Palladium-catalysed diastereodivergent inverse-electron-demand oxa-Diels–Alder reactions of in situ formed cyclopentadienones via ligand-control

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Supplementary Information

1. General methods

Unless otherwise noted, the reactions were carried out under ambient atmosphere; when the reactions required heating, the heat source was oil bath. ^{1}H NMR (400 MHz), ^{13}C NMR (100 MHz) were recorded on Varian INOVA-400/54, Agilent DD2-600/54 or Bruker Ascend^{TM} 400 instruments (Chemical shifts were reported in ppm from tetramethylsilane with the solvent resonance as the internal standard in $CDCl_3$ solution, unless otherwise noted). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, dd = double doublet, ddd = double double doublet, dt = double triplet, m = multiplet and coupling constants (J) are reported in Hertz (Hz). High resolution mass spectra (HRMS) were recorded on a Waters SYNAPT G2 or Agilent G1969-85000 using a time-of-flight mass spectrometer equipped with electrospray ionization (ESI) source. X-ray diffraction experiments were carried out on an Agilent Gemini and the data obtained were deposited at the Cambridge Crystallographic Data Centre. In each case, diastereomeric ratio was determined by ^{1}H NMR analysis or HPLC and enantiomeric excess was determined by HPLC analysis (Agilent Technologies: 1220 Infinity II, 1200 Series, 1260 Infinity) on a chiral column in comparison with authentic racemate, using a Daicel Chiralpak AD-H Column (250 × 4.6 mm), Daicel Chiralpak IA Column (250 × 4.6 mm), Daicel Chiralpak IE Column (250 × 4.6 mm) or IF Column (250 × 4.6 mm). UV detection was monitored at 220 nm or 254 nm. Optical rotation was measured in $CHCl_3$ solution at 25 °C on Perkin-Elmer PL341. Column chromatography was performed on silica gel (200-300 mesh) eluting with EtOAc or acetone and petroleum ether. TLC was performed on glass-backed silica plates. UV light, I_2, and solution of potassium permanganate were used to visualize products or starting materials. All chemicals were used without purification as commercially available unless otherwise noted. Petroleum ether was distilled. THF was freshly distilled from sodium/benzophenone before use. $CHCl_3$ was washed with water and distilled from anhydrous $CaCl_2$. Dichloromethane (DCM) was treated with 5% Na_2CO_3 aqueous solution followed by water. Toluene was freshly distilled from CaH_2 under an atmosphere of dry argon. Experiments involving moisture and/or air sensitive components were performed under a positive pressure of argon in oven-dried glassware equipped with a rubber septum inlet. Dried solvents and liquid reagents were transferred by oven-dried syringe. The γ-functionalized 2-cyclopentenones **1**,[1] α-cyano chalcones **2**,[2a,2c] alkylidene pyrazolones **5**,[3] ethyl 2-benzoylacrylate **7**,[4] 1-phenylprop-2-en-1-one **9**[4] and chiral ligands **L1–L16**[1b,5] were prepared according to the literature procedures. Compounds **1a**,[1a] **1b–1f**,[1b] **2a–2n**[2b]

(**2g**[2c]), **5a–5e**,[3] **7**[4], **9**[4], **L1–L2**[5] and **L3–L16**[1b] are known compounds and the spectroscopic data were consistent with the literature report.

Table S1. Summary of data and instruments

Data	Instrument
^{1}H NMR and ^{13}C NMR	Varian INOVA-400/54 or Agilent DD2-600/54 or Bruker Ascend^{TM} 400
High resolution mass spectra (HRMS)	Waters SYNAPT G2 or Agilent G1969-85000 (ESI source)
X-ray diffraction	Agilent Gemini diffractometer
HPLC analysis	Agilent 1220 Infinity II, 1200 Series, 1260 Infinity Daicel Chiralpak columns (AD-H, IA, IE, IF)
Optical rotation	Perkin-Elmer PL341
Melting point	WRX-4 melting-point apparatus (Shanghai YiCe Apparatus & Equiments Co., Ltd) with capillary

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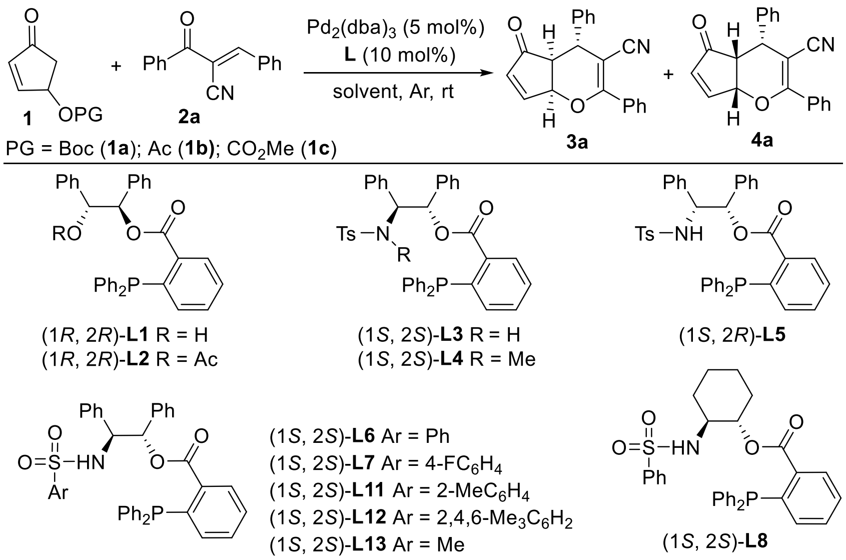
2. Detailed screening conditions of asymmetric oxa-DA reaction of 2-cyclopentenones 1 and 1-oxadiene 2a

Table S1 Detailed screening conditions for synthesis of **3a**[a]

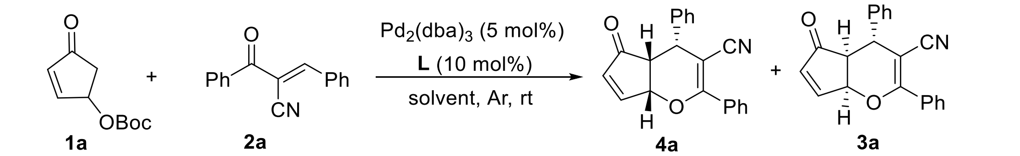


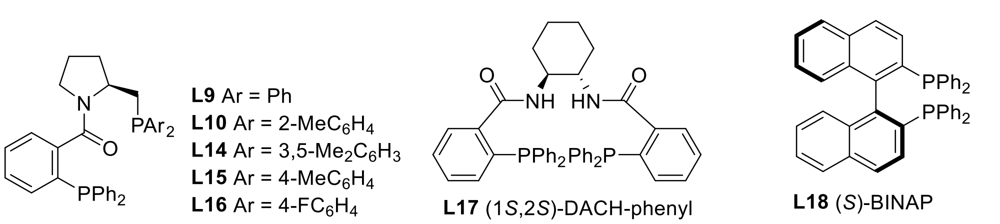
Entry	Pd source	L	Solvent	Time (h)	Yield[b] (%)	dr[c] (**3a**:**4a**)	ee[d] (%)(**3a/4a**)
1[e]	$Pd_2(dba)_3$	-	$CHCl_3$	18	48	1:15	-
2	$Pd_2(dba)_3$	**L1**	$CHCl_3$	8	90	5:1	–99/80
3	$Pd_2(dba)_3$	**L2**	$CHCl_3$	10	83	1:3	–65/43
4	$Pd_2(dba)_3$	**L3**	$CHCl_3$	12	94	8:1	93/66
5	$Pd_2(dba)_3$	**L4**	$CHCl_3$	24	85	1:1	–3/–11
6	$Pd_2(dba)_3$	**L5**	$CHCl_3$	12	92	4:1	99/–82
7	$Pd_2(dba)_3$	**L6**	$CHCl_3$	36	82	10:1	99/–73
8	$Pd_2(dba)_3$	**L7**	$CHCl_3$	40	89	10:1	94/–55
9	$Pd_2(dba)_3$	**L11**	$CHCl_3$	24	77	7:1	98/–80
10	$Pd_2(dba)_3$	**L12**	$CHCl_3$	40	74	2:1	96/–60
11	$Pd_2(dba)_3$	**L13**	$CHCl_3$	12	77	6:1	98/–80
12	$Pd_2(dba)_3$	**L8**	$CHCl_3$	48	90	5:1	93/–70
13[f]	$Pd_2(dba)_3$	**L6**	$CHCl_3$	36	72	9:1	98/–55

14[g]	$Pd_2(dba)_3$	**L6**	$CHCl_3$	48	40	13:1	94/–71
15	$Pd_2(dba)_3$	**L6**	toluene	48	78	9:1	97/–88
16	$Pd_2(dba)_3$	**L6**	THF	48	78	5:1	93/–88
17	$Pd_2(dba)_3$	**L6**	DCE	48	67	17:1	99/-
18	**$Pd_2(dba)_3$**	**L6**	**DCM**	**30**	**92**	**18:1**	**99/-**
19[h]	$Pd_2(dba)_3$	**L6**	DCM	24	74	18:1	>99
20[i]	$Pd_2(dba)_3$	**L6**	DCM	24	64	18:1	>99
21[j]	$Pd_2(dba)_3$	**L6**	DCM	40	78	11:1	99
22	$Pd(OAc)_2$	**L6**	DCM	30	-	-	-
23	$Pd(\eta^3\text{-}C_3H_5)_2Cl_2$	**L6**	DCM	30	-	-	-
24	$Pd(dba)_2$	**L6**	DCM	30	80	15:1	99
25	$Pd_2(dba)_3{\cdot}CHCl_3$	**L6**	DCM	30	66	17:1	>99
26[k]	$Pd_2(dba)_3$	**L6**	DCM	30	83	18:1	>99

[a] Unless noted otherwise, reactions were performed with **1a** (0.1 mmol, 2.0 equiv), **2a** (0.05 mmol, 1.0 equiv), $Pd_2(dba)_3$ (5 mol%), and **L** (10 mol%) in solvent (0.05 M, 1.0 mL) under Ar at room temperature. [b] Yield of the isolated inseparable diastereomers. [c] Determined by ^{1}H NMR analysis. [d] Determined by HPLC analysis on a chiral stationary phase. [e] With $Pd(PPh_3)_4$ (5 mol%). [f] With **1b**. [g] With **1c**. [h] With **L6** (15 mol%). [i] With **L6** (20 mol%). [j] With $Pd_2(dba)_3$ (2.5 mol%) and **L6** (5 mol%). [k] On a 0.1 mmol scale.

Table S2 Optimization conditions for asymmetric [4 + 2] cycloaddition reaction between cyclic enone **1a** and 1-oxadiene **2a** for synthesis of **4a**[a]



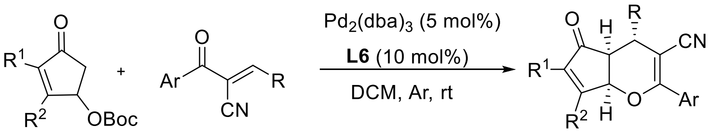


Entry	L	Solvent	Time (h)	Yield[b] (%)	dr[c] (**4a**:**3a**)	ee[d] (%)(**4a**/**3a**)
1	**L9**	$CHCl_3$	12	91	4:1	77/–60
2	**L17**	$CHCl_3$	12	30	3:1	–40/78
3	**L18**	$CHCl_3$	12	-	-	-
4	**L9**	DCM	12	70	1:1	76/–65
5	**L9**	DCE	12	60	1:1	96/–68
6	**L9**	THF	18	45	2:1	94/–60
7	**L9**	toluene	18	50	3:1	96/–15
8	**L9**	$CHCl_3$/toluene[e]	12	92	4:1	87/–73
9	**L10**	$CHCl_3$/toluene[e]	20	95	4:1	89/–84

10	**L14**	$CHCl_3$/toluene[e]	12	86	3:1	87/–68
11	**L15**	$CHCl_3$/toluene[e]	12	93	3:1	82/–63
12	**L16**	$CHCl_3$/toluene[e]	12	90	4:1	88/–72
13[f]	**L10**	$CHCl_3$/toluene[e]	20	88	5:1	90/–83

[a] Unless noted otherwise, reactions were performed with **1a** (0.06 mmol, 2.0 equiv), **2a** (0.03 mmol, 1.0 equiv), $Pd_2(dba)_3$ (5 mol%), and **L** (10 mol%) in solvent (0.05 M, 1.0 mL) under Ar at room temperature. [b] Yield of the isolated inserarable diastereomers. [c] Determined by ^{1}H NMR analysis. [d] Determined by HPLC analysis on a chiral stationary phase. [e] $CHCl_3$:toluene = 1:1. [f] On a 0.1 mmol scale.

3. General procedure for synthesis of *exo*-cycloadducts 3



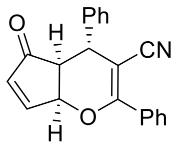
1 **2** **3**

General procedure A: To an oven-dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (1.0 mL) was added via syringe and the mixture was stirred for 20 min. The mixture of 1-oxadiene **2** (0.1 mmol) and carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry DCM (1.0 mL) was transferred to the catalytic solution in one portion, and the mixture was stirred at room temperature (20−25 °C) for the indicated time. After complete completion monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (EtOAc/petroleum ether or acetone/petroleum ether) to afford the cycloadduct **3** (**3a–3m**).

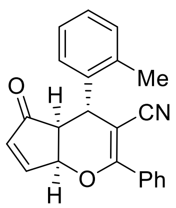
The corresponding racemates were generally obtained under the catalysis of $Pd_2(dba)_3$ (1.4 mg, 0.0015 mmol, 5.0 mol%) and 1,3-bis(diphenylphosphino)propane (2.2 mg, 0.0029 mmol, 10 mol%) on a 0.03 mmol scale.

General procedure B: To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%), **L6** (6.4 mg, 0.010 mmol, 10 mol%), (*E*)-2-benzoyl-3-phenylacrylonitrile **2a** (23.3 mg, 0.100 mmol) and carbonate **1** (**1d–1f**) (0.2 mmol). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed toluene (2.0 mL) was added via syringe and it was allowed to stir at 50 °C for 22 h. After completion monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/5) to afford the cycloadduct **3** (**3n–3p**).

The corresponding racemates were obtained under the catalysis of $Pd_2(dba)_3$ (1.4 mg, 0.0015 mmol, 5.0 mol%) and (±)-**L6** (1.9 mg, 0.0030 mmol, 10 mol%) on a 0.03 mmol scale.

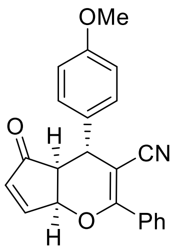


Synthesis of 3a: **General procedure A:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (1.0 mL) was added via syringe and the mixture was stirred for 20 min. The mixture of (*E*)-2-benzoyl-3-phenylacrylonitrile **2a** (23.3 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry DCM (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature for 30 h. After complete consumption of **2a** monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/5) to afford the cycloadduct **3a**: 26.2 mg (0.0837 mmol) as a white solid, 83% yield, 18:1 dr; mp 122–124 °C; $[\alpha]_D^{25}$ = +15.6 (*c* = 1.23 in $CHCl_3$); >99% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), major diastereomer: t_R = 10.52 min (major), t_R = 12.68 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.75–7.12 (m, 2H), 7.49 (dd, *J* = 5.8, 2.8 Hz, 1H), 7.46–7.41 (m, 3H), 7.40–7.38 (m, 4H), 7.34–7.29 (m, 1H), 6.46 (d, *J* = 5.8 Hz, 1H), 5.71 (dd, *J* = 6.8, 2.7 Hz, 1H), 4.17 (d, *J* = 1.9 Hz, 1H), 3.02 (dd, *J* = 6.8, 1.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 204.2, 163.3, 156.6, 140.8, 136.3, 132.6, 131.3, 129.3, 128.5, 127.8, 127.7, 127.3, 119.1, 89.1, 77.0, 50.5, 39.6; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{15}NO_2Na^+$ 336.0995; Found 336.0996.

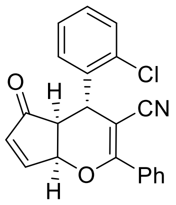


Synthesis of 3b: **General procedure A:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of (*E*)-2-benzoyl-3-(*o*-tolyl)acrylonitrile **2b** (26.3 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry DCM (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature for 24 h. After complete consumption of **2b** monitored by

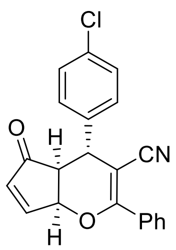
TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/5) to afford the cycloadduct **3b**: 31.1 mg (0.0951 mmol) as a white solid, 90% yield, 17:1 dr; mp 173–175 °C; $[\alpha]_D^{25}$ = –36.1 (*c* = 1.40 in $CHCl_3$); 96% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), major diastereomer: t_R = 9.75 min (major), t_R = 12.04 min (minor); ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.77–7.74 (m, 2H), 7.69 (dd, *J* = 5.7, 2.8 Hz, 1H), 7.49–7.41 (m, 3H), 7.28–7.19 (m, 4H), 6.46 (d, *J* = 5.7 Hz, 1H), 5.61 (dd, *J* = 6.8, 2.8 Hz, 1H), 4.44 (d, *J* = 1.7 Hz, 1H), 2.84 (dd, *J* = 6.8, 1.7 Hz, 1H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 204.3, 163.8, 156.8, 138.6, 136.1, 135.9, 132.6, 131.4, 131.3, 128.6, 127.9, 127.7, 126.8, 126.3, 119.3, 88.3, 76.6, 49.6, 35.5, 19.5; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{22}H_{17}NO_2Na^+$ 350.1151; Found 350.1148.



Synthesis of 3c: **General procedure A:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of (*E*)-2-benzoyl-3-(4-methoxyphenyl)acrylonitrile **2c** (26.3 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry DCM (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature for 24 h. After complete consumption of **2c** monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/5) to afford the cycloadduct **3c**: 30.5 mg (0.0889 mmol) as a white solid, 89% yield, 18:1 dr; mp 48–50 °C; $[\alpha]_D^{25}$ = –3.8 (*c* = 1.37 in $CHCl_3$); 97% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 20/80, flow rate = flow rate = 1.0 mL/min, λ = 254 nm), major diastereomer: t_R = 16.04 min (major), t_R = 20.91 min (minor); ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.74–7.71 (m, 2H), 7.67 (dd, *J* = 5.7, 2.7 Hz, 1H), 7.48–7.39 (m, 3H), 7.33–7.29 (m, 2H), 6.93–6.88 (m, 2H), 6.46 (d, *J* = 5.7, 1H), 5.70 (dd, *J* = 6.9, 2.7, 1H), 4.11 (d, *J* = 2.1 Hz, 1H), 3.80 (s, 3H), 2.99 (dd, *J* = 6.9, 2.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 204.3, 163.1, 159.1, 156.6, 136.3, 132.8, 132.6, 131.2, 128.5, 128.4, 127.8, 119.1, 114.7, 89.6, 77.1, 55.4, 50.7, 39.0; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{22}H_{17}NO_3Na^+$ 366.1101; Found 350.1106.

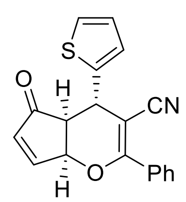


Synthesis of 3d: **General procedure A:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed toluene (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of (*E*)-2-benzoyl-3-(2-chlorophenyl) acrylonitrile **2d** (26.7 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry toluene (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at 30 °C for 28 h. After complete consumption of **2d** monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/5) to afford the cycloadduct **3d**: 28.8 mg (0.0830 mmol) as a white solid, 83% yield, >19:1 dr; mp 190–192 °C; $[\alpha]_D^{25} = -8.6$ (c = 1.42 in $CHCl_3$); 86% ee, determined by HPLC analysis (Chiralpak AD-H, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), t_R = 12.58 min (major), t_R = 15.58 min (minor); ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.79–7.76 (m, 2H), 7.68 (dd, J = 5.8, 2.8 Hz, 1H), 7.51–7.42 (m, 4H), 7.35–7.25 (m, 3H), 6.47 (d, J = 5.8 Hz, 1H), 5.56 (dd, J = 6.8, 2.8 Hz, 1H), 4.68 (d, J = 2.2 Hz, 1H), 3.08 (dd, J = 6.8, 2.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 203.8, 165.1, 156.6, 137.1, 136.5, 134.2, 132.7, 131.8, 130.9, 129.6, 128.9, 128.8, 128.2, 127.8, 119.2, 87.7, 77.2, 49.1, 36.7; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{14}{}^{35}ClNO_2Na^+$ 370.0605; Found 370.0606; Calcd for $C_{21}H_{14}{}^{37}ClNO_2Na^+$ 372.0576; Found 372.0584.

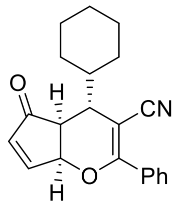


Synthesis of 3e: **General procedure A:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of (*E*)-2-benzoyl-3-(4-chlorophenyl)acrylonitrile **2e** (26.7 mg, 0.1 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry DCM (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature for 48 h. After complete consumption of **2e** monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/5) to afford the cycloadduct **2e**: 28.2 mg

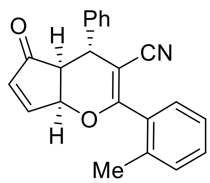
(0.0813 mmol) as a white solid, 81% yield, 18:1 dr; mp 140–141 °C; $[\alpha]_D^{25}$ = +12.9 (c = 1.03 in $CHCl_3$); 94% ee, determined by HPLC analysis (Chiralpak ID, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), major diastereomer: t_R = 26.32 min (minor), t_R = 27.89 min (major); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.74–7.71 (m, 2H), 7.69 (dd, J = 5.7, 2.8 Hz, 1H), 7.48–7.40 (m, 3H), 7.37–7.32 (m, 4H), 6.48 (d, J = 5.7 Hz, 1H), 5.70 (dd, J = 6.8, 2.8 Hz, 1H), 4.13 (d, J = 2.1 Hz, 1H), 2.98 (dd, J = 6.8, 2.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 203.9, 163.6, 156.6, 139.2, 136.4, 133.7, 132.3, 131.4, 129.5, 128.7, 128.6, 127.8, 118.9, 88.8, 77.0, 50.4, 39.1; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{14}{}^{35}ClNO_2Na^+$ 370.0605; Found 370.0603; Calcd for $C_{21}H_{14}{}^{37}ClNO_2Na^+$ 372.0576; Found 372.0574.



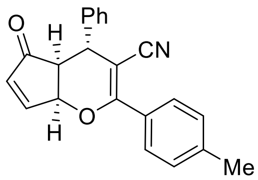
Synthesis of 3f: **General procedure A:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of (*E*)-2-benzoyl-3-(thiophen-2-yl)acrylonitrile **2f** (23.9 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry DCM (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature for 24 h. After complete consumption of **2f** monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/5) to afford the cycloadduct **3f**: 25.1 mg (0.0787 mmol) as a white solid, 79% yield, 17:1 dr; mp 119–120 °C; $[\alpha]_D^{25}$ = +50.40 (c = 1.32 in $CHCl_3$); >99% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), major diastereomer: t_R = 26.32 min (major), t_R = 27.89 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.73–7.66 (m, 2H), 7.67 (dd, J = 5.7, 2.8 Hz, 1H), 7.48–7.39 (m, 3H), 7.24 (dd, J = 5.1, 1.3 Hz, 1H), 7.08–7.06 (m, 1H), 6.98 (dd, J = 5.1, 3.5 Hz, 1H), 6.47 (d, J = 5.7 Hz, 1H), 5.78 (dd, J = 6.9, 2.8 Hz, 1H), 4.47 (d, J = 1.9 Hz, 1H), 3.15 (dd, J = 6.9, 1.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 203.6, 163.5, 156.5, 144.0, 136.6, 132.4, 131.4, 128.5, 127.8, 127.3, 125.4, 125.1, 118.8, 89.7, 77.1, 51.1, 35.1; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{19}H_{13}NO_2SNa^+$ 342.0559; Found 342.0554.



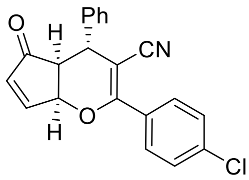
Synthesis of 3g: **General procedure A:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (1.0 mL) was added via syringe and the mixture was stirred for 20 min. The mixture of (*E*)-2-benzoyl-3-cyclohexylacrylonitrile **2g** (24.0 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.200 mmol) dissolved in dry DCM (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature for 48 h. The corresponding racemate was obtained under the catalysis of $Pd_2(dba)_3$ (1.4 mg, 0.0015 mmol, 5.0 mol%) and (±)-**L6** (1.9 mg, 0.0030 mmol, 10 mol%) in 0.03 mmol scale. After completion, the crude product was concentrated and purified by flash chromatography on silica gel (EtOAc/petroleum ether = 1/6) to afford the cycloadduct **3g**: 17.6 mg (0.0552 mmol) as a sem-solid, 50% yield for inseparable diastereomers, 2:1 dr; $[\alpha]_D^{25}$ = +108.9 (*c* = 0.81 in $CHCl_3$); 98%/60% ee, determined by HPLC analysis (Chiralpak AD-H, *i*-PrOH/*n*-hexane = 10/90, flow rate = 1.0 mL/min, λ = 254 nm), major diastereomer: t_R = 11.68 min (major), t_R = 14.07 min (minor); minor diastereomer: t_R = 13.66 min (major), t_R = 15.32 min (minor); ^1H NMR for major diastereomer (400 MHz, $CDCl_3$) δ (ppm) 7.71–7.66 (m, 2H), 7.60 (dd, *J* = 5.7, 2.7 Hz, 1H), 7.44–7.40 (m, 3H), 6.43 (d, *J* = 5.7 Hz, 1H), 5.60–5.58 (m, 1H), 2.86 (dd, *J* = 7.0, 1.3 Hz, 1H), 2.79 (d, *J* = 6.2 Hz, 1H), 1.96–1.81 (m, 4H), 1.29–1.07 (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 206.2, 163.1, 156.7, 136.8, 132.7, 131.1, 128.5, 127.8, 120.1, 89.2, 78.0, 45.8, 42.3, 40.6, 30.9, 30.5, 26.3, 26.22, 26.16; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{21}NO_2Na^+$ 342.1465 ; Found 342.1463.



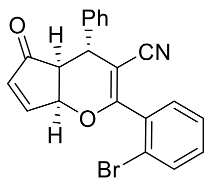
Synthesis of 3h: **General procedure A:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of (*E*)-2-(2-methylbenzoyl)-3-phenylacrylonitrile **2h** (24.7 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry DCM (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature for 48 h. After complete consumption of **2h** monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/5) to afford the cycloadduct **3h**: 31.7 mg (0.0969 mmol) as a white solid, 97% yield, 10:1 dr; mp 119–120 °C; $[\alpha]_D^{25}$ = –44.4 (*c* = 1.14 in $CHCl_3$); 98% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane= 20/80, flow rate = 1.0 mL/min, λ = 254 nm), major diastereomer: t_R = 10.99 min (major), t_R = 12.51 min (minor); ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.69 (dd, *J* = 5.8, 2.9 Hz, 1H), 7.45–7.40 (m, 4H), 7.38–7.30 (m, 2H), 7.28–7.24 (m, 1H), 7.25–7.19 (m, 2H), 6.50 (d, *J* = 5.8 Hz, 1H), 5.66 (dd, *J* = 6.7, 2.9 Hz, 1H), 4.18 (d, *J* = 1.8 Hz, 1H), 2.94 (dd, *J* = 6.7, 1.8 Hz, 1H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 203.9, 164.9, 156.9, 141.4, 136.5, 135.4, 132.7, 130.7, 130.6, 129.4, 129.3, 127.8, 127.3, 126.0, 118.2, 90.6, 76.1, 49.7, 37.9, 19.6; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{22}H_{17}NO_2Na^+$ 350.1151; Found 350.1155.



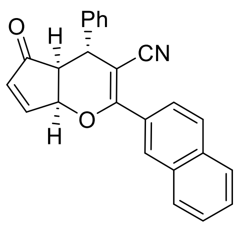
Synthesis of 3i: **General procedure A:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of (*E*)-2-(4-methylbenzoyl)-3-phenylacrylonitrile **2i** (24.7 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry DCM (1.0 mL) was transferred to the solution in one portion and it was allowed to stir at room temperature for 48 h. After complete consumption of **2i** monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/5) to afford the cycloadduct **3i**: 30.8 mg (0.0942 mmol) as a white solid, 94% yield, >19:1 dr; mp 134–136 °C; $[\alpha]_D^{25}$ = +59.0 (*c* = 1.00 in $CHCl_3$); >99% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), t_R = 11.17 min (major), t_R = 15.66 min (minor); ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.68 (dd, *J* = 5.7, 2.7 Hz, 1H), 7.66–7.61 (m, 2H), 7.41–7.37 (m, 4H), 7.34–7.29 (m, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 6.47 (d, *J* = 5.7 Hz, 1H), 5.70 (dd, *J* = 6.9, 2.8 Hz, 1H), 4.16 (d, *J* = 2.0 Hz, 1H), 3.03 (dd, *J* = 6.9, 2.0 Hz, 1H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 204.4, 163.5, 156.7, 141.8, 140.8, 136.3, 129.7, 129.3, 129.2, 127.8, 127.7, 127.3, 119.4, 88.3, 77.0, 50.6, 39.7, 21.5; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{22}H_{17}NO_2Na^+$ 350.1151; Found 350.1149.



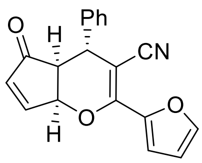
Synthesis of 3j: **General procedure A:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of (*E*)-2-(4-chlorobenzoyl)-3-phenylacrylonitrile **2j** (26.7 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry DCM (1.0 mL) was transferred to the solution in one portion and it was allowed to stir at room temperature for 30 h. After complete consumption of **2j** monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/5) to afford the cycloadduct **3j**: 31.3 mg (0.0902 mmol) as a white solid, 90% yield, 16:1 dr; mp 105–107 °C; $[\alpha]_D^{25}$ = +46.4 (*c* = 1.13 in $CHCl_3$); >99% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), major diastereomer: t_R = 14.96 min (major), t_R = 21.54 min (minor); ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.71–7.65 (m, 3H), 7.41–7.37 (m, 6H), 7.33–7.31 (m, 1H), 6.47 (d, *J* = 5.7 Hz, 1H), 5.72 (dd, *J* = 6.8, 2.8 Hz, 1H), 4.17 (d, *J* = 2.0 Hz, 1H), 3.03 (dd, *J* = 6.8, 2.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 204.0, 162.0, 156.4, 140.6, 137.4, 136.4, 130.9, 129.3, 129.2, 128.8, 127.8, 127.3, 118.8, 89.5, 77.1, 50.4, 39.5; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{14}{}^{35}ClNO_2Na^+$ 370.0605; Found 370.0605; Calcd for $C_{21}H_{14}{}^{37}ClNO_2Na^+$ 372.0576; Found 372.0580.



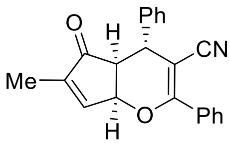
Synthesis of 3k: **General procedure A:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of (*E*)-2-(2-bromobenzoyl)-3-phenylacrylonitrile **2k** (31.1 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry DCM (1.0 mL) was transferred to the solution in one portion and it was allowed to stir at room temperature for 20 h. After complete consumption of **2k** monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/5) to afford the cycloadduct **3k**: 36.4 mg (0.0931 mmol) as a white solid, 93% yield, 10:1 dr; mp 198–199 °C; $[\alpha]_D^{25}$ = –68.4 (c = 1.45 in $CHCl_3$); 97% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), major diastereomer: t_R = 14.65 min (major), t_R = 16.25 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.70 (dd, J = 5.8, 2.9 Hz, 1H), 7.66–7.58 (m, 1H), 7.47–7.41 (m, 4H), 7.36–7.28 (m, 4H), 6.47 (d, J = 5.8 Hz, 1H), 5.64 (dd, J = 6.6, 2.9 Hz, 1H), 4.15 (d, J = 2.2 Hz, 1H), 2.90 (dd, J = 6.6, 2.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 203.7, 163.5, 156.9, 141.1, 135.4, 134.3, 133.4, 132.0, 131.1, 129.4, 127.9, 127.7, 127.5, 122.1, 117.7, 91.5, 76.2, 49.8, 37.7; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{14}{}^{79}BrNO_2Na^+$ 414.0100; Found 414.0108; $C_{21}H_{14}{}^{81}BrNO_2Na^+$ 416.0080; Found 416.0088.



Synthesis of 3l: **General procedure A:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of (*E*)-2-(2-naphthoyl)-3-phenylacrylonitrile **12l** (28.3 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry DCM (1.0 mL) was transferred to the solution in one portion and it was allowed to stir at room temperature for 30 h. After complete consumption of **2l** monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/5) to afford the cycloadduct **3l**: 32.7 mg (0.0901 mmol) as a white solid, 90% yield, 18:1 dr; mp: 158–160 °C; $[\alpha]_D^{25}$ = +112.0 (c = 1.22 in $CHCl_3$); 99% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), major diastereomer: t_R = 14.76 min (major), t_R = 18.80 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.26 (d, J = 1.9 Hz, 1H), 7.90–7.82 (m, 3H), 7.76 (dd, J = 8.6, 1.9 Hz, 1H), 7.72 (dd, J = 5.8, 2.8 Hz, 1H), 7.57–7.49 (m, 2H), 7.45–7.38 (m, 4H), 7.34–7.30 (m, 1H), 6.48 (d, J = 5.8 Hz, 1H), 5.75 (dd, J = 6.9, 2.8 Hz, 1H), 4.22 (d, J = 1.9 Hz, 1H), 3.05 (dd, J = 6.9, 1.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 204.3, 163.3, 156.7, 140.8, 136.4, 134.4, 132.5, 129.8, 129.3, 128.9, 128.6, 128.3, 127.9, 127.8, 127.7, 127.4, 126.9, 124.1, 119.2, 89.4, 77.2, 50.6, 39.8; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{25}H_{17}NO_2Na^+$ 386.1151; Found 386.1155.

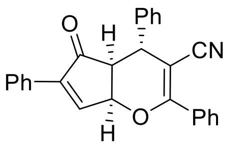


Synthesis of 3m: **General procedure A:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of (*E*)-2-(furan-2-carbonyl)-3-phenylacrylonitrile **2m** (22.3 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry DCM (1.0 mL) was transferred to the solution in one portion and it was allowed to stir at room temperature for 36 h. After complete consumption of **2m** monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/5) to afford the cycloadduct **3m**: 24.2 mg (0.0799 mmol) as a white solid, 80% yield, >19:1 dr; mp 140–142 °C; $[\alpha]_D^{25}$ = +48.2 (*c* = 0.66 in $CHCl_3$); 98% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), t_R = 13.69 min (minor), t_R = 16.33 min (major); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.61 (dd, *J* = 5.7, 2.7 Hz, 1H), 7.55 (d, *J* = 1.8 Hz, 1H), 7.41–7.34 (m, 4H), 7.33–7.28 (m, 1H), 7.02 (d, *J* = 3.6 Hz, 1H), 6.50 (dd, *J* = 3.6, 1.8 Hz, 1H), 6.45 (d, *J* = 5.7 Hz, 1H), 5.70 (dd, *J* = 6.9, 2.7 Hz, 1H), 4.16 (d, *J* = 2.0 Hz, 1H), 3.05 (dd, *J* = 6.9, 2.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 204.3, 156.7, 153.1, 146.4, 145.0, 140.4, 136.7, 129.3, 127.7, 127.3, 118.2, 114.1, 111.9, 87.2, 77.1, 50.6, 39.8; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{19}H_{13}NO_3Na^+$ 326.0788; Found 326.0789.

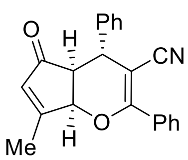


Synthesis of 3n: **General procedure B:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%), **L6** (6.4 mg, 0.010 mmol, 10 mol%), (*E*)-2-benzoyl-3-phenylacrylonitrile **2a** (23.3 mg, 0.100 mmol) and *tert*-butyl (3-methyl-4-oxocyclopent-2-en-1-yl) carbonate **1d** (42.4 mg, 0.200 mmol). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed toluene (2.0 mL) was added via syringe and it was allowed to stir at 50 °C for 22 h. After complete consumption of **2a** monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/15) to afford the cycloadduct **3n**: 28.1 mg (0.0859 mmol) as a semi-solid, 86% yield, >19:1 dr; $[\alpha]_D^{25}$ = –22.1 (*c* = 0.15 in $CHCl_3$); 81% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), t_R = 9.87 min (major), t_R = 16.15 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm)

7.77–7.71 (m, 2H), 7.48–7.35 (m, 7H), 7.33–7.27 (m, 2H), 5.62 (ddd, J = 6.8, 2.9, 1.4 Hz, 1H), 4.18 (d, J = 1.9 Hz, 1H), 3.04 (dd, J = 6.8, 1.9 Hz, 1H), 1.91 (t, J = 1.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 204.5, 163.4, 150.4, 145.5, 141.0, 132.7, 131.2, 129.3, 128.5, 127.9, 127.7, 127.3, 119.4, 88.8, 75.9, 50.8, 39.9, 10.4; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{22}H_{17}NO_2Na^+$ 350.1151; Found 350.1154.

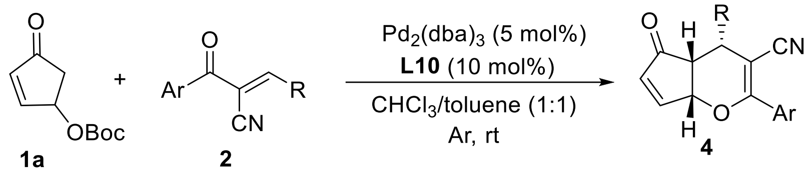


Synthesis of 3o: **General procedure B:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%), **L6** (6.4 mg, 0.010 mmol, 10 mol%), (*E*)-2-benzoyl-3-phenylacrylonitrile **2a** (23.3 mg, 0.100 mmol) and *tert*-butyl (4-oxo-3-phenylcyclopent-2-en-1-yl) carbonate **1e** (54.8 mg, 0.200 mmol). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed toluene (2.0 mL) was added via syringe and it was allowed to stir at 50 °C for 24 h. After complete consumption of **2a** monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/15) to afford the cycloadduct **3o**: 31.8 mg (0.0817 mmol) as a white solid, 82% yield, >19:1 dr; mp 48–50 °C; $[\alpha]_D^{25}$ = −100.0 (c = 0.11 in $CHCl_3$); 53% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 40/60, flow rate = 1.0 mL/min, λ = 254 nm), t_R = 7.93 min (major), t_R = 15.10 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.82–7.71 (m, 5H), 7.47–7.37 (m, 10H), 7.35–7.29 (m, 1H), 5.73 (dd, J = 6.8, 3.1 Hz, 1H), 4.29 (d, J = 2.0 Hz, 1H), 3.22 (dd, J = 6.8, 2.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 202.4, 163.6, 149.3, 145.1, 140.9, 132.7, 131.2, 130.1, 129.5, 129.3, 128.8, 128.5, 127.9, 127.79, 127.76, 127.4, 119.3, 88.7, 75.0, 52.1, 39.8; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{27}H_{19}NO_2Na^+$ 412.1308; Found 412.1312.



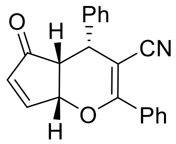
Synthesis of 3p: **General procedure B:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%), **L6** (6.4 mg, 0.010 mmol, 10 mol%), (*E*)-2-benzoyl-3-phenylacrylonitrile **2a** (23.3 mg, 0.100 mmol) and *tert*-butyl (4-oxo-3-phenylcyclopent-2-en-1-yl) carbonate **1f** (42.4 mg, 0.200 mmol). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed toluene (2.0 mL) was added via syringe and it was allowed to stir at 50 °C for 26 h. After complete consumption of **2a** monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/10) to afford the cycloadduct **3p**: 11.8 mg (0.0361 mmol) as a white solid, 36% yield, 10:1 dr; mp 138–140 °C; $[\alpha]_D^{25}$ = +22.0 (c = 0.10 in $CHCl_3$); 20% ee, determined by HPLC analysis (Chiralpak AD-H, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), t_R = 14.26 min (major), t_R = 15.22 min (minor); ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.76–7.71 (m, 2H), 7.48–7.41 (m, 3H), 7.41–7.35 (m, 4H), 7.34–7.29 (m, 1H), 6.18–6.15 (m, 1H), 5.42 (d, J = 6.9 Hz, 1H), 4.18 (d, J = 2.0 Hz, 1H), 3.03 (dd, J = 6.9, 2.0 Hz, 1H), 2.33–2.30 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 203.5, 170.6, 163.3, 141.0, 132.6, 132.0, 131.1, 129.3, 128.6, 127.8, 127.7, 127.3, 119.2, 88.7, 79.4, 51.5, 39.2, 16.9; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{22}H_{17}NO_2Na^+$ 350.1151; Found 350.1151.

4. General procedure for synthesis of *endo*-cycloadducts 4

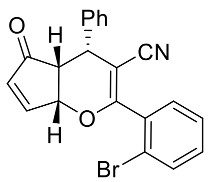


General procedure C: To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L10** (5.9 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed toluene (1.0 mL) was added via syringe and the mixture was stirred for 20 min. The mixture of 1-oxadiene **2** (0.1 mmol) and carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry $CHCl_3$ (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature (20–25 °C) for the indicated time. After complete consumption of **2** monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (EtOAc/petroleum ether or acetone/petroleum ether) to afford the cycloadduct **4** (**4a–4g**).

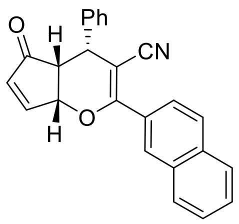
The corresponding racemates were obtained under the catalysis of $Pd_2(dba)_3$ (1.4 mg, 0.0015 mmol, 5.0 mol%) and 1,3-bis(diphenylphosphino)propane (2.2 mg, 0.0029 mmol, 10 mol%) on a 0.03 mmol scale.



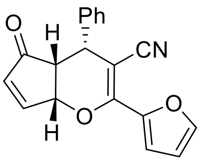
Synthesis of 4a: **General procedure C:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L10** (5.9 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed toluene (1.0 mL) was added via syringe and the mixture was stirred for 20 min. The mixture of (*E*)-2-benzoyl-3-phenylacrylonitrile **2a** (23.3 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry $CHCl_3$ (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature for 20 h. After complete consumption of **2a** monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/5) to afford the cycloadduct **4a**: 27.5 mg (0.0879 mmol) as a white solid, 88% yield, 5:1 dr; mp 50–52 °C; $[\alpha]_D^{25}$ = –144.1 (*c* = 1.40 in $CHCl_3$); 90% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), major diastereomer: t_R = 8.77 min (minor), t_R = 9.72 min (major); ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.90–7.88 (m, 2H), 7.66 (dd, *J* = 5.8, 2.2 Hz, 1H), 7.52–7.38 (m, 4H), 7.22–7.20 (m, 2H), 7.13–7.10 (m, 2H), 6.06 (dd, *J* = 5.8, 1.6 Hz, 1H), 5.52 (dt, *J* = 6.8, 1.6 Hz, 1H), 4.27 (d, *J* = 9.0 Hz, 1H), 3.35 (dd, *J* = 9.0, 6.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 203.2, 165.6, 158.5, 137.4, 136.3, 132.3, 131.5, 129.4, 128.7, 128.5, 128.1, 127.8, 119.2, 91.1, 79.1, 49.4, 41.9. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{15}NO_2Na^+$ 336.0995; Found 336.0991.



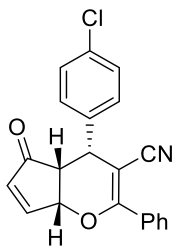
Synthesis of 4b: **General procedure C:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L10** (5.9 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed toluene (1.0 mL) was added via syringe and the mixture was stirred for 20 min. The mixture of (*E*)-2-(2-bromobenzoyl)-3-phenylacrylonitrile **2k** (31.1 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry $CHCl_3$ (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature for 20 h. After complete consumption of **2k** monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/5) to afford the cycloadduct **4b**: 35.2 mg (0.0900 mmol) as a white solid, 90% yield, 5:1 dr; mp 139–141 °C; $[\alpha]_D^{25}$ = –84.8 (*c* = 0.79 in $CHCl_3$); 80% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), major diatereomer: t_R = 8.57 min (major), t_R = 9.81 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.73–7.68 (m, 1H), 7.64 (dd, *J* = 5.8, 2.3 Hz, 1H), 7.50 (dd, *J* = 7.2, 2.1 Hz, 1H), 7.43–7.35 (m, 3H), 7.26–7.24 (m, 2H), 7.19–7.14 (m, 2H), 6.06 (dd, *J* = 5.8, 2.1 Hz, 1H), 5.67 (dt, *J* = 6.8, 2.1 Hz, 1H), 4.26 (d, *J* = 9.1 Hz, 1H), 3.37 (dd, *J* = 9.1, 6.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 203.0, 166.0, 158.6, 137.4, 136.3, 133.8, 133.6, 132.4, 131.8, 129.3, 128.6, 128.0, 127.8, 122.3, 117.8, 95.5, 79.5, 48.8, 40.9; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{14}{}^{79}BrNO_2Na^+$ 414.0100; Found 414.0102; Calcd for $C_{21}H_{14}{}^{81}BrNO_2Na^+$ 416.0080; Found 416.0086.



Synthesis of 4c: **General procedure C:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L10** (5.9 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed toluene (1.0 mL) was added via syringe and the mixture was stirred for 20 min. The mixture of (*E*)-2-(2-naphthoyl)-3-phenylacrylonitrile **2l** (28.3 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry $CHCl_3$ (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature for 20 h. After complete consumption of **2l** monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/5) to afford the cycloadduct **4c**: 31.4 mg (0.0865 mmol) as a white solid, 87% yield, 5:1 dr; mp 143–145 °C; $[\alpha]_D^{25}$ = –106.5 (*c* = 1.55 in $CHCl_3$); 86% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 10/90, flow rate = 1.0 mL/min, λ = 254 nm), major diastereomer: t_R = 17.54 min (major), t_R = 18.84 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.99 (d, *J* = 8.3 Hz, 1H), 7.94–7.91 (m, 1H), 7.81–7.85 (m, 1H), 7.73–7.68 (m, 1H), 7.60 (dd, *J* = 5.8, 2.2 Hz, 1H), 7.59–7.48 (m, 4H), 7.28–7.26 (m, 2H), 7.23–7.21 (m, 2H), 6.07 (dd, *J* = 5.8, 2.0 Hz, 1H), 5.67 (dt, *J* = 6.9, 2.0 Hz, 1H), 4.32 (d, *J* = 9.1 Hz, 1H), 3.45 (dd, *J* = 9.1, 6.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 203.1, 166.8, 158.6, 137.4, 136.7, 133.8, 131.8, 130.7, 130.1, 129.4, 129.1, 128.9, 128.7, 128.0, 127.3, 126.6, 125.2, 124.6, 118.3, 94.8, 78.8, 48.6, 40.9; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{25}H_{17}NO_2Na^+$ 386.1151; Found 386.1149.

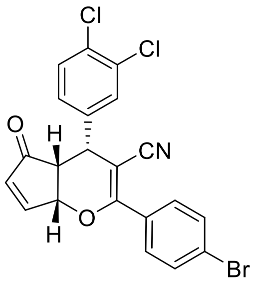


Synthesis of 4d: **General procedure C:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L10** (5.9 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed toluene (1.0 mL) was added via syringe and the mixture was stirred for 20 min. The mixture of (*E*)-2-(furan-2-carbonyl)-3-phenylacrylonitrile **2m** (22.3 mg, 0.1 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry $CHCl_3$ (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature for 22 h. After complete consumption of **2m** monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/5) to afford the cycloadduct **4d**: 28.0 mg (0.0924 mmol) as a white solid, 92% yield, 6:1 dr; mp 116–118 °C; $[\alpha]_D^{25}$ = –220.5 (*c* = 0.96 in $CHCl_3$); 92% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), major diastereomer: t_R = 8.85 min (minor), t_R = 10.06 min (major); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.67 (dd, *J* = 5.8, 2.3 Hz, 1H), 7.63–7.60 (m, 1H), 7.37 (d, *J* = 4.4 Hz, 1H), 7.21–7.18 (m, 2H), 7.14 (d, *J* = 3.5 Hz, 1H), 7.12–7.08 (m, 2H), 6.56 (dd, *J* = 3.5, 1.8 Hz, 1H), 6.10 (dd, *J* = 5.8, 1.8 Hz, 1H), 5.46 (dt, *J* = 6.8, 2.0 Hz, 1H), 4.26 (d, *J* = 8.9 Hz, 1H), 3.32 (dd, *J* = 8.9, 6.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 203.0, 158.3, 155.5, 146.2, 145.2, 137.8, 136.2, 129.3, 128.5, 127.8, 118.2, 114.5, 112.1, 89.2, 78.8, 49.6, 41.7; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{19}H_{13}NO_3Na^+$ 326.0788; Found 326.0782.

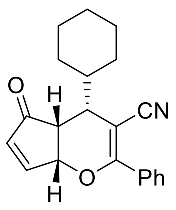


Synthesis of 4e: **General procedure C:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L10** (5.9 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed toluene (1.0 mL) was added via syringe and the mixture was stirred for 20 min. The mixture of (*E*)-2-benzoyl-3-(4-chlorophenyl)acrylonitrile **2e** (26.7 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry $CHCl_3$ (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature for 20 h. After complete consumption of **2e** monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/5) to afford the cycloadduct **4e**: 30.8 mg

(0.0888 mmol) as a white solid, 89% yield, 7:1 dr; mp 53–54 °C; $[\alpha]_D^{25}$ = –168.0 (c = 1.08 in $CHCl_3$); 85% ee, determined by HPLC analysis (Chiralpak ID, *i*-PrOH/*n*-hexane = 30/70, flow rate = 1.0 mL/min, λ = 254 nm), major diastereomer: t_R = 14.75 min (minor), t_R = 15.74 min (major); ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.89–7.87 (m, 2H), 7.68 (dd, J = 5.8, 2.3 Hz, 1H), 7.53–7.45 (m, 3H), 7.21–7.18 (m, 2H), 7.08–7.05 (m, 2H), 6.12 (dd, J = 5.8, 1.7 Hz, 1H), 5.53 (dt, J = 6.8, 2.0 Hz, 1H), 4.17 (d, J = 9.0 Hz, 1H), 3.27 (dd, J = 9.0, 6.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 201.9, 164.7, 157.5, 136.6, 133.9, 132.8, 131.0, 130.7, 129.7, 127.70, 127.65, 127.0, 117.9, 89.8, 78.1, 48.1, 40.2; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{14}{}^{35}ClNO_2Na^+$ 370.0605; Found 370.0608; $[M + H]^+$ Calcd for $C_{21}H_{15}{}^{37}ClNO_2^+$ 350.0756; Found 350.0760.

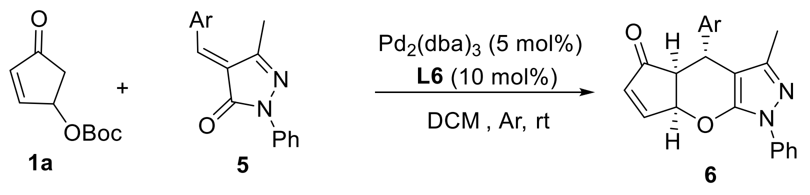


Synthesis of 4f: **General procedure C:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L10** (5.9 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed toluene (1.0 mL) was added via syringe and the mixture was stirred for 20 min. The mixture of (*E*)-2-(4-bromobenzoyl)-3-(3,4-dichlorophenyl)acrylonitrile **2n** (37.9 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry $CHCl_3$ (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature for 20 h. After complete consumption of **2n** monitored by TLC, the crude product was concentrated and purified by flash chromatography on silica gel (acetone/petroleum ether = 1/5) to afford the cycloadduct **4f**: 36.7 mg (0.0800 mmol) as a white solid, 80% yield, 8:1 dr; mp 165–167 °C; $[\alpha]_D^{25}$ = –96.5 (c = 0.96 in $CHCl_3$); 90% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 10/90, flow rate = 1.0 mL/min, λ = 254 nm), major diastereomer: t_R = 18.23 min (minor), t_R = 19.32 min (major); ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.80–7.74 (m, 2H), 7.72 (dd, J = 5.8, 2.3 Hz, 1H), 7.65–7.60 (m, 2H), 7.31 (d, J = 8.3 Hz, 1H), 7.19 (d, J = 2.3 Hz, 1H), 6.96 (dd, J = 8.3, 2.3 Hz, 1H), 6.20 (dd, J = 5.8, 1.7 Hz, 1H), 5.53 (dt, J = 6.9, 2.0 Hz, 1H), 4.21 (d, J = 9.1 Hz, 1H), 3.35 (dd, J = 9.1, 6.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 202.5, 164.9, 158.4, 138.0, 136.6, 132.7, 132.3, 132.1, 131.1, 130.7, 130.5, 129.5, 128.7, 126.5, 118.4, 91.1, 79.2, 48.7, 40.9; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{13}{}^{79}Br^{35}Cl_2NO_2^+$ 459.9501; Found 459.9503; Calcd for $C_{21}H_{13}{}^{81}Br^{37}Cl_2NO_2^+$ 461.9481; Found 461.9487.



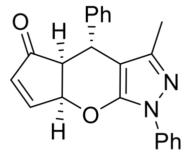
Synthesis of 4g: **General procedure C:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%) and **L10** (5.9 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed toluene (1.0 mL) was added via syringe and the mixture was stirred for 20 min. The mixture of (*E*)-2-benzoyl-3-cyclohexylacrylo nitrile **2g** (24.0 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry $CHCl_3$ (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature for 48 h. The corresponding racemate was obtained under the catalysis of $Pd_2(dba)_3$ (1.4 mg, 0.0015 mmol, 5.0 mol%) and (±)-**L6** (1.9 mg, 0.0030 mmol, 10 mol%) in 0.03 mmol scale. After completion, the crude product was concentrated and purified by flash chromatography on silica gel (EtOAc/petroleum ether = 1/6) to afford the cycloadduct **4g**: 21.8 mg (0.0681 mmol) as a sem-solid, 68% yield, >19:1 dr; $[\alpha]_D^{25}$ = –162.7 (*c* = 0.82 in $CHCl_3$); 85% ee, determined by HPLC analysis (Chiralpak AD-H, *i*-PrOH/*n*-hexane = 10/90, flow rate = 1.0 mL/min, λ = 254 nm), t_R = 13.31 min (minor), t_R = 16.96 min (major); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.80–7.76 (m, 2H), 7.56 (dd, *J* = 5.8, 2.7 Hz, 1H), 7.48–7.39 (m, 3H), 6.38 (d, *J* = 5.8 Hz, 1H), 5.58 (ddd, *J* = 6.8, 2.7, 0.8 Hz, 1H), 3.27 (t, *J* = 6.4 Hz, 1H), 2.51 (dd, *J* = 8.9, 5.8 Hz, 1H), 2.16–2.08 (m, 3H), 1.83–1.77 (m, 1H), 1.76–1.67 (m, 2H), 1.52–1.32 (m, 2H), 1.28–1.06 (m, 2H), 0.98–0.84 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 204.8, 166.0, 155.7, 139.2, 132.3, 131.3, 128.6, 127.9, 118.4, 93.3, 81.1, 47.7, 40.9, 36.5, 32.9, 31.4, 26.3, 26.2, 25.8; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{22}NO_2^+$ 320.1645 ; Found 320.1644.

5. General procedure for synthesis of cycloadducts 6

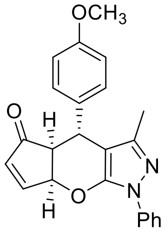


General procedure D: To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%), **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of alkylidene pyrazolones **5** (0.1 mmol) and carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry DCM (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature for the indicated time. After complete consumption of **5** monitored by TLC, the crude product was purified by flash chromatography on silica gel (EtOAc/petroleum ether) to afford the cycloadduct **6** (**6a–6e**).

The corresponding racemates were obtained under the catalysis of $Pd(PPh_3)_4$ (1.7 mg, 0.015 mmol, 5 mol%) on a 0.03 mmol scale.

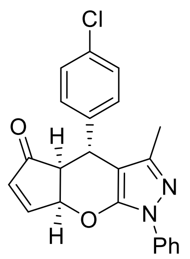


Synthesis of 6a: **General procedure D**: To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%), **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of (*E*)-4-benzylidene-5-methyl-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-one **5a** (26.2 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry DCM (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature for 20 h. After complete consumption of **5a** monitored by TLC, the crude product was purified by flash chromatography on silica gel (EtOAc/petroleum ether = 1/10) to afford the cycloadduct **6a**: 30.6 mg (0.0895 mmol) as a colorless semi-solid, 89% yield, >19:1 dr; $[\alpha]_D^{25}$ = +95.9 (*c* = 1.48 in $CHCl_3$); 98% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), t_R = 6.03 min (major), t_R = 7.04 min (minor); ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.74–7.69 (m, 2H), 7.64 (dd, *J* = 5.8, 2.8 Hz, 1H), 7.44–7.37 (m, 2H), 7.35–7.19 (m, 6H), 6.35 (d, *J* = 5.8 Hz, 1H), 5.73 (dd, *J* = 6.2, 2.8 Hz, 1H), 4.52 (d, *J* = 1.5 Hz, 1H), 2.91 (dd, *J* = 6.2, 1.5 Hz, 1H), 2.05 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 205.0, 156.8, 147.9, 146.5, 143.8, 138.5, 135.4, 129.01, 128.98, 127.3, 126.9, 125.7, 120.4, 98.5, 79.1, 52.3, 34.9, 12.7; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{19}N_2O_2^+$ 343.1441; Found 343.1449.

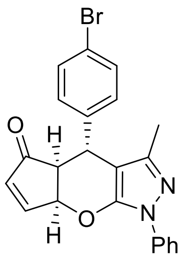


Synthesis of 6b: **General procedure D**: To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%), **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of (*E*)-4-(4-methoxybenzylidene)-5-

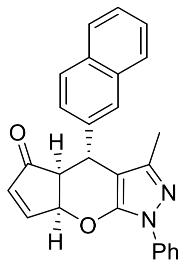
methyl-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-one **5b** (29.2 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry DCM (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature for 4 h. After complete consumption of **5b** monitored by TLC, the crude product was purified by flash chromatography on silica gel (EtOAc/petroleum ether = 1/10) to afford the cycloadduct **6b**: 35.0 mg (0.0941 mmol) as a colorless semi-solid, 94% yield, >19:1 dr; $[\alpha]_D^{25}$ = +54.8 (c = 2.39 in $CHCl_3$); 98% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), t_R = 7.46 min (major), t_R = 8.56 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.74–7.68 (m, 2H), 7.62 (dd, J = 5.8, 2.8 Hz, 1H), 7.44–7.37 (m, 2H), 7.24–7.17 (m, 3H), 6.88–6.83 (m, 2H), 6.34 (d, J = 5.8 Hz, 1H), 5.71 (dd, J = 6.2, 2.8 Hz, 1H), 4.46 (d, J = 1.6 Hz, 1H), 3.78 (s, 3H), 2.87 (dd, J = 6.2, 1.6 Hz, 1H), 2.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 205.1, 158.5, 156.8, 147.9, 146.5, 138.5, 135.8, 135.4, 129.0, 128.3, 125.7, 120.3, 114.3, 98.8, 79.2, 55.3, 52.5, 34.2, 12.7; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{23}H_{21}N_2O_3^+$ 373.1547; Found 373.1552.



Synthesis of 6c: **General procedure D**: To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%), **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of (*E*)-4-(4-chlorobenzylidene)-5-methyl-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-one **5c** (29.6 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry DCM (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature for 20 h. After complete consumption of **5c** monitored by TLC, the crude product was purified by flash chromatography on silica gel (EtOAc/petroleum ether = 1/10) to afford the cycloadduct **6c**: 35.8 mg (0.0952 mmol) as a colorless semi-solid, 95% yield, >19:1 dr; $[\alpha]_D^{25}$ = +49.3 (c = 2.04 in $CHCl_3$); 96% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), t_R = 6,36 min (major), t_R = 7.57 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.71 (d, J = 7.9 Hz, 2H), 7.64 (dd, J = 5.7, 2.7 Hz, 1H), 7.41 (t, J = 7.9 Hz, 2H), 7.33–7.18 (m, 5H), 6.36 (d, J = 5.7 Hz, 1H), 5.71 (dd, J = 6.0, 2.7 Hz, 1H), 4.49 (s, 1H), 2.87–2.82 (m, 1H), 2.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 204.7, 156.9, 147.9, 146.4, 142.3, 138.3, 135.4, 132.8, 129.1, 129.0, 128.7, 125.8, 120.4, 98.0, 79.0, 52.1, 34.4, 12.7; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{18}{}^{35}ClN_2O_2^+$ 377.1051; Found 377.1057; Calcd for $C_{22}H_{18}{}^{37}ClN_2O_2^+$ 379.1022; Found 379.1042.

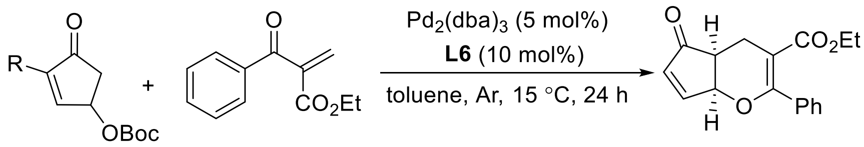


Synthesis of 6d: **General procedure D**: To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%), **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of (*E*)-4-(4-bromobenzylidene)-5-methyl-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-one **5d** (34.0 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry DCM (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature for 26 h. After complete consumption of **5d** monitored by TLC, the crude product was purified by flash chromatography on silica gel (EtOAc/petroleum ether = 1/10) to afford the cycloadduct **6d**: 34.4 mg (0.0817 mmol) as a colorless semi-solid, 82% yield, >19:1 dr; $[\alpha]_D^{25}$ = +200.0 (c = 1.81 in $CHCl_3$); 97% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), t_R = 6.97 min (major), t_R = 8.42 min (minor); ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.71 (d, J = 8.2 Hz, 2H), 7.64 (dd, J = 5.7, 2.4 Hz, 1H), 7.46–7.39 (m, 4H), 7.27–7.20 (m, 1H), 7.16 (d, J = 8.2 Hz, 2H), 6.36 (d, J = 5.7 Hz, 1H), 5.70 (dd, J = 6.0, 2.4 Hz, 1H), 4.47 (s, 1H), 2.84 (d, J = 6.0 Hz, 1H), 2.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 204.6, 156.9, 147.9, 146.4, 142.8, 138.3, 135.4, 132.1, 129.1, 129.0, 125.8, 120.8, 120.4, 97.9, 79.0, 52.1, 34.5, 12.7; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{18}{}^{79}BrN_2O_2^+$ 421.0546; Found 421.0541; $C_{22}H_{18}{}^{81}BrN_2O_2^+$ 423.0526; Found 423.0522.



Synthesis of 6e: **General procedure D**: To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%), **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of (*E*)-5-methyl-4-(naphthalen-2-ylmethylene)-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-one **5e** (31.2 mg, 0.1 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry DCM (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature for 20 h. After complete consumption of **5e** monitored by TLC, the crude product was purified by flash chromatography on silica gel (EtOAc/petroleum ether = 1/10) to afford the cycloadduct **6e**: 35.2 mg (0.0898 mmol) as a colorless semi-solid, 90% yield, >19:1 dr; $[\alpha]_D^{25}$ = –20.0 (c = 3.72 in $CHCl_3$); 98% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 10/90, flow rate = 1.0 mL/min, λ = 254 nm), t_R = 10.52 min (minor), t_R = 12.30 min (major); ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.84–7.74 (m, 5H), 7.67–7.62 (m, 2H), 7.50–7.36 (m, 5H), 7.28–7.20 (m, 1H), 6.37 (d, J = 5.8 Hz, 1H), 5.72 (dd, J = 5.8, 2.2 Hz, 1H), 4.69 (s, 1H), 2.97 (d, J = 6.0 Hz, 1H), 2.05 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 205.0, 156.9, 148.1, 146.7, 141.0, 138.5, 135.4, 133.5, 132.5, 129.1, 129.0, 127.9, 127.7, 126.4, 125.9, 125.75, 125.69, 125.6, 120.4, 98.1, 79.1, 52.2, 35.0, 12.7; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{26}H_{20}N_2O_2Na^+$ 415.1417; Found 415.1411.

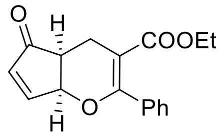
6. General procedure for synthesis of cycloadducts 8 and 10



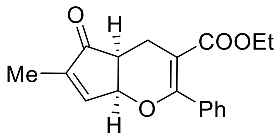
1 7 8

General procedure E: To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%), **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed toluene (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of 1-oxadiene **7** (20.4 mg, 0.100 mmol) and 2-cyclopentenone **1** (0.2 mmol) dissolved in dry toluene (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at 15 °C for the indicated time. After complete consumption of **7** monitored by TLC, the crude product was directly purified by flash chromatography on silica gel (EtOAc or acetone/petroleum ether) to afford the cycloadduct **8** (**8a–8c**).

The corresponding racemates were obtained under the catalysis of $Pd_2(dba)_3$ (1.4 mg, 0.0015 mmol, 5.0 mol%) and (±)-**L6** (1.9 mg, 0.0030 mmol, 10 mol%) on a 0.03 mmol scale.

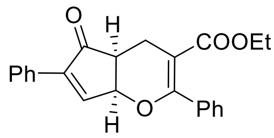


Synthesis of 8a: **General procedure E:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%), **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed toluene (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of ethyl 2-benzoylacrylate **7** (20.4 mg, 0.100 mmol) and 2-cyclopentenone **1a** (40.0 mg, 0.202 mmol) dissolved in dry toluene (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at 15 °C for 24 h. After complete consumption of **7** monitored by TLC, the crude product was purified by flash chromatography on silica gel (acetone/petroleum ether = 1/20) to afford the cycloadduct **8a**: 15.8 mg (0.0556 mmol) as a semi-solid, 56% yield, >19:1 dr; $[\alpha]_D^{25}$ = +133.3 (*c* = 0.15 in $CHCl_3$); 90% ee, determined by HPLC analysis (Chiralpak IF, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), t_R = 11.41 min (minor), t_R = 12.96 min (major); ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.63 (dd, *J* = 5.7, 2.4 Hz, 1H), 7.41–7.32 (m, 3H), 7.31–7.27 (m, 2H), 6.43 (d, *J* = 5.7 Hz, 1H), 5.46–5.40 (m, 1H), 4.02–3.94 (m, 2H), 3.00–2.95 (m, 1H), 2.81 (dd, *J* = 15.0, 7.7 Hz, 1H), 2.69 (dd, *J* = 15.0, 5.1 Hz, 1H), 0.98 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 207.1, 167.4, 162.7, 158.2, 136.8, 135.5, 129.6, 128.6, 127.8, 107.1, 77.6, 60.3, 45.7, 21.9, 13.7; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{17}H_{16}O_4Na^+$ 307.0941, found 307.0939.

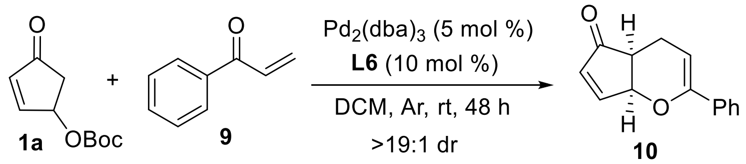


Synthesis of 8b: **General procedure E:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%), **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed toluene (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of ethyl 2-benzoylacrylate **7** (20.4 mg, 0.100 mmol) and *tert*-butyl (3-methyl-4-oxocyclopent-2-en-1-yl) carbonate **1d** (42.4 mg, 0.200 mmol) dissolved in dry toluene (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at 15 °C for 24 h. After complete consumption of **7** monitored by TLC, the crude product was purified by flash chromatography on silica gel (acetone/petroleum ether = 1/20) to afford the cycloadduct **8a**: 17.8 mg (0.0581 mmol) as a semi-solid, 58% yield, >19:1 dr; $[\alpha]_D^{25}$ = +200.0 (*c* = 0.12 in $CHCl_3$); 93% ee, determined by HPLC analysis (Chiralpak IF, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), t_R = 6.76 min (major), t_R = 7.36 min (minor); ^1H NMR (400 MHz,

$CDCl_3$) δ (ppm) 7.40–7.28 (m, 5H), 7.27–7.24 (m, 1H), 5.34–5.27 (m, 1H), 4.02–3.94 (m, 2H), 3.02–2.94 (m, 1H), 2.84–2.75 (m, 1H), 2.72–2.64 (m, 1H), 1.90–1.85 (m Hz, 3H), 1.03–3.96 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 207.1, 167.5, 162.9, 151.9, 145.7, 135.6, 129.5, 128.7, 127.8, 106.9, 76.1, 60.2, 45.9, 22.1, 13.8, 10.3; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{18}H_{18}O_4Na^+$ 321.1097; Found 321.1105.

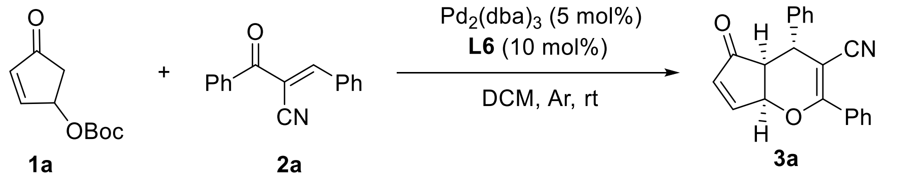


Synthesis of 8c: **General procedure E:** To an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%), **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed toluene (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of ethyl 2-benzoylacrylate **7** (20.4 mg, 0.100 mmol) and *tert*-butyl (4-oxo-3-phenylcyclopent-2-en-1-yl) carbonate **1e** (54.8 mg, 0.200 mmol) dissolved in dry toluene (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at 15 °C for 24 h. After complete consumption of **7** monitored by TLC, the crude product was purified by flash chromatography on silica gel (acetone/petroleum ether = 1/20) to afford the cycloadduct **8c**: 18.1 mg (0.0503 mmol) as a semi-solid, 50% yield, >19:1 dr; $[\alpha]_D^{25}$ = +200.0 (*c* = 0.11 in $CHCl_3$); 90% ee, determined by HPLC analysis (Chiralpak IE, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), t_R = 23.29 min (major), t_R = 36.56 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.79–7.73 (m, 2H), 7.73–7.70 (m, 1H), 7.45–7.38 (m, 3H), 7.38–7.29 (m, 5H), 5.48–5.43 (m, 1H), 4.03–3.91 (m, 2H), 3.23–3.13 (m, 1H), 2.92–2.84 (m, 1H), 2.83–2.75 (m, 1H), 1.00–0.94 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 204.9, 167.4, 162.9, 151.2, 145.5, 135.7, 130.0, 129.6, 129.5, 128.7, 127.8, 127.7, 106.9, 75.4, 60.2, 47.2, 22.2, 13.7; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{23}H_{20}O_4Na^+$ 383.1254; Found 383.1262.



Synthesis of 10: an oven dried 10 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (4.6 mg, 0.0050 mmol, 5.0 mol%), **L6** (6.4 mg, 0.010 mmol, 10 mol%). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (1.0 mL) was added via syringe and the mixture was stirred for 30 min. The mixture of 1-phenylprop-2-en-1-one **9** (13.2 mg, 0.100 mmol) and *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (40.0 mg, 0.202 mmol) dissolved in dry DCM (1.0 mL) was transferred to the catalytic solution in one portion and it was allowed to stir at room temperature for 48 h. After complete consumption of **9** monitored by TLC, the crude product was purified by flash chromatography on silica gel (EtOAc/DCM/petroleum ether = 1/60/60) to afford the cycloadduct **10**: 12.1 mg (0.0571 mmol) as a semi-solid, 57% yield, >19:1 dr; $[\alpha]_D^{25}$ = +10.4 (c = 0.52 in $CHCl_3$); 96% ee, determined by HPLC analysis (Chiralpak IA, *i*-PrOH/*n*-hexane = 5/95, 1.0 mL/min, λ = 254 nm), t_R = 11.21 min (major), t_R = 11.89 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.56 (dd, J = 5.7, 2.5 Hz, 1H), 7.53–7.49 (m, 2H), 7.35–7.25 (m, 3H), 6.32 (d, J = 5.7 Hz, 1H), 5.73 (dd, J = 6.3, 4.2 Hz, 1H), 5.47 (ddd, J = 6.3, 2.5, 0.8 Hz, 1H), 2.89–2.83 (m, 1H), 2.59–2.41 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 208.8, 158.9, 151.4, 136.6, 135.0, 128.29, 128.27, 124.1, 101.4, 77.2, 45.4, 20.7; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{14}H_{12}O_2Na^+$ 235.0730; Found 235.0728.

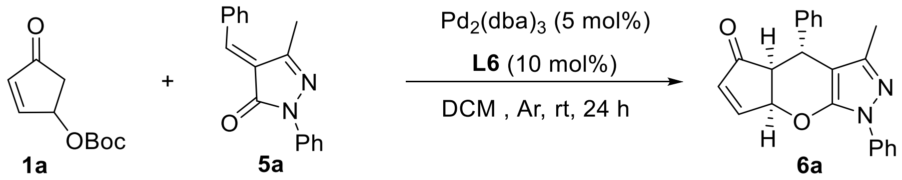
7. Asymmetric reaction on a 1.0 mmol and gram scale



1.0 mmol-scale reaction: To an oven dried 50 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (45.7 mg, 0.0500 mmol) and **L6** (64.2 mg, 0.100 mmol). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (10 mL) was added via syringe and the mixture was stirred for 30 min. (*E*)-2-Benzoyl-3-phenylacrylonitrile **2a** (233.0 mg, 0.9999 mmol) in dry DCM (8.0 mL) was transferred to the catalytic solution in one portion. Then *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (400.0 mg, 2.020 mmol) in dry DCM (2.0 mL) was added in four potions for 4 h by syringe. The mixture was allowed to stir at room temperature for another 26 h. After complete consumption of **2a** monitored by TLC, the mixture was filtered through a celite pad and concentrated in vacuo. The residue was purified by flash chromatography on silica gel (acetone/petroleum ether = 1/5) to afford the cycloadduct **3a**: 304.0 mg (0.9701 mmol), as a white solid, 97% yield, 18:1 dr, 98% ee.

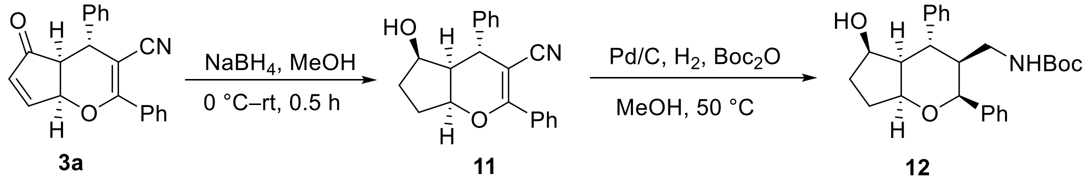
Gram-scale reaction: To an oven dried 100 mL Schlenk tube equipped with a stir bar were added

$Pd_2(dba)_3$ (206 mg, 0.225 mmol) and **L6** (289 mg, 0.450 mmol). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (45 mL) was added via syringe and the mixture was stirred for 30 min. (*E*)-2-Benzoyl-3-phenylacrylonitrile **2a** (1.05 g, 4.51 mmol) in dry DCM (25 mL) was transferred to the catalytic solution in one portion. Then *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (1.78 g, 8.99 mmol) in dry DCM (20 mL) was added in four potions for 8 h by syringe. The mixture was allowed to stir at room temperature for another 40 h. After complete consumption of **2a** monitored by TLC, the mixture was filtered through a celite pad and concentrated in vacuo. The residue was purified by flash chromatography on silica gel (acetone/petroleum ether = 1/10 to 1/7) to afford the cycloadduct **3a**: 1.35 g (4.30 mmol), as a white solid, 96% yield, 19:1 dr, 98% ee.



To an oven dried 50 mL Schlenk tube equipped with a stir bar were added $Pd_2(dba)_3$ (45.7 mg, 0.0500 mmol) and **L6** (64.2 mg, 0.100 mmol). The tube was evacuated and back-filled with argon for three times. Then distilled and degassed DCM (10 mL) was added via syringe and the mixture was stirred for 30 min. (*E*)-4-benzylidene-5-methyl-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-one **5a** (262.3 mg, 0.100 mmol) in dry DCM (8.0 mL) was transferred to the catalytic solution in one portion. Then *tert*-butyl (4-oxocyclopent-2-en-1-yl) carbonate **1a** (400.0 mg, 2.020 mmol) in dry DCM (2.0 mL) was added in two potions by syringe. The mixture was stirred at room temperature for 24 h totally. After complete consumption of **5a** monitored by TLC, the resulting mixture was filtered through a celite pad and concentrated in vacuo. The residue was purified by flash chromatography on silica gel (acetone/petroleum ether = 1/5 to 1/3) to afford the cycloadduct **6a**: 263.0 mg (0.7681 mmol), as a white solid, 77% yield, >19:1 dr, 96% ee.

8. Synthetic transformations

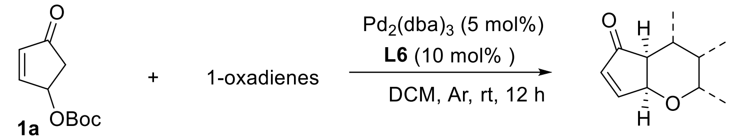


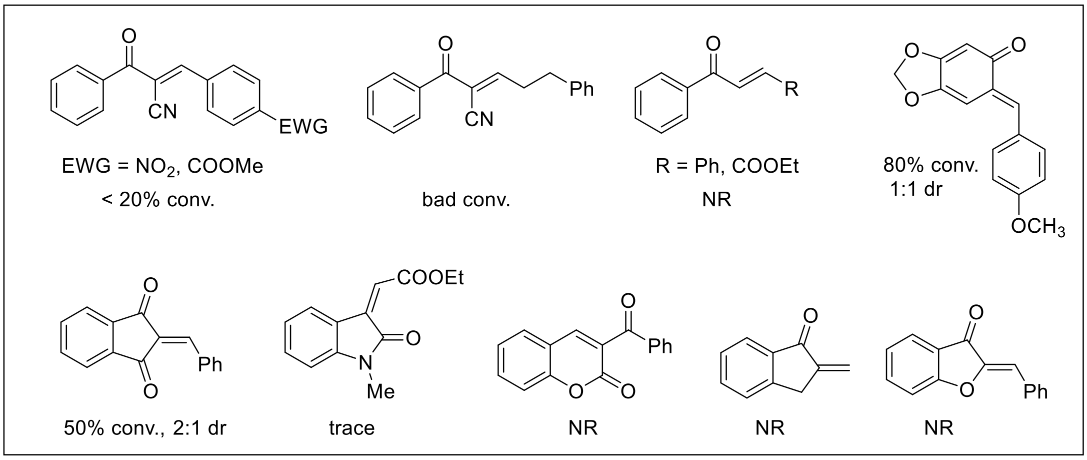
To a 10 mL oven dried tube were added **3a** (62.8 mg, 0.201 mmol, 98% ee) and MeOH (2.0 mL). The reaction was cooled to 0 °C and $NaBH_4$ (22.8 mg, 0.6 mmol) was added in one portion. After warming to room termperature, the mixture was stirred for 20 min until the consumption of **3a**, and then it was quenchen by water and extracted by EtOAc. The organic layer was dried by Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (EtOAc/petroleum ether = 1/5) to the reduction product **11**: 61.1 mg (0.193 mmol) as a white solid, 96% yield, 8:1 dr; mp 157–158 °C; $[\alpha]_D^{25}$ = –148.2 (*c* = 1.41 in $CHCl_3$); 99% ee, determined by HPLC analysis (Chiralpak AD-H, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 mL/min, λ = 254 nm), major diastereomer: t_R = 7.90 min (major), t_R = 20.48 min (minor); ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.84–7.76 (m, 2H), 7.47–7.41 (m, 3H), 7.37–7.35 (m, 2H), 7.34–7.27 (m, 3H), 4.54 (t, *J* = 4.1 Hz, 1H), 4.46–4.38 (m, 1H), 3.94 (s, 1H), 2.34–2.24 (m, 1H), 2.21–2.12 (m, 1H), 2.07–2.02 (m, 1H), 1.90–1.78 (m, 2H), 1.74 (brs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 165.9, 143.8, 133.5, 130.7, 129.1, 128.4, 128.2, 127.6, 127.3, 120.4, 86.7, 77.9, 74.1, 50.5, 38.9, 33.3, 30.8; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{20}NO_2^+$ 318.1489; Found 318.1495. Its absolute configuration was confirmed by X-ray diffraction in Section 10.

The alcohol **11** (32.3 mg, 0.102 mmol, 99% ee, 8:1 dr), Pd/C (32.0 mg, 10 wt %) and Boc_2O (70 *μ*L, 0.31 mmol) were stirred in MeOH (2.0 mL). The mixture was degassed, and charged with hydrogen balloon and stirred at 50 °C for 48 h. Then the mixture was filtered by celite, concentrated and purified by flash chromatography on silica gel (EtOAc/petroleum ether = 1/10) to give the product **12**: 25.4 mg (0.0600 mmol) as a white solid, 60% yield, >19:1 dr; mp 126–128 °C; $[\alpha]_D^{25}$ = –34.4 (*c* = 0.71 in $CHCl_3$); 98% ee, determined by HPLC analysis (Chiralpak AD-H, *i*-PrOH/*n*-hexane = 5/95, flow rate = 1.0 mL/min, λ = 220 nm), t_R = 13.58 min (minor), t_R = 18.35 min (major); ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.38–7.29 (m, 8H), 7.26–7.21 (m, 2H), 4.92 (d, *J* = 5.6 Hz, 1H), 4.43–4.38 (m, 1H), 4.20–4.10 (m, 2H), 3.45 (t, *J* = 6.8 Hz, 1H), 2.96–2.86 (m, 1H), 2.74–2.50 (m, 2H), 2.38–2.28 (m, 1H), 2.25 –2.15 (m, 2H), 2.14–2.03 (m, 1H), 1.99–1.91 (m, 1H), 1.75–1.64 (m, 1H), 1.38 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 156.1, 145.9, 140.2, 128.8, 128.4, 128.1, 127.5, 126.6, 126.4, 79.0, 78.2, 77.5, 74.0, 50.0, 43.9, 40.1, 38.0, 33.1, 30.7, 28.4; HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{26}H_{33}NO_4Na^+$ 446.2302; Found 446.2307.

9. Exploration of other substrates

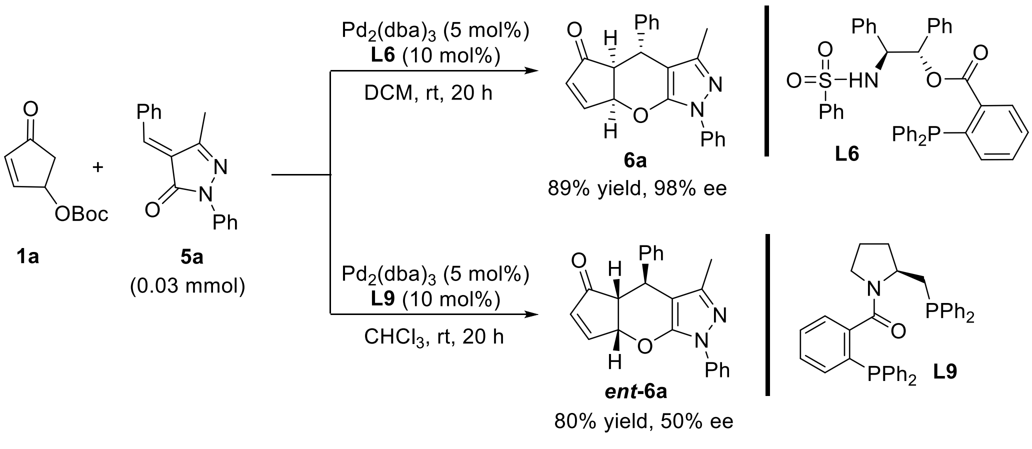
9.1 Exploration of more 1-oxadienes



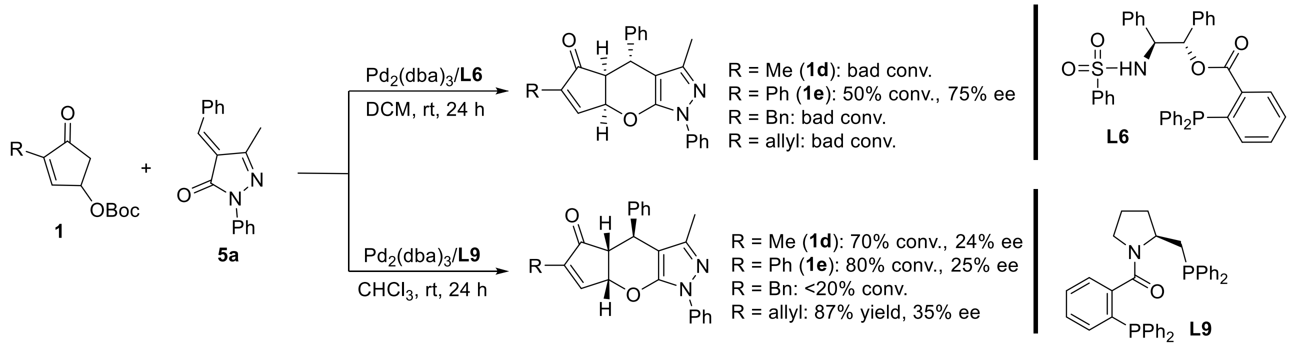


9.2 More exploration for the reaction of alkylidene pyrazolone 5a

We tried to develop diastereodivergent oxa-DA reaction of **1a** and alkylidene pyrazolone **5a**. Bifunctional ligand **L6** and bisphosphine **L9** were employed, respectively. It was found that **6a** was afforded in good results with **L6**, while the enantiomer of **6a** (***ent*-6a**), instead of its diastereomer, was obtained by using **L9**. This is different from the sanario of oxa-DA reaction between **1a** and acyclic α-cyano chalcone **2a**, possibly because the π-π interactions between the in-situ formed η^2-Pd(0)-cyclopentadienone complex and alkylidene pyrazolone of **5a** play an important role in the stereodetermining step, which overcome the impact of different ligands (also see the SI of previous work: *Angew. Chem., Int. Ed.* **2021**, *60*, 26762).

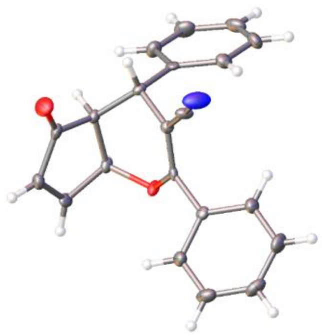


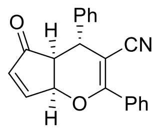
9.3 Exploration of substituted 2-cyclopentenones 1 with alkylidene pyrazolone 5a



10. Crystal data and structural refinement

Procedure for the recrystallization of 3a: To a 10 mL tube containing **3a** (30 mg) were added EtOAc (0.3 mL) and *n*-hexane (2.0 mL). The mixture was heated until a clear solution was formed, which was kept aside and sealed by a piece of weighing paper with a tiny hole at room temperature to obtain crystals. The crystals were subjected for single crystal XRD to determine the absolute configuration of **3a**. The data were collected by an Agilent Gemini equipped with a Cu radiation source (Kα = 1.54184 Å) at 170(20) K. CCDC 1996953 (**3a**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif.





