# **Supporting Information**

# Palladium-Catalyzed Cross-Electrophile Coupling Reaction involving Sulfur Dioxide for the Direct Synthesis of Diverse Functionalized Sulfones

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# **Table of Content**

General information and Materials:	S2
Optimization Table	S3
General Procedures	S4
The procedure for the gram scale reactions:	S6
Mechanistic Experiments	S8
Computational Details	S11
X-Ray Crystal Structures	S35
Characterization data of products	S36

### **General information and Materials**

Unless otherwise noted, all reactions or reagents were obtained from commercial suppliers and used as received. Unless otherwise noted, all strict water-free and oxygen-free conditions were carried in an argon atmosphere glovebox (Vigor, SGI800-750TS-F). The substrates and reagents for catalytic reactions were degassed and stored in the glovebox, unless otherwise noted. All work-up and purification procedures were carried out with reagent-grade solvents in air.

Thin Layer Chromatography analyses were performed on silica gel coated glass plates (0.25 mm) with fluorescence indicator UV254. For detection of spots, irradiation of UV light at 254 nm or staining reagent using phosphomolybdic acid solution was used. Flash column chromatography was conducted with silica gel 60 (particle size 230–400 mesh, Huanghai) at room temperature and under elevated pressure.

Gas Chromatography (GC) analysis was conducted on a Shimadzu GC-2030 instrument equipped with a Rtx-5 column (30 m  $\times$  0.25 mm) with dodecane as an internal standard. GC-MS analysis was conducted on Agilent 5977B GC/MSD instrument equipped with a HP-5MS UI column (30 m  $\times$  0.25 mm). <sup>1</sup>H NMR, <sup>13</sup>C NMR and <sup>19</sup>F NMR spectra were recorded at 400 MHz, 101 MHz and 376 MHz, respectively in CDCl<sub>3</sub> (or DMSO-*d*<sub>6</sub>) at room temperature. <sup>1</sup>H NMR was reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quadruplet, m = multiplet), coupling constant (*J* values) in Hz and integration.

## **Optimization Table**



<sup>a</sup>Yields determined by GC analysis using n-dodecane as the internal standard; <sup>b</sup> Isolated yield in the parenthesis.

The initial study started with the attempts on the introduction of SO<sub>2</sub> into allylic acetate and aryl iodide (Table S1). (E)-4-phenylbut-3-en-2-yl 1, 1-iodo-4-methylbenzene 2 and DABSO were employed as the substrates to evaluate this Pd-catalyzed multicomponent cross-electrophile coupling reaction. After evaluation of a range of reaction parameters, we found that a combination of Pd(OAc)<sub>2</sub> (5 mol%), BIPHEP (5 mol%), and TEA (2.5 equiv) in DMF (1 mL) at 80 °C provided the best results, giving rise to 3 in 81% isolated yield (Table S1, entry 1). When Pd(OAc)<sub>2</sub> was replaced by other palladium sources such as Pd(TFA)<sub>2</sub>, Pd(acac)<sub>2</sub> and Pd<sub>2</sub>(dba)<sub>3</sub>, the efficiency of the reaction decreased slightly (entries 2-4). A comparison of entries 5-11 reveals that the characteristic of the ligand played an important role, with bidentate phosphine ligand (L1) providing the best interplay between electronic and steric effects. It was found that the type of the base has a significant impact on the reaction (entries 12-14). Switching the TEA to DIPEA caused a precipitously decrease in the yield, moreover, no desired product was detected when other bases such as DBU and DMAP were used. Various inorganic SO<sub>2</sub> surrogates such as Na<sub>2</sub>S<sub>2</sub>O<sub>5</sub>, K<sub>2</sub>S<sub>2</sub>O<sub>5</sub>,  $Na_2S_2O_8$  or  $K_2S_2O_8$  were tested, however, no reaction was observed (entries 15-18). Finally, a control experiment demonstrated that the catalyst and ligand were essential to this transformation (entry 19).

### **General Procedures**



In an argon fulfilled glovebox, allylic acetate (0.2 mmol, 1 equiv), aryl iodide (0.24 mmol, 1.2 equiv), Pd(OAc)<sub>2</sub> (2.2 mg, 0.01 mmol, 0.05 equiv), BIPHEP (5.2 mg, 0.01 mmol, 0.05 equiv), DABSO (72.1 mg, 1.5 equiv), and TEA (0.5 mmol, 2.5 equiv) were added as this order into an ovendried 4 mL vial with a magnetic stirring bar, followed by addition of DMF (1.0 mL). The vial was sealed and removed out of the glovebox, then heated to 80 °C using heating mantle with 600-700 rpm stirring speed. After 16 h, the vial was cooled to room temperature. The mixture was passed through a short silica gel pad with EtOAc. The filtrate was washed by H<sub>2</sub>O (3×5 mL), dried over anhydrous  $Na_2SO_4$ , then concentrated and the residue was purified by flash column chromatography to give the desired products **3-51**.



Figure S1 | The heat source used in this study.





In an argon fulfilled glovebox, allylic acetate (0.2 mmol, 1 equiv), alkene-tethered aryl halide (0.24 mmol, 1.2 equiv),  $Pd(OAc)_2$  (2.2 mg, 0.01 mmol, 0.05 equiv), BIPHEP (2.6 mg, 0.005 mmol, 0.025 equiv), DABSO (72.1 mg, 1.5 equiv), and TEA (0.5 mmol, 2.5 equiv) were added as this order into an oven-dried 4 mL vial with a magnetic stirring bar, followed by addition of DMF (1.0 mL). The vial was sealed and removed out of the glovebox, then heated to 80 °C using heating mantle with 600-700 rpm stirring speed. After 16 h, the vial was cooled to room temperature. The mixture was passed through a short silica gel pad with EtOAc. The filtrate was washed by H<sub>2</sub>O ( $3 \times 5 mL$ ), dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, then concentrated and the residue was purified by flash column chromatography to give the desired products **52-67**, **73-84**.

# General procedure 3: Synthesis of sulfone-containing hetero- and carbocyclic scaffolds (compounds 68-72)



In an argon fulfilled glovebox, allylic acetate (0.2 mmol, 1 equiv), alkene-tethered aryl halide (0.24 mmol, 1.2 equiv), Pd(OAc)<sub>2</sub> (2.2 mg, 0.01 mmol, 0.05 equiv), BIPHEP (2.6 mg, 0.005 mmol, 0.025 equiv), PPh<sub>3</sub> (2.6 mg, 0.01 mmol, 0.05 equiv) DABSO (72.1 mg, 1.5 equiv), and TEA (0.5 mmol, 2.5 equiv) were added as this order into an oven-dried 4 mL vial with a magnetic stirring bar,

followed by addition of DMF (1.0 mL). The vial was sealed and removed out of the glovebox, then heated to 80 °C using heating mantle with 600-700 rpm stirring speed. After 16 h, the vial was cooled to room temperature. The mixture was passed through a short silica gel pad with EtOAc. The filtrate was washed by  $H_2O$  (3×5 mL), dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, then concentrated and the residue was purified by flash column chromatography to give the desired products **68-72**.



In an argon fulfilled glovebox, propargyl acetate (0.2 mmol, 1 equiv), 4-lodotoluene (0.24 mmol, 1.2 equiv), Pd(OAc)<sub>2</sub> (4.5 mg, 0.02 mmol, 0.1 equiv), DPEPhos (10.8 mg, 0.02 mmol, 0.1 equiv), DABSO (72.1 mg, 1.5 equiv), and TEA (0.5 mmol, 2.5 equiv) were added as this order into an ovendried 4 mL vial with a magnetic stirring bar, followed by addition of DMF (1.0 mL). The vial was sealed and removed out of the glovebox, then heated to 80 °C using heating mantle with 600-700 rpm stirring speed. After 16 h, the vial was cooled to room temperature. The mixture was passed through a short silica gel pad with EtOAc. The filtrate was washed by H<sub>2</sub>O (3×5 mL), dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, then concentrated and the residue was purified by flash column chromatography to give the desired products **85-89**.

#### General procedure 5: Synthesis of propargyl-alkyl sulfones (compounds 90-94)



In an argon fulfilled glovebox, propargyl acetate (0.2 mmol, 1 equiv), *N*-(2-iodophenyl)-*N*-methylmethacrylamide (0.24 mmol, 1.2 equiv), Pd(OAc)<sub>2</sub> (4.5 mg, 0.02 mmol, 0.1 equiv), DPEPhos (5.4 mg, 0.01 mmol, 0.05 equiv), DABSO (72.1 mg, 1.5 equiv), and TEA (0.5 mmol, 2.5 equiv) were added as this order into an oven-dried 4 mL vial with a magnetic stirring bar, followed by addition of DMF (1.0 mL). The vial was sealed and removed out of the glovebox, then heated to 80 °C using heating mantle with 600-700 rpm stirring speed. After 16 h, the vial was cooled to room temperature. The mixture was passed through a short silica gel pad with EtOAc. The filtrate was washed by H<sub>2</sub>O ( $3\times5$  mL), dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, then concentrated and the residue was purified by flash column chromatography to give the desired products **90-94**.

#### The procedure for the gram scale reactions:

1) Synthesis of compound 43





43, 83 % yield

In an argon fulfilled glovebox, (E)-4-(6-methoxypyridin-3-yl)but-3-en-2-yl acetate **95** (1.1 g, 5.0 mmol), 5-iodo-1H-indole **50** (6.0 mmol, 1.2 equiv), Pd(OAc)<sub>2</sub> (56.0 mg, 0.25 mmol, 0.05 equiv), BIPHEP (130.6 mg, 0.25 mmol, 0.05 equiv), DABSO (7.5 mmol, 1.5 equiv) and TEA (12.5 mmol, 2.5 equiv) were added as this order into an oven-dried 100 mL seal-tube with a magnetic stirring bar, followed by addition of DMF (25 mL). The tube was sealed and removed out of the glovebox, then heated to 80 °C using oil bath with 600 rpm stirring speed. After 16 h, the seal-tube was cooled to room temperature. The mixture was passed through a short silica gel pad with EtOAc. The filtrate was washed by H<sub>2</sub>O (3×50 mL), dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, then concentrated and the residue was purified by flash column chromatography using petroleum/ethyl acetate (1:1) as eluent to give the desired product **43** as a white solid (1.421 g, 83% yield).



In an argon fulfilled glovebox, (E)-3-(4-bromophenyl)allyl acetate **96** (1.0 g, 3.9 mmol), *N*-(2-iodophenyl)-*N*-methylmethacrylamide **83** (4.7 mmol, 1.2 equiv),  $Pd(OAc)_2$  (43.8 mg, 0.195 mmol, 0.05 equiv), BIPHEP (50.9 mg, 0.025 equiv), DABSO (5.85 mmol, 1.5 equiv) and TEA (9.75 mmol, 2.5 equiv) were added as this order into an oven-dried 100 mL seal-tube with a magnetic stirring bar, followed by addition of DMF (20 mL). The tube was sealed and removed out of the glovebox, then heated to 80 °C using oil bath with 600 rpm stirring speed. After 16 h, the seal-tube was cooled to room temperature. The mixture was passed through a short silica gel pad with EtOAc. The filtrate was washed by H<sub>2</sub>O (3×50 mL), dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, then concentrated and the residue was purified by flash column chromatography using petroleum/ethyl acetate (2:1) as eluent to give the desired product **97** as a white solid (1.355 g, 80% yield).



Figure S2 | The heat source used in the gram scale reaction.

#### **Mechanistic Experiments**



In an argon fulfilled glovebox, (*E*)-4-phenylbut-3-en-2-yl acetate **1** (0.2 mmol, 1 equiv), Pd(OAc)<sub>2</sub> (2.2 mg, 0.01 mmol, 0.05 equiv), BIPHEP (5.2 mg, 0.01 mmol, 0.05 equiv), DABSO (72.1 mg, 1.5 equiv), and TEA (0.5 mmol, 2.5 equiv) were added as this order into an oven-dried 4 mL vial with a magnetic stirring bar, followed by addition of DMF (1.0 mL). The vial was sealed and removed out of the glovebox, then heated to 80 °C using heating mantle with 600 rpm stirring speed. After 16 h, the vial was cooled to room temperature. The mixture was passed through a short silica gel pad with EtOAc. The filtrate was washed by H<sub>2</sub>O (3×5 mL), dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, then concentrated and the residue was purified by flash column chromatography using petroleum/ethyl acetate (100:1) as eluent to give the compound **98** as a colorless oil (18.2 mg, 70% yield).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.33 (d, *J* = 7.6 Hz, 2H), 7.24 (t, *J* = 7.6 Hz, 2H), 7.16 (d, *J* = 7.2 Hz, 1H), 6.71 (dd, *J* = 15.6, 10.4 Hz, 1H), 6.51 – 6.38 (m, 2H), 5.25 (d, *J* = 16.8 Hz, 1H), 5.09 (d, *J* = 10.0 Hz, 1H).



In an argon fulfilled glovebox, (*E*)-4-phenylbut-3-en-2-yl acetate **1** (0.2 mmol, 1 equiv), Pd(OAc)<sub>2</sub> (2.2 mg, 0.01 mmol, 0.05 equiv), BIPHEP (5.2 mg, 0.01 mmol, 0.05 equiv), DABSO (72.1 mg, 1.5 equiv), and TEA (0.5 mmol, 2.5 equiv) were added as this order into an oven-dried 4 mL vial with a magnetic stirring bar, followed by addition of DMF (1.0 mL). The vial was sealed and removed out of the glovebox, then heated to 80 °C using heating mantle with 600 rpm stirring speed. After 16 h, the resulting mixture was cooled to room temperature before adding *t*-butylbromoacetate (0.6 mmol, 3 equiv). The reaction was left to stir at room temperature for an additional 3 hours. The mixture was passed through a short silica gel pad with EtOAc. The filtrate was washed by H<sub>2</sub>O (3×5 mL), dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, then concentrated and the residue was purified by flash column chromatography using petroleum/ethyl acetate (100:1) as eluent to give the compound **98** as a colorless oil (18.0 mg, 69% yield). *No sulfone product 99 was detected in the reaction.* 



In an argon fulfilled glovebox, 1-iodo-4-methylbenzene **2** (0.2 mmol, 1 equiv),  $Pd(OAc)_2$  (2.2 mg, 0.01 mmol, 0.05 equiv), BIPHEP (5.2 mg, 0.01 mmol, 0.05 equiv), DABSO (72.1 mg, 1.5 equiv), and TEA (0.5 mmol, 2.5 equiv) were added as this order into an oven-dried 4 mL vial with a magnetic stirring bar, followed by addition of DMF (1.0 mL). The vial was sealed and removed out of the glovebox, then heated to 80 °C using heating mantle with 600 rpm stirring speed. After 16 h, the resulting mixture was cooled to room temperature before adding *t*-butylbromoacetate (0.6 mmol, 3 equiv). The reaction was left to stir at room temperature for an additional 3 hours. The mixture was passed through a short silica gel pad with EtOAc. The filtrate was washed by H<sub>2</sub>O (3×5 mL), dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, then concentrated and the residue was purified by flash column chromatography using petroleum/ethyl acetate (3:1) as eluent to give the compound **100** as a colorless oil (38.4 mg, 71% yield).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.75 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 7.2 Hz, 2H), 3.94 (d, *J* = 2.0 Hz, 2H), 2.38 (s, 3H), 1.30 (d, *J* = 2.0 Hz, 9H).





In an argon fulfilled glovebox, (*E*)-4-phenylbut-3-en-2-yl acetate **1** (0.2 mmol, 1 equiv), sodium 4-methylbenzenesulfinate **101** (0.24 mmol, 1.2 equiv),  $Pd(OAc)_2$  (2.2 mg, 0.01 mmol, 0.05 equiv) and BIPHEP (5.2 mg, 0.01 mmol, 0.05 equiv) were added as this order into an oven-dried 4 mL vial with a magnetic stirring bar, followed by addition of DMF (1.0 mL). The vial was sealed and removed out of the glovebox, then heated to 80 °C using heating mantle with 600 rpm stirring speed. After 16 h, the vial was cooled to room temperature. The mixture was passed through a short silica gel pad with EtOAc. The filtrate was washed by H<sub>2</sub>O (3×5 mL), dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, then concentrated and the residue was purified by flash column chromatography using petroleum/ethyl acetate (10:1) as eluent to give the compound **3** as a white solid (45.2 mg, 79% yield).



In an argon fulfilled glovebox, (*E*)-4-phenylbut-3-en-2-yl acetate **1** (0.2 mmol, 1 equiv), sodium 4-methylbenzenesulfinate **101** (0.24 mmol, 1.2 equiv) were added as this order into an oven-dried 4 mL vial with a magnetic stirring bar, followed by addition of DMF (1.0 mL). The vial was sealed and removed out of the glovebox, then heated to 80 °C using heating mantle with 600 rpm stirring speed. After 16 h, the vial was cooled to room temperature. The mixture was passed through a short silica gel pad with EtOAc. The filtrate was analyzed by GC-MS and GC, *no desired product 3 was found in this reaction.* 

#### **Computational Details**

#### **Computational Methods**

All the calculations were performed with Gaussian 16 package. <sup>[1]</sup> Geometries were optimized in gas phase by using unrestricted MN15<sup>[2]</sup> and a mixed basis set of SDD<sup>[3]</sup> for Pd, P, and I, and 6- $31G(d,p)^{[4]}$  basis set for all other atoms at temperature of 353K. Optimized geometries were verified by frequency computations as minima (zero imaginary frequencies) or transition state (a single imaginary frequency) at the same level of theory. The transition states (TSs) were also confirmed by viewing normal mode vibrational vector. Solvent effect was included by single-point energy calculation using SMD model with toluene as the solvent and MN15 method with def2-TZVP basis set for Pd, P, and I, and 6-311++G(d,p) basis set for other atoms. <sup>[5]</sup> All relative Gibbs free energies

and electronic energies were reported in kcal/mol.

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**Figure S3.** The DFT studies of allyl-sulfonylated first (left) and aryl-sulfonylated first (right) by Pd Catalyst. Relative free energies (electronic energies) are in kcal/mol at 353 K and 1 atm.

**Table S2.** Listed are the zero-point vibrational energy correction (cZPE), enthalpy correction (cH), Gibbs free energy correction (cG) and imaginary frequencies (IF) determined in the gas-phase

Geometry	cZPE <sub>353,gas</sub>	cH <sub>353,gas</sub>	cG <sub>353,gas</sub>	E <sub>0,sol</sub>	IF
OAc	0.048552	0.055367	0.014662	-228.438375	-
P_ligand	0.529418	0.575252	0.440302	-2069.826232	-
cinnamyl_acetate	0.233719	0.253874	0.178953	-615.592189	-
PhI	0.090533	0.099638	0.051465	-528.398678	-
Cat	1.063503	1.156625	0.927562	-4267.483608	-
TS1	0.621046	0.678283	0.521788	-2725.991718	-74.097
INT1	0.623492	0.680962	0.524061	-2726.043839	-
TS1b'	0.763845	0.831466	0.655557	-2813.179026	-261.574
TS1b	0.763502	0.831650	0.651337	-2813.191669	-186.482
INT1b	0.713894	0.774965	0.613442	-2584.759652	-
TS2	0.632852	0.694305	0.531265	-3274.448915	-151.888
TS2'	0.632966	0.694646	0.529537	-3274.44501	-189.083
INT2	0.634734	0.696091	0.533014	-3274.498901	-
INT2'	0.634528	0.696424	0.529761	-3274.496594	-
TS2b	0.722756	0.788044	0.617842	-3133.152113	-192.048
INT2b	0.724559	0.790054	0.619237	-3133.17199	-
INT3	0.585692	0.642227	0.488362	-2722.974221	-
INT4	0.098213	0.109668	0.057060	-779.962497	-
INT5	0.813791	0.887141	0.698512	-3364.73786	-
TS3	0.812869	0.885969	0.693672	-3364.713385	-133.088
TS3'	0.812745	0.885504	0.698118	-3364.705912	-87.564
INT6	0.815686	0.888194	0.699510	-3364.743961	-
Prd	0.283005	0.308014	0.221082	-1167.110803	-

geometries at 353 K and 1 atm. Single-point solvent (n,n-dimethylformamide) corrected SCF Done energies (E) are also presented. All energies values are given in Hartree.

