

Supporting Information

Catalytic asymmetric oxidative carbonylation –induced kinetic resolution of sterically hindered benzylamines to chiral isoindolinones

Qiu-Qi Mu^{‡a,b,c}, Yi-Xue Nie^{‡b}, Hang Li^{‡b}, Xing-Feng Bai^{*b,c}, Xue-Wei Liu^{a,d},
Zheng Xu^b, and Li-Wen Xu^{*b,c}

^a *Institute of Advanced Synthesis (IAS), Northwestern Polytechnical University (NPU), Xi'an 710072, China. Yangtze River Delta Research Institute of NPU, Taicang Jiangsu, 215400, China.*

^b *Key Laboratory of Organosilicon Chemistry and Material Technology of Ministry of Education, and Key Laboratory of Organosilicon Material Technology of Zhejiang Province, Hangzhou Normal University, Hangzhou 311121, P. R. China*

^c *State Key Laboratory for Oxo Synthesis and Selective Oxidation, Suzhou Research Institute (SRI), Lanzhou Institute of Chemical Physics (LICP), University of the Chinese Academy of Sciences (UCAS), Lanzhou 730000, P. R. China*

^e *Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371*

*liwenxu@hznu.edu.cn, xuewei@ntu.edu.sg

‡ (Q.-Q. Mu, Y.-X. Nie) *These authors contributed equally.*

Table of Contents

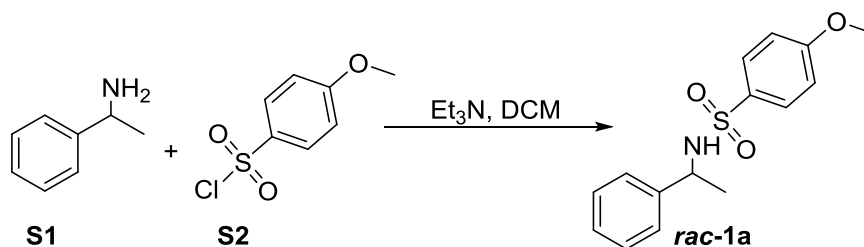
1. General Considerations	S2
2. Experimental procedures and Compound characterizations	S3
2.1 General procedure for the preparation of <i>rac</i> -1a-k and characterization data ...	S3
2.2 Kinetic resolution of Benzylamines and characterization data	S10
3. Computational studies	S25
4. X-ray structure of (<i>S</i>)-2h	S52
5. Reference	S52
6. NMR Spectra	S53
7. HPLC Chromatograms	S75

1. General Considerations

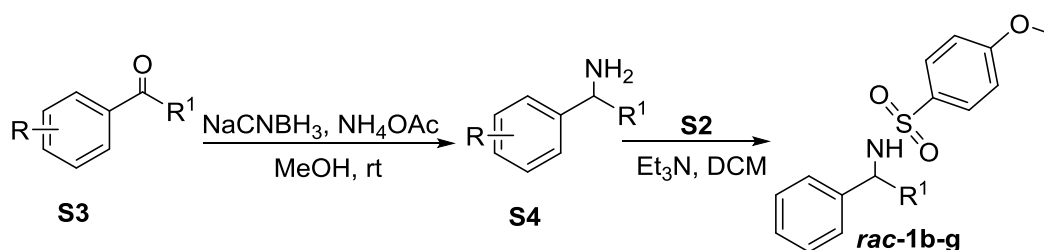
Unless specifically stated, all commercial materials and solvents were used without further purification. Reactions were monitored by thin layer chromatography (TLC) using silica gel plates. Flash column chromatography was performed over silica (300 - 400 mesh). Nuclear magnetic resonance (NMR) spectra were recorded with Bruker 400 MHz spectrometer. ^1H and ^{13}C chemical shifts are reported in ppm downfield of tetramethylsilane and referenced to residual solvent peak (CDCl_3 , $\delta\text{H} = 7.26$ and $\delta\text{C} = 77.16$). Multiplicities were given as: s (singlet); d (doublet); dd (doublets of doublet); t (triplet); q (quartet); or m (multiplets). High resolution mass spectra (HRMS) of the products were obtained on a Bruker Daltonics micro TOF-spectrometer. Enantiomeric excesses were determined on an Agilent 1260 Chiral HPLC using AD, OD columns. Optical rotations were obtained on a SGW-3 polarimeter. Computational study was conducted using Gauss 09 with B3LYP and the LANL2DZ basis set for Pd and Cs, 6-31G(d,p) basis set for other atoms. Activation free energies are given in kcal/mol. Infrared spectra (FT-IR) were recorded using a BRUKER VERTEX 70 Spectrometer and analyzed as thin films, with absorption maxima (ν_{max}) being quoted in wavenumbers (cm^{-1}); Melting points (m.p.) were recorded using a JM 628 X-4 melting point apparatus.

2. Experimental procedures and Compound characterizations

2.1 General procedure for the preparation of *rac*-1a-k and characterization data



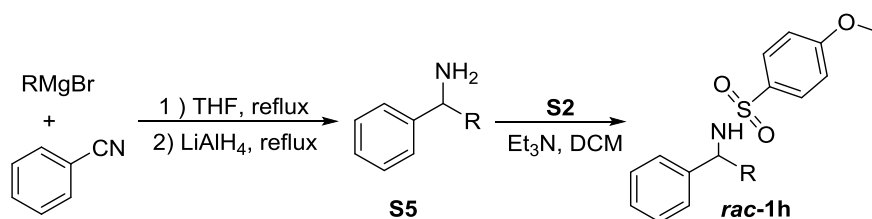
Procedure A: synthesis of *rac*-1a. Following a literature procedure^[1]. To a solution of **S1** phenylethylamine (5 mmol, 1.0 equiv.) and triethylamine (7.5 mmol, 1.5 equiv.) in CH₂Cl₂ (30 mL) at 0 °C was added drop wise a solution of the corresponding **S2** sulfonyl chloride (6 mmol, 1.2 equiv) in CH₂Cl₂ (10 mL). The resulting solution was stirred at room temperature for overnight. Water (50 mL) was added, and the aqueous layer was extracted with dichloromethane (3 × 20 mL). The combined organic layer was dried (Na₂SO₄) and concentrated, the product *rac*-1a was obtained through chromatography.



Procedure B: synthesis of *rac*-1b-g. Following a literature procedure^[2,3]. **S3** Ketone (10 mmol, 1.0 equiv), ammonium acetate (60 mmol, 6.0 equiv) and sodium cyanoborohydride (NaCNBH₃) (15 mmol, 1.5 equiv) were dissolved in MeOH (30 mL) and the solution was stirred at room temperature for overnight. After removing the solvents in vacuo, the residue was dissolved in 4M NaOH (50 mL) and extracted with CH₂Cl₂ (3×30 mL). The combined layers were concentrated and extracted with 6M HCl (3×30 mL). The aqueous layer was basified with concentrated NaOH and extracted with CH₂Cl₂ (3×30 mL). The combined organic layers were dried over anhydrous Na₂SO₄ and evaporated under reduced pressured to give crude amine **S4**,

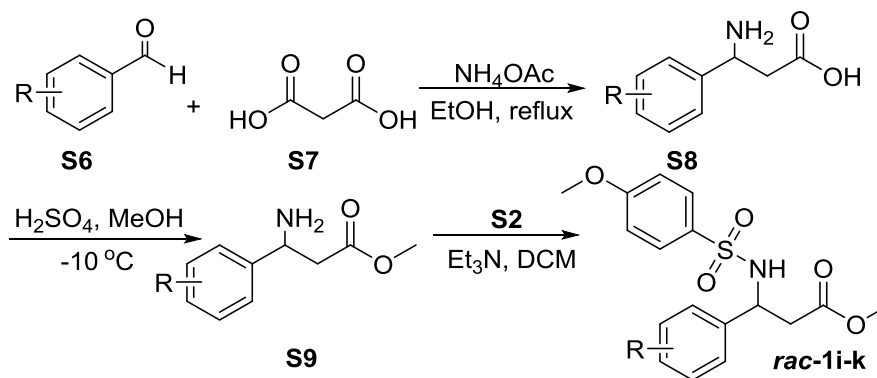
which could be used directly in the next step without further purification.

To a solution of crude amine **S4** and triethylamine (1.5 equiv.) in CH₂Cl₂ (30 mL) at 0 °C was added drop wise a solution of the corresponding **S2** sulfonyl chloride (1.2 equiv) in CH₂Cl₂ (10 mL). The resulting solution was stirred at room temperature for overnight. Water (50 mL) was added, and the aqueous layer was extracted with CH₂Cl₂ (3 × 20 mL). The combined organic layer was dried (Na₂SO₄) and concentrated, the product **rac-1b-g** was obtained through chromatography.



Procedure C: synthesis of **rac-1g**. Following a literature procedure ^[4,5]. To a flame-dried 100 mL three-necked round-bottomed flask, aryl nitrile (10 mmol, 1.0 equiv.) and THF (20 mL) was added. Fill the flask with argon and equip with a refluxing condenser. Cool down the solution to 0 °C and then add the corresponding Grignard reagent (12 mmol, 1.2 equiv.) slowly. The reaction mixture was heated to reflux for 24 h and then cooled to 0 °C. To this mixture was transferred a suspension of LiAlH₄ (10 mmol, 1.0 equiv) in THF (20 mL) and heated to reflux, which was maintained for 12 h. The reaction mixture was cooled to 0 °C, and carefully quenched by slow addition of water (1 mL), then 10 % aq NaOH (1 mL), and finally water (2 mL). The mixture was filtered through a Celite pad and washed with DCM. The combined organic layer was washed with brine and dried over Na₂SO₄, filtered and concentrated under reduce pressure to afford crude amine **S5**, which could be used directly in the next step without further purification.

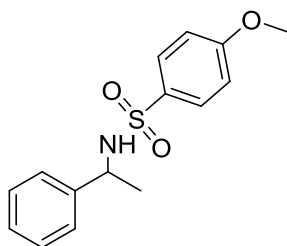
To a solution of crude amine **S5** and triethylamine (1.5 equiv.) in CH₂Cl₂ (30 mL) at 0 °C was added drop wise a solution of the corresponding **S2** sulfonyl chloride (1.2 equiv) in CH₂Cl₂ (10 mL). The resulting solution was stirred at room temperature for overnight. Water (50 mL) was added, and the aqueous layer was extracted with CH₂Cl₂ (3 × 20 mL). The combined organic layer was dried (Na₂SO₄) and concentrated, the product **rac-1h** was obtained through chromatography.



Procedure D: synthesis of *rac-1i-1k*. Following a literature procedure^[6]. In a 50 mL round bottom flask, benzaldehyde **S6** (10 mmol, 1.0 equiv) was dissolved in ethanol (10 mL). Malonic acid **S7** (10 mmol, 1.0 equiv) and ammonium acetate (20 mmol, 2.0 equiv) were added to the reaction and the resulting mixture was reflux for overnight. After stirring overnight, the reaction mixture was allowed to cool to room temperature and the resulting solid was filtered. The solid was washed with methanol and dried in vacuo to give the intermediate **S8**.

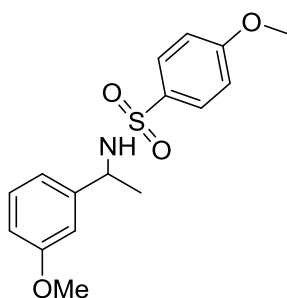
S8 was added to a round bottom flask followed by addition of methanol. The reaction mixture was cooled to $-10\text{ }^\circ\text{C}$ followed by the addition of conc. sulfuric acid (0.4 mL) in one portion. The reaction mixture was stirred at room temperature for 6 h and concentrated in vacuo. The reaction mixture was treated with sodium hydroxide solution (2.0 M) and extracted with CH_2Cl_2 ($3 \times 20\text{ mL}$). The combined organic phase was dried over Na_2SO_4 and concentrated in vacuo to give the product **S9**, which could be used directly in the next step without further purification.

To a solution of crude amine **S9** and triethylamine (1.5 equiv.) in CH_2Cl_2 (30 mL) at $0\text{ }^\circ\text{C}$ was added drop wise a solution of the corresponding **S2** sulfonyl chloride (1.2 equiv) in CH_2Cl_2 (10 mL). The resulting solution was stirred at room temperature for overnight. Water (50 mL) was added, and the aqueous layer was extracted with CH_2Cl_2 ($3 \times 20\text{ mL}$). The combined organic layer was dried (Na_2SO_4) and concentrated, the product *rac-1i-k* were obtained through chromatography.



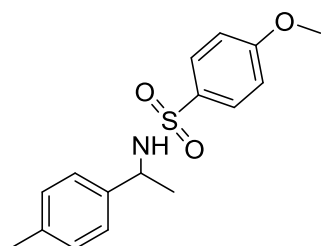
4-methoxy-*N*-(1-phenylethyl)benzenesulfonamide (*rac*-1a)^[7]

White solid, 1.25 g, 85% yield. Analytical data for **1a**: ¹H NMR (400 MHz, CDCl₃) δ 7.66 (d, *J* = 8.0 Hz, 2H), 7.19 (t, *J* = 8.0, 4.0 Hz, 3H), 7.11 (d, *J* = 4.0 Hz, 2H), 6.84 (d, *J* = 8.0 Hz, 2H), 5.00 (s, 1H), 4.48-4.41 (m, 1H), 3.82 (s, 3H), 1.42 (d, *J* = 4.0 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 162.6, 142.1, 132.3, 129.1, 128.5, 127.4, 126.1, 113.9, 55.5, 53.6, 23.5. HRMS (ESI-TOF) Calcd for C₁₅H₁₇NNaO₃S [M+Na]⁺: 314.0821, found: 314.0829.



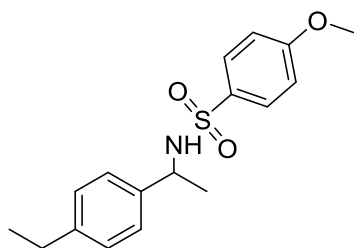
4-methoxy-*N*-(1-(3-methoxyphenyl)ethyl)benzenesulfonamide (*rac*-1b)

White solid, 65% yield, mp: 95-98 °C. Analytical data for **1b**: ¹H NMR (400 MHz, CDCl₃) δ 7.66 (d, *J* = 8.0 Hz, 2H), 7.09 (d, *J* = 4.0, 1H), 6.83-6.81 (t, *J* = 4.0 Hz, 2H), 6.70-6.68 (m, 2H), 6.60 (t, *J* = 4.0 Hz, 1H), 5.34 (d, *J* = 8.0, 1H), 4.44-4.37 (m, 1H), 3.82 (s, 3H), 3.69 (s, 3H), 1.40 (d, *J* = 4.0 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 162.8, 159.8, 143.9, 132.4, 129.7, 129.4, 118.6, 114.1, 113.1, 111.9, 55.8, 55.3, 53.8, 23.8. HRMS (ESI-TOF) Calcd for C₁₆H₁₉NNaO₄S [M+Na]⁺: 344.0927, found: 344.0937.



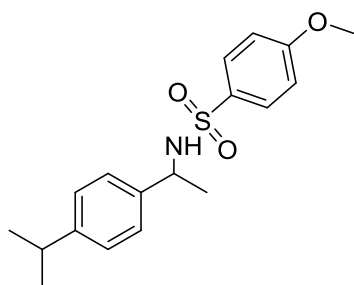
4-methoxy-*N*-(1-(*p*-tolyl)ethyl)benzenesulfonamide (*rac*-1c)

White solid, 70% yield. mp: 92-95 °C. Analytical data for **1c**: ¹H NMR (400 MHz, CDCl₃) δ 7.72-7.69 (m, 2H), 7.03 (s, 4H), 6.88-6.85 (m, 2H), 5.45 (d, *J* = 4.0 Hz, 1H), 4.46-4.39 (m, 1H), 3.86 (s, 3H), 2.30 (s, 3H), 1.44 (d, *J* = 8.0 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 162.6, 139.2, 137.0, 132.3, 129.2, 129.1, 126.1, 113.9, 55.5, 53.4, 23.5, 21.0. HRMS (ESI-TOF) Calcd for C₁₆H₁₉NNaO₃S [M+Na]⁺: 328.0978, found: 328.0989.



***N*-(1-(4-ethylphenyl)ethyl)-4-methoxybenzenesulfonamide (*rac*-1d)**

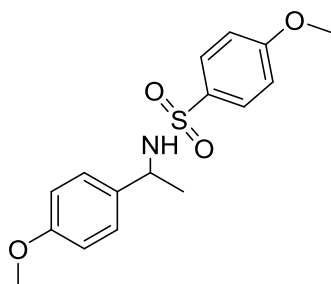
White solid, 75% yield, mp: 81-84 °C. Analytical data for **1d**: ¹H NMR (400 MHz, CDCl₃) δ 7.66-7.64 (m, 2H), 7.00 (s, 4H), 6.83-6.80 (m, 2H), 5.34 (d, *J* = 8.0 Hz, 1H), 4.43-4.40 (t, *J* = 8.0, 4.0 Hz, 1H), 3.82 (s, 3H), 2.59-2.53 (m, 2H), 1.41 (d, *J* = 8.0 Hz, 3H), 1.20 (t, *J* = 8.0 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 162.7, 143.6, 139.5, 132.5, 129.4, 128.1, 126.3, 114.1, 55.7, 53.6, 28.6, 23.7, 15.8. HRMS (ESI-TOF) Calcd for C₁₇H₂₁NNaO₃S [M+Na]⁺: 342.1134, found: 342.1149.



***N*-(1-(4-isopropylphenyl)ethyl)-4-methoxybenzenesulfonamide (*rac*-1e)**

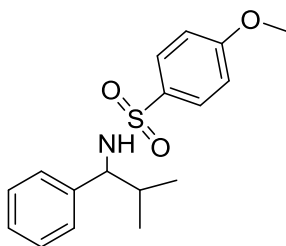
White solid, 55% yield, mp: 74-77 °C. Analytical data for **1d**: ¹H NMR (400 MHz, CDCl₃) δ 7.65-7.63 (m, 2H), 7.04-7.00 (m, 4H), 6.82-6.80 (m, 2H), 5.20 (s, 1H), 4.46-4.39 (m, 1H), 3.82 (s, 3H), 2.85-2.78 (m, 1H), 1.42 (d, *J* = 8.0 Hz, 3H), 1.20 (s, 3H), 1.18 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 162.5, 148.0, 139.3, 132.3, 129.2, 126.4, 126.1, 113.8, 55.5, 53.4, 33.7, 23.9, 23.5. HRMS (ESI-TOF) Calcd for

C₁₈H₂₃NNaO₃S [M+Na]⁺: 356.1291, found: 356.1304.



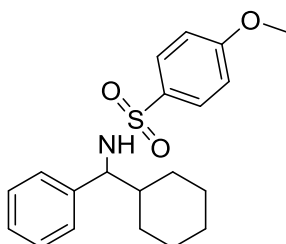
4-methoxy-N-(1-(4-methoxyphenyl)ethyl)benzenesulfonamide (*rac*-1f)

White solid, 53% yield, mp: 114-117 °C. Analytical data for **1f**: ¹H NMR (400 MHz, CDCl₃) δ 7.66-7.63 (m, 2H), 7.02 (t, *J* = 8.0, 4.0 Hz, 2H), 6.85-6.82 (m, 2H), 6.73-6.69 (m, 2H), 4.99 (d, *J* = 8.0 Hz, 1H), 4.41 (t, *J* = 8.0 Hz, 1H), 3.83 (s, 3H), 3.74 (s, 3H), 1.40 (d, *J* = 4.0 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 163.1, 159.4, 134.7, 132.8, 129.7, 127.8, 114.4, 114.4 (d, *J* = 9.0 Hz), 56.1, 55.8, 53.6, 24.0. HRMS (ESI-TOF) Calcd for C₁₆H₁₉NNaO₄S [M+Na]⁺: 344.0927, found: 344.0936.



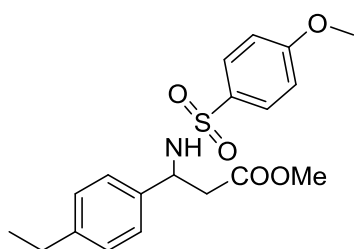
4-methoxy-N-(2-methyl-1-phenylpropyl)benzenesulfonamide (*rac*-1g)

White solid, 79% yield, mp: 117-120 °C. Analytical data for **1g**: ¹H NMR (400 MHz, CDCl₃) δ 7.59-7.55 (m, 2H), 7.13-7.12 (m, 3H), 6.98-6.96 (m, 2H), 6.75 (t, *J* = 8.0, 4.0 Hz, 2H), 5.57 (d, *J* = 12.0 Hz, 1H), 4.05 (t, *J* = 8.0 Hz, 1H), 3.81 (s, 3H), 1.99-1.90 (m, 1H), 0.99 (d, *J* = 8.0 Hz, 3H), 0.76 (d, *J* = 8.0 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 162.6, 140.2, 132.5, 129.3, 128.3, 127.2, 127.2, 113.9, 64.4, 55.7, 34.6, 19.6, 19.1. HRMS (ESI-TOF) Calcd for C₁₇H₂₁NNaO₃S [M+Na]⁺: 342.1134, found: 342.1133.



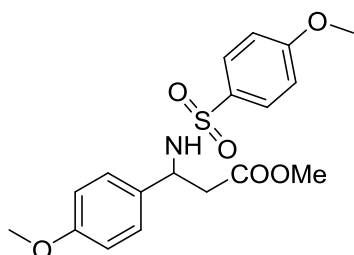
***N*-(cyclohexyl (phenyl)methyl)-4-methoxybenzenesulfonamid (*rac*-1h)**

White solid, 68% yield, mp: 153-156 °C. Analytical data for **1h**: ¹H NMR (400 MHz, CDCl₃) δ 7.54-7.50 (m, 2H), 7.10-7.06 (m, 3H), 6.93-6.90 (m, 2H), 6.71-6.67 (m, 2H), 5.58 (d, *J* = 12.0 Hz, 1H), 4.02 (t, *J* = 8.0 Hz, 1H), 3.98 (s, 3H), 1.98 (d, *J* = 12.0 Hz, 1H), 1.72 (t, *J* = 12.0 Hz, 1H), 1.58-1.50 (m, 3H), 1.28 (d, *J* = 12.0 Hz, 1H), 1.16-1.03 (m, 3H), 0.98-0.82 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 162.5, 140.2, 132.6, 129.3, 128.3, 127.2, 127.1, 113.9, 63.7, 55.7, 43.9, 30.0, 29.7, 26.4, 26.1. HRMS (ESI-TOF) Calcd for C₂₀H₂₅NNaO₃S [M+Na]⁺: 382.1447, found: 382.1437.



Methyl 3-(4-ethylphenyl)-3-((4-methoxyphenyl)sulfonamide)propanoate (*rac*-1i)

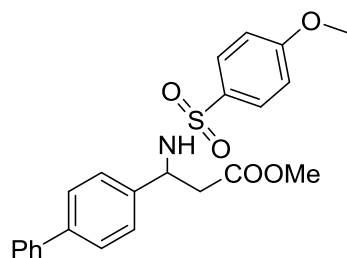
White solid, 45% yield, mp: 86-89 °C. Analytical data for **1i**: ¹H NMR (400 MHz, CDCl₃) δ 7.65-7.61 (m, 2H), 7.00 (s, 4H), 6.84-6.81 (m, 2H), 5.70 (d, *J* = 8.0 Hz, 1H), 4.71 (m, 1H), 3.82 (s, 3H), 3.57 (s, 3H), 2.89 (dd, *J* = 16.0, 8.0 Hz, 1H), 2.79 (dd, *J* = 16.0, 8.0 Hz, 1H), 2.59 (q, *J* = 8.0 Hz, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 171.1, 162.6, 143.8, 136.5, 131.9, 129.2, 128.0, 126.4, 113.9, 55.5, 54.1, 51.9, 41.1, 28.4, 15.5. HRMS (ESI-TOF) Calcd for C₁₉H₂₃NNaO₅S [M+Na]⁺: 400.1189, found: 400.1178.



Methyl 3-(4-methoxyphenyl)-3-((4-methoxyphenyl)sulfonamide)propanoate (*rac*-1j)

White solid, 49% yield, mp: 94-97 °C. Analytical data for **1j**: ¹H NMR (400 MHz, CDCl₃) δ 7.65-7.61 (m, 2H), 7.02 (d, *J* = 8.0 Hz, 2H), 6.84-6.82 (m, 2H), 6.71-6.69

(m, 2H), 5.74 (d, $J = 8.0$ Hz, 1H), 4.69-4.64 (m, 1H), 3.83 (s, 3H), 3.74 (s, 3H), 3.56 (s, 3H), 2.88 (dd, $J = 16.0, 8.0$ Hz, 1H), 2.77 (dd, $J = 16.0, 8.0$ Hz, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 171.2, 162.7, 159.1, 132.0, 131.4, 129.3, 127.7, 114.0, 113.9, 55.6, 55.2, 53.9, 51.9, 41.3. HRMS (ESI-TOF) Calcd for $\text{C}_{18}\text{H}_{21}\text{NNaO}_6\text{S}$ $[\text{M}+\text{Na}]^+$: 402.0982, found: 402.0991.



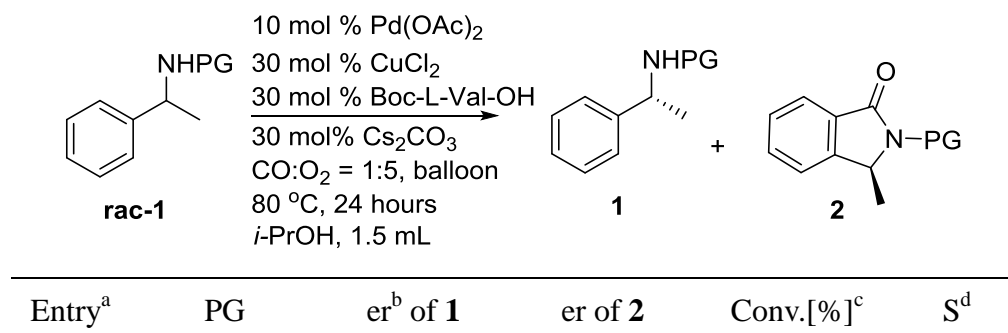
Methyl 3-((1,1'-biphenyl)-4-yl)-3-((4-methoxyphenyl)sulfonamide)propanoate (*rac*-1k)

White solid, 51% yield, mp: 152-155 °C. Analytical data for **1k**: ^1H NMR (400 MHz, CDCl_3) δ 7.64-7.62 (m, 2H), 7.52-7.49 (m, 2H), 7.44-7.32 (m, 5H), 7.17 (d, $J = 8.0$ Hz, 2H), 6.81-6.79 (m, 2H), 5.85 (d, $J = 8.0$ Hz, 1H), 4.81 (q, $J = 8.0$ Hz, 1H), 3.74 (s, 3H), 3.59 (s, 3H), 2.92 (dd, $J = 16.0, 4.0$ Hz, 1H), 2.84 (dd, $J = 16.0, 8.0$ Hz, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 171.1, 162.7, 140.6, 140.4, 138.2, 133.8, 131.9, 129.2, 128.8, 127.4, 127.2, 127.0, 126.9, 115.1, 113.9, 55.5, 54.1, 52.0, 41.0. HRMS (ESI-TOF) Calcd for $\text{C}_{23}\text{H}_{23}\text{NNaO}_5\text{S}$ $[\text{M}+\text{Na}]^+$: 448.1189, found: 448.1175.

2.2 Kinetic resolution of Benzylamines and characterization data

Optimization of reaction conditions

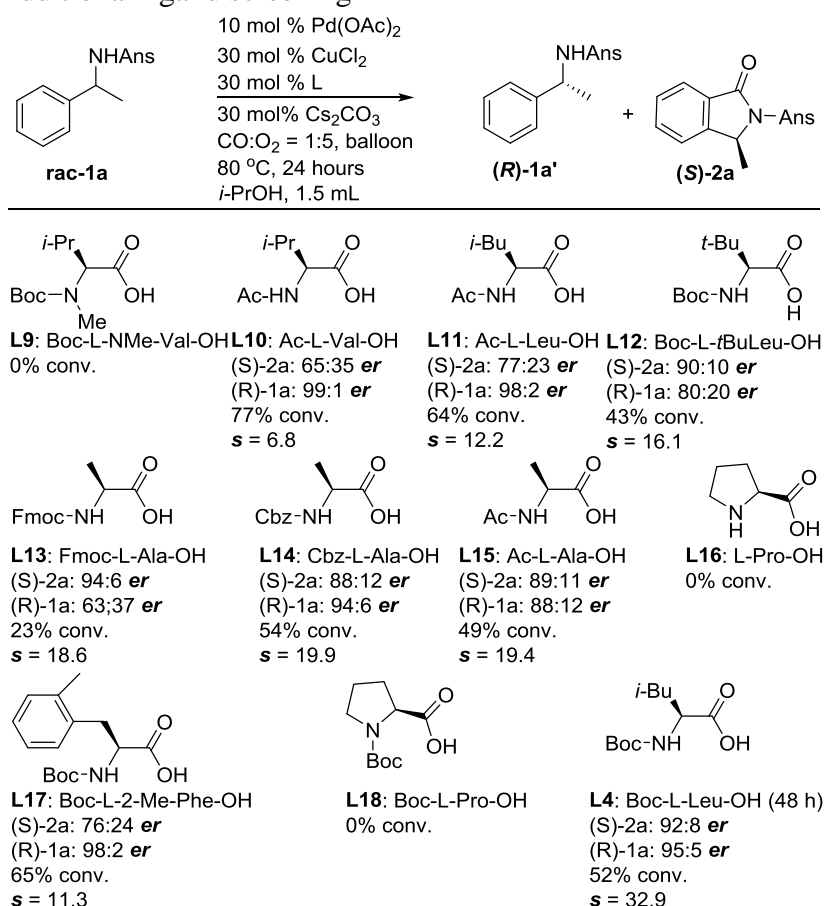
Table S1. Screening of Protecting groups ^a



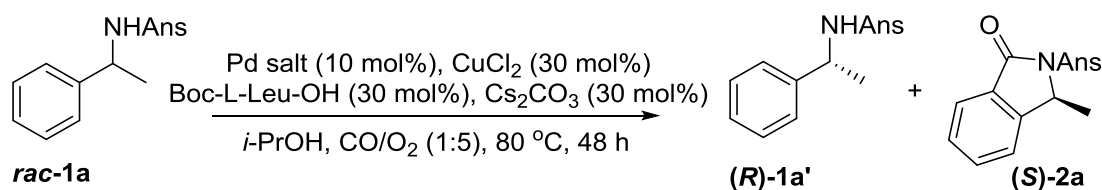
1	Ms	93:7	90:10	52	23.8
2 ^f	Ans	91:9	92:8	49	32.1
3 ^g	Ns	82:18	88:12	46	13.5
4	Tf	70:30	90:10	33	14.2
5	Boc	-	-	N.D. ^e	-
6	Ts	95:5	87:13	55	19.8

^aReaction conditions: **rac-1** (0.1 mmol), Pd(OAc)₂ (10 mmol%), CuCl₂ (30 mmol%), Boc-L-Val-OH (30 mmol%), Cs₂CO₃ (30 mmol%), CO/O₂=1:5 (1 atm), *i*-PrOH (1.0 mL), 80 °C, 48 h. ^bDetermined by HPLC analysis on a chiral stationary phase. ^cDetermined by HPLC analysis on a chiral stationary phase. Conversion (C) = ee₁/(ee₁+ee₂), where ee₁ is the enantiomeric excess of the recovered **1** and ee₂ is the enantiomeric excess of **2**. ^ds = ln[(1-C)(1-ee)]/ln[(1-C)(1+ee)], where ee = ee₁/100 and C = conversion/100. s = selectivity factor. ^eN.D.= not determined. ^fAns = 4-methoxybenzenesulfonamide. ^gNs = 4-nitrobenzenesulfonamide.

Table S2. Additional ligand screening^a

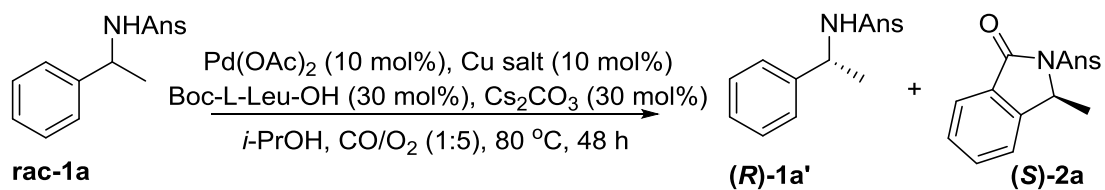


^aReaction conditions: **rac-1** (0.1 mmol), Pd(OAc)₂ (10 mmol%), CuCl₂ (30 mmol%), Ligand (30 mmol%), Cs₂CO₃ (30 mmol%), CO/O₂=1:5 (1 atm), *i*-PrOH (1.0 mL), 80 °C, 48 h. ^bDetermined by HPLC analysis on a chiral stationary phase. ^cDetermined by HPLC analysis on a chiral stationary phase. Conversion (C) = ee₁/(ee₁+ee₂), where ee₁ is the enantiomeric excess of the recovered **1** and ee₂ is the enantiomeric excess of **2**. ^ds = ln[(1-C)(1-ee)]/ln[(1-C)(1+ee)], where ee = ee₁/100 and C = conversion/100. s = selectivity factor.

Table S3. Screening of Pd catalyst ^a

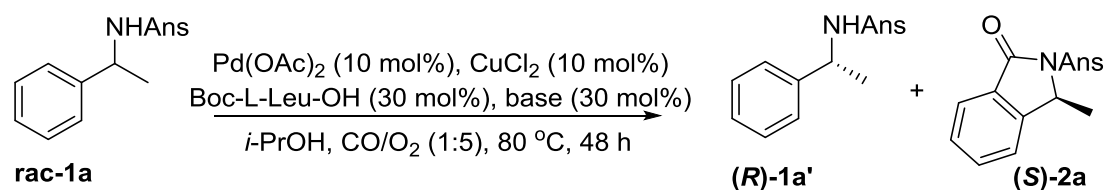
Entry ^a	Pd salt	Er [%] ^b		Conv.[%] ^c	s ^d
		1a'	2a		
1	PdCl ₂	-	-	0	-
2	Pd(TFA) ₂	-	-	0	-
3	Pd(CH ₃ CN) ₂ Cl ₂	52:48	94:6	4	51

^aReaction conditions: **rac-1a** (0.1 mmol), Pd salt (10 mmol%), CuCl₂ (30 mmol%), Boc-L-Leu-OH (30 mmol%), Cs₂CO₃ (30 mmol%), CO/O₂=1:5 (1 atm), *i*-PrOH (1.0 mL), 80 °C, 48 h. ^bDetermined by HPLC analysis on a chiral stationary phase. ^cDetermined by HPLC analysis on a chiral stationary phase. Conversion (*C*) = $ee_1/(ee_1+ee_2)$, where ee_1 is the enantiomeric excess of the recovered **1a'** and ee_2 is the enantiomeric excess of **2a**. ^d $s = \ln[(1-C)(1-ee)]/\ln[(1-C)(1+ee)]$, where $ee = ee_1/100$ and $C = \text{conversion}/100$. *s* = selectivity factor.

Table S4. Screening of Cu salts^a

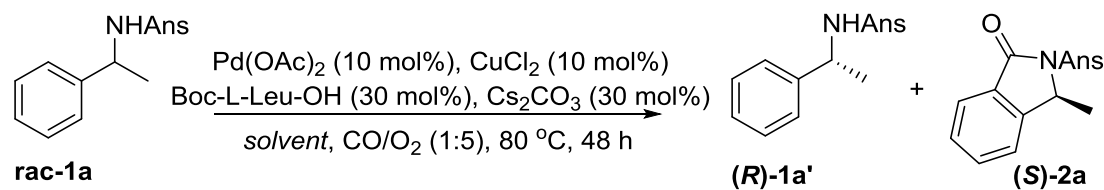
Entry ^a	Cu salt	Er [%] ^b		Conv.[%] ^c	s ^d
		1a	2a		
1	Cu(OAc) ₂	68:32	87:13	33	9.1
2	Cu(TFA) ₂ ·XH ₂ O	62:38	91:9	23	11.6
3	Cu(OTf) ₂	56:44	89:11	13	10.3

^aReaction conditions: **rac-1a** (0.1 mmol), Pd(OAc)₂ (10 mmol%), Cu salt (30 mmol%), Boc-L-Leu-OH (30 mmol%), Cs₂CO₃ (30 mmol%), CO/O₂=1:5 (1 atm), *i*-PrOH (1.0 mL), 80 °C, 48 h. ^bDetermined by HPLC analysis on a chiral stationary phase. ^cDetermined by HPLC analysis on a chiral stationary phase. Conversion (*C*) = $ee_1/(ee_1+ee_2)$, where ee_1 is the enantiomeric excess of the recovered **1a'** and ee_2 is the enantiomeric excess of **2a**. ^d $s = \ln[(1-C)(1-ee)]/\ln[(1-C)(1+ee)]$, where $ee = ee_1/100$ and $C = \text{conversion}/100$. *s* = selectivity factor.

Table S5. Screening of base^a

Entry ^a	Base	Er [%] ^b		Conv.[%] ^c	<i>s</i> ^d
		1a	2a		
1	K_2CO_3	83:17	94:6	43	29.7
2	CsPivO	-	-	0	-
3	Ag_2CO_3	-	-	0	-

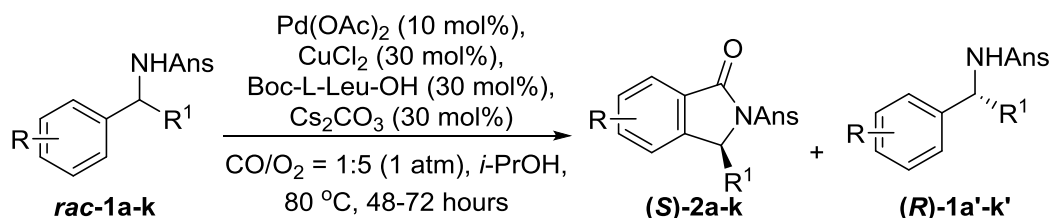
^aReaction conditions: **rac-1a** (0.1 mmol), $\text{Pd}(\text{OAc})_2$ (10 mmol%), CuCl_2 (30 mmol%), Boc-L-Leu-OH (30 mmol%), base (30 mmol%), $\text{CO}/\text{O}_2=1:5$ (1 atm), *i*-PrOH (1.0 mL), 80 °C, 48 h. ^bDetermined by HPLC analysis on a chiral stationary phase. ^cDetermined by HPLC analysis on a chiral stationary phase. Conversion (*C*) = $ee_1/(ee_1+ee_2)$, where ee_1 is the enantiomeric excess of the recovered **1a'** and ee_2 is the enantiomeric excess of **2a**. ^d $s = \ln[(1-C)(1-ee)]/\ln[(1-C)(1+ee)]$, where $ee = ee_1/100$ and *C* = conversion/100. *s* = selectivity factor.

Table S6. Screening of solvent^a

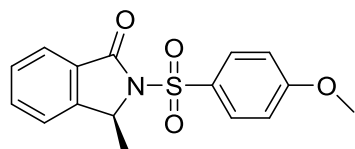
Entry ^a	solvent	Er [%] ^b		Conv.[%] ^c	<i>s</i> ^d
		1a	2a		
1	CH_3CN	61:39	79:21	28	4.5
2	DCE	51:49	57:43	13	1.3
3	dioxane	53:47	72:28	12	2.7
4	HFIP	-	-	0	-
5	TFE	-	-	0	-

^aReaction conditions: **rac-1a** (0.1 mmol), $\text{Pd}(\text{OAc})_2$ (10 mmol%), CuCl_2 (30 mmol%), Boc-L-Leu-OH (30 mmol%), Cs_2CO_3 (30 mmol%), $\text{CO}/\text{O}_2=1:5$ (1 atm), solvent (1.0 mL), 80 °C, 48 h. ^bDetermined by HPLC analysis on a chiral stationary phase. ^cDetermined by HPLC analysis on a chiral stationary phase. Conversion (*C*) = $ee_1/(ee_1+ee_2)$, where ee_1 is the enantiomeric excess of the recovered **1a'** and ee_2 is the enantiomeric excess of **2a**. ^d $s = \ln[(1-C)(1-ee)]/\ln[(1-C)(1+ee)]$, where $ee = ee_1/100$ and *C* = conversion/100. *s* = selectivity factor.

Kinetic resolution of benzylamines via Pd/Cu-cocatalyzed C-H amine carbonylation

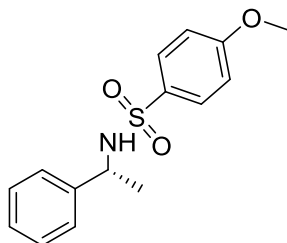


To a 25 mL reaction tube, **rac-1a-k** (0.2 mmol, 1.0 equiv.), Pd(OAc)_2 (10 mol%), Boc-L-Leu-OH (30 mol%), CuCl_2 (30 mol%) and Cs_2CO_3 (30 mol%) were added. Evacuated the reaction tube and refilled it with the CO/O_2 gas mixture through the balloon and then *i*-PrOH (3 mL) was added. The resulting solution was heated to 80 °C for 48-72 hours. After the reaction finished, cool down the mixture to room temperature and release the CO/O_2 gas mixture carefully in the fume hood. The reaction mixture was passed through a short column of silica gel and eluted with EtOAc (50 ml), the eluent was concentrated under vacuum. The resulting residue was purified by column chromatography to give the desired product. The ee value was determined on a Agilent Technologies HPLC system using commercially available chiral columns as described below.