3a

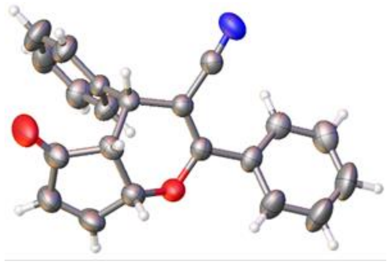
CCDC 1996953

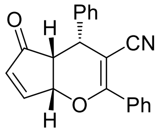
(ellipsoid contour probability 50%)

Identification code	**3a**
Empirical formula	$C_{21}H_{15}NO_2$
Formula weight	313.34
Temperature/K	170(20)
Crystal system	orthorhombic
Space group	$P2_12_12_1$

a/Å	8.6996(2)
b/Å	10.0320(3)
c/Å	18.0221(6)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1572.86(8)
Z	4
ρ_{calc}g/cm^3	1.323
μ/mm^{-1}	0.681
F(000)	656.0
Crystal size/mm^3	0.7 × 0.6 × 0.5
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	9.816 to 134.054
Index ranges	$-10 \le h \le 10$, $-7 \le k \le 11$, $-21 \le l \le 21$
Reflections collected	6745
Independent reflections	2801 [R_{int} = 0.0297, R_{sigma} = 0.0313]
Data/restraints/parameters	2801/0/217
Goodness-of-fit on F^2	1.090
Final R indexes [I >=2σ (I)]	R_1 = 0.0517, wR_2 = 0.1348
Final R indexes [all data]	R_1 = 0.0521, wR_2 = 0.1355
Largest diff. peak/hole / e Å^{-3}	0.33/–0.44
Flack parameter	0.04(14)

Procedure for the recrystallization of 4a: To a 10 mL tube containing **4a** (15 mg) were added EtOAc (0.2 mL) and *n*-hexane (2.5 mL). The mixture was heated until a clear solution was formed, which was kept aside and sealed by a piece of weighing paper with a tiny hole at room temperature to obtain crystals. The crystals were subjected for single crystal XRD to determine the absolute configuration of **4a**. The data were collected by an Agilent Gemini equipped with a Cu radiation source (Kα = 1.54184 Å) at 292.28(10) K. CCDC 1996954 (**4a**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif.





4a

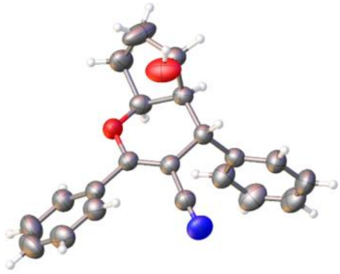
CCDC 1996954

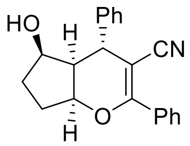
(ellipsoid contour probability 50%)

Identification code	**4a**
Empirical formula	$C_{21}H_{15}NO_2$
Formula weight	313.34
Temperature/K	292.28(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	6.63882(14)
b/Å	14.4059(4)
c/Å	17.5126(5)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1674.88(7)
Z	4
ρ_{calc}g/cm^3	1.243
μ/mm^{-1}	0.640
F(000)	656.0
Crystal size/mm^3	0.65 × 0.5 × 0.4
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.946 to 142.474
Index ranges	$-8 \leq h \leq 6$, $-17 \leq k \leq 16$, $-20 \leq l \leq 21$
Reflections collected	8987
Independent reflections	3195 [R_{int} = 0.0376, R_{sigma} = 0.0313]
Data/restraints/parameters	3195/0/217
Goodness-of-fit on F^2	1.061
Final R indexes [I >=2σ (I)]	R_1 = 0.0469, wR_2 = 0.1242

Final R indexes [all data]	$R_1 = 0.0502$, $wR_2 = 0.1291$
Largest diff. peak/hole / e Å^{-3}	0.17/–0.23
Flack parameter	0.0(2)

Procedure for the recrystallization of 11: To a 10 mL tube containing **11** (20 mg) were added EtOAc (0.5 mL) and *n*-hexane (2.0 mL). The mixture was heated until a clear solution was formed, which was kept aside and sealed by a piece of weighing paper with a tiny hole at room temperature to obtain crystals. The crystals were subjected for single crystal XRD to determine the absolute configuration of **11**. The data were collected by an Agilent Gemini equipped with a Cu radiation source (Kα = 1.54184 Å) at 295.2(2) K. CCDC 2125794 (**11**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif.





11
CCDC 2125794

(ellipsoid contour probability 50%)

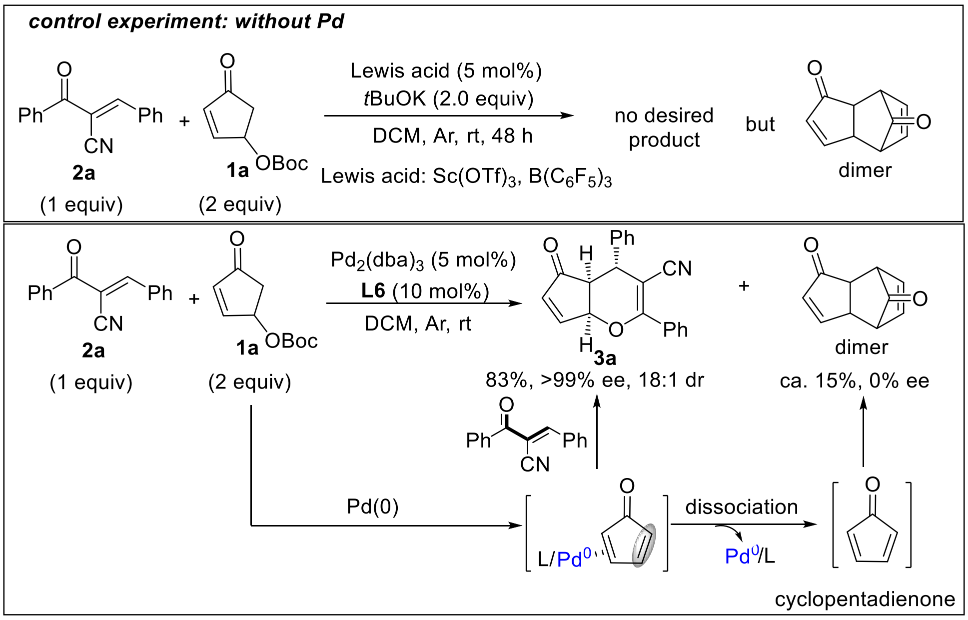
Identification code	**11**
Empirical formula	$C_{21}H_{19}NO_2$
Formula weight	317.37
Temperature/K	295.2(2)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	7.7662(2)
b/Å	12.8859(3)
c/Å	16.6700(6)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1668.23(9)

Z	4
ρ_{calc}g/cm^3	1.264
μ/mm^{-1}	0.643
F(000)	672.0
Crystal size/mm^3	0.5 × 0.1 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.674 to 141.22
Index ranges	$-9 \le h \le 9$, $-9 \le k \le 15$, $-18 \le l \le 20$
Reflections collected	9019
Independent reflections	3165 [R_{int} = 0.0434, R_{sigma} = 0.0341]
Data/restraints/parameters	3165/0/218
Goodness-of-fit on F^2	1.041
Final R indexes [I>=2σ (I)]	R_1 = 0.0506, wR_2 = 0.1388
Final R indexes [all data]	R_1 = 0.0551, wR_2 = 0.1452
Largest diff. peak/hole / e Å^{-3}	0.19/–0.20
Flack parameter	–0.1(2)

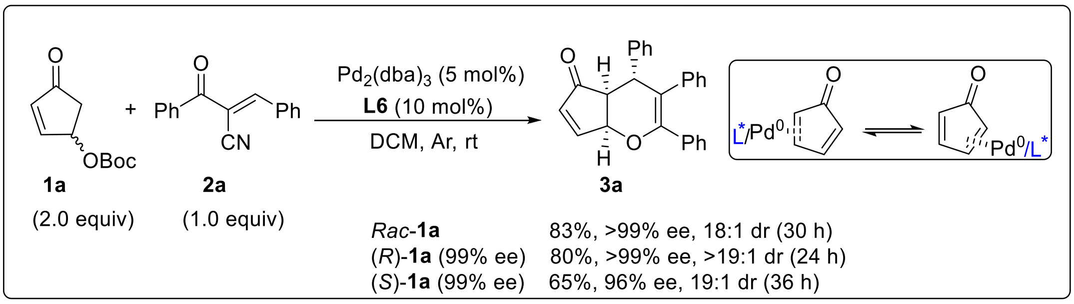
11. Mechanism studies

11.1 Control experiments

The reaction between **1a** and **2a** under the catalysis of some Lewis acids, such as $Sc(OTf)_3$ and $B(C_6F_5)_3$, has also been carried out. No desired cycloadduct but the dimer from **1a** was detected. Besides, the dimerization side product, possibly as the Diels–Alder adduct from in situ-generated cyclopentadienone intermediate, was racemic even under the chiral catalytic conditions, whereas the desired cycloadduct **3a** obtained in the same batch showed high enantioselectivity. These results indicated that the dimerization process was not catalysed by Pd(0), but from the dissociated cyclopentadienone.



Both (*R*)-**1a** (99% ee) and (*S*)-**1a** (99% ee) were prepared, and applied to the reaction with 1-oxadiene **2a** under the standard conditions, respectively. The two enantiomers gave comparable results with those from racemic **1a**, and both afforded chiral product **3a** as the major diastereomer, indicating that both enantiomers could participate in the reaction. Although the rate in the first Pd-oxidative insertion step might be different under the asymmetric conditions, they would undergo the same pathway in the enantiodetermining step (also see *Angew. Chem., Int. Ed.* **2021**, *60*, 26762).



11.2 DFT caculations

In this article, all calculations were performed by Gaussian 09 software packages.[6] The conformations of intermediates were generated by SYBYL-X 2.0 GA Conf. search module and initially optimized and screened by SYBYL-X 2.0.[7] All geometries were optimized with the dispersion corrected functional B3LYP-D3[8] which was a good function to estimate the hydrogen bond and π-π interactions. Moreover, the 6-31G (d)[9] basis was set to the light atoms (C, H, O, N, S, P) and the transition metal Pd was described with the SDD basis.[10] The optimized structures or transition structures were confirmed by normal vibrational mode analysis. The optimized structures have no imaginary frequency but transition structures have only one imaginary frequency. Transition structures were also verified by intrinsic reaction coordinate (IRC) calculations. Single-point energies were computed on the dispersion corrected B3LYP-D3 functional. Besides, the 6-311G++(d, p) basis set[11] was applied to the light atoms (C, H, O, N, S and P), and the transition metal Pd atom was described with the SDD basis set. To estimate the solvent effects, the polarization continuum model (PCM)[12] was applied in this work. The dielectric constant (eps) of DCM was set as 8.93.[13] Moreover, the dielectric constant of binary mixed solvents was calculated as follows,[14]

$$\varepsilon_m = \varphi_1\varepsilon_1 + \varphi_2\varepsilon_2 \qquad (1)$$

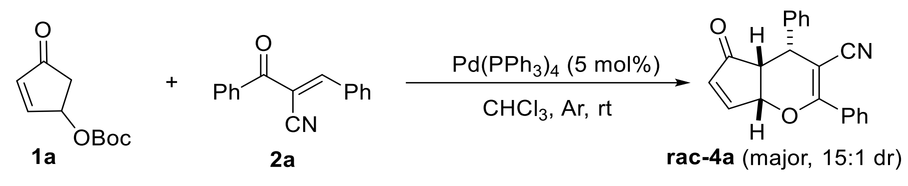
where ε_m, ε_1, ε_2 represent the dielectric constants of the mixture and solvents 1 and 2, respectively. φ_1 and φ_2 represent the volume fractions of the solvents 1 and 2 in the mixture. In the case of binary mixed solvents, the dielectric constant of $CHCl_3$ is 4.7113,[16] and the dielectric constant of toluene is 2.3741,[16] so the electronic constant of mixture solvent in this article is 3.5427. All energies reported throughout the text are in kcal/mol, and the bond length unit is angstroms (Å), and structures were generated by GaussView 6[15] and CYL view.[16]

To gain more sight into the cycloaddition reaction, we carried out DFT calculations on the [4 + 2] cycloaddition between **1a** and **2a** under the catalysis of Pd with different ligand as a model reaction.

11.2.1 Possible pathway for the [4 + 2] cycloaddition of 1-oxadiene 2a

After the formation of the active intermediate as a cyclopentandienone η^2-Pd(0) complex, **A-INT2** could react with **2a** to generated the final product **3a** or **4a**. Several possible pathways, involving stepwise and concerted processes, were proposed and calculated as shown in Fig. S1.

1) With PPh_3 as the ligand



Pathway A (*concerted process*): Intermediate **A-INT2** approached **2a** from the opposite side of the Pd via **A-TS2**. The energy barrier of **A-TS2** was reasonable with a value of 17.3 kcal/mol and the energy of **A-INT3** was –3.1 kcal/mol, suggesting the concerted process was possible.

Pathway B (*stepwise process*): The α'-position of intermediate **A-INT2** attacked **2a**, giving **B-INT2** as a η^3-complex via **B-TS2**, then the oxygen anion attacked the π-allylpalladium moiety to furnish **rac-4a**. Compared with the concerted process, the energy barrier of the stepwise process for the step of C–C bond formation via **B-TS2** was slightly higher with a value of 18.1 kcal/mol. The energy of the following C-O bond formation employed a lower value of 12.5 kcal/mol.

Pathway C (*stepwise process*): Another possibility, that **2a** added with **A-INT2** from the same side of the Pd coordination, was also proposed. As there was not enough space for two PPh_3 ligand and **2a** in the same side, one ligand might be left and **2a** acted as the ligand by O-Pd coordinated bond in **A-INT2′**. It also would promote sequential C-C and C-O bond formation to generate **rac-4a**. The related energy of **C-TS2** and **C-TS3** was quite high with a value of 36.0 kcal/mol and 32.3 kcal/mol, respectively. **A-INT2′** was not so stable with a value of 21.1 kcal/mol, so **Pathway C** would not be favored.

Pathway D (*oxidative cyclisation like those catalysed by Ni/Ru*): We also calculated the reaction possibility of oxidative cyclisation pathway for our reaction, in which the Pd-coordinated double bond would participate in the reaction. We found the energy of **D-TS2A–B** was much higher than that of **A-TS2**. There results suggested the reaction mode of oxidative cyclisation pathway was unfavorable.

The results indicated that with PPh_3 as the ligand, the cycloaddition between 1a and 2a might proceed through a concerted Diels–Alder cycloaddition pathway, while the stepwise pathway would not be completely ruled out because of the small difference for their energy barriers.

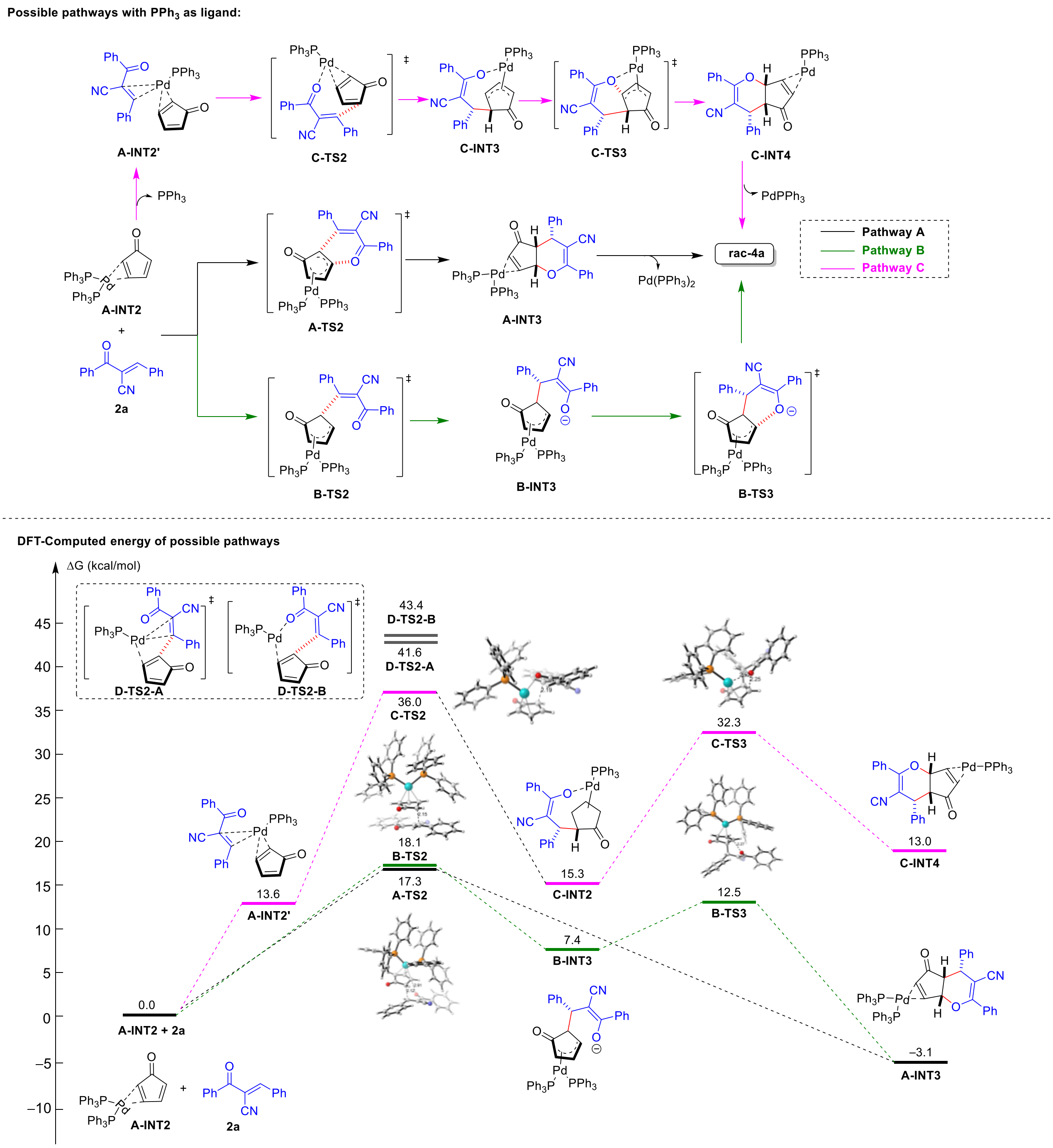
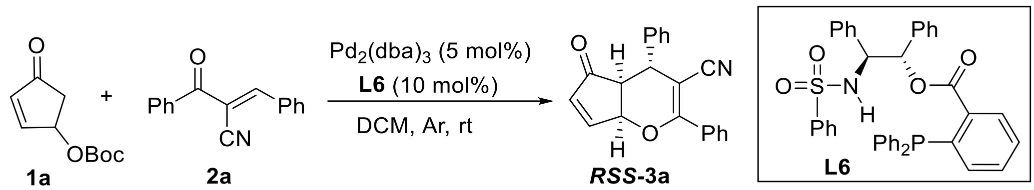


Fig. S1 Computed potential energy surface of the reaction of **A-INT2** and **2a** at the B3LYP-D3/6-31(d)//B3LYP-D3/6-311++G(d,p) and SDD for Pd (chloroform) level and is given in kcal/mol relative to the sum energy of **A-INT2** and **2a**.

2) With chiral bifunctional L6 as the ligand



We further conducted comprehensive computational calculations to elucidate the results with bifunctional **L6** as the ligand. As **L6** is a monophosphine ligand, there are many conformations of transition state (TS) to form the product **3a**. After considering three pathways similar to those with PPh_3 as the ligand, various conformations of **TS2** to form **3a** were generated by SYBYL-X2.0 Ga.conf module and calculated and calculated by Gaussian 09.

Firstly, a concerted pathway was proposed and calculated (Fig. S2). In these conformations, the phosphine atom and the O atom of carbonyl would coordinate to Pd(0). The energy differences of each conformation resulted from the molecular flexibility of ligand **L6**. We found some *π-π* interactions of phenyls in most conformations, obviously in **L6-*RSS*-TS2** and **L6-*RSS*-TS4**. There are H-bonding interactions between NH of **L6** and different heteroatoms in **L6-*RSS*-TS1**, **L6-*RSS*-TS3**, and **L6-*RSS*-TS5**. Among them, **L6-*RSS*-TS1**, in which the NH was bonding to the O atom of cyclopentadienone, has the lowest energy.

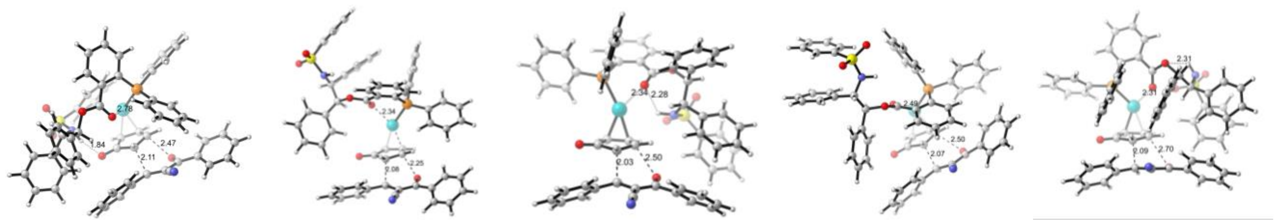


Fig. S2 The calculated structures of TSs to form **3a** via concerted process at the B3LYP-D3/6-31(d)// B3LYP-D3/6-311++G(d,p) SDD for Pd (dichloromethane) level and are given in kcal/mol relative to the sum energy of **L6-*RSS*-TS1**.

Similarly, the TSs for the stepwise process were calculated as shown in Fig. S3 under the same coordination model. The energy barrier for the concerted process was lower than that of the stepwise process (**L6-*RSS*-TS1**, 0 kcal/mol *VS* **L6-*RSS*-TS10**, 1.5 kcal/mol). **L6-*RSS*-TS6** (0.6 kcal/mol) has the lowest energy, but still slightly higher than that via the concerted pathway. Moreover, the TSs proposed as **Pathway C** also was calculated as shown in Fig. S3. The energies of these TSs were higher than those of other two pathways.

<u>The results imply that the concerted pathway is more favored, but the stepwise pathway also could</u>

not be ruled out as the difference for the energy barrier is small (0.6 kcal/mol).

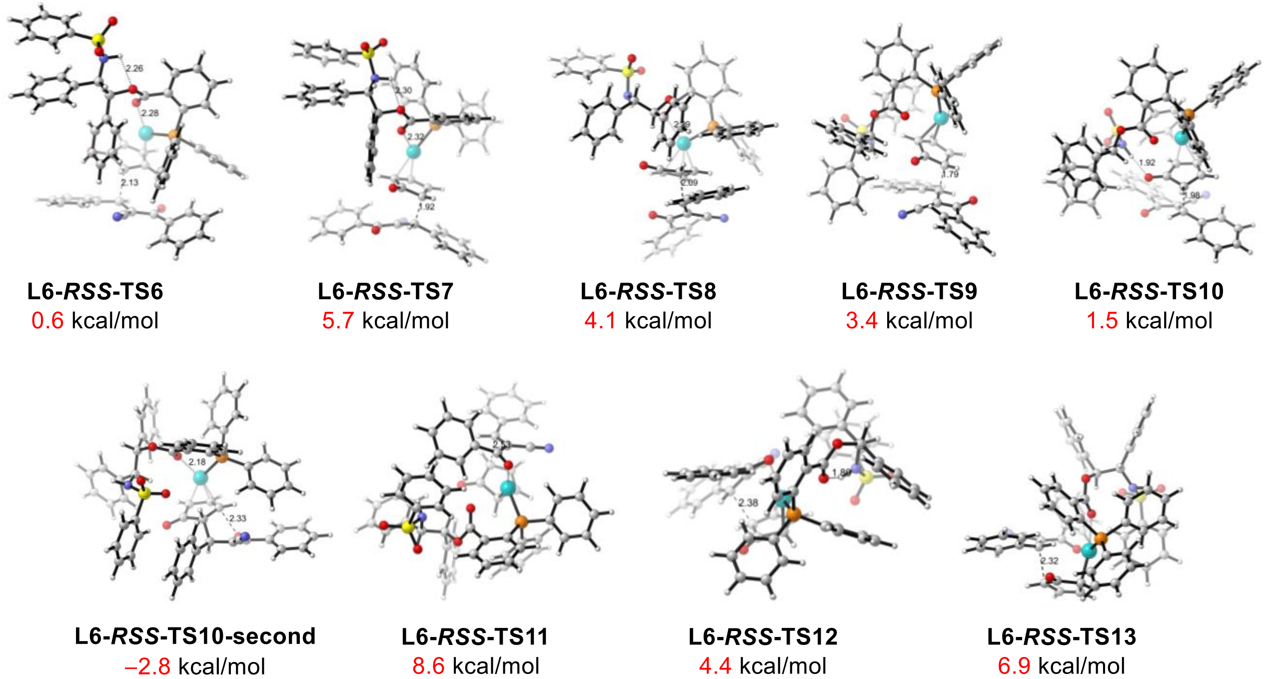
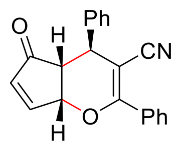


Fig. S3 The calculated structures of TSs to form **3a** via stepwise process at the B3LYP-D3/6-31(d)// B3LYP-D3/6-311++G(d,p) SDD for Pd (dichloromethane) level and are given in kcal/mol relative to the sum energy of **L6-*RSS*-TS1**.

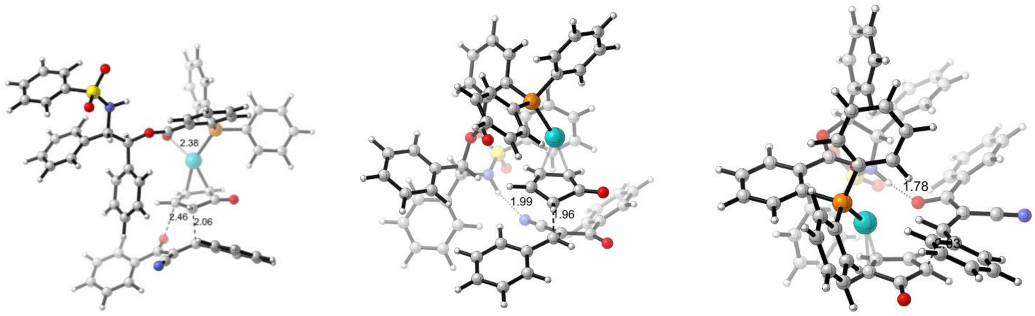
Stereoselectivity with L6:

Using the same methods, we calculated the TSs to produce other stereoisomers via the concerted pathway. As shown in Fig. S4, it was found that the **L6-*RSS*-TS1** with the lowest energy would result in the ***RSS*-3a** (the enantiomer of **3a**), and the energy is higher than that for **L6-*SRR*-TS1** with a value of 2.2 kcal/mol. According to Van't Hoff equation, we predicted that the ee value was 95%, which is similar to the experimental results (>99% ee).

For the diastereoselectivity, the energies of **L6-*SSS*-TS1** and **L6-*RRR*-TS1** for ***SSS*-3a** and ***RRR*-3a** were 2.5 kcal/mol and 1.8 kcal/mol higher than that of **L6-*SRR*-TS1**, respectively (Fig. S5 and S6). According to Van't Hoff equation, we predicted that the dr value was 16:1, comparable with the experimental data (18:1 dr).

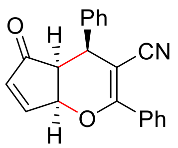


***SRR*-3a**

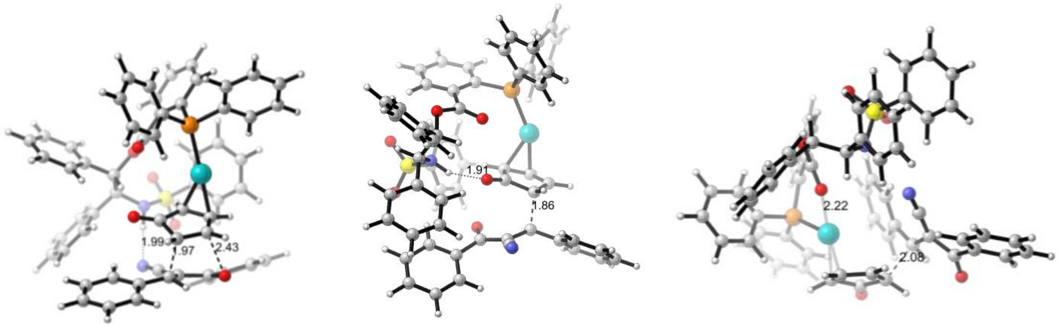


L6-*SRR*-TS1 2.2 kcal/mol | **L6-*SRR*-TS2** 2.8 kcal/mol | **L6-SRR-TS3** 4.0 kcal/mol

Fig. S4 The calculated structures of TSs to form ***SRR*-3a** at the B3LYP-D3/6-31(d) // B3LYP-D3/6-311++G(d,p) SDD for Pd (dichloromethane) level and are given in kcal/mol relative energy of **L6-*SRR*-TS1**.

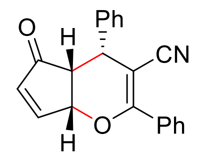


***SSS*-3a**

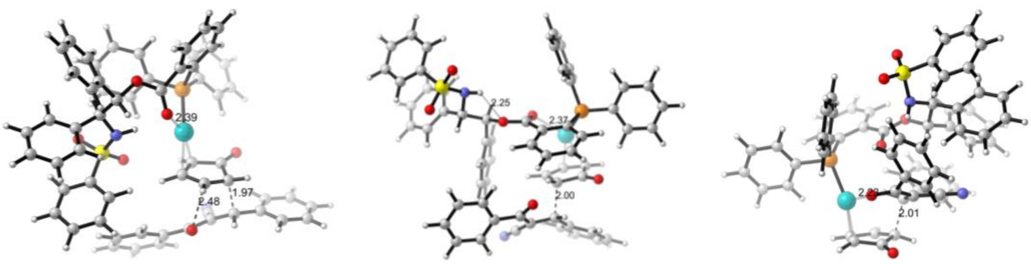


L6-*SSS*-TS1 2.5 kcal/mol | **L6-*SSS*-TS2** 5.5 kcal/mol | **L6-*SSS*-TS3** 4.8 kcal/mol

Fig. S5 The calculated structures of TSs to form ***SSS*-3a** at the B3LYP-D3/6-31(d) // B3LYP-D3/6-311++G(d,p) SDD for Pd (dichloromethane) level and are given in kcal/mol relative energy of **L6-*SRR*-TS1**.



***RRR*-3a**



L6-*RRR*-TS1 3.2 kcal/mol | **L6-*RRR*-TS2** 3.1 kcal/mol | **L6-*RRR*-TS3** 1.8 kcal/mol

Fig. S6 The calculated structures of TSs to form ***RRR*-3a** at the B3LYP-D3/6-31(d) // B3LYP-D3/6-311++G(d,p) SDD for Pd (dichloromethane) level and are given in kcal/mol relative energy of **L6-*SRR*-TS1**.

As summarised in Fig. S7, the cycloaddition between 1a and 2a under the catalysis of Pd and L6 might undergo a concerted pathway, and the transition state L6-RSS-TS1 with the lowest energy

might be responsible for the high levels of stereoselectivity.

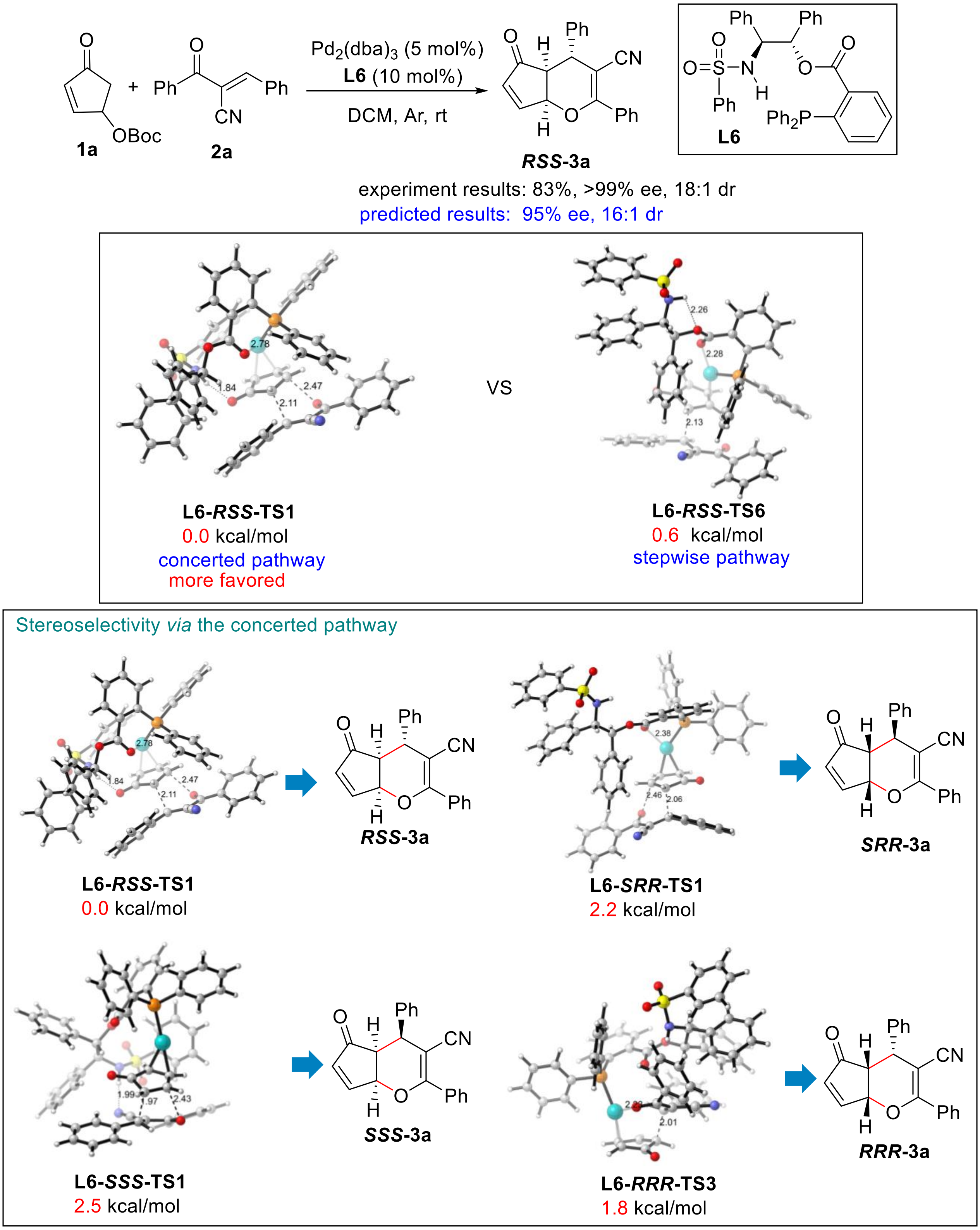
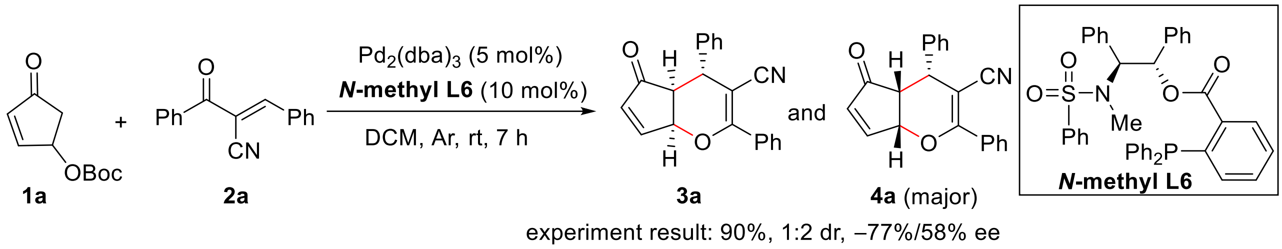


Fig. S7 The summary structures of TSs to form **3a** at the B3LYP-D3/6-31(d) // B3LYP-D3/6-311++G(d,p) SDD for Pd (dichloromethane) level and are given in kcal/mol relative energy of **L6-SRR-TS1**.

3) With monophosphine *N*-methyl protected L6 as the ligand



In order to elucidate the effect of NH group of ligand **L6**, *N*-methyl protected **L6** was prepared and tested. Although high catalytic activity was observed, both diastereoselectivity and enantioselectivity were dramatically decreased, as outlined above. To comprehensively calculate the stereoselectivity catalysed by ***N*-methyl L6**, many TSs would be considered and the calculations would be time consuming. To simply compare the difference, we calculated the conformations for **L6-INT2** and ***N*-methyl L6-INT2**. More than 10 conformations of **L6-INT2** and ***N*-methyl L6-INT2** were generated by SYBYL-X2.0 Ga.conf module and calculated by Gaussian 09. The one with the lowest energy was shown in Fig. S8. There is an H-bonding interaction between the NH and the O atom of cyclopentadienone in **L6-INT2**, which is consistent with the **L6-RSS-TS1** (the TS to form **3a** with the lowest energy). However, because of the additional N-methyl, there is no H-bonding interaction in ***N*-methyl L6-INT2**, and the conformation with the lowest energy is totally different from **L6-INT2**, which might be the reason for the bad stereoselectivity control for ***N*-methyl L6**.

Fig. S8. The calculated structures of **L6-INT2** and ***N*-methyl L6-INT2** at the B3LYP-D3/6-31(d) level.

4) With chiral bisphosphine L10 as the ligand

In the presence of **L10**, various conformations of the transition states in the key step for both pathways were generated by SYBYL-X2.0 Ga.conf module and calculated and calculated by Gaussian 09. The reactants and catalyst may have π-π interactions, so the B3LYP-D3 functional was adopted in the calculations. As **TS2** was the rate-limited step for the formation of C-C bond and the chiral center, the transition states via a concerted or stepwise pathway listed in Fig. S9 were considered. ***<u>The calculation results showed that the reaction via the concerted [4 + 2] pathway is more favorable</u>***, as the rate-limited step has a lower energy barrier (**L10-RRR-TS1**, 0 kcal/mol; **L10-RRR-TS3**, 5.9 kcal/mol) for the concerted pathway.

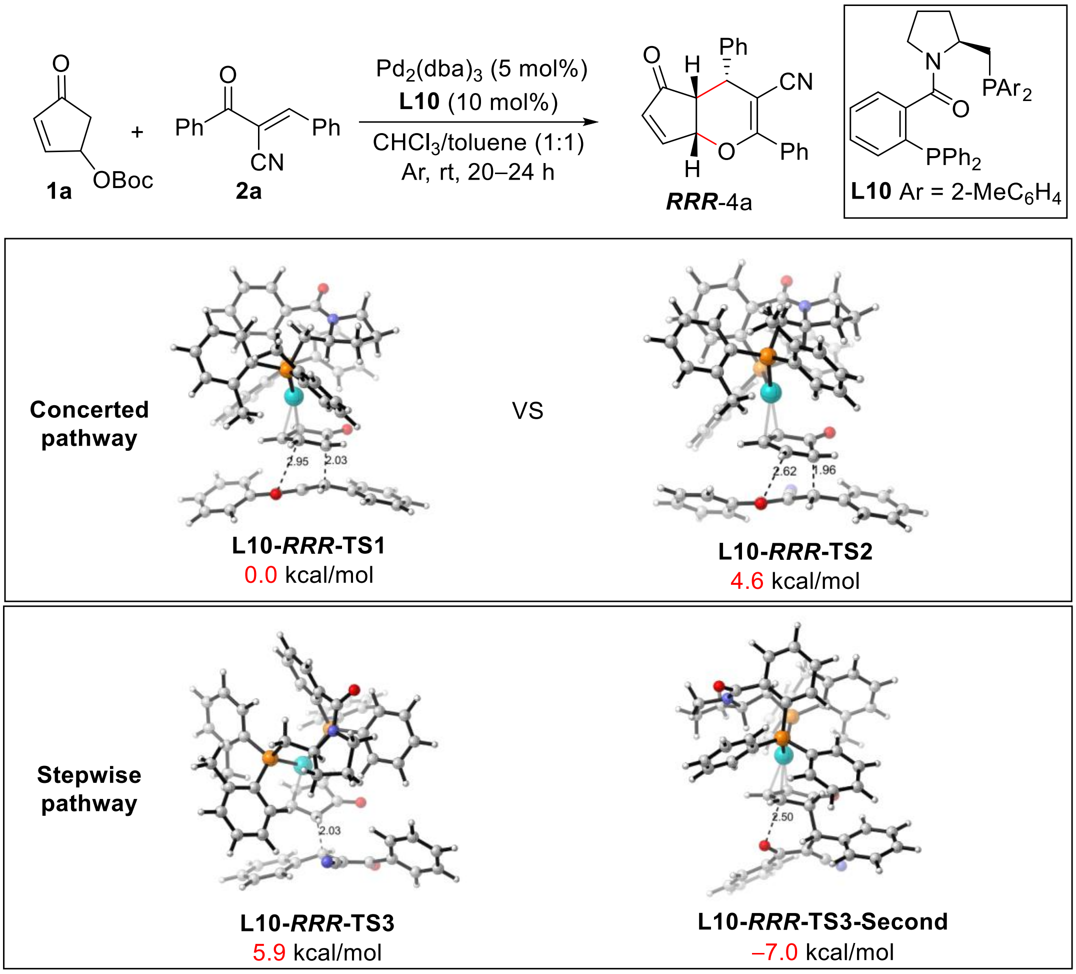
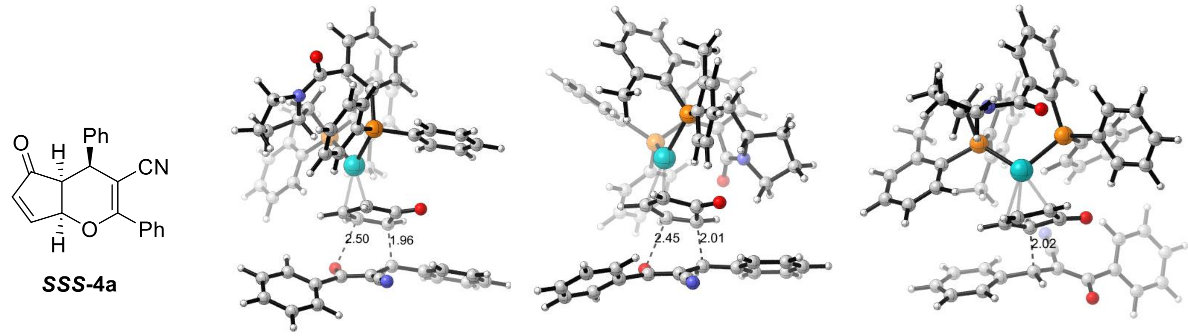


Fig. S9 The calculated structures of ***RRR*-4a** along synergetic reaction mechanism and stepwise reaction mechanism at the B3LYP-D3/6-31(d)// B3LYP-D3/6-311++G(d,p) SDD for Pd ($CHCl_3$/toluene = 1:1) level.

<u>Stereoselectivity with L10:</u>

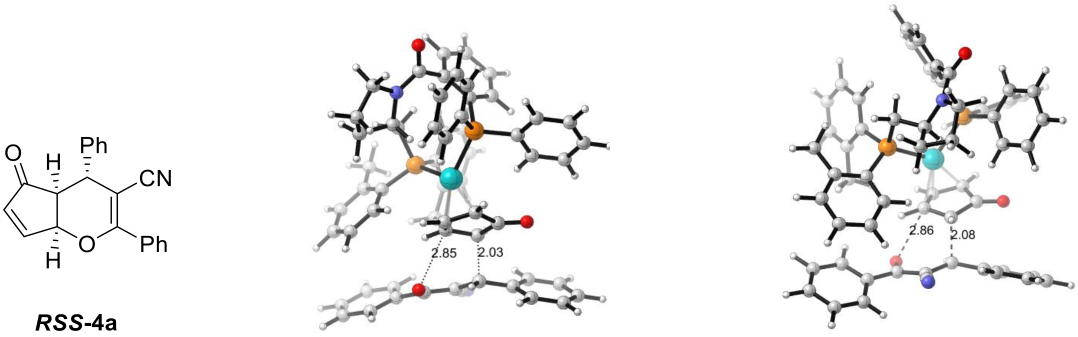
According to the above results, only the concerted pathway was considered for the models of other stereoisomers. Firstly, we calculated the enantioselectivity and found energy difference of **L10-*RRR*-TS1** and **L10-*SSS*-TS1** with a value of 1.9 kcal/mol (Fig. S10). According to Van't Hoff equation, we predicted that the ee value was 92%, which is similar to the experimental value (90% ee). In addition, **L10-*RSS*-TS1** and **L10-*SRR*-TS1** were selected as the one with the lowest energy to form ***RSS*-4a** and ***SRR*-4a**, respectively (Fig. S11). The energies of **L10-*RSS*-TS1** and **L10-*SRR*-TS1** were 2.8

kcal/mol and 1.2 kcal/mol higher than **L10-*RRR*-TS1**. According to Van't Hoff equation, we predicted that the dr value was 7:1, which is close to the experimental data (5:1 dr).



L10-*SSS*-TS1 1.9 kcal/mol　**L10-*SSS*-TS1** 4.3 kcal/mol　**L10-*SSS*-TS1** 7.1 kcal/mol

Fig. S10 The calculated structures of **SSS-4a** along synergetic reaction mechanism and stepwise reaction mechanism at the B3LYP-D3/6-31(d)// B3LYP-D3/6-311++G(d,p) SDD for Pd ($CHCl_3$/toluene = 1:1) level.



L10-*RSS*-TS1 2.8 kcal/mol　**L10-*RSS*-TS1** 1.2 kcal/mol

Fig. S11 The calculated structures of ***RSS*-4a and *SRR*-4a** along synergetic reaction mechanism reaction mechanism at the B3LYP-D3/6-31(d)// B3LYP-D3/6-311++G(d,p) SDD for Pd ($CHCl_3$/toluene = 1:1) level.

<u>As summarised in Fig. S12, the cycloaddition between 1a and 2a under the catalysis of Pd and L10 might undergo a concerted oxa-Diels–Alder cycloaddition pathway, and the transition state L10-RRR-TS1 with the lowest energy might be responsible for the high levels of stereoselectivity.</u>

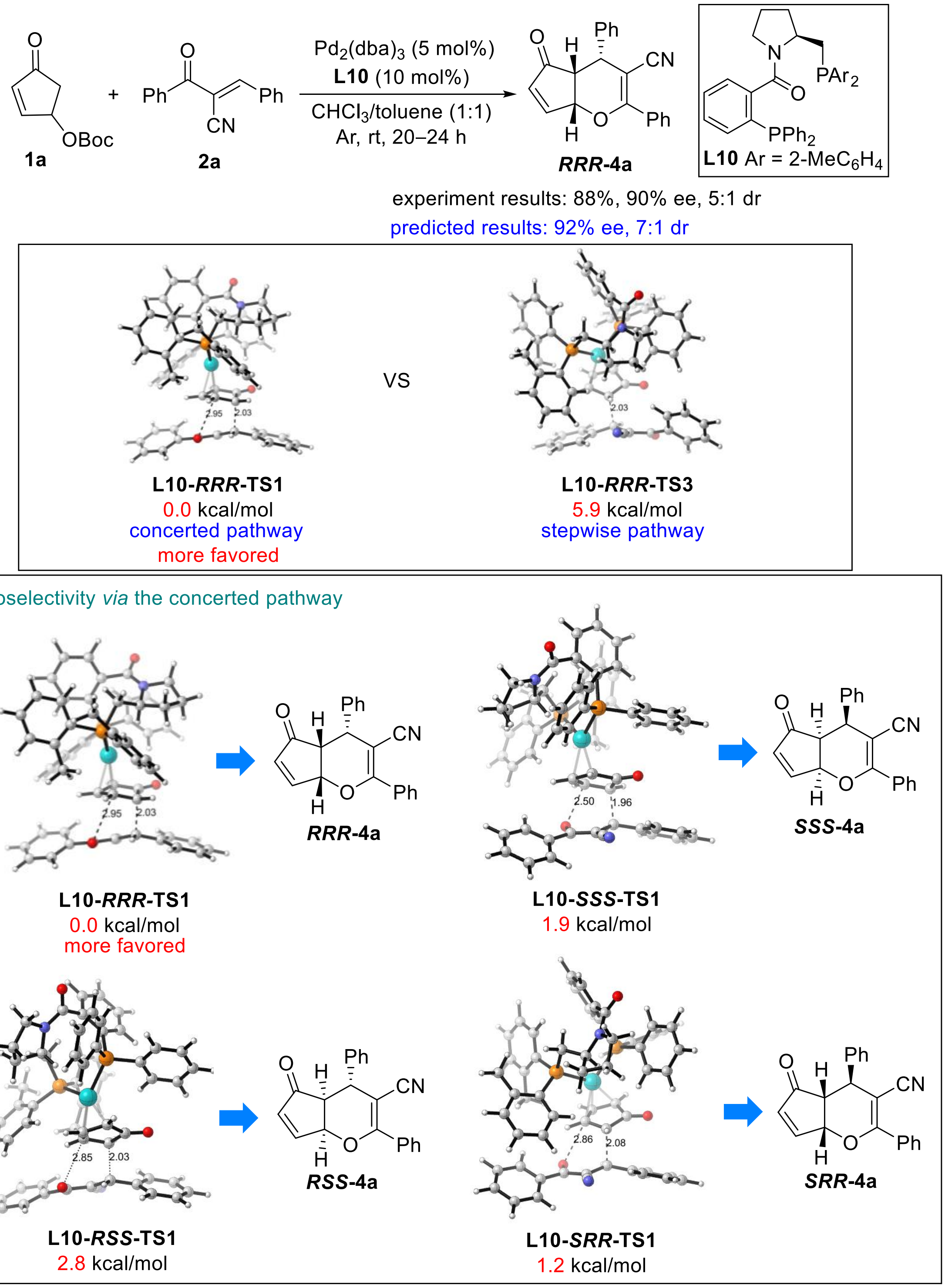


Fig. S12 The summary structures of TSs to form **4a** at the B3LYP-D3/6-31(d) // B3LYP-D3/6-311++G(d,p) SDD for Pd ($CHCl_3$:toluene=1:1) level and are given in kcal/mol relative energy of **L10-*RRR*-TS1**.

5) Reference

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Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, Jr. J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S.Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V.Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O.Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, Gaussian, Inc., Wallingford, CT, USA, 2009.

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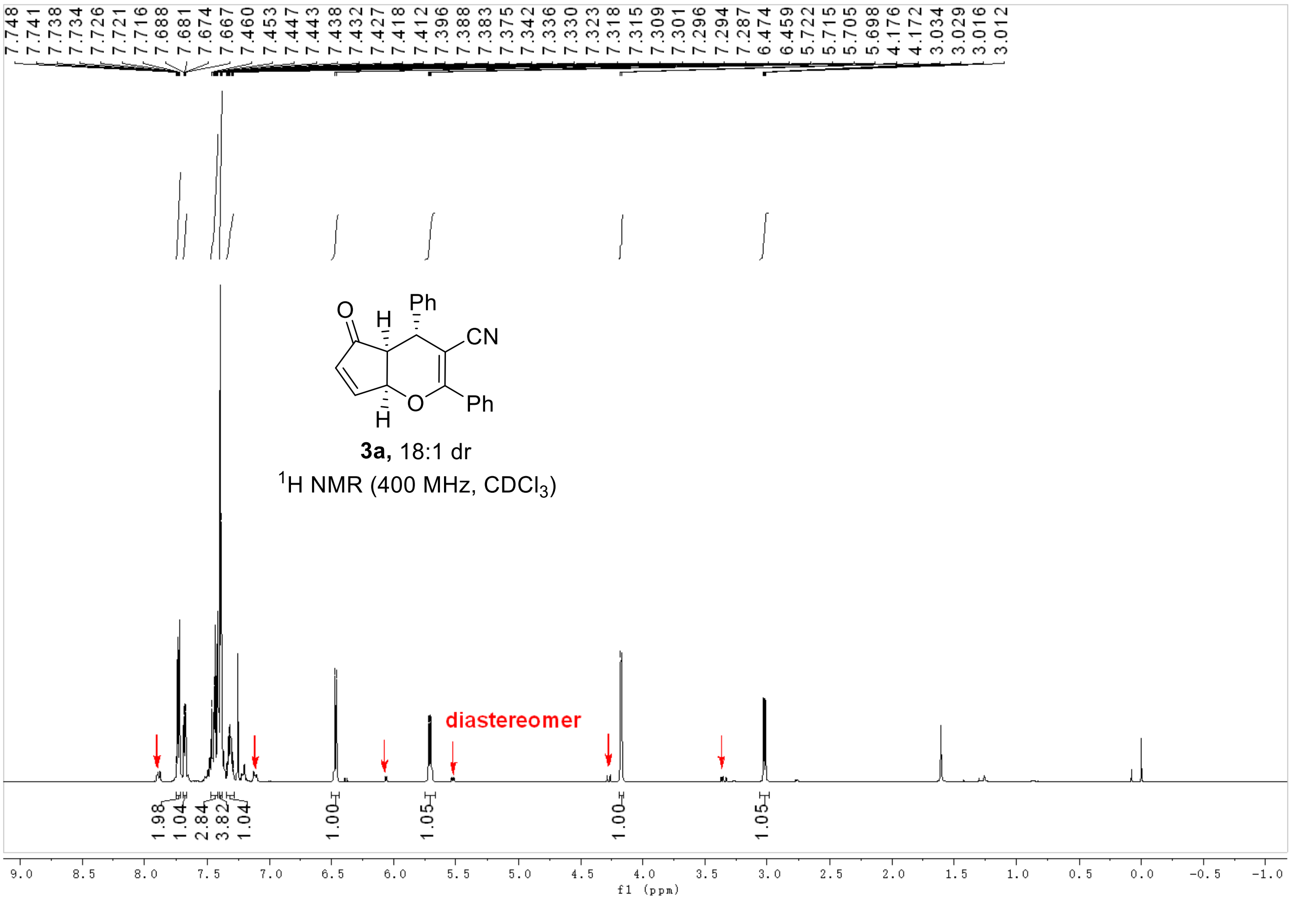
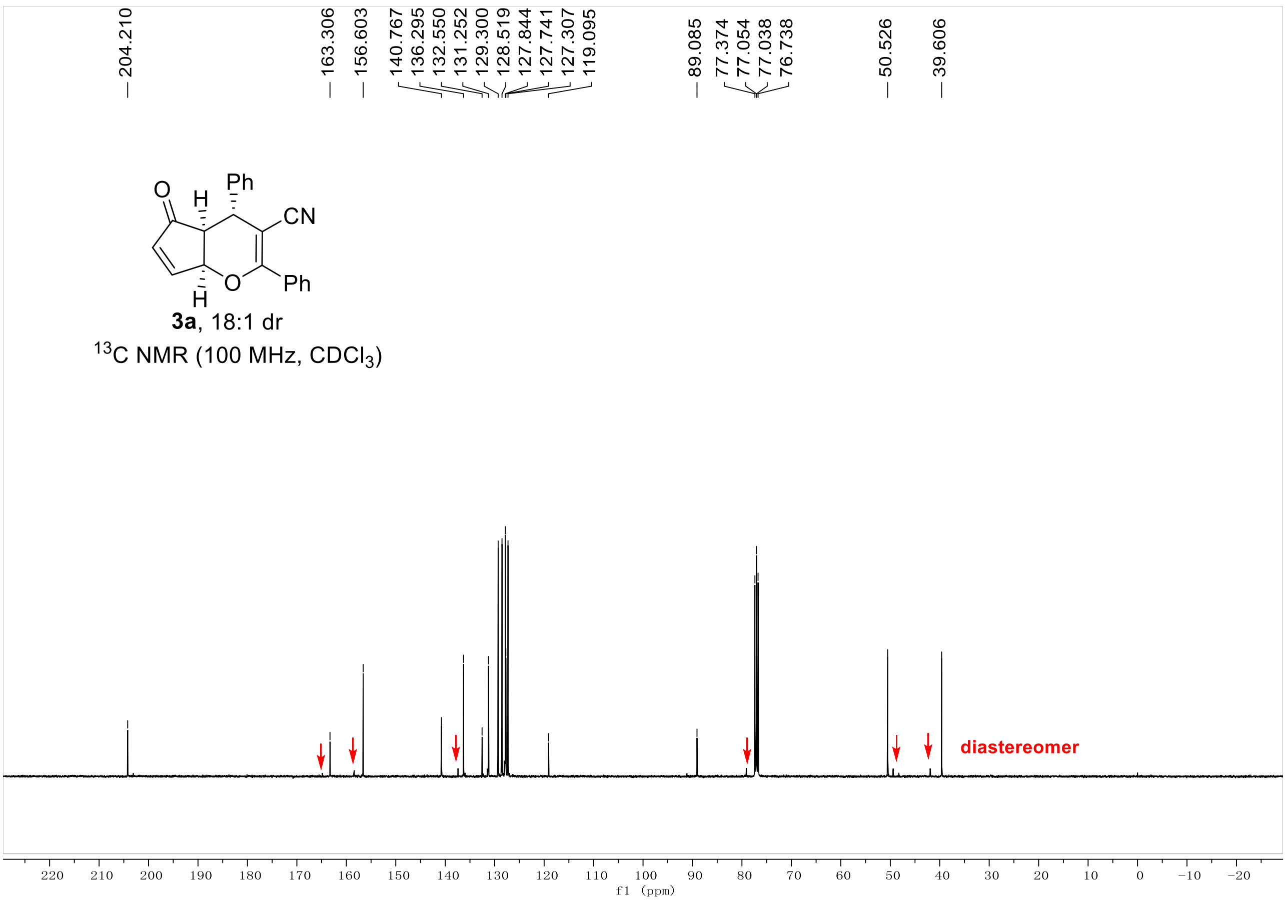
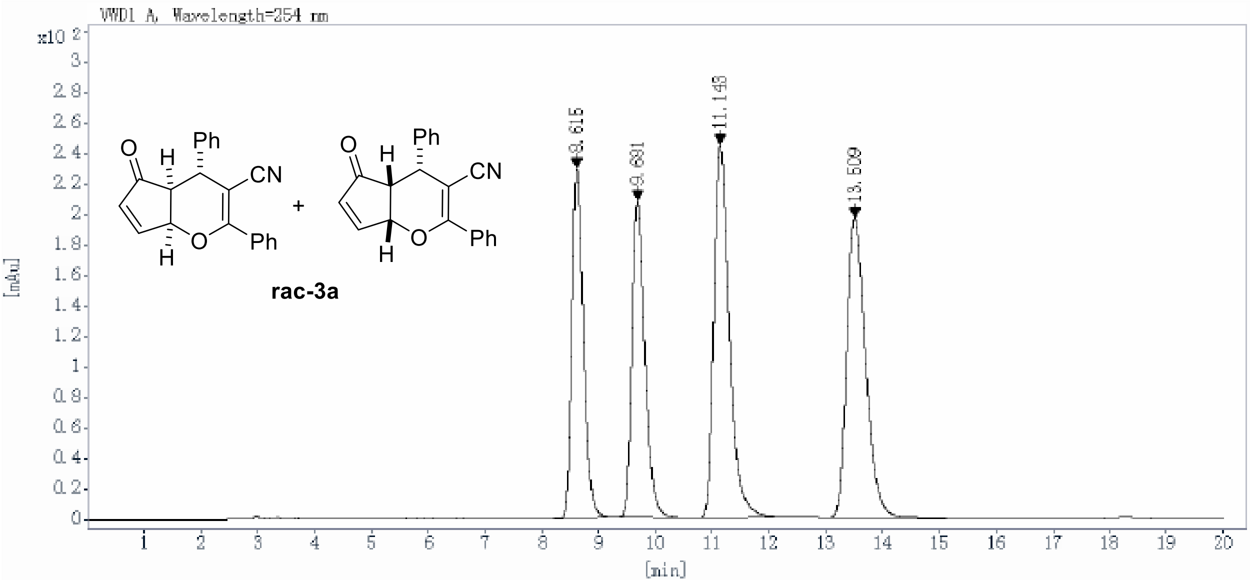
12. NMR, HRMS spectra and HPLC chromatograms







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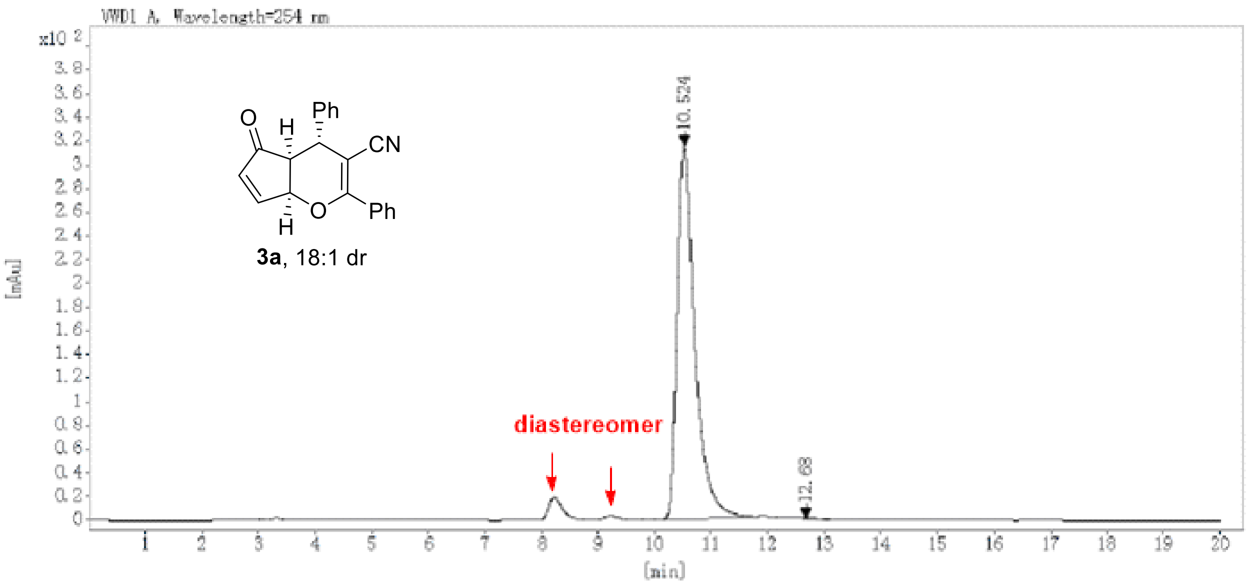

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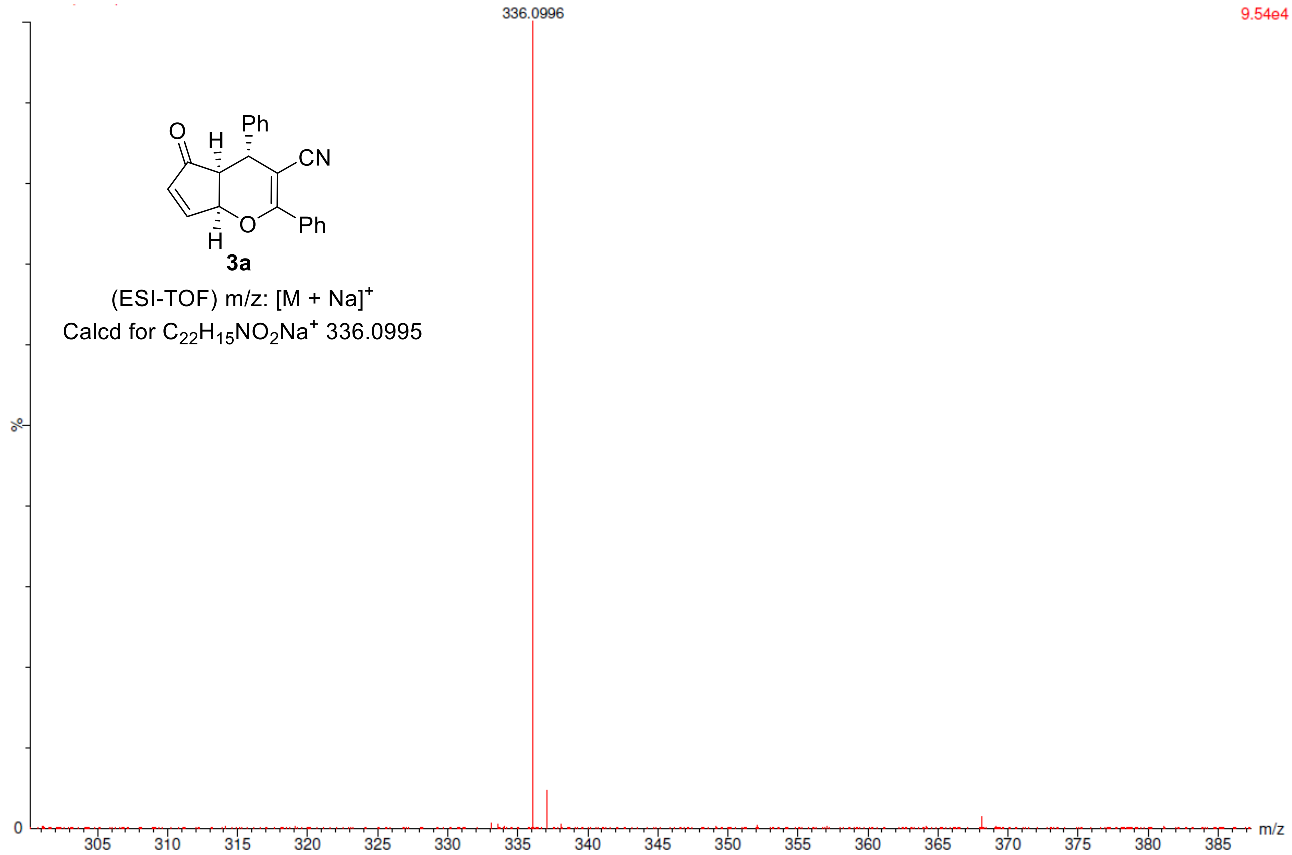
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9.54e4
3a
(ESI-TOF) m/z: [M + Na]+
Calcd for $C_{22}H_{15}NO_2Na^+$ 336.0995
%
0
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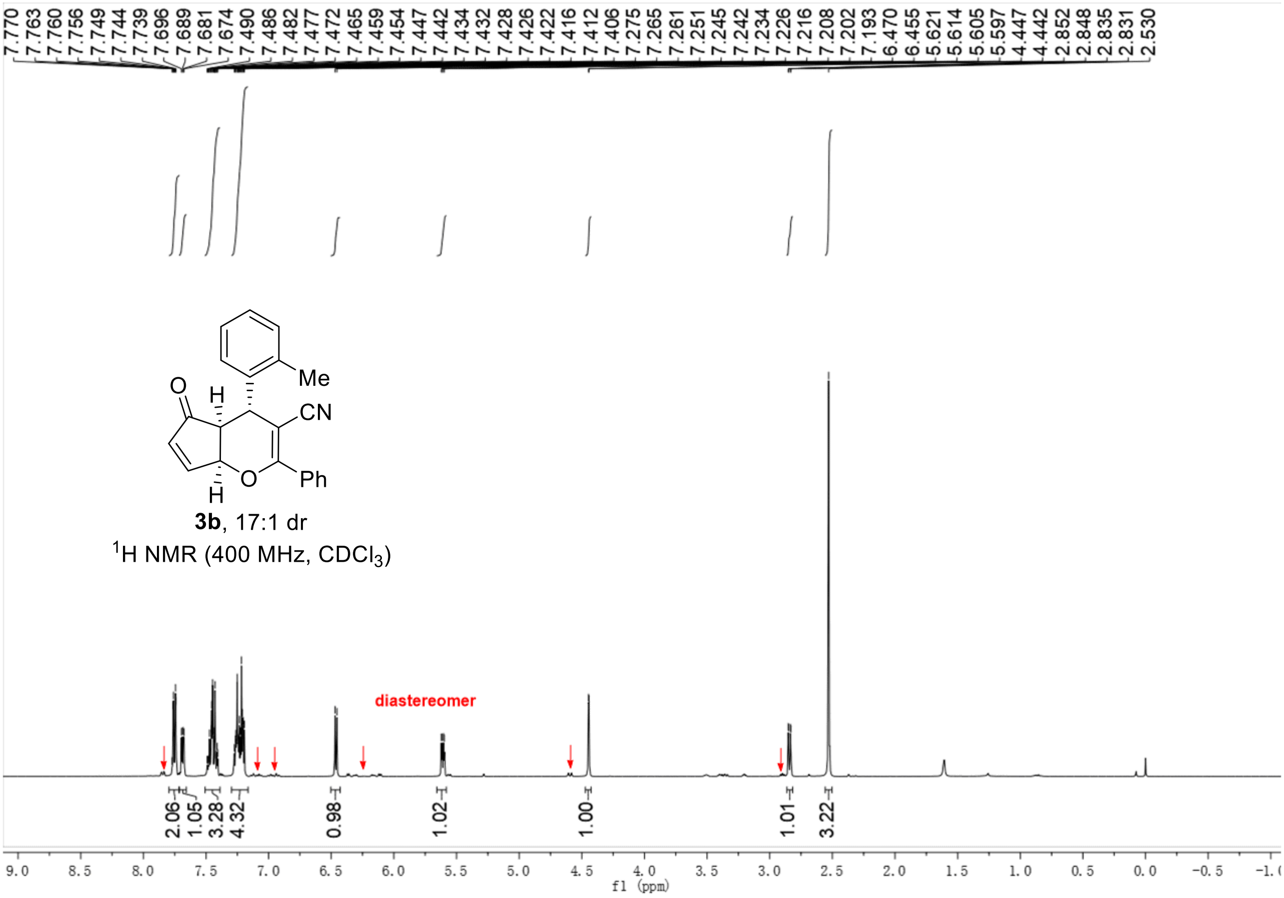
310
315
320
325
330
335
340
345
350
355
360
365
370
375
380
385
m/z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7.482
7.477
7.472
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7.459
7.454
7.447
7.442
7.434
7.432
7.428
7.426
7.422
7.416
7.412
7.406
7.275
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7.245
7.242
7.234
7.226
7.216
7.208
7.202
7.193
6.470
6.455
5.621
5.614
5.605
5.597
4.447
4.442
2.852
2.848
2.835
2.831
2.530
Me
CN
O
H
H
O
Ph
3b, 17:1 dr
1H NMR (400 MHz, CDCl3)
diastereomer
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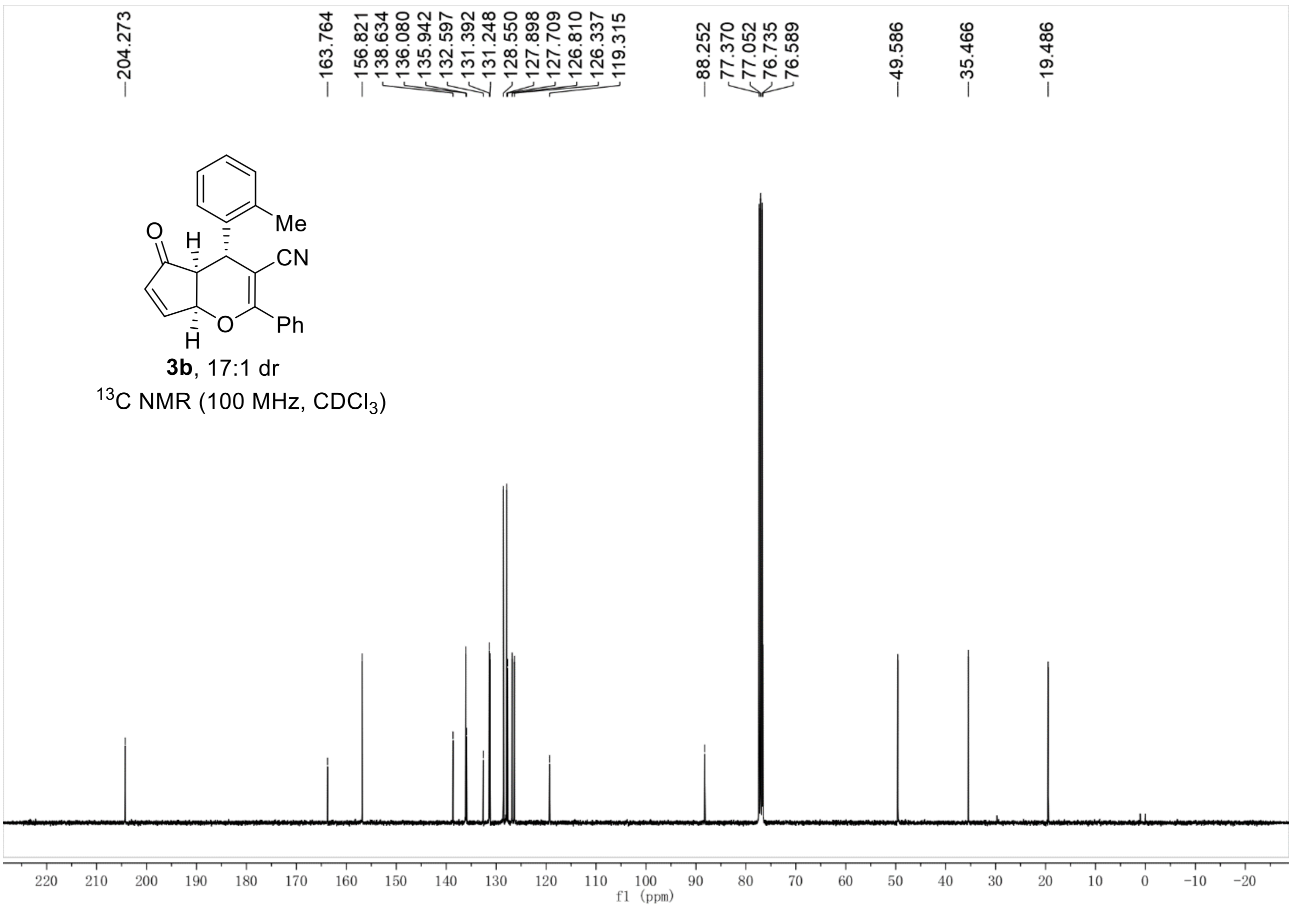
1.05
3.28
4.32
0.98
1.02
1.00
1.01
3.22
fl (ppm)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136.080
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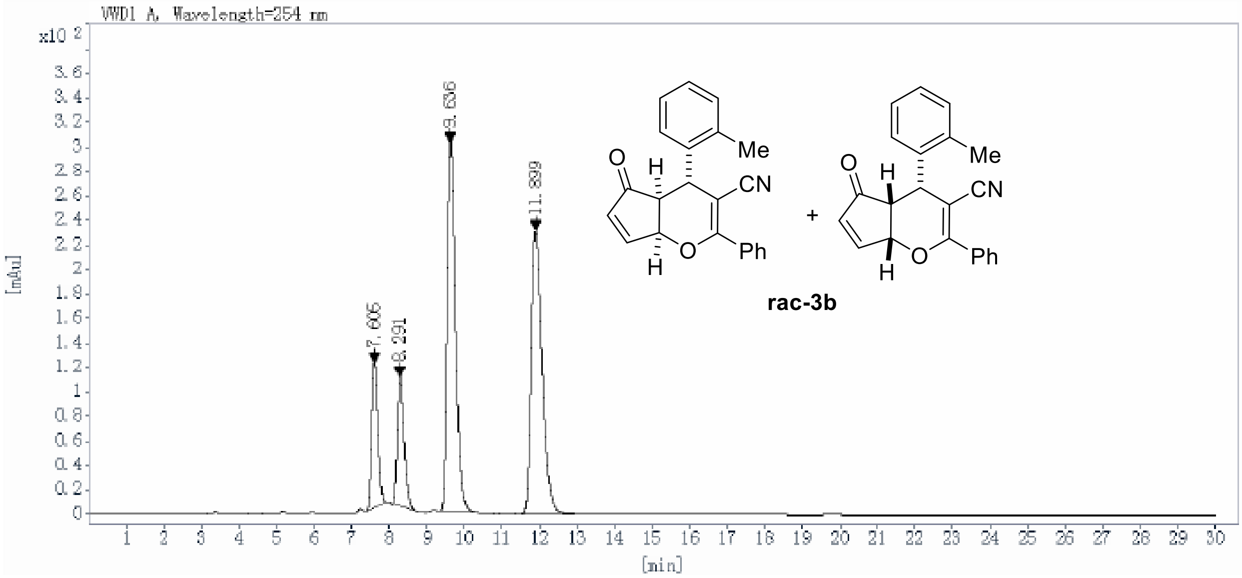
126.810
126.337
119.315
88.252
77.370
77.052
76.735
76.589
49.586
35.466
19.486
Me
CN
O
H
H
O
Ph
3b, 17:1 dr
13C NMR (100 MHz, CDCl3)
fl (ppm)



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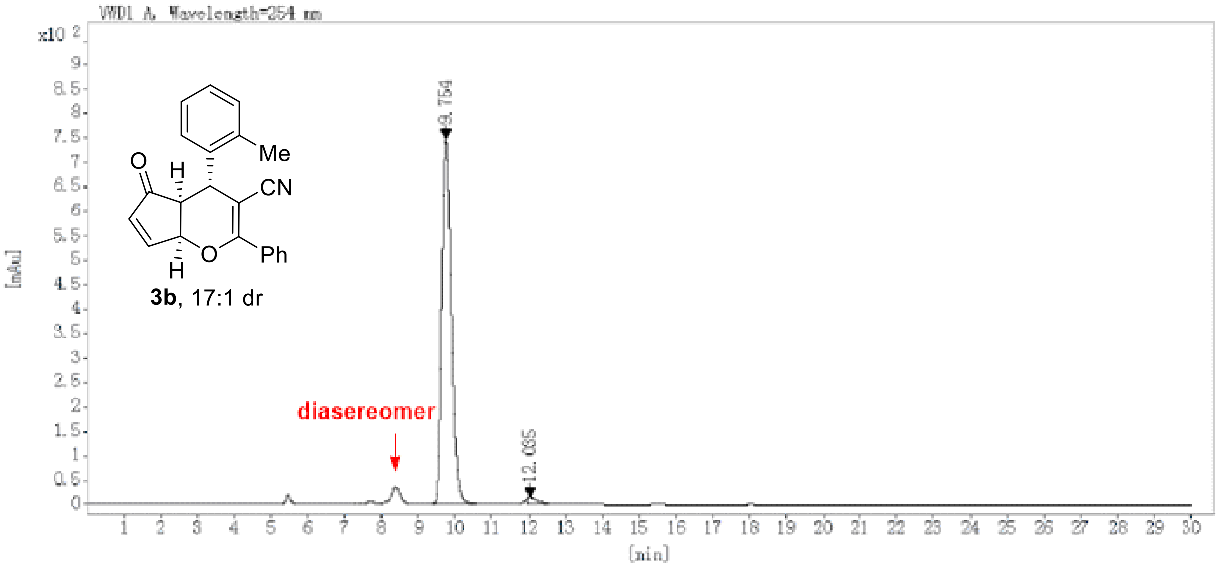

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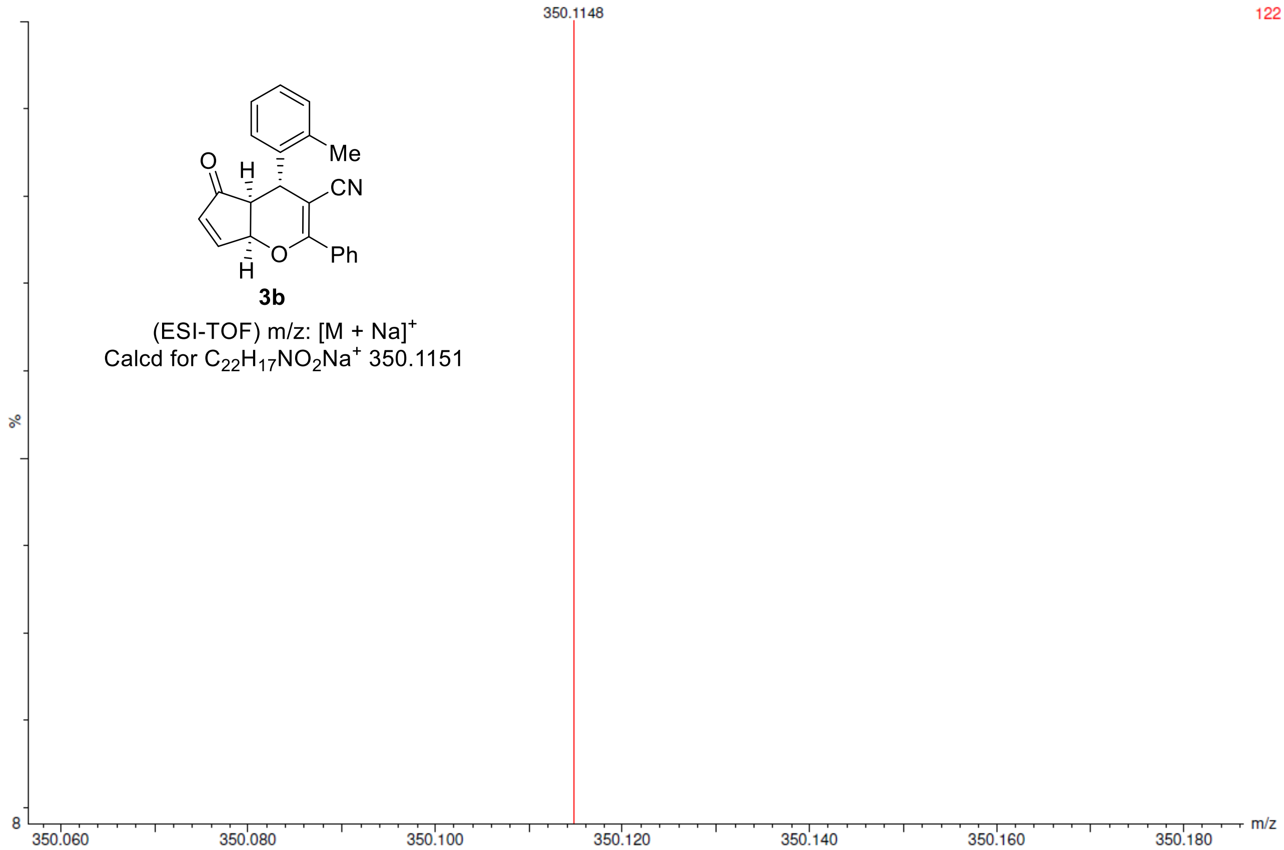

3b

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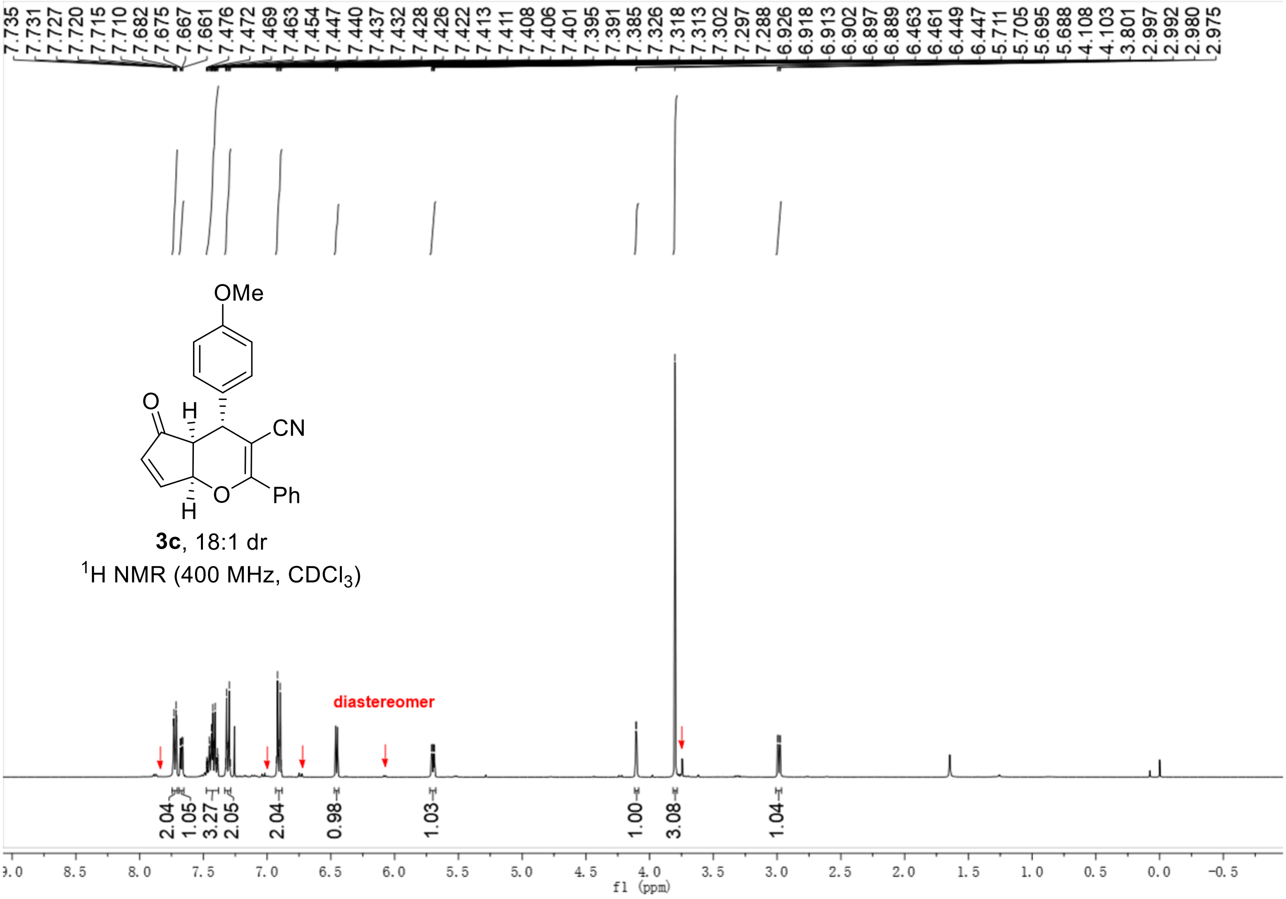
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OMe
O
H
CN
H
O
Ph
3c, 18:1 dr
^{1}H NMR (400 MHz, $CDCl_3$)
diastereomer
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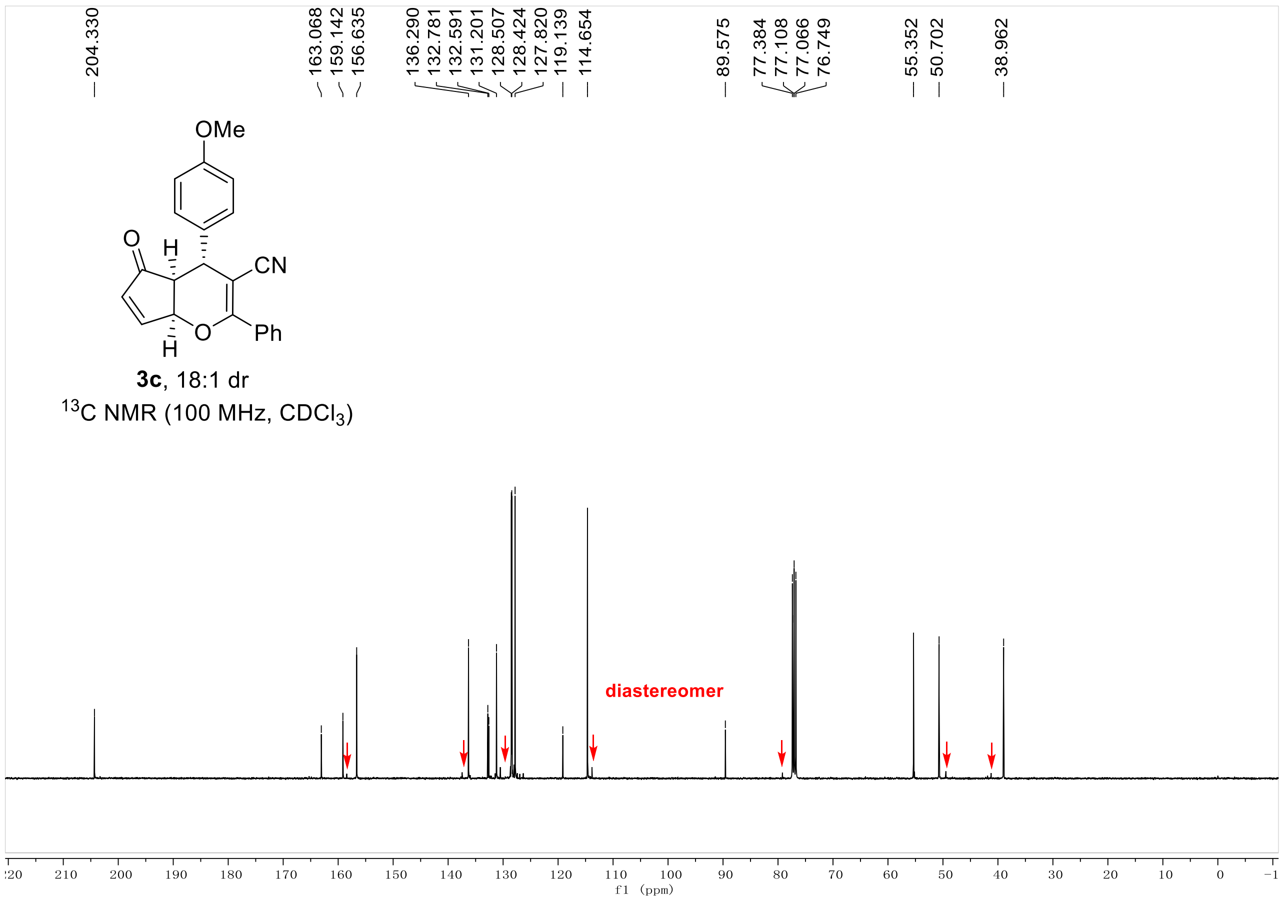
f1 (ppm)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89.575
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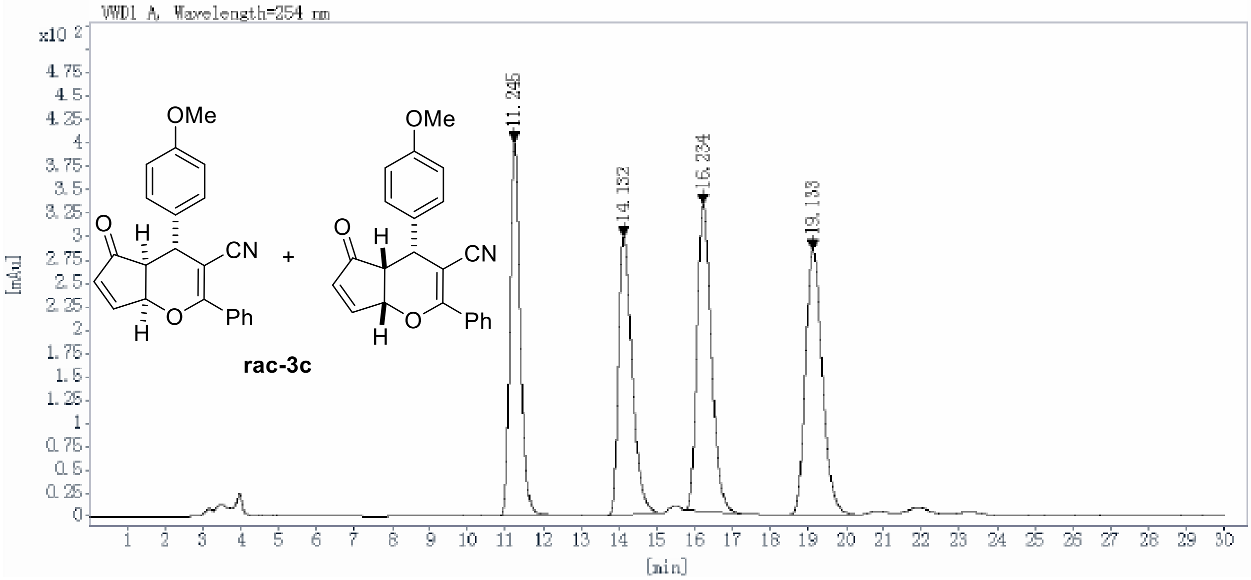
55.352 50.702
38.962
OMe
O
H
CN
H
O
Ph
3c, 18:1 dr
^{13}C NMR (100 MHz, $CDCl_3$)
diastereomer
f1 (ppm)



