target compound **5d** in CDCl₃

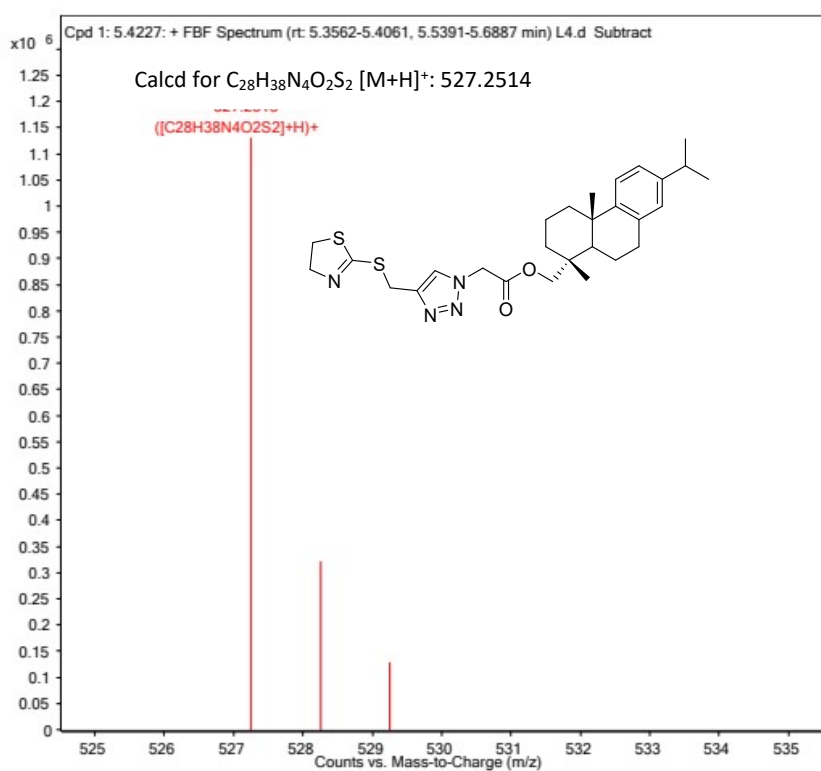


Figure S25 HRMS-ESI spectrum of the target compound **5d**

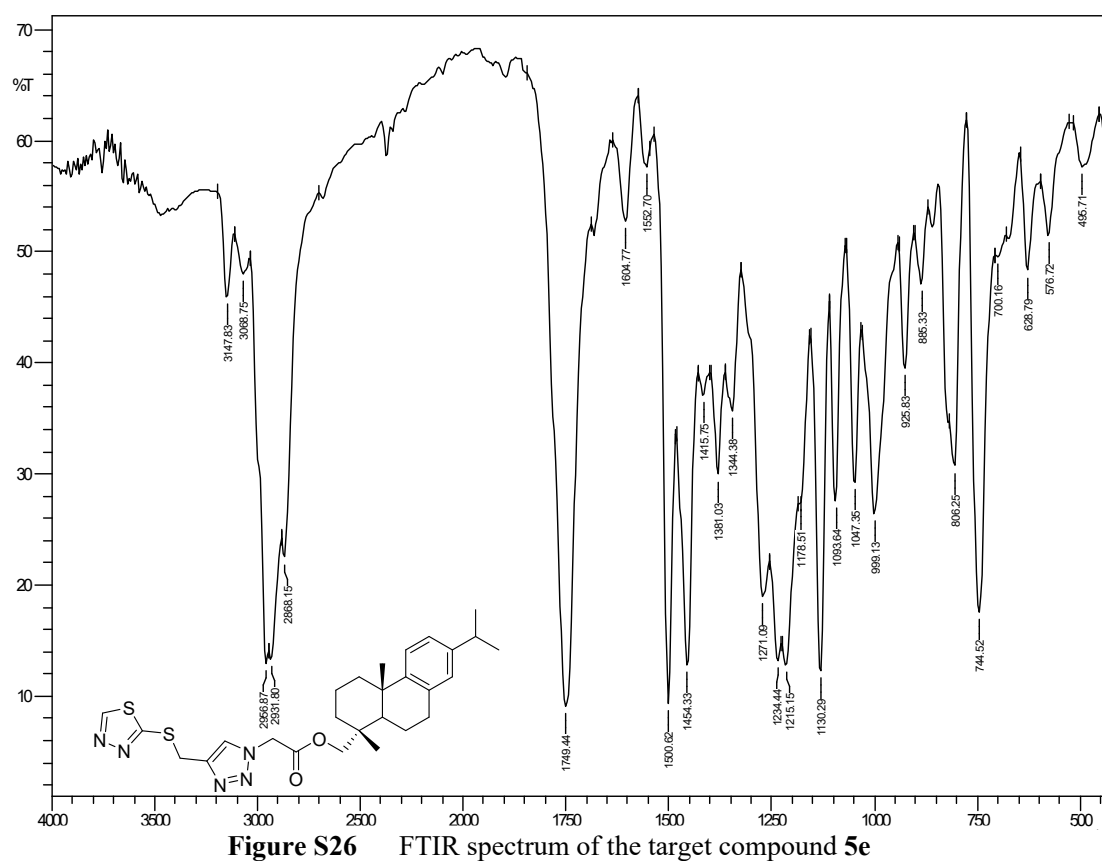


Figure S26 FTIR spectrum of the target compound **5e**

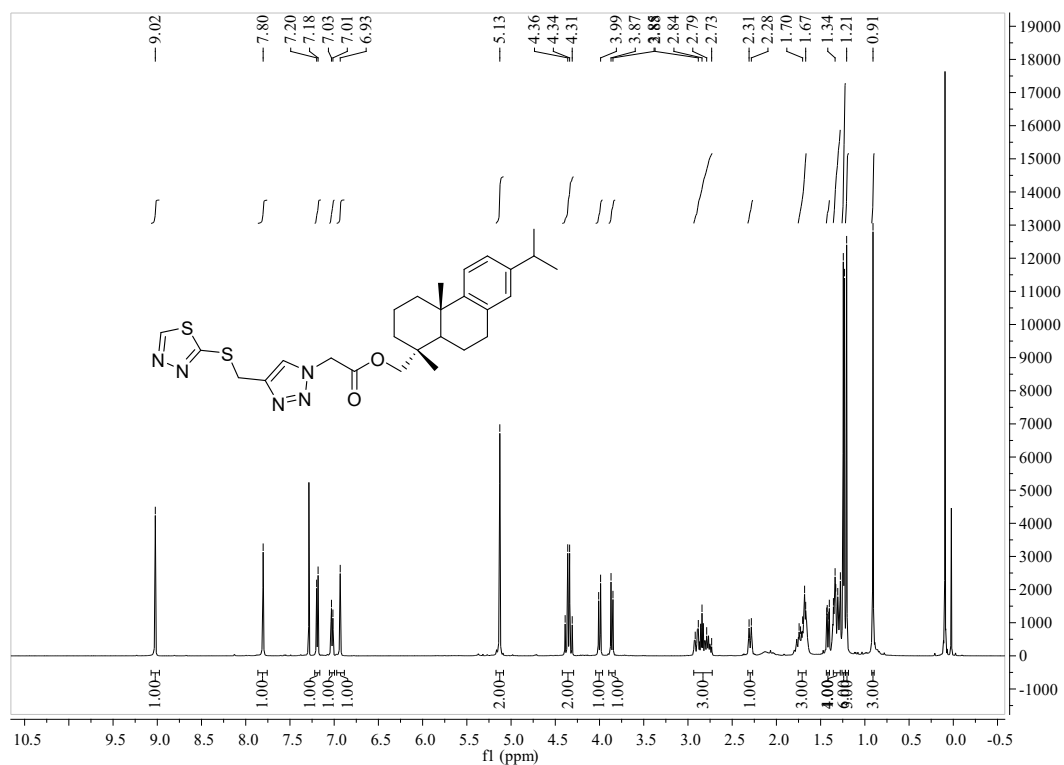


Figure S27 ¹H-NMR spectrum of the target compound **5e** in CDCl₃

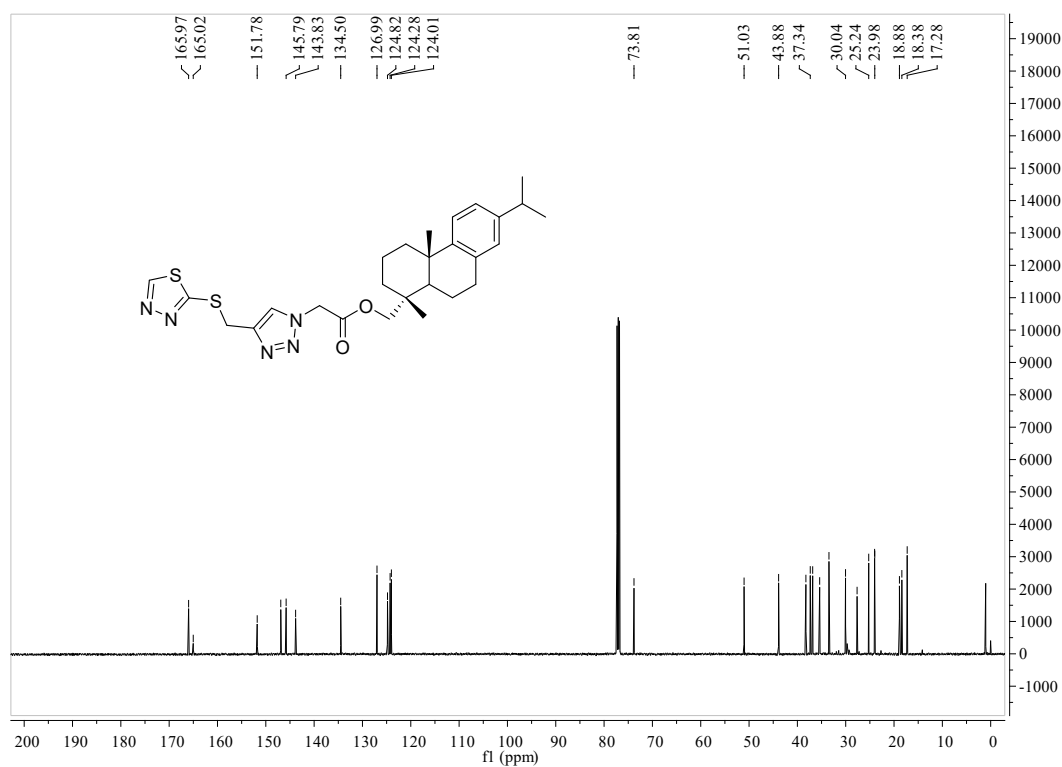


Figure S28 ^{13}C -NMR spectrum of the target compound **5e** in CDCl_3

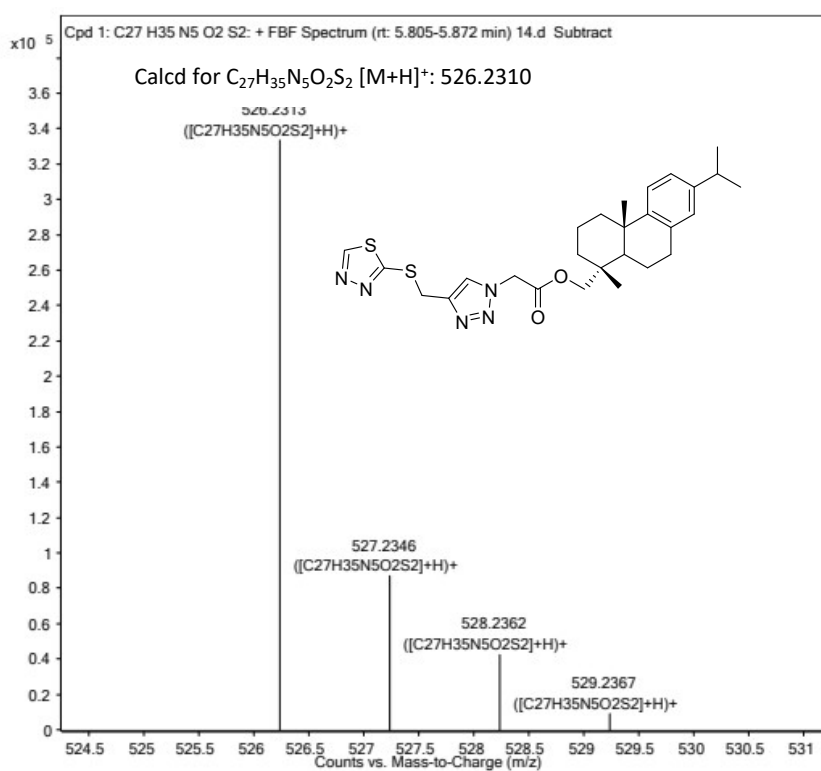


Figure S29 HRMS-ESI spectrum of the target compound **5e**

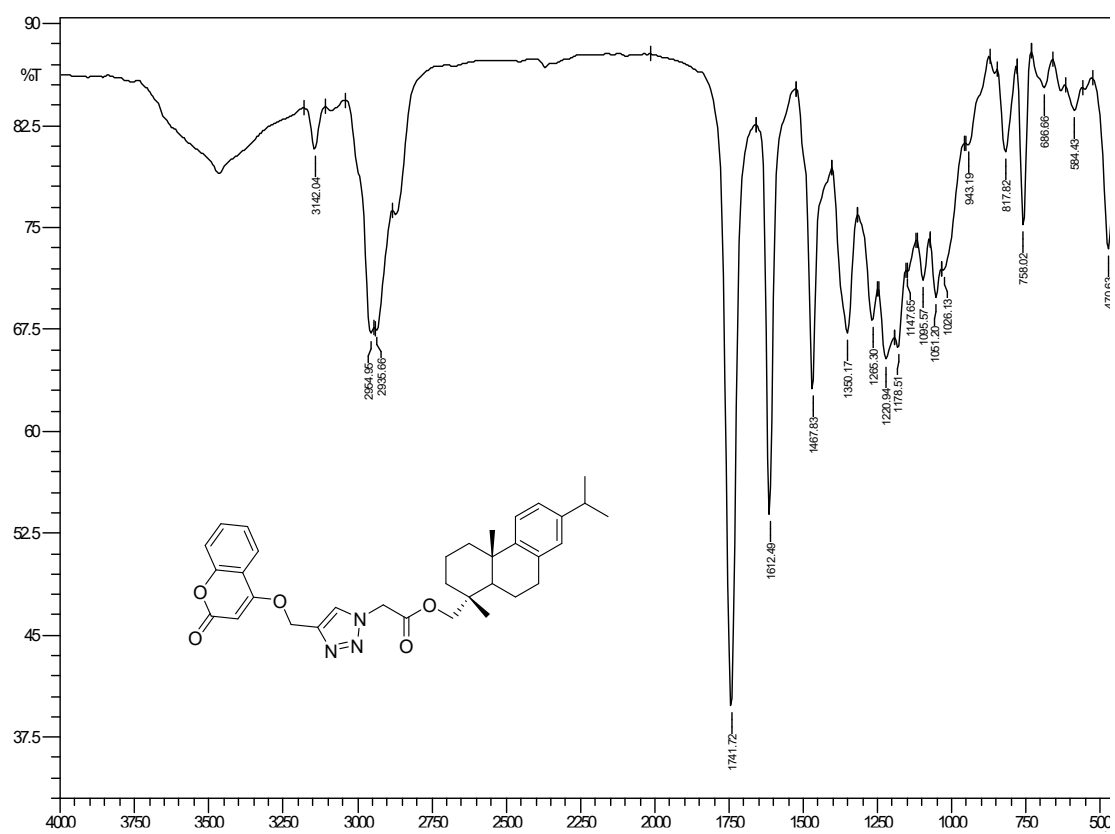


Figure S30 FTIR spectrum of the target compound **5f**

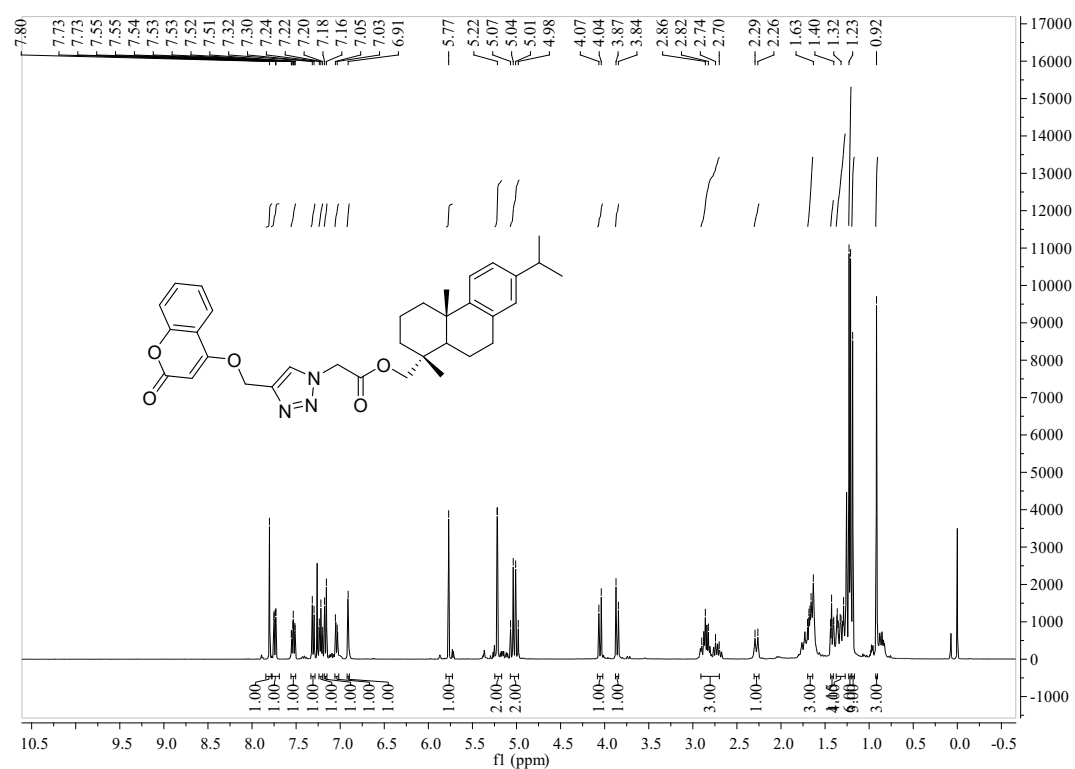


Figure S31 ¹H-NMR spectrum of the target compound **5f** in CDCl₃

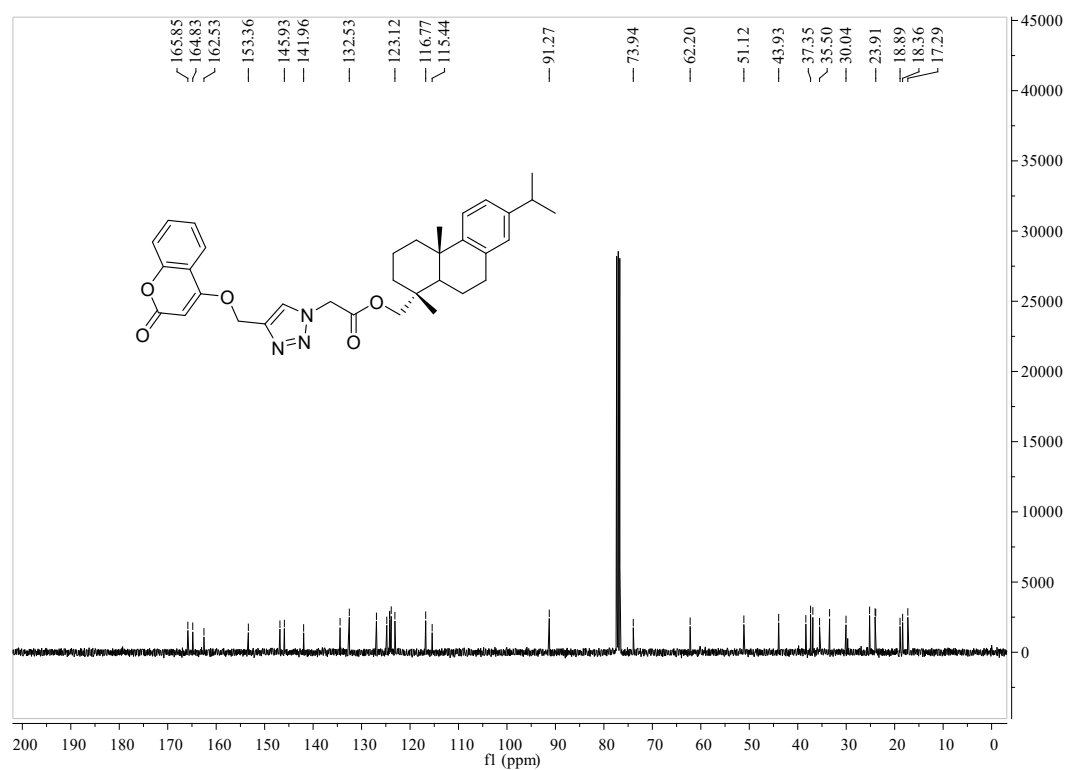


Figure S32 ^{13}C -NMR spectrum of the target compound **5f** in CDCl_3

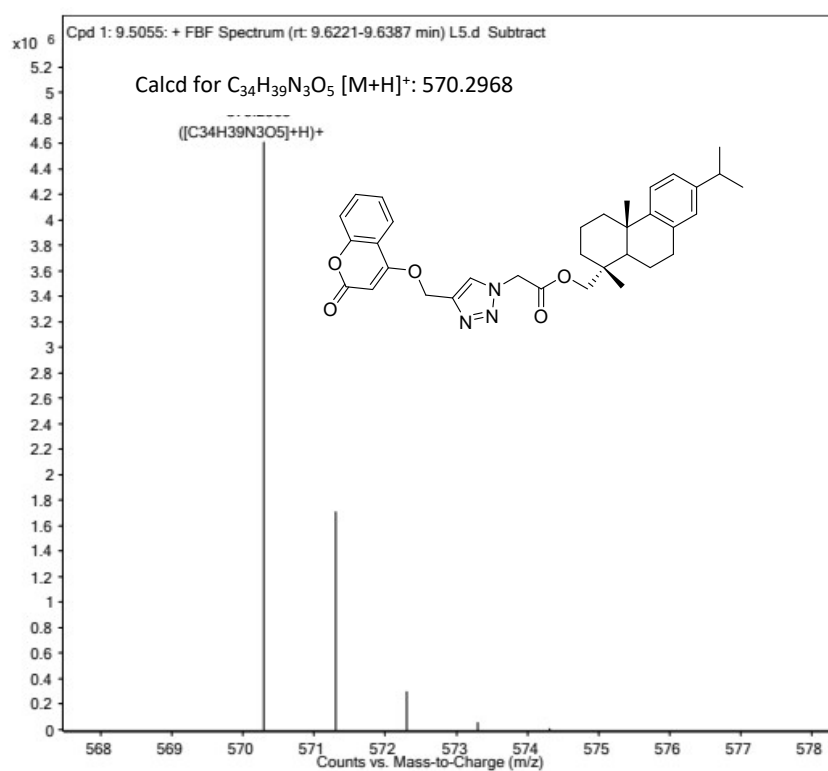


Figure S33 HRMS-ESI spectrum of the target compound **5f**

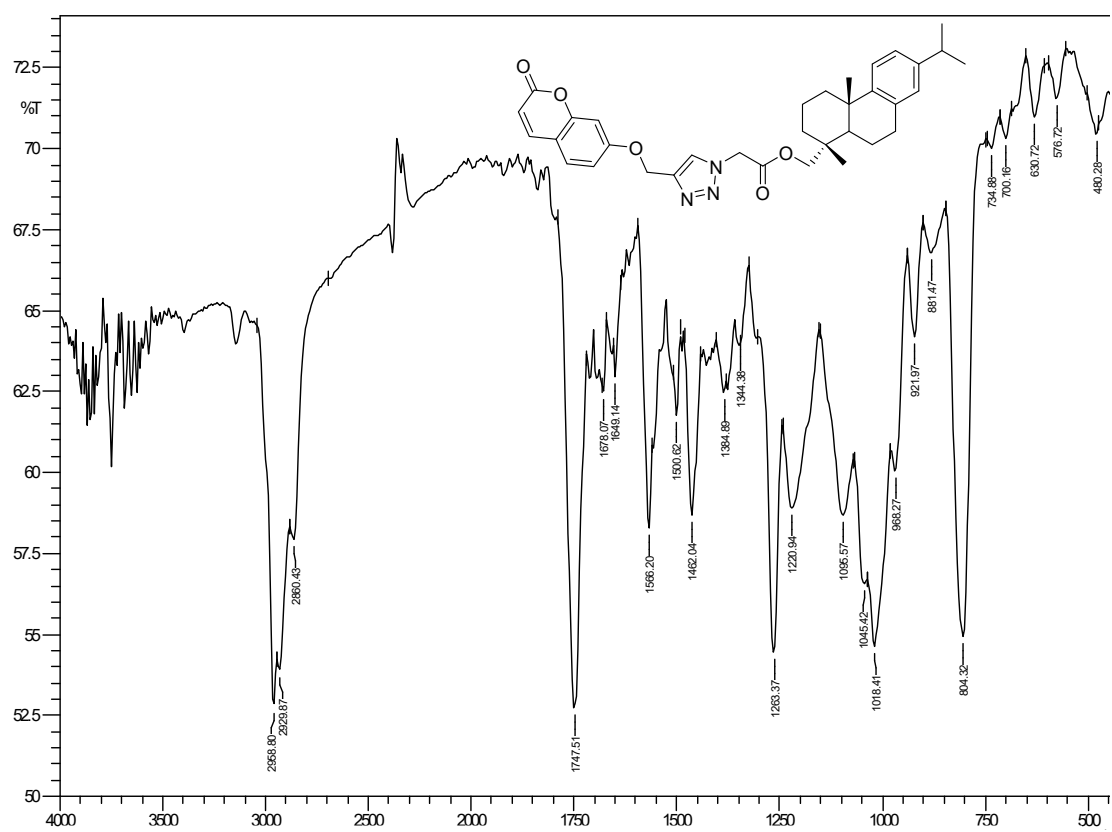


Figure S34 FTIR spectrum of the target compound **5g**

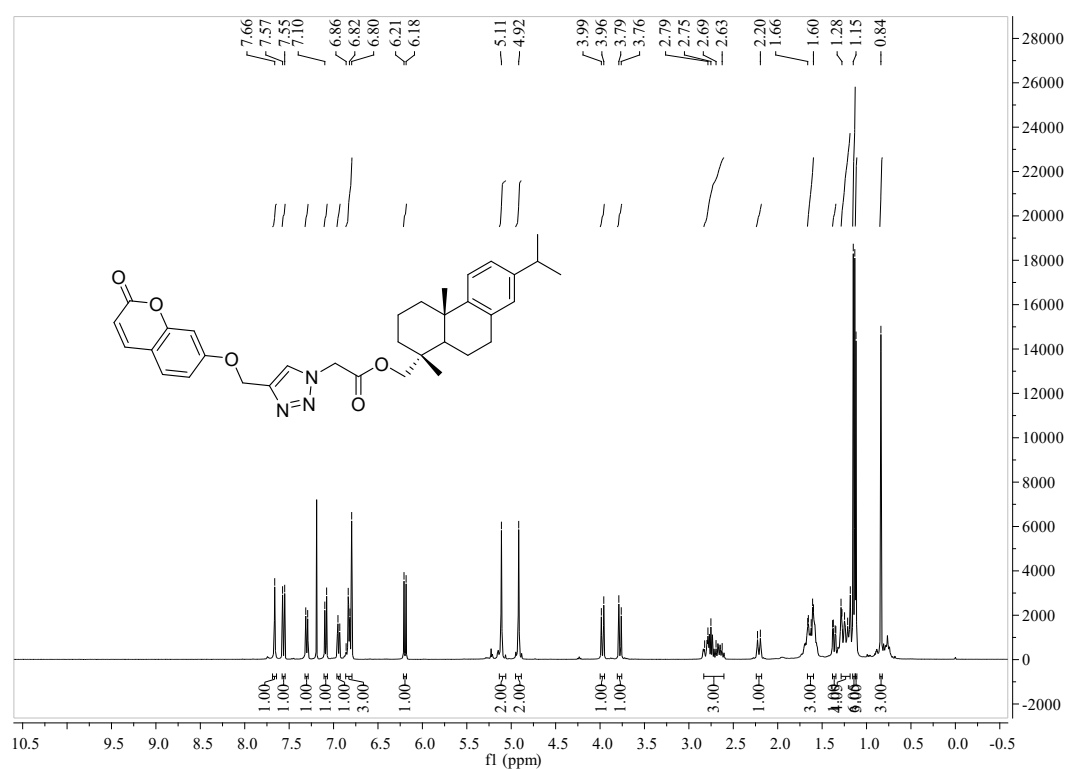