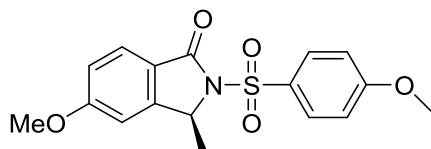


(S)-2-((4-methoxyphenyl)sulfonyl)-3-methylisoindolin-1-one (2a). Following the general procedure, the product was isolated by column chromatography with petroleum ether/EA (10 : 1) as the eluent to give a semi-solid. ^1H NMR (400 MHz, CDCl_3) δ 8.12 (d, $J = 8.0$ Hz, 2H), 7.80 (d, $J = 8.0$ Hz, 1H), 7.67 (t, $J = 4.0, 8.0$ Hz, 1H), 7.49-7.43 (m, 2H), 7.01 (d, $J = 8.0$ Hz, 2H), 5.34-5.29 (m, 1H), 3.87 (s, 3H), 1.81 (d, $J = 8.0$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 166.3, 163.8, 147.4 (d, $J = 3.6$ Hz), 134.0, 130.6, 130.5, 128.9, 128.7, 124.9, 122.1, 58.6, 55.6, 21.4. IR (neat) 2918, 2849, 1720, 1465, 1355, 1260, 1183, 1160, 1107, 1087, 1024, 832, 803, 789, 757 cm^{-1} . HRMS (ESI-TOF) Calcd for $\text{C}_{16}\text{H}_{15}\text{NNaO}_4\text{S}$ $[\text{M}+\text{Na}]^+$: 340.0614, found:

340.0623. Optical rotation: $[\alpha]_{\text{D}}^{25} = -12.0$ ($c = 0.75$, CHCl_3). HPLC: Chiralpak AD-H column (hexanes: isopropanol = 85:15, 1.0 mL/min, 254 nm); $t_{\text{R}} = 30.9$ min (minor), $t_{\text{R}} = 43.4$ min (major); 92:8 er.

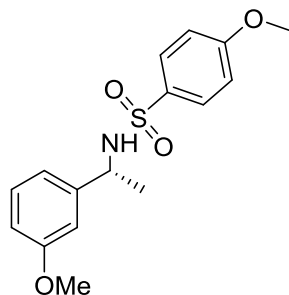


(R)-4-methoxy-N-(1-phenylethyl)benzenesulfonamide (1a'). $[\alpha]_{\text{D}}^{25} = -16.1$ ($c = 0.25$, CHCl_3). HPLC: Chiralpak AD-H column (hexanes: isopropanol = 90:10, 1.0 mL/min, 254 nm); $t_{\text{R}} = 21.1$ min (minor), $t_{\text{R}} = 23.3$ min (major); 95:5 er.

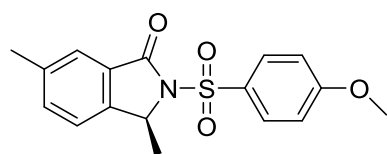


(S)-5-methoxy-2-((4-methoxyphenyl)sulfonyl)-3-methylisoindolin-1-one (2b).

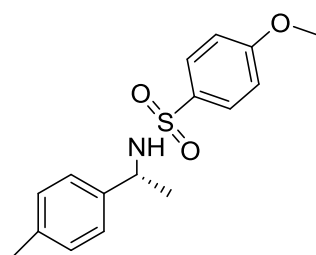
Following the general procedure, the product was isolated by column chromatography with petroleum ether/EA (10 : 1) as the eluent to give a semi-solid. ^1H NMR (400 MHz, CDCl_3) δ 8.07 (d, $J = 8.0$ Hz, 2H), 7.67 (d, $J = 8.0$ Hz, 1H), 6.97-6.93 (m, 3H), 6.84 (d, $J = 4.0$ Hz, 1H), 5.22-5.17 (m, 1H), 3.86 (s, 3H), 3.84(s, 3H), 1.75 (d, $J = 4.0$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 165.8, 164.5, 163.5, 149.9, 130.6, 130.0, 126.3, 121.1, 116.1, 114.0, 106.6, 57.9, 55.5, 21.5. IR (neat) 1726, 1593, 1495, 1357, 1322, 1281, 1260, 1183, 1157, 1109, 1080, 1020, 832, 811, 801, 766 cm^{-1} . HRMS (ESI-TOF) Calcd for $\text{C}_{17}\text{H}_{17}\text{NNaO}_5\text{S}$ $[\text{M}+\text{Na}]^+$: 370.0720, found: 370.0709. Optical rotation: $[\alpha]_{\text{D}}^{25} = -16.8$ ($c = 2.08$, CHCl_3). HPLC: Chiralpak AD-H column (hexanes: isopropanol = 85:15, 1.0 mL/min, 254 nm); $t_{\text{R}} = 16.2$ min (minor), $t_{\text{R}} = 20.4$ min (major); 60:40 er.



(R)-4-methoxy-N-(1-(3-methoxyphenyl)ethyl)benzenesulfonamide (1b'). $[\alpha]_{\text{D}}^{25} = -43.5$ ($c = 0.865$, CHCl_3). HPLC: Chiralpak AD-H column (hexanes: isopropanol = 90:10, 1.0 mL/min, 254 nm); $t_{\text{R}} = 24.6$ min (minor), $t_{\text{R}} = 31.7$ min (major); 99:1 er.

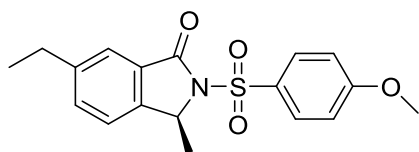


(S)-2-((4-methoxyphenyl)sulfonyl)-3,6-dimethylisoindolin-1-one (2c). Following the general procedure, the product was isolated by column chromatography with petroleum ether/EA (10 : 1) as the eluent to give a semi-solid. ^1H NMR (400 MHz, CDCl_3) δ 8.09 (d, $J = 8.0$ Hz, 2H), 7.55 (s, 1H), 7.45 (d, $J = 8.0$ Hz, 1H), 7.31 (d, $J = 8.0$ Hz, 1H), 6.99 (d, $J = 12.0$ Hz, 2H), 5.26-5.22 (m, 1H), 3.85 (s, 3H), 2.39 (s, 3H), 1.76 (d, $J = 8.0$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 166.5, 163.7, 144.7, 138.9, 135.1, 130.6, 130.4, 128.9, 124.7, 122.1, 114.0, 58.4, 55.6, 21.5, 21.2. IR (neat) 2918, 1721, 1593, 1495, 1354, 1301, 1260, 1157, 1132, 1087, 1023, 925, 829, 809, 788, 744 cm^{-1} . HRMS (ESI-TOF) Calcd for $\text{C}_{17}\text{H}_{17}\text{NNaO}_4\text{S}$ $[\text{M}+\text{Na}]^+$: 354.0770, found: 354.0760. Optical rotation: $[\alpha]_{\text{D}}^{25} = -17.0$ ($c = 1.02$, CHCl_3). HPLC: Chiralpak AD-H column (hexanes: isopropanol = 90:10, 1.0 mL/min, 254 nm); $t_{\text{R}} = 43.7$ min (major), $t_{\text{R}} = 50.2$ min (minor); 87:13 er.



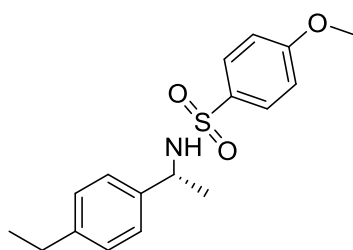
(R)-4-methoxy-N-(1-(p-tolyl)ethyl)benzenesulfonamide (1c'). $[\alpha]_{\text{D}}^{25} = -37.0$ ($c = 0.725$, CHCl_3). HPLC: Chiralpak OD-H column (hexanes: isopropanol = 90:10, 0.5

mL/min, 254 nm); $t_R = 30.4$ min (minor), $t_R = 33.7$ min (major); 90:10 er.

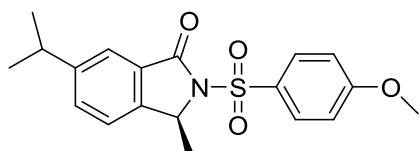


(S)-6-ethyl-2-((4-methoxyphenyl)sulfonyl)-3-methylisoindolin-1-one (2d).

Following the general procedure, the product was isolated by column chromatography with petroleum ether/EA (10 : 1) as the eluent to give a semi-solid. ^1H NMR (400 MHz, CDCl_3) δ 8.10-8.06 (m, 2H), 7.59 (s, 1H), 7.47-7.45 (m, 1H), 7.33 (d, $J = 8.0$ Hz, 1H), 6.99-6.96 (m, 2H), 5.27-5.22 (m, 1H), 3.85 (s, 3H), 2.72 (q, $J = 8.0$ Hz, 2H), 1.77 (d, $J = 8.0$ Hz, 3H), 1.23 (t, $J = 8.0$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 166.7, 163.9, 145.5, 145.0, 134.2, 130.8, 130.6, 129.1, 123.7, 122.3, 114.1, 58.6, 55.7, 28.6, 21.6, 15.5. IR (neat) 1727, 1594, 1495, 1438, 1346, 1324, 1302, 1258, 1183, 1158, 1085, 1021, 833, 802, 767 cm^{-1} . HRMS (ESI-TOF) Calcd for $\text{C}_{15}\text{H}_{21}\text{NNaO}_6\text{S}$ $[\text{M}+\text{Na}]^+$: 366.0982, found: 368.0994. Optical rotation: $[\alpha]_{\text{D}}^{25} = -21.3$ ($c = 1.5$, CHCl_3). HPLC: Chiralpak AD-H column (hexanes: isopropanol = 90:10, 1.0 mL/min, 254 nm); $t_R = 33.5$ min (major), $t_R = 43.8$ min (minor); 95:5 er.



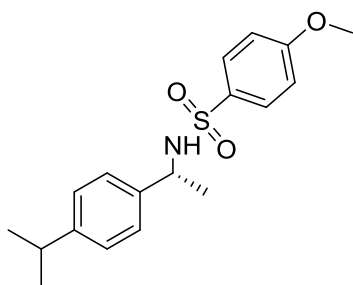
(R)-N-(1-(4-ethylphenyl)ethyl)-4-methoxybenzenesulfonamide (1d'). $[\alpha]_{\text{D}}^{25} = -10.5$ ($c = 0.25$, CHCl_3). HPLC: Chiralpak AD-H column (hexanes: isopropanol = 90:10, 0.5 mL/min, 254 nm); $t_R = 35.1$ min (major), $t_R = 38.3$ min (minor); 81:19 er.



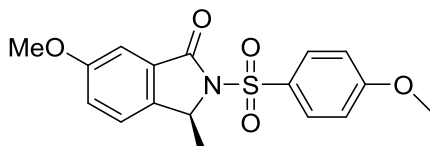
(S)-6-isopropyl-2-((4-methoxyphenyl)sulfonyl)-3-methylisoindolin-1-one (2e).

Following the general procedure, the product was isolated by column chromatography with petroleum ether/EA (10 : 1) as the eluent to give a semi-solid. ^1H NMR (400

MHz, CDCl₃) δ 8.10-8.06 (m, 2H), 7.62 (s, 1H), 7.51-7.48 (m, 1H), 7.34 (d, *J* = 8.0 Hz, 1H), 6.99-6.95 (m, 2H), 5.29-5.22 (m, 1H), 3.85 (s, 3H), 2.99-2.93 (m, 1H), 1.77 (d, *J* = 8.0 Hz, 3H), 1.28-1.22 (m, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 165.6, 162.7, 149.1, 144.0, 131.9, 129.6, 129.4, 127.9, 121.2, 121.1, 113.0, 57.5, 54.6, 32.9, 22.8, 20.5. IR (neat) 1722, 1594, 1496, 1354, 1303, 1260, 1177, 1160, 1130, 1106, 1087, 1024, 833, 807, 785, 739 cm⁻¹. HRMS (ESI-TOF) Calcd for C₁₉H₂₁NNaO₄S [M+Na]⁺: 382.1083, found: 382.1071. Optical rotation: [α]_D²⁵ = -32.9 (c = 1.0, CHCl₃). HPLC: Chiralpak AD-H column (hexanes: isopropanol = 85:15, 1.0 mL/min, 254 nm); t_R = 14.9 min (major), t_R = 21.9 min (minor); 95:5 er.



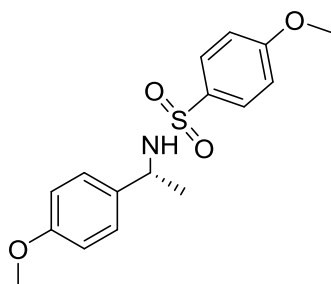
(*R*)-*N*-(1-(4-isopropylphenyl)ethyl)-4-methoxybenzenesulfonamide (1e'). [α]_D²⁵ = -5.8 (c = 0.4, CHCl₃). HPLC: Chiralpak AD-H column (hexanes: isopropanol = 90:10, 1.0 mL/min, 254 nm); t_R = 10.2 min (major), t_R = 13.8 min (minor); 67:33 er.



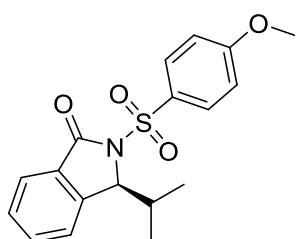
(*S*)-6-methoxy-2-((4-methoxyphenyl)sulfonyl)-3-methylisoindolin-1-one (2f).

Following the general procedure, the product was isolated by column chromatography with petroleum ether/EA (10 : 1) as the eluent to give a semi-solid. ¹H NMR (400 MHz, CDCl₃) δ 8.10-8.06 (m, 2H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.19 (m, 2H), 7.00-6.96 (m, 2H), 5.24-5.19 (m, 1H), 3.85 (s, 3H), 3.80 (s, 3H), 1.75 (d, *J* = 8.0 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 166.7, 164.1, 160.5, 140.1, 130.8, 130.4, 123.6, 123.1, 114.3, 106.9, 58.6, 56.0, 55.9, 21.8. IR (neat) 2918, 1722, 1495, 1358, 1323, 1307, 1280, 1260, 1159, 1082, 931, 830, 810, 801, 784, 749 cm⁻¹. HRMS (ESI-TOF) Calcd for C₁₇H₁₇NNaO₅S [M+Na]⁺: 370.0720, found: 370.0727. Optical rotation: [α]_D²⁵ = -6.4 (c = 0.78, CHCl₃). HPLC: Chiralpak AD-H column (hexanes: isopropanol = 85:15,

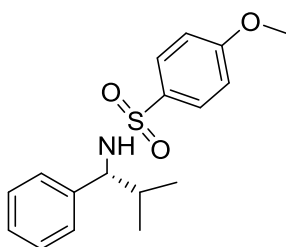
1.0 mL/min, 254 nm); $t_R = 28.5$ min (major), $t_R = 31.6$ min (minor); 96:4 er.



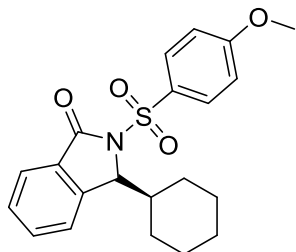
(R)-4-methoxy-N-(1-(4-methoxyphenyl)ethyl)benzenesulfonamide (1f'). $[\alpha]_D^{25} = -22.2$ ($c = 2.38$, CHCl_3). HPLC: Chiralpak AD-H column (hexanes: isopropanol = 90:10, 1.0 mL/min, 254 nm); $t_R = 30.2$ min (minor), $t_R = 32.1$ min (major); 82:18 er.



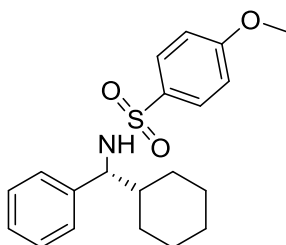
(S)-3-isopropyl-2-((4-methoxyphenyl)sulfonyl)isoindolin-1-one (2g). Following the general procedure, the product was isolated by column chromatography with petroleum ether/EA (10 : 1) as the eluent to give a semi-solid. ^1H NMR (400 MHz, CDCl_3) δ 8.11 (d, $J = 8.0$ Hz, 2H), 7.81 (d, $J = 8.0$ Hz, 1H), 7.61 (t, $J = 8.0, 4.0$ Hz, 1H), 7.48-7.45 (m, 2H), 7.00 (d, $J = 8.0$ Hz, 2H), 5.25 (d, $J = 4.0$ Hz, 1H), 3.86 (s, 3H), 2.99-2.91 (m, 1H), 1.28 (d, $J = 8.0$ Hz, 3H), 0.29 (d, $J = 4.0$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 165.5, 162.6, 142.4, 132.1, 129.4, 127.6, 123.8, 122.6, 112.9, 66.3, 54.5, 29.9, 18.3, 13.1. IR (neat) 2919, 1719, 1593, 1365, 1355, 1293, 1261, 1185, 1168, 1153, 1085, 1068, 1017, 828, 801, 748 cm^{-1} . HRMS (ESI-TOF) Calcd for $\text{C}_{18}\text{H}_{19}\text{NNaO}_4\text{S}$ $[\text{M}+\text{Na}]^+$: 368.0927, found: 368.0921. Optical rotation: $[\alpha]_D^{25} = -22.3$ ($c = 1.07$, CHCl_3). HPLC: Chiralpak OD-H column (hexanes: isopropanol = 90:10, 0.5 mL/min, 254 nm); $t_R = 33.1$ min (minor), $t_R = 35.8$ min (major); 90:10 er.



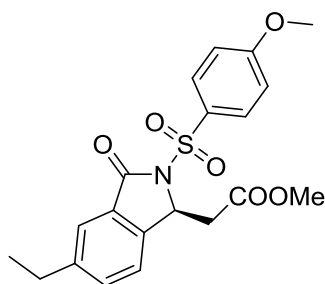
(R)-4-methoxy-N-(2-methyl-1-phenylpropyl)benzenesulfonamide (1g'). $[\alpha]_{\text{D}}^{25} = -6.6$ ($c = 1.17$, CHCl_3). HPLC: Chiralpak AD-H column (hexanes: isopropanol = 90:10, 1.0 mL/min, 254 nm); $t_{\text{R}} = 13.0$ min (major), $t_{\text{R}} = 15.0$ min (minor); 59:41 er.



(S)-3-cyclohexyl-2-((4-methoxyphenyl)sulfonyl)isoindolin-1-one (2h). Following the general procedure, the product was isolated by column chromatography with petroleum ether/EA (10 : 1) as the eluent to give a semi-solid. ^1H NMR (400 MHz, CDCl_3) δ 8.12 (d, $J = 8.0$ Hz, 2H), 7.80 (d, $J = 8.0$ Hz, 1H), 7.61 (t, $J = 8.0, 4.0$ Hz, 1H), 7.47 (t, $J = 8.0, 4.0$ Hz, 2H), 7.00 (d, $J = 8.0$ Hz, 2H), 5.22 (d, $J = 4.0$ Hz, 1H), 3.86 (s, 3H), 2.57-2.51 (m, 1H), 2.03 (d, $J = 12.0$ Hz, 1H), 1.86 (d, $J = 12.0$ Hz, 1H), 1.63 (s, 1H), 1.48-1.32 (m, 3H), 1.25 (s, 1H), 1.02-0.97 (m, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 166.9, 164.1, 144.4, 133.5, 130.9, 130.8, 130.7, 128.9, 125.1, 124.1, 114.3, 67.4, 55.9, 41.6, 30.3, 26.9, 26.5, 25.8, 25.4. IR (neat) 2920, 1721, 1362, 1287, 1259, 1184, 1164, 1085, 1044, 1021, 869, 830, 816, 798, 775, 748 cm^{-1} . HRMS (ESI-TOF) Calcd for $\text{C}_{21}\text{H}_{23}\text{NNaO}_4\text{S}$ $[\text{M}+\text{Na}]^+$: 408.1240, found: 408.1230. Optical rotation: $[\alpha]_{\text{D}}^{25} = -18.6$ ($c = 0.81$, CHCl_3). HPLC: Chiralpak AD-H column (hexanes: isopropanol = 90:10, 0.5 mL/min, 254 nm); $t_{\text{R}} = 28.9$ min (major), $t_{\text{R}} = 30.5$ min (minor); 89:11 er.

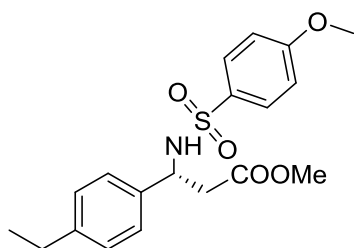


(R)-N-(cyclohexyl (phenyl)methyl)-4-methoxybenzenesulfonamid (1h'). $[\alpha]_{\text{D}}^{25} = -10.2$ ($c = 2.48$, CHCl_3). HPLC: Chiralpak AD-H column (hexanes: isopropanol = 90:10, 1.0 mL/min, 254 nm); $t_{\text{R}} = 14.2$ min (major), $t_{\text{R}} = 17.4$ min (minor); 87:13 er.



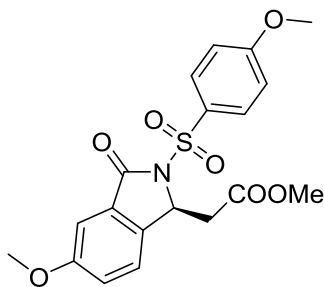
(S)-methyl-2-(5-ethyl-2-((4-methoxyphenyl)sulfonyl)-3-oxoisindolin-1-yl)acetate

(2i). Following the general procedure, the product was isolated by column chromatography with petroleum ether/EA (10 : 1) as the eluent to give a semi-solid. ¹H NMR (400 MHz, CDCl₃) δ 8.02 (d, *J* = 12.0 Hz, 2H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 1H), 6.92 (d, *J* = 8.0 Hz, 2H), 5.49 (q, *J* = 4.0 Hz, 1H), 3.78 (s, 3H), 3.61 (s, 3H), 3.52-3.47 (m, 1H), 2.82 (q, *J* = 8.0 Hz, 1H), 2.64-2.59 (m, 2H), 1.16 (t, *J* = 8.0 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 168.7, 164.9, 162.1, 144.4, 141.1, 132.5, 128.9, 128.4, 127.6, 121.8, 121.0, 112.6, 56.7, 54.0, 52.6, 50.1, 37.3, 27.0, 13.6. IR (neat) 2959, 2920, 2850, 1728, 1496, 1357, 1291, 1259, 1155, 1131, 1086, 1019, 915, 900, 832, 799, 716 cm⁻¹. HRMS (ESI-TOF) Calcd for C₂₀H₂₁NNaO₆S [M+Na]⁺:426.0982, found: 426.0969. Optical rotation: [α]_D²⁵ = -43.1 (c = 2.11, CHCl₃). HPLC: Chiralpak AD-H column (hexanes: isopropanol = 85:15, 1.0 mL/min, 254 nm); t_R = 39.2 min (minor), t_R = 48.7 min (major); 91:9 er.

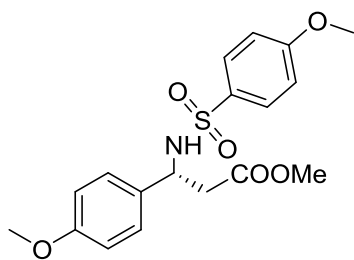


(R)-Methyl 3-(4-ethylphenyl)-3-((4-methoxyphenyl)sulfonamide)propanoate (1i')

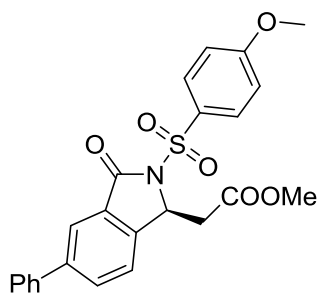
[α]_D²⁵ = -27.3 (c = 1.77, CHCl₃). HPLC: Chiralpak OD-H column (hexanes: isopropanol = 90:10, 0.5 mL/min, 254 nm); t_R = 48.3 min (minor), t_R = 51.6 min (major); 80:20 er.



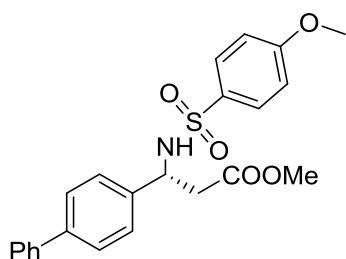
(S)-methyl-2-(5-methoxy-2-((4-methoxyphenyl)sulfonyl)-3-oxoisindolin-1-yl)acetate (2j). Following the general procedure, the product was isolated by column chromatography with petroleum ether/EA (10 : 1) as the eluent to give a semi-solid. ^1H NMR (400 MHz, CDCl_3) δ 8.02 (d, $J = 12.0$ Hz, 2H), 7.30 (d, $J = 8.0$ Hz, 1H), 7.14-7.07 (m, 2H), 6.92 (d, $J = 8.0$ Hz, 2H), 5.46 (dd, $J = 8.0, 4.0$ Hz, 1H), 3.78 (s, 3H), 3.73 (s, 3H), 3.60 (s, 3H), 3.51 (dd, $J = 16.0, 4.0$ Hz, 1H), 2.82 (q, $J = 8.0$ Hz, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 170.3, 167.0, 163.9, 160.8, 138.1, 130.6, 124.2, 122.7, 114.2, 107.2, 58.5, 55.9, 51.8, 39.1. IR (neat) 1726, 1593, 1495, 1357, 1322, 1281, 1260, 1183, 1157, 1109, 1080, 1020, 832, 811, 766, 717 cm^{-1} . HRMS (ESI-TOF) Calcd for $\text{C}_{19}\text{H}_{19}\text{NNaO}_7\text{S}$ $[\text{M}+\text{Na}]^+$:428.0774, found: 428.0764. Optical rotation: $[\alpha]_{\text{D}}^{25} = -31.6$ ($c = 1.3$, CHCl_3). HPLC: Chiralpak AD-H column (hexanes: isopropanol = 85:15, 0.5 mL/min, 254 nm); $t_{\text{R}} = 102.0$ min (minor), $t_{\text{R}} = 106.9$ min (major); 96:4 er.



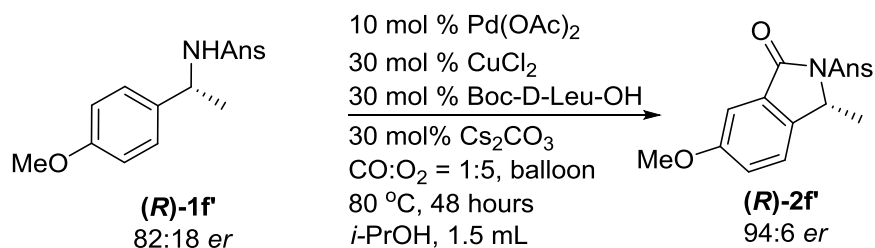
(R)-Methyl 3-(4-methoxyphenyl)-3-((4-methoxyphenyl)sulfonamide)propanoate (1j'). $[\alpha]_{\text{D}}^{25} = -23.2$ ($c = 1.80$, CHCl_3). HPLC: Chiralpak AD-H column (hexanes: isopropanol = 90:10, 1.0 mL/min, 254 nm); $t_{\text{R}} = 63.2$ min (major), $t_{\text{R}} = 69.0$ min (minor); 72:28 er.



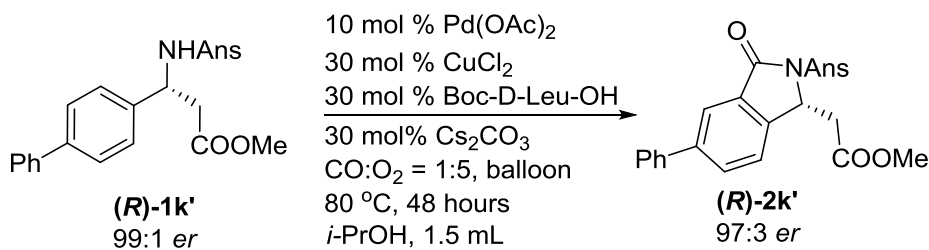
(S)-methyl-2-(2-((4-methoxyphenyl)sulfonyl)-3-oxo-5-phenylisoindolin-1-yl)acetate (2k). Following the general procedure, the product was isolated by column chromatography with petroleum ether/EA (10 : 1) as the eluent to give a semi-solid. ^1H NMR (400 MHz, CDCl_3) δ 8.12 (d, $J = 12.0$ Hz, 2H), 7.97 (s, 1H), 7.85-7.82 (m, $J = 4.0$ Hz, 1H), 7.56-7.54 (m, 3H), 7.46 (t, $J = 4.0, 8.0$ Hz, 2H), 7.40 (t, $J = 8.0$ Hz, 1H), 7.01 (d, $J = 8.0$ Hz, 2H), 5.64 (dd, $J = 8.0, 1$ Hz), 3.86 (s, 3H), 3.70 (s, 3H), 3.65 (dd, $J = 16.0, 4.0$ Hz, 1H), 2.97 (q, $J = 8.0$ Hz, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 170.5, 166.5, 164.2, 144.1, 142.8, 139.4, 133.4, 130.8, 129.2, 128.3, 127.3, 123.6, 123.2, 114.3, 58.4, 55.8, 52.2, 39.4. IR (neat) 1722, 1356, 1302, 1261, 1198, 1180, 1157, 1137, 1088, 1019, 981, 833, 806, 759, 718 cm^{-1} . HRMS (ESI-TOF) Calcd for $\text{C}_{24}\text{H}_{21}\text{NNaO}_6\text{S}$ $[\text{M}+\text{Na}]^+$: 474.0982, found: 474.0971. Optical rotation: $[\alpha]_{\text{D}}^{25} = -23.9$ ($c = 2.84$, CHCl_3). HPLC: Chiralpak AD-H column (hexanes: isopropanol = 85:15, 1.0 mL/min, 254 nm); $t_{\text{R}} = 65.5$ min (minor), $t_{\text{R}} = 85.8$ min (major); 89:11 er.



(R)-Methyl-3-([1,1'-biphenyl]-4-yl)-3-((4-methoxyphenyl)sulfonamide)propanoate (1k'). $[\alpha]_{\text{D}}^{25} = -13.4$ ($c = 1.0$, CHCl_3). HPLC: Chiralpak AD-H column (hexanes: isopropanol = 90:10, 1.0 mL/min, 254 nm); $t_{\text{R}} = 61.5$ min (major), $t_{\text{R}} = 67.2$ min (minor); 99:1 er.



(R)-6-methoxy-2-((4-methoxyphenyl)sulfonyl)-3-methylisoindolin-1-one (2f'). To a 25 mL reaction tube, **(R)-1f'** (33 mg, 0.1 mmol, 1.0 equiv.), Pd(OAc)₂ (10 mol%), Boc-D-Leu-OH (30 mol%), CuCl₂ (30 mol%) and Cs₂CO₃ (30 mol%) were added. Evacuated the reaction tube and refilled it with the CO/O₂ gas mixture through the balloon and then *i*-PrOH (1.5 mL) was added. The resulting solution was heated to 80 °C for 48 hours. After the reaction finished, cool down the mixture to room temperature and release the CO/O₂ gas mixture carefully in the fume hood. The reaction mixture was passed through a short column of silica gel and eluted with EtOAc (50 ml), the eluent was concentrated under vacuum. The resulting residue was purified by column chromatography to give the desired product **(R)-2f'** (21 mg, 60% yield). $[\alpha]_D^{25} = 23.0$ (*c* = 0.4, CHCl₃). HPLC: Chiralpak AD-H column (hexanes: isopropanol = 85:15, 1.0 mL/min, 254 nm); *t*_R = 28.8 min (minor), *t*_R = 31.9 min (major); 94:6 *er*.



(R)-methyl-2-(2-((4-methoxyphenyl)sulfonyl)-3-oxo-5-phenylisoindolin-1-yl)acetate (2k'). To a 25 mL reaction tube, **(R)-1k'** (43 mg, 0.1 mmol, 1.0 equiv.), Pd(OAc)₂ (10 mol%), Boc-D-Leu-OH (30 mol%), CuCl₂ (30 mol%) and Cs₂CO₃ (30 mol%) were added. Evacuated the reaction tube and refilled it with the CO/O₂ gas mixture through the balloon and then *i*-PrOH (1.5 mL) was added. The resulting solution was heated to 80 °C for 48 hours. After the reaction finished, cool down the mixture to room temperature and release the CO/O₂ gas mixture carefully in the fume hood. The

reaction mixture was passed through a short column of silica gel and eluted with EtOAc (50 ml), the eluent was concentrated under vacuum. The resulting residue was purified by column chromatography to give the desired product **(R)-2k'** (30 mg, 66.4% yield). $[\alpha]_D^{25} = 17.3$ ($c = 1.5$, CHCl_3). HPLC: Chiralpak AD-H column (hexanes: isopropanol = 85:15, 1.0 mL/min, 254 nm); $t_R = 64.1$ min (major), $t_R = 83.8$ min (minor); 97:3 er.

3. Computational studies

All calculations were performed with the Gaussian 09 suites of programs.¹² Geometry optimization for all stationary points along the reaction paths without any symmetry constraints was conducted with the M06L functional.¹³ The standard 6-31G(d,p) basis was employed for the C, H, O, N and S atoms, whereas the SDD valence basis set¹⁴ in combination with the corresponding effective core potential were used for the Pd and Cs atoms. Frequency calculations were performed for each optimized structure at the same level of theory to characterize the stationary points as minima or saddle points. The connectivity of the stationary points was verified by IRC¹⁶ runs or the vibrational mode of the imaginary frequencies. The zero-point correction, thermal corrections, and entropic corrections were determined from the frequency calculations. The reported enthalpies and Gibbs free energies (in kcal/mol at 298.15 K and 1 atm) were obtained from the single-point energy calculations on the optimized geometries at the M06L/Def2TZVP¹⁷ level of theory combined with the above mentioned corrections.

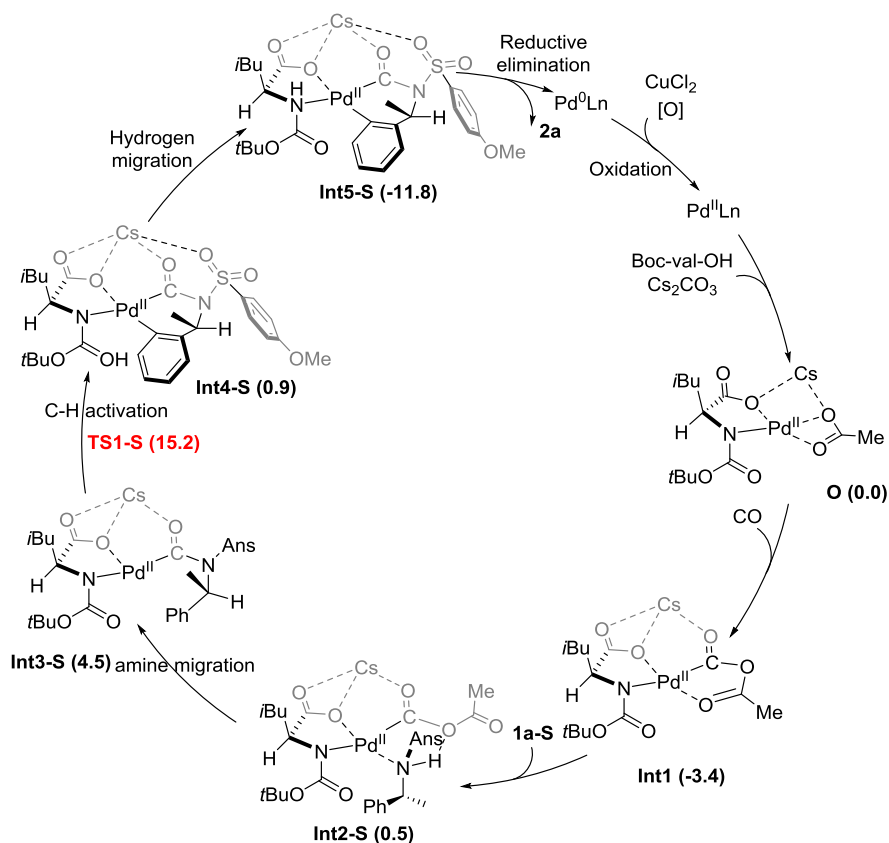


Figure S1. Propose catalytic cycle for the kinetic resolution of benzylamine

Table S7

Systems	ΔE^d	ΔH^d	ΔS^e	ΔG^d
O	0.0	0.0	0.0	0.0
Int1	-14.6	-15.2	-39.3	-3.4
Int2-R	-25.6	-26.8	-101.6	3.5
Int2-S	-27.2	-28.4	-97.1	0.5
Int3-R	-12.2	-12.8	-59.4	4.9
Int3-S	-9.9	-10.4	-50.1	4.5
Int4-R	-13.6	-14.2	-55.2	2.2
Int4-S	-13.3	-13.9	-49.7	0.9
Int5-R	-24.1	-24.7	-60.7	-6.6
Int5-S	-26.3	-26.9	-50.4	-11.8
TS1-R	-1.3	-1.9	-58.8	15.7
TS1-S	0.9	0.3	-49.9	15.2
TS2-R	5.6	5.0	-58.1	22.3
TS2-S	3.1	2.5	-53.1	18.4

[a] Basis set (BS) refers to the standard 6-31G(d,p) basis for C, H, O, N atoms and LANL2DZ valence basis set in combination with the corresponding effective core potential for Pd. [b] Relative activation energy and reaction parameters were calculated based on those of free O. [c] Parameters for all the transition state (TSs) should read as those with double dagger like ΔE^\ddagger , ΔH^\ddagger , ΔS^\ddagger , and ΔG^\ddagger . [d] In kcal/mol. [e] In kcal/(mol K).

B3-LYP geometries for all the optimized

compounds and transition states.