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14.132	BB	0.38	298.2646	7418.5083	22.9893
16.234	BB	0.40	328.1206	8593.4014	26.6302
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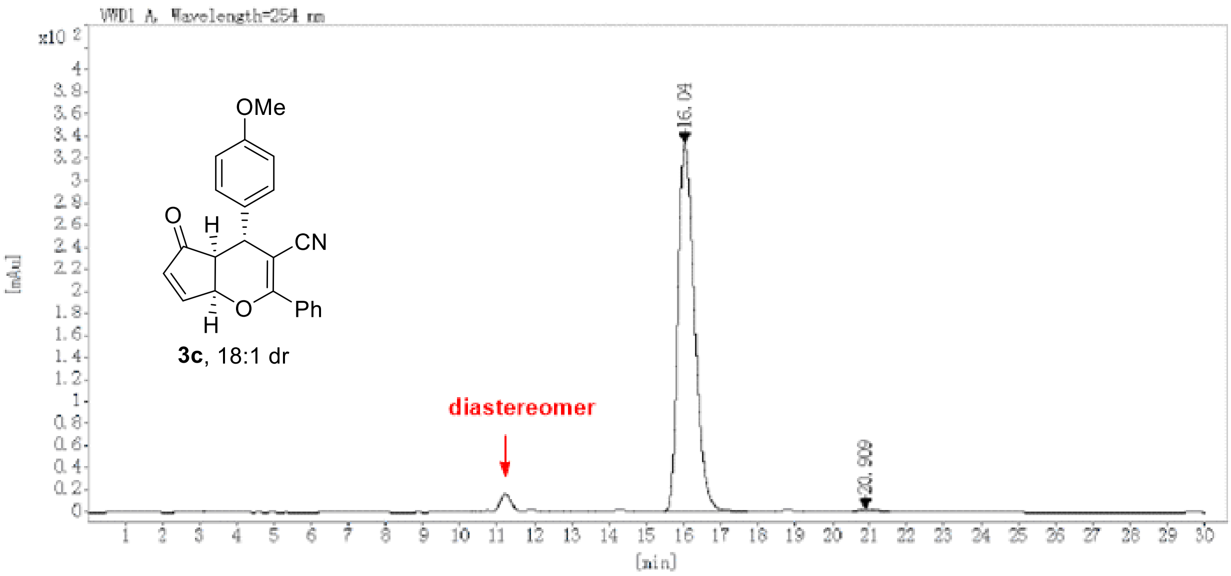

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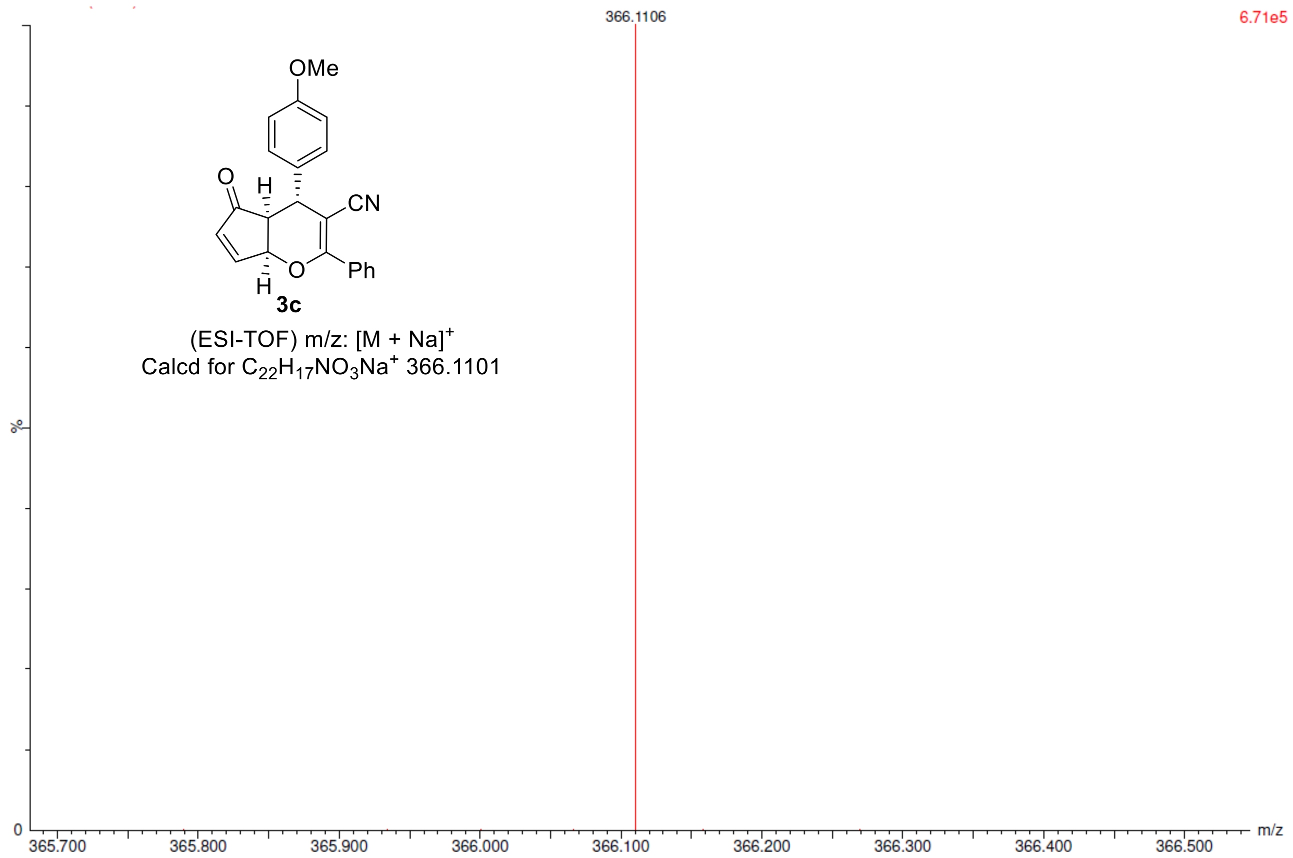
OMe
O
H
CN
Ph
O
H
3c
(ESI-TOF) m/z: [M + Na]+
Calcd for C22H17NO3Na+ 366.1101
366.1106
6.71e5
%
0
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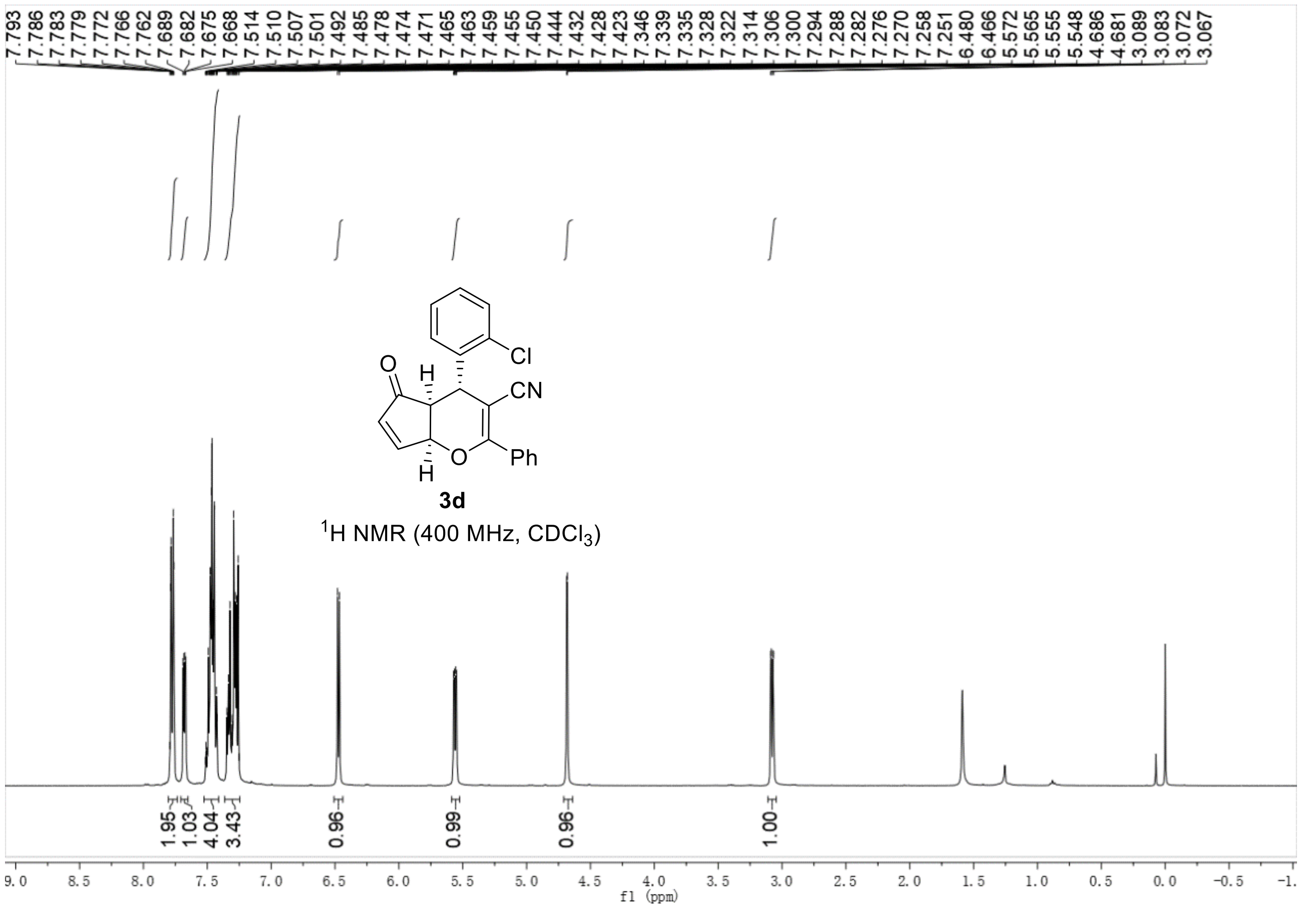
365.800
365.900
366.000
366.100
366.200
366.300
366.400
366.500
m/z


7.793 7.786 7.783 7.779 7.772 7.766 7.762 7.689 7.682 7.675 7.668 7.514 7.510 7.507 7.501 7.492 7.485 7.478 7.474 7.471 7.465 7.463 7.459 7.455 7.450 7.444 7.432 7.428 7.423 7.346 7.339 7.335 7.328 7.322 7.314 7.306 7.300 7.294 7.288 7.282 7.276 7.270 7.258 7.251 6.480 6.466 5.572 5.565 5.555 5.548 4.686 4.681 3.089 3.083 3.072 3.067
O
H
Cl
CN
H
O
Ph
3d
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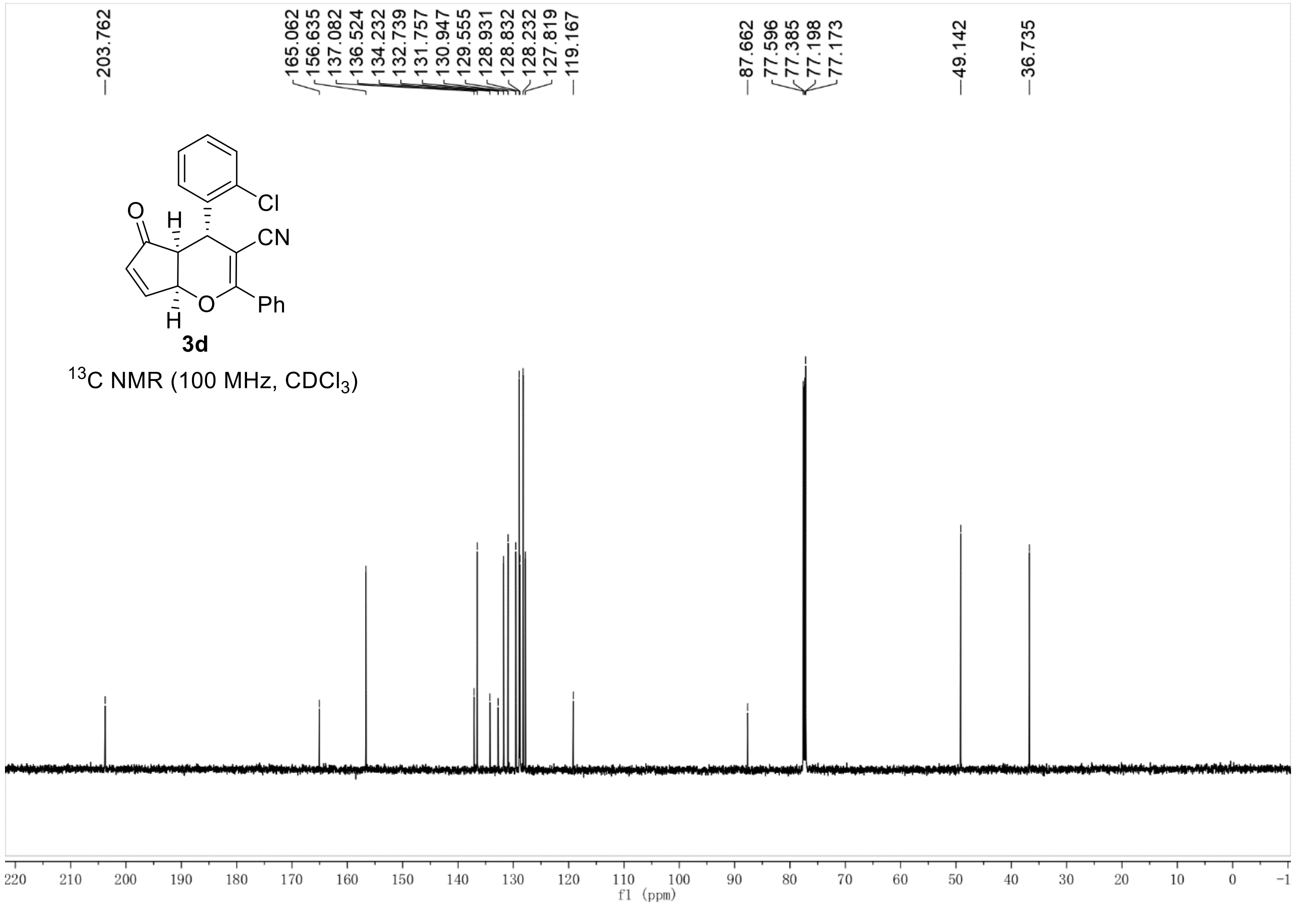
f1 (ppm)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49.142
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O
H
Cl
CN
H
O
Ph
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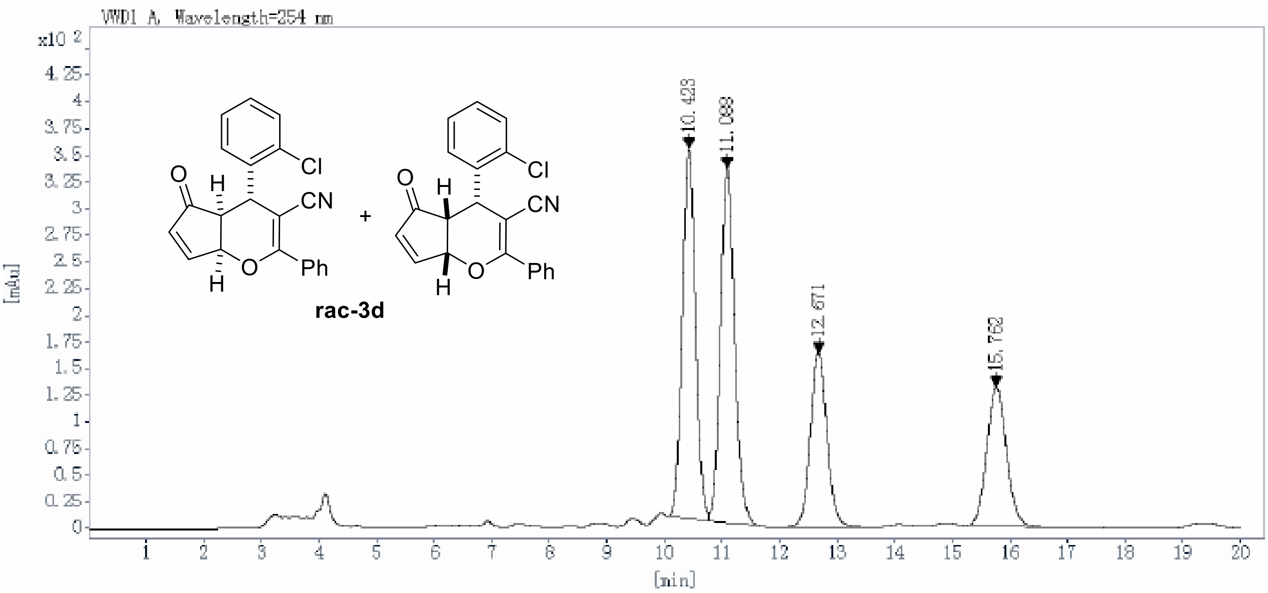
f1 (ppm)



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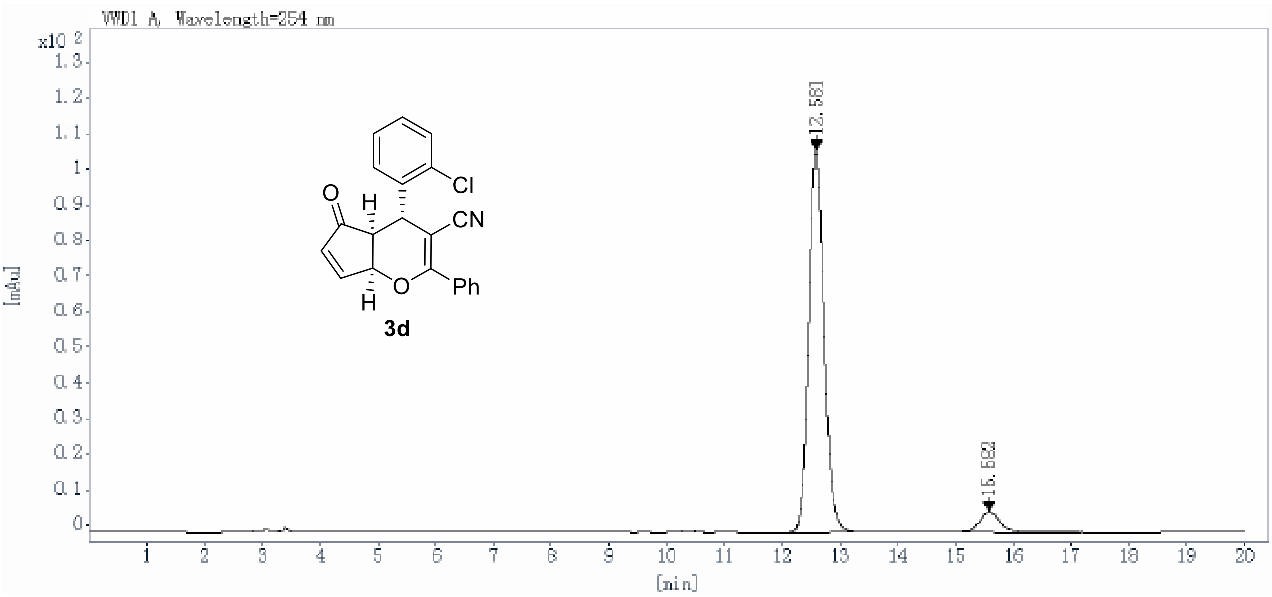

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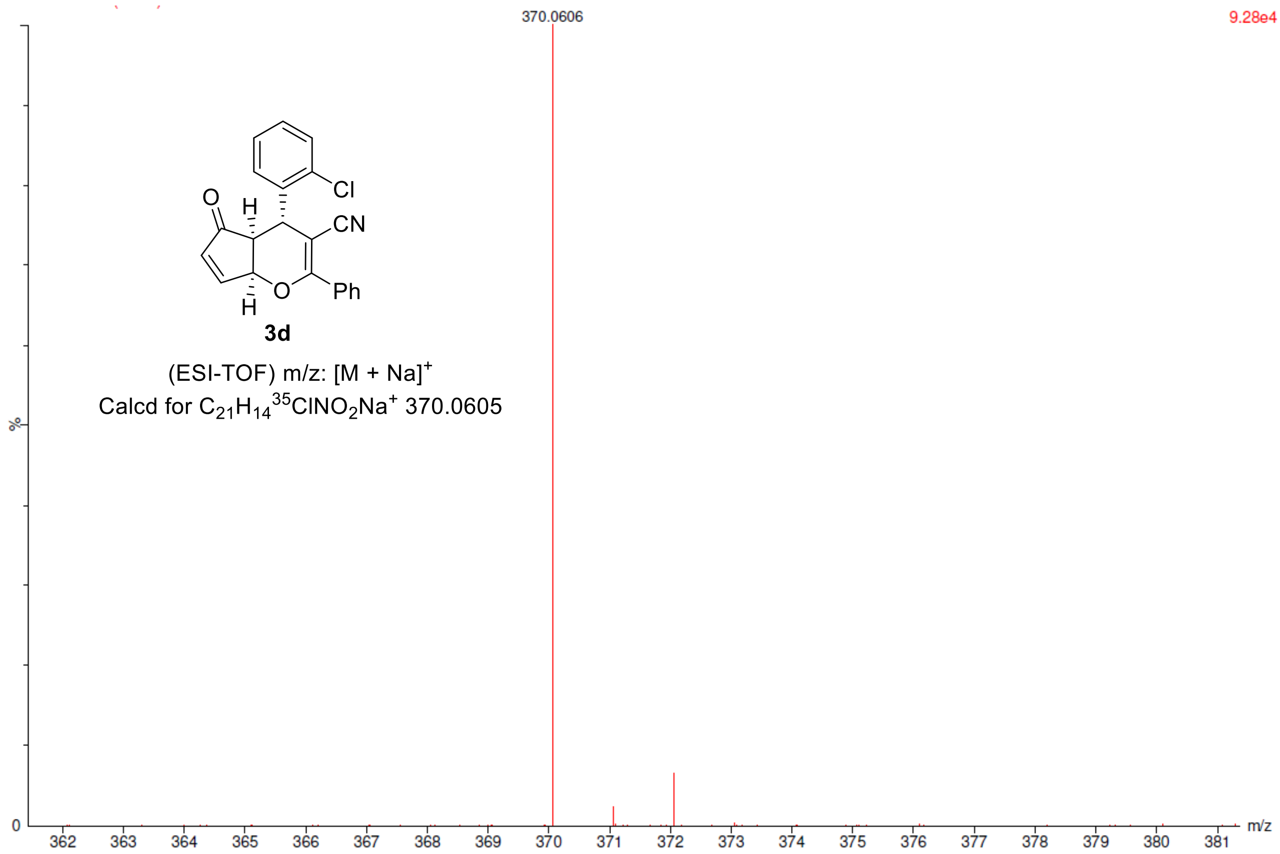
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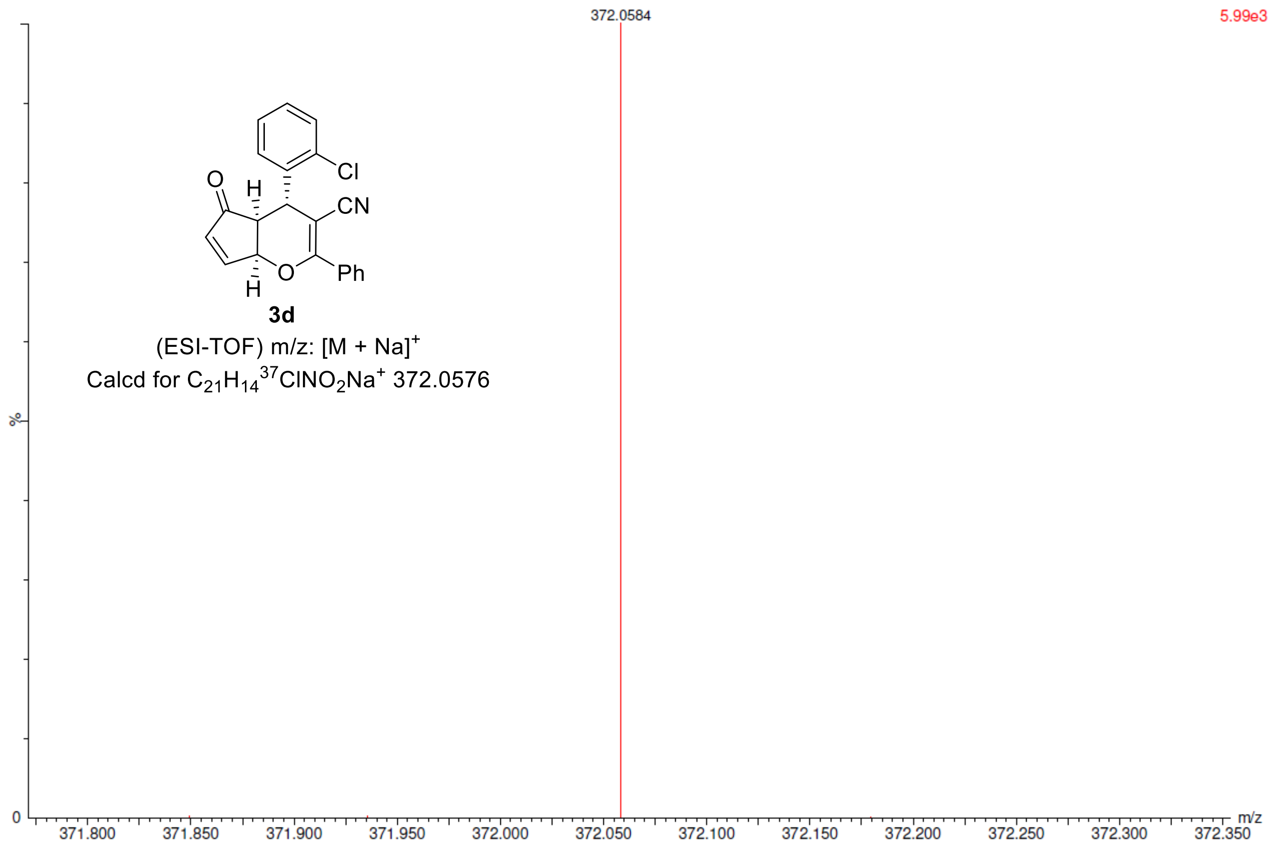
CN
Ph
H
O
3d
(ESI-TOF) m/z: [M + Na]+
Calcd for $C_{21}H_{14}{}^{35}ClNO_2Na^+$ 370.0605
%
0
362
363
364
365
366
367
368
369
370
371
372
373
374
375
376
377
378
379
380
381
m/z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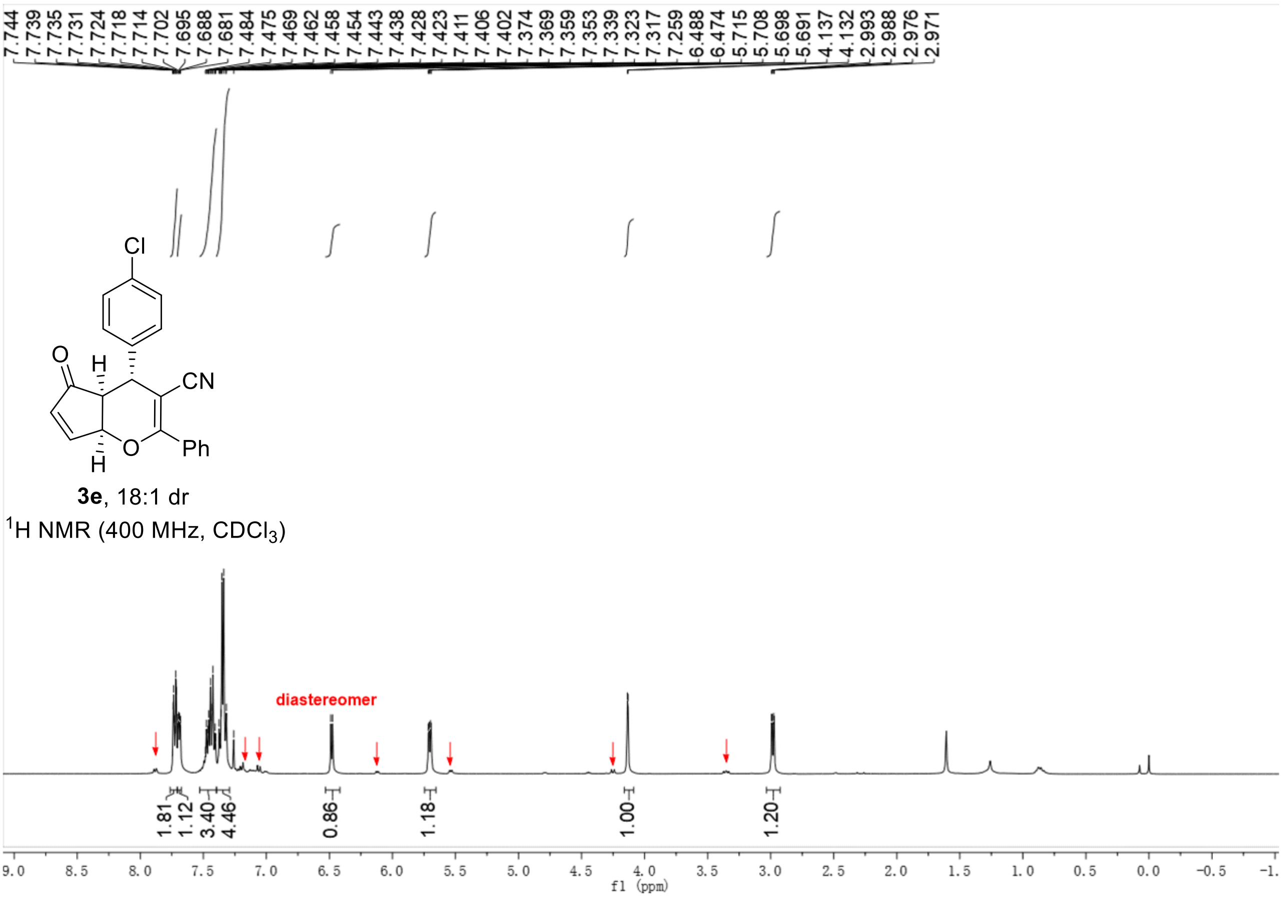
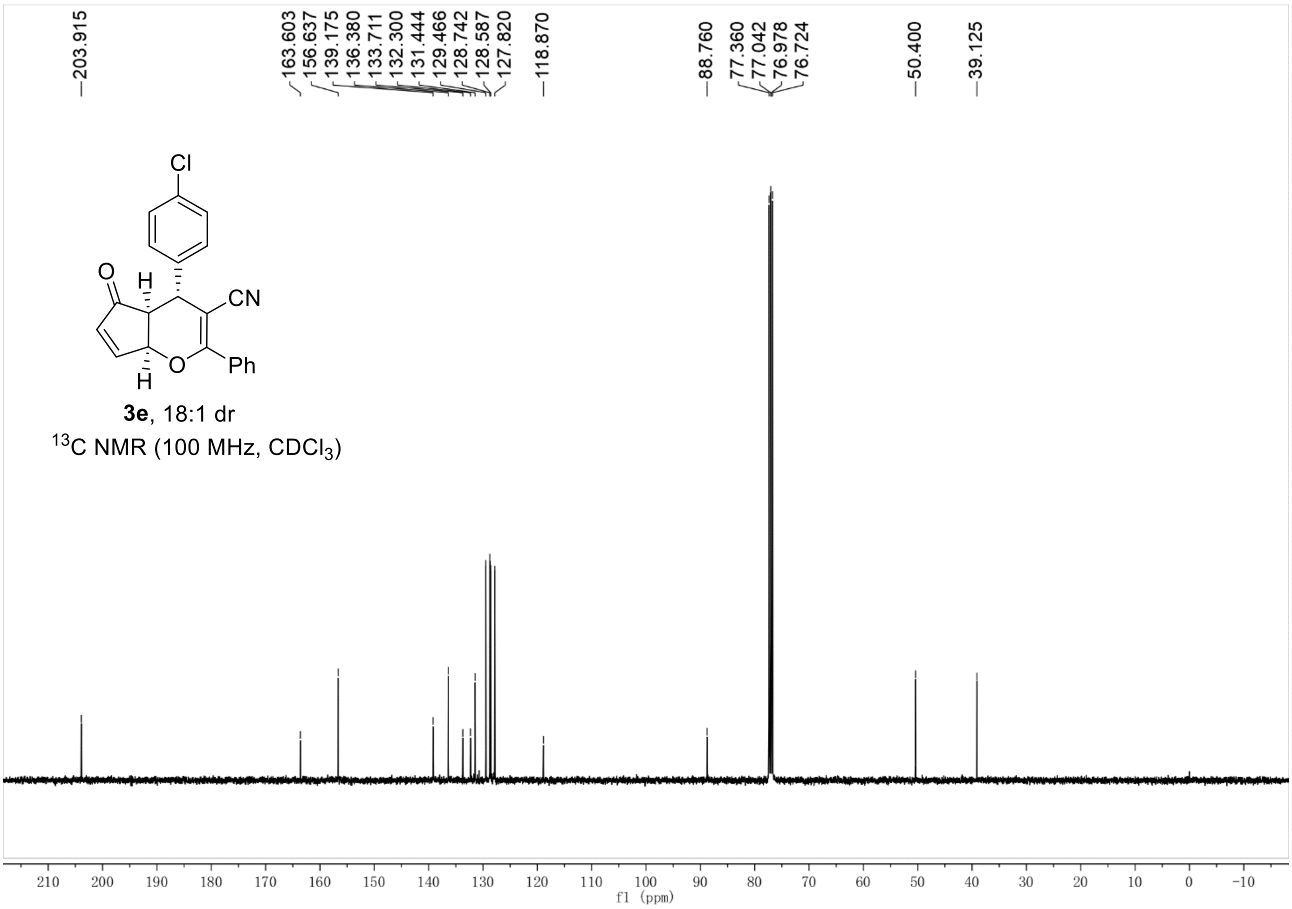
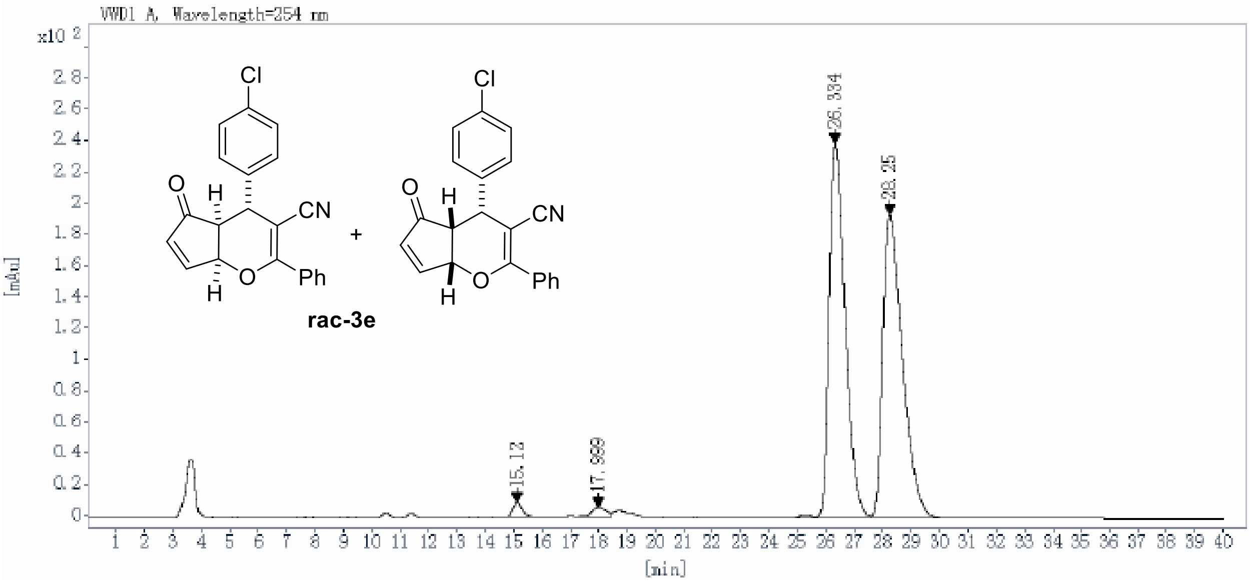
5.99e3
Cl
O
H
CN
Ph
H
O
3d
(ESI-TOF) m/z: [M + Na]+
Calcd for $C_{21}H_{14}{}^{37}ClNO_2Na^+$ 372.0576
%
0
371.800
371.850
371.900
371.950
372.000
372.050
372.100
372.150
372.200
372.250
372.300
372.350
m/z



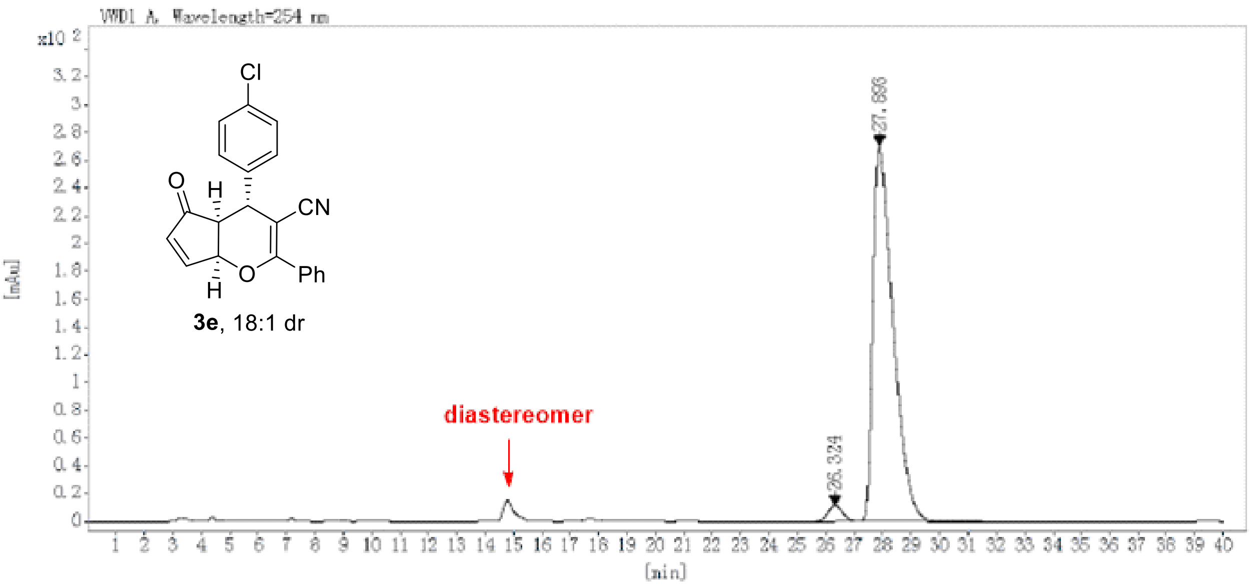
3e, 18:1 dr
^{1}H NMR (400 MHz, $CDCl_3$)



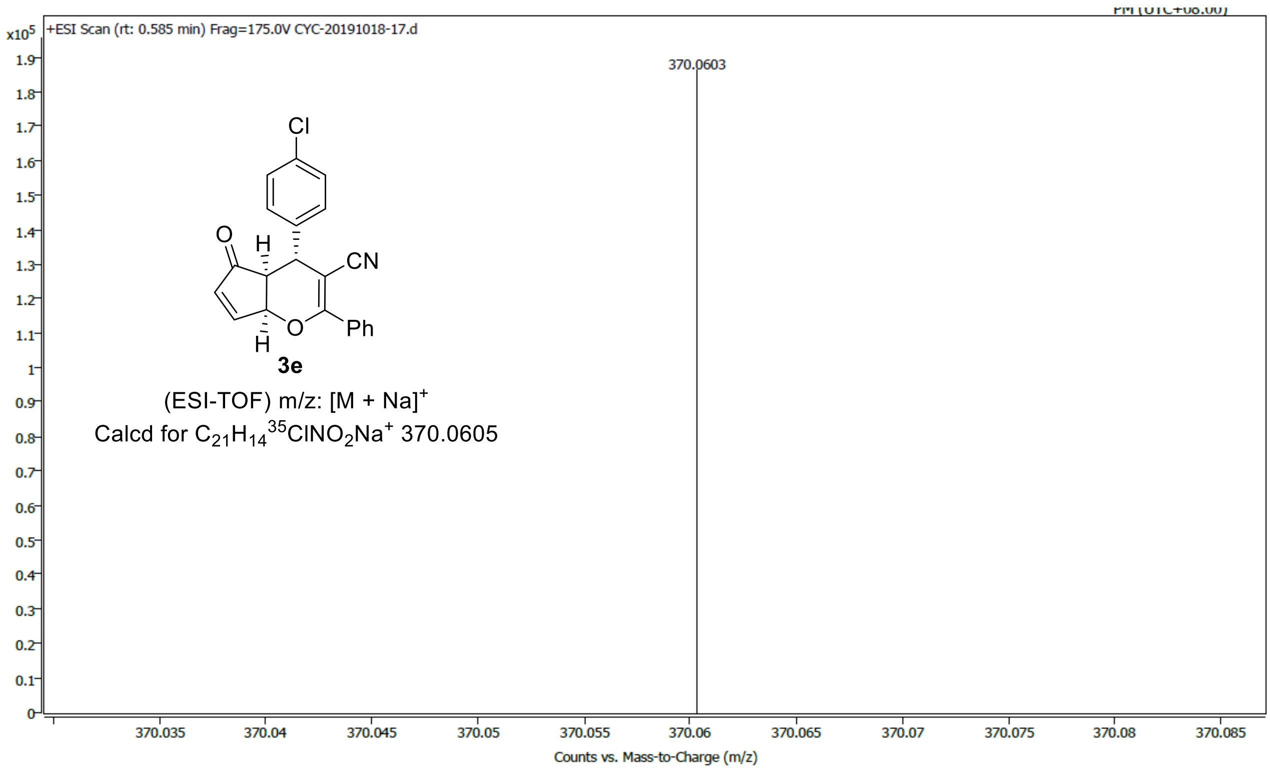
3e, 18:1 dr
^{13}C NMR (100 MHz, $CDCl_3$)

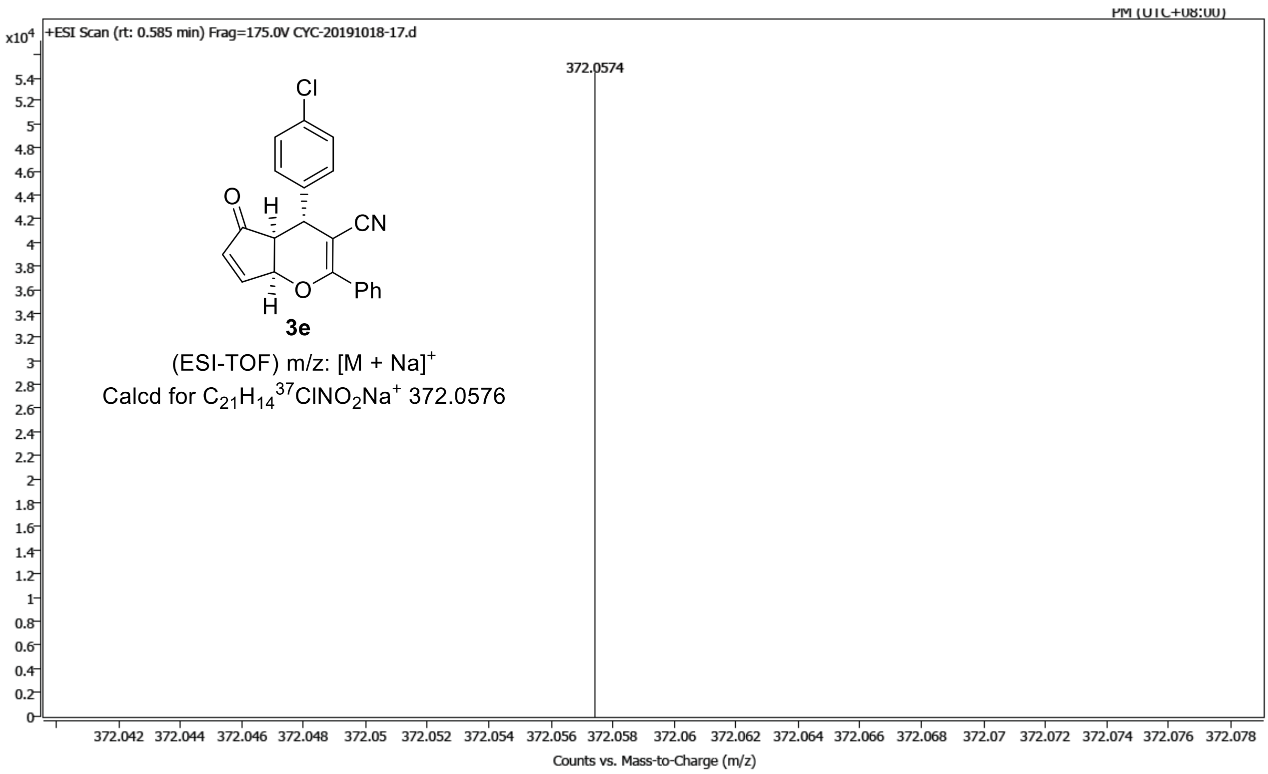


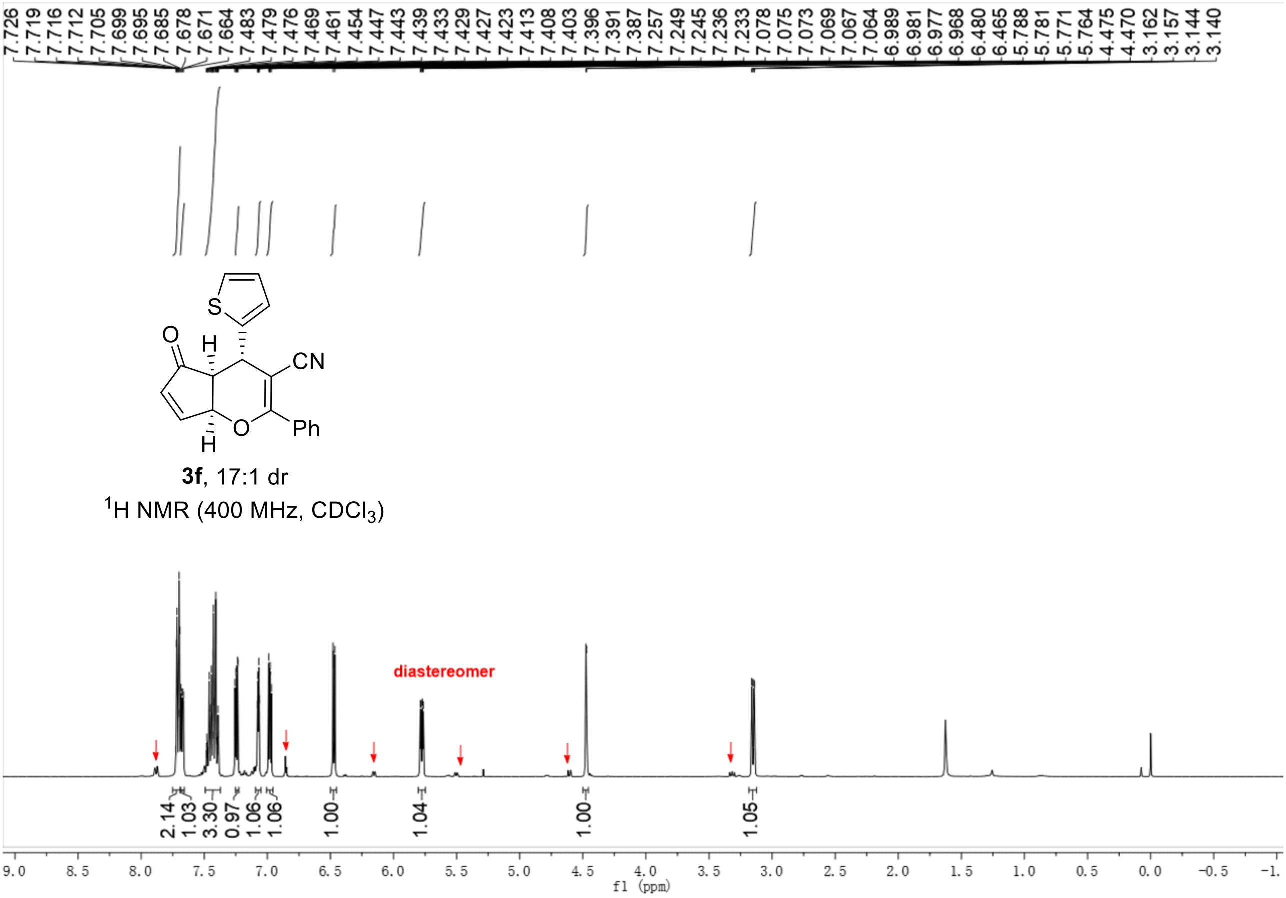
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
15.120	BB	0.36	9.2142	217.0491	1.1317
17.999	BV	0.52	5.8634	201.1309	1.0487
26.334	VV R	0.60	239.5816	9417.1592	49.1010
28.250	VB	0.73	194.0842	9343.8389	48.7187
			Totals:	19179.1781	100.0000

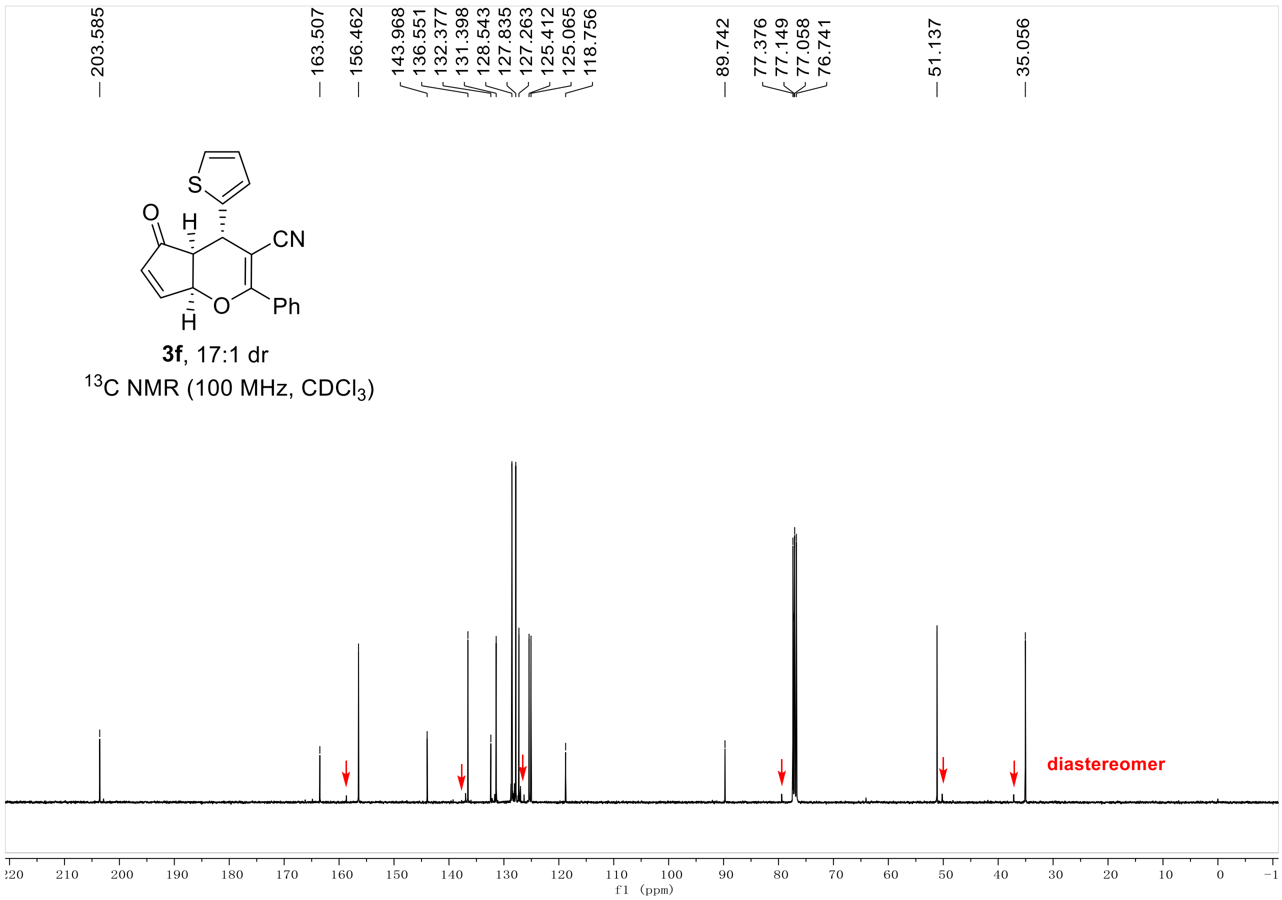


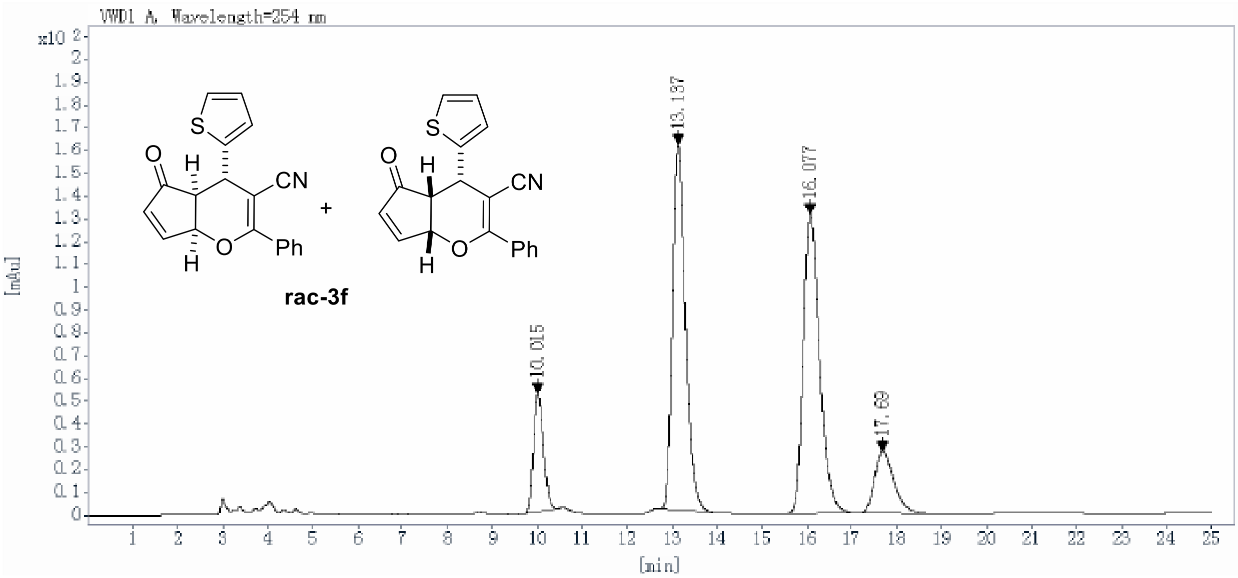
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
26.324	BB	0.56	11.5914	416.9321	3.0397
27.893	BB	0.74	270.0060	13299.4385	96.9603
			Totals:	13716.3706	100.0000


+ESI Scan (rt: 0.585 min) Frag=175.0V CYC-20191018-17.d
x10^5
370.0603
Cl
O
H
CN
O
Ph
H
3e
(ESI-TOF) m/z: [M + Na]+
Calcd for C21H14 35ClNO2Na+ 370.0605
Counts vs. Mass-to-Charge (m/z)

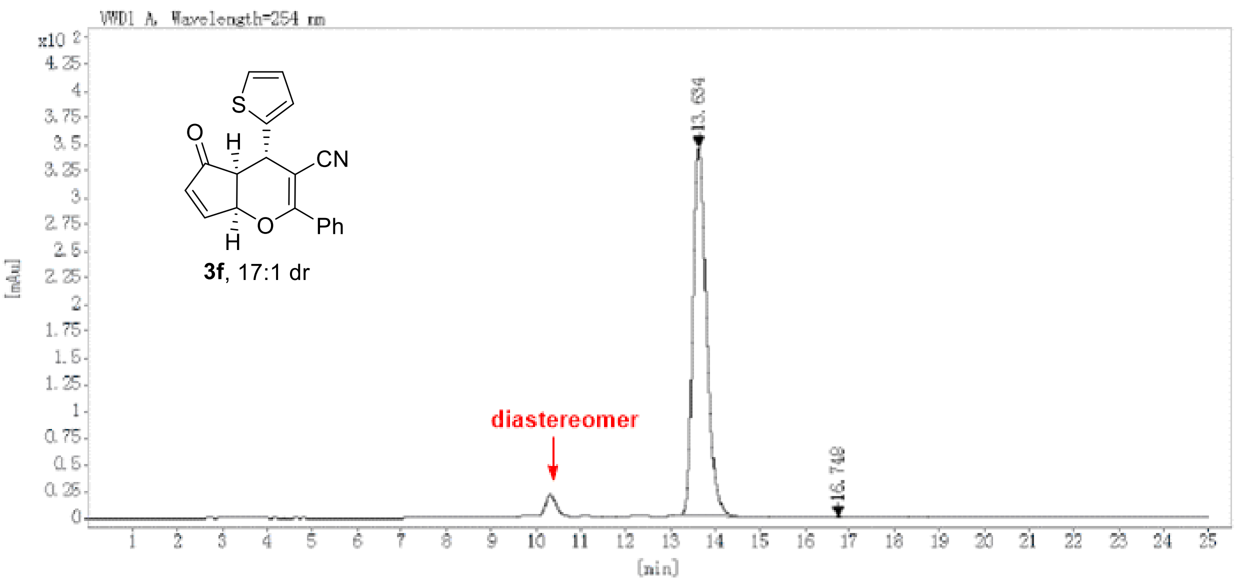

+ESI Scan (rt: 0.585 min) Frag=175.0V CYC-20191018-17.d
x10^4
372.0574
Cl
O
H
CN
O
Ph
H
3e
(ESI-TOF) m/z: [M + Na]+
Calcd for C21H14 37ClNO2Na+ 372.0576
Counts vs. Mass-to-Charge (m/z)


3f, 17:1 dr
1H NMR (400 MHz, CDCl3)
diastereomer
f1 (ppm)

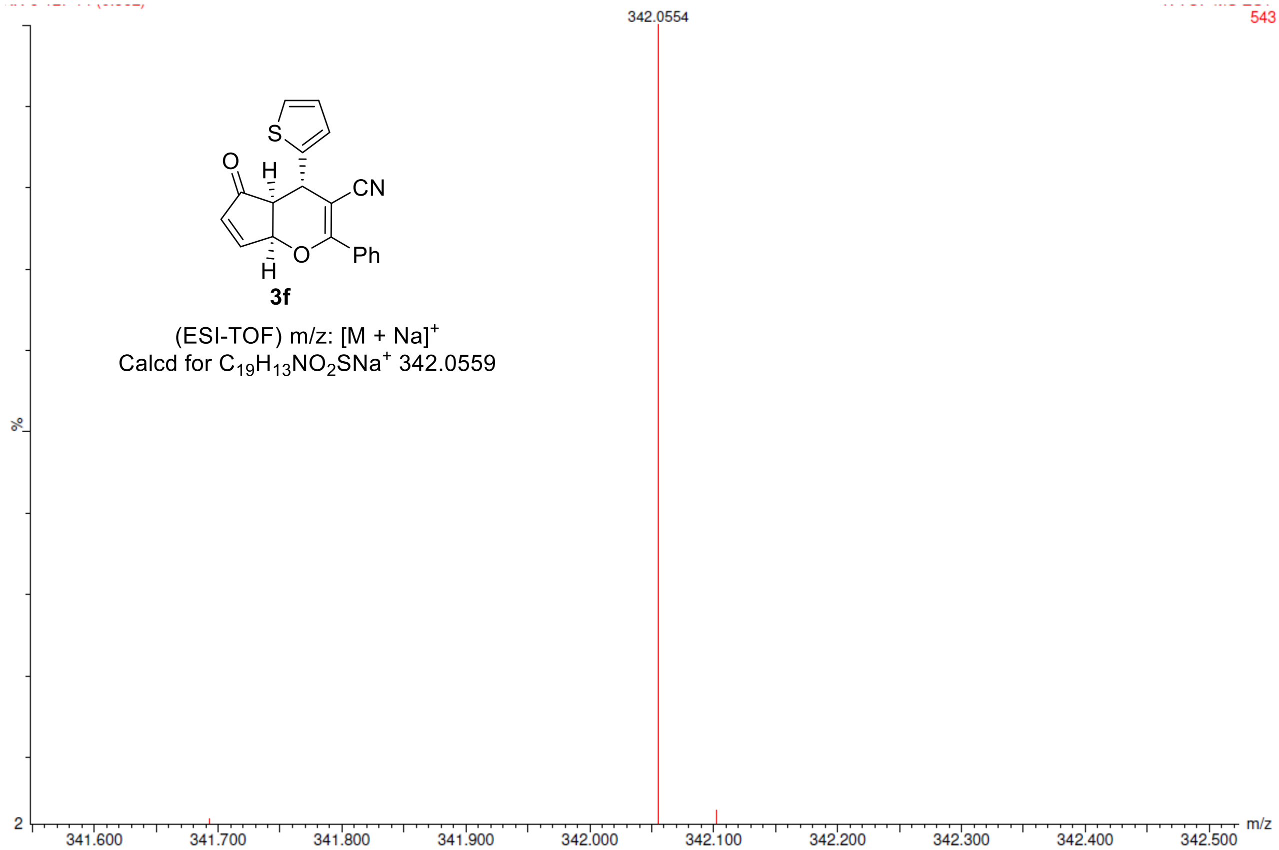

3f, 17:1 dr
13C NMR (100 MHz, CDCl3)
diastereomer
f1 (ppm)

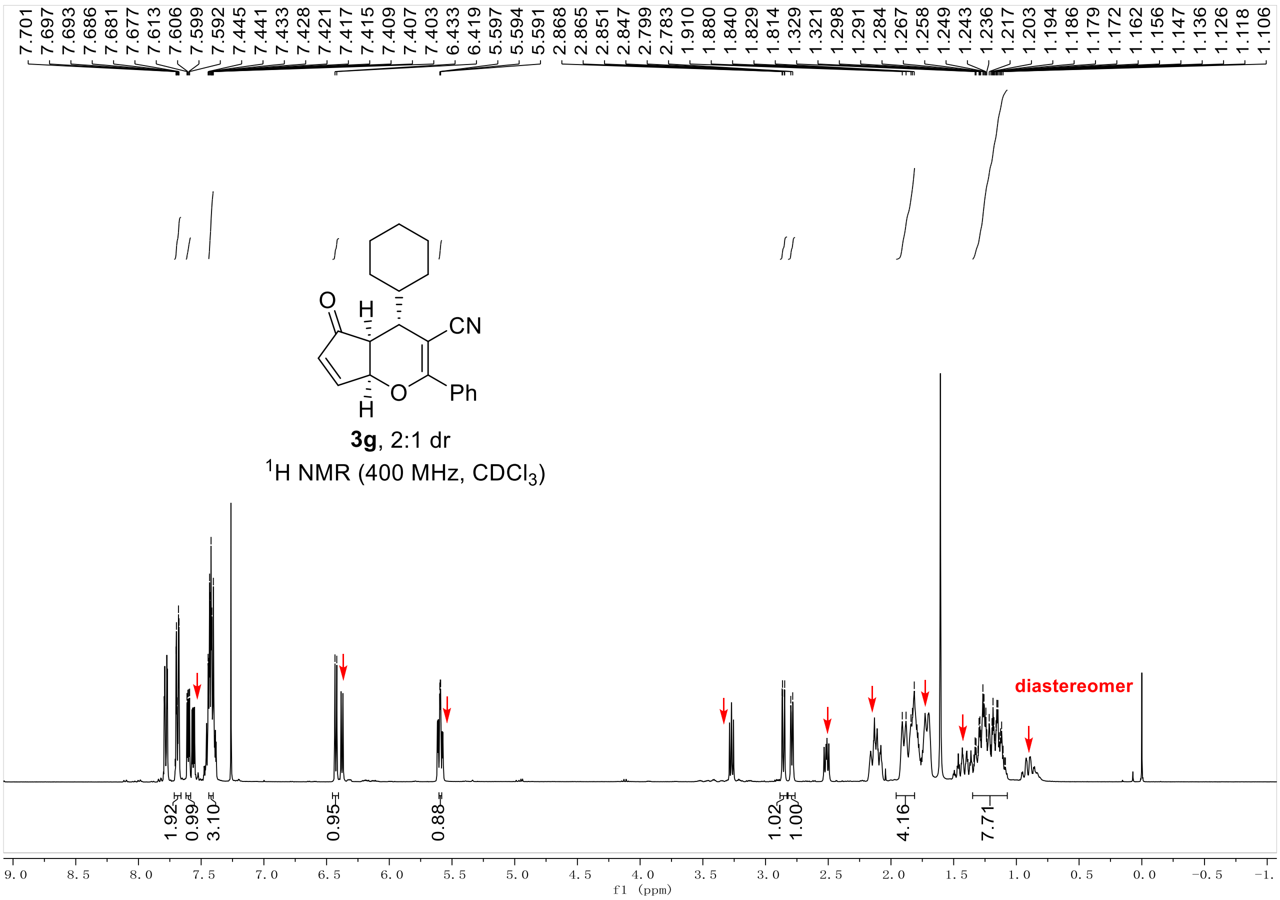


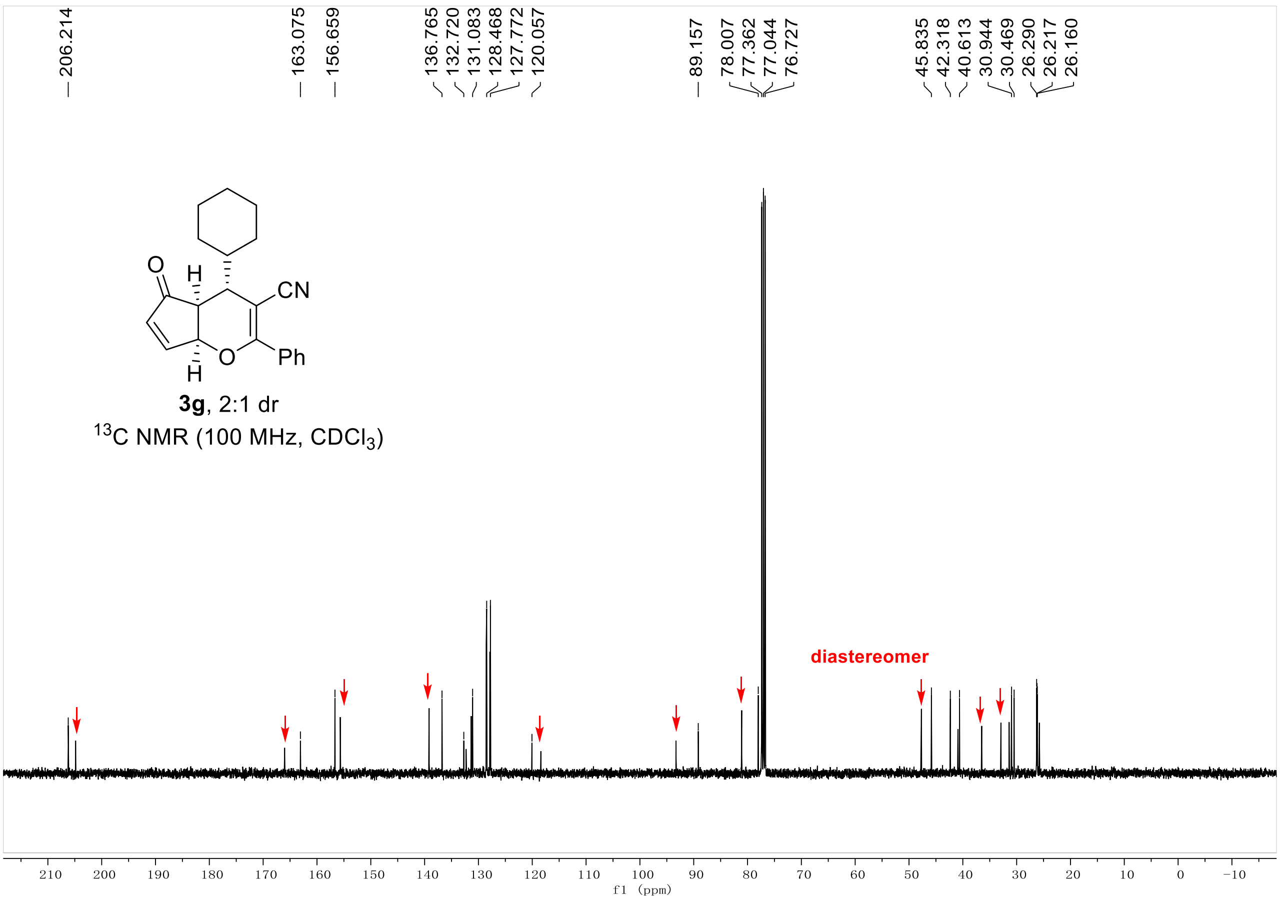
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
10.015	BV R	0.24	51.9649	791.4584	9.7328
13.137	BB	0.31	160.2263	3221.9548	39.6212
16.077	BB	0.39	131.5512	3307.4590	40.6727
17.690	BB	0.45	27.2641	811.0231	9.9734
			Totals:	8131.8953	100.0000

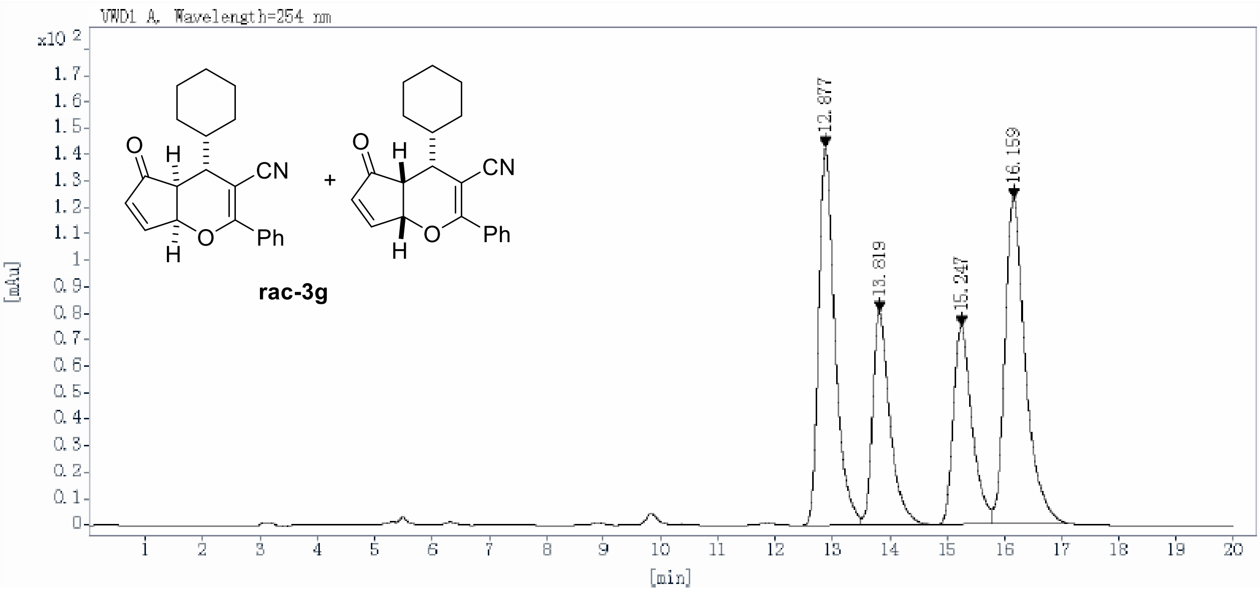


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
13.634	BB	0.32	344.7734	7229.2607	99.7939
16.748	BB	0.37	0.6252	14.9277	0.2061
			Totals:	7244.1884	100.0000

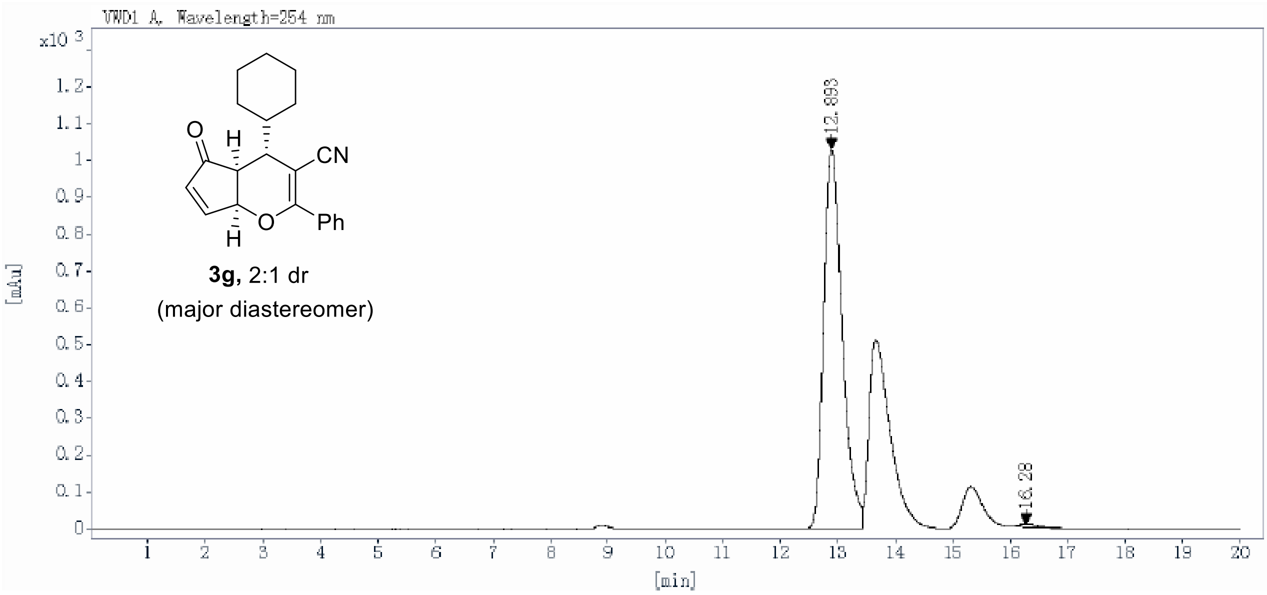

342.0554
543
3f
(ESI-TOF) m/z: [M + Na]+
Calcd for C19H13NO2SNa+ 342.0559
%
2
341.600
341.700
341.800
341.900
342.000
342.100
342.200
342.300
342.400
342.500
m/z


7.701
7.697
7.693
7.686
7.681
7.677
7.613
7.606
7.599
7.592
7.445
7.441
7.433
7.428
7.421
7.417
7.415
7.409
7.407
7.403
6.433
6.419
5.597
5.594
5.591
2.868
2.865
2.851
2.847
2.799
2.783
1.910
1.880
1.840
1.829
1.814
1.329
1.321
1.298
1.291
1.284
1.267
1.258
1.249
1.243
1.236
1.217
1.203
1.194
1.186
1.179
1.172
1.162
1.156
1.147
1.136
1.126
1.118
1.106
O
H
CN
H
O
Ph
3g, 2:1 dr
1H NMR (400 MHz, CDCl3)
diastereomer
1.92
0.99
3.10
0.95
0.88
1.02
1.00
4.16
7.71
f1 (ppm)

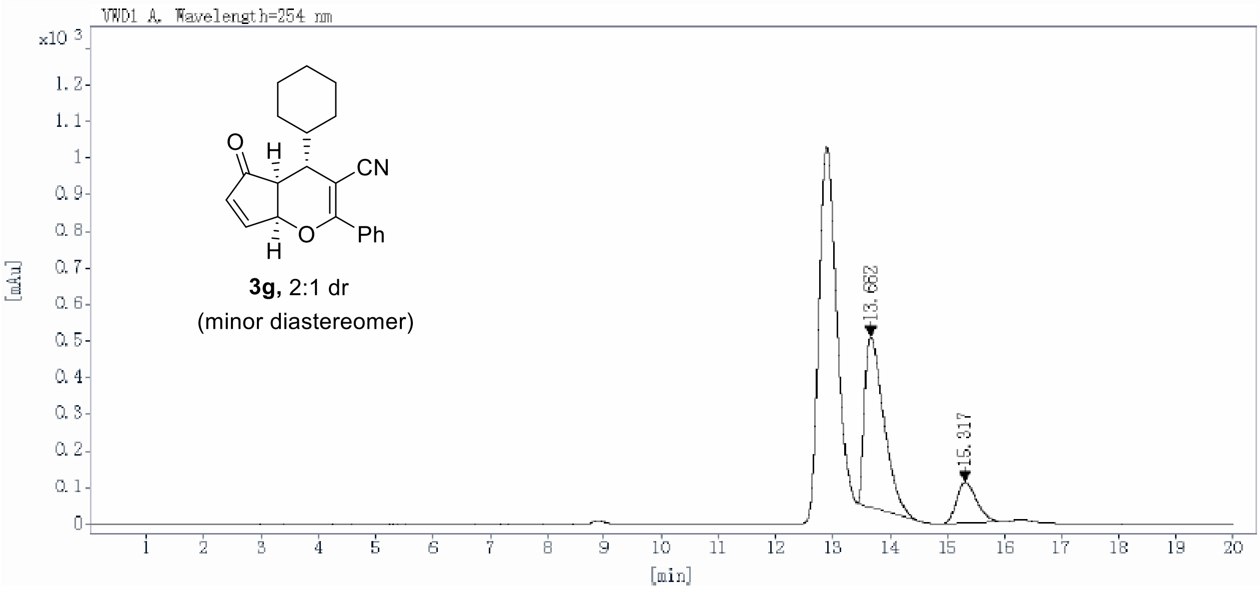

206.214
163.075
156.659
136.765
132.720
131.083
128.468
127.772
120.057
89.157
78.007
77.362
77.044
76.727
45.835
42.318
40.613
30.944
30.469
26.290
26.217
26.160
O
H
CN
H
O
Ph
3g, 2:1 dr
13C NMR (100 MHz, CDCl3)
diastereomer
f1 (ppm)



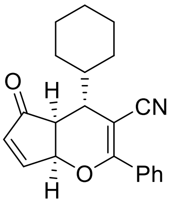
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
12.877	BV	0.30	142.6112	2833.3311	30.4664
13.819	VB	0.32	80.4895	1696.7388	18.2448
15.247	BV	0.34	74.8907	1690.3802	18.1764
16.159	VBA	0.38	122.9815	3079.4075	33.1124
			Totals:	9299.8575	100.0000



Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
12.893	BBAS	0.35	1029.2600	23120.9766	99.0647
16.280	BBA	0.36	9.2756	218.2867	0.9353
			Totals:	23339.2632	100.0000



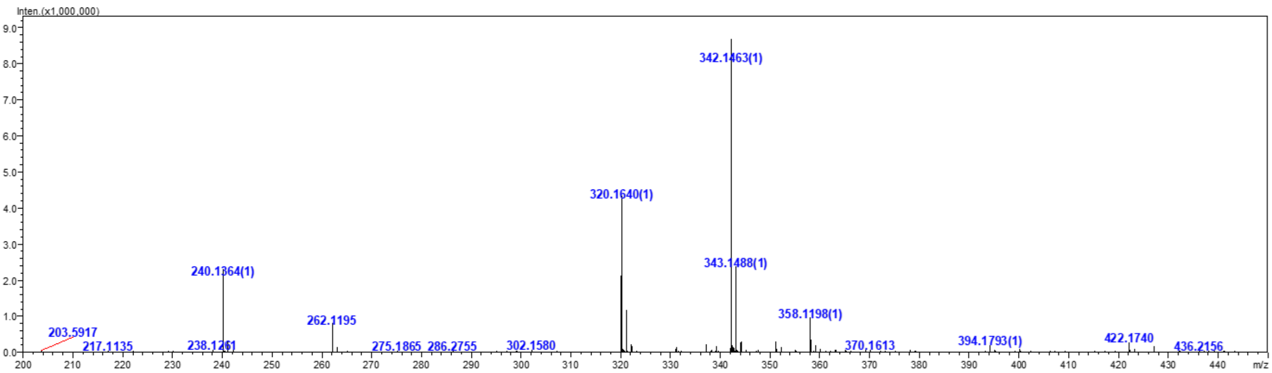
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
13.662	BB	0.36	466.5966	10972.2412	80.0650
15.317	BBA	0.38	111.9197	2731.9302	19.9350
			Totals:	13704.1714	100.0000

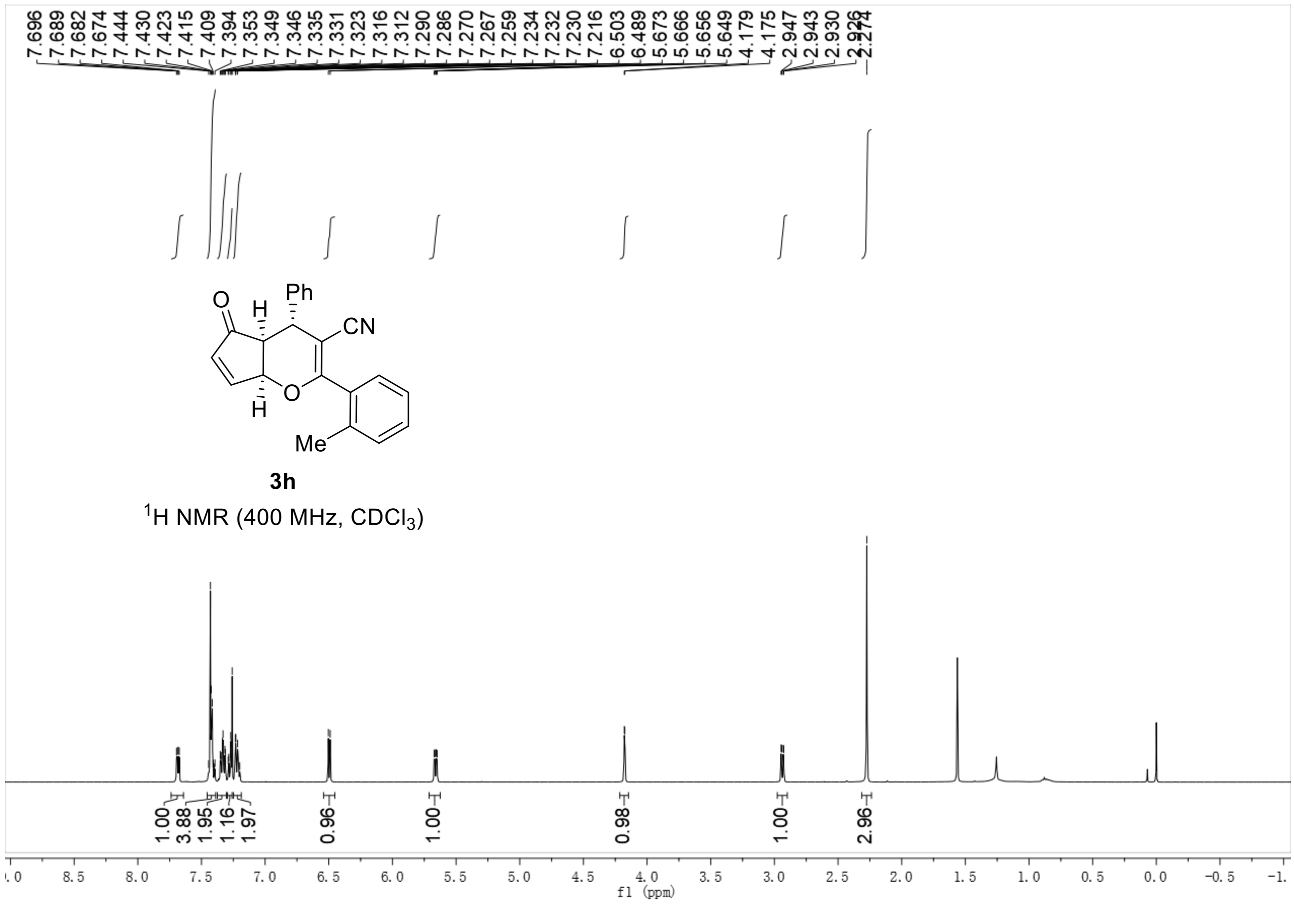


3g

(ESI-TOF) m/z: $[M + Na]^+$

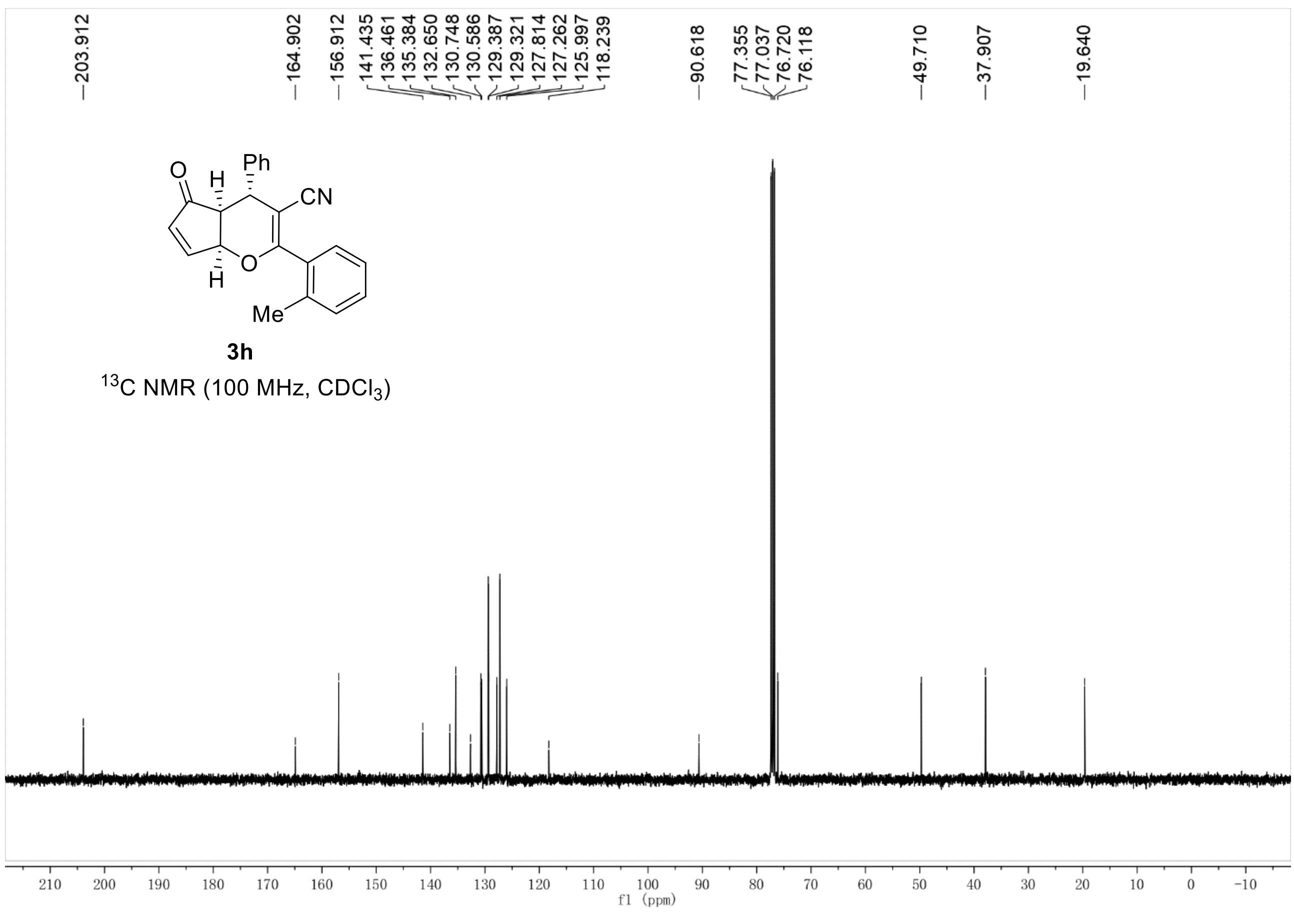
Calcd for $C_{21}H_{21}NO_2Na^+$ 342.1465





