SUPPORTING INFORMATION

Kinetic Resolution of 1-(1-Alkynyl)cyclopropyl Ketones *via* Gold-Catalyzed Divergent (4+4) Cycloadditions: Stereoselective Access to Furan Fused Eight-Membered Heterocycles

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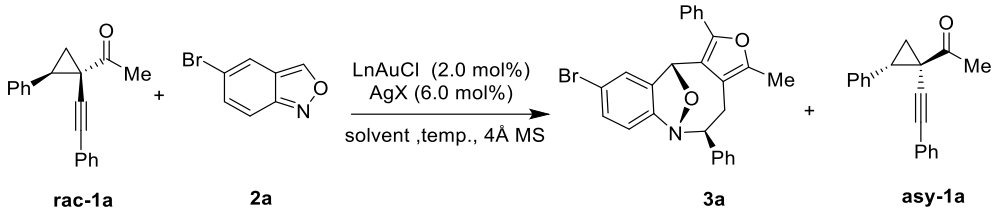
1. General information

Unless otherwise noted, all the reactions for the preparation of the substrates were performed in oven-dried glassware under nitrogen atmosphere with freshly distilled solvents. The catalytic reactions were performed under nitrogen atmosphere. The solvents were purified by distillation from calcium hydride unless otherwise noted. The AgOTf was purchased from Sigma-Aldrich manufacturer and conduct timely moisture removal. All other commercial reagents were used without further purification unless otherwise indicated. ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker 400 MHz spectrometer (ADVNCE III) using chloroform-*d* ($CDCl_3$) and dimethyl sulphoxide-*d6* (DMSO- *d6*) as the internal standard. Chemical shifts were reported in parts per million (ppm), and the residual solvent peak was used as an internal reference: proton (chloroform δ 7.26), carbon (chloroform δ 77.10) or tetramethylsilane (TMS δ 0.00) was used as a reference. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), coupling constants (Hz) and integration. The enantiomeric excesses (e.e.) was determined by HPLC analysis on LC-20AD/T LPGE KIT using Daicel CHIRALPAK® column. X-ray diffraction analyses were carried out on a microcrystalline powder using a Rigaku Oxford Diffraction XtaLAB Synergy-S diffractometer using Cu radiation (λ = 1.54184 Å). If not specially mentioned, flash column chromatography was performed using 200-300 silica gel purchased from Yantai Chemicals (China). High-resolution mass spectra (HRMS) were recorded on a Bruker Apex IV FTMS mass spectrometer using ESI (electrospray ionization) as ionization method. Optical rotations were recorded on an AUTOPOL II digital polarimeter at 589 nm and are recorded as $[\alpha]_D^T$ (concentration in grams/100 mL solvent). The racemic 1-(1-alkynyl) cyclopropyl ketones [1-2], *ortho*-quinone methides [3-4] and anthranils [5-6] were prepared according to the reported procedures. The chiral gold catalyst [7] was prepared according to the reported procedures.

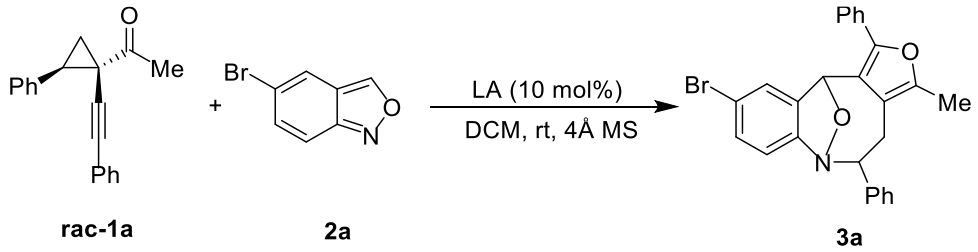
2. Reaction optimizations

General procedure for the reaction optimization



To a dried tube was added LnAuCl (2.0 mol%) and AgX (6.0 mol%) in the glove box, and the solvent (0.5 mL) was added. The mixture was stirred at room temperature for 10 min. Then the precipitate was removed and the remaining solution was transferred into a solution of cyclopropyl ketone **1a** (0.1 mmol, 1.0 equiv.) and anthranils **2a** (x mmol) with 4 Å molecular sieves 150 mg in solvent (0.5 mL). The reaction was then stirred at the corresponding temperature. After the reaction was complete as monitored by TLC and HPLC analysis, it was filtered through a short pad of silica gel to remove catalyst rapidly. Then the solvent was removed under reduced pressure, and the residue was purified by a silica gel column using ethyl acetate/ petroleum ether (1/60-1/10) as the eluent to give aim product **3a** and **asy-1a**.

Table 1. Investigation of metal catalysts



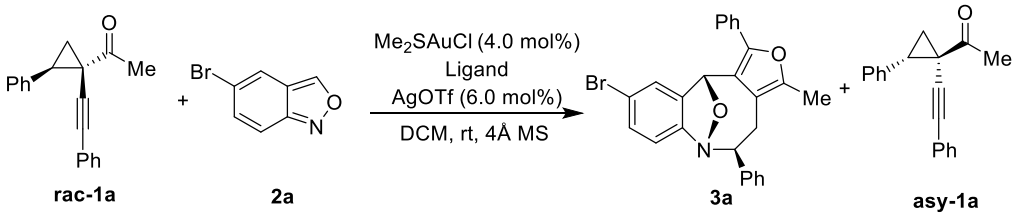
rac-1a 2a 3a

Entry	LA	yield
1	$Cu(OTf)_2$	trace
2	CuOTf	NR
3	$Sc(OTf)_3$	NR
4	$Zn(OTf)_2$	NR
5	AgOTf	10%
6	PPh_3AuCl	21%
7	PPh_3AuOTf	86%

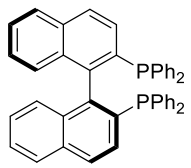
Unless otherwise indicated, all reactions were performed with **1a** (0.1 mmol) and **2a** (0.1 mmol) in the presence of catalyst (10 mol%) in DCM (1.0 mL) at room temperature under nitrogen atmosphere. [b] Isolated yield of product **3a**.

After screening Lewis acid, PPh_3AuOTf was beneficial to this reaction.

Table 2. Investigation of chiral ligands



rac-1a **2a** **3a** **asy-1a**



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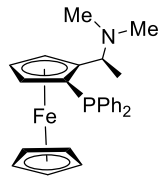

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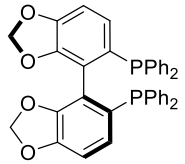

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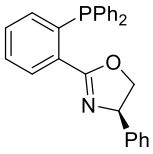

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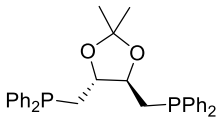

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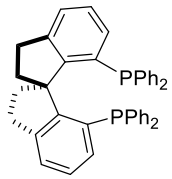

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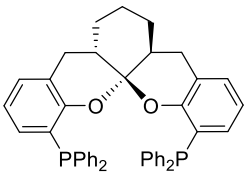

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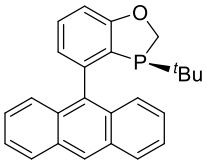

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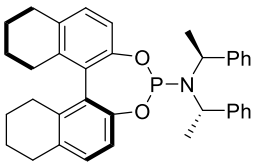

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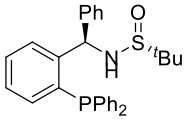

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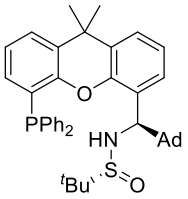

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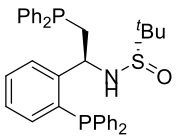

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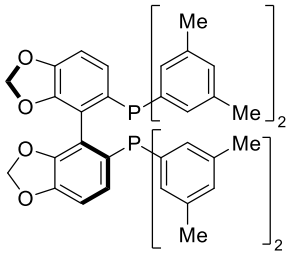
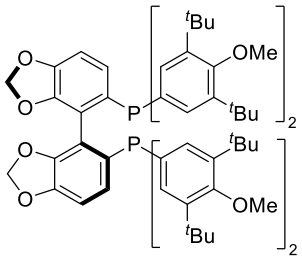
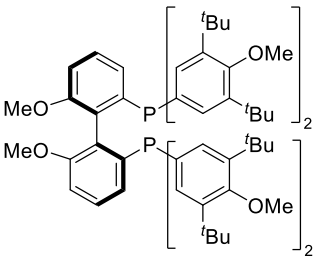


L13



L14



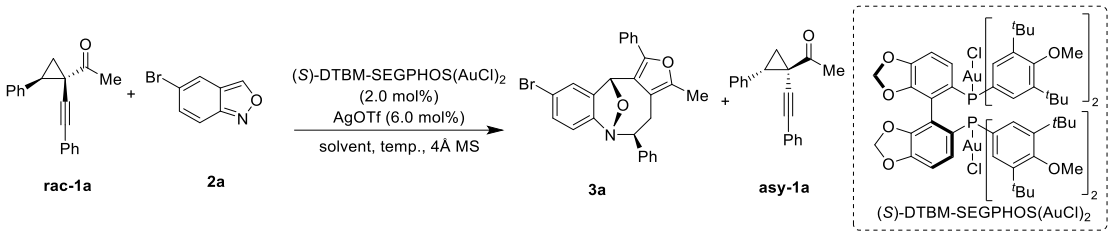
L15

Entry	ligand	yield [b] (**3a**)	ee [c] (**3a**)	yield [b](**1a**)	ee [c] (**1a**)	time	*s*
1	**L1**	12%	15%	65%	25%	18 h	2
2	**L2**	15%	8%	34%	36%	18 h	2
3	**L3**	15%	62%	57%	25%	18 h	5
4	**L4**	trace	--	--	--	18 h	--
5	**L5**	21%	20%	25%	35%	18 h	2
6	**L6**	26%	21%	35%	26%	18 h	2
7	**L7**	35%	29%	28%	21%	18 h	2
8	**L8**	29%	38%	25%	39%	18 h	3
9	**L9**	42%	8%	41%	10%	4 h	1
10	**L10**	36%	15%	43%	38%	18 h	2
11	**L11**	28%	31%	38%	42%	18 h	3
12	**L12**	31%	25%	42%	44%	18 h	2
13	**L13**	21%	61%	58%	45%	10 h	6
14	**L14**	43%	65%	40%	90%	2 h	14
15	**L15**	35%	55%	37%	75%	2 h	7

[a] Unless otherwise indicated, all reactions were performed with **1a** (0.1 mmol) and **2a** (0.07 mmol) in the presence of Me_2SAuCl (4.0 mol%), ligand, AgOTf (6.0 mol%) in DCM (1.0 mL) at room temperature under nitrogen atmosphere. [b] Isolated yield of product **3a**. [c] Determined by HPLC analysis. [d] Selectivity (s) values were calculated through the equation $s = \ln[(1 - C)(1 - ee_{1a})]/\ln[(1 - C)(1 + ee_{1a})]$, where C is the conversion; $C = ee_{1a}/(ee_{1a} + ee_{3a})$.

After optimization, **L14** was selected for the following reaction optimization.

Table 3. Investigation of solvents and temperature

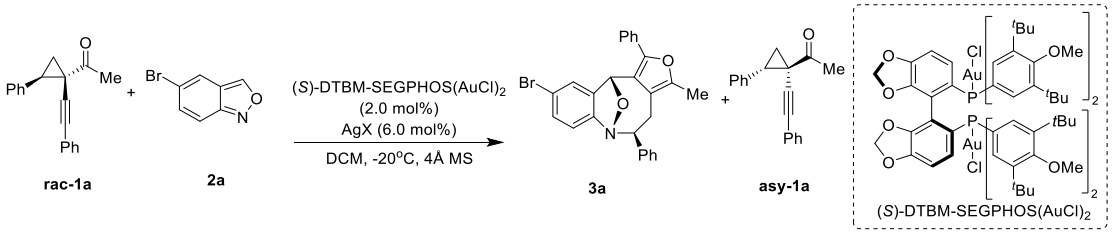


Entry	temp.	sol.	yield (**3a**)[b]	ee (**3a**)[c]	yield (**1a**)[b]	ee (**1a**)[c]	time	*s*
1	rt	THF	trace	--	--	--	18 h	--
2	rt	DCE	36%	60%	41%	92%	2 h	12
3	rt	Toluene	15%	60%	35%	81%	6 h	10
4	rt	$CHCl_3$	30%	61%	40%	88%	8 h	12
5	rt	MeCN	trace	--	--	--	24 h	--
6	0 ºC	DCM	44%	70%	46%	94%	6 h	19
7	-10 ºC	DCM	46%	77%	43%	92%	12 h	25
8	-20 ºC	DCM	45%	87%	44%	90%	24 h	44
9	-30 ºC	DCM	25%	90%	61%	46%	38 h	30

Unless otherwise indicated, all reactions were performed with **1a** (0.1 mmol) and **2a** (0.07 mmol) in the presence of (*S*)-DTBM-SEGPHOS(AuCl)$_2$ (2.0 mol%), AgOTf (6.0 mol%) in solvent (1.0 mL) under nitrogen atmosphere. [b] Isolated yield of product **3a**. [c] Determined by HPLC analysis.

After optimization, the reaction showed the optimal result with DCM as the solvent at -20 ºC.

Table 4. Investigation of silver salts

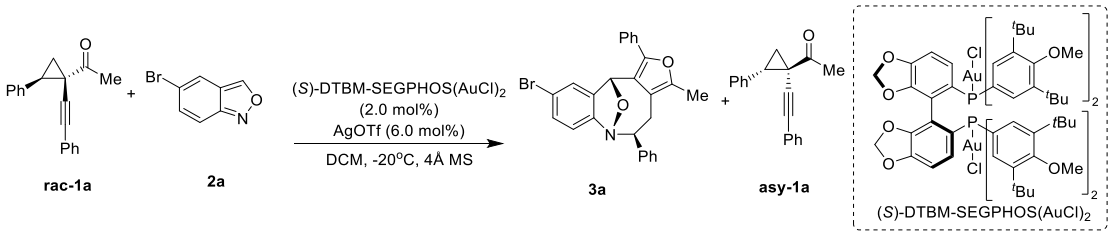


Entry	AgX	yield (**3a**)[b]	ee (**3a**)[c]	yield (**1a**)[b]	ee (**1a**)[c]	time	*s*
1	AgOTf	45%	87%	44%	91%	24 h	45
2	$AgSbF_6$	36%	75%	41%	79%	24 h	17
3	$AgNTf_2$	43%	78%	45%	83%	24 h	21
4	$AgClO_4$	36%	83%	40%	78%	24 h	25
5	$AgPF_6$	28%	88%	54%	57%	24 h	28
6	$AgBF_4$	35%	74%	41%	64%	24 h	13

Unless otherwise indicated, all reactions were performed with **1a** (0.1 mmol) and **2a** (0.07 mmol) in the presence of (*S*)-DTBM-SEGPHOS$(AuCl)_2$ (2.0 mol%), AgOTf (6.0 mol%) in DCM (1.0 mL) under nitrogen atmosphere. [b] Isolated yield of product **3a**. [c] Determined by HPLC analysis.

After optimization, AgOTf was selected for the following investigation.

Table 5. Investigation of 1a/2a ratio

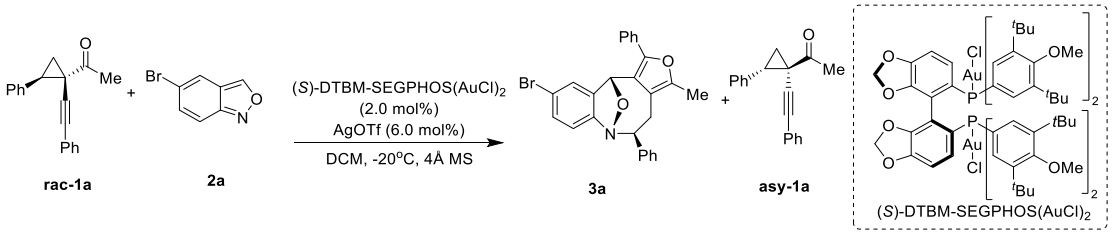


Entry	**1a**/**2a**	yield (**3a**)[b]	ee (**3a**)[c]	yield (**1a**)[b]	ee (**1a**)[c]	time	*s*
1	1:0.5	31%	89%	54%	65%	24 h	34
2	1:0.7	45%	87%	44%	91%	24 h	45
3	1:1	46%	79%	38%	96%	24 h	33

Unless otherwise indicated, all reactions were performed with **1a** (0.1 mmol) and **2a** (0.05-0.1 mmol) in the presence of (*S*)-DTBM-SEGPHOS$(AuCl)_2$ (2.0 mol%), AgOTf (6.0 mol%) in DCM (1.0 mL) under nitrogen atmosphere. [b] Isolated yield of product **3a**. [c] Determined by HPLC analysis.

After optimization, the reaction with **1a**/**2a** ratio = 1:0.7 showed the optimal result.

Table 6. Investigation of reaction concentration



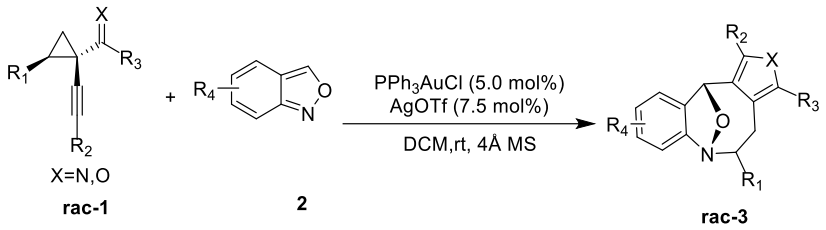
Entry	conc.	yield (**3a**)[b]	ee (**3a**)[c]	yield (**1a**)[b]	ee (**1a**)[c]	time	*s*
1	0.05 M	38%	87%	43%	81%	24 h	36
2	0.1 M	45%	87%	44%	90%	24 h	44
3	0.2 M	43%	86%	42%	91%	24 h	42

Unless otherwise indicated, all reactions were performed with **1a** (0.1 mmol) and **2a** (0.07 mmol) in the presence of (*S*)-DTBM-SEGPHOS(AuCl)$_2$ (2.0 mol%), AgOTf (6.0 mol%) in DCM (0.5-2.0 mL) under nitrogen atmosphere. [b] Isolated yield of product **3a**. [c] Determined by HPLC analysis.

After optimization, the beat result was obtained with the reaction concentration as 0.1 M.

3. Representative procedure and data for the products of 3 and 5.

General procedure for synthesis the racemic heterocycles 3 and 5

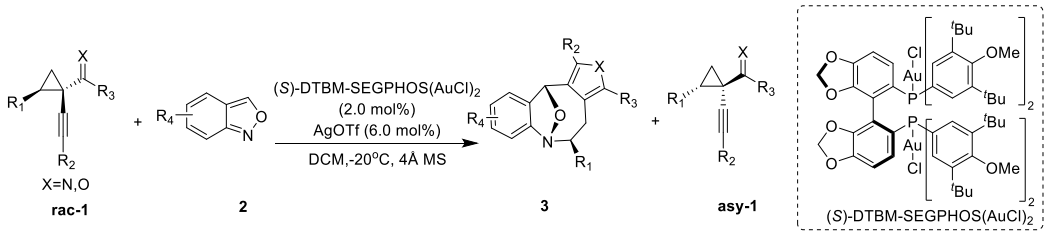


To a dried flask was added PPh_3AuCl (5.0 mol%) and AgOTf (7.5 mol%) in the glove box, and the DCM (0.5 mL) was added. The mixture was stirred at room temperature for 10 min. Then the precipitate was removed and the remaining solution was transferred into a solution of cyclopropyl ketone **1** (0.12 mmol, 1.2 equiv.) and anthranils **2** (0.1 mmol, 1.0 equiv.) with 4 Å molecular sieves 300 mg in DCM (0.5 mL) at room temperature. The reaction was stirred at room temperature. After it was complete, the reaction was filtered through a short pad of silica gel to remove catalyst rapidly. Then the filtrate was removed under reduced pressure, and the residue was purified by a silica gel column using ethyl acetate/ petroleum ether (1/60-1/10) as the eluent to give racemic product **3**.

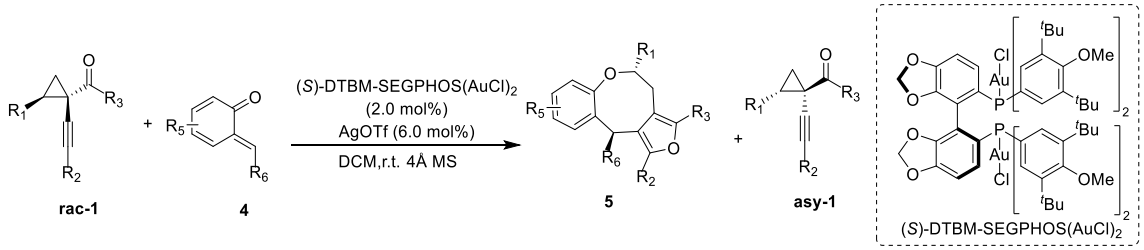
To a dried flask was added PPh_3AuCl (5.0 mol%) and AgOTf (7.5 mol%) in the glove box, and the DCM (0.5 mL) was added. The mixture was stirred at room temperature for 10 min. Then the precipitate was removed and the remaining solution was transferred into a solution of cyclopropyl ketone **1** (0.1 mmol, 1.0 equiv.) and *o*-quinone methides **4** (0.15 mmol, 1.5 equiv.) with 4 Å molecular sieves 300 mg in DCM (0.5 mL) at room temperature. The reaction was stirred at room temperature. After it was

complete, the reaction was filtered through a short pad of silica gel to remove catalyst rapidly. Then the filtrate was removed under reduced pressure, and the residue was purified by a silica gel column using ethyl acetate/ petroleum ether (1/20-1/10) as the eluent to give racemic product **5**.

General procedure for synthesis the chiral heterocycles 3 and 5

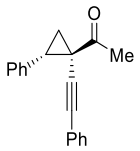


General procedure 1: To a dried flask was added (*S*)-DTBM-SEGPHOS(AuCl)$_2$ (2.0 mol%) and AgOTf (6.0 mol%) in the glove box, and the DCM (1.0 mL) was added. The mixture was stirred at room temperature for 10 min. Then the precipitate was removed and the remaining solution was transferred into a solution of cyclopropyl ketone **1** (0.2 mmol, 1.0 equiv.) and anthranils **2** (0.14 mmol, 0.7 equiv.) with 4 Å molecular sieves 300 mg in DCM (1.0 mL) at -20 ºC. The reaction was then stirred at -20 ºC for 12-96 h. After the reaction was complete as monitored by TLC and HPLC analysis, it was filtered through a short pad of silica gel to remove catalyst rapidly. Then the solvent was removed under reduced pressure, and the residue was purified by a silica gel column using ethyl acetate/ petroleum ether (1/60-1/10) as the eluent to give aim product **3**.



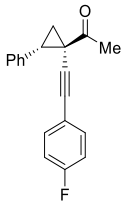
General procedure 2: To a dried tube was added (S)-DTBM-SEGPHOS(AuCl)$_2$ (2.0 mol%) and AgOTf (6.0 mol%) in the glove box, and the DCM (1.0 mL) was added. The mixture was stirred at room temperature for 10 min. Then the precipitate was removed and the remaining solution was transferred into a solution of cyclopropyl

ketone **1** (0.2 mmol, 1.0 equiv.) and *ortho*-quinone methides **4** (0.13 mmol, 0.65 equiv.) with 4 Å molecular sieves 300 mg in DCM (1.0 mL) at room temperature. The reaction was then stirred at room temperature for 2 h-48 h. After the reaction was complete as monitored by TLC and HPLC analysis, it was filtered through a short pad of silica gel to remove catalyst rapidly. Then the solvent was removed under reduced pressure, and the residue was purified by a silica gel column using ethyl acetate/ petroleum ether (1/60-1/10) as the eluent to give aim product **5**.



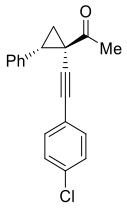
1-((1R,2S)-2-phenyl-1-(phenylethynyl)cyclopropyl)ethan-1-one (1a)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.85 (dd, *J* = 8.0, 4.2 Hz, 1H), 2.20 (dd, *J* = 9.1, 4.3 Hz, 1H), 2.59 (s, 3H), 3.04 (t, *J* = 8.5 Hz, 1H), 7.10-7.15 (m, 2H), 7.17-7.26 (m, 3H), 7.26-7.32 (m, 3H), 7.32-7.38 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.5, 29.7, 33.4, 39.2, 84.4, 87.4, 123.0, 127.3, 128.0, 128.1, 128.3, 128.7, 131.4, 135.9, 205.0.



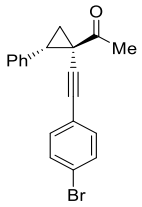
1-((1R,2S)-1-((4-fluorophenyl)ethynyl)-2-phenylcyclopropyl)ethan-1-one (1b)

Yellow oil, 25 mg, 45% yield; 91% ee; $[\alpha]_D^{20.0}$ =46.5 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99/1, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =5.6 min, t (minor) =5.2 min]; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.87 (dd, *J* = 7.9, 4.3 Hz, 1H), 2.22 (dd, *J* = 9.1, 4.3 Hz, 1H), 2.60 (s, 3H), 3.07 (t, *J* = 8.5 Hz, 1H), 6.89-6.97 (m, 2H), 7.06-7.13 (m, 2H), 7.27-7.43 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.4, 29.7, 33.3, 39.2, 83.3, 87.1, 115.5 (d, *J* = 22.0 Hz), 119.05 (d, *J* = 3.5 Hz), 127.4, 128.0, 128.8, 133.3 (d, *J* = 8.3 Hz), 135.9, 162.3 (d, *J* = 249.2 Hz), 204.8.



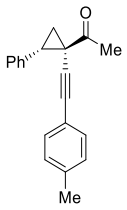
1-((1R,2S)-1-((4-chlorophenyl)ethynyl)-2-phenylcyclopropyl)ethan-1-one (1c)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.86 (dd, *J* = 7.9, 4.3 Hz, 1H), 2.20 (dd, *J* = 9.0, 4.3 Hz, 1H), 2.57 (s, 3H), 3.05 (t, *J* = 8.5 Hz, 1H), 7.00-7.05 (m, 2H), 7.17-7.22 (m, 2H), 7.26-7.39 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.5, 29.7, 33.3, 39.3, 83.3, 88.5, 121.5, 127.4, 128.1, 128.6, 128.7, 132.6, 134.1, 135.8, 204.6; HRMS (ESI) m/z calcd for $C_{19}H_{15}ClO$ $[M+H]^+$: 295.0884, found: 295.0880.



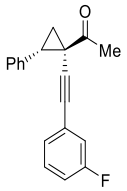
1-((1R,2S)-1-((4-bromophenyl)ethynyl)-2-phenylcyclopropyl)ethan-1-one (1d)

Yellow oil, 30.3 mg, 45% yield; >99% ee; $[\alpha]_D^{20.0}$ =65.6 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99/1, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =10.3 min, t (minor) =8.6 min];^{1}H NMR (400 MHz, $CDCl_3$) δ 1.86 (dd, *J* = 8.0, 4.3 Hz, 1H), 2.20 (dd, *J* = 9.1, 4.3 Hz, 1H), 2.57 (s, 3H), 3.05 (t, *J* = 8.5 Hz, 1H), 6.92-6.98 (m, 2H), 7.24-7.31 (m, 3H), 7.32-7.38 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.5, 29.7, 33.3, 39.3, 83.4, 88.8, 122.0, 122.2, 127.4, 128.1, 128.7, 131.5, 132.8, 135.8, 204.5.



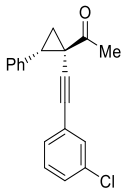
1-((1R,2S)-2-phenyl-1-(p-tolylethynyl)cyclopropyl)ethan-1-one (1e)

Yellow oil, 23 mg, 42% yield; 95% ee; $[\alpha]_D^{20.0}$=76.7 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99/1, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =7.2 min, t (minor) =6.5 min];^{1}H NMR (400 MHz, $CDCl_3$) δ 1.83 (dd, *J* = 8.0, 4.2 Hz, 1H), 2.18 (dd, *J* = 9.1, 4.2 Hz, 1H), 2.30 (s, 3H), 2.58 (s, 3H), 3.02 (t, *J* = 8.5 Hz, 1H), 7.01-7.03 (m, 4H), 7.25-7.30 (m, 3H), 7.30-7.37 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.5, 26.5, 29.7, 33.4, 39.2, 84.5, 86.6, 119.9, 127.2, 128.0, 128.7, 129.0, 131.3, 136.0, 138.2, 205.2.



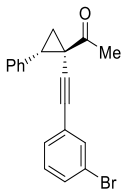
1-((1R,2S)-1-((3-fluorophenyl)ethynyl)-2-phenylcyclopropyl)ethan-1-one (1f)

Yellow oil, 24.4 mg, 44% yield; 93% ee; $[\alpha]_D^{20.0}$=42.6 (0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =7.2 min, t (minor) =7.6 min]; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.87 (dd, *J* = 8.0, 4.3 Hz, 1H), 2.20 (dd, *J* = 9.1, 4.3 Hz, 1H), 2.57 (s, 3H), 3.06 (t, *J* = 8.5 Hz, 1H), 6.78 (ddd, *J* = 9.4, 2.6, 1.4 Hz, 1H), 6.89 (dt, *J* = 7.6, 1.2 Hz, 1H), 6.94 (tdd, *J* = 8.5, 2.6, 1.0 Hz, 1H), 7.17 (td, *J* = 8.0, 5.9 Hz, 1H), 7.24-7.40 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.5, 29.7, 33.2, 39.3, 83.2 (d, *J* = 3.4 Hz), 88.6, 115.4 (d, *J* = 21.2 Hz), 118.2 (d, *J* = 22.7 Hz), 124.8 (d, *J* = 9.6 Hz), 127.2 (d, *J* = 3.0 Hz), 127.4, 128.1, 128.7, 129.8 (d, *J* = 8.6 Hz), 135.8, 162.3 (d, *J* = 246.5 Hz), 204.5; HRMS (ESI) m/z calcd for $C_{19}H_{15}FO$ $[M+H]^+$:279.1180, found:279.1177.



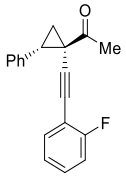
1-((1R,2S)-1-((3-chlorophenyl)ethynyl)-2-phenylcyclopropyl)ethan-1-one (1g)

Yellow oil, 25.3 mg, 43% yield; 87% ee; $[\alpha]_D^{20.0}$=41.6 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99/1, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =10.7 min, t (minor) =9.6 min];^{1}H NMR (400 MHz, $CDCl_3$) δ 1.86 (dd, *J* = 8.0, 4.3 Hz, 1H), 2.20 (dd, *J* = 9.1, 4.3 Hz, 1H), 2.57 (s, 3H), 3.06 (t, *J* = 8.5 Hz, 1H), 6.97 (dt, *J* = 7.7, 1.3 Hz, 1H), 7.07 (t, *J* = 1.8 Hz, 1H), 7.14 (t, *J* = 7.9 Hz, 1H), 7.21 (ddd, *J* = 8.1, 2.2, 1.2 Hz, 1H), 7.25-7.29 (m, 2H), 7.30-7.33 (m, 1H), 7.33-7.39 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.5, 29.7, 33.3, 39.4, 83.1, 88.9, 124.7, 127.5, 128.1, 128.3, 128.7, 129.4, 129.5, 131.3, 134.0, 135.7, 204.4; HRMS (ESI) m/z calcd for $C_{19}H_{15}ClO$ [M+H]+:295.0884, found:295.0880.



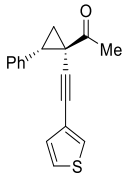
1-((1R,2S)-1-((3-bromophenyl)ethynyl)-2-phenylcyclopropyl)ethan-1-one (1h)

Yellow oil, 29 mg, 43% yield; 83% ee; $[\alpha]_D^{20.0}$=71.8 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =6.2 min, t (minor) = 5.9 min];^{1}H NMR (400 MHz, $CDCl_3$) δ 1.86 (dd, *J* = 8.0, 4.3 Hz, 1H), 2.20 (dd, *J* = 9.1, 4.3 Hz, 1H), 2.57 (s, 3H), 3.06 (t, *J* = 8.5 Hz, 1H), 7.02 (dt, *J* = 7.8, 1.3 Hz, 1H), 7.08 (t, *J* = 7.8 Hz, 1H), 7.23 (t, *J* = 1.7 Hz, 1H), 7.27 (dd, *J* = 7.9, 1.6 Hz, 2H), 7.30-7.39 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.5, 29.7, 33.3, 39.4, 82.9, 89.1, 122.0, 125.0, 127.5, 128.1, 128.7, 129.7, 129.9, 131.2, 134.2, 135.7, 204.4; HRMS (ESI) m/z calcd for $C_{19}H_{15}BrO$ $[M+H]^+$:339.0379, found:339.0377.



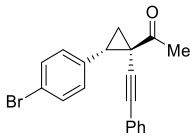
1-((1R,2S)-1-((2-fluorophenyl)ethynyl)-2-phenylcyclopropyl)ethan-1-one (1i)

Yellow oil, 21.3 mg, 38% yield; 90% ee; $[\alpha]_D^{20.0}$=72.9 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =5.7 min, t (minor) =5.3 min];^{1}H NMR (400 MHz, $CDCl_3$) δ 1.89 (dd, *J* = 8.0, 4.3 Hz, 1H), 2.22 (dd, *J* = 9.1, 4.2 Hz, 1H), 2.61 (s, 3H), 3.06 (t, *J* = 8.5 Hz, 1H), 6.95-7.09 (m, 3H), 7.18-7.24 (m, 1H), 7.25-7.37 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.7, 29.7, 33.5, 39.3, 78.2, 92.7 (d, *J* = 3.3 Hz), 111.6 (d, *J* = 15.0 Hz), 115.4 (d, *J* = 20.8 Hz), 123.9 (d, *J* = 3.7 Hz), 127.4, 128.1, 128.7, 129.7 (d, *J* = 8.0 Hz), 133.2, 135.7, 162.9 (d, *J* = 251.2 Hz), 204.7; HRMS (ESI) m/z calcd for $C_{19}H_{15}FO$ $[M+H]^+$:279.1180, found:279.1177.



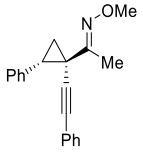
1-((1R,2S)-2-phenyl-1-(thiophen-3-ylethynyl)cyclopropyl)ethan-1-one (1j)

Yellow oil, 21 mg, 39% yield; 82% ee; $[\alpha]_D^{20.0}$=25.6 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99/1, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =9.5 min, t (minor) =8.5 min];^{1}H NMR (400 MHz, $CDCl_3$) δ 1.83 (dd, *J* = 8.0, 4.2 Hz, 1H), 2.19 (dd, *J* = 9.1, 4.2 Hz, 1H), 2.57 (s, 3H), 3.02 (t, *J* = 8.5 Hz, 1H), 6.81 (dd, *J* = 4.9, 1.2 Hz, 1H), 7.13 (dd, *J* = 3.0, 1.2 Hz, 1H), 7.17 (dd, *J* = 4.9, 3.0 Hz, 1H), 7.24-7.31 (m, 3H), 7.31-7.39 (m, 2H);^{13}C NMR (100 MHz, $CDCl_3$) δ 26.5, 29.7, 33.4, 39.2, 79.5, 86.9, 122.0, 125.2, 127.3, 128.0, 128.4, 128.7, 129.7, 135.9, 204.9; HRMS (ESI) m/z calcd for $C_{17}H_{14}OS$ [M+H]+:267.0838, found:267.0835.



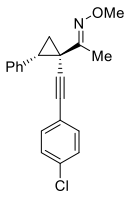
1-((1R,2S)-2-(4-bromophenyl)-1-(phenylethynyl)cyclopropyl)ethan-1-one (1k)

Yellow oil, 27.6 mg, 41% yield; 88% ee; $[\alpha]_D^{20.0}$=42.3 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =5.9 min, t (minor) =6.2 min];^{1}H NMR (400 MHz, $CDCl_3$) δ 1.78 (dd, *J* = 7.9, 4.4 Hz, 1H), 2.18 (dd, *J* = 9.1, 4.4 Hz, 1H), 2.58 (s, 3H), 2.98 (t, *J* = 8.4 Hz, 1H), 7.09-7.21 (m, 4H), 7.26 (dd, *J* = 5.5, 2.1 Hz, 3H), 7.46 (d, *J* = 8.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.6, 29.7, 33.2, 38.2, 84.8, 86.9, 121.2, 122.8, 128.3, 128.4, 130.4, 131.1, 131.4, 135.1, 204.7.



(E)-1-((1R,2S)-2-phenyl-1-(phenylethynyl)cyclopropyl)ethan-1-one-O-methyl oxime (1l)

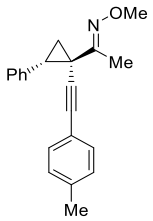
Yellow oil, 21.3 mg, 37% yield; 85% ee; $[\alpha]_D^{20.0}$=42.3 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99.8/0.2, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =11.3 min, t (minor) =9.8 min]; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.67 (dd, *J* = 7.4, 5.1 Hz, 1H), 2.13 (s, 3H), 2.16 (dd, *J* = 5.5, 3.3 Hz, 1H), 2.67 (dd, *J* = 8.9, 7.4 Hz, 1H), 3.87 (s, 3H), 7.03-7.11 (m, 2H), 7.14-7.22 (m, 3H), 7.22 -7.28 (m, 1H) 7.29-7.36 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.0, 21.0, 26.6, 34.4, 61.7, 82.3, 88.7, 123.4, 126.7, 127.7, 127.9, 128.1, 128.6, 131.5, 137.3, 156.0.



(E)-1-((1R,2S)-1-((4-chlorophenyl)ethynyl)-2-phenylcyclopropyl)ethan-1-one-O-methyl oxime (1m)

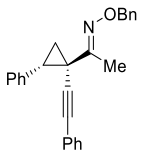
Yellow oil, 26 mg, 40% yield; 85% ee; $[\alpha]_D^{20.0}$=123.8 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99.8/0.2, v = 1.0 mL•min^{-1}, λ = 254

nm, t (major) =7.6 min, t (minor) =6.8 min];^{1}H NMR (400 MHz, $CDCl_3$) δ 1.67 (dd, *J* = 7.4, 5.1 Hz, 1H), 2.11 (s, 3H), 2.16 (dd, *J* = 5.5, 3.3 Hz, 1H), 2.69 (t, *J* = 8.2 Hz, 1H), 3.87 (s, 3H), 6.97 (d, *J* = 8.3 Hz, 2H), 7.15 (d, *J* = 8.3 Hz, 2H), 7.24-7.36 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.0, 20.9, 26.6, 34.4, 61.7, 81.2, 89.9, 121.8, 126.8, 127.9, 128.4, 128.6, 132.7, 133.7, 137.2, 155.7; HRMS (ESI) m/z calcd for $C_{20}H_{18}ClNO$ $[M+H]^+$:324.1150, found: 324.1055.



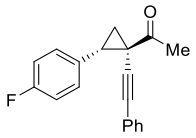
(E)-1-((1R,2S)-2-phenyl-1-(p-tolylethynyl)cyclopropyl)ethan-1-one-O-methyl oxime (1n)

Yellow oil, 22.4 mg, 37% yield; 83% ee; $[\alpha]_D^{20.0}$=32.1 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99.8/0.2, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =5.0 min, t (minor) =4.8 min];^{1}H NMR (400 MHz, $CDCl_3$) δ 1.58 (dd, *J* = 7.4, 4.9 Hz, 1H), 2.05 (s, 3H), 2.06-2.10 (m, 1H), 2.20 (s, 3H), 2.58 (dd, *J* = 8.9, 7.4 Hz, 1H), 3.79 (s, 3H), 6.91 (s, 4H), 7.16-7.20 (m, 1H), 7.22-7.28 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.0, 20.9, 21.5, 26.7, 34.3, 61.7, 82.4, 87.9, 120.3, 126.7, 127.9, 128.6, 128.9, 131.4, 137.3, 137.8, 156.1; HRMS (ESI) m/z calcd for $C_{21}H_{21}NO$ $[M+H]^+$:304.1696, found:304.1693.



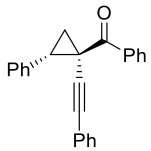
(E)-1-((1R,2S)-2-phenyl-1-(phenylethynyl)cyclopropyl)ethan-1-one-O-benzyl oxime (1o)

Yellow oil, 27.7 mg, 38% yield; 83% ee; $[\alpha]_D^{20.0}$=83.1 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99.8/0.2, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =6.7 min, t (minor) =6.3 min];^{1}H NMR (400 MHz, $CDCl_3$) δ 1.66 (dd, *J* = 7.4, 4.9 Hz, 1H), 2.13-2.21 (m, 1H), 2.17 (s, 3H), 2.65 (dd, *J* = 8.9, 7.4 Hz, 1H), 5.10 (s, 2H), 7.05-7.11 (m, 2H), 7.14-7.21 (m, 3H), 7.23-7.27 (m, 1H), 7.28-7.35 (m, 5H), 7.35-7.41 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.3, 21.1, 26.7, 34.7, 76.0, 82.3, 88.7, 123.4, 126.7, 127.7, 127.8, 127.9, 128.1, 128.3, 128.4, 128.6, 131.5, 137.3, 138.1, 156.5; HRMS (ESI) m/z calcd for $C_{26}H_{23}NO$ $[M+H]^+$:366.1852, found:366.1849.



1-((1*R*,2*S*)-2-(4-fluorophenyl)-1-(phenylethynyl)cyclopropyl)ethan-1-one (1p)

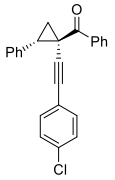
Yellow oil, 19 mg, 34% yield; 93% ee, $[\alpha]_D^{20.0}$= 97.7(0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 7.1 min, t (minor) =7.7 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 1.79 (dd, *J* = 4.3, 7.9 Hz, 1H), 2.19 (dd, *J* = 4.3, 9.1 Hz, 1H), 2.59 (s, 3H), 3.01 (t, *J* = 8.5 Hz, 1H), 7.00-7.07 (t, *J* = 8.7 Hz, 2H), 7.12-7.19 (m, 2H), 7.21-7.29 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) 26.8, 29.7, 33.2, 38.3, 84.6, 87.2, 114.9 (d, *J* = 21.5 Hz), 122.9, 128.2, 128.4, 130.3 (d, *J* = 8.1 Hz), 131.4, 131.8 (d, *J* = 3.2 Hz), 162.1 (d, *J* = 245.9 Hz), 204.8; HRMS (ESI) m/z calcd for $C_{19}H_{15}FO$ [M+H]+:279.1180, found:279.1177.



phenyl((1*R*,2*S*)-2-phenyl-1-(phenylethynyl)cyclopropyl)methanone (1q)

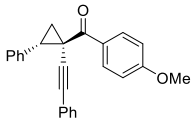
Yellow oil, 23.8 mg, 37% yield; 90% ee, $[\alpha]_D^{20.0}$= 39.7(c = 0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 6.0 min, t (minor) =5.6 min]**;**^{1}H NMR (400 MHz, $CDCl_3$) *δ* 1.94 (dd, *J* = 7.8, 4.7 Hz, 1H), 2.50 (dd, *J* = 9.1, 4.7 Hz, 1H), 3.03 (dd, *J* = 9.1, 7.8 Hz, 1H),

7.01-6.95 (m, 2H), 7.18-7.10 (m, 3H), 7.34-7.29 (m, 1H), 7.45-7.36 (m, 6H), 7.55-7.48 (m, 1H), 8.11-8.05 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.6, 32.1, 38.1, 85.0, 88.3, 123.1, 127.4, 127.9, 128.0, 128.1, 128.2, 128.8, 129.3, 131.2, 132.6, 135.8, 136.8, 196.8.



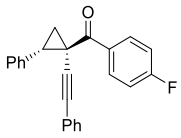
((1*R*,2*S*)-1-((4-chlorophenyl)ethynyl)-2-phenylcyclopropyl)(phenyl)methanone (1r)

Yellow oil, 27.8 mg, 39% yield; 99% ee, $[\alpha]_D^{20.0}$=78.4 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 6.6 min, t (minor) =5.9 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.89 (dd, *J* = 7.9, 4.7 Hz, 1H), 2.44 (dd, *J* = 9.0, 4.7 Hz, 1H), 2.98 (t, *J* = 8.4 Hz, 1H), 6.78-6.84 (m, 2H), 7.05 (d, *J* = 8.5 Hz, 2H), 7.26-7.39 (m, 7H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.98 (d, *J* = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.6, 32.1, 38.2, 83.9, 89.4, 121.6, 127.5, 128.1, 128.2, 128.5, 128.7, 128.8, 129.2, 132.4, 132.7, 135.8, 136.8, 196.7; HRMS (ESI) m/z calcd for $C_{24}H_{17}ClO$ $[M+H]^+$:357.1041, found: 357.1044.



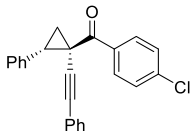
4-methoxyphenyl)((1*R*,2*S*)-2-phenyl-1-(phenylethynyl)cyclopropyl)methanone (1s)

Yellow oil, 22 mg, 31% yield; >99% ee, $[\alpha]_D^{20.0}$= 97.1 (0.1, CH_2Cl_2); [Daicel Chiralpak IA-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 6.5 min, t (minor) =7.2 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.78 (dd, *J* = 4.7, 7.8 Hz, 1H), 2.36 (dd, *J* = 4.7, 9.0 Hz, 1H), 2.83 (dd, *J* = 7.7, 9.1 Hz, 1H), 3.66 (s, 3H), 6.77 (d, *J* = 8.9 Hz, 2H), 6.88-6.96 (m, 2H), 6.98-7.10 (m, 3H), 7.15-7.29 (m, 5H), 8.02 (d, *J* = 8.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 22.9, 31.7, 37.2, 55.5, 84.7, 88.6, 113.2, 123.2, 127.3, 127.9, 128.1, 128.7, 129.4, 131.3, 131.8, 136.1, 163.3, 194.6. HRMS (ESI) m/z calcd for $C_{25}H_{20}O_2$ $[M+H]^+$:353.1536, found:353.1538.



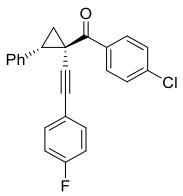
(4-fluorophenyl)((1*R*,2*S*)-2-phenyl-1-(phenylethynyl)cyclopropyl)methanone (1t)

Yellow oil, 24 mg, 35% yield; 95% ee, $[\alpha]_D^{20.0}$= 92.3 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99/1, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 7.5 min, t (minor) =7.0 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) 1.96 (dd, *J* = 7.9, 4.7 Hz, 1H), 2.51 (dd, *J* = 9.1, 4.7 Hz, 1H), 3.01 (t, *J* = 8.5 Hz, 1H), 6.99 (d, *J* = 5.8 Hz, 2H), 7.10 (t, *J* = 8.7 Hz, 2H), 7.15-7.22 (m, 3H), 7.30-7.45 (m, 5H), 8.12 (dd, *J* = 8.7, 5.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 23.6, 32.0, 38.1, 85.2, 88.0, 115.1 (d, *J* = 21.9 Hz), 122.9, 127.5, 128.0, 128.0, 128.2, 128.7, 131.2, 132.0 (d, *J* = 9.2 Hz), 133.0 (d, *J* = 3.0 Hz), 135.7, 165.5 (d, *J* = 254.2 Hz), 195.1; HRMS (ESI) m/z calcd for $C_{24}H_{17}FO$ $[M+H]^+$:341.1336, found:341.1339.



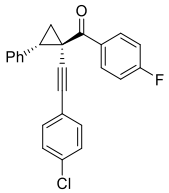
(4-chlorophenyl)((1*R*,2*S*)-2-phenyl-1-(phenylethynyl)cyclopropyl)methanone (1u)

Yellow oil, 26 mg, 37% yield; 95% ee, $[\alpha]_D^{20.0}$=139.4 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99/1, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 7.7 min, t (minor) =7.3 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 1.96 (dd, *J* = 7.9, 4.7 Hz, 1H), 2.51 (dd, *J* = 9.1, 4.7 Hz, 1H), 3.02 (t, *J* = 8.5 Hz, 1H), 6.96-7.02 (m, 2H), 7.22-7.15 (m, 3H), 7.34-7.42 (m, 7H), 8.03 (d, *J* = 8.6 Hz, 2H);^{13}C NMR (100 MHz, $CDCl_3$) *δ* 23.8, 32.1, 38.4, 85.2, 87.9, 122.9, 127.5, 128.1, 128.2, 128.4, 128.5, 128.7, 130.8, 131.2, 135.1, 135.6, 139.0, 195.6; HRMS (ESI) m/z calcd for $C_{24}H_{17}ClO$ $[M+H]^+$:357.1041, found: 357.1042.