Figure S35 ¹H-NMR spectrum of the target compound **5g** in CDCl₃

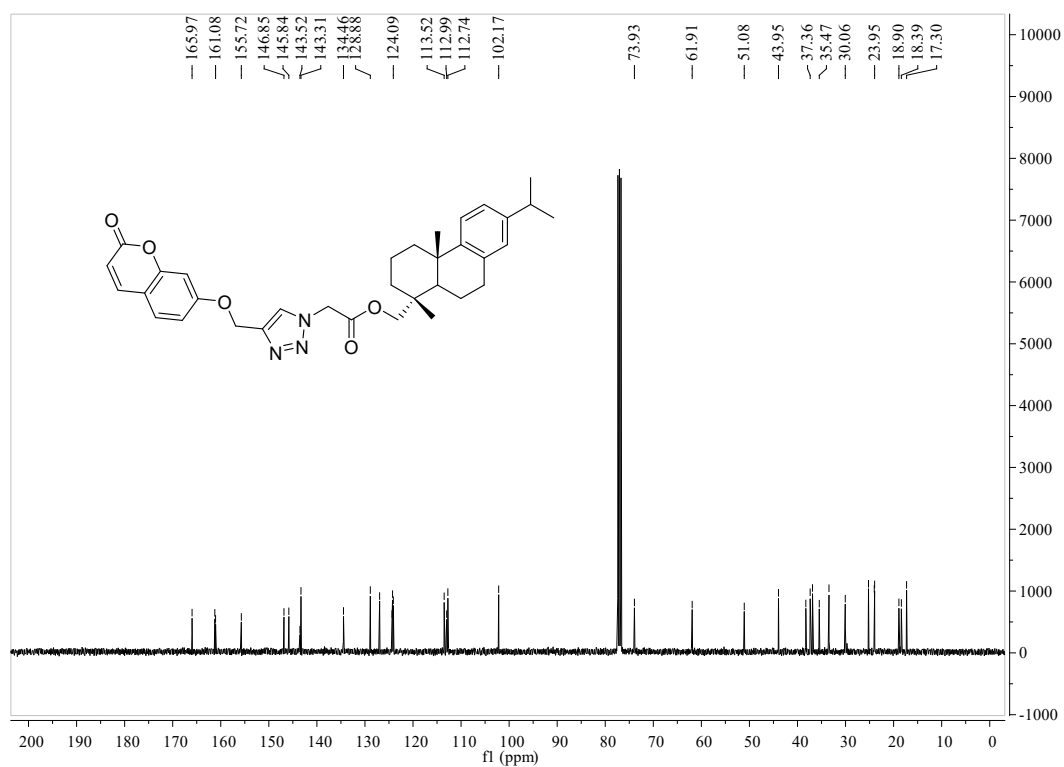


Figure S36 ^{13}C -NMR spectrum of the target compound **5g** in CDCl_3

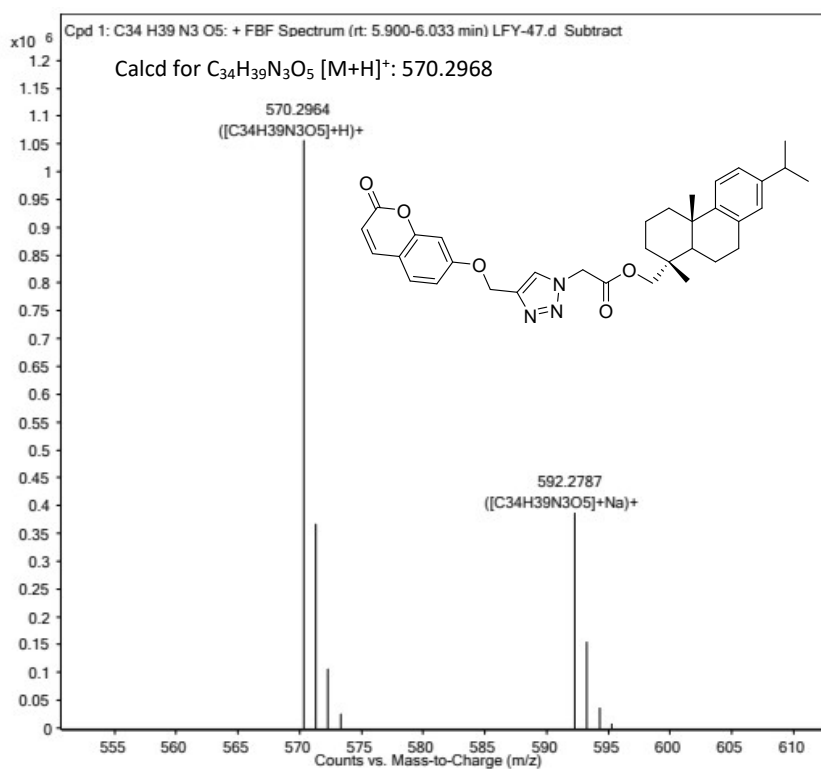


Figure S37 HRMS-ESI spectrum of the target compound **5g**

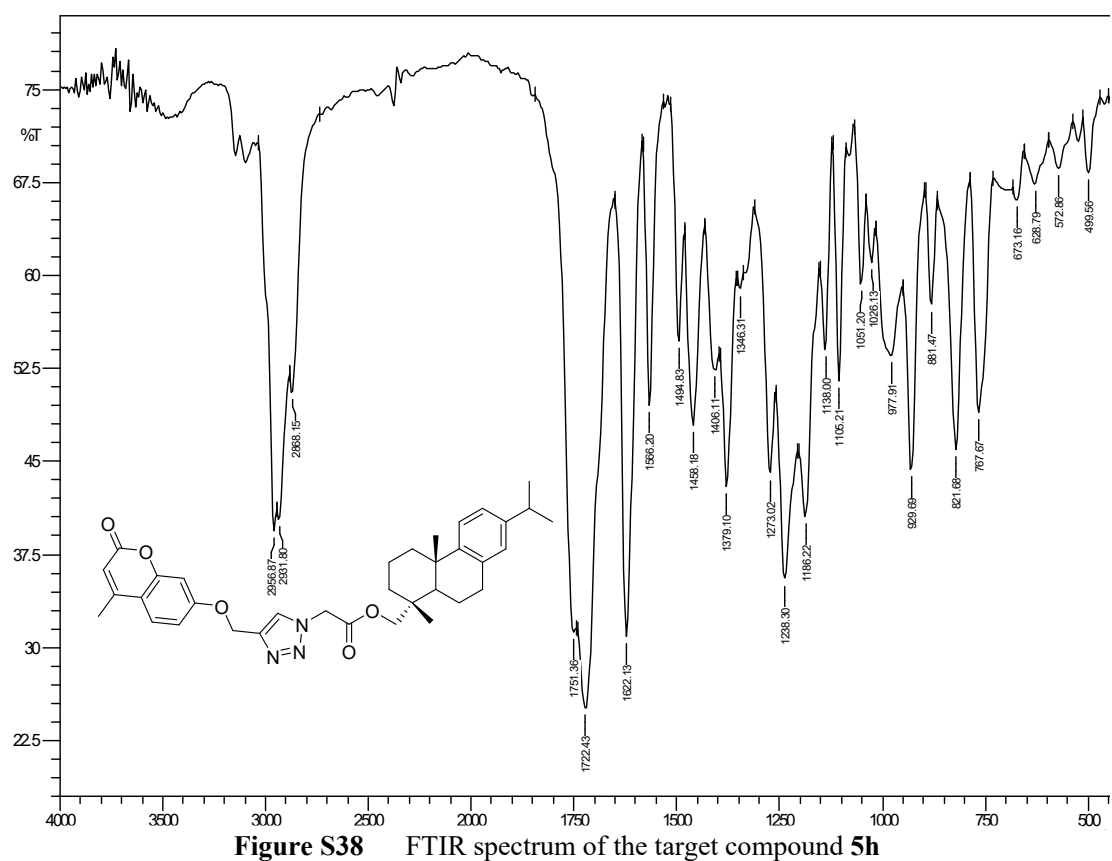


Figure S38 FTIR spectrum of the target compound **5h**

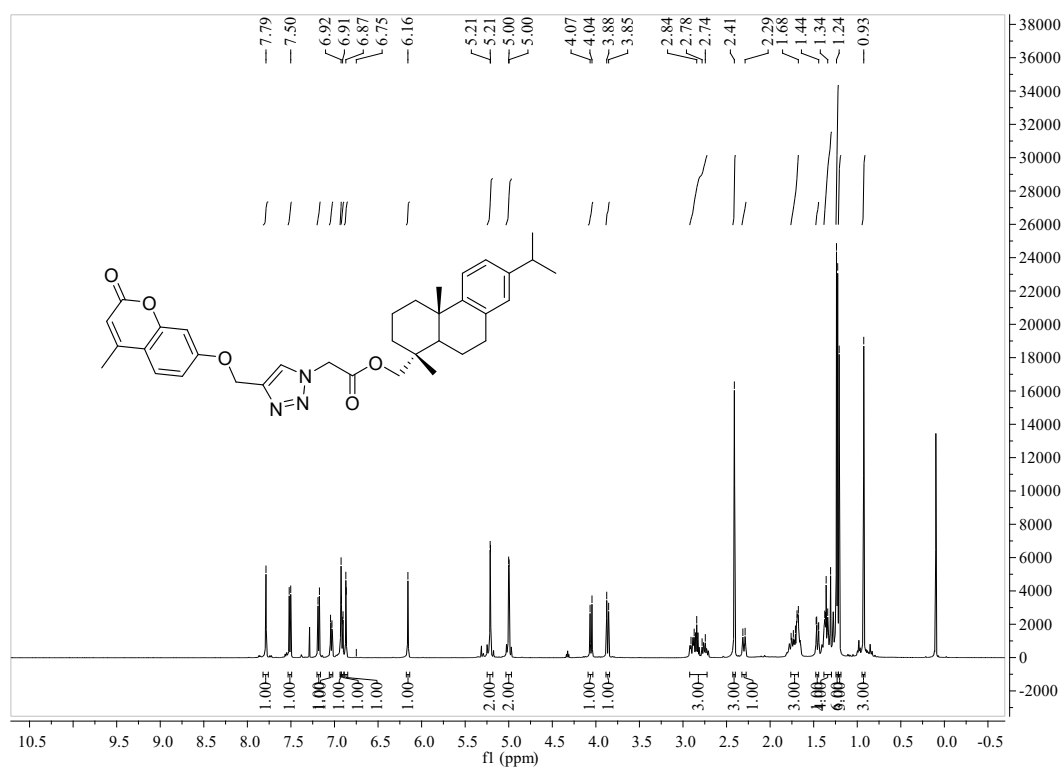


Figure S39 ¹H-NMR spectrum of the target compound **5h** in CDCl₃

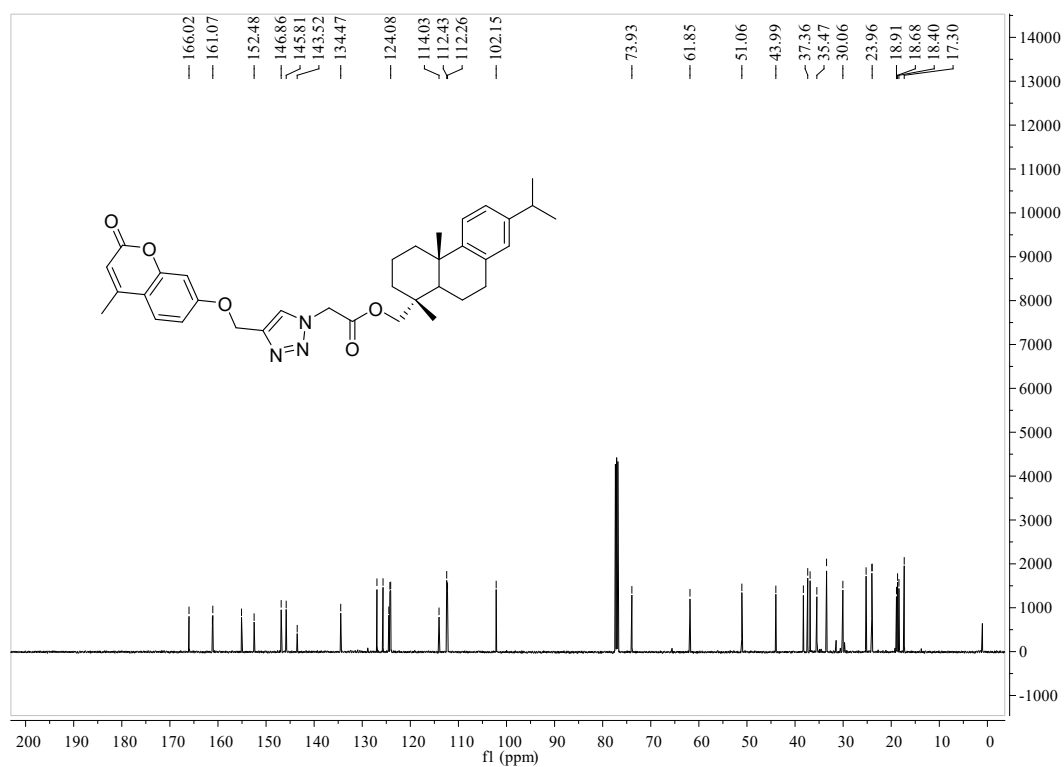


Figure S40 ^{13}C -NMR spectrum of the target compound **5h** in CDCl_3

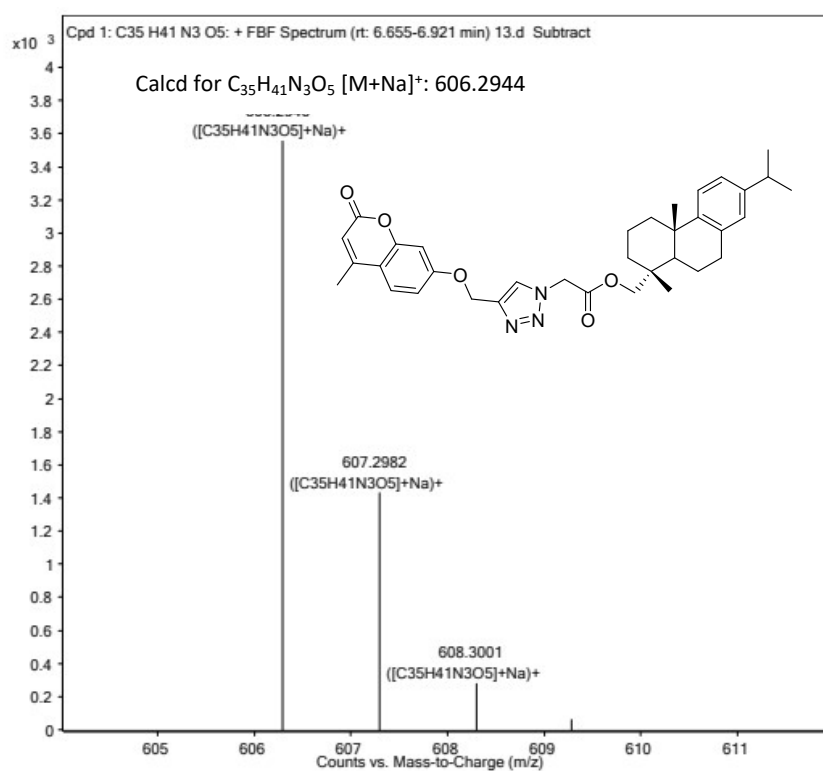


Figure S41 HRMS-ESI spectrum of the target compound **5h**

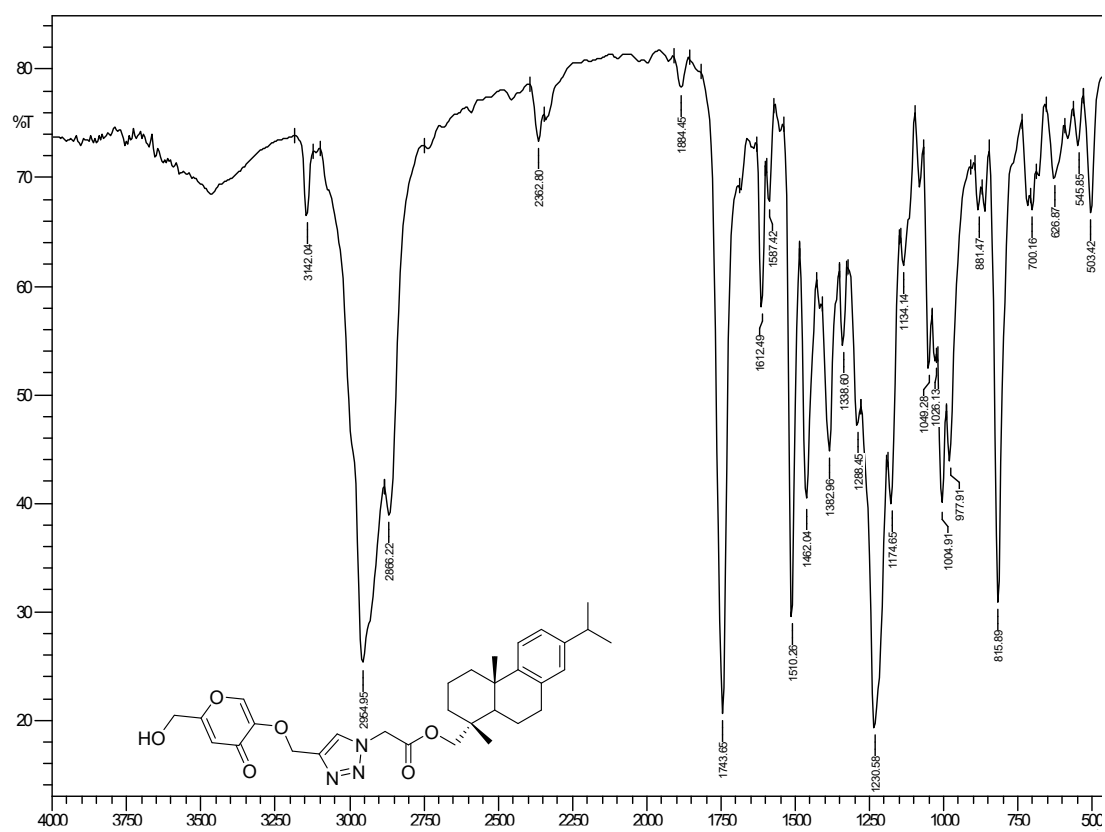


Figure S42 FTIR spectrum of the target compound **5i**

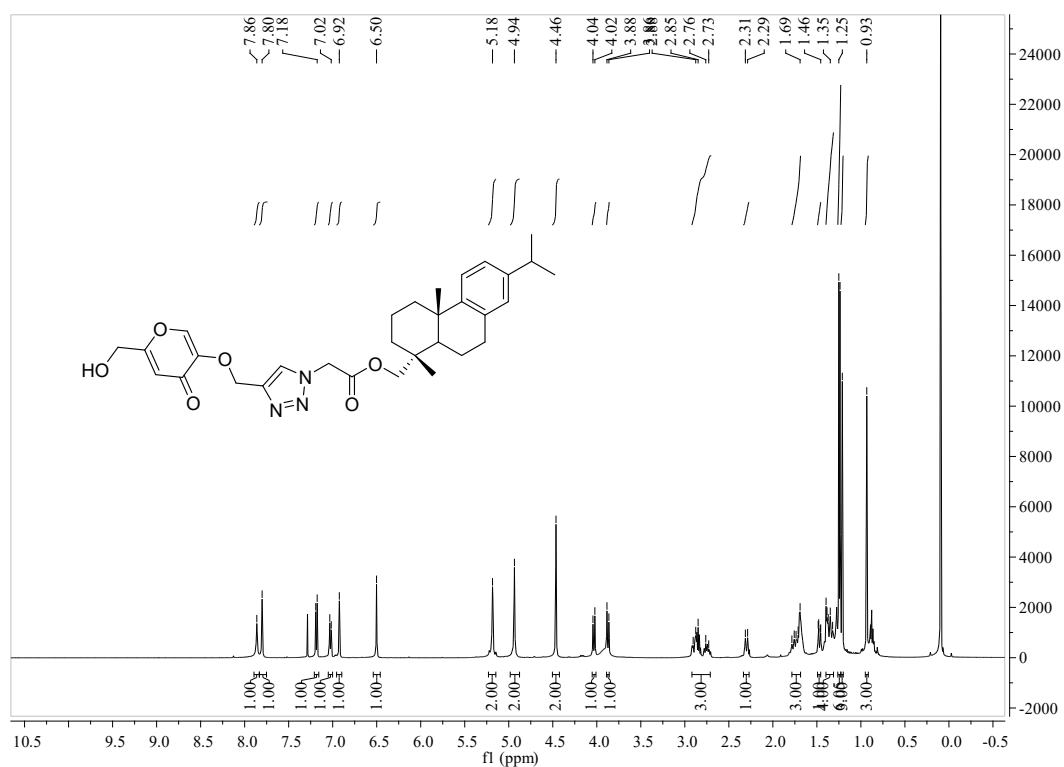


Figure S43 ¹H-NMR spectrum of the target compound **5i** in CDCl₃

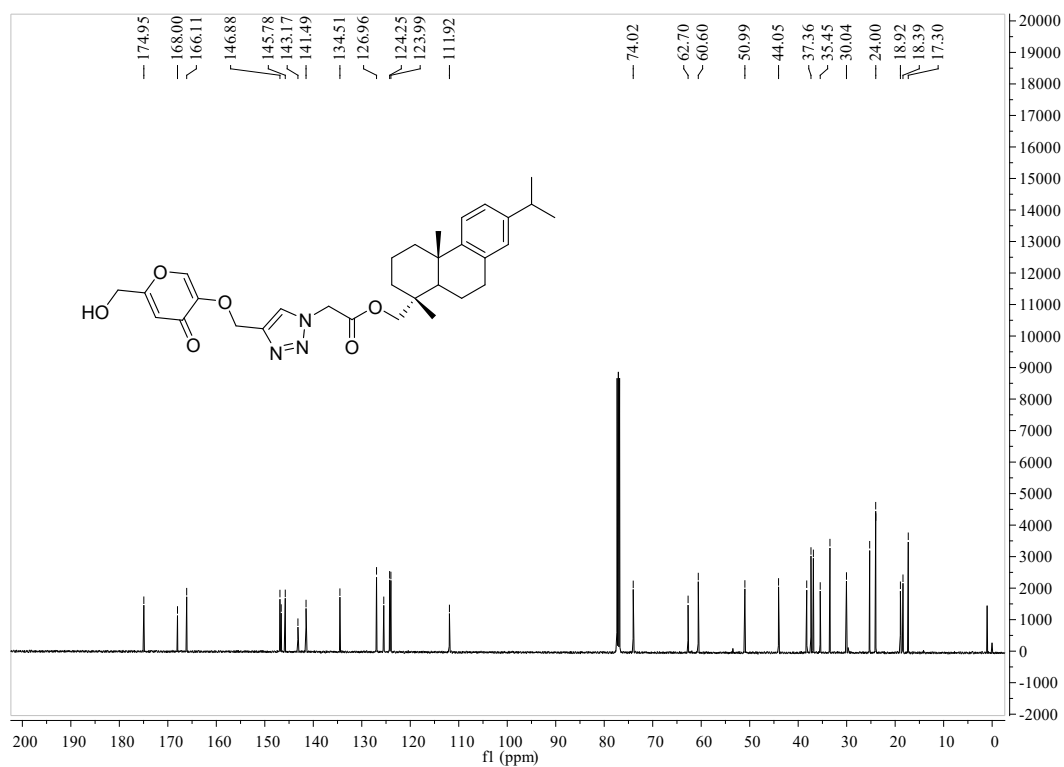


Figure S44 ^{13}C -NMR spectrum of the target compound **5i** in CDCl_3

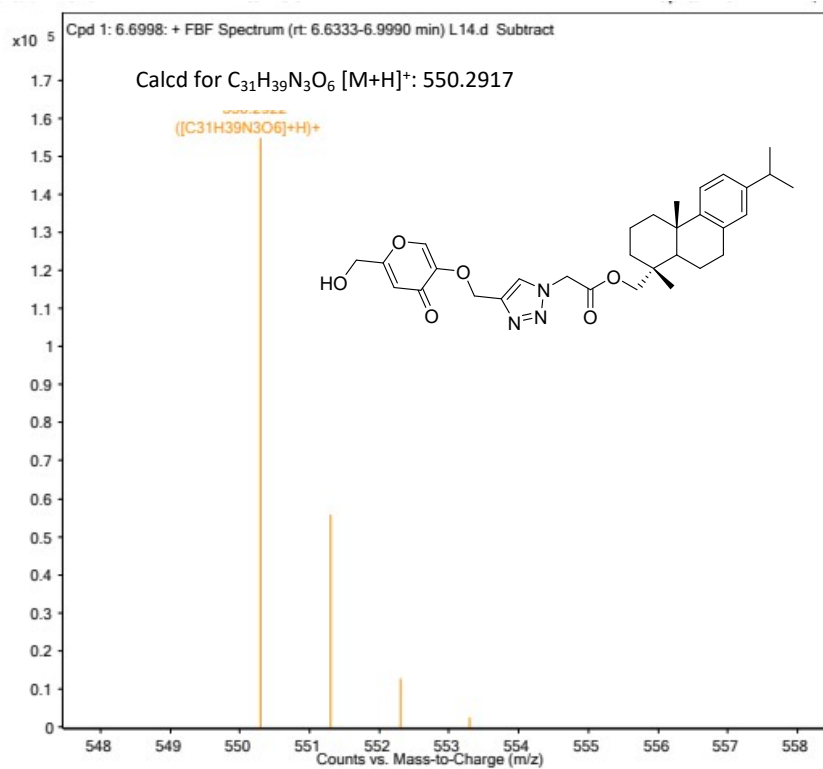


Figure S45 HRMS-ESI spectrum of the target compound **5i**