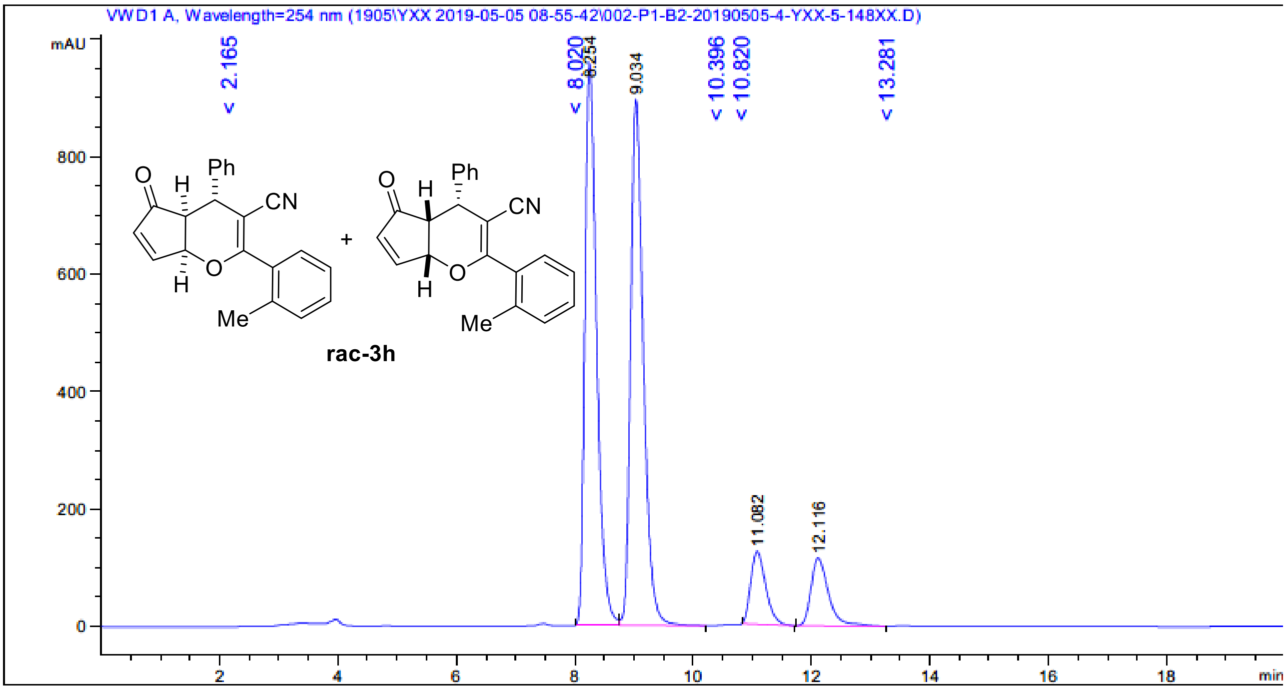
3h

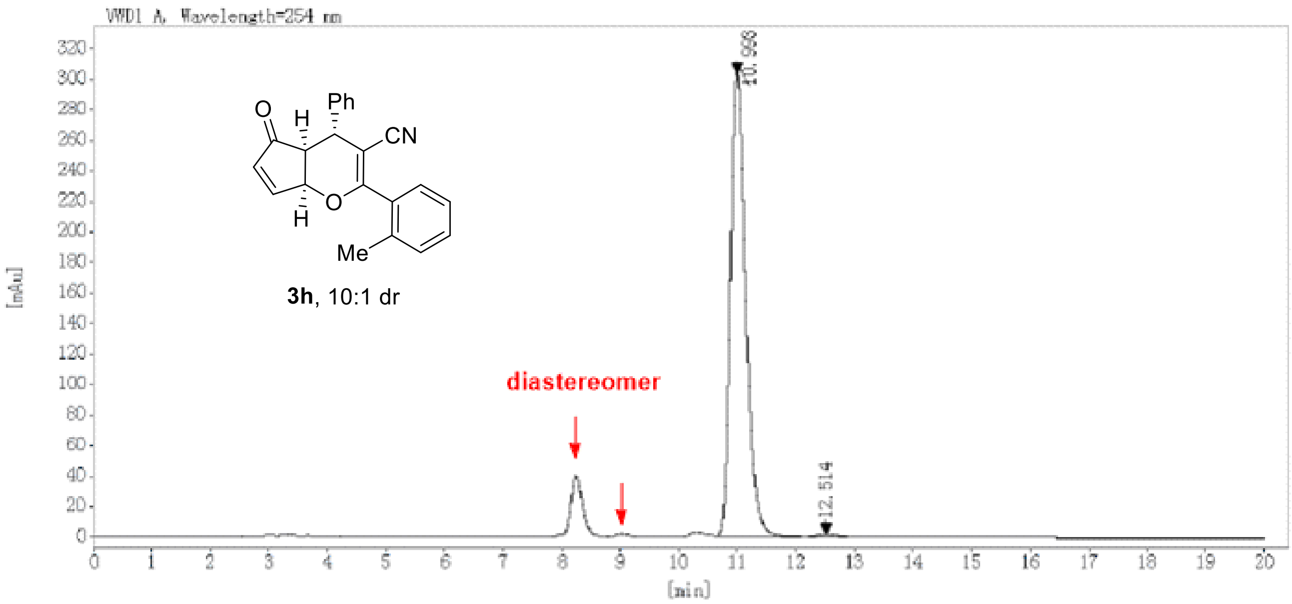
^{1}H NMR (400 MHz, $CDCl_3$)



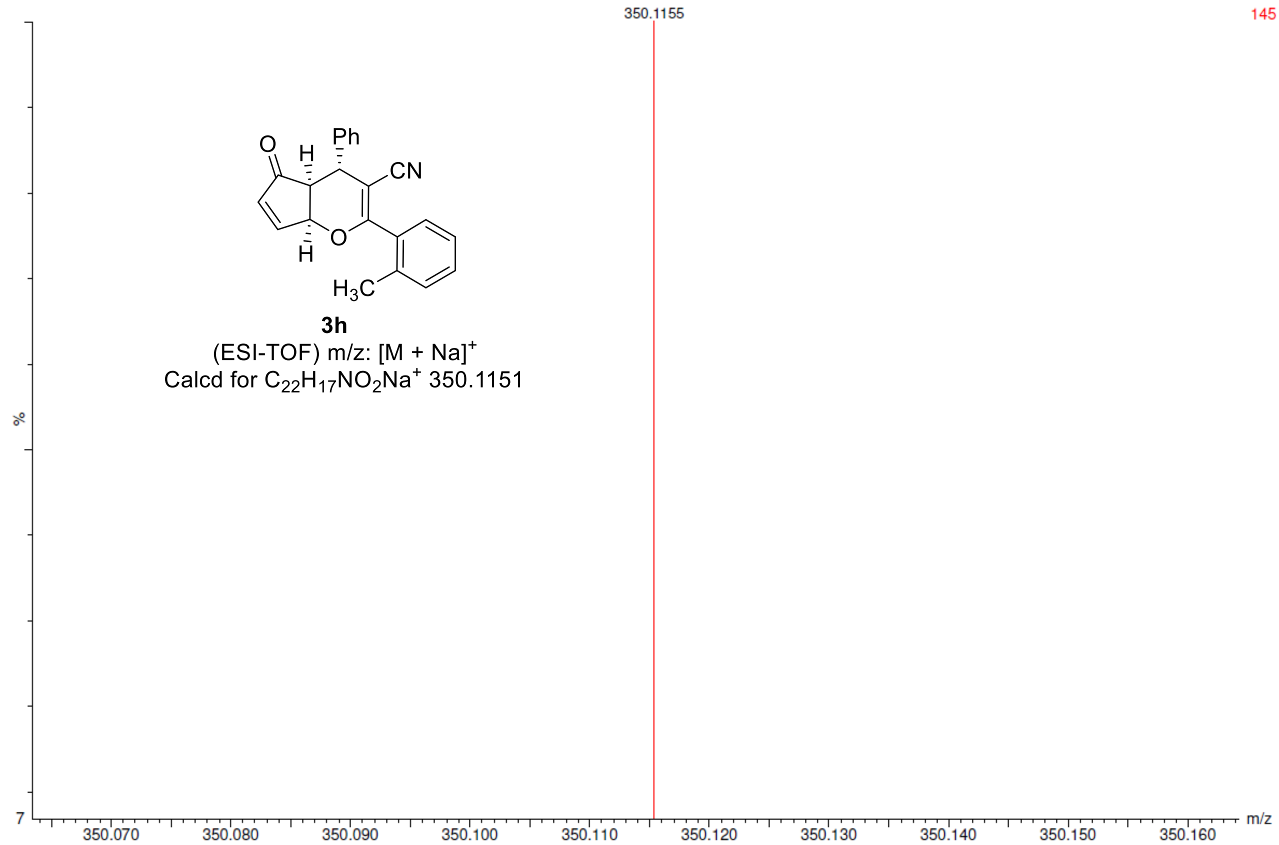
3h

^{13}C NMR (100 MHz, $CDCl_3$)

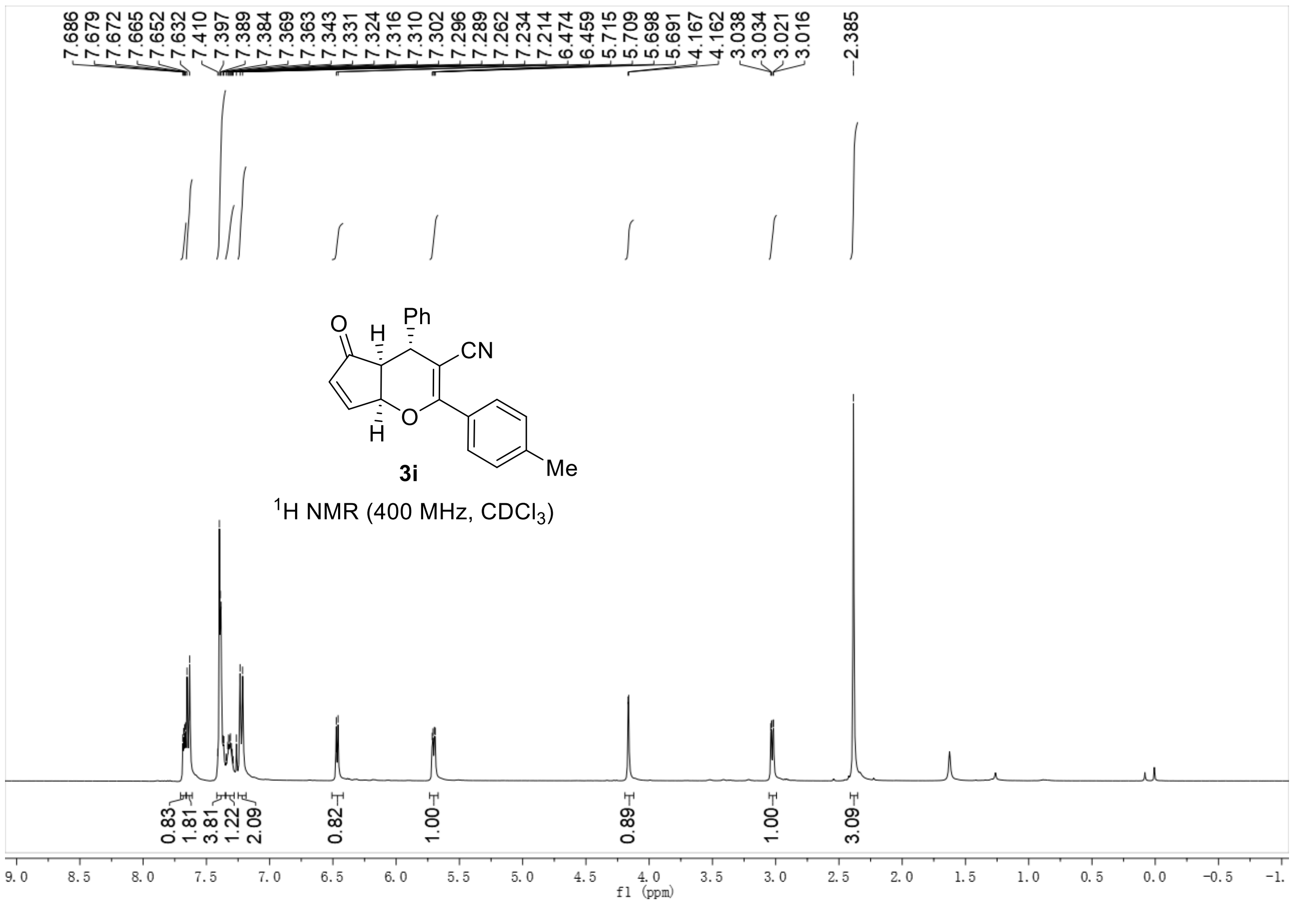


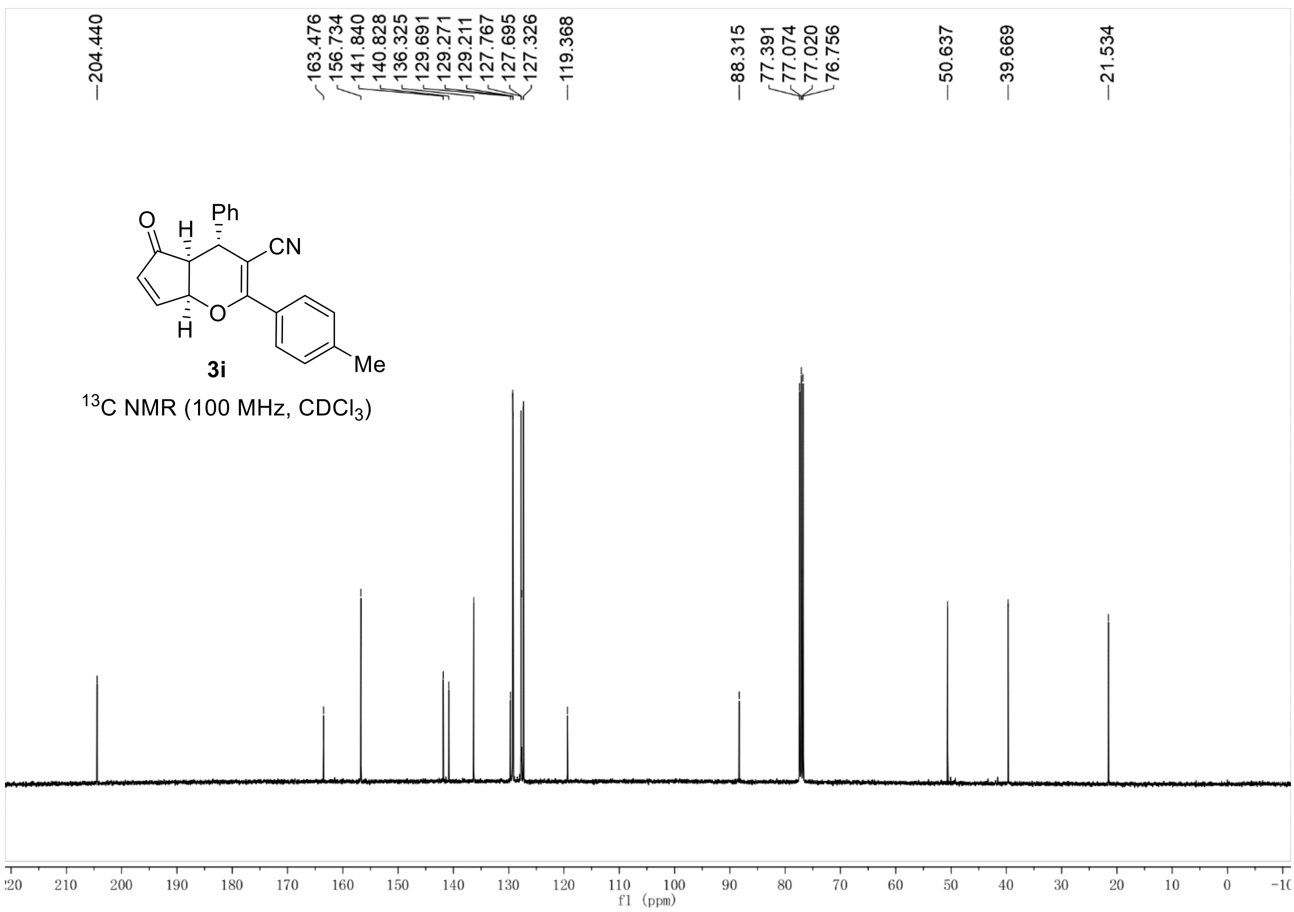


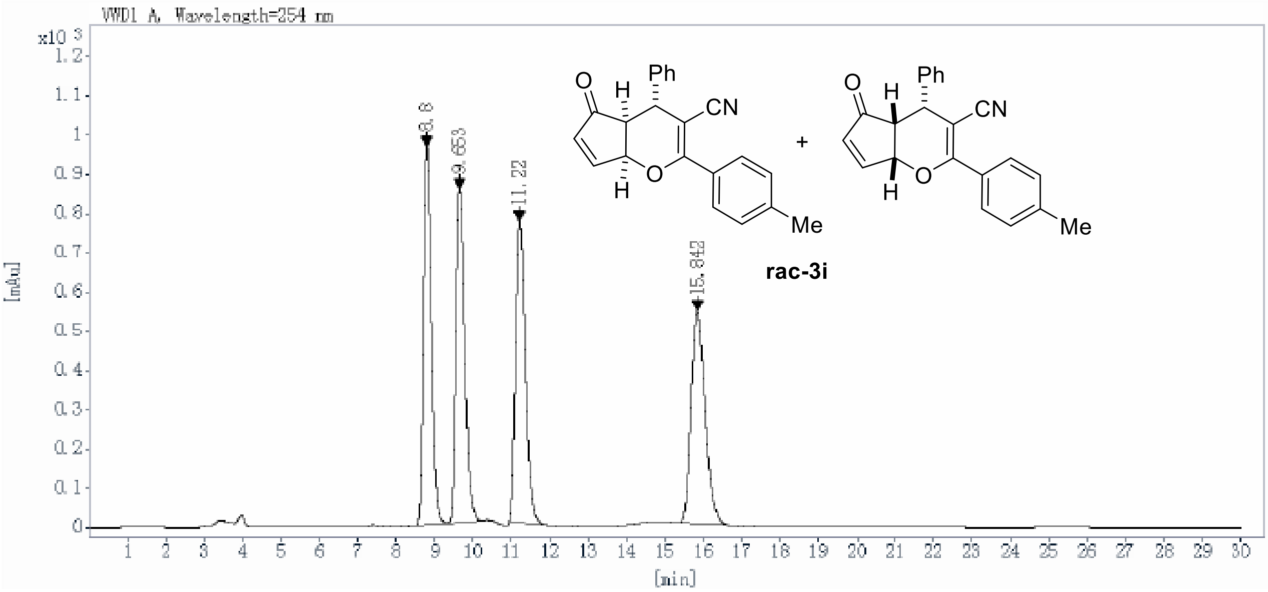
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
10.993	BB	0.28	303.6809	5503.7461	99.1078
12.514	BBA	0.34	2.2286	49.5450	0.8922
			Totals:	5553.2911	100.0000



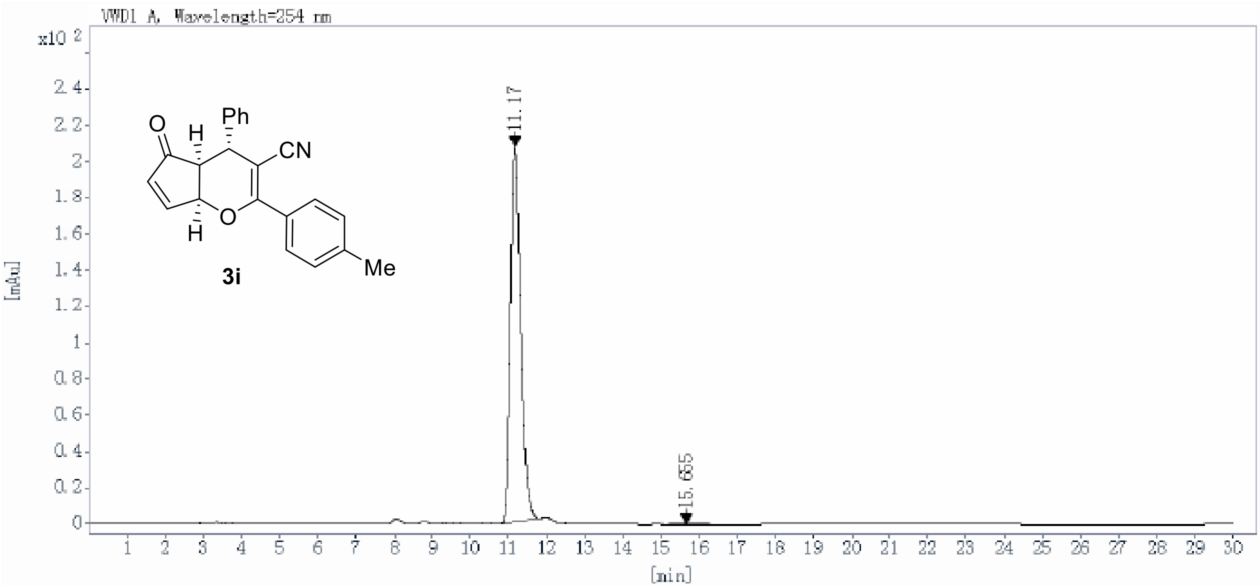
350.1155
145
Ph
CN
O
H
H
O
H_3C
3h
(ESI-TOF) m/z: [M + Na]$^+$
Calcd for $C_{22}H_{17}NO_2Na^+$ 350.1151
%
7
350.070
350.080
350.090
350.100
350.110
350.120
350.130
350.140
350.150
350.160
m/z


O
H
Ph
CN
H
O
Me
3i
¹H NMR (400 MHz, CDCl₃)
f1 (ppm)

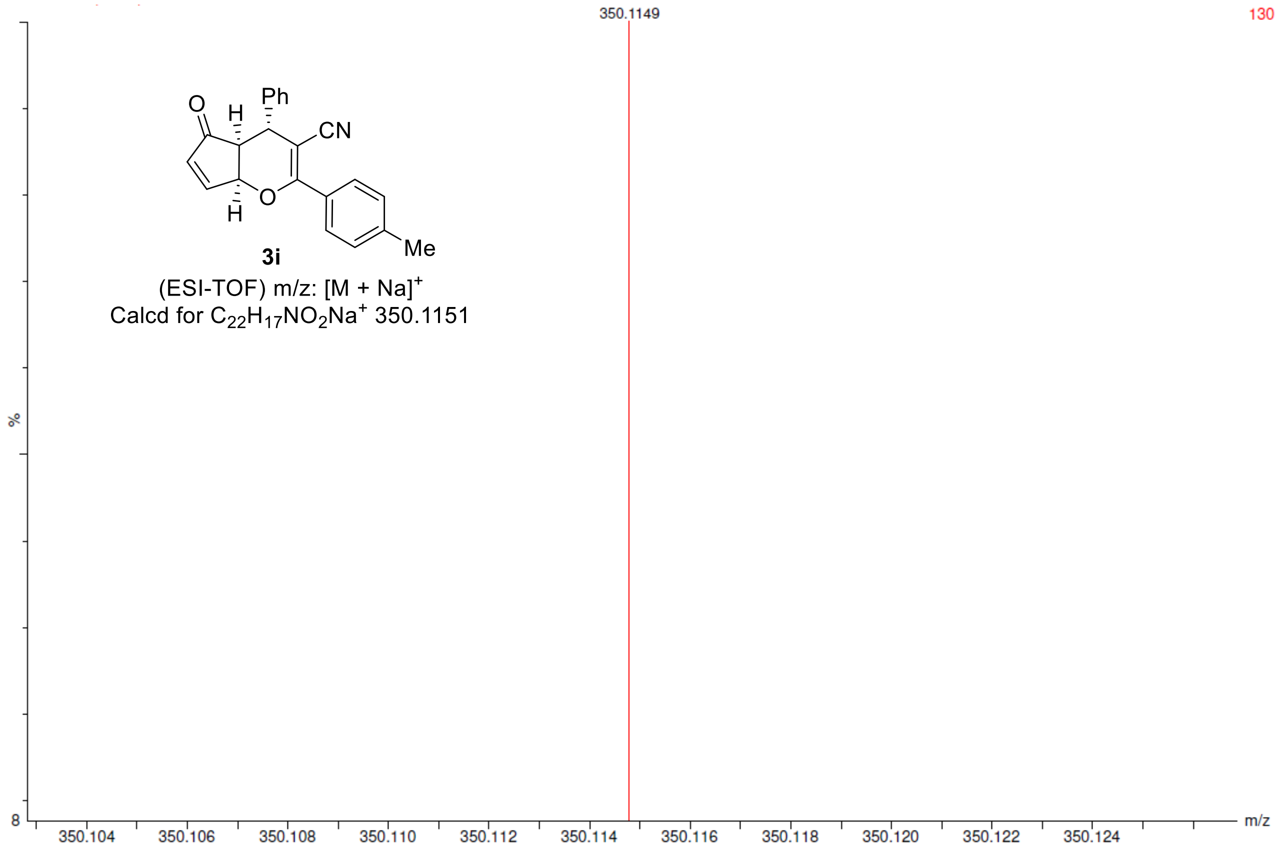

O
H
Ph
CN
H
O
Me
3i
¹³C NMR (100 MHz, CDCl₃)
f1 (ppm)

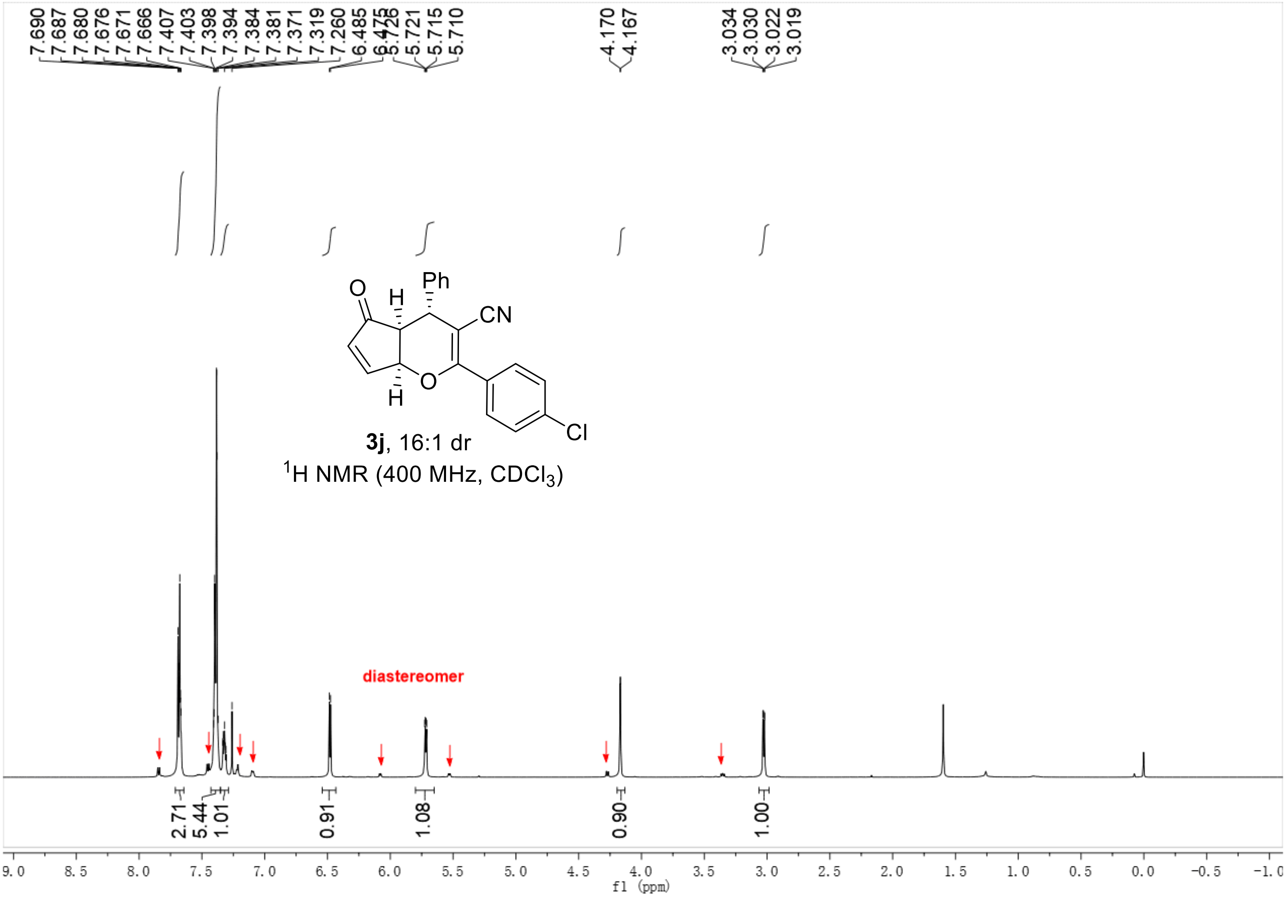


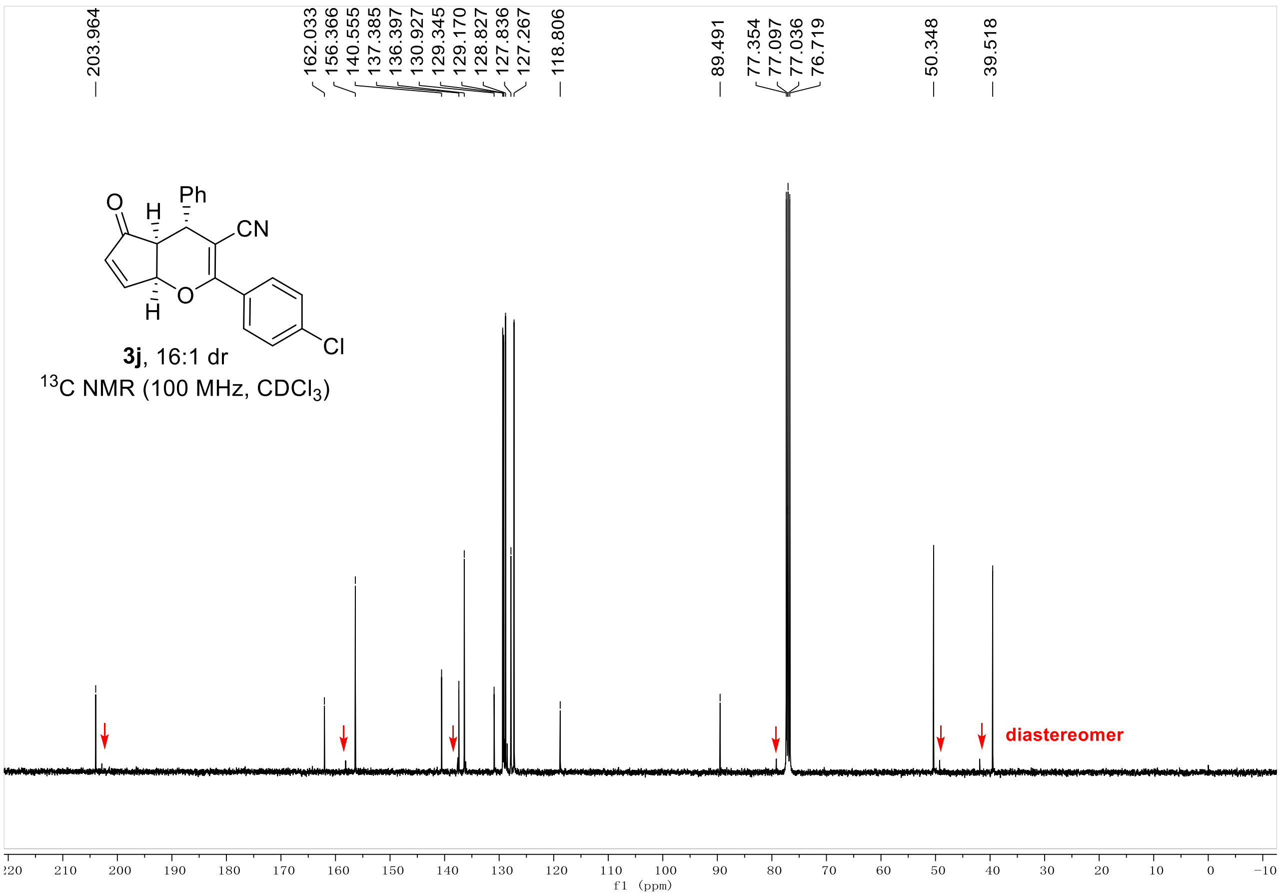
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
8.800	BV	0.22	963.5249	13632.5859	24.9895
9.653	VB	0.25	849.4219	13552.3447	24.8424
11.220	BB	0.27	769.3521	13612.4707	24.9526
15.842	BB	0.39	541.3206	13755.9268	25.2156
			Totals:	54553.3281	100.0000

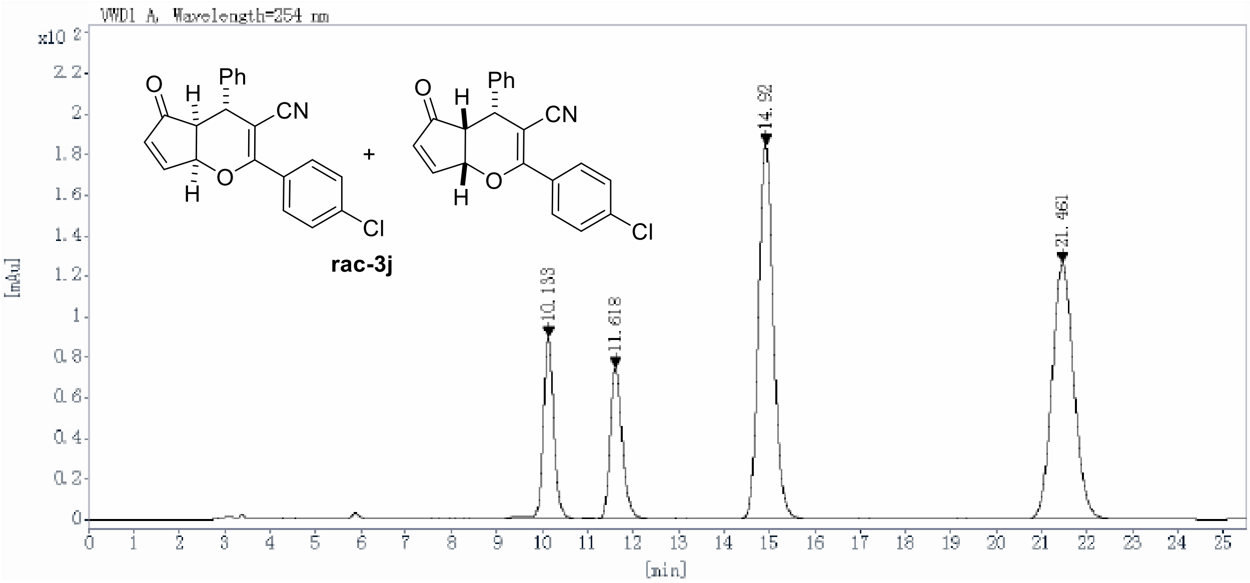


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
11.170	BB	0.28	207.1306	3820.0989	99.6766
15.655	BB	0.40	0.4610	12.3942	0.3234
			Totals:	3832.4931	100.0000

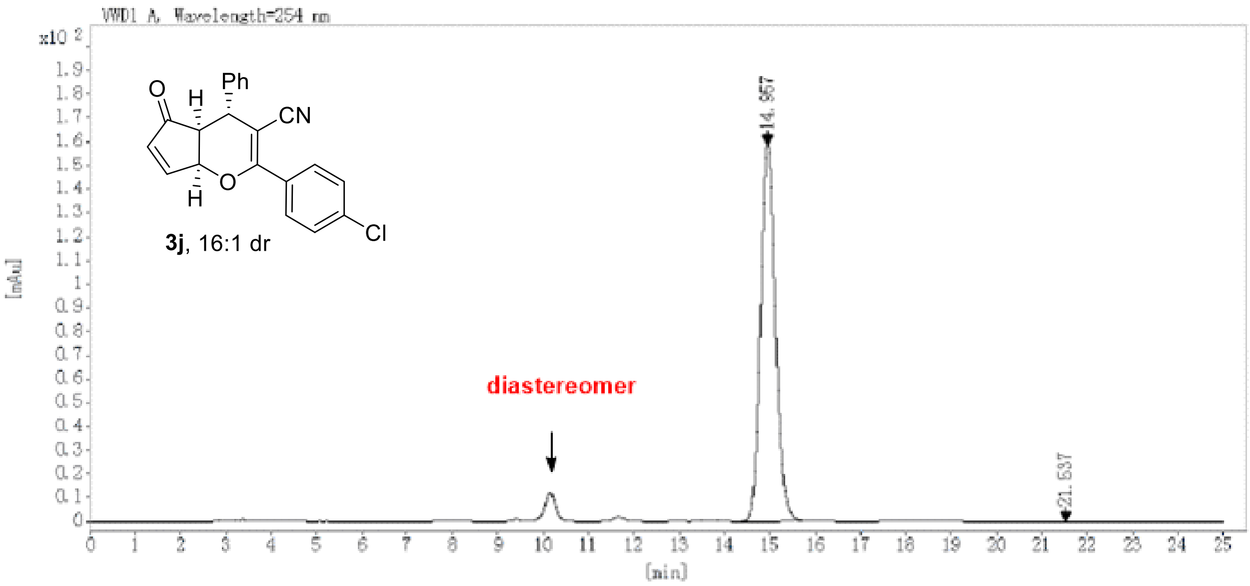

350.1149
130
Ph
H
O
CN
H
O
Me
3i
(ESI-TOF) m/z: [M + Na]+
Calcd for C22H17NO2Na+ 350.1151
%
8
350.104
350.106
350.108
350.110
350.112
350.114
350.116
350.118
350.120
350.122
350.124
m/z


7.690
7.687
7.680
7.676
7.671
7.666
7.407
7.403
7.398
7.394
7.384
7.381
7.371
7.319
7.260
6.485
6.475
5.726
5.721
5.715
5.710
4.170
4.167
3.034
3.030
3.022
3.019
Ph
CN
O
H
H
Cl
3j, 16:1 dr
^{1}H NMR (400 MHz, CDCl$_3$)
diastereomer
2.71
5.44
1.01
0.91
1.08
0.90
1.00
f1 (ppm)

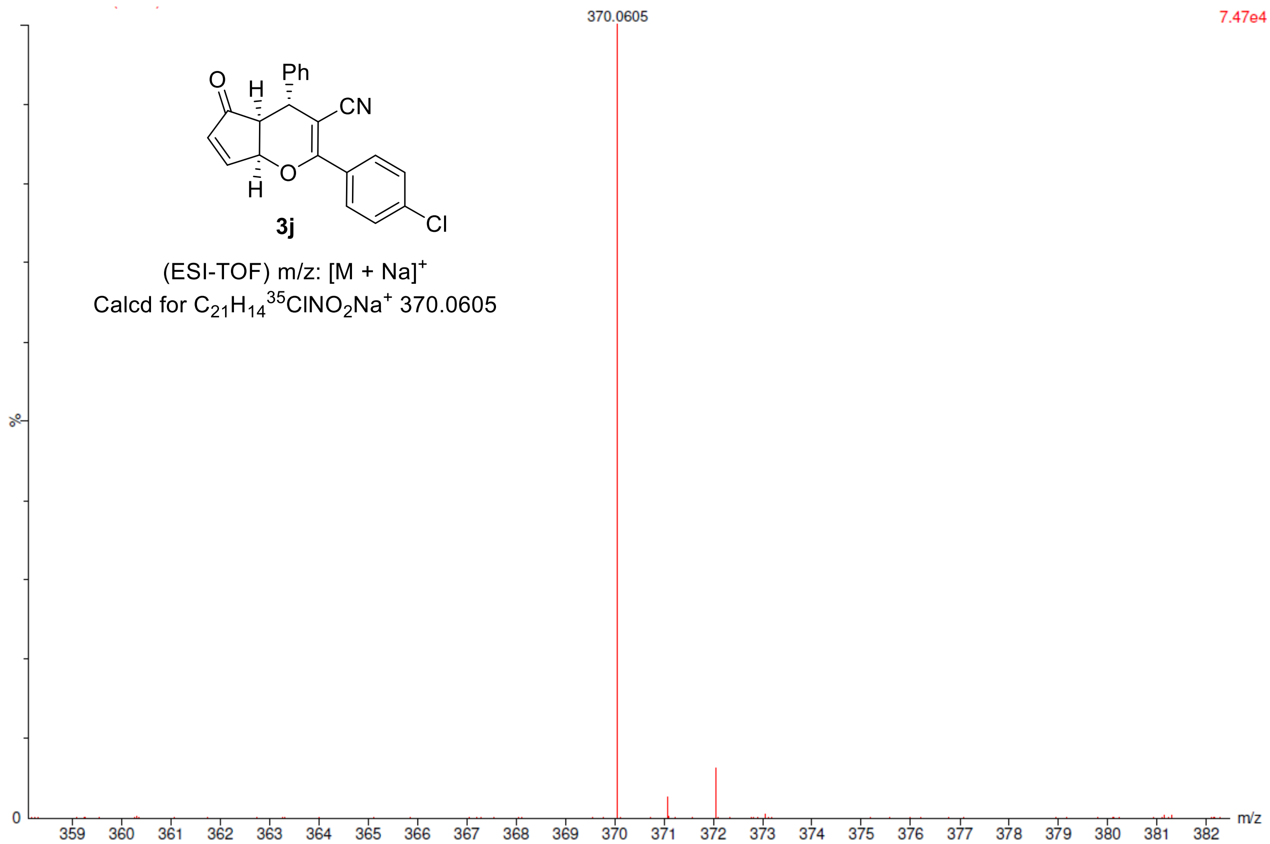

203.964
162.033
156.366
140.555
137.385
136.397
130.927
129.345
129.170
128.827
127.836
127.267
118.806
89.491
77.354
77.097
77.036
76.719
50.348
39.518
Ph
CN
O
H
H
Cl
3j, 16:1 dr
^{13}C NMR (100 MHz, CDCl$_3$)
diastereomer
f1 (ppm)

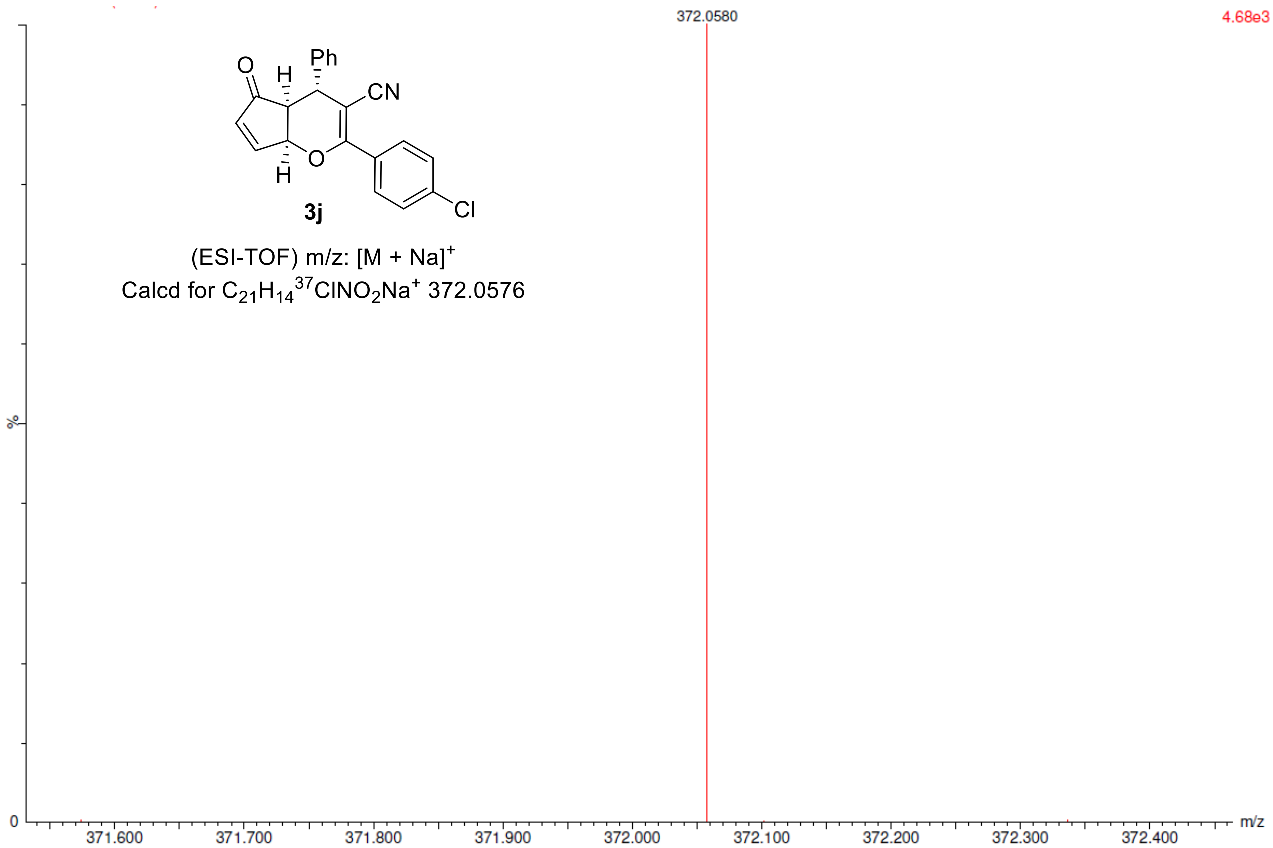


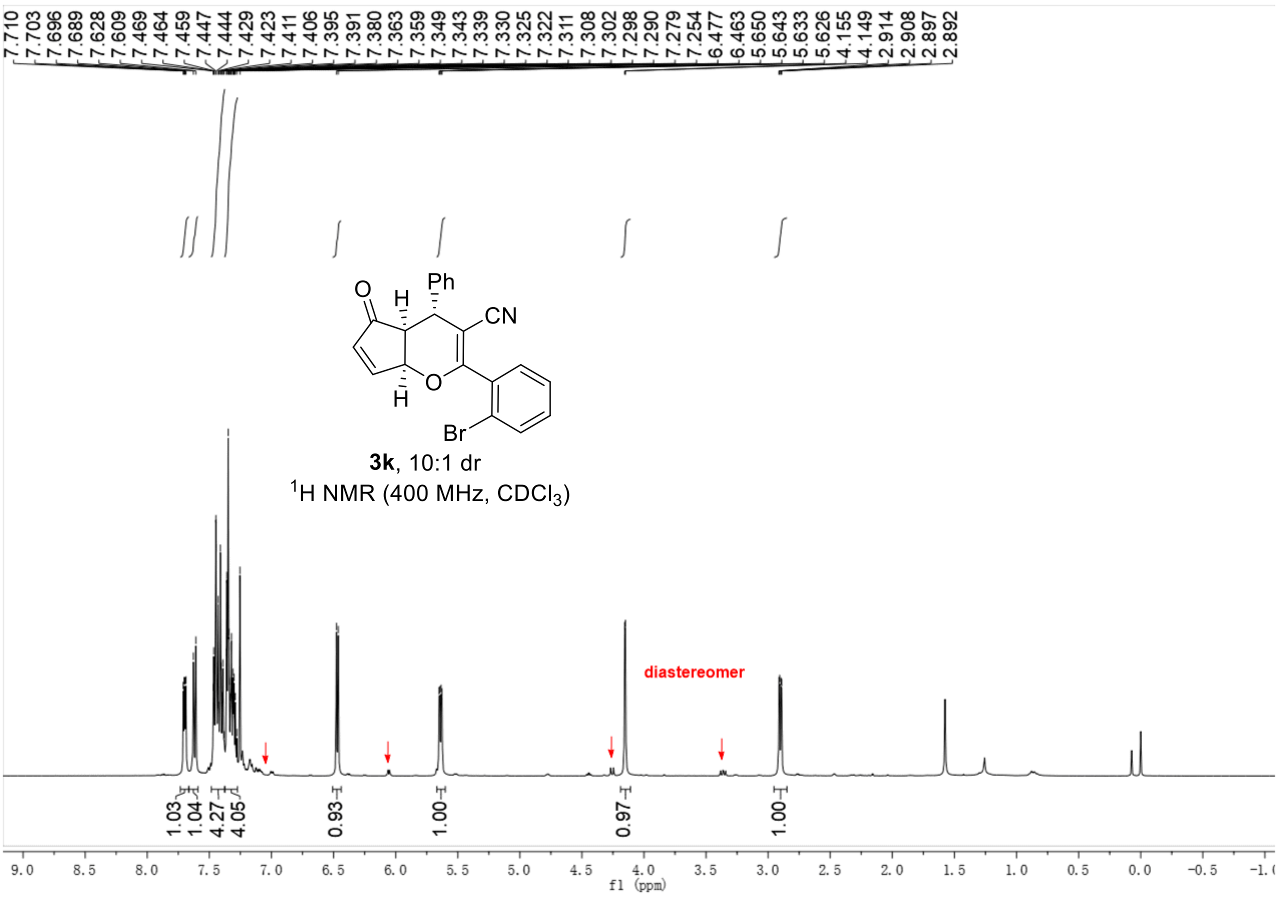
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
10.133	VB R	0.24	89.4702	1426.9749	12.6607
11.618	VB R	0.28	74.6380	1382.1534	12.2630
14.920	BB	0.35	184.5390	4235.5420	37.5794
21.461	BB	0.52	126.3961	4226.2314	37.4968
			Totals:	11270.9017	100.0000

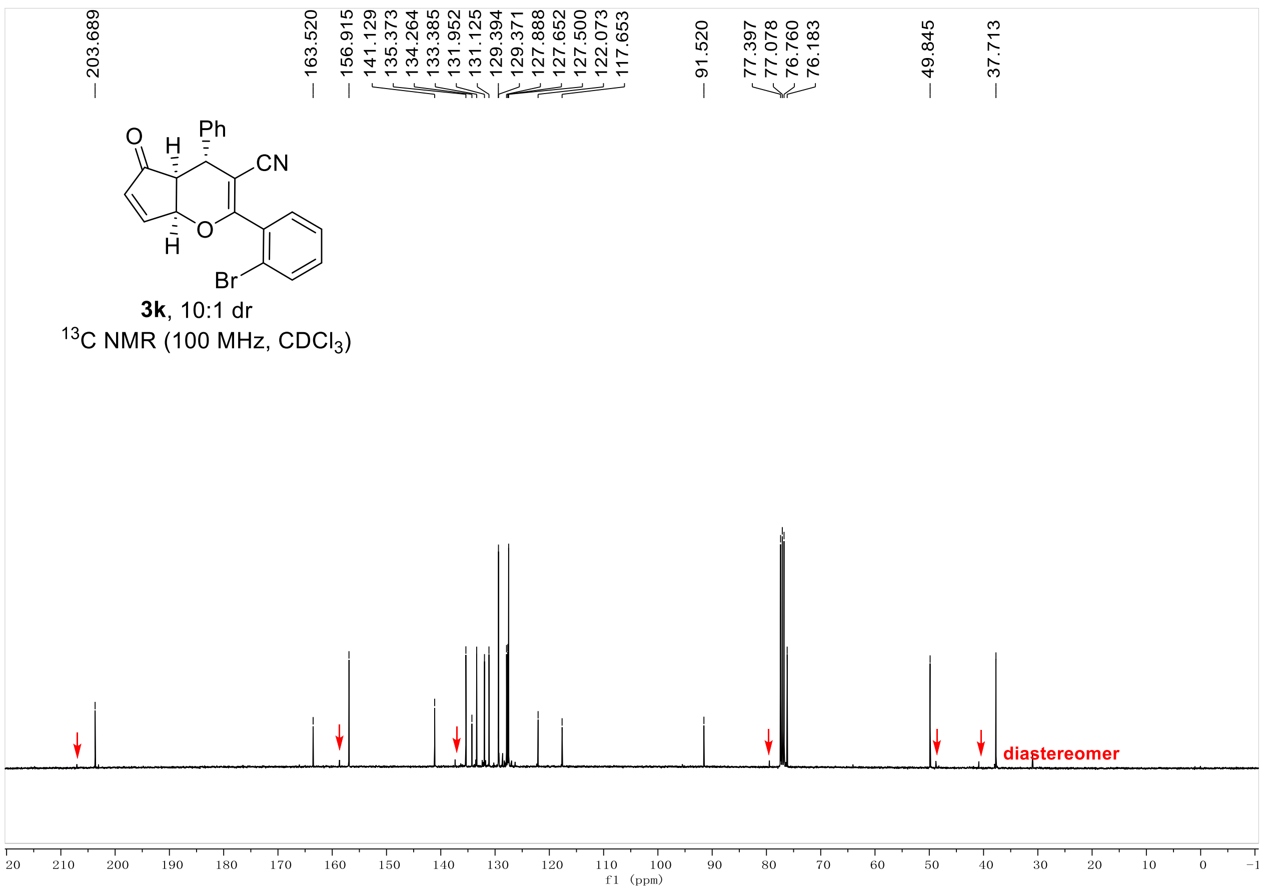


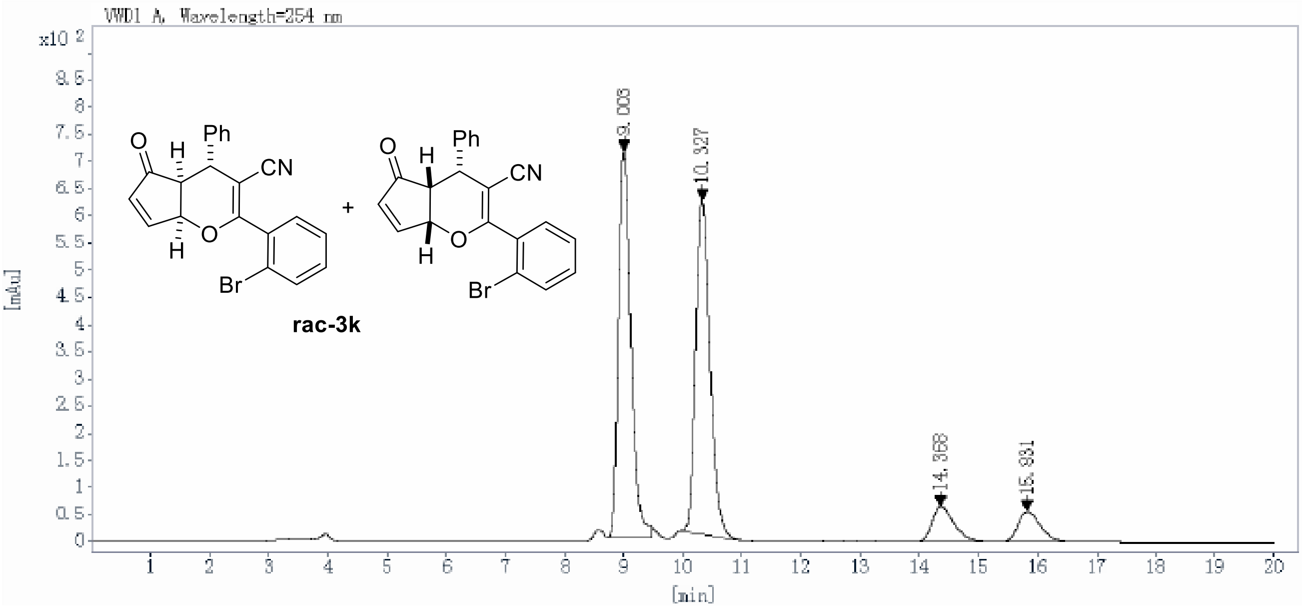
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
14.957	BB S	0.35	158.3622	3633.9900	99.9784
21.537	BB	0.30	0.0307	0.7857	0.0216
			Totals:	3634.7757	100.0000


370.0605
7.47e4
3j
(ESI-TOF) m/z: [M + Na]$^+$
Calcd for $C_{21}H_{14}{}^{35}ClNO_2Na^+$ 370.0605
%
m/z

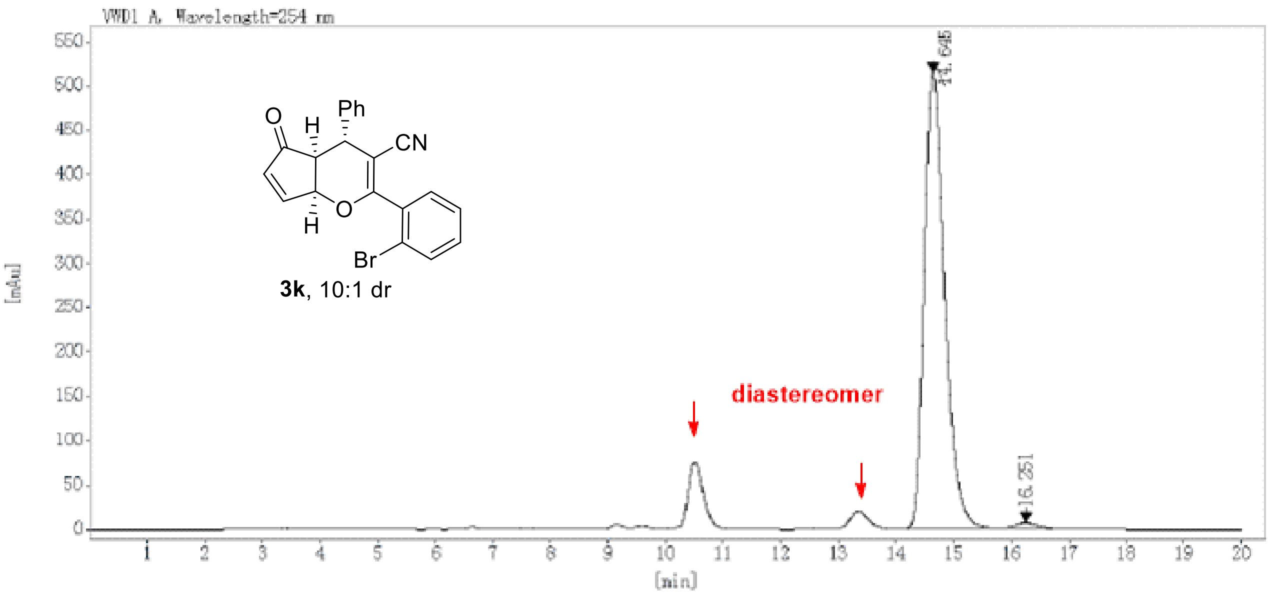

372.0580
4.68e3
3j
(ESI-TOF) m/z: [M + Na]$^+$
Calcd for $C_{21}H_{14}{}^{37}ClNO_2Na^+$ 372.0576
%
m/z


7.710
7.703
7.696
7.689
7.628
7.609
7.469
7.464
7.459
7.447
7.444
7.429
7.423
7.411
7.406
7.395
7.391
7.380
7.363
7.359
7.349
7.343
7.339
7.330
7.325
7.322
7.311
7.308
7.302
7.298
7.290
7.279
7.254
6.477
6.463
5.650
5.643
5.633
5.626
4.155
4.149
2.914
2.908
2.897
2.892
Ph
O
H
CN
H
O
Br
3k, 10:1 dr
^{1}H NMR (400 MHz, $CDCl_3$)
diastereomer
1.03
1.04
4.27
4.05
0.93
1.00
0.97
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

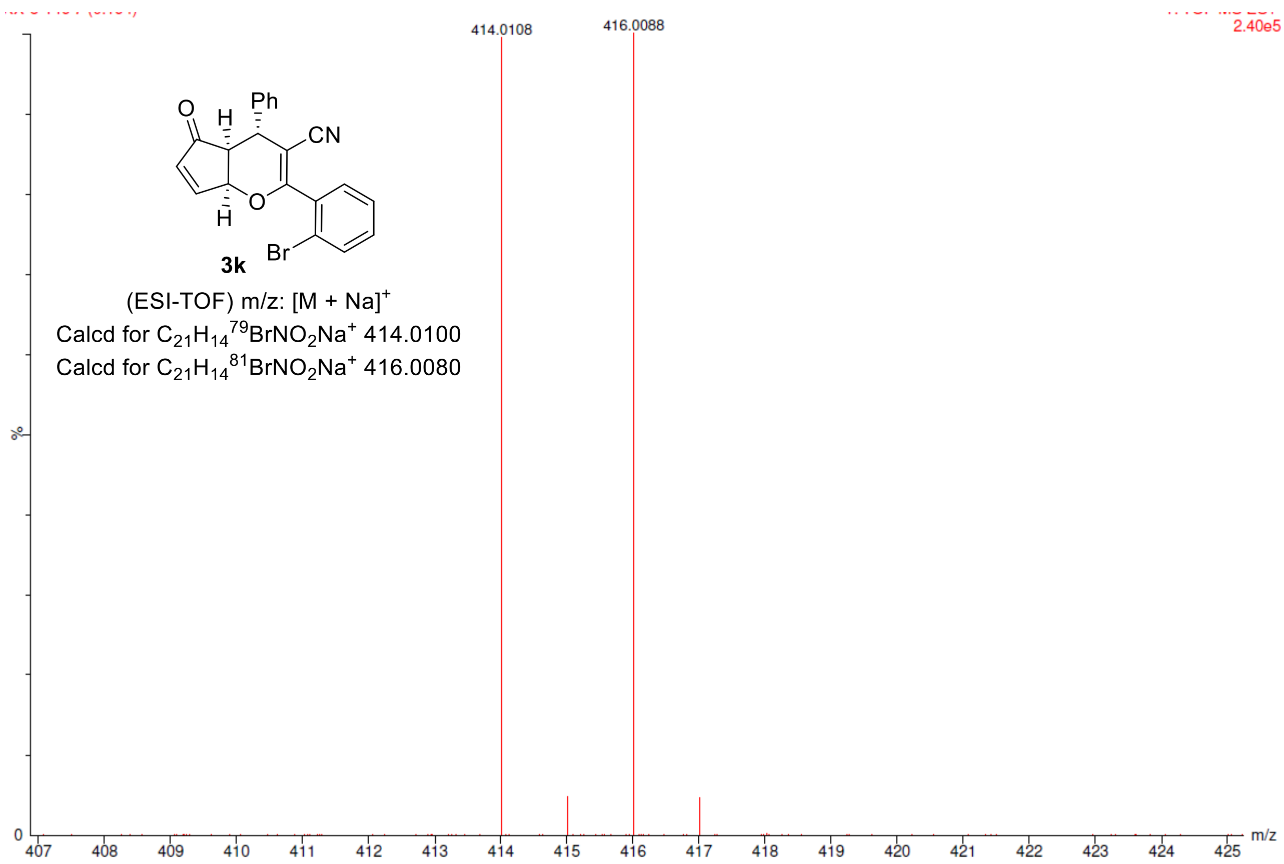

203.689
163.520
156.915
141.129
135.373
134.264
133.385
131.952
131.125
129.394
129.371
127.888
127.652
127.500
122.073
117.653
91.520
77.397
77.078
76.760
76.183
49.845
37.713
Ph
O
H
CN
H
O
Br
3k, 10:1 dr
^{13}C NMR (100 MHz, $CDCl_3$)
diastereomer
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

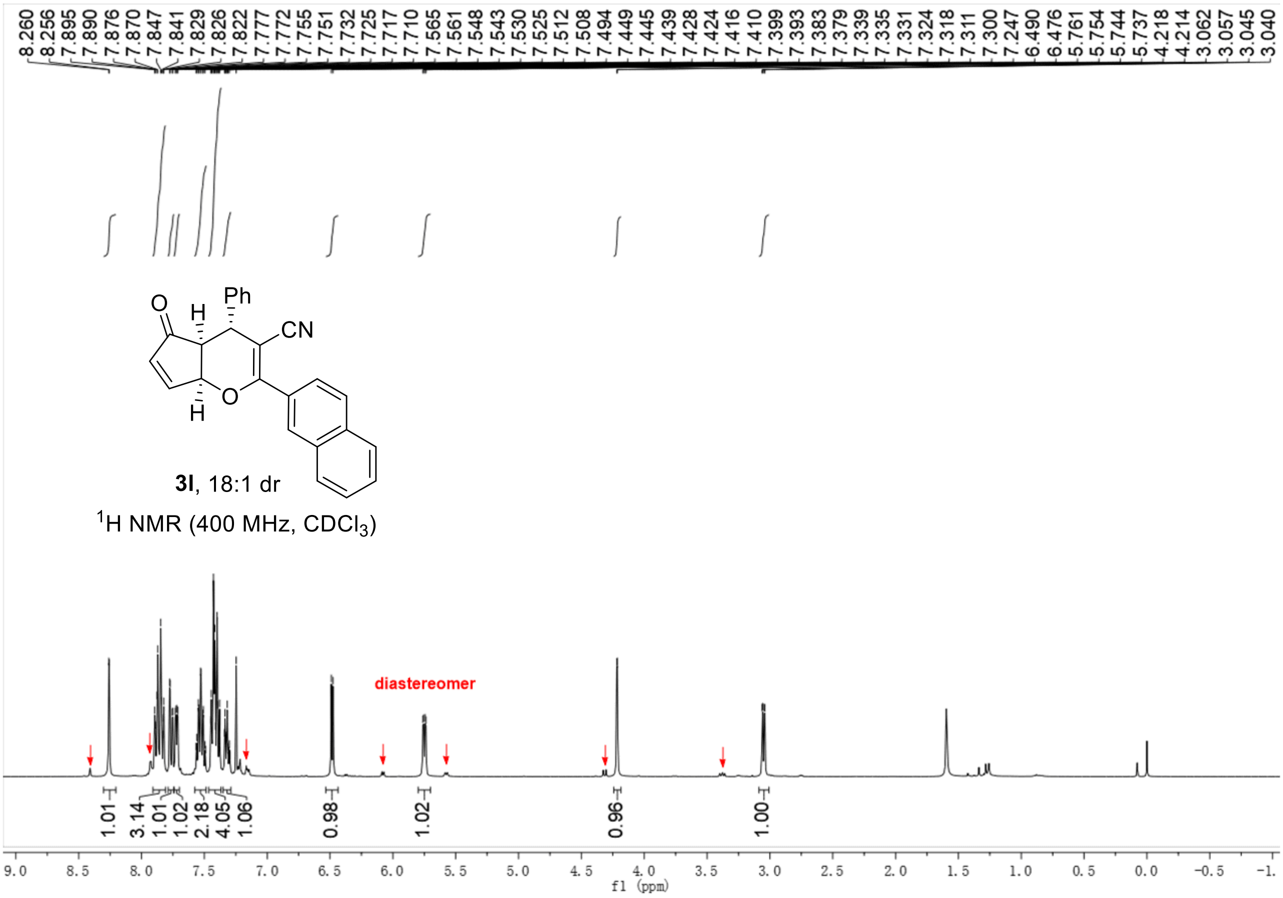


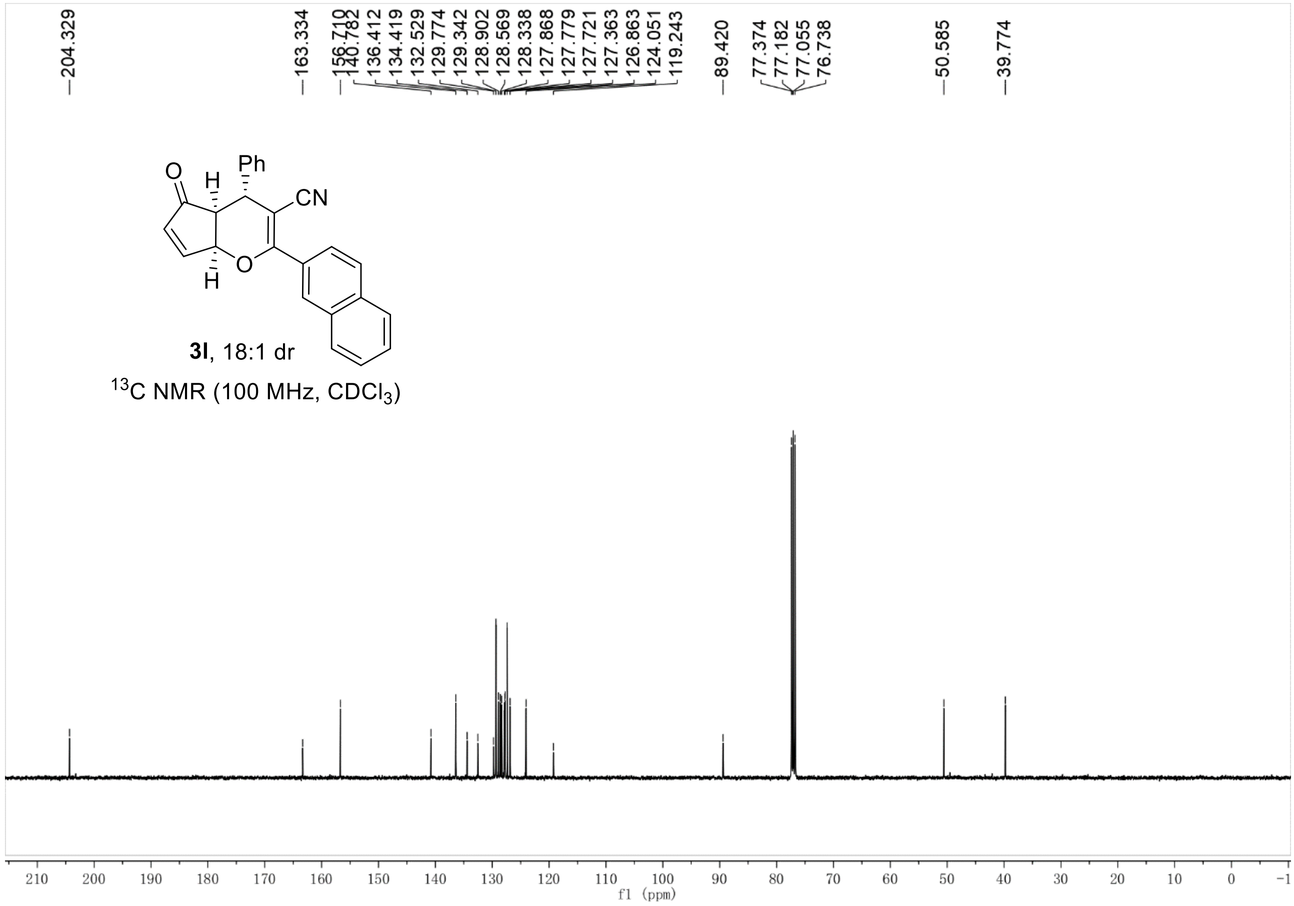
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
9.003	BBAS	0.22	710.2631	10358.5703	43.3062
10.327	BBA	0.26	613.9765	10333.4502	43.2012
14.368	BV	0.39	65.9368	1712.9633	7.1614
15.831	VBA	0.41	56.6327	1514.3987	6.3313

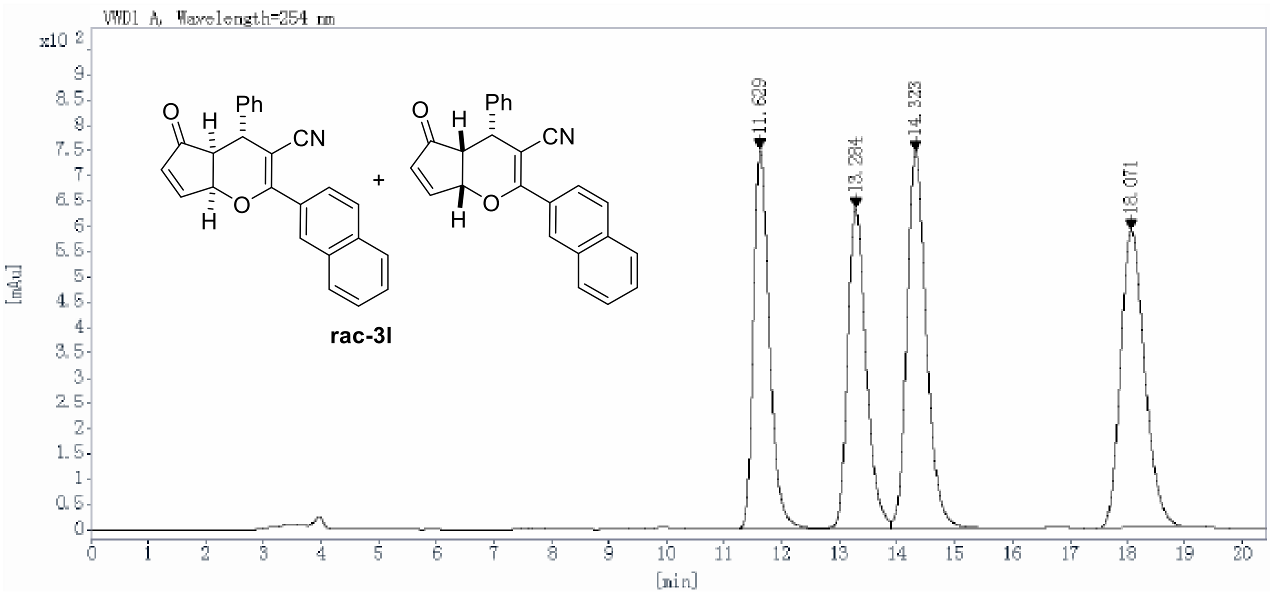


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
14.645	BB	0.38	515.1614	12695.1729	98.6395
16.251	BB	0.42	6.4664	175.0968	1.3605
			Totals:	12870.2697	100.0000

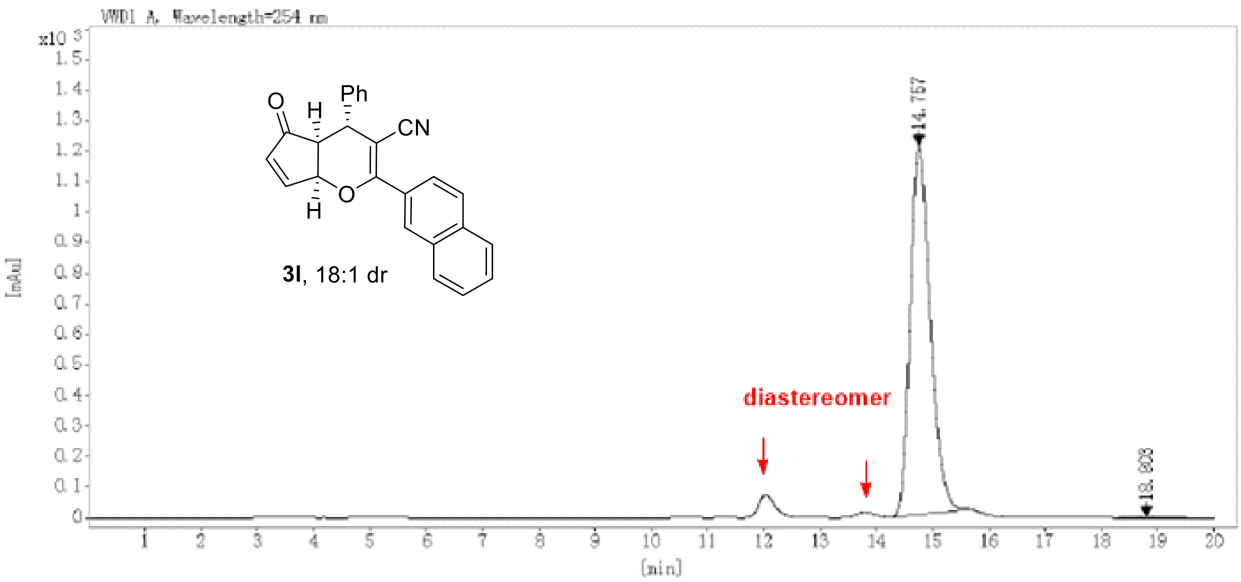

414.0108
416.0088
2.40e5
3k
(ESI-TOF) m/z: [M + Na]+
Calcd for $C_{21}H_{14}{}^{79}BrNO_2Na^+$ 414.0100
Calcd for $C_{21}H_{14}{}^{81}BrNO_2Na^+$ 416.0080
%
0
407 408 409 410 411 412 413 414 415 416 417 418 419 420 421 422 423 424 425
m/z


8.260 8.256 7.895 7.890 7.876 7.870 7.847 7.841 7.829 7.826 7.822 7.777 7.772 7.755 7.751 7.732 7.725 7.717 7.710 7.565 7.561 7.548 7.543 7.530 7.525 7.512 7.508 7.494 7.449 7.445 7.439 7.428 7.424 7.416 7.410 7.399 7.393 7.383 7.379 7.339 7.335 7.331 7.324 7.318 7.311 7.300 7.247 6.490 6.476 5.761 5.754 5.744 5.737 4.218 4.214 3.062 3.057 3.045 3.040
O
H
Ph
CN
O
H
3l, 18:1 dr
^{1}H NMR (400 MHz, $CDCl_3$)
diastereomer
1.01 3.14 1.01 1.02 2.18 4.05 1.06 0.98 1.02 0.96 1.00
f1 (ppm)

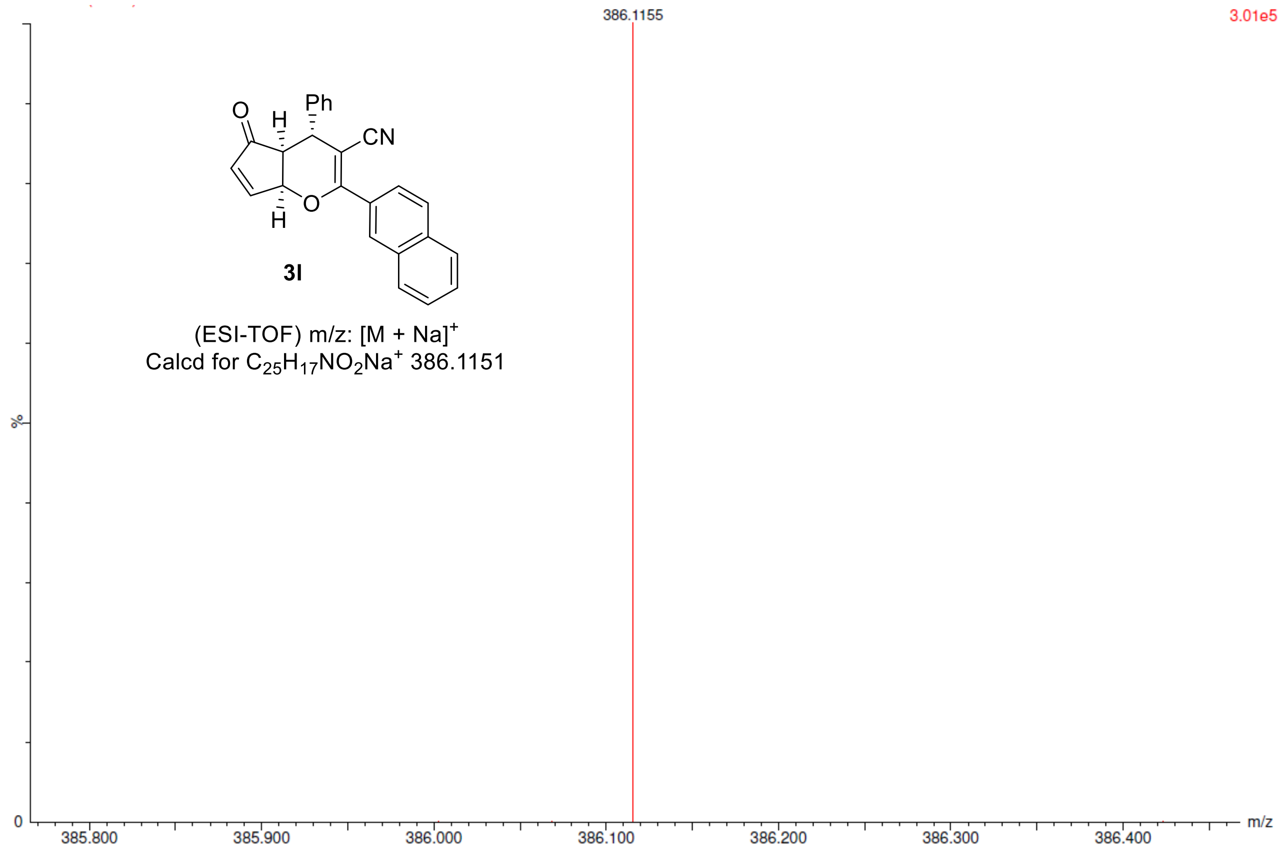

204.329 163.334 156.710 140.782 136.412 134.419 132.529 129.774 129.342 128.902 128.569 128.338 127.868 127.779 127.721 127.363 126.863 124.051 119.243 89.420 77.374 77.182 77.055 76.738 50.585 39.774
O
H
Ph
CN
O
H
3l, 18:1 dr
^{13}C NMR (100 MHz, $CDCl_3$)
f1 (ppm)



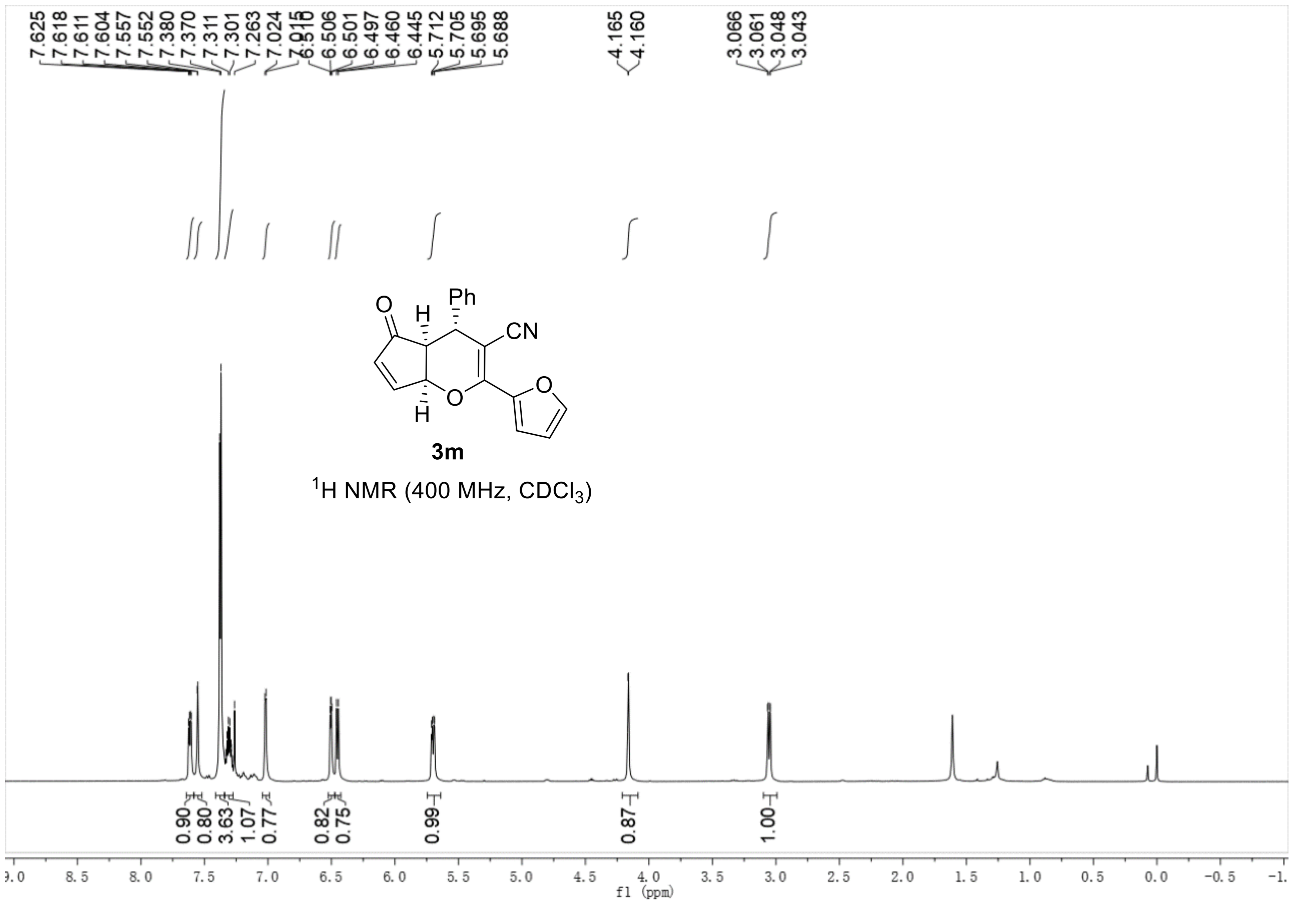
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
11.629	BV	0.30	750.8439	14501.5811	22.7894
13.284	VV	0.34	634.7147	14269.2510	22.4243
14.323	VB	0.36	747.1033	17743.6133	27.8843
18.071	BBA	0.45	587.5760	17118.5625	26.9020
			Totals:	63633.0078	100.0000