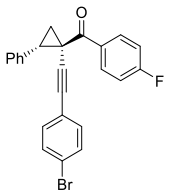
(4-chlorophenyl)((1R,2S)-1-((4-fluorophenyl)ethynyl)-2-phenylcyclopropyl) methanone (1v)

Yellow oil, 28.4 mg, 38% yield; 92% ee; $[\alpha]_D^{20.0}$ = 88.1 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99/1, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =7.5 min, t (minor) =6.9 min]; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.96 (dd, *J* = 7.9, 4.8 Hz, 1H), 2.50 (dd, *J* = 9.1, 4.7 Hz, 1H), 3.02 (t, *J* = 8.5 Hz, 1H), 6.86 (t, *J* = 8.7 Hz, 2H), 6.95 (dd, *J* = 8.6, 5.6 Hz, 2H), 7.31-7.45 (m, 7H), 8.01 (d, *J* = 8.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.7, 32.0, 38.3, 84.1, 87.5, 115.5 (d, *J* = 22.1 Hz), 118.9 (d, *J* = 3.5 Hz), 127.6, 128.2, 128.4, 128.7, 130.7, 133.1 (d, *J* = 8.4 Hz), 135.1, 135.6, 139.1, 162.3 (d, *J* = 249.3 Hz), 195.5; HRMS (ESI) m/z calcd. for $C_{24}H_{16}ClFO$ $[M+H]^+$: 375.0946, found: 375.0947.



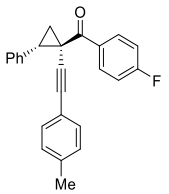
(1R,2S)-1-((4-chlorophenyl)ethynyl)-2-phenylcyclopropyl)(4-fluorophenyl) methanone (1w)

Yellow oil, 27 mg, 36% yield; 92% ee; $[\alpha]_D^{20.0}$=135.9 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =5.8 min, t (minor) =5.6 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 1.95 (dd, *J* = 4.8, 7.9 Hz, 1H), 2.49 (dd, *J* = 4.8, 9.1 Hz, 1H), 3.03 (t, *J* = 8.5 Hz, 1H), 6.89 (d, *J* = 8.2 Hz, 2H), 7.06-7.15 (m, 4H), 7.28-7.42 (m, 5H), 8.10 (dd, *J* = 8.5, 5.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 23.5, 31.9, 38.0, 84.0, 89.1, 115.2 (d, *J* = 21.8 Hz), 121.4, 127.5, 128.2, 128.5, 128.7, 131.9 (d, *J* = 9.2 Hz), 132.4, 133.0 (d, *J* = 3.1 Hz), 134.0, 135.6, 165.5 (d, *J* = 254.5 Hz), 194.9; HRMS (ESI) m/z calcd. for $C_{24}H_{16}ClFO$ $[M+H]^+$: 375.0946, found: 375.0948.



((1R,2S)-1-((4-bromophenyl)ethynyl)-2-phenylcyclopropyl)(4-fluorophenyl) methanone (1x)

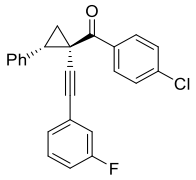
Yellow oil, 40 mg, 48% yield; 96% ee; $[\alpha]_D^{20.0}$=130.8 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =6.0 min, t (minor) =5.6 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.95 (dd, *J* = 7.8, 4.8 Hz, 1H); 2.50 (dd, *J* = 9.0, 4.7 Hz, 1H), 3.03 (t, *J* = 8.4 Hz, 1H), 6.82 (d, *J* = 8.0 Hz, 2H), 7.10 (t, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.2 Hz, 2H), 7.43-7.32 (m, 5H), 8.10 (dd, *J* = 8.5, 5.5 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.5, 32.0, 38.1, 84.1, 89.4, 115.2 (d, *J* = 21.8 Hz), 121.8, 122.2, 127.6, 128.2, 128.7, 131.5, 131.9 (d, *J* = 9.2 Hz), 132.6, 133.0 (d, *J* = 3.0 Hz), 135.6, 165.5 (d, *J* = 254.5 Hz), 194.9; HRMS (ESI) m/z calcd. for $C_{24}H_{16}BrFO$ $[M+H]^+$: 419.0441, found: 419.0441.



(4-fluorophenyl)-((1R,2S)-2-phenyl-1-(p-tolylethynyl)cyclopropyl)methanone (1y)

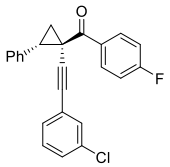
Yellow oil, 27.6 mg, 39% yield; 94% ee; $[\alpha]_D^{20.0}$ =128.7 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99/1, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 7.0 min, t (minor) =6.5 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 1.93 (dd, *J* =4.7, 7.8 Hz, 1H), 2.27 (s, 3H), 2.49 (dd, *J* = 4.7, 9.1 Hz, 1H), 2.99 (t, *J* = 8.5 Hz, 1H), 6.89 (d, *J* = 7.9 Hz, 2H), 6.97 (d, *J* = 7.9 Hz, 2H), 7.08 (t, *J* = 8.6 Hz, 2H), 7.28-7.41 (m, 5H), 8.12 (dd, *J* = 8.6, 5.7 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 21.5, 23.6, 32.1, 38.1, 85.2, 87.2, 115.1 (d, *J* = 21.9 Hz), 119.8, 127.4, 128.2, 128.7, 129.0, 131.1,

132.0 (d, J = 9.2 Hz), 133.1 (d, J = 3.1 Hz), 135.8, 138.2, 165.5 (d, J = 254.1 Hz), 195.3; HRMS (ESI) m/z calcd. for $C_{25}H_{19}FO$ $[M+H]^+$: 355.1493, found: 355.1493.



(4-chlorophenyl)((1*R*,2*S*)-1-((3-fluorophenyl)ethynyl)-2-phenylcyclopropyl)-Methanone (1z)

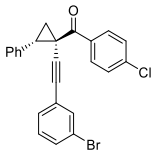
Yellow oil, 27 mg, 36% yield; 91% ee, $[\alpha]_D^{20.0}$ = 99.5 (c = 0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99/1, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 7.8 min, t (minor) =8.6 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.98 (dd, J = 7.9, 4.8 Hz, 1H), 2.52 (dd, J = 9.1, 4.8 Hz, 1H), 3.04 (t, J = 8.5 Hz, 1H), 6.62-6.69 (m, 1H), 6.76 (dd, J = 7.6, 1.3 Hz, 1H), 6.90 (td, J = 8.5, 2.6 Hz, 1H), 7.11 (td, J = 8.0, 5.9 Hz, 1H), 7.31-7.37 (m, 3H), 7.38-7.43 (m, 4H), 7.96-8.04 (m, 2H);^{13}C NMR (100 MHz, $CDCl_3$) δ 23.7, 32.0, 38.4, 84.0 (d, J = 3.4 Hz), 89.0, 115.4 (d, J = 21.1 Hz) 118.0 (d, J = 22.6 Hz), 124.6 (d, J = 9.5 Hz), 127.1 (d, J = 3.0 Hz), 127.7, 128.3, 128.4, 128.7, 129.8 (d, J = 8.7 Hz), 130.7, 135.0, 135.5, 139.2, 162.2 (d, J = 245.0 Hz), 195.3; HRMS (ESI) m/z calcd for $C_{24}H_{16}ClFO$ $[M+H]^+$:375.0946, found: 375.0951.



((1R,2S)-1-((3-chlorophenyl)ethynyl)-2-phenylcyclopropyl)(4-fluorophenyl) methanone (1a')

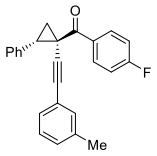
Yellow oil, 30 mg, 40% yield; >99% ee; $[\alpha]_D^{20.0}$= 85.9 (0.1, CH_2Cl_2); [Daicel Chiralpak IA-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99/1, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =7.7 min, t (minor) =8.1 min]; ^{1}H NMR (400 MHz, CDCl3) δ 1.97 (dd, J = 7.9, 4.8 Hz, 1H), 2.52 (dd, J = 9.1, 4.8 Hz, 1H), 3.03 (t, J = 8.5 Hz, 1H), 6.85 (d, J = 7.8 Hz, 1H), 6.94 (t, J = 1.8 Hz, 1H), 7.05-7.15 (m, 3H), 7.17 (dt, J = 8.1, 1.5 Hz, 1H), 7.33-7.47 (m, 5H), 8.09 (dd, J = 8.7, 5.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.5, 31.9, 38.2, 83.7, 89.5, 115.3 (d, J = 21.9 Hz), 124.6, 127.6, 128.2, 128.3, 128.7, 129.3, 129.4,

131.1, 131.9 (d, J = 9.2 Hz), 133.0 (d, J = 3.0 Hz), 134.0, 135.5, 165.5 (d, J = 254.4 Hz), 194.8; HRMS (ESI) m/z calcd. for $C_{24}H_{16}ClFO$ $[M+H]^+$: 375.0946, found: 375.0949.



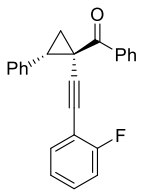
((1*R*,2*S*)-1-((3-bromophenyl)ethynyl)-2-phenylcyclopropyl)(4-chlorophenyl) methanone (1b')

Yellow oil, 31 mg, 36% yield; 96% ee, $[\alpha]_D^{20.0} = 53.0$ (c = 0.1, CH_2Cl_2); [Daicel Chiralpak IJ-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 95/5, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 13.2 min, t (minor) =16.2 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.03 (dd, J = 7.9, 4.8 Hz, 1H), 2.52 (dd, J = 9.1, 4.7 Hz, 1H), 3.08 (t, J = 8.5 Hz, 1H), 6.90 (dd, J = 7.5, 1.9 Hz, 1H), 7.00-7.11 (m, 2H), 7.31 (d, J = 5.5 Hz, 1H), 7.40 (dt, J = 13.7, 4.0 Hz, 7H), 8.07 (d, J = 8.5 Hz, 2H);^{13}C NMR (100 MHz, $CDCl_3$) δ 24.0, 32.2, 38.4, 83.9, 92.4, 125.0, 125.1, 126.8, 127.6, 128.3, 128.4, 128.9, 129.2, 130.9, 132.3, 133.3, 135.0, 135.4, 139.1, 195.3; HRMS (ESI) m/z calcd. for $C_{24}H_{16}BrClO$ $[M+H]^+$: 435.0146, found: 435.0144.



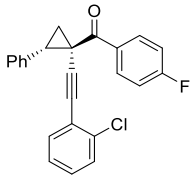
(4-fluorophenyl)-((1*R*,2*S*)-2-phenyl-1-(m-tolylethynyl)cyclopropyl)methanone(1c')

Yellow oil, 26 mg, 37% yield; 94% ee, $[\alpha]_D^{20.0}$= 100.8 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99/1, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 7.0 min, t (minor) =6.4 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.94 (dd, J = 7.8, 4.7 Hz, 1H), 2.23 (s, 3H), 2.51 (dd, J = 9.1, 4.7 Hz, 1H), 3.00 (t, J = 8.2 Hz, 1H), 6.77-6.83 (m, 2H), 7.01-7.13(m, 4H), 7.33-7.43 (m, 5H), 8.09-8.16 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.2, 23.5, 32.0, 38.1, 85.3, 87.7, 115.1 (d, J = 21.8 Hz), 122.7, 127.5, 128.1, 128.2, 128.3, 128.7, 128.9, 131.8, 132.0 (d, J = 9.2 Hz), 133.1 (d, J = 2.9 Hz), 135.8, 137.9, 165.5 (d, J = 254.2 Hz), 195.2; HRMS (ESI) m/z calcd for $C_{25}H_{19}FO$ $[M+H]^+$:355.1493, found: 355.1490.



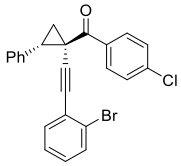
1-((1*R*,2*S*)-1-((2-fluorophenyl)ethynyl)-2-phenylcyclopropyl)ethan-1-one (1d')

Yellow oil, 29.2 mg, 43% yield; 99% ee, $[\alpha]_D^{20.0} = 103.0$ (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99/1, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 8.0 min, t (minor) =8.4 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.00 (dd, J = 7.7, 4.7 Hz, 1H), 2.53 (dd, J = 9.0, 4.6 Hz, 1H), 3.08 (t, J = 8.4 Hz, 1H), 6.89-6.96 (m, 3H), 7.12-7.20 (m, 1H), 7.29-7.35 (m, 1H), 7.38 (d, J = 3.9 Hz, 4H), 7.44 (t, J = 7.6 Hz, 2H), 7.54 (t, J = 7.4 Hz, 1H), 8.10 (d, J = 8.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 24.1, 32.3, 38.4, 78.7, 93.4 (d, J = 3.0 Hz), 111.7 (d, J = 15.6 Hz), 115.4 (d, J = 20.7 Hz), 123.7 (d, J = 3.8 Hz), 127.4, 128.0, 128.2, 128.8, 129.4, 129.5 (d, J = 7.8 Hz), 132.7, 133.2, 135.6, 136.7 162.8 (d, J = 251.7 Hz), 196.6; HRMS (ESI) m/z calcd for $C_{24}H_{17}FO$ $[M+H]^+$:341.1336, found:341.1337.



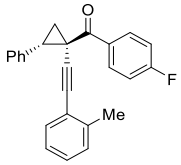
((1R,2S)-1-((2-chlorophenyl)ethynyl)-2-phenylcyclopropyl)(4-fluorophenyl) methanone (1e')

Yellow oil, 33 mg, 44% yield; 98% ee; $[\alpha]_D^{20.0}$=106.5 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99/1, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =7.6 min, t (minor) =7.0 min]**;**^{1}H NMR (400 MHz, $CDCl_3$) δ 2.01 (dd, J = 7.9, 4.7 Hz, 1H), 2.51 (dd, J = 9.1, 4.7 Hz, 1H), 3.09 (t, J = 8.5 Hz, 1H), 6.92 (d, J = 7.6 Hz, 1H), 7.03 (t, J = 7.5 Hz, 1H), 7.06-7.14 (m, 3H), 7.23 (d, J = 7.7 Hz, 1H), 7.29 -7.33 (m, 1H), 7.37 (d, J = 5.0 Hz, 4H), 8.17 (dd, J = 8.6, 5.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 24.0, 32.1, 38.2, 82.2, 93.2, 115.2 (d, J = 21.9 Hz), 122.8 126.3, 127.5, 128.3, 128.8, 129.0, 129.1, 132.2 (d, J = 9.3 Hz), 133.0 (d, J = 3.0 Hz), 133.1, 135.5, 135.6, 166.5 (d, J = 254.1 Hz), 194.9; HRMS (ESI) m/z calcd. for $C_{24}H_{16}ClFO$ $[M+H]^+$: 375.0946, found: 375.0949.



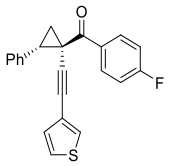
((1R,2S)-1-((2-bromophenyl)ethynyl)-2-phenylcyclopropyl)(4-chlorophenyl) methanone (1f')

Yellow oil, 40 mg, 46% yield; >99% ee; $[\alpha]_D^{20.0}$= 77.9 (0.1, CH_2Cl_2); [Daicel Chiralpak IJ-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =10.3 min, t (minor) =14.4 min]; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.03 (dd, *J* = 7.9, 4.8 Hz, 1H), 2.52 (dd, *J* = 9.1, 4.8 Hz, 1H), 3.08 (t, *J* = 8.5 Hz, 1H), 6.91 (d, *J* = 7.9 Hz, 1H), 7.00-7.13 (m, 2H), 7.29-7.38 (m, 1H), 7.34-7.47 (m, 7H), 8.07 (d, *J* = 8.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 24.0, 32.2, 38.4, 83.9, 92.4, 124.9, 125.0, 126.8, 127.6, 128.3, 128.4, 128.9, 129.2, 130.9, 132.3, 133.3, 135.0, 135.4, 139.1, 195.3; HRMS (ESI) m/z calcd. for $C_{24}H_{16}BrClO$ $[M+H]^+$: 435.0146, found: 435.0149.



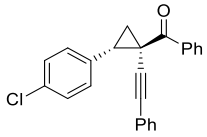
(4-fluorophenyl)((1*R*,2*S*)-2-phenyl-1-(o-tolylethynyl)cyclopropyl)methanone (1g')

Yellow oil, 28 mg, 40% yield; 99% ee, $[\alpha]_D^{20.0}$=121.9 (0.1, CH_2Cl_2); [Daicel Chiralpak IH-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 5.6 min, t (minor) =5.2 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 1.91 (s, 3H), 1.95 (dd, *J* = 7.9, 4.8 Hz, 1H), 2.50 (dd, *J* = 9.1, 4.7 Hz, 1H), 3.03 (t, *J* = 8.2 Hz, 1H), 6.91-7.05 (m, 3H), 7.06-7.14 (m, 3H), 7.29-7.34 (m, 1H), 7.35-7.39 (m, 4H), 8.10-8.18 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 20.3, 23.3, 32.2, 37.7, 84.3, 91.6, 115. 2 (d, *J* = 21.8 Hz), 122.7, 125.4, 127.5, 128.0, 128.3, 128.8, 129.3, 131.7, 132.0 (d, *J* = 9.2 Hz), 133.1 (d, *J* = 3.1 Hz), 135.8, 140.0, 165.4 (d, *J* = 254.2 Hz), 195.2; HRMS (ESI) m/z calcd for $C_{25}H_{19}FO$ $[M+H]^+$:355.1493, found: 355.1493.



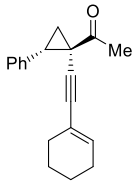
(4-fluorophenyl)((1R,2S)-2-phenyl-1-(thiophen-3-ylethynyl)cyclopropyl) methanone (1h')

Yellow oil, 25 mg, 36% yield; >99% ee; $[\alpha]_D^{20.0}$ =104.1 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99/1, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =8.8 min, t (minor) =8.1 min]; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.93 (dd, *J* = 7.8, 4.8 Hz, 1H), 2.50 (dd, *J* = 9.1, 4.7 Hz, 1H), 2.98 (dd, *J* = 9.0, 7.9 Hz, 1H), 6.71 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.03 (dd, *J* = 3.1, 1.2 Hz, 1H), 7.06-7.15 (m, 3H), 7.30-7.43 (m, 5H), 8.02-8.19 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.4, 32.0, 38.0, 80.3, 87.5, 115.2 (d, *J* = 21.9 Hz), 121.9, 125.2, 127.5, 128.2, 128.3, 128.7, 129.5, 132.0 (d, *J* = 9.2 Hz), 133.0 (d, *J* = 2.9 Hz), 135.7, 165.5 (d, *J* = 254.2 Hz), 195.0; HRMS (ESI) m/z calcd. for $C_{22}H_{15}FOS$ $[M+H]^+$: 347.0900, found: 347.0901.



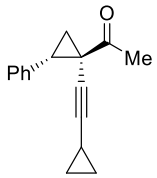
((1*R*,2*S*)-2-(4-chlorophenyl)-1-(phenylethynyl)cyclopropyl-(phenyl)-methanone(1i')

Yellow oil; 29 mg, 41% yield; 98% ee, $[\alpha]_D^{20.0}$=86.6 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99/1, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 7.3 min, t (minor) =8.2 min]**;** H NMR (400 MHz, $CDCl_3$) δ 1.90 (dd, *J* = 7.8, 4.8 Hz, 1H), 2.50 (dd, *J* = 9.1, 4.8 Hz, 1H), 3.00 (t, *J* = 8.4 Hz, 1H), 7.01 (dd, *J* = 7.9, 1.7 Hz, 2H), 7.14-7.24 (m, 3H), 7.30 (d, *J* = 8.5 Hz, 2H), 7.37 (d, *J* = 8.5 Hz, 2H), 7.44 (dd, *J* = 8.4, 7.0 Hz, 2H), 7.51-7.58 (m, 1H), 8.02-8.09 (m, 2H); ^{13}C NMR (100 MHz) *δ* 23.8, 32.1, 37.0, 85.3, 87.8, 122.9, 128.0, 128.1, 128.2, 128.3, 129.3, 130.0, 131.2, 132.8, 133.2, 134.5, 136.7, 196.5; HRMS (ESI) m/z calcd for $C_{24}H_{17}ClO$ $[M+H]^+$:357.1041, found: 357.1039.



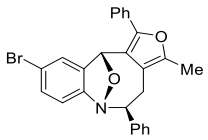
1-((1R,2S)-1-(cyclohex-1-en-1-ylethynyl)-2-phenylcyclopropyl)ethan-1-one (1j')

Yellow oil, 21 mg, 39% yield; $[\alpha]_D^{20.0}$ = 56.2 (0.1, CH_2Cl_2); 38% ee; [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 95/5, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =4.5 min, t (minor) =4.3 min];^{1}H NMR (400 MHz, $CDCl_3$) δ 1.45-1.57 (m, 4H), 1.71 (dd, *J* = 7.9, 4.2 Hz, 1H), 1.87 (tq, *J* = 4.9, 2.1 Hz, 2H), 2.00 (td, *J* = 5.8, 2.9 Hz, 2H), 2.11 (dd, *J* = 9.1, 4.2 Hz, 1H), 2.51 (s, 3H), 2.94 (dd, *J* = 9.1, 8.0 Hz, 1H), 5.81 (tt, *J* = 4.0, 1.9 Hz, 1H), 7.20-7.27 (m, 3H), 7.28-7.34 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.5, 22.3, 25.6, 26.5, 28.9, 29.5, 33.4, 39.0, 84.4, 86.4, 120.5, 127.1, 127.9, 128.7, 134.1, 136.1, 205.4;



1-((1R,2S)-1-(cyclopropylethynyl)-2-phenylcyclopropyl)ethan-1-one (1j'')

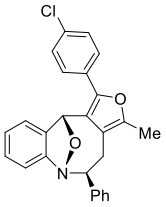
Yellow oil, 18 mg, 41% yield; $[\alpha]_D^{20.0}$ = 66.3 (0.1, CH_2Cl_2); 18% ee; [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =4.8 min, t (minor) =4.6 min];^{1}H NMR (400 MHz, $CDCl_3$) δ 0.32-0.36 (m, 2H), 0.59 (dd, *J* = 8.3, 2.6 Hz, 2H), 1.01-1.15 (m, 1H), 1.63 (dd, *J* = 7.9, 4.1 Hz, 1H), 2.02 (dd, *J* = 9.1, 4.1 Hz, 1H), 2.48 (s, 3H), 2.85 (t, *J* = 8.5 Hz, 1H), 7.15-7.21 (m, 2H), 7.22-7.27 (m, 1H), 7.27-7.33 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ0.5, 7.9, 8.1, 26.2, 29.5, 32.9, 38.5, 72.7, 88.0, 127.0, 127.8, 128.7, 136.3, 205.9;



(5S,6R,11R)-9-bromo-3-methyl-1,5-diphenyl-4,5-dihydro-11H-6,11-epoxybenzo [b]furo[3,4-e] azocine (3a)

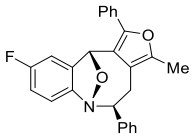
White solid, m.p. = 236-238 ℃; 41 mg, 45% yield; 87% ee; $[\alpha]_D^{20.0}$= 546.0 (0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =5.9 min, t (minor) =6.7 min]**;**^{1}H NMR (400 MHz, $CDCl_3$) δ 2.27 (s, 3H), 2.73 (dd, *J* = 16.2, 4.3 Hz, 1H), 3.00 (dd, *J* = 16.1, 2.7 Hz, 1H), 4.67 (dd, *J* = 5.2, 2.6 Hz, 1H), 6.24 (s, 1H), 7.01-7.12 (m, 1H), 7.27 (t, *J* = 7.3 Hz,

1H), 7.35 (t, *J* = 7.6 Hz, 3H), 7.44 (dd, *J* = 11.3, 7.5 Hz, 4H), 7.57 (d, *J* = 7.1 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 25.5, 71.3, 77.6, 115.3, 117.8, 118.4, 124.2, 125.4, 126.0, 127.5, 127.9, 128.2, 128.4, 128.9, 130.5, 131.6, 137.4, 139.9, 145.7, 147.6, 148.5; HRMS (ESI) m/z calcd. for $C_{26}H_{20}BrNO_2$ $[M+H]^+$: 458.0750, found: 458.0754.



(5S,6R,11R)-1-(4-chlorophenyl)-3-methyl-5-phenyl-4,5-dihydro-11H-6,11-epoxy-benzo[b]furo[3,4-e]azocine (3b)

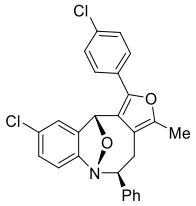
White solid, m.p. = 100-102 ℃; 32 mg, 39% yield; 89% ee; $[\alpha]_D^{20.0}$=275.1 (0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =6.5 min, t (minor) =8.2 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.25 (s, 3H), 2.69 (ddd, *J* = 16.1, 5.2, 1.5 Hz, 1H), 2.99 (dd, *J* = 16.1, 2.9 Hz, 1H), 4.69 (dd, *J* = 5.1, 2.8 Hz, 1H), 6.23 (s, 1H), 7.14-7.21 (m, 2H), 7.25-7.30 (m, 1H), 7.31-7.44 (m, 6H), 7.50-7.56 (m, 2H), 7.59 (d, *J* = 7.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 25.4, 71.4, 77.6, 113.7, 118.8, 122.0, 125.3, 125.4, 127.1, 127.4, 128.1, 128.4, 128.7, 129.0, 129.3, 133.4, 134.8, 140.3, 144.2, 147.7, 149.3; HRMS (ESI) m/z calcd. for $C_{26}H_{20}ClNO_2$ $[M+H]^+$: 414.1255, found: 414.1251.



(5S,6R,11R)-9-fluoro-3-methyl-1,5-diphenyl-4,5-dihydro-11H-6,11-epoxybenzo[b] furo[3,4-e] azocine (3c)

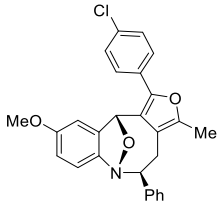
White solid, m.p. = 156-158 ℃; 35 mg, 44% yield; 91% ee; $[\alpha]_D^{20.0}$=217.0 (0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =5.9 min, t (minor) =6.9 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.27 (s, 3H), 2.73 (dd, *J* = 16.1, 5.1 Hz, 1H), 3.00 (dd, *J* = 16.1, 2.8 Hz, 1H), 4.65 (dd, *J* = 5.2, 2.8 Hz, 1H), 6.25 (s, 1H), 7.05 (dd, *J* = 8.4, 2.4 Hz, 2H), 7.11

(dd, J = 8.3, 4.3 Hz, 1H), 7.25-7.31 (m, 1H), 7.31-7.39 (m, 3H), 7.44 (t, J = 7.6 Hz, 2H), 7.57 (dd, J = 7.5, 4.6 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 25.5, 71.6, 77.8 (d, J = 2.4 Hz), 109.6 (d, J = 25.0 Hz), 114.6 (d, J = 8.9 Hz), 115.4 (d, J = 24.0 Hz), 118.5, 124.2, 126.0, 127.5, 127.9, 128.2, 128.4, 128.9, 130.6, 136.9 (d, J = 8.2 Hz), 140.2, 145.2 (d, J = 2.2 Hz), 145.6, 147.5, 160.6 (d, J = 243.3 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -112.8; HRMS (ESI) m/z calcd. for $C_{26}H_{20}FNO_2$ $[M+H]^+$: 398.1551, found: 398.1553.



(5S,6R,11R)-9-chloro-1-(4-chlorophenyl)-3-methyl-5-phenyl-4,5-dihydro-11H-6,11-epoxybenzo[b]furo[3,4-e]azocine (3d)

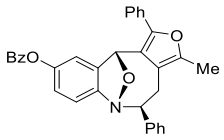
White solid, m.p. = 176-178 ℃; 37.5 mg, 42% yield; 84% ee; $[\alpha]_D^{20.0}$=316.3 (0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =10.5 min, t (minor) =8.8 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.27 (s, 3H), 2.72 (ddd, J = 16.0, 5.2, 1.5 Hz, 1H), 3.01 (dd, J = 16.2, 2.8 Hz, 1H), 4.67 (dd, J = 5.0, 2.5 Hz, 1H), 6.19 (s, 1H), 7.11 (d, J = 8.2 Hz, 1H), 7.26 -7.38 (m, 5H), 7.39-7.44 (m, 2H), 7.48-7.52 (m, 2H), 7.56 (d, J = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 25.4, 71.3, 77.5, 114.8, 118.6, 122.4, 124.7, 127.1, 127.6, 128.1, 128.5, 128.8, 129.1, 129.2, 130.5, 133.6, 136.7, 139.9, 144.5, 147.9, 148.0; HRMS (ESI) m/z calcd. for $C_{26}H_{19}Cl_2NO_2$ $[M+H]^+$: 448.0866, found: 448.0866.



(5S,6R,11R)-1-(4-chlorophenyl)-9-methoxy-3-methyl-5-phenyl-4,5-dihydro-11H-6,11-epoxybenzo[b]furo[3,4-e]azocine (3e)

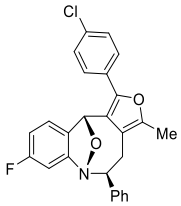
White solid, m.p. = 82-84 ℃; 29 mg, 33% yield; 88% ee; $[\alpha]_D^{20.0}$= 448.3 (0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =10.5 min, t (minor) =12.0 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.26 (s, 3H), 2.72 (ddd, J = 16.2, 5.1, 1.5 Hz, 1H), 2.97 (dd, J = 16.1, 2.7 Hz,

1H), 3.81 (s, 3H), 4.62 (dd, *J* = 5.1, 2.6 Hz, 1H), 6.18 (s, 1H), 6.84 (d, *J* = 2.4 Hz, 1H), 6.88 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.09 (d, *J* = 8.4 Hz, 1H), 7.25-7.31 (m, 1H), 7.35 (t, *J* = 7.5 Hz, 2H), 7.38-7.43 (m, 2H), 7.52 (d, *J* = 8.6 Hz, 2H), 7.58 (d, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 25.2, 55.9, 71.4, 77.8, 107.8, 114.0, 114.3, 118.9, 125.2, 127.1, 127.4, 128.2, 128.4, 129.1, 129.3, 133.4, 136.2, 140.3, 142.5, 144.3, 147.7, 157.8; HRMS (ESI) m/z calcd. for $C_{27}H_{22}ClNO_3$ $[M+H]^+$: 444.1361, found: 444.1359.



(5S,6R,11R)-3-methyl-1,5-diphenyl-4,5-dihydro-11H-6,11-epoxybenzo[b]furo [3,4-e] azocin-8-yl benzoate (3f)

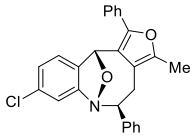
White solid, m.p. = 176-178 ℃; 38 mg, 38% yield; 86% ee; $[\alpha]_D^{20.0}$= 224.6 (0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 80/20, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =7.6 min, t (minor) =5.7 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.27 (s, 3H), 2.80 (dd, *J* = 16.1, 5.2 Hz, 1H), 3.01 (dd, *J* = 16.1, 2.7 Hz, 1H), 4.70 (dd, *J* = 5.1, 2.6 Hz, 1H), 6.29 (s, 1H), 7.22 (d, *J* = 6.0 Hz, 3H), 7.23-7.32 (m, 2H), 7.35 (t, *J* = 7.5 Hz, 2H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.50 (t, *J* = 7.7 Hz, 2H), 7.55-7.65 (m, 5H), 8.13-8.31 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 25.5, 71.5, 77.8, 114.3, 115.9, 118.6, 122.0, 124.4, 126.0, 127.4, 127.8, 128.3, 128.4, 128.7, 128.8, 129.4, 130.2, 130.6, 133.8, 136.5, 140.2, 145.6, 147.0, 147.5, 148.4, 165.4; HRMS (ESI) m/z calcd. for $C_{33}H_{25}NO_4$ $[M+H]^+$: 500.1856, found: 500.1858.



(5S,6R,11R)-1-(4-chlorophenyl)-8-fluoro-3-methyl-5-phenyl-4,5-dihydro-11H-6,11-epoxybenzo[b]furo[3,4-e]azocine (3g)

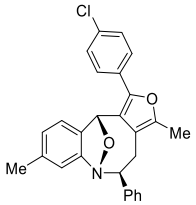
White solid, m.p. = 102-104 ℃; 37 mg, 43% yield; 90% ee; $[\alpha]_D^{20.0}$= 437.0 (0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =8.3 min, t (minor) =9.8 min]**;** ^{1}H NMR (400

MHz, $CDCl_3$) δ 2.27 (s, 3H), 2.73 (ddd, *J* = 16.2, 5.1, 1.5 Hz, 1H), 3.04 (dd, *J* = 16.1, 2.9 Hz, 1H), 4.68 (dd, *J* = 5.1, 2.9 Hz, 1H), 6.20 (s, 1H), 6.83-6.94 (m, 2H), 7.25-7.32 (m, 2H), 7.32-7.43 (m, 4H), 7.48-7.54 (m, 2H), 7.57 (d, *J* = 7.5 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 25.6, 71.4, 77.5, 101.9 (d, *J* = 26.1 Hz), 112.2 (d, *J* = 23.3 Hz), 118.6, 122.9 (d, *J* = 10.0 Hz), 125.2, 127.0, 127.6, 128.1, 128.5, 129.1, 129.2, 130.4 (d, *J* = 2.4 Hz), 133.5, 139.9, 144.2, 147.9, 151.1 (d, *J* = 10.8 Hz), 163.2 (d, *J* = 246.2 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -112.8; HRMS (ESI) m/z calcd. for $C_{26}H_{19}ClFNO_2$ $[M+H]^+$: 432.1161, found: 432.1163.



(5S,6R,11R)-8-chloro-3-methyl-1,5-diphenyl-4,5-dihydro-11H-6,11-epoxybenzo [b]furo[3,4-e] azocine (3h)

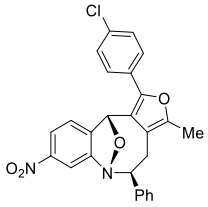
White solid, m.p. = 110-112 ℃; 31 mg, 38% yield; 87% ee; $[\alpha]_D^{20.0}$ = 421.2 (0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 95/5, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =9.1 min, t (minor) =11.6 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.26 (s, 3H), 2.75 (dd, *J* = 16.1, 4.6 Hz, 1H), 3.03 (dd, *J* = 16.1, 2.9 Hz, 1H), 4.68 (dd, *J* = 2.9, 4.6 Hz, 1H), 6.26 (s, 1H), 7.12-7.19 (m, 2H), 7.25-7.30 (m, 2H), 7.31-7.39 (m, 3H), 7.43 (t, *J* = 7.7 Hz, 2H), 7.53-7.62 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 25.8, 71.6, 77.7, 114.2, 118.4, 122.9, 124.5, 125.4, 126.0, 127.5, 127.8, 128.1, 128.4, 128.8, 130.6, 133.8, 134.3, 140.0, 145.5, 147.5, 150.9; HRMS (ESI) m/z calcd. for $C_{26}H_{20}ClNO_2$ $[M+H]^+$: 414.1255, found: 414.1258.



(5S,6R,11R)-1-(4-chlorophenyl)-3,8-dimethyl-5-phenyl-4,5-dihydro-11H-6,11-epoxybenzo[b]furo[3,4-e] azocine (3i)

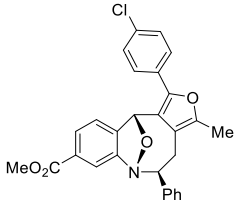
White solid, m.p. = 194-196 ℃; 33 mg, 39% yield; 88% ee; $[\alpha]_D^{20.0}$ = 274.8 (0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 90/10,

v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =7.5 min, t (minor) =8.0 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.24 (s, 3H), 2.41 (s, 3H), 2.71 (ddd, *J* = 16.0, 5.0, 1.5 Hz, 1H), 2.98 (dd, *J* = 16.0, 2.9 Hz, 1H), 4.66 (dd, *J* = 5.1, 2.9 Hz, 1H), 6.19 (s, 1H), 6.97 (d, *J* = 8.1 Hz, 2H), 7.19 (d, *J* = 7.5 Hz, 1H), 7.24 -7.30 (m, 1H), 7.32-7.42 (m, 4H), 7.50-7.54 (m, 2H), 7.59 (d, *J* = 7.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 21.7, 25.5, 71.4, 77.6, 114.2, 118.9, 121.5, 125.7, 126.1, 127.0, 127.4, 128.1, 128.4, 129.0, 129.4, 132.0, 133.3, 138.9, 140.4, 144.0, 147.6, 149.6; HRMS (ESI) m/z calcd. for $C_{27}H_{22}ClNO_2$ $[M+H]^+$: 428.1412, found: 428.1412.



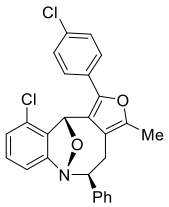
(5S,6R,11R)-1-(4-chlorophenyl)-3-methyl-8-nitro-5-phenyl-4,5-dihydro-11H-6,11-epoxybenzo[b]furo[3,4-e]azocine (3j)

White solid, m.p. = 180-182 ℃; 33 mg, 36% yield; 88% ee; $[\alpha]_D^{20.0}$= 429.8 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 80/20, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =6.9 min, t (minor) =7.6 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.20 (s, 3H), 2.63 (ddd, *J* = 16.2, 5.1, 1.5 Hz, 1H), 3.03 (dd, *J* = 16.2, 3.1 Hz, 1H), 4.71 (dd, *J* = 5.2, 3.1 Hz, 1H), 6.24 (s, 1H), 7.21-7.27 (m, 1H), 7.30 (dd, *J* = 8.3, 6.6 Hz, 2H), 7.32-7.39 (m, 3H), 7.42-7.46 (m, 2H), 7.47-7.53 (m, 2H), 7.94 (d, *J* = 1.9 Hz, 1H), 7.99 (dd, *J* = 8.2, 2.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 26.0, 71.7, 77.6, 109.3, 118.3, 121.2, 122.5, 123.9, 127.1, 127.8, 128.0, 128.6, 128.9, 129.2, 133.9, 139.5, 141.6, 144.6, 148.3, 148.9, 150.8; HRMS (ESI) m/z calcd. for $C_{26}H_{19}ClN_2O_4$ $[M+H]^+$: 459.1106, found: 459.1109.



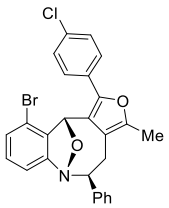
Methyl-(5S,6R,11R)-1-(4-chlorophenyl)-3-methyl-5-phenyl-4,5-dihydro-11H-6,11-epoxybenzo[b]furo[3,4-e]azocine-8-carboxylate (3k)

White solid, m.p. = 100-102 ℃; 40.6 mg, 43% yield; 90% ee; $[\alpha]_D^{20.0}$= 443.0 (0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =20.6 min, t (minor) =14.5 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.26 (s, 3H), 2.69 (ddd, *J* = 16.2, 5.1, 1.5 Hz, 1H), 3.02 (dd, *J* = 16.2, 2.8 Hz, 1H), 3.95 (s, 3H), 4.75 (dd, *J* = 5.2, 2.8 Hz, 1H), 6.26 (s, 1H), 7.27-7.33 (m, 1H), 7.34-7.44 (m, 5H), 7.52 (d, *J* = 8.6 Hz, 2H), 7.58 (d, *J* = 7.4 Hz, 2H), 7.85 (d, *J* = 1.3 Hz, 1H), 7.89 (dd, *J* = 7.8, 1.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 25.5, 52.5, 71.3, 77.6, 114.9, 118.7, 121.9, 124.6, 127.1, 127.2, 127.6, 128.1, 128.5, 129.0, 129.1, 131.1, 133.6, 139.6, 139.9, 144.4, 147.9, 149.8, 166.5; HRMS (ESI) m/z calcd. for $C_{28}H_{22}ClNO_4$ $[M+H]^+$: 472.1310, found: 472.1310.



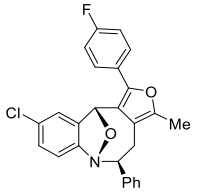
(5S,6R,11S)-10-chloro-1-(4-chlorophenyl)-3-methyl-5-phenyl-4,5-dihydro-11H-6,11-epoxybenzo[b]furo[3,4-e] azocine (3l)

White solid, m.p. = 190-192 ℃; 34 mg, 38% yield; 93% ee; $[\alpha]_D^{20.0}$= 541.8 (0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =5.2 min, t (minor) =5.6 min]; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.27 (s, 3H), 2.69 (ddd, *J* = 16.1, 5.1, 1.5 Hz, 1H), 2.95 (dd, *J* = 16.1, 2.3 Hz, 1H), 4.69 (dd, *J* = 5.1, 2.2 Hz, 1H), 6.32 (s, 1H), 7.09 (d, *J* = 7.8 Hz, 1H), 7.14 (d, *J* = 7.9 Hz, 1H), 7.22-7.41 (m, 6H), 7.51-7.60 (m, 2H), 7.74 (d, J = 8.5 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 24.9, 71.2, 77.8, 112.2, 118.7, 123.3, 125.8, 127.1, 127.6, 128.2, 128.4, 128.6, 128.9, 129.3, 130.2, 132.9, 133.2, 139.4, 144.8, 147.7, 151.2; HRMS (ESI) m/z calcd. for $C_{26}H_{19}Cl_2NO_2$ $[M+H]^+$: 448.0866, found: 448.0871.



(5S,6R,11S)-10-bromo-1-(4-chlorophenyl)-3-methyl-5-phenyl-4,5-dihydro-11H-6,11-epoxybenzo[b]furo[3,4-e] azocine (3m)

White solid, m.p. = 212-214 ℃; 39 mg, 40% yield; 94% ee; $[\alpha]_D^{20.0}$= 483.8 (0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =5.3 min, t (minor) =5.8 min];^{1}H NMR (400 MHz, $CDCl_3$) δ 2.26 (s, 3H), 2.66 (ddd, *J* = 16.4, 5.3, 1.6 Hz, 1H), 2.94 (dd, *J* = 16.3, 2.3 Hz, 1H), 4.69 (dd, *J* = 5.1, 2.2 Hz, 1H), 6.28 (s, 1H), 7.13 (d, *J* = 7.5 Hz, 1H), 7.24 (d, *J* = 6.8 Hz, 1H), 7.29 (d, *J* = 7.5 Hz, 2H), 7.31-7.41 (m, 4H), 7.56 (d, *J* = 7.3 Hz, 2H), 7.74-7.82 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 24.9, 71.3, 79.0, 112.7, 116.7, 118.7, 123.3, 127.2, 127.6, 128.2, 128.4, 128.7, 128.8, 129.4, 130.3, 133.2, 135.2, 139.4, 144.7, 147.7, 150.9; HRMS (ESI) m/z calcd. for $C_{26}H_{19}BrClNO_2$ $[M+H]^+$: 492.0360, found: 492.0365.



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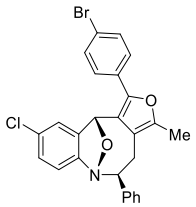
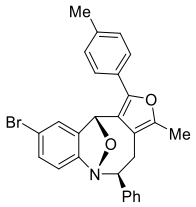
(5S,6R,11R)-9-chloro-5-(4-fluorophenyl)-3-methyl-1-phenyl-4,5-dihydro-11H-6,11-epoxybenzo[b]furo[3,4-e] azocine (3n)

White solid, m.p. = 192-194 ℃; 34.6 mg, 40% yield; 88% ee; $[\alpha]_D^{20.0}$= 335.1 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =9.2 min, t (minor) =12.8 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.26 (s, 3H), 2.72 (dd, *J* = 16.3, 5.0 Hz, 1H), 3.00 (dd, *J* = 16.2, 2.7 Hz, 1H), 4.67 (dd, *J* = 5.3, 2.6 Hz, 1H), 6.15 (s, 1H), 7.06-7.20 (m, 3H), 7.23-7.39 (m, 5H), 7.49-7.63 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 25.3, 71.3, 77.6, 114.8, 116.0 (d, *J* = 21.8 Hz), 118.4, 122.4, 124.0, 126.9 (d, *J* = 3.5 Hz), 127.5, 127.8 (d, *J* = 8.1 Hz), 128.1, 128.4, 128.8, 130.4, 136.9, 139.9, 144.8, 147.5, 148.0, 162.4 (d, *J* = 248.0 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -113.2; HRMS (ESI) m/z calcd. for $C_{26}H_{19}ClFNO_2$ $[M+H]^+$: 432.1161, found: 432.1164.



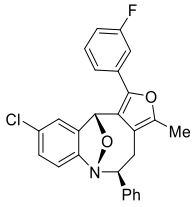
(5S,6R,11R)-1-(4-bromophenyl)-9-chloro-3-methyl-5-phenyl-4,5-dihydro-11H-6,11-epoxybenzo[b]furo[3,4-e] azocine (3o)

White solid, m.p. = 186-188 ℃; 44 mg, 45% yield; 80% ee; $[\alpha]_D^{20.0}$= 231.0 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =10.9 min, t (minor) =15.7 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.26 (s, 3H), 2.71 (ddd, *J* = 16.2, 5.0, 1.6 Hz, 1H), 3.00 (dd, *J* = 16.2, 2.7 Hz, 1H), 4.66 (dd, *J* = 5.2, 2.7 Hz, 1H), 6.18 (s, 1H), 7.10 (d, *J* = 8.2 Hz, 1H), 7.23-7.38 (m, 5H), 7.42 (d, *J* = 8.5 Hz, 2H), 7.55 (dd, *J* = 8.0, 3.4 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 25.4, 71.3, 77.5, 114.8, 118.6, 121.7, 122.4, 124.8, 127.3, 127.6, 128.1, 128.4, 128.8, 129.5, 130.4, 132.0, 136.6, 139.8, 144.4, 147.9; HRMS (ESI) m/z calcd. for $C_{26}H_{19}BrClNO_2$ $[M+H]^+$: 492.0360, found: 492.0365.



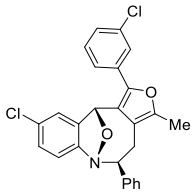
(5S,6R,11R)-9-bromo-3-methyl-5-phenyl-1-(p-tolyl)-4,5-dihydro-11H-6,11-epoxybenzo[b]furo[3,4-e] azocine (3p)

White solid, m.p. = 178-180 ℃; 37 mg, 39% yield; 84% ee; $[\alpha]_D^{20.0}$= 216.4 (0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =7.7 min, t (minor) =8.6 min]; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.26 (s, 3H), 2.39 (s, 3H), 2.73 (dd, *J* = 16.1, 5.1 Hz, 1H), 3.00 (dd, *J* = 16.1, 2.6 Hz, 1H), 4.67 (dd, *J* = 4.7, 2.4 Hz, 1H), 6.22 (s, 1H), 7.06 (d, *J* = 8.7 Hz, 1H), 7.22-7.31 (m, 3H), 7.34 (dd, *J* = 8.3, 6.6 Hz, 2H), 7.43 -7.48 (m, 4H), 7.57 (d, *J* = 7.5 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 21.4, 25.5, 71.3, 77.6, 115.2, 117.8, 118.3, 123.6, 125.4, 126.0, 127.5, 127.8, 128.2, 128.4, 129.6, 131.5, 137.6, 137.8, 140.0, 145.9, 147.2, 148.5; HRMS (ESI) m/z calcd. for $C_{27}H_{22}BrNO_2$ $[M+H]^+$: 472.0907, found: 472.0906.