**Table S3.** Cartesian coordinates (in Å) of related structures which were calculated at the M N15/6-31G(d,p)+SDD(Pd) level of theory

OAc anion			С	1.762668	-2.375651	-0.499014	
0	0.688921	1.166683	-0.000133	С	1.280965	-3.306710	-1.422746
С	0.218674	0.002120	0.000264	С	0.306305	-2.936394	-2.346755
0	0.805885	-1.106535	-0.000130	С	-0.186946	-1.631594	-2.341587
С	-1.346311	-0.057585	0.000058	С	-0.278669	0.692487	-1.414238
н	-1.737640	0.469460	0.880274	С	-1.268492	1.067340	-0.483552
н	-1.737522	0.470828	-0.879385	С	-1.762336	2.374502	-0.502795
Н	-1.717465	-1.088682	-0.000717	С	-1.280685	3.303904	-1.428219
				С	-0.306305	2.931842	-2.351826
P_ligand			С	0.186777	1.626989	-2.344500	
С	0.278575	-0.695422	-1.413044	н	2.530167	-2.671414	0.211851
С	1.268597	-1.068543	-0.481871	н	1.674789	-4.320021	-1.419712

Н	-0.076162	-3.658158	-3.063507
Н	-0.969590	-1.334981	-3.037298
н	-2.529619	2.671592	0.207754
н	-1.674320	4.317291	-1.426812
н	0.076098	3.652315	-3.069909
н	0.969242	1.329067	-3.039850
Р	1.852576	0.240562	0.715382
Р	-1.852564	-0.239664	0.715946
С	2.883469	1.255575	-0.450928
С	2.831380	2.647745	-0.336543
С	3.628926	0.679463	-1.487744
С	3.510317	3.458090	-1.248104
н	2.225946	3.091158	0.451216
С	4.308902	1.486957	-2.399079
н	3.658523	-0.404983	-1.584652
С	4.246350	2.877890	-2.281298
н	3.455687	4.539855	-1.157973
Н	4.882470	1.033559	-3.203555
н	4.769322	3.507330	-2.996816
С	3.100022	-0.703539	1.709160
С	4.484859	-0.573665	1.570775
С	2.589682	-1.573487	2.684851
С	5.345819	-1.303898	2.394091
Н	4.893436	0.100437	0.822112
С	3.448603	-2.314140	3.493320
Н	1.509967	-1.664773	2.800809
С	4.831844	-2.177570	3.350994
Н	6.421261	-1.191476	2.281755
Н	3.040765	-2.989981	4.240567
Н	5.504235	-2.747102	3.987209
С	-3.099619	0.706418	1.708331
С	-2.588899	1.578266	2.682124
С	-4.484510	0.576426	1.570594
С	-3.447509	2.320581	3.489398
Н	-1.509140	1.669701	2.797547
С	-5.345154	1.308348	2.392738
Н	-4.893373	-0.099082	0.823354
С	-4.830805	2.183839	3.347777
Н	-3.039386	2.997863	4.235182
Н	-6.420641	1.195815	2.280941
Н	-5.502950	2.754674	3.983084
С	-2.883925	-1.256322	-0.448541
С	-2.831958	-2.648326	-0.332058
С	-3.629639	-0.681709	-1.486004
С	-3.511221	-3.459982	-1.242205

Н	-2.226366	-3.090607	0.456215
С	-4.309948	-1.490517	-2.395930
Н	-3.659180	0.402590	-1.584543
С	-4.247483	-2.881275	-2.276075
Н	-3.456672	-4.541614	-1.150451
Н	-4.883707	-1.038279	-3.200921
Н	-4.770708	-3.511746	-2.990500
cinna	amyl_acetate		
С	-0.303325	0.504088	0.062352
С	0.708076	-0.034850	-0.629436
Н	-0.142755	0.970346	1.035199
Н	0.477100	-0.511274	-1.584852
С	-1.710413	0.545341	-0.449430
Н	-1.805158	-0.046146	-1.367480
С	2.128350	-0.075879	-0.242005
С	3.010247	-0.867730	-0.992162
С	2.643304	0.644530	0.848219
С	4.360848	-0.953708	-0.659307
Н	2.623423	-1.424429	-1.843745
С	3.991021	0.559528	1.182776
Н	1.985809	1.285056	1.430783
С	4.856087	-0.241148	0.432091
Н	5.025510	-1.575743	-1.252889
Н	4.371833	1.125156	2.029154
Н	5.908787	-0.302766	0.694261
С	-2.198243	1.968589	-0.696699
Н	-1.572898	2.453776	-1.451479
Н	-3.232093	1.950857	-1.051390
Н	-2.142057	2.550503	0.229161
0	-2.540588	-0.063580	0.565462
С	-3.723935	-0.552799	0.152257
0	-4.106996	-0.499039	-0.997333
С	-4.484426	-1.167638	1.297458
Н	-3.895519	-1.975904	1.739527
Н	-4.648887	-0.418076	2.076367
Н	-5.437975	-1.550343	0.935678
Phl			
I	-1.560493	0.000000	-0.000001
С	0.575986	0.000005	0.000000
С	1.256302	-1.215557	0.000001
С	1.256305	1.215559	0.000001
С	2.652347	-1.207040	0.000002
Н	0.709643	-2.153520	0.000000

С	2.652356	1.207035	0.000002	Н	3.025405	3.415214	-2.931348
Н	0.709660	2.153529	0.000001	С	-0.666751	4.446445	-2.338784
С	3.351312	-0.000002	0.000003	Н	-0.810175	2.610515	-1.190908
Н	3.190789	-2.150939	0.000003	С	0.170852	5.256952	-3.103119
Н	3.190795	2.150936	0.000003	Н	2.159121	5.514982	-3.901020
Н	4.437610	-0.000009	0.000003	Н	-1.707786	4.718477	-2.179811
				н	-0.208392	6.177113	-3.540471
Ca	at			С	1.153373	-2.874755	1.995943
С	4.063637	0.718457	0.217253	С	-0.170327	-3.265965	1.781563
С	3.139429	1.693049	-0.219039	С	1.989717	-3.697252	2.761898
С	3.272773	3.009264	0.246424	С	-0.666550	-4.446485	2.339030
С	4.283051	3.369336	1.136002	Н	-0.810011	-2.610867	1.190649
С	5.211310	2.415794	1.548453	С	1.502179	-4.882944	3.309167
С	5.105096	1.113130	1.069654	н	3.025328	-3.414531	2.932098
С	4.063547	-0.718623	-0.217471	С	0.171014	-5.256658	3.103769
С	3.139356	-1.693136	0.219018	н	-1.707512	-4.718713	2.179908
С	3.272593	-3.009409	-0.246323	н	2.159157	-5.514178	3.902165
С	4.282693	-3.369593	-1.136050	н	-0.208195	-6.176752	3.541293
С	5.210916	-2.416111	-1.548740	С	2.514996	-0.420234	2.723034
С	5.104852	-1.113410	-1.070011	С	1.880606	0.682117	3.298191
Н	2.566479	3.764851	-0.091287	С	3.757960	-0.830508	3.220604
Н	4.351245	4.395753	1.489123	С	2.479143	1.378144	4.350428
Н	6.011066	2.679916	2.234897	н	0.920884	1.000454	2.896696
Н	5.820110	0.356679	1.386500	С	4.348646	-0.151440	4.284744
Н	2.566352	-3.764938	0.091627	Н	4.290092	-1.650884	2.740444
Н	4.350789	-4.396037	-1.489110	С	3.712283	0.958042	4.847727
Н	6.010533	-2.680316	-2.235313	н	1.980642	2.249372	4.768750
Н	5.819869	-0.357026	-1.387010	н	5.315553	-0.474659	4.662995
Ρ	1.678882	1.236298	-1.274339	Н	4.182964	1.496428	5.666548
Ρ	1.678888	-1.236241	1.274351	Pd	-0.000081	0.000028	0.000047
С	2.514981	0.420344	-2.723053	Р	-1.678830	-1.237201	-1.273633
С	1.880790	-0.682225	-3.298029	Р	-1.678884	1.237159	1.273566
С	3.757819	0.830833	-3.220747	С	-3.139322	-1.693321	-0.217995
С	2.479417	-1.378246	-4.350211	С	-2.514949	-0.422166	-2.722849
Н	0.921168	-1.000700	-2.896403	С	-1.153275	-2.876197	-1.994033
С	4.348577	0.151786	-4.284864	С	-3.139367	1.693197	0.217881
Н	4.289816	1.651359	-2.740699	С	-1.153368	2.876207	1.993890
С	3.712422	-0.957902	-4.847663	С	-2.515082	0.422176	2.722771
Н	1.981098	-2.249644	-4.768393	С	-4.063498	-0.718471	0.217807
Н	5.315384	0.475171	-4.663228	С	-3.272593	-3.009260	0.248260
Н	4.183163	-1.496271	-5.666460	С	-1.880788	0.680035	-3.298559
С	1.153335	2.874885	-1.995717	С	-3.757762	-0.833044	-3.220280
С	1.989717	3.697719	-2.761284	С	-1.989578	-3.699405	-2.759281
С	-0.170469	3.265850	-1.781532	С	0.170469	-3.267129	-1.779402
С	1.502115	4.883484	-3.308334	С	-4.063518	0.718322	-0.217886

С	-3.272665	3.009126	-0.248406	Н	-6.010
С	0.170475	3.266964	1.779554	Н	-4.18
С	-1.989786	3.699599	2.758812	н	0.208
С	-1.881066	-0.680144	3.298411	н	-6.010
С	-3.757865	0.833146	3.220199	Н	0.208
С	-5.104811	-1.112640	1.070611	н	-4.183
С	-4.282727	-3.368805	1.138216		
Н	-2.566343	-3.765043	-0.089106	TS1	
С	-2.479438	1.375335	-4.351204	С	1.574
Н	-0.921177	0.998795	-2.897139	С	2.047
С	-4.348548	-0.154718	-4.284841	С	2.379
Н	-4.289719	-1.653280	-2.739688	С	2.293
С	-1.501960	-4.885513	-3.305576	С	1.87
Н	-3.025215	-3.416924	-2.929709	С	1.526
С	0.666765	-4.448075	-2.335897	С	1.097
Н	0.810131	-2.611517	-1.189040	С	-0.173
С	-5.104869	1.112461	-1.070669	С	-0.572
С	-4.282801	3.368631	-1.138364	С	0.27
Н	-2.566429	3.764923	0.088953	С	1.528
С	0.666775	4.447880	2.336110	С	1.922
Н	0.810187	2.611226	1.189377	н	2.702
С	-1.502167	4.885686	3.305151	н	2.553
Н	-3.025532	3.417304	2.928900	Н	1.802
С	-2.479813	-1.375445	4.351009	Н	1.164
Н	-0.921499	-0.999025	2.896978	Н	-1.55
С	-4.348744	0.154821	4.284706	Н	-0.058
Н	-4.289747	1.653454	2.739654	Н	2.198
С	-5.210926	-2.415017	1.550231	Н	2.899
Н	-5.819797	-0.356018	1.387108	Р	2.00
Н	-4.350863	-4.395009	1.491965	Р	-1.218
С	-3.712432	0.954622	-4.848369	С	2.678
Н	-1.981155	2.246477	-4.769965	С	1.869
Н	-5.315342	-0.478390	-4.662994	С	3.948
С	-0.170762	-5.258961	-3.099915	С	2.324
Н	-2.158911	-5.517285	-3.898031	Н	0.880
Н	1.707754	-4.720085	-2.176590	С	4.403
С	-5.211007	2.414816	-1.550327	Н	4.578
Н	-5.819861	0.355823	-1.387114	С	3.589
Н	-4.350957	4.394821	-1.492148	Н	1.689
С	-0.170854	5.258926	3.099847	Н	5.390
Н	1.707840	4.719747	2.177059	Н	3.943
Н	-2.159207	5.517609	3.897344	С	3.332
С	-3.712765	-0.954626	4.848184	С	4.558
Н	-1.981638	-2.246680	4.769704	С	3.08
Н	-5.315507	0.478583	4.662860	С	5.526

H	-6.010572	-2.678721	2.236962
Н	-4.183186	1.492434	-5.667525
Н	0.208495	-6.179394	-3.536683
Н	-6.010672	2.678491	-2.237048
Н	0.208413	6.179337	3.536653
Н	-4.183604	-1.492448	5.667285
TS1			
С	1.574976	2.465946	-0.514520
С	2.047247	1.260866	-1.072460
С	2.379693	1.224486	-2.435070
С	2.293806	2.362180	-3.232732
С	1.875433	3.569117	-2.672785
С	1.526725	3.610131	-1.326842
С	1.097702	2.641668	0.897811
С	-0.173262	2.217187	1.343014
С	-0.572553	2.511049	2.652035
С	0.271036	3.195845	3.525347
С	1.528174	3.612218	3.091386
С	1.922012	3.349405	1.781381
Н	2.702770	0.284150	-2.875894
Н	2.553700	2.303524	-4.286378
Н	1.802731	4.466386	-3.281199
Н	1.164734	4.535617	-0.884229
Н	-1.555801	2.198188	2.993419
Н	-0.058675	3.406700	4.539334
Н	2.198001	4.140539	3.764369
Н	2.899174	3.671337	1.427846
Р	2.001400	-0.339198	-0.138779
Р	-1.218829	1.148720	0.244926
С	2.678132	0.061319	1.538947
С	1.869725	-0.188913	2.650790
С	3.948293	0.620137	1.713362
С	2.324335	0.132405	3.931247
Н	0.880297	-0.622583	2.495790
С	4.403562	0.935273	2.992125
Н	4.578638	0.818412	0.849037
С	3.589469	0.694184	4.101605
Н	1.689184	-0.054856	4.793089
Н	5.390991	1.370183	3.124497
н	3.943623	0.943691	5.098608
С	3.332752	-1.390223	-0.882121
С	4.558930	-0.896135	-1.345578
С	3.086752	-2.767067	-0.922402
С	5 526374	-1.770991	-1 838329

Н	4.747980	0.175797	-1.345450	С	1.847621	1.774617	-0.750672
С	4.060058	-3.643064	-1.405729	С	2.530542	2.036788	-1.943715
н	2.123552	-3.137915	-0.569318	С	2.485772	3.298017	-2.536357
С	5.279402	-3.145283	-1.864638	С	1.769360	4.324891	-1.926367
н	6.473007	-1.380229	-2.202467	С	1.109291	4.078265	-0.725035
Н	3.862110	-4.711319	-1.429377	С	0.407029	2.662468	1.177634
н	6.035513	-3.825161	-2.248441	С	-0.789142	1.943183	1.375153
С	-2.857125	1.016534	1.081105	С	-1.370464	1.921005	2.648895
С	-2.938897	0.139391	2.173755	С	-0.777467	2.574936	3.726458
С	-4.027272	1.586646	0.571376	С	0.405468	3.286167	3.537630
С	-4.169705	-0.150137	2.758044	С	0.972406	3.339763	2.268301
Н	-2.031832	-0.346181	2.534537	н	3.103983	1.245948	-2.418070
С	-5.262986	1.282005	1.148307	н	3.017732	3.474893	-3.467264
Н	-3.978576	2.251363	-0.287218	н	1.725741	5.312502	-2.377393
С	-5.337450	0.417363	2.239907	н	0.545625	4.870161	-0.236170
Н	-4.219965	-0.835815	3.599629	н	-2.304449	1.390226	2.803175
Н	-6.169467	1.720873	0.739310	н	-1.246066	2.531804	4.705741
Н	-6.301252	0.178321	2.681379	н	0.882426	3.798914	4.368234
С	-1.511335	2.219133	-1.227580	н	1.896586	3.889088	2.103846
С	-1.350972	1.655014	-2.495612	Р	1.829832	0.061404	-0.029896
С	-1.830073	3.576853	-1.097462	Р	-1.540495	0.908502	0.023796
С	-1.507211	2.450381	-3.633504	С	2.468141	0.346454	1.674184
н	-1.086393	0.599668	-2.575486	С	1.810225	-0.258359	2.748435
С	-1.985959	4.367598	-2.234432	С	3.535539	1.222910	1.906424
Н	-1.938303	4.009053	-0.102901	С	2.219134	0.017959	4.054773
С	-1.821205	3.802994	-3.502927	н	0.979763	-0.935616	2.550591
Н	-1.375019	2.012740	-4.619602	С	3.948338	1.486862	3.211045
Н	-2.230461	5.422088	-2.134390	н	4.023827	1.711575	1.063765
Н	-1.937257	4.421644	-4.389325	С	3.285395	0.887451	4.285192
Pd	-0.269059	-1.061294	-0.255292	н	1.703294	-0.446999	4.890417
I	-1.412499	-3.346234	1.052401	н	4.778551	2.164867	3.391150
С	-1.908446	-2.194221	-0.869027	н	3.601870	1.099964	5.303123
С	-1.158497	-2.573098	-2.005627	С	3.159590	-0.794753	-0.978582
С	-3.193191	-1.618054	-1.000531	С	4.457384	-0.963145	-0.496819
С	-1.652235	-2.220995	-3.280313	С	2.813441	-1.299149	-2.239375
Н	-0.275394	-3.198255	-1.907057	С	5.408787	-1.623756	-1.278383
С	-3.649189	-1.296350	-2.266735	Н	4.725354	-0.601928	0.492068
Н	-3.780655	-1.389557	-0.114342	С	3.767597	-1.939988	-3.024107
С	-2.875940	-1.583234	-3.411318	н	1.783487	-1.209567	-2.585961
Н	-1.079101	-2.496656	-4.162496	С	5.068570	-2.104925	-2.541101
Н	-4.614484	-0.807037	-2.373640	н	6.415437	-1.764674	-0.894131
Н	-3.259315	-1.335033	-4.397306	н	3.491183	-2.333183	-3.998391
				н	5.810835	-2.619653	-3.145289
INT1				С	-3.326996	0.713526	0.462887
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С	-4.354133	1.329174	-0.256545	С	-1.116927	4.634310	-1.228102
С	-4.980015	-0.449807	1.802512	С	-1.166227	4.007111	0.014520
Н	-2.852823	-0.716428	2.005466	н	-1.875552	-0.184249	3.580760
С	-5.687742	1.060937	0.059101	н	-0.840295	1.138555	5.381292
Н	-4.126129	1.998768	-1.079763	н	0.400950	3.235036	4.829283
С	-6.003070	0.175055	1.086781	Н	0.554070	3.970821	2.462040
н	-5.214808	-1.164977	2.585851	н	1.181184	2.629819	-2.723451
н	-6.479174	1.539935	-0.511077	н	-0.224759	4.609723	-3.193615
Н	-7.041909	-0.040863	1.321300	Н	-1.739488	5.503668	-1.421515
С	-1.534041	2.008706	-1.452725	н	-1.833526	4.377737	0.789714
С	-0.994019	1.545964	-2.654090	Р	-1.828748	0.024343	0.604576
С	-2.039845	3.312347	-1.367038	Р	1.445297	0.831362	-0.415211
С	-0.964908	2.383701	-3.771473	С	-2.978010	1.167669	-0.268859
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С	-2.023263	4.140841	-2.486405	С	-3.988571	1.843232	0.426381
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н	-2.420002	5.150410	-2.420408	Н	-4.139976	1.640764	1.486323
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Pd	-0.316903	-1.111774	-0.140409	Н	-3.369617	2.588640	-3.331476
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С	-2.873460	-1.805738	-1.452708	С	-2.873386	-1.281363	1.384701
С	-2.521164	-3.061900	0.570818	С	-4.224374	-1.452736	1.075744
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Н	-4.130815	-4.360032	1.166922	Н	-5.977935	-2.671217	1.342425
Н	-5.589307	-3.741947	-0.754932	Н	-2.433796	-4.017606	3.375415
				Н	-4.849582	-4.299282	2.841134
TS1b'				С	2.714638	0.743816	-1.751815
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С	-1.322252	0.715371	3.327873	С	3.231543	-0.026500	-3.987151
С	-0.743724	1.467494	4.349898	Н	1.257279	-0.107270	-3.105375
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С	0.027444	3.053834	2.717080	н	4.393381	1.456883	-0.594917
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С	0.516669	3.014958	-1.953990	Н	6.039738	1.058656	-2.398901
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С	2.378684	0.291734	2.162422	С	2.159390	-4.333834	1.295089
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С	3.024861	0.590129	3.363683	С	1.476959	-2.119397	-1.693955
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н	3.033825	-0.143196	4.165968	С	2.424206	-2.356967	-2.698238
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Pd	0.043377	-1.060022	-0.414493	н	2.123513	-5.397035	1.515803
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С	-2.906016	-0.859801	-3.982262	н	2.937262	-2.186676	-4.781565
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н	-1.599440	-3.791340	3.363903	С	1.888
н	-1.707354	-6.041535	-0.306282	н	2.507
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Pd	-0.222446	0.798172	0.412300	н	1.153
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С	-4.154659	-0.996192	3.466365	С	5.092
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Н	1.938593	3.558147	0.086672	н	5.3494
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С	0.600247	-4.258605	-1.753195
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С	1.888926	-3.639172	0.182177
н	2.507014	1.176735	2.864881
Н	2.080207	0.078708	5.032309
Н	1.153622	-2.235747	5.092309
н	0.679034	-3.422762	2.962364
Н	-1.181402	-3.114949	-2.094453
Н	0.431331	-4.899955	-2.613431
Н	2.420850	-5.246561	-1.146849
Н	2.744816	-3.786221	0.836923
Р	2.003508	0.380055	0.061611
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С	3.134222	-0.677238	-0.916492
С	2.772298	-1.019333	-2.222370
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С	4.728610	-2.426815	-2.382579
Н	3.289199	-2.172770	-3.967789
Н	5.992749	-2.498617	-0.634908
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С	4.732385	3.484860	0.285412
Н	4.776394	1.442467	-0.411589
С	2.655707	4.226989	1.280536
Н	1.060254	2.769063	1.318055
С	3.973928	4.485696	0.890982