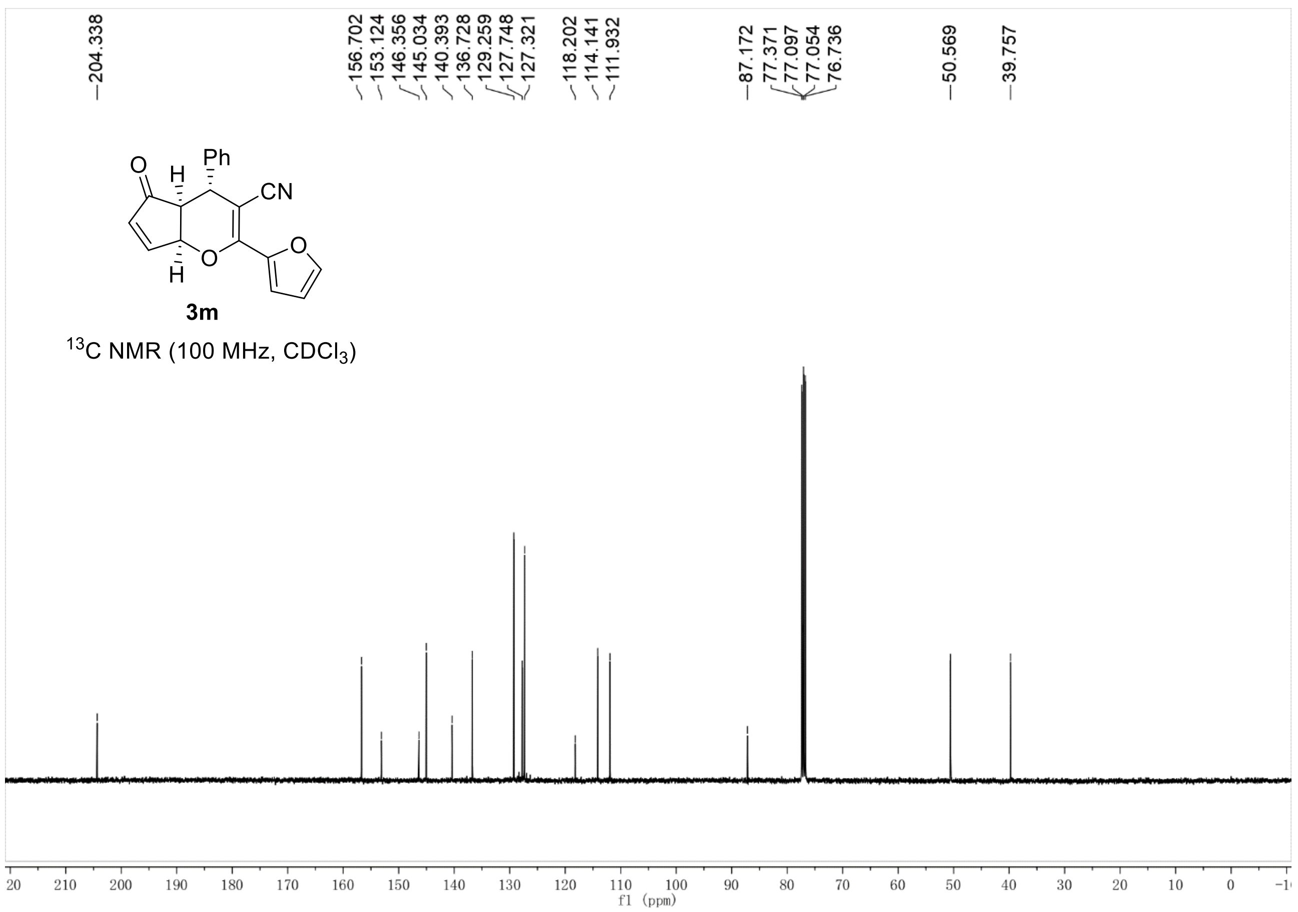


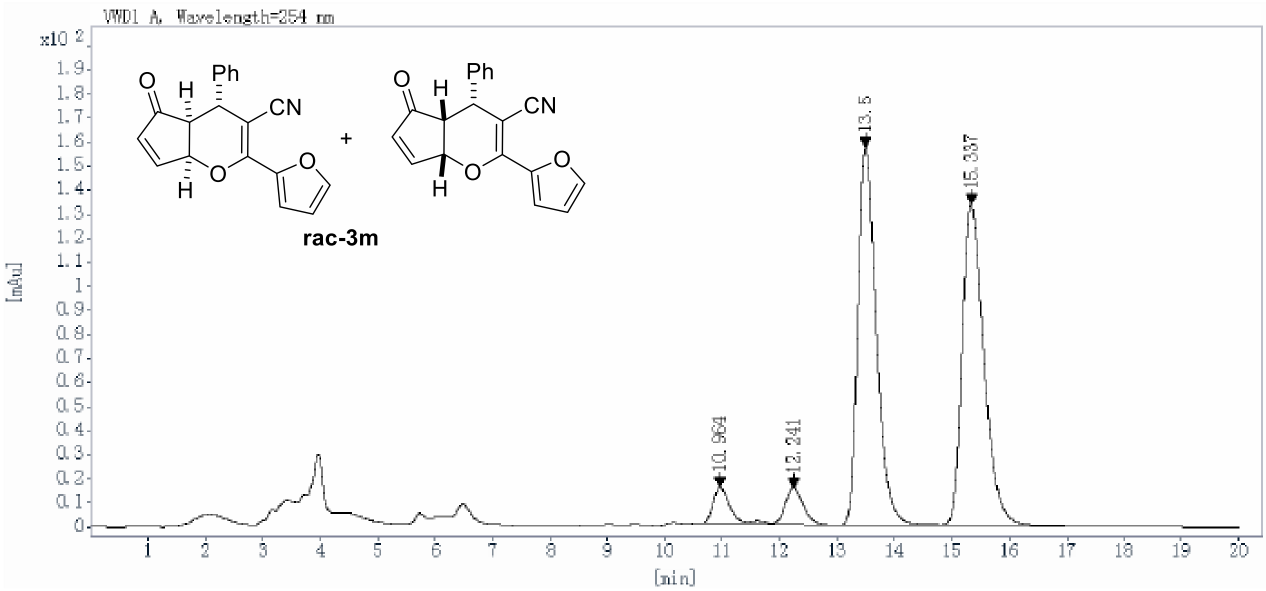
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
14.757	BBA	0.38	1205.6920	29927.0566	99.5783
18.803	BBA	0.50	3.7966	126.7469	0.4217
			Totals:	30053.8035	100.0000



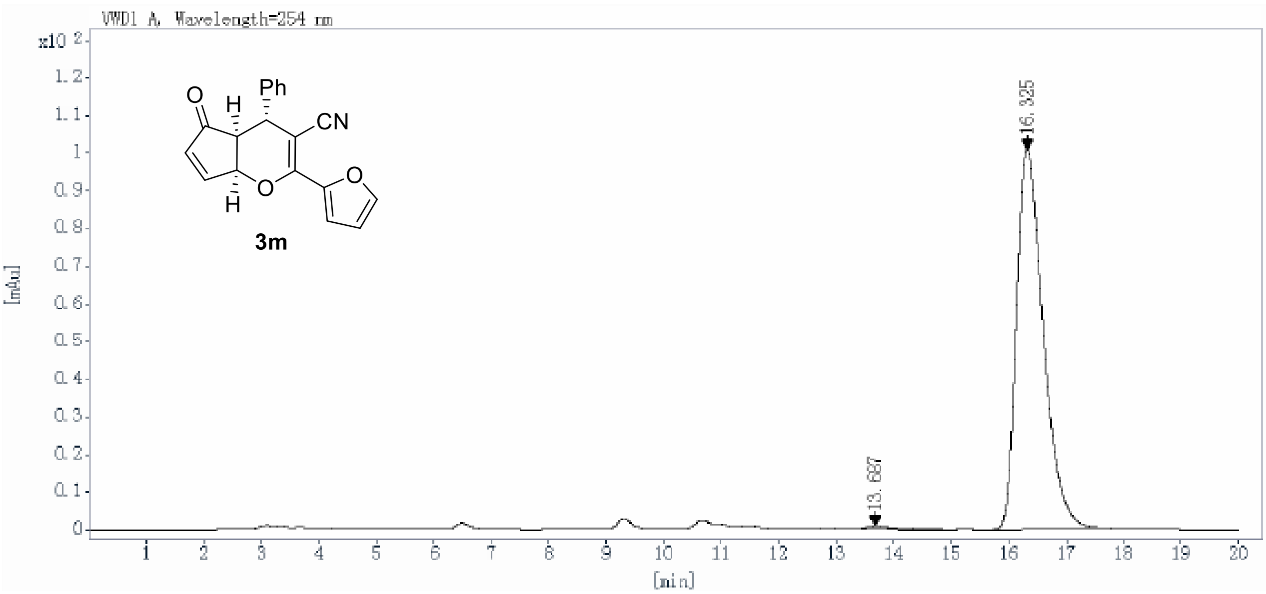
386.1155
3.01e5
O
H
Ph
CN
H
O
3l
(ESI-TOF) m/z: [M + Na]+
Calcd for C25H17NO2Na+ 386.1151
%
0
385.800
385.900
386.000
386.100
386.200
386.300
386.400
m/z


7.625
7.618
7.611
7.604
7.557
7.552
7.380
7.370
7.311
7.301
7.263
7.024
7.015
6.510
6.506
6.501
6.497
6.460
6.445
5.712
5.705
5.695
5.688
4.165
4.160
3.066
3.061
3.048
3.043
O
H
Ph
CN
O
H
O
3m
^{1}H NMR (400 MHz, $CDCl_3$)
0.90
0.80
3.63
1.07
0.77
0.82
0.75
0.99
0.87
1.00
f1 (ppm)

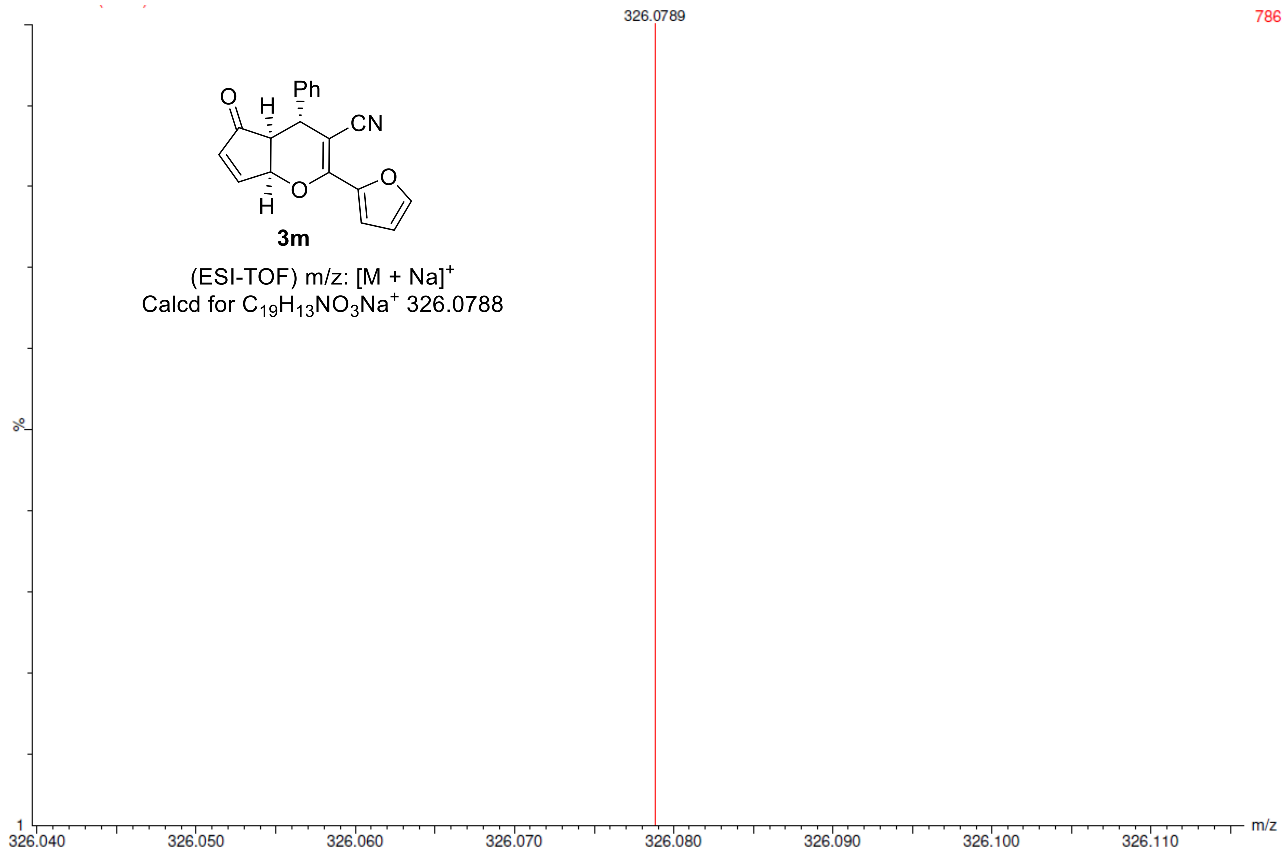

204.338
156.702
153.124
146.356
145.034
140.393
136.728
129.259
127.748
127.321
118.202
114.141
111.932
87.172
77.371
77.097
77.054
76.736
50.569
39.757
O
H
Ph
CN
O
H
O
3m
^{13}C NMR (100 MHz, $CDCl_3$)
f1 (ppm)



Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
10.964	BV R	0.33	15.2030	332.0816	4.3063
12.241	VB	0.34	15.3141	336.7136	4.3664
13.500	BB	0.34	156.7655	3516.8328	45.6050
15.337	BBA	0.41	133.5784	3525.8833	45.7223
			Totals:	7711.5112	100.0000

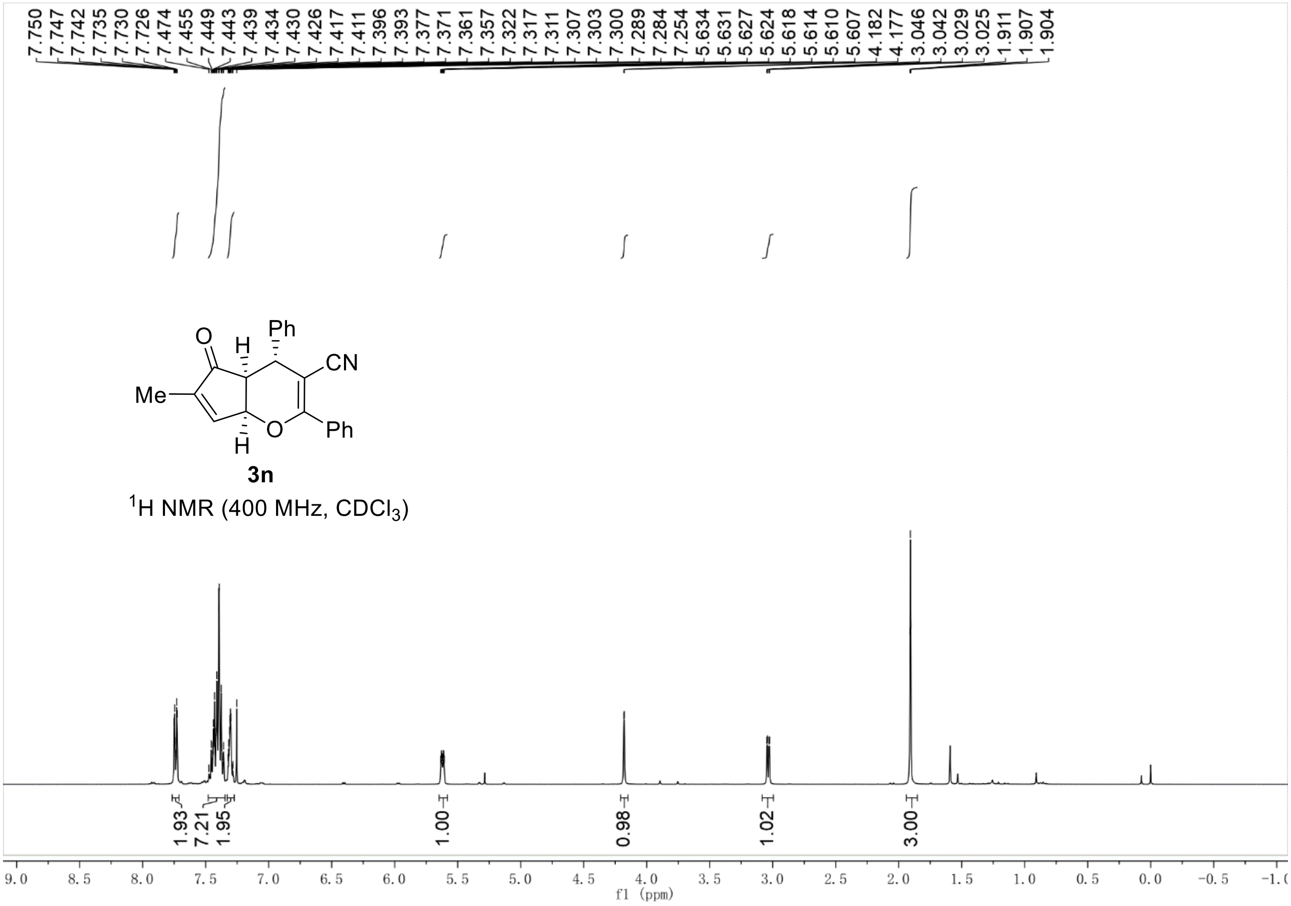


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
13.687	BBA	0.54	0.8300	31.0941	0.9445
16.325	BBA	0.50	100.7077	3261.1772	99.0555
			Totals:	3292.2713	100.0000



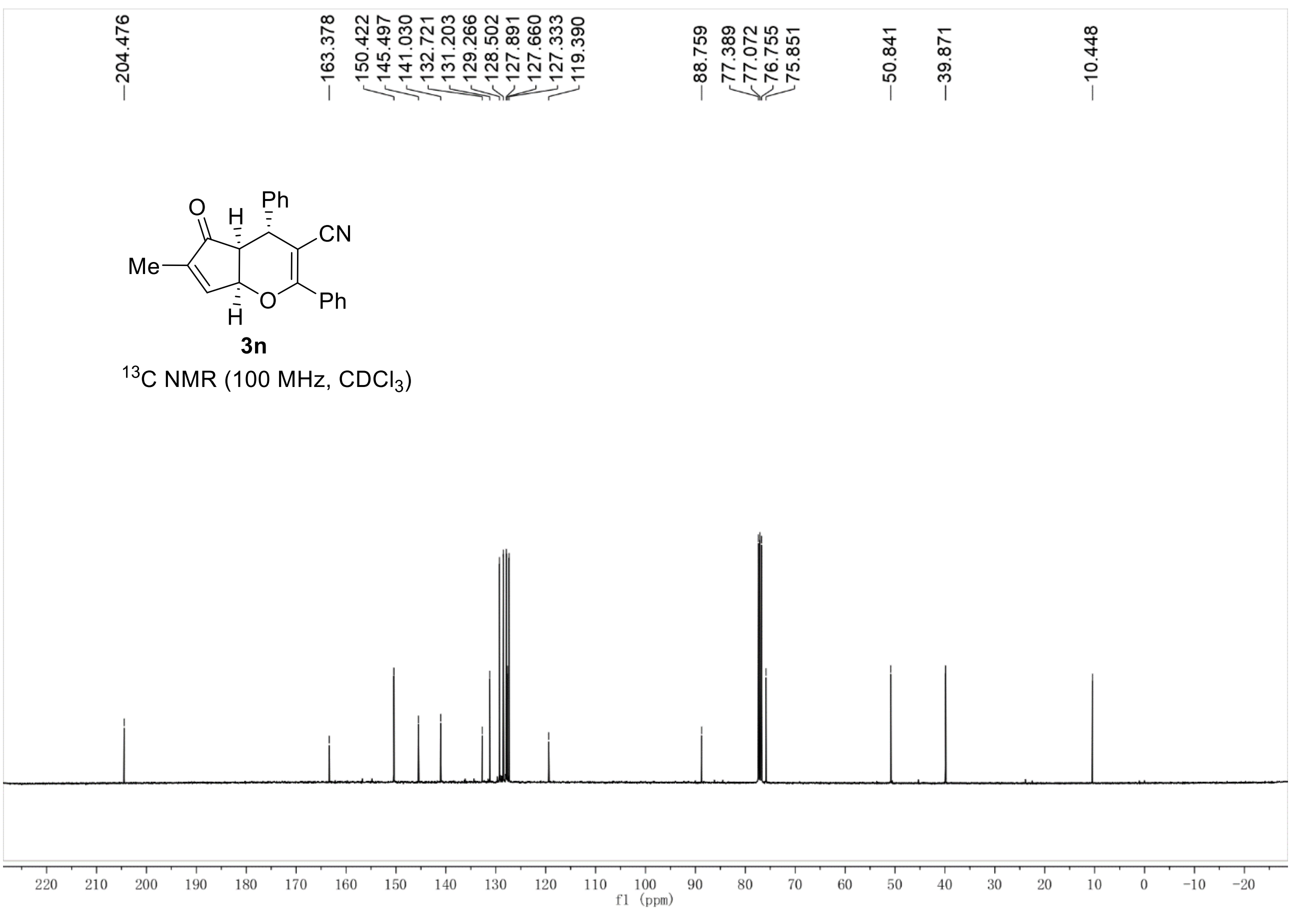
3m

(ESI-TOF) m/z: $[M + Na]^+$
Calcd for $C_{19}H_{13}NO_3Na^+$ 326.0788



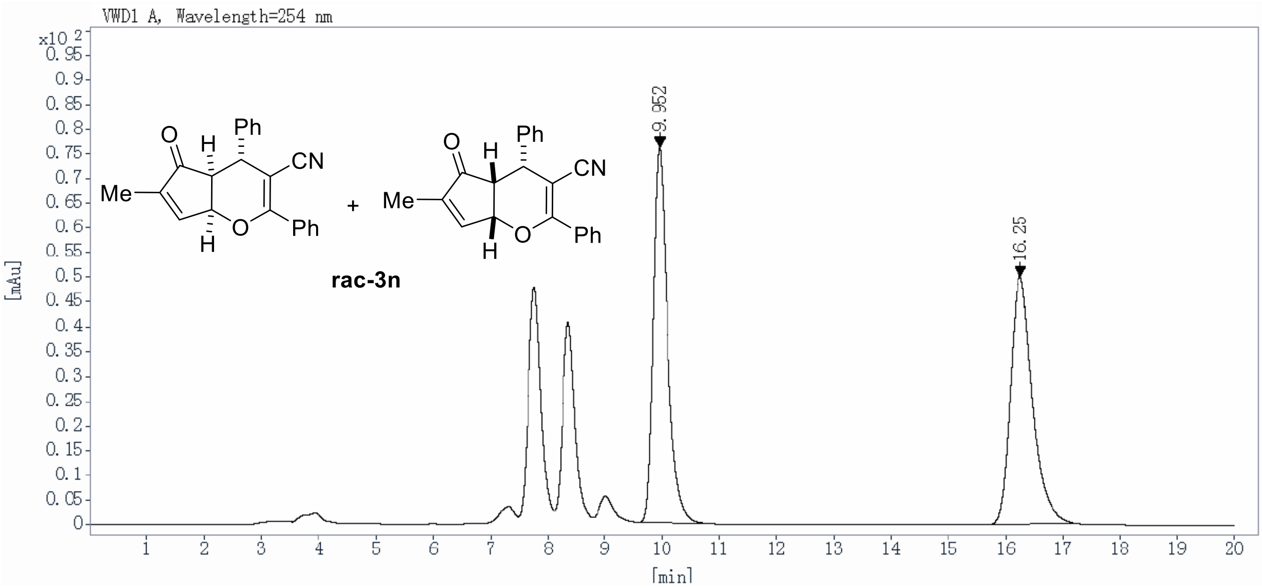
3n

^1H NMR (400 MHz, $CDCl_3$)

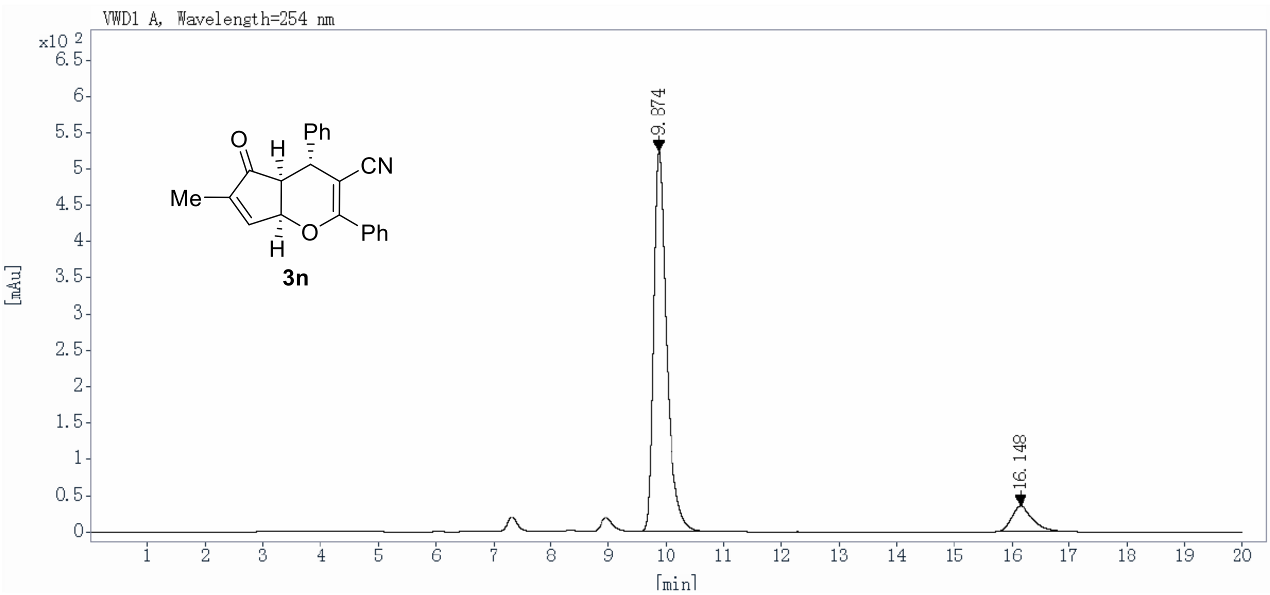


3n

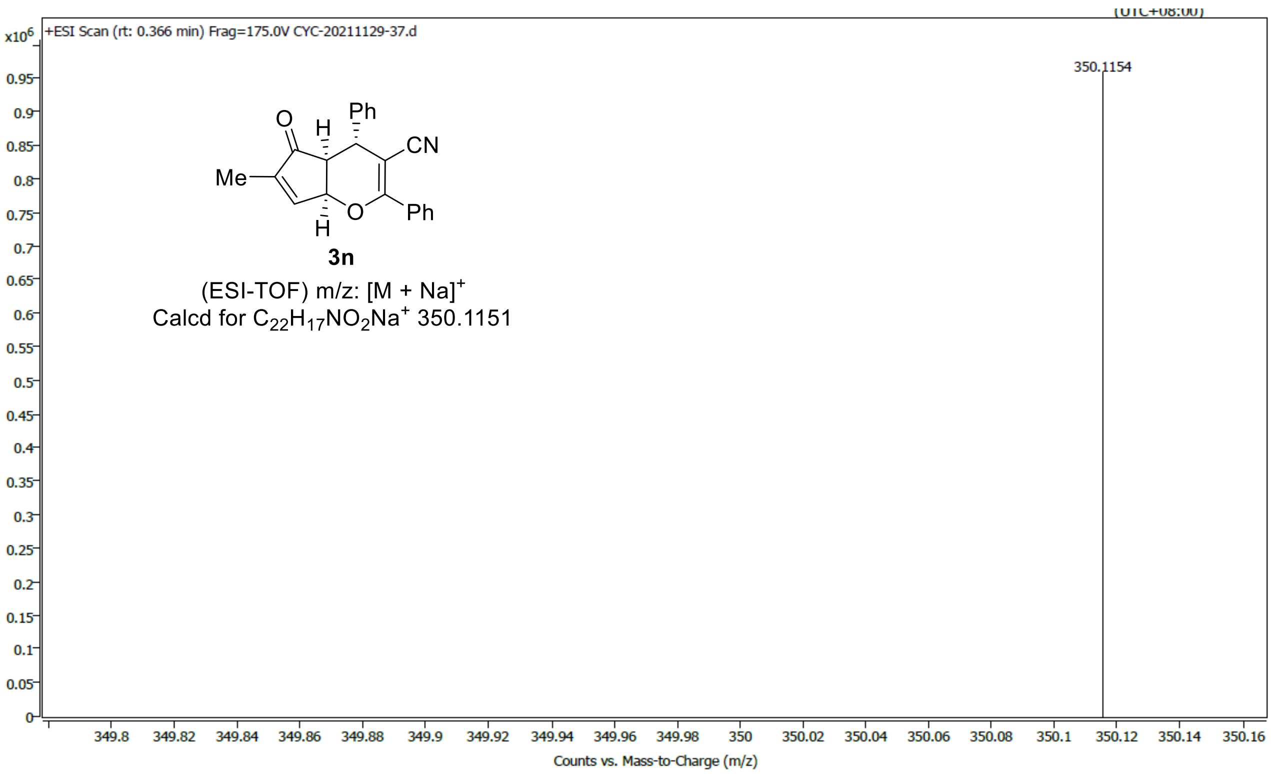
^{13}C NMR (100 MHz, $CDCl_3$)

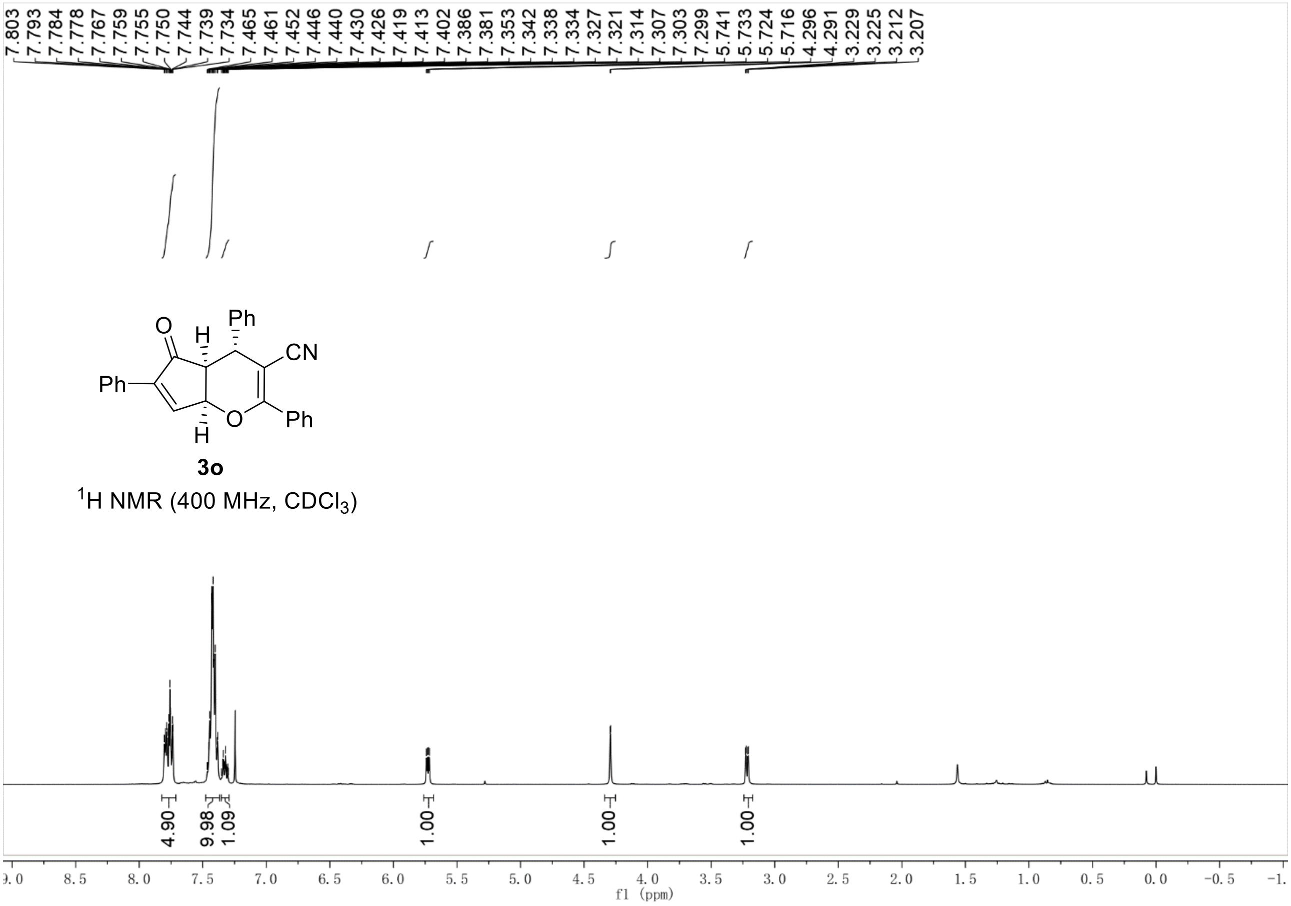


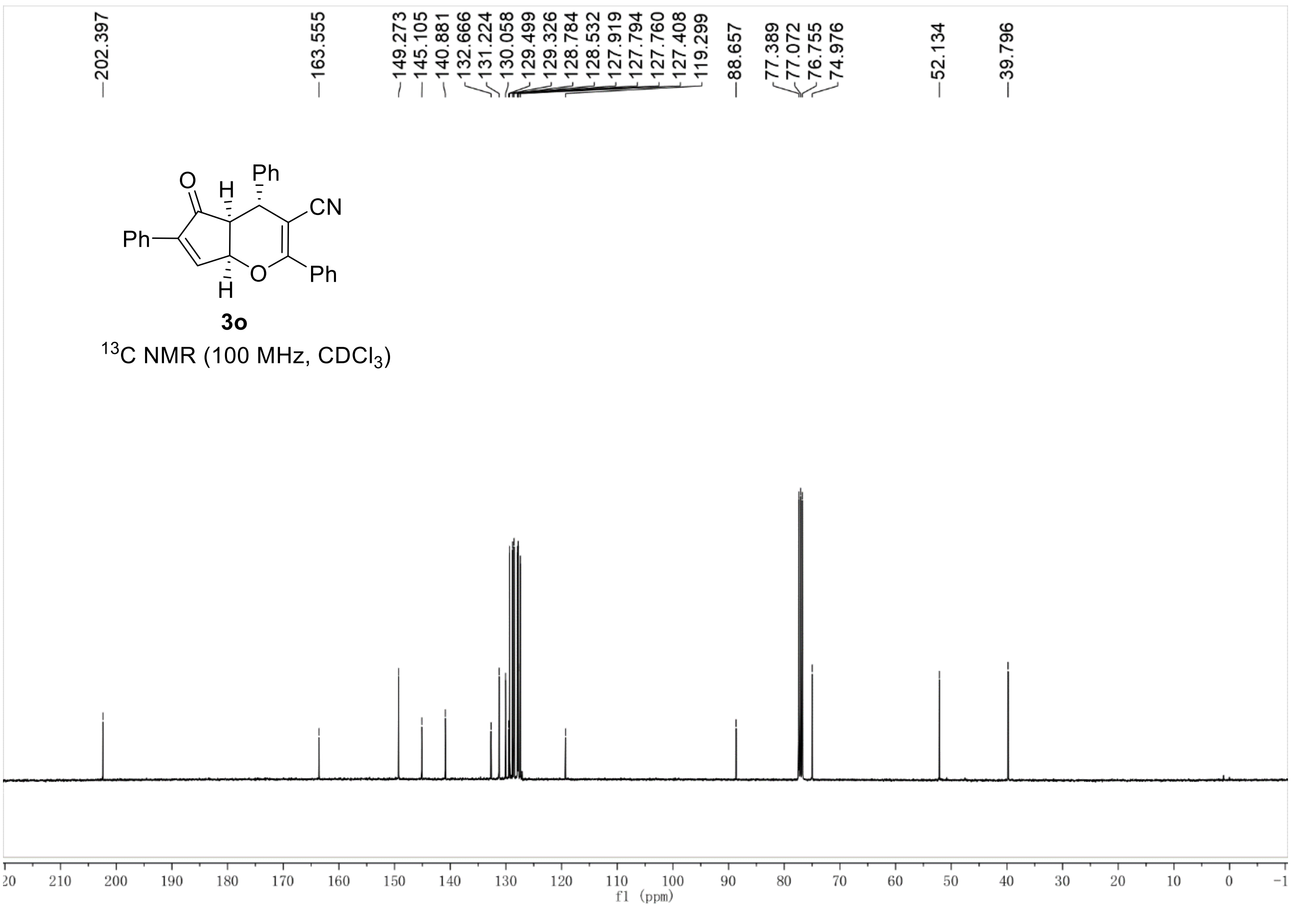
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
9.952	BBA	0.26	76.0133	1316.4818	49.5884
16.250	BBA	0.41	50.0722	1338.3352	50.4116
			Totals:	2654.8170	100.0000

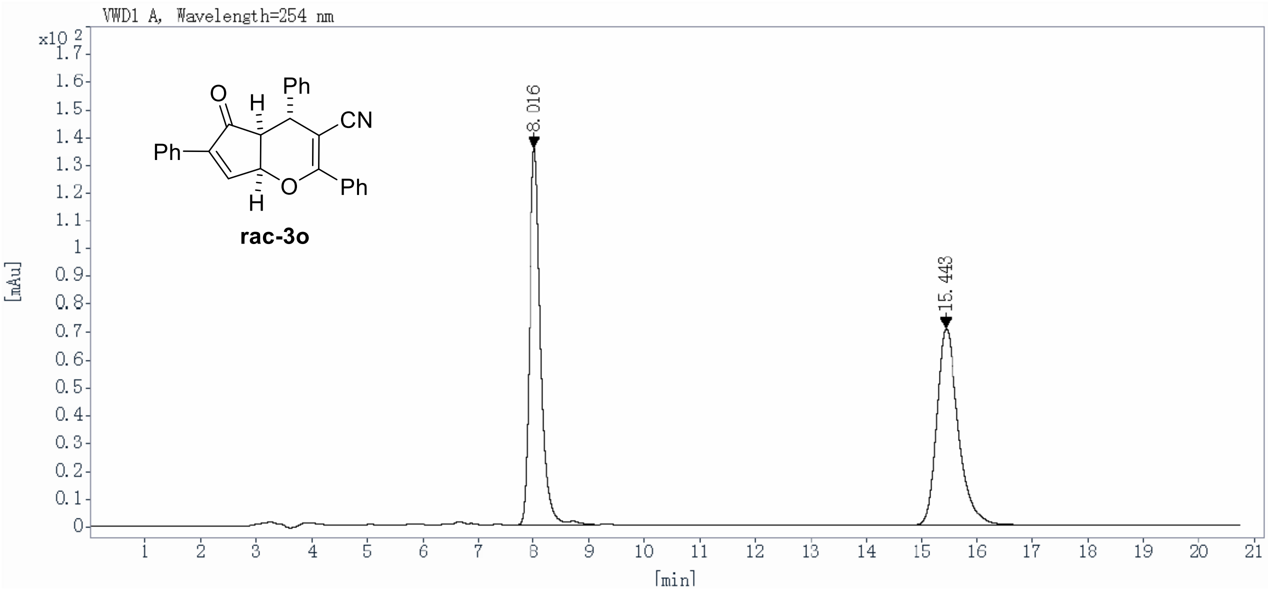


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
9.874	BBA	0.23	524.3347	8095.6279	90.3292
16.148	BBA	0.37	35.4706	866.7331	9.6708
			Totals:	8962.3610	100.0000

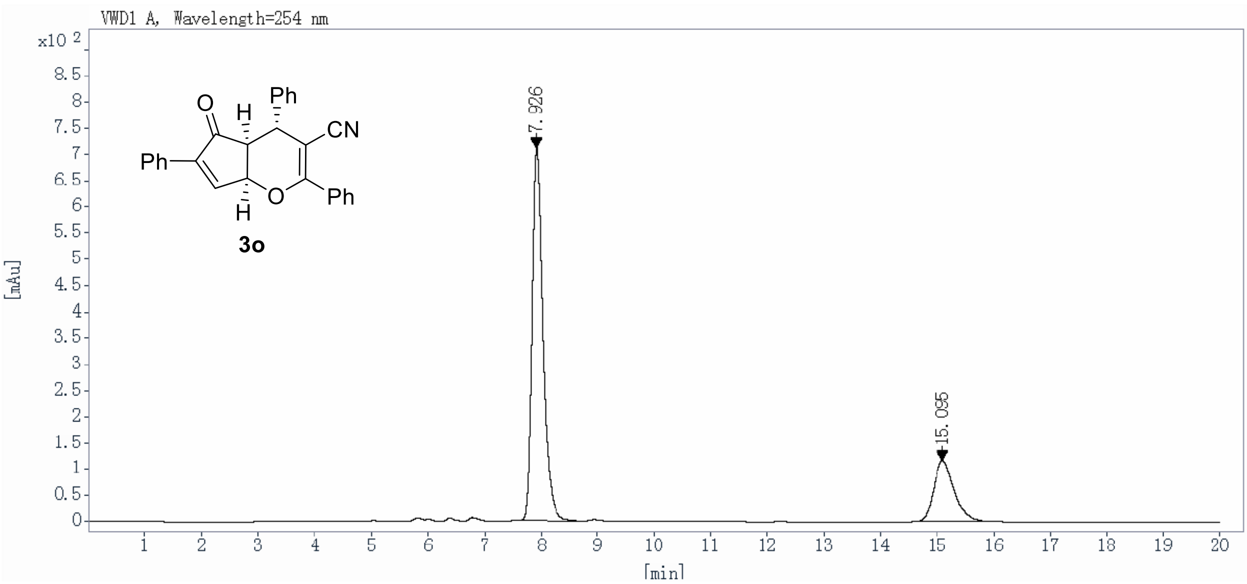

(UTC+08:00)
x10^6
+ESI Scan (rt: 0.366 min) Frag=175.0V CYC-20211129-37.d
350.1154
O
H
Ph
CN
Me
O
Ph
H
3n
(ESI-TOF) m/z: [M + Na]+
Calcd for C22H17NO2Na+ 350.1151
0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
0.55
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
349.8
349.82
349.84
349.86
349.88
349.9
349.92
349.94
349.96
349.98
350
350.02
350.04
350.06
350.08
350.1
350.12
350.14
350.16
Counts vs. Mass-to-Charge (m/z)


7.803
7.793
7.784
7.778
7.767
7.759
7.755
7.750
7.744
7.739
7.734
7.465
7.461
7.452
7.446
7.440
7.430
7.426
7.419
7.413
7.402
7.386
7.381
7.353
7.342
7.338
7.334
7.327
7.321
7.314
7.307
7.303
7.299
5.741
5.733
5.724
5.716
4.296
4.291
3.229
3.225
3.212
3.207
O
H
Ph
CN
Ph
O
Ph
H
3o
^{1}H NMR (400 MHz, $CDCl_3$)
4.90
9.98
1.09
1.00
1.00
1.00
f1 (ppm)

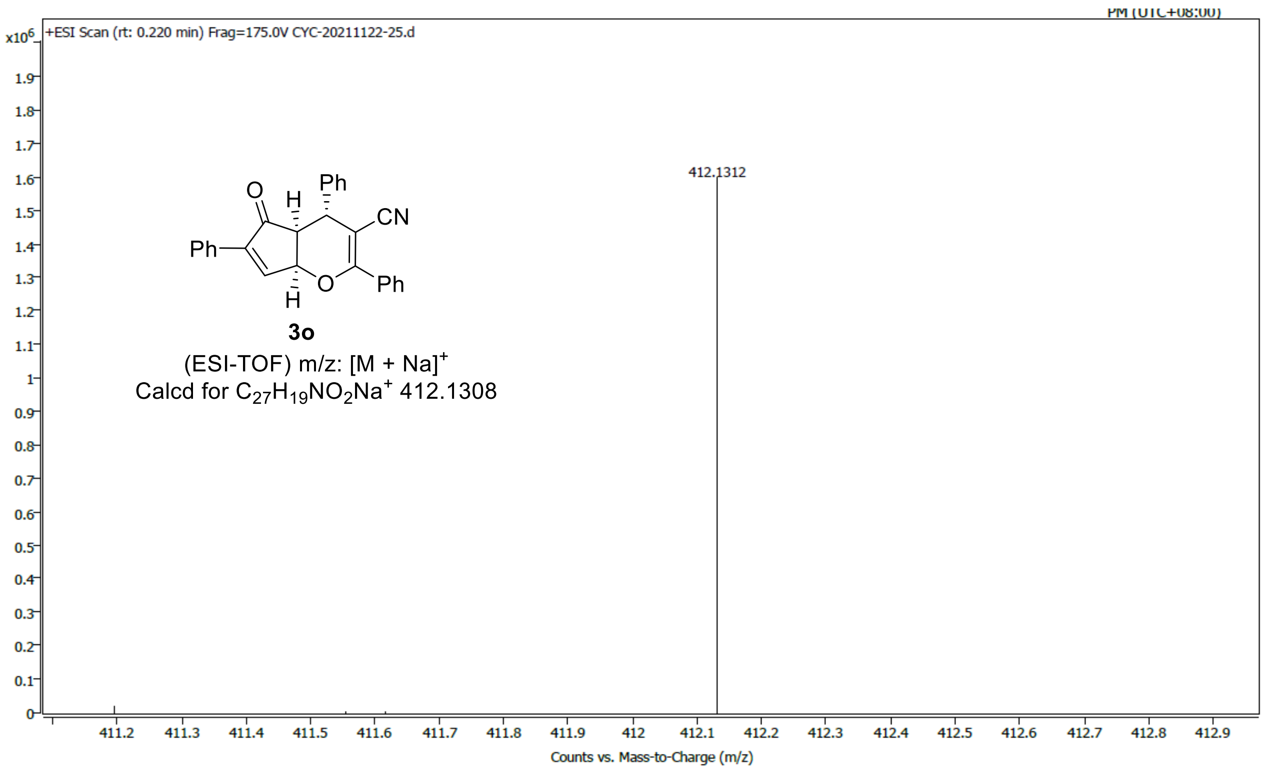

202.397
163.555
149.273
145.105
140.881
132.666
131.224
130.058
129.499
129.326
128.784
128.532
127.919
127.794
127.760
127.408
119.299
88.657
77.389
77.072
76.755
74.976
52.134
39.796
O
H
Ph
CN
Ph
O
Ph
H
3o
^{13}C NMR (100 MHz, $CDCl_3$)
f1 (ppm)

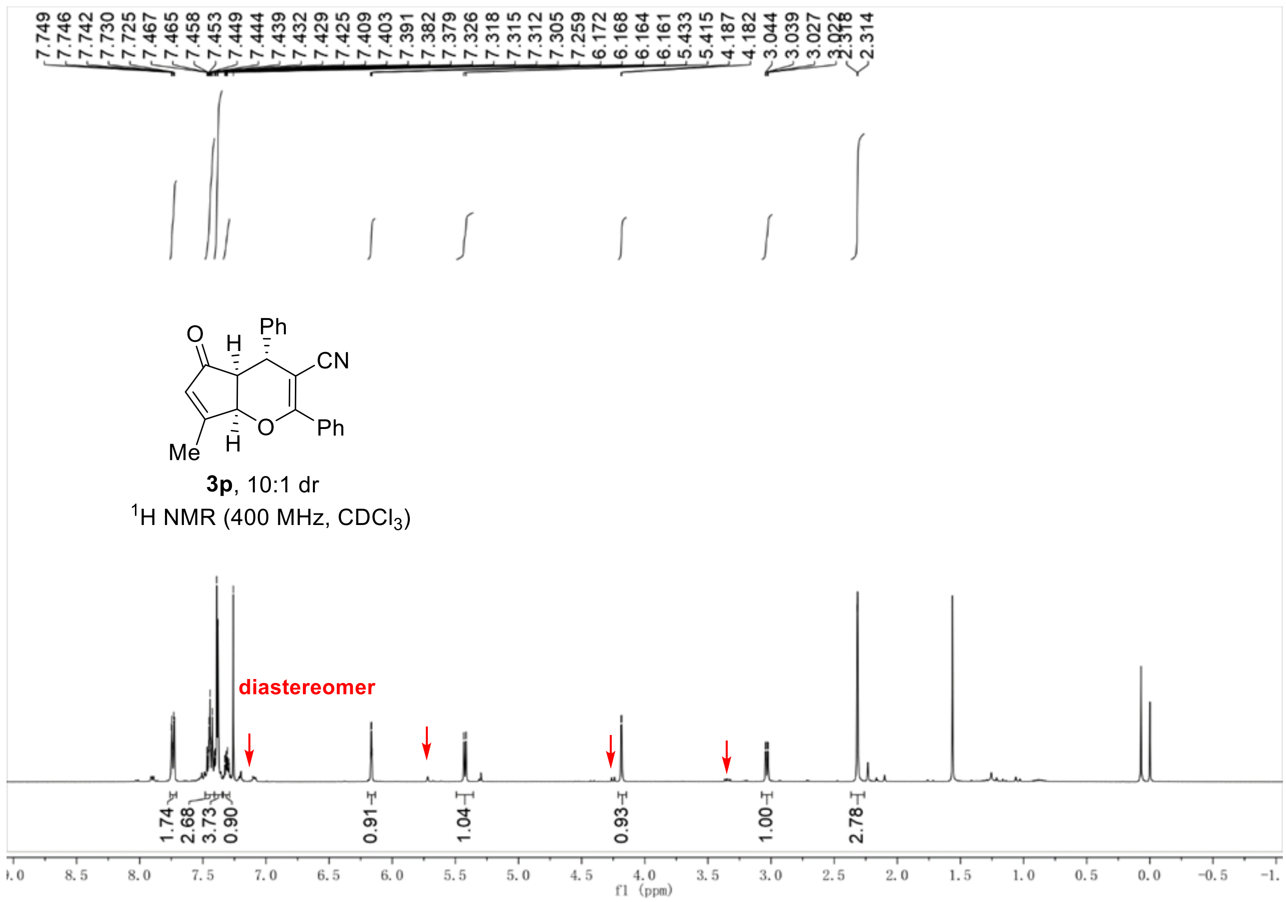


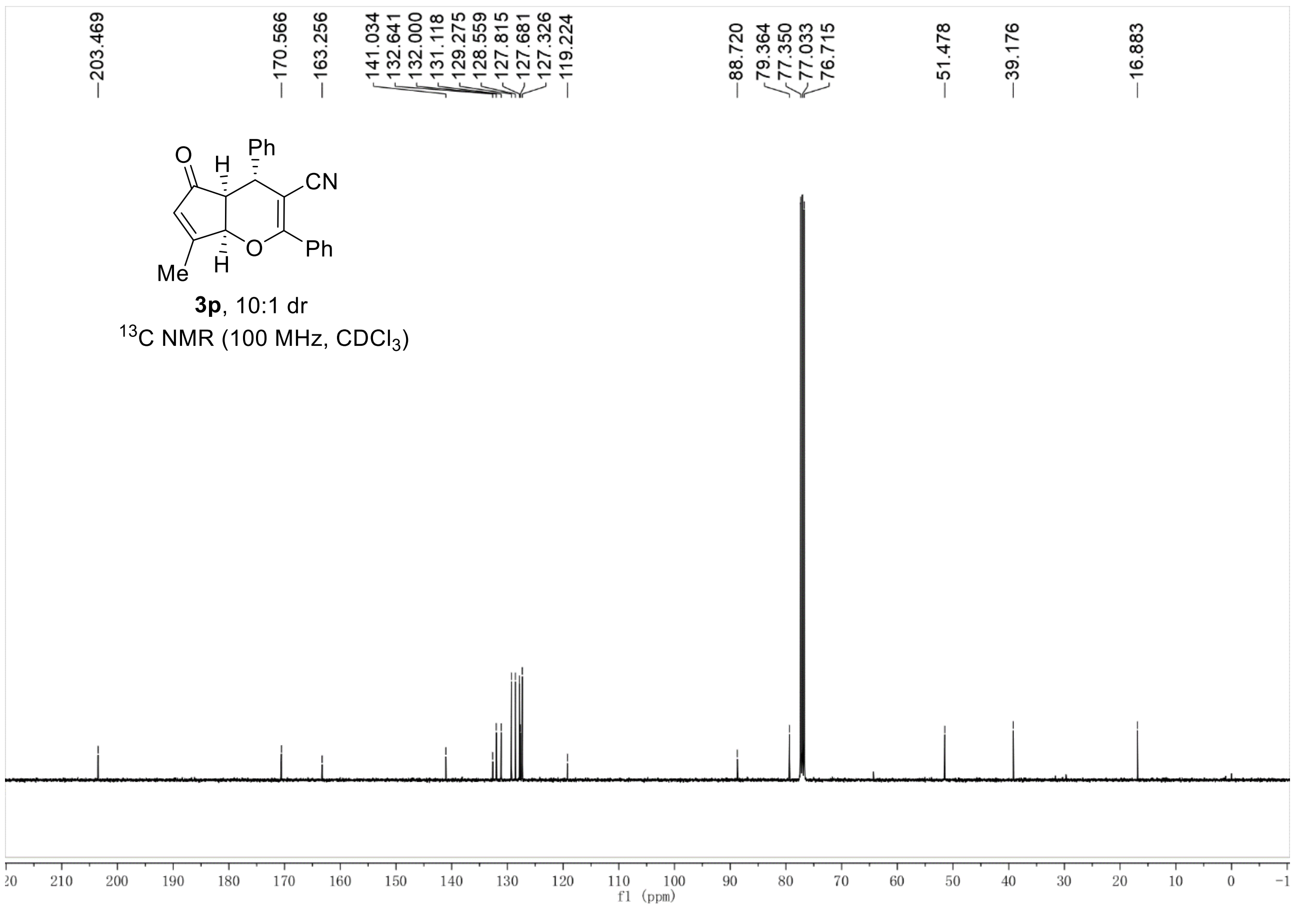
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
8.016	BV R	0.21	135.8665	1894.4500	49.8049
15.443	BB	0.41	71.1650	1909.2932	50.1951
			Totals:	3803.7432	100.0000

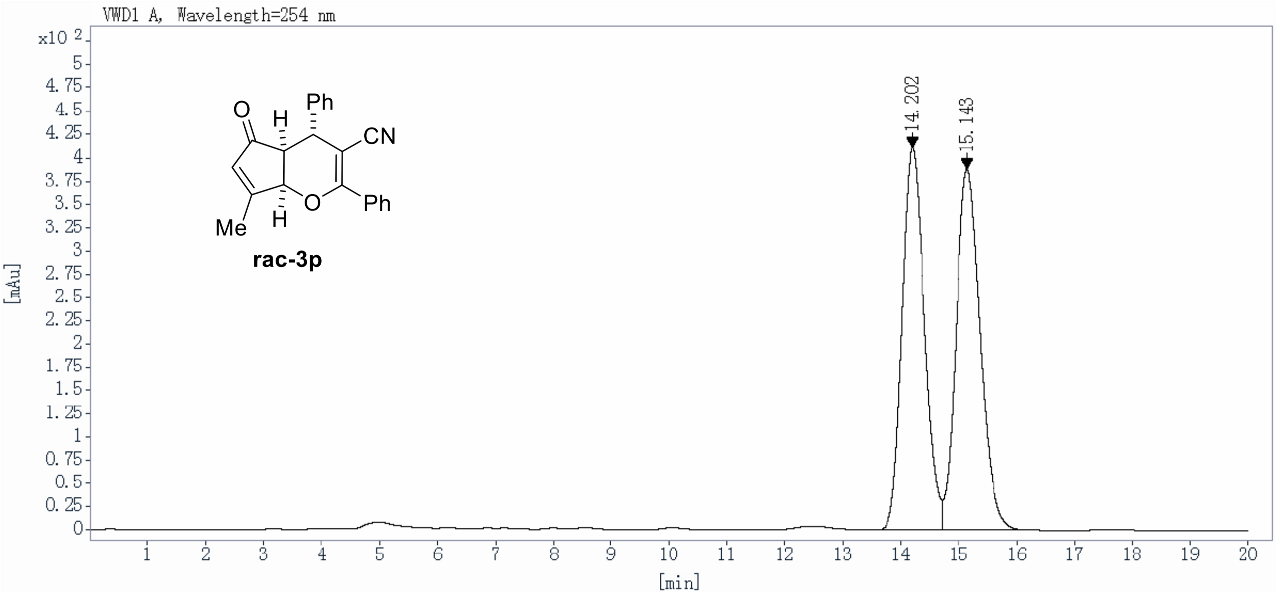


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
7.926	BBA	0.20	711.0656	9270.9961	76.5622
15.095	BBA	0.38	115.2938	2838.1104	23.4378
			Totals:	12109.1064	100.0000

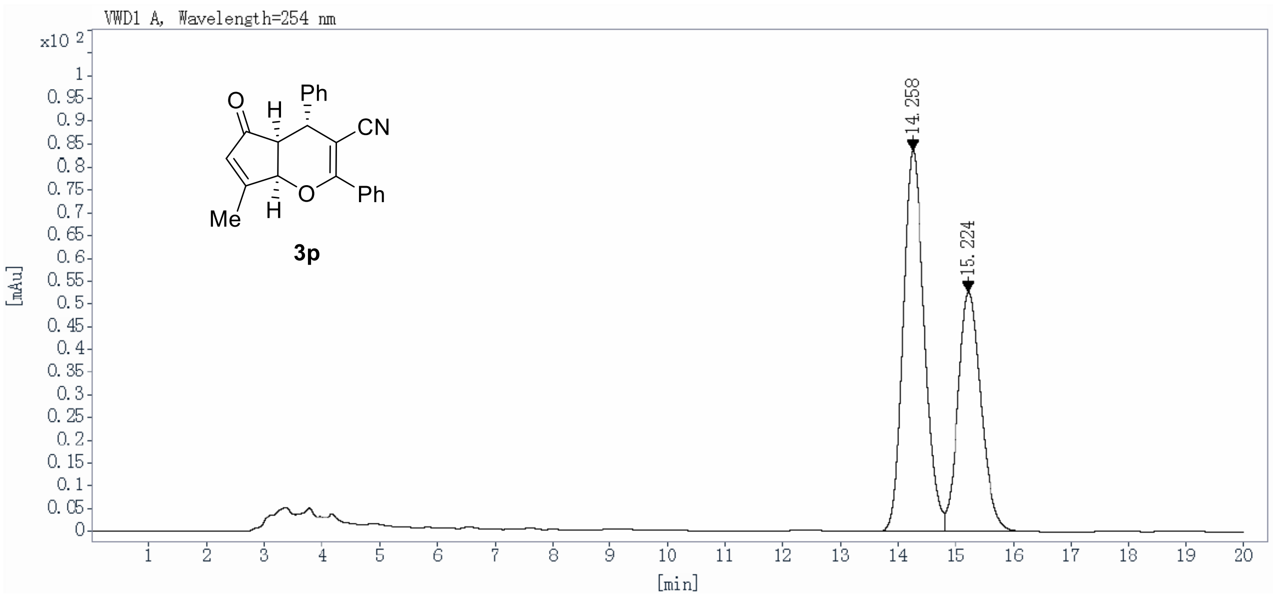

PM (UTC+08:00)
+ESI Scan (rt: 0.220 min) Frag=175.0V CYC-20211122-25.d
x10^6
412.1312
3o
(ESI-TOF) m/z: [M + Na]+
Calcd for C27H19NO2Na+ 412.1308
Counts vs. Mass-to-Charge (m/z)


7.749
7.746
7.742
7.730
7.725
7.467
7.465
7.458
7.453
7.449
7.444
7.439
7.432
7.429
7.425
7.409
7.403
7.391
7.382
7.379
7.326
7.318
7.315
7.312
7.305
7.259
6.172
6.168
6.164
6.161
5.433
5.415
4.187
4.182
3.044
3.039
3.027
3.022
2.318
2.314
O
H
Ph
CN
Ph
O
H
Me
3p, 10:1 dr
^{1}H NMR (400 MHz, $CDCl_3$)
diastereomer
1.74
2.68
3.73
0.90
0.91
1.04
0.93
1.00
2.78
f1 (ppm)

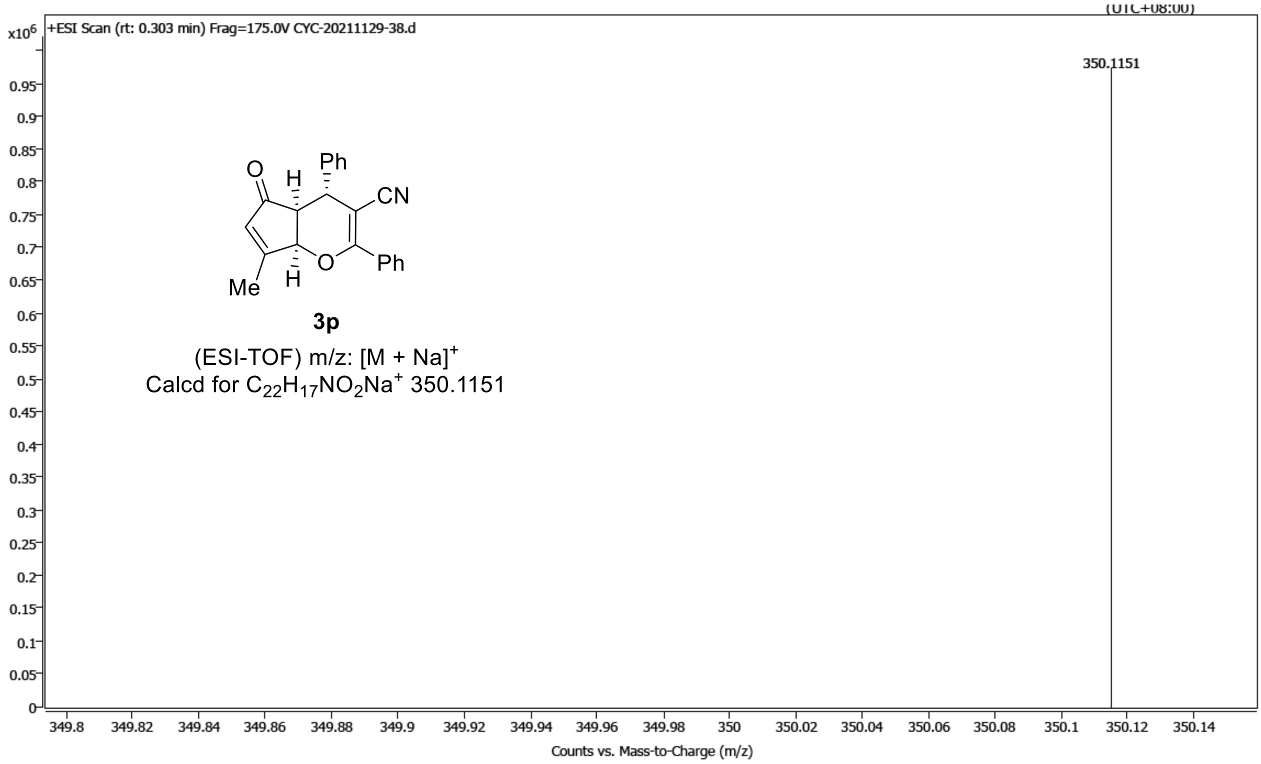

203.469
170.566
163.256
141.034
132.641
132.000
131.118
129.275
128.559
127.815
127.681
127.326
119.224
88.720
79.364
77.350
77.033
76.715
51.478
39.176
16.883
O
H
Ph
CN
Ph
O
H
Me
3p, 10:1 dr
^{13}C NMR (100 MHz, $CDCl_3$)
f1 (ppm)

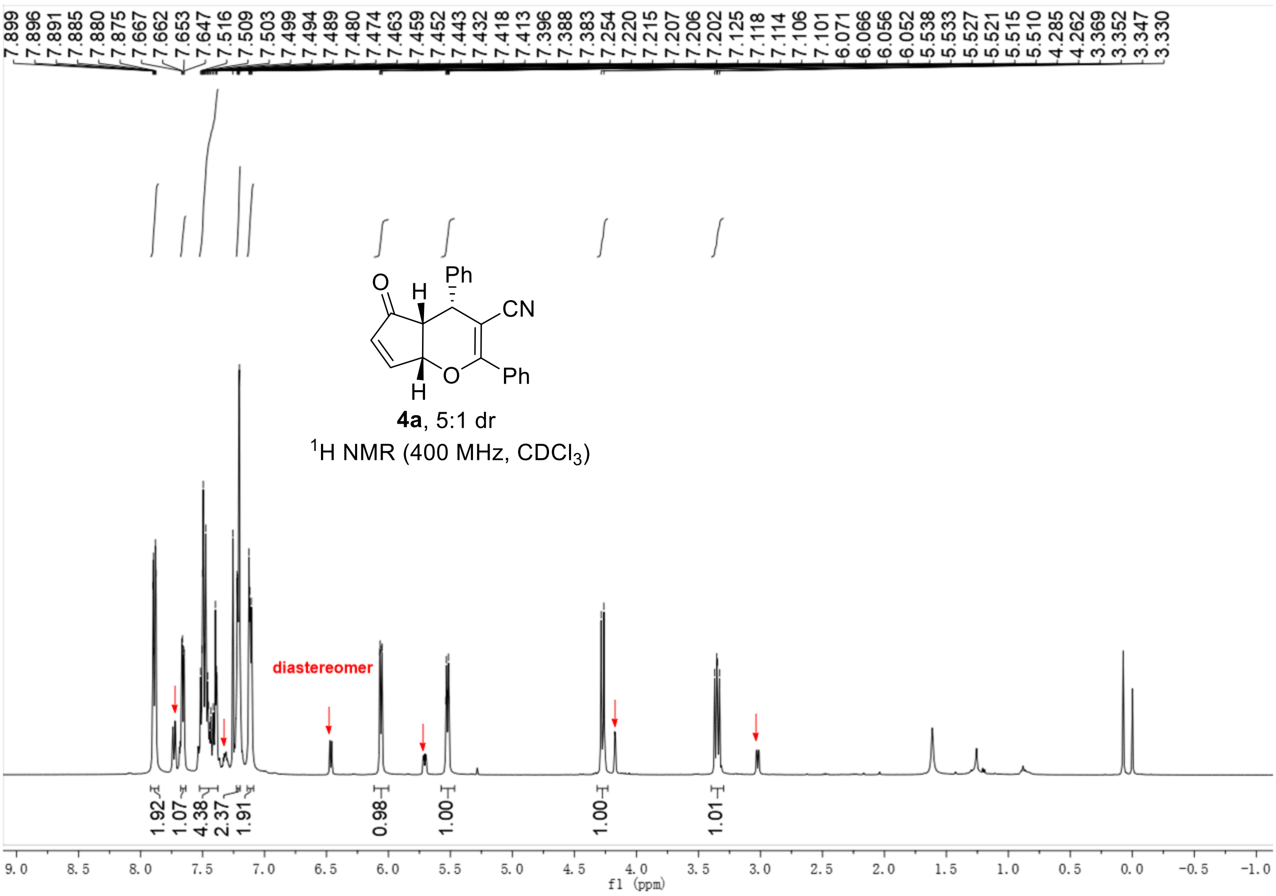


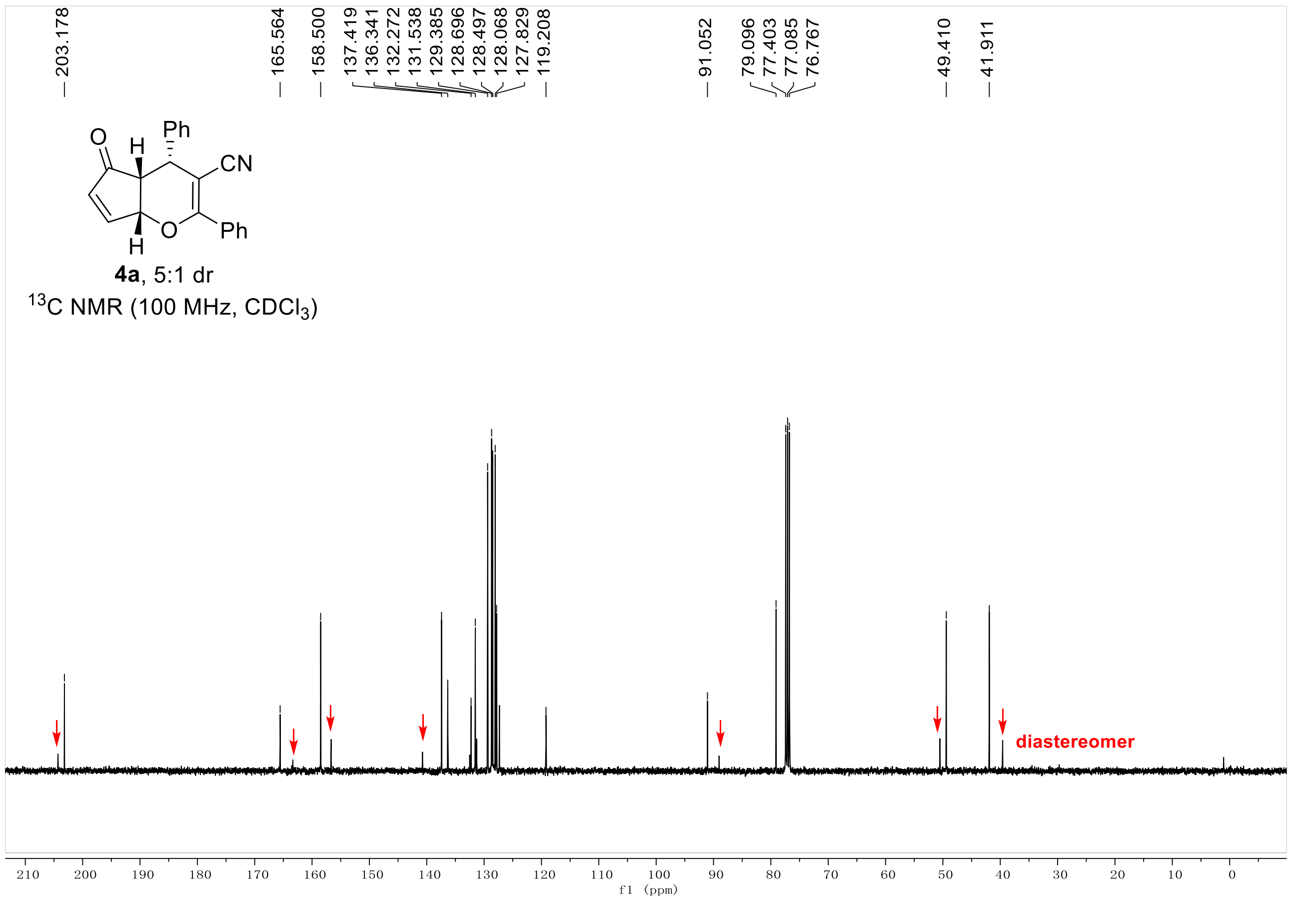
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
14.202	BV	0.42	410.8588	11031.6279	49.4929
15.143	VBA	0.45	388.9830	11257.6689	50.5071
			Totals:	22289.2969	100.0000

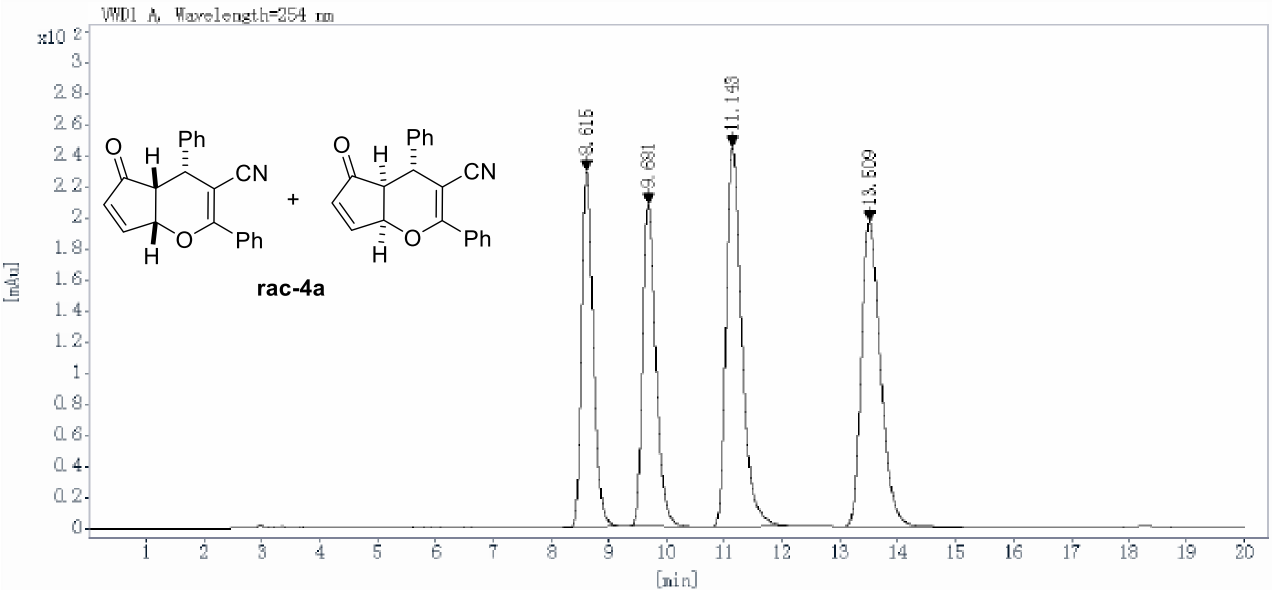


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
14.258	BV	0.40	83.6423	2141.2937	59.4186
15.224	VBA	0.43	52.8324	1462.4504	40.5814
			Totals:	3603.7441	100.0000

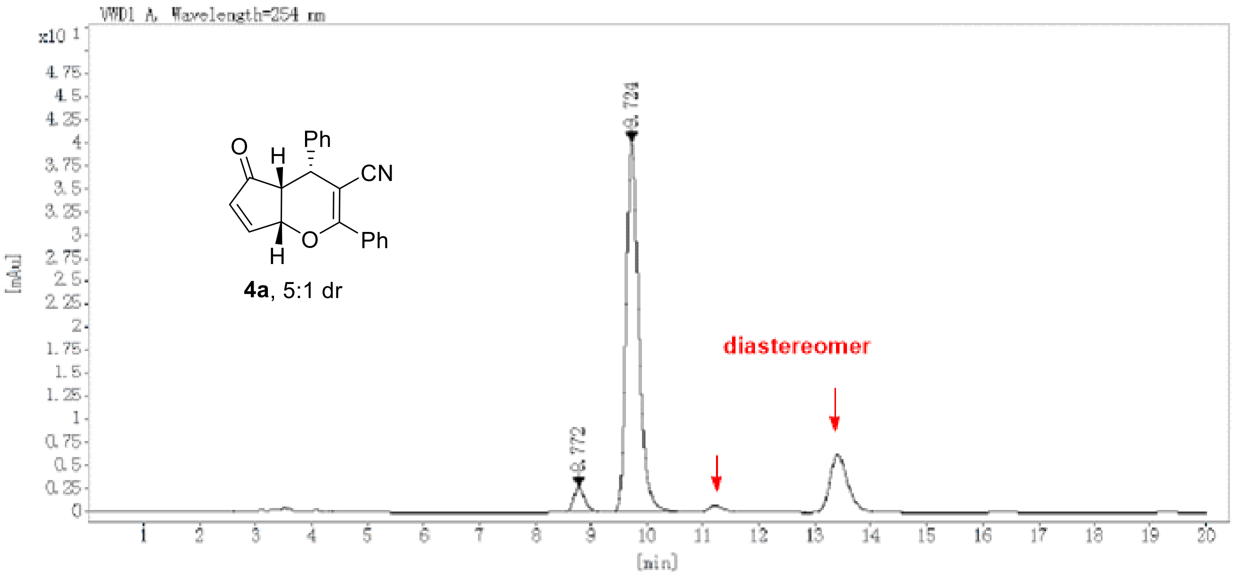

(UTC+08:00)
x10^6 +ESI Scan (rt: 0.303 min) Frag=175.0V CYC-20211129-38.d
350.1151
3p
(ESI-TOF) m/z: [M + Na]+
Calcd for C22H17NO2Na+ 350.1151
Counts vs. Mass-to-Charge (m/z)


7.899
7.896
7.891
7.885
7.880
7.875
7.667
7.662
7.653
7.647
7.516
7.509
7.503
7.499
7.494
7.489
7.480
7.474
7.463
7.459
7.452
7.443
7.432
7.418
7.413
7.396
7.388
7.383
7.254
7.220
7.215
7.207
7.206
7.202
7.125
7.118
7.114
7.106
7.101
6.071
6.066
6.056
6.052
5.538
5.533
5.527
5.521
5.515
5.510
4.285
4.262
3.369
3.352
3.347
3.330
O
H
Ph
CN
O
Ph
H
4a, 5:1 dr
1H NMR (400 MHz, CDCl3)
diastereomer
1.92
1.07
4.38
2.37
1.91
0.98
1.00
1.00
1.01
f1 (ppm)

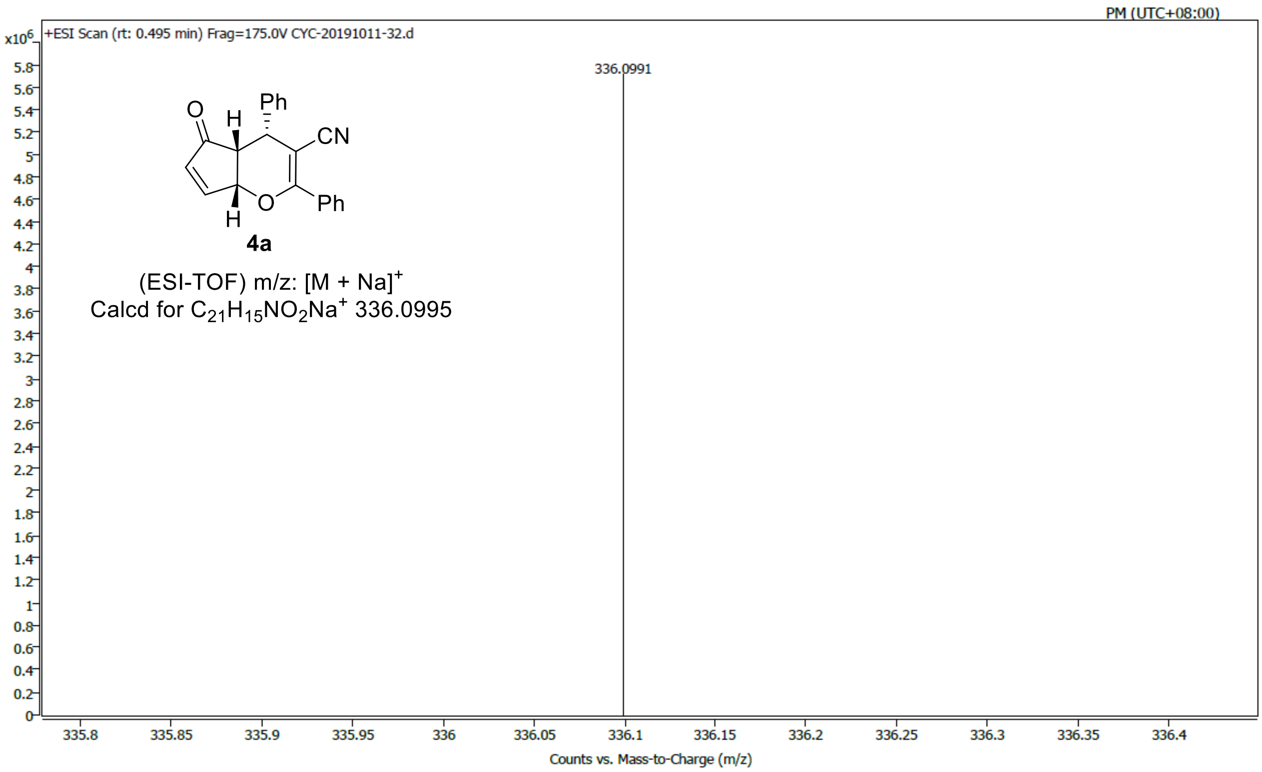

203.178
165.564
158.500
137.419
136.341
132.272
131.538
129.385
128.696
128.497
128.068
127.829
119.208
91.052
79.096
77.403
77.085
76.767
49.410
41.911
O
H
Ph
CN
O
Ph
H
4a, 5:1 dr
13C NMR (100 MHz, CDCl3)
diastereomer
f1 (ppm)

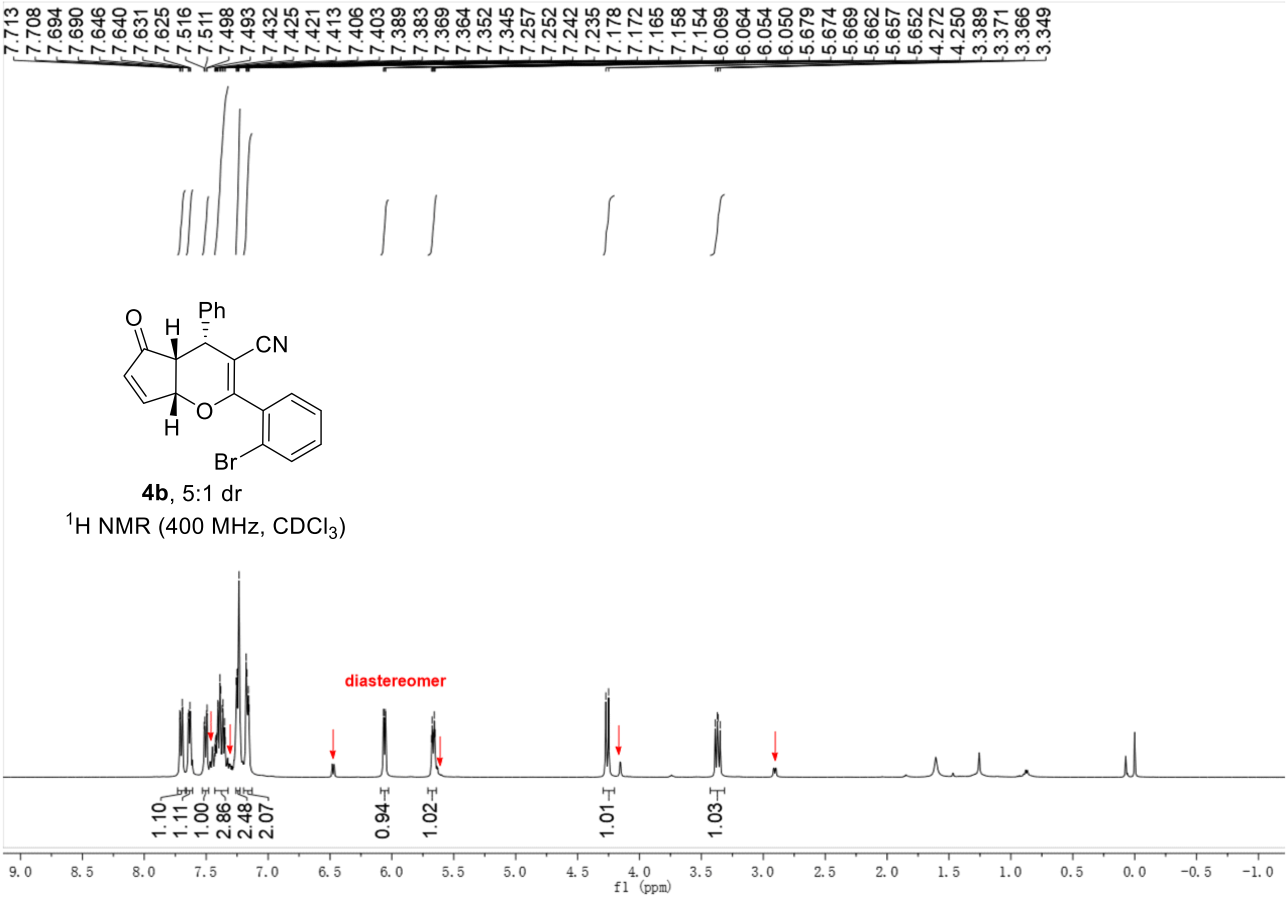


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
8.615	BB	0.21	229.5542	3202.6465	20.3367
9.681	BB	0.25	207.5817	3316.2485	21.0580
11.143	BB	0.29	244.6759	4652.0371	29.5402
13.509	BBA	0.36	196.7071	4577.2104	29.0651
			Totals:	15748.1426	100.0000



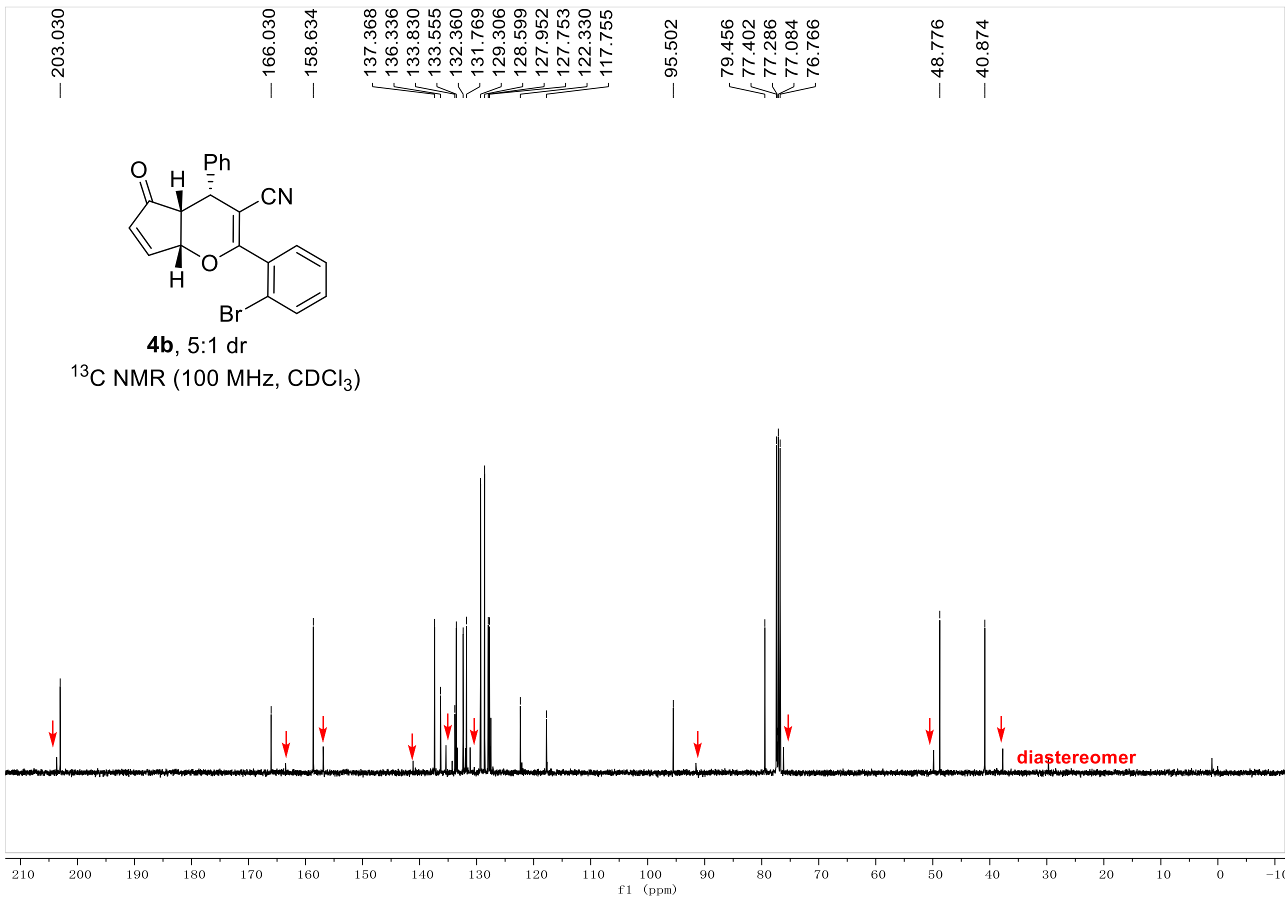
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
8.772	BBA	0.20	2.5872	33.8737	5.0749
9.724	BB	0.24	40.1205	633.6027	94.9251
			Totals:	667.4763	100.0000


PM (UTC+08:00)
+ESI Scan (rt: 0.495 min) Frag=175.0V CYC-20191011-32.d
x10^6
336.0991
4a
(ESI-TOF) m/z: [M + Na]+
Calcd for C21H15NO2Na+ 336.0995
Counts vs. Mass-to-Charge (m/z)