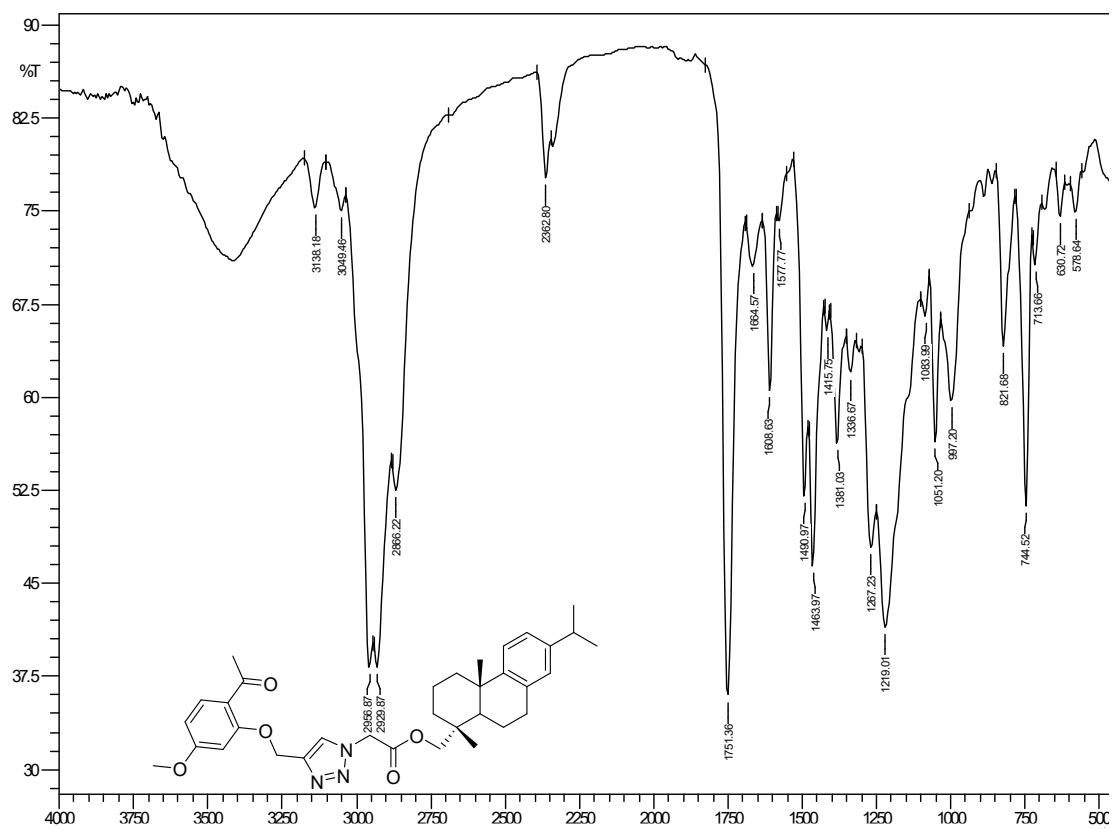


Figure S46 FTIR spectrum of the target compound **5i**

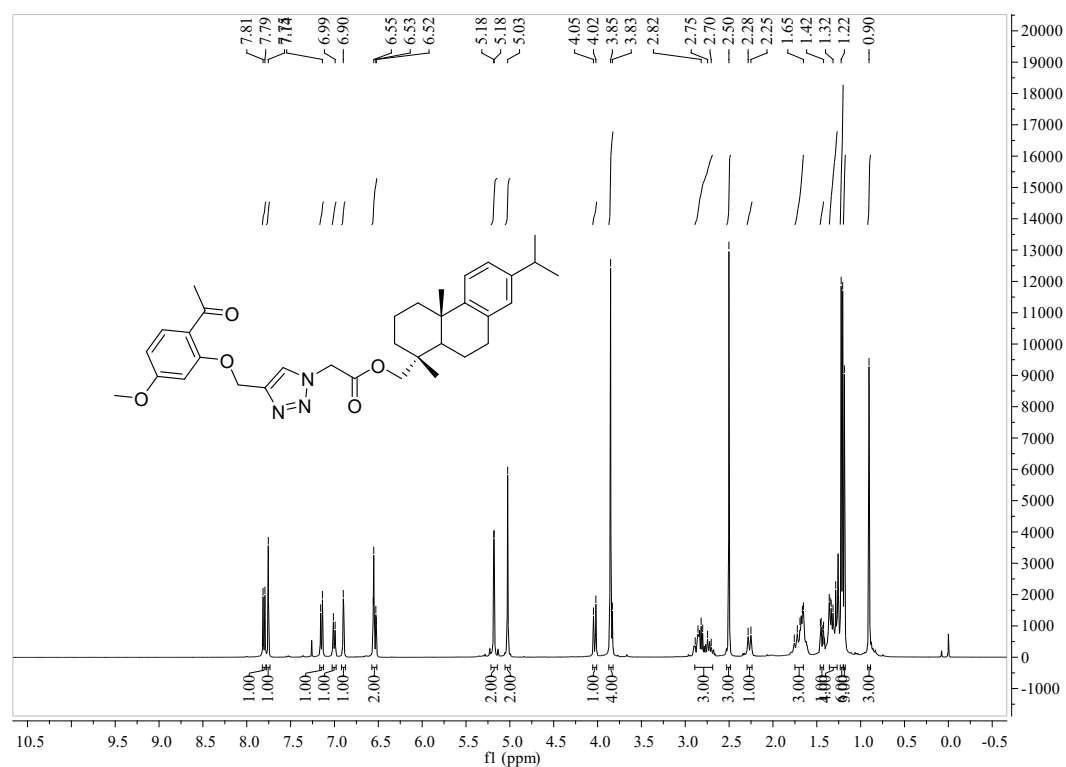


Figure S47 ¹H-NMR spectrum of the target compound **5j** in CDCl₃

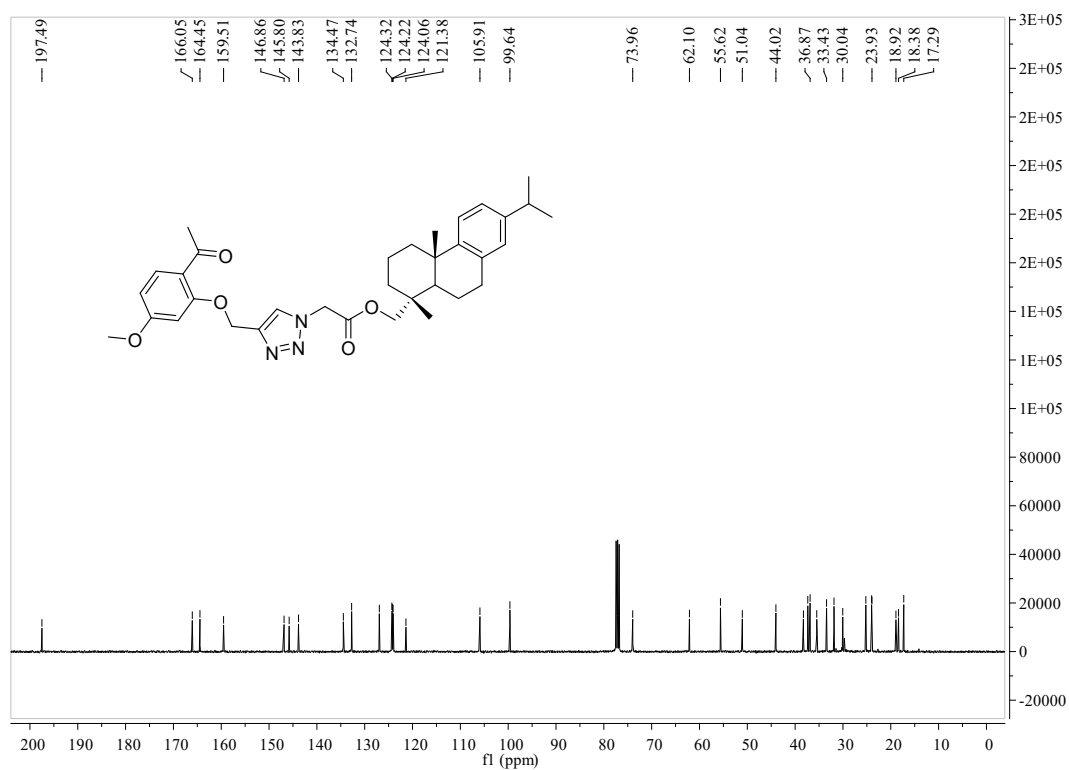


Figure S48 ^{13}C -NMR spectrum of the target compound **5i** in CDCl_3

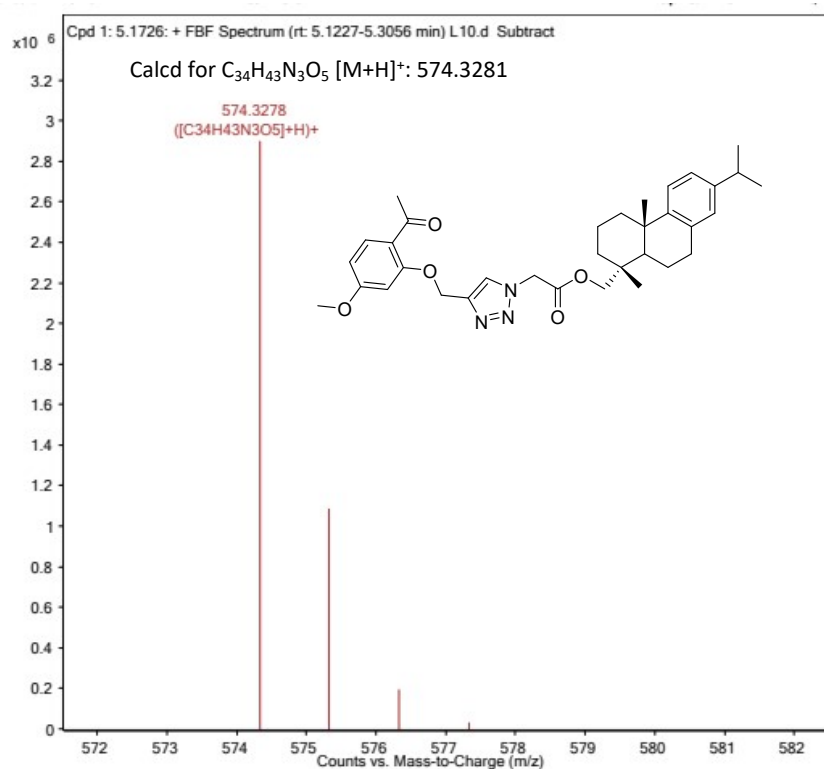


Figure S49 HRMS-ESI spectrum of the target compound **5j**

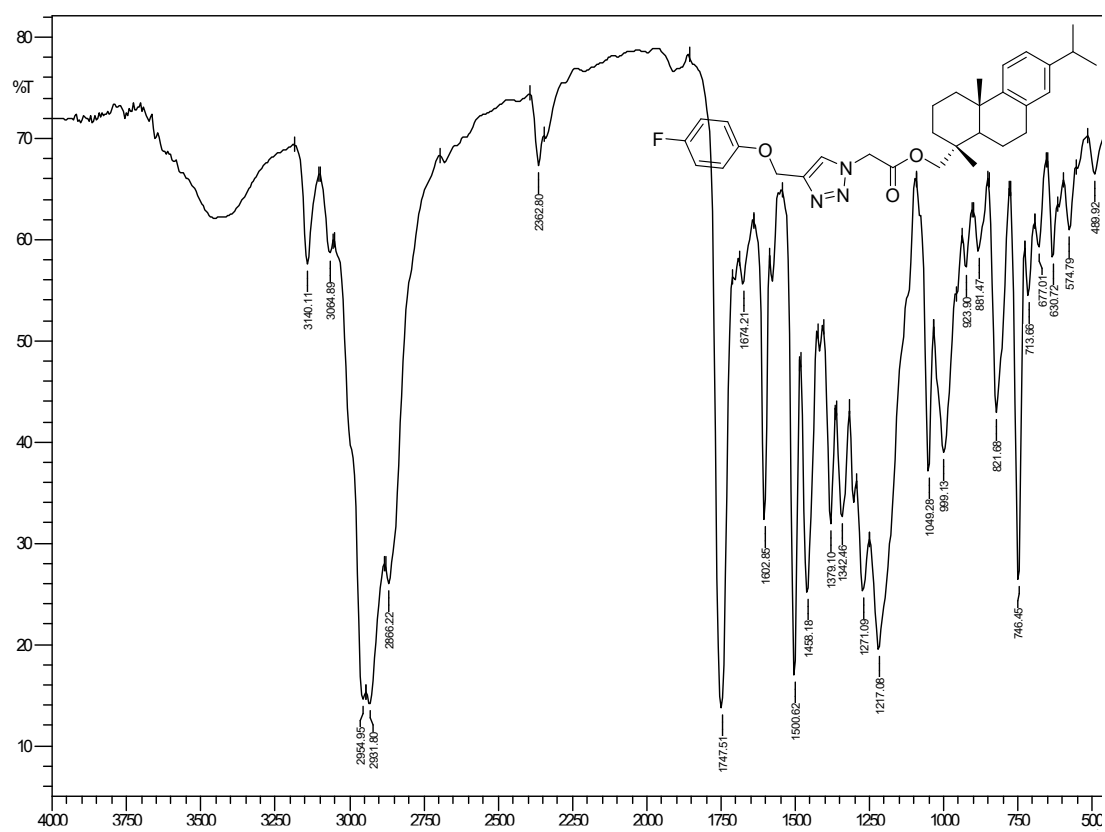


Figure S50 FTIR spectrum of the target compound **5k**

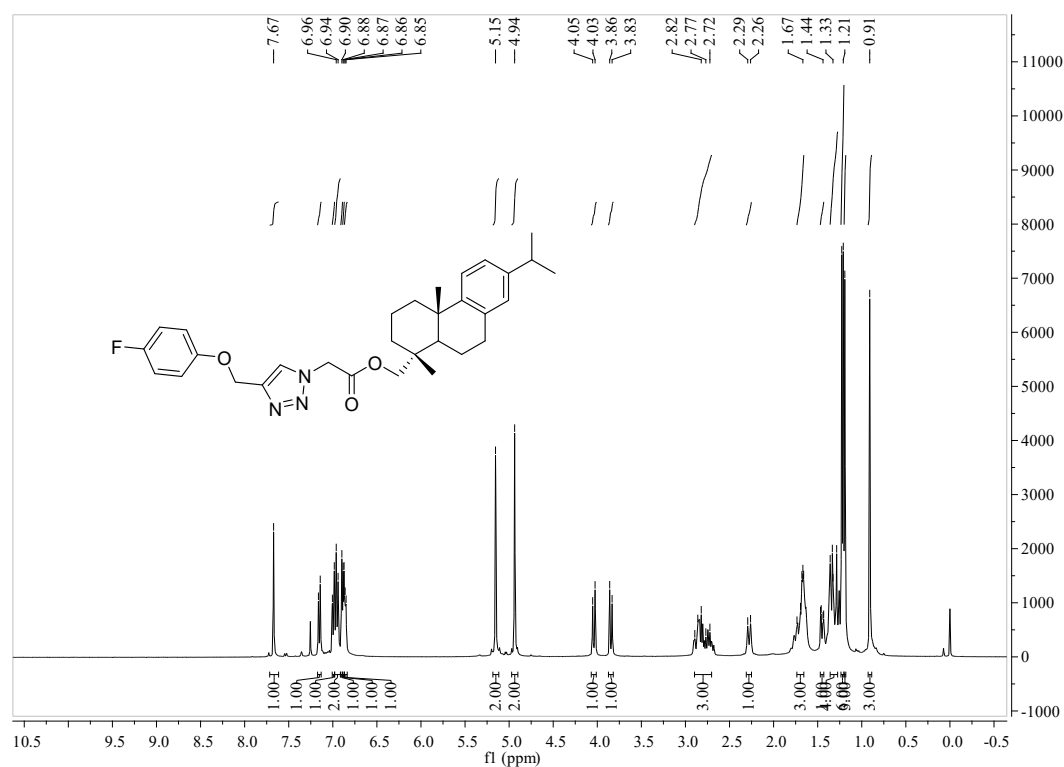


Figure S51 ^1H -NMR spectrum of the target compound **5k** in CDCl_3

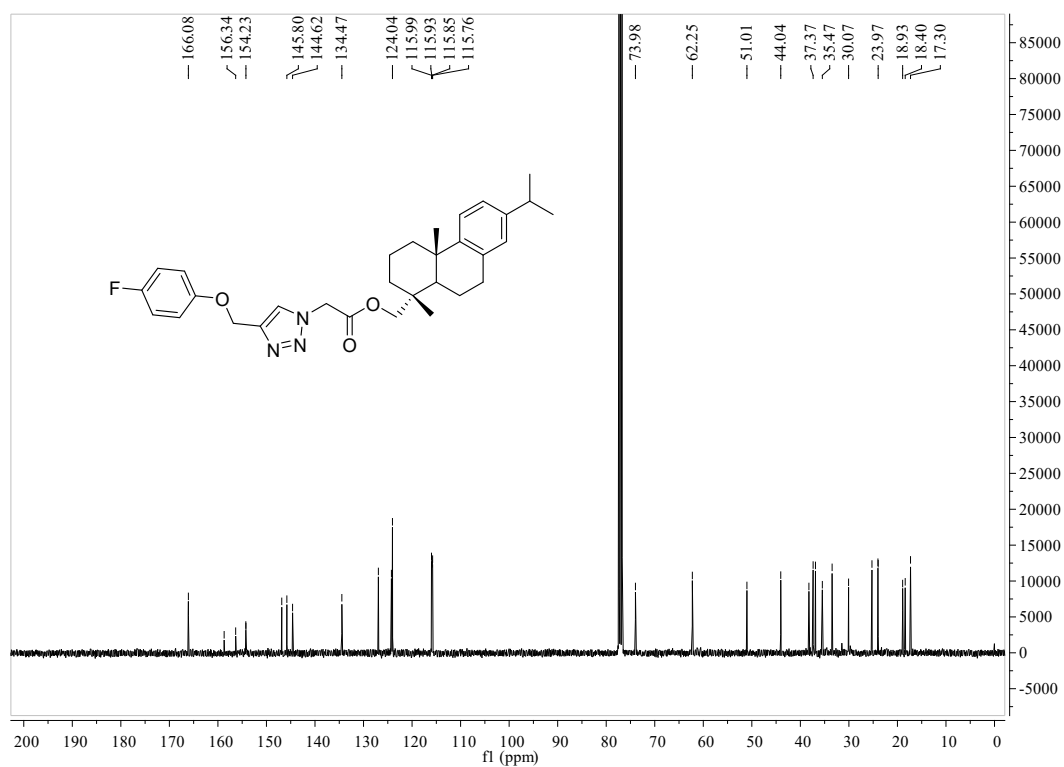


Figure S52 ¹³C-NMR spectrum of the target compound **5k** in CDCl₃

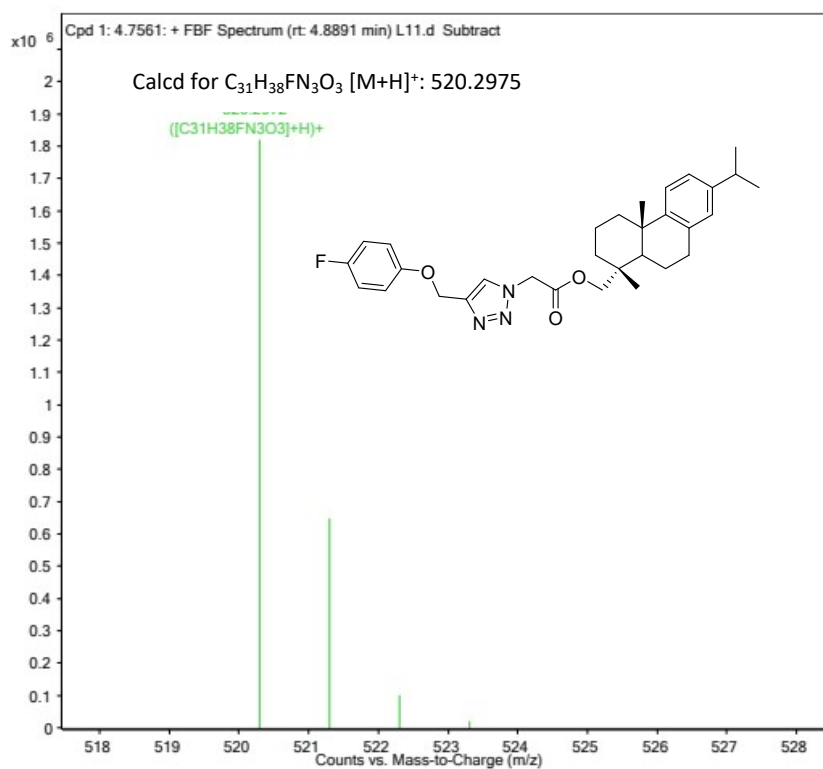


Figure S53 HRMS-ESI spectrum of the target compound **5k**

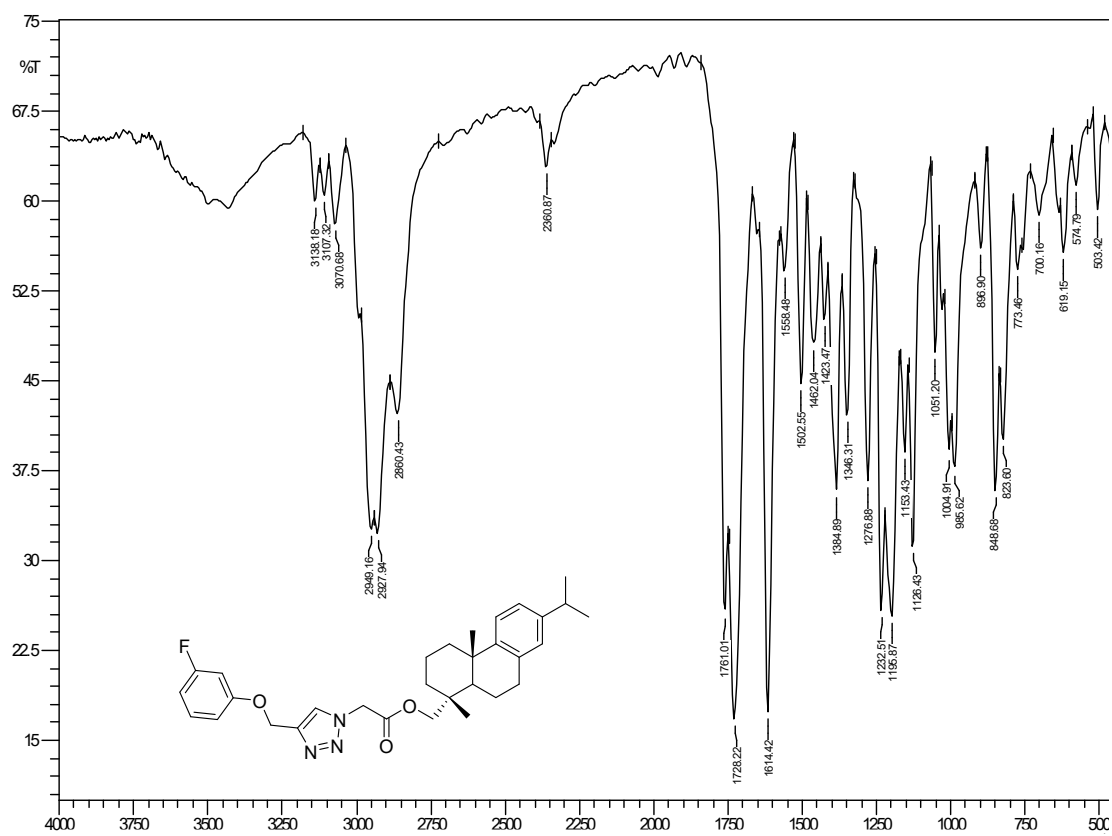


Figure S54 FTIR spectrum of the target compound **5l**

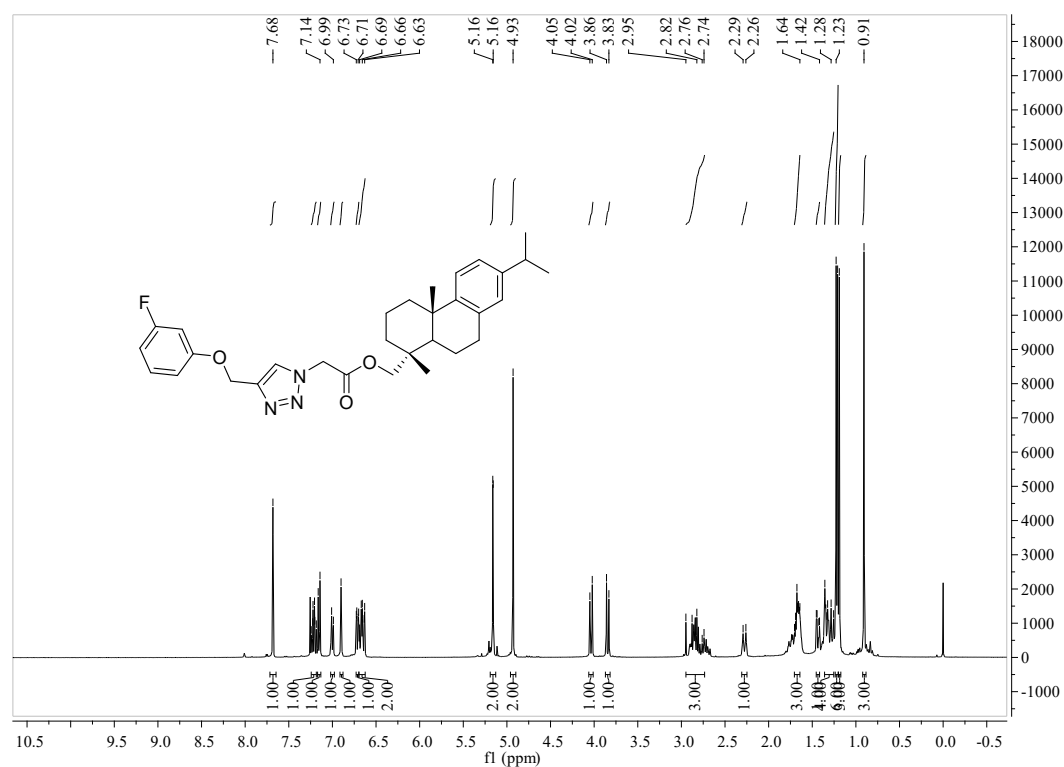


Figure S55 ¹H-NMR spectrum of the target compound **5l** in CDCl₃

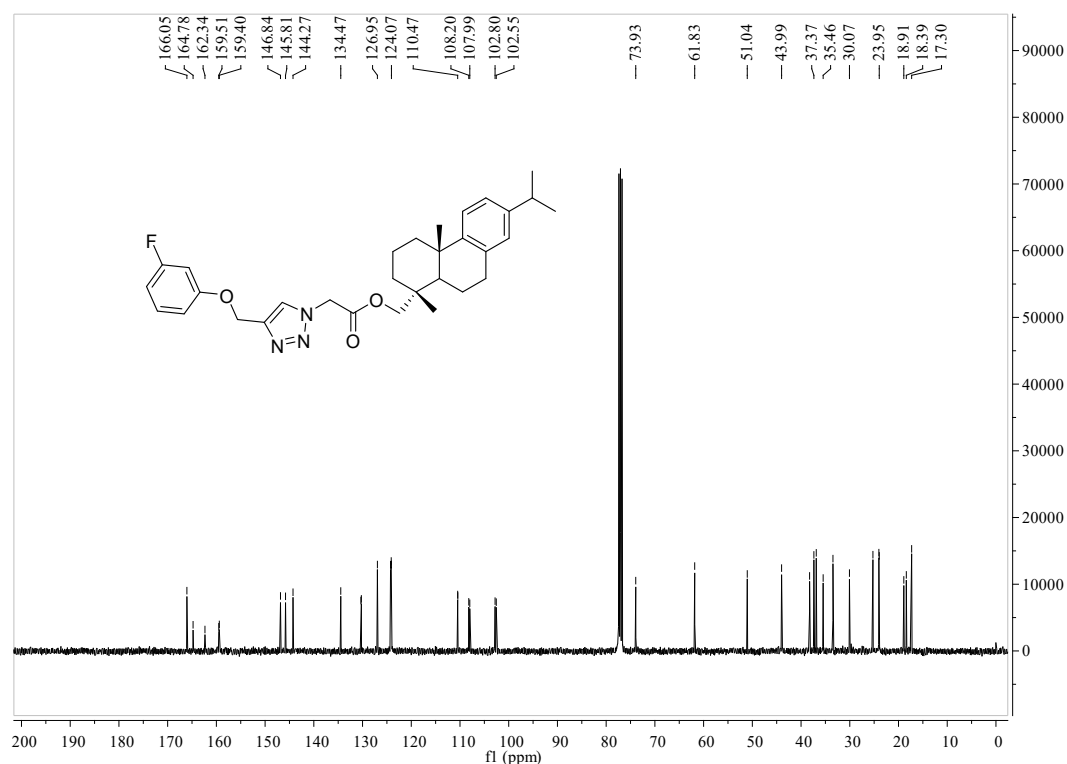