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н	2.063744	5.004904	1.754566	н	0.368031	1.758351	-3.202763
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н	-3.651609	-1.206542	-4.392649	С	0.903580	2.310882	-0.968153
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н	-1.198198	0.992160	2.077820	н	-0.430061	4.346747	4.088325
С	-2.541123	-2.347470	3.548140	н	0.306842	4.666184	1.736420
н	-2.311297	-3.131216	1.548168	н	2.121538	2.017630	-2.722728
С	-2.383370	-1.231801	4.375464	н	1.221154	3.967022	-3.930669
н	-1.775933	0.832864	4.501519	н	-0.500143	5.414958	-2.851434
н	-2.910629	-3.283052	3.958293	н	-1.301520	4.863544	-0.563200
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Pd	-0.093062	0.979252	-0.878630	Р	1.563362	0.823770	-0.068221
С	0.529422	2.487535	-2.400218	С	-2.339620	1.369827	-1.373412
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н	-0.513748	3.776295	-1.030824	С	-2.242716	1.807095	-3.743294
н	-2.001868	1.527569	-2.576926	н	-1.102682	0.258956	-2.737481
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н	1.878535	3.835489	-3.355862	С	-5.472762	-1.851813	1.760479

Н	-6.630418	-0.771694	0.297407	С	2.335921	1.677470	-2.475742
Н	-4.052844	-2.802213	3.080285	С	2.256967	2.840117	-3.241957
Н	-6.325594	-2.404720	2.145123	С	1.679256	3.986081	-2.701747
С	2.991218	0.330176	-1.125128	С	1.196386	3.958052	-1.395666
С	2.702799	-0.461728	-2.243654	С	0.728272	2.910008	0.786413
С	4.305344	0.736399	-0.877264	С	-0.423970	2.260647	1.273829
С	3.723713	-0.823940	-3.122731	С	-0.836063	2.468421	2.593751
н	1.680134	-0.806548	-2.409307	С	-0.120355	3.314578	3.439642
С	5.325696	0.354590	-1.748937	С	1.012115	3.971504	2.962628
н	4.536952	1.329990	0.002921	С	1.421203	3.773471	1.645948
С	5.035751	-0.417736	-2.874974	н	2.814915	0.799470	-2.896581
н	3.494686	-1.441071	-3.987253	н	2.655565	2.846084	-4.252658
Н	6.348226	0.662899	-1.547879	н	1.608347	4.898595	-3.287149
н	5.832616	-0.709089	-3.554095	н	0.743864	4.846165	-0.960088
С	2.198477	1.587783	1.482758	н	-1.724757	1.963178	2.962697
С	1.825569	1.040148	2.713477	н	-0.452145	3.460230	4.463880
С	2.934790	2.779471	1.428245	н	1.580828	4.631198	3.612102
С	2.221848	1.676943	3.892641	н	2.313986	4.267383	1.269112
н	1.210123	0.139071	2.744980	Р	1.846690	0.047901	-0.198985
С	3.329993	3.404489	2.608967	Р	-1.361134	1.097529	0.184041
н	3.173675	3.225363	0.463264	С	2.635953	0.633970	1.364233
С	2.973379	2.850489	3.841899	С	2.049686	0.459514	2.616730
Н	1.928494	1.255650	4.850273	С	3.834959	1.349452	1.237504
Н	3.905250	4.325733	2.568835	С	2.669577	0.998683	3.746389
Н	3.276382	3.342076	4.762857	н	1.120064	-0.096945	2.704171
Pd	0.019121	-1.015434	-0.009614	С	4.453835	1.875905	2.368685
I	-1.590276	-2.632859	-1.463803	Н	4.277179	1.493891	0.252234
С	1.596139	-2.587255	0.485307	С	3.867878	1.700838	3.625243
С	2.720997	-2.010979	1.118194	Н	2.208022	0.867157	4.721131
С	1.811066	-3.428909	-0.625720	н	5.388209	2.421977	2.270192
С	4.004382	-2.220334	0.634515	н	4.347472	2.114304	4.508761
Н	2.554742	-1.448487	2.035898	С	3.081604	-1.083382	-0.980639
С	3.099608	-3.639219	-1.115851	С	2.847463	-1.575006	-2.272754
Н	0.962993	-3.921425	-1.094594	С	4.181757	-1.546946	-0.255085
С	4.191146	-3.030432	-0.492738	С	3.729232	-2.486433	-2.847500
Н	4.860290	-1.767931	1.129170	н	1.965506	-1.260697	-2.829325
Н	3.254446	-4.280937	-1.979694	С	5.056297	-2.470690	-0.831266
Н	5.194802	-3.195159	-0.877903	н	4.345284	-1.210836	0.764381
0	1.075675	-3.878784	2.830837	С	4.837935	-2.934847	-2.126301
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TS2'				С	-2.961779	0.788138	1.043525
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Н	-2.051063	-0.799322	2.195872	С	3.385204	-2.936489	1.966566
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Н	-4.133779	-1.316557	3.445168	н	-0.380458	-1.737348	-5.198851
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С	-1.686716	2.159387	-1.291051	н	3.326977	-0.824953	2.332307
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Н	-2.109488	4.489522	-4.361992	н	-0.344256	-1.902233	2.542422
Pd	-0.279293	-0.958264	-0.302085	С	-0.670960	-5.356304	0.785109
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С	2.039774	-2.416248	-2.913690	н	4.290532	2.192069	-0.238397
С	2.055292	-2.353074	-0.432135	С	4.414891	2.907153	3.086355
С	2.383850	-1.309560	0.457100	н	2.983002	2.229089	4.553255

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н	5.000107	3.477654	3.802724	Н	-4.292535	-1.370900	2.357010
С	2.512812	0.668478	-1.623789	Н	-3.152836	1.005701	-2.468279
С	1.667526	1.149073	-2.624649	Н	-4.594562	-0.737517	-3.453151
С	3.815968	0.263755	-1.931836	Н	-5.054413	-2.835901	-2.182423
С	2.130514	1.228006	-3.937411	Н	-4.024876	-3.159328	0.056363
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н	1.470509	1.590962	-4.720855	С	-1.144030	-4.173745	-0.695686
н	5.298162	0.060666	-3.481383	С	-1.344241	-3.370828	-3.363639
н	3.795882	0.911915	-5.268733	Н	-0.296160	-1.578488	-2.737548
Pd	-0.375236	0.602115	0.760893	С	-1.765897	-5.003675	-1.626293
I	-2.536688	0.420162	2.317342	Н	-1.091938	-4.463392	0.353396
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S	0.250429	3.605133	0.477227	Н	-1.428441	-3.054946	-4.399703
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INT2	1			С	-1.902212	2.686230	-1.023887
С	-2.391553	-1.577266	1.391333	C	-1.268980	2.745423	-2.271909
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Н	0.516167	-2.361329	2.990812	С	-3.607662	1.658183	1.913245
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Н	-1.153809	1.700119	4.917980	С	-3.075666	3.192060	-0.254285
Н	-5.163293	1.950401	3.372862	С	-3.039969	2.563539	-2.982207
Н	-3.592042	1.974025	5.297593	н	-1.931788	0.793473	-2.398752
Pd	0.614972	0.478292	-0.398190	С	-3.693933	4.038304	-1.172025
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S	1.355831	2.645787	-0.199308	С	-3.669495	3.725509	-2.534401
0	1.694922	3.389409	-1.422165	н	-3.027801	2.323254	-4.041302
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С	2.894258	2.336663	0.671120	н	-4.147365	4.390497	-3.248331
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С	2.840393	2.006002	2.025184	С	-4.126185	0.105883	1.265862
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Н	4.091071	2.643164	-1.079821	С	-4.989874	-0.730747	1.978272
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С	5.235190	1.688004	1.996409	н	-1.163775	-0.921365	2.616342
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С	0.374631	2.924350	0.986671	С	2.179410	-0.942189	-2.963938
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С	-0.770026	2.070188	2.956545	С	2.985420	-1.566756	-3.913814
С	0.014902	2.882995	3.773681	Н	1.097971	-0.901443	-3.104103
С	0.972874	3.720752	3.204536	С	4.936151	-1.073077	-2.573120
С	1.135110	3.751122	1.820214	н	4.580327	-0.035868	-0.719789
С	0.554873	3.028469	-0.494891	С	4.366759	-1.635645	-3.715409
С	1.109627	2.015484	-1.303781	н	2.537270	-2.003669	-4.801491
С	1.219380	2.221039	-2.683304	Н	6.009272	-1.130009	-2.415323
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С	0.220927	4.407706	-2.476609	С	2.624843	0.836684	0.887188
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Н	1.586392	4.358405	3.834442	н	1.544170	-0.456601	2.222713
Н	1.875245	4.406299	1.367120	С	4.375345	2.181994	1.867443
Н	1.668492	1.458303	-3.311439	н	3.826677	2.254175	-0.219564
Н	0.859545	3.537442	-4.344661	С	4.096550	1.617890	3.116253
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н	1.019215	-2.728139	-1.621919	С	-2.747614	1.143526	-2.089009
С	1.531577	-2.929955	0.511492	С	-3.659108	2.482357	-0.269262
С	2.918999	-2.912800	0.304421	С	-3.508912	1.879193	-2.997830
С	1.051624	-3.025200	1.831408	н	-2.108808	0.327565	-2.418928
С	3.798747	-2.960715	1.386007	С	-4.423450	3.203246	-1.184061
н	3.303596	-2.888282	-0.712983	н	-3.698502	2.720906	0.792823
С	1.932023	-3.100035	2.909172	С	-4.340998	2.904935	-2.547016
н	-0.025304	-3.035042	2.005692	н	-3.455641	1.646161	-4.057199
С	3.311247	-3.054721	2.690949	н	-5.078266	3.996980	-0.836448
н	4.870441	-2.947545	1.206046	н	-4.933555	3.472168	-3.259306
н	1.542845	-3.186370	3.920512	С	-2.754744	-0.522142	1.541775
Н	3.999841	-3.105073	3.529432	С	-4.123125	-0.694255	1.330985
С	-2.305924	-5.320699	-1.533483	С	-2.070813	-1.317515	2.473782
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Н	-3.324872	-5.137057	-1.889968	н	-4.639370	-0.101871	0.579858
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S	-2.959890	-2.632183	-0.514047	С	-4.142061	-2.431958	3.017122
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н	2.144219	4.450036	-1.017893	С	4.943806	2.748989	-0.744536
н	0.884165	-0.156433	-3.726900	Н	3.689343	1.912230	-2.292043
н	-0.393790	1.316923	-5.242882	С	5.219654	2.782904	0.625901
н	-1.094678	3.585537	-4.472676	Н	4.691338	2.020268	2.574838
н	-0.540689	4.319302	-2.165005	Н	5.517909	3.364948	-1.431963
Р	-1.105999	1.119347	0.735273	Н	6.011724	3.425377	1.002200
Р	1.793134	0.092321	-0.940906	Pd	0.207818	-0.912301	0.514775
С	-2.315546	1.768026	-0.493948	С	-1.037258	-3.509345	1.688109
С	-2.640745	0.982052	-1.601879	С	0.049681	-2.682335	1.921078
С	-2.838850	3.061086	-0.361058	С	1.222035	-2.644980	1.075458
С	-3.519077	1.486002	-2.564576	Н	0.018946	-2.084415	2.834500
н	-2.197166	-0.008190	-1.705282	Н	1.217366	-3.349452	0.237827
С	-3.711172	3.558565	-1.327182	С	2.570918	-2.334327	1.600468
н	-2.548342	3.676402	0.490504	С	2.783969	-1.776666	2.874711
С	-4.052984	2.766964	-2.427892	С	3.694191	-2.589961	0.794220
н	-3.780032	0.870707	-3.421604	С	4.068150	-1.452989	3.307843
н	-4.120237	4.560674	-1.226068	Н	1.937128	-1.586502	3.530864
н	-4.733683	3.155694	-3.181378	С	4.974733	-2.243841	1.218574
С	-2.005008	1.064558	2.353004	Н	3.548944	-3.056534	-0.178827
С	-3.335099	1.463584	2.512114	С	5.169588	-1.668909	2.476310
С	-1.327439	0.493264	3.441144	Н	4.209315	-1.024886	4.297539
С	-3.980371	1.282652	3.738381	Н	5.823288	-2.433087	0.565509
н	-3.875868	1.890441	1.671666	Н	6.169184	-1.404370	2.810340
С	-1.965193	0.332495	4.670034	С	-2.207207	-3.556605	2.622880
н	-0.293179	0.171406	3.306184	Н	-2.329272	-2.598735	3.142281
С	-3.299477	0.720732	4.817574	Н	-3.135160	-3.794486	2.096428
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н	-1.427223	-0.104955	5.507108	Н	-0.920634	-4.337496	0.991378
н	-3.805159	0.581799	5.769266	0	-2.427173	-4.114689	-1.508854
С	2.564289	-1.200085	-2.010090				
С	1.741022	-2.267329	-2.401674	INT	6		
С	3.927070	-1.217599	-2.321529	S	-4.496611	0.785092	2.107351
С	2.286570	-3.340115	-3.106984	0	-5.243313	-0.025831	3.070482
н	0.683572	-2.264726	-2.125865	С	-5.273588	0.578066	0.518637
С	4.467797	-2.301038	-3.017439	С	-5.090161	1.559669	-0.457166
н	4.575433	-0.410276	-1.992652	С	-6.033100	-0.565868	0.277117
С	3.650901	-3.362209	-3.408627	С	-5.675572	1.379877	-1.710020
н	1.644751	-4.164754	-3.405040	Н	-4.498851	2.441846	-0.221730
н	5.530405	-2.317302	-3.245911	С	-6.622532	-0.731187	-0.977198
н	4.076550	-4.207343	-3.943479	Н	-6.165494	-1.292127	1.074681
С	3.186026	1.136644	-0.341325	С	-6.442056	0.238439	-1.965957
С	3.458985	1.176052	1.025542	Н	-5.545063	2.135301	-2.480246
С	3.926595	1.928996	-1.228652	Н	-7.227590	-1.610942	-1.179825
С	4.480177	1.996745	1.508746	Н	-6.906837	0.108587	-2.940173
Н	2.860442	0.568834	1.701533	С	2.876600	-1.550807	-1.409515

С	1.524830	-1.797130	-1.729714	С	3.540074	3.260734	1.565587
С	1.130651	-1.833770	-3.071673	С	1.957703	3.226815	3.870251
С	2.049379	-1.612814	-4.096807	н	0.975890	1.522088	2.964387
С	3.387391	-1.377249	-3.787880	С	3.723549	4.226186	2.557766
С	3.791559	-1.370512	-2.455012	н	4.148006	3.288362	0.665297
С	3.424375	-1.533212	-0.010847	С	2.938176	4.208408	3.710465
С	3.279465	-0.454203	0.887962	н	1.334184	3.215962	4.760155
С	3.859041	-0.537108	2.159202	н	4.480543	4.995040	2.426827
С	4.572357	-1.668808	2.552756	н	3.082384	4.963424	4.478710
С	4.732095	-2.730347	1.664042	С	2.888474	1.598397	-1.129382
С	4.171755	-2.648610	0.391332	С	1.997911	1.939718	-2.150473
н	0.091723	-2.036190	-3.318254	С	4.269650	1.677865	-1.348508
н	1.718532	-1.634514	-5.131736	С	2.488077	2.366617	-3.386281
н	4.114405	-1.203116	-4.576336	н	0.924930	1.863786	-1.973441
н	4.833227	-1.188104	-2.200428	С	4.756275	2.106992	-2.582072
н	3.746018	0.294955	2.850338	н	4.958078	1.375065	-0.559592
н	5.007248	-1.713550	3.547779	С	3.863638	2.449188	-3.602013
н	5.285141	-3.618454	1.957515	н	1.788651	2.636180	-4.173570
н	4.280581	-3.474140	-0.308786	н	5.828263	2.166790	-2.752375
Р	0.266528	-1.906252	-0.372602	н	4.244096	2.779086	-4.565456
Р	2.184298	0.978940	0.455640	Pd	-0.107446	0.293160	0.475262
С	0.888178	-3.280627	0.681585	С	-2.846007	0.043961	1.884955
С	1.025760	-3.047777	2.052574	С	-2.174796	0.681782	0.699723
С	1.303631	-4.499372	0.131511	С	-1.463866	1.900699	0.804037
С	1.577156	-4.032603	2.874442	Н	-2.640841	0.405398	-0.246926
н	0.725868	-2.079394	2.454562	н	-1.349386	2.353024	1.790966
С	1.849429	-5.483252	0.954192	С	-1.203126	2.805360	-0.340515
Н	1.212847	-4.662566	-0.942006	С	-1.725111	2.585681	-1.629380
С	1.988085	-5.247251	2.325032	С	-0.355560	3.915292	-0.156822
Н	1.695647	-3.846505	3.938439	С	-1.387698	3.425569	-2.692481
Н	2.173038	-6.429663	0.528778	Н	-2.409226	1.756066	-1.801963
Н	2.421154	-6.012433	2.964091	С	-0.020884	4.750835	-1.217424
С	-1.299254	-2.511448	-1.143483	Н	0.058859	4.095226	0.834868
С	-1.875308	-3.750460	-0.855492	С	-0.529590	4.508537	-2.497516
С	-2.033232	-1.566867	-1.878807	Н	-1.805797	3.234143	-3.678363
С	-3.180539	-4.028817	-1.274547	Н	0.643310	5.594501	-1.047068
н	-1.324872	-4.486256	-0.274623	Н	-0.267828	5.160577	-3.326510
С	-3.330661	-1.844535	-2.297694	С	-2.978347	-1.471518	1.784743
Н	-1.589907	-0.588205	-2.070960	Н	-1.976253	-1.915390	1.804504
С	-3.912062	-3.077430	-1.983512	Н	-3.573993	-1.871385	2.609366
Н	-3.628500	-4.988424	-1.030010	Н	-3.445758	-1.752456	0.831431
н	-3.900694	-1.090063	-2.834415	Н	-2.348897	0.341974	2.819488
н	-4.936001	-3.285833	-2.283259	0	-4.313646	2.218155	2.326295
С	2.559702	2.276545	1.719526				
С	1.763209	2.271782	2.873490	Prd			

С	1.079511	-0.497771	-0.662669
С	1.992889	0.474050	-0.531186
Н	1.344421	-1.548181	-0.544309
н	1.665512	1.506947	-0.664852
С	-0.368097	-0.225307	-0.937226
Н	-0.512482	0.808797	-1.276042
С	3.424055	0.302380	-0.238595
С	4.285374	1.395722	-0.412403
С	3.967431	-0.912685	0.210143
С	5.651971	1.279499	-0.166002
Н	3.871302	2.344709	-0.747883
С	5.331393	-1.030304	0.456406
Н	3.314212	-1.763460	0.386548
С	6.180228	0.063661	0.266554
Н	6.302558	2.138139	-0.308973
Н	5.734964	-1.976321	0.807500
н	7.244614	-0.031019	0.463759
С	-0.988819	-1.238920	-1.892580

Н	-0.446341	-1.224813	-2.842064
Н	-2.042414	-1.022014	-2.090670
Н	-0.912459	-2.242382	-1.460846
S	-1.207348	-0.284310	0.677221
0	-0.676974	0.810954	1.481446
0	-1.149760	-1.669067	1.141458
С	-2.901601	0.096105	0.306770
С	-3.280468	1.433837	0.192640
С	-3.811738	-0.946735	0.135419
С	-4.606970	1.731131	-0.115579
Н	-2.545969	2.215214	0.369382
С	-5.136668	-0.636742	-0.169022
Н	-3.471988	-1.971692	0.257752
С	-5.529105	0.697556	-0.297573
Н	-4.924457	2.766171	-0.204015
Н	-5.863362	-1.433335	-0.300552
Н	-6.562990	0.934246	-0.534090

# X-Ray Crystal Structures



Table S4 Crystal data and stru	acture refinement for compound 85
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Identification code	85		
Empirical formula	C <sub>18</sub> H <sub>18</sub> O <sub>2</sub> S		
Formula weight	298.38		
Temperature/K	290.0		
Crystal system	monoclinic		
Space group	P21/n		
a/Å	11.7968(3)		
b/Å	7.4154(2)		
c/Å	18.6524(5)		
α/°	90		
β/°	104.9740(10)		
γ/°	90		
Volume/Å <sup>3</sup>	1576.27(7)		
Z	4		
ρ <sub>calc</sub> g/cm <sup>3</sup>	1.257		
µ/mm <sup>-1</sup>	0.207		
F(000)	632.0		
Crystal size/mm <sup>3</sup>	0.3 × 0.3 × 0.2		
Radiation	ΜοΚα (λ = 0.71073)		
2Θ range for data collection/° 4.522 to 55.07			
Index ranges	$-13 \le h \le 15, -9 \le k \le 9, -24 \le l \le 24$		
Reflections collected	36614		
Independent reflections	3618 [ $R_{int}$ = 0.0655, $R_{sigma}$ = 0.0359]		
Data/restraints/parameters	3618/0/193		
Goodness-of-fit on F <sup>2</sup>	1.029		
Final R indexes [I>=2σ (I)]	R <sub>1</sub> = 0.0395, wR <sub>2</sub> = 0.0996		
Final R indexes [all data]	$R_1 = 0.0549, wR_2 = 0.1095$		
Largest diff. peak/hole / e Å <sup>-3</sup> 0.18/-0.34			

## **Characterization data of products**

(*E*)-1-methyl-4-((4-phenylbut-3-en-2-yl)sulfonyl)benzene (3).



