Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Asymmetric synthesis of tricyclic 6,5,5-fused polycycles by desymmetric Pauson-Khand reaction

Qi Teng[#], *Dong Chen*[#], *Chen-Ho Tong and Zhenghu Xu*[*]
xuzh@sdu.edu.cn

CONTENT:

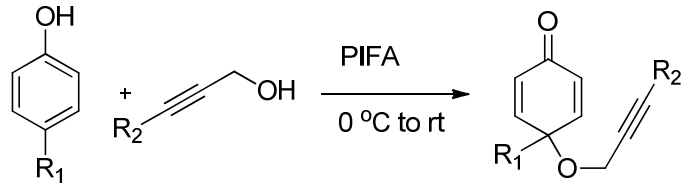
1. General Information

Unless otherwise noted, analytic grade solvents were used for the chromatography, and all the reagents were obtained commercially and used without further purification. All reactions were performed under nitrogen atmosphere and in a flame-dried or oven-dried glassware with magnetic stirring. Reactions were monitored by TLC. Solvents were dried with CaH_2. All NMR spectra were recorded on Bruker-500 MHz spectrometer. The chemical shifts (δ) and coupling constants (*J*) were expressed in ppm and Hz respectively. All ^1H NMR experiments are reported in δ units, parts per million (ppm), and were measured relative to the signals for TMS. All ^{13}C NMR spectra are reported in ppm relative to deuterochloroform (77.16 ppm) and were obtained with ^1H decoupling. HRMS were measured on the Q-TOF6510 instruments.

2. Preparation of Starting Materials

(1) General procedure for the synthesis of *O*-Tethered Alkynes

1a-1p were prepared according to the previously reported procedure.[1],[2]



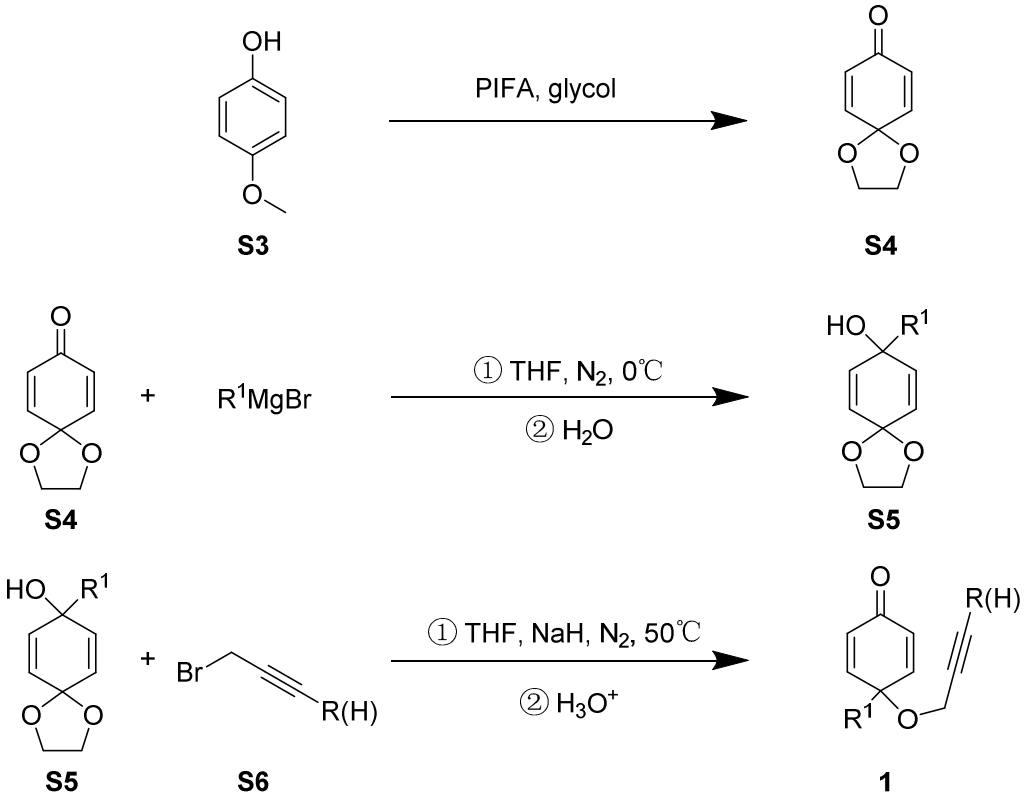
S1 **S2** **1**

The meso-1,6-dienyne substrates **1** were prepared from commercially available 4-substituted phenols **S1** and 3-substituted propargyl alcohol S2 using standard procedures[1] as following:

To a stirred solution of 4-substitude phenol **S1** (1.0 mmol) in 1 mL of 3-substitude propargyl alcohol **S2** was added [bis(trifluoroacetoxy)iodo]benzene (PIFA, 516 mg, 1.2 mmol, 1.2 equiv.) in several portions at 0 °C. The resulting reaction mixture was stirred at room temperature for overnight. Then the reaction mixture was diluted with water (10 mL) and extracted with ethyl acetate (15 mL × 3). The combined organic solvent was washed with brine (15 mL), dried over anhydrous sodium sulfate. The solvent was removed under reduced pressure and the residue was

purified by a silica gel column chromatography (petroleum ether) to give the desired products **1a-1h**, **1j**, **1k** and **1m**.

General procedure for the synthesis of **1i**, **1l** and **1n-1p**:

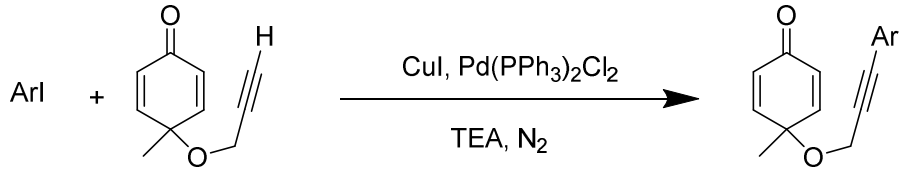


To a stirred suspension of PIFA (4.50 g, 10.5 mmol) in ethylene glycol (40 mL) was added a solution of 4-methoxyphenol (1.00 g, 8.06 mmol) in CH_2Cl_2 (5 mL) and ethylene glycol (5 mL) at room temperature. After 20 minutes, the reaction mixture was quenched with $NaHCO_3$ (saturated aqueous solution, 50 mL). After 10 minutes, the resultant solution was extracted with CH_2Cl_2 (3 × 100 mL). Then the combined organic layers were dried over anhydrous sodium sulfate and concentrated in vacuo. The crude material was purified by column chromatography (silica gel, petroleum ether/ ethyl acetate: 4/1) to afford product 1,4-dioxaspiro[4.5]deca-6,9-dien-8-one (**S4**).

To a well-stirred solution of **S4** (1.0 mmol) in 1 mL of tetrahydrofuran was dropwise added Grignard reagent (1mol/L in tetrahydrofuran, 1.2equiv) at 0 ^{o}C under nitrogen atmosphere. After 20 minutes, the resulting mixture was quenched with water (50 mL) and extracted with dichloromethane (3 × 50 mL). The combined

organic layers were then dried over anhydrous sodium sulfate and concentrated in vacuo to afford crude product **S5**. The crude product **S5** could be used for the next step with no further purification.

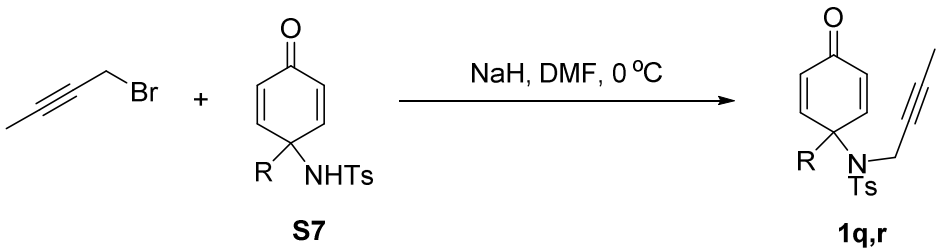
To a solution of crude product **S5** in 10 mL tetrahydrofuran was added NaH (60% in mineral oil, 5.0 mmol, 5.0 equiv.) in several portions at 0 ^{o}C under nitrogen atmosphere, followed by the addition of β-brominated alkynes (**S6**, 3.0 mmol, 3.0 equiv.). Then the mixture was heated at 50 ^{o}C overnight. The resulting solution was quenched with 10 mL of water at 0 ^{o}C and acidified with hydrochloric acid (6 mol/L, 0.9 mL). The resulting mixture was stirred at room temperature to hydrolyze the ketal. After two hours, the mixture was extracted with dichloromethane (50 mL × 3). The combined organic layers were dried over anhydrous sodium sulfate and concentrated in vacuo. The crude material was then purified by a silica gel column chromatography to give the desired products **1i**, **1l** and **S7**, precursor of **1n-1p**.



S7 **1n-1p**

To a solution of *O*-tethered alkyne **1l** (10.0 mmol, 1.0 equiv.) in degassed triethylamine (TEA, 1 mol/L, 10mL) was added $Pd(PPh_3)_2Cl_2$ (3 mol%), CuI (1.5 mol%) and substituted iodobenzene (15 mmol, 1.5 equiv.) under nitrogen atmosphere. The mixture was stirred at 65 ^{o}C. After five hours, the reaction was cooled to room temperature. The solution was washed with saturated ammonium chloride solution and extracted with dichloromethane. The combined organic layers were dried over anhydrous sodium sulfate and concentrated in vacuo. The crude material was purified by column chromatography (silica gel, petroleum ether/ ethyl acetate: 12/1 to 8/1) to give the desired products **1p-1t**.

(2) General procedure for the synthesis of *N*-Tethered Alkynes[3]

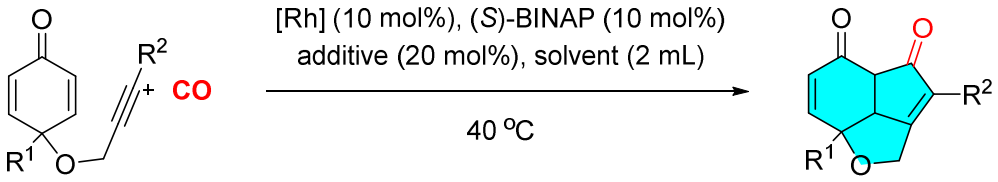


S7 **1q,r**

To a well-stirred solution of substrate **S3** (1 equiv.) in dimethyl formamide (DMF, 0.5 mol/L) was added NaH (2.0 equiv.) in several portion at 0 ℃ under nitrogen atmosphere. The resulting reaction mixture was added 1-bromo-2-butyne (1.5 equiv.) at 0 ℃ and stirred for 30 min. The reaction mixture was quenched by saturated aqueous NH_4Cl and extracted with 1:1 ratio of hexanes/EtOAc (3 times). The combined organic solvent was dried over anhydrous Na_2SO_4, filtered and evaporated under reduced pressure. The residue was purified by flash column chromatography (EtOAc/Hexane) to afford **1q** and **1r**.

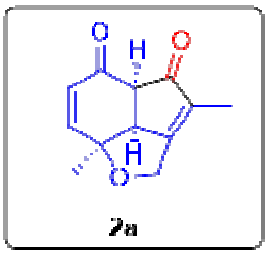
3. Standard Procedure for the Pauson-Khand Reaction

General Procedure for Rhodium-Catalyzed Asymmetric Synthesis of Fused tricyclic Scaffold

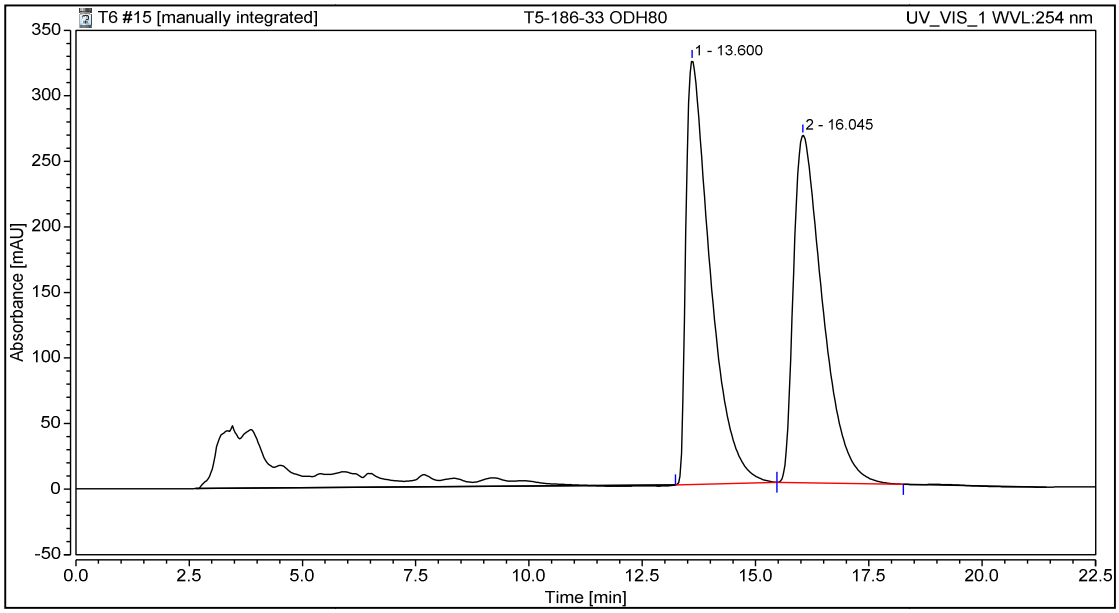


1a **2a**

To a mixture of reactant **1** (0.1 mmol), $[Rh(CO)_2Cl]_2$ (0.005 mmol, 5.0 mol%), (S)-BINAP (0.010 mmol, 10 mol%), $AgNTf_2$ (0.010 mmol, 10 mol%), CH_3OLi (0.020 mmol, 20 mol%), DCM (2 mL) was added under atmosphere of carbon monoxide (0.1 atm) and nitrogen (0.9 atm). Then the reaction mixture was stirred at 40 °C overnight under atmosphere above. The solvent was evaporated under reduce pressure when the reaction completed. The mixture was further purified by column chromatography (silica gel, petroleum ether/ ethyl acetate: 4/1 to 1.5/1) to afford the desired product **2**.

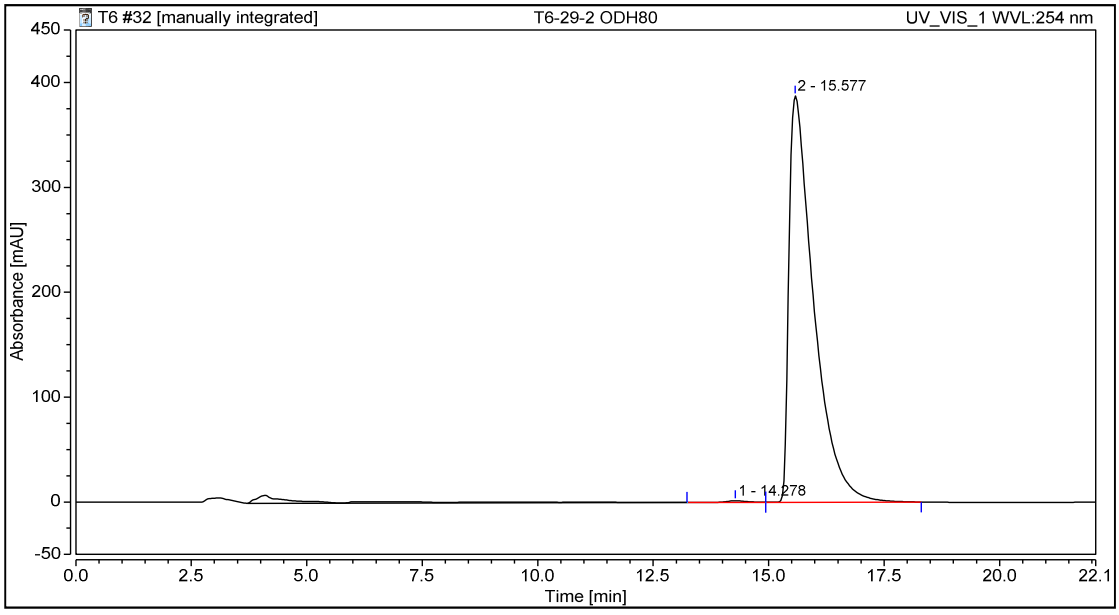


White solid. 91% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.58 (dd, *J* = 10.3, 1.6 Hz, 1H), 5.77 (d, *J* = 10.3 Hz, 1H), 4.82 (d, *J* = 15.7 Hz, 1H), 4.63 (d, *J* = 15.7 Hz, 1H), 3.69 (d, *J* = 5.8 Hz, 1H), 3.41 (dd, *J* = 3.4, 1.7 Hz, 1H), 1.76 (s, 3H), 1.61 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.9, 187.4, 176.0, 151.4, 132.7, 126.5, 76.6, 65.7, 58.7, 50.1, 26.6, 9.3. HRMS (ESI, m/z) calcd for $C_{12}H_{12}O_3$ $[M+H]^+$ 205.0859, found 205.0859. >99% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 80/20, detected at 254 nm, flow rate 1 mL/min, Retention times: 14.3 min (minor), 15.6 min (major).



Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	13.600	200.964	323.450	50.36	54.94
2	16.045	198.119	265.264	49.64	45.06
Total:		**399.083**	**588.715**	**100.00**	**100.00**

Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	14.278	0.854	1.566	0.35	0.40
2	15.577	241.118	387.456	99.65	99.60



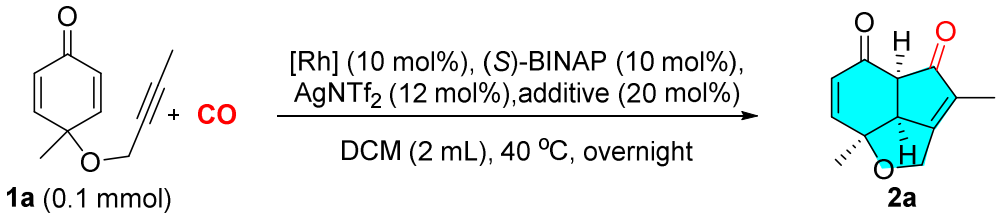
4. Scale-up Experiment

To a mixture of reactant **1a** (1.8 mmol), $[Rh(CO)_2Cl]_2$ (0.050 mmol, 2.8 mol%), (S)-BINAP (0.100 mmol, 5.6 mol%), $AgNTf_2$ (0.100 mmol, 5.6 mol%), CH_3OLi (0.200 mmol, 11 mol%), DCM (30 mL) was added under atmosphere of carbon monoxide (0.1 atm) and nitrogen (0.9 atm). Then the reaction mixture was stirred at

40 °C for 40 hours under atmosphere above. The solvent was evaporated under reduce pressure when the reaction completed. The mixture was further purified by column chromatography (silica gel, petroleum ether/ ethyl acetate: 2/1) to afford product **2a**.

5. Investigation of the Additives

The investigation was carried out with standard reaction under optimized conditions but changing MeOLi to other additives. The results were shown as follow.

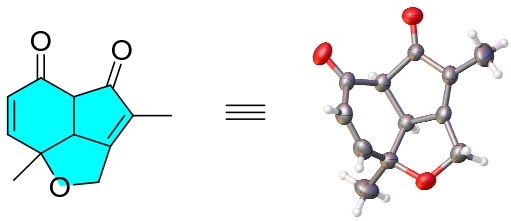


1a (0.1 mmol) **2a**

Entry	additive	T/°C	Yield/%
1	MeONa	40	55
2	DBU	40	0
3	$LiNTf_2$	40	77
4	MeOLi	40	91

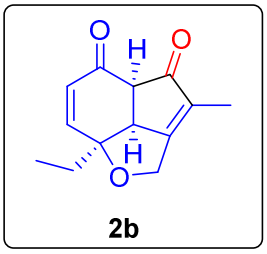
6. X-ray Crystallography

The crystal of **2a** suitable for XRD analysis was prepared by recrystallization from a mixed solvent of dichloromethane and petroleum ether. CCDC 2049470 (**2a**) contains the supplementary crystallographic data for this paper. The crystallographic data can be obtained free from The Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/ci.



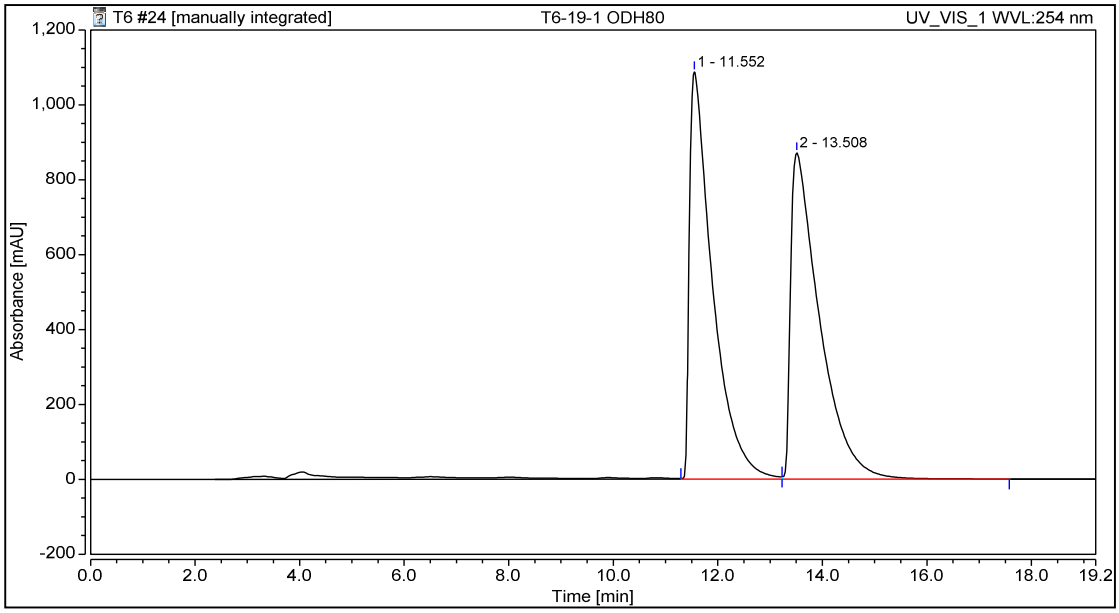
2a CCDC: 2049470

7. Characterization of Compound 2

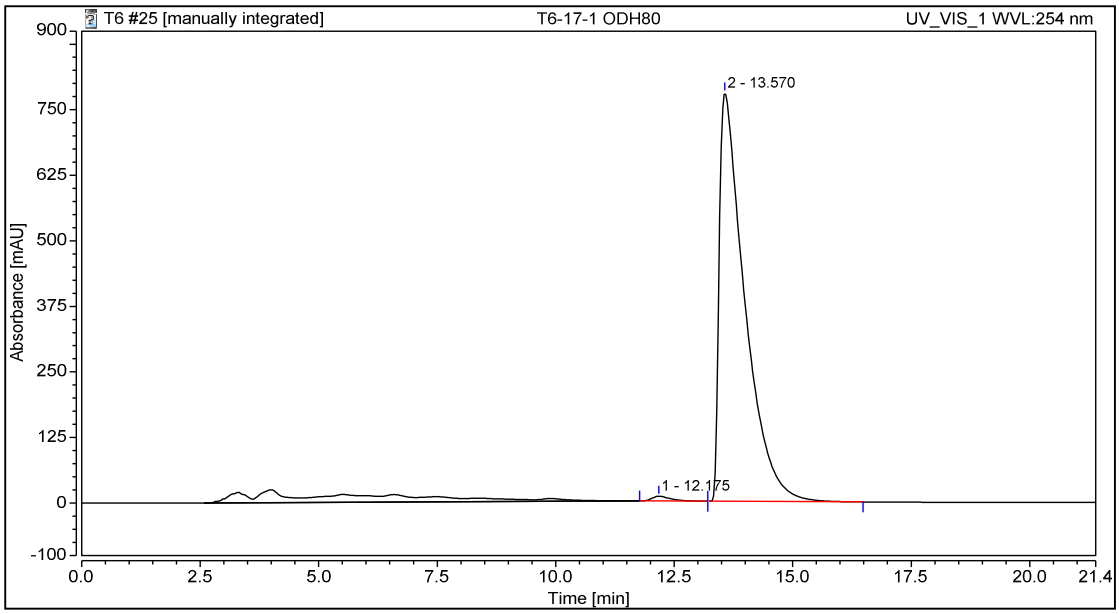


2b

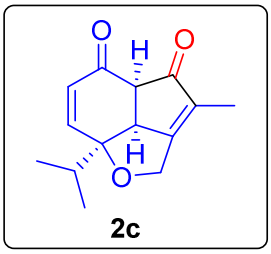
Yellow solid. 70% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.43 (dd, *J* = 10.4, 1.6 Hz, 1H), 5.79 (d, *J* = 10.4 Hz, 1H), 4.73 (d, *J* = 15.6 Hz, 1H), 4.59 (d, *J* = 15.6 Hz, 1H), 3.58 (d, *J* = 5.8 Hz, 1H), 3.41 – 3.25 (m, 1H), 1.85 (qd, *J* = 7.5, 2.7 Hz, 2H), 1.69 (s, 3H), 0.89 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.0, 187.6, 175.9, 150.1, 132.4, 127.7, 79.9, 65.6, 59.2, 48.3, 32.4, 9.3, 8.3. HRMS (ESI, m/z) calcd for $C_{13}H_{14}O_3$ $[M+H]^+$ 219.1016, found 219.1024. $[\alpha]^{23}_D$ = -116.6° (c 0.26, $CHCl_3$); 98% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 80/20, detected at 254 nm, flow rate 1 mL/min, Retention times: 12.2 min (minor), 13.6 min (major).



Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	11.552	555.945	1087.559	49.90	55.50
2	13.508	558.261	871.836	50.10	44.50
Total:		**1114.206**	**1959.395**	**100.00**	**100.00**

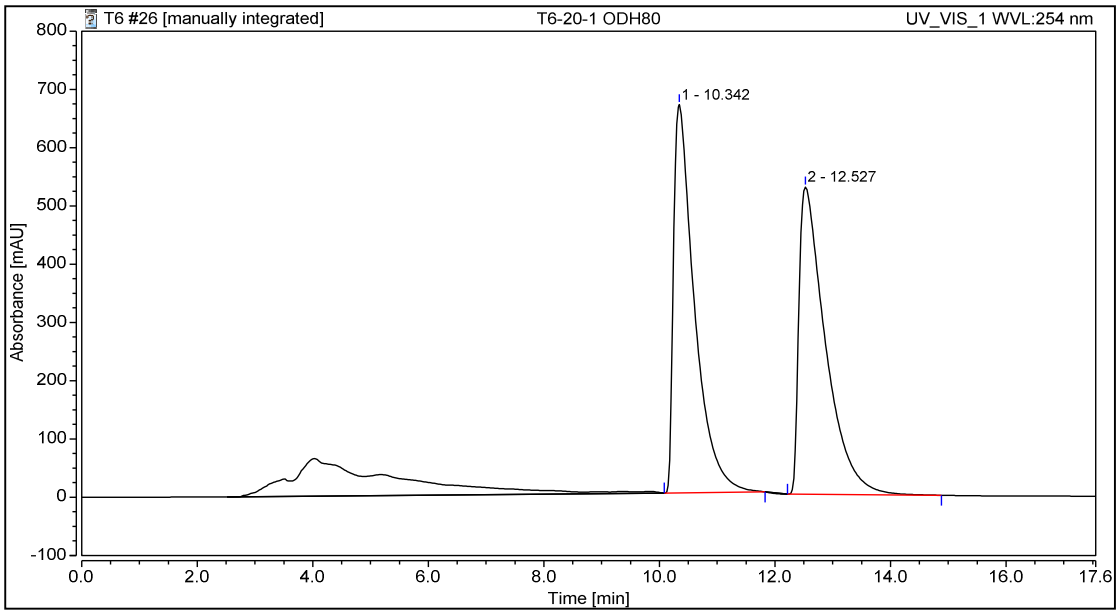


Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	12.175	4.012	8.997	0.82	1.14
2	13.570	484.075	778.818	99.18	98.86
Total:		**488.086**	**787.815**	**100.00**	**100.00**

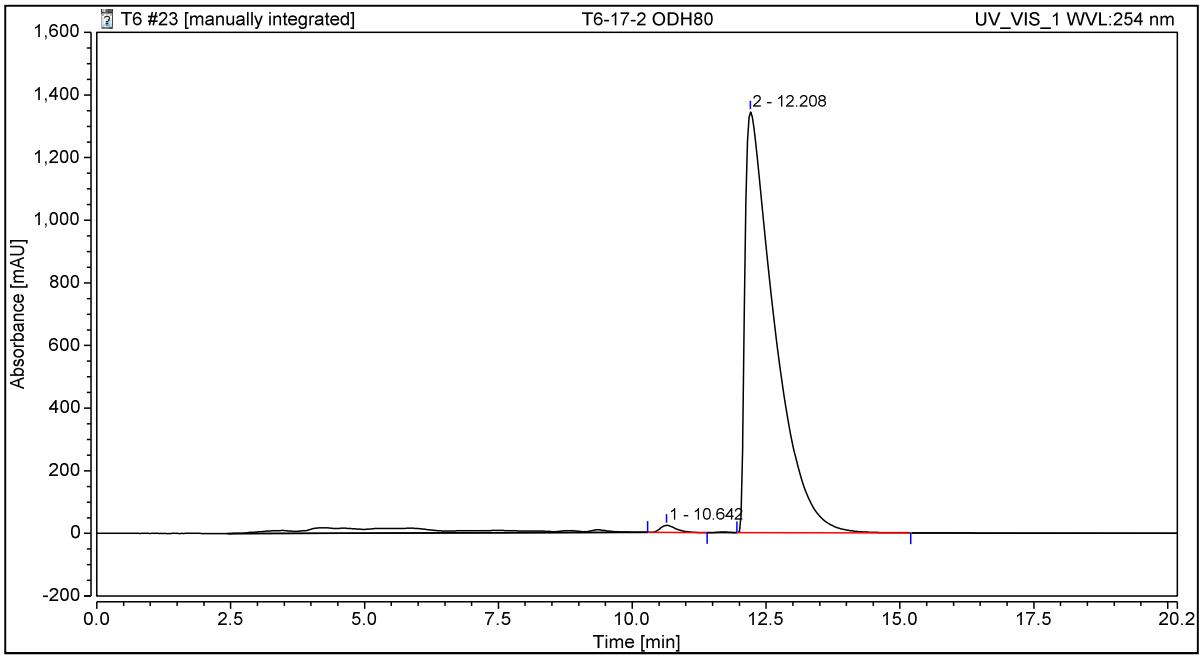


2c

Yellow solid. 68% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.49 (dd, J = 10.5, 1.4 Hz, 1H), 5.91 (d, J = 10.5 Hz, 1H), 4.77 (d, J = 15.5 Hz, 1H), 4.67 (d, J = 15.5 Hz, 1H), 3.62 (d, J = 5.8 Hz, 1H), 3.37 (d, J = 1.6 Hz, 1H), 2.21 – 2.05 (m, 1H), 1.75 (s, 3H), 1.02 (d, J = 6.9 Hz, 3H), 0.96 (d, J = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.1, 187.6, 175.9, 148.4, 132.4, 128.5, 82.2, 65.6, 59.8, 47.5, 37.3, 17.5, 17.0, 9.3. HRMS (ESI, m/z) calcd for $C_{14}H_{16}O_3$ $[M+H]^+$ 233.1172, found 233.1175. $[\alpha]^{23}_D$ = -97.0° (c 0.13, $CHCl_3$); 98% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 80/20, detected at 254 nm, flow rate 1 mL/min, Retention times: 10.6 min (minor), 12.2 min (major).

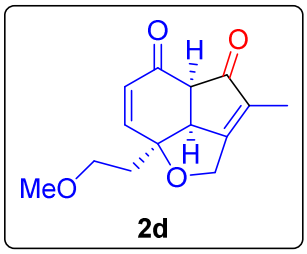


Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	10.342	279.566	666.368	49.97	55.82
2	12.527	279.953	527.479	50.03	44.18
Total:		**559.519**	**1193.847**	**100.00**	**100.00**



Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	10.642	8.064	22.692	0.93	1.66
2	12.208	860.159	1343.428	99.07	98.34

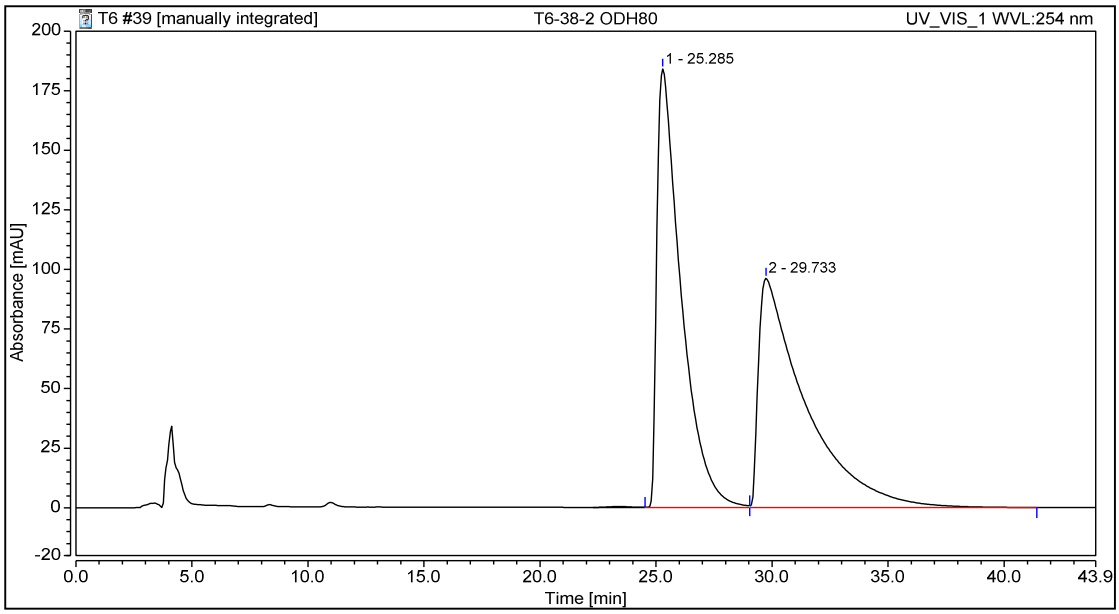
Total:	**868.223**	**1366.120**	**100.00**	**100.00**

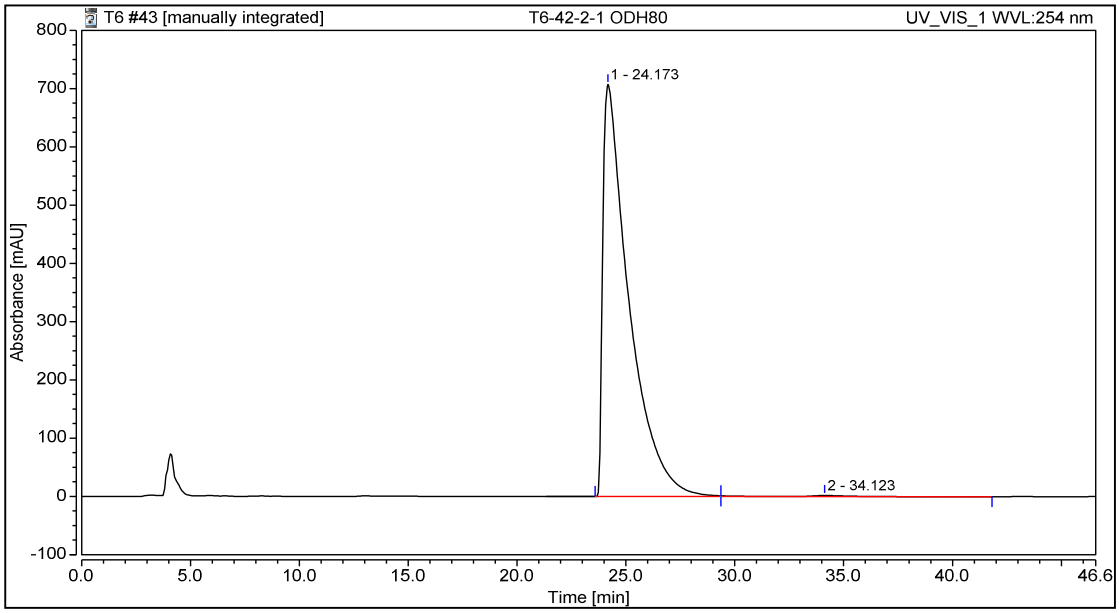


2d

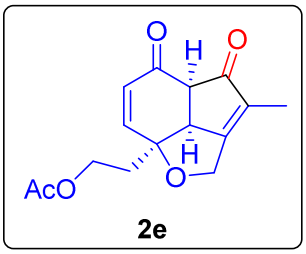
White solid. 86% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.43 (dd, *J* = 10.4, 1.5 Hz, 1H), 5.86 (d, *J* = 10.3 Hz, 1H), 4.77 (d, *J* = 15.5 Hz, 1H), 4.61 (d, *J* = 15.5 Hz, 1H), 3.69 (d, *J* = 5.7 Hz, 1H), 3.56 – 3.50 (m, 1H), 3.49 (dd, *J* = 3.5, 1.9 Hz, 1H), 3.22 (ddd, *J* = 11.0, 10.0, 3.3 Hz, 1H), 3.18 (s, 3H), 2.22 (ddd, *J* = 14.4, 11.1, 4.7 Hz, 1H), 2.06 (dt, *J* = 14.2, 3.5 Hz, 1H), 1.75 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.6, 187.9, 176.2, 148.7, 132.5, 128.3, 78.9, 68.1, 65.1, 60.0, 58.6, 50.3, 39.0, 9.3. HRMS (ESI, m/z) calcd for $C_{14}H_{16}O_4$ $[M+H]^+$ 249.1121, found 249.1144. $[\alpha]17_D$ = -73.4° (c 0.38, $CHCl_3$); >99% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 80/20, detected at 254 nm, flow rate 1 mL/min, Retention times: 27.2 min (major), 34.1 min (major).

Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	25.285	222.573	183.951	49.76	65.67
2	29.733	224.715	96.170	50.24	34.33
Total:		**447.288**	**280.121**	**100.00**	**100.00**



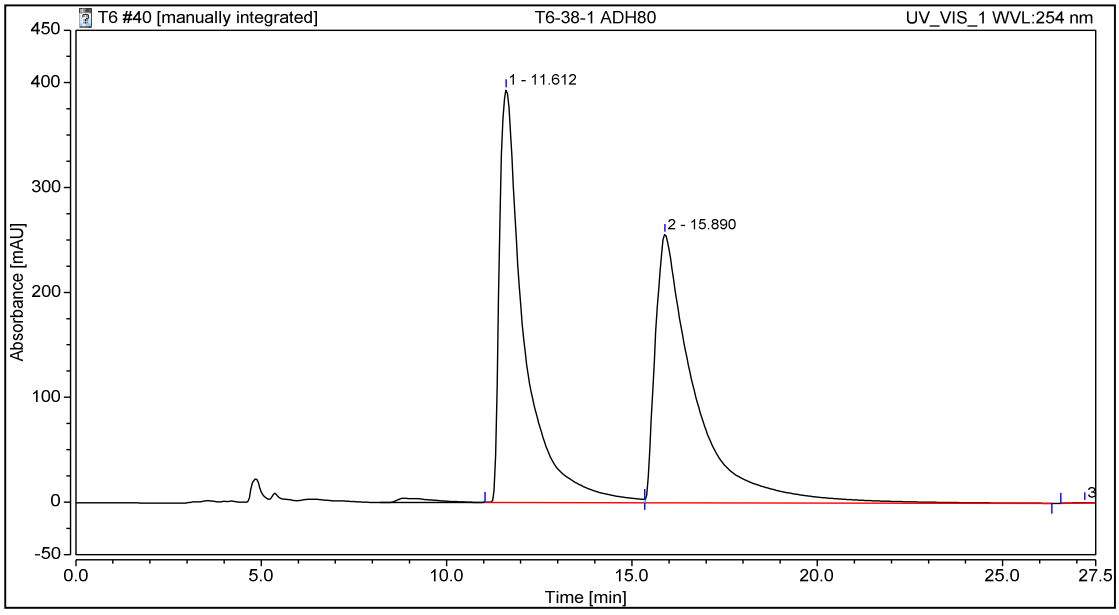


Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	24.173	981.700	707.029	99.51	99.73
2	34.123	4.792	1.917	0.49	0.27
Total:		**986.492**	**708.946**	**100.00**	**100.00**



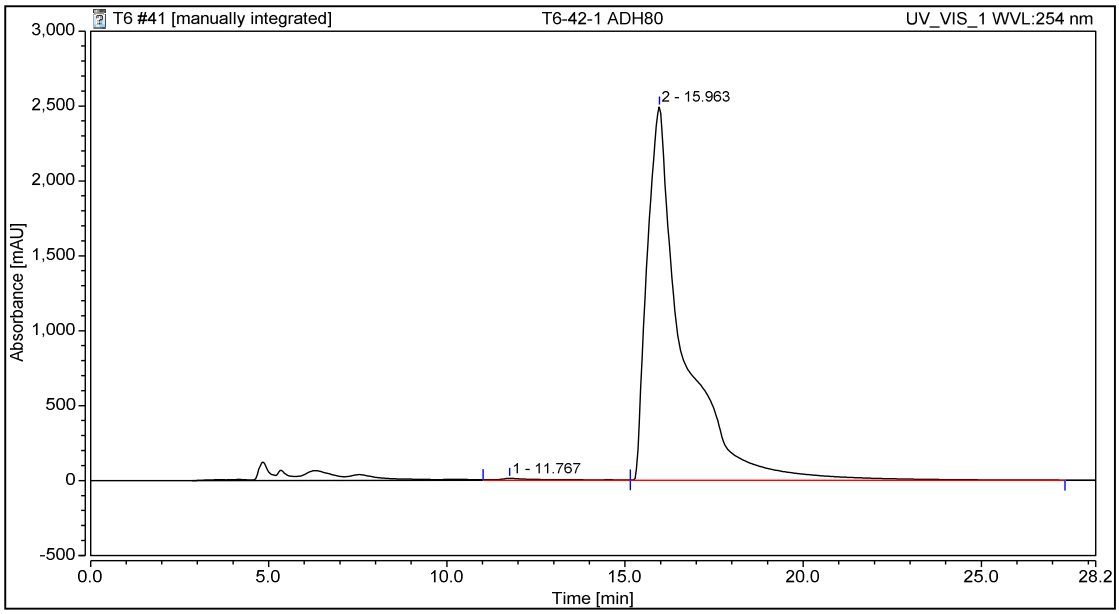
2e

White solid. 60% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.51 (dd, *J* = 10.4, 1.3 Hz, 1H), 5.86 (d, *J* = 10.4 Hz, 1H), 4.79 (d, *J* = 15.6 Hz, 1H), 4.64 (d, *J* = 15.6 Hz, 1H), 4.33 (ddd, *J* = 17.2, 12.3, 6.0 Hz, 1H), 4.01 (ddd, *J* = 11.7, 9.1, 5.1 Hz, 1H), 3.69 (d, *J* = 5.8 Hz, 1H), 3.55 – 3.41 (m, 1H), 2.24 (qt, *J* = 14.6, 5.3 Hz, 2H), 2.03 (s, 3H), 1.77 (s, 3H). 13C NMR (126 MHz, CDCl3) δ 199.7, 187.2, 175.5, 170.5, 149.0, 132.8, 128.1, 78.0, 65.4, 60.0, 59.2, 49.3, 38.2, 20.9, 9.3. HRMS (ESI, m/z) calcd for $C_{15}H_{16}O_5$ $[M+H]^+$ 277.1071, found 277.1091. $[\alpha]^{17}_D$ = 46.6° (c 0.16, $CHCl_3$); 98% ee; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5u column; hexane/2-propanol = 80/20, detected at 254 nm, flow rate 1 mL/min, Retention times: 11.8 min (minor), 16.0 min (major).

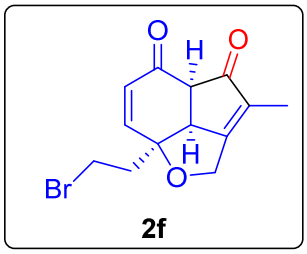


Integration Results

No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	11.612	308.814	393.615	49.35	60.57
2	15.890	316.740	255.950	50.62	39.39
3	27.213	0.147	0.271	0.02	0.04
Total:		**625.701**	**649.836**	**100.00**	**100.00**

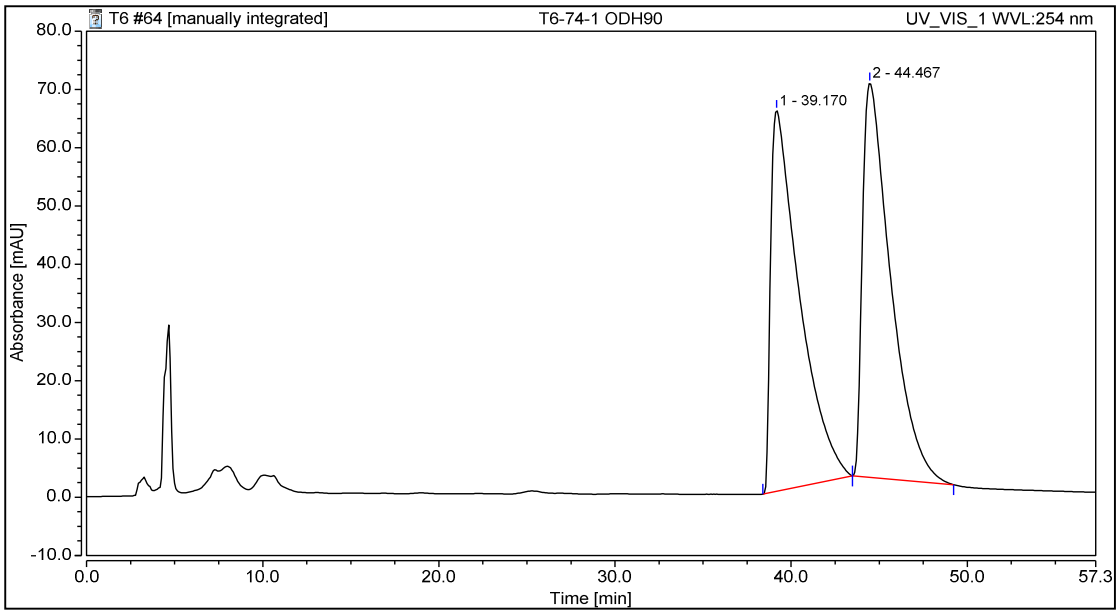


Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	11.767	24.063	14.324	0.82	0.57
2	15.963	2910.560	2491.925	99.18	99.43
Total:		**2934.623**	**2506.249**	**100.00**	**100.00**

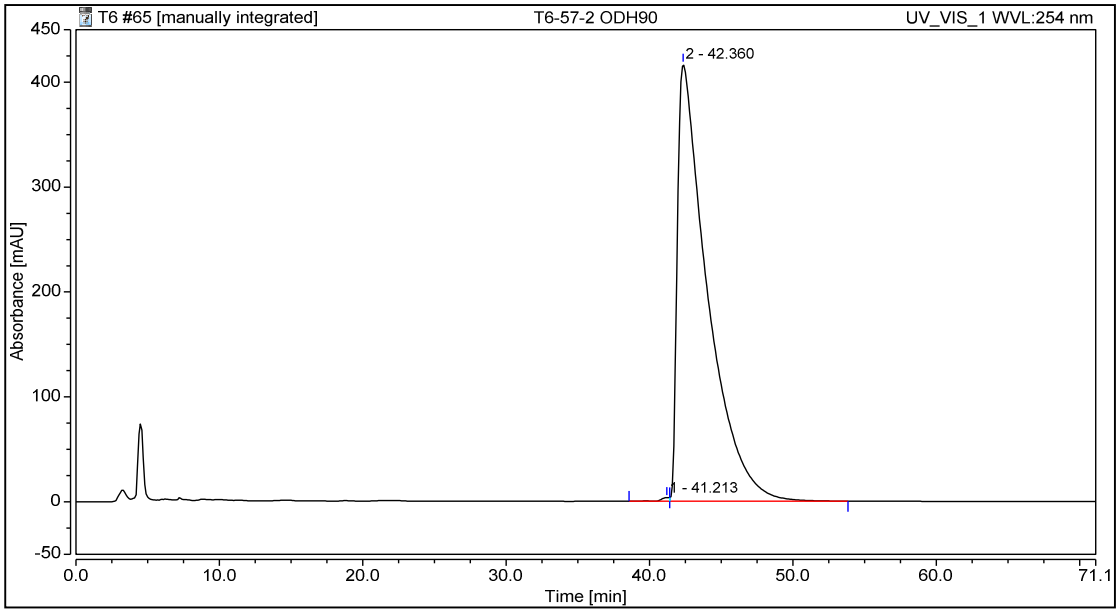


2f

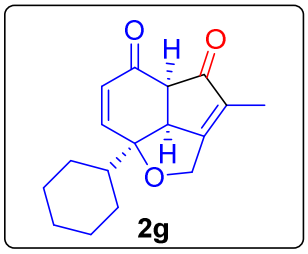
White solid. 65% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.52 (dd, *J* = 10.4, 1.5 Hz, 1H), 5.88 (d, *J* = 10.4 Hz, 1H), 4.80 (d, *J* = 15.6 Hz, 1H), 4.65 (d, *J* = 15.5 Hz, 1H), 3.77 (d, *J* = 5.8 Hz, 1H), 3.64 – 3.45 (m, 2H), 3.37 (dt, *J* = 10.3, 7.8 Hz, 1H), 2.55 – 2.42 (m, 2H), 1.77 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.53 (s), 187.05 (s), 174.8, 148.7, 132.8, 128.2, 78.5, 65.5, 59.1, 48.5, 42.6, 25.8, 9.4. HRMS (ESI, m/z) calcd for $C_{13}H_{13}BrO_3$ $[M+H]^+$ 297.0121, found 297.0113. $[\alpha]^{17}_D$ = -97.4° (c 0.16, $CHCl_3$); >99% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 90/10, detected at 254 nm, flow rate 1 mL/min, Retention times: 41.2 min (minor), 42.4 min (major).



Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	24.173	981.700	707.029	99.51	99.73
2	34.123	4.792	1.917	0.49	0.27
Total:		**986.492**	**708.946**	**100.00**	**100.00**

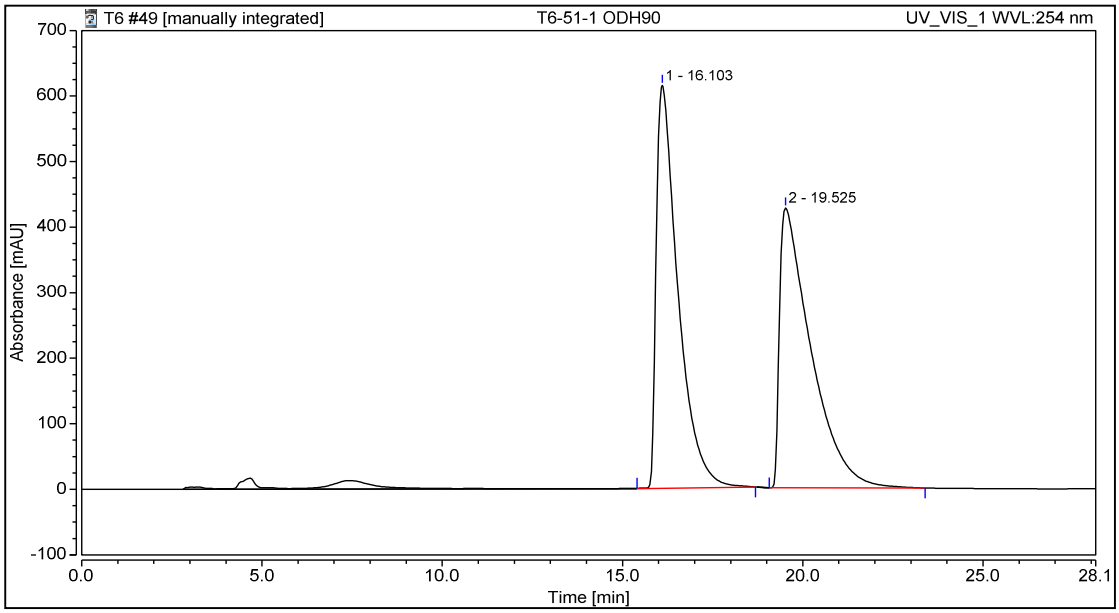


Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	41.213	2.492	3.502	0.25	0.83
2	42.360	1008.759	416.723	99.75	99.17
Total:		**1011.251**	**420.225**	**100.00**	**100.00**

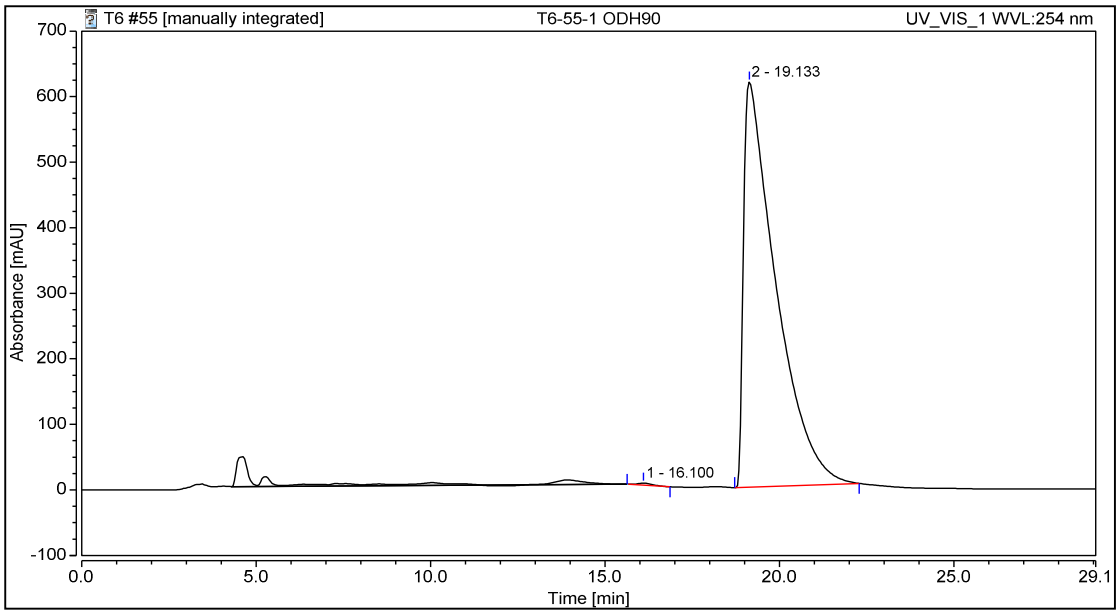


2g

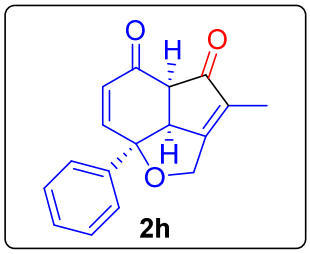
White solid. 60% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.49 (dd, *J* = 10.5, 1.4 Hz, 1H), 5.88 (d, *J* = 10.5 Hz, 1H), 4.75 (d, *J* = 15.5 Hz, 1H), 4.65 (d, *J* = 15.5 Hz, 1H), 3.61 (d, *J* = 5.8 Hz, 1H), 3.45 – 3.30 (m, 1H), 1.96 (d, *J* = 12.5 Hz, 1H), 1.79 (ddd, *J* = 9.4, 6.9, 3.5 Hz, 2H), 1.75 (s, 3H), 1.70 (d, *J* = 18.0 Hz, 2H), 1.35 – 1.19 (m, 3H), 1.18 – 1.05 (m, 1H), 1.04 – 0.93 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.1, 187.8, 175.9, 149.1, 132.2, 128.1, 81.8, 65.4, 59.9, 47.8, 47.4, 27.9, 27.2, 26.2, 26.2, 26.0, 9.3. HRMS (ESI, m/z) calcd for $C_{17}H_{20}O_3$ $[M+H]^+$ 273.1485, found 273.1487. $[\alpha]^{17}_D$ = 34.2° (c 0.20, $CHCl_3$); >99% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 90/10, detected at 254 nm, flow rate 1 mL/min, Retention times: 16.1 min (minor), 19.1 min (major).



Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	16.103	428.113	614.615	49.96	59.00
2	19.525	428.841	427.168	50.04	41.00
Total:		**856.954**	**1041.783**	**100.00**	**100.00**

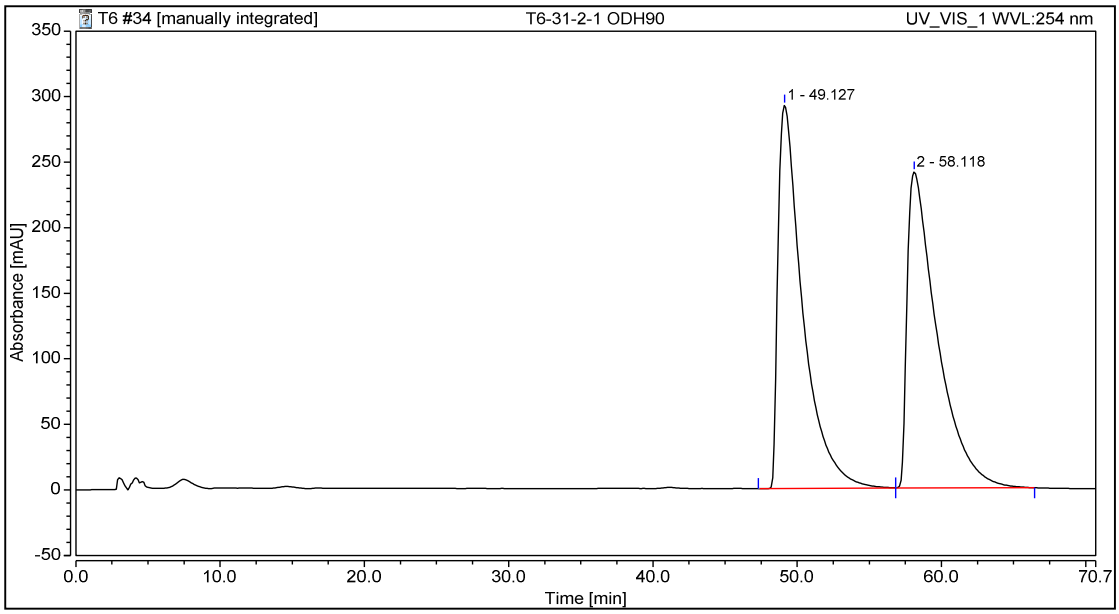


Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	16.100	1.430	2.982	0.22	0.48
2	19.133	663.453	617.988	99.78	99.52
Total:		**664.883**	**620.970**	**100.00**	**100.00**

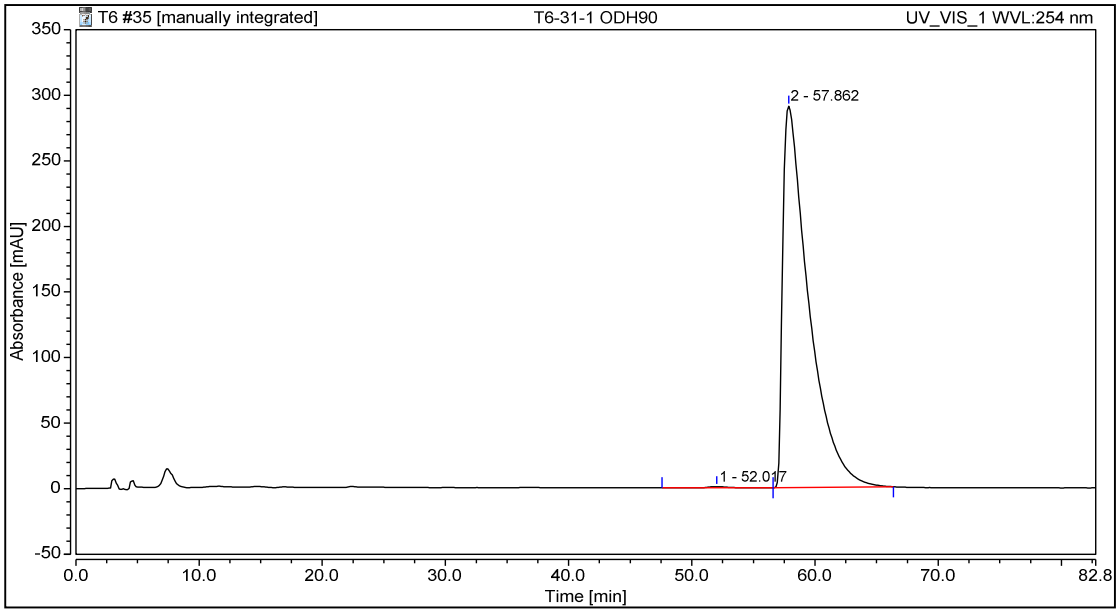


2h

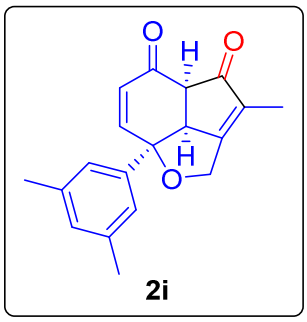
White solid. 80% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 – 7.31 (m, 5H), 6.61 (dd, *J* = 10.3, 1.6 Hz, 1H), 5.91 (d, *J* = 10.3 Hz, 1H), 4.99 (d, *J* = 15.4 Hz, 1H), 4.87 (d, *J* = 15.4 Hz, 1H), 3.79 (d, *J* = 5.8 Hz, 1H), 3.73 – 3.55 (m, 1H), 1.82 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.7, 187.0, 176.6, 151.5, 134.6, 129.7, 129.2, 128.8, 128.3, 126.9, 76.2, 67.2, 60.1, 50.3, 26.4. HRMS (ESI, m/z) calcd for $C_{17}H_{14}O_3$ $[M+H]^+$ 267.1016, found 207.1017. $[\alpha]^{17}_D$ = -218.7° (c 0.81, $CHCl_3$); >99% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 90/10, detected at 254 nm, flow rate 1 mL/min, Retention times: 57.0 min (minor), 57.9 min (major).



Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	49.127	581.078	292.395	50.05	54.80
2	58.118	579.976	241.195	49.95	45.20
Total:		**1161.055**	**533.589**	**100.00**	**100.00**

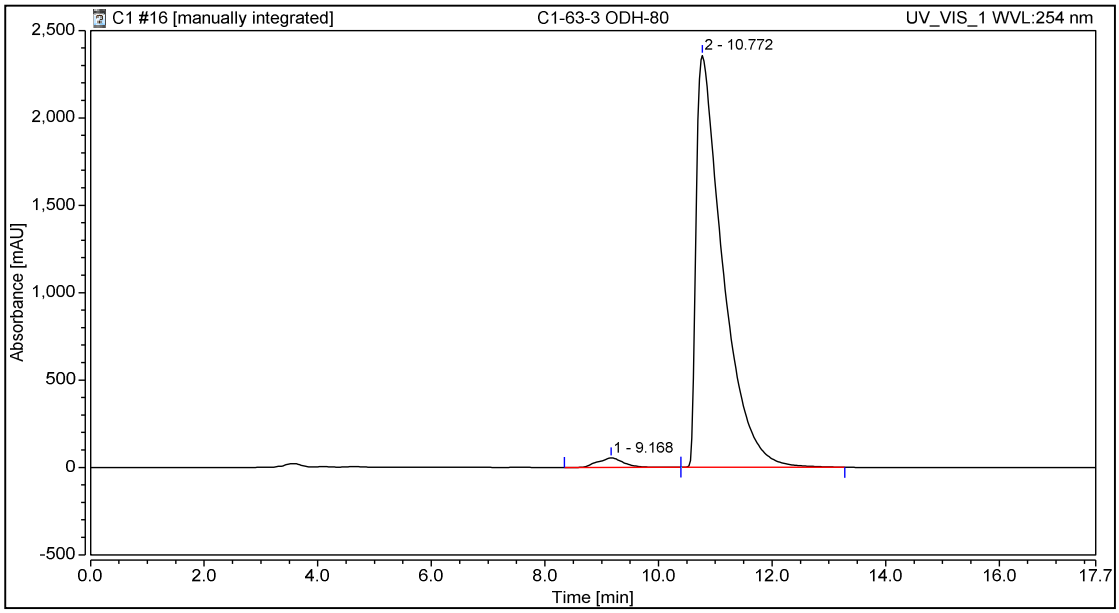


Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	52.017	1.239	0.853	0.17	0.29
2	57.862	710.943	290.985	99.83	99.71
Total:		**712.182**	**291.838**	**100.00**	**100.00**

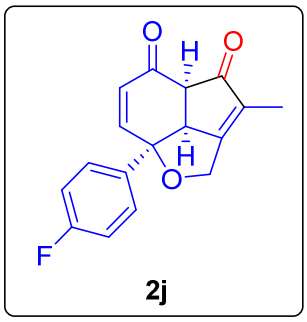


2i

White solid. 57% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.03 (s, 2H), 6.97 (s, 1H), 6.60 (dd, *J* = 10.3, 1.5 Hz, 1H), 5.90 (d, *J* = 10.3 Hz, 1H), 4.98 (d, *J* = 15.4 Hz, 1H), 4.85 (d, *J* = 15.4 Hz, 1H), 3.80 (d, *J* = 5.8 Hz, 1H), 3.74 – 3.63 (m, 1H), 2.33 (s, 6H), 1.81 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.6, 187.8, 175.2, 149.9, 141.1, 138.8, 132.8, 130.0, 126.4, 122.85, 80.0, 65.9, 59.0, 51.5, 21.5, 9.4. HRMS (ESI, m/z) calcd for $C_{19}H_{18}O_3$ $[M+H]^+$ 295.1329, found 295.1325. $[\alpha]^{16}_D$ = -245.2° (c 0.49, $CHCl_3$); 96% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 80/20, detected at 254 nm, flow rate 1 mL/min, Retention times: 9.2 min (minor), 10.8 min (major)

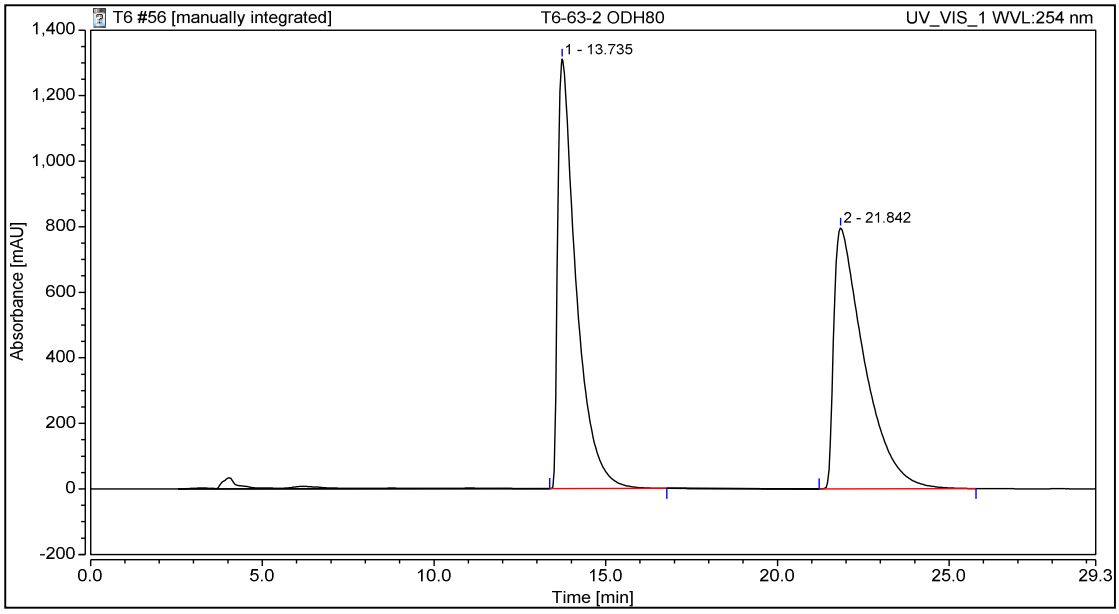


Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	9.168	28.976	54.684	2.21	2.27
2	10.772	1279.795	2357.296	97.79	97.73
Total:		**1308.771**	**2411.980**	**100.00**	**100.00**

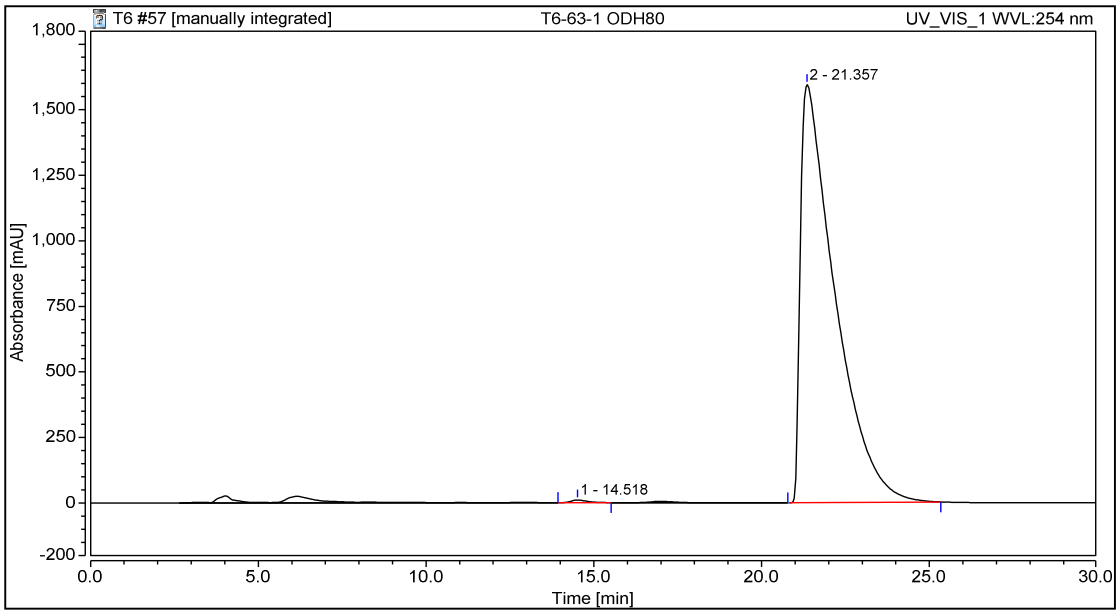


2j

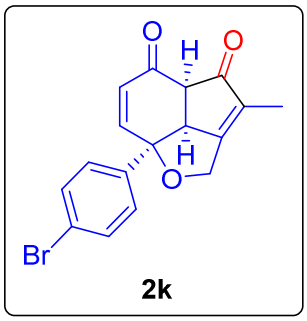
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (ddd, *J* = 7.0, 5.1, 2.5 Hz, 2H), 7.17 – 7.04 (m, 2H), 6.59 (dd, *J* = 10.3, 1.5 Hz, 1H), 5.92 (d, *J* = 10.3 Hz, 1H), 5.00 (d, *J* = 15.5 Hz, 1H), 4.86 (d, *J* = 15.5 Hz, 1H), 3.78 (d, *J* = 5.8 Hz, 1H), 3.71 – 3.54 (m, 1H), 1.82 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.3, 187.5, 174.9, 162.5 (d, *J* = 247.9 Hz), 149.4, 137.0 (d, *J* = 3.2 Hz), 133.0, 127.1 (d, *J* = 8.2 Hz), 126.7, 115.9 (d, *J* = 21.7 Hz), 79.6, 66.0, 58.8, 51.8, 9.4. 78% yield. HRMS (ESI, m/z) calcd for $C_{17}H_{13}FO_3$ $[M+H]^+$ 285.0921, found 285.0925. $[\alpha]^{17}_D$ = -213.3° (c 0.63, $CHCl_3$); >99% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 80/20, detected at 254 nm, flow rate 1 mL/min, Retention times: 14.5 min (minor), 21.4 min (major).



Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	13.735	815.822	1310.226	49.95	62.22
2	21.842	817.494	795.454	50.05	37.78
Total:		**1633.316**	**2105.680**	**100.00**	**100.00**

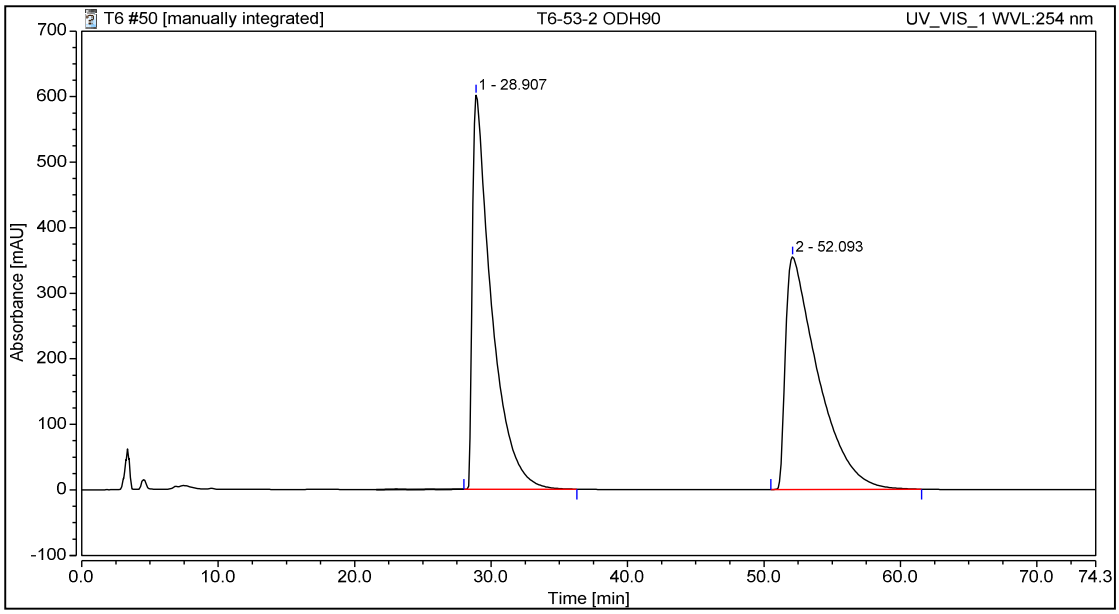


Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	14.518	5.289	9.873	0.28	0.62
2	21.357	1903.349	1595.223	99.72	99.38
Total:		**1908.638**	**1605.096**	**100.00**	**100.00**

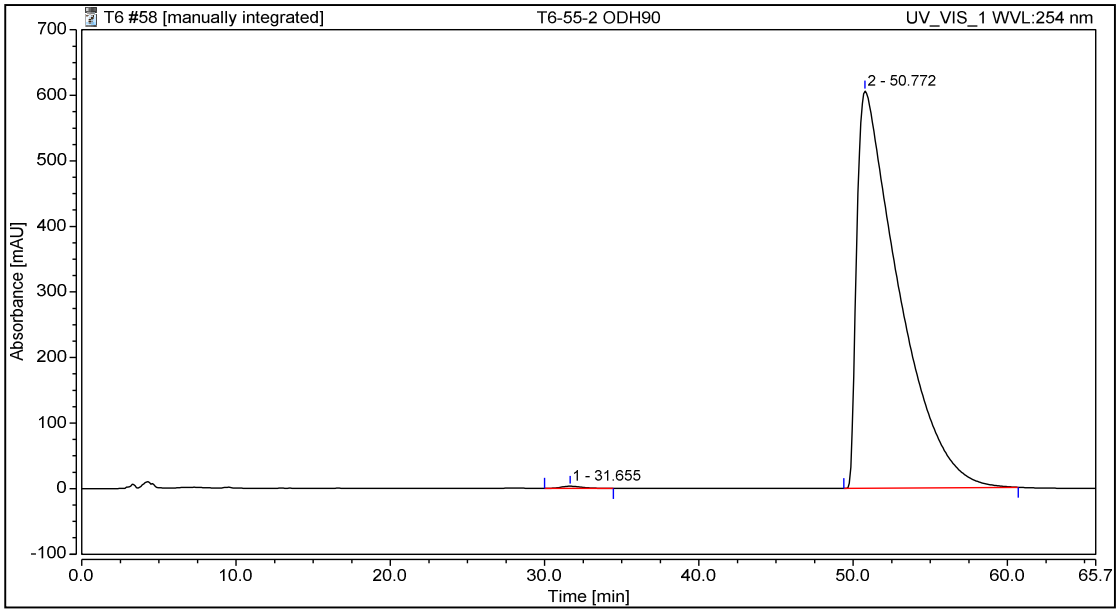


2k

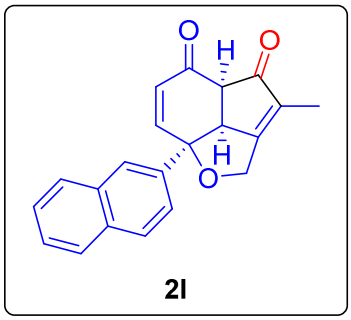
White solid. 84% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 – 7.46 (m, 2H), 7.40 – 7.28 (m, 2H), 6.57 (dd, *J* = 10.3, 1.6 Hz, 1H), 5.92 (d, *J* = 10.3 Hz, 1H), 4.99 (d, *J* = 15.4 Hz, 1H), 4.86 (d, *J* = 15.5 Hz, 1H), 3.77 (d, *J* = 5.8 Hz, 1H), 3.69 – 3.56 (m, 1H), 1.81 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.1, 187.4, 174.6, 149.1, 140.3, 133.1, 132.1, 127.0, 126.9, 122.5, 79.6, 66.0, 58.7, 51.7, 9.4. HRMS (ESI, m/z) calcd for $C_{17}H_{13}BrO_3$ $[M+H]^+$ 345.0121, found 345.0123. $[\alpha]^{17}_D$ = -199.0° (c 0.50, $CHCl_3$); >99% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 90/10, detected at 254 nm, flow rate 1 mL/min, Retention times: 31.7 min (minor), 50.8 min (major).



Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	28.907	976.513	601.434	49.98	62.90
2	52.093	977.309	354.697	50.02	37.10
Total:		**1953.822**	**956.132**	**100.00**	**100.00**

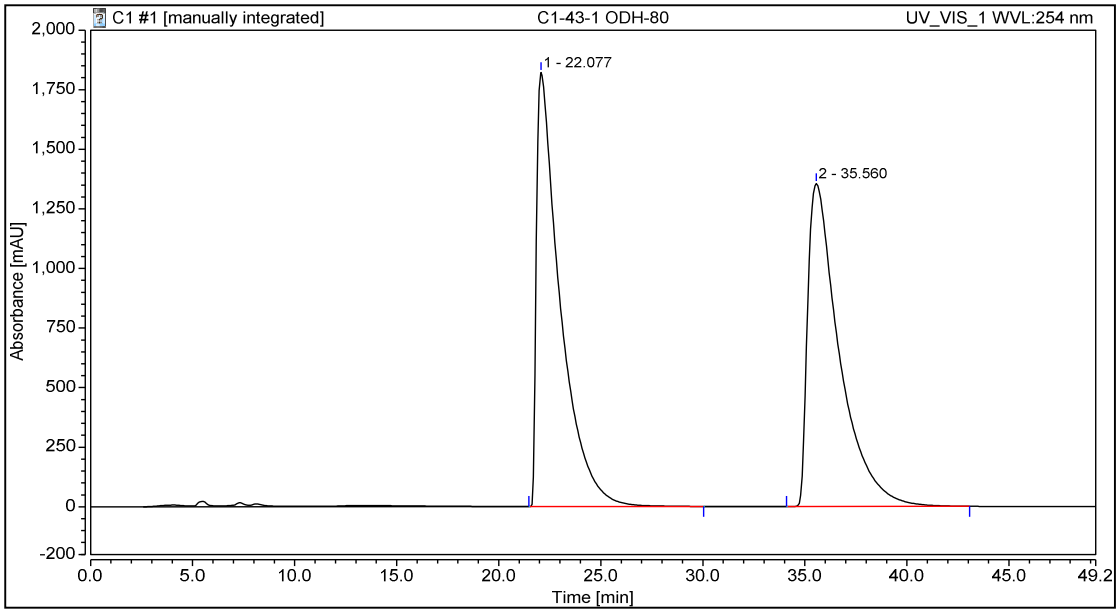


Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	31.655	5.001	3.252	0.26	0.53
2	50.772	1911.510	606.015	99.74	99.47
Total:		**1916.511**	**609.268**	**100.00**	**100.00**

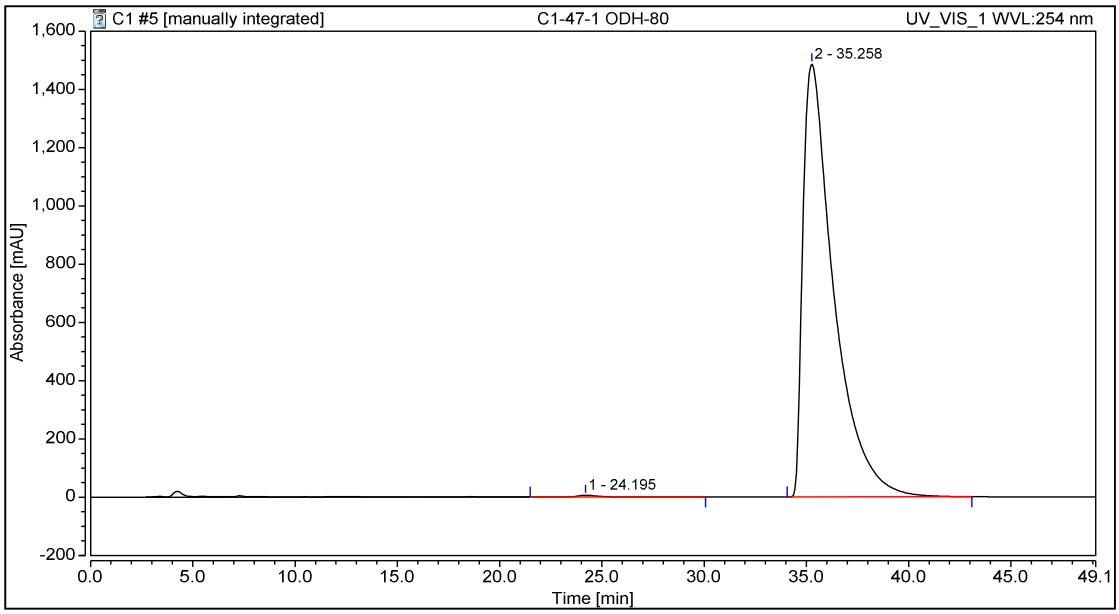


2l

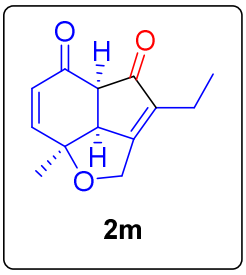
White solid. 56% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 – 7.75 (m, 4H), 7.64 – 7.38 (m, 3H), 6.68 (dd, *J* = 10.3, 1.6 Hz, 1H), 5.98 (d, *J* = 10.3 Hz, 1H), 5.15 – 5.00 (m, 1H), 4.93 (d, *J* = 15.4 Hz, 1H), 3.84 (d, *J* = 5.8 Hz, 1H), 3.74 (ddd, *J* = 29.7, 15.7, 4.1 Hz, 1H), 1.84 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.5, 187.7, 175.0, 149.6, 138.4, 133.1, 133.0, 133.0, 129.07, 128.2, 127.7, 126.8, 126.8, 126.7, 124.3, 122.7, 80.1, 66.1, 58.9, 51.7, 9.4. HRMS (ESI, m/z) calcd for $C_{21}H_{16}O_3$ $[M+H]^+$ 317.1172, found 317.1169. $[\alpha]^{16}_D$ = -253.2° (c 0.60, $CHCl_3$); >99% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 80/20, detected at 254 nm, flow rate 1 mL/min, Retention times: 24.2 min (minor), 35.3 min (major).



Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	22.077	2440.345	1820.914	50.11	57.35
2	35.560	2429.909	1354.067	49.89	42.65
Total:		**4870.254**	**3174.981**	**100.00**	**100.00**

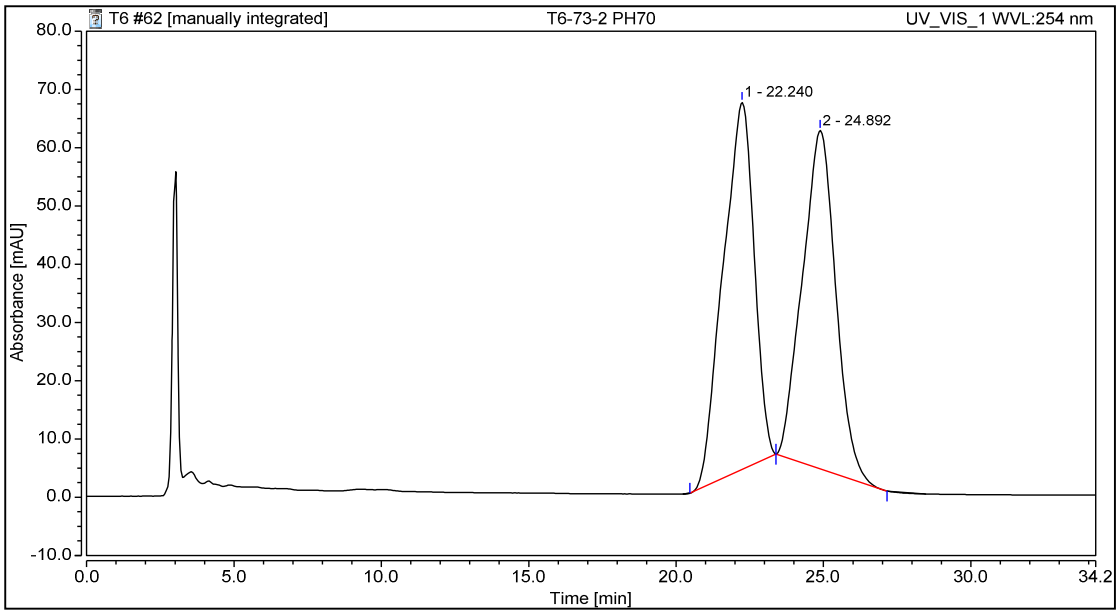


Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	24.195	6.838	5.932	0.26	0.40
2	35.258	2601.655	1486.663	99.74	99.60
Total:		**2608.493**	**1492.595**	**100.00**	**100.00**

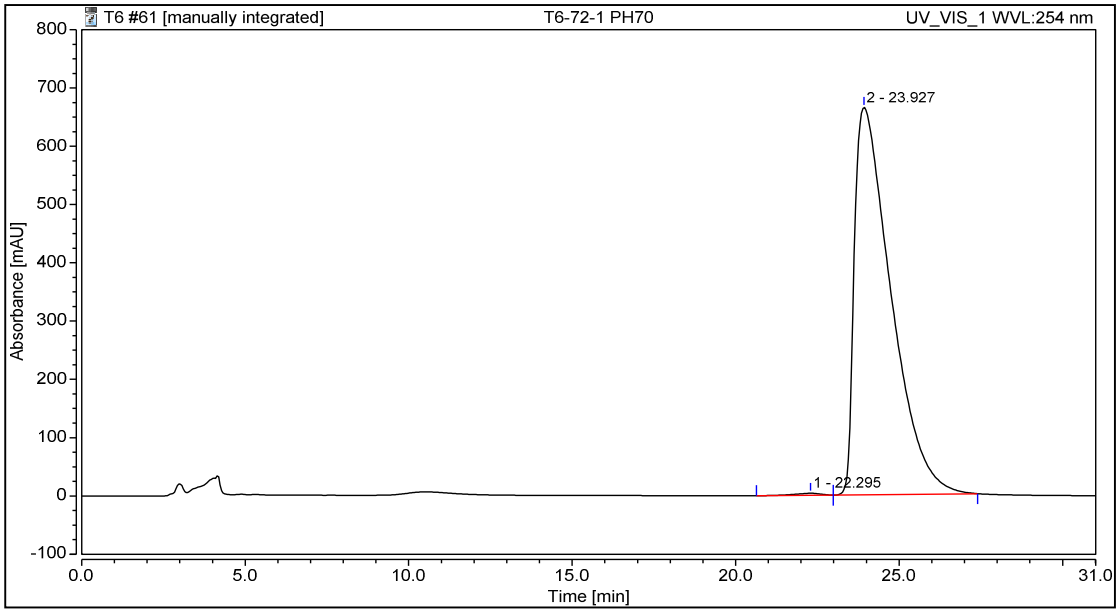


2m

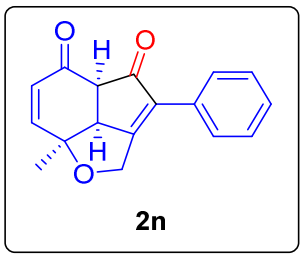
White solid. 86% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.59 (dd, J = 10.3, 1.6 Hz, 1H), 5.77 (d, J = 10.3 Hz, 1H), 4.85 (d, J = 15.8 Hz, 1H), 4.68 (d, J = 15.8 Hz, 1H), 3.67 (d, J = 5.8 Hz, 1H), 3.48 – 3.30 (m, 1H), 2.35 – 2.10 (m, 2H), 1.61 (s, 3H), 1.04 (t, J = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.5, 187.4, 175.2, 151.4, 138.3, 126.6, 76.4, 65.8, 60.0, 53.4, 26.4, 17.9, 12.0. HRMS (ESI, m/z) calcd for $C_{13}H_{14}O_3$ $[M+H]^+$ 219.1016, found 219.1023. $[\alpha]^{16}_D$ = -17.8° (c 0.63, $CHCl_3$); >99% ee; Chiral HPLC analysis of the product: Phenomenex 00G-4457-E0 250X4.6 mm 5u column; hexane/2-propanol = 70/30, detected at 254 nm, flow rate 1 mL/min, Retention times: 22.3 min (minor), 23.9 min (major).



Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	22.240	76.860	63.035	50.25	52.03
2	24.892	76.108	58.121	49.75	47.97
Total:		**152.968**	**121.156**	**100.00**	**100.00**

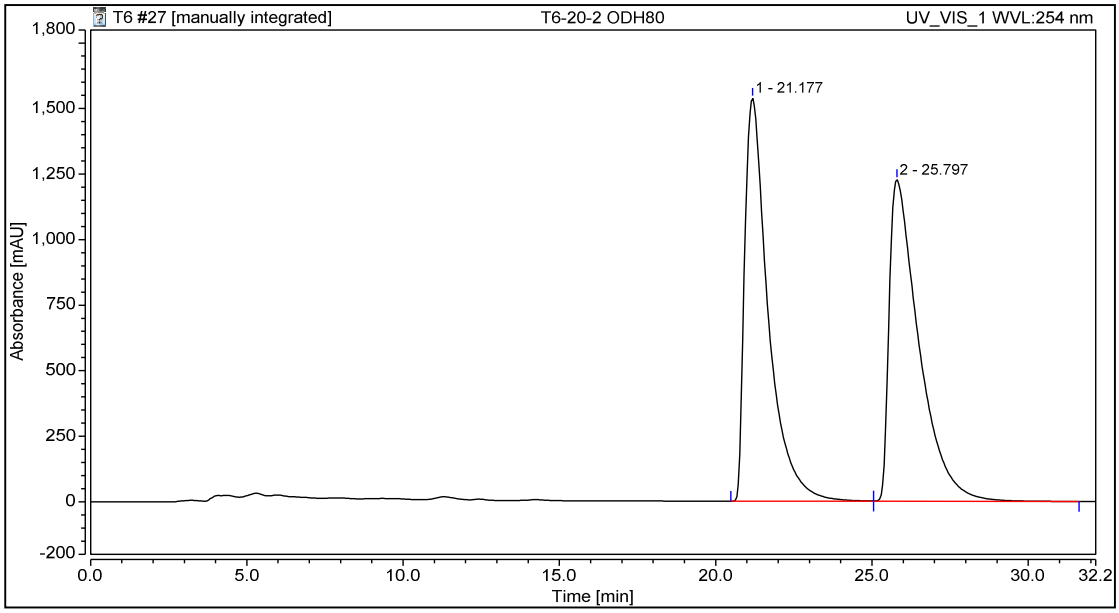


Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	22.295	3.187	3.563	0.37	0.53
2	23.927	861.772	665.054	99.63	99.47
Total:		**864.960**	**668.617**	**100.00**	**100.00**

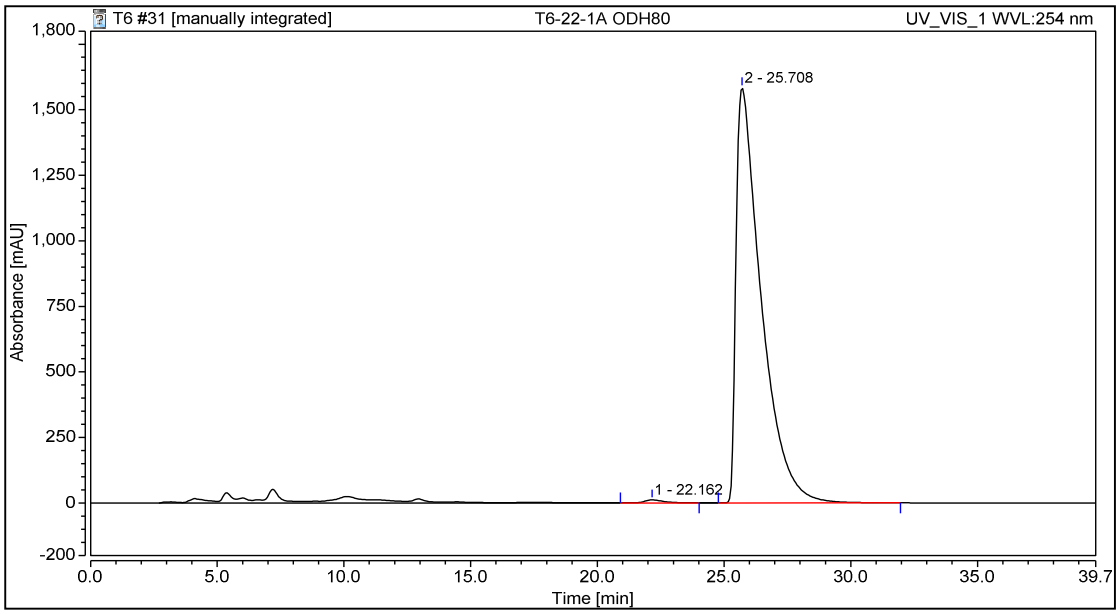


2n

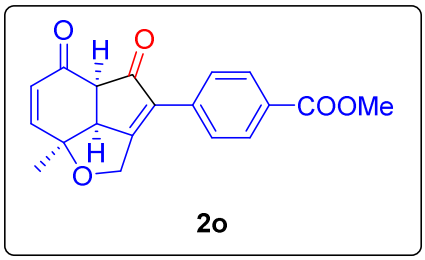
White solid. 65% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 – 7.31 (m, 5H), 6.60 (dd, *J* = 10.3, 1.1 Hz, 1H), 5.81 (d, *J* = 10.3 Hz, 1H), 5.17 (d, *J* = 16.7 Hz, 1H), 4.76 (dd, *J* = 16.6, 1.5 Hz, 1H), 3.85 (d, *J* = 6.0 Hz, 1H), 3.58 (d, *J* = 4.5 Hz, 1H), 1.67 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.7, 187.0, 176.6, 151.5, 134.6, 129.7, 129.2, 128.8, 128.3, 126.9, 76.6, 67.2, 60.1, 50.3, 26.4. HRMS (ESI, m/z) calcd for $C_{21}H_{16}O_3$ $[M+H]^+$ 267.1016, found 267.1019. 99% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 80/20, detected at 254 nm, flow rate 1 mL/min, Retention times: 22.2 min (minor), 25.7 min (major).



Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	21.177	1349.487	1537.035	50.02	55.62
2	25.797	1348.474	1226.494	49.98	44.38
Total:		**2697.960**	**2763.529**	**100.00**	**100.00**

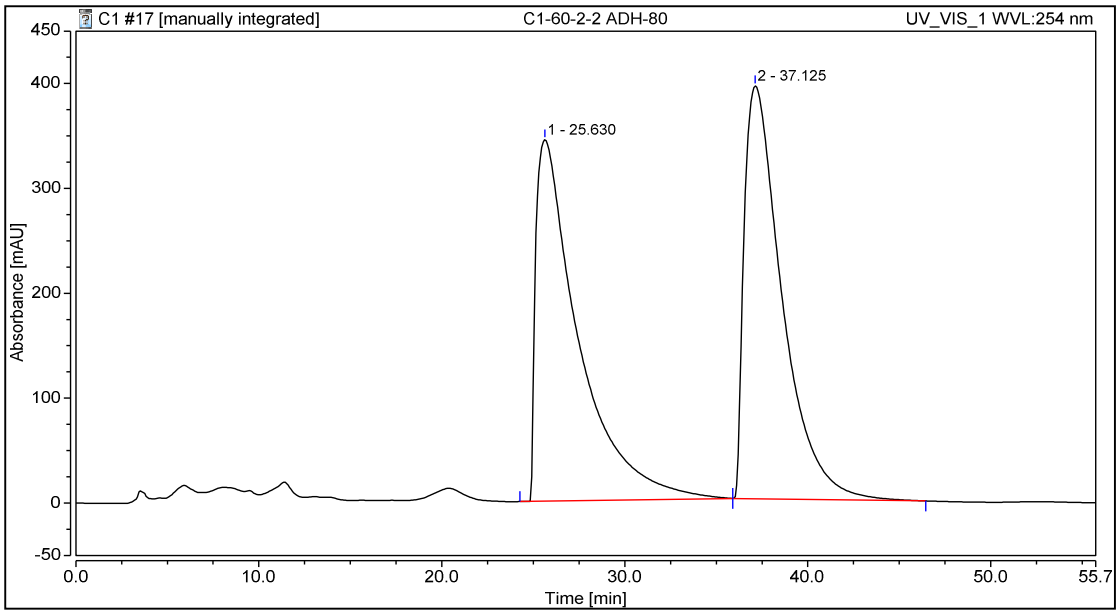


Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	22.162	9.941	11.417	0.54	0.72
2	25.708	1822.960	1582.922	99.46	99.28
Total:		**1832.901**	**1594.339**	**100.00**	**100.00**

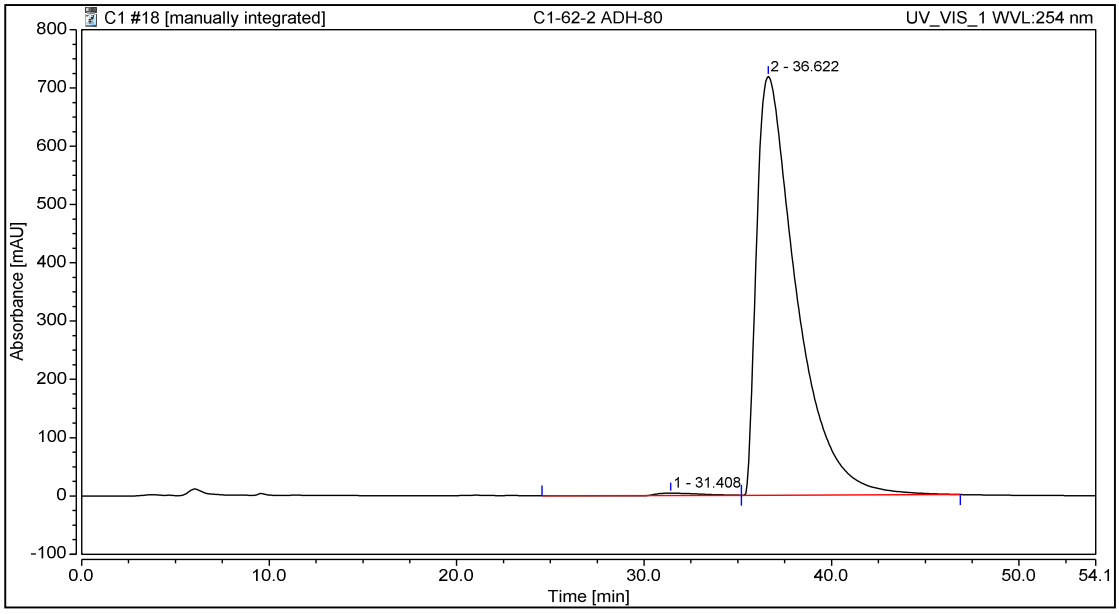


2o

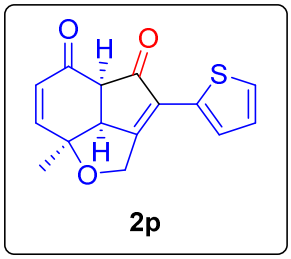
White solid. 79% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.5 Hz, 2H), 7.55 (d, *J* = 8.4 Hz, 2H), 6.62 (dd, *J* = 10.3, 1.5 Hz, 1H), 5.83 (d, *J* = 10.3 Hz, 1H), 5.20 (dd, *J* = 16.9, 1.1 Hz, 1H), 4.77 (dd, *J* = 16.9, 1.7 Hz, 1H), 3.92 (s, 3H), 3.87 (d, *J* = 6.0 Hz, 1H), 3.70 – 3.57 (m, 1H), 1.68 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.3, 186.6, 178.8, 166.4, 151.5, 133.9, 133.7, 130.4, 129.9, 128.1, 127.0, 76.2, 67.2, 60.1, 52.3, 50.6, 26.3. HRMS (ESI, m/z) calcd for $C_{19}H_{16}O_5$ $[M+H]^+$ 325.1071, found 325.1076. $[\alpha]^{17}_D$ = -52.5° (c 0.83, $CHCl_3$); >99% ee; Chiral HPLC analysis of the product: Daicel Chiralpak AD-H 250X4.6 mm 5u column; hexane/2-propanol = 80/20, detected at 254 nm, flow rate 1 mL/min, Retention times: 31.4 min (minor), 36.6 min (major).



Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	25.630	929.197	344.582	49.58	46.67
2	37.125	944.765	393.680	50.42	53.33
Total:		**1873.961**	**738.262**	**100.00**	**100.00**

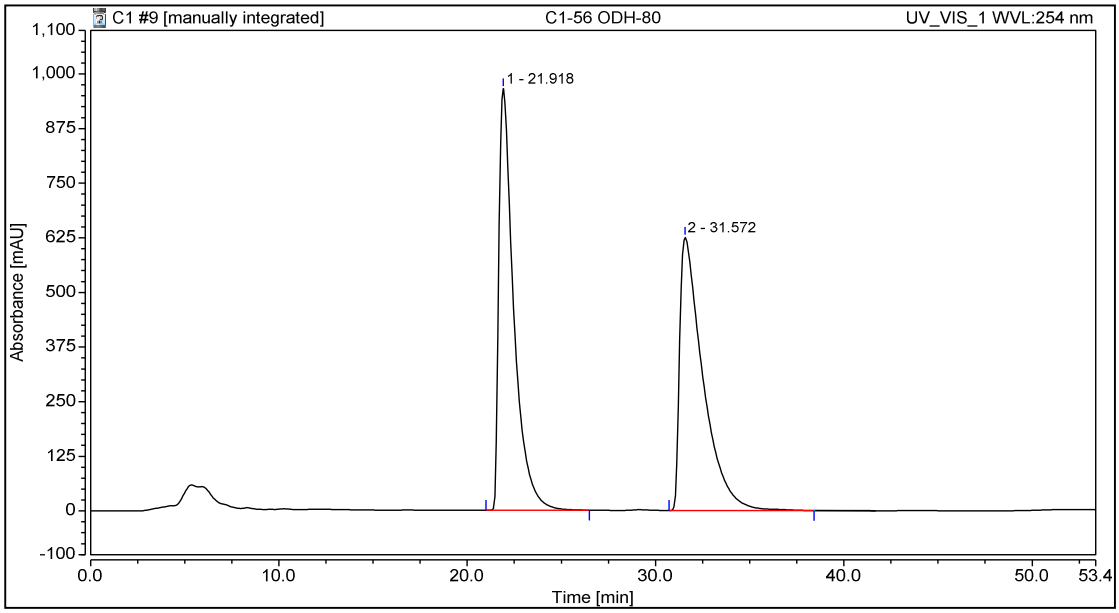


Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	31.408	9.006	3.989	0.50	0.55
2	36.622	1776.116	718.712	99.50	99.45
Total:		**1785.123**	**722.700**	**100.00**	**100.00**

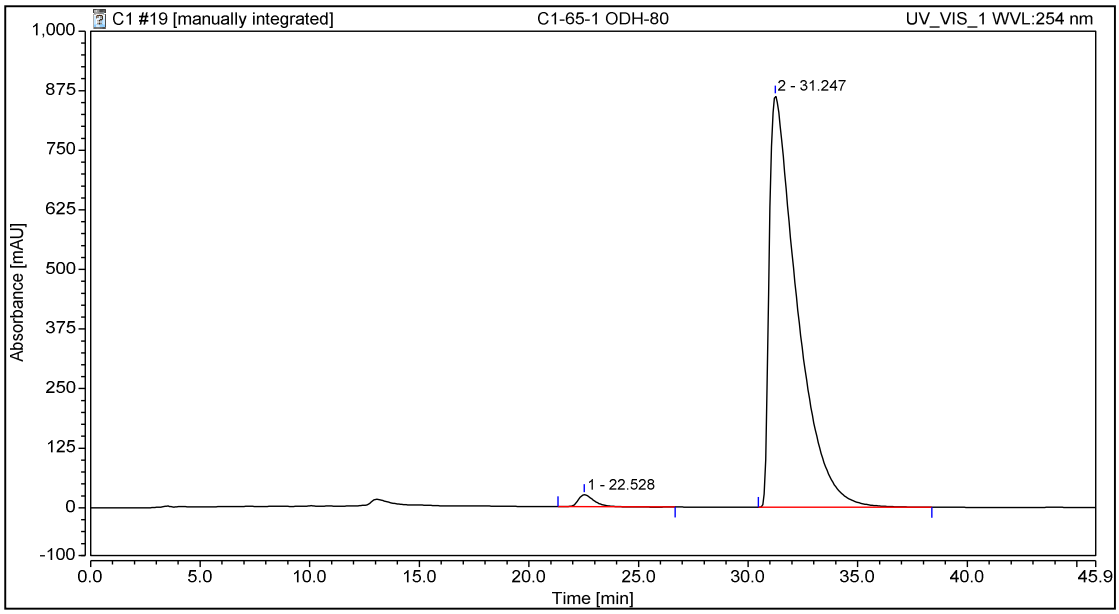


2p

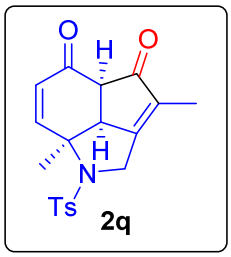
White solid. 60% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (d, *J* = 3.6 Hz, 1H), 7.43 (d, *J* = 5.0 Hz, 1H), 7.20 – 7.05 (m, 1H), 6.67 – 6.56 (m, 1H), 5.81 (d, *J* = 10.3 Hz, 1H), 5.06 (dd, *J* = 17.1, 1.8 Hz, 1H), 4.85 (dd, *J* = 17.1, 2.1 Hz, 1H), 3.84 (d, *J* = 5.9 Hz, 1H), 3.58 (dt, *J* = 12.8, 5.4 Hz, 1H), 1.66 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.4, 186.6, 172.9, 151.3, 131.5, 128.9, 127.8, 127.7, 127.5, 127.1, 76.5, 67.0, 59.4, 50.6, 26.3. 97% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 80/20, detected at 254 nm, flow rate 1 mL/min, Retention times: 22.5 min (minor), 31.2 min (major).



Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	21.918	890.410	964.679	49.88	60.68
2	31.572	894.625	625.086	50.12	39.32
Total:		**1785.034**	**1589.765**	**100.00**	**100.00**

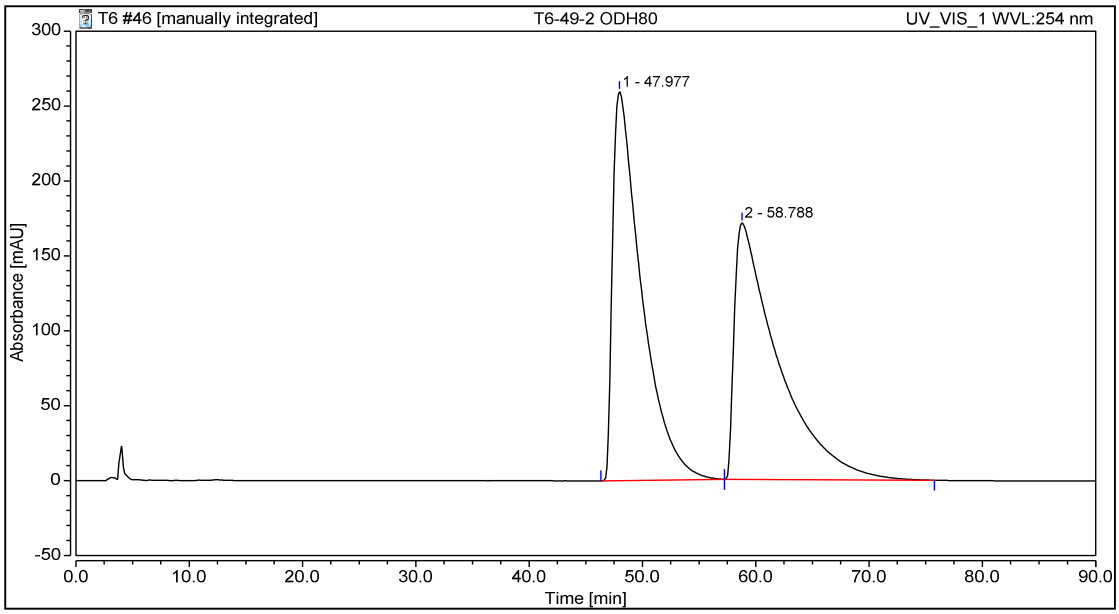


Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	22.528	20.687	25.273	1.60	2.85
2	31.247	1272.386	862.840	98.40	97.15
Total:		**1293.073**	**888.113**	**100.00**	**100.00**

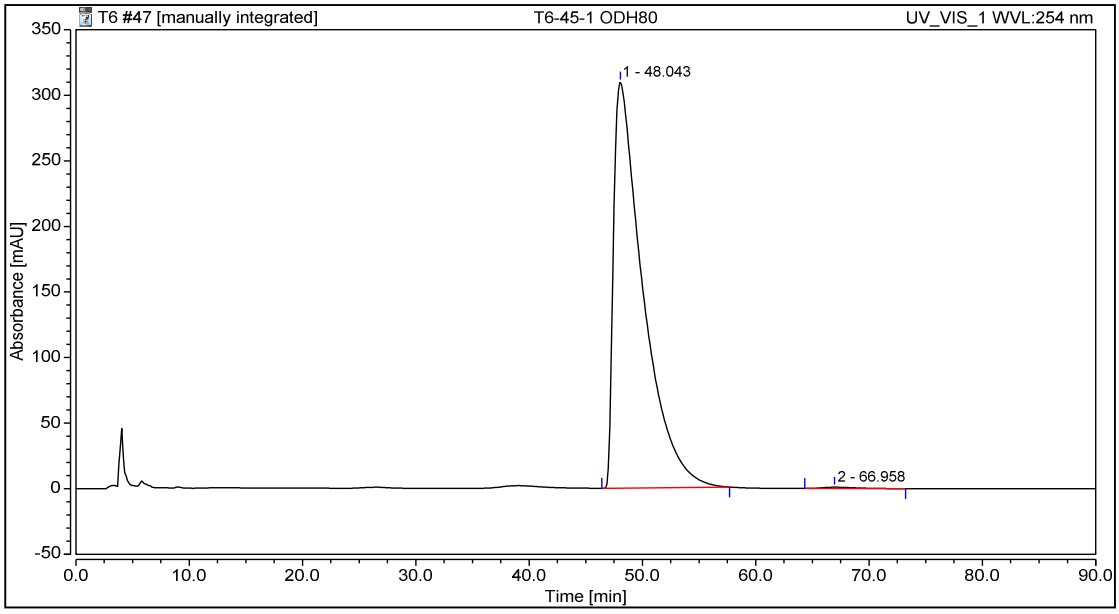


2q

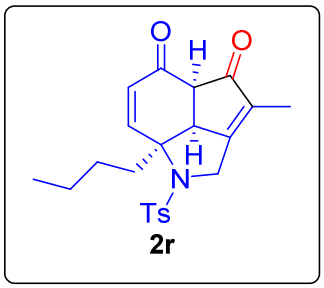
White solid. 75% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 (d, J = 8.3 Hz, 2H), 7.36 (d, J = 8.2 Hz, 2H), 7.13 (dd, J = 10.4, 1.4 Hz, 1H), 5.77 (d, J = 10.4 Hz, 1H), 4.56 (d, J = 15.5 Hz, 1H), 4.39 – 4.25 (m, 1H), 3.59 (d, J = 6.0 Hz, 1H), 3.48 – 3.38 (m, 1H), 2.46 (s, 3H), 1.82 (s, 3H), 1.76 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 198.2, 186.1, 167.7, 150.4, 144.1, 138.1, 133.9, 130.0, 126.9, 125.5, 63.5, 58.0, 52.5, 48.6, 27.3, 21.6, 9.1. HRMS (ESI, m/z) calcd for $C_{19}H_{19}NO_4S$ $[M+H]^+$ 358.1108, found 358.1124. $[\alpha]^{16}_D$ = 164.3° (c 0.10, $CHCl_3$); >99% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 80/20, detected at 254 nm, flow rate 1 mL/min, Retention times: 48.0 min (major), 67.0 (minor).



Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	47.977	765.414	259.674	50.08	60.28
2	58.788	763.053	171.137	49.92	39.72
Total:		**1528.468**	**430.811**	**100.00**	**100.00**

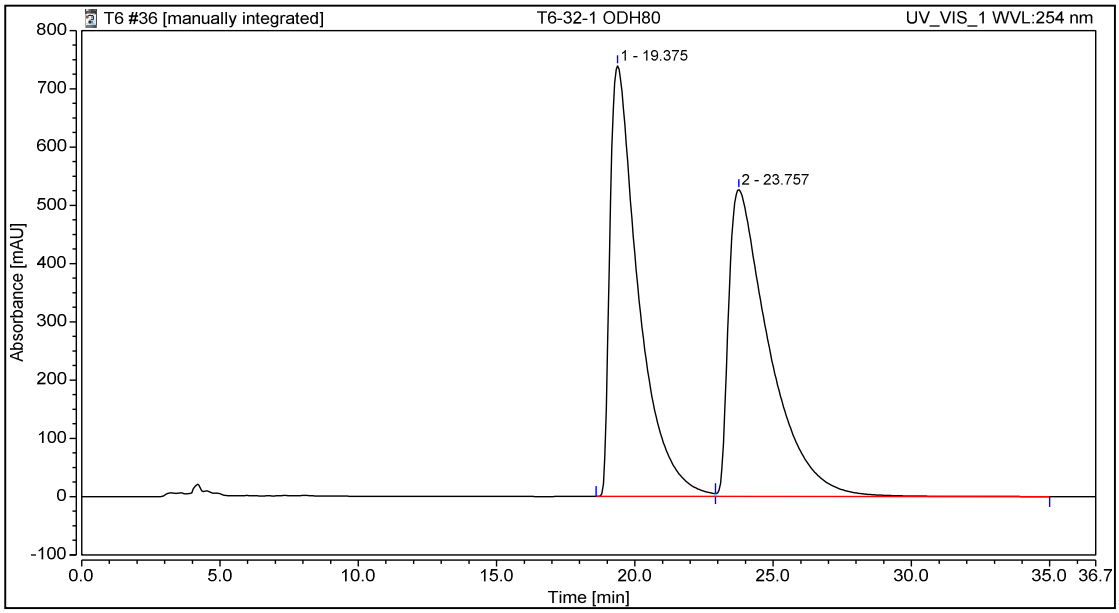


Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	48.043	929.652	309.715	99.63	99.66
2	66.958	3.435	1.048	0.37	0.34
Total:		**933.087**	**310.763**	**100.00**	**100.00**

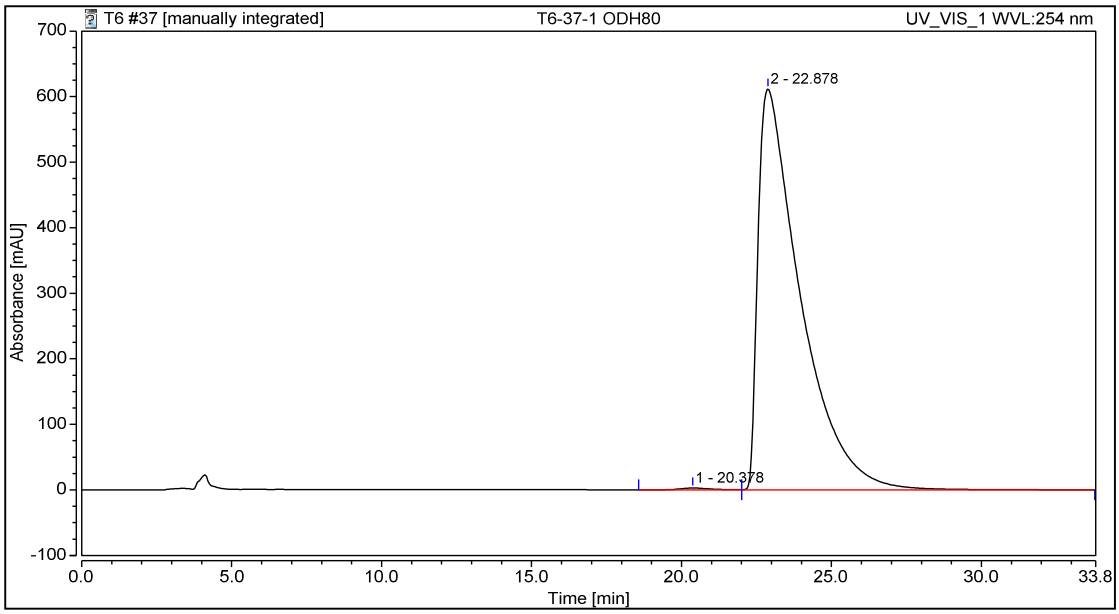


2r

White solid. 96% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.3 Hz, 2H), 7.36 (d, *J* = 8.2 Hz, 2H), 7.06 (dd, *J* = 10.5, 1.3 Hz, 1H), 5.89 (d, *J* = 10.5 Hz, 1H), 4.56 (d, *J* = 15.3 Hz, 1H), 4.25 (d, *J* = 15.3 Hz, 1H), 3.55 (d, *J* = 6.0 Hz, 1H), 3.47 – 3.38 (m, 1H), 2.55 – 2.47 (m, 1H), 2.46 (s, 3H), 1.89 (td, *J* = 12.9, 5.1 Hz, 1H), 1.74 (d, *J* = 8.7 Hz, 3H), 1.38 – 1.29 (m, 2H), 1.26 (t, *J* = 7.1 Hz, 1H), 1.22 – 1.08 (m, 2H), 0.86 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 198.4, 186.5, 167.9, 148.4, 144.1, 138.1, 133.5, 129.9, 127.0, 67.7, 59.3, 50.5, 48.5, 38.8, 26.8, 22.6, 21.6, 13.8, 9.1. >99% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 80/20, detected at 254 nm, flow rate 1 mL/min, Retention times:

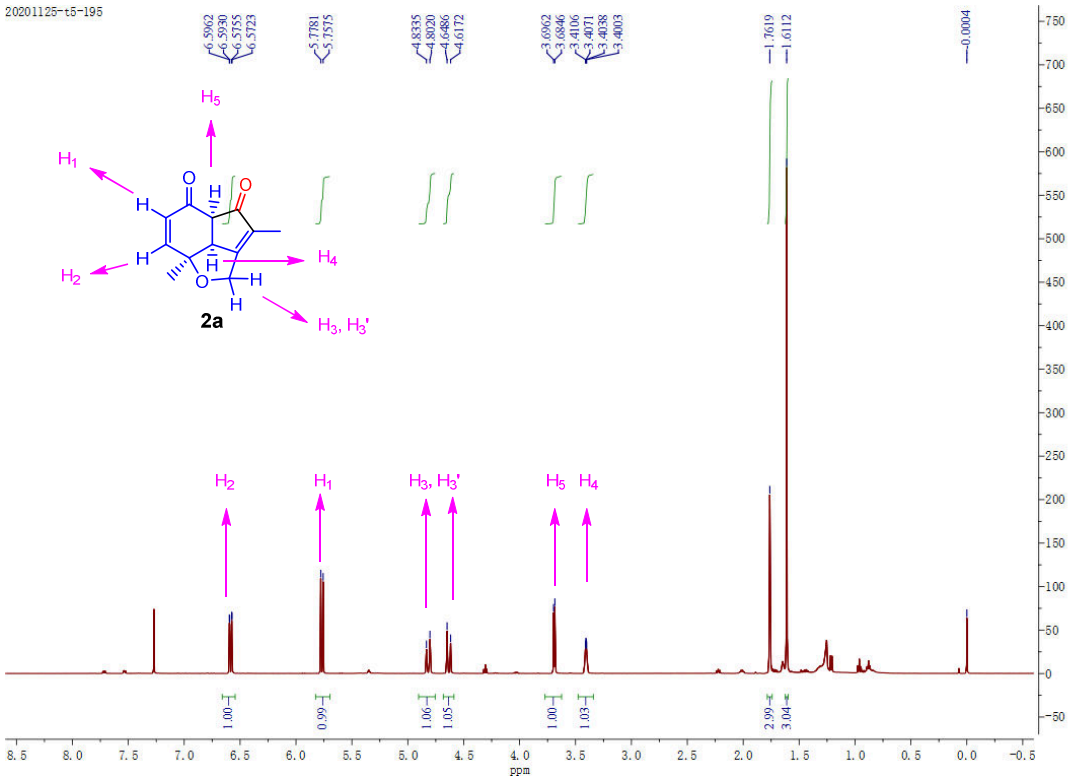


Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	19.375	884.997	739.284	49.66	58.40
2	23.757	897.133	526.677	50.34	41.60
Total:		**1782.130**	**1265.961**	**100.00**	**100.00**



Integration Results					
No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	20.378	3.119	2.782	0.31	0.45
2	22.878	1000.851	611.619	99.69	99.55
Total:		**1003.970**	**614.402**	**100.00**	**100.00**

8. NMR and HRMS Spectra of All Compounds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5.7781
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4.6486
4.6172
3.6962
3.6846
3.4106
3.4071
3.4038
3.4003
1.7619
1.6112
0.0004
H5
H1
H2
H4
H3, H3'
2a
H2
H1
H3, H3'
H5
H4
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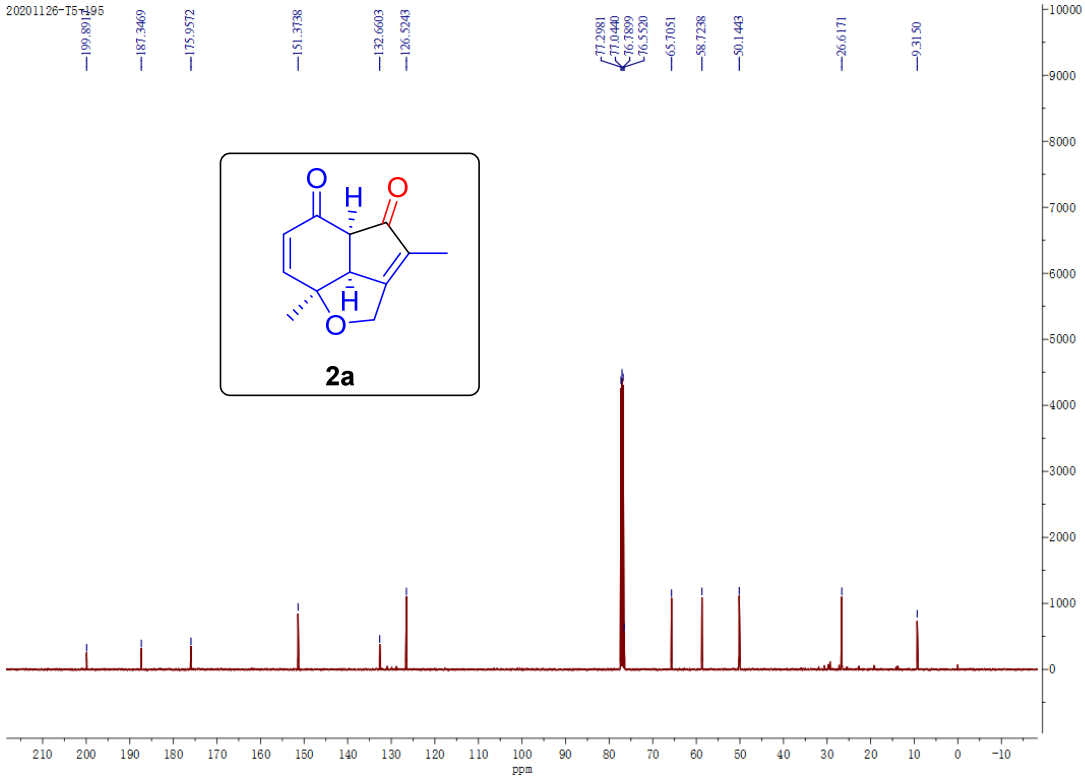
0.99
1.06
1.05
1.00
1.03
2.99
3.04
ppm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126.5243
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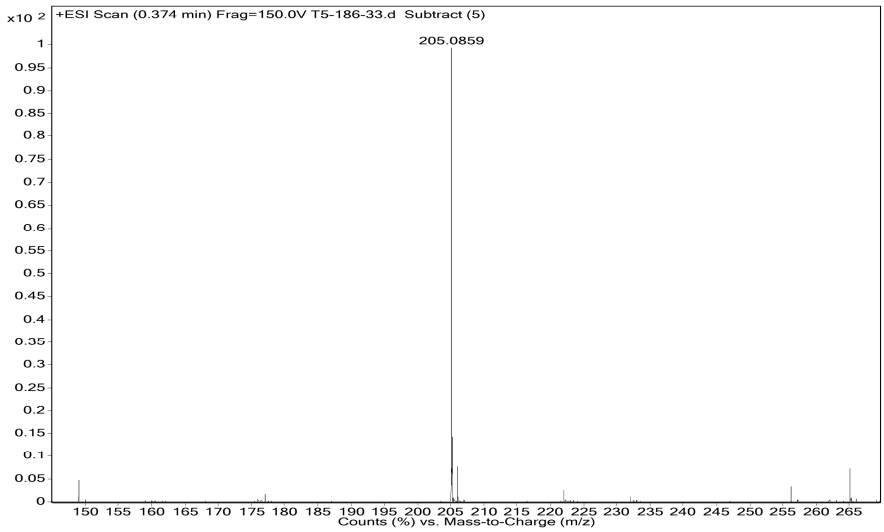
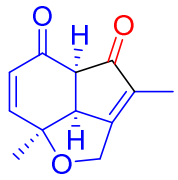
77.0440
76.7899
76.5520
65.7051
58.7238
50.1443
26.6171
9.3150
2a
ppm

Sample Name	T5-186-33	Position	P1-F3	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	T5-186-33.d	ACQ Method	0103.m	Comment		Acquired Time	11/17/2020 8:23:48 AM

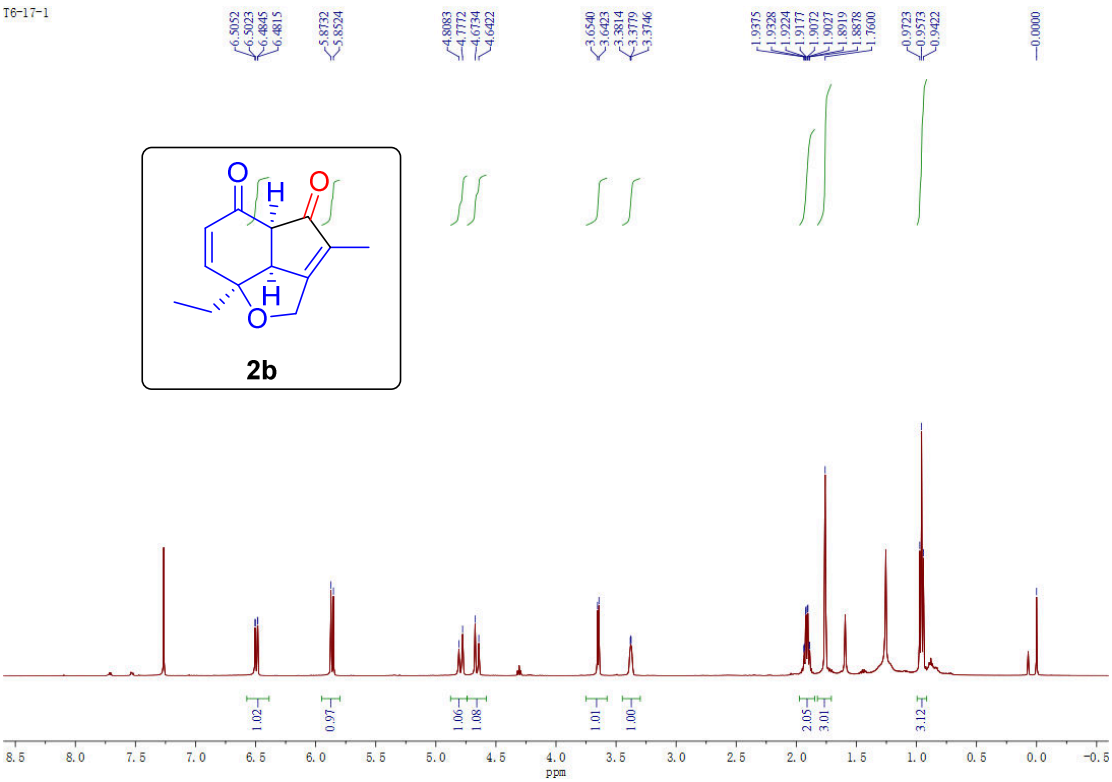




2a

Molecular Weight: 204.22Chemical Formula: $C_{12}H_{12}O_3$
Exact Mass: 204.0786
Molecular Weight: 204.2250
m/z: 204.0786 (100.0%), 205.0820 (13.0%)

HRMS (ESI, m/z) calcd for $C_{12}H_{12}O_3$ $[M+H]^+$ 205.0859, found 205.0859.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3.6540
3.6423
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3.3746
1.9375
1.9328
1.9224
1.9177
1.9072
1.9027
1.8919
1.8878
1.7600
0.9723
0.9573
0.9422
0.0000
2b
1.02
0.97
1.06
1.08
1.01
1.00
2.05
3.01
3.12
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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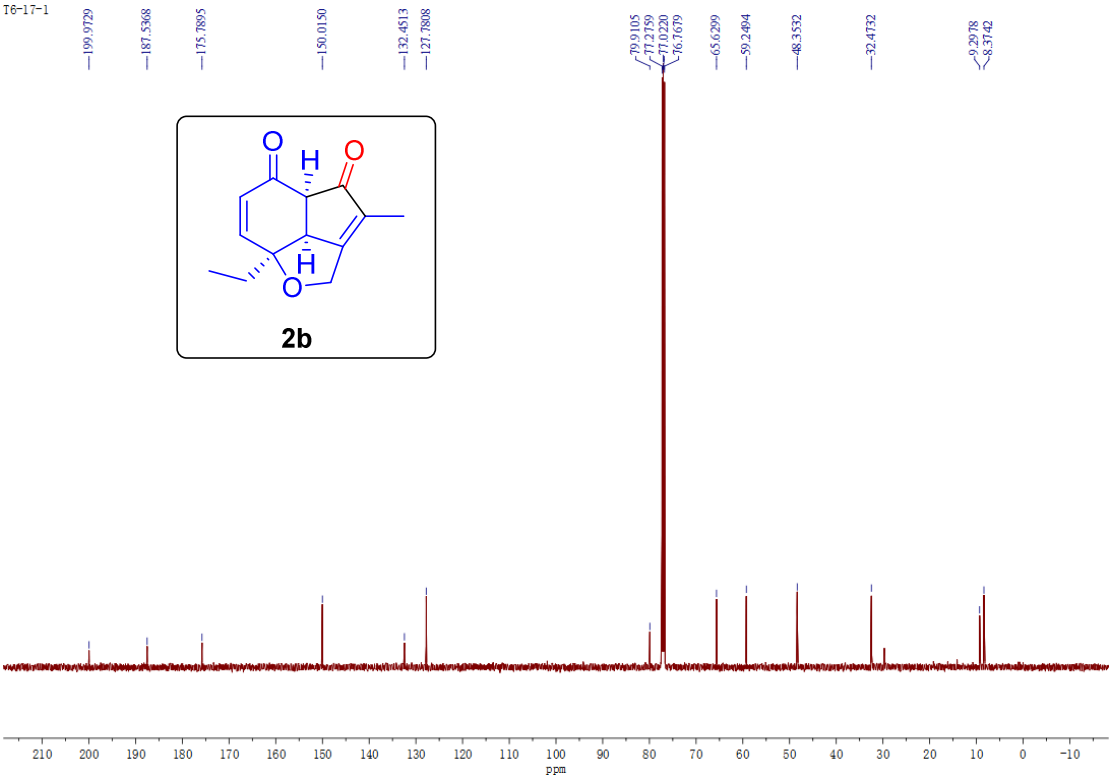
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65.6299
59.2494
48.3532
32.4732
9.2978
8.3742
2b
210
200
190
180
170
160
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40
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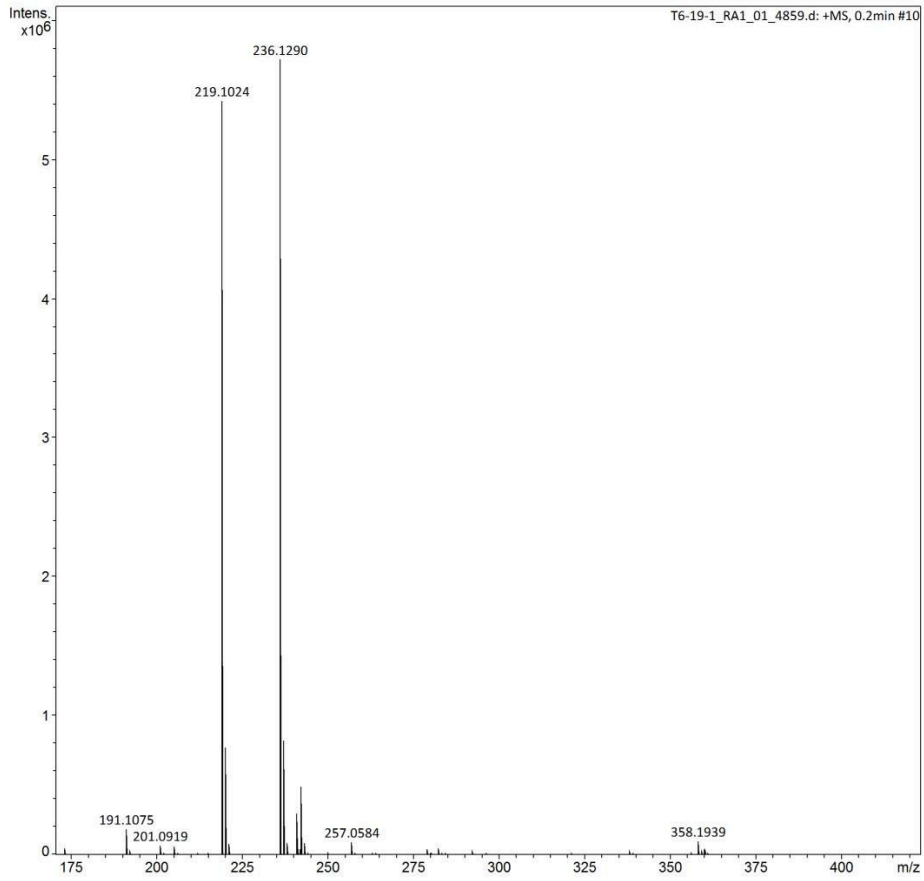
Display Report

Analysis Info

Analysis Name	D:\Data\fenglei\T6-19-1_RA1_01_4859.d	Acquisition Date	4/28/2021 3:28:51 PM
Method	1225-1.m	Operator	Demo User
Sample Name	T6-19-1	Instrument	impact II 1825265.10256
Comment			

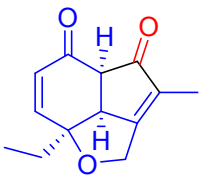
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	2600 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



T6-19-1_RA1_01_4859.d

Bruker Compass DataAnalysis 4.4 printed: 4/28/2021 3:54:37 PM by: demo Page 1 of 1

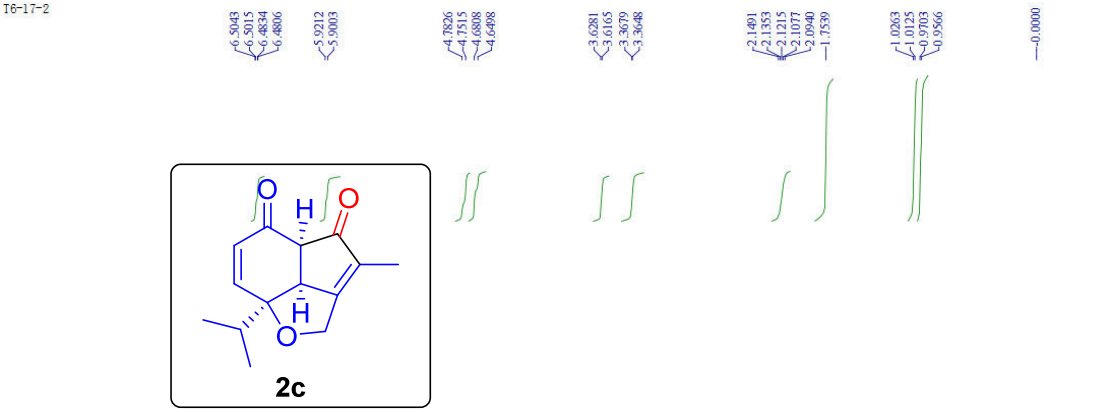


2b

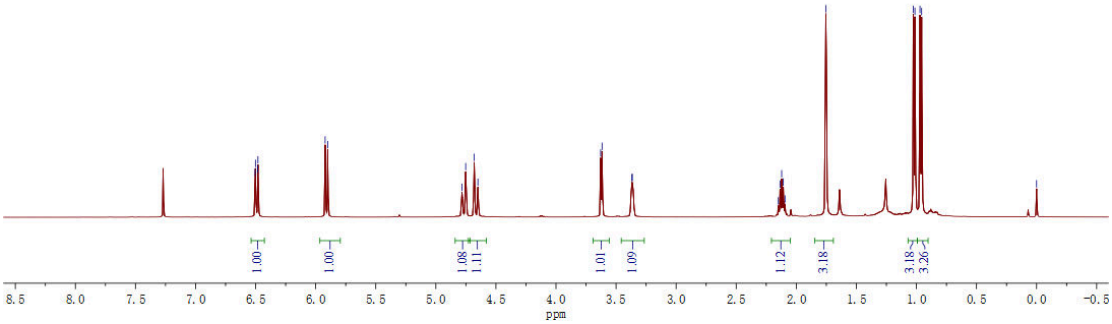
Chemical Formula: $C_{13}H_{14}O_3$
Exact Mass: 218.0943
Molecular Weight: 218.2520
m/z: 218.0943 (100.0%), 219.0976 (14.1%)

HRMS (ESI, m/z) calcd for $C_{13}H_{14}O_3$ $[M+H]^+$ 219.1016, found 219.1024.