(5S,6R,11R)-9-chloro-1-(3-fluorophenyl)-3-methyl-5-phenyl-4,5-dihydro-11H-6,11-epoxybenzo[b]furo[3,4-e] azocine (3q)

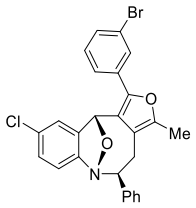
White solid, m.p. = 188-190 ℃; 33 mg, 38% yield; 95% ee; $[\alpha]_D^{20.0}$= 348.5 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =10.0 min, t (minor) =13.8 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.27 (s, 3H), 2.73 (ddd, *J* = 16.2, 5.2, 1.5 Hz, 1H), 3.02 (dd, *J* = 16.1, 2.8 Hz, 1H), 4.67 (dd, *J* = 5.2, 2.8 Hz, 1H), 6.24 (s, 1H), 6.98-7.06 (m, 1H), 7.11 (d, *J* = 8.1 Hz, 1H), 7.28 (d, *J* = 2.9 Hz, 1H), 7.29-7.36 (m, 5H), 7.36-7.44 (m, 2H), 7.56 (dd, *J* = 7.5, 1.7 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 25.5, 71.4, 77.5, 112.8 (d, *J* = 23.3 Hz), 114.7 (d, *J* = 21.0 Hz), 114.8, 118.7, 121.4 (d, *J* = 3.0 Hz), 122.4, 125.2, 127.6, 128.1, 128.5, 128.8, 130.4, 130.5, 130.6, 132.6 (d, *J* = 8.4 Hz), 136.7, 139.9, 144.3 (d, *J* = 2.5 Hz), 148.0 (d, *J* = 9.9 Hz), 163.1 (d, *J* = 246.2 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -112.0; HRMS (ESI) m/z calcd. for $C_{26}H_{19}ClFNO_2$ $[M+H]^+$: 432.1161, found: 432.1163.



(5S,6R,11R)-9-chloro-1-(3-chlorophenyl)-3-methyl-5-phenyl-4,5-dihydro-11H-6,11-epoxybenzo[b]furo[3,4-e] azocine (3r)

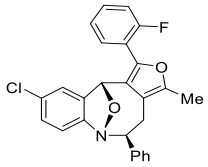
White solid, m.p. = 178-180 ℃; 34 mg, 38% yield; 87% ee; $[\alpha]_D^{20.0}$= 429.9 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =8.1min, t (minor) =11.1 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.27 (s, 3H), 2.71 (dd, *J* = 16.2, 4.6 Hz, 1H), 3.00 (dd, *J* = 16.1, 2.8 Hz, 1H), 4.66 (dd, *J* = 5.2, 2.7 Hz, 1H), 6.21 (s, 1H), 7.10 (d, *J* = 8.2 Hz, 1H), 7.25-7.39 (m, 6H), 7.41-7.48 (m, 2H), 7.53- 7.59 (m, 2H), 7.74 (t, *J* = 1.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 25.4, 71.3, 77.4, 114.8, 118.7, 122.4, 123.1, 124.2, 125.3, 127.6,

128.1, 128.4, 128.8, 128.9, 130.3, 130.4, 130.7, 132.4, 136.6, 139.8, 143.9, 148.0, 148.2; HRMS (ESI) m/z calcd. for $C_{26}H_{19}Cl_2NO_2$ $[M+H]^+$: 448.0866, found: 448.0870.



(5S,6R,11R)-1-(3-bromophenyl)-9-chloro-3-methyl-5-phenyl-4,5-dihydro-11H-6,11-epoxybenzo[b]furo[3,4-e] azocine (3s)

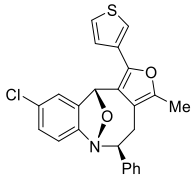
White solid, m.p. = 182-184 ℃; 35 mg, 36% yield; 94% ee; $[\alpha]_D^{20.0}$= 417.9 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =6.6 min, t (minor) =9.6 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.27 (s, 3H), 2.71 (dd, *J* = 16.1, 5.1, 1.5 Hz, 1H), 3.00 (dd, *J* = 16.1, 2.8 Hz, 1H), 4.66 (dd, *J* = 5.1, 2.7 Hz, 1H), 6.22 (s, 1H), 7.10 (d, *J* = 8.2 Hz, 1H), 7.25-7.39 (m, 7H), 7.40-7.45 (m, 1H), 7.52-7.61 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 25.4, 71.3, 77.4, 114.8, 118.7, 122.4, 123.8, 125.2, 125.9, 127.6, 127.8, 128.1, 128.5, 128.8, 130.1, 130.5, 132.2, 134.9, 136.6, 139.8, 144.0, 148.0, 148.2; HRMS (ESI) m/z calcd. for $C_{26}H_{19}BrClNO_2$ $[M+H]^+$: 492.0360, found: 492.0363.



(5S,6R,11R)-9-chloro-1-(2-fluorophenyl)-3-methyl-5-phenyl-4,5-dihydro-11H-6,11-epoxybenzo[b]furo[3,4-e] azocine (3t)

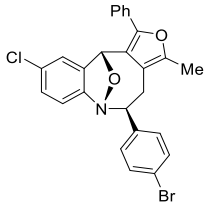
White solid, m.p. = 202-204 ℃; 27 mg, 31% yield; 94% ee; $[\alpha]_D^{20.0}$= 363.4 (0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 80/20, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =10.1 min, t (minor) =11.2 min];^{1}H NMR (400 MHz, $CDCl_3$) δ 2.28 (s, 3H), 2.76 (ddd, *J* = 16.1, 5.1, 1.5 Hz, 1H), 2.98 (dd, *J* = 16.1, 2.4 Hz, 1H), 4.68 (dd, *J* = 4.8, 1.9 Hz, 1H), 6.03 (d, *J* = 4.2 Hz, 1H), 7.10 (d, *J* = 8.3 Hz, 1H), 7.14-7.24 (m, 2H), 7.26-7.31 (m, 2H), 7.31-7.39 (m, 3H), 7.43 (d, *J* = 2.0 Hz, 1H), 7.55-7.63 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 25.0, 71.1, 78.0 (d, *J* = 10.3 Hz), 114.5, 116.1 (d, *J* = 22.6 Hz), 118.4, 118.7 (d, *J* = 13.8 Hz), 123.5 (d, *J* = 9.2

Hz), 124.7 (d, *J* = 3.3 Hz), 126.5, 127.5, 128.1, 128.4, 128.6, 129.6 (d, *J* = 3.3 Hz), 129.7 (d, *J* = 7.3 Hz), 130.6, 136.7, 139.2, 139.8, 147.9, 148.8, 158.2 (d, *J* = 245.5 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -114.4; HRMS (ESI) m/z calcd. for $C_{26}H_{19}ClFNO_2$ $[M+H]^+$: 432.1161, found: 432.1165.



(5S,6R,11R)-9-chloro-3-methyl-5-phenyl-1-(thiophen-3-yl)-4,5-dihydro-11H-6,11-epoxybenzo[b]furo[3,4-e]azocine (3u)

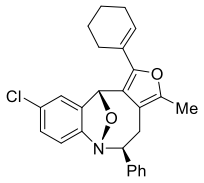
White solid, m.p. = 180-182 ℃; 31 mg, 37% yield; 90% ee; $[\alpha]_D^{20.0}$= 310.3 (0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =6.3 min, t (minor) =7.1 min];^{1}H NMR (400 MHz, $CDCl_3$) δ 2.24 (s, 3H), 2.71 (ddd, *J* = 16.2, 5.1, 1.5 Hz, 1H), 2.99 (dd, *J* = 16.1, 2.8 Hz, 1H), 4.67 (dd, *J* = 5.2, 2.8 Hz, 1H), 6.22 (s, 1H), 7.10 (d, *J* = 8.3 Hz, 1H), 7.25 (d, *J* = 4.3 Hz, 1H), 7.27-7.32 (m, 2H), 7.31-7.38 (m, 3H), 7.38-7.43 (m, 2H), 7.56 (d, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 25.5, 71.5, 77.6, 114.8, 118.0, 120.5, 122.4, 123.5, 125.4, 126.6, 127.5, 128.2, 128.4, 128.7, 130.4, 131.6, 137.0, 140.0, 142.1, 147.0, 148.0; HRMS (ESI) m/z calcd. for $C_{24}H_{18}ClNO_2S$ $[M+H]^+$: 420.0820, found: 420.0818.



(5S,6R,11R)-5-(4-bromophenyl)-9-chloro-3-methyl-1-phenyl-4,5-dihydro-11H-6,11-epoxybenzo[b]furo[3,4-e]azocine (3v)

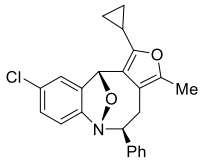
White solid, m.p. = 176-178 ℃; 37 mg, 38% yield; 86% ee; $[\alpha]_D^{20.0}$= 255.1 (0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 80/20, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =8.5 min, t (minor) =7.1 min]; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.26 (s, 3H), 2.73 (ddd, *J* = 16.3, 5.1, 1.6 Hz, 1H), 2.94 (dd, *J* = 16.2, 2.6 Hz, 1H), 4.62 (dd, *J* = 5.2, 2.6 Hz, 1H), 6.23 (s, 1H), 7.08-7.14 (m, 1H), 7.30-7.37

(m, 3H), 7.41-7.51 (m, 6H), 7.54-7.59 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 25.3, 70.7, 77.6, 114.8, 118.0, 121.6, 122.6, 124.0, 126.1, 128.0, 128.8, 128.9, 130.0, 130.4, 130.6, 131.5, 137.0, 138.9, 145.9, 147.6, 147.7; HRMS (ESI) m/z calcd. for $C_{26}H_{19}BrClNO_2$ $[M+H]^+$: 492.0360, found: 492.0365.



(5S,6R,11R)-9-chloro-1-(cyclohex-1-en-1-yl)-3-methyl-5-phenyl-4,5-dihydro-11H-6,11-epoxybenzo[b]furo[3,4-e]azocine (3w)

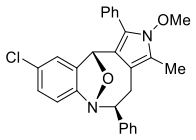
White solid, m.p. = 84-86 ℃; 29 mg, 35% yield; $[\alpha]_D^{20.0}$ = 115.2 (0.1, CH_2Cl_2); 63% ee; [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), n-hexane/2-propanol = 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =5.5 min, t (minor) =6.5 min]; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.62-1.81 (m, 4H), 2.19 (s, 3H), 2.21-2.35 (m, 3H), 2.48-2.59 (m, 1H), 2.67 (ddd, *J* = 16.1, 5.1, 1.5 Hz, 1H), 2.94 (dd, *J* = 16.1, 2.5 Hz, 1H), 4.64 (d, *J* = 2.8 Hz, 1H), 6.05 (dt, *J* = 4.1, 2.1 Hz, 1H), 6.13 (s, 1H), 7.09 (d, *J* = 8.2 Hz, 1H), 7.23 (d, *J* = 2.0 Hz, 1H), 7.29 (dt, *J* = 7.3, 1.8 Hz, 2H), 7.32-7.38 (m, 2H), 7.56 (dd, *J* = 7.5, 1.7 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.5, 22.1, 22.6, 25.2, 25.7, 26.7, 71.2, 77.8, 114.7, 117.6, 122.5, 122.8, 126.4, 127.4, 128.2, 128.3, 128.4, 128.5, 130.3, 137.4, 140.1, 146.0, 147.9, 148.0; HRMS (ESI) m/z calcd. for $C_{26}H_{24}ClNO_2$ $[M+H]^+$: 418.1568, found: 418.1565.



(5S,6R,11R)-9-chloro-1-cyclopropyl-3-methyl-5-phenyl-4,5-dihydro-11H-6,11-epoxybenzo[b]furo[3,4-e]azocine (3w')

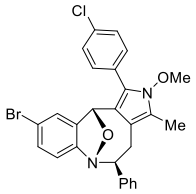
White solid, m.p. = 86-88℃; 24 mg, 32% yield; $[\alpha]_D^{20.0}$ = 135.2 (0.1, CH_2Cl_2); 38% ee; [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =6.6 min, t (minor) =7.5 min]; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.80-0.97 (m, 4H), 1.79-1.91 (m, 1H), 2.11 (s, 3H), 2.56-2.65 (m, 1H), 2.90

(dd, *J* = 16.1, 2.8 Hz, 1H), 4.63 (dd, *J* = 5.1, 2.7 Hz, 1H), 5.99 (s, 1H), 7.06 (d, *J* = 8.3 Hz, 1H), 7.19 (d, *J* = 1.9 Hz, 1H), 7.23-7.29 (m, 2H), 7.30-7.36 (m, 2H), 7.54 (dd, *J* = 7.3, 1.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 6.0, 6.6, 7.3, 11.3, 25.2, 71.6, 77.6, 114.7, 116.7, 122.5, 123.2, 127.4, 128.2, 128.3, 128.4, 130.3, 137.8, 140.1, 145.1, 147.3, 147.9; HRMS (ESI) m/z calcd. for $C_{23}H_{20}ClNO_2$ $[M+H]^+$: 378.1255, found: 378.1260.



(5S,6R,11R)-9-chloro-2-methoxy-3-methyl-1,5-diphenyl-2,4,5,11-tetrahydro-6,11-epoxybenzo[b]pyrrolo[3,4-e] azocine (3x)

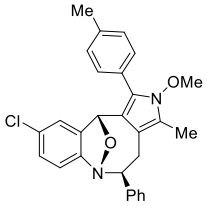
White solid, m.p. = 78-80 ℃; 34 mg, 38% yield; 82% ee; $[\alpha]_D^{20.0}$= 329.6 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =9.7 min, t (minor) =13.2 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.22 (s, 3H), 2.77 (dd, *J* = 16.2, 4.9 Hz, 1H), 3.01 (dd, *J* = 16.1, 2.8 Hz, 1H), 3.56 (s, 3H), 4.67 (dd, *J* = 5.0, 2.7 Hz, 1H), 5.92 (s, 1H), 7.10 (d, *J* = 8.2 Hz, 1H), 7.23 -7.28 (m, 3H), 7.29-7.38 (m, 3H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.49 -7.57 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 8.5, 26.0, 65.6, 72.2, 78.8, 112.0, 114.7, 118.9, 122.4, 123.2, 127.3, 127.5, 128.0, 128.3, 128.4, 128.6, 129.3, 129.6, 130.1, 138.0, 140.5, 148.1; HRMS (ESI) m/z calcd. for $C_{27}H_{23}ClN_2O_2$ $[M+H]^+$: 443.1521, found: 443.1521.



(5S,6R,11R)-9-bromo-1-(4-chlorophenyl)-2-methoxy-3-methyl-5-phenyl-2,4,5,11-tetrahydro-6,11-epoxybenzo[b]pyrrolo[3,4-e] azocine (3y)

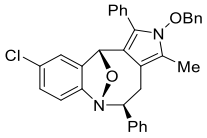
White solid, m.p. = 94-96 ℃; 39.5 mg, 38% yield; 88% ee; $[\alpha]_D^{20.0}$= 318.4 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 95/5, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =8.6 min, t (minor) =11.4 min]; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.22 (s, 3H), 2.75 (ddd, *J* = 16.1, 5.1, 1.5 Hz, 1H), 3.01 (dd, *J* = 16.1,

2.7 Hz, 1H), 3.55 (s, 3H), 4.67 (dd, *J* = 5.2, 2.6 Hz, 1H), 5.87 (s, 1H), 7.06 (d, *J* = 8.2 Hz, 1H), 7.26 (d, *J* = 7.3 Hz, 1H), 7.29-7.37 (m, 3H), 7.39-7.43 (m, 1H), 7.43-7.45 (m, 4H), 7.50-7.56 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 8.5, 25.8, 65.6, 72.1, 78.5, 112.2, 115.3, 117.6, 119.2, 121.9, 122.9, 125.3, 127.3, 128.0, 128.2, 128.3, 128.9, 130.4, 131.0, 133.4, 138.1, 140.3, 148.5; HRMS (ESI) m/z calcd. for $C_{27}H_{22}BrClN_2O_2$ $[M+H]^+$: 521.0626, found: 521.0628.



(5S,6R,11R)-9-chloro-2-methoxy-3-methyl-5-phenyl-1-(p-tolyl)-2,4,5,11-tetrahydro-6,11-epoxybenzo[b]pyrrolo[3,4-e]azocine (3z)

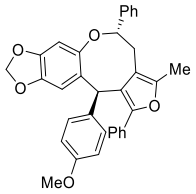
White solid, m.p. = 100-102 ℃; 36 mg, 39% yield; 90% ee; $[\alpha]_D^{20.0}$= 311.5 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 95/5, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =6.5 min, t (minor) =9.2 min]; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.21 (s, 3H), 2.40 (s, 3H), 2.77 (dd, *J* = 16.5, 4.8 Hz, 1H), 3.01 (dd, *J* = 16.1, 2.7 Hz, 1H), 3.56 (s, 3H), 4.66 (dd, *J* = 5.1, 2.6 Hz, 1H), 5.91 (s, 1H), 7.10 (d, *J* = 8.2 Hz, 1H), 7.21-7.29 (m, 5H), 7.32 (t, *J* = 7.5 Hz, 2H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.54 (d, *J* = 7.5 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 8.5, 21.4, 25.9, 65.5, 72.2, 78.8, 111.8, 114.7, 118.5, 122.1, 122.4, 123.3, 126.7, 127.3, 127.9, 128.3, 128.4, 129.2, 129.3, 130.0, 137.3, 138.1, 140.5, 148.0; HRMS (ESI) m/z calcd. for $C_{28}H_{25}ClN_2O_2$ $[M+H]^+$: 457.1677, found: 457.1679.



(5S,6R,11R)-2-(benzyloxy)-9-chloro-3-methyl-1,5-diphenyl-2,4,5,11-tetrahydro-6,11-epoxybenzo[b]pyrrolo[3,4-e]azocine (3a')

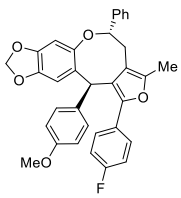
White solid, m.p. = 92-94 ℃; 37.3 mg, 36% yield; 89% ee; $[\alpha]_D^{20.0}$= 282.8 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =7.2 min, t (minor) =9.8 min]; ^{1}H NMR (400 MHz,

$CDCl_3$) δ 2.15 (s, 3H), 2.77 (dd, *J* = 16.3, 5.0 Hz, 1H), 3.00 (dd, *J* = 16.1, 2.7 Hz, 1H), 4.56 (d, *J* = 9.6 Hz, 1H), 4.62 (d, *J* = 9.6 Hz, 1H), 4.67 (dd, *J* = 5.2, 2.7 Hz, 1H), 5.97 (s, 1H), 7.03-7.08 (m, 2H), 7.11 (d, *J* = 8.3 Hz, 1H), 7.22 (d, *J* = 1.9 Hz, 1H), 7.25-7.30 (m, 4H), 7.30-7.40 (m, 4H), 7.47 (t, *J* = 7.7 Hz, 2H), 7.51-7.57 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 8.7, 26.0, 72.3, 78.8, 80.4, 111.8, 114.7, 118.7, 122.4, 122.9, 123.6, 127.3, 127.5, 128.0, 128.3, 128.4, 128.6, 129.2, 129.5, 129.7, 129.8, 130.1, 133.6, 138.1, 140.5, 148.0; HRMS (ESI) m/z calcd. for $C_{33}H_{27}ClN_2O_2$ $[M+H]^+$: 519.1834, found: 519.1837.



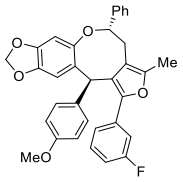
(5*S*,12*S*)-12-(4-methoxyphenyl)-3-methyl-1,5-diphenyl-4,5-dihydro-12*H*-[1,3]dioxolo[4',5':4,5]benzo[1,2-*b*]furo[3,4-*e*]oxocine (5a)

White solid, m.p. =186-187 ℃; 39 mg, 38% yield; 90% ee; $[\alpha]_D^{20.0}$ = 102.3 (0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 7.3 min, t (minor) =6.3 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 2.18 (s, 3H), 2.66 (dd, *J* = 4.2, 15.7 Hz, 1H), 2.77 (dd, *J* = 10.4, 15.7 Hz, 1H), 3.77 (s, 3H), 5.13 (dd, *J* = 4.1, 10.3 Hz, 1H), 5.44 (s, 1H), 5.91 (d, *J* = 1.4 Hz, 1H), 5.92 (d, *J* = 1.4 Hz, 1H), 6.30 (s, 1H), 6.72-6.83 (m, 3H), 7.05 (d, *J* = 8.4 Hz, 2H), 7.16-7.26 (m, 3H), 7.27-7.36 (m, 5H), 7.45 (d, *J* = 7.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 11.9, 30.3, 45.7, 55.3, 82.8, 101.4, 105.8, 111.3, 113.6, 117.4, 121.2, 126.5, 126.8, 127.1, 127.3, 127.8, 128.3, 128.4, 128.5, 131.5, 137.3, 142.2, 143.8, 146.8, 147.8, 148.6, 150.8, 157.8; HRMS (ESI) m/z calcd for $C_{34}H_{28}O_5$ $[M+H]^+$:517.2010, found:517.2006.



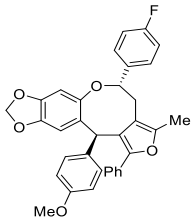
(5*S*,12*S*)-1-(4-fluorophenyl)-12-(4-methoxyphenyl)-3-methyl-5-phenyl-4,5-dihydro-12*H*-[1,3]dioxolo[4',5':4,5]benzo[1,2-*b*]furo[3,4-*e*]oxocine (5b)

White solid, m.p. =90-91 ℃； 33 mg, 31% yield; 86% ee; $[\alpha]_D^{20.0}$= 152.6 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 8.2 min, t (minor) =7.8 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 2.16 (s, 3H), 2.67 (dd, *J* = 4.2, 15.7 Hz, 1H), 2.76 (dd, *J* = 10.0, 15.7 Hz, 1H), 3.77 (s, 3H), 5.12 (dd, *J* = 4.2, 10.0 Hz, 1H), 5.35 (s, 1H), 5.92 (d, *J* = 1.4 Hz, 1H), 5.93 (d, *J* = 1.5 Hz, 1H), 6.29 (s, 1H), 6.72 (s, 1H), 6.78 (d, *J* = 8.7 Hz, 2H), 6.97-7.09 (m, 4H), 7.21 (d, *J* = 7.1 Hz, 2H), 7.26-7.35 (m, 3H), 7.37-7.44 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 11.9, 30.1, 45.8, 55.3, 82.9, 101.5, 105.8, 111.1, 113.6, 115.5 (d, *J* = 21.6 Hz), 117.3, 121.1, 126.5, 127.3, 127.7 (d, *J* = 3.2 Hz), 127.8, 128.4, 128.5, 128.6 (d, *J* = 8.0 Hz), 137.1, 142.0, 143.9, 146.8, 147.6, 147.7, 150.7, 157.8, 162.0 (d, *J* = 247.0 Hz);^{19}F NMR (377 MHz, $CDCl_3$) δ -114.6; HRMS (ESI) m/z calcd for $C_{34}H_{27}FO_5$ $[M+H]^+$: 535.1915, found: 535.1915.



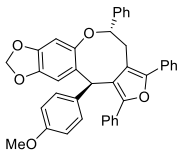
(5*S*,12*S*)-1-(3-fluorophenyl)-12-(4-methoxyphenyl)-3-methyl-5-phenyl-4,5-dihydro-12*H*-[1,3]dioxolo[4',5':4,5]benzo[1,2-*b*]furo[3,4-*e*]oxocine (5c)

White solid, m.p. =122-123 ℃; 33 mg, 31% yield; 95% ee; $[\alpha]_D^{20.0}$= 70.8 (0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 7.6 min, t (minor) =6.9 min]**;**^{1}H NMR (400 MHz, $CDCl_3$) *δ* 2.16 (s, 3H), 2.76 (dd, *J* = 15.6, 9.8 Hz, 1H), 2.69 (dd, *J* = 15.6, 4.2 Hz, 1H), 3.77 (s, 3H), 5.12 (dd, *J* = 4.0, 9.5 Hz, 1H), 5.42 (s, 1H), 5.92 (d, *J* = 1.3 Hz, 1H), 5.93 (d, *J* = 1.3 Hz, 1H), 6.27 (s, 1H), 6.74 (s, 1H), 6.78 (d, *J* = 8.7 Hz, 2H), 6.89-6.97 (m, 1H), 7.04 (d, *J* = 8.5 Hz, 2H), 7.15-7.24 (m, 4H), 7.24-7.34 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 11.9, 29.9, 45.8, 55.3, 82.8, 101.5, 105.9, 111.1, 113.4 (d, *J* = 23.0 Hz), 113.7, 113.8 (d, *J* = 21.5 Hz), 117.7, 122.1 (d, *J* = 2.8 Hz), 122.5, 126.6, 126.7, 127.8, 128.4 (d, *J* = 6.1 Hz), 128.5, 129.9, 130.0, 133.5 (d, *J* = 8.5 Hz), 136.9, 141.9, 143.9, 146.9, 148.3, 150.5, 157.9, 162.9 (d, *J* = 244.9 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -112.8; HRMS (ESI) m/z calcd for $C_{34}H_{27}FO_5$ $[M+H]^+$:535.1915, found:535.1919.



(5*S*,12*S*)-5-(4-fluorophenyl)-12-(4-methoxyphenyl)-3-methyl-1-phenyl-4,5-dihydro-12*H*-[1,3]dioxolo[4',5':4,5]benzo[1,2-*b*]furo[3,4-*e*]oxocine (5d)

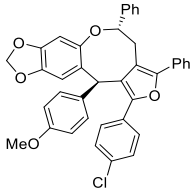
White solid, m.p. =121-122 ℃; 29 mg, 27% yield; 89% ee; $[\alpha]_D^{20.0}$=73.4 (0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 7.7 min, t (minor) =6.4 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 2.18 (s, 3H), 2.63-2.76 (m, 2H), 3.76 (s, 3H), 5.11 (dd, *J* = 4.2, 9.8 Hz, 1H), 5.44 (s, 1H), 5.91 (d, *J* = 1.2 Hz, 1H), 5.92 (d, *J* = 1.2 Hz, 1H), 6.25 (s, 1H), 6.74 (s, 1H), 6.78 (d, *J* = 8.7 Hz, 2H), 6.96-7.06 (m, 4H), 7.14-7.20 (m, 2H), 7.21-7.25 (m, 1H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.42-7.47 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 11.9, 30.2, 45.7, 55.3, 82.2, 101.5, 105.6, 111.3, 113.6, 115.2 (d, *J* = 21.3 Hz), 117.1, 121.3, 126.8, 127.2, 127.5, 128.2 (d, *J* = 8.0 Hz), 128.4, 128.5, 131.5, 137.3, 137.9 (d, *J* = 2.6 Hz), 143.9, 146.8, 147.8, 148.6, 150.5, 157.8, 162.3 (d, *J* = 246.1 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -114.6; HRMS (ESI) m/z calcd for $C_{34}H_{27}FO_5$ $[M+H]^+$:535.1915, found: 535.1915.



(5*S*,12*S*)-12-(4-methoxyphenyl)-1,3,5-triphenyl-4,5-dihydro-12*H*-[1,3]dioxolo [4',5':4,5]benzo[1,2-*b*]furo[3,4-*e*]oxocine (5e)

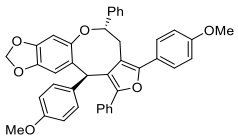
White solid, m.p. =183-185 ℃, 37 mg, 32% yield; 90% ee; $[\alpha]_D^{20.0}$= 82.3 (0.1, CH_2Cl_2); [Daicel Chiralpak IA-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 7.0 min, t (minor) =5.6 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 2.88 (dd, *J* = 16.0, 4.1 Hz, 1H), 3.14 (dd, *J* = 16.0, 11.4 Hz, 1H), 3.79 (s, 3H), 5.26 (dd, *J* = 11.3, 4.0 Hz, 1H), 5.56 (s, 1H), 5.93 (d, *J* = 1.3 Hz, 1H), 5.96 (d, *J* = 1.4 Hz, 1H), 6.38 (s, 1H), 6.83 (dd, *J* = 6.2, 2.6 Hz, 3H), 7.09-7.15 (m, 4H), 7.24 (d, *J* = 3.2 Hz, 1H), 7.26-7.43 (m, 8H), 7.53-7.58 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 32.9,

45.7, 55.4, 82.8, 101.5, 105.4, 111.7, 113.8, 119.6, 122.0, 125.4, 126.2, 126.8, 127.3, 127.5, 127.7, 127.8, 128.1, 128.4, 128.5, 128.6, 131.1, 131.3, 137.1, 142.3, 143.8, 146.9, 149.4, 150.7, 152.3, 158.0; HRMS (ESI) m/z calcd for $C_{39}H_{30}O_5$ $[M+H]^+$:579.2166, found:579.2163.



(5*S*,12*S*)-1-(4-chlorophenyl)-12-(4-methoxyphenyl)-3,5-diphenyl-4,5-dihydro-12*H*-[1,3]dioxolo[4',5':4,5]benzo[1,2-*b*]furo[3,4-*e*]oxocine (5f)

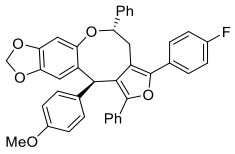
White solid, m.p. =234-236 ℃; 42 mg, 34% yield; 92% ee; $[\alpha]_D^{20.0}$= 82.3 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 8.0 min, t (minor) =7.1 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.91 (dd, *J* = 16.0, 4.0 Hz, 1H), 3.12 (dd, *J* = 16.0, 11.3 Hz, 1H), 3.81 (s, 3H), 5.26 (dd, *J* = 11.3, 3.9 Hz, 1H), 5.48 (s, 1H), 5.95 (s, 1H), 5.96 (s, 1H), 6.35 (s, 1H), 6.80-6.86 (m, 3H), 7.08-7.16 (m, 4H), 7.23-7.33 (m, 4H), 7.35-7.40 (m, 4H), 7.49 (d, *J* = 8.5 Hz, 2H), 7.54 (d, *J* = 7.9 Hz, 2H);^{13}C NMR (100 MHz, $CDCl_3$) δ 32.4, 45.8, 55.4, 82.9, 101.6, 105.5, 111.5, 113.9, 119.7, 122.6, 125.5, 126.3, 126.9, 127.5, 127.8, 128.2, 128.4, 128.5, 128.6, 128.9, 129.5, 131.1, 133.6, 136.8, 142.0, 143.9, 147.0, 149.4, 149.7, 152.0, 158.1; HRMS (ESI) m/z calcd for $C_{39}H_{29}ClO_5$ $[M+H]^+$:613.1776, found:613.1777.



(5*S*,12*S*)-3,12-bis(4-methoxyphenyl)-1,5-diphenyl-4,5-dihydro-12*H*-[1,3]dioxolo-[4',5':4,5]benzo[1,2-*b*]furo[3,4-*e*]oxocine (5g)

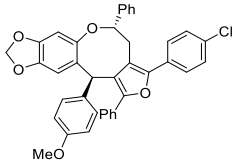
White solid, m.p. =120-122 ℃; 32 mg, 26% yield; 90% ee; $[\alpha]_D^{20.0}$= 99.8(0.1, CH_2Cl_2); [Daicel Chiralpak IA-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 9.7 min, t (minor) =7.7 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.84 (dd, *J* = 4.1,16.0 Hz, 1H), 3.09 (dd, *J* = 11.5, 16.0 Hz, 1H), 3.79 (s, 3H),

3.81 (s, 3H), 5.24 (dd, *J* = 4.0, 11.5 Hz, 1H), 5.54 (s, 1H), 5.94 (d, *J* = 1.4 Hz, 1H), 5.97 (d, *J* = 1.4 Hz, 1H), 6.37 (s, 1H), 6.80-6.86 (m, 3H), 6.88-6.92 (m, 2H), 7.09-7.17 (m, 4H), 7.24-7.32 (m, 4H), 7.39 (t, *J* = 7.6 Hz, 2H), 7.46-7.50 (m, 2H), 7.52-7.57 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 32.8, 45.7, 55.3, 55.4, 82.9, 101.5, 105.4, 111.7, 113.8, 114.0, 118.2, 121.8, 124.1, 125.6, 126.2, 127.4, 127.6, 127.7, 128.2, 128.3, 128.4, 128.6, 131.2, 137.1, 142.3, 143.7, 146.9, 149.5, 150.0, 152.2, 158.0, 159.0; HRMS (ESI) m/z calcd for $C_{40}H_{32}O_6$ $[M+H]^+$:609.2272, found:609.2271.



(5*S*,12*S*)-3-(4-fluorophenyl)-12-(4-methoxyphenyl)-1,5-diphenyl-4,5-dihydro-12*H*-[1,3]dioxolo[4',5':4,5]benzo[1,2-*b*]furo[3,4-*e*]oxocine (5h)

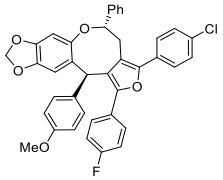
White solid, m.p. =198-199 ℃; 43 mg, 36% yield; 97% ee; $[\alpha]_D^{20.0}$= 49.0 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 8.9 min, t (minor) =8.0 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.83 (dd, *J* = 15.9, 4.3 Hz, 1H), 3.08 (dd, *J* = 16.0, 11.3 Hz, 1H), 3.79 (s, 3H), 5.25 (dd, *J* = 11.2, 4.2 Hz, 1H), 5.56 (s, 1H), 5.95 (s, 1H), 5.97 (s, 1H), 6.41 (s, 1H), 6.81-6.84 (m, 3H), 7.02-7.08 (m, 2H), 7.09-7.13 (m, 4H), 7.25-7.35 (m, 4H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.51 (dd, *J* = 8.6, 5.5 Hz, 2H), 7.55 (d, *J* = 7.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.1, 45.6, 55.4, 82.8, 101.6, 105.3, 111.7, 113.8, 115.6 (d, *J* = 21.6 Hz), 119.2, 122.0, 125.2, 126.1, 127.4, 127.5 (d, *J* = 3.0 Hz), 127.8 (d, *J* = 13.0 Hz), 128.1, 128.3, 128.4, 128.5, 128.6, 131.0, 137.0, 142.2, 143.8, 146.9, 148.6, 150.7, 152.4, 158.0, 162.0 (d, *J* = 247.5 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -114.1; HRMS (ESI) m/z calcd for $C_{39}H_{29}FO_5$ $[M+H]^+$:597.2072 found:597.2075.



(5*S*,12*S*)-3-(4-chlorophenyl)-12-(4-methoxyphenyl)-1,5-diphenyl-4,5-dihydro-12*H*-[1,3]dioxolo[4',5':4,5]benzo[1,2-*b*]furo[3,4-*e*]oxocine(5i)

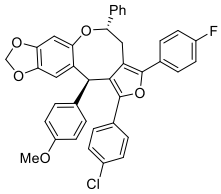
white solid, m.p. =130-131 ℃; 36 mg, 29% yield; 99% ee; $[\alpha]_D^{20.0}$= 94.7 (0.1, CH_2Cl_2);

[Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99/1, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 14.2 min, t (minor) =12.5 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 2.83 (dd, *J* = 16.0, 4.3 Hz, 1H), 3.09 (dd, *J* = 16.0, 11.2 Hz, 1H), 3.79 (s, 3H), 5.26 (dd, *J* = 11.2, 4.3 Hz, 1H), 5.57 (s, 1H), 5.94 (d, *J* = 1.2 Hz, 1H), 5.97 (d, *J* = 1.2 Hz, 1H), 6.41 (s, 1H), 6.80-6.86 (m, 3H), 7.06-7.13 (m, 4H), 7.22-7.29 (m, 2H), 7.28-7.36 (m, 4H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.43-7.48 (m, 2H) 7.55 (d, *J* = 8.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 33.3, 45.5, 55.4, 82.8, 101.6, 105.3, 111.7, 113.9, 120.0, 122.2, 125.1, 126.0, 127.6, 127.7, 127.8, 128.0, 128.1, 128.5, 128.7, 128.7, 129.7, 130.9, 133.1, 136.9, 142.1, 143.8, 147.0, 148.3, 151.0, 152.5, 158.1; HRMS (ESI) m/z calcd for $C_{39}H_{29}ClO_5$ $[M+H]^+$:613.1776, found: 613.1777.



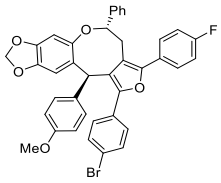
(5S,12S)-3-(4-chlorophenyl)-1-(4-fluorophenyl)-12-(4-methoxyphenyl)-5-phenyl-4,5-dihydro-12H-[1,3] dioxolo[4',5':4,5]benzo[1,2-b]furo[3,4-e]oxocine (5j)

White solid, m.p. = 110-112 ℃; 35.2 mg, 286% yield; 93% ee; $[\alpha]_D^{20.0}$= 81.6 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =8.4 min, t (minor) =7.5 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.85 (dd, *J* = 15.9, 4.1 Hz, 1H), 3.05 (dd, *J* = 16.0, 10.9 Hz, 1H), 3.79 (s, 3H), 5.24 (dd, *J* = 11.0, 4.0 Hz, 1H), 5.48 (s, 1H), 5.93 (s, 1H) 5.95 (s, 1H), 6.36 (s, 1H), 6.78 (s, 1H), 6.83 (d, *J* = 8.6 Hz, 2H), 7.00-7.16 (m, 6H), 7.23-7.30 (m, 3H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.45-7.48 (m, 2H), 7.55 (d, *J* = 7.3 Hz, 2H);^{13}C NMR (100 MHz, $CDCl_3$) δ 33.0, 45.6, 55.4, 82.8, 101.6, 105.4, 111.5, 113.9, 115.7 (d, *J* = 21.7 Hz), 119.3, 122.1, 125.1, 126.1, 127.2 (d, *J* = 3.3 Hz), 127.8, 127.9, 128.2, 128.5, 128.8, 129.4 (d, *J* = 8.2 Hz) 129.6, 133.2, 136.8, 142.0, 143.9, 147.1, 148.4, 150.1, 152.3, 158.1, 162.5 (d, *J* = 247.7 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -112.9; HRMS (ESI) m/z calcd. for $C_{39}H_{28}ClFO_4$ $[M+H]^+$: 631.1682, found: 631.1680.



(5S,12S)-1-(4-chlorophenyl)-3-(4-fluorophenyl)-12-(4-methoxyphenyl)-5-phenyl-4,5-dihydro-12H-[1,3] dioxolo[4',5':4,5]benzo[1,2-b]furo[3,4-e]oxocine (5k)

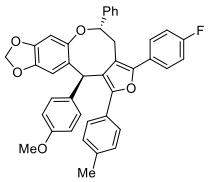
White solid, m.p. = 144-146 ℃; 48 mg, 38% yield; 90% ee; $[\alpha]_D^{20.0}$= 65.8 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =8.4 min, t (minor) =7.4 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.85 (dd, *J* = 4.1, 15.9 Hz, 1H), 3.05 (dd, *J* = 10.9, 16.0 Hz, 1H), 3.79 (s, 3H), 5.24 (dd, *J* = 4.0, 11.0 Hz, 1H), 5.48 (s, 1H), 5.93 (s, 1H), 5.95 (s, 1H), 6.36 (s, 1H), 6.78 (s, 1H), 6.83 (d, *J* = 8.6 Hz, 2H), 7.00 -7.16 (m, 6H), 7.23-7.30 (m, 3H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.42 -7.52 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 32.5, 45.7, 55.4, 82.8, 101.6, 105.5, 113.9, 115.6 (d, *J* = 21.7 Hz), 119.3, 122.8, 125.4, 126.2, 127.3 (d, *J* = 3.4 Hz), 127.8, 127.9, 128.2, 128.5, 128.6 (d, *J* = 7.9 Hz), 128.7, 128.9, 129.5, 133.8, 136.7, 142.0, 143.9, 147.1, 148.9, 149.4, 152.1, 158.2, 162.2 (d, *J* = 247.7 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -113.9; HRMS (ESI) m/z calcd. for $C_{39}H_{28}ClFO_4$ $[M+H]^+$: 631.1682, found: 631.1683.



(5S,12S)-1-(4-bromophenyl)-3-(4-fluorophenyl)-12-(4-methoxyphenyl)-5-phenyl-4,5-dihydro-12H-[1,3] dioxolo[4',5':4,5]benzo[1,2-b]furo[3,4-e]oxocine (5l)

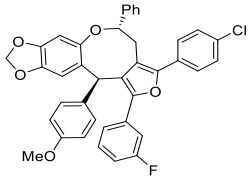
White solid, m.p. = 134-136 ℃; 39 mg, 29% yield; 95% ee; $[\alpha]_D^{20.0}$= 52.1 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =8.8 min, t (minor) =7.7 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.85 (dd, *J* = 15.9, 4.2 Hz, 1H), 3.05 (dd, *J* = 15.9, 10.9 Hz, 1H), 3.79 (s, 3H), 5.24 (dd, *J* = 11.0, 4.1 Hz, 1H), 5.48 (s, 1H), 5.93 (s, 1H), 5.96 (s, 1H), 6.36 (s, 1H),

6.78 (s, 1H), 6.83 (d, *J* = 8.4 Hz, 2H), 7.01-7.07 (m, 3H), 7.09 -7.14 (m, 3H), 7.22-7.30 (m, 3H), 7.40 (d, *J* = 8.3 Hz, 2H), 7.47 (dd, *J* = 8.6, 5.3 Hz, 2H), 7.52 (d, *J* = 8.3 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 32.5, 45.7, 55.4, 82.8, 101.6, 105.5, 111.5, 113.9, 115.6 (d, *J* = 21.7 Hz), 119.4, 121.9, 122.8, 125.3, 126.2, 127.3 (d, *J* = 3.3 Hz), 127.8, 128.2, 128.5, 128.6 (d, *J* = 8.1 Hz), 128.8, 129.9, 131.8, 136.7, 142.0, 143.9, 147.1, 149.0, 149.4, 152.0, 158.1, 162.2 (d, *J* = 247.9 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -113.6; HRMS (ESI) m/z calcd. for $C_{39}H_{28}BrFO_4$ $[M+H]^+$: 675.1177, found: 675.1174.



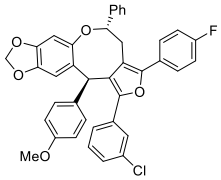
(5S,12S)-3-(4-fluorophenyl)-12-(4-methoxyphenyl)-5-phenyl-1-(p-tolyl)-4,5-dihydro-12H-[1,3] dioxolo[4',5':4,5]benzo[1,2-b]furo[3,4-e]oxocine (5m)

White solid, m.p. = 94-96 ℃; 38 mg, 31% yield; 91% ee; $[\alpha]_D^{20.0}$= 65.0 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 7.8 min, t (minor) =7.1 min]**;**^{1}H NMR (400 MHz, $CDCl_3$) *δ* 2.37 (s, 3H), 2.83 (dd, *J* = 4.2, 15.9 Hz, 1H), 3.07 (dd, *J* = 11.2, 15.9 Hz, 1H), 3.79 (s, 3H), 5.25 (dd, *J* = 4.1, 11.2 Hz, 1H), 5.54 (s, 1H), 5.93 (s, 1H), 5.96 (s, 1H), 6.39 (s, 1H), 6.81 (d, *J* = 3.6 Hz, 2H), 6.83 (s, 1H), 7.04 (t, *J* = 8.5 Hz, 2H), 7.10 (t, *J* = 7.2 Hz, 4H), 7.19-7.30 (m, 5H), 7.44 (d, *J* = 7.9 Hz, 2H), 7.49 (dd, *J* = 5.6, 8.3 Hz, 2H);^{13}C NMR (100 MHz, $CDCl_3$) *δ* 21.4, 33.1, 45.7, 55.4, 82.8, 101.5, 105.3, 111.7, 113.9, 115.5 (d, *J* = 21.7 Hz), 119.2, 121.5, 125.4, 126.1, 127.5, 127.6 (d, *J* = 3.3 Hz), 127.7, 128.2, 128.3, 128.4 (d, *J* = 8.2 Hz), 128.5, 129.4, 137.1, 137.8, 142.3, 143.8, 146.9, 148.3, 150.9, 152.4, 158.1, 162.0 (d, *J* = 247.7 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -114.3; HRMS (ESI) m/z calcd. for $C_{40}H_{31}FO_5$ $[M+H]^+$: 611.2228, found: 611.2232.



(5*S*,12*S*)-1-(3-fluorophenyl)-12-(4-methoxyphenyl)-3-methyl-5-phenyl-4,5-dihydro-12*H*-[1,3]dioxolo[4',5':4,5]benzo[1,2-*b*]furo[3,4-*e*]oxocine (5n)

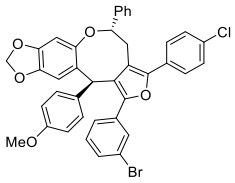
White solid, m.p. =192-193 ℃; 52 mg, 41% yield; 92% ee; $[\alpha]_D^{20.0}$= 152.6 (0.1, CH_2Cl_2); [Daicel Chiralpak IA-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99/1, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 10.0 min, t (minor) =8.4 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.85 (dd, *J* = 15.9, 4.2 Hz, 1H), 3.07 (dd, *J* = 15.9, 11.0 Hz, 1H), 3.79 (s, 3H), 5.24 (dd, *J* = 10.9, 4.2 Hz, 1H), 5.55 (s, 1H), 5.95 (s, 1H), 5.97 (s, 1H), 6.38 (s, 1H), 6.80-6.87 (m, 3H), 7.02 (t, *J* = 8.1 Hz, 1H), 7.06-7.13 (m, 4H), 7.23-7.38 (m, 8H), 7.45 (d, *J* = 8.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 32.7, 45.6, 55.4, 82.8, 101.6, 105.4, 111.5, 113.9, 114.3 (d, *J* = 23.1 Hz), 114.8 (d, *J* = 21.0 Hz), 120.1, 123.0 (d, *J* = 2.7 Hz), 123.3, 125.1, 126.1, 127.9, 128.0, 128.2, 128.5, 128.8, 129.5, 130.2 (d, *J* = 8.5 Hz), 132.9 (d, *J* = 8.4 Hz), 133.4, 136.6, 141.9, 144.0, 147.1, 148.8, 149.5, 152.2, 158.2, 162.9 (d, *J* = 245.8 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -113.6; HRMS (ESI) m/z calcd for $C_{39}H_{28}ClFO_5$ $[M+H]^+$:631.1682, found: 631.1687.



(5S,12S)-1-(3-chlorophenyl)-3-(4-fluorophenyl)-12-(4-methoxyphenyl)-5-phenyl-4,5-dihydro-12H-[1,3] dioxolo[4',5':4,5]benzo[1,2-b]furo[3,4-e]oxocine (5o)

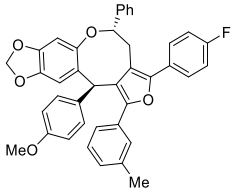
White solid, m.p. = 94-96 ℃; 45.4 mg, 36% yield; 92% ee; $[\alpha]_D^{20.0}$= 76.9 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =9.4 min, t (minor) =8.0 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.85 (dd, *J* = 15.9, 4.2 Hz, 1H), 3.05 (dd, *J* = 15.9, 10.9 Hz, 1H), 3.79 (s, 3H), 5.25 (dd, *J* = 10.9, 4.1 Hz, 1H), 5.52 (s, 1H), 5.94 (s, 1H), 5.97 (s, 1H), 6.38 (s, 1H), 6.79-6.90 (m, 3H), 7.01-7.17 (m, 6H), 7.23-7.35 (m, 5H), 7.39 (d, *J* = 7.2 Hz, 1H), 7.48 (dd, *J* = 8.5, 5.3 Hz, 2H), 7.58 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 32.6, 45.6, 55.4,

82.8, 101.6, 105.4, 111.5, 113.9, 115.5, 115.7, 119.3, 123.3, 125.2, 125.3, 126.1, 127.2 (d, *J* = 3.1 Hz), 127.4, 127.7, 127.8, 128.2, 128.5, 128.7 (d, *J* = 8.1 Hz), 129.9, 132.7, 134.6, 136.7, 142.0, 144.0, 147.1, 149.1 (d, *J* = 18.6 Hz), 152.2, 158.1, 162.2 (d, *J* = 248.3 Hz);^{19}F NMR (377 MHz, $CDCl_3$) δ -113.6; HRMS (ESI) m/z calcd. for $C_{39}H_{28}ClFO_4$ $[M+H]^+$: 631.1682, found: 631.1680.