CO

O	0.00000000	0.00000000	0.48912700
C	0.00000000	0.00000000	-0.65216900

HAc

C	-0.13417400	-0.13659200	0.00001300
C	1.36567100	0.01235700	-0.00004000
H	1.70310400	0.56786000	-0.88075100
H	1.70309200	0.56439500	0.88285700
H	1.83338700	-0.97037000	-0.00192400
O	-0.82717100	1.03521500	-0.00007100
O	-0.72477500	-1.18464400	0.00001600
H	-0.21299300	1.77895100	0.00042400

a-R

C	-1.32515600	-0.47405300	-0.21936200
S	0.04720700	1.86076700	0.05000300
N	-1.07900800	0.89343900	-0.71506300
H	-1.02505900	0.98827100	-1.72333600
O	-0.37445200	1.94511200	1.44328900
O	0.19292300	3.02216400	-0.81735400
C	1.57895600	0.96081100	0.03455900
C	2.38533300	0.98700600	-1.10822300
C	1.92004100	0.16024100	1.12025500
C	3.52507900	0.20684700	-1.16075800
H	2.11584500	1.63280100	-1.93909900
C	3.06440800	-0.63028200	1.07208600
H	1.29379300	0.17373000	2.00747900
C	3.86714600	-0.61141800	-0.07341800
H	4.17629700	0.21304500	-2.02858600
H	3.32632200	-1.24513200	1.92587600
C	-2.82013800	-0.68766100	-0.06329100
C	-3.48422000	-1.79416500	-0.59151700
C	-3.55258600	0.25633100	0.66488000
C	-4.85565600	-1.95686000	-0.39702300
H	-2.93792500	-2.54014800	-1.16259300
C	-4.91688200	0.09273200	0.86311000
H	-3.03113400	1.12319700	1.06503500
C	-5.57443500	-1.01633300	0.33084800
H	-5.35973400	-2.82202400	-0.81952600
H	-5.47164600	0.83300700	1.43317200
H	-6.64274700	-1.14330800	0.48279700

O	4.99882300	-1.34007600	-0.22720000
C	5.38252500	-2.17926000	0.84579200
H	4.61877500	-2.93792000	1.05711700
H	6.30116700	-2.67191300	0.52911900
H	5.57570700	-1.60350100	1.75924500
H	-0.89118300	-0.49381200	0.79119800
C	-0.61203100	-1.51426600	-1.06800800
H	-1.00817200	-1.53029800	-2.08975300
H	0.45889900	-1.29980300	-1.11973300
H	-0.73412700	-2.51814100	-0.65246900
a-S			
C	-1.44726900	0.18449000	0.73590000
S	0.21770400	2.15406000	-0.21026300
N	-1.22444700	1.28178000	-0.23310800
H	-1.38136900	0.97834100	-1.19039600
O	0.29931400	2.83105800	1.07648000
O	0.22427400	2.86855000	-1.48014300
C	1.52385000	0.94922600	-0.25148500
C	1.98897100	0.47334500	-1.48130300
C	2.04220700	0.44852800	0.93922300
C	2.97233200	-0.49749800	-1.51287600
H	1.59029200	0.88989800	-2.40159900
C	3.02930900	-0.53206200	0.91430100
H	1.68631200	0.84659400	1.88525000
C	3.49479000	-1.00866400	-0.31564500
H	3.36379700	-0.87640800	-2.45112000
H	3.43110300	-0.90807000	1.84826800
C	-2.62054500	-0.62795600	0.24201600
C	-2.53152200	-2.01680700	0.14389600
C	-3.82355400	0.00064800	-0.09549100
C	-3.62494600	-2.76960300	-0.27660000
H	-1.59502500	-2.50947500	0.39964300
C	-4.91442400	-0.74953100	-0.52103300
H	-3.89196000	1.08397400	-0.02706700
C	-4.81848700	-2.13693400	-0.61074200
H	-3.54147400	-3.85038300	-0.34889400
H	-5.84326300	-0.25010900	-0.78306100
H	-5.67163700	-2.72199400	-0.94218000
H	-0.56516800	-0.48012200	0.76950000
C	-1.70080900	0.73537500	2.13294600
H	-0.84470300	1.29792100	2.50941400
H	-2.56269900	1.40822900	2.12162300
H	-1.91521300	-0.08892900	2.81872300
O	4.45071700	-1.95801300	-0.45704300

C	5.01528700	-2.49435300	0.72475500
H	4.25826200	-2.99094900	1.34458800
H	5.75218500	-3.22787000	0.40008800
H	5.51283200	-1.72007300	1.32165800
O			
C	-1.38070700	1.15402000	-0.11461800
H	-2.00838000	1.25908100	-1.01163600
C	-0.07110900	1.85922700	-0.43081500
O	0.01247000	3.05333700	-0.68724700
C	-2.10470400	1.82272400	1.06597000
H	-1.38881100	1.93143000	1.89327000
C	-2.03961500	-1.20685800	-0.16269100
C	-4.42496100	-1.49275200	-0.62776500
C	-4.25674000	-2.32632600	-1.88974100
H	-5.18530500	-2.86688300	-2.10318900
H	-4.03999500	-1.67865800	-2.74493800
H	-3.44563400	-3.04529400	-1.77786800
C	-5.55260400	-0.48717400	-0.80066700
H	-5.66061400	0.12997500	0.09632200
H	-5.35515300	0.17653600	-1.64759900
H	-6.49958600	-1.00538700	-0.97994700
C	-4.66942300	-2.35536100	0.60190400
H	-3.87146000	-3.08544600	0.73569100
H	-4.72650900	-1.72786600	1.49713000
H	-5.62320100	-2.88366100	0.49878700
O	1.01026500	1.10042700	-0.42011900
O	-3.26186400	-0.63504300	-0.42542700
O	-1.82464700	-2.41264900	-0.18226700
N	-1.12572800	-0.25667700	0.15262600
Pd	0.78912600	-0.80373400	0.20224900
Cs	3.83551500	1.11703100	-0.48362500
C	2.32296400	-2.69515700	0.81262700
O	2.81269200	-1.57467200	0.40370200
O	1.07460900	-2.82969600	0.90678400
C	3.24595500	-3.82036200	1.15513600
H	3.76803400	-4.15834000	0.25561600
H	4.00761400	-3.48535700	1.86378300
H	2.69187700	-4.65725000	1.57889500
H	-2.87054300	1.11628000	1.41321400
C	-2.76075900	3.17038400	0.76218100
H	-2.01555700	3.80101400	0.26173000
C	-3.96327900	3.01355000	-0.16069100
H	-4.39472300	3.98660600	-0.41851000
H	-3.71080100	2.50678600	-1.09747700

H	-4.75010100	2.42220400	0.32437500
C	-3.17904200	3.84958500	2.05973900
H	-3.89838300	3.23025600	2.61094400
H	-2.32245700	4.02224700	2.71989800
H	-3.65740400	4.81687600	1.87217000
Int1			
C	1.07359500	-1.32193300	-0.31919200
H	1.65265900	-1.85661900	-1.08423000
C	-0.39668400	-1.50960300	-0.64645200
O	-0.89867800	-2.57486500	-1.01732500
C	1.40227300	-1.96283100	1.04696200
H	0.90782100	-1.36491900	1.82724800
C	2.64271000	0.54615300	-0.41936200
C	4.95837000	-0.22971600	-0.65128900
C	5.30291500	0.63691300	-1.85476200
H	6.39038100	0.73417000	-1.94527500
H	4.92771600	0.17511800	-2.77348200
H	4.86063100	1.62794900	-1.75311600
C	5.55422100	-1.62089200	-0.80850500
H	5.28840900	-2.25336100	0.04430200
H	5.18198700	-2.10070400	-1.71827100
H	6.64554100	-1.56469100	-0.86840600
C	5.42786200	0.39852900	0.65408500
H	5.01448400	1.39918300	0.77617200
H	5.11564100	-0.21791800	1.50382700
H	6.52146500	0.45958300	0.66592600
C	-0.52269100	3.98412800	0.75027200
C	-0.25748200	5.40338000	1.11836900
H	0.81438900	5.58616000	1.16034500
H	-0.72128700	6.06821100	0.38608400
H	-0.71431200	5.62781900	2.08499600
O	-1.16866200	-0.46348800	-0.45563100
O	3.53075900	-0.49847800	-0.60307000
O	2.99199700	1.72136800	-0.37484400
N	1.37387700	0.10188400	-0.31782000
Pd	-0.29113800	1.27824900	0.02125700
C	-2.00621700	2.16205600	0.28268300
O	-3.16880500	1.87112400	0.23198400
O	0.41233500	3.19115100	0.54222200
O	-1.79131900	3.65957200	0.66858400
Cs	-3.87074600	-1.24362500	-0.52135100
H	2.47845100	-1.81130800	1.18627700
C	1.04714800	-3.45015000	1.20930200
H	0.93635100	-3.88576100	0.20671200

C	-0.27812100	-3.63536800	1.94168100
H	-1.08945400	-3.09131800	1.44831500
H	-0.56835600	-4.69082200	1.98998600
H	-0.20189100	-3.26573400	2.97238800
C	2.15610800	-4.19671900	1.94056400
H	1.91440200	-5.25723500	2.07331300
H	3.10515900	-4.13506900	1.39847800
H	2.32100600	-3.77075400	2.93815200
Int2-R			
C	3.09174500	1.31388300	0.46641900
H	3.81509200	2.10118100	0.22188000
C	3.75142400	-0.00864400	0.08850200
O	4.84168400	-0.35160900	0.56071400
C	2.81391500	1.33616900	1.97522400
H	2.05919000	0.56095500	2.18040000
C	1.59920200	2.57145200	-1.00011600
C	2.29673800	4.89677500	-1.36928300
C	2.36176100	4.81752300	-2.88841000
H	2.33634800	5.82679500	-3.31388400
H	3.29723800	4.34383800	-3.20196700
H	1.52661700	4.24172900	-3.28605700
C	3.47295800	5.70154700	-0.83501000
H	3.42832200	5.78170500	0.25497100
H	4.42035300	5.22490400	-1.10418600
H	3.46327800	6.71210700	-1.25522200
C	0.98637400	5.50022200	-0.88131900
H	0.13132600	4.96620800	-1.29527100
H	0.93745000	5.45572700	0.21265000
H	0.92590800	6.55259900	-1.17867400
O	3.09555800	-0.79609600	-0.73181600
O	2.50437800	3.58748000	-0.77052100
O	0.64338100	2.71007200	-1.77463900
N	1.85680800	1.47339400	-0.27960900
C	0.68828200	-2.33015500	-1.12466300
O	1.35034200	-3.33090100	-0.95145100
Pd	1.07436700	-0.43676800	-0.67513400
C	-1.65539600	1.21566700	-0.60724200
S	-1.41681000	-0.91730200	1.24146400
N	-1.07206800	-0.15350100	-0.31929900
H	-1.44262300	-0.82172900	-1.00542600
O	-0.68979600	-0.18156300	2.26375600
O	-1.15965000	-2.33618700	0.99945800
C	-3.14738500	-0.68943600	1.47280500
C	-4.02894900	-1.34928300	0.61728500

C	-3.61082700	0.19282800	2.45046300
C	-5.38877300	-1.10220000	0.71635400
H	-3.65721000	-2.03155200	-0.14460500
C	-4.96876300	0.43286800	2.55493300
H	-2.90178800	0.68339800	3.11066100
C	-5.85926700	-0.19047600	1.67016600
H	-6.06536300	-1.58864800	0.02333700
H	-5.36701100	1.11798900	3.29579000
O	-0.58583500	-2.42875500	-1.81796300
O	-2.63901400	-3.21180600	-1.97035200
C	-1.48683300	-3.45941600	-1.69106400
C	-1.00403400	-4.78989800	-1.21739000
H	-0.18835000	-5.15882500	-1.84043100
H	-0.60655500	-4.69545500	-0.20469700
H	-1.84361400	-5.48424400	-1.22772300
C	-3.09021300	1.12065700	-1.08649100
C	-4.11769300	1.88641600	-0.53164400
C	-3.39982700	0.27289000	-2.15943700
C	-5.41746100	1.80383900	-1.02760800
H	-3.90738500	2.55180900	0.30114700
C	-4.69733300	0.17704200	-2.64698300
H	-2.61945900	-0.32971900	-2.62292100
C	-5.71346300	0.94670700	-2.08302400
H	-6.20261600	2.40542000	-0.57434400
H	-4.91101100	-0.49394400	-3.47436900
H	-6.72720800	0.88481800	-2.47199300
Cs	4.13310900	-3.28951200	0.35068600
H	3.72832200	1.05708300	2.51789000
C	2.29668500	2.68375300	2.47767100
H	1.53173000	3.02455200	1.76329400
C	1.63833400	2.53345700	3.84213800
H	2.35259300	2.14974500	4.58202600
H	1.26636600	3.49297700	4.21774200
H	0.79571000	1.83511700	3.80226000
C	3.40271400	3.72939900	2.51256400
H	3.01341400	4.71112500	2.80637200
H	4.17939700	3.45315200	3.23724600
H	3.87837400	3.84495000	1.53423900
H	-1.02661500	1.54954000	-1.44373000
C	-1.38636500	2.19345100	0.51552600
H	-0.33819600	2.12659900	0.81546500
H	-1.57245100	3.20570500	0.14894100
H	-2.01453900	2.02776900	1.39547100
O	-7.15862100	0.16040800	1.80522800

C	-8.07663200	-0.38353700	0.87348700
H	-9.04548700	0.05161100	1.11611000
H	-7.80144900	-0.11893600	-0.15540500
H	-8.13910000	-1.47531200	0.95796100
Int2-S			
C	3.11992500	1.14782200	0.44435100
H	3.86196900	1.94091400	0.29393000
C	3.74897100	-0.16875700	0.00571000
O	4.87047500	-0.52556700	0.38505900
C	2.79680800	1.02562400	1.94469900
H	2.06683200	0.20924100	2.05707700
C	1.64165500	2.56397800	-0.90743500
C	2.20940200	4.94479300	-0.88593400
C	2.28375800	5.12677600	-2.39645600
H	2.21879100	6.19245900	-2.64291500
H	3.24087500	4.75336800	-2.77401000
H	1.47804700	4.59382000	-2.89860000
C	3.33185200	5.72475500	-0.21669500
H	3.28534700	5.62467900	0.87101900
H	4.30740800	5.36060100	-0.55282200
H	3.25571000	6.78716100	-0.46816400
C	0.86199900	5.36914300	-0.31743700
H	0.04725500	4.82244000	-0.79333100
H	0.83000700	5.17488000	0.76001300
H	0.71135800	6.44279900	-0.47427800
O	3.00900700	-0.96507900	-0.73150400
O	2.49846500	3.56743200	-0.50708500
O	0.72028300	2.76681700	-1.70484700
N	1.92170300	1.38347400	-0.34163700
C	0.50095900	-2.37230000	-0.87236600
O	1.18792000	-3.36732300	-0.75346100
Pd	1.02504500	-0.44974400	-0.72630400
C	-1.65019700	1.04571700	-1.59244000
S	-1.32171400	0.63052600	1.14244600
N	-1.07301700	0.13869200	-0.54112200
H	-1.51251000	-0.78611000	-0.61824800
O	-1.21687000	2.08032700	1.18599300
O	-0.43589900	-0.25227400	1.89385300
C	-2.98471100	0.13410200	1.46793300
C	-3.29883400	-1.22210300	1.42685900
C	-3.97457000	1.09915200	1.66022500
C	-4.62008400	-1.62728800	1.55510300
H	-2.52313100	-1.96416200	1.25842900
C	-5.28790200	0.69650300	1.80520700

H	-3.70520800	2.15036600	1.66741800
C	-5.61956500	-0.66353300	1.73238300
H	-4.85514000	-2.68321200	1.48641400
H	-6.08668600	1.41882800	1.93760300
O	-0.94936100	-2.56741800	-1.00139800
O	-2.75653200	-3.82914800	-0.80911000
C	-1.60732900	-3.75971500	-1.18050000
C	-0.88422100	-4.86456600	-1.88342700
H	-0.27379700	-4.48933500	-2.70644700
H	-0.20017900	-5.35606100	-1.18955300
H	-1.61826000	-5.58502000	-2.24382800
C	-3.15690800	1.12803900	-1.54664100
C	-3.77193700	2.37713300	-1.44158800
C	-3.96065800	-0.01352500	-1.64327100
C	-5.16024200	2.48883100	-1.43672000
H	-3.14694500	3.26413700	-1.35472600
C	-5.34640600	0.09393100	-1.61671300
H	-3.50233900	-1.00153000	-1.70744000
C	-5.95098000	1.34683300	-1.51965200
H	-5.62351900	3.46864900	-1.35504700
H	-5.95798100	-0.80408600	-1.66817700
H	-7.03451800	1.42785000	-1.49788200
Cs	4.08113800	-3.44126700	0.27806800
H	3.71034100	0.72810700	2.48074800
C	2.21848500	2.29494000	2.56552000
H	1.43012300	2.65711700	1.89060900
C	1.57784900	1.98627600	3.91167800
H	2.31852700	1.58560800	4.61660600
H	1.14963900	2.88627200	4.36632100
H	0.77847300	1.24617000	3.80842300
C	3.28256300	3.37510600	2.70322800
H	2.85159500	4.31634800	3.06403500
H	4.05409200	3.07044300	3.42258500
H	3.77261000	3.58144900	1.74727100
O	-6.94146300	-0.94511700	1.82416100
C	-7.32330800	-2.30206900	1.70208500
H	-8.40959700	-2.31878200	1.78226400
H	-7.02276500	-2.71877200	0.73246800
H	-6.89142500	-2.91755600	2.50090900
H	-1.20342500	2.02355400	-1.40550600
C	-1.14738300	0.54431600	-2.93541000
H	-1.46594300	-0.48806900	-3.12307300
H	-1.55047300	1.17430600	-3.73276700
H	-0.05538000	0.60474400	-2.96796800

Int3-R

C	1.16525900	3.40292600	0.82512500
H	1.81035600	4.27231700	0.99924700
C	0.19123400	3.72963800	-0.28782800
C	0.64982200	4.40899500	-1.42873500
C	-0.20477000	4.65194900	-2.49060100
H	1.69118600	4.71898400	-1.47553500
C	-2.00224400	3.53701800	-1.33781000
C	-1.52992000	4.19718900	-2.45880700
H	0.16331600	5.18426800	-3.36382200
H	-3.02782700	3.18918800	-1.25393500
H	-2.18444000	4.37368700	-3.30738900
S	3.56280600	1.99061200	0.97380700
C	3.31253300	0.27465600	1.40707300
C	2.06064300	-0.19373500	1.79512900
C	4.39606700	-0.60354600	1.33009300
C	1.86069900	-1.54442000	2.05188300
H	1.20776200	0.47850800	1.83327300
C	4.21159500	-1.94978700	1.61096000
H	5.36842000	-0.22824100	1.02475200
C	2.93527700	-2.43436300	1.94623400
H	0.86170700	-1.89547500	2.28372400
H	5.03747600	-2.65357400	1.55741900
O	3.60076800	2.82802800	2.16957900
O	4.65897900	2.03179800	0.01767500
N	2.05327300	2.35981000	0.24042600
C	1.53858100	1.48486200	-0.74805400
O	2.31037500	0.79442600	-1.39728500
C	-2.16244500	-1.32726100	-0.12666600
H	-2.48780400	-1.80335400	0.80786400
C	-0.73135000	-1.76364400	-0.37833900
O	-0.35981600	-2.94277500	-0.24317300
C	-3.06522400	-1.85074200	-1.26097600
H	-2.72595600	-1.40162000	-2.20576500
C	-3.18509700	-3.36756700	-1.41639700
H	-2.22134600	-3.76133200	-1.76829600
C	-3.30526400	0.67125000	0.58510900
C	-5.50347900	0.12189800	1.54450800
C	-5.34382900	0.87844700	2.85532800
H	-6.32672500	1.07469600	3.29739500
H	-4.76649300	0.28173500	3.56854300
H	-4.82973100	1.82566900	2.69096000
C	-6.19135400	-1.21580300	1.77715100
H	-6.28624000	-1.76830100	0.83614800

H	-5.61659400	-1.83119900	2.47578800
H	-7.19301800	-1.06587600	2.19163100
C	-6.27251200	0.93069900	0.50836300
H	-5.80355000	1.89977900	0.33960000
H	-6.31102700	0.38687700	-0.44160900
H	-7.30169400	1.08695800	0.84883200
O	0.10221800	-0.86024700	-0.80410100
O	-4.20627300	-0.28008800	1.02452300
O	-3.50534200	1.88102000	0.75527700
N	-2.23539600	0.12604400	-0.01243600
Pd	-0.42074200	1.12419600	-0.57304800
C	-1.15702000	3.31884300	-0.22892900
H	-1.62760700	2.96426000	0.68539300
Cs	2.56198400	-2.21260700	-1.55092200
C	0.51704200	3.00302800	2.13821900
H	-0.09855500	3.82294900	2.51896000
H	-0.13546600	2.13076700	2.01322800
H	1.27972400	2.77403300	2.88352000
O	2.82499900	-3.77558500	2.08333300
C	1.51673700	-4.29213500	2.33017100
H	0.82022500	-4.00987800	1.53014700
H	1.62998200	-5.37466300	2.36634900
H	1.13115500	-3.93840500	3.29326300
H	-4.06413400	-1.43998900	-1.06563300
C	-4.24781800	-3.68300600	-2.46179100
H	-4.32807300	-4.75967900	-2.64612500
H	-5.23324300	-3.33242900	-2.12861900
H	-4.03562000	-3.19344400	-3.41866700
C	-3.50607100	-4.05244800	-0.09323000
H	-4.36653200	-3.57812700	0.39617600
H	-3.74976700	-5.10994100	-0.24358100
H	-2.65467300	-3.99980500	0.59110600

Int3-S

C	1.05940300	-1.92661000	1.75533800
H	1.84774500	-2.41726000	2.33729900
C	0.54899500	-2.89618300	0.71544700
C	1.48492700	-3.67917600	0.02523200
C	-0.80768000	-2.96430300	0.34249200
C	1.09268200	-4.48405000	-1.03278300
H	2.53023400	-3.63604800	0.32644400
C	-1.18698000	-3.75592000	-0.76072200
H	-1.60615400	-2.53565400	0.94946500
C	-0.24285300	-4.50325500	-1.44653100
H	1.83147900	-5.08973600	-1.55152600

H	-2.23913000	-3.76170400	-1.02439500
H	-0.54074100	-5.11477900	-2.29299800
S	2.94886400	0.07884100	1.70201700
C	4.42327700	-0.20970100	0.75978800
C	4.50343300	-1.17585000	-0.24360500
C	5.53722300	0.55603800	1.09505600
C	5.70119100	-1.37009900	-0.90833200
H	3.62540100	-1.75341000	-0.51493600
C	6.74229500	0.36391000	0.42988100
H	5.46684300	1.30415200	1.87981400
C	6.82652300	-0.60407600	-0.57749400
H	5.79144600	-2.10805200	-1.69840200
H	7.60244600	0.96489000	0.70199300
O	3.12410100	-0.47168600	3.04303900
O	2.60232100	1.49890800	1.56464900
N	1.75104400	-0.87135900	0.96128300
C	1.20242500	-0.43967000	-0.28836700
O	1.89517100	0.29047300	-0.98411300
C	-3.17157800	1.02751300	-0.61642300
H	-3.97345000	1.19742500	-1.34821100
C	-1.96127700	1.80313400	-1.10341600
O	-2.00479100	3.02138100	-1.31680800
C	-3.63157000	1.59805900	0.74155700
H	-2.79823400	1.49750000	1.45530800
C	-4.17111000	3.02968000	0.77091800
H	-3.33891200	3.72351800	0.59556800
C	-3.85335100	-1.26804600	-0.31163900
C	-6.29383000	-1.41427400	-0.05502500
C	-6.53761800	-2.59876000	-0.97934400
H	-7.50122700	-3.06478900	-0.74552800
H	-6.56750900	-2.26558400	-2.02128600
H	-5.74683300	-3.34047000	-0.87084700
C	-7.38858100	-0.37089400	-0.22660100
H	-7.22236200	0.47744800	0.44578500
H	-7.40604700	0.00604400	-1.25340900
H	-8.36811500	-0.80267800	0.00151700
C	-6.20550700	-1.83798600	1.40519800
H	-5.43556000	-2.59494300	1.55146300
H	-5.97442300	-0.97264400	2.03613100
H	-7.16905800	-2.24288500	1.73244600
O	-0.83339200	1.15803200	-1.24798400
O	-5.09924100	-0.68963700	-0.45712500
N	-2.85726400	-0.39277600	-0.50675600
Pd	-0.75781100	-0.75318200	-0.50453400

Cs	1.13514000	3.22393300	-0.60138800
O	-3.72148800	-2.46854400	-0.03998100
C	0.02518500	-1.35214200	2.70451900
H	0.51473000	-0.70579500	3.43601900
H	-0.72271200	-0.76105600	2.16201300
H	-0.49309300	-2.15112700	3.24232500
O	7.94680400	-0.87088100	-1.28976000
C	9.10121200	-0.10696900	-0.99836100
H	9.87628000	-0.46110200	-1.67693200
H	8.93055800	0.96334100	-1.17020900
H	9.43264800	-0.25300500	0.03729800
H	-4.42170700	0.92892600	1.10459100
C	-5.20685800	3.26994000	-0.32041900
H	-5.98531400	2.49636900	-0.30205900
H	-5.69932500	4.23986700	-0.19145800
H	-4.74436800	3.26111500	-1.31099400
C	-4.76024000	3.31111800	2.14823600
H	-5.10850500	4.34589400	2.23600800
H	-5.62104600	2.65761200	2.34214500
H	-4.03196600	3.13322900	2.94754300

Int4-R

C	1.11272600	3.51482000	0.43073500
H	1.73513400	4.41532100	0.43734800
C	-0.07926200	3.76301300	-0.46847000
C	-0.39911500	5.07332500	-0.82435400
C	-1.51620000	5.34599200	-1.61150900
H	0.23825400	5.88953400	-0.48458400
C	-1.99081200	2.98178600	-1.70532800
C	-2.31222500	4.29511500	-2.05422900
H	-1.75456500	6.37060900	-1.88327100
H	-2.61848800	2.16861500	-2.07266100
H	-3.18050400	4.49338100	-2.67908100
S	3.64284300	2.41939800	0.27081400
C	3.77491800	0.76862000	0.94239800
C	2.77890100	0.28021100	1.77938900
C	4.81671000	-0.05919700	0.52694500
C	2.77478800	-1.05529000	2.16089500
H	1.94587100	0.91428700	2.07067600
C	4.83205300	-1.38966400	0.92070800
H	5.57796900	0.33549600	-0.13879800
C	3.78530000	-1.90332900	1.70164900
H	1.94162600	-1.43270200	2.74098900
H	5.62304500	-2.06223600	0.59990300
O	3.76967500	3.40423700	1.34245600

O	4.51068300	2.48814700	-0.89572300
N	1.97396900	2.44962300	-0.15215500
C	1.44336100	1.31960100	-0.78595200
O	2.19529500	0.55703800	-1.39629800
C	-2.19659600	-1.64663900	0.21525500
H	-2.72194700	-2.08923800	1.07199000
C	-0.72966400	-2.09259900	0.31107000
O	-0.47088700	-3.31093900	0.34783300
C	-2.86928600	-2.13818300	-1.07457100
H	-2.34638000	-1.68299300	-1.92949100
C	-2.98391700	-3.64985700	-1.27333800
H	-1.97282500	-4.05710900	-1.39910100
C	-3.35363700	0.36461700	0.70874300
C	-5.73485200	0.19630200	1.38223600
C	-5.71842100	1.10593100	2.59783700
H	-6.74509400	1.38300200	2.85568300
H	-5.28460900	0.58706700	3.45702300
H	-5.15107400	2.01851500	2.41447700
C	-6.53056600	-1.06827200	1.65605500
H	-6.51196400	-1.73109100	0.78637700
H	-6.11502900	-1.61043000	2.50941800
H	-7.57101700	-0.81737300	1.87818300
C	-6.24461200	0.88775200	0.12908900
H	-5.70864300	1.81388000	-0.07935500
H	-6.15550200	0.22420900	-0.73662400
H	-7.30410400	1.12866300	0.25713800
O	0.17029500	-1.17806600	0.32504400
O	-4.38189600	-0.35603900	1.14109000
O	-3.48772100	1.68884600	0.77839700
N	-2.27697700	-0.18594700	0.27406300
Pd	-0.40315000	0.80873100	-0.34748800
C	-0.88339600	2.68695400	-0.89304800
H	-2.68146200	2.08623700	0.38573200
Cs	2.22862400	-2.41896900	-1.32175100
C	0.69007500	3.21489400	1.86467400
H	0.07910000	4.03705200	2.25013200
H	0.08564400	2.29963000	1.89587900
H	1.56147900	3.10480700	2.51557600
O	3.78385000	-3.25225100	1.88516000
C	2.63817700	-3.80788000	2.52350500
H	1.71507700	-3.57758000	1.97039900
H	2.79883900	-4.88538900	2.53746600
H	2.53990600	-3.44711400	3.55375000
H	-3.88426500	-1.71094500	-1.08343400

C	-3.79187100	-3.93229100	-2.53359200
H	-3.84547700	-5.00520100	-2.74496700
H	-4.82184400	-3.56835500	-2.42772000
H	-3.36242100	-3.43889500	-3.41266300
C	-3.60082100	-4.33292000	-0.06004900
H	-4.55061500	-3.85786000	0.22089300
H	-3.80927300	-5.38831800	-0.26397400
H	-2.92359400	-4.28656800	0.79694500
Int4-S			
C	-1.16774700	1.45335400	1.97113600
H	-1.94526700	1.81131000	2.65221400
C	-0.64191900	2.63594000	1.19325700
C	-0.94520600	3.92577600	1.62825100
C	0.12174600	2.42513400	0.02986100
C	-0.51610500	5.04119200	0.91068600
H	-1.53593600	4.05764800	2.53525300
C	0.48953800	3.56207700	-0.71038800
H	2.45850900	2.65323100	-0.40697600
C	0.18988300	4.85482200	-0.27157600
H	-0.75594900	6.04199700	1.25961500
H	1.00540000	3.44398300	-1.66423800
H	0.49851500	5.71248300	-0.86533600
S	-3.21951500	-0.35101300	1.63754500
C	-4.58144800	0.13514100	0.62042900
C	-5.30669700	1.27753300	0.97172000
C	-4.92998300	-0.61120100	-0.49933400
C	-6.38195100	1.66767000	0.19490500
H	-5.02929800	1.83971300	1.85798300
C	-6.01281600	-0.22539000	-1.27912900
H	-4.34004900	-1.48120000	-0.76137000
C	-6.73968300	0.91986500	-0.93528200
H	-6.96684400	2.54718800	0.44185100
H	-6.27771400	-0.81281800	-2.15074300
O	-3.45765400	0.16558600	2.98191500
O	-2.98214600	-1.78679100	1.44668800
N	-1.85824900	0.51061100	1.04732500
C	-1.33607500	0.13842100	-0.20713700
O	-2.00146800	-0.60999700	-0.92255300
C	3.24280500	-1.03942700	-0.61959600
H	3.99215200	-1.21803300	-1.40299300
C	2.07510200	-1.99354900	-0.89490800
O	2.26699700	-3.21855400	-0.80996100
C	3.88831500	-1.31040400	0.74800500
H	3.12119900	-1.17725900	1.52548800

C	4.59864000	-2.65239900	0.94100200
H	3.83800400	-3.43931400	0.99618900
C	3.69140700	1.27290100	-0.75233500
C	6.08752700	1.90737200	-0.67029800
C	6.11649200	3.02968200	-1.69291300
H	7.03164200	3.61540500	-1.56161000
H	6.12119200	2.62174300	-2.70741300
H	5.26210900	3.69855200	-1.58778300
C	7.29043000	0.99339300	-0.82916500
H	7.25943300	0.18377400	-0.09392800
H	7.31027500	0.54926900	-1.82784500
H	8.21465900	1.55881100	-0.68240200
C	5.98573500	2.41101500	0.75923500
H	5.14017400	3.08526300	0.89829400
H	5.88917600	1.57158600	1.45527400
H	6.90063100	2.95314600	1.01610700
O	0.94001500	-1.47101700	-1.19017100
O	4.97068100	0.98133300	-0.96715500
N	2.79057900	0.35928600	-0.67944400
Pd	0.56316100	0.54733500	-0.54741500
Cs	-0.94266100	-3.43463800	-0.20315200
O	3.40191100	2.57068300	-0.65360800
C	-0.10711200	0.73022600	2.79215800
H	-0.55362900	-0.09099800	3.36200900
H	0.67213200	0.33046000	2.13144300
H	0.36190700	1.42283500	3.49761500
O	-7.80622900	1.38400800	-1.62974500
C	-8.18872100	0.66895900	-2.78826800
H	-9.04734400	1.19857100	-3.20005200
H	-7.38408900	0.64852100	-3.53358000
H	-8.47953800	-0.36177600	-2.54976700
H	4.62859900	-0.51536700	0.91757600
C	5.51500600	-2.98295900	-0.22944700
H	6.18104200	-2.14127500	-0.46413900
H	6.14540900	-3.84971300	-0.00513900
H	4.93165300	-3.21799300	-1.12370900
C	5.37481900	-2.61783000	2.25188700
H	5.85111600	-3.58076300	2.46356500
H	6.16944100	-1.86012900	2.21546300
H	4.72940300	-2.37011600	3.10182100
Int5-R			
C	-3.58660900	0.76690900	0.28346700
H	-4.45830900	1.42306100	0.19744200
C	-3.89125400	-0.54403400	-0.40263400

C	-5.22127000	-0.90015600	-0.63153000
C	-5.53842900	-2.13729200	-1.18535400
H	-6.01491300	-0.19927900	-0.37280200
C	-3.18563200	-2.66418400	-1.29446700
C	-4.51565900	-3.02027800	-1.51912500
H	-6.57626500	-2.40528300	-1.36349000
H	-2.39829700	-3.36369500	-1.58001500
H	-4.75066600	-3.98662000	-1.96031000
S	-2.40244700	3.20133500	-0.29098800
C	-0.73546300	3.38318200	0.32624200
C	-0.27296700	2.52756800	1.31859100
C	0.12202400	4.30714000	-0.26740300
C	1.06861400	2.53151700	1.67969400
H	-0.94389200	1.79640600	1.76327100
C	1.45754800	4.33903300	0.10800300
H	-0.25607300	4.95976300	-1.04840700
C	1.94495400	3.41878400	1.04874400
H	1.42340900	1.80620600	2.40395300
H	2.15337100	5.04102000	-0.34305700
O	-3.36060800	3.53271000	0.75919300
O	-2.46476800	3.86433400	-1.58441900
N	-2.49107100	1.48336600	-0.43201200
C	-1.39708300	0.83152200	-0.99746100
O	-0.61434000	1.45018500	-1.71920100
C	1.43580400	-2.85139100	-0.06757800
H	2.14433500	-3.51657300	0.44134600
C	1.98004900	-1.41433700	0.06598200
O	3.20589300	-1.23917500	-0.03890800
C	1.29567300	-3.25134800	-1.53816700
H	0.51280500	-2.61561300	-1.98656300
C	2.56586400	-3.18026200	-2.38474000
H	2.88785400	-2.12856100	-2.42000100
C	-0.07414700	-2.84082100	1.92905300
C	0.96178500	-1.55448600	3.71266900
C	-0.14959800	-0.52695700	3.56826200
H	-0.04258700	0.25374100	4.32846100
H	-0.08125700	-0.06694200	2.57446100
H	-1.13672200	-0.97979800	3.67232600
C	2.32213000	-0.87966600	3.74204500
H	3.12529300	-1.62017000	3.78656500
H	2.46062900	-0.29054200	2.83006700
H	2.40335200	-0.22425100	4.61479600
C	0.75931900	-2.48543800	4.89245600
H	-0.19916500	-3.00050100	4.81610300

H	1.55939600	-3.22964000	4.93778100
H	0.77681700	-1.91170400	5.82454300
O	1.12274600	-0.46906500	0.20163900
O	1.04478800	-2.33882900	2.46754700
O	-1.10223700	-3.13253100	2.50269900
N	0.09478300	-2.96572900	0.54115000
Pd	-0.95220300	-0.95396700	-0.32022300
C	-2.85188900	-1.43246900	-0.71782400
Cs	2.36438800	1.35438900	-1.75561300
C	-3.27409800	0.55362200	1.75947000
H	-4.11612000	0.05343500	2.24668000
H	-2.39959100	-0.10102700	1.85774700
H	-3.09706700	1.50346200	2.27240000
O	3.29474600	3.41055700	1.22708200
C	3.82662200	2.36446400	2.02941000
H	3.57628600	1.37607800	1.61643300
H	4.90739100	2.50108000	2.02319800
H	3.46272000	2.41981100	3.06231500
H	0.90865300	-4.28242700	-1.57910300
C	2.25836000	-3.64006700	-3.80388200
H	3.13467100	-3.54706600	-4.45308700
H	1.95708600	-4.69426100	-3.81409300
H	1.44230500	-3.06420200	-4.25335400
C	3.70803700	-3.98349400	-1.77663000
H	3.40761600	-5.02564300	-1.60904800
H	4.57494000	-3.99870200	-2.44501900
H	4.02737500	-3.55253100	-0.82439000
H	-0.48809900	-3.71063300	0.17486800
Int5-S			
C	-1.31097100	-0.78429700	2.55154600
H	-2.21659500	-1.03327600	3.11162500
C	-0.74549600	0.49581200	3.11571500
C	-1.11462000	0.88556500	4.40583200
C	0.18618600	1.25016500	2.38961700
C	-0.56789700	2.02679400	4.98535100
H	-1.83842900	0.28632900	4.95917000
C	0.72053400	2.40551700	2.97649100
C	0.35095500	2.78730300	4.26644100
H	-0.86442500	2.32417900	5.98773500
H	1.42980000	3.01771000	2.41843000
H	0.77648600	3.68705000	4.70604500
S	-3.04232200	-1.61276700	0.58592800
C	-4.26592500	-0.50337400	-0.03466100
C	-5.17542100	0.05602300	0.86837500

C	-4.33230400	-0.20639400	-1.39070200
C	-6.15125200	0.91697800	0.40402500
H	-5.11749700	-0.19973900	1.92175200
C	-5.31583000	0.65407800	-1.86163800
H	-3.60573200	-0.64205800	-2.06598800
C	-6.22603300	1.22204300	-0.96271800
H	-6.87388000	1.36668900	1.07647000
H	-5.36130200	0.88136000	-2.92050900
O	-3.57551900	-2.25593500	1.78220600
O	-2.54500000	-2.44358500	-0.51727800
N	-1.75548700	-0.60712100	1.14298200
C	-0.99005600	0.05063300	0.17290800
O	-1.39617400	0.09113200	-0.98916200
C	3.70189800	-0.18059400	0.15243600
H	4.73883500	-0.05995000	-0.18616400
C	2.87485000	-0.62048600	-1.07497400
O	3.33337100	-1.52365900	-1.79203900
C	3.63663400	-1.20017800	1.29386600
H	2.61991800	-1.15820400	1.71689900
C	3.99054400	-2.64770800	0.96116100
H	3.26936100	-3.00724200	0.21224100
C	3.32976900	2.30326300	0.00571100
C	3.36377000	3.03899200	-2.31049700
C	1.87960100	3.35818100	-2.24332500
H	1.59899600	3.96150400	-3.11203700
H	1.29206500	2.43466200	-2.25589600
H	1.63066300	3.92076500	-1.34150200
C	3.69916400	2.26325500	-3.57126700
H	4.75522000	1.98054000	-3.58455800
H	3.09902100	1.35109300	-3.62417600
H	3.49416200	2.87526900	-4.45417700
C	4.23954400	4.26953400	-2.15863400
H	4.00786600	4.80727600	-1.23875100
H	5.29708400	3.99027200	-2.14808100
H	4.07685200	4.94059000	-3.00819000
O	1.73064900	-0.06374200	-1.24947800
O	3.69170300	2.05835100	-1.25385300
N	3.19234100	1.09420600	0.70406000
Pd	0.81999800	0.68341900	0.59244000
Cs	0.17506000	-2.41910600	-2.01791200
O	3.10844800	3.38284900	0.51995800
C	-0.34642900	-1.96318000	2.64607000
H	-0.82774600	-2.88787400	2.30907100
H	0.53519600	-1.76730700	2.02233100

H	-0.00843100	-2.10512300	3.67695500
O	-7.21702600	2.07347600	-1.31639600
C	-7.32106600	2.41903700	-2.68445000
H	-8.16487000	3.10406400	-2.75934600
H	-6.41376300	2.92022100	-3.04355400
H	-7.51293100	1.53803400	-3.30950800
H	4.30837500	-0.85420400	2.09589600
C	5.38192700	-2.77191700	0.35575700
H	6.13908500	-2.34563200	1.02638600
H	5.64667700	-3.82137500	0.19087300
H	5.43222300	-2.25832800	-0.60721800
C	3.85219100	-3.50069000	2.21589700
H	4.04967500	-4.55636500	2.00476300
H	4.56754100	-3.18321900	2.98442100
H	2.85013000	-3.42652500	2.65303100
H	3.35210100	1.22982700	1.69667500
TS1-R			
C	0.37011900	3.41010000	0.73068900
H	0.85192900	4.33435600	1.06412800
C	-0.54043500	3.73829400	-0.42947400
C	-0.48691700	5.00614400	-1.00307500
C	-1.26639900	5.31047100	-2.11704500
H	0.18242700	5.75662600	-0.58609000
C	-2.14709900	3.07308500	-2.10553800
C	-2.09895100	4.34065100	-2.67310000
H	-1.21943900	6.30484000	-2.55365400
H	-2.81562600	2.31956800	-2.51989900
H	-2.70648600	4.57741100	-3.54271200
S	2.96974000	2.54129700	1.07531300
C	3.10183600	0.80575800	1.48161500
C	1.97744100	0.07462900	1.85093600
C	4.34495900	0.17952200	1.38148900
C	2.06922400	-1.29361800	2.07597200
H	1.00204200	0.55138700	1.90177600
C	4.45112300	-1.18124600	1.63045700
H	5.21186300	0.76141800	1.08370100
C	3.30767900	-1.93190600	1.94988300
H	1.16870000	-1.85654500	2.29233800
H	5.40735100	-1.69259300	1.56093200
O	2.69676600	3.31278500	2.28603900
O	4.11124500	2.87790000	0.23721100
N	1.48701100	2.56503900	0.20423600
C	1.28625500	1.57724600	-0.78752900
O	2.26527400	1.04271200	-1.30444300

C	-2.00631600	-1.82569000	-0.21650300
H	-2.30781100	-2.16884700	0.78381100
C	-0.50814400	-2.12627600	-0.35557100
O	-0.06892500	-3.26208700	-0.11180800
C	-2.84339200	-2.59225400	-1.25069700
H	-2.55989000	-2.24119300	-2.25327500
C	-2.79061900	-4.11879300	-1.19691600
H	-1.77407900	-4.43791500	-1.46126400
C	-3.18301900	0.20843400	0.32984900
C	-5.11281800	-0.03011200	1.84475000
C	-4.47067800	0.72691400	2.99647600
H	-5.23496700	0.98623000	3.73587500
H	-3.72222500	0.10146000	3.49296500
H	-3.99249500	1.64500800	2.65388000
C	-5.79619500	-1.29305400	2.34405000
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H	-5.08798500	-1.93304900	2.87814700
H	-6.61425500	-1.03905100	3.02400400
C	-6.08588200	0.82943300	1.05426800
H	-5.60959400	1.74058500	0.69239100
H	-6.47646800	0.27108000	0.19843200
H	-6.93268900	1.10436800	1.69132800
O	0.26648800	-1.16516600	-0.74856600
O	-4.07932800	-0.57957500	0.95744100
O	-3.28345600	1.48416700	0.39712200
N	-2.22666700	-0.39241000	-0.33762100
Pd	-0.52774400	0.78769000	-0.82174500
C	-1.38620000	2.74049800	-0.96627700
H	-2.22668400	2.01130100	-0.19419900
Cs	2.90280900	-1.90770000	-1.51896100
C	-0.35223400	2.79263900	1.92005100
H	-1.14429100	3.46532700	2.26340900
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H	0.34364900	2.63414400	2.74727200
O	3.48352900	-3.27284200	2.04612200
C	2.31956700	-4.05907600	2.29899400
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C	-3.76482200	-4.69591100	-2.21617200
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H	-3.56326300	-4.32464300	-3.22695000

C	-3.08858200	-4.64493900	0.20158700
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H	-3.20356000	-5.73409400	0.19892600
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H	-1.57037000	2.16010500	2.38244300
C	-0.56171000	2.80901600	0.62919000
C	-1.38060600	3.93742700	0.58503400
C	0.41839900	2.59254900	-0.36771900
C	-1.25838700	4.86573900	-0.44687200
H	-2.13039600	4.08452300	1.36223500
C	0.49771900	3.53708100	-1.41180700
H	1.71918000	2.31289600	-0.15785200
C	-0.32077400	4.65942600	-1.45616100
H	-1.89698100	5.74506800	-0.46359100
H	1.25860700	3.39570100	-2.17705700
H	-0.22513200	5.37625800	-2.26765200
S	-2.80952900	-0.19199000	1.79585100
C	-4.26709300	0.18435700	0.86348700
C	-4.43741900	1.46100800	0.32335800
C	-5.26039700	-0.77800500	0.73579900
C	-5.60469800	1.76637900	-0.34949900
H	-3.64196000	2.19891300	0.40511300
C	-6.44117200	-0.47319200	0.06571700
H	-5.10778500	-1.76663500	1.15773800
C	-6.61470200	0.80275400	-0.47989100
H	-5.76018100	2.74360600	-0.79376800
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O	-2.90321500	0.42527900	3.11614600
O	-2.56915500	-1.63758700	1.70409000
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O	-1.96180100	-0.58248200	-0.89895300
C	3.28248400	-1.09420300	-0.85145400
H	4.08092600	-1.22986700	-1.59437100
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O	2.32553700	-3.23853300	-1.39195900
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H	2.97369100	-1.43026300	1.25174300
C	4.48522100	-2.87037400	0.66816500
H	3.72609000	-3.65049900	0.53373300
C	3.54714100	1.29842300	-0.48784400
C	5.79608800	2.06488800	0.16003500