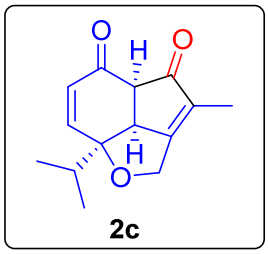
T6-17-2



2c



T6-17-2



2c

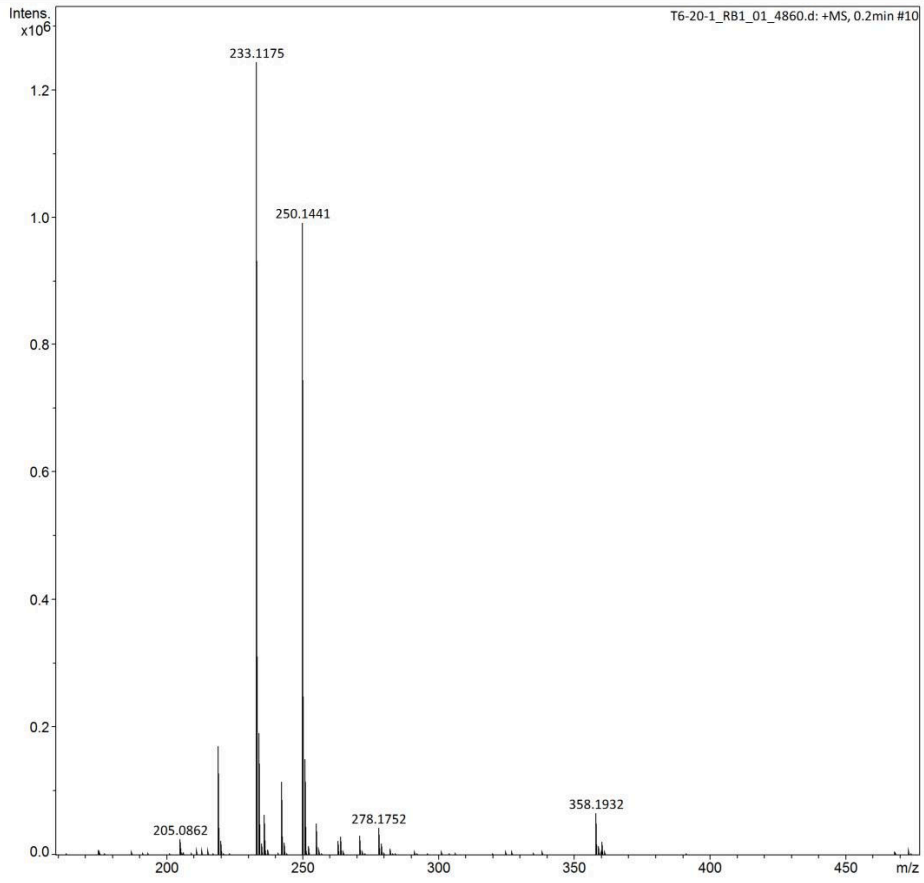
Display Report

Analysis Info

Analysis Name	D:\Data\fenglei\T6-20-1_RB1_01_4860.d	Acquisition Date	4/28/2021 3:31:16 PM
Method	1225-1.m	Operator	Demo User
Sample Name	T6-20-1	Instrument	impact II 1825265.10256
Comment			

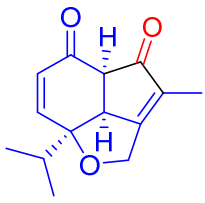
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	2600 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



T6-20-1_RB1_01_4860.d

Bruker Compass DataAnalysis 4.4 printed: 4/28/2021 3:56:57 PM by: demo Page 1 of 1



2c

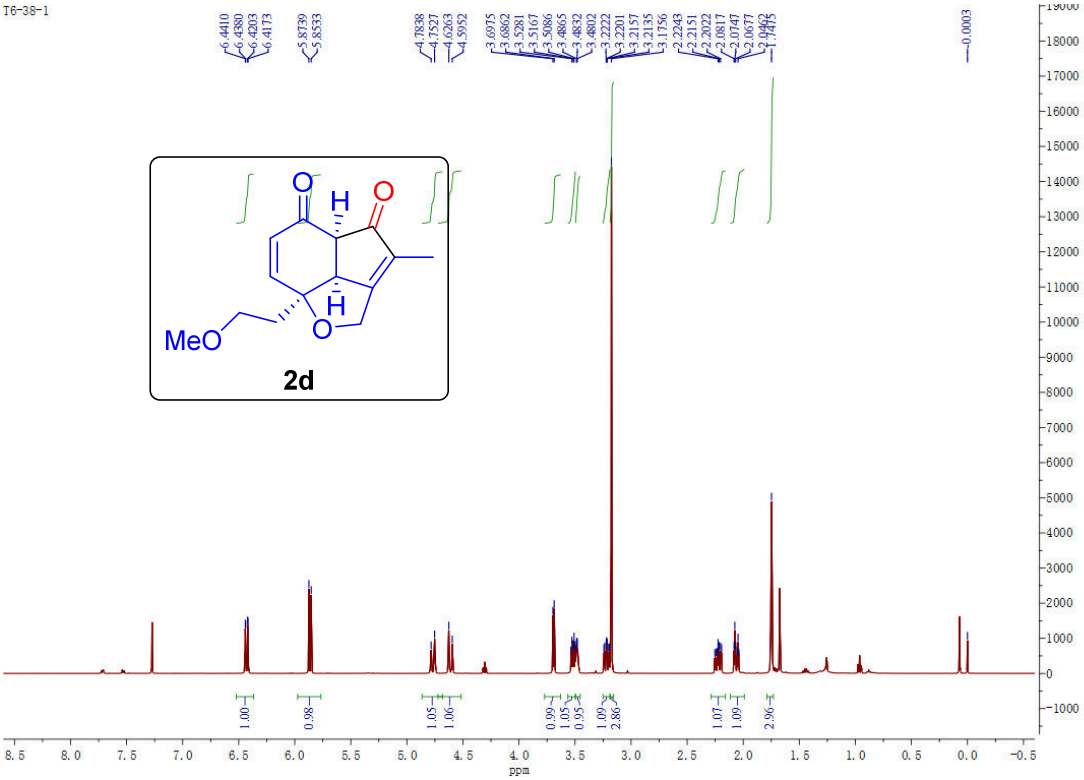
Chemical Formula: $C_{14}H_{16}O_3$

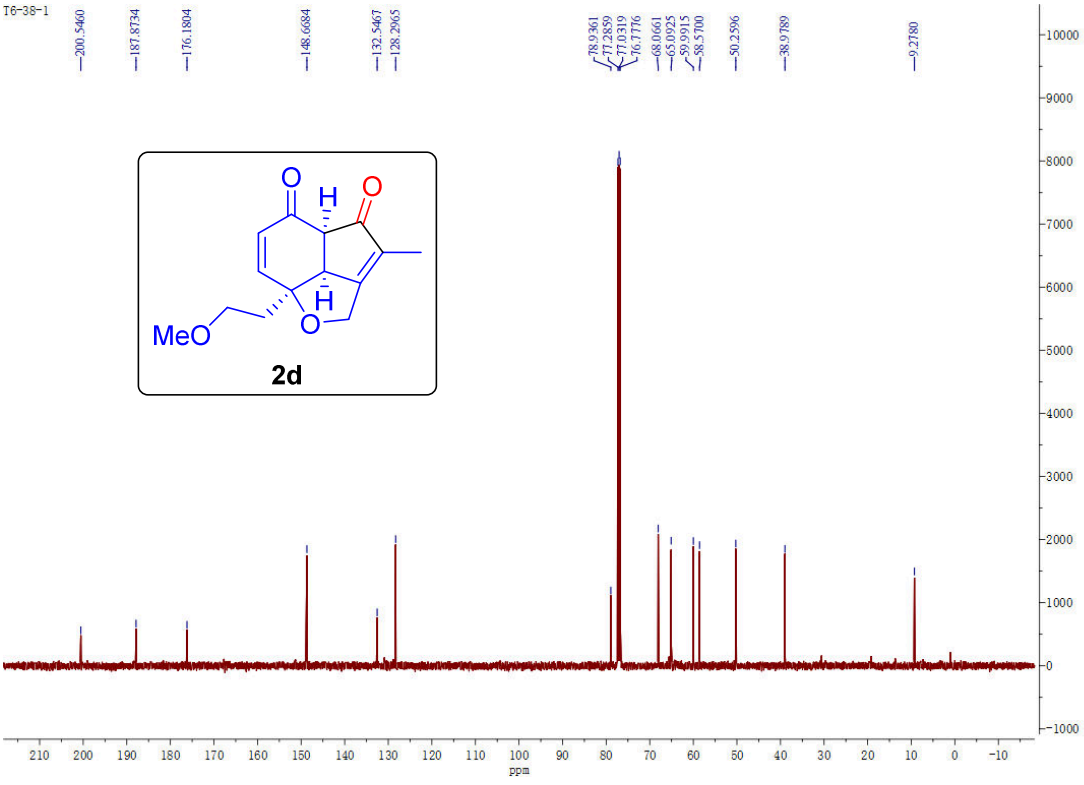
Exact Mass: 232.1099

Molecular Weight: 232.2790

m/z: 232.1099 (100.0%), 233.1133 (15.1%), 234.1167 (1.1%)

HRMS (ESI, m/z) calcd for $C_{14}H_{16}O_3$ $[M+H]^+$ 233.1172, found 233.1175.


T6-38-1
MeO
2d


T6-38-1
MeO
2d

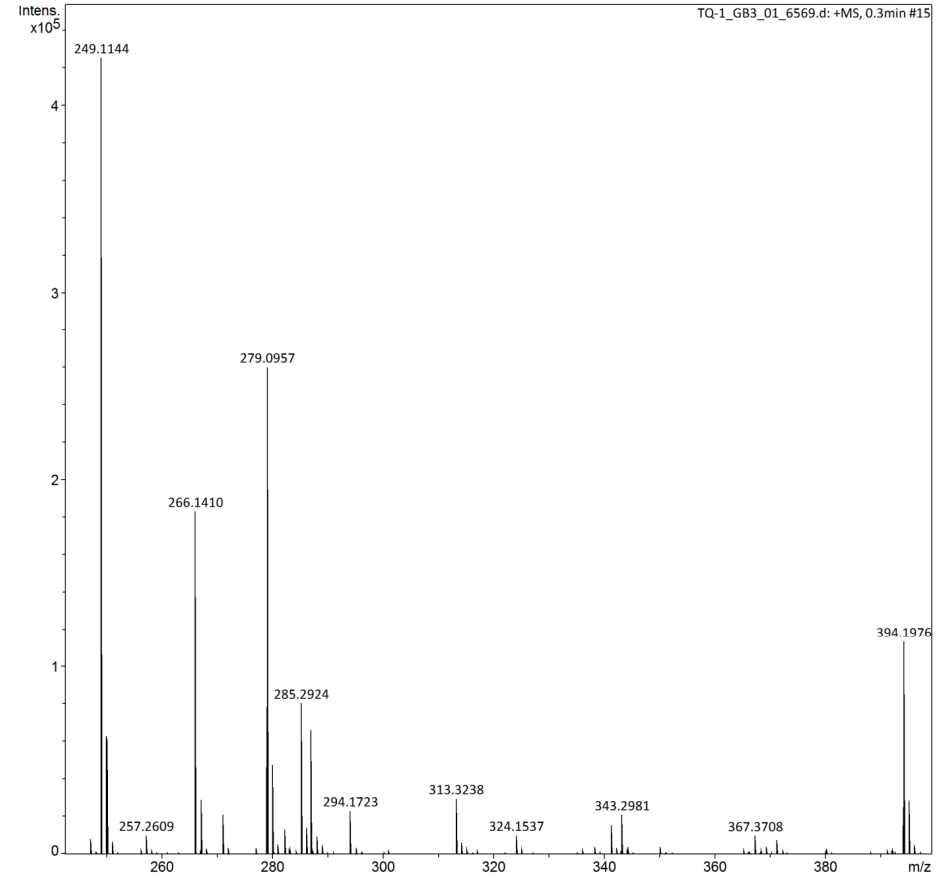
Display Report

Analysis Info

Analysis Name	D:\Data\fenglei\TQ-1_GB3_01_6569.d	Acquisition Date	6/18/2021 5:01:11 PM
Method	1225-1.m	Operator	Demo User
Sample Name	TQ-1	Instrument	impact II 1825265.10256
Comment			

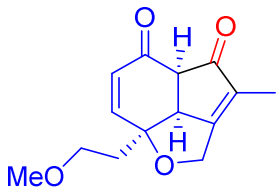
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	2600 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



TQ-1_GB3_01_6569.d

Bruker Compass DataAnalysis 4.4 printed: 6/18/2021 5:11:57 PM by: demo Page 1 of 1



2d

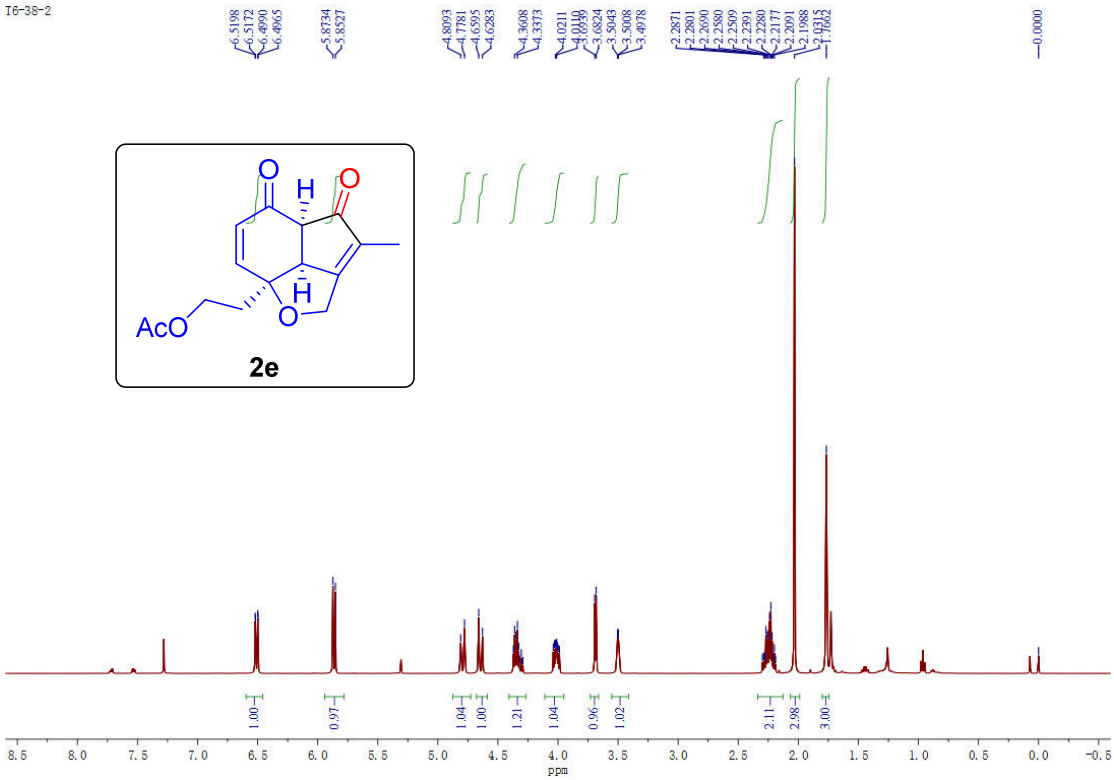
Chemical Formula: $C_{14}H_{16}O_4$

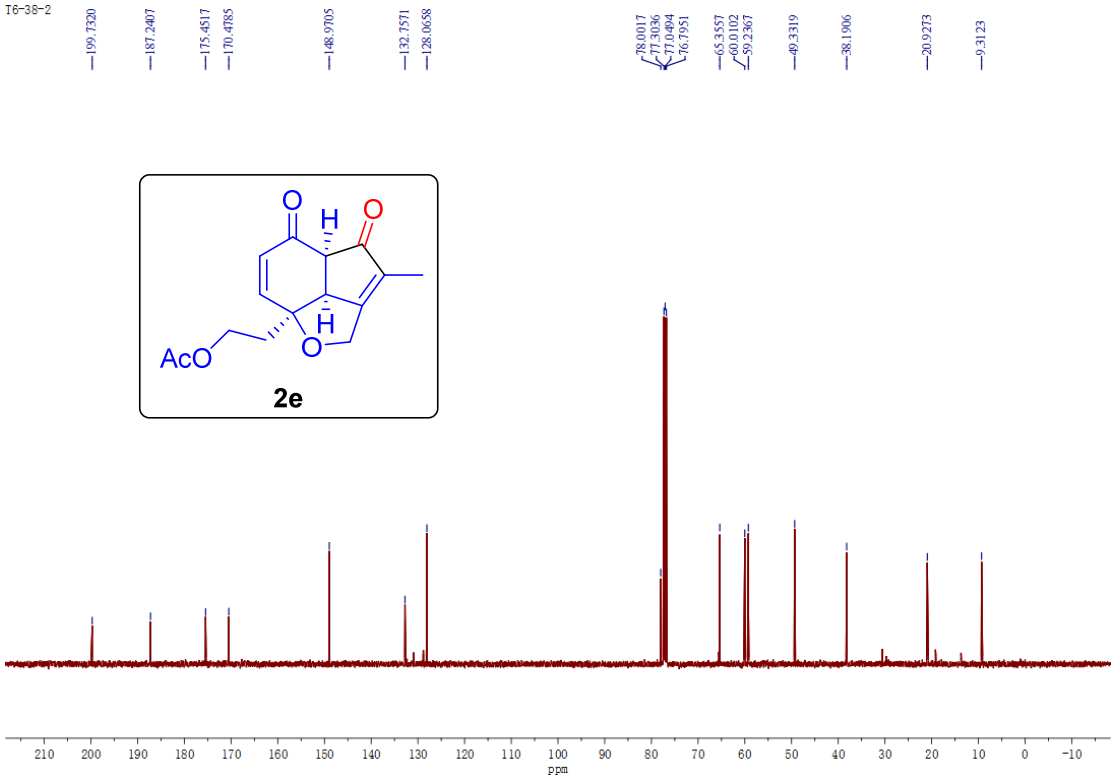
Exact Mass: 248.1049

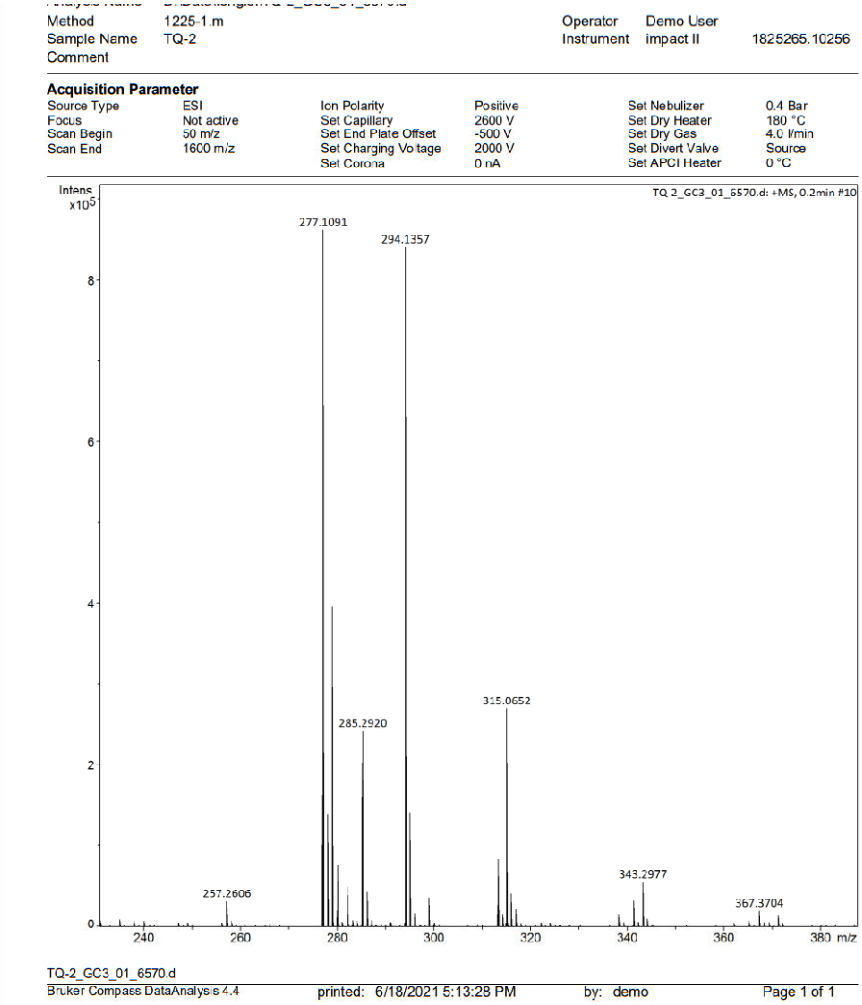
Molecular Weight: 248.2780

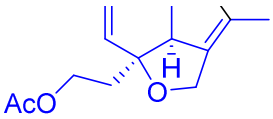
m/z: 248.1049 (100.0%), 249.1082 (15.1%), 250.1116 (1.1%)

HRMS (ESI, m/z) calcd for $C_{14}H_{16}O_4$ $[M+H]^+$ 249.1121, found 249.1144.


T6-38-2
2e
ppm


T6-38-2
2e
ppm

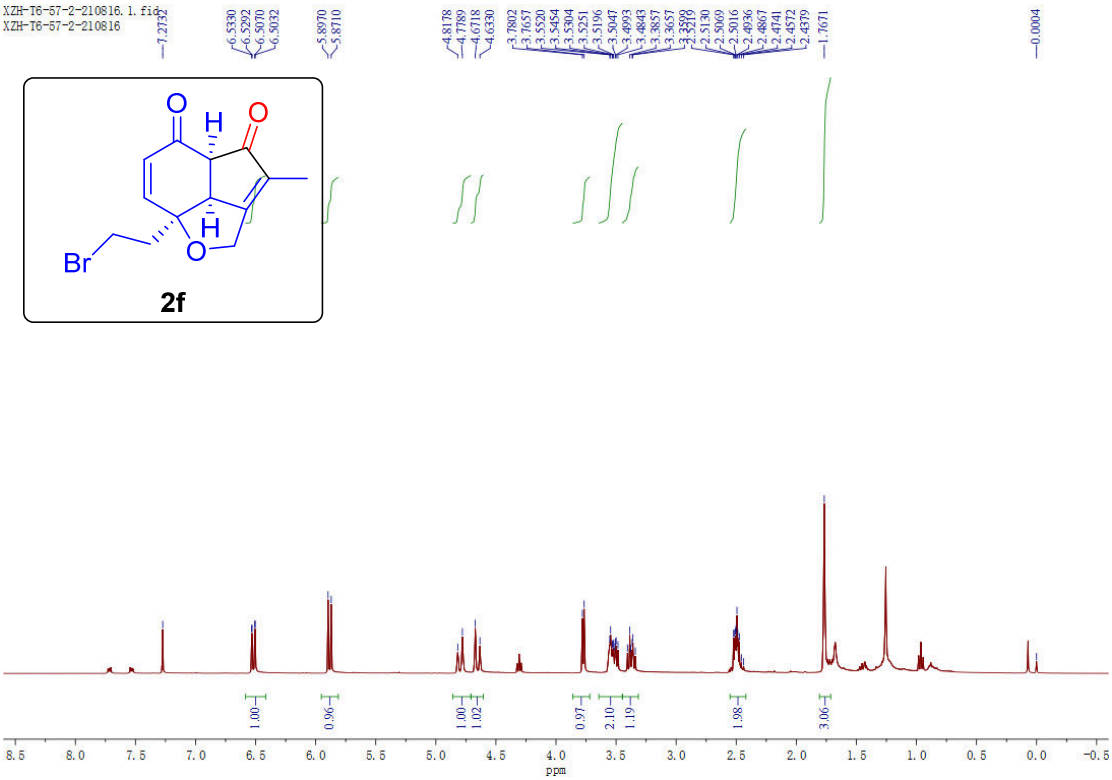


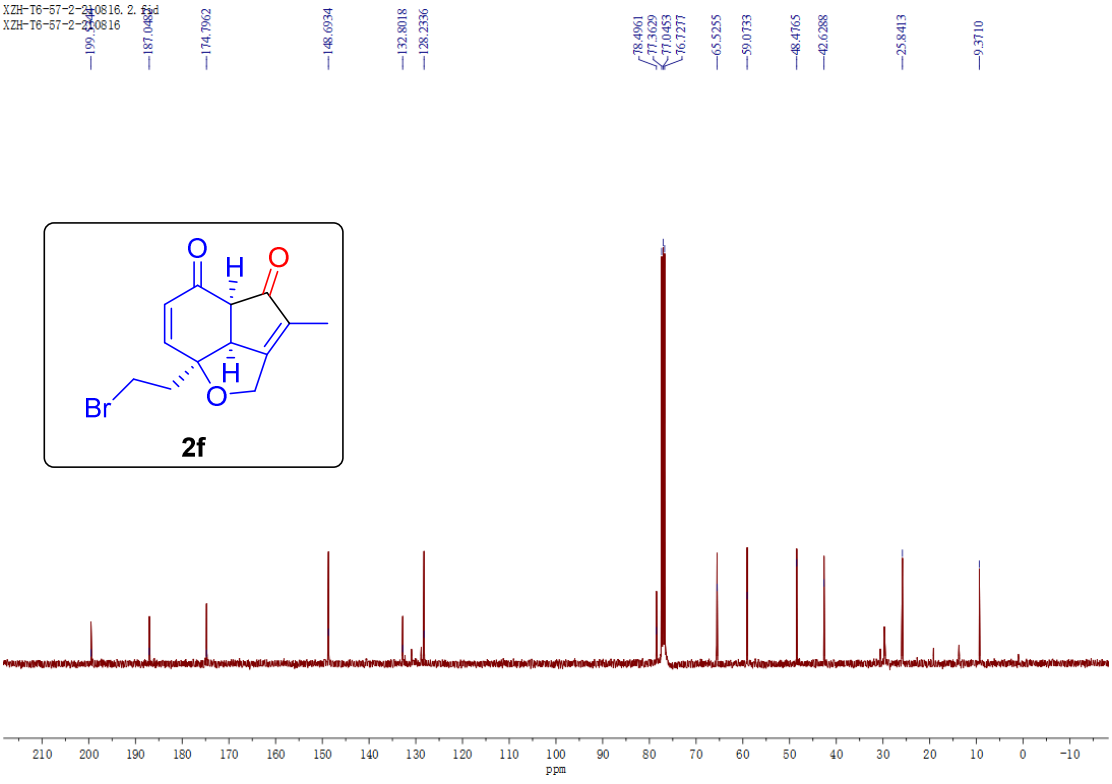


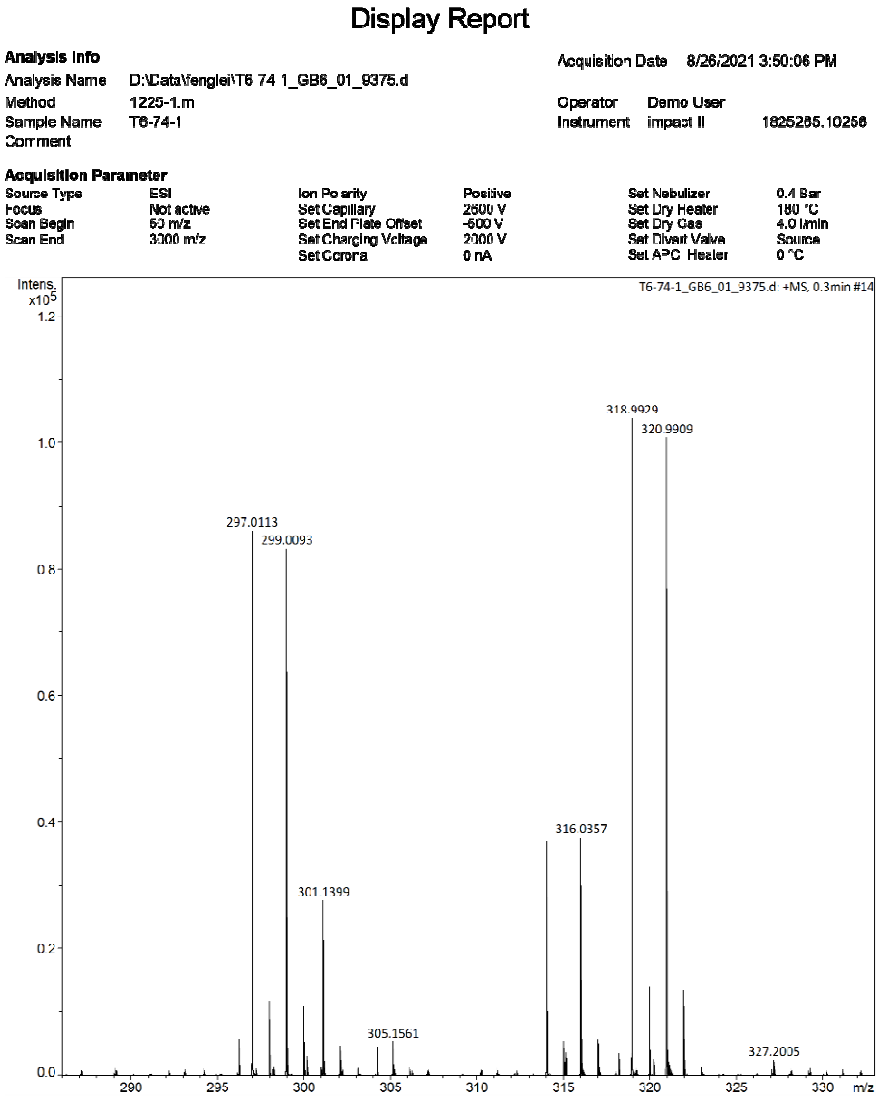
2e

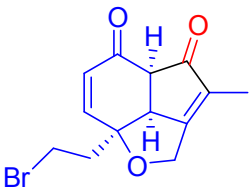
Chemical Formula: $C_{15}H_{16}O_5$
Exact Mass: 276.0998
Molecular Weight: 276.2880
m/z: 276.0998 (100.0%), 277.1031 (16.2%), 278.1065 (1.2%), 278.1040 (1.0%)

HRMS (ESI, m/z) calcd for $C_{15}H_{16}O_5$ $[M+H]^+$ 277.1071, found 277.1091.


XZH-T6-57-2-210816.1.fid
XZH-T6-57-2-210816
2f
ppm


XZH-T6-57-2-210816.2.fid
XZH-T6-57-2-210816
2f
ppm

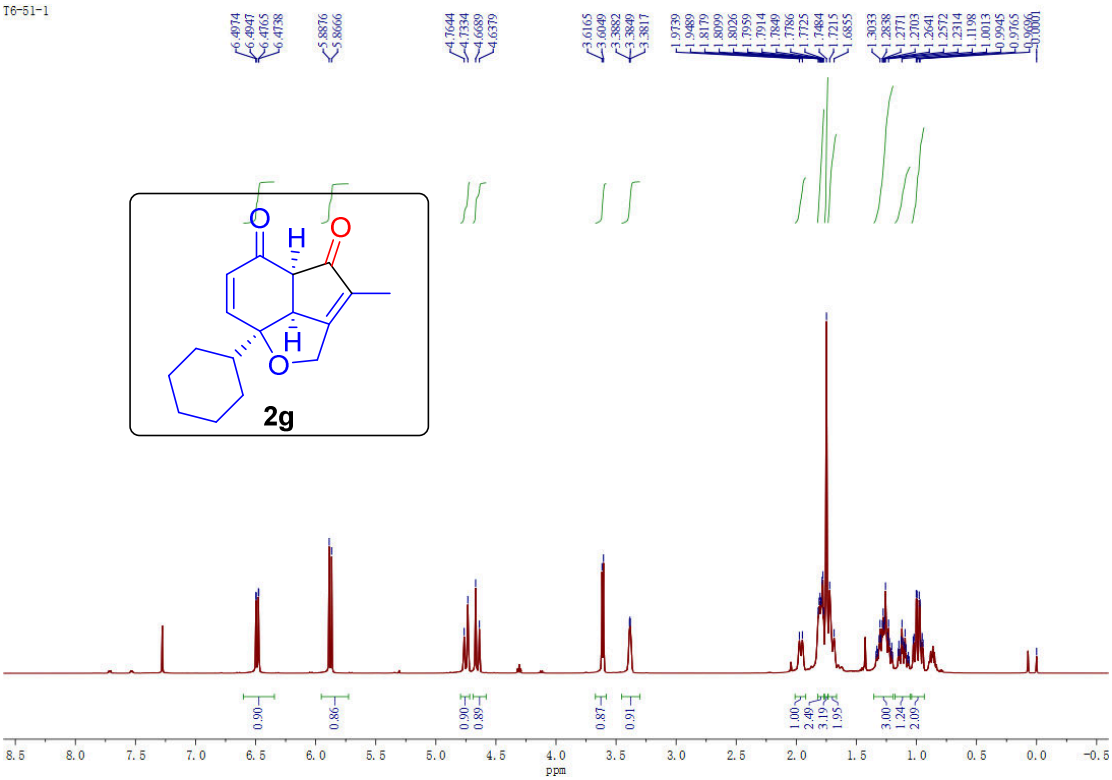


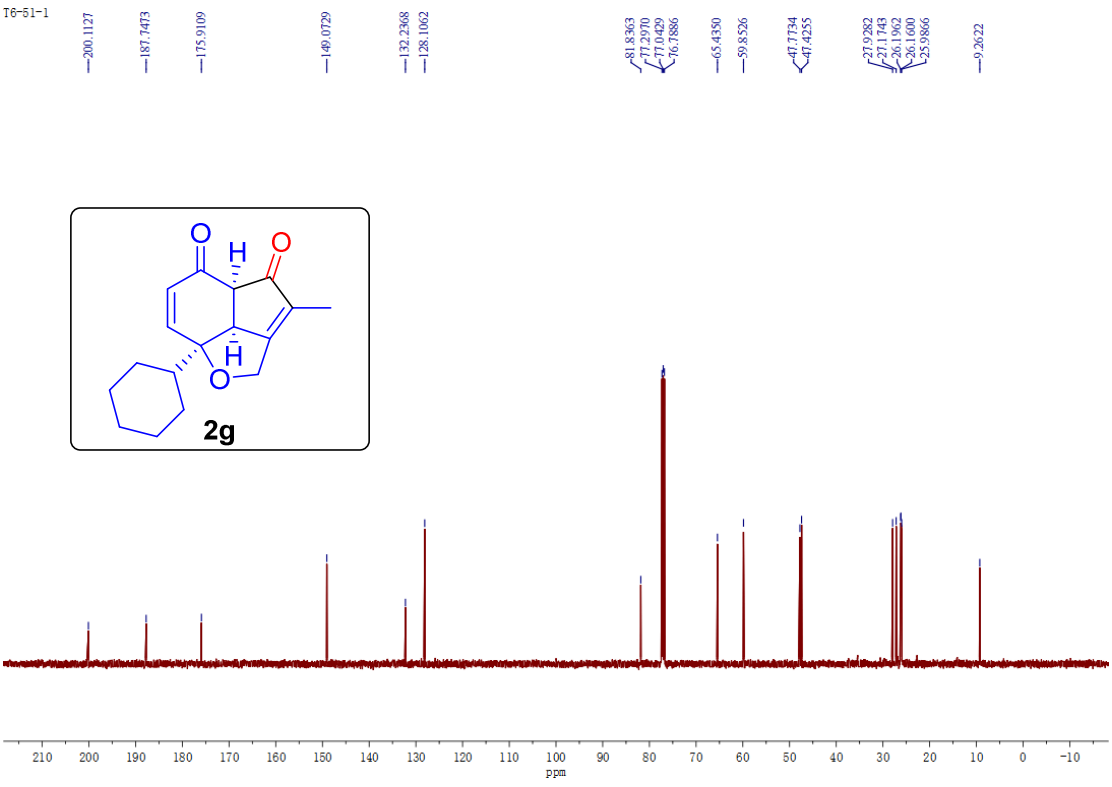


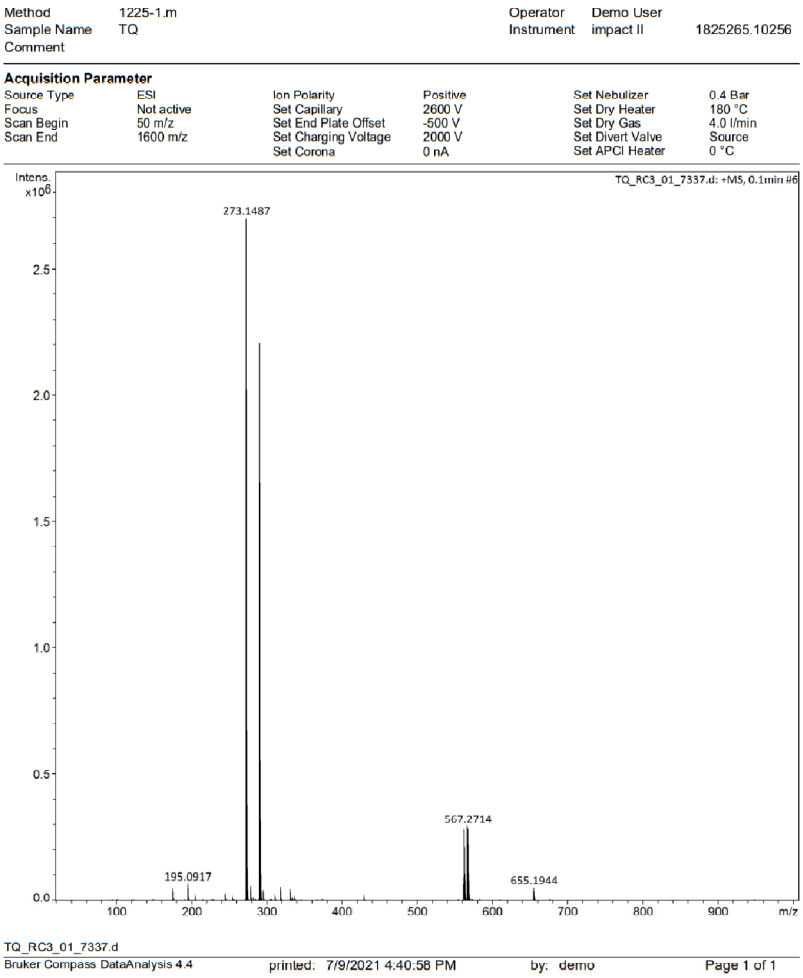
2f

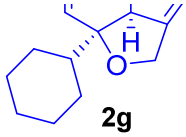
Chemical Formula: $C_{13}H_{13}BrO_3$
Exact Mass: 296.0048
Molecular Weight: 297.1480
m/z: 296.0048 (100.0%), 298.0028 (97.3%), 297.0082 (14.1%), 299.0061 (13.7%)

HRMS (ESI, m/z) calcd for $C_{13}H_{13}BrO_3$ $[M+H]^+$ 297.0121, found 297.0113.