(5*S*,12*S*)-1-(3-bromophenyl)-3-(4-chlorophenyl)-12-(4-methoxyphenyl)-5-phenyl-4,5-dihydro-12*H*-[1,3]dioxolo[4',5':4,5]benzo[1,2-*b*]furo[3,4-*e*]oxocine (5p)

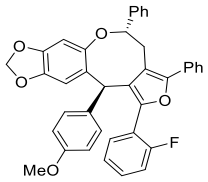
White solid, m.p. =110-111 ℃; 40 mg, 29% yield; 96% ee; $[\alpha]_D^{20.0}$=100.8 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 12.5 min, t (minor) =9.3 min]**;**^{1}H NMR (400 MHz, $CDCl_3$) *δ* 2.92 (dd, *J* = 15.7, 4.7 Hz, 1H), 3.05 (dd, *J* = 15.7, 8.8 Hz, 1H), 3.77 (s, 3H), 5.27 (dd, *J* = 8.9, 4.5 Hz, 1H), 5.32 (s, 1H), 5.91 (s, 1H), 5.94 (s, 1H), 6.50 (s, 2H), 6.77 (d, *J* = 8.5 Hz, 2H), 7.07 (d, *J* = 8.3 Hz, 2H), 7.13 (d, *J* = 7.2 Hz, 2H), 7.16-7.22 (m, 2H), 7.22-7.26 (m, 4H), 7.26-7.32 (m, 4H), 7.62 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 32.6, 45.2, 55.4, 83.2, 101.5, 104.6, 111.4, 113.8, 118.1, 124.7, 125.0, 125.3, 126.1, 127.0, 127.8, 127.9, 128.4, 128.6, 128.8, 129.7, 130.4, 132.4, 132.7, 133.0, 133.1, 136.4, 141.5, 143.7, 146.9, 148.9, 150.0, 152.0, 158.1; HRMS (ESI) m/z calcd for $C_{39}H_{28}BrClO_5$ $[M+H]^+$:691.0881, found: 691.0879.



(5*S*,12*S*)-3-(4-fluorophenyl)-12-(4-methoxyphenyl)-5-phenyl-1-(m-tolyl)-4,5-dihydro-12*H*-[1,3]dioxolo[4',5':4,5]benzo[1,2-*b*]furo[3,4-*e*]oxocine (5q)

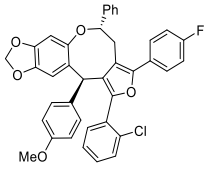
White solid, m.p. =108-109 ℃; 38 mg, 31% yield; 92% ee; $[\alpha]_D^{20.0}$= 96.0 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 99/1, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 8.3 min, t (minor) =7.2 min]**;**^{1}H NMR (400 MHz,

$CDCl_3$) δ 2.37 (s, 3H), 2.82 (dd, J = 15.9, 4.3 Hz, 1H), 3.07 (dd, J = 15.9, 11.2 Hz, 1H), 3.80 (s, 3H), 5.26 (dd, J = 11.2, 4.3 Hz, 1H), 5.56 (s, 1H), 5.95 (d, J = 1.4 Hz, 1H), 5.98 (d, J = 1.4 Hz, 1H), 6.41 (s, 1H), 6.83 (d, J = 8.3 Hz, 3H), 7.02-7.16 (m, 7H), 7.24-7.26 (m, 1H), 7.26-7.35 (m, 4H), 7.39 (s, 1H),7.47- 7.54 (m, 2H);^{13}C NMR (101 MHz, $CDCl_3$) δ 21.6, 33.1, 45.7, 55.4, 82.8, 101.6, 105.3, 111.7, 113.9, 115.5 (d, J = 21.6 Hz), 119.2, 121.9, 124.6, 125.3, 126.1, 127.6 (d, J = 3.3 Hz), 127.7, 128.2, 128.3 (d, J = 14.7 Hz), 128.4, 128.5, 128.6, 128.7, 131.0, 137.1, 138.3, 142.2, 143.8, 147.0, 148.5, 150.9, 152.5, 158.1, 162.0 (d, J = 247.5 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -114.2; HRMS (ESI) m/z calcd for $C_{40}H_{31}FO_5$ $[M+H]^+$:611.2228, found: 611.2233.



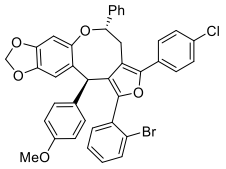
(5*S*,12*S*)-3-(4-fluorophenyl)-12-(4-methoxyphenyl)-5-phenyl-1-(m-tolyl)-4,5-dihydro-12*H*-[1,3]dioxolo[4',5':4,5]benzo[1,2-*b*]furo[3,4-*e*]oxocine (5r)

White solid, m.p. =117-118 ℃ 43 mg, 36% yield; 91% ee; $[\alpha]_D^{20.0}$= 95.5 (0.1, CH_2Cl_2); [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 5.6 min, t (minor) =5.2 min]**;**^{1}H NMR (400 MHz, $CDCl_3$) δ 2.88 (dd, J = 4.2, 15.8 Hz, 1H), 3.13 (dd, J = 10.2, 15.8 Hz, 1H), 3.78 (s, 3H), 5.27 (dd, J = 4.2, 10.0 Hz, 1H), 5.42 (s, 1H), 5.91 (s, 1H), 5.94 (s, 1H), 6.46 (s, 1H), 6.63 (s, 1H), 6.79 (d, J = 8.5 Hz, 2H), 7.06-7.17 (m, 6H), 7.19-7.28 (m, 4H), 7.27-7.38 (m, 4H), 7.45 (d, J = 7.7 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.0, 45.3, 55.4, 83.1, 101.5, 104.8, 111.8, 113.8, 116.1 (d, J = 22.0 Hz), 118.5, 119.4 (d, J = 14.6 Hz), 124.0 (d, J = 3.5 Hz), 124.5, 125.1, 126.0, 126.7, 127.4, 127.7, 128.3, 128.4, 128.5, 130.3 (d, J = 8.1 Hz), 131.2, 131.4 (d, J = 2.3 Hz), 136.7, 141.9, 143.6, 145.7, 146.8, 150.4, 152.3, 158.0, 160.1 (d, J = 250.4 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -111.8; HRMS (ESI) m/z calcd for $C_{39}H_{29}FO_5$ $[M+H]^+$:597.2072, found:597.2073.



(5S,12S)-1-(2-chlorophenyl)-3-(4-fluorophenyl)-12-(4-methoxyphenyl)-5-phenyl-4,5-dihydro-12H-[1,3] dioxolo[4',5':4,5]benzo[1,2-b]furo[3,4-e]oxocine (5s)

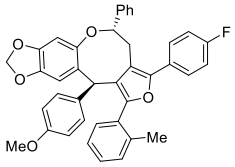
White solid, m.p. = 88-90 ℃; 38 mg, 30% yield; 94% ee; $[\alpha]_D^{20.0}$= 123.6 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 10.4 min, t (minor) =8.4 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 2.91 (dd, *J* = 15.6, 4.6 Hz, 1H), 3.02 (dd, *J* = 15.7, 8.8 Hz, 1H), 3.77 (s, 3H), 5.27 (dd, *J* = 9.2, 4.9 Hz, 1H), 5.35 (s, 1H), 5.91 (d, *J* = 1.4 Hz, 1H), 5.94 (d, *J* = 1.4 Hz, 1H), 6.50 (d, *J* = 2.1 Hz, 2H), 6.77 (d, *J* = 8.6 Hz, 2H), 6.97 (t, *J* = 8.7 Hz, 2H), 7.06 (d, *J* = 8.4 Hz, 2H), 7.13 (d, *J* = 7.1 Hz, 2H), 7.21 (d, *J* = 4.3 Hz, 2H), 7.23 -7.35 (m, 6H), 7.42 (d, *J* = 7.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 32.5, 45.2, 55.4, 83.3, 101.5, 104.6, 111.4, 113.8, 115.4 (d, *J* = 21.5 Hz), 117.3, 124.9, 125.5, 126.1, 126.4, 127.4 (d, *J* = 3.3 Hz), 127.8, 128.4, 128.5 (d, *J* = 8.0 Hz), 128.9, 129.9, 130.1, 130.5, 132.5, 135.1, 136.5, 141.5, 143.7, 146.9, 148.4, 149.3, 152.0, 158.1, 162.1 (d, *J* = 247.3 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -114.2; HRMS (ESI) m/z calcd. for $C_{39}H_{28}ClFO_4$ $[M+H]^+$: 631.1682, found: 631.1683.



(5S,12S)-1-(2-bromophenyl)-3-(4-chlorophenyl)-12-(4-methoxyphenyl)-5-phenyl-4,5-dihydro-12H-[1,3] dioxolo[4',5':4,5]benzo[1,2-b]furo[3,4-e]oxocine (5t)

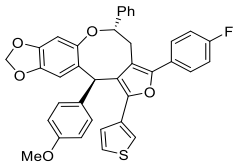
White solid, m.p. = 100-102 ℃; 52.4 mg, 38% yield; 95% ee; $[\alpha]_D^{20.0}$= 72.4 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =10.1 min, t (minor) =8.3 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.84 (dd, *J* = 15.9, 4.4 Hz, 1H), 3.06 (dd, *J* = 15.9, 10.9 Hz, 1H), 3.80 (s, 3H), 5.25 (dd, *J* = 10.8, 4.3 Hz, 1H), 5.52 (s, 1H), 5.95 (d, *J* = 1.4 Hz, 1H), 5.98 (d, *J* = 1.4 Hz, 1H), 6.39 (s, 1H), 6.76-6.95 (m, 3H), 7.08 (d, *J* = 8.6 Hz, 4H), 7.22-7.30 (m, 4H), 7.33 (d, *J* = 8.5 Hz, 2H), 7.41 -7.51 (m, 4H), 7.73 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 32.9, 45.6, 55.4, 82.8, 101.6, 105.3, 111.6, 114.0, 120.1, 122.8, 123.4, 124.9, 125.8, 126.1, 127.9, 128.0, 128.2, 128.5, 128.8, 129.4, 130.1, 130.4, 130.8, 132.8, 133.4,

136.6, 141.9, 144.0, 147.1, 148.9, 149.2, 152.3, 158.2; HRMS (ESI) m/z calcd. for $C_{39}H_{28}BrClO_5$ $[M+H]^+$: 691.0881, found: 691.0879.



(5*S*,12*S*)-3-(4-fluorophenyl)-12-(4-methoxyphenyl)-5-phenyl-1-(o-tolyl)-4,5-dihydro-12*H*-[1,3]dioxolo[4',5':4,5]benzo[1,2-*b*]furo[3,4-*e*]oxocine (5u)

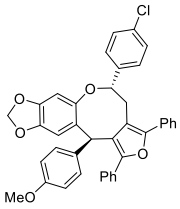
White solid, m.p. =82-84 ℃; 49 mg, 40% yield; 92% ee; $[\alpha]_D^{20.0}$= 92.8 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 6.3 min, t (minor) =5.6 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.32 (s, 3H), 2.86 (dd, *J* = 15.7, 3.7 Hz, 1H), 3.11 (dd, *J* = 15.7, 10.5 Hz, 1H), 3.79 (s, 3H), 5.27 (t, *J* = 7.9 Hz, 2H), 5.91 (s, 1H), 5.96 (s, 1H), 6.49 (s, 1H), 6.59 (s, 1H), 6.82 (d, *J* = 8.5 Hz, 2H), 7.00 (t, *J* = 8.6 Hz, 2H), 7.04-7.11 (m, 4H), 7.18-7.22 (m, 2H), 7.22-7.30 (m, 5H), 7.38-7.45 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 20.6, 33.8, 45.4, 55.4, 82.8, 101.5, 104.7, 111.9, 113.9, 115.4 (d, *J* = 21.8 Hz), 117.7, 122.9, 124.7, 125.6, 125.8, 127.6, 127.7 (d, *J* = 3.7 Hz), 128.1 (d, *J* = 8.1 Hz), 128.2, 128.4, 129.1, 130.4, 130.6, 130.9, 137.1, 138.7, 142.0, 143.6, 146.8, 148.4, 151.4, 152.7, 158.0, 161.9 (d, *J* = 247.1 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -114.6; HRMS (ESI) m/z calcd for $C_{40}H_{31}FO_5$ $[M+H]^+$:611.2228, found:611.2229.



(5S,12S)-3-(4-fluorophenyl)-12-(4-methoxyphenyl)-5-phenyl-1-(thiophen-3-yl)-4,5-dihydro-12H-[1,3] dioxolo[4',5':4,5]benzo[1,2-b]furo[3,4-e]oxocine (5v)

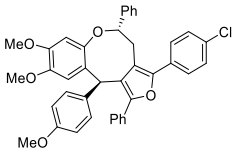
White solid, m.p. = 104-106 ℃; 27 mg, 22% yield; 96% ee; $[\alpha]_D^{20.0}$= 86.8 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =10.7 min, t (minor) =9.2 min]**;**^{1}H NMR (400 MHz, $CDCl_3$) δ 2.91 (dd, *J* = 15.8, 3.8 Hz, 1H), 3.05 (dd, *J* = 15.9, 11.2 Hz, 1H), 3.80 (s, 3H), 5.25 (dd, *J* = 11.2, 3.7 Hz, 1H), 5.49 (s, 1H), 5.94 (d, *J* = 1.4 Hz, 1H), 5.95 (d, *J* = 1.4 Hz, 1H), 6.23 (s, 1H), 6.79-6.90 (m, 3H), 7.06 (t, *J* = 8.7 Hz, 2H), 7.10 -7.20 (m, 4H),

7.23-7.31 (m, 4H), 7.35 (d, J = 2.1 Hz, 2H), 7.46 -7.54 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.2, 46.0, 55.3, 82.8, 101.5, 105.8, 111.3, 113.8, 115.6 (d, J = 21.7 Hz), 119.2, 121.7, 121.8, 125.9, 126.4, 126.6, 126.7, 127.4 (d, J = 3.0 Hz), 127.9, 128.3, 128.5, 128.7 (d, J = 8.0 Hz), 131.9, 136.8, 141.8, 143.9, 146.9, 147.1, 148.0, 151.1, 158.0, 160.9 (d, J = 247.5 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -114.0; HRMS (ESI) m/z calcd. for $C_{37}H_{27}FO_4S$ $[M+H]^+$: 603.1636, found: 603.1641.



(5S,12S)-3-(4-fluorophenyl)-12-(4-methoxybenzyl)-1,5-diphenyl-4,5-dihydro-12*H*-[1,3]dioxolo[4',5':4,5]benzo[1,2-*b*]furo[3,4-*e*]oxocine(5w)

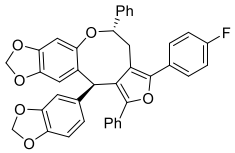
White solid, m.p. =138-139 °C; 48 mg, 39% yield; 90% ee; $[\alpha]_D^{20.0}$= 66.2(0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 6.5 min, t (minor) =5.7 min]**;** ^{1}H NMR (400 MHz,) δ 2.86 (dd, J = 16.0, 4.2 Hz, 1H), 3.08 (dd, J = 16.0, 11.2 Hz, 1H), 3.79 (s, 3H), 5.22 (dd, J = 11.1, 4.1 Hz, 1H), 5.56 (s, 1H), 5.94 (d, J = 1.4 Hz, 1H), 5.97 (d, J = 1.4 Hz, 1H), 6.36 (s, 1H), 6.80-6.86 (m, 3H), 7.03-7.07 (m, 2H), 7.10 (d, J = 8.4 Hz, 2H), 7.22-7.25 (m, 2H), 7.27-7.30 (m, 1H),7.31-7.43 (m, 5H), 7.51-7.58 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 32.8, 45.6, 55.4, 82.2, 101.6, 105.2, 111.7, 113.8, 119.1, 122.0, 125.5, 126.7, 127.4, 127.5, 127.6, 127.8, 128.1, 128.5, 128.6, 128.7, 131.1, 131.2, 133.5, 137.0, 140.7, 143.9, 147.0, 149.5, 150.6, 152.0, 158.0; HRMS (ESI) m/z calcd for $C_{39}H_{29}ClO_5$ $[M+H]^+$:613.1776, found: 613.1781.



(5*S*,11*S*)-3-(4-chlorophenyl)-8,9-dimethoxy-11-(4-methoxyphenyl)-1,5-diphenyl-4,5-dihydro-11*H*-benzo[*b*]furo[3,4-*e*]oxocine (5x)

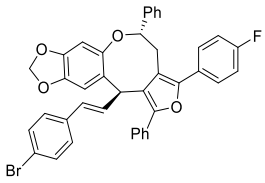
White solid, m.p. =91-93 °C; 50 mg, 40% yield; 86% ee; $[\alpha]_D^{20.0}$=135.6 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 80/20, v = 1.0

mL•min^{-1}, λ = 254 nm, t (major) = 5.8 min, t (minor) =6.5 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.84 (dd, J = 16.0, 4.2 Hz, 1H), 3.10 (dd, J = 16.0, 11.2 Hz, 1H), 3.73 (s, 3H), 3.80 (s, 3H), 3.89 (s, 3H), 5.32 (dd, J = 11.2, 4.1 Hz, 1H), 5.59 (s, 1H), 6.40 (s, 1H), 6.81-6.88 (m, 3H), 7.09-7.16 (m, 4H), 7.24-7.35 (m, 6H), 7.40 (t, J = 7.4 Hz, 2H), 7.44-7.49 (m, 2H), 7.54-7.58 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.2, 45.4, 55.4, 55.9, 56.6, 82.5, 107.6, 113.9, 115.6, 119.9, 122.4, 123.6, 126.2, 127.6, 127.7, 127.8, 128.0, 128.1, 128.5, 128.6, 128.7, 129.7, 131.0, 133.0, 137.1, 142.4, 145.1, 148.3, 148.4, 150.9, 151.5, 158.1; HRMS (ESI) m/z calcd for $C_{40}H_{33}ClO_5$ $[M+H]^+$:629.2089, found: 629.2093.



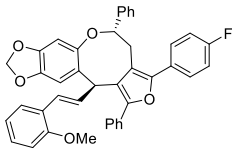
(5*S*,12*S*)-12-(benzo[*d*][1,3]dioxol-5-yl)-3-(4-fluorophenyl)-1,5-diphenyl-4,5-dihydro-12*H*-[1,3]dioxolo[4',5':4,5]benzo[1,2-*b*]furo[3,4-*e*]oxocine (5y)

White solid, m.p. =84-86 ℃; 51 mg, 42% yield; 95% ee; $[\alpha]_D^{20.0}$= 203.2 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 6.9 min, t (minor) =6.4 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.91 (dd, J = 15.9, 4.1 Hz, 1H), 3.09 (dd, J = 15.9, 11.1 Hz, 1H), 5.30 (dd, J = 11.1, 4.0 Hz, 1H), 5.50 (s, 1H), 5.92 (d, J = 1.4 Hz, 1H), 5.94 (d, J = 1.3 Hz, 1H), 5.95 (d, J = 1.4 Hz, 1H), 5.97 (d, J = 1.4 Hz, 1H), 6.37 (s, 1H), 6.66 (s, 1H), 6.69 (s, 1H), 6.73 (d, J = 8.1 Hz, 1H), 6.79 (s, 1H), 7.05 (t, J = 8.7 Hz, 2H), 7.14-7.19 (m, 2H), 7.25 (d, J = 3.4 Hz, 1H), 7.25-7.30 (m, 1H), 7.20-7.35 (m, 2H), 7.41 (t, J = 7.6 Hz, 2H), 7.47-7.52 (m, 2H), 7.52-7.57 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 32.5, 46.1, 82.8, 101.1, 101.6, 105.4, 108.0 (d, J = 10.5 Hz), 111.6, 115.6 (d, J = 21.7 Hz), 119.1, 120.3, 121.9, 125.4, 126.2, 127.3, 127.4 (d, J = 3.0 Hz), 127.8, 127.9, 128.5, 128.6, 128.7, 128.8, 140.0, 139.1, 142.0, 143.9, 145.9, 147.1, 147.9, 148.7, 150.6, 151.9, 162.1 (d, J = 247.6 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -113.6; HRMS (ESI) m/z calcd for $C_{39}H_{27}FO_6$ $[M+H]^+$:611.1864, found: 611.1859.



(5S,12S)-12-((*E*)-4-bromostyryl)-3-(4-fluorophenyl)-1,5-diphenyl-4,5-dihydro-12*H*-[1,3]dioxolo[4',5':4,5]benzo[1,2-*b*]furo[3,4-*e*]oxocine (5z)

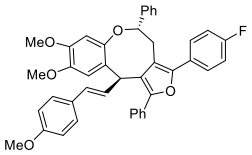
White solid, m.p. =88-89 ℃; 52 mg, 39% yield; 92% ee; $[\alpha]_D^{20.0}$= 288.5 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 9.8 min, t (minor) = 9.3 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.19 (br, 2H), 5.14 (br, 1H), 5.44 (br, 1H), 5.93 (d, *J* = 1.4 Hz, 1H), 5.94 (d, *J* = 1.4 Hz, 1H), 6.28-6.36 (m, 1H), 6.41 (s, 1H), 6.59-6.66 (m, 1H), 6.81 (s, 1H), 7.05 (t, *J* = 8.7 Hz, 2H), 7.11-7.18 (m, 1H), 7.30-7.36 (m, 4H), 7.36-7.42 (m, 4H), 7.43-7.49 (m, 5H), 7.60-7.64 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.7, 44.1, 83.7, 101.6, 105.3, 110.2, 115.6 (d, *J* = 21.8 Hz), 118.8, 121.1, 121.6, 126.1, 126.4, 127.3 (d, *J* = 3.3 Hz), 127.8, 127.9, 128.1, 128.3, 128.6 (d, *J* = 17.3 Hz), 128.7, 129.1, 129.4, 130.7, 131.2, 131.4, 131.7, 136.2, 142.1, 144.2, 146.9, 148.7, 151.5, 162.1 (d, *J* = 247.8 Hz); HRMS (ESI) m/z calcd for $C_{40}H_{28}BrFO_4$ $[M+H]^+$: 671.1205, found: 671.1200.



(5S,12S)-3-(4-fluorophenyl)-12-((*E*)-2-methoxystyryl)-1,5-diphenyl-4,5-dihydro-12*H*-[1,3]dioxolo[4',5':4,5]benzo[1,2-*b*]furo[3,4-*e*]oxocine (5a')

White solid, m.p. =89-90 ℃; 50 mg, 40% yield; 90% ee; $[\alpha]_D^{20.0}$= 207.4 (0.1, CH_2Cl_2); [Daicel Chiralpak IA-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 6.2 min, t (minor) =6.5 min]**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.10-3.32 (m, 2H), 3.77 (s, 3H), 5.14 (br, 1H), 5.61 (br, 1H), 5.92 (s, 1H), 5.95 (s, 1H), 6.45 (s, 1H), 6.52-6.61 (m, 1H), 6.66-6.77 (m, 1H), 6.82-6.90 (m, 3H), 7.05 (t, *J* = 8.7 Hz, 2H), 7.21 (d, *J* = 7.5 Hz, 1H), 7.27-7.39 (m, 7H), 7.41-7.49 (m, 4H), 7.62 (d, *J* = 3.2 Hz, 2H);^{13}C NMR (100 MHz, $CDCl_3$) δ 29.8, 33.0, 55.4, 83.8, 100.0, 101.5, 105.0, 110.7, 115.5 (d, *J* = 21.8 Hz), 119.2, 120.7, 125.1, 125.9, 126.0 (d, *J* = 2.7

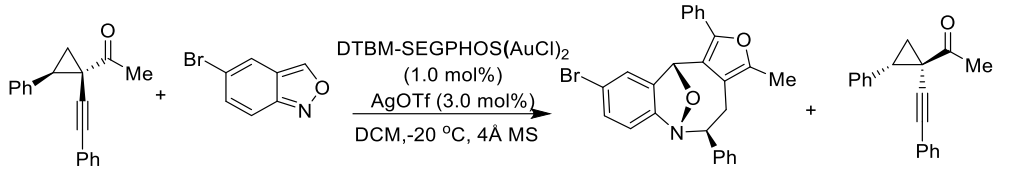
Hz), 126.6, 127.0, 127.4, 127.5, 127.8, 127.9, 128.0, 128.1, 128.4, 128.5, 128.6, 128.7, 128.9 (d, *J* = 11.2 Hz), 131.0, 142.6, 144.1, 146.7, 148.5, 152.3, 156.6, 162.0 (d, *J* = 247.4 Hz); HRMS (ESI) m/z calcd for $C_{41}H_{31}FO_5$ $[M+H]^+$:623.2228, found: 623.2225.



(5*S*,11*S*)-3-(4-fluorophenyl)-8,9-dimethoxy-11-((*E*)-4-methoxystyryl)-1,5-diphenyl-4,5-dihydro-11*H*-benzo[*b*]furo[3,4-*e*]oxocine (5b')

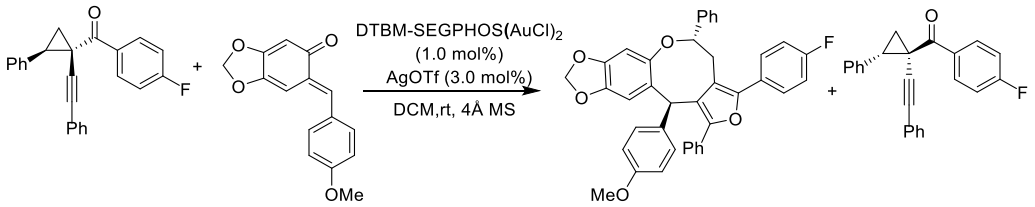
White solid, m.p. =90-91 ℃; 53 mg, 42% yield; 95% ee; $[\alpha]_D^{20.0}$= 227.7 (0.1, CH_2Cl_2); [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 80/20, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) = 7.3 min, t (minor) =8.1 min]**;** ^{1}H NMR (400 MHz) δ 3.13-3.24 (m, 2H), 3.73 (s, 3H), 3.79 (s, 3H), 3.88 (s, 3H), 5.13 (s, 1H), 5.60 (s, 1H), 6.32 (d, *J* = 16.1 Hz, 1H), 6.40 (s, 1H), 6.52 (dd, *J* = 16.0, 4.4 Hz, 1H), 6.78-6.86 (m, 3H), 7.03 (t, *J* = 8.7 Hz, 2H), 7.26-7.40 (m, 7H), 7.23-7.48 (m, 5H), 7.62-7.66 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 44.0, 55.4, 56.0, 56.4, 83.4, 107.6, 114.0, 114.1, 115.5 (d, *J* = 21.6 Hz), 118.8, 122.2, 124.8, 126.3, 127.4, 127.5, 127.6, 127.7, 127.8, 127.9, 128.5, 128.6, 128.7, 129.0, 130.1, 131.2, 132.3, 142.4, 145.4, 148.2, 148.6, 149.7, 150.7, 159.1, 162.0 (d, *J* = 247.1 Hz); HRMS (ESI) m/z calcd for $C_{42}H_{35}FO_5$ $[M+H]^+$:639.2541, found: 639.2546.

4. Large-scale reaction and synthetic transformations



rac-1a, 5 mmol **2a,** 3.5 mmol **3a,** 38% yield, 90% ee, **0.87 g** **asy-1a,** 46% yield 85% ee, **0.60 g**

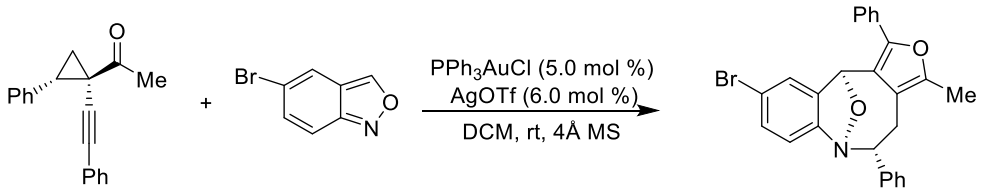
To a dried tube was added (*S*)-DTBM-SEGPHOS(AuCl)$_2$ (1.0 mol%) and AgOTf (3.0 mol%) in the glove box, and the DCM (10.0 mL) was added. The mixture was stirred at room temperature for 10 min. Then the precipitate was removed and the remaining solution was transferred into a solution of cyclopropyl ketone **1a** (5.0 mmol, 1.0 equiv.) and anthranils **2a** (3.5 mmol, 0.7 equiv.) with 4 Å molecular sieves 10.0 g in DCM (40 mL) at -20 °C. The reaction was then stirred at -20°C for 24 h. After the reaction was complete as monitored by TLC and HPLC analysis, it was filtered through a short pad of silica gel to remove catalyst rapidly. Then the solvent was removed under reduced pressure, and the residue was purified by a silica gel column using ethyl acetate/ petroleum ether (1/60-1/10) as the eluent to give aim product **3a** as white solid (0.87 g) with 38% yield and 90% ee and chiral **1a** (0.6 g) as yellow oil with 46% yield and 85% ee. [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =5.7 min, t (minor) =6.4 min]**.**



rac-1t, 5.0 mmol **4a,** 3.2 mmol **5h**, 37% yield 95% ee, **1.1 g** **asy-1t**, 41% yield 97% ee, **0.7 g**

To a dried tube was added (*S*)-DTBM-SEGPHOS(AuCl)$_2$ (1.0 mol%) and AgOTf (3.0 mol%) in the glove box, and the DCM (10.0 mL) was added. The mixture was stirred at room temperature for 10 min. Then the precipitate was removed and the remaining solution was transferred into a solution of cyclopropyl ketone **1t** (5.0 mmol, 1.0 equiv.) and *ortho*-quinone methides **4a** (3.2 mmol, 0.65 equiv.) with 4 Å molecular sieves 10.0

g in DCM (10 mL) at room temperature. The reaction was then stirred at room temperature for 8 h. After the reaction was complete as monitored by TLC and HPLC analysis, it was filtered through a short pad of silica gel to remove catalyst rapidly. Then the solvent was removed under reduced pressure, and the residue was purified by a silica gel column using ethyl acetate/ petroleum ether (1/60-1/10) as the eluent to give aim product **5h** as white solid (1.1 g) with 37% yield and 95% ee and chiral **1t** (0.7 g) as yellow oil with 41% yield and 97% ee. [Daicel Chiralpak IB-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =8.0 min, t (minor) =7.2 min]**.**

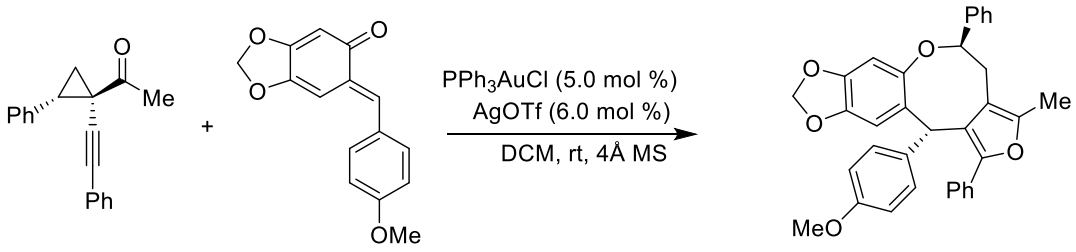


asy-1a
93% ee

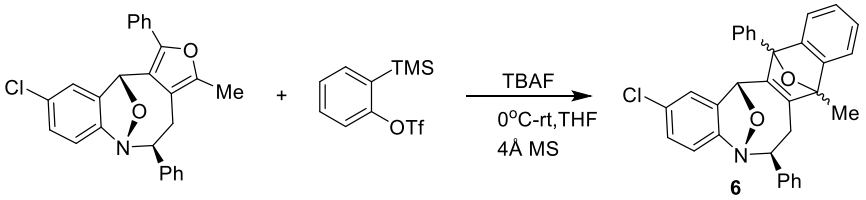
2a

3a',83% ee
82% yield

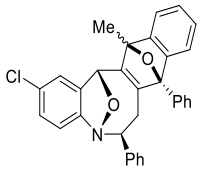
To a dried tube was added PPh_3AuCl (5.0 mol%) and AgOTf (6.0 mol%) in the glove box, and the DCM (0.5 mL) was added. The mixture was stirred at room temperature for 10 min. Then the precipitate was removed and the remaining solution was transferred into a solution of chiral cyclopropyl ketone **1a** (0.2 mmol, 1.0 equiv.) and anthranils **2a** (0.22 mmol, 1.1 equiv.) with 4 Å molecular sieves 300 mg in DCM (1.5 mL) at room temperature. The reaction was stirred at room temperature. The reaction was monitored by TLC. Then the solvent was removed under reduced pressure, and the residue was purified by a silica gel column using ethyl acetate/ petroleum ether (1/60-1/10) as the eluent to give aim product **3a'**as white solid with 82% yield and 83% ee [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/tetrahydrofuran= 90/10, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =7.1 min, t (minor) =6.4 min]**.**



To a dried tube was added PPh_3AuCl (5.0 mol%) and AgOTf (6.0 mol%) in the glove box, and the DCM (0.5 mL) was added. The mixture was stirred at room temperature for 10 min. Then the precipitate was removed and the remaining solution was transferred into a solution of chiral cyclopropyl ketone **1a** (0.2 mmol, 1.0 equiv.) and anthranils **2a** (0.3 mmol, 1.5 equiv.) with 4 Å molecular sieves 300 mg in DCM (1.5 mL) at room temperature. The reaction was stirred at room temperature. After the reaction was complete as monitored by TLC, the solvent was removed under reduced pressure, and the residue was purified by a silica gel column using ethyl acetate/ petroleum ether (1/60-1/10) as the eluent to give aim product **5a'**as white solid with 74% yield and 86% ee [Daicel Chiralpak IC-3 (0.45 cm × 25 cm), *n*-hexane/2-propanol = 97/3, v = 1.0 mL•min^{-1}, λ = 254 nm, t (major) =6.3 min, t (minor) =7.1 min]**.**

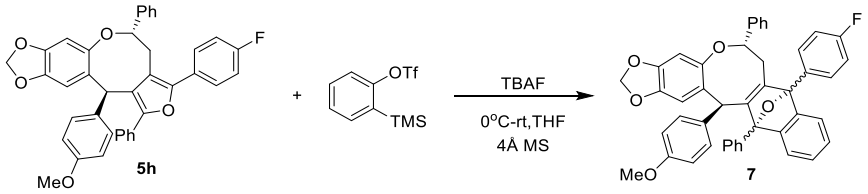


TBAF (0.4 mL, 1 mol/L in THF) was slowly added dropwise to a stirred solution of 4 Å MS (120 mg), chiral product (0.1 mmol) and the triflate (0.3 mmol) in dry THF (1.0 mL) at 0 ºC under nitrogen. Then the mixture was stirred at room temperature for 2 h, the solution was quenched with saturated ammonium chloride and extracted with ethyl acetate. The combined organic phase was dried over Na_2SO_4 and concentrated in vacuum. The residue was purified by flash chromatography on silica gel with EA/PE=1/30 to afford aim product as white solid (62% yield, 1.5:1 dr).



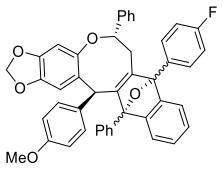
(5R,6S,8S,14R)-2-chloro-13-methyl-6,8-diphenyl-7,8,13,14-tetrahydro-6H-5,14:8,13-diepoxybenzo[b]naphtho[2,3-e] azocine (6)

White solid, m.p. = 124-126 ℃; 30 mg, 62% yield; $[\alpha]_D^{20.0}$ = 69.2 (0.1, CH_2Cl_2);^{1}H NMR (400 MHz, $CDCl_3$) δ 1.87 (s, 2H), 1.94 (s, 3H), 2.03 (dd, *J* = 17.4, 5.7 Hz, 1H), 2.71 (d, *J* = 17.3 Hz, 1H), 3.14 (ddd, *J* = 17.2, 11.9, 3.2 Hz, 2H), 4.46 (t, *J* = 4.9 Hz, 1H), 5.57 (d, *J* = 8.7 Hz, 1H), 5.63 (dd, *J* = 6.0, 3.0 Hz, 1H), 5.75 -5.95 (m, 3H), 6.53 (d, *J* = 2.5 Hz, 1H), 6.65-6.71 (m, 2H), 6.76- 6.81 (m, 3H), 6.84 -6.94 (m, 2H), 6.95-7.03 (m, 3H), 7.06 (dd, *J* = 5.5, 3.6 Hz, 2H), 7.21 (d, *J* = 7.1 Hz, 1H), 7.26 - 7.30 (m, 2H), 7.31 -7.38 (m, 4H), 7.40 (t, *J* = 7.5 Hz, 2H), 7.46 -7.52 (m, 1H), 7.51-7.61 (m, 6H), 7.76-7.85 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.3, 13.9, 29.5, 29.9, 71.9, 72.3, 79.5, 87.3, 89.3, 89.7, 91.6, 92.4, 113.9, 115.1, 118.2, 118.4, 120.4, 120.6, 120.8, 121.0, 121.1, 123.6, 124.3, 124.7, 124.9, 125.1, 126.6, 127.0, 127.6, 127.7, 127.8, 128.0, 128.1, 128.3, 128.6, 128.7, 128.8, 128.9, 129.0, 129.2, 129.3, 129.5, 129.6, 131.0, 133.9, 134.1, 134.2, 140.8, 141.1, 141.8, 142.6, 147.6, 147.7, 148.7, 149.4, 151.2, 151.3, 151.7, 151.7, 152.4; HRMS (ESI) m/z calcd. for $C_{32}H_{24}ClNO_2$ $[M+H]^+$: 490.1568, found: 490.1567.



TBAF (0.4 mL, 1 mol/L in THF) was slowly added dropwise to a stirred solution of 4 Å MS (120 mg), chiral product (0.1 mmol) and the triflate (0.3 mmol) in dry THF (1.0 mL) at 0 ºC under nitrogen. Then the mixture was stirred at room temperature for 6 h, the solution was quenched with saturated ammonium chloride and extracted with ethyl acetate. The combined organic phase was dried over Na_2SO_4 and concentrated in

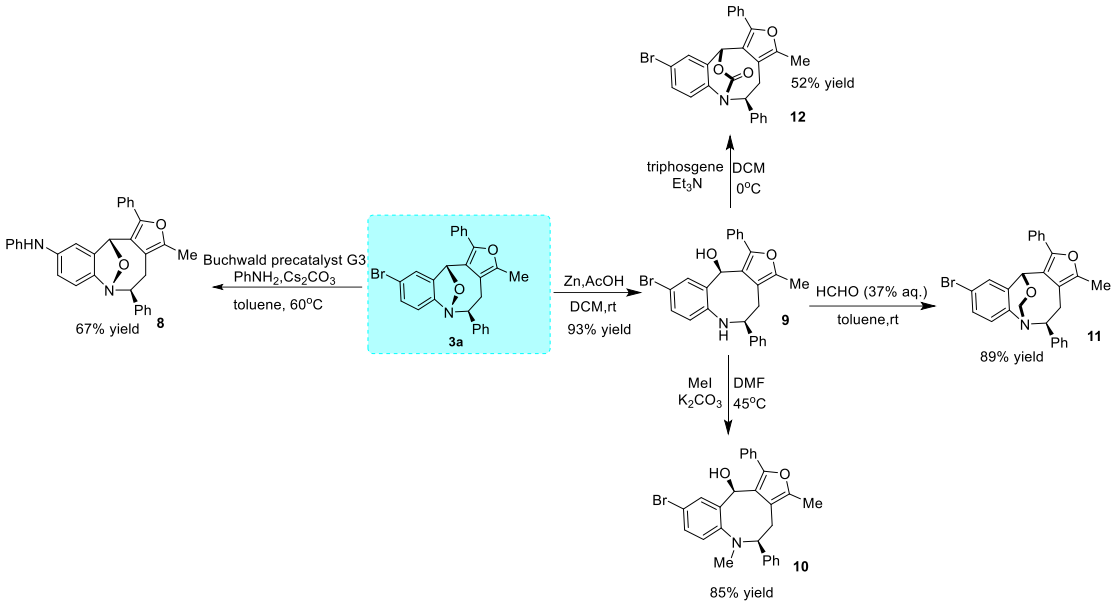
vacuum. The residue was purified by flash chromatography on silica gel with EA/PE=1/20 to afford aim product as white solid (72% yield, 1.5:1 dr).

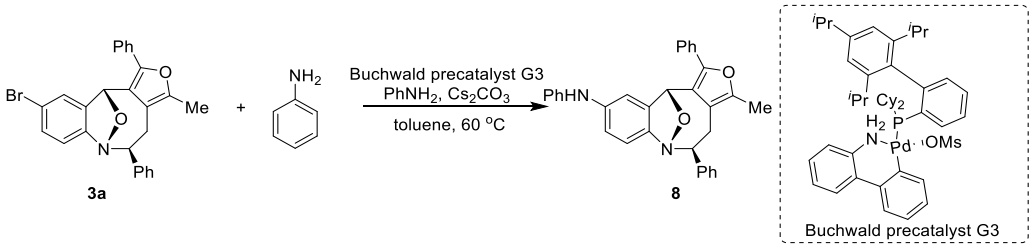


(6S,14S)-8-(4-fluorophenyl)-14-(4-methoxyphenyl)-6,13-diphenyl-7,8,13,14-tetrahydro-6H-8,13-epoxy[1,3]dioxolo[4',5':4,5]benzo[1,2-b]naphtho[2,3-e]oxocine (7)

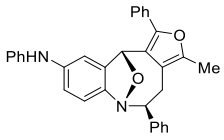
White solid, m.p. =96-98 ℃; 48.3 mg, 72% yield; 1:1.5 dr**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.39 (dd, *J* = 16.4, 11.7 Hz, 1H), 2.55 (dd, *J* = 16.4, 3.5 Hz, 1H), 2.76 (dd, *J* = 8.3, 6.3 Hz, 1H), 3.73 (s, 3H), 3.79 (s, 1.5H), 4.65 (s, 0.5H), 4.79-4.83 (m, 0.5H), 4.84 (d, *J* = 3.8 Hz, 1H), 4.95 (d, *J* = 11.3 Hz, 1H), 5.75-5.83 (m, 3.5H), 5.89 (d, *J* = 1.4 Hz, 1H), 6.37 (s, 0.5H), 6.48 (d, *J* = 8.6 Hz, 1H), 6.57 (s, 1H), 6.61 (d, *J* = 8.7 Hz, 1H), 6.65-6.70 (m, 2H), 6.92 (t, *J* = 7.4 Hz, 1H), 6.95-7.01 (m, 3.5H), 7.02-7.14 (m, 5H), 7.16-7.22 (m, 6H), 7.27 (dd, *J* = 5.1, 2.4 Hz, 3.5H), 7.31-7.41 (m, 5.5H), 7.49 (dd, *J* = 6.7, 3.1 Hz, 1H), 7.53-7.57 (m, 1H), 7.73 (d, *J* = 7.6 Hz, 2H), 7.79-7.85 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.9, 32.3, 48.1, 49.9, 55.3, 55.4, 80.6, 81.7, 92.5, 93.5, 93.5, 94.0, 101.3, 105.3, 105.8, 109.4, 110.8, 113.3, 113.5, 115.4 (d, *J* = 21.4 Hz), 115.8 (d, *J* = 21.4 Hz), 118.8, 119.7, 120.2, 121.9, 123.1 (d, *J* =3.6 Hz), 124.4, 124.8, 124.8, 125.0, 126.5, 126.6, 126.7, 127.3, 127.7, 127.8, 127.9, 128.0, 128.1, 128.2, 128.3, 128.4, 128.5, 128.6, 128.9, 129.2 (d, *J* = 8.0 Hz), 130.6 (d, *J* = 8.2 Hz), 131.1 (d, *J* =3.6 Hz), 131.3, 131.9, 135.3, 135.4, 135.5, 137.1, 140.0, 141.3, 143.5, 144.0, 145.8, 146.5, 146.6, 147.6, 148.7, 149.7, 150.6, 150.9, 151.2, 151.8, 151.9, 153.8, 157.7, 158.3, 162.6 (d, *J* = 191.9 Hz), 163.3 (d, *J* = 176.8 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -114.1, -113.1; HRMS (ESI) m/z calcd for $C_{45}H_{33}FO_5$ $[M+H]^+$:673.2445, found: 673.2449.

Synthetic transformations of 3a:





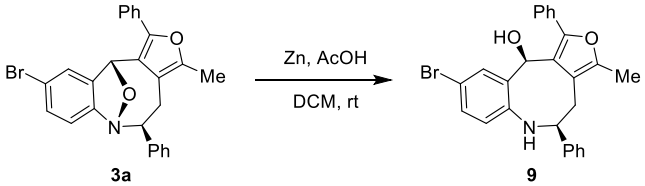
Under nitrogen atmosphere, a dried flask was added **3a** (46 mg, 0.1 mmol), aniline (19 mg, 0.2 mmol), palladium complex (9 mg, 10 mol%), cesium carbonate (39 mg, 0.12 mmol), and 1.0 mL degassed toluene. Then the mixture was stirred at 60 °C overnight. The solution was quenched with water and extracted with DCM. The combined organic phase was dried over Na_2SO_4 and concentrated in vacuum. The residue was purified by flash chromatography on silica gel with EA/PE=1/5 to afford aim product as yellow solid (31.4 mg, 67% yield).



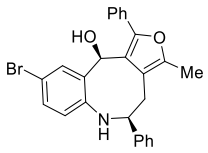
(5S,6R,11R)-3-methyl-N,1,5-triphenyl-4,5-dihydro-11H-6,11-epoxybenzo[b]furo-[3,4-e]azocin-9-amine (8)

Yellow solid, m.p. =102-104 °C; 31.4 mg, 67% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ

2.27 (s, 3H), 2.81 (dd, *J* = 16.1, 4.6 Hz, 1H), 2.99 (dd, *J* = 16.0, 2.9 Hz, 1H), 4.63 (dd, *J* = 5.0, 2.8 Hz, 1H), 5.69 (s, 1H), 6.22 (s, 1H), 6.90 (t, *J* = 7.3 Hz, 1H), 6.98 (d, *J* = 7.9 Hz, 2H), 7.07 (d, *J* = 3.3 Hz, 3H), 7.21-7.28 (m, 3H), 7.28-7.37 (m, 3H), 7.40 (t, *J* = 7.7 Hz, 2H), 7.53-7.62 (m, 4H); 13C NMR (101 MHz, CDCl3) δ 11.6, 25.5, 71.6, 77.9, 112.7, 114.4, 117.2, 118.8, 119.1, 120.8, 124.8, 126.0, 127.3, 127.7, 128.2, 128.4, 128.8, 129.5, 120.8, 136.5, 140.5, 140.8, 143.5, 143.7, 145.5, 147.3; HRMS (ESI) m/z calcd. for $C_{32}H_{26}N_2O_2$ $[M+H]^+$: 471.2067, found: 471.2065.



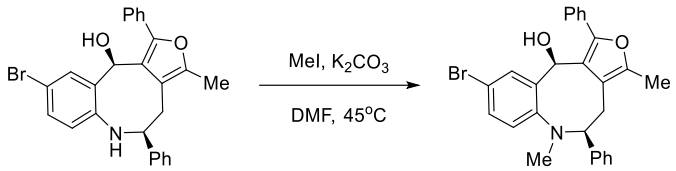
To a solution of **3a** (229 mg, 0.5 mmol) in dichloromethane (10 mL) was added zinc powder (975 mg, 15 mmol) followed by AcOH (150 mg, 2.5 mmol), and the reaction was stirred at room temperature for 3 h. Upon completion, the reaction mixture was filtered over celite bed. The filtrate was washed with saturated $NaHCO_3$ three times. The organic phase was washed by saturated NaCl, dried over anhydrous Na_2SO_4. Then the solvent was removed under reduced pressure to afford aim product as white solid (214 mg, 93% yield).



(5S,11R)-9-bromo-3-methyl-1,5-diphenyl-4,5,6,11-tetrahydrobenzo[b]furo[3,4-e] azocin-11-ol (9)

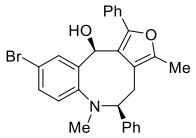
White solid, m.p. =108-110 ℃; 214 mg, 93% yield;^{1}H NMR (400 MHz, $CDCl_3$) δ 1.76 (s, 3H), 2.44 (d, *J* = 3.6 Hz, 2H), 4.47 (t, *J* = 3.7 Hz, 1H), 5.59 (s, 1H), 7.13 (d, *J* = 8.3 Hz, 1H), 7.23-7.33 (m, 5H), 7.32-7.37 (m, 2H), 7.42-7.52 (m, 3H), 7.89 (d, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.0, 29.4, 65.8, 69.8, 113.4, 119.2, 123.5, 126.6,

127.0, 127.5, 127.7, 128.5, 128.7, 129.0, 131.0, 132.0, 132.1, 141.6, 142.1, 144.7, 148.6, 149.4; HRMS (ESI) m/z calcd. for $C_{26}H_{22}BrNO_2$ $[M+H]^+$: 460.0907, found: 460.0910.