C	5.84781200	3.36062300	-0.63184500
H	6.62274300	4.01590100	-0.22077100
H	6.09714600	3.15663200	-1.67708200
H	4.89091700	3.88151700	-0.59411400
C	7.12329400	1.32664900	0.08404400
H	7.07391700	0.38327600	0.63718400
H	7.38050300	1.09936600	-0.95396500
H	7.92273900	1.93713400	0.51369500
C	5.39400700	2.28475100	1.61041400
H	4.45554200	2.83373800	1.69037600
H	5.28789100	1.32519500	2.12776400
H	6.17527400	2.85519900	2.12243600
O	0.92574700	-1.52640200	-1.26613200
O	4.88379100	1.11574700	-0.48983200
N	2.80078600	0.27961800	-0.83813800
Pd	0.70067300	0.48579900	-0.75758900
Cs	-1.03797300	-3.43824900	-0.36154300
O	3.04946300	2.43779900	-0.18155400
C	0.35726500	1.25155700	2.45503100
H	0.03426300	0.53708900	3.21719100
H	1.08767700	0.75920000	1.80384900
H	0.85393900	2.08837000	2.95537100
O	-7.71962400	1.20220700	-1.15512400
C	-8.75454300	0.25339900	-1.32101200
H	-9.53973700	0.75645300	-1.88394200
H	-8.41083700	-0.62434600	-1.88288300
H	-9.15733000	-0.07850300	-0.35564600
H	4.53641600	-0.74314000	0.84792200
C	5.55195200	-3.07705400	-0.39950100
H	6.24858600	-2.22817500	-0.43159900
H	6.14046700	-3.97896500	-0.20056500
H	5.10042900	-3.18720500	-1.38900100
C	5.08113300	-2.99785500	2.06516500
H	5.52808500	-3.98453400	2.22524100
H	5.87130200	-2.25128400	2.22124200
H	4.32831600	-2.84055700	2.84567200
TS2-R			
C	3.05204800	0.87255100	-0.26164700
H	2.81760100	1.33273300	0.70828400
C	4.52920400	1.06258200	-0.51640900
C	5.22580700	2.05493200	0.17336500
C	6.56689600	2.30238500	-0.10331000
H	4.71113300	2.62646600	0.94390900
C	6.54059200	0.55345900	-1.75866700

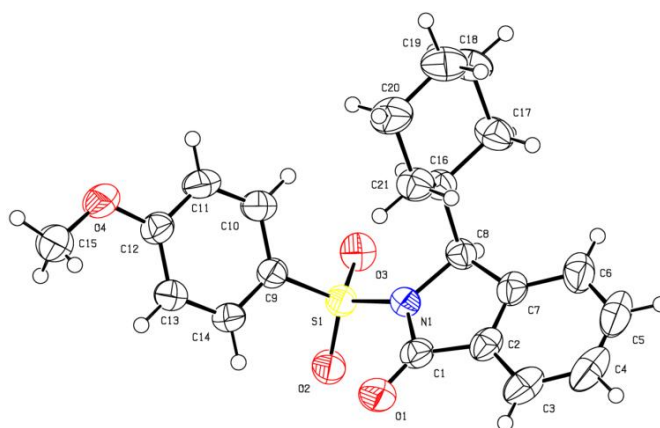
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H	7.05375900	-0.04227400	-2.50906100
H	8.27619100	1.74037500	-1.28681600
S	2.92885500	-1.34341900	1.32554100
C	1.23855900	-1.41729400	1.90265000
C	0.41803100	-0.29652900	1.77777300
C	0.72898300	-2.60521700	2.42498400
C	-0.92845500	-0.36909700	2.11343000
H	0.81119600	0.63854600	1.38324800
C	-0.60539800	-2.67357000	2.80188100
H	1.38136700	-3.46937100	2.51643800
C	-1.45163900	-1.56559300	2.62171300
H	-1.56158500	0.49899300	1.95543000
H	-1.02461400	-3.57925700	3.23254000
O	3.66823200	-0.37606300	2.12723100
O	3.39940800	-2.70800300	1.15711700
N	2.70002900	-0.56667500	-0.20307300
C	1.62413300	-1.05922400	-0.99617600
O	1.38791800	-2.25988600	-1.02148600
C	-2.59066900	1.05813100	-0.84677900
H	-3.00998700	1.26636000	0.14911000
C	-2.41982700	-0.46201300	-0.94858400
O	-3.30269000	-1.21691100	-0.50267500
C	-3.57590600	1.58478000	-1.89806900
H	-3.15079300	1.39223700	-2.89260500
C	-5.00572100	1.05049900	-1.82604000
H	-4.98040700	-0.03135500	-2.01414300
C	-0.91020500	2.65967700	-0.19477300
C	-1.52946200	4.21930900	1.61239600
C	-0.56192900	3.63010700	2.62700400
H	-0.45284100	4.32048000	3.46919100
H	-0.94472000	2.68370500	3.02399600
H	0.42295800	3.45838500	2.19244600
C	-2.88933000	4.45904900	2.24852200
H	-3.60360800	4.82487100	1.50604700
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H	-2.81111400	5.19844600	3.05024700
C	-0.99400100	5.48914500	0.97291000
H	-0.03005900	5.31236400	0.49532100
H	-1.69598400	5.86321600	0.22227200
H	-0.87084700	6.26397000	1.73611400
O	-1.34849100	-0.91334700	-1.52016300
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O	0.30975100	3.04262100	-0.12681500
N	-1.29218000	1.69053500	-0.99496500
Pd	0.33413900	0.36806400	-1.43062800
C	5.19922400	0.30999800	-1.48335600
Cs	-1.25396500	-3.64935400	-0.56877100
C	2.19659200	1.54570800	-1.32689700
H	2.44498800	1.18184900	-2.33180000
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H	-3.34924900	0.22657600	3.26268500
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H	-5.42462000	1.56160500	-3.90349500
C	-5.61916600	1.26482800	-0.44758200
H	-5.52530000	2.31312900	-0.13278000
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H	-5.12850700	0.63851000	0.30361600
H	4.66565500	-0.48134900	-2.00544800
TS2-S			
C	1.38769000	1.71245800	-2.04913000
H	1.88606500	2.07459000	-2.95472700
C	1.68188100	2.70148100	-0.93919500
C	2.48243800	3.81502500	-1.20132600
C	1.18437600	2.51806200	0.35464700
C	2.78394700	4.72769100	-0.19279800
H	2.89402200	3.94457000	-2.19979700
C	1.48228900	3.42855300	1.36293300
C	2.28476100	4.53573800	1.09281100
H	3.41288900	5.58652400	-0.41174300
H	1.08523700	3.27331600	2.36302000
H	2.51867300	5.24625000	1.88145000
S	3.67526800	0.16939000	-1.89059100
C	4.21469000	0.07539000	-0.20613300
C	4.44082900	1.25333500	0.51236200
C	4.41113800	-1.16843100	0.38293800
C	4.86114000	1.17585500	1.82689700
H	4.29213300	2.21944200	0.03745600
C	4.84364900	-1.24922200	1.70219400

H	4.22513500	-2.06215200	-0.20300100
C	5.06685500	-0.07353800	2.42756800
H	5.04479200	2.07153600	2.41170400
H	5.00945100	-2.22144500	2.15333100
O	4.15967100	1.42610800	-2.45343900
O	3.94399000	-1.10689400	-2.53430100
N	1.96184300	0.37416400	-1.77720200
C	1.15867800	-0.61544600	-1.19706600
O	1.63240300	-1.69770900	-0.85128500
C	-3.41846500	-0.62289900	0.38715600
H	-3.55919700	-0.25575100	1.41881600
C	-2.50975500	-1.85885400	0.50352100
O	-2.95035200	-2.96508500	0.83708200
C	-4.79453400	-0.97203300	-0.19174100
H	-4.65287300	-1.63908600	-1.05259600
C	-5.77279800	-1.60665700	0.79916100
H	-5.23823100	-2.41286700	1.31813200
C	-2.90484900	1.66600200	-0.25151000
C	-4.11008200	3.46133700	0.90738500
C	-2.88312000	3.92544300	1.67828800
H	-3.07741400	4.90937300	2.11696800
H	-2.66352700	3.23115400	2.49586200
H	-2.00551900	3.99901600	1.03526000
C	-5.32305100	3.39427300	1.82074400
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H	-3.53598000	4.38394800	-0.96780500
H	-5.25047300	3.93104600	-0.86434600
H	-4.65719600	5.34312400	0.02273400
O	-1.24276600	-1.68424500	0.25600700
O	-3.94993100	2.05613800	0.50250000
N	-2.71330300	0.37389000	-0.39612000
Pd	-0.72688500	-0.06757300	-0.94616700
Cs	0.00325900	-4.19520900	-0.11035100
O	-2.13316500	2.51999400	-0.80689900
C	-0.10010100	1.53846900	-2.33017900
H	-0.25712000	0.88977200	-3.19942400
H	-1.11243000	1.81744400	-1.39929100
H	-0.48159200	2.51656400	-2.65295400
O	5.48919700	-0.03996500	3.71644000
C	5.71880200	-1.27836100	4.35583400
H	6.04766100	-1.04134200	5.36729200

H	4.80479200	-1.88419800	4.40627500
H	6.49997700	-1.85814700	3.84785900
H	-5.23918700	-0.04767600	-0.58548900
C	-6.25904800	-0.58974800	1.82505200
H	-6.80013600	0.22800700	1.33160900
H	-6.94092700	-1.04760900	2.54947400
H	-5.43704700	-0.13684100	2.38881400
C	-6.95525100	-2.21120800	0.05443900
H	-7.67546600	-2.66962300	0.74054400
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H	-6.63171900	-2.98062000	-0.65435600
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4. X-ray structure of (S)-2h (CCDC 1971018)

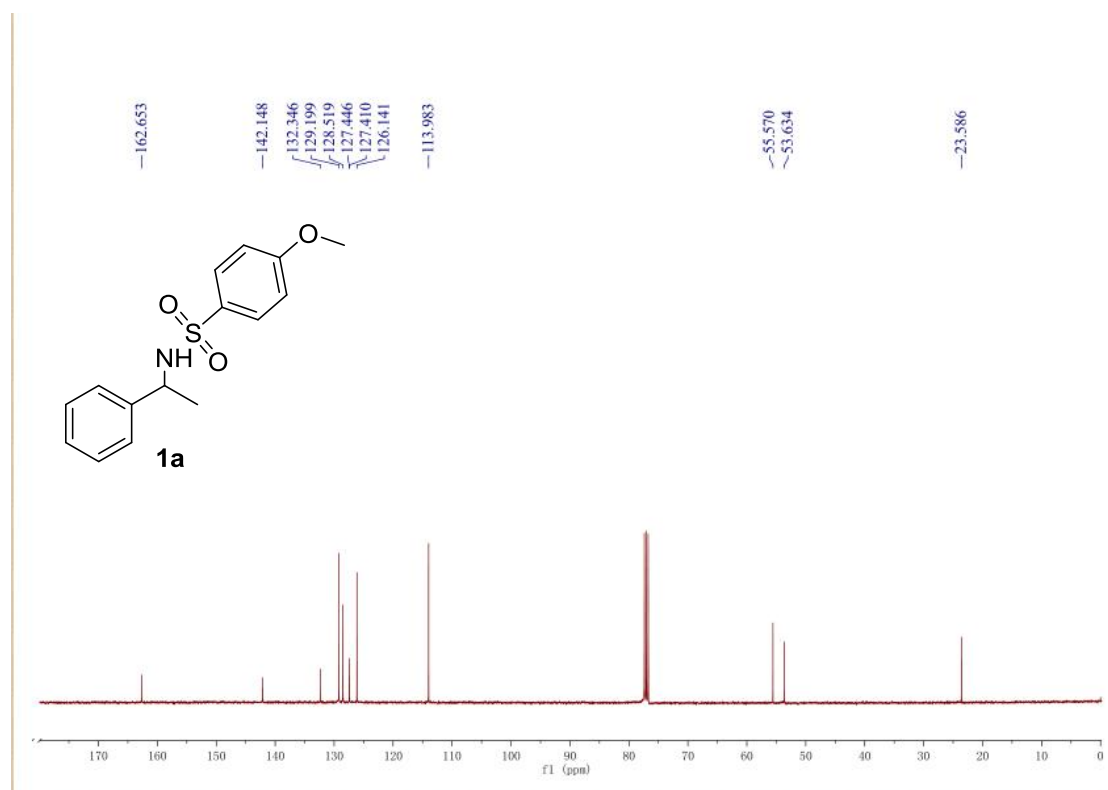
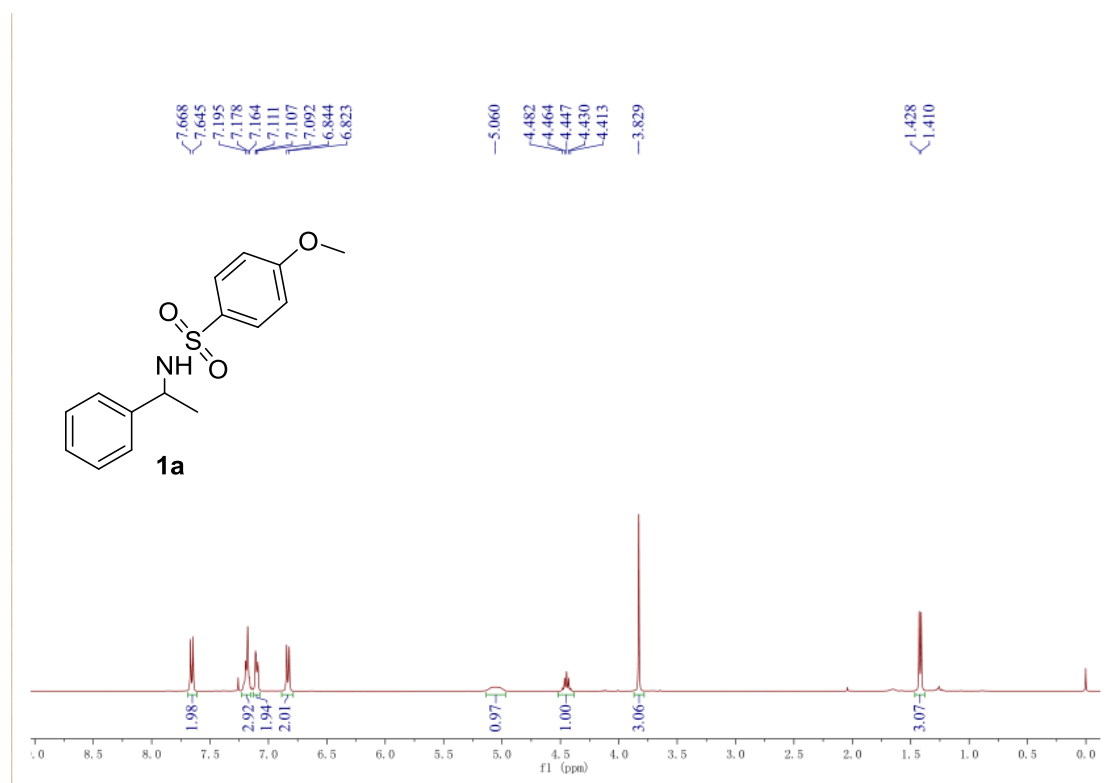


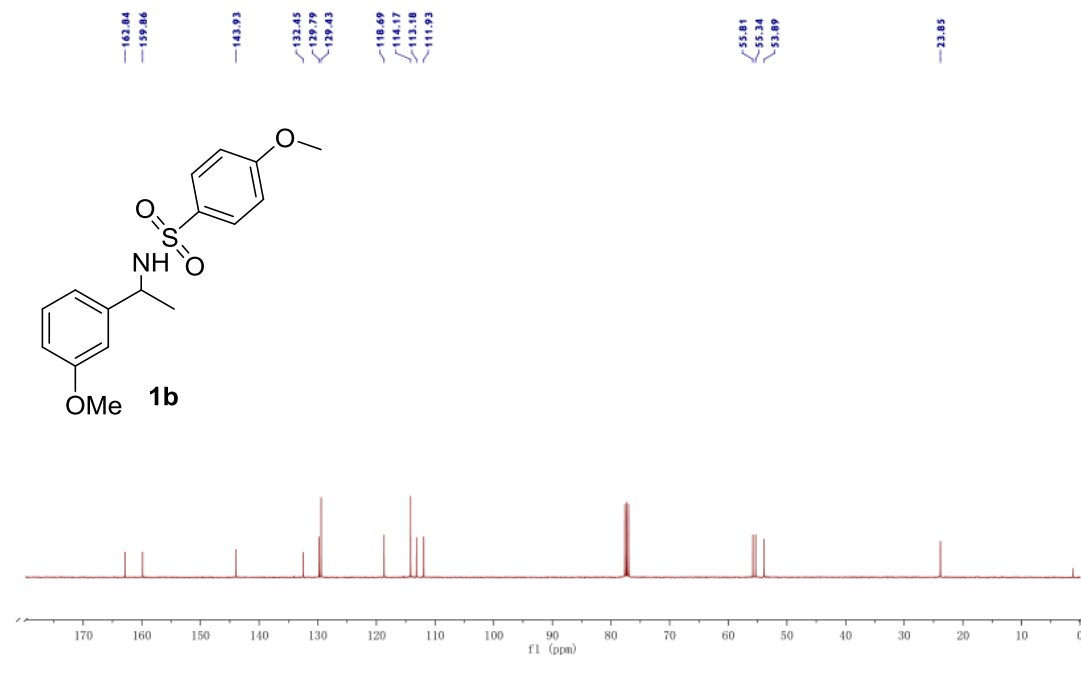
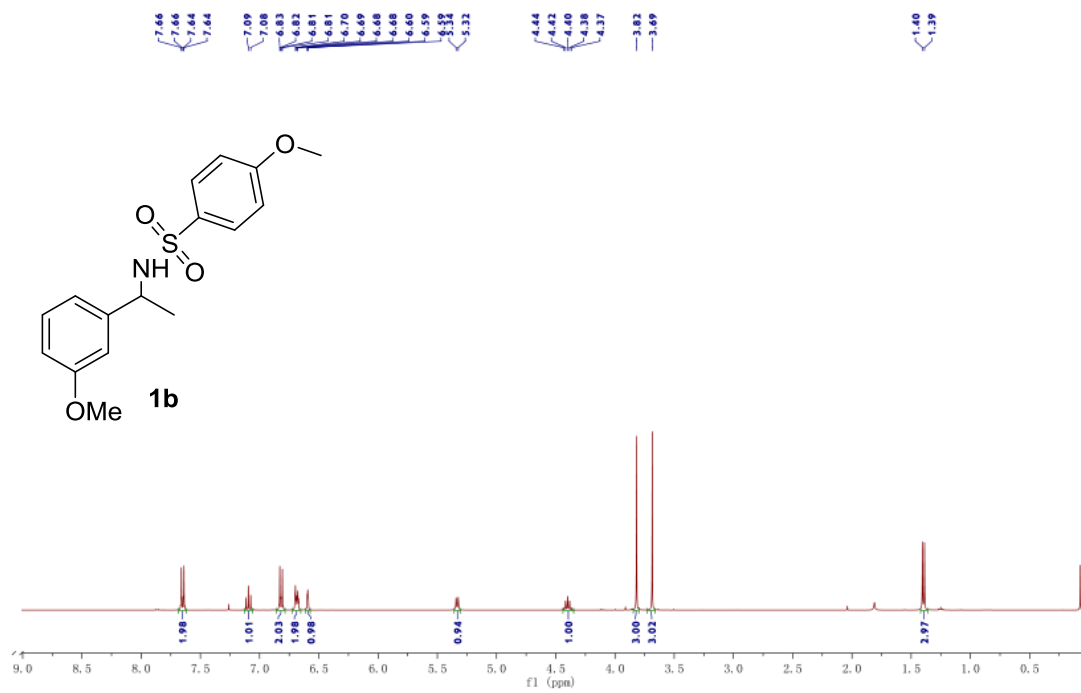
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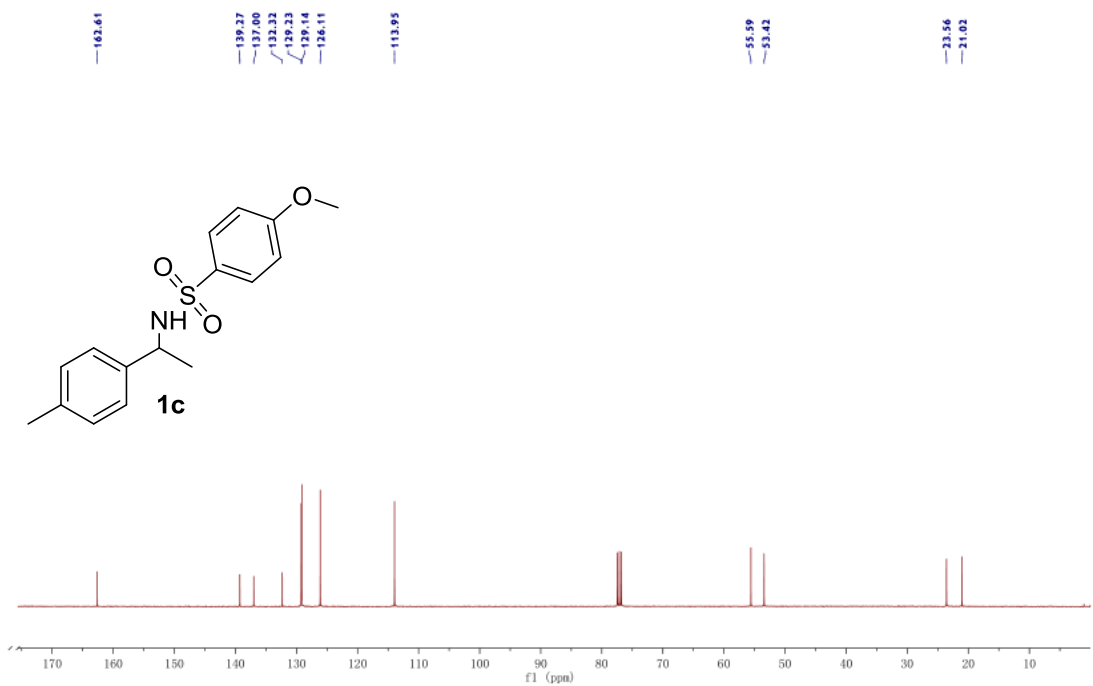
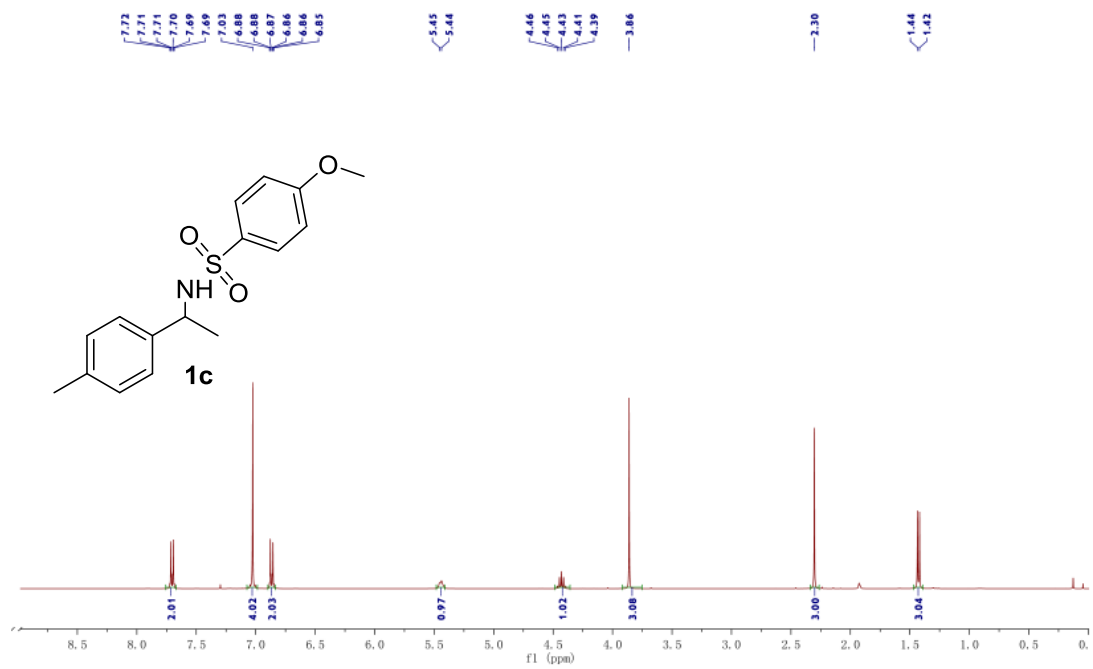
5. Reference

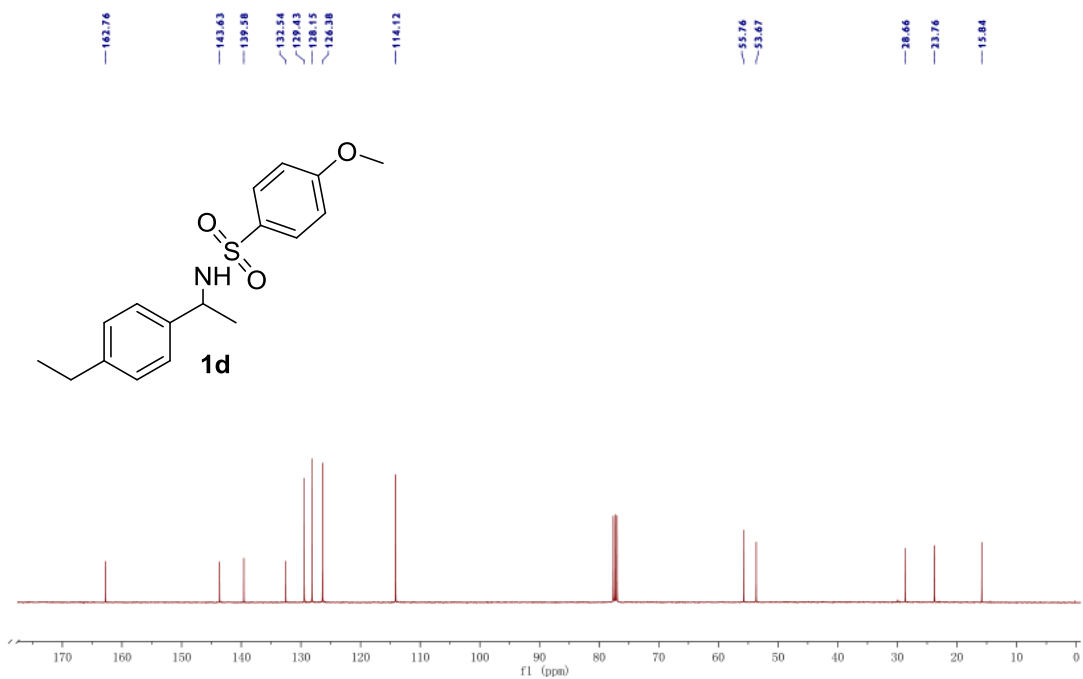
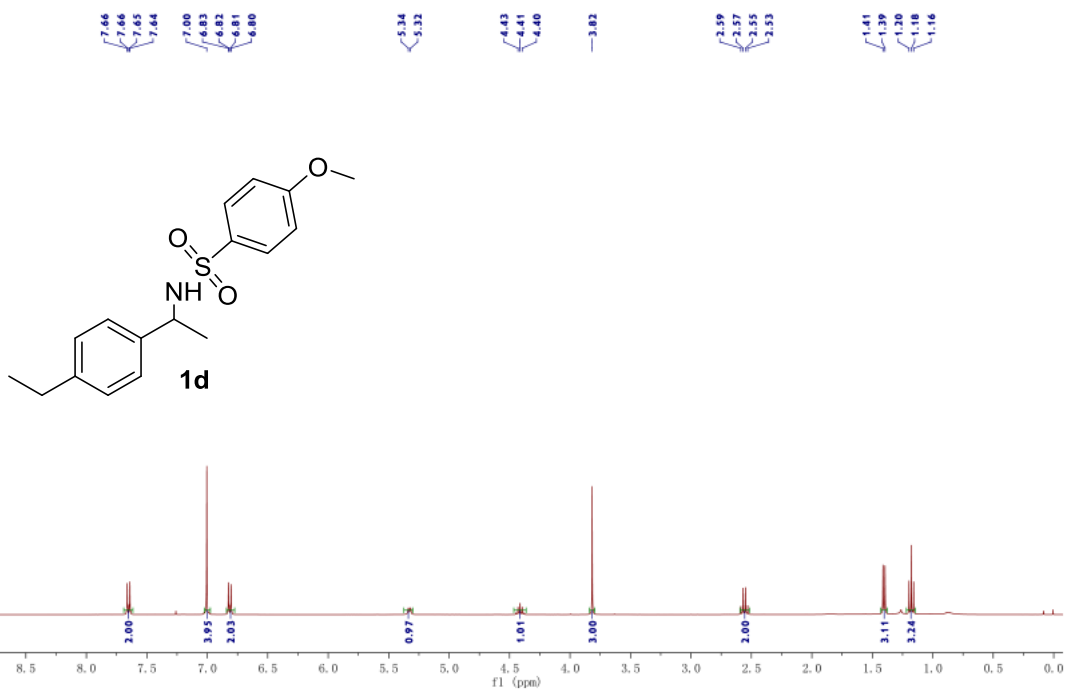
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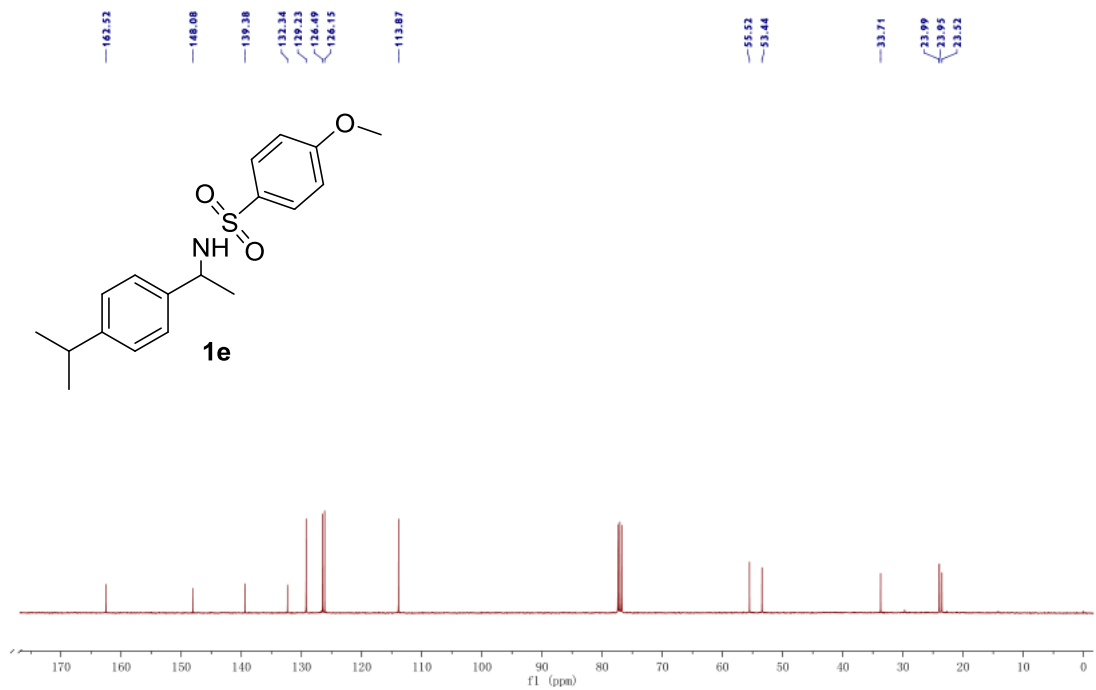
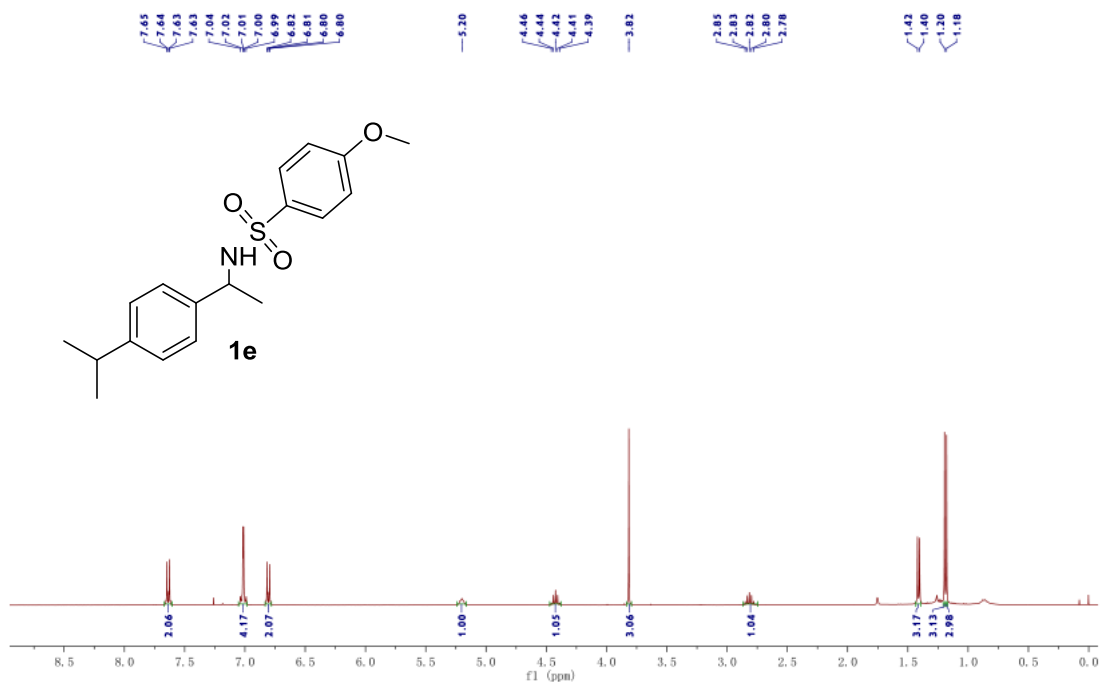
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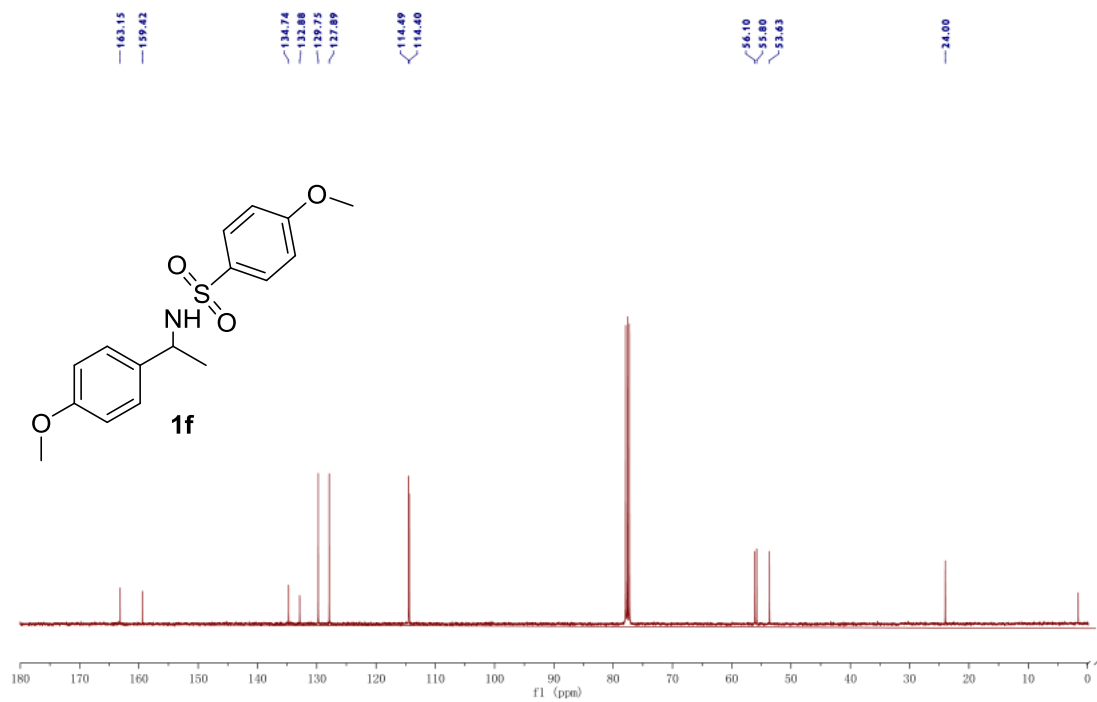
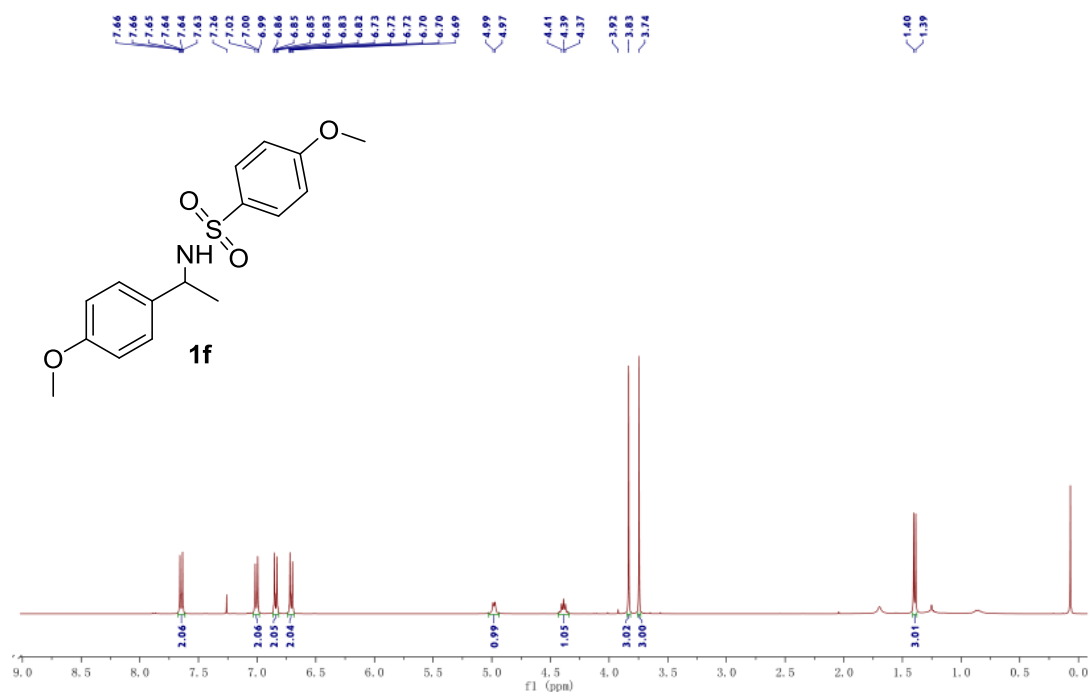