The product (46.4 mg, 81% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.64 (d, *J* = 8.0 Hz, 2H), 7.24-7.18 (m, 7H), 6.26 (d, *J* = 16.0 Hz, 1H), 6.00 (dd, *J* = 16.0 Hz, 8.4 Hz, 1H), 3.80-3.72 (m, 1H), 2.34 (s, 3H), 1.45 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  144.6, 136.3, 135.9, 134.0, 129.5, 129.3, 128.7, 128.3, 126.6, 122.3, 64.1, 21.6, 13.6; HRMS Calculated for C<sub>17</sub>H<sub>18</sub>O<sub>2</sub>S (M+Na<sup>+</sup>): 309.0920; Found: 309.0917.






methyl (E)-3-(4-((4-phenylbut-3-en-2-yl)sulfonyl)phenyl)propanoate (4).



The product (58.1 mg, 81% yield) as yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 3/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.69-7.65 (m, 2H), 7.27-7.18 (m, 7H), 6.24 (d, J = 16.0 Hz, 1H), 5.99 (dd, J = 16.0 Hz, 8.4 Hz, 1H), 3.80-3.73 (m, 1H), 3.56 (s, 3H), 2.94 (t, J = 7.6 Hz, 2H), 2.56 (t, J = 7.6 Hz, 2H), 1.46 (d, J = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  172.6, 147.0, 136.4, 135.8, 134.9, 129.5, 128.8, 128.6, 128.3, 126.5, 122.1, 64.0, 51.7, 34.9, 30.7, 13.5; HRMS Calculated for C<sub>20</sub>H<sub>22</sub>O<sub>4</sub>S (M+Na<sup>+</sup>): 381.1131; Found: 381.1130.



<sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of compound 4



(E)-1-((4-phenylbut-3-en-2-yl)sulfonyl)-4-(prop-1-en-2-yl)benzene (5)



The product (51.9 mg, 83% yield) as light yellow oil was purified with silica gel chromatography (petroleum ether/ethyl acetate = 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.71 (d, *J* = 7.6 Hz, 2H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.24-7.18 (m, 5H), 6.27 (d, *J* = 16.0 Hz, 1H), 6.02 (dd, *J* = 15.6 Hz, 8.0 Hz, 1H), 5.40 (s, 1H), 5.16 (s, 1H), 3.82-3.75 (m, 1H), 2.08 (s, 3H), 1.47 (d, *J* = 6.4 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  146.6, 141.8, 136.5, 135.9, 135.5, 129.4, 128.7, 128.4, 126.6, 125.8, 122.1, 115.8, 64.1, 21.6, 13.6; HRMS Calculated for C<sub>19</sub>H<sub>20</sub>O<sub>2</sub>S (M+Na<sup>+</sup>): 335.1076; Found: 335.1076.







methyl (E)-4-((4-phenylbut-3-en-2-yl)sulfonyl)benzoate (6).



The product (37.0 mg, 56% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.09 (d, *J* = 8.4 Hz, 2H), 7.85 (d, *J* = 8.8 Hz, 2H), 7.25-7.17 (m, 5H), 6.24 (d, *J* = 16.0 Hz, 1H), 5.99 (dd, *J* = 16.0 Hz, 8.4 Hz, 1H), 3.88 (s, 3H), 3.85-3.78 (m, 1H), 1.49 (d, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  165.6, 141.0, 136.9, 135.6, 134.8, 130.0, 129.4, 128.7, 128.6, 126.6, 121.6, 64.2, 52.7, 13.4; HRMS Calculated for C<sub>18</sub>H<sub>18</sub>O<sub>4</sub>S (M+Na<sup>+</sup>): 353.0818; Found: 353.0817.







(E)-1-((4-phenylbut-3-en-2-yl)sulfonyl)-4-(trifluoromethyl)benzene (7).



The product (53.1 mg, 78% yield) as light yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.90 (d, *J* = 8.0 Hz, 2H), 7.70 (d, *J* = 8.0 Hz, 2H), 7.24-7.18 (m, 5H), 6.24 (d, *J* = 16.0 Hz, 1H), 6.00 (dd, *J* = 16.0 Hz, 8.0 Hz, 1H), 3.85-3.78 (m, 1H), 1.50 (d, *J* = 6.4 Hz, 3H); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>)  $\delta$  -63.18 (s, 1F); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  140.6, 137.1, 135.5, 135.4 (q, *J* = 33.3 Hz), 130.0, 128.8, 128.7, 126.6, 126.0 (q, *J* = 4.0 Hz), 123.1 (q, *J* = 273.7 Hz), 121.4, 64.3, 13.4; HRMS Calculated for C<sub>17</sub>H<sub>15</sub>F<sub>3</sub>O<sub>2</sub>S (M+Na<sup>+</sup>): 363.0637; Found: 363.0637.





 $^{19}F$  NMR spectrum (376 MHz, CDCl\_3) of compound 7



<sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of compound 7



160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 f1 (ppm) (E)-1-((4-phenylbut-3-en-2-yl)sulfonyl)-4-(trifluoromethoxy)benzene (8).



The product (53.5 mg, 75% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.83-7.80 (m, 2H), 7.27-7.18 (m, 7H), 6.23 (d, J = 15.6 Hz, 1H), 5.99 (dd, J = 16.0 Hz, 8.4 Hz, 1H), 3.82-3.75 (m, 1H), 1.49 (d, J = 7.2 Hz, 3H); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>)  $\delta$  -57.68 (s, 1F); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  153.0, 137.0, 135.6, 135.2, 131.6, 128.8, 128.6, 126.6, 121.7, 120.6, 120.2 (q, J = 260.6 Hz), 64.4, 13.4; HRMS Calculated for C<sub>17</sub>H<sub>15</sub>F<sub>3</sub>O<sub>3</sub>S (M+Na<sup>+</sup>): 379.0586; Found: 379.0585.



<sup>19</sup>F NMR spectrum (376 MHz, CDCl<sub>3</sub>) of compound 8



<sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of compound 8





(E)-4-(4-((4-phenylbut-3-en-2-yl)sulfonyl)phenoxy)butanenitrile (9).



The product (60.4 mg, 85% yield) as yellow oil was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  7.69-7.66 (m, 2H), 7.24-7.18 (m, 5H), 6.89-6.86 (m, 2H), 6.27 (d, *J* = 16.0 Hz, 1H), 6.00 (dd, *J* = 16.0 Hz, 8.0 Hz, 1H), 4.04 (t, *J* = 6.0 Hz, 2H), 3.79-3.71 (m, 1H), 2.51 (t, *J* = 6.8 Hz, 2H), 2.11-2.04 (m, 2H), 1.45 (d, *J* = 7.2 Hz, 3H); <sup>13</sup>**C NMR (101 MHz, CDCl<sub>3</sub>)**  $\delta$  162.4, 136.2, 135.8, 131.4, 128.9, 128.6, 128.3, 126.5, 122.2, 118.9, 114.4, 65.7, 64.1, 25.1, 14.1, 13.6; **HRMS** Calculated for C<sub>20</sub>H<sub>21</sub>NO<sub>3</sub>S (M+Na<sup>+</sup>): 378.1134; Found: 378.1132.





## (E)-1-phenoxy-4-((4-phenylbut-3-en-2-yl)sulfonyl)benzene (10).



The product (64.9 mg, 89% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.80 (d, *J* = 8.8 Hz, 2H), 7.44-7.39 (m, 2H), 7.35-7.29 (m, 5H), 7.26-7.22 (m, 1H), 7.07-7.04 (m, 4H), 6.38 (d, *J* = 16.0 Hz, 1H), 6.11 (dd, *J* = 16.0 Hz, 8.0 Hz, 1H), 3.91-3.84 (m, 1H), 1.58 (d, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  162.4, 155.0, 136.4, 135.9, 131.6, 130.4, 130.2, 128.7, 128.4, 126.6, 125.1, 122.3, 120.3, 117.3, 64.3, 13.6; HRMS Calculated for C<sub>22</sub>H<sub>20</sub>O<sub>3</sub>S (M+Na<sup>+</sup>): 387.1025; Found: 387.1025.



<sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of compound 10



(E)-5-((4-phenylbut-3-en-2-yl)sulfonyl)-2,3-dihydrobenzofuran (11).



The product (52.8 mg, 84% yield) as yellow oil was purified with silica gel chromatography (petroleum ether/ethyl acetate = 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.55-7.51 (m, 2H), 7.24-7.18 (m, 5H), 6.75 (d, *J* = 8.0 Hz, 1H), 6.26 (d, *J* = 16.0 Hz, 1H), 6.00 (dd, *J* = 16.0 Hz, 8.0 Hz, 1H), 4.57 (t, *J* = 8.8 Hz, 2H), 3.77-3.70 (m, 1H), 3.15-3.06 (m, 2H), 1.45 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  164.6, 136.2, 135.9, 130.9, 128.6, 128.31, 128.27, 128.1, 126.5, 122.5, 109.3, 72.4, 64.2, 28.8, 13.7; HRMS Calculated for C<sub>18</sub>H<sub>18</sub>O<sub>3</sub>S (M+Na<sup>+</sup>): 337.0869; Found: 337.0869.

<sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 11





#### (E)-methyl(4-((4-phenylbut-3-en-2-yl)sulfonyl)phenyl)sulfane (12).



The product (52.2 mg, 82% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.62 (d, *J* = 8.4 Hz, 2H), 7.26-7.16 (m, 7H), 6.27 (d, *J* = 16.0 Hz, 1H), 6.00 (dd, *J* = 16.0 Hz, 8.4 Hz, 1H), 3.80-3.72 (m, 1H), 2.42 (s, 3H), 1.46 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  147.2, 136.4, 135.9, 132.5, 129.6, 128.7, 128.4, 126.6, 125.0, 122.2, 64.2, 14.7, 13.6; HRMS Calculated for C<sub>17</sub>H<sub>18</sub>O<sub>2</sub>S<sub>2</sub> (M+Na<sup>+</sup>): 341.0640; Found: 341.0640.

# $^1\text{H}$ NMR spectrum (400 MHz, CDCl\_3) of compound 12



<sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of compound 12



100 90 f1 (ppm) 

(E)-1-fluoro-4-((4-phenylbut-3-en-2-yl)sulfonyl)benzene (13).



The product (42.4 mg, 73% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.77 (dd, J = 8.4 Hz, 5.2 Hz, 2H), 7.26-7.18 (m, 5H), 7.10 (t, J = 8.4 Hz, 2H), 6.24 (d, J = 16.0 Hz, 1H), 5.99 (dd, J = 16.0 Hz, 8.4 Hz, 1H), 3.81-3.74 (m, 1H), 1.48 (d, J = 6.8 Hz, 3H); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>)  $\delta$  -103.44 (s, 1F); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  165.9 (d, J = 257.6 Hz), 136.7, 135.7, 133.0 (d, J = 4.0 Hz), 132.2 (d, J = 10.1 Hz), 128.7, 128.5, 126.6, 121.9, 116.2 (d, J = 22.2 Hz), 64.3, 13.5; HRMS Calculated for C<sub>16</sub>H<sub>15</sub>FO<sub>2</sub>S (M+Na<sup>+</sup>): 313.0669; Found: 313.0666.



<sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 13



<sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of compound 13



(E)-2-(4-fluorophenyl)-5-(2-methyl-5-((4-phenylbut-3-en-2-yl)sulfonyl)benzyl)thiophene (14).



The product (63.9 mg, 67% yield) as light yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.62 (s, 1H), 7.57 (d, *J* = 7.6 Hz, 1H), 7.38 – 7.31 (m, 2H), 7.23 (d, *J* = 7.6 Hz, 1H), 7.19 – 7.16 (m, 5H), 6.94 (t, *J* = 8.4 Hz, 2H), 6.83 (d, *J* = 3.6 Hz, 1H), 6.42 (d, *J* = 2.8 Hz, 1H), 6.26 (d, *J* = 15.6 Hz, 1H), 6.00 (dd, *J* = 15.6, 8.0 Hz, 1H), 4.03 (s, 2H), 3.81 – 3.74 (m, 1H), 2.29 (s, 3H), 1.46 (d, *J* = 6.8 Hz, 3H); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>)  $\delta$  -114.84 (s, 1F); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  162.1 (d, *J* = 247.5 Hz), 143.3, 141.9, 141.4, 139.2, 136.3, 135.9, 134.7, 131.0, 130.6 (d, *J* = 3.0 Hz), 130.1, 128.6, 128.3, 127.8, 127.2 (d, *J* = 8.1 Hz), 126.6, 126.3, 122.8, 122.3, 115.8 (d, *J* = 22.2 Hz), 64.2, 33.9, 19.8, 13.6; HRMS Calculated for C<sub>28</sub>H<sub>25</sub>FO<sub>2</sub>S<sub>2</sub> (M+Na<sup>+</sup>): 499.1172; Found: 499.1173.

<sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 14





<sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of compound 14



(E)-1-chloro-4-((4-phenylbut-3-en-2-yl)sulfonyl)benzene (15).



The product (44.2 mg, 72% yield) as yellow oil was purified with silica gel chromatography (petroleum ether/ethyl acetate = 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.69 (d, J = 8.4 Hz, 2H), 7.40 (d, J = 8.4 Hz, 2H), 7.24 – 7.18 (m, 5H), 6.26 (d, J = 15.6 Hz, 1H), 5.99 (dd, J = 16.0, 8.4 Hz, 1H), 3.81 – 3.74 (m, 1H), 1.47 (d, J = 7.2 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  140.5, 136.8, 135.6, 135.5, 130.8, 129.2, 128.7, 128.6, 126.6, 121.8, 64.2, 13.5; HRMS Calculated for C<sub>16</sub>H<sub>15</sub>ClO<sub>2</sub>S (M+Na<sup>+</sup>): 329.0373; Found: 329.0374.



<sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 15



#### (E)-1-bromo-4-((4-phenylbut-3-en-2-yl)sulfonyl)benzene (16).



The product (45.7 mg, 65% yield) as light yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.63-7.60 (m, 2H), 7.58-7.56 (m, 2H), 7.25-7.18 (m, 5H), 6.26 (d, *J* = 16.0 Hz, 1H), 5.99 (dd, *J* = 16.0 Hz, 8.4 Hz, 1H), 3.81-3.74 (m, 1H), 1.47 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  136.8, 136.0, 135.6, 132.2, 130.9, 129.1, 128.7, 128.6, 126.6, 121.7, 64.2, 13.5; HRMS Calculated for C<sub>16</sub>H<sub>15</sub>BrO<sub>2</sub>S (M+Na<sup>+</sup>): 372.9868; Found: 372.9870.



 $^{13}C$  NMR spectrum (101 MHz, CDCl\_3) of compound 16



fl (ppm) 

(E)-4-((4-phenylbut-3-en-2-yl)sulfonyl)phenyl 4-methylbenzenesulfonate (17).



The product (56.6 mg, 64% yield) as light yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.80 (d, *J* = 8.8 Hz, 2H), 7.65 (d, *J* = 8.0 Hz, 2H), 7.34-7.24 (m, 7H), 7.14 (d, *J* = 8.4 Hz, 2H), 6.29 (d, *J* = 16.0 Hz, 1H), 6.05 (dd, *J* = 16.0 Hz, 8.4 Hz, 1H), 3.90-3.82 (m, 1H), 2.44 (s, 3H), 1.57 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  153.4, 146.1, 136.8, 135.61, 135.58, 131.6, 131.2, 130.0, 128.8, 128.6, 128.4, 126.6, 122.9, 121.8, 64.3, 21.7, 13.3; HRMS Calculated for C<sub>23</sub>H<sub>22</sub>O<sub>5</sub>S<sub>2</sub> (M+Na<sup>+</sup>): 465.0801; Found: 465.0802.



<sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 17



(E)-1-(4-((4-phenylbut-3-en-2-yl)sulfonyl)phenyl)-1H-pyrrole (18).



The product (58.0 mg, 86% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.79 (d, *J* = 8.4 Hz, 2H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.23-7.19 (m, 5H), 7.06-7.05 (m, 2H), 6.31-6.30 (m, 2H), 6.27 (d, *J* = 16.0 Hz, 1H), 6.02 (dd, *J* = 15.6 Hz, 8.0 Hz, 1H), 3.83-3.76 (m, 1H), 1.49 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  144.5, 136.6, 135.7, 133.1, 131.2, 128.7, 128.5, 126.6, 122.0, 119.3, 119.0, 112.1, 64.3, 13.6; HRMS Calculated for C<sub>20</sub>H<sub>19</sub>NO<sub>2</sub>S (M+H<sup>+</sup>): 338.1209; Found: 338.1209.



 $^{13}C$  NMR spectrum (101 MHz, CDCl\_3) of compound 18



fl (ppm) 

(E)-2-methoxy-5-((4-phenylbut-3-en-2-yl)sulfonyl)pyridine (19).



The product (51.0 mg, 84% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, Chloroform-*d*)  $\delta$  8.54 (d, *J* = 2.4 Hz, 1H), 7.82 (dd, *J* = 8.8 Hz, 2.4 Hz, 1H), 7.25-7.19 (m, 5H), 6.71 (d, *J* = 8.8 Hz, 1H), 6.30 (d, *J* = 15.6 Hz, 1H), 6.02 (dd, *J* = 16.0 Hz, 8.4 Hz, 1H), 3.92 (s, 3H), 3.81-3.74 (m, 1H), 1.49 (d, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  167.1, 149.7, 139.3, 136.8, 135.7, 128.7, 128.6, 126.6, 126.1, 121.9, 111.1, 64.6, 54.4, 13.6; HRMS Calculated for C<sub>16</sub>H<sub>17</sub>NO<sub>3</sub>S (M+H<sup>+</sup>): 304.1002; Found: 304.1000.







(E)-4-(5-((4-phenylbut-3-en-2-yl)sulfonyl)pyridin-2-yl)morpholine (20).



The product (66.0 mg, 92% yield) as yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 3/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.45 (s, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.24-7.18 (m, 5H), 6.47 (d, *J* = 8.4 Hz, 1H), 6.34 (d, *J* = 15.6 Hz, 1H), 6.04 (dd, *J* = 15.6 Hz, 7.6 Hz, 1H), 3.76-3.70 (m, 5H), 3.57 (s, 4H), 1.46 (d, *J* = 6.4 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  160.5, 150.2, 138.3, 136.4, 135.9, 128.7, 128.4, 126.6, 122.3, 120.7, 104.9, 66.4, 64.5, 44.8, 13.7; HRMS Calculated for C<sub>19</sub>H<sub>22</sub>N<sub>2</sub>O<sub>3</sub>S (M+ H<sup>+</sup>): 359.1424; Found: 359.1425.

## $^1H$ NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 20



 $^{13}C$  NMR spectrum (101 MHz, CDCl\_3) of compound 20



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(*E*)-3-((4-phenylbut-3-en-2-yl)sulfonyl)thiophene (21).



The product (34.0 mg, 61% yield) as yellow oil was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.03-8.02 (m, 1H), 7.44-7.41 (m, 1H), 7.37-7.29 (m, 6H), 6.40 (d, *J* = 16.0 Hz, 1H), 6.14 (dd, *J* = 16.0 Hz, 8.4 Hz, 1H), 3.93-3.86 (m, 1H), 1.60 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  137.4, 136.6, 135.8, 133.7, 128.7, 128.5, 127.6, 127.1, 126.6, 122.0, 64.3, 13.4; HRMS Calculated for C<sub>14</sub>H<sub>14</sub>O<sub>2</sub>S<sub>2</sub> (M+Na<sup>+</sup>): 301.0327; Found: 301.0334.



<sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 21



(E)-5-((4-phenylbut-3-en-2-yl)sulfonyl)-1H-indole (22).