T6-61-1
2g
ppm


T6-61-1
2g
ppm





2g

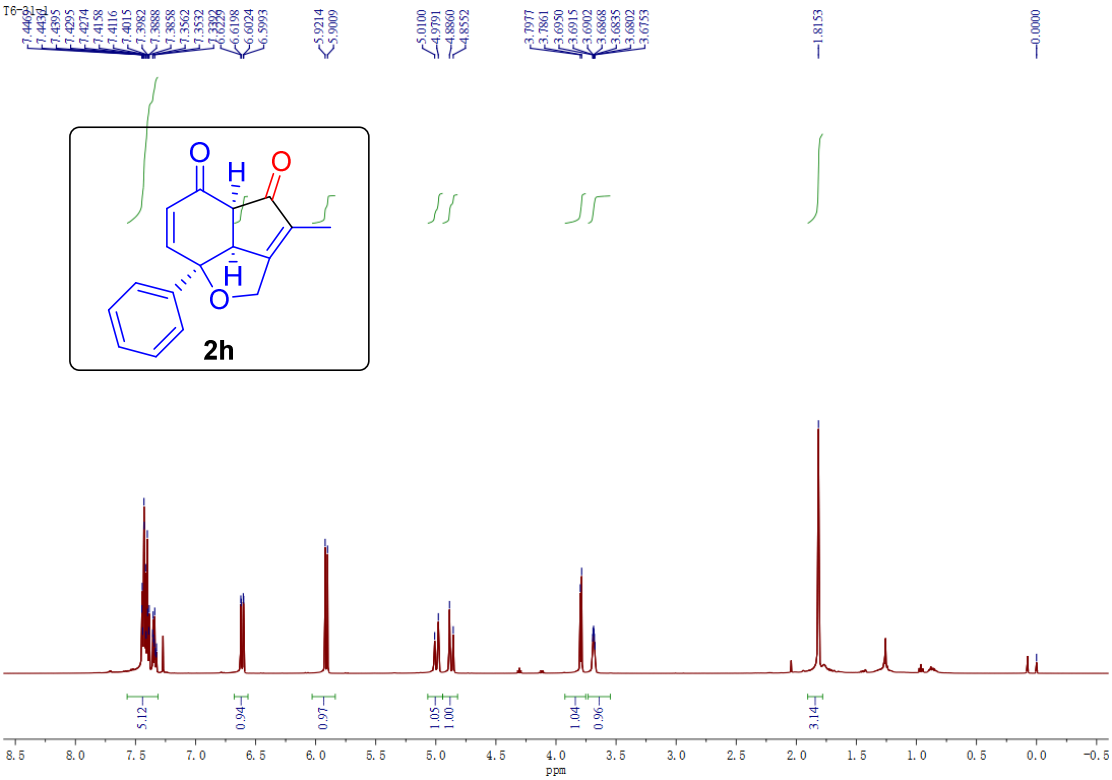
Chemical Formula: $C_{17}H_{20}O_3$

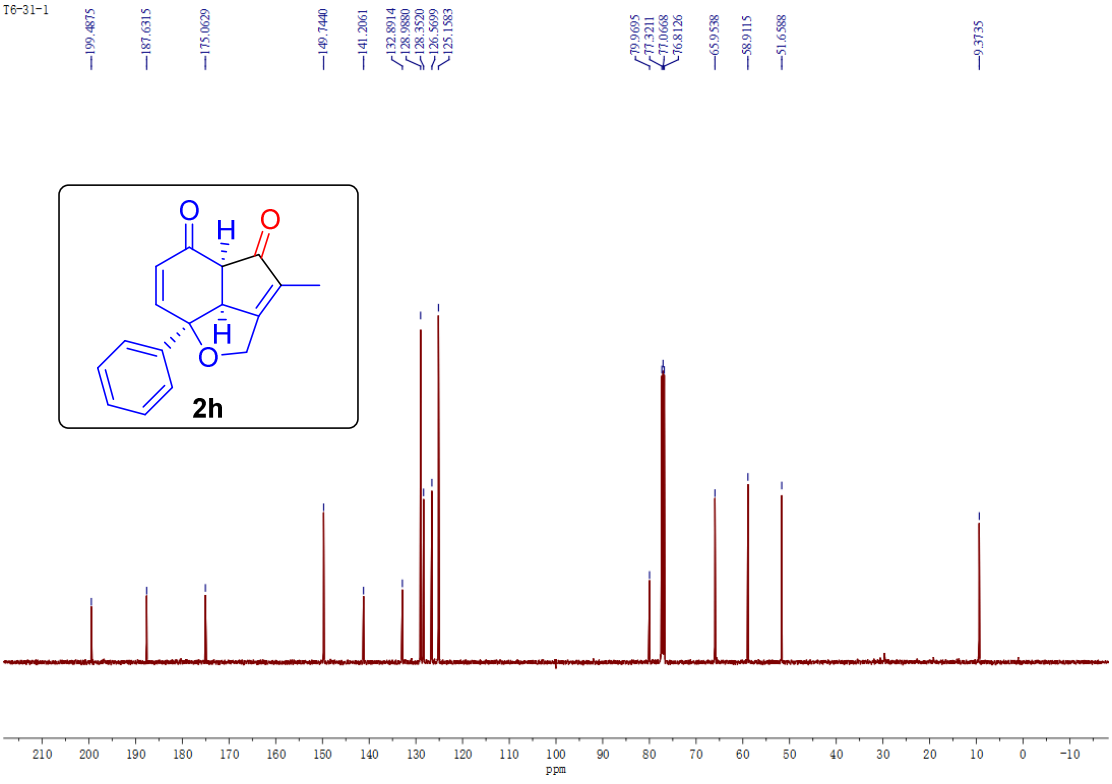
Exact Mass: 272.1412

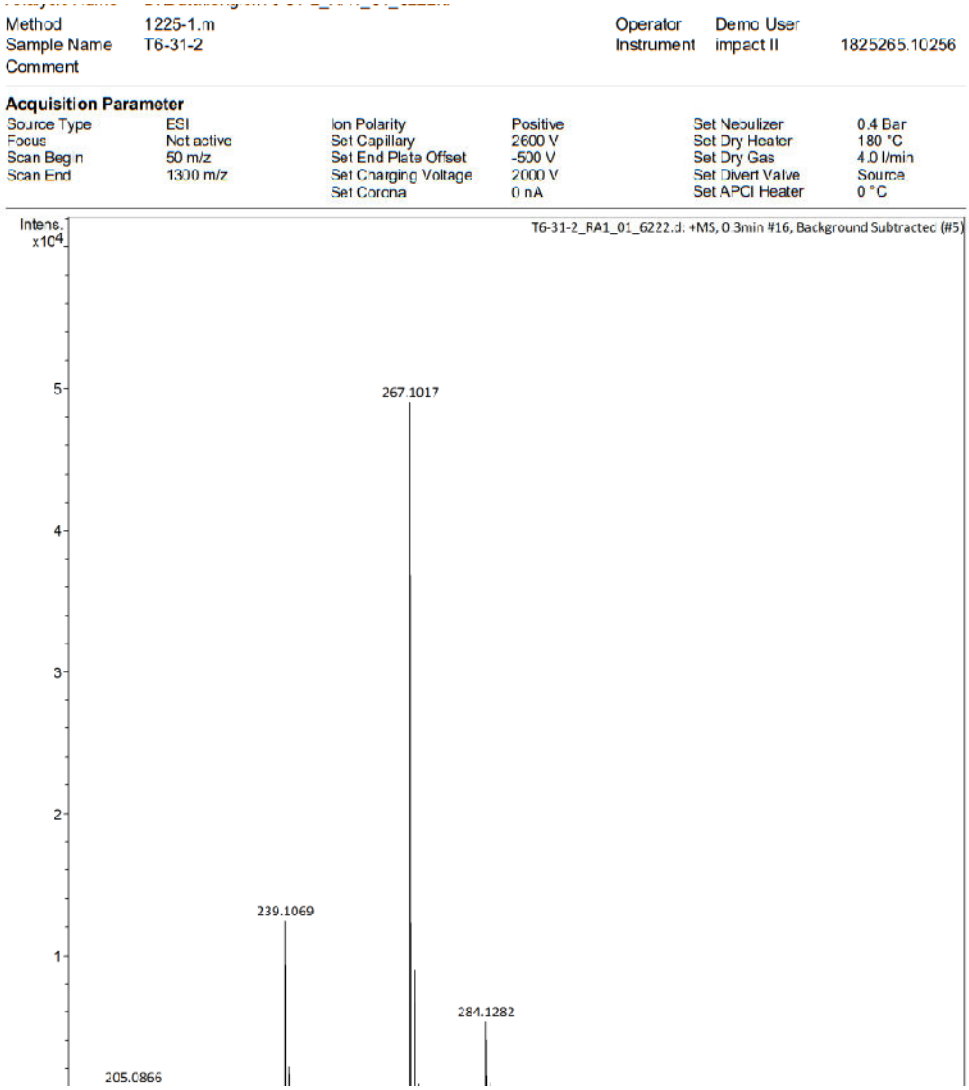
Molecular Weight: 272.3440

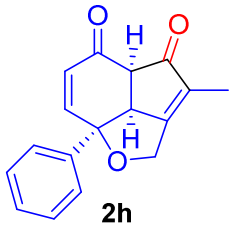
m/z: 272.1412 (100.0%), 273.1446 (18.4%), 274.1480 (1.6%)

HRMS (ESI, m/z) calcd for $C_{17}H_{20}O_3$ $[M+H]^+$ 273.1485, found 273.1487.


T6-31-1
2h
ppm


T6-31-1
2h
ppm

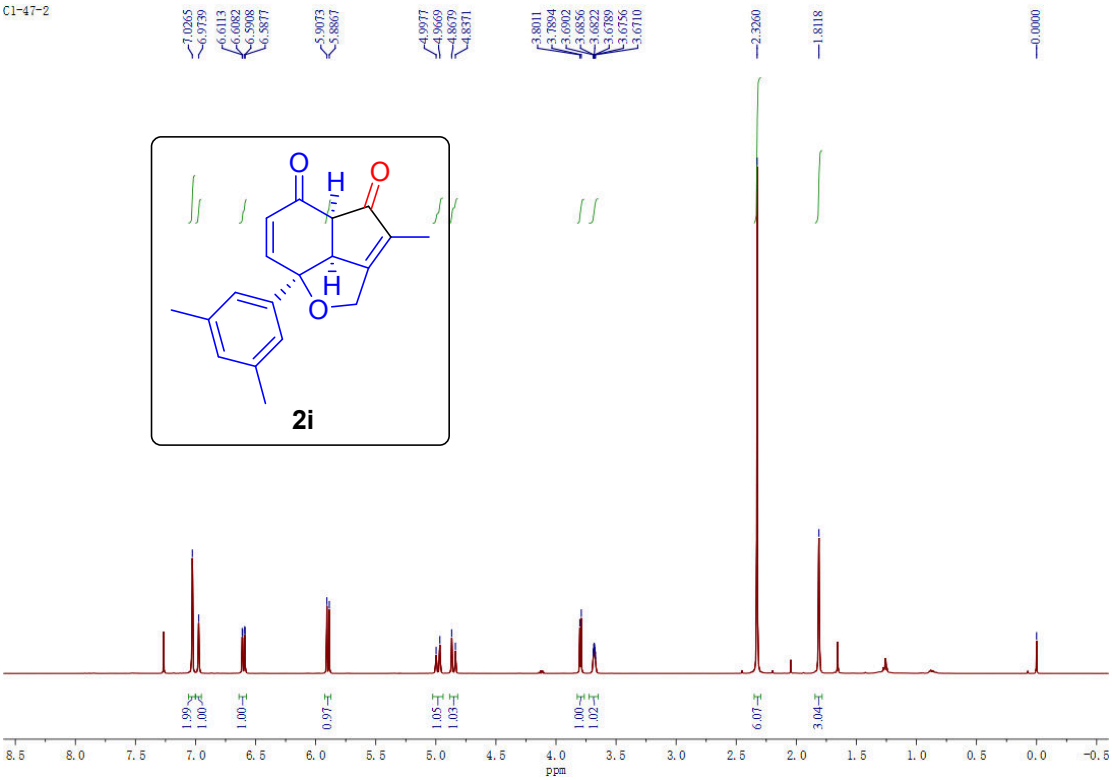




2h

Chemical Formula: $C_{17}H_{14}O_3$
Exact Mass: 266.0943
Molecular Weight: 266.2960
m/z: 266.0943 (100.0%), 267.0976 (18.4%), 268.1010 (1.6%)

HRMS (ESI, m/z) calcd for $C_{17}H_{14}O_3$ $[M+H]^+$ 267.1016, found 267.1017.


C1-47-2
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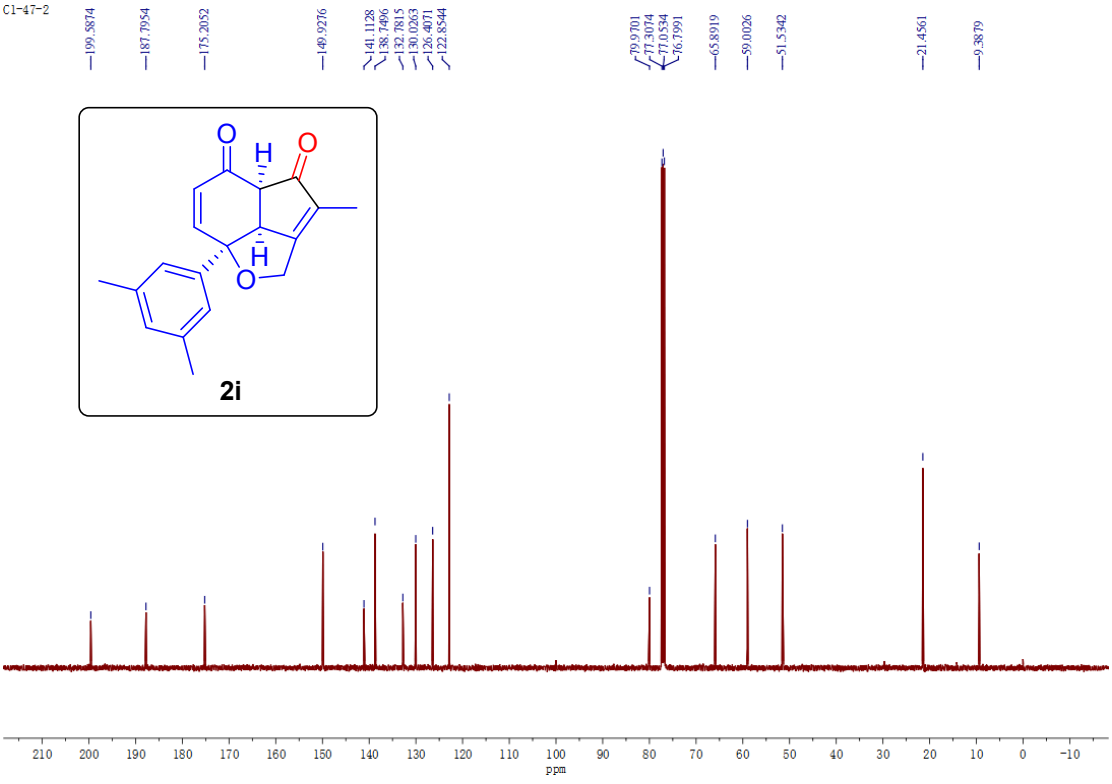
6.9739
6.6113
6.6082
6.5908
6.5877
5.9073
5.8867
4.9977
4.9669
4.8679
4.8371
3.8011
3.7894
3.6902
3.6856
3.6822
3.6789
3.6756
3.6710
2.3260
1.8118
0.0000
O
H
O
H
O
2i
1.99
1.00
1.00
0.97
1.05
1.03
1.00
1.02
6.07
3.04
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
ppm


C1-47-2
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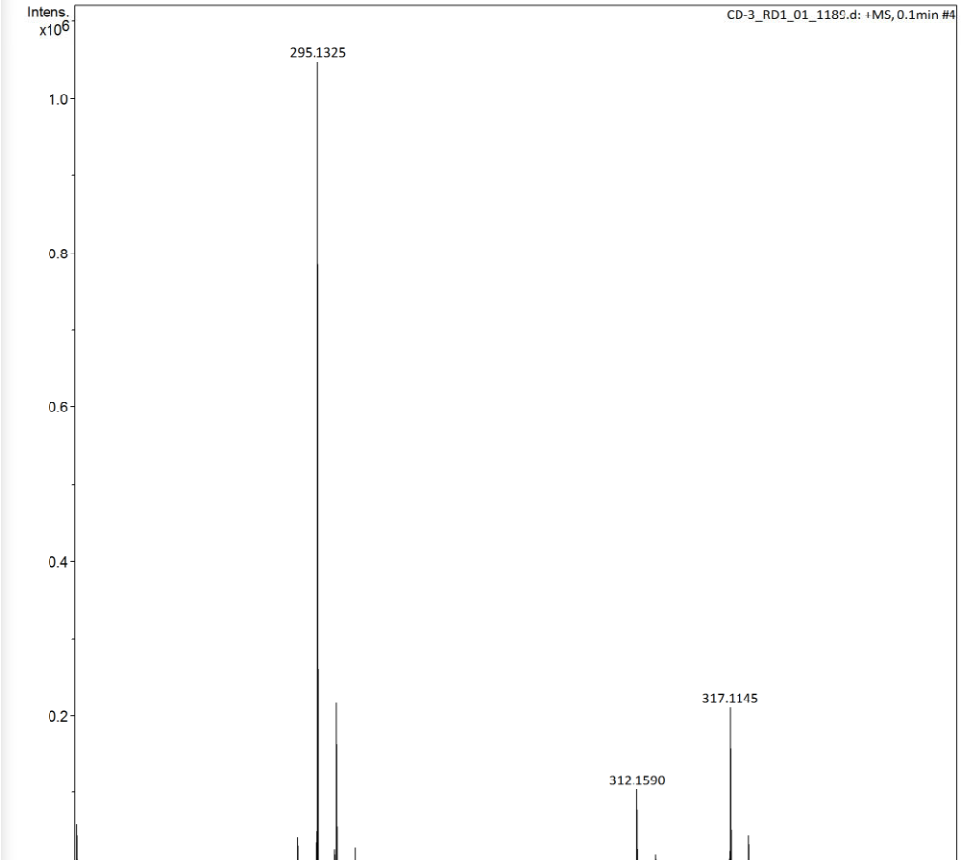
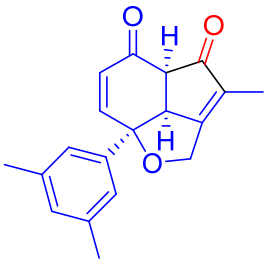
187.7954
175.2052
149.9276
141.1128
138.7496
132.7815
130.0263
126.4071
122.8544
79.9701
77.3074
77.0534
76.7991
65.8919
59.0026
51.5342
21.4561
9.3879
O
H
O
H
O
2i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
ppm

Sample Name	CD-3	Instrument	impact II 1825265.10256
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	2600 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

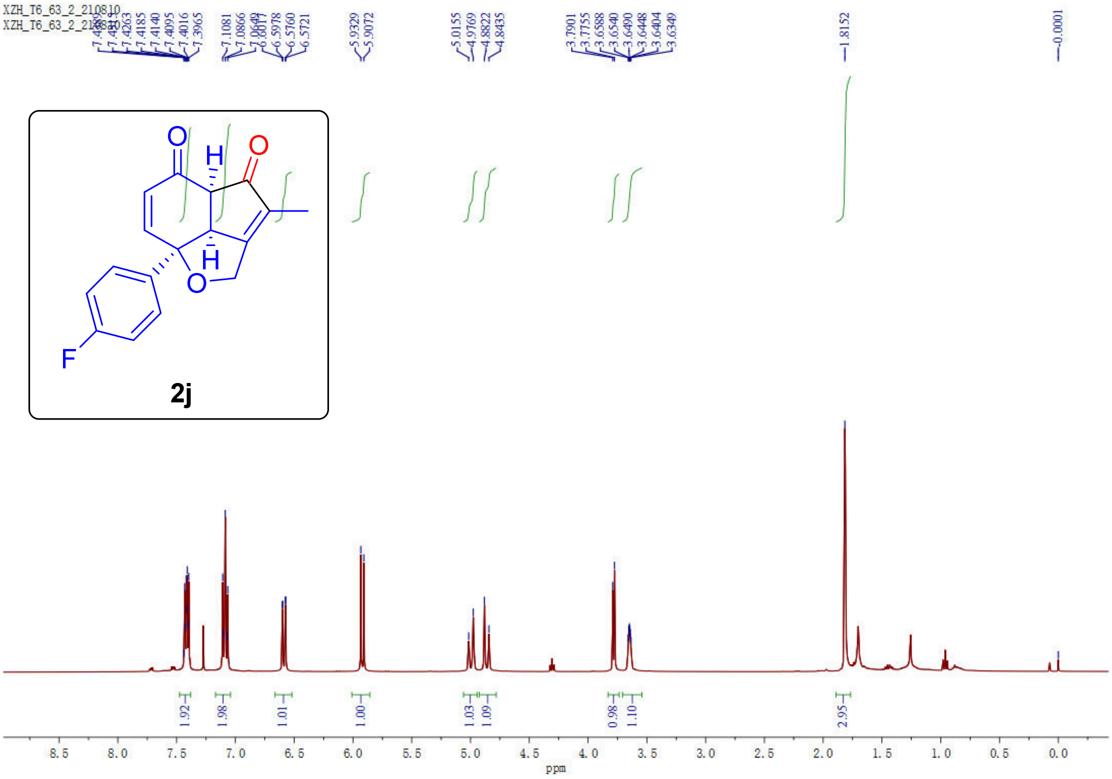




2i

Chemical Formula: $C_{19}H_{18}O_3$
Exact Mass: 294.1256
Molecular Weight: 294.3500
m/z: 294.1256 (100.0%), 295.1289 (20.5%), 296.1323 (2.0%)

HRMS (ESI, m/z) calcd for $C_{19}H_{18}O_3$ $[M+H]^+$ 295.1329, found 295.1325.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7.4016
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7.1081
7.0866
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6.5760
6.5721
5.9329
5.9072
5.0155
4.9769
4.8822
4.8435
3.7901
3.7755
3.6588
3.6540
3.6490
3.6448
3.6404
3.6349
1.8152
-0.0001
O
H
O
H
O
F
2j
1.92
1.98
1.01
1.00
1.03
1.09
0.98
1.10
2.95
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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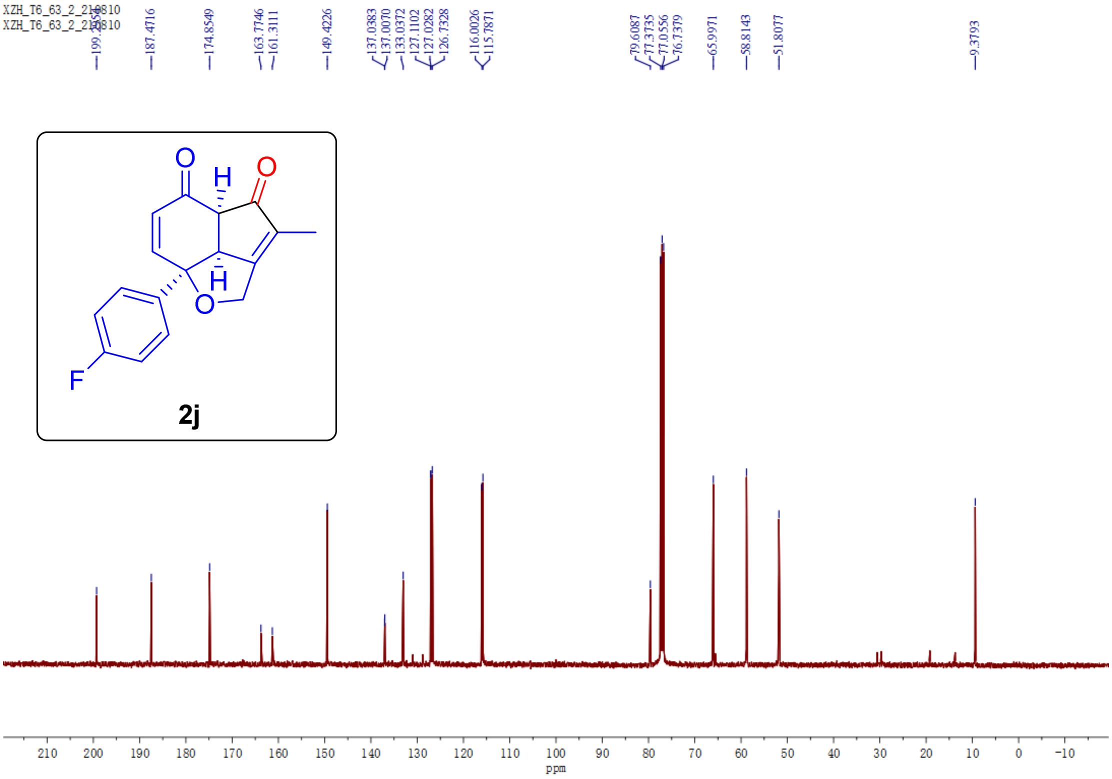
2.0
1.5
1.0
0.5
0.0
ppm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163.7746
161.3111
149.4226
137.0383
137.0070
133.0372
127.1102
127.0282
126.7328
116.0026
115.7871
79.6087
77.3735
77.0556
76.7379
65.9971
58.8143
51.8077
9.3793
O
H
O
H
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F
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210
200
190
180
170
160
150
140
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110
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90
80
70
60
50
40
30
20
10
0
-10
ppm

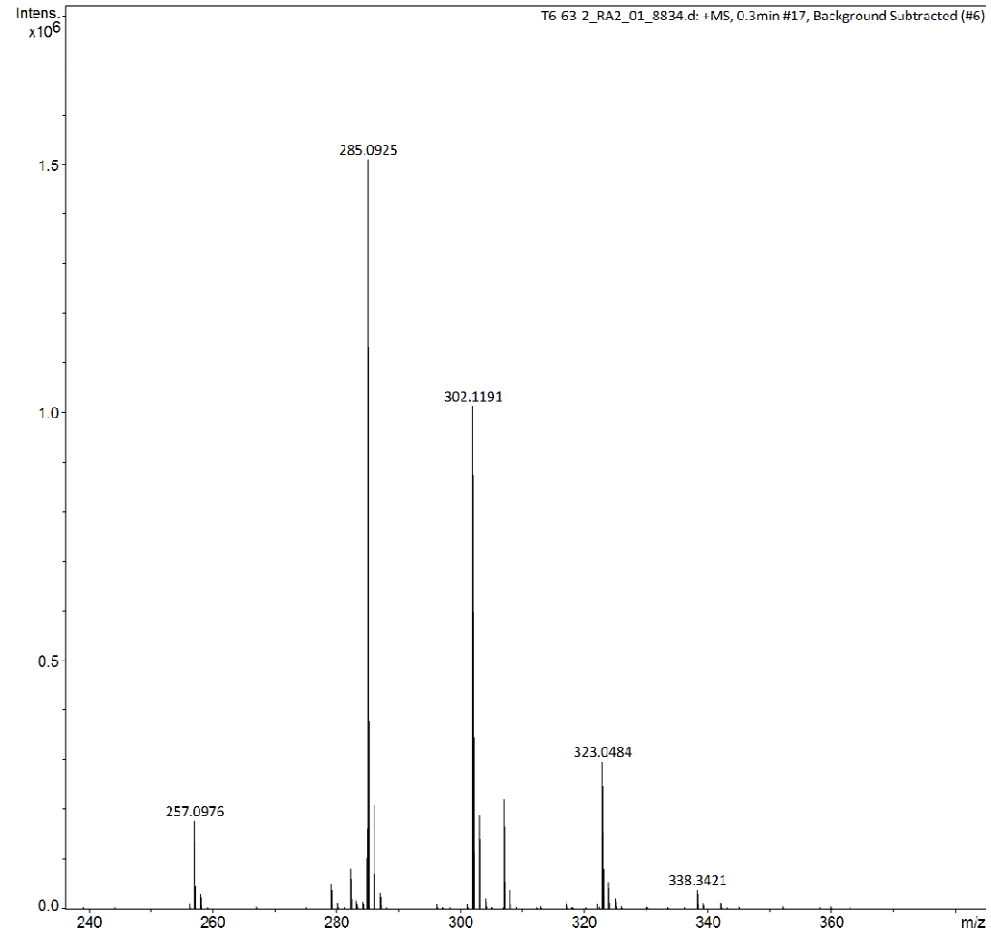
Display Report

Analysis Info

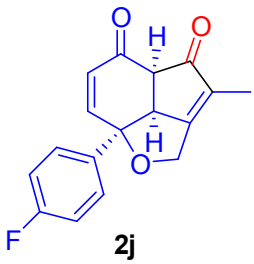
Analysis Name	D:\Data\Yenglei\T6-63-2_RA2_01_8834.d	Acquisition Date	8/12/2021 3:21:45 PM
Method	1225-1.m	Operator	Demo User
Sample Name	T6-63-2	Instrument	Impact II 1825265.10256
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	2600 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



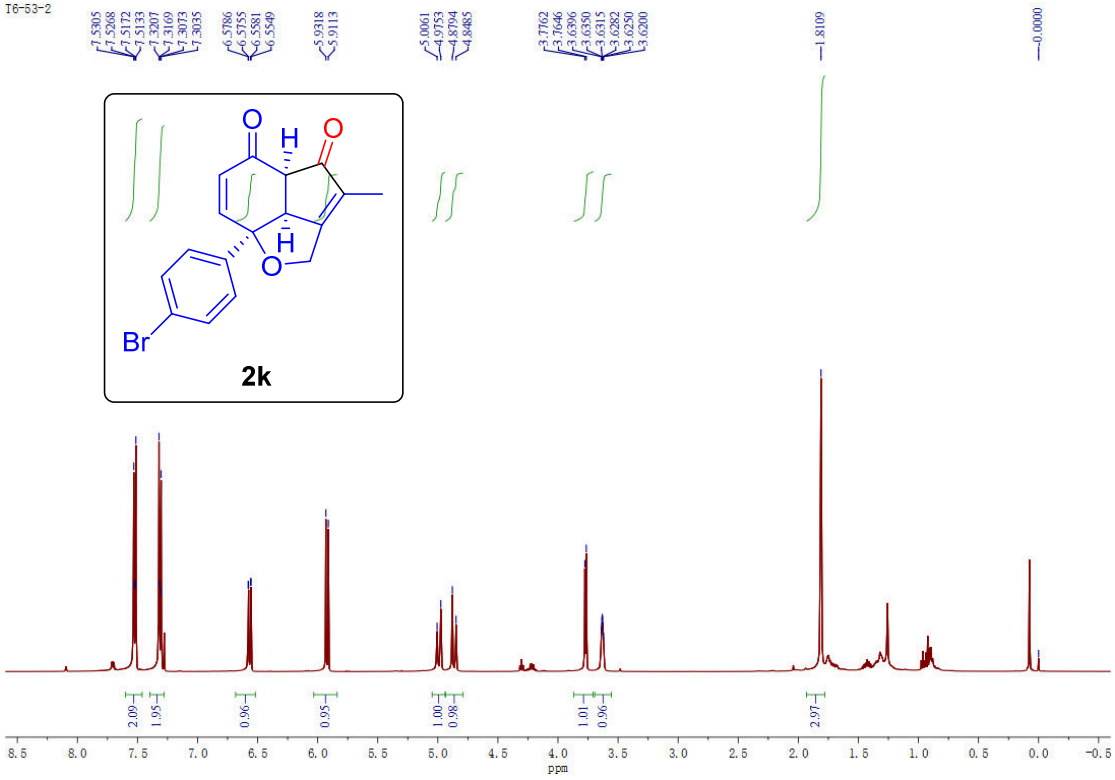
T6-63-2_RA2_01_8834.d
Bruker Compass DataAnalysis 4.4 printed: 8/12/2021 3:23:35 PM by: demo Page 1 of 1



2j

Chemical Formula: $C_{17}H_{13}FO_3$
Exact Mass: 284.0849
Molecular Weight: 284.2864
m/z: 284.0849 (100.0%), 285.0882 (18.4%), 286.0916 (1.6%)

HRMS (ESI, m/z) calcd for $C_{17}H_{13}FO_3$ $[M+H]^+$ 285.0921, found 285.0925.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7.5172
7.5133
7.3207
7.3169
7.3073
7.3035
6.5786
6.5755
6.5581
6.5549
5.9318
5.9113
5.0061
4.9753
4.8794
4.8485
3.7762
3.7646
3.6396
3.6330
3.6315
3.6282
3.6250
3.6200
1.8109
0.0000
O
H
O
H
O
Br
2k
2.09
1.95
0.96
0.95
1.00
0.98
1.01
0.96
2.97
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.5
3.0
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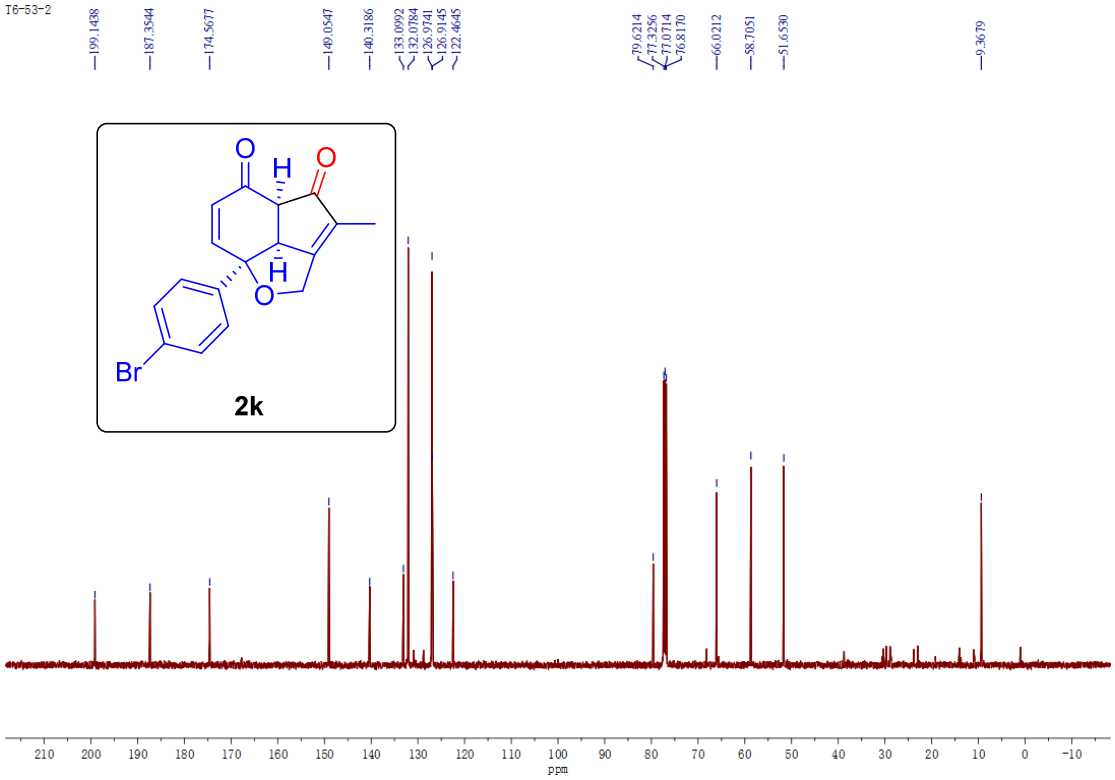
1.5
1.0
0.5
0.0
-0.5
ppm