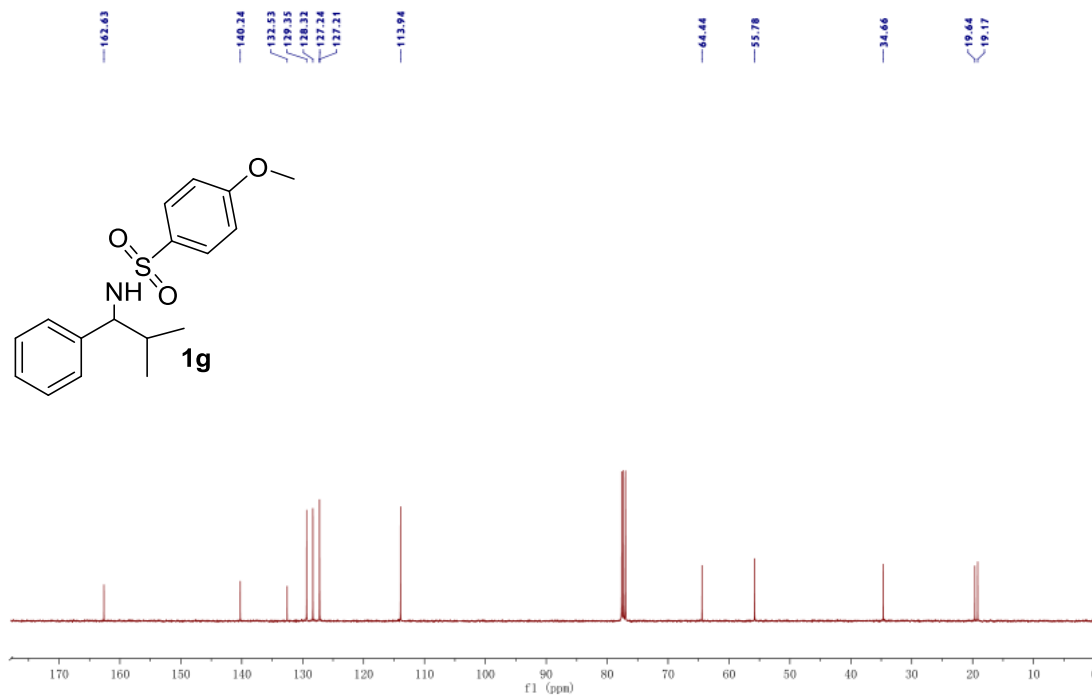
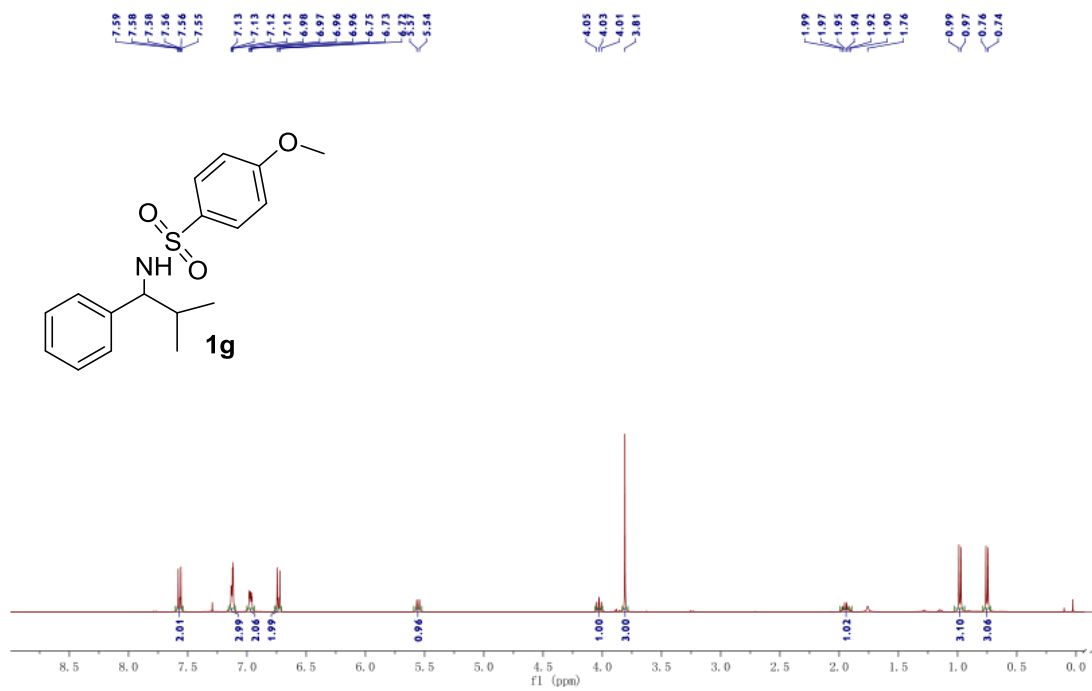


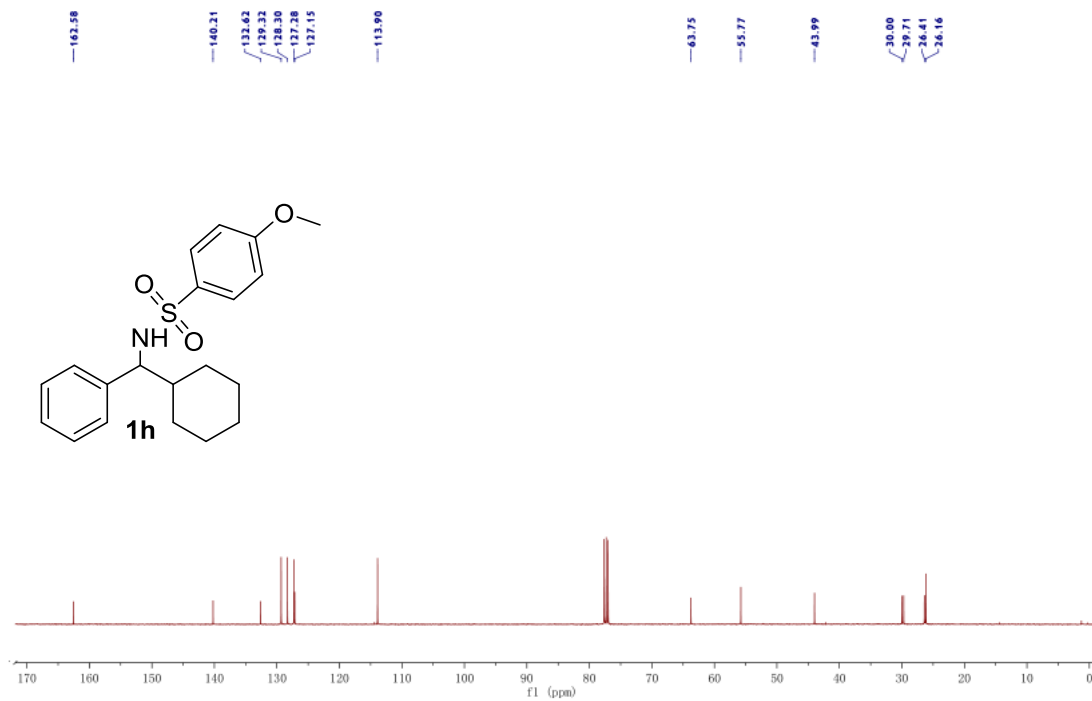
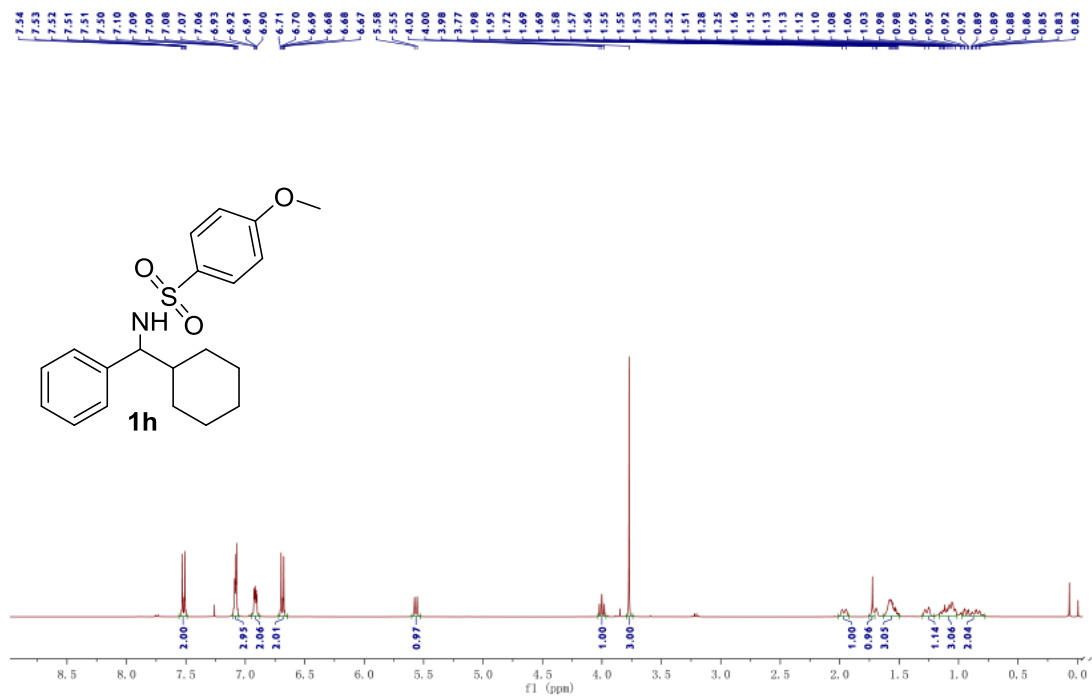


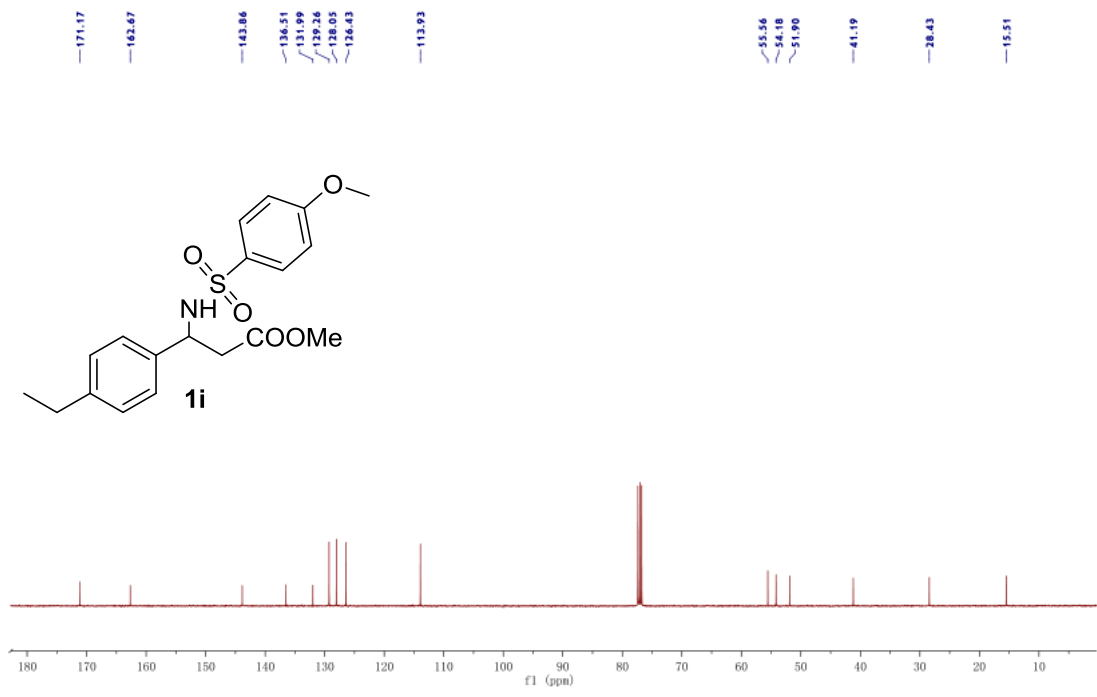
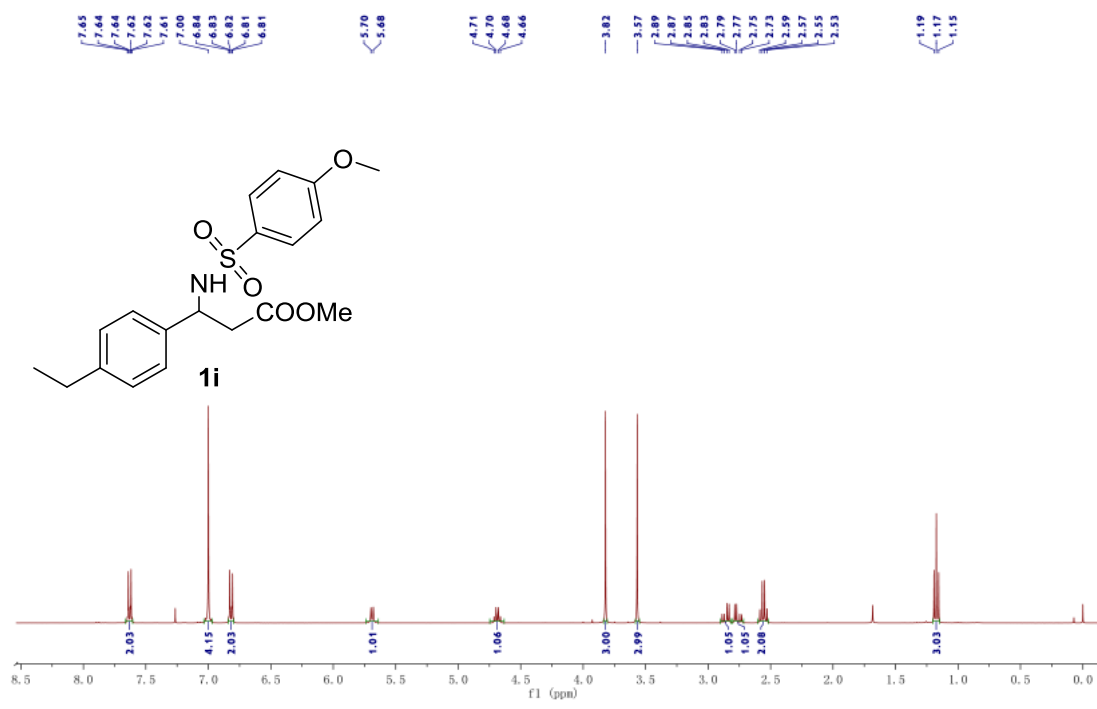


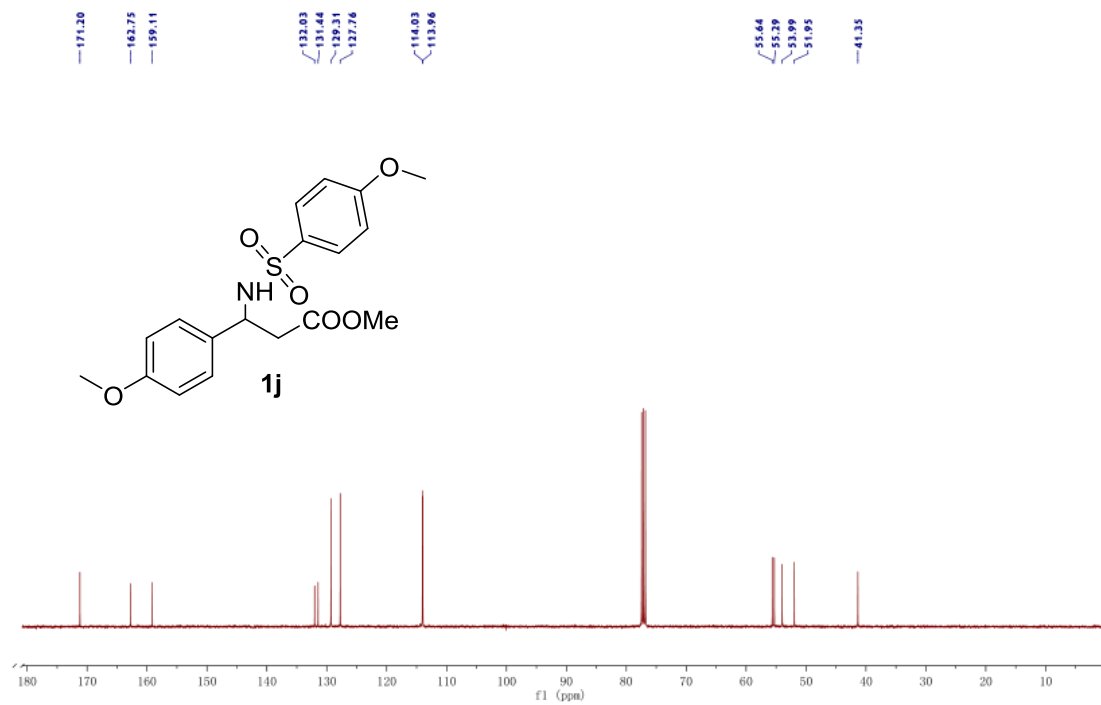
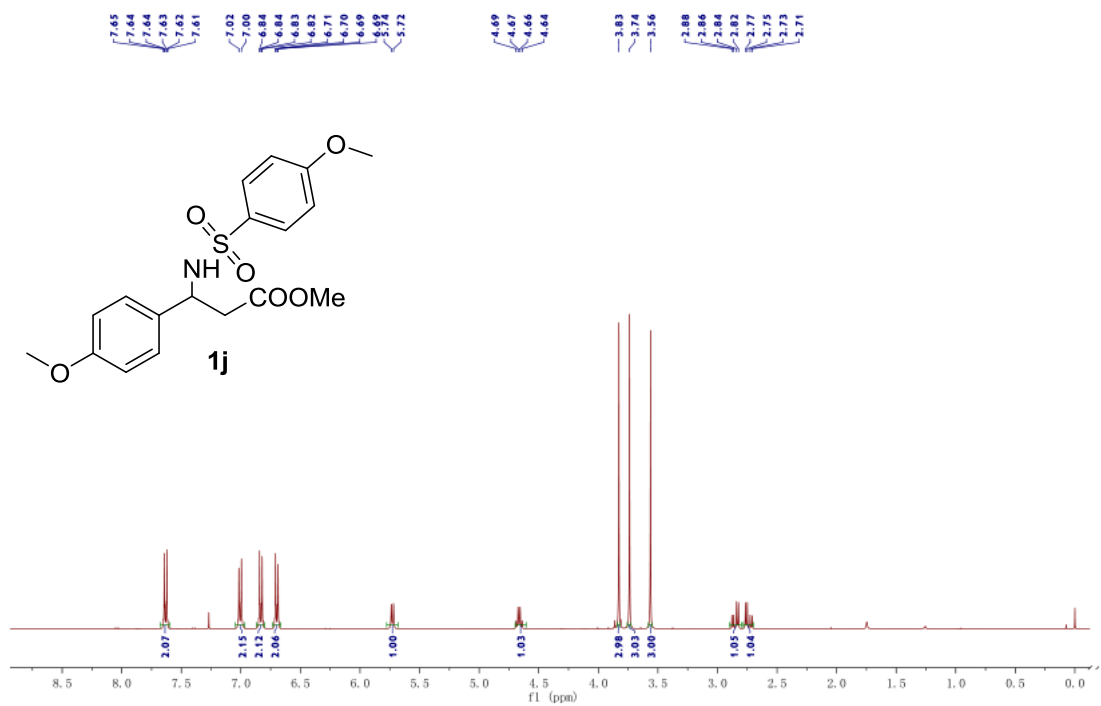


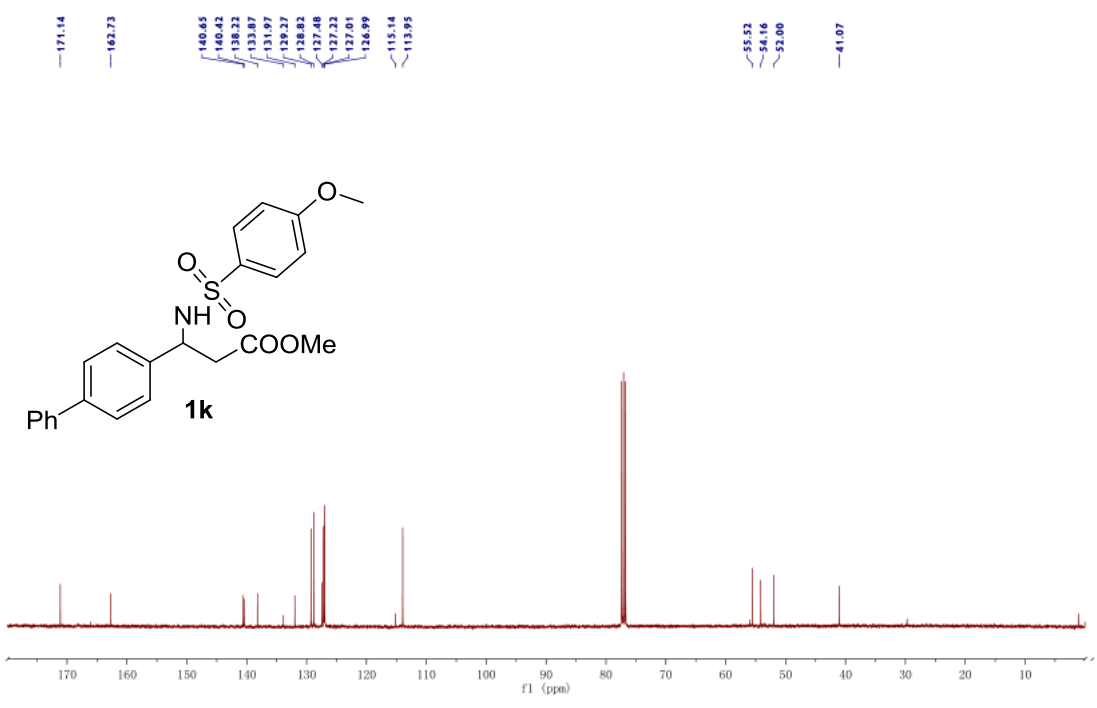
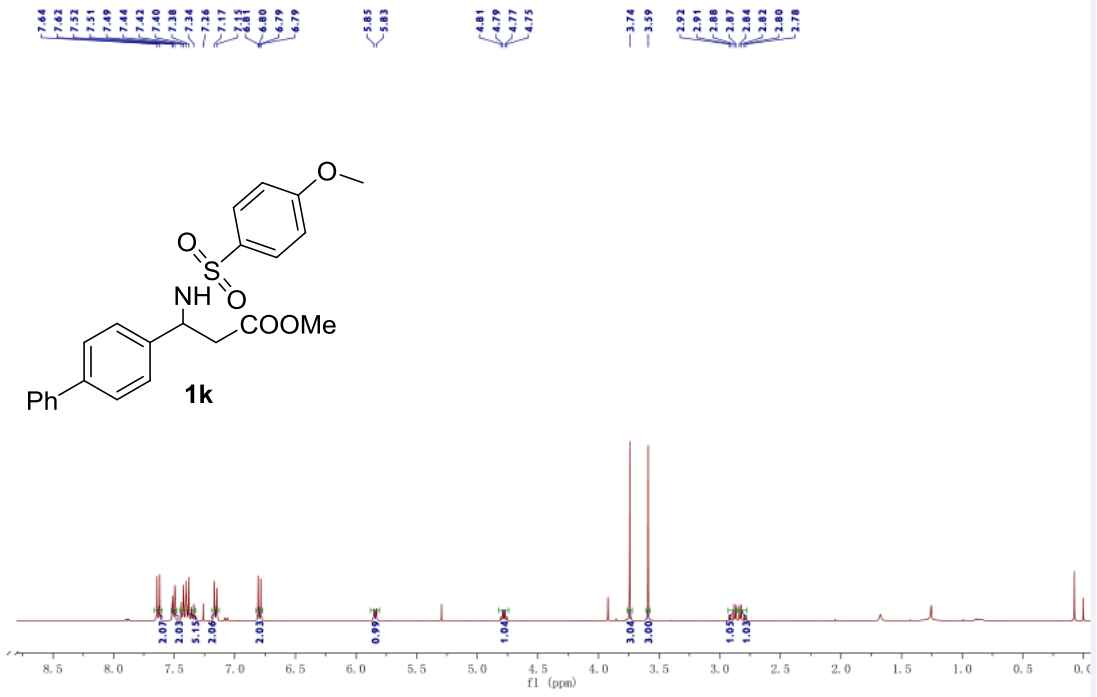


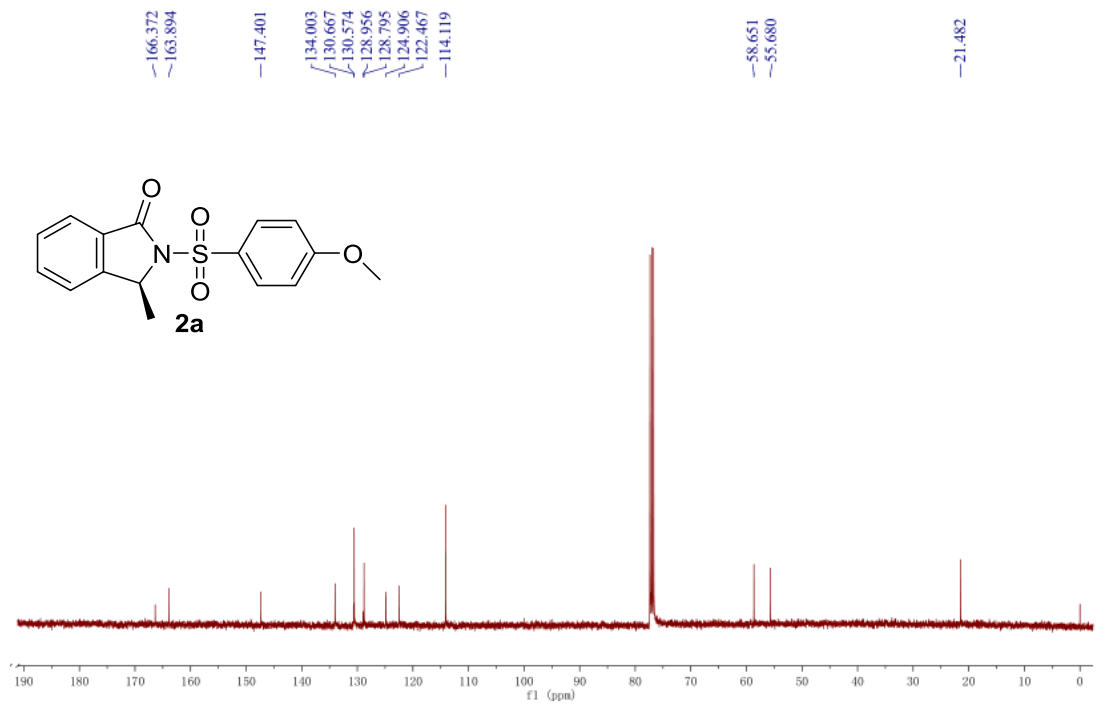
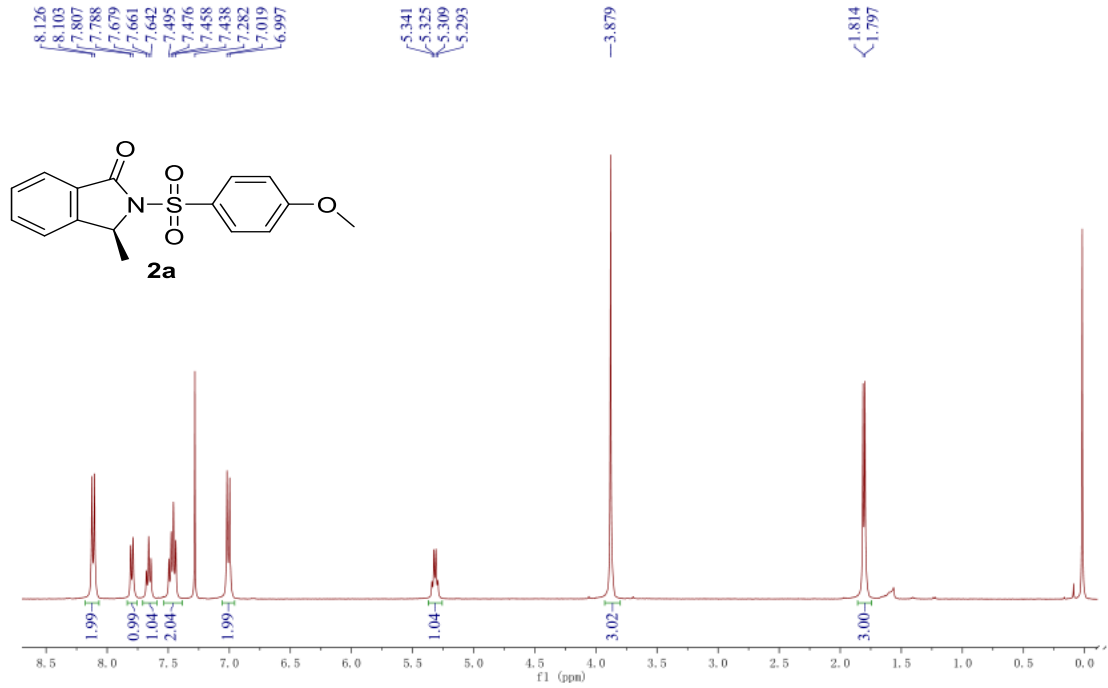


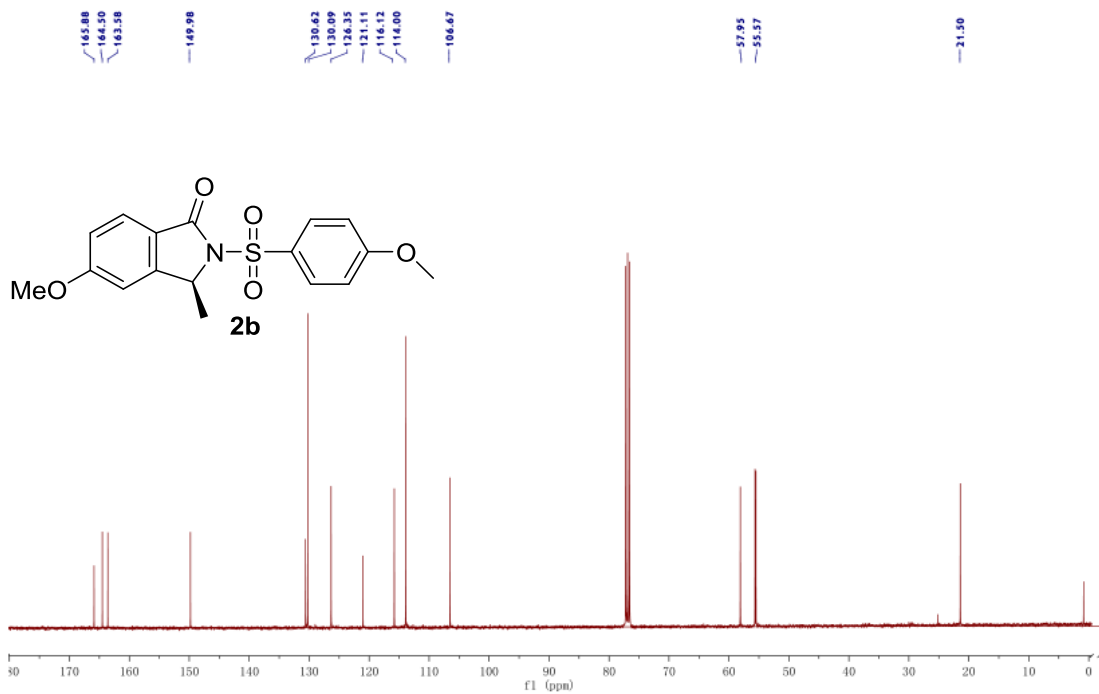
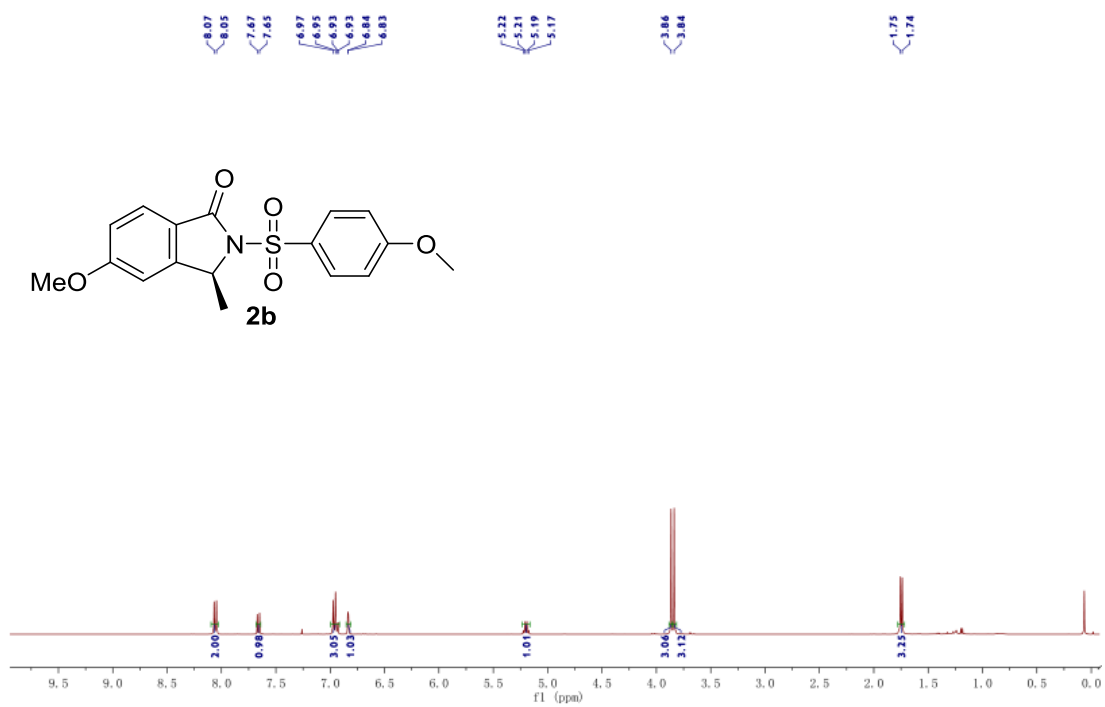


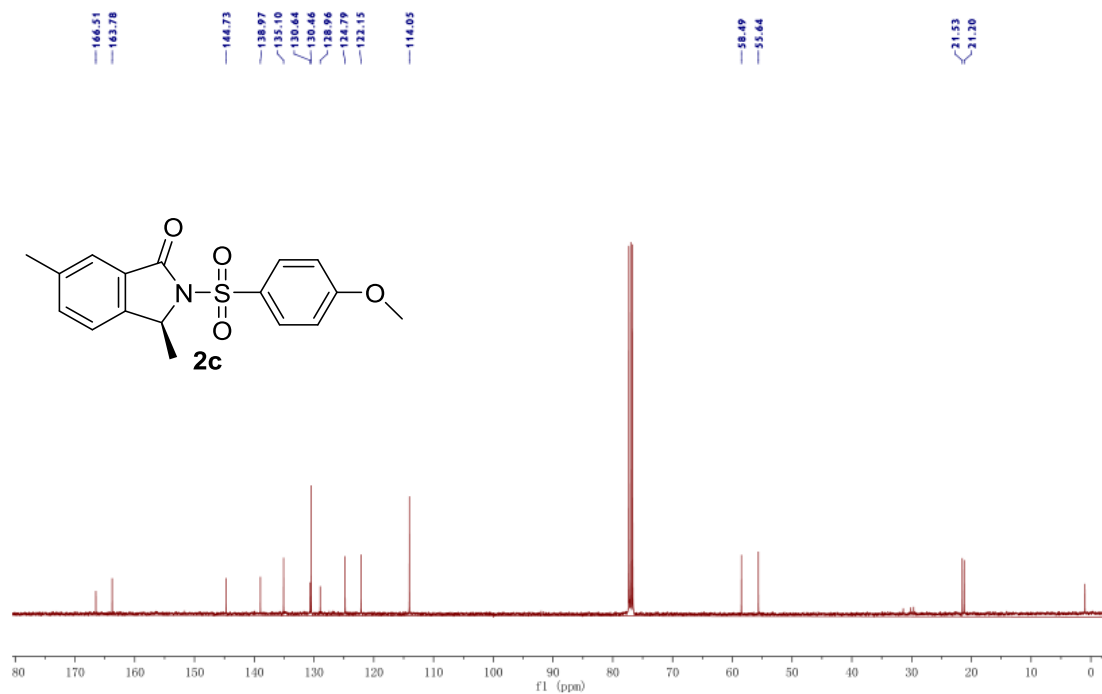
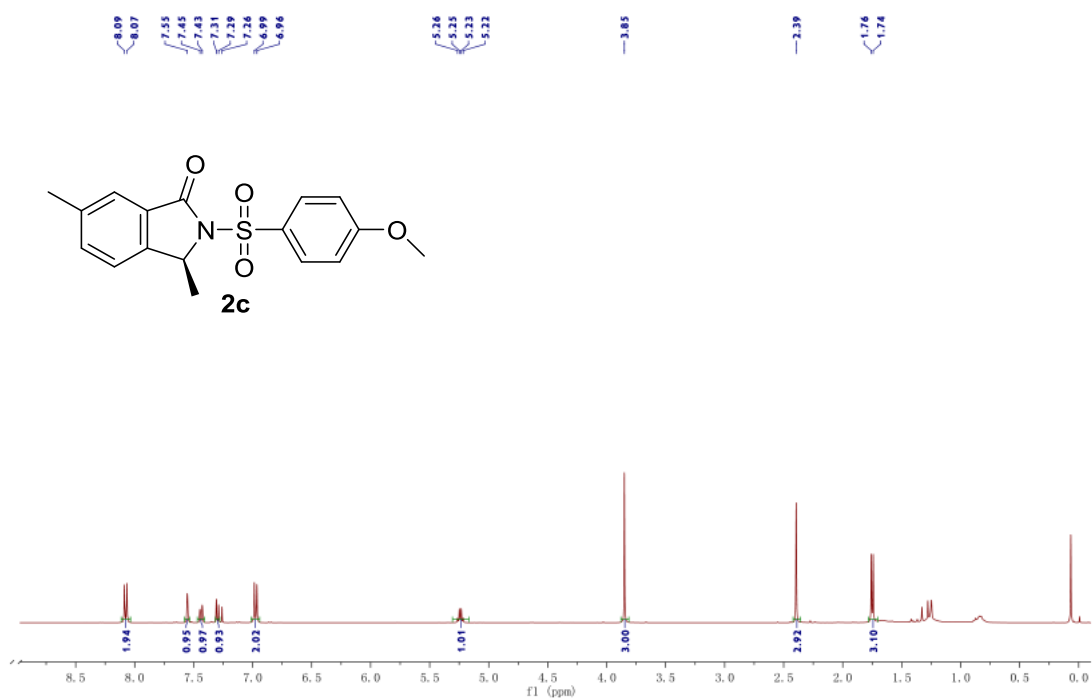


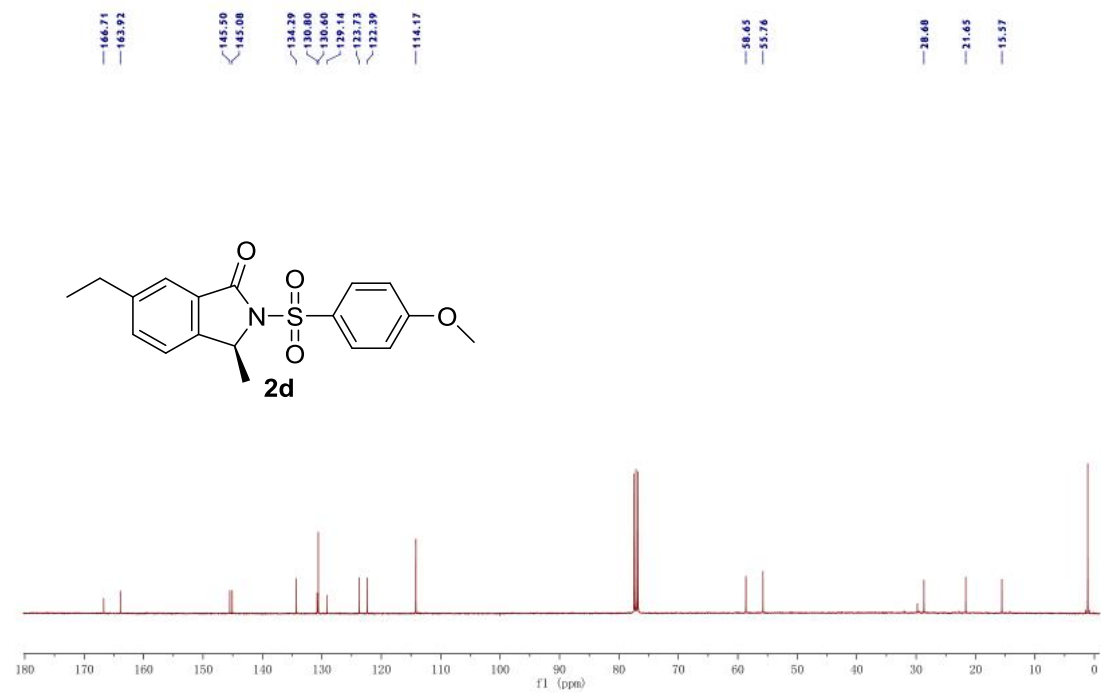
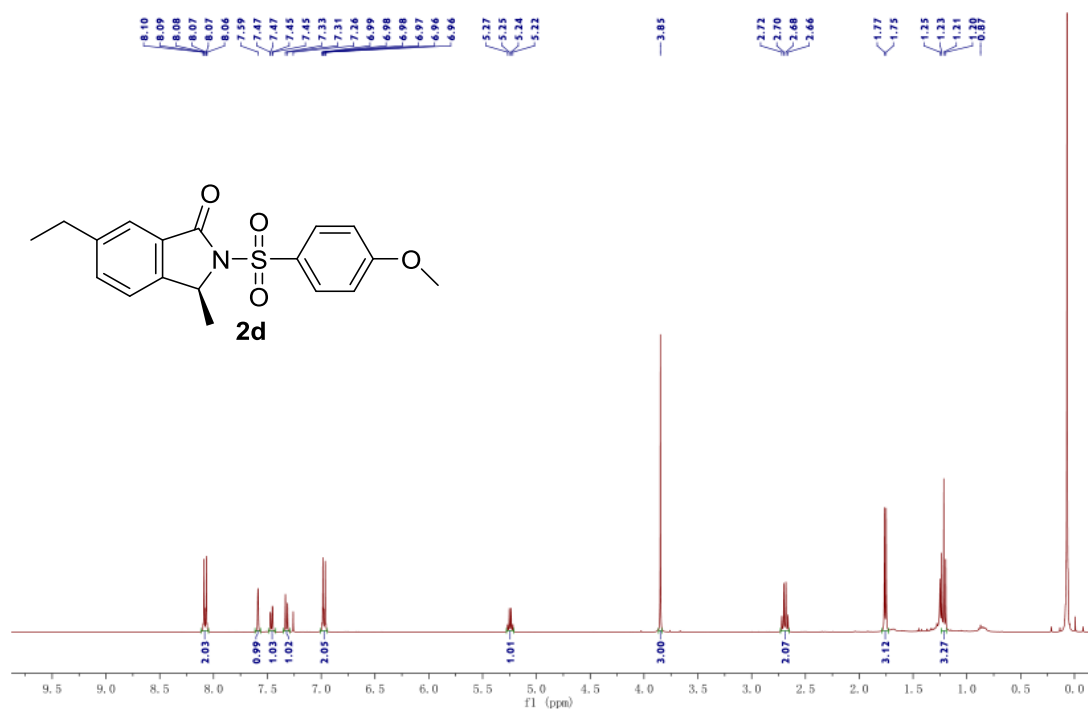