The product (52.9 mg, 85% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  9.01 (s, 1H), 7.49 (dd, J = 8.8 Hz, 1.6 Hz, 1H), 7.35 (d, J = 8.4 Hz, 1H), 7.22-7.14 (m, 6H), 6.51 (s, 1H), 6.29 (d, J = 16.0 Hz, 1H), 6.01 (dd, J = 15.6 Hz, 8.0 Hz, 1H), 3.86-3.79 (m, 1H), 1.44 (d, J = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  138.4, 136.2, 136.0, 128.6, 128.2, 127.4, 126.9, 126.6, 123.4, 122.5, 122.0, 111.5, 103.8, 64.4, 14.1; HRMS Calculated for C<sub>18</sub>H<sub>17</sub>NO<sub>2</sub>S (M+Na<sup>+</sup>): 334.0872; Found: 334.0872.



 $^{13}C$  NMR spectrum (101 MHz, CDCl\_3) of compound 21



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(E)-4-((4-phenylbut-3-en-2-yl)sulfonyl)phenol (23).



The product (51.9 mg, 90% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.56 (d, *J* = 8.4 Hz, 2H), 7.23-7.18 (m, 5H), 6.84 (d, *J* = 8.4 Hz, 2H), 6.29 (d, *J* = 16.0 Hz, 1H), 5.96 (dd, *J* = 16.0 Hz, 8.4 Hz, 1H), 3.80-3.72 (m, 1H), 1.44 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  161.3, 136.8, 135.8, 131.6, 128.7, 128.5, 127.3, 126.6, 121.8, 115.9, 64.4, 13.7; HRMS Calculated for C<sub>16</sub>H<sub>16</sub>O<sub>3</sub>S (M+Na<sup>+</sup>): 311.0712; Found: 311.0711.



<sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 23



#### (E)-(4-((4-phenylbut-3-en-2-yl)sulfonyl)phenyl)methanol (24).



The product (44.2 mg, 73% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.68 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 8.4 Hz, 2H), 7.25-7.17 (m, 5H), 6.26 (d, *J* = 15.6 Hz, 1H), 5.98 (dd, *J* = 16.0 Hz, 8.4 Hz, 1H), 4.69 (s, 2H), 3.80-3.73 (m, 1H), 2.09 (s, 1H), 1.45 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  147.4, 136.6, 135.8, 135.6, 129.4, 128.7, 128.5, 126.7, 126.6, 121.9, 64.1, 64.1, 13.6; HRMS Calculated for C<sub>17</sub>H<sub>18</sub>O<sub>3</sub>S (M+Na<sup>+</sup>): 325.0869; Found: 325.0868.



<sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of compound 24





(E)-4-((4-phenylbut-3-en-2-yl)sulfonyl)aniline (25).



The product (35.1 mg, 61% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.49 (d, *J* = 8.8 Hz, 2H), 7.24-7.18 (m, 5H), 6.56 (d, *J* = 8.8 Hz, 2H), 6.29 (d, *J* = 16.0 Hz, 1H), 6.01 (dd, *J* = 16.0 Hz, 8.0 Hz, 1H), 4.14 (s, 2H), 3.76-3.68 (m, 1H), 1.43 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  151.5, 136.1, 136.0, 131.4, 128.6, 128.2, 126.6, 124.7, 122.8, 113.8, 64.2, 13.8; HRMS Calculated for C<sub>16</sub>H<sub>17</sub>NO<sub>2</sub>S (M+Na<sup>+</sup>): 310.0872; Found: 310.0869.



<sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 25



(E)-4-((4-phenylbut-3-en-2-yl)sulfonyl)benzamide (26).



The product (40.4 mg, 64% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 1/4). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  8.21 (s, 1H), 8.07 (d, *J* = 8.4 Hz, 2H), 7.91 (d, *J* = 8.4 Hz, 2H), 7.66 (s, 1H), 7.38-7.26 (m, 5H), 6.47 (d, *J* = 15.6 Hz, 1H), 6.10 (dd, *J* = 16.0 Hz, 8.4 Hz, 1H), 4.35-4.28 (m, 1H), 1.40 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  166.6, 139.3, 139.0, 136.2, 135.7, 128.81, 128.75, 128.4, 128.2, 126.5, 122.0, 62.4, 13.2; HRMS Calculated for C<sub>17</sub>H<sub>17</sub>NO<sub>3</sub>S (M+H<sup>+</sup>): 316.1002; Found: 316.1003.
## <sup>1</sup>H NMR spectrum (400 MHz, DMSO-*d*<sub>6</sub>) of compound **26**



<sup>13</sup>C NMR spectrum (101 MHz, DMSO-*d*<sub>6</sub>) of compound 26



140 130 120 fl (ppm) 

(E)-4-(4-((4-phenylbut-3-en-2-yl)sulfonyl)phenyl)pent-4-enoic acid (27).



The product (51.9 mg, 70% yield) as yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 1/1). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  12.15 (s, 1H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.69 (d, *J* = 8.4 Hz, 2H), 7.37 – 7.27 (m, 5H), 6.45 (d, *J* = 16.0 Hz, 1H), 6.10 (dd, *J* = 16.0, 8.4 Hz, 1H), 5.51 (s, 1H), 5.25 (s, 1H), 4.28 – 4.21 (m, 1H), 2.74 (t, *J* = 7.6 Hz, 2H), 2.36 (t, *J* = 7.6 Hz, 2H), 1.40 (d, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  173.7, 145.4, 145.2, 136.1, 135.9, 135.8, 129.0, 128.7, 128.3, 126.47, 126.46, 122.2, 115.5, 62.5, 32.4, 29.3, 13.3; HRMS Calculated for C<sub>21</sub>H<sub>22</sub>O<sub>4</sub>S (M+Na<sup>+</sup>): 393.1131; Found: 393.1130.



<sup>1</sup>H NMR spectrum (400 MHz, DMSO- $d_6$ ) of compound 27

#### <sup>13</sup>C NMR spectrum (101 MHz, DMSO-*d*<sub>6</sub>) of compound 27



(E)-4-(4-((4-(4-(tert-butyl)phenyl)but-3-en-2-yl)sulfonyl)phenyl)morpholine (28).



The product (71.1 mg, 86% yield) as yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 10/1). <sup>1</sup>H NMR (400 MHz, Chloroform-*d*)  $\delta$  7.59 (d, *J* = 8.8 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 7.16 (d, *J* = 8.4 Hz, 2H), 6.79 (d, *J* = 8.8 Hz, 2H), 6.26 (d, *J* = 16.0 Hz, 1H), 5.97 (dd, *J* = 16.0 Hz, 8.4 Hz, 1H), 3.77-3.71 (m, 5H), 3.21-3.19 (m, 4H), 1.43 (d, *J* = 6.8 Hz, 3H), 1.23 (s, 9H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  154.2, 151.4, 135.7, 133.3, 131.0, 126.3, 125.54, 125.50, 121.8, 113.3, 66.4, 64.2, 47.4, 34.6, 31.2, 13.8; HRMS Calculated for C<sub>24</sub>H<sub>31</sub>NO<sub>3</sub>S (M+H<sup>+</sup>): 414.2097; Found: 414.2098.

## $^1H$ NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound $\mathbf{28}$



 $^{13}C$  NMR spectrum (101 MHz, CDCl\_3) of compound  $\mathbf{28}$ 



170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 fl (ppm) (E)-5-methoxy-2-((4-(4-methoxyphenyl)but-3-en-2-yl)sulfonyl)pyridine (29).



The product (55.3 mg, 83% yield) as brown solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  8.53 (s, 1H), 7.81 (d, *J* = 8.8 Hz, 1H), 7.16 (d, *J* = 8.0 Hz, 2H), 6.76 (d, *J* = 7.6 Hz, 2H), 6.70 (d, *J* = 8.4 Hz, 1H), 6.23 (d, *J* = 15.6 Hz, 1H), 5.86 (dd, *J* = 15.6 Hz, 8.0 Hz, 1H), 3.91 (s, 3H), 3.73 (s, 3H), 1.47 (d, *J* = 6.4 Hz, 3H); <sup>13</sup>**C NMR (101 MHz, CDCl<sub>3</sub>)**  $\delta$  167.1, 159.9, 149.6, 139.3, 136.3, 128.4, 127.9, 126.2, 119.4, 114.1, 111.0, 64.6, 55.3, 54.4, 13.6; **HRMS** Calculated for C<sub>17</sub>H<sub>19</sub>NO<sub>4</sub>S (M+H<sup>+</sup>): 334.1108; Found: 334.1107.

<sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 29





(E)-5-((4-(4-(trifluoromethyl)phenyl)but-3-en-2-yl)sulfonyl)-2,3-dihydrobenzofuran (30).



The product (52.0 mg, 68% yield) as yellow oil was purified with silica gel chromatography (petroleum ether/ethyl acetate = 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.56-7.47 (m, 4H), 7.32 (d, J = 8.0 Hz, 2H), 6.76 (d, J = 8.4 Hz, 1H), 6.33 (d, J = 16.0 Hz, 1H), 6.13 (dd, J = 16.0 Hz, 8.4 Hz, 1H), 4.59 (t, J = 8.8 Hz, 2H), 3.80-3.73 (m, 1H), 3.18-3.09 (m, 2H), 1.46 (d, J = 7.2 Hz, 3H); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>)  $\delta$  -62.62 (s, 1F); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  164.8, 139.4, 134.8, 131.0, 130.0 (q, J = 32.3 Hz), 128.3, 128.3, 126.7, 126.4, 125.6 (q, J = 4.0 Hz), 125.3, 124.0 (q, J = 272.7 Hz), 109.5, 72.4, 64.1, 28.9, 13.7; HRMS Calculated for C<sub>19</sub>H<sub>17</sub>F<sub>3</sub>O<sub>3</sub>S (M+Na<sup>+</sup>): 405.0743; Found: 405.0742.

# $^1\text{H}$ NMR spectrum (400 MHz, CDCl\_3) of compound 30



 $^{19}F$  NMR spectrum (376 MHz, CDCl\_3) of compound 30



<sup>10</sup> O -10 -20 -30 -40 -50 -60 70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 f1 (ppm)

## <sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of compound **30**



methyl (E)-4-(3-((4-(tert-butyl)phenyl)sulfonyl)but-1-en-1-yl)benzoate (31).



The product (52.6 mg, 68% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.90 (d, *J* = 8.0 Hz, 2H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.25 (d, *J* = 8.4 Hz, 2H), 6.29 (d, *J* = 16.0 Hz, 1H), 6.13 (dd, *J* = 16.0 Hz, 8.4 Hz, 1H), 3.84 (s, 3H), 3.81-3.76 (m, 1H), 1.48 (d, *J* = 6.8 Hz, 3H), 1.25 (s, 9H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  166.7, 157.8, 140.3, 135.5, 133.9, 130.0, 129.8, 129.2, 126.5, 126.0, 125.0, 64.1, 52.2, 35.3, 31.1, 13.6; HRMS Calculated for C<sub>22</sub>H<sub>26</sub>O<sub>4</sub>S (M+Na<sup>+</sup>): 409.1444; Found: 409.1443.

## $^1H$ NMR spectrum (400 MHz, CDCl\_3) of compound 31



 $^{13}C$  NMR spectrum (101 MHz, CDCl\_3) of compound 31



180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 f1 (ppm) (E)-methyl(4-((4-(methylsulfonyl)phenyl)but-3-en-2-yl)sulfonyl)phenyl)sulfane (32).



The product (57.9 mg, 73% yield) as yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.82 (d, *J* = 8.4 Hz, 2H), 7.63 (d, *J* = 8.8 Hz, 2H), 7.41 (d, *J* = 8.4 Hz, 2H), 7.23 (d, *J* = 8.4 Hz, 2H), 6.37 (d, *J* = 16.0 Hz, 1H), 6.19 (dd, *J* = 16.0 Hz, 8.0 Hz, 1H), 3.86-3.78 (m, 1H), 2.99 (s, 3H), 2.45 (s, 3H), 1.47 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  147.7, 141.1, 139.9, 134.6, 132.3, 129.5, 127.9, 127.3, 126.4, 125.0, 64.0, 44.5, 14.7, 13.6; HRMS Calculated for C<sub>18</sub>H<sub>20</sub>O<sub>4</sub>S<sub>3</sub> (M+Na<sup>+</sup>): 419.0416; Found: 419.0416.





#### <sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of compound 32



(E)-4-(4-((4-(4-fluorophenyl)but-3-en-2-yl)sulfonyl)phenoxy)butanenitrile (33).



The product (54.5 mg, 73% yield) as yellow oil was purified with silica gel chromatography (petroleum ether/ethyl acetate = 3/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.67 (d, J = 8.8 Hz, 2H), 7.22-7.17 (m, 2H), 6.95-6.87 (m, 4H), 6.25 (d, J = 16.0 Hz, 1H), 5.92 (dd, J = 16.0 Hz, 8.0 Hz, 1H), 4.05 (t, J = 5.6 Hz, 2H), 3.78-3.70 (m, 1H), 2.53 (t, J = 7.2 Hz, 2H), 2.12-2.06 (m, 2H), 1.44 (d, J = 7.2 Hz, 3H); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>)  $\delta$  -113.00 (s, 1F); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  162.7 (d, J = 249.5 Hz), 162.5, 135.1, 132.1 (d, J = 3.0 Hz), 131.5, 129.0, 128.2 (d, J = 8.1 Hz), 121.9 (d, J = 2.0 Hz), 118.9, 115.6 (d, J = 22.2 Hz), 114.5, 65.7, 64.1, 25.1, 14.1, 13.7; HRMS Calculated for C<sub>20</sub>H<sub>20</sub>FNO<sub>3</sub>S (M+Na<sup>+</sup>): 396.1040; Found: 396.1040.

# <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound **33**



 $^{19}F$  NMR spectrum (376 MHz, CDCl\_3) of compound  ${\bf 33}$ 



<sup>10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210</sup> f1 (ppm)

## <sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of compound 33



methyl (E)-3-(4-((4-(4-chlorophenyl)but-3-en-2-yl)sulfonyl)phenyl)propanoate (34).



The product (58.8 mg, 75% yield) as brown oil was purified with silica gel chromatography (petroleum ether/ethyl acetate = 3/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.66 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 7.19 (d, *J* = 8.4 Hz, 2H), 7.12 (d, *J* = 8.4 Hz, 2H), 6.21 (d, *J* = 16.0 Hz, 1H), 5.97 (dd, *J* = 16.0 Hz, 8.4 Hz, 1H), 3.79-3.72 (m, 1H), 3.57 (s, 3H), 2.94 (t, *J* = 7.6 Hz, 2H), 2.57 (t, *J* = 7.6 Hz, 2H), 1.44 (d, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  172.6, 147.1, 135.2, 134.9, 134.3, 134.1, 129.5, 128.84, 128.82, 127.8, 122.7, 64.0, 51.7, 34.9, 30.7, 13.5; HRMS Calculated for C<sub>20</sub>H<sub>21</sub>ClO<sub>4</sub>S (M+Na<sup>+</sup>): 415.0741; Found: 415.0742.

### <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound **34**







220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 f1 (ppm) (E)-1-bromo-4-(3-((4-(prop-1-en-2-yl)phenyl)sulfonyl)but-1-en-1-yl)benzene (35).



The product (50.9 mg, 65% yield) as yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.69 (d, *J* = 8.4 Hz, 2H), 7.49 (d, *J* = 8.4 Hz, 2H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.07 (d, *J* = 8.4 Hz, 2H), 6.22 (d, *J* = 16.0 Hz, 1H), 6.01 (dd, *J* = 16.0 Hz, 8.0 Hz, 1H), 5.40 (s, 1H), 5.17 (s, 1H), 3.81-3.73 (m, 1H), 2.08 (s, 3H), 1.45 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  146.63, 141.73, 135.37, 135.29, 134.78, 131.80, 129.32, 128.09, 125.86, 122.88, 122.31, 115.89, 64.02, 21.56, 13.58; HRMS Calculated for C<sub>19</sub>H<sub>19</sub>BrO<sub>2</sub>S (M+Na<sup>+</sup>): 413.0181; Found: 413.0183.



#### <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound **35**

## $^{13}C$ NMR spectrum (101 MHz, CDCl\_3) of compound 35



(E)-4-(3-tosylbut-1-en-1-yl)phenyl 4-methylbenzenesulfonate (36).



The product (65.8 mg, 72% yield) as yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.62 (d, *J* = 8.0 Hz, 4H), 7.25-7.22 (m, 4H), 7.12 (d, *J* = 8.4 Hz, 2H), 6.84 (d, *J* = 8.4 Hz, 2H), 6.25 (d, *J* = 16.0 Hz, 1H), 5.95 (dd, *J* = 16.0 Hz, 8.0 Hz, 1H), 3.78-3.71 (m, 1H), 2.37 (s, 3H), 2.35 (s, 3H), 1.41 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  149.3, 145.5, 144.8, 134.91, 134.88, 134.0, 132.2, 129.8, 129.6, 129.2, 128.5, 127.7, 123.2, 122.6, 63.9, 21.7, 21.6, 13.7; HRMS Calculated for C<sub>24</sub>H<sub>24</sub>O<sub>5</sub>S<sub>2</sub> (M+Na<sup>+</sup>): 479.0957; Found: 479.0959.

# $^1\text{H}$ NMR spectrum (400 MHz, CDCl\_3) of compound 36



 $^{13}C$  NMR spectrum (101 MHz, CDCl\_3) of compound 36



90 80 fl (ppm) 

(E)-4-(3-((3,4-dimethylphenyl)sulfonyl)but-1-en-1-yl)phenyl acetate (37).



The product (44.5 mg, 62% yield) as brown solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.50 (s, 1H), 7.46 (d, *J* = 7.6 Hz, 1H), 7.22-7.16 (m, 3H), 6.96 (d, *J* = 8.0 Hz, 2H), 6.25 (d, *J* = 15.6 Hz, 1H), 5.96 (dd, *J* = 16.0 Hz, 8.4 Hz, 1H), 3.78-3.71 (m, 1H), 2.24-2.20 (m, 9H), 1.44 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  169.4, 150.6, 143.4, 137.7, 135.2, 134.1, 133.8, 130.0, 127.6, 126.8, 122.7, 121.8, 64.0, 21.1, 20.0, 19.7, 13.6; HRMS Calculated for C<sub>20</sub>H<sub>22</sub>O<sub>4</sub>S (M+Na<sup>+</sup>): 381.1131; Found: 381.1129.





## $^{13}C$ NMR spectrum (101 MHz, CDCl\_3) of compound 37



(E)-N-(4-(3-((4-(prop-1-en-2-yl)phenyl)sulfonyl)but-1-en-1-yl)phenyl)acetamide (38).



The product (52.5 mg, 71% yield) as brown solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.07 (s, 1H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.52 (d, *J* = 8.0 Hz, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 6.35 (d, *J* = 16.0 Hz, 1H), 6.01 (dd, *J* = 15.6 Hz, 8.0 Hz, 1H), 5.50 (s, 1H), 5.27 (s, 1H), 3.92-3.84 (m, 1H), 2.17-2.16 (m, 6H), 1.54 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  168.9, 146.7, 141.7, 138.4, 136.2, 135.3, 131.6, 129.3, 127.3, 125.9, 120.4, 119.9, 116.0, 64.2, 24.5, 21.5, 13.8; HRMS Calculated for C<sub>21</sub>H<sub>23</sub>NO<sub>3</sub>S (M+Na<sup>+</sup>): 392.1291; Found: 392.1290.

## <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound **38**



<sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of compound 38



180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 f1 (ppm) (E)-N,N-diphenyl-4-((4-(thiophen-2-yl)but-3-en-2-yl)sulfonyl)aniline (39).



The product (70.4 mg, 79% yield) as yellow oil was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.49 (d, *J* = 8.8 Hz, 2H), 7.25-7.17 (m, 5H), 7.08-7.02 (m, 8H), 6.89 (d, *J* = 8.4 Hz, 2H), 6.31 (d, *J* = 16.0 Hz, 1H), 5.87 (dd, *J* = 16.0 Hz, 8.4 Hz, 1H), 3.75-3.67 (m, 1H), 1.44 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  152.5, 146.0, 138.7, 130.6, 130.2, 129.8, 127.2, 126.3, 126.1, 125.1, 124.8, 123.3, 122.3, 119.0, 64.3, 13.7; HRMS Calculated for C<sub>26</sub>H<sub>23</sub>NO<sub>2</sub>S<sub>2</sub> (M+Na<sup>+</sup>): 468.1062; Found: 468.1064.



<sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound **39** 

#### <sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of compound 39



(E)-9-(4-((4-(benzo[b]thiophen-2-yl)but-3-en-2-yl)sulfonyl)phenyl)-9H-carbazole (40).