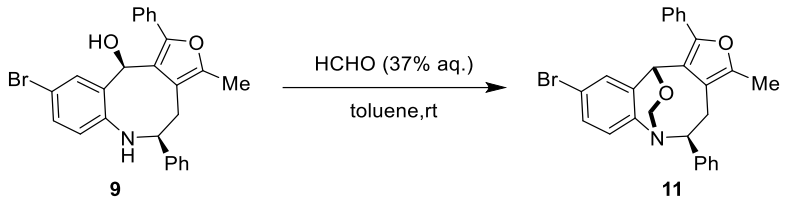
9 **10**

To a solution of product **9** (0.05 mmol, 23 mg) in DMF (0.5 mL) was added MeI (13 mg, 0.09 mmol) and K_2CO_3 (1.0 mmol, 14 mg), then the reaction mixture was stirred at 45 °C for 6 h. Upon completion, the organic phase was washed by water and aqueous layer was extracted with ethyl acetate. The combined organic phase was dried over Na_2SO_4 and concentrated in vacuum. Then the crude product was purified by silica gel column chromatography with PE/ EA= 10/1 to give product **10** as a white solid (20 mg, 85% yield).

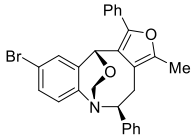


(5S,11R)-9-bromo-3,6-dimethyl-1,5-diphenyl-4,5,6,11-tetrahydrobenzo[b]furo [3,4-e] azocin-11-ol (10)

White solid, m.p. = 90-92 °C; 20 mg, 85% yield; $[\alpha]_D^{20.0}$= 129.8 (0.1, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.62 (s, 3H), 2.28 (d, *J* = 3.3 Hz, 2H), 2.65 (s, 3H), 3.94 (t, *J* = 3.5 Hz, 1H), 5.54 (d, *J* = 11.1 Hz, 1H), 6.87 (d, *J* = 11.2 Hz, 1H), 7.17-7.27 (m, 5H), 7.32-7.39 (m, 2H), 7.41 (d, *J* = 8.5 Hz, 1H), 7.46-7.56 (m, 3H), 7.90 -7.95 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 10.7, 30.8, 40.9, 69.6, 74.3, 113.8, 119.6, 123.5, 125.0, 126.6, 127.4, 127.5, 127.6, 128.4, 128.8, 131.1, 131.8, 131.9, 140.3, 142.2, 148.7, 149.1, 150.1; HRMS (ESI) m/z calcd. for $C_{27}H_{24}BrNO_2$ $[M+H]^+$: 474.1063, found: 474.1065.

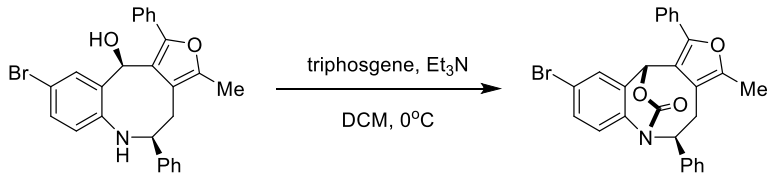


To a solution of product **9** (0.05 mmol, 23 mg) in toluene (1.0 mL) was added 37% formaldehyde solution (0.1 mL), then the reaction mixture was stirred at room temperature. Upon completion, water was added to the mixture and aqueous layer was extracted with ethyl acetate. The combined organic phase was dried over Na_2SO_4 and concentrated in vacuum. Then the crude product was purified by silica gel column chromatography with PE/ EA= 10/1 to give product **11** as a white solid (21 mg, 89% yield).



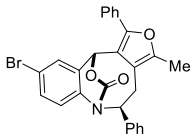
(5S,6R,11R)-9-bromo-3-methyl-1,5-diphenyl-4,5-dihydro-11H-11,6-(epoxymethano) benzo[b]furo[3,4-e] azocine (11)

White solid, m.p. = 122-124 ℃; 21 mg, 89% yield; $[\alpha]_D^{20.0}$= 92.8 (0.1, CH_2Cl_2);^{1}H NMR (400 MHz, $CDCl_3$) δ 2.24 (s, 3H), 3.05 (dd, *J* = 15.1, 3.3 Hz, 1H), 3.45 (dd, *J* = 15.5, 11.4 Hz, 1H), 4.44 (dd, *J* = 11.9, 3.3 Hz, 1H), 4.50 (d, *J* = 9.8 Hz, 1H), 5.00 (d, *J* = 9.8 Hz, 1H), 6.20 (s, 1H), 6.93 (d, *J* = 2.2 Hz, 1H), 7.01 (d, *J* = 8.3 Hz, 1H), 7.29 (dd, *J* = 8.3, 2.2 Hz, 1H), 7.32-7.40 (m, 2H), 7.46 (q, *J* = 7.4 Hz, 4H), 7.59 (dd, *J* = 7.2, 4.9 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.9, 30.4, 66.4, 68.7, 74.8, 115.6, 117.5, 126.1, 126.9, 127.0, 127.4, 127.5, 127.6, 127.9, 128.8, 128.9, 131.2, 131.3, 140.0, 143.0, 146.1, 147.6, 148.2; HRMS (ESI) m/z calcd. for $C_{27}H_{22}BrNO_2$ $[M+H]^+$: 472.0907, found: 472.0906.



9 12

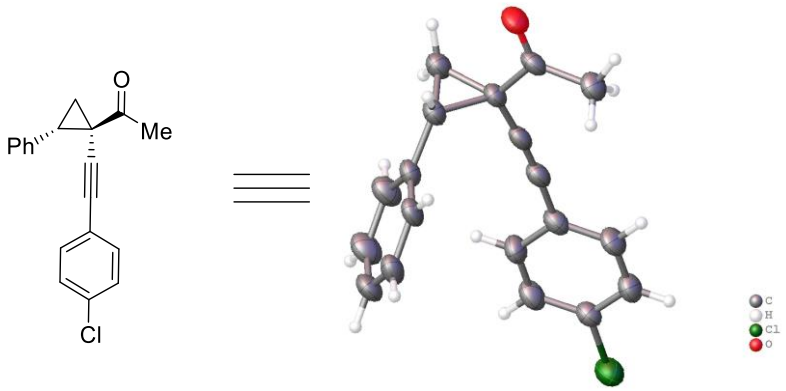
To a solution of product **9** (0.05 mmol, 23 mg) in DCM (1.0 mL) was added Et_3N (42 uL, 0.3 mmol) and the mixture was cooled to 0°C. Then to this solution was added a solution of triphosgene (15 mg, 0.05 mmol) dropwise over 10 min. The reaction mixture was stirred at 0 °C. Upon completion, the mixture was quenched with saturated ammonium chloride and the aqueous layer was extracted with DCM. The combined organic layers were washed with brine, dried over sodium sulfate, filtered, concentrated, and purified by silica gel column chromatography with PE/ EA=6/1 to give product **12** as a white solid (12.7 mg, 52% yield).



(5S,6R,11R)-9-bromo-3-methyl-1,5-diphenyl-4,5-dihydro-11H-11,6-(epoxymethano) benzo[b]furo[3,4-e]azocin-13-one (12)

White solid, m.p. = 92-94 °C; 12.7 mg, 52% yield; $[\alpha]_D^{20.0}$= 112.8 (0.1, CH_2Cl_2);^{1}H NMR (400 MHz, $CDCl_3$) δ 2.30 (s, 3H), 3.02 (dd, *J* = 16.0, 4.9 Hz, 1H), 3.43 (dd, *J* = 16.0, 8.9 Hz, 1H), 4.92 (dd, *J* = 8.9, 4.9 Hz, 1H), 6.17 (s, 1H), 7.15 (d, *J* = 8.4 Hz, 1H), 7.21 (d, *J* = 2.1 Hz, 1H), 7.36 (t, *J* = 7.3 Hz, 1H), 7.40-7.49 (m, 4H), 7.49-7.55 (m, 2H), 7.58 (dd, *J* = 8.3, 1.4 Hz, 2H), 7.66 (d, *J* = 7.4 Hz, 2H);^{13}C NMR (100 MHz, $CDCl_3$) δ 12.5, 31.0, 69.7, 74.0, 113.7, 118.5, 120.9, 123.3, 126.6, 127.7, 128.0, 128.4, 128.6, 129.0, 129.1, 130.0, 132.8, 136.0, 139.9, 142.2, 149.8, 151.1, 156.6; HRMS (ESI) m/z calcd. for $C_{27}H_{20}BrNO_3$ $[M+H]^+$: 486.0699, found: 486.0704.

5. X-ray crystallography data



1c CCDC **2301807**

Table 7 Crystal data and structure refinement for 1c.

Identification code	cu_230410D_0m
Empirical formula	$C_{19}H_{15}ClO$
Formula weight	294.76
Temperature/K	173.0
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	5.4676(8)
b/Å	10.7252(15)
c/Å	26.292(4)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1541.8(4)
Z	4
ρ_{calc}g/cm^3	1.270
μ/mm^{-1}	2.143
F(000)	616.0

Crystal size/mm^3	0.03 × 0.03 × 0.01
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	6.724 to 133.134
Index ranges	-6 ≤ h ≤ 6, -12 ≤ k ≤ 12, -30 ≤ l ≤ 31
Reflections collected	9671
Independent reflections	2702 [R_{int} = 0.0801, R_{sigma} = 0.0708]
Data/restraints/parameters	2702/0/191
Goodness-of-fit on F^2	1.013
Final R indexes [I>=2σ (I)]	R_1 = 0.0481, wR_2 = 0.1196
Final R indexes [all data]	R_1 = 0.0595, wR_2 = 0.1274
Largest diff. peak/hole / e Å^{-3}	0.23/-0.43
Flack parameter	0.057(18)

Table 8 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for cu_230410D_0m. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cl1	11179(2)	4699.8(10)	1572.1(4)	56.0(4)
O1	227(6)	8083(3)	4651.7(12)	57.0(9)
C1	6172(9)	5872(4)	2852.2(15)	42.5(10)
C2	2724(10)	3483(4)	3961.3(18)	55.9(12)
C3	7512(10)	4334(4)	2243.0(17)	50.6(11)
C4	1758(8)	6620(4)	4066.5(15)	41.5(10)
C5	5052(9)	4169(4)	4680.4(17)	46.1(10)
C6	-550(9)	5836(4)	4104.8(18)	50.7(11)
C7	7926(9)	6681(4)	2662.6(17)	50.7(11)
C8	4586(8)	6219(4)	3265.0(16)	43.5(10)

C9	4308(11)	2482(4)	3905.6(19)	63.3(14)
C10	3303(8)	6440(3)	3624.4(16)	41.8(10)
C11	9485(9)	6332(4)	2271.7(17)	50.7(11)
C12	1518(8)	5465(4)	4433.2(16)	44.0(10)
C13	3865(9)	8712(4)	4229.7(16)	49.9(11)
C14	1807(9)	7841(4)	4338.8(16)	44.6(10)
C15	6634(9)	3174(4)	4621.4(18)	54.7(12)
C16	5978(9)	4687(4)	2635.1(16)	48.8(10)
C17	6257(10)	2326(4)	4231.7(18)	58.1(12)
C18	3094(8)	4343(4)	4349.7(15)	42.2(10)
C19	9253(8)	5148(4)	2065.7(15)	43.3(10)

Table 9 Anisotropic Displacement Parameters ($Å^2×10^3$) for cu_230410D_0m.

The Anisotropic displacement factor exponent takes the form: -

$2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	61.6(8)	41.3(6)	65.2(6)	-2.0(5)	12.8(5)	6.6(5)
O1	61(2)	31.5(16)	78(2)	-5.6(14)	19.0(17)	6.5(14)
C1	50(3)	27(2)	51(2)	-1.1(17)	-3(2)	6(2)
C2	61(3)	33(2)	73(3)	-7(2)	-9(2)	4(2)
C3	61(3)	27(2)	63(3)	-5.8(19)	-1(2)	0(2)
C4	41(3)	22.4(19)	61(2)	-0.7(17)	3.2(18)	3.1(16)
C5	51(3)	21.8(19)	66(3)	0.3(18)	-3(2)	-2.9(18)
C6	45(3)	31(2)	76(3)	1(2)	0(2)	2(2)
C7	56(3)	26(2)	70(3)	-9.8(19)	4(2)	-1(2)
C8	44(3)	25(2)	62(2)	-0.5(17)	-2(2)	4.7(18)
C9	75(4)	35(3)	79(3)	-12(2)	-1(3)	5(2)

C10	43(3)	20.2(18)	62(2)	0.0(17)	-4(2)	3.6(17)
C11	54(3)	29(2)	69(3)	-2.2(19)	3(2)	-4(2)
C12	45(3)	26(2)	60(2)	2.1(17)	2.7(19)	1.7(19)
C13	54(3)	31(2)	66(2)	-6.7(19)	2(2)	-2(2)
C14	49(3)	25(2)	60(2)	-0.1(17)	0(2)	9.8(18)
C15	51(3)	29(2)	84(3)	7(2)	-4(2)	-4(2)
C16	54(3)	27(2)	66(2)	-1.2(19)	9(2)	-4(2)
C17	58(3)	26(2)	91(3)	2(2)	4(3)	7(2)
C18	45(3)	22.8(19)	59(2)	2.2(16)	3.3(19)	-1.7(17)
C19	46(3)	29(2)	54(2)	-0.5(17)	2.1(18)	5.2(19)

Table 10 Bond Lengths for cu_230410D_0m.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C19	1.739(4)	C4	C14	1.493(5)
O1	C14	1.221(5)	C5	C15	1.383(6)
C1	C7	1.386(6)	C5	C18	1.392(6)
C1	C8	1.439(6)	C6	C12	1.477(6)
C1	C16	1.397(5)	C7	C11	1.387(6)
C2	C9	1.388(7)	C8	C10	1.200(6)
C2	C18	1.391(6)	C9	C17	1.378(7)
C3	C16	1.382(6)	C11	C19	1.386(6)
C3	C19	1.373(6)	C12	C18	1.496(5)
C4	C6	1.520(6)	C13	C14	1.490(6)
C4	C10	1.450(6)	C15	C17	1.385(7)
C4	C12	1.575(5)			

Table 11 Bond Angles for cu_230410D_0m.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C7	C1	C8	121.7(4)	C19	C11	C7	118.7(4)
C7	C1	C16	118.4(4)	C6	C12	C4	59.6(3)
C16	C1	C8	119.9(4)	C6	C12	C18	124.8(4)
C9	C2	C18	120.0(5)	C18	C12	C4	119.7(3)
C19	C3	C16	120.0(4)	O1	C14	C4	119.8(4)
C6	C4	C12	57.0(3)	O1	C14	C13	122.0(4)
C10	C4	C6	117.6(4)	C13	C14	C4	118.1(4)
C10	C4	C12	115.8(3)	C5	C15	C17	119.8(5)
C10	C4	C14	119.4(4)	C3	C16	C1	120.5(4)
C14	C4	C6	117.9(4)	C9	C17	C15	119.7(4)
C14	C4	C12	113.4(3)	C2	C18	C5	118.8(4)
C15	C5	C18	121.0(4)	C2	C18	C12	123.9(4)
C12	C6	C4	63.4(3)	C5	C18	C12	117.3(4)
C1	C7	C11	121.5(4)	C3	C19	Cl1	119.8(3)
C10	C8	C1	175.8(4)	C3	C19	C11	120.9(4)
C17	C9	C2	120.7(4)	C11	C19	Cl1	119.3(3)
C8	C10	C4	176.2(4)				

Table 12 Torsion Angles for cu_230410D_0m.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C1	C7	C11	C19	0.6(7)	C10	C4	C6	C12	104.2(4)
C2	C9	C17	C15	0.3(8)	C10	C4	C12	C6	-107.4(4)
C4	C6	C12	C18	-106.9(4)	C10	C4	C12	C18	7.9(6)
C4	C12	C18	C2	-74.6(5)	C10	C4	C14	O1	167.1(4)

C4 C12 C18 C5	104.7(4)	C10 C4 C14 C13	-15.1(6)
C5 C15 C17 C9	0.0(7)	C12 C4 C14 O1	-50.9(5)
C6 C4 C12 C18	115.4(4)	C12 C4 C14 C13	126.9(4)
C6 C4 C14 O1	12.8(6)	C14 C4 C6 C12	-101.1(4)
C6 C4 C14 C13	-169.3(4)	C14 C4 C12 C6	109.1(4)
C6 C12 C18 C2	-2.8(7)	C14 C4 C12 C18	-135.5(4)
C6 C12 C18 C5	176.5(4)	C15 C5 C18 C2	1.0(6)
C7 C1 C16 C3	0.4(6)	C15 C5 C18 C12	-178.3(4)
C7 C11 C19 Cl1	179.5(3)	C16 C1 C7 C11	-0.8(7)
C7 C11 C19 C3	0.2(7)	C16 C3 C19 Cl1	-180.0(4)
C8 C1 C7 C11	178.6(4)	C16 C3 C19 C11	-0.6(7)
C8 C1 C16 C3	-179.1(4)	C18 C2 C9 C17	0.0(8)
C9 C2 C18 C5	-0.7(7)	C18 C5 C15 C17	-0.7(6)
C9 C2 C18 C12	178.7(4)	C19 C3 C16 C1	0.3(7)

Table 13 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for cu_230410D_0m.

Atom	***x***	***y***	***z***	**U(eq)**
H2	1386.45	3581.78	3734.13	67
H3	7362.72	3528.12	2096.21	61
H5	5305.52	4743.29	4950.58	55
H6A	-1989.14	6217.37	4271.79	61
H6B	-947.25	5286.64	3813.54	61
H7	8062.74	7493.57	2803.7	61
H9	4045.95	1897.55	3639.57	76
H11	10688.64	6893.98	2147.39	61

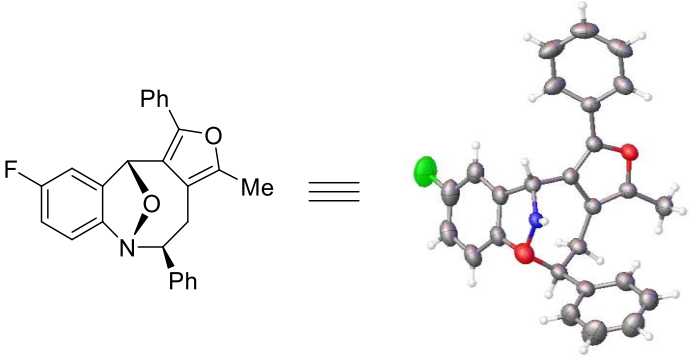
H12	1301.29	5693.66	4799.16	53
H13A	3587.26	9502.2	4407.52	75
H13B	3957.32	8864.42	3862.66	75
H13C	5402.94	8341.32	4346.99	75
H15	7974.87	3071.4	4847.43	66
H16	4781.26	4119.52	2757.94	59
H17	7337.71	1639.66	4189.53	70

Experimental

Single crystals of $C_{19}H_{15}ClO$ were from hexane. A suitable crystal was selected and on a diffractometer. The crystal was kept at 173.0 K during data collection. Using Olex2 [1], the structure was solved with the Unknown [2] structure solution program using Unknown and refined with the Unknown [3] refinement package using Unknown minimisation.

Crystal structure determination of [cu_230410D_0m]

Crystal Data for $C_{19}H_{15}ClO$ (M =294.76 g/mol): orthorhombic, space group $P2_12_12_1$ (no. 19), a = 5.4676(8) Å, b = 10.7252(15) Å, c = 26.292(4) Å, V = 1541.8(4) Å^3, Z = 4, T = 173.0 K, μ(CuKα) = 2.143 mm^{-1}, $Dcalc$ = 1.270 g/cm^3, 9671 reflections measured (6.724° ≤ 2Θ ≤ 133.134°), 2702 unique (R_{int} = 0.0801, R_{sigma} = 0.0708) which were used in all calculations. The final R_1 was 0.0481 (I > 2σ(I)) and wR_2 was 0.1274 (all data).



4c

CCDC **2301808**

Table 14 Crystal data and structure refinement for CCDC 2301808.

Identification code	cu_220601G_0m
Empirical formula	$C_{26}H_{20}FNO_2$
Formula weight	397.43
Temperature/K	293
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	7.228(2)
b/Å	10.686(3)
c/Å	25.745(7)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1988.6(10)
Z	4
ρ_{calc}g/cm^3	1.327
μ/mm^{-1}	0.730
F(000)	832.0
Crystal size/mm^3	0.05 × 0.03 × 0.02
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	12.72 to 134.086
Index ranges	$-8 \leq h \leq 8$, $-10 \leq k \leq 12$, $-30 \leq l \leq 30$
Reflections collected	13101
Independent reflections	3440 [R_{int} = 0.0249, R_{sigma} = 0.0210]
Data/restraints/parameters	3440/24/272
Goodness-of-fit on F^2	1.062
Final R indexes [I>=2σ (I)]	R_1 = 0.0299, wR_2 = 0.0786

Final R indexes [all data]	R_1 = 0.0303, wR_2 = 0.0790
Largest diff. peak/hole / e Å^{-3}	0.12/-0.13
Flack parameter	0.03(4)

Table 15 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for cu_220601G_0m. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
F1	7902(3)	2315.5(15)	4403.5(6)	87.0(5)
O1	5952.0(16)	4541.6(11)	7050.7(4)	38.2(3)
C1	7376(2)	4949.1(16)	6300.8(6)	35.0(4)
C4	10556(3)	3021(2)	7813.4(9)	58.9(6)
C6	11796(4)	2332(2)	7530.7(11)	66.7(7)
C8	4693(2)	6193.7(18)	5843.0(6)	38.0(4)
C10	7765(3)	3452(2)	4640.7(9)	60.3(6)
C12	5562(2)	5513.1(16)	6291.1(6)	35.1(4)
C14	5317(3)	8597.9(19)	6397.3(7)	47.2(4)
C16	7544(2)	4362.7(16)	6769.2(6)	35.9(4)
C18	5456(3)	9728(2)	6657.3(8)	55.8(5)
C20	5809(2)	7256.5(18)	5589.0(6)	38.8(4)
C22	6305(4)	10722(2)	6429.7(10)	65.1(6)
C24	6019(2)	8442.4(18)	5902.2(7)	40.6(4)
C26	6855(3)	5590(2)	4596.1(7)	53.8(5)
C13	8324(2)	4739.5(19)	5361.7(7)	42.3(4)
C7	8457(3)	3566(2)	5135.8(8)	51.6(5)
C15	4774(2)	5252.3(16)	6752.5(7)	36.2(4)
C2	6869(3)	9474(2)	5675.0(9)	60.9(6)

C17	11658(4)	2297(2)	6996.2(11)	70.2(7)
C9	8998(2)	3648.4(16)	7027.3(7)	39.0(4)
C19	10251(3)	2935(2)	6747.7(9)	54.7(5)
C5	7574(3)	5730.8(19)	5090.3(7)	43.1(4)
C21	6959(3)	4420(3)	4371.5(8)	61.9(6)
C11	3016(3)	5632(2)	7003.9(8)	48.3(5)
C23	7001(4)	10594(2)	5937.6(12)	75.5(7)
C3	9163(3)	3678(2)	7567.4(7)	47.5(4)
O2	8898.6(17)	6557.3(12)	5812.3(4)	40.8(3)
N1	7649(2)	6868.3(15)	5382.7(5)	41.2(4)
C25	8813(2)	5209.0(18)	5896.4(6)	39.1(4)

Table 16 Anisotropic Displacement Parameters ($Å^2×10^3$) for cu_220601G_0m. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F1	105.4(12)	76.6(10)	79.0(9)	-34.8(8)	6.4(9)	-11.9(9)
O1	37.5(6)	41.9(7)	35.1(5)	7.6(5)	1.0(5)	-2.0(5)
C1	32.8(8)	40.0(9)	32.3(7)	0.0(7)	-2.2(6)	1.1(7)
C4	57.0(12)	65.6(14)	54.2(11)	23.7(10)	-17.7(10)	-10.7(11)
C6	66.3(14)	48.7(12)	85.2(16)	12.2(12)	-32.1(13)	6.6(11)
C8	31.3(8)	46.5(9)	36.1(8)	4.8(7)	-3.7(6)	-0.8(7)
C10	62.9(13)	64.5(14)	53.6(11)	-19.2(11)	10.5(11)	-14.0(11)
C12	30.8(8)	38.7(9)	35.6(7)	4.0(7)	-1.7(6)	-2.4(7)
C14	53.2(11)	47.8(11)	40.7(9)	6.1(8)	-1.5(8)	-3.5(9)
C16	36.1(8)	37.0(9)	34.5(8)	1.3(7)	-2.2(7)	-1.2(7)
C18	57.8(12)	60.6(13)	49.2(10)	-4.9(9)	-1.5(9)	-1.4(11)

C20	35.7(8)	48.1(10)	32.8(8)	8.1(7)	-2.3(7)	1.2(8)
C22	59.1(13)	54.3(13)	81.9(16)	-12.1(12)	3.0(12)	-7.2(11)
C24	34.9(8)	45.3(10)	41.7(8)	9.7(7)	-2.2(7)	2.5(7)
C26	53.4(11)	73.7(14)	34.4(9)	2.8(9)	2.1(9)	-4.3(11)
C13	38.3(8)	52.4(11)	36.1(8)	-0.6(8)	6.5(7)	-2.4(8)
C7	51.5(11)	52.6(12)	50.8(10)	-2.3(9)	10.8(9)	-3.1(9)
C15	32.6(8)	36.0(9)	39.9(8)	4.2(7)	-1.2(7)	-2.3(7)
C2	62.1(13)	55.4(13)	65.1(13)	7.6(11)	22.2(11)	-6.7(11)
C17	70.3(15)	53.5(13)	86.8(16)	-14.5(12)	-26.1(13)	26.1(12)
C9	39.7(8)	34.0(9)	43.2(9)	3.7(7)	-7.5(7)	-3.7(7)
C19	61.3(12)	47.6(11)	55.2(11)	-9.9(9)	-15.6(10)	14.6(10)
C5	41.4(9)	54.1(11)	33.8(8)	2.0(8)	5.9(7)	-3.5(9)
C21	59.7(13)	87.5(17)	38.6(10)	-11.7(11)	1.7(10)	-13.6(13)
C11	38.2(9)	56.6(12)	50.1(10)	7.8(9)	9.1(8)	0.1(8)
C23	74.6(16)	50.1(13)	101.9(19)	4.6(13)	24.4(15)	-17.4(12)
C3	42.5(9)	57.8(11)	42.3(9)	11.7(9)	-3.3(8)	-6.5(9)
O2	36.1(6)	47.5(7)	38.8(6)	2.8(5)	-1.9(5)	-3.0(5)
N1	41.2(8)	50.7(9)	31.8(7)	5.0(6)	0.7(6)	0.0(7)
C25	32.8(8)	46.4(10)	38.0(8)	3.0(7)	-0.2(7)	1.7(7)

Table 17 Bond Lengths for cu_220601G_0m.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
F1	C10	1.363(3)	C20	C24	1.510(3)
O1	C16	1.373(2)	C20	N1	1.491(2)
O1	C15	1.375(2)	C22	C23	1.370(4)
C1	C12	1.443(2)	C24	C2	1.391(3)

C1	C16	1.364(2)	C26	C5	1.383(3)
C1	C25	1.497(2)	C26	C21	1.380(4)
C4	C6	1.369(4)	C13	C7	1.386(3)
C4	C3	1.381(3)	C13	C5	1.380(3)
C6	C17	1.380(4)	C13	C25	1.507(2)
C8	C12	1.502(2)	C15	C11	1.483(3)
C8	C20	1.539(3)	C2	C23	1.378(4)
C10	C7	1.374(3)	C17	C19	1.381(3)
C10	C21	1.375(4)	C9	C19	1.385(3)
C12	C15	1.346(2)	C9	C3	1.396(3)
C14	C18	1.385(3)	C5	N1	1.431(3)
C14	C24	1.382(3)	O2	N1	1.4664(19)
C16	C9	1.459(2)	O2	C25	1.458(2)
C18	C22	1.359(3)			

Table 18 Bond Angles for cu_220601G_0m.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C16	O1	C15	107.50(12)	C7	C13	C25	131.94(18)
C12	C1	C25	122.75(15)	C5	C13	C7	120.62(18)
C16	C1	C12	106.74(15)	C5	C13	C25	107.41(17)
C16	C1	C25	129.66(16)	C10	C7	C13	116.4(2)
C6	C4	C3	120.4(2)	O1	C15	C11	115.97(14)
C4	C6	C17	119.8(2)	C12	C15	O1	110.20(15)
C12	C8	C20	117.70(14)	C12	C15	C11	133.69(16)
F1	C10	C7	117.9(2)	C23	C2	C24	120.8(2)
F1	C10	C21	118.4(2)	C6	C17	C19	120.1(2)

C7	C10	C21	123.7(2)	C19	C9	C16	121.47(16)
C1	C12	C8	126.56(15)	C19	C9	C3	118.32(18)
C15	C12	C1	106.40(15)	C3	C9	C16	120.21(17)
C15	C12	C8	126.96(16)	C17	C19	C9	120.8(2)
C24	C14	C18	121.61(19)	C26	C5	N1	126.19(19)
O1	C16	C9	115.85(14)	C13	C5	C26	122.0(2)
C1	C16	O1	109.15(15)	C13	C5	N1	111.78(15)
C1	C16	C9	134.98(16)	C10	C21	C26	119.58(19)
C22	C18	C14	120.4(2)	C22	C23	C2	121.0(2)
C24	C20	C8	116.45(14)	C4	C3	C9	120.5(2)
N1	C20	C8	114.43(15)	C25	O2	N1	108.05(13)
N1	C20	C24	109.50(15)	C5	N1	C20	112.97(14)
C18	C22	C23	119.1(2)	C5	N1	O2	103.15(13)
C14	C24	C20	123.81(17)	O2	N1	C20	110.12(12)
C14	C24	C2	117.04(19)	C1	C25	C13	114.24(15)
C2	C24	C20	119.03(17)	O2	C25	C1	108.42(14)
C21	C26	C5	117.6(2)	O2	C25	C13	101.72(14)

Table 19 Torsion Angles for cu_220601G_0m.

A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
F1	C10	C7	C13	178.92(19)	C24	C14	C18	C22	-0.4(3)
F1	C10	C21	C26	-178.0(2)	C24	C20	N1	C5	178.62(14)
O1	C16	C9	C19	150.92(18)	C24	C20	N1	O2	63.89(17)
O1	C16	C9	C3	-29.5(2)	C24	C2	C23	C22	0.2(4)
C1	C12	C15	O1	-1.1(2)	C26	C5	N1	C20	73.8(2)
C1	C12	C15	C11	174.4(2)	C26	C5	N1	O2	-167.37(18)

C1	C16	C9	C19	-31.0(3)	C13	C5	N1	C20	-106.20(17)
C1	C16	C9	C3	148.6(2)	C13	C5	N1	O2	12.66(18)
C4	C6	C17	C19	-1.3(4)	C7	C10	C21	C26	1.6(4)
C6	C4	C3	C9	0.0(3)	C7	C13	C5	C26	2.9(3)
C6	C17	C19	C9	2.1(4)	C7	C13	C5	N1	-177.11(16)
C8	C12	C15	O1	175.84(16)	C7	C13	C25	C1	-81.3(2)
C8	C12	C15	C11	-8.7(3)	C7	C13	C25	O2	162.09(19)
C8	C20	C24	C14	1.7(3)	C15	O1	C16	C1	-0.05(19)
C8	C20	C24	C2	-174.28(18)	C15	O1	C16	C9	178.54(15)
C8	C20	N1	C5	45.79(18)	C19	C9	C3	C4	0.7(3)
C8	C20	N1	O2	-68.95(17)	C5	C26	C21	C10	-0.3(3)
C12	C1	C16	O1	-0.61(19)	C5	C13	C7	C10	-1.6(3)
C12	C1	C16	C9	-178.8(2)	C5	C13	C25	C1	96.56(19)
C12	C1	C25	C13	-66.0(2)	C5	C13	C25	O2	-20.01(18)
C12	C1	C25	O2	46.7(2)	C21	C10	C7	C13	-0.6(3)
C12	C8	C20	C24	-71.4(2)	C21	C26	C5	C13	-1.9(3)
C12	C8	C20	N1	58.1(2)	C21	C26	C5	N1	178.11(19)
C14	C18	C22	C23	0.8(4)	C3	C4	C6	C17	0.3(4)
C14	C24	C2	C23	0.2(4)	C3	C9	C19	C17	-1.8(3)
C16	O1	C15	C12	0.75(19)	N1	C20	C24	C14	-130.04(18)
C16	O1	C15	C11	-175.63(15)	N1	C20	C24	C2	53.9(2)
C16	C1	C12	C8	-175.91(17)	N1	O2	C25	C1	-92.62(14)
C16	C1	C12	C15	1.05(19)	N1	O2	C25	C13	28.12(16)
C16	C1	C25	C13	126.1(2)	C25	C1	C12	C8	13.7(3)
C16	C1	C25	O2	-121.3(2)	C25	C1	C12	C15	-169.31(16)
C16	C9	C19	C17	177.9(2)	C25	C1	C16	O1	168.85(16)
C16	C9	C3	C4	-178.89(18)	C25	C1	C16	C9	-9.4(3)

C18	C14	C24	C20	-176.27(18)	C25	C13	C7	C10	176.08(19)
C18	C14	C24	C2	-0.2(3)	C25	C13	C5	C26	-175.27(17)
C18	C22	C23	C2	-0.7(4)	C25	C13	C5	N1	4.7(2)
C20	C8	C12	C1	-52.0(3)	C25	O2	N1	C20	94.99(15)
C20	C8	C12	C15	131.61(19)	C25	O2	N1	C5	-25.83(16)
C20	C24	C2	C23	176.5(2)					

Table 20 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for cu_220601G_0m.

Atom	***x***	***y***	***z***	**U(eq)**
H4	10652.9	3046.78	8173.48	71
H6	12727.92	1888.61	7698.4	80
H8A	3526.66	6540.58	5961.43	46
H8B	4407.88	5582.76	5576.06	46
H14	4737.36	7926.87	6559.83	57
H18	4964.71	9808.31	6989.55	67
H20	5089.47	7500.2	5282.54	47
H22	6412.25	11478.11	6605.8	78
H26	6320.87	6260.77	4421.24	65
H7	8984.88	2892.24	5309.68	62
H2	7354.16	9407.08	5341.59	73
H17	12513.13	1842.65	6803.04	84
H19	10143.41	2885.01	6388.37	66
H21	6485.88	4286.75	4040.13	74
H11A	3259.19	6272.04	7256.52	72
H11B	2468.9	4921.05	7172.36	72

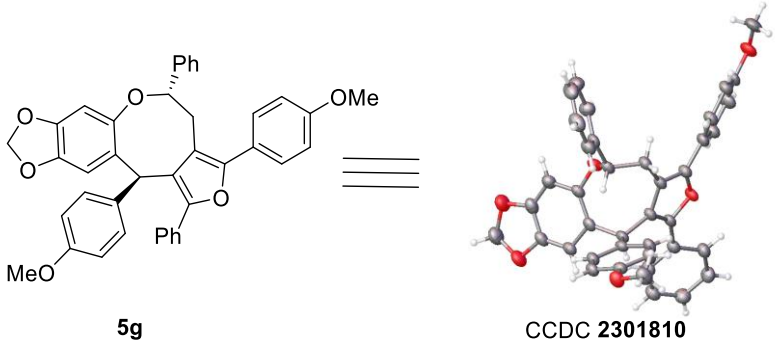
H11C	2180.15	5949.06	6745.6	72
H23	7570.42	11273.91	5778.39	91
H3	8328.18	4143.13	7763.08	57
H25	10020.87	4885.43	6005.48	47

Experimental

Single crystals of $C_{26}H_{20}FNO_2$ were from ether. A suitable crystal was selected and on a diffractometer. The crystal was kept at 293 K during data collection. Using Olex2 [1], the structure was solved with the Unknown [2] structure solution program using Unknown and refined with the Unknown [3] refinement package using Unknown minimization.

Crystal structure determination of [cu_220601G_0m]

Crystal Data for $C_{26}H_{20}FNO_2$ (*M* =397.43 g/mol): orthorhombic, space group $P2_12_12_1$ (no. 19), *a* = 7.228(2) Å, *b* = 10.686(3) Å, *c* = 25.745(7) Å, *V* = 1988.6(10) $Å^3$, *Z* = 4, *T* = 293 K, μ(CuKα) = 0.730 mm^{-1}, *Dcalc* = 1.327 g/cm^3, 13101 reflections measured (12.72° ≤ 2Θ ≤ 134.086°), 3440 unique (R_{int} = 0.0249, R_{sigma} = 0.0210) which were used in all calculations. The final R_1 was 0.0299 (I > 2σ(I)) and wR_2 was 0.0790 (all data).



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CCDC **2301810**

Table 21 Crystal data and structure refinement for CCDC 2301810.

Identification code	220225A_auto
Empirical formula	$C_{40}H_{32}O_6$

Formula weight	608.65
Temperature/K	173(2)
Crystal system	triclinic
Space group	P-1
a/Å	12.1952(3)
b/Å	12.2266(3)
c/Å	12.7568(4)
α/°	78.461(2)
β/°	62.446(3)
γ/°	64.147(3)
Volume/Å^3	1517.57(9)
Z	2
ρ_{calc}g/cm^3	1.332
μ/mm^{-1}	0.717
F(000)	640.0
Crystal size/mm^3	0.07 × 0.06 × 0.05
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.818 to 134.136
Index ranges	-14 ≤ h ≤ 14, -14 ≤ k ≤ 14, -15 ≤ l ≤ 15
Reflections collected	41062
Independent reflections	5401 [R_{int} = 0.0970, R_{sigma} = 0.0489]
Data/restraints/parameters	5401/0/417
Goodness-of-fit on F^2	1.055
Final R indexes [I>=2σ (I)]	R_1 = 0.0496, wR_2 = 0.1226
Final R indexes [all data]	R_1 = 0.0611, wR_2 = 0.1296
Largest diff. peak/hole / e Å^{-3}	0.32/-0.26

Table 22 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 220225A_auto. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	6333.1(12)	4859.7(10)	3390.6(12)	34.0(3)
O2	4737.1(16)	10152.7(12)	1411.2(14)	48.4(4)
O3	8969.7(15)	-1199.7(12)	586.2(14)	48.7(4)
O4	5190.1(12)	3468.1(11)	1231.4(12)	35.4(3)
O5	8645.4(16)	-110.8(13)	-1029.3(13)	51.9(4)
O6	772.5(13)	1503.5(12)	6504.1(12)	40.4(3)
C1	6566.5(18)	3644.5(15)	3545.6(16)	30.9(4)
C2	5982(2)	8177.4(18)	1794(2)	47.3(5)
C3	7794.0(19)	598.5(17)	-22.5(18)	39.2(5)
C4	7727.4(17)	2916.9(16)	3808.6(16)	30.5(4)
C5	3765(2)	7582.6(16)	2875.6(18)	37.8(4)
C6	6292.5(17)	1663.4(15)	2207.4(17)	31.1(4)
C7	3622(2)	8755.8(17)	2438.5(18)	38.8(4)
C8	5621.5(17)	3447.3(15)	3405.0(16)	29.5(4)
C9	3522(2)	11048.3(18)	1393(2)	54.2(6)
C10	4258.5(18)	2096.0(15)	4257.8(16)	29.8(4)
C11	3291.8(19)	2868.8(16)	5196.3(18)	36.6(4)
C12	3830.9(17)	3862.8(15)	2133.8(17)	31.4(4)
C13	6831.9(19)	1751.4(17)	89.4(18)	37.7(4)
C14	4755.6(18)	4607.7(15)	3140.2(17)	31.1(4)
C15	9977(2)	1603.5(19)	4302.2(19)	42.7(5)
C16	5004.1(19)	6696.6(16)	2757.2(17)	33.9(4)
C17	-309(2)	2355(2)	7409(2)	48.5(5)
C18	4042.4(18)	1105.6(16)	4120.4(17)	32.0(4)

C19	9489(2)	-1207(2)	-662(2)	51.3(6)
C20	5242.8(18)	5432.1(16)	3127.2(17)	32.5(4)
C21	2099(2)	2723.1(17)	5967.8(18)	38.1(4)
C22	2880.0(19)	935.5(16)	4884.9(17)	33.7(4)
C23	4740(2)	9046.3(16)	1887.1(18)	38.5(5)
C24	3616.8(18)	4880.0(16)	2831.3(18)	33.4(4)
C25	9284(2)	2833.5(19)	4531.4(19)	41.4(5)
C26	6076.4(18)	2277.5(15)	1220.5(17)	32.0(4)
C27	9562.3(19)	1025.9(18)	3819.0(19)	40.2(5)
C28	5606.6(18)	2203.7(15)	3451.0(16)	29.8(4)
C29	1641(2)	4161.3(17)	2162(2)	40.2(5)
C30	2845.4(18)	4324.8(15)	1583.7(17)	33.0(4)
C31	3084(2)	4967.0(19)	534(2)	43.7(5)
C32	8172.7(19)	3488.6(17)	4293.2(18)	37.0(4)
C33	6116(2)	7026.2(18)	2212(2)	43.7(5)
C34	7266.7(18)	457.5(16)	2039.2(18)	33.4(4)
C35	694(2)	4646(2)	1701(2)	51.7(6)
C36	7989.8(18)	-35.8(16)	934.0(18)	36.2(4)
C37	2142(2)	5452(2)	72(2)	52.2(6)
C38	8456.5(18)	1676.9(16)	3569.3(18)	35.7(4)
C39	944(2)	5299(2)	656(2)	54.8(6)
C40	1891.6(18)	1751.5(16)	5802.6(17)	32.0(4)

Table 23 Anisotropic Displacement Parameters ($Å^2×10^3$) for 220225A_auto. The Anisotropic displacement factor exponent takes the form: -$2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	38.2(7)	22.1(6)	51.2(8)	4.1(5)	-24.4(6)	-15.9(5)

O2	64.1(9)	25.8(7)	65.4(10)	12.5(6)	-33.2(8)	-25.4(7)
O3	47.5(8)	29.2(7)	54.3(9)	-6.6(6)	-15.9(7)	-5.9(6)
O4	35.6(7)	24.3(6)	42.3(7)	7.0(5)	-15.2(6)	-12.8(5)
O5	55.0(9)	38.6(8)	45.5(9)	-7.8(7)	-11.6(7)	-11.6(7)
O6	36.1(7)	37.7(7)	46.7(8)	-0.2(6)	-11.2(6)	-20.9(6)
C1	37.3(9)	20.2(8)	38.4(10)	3.4(7)	-16.7(8)	-14.9(7)
C2	48.8(12)	35.0(11)	70.3(15)	11.8(10)	-29.2(11)	-27.8(10)
C3	38.3(10)	33.3(10)	43.2(11)	-3.0(9)	-10.0(9)	-18.6(8)
C4	30.7(9)	27.0(9)	36.1(10)	3.5(7)	-13.9(8)	-15.2(7)
C5	39.3(10)	27.5(9)	49.8(12)	2.8(8)	-18.9(9)	-17.2(8)
C6	31.7(9)	24.0(8)	41.6(10)	1.1(8)	-14.8(8)	-15.8(7)
C7	42.0(10)	26.0(9)	48.9(12)	0.7(8)	-21.0(9)	-12.5(8)
C8	31.6(9)	21.8(8)	38.2(10)	2.2(7)	-15.0(8)	-14.0(7)
C9	68.3(15)	23.7(10)	68.0(15)	9.8(10)	-31.5(13)	-17.5(10)
C10	35.3(9)	22.6(8)	37.3(10)	7.1(7)	-19.5(8)	-15.0(7)
C11	42.2(10)	25.6(9)	46.3(11)	-0.3(8)	-17.6(9)	-18.2(8)
C12	32.9(9)	22.2(8)	39.4(10)	4.1(7)	-14.2(8)	-14.2(7)
C13	41.9(10)	31.6(10)	40.4(11)	5.0(8)	-16.1(9)	-18.7(8)
C14	32.6(9)	21.3(8)	41.7(10)	1.6(7)	-15.8(8)	-13.3(7)
C15	36.2(10)	42.8(11)	53.0(13)	4.0(9)	-23.8(9)	-15.3(9)
C16	41.9(10)	23.5(9)	43.4(11)	2.0(8)	-20.2(9)	-17.5(8)
C17	39.2(11)	44.8(12)	50.9(13)	-1.4(10)	-7.6(10)	-19.4(9)
C18	34.8(9)	23.6(8)	41.0(10)	0.9(7)	-18.0(8)	-12.7(7)
C19	46.2(12)	40.7(12)	54.0(14)	-10.7(10)	-13.7(10)	-10.0(10)
C20	34.9(9)	23.8(8)	43.7(11)	3.6(8)	-19.6(8)	-14.0(7)
C21	39.8(10)	28.1(9)	42.5(11)	-3.9(8)	-11.5(9)	-14.9(8)
C22	39.2(10)	25.8(9)	44.2(11)	3.5(8)	-20.8(9)	-17.7(8)

C23	55.5(12)	23.6(9)	46.6(11)	4.8(8)	-25.7(10)	-22.0(9)
C24	34.8(9)	23.6(8)	45.1(11)	1.6(8)	-19.3(8)	-12.6(7)
C25	42.6(11)	43.6(11)	50.4(12)	0.3(9)	-24.6(10)	-22.5(9)
C26	32.9(9)	22.9(8)	42.6(11)	4.0(8)	-16.2(8)	-14.6(7)
C27	36.1(10)	30.5(10)	53.5(12)	0.6(9)	-20.0(9)	-11.8(8)
C28	33.9(9)	19.9(8)	39.4(10)	4.3(7)	-17.8(8)	-13.4(7)
C29	41.7(11)	31.9(10)	53.1(12)	3.6(9)	-21.2(9)	-20.1(8)
C30	37.3(10)	21.8(8)	45.1(11)	0.1(8)	-19.2(8)	-14.4(7)
C31	46.9(11)	43.4(11)	50.7(12)	9.1(10)	-25.5(10)	-24.8(10)
C32	40.4(10)	30.5(9)	45.8(11)	0.0(8)	-19.7(9)	-17.2(8)
C33	42.8(11)	31.1(10)	65.5(14)	7.1(9)	-28.0(10)	-19.2(9)
C34	35.3(9)	24.6(9)	44.7(11)	4.5(8)	-19.2(8)	-15.1(7)
C35	43.4(11)	42.6(12)	81.3(17)	-1.6(12)	-31.7(12)	-21.0(10)
C36	32.8(9)	24.2(9)	49.4(12)	-1.5(8)	-14.8(9)	-11.6(7)
C37	63.9(14)	49.0(13)	57.5(14)	12.1(11)	-38.6(12)	-25.3(11)
C38	34.6(9)	29.5(9)	48.3(11)	-0.6(8)	-19.0(9)	-15.3(8)
C39	58.7(14)	44.7(12)	80.6(17)	-3.0(12)	-47.3(13)	-16.6(11)
C40	33.2(9)	28.1(9)	38.4(10)	7.6(8)	-18.1(8)	-15.4(7)

Table 24 Bond Lengths for 220225A_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C1	1.376(2)	C8	C28	1.518(2)
O1	C20	1.371(2)	C10	C11	1.375(3)
O2	C9	1.415(3)	C10	C18	1.404(2)
O2	C23	1.367(2)	C10	C28	1.533(2)
O3	C19	1.416(3)	C11	C21	1.395(3)
O3	C36	1.389(2)	C12	C24	1.533(2)
O4	C12	1.437(2)	C12	C30	1.512(3)