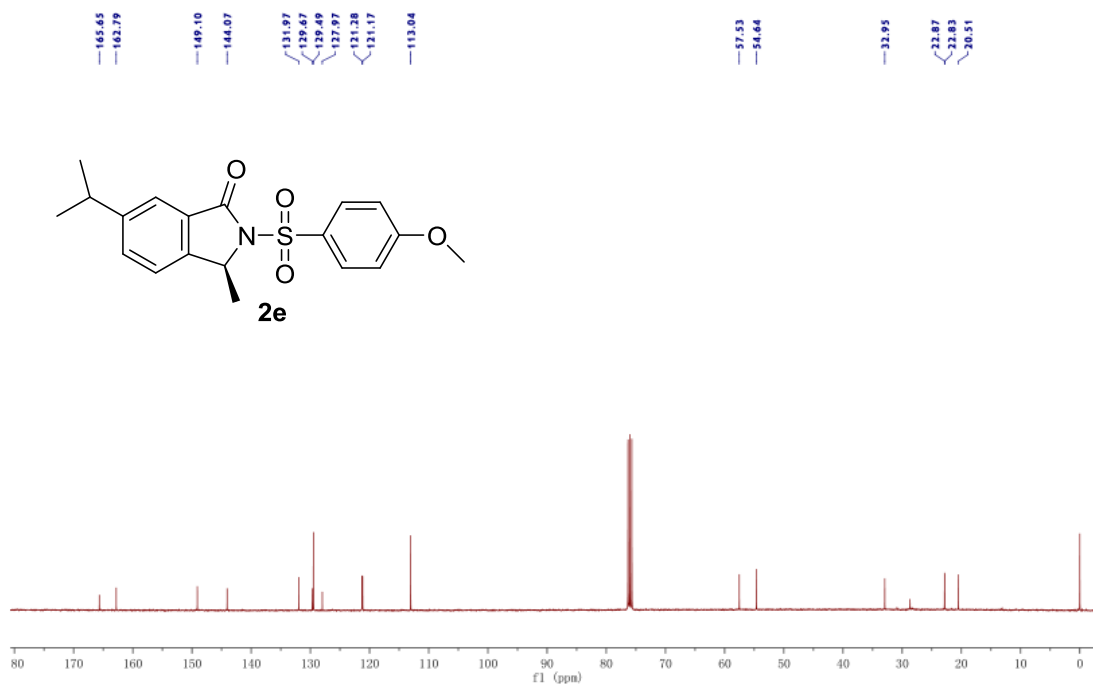
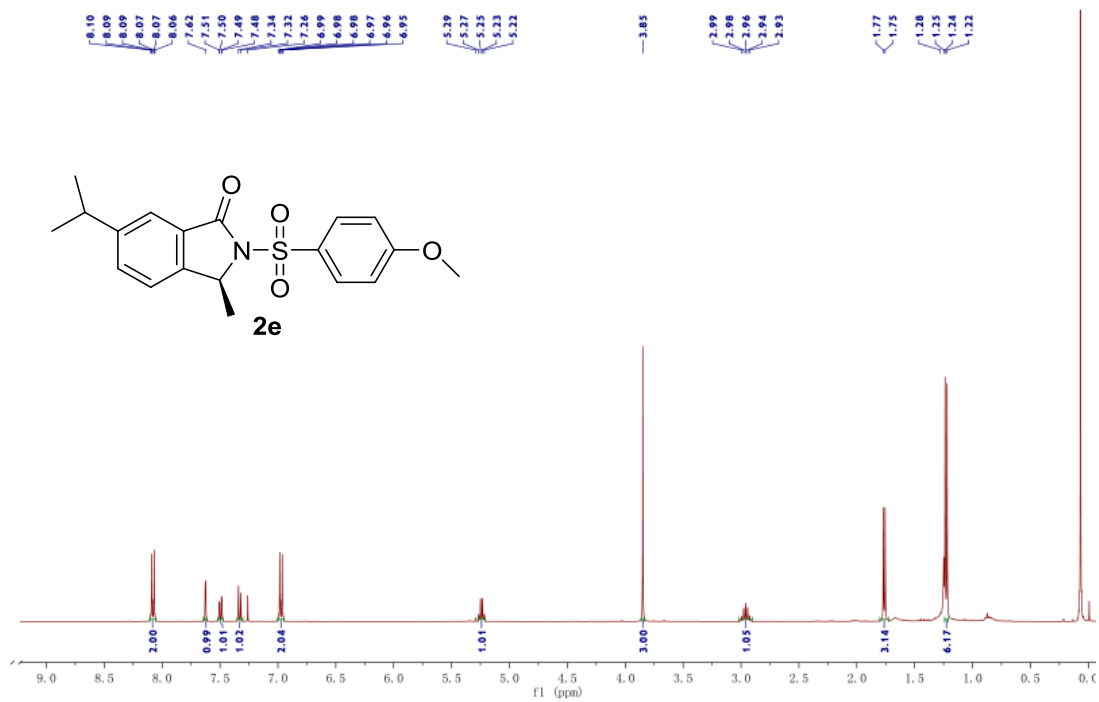


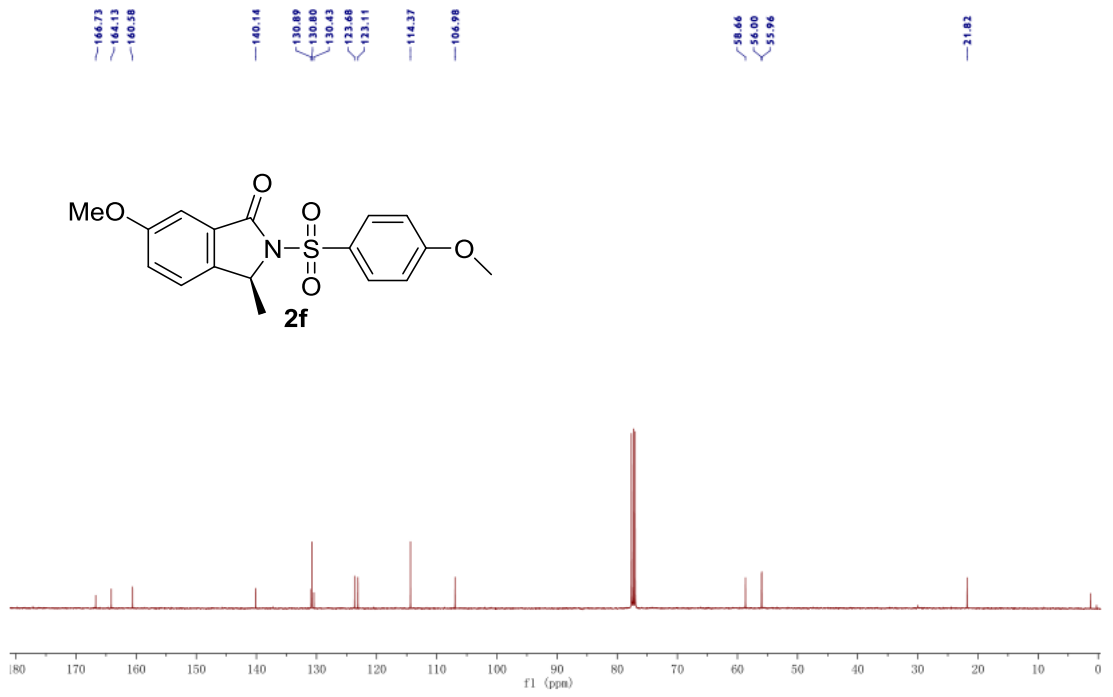
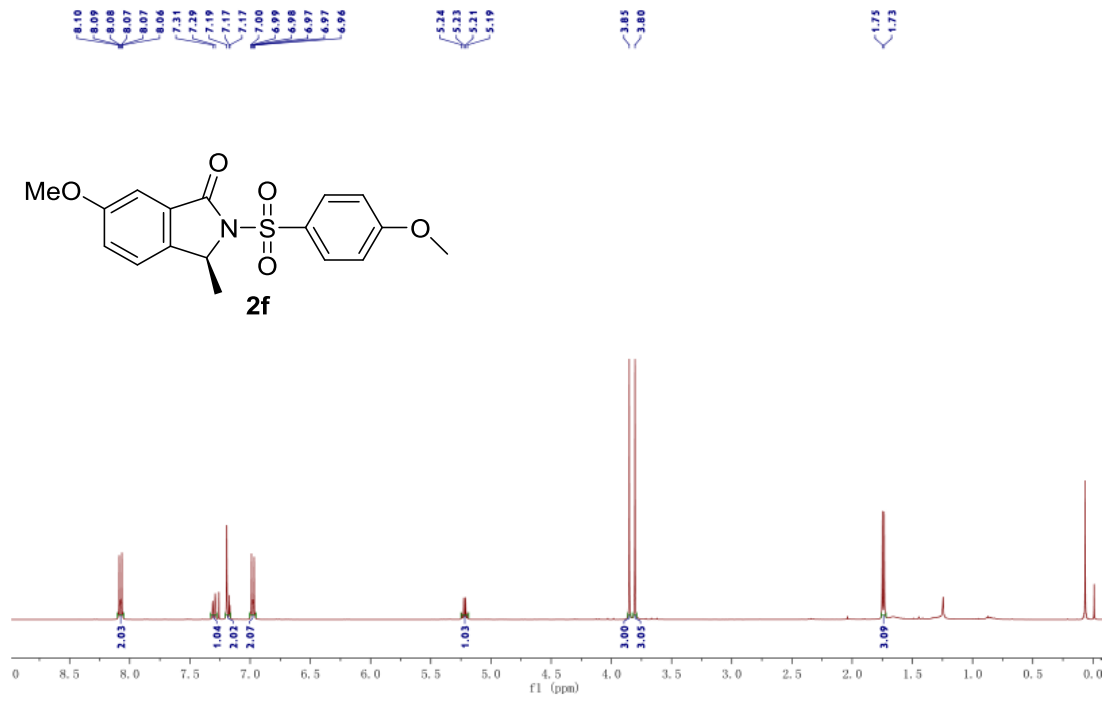


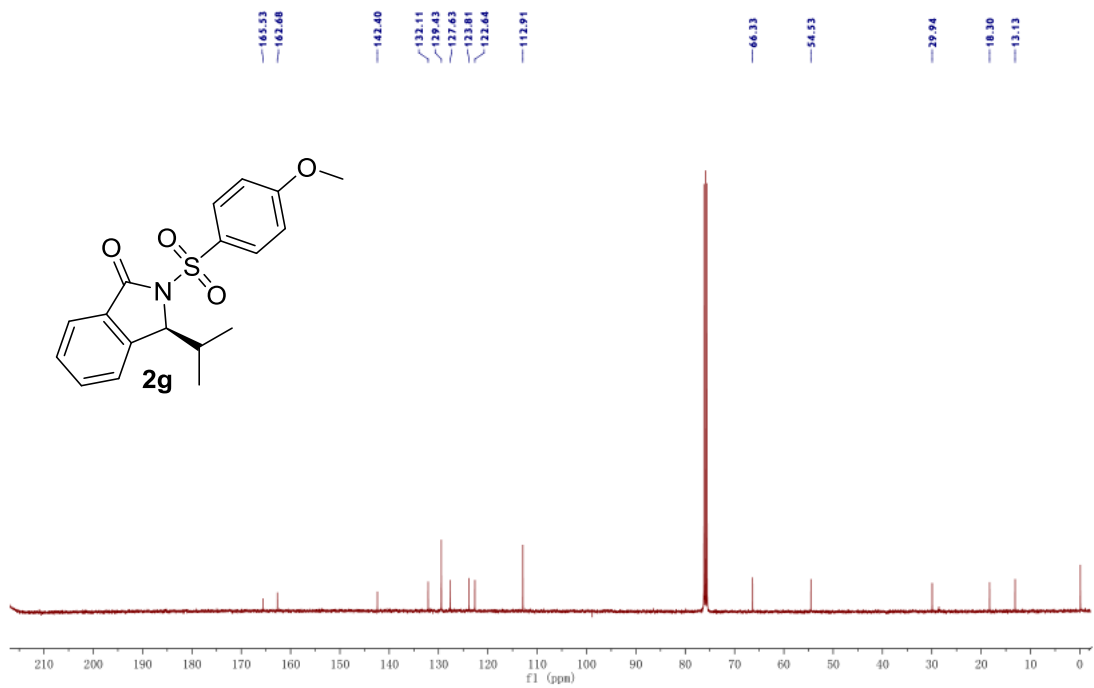
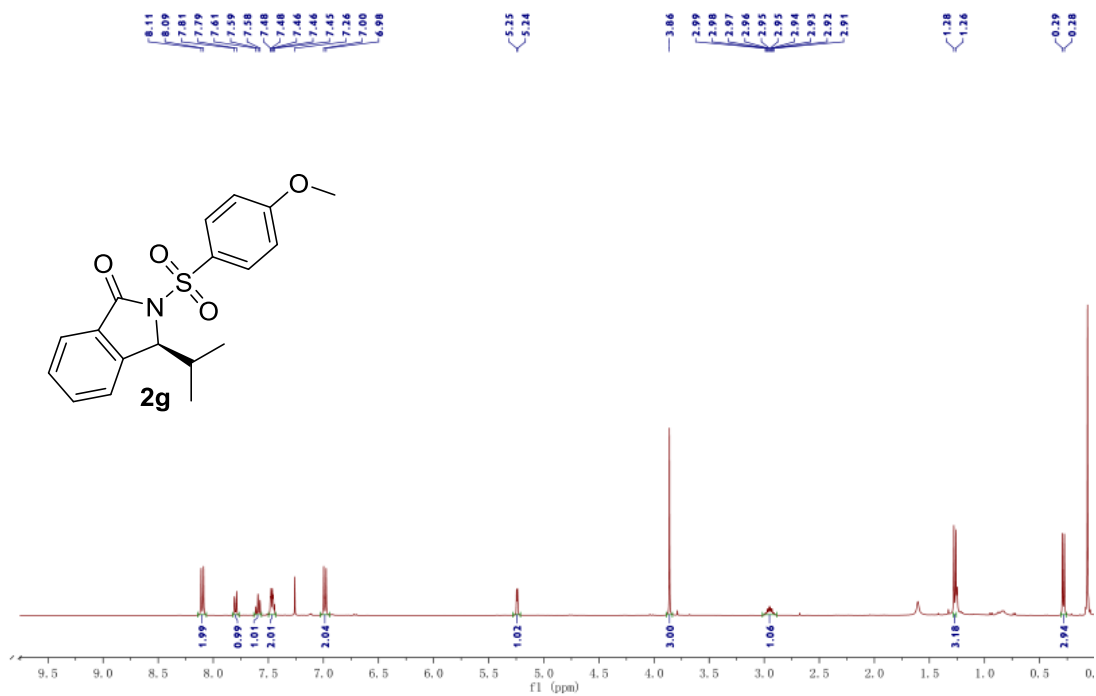


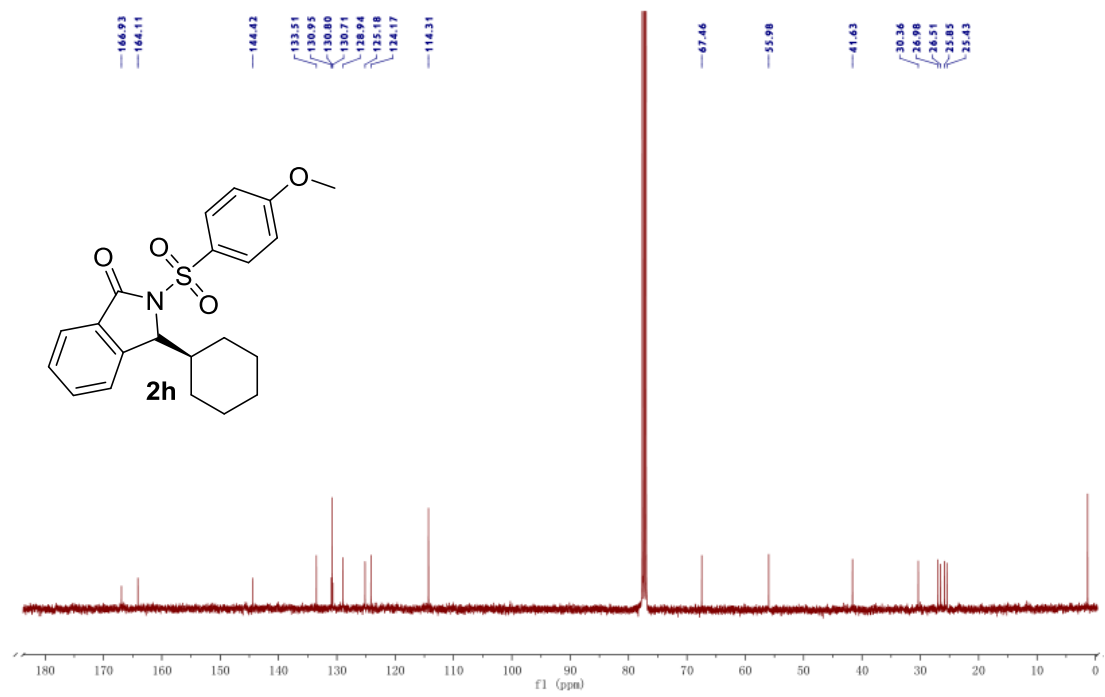
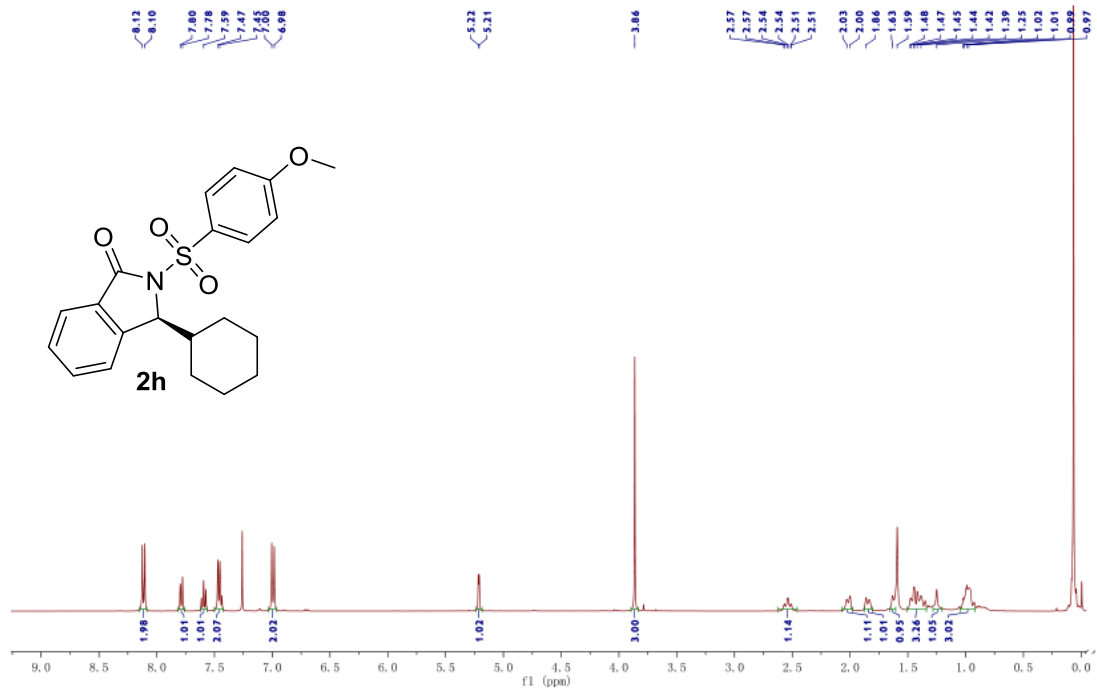


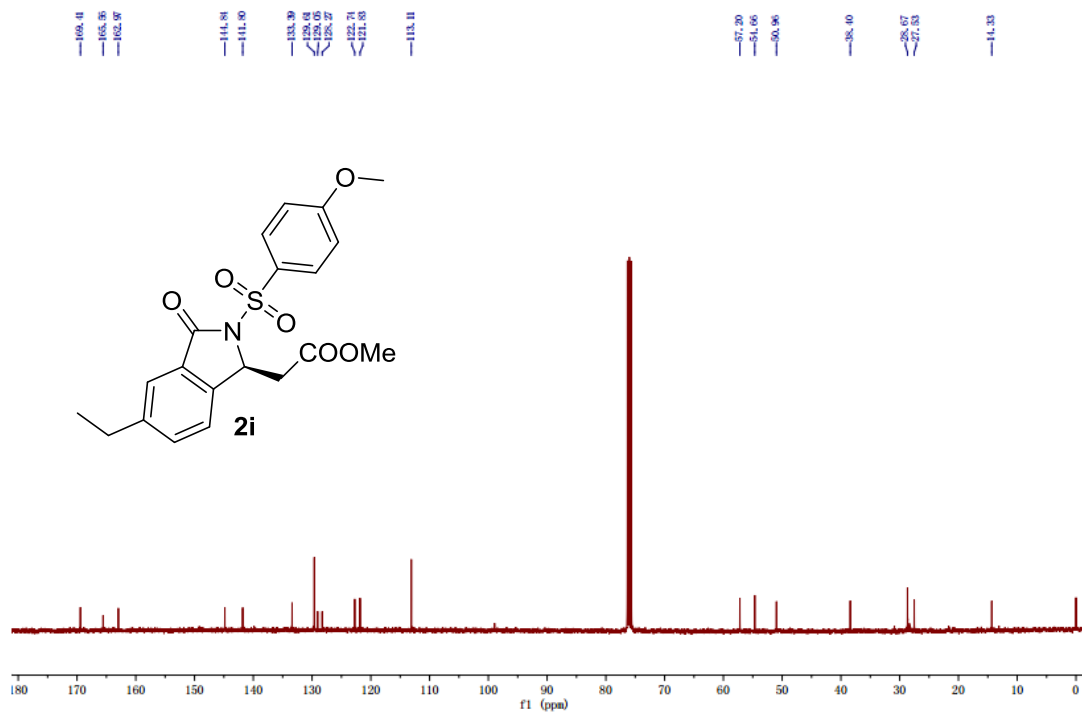
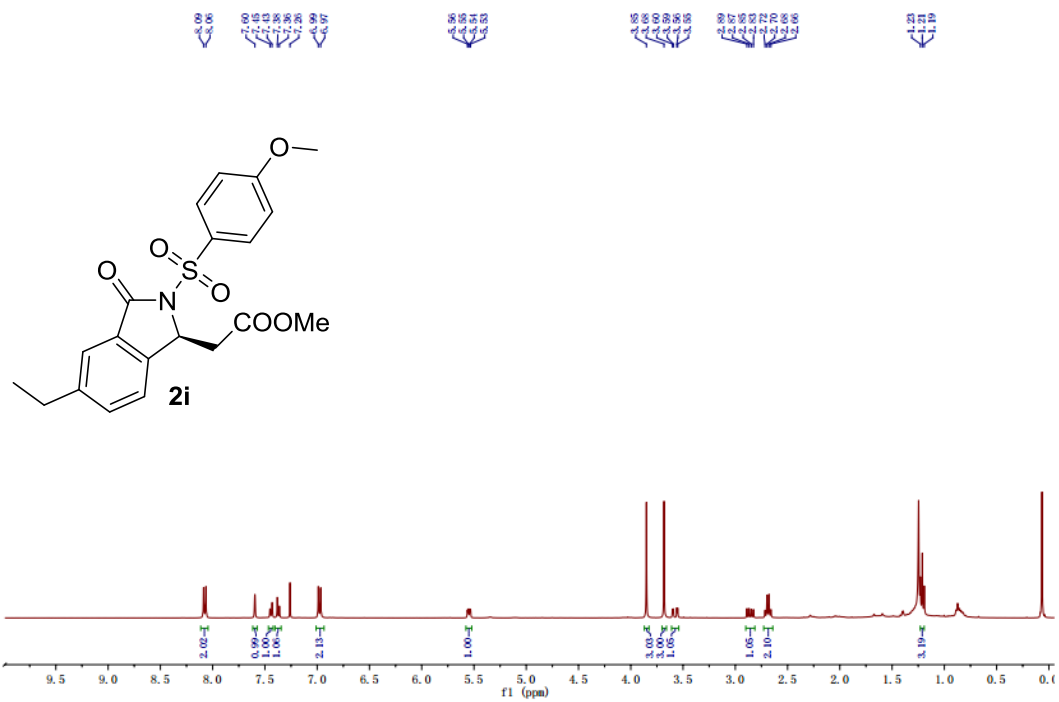


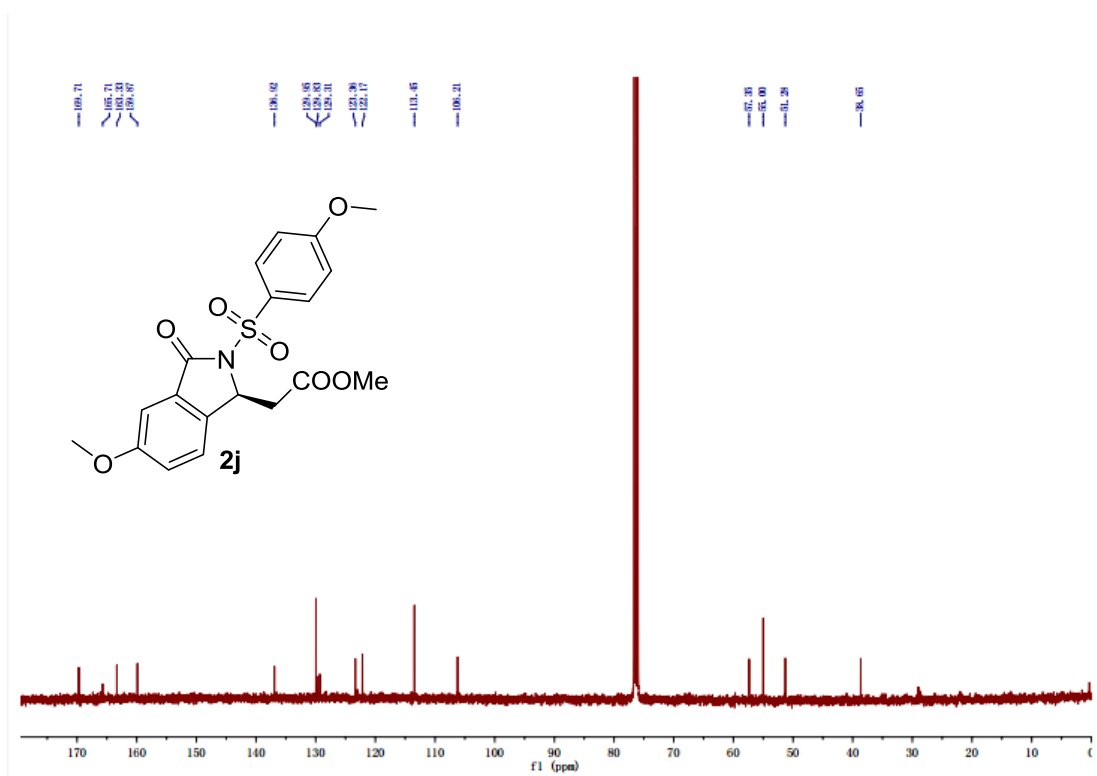
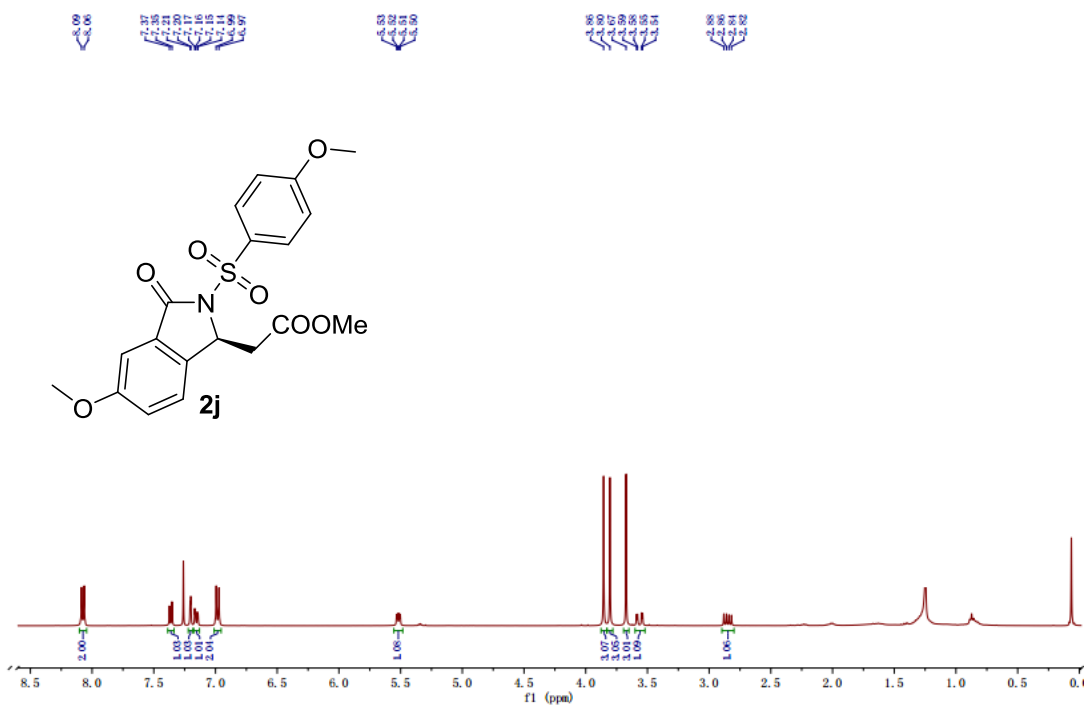


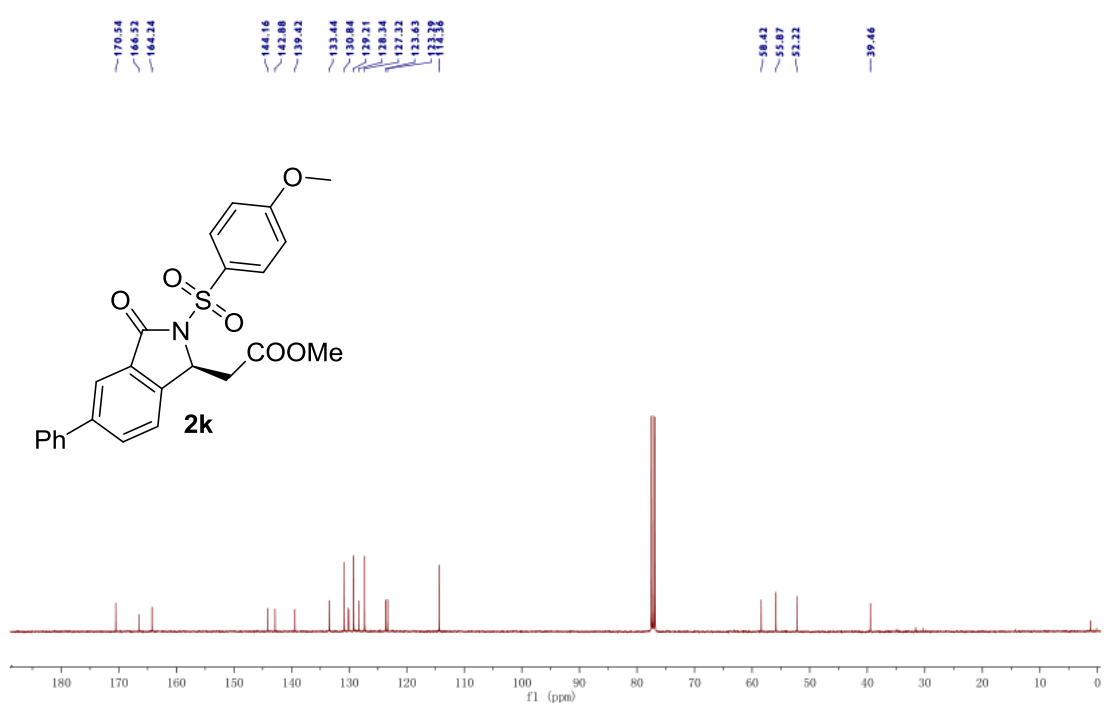
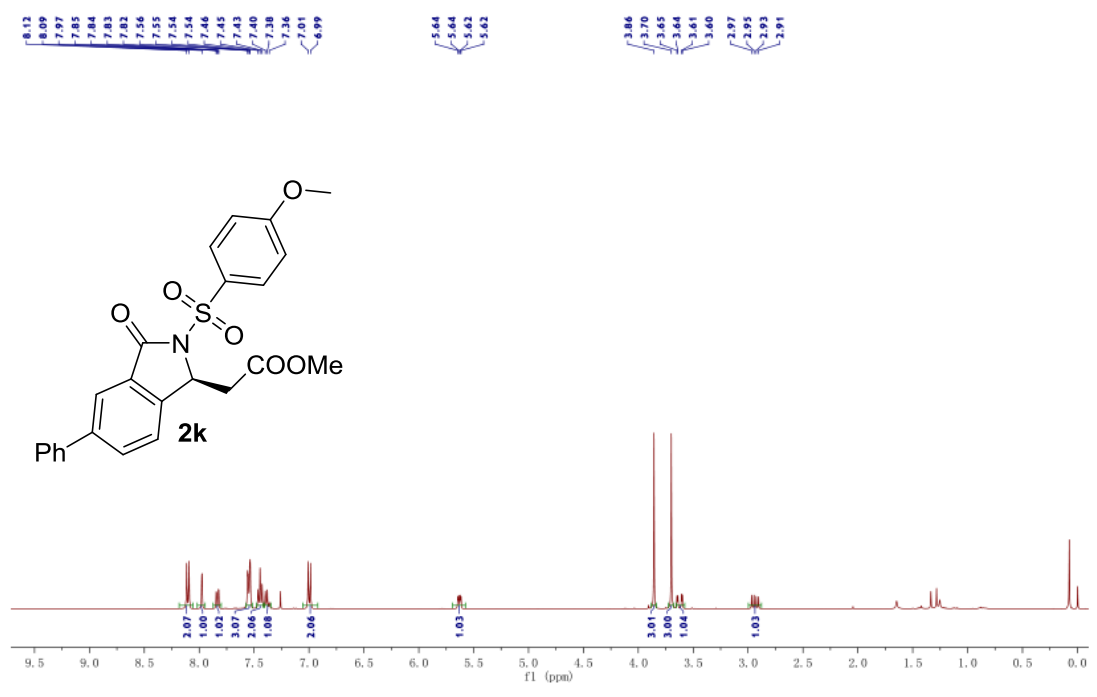






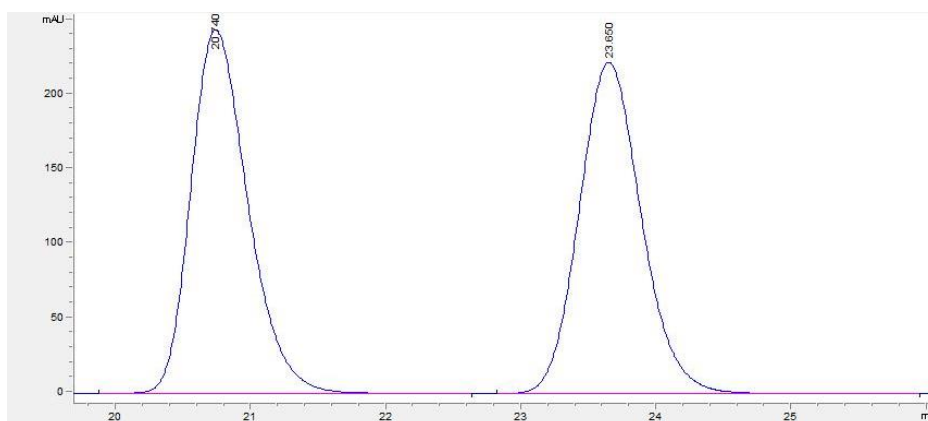
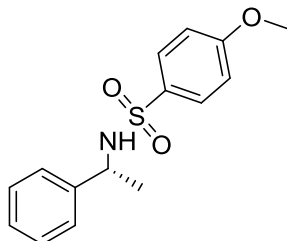






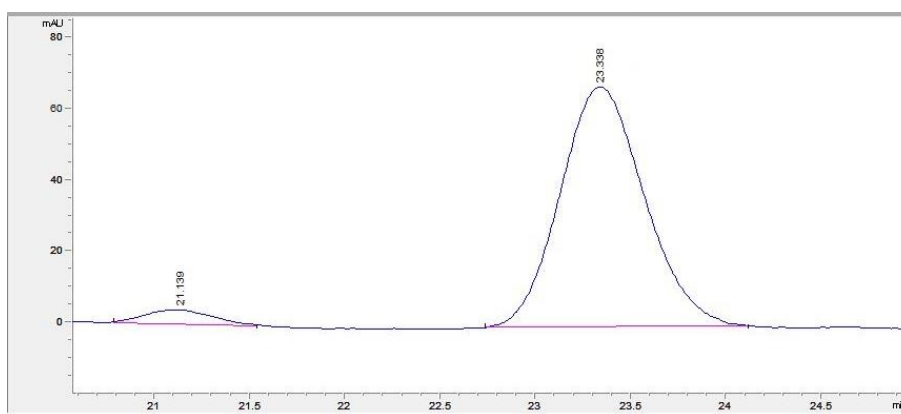
7. HPLC Chromatograms

(*R*)-4-methoxy-*N*-(1-phenylethyl)benzenesulfonamide (1a')



Area Percent Report

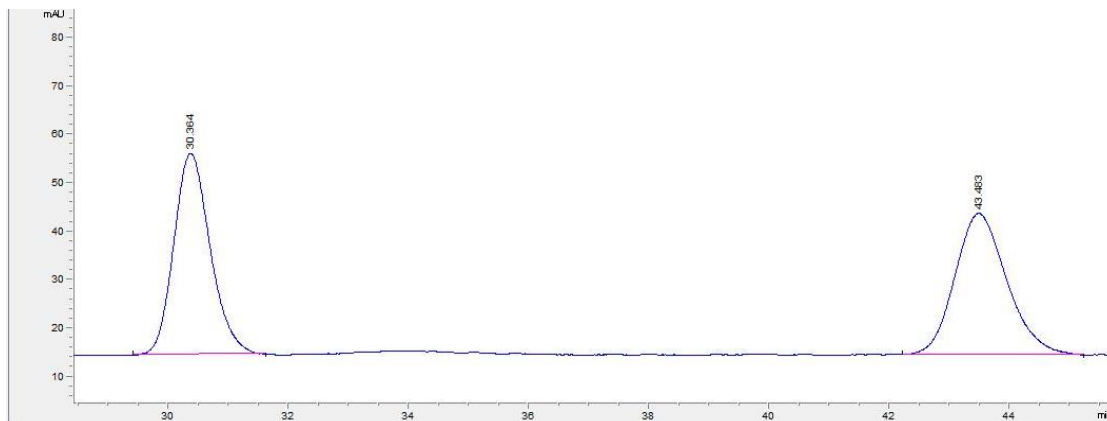
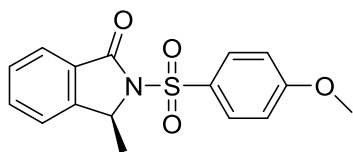
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	20.74	7175.6	50.138	244.3
2	23.65	7136	49.862	222.3



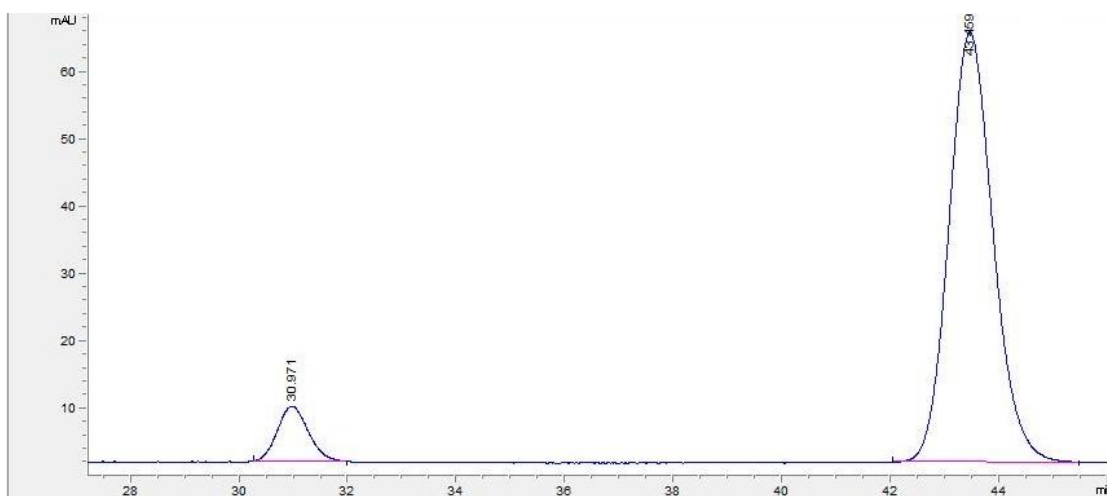
Area Percent Report

Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	21.139	102.7	4.690	4.1
2	23.338	2087.7	95.310	67.6