T6-53-2
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149.0547
140.3186
133.0992
132.0784
126.9741
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122.4645
79.6214
77.3256
77.0714
76.8170
66.0212
58.7051
51.6530
9.3679
O
H
O
H
O
Br
2k
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
ppm

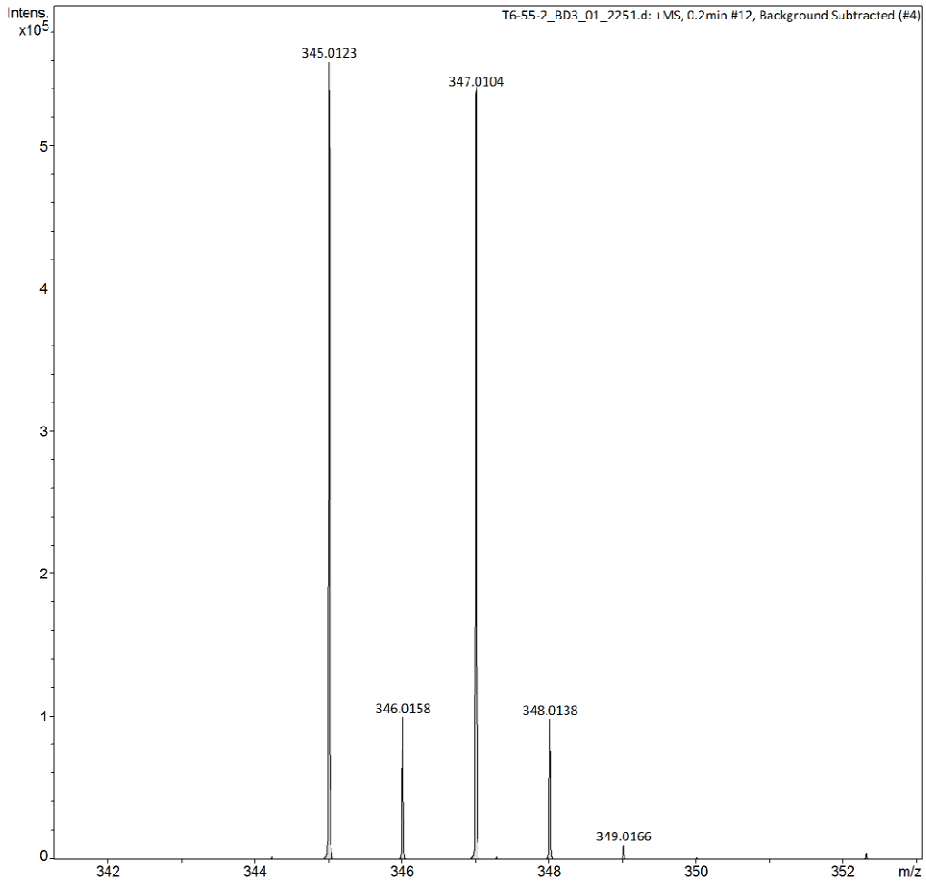
Display Report

Analysis Info

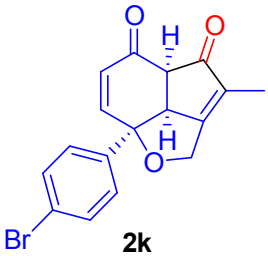
Analysis Name	D:\data\lengjie\T6-55-2_BD3_01_2251.d	Acquisition Date	12/10/2021 1:35:30 PM
Method	1008-ms.m	Operator	Demo User
Sample Name	T6-55-2	Instrument	impact II 1825285.10258
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	2600 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



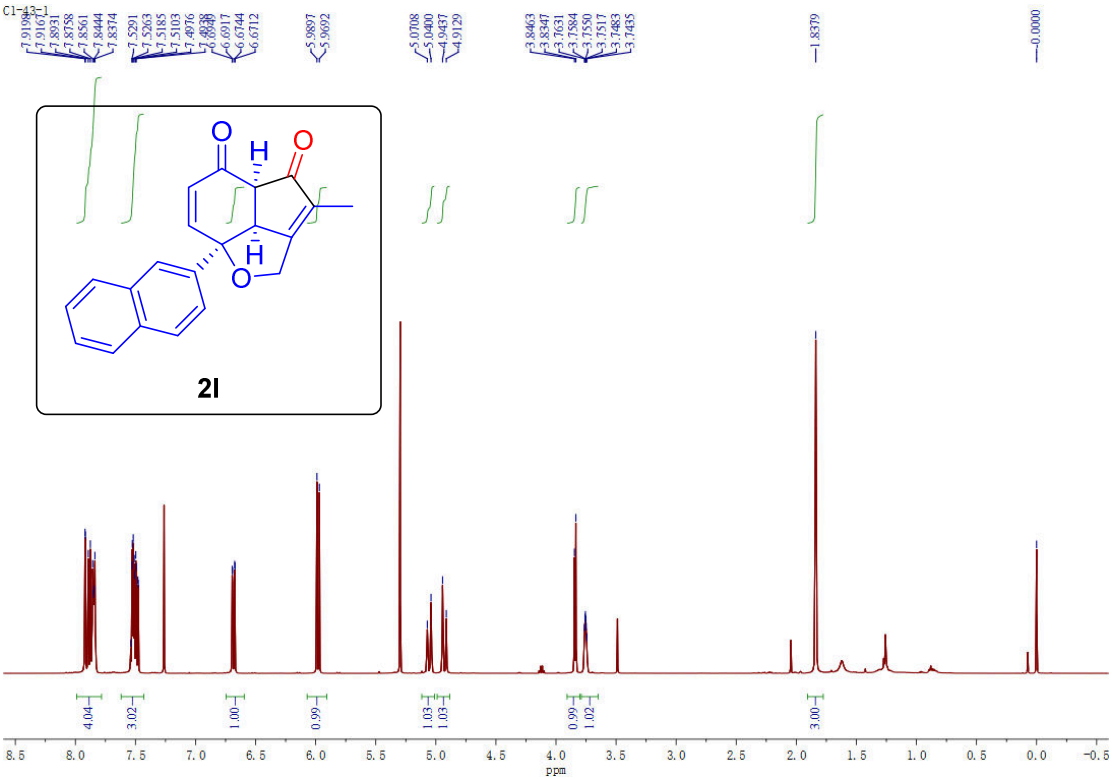
T6-55-2_BD3_01_2251.d
Bruker Compass DataAnalysis 4.4 printed: 12/10/2021 1:37:53 PM by: demo Page 1 of 1

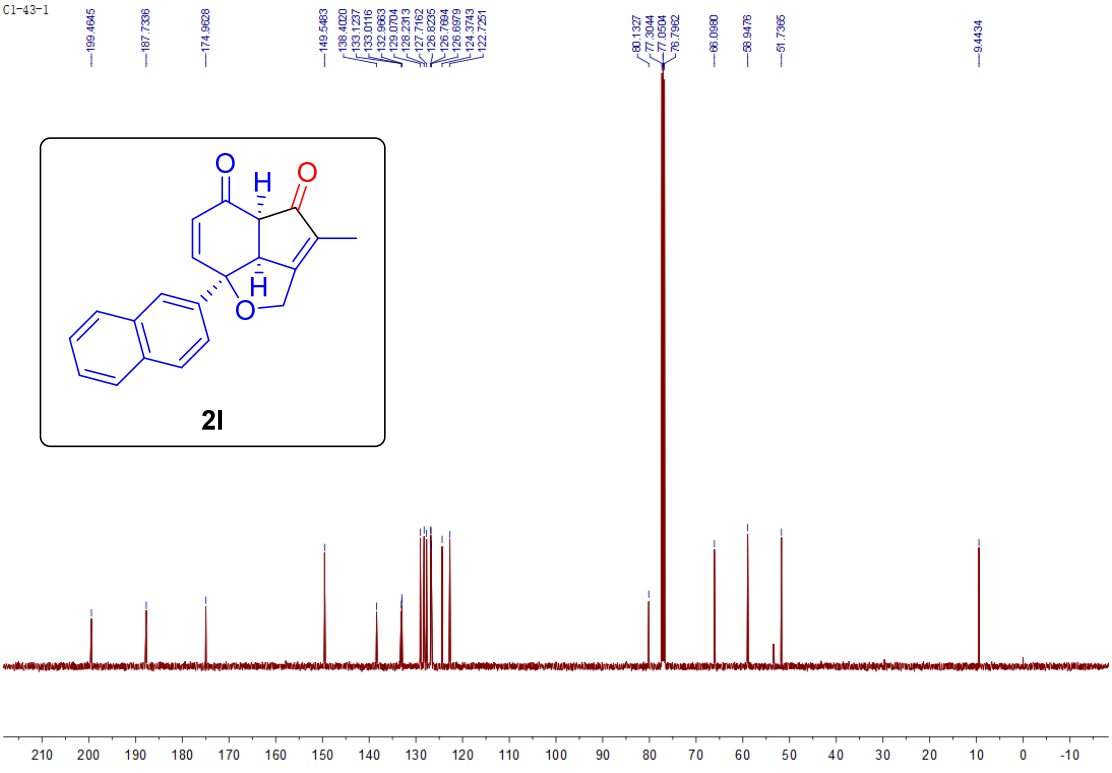


2k

Chemical Formula: $C_{17}H_{13}BrO_3$
Exact Mass: 344.0048
Molecular Weight: 345.1920
m/z: 344.0048 (100.0%), 346.0028 (97.3%), 345.0082 (18.4%), 347.0061 (17.9%), 346.0115 (1.6%), 348.0095 (1.5%)

HRMS (ESI, m/z) calcd for $C_{17}H_{13}BrO_3$ $[M+H]^+$ 345.0121, found 345.0123.


C1-43-1
2l


C1-43-1
2l

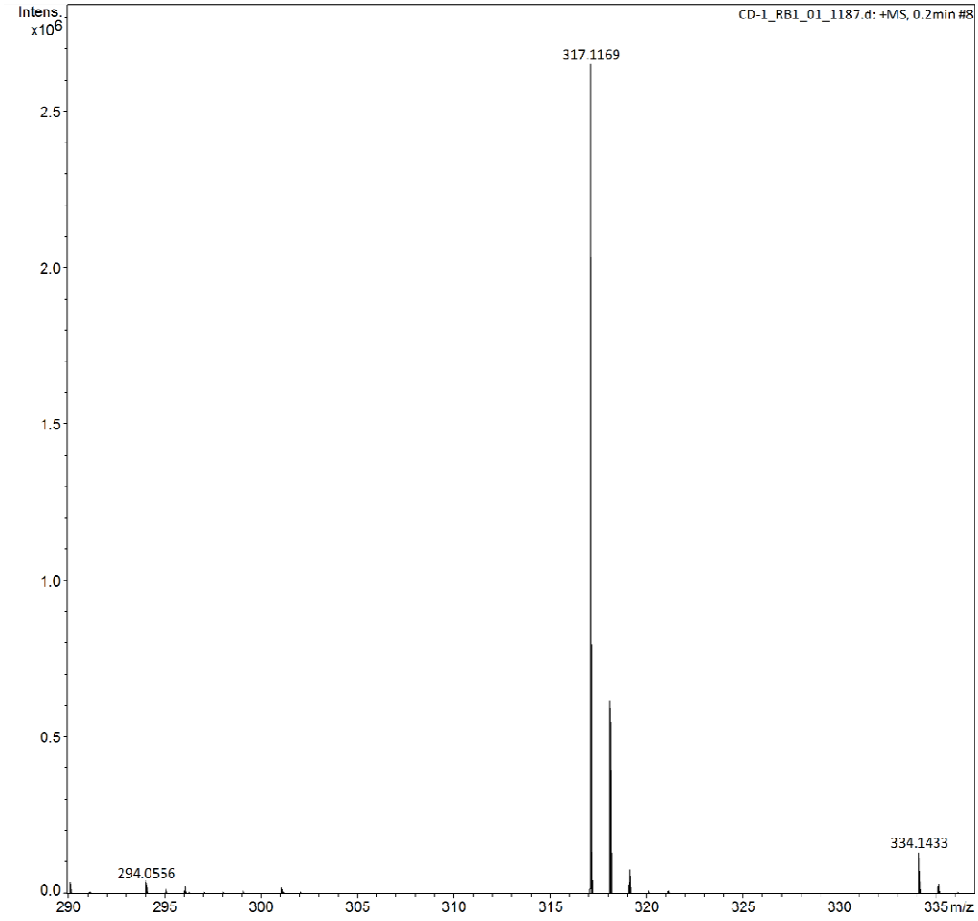
Display Report

Analysis Info

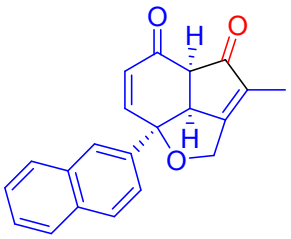
Analysis Name	D:\data\fengjel\CD-1_RB1_01_1187.d	Acquisition Date	11/12/2021 4:08:05 PM
Method	1008-ms.m	Operator	Demo User
Sample Name	CD-1	Instrument	impact II 1825255.10256
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	2600 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



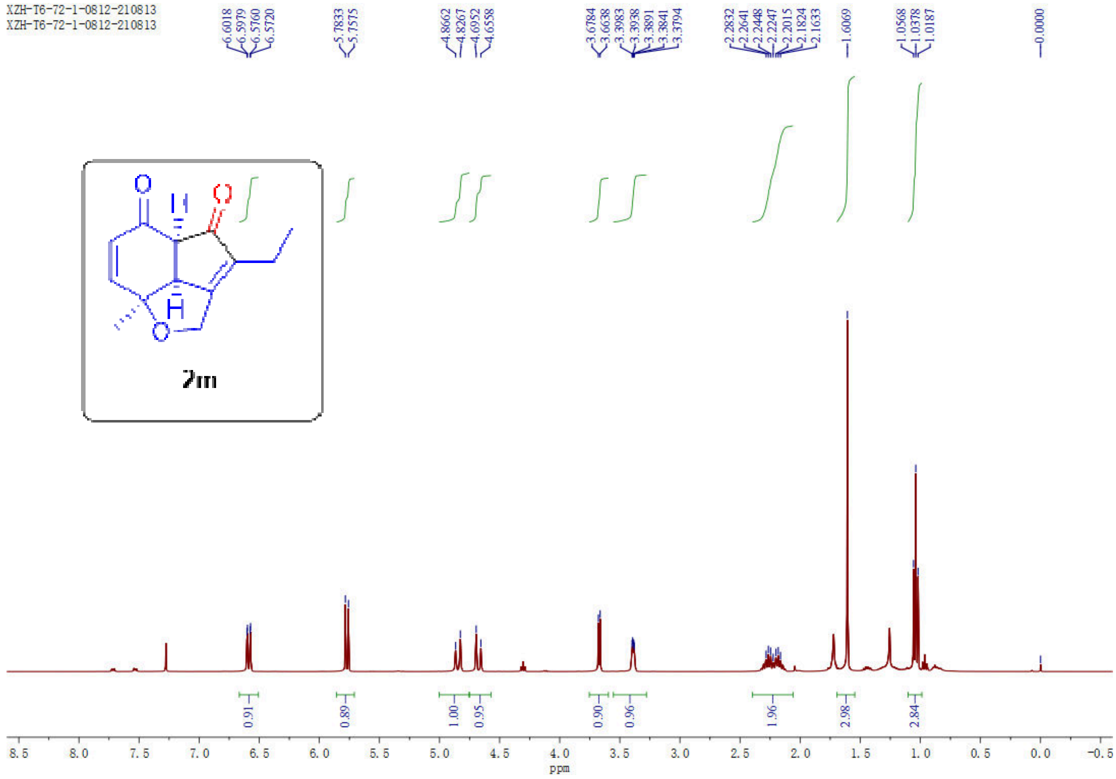
CD-1_RB1_01_1187.d
Bruker Compass DataAnalysis 4.4 printed: 11/12/2021 4:08:45 PM by: demo Page 1 of 1



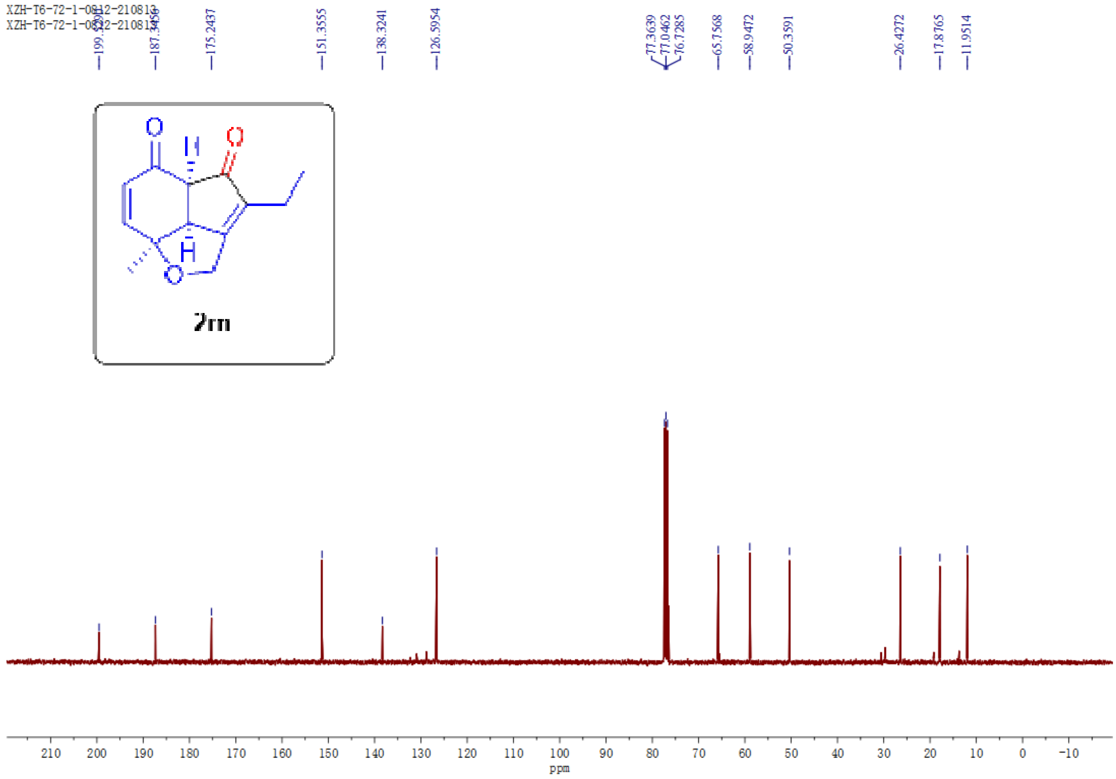
2l

Chemical Formula: $C_{21}H_{16}O_3$
Exact Mass: 316.1099
Molecular Weight: 316.3560
m/z: 316.1099 (100.0%), 317.1133 (22.7%), 318.1167 (2.5%)

HRMS (ESI, m/z) calcd for $C_{21}H_{16}O_3$ $[M+H]^+$ 317.1172, found 317.1169.



XZH-T6-72-1-0812-210813
XZH-T6-72-1-0812-210813
6.6018
6.5979
6.5760
6.5720
5.7833
5.7575
4.8662
4.8267
4.6952
4.6558
3.6784
3.6638
3.3983
3.3938
3.3891
3.3841
3.3794
2.2832
2.2641
2.2448
2.2247
2.2015
2.1824
2.1633
1.6069
1.0568
1.0378
1.0187
0.0000
2m
0.91
0.89
1.00
0.95
0.90
0.96
1.96
2.98
2.84
ppm



XZH-T6-72-1-0812-210813
XZH-T6-72-1-0812-210813
175.2437
151.3555
138.3241
126.5954
77.3639
77.0462
76.7285
65.7568
58.9472
50.3591
26.4272
17.8765
11.9514
2m
ppm

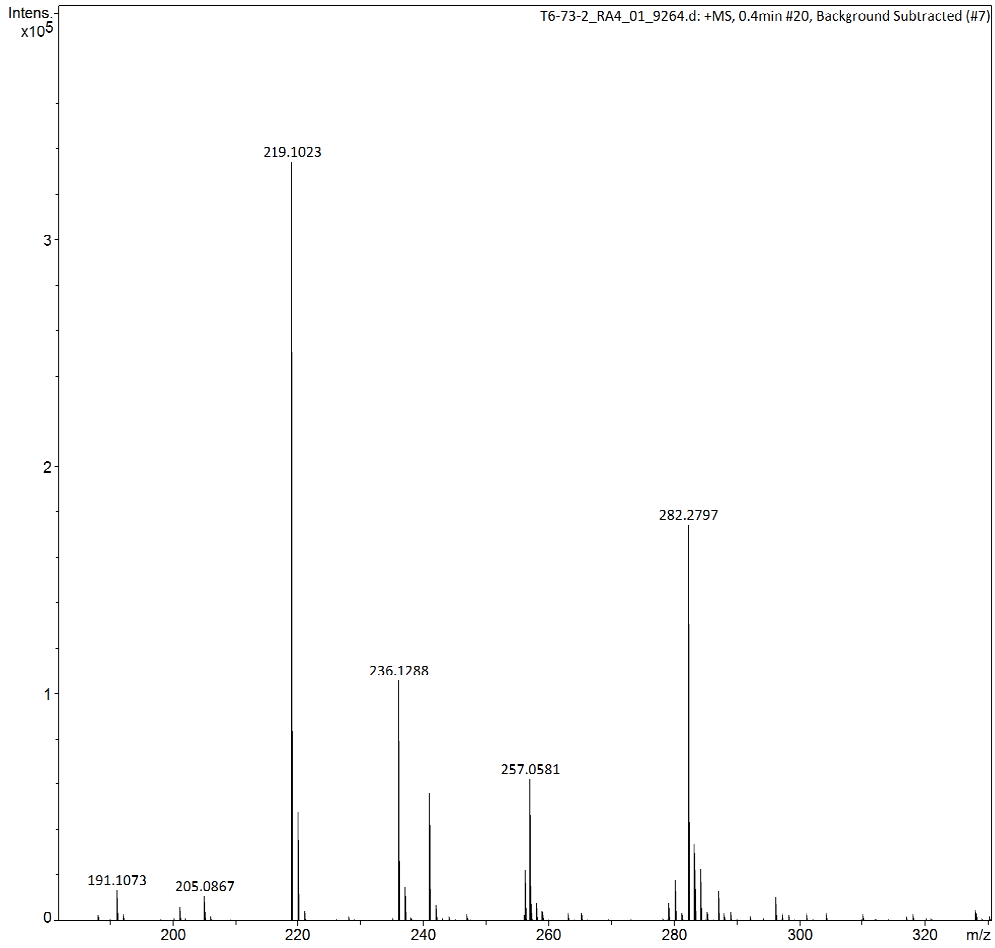
Display Report

Analysis Info

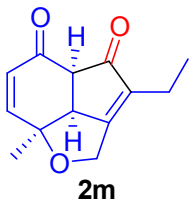
Analysis Name	D:\Data\fenglei\T6-73-2_RA4_01_9264.d	Acquisition Date	8/25/2021 2:28:25 PM
Method	1225-1.m	Operator	Demo User
Sample Name	T6-73-2	Instrument	impact II 1825265.10256
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	2600 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



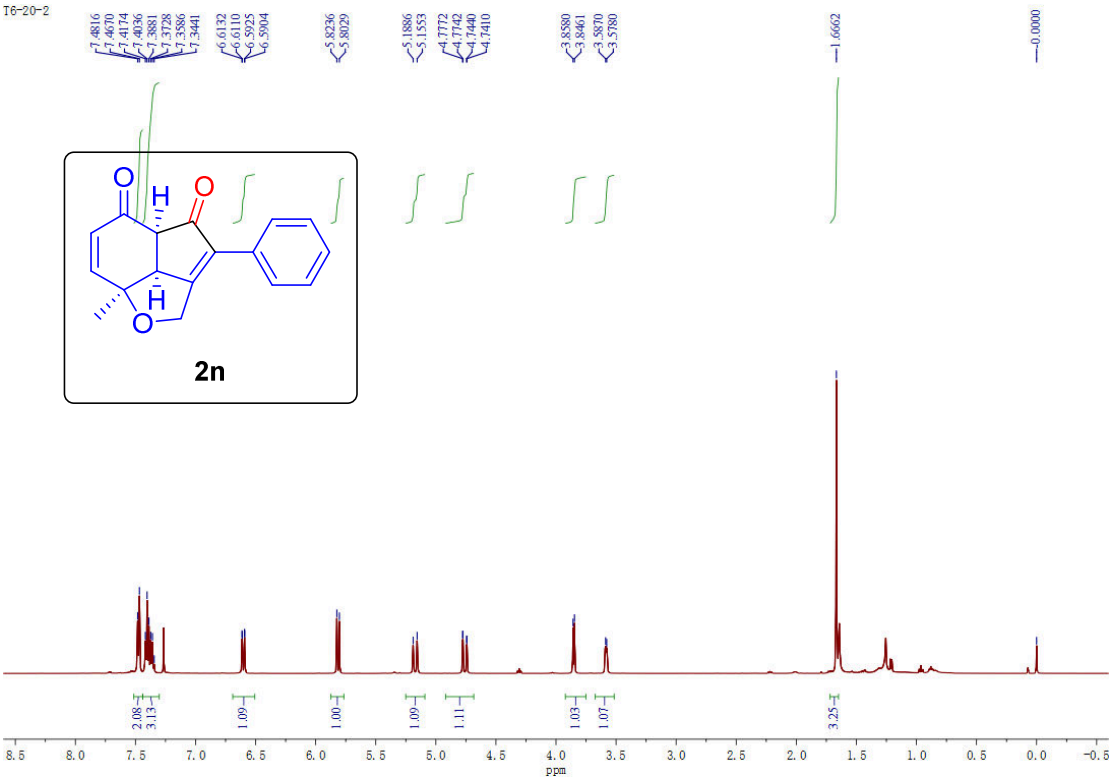
T6-73-2_RA4_01_9264.d
Bruker Compass DataAnalysis 4.4 printed: 8/25/2021 2:29:53 PM by: demo Page 1 of 1

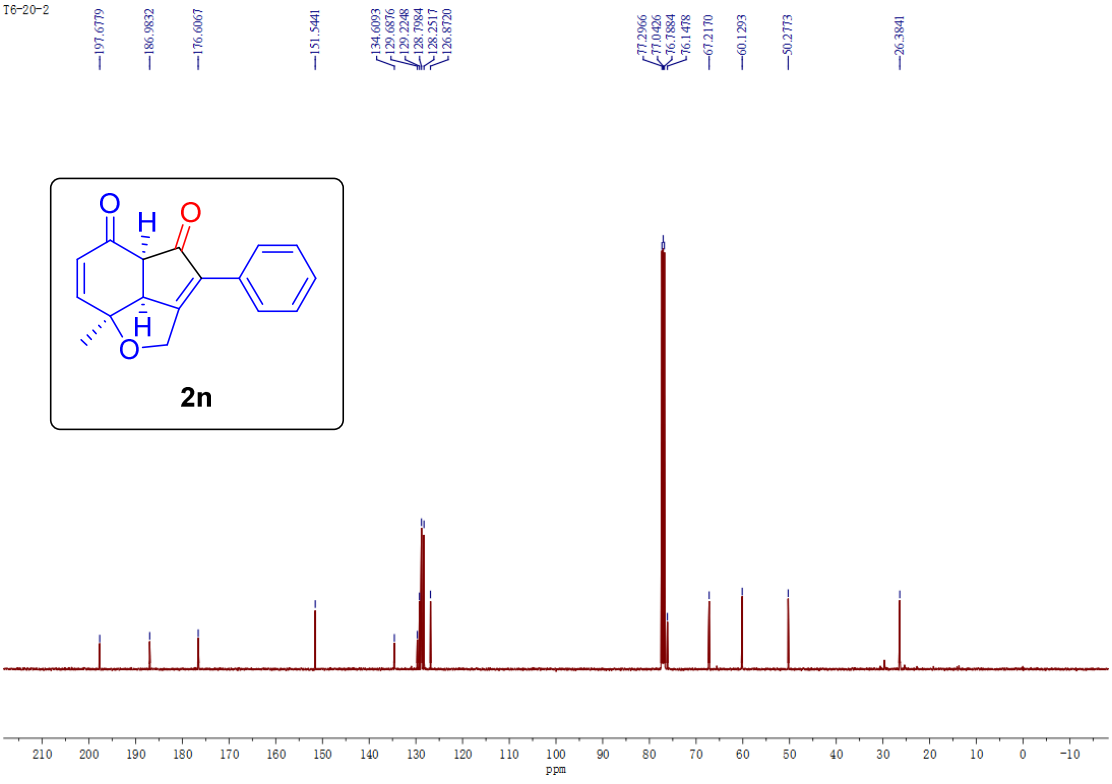


2m

Chemical Formula: $C_{13}H_{14}O_3$
Exact Mass: 218.0943
Molecular Weight: 218.2520
m/z: 218.0943 (100.0%), 219.0976 (14.1%)

HRMS (ESI, m/z) calcd for $C_{13}H_{14}O_3$ $[M+H]^+$ 219.1016, found 219.1023.


T6-20-2
7.4816
7.4670
7.4174
7.4036
7.3681
7.3728
7.3586
7.3441
6.6132
6.6110
6.5925
6.5904
5.8236
5.8029
5.1886
5.1553
4.7772
4.7742
4.7440
4.7410
3.8580
3.8461
3.5870
3.5780
1.6662
0.0000
2n
2.08
3.13
1.09
1.00
1.09
1.11
1.03
1.07
3.25
ppm


T6-20-2
197.6779
186.9832
176.6067
151.5441
134.6093
129.6876
129.2248
128.7984
128.2517
126.8720
77.2966
77.0426
76.7884
76.1478
67.2170
60.1293
50.2773
26.3841
2n
ppm

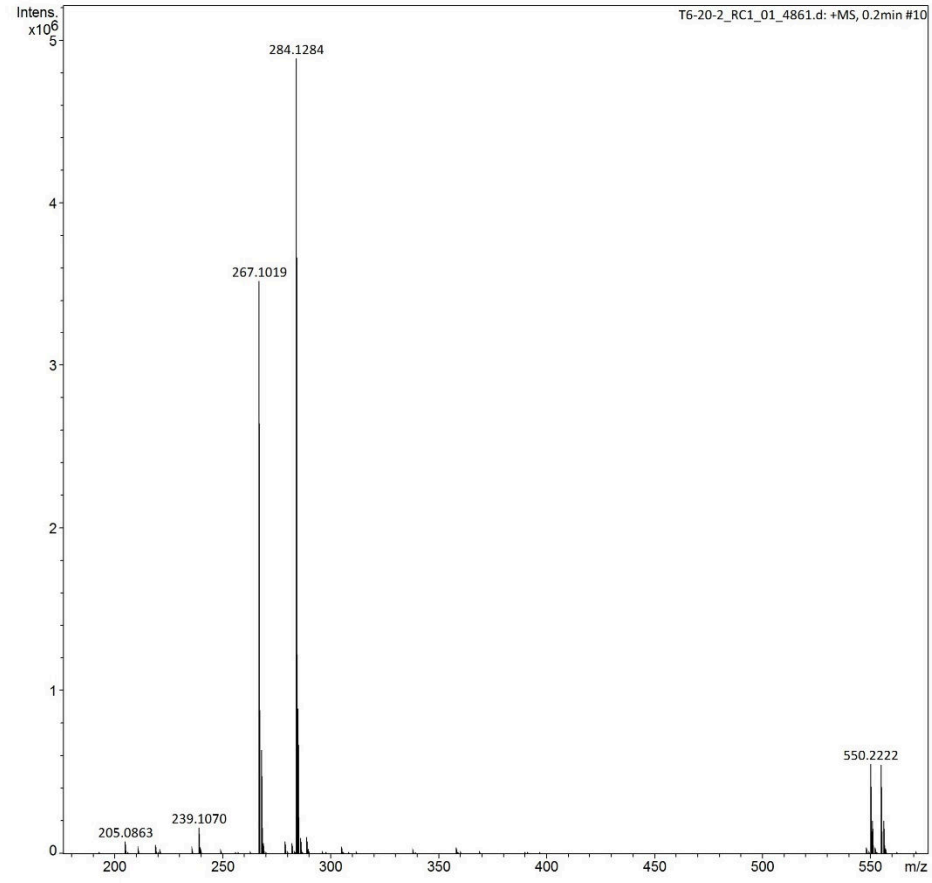
Display Report

Analysis Info

Analysis Name	D:\Data\fenglei\T6-20-2_RC1_01_4861.d	Acquisition Date	4/28/2021 3:33:43 PM
Method	1225-1.m	Operator	Demo User
Sample Name	T6-20-2	Instrument	impact II 1825265.10256
Comment			

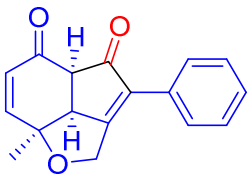
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	2600 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



T6-20-2_RC1_01_4861.d

Bruker Compass DataAnalysis 4.4 printed: 4/28/2021 3:57:48 PM by: demo Page 1 of 1



2n

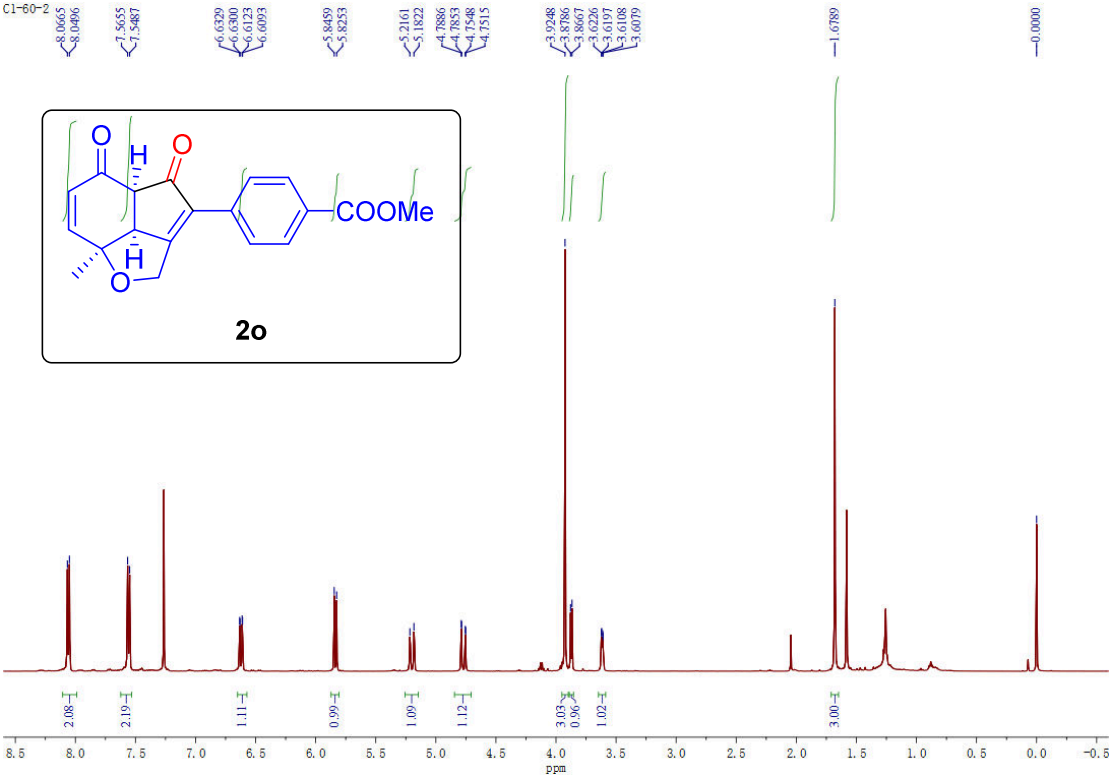
Chemical Formula: $C_{17}H_{14}O_3$

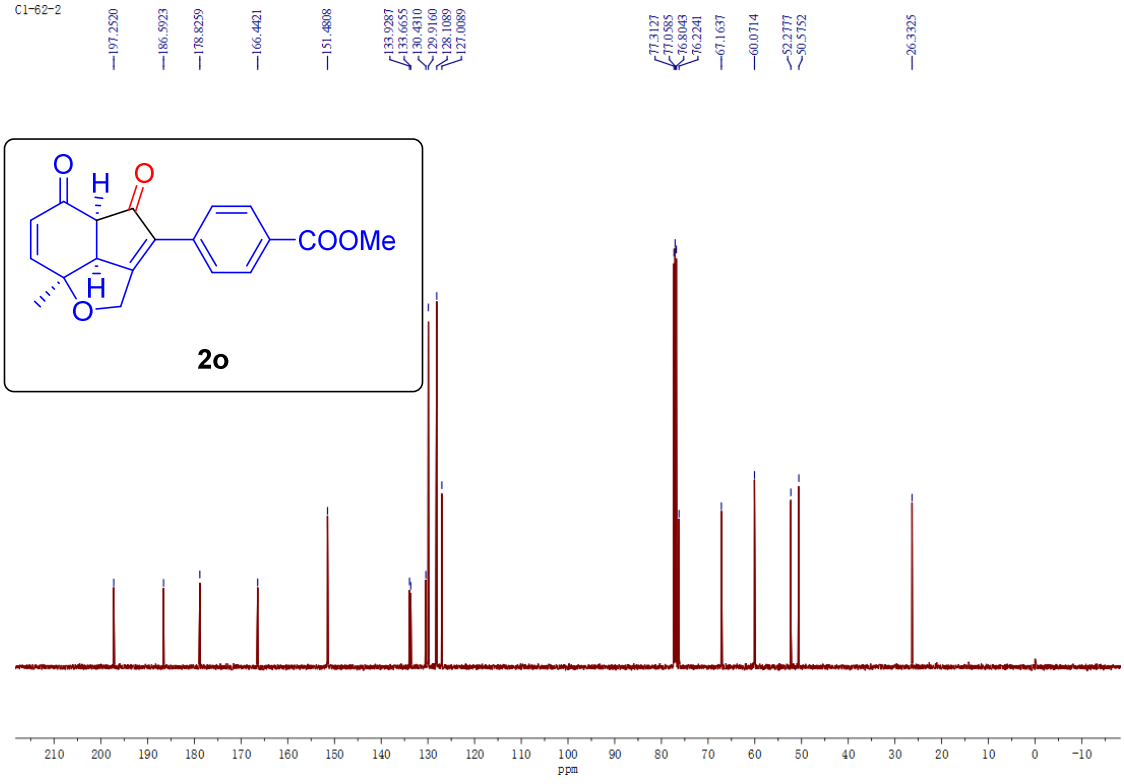
Exact Mass: 266.0943

Molecular Weight: 266.2960

m/z: 266.0943 (100.0%), 267.0976 (18.4%), 268.1010 (1.6%)

HRMS (ESI, m/z) calcd for $C_{17}H_{14}O_3$ $[M+NH_4]^+$ 284.1281, found 284.1284.