The product (64.2 mg, 65% yield) as brown oil was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.58 (s, 1H), 8.03 (d, *J* = 7.6 Hz, 1H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.66-7.62 (m, 1H), 7.55-7.51 (m, 3H), 7.44-7.40 (m, 3H), 7.38 (d, *J* = 7.2 Hz, 1H), 7.34-7.30 (m, 2H), 7.25-7.19 (m, 3H), 6.96 (s, 1H), 6.54 (d, *J* = 15.6 Hz, 1H), 5.96 (dd, *J* = 15.6 Hz, 8.0 Hz, 1H), 3.91-3.84 (m, 1H), 1.50 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  143.5, 141.9, 141.0, 139.8, 139.1, 136.5, 130.2, 129.8, 128.4, 127.4, 127.3, 127.1, 126.8, 125.1, 124.7, 124.6, 124.1, 123.7, 123.3, 122.8, 122.67, 122.3, 121.3, 120.9, 110.4, 109.7, 64.5, 13.8; HRMS Calculated for C<sub>30</sub>H<sub>23</sub>NO<sub>2</sub>S<sub>2</sub> (M+Na<sup>+</sup>): 516.1062; Found: 516.1064.

## $^1H$ NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 40



 $^{13}C$  NMR spectrum (101 MHz, CDCl\_3) of compound 40



fl (ppm)  $\frac{1}{70}$ -1 

(E)-6-(3-((4-ethylphenyl)sulfonyl)but-1-en-1-yl)quinoline (41).



The product (49.2 mg, 70% yield) as yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.80-8.78 (m, 1H), 8.02 (d, J = 8.4 Hz, 1H), 7.97 (d, J = 8.8 Hz, 1H), 7.69-7.62 (m, 3H), 7.55 (s, 1H), 7.33-7.30 (m, 1H), 7.24 (d, J = 7.6 Hz, 2H), 6.45 (d, J = 16.0 Hz, 1H), 6.17 (dd, J = 16.0 Hz, 8.4 Hz, 1H), 3.87-3.80 (m, 1H), 2.63 (q, J = 7.2 Hz, 2H), 1.49 (d, J = 6.8 Hz, 3H), 1.16 (t, J = 7.2 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  150.9, 150.4, 148.0, 136.3, 135.6, 134.15, 134.12, 129.7, 129.4, 128.4, 128.3, 127.2, 126.3, 123.9, 121.6, 64.1, 28.8, 15.1, 13.7; HRMS Calculated for C<sub>17</sub>H<sub>19</sub>NO<sub>4</sub>S (M+H<sup>+</sup>): 352.1366; Found: 352.1368.





## $^{13}C$ NMR spectrum (101 MHz, CDCl\_3) of compound 41



(E)-2-(3-((2,3-dihydrobenzofuran-5-yl)sulfonyl)but-1-en-1-yl)benzofuran (42).



The product (36.9 mg, 52% yield) as yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.57 – 7.53 (m, 2H), 7.43 (d, J = 7.6 Hz, 1H), 7.35 (d, J = 8.4 Hz, 1H), 7.23 – 7.18 (m, 1H), 7.12 (t, J = 7.2 Hz, 1H), 6.76 (d, J = 8.4 Hz, 1H), 6.49 (s, 1H), 6.26 – 6.25 (m, 2H), 4.58 (t, J = 8.8 Hz, 2H), 3.81 – 3.74 (m, 1H), 3.12 (t, J = 8.8 Hz, 2H), 1.46 (d, J = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  164.8, 154.9, 153.3, 131.1, 128.6, 128.3, 128.2, 126.5, 125.1, 124.3, 124.2, 123.0, 121.2, 111.1, 109.5, 106.0, 72.4, 64.1, 28.9, 13.7; HRMS Calculated for C<sub>20</sub>H<sub>18</sub>O<sub>4</sub>S (M+Na<sup>+</sup>): 377.0818; Found: 377.0817.

# <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 42



# $^{13}C$ NMR spectrum (101 MHz, CDCl\_3) of compound 42



150 140 130 120 100 90 f1 (ppm) 

(E)-5-((4-(6-methoxypyridin-3-yl)but-3-en-2-yl)sulfonyl)-1H-indole (43).



The product (62.3 mg, 91% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 1/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  9.15 (s, 1H), 8.09 (s, 1H), 7.86 (s, 1H), 7.53 (d, *J* = 8.4 Hz, 1H), 7.48 (d, *J* = 8.4 Hz, 1H), 7.39 (d, *J* = 8.4 Hz, 1H), 7.27 (s, 1H), 6.64 (d, *J* = 8.4 Hz, 1H), 6.55 (s, 1H), 6.19 (d, *J* = 16.0 Hz, 1H), 5.93 (dd, *J* = 16.0 Hz, 8.4 Hz, 1H), 3.87 (s, 3H), 3.83-3.78 (m, 1H), 1.44 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  163.3, 144.4, 138.4, 136.8, 131.7, 127.4, 127.0, 125.7, 123.4, 122.7, 122.0, 111.5, 111.2, 103.9, 64.3, 54.4, 14.0; HRMS Calculated for C<sub>18</sub>H<sub>18</sub>N<sub>2</sub>O<sub>3</sub>S (M+H<sup>+</sup>): 343.1111; Found: 343.1112.





### <sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of compound 43



1-(cinnamylsulfonyl)-4-((1s,4r)-4-propylcyclohexyl)benzene (44).



The product (55.9 mg, 73% yield) as yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 10/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.70 (d, J = 8.0 Hz, 2H), 7.27 (d, J = 8.4 Hz, 2H), 7.23-7.18 (m, 5H), 6.30 (d, J = 16.0 Hz, 1H), 6.07-5.99 (m, 1H), 3.85 (d, J = 7.6 Hz, 2H), 2.46 (t, J = 12.4 Hz, 1H), 1.83-1.77 (m, 4H), 1.41-1.32 (m, 2H), 1.30-1.11 (m, 5H), 1.02-0.92 (m, 2H), 0.82 (t, J = 7.2 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  154.4, 139.1, 135.9, 135.8, 128.64, 128.59, 128.5, 127.6, 126.6, 115.3, 60.6, 44.7, 39.6, 36.9, 34.0, 33.3, 20.0, 14.4; HRMS Calculated for C<sub>24</sub>H<sub>30</sub>O<sub>2</sub>S (M+Na<sup>+</sup>): 405.1859; Found: 405.1858.

# $^1\text{H}$ NMR spectrum (400 MHz, CDCl\_3) of compound 44







(E)-5-((1-phenylpent-1-en-3-yl)sulfonyl)-1H-indole (45).



The product (52.7 mg, 81% yield) as light yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>**H NMR (400 MHz, DMSO-***d*<sub>6</sub>**)**  $\delta$  11.65 (s, 1H), 8.08 (s, 1H), 7.58-7.54 (m, 2H), 7.51-7.48 (m, 1H), 7.35-7.25 (m, 5H), 6.64 (s, 1H), 6.43 (d, *J* = 15.6 Hz, 1H), 5.95 (dd, *J* = 16.0 Hz, 9.6 Hz, 1H), 3.91-3.85 (m, 1H), 2.02-1.93 (m, 1H), 1.70-1.58 (m, 1H), 0.87 (t, *J* = 7.6 Hz, 3H); <sup>13</sup>**C NMR (101 MHz, DMSO-***d*<sub>6</sub>**)**  $\delta$  138.1, 137.1, 135.9, 128.7, 128.1, 127.8, 127.0, 126.4, 122.3, 121.6, 120.8, 111.7, 102.8, 69.7, 21.1, 11.1; **HRMS** Calculated for C<sub>19</sub>H<sub>19</sub>NO<sub>2</sub>S (M+Na<sup>+</sup>): 348.1029; Found: 348.1028.



#### <sup>1</sup>H NMR spectrum (400 MHz, DMSO- $d_6$ ) of compound 45

#### <sup>13</sup>C NMR spectrum (101 MHz, DMSO-*d*<sub>6</sub>) of compound 45



(E)-5-((1-phenylhex-1-en-3-yl)sulfonyl)-1H-indole (46).



The product (50.2 mg, 74% yield) as pink solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  11.65 (s, 1H), 8.07 (s, 1H), 7.58-7.54 (m, 2H), 7.50-7.47 (m, 1H), 7.33-7.24 (m, 5H), 6.64 (s, 1H), 6.43 (d, *J* = 16.0 Hz, 1H), 5.95 (dd, *J* = 15.2 Hz, 8.8 Hz, 1H), 3.97-3.91 (m, 1H), 1.92-1.84 (m, 1H), 1.69-1.59 (m, 1H), 1.39-1.17 (m, 2H), 0.83 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  138.1, 136.9, 135.9, 128.7, 128.1, 127.7, 127.0, 126.4, 122.3, 121.9, 120.8, 111.7, 102.8, 68.2, 29.6, 19.4, 13.5; HRMS Calculated for C<sub>20</sub>H<sub>21</sub>NO<sub>2</sub>S (M+Na<sup>+</sup>): 362.1185; Found: 362.1185.

## <sup>1</sup>H NMR spectrum (400 MHz, DMSO-*d*<sub>6</sub>) of compound 46



<sup>13</sup>C NMR spectrum (101 MHz, DMSO-*d*<sub>6</sub>) of compound 46



(E)-5-((5-methyl-1-phenylhex-1-en-3-yl)sulfonyl)-1H-indole (47).



The product (55.1 mg, 78% yield) as pink solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  11.65 (s, 1H), 8.08 (s, 1H), 7.58-7.54 (m, 2H), 7.51-7.48 (m, 1H), 7.33-7.27 (m, 5H), 6.64 (s, 1H), 6.47 (d, *J* = 15.6 Hz, 1H), 5.94 (dd, *J* = 15.6 Hz, 9.2 Hz, 1H), 4.00-3.94 (m, 1H), 1.72-1.63 (m, 2H), 1.58-1.48 (m, 1H), 0.86 (d, *J* = 6.8 Hz, 3H), 0.78 (d, *J* = 6.4 Hz, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  138.1, 136.9, 136.0, 128.7, 128.10, 128.07, 127.7, 127.0, 126.4, 122.3, 122.0, 120.9, 111.6, 102.8, 67.1, 36.2, 25.0, 23.5, 20.7; HRMS Calculated for C<sub>21</sub>H<sub>23</sub>NO<sub>2</sub>S (M+Na<sup>+</sup>): 376.1342; Found: 376.1342.





#### <sup>13</sup>C NMR spectrum (101 MHz, DMSO-*d*<sub>6</sub>) of compound 47



5-(cinnamylsulfonyl)-1*H*-indole (51).



The product (42.8 mg, 72% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  11.66 (s, 1H), 8.13 (s, 1H), 7.61-7.54 (m, 3H), 7.34-7.23 (m, 5H), 6.65 (s, 1H), 6.49 (d, *J* = 16.0 Hz, 1H), 6.14-6.06 (m, 1H), 4.17 (d, *J* = 7.2 Hz, 2H); <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  138.1, 137.6, 135.9, 129.2, 128.7, 128.2, 127.0, 126.4, 121.5, 120.1, 116.7, 111.9, 102.8, 59.8; HRMS Calculated for C<sub>17</sub>H<sub>15</sub>NO<sub>2</sub>S (M+Na<sup>+</sup>): 320.0716; Found: 320.0715.

# <sup>1</sup>H NMR spectrum (400 MHz, DMSO- $d_6$ ) of compound 51



<sup>13</sup>C NMR spectrum (101 MHz, DMSO-*d*<sub>6</sub>) of compound **51** 



3-((cinnamylsulfonyl)methyl)-1,3,5-trimethylindolin-2-one (52).



The product (62.8 mg, 85% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.34-7.32 (m, 2H), 7.28-7.21 (m, 3H), 7.10 (s, 1H), 7.06 (d, *J* = 7.6 Hz, 1H), 6.72 (d, *J* = 7.6 Hz, 1H), 6.57 (d, *J* = 16.0 Hz, 1H), 6.12-6.04 (m, 1H), 3.62 (dd, *J* = 14.0 Hz, 7.2 Hz, 1H), 3.57 (d, *J* = 14.8 Hz, 1H), 3.46-3.40 (m, 2H), 3.16 (s, 3H), 2.30 (s, 3H), 1.35 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.8, 141.0, 139.0, 135.6, 132.0, 130.5, 129.3, 128.70, 128.65, 126.7, 124.3, 115.3, 108.5, 59.4, 57.0, 45.6, 26.6, 24.9, 21.2; HRMS Calculated for C<sub>21</sub>H<sub>23</sub>NO<sub>3</sub>S (M+H<sup>+</sup>): 370.1471; Found: 370.1472.



#### <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound **52**


3-((cinnamylsulfonyl)methyl)-5-methoxy-1,3-dimethylindolin-2-one (53).



The product (68.6 mg, 89% yield) as light yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.35-7.32 (m, 2H), 7.28-7.21 (m, 3H), 6.92 (s, 1H), 6.78 (d, *J* = 8.8 Hz, 1H), 6.73 (d, *J* = 8.4 Hz, 1H), 6.59 (d, *J* = 16.0 Hz, 1H), 6.12-6.05 (m, 1H), 3.73 (s, 3H), 3.64 (dd, *J* = 14.4 Hz, 7.2 Hz, 1H), 3.56 (d, *J* = 14.8 Hz, 1H), 3.45 (dd, *J* = 15.2 Hz, 7.6 Hz, 1H), 3.42 (d, *J* = 14.8 Hz, 1H), 3.16 (s, 3H), 1.36 (s, 3H).<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.5, 156.0, 139.2, 136.7, 135.6, 131.9, 128.7, 126.8, 115.2, 112.8, 111.4, 109.0, 59.5, 56.9, 55.8, 46.0, 26.7, 24.9; HRMS Calculated for C<sub>21</sub>H<sub>23</sub>NO<sub>4</sub>S (M+H<sup>+</sup>): 386.1421; Found: 386.1422.



<sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of compound 53



3-((cinnamylsulfonyl)methyl)-1,3-dimethyl-2-oxoindoline-5-carbonitrile (54).



The product (48.7 mg, 64% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 1/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.66-7.62 (m, 2H), 7.43 (d, *J* = 7.2 Hz, 2H), 7.37-7.29 (m, 3H), 6.96 (d, *J* = 8.0 Hz, 1H), 6.72 (d, *J* = 16.0 Hz, 1H), 6.20-6.13 (m, 1H), 3.78 (dd, *J* = 14.0 Hz, 7.6 Hz, 1H), 3.73 (d, *J* = 15.2 Hz, 1H), 3.64 (dd, *J* = 14.1 Hz, 7.3 Hz, 1H), 3.54 (d, *J* = 14.4 Hz, 1H), 3.28 (s, 3H), 1.44 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.8, 147.2, 139.5, 135.4, 134.2, 131.7, 128.9, 128.8, 127.1, 126.8, 119.0, 114.7, 109.2, 105.8, 59.9, 56.5, 45.2, 26.9, 24.9; HRMS Calculated for C<sub>21</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub>S (M+H<sup>+</sup>): 381.1267; Found: 381.1267.





3-((cinnamylsulfonyl)methyl)-1,3-dimethyl-5-(trifluoromethyl)indolin-2-one (55).



The product (67.8 mg, 80% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.56-7.53 (m, 2H), 7.34 (d, *J* = 7.6 Hz, 2H), 7.29-7.22 (m, 3H), 6.90 (d, *J* = 8.0 Hz, 1H), 6.61 (d, *J* = 16.0 Hz, 1H), 6.13-6.05 (m, 1H), 3.68-3.60 (m, 2H), 3.50-3.43 (m, 2H), 3.21 (s, 3H), 1.37 (s, 3H); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>)  $\delta$  -61.2 (s, 3F); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.0, 146.4, 139.3, 135.4, 131.1, 128.81, 128.77, 126.8-126.7 (m, 2C), 124.8 (q, *J* = 33.3 Hz), 124.3 (q, *J* = 272.7 Hz), 120.7 (q, *J* = 4.0 Hz), 115.0, 108.6, 60.0, 56.6, 45.5, 26.9, 24.9; HRMS Calculated for C<sub>21</sub>H<sub>20</sub>F<sub>3</sub>NO<sub>3</sub>S (M+H<sup>+</sup>): 424.1189; Found: 424.1190.

## $^1\text{H}$ NMR spectrum (400 MHz, CDCl\_3) of compound 55



 $^{19}F$  NMR spectrum (376 MHz, CDCl\_3) of compound 55



<sup>10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210</sup> f1 (ppm)



Methyl 3-((cinnamylsulfonyl)methyl)-1,3-dimethyl-2-oxoindoline-6-carboxylate (56).



The product (70.3 mg, 85% yield) as light yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 1/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.76 (d, *J* = 8.0 Hz, 1H), 7.48 (s, 1H), 7.36-7.21 (m, 6H), 6.61 (d, *J* = 16.0 Hz, 1H), 6.11-6.03 (m, 1H), 3.85 (s, 3H), 3.70-3.63 (m, 2H), 3.53 (dd, *J* = 14.0 Hz, 7.2 Hz, 1H), 3.46 (d, *J* = 14.8 Hz, 1H), 3.22 (s, 3H), 1.37 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.7, 166.5, 139.3, 135.7, 135.5, 130.9, 128.7, 126.8, 124.4, 123.4, 114.9, 109.4, 59.7, 56.6, 52.3, 45.7, 26.8, 24.9; HRMS Calculated for C<sub>22</sub>H<sub>23</sub>NO<sub>5</sub>S (M+H<sup>+</sup>): 414.1370; Found: 414.1371.



<sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of compound 56



6-chloro-3-((cinnamylsulfonyl)methyl)-1,3-dimethylindolin-2-one (57).



The product (71.0 mg, 91% yield) as light yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.45-7.43 (m, 2H), 7.39-7.30 (m, 4H), 7.10 (d, *J* = 8.0 Hz, 1H), 6.92 (s, 1H), 6.71 (d, *J* = 16.0 Hz, 1H), 6.22-6.14 (m, 1H), 3.77 (dd, *J* = 14.0 Hz, 7.6 Hz, 1H), 3.70 (d, *J* = 15.6 Hz, 1H), 3.65 (dd, *J* = 14.0 Hz, 7.2 Hz, 1H), 3.53 (d, *J* = 14.4 Hz, 1H), 3.26 (s, 3H), 1.44 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.9, 144.5, 139.3, 135.5, 134.7, 128.9, 128.7, 126.8, 124.6, 122.4, 114.9, 109.5, 59.7, 56.7, 45.2, 26.7, 24.9; HRMS Calculated for C<sub>20</sub>H<sub>20</sub>CINO<sub>3</sub>S (M+H<sup>+</sup>): 390.0925; Found: 390.0924.







3-butyl-3-((cinnamylsulfonyl)methyl)-5-methoxy-1-methylindolin-2-one (58).



The product (70.1 mg, 82% yield) as brown solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.46-7.43 (m, 2H), 7.39-7.31 (m, 3H), 6.96 (s, 1H), 6.89 (d, J = 8.4 Hz, 1H), 6.83 (d, J = 8.4 Hz, 1H), 6.69 (d, J = 16.8 Hz, 1H), 6.22-6.14 (m, 1H), 3.84 (s, 3H), 3.72 (dd, J = 14.4 Hz, 7.6 Hz, 1H), 3.67 (d, J = 14.8 Hz, 1H), 3.52-3.47 (m, 2H), 3.26 (s, 3H), 1.91-1.74 (m, 2H), 1.36-1.10 (m, 3H), 1.04-0.93 (m, 1H), 0.78 (t, J = 6.8 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  176.9, 155.9, 139.1, 137.8, 135.6, 130.2, 128.7, 128.6, 126.8, 115.3, 112.6, 111.6, 108.8, 59.6, 56.9, 55.8, 50.0, 38.3, 26.6, 25.1, 22.5, 13.7; HRMS Calculated for C<sub>24</sub>H<sub>29</sub>NO<sub>4</sub>S (M+H<sup>+</sup>): 428.1890; Found: 428.1897.







3-benzyl-3-((cinnamylsulfonyl)methyl)-5-methoxy-1-methylindolin-2-one (59).



The product (73.9 mg, 80% yield) as brown solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.46-7.44 (m, 2H), 7.40-7.33 (m, 3H), 7.15-7.07 (m, 3H), 6.92 (s, 1H), 6.84-6.79 (m, 3H), 6.73 (d, *J* = 16.0 Hz, 1H), 6.58 (d, *J* = 8.4 Hz, 1H), 6.25-6.17 (m, 1H), 3.87-3.78 (m, 5H), 3.65-3.58 (m, 2H), 3.08 (s, 2H), 3.01 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  176.2, 155.5, 139.3, 137.4, 135.6, 133.6, 130.1, 129.1, 128.73, 128.69, 127.7, 127.1, 126.8, 115.2, 113.2, 112.2, 108.7, 59.8, 56.0, 55.9, 51.4, 44.4, 26.3; HRMS Calculated for C<sub>27</sub>H<sub>27</sub>NO<sub>4</sub>S (M+H<sup>+</sup>): 462.1734; Found: 462.1736.