(S)-2-((4-methoxyphenyl)sulfonyl)-3-methylisoindolin-1-one (2a)

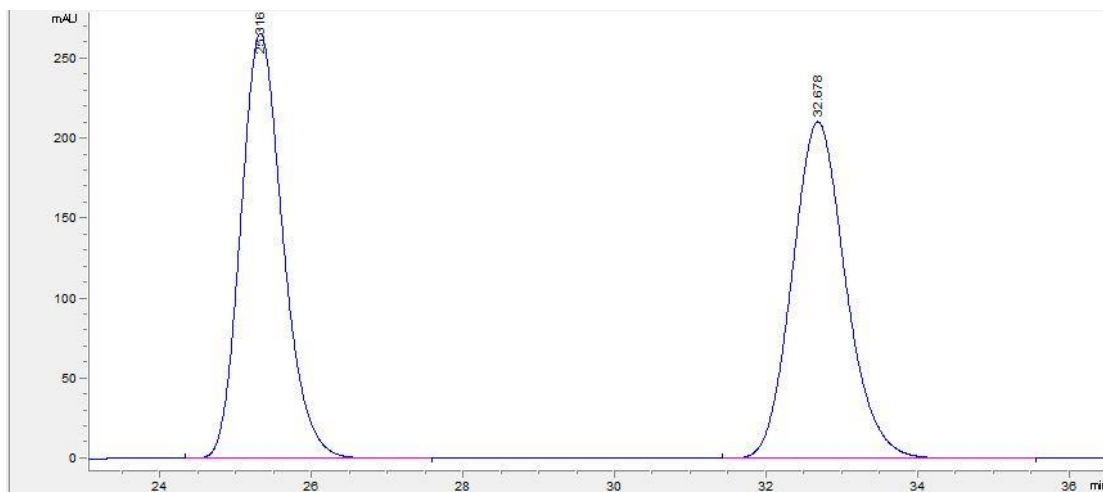
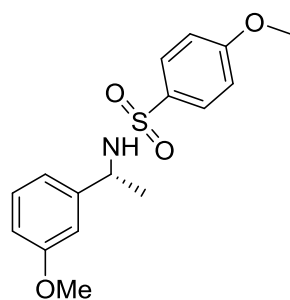


Area Percent Report				
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	30.364	1751.4	49.957	41.6
2	43.483	1754.4	50.043	29.2



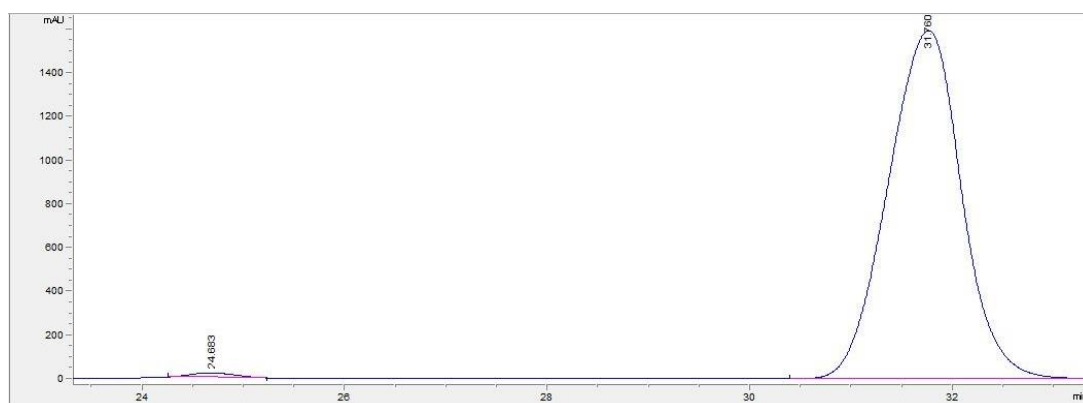
Area Percent Report				
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	30.971	323.2	8.228	8.2
2	43.459	3604.5	91.772	63.9

(R)-4-methoxy-N-(1-3-methoxyphenyl)ethylbenzenesulfonamide (1b')



Area Percent Report

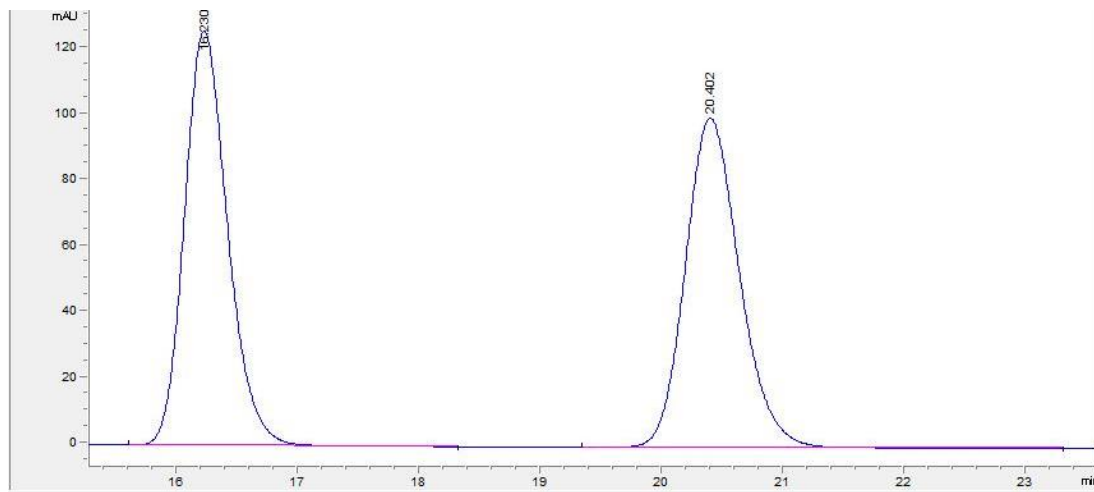
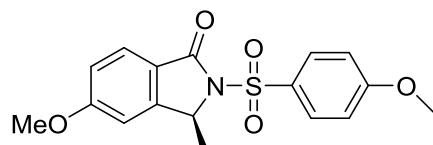
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	25.316	10277.6	49.879	266
2	32.678	10327.5	50.121	210.6



Area Percent Report

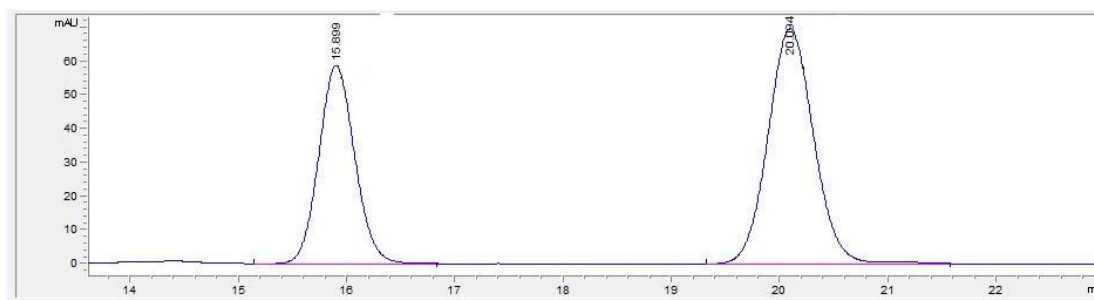
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	24.683	741.3	0.915	22.7
2	31.76	80313.9	99.085	1592.8

(S)-5-methoxy-2-((4-methoxyphenyl)sulfonyl)-3-methylisoindolin-1-one (2b)



Area Percent Report

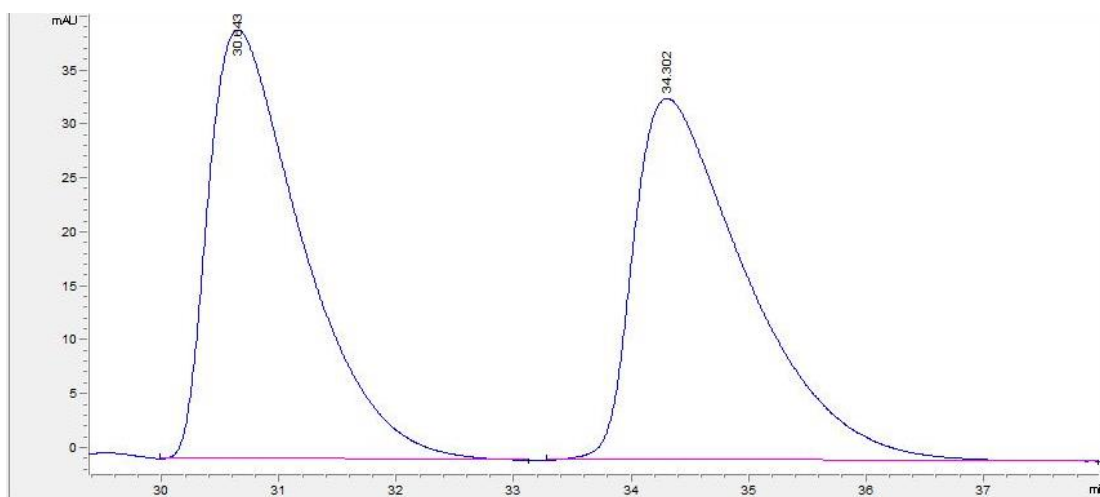
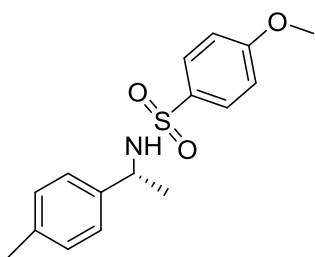
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	16.23	3116	50.069	125.9
2	20.402	3107.3	49.931	100



Area Percent Report

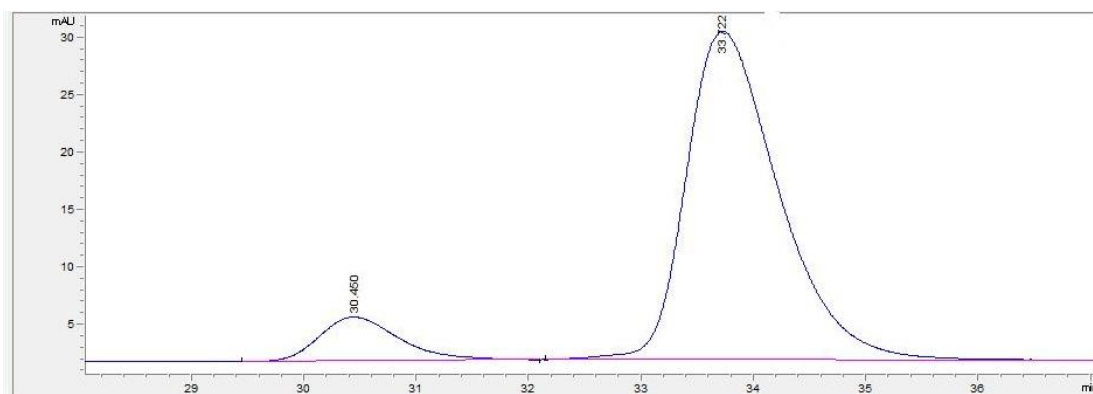
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	15.899	1405	40.018	59.2
2	20.094	2105.9	59.982	70.1

(R)-4-methoxy-N-(1-(p-tolyl)ethyl)benzenesulfonamide (1c')



Area Percent Report

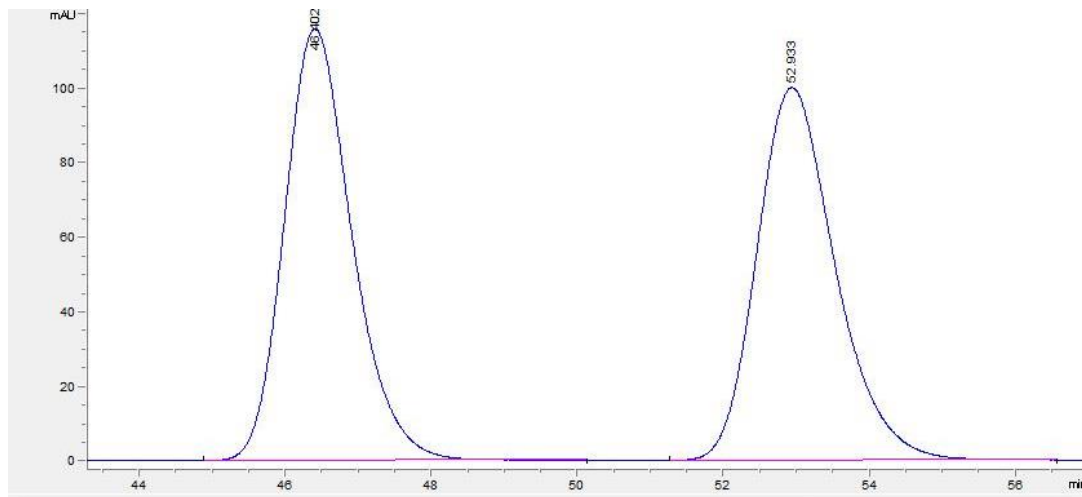
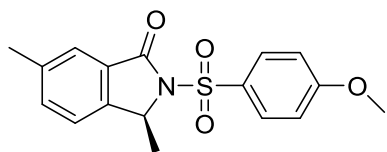
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	30.643	2219.9	49.526	39.8
2	34.302	2262.4	50.474	33.6



Area Percent Report

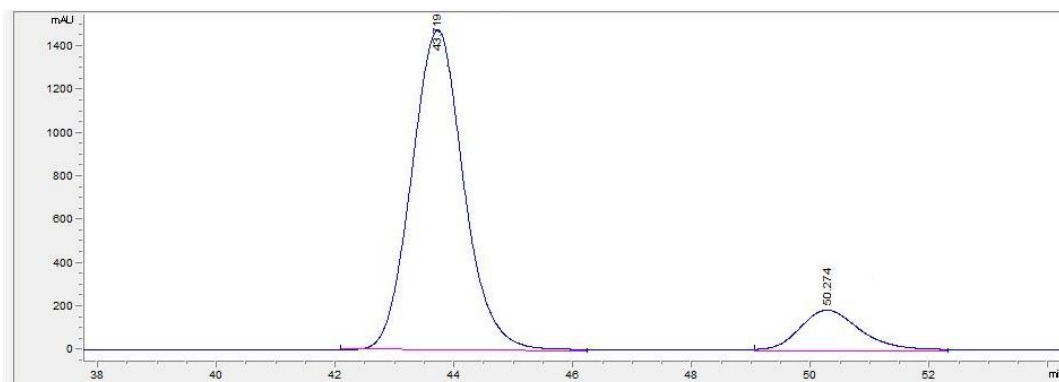
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	30.450	191.7	10.430	3.8
2	33.722	1646.6	89.570	28.6

(S)-2-((4-methoxyphenyl)sulfonyl)-3,6-dimethylisoindolin-1-one (2c)



Area Percent Report

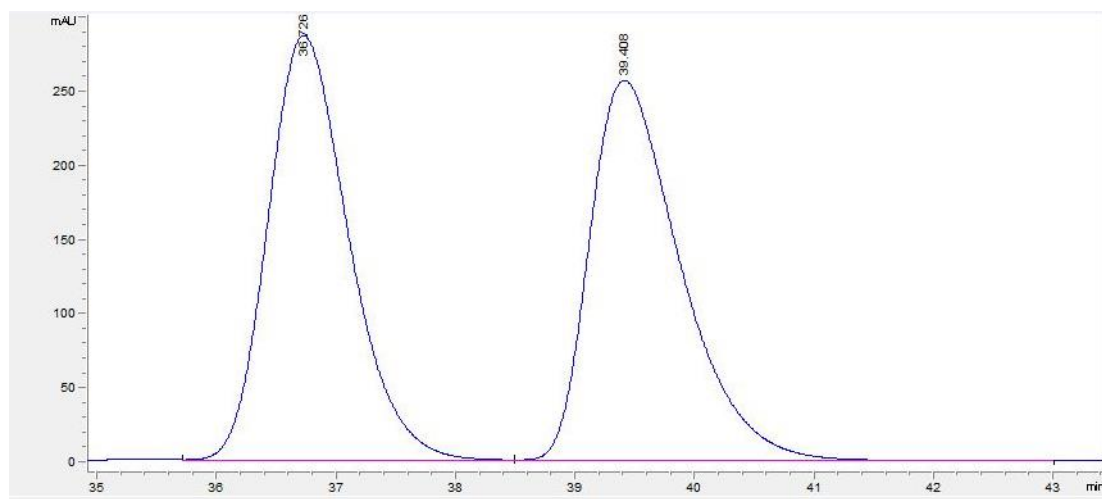
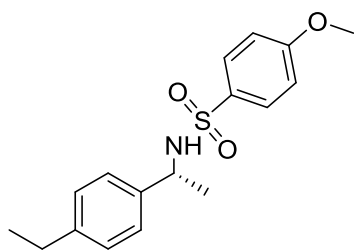
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	46.402	7445.5	49.954	115.7
2	52.933	7459.2	50.046	99.9



Area Percent Report

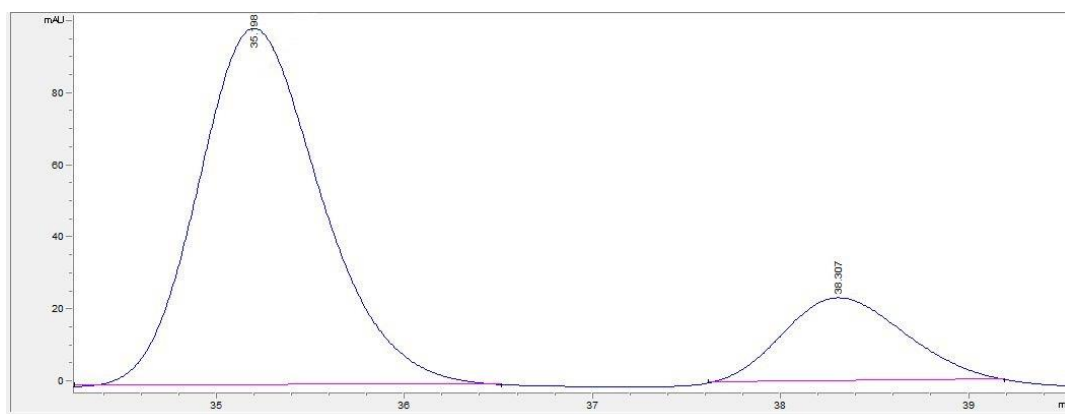
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	43.719	89834.8	86.750	1475.5
2	50.274	13720.6	13.250	188.6

(R)-N-(1-(4-ethylphenyl)ethyl)-4-methoxybenzenesulfonamide (1d')



Area Percent Report

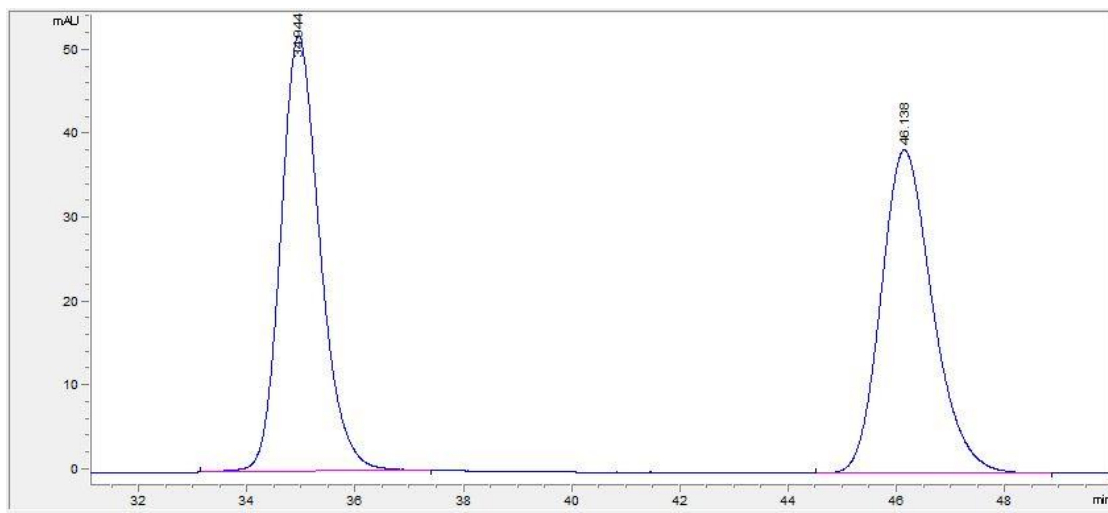
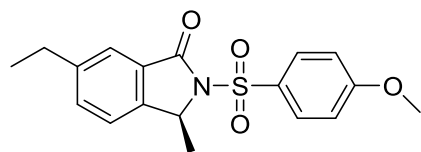
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	36.726	13571.4	49.931	287.2
2	39.408	136.08.7	50.069	256.9



Area Percent Report

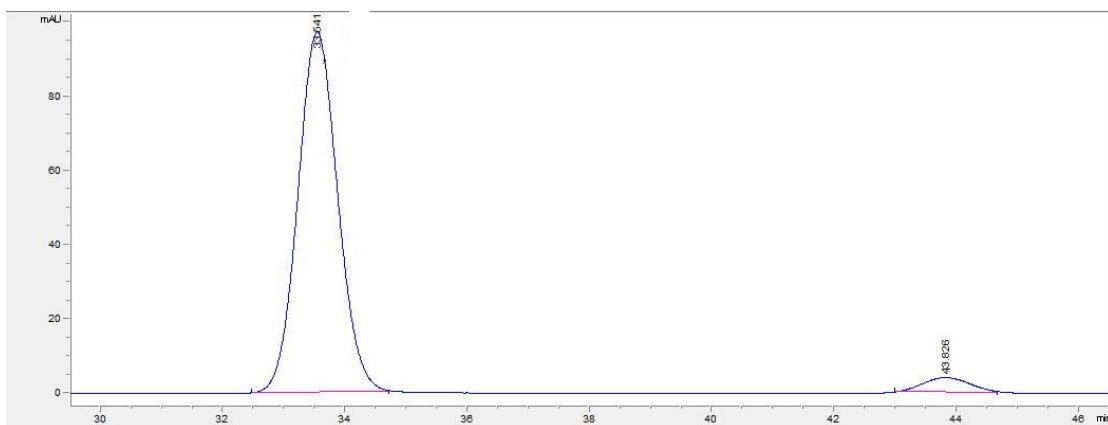
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	35.198	4494.3	81.163	99.1
2	38.307	1043.1	18.837	23.2

(S)-6-ethyl-2-((4-methoxyphenyl)sulfonyl)-3-methylisindolin-1-one (2d)



Area Percent Report

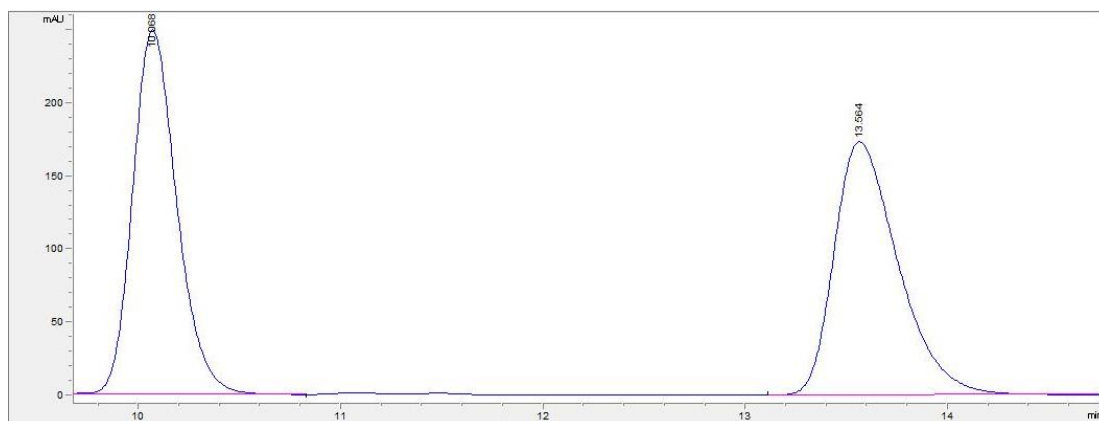
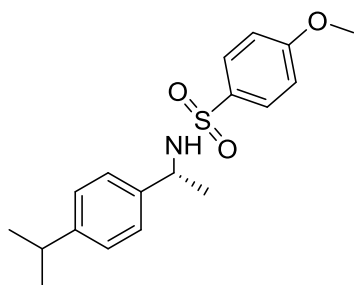
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	34.944	2626.3	50.780	51.9
2	46.138	2545.7	49.220	38.5



Area Percent Report

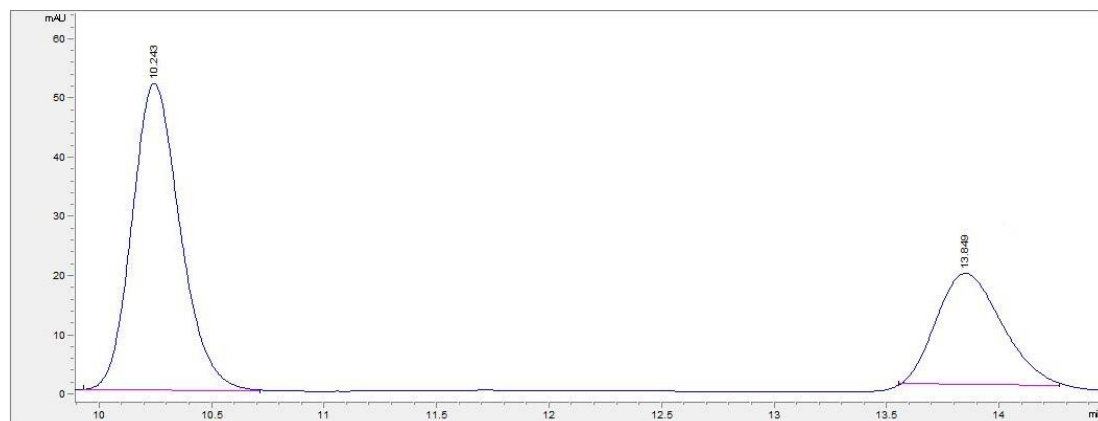
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	33.541	4425.9	95.087	97.3
2	43.826	228.7	4.913	4.1

(R)-N-(1-(4-isopropylphenyl)ethyl)-4-methoxybenzenesulfonamide (1e')



Area Percent Report

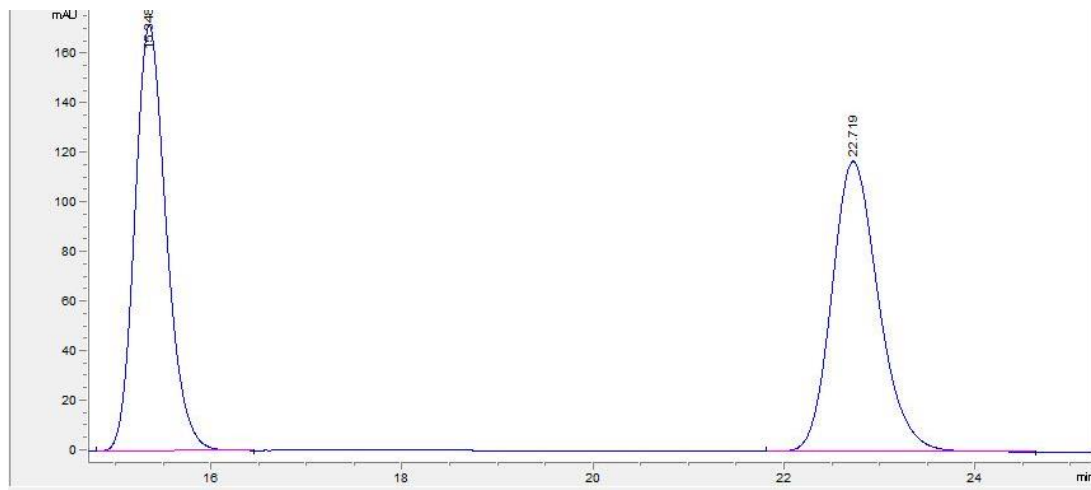
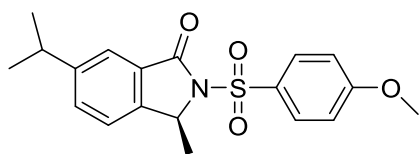
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	10.068	3821.9	50.029	250
2	13.564	3817.5	49.971	173.3



Area Percent Report

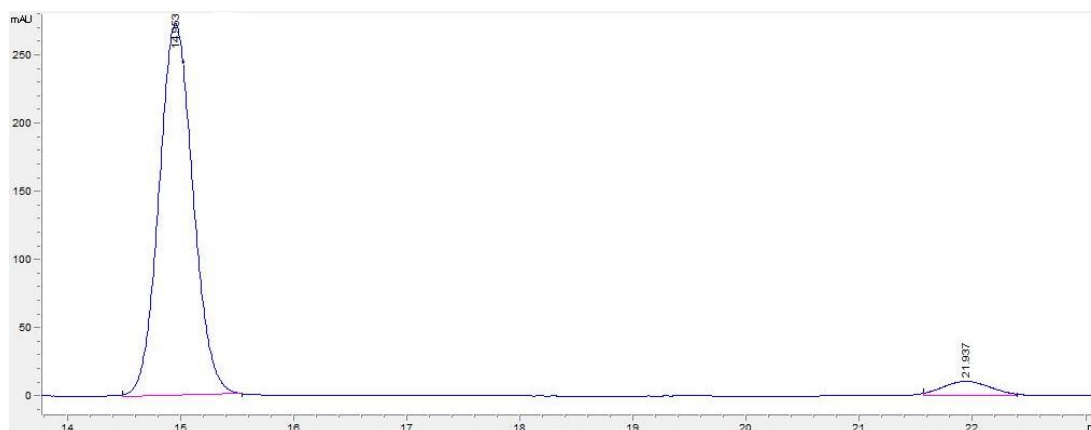
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	10.243	776.3	67.118	52
2	13.849	380.3	32.882	18.8

(S)-6-isopropyl-2-((4-methoxyphenyl)sulfonyl)-3-methylisoindolin-1-one (2e)



Area Percent Report

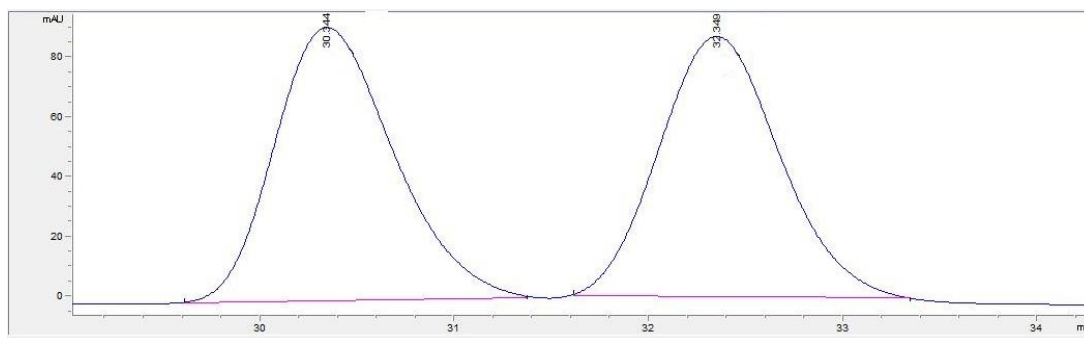
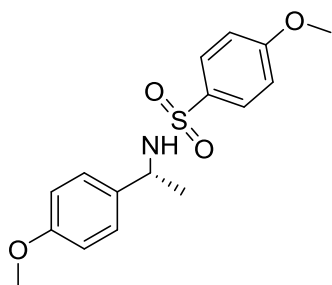
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	15.348	3945.9	49.812	171.7
2	22.719	3975.7	50.188	117.1



Area Percent Report

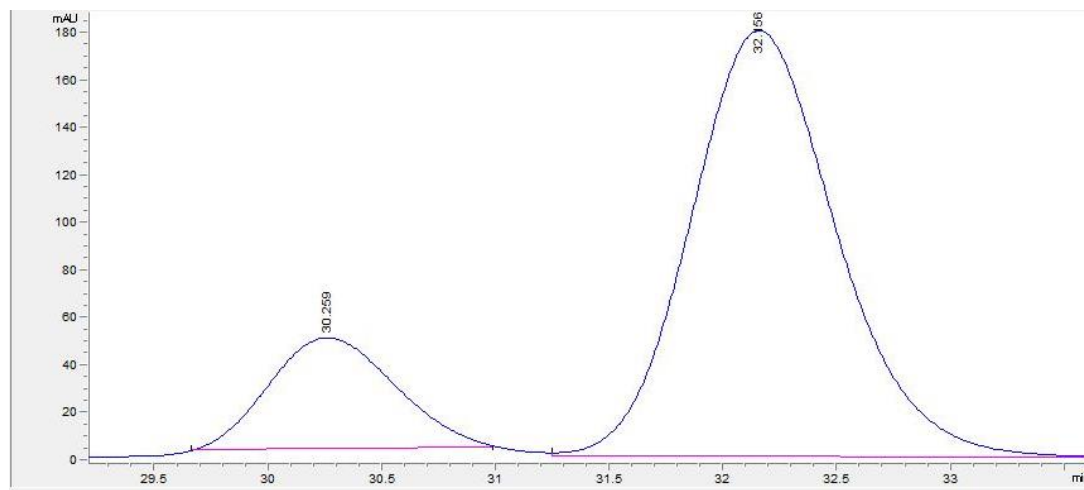
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	14.953	5706.8	95.037	272.9
2	21.937	298	4.963	10.3

(R)-4-methoxy-N-(1-(4-methoxyphenyl)ethyl)benzenesulfonamide (1f')



Area Percent Report

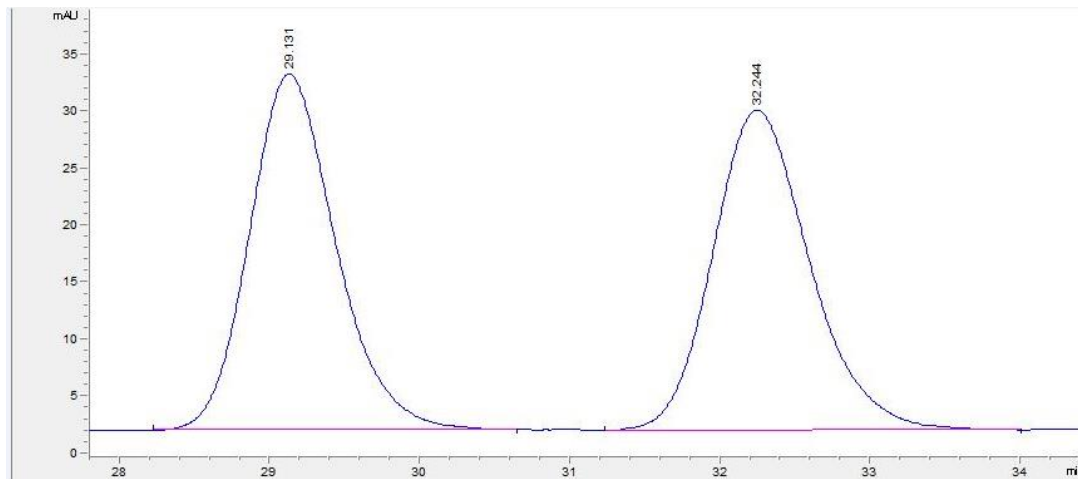
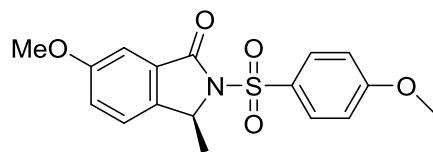
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	30.344	3906.9	50.913	91.6
2	32.349	3766.7	49.087	49.087



Area Percent Report

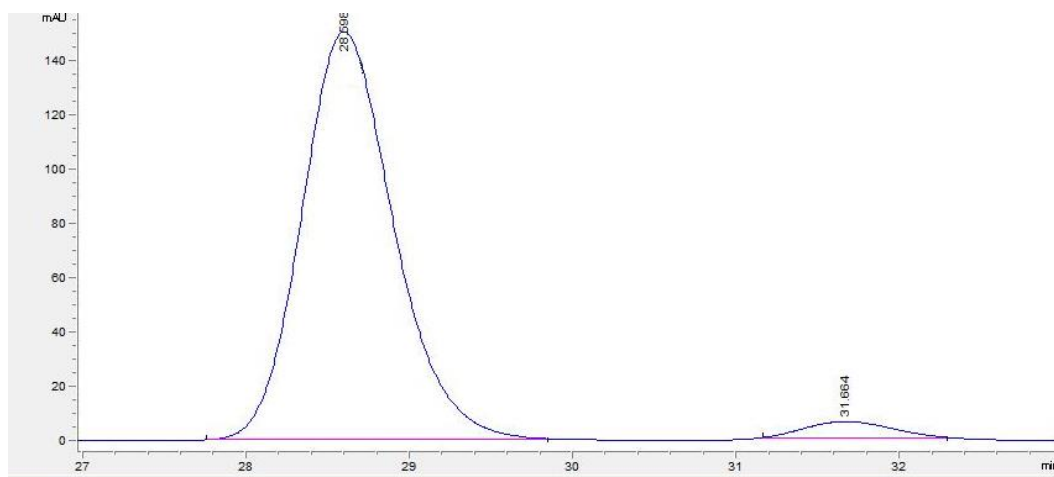
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	30.259	1815.7	18.418	47
2	32.156	8042.8	81.582	179.7

(S)-6-methoxy-2-((4-methoxyphenyl)sulfonyl)-3-methylisoindolin-1-one (2f)



Area Percent Report

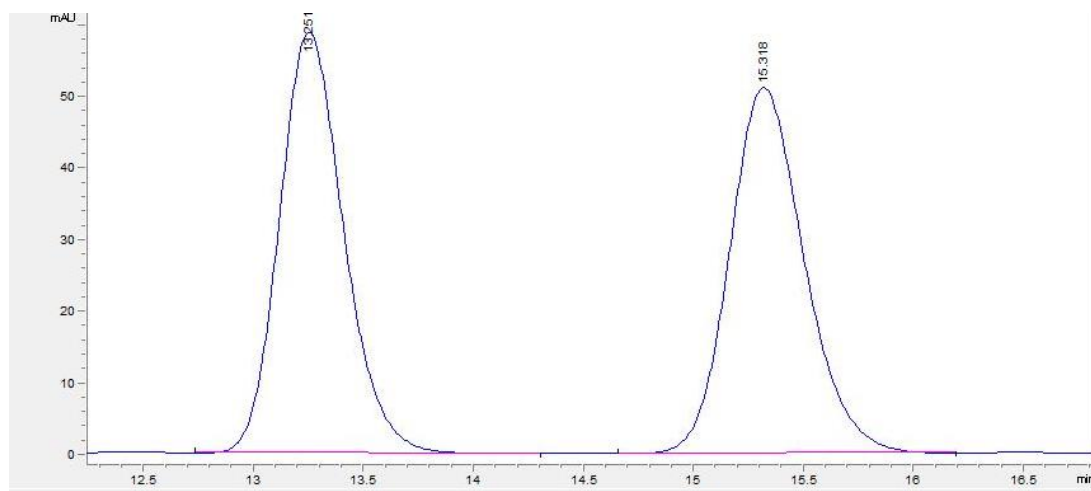
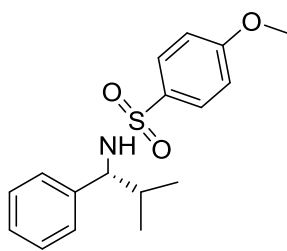
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	29.131	1251	49.751	31.2
2	32.244	1263.5	50.249	28.1



Area Percent Report

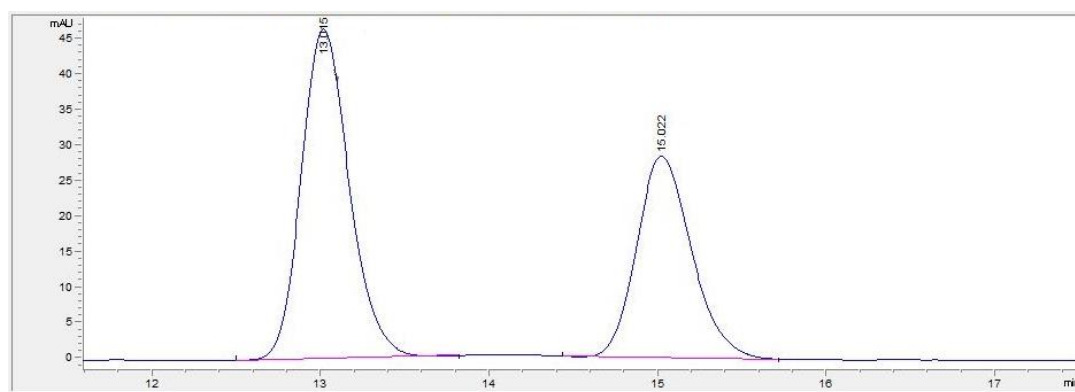
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	28.598	5878.3	96.328	150.3
2	31.664	224.1	3.672	6.1

(R)-4-methoxy-N-(2-methyl-1-phenylpropyl)benzenesulfonamide (1g')