C1-60-2
8.0665
8.0496
7.5655
7.5487
6.6329
6.6300
6.6123
6.6093
5.8459
5.8253
5.2161
5.1822
4.7886
4.7853
4.7548
4.7515
3.9248
3.8786
3.8667
3.6226
3.6197
3.6108
3.6079
1.6789
0.0000
O
H
O
COOMe
H
O
2o
2.08
2.19
1.11
0.99
1.09
1.12
3.03
0.96
1.02
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm


C1-62-2
197.2520
186.5923
178.8259
166.4421
151.4808
133.9287
133.6655
130.4310
129.9160
128.1089
127.0089
77.3127
77.0585
76.8043
76.2241
67.1637
60.0714
52.2777
50.5752
26.3325
O
H
O
COOMe
H
O
2o
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
ppm

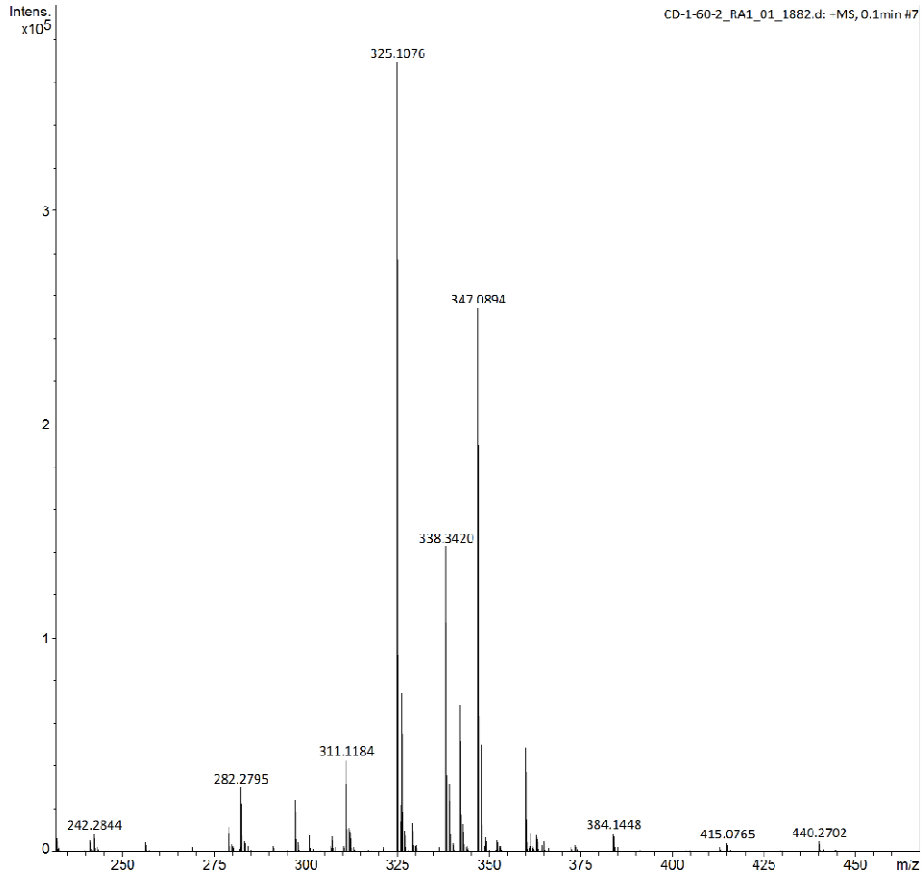
Display Report

Analysis Info

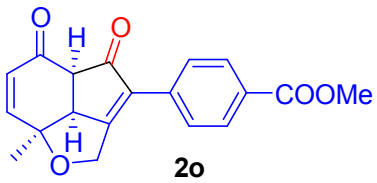
Analysis Name	D:\data\fengei\CD-1-60-2_RA1_01_1882.d	Acquisition Date	12/2/2021 4:03:56 PM
Method	1008-ms.m	Operator	Demo User
Sample Name	CD-1-60-2	Instrument	impact II 1825265.10256
Commen:			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	2600 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APC Heater	0 °C



CD-1-60-2_RA1_01_1882.d
Bruker Compass DataAnalysis 4.4 printed: 12/2/2021 4:06:56 PM by: demo Page 1 of 1



2o

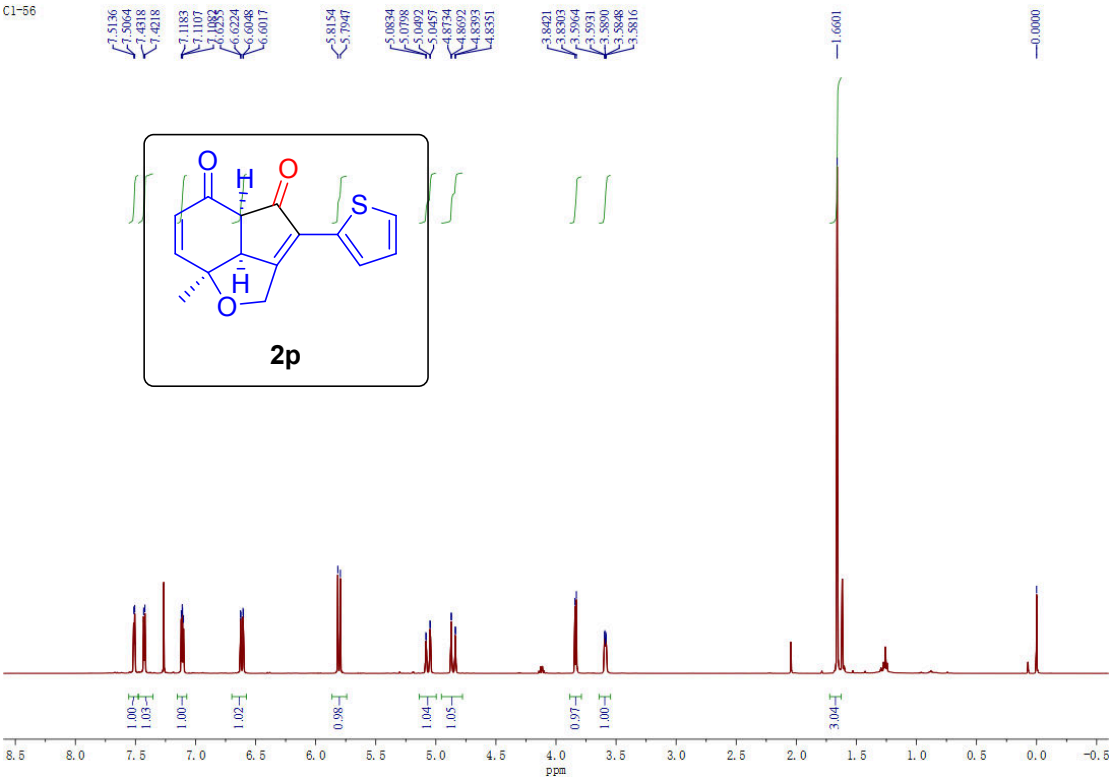
Chemical Formula: $C_{19}H_{16}O_5$

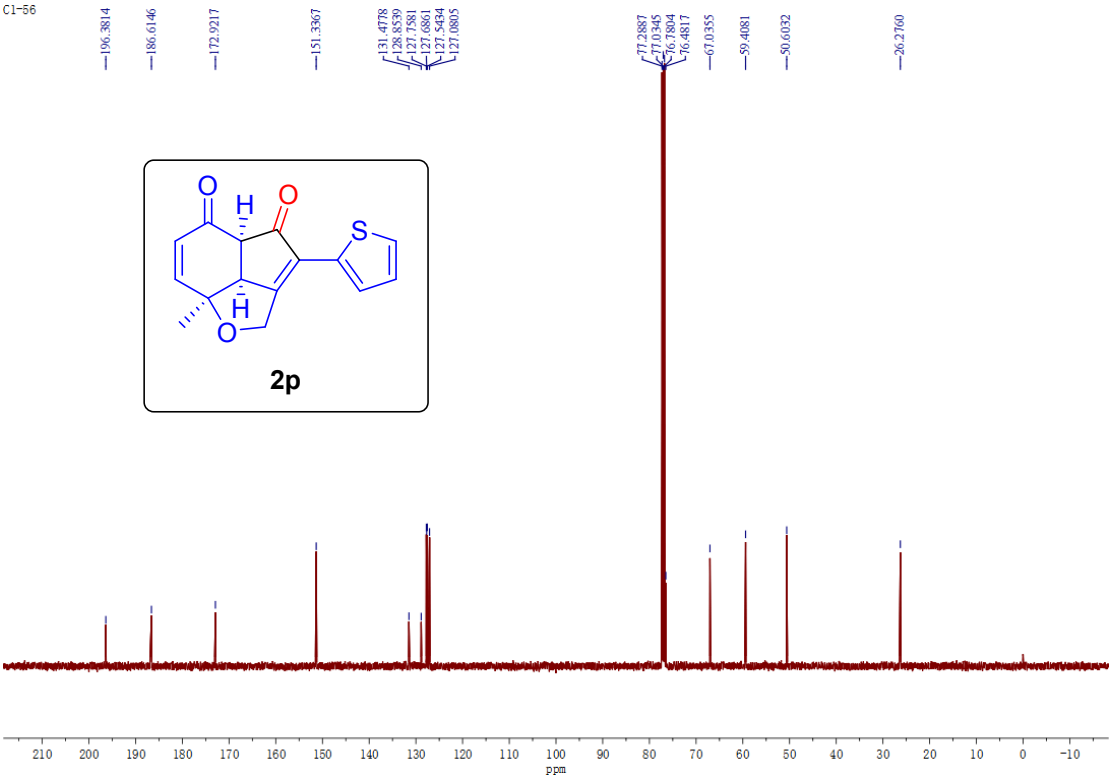
Exact Mass: 324.0998

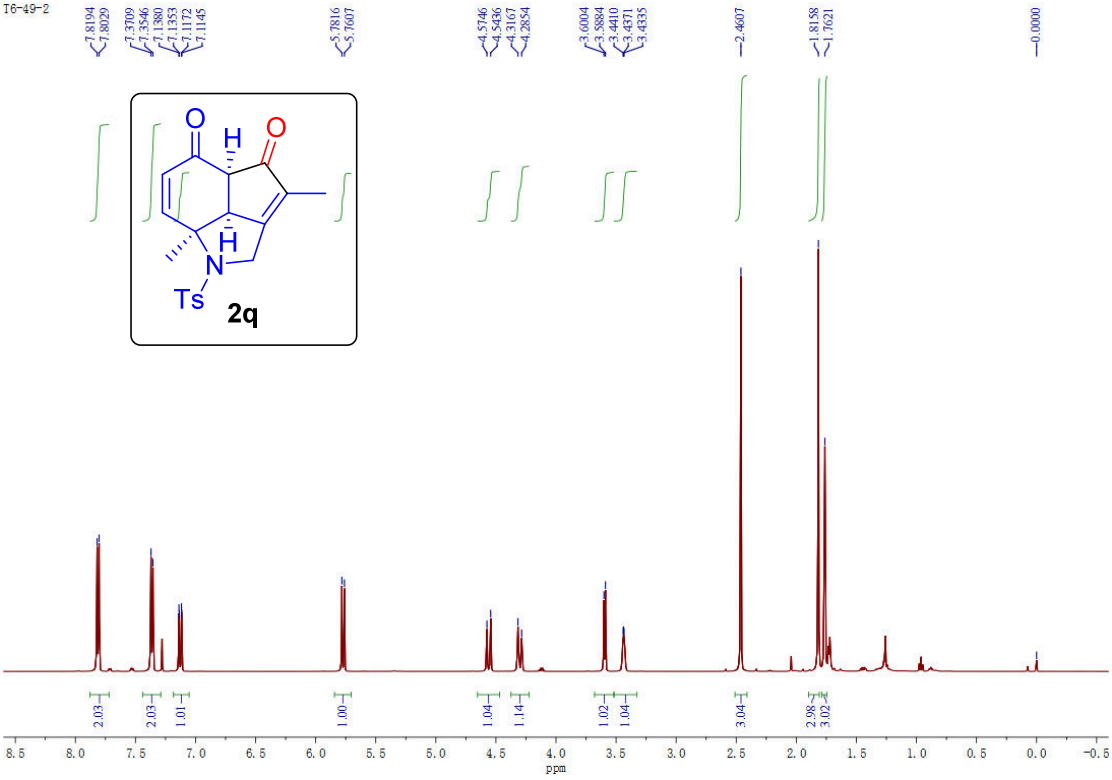
Molecular Weight: 324.3320

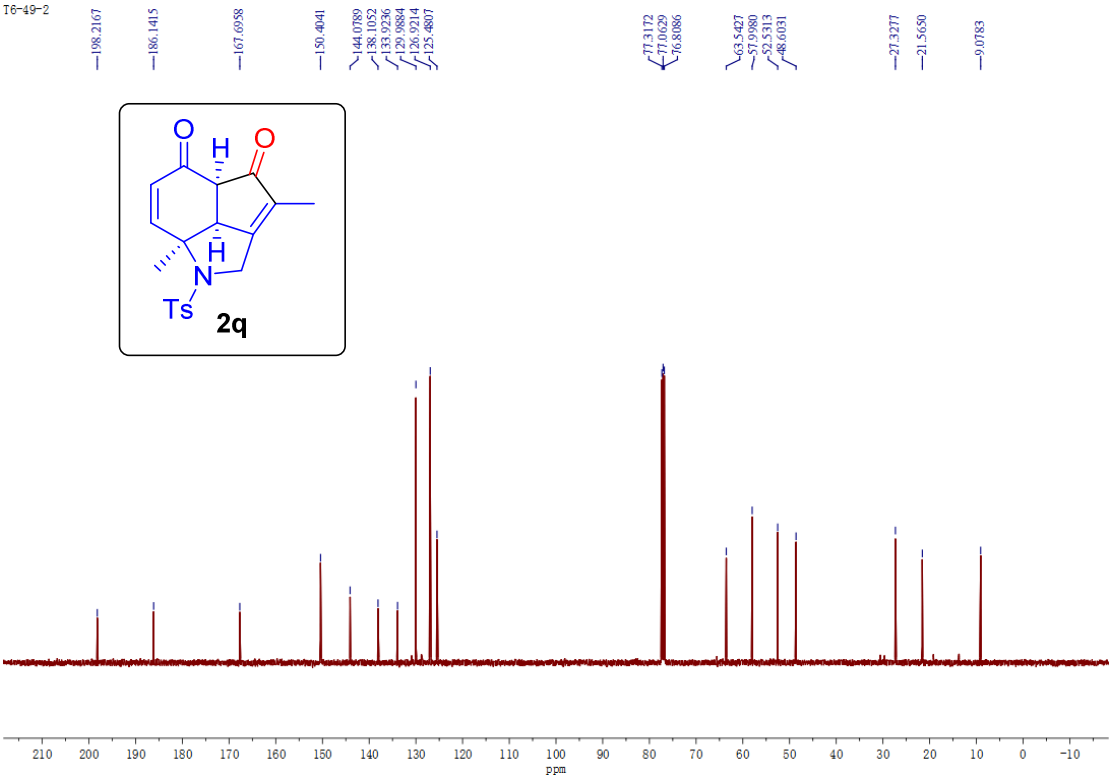
m/z: 324.0998 (100.0%), 325.1031 (20.5%), 326.1065 (2.0%), 326.1040 (1.0%)

HRMS (ESI, m/z) calcd for $C_{19}H_{16}O_5$ $[M+H]^+$ 325.1071, found 325.1076


C1-66
7.5136
7.5064
7.4318
7.4218
7.1183
7.1107
7.1032
6.6224
6.6048
6.6017
5.8154
5.7947
5.0834
5.0798
5.0492
5.0457
4.8734
4.8692
4.8393
4.8351
3.8421
3.8303
3.5964
3.5931
3.5890
3.5848
3.5816
1.6601
0.0000
1.00
1.03
1.00
1.02
0.98
1.04
1.05
0.97
1.00
3.04
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm
O
H
O
S
H
O
2p


C1-66
196.3814
186.6146
172.9217
151.3367
131.4778
128.8539
127.7581
127.6861
127.5434
127.0805
77.2887
77.0345
76.7804
76.4817
67.0355
59.4081
50.6032
26.2760
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
ppm
O
H
O
S
H
O
2p


T6-49-2
7.8194
7.8029
7.3709
7.3546
7.1380
7.1353
7.1172
7.1145
5.7816
5.7607
4.5746
4.5436
4.3167
4.2854
3.6004
3.5884
3.4410
3.4371
3.4335
2.4607
1.8158
1.7621
0.0000
2.03
2.03
1.01
1.00
1.04
1.14
1.02
1.04
3.04
2.98
3.02
ppm
2q


T6-49-2
198.2167
186.1415
167.6958
150.4041
144.0789
138.1052
133.9236
129.9884
126.9214
125.4807
77.3172
77.0629
76.8086
63.5427
57.9980
52.5313
48.6031
27.3277
21.5650
9.0783
ppm
2q

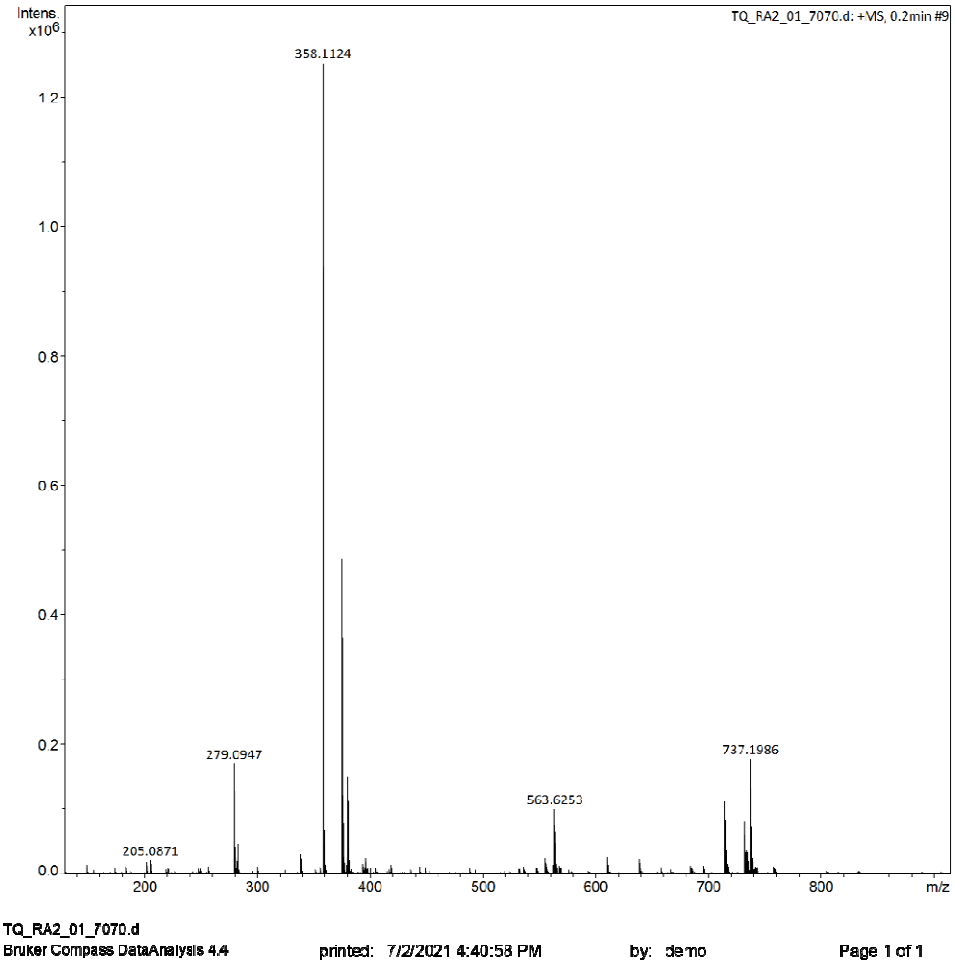
Display Report

Analysis Info

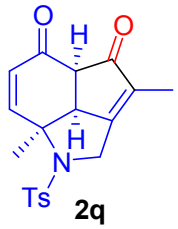
Analysis Name	D:\Data\fenglei\TQ_RA2_01_7070.d	Acquisition Date	7/2/2021 4:35:33 PM
Method	1225-1.m	Operator	Demo User
Sample Name	TQ	Instrument	Impact II 18255265.10256
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	2600 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1800 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



TQ_RA2_01_7070.d
Bruker Compass DataAnalysis 4.4 printed: 7/2/2021 4:40:58 PM by: demo Page 1 of 1



2q

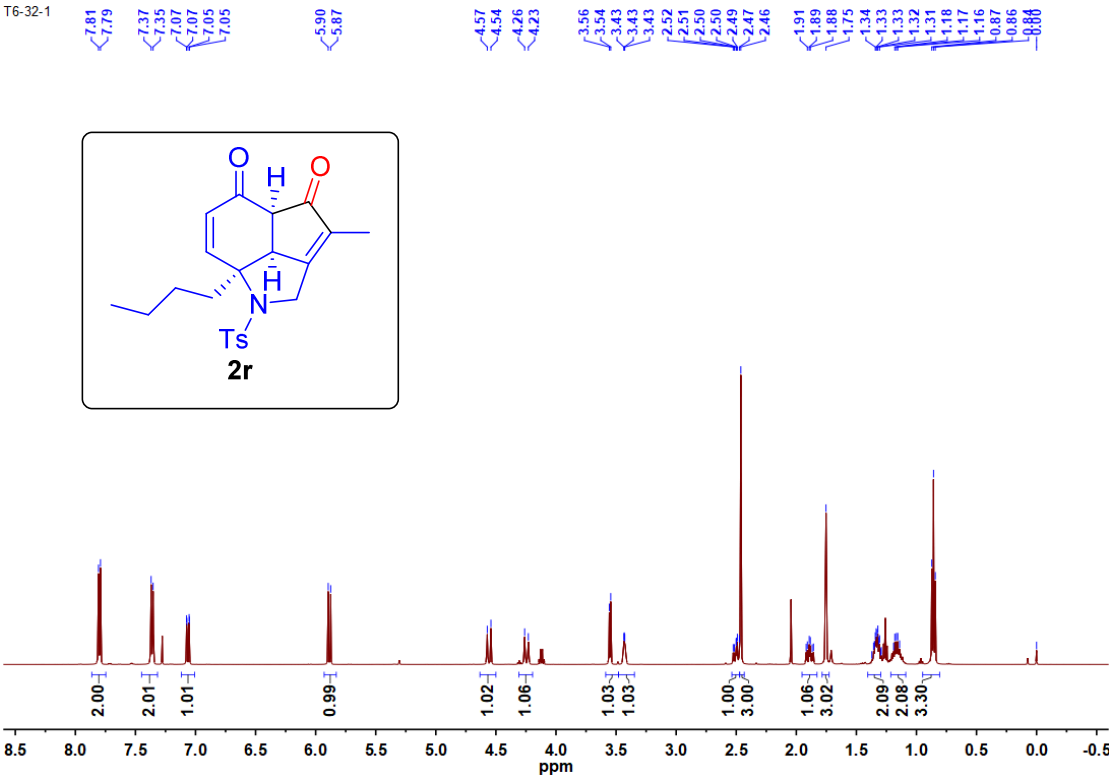
Chemical Formula: $C_{19}H_{19}NO_4S$

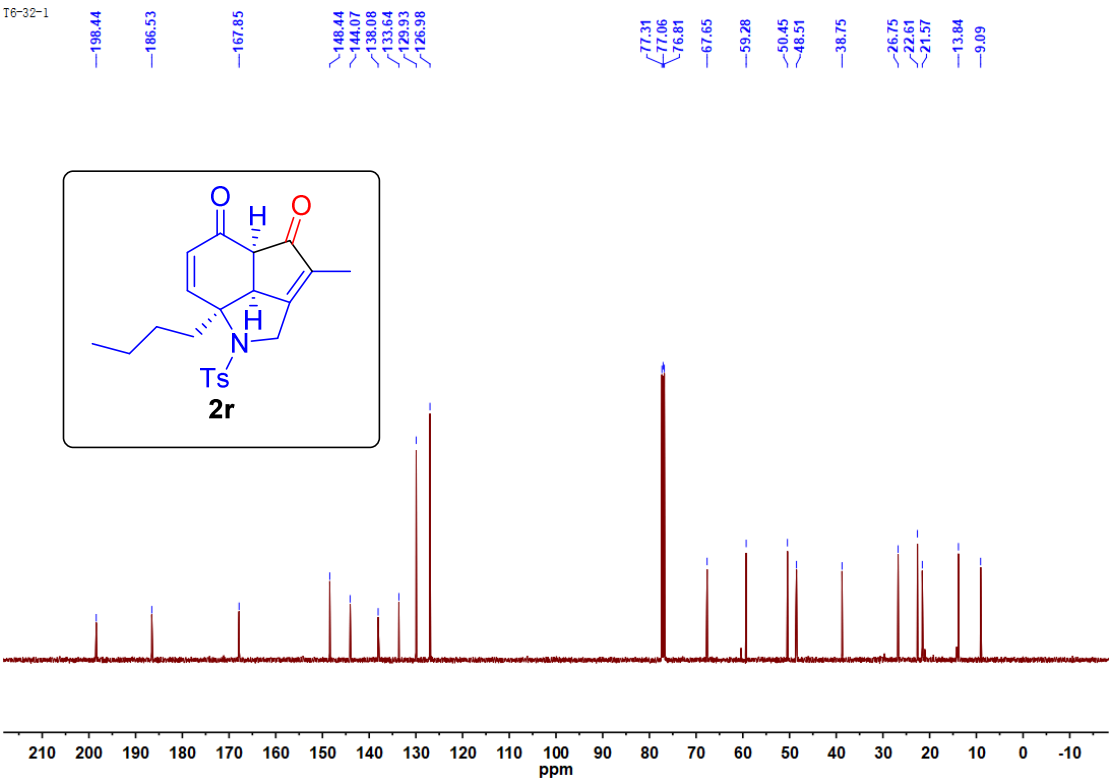
Exact Mass: 357.1035

Molecular Weight: 357.4240

m/z: 357.1035 (100.0%), 358.1068 (20.5%), 359.0993 (4.5%), 359.1102 (2.0%)

HRMS (ESI, m/z) calcd for $C_{19}H_{19}NO_4S$ $[M+H]^+$ 358.1108, found 358.1124.


T6-32-1
7.81
7.79
7.37
7.35
7.07
7.07
7.05
7.05
5.90
5.87
4.57
4.54
4.26
4.23
3.56
3.54
3.43
3.43
3.43
2.52
2.51
2.50
2.50
2.49
2.47
2.46
1.91
1.89
1.88
1.75
1.34
1.33
1.33
1.32
1.31
1.18
1.17
1.16
0.87
0.86
0.84
0.00
O
H
O
H
N
Ts
2r
2.00
2.01
1.01
0.99
1.02
1.06
1.03
1.03
1.00
3.00
1.06
3.02
2.09
2.08
3.30
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm


T6-32-1
198.44
186.53
167.85
148.44
144.07
138.08
133.64
129.93
126.98
77.31
77.06
76.81
67.65
59.28
50.45
48.51
38.75
26.75
22.61
21.57
13.84
9.09
O
H
O
H
N
Ts
2r
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
ppm

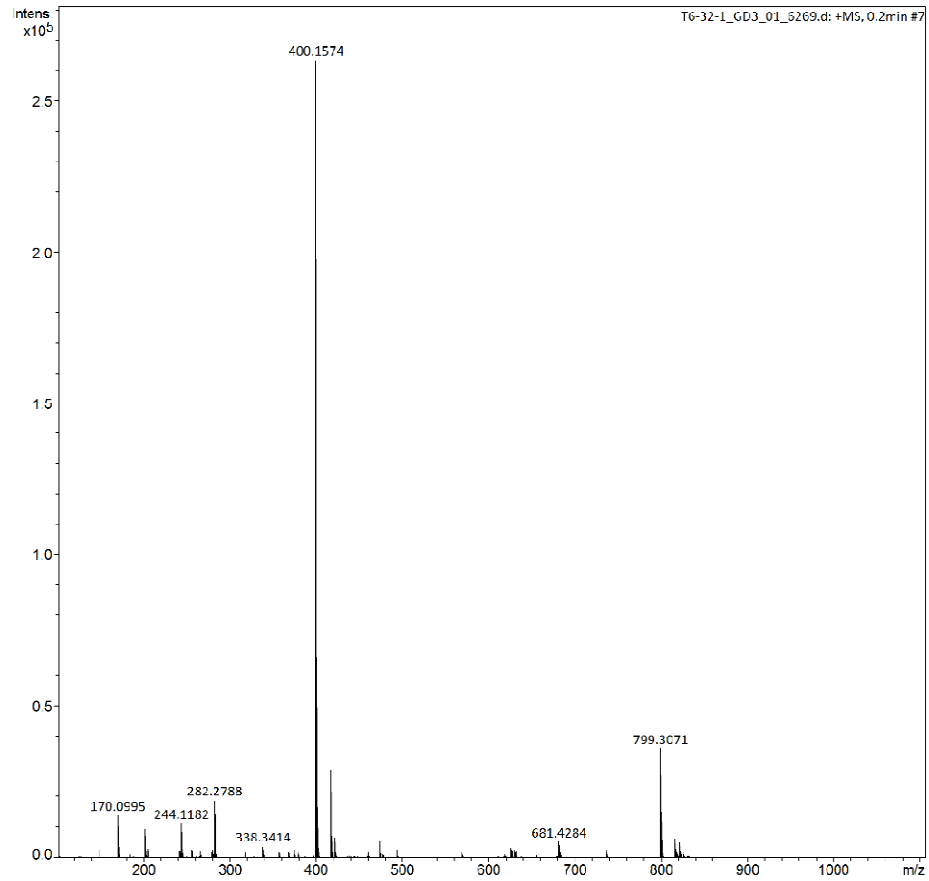
Display Report

Analysis Info

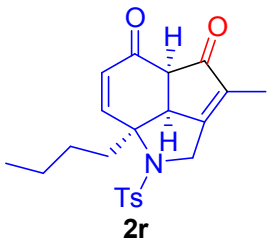
Analysis Name	D:\Data\fenglei\T6-32-1_GD3_01_6269.d	Acquisition Date	6/9/2021 4:33:23 PM
Method	1225-1.m		
Sample Name	T6-32-1	Operator	Demo User
Comment		Instrument	impact II 1825265.10256

Acquisition Parameter

Source Type	ESI	on Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	2600 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Va ve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



T6-32-1_GD3_01_6269.d
Bruker Compass DataAnalysis 4.4 printed: 6/9/2021 4:35:35 PM by: demo Page 1 of 1



2r

Chemical Formula: $C_{22}H_{25}NO_4S$
Exact Mass: 399.1504
Molecular Weight: 399.5050
m/z: 399.1504 (100.0%), 400.1538 (23.8%), 401.1462 (4.5%), 401.1571 (2.7%), 402.1496 (1.1%)

HRMS (ESI, m/z) calcd for $C_{22}H_{25}NO_4S$ $[M+H]^+$ 400.1577, found 400.1574.

9. Reference

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