Figure S56 ^{13}C -NMR spectrum of the target compound **5l** in CDCl_3

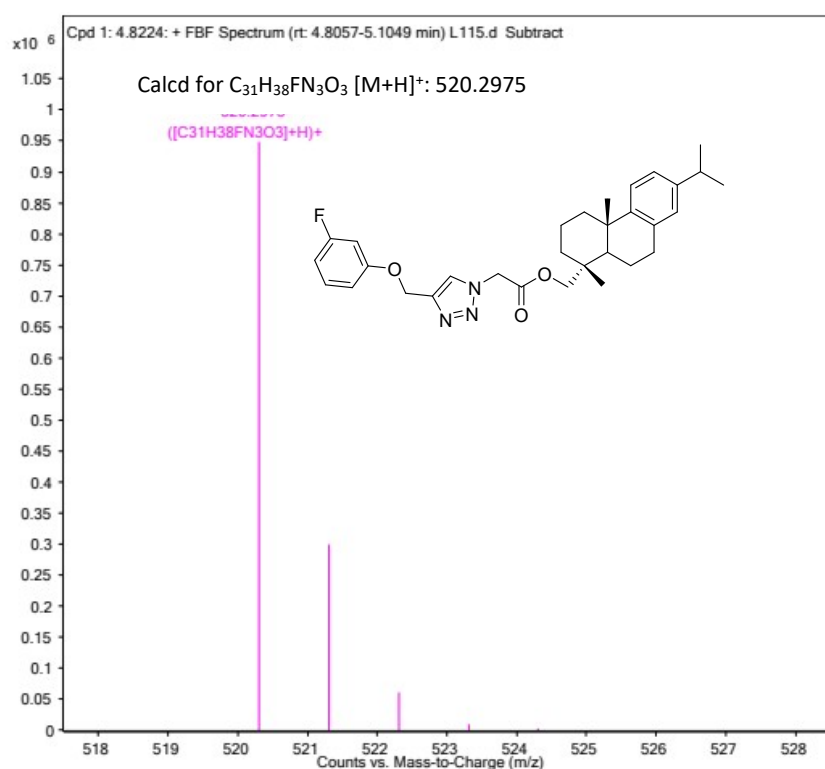


Figure S57 HRMS-ESI spectrum of the target compound **5l**

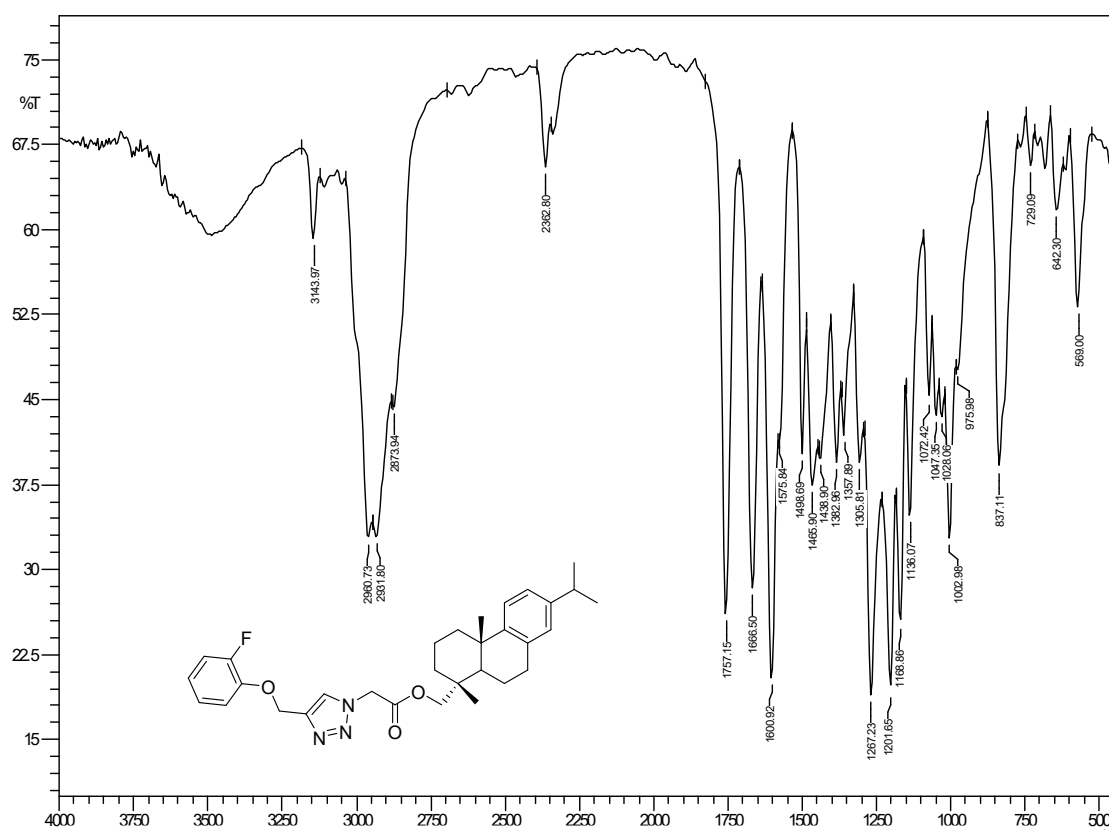


Figure 58. FTIR spectrum of the target compound **5m**

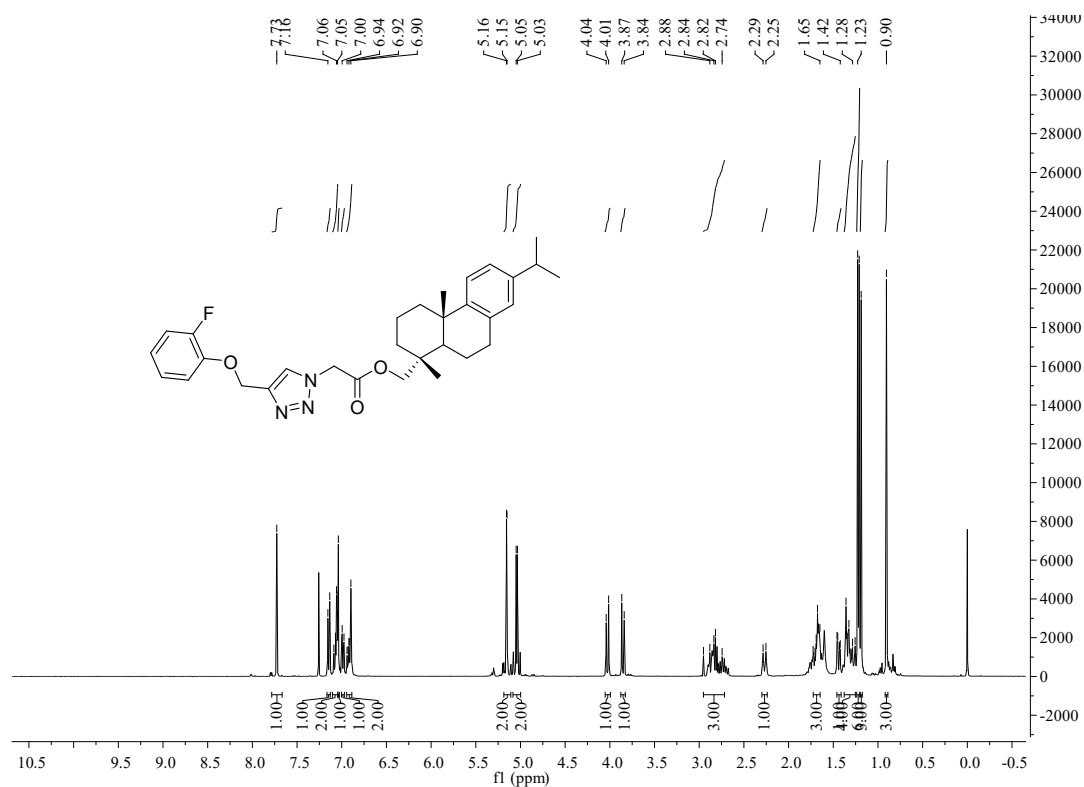


Figure S59 ¹H-NMR spectrum of the target compound **5m** in CDCl₃

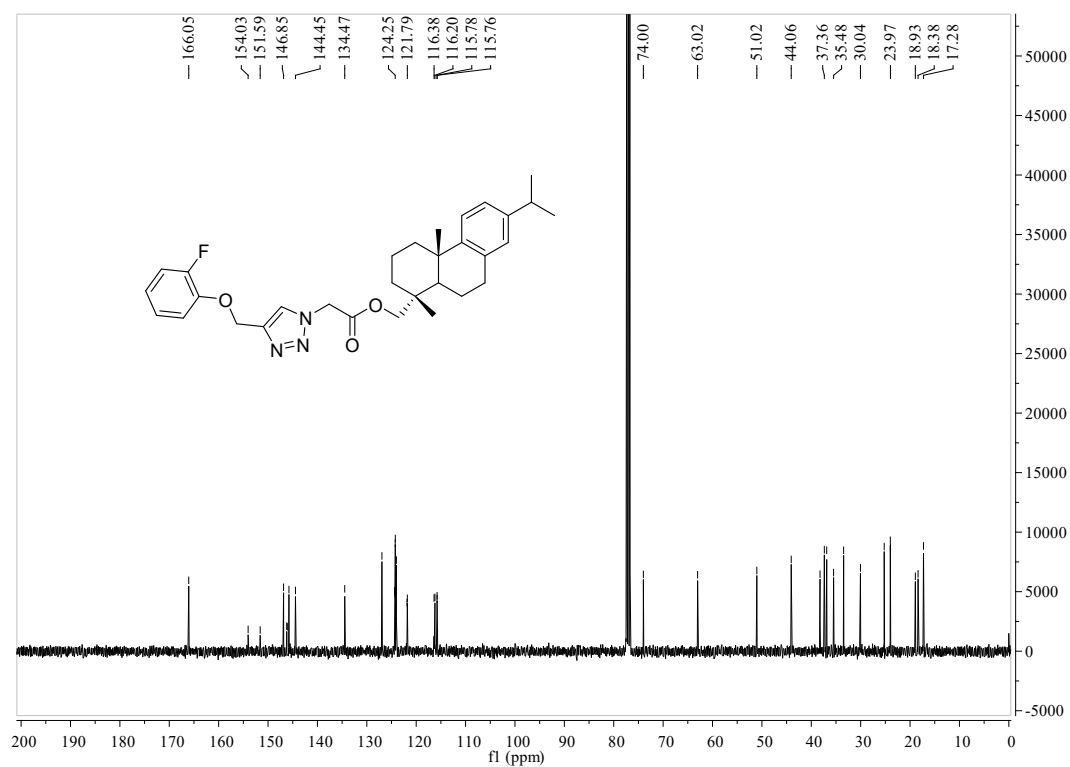


Figure S60 ¹³C-NMR spectrum of the target compound **5m** in CDCl₃

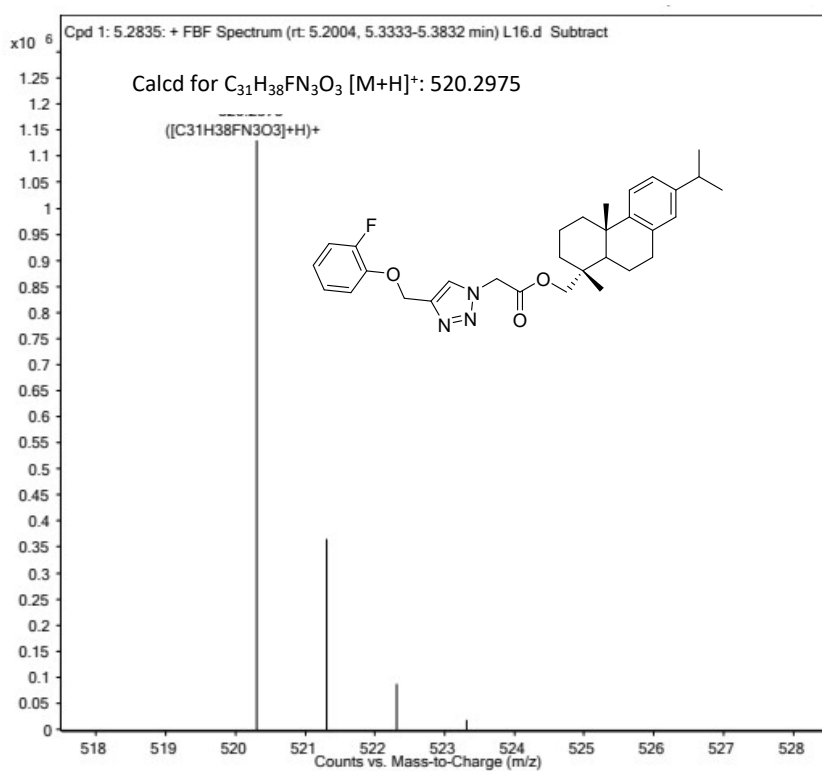


Figure S61 HRMS-ESI spectrum of the target compound **5m**

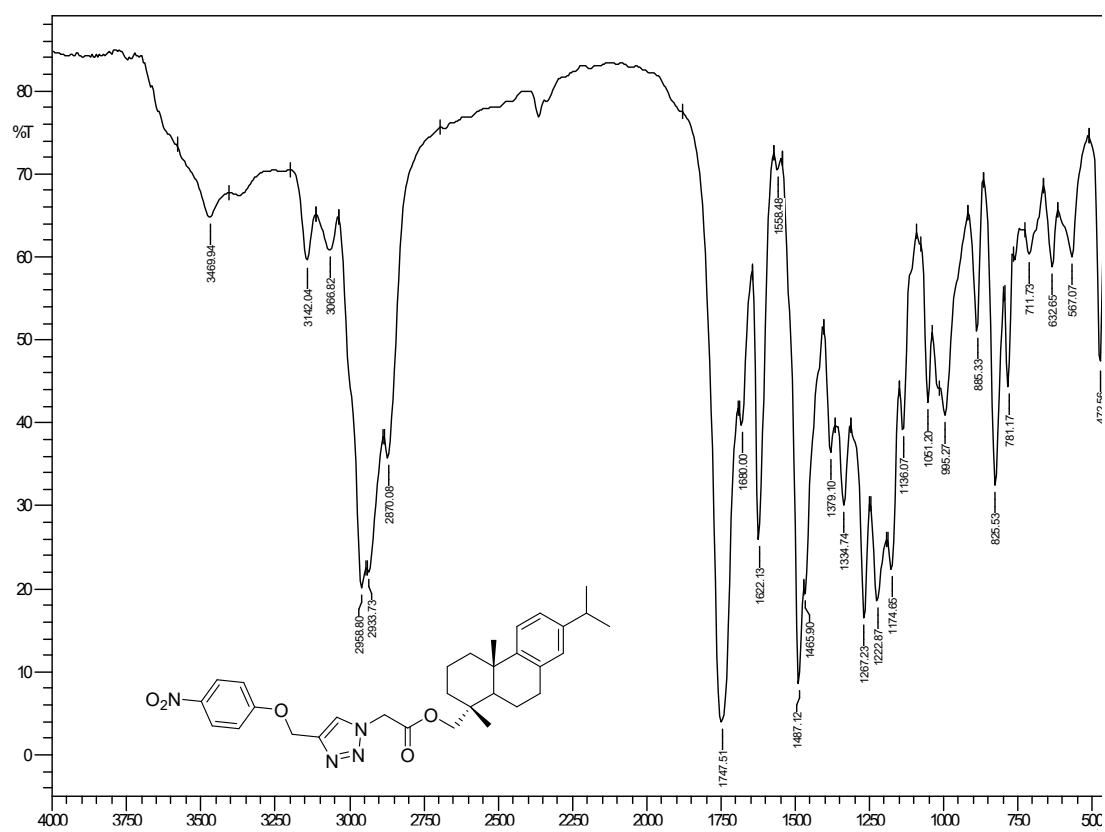


Figure S62 FTIR spectrum of the target compound **5n**

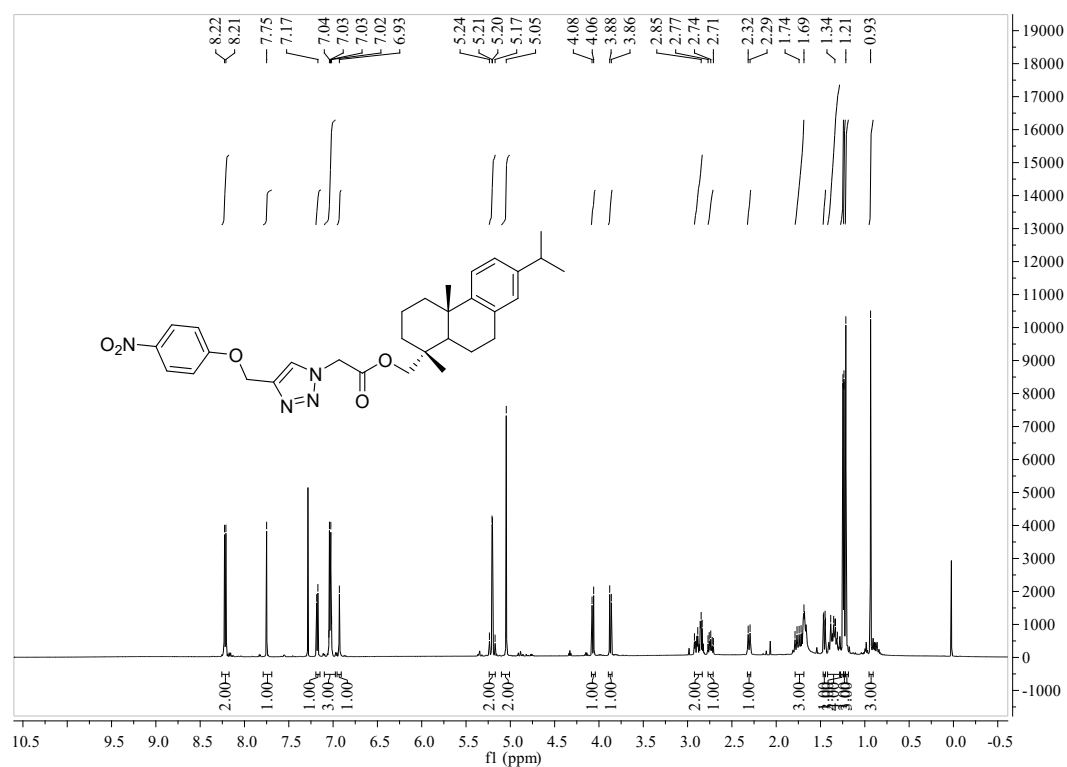


Figure S63 ¹H-NMR spectrum of the target compound **5n** in CDCl₃

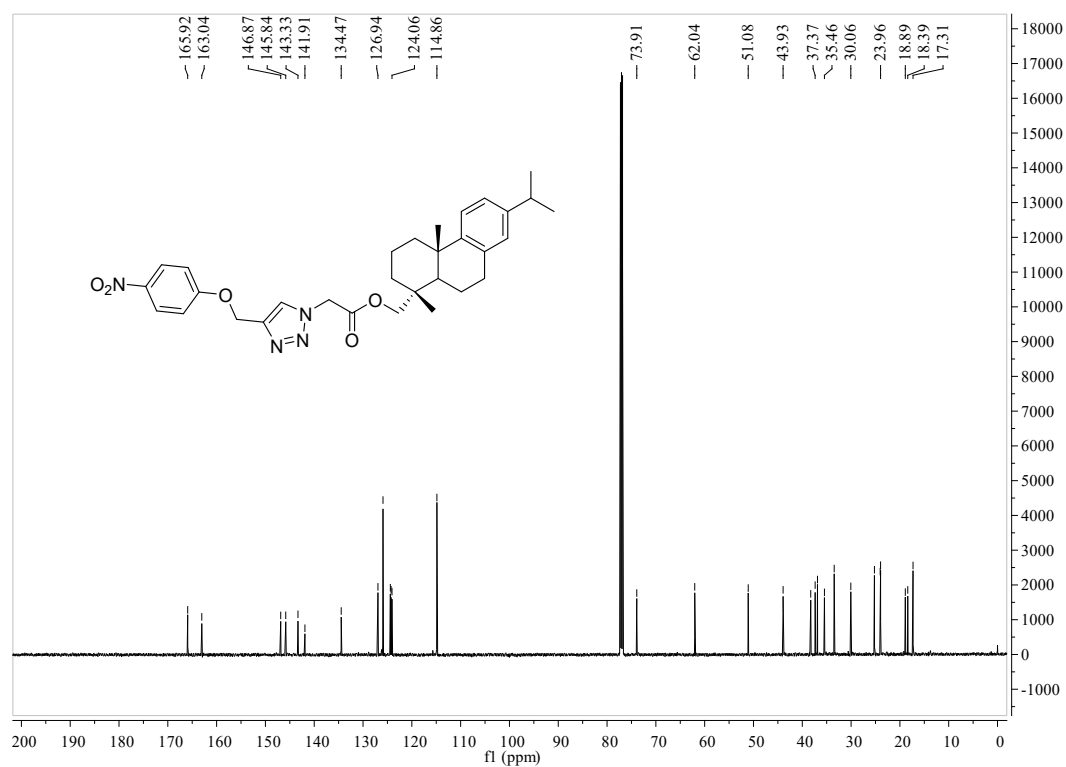


Figure S64 ^{13}C -NMR spectrum of the target compound **5n** in CDCl_3

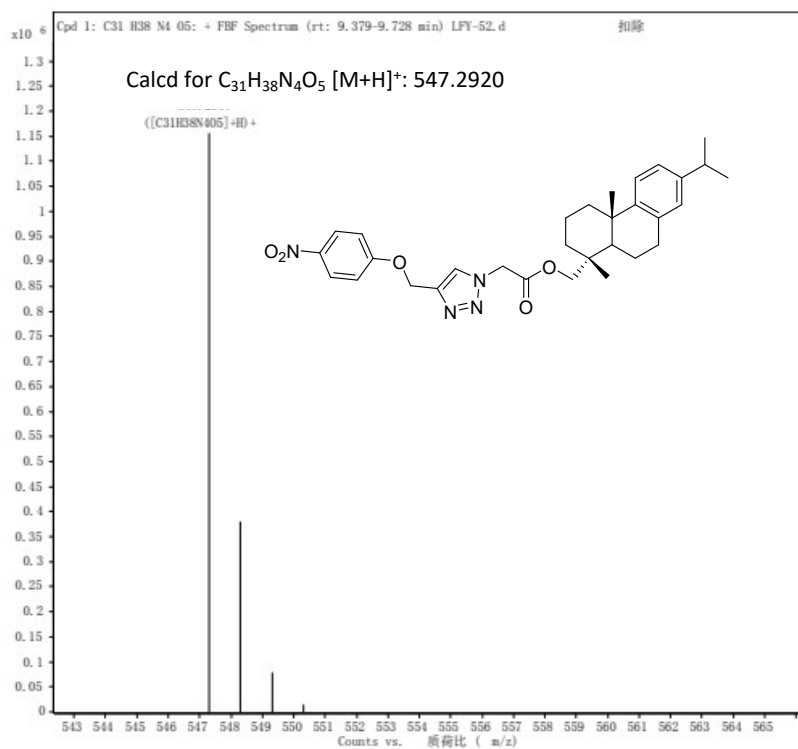


Figure S65 HRMS-ESI spectrum of the target compound **5n**

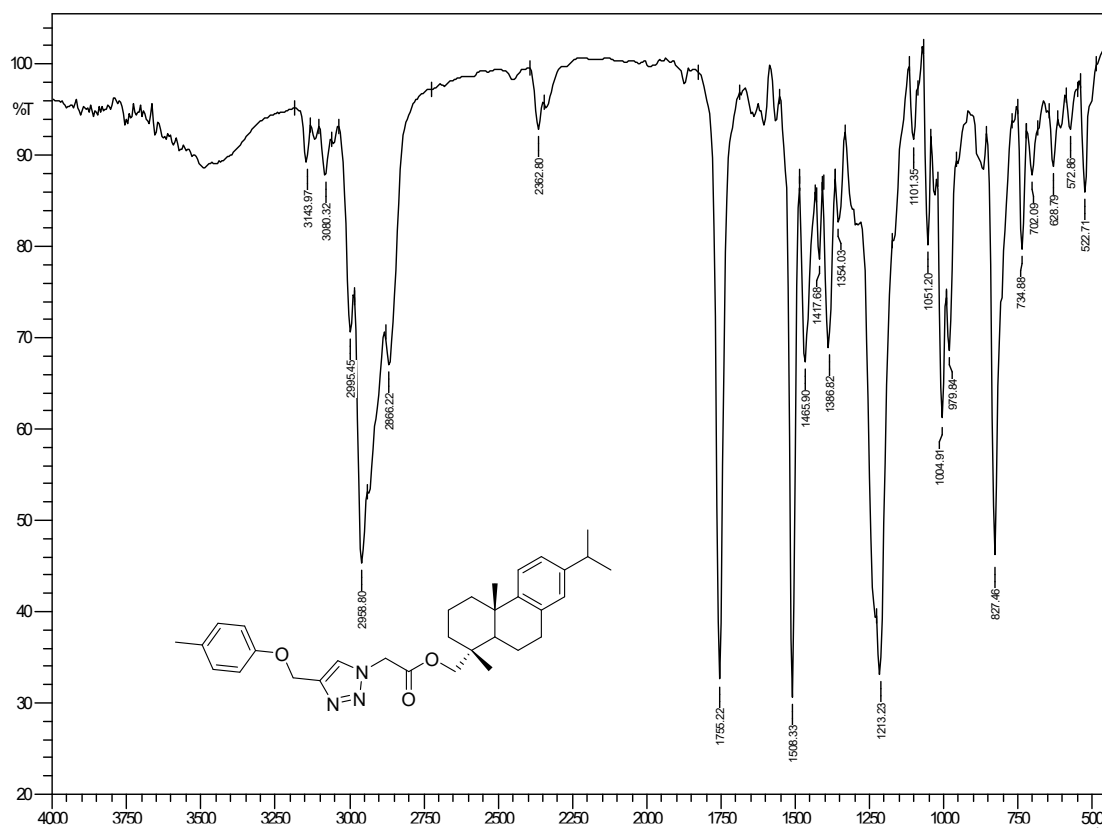


Figure S66 FTIR spectrum of the target compound **5o**

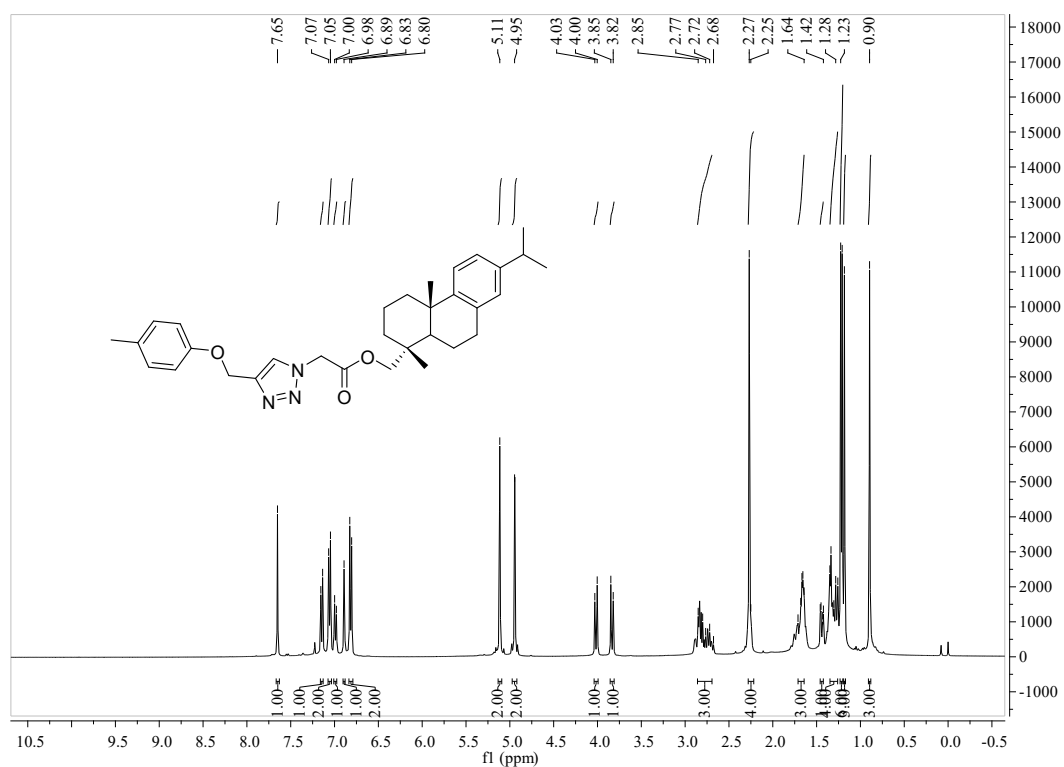