Area Percent Report

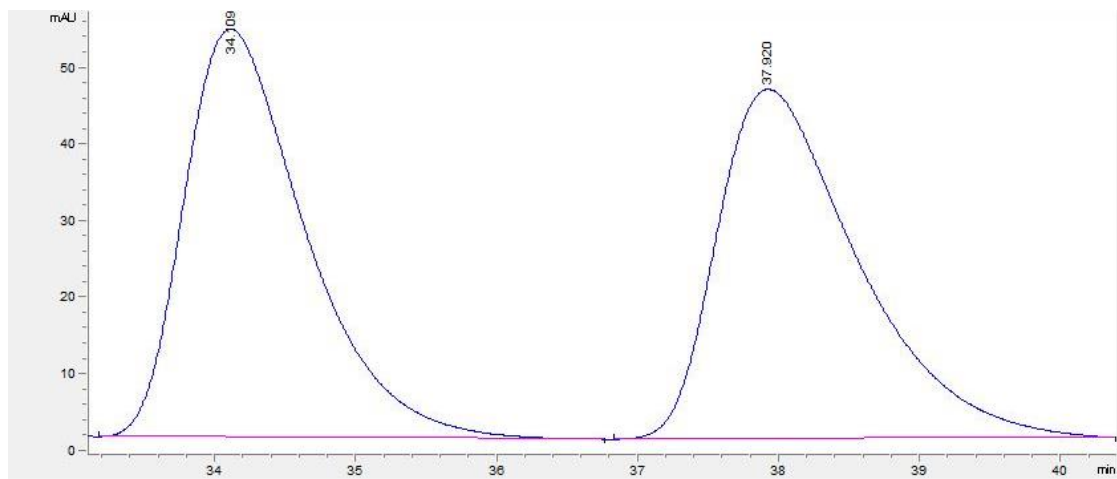
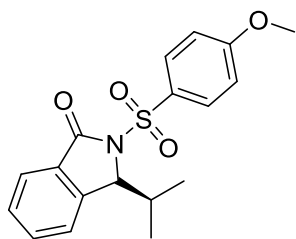
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	13.251	1198.4	49.855	58.8
2	15.318	1205.4	50.145	51.1



Area Percent Report

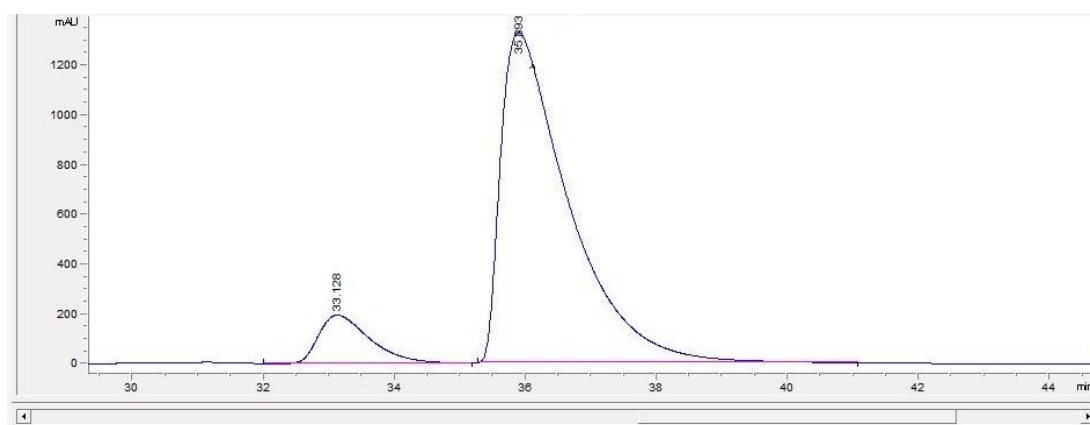
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	13.015	919.2	58.885	46.4
2	15.022	641.8	41.115	28.4

(S)-3-isopropyl-2-((4-methoxyphenyl)sulfonyl)isoindolin-1-one (2g)



Area Percent Report

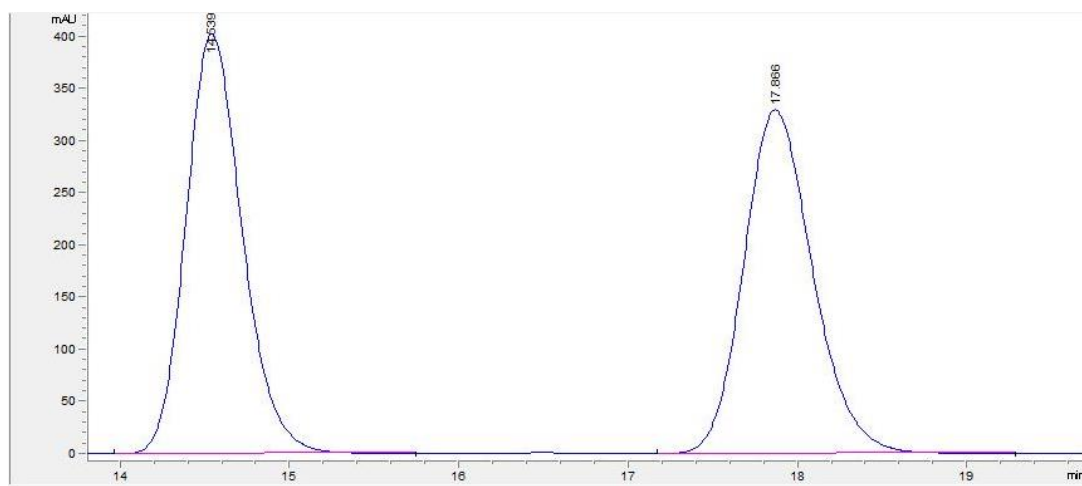
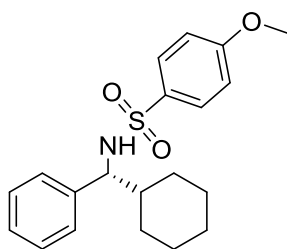
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	34.109	3181.1	50.070	53.3
2	37.92	3172.2	49.930	45.6



Area Percent Report

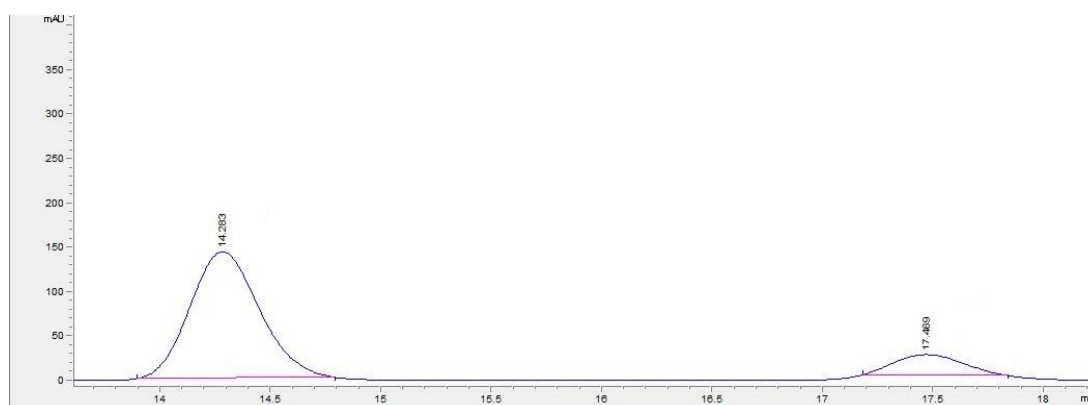
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	33.128	10468.4	9.873	193.9
2	35.893	95563.8	90.127	1327.1

(R)-N-(cyclohexyl (phenyl)methyl)-4-methoxybenzenesulfonamid (1h')



Area Percent Report

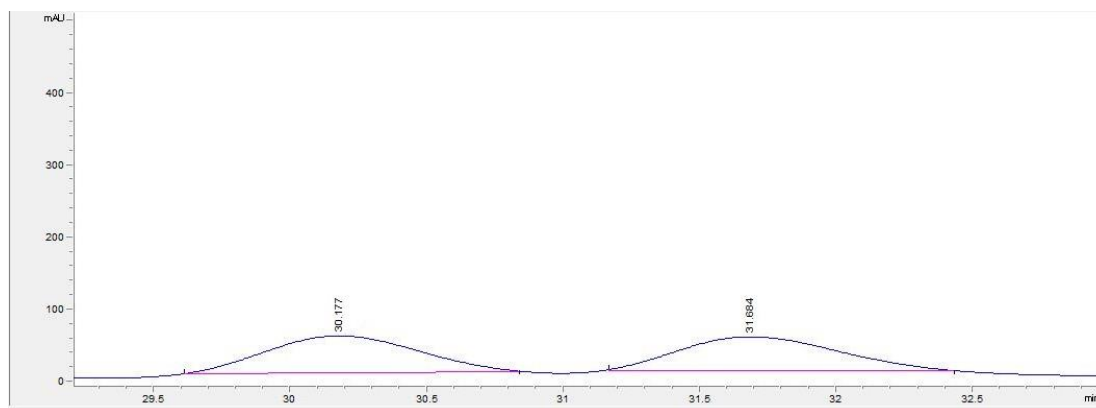
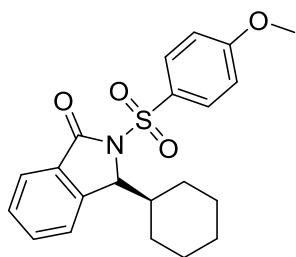
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	14.539	9335.8	49.977	402.7
2	17.866	9344.3	50.023	329.6



Area Percent Report

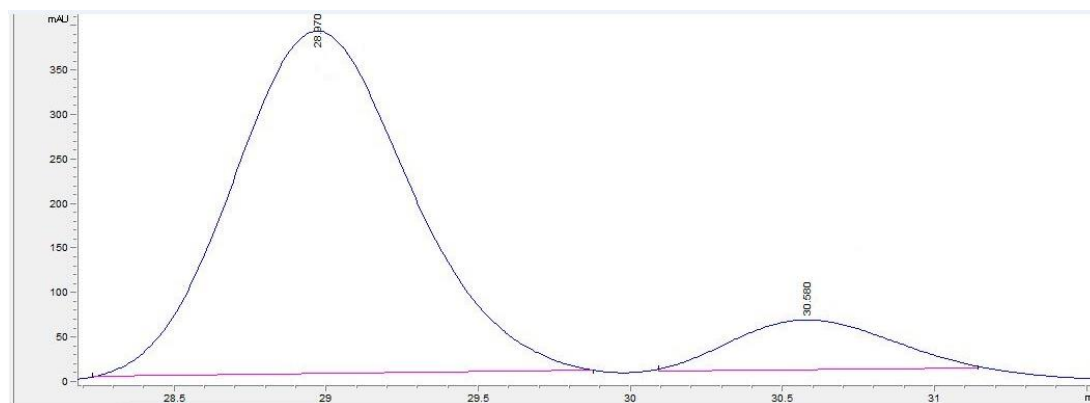
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	14.283	3110.4	86.509	142.6
2	17.469	485.1	13.491	22.9

(S)-3-cyclohexyl-2-((4-methoxyphenyl)sulfonyl)isoindolin-1-one (2h)



Area Percent Report

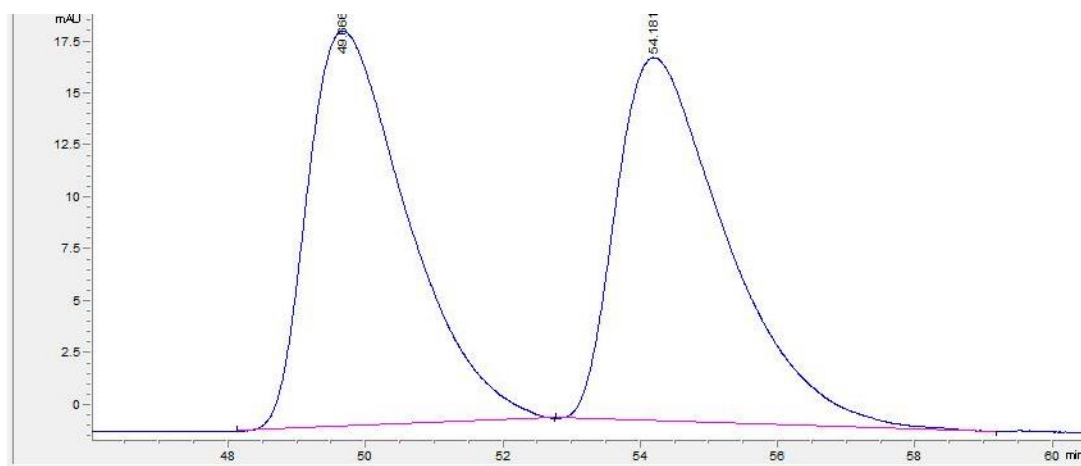
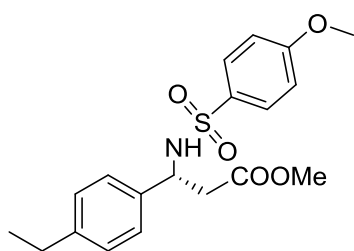
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	30.177	2067	50.019	52.6
2	31.684	1984.4	49.981	48.3



Area Percent Report

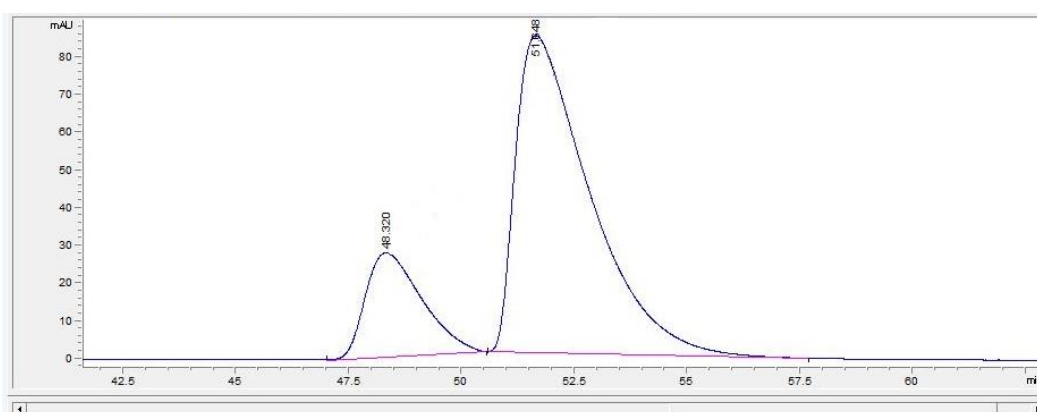
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	28.97	15625.2	88.815	385.8
2	30.58	1967.8	11.185	55.8

(R)-Methyl 3-(4-ethylphenyl)-3-((4-methoxyphenyl)sulfonamide)propanoate (1i')



Area Percent Report

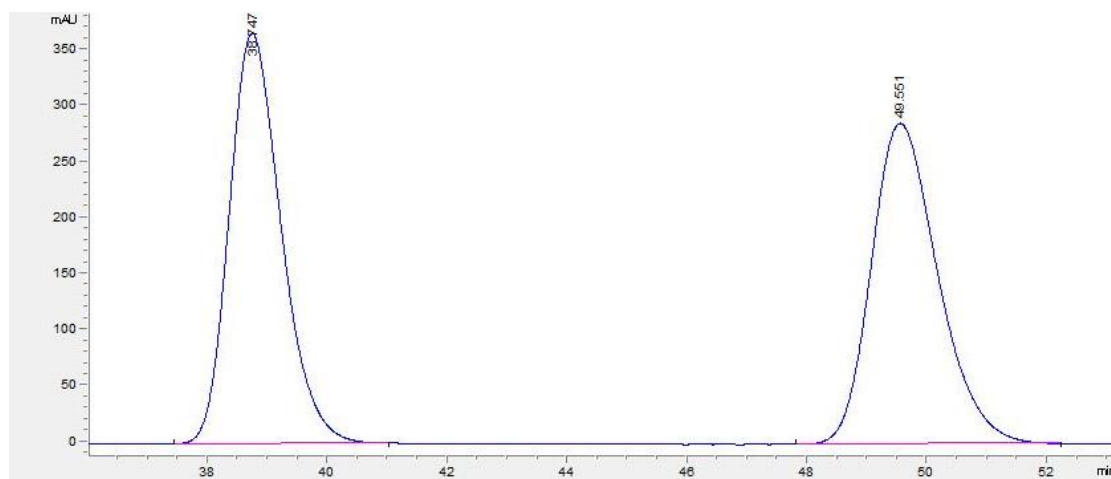
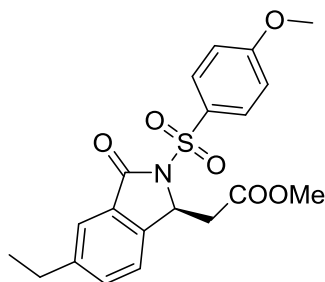
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	49.666	1936	49.657	19.1
2	54.181	1962.8	50.343	17.5



Area Percent Report

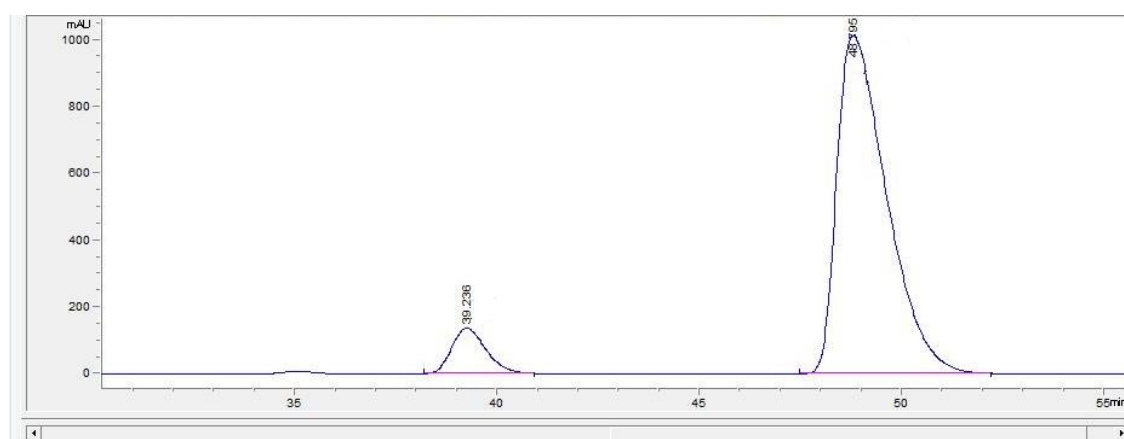
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	48.32	2424.5	20.056	27.8
2	51.648	9664.2	79.944	84.2

**(S)-methyl-2-(5-ethyl-2-((4-methoxyphenyl)sulfonyl)-3-oxoisindolin-1-yl)acetate
(2i)**



Area Percent Report

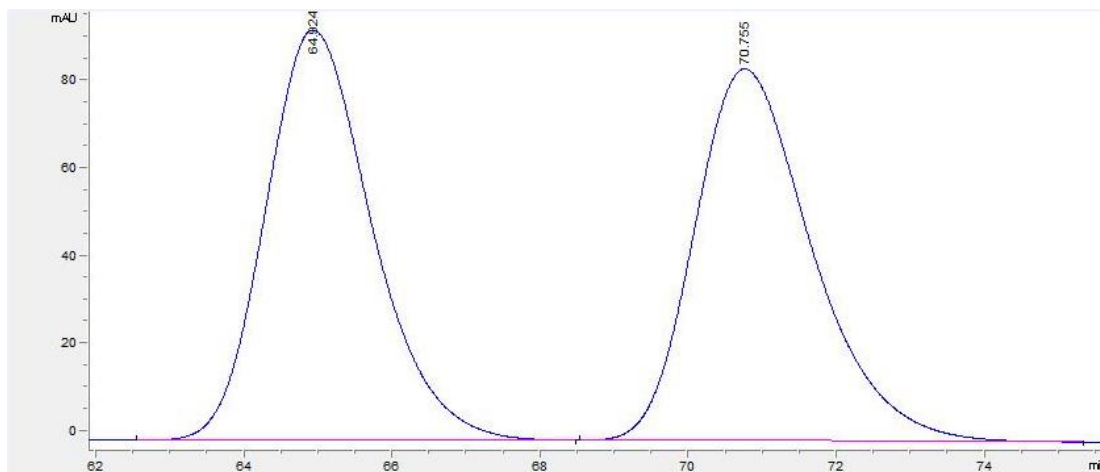
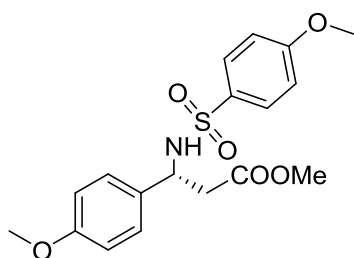
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	38.747	22049.4	49.969	366.2
2	49.551	22076.9	50.031	286.2



Area Percent Report

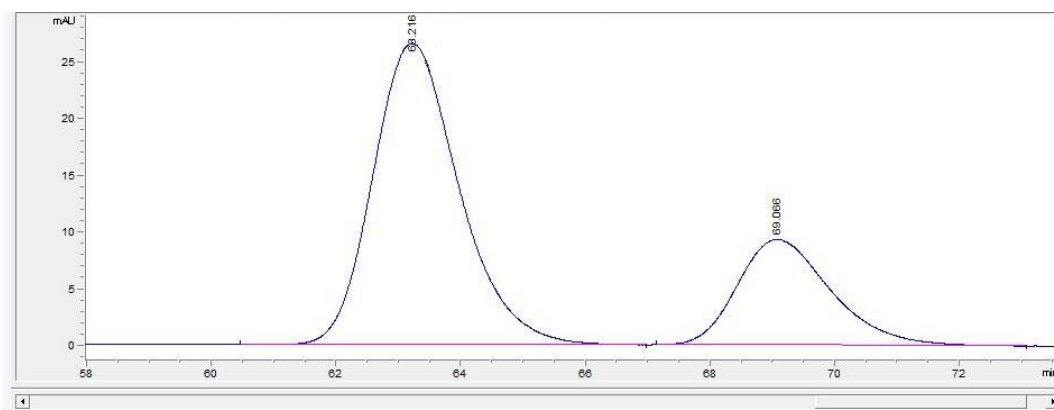
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	39.236	8033.4	8.509	136.1
2	48.795	86372.2	91.491	1013.9

(R)-Methyl 3-(4-methoxyphenyl)-3-((4-methoxyphenyl)sulfonamide)propanoate (1j)



Area Percent Report

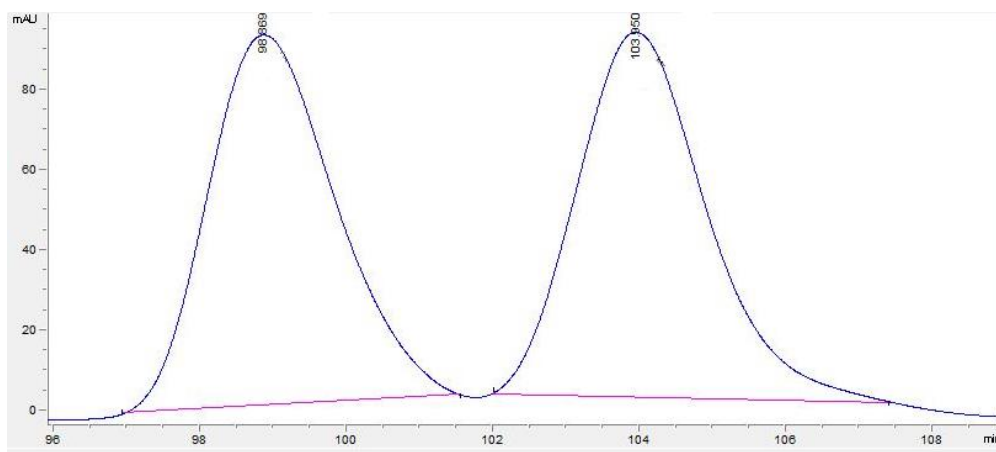
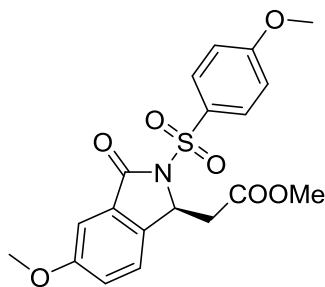
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	64.924	9361	49.997	93.7
2	70.755	9362.1	50.003	85



Area Percent Report

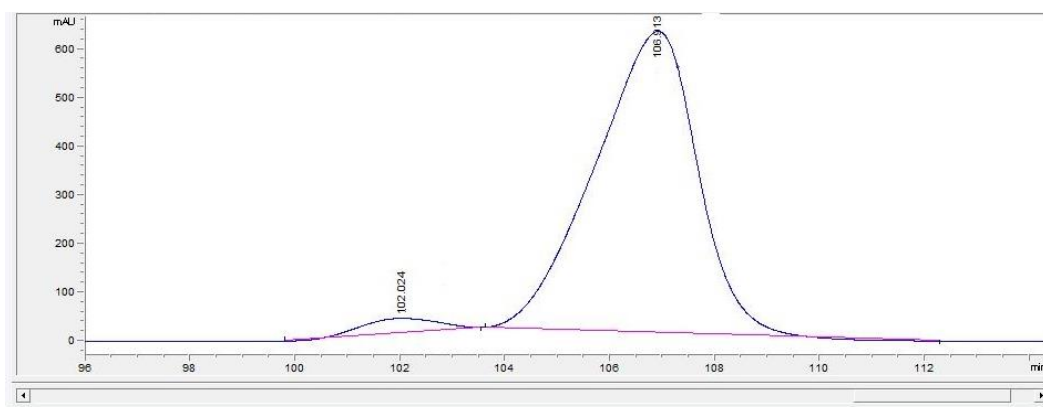
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	63.216	2559.4	72.491	26.5
2	69.066	971.2	27.509	9.3

(S)-methyl-2-(5-methoxy-2-((4-methoxyphenyl)sulfonyl)-3-oxoisindolin-1-yl)acetate (2j)



Area Percent Report

Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	98.869	11116	49.812	92.4
2	103.95	11199.9	50.188	91.1

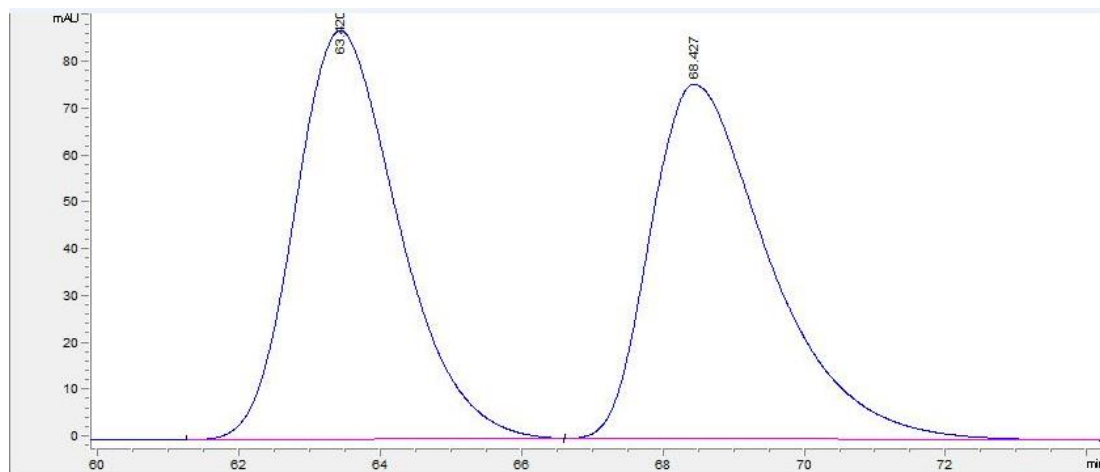
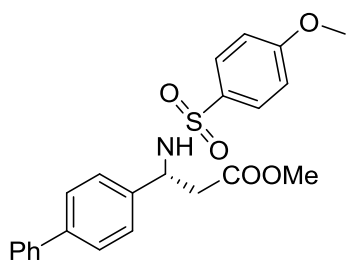


Area Percent Report

m

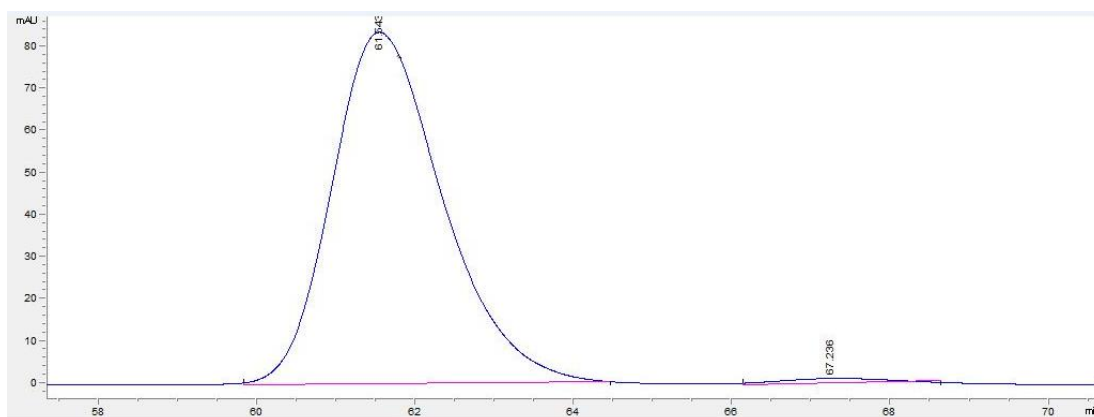
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	102.024	3163	3.597	30.7
2	106.913	84777.7	96.403	620.2

**(R)-Methyl
3-([1,1'-biphenyl]-4-yl)-3-((4-methoxyphenyl)sulfonamide)propanoate (1k')**



Area Percent Report

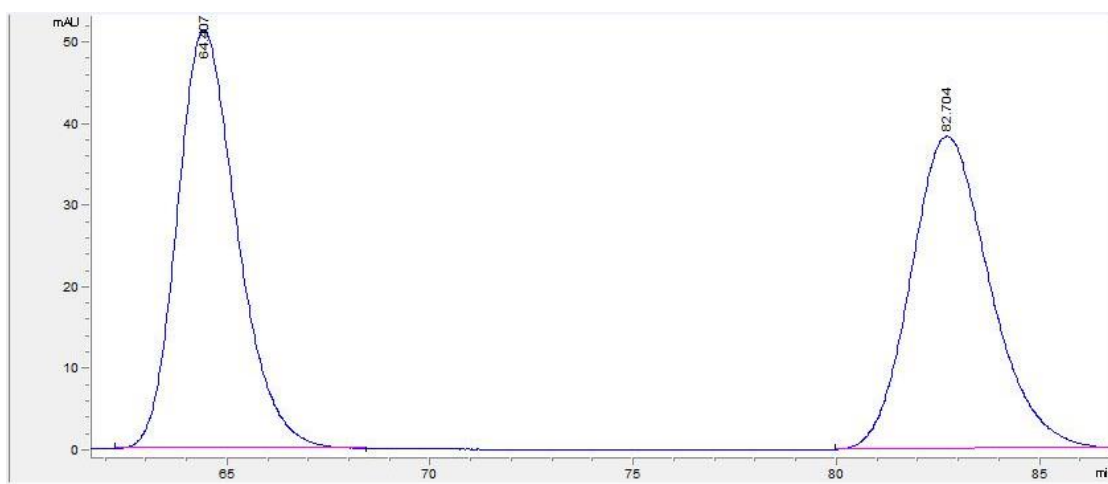
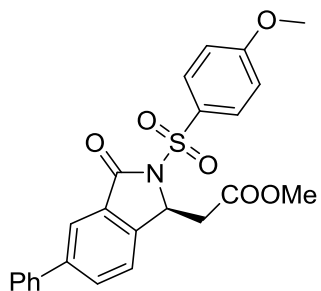
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	63.42	8891.1	50.016	87.4
2	68.427	8885.2	49.984	75.8



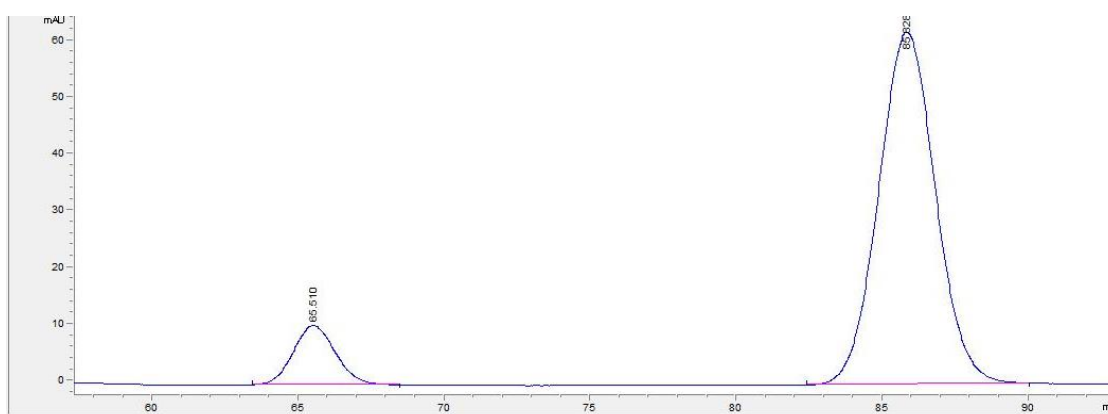
Area Percent Report

Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	61.543	8161.1	98.716	83.6
2	67.236	106.1	1.284	1.2

(S)-methyl-2-(2-((4-methoxyphenyl)sulfonyl)-3-oxo-5-phenylisoindolin-1-yl)acetate (2k)

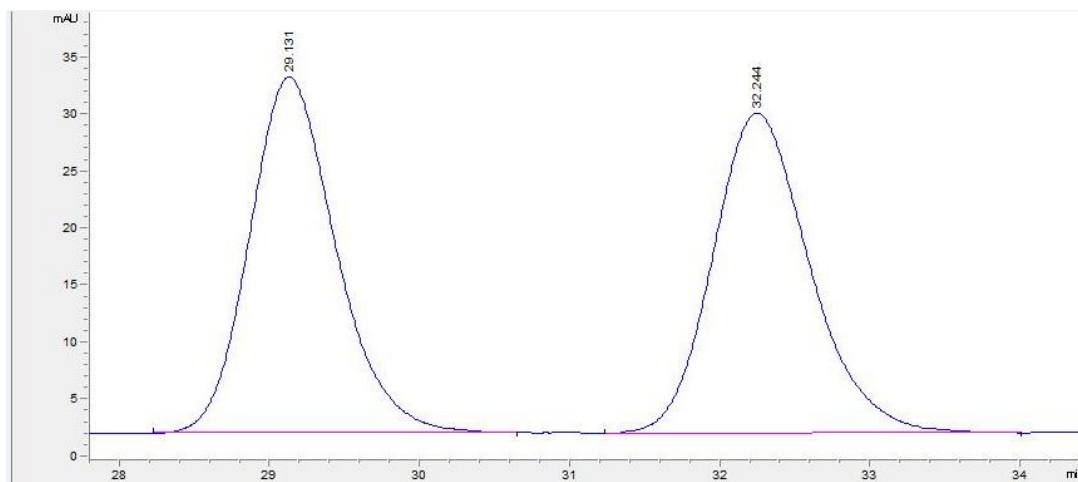
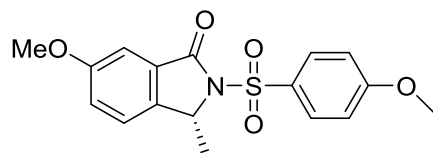


Area Percent Report				
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	64.407	5262.9	50.464	51.2
2	82.704	5166.1	49.536	38.3



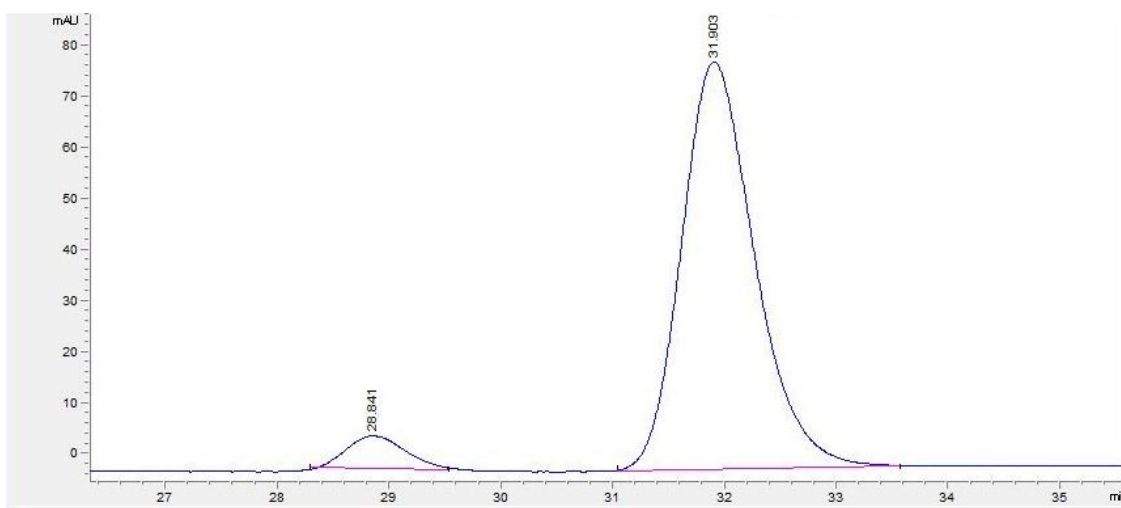
Area Percent Report				
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	65.51	1045.8	11.076	10.4
2	85.828	8396.4	88.924	62

(R)-6-methoxy-2-((4-methoxyphenyl)sulfonyl)-3-methylisoindolin-1-one (2f')



Area Percent Report

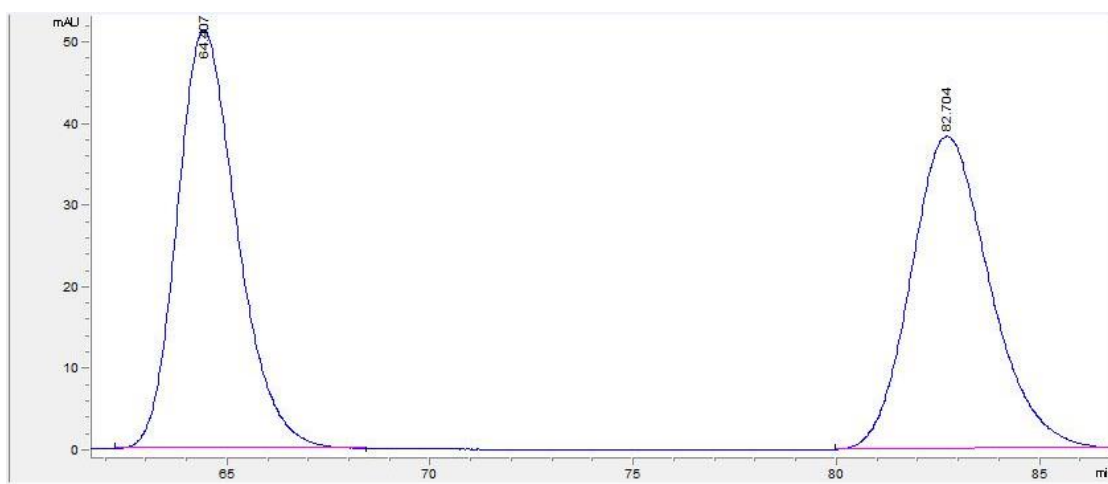
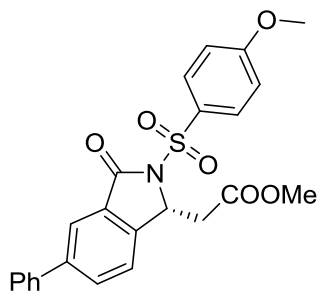
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	29.131	1251	49.751	31.2
2	32.244	1263.5	50.249	28.1



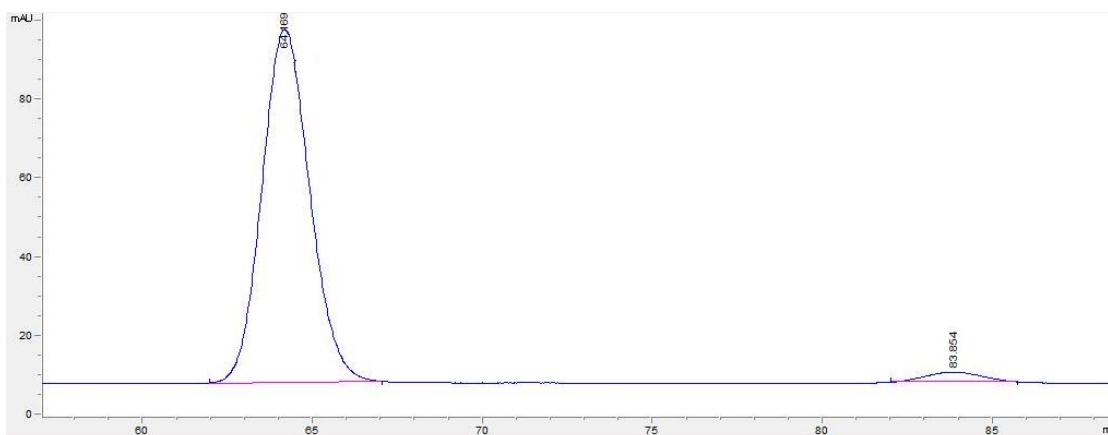
Area Percent Report

Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	28.841	238.6	6.139	6.5
2	31.903	3648.4	93.861	79.9

(R)-methyl-2-(2-((4-methoxyphenyl)sulfonyl)-3-oxo-5-phenylisoindolin-1-yl)acetate (2k')



Area Percent Report				
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	64.407	5262.9	50.464	51.2
2	82.704	5166.1	49.536	38.3



Area Percent Report				
Peak	RetTime [min]	Area [mAU*s]	Area %	Height [mAU]
1	64.169	8813.9	96.681	89.7
2	83.854	302.6	3.319	2.6