3-(4-(tert-butyl)phenyl)-3-((cinnamylsulfonyl)methyl)-5-methoxy-1-methylindolin-2-one (60).



The product (78.6 mg, 78% yield) as light yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  7.35-7.33 (m, 2H), 7.28-7.18 (m, 7H), 6.99 (s, 1H), 6.85 (d, *J* = 8.4 Hz, 1H), 6.77 (d, *J* = 8.8 Hz, 1H), 6.66 (d, *J* = 15.6 Hz, 1H), 6.15-6.07 (m, 1H), 4.15 (d, *J* = 14.8 Hz, 1H), 3.77-3.70 (m, 5H), 3.46 (dd, *J* = 14.0 Hz, 7.6 Hz, 1H), 3.14 (s, 3H), 1.16 (s, 9H); <sup>13</sup>**C NMR (101 MHz, CDCl<sub>3</sub>)**  $\delta$  176.1, 155.7, 151.1, 139.2, 137.9, 135.6, 134.7, 129.9, 128.72, 128.67, 126.8, 126.2, 125.9, 115.3, 113.6, 113.3, 109.3, 59.8, 57.6, 55.9, 53.0, 34.4, 31.2, 27.0; **HRMS** Calculated for C<sub>30</sub>H<sub>33</sub>NO<sub>4</sub>S (M+H<sup>+</sup>): 504.2203; Found: 504.2206.





3-((cinnamylsulfonyl)methyl)-3-cyclohexyl-5-methoxy-1-methylindolin-2-one (61).



The product (76.2 mg, 84% yield) as light yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  7.46-7.43 (m, 2H), 7.39-7.31 (m, 3H), 6.92-6.87 (m, 2H), 6.81 (d, *J* = 8.4 Hz, 1H), 6.72 (d, *J* = 15.6 Hz, 1H), 6.23-6.15 (m, 1H), 3.84 (s, 3H), 3.78-3.71 (m, 2H), 3.63 (d, *J* = 14.4 Hz, 1H), 3.49 (dd, *J* = 13.6 Hz, 7.2 Hz, 1H), 3.25 (s, 3H), 1.85-1.73 (m, 2H), 1.65-1.57 (m, 3H), 1.51-1.47 (m, 1H), 1.24-1.13 (m, 3H), 1.05-0.96 (m, 1H), 0.86-0.76 (m, 1H); <sup>13</sup>**C NMR (101 MHz, CDCl<sub>3</sub>)**  $\delta$  177.0, 155.4, 139.0, 138.2, 135.7, 129.4, 128.7, 128.6, 126.7, 115.4, 112.6, 112.1, 108.5, 59.5, 55.8, 55.5, 53.2, 46.0, 26.7, 26.4, 26.3(m, 2C), 25.9, 25.8; **HRMS** Calculated for C<sub>26</sub>H<sub>31</sub>NO<sub>4</sub>S (M+H<sup>+</sup>): 454.2047; Found: 454.2049.

### <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 61

845 845 7789 885 885 7789 845 7789 845 7789 7789 11134 1159 11134 1159 11134 1159 11134 1159 11134 1159 11134 1159 11134 11135 111135 111135 11135 11115 11115 1115 1115 1115 1115 1115 1115 1115 1111 8 3.054 500 2 95 0.0 7.5 7.0 6.5 6.0 5.5 3.0 9.0 8.5 8.0 5.0 4.5 f1 (ppm) 3.5 2.5 2.0 1.0 0.5 40



tert-butyl 3-((cinnamylsulfonyl)methyl)-3-methyl-2-oxoindoline-1-carboxylate (62).



The product (63.6 mg, 72% yield) as yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.93 (d, *J* = 8.0 Hz, 1H), 7.44-7.32 (m, 7H), 7.28-7.23 (m, 1H), 6.68 (d, *J* = 16.0 Hz, 1H), 6.21-6.13 (m, 1H), 3.76 (d, *J* = 14.8 Hz, 1H), 3.70 (dd, *J* = 14.4 Hz, 7.6 Hz, 1H), 3.59-3.52 (m, 2H), 1.68 (s, 9H), 1.50 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  176.7, 149.0, 139.4, 139.3, 135.5, 129.3, 129.2, 128.7, 126.8, 124.4, 123.2, 115.7, 115.0, 59.5, 57.4, 46.2, 28.1, 26.1; HRMS Calculated for C<sub>24</sub>H<sub>27</sub>NO<sub>5</sub>S (M+Na<sup>+</sup>): 464.1502; Found: 464.1504.



<sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of compound 62



1-acetyl-3-((cinnamylsulfonyl)methyl)-5-methoxy-3-methylindolin-2-one (63).



The product (52.9 mg, 64% yield) as yellow oil was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.28 (d, *J* = 8.8 Hz, 1H), 7.46-7.43 (m, 2H), 7.41-7.33 (m, 3H), 6.95-6.92 (m, 2H), 6.62 (d, *J* = 15.6 Hz, 1H), 6.18-6.10 (m, 1H), 3.87 (s, 3H), 3.71-3.61 (m, 2H), 3.56 (dd, *J* = 14.0 Hz, 6.4 Hz, 1H), 3.32 (dd, *J* = 14.4 Hz, 8.4 Hz, 1H), 2.71 (s, 3H), 1.49 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.7, 170.7, 157.1, 139.3, 135.4, 133.2, 130.6, 128.9, 128.8, 126.8, 118.3, 114.9, 113.2, 110.0, 59.3, 57.9, 55.7, 46.3, 26.4, 26.1; HRMS Calculated for C<sub>22</sub>H<sub>23</sub>NO<sub>5</sub>S (M+H<sup>+</sup>): 414.1370; Found: 414.1371.





ethyl 2-(3-((cinnamylsulfonyl)methyl)-5-methoxy-3-methyl-2-oxoindolin-1-yl) acetate (64).



The product (75.0 mg, 82% yield) as yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.34-7.32 (m, 2H), 7.28-7.20 (m, 3H), 6.96 (s, 1H), 6.75 (d, *J* = 8.8 Hz, 1H), 6.64-6.58 (m, 2H), 6.13-6.05 (m, 1H), 4.59 (d, *J* = 17.6 Hz, 1H), 4.20 (d, *J* = 17.6 Hz, 1H), 4.12 (q, *J* = 6.8 Hz, 2H), 3.72 (s, 3H), 3.67 (dd, *J* = 14.0 Hz, 8.4 Hz, 1H), 3.57 (d, *J* = 14.8 Hz, 1H), 3.51 (dd, *J* = 14.0 Hz, 7.6 Hz, 1H), 3.44 (d, *J* = 14.8 Hz, 1H), 1.42 (s, 3H), 1.17 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.6, 167.5, 156.2, 139.2, 135.6, 135.2, 131.6, 128.7, 128.6, 126.8, 115.1, 113.0, 111.5, 109.1, 61.7, 59.4, 56.6, 55.8, 46.1, 41.7, 25.2, 14.1; HRMS Calculated for C<sub>24</sub>H<sub>27</sub>NO<sub>6</sub>S (M+H<sup>+</sup>): 458.1632; Found: 458.1635.



<sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of compound 64



1-benzyl-3-((cinnamylsulfonyl)methyl)-5-methoxy-3-methylindolin-2-one (65).



The product (83.1 mg, 90% yield) as yellow oil was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.34-7.31 (m, 2H), 7.27-7.15 (m, 8H), 6.91 (s, 1H), 6.64-6.54 (m, 3H), 6.13-6.05 (m, 1H), 4.93 (d, *J* = 15.6 Hz, 1H), 4.78 (d, *J* = 15.6 Hz, 1H), 3.70-3.62 (m, 5H), 3.50 (dd, *J* = 14.4 Hz, 7.6 Hz, 1H), 3.46 (d, *J* = 14.4 Hz, 1H), 1.40 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.7, 155.9, 139.2, 135.69, 135.68, 135.6, 132.0, 128.74, 128.69, 128.6, 127.5, 127.2, 126.8, 115.2, 112.7, 111.3, 110.2, 59.5, 56.6, 55.7, 46.1, 44.2, 25.7; HRMS Calculated for C<sub>27</sub>H<sub>27</sub>NO<sub>4</sub>S (M+H<sup>+</sup>): 462.1734; Found: 462.1736.





3-((cinnamylsulfonyl)methyl)-3-methyl-1-propylindolin-2-one (66).



The product (61.4 mg, 80% yield) as yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.45-7.32 (m, 7H), 7.13 (t, *J* = 7.6 Hz, 1H), 6.95 (d, *J* = 7.6 Hz, 1H), 6.69 (d, *J* = 16.0 Hz, 1H), 6.23-6.15 (m, 1H), 3.78-3.69 (m, 4H), 3.60 (dd, *J* = 14.0 Hz, 7.2 Hz, 1H), 3.54 (d, *J* = 14.4 Hz, 1H), 1.82-1.73 (m, 2H), 1.47 (s, 3H), 1.01 (t, *J* = 7.6 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.8, 142.8, 139.1, 135.6, 130.7, 128.8, 128.7, 128.6, 126.7, 123.6, 122.3, 115.3, 109.0, 59.5, 56.7, 45.5, 41.9, 25.3, 20.5, 11.4; HRMS Calculated for C<sub>22</sub>H<sub>25</sub>NO<sub>3</sub>S (M+H<sup>+</sup>): 384.1628; Found: 384.1628.





3-((cinnamylsulfonyl)methyl)-3-methylindolin-2-one (67).



The product (28.7 mg, 42% yield) as yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.63 (s, 1H), 7.33-7.31 (m, 2H), 7.27-7.21 (m, 4H), 7.18-7.14 (m, 1H), 7.00 (t, *J* = 7.6 Hz, 1H), 6.87 (d, *J* = 7.6 Hz, 1H), 6.58 (d, *J* = 15.6 Hz, 1H), 6.12-6.04 (m, 1H), 3.66-3.61 (m, 2H), 3.54-3.48 (m, 2H), 1.39 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  180.0, 140.7, 139.4, 135.6, 130.8, 129.0, 128.74, 128.71, 126.8, 123.8, 122.5, 115.0, 110.8, 59.5, 57.0, 46.0, 25.2; HRMS Calculated for C<sub>19</sub>H<sub>19</sub>NO<sub>3</sub>S (M+H<sup>+</sup>): 342.1158; Found: 342.1158.







1-(3-((cinnamylsulfonyl)methyl)-3-methylindolin-1-yl)ethan-1-one (68).



The product (50.3 mg, 68% yield) as yellow oil was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.14 (d, *J* = 8.0 Hz, 1H), 7.32-7.18 (m, 6H), 7.06 (d, *J* = 7.2 Hz, 1H), 7.00 (t, *J* = 7.2 Hz, 1H), 6.49 (d, *J* = 15.6 Hz, 1H), 6.12-6.05 (m, 1H), 4.47 (d, *J* = 10.8 Hz, 1H), 3.78 (d, *J* = 10.8 Hz, 1H), 3.60 (d, *J* = 7.2 Hz, 2H), 3.19 (dd, *J* = 26.4 Hz, 14.4 Hz, 2H), 2.13 (s, 3H), 1.61 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  169.0, 141.7, 139.4, 136.6, 135.3, 129.2, 128.9, 128.8, 126.8, 124.2, 122.3, 117.5, 114.8, 60.03, 59.95, 59.0, 42.7, 25.7, 24.1; HRMS Calculated for C<sub>21</sub>H<sub>23</sub>NO<sub>3</sub>S (M+H<sup>+</sup>): 370.1471; Found: 370.1470.





## 1-((cinnamylsulfonyl)methyl)-1-methyl-2,3-dihydro-1*H*-indene (69).



The product (58.8 mg, 90% yield) as yellow oil was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.28-7.13 (m, 9H), 6.26 (d, *J* = 16.0 Hz, 1H), 6.10-6.02 (m, 1H), 3.51 (dd, *J* = 14.4 Hz, 6.8 Hz, 1H), 3.42 (dd, *J* = 14.0 Hz, 8.4 Hz, 1H), 3.29 (d, *J* = 14.4 Hz, 1H), 2.98 (d, *J* = 14.4 Hz, 1H), 2.85-2.81 (m, 2H), 2.41-2.34 (m, 1H), 2.03-1.95 (m, 1H), 1.54 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  148.1, 143.1, 138.8, 135.6, 128.7, 128.6, 127.7, 126.67, 126.63, 125.1, 123.2, 115.8, 59.8, 59.3, 46.6, 39.5, 30.1, 26.1; HRMS Calculated for C<sub>20</sub>H<sub>22</sub>O<sub>2</sub>S (M+Na<sup>+</sup>): 349.1233; Found: 349.1238.





## 4-((cinnamylsulfonyl)methyl)-4-methylisochromane (70).



The product (56.2 mg, 82% yield) as brown oil was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.52-7.48 (m, 1H), 7.40-7.27 (m, 7H), 7.06-7.04 (m, 1H), 6.45 (d, *J* = 16.0 Hz, 1H), 6.22-6.14 (m, 1H), 4.86 (s, 2H), 4.33 (d, *J* = 11.6 Hz, 1H), 3.72 (dd, *J* = 14.0 Hz, 7.2 Hz, 1H), 3.60-3.55 (m, 2H), 3.43 (s, 2H), 1.64 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  138.9, 138.8, 135.6, 133.7, 128.7, 128.6, 127.3, 127.1, 126.67, 126.65, 124.5, 115.6, 73.0, 68.6, 59.9, 58.6, 37.0, 21.6; HRMS Calculated for C<sub>20</sub>H<sub>22</sub>O<sub>3</sub>S (M+H<sup>+</sup>): 343.1362; Found: 343.1363.





Diethyl 4-((cinnamylsulfonyl)methyl)-4-methyl-3,4-dihydronaphthalene-2,2(1*H*)dicarboxylate (71).



The product (69.8 mg, 72% yield) as white oil was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.31-7.12 (m, 9H), 6.39 (d, J = 16.0 Hz, 1H), 6.07-6.00 (m, 1H), 4.12-3.95 (m, 4H), 3.39-3.34 (m, 1H), 3.30-3.18 (m, 4H), 3.11 (d, J = 16.0 Hz, 1H), 2.90 (d, J = 14.4 Hz, 1H), 2.38 (d, J = 14.8 Hz, 1H), 1.56 (s, 3H), 1.15-1.06 (m, 6H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  171.6, 171.1, 139.4, 138.8, 135.6, 134.3, 129.4, 128.7, 128.6, 127.4, 127.1, 126.7, 126.4, 115.5, 61.9, 61.8, 61.5, 59.8, 53.0, 40.1, 37.4, 34.9, 29.6, 13.9, 13.9; HRMS Calculated for C<sub>27</sub>H<sub>32</sub>O<sub>6</sub>S (M+H<sup>+</sup>): 485.1992; Found: 485.2000.







11-(cinnamylsulfonyl)-10b-methyl-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one (72).



The product (33.2 mg, 40% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 1/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.92 (d, *J* = 7.6 Hz, 1H), 7.85 (d, *J* = 7.6 Hz, 1H), 7.78-7.71 (m, 3H), 7.63-7.59 (m, 1H), 7.38-7.33 (m, 1H), 7.24-7.16 (m, 4H), 7.14-7.11 (m, 2H), 6.04 (d, *J* = 16.0 Hz, 1H), 5.53-5.45 (m, 1H), 4.54 (s, 1H), 2.89-2.76 (m, 2H), 1.75 (s, 3H); <sup>13</sup>C NMR (151 MHz, CDCl<sub>3</sub>)  $\delta$  166.6, 145.4, 139.6, 138.9, 135.4, 133.0, 132.9, 131.4, 129.8, 128.7, 128.4, 128.3, 127.2, 126.8, 126.7, 125.2, 124.6, 117.3, 112.5, 73.3, 72.5, 55.0, 30.2; HRMS Calculated for C<sub>25</sub>H<sub>21</sub>NO<sub>3</sub>S (M+Na<sup>+</sup>): 438.1134; Found: 438.1136.



<sup>13</sup>C NMR spectrum (151 MHz, CDCl<sub>3</sub>) of compound 72



(E)-1-benzyl-3-methyl-3-(((3-(p-tolyl)allyl)sulfonyl)methyl)indolin-2-one (73).



The product (74.0 mg, 83% yield) as brown solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.29-7.19 (m, 7H), 7.17-7.09 (m, 2H), 7.06-7.05 (m, 2H), 6.98 (t, J = 7.2 Hz, 1H), 6.66 (d, J = 8.0 Hz, 1H), 6.53 (d, J = 15.6 Hz, 1H), 6.05-5.98 (m, 1H), 4.96 (d, J = 16.0 Hz, 1H), 4.79 (d, J = 15.6 Hz, 1H), 3.66-3.58 (m, 2H), 3.50-3.45 (m, 2H), 2.25 (s, 3H), 1.40 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.0, 142.4, 139.0, 138.7, 135.6, 132.8, 130.5, 129.4, 128.8, 128.7, 127.5, 127.2, 126.7, 123.5, 122.6, 114.0, 109.8, 59.6, 56.6, 45.6, 44.2, 25.6, 21.2; HRMS Calculated for C<sub>27</sub>H<sub>27</sub>NO<sub>3</sub>S (M+H<sup>+</sup>): 446.1784; Found: 446.1787.







(E)-6-chloro-3-(((3-(4-methoxyphenyl)allyl)sulfonyl)methyl)-1,3-dimethylindolin-2-one (74).



The product (63.0 mg, 75% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, Chloroform-*d*)  $\delta$  7.28-7.26 (m, 2H), 7.20 (d, J = 8.0 Hz, 1H), 7.00 (d, J = 7.6 Hz, 1H), 6.82-6.78 (m, 3H), 6.54 (d, J = 16.0 Hz, 1H), 5.96-5.88 (m, 1H), 3.74 (s, 3H), 3.64 (dd, J = 14.4 Hz, 7.6 Hz, 1H), 3.58 (d, J = 14.4 Hz, 1H), 3.52 (dd, J = 14.4 Hz, 7.6 Hz, 1H), 3.41 (d, J = 14.4 Hz, 1H), 3.16 (s, 3H), 1.34 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.0, 160.0, 144.5, 138.8, 134.7, 128.9, 128.3, 128.1, 124.6, 122.4, 114.1, 112.4, 109.5, 59.9, 56.6, 55.3, 45.3, 26.7, 24.9; HRMS Calculated for C<sub>21</sub>H<sub>22</sub>ClNO<sub>4</sub>S (M+Na<sup>+</sup>): 442.0850; Found: 442.0852.



f1 (ppm) ò 

(*E*)-3-(((3-(benzo[*d*][1,3]dioxol-5-yl)allyl)sulfonyl)methyl)-1-ethyl-5-methoxy-3methylindolin-2-one (75).



The product (67.4 mg, 76% yield) as yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  6.99 (s, 1H), 6.94 (s, 1H), 6.86-6.80 (m, 3H), 6.76 (d, J = 8.0 Hz, 1H), 6.57 (d, J = 16.0 Hz, 1H), 6.01-5.94 (m, 3H), 3.86-3.79 (m, 4H), 3.75-3.67 (m, 2H), 3.63 (d, J = 14.8 Hz, 1H), 3.52 (dd, J = 14.0 Hz, 7.2 Hz, 1H), 3.46 (d, J = 14.8 Hz, 1H), 1.42 (s, 3H), 1.27 (t, J = 7.6 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.1, 155.8, 148.2, 148.1, 138.7, 135.7, 132.2, 130.1, 121.9, 113.2, 112.8, 111.5, 109.2, 108.3, 105.8, 101.3, 59.5, 56.7, 55.8, 45.9, 35.0, 25.2, 12.3; HRMS Calculated for C<sub>23</sub>H<sub>25</sub>NO<sub>6</sub>S (M+H<sup>+</sup>): 444.1475; Found: 444.1477.







(*E*)-1-(3,5-dimethylbenzyl)-3-(((3-(4-fluorophenyl)allyl)sulfonyl)methyl)-5-methoxy-3-methylindolin-2-one (76).



The product (73.1 mg, 72% yield) as brown solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1).<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.31-7.27 (m, 2H), 6.96-6.91 (m, 3H), 6.85 (s, 2H), 6.79 (s, 1H), 6.65 (d, J = 8.4 Hz, 1H), 6.61-6.53 (m, 2H), 6.04-5.97 (m, 1H), 4.85 (d, J = 15.6 Hz, 1H), 4.70 (d, J = 15.6 Hz, 1H), 3.70-3.62 (m, 5H), 3.53-3.43 (m, 2H), 2.17 (s, 6H), 1.42 (s, 3H); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>)  $\delta$  -112.53 (s, 1F); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.7, 164.1, 161.6, 156.0, 138.3, 138.0, 135.8, 135.6, 132.0, 131.9 (d, J = 3.0 Hz), 129.2, 128.4 (d, J = 8.1 Hz), 125.0, 115.8, 115.6, 114.9 (d, J = 2.0 Hz), 112.8, 111.2, 110.2, 59.4, 56.8, 55.7, 46.2, 44.2, 25.7, 21.3; HRMS Calculated for C<sub>29</sub>H<sub>30</sub>FNO<sub>4</sub>S (M+H<sup>+</sup>): 508.1952; Found: 508.1956.