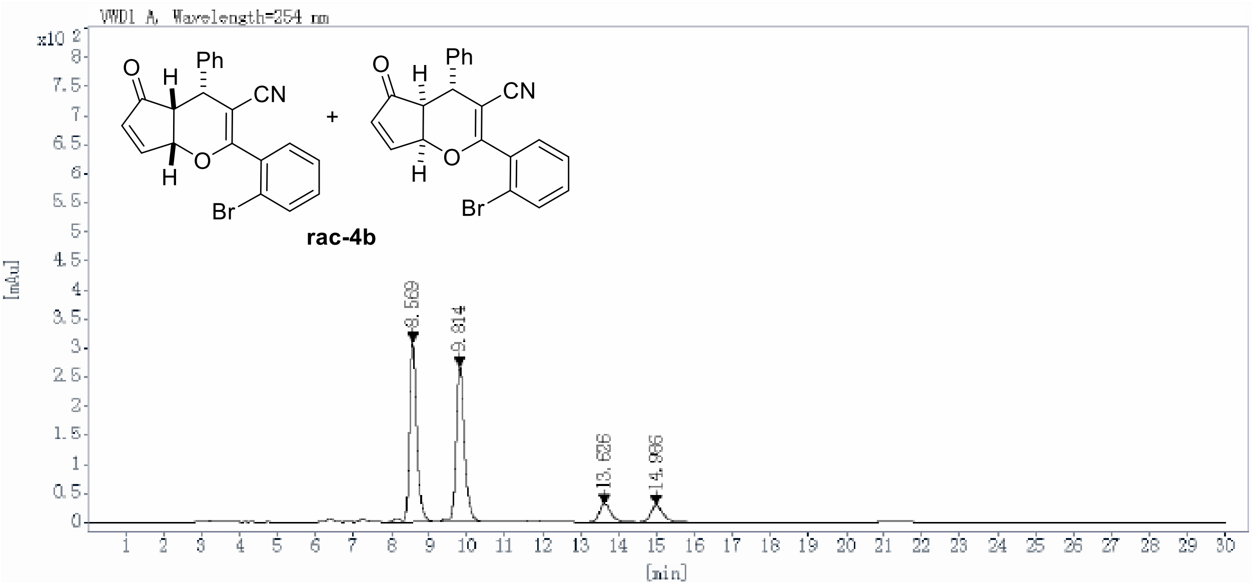
4b, 5:1 dr

^{1}H NMR (400 MHz, $CDCl_3$)

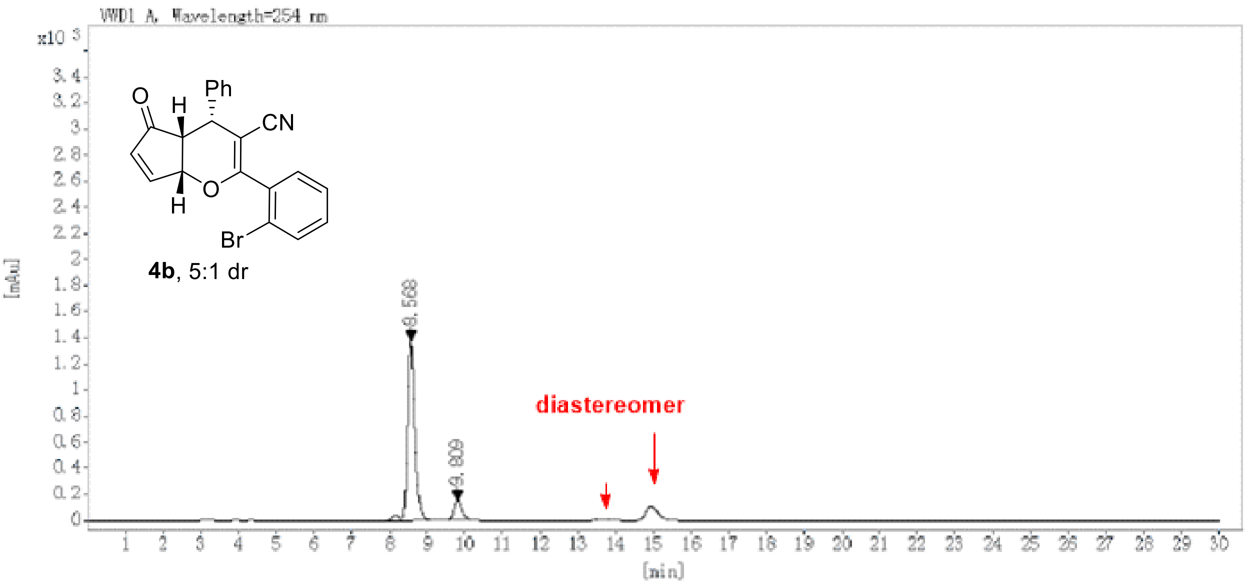


4b, 5:1 dr

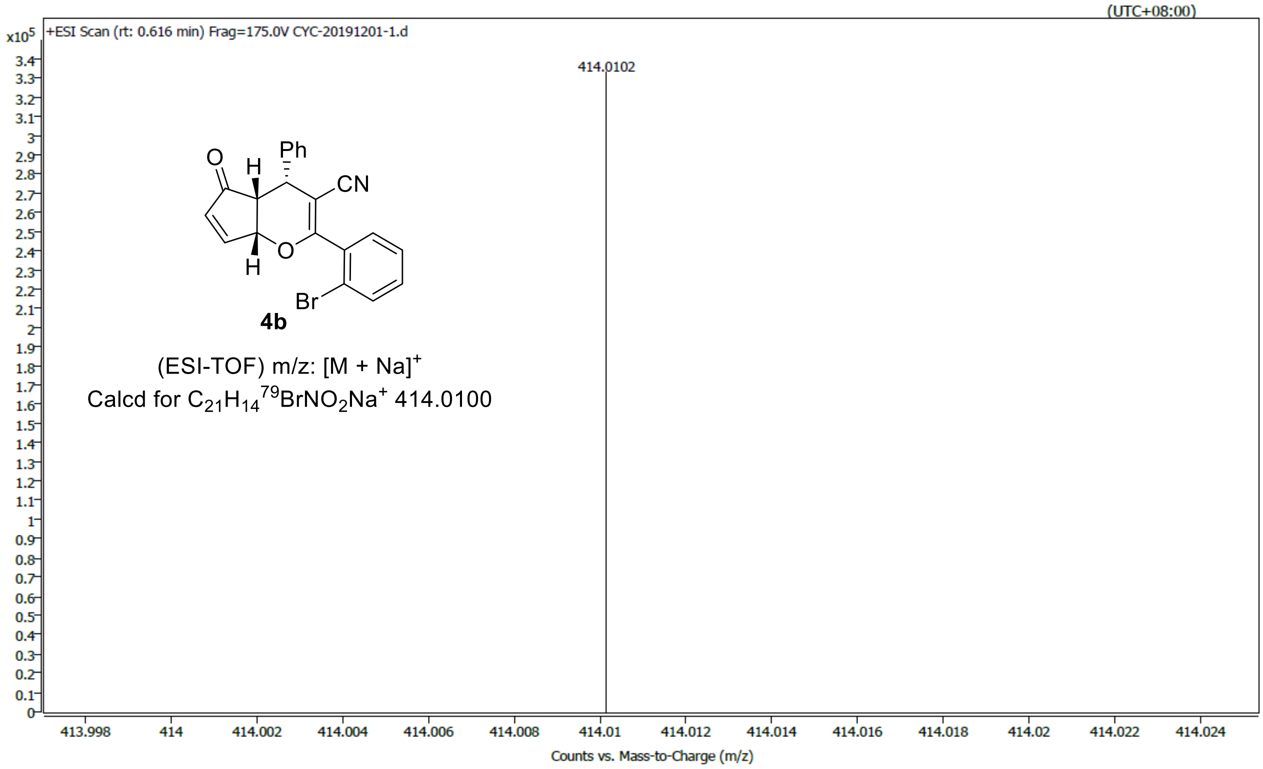
^{13}C NMR (100 MHz, $CDCl_3$)

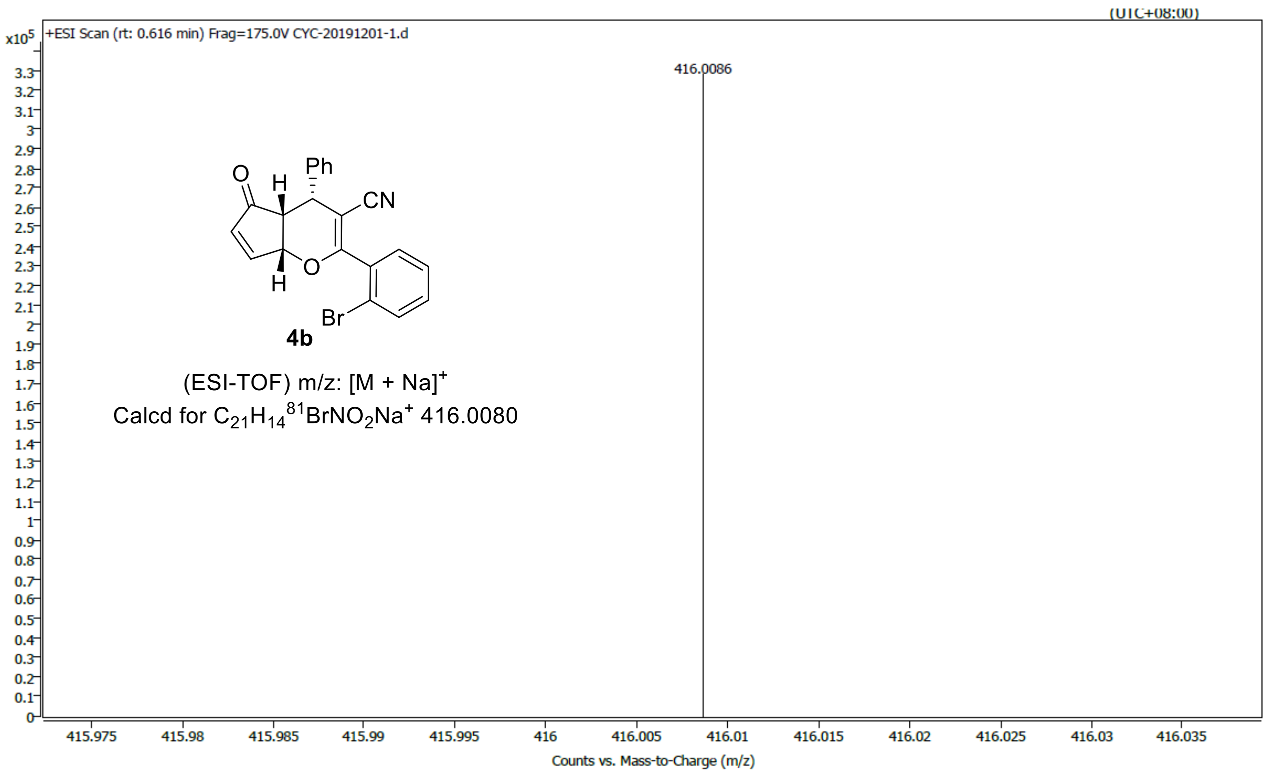


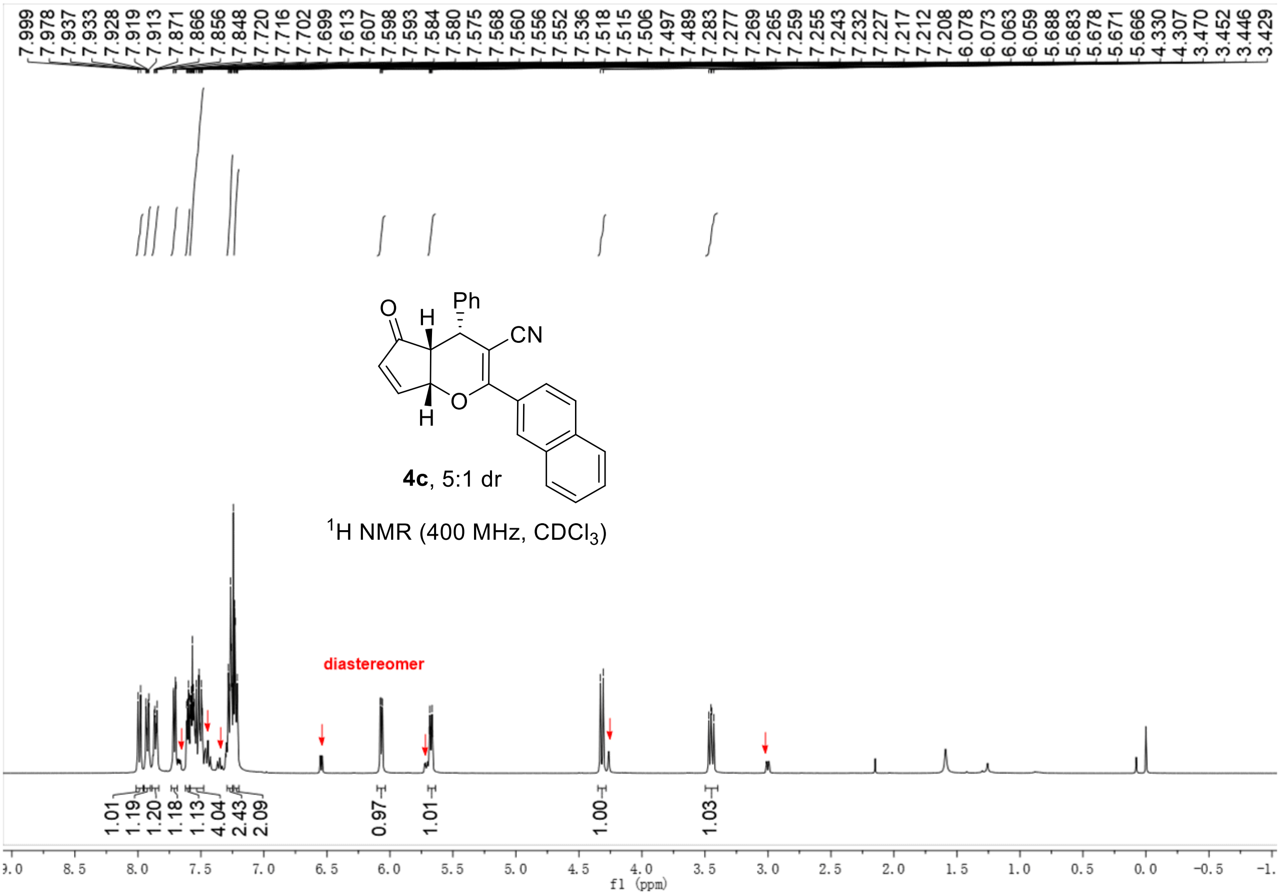
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
8.569	VB R	0.20	309.5046	4089.5901	43.0793
9.814	VB R	0.23	267.5630	4079.8186	42.9764
13.626	BB	0.32	31.5454	669.9623	7.0573
14.986	BB	0.35	28.4337	653.7908	6.8870
			Totals:	9493.1617	100.0000

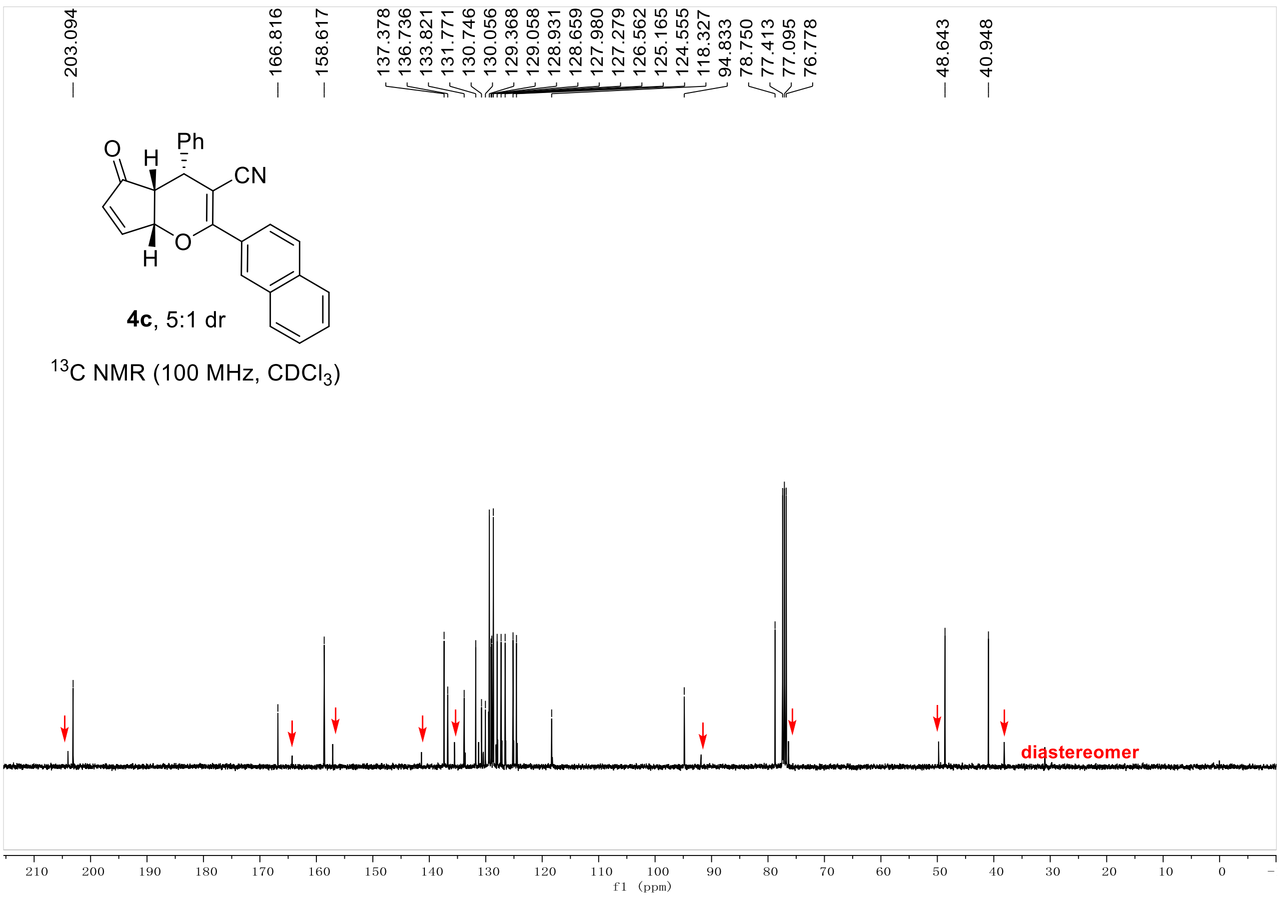


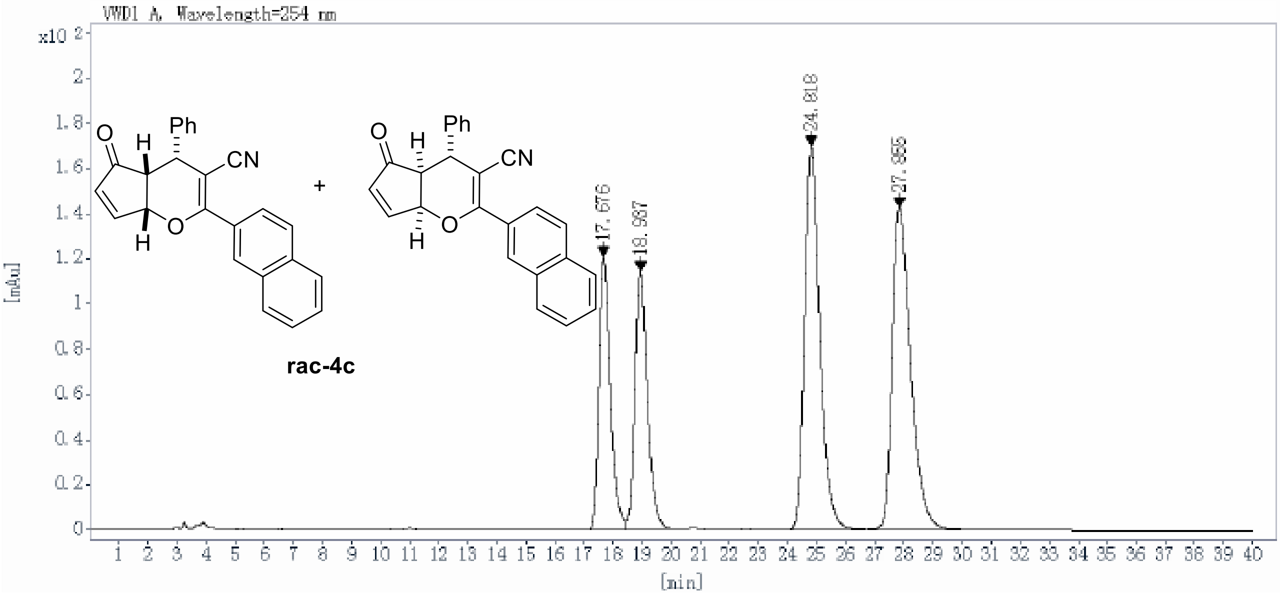
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
8.568	VB R	0.20	1376.3375	18354.5313	90.0408
9.809	BBA	0.21	146.5357	2030.1547	9.9592
			Totals:	20384.6859	100.0000


(UTC+08:00)
+ESI Scan (rt: 0.616 min) Frag=175.0V CYC-20191201-1.d
x10^5
414.0102
4b
(ESI-TOF) m/z: [M + Na]+
Calcd for $C_{21}H_{14}{}^{79}BrNO_2Na^+$ 414.0100
Counts vs. Mass-to-Charge (m/z)

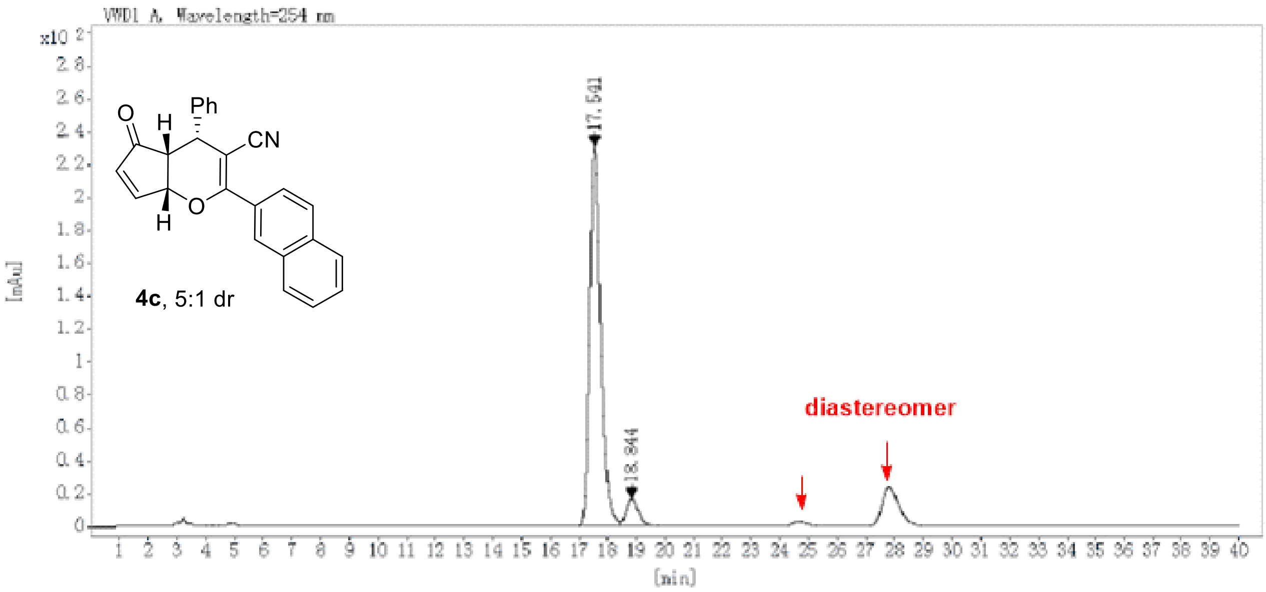

(UTC+08:00)
+ESI Scan (rt: 0.616 min) Frag=175.0V CYC-20191201-1.d
x10^5
416.0086
4b
(ESI-TOF) m/z: [M + Na]+
Calcd for $C_{21}H_{14}{}^{81}BrNO_2Na^+$ 416.0080
Counts vs. Mass-to-Charge (m/z)


7.999
7.978
7.937
7.933
7.928
7.919
7.913
7.871
7.866
7.856
7.848
7.720
7.716
7.702
7.699
7.613
7.607
7.598
7.593
7.584
7.580
7.575
7.568
7.560
7.556
7.552
7.536
7.518
7.515
7.506
7.497
7.489
7.283
7.277
7.269
7.265
7.259
7.255
7.243
7.232
7.227
7.217
7.212
7.208
6.078
6.073
6.063
6.059
5.688
5.683
5.678
5.671
5.666
4.330
4.307
3.470
3.452
3.446
3.429
Ph
CN
O
H
H
O
4c, 5:1 dr
1H NMR (400 MHz, CDCl3)
diastereomer
1.01
1.19
1.20
1.18
1.13
4.04
2.43
2.09
0.97
1.01
1.00
1.03
f1 (ppm)

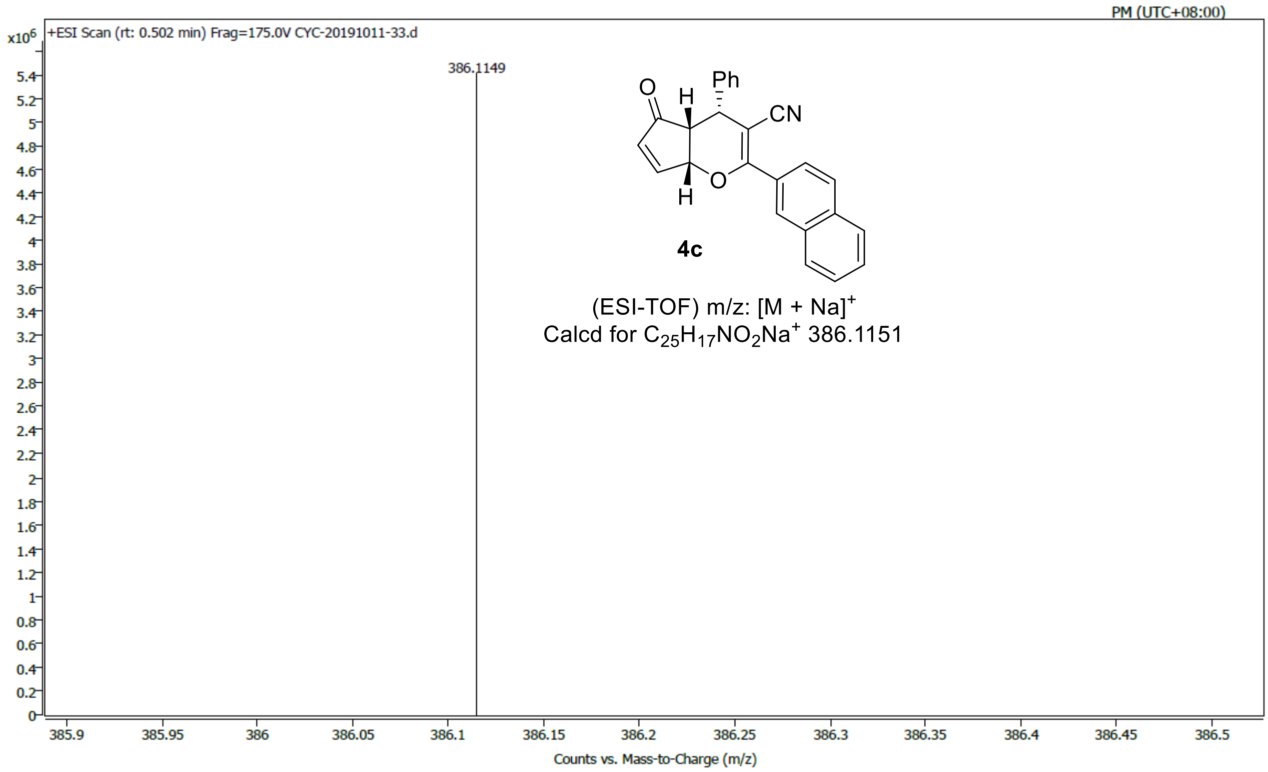

203.094
166.816
158.617
137.378
136.736
133.821
131.771
130.746
130.056
129.368
129.058
128.931
128.659
127.980
127.279
126.562
125.165
124.555
118.327
94.833
78.750
77.413
77.095
76.778
48.643
40.948
Ph
CN
O
H
H
O
4c, 5:1 dr
13C NMR (100 MHz, CDCl3)
diastereomer
f1 (ppm)

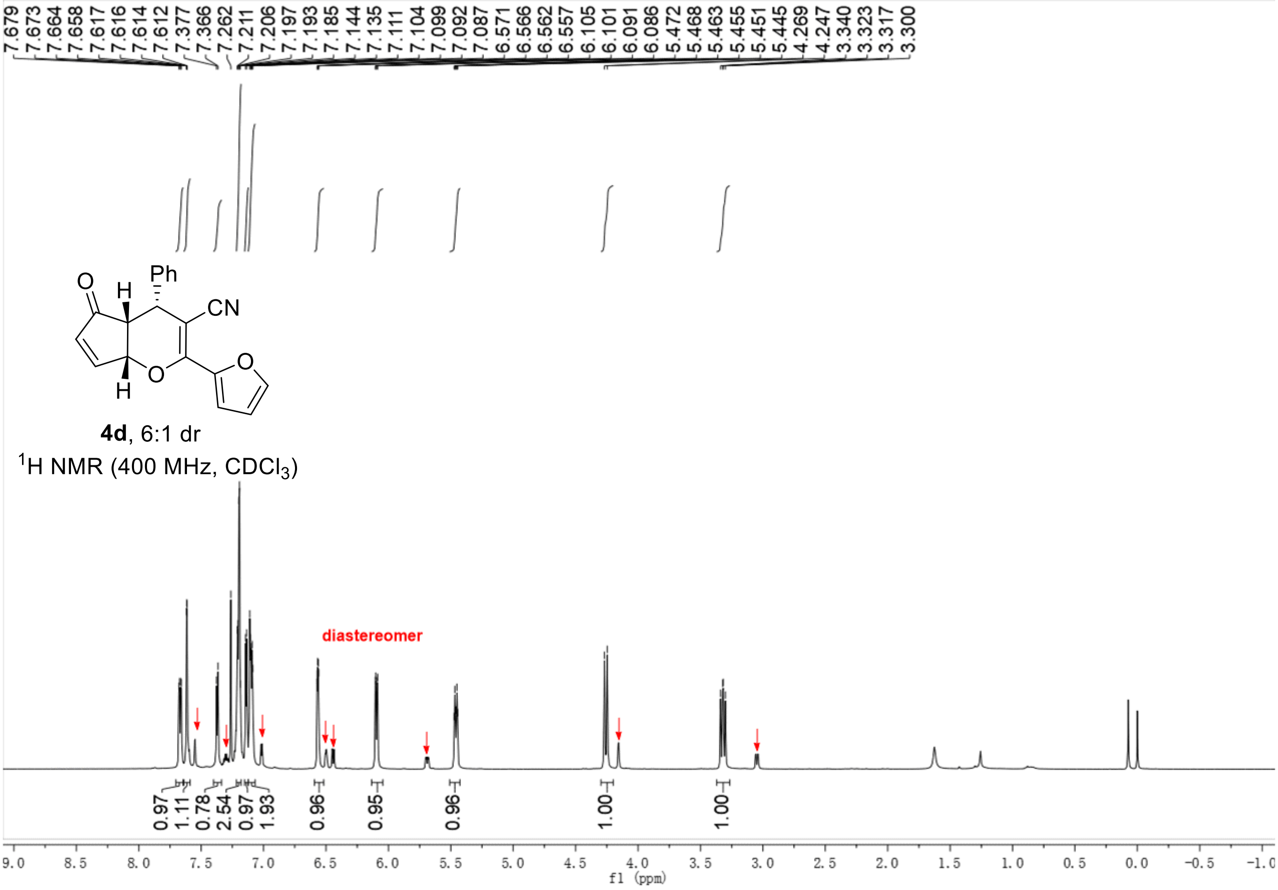


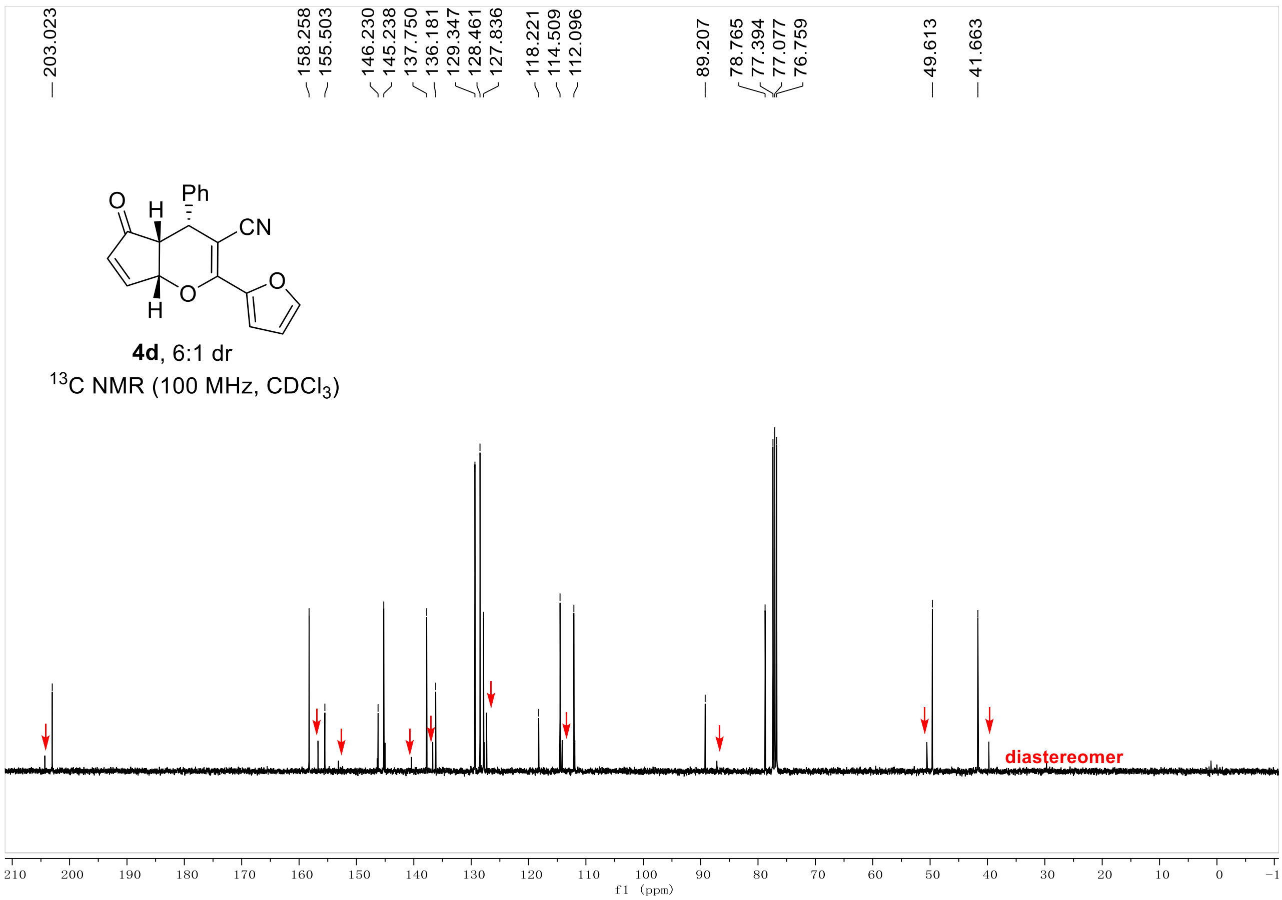
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
17.676	BV	0.42	120.6189	3305.0874	17.2675
18.937	VB	0.44	114.3205	3342.7715	17.4643
24.818	BB	0.56	169.4804	6229.9575	32.5485
27.855	BB	0.67	142.5582	6262.7388	32.7197
			Totals:	19140.5552	100.0000

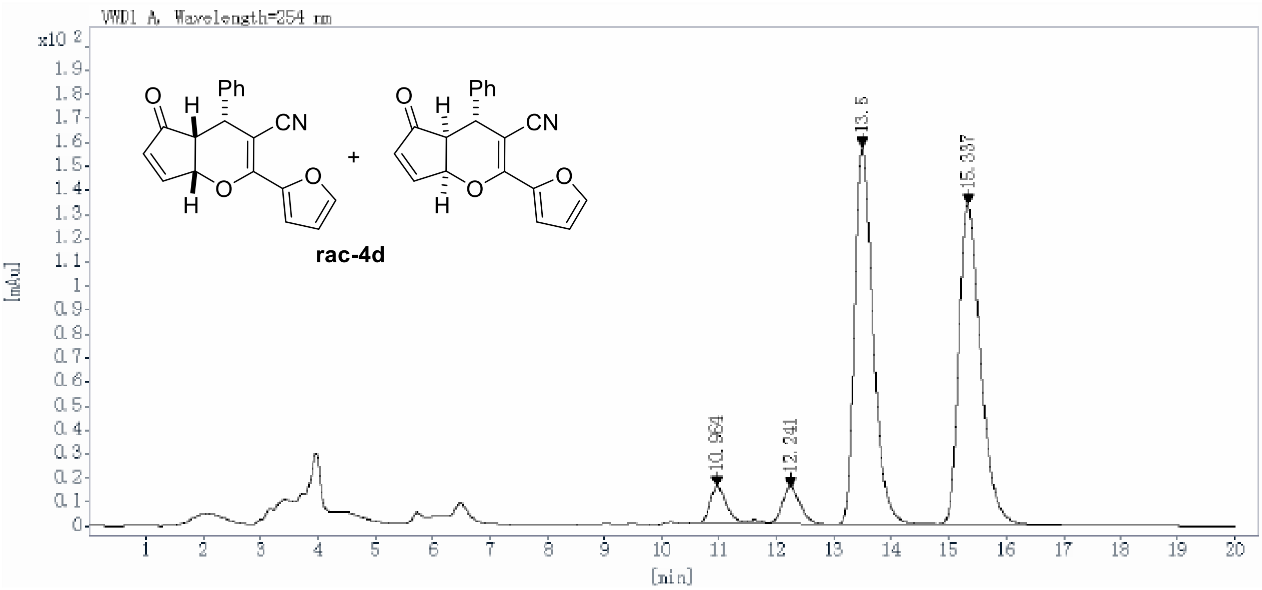


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
17.541	BV	0.41	230.2973	6199.3047	92.8358
18.844	VB S	0.44	16.4102	478.4063	7.1642
			Totals:	6677.7110	100.0000

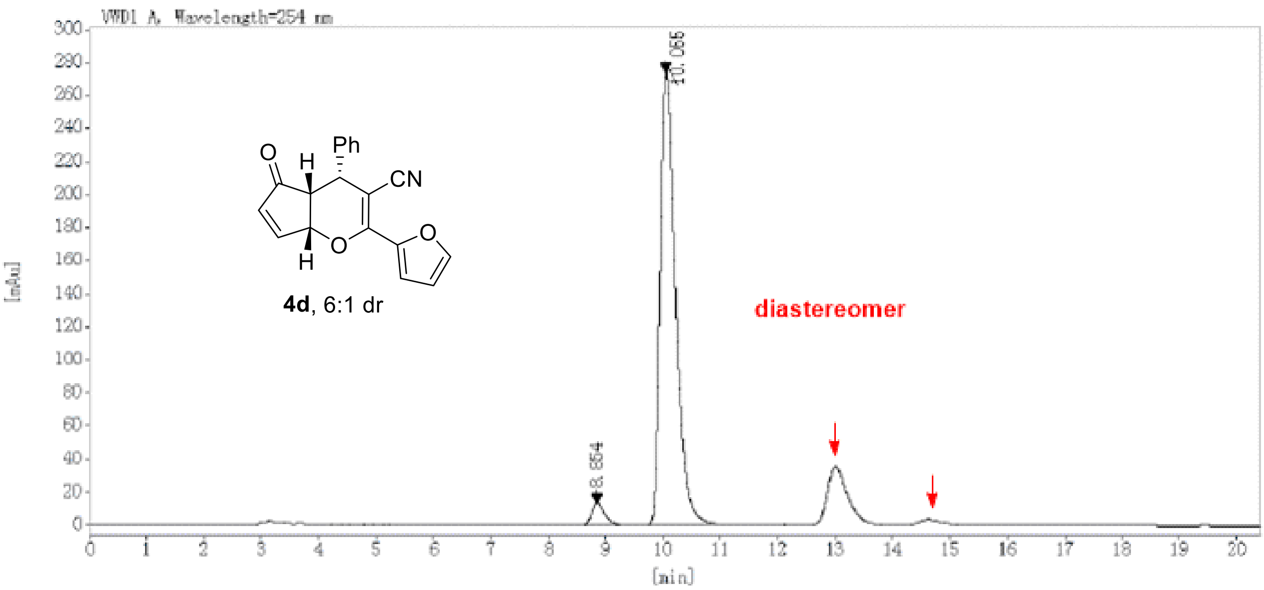

PM (UTC+08:00)
x10^6
+ESI Scan (rt: 0.502 min) Frag=175.0V CYC-20191011-33.d
386.1149
O
H
Ph
CN
H
O
4c
(ESI-TOF) m/z: [M + Na]+
Calcd for C25H17NO2Na+ 386.1151
5.4
5.2
5
4.8
4.6
4.4
4.2
4
3.8
3.6
3.4
3.2
3
2.8
2.6
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
385.9
385.95
386
386.05
386.1
386.15
386.2
386.25
386.3
386.35
386.4
386.45
386.5
Counts vs. Mass-to-Charge (m/z)


7.679
7.673
7.664
7.658
7.617
7.616
7.614
7.612
7.377
7.366
7.262
7.211
7.206
7.197
7.193
7.185
7.144
7.135
7.111
7.104
7.099
7.092
7.087
6.571
6.566
6.562
6.557
6.105
6.101
6.091
6.086
5.472
5.468
5.463
5.455
5.451
5.445
4.269
4.247
3.340
3.323
3.317
3.300
Ph
O
H
CN
O
O
H
4d, 6:1 dr
1H NMR (400 MHz, CDCl3)
diastereomer
0.97
1.11
0.78
2.54
0.97
1.93
0.96
0.95
0.96
1.00
1.00
f1 (ppm)

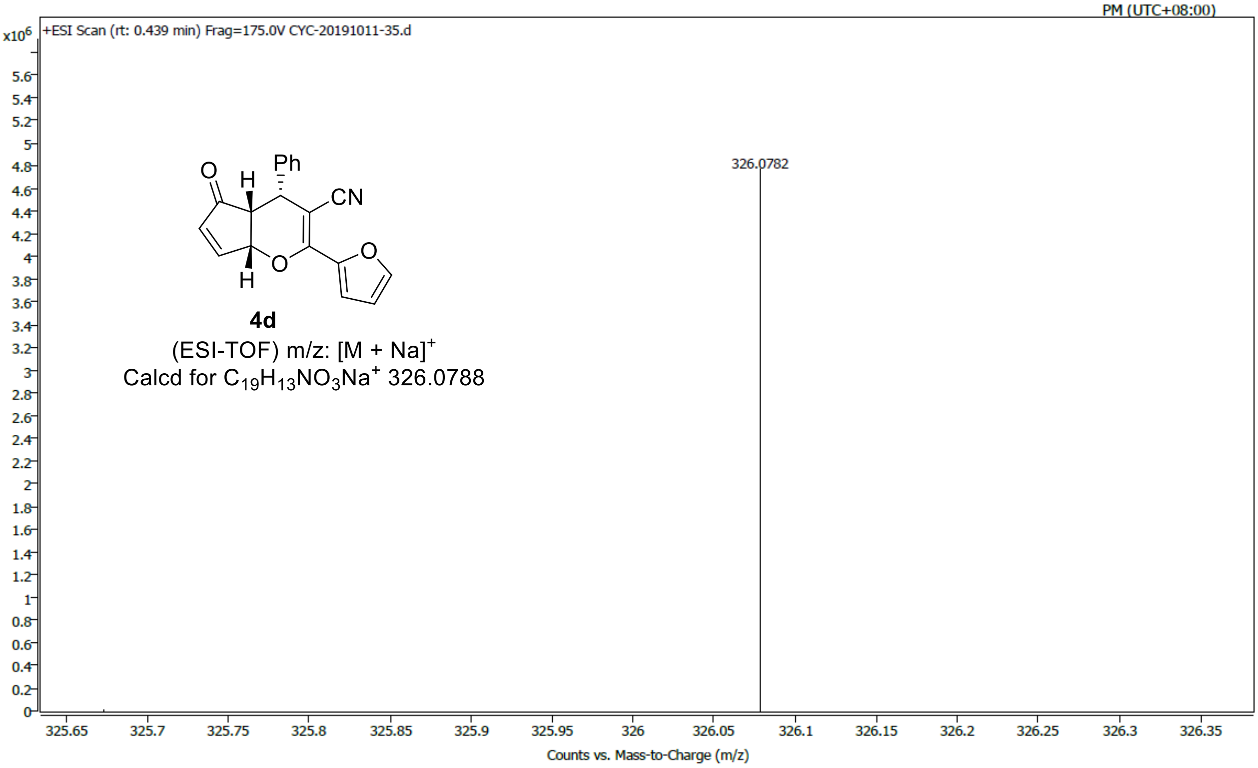

203.023
158.258
155.503
146.230
145.238
137.750
136.181
129.347
128.461
127.836
118.221
114.509
112.096
89.207
78.765
77.394
77.077
76.759
49.613
41.663
Ph
O
H
CN
O
O
H
4d, 6:1 dr
13C NMR (100 MHz, CDCl3)
diastereomer
f1 (ppm)

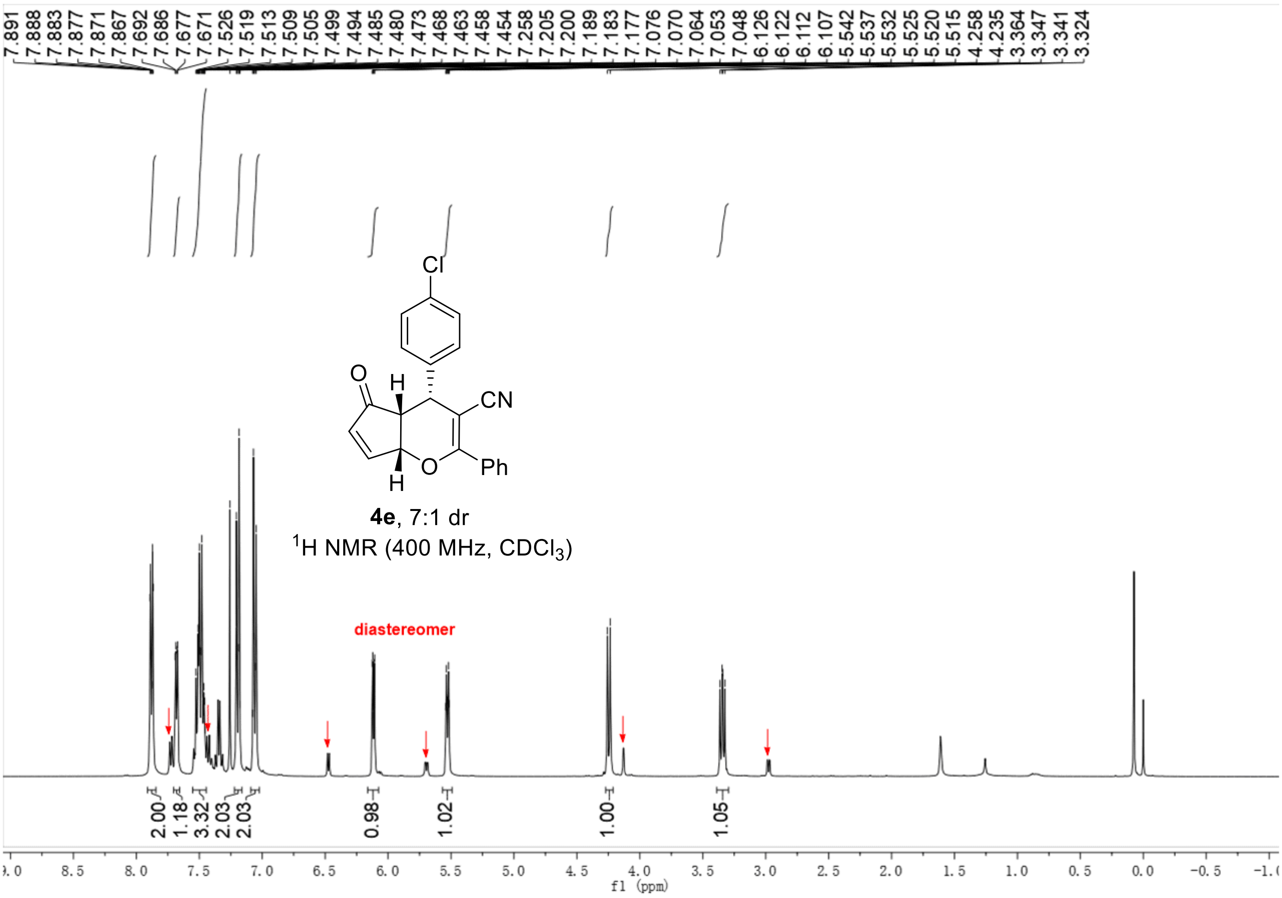


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
10.964	BV R	0.33	15.2030	332.0816	4.3063
12.241	VB	0.34	15.3141	336.7136	4.3664
13.500	BB	0.34	156.7655	3516.8328	45.6050
15.337	BBA	0.41	133.5784	3525.8833	45.7223
			Totals:	7711.5112	100.0000

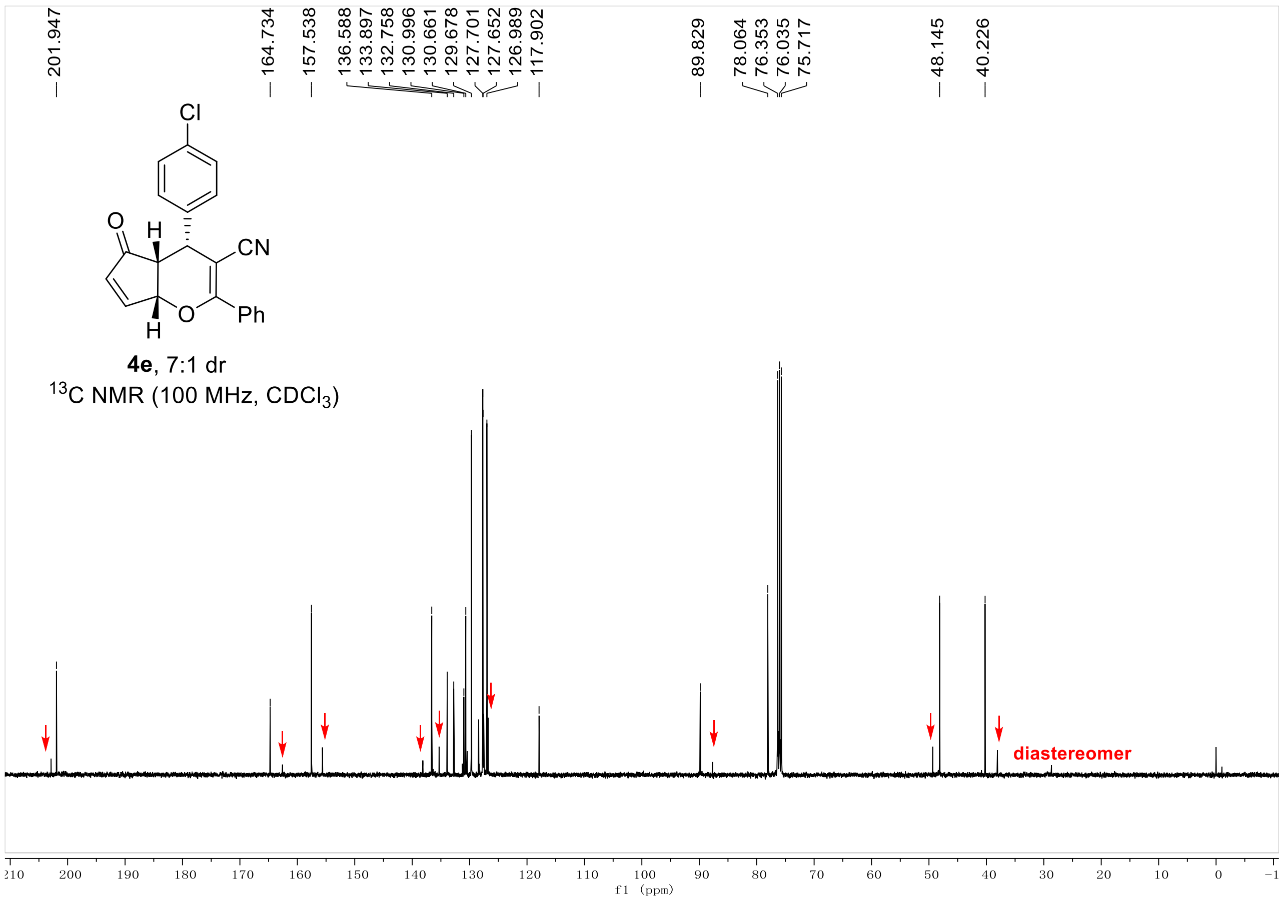


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
8.854	BB	0.25	13.4446	217.9788	4.0912
10.055	BB	0.29	274.0526	5109.9829	95.9088
			Totals:	5327.9617	100.0000

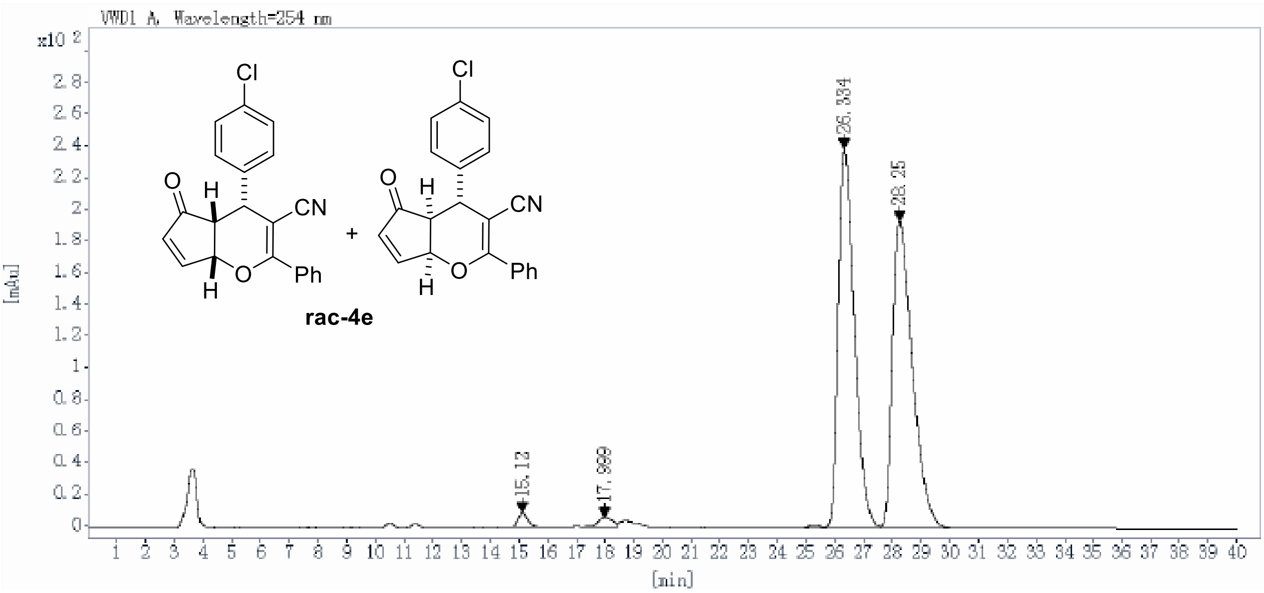

PM (UTC+08:00)
x10^6
+ESI Scan (rt: 0.439 min) Frag=175.0V CYC-20191011-35.d
326.0782
O
H
Ph
CN
O
O
H
4d
(ESI-TOF) m/z: [M + Na]+
Calcd for C19H13NO3Na+ 326.0788
Counts vs. Mass-to-Charge (m/z)



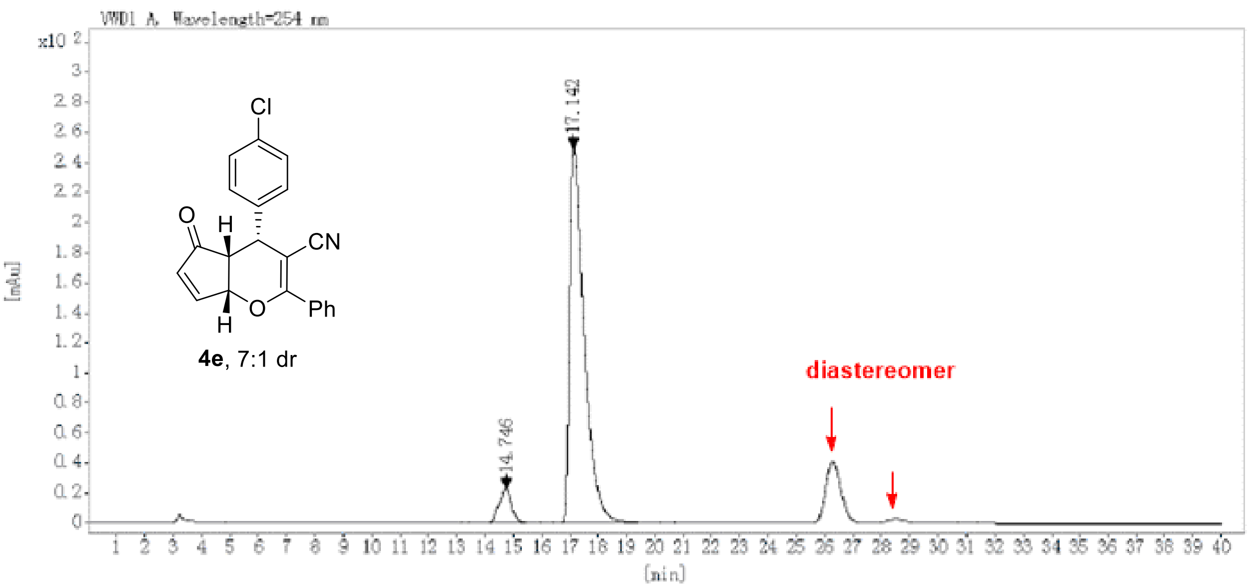
7.891
7.888
7.883
7.877
7.871
7.867
7.692
7.686
7.677
7.671
7.526
7.519
7.513
7.509
7.505
7.499
7.494
7.485
7.480
7.473
7.468
7.463
7.458
7.454
7.258
7.205
7.200
7.189
7.183
7.177
7.076
7.070
7.064
7.053
7.048
6.126
6.122
6.112
6.107
5.542
5.537
5.532
5.525
5.520
5.515
4.258
4.235
3.364
3.347
3.341
3.324
Cl
O
H
CN
H
O
Ph
4e, 7:1 dr
¹H NMR (400 MHz, CDCl₃)
diastereomer
2.00
1.18
3.32
2.03
2.03
0.98
1.02
1.00
1.05
f1 (ppm)



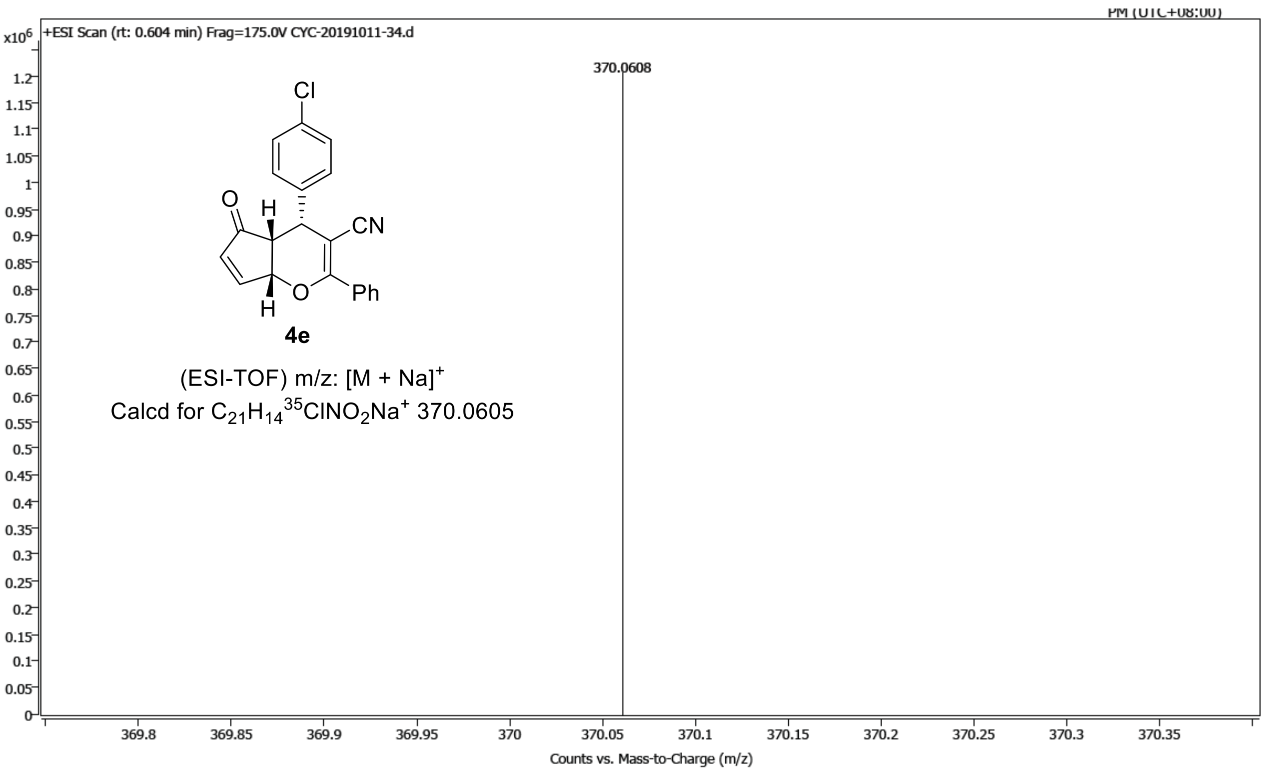
201.947
164.734
157.538
136.588
133.897
132.758
130.996
130.661
129.678
127.701
127.652
126.989
117.902
89.829
78.064
76.353
76.035
75.717
48.145
40.226
Cl
O
H
CN
H
O
Ph
4e, 7:1 dr
¹³C NMR (100 MHz, CDCl₃)
diastereomer
f1 (ppm)

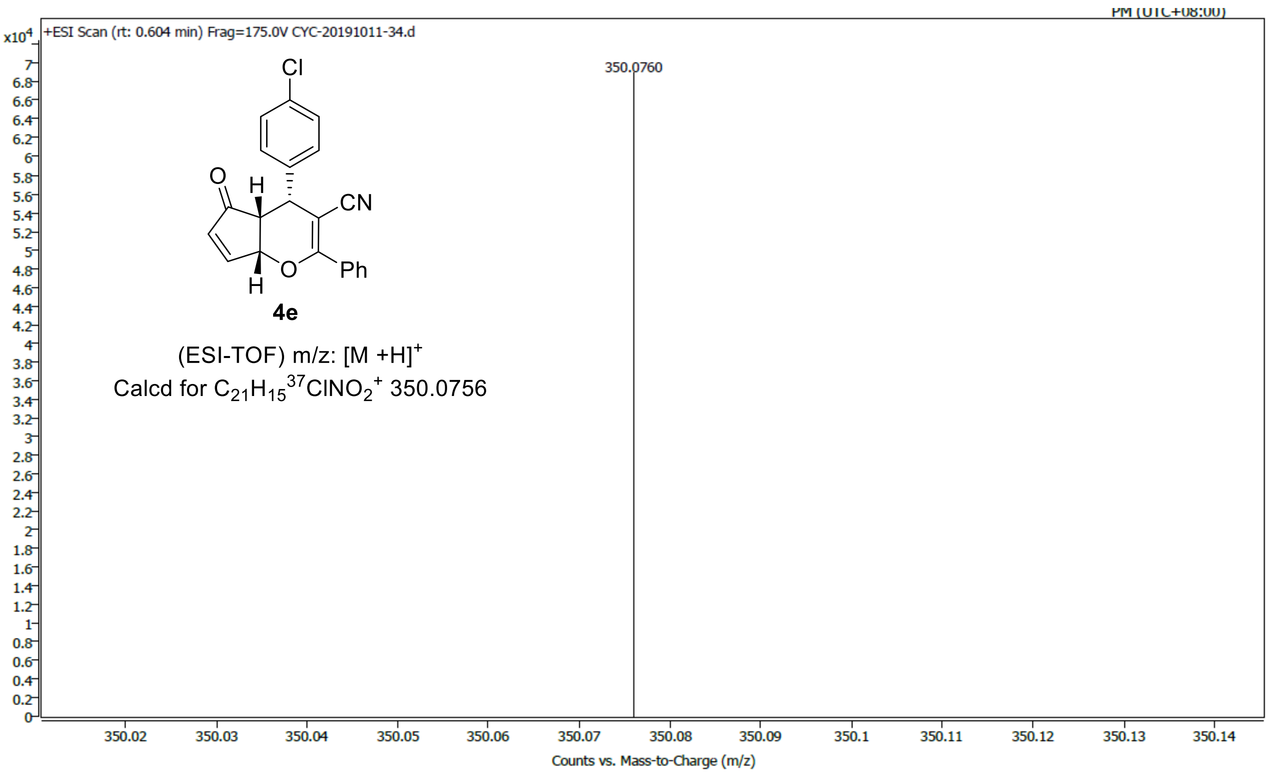


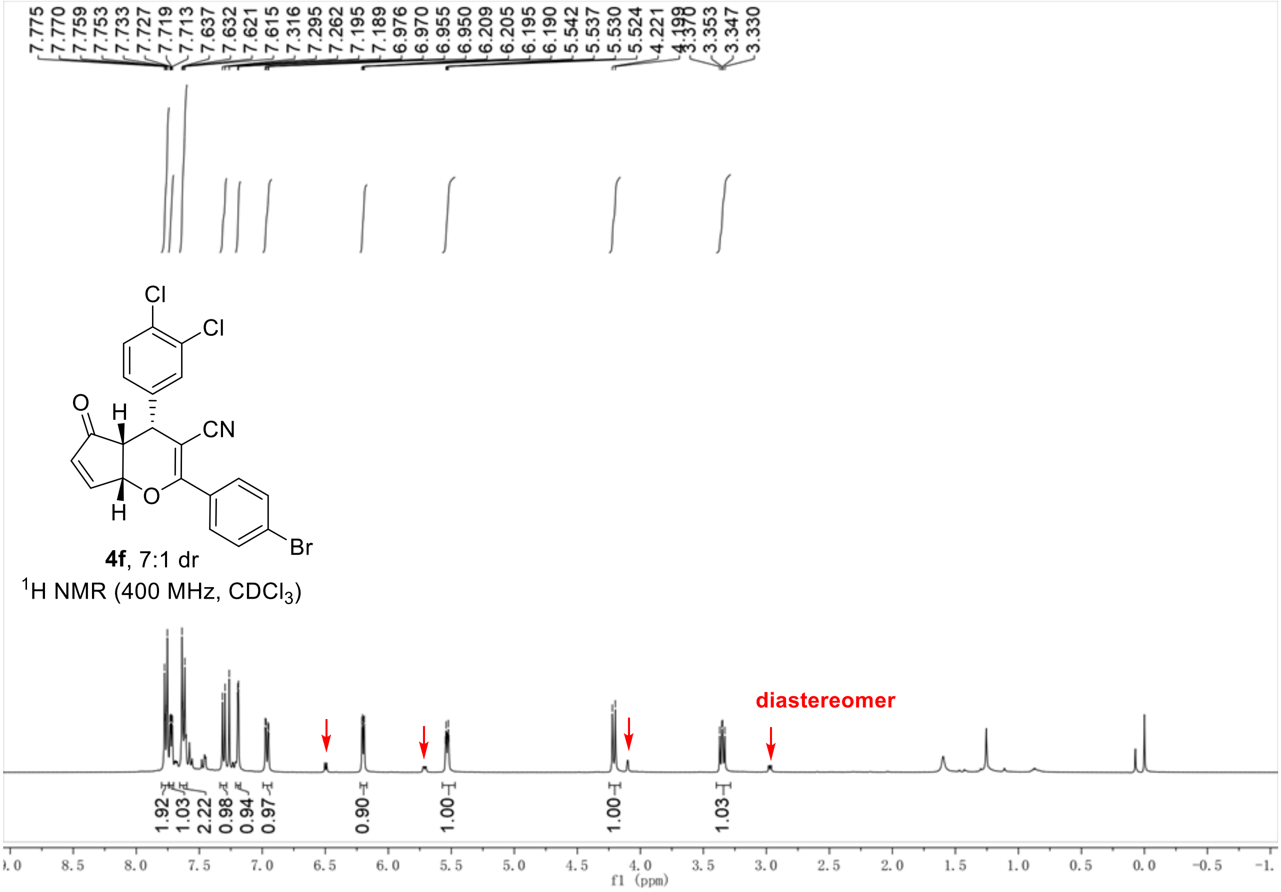
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
15.120	BB	0.36	9.2142	217.0491	1.1317
17.999	BV	0.52	5.8634	201.1309	1.0487
26.334	VV R	0.60	239.5816	9417.1592	49.1010
28.250	VB	0.73	194.0842	9343.8389	48.7187
			Totals:	19179.1781	100.0000

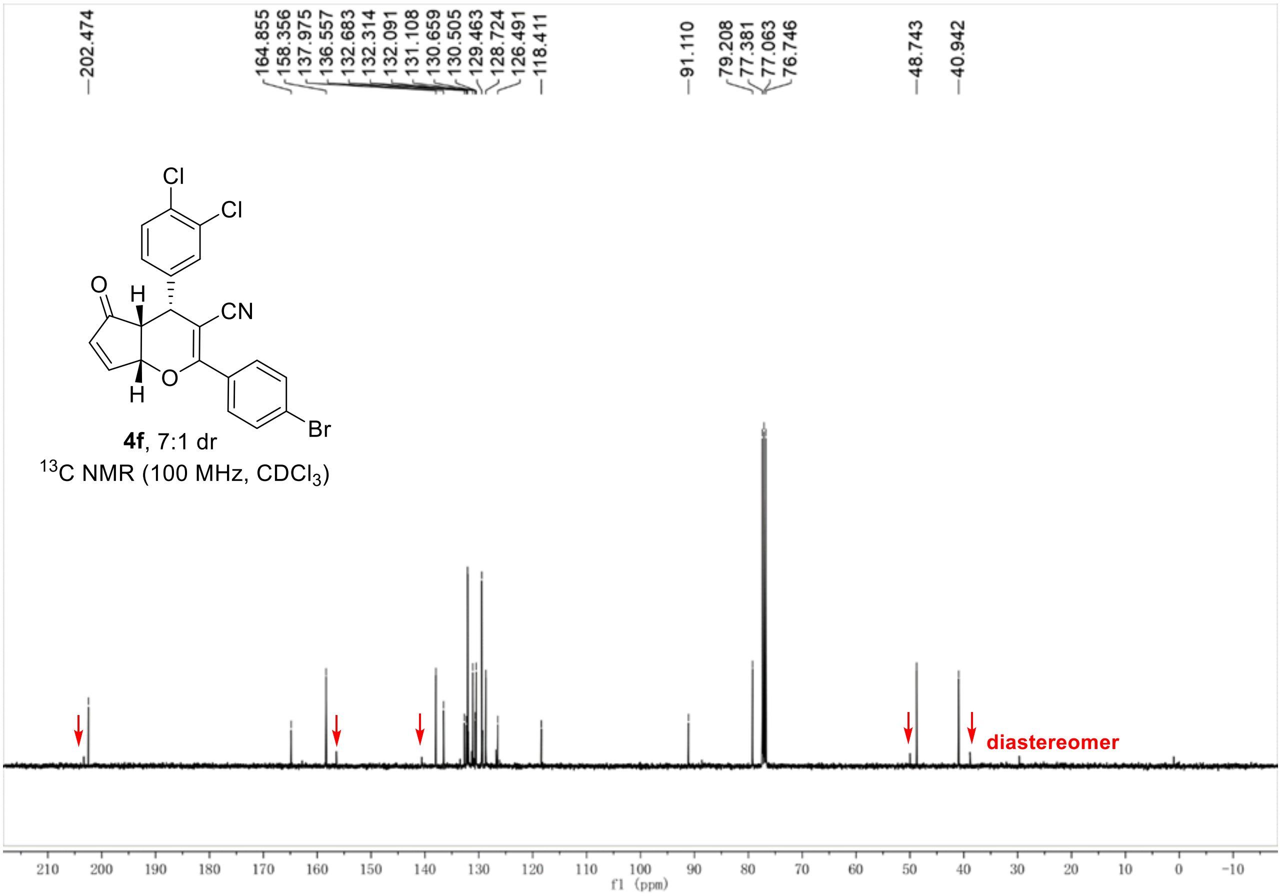


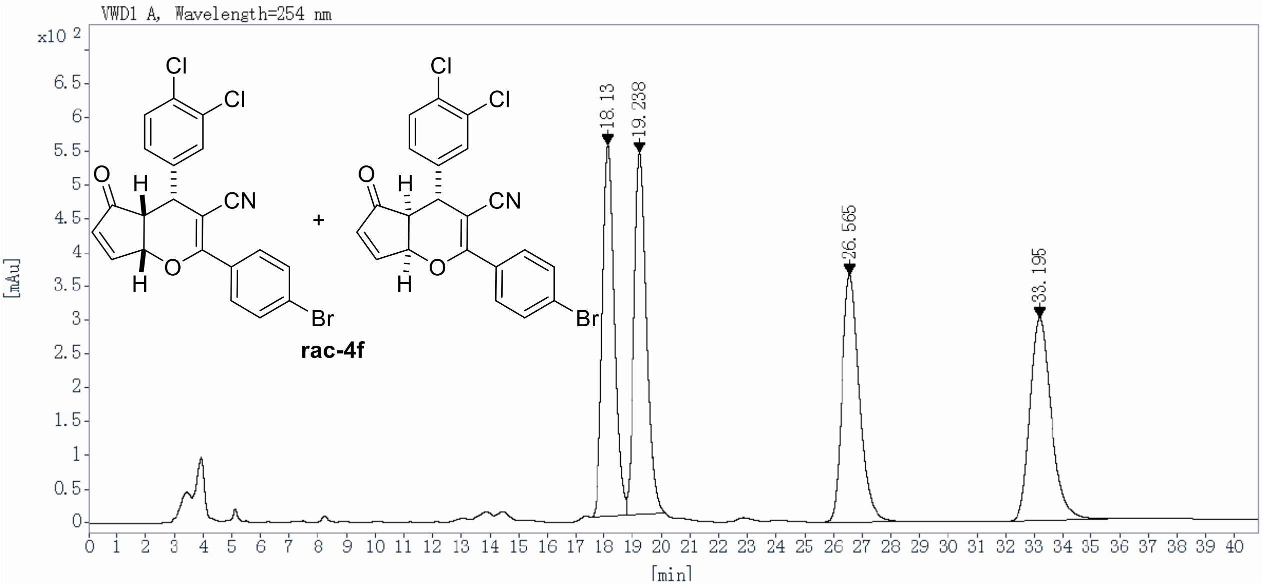
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
14.746	BB	0.43	23.0988	696.2591	7.2967
17.142	BB	0.52	248.8531	8845.8975	92.7033
			Totals:	9542.1566	100.0000


PM (UTC+08:00)
+ESI Scan (rt: 0.604 min) Frag=175.0V CYC-20191011-34.d
x10^6
370.0608
Cl
O
H
CN
H
O
Ph
4e
(ESI-TOF) m/z: [M + Na]+
Calcd for C21H14 35ClNO2Na+ 370.0605
Counts vs. Mass-to-Charge (m/z)

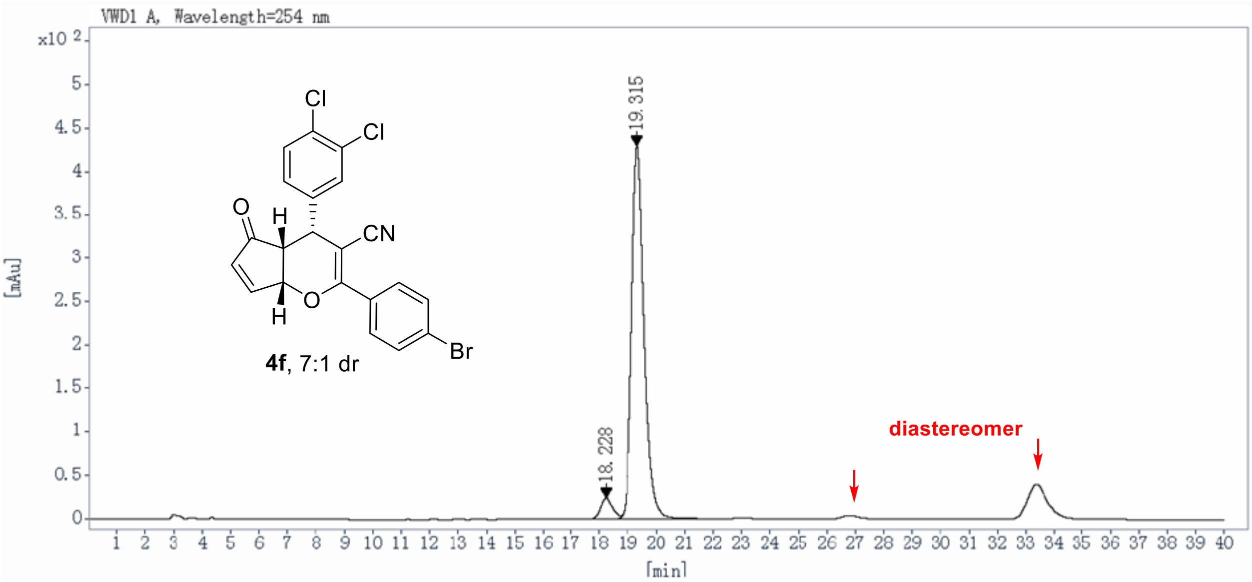

PM (UTC+08:00)
+ESI Scan (rt: 0.604 min) Frag=175.0V CYC-20191011-34.d
x10^4
350.0760
Cl
O
H
CN
H
O
Ph
4e
(ESI-TOF) m/z: [M +H]+
Calcd for C21H15 37ClNO2+ 350.0756
Counts vs. Mass-to-Charge (m/z)


7.775
7.770
7.759
7.753
7.733
7.727
7.719
7.713
7.637
7.632
7.621
7.615
7.316
7.295
7.262
7.195
7.189
6.976
6.970
6.955
6.950
6.209
6.205
6.195
6.190
5.542
5.537
5.530
5.524
4.221
4.199
3.370
3.353
3.347
3.330
Cl
Cl
O
H
CN
H
O
Br
4f, 7:1 dr
^{1}H NMR (400 MHz, $CDCl_3$)
diastereomer
1.92
1.03
2.22
0.98
0.94
0.97
0.90
1.00
1.00
1.03
f1 (ppm)

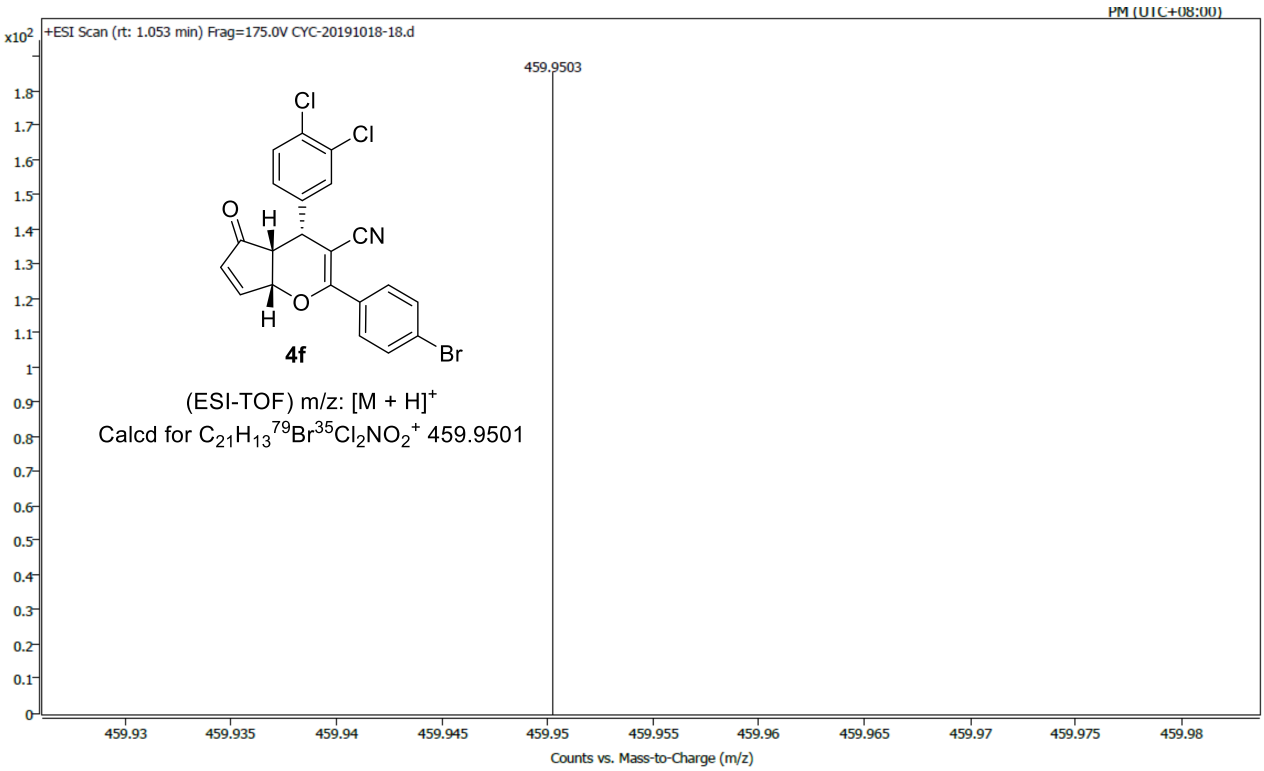

202.474
164.855
158.356
137.975
136.557
132.683
132.314
132.091
131.108
130.659
130.505
129.463
128.724
126.491
118.411
91.110
79.208
77.381
77.063
76.746
48.743
40.942
Cl
Cl
O
H
CN
H
O
Br
4f, 7:1 dr
^{13}C NMR (100 MHz, $CDCl_3$)
diastereomer
f1 (ppm)

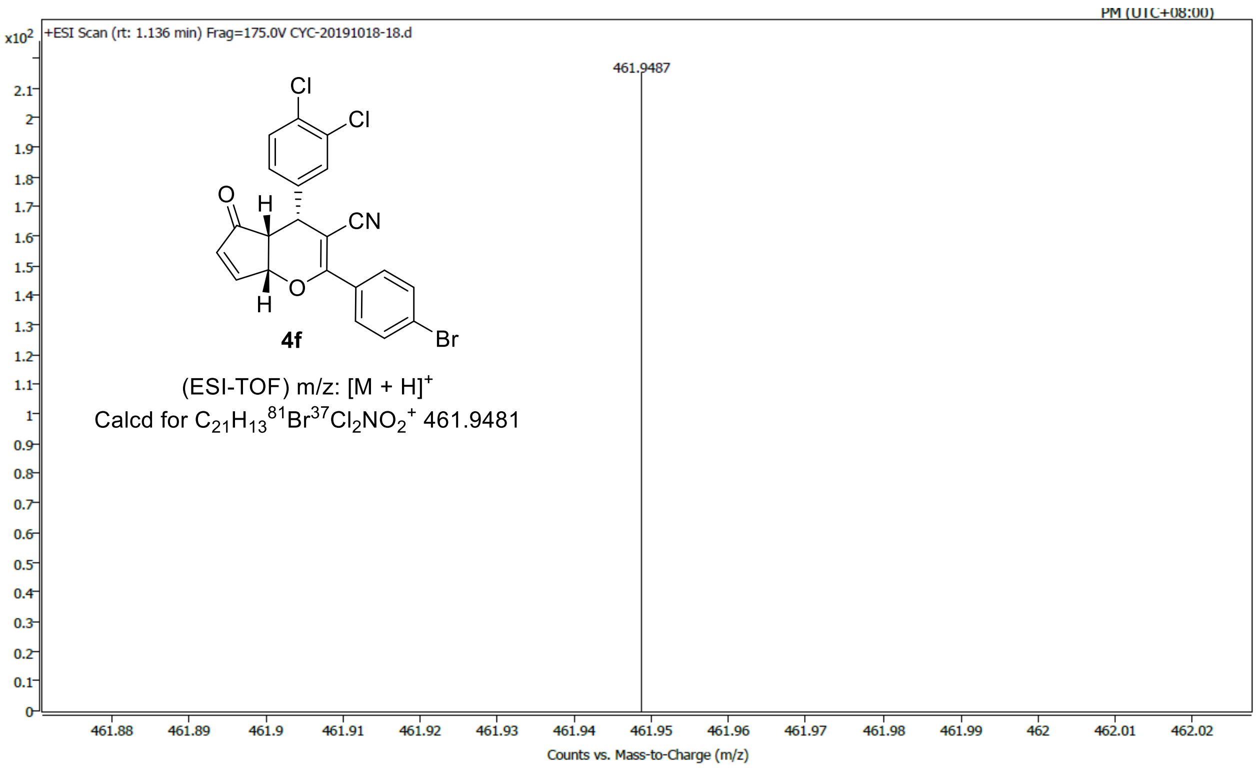


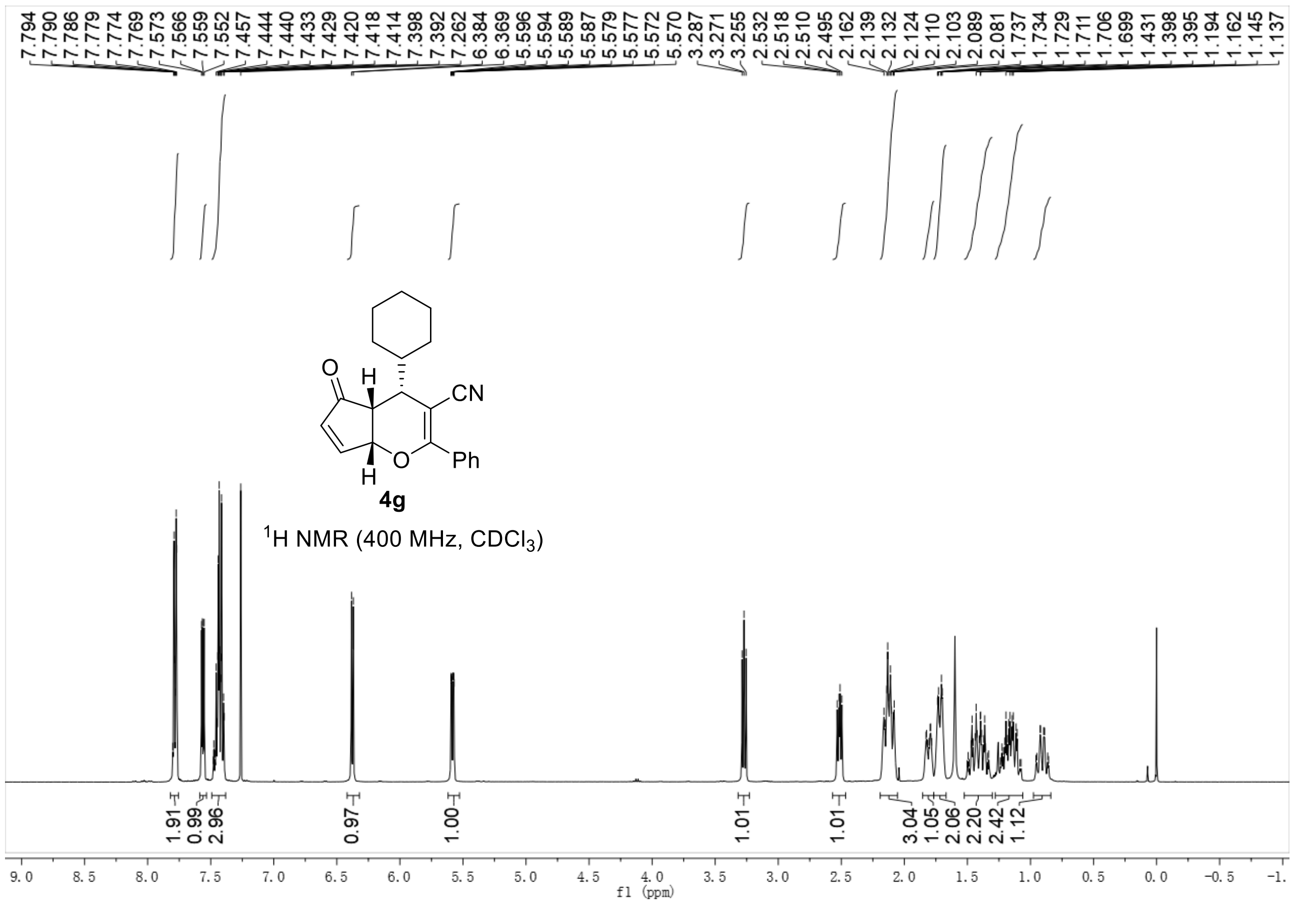
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
18.130	BV	0.45	550.7127	15925.7783	25.2951
19.238	VBA	0.46	536.3328	16159.5137	25.6664
26.565	BB	0.64	366.4348	15355.6523	24.3896
33.195	BB	0.79	300.3666	15518.8682	24.6488
			Totals:	62959.8125	100.0000