Figure S67 ¹H-NMR spectrum of the target compound **5o** in CDCl₃

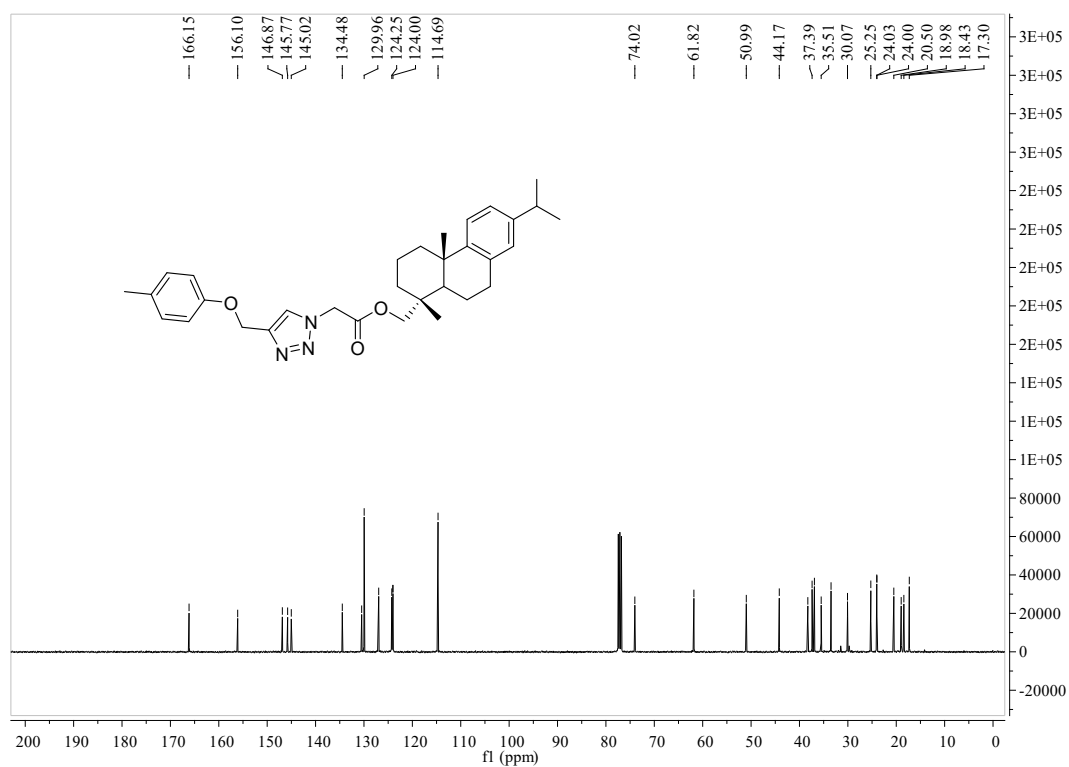


Figure S68 ¹³C-NMR spectrum of the target compound **5o** in CDCl₃

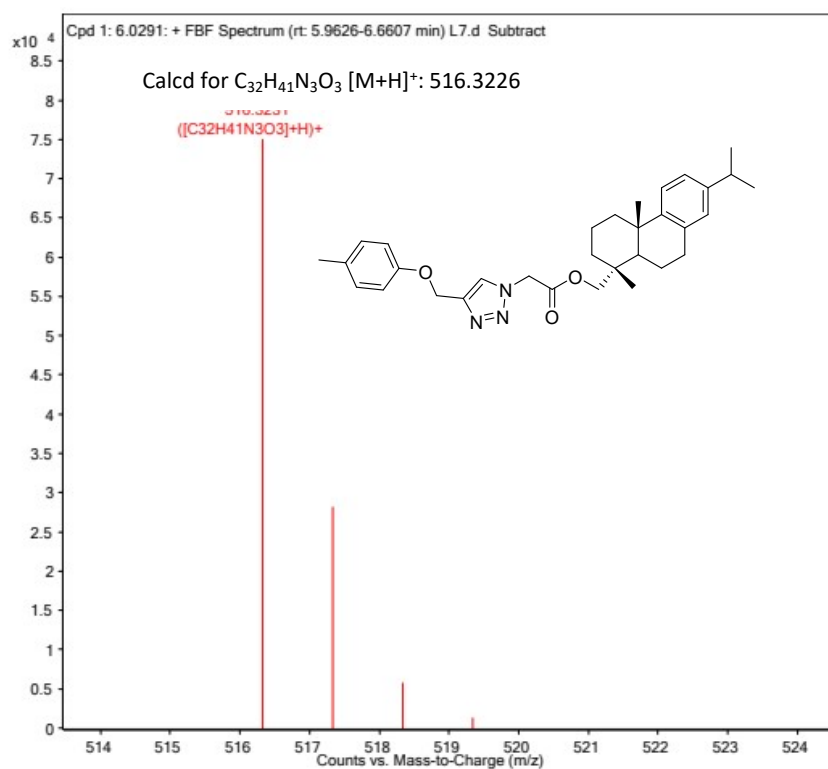


Figure S69 HRMS-ESI spectrum of the target compound **5o**

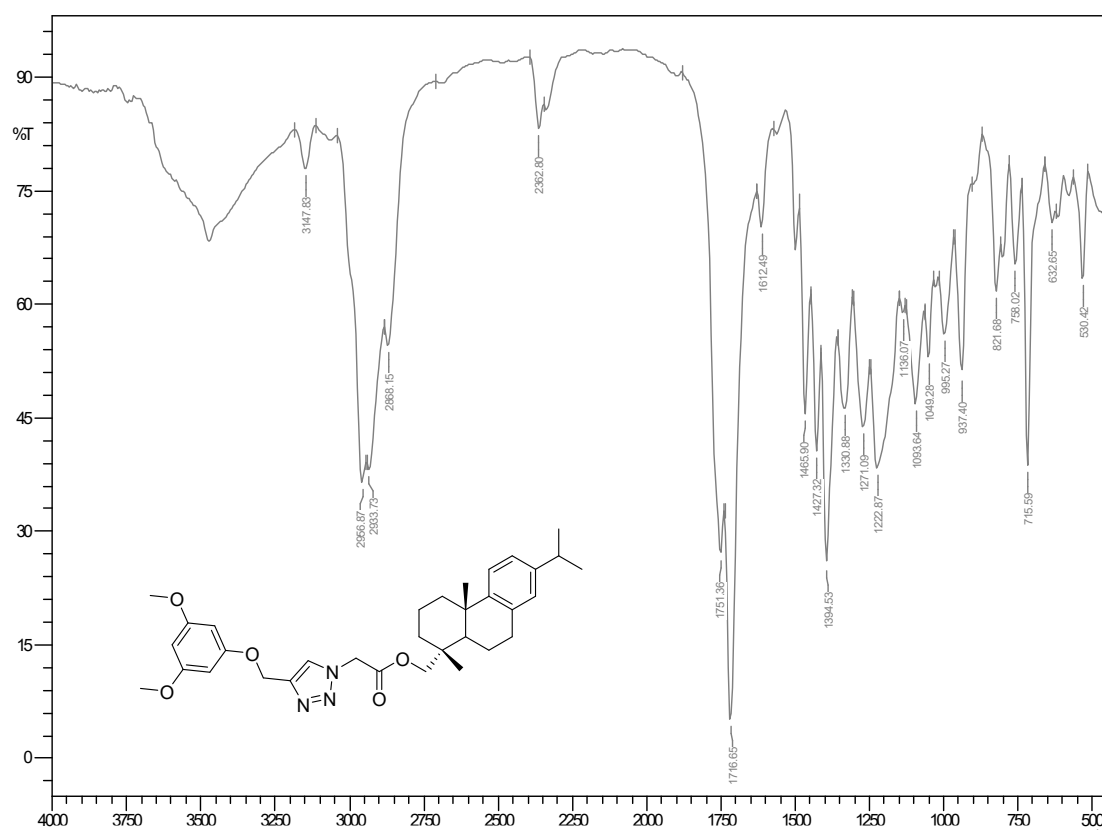


Figure S70 FTIR spectrum of the target compound **5p**

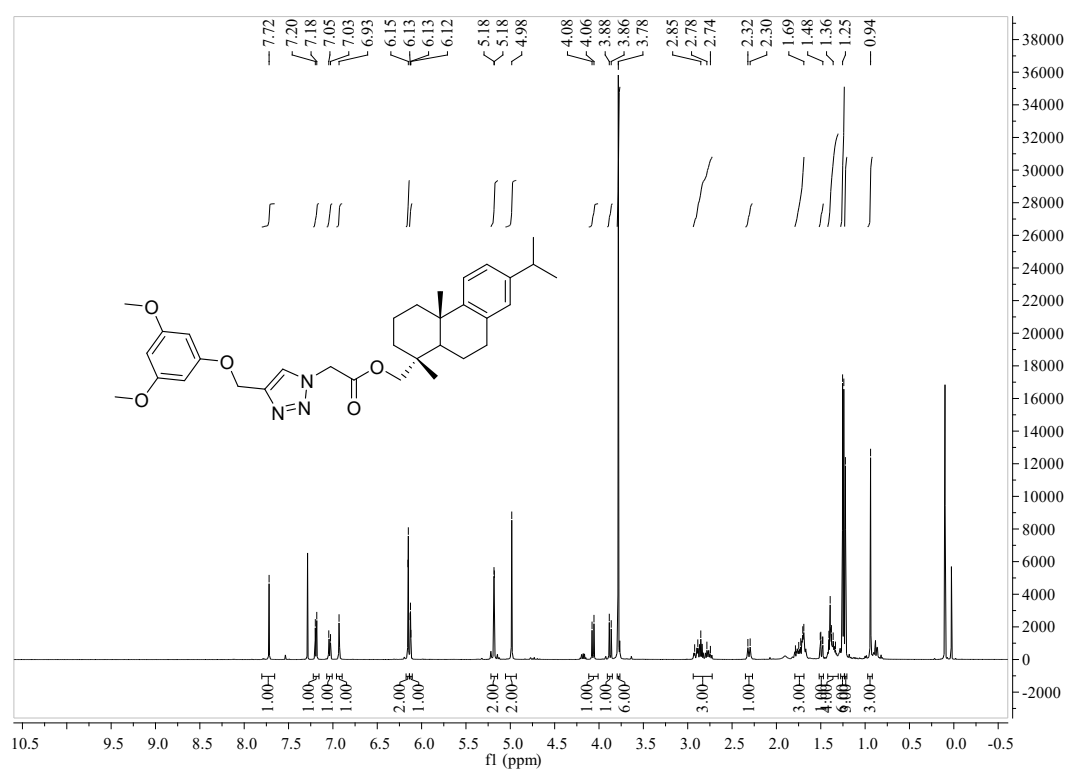


Figure S71 ¹H-NMR spectrum of the target compound **5p** in CDCl₃

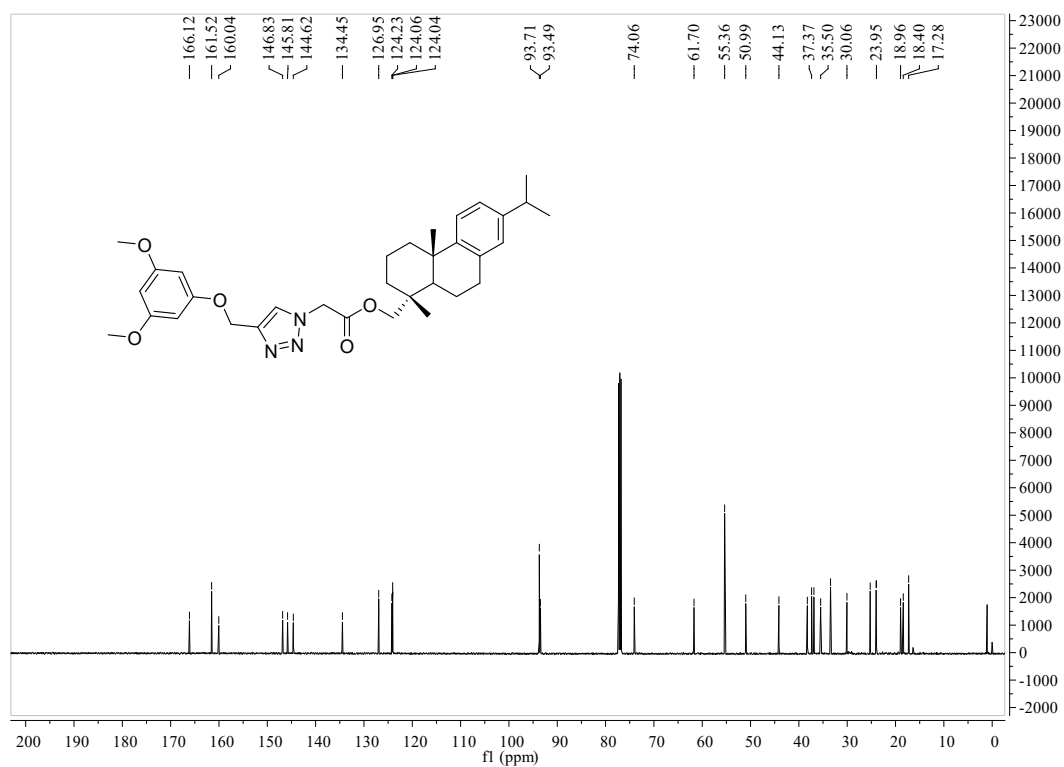


Figure S72 ^{13}C -NMR spectrum of the target compound **5p** in CDCl_3

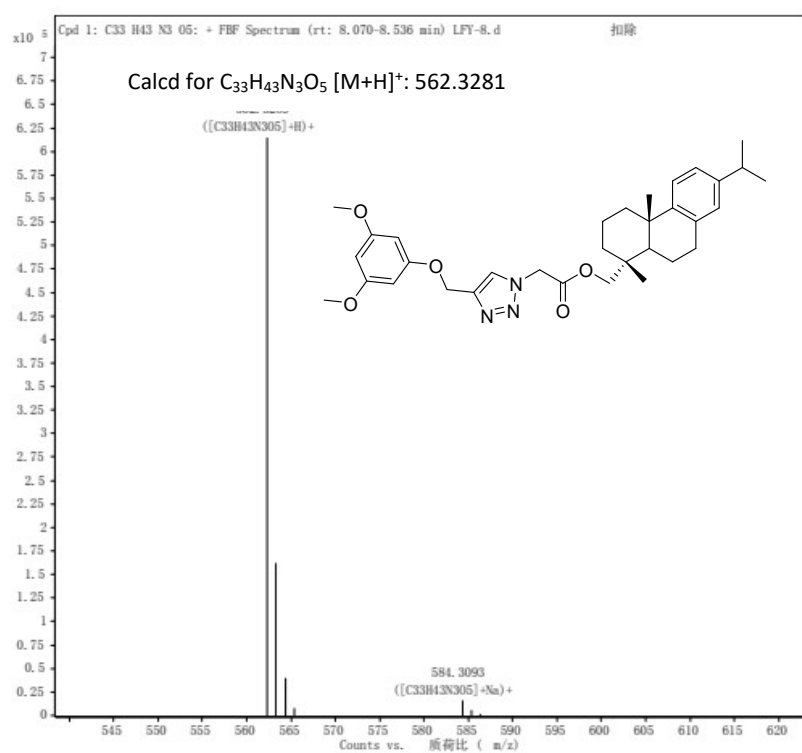


Figure S73 HRMS-ESI spectrum of the target compound **5p**

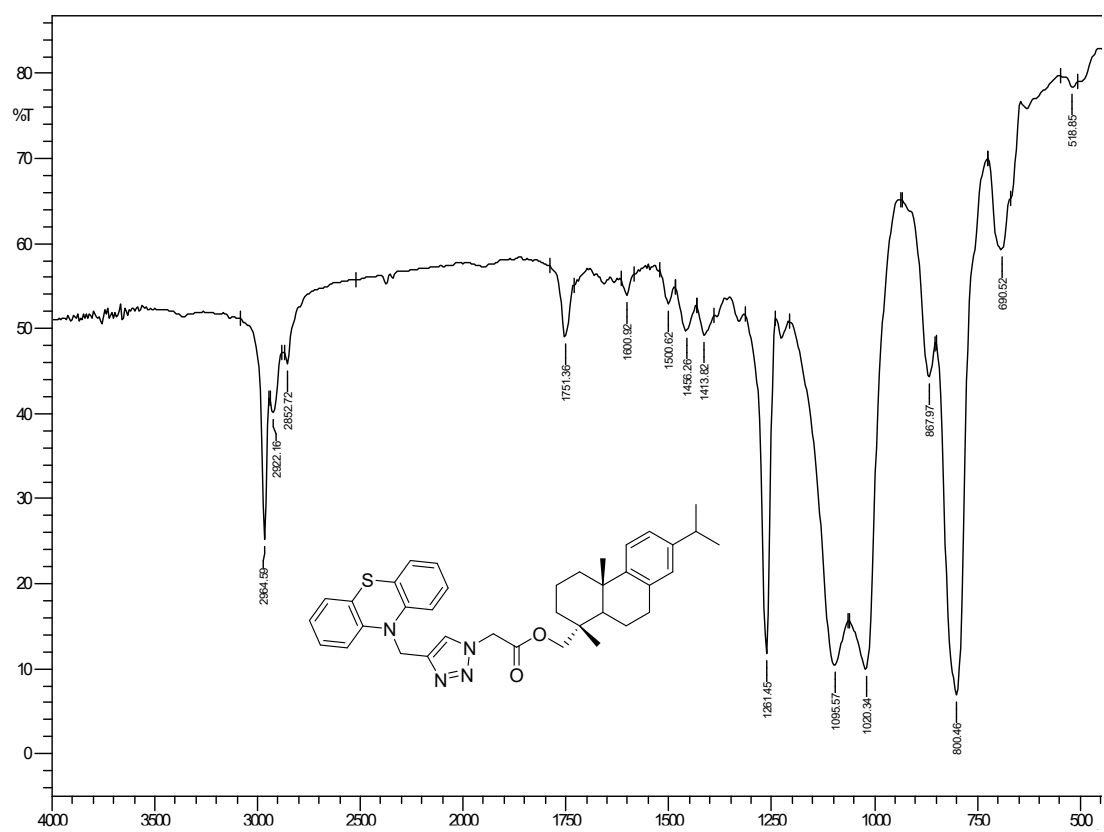


Figure S74 FTIR spectrum of the target compound **5q**

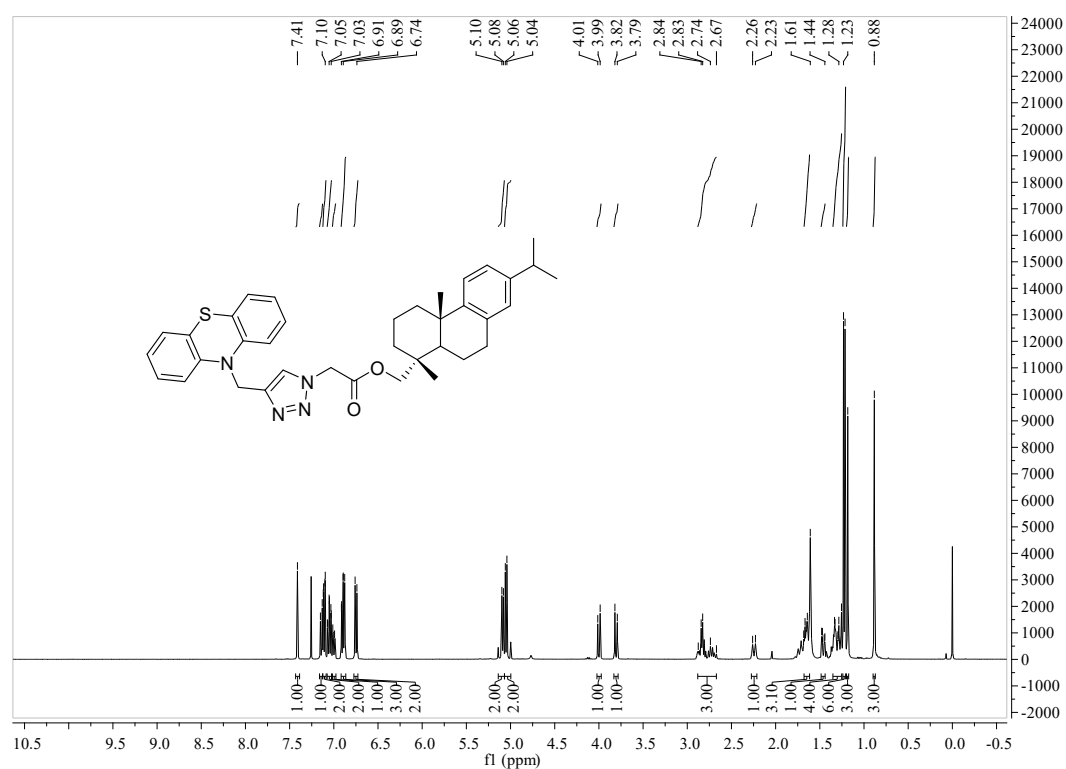


Figure S75 ¹H-NMR spectrum of the target compound **5q** in CDCl₃

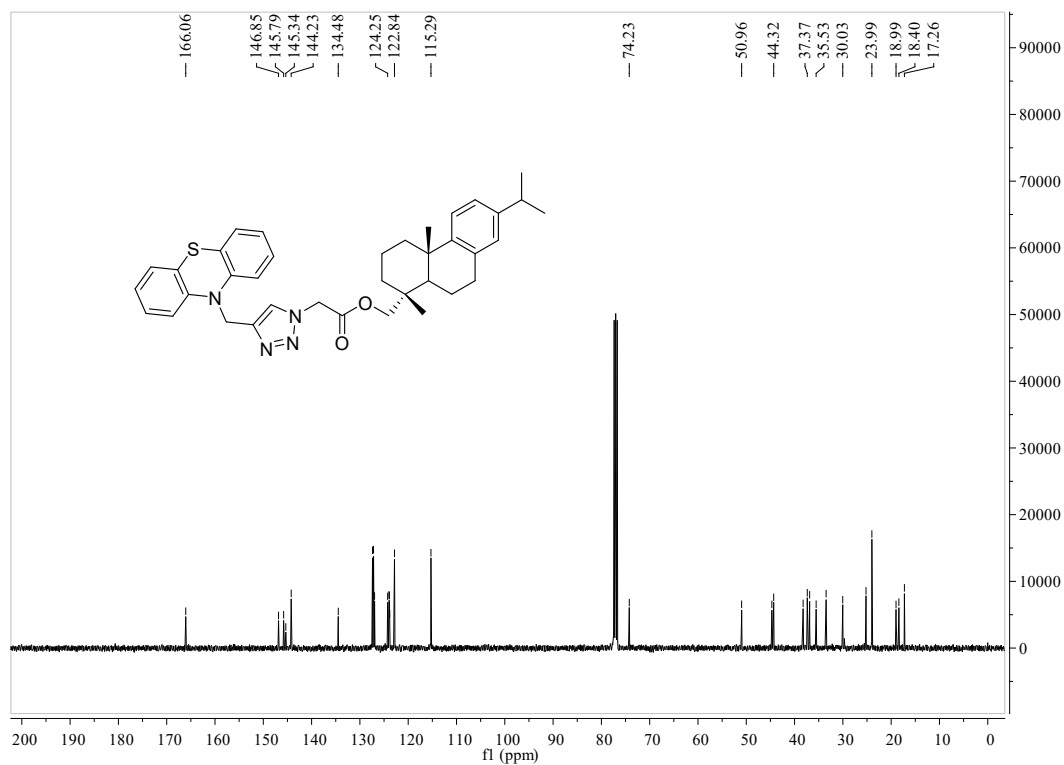


Figure S76 ^{13}C -NMR spectrum of the target compound **5q** in CDCl_3

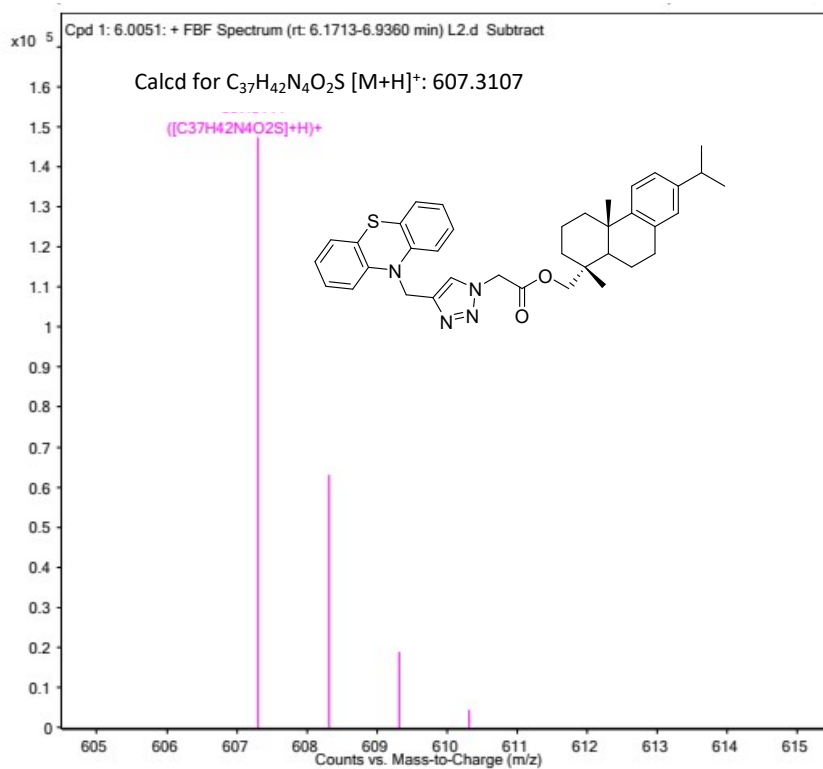


Figure S77 HRMS-ESI spectrum of the target compound **5q**