O4	C26	1.382(2)	C13	C26	1.403(3)
O5	C3	1.381(2)	C14	C20	1.370(2)
O5	C19	1.437(3)	C14	C24	1.499(3)
O6	C17	1.425(2)	C15	C25	1.379(3)
O6	C40	1.370(2)	C15	C27	1.382(3)
C1	C4	1.459(3)	C16	C20	1.463(2)
C1	C8	1.367(2)	C16	C33	1.406(3)
C2	C23	1.385(3)	C18	C22	1.379(3)
C2	C33	1.368(3)	C21	C40	1.390(3)
C3	C13	1.366(3)	C22	C40	1.390(3)
C3	C36	1.370(3)	C25	C32	1.381(3)
C4	C32	1.407(3)	C27	C38	1.383(3)
C4	C38	1.393(2)	C29	C30	1.392(3)
C5	C7	1.397(3)	C29	C35	1.387(3)
C5	C16	1.380(3)	C30	C31	1.383(3)
C6	C26	1.405(3)	C31	C37	1.383(3)
C6	C28	1.537(3)	C34	C36	1.362(3)
C6	C34	1.412(2)	C35	C39	1.385(4)
C7	C23	1.383(3)	C37	C39	1.378(3)
C8	C14	1.440(2)			

Table 25 Bond Angles for 220225A_auto.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C20	O1	C1	107.74(13)	C33	C16	C20	117.94(17)
C23	O2	C9	117.77(16)	C22	C18	C10	120.89(17)
C36	O3	C19	105.39(16)	O3	C19	O5	108.66(16)
C26	O4	C12	119.60(13)	O1	C20	C16	113.76(14)
C3	O5	C19	104.90(16)	C14	C20	O1	109.75(15)

C40	O6	C17	117.90(14)	C14	C20	C16	135.86(18)
O1	C1	C4	113.55(14)	C40	C21	C11	119.19(17)
C8	C1	O1	109.44(15)	C18	C22	C40	120.41(16)
C8	C1	C4	137.01(16)	O2	C23	C2	115.09(17)
C33	C2	C23	120.41(18)	O2	C23	C7	125.27(19)
C13	C3	O5	128.1(2)	C7	C23	C2	119.64(17)
C13	C3	C36	121.58(19)	C14	C24	C12	113.82(15)
C36	C3	O5	110.30(17)	C15	C25	C32	120.58(18)
C32	C4	C1	119.18(16)	O4	C26	C6	124.60(16)
C38	C4	C1	123.26(16)	O4	C26	C13	113.04(16)
C38	C4	C32	117.53(17)	C13	C26	C6	122.21(17)
C16	C5	C7	121.47(17)	C15	C27	C38	120.23(18)
C26	C6	C28	125.85(16)	C8	C28	C6	111.57(14)
C26	C6	C34	117.57(17)	C8	C28	C10	115.84(14)
C34	C6	C28	116.52(17)	C10	C28	C6	114.71(14)
C23	C7	C5	119.54(18)	C35	C29	C30	120.6(2)
C1	C8	C14	106.73(14)	C29	C30	C12	120.15(17)
C1	C8	C28	124.15(16)	C31	C30	C12	121.18(16)
C14	C8	C28	129.01(16)	C31	C30	C29	118.59(18)
C11	C10	C18	117.87(16)	C37	C31	C30	120.97(19)
C11	C10	C28	122.34(15)	C25	C32	C4	120.78(18)
C18	C10	C28	119.47(15)	C2	C33	C16	121.28(19)
C10	C11	C21	122.04(16)	C36	C34	C6	119.23(18)
O4	C12	C24	107.28(13)	C39	C35	C29	119.9(2)
O4	C12	C30	110.37(15)	C3	C36	O3	109.73(18)
C30	C12	C24	110.41(14)	C34	C36	O3	128.23(19)
C3	C13	C26	117.30(19)	C34	C36	C3	122.02(17)

C8	C14	C24	128.21(15)	C39	C37	C31	120.1(2)
C20	C14	C8	106.32(16)	C27	C38	C4	121.30(17)
C20	C14	C24	125.28(16)	C37	C39	C35	119.8(2)
C25	C15	C27	119.57(19)	O6	C40	C21	124.77(17)
C5	C16	C20	124.41(16)	O6	C40	C22	115.68(15)
C5	C16	C33	117.61(17)	C22	C40	C21	119.53(16)

Table 26 Torsion Angles for 220225A_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C1	C4	C32	22.8(2)	C16	C5	C7	C23	-0.8(3)
O1	C1	C4	C38	-155.11(17)	C17	O6	C40	C21	5.6(3)
O1	C1	C8	C14	0.4(2)	C17	O6	C40	C22	-175.93(18)
O1	C1	C8	C28	176.75(16)	C18	C10	C11	C21	-2.8(3)
O4	C12	C24	C14	-44.8(2)	C18	C10	C28	C6	30.7(2)
O4	C12	C30	C29	146.42(16)	C18	C10	C28	C8	162.91(17)
O4	C12	C30	C31	-36.8(2)	C18	C22	C40	O6	179.47(17)
O5	C3	C13	C26	179.10(17)	C18	C22	C40	C21	-1.9(3)
O5	C3	C36	O3	-1.0(2)	C19	O3	C36	C3	6.9(2)
O5	C3	C36	C34	-179.58(16)	C19	O3	C36	C34	-174.62(19)
C1	O1	C20	C14	1.5(2)	C19	O5	C3	C13	177.3(2)
C1	O1	C20	C16	-170.94(16)	C19	O5	C3	C36	-5.3(2)
C1	C4	C32	C25	-178.71(18)	C20	O1	C1	C4	178.79(15)
C1	C4	C38	C27	179.11(18)	C20	O1	C1	C8	-1.1(2)
C1	C8	C14	C20	0.5(2)	C20	C14	C24	C12	141.25(19)
C1	C8	C14	C24	175.64(18)	C20	C16	C33	C2	177.0(2)
C1	C8	C28	C6	-95.9(2)	C23	C2	C33	C16	-0.8(4)
C1	C8	C28	C10	130.38(19)	C24	C12	C30	C29	-95.15(19)
C3	O5	C19	O3	9.5(2)	C24	C12	C30	C31	81.6(2)

C3	C13	C26	O4	176.17(15)	C24	C14	C20	O1	-176.53(16)
C3	C13	C26	C6	0.6(3)	C24	C14	C20	C16	-6.5(4)
C4	C1	C8	C14	-179.5(2)	C25	C15	C27	C38	-0.1(3)
C4	C1	C8	C28	-3.1(3)	C26	O4	C12	C24	119.20(16)
C5	C7	C23	O2	179.21(19)	C26	O4	C12	C30	-120.47(16)
C5	C7	C23	C2	-1.2(3)	C26	C6	C28	C8	-46.5(2)
C5	C16	C20	O1	-154.21(19)	C26	C6	C28	C10	87.7(2)
C5	C16	C20	C14	36.1(4)	C26	C6	C34	C36	2.9(2)
C5	C16	C33	C2	-1.1(3)	C27	C15	C25	C32	0.6(3)
C6	C34	C36	O3	-178.90(17)	C28	C6	C26	O4	-0.9(3)
C6	C34	C36	C3	-0.6(3)	C28	C6	C26	C13	174.21(16)
C7	C5	C16	C20	-176.06(19)	C28	C6	C34	C36	-174.51(15)
C7	C5	C16	C33	2.0(3)	C28	C8	C14	C20	-175.61(18)
C8	C1	C4	C32	-157.3(2)	C28	C8	C14	C24	-0.5(3)
C8	C1	C4	C38	24.8(3)	C28	C10	C11	C21	-176.24(18)
C8	C14	C20	O1	-1.3(2)	C28	C10	C18	C22	175.36(17)
C8	C14	C20	C16	168.8(2)	C29	C30	C31	C37	0.8(3)
C8	C14	C24	C12	-33.0(3)	C29	C35	C39	C37	0.8(3)
C9	O2	C23	C2	175.1(2)	C30	C12	C24	C14	-165.07(15)
C9	O2	C23	C7	-5.3(3)	C30	C29	C35	C39	0.0(3)
C10	C11	C21	C40	1.5(3)	C30	C31	C37	C39	0.0(3)
C10	C18	C22	C40	0.6(3)	C31	C37	C39	C35	-0.8(4)
C11	C10	C18	C22	1.7(3)	C32	C4	C38	C27	1.2(3)
C11	C10	C28	C6	-156.01(17)	C33	C2	C23	O2	-178.4(2)
C11	C10	C28	C8	-23.8(3)	C33	C2	C23	C7	2.0(3)
C11	C21	C40	O6	179.35(18)	C33	C16	C20	O1	27.8(3)
C11	C21	C40	C22	0.9(3)	C33	C16	C20	C14	-142.0(2)

C12	O4	C26	C6	-49.5(2)	C34	C6	C26	O4	-178.02(15)
C12	O4	C26	C13	134.98(16)	C34	C6	C26	C13	-2.9(2)
C12	C30	C31	C37	-175.98(19)	C34	C6	C28	C8	130.65(16)
C13	C3	C36	O3	176.65(16)	C34	C6	C28	C10	-95.10(18)
C13	C3	C36	C34	-1.9(3)	C35	C29	C30	C12	176.04(18)
C14	C8	C28	C6	79.6(2)	C35	C29	C30	C31	-0.8(3)
C14	C8	C28	C10	-54.1(3)	C36	O3	C19	O5	-10.1(2)
C15	C25	C32	C4	-0.2(3)	C36	C3	C13	C26	1.9(3)
C15	C27	C38	C4	-0.8(3)	C38	C4	C32	C25	-0.7(3)

Table 27 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 220225A_auto.

Atom	*x*	*y*	*z*	U(eq)
H2	6729.29	8377.86	1445.95	57
H5	3009.57	7394.19	3254.92	45
H7	2781.01	9337.76	2517.63	47
H9A	3226.47	10737.29	983.61	81
H9B	3669.41	11759.51	995.16	81
H9C	2846.11	11255.81	2189.64	81
H11	3437.37	3508.44	5320.56	44
H12	3706.49	3183.35	2663.6	38
H13	6683.83	2170.42	-557.87	45
H15	10719.3	1165.24	4471.67	51
H17A	-593.13	3142.92	7064.78	73
H17B	-13.48	2392.05	7974.96	73
H17C	-1048.53	2102.99	7796.3	73
H18	4692.06	557.17	3505.46	38
H19A	9502.66	-1909.8	-919.3	62

H19B	10402.86	-1251.68	-1015.5	62
H21	1451.66	3269.34	6585	46
H22	2756.58	270.61	4785.95	40
H24A	3493.95	5620.58	2368.24	40
H24B	2796.54	5025.35	3555.13	40
H25	9566.7	3225.54	4849.36	50
H27	10028.06	196.6	3661.1	48
H28	6207.65	1681.29	3821.76	36
H29	1469.29	3722.95	2863.4	48
H31	3889.31	5074.36	133.32	52
H32	7713.32	4317.41	4454.89	44
H33	6959.37	6450.37	2133.89	52
H34	7412.92	5.52	2675.68	40
H35	-108.84	4532.11	2092.99	62
H37	2316.73	5882.08	-634.6	63
H38	8194.68	1278.93	3235.09	43
H39	305.66	5633.56	350.29	66

Experimental

Single crystals of $C_{26}H_{20}FNO_2$ were from ether. A suitable crystal was selected and on a diffractometer. The crystal was kept at 293 K during data collection. Using Olex2 [1]the structure was solved with the olex2.solve [2] structure solution program using Charge Flipping and refined with the olex2.refine [3] refinement package using Gauss-Newton minimisation.

Crystal structure determination of CCDC 2301810

Crystal Data for $C_{40}H_{32}O_6$ (M =608.65 g/mol): triclinic, space group P-1 (no. 2), a = 12.1952(3) Å, b = 12.2266(3) Å, c = 12.7568(4) Å, α = 78.461(2)°, β = 62.446(3)°, γ = 64.147(3)°, V = 1517.57(9) Å^3, Z = 2, T = 173(2) K, μ(Cu Kα) = 0.717 mm^{-1}, *Dcalc* = 1.332 g/cm^3, 41062 reflections measured (7.818° ≤ 2Θ ≤ 134.136°),

5401 unique (R_{int} = 0.0970, R_{sigma} = 0.0489) which were used in all calculations. The final R_1 was 0.0496 ($I > 2\sigma(I)$) and wR_2 was 0.1296 (all data).

6. Computational calculations

6.1 Computational details.

All DFT calculations were carried out using the CP2K code.[8] All calculations employed a mixed Gaussian and planewave basis sets. Core electrons were represented with norm-conserving Goedecker-Teter-Hutter pseudopotentials,[9-11]and the valence electron wavefunction was expanded in a double-zeta basis set with polarization functions[12] along with an auxiliary plane wave basis set with an energy cutoff of 400 eV. The generalized gradient approximation exchange-correlation functional of Perdew, Burke, and Enzerhof (PBE)[13] was used. Each configuration was optimized with the Broyden-Fletcher-Goldfarb-Shanno (BGFS) algorithm with SCF convergence criteria of 1.0×10^{-6} au. To compensate the long-range van der Waals dispersion interaction between the adsorbate and the skeleton, the DFT-D3 scheme[14] with an empirical damped potential term was added into the energies obtained from exchange-correlation functional in all calculations. Transition states of elementary steps in the reaction routes were located using the climbing image nudged elastic band (CI-NEB) method [15-16] with seven intermediate images along the reaction pathway between the initial and the final states. Each identified transition state was further confirmed by the vibrational frequency analysis.

The Gibbs free energy change for each elementary step was calculated at 298.15 K, defining as follows:

$$\Delta G = \Delta E_{DFT} + \Delta E_{ZPE} - T\Delta S$$

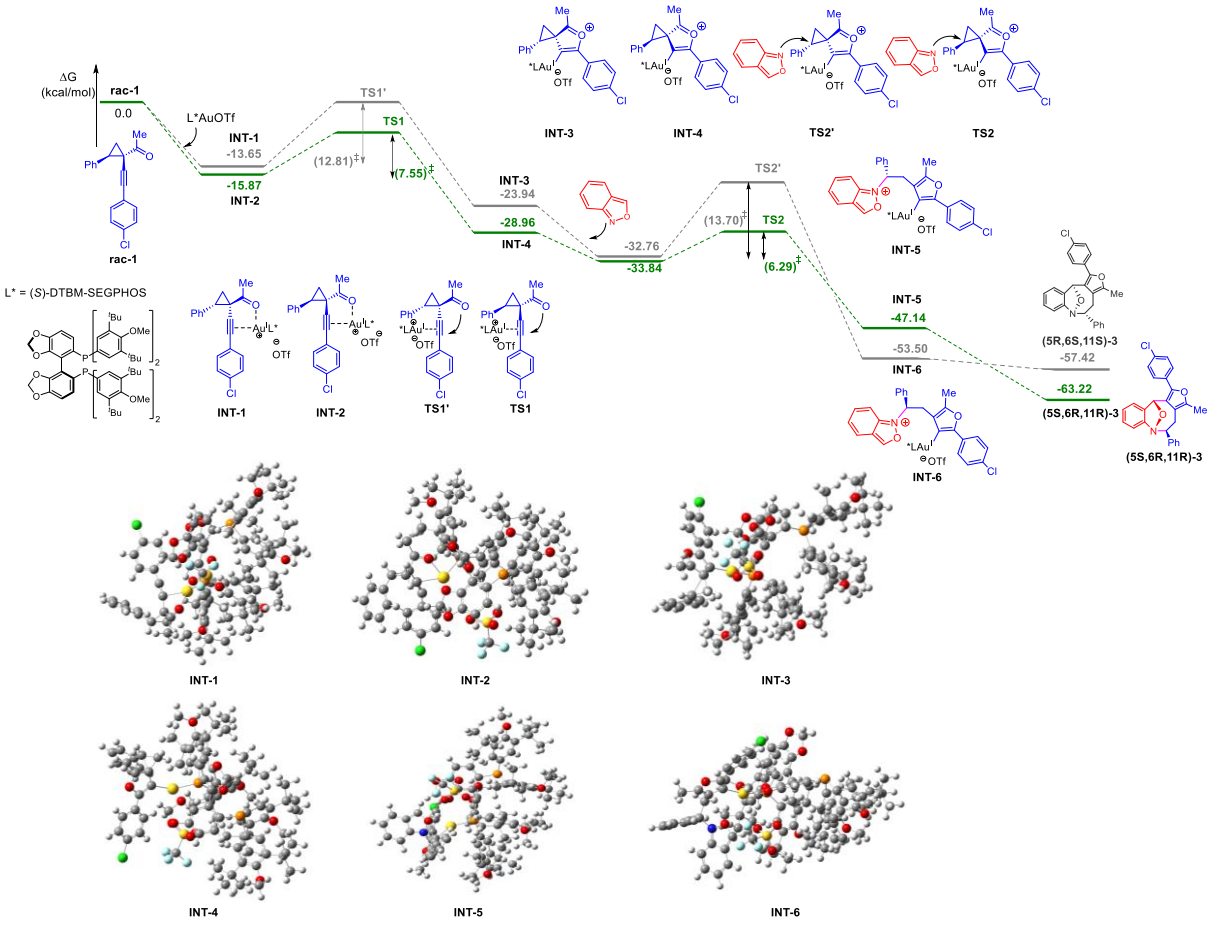
where ΔE is the difference of electronic energy calculated with CP2K, ΔE_{ZPE} is the difference of zero-point energy (ZEP), and $T\Delta S$ is the changed entropy value. E_{ZPE} and TS were calculated using the following equations for each reaction intermediates,

$$E_{ZPE} = \frac{1}{2}\sum_i h\nu_i$$

$$TS = \sum_i h\nu_i \left(\frac{1}{e^{h\nu_i/k_BT}}\right) - k_BT\sum_i \ln\left(1 - e^{-h\nu_i/k_BT}\right)$$

where h, v_i, and k_B are Planck's constant, vibrational frequencies, and Boltzmann constant, respectively.

6.2 DFT calculations



6.3 Calculation data of intermediates

Table 28 Calculation data of DTBM-SEGPHOS(AuCl)$_2$

cm-1	x_i	pf	TS (kcal/mol)	E_{ZEP} (kcal/mol)
74.855699	0.36122984	2.023660129	1.174640734	0.107011367
77.881367	0.375830754	1.98448102	1.15189908	0.111336768
180.971211	0.873309615	1.166649117	0.677185638	0.258710786
		sum	3.003725451	0.477058922

Table 29 Calculation data of anthranil

cm-1	x_i	pf	TS(kcal/mol)	E_{ZEP}(kcal/mol)
131.635392	0.635230614	1.470412602	0.853506235	0.188181842

286.05719	1.38042119	0.753408907	0.437318885	0.408938417
457.283031	2.206702742	0.389518501	0.226097402	0.653717527
624.156972	3.011983407	0.206283074	0.119737745	0.892275297
764.323437	3.688382271	0.119952703	0.069626974	1.092652894
849.804391	4.100886219	0.085742322	0.049769437	1.214853794
943.939344	4.555151619	0.058965228	0.034226577	1.34942618
1008.566487	4.867021695	0.045474373	0.026395762	1.441815123
1169.66256	5.644420189	0.023579778	0.013686966	1.67211303
1350.31974	6.516214414	0.011133798	0.006462653	1.930374894
1470.6819	7.097043998	0.006705896	0.003892461	2.102440879
1640.30909	7.915610969	0.003255327	0.001889566	2.344934607
3194.25113	15.41444191	3.31756E-06	1.92569E-06	4.566401561
170.94853	0.824943338	1.220322169	0.708340352	0.244382675
377.101356	1.819771433	0.528768353	0.306925475	0.539092311
560.89271	2.706690162	0.262707043	0.15248924	0.801834686
725.047173	3.498847489	0.139774095	0.081132372	1.036504775
788.217408	3.80368699	0.109251495	0.06341542	1.126810968
901.768802	4.35164997	0.069774574	0.0405009	1.289140491
971.846195	4.689821223	0.052722032	0.030602692	1.389320942
1138.49929	5.494036174	0.026800111	0.01555622	1.627563003
1241.56985	5.991421967	0.017519973	0.010169531	1.774909451
1381.45458	6.666461243	0.009770228	0.005671164	1.974884281
1517.36538	7.322323643	0.005501354	0.003193281	2.169178119
3178.33646	15.33764279	3.56563E-06	2.06968E-06	4.543650453
3195.94537	15.42261778	3.29219E-06	1.91096E-06	4.568823596
222.245163	1.072484605	0.976610518	0.566877055	0.317714738
440.354116	2.125009173	0.415403983	0.241122722	0.629516479
573.281741	2.766475693	0.250585877	0.145453465	0.819545657
758.011647	3.657923576	0.122944099	0.07136334	1.083629756

793.296189	3.828195575	0.107098607	0.062165768	1.134071435
904.183229	4.363301229	0.069107183	0.04011351	1.292592081
974.0772	4.700587345	0.052251501	0.03032957	1.392510317
1155.14768	5.574376005	0.025029899	0.014528694	1.651363017
1269.80395	6.127670771	0.015581743	0.009044478	1.815272038
1401.54671	6.763419518	0.008978566	0.005211641	2.003607372
1559.86453	7.527411016	0.004591179	0.002664966	2.229933566
3186.43587	15.37672796	3.43716E-06	1.99511E-06	4.555229114
3241.11254	15.64058022	2.68257E-06	1.55711E-06	4.633393175
		sum	4.449491975	66.50260054

Table 30 Calculation data of race-1

cm-1	x_i	pf	TS(kcal/mol)	E_{ZEP}(kcal/mol)
145.819629	0.703679239	1.371812405	0.796273399	0.208459184
98.758838	0.476578801	1.750532419	1.016102781	0.141182548
108.440145	0.523297715	1.658937201	0.96293601	0.155022642
145.5811	0.702528174	1.373383717	0.797185473	0.20811819
231.335907	1.116353649	0.940292999	0.545796422	0.330710581
299.689509	1.446206433	0.713884805	0.414376979	0.428426754
391.370058	1.888627659	0.500661408	0.290610698	0.559490401
415.154087	2.003401832	0.457218876	0.265394326	0.593491306
471.007163	2.272931047	0.36973238	0.214612478	0.673337117
533.447993	2.57425067	0.291642456	0.169284903	0.762600576
600.25089	2.896620244	0.226058117	0.13121624	0.858099909
638.948279	3.083361559	0.194900437	0.113130653	0.913420487
706.054057	3.407192741	0.150458509	0.087334178	1.00935281
765.524584	3.694178625	0.119391439	0.069301186	1.094370016
824.704075	3.979760062	0.094665888	0.054949152	1.178971167
895.672605	4.322231659	0.071487483	0.041495164	1.280425559

943.810619	4.554530433	0.058995619	0.034244217	1.349242159
957.246368	4.619367092	0.055903929	0.032449635	1.368449486
1001.65487	4.833668401	0.046760459	0.027142275	1.431934485
1033.5636	4.987649837	0.041102887	0.023858317	1.477550218
1081.72971	5.220084184	0.033799316	0.019618934	1.54640698
1115.28557	5.382014131	0.029472958	0.017107683	1.594377394
1183.88523	5.713054298	0.022238316	0.01290831	1.69244532
1238.38522	5.976053939	0.017752825	0.010304691	1.770356799
1324.42941	6.391275866	0.01240803	0.007202285	1.893362878
1364.56193	6.584942668	0.010488386	0.006088021	1.950735074
1433.37023	6.916989719	0.007851506	0.004557434	2.04910128
1461.98156	7.0550589	0.006957405	0.00403845	2.090003139
1555.89921	7.508275665	0.004669422	0.002710383	2.224264875
1612.05192	7.779250822	0.003674034	0.002132606	2.304539036
3022.81572	14.58714905	7.20524E-06	4.18231E-06	4.32132286
3140.89711	15.15697237	4.22445E-06	2.4521E-06	4.49012833
3175.49247	15.32391858	3.61186E-06	2.09652E-06	4.539584768
3187.06784	15.37977768	3.42733E-06	1.9894E-06	4.556132567
3199.40858	15.43933015	3.24092E-06	1.8812E-06	4.573774497
57.993267	0.279857096	2.276733133	1.32153786	0.082905362
101.404215	0.489344551	1.724606502	1.00105399	0.144964296
117.827057	0.568595973	1.577948098	0.915925597	0.168441878
150.711608	0.727286377	1.34018694	0.777916285	0.215452604
255.327595	1.232129919	0.852203624	0.49466463	0.365008349
314.175789	1.516112622	0.674437245	0.391479502	0.449135887
402.170249	1.940745952	0.480427164	0.278865659	0.574930017
448.823243	2.165878491	0.402243363	0.233483593	0.641623679
508.26172	2.452709712	0.320946943	0.186294797	0.726595067
544.947476	2.629743525	0.279155934	0.162037057	0.779039877

619.787273	2.990896627	0.209767478	0.12176028	0.886028512
667.467414	3.220985851	0.174647273	0.101374632	0.954190551
713.260566	3.441969066	0.14631487	0.084928988	1.01965501
795.441565	3.838548478	0.106201527	0.061645055	1.137138397
830.291139	4.006721459	0.09260526	0.053753053	1.186958259
902.201633	4.353738675	0.069654476	0.040431189	1.289759253
953.703294	4.602269342	0.056703666	0.032913845	1.363384418
975.10884	4.705565712	0.052035299	0.030204075	1.393985117
1010.67117	4.877178227	0.045089592	0.026172415	1.444823913
1045.00961	5.042884614	0.039239848	0.02277691	1.493913066
1093.09861	5.274946867	0.032268651	0.018730453	1.562659598
1167.07637	5.631940066	0.023832025	0.013833384	1.668415896
1191.27102	5.748695791	0.021571314	0.012521146	1.703003818
1290.04105	6.225328591	0.014322948	0.008313806	1.844202363
1344.13749	6.486380828	0.011425907	0.006632208	1.92153694
1380.7219	6.662925553	0.009800353	0.00568865	1.973836862
1442.05414	6.958895507	0.007568848	0.004393365	2.061515525
1489.02377	7.185556002	0.006204544	0.003601449	2.128661831
1590.13112	7.673467971	0.004034952	0.002342102	2.273201737
1741.09419	8.401967843	0.002110487	0.00122504	2.489013829
3105.05792	14.98402381	4.9683E-06	2.88386E-06	4.43889374
3149.86258	15.20023686	4.05642E-06	2.35456E-06	4.502945077
3180.64284	15.34877263	3.52856E-06	2.04817E-06	4.546947577
3191.05548	15.39902073	3.36595E-06	1.95378E-06	4.561833164
3201.76877	15.45071969	3.20644E-06	1.86119E-06	4.577148555
74.883357	0.361363309	2.023294706	1.174428622	0.107050906
106.669548	0.514753376	1.675035208	0.972280156	0.152491451
125.343115	0.604866083	1.517854391	0.88104399	0.179186599
168.040815	0.810911628	1.236552544	0.717761331	0.240225896

283.450519	1.367842223	0.761249101	0.441869754	0.405212002
326.73351	1.576712197	0.642202064	0.372768477	0.467088013
413.92181	1.997455255	0.459370973	0.266643518	0.591729681
453.056061	2.186304727	0.395824865	0.229757954	0.647674783
519.16128	2.505307529	0.307924196	0.178735697	0.742176738
563.784629	2.720645645	0.259827314	0.15081769	0.805968883
632.629378	3.052868549	0.199686551	0.11590877	0.904387184
695.286224	3.355230597	0.15686172	0.091050944	0.993959452
762.393114	3.679067145	0.120860025	0.070153632	1.089893364
798.003555	3.850911829	0.10513973	0.061028731	1.140800938
837.667858	4.042319164	0.089950737	0.052212226	1.197503786
927.467438	4.47566343	0.062979504	0.036556678	1.325878458
954.565621	4.606430658	0.056508011	0.032800276	1.364617173
997.012523	4.811265933	0.047643982	0.027655119	1.425297938
1013.34203	4.890066935	0.04460584	0.025891619	1.448642086
1060.64055	5.118314582	0.036827364	0.021376575	1.516258573
1106.8788	5.341445689	0.030503412	0.017705814	1.582359327
1177.26777	5.681120513	0.022852958	0.013265081	1.682985199
1224.30843	5.908123815	0.018818749	0.01092341	1.750233059
1315.60619	6.348697827	0.012874029	0.007472776	1.880749484
1358.23204	6.554396637	0.010770586	0.006251825	1.941686064
1404.59323	6.778121052	0.008864148	0.005145227	2.00796258
1450.35026	6.998929939	0.007308144	0.004242038	2.073375396
1498.17575	7.229720586	0.005968333	0.00346434	2.141745226
1598.39187	7.713331748	0.003895021	0.002260879	2.285011053
2270.27312	10.95561737	0.000208745	0.000121167	3.245511485
3121.48328	15.06328739	4.61245E-06	2.67731E-06	4.462374925
3173.00349	15.31190757	3.65282E-06	2.12029E-06	4.536026606
3186.98042	15.3793558	3.42868E-06	1.99019E-06	4.556007589

3195.59355	15.42092001	3.29744E-06	1.91401E-06	4.568320644
3219.84283	15.53793934	2.9542E-06	1.71478E-06	4.602986658
		sum	18.58249273	176.2543206

Table 31 Calculation data of INT-1

cm-1	x_i	pf	TS(kcal/mol)	E_{ZEP}(kcal/mol)
171.397748	0.827111121	1.217842083	0.706900777	0.245024863
31.330239	0.151189788	2.890171247	1.6776102	0.04478873
54.51582	0.263076041	2.338190887	1.357211232	0.077934112
97.065824	0.468408853	1.767505844	1.025955065	0.138762268
125.521491	0.605726869	1.516474936	0.880243281	0.1794416
146.38852	0.706424526	1.368076028	0.794104606	0.209272452
235.410873	1.136018142	0.924565502	0.53666734	0.336536025
290.161076	1.400225241	0.741253118	0.430263014	0.414805204
394.654602	1.904477825	0.494415591	0.286985292	0.564185883
424.944676	2.050648107	0.440484138	0.255680587	0.607487626
468.885215	2.262691199	0.372724236	0.216349111	0.670303647
550.999169	2.658947074	0.272797416	0.158346232	0.787691189
599.2429	2.891756005	0.226931219	0.131723034	0.856658918
657.912949	3.174879036	0.181194184	0.10517481	0.940531786
717.174798	3.460857907	0.144110639	0.083649534	1.025250673
779.558022	3.761899542	0.113018772	0.065602149	1.11443178
836.454581	4.036464274	0.090382236	0.052462691	1.195769323
901.519028	4.35044464	0.069843971	0.040541182	1.288783422
954.11105	4.604237043	0.056611068	0.032860096	1.363967333
979.296293	4.725773031	0.051166579	0.029699823	1.399971369
1009.07413	4.869471405	0.045381276	0.026341723	1.44254083
1027.22788	4.957075663	0.042170702	0.024478134	1.46849287
1086.68406	5.243992304	0.033123808	0.019226832	1.553489564

1119.0636	5.400245704	0.029020959	0.016845319	1.599778348
1185.90658	5.722808692	0.022053801	0.012801207	1.695334978
1249.18023	6.028147231	0.016975522	0.009853502	1.785789008
1326.29518	6.400279509	0.012311622	0.007146325	1.896030133
1362.61563	6.575550451	0.010574377	0.006137935	1.947952707
1431.90181	6.909903571	0.007900314	0.004585766	2.047002067
1454.19518	7.017484287	0.007190324	0.004173649	2.078871969
1557.30616	7.515065144	0.004641511	0.002694182	2.226276203
1611.07534	7.774538162	0.003689414	0.002141534	2.303142949
3018.53006	14.56646783	7.34605E-06	4.26404E-06	4.315196217
3128.99537	15.09953835	4.45828E-06	2.58782E-06	4.473113973
3178.80913	15.33992372	3.558E-06	2.06525E-06	4.544326162
3192.02419	15.40369543	3.35121E-06	1.94522E-06	4.563218004
3199.71591	15.44081323	3.23641E-06	1.87859E-06	4.574213846
146.541194	0.707161282	1.367075966	0.793524116	0.20949071
40.285193	0.194403553	2.639392323	1.532044679	0.057590453
63.62099	0.307014701	2.184777832	1.268162078	0.090950579
100.234086	0.48369788	1.735986599	1.007659608	0.143291516
136.821251	0.660255923	1.433096132	0.831845757	0.195595384
162.560397	0.784464871	1.268006376	0.73601882	0.232391262
250.685468	1.209728488	0.86843312	0.504085099	0.358372109
308.964231	1.490963298	0.688339911	0.399549354	0.441685607
403.054285	1.945012029	0.478808986	0.277926382	0.576193807
453.331663	2.187634695	0.395410561	0.229517469	0.648068775
509.451595	2.458451671	0.319499172	0.185454433	0.728296075
562.318086	2.713568574	0.26128379	0.151663107	0.803872358
612.630821	2.956361861	0.215597907	0.125144573	0.875797872
682.773977	3.294850465	0.164633182	0.095561917	0.976072335
720.585403	3.477316404	0.142216178	0.082549887	1.030126368

803.339138	3.876659659	0.102961197	0.059764194	1.14842852
853.765385	4.120000719	0.084410409	0.048996323	1.220516307
916.122634	4.420917007	0.065896496	0.038249856	1.309660281
961.267756	4.638773034	0.055009439	0.031930425	1.374198336
981.059517	4.73428179	0.050804997	0.029489942	1.402492019
1013.1914	4.889340033	0.044632989	0.025907377	1.448426747
1045.45311	5.045024833	0.039169332	0.022735979	1.494547088
1094.03101	5.279446352	0.032146145	0.018659344	1.563992534
1172.62171	5.658700112	0.02329434	0.013521283	1.676343339
1188.29646	5.734341509	0.021837567	0.012675693	1.698751481
1297.3904	6.260794192	0.013890849	0.008062993	1.854708756
1344.06867	6.486048705	0.011429201	0.00663412	1.921438551
1380.17465	6.660284703	0.009822913	0.005701745	1.973054532
1441.13617	6.954465651	0.00759825	0.004410431	2.060203217
1488.76976	7.18433023	0.006211229	0.00360533	2.128298706
1590.96195	7.677477336	0.004020657	0.002333805	2.274389478
1650.56553	7.965105263	0.003115277	0.001808273	2.359596885
3098.11805	14.95053422	5.12673E-06	2.97583E-06	4.428972726
3153.22274	15.21645194	3.99517E-06	2.31901E-06	4.507748662
3188.32991	15.38586802	3.40778E-06	1.97806E-06	4.557936782
3193.67666	15.41166974	3.32621E-06	1.93071E-06	4.565580329
3203.77261	15.46038959	3.17745E-06	1.84436E-06	4.580013182
118.445922	0.571582419	1.572849129	0.912965882	0.169326588
53.629943	0.25880108	2.354481629	1.366667252	0.07666769
70.851698	0.341907803	2.078070843	1.206223626	0.101287373
119.139142	0.574927678	1.567170776	0.909669861	0.170317593
139.927194	0.675244218	1.411464988	0.819289882	0.200035543
178.143715	0.859665017	1.181447144	0.685775205	0.254668686
269.866406	1.302289606	0.80367355	0.466495176	0.385792578

328.70571	1.586229408	0.63729582	0.369920629	0.469907408
415.373736	2.004461789	0.456836364	0.265172295	0.593805309
459.10836	2.215511201	0.386826665	0.224534916	0.65632696
527.157784	2.543896118	0.298703624	0.173383583	0.75360829
573.844185	2.769189869	0.250048774	0.145141702	0.820349709
635.886534	3.06858655	0.197205428	0.114468593	0.909043512
699.418569	3.375171982	0.154373852	0.089606853	0.999866923
769.180736	3.711822054	0.11769856	0.068318548	1.099596737
831.108135	4.010664023	0.092307584	0.053580266	1.188126211
859.675676	4.148521907	0.08246007	0.047864241	1.228965474
937.767364	4.525367603	0.060439516	0.035082333	1.34060291
969.692133	4.679426403	0.053180223	0.03086865	1.386241562
989.381884	4.774442891	0.049131453	0.028518527	1.414389415
1023.83568	4.940705993	0.042753417	0.024816374	1.46364349
1067.3545	5.150713964	0.035835875	0.020801061	1.525856624
1112.91947	5.370596079	0.02975951	0.017274014	1.59099489
1175.24263	5.67134784	0.023044339	0.013376168	1.680090125
1224.65234	5.909783439	0.018791978	0.010907871	1.750724709
1308.5172	6.314488616	0.013260789	0.007697272	1.870615287
1356.25532	6.544857648	0.010860225	0.006303857	1.938860217
1402.80611	6.769496949	0.008931093	0.005184085	2.005407761
1444.77605	6.972030561	0.007482323	0.004343141	2.065406677
1494.54806	7.212214467	0.006060888	0.003518064	2.136559182
1594.16015	7.692910805	0.003966096	0.002302135	2.278961516
2227.62334	10.74980306	0.000252034	0.000146294	3.18454069
3113.47104	15.02462284	4.78274E-06	2.77616E-06	4.45092087
3173.89337	15.31620185	3.63812E-06	2.11176E-06	4.537298752
3189.60886	15.39203979	3.38809E-06	1.96663E-06	4.559765118
3199.20097	15.43832828	3.24397E-06	1.88297E-06	4.573477703

3225.14611	15.56353128	2.88401E-06	1.67404E-06	4.61056806
		sum	25.68990311	177.3360798

Table 32 The calculation data of INT-2

cm-1	x_i	pf	TS(kcal/mol)	E_{ZEP}(kcal/mol)
127.906206	0.617234746	1.498230294	0.869653113	0.182850714
59.515631	0.287203542	2.250993949	1.306597459	0.085081686
75.122582	0.362517733	2.020139755	1.17259732	0.107392895
107.511589	0.518816799	1.667344962	0.967816325	0.153695207
122.249783	0.589938644	1.542112871	0.895124912	0.174764468
160.500952	0.774526643	1.280129692	0.743055841	0.229447144
223.771362	1.079849556	0.970390738	0.563266762	0.319896544
291.354259	1.405983163	0.737761227	0.428236133	0.416510941
391.697372	1.890207172	0.500035319	0.290247283	0.559958319
407.765041	1.967744642	0.470280879	0.272976212	0.582928156
465.840818	2.247999906	0.377059222	0.218865369	0.665951472
528.171255	2.548786808	0.297554651	0.172716658	0.755057116
576.289483	2.780990101	0.247726702	0.143793847	0.823845431
630.071097	3.040523097	0.201656518	0.117052244	0.900729945
709.562247	3.424122152	0.148427393	0.086155209	1.014368008
771.033634	3.720763552	0.116849488	0.067825702	1.102245582
829.336705	4.002115664	0.092954186	0.053955588	1.18559383
882.414627	4.258252866	0.075353979	0.043739486	1.261472368
949.462013	4.581802266	0.057675553	0.03347798	1.357321215
974.754649	4.703856499	0.052109429	0.030247104	1.393478777
1000.88453	4.829951004	0.046905962	0.027226733	1.430833236
1034.69221	4.993096117	0.040915444	0.023749515	1.479163633
1081.9195	5.221000045	0.033773195	0.019603771	1.546678297
1130.12886	5.453643136	0.02773554	0.016099193	1.615596898

1181.16728	5.69993833	0.022488791	0.013053699	1.688559822
1235.01584	5.9597944	0.018002471	0.010449598	1.765540044
1318.45759	6.362457759	0.012721592	0.007384293	1.88482575
1361.78078	6.57152174	0.010611473	0.006159467	1.946759234
1423.37657	6.868763469	0.008189616	0.004753692	2.03481465
1453.4443	7.013860798	0.007213186	0.004186919	2.07779854
1554.48824	7.501466757	0.004697579	0.002726726	2.222247793
1612.4983	7.78140492	0.003667024	0.002128537	2.30517717
3008.73774	14.51921322	7.67813E-06	4.4568E-06	4.30119743
3129.67306	15.10280869	4.44463E-06	2.5799E-06	4.474082783
3174.43975	15.3188385	3.62913E-06	2.10654E-06	4.538079838
3179.65149	15.3439887	3.54445E-06	2.05739E-06	4.545530376
3199.30986	15.43885374	3.24237E-06	1.88205E-06	4.573633364
29.313415	0.141457235	2.956591172	1.716163882	0.041905542
61.924151	0.298826295	2.211605256	1.283734152	0.088524831
89.025209	0.429607397	1.852538311	1.075312464	0.127267656
110.504105	0.533257731	1.640515313	0.952242959	0.157973214
134.625952	0.649662107	1.448705247	0.840906123	0.192457053
171.431758	0.827275243	1.217654612	0.706791959	0.245073483
257.546013	1.2428353	0.844576956	0.490237704	0.36817973
312.153596	1.506354161	0.679794171	0.394588949	0.446245023
399.565375	1.928175657	0.485228302	0.281652497	0.57120617
422.378527	2.038264687	0.444808654	0.258190768	0.603819139
477.528119	2.30439911	0.360688002	0.209362636	0.682659272
538.348435	2.597898648	0.286255593	0.166158079	0.769606095
603.643369	2.912991271	0.223143577	0.129524484	0.862949691
673.175117	3.248529414	0.170846079	0.099168215	0.962350105
734.201014	3.54302102	0.134889916	0.078297333	1.04959082
781.663102	3.77205799	0.112091595	0.065063966	1.117441137

830.487523	4.007669146	0.092533623	0.053711471	1.187239003
899.09067	4.338726156	0.070522138	0.040934827	1.285311918
954.738825	4.607266486	0.056468791	0.032777511	1.36486478
995.583342	4.804369159	0.047919219	0.027814881	1.423254825
1012.71657	4.887048664	0.044718672	0.025957113	1.447747948
1044.46542	5.040258559	0.03932654	0.02282723	1.493135119
1095.24215	5.285290949	0.031987691	0.018567369	1.565723948
1172.6893	5.659026299	0.023287859	0.013517521	1.67643997
1195.46089	5.768914735	0.021201637	0.012306566	1.708993514
1281.90633	6.18607302	0.014816536	0.008600311	1.832573223
1341.96097	6.475877609	0.01153052	0.006692932	1.918425448
1374.38324	6.632337235	0.010064796	0.005842147	1.964775324
1431.57879	6.908344764	0.007911091	0.004592021	2.046540283
1474.8996	7.117397251	0.006587203	0.003823565	2.108470362
1586.93784	7.658058216	0.004090358	0.002374263	2.268636724
1746.4564	8.427844171	0.002062225	0.001197026	2.496679478
3091.80758	14.92008186	5.27517E-06	3.06199E-06	4.419951464
3137.67742	15.14143518	4.28648E-06	2.4881E-06	4.485525565
3178.08435	15.33642618	3.5697E-06	2.07205E-06	4.543290044
3192.53503	15.40616055	3.34346E-06	1.94073E-06	4.563948278
3205.77167	15.4700364	3.14879E-06	1.82772E-06	4.58287097
43.855293	0.211631722	2.554771754	1.482926369	0.062694156
73.166743	0.353079475	2.04624035	1.187747503	0.104596889
101.11752	0.487961052	1.727382084	1.002665086	0.144554446
111.661071	0.538840882	1.630345712	0.946339978	0.159627177
141.180938	0.681294389	1.402879162	0.814306209	0.201827856
187.984856	0.907155239	1.131040064	0.656516236	0.268737274
281.496813	1.358414258	0.767187199	0.445316544	0.402419045
357.778146	1.726523755	0.569514514	0.330576729	0.511468454

403.143128	1.945440757	0.478646677	0.277832169	0.576320814
439.01005	2.118523137	0.41753243	0.242358187	0.627595045
512.799606	2.474608109	0.315460138	0.183109961	0.733082287
551.707783	2.66236662	0.272062239	0.157919496	0.788704201
627.892221	3.030008533	0.203349189	0.118034761	0.897615092
697.333484	3.365110024	0.15562437	0.09033272	0.996886151
765.464145	3.693886966	0.11941962	0.069317544	1.094283614
793.589002	3.829608597	0.106975739	0.062094449	1.134490031
872.862685	4.212158226	0.078263946	0.045428586	1.24781721
928.777493	4.481985339	0.062650807	0.036365884	1.327751272
1557.9051	7.517955472	0.00462968	0.002687314	2.227132439
1000.1762	4.826532848	0.04704014	0.027304617	1.429820636
1015.56365	4.900787787	0.044207287	0.025660277	1.45181805
1064.76544	5.138219987	0.03621511	0.02102119	1.522155386
1117.02267	5.390396805	0.029264291	0.016986562	1.596860693
1174.51812	5.667851609	0.023113184	0.01341613	1.679054395
1213.61613	5.856526189	0.019669838	0.011417428	1.734947686
1313.39669	6.338035481	0.012993377	0.007542052	1.877590852
1352.52969	6.526878902	0.011031162	0.006403077	1.933534161
1401.24473	6.761962254	0.008989986	0.005218269	2.003175669
1433.51608	6.917693549	0.007846674	0.00455463	2.049309784
1495.01247	7.214455562	0.006048961	0.003511141	2.137223088
1594.28369	7.693506994	0.003964003	0.00230092	2.279138133
2058.21788	9.932306104	0.000531112	0.000308286	2.942363944
3115.69842	15.03537148	4.73479E-06	2.74832E-06	4.454105065
3155.98596	15.22978636	3.94549E-06	2.29017E-06	4.511698875
3178.81861	15.3399695	3.55785E-06	2.06516E-06	4.544339721
3192.75843	15.40723862	3.34008E-06	1.93876E-06	4.564267646
3237.28744	15.62212151	2.72951E-06	1.58436E-06	4.627924934

		sum	25.94141102	177.221688

Table 33 The calculation data of TS1’

cm-1	x_i	pf	TS(kcal/mol)	E_{ZEP} (kcal/mol)
118.958758	0.574057202	1.56864499	0.910525574	0.170059722
189.192445	0.91298268	1.125060976	0.653045653	0.270463605
129.702251	0.625901889	1.484726471	0.861814771	0.185418284
63.842279	0.308082572	2.181332868	1.266162436	0.091266926
83.294847	0.40195449	1.918121306	1.113380348	0.11907571
122.419955	0.59075984	1.540761542	0.894340528	0.175007741
202.909238	0.979175569	1.060059805	0.615315491	0.290072704
277.195092	1.337655518	0.780452335	0.453016339	0.396269439
375.312588	1.811139406	0.532407178	0.309037644	0.536535144
398.615048	1.923589681	0.486992262	0.282676394	0.569847612
470.945926	2.272635536	0.369818383	0.214662398	0.673249575
524.231094	2.529772842	0.302046246	0.17532382	0.749424385
592.57442	2.859576037	0.232790628	0.13512415	0.847125868
631.005311	3.045031317	0.200934964	0.116633416	0.902065468
698.551711	3.370988801	0.154892562	0.08990794	0.99862769
759.848594	3.666788099	0.122066158	0.070853736	1.086255798
1808.73881	8.728399305	0.001575478	0.000914492	2.585716463
886.211317	4.276574487	0.074226573	0.043085079	1.266899997
944.468573	4.55770551	0.058840443	0.034154145	1.350182749
968.194159	4.672197656	0.053501125	0.031054919	1.384100105
1001.59607	4.833384671	0.046771549	0.027148712	1.431850432
1028.97854	4.965523793	0.04187299	0.024305326	1.470995559
1085.03677	5.236042981	0.033346943	0.019356352	1.551134643
1116.36188	5.387208032	0.029343498	0.017032538	1.595916045
1189.45984	5.739955568	0.021733055	0.012615029	1.700414599
1240.01559	5.983921573	0.017633242	0.010235278	1.772687521