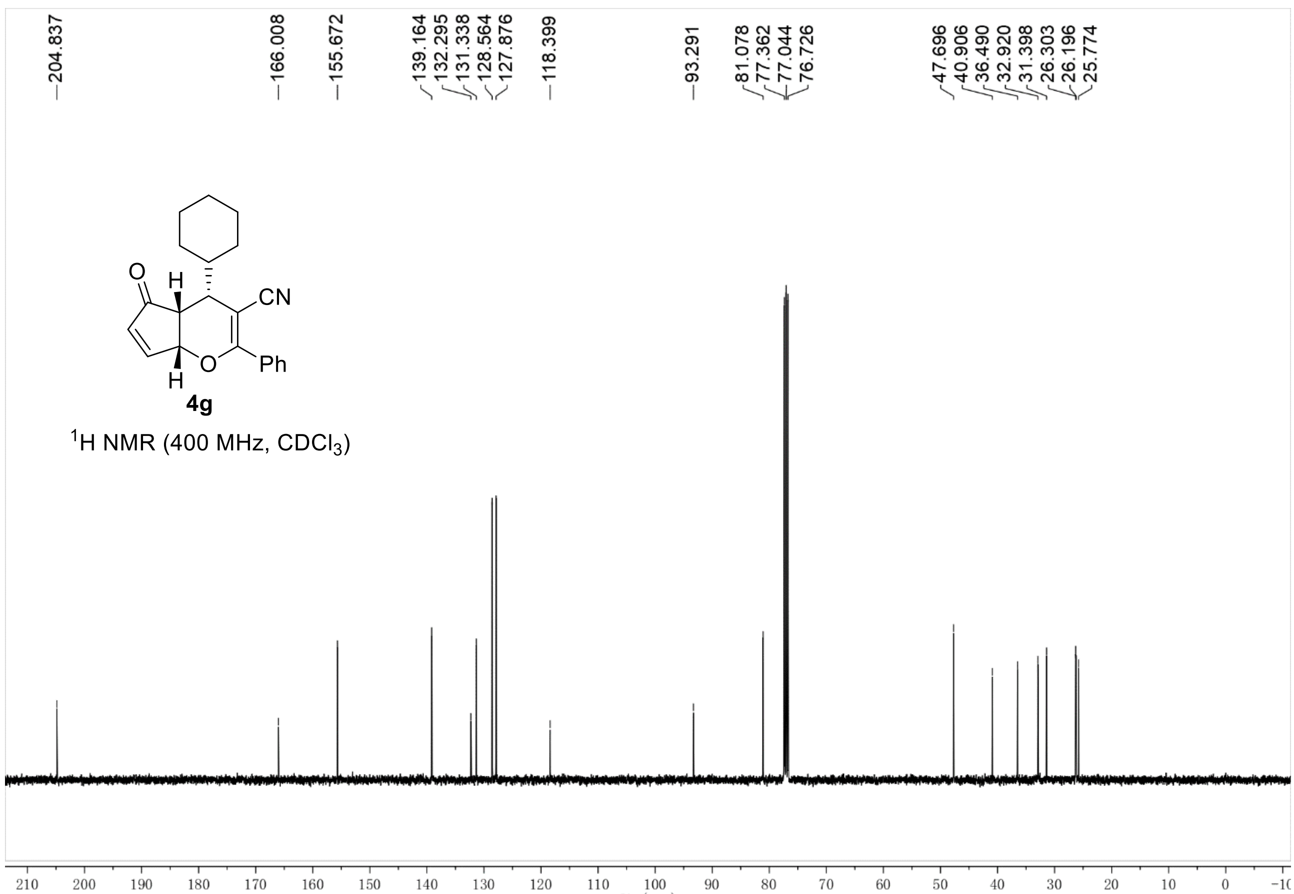


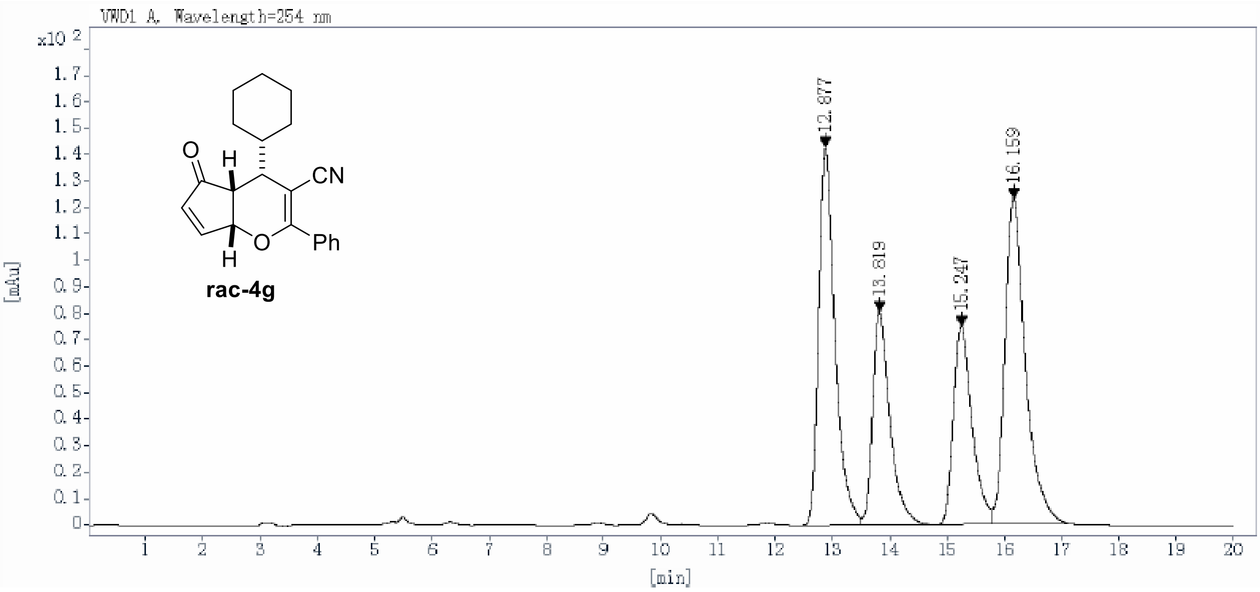
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
18.228	BV E	0.43	24.2505	676.3956	4.9863
19.315	VB R	0.46	429.4350	12888.7764	95.0137
			Totals:	13565.1720	100.0000


PM (UTC+08:00)
+ESI Scan (rt: 1.053 min) Frag=175.0V CYC-20191018-18.d
x10^2
459.9503
4f
(ESI-TOF) m/z: [M + H]+
Calcd for C21H13 79Br35Cl2NO2+ 459.9501
Counts vs. Mass-to-Charge (m/z)

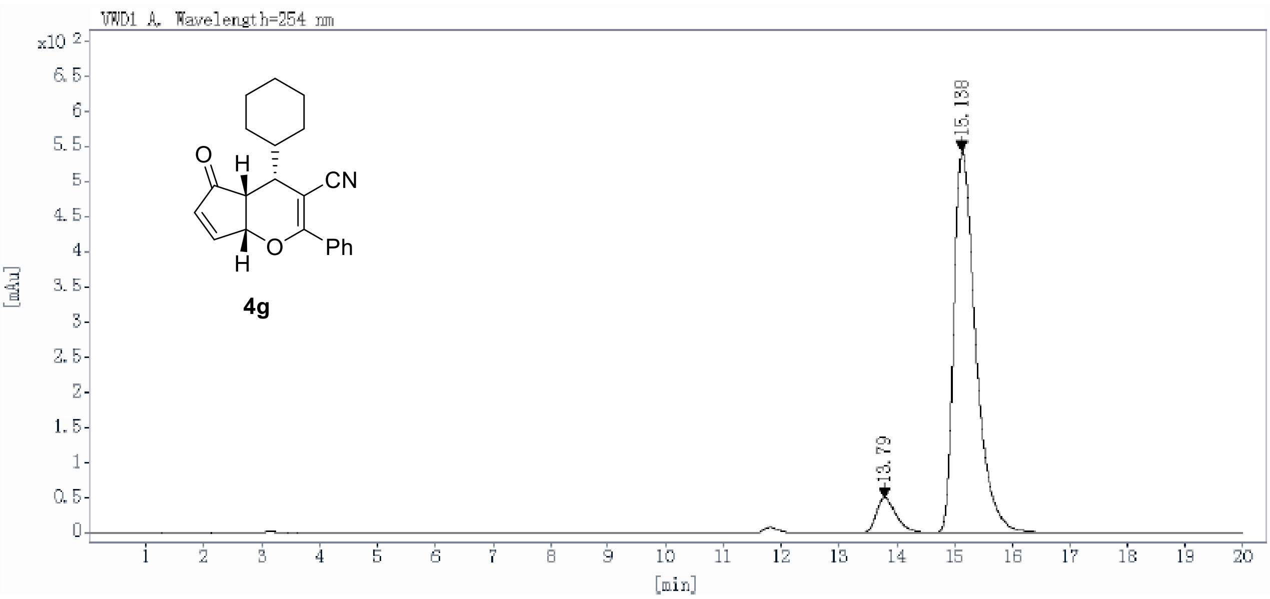

PM (UTC+08:00)
+ESI Scan (rt: 1.136 min) Frag=175.0V CYC-20191018-18.d
x10^2
461.9487
4f
(ESI-TOF) m/z: [M + H]+
Calcd for C21H13 81Br37Cl2NO2+ 461.9481
Counts vs. Mass-to-Charge (m/z)


7.794 7.790 7.786 7.779 7.774 7.769 7.573 7.566 7.559 7.552 7.457 7.444 7.440 7.433 7.429 7.420 7.418 7.414 7.398 7.392 7.262 6.384 6.369 5.596 5.594 5.589 5.587 5.579 5.577 5.572 5.570 3.287 3.271 3.255 2.532 2.518 2.510 2.495 2.162 2.139 2.132 2.124 2.110 2.103 2.089 2.081 1.737 1.734 1.729 1.711 1.706 1.699 1.431 1.398 1.395 1.194 1.162 1.145 1.137
O
H
CN
O
Ph
H
4g
1H NMR (400 MHz, CDCl3)
1.91 0.99 2.96 0.97 1.00 1.01 1.01 3.04 1.05 2.06 2.20 2.42 1.12
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)

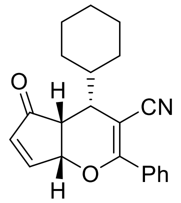

204.837 166.008 155.672 139.164 132.295 131.338 128.564 127.876 118.399 93.291 81.078 77.362 77.044 76.726 47.696 40.906 36.490 32.920 31.398 26.303 26.196 25.774
O
H
CN
O
Ph
H
4g
1H NMR (400 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
12.877	BV	0.30	142.6112	2833.3311	30.4664
13.819	VB	0.32	80.4895	1696.7388	18.2448
15.247	BV	0.34	74.8907	1690.3802	18.1764
16.159	VBA	0.38	122.9815	3079.4075	33.1124
			Totals:	9299.8575	100.0000



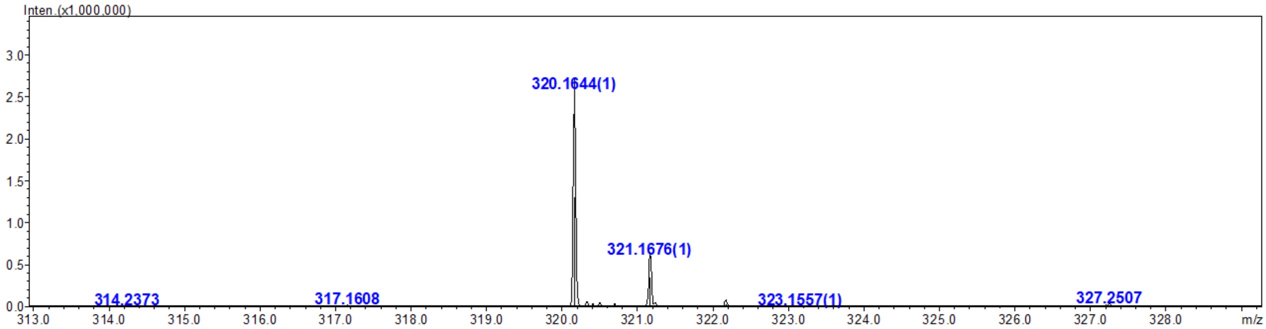
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
13.790	BB	0.36	49.2888	1161.0352	7.5383
15.138	BBA	0.41	541.8414	14240.7871	92.4617
			Totals:	15401.8223	100.0000

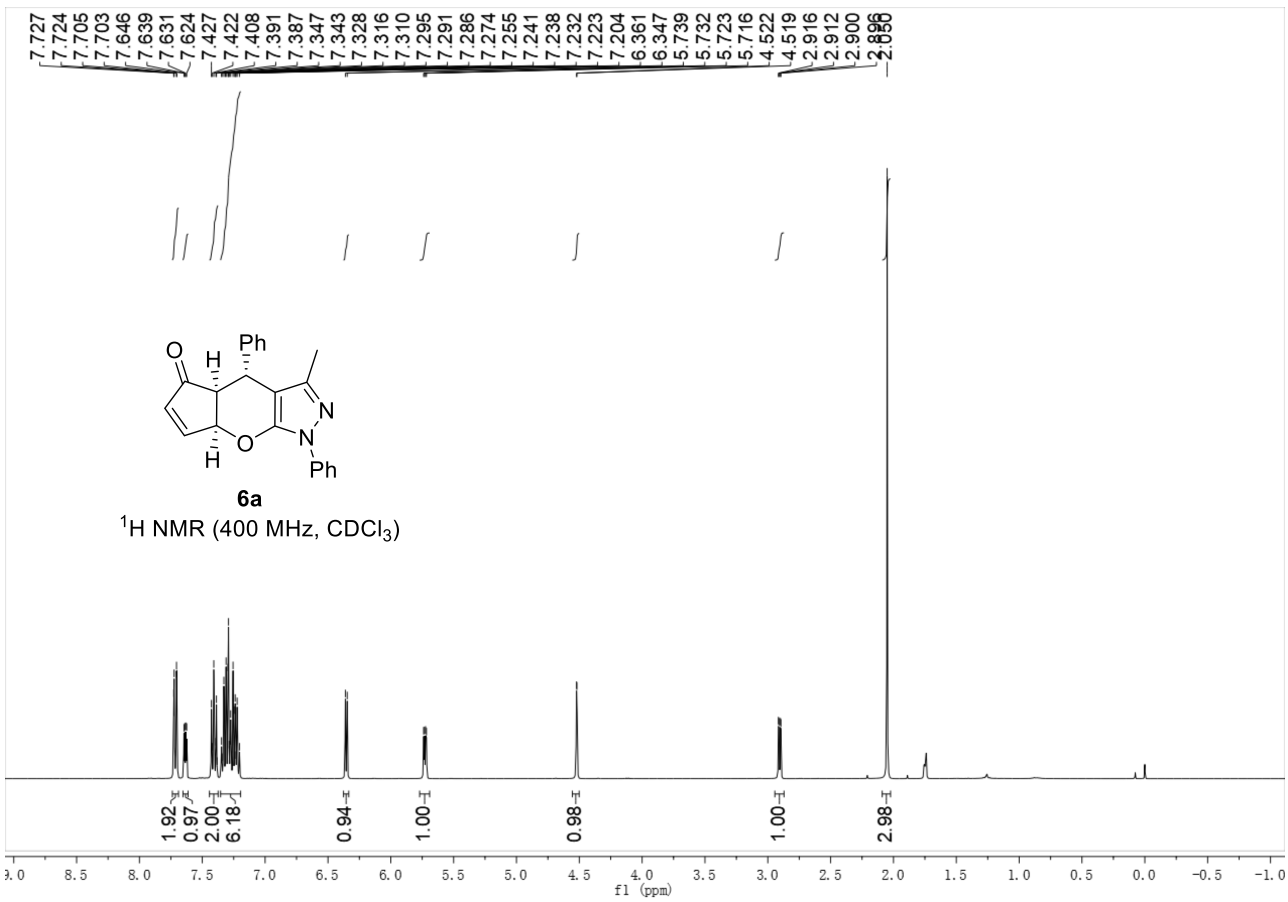


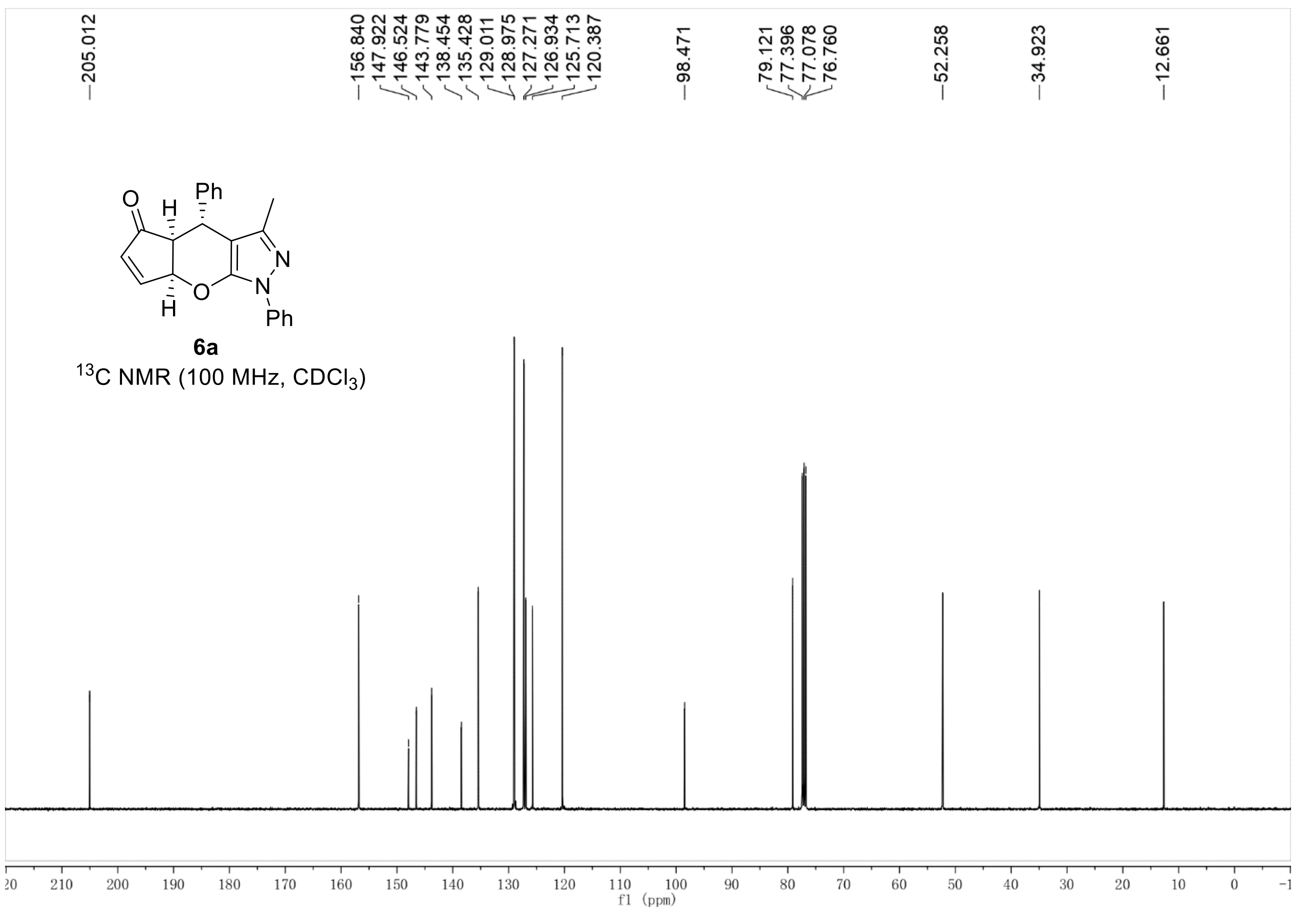
4g

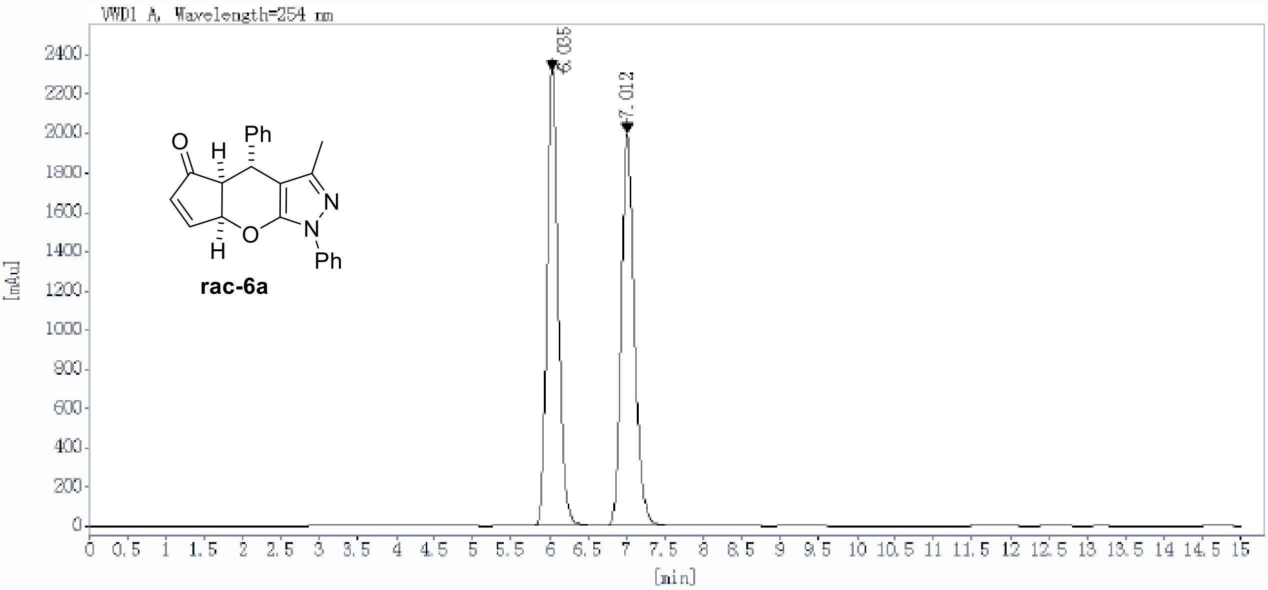
(ESI-TOF) m/z: $[M+H]^+$

Calcd for $C_{21}H_{22}NO_2^+$ 320.1645

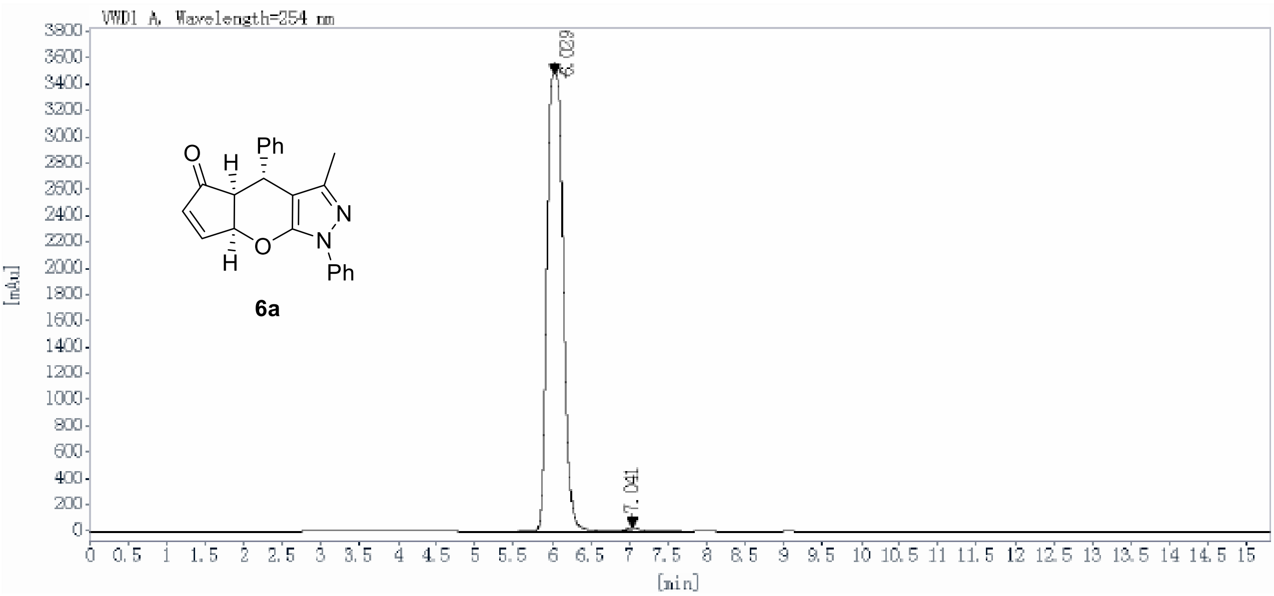



7.727
7.724
7.705
7.703
7.646
7.639
7.631
7.624
7.427
7.422
7.408
7.391
7.387
7.347
7.343
7.328
7.316
7.310
7.295
7.291
7.286
7.274
7.255
7.241
7.238
7.232
7.223
7.204
6.361
6.347
5.739
5.732
5.723
5.716
4.522
4.519
2.916
2.912
2.900
2.896
2.050
6a
1H NMR (400 MHz, CDCl3)
1.92
0.97
2.00
6.18
0.94
1.00
0.98
1.00
2.98
f1 (ppm)

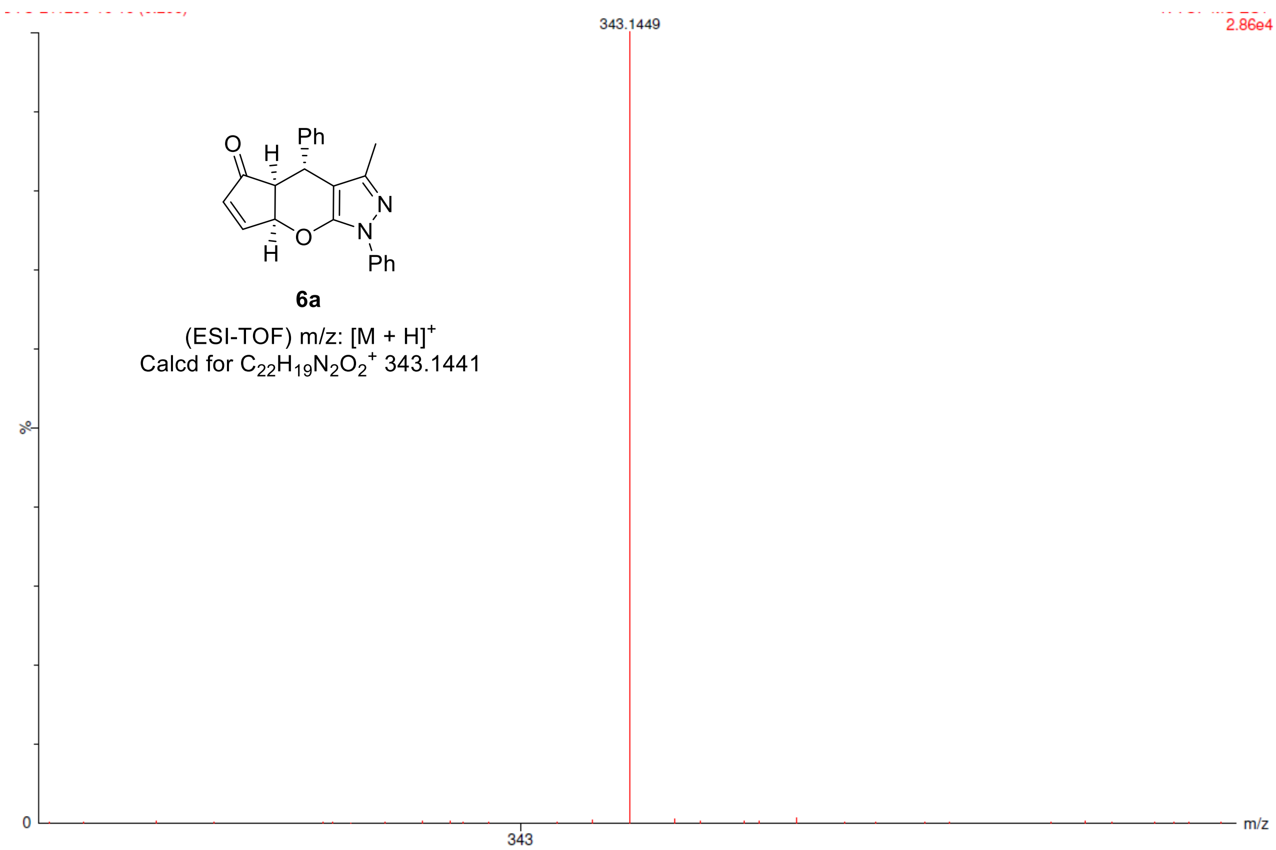

205.012
156.840
147.922
146.524
143.779
138.454
135.428
129.011
128.975
127.271
126.934
125.713
120.387
98.471
79.121
77.396
77.078
76.760
52.258
34.923
12.661
6a
13C NMR (100 MHz, CDCl3)
f1 (ppm)

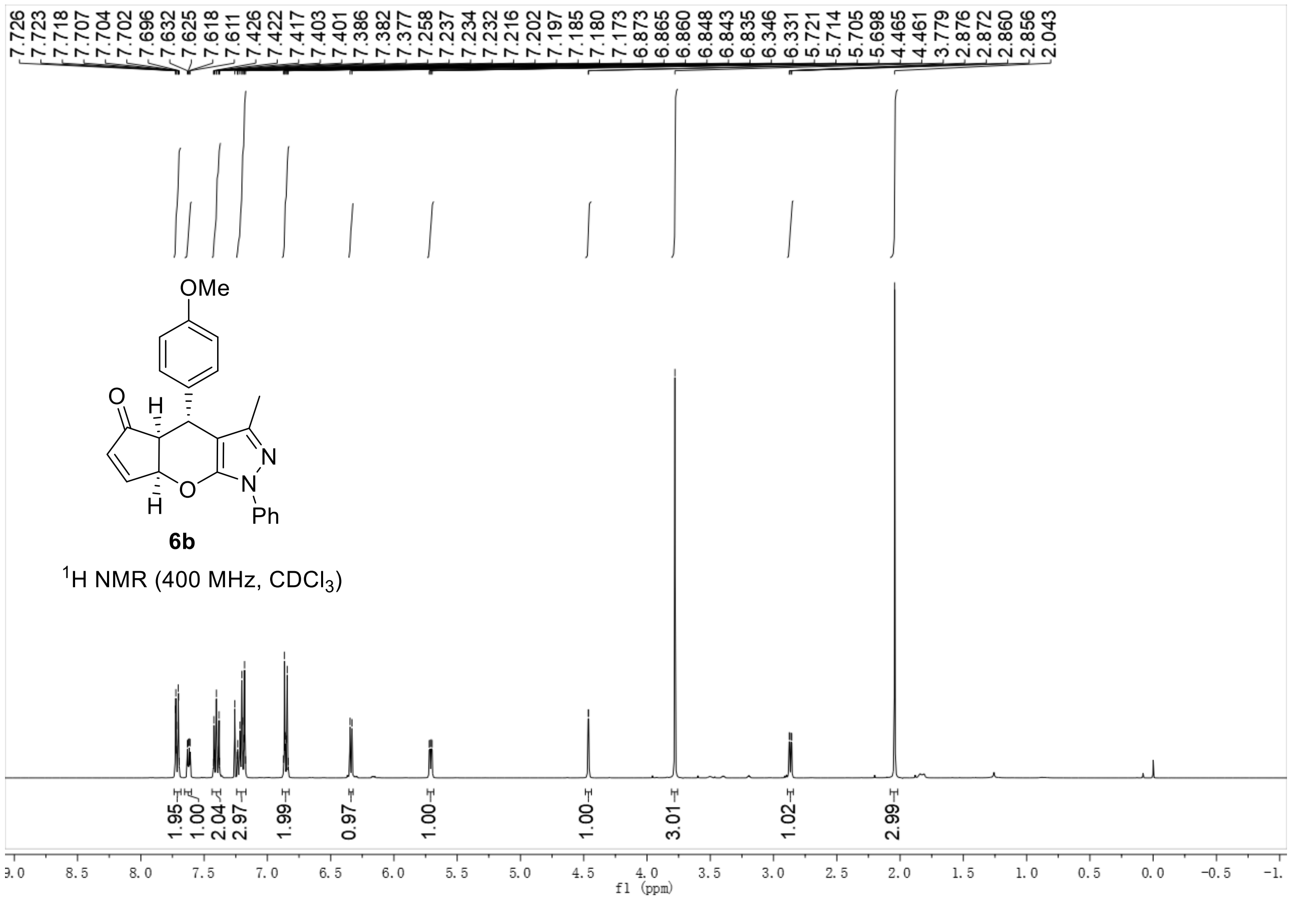


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
6.035	BB	0.15	2323.3459	23177.2988	49.9703
7.012	BBA	0.17	1999.8958	23204.8262	50.0297
			Totals:	46382.1250	100.0000



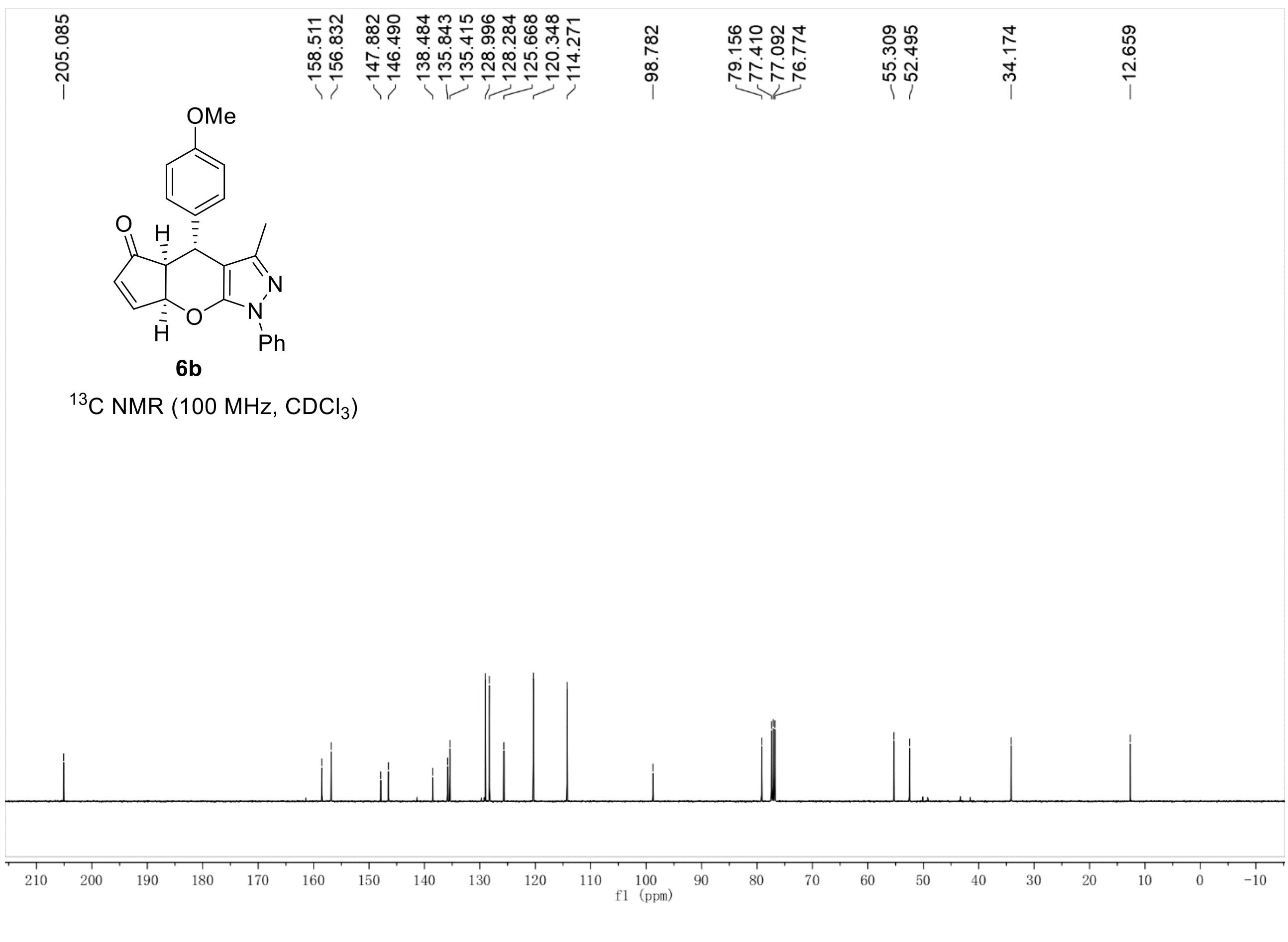
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
6.029	VV R	0.23	3481.2048	50506.1758	99.1479
7.041	VB E	0.21	29.4845	434.0825	0.8521
			Totals:	50940.2582	100.0000


343.1449
2.86e4
Ph
O
H
N
N
O
H
Ph
6a
(ESI-TOF) m/z: [M + H]$^+$
Calcd for $C_{22}H_{19}N_2O_2^+$ 343.1441
%
0
343
m/z



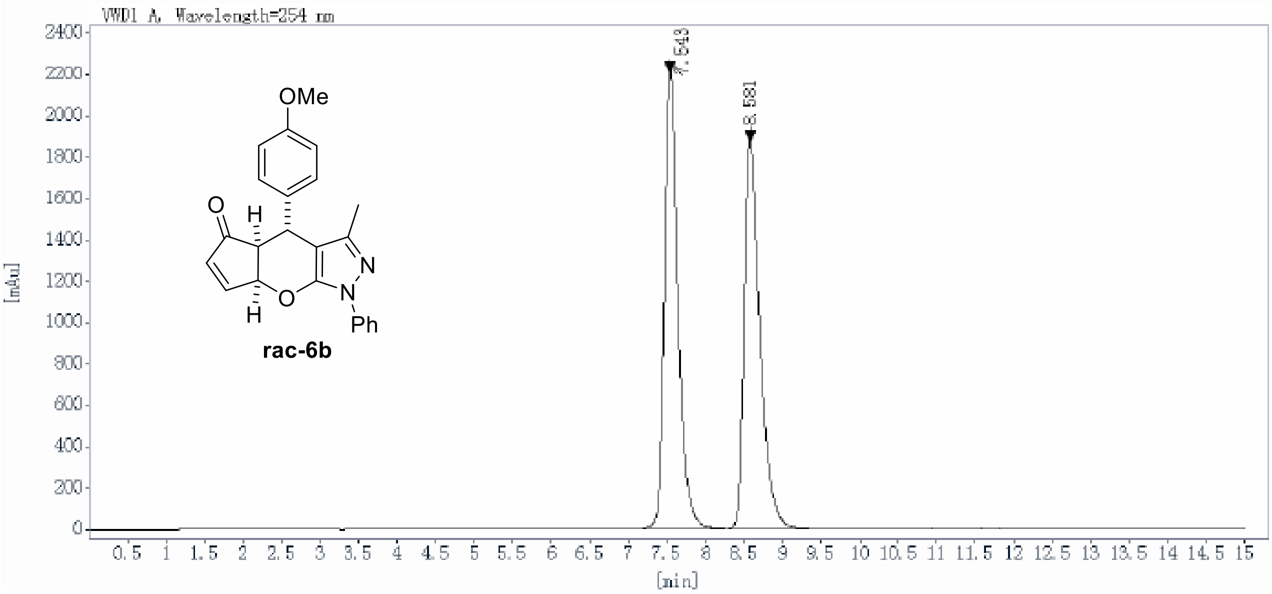
6b

^1H NMR (400 MHz, $CDCl_3$)

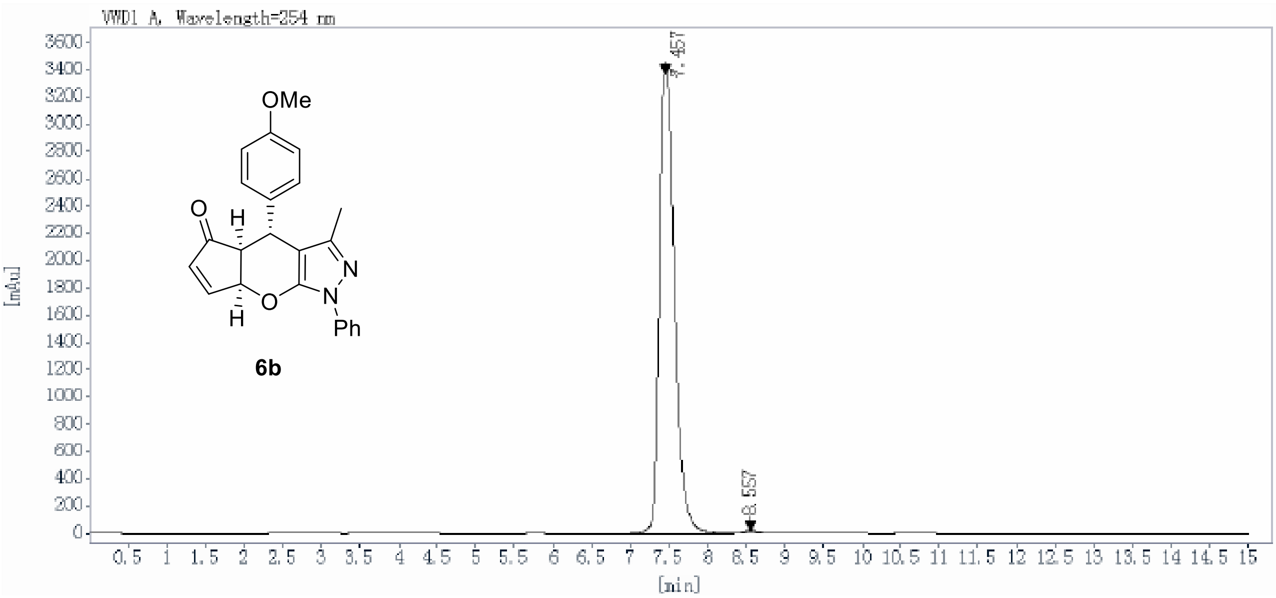


6b

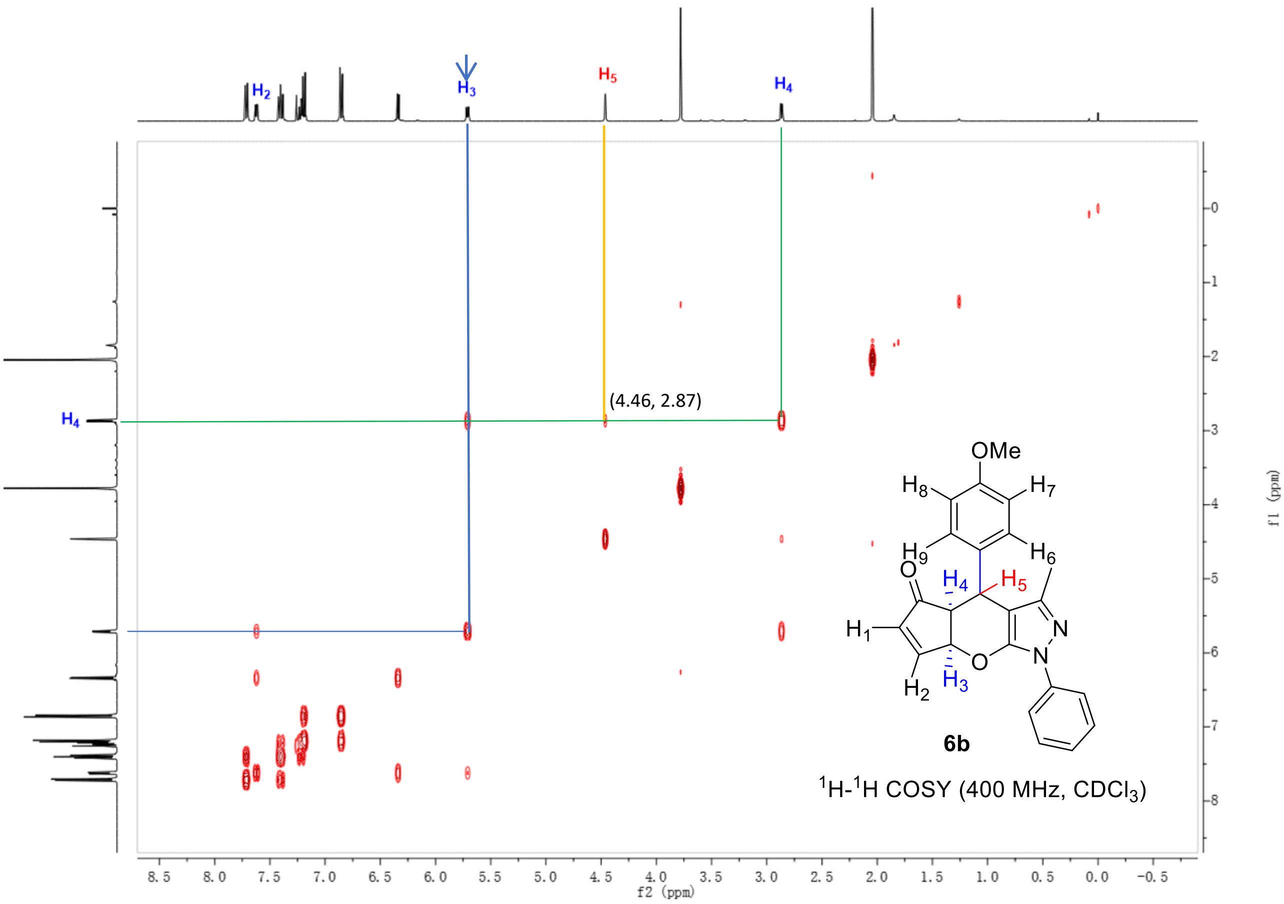
^{13}C NMR (100 MHz, $CDCl_3$)



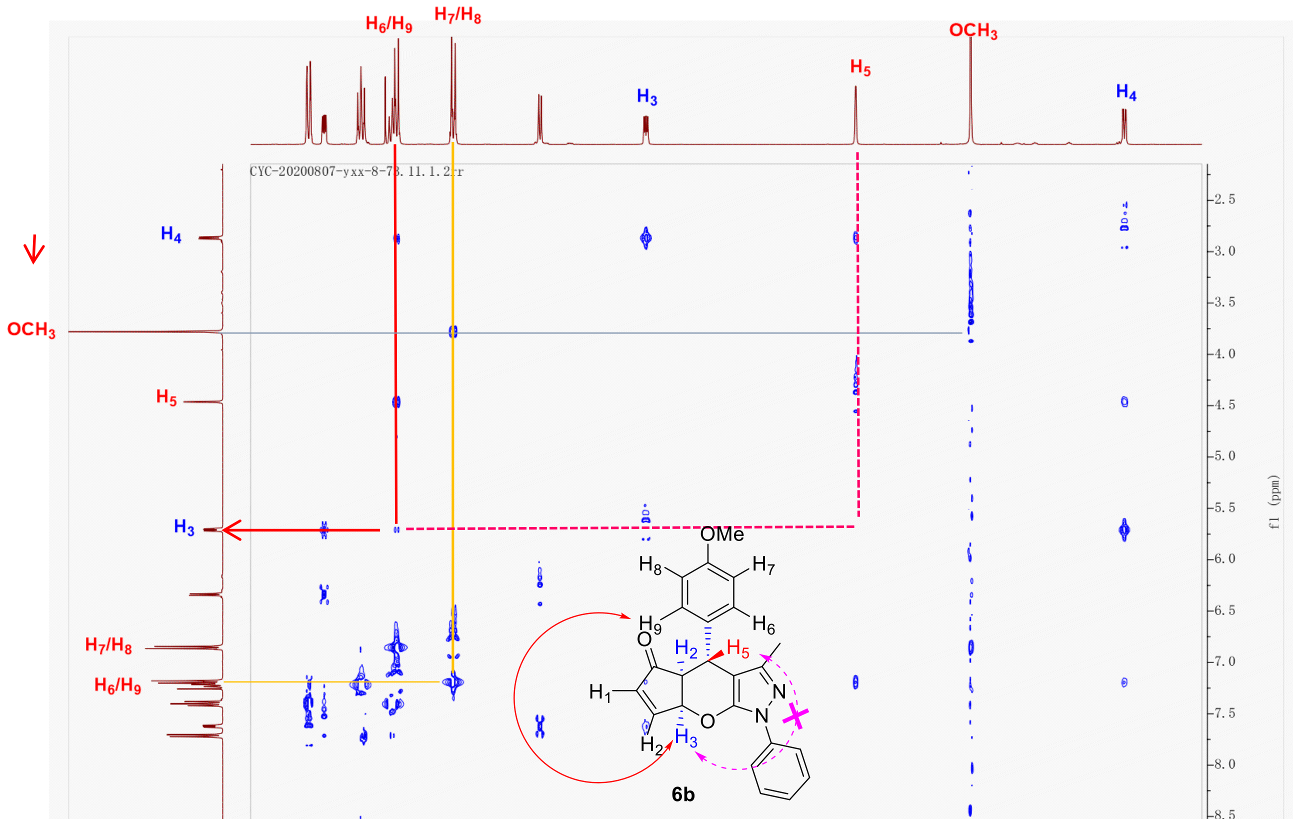
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
7.543	BB	0.18	2213.2488	27012.1094	50.1838
8.581	BBA	0.21	1876.7942	26814.2461	49.8162
			Totals:	53826.3555	100.0000



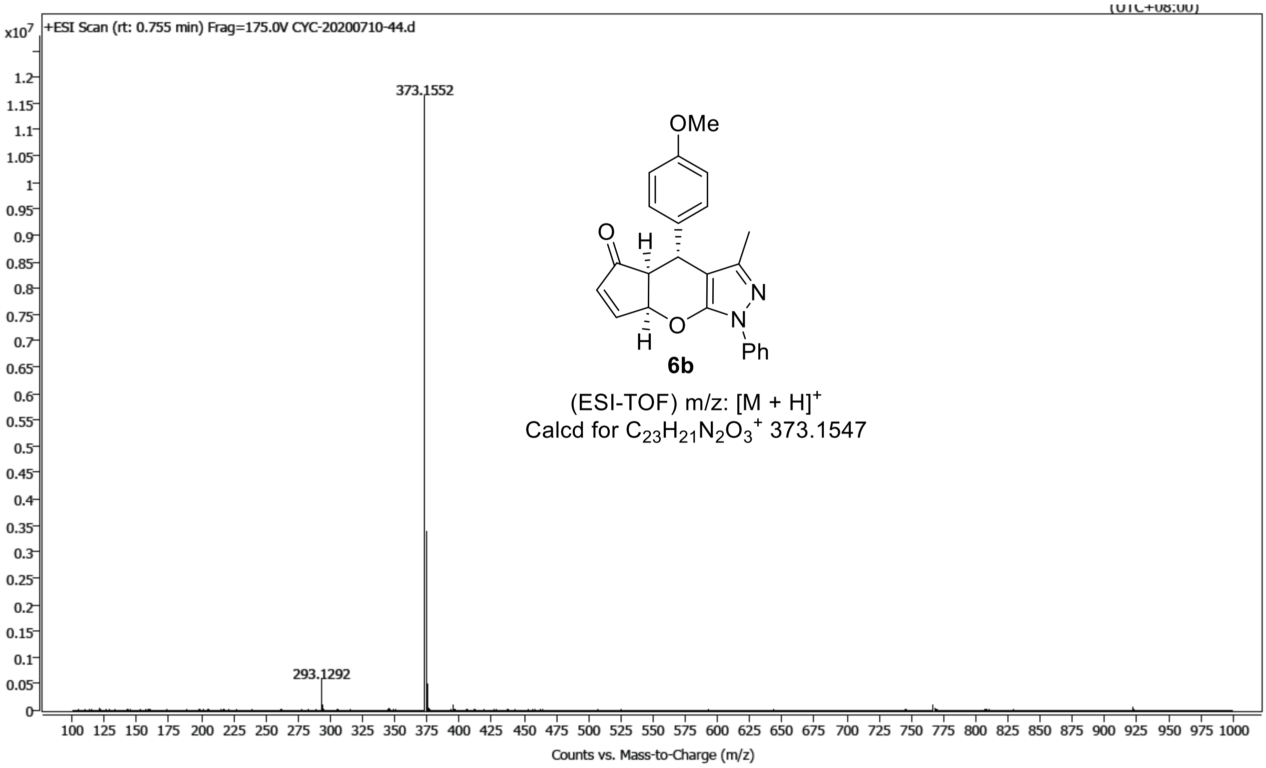
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
7.457	BV R	0.21	3370.2249	46629.3516	99.2244
8.557	VB E	0.26	19.8815	364.4952	0.7756
			Totals:	46993.8468	100.0000

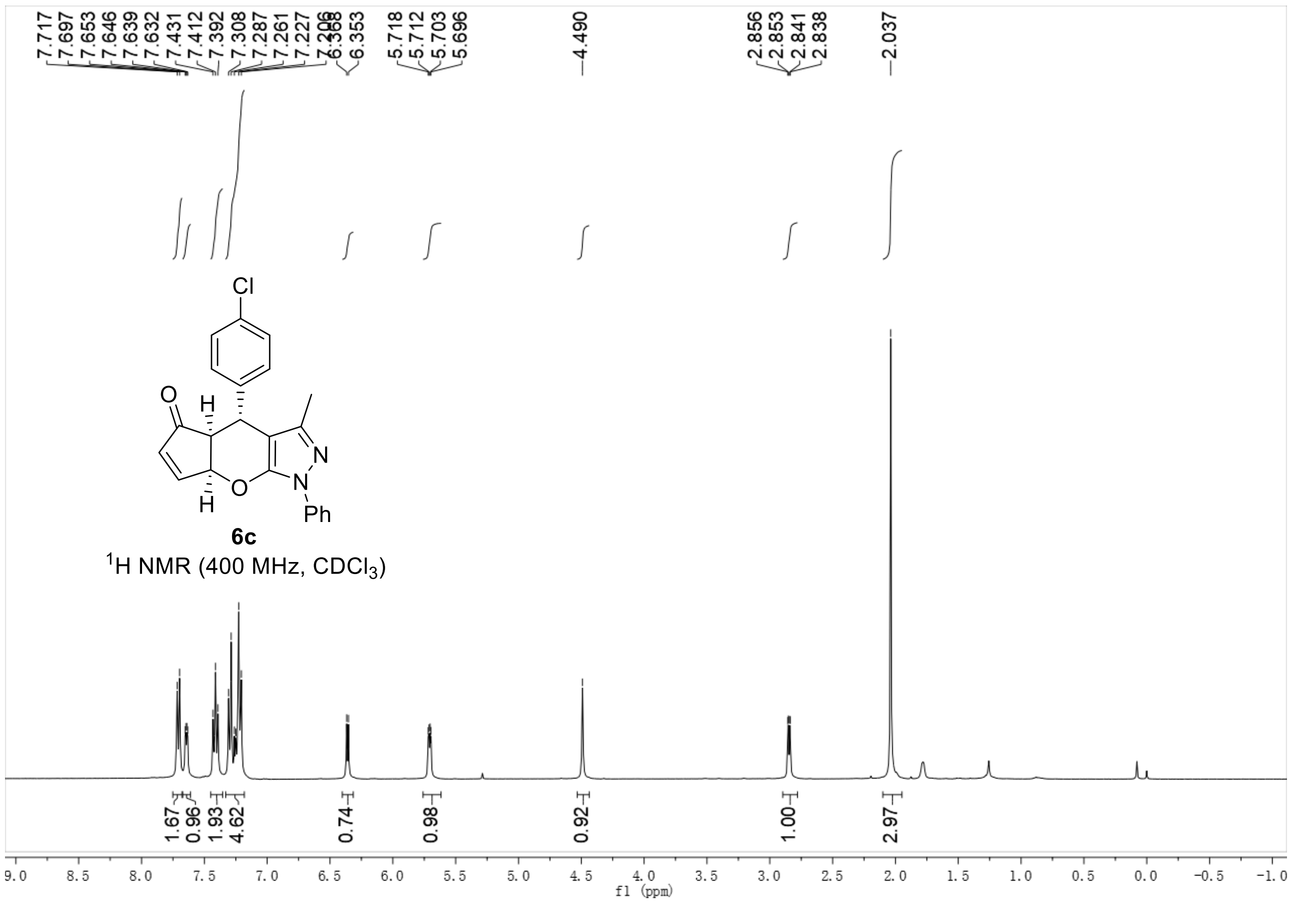


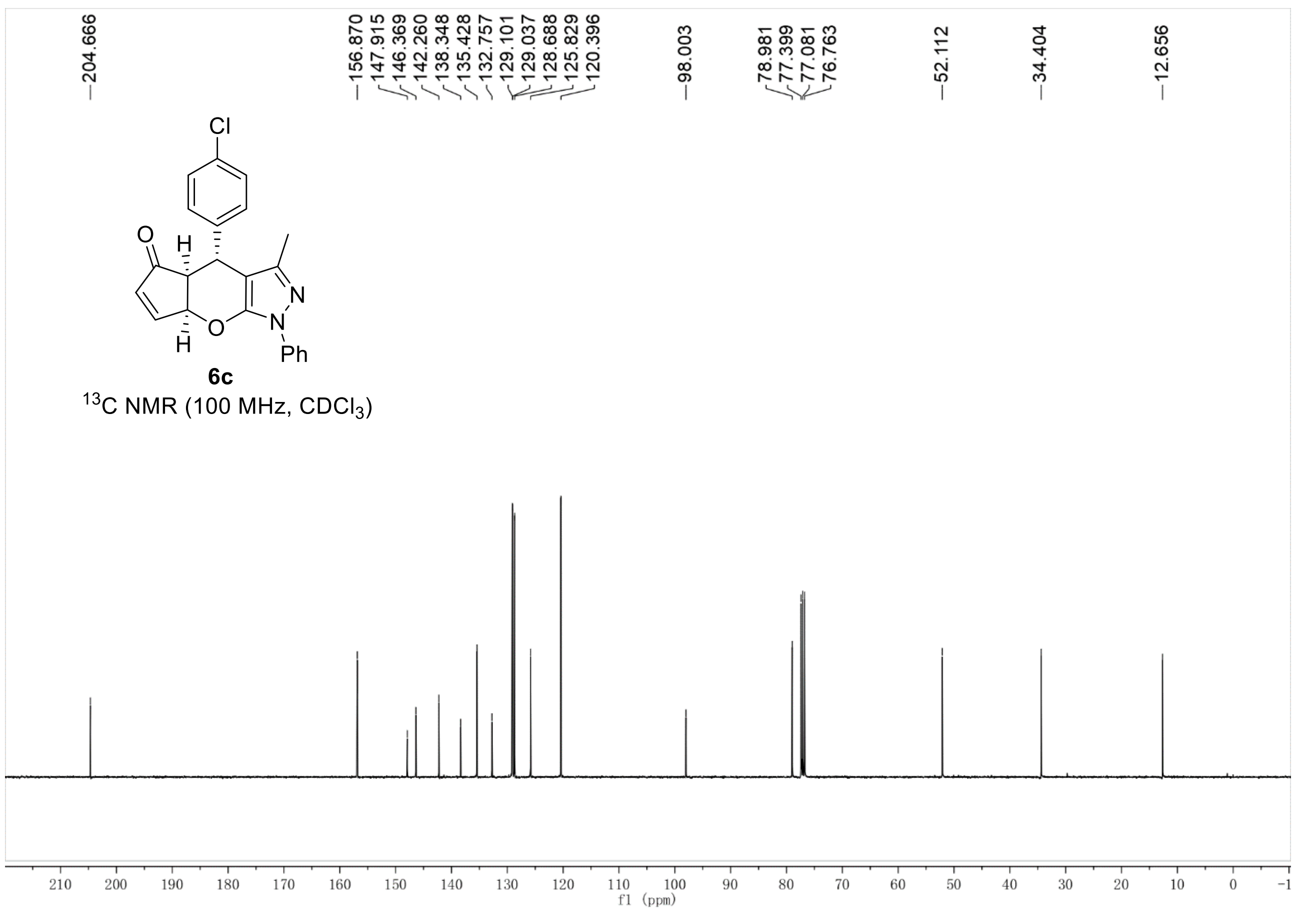
^{1}H-^{1}H COSY (400 MHz, $CDCl_3$)

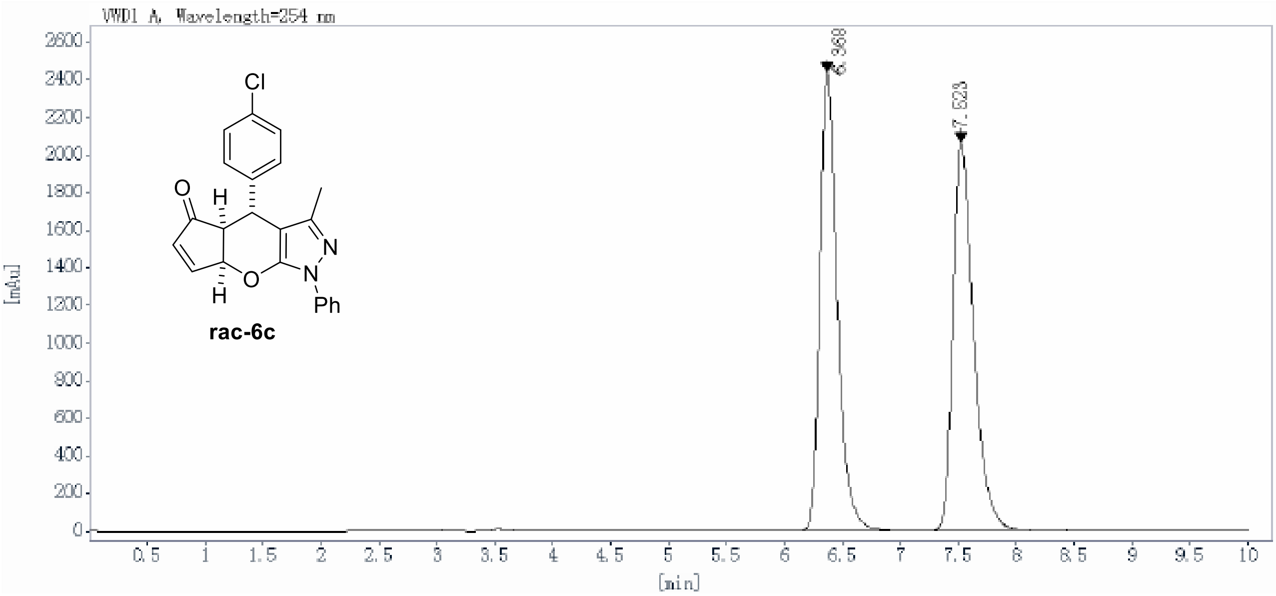


NOESY (400 MHz, $CDCl_3$)

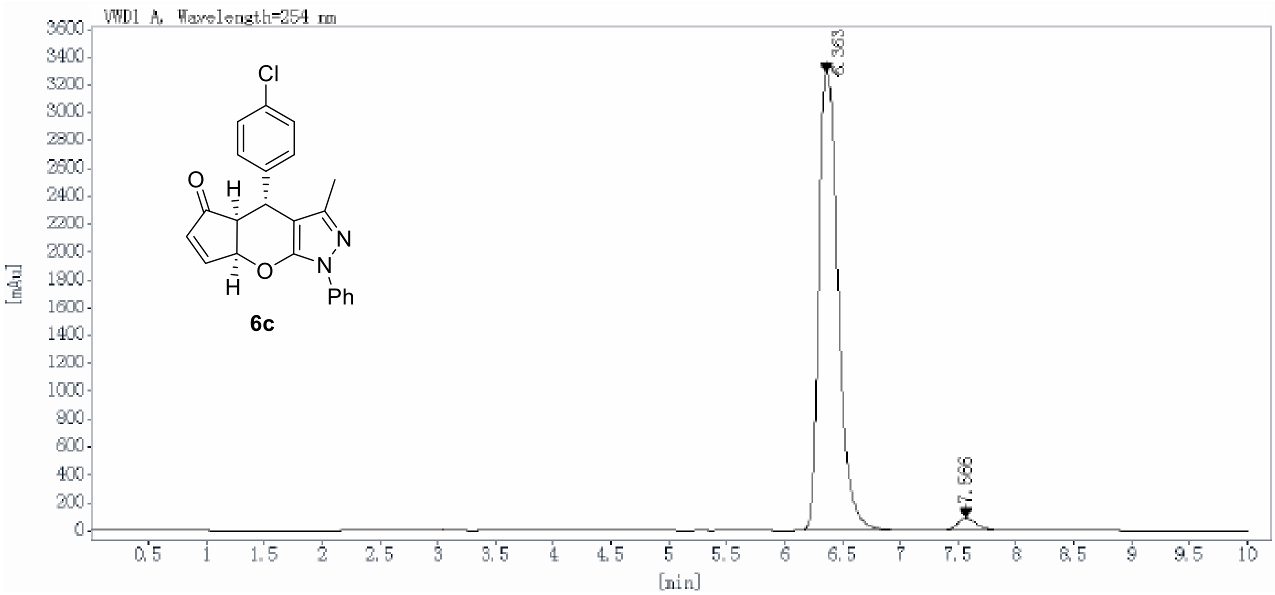

(UTC+08:00)
x10^7
+ESI Scan (rt: 0.755 min) Frag=175.0V CYC-20200710-44.d
373.1552
293.1292
OMe
O
H
H
O
N
N
Ph
6b
(ESI-TOF) m/z: [M + H]$^+$
Calcd for $C_{23}H_{21}N_2O_3^+$ 373.1547
Counts vs. Mass-to-Charge (m/z)


7.717
7.697
7.653
7.646
7.639
7.632
7.431
7.412
7.392
7.308
7.287
7.261
7.227
7.206
6.368
6.353
5.718
5.712
5.703
5.696
4.490
2.856
2.853
2.841
2.838
2.037
Cl
O
H
N
N
O
H
Ph
6c
^{1}H NMR (400 MHz, $CDCl_3$)
1.67
0.96
1.93
4.62
0.74
0.98
0.92
1.00
2.97
f1 (ppm)

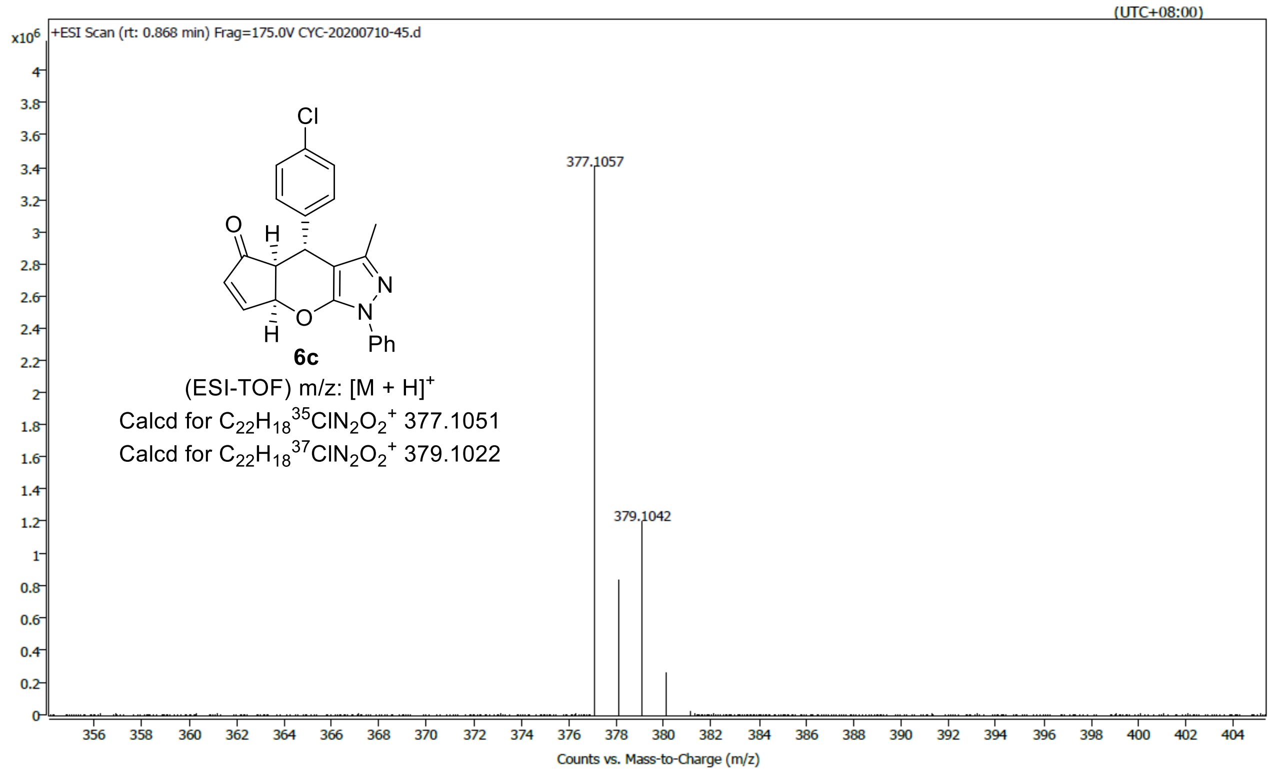

204.666
156.870
147.915
146.369
142.260
138.348
135.428
132.757
129.101
129.037
128.688
125.829
120.396
98.003
78.981
77.399
77.081
76.763
52.112
34.404
12.656
Cl
O
H
N
N
O
H
Ph
6c
^{13}C NMR (100 MHz, $CDCl_3$)
f1 (ppm)

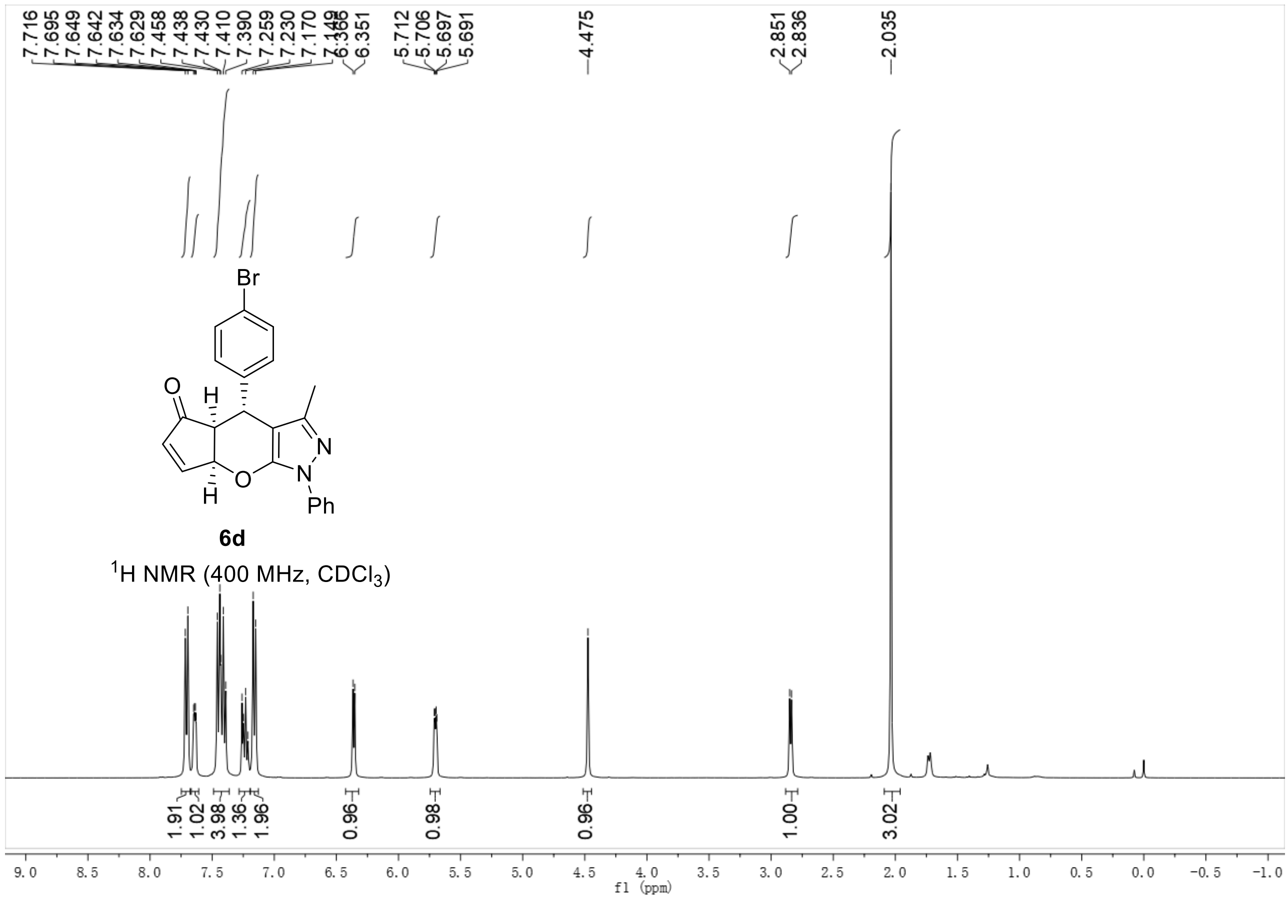


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
6.368	BBA	0.16	2440.3694	25342.8145	49.9289
7.523	BBA	0.19	2060.0010	25415.0410	50.0711
			Totals:	50757.8555	100.0000

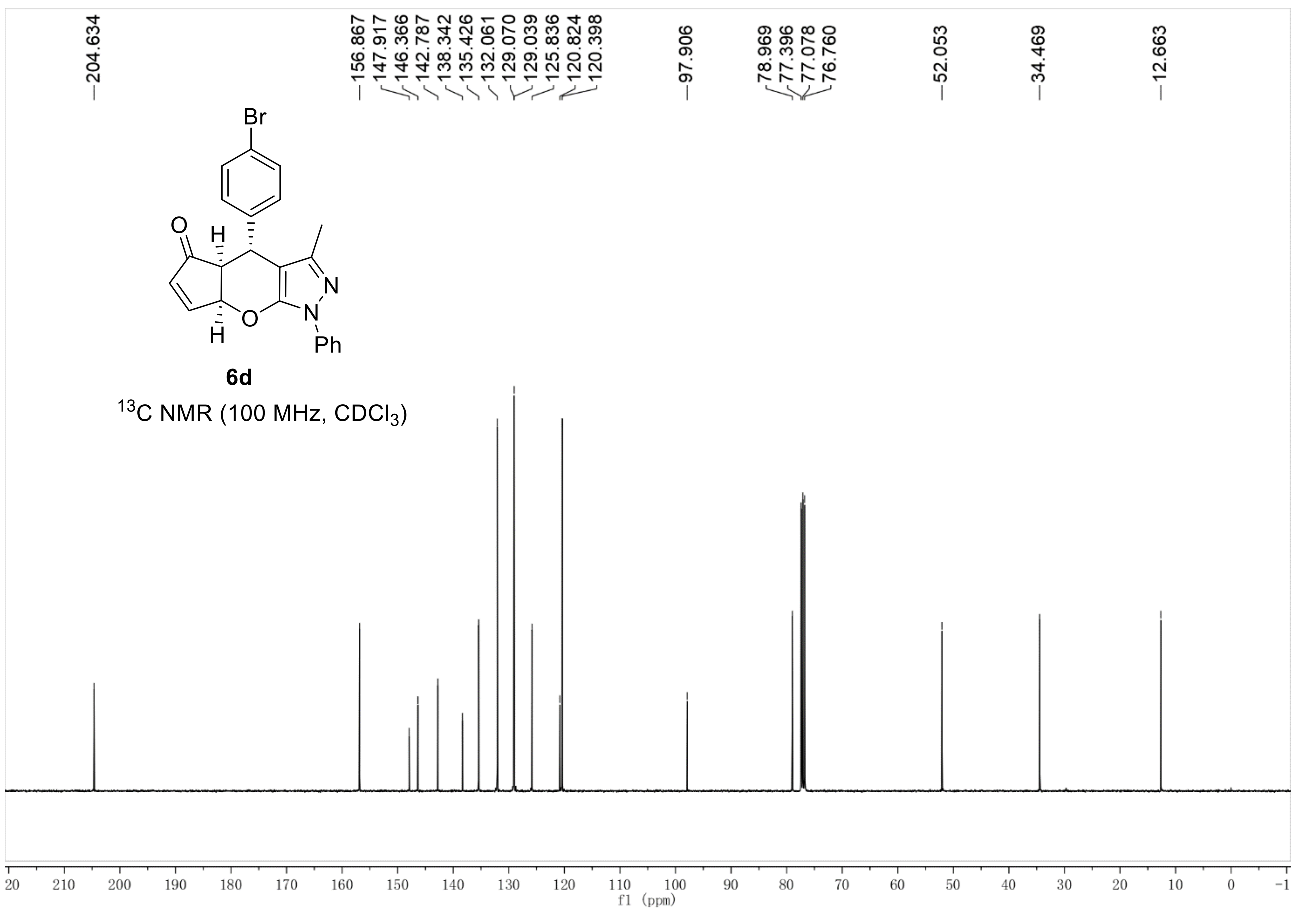


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
6.363	BBA	0.18	3286.7825	38264.1719	97.3903
7.566	BB	0.18	85.2903	1025.3364	2.6097
			Totals:	39289.5083	100.0000

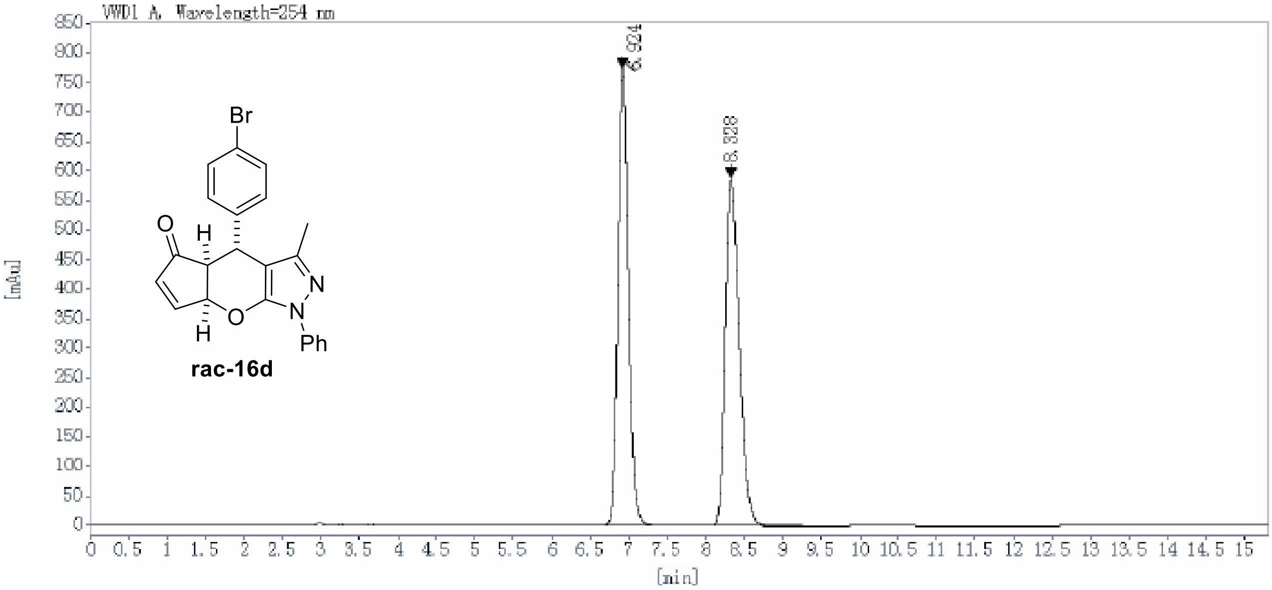

(UTC+08:00)
x10^6
+ESI Scan (rt: 0.868 min) Frag=175.0V CYC-20200710-45.d
Cl
O
H
H
N
N
O
Ph
6c
(ESI-TOF) m/z: [M + H]+
Calcd for C22H18 35ClN2O2+ 377.1051
Calcd for C22H18 37ClN2O2+ 379.1022
377.1057
379.1042
Counts vs. Mass-to-Charge (m/z)



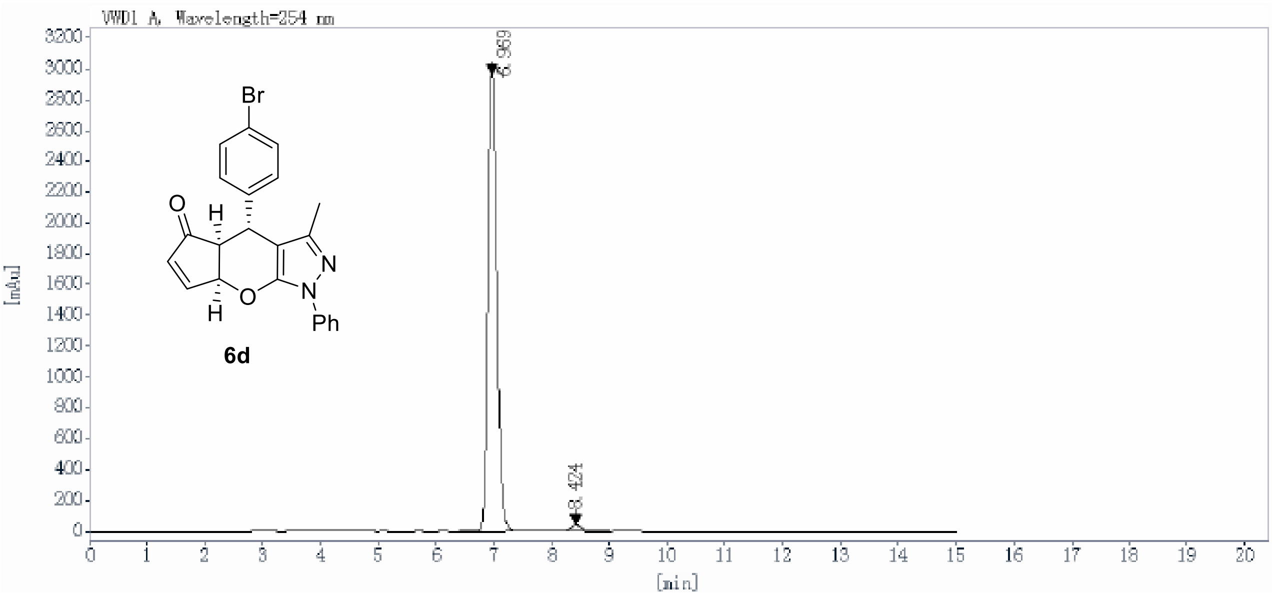
7.716
7.695
7.649
7.642
7.634
7.629
7.458
7.438
7.430
7.410
7.390
7.259
7.230
7.170
7.149
6.365
6.351
5.712
5.706
5.697
5.691
4.475
2.851
2.836
2.035
Br
O
H
N
N
H
O
Ph
6d
1H NMR (400 MHz, CDCl3)
1.91
1.02
3.98
1.36
1.96
0.96
0.98
0.96
1.00
3.02
f1 (ppm)



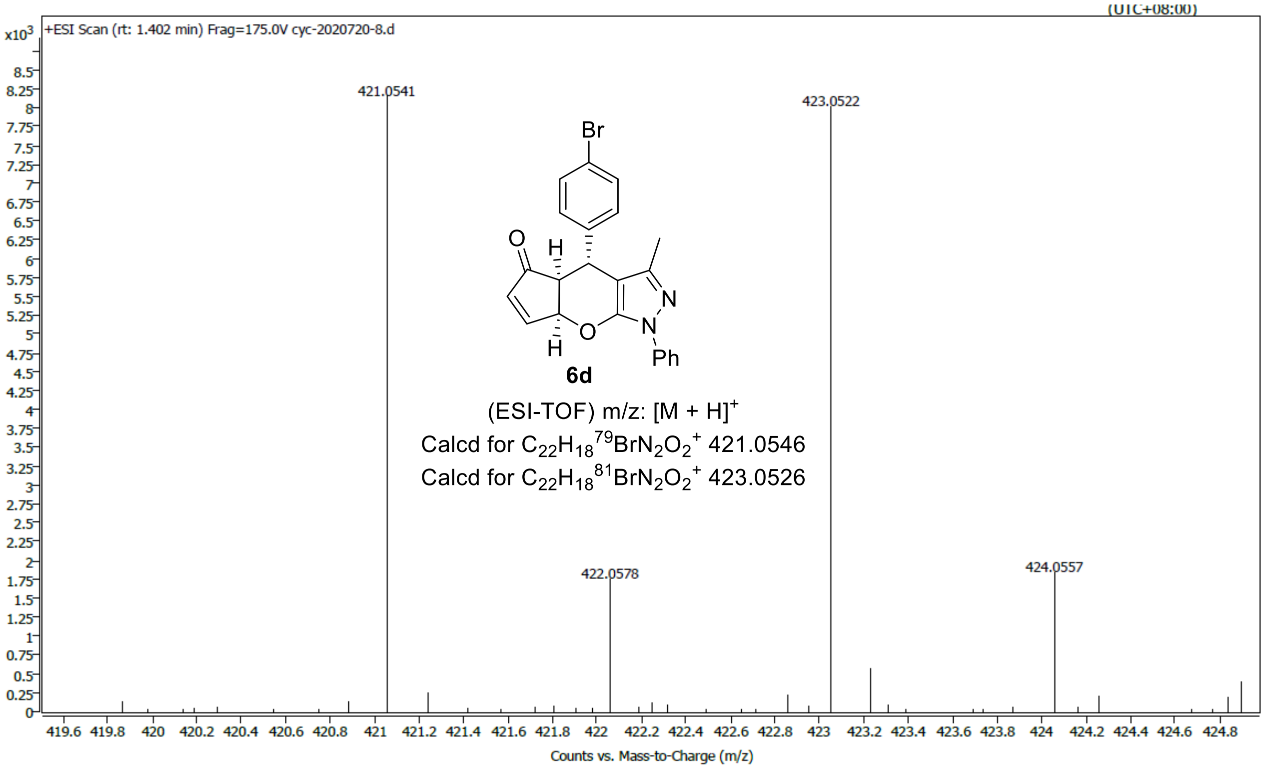
204.634
156.867
147.917
146.366
142.787
138.342
135.426
132.061
129.070
129.039
125.836
120.824
120.398
97.906
78.969
77.396
77.078
76.760
52.053
34.469
12.663
Br
O
H
N
N
H
O
Ph
6d
13C NMR (100 MHz, CDCl3)
f1 (ppm)