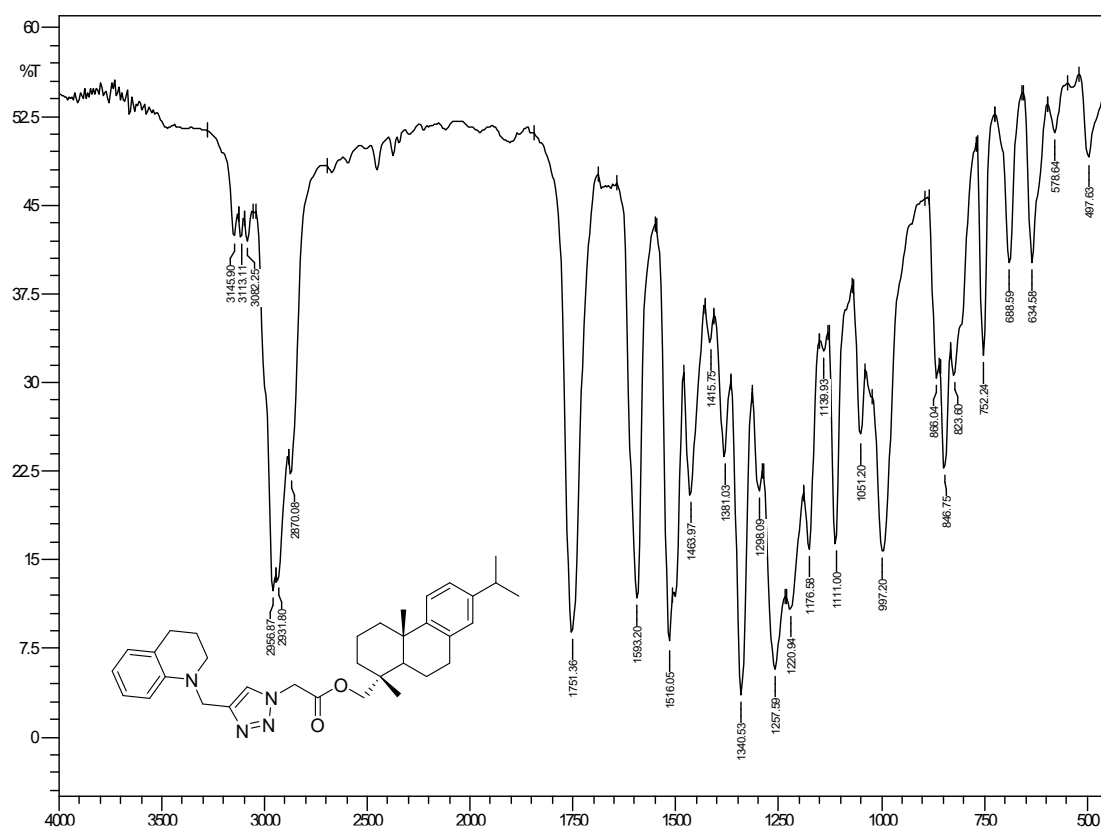


Figure S78 FTIR spectrum of the target compound **5r**

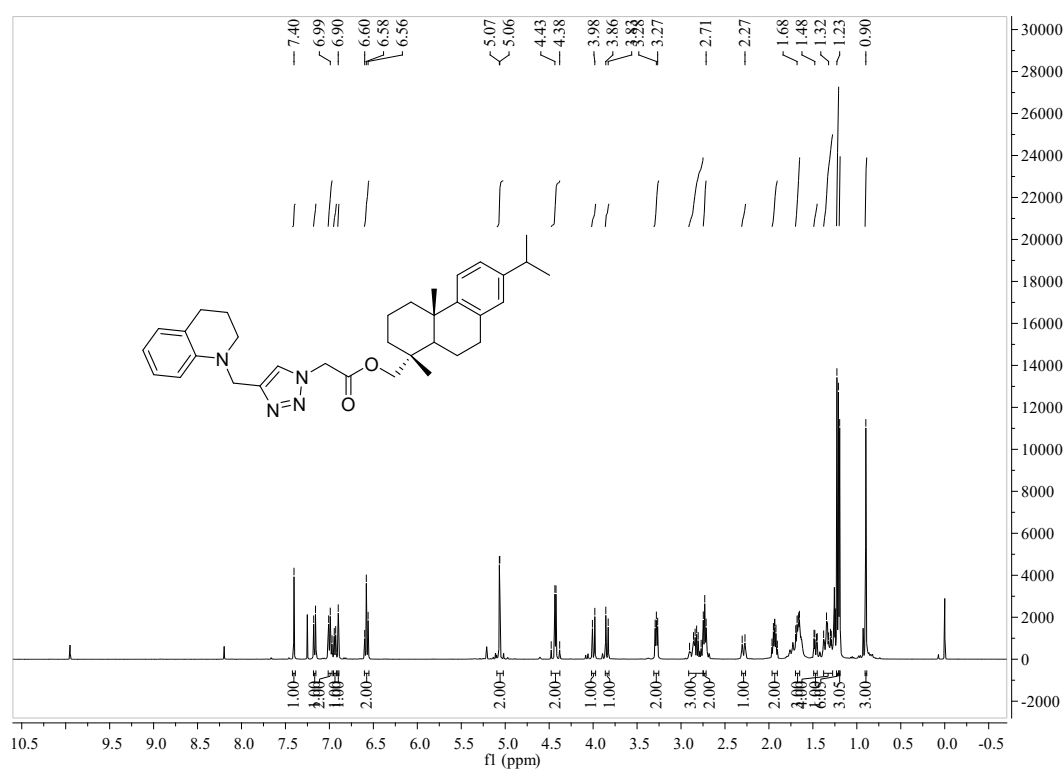


Figure S79 ¹H-NMR spectrum of the target compound **5r** in CDCl₃

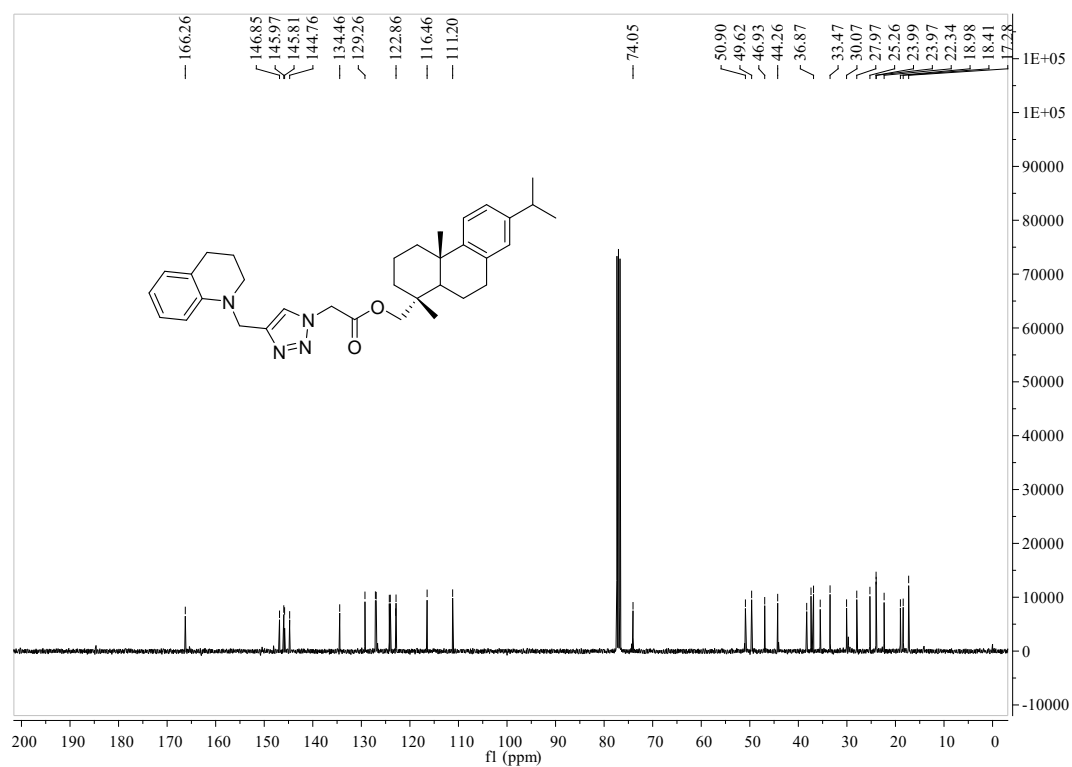


Figure S80 ^{13}C -NMR spectrum of the target compound **5r** in CDCl_3

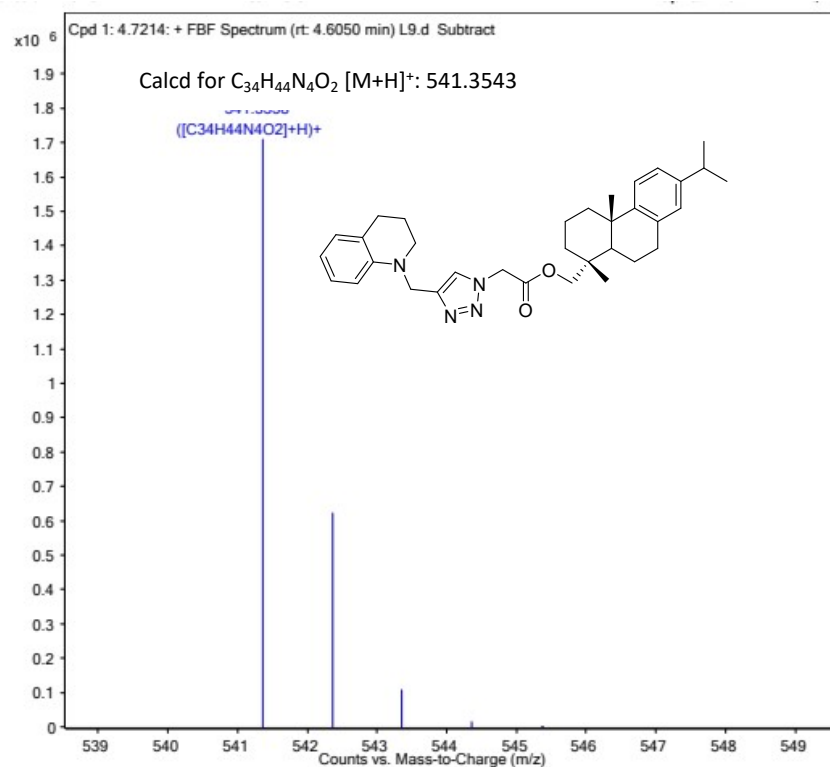


Figure S81 HRMS-ESI spectrum of the target compound **5r**

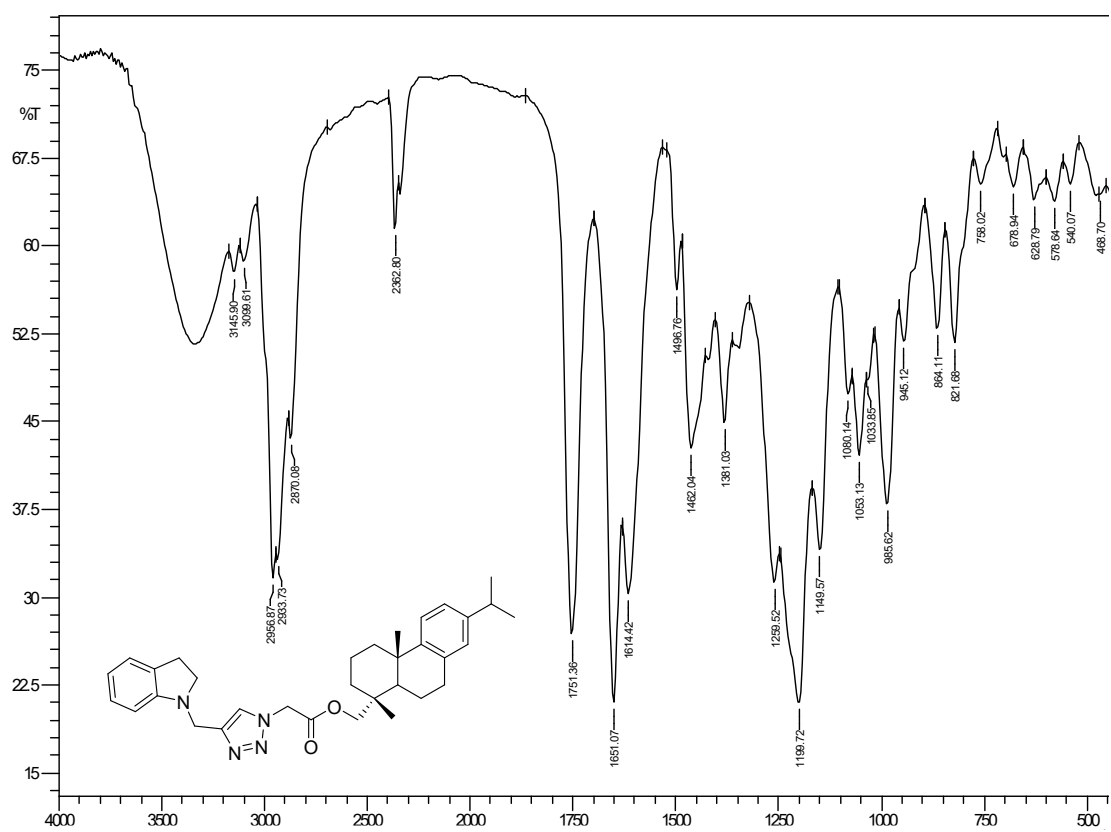


Figure S82 FTIR spectrum of the target compound **5s**

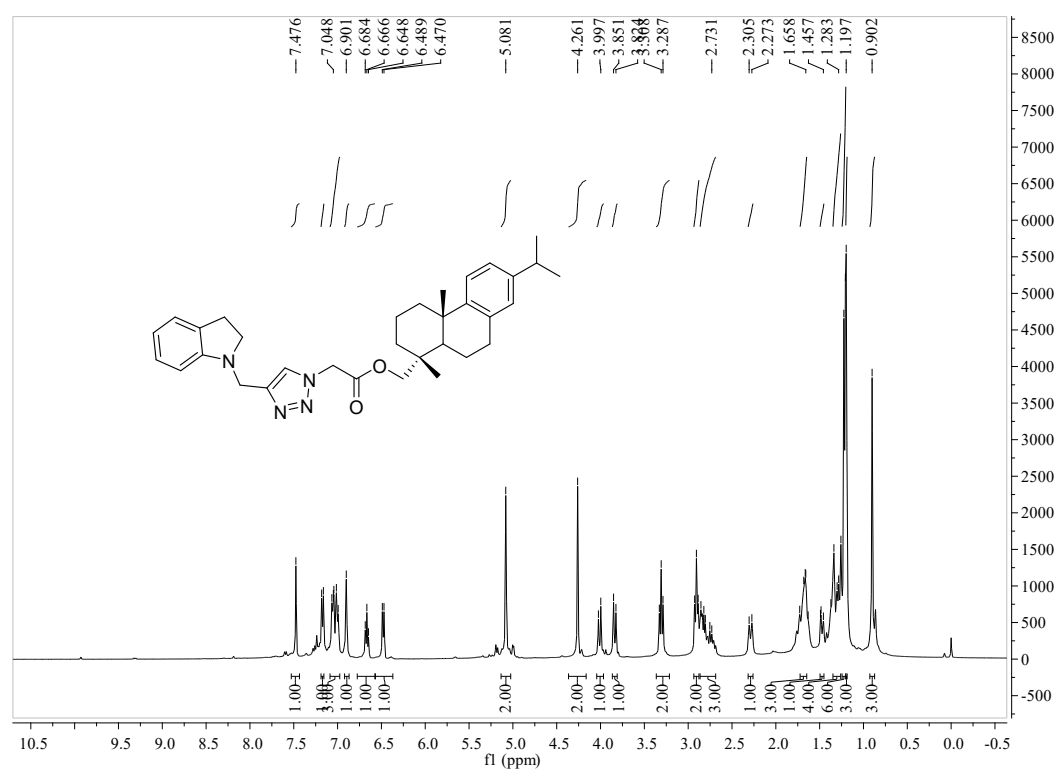


Figure S83 ¹H-NMR spectrum of the target compound **5s** in CDCl₃

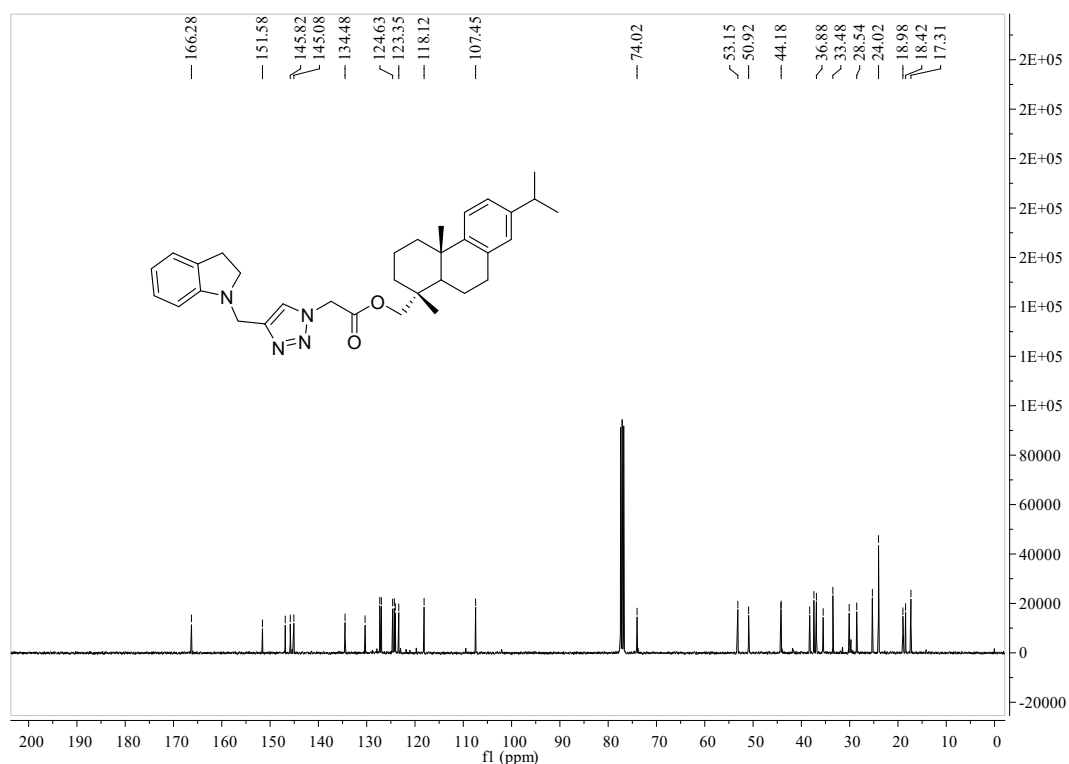


Figure S84 ¹³C-NMR spectrum of the target compound **5s** in CDCl₃

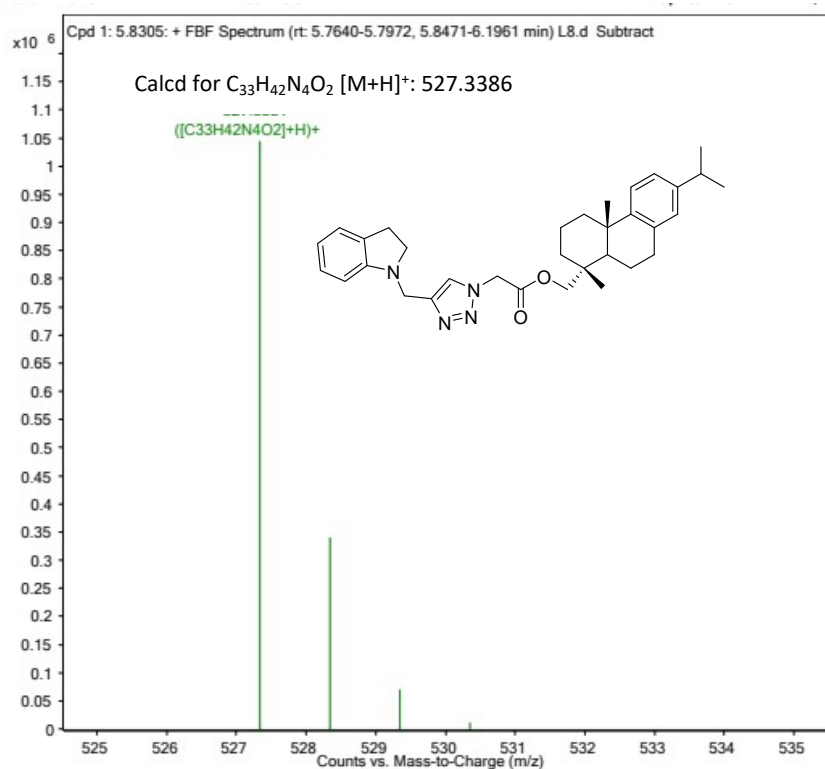


Figure S85 HRMS-ESI spectrum of the target compound **5s**

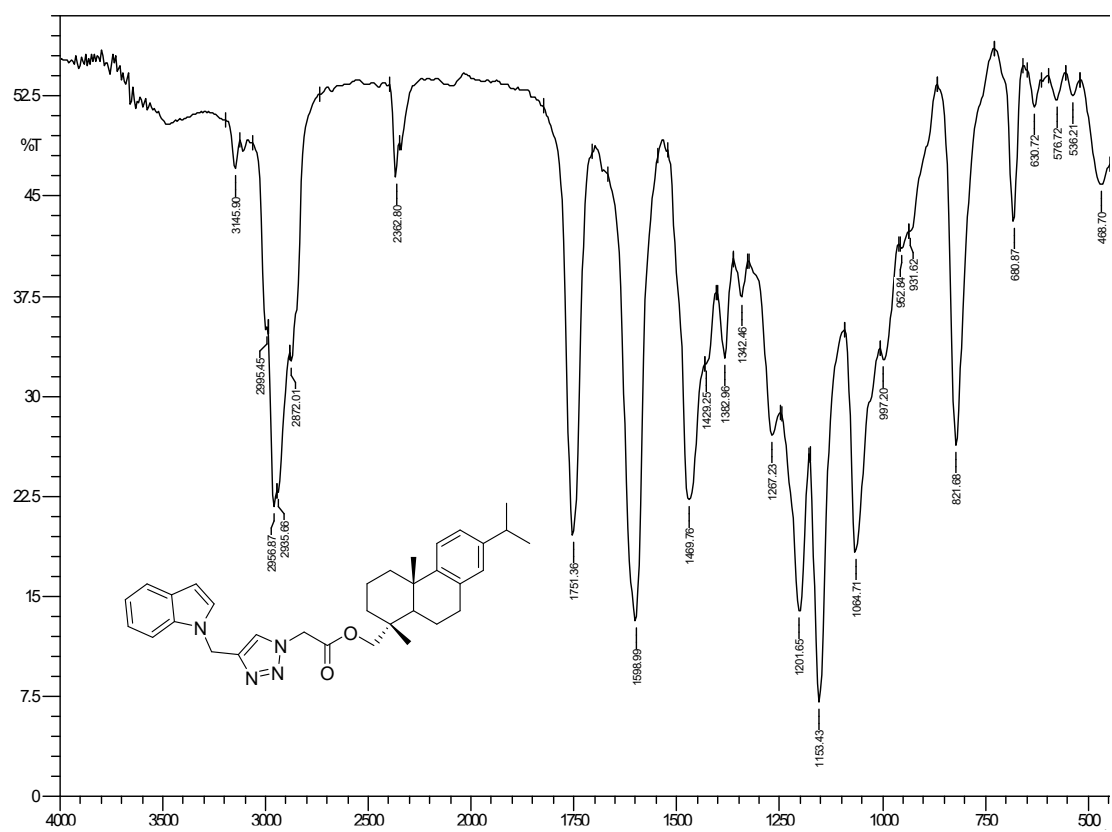


Figure S86 FTIR spectrum of the target compound **5t**

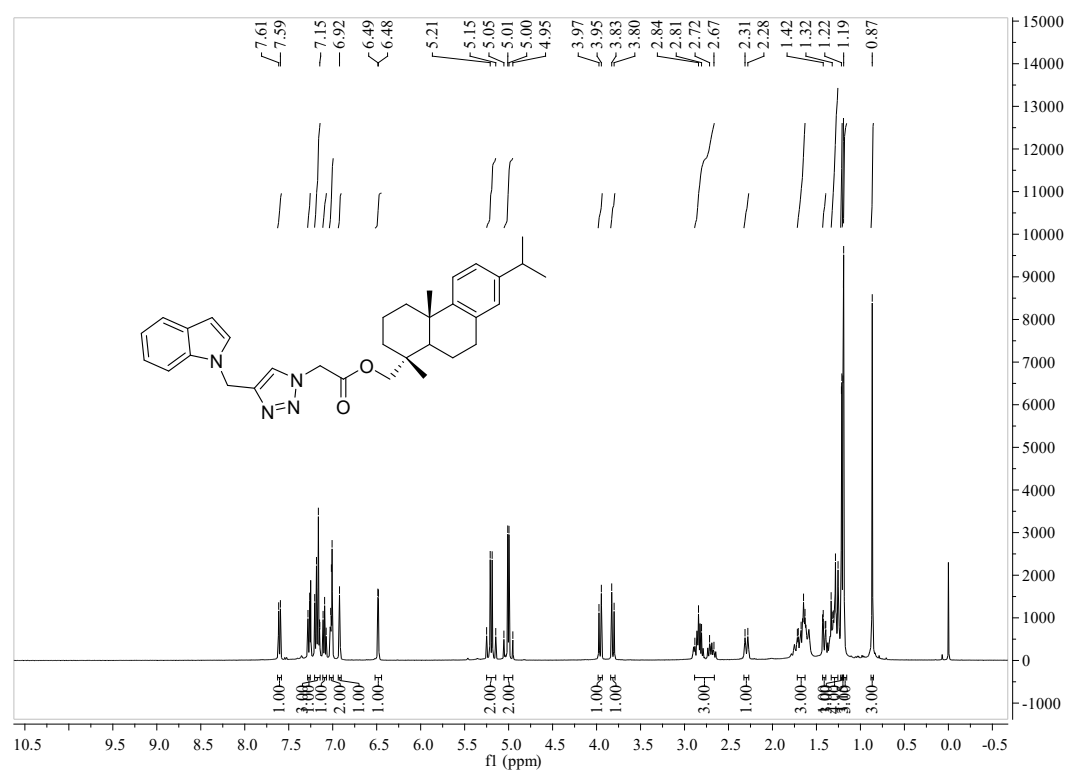


Figure S87 ¹H-NMR spectrum of the target compound **5t** in CDCl₃

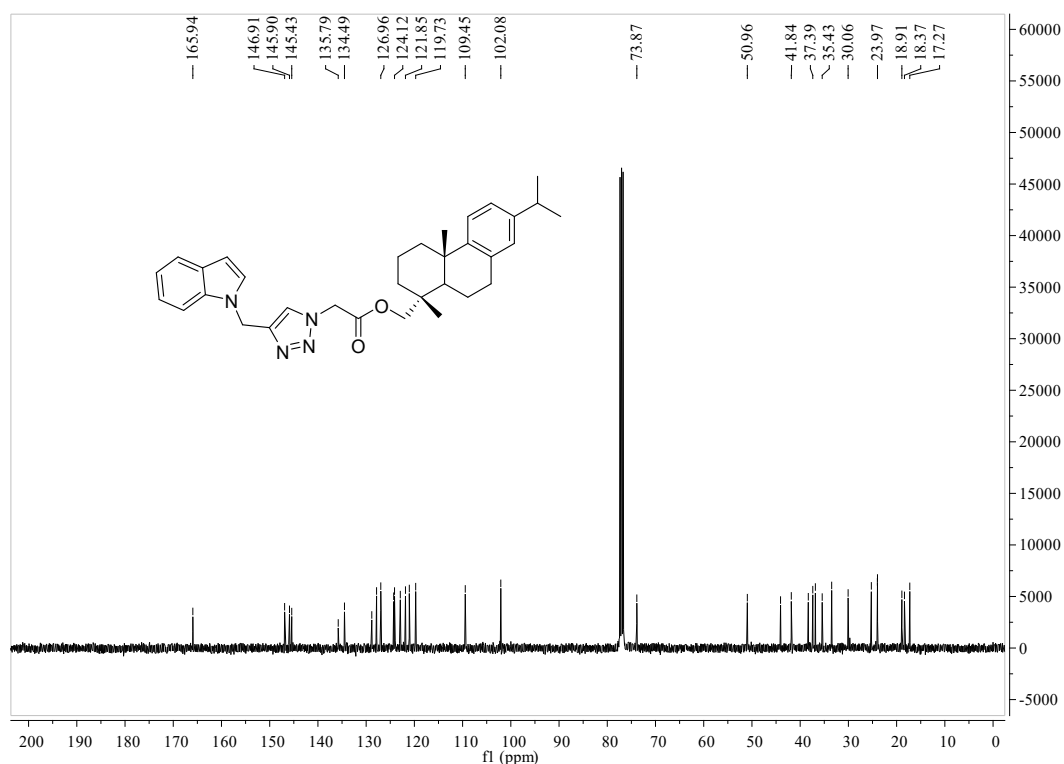


Figure S88 ^{13}C -NMR spectrum of the target compound **5t** in CDCl_3