1320.32392	6.371464113	0.012622773	0.007326934	1.887493809
1353.31718	6.530679098	0.010994813	0.006381978	1.934659938
1435.17558	6.92570175	0.007791903	0.004522838	2.051682148
1460.30526	7.046969618	0.007006915	0.004067189	2.087606756
1540.98112	7.436285698	0.004975702	0.002888164	2.20293844
1604.82994	7.744399815	0.003789285	0.002199504	2.294214712
3019.02087	14.56883633	7.32978E-06	4.2546E-06	4.315897868
3138.89355	15.14730382	4.26294E-06	2.47444E-06	4.487264099
3163.4344	15.26573016	3.81462E-06	2.21421E-06	4.52234693
3184.96527	15.36963132	3.46013E-06	2.00845E-06	4.553126793
3198.44594	15.43468473	3.25509E-06	1.88943E-06	4.57239833
108.954067	0.52577774	1.654316103	0.960253677	0.155757328
161.919612	0.781372646	1.271760282	0.738197788	0.231475216
32.33457	0.15603637	2.858680013	1.659331	0.046224491
67.268378	0.324615838	2.129491942	1.236071186	0.09616477
94.929248	0.458098415	1.78936954	1.038645926	0.135707886
141.906673	0.684796555	1.397946648	0.811443114	0.202865344
267.491766	1.290830347	0.811371191	0.470963299	0.382397867
287.404789	1.386924275	0.749392199	0.434987373	0.410864902
383.439698	1.850358259	0.516083866	0.299562719	0.548153406
431.606574	2.082796312	0.429457059	0.24927988	0.617011267
486.512014	2.347752535	0.348589112	0.202339793	0.695502368
528.641211	2.551054666	0.297023342	0.172408258	0.755728951
607.801884	2.933058944	0.21962078	0.127479665	0.868894574
658.598163	3.178185662	0.180716861	0.104897746	0.941511347
707.631837	3.414806606	0.149541732	0.086802031	1.011608355
768.737049	3.709680962	0.117902756	0.068437075	1.098962456
839.127661	4.049363709	0.089434194	0.051912397	1.199590674
913.829292	4.409850067	0.066501817	0.038601217	1.306381791

963.865227	4.651307605	0.054439048	0.03159934	1.377911599
980.00876	4.72921117	0.051020176	0.029614843	1.40098989
1005.40743	4.851777099	0.04605789	0.026734466	1.437299037
1055.97465	5.095798435	0.037532022	0.021785596	1.50958835
1089.83248	5.259185574	0.032701362	0.018981622	1.557990445
1167.7387	5.635136256	0.023767175	0.013795741	1.669362741
1192.07767	5.752588394	0.021499658	0.012479553	1.70415697
1286.60067	6.2087264	0.014529708	0.008433821	1.839284101
1326.53662	6.401444602	0.0122992	0.007139115	1.896375282
1385.10414	6.684072861	0.009621519	0.005584845	1.980101578
1442.4369	6.96074258	0.007556622	0.004386268	2.062062705
1475.60122	7.120783036	0.006567659	0.003812221	2.109473373
1581.72477	7.632901619	0.004182423	0.002427702	2.261184289
1736.95262	8.381981936	0.002148524	0.001247118	2.483093168
3103.59061	14.97694303	5.00138E-06	2.90307E-06	4.436796118
3141.75885	15.16113087	4.20801E-06	2.44255E-06	4.491360251
3165.17315	15.27412081	3.7847E-06	2.19684E-06	4.524832591
3187.97361	15.38414862	3.41329E-06	1.98126E-06	4.557427423
3206.05463	15.47140186	3.14475E-06	1.82538E-06	4.583275477
196.766417	0.949532265	1.088525871	0.631838721	0.281291119
149.50548	0.721465986	1.347879705	0.782381578	0.213728361
45.121492	0.217741996	2.526417563	1.466468078	0.064504275
70.726383	0.341303072	2.079823988	1.207241245	0.101108226
105.072305	0.507045589	1.689798276	0.980849431	0.150208083
193.583349	0.934171789	1.103681076	0.640635613	0.276740705
270.993966	1.307730852	0.800048604	0.464391063	0.387404503
296.975019	1.433107166	0.72156259	0.418833576	0.424546204
395.789742	1.909955651	0.492275961	0.285743336	0.565808643
450.131364	2.172191068	0.400248612	0.232325733	0.643493728

510.10645	2.461611794	0.318705146	0.184993538	0.729232236
570.445177	2.752787335	0.253311869	0.147035777	0.815490594
626.790954	3.024694168	0.204209952	0.118534394	0.896040755
696.407116	3.360639666	0.156183088	0.09065703	0.995561844
723.304654	3.490438646	0.140722982	0.081683156	1.034013724
788.07863	3.803017291	0.109310905	0.063449904	1.126612575
849.46455	4.099246254	0.085857536	0.049836313	1.214367968
935.286722	4.513396812	0.061042043	0.035432072	1.337056662
964.992703	4.656748446	0.054193245	0.031456662	1.379523404
989.715106	4.776050915	0.049065568	0.028480284	1.414865778
1019.26541	4.918651291	0.043550852	0.025279247	1.457109967
1068.62522	5.156846065	0.035651156	0.020693841	1.527673208
1105.48993	5.334743453	0.030676986	0.017806566	1.580373845
1171.0439	5.651086126	0.023446113	0.01360938	1.674087759
1214.28147	5.859736884	0.019615802	0.011386062	1.735898829
1312.32665	6.332871798	0.013051564	0.007575827	1.876061153
1352.45308	6.52650923	0.011034705	0.006405134	1.933424649
1402.0532	6.765863654	0.008959444	0.005200541	2.004331427
1451.12949	7.00269026	0.007284114	0.00422809	2.07448936
1495.40974	7.216372704	0.006038777	0.003505229	2.137791026
1586.55018	7.656187491	0.004097135	0.002378197	2.268082537
2043.86622	9.86304953	0.000565595	0.000328301	2.921847254
3112.45048	15.01969796	4.80488E-06	2.78901E-06	4.449461916
3155.27129	15.22633759	3.95828E-06	2.2976E-06	4.510677204
3178.26873	15.33731595	3.56672E-06	2.07032E-06	4.54355363
3192.97368	15.40827735	3.33682E-06	1.93687E-06	4.564575359
3209.71295	15.48905575	3.09303E-06	1.79536E-06	4.588505297
		sum	25.40944451	177.5672058

Table 34 The calculation data of TS1

cm-1	x_i	pf	TS(kcal/mol)	E_{ZEP}(kcal/mol)
2622.689688	12.65626786	4.35297E-05	2.5267E-05	3.749315196
150.770739	0.727571724	1.339811521	0.777698372	0.215537136
144.458067	0.697108773	1.380819307	0.801501487	0.206512737
58.394887	0.281795187	2.269876893	1.317558131	0.083479505
103.909416	0.501433855	1.700694651	0.987174271	0.148545653
152.686693	0.73681751	1.327733191	0.770687462	0.218276124
211.297488	1.0196546	1.022760844	0.593665177	0.302064284
266.845709	1.287712681	0.813480497	0.472187653	0.381474284
309.191901	1.492061961	0.687725911	0.399192956	0.442011077
400.802588	1.934146054	0.482941772	0.280325272	0.572974851
444.752676	2.146235227	0.408515208	0.237124108	0.635804523
508.852015	2.455558288	0.320227895	0.185877423	0.727438935
568.692646	2.744330177	0.255010556	0.148021786	0.81298523
624.372693	3.013024408	0.206112522	0.119638748	0.892583685
687.631602	3.318291821	0.161572875	0.093785551	0.983016644
751.302025	3.625545071	0.126202899	0.073254922	1.07403789
792.811747	3.825857812	0.107302184	0.062283935	1.133378891
857.963194	4.140258012	0.083020654	0.048189634	1.226517363
943.640271	4.553708388	0.059035859	0.034267575	1.348998635
979.881153	4.728595379	0.051046367	0.029630046	1.400807467
1005.24504	4.850993461	0.04608808	0.02675199	1.437066891
1079.34141	5.208558982	0.034129711	0.019810712	1.542992734
1128.30161	5.444825384	0.027943924	0.01622015	1.612984711
1170.17169	5.646877103	0.023530426	0.013658319	1.67284087
1197.95213	5.780936707	0.020984763	0.012180681	1.712554925
1293.62602	6.242628499	0.014110557	0.008190523	1.849327318
1352.08404	6.524728356	0.011051785	0.006415048	1.932897079
1399.38347	6.75298037	0.009060687	0.005259308	2.00051486

1438.69875	6.942703455	0.007676862	0.004456062	2.056718763
1474.76064	7.116726688	0.00659108	0.003825816	2.108271713
1578.72984	7.618449047	0.004236232	0.002458936	2.256902833
1707.55867	8.240136055	0.002438603	0.001415496	2.441072493
3000.73381	14.48058876	7.96064E-06	4.62078E-06	4.28975525
3120.29078	15.05753276	4.63741E-06	2.6918E-06	4.460670163
3183.80874	15.36405028	3.47831E-06	2.019E-06	4.551473456
3193.78532	15.41219407	3.32457E-06	1.92976E-06	4.565735657
3196.75185	15.4265096	3.28018E-06	1.90399E-06	4.569976516
576.076576	2.779962679	0.24792804	0.143910714	0.823541066
121.583957	0.586725579	1.547419357	0.89820508	0.173812624
32.152684	0.155158646	2.864309651	1.662598744	0.045964472
72.9962	0.352256488	2.048549915	1.189088098	0.104353086
118.437299	0.571540807	1.572919983	0.913007009	0.16931426
171.378627	0.827018849	1.217947501	0.706961967	0.244997528
239.002045	1.153347998	0.910975952	0.528779238	0.341669853
279.040767	1.34656216	0.774728462	0.449693897	0.398907958
366.161243	1.76697792	0.551442201	0.320086591	0.523452667
411.90518	1.987723639	0.462915431	0.268700912	0.58884677
479.31223	2.313008663	0.35825233	0.207948841	0.685209781
532.815143	2.571196737	0.292345361	0.169692907	0.761695873
597.594232	2.883800056	0.228366345	0.132556059	0.854302034
633.472869	3.056938969	0.199041136	0.115534137	0.905593012
704.264059	3.398554779	0.151505167	0.087941714	1.006793884
765.843679	3.695718476	0.119242761	0.069214885	1.094826184
825.045761	3.98140893	0.094538607	0.054875272	1.17945963
874.524676	4.220178467	0.077749951	0.045130236	1.25019314
945.62704	4.563295904	0.058568182	0.03399611	1.351838857
984.429305	4.750543317	0.050120825	0.029092812	1.407309363

1023.56648	4.9394069	0.042799994	0.024843409	1.463258645
1085.45665	5.238069222	0.033289929	0.019323258	1.5517349
1148.23998	5.541041618	0.025750137	0.014946759	1.641487979
1178.49546	5.687044984	0.022737691	0.013198174	1.684740274
1225.17184	5.912290381	0.018751611	0.010884439	1.75146737
1321.0631	6.375031142	0.012583843	0.007304337	1.888550512
1356.62075	6.546621083	0.010843599	0.006294206	1.93938262
1403.90249	6.774787721	0.008889965	0.005160212	2.006975109
1461.4086	7.052293962	0.006974289	0.004048251	2.089184049
1540.8013	7.435417934	0.004979511	0.002890375	2.202681372
1579.31512	7.621273394	0.004225664	0.002452801	2.257739523
1797.42772	8.673815566	0.001654543	0.000960385	2.569546479
1546.5053	7.462943647	0.004860051	0.002821034	2.210835638
1128.80817	5.447269862	0.027886004	0.01618653	1.613708868
3187.63188	15.38249953	3.41858E-06	1.98433E-06	4.556938893
3194.19294	15.41416112	3.31844E-06	1.9262E-06	4.56631838
3201.62558	15.45002868	3.20852E-06	1.8624E-06	4.57694385
213.158036	1.028633014	1.014721729	0.588998844	0.304724065
156.382213	0.754650916	1.304896256	0.757431682	0.223559123
41.61883	0.200839262	2.606929375	1.513201446	0.059496978
75.740548	0.365499841	2.012037167	1.167894143	0.10827632
144.474424	0.697187707	1.38071056	0.801438365	0.20653612
197.744731	0.954253297	1.083924352	0.629167753	0.282689686
248.691232	1.200104938	0.875520066	0.508198742	0.355521212
293.701843	1.417311858	0.730945729	0.424280053	0.419866974
390.269649	1.883317434	0.502772286	0.291835965	0.557917291
442.79053	2.136766533	0.411573767	0.23889946	0.632999501
501.614214	2.420630958	0.329155788	0.19105965	0.717092001
540.345864	2.607537606	0.2840881	0.16489995	0.772461557

604.661981	2.917906769	0.222275631	0.129020682	0.864405867
679.485716	3.278982362	0.16673651	0.096782801	0.97137154
707.50364	3.414187968	0.14961602	0.086845152	1.011425088
780.961624	3.76867288	0.112399741	0.06524283	1.116438326
829.149719	4.001213329	0.093022693	0.053995354	1.18532652
896.860801	4.327965516	0.07115047	0.041299544	1.282124167
971.482832	4.688067748	0.052799055	0.030647399	1.388801489
992.758147	4.790735665	0.048467842	0.028133332	1.419216015
1030.11803	4.971022576	0.041680308	0.024193483	1.472624529
1116.59066	5.388312071	0.029316051	0.017016606	1.596243107
1153.54843	5.566658503	0.025194883	0.01462446	1.64907677
1192.77782	5.755967105	0.02143765	0.012443561	1.705157886
1257.60967	6.068825018	0.016391736	0.009514642	1.797839467
1332.06168	6.428106822	0.012018264	0.006976044	1.904273745
1369.0719	6.606706351	0.010291749	0.005973882	1.957182386
1435.43953	6.92697547	0.007783226	0.004517801	2.052059477
1470.5219	7.096271889	0.00671044	0.003895099	2.102212148
1559.29065	7.524641673	0.004602422	0.002671492	2.229113171
1674.16266	8.078977536	0.002815197	0.001634091	2.393330608
2736.06481	13.20338019	2.61961E-05	1.52056E-05	3.911392723
3100.64596	14.96273311	5.06845E-06	2.942E-06	4.432586546
3180.91528	15.35008733	3.52421E-06	2.04564E-06	4.547337046
3190.53388	15.39650364	3.37392E-06	1.9584E-06	4.561087496
3195.99809	15.42287223	3.2914E-06	1.91051E-06	4.568898973
3231.0812	15.59217214	2.80743E-06	1.62958E-06	4.61905268
		sum	23.62384115	177.4808114

Table 35 The calculation data of INT3

cm-1	x_i	pf	TS(kcal/mol)	E_{ZEP}(kcal/mol)
171.76382	0.828877669	1.21582638	0.705730755	0.245548188

50.250358	0.242492276	2.41923193	1.404251795	0.071836341
77.813613	0.375503794	1.985341199	1.152398374	0.111239909
113.28173	0.546661668	1.61628452	0.938178109	0.16194402
139.080099	0.671156407	1.417312992	0.822684377	0.198824562
176.206289	0.850315614	1.191739873	0.691749656	0.251899003
232.420312	1.121586643	0.936075242	0.54334821	0.332260813
299.239144	1.444033115	0.715152201	0.415112644	0.427782926
391.929926	1.891329404	0.499590984	0.289989367	0.560290771
412.246931	1.989372821	0.462312787	0.268351105	0.589335326
499.34929	2.409701154	0.332000033	0.192710602	0.713854136
567.130045	2.736789561	0.256534542	0.148906389	0.810751385
627.579822	3.028500995	0.203593005	0.118176285	0.897168496
689.709883	3.328320946	0.160280415	0.093035338	0.985987689
769.049178	3.711187197	0.117759071	0.068353672	1.099408666
802.640005	3.873285865	0.103244157	0.059928439	1.147429062
839.061476	4.049044322	0.089457551	0.051925954	1.199496058
939.301381	4.532770282	0.060069797	0.034867728	1.342795893
968.855099	4.675387143	0.053359306	0.030972599	1.385044965
993.22036	4.792966158	0.048377671	0.028080992	1.41987678
1015.64974	4.901203221	0.044191913	0.025651353	1.451941119
1053.8446	5.08551948	0.03785804	0.021974834	1.506543294
1113.84792	5.375076488	0.029646747	0.01720856	1.592322175
1163.76474	5.615959191	0.024158866	0.0140231	1.663681693
1189.17247	5.738568821	0.021758825	0.012629988	1.700003787
1295.43479	6.251357049	0.014004568	0.008129001	1.85191308
1327.87694	6.40791258	0.012230464	0.007099216	1.898291367
1386.30708	6.689877883	0.00957299	0.005556676	1.981821268
1426.5107	6.883887804	0.008082072	0.004691268	2.03929511
1461.45059	7.052496612	0.00697305	0.004047532	2.089244082

1506.2921	7.268887495	0.005766255	0.003347043	2.1533481
1572.27875	7.587318115	0.004354462	0.002527563	2.247680551
3010.46512	14.527549	7.61849E-06	4.42218E-06	4.303666836
3119.05454	15.05156707	4.66343E-06	2.7069E-06	4.458902876
3157.89681	15.2390075	3.91149E-06	2.27044E-06	4.514430561
3180.81788	15.34961732	3.52577E-06	2.04654E-06	4.547197811
3195.38439	15.41991068	3.30057E-06	1.91583E-06	4.568021638
126.956827	0.612653344	1.505450038	0.873843839	0.181493511
58.828638	0.283888332	2.262525589	1.313291041	0.084099582
86.502469	0.417433455	1.880859099	1.091751366	0.123661226
119.472912	0.576538346	1.564449191	0.908090108	0.17079474
147.93528	0.713888699	1.357996138	0.788253698	0.211483652
183.748584	0.886712335	1.152364606	0.668894142	0.262681232
266.297863	1.28506895	0.815274239	0.473228837	0.380691101
323.834462	1.562722312	0.649489646	0.37699858	0.462943624
397.848973	1.919892846	0.488419071	0.28350459	0.568752456
436.511122	2.106464104	0.421519231	0.24467234	0.624022655
499.817023	2.411958285	0.331410669	0.192368504	0.714522793
592.855335	2.860931644	0.232540849	0.134979164	0.847527455
653.555793	3.153852785	0.18425808	0.106953259	0.934302932
710.244343	3.427413731	0.14803557	0.085927774	1.015343112
775.339608	3.741542815	0.114899069	0.066693574	1.108401268
817.151253	3.943312541	0.097521929	0.056606951	1.168173888
890.009933	4.294905401	0.073114897	0.042439803	1.27233038
943.426645	4.552677496	0.05908636	0.034296888	1.348693242
976.901932	4.714218605	0.051661575	0.029987145	1.396548465
997.460164	4.813426106	0.047558088	0.027605262	1.425937871
1022.62865	4.934881225	0.042962639	0.024937817	1.461917951
1077.20699	5.198258973	0.034427634	0.019983643	1.539941441

1120.93511	5.409276974	0.028799557	0.016716806	1.602453787
1169.34003	5.642863752	0.023611094	0.013705144	1.671651948
1240.2905	5.985248216	0.017613156	0.010223619	1.773080528
1317.15691	6.356181104	0.012790907	0.007424528	1.882966343
1358.23406	6.554406405	0.010770495	0.006251772	1.941688957
1405.51936	6.782590237	0.00882965	0.005125202	2.00928654
1434.32817	6.921612404	0.007819824	0.004539045	2.050470713
1475.78732	7.12168113	0.006562485	0.003809218	2.109739426
1544.11562	7.451411781	0.004909752	0.002849883	2.207419418
1594.22808	7.693238638	0.003964945	0.002301466	2.279058634
3086.78233	14.89583161	5.39642E-06	3.13237E-06	4.412767526
3127.21452	15.09094454	4.49436E-06	2.60877E-06	4.470568128
3164.36597	15.27022561	3.79856E-06	2.20489E-06	4.52367867
3190.7781	15.39768221	3.37019E-06	1.95624E-06	4.561436638
3196.98263	15.42762327	3.27675E-06	1.902E-06	4.570306429
37.41449	0.180550451	2.713102194	1.574829837	0.053486585
68.147956	0.328860402	2.116615995	1.228597297	0.097422188
103.628349	0.500077515	1.703347342	0.988714035	0.148143848
126.786053	0.611829243	1.506754808	0.874601198	0.181249378
149.2298	0.720135642	1.349647478	0.783407688	0.213334257
228.131762	1.100891463	0.952895635	0.553111667	0.326130036
285.474231	1.377608015	0.755154177	0.438331933	0.408105037
338.038352	1.631265776	0.614629125	0.356763666	0.483249061
408.218481	1.9699328	0.469468326	0.272504563	0.58357638
453.146901	2.186743092	0.39568826	0.22967866	0.647804645
540.098672	2.606344736	0.28435546	0.16505514	0.772108179
616.932925	2.97712245	0.212074337	0.123099305	0.881948025
685.151822	3.30632519	0.163128203	0.094688347	0.979471628
714.963352	3.45018617	0.145352006	0.08437009	1.022089259

785.11703	3.78872555	0.110586188	0.064190147	1.122378764
827.115207	3.99139542	0.093771245	0.054429853	1.182418046
927.390806	4.475293628	0.062998783	0.036567868	1.325768907
962.997972	4.647122508	0.054628854	0.031709513	1.376671799
991.161888	4.783032625	0.048780501	0.028314816	1.416934053
1007.58639	4.862292034	0.04565464	0.026500398	1.440414
1041.01083	5.023587776	0.039881221	0.023149197	1.488196536
1087.87125	5.249721311	0.032963895	0.019134011	1.555186735
1159.91591	5.59738596	0.024544208	0.014246773	1.658179526
1182.4456	5.706107111	0.022370646	0.012985121	1.690387273
1242.36245	5.995246794	0.017462485	0.010136162	1.776042524
1325.50827	6.396482131	0.012352194	0.007169875	1.894905191
1369.894	6.610673554	0.010256296	0.005953304	1.958357637
1406.82533	6.788892419	0.008781226	0.005097094	2.011153509
1447.286	6.984142788	0.007403396	0.004297327	2.068994824
1496.8398	7.22327372	0.006002255	0.00348403	2.139835395
1568.93975	7.571205171	0.004416924	0.002563819	2.242907224
1601.6228	7.728923195	0.0038416	0.00222987	2.28962989
3092.57273	14.92377423	5.25694E-06	3.05141E-06	4.4210453
3155.7681	15.22873503	3.94938E-06	2.29243E-06	4.511387427
3171.28133	15.30359698	3.68142E-06	2.1369E-06	4.533564663
3193.50205	15.41082712	3.32884E-06	1.93224E-06	4.565330708
3206.92737	15.47561343	3.13233E-06	1.81817E-06	4.584523121
		sum	24.22384253	177.9442502

Table 36 The calculation data of INT4

cm-1	x_i	pf	TS(kcal/mol)	E_{ZEP}(kcal/mol)
1476.167746	7.12351693	0.00655192	0.003803085	2.110283267
111.163044	0.536437561	1.634709717	0.94887308	0.158915213
28.48218	0.137445959	2.985311235	1.732834544	0.040717234

87.083232	0.420236033	1.874264671	1.087923607	0.124491466
112.219979	0.541537994	1.625472461	0.943511283	0.160426174
160.847291	0.776197965	1.278078974	0.741865495	0.229942259
206.786646	0.997886709	1.0425999	0.605180827	0.295615725
266.983268	1.288376497	0.813030839	0.471926648	0.381670934
361.914481	1.746484395	0.560519731	0.325355675	0.517381629
400.925319	1.934738315	0.48271556	0.280193967	0.573150304
472.177553	2.278578977	0.368092505	0.213660606	0.67501027
559.244861	2.698738166	0.264361905	0.15344981	0.799478972
636.912189	3.073536035	0.196430349	0.114018696	0.910509756
682.615748	3.294086902	0.164733803	0.095620323	0.975846136
717.06214	3.460314255	0.14417363	0.083686097	1.025089621
777.046558	3.749780014	0.114134616	0.066249844	1.11084147
840.729014	4.057091331	0.088870855	0.051585404	1.201879918
946.115579	4.565653438	0.058453732	0.033929677	1.352537258
974.511417	4.702682738	0.052160396	0.030276688	1.39313106
993.919607	4.796340502	0.048241567	0.028001989	1.420876402
1018.75688	4.916197316	0.043640466	0.025331264	1.456382996
1084.1215	5.231626183	0.033471552	0.019428681	1.549826203
1126.46395	5.43595742	0.02815503	0.016342687	1.61035765
1179.53424	5.692057778	0.022640605	0.01314182	1.686225273
1228.95231	5.930533715	0.018460385	0.010715397	1.756871807
1287.64892	6.213784941	0.014466403	0.008397075	1.840782652
1344.40009	6.487648052	0.011413348	0.006624919	1.921912345
1395.63996	6.734915384	0.009204541	0.005342809	1.995163257
1434.48722	6.922379919	0.007814576	0.004535999	2.050698083
1456.75997	7.029861145	0.007112769	0.004128632	2.082538511
1530.10542	7.383802998	0.005211347	0.003024945	2.187390872
1589.46706	7.670263433	0.004046413	0.002348755	2.272252419

2965.78205	14.31192268	9.32054E-06	5.41014E-06	4.239789313
3073.5885	14.8321624	5.72815E-06	3.32492E-06	4.393906049
3137.3225	15.13972241	4.29337E-06	2.4921E-06	4.485018171
3184.61027	15.36791819	3.4657E-06	2.01168E-06	4.552619291
3194.30151	15.41468503	3.31681E-06	1.92525E-06	4.566473584
678.315729	3.273336376	0.167491137	0.097220827	0.969698963
149.986733	0.72378836	1.344802183	0.78059522	0.214416345
53.261228	0.257021778	2.361342427	1.370649626	0.076140587
87.575165	0.422609945	1.868714202	1.084701818	0.125194718
135.149737	0.652189727	1.444956378	0.838730079	0.193205839
173.131296	0.835476674	1.208338738	0.701384527	0.247503089
217.213341	1.048202629	0.997481471	0.578991674	0.310521403
307.874792	1.485706011	0.691286523	0.401259726	0.440128179
373.771068	1.80370052	0.535564237	0.31087017	0.534331435
418.293024	2.018549346	0.451783651	0.26223943	0.597978632
519.983593	2.50927575	0.306963183	0.178177874	0.743352291
613.201611	2.959116313	0.215127157	0.124871325	0.876613855
663.24828	3.20062565	0.177509579	0.103036068	0.948159009
707.701453	3.415142551	0.149501406	0.086778624	1.011707875
763.2264	3.683088319	0.120467541	0.069925813	1.091084604
809.011662	3.904033459	0.100692838	0.058447517	1.156537783
864.98676	4.174151512	0.080744607	0.046868495	1.236558034
955.845436	4.612606639	0.056218833	0.032632422	1.366446757
978.11778	4.720085901	0.051409642	0.02984091	1.398286604
999.975019	4.825561998	0.047078317	0.027326777	1.429533029
1034.56003	4.992458292	0.040937353	0.023762232	1.478974683
1088.7788	5.254100849	0.032842156	0.019063346	1.556484137
1155.88084	5.577914002	0.024954615	0.014484995	1.652411119
1181.07664	5.699500911	0.022497192	0.013058575	1.68843024

1233.86055	5.954219323	0.018088855	0.010499741	1.763888474
1295.92855	6.253739773	0.01397577	0.008112285	1.852618942
1370.1004	6.611669604	0.010247414	0.005948148	1.958652709
1412.62128	6.816861844	0.008569439	0.004974161	2.019439221
1444.31319	6.969796965	0.007496968	0.004351642	2.064744992
1495.59194	7.21725191	0.006034112	0.003502522	2.138051483
1547.87803	7.469568001	0.004831725	0.002804592	2.212798049
1621.04614	7.822654068	0.003535313	0.002052085	2.31739689
1013.07866	4.888796019	0.044653317	0.025919177	1.448265588
3130.77317	15.10811746	4.42255E-06	2.56709E-06	4.475655465
3150.94738	15.20547178	4.03654E-06	2.34302E-06	4.504495879
3188.28071	15.3856306	3.40854E-06	1.9785E-06	4.557866448
3195.21163	15.41907699	3.30315E-06	1.91733E-06	4.567774664
219.218663	1.057879676	0.989095891	0.574124235	0.313388148
111.828575	0.539649203	1.628882526	0.945490667	0.159866635
71.117285	0.343189441	2.074365731	1.204072981	0.101667048
94.089602	0.45404655	1.798101448	1.043714393	0.134507554
148.252965	0.715421746	1.355939996	0.787060203	0.211937805
186.490137	0.8999422	1.138501478	0.66084724	0.26660047
251.201893	1.212220591	0.866609258	0.503026432	0.359110374
337.237319	1.627400245	0.616539691	0.357872661	0.48210393
390.07125	1.882360024	0.503153857	0.292057449	0.557633666
455.706252	2.199093707	0.391859004	0.227455955	0.651463413
548.353212	2.646178525	0.275559833	0.159949687	0.783908611
616.655232	2.975782391	0.212300077	0.123230336	0.881551044
666.614203	3.216868526	0.175222474	0.10170851	0.952970827
711.854971	3.43518611	0.14711432	0.085393031	1.017645615
767.669704	3.704530293	0.118395376	0.068723018	1.097436613
823.87453	3.975756941	0.094975587	0.055128918	1.177785275

887.718618	4.283848243	0.073783519	0.042827906	1.269054787
968.611825	4.67421318	0.053411463	0.031002874	1.384697188
991.379363	4.784082091	0.04873779	0.028290024	1.417244948
1001.06756	4.830834268	0.046871351	0.027206642	1.431094896
1061.47573	5.122344915	0.036702593	0.021304151	1.517452526
1116.9705	5.390145054	0.029270537	0.016990187	1.596786113
1169.52245	5.643744082	0.023593376	0.013694859	1.671912738
1195.26401	5.767964683	0.021218868	0.012316568	1.708712069
1258.61965	6.073698861	0.016323117	0.009474812	1.799283303
1333.49019	6.435000319	0.011946655	0.006934478	1.906315887
1381.9268	6.668740032	0.009750861	0.005659922	1.975559353
1432.62255	6.913381614	0.007876321	0.004571839	2.048032409
1448.9841	6.992337284	0.007350461	0.004266601	2.071422376
1514.70945	7.309506973	0.00556378	0.003229516	2.165381286
1550.56723	7.482545198	0.004776702	0.002772654	2.216642436
1931.92865	9.322874361	0.000922496	0.000535466	2.761824806
3069.18054	14.81089098	5.84344E-06	3.39184E-06	4.387604566
3132.56818	15.11677959	4.38677E-06	2.54631E-06	4.478221549
3164.63249	15.27151177	3.79398E-06	2.20223E-06	4.524059683
3190.31032	15.39542484	3.37734E-06	1.96039E-06	4.56076791
3201.56045	15.44971441	3.20947E-06	1.86295E-06	4.576850747
		sum	22.8753629	177.9498502

Table 37 The calculation data of TS2’

cm-1	x_i	pf	TS(kcal/mol)	E_{ZEP}(kcal/mol)
2160.168822	10.42428899	0.000339336	0.000196969	3.088109824
399.210267	1.926462019	0.485886662	0.282034644	0.570698519
163.656916	0.789756323	1.261620309	0.732312004	0.233958811
170.478212	0.822673733	1.222926524	0.709852059	0.243710323
48.388726	0.233508631	2.456805077	1.426061262	0.06917501

86.634901	0.41807253	1.879351362	1.090876195	0.123850546
126.42201	0.610072487	1.50954246	0.8762193	0.180728954
172.62761	0.833046045	1.211088991	0.70298092	0.246783035
225.290152	1.087178755	0.964251093	0.559702983	0.322067759
287.003631	1.384988413	0.750585324	0.435679926	0.41029142
323.140717	1.559374519	0.651247059	0.378018676	0.461951868
387.588378	1.870378472	0.507954713	0.294844124	0.55408423
421.589142	2.034455365	0.446147671	0.258968006	0.602690659
476.824113	2.301001801	0.361653667	0.20992316	0.681652847
551.720268	2.662426869	0.272049304	0.157911988	0.788722049
591.066228	2.852297981	0.234136135	0.135905154	0.844969804
630.16312	3.040967171	0.201585331	0.117010924	0.900861498
694.498621	3.351429875	0.157340268	0.091328719	0.99283352
721.554274	3.481991868	0.141682406	0.082240058	1.031511435
747.108628	3.605309068	0.128281727	0.074461585	1.068043141
797.675452	3.849328508	0.105275136	0.061107328	1.140331892
815.97004	3.937612382	0.097976043	0.056870543	1.166485263
880.240733	4.247762344	0.076006926	0.044118491	1.258364637
897.21502	4.329674864	0.071050299	0.041241399	1.282630547
943.990598	4.555398955	0.058953132	0.034219556	1.349499451
958.510583	4.625467793	0.055621221	0.032285536	1.370256768
973.407504	4.697355604	0.052392315	0.030411306	1.39155294
983.468861	4.745908519	0.050314912	0.02920547	1.405936342
1008.04713	4.864515419	0.045569811	0.026451159	1.44107266
1070.42427	5.165527714	0.035391216	0.020542957	1.530245075
1112.181	5.367032452	0.029849497	0.017326247	1.589939195
1148.15	5.540607423	0.025759651	0.014952281	1.641359352
1183.41223	5.710771726	0.022281711	0.012933498	1.691769127
1219.78412	5.88629096	0.019174403	0.01112985	1.743765255

1275.52462	6.155276908	0.015215347	0.008831802	1.823450129
1304.32459	6.294256431	0.013494848	0.007833133	1.864621668
1352.50265	6.526748454	0.011032412	0.006403803	1.933495517
1382.74777	6.672701768	0.009717279	0.005640429	1.976732985
1398.83689	6.750342778	0.009081553	0.00527142	1.999733495
1427.80195	6.890118943	0.008038169	0.004665784	2.041141034
1462.24398	7.056325251	0.006949685	0.00403397	2.090378285
1516.04079	7.315931588	0.005532401	0.003211302	2.167284526
1555.71837	7.507402964	0.004673022	0.002712472	2.224006345
1608.46474	7.761940245	0.003730842	0.00216558	2.29941092
2383.79935	11.50345894	0.000126225	7.32678E-05	3.407805042
3084.45502	14.88460074	5.45351E-06	3.16551E-06	4.409440475
1152.76477	5.562876852	0.025276113	0.01467161	1.647956487
2175.29307	10.49727382	0.000317467	0.000184275	3.109730981
3185.75069	15.37342151	3.44784E-06	2.00131E-06	4.554249606
3195.69038	15.4213873	3.29599E-06	1.91317E-06	4.568459075
1204.32733	5.811701369	0.020439571	0.011864222	1.721668703
593.084018	2.862035195	0.232337705	0.134861249	0.847854373
236.193668	1.139795662	0.921581944	0.534935524	0.337655085
119.343499	0.57591384	1.56550348	0.908702074	0.170609736
153.262323	0.739595317	1.324136598	0.768599807	0.219099026
63.534242	0.306596083	2.186131622	1.26894789	0.090826566
110.145269	0.531526102	1.643692112	0.954086944	0.157460234
144.016485	0.694977838	1.383760142	0.803208505	0.205881465
201.238898	0.971115038	1.067700822	0.619750747	0.287684838
247.988946	1.196715929	0.878032521	0.509657106	0.354517245
289.322658	1.396179302	0.743718107	0.431693826	0.413606628
338.856925	1.635215949	0.612683378	0.35563425	0.484419268
396.35472	1.912682055	0.491214627	0.285127281	0.566616318

451.428251	2.178449433	0.398280871	0.231183551	0.645347717
487.294384	2.351528005	0.347554859	0.201739457	0.696620819
569.009571	2.745859557	0.254702545	0.147843	0.813438296
618.463225	2.984507192	0.210834514	0.122379645	0.884135694
650.033587	3.136855737	0.186771466	0.108412163	0.929267697
703.70605	3.395862005	0.151832885	0.088131939	1.005996172
741.198971	3.576790939	0.131267526	0.076194703	1.05959488
758.339114	3.659503828	0.122787147	0.071272237	1.084097893
807.953016	3.898924769	0.101112485	0.058691102	1.155024376
829.620604	4.00348567	0.092850265	0.053895267	1.185999683
891.824175	4.303660357	0.072589642	0.042134916	1.274923963
906.09277	4.372516067	0.06858372	0.039809665	1.295321901
949.424769	4.581622539	0.057684158	0.033482975	1.357267972
966.811795	4.665526807	0.053798922	0.031227776	1.382123921
976.58323	4.71268065	0.05172781	0.030025592	1.396092859
1002.42068	4.837363986	0.046616243	0.027058564	1.433029271
1020.73697	4.925752583	0.04329253	0.025129303	1.459213666
1079.73808	5.210473214	0.034074619	0.019778734	1.54355981
1128.26176	5.444633071	0.027948486	0.016222798	1.61292774
1161.86744	5.606803429	0.02434808	0.01413293	1.660969374
1189.78764	5.741537436	0.021703694	0.012597987	1.700883215
1241.2421	5.989840326	0.0175438	0.010183361	1.774440902
1286.9374	6.210351352	0.014509343	0.008422	1.839765479
1320.72181	6.373384209	0.012601803	0.007314762	1.888062621
1368.33293	6.603140355	0.010323719	0.00599244	1.956125989
1388.85242	6.70216089	0.009471095	0.005497531	1.985460008
1412.75947	6.817528734	0.008564451	0.004971266	2.019636782
1443.10029	6.963943875	0.007535477	0.004373995	2.063011062
1467.9042	7.08363969	0.006785208	0.003938498	2.098469963

1536.37178	7.414042506	0.005074266	0.002945376	2.196349078
1565.66837	7.555418539	0.004478976	0.002599837	2.238230564
1638.85941	7.908615264	0.003275616	0.001901343	2.342862187
3012.24769	14.53615112	7.55742E-06	4.38673E-06	4.306215143
3093.71024	14.92926353	5.22997E-06	3.03575E-06	4.42267146
3162.28054	15.26016201	3.83461E-06	2.22581E-06	4.52069741
3178.08808	15.33644419	3.56964E-06	2.07201E-06	4.543295378
3186.41716	15.37663767	3.43745E-06	1.99528E-06	4.555202365
3196.36766	15.42465565	3.28589E-06	1.90731E-06	4.569427299
3206.45339	15.47332614	3.13907E-06	1.82209E-06	4.58384553
476.435274	2.299125387	0.362188135	0.210233394	0.681096975
178.098654	0.859447566	1.181685106	0.685913331	0.254604269
97.055752	0.468360249	1.767607737	1.02601421	0.138747869
42.22998	0.203788478	2.592401309	1.504768578	0.060370659
69.607466	0.335903534	2.095619339	1.216409713	0.099508658
117.570077	0.567355869	1.580073712	0.917159417	0.168074507
151.704102	0.732075838	1.333906783	0.774270945	0.216871442
202.210275	0.975802595	1.06324835	0.617166294	0.289073488
252.497379	1.218472195	0.86205436	0.500382525	0.36096236
316.457882	1.527125278	0.668448249	0.388003168	0.452398296
381.940973	1.843125888	0.519054	0.301286744	0.546010876
399.556944	1.928134972	0.485243922	0.281661564	0.571194118
470.286115	2.269451498	0.370746313	0.215201019	0.67230633
503.853721	2.431438108	0.326367262	0.18944104	0.72029353
574.318248	2.771477547	0.249596945	0.144879436	0.821027415
624.587157	3.014059343	0.205943099	0.119540406	0.892890276
677.071902	3.267334061	0.16829701	0.097688599	0.967920827
710.697046	3.429598332	0.147776071	0.085777147	1.015990282
744.604834	3.593226553	0.12953866	0.075191177	1.064463795

790.368571	3.81406782	0.108334575	0.06288319	1.129886203
813.719868	3.926753766	0.098846762	0.057375955	1.163268488
836.26862	4.035566885	0.090448549	0.052501182	1.195503479
892.193397	4.305442106	0.072483192	0.042073127	1.275451792
930.08328	4.488286653	0.06232483	0.03617667	1.329617984
954.304236	4.605169297	0.056567248	0.032834661	1.364243506
969.714499	4.679534335	0.053175446	0.030865877	1.386273536
981.262234	4.735260038	0.050763585	0.029465904	1.402781817
1006.71455	4.858084811	0.045815576	0.026593814	1.439167645
1036.07814	4.999784204	0.040686394	0.023616562	1.481144924
1092.25289	5.270865724	0.032380158	0.018795178	1.561450594
1129.37203	5.449990876	0.027821668	0.016149186	1.614514946
1176.92971	5.679489172	0.022884797	0.013283562	1.682501927
1198.68185	5.784458089	0.020921649	0.012144046	1.713598105
1254.09387	6.051858902	0.016632804	0.00965457	1.792813395
1297.68964	6.262238268	0.013873527	0.008052938	1.855136551
1345.12115	6.491127678	0.011378933	0.006604942	1.922943155
1377.22687	6.646059676	0.009945309	0.00577279	1.968840485
1395.1536	6.732568385	0.009223394	0.005353752	1.994467978
1419.81052	6.851554848	0.008313685	0.004825708	2.029716738
1454.85701	7.020678074	0.007170233	0.004161987	2.079818102
1497.71034	7.227474626	0.00598013	0.003471188	2.141079879
1551.86561	7.488810767	0.004750358	0.002757362	2.21849856
1585.10666	7.649221551	0.004122468	0.002392901	2.266018934
1682.35238	8.118498501	0.002717857	0.00157759	2.405038369
3036.44654	14.65292708	6.77502E-06	3.93258E-06	4.34080906
3122.13826	15.0664481	4.5988E-06	2.66939E-06	4.46331126
3166.83465	15.28213868	3.75632E-06	2.18037E-06	4.527207819
3183.76858	15.36385648	3.47895E-06	2.01937E-06	4.551416045

3191.19031	15.3996714	3.3639E-06	1.95259E-06	4.562025919
3201.64496	15.45012219	3.20824E-06	1.86223E-06	4.576971549
3222.21336	15.5493788	2.92262E-06	1.69645E-06	4.606375503
		sum	28.07199145	244.9110062

Table 38 The calculation data of TS2

cm-1	x_i	pf	TS(kcal/mol)	E_{ZEP}(kcal/mol)
1056.689754	5.099249305	0.037423183	0.02172242	1.510610642
269.91398	1.302519183	0.803520216	0.466406173	0.385860589
116.977128	0.564494485	1.584997029	0.920017174	0.167226846
159.776078	0.771028631	1.284437548	0.745556352	0.228410887
35.527932	0.171446521	2.764707736	1.604784458	0.050789621
75.513991	0.364406549	2.014999844	1.16961384	0.107952441
111.863205	0.539816316	1.628580312	0.945315246	0.159916141
148.226537	0.715294213	1.356110863	0.787159383	0.211900024
190.901473	0.921229907	1.116672905	0.648176767	0.272906778
244.797201	1.181313581	0.889562559	0.516349758	0.349954427
300.487087	1.450055292	0.711646536	0.413077768	0.429566947
372.138995	1.795824654	0.538928318	0.312822863	0.531998275
393.090323	1.896929112	0.497379994	0.28870599	0.561949638
431.350815	2.0815621	0.429875153	0.249522564	0.616645642
513.581832	2.478382884	0.314523774	0.182566445	0.734200533
570.181743	2.751516087	0.253566501	0.147183579	0.815113997
612.209843	2.954330355	0.215945743	0.125346476	0.875196055
647.842907	3.12628421	0.188351415	0.10932925	0.926135969
697.585707	3.366327172	0.155472582	0.090244614	0.997246721
728.798029	3.51694793	0.137752476	0.079958915	1.041866881
753.193682	3.634673607	0.125275802	0.072716786	1.076742144
825.535223	3.983770919	0.094356567	0.054769606	1.18015935
841.775442	4.06214106	0.088504583	0.051372801	1.203375859

881.540303	4.254033656	0.075615936	0.043891539	1.260222461
924.758077	4.462588914	0.063664586	0.036954336	1.32200524
949.560689	4.582278445	0.05765276	0.03346475	1.357462279
973.594462	4.698257804	0.052352968	0.030388467	1.39182021
991.206809	4.7832494	0.048771676	0.028309693	1.41699827
1005.65133	4.852954054	0.046012582	0.026708167	1.4376477
1057.215	5.10178397	0.037343435	0.02167613	1.511361516
1110.69283	5.359850992	0.030031645	0.017431975	1.587811747
1139.14118	5.497133703	0.026729658	0.015515325	1.62848062
1172.44962	5.657869646	0.023310847	0.013530864	1.676097321
1219.07749	5.882880988	0.019230539	0.011162435	1.742755079
1240.14241	5.98453359	0.017623973	0.010229898	1.772868826
1303.636	6.29093349	0.013533674	0.007855669	1.863637274
1336.92832	6.451591681	0.011776012	0.006835428	1.911230942
1369.0806	6.606748363	0.010291373	0.005973664	1.957194832
1395.33356	6.733436805	0.009216414	0.0053497	1.99472524
1426.23291	6.882547283	0.008091548	0.004696768	2.038897992
1454.52182	7.019060577	0.007180401	0.004167889	2.079338932
1514.84721	7.310171725	0.005560525	0.003227626	2.165578214
1555.03061	7.504084067	0.004686736	0.002720432	2.223023149
1578.91759	7.619355074	0.004232839	0.002456967	2.257171236
1691.71174	8.163663796	0.00261067	0.001515373	2.418418216
3018.88613	14.56818609	7.33424E-06	4.25719E-06	4.31570524
3134.27955	15.12503812	4.35292E-06	2.52667E-06	4.48066807
3176.70629	15.32977609	3.59206E-06	2.08502E-06	4.541320007
3184.00093	15.36497771	3.47529E-06	2.01724E-06	4.551748198
3190.94145	15.39847047	3.36769E-06	1.95479E-06	4.561670154
3202.94995	15.45641968	3.18932E-06	1.85125E-06	4.578837129
539.290627	2.602445367	0.285231162	0.165563444	0.770953023

250.760341	1.210089801	0.868168402	0.503931443	0.358479145
187.64227	0.905502028	1.132744242	0.657505432	0.268247524
145.215683	0.700764787	1.375796314	0.798585873	0.207595801
164.301547	0.792867108	1.257887996	0.73014557	0.234880356
81.711404	0.394313296	1.937062896	1.124375061	0.116812069
124.017742	0.598470253	1.528169693	0.887031544	0.177291887
161.219102	0.777992207	1.275882829	0.740590735	0.230473789
214.244591	1.033876384	1.01006488	0.586295759	0.30627737
270.004873	1.302957804	0.803227358	0.466236182	0.385990526
333.577353	1.609738411	0.625351914	0.362987747	0.476871757
376.93248	1.818956491	0.529110767	0.30712423	0.538850891
403.249121	1.945952246	0.47845311	0.277719813	0.576472338
488.789654	2.358743703	0.345586698	0.20059703	0.698758411
533.0569	2.57236338	0.292076646	0.16953693	0.762041482
589.62917	2.845363196	0.235425233	0.136653415	0.84291543
623.394702	3.008304934	0.206886835	0.1200882	0.89118558
660.522204	3.187470473	0.179383065	0.104123539	0.944261896
721.550698	3.481974611	0.141684373	0.082241199	1.031506323
737.91774	3.56095676	0.132954166	0.077173719	1.054904135
763.476244	3.684293987	0.120350102	0.069857646	1.091441773
831.276557	4.011476774	0.092246333	0.053544713	1.188366981
850.542918	4.104450116	0.085492459	0.049624403	1.215909569
893.312176	4.310840978	0.072161559	0.041886434	1.277051163
927.768932	4.477118344	0.062903711	0.036512683	1.326309464
952.847024	4.598137255	0.056898596	0.033026993	1.362160321
980.702412	4.732558515	0.050878028	0.029532333	1.401981513
993.948026	4.796477643	0.048236043	0.027998783	1.420917029
1017.32138	4.909270005	0.043894402	0.025478662	1.454330838
1081.61719	5.219541203	0.033814812	0.019627928	1.546246126

1117.9563	5.394902202	0.029152733	0.016921808	1.598195379
1152.91313	5.563592771	0.025260715	0.014662672	1.648168572
1184.80812	5.717507844	0.022153887	0.012859302	1.693764646
1228.54504	5.92856834	0.018491546	0.010733484	1.756289581
1252.23514	6.042889266	0.016761646	0.009729357	1.790156215
1311.70469	6.32987045	0.013085502	0.007595526	1.875172029
1345.90909	6.494929988	0.011341442	0.00658318	1.924069558
1376.26475	6.641416771	0.009985581	0.005796166	1.967465062
1406.84719	6.788997947	0.008780418	0.005096625	2.011184771
1447.31409	6.98427836	0.007402517	0.004296817	2.069034986
1467.14427	7.07997248	0.006807067	0.003951186	2.097383582
1522.54291	7.347308755	0.005381632	0.003123787	2.176579753
1557.79534	7.517425805	0.004631846	0.002688571	2.226975529
1593.10976	7.687841952	0.003983935	0.002312489	2.27745991
1905.43257	9.1950127	0.001035348	0.000600972	2.723946841
3070.32237	14.81640109	5.81335E-06	3.37438E-06	4.389236889
3135.89009	15.13281006	4.3213E-06	2.50831E-06	4.482970442
3178.57369	15.3387876	3.5618E-06	2.06746E-06	4.543989594
3185.72103	15.37327838	3.44831E-06	2.00158E-06	4.554207205
3193.77411	15.41213999	3.32474E-06	1.92986E-06	4.565719636
3204.98309	15.46623096	3.16006E-06	1.83427E-06	4.581743639
374.613954	1.80776802	0.53383555	0.309866748	0.535536399
135.803086	0.655342582	1.440301925	0.836028385	0.194139847
181.252812	0.874668532	1.165189577	0.676338442	0.259113354
143.199408	0.691034884	1.389227452	0.806382025	0.204713397
168.270389	0.81201948	1.235259808	0.717010957	0.240554088
94.484887	0.45595407	1.793980678	1.041322477	0.135072641
135.574877	0.654241318	1.441924954	0.836970478	0.193813606
178.167843	0.859781451	1.181319754	0.685701261	0.254703179