 $^{19}F$  NMR spectrum (376 MHz, CDCl\_3) of compound 76





(*E*)-1-(4-(*tert*-butyl)benzyl)-3-(((3-(4-chlorophenyl)allyl)sulfonyl)methyl)-5-methoxy-3-methylindolin-2-one (77).



The product (82.8 mg, 75% yield) as yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1).<sup>1</sup>H NMR (400 MHz, CDCl3)  $\delta$  7.26-7.15 (m, 8H), 6.91 (s, 1H), 6.66-6.54 (m, 3H), 6.11-6.04 (m, 1H), 4.89 (d, *J* = 15.6 Hz, 1H), 4.76 (d, *J* = 15.6 Hz, 1H), 3.71-3.61 (m, 5H), 3.57-3.51 (m, 1H), 3.45 (d, *J* = 14.4 Hz, 1H), 1.41 (s, 3H), 1.19 (s, 9H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.6, 156.0, 150.5, 138.0, 135.8, 134.4, 134.1, 132.6, 132.0, 128.9, 128.0, 126.9, 125.7, 115.9, 112.8, 111.3, 110.3, 59.4, 56.9, 55.8, 46.2, 43.9, 34.5, 31.3, 25.7; HRMS Calculated for C<sub>31</sub>H<sub>34</sub>CINO<sub>4</sub>S (M+H<sup>+</sup>): 552.1970; Found: 552.1975.



 $^{13}C$  NMR spectrum (101 MHz, CDCl\_3) of compound 77



(*E*)-2-(3-(((3-(4-bromophenyl)allyl)sulfonyl)methyl)-5-methoxy-3-methyl-2-oxoindolin-1-yl)acetate (78).



The product (75.1 mg, 70% yield) as yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.38 (d, *J* = 8.4 Hz, 2H), 7.19 (d, *J* = 8.4 Hz, 2H), 6.95 (d, *J* = 2.0 Hz, 1H), 6.75 (dd, *J* = 8.4 Hz, 2.0 Hz, 1H), 6.63 (d, *J* = 8.4 Hz, 1H), 6.54 (d, *J* = 15.6 Hz, 1H), 6.12-6.04 (m, 1H), 4.57 (d, *J* = 17.6 Hz, 1H), 4.22 (d, *J* = 17.6 Hz, 1H), 4.13 (q, *J* = 7.2 Hz, 2H), 3.72 (s, 3H), 3.67 (dd, *J* = 14.0 Hz, 7.6 Hz, 1H), 3.58 (d, *J* = 15.2 Hz, 1H), 3.53 (dd, *J* = 14.0 Hz, 7.6 Hz, 1H), 3.43 (d, *J* = 14.8 Hz, 1H), 1.43 (s, 3H), 1.18 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.6, 167.5, 156.2, 138.1, 135.2, 134.6, 131.8, 131.6, 128.3, 122.6, 115.9, 113.0, 111.6, 109.1, 61.8, 59.3, 56.9, 55.8, 46.2, 41.7, 25.2, 14.1; HRMS Calculated for C<sub>24</sub>H<sub>26</sub>BrNO<sub>6</sub>S (M+H<sup>+</sup>): 536.0737; Found: 536.0743.







(*E*)-3-cyclohexyl-3-(((3-(furan-2-yl)allyl)sulfonyl)methyl)-5-methoxy-1-methylindolin-2-one (79).



The product (48.8 mg, 55% yield) as brown oil was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.37 (s, 1H), 6.89-6.84 (m, 2H), 6.77 (d, J = 8.4 Hz, 1H), 6.51 (d, J = 16.0 Hz, 1H), 6.39-6.38 (m, 1H), 6.34 (d, J = 3.2 Hz, 1H), 6.09-6.02 (m, 1H), 3.81 (s, 3H), 3.71-3.64 (m, 2H), 3.59 (d, J = 14.4 Hz, 1H), 3.41 (dd, J = 14.4, 7.2 Hz, 1H), 3.21 (s, 3H), 1.80-1.71 (m, 2H), 1.63-1.54 (m, 3H), 1.29-1.25 (m, 1H), 1.19-1.11 (m, 3H), 1.03-0.96 (m, 1H), 0.78-0.74 (m, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.1, 155.5, 151.4, 142.9, 138.2, 129.4, 126.9, 113.5, 112.5, 112.3, 111.5, 110.0, 108.5, 59.3, 55.8, 55.6, 53.3, 46.1, 26.7, 26.5, 26.3, 26.0, 25.8; HRMS Calculated for C<sub>24</sub>H<sub>29</sub>NO<sub>5</sub>S (M+H<sup>+</sup>): 444.1839; Found: 444.1841.





<sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of compound 79



methyl (*E*)-3-(((3-(4-fluorophenyl)-1-isopropyl-1*H*-indol-2-yl)allyl)sulfonyl)methyl)-1,3-dimethyl-2-oxoindoline-6-carboxylate (80).



The product (83.6 mg, 71% yield) as brown solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 1/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.72 (d, *J* = 7.6 Hz, 1H), 7.47-7.44 (m, 2H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.35-7.31 (m, 2H), 7.21 (d, *J* = 6.8 Hz, 1H), 7.13 (t, *J* = 8.0 Hz, 1H), 7.08-6.98 (m, 3H), 6.69 (d, *J* = 16.0 Hz, 1H), 5.61-5.53 (m, 1H), 4.77-4.70 (m, 1H), 3.84 (s, 3H), 3.55 (dd, *J* = 13.6 Hz, 7.6 Hz, 1H), 3.41-3.32 (m, 2H), 3.20-3.12 (m, 4H), 1.57 (d, *J* = 6.8 Hz, 6H), 1.31 (s, 3H); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>)  $\delta$  -115.87 (s, 1F); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.5, 166.5, 161.57 (d, *J* = 246.4 Hz), 143.6, 135.5, 135.3, 132.3 (d, *J* = 8.1 Hz), 132.1, 131.2 (d, *J* = 3.0 Hz), 131.0, 129.3, 128.3, 124.5, 123.2, 122.5, 120.8, 119.9, 119.8, 116.1, 115.6 (d, *J* = 21.2 Hz), 111.8, 109.5, 59.6, 57.1, 52.3, 48.0, 45.6, 26.8, 24.8, 21.8; HRMS Calculated for C<sub>33</sub>H<sub>33</sub>FN<sub>2</sub>O<sub>5</sub>S (M+H<sup>+</sup>): 589.2167; Found: 589.2173.







<sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of compound 80



(E)-1,3-dimethyl-3-(((3-phenylbut-2-en-1-yl)sulfonyl)methyl)indolin-2-one (81).



The product (44.3 mg, 60% yield) as brown solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.33-7.20 (m, 7H), 7.03 (t, *J* = 7.6 Hz, 1H), 6.83 (d, *J* = 8.0 Hz, 1H), 5.68 (t, *J* = 8.0 Hz, 1H), 3.66 (dd, *J* = 14.4 Hz, 8.0 Hz, 1H), 3.58-3.51 (m, 2H), 3.46 (d, *J* = 14.4 Hz, 1H), 3.18 (s, 3H), 1.98 (s, 3H), 1.38 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.0, 144.9, 143.4, 142.0, 130.5, 129.0, 128.4, 128.0, 126.0, 123.6, 122.7, 112.3, 108.8, 58.0, 55.9, 45.6, 26.6, 25.0, 16.7; HRMS Calculated for C<sub>21</sub>H<sub>23</sub>NO<sub>3</sub>S (M+H<sup>+</sup>): 370.1471; Found: 370.1472.



<sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 81



(E)-3-((hex-2-en-1-ylsulfonyl)methyl)-1,3-dimethylindolin-2-one (82).



The product (54.6 mg, 85% yield) as brown oil was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.30-7.24 (m, 2H), 7.03 (t, *J* = 7.6 Hz, 1H), 6.82 (d, *J* = 7.6 Hz, 1H), 5.76-5.68 (m, 1H), 5.40-5.33 (m, 1H), 3.52 (d, *J* = 14.4 Hz, 1H), 3.42 (d, *J* = 14.0 Hz, 1H), 3.38 (dd, *J* = 14.4 Hz, 7.2 Hz, 1H), 3.25 (dd, *J* = 14.0 Hz, 7.2 Hz, 1H), 3.18 (s, 3H), 2.00 (q, *J* = 7.2 Hz, 2H), 1.38-1.33 (m, 5H), 0.84 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.9, 143.3, 141.7, 130.4, 128.9, 123.6, 122.5, 116.1, 108.7, 59.1, 56.6, 45.5, 34.6, 26.6, 24.8, 21.9, 13.6; HRMS Calculated for C<sub>17</sub>H<sub>23</sub>NO<sub>3</sub>S (M+H<sup>+</sup>): 322.1471; Found: 322.1471.



#### 3-((cinnamylsulfonyl)methyl)-1,3-dimethylindolin-2-one (84).



The product (66.1 mg, 93% yield) as white solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.44-7.30 (m, 7H), 7.15 (t, *J* = 7.6 Hz, 1H), 6.94 (d, *J* = 7.6 Hz, 1H), 6.68 (d, *J* = 16.0 Hz, 1H), 6.22-6.14 (m, 1H), 3.74-3.67 (m, 2H), 3.59-3.54 (m, 2H), 3.29 (s, 3H), 1.47 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.9, 143.4, 139.2, 135.6, 130.4, 129.0, 128.71, 128.68, 126.8, 123.5, 122.6, 115.2, 108.8, 59.5, 57.0, 45.6, 26.6, 24.9; HRMS Calculated for C<sub>20</sub>H<sub>21</sub>NO<sub>3</sub>S (M+H<sup>+</sup>): 356.1315; Found: 356.1316.



<sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 84



1-methyl-4-((2-methyl-4-phenylbut-3-yn-2-yl)sulfonyl)benzene (85).



The product (46.0 mg, 77% yield) as yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.82 (d, *J* = 8.4 Hz, 2H), 7.28-7.22 (m, 7H), 2.38 (s, 3H), 1.61 (s, 6H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  145.0, 132.1, 131.7, 131.0, 129.2, 128.8, 128.3, 122.1, 87.6, 86.4, 59.4, 23.4, 21.7; HRMS Calculated for C<sub>18</sub>H<sub>18</sub>O<sub>2</sub>S (M+Na<sup>+</sup>): 321.0920; Found: 321.0920.



1-methoxy-3-(3-methyl-3-tosylbut-1-yn-1-yl)benzene (86).



The product (47.9 mg, 73% yield) as brown solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.82 (d, *J* = 8.4 Hz, 2H), 7.26 (d, *J* = 8.0 Hz, 2H), 7.13 (t, *J* = 8.0 Hz, 1H), 6.87-6.78 (m, 3H), 3.72 (s, 3H), 2.37 (s, 3H), 1.61 (s, 6H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  159.3, 145.0, 132.1, 130.9, 129.4, 129.2, 124.2, 123.0, 116.6, 115.3, 87.3, 86.3, 59.4, 55.3, 23.4, 21.7; HRMS Calculated for C<sub>19</sub>H<sub>20</sub>O<sub>3</sub>S (M+Na<sup>+</sup>): 351.1025; Found: 351.1030.





methyl 4-(3-methyl-3-tosylbut-1-yn-1-yl)benzoate (87).



The product (52.0 mg, 73% yield) as brown solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.90 (d, *J* = 8.0 Hz, 2H), 7.81 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 7.26 (d, *J* = 7.6 Hz, 2H), 3.84 (s, 3H), 2.38 (s, 3H), 1.62 (s, 6H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  166.4, 145.2, 131.9, 131.6, 130.9, 130.0, 129.5, 129.2, 126.7, 90.5, 85.5, 59.4, 52.3, 23.3, 21.7; HRMS Calculated for C<sub>20</sub>H<sub>20</sub>O<sub>4</sub>S (M+Na<sup>+</sup>): 379.0975; Found: 379.0974.



1-chloro-3-(3-methyl-3-tosylbut-1-yn-1-yl)benzene (88).



The product (49.3 mg, 74% yield) as brown solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.90 (d, *J* = 8.0 Hz, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.34-7.32 (m, 2H), 7.27-7.23 (m, 2H), 2.49 (s, 3H), 1.70 (s, 6H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  145.2, 134.2, 132.0, 131.6, 130.9, 129.8, 129.6, 129.3, 129.1, 123.7, 88.9, 84.9, 59.3, 23.3, 21.7; HRMS Calculated for C<sub>18</sub>H<sub>17</sub>ClO<sub>2</sub>S (M+Na<sup>+</sup>): 355.0530; Found: 355.0530.



<sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 88



### 3-(3-methyl-3-tosylbut-1-yn-1-yl)thiophene (89).



The product (38.4 mg, 63% yield) as brown solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 5/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.81 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 3.2 Hz, 1H), 7.26 (d, *J* = 8.0 Hz, 2H), 7.19-7.17 (m, 1H), 6.95 (d, *J* = 5.2 Hz, 1H), 2.38 (s, 3H), 1.60 (s, 6H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  145.0, 132.1, 131.0, 129.7, 129.4, 129.2, 125.5, 121.1, 87.1, 81.7, 59.4, 23.4, 21.7; HRMS Calculated for C<sub>16</sub>H<sub>16</sub>O<sub>2</sub>S<sub>2</sub> (M+Na<sup>+</sup>): 327.0484; Found: 327.0479.



f1 (ppm) 

1,3-dimethyl-3-(((2-methyl-4-phenylbut-3-yn-2-yl)sulfonyl)methyl)indolin-2-one (90).



The product (45.8 mg, 60% yield) as yellow oil was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  7.54-7.49 (m, 3H), 7.39-7.33 (m, 4H), 7.12 (t, *J* = 7.6 Hz, 1H), 6.91 (d, *J* = 7.6 Hz, 1H), 4.12 (d, *J* = 13.6 Hz, 1H), 3.75 (d, *J* = 13.6 Hz, 1H), 3.29 (s, 3H), 1.68 (d, *J* = 10.8 Hz, 6H), 1.53 (s, 3H); <sup>13</sup>**C NMR (101 MHz, CDCl<sub>3</sub>)**  $\delta$  178.1, 143.3, 132.0, 130.3, 129.0, 128.8, 128.4, 124.4, 122.5, 121.8, 108.5, 87.0, 86.5, 59.1, 52.6, 45.2, 26.7, 25.3, 23.1, 22.5; **HRMS** Calculated for C<sub>22</sub>H<sub>23</sub>NO<sub>3</sub>S (M+Na<sup>+</sup>): 404.1291; Found: 404.1295.







3-(((4-(3-methoxyphenyl)-2-methylbut-3-yn-2-yl)sulfonyl)methyl)-1,3-dimethylindolin-2-one (91).



The product (51.0 mg, 62% yield) as brown solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.39 (d, *J* = 7.2 Hz, 1H), 7.24 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.6 Hz, 1H), 7.04-6.99 (m, 3H), 6.86-6.80 (m, 2H), 4.03 (d, *J* = 13.6 Hz, 1H), 3.75 (s, 3H), 3.64 (d, *J* = 13.6 Hz, 1H), 3.18 (s, 3H), 1.57 (d, *J* = 8.8 Hz, 6H), 1.42 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.0, 159.3, 143.3, 130.3, 129.4, 128.8, 124.4, 124.3, 122.7, 122.5, 116.7, 115.8, 108.5, 86.9, 86.2, 59.1, 55.4, 52.6, 45.2, 26.7, 25.3, 23.0, 22.5; HRMS Calculated for C<sub>23</sub>H<sub>25</sub>NO<sub>4</sub>S (M+Na<sup>+</sup>): 434.1397; Found: 434.1399.



methyl 4-(3-(((1,3-dimethyl-2-oxoindolin-3-yl)methyl)sulfonyl)-3-methylbut-1-yn-1yl)benzoate (92).



The product (52.7 mg, 60% yield) as yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 1/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.94 (d, *J* = 8.0 Hz, 2H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 7.6 Hz, 1H), 7.25 (t, *J* = 7.6 Hz, 1H), 7.02 (t, *J* = 7.6 Hz, 1H), 6.82 (d, *J* = 8.0 Hz, 1H), 4.04 (d, *J* = 13.6 Hz, 1H), 3.85 (s, 3H), 3.63 (d, *J* = 13.6 Hz, 1H), 3.19 (s, 3H), 1.58 (d, *J* = 3.2 Hz, 6H), 1.43 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.0, 166.4, 143.2, 131.9, 130.2, 129.5, 128.9, 126.3, 124.3, 122.5, 108.5, 89.3, 86.2, 59.1, 52.7, 52.3, 45.2, 26.6, 25.2, 22.7, 22.6; HRMS Calculated for C<sub>24</sub>H<sub>25</sub>NO<sub>5</sub>S (M+Na<sup>+</sup>): 462.1346; Found: 462.1349.







3-(((4-(3-chlorophenyl)-2-methylbut-3-yn-2-yl)sulfonyl)methyl)-1,3-dimethylindolin-2-one (93).



The product (52.4 mg, 63% yield) as brown solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.42 – 7.39 (m, 2H), 7.34 – 7.32 (m, 1H), 7.28 – 7.18 (m, 3H), 7.03 (t, *J* = 7.6 Hz, 1H), 6.82 (d, *J* = 7.6 Hz, 1H), 4.02 (d, *J* = 13.6 Hz, 1H), 3.62 (d, *J* = 13.6 Hz, 1H), 3.19 (s, 3H), 1.57 (d, *J* = 6.0 Hz, 6H), 1.43 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.0, 143.3, 134.2, 131.8, 130.2, 130.1, 129.6, 129.3, 128.9, 124.3, 123.4, 122.6, 108.5, 87.7, 85.6, 59.1, 52.7, 45.2, 26.7, 25.3, 22.8, 22.6; HRMS Calculated for C<sub>22</sub>H<sub>22</sub>CINO<sub>3</sub>S (M+Na<sup>+</sup>): 438.0901; Found: 438.0909.





1,3-dimethyl-3-(((2-methyl-4-(thiophen-3-yl)but-3-yn-2-yl)sulfonyl)methyl)indolin-2-one (94).



The product (42.6 mg, 55% yield) as brown oil was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.52 (dd, *J* = 3.2 Hz, 1.2 Hz, 1H), 7.40 (d, *J* = 6.8 Hz, 1H), 7.25-7.21 (m, 2H), 7.11 (dd, *J* = 4.8 Hz, 0.8 Hz, 1H), 7.03 (t, *J* = 7.6 Hz, 1H), 6.82 (d, *J* = 7.6 Hz, 1H), 4.04 (d, *J* = 13.6 Hz, 1H), 3.63 (d, *J* = 14.0 Hz, 1H), 3.19 (s, 3H), 1.56 (d, *J* = 6.0 Hz, 6H), 1.43 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.1, 143.3, 130.3, 130.2, 130.0, 128.9, 125.5, 124.4, 122.5, 120.8, 108.5, 86.1, 82.3, 59.2, 52.6, 45.2, 26.7, 25.3, 22.9, 22.6; HRMS Calculated for C<sub>20</sub>H<sub>21</sub>NO<sub>3</sub>S<sub>2</sub> (M+Na<sup>+</sup>): 410.0855; Found: 410.0855.





(E)-3-(((3-(4-bromophenyl)allyl)sulfonyl)methyl)-1,3-dimethylindolin-2-one (97).



The product (1.4 g, 80% yield) as light yellow solid was purified with silica gel chromatography (petroleum ether/ethyl acetate = 2/1). <sup>1</sup>**H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  7.41 – 7.37 (m, 2H), 7.30 – 7.26 (m, 2H), 7.21 – 7.17 (m, 2H), 7.05 (t, *J* = 7.6 Hz, 1H), 6.84 (d, *J* = 7.6 Hz, 1H), 6.52 (d, *J* = 16.0 Hz, 1H), 6.11 – 6.03 (m, 1H), 3.63 – 3.58 (m, 2H), 3.51 – 3.42 (m, 2H), 3.19 (s, 3H), 1.38 (s, 3H); <sup>13</sup>**C NMR (101 MHz, CDCl<sub>3</sub>)**  $\delta$  177.9, 143.4, 138.0, 134.5, 131.9, 130.4, 129.1, 128.3, 123.5, 122.7, 115.9, 108.8, 59.4, 57.3, 45.6, 26.7, 25.0; **HRMS** Calculated for C<sub>20</sub>H<sub>20</sub>BrNO<sub>3</sub>S (M+Na<sup>+</sup>): 456.0239; Found: 456.0246.