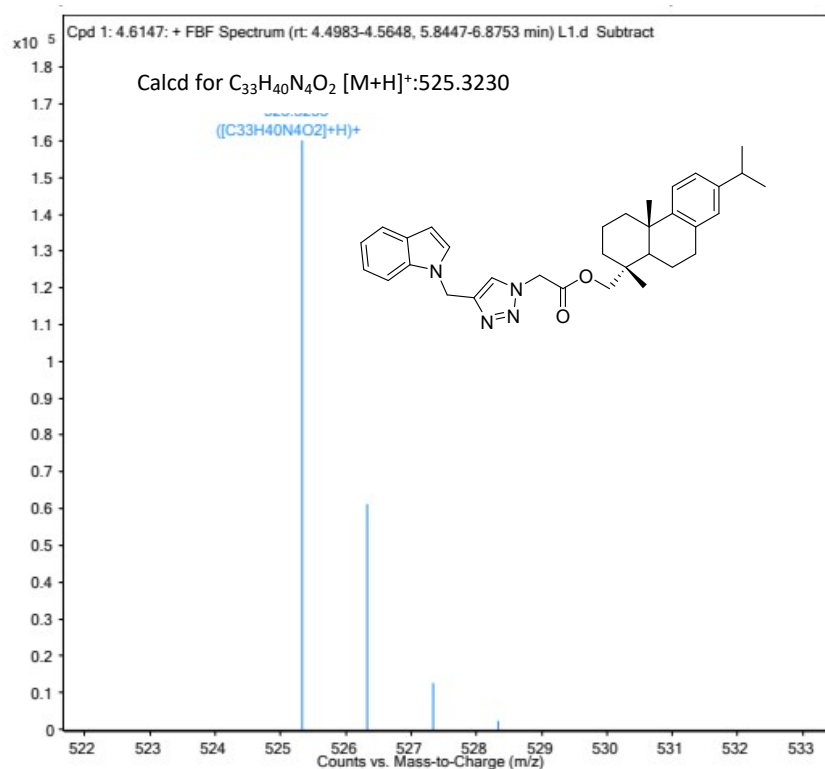


Figure S89 HRMS-ESI spectrum of the target compound **5t**

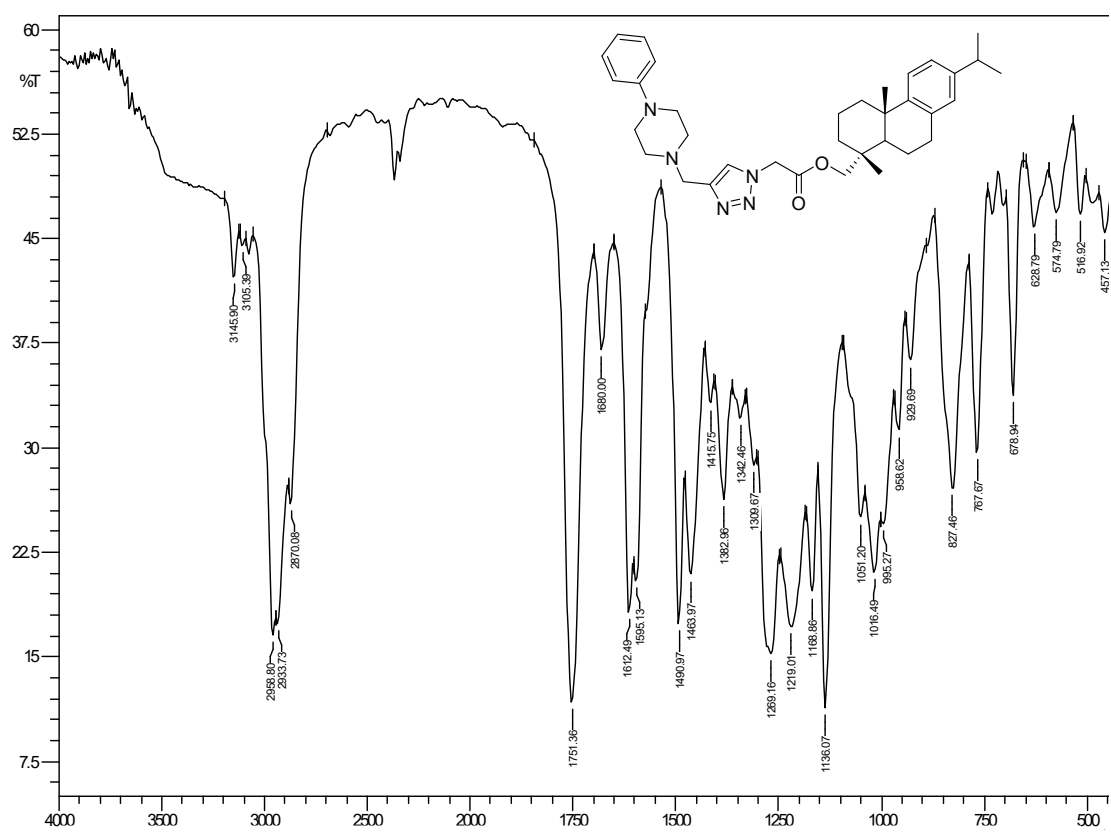


Figure S90. FTIR spectrum of the target compound **5u**

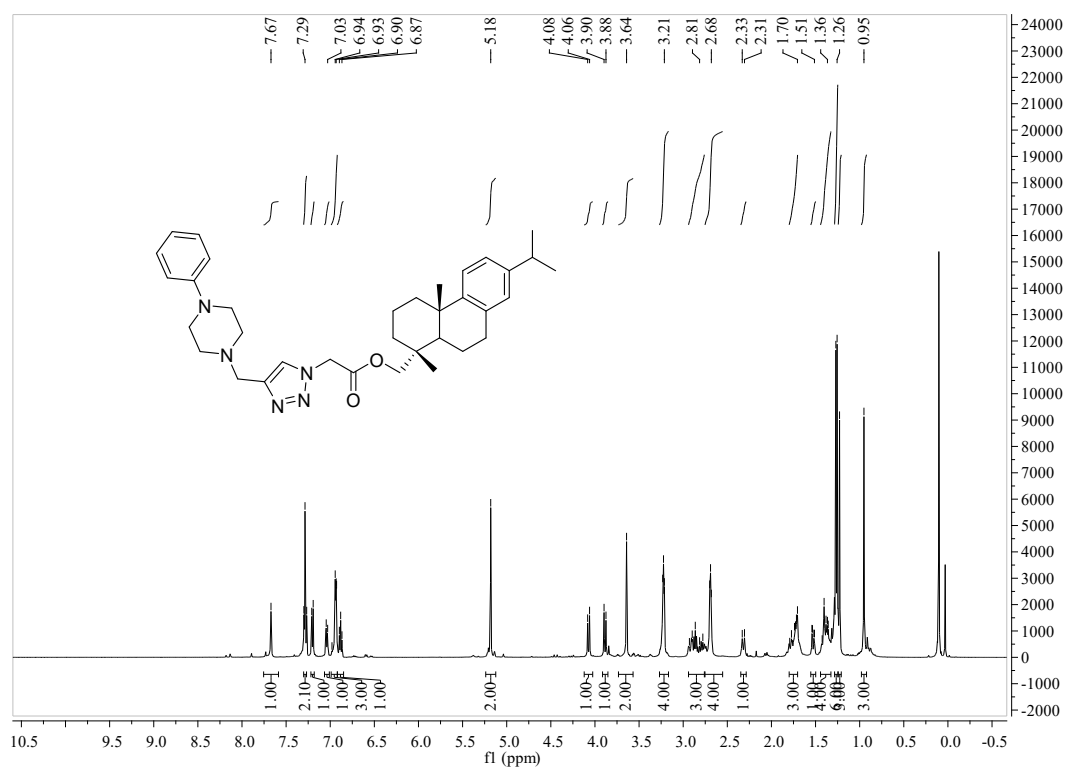


Figure S91 ¹H-NMR spectrum of the target compound **5u** in CDCl₃

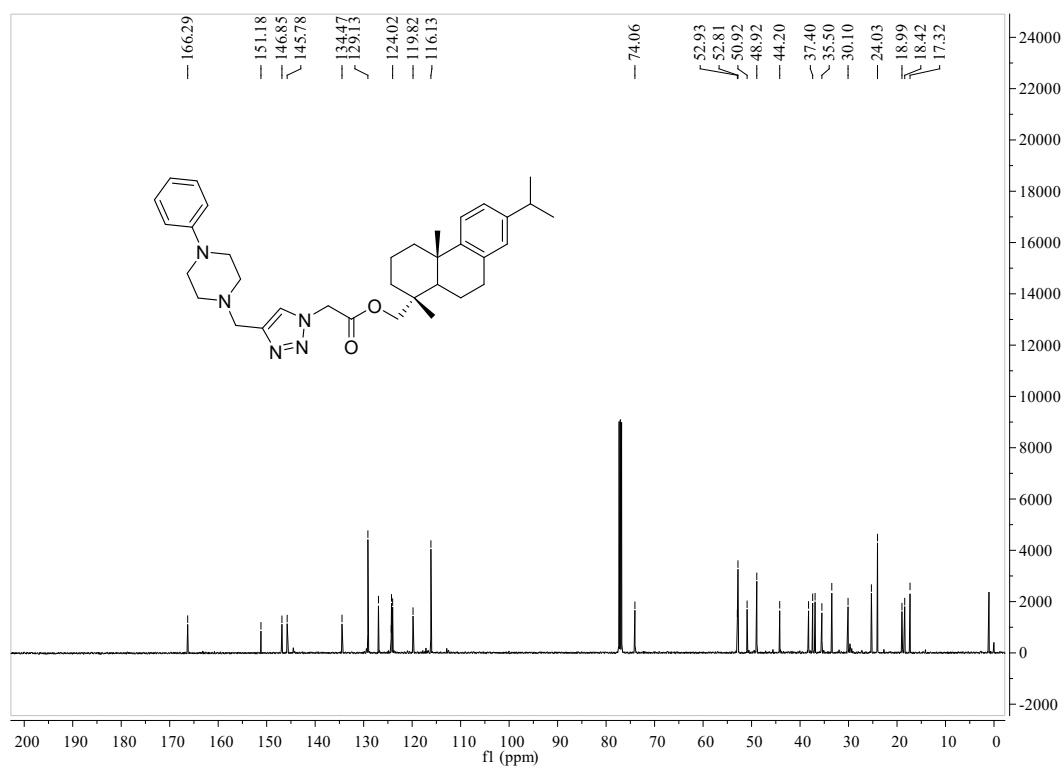


Figure S92 ^{13}C -NMR spectrum of the target compound **5u** in CDCl_3

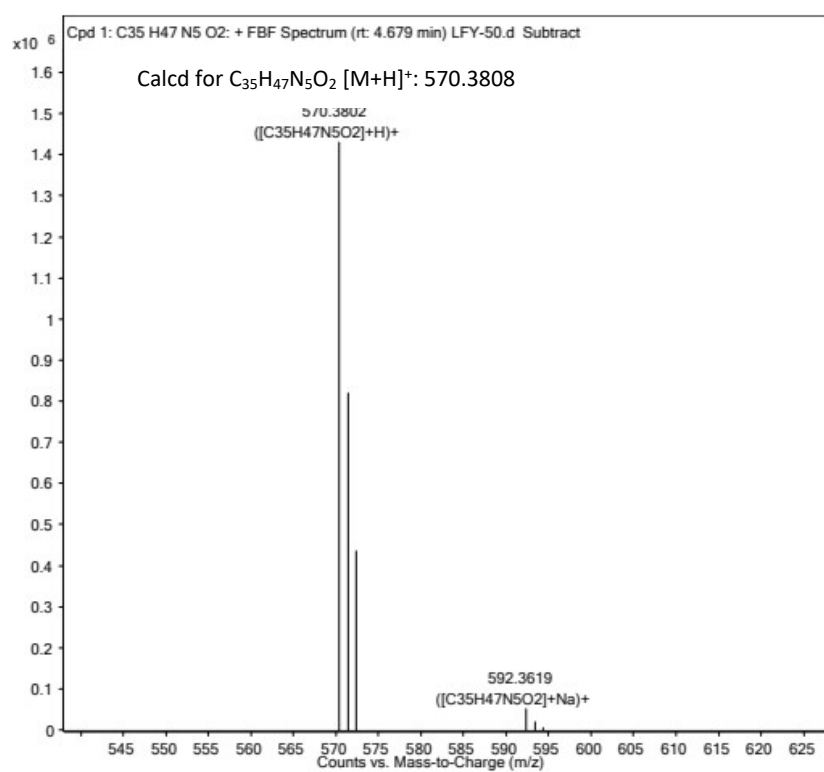


Figure S93 HRMS-ESI spectrum of the target compound **5u**

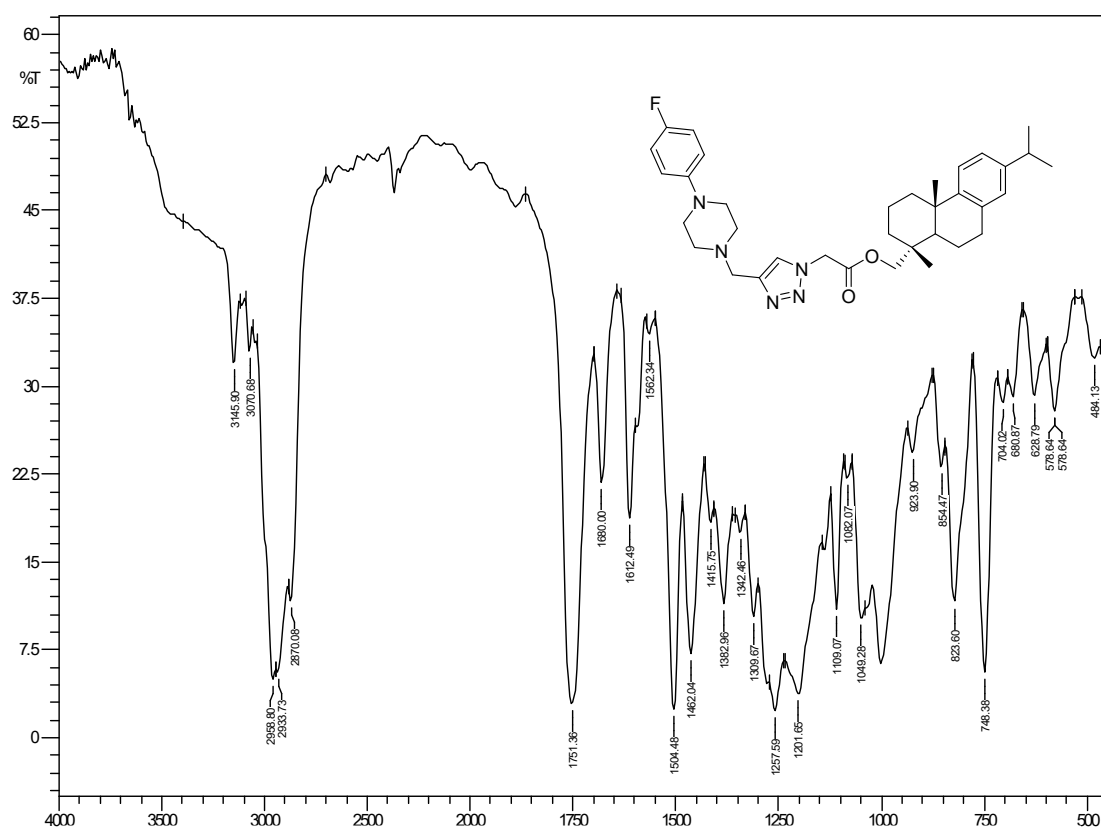


Figure S94. FTIR spectrum of the target compound **5v**

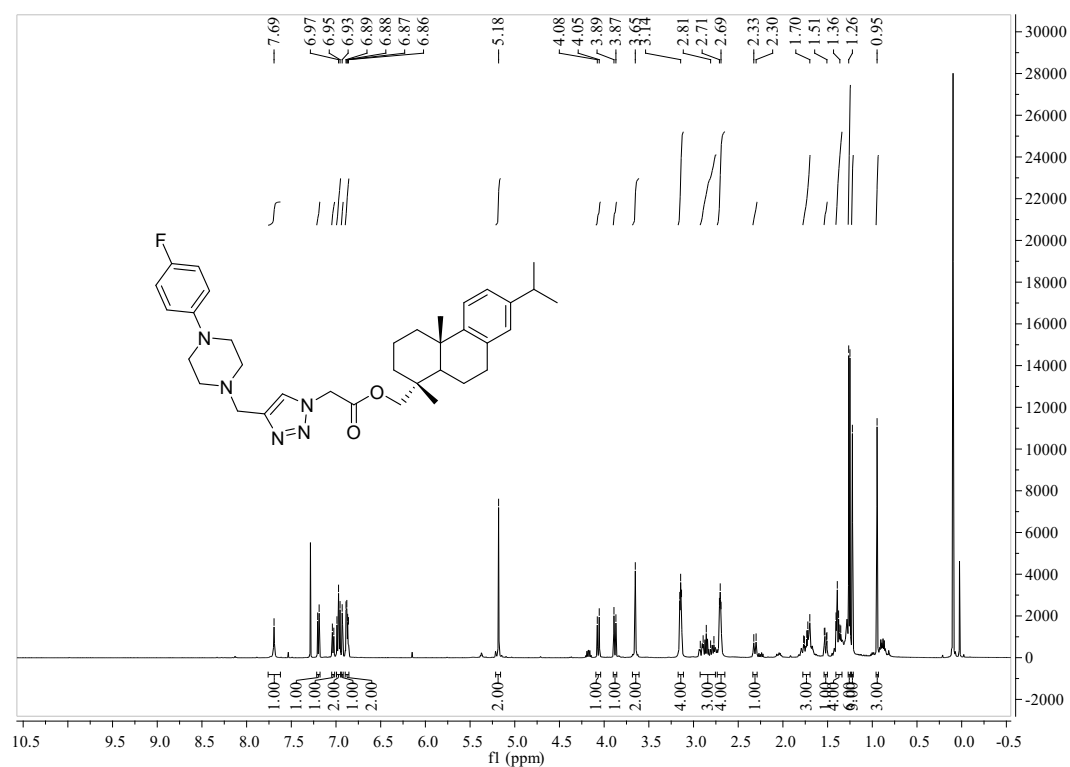


Figure S95 ¹H-NMR spectrum of the target compound **5v** in CDCl₃

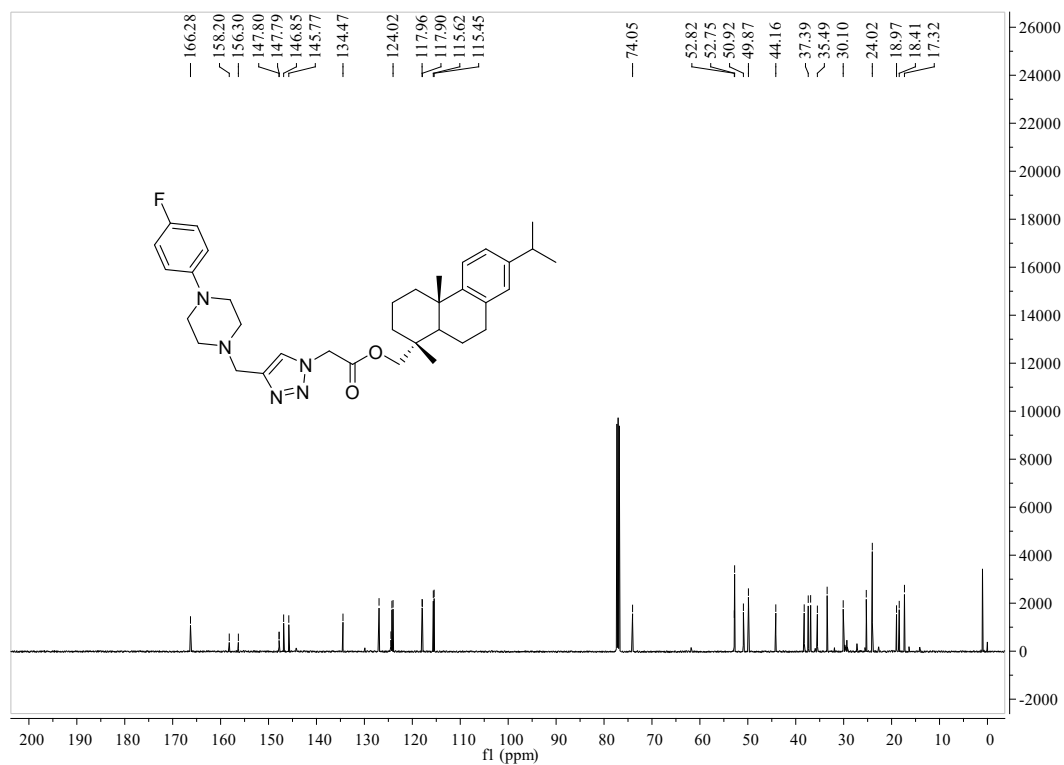


Figure S96 ¹³C-NMR spectrum of the target compound **5v** in CDCl₃

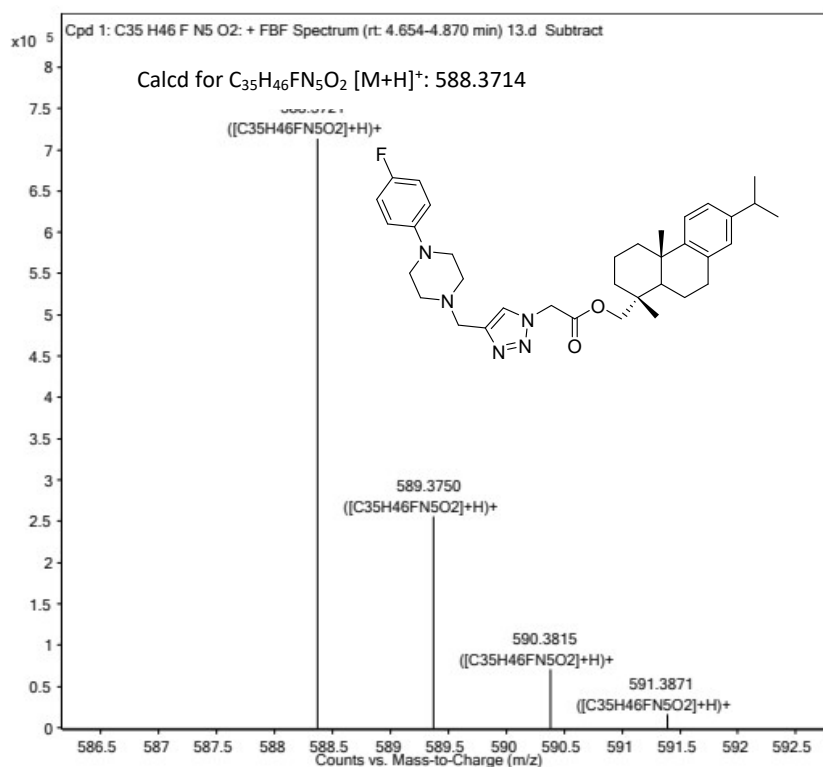


Figure S97 HRMS-ESI spectrum of the target compound **5v**

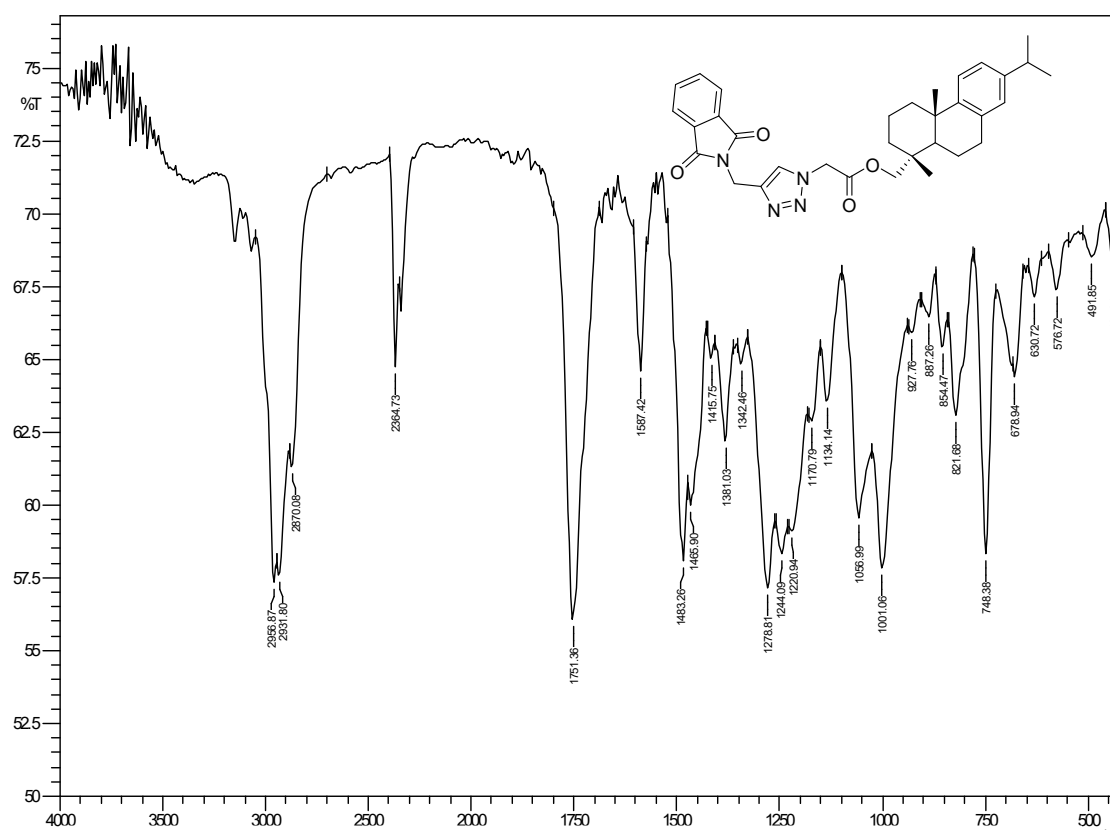


Figure S98. FTIR spectrum of the target compound **5w**

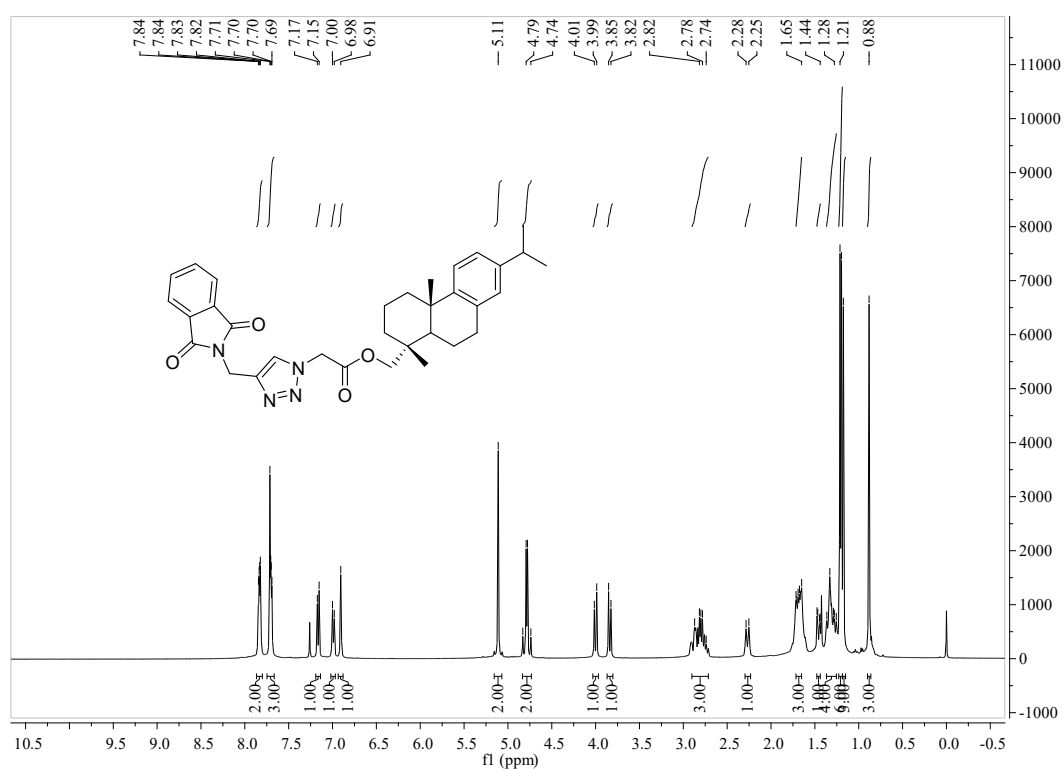