223.888178	1.080413273	0.969916754	0.562991636	0.320063541
292.874659	1.413320131	0.733338965	0.425669215	0.418684458
354.0458	1.708512638	0.577763363	0.335364803	0.506132809
390.771342	1.885738445	0.501808755	0.29127668	0.558634496
412.722338	1.991666984	0.461475799	0.267865272	0.590014953
504.077321	2.432517131	0.326090137	0.189280182	0.720613181
542.112976	2.616065127	0.282183997	0.163794707	0.774987765
600.904999	2.899776767	0.225493292	0.130888385	0.859035003
632.041355	3.050030937	0.20013769	0.116170635	0.903546564
667.258181	3.219976159	0.17478816	0.10145641	0.953891438
723.589436	3.491812913	0.14056748	0.081592895	1.034420839
743.688437	3.588804312	0.130001664	0.075459929	1.063153743
780.359589	3.76576765	0.112664855	0.065396717	1.115577676
835.513167	4.031921309	0.090718422	0.052657831	1.194423507
861.779331	4.158673478	0.081776432	0.047467421	1.231972794
917.288634	4.426543753	0.065590778	0.038072401	1.311327158
940.481826	4.538466735	0.059786782	0.034703451	1.34448342
971.08278	4.686137224	0.05288398	0.030696695	1.388229588
984.252134	4.749688346	0.050156573	0.029113562	1.407056084
1000.23511	4.826817119	0.047028967	0.027298131	1.429904849
1026.12879	4.95177178	0.042358658	0.024587234	1.466921639
1091.49486	5.267207693	0.032480423	0.018853377	1.560366932
1130.10521	5.453528999	0.027738228	0.016100753	1.615563086
1170.71024	5.649475984	0.023478332	0.013628081	1.673610767
1188.81831	5.736859772	0.021790626	0.012648446	1.699497495
1234.22915	5.95599806	0.018061251	0.010483717	1.76441541
1276.92589	6.162038964	0.01512689	0.008780457	1.825453332
1327.44307	6.405818862	0.012252673	0.007112108	1.89767112
1362.24535	6.573763598	0.010590814	0.006147476	1.947423366

1378.06906	6.650123799	0.009910189	0.005752404	1.970044447
1410.36769	6.805986748	0.008651185	0.005021611	2.016217564
1453.62668	7.014740906	0.007207626	0.004183692	2.078059265
1485.3977	7.168057768	0.006300649	0.003657234	2.123478123
1541.25119	7.437588951	0.004969985	0.002884846	2.203324518
1570.27127	7.577630664	0.004391911	0.0025493	2.244810723
1633.44828	7.882502854	0.003352452	0.001945943	2.3351266
3004.60212	14.499256	7.82284E-06	4.54079E-06	4.295285267
3081.12851	14.86854806	5.53616E-06	3.21349E-06	4.404684999
3170.7865	15.30120906	3.68968E-06	2.14169E-06	4.53285726
3182.12793	15.35593919	3.5049E-06	2.03443E-06	4.549070613
3188.24795	15.3854725	3.40905E-06	1.97879E-06	4.557819612
3197.05774	15.42798576	3.27563E-06	1.90135E-06	4.570413815
3209.65593	15.48878062	3.09383E-06	1.79583E-06	4.588423791
		sum	28.45055214	244.657961

Table 39 The calculation data of INT6

cm-1	x_i	pf	TS(kcal/mol)	E_{ZEP}(kcal/mol)
272.713769	1.316030076	0.794556631	0.461203228	0.38986308
118.746676	0.573033762	1.570381279	0.911533409	0.169756536
72.620581	0.35044387	2.053656188	1.192052053	0.103816113
93.58712	0.451621732	1.803365649	1.046770018	0.133789221
118.171849	0.570259829	1.575103806	0.914274617	0.168934781
159.543522	0.76990639	1.285824156	0.746361213	0.228078432
198.745438	0.959082392	1.079244503	0.626451318	0.284120266
222.827439	1.075294484	0.974231569	0.565496186	0.318547142
275.767244	1.330765177	0.784914263	0.455606281	0.394228232
318.476019	1.536864167	0.663201202	0.384957501	0.455283362
369.497151	1.783075953	0.544421246	0.316011253	0.528221577
416.70474	2.010884792	0.45452549	0.26383094	0.595708071

456.763403	2.204195183	0.390288252	0.226544207	0.652974683
512.878483	2.474988745	0.315365593	0.183055082	0.733195047
561.63508	2.710272604	0.261964834	0.152058422	0.802895954
613.266853	2.95943115	0.215073414	0.124840129	0.876707123
652.562516	3.149059545	0.18496353	0.10736274	0.932882975
700.403552	3.379925198	0.153786495	0.089265919	1.001275024
732.916372	3.536821746	0.135565287	0.078689354	1.047754336
761.656231	3.675511182	0.121208129	0.07035569	1.08883994
802.490302	3.872563446	0.103304843	0.059963665	1.147215051
826.69179	3.989352144	0.09392776	0.054520703	1.181812742
874.855336	4.221774127	0.077648078	0.045071104	1.250665842
913.405117	4.407803133	0.066614364	0.038666545	1.305775404
956.275227	4.614680674	0.056122042	0.032576239	1.367061173
979.67692	4.727609816	0.051088314	0.029654394	1.400515502
999.11979	4.821434934	0.047240945	0.027421175	1.428310421
1011.08915	4.879195242	0.045013554	0.026128278	1.445421437
1034.95849	4.994381143	0.040871338	0.023723914	1.479544312
1080.43773	5.213849517	0.033977659	0.019722453	1.544560012
1110.20375	5.357490842	0.030091742	0.017466859	1.587112572
1166.38293	5.628593726	0.023900106	0.013872902	1.66742457
1179.47467	5.691770312	0.022646161	0.013145045	1.686140114
1230.56251	5.938304039	0.018337688	0.010644176	1.759173702
1264.20916	6.100672057	0.015948401	0.009257306	1.807273891
1294.74863	6.248045859	0.014044683	0.008152286	1.850932167
1329.92572	6.417799318	0.012126121	0.00703865	1.901220232
1364.60023	6.585127535	0.0104867	0.006087043	1.950789839
1400.80807	6.759855052	0.009006524	0.005227869	2.002551428
1434.5421	6.922644791	0.007812766	0.004534948	2.050776549
1456.99668	7.031003437	0.007105653	0.004124502	2.082876906

1497.18302	7.224929986	0.005993522	0.003478961	2.14032605
1566.21449	7.558053907	0.004468558	0.00259379	2.23901127
1596.40358	7.703736906	0.003928258	0.002280172	2.28216866
1620.83359	7.821628379	0.003538531	0.002053953	2.317093038
3014.41661	14.5466176	7.48377E-06	4.34398E-06	4.309315752
3079.55231	14.86094183	5.57576E-06	3.23647E-06	4.402431717
3166.17755	15.27896777	3.76752E-06	2.18687E-06	4.526268461
3180.92388	15.35012883	3.52407E-06	2.04556E-06	4.547349341
3189.14249	15.38978925	3.39526E-06	1.97079E-06	4.559098414
1200.4579	5.793028714	0.020768807	0.012055328	1.716137082
136.360978	0.658034792	1.436346451	0.833732416	0.194937392
43.609751	0.210446814	2.560365608	1.486173341	0.062343137
76.568553	0.36949553	2.001285913	1.16165354	0.10946001
96.672529	0.466510936	1.77149278	1.028269297	0.138200026
133.612932	0.644773594	1.456000172	0.845140488	0.191008871
177.126386	0.85475571	1.186836059	0.68890322	0.253214345
211.002947	1.018233239	1.024041106	0.594408309	0.301643217
231.569068	1.11747881	0.93938412	0.54526886	0.331043901
303.995289	1.466984761	0.701895099	0.407417511	0.434582163
332.43387	1.604220325	0.628133239	0.364602177	0.475237069
391.50378	1.889272959	0.500405524	0.29046217	0.559681566
419.494573	2.02434764	0.449720724	0.261041997	0.599696329
484.42389	2.337675912	0.351364571	0.203950818	0.692517251
533.179429	2.572954666	0.291940546	0.16945793	0.762216645
580.095539	2.799356919	0.244154298	0.141720233	0.82928645
628.815859	3.034465717	0.202629979	0.117617293	0.898935496
663.785118	3.20321626	0.177142878	0.102823215	0.948926456
713.46716	3.442966023	0.146197721	0.084860988	1.01995035
745.376788	3.596951758	0.129149869	0.074965502	1.065567357

764.853787	3.690941572	0.119704571	0.069482945	1.093411066
806.301517	3.890955159	0.101770508	0.059073054	1.152663445
839.428863	4.050817215	0.089327972	0.05185074	1.200021263
900.896846	4.347442188	0.070017125	0.04064169	1.28789397
922.727101	4.452788068	0.064182848	0.037255163	1.31910182
961.281256	4.638838181	0.055006459	0.031928695	1.374217635
981.617702	4.736975414	0.050691047	0.029423799	1.403289983
1000.27793	4.827023736	0.047020847	0.027293418	1.429966057
1022.79201	4.935669544	0.042934265	0.024921347	1.462151484
1041.39155	5.025425043	0.039819721	0.023113499	1.488740812
1087.36031	5.247255657	0.033032627	0.019173906	1.554456306
1138.77725	5.495377521	0.02676958	0.015538498	1.627960366
1168.61499	5.639364963	0.023681639	0.013746092	1.67061546
1194.19062	5.76278482	0.021313058	0.01237124	1.707177577
1238.43999	5.976318256	0.017748795	0.010302351	1.770435101
1269.61264	6.126747555	0.015594143	0.009051676	1.814998542
1313.469	6.338384412	0.012989454	0.007539775	1.87769422
1335.53152	6.444851129	0.011845049	0.006875501	1.909234108
1373.72237	6.629148072	0.010092766	0.005858382	1.963830561
1406.64839	6.788038597	0.008787771	0.005100893	2.010900571
1438.51513	6.941817339	0.007682816	0.004459518	2.056456258
1463.60746	7.062904987	0.00690971	0.004010766	2.092327477
1516.48518	7.318076082	0.005521966	0.003205245	2.167919814
1566.94326	7.561570749	0.004454692	0.002585742	2.240053106
1600.18775	7.721998109	0.003865238	0.002243591	2.287578391
2698.02949	13.01983381	3.10672E-05	1.80331E-05	3.857018618
3030.8626	14.62598077	6.94808E-06	4.03304E-06	4.332826437
3113.28462	15.02372328	4.78678E-06	2.7785E-06	4.450654382
3171.57794	15.30502832	3.67648E-06	2.13403E-06	4.533988684

3184.53512	15.36755554	3.46688E-06	2.01237E-06	4.552511861
3189.96886	15.39377705	3.38257E-06	1.96342E-06	4.560279767
3206.54879	15.47378652	3.13771E-06	1.8213E-06	4.583981912
175.258306	0.845740949	1.196822372	0.694699811	0.250543796
53.245422	0.256945504	2.361637607	1.370820964	0.076117991
81.244326	0.392059326	1.942722202	1.127660025	0.116144349
104.698847	0.505243399	1.693283852	0.982872646	0.149674199
147.248262	0.710573368	1.362459118	0.79084425	0.210501513
191.251879	0.922920855	1.114963643	0.64718462	0.273407708
218.726653	1.055505392	0.991144894	0.575313586	0.312684786
264.946618	1.278548271	0.819718515	0.475808533	0.378759403
309.511827	1.493605822	0.686864144	0.39869274	0.442468433
343.671944	1.658451702	0.601372634	0.349068888	0.491302668
398.295977	1.922049945	0.487586002	0.283021033	0.569391479
448.786654	2.165701924	0.402299302	0.233516063	0.641571372
495.899619	2.393054137	0.336379069	0.19525243	0.708922594
553.659858	2.671786714	0.27004703	0.156749761	0.791494826
587.798653	2.836529702	0.237077304	0.137612366	0.840298581
639.526973	3.086154153	0.194467721	0.112879482	0.91424777
695.456811	3.356053796	0.156758256	0.090990888	0.994203318
727.4012	3.510207276	0.138502013	0.080393987	1.039870018
757.97625	3.657752762	0.122961076	0.071373195	1.083579154
769.380712	3.712787075	0.117606637	0.068265192	1.099882616
818.915843	3.951827892	0.096847317	0.05621537	1.170696491
852.214699	4.1125176	0.084929444	0.049297598	1.218299495
908.663034	4.384919345	0.067885175	0.039404192	1.29899627
945.824703	4.564249763	0.058521849	0.033969216	1.35212143
975.005284	4.705065983	0.052056962	0.030216649	1.393837077
990.636128	4.780495475	0.048883909	0.028374839	1.416182443

1008.74093	4.867863487	0.045442361	0.026377181	1.442064497
1027.66805	4.959199765	0.042095657	0.024434574	1.469122118
1066.59282	5.147038338	0.035947041	0.020865588	1.52476775
1089.52466	5.257700133	0.032742432	0.019005462	1.557550396
1149.16039	5.545483254	0.025653018	0.014890386	1.642803777
1171.49575	5.653266601	0.02340255	0.013584094	1.674733706
1213.06189	5.853851568	0.019714964	0.011443621	1.734155352
1251.7723	6.040655723	0.01679388	0.009748067	1.789494546
1284.23301	6.197300824	0.014673689	0.008517395	1.835899368
1315.56549	6.348501446	0.012876218	0.007474047	1.880691308
1362.06562	6.572896278	0.010598802	0.006152112	1.94716643
1396.71708	6.740113223	0.009162922	0.005318651	1.996703074
1415.20983	6.829353364	0.008476477	0.004920201	2.023139731
1444.4994	6.97069555	0.007491073	0.00434822	2.065011191
1470.42394	7.095799136	0.006713223	0.003896714	2.102072098
1535.90737	7.411801391	0.005084303	0.002951202	2.195685166
1590.72191	7.67631897	0.004024782	0.002336199	2.274046322
1614.53307	7.791224079	0.00363524	0.002110088	2.308086015
3008.54896	14.51830221	7.68468E-06	4.4606E-06	4.300927549
3064.11341	14.78643859	5.97882E-06	3.47043E-06	4.380360745
3159.32282	15.24588902	3.88632E-06	2.25583E-06	4.516469153
3176.21364	15.32739871	3.60008E-06	2.08968E-06	4.54061573
3187.54103	15.38206113	3.41999E-06	1.98514E-06	4.556809023
3196.64047	15.42597212	3.28183E-06	1.90495E-06	4.569817292
3207.80491	15.47984817	3.1199E-06	1.81096E-06	4.585777627
		sum	28.58463531	244.6952004

Table 40 The calculation data of INT5

cm-1	x_i	pf	TS(kcal/mol)	E_{ZEP}(kcal/mol)
148.806909	0.718094904	1.352366129	0.784985739	0.212729706

162.349332	0.783446338	1.269241054	0.736735493	0.23208953
177.379067	0.855975068	1.185494345	0.688124417	0.25357557
106.489098	0.513882582	1.67669148	0.973241545	0.152233486
121.444128	0.586050809	1.548537666	0.898854206	0.173612729
156.819014	0.756758779	1.302236024	0.755887541	0.22418356
175.587009	0.847327165	1.195056595	0.693674859	0.251013699
219.695699	1.060181701	0.987114436	0.572974092	0.314070104
255.017166	1.230631887	0.853277438	0.49528793	0.364564569
311.127902	1.501404487	0.68252945	0.396176651	0.444778723
367.018768	1.771116064	0.549628272	0.319033689	0.524678558
414.866744	2.002015206	0.457719774	0.265685074	0.593080529
459.088891	2.215417249	0.386855277	0.224551524	0.656299128
507.636224	2.449691267	0.321710616	0.186738074	0.725700878
546.516	2.637312724	0.277494046	0.161072408	0.78128219
617.834306	2.981472228	0.211343199	0.122674913	0.883236611
636.444243	3.071277876	0.196783605	0.114223745	0.909840795
697.026871	3.363630407	0.155809083	0.090439937	0.996447827
718.044166	3.465053201	0.143625438	0.083367897	1.026493495
739.415113	3.568182607	0.132181899	0.076725454	1.057044732
785.840878	3.792218611	0.110273177	0.064008458	1.123413555
844.873333	4.077090499	0.087428772	0.050748342	1.207804507
867.144627	4.184564693	0.080057504	0.046469664	1.239642853
932.127228	4.498150097	0.061817866	0.035882401	1.332539948
964.863565	4.656125267	0.054221344	0.031472972	1.379338792
980.548414	4.731815369	0.050909553	0.029550632	1.401761362
1002.21241	4.836358937	0.046655421	0.027081305	1.432731534
1016.07531	4.903256872	0.044115987	0.025607282	1.452549496
1034.43786	4.991868728	0.040957614	0.023773993	1.47880003
1083.3386	5.227848152	0.033578497	0.019490758	1.548706992

1113.08518	5.371395709	0.029739355	0.017262314	1.591231774
1164.94903	5.621674213	0.024041484	0.013954965	1.665374722
1183.31131	5.710284719	0.02229098	0.012938879	1.691624854
1212.65529	5.851889475	0.019748131	0.011462873	1.733574098
1257.7002	6.069261906	0.016385573	0.009511065	1.797968892
1295.94044	6.25379715	0.013975077	0.008111883	1.85263594
1335.90075	6.446632926	0.011826762	0.006864886	1.909761951
1363.37674	6.579223346	0.010540668	0.006118368	1.949040772
1397.88471	6.74574785	0.009118015	0.005292584	1.998372286
1438.69146	6.942668276	0.007677098	0.004456199	2.056708341
1452.94617	7.011456986	0.007228392	0.004195746	2.07708643
1496.87182	7.223428214	0.00600144	0.003483557	2.139881162
1561.84004	7.53694421	0.00455268	0.002642619	2.232757696
1594.16748	7.692946168	0.003965972	0.002302062	2.278971992
1634.19849	7.886123148	0.003341694	0.001939698	2.336199083
3005.41973	14.50320154	7.79401E-06	4.52406E-06	4.296454101
3111.41358	15.01469423	4.82747E-06	2.80212E-06	4.4479796
3170.0032	15.29742913	3.7028E-06	2.1493E-06	4.531737486
3179.79083	15.34466112	3.54221E-06	2.05609E-06	4.545729576
3190.60496	15.39684667	3.37283E-06	1.95777E-06	4.561189117
3198.53018	15.43509129	3.25385E-06	1.88871E-06	4.57251877
126.556827	0.610723071	1.508509109	0.875619488	0.180921684
164.630749	0.794455732	1.255988196	0.729042824	0.235350973
85.796478	0.414026567	1.888937083	1.096440261	0.122651963
109.202147	0.526974895	1.652093562	0.958963595	0.156111976
126.751084	0.611660494	1.507022213	0.874756414	0.181199388
164.431363	0.793493559	1.257138336	0.729710427	0.235065937
187.345707	0.904070909	1.134222335	0.658363396	0.267823567
235.512783	1.136509927	0.924176401	0.536441485	0.336681713

285.689088	1.378644846	0.754510394	0.437958247	0.40841219
329.318012	1.589184183	0.635780981	0.369041336	0.470782736
403.886805	1.949029506	0.477290269	0.277044838	0.577383952
423.079902	2.0416493	0.443622383	0.257502193	0.604821803
468.843476	2.26248978	0.372783329	0.216383412	0.670243978
526.895058	2.542628286	0.29900219	0.173556887	0.753232705
569.705581	2.74921828	0.254027388	0.147451103	0.81443329
627.158561	3.026468123	0.203922233	0.118367387	0.896566275
664.55685	3.206940393	0.17661701	0.102517973	0.9500297
706.574384	3.409703674	0.150155572	0.087158337	1.010096653
733.47085	3.539497481	0.135273384	0.078519918	1.048547
755.104935	3.643896707	0.124345773	0.072176947	1.079474412
814.323796	3.929668131	0.098612338	0.057239883	1.164131844
861.475112	4.157205414	0.081874957	0.04752461	1.231537892
868.748307	4.192303544	0.079550522	0.046175384	1.241935424
942.827364	4.549785557	0.059228252	0.03437925	1.347836528
973.784731	4.699175982	0.052312952	0.03036524	1.392092212
984.921018	4.752916168	0.050021741	0.029035298	1.4080123
1006.2901	4.85603655	0.045894125	0.026639408	1.438560865
1019.37431	4.919176799	0.043531684	0.025268121	1.457265644
1044.31371	5.039526445	0.039350741	0.022841278	1.492918236
1087.00653	5.245548447	0.033080297	0.019201576	1.553950558
1136.64327	5.485079572	0.027004845	0.015675059	1.624909683
1170.03186	5.646202337	0.02354397	0.013666181	1.672640976
1192.58786	5.755050423	0.021454457	0.012453316	1.704886326
1235.83239	5.963734783	0.017941659	0.0104143	1.76670735
1269.21083	6.124808567	0.01562022	0.009066812	1.814424133
1320.33922	6.371537941	0.012621966	0.007326465	1.88751568
1347.50159	6.502614892	0.011266037	0.006539411	1.926346148

1371.67176	6.619252465	0.010180038	0.00590904	1.960899069
1406.44053	6.787035535	0.008795467	0.00510536	2.010603423
1449.31715	6.993944463	0.007340123	0.0042606	2.07189849
1464.79414	7.068631518	0.006875103	0.003990678	2.094023915
1519.3285	7.331797023	0.005455655	0.003166755	2.17198453
1564.0507	7.547612187	0.004509975	0.002617831	2.235917996
1595.8004	7.700826122	0.003938397	0.002286056	2.281306364
1910.90483	9.22142008	0.001010975	0.000586824	2.73176981
2244.96256	10.83347664	0.000233454	0.000135509	3.209328299
3155.04548	15.22524793	3.96233E-06	2.29995E-06	4.510354402
3176.64637	15.32948696	3.59303E-06	2.08559E-06	4.541234356
3186.66822	15.37784923	3.43354E-06	1.99301E-06	4.555561281
3195.00708	15.41808991	3.30622E-06	1.91911E-06	4.567482252
3201.36089	15.44875137	3.21237E-06	1.86463E-06	4.576565457
56.389528	0.272117961	2.304599267	1.337712857	0.080612707
70.178171	0.338657575	2.087530831	1.21171471	0.10032452
94.766161	0.457311409	1.791059296	1.039626751	0.135474742
118.800509	0.573293543	1.569940245	0.91127741	0.169833494
142.208439	0.686252782	1.395903667	0.810257258	0.203296739
173.715627	0.83829647	1.205159301	0.699539011	0.24833843
191.82797	0.925700887	1.112161248	0.64555796	0.27423127
249.68771	1.204913625	0.87197012	0.506138163	0.356945745
298.439001	1.440171879	0.717410223	0.41642332	0.426639067
335.617262	1.619582364	0.620423535	0.360127052	0.479787947
404.759795	1.953242279	0.475703084	0.27612355	0.578631951
450.086201	2.171973125	0.400317314	0.232365611	0.643429164
482.175359	2.326825215	0.354377919	0.205699926	0.689302821
541.919135	2.615129712	0.282392251	0.163915588	0.774710656
598.135592	2.886412488	0.227894132	0.132281961	0.855075945

632.030585	3.049978964	0.200145962	0.116175437	0.903531168
687.887822	3.319528258	0.161412992	0.093692746	0.983382928
709.538675	3.424008401	0.148440952	0.086163079	1.014334311
736.34825	3.553382899	0.133768298	0.077646285	1.052660441
782.295617	3.775110307	0.111814441	0.064903091	1.118345361
836.738302	4.037833421	0.090281153	0.052404017	1.196174921
863.423659	4.166608483	0.081245875	0.047159458	1.234323474
897.463934	4.330876044	0.070979988	0.041200587	1.282986387
944.640051	4.558533009	0.058800066	0.034130708	1.350427889
978.266628	4.720804194	0.051378881	0.029823054	1.398499392
997.728514	4.814721078	0.047506669	0.027575415	1.426321496
1007.88744	4.86374482	0.045599195	0.026468215	1.440844376
1030.5048	4.972889044	0.041615101	0.024155634	1.473177454
1077.82276	5.201230483	0.034341426	0.019933603	1.540821727
1097.14125	5.294455388	0.031740757	0.018424036	1.568438837
1144.42911	5.522651589	0.026156068	0.015182383	1.636040084
1176.53184	5.677569148	0.022922325	0.013305345	1.681933136
1205.92451	5.819408872	0.02030516	0.011786202	1.723951987
1248.54472	6.025080461	0.017020348	0.009879522	1.784880503
1283.66596	6.194564411	0.014708379	0.008537531	1.835088728
1331.56974	6.425732871	0.012043021	0.006990415	1.903570482
1361.3087	6.569243627	0.010632506	0.006171676	1.946084362
1386.84694	6.692483071	0.009551289	0.00554408	1.982593033
1427.46034	6.888470427	0.008049761	0.004672513	2.040652675
1452.49214	7.009265976	0.007242279	0.004203806	2.076437362
1471.03437	7.098744863	0.006695897	0.003886657	2.102944746
1529.50239	7.380892972	0.005224729	0.003032712	2.186528801
1584.28613	7.645261905	0.004136937	0.0024013	2.264845922
1610.16028	7.770122378	0.003703883	0.002149932	2.301834809

2998.31833	14.46893244	8.04791E-06	4.67144E-06	4.286302161
3084.36652	14.8841737	5.4557E-06	3.16678E-06	4.409313968
3160.3575	15.25088201	3.86815E-06	2.24528E-06	4.517948287
3178.93154	15.34051445	3.55603E-06	2.06411E-06	4.544501158
3187.11236	15.3799925	3.42664E-06	1.989E-06	4.556196205
3196.92055	15.42732372	3.27767E-06	1.90254E-06	4.570217691
3221.61973	15.54651409	2.9305E-06	1.70102E-06	4.605526857
		sum	28.15036926	245.2437758

Table 41 The calculation data of (5R, 6S, 11S)-3

cm-1	x_i	pf	TS(kcal/mol)	E_{ZEP}(kcal/mol)
182.72824	0.881788479	1.157583946	0.671923726	0.26122258
22.915742	0.110584096	3.202488375	1.858895789	0.032759628
75.71571	0.36537998	2.01236153	1.168082421	0.108240812
135.532333	0.654036014	1.442227852	0.837146296	0.193752787
164.953338	0.796012444	1.254130624	0.72796459	0.235812136
218.282151	1.053360367	0.993000739	0.576390818	0.31204934
276.963889	1.336539806	0.781172817	0.453434545	0.395938918
333.687658	1.610270708	0.625084329	0.362832426	0.477029445
389.036534	1.877366813	0.505148782	0.29321541	0.556154468
426.779869	2.059504166	0.437417863	0.253900757	0.61011116
466.050781	2.24901312	0.376758631	0.21869089	0.666251628
541.399774	2.612623441	0.282950973	0.164239901	0.773968194
597.766583	2.884631768	0.228215905	0.132468735	0.854548422
613.526613	2.960684669	0.214859564	0.124715999	0.877078468
674.467201	3.254764601	0.169996757	0.098675223	0.964197228
712.924145	3.440345605	0.146505831	0.085039832	1.019174073
743.714219	3.588928728	0.129988616	0.075452356	1.0631906
775.617646	3.742884538	0.114774215	0.066621102	1.108798742
817.970435	3.947265653	0.09720819	0.05642484	1.169344965

843.58527	4.070874715	0.08787454	0.05100709	1.205963133
881.85007	4.255528493	0.075523026	0.04383761	1.260665295
917.887991	4.429436059	0.065434164	0.037981493	1.31218398
945.144632	4.560967956	0.058681408	0.034061833	1.351149222
962.730229	4.645830465	0.054687581	0.031743601	1.376289042
988.665144	4.770984132	0.049273457	0.028600953	1.413364786
1008.72754	4.867798895	0.045444817	0.026378606	1.442045363
1025.80502	4.950209393	0.04241418	0.024619462	1.466458794
1088.26644	5.251628377	0.03291083	0.019103209	1.555751688
1113.92027	5.375425602	0.029637978	0.01720347	1.592425597
1165.67224	5.625164166	0.023970077	0.013913516	1.666408591
1178.58611	5.687482428	0.022729203	0.013193247	1.684869863
1212.13343	5.849371125	0.019790782	0.01148763	1.732828058
1251.83519	6.040959249	0.016789496	0.009745523	1.789584463
1282.33886	6.188160277	0.014789878	0.008584837	1.833191556
1317.20778	6.356426592	0.012788189	0.00742295	1.883039067
1344.45431	6.487909681	0.011410757	0.006623414	1.92198985
1379.74559	6.658214229	0.009840636	0.005712032	1.972441171
1438.5054	6.941770424	0.007683132	0.004459701	2.05644236
1454.82813	7.020538718	0.007171108	0.004162495	2.079776819
1483.35083	7.158180199	0.006355542	0.003689097	2.120551975
1578.91343	7.619334989	0.004232914	0.00245701	2.257165286
1600.58496	7.723914899	0.003858681	0.002239785	2.288146224
1628.46505	7.858455348	0.003424779	0.001987925	2.328002725
3019.40924	14.57071046	7.31694E-06	4.24714E-06	4.316453061
2584.05872	12.46984708	5.17343E-05	3.00294E-05	3.694089575
3179.84863	15.34494005	3.54128E-06	2.05555E-06	4.545812208
3185.10922	15.37032599	3.45788E-06	2.00714E-06	4.553332582
3190.20564	15.39491968	3.37894E-06	1.96132E-06	4.56061826

1197.49343	5.778723166	0.021024532	0.012203765	1.711899181
178.823229	0.862944135	1.177866866	0.68369702	0.255640098
54.702347	0.263976161	2.334794905	1.355240023	0.078200765
89.145647	0.430188593	1.851207003	1.074539702	0.12743983
136.893857	0.660606297	1.43258448	0.831548766	0.195699179
181.221139	0.874515688	1.165353611	0.676433656	0.259068076
242.825457	1.17179857	0.896778052	0.520538016	0.347135683
289.82768	1.398616377	0.742232194	0.430831322	0.414328592
355.757457	1.716772552	0.573964654	0.333159829	0.50857974
391.554334	1.889516916	0.500308822	0.290406039	0.559753836
436.308701	2.105487284	0.421843865	0.244860775	0.623733281
493.617781	2.382042711	0.339307179	0.196952061	0.70566055
557.285297	2.689281932	0.266343107	0.154599806	0.796677641
598.60809	2.888692613	0.227482763	0.13204318	0.855751414
635.950258	3.068894062	0.197157186	0.114440591	0.90913461
679.516726	3.279132006	0.166716554	0.096771218	0.971415871
721.955002	3.483925654	0.141462202	0.082112239	1.032084304
751.402514	3.626029999	0.126153483	0.073226239	1.074181546
779.842307	3.763271411	0.112893129	0.065529219	1.114838185
822.252007	3.96792716	0.095584159	0.055482166	1.175465767
854.597443	4.124015966	0.084133171	0.048835399	1.221705791
890.501947	4.297279705	0.072972089	0.042356909	1.273033748
924.237116	4.460074921	0.063797137	0.037031276	1.321260491
947.034125	4.57008605	0.058239129	0.03380511	1.353850382
964.926971	4.656431244	0.054207546	0.031464963	1.379429436
998.515196	4.818517356	0.047356241	0.027488099	1.427446112
1021.701	4.930404666	0.043124107	0.025031542	1.460591807
1030.9331	4.97495585	0.04154301	0.024113788	1.473789729
1093.07648	5.274840113	0.032271563	0.018732144	1.562627974

1143.43892	5.517873222	0.026262557	0.015244195	1.634624532
1168.57421	5.639168172	0.023685613	0.013748398	1.670557163
1184.45266	5.715792531	0.022186368	0.012878157	1.693256498
1216.59217	5.870887613	0.019429254	0.01127778	1.73920214
1264.28418	6.101034099	0.015943429	0.00925442	1.807381143
1294.6856	6.24774171	0.014048373	0.008154428	1.850842065
1320.76921	6.373612908	0.012599308	0.007313313	1.888130372
1355.9669	6.543465815	0.010873365	0.006311484	1.938447898
1402.50469	6.768042426	0.008942432	0.005190667	2.00497687
1441.89016	6.958104191	0.007574092	0.004396409	2.061281104
1457.1898	7.031935387	0.007099853	0.004121135	2.083152988
1488.12942	7.181240148	0.006228113	0.00361513	2.127383295
1588.30288	7.664645509	0.004066582	0.002360462	2.270588155
1604.55117	7.743054574	0.003793805	0.002202127	2.293816195
2991.43017	14.43569236	8.30204E-06	4.81895E-06	4.276455062
3059.6135	14.76472345	6.10167E-06	3.54174E-06	4.373927815
3121.6661	15.06416963	4.60864E-06	2.6751E-06	4.462636279
3180.59181	15.3485264	3.52938E-06	2.04864E-06	4.546874632
3187.98923	15.38422401	3.41305E-06	1.98112E-06	4.557449757
3193.60886	15.41134252	3.32723E-06	1.9313E-06	4.565483392
3202.83054	15.45584342	3.19104E-06	1.85225E-06	4.578666417
144.004933	0.694922092	1.383837206	0.803253238	0.205864951
68.906251	0.332519693	2.105650552	1.222232367	0.098506223
102.70743	0.495633453	1.7120917	0.993789729	0.146827331
143.112321	0.69061463	1.389812162	0.806721422	0.204588901
208.600769	1.006641091	1.034561109	0.600514682	0.298209139
256.887208	1.239656117	0.84683326	0.491547384	0.367237923
315.870459	1.524290562	0.669984172	0.3888947	0.451558535
372.592876	1.798014939	0.537990527	0.312278519	0.532647129

406.988094	1.963995343	0.471676527	0.273786321	0.581817457
449.556585	2.169417367	0.401123855	0.232833771	0.642672041
515.585495	2.488051925	0.312137818	0.181181509	0.737064907
569.900616	2.750159457	0.253838511	0.147341468	0.814712106
609.409229	2.940815481	0.218273701	0.126697748	0.871192385
640.831549	3.092449622	0.193495643	0.112315236	0.916112751
693.520947	3.346711931	0.157936267	0.091674669	0.991435867
738.745627	3.56495188	0.132526649	0.076925566	1.056087656
772.505304	3.727865364	0.116179322	0.067436701	1.104349435
789.063787	3.807771346	0.108889842	0.063205497	1.128020925
827.165972	3.991640396	0.093752496	0.054418971	1.182490618
868.602919	4.191601948	0.079596357	0.046201989	1.241727582
905.699374	4.370617663	0.068691248	0.039872079	1.294759514
935.710625	4.515442433	0.060938671	0.035372069	1.337662661
957.544822	4.620807337	0.055837062	0.032410822	1.368876146
977.739313	4.71825954	0.051487935	0.029886355	1.397745559
1002.59103	4.838186041	0.046584221	0.027039977	1.433272798
1022.5294	4.934402286	0.042979886	0.024947828	1.461776069
1059.36458	5.112157152	0.03701878	0.021487683	1.514434485
1107.795	5.345867013	0.030389431	0.017639654	1.583669108
1160.16317	5.598579153	0.024519273	0.0142323	1.658533
1173.2817	5.661885014	0.023231138	0.013484597	1.67728684
1190.33635	5.744185356	0.021654634	0.01256951	1.701667639
1233.13216	5.95070432	0.018143527	0.010531475	1.762847183
1267.06721	6.114464137	0.015760057	0.009147981	1.811359681
1305.49047	6.299882593	0.013429359	0.007795119	1.866288372
1335.85822	6.446427694	0.011828867	0.006866108	1.909701153
1372.31033	6.622334001	0.010152782	0.005893219	1.961811948
1418.04346	6.843027587	0.008375845	0.004861789	2.027190607

1449.08828	6.992840014	0.007347226	0.004264723	2.071571306
1466.18734	7.07535465	0.00683469	0.00396722	2.096015588
1558.2667	7.519700434	0.004622551	0.002683176	2.227649369
1597.32872	7.708201318	0.003912759	0.002271175	2.283491205
1606.63823	7.753126053	0.003760098	0.002182562	2.296799788
3012.99219	14.53974383	7.53206E-06	4.37201E-06	4.307279454
3067.35516	14.80208225	5.89185E-06	3.41995E-06	4.38499505
3169.87476	15.29680932	3.70495E-06	2.15055E-06	4.531553874
3182.15535	15.35607153	3.50447E-06	2.03418E-06	4.549109817
3188.48202	15.38660204	3.40544E-06	1.9767E-06	4.55815423
3197.00847	15.42774796	3.27637E-06	1.90178E-06	4.570343369
3208.55732	15.48347905	3.10928E-06	1.80479E-06	4.586853246
		sum	23.87861083	243.3620445

Table 42 The calculation data of (5S, 6R, 11R)-3

cm-1	x_i	pf	TS(kcal/mol)	E_{ZEP}(kcal/mol)
182.72824	0.881788479	1.157583946	0.671923726	0.26122258
22.915742	0.110584096	3.202488375	1.858895789	0.032759628
75.71571	0.36537998	2.01236153	1.168082421	0.108240812
135.532333	0.654036014	1.442227852	0.837146296	0.193752787
164.953338	0.796012444	1.254130624	0.72796459	0.235812136
218.282151	1.053360367	0.993000739	0.576390818	0.31204934
276.963889	1.336539806	0.781172817	0.453434545	0.395938918
333.687658	1.610270708	0.625084329	0.362832426	0.477029445
389.036534	1.877366813	0.505148782	0.29321541	0.556154468
426.779869	2.059504166	0.437417863	0.253900757	0.61011116
466.050781	2.24901312	0.376758631	0.21869089	0.666251628
541.399774	2.612623441	0.282950973	0.164239901	0.773968194
597.766583	2.884631768	0.228215905	0.132468735	0.854548422
613.526613	2.960684669	0.214859564	0.124715999	0.877078468

674.467201	3.254764601	0.169996757	0.098675223	0.964197228
712.924145	3.440345605	0.146505831	0.085039832	1.019174073
743.714219	3.588928728	0.129988616	0.075452356	1.0631906
775.617646	3.742884538	0.114774215	0.066621102	1.108798742
817.970435	3.947265653	0.09720819	0.05642484	1.169344965
843.58527	4.070874715	0.08787454	0.05100709	1.205963133
881.85007	4.255528493	0.075523026	0.04383761	1.260665295
917.887991	4.429436059	0.065434164	0.037981493	1.31218398
945.144632	4.560967956	0.058681408	0.034061833	1.351149222
962.730229	4.645830465	0.054687581	0.031743601	1.376289042
988.665144	4.770984132	0.049273457	0.028600953	1.413364786
1008.72754	4.867798895	0.045444817	0.026378606	1.442045363
1025.80502	4.950209393	0.04241418	0.024619462	1.466458794
1088.26644	5.251628377	0.03291083	0.019103209	1.555751688
1113.92027	5.375425602	0.029637978	0.01720347	1.592425597
1165.67224	5.625164166	0.023970077	0.013913516	1.666408591
1178.58611	5.687482428	0.022729203	0.013193247	1.684869863
1212.13343	5.849371125	0.019790782	0.01148763	1.732828058
1251.83519	6.040959249	0.016789496	0.009745523	1.789584463
1282.33886	6.188160277	0.014789878	0.008584837	1.833191556
1317.20778	6.356426592	0.012788189	0.00742295	1.883039067
1344.45431	6.487909681	0.011410757	0.006623414	1.92198985
1379.74559	6.658214229	0.009840636	0.005712032	1.972441171
1438.5054	6.941770424	0.007683132	0.004459701	2.05644236
1454.82813	7.020538718	0.007171108	0.004162495	2.079776819
1483.35083	7.158180199	0.006355542	0.003689097	2.120551975
1578.91343	7.619334989	0.004232914	0.00245701	2.257165286
1600.58496	7.723914899	0.003858681	0.002239785	2.288146224
1628.46505	7.858455348	0.003424779	0.001987925	2.328002725

3019.40924	14.57071046	7.31694E-06	4.24714E-06	4.316453061
3084.05872	14.88268835	5.4633E-06	3.17119E-06	4.408873946
3179.84863	15.34494005	3.54128E-06	2.05555E-06	4.545812208
3185.10922	15.37032599	3.45788E-06	2.00714E-06	4.553332582
3190.20564	15.39491968	3.37894E-06	1.96132E-06	4.56061826
3197.49343	15.43008826	3.26917E-06	1.8976E-06	4.571036664
178.823229	0.862944135	1.177866866	0.68369702	0.255640098
54.702347	0.263976161	2.334794905	1.355240023	0.078200765
89.145647	0.430188593	1.851207003	1.074539702	0.12743983
136.893857	0.660606297	1.43258448	0.831548766	0.195699179
181.221139	0.874515688	1.165353611	0.676433656	0.259068076
242.825457	1.17179857	0.896778052	0.520538016	0.347135683
289.82768	1.398616377	0.742232194	0.430831322	0.414328592
355.757457	1.716772552	0.573964654	0.333159829	0.50857974
391.554334	1.889516916	0.500308822	0.290406039	0.559753836
436.308701	2.105487284	0.421843865	0.244860775	0.623733281
493.617781	2.382042711	0.339307179	0.196952061	0.70566055
557.285297	2.689281932	0.266343107	0.154599806	0.796677641
598.60809	2.888692613	0.227482763	0.13204318	0.855751414
635.950258	3.068894062	0.197157186	0.114440591	0.90913461
679.516726	3.279132006	0.166716554	0.096771218	0.971415871
721.955002	3.483925654	0.141462202	0.082112239	1.032084304
751.402514	3.626029999	0.126153483	0.073226239	1.074181546
779.842307	3.763271411	0.112893129	0.065529219	1.114838185
822.252007	3.96792716	0.095584159	0.055482166	1.175465767
854.597443	4.124015966	0.084133171	0.048835399	1.221705791
890.501947	4.297279705	0.072972089	0.042356909	1.273033748
924.237116	4.460074921	0.063797137	0.037031276	1.321260491
947.034125	4.57008605	0.058239129	0.03380511	1.353850382

964.926971	4.656431244	0.054207546	0.031464963	1.379429436
998.515196	4.818517356	0.047356241	0.027488099	1.427446112
1021.701	4.930404666	0.043124107	0.025031542	1.460591807
1030.9331	4.97495585	0.04154301	0.024113788	1.473789729
1093.07648	5.274840113	0.032271563	0.018732144	1.562627974
1143.43892	5.517873222	0.026262557	0.015244195	1.634624532
1168.57421	5.639168172	0.023685613	0.013748398	1.670557163
1184.45266	5.715792531	0.022186368	0.012878157	1.693256498
1216.59217	5.870887613	0.019429254	0.01127778	1.73920214
1264.28418	6.101034099	0.015943429	0.00925442	1.807381143
1294.6856	6.24774171	0.014048373	0.008154428	1.850842065
1320.76921	6.373612908	0.012599308	0.007313313	1.888130372
1355.9669	6.543465815	0.010873365	0.006311484	1.938447898
1402.50469	6.768042426	0.008942432	0.005190667	2.00497687
1441.89016	6.958104191	0.007574092	0.004396409	2.061281104
1457.1898	7.031935387	0.007099853	0.004121135	2.083152988
1488.12942	7.181240148	0.006228113	0.00361513	2.127383295
1588.30288	7.664645509	0.004066582	0.002360462	2.270588155
1604.55117	7.743054574	0.003793805	0.002202127	2.293816195
1691.43017	8.162305048	0.002613833	0.001517209	2.418015698
1759.6135	8.491336139	0.00194837	0.001130938	2.515488451
3121.6661	15.06416963	4.60864E-06	2.6751E-06	4.462636279
3180.59181	15.3485264	3.52938E-06	2.04864E-06	4.546874632
3187.98923	15.38422401	3.41305E-06	1.98112E-06	4.557449757
3193.60886	15.41134252	3.32723E-06	1.9313E-06	4.565483392
3202.83054	15.45584342	3.19104E-06	1.85225E-06	4.578666417
144.004933	0.694922092	1.383837206	0.803253238	0.205864951
68.906251	0.332519693	2.105650552	1.222232367	0.098506223
102.70743	0.495633453	1.7120917	0.993789729	0.146827331

143.112321	0.69061463	1.389812162	0.806721422	0.204588901
208.600769	1.006641091	1.034561109	0.600514682	0.298209139
256.887208	1.239656117	0.84683326	0.491547384	0.367237923
315.870459	1.524290562	0.669984172	0.3888947	0.451558535
372.592876	1.798014939	0.537990527	0.312278519	0.532647129
406.988094	1.963995343	0.471676527	0.273786321	0.581817457
449.556585	2.169417367	0.401123855	0.232833771	0.642672041
515.585495	2.488051925	0.312137818	0.181181509	0.737064907
569.900616	2.750159457	0.253838511	0.147341468	0.814712106
609.409229	2.940815481	0.218273701	0.126697748	0.871192385
640.831549	3.092449622	0.193495643	0.112315236	0.916112751
693.520947	3.346711931	0.157936267	0.091674669	0.991435867
738.745627	3.56495188	0.132526649	0.076925566	1.056087656
772.505304	3.727865364	0.116179322	0.067436701	1.104349435
789.063787	3.807771346	0.108889842	0.063205497	1.128020925
827.165972	3.991640396	0.093752496	0.054418971	1.182490618
868.602919	4.191601948	0.079596357	0.046201989	1.241727582
905.699374	4.370617663	0.068691248	0.039872079	1.294759514
935.710625	4.515442433	0.060938671	0.035372069	1.337662661
957.544822	4.620807337	0.055837062	0.032410822	1.368876146
977.739313	4.71825954	0.051487935	0.029886355	1.397745559
1002.59103	4.838186041	0.046584221	0.027039977	1.433272798
1022.5294	4.934402286	0.042979886	0.024947828	1.461776069
1059.36458	5.112157152	0.03701878	0.021487683	1.514434485
1107.795	5.345867013	0.030389431	0.017639654	1.583669108
1160.16317	5.598579153	0.024519273	0.0142323	1.658533
1173.2817	5.661885014	0.023231138	0.013484597	1.67728684
1190.33635	5.744185356	0.021654634	0.01256951	1.701667639
1233.13216	5.95070432	0.018143527	0.010531475	1.762847183

1267.06721	6.114464137	0.015760057	0.009147981	1.811359681
1305.49047	6.299882593	0.013429359	0.007795119	1.866288372
1335.85822	6.446427694	0.011828867	0.006866108	1.909701153
1372.31033	6.622334001	0.010152782	0.005893219	1.961811948
1418.04346	6.843027587	0.008375845	0.004861789	2.027190607
1449.08828	6.992840014	0.007347226	0.004264723	2.071571306
1466.18734	7.07535465	0.00683469	0.00396722	2.096015588
1558.2667	7.519700434	0.004622551	0.002683176	2.227649369
1597.32872	7.708201318	0.003912759	0.002271175	2.283491205
1606.63823	7.753126053	0.003760098	0.002182562	2.296799788
3012.99219	14.53974383	7.53206E-06	4.37201E-06	4.307279454
3067.35516	14.80208225	5.89185E-06	3.41995E-06	4.38499505
3169.87476	15.29680932	3.70495E-06	2.15055E-06	4.531553874
3182.15535	15.35607153	3.50447E-06	2.03418E-06	4.549109817
3188.48202	15.38660204	3.40544E-06	1.9767E-06	4.55815423
3197.00847	15.42774796	3.27637E-06	1.90178E-06	4.570343369
3208.55732	15.48347905	3.10928E-06	1.80479E-06	4.586853246
		sum	23.86902189	243.2190876

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