Figure S99 ¹H-NMR spectrum of the target compound **5w** in CDCl₃

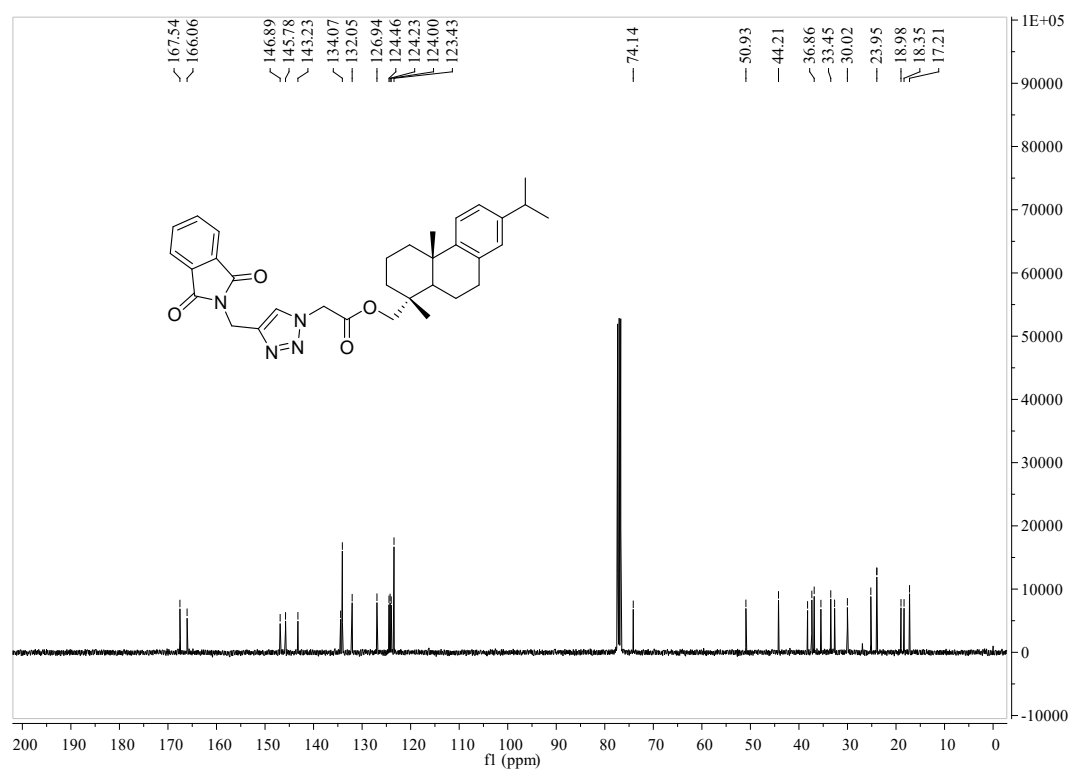


Figure S100 ^{13}C -NMR spectrum of the target compound **5w** in CDCl_3

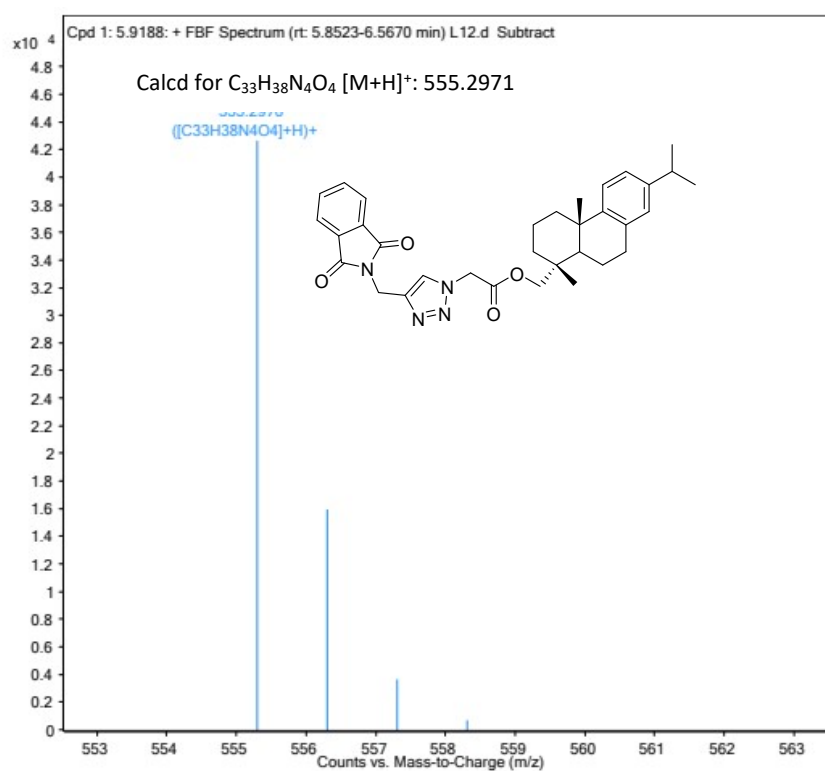


Figure S101 HRMS-ESI spectrum of the target compound **5w**

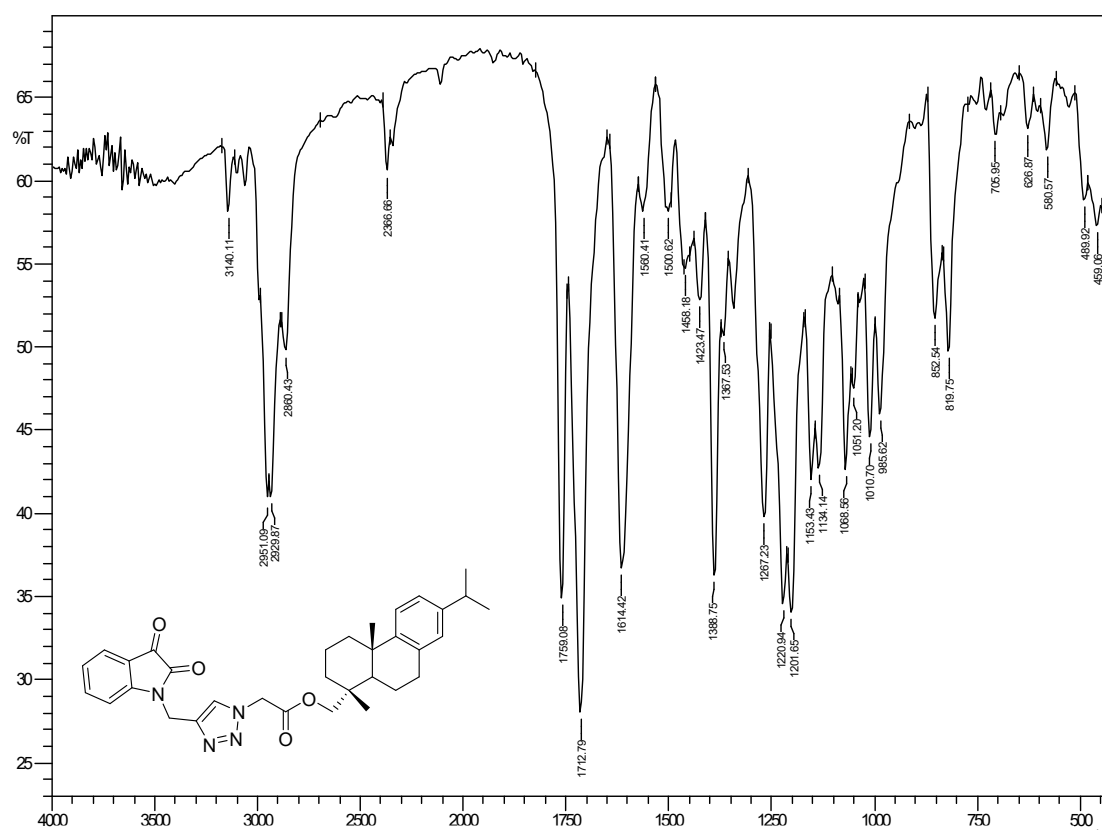


Figure S102. FTIR spectrum of the target compound **5x**

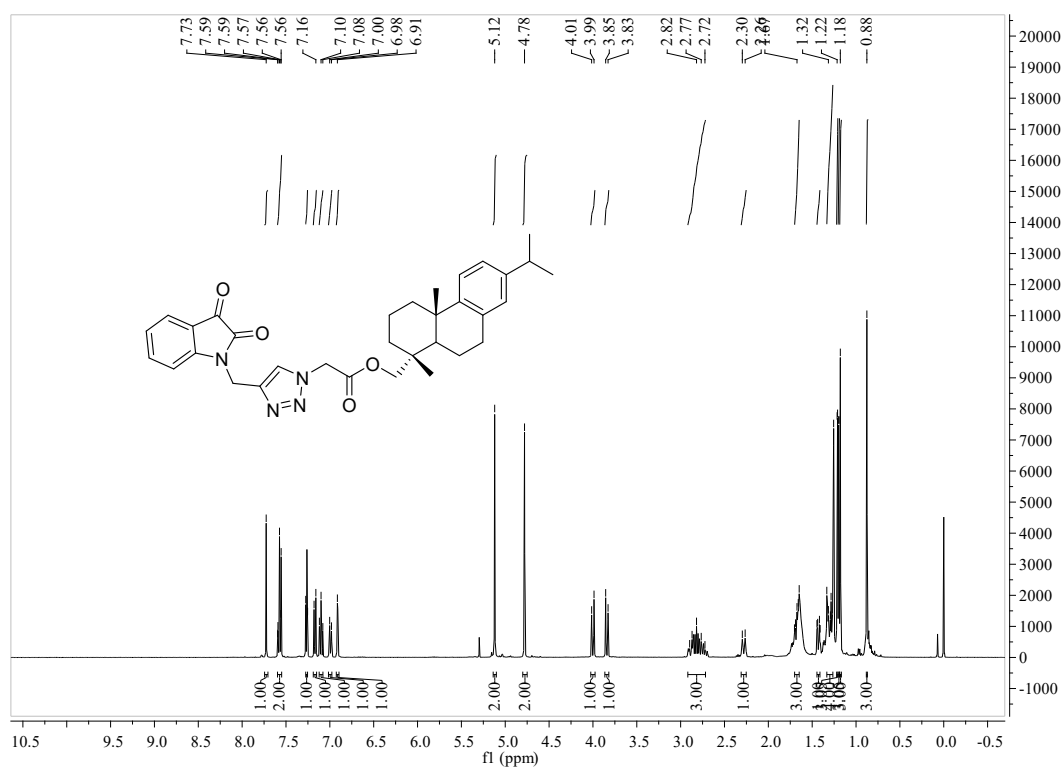


Figure S103 ¹H-NMR spectrum of the target compound **5x** in CDCl₃

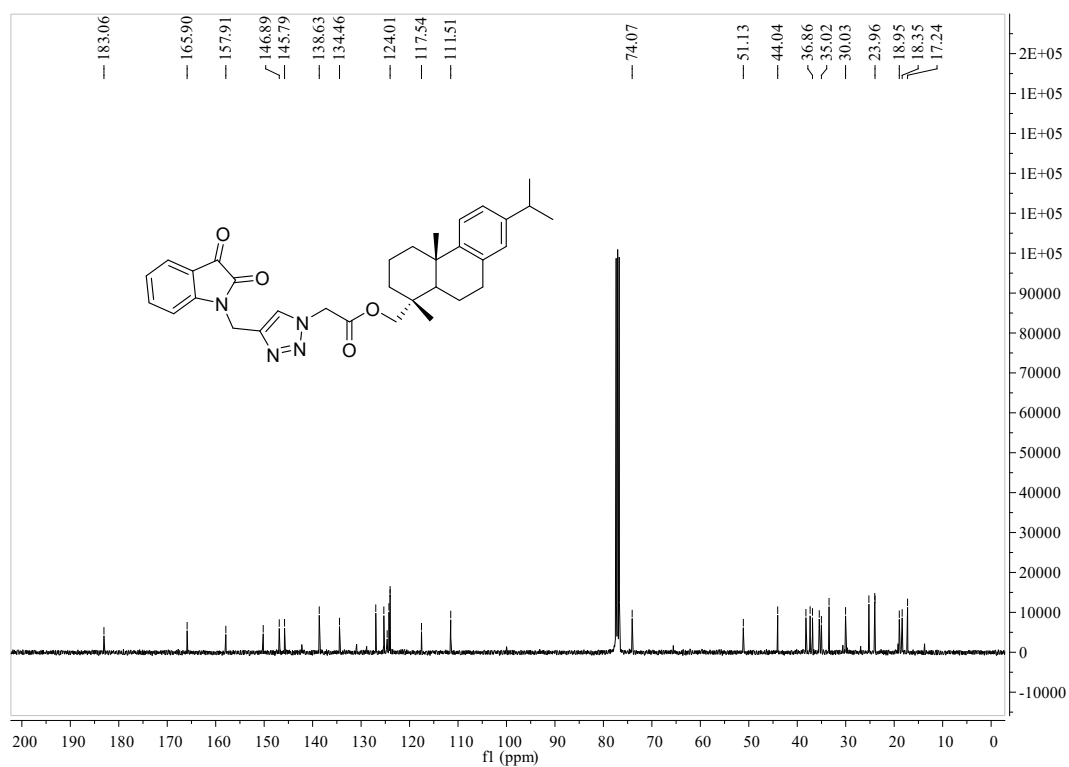


Figure S104 ^{13}C -NMR spectrum of the target compound **5x** in CDCl_3

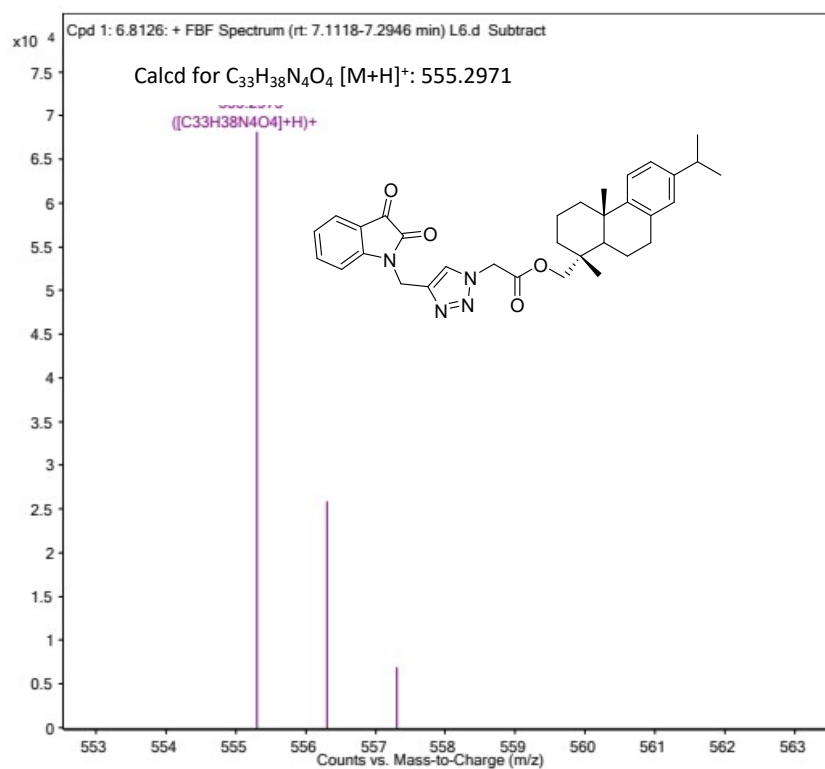


Figure S105 HRMS-ESI spectrum of the target compound **5x**

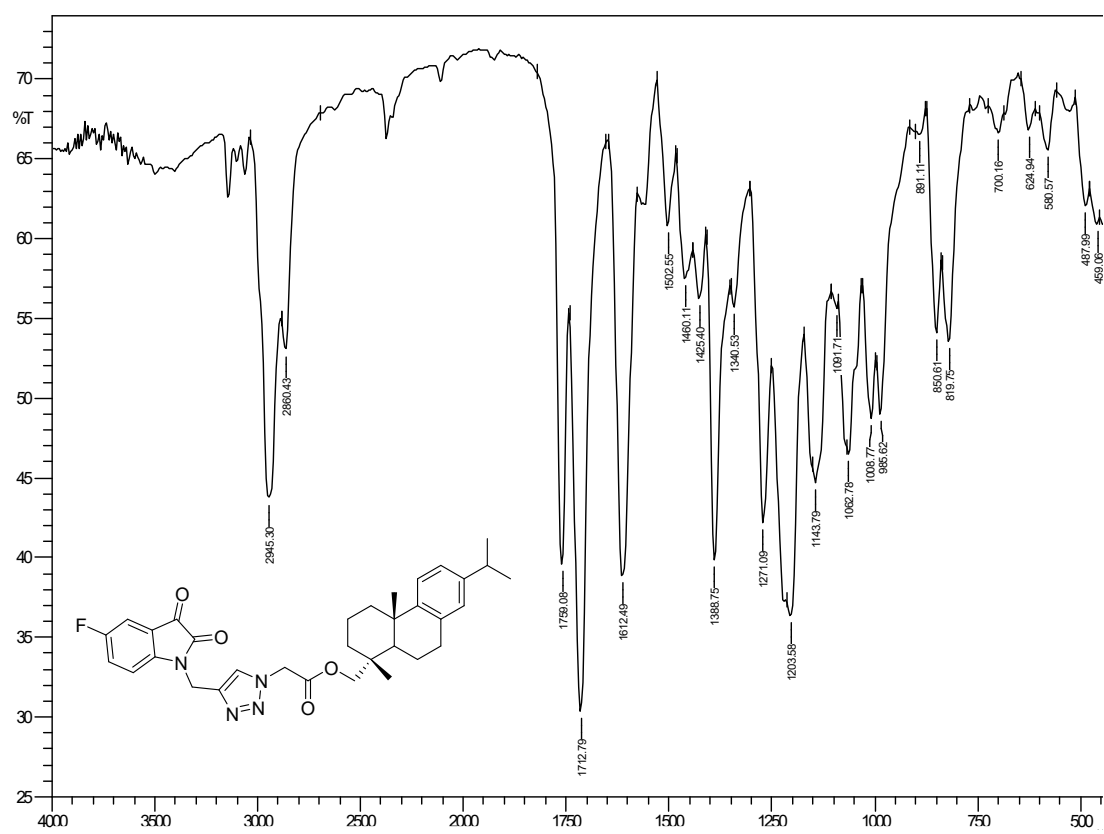


Figure S106. FTIR spectrum of the target compound **5x**

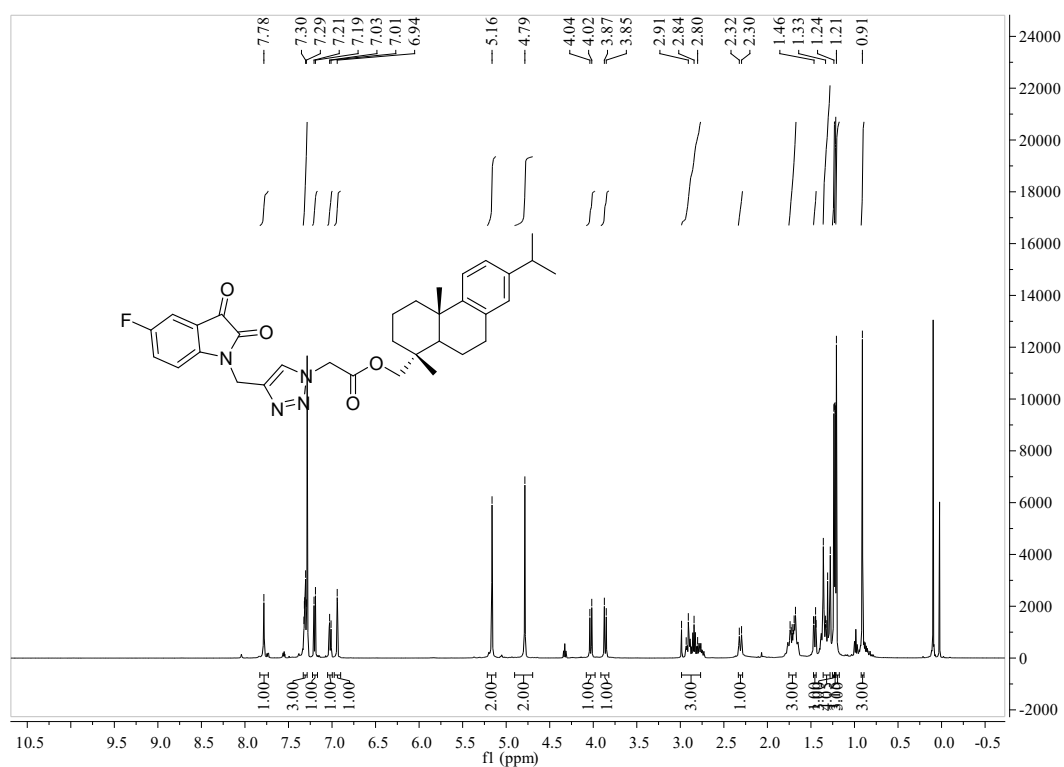


Figure S107 ¹H-NMR spectrum of the target compound **5y** in CDCl₃

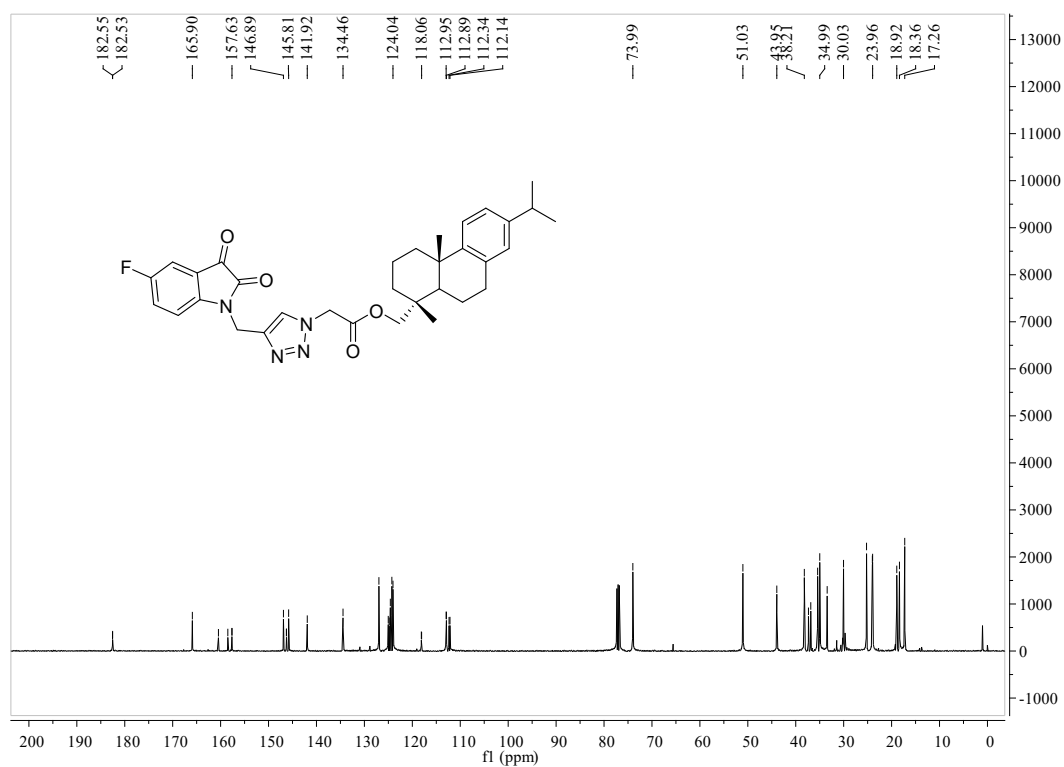


Figure S108 ^{13}C -NMR spectrum of the target compound **5y** in CDCl_3

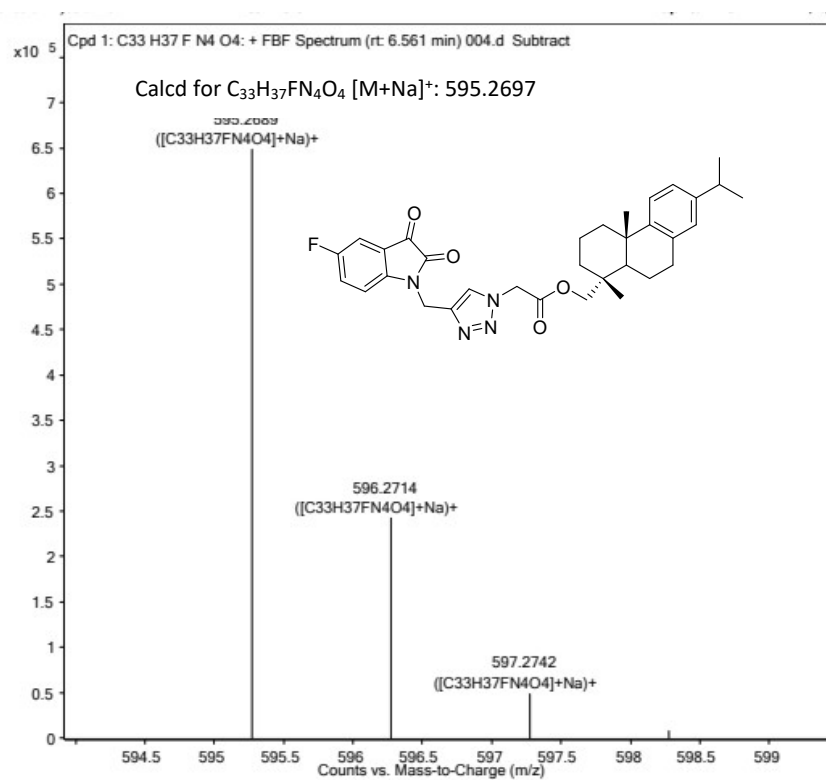


Figure S109 HRMS-ESI spectrum of the target compound **5y**