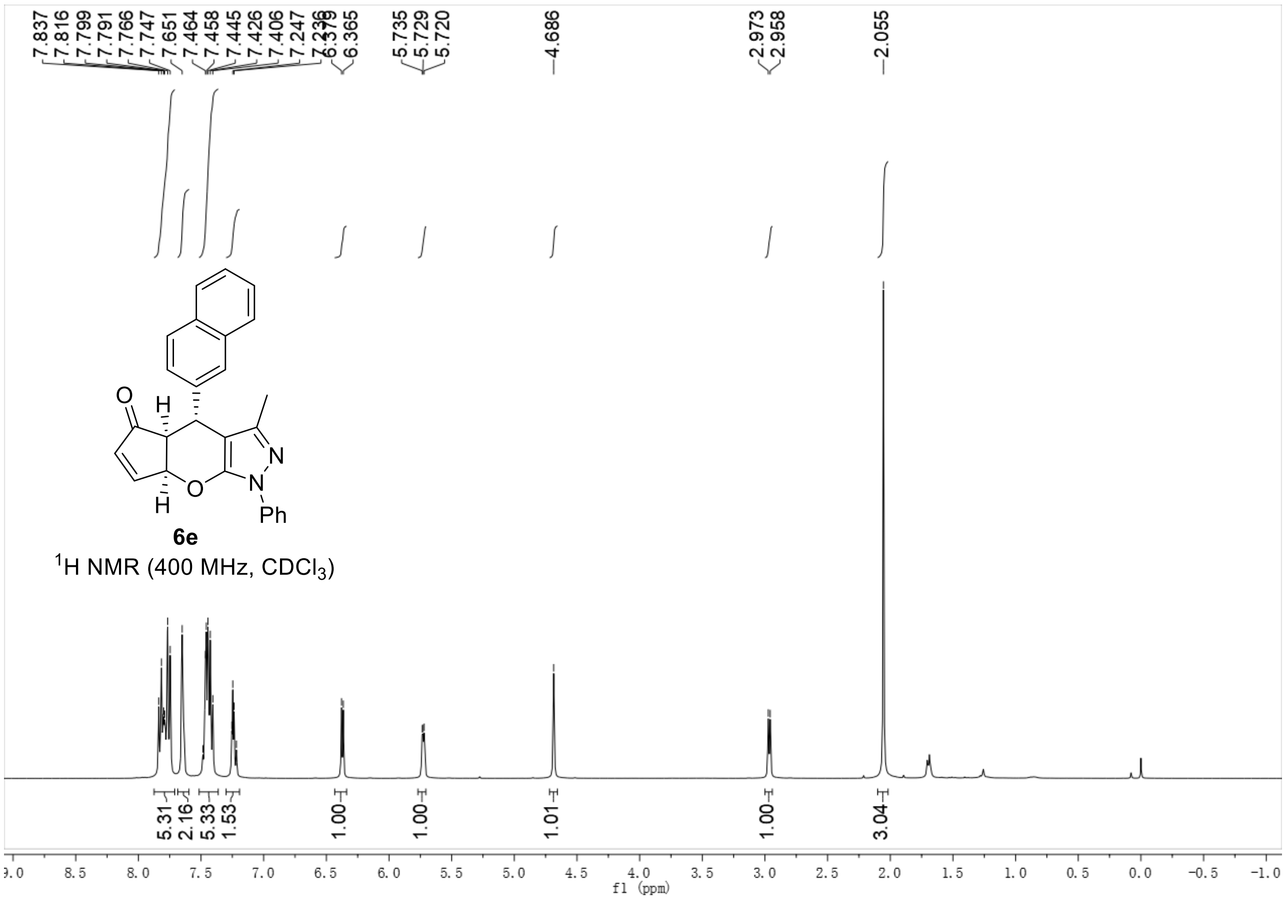


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
6.924	VB R	0.15	774.3711	7436.1001	50.0099
8.328	BB	0.20	587.5632	7433.1489	49.9901
			Totals:	14869.2490	100.0000



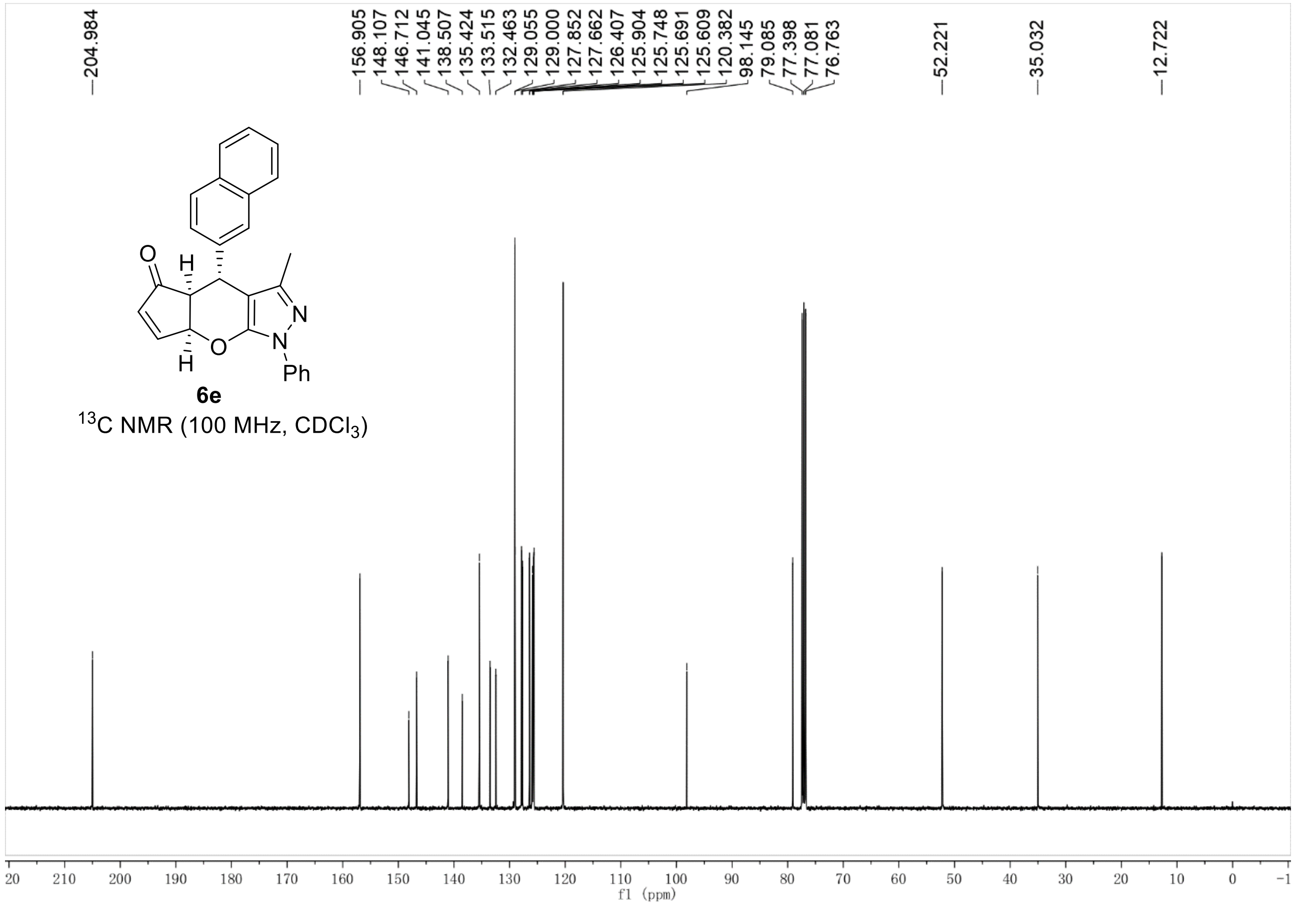
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
6.969	VB R	0.17	2968.4609	32119.7676	98.2940
8.424	BB	0.20	43.6259	557.4812	1.7060
			Totals:	32677.2488	100.0000


(UTC+08:00)
+ESI Scan (rt: 1.402 min) Frag=175.0V cyc-2020720-8.d
x10^3
421.0541
423.0522
422.0578
424.0557
Br
O
H
H
O
N
N
Ph
6d
(ESI-TOF) m/z: [M + H]+
Calcd for C22H18 79BrN2O2+ 421.0546
Calcd for C22H18 81BrN2O2+ 423.0526
Counts vs. Mass-to-Charge (m/z)



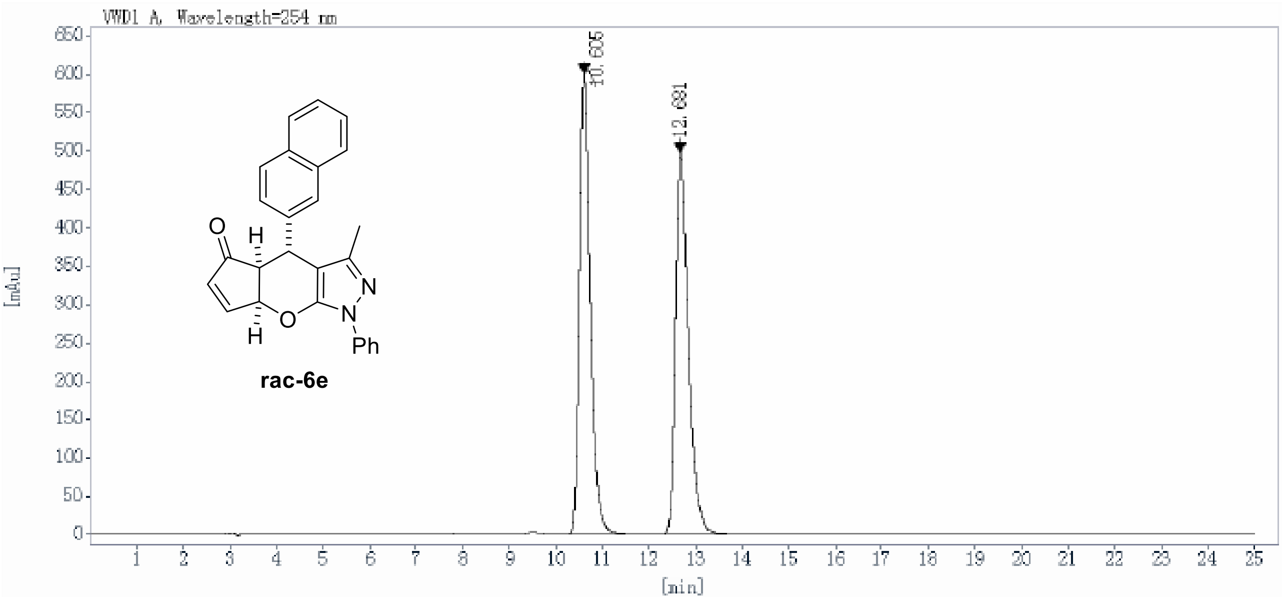
6e

^1H NMR (400 MHz, $CDCl_3$)

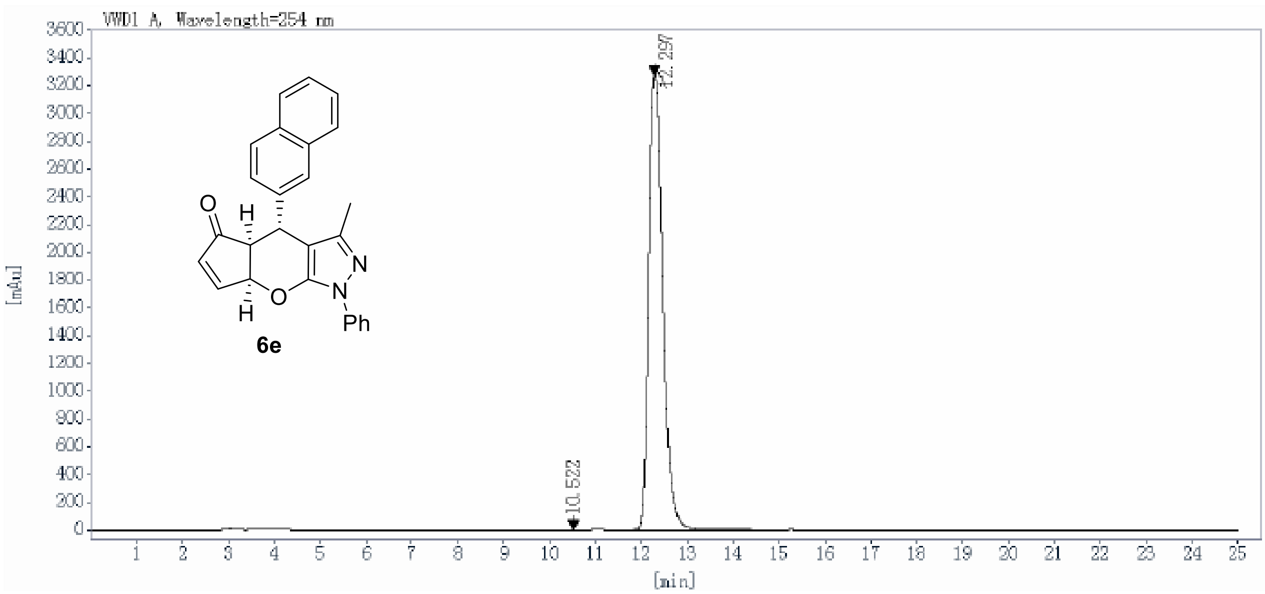


6e

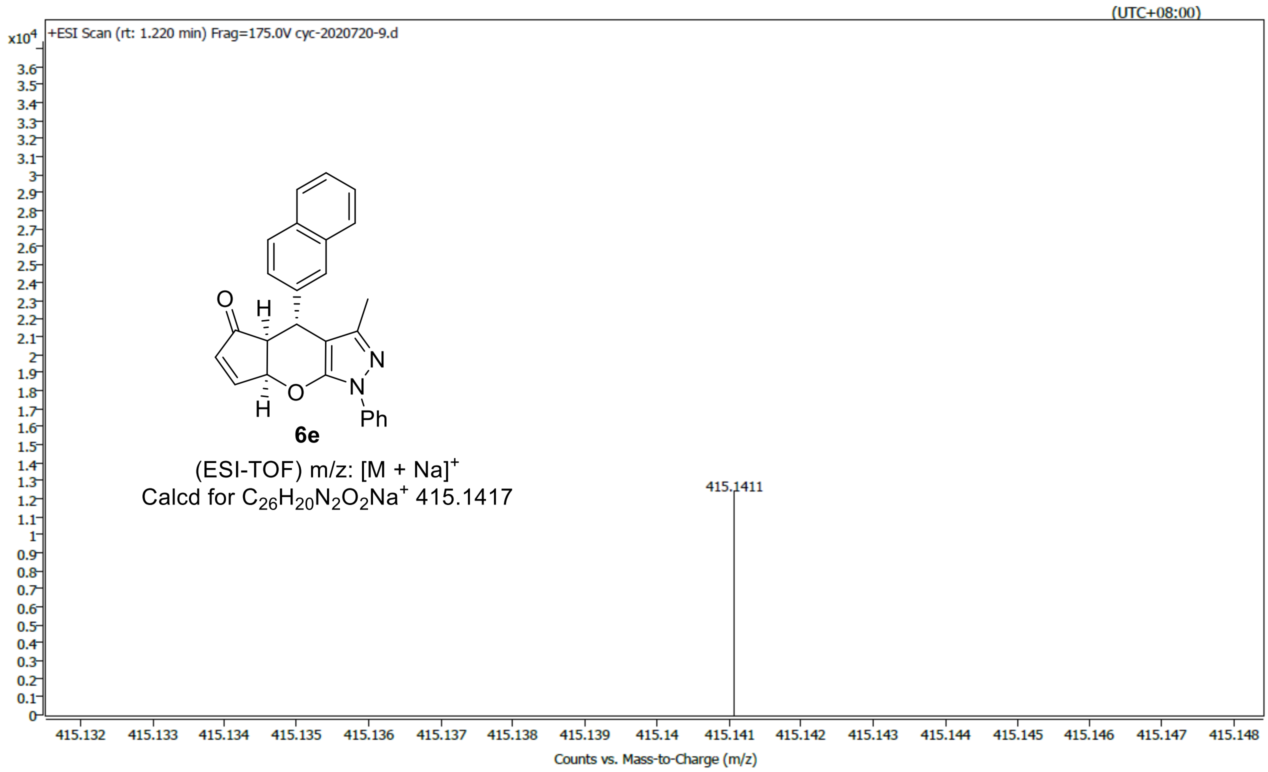
^{13}C NMR (100 MHz, $CDCl_3$)



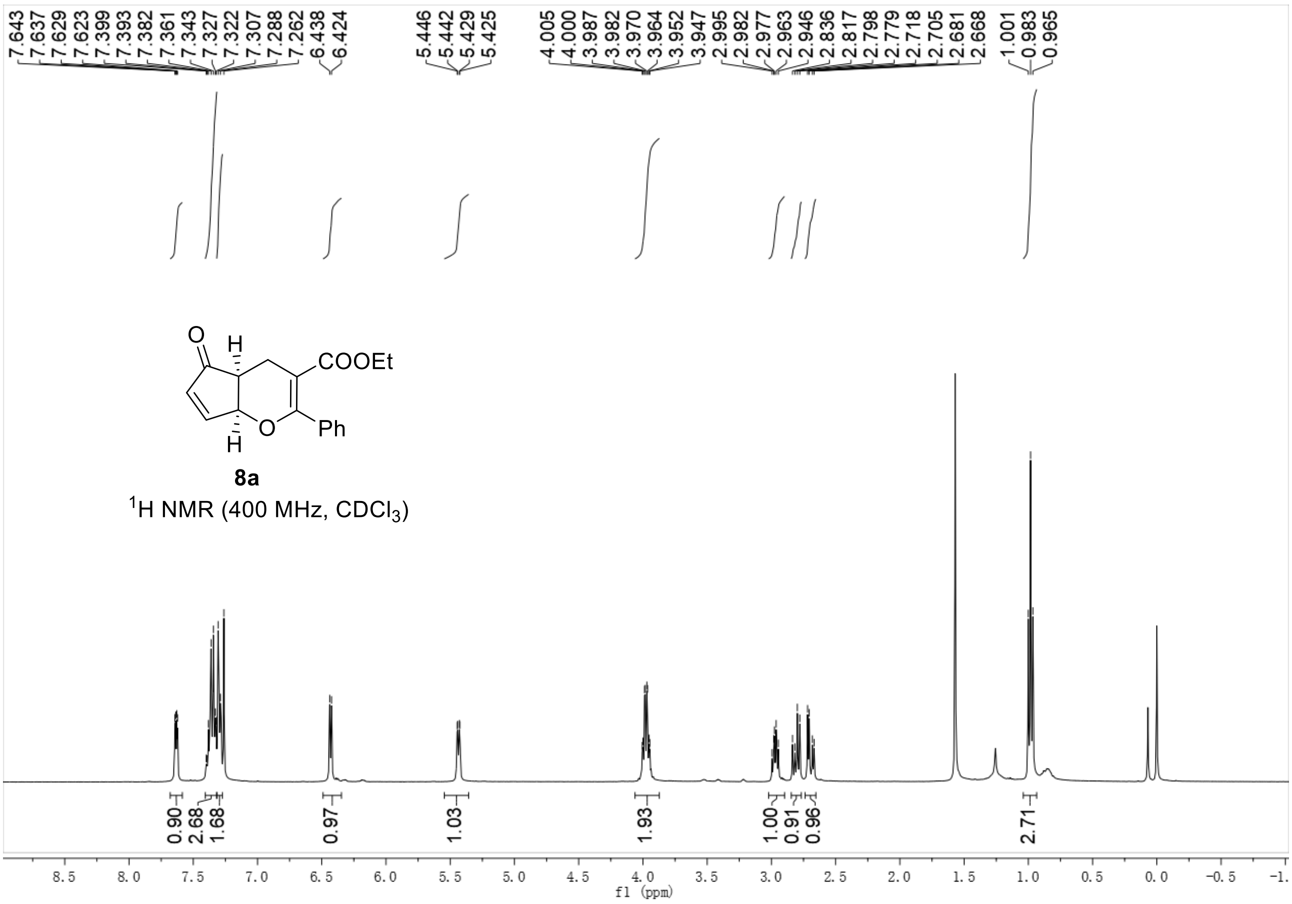
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
10.605	BB	0.24	601.2844	9641.2383	50.0396
12.681	BB	0.29	496.9016	9625.9736	49.9604
			Totals:	19267.2119	100.0000



Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
10.522	BB	0.32	0.1539	3.1278	0.0045
12.297	BBA	0.33	3277.3005	69905.7109	99.9955
			Totals:	69908.8387	100.0000

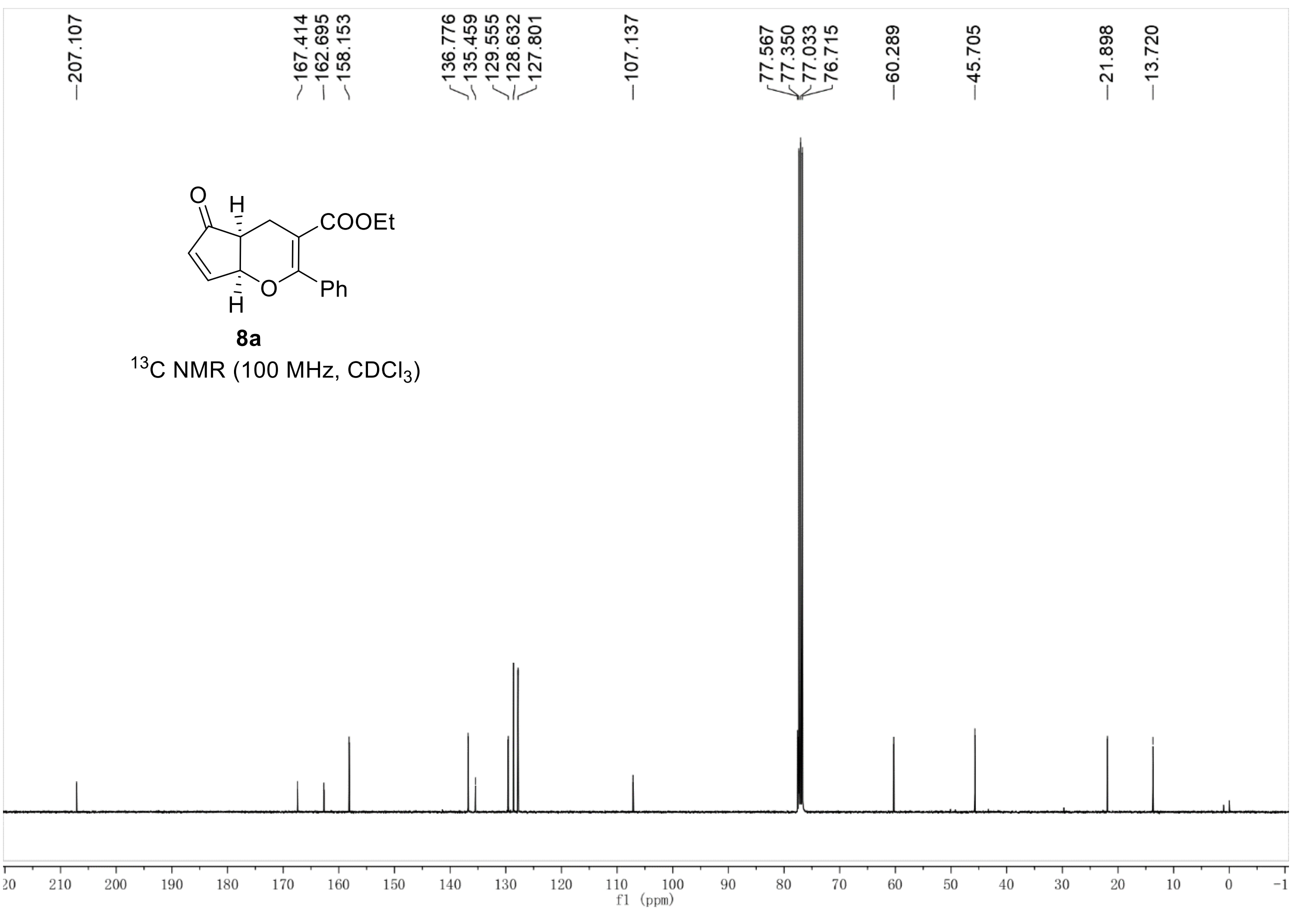


(UTC+08:00)
+ESI Scan (rt: 1.220 min) Frag=175.0V cyc-2020720-9.d
x10^4
6e
(ESI-TOF) m/z: [M + Na]+
Calcd for C26H20N2O2Na+ 415.1417
415.1411
Counts vs. Mass-to-Charge (m/z)



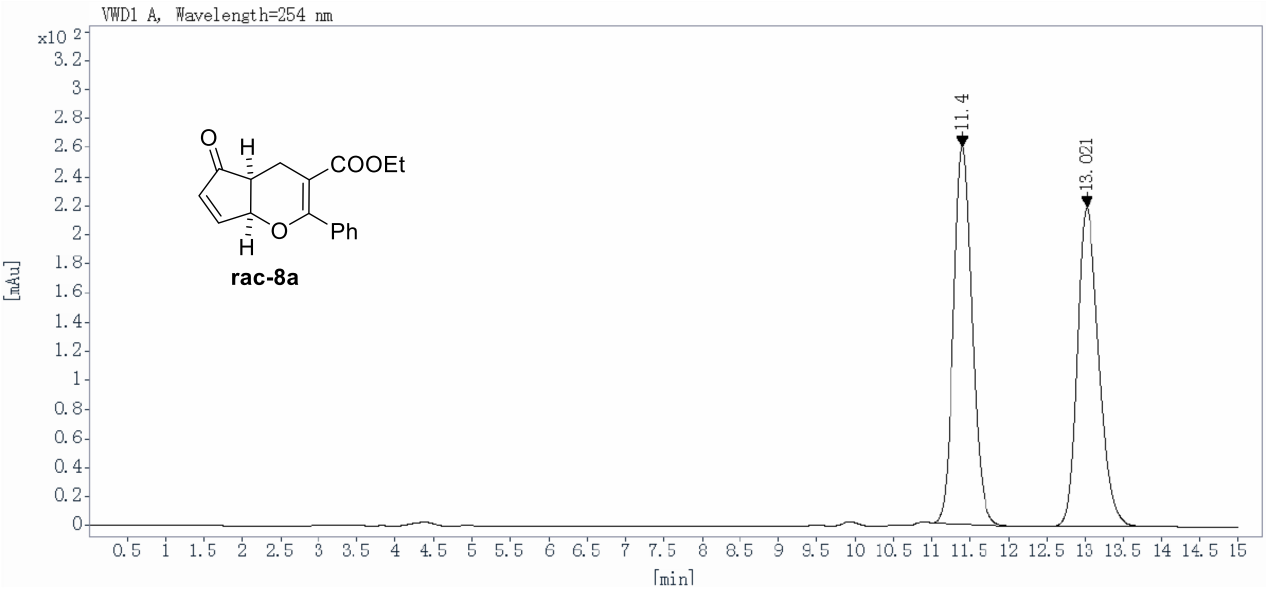
8a

^{1}H NMR (400 MHz, $CDCl_3$)

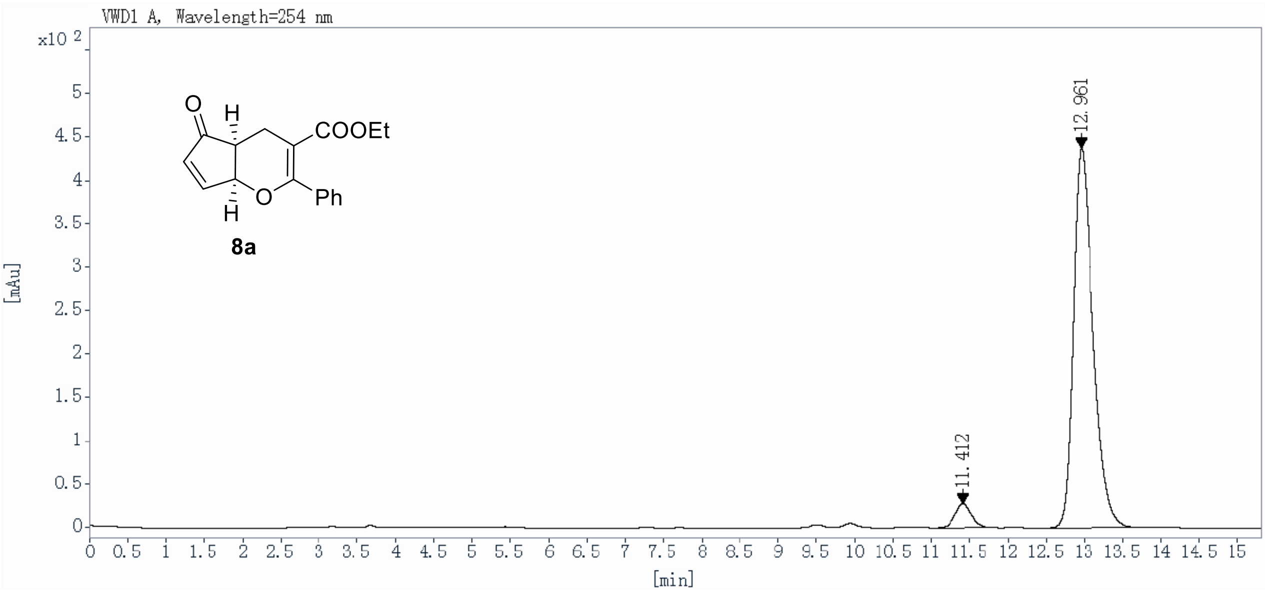


8a

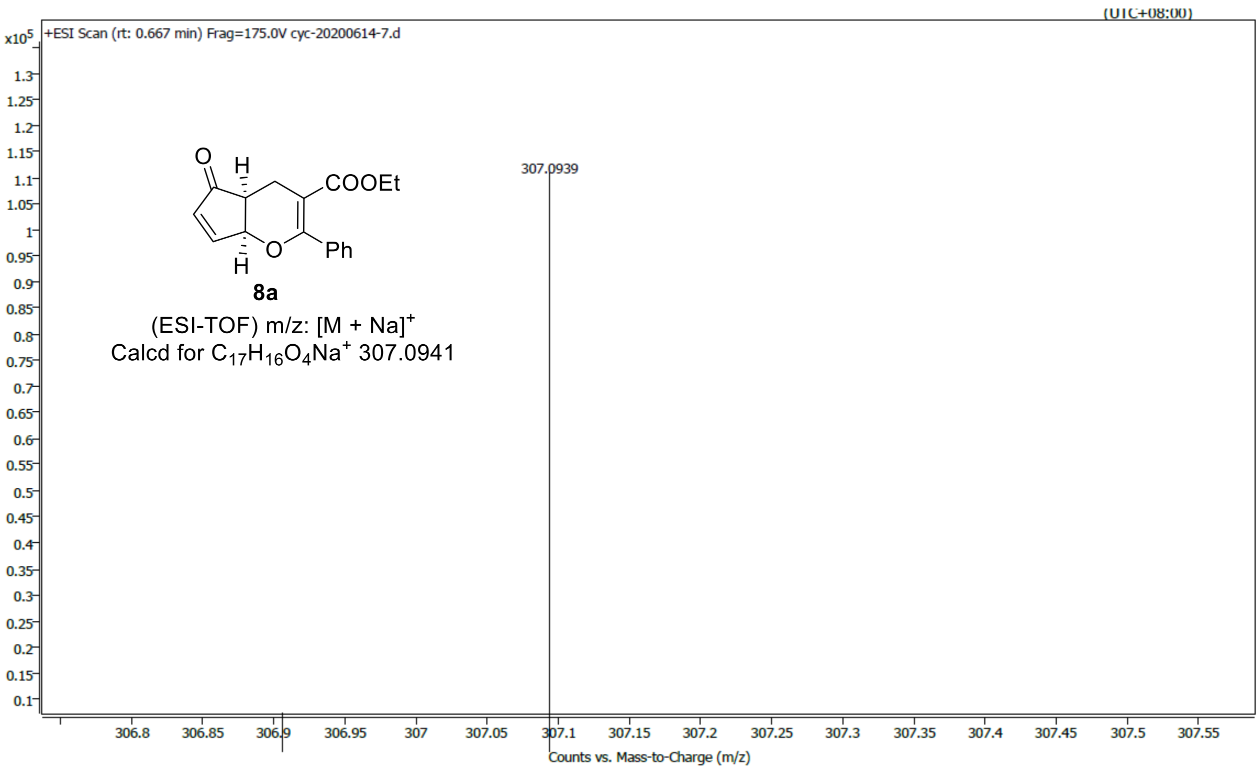
^{13}C NMR (100 MHz, $CDCl_3$)

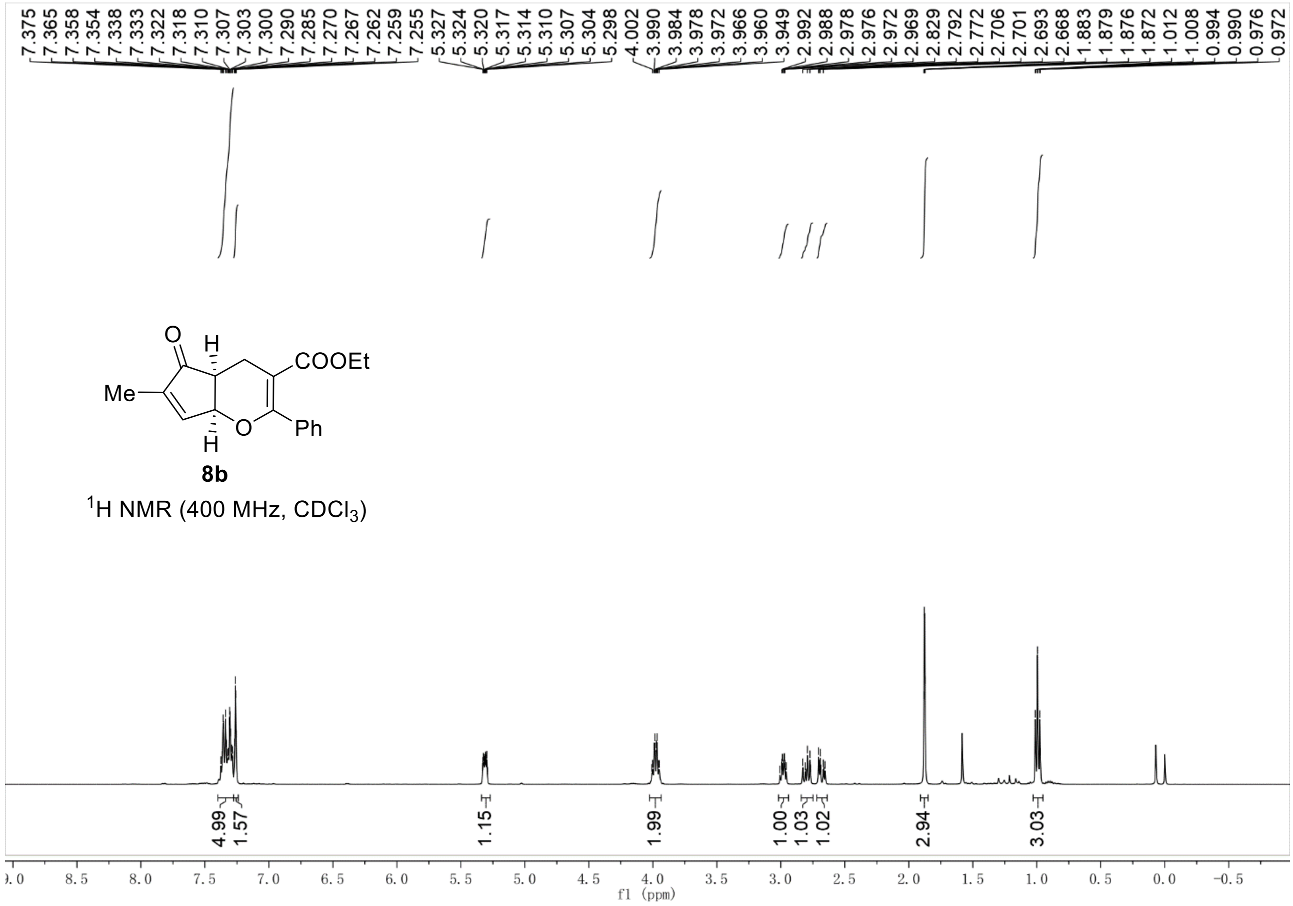


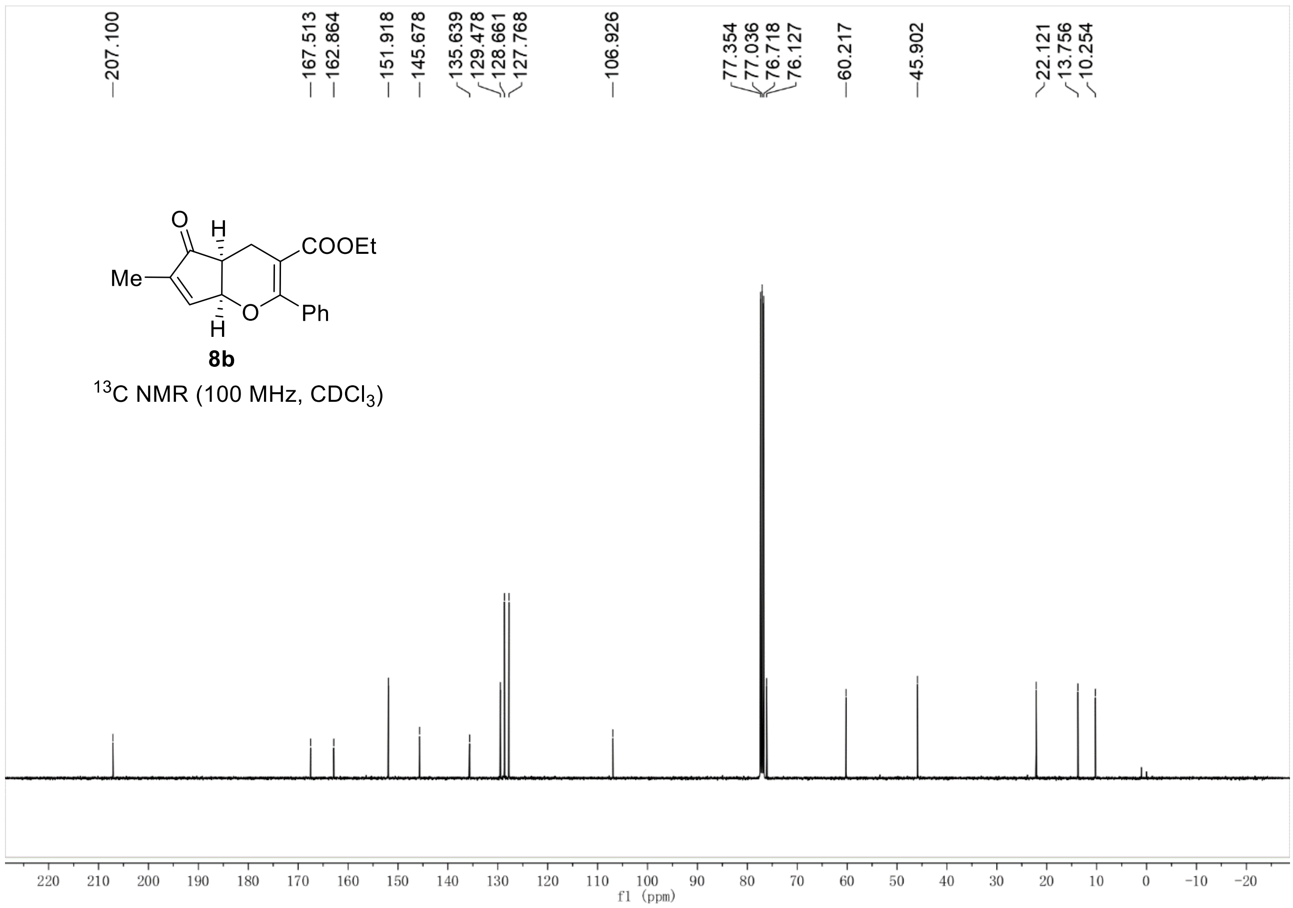
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
11.400	BB	0.26	259.8564	4371.8726	50.5844
13.021	BBA	0.30	219.5111	4270.8550	49.4156
			Totals:	8642.7275	100.0000

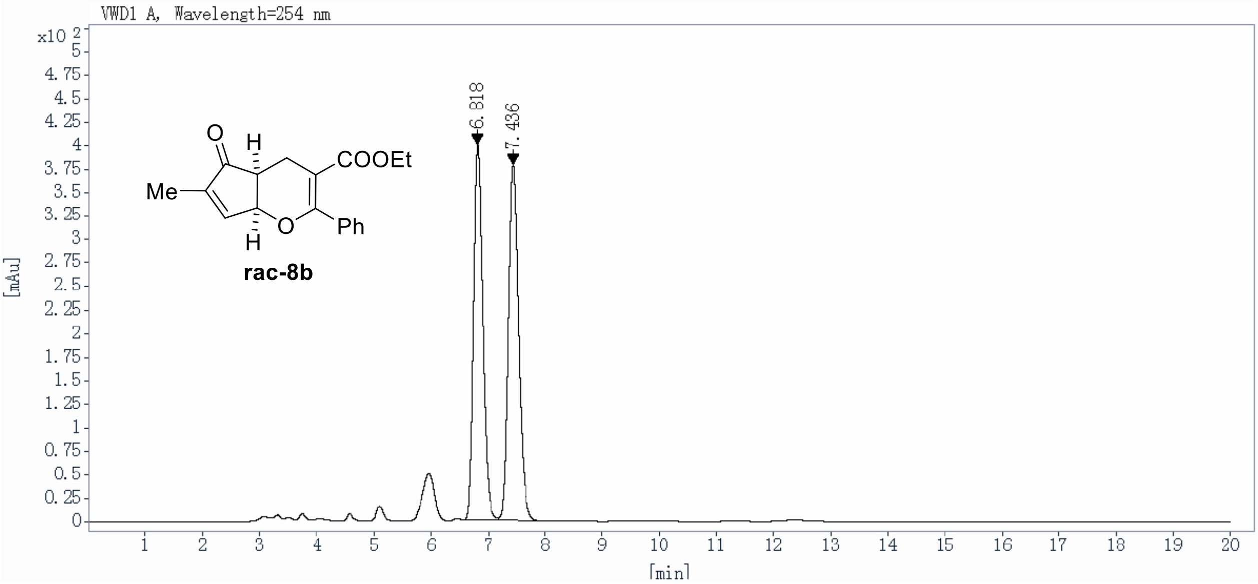


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
11.412	BBA	0.22	28.2433	407.9403	5.0318
12.961	BBA	0.27	437.1207	7699.2383	94.9682
			Totals:	8107.1786	100.0000

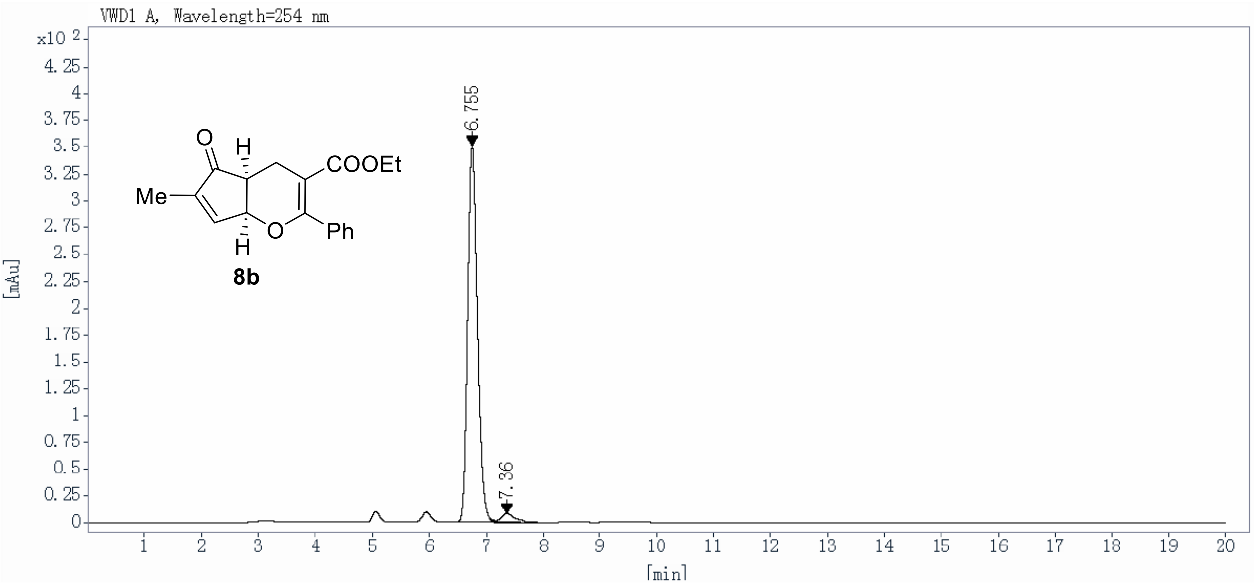

(UTC+08:00)
x10^5
+ESI Scan (rt: 0.667 min) Frag=175.0V cyc-20200614-7.d
1.3
1.25
1.2
1.15
1.1
1.05
1
0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
0.55
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
307.0939
O
H
COOEt
O
Ph
H
8a
(ESI-TOF) m/z: [M + Na]+
Calcd for C17H16O4Na+ 307.0941
306.8
306.85
306.9
306.95
307
307.05
307.1
307.15
307.2
307.25
307.3
307.35
307.4
307.45
307.5
307.55
Counts vs. Mass-to-Charge (m/z)


7.375 7.365 7.358 7.354 7.338 7.333 7.322 7.318 7.310 7.307 7.303 7.300 7.290 7.285 7.270 7.267 7.262 7.259 7.255 5.327 5.324 5.320 5.317 5.314 5.310 5.307 5.304 5.298 4.002 3.990 3.984 3.978 3.972 3.966 3.960 3.949 2.992 2.988 2.978 2.976 2.972 2.969 2.829 2.792 2.772 2.706 2.701 2.693 2.668 1.883 1.879 1.876 1.872 1.012 1.008 0.994 0.990 0.976 0.972
O
H
COOEt
Me
O
Ph
H
8b
1H NMR (400 MHz, CDCl3)
4.99 1.57 1.15 1.99 1.00 1.03 1.02 2.94 3.03
f1 (ppm)

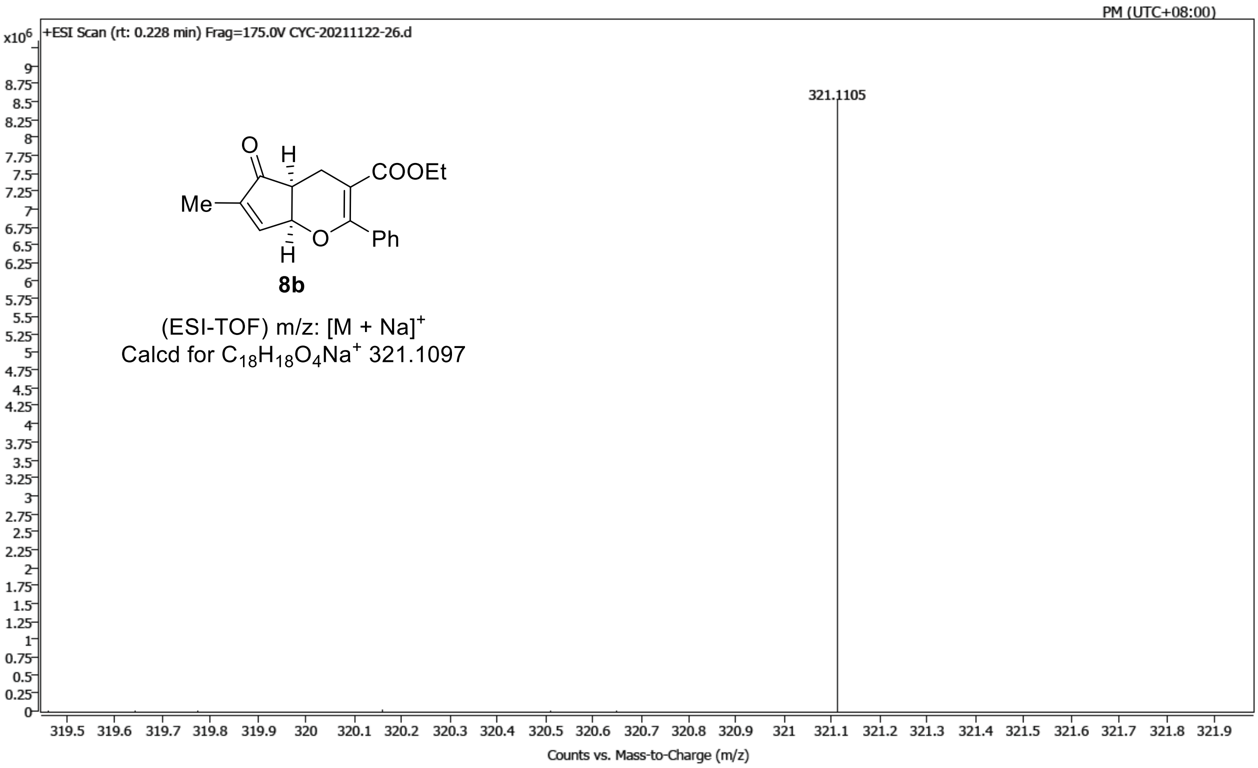

207.100 167.513 162.864 151.918 145.678 135.639 129.478 128.661 127.768 106.926 77.354 77.036 76.718 76.127 60.217 45.902 22.121 13.756 10.254
O
H
COOEt
Me
O
Ph
H
8b
13C NMR (100 MHz, CDCl3)
f1 (ppm)

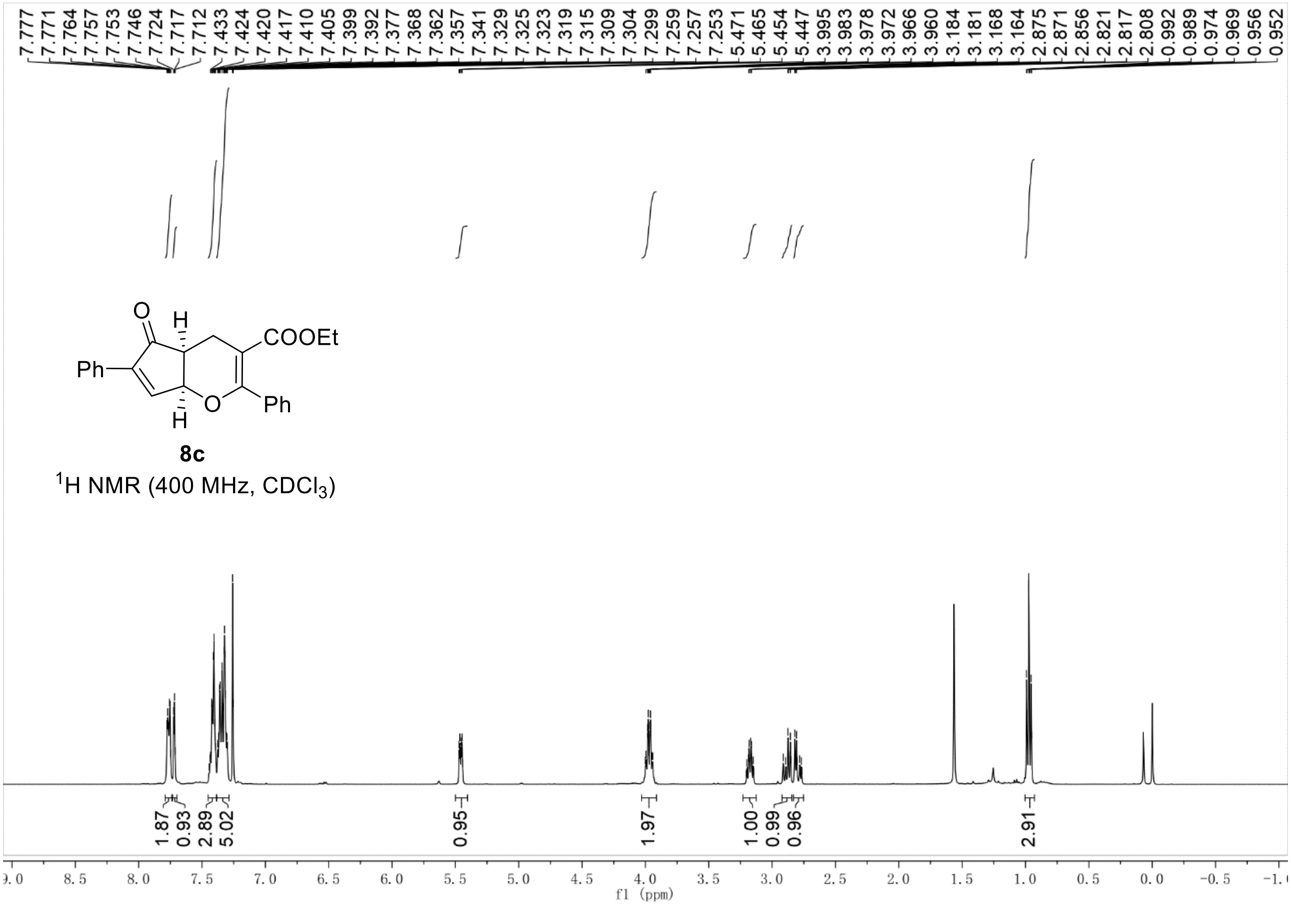


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
6.818	BV	0.17	400.1830	4452.7285	48.9374
7.436	VBA	0.19	379.3825	4646.1040	51.0626
			Totals:	9098.8325	100.0000



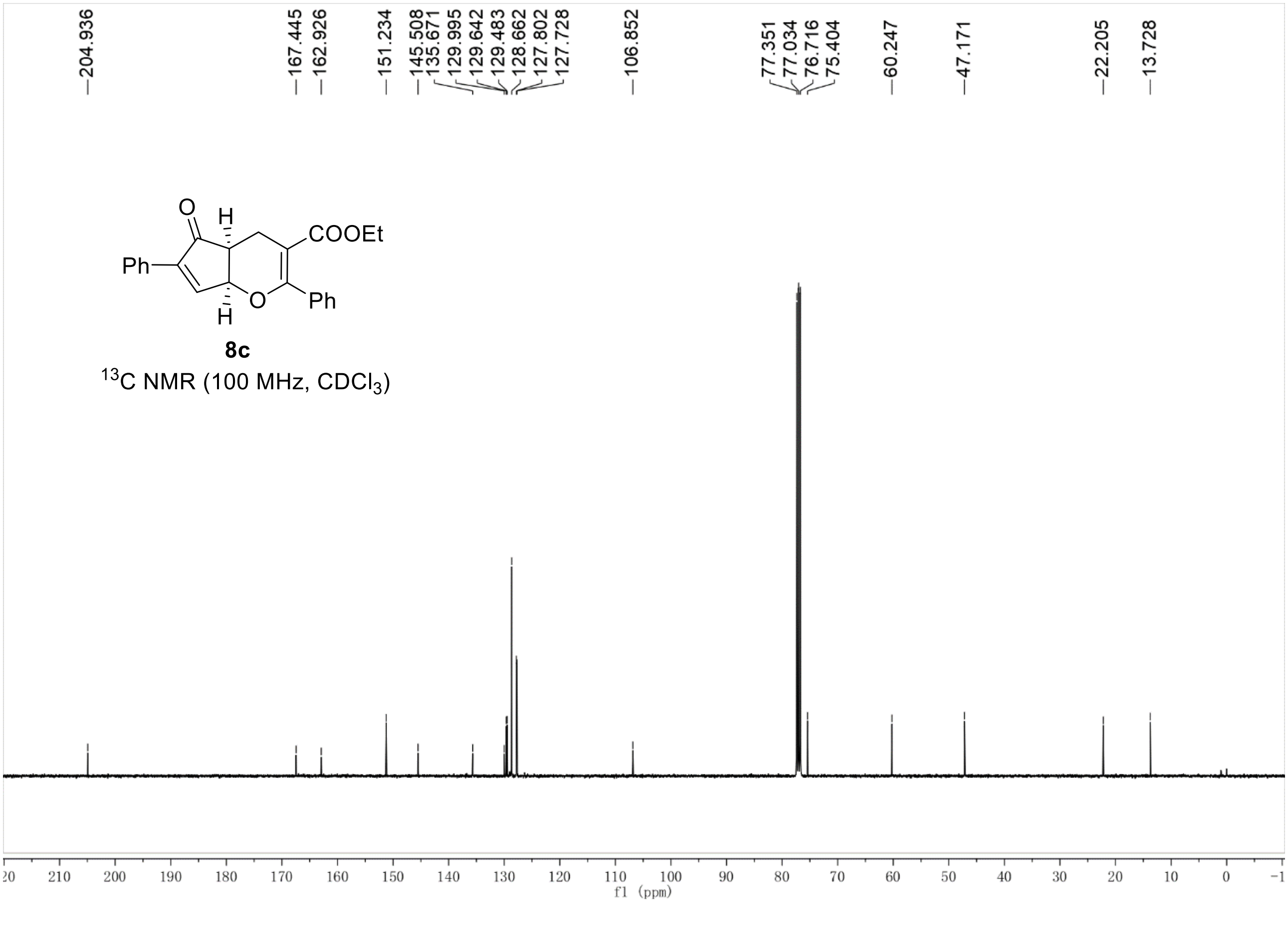
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
6.755	VV R	0.18	350.7076	4081.3738	96.5491
7.360	VBAE	0.25	8.4640	145.8802	3.4509
			Totals:	4227.2540	100.0000


PM (UTC+08:00)
+ESI Scan (rt: 0.228 min) Frag=175.0V CYC-20211122-26.d
x10^6
321.1105
8b
(ESI-TOF) m/z: [M + Na]+
Calcd for C18H18O4Na+ 321.1097
Counts vs. Mass-to-Charge (m/z)



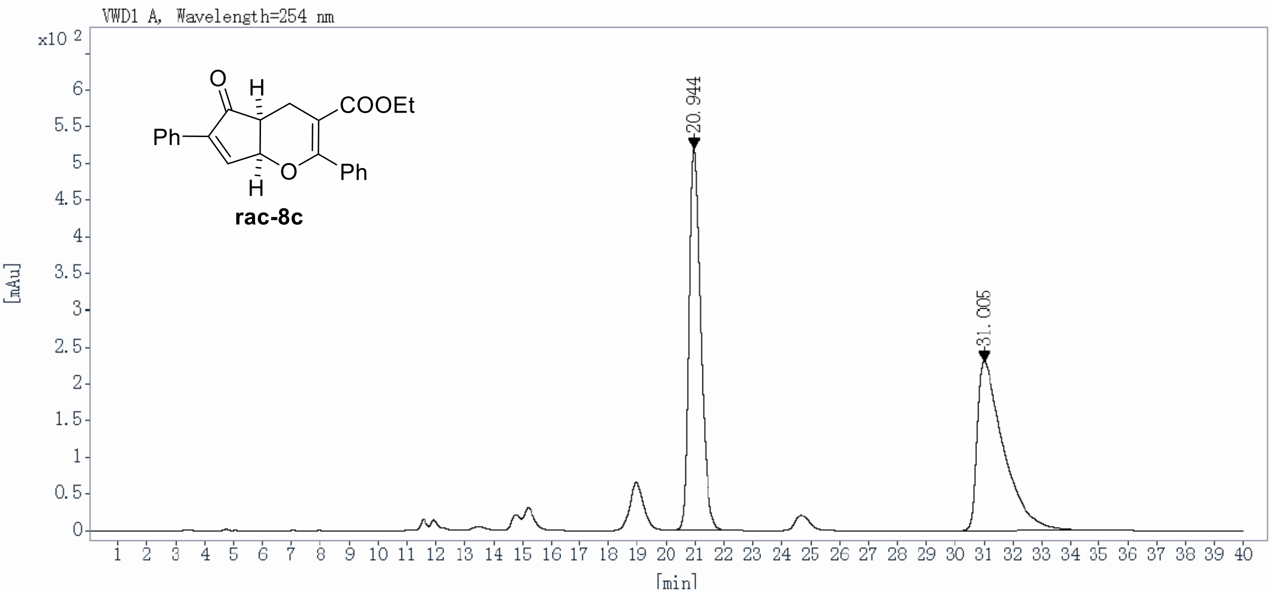
8c

^{1}H NMR (400 MHz, $CDCl_3$)

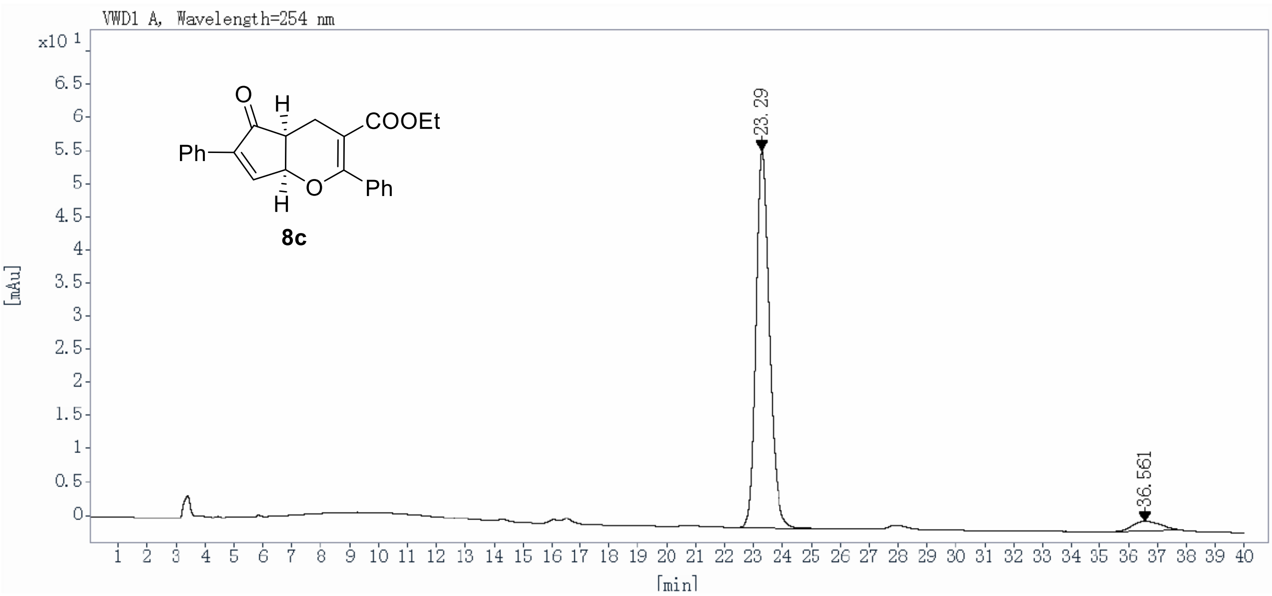


8c

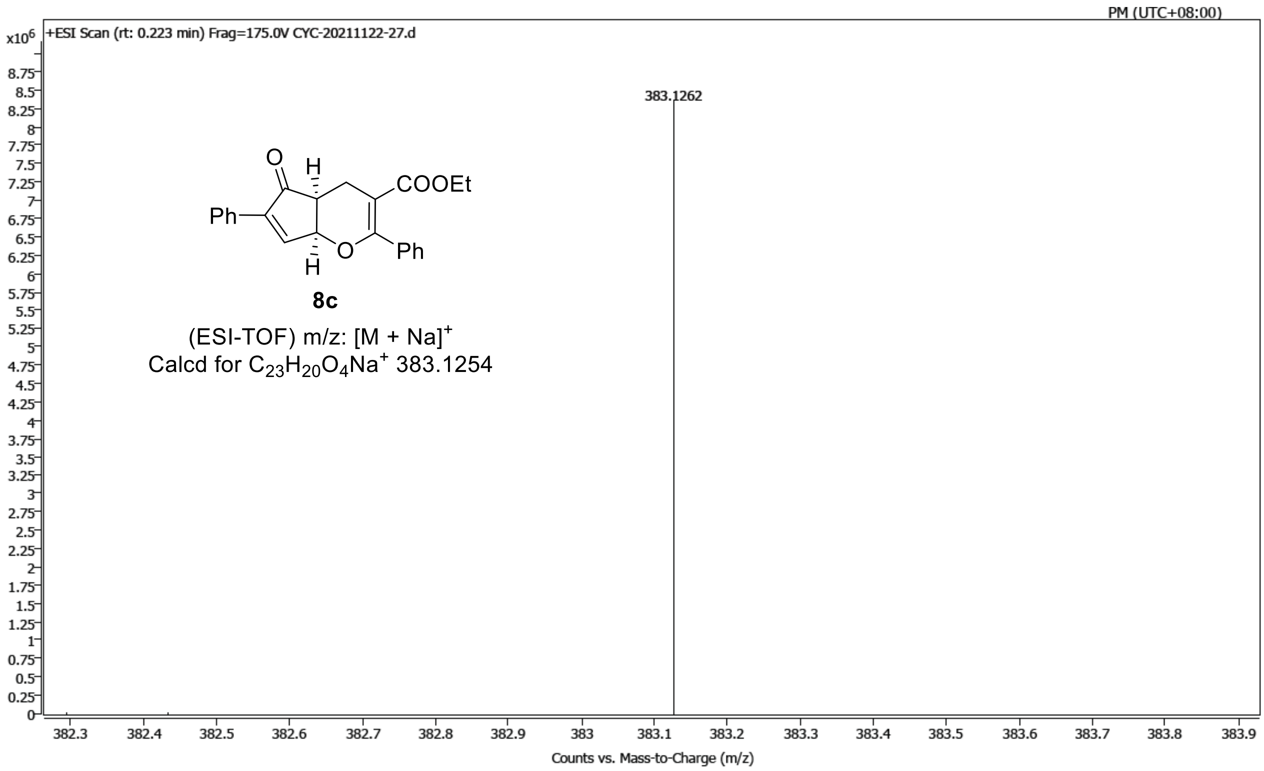
^{13}C NMR (100 MHz, $CDCl_3$)

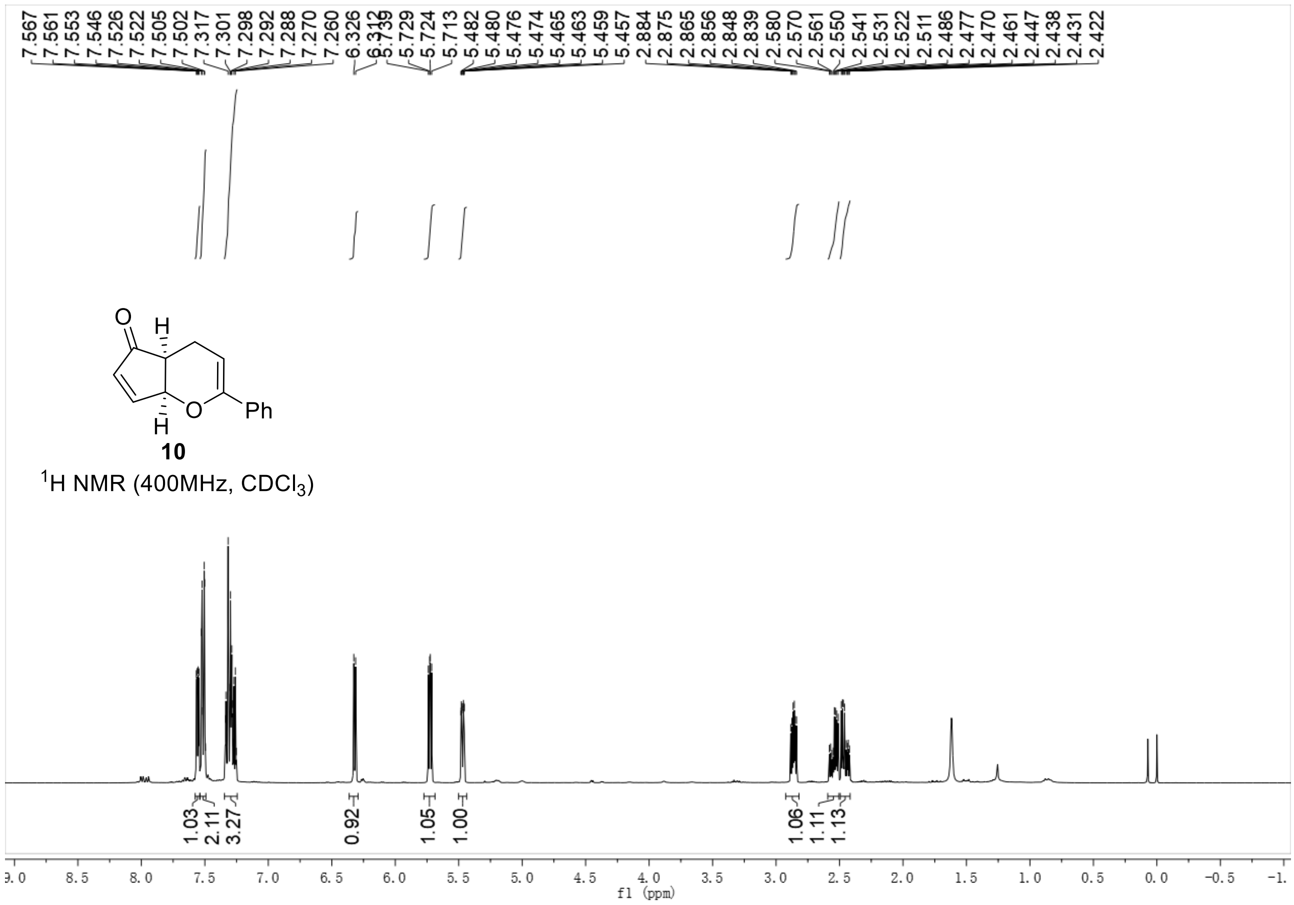


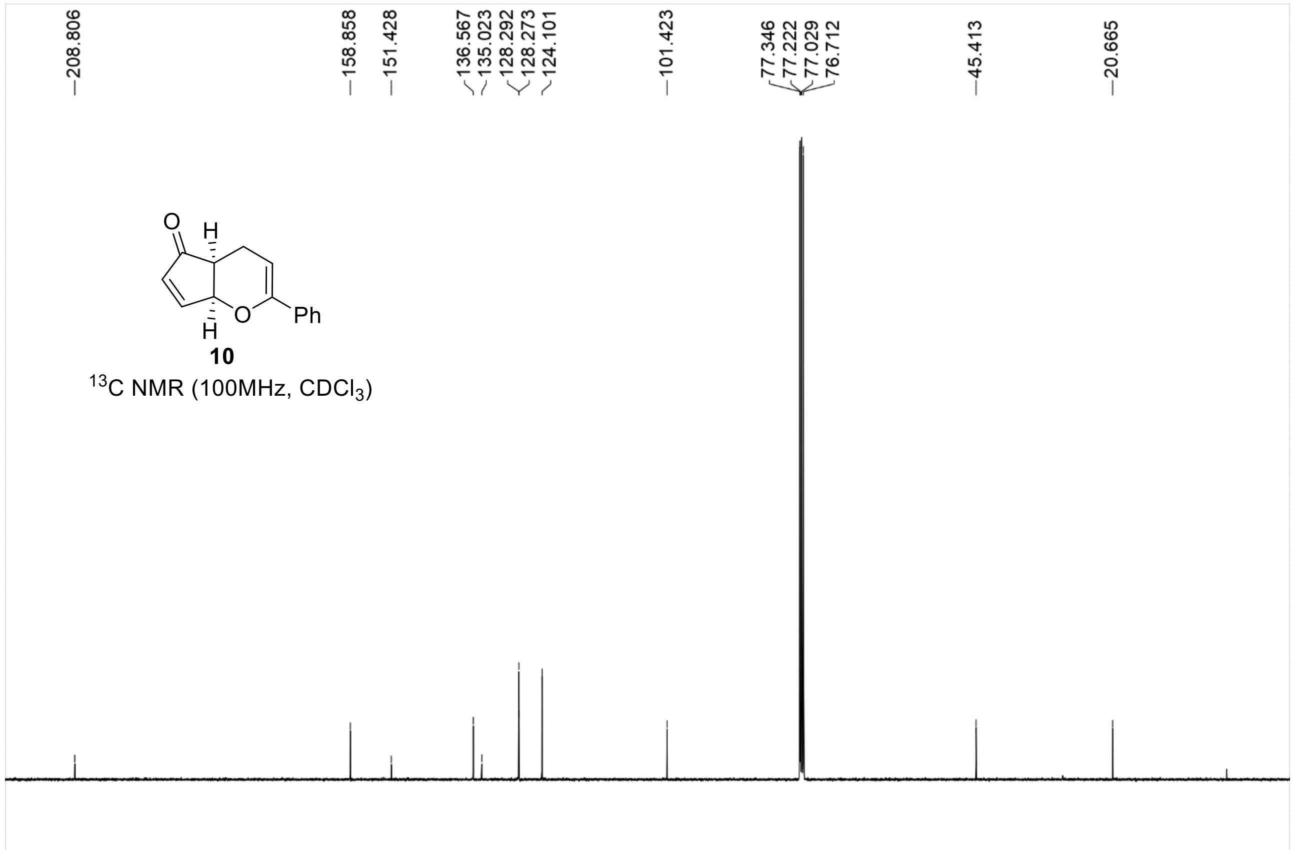
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
20.944	BBA	0.43	520.0304	14526.2070	49.8704
31.005	BBA	0.92	231.5387	14601.6865	50.1296
			Totals:	29127.8936	100.0000

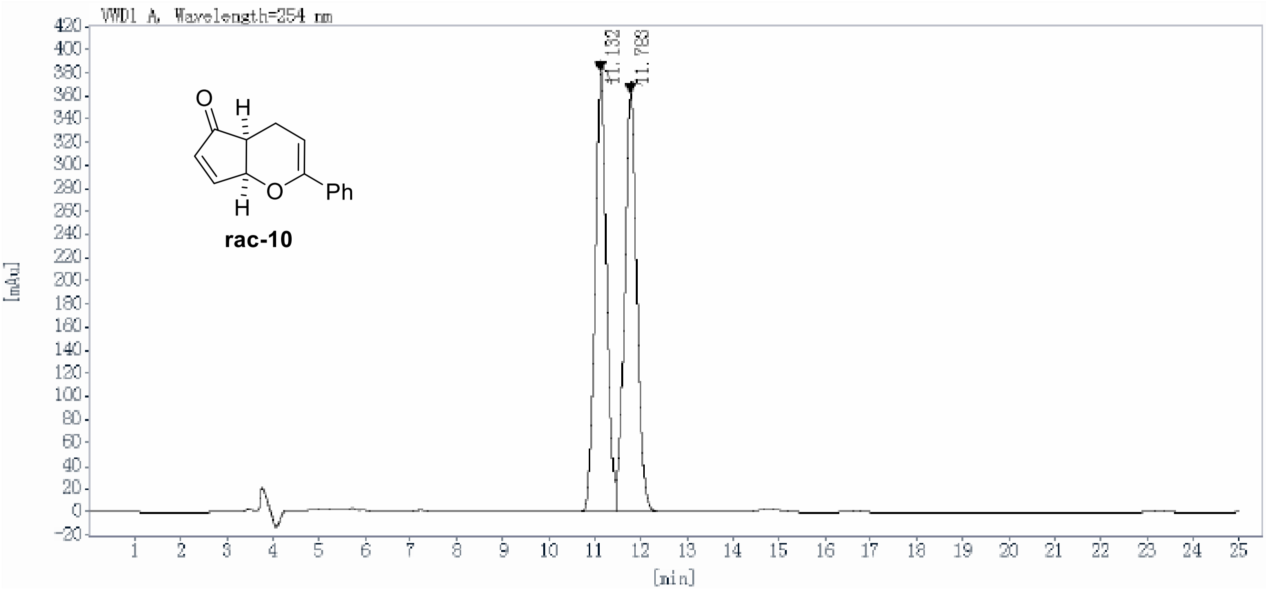


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
23.290	BBA	0.49	56.7829	1805.9852	95.0648
36.561	BBA	0.94	1.3797	93.7553	4.9352
			Totals:	1899.7405	100.0000

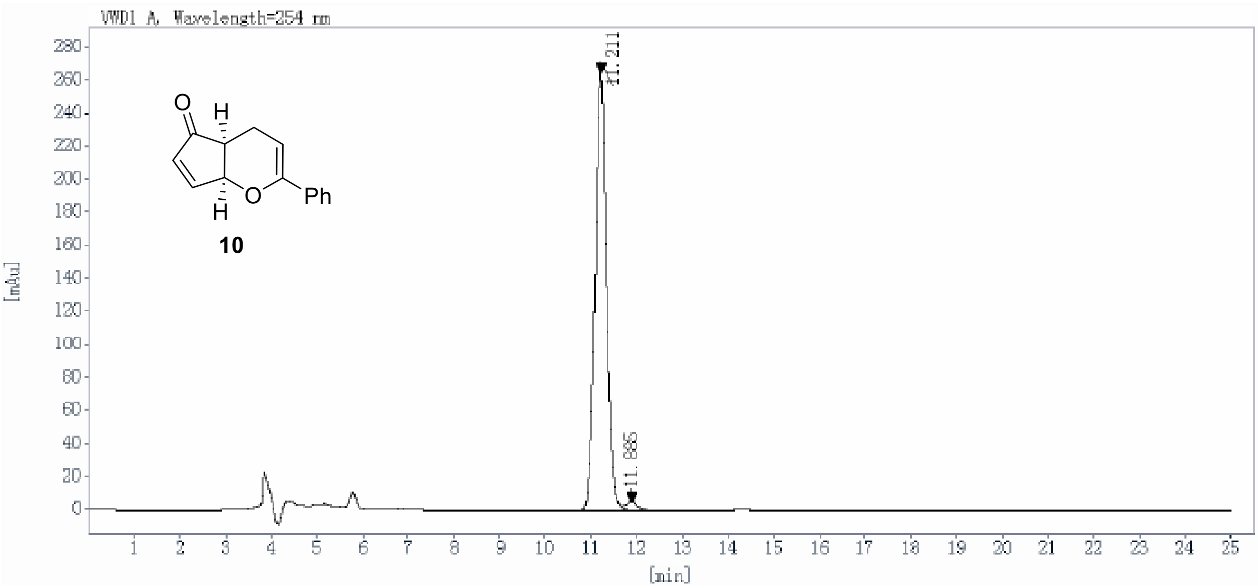

PM (UTC+08:00)
x10^6
+ESI Scan (rt: 0.223 min) Frag=175.0V CYC-20211122-27.d
383.1262
O
H
COOEt
Ph
O
Ph
H
8c
(ESI-TOF) m/z: [M + Na]+
Calcd for C23H20O4Na+ 383.1254
Counts vs. Mass-to-Charge (m/z)


7.567 7.561 7.553 7.546 7.526 7.522 7.505 7.502 7.317 7.301 7.298 7.292 7.288 7.270 7.260 6.326 6.312 5.739 5.729 5.724 5.713 5.482 5.480 5.476 5.474 5.465 5.463 5.459 5.457 2.884 2.875 2.865 2.856 2.848 2.839 2.580 2.570 2.561 2.550 2.541 2.531 2.522 2.511 2.486 2.477 2.470 2.461 2.447 2.438 2.431 2.422
O
H
H
O
Ph
10
1H NMR (400MHz, CDCl3)
1.03
2.11
3.27
0.92
1.05
1.00
1.06
1.11
1.13
f1 (ppm)

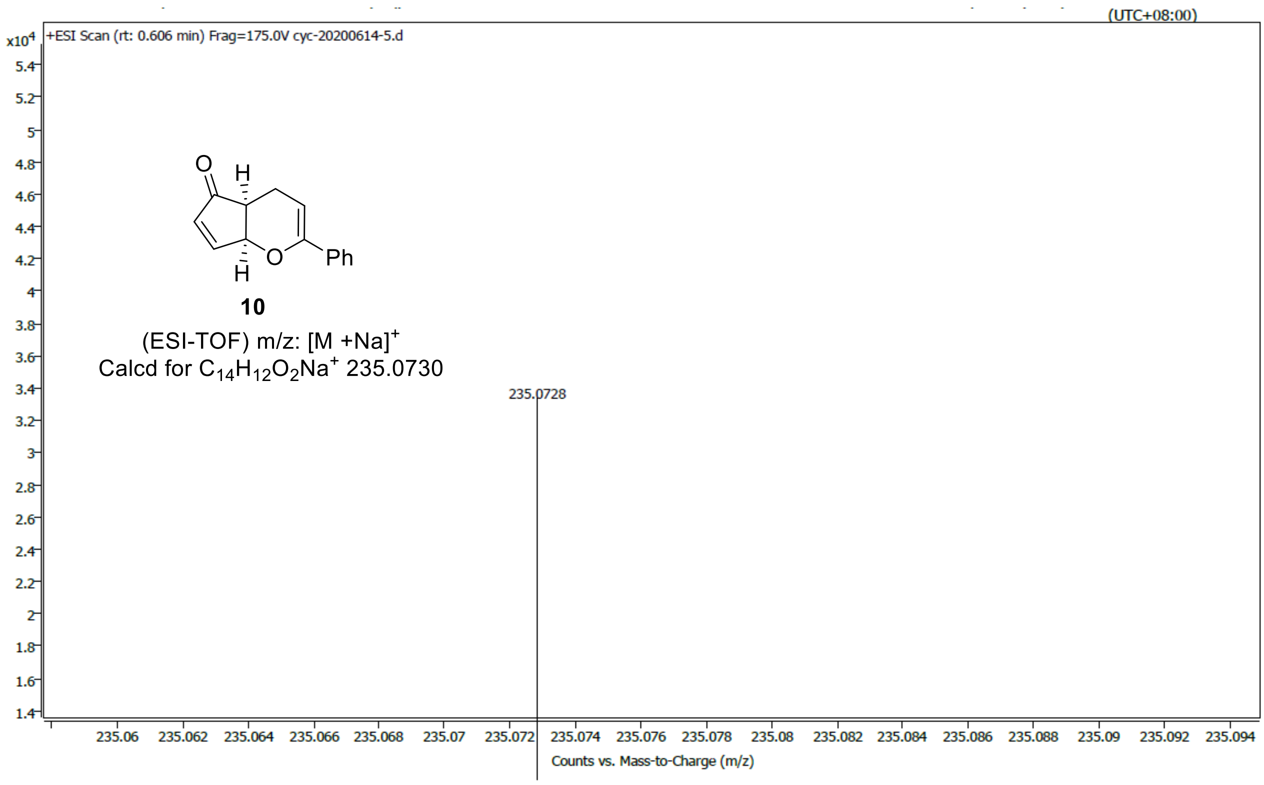

208.806 158.858 151.428 136.567 135.023 128.292 128.273 124.101 101.423 77.346 77.222 77.029 76.712 45.413 20.665
O
H
H
O
Ph
10
13C NMR (100MHz, CDCl3)
f1 (ppm)

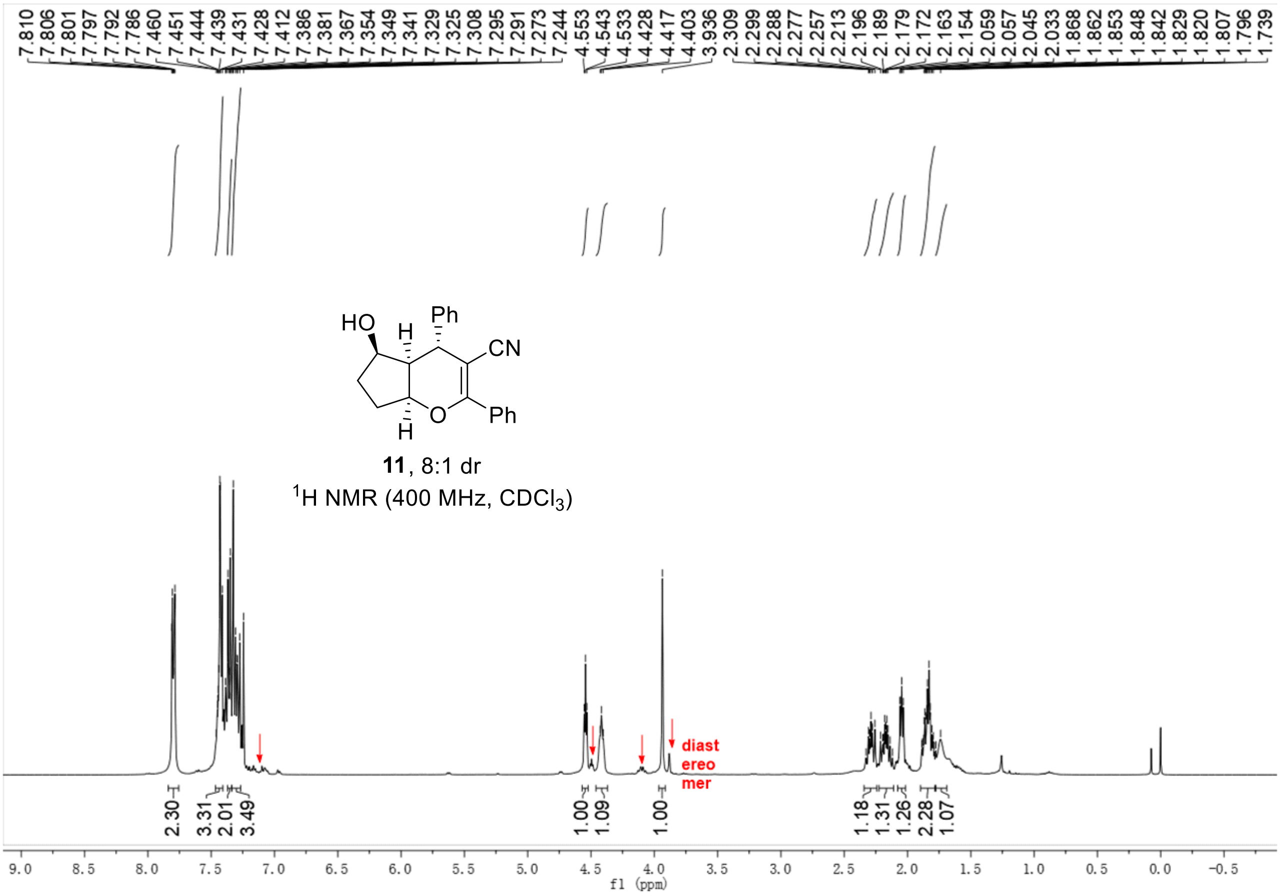


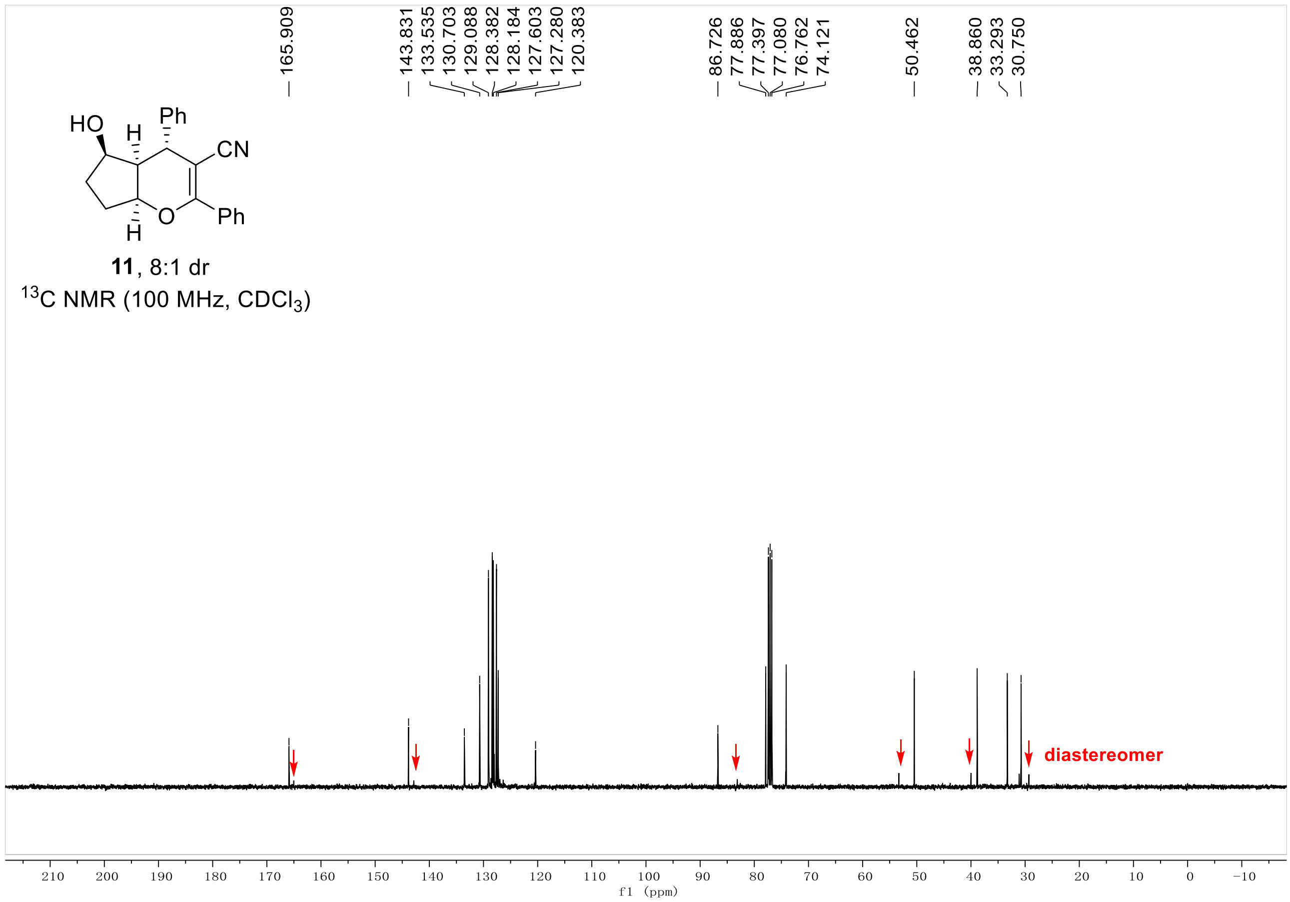
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
11.132	BV	0.26	381.6285	6554.5625	49.6704
11.783	VB	0.27	362.4886	6641.5615	50.3296
			Totals:	13196.1240	100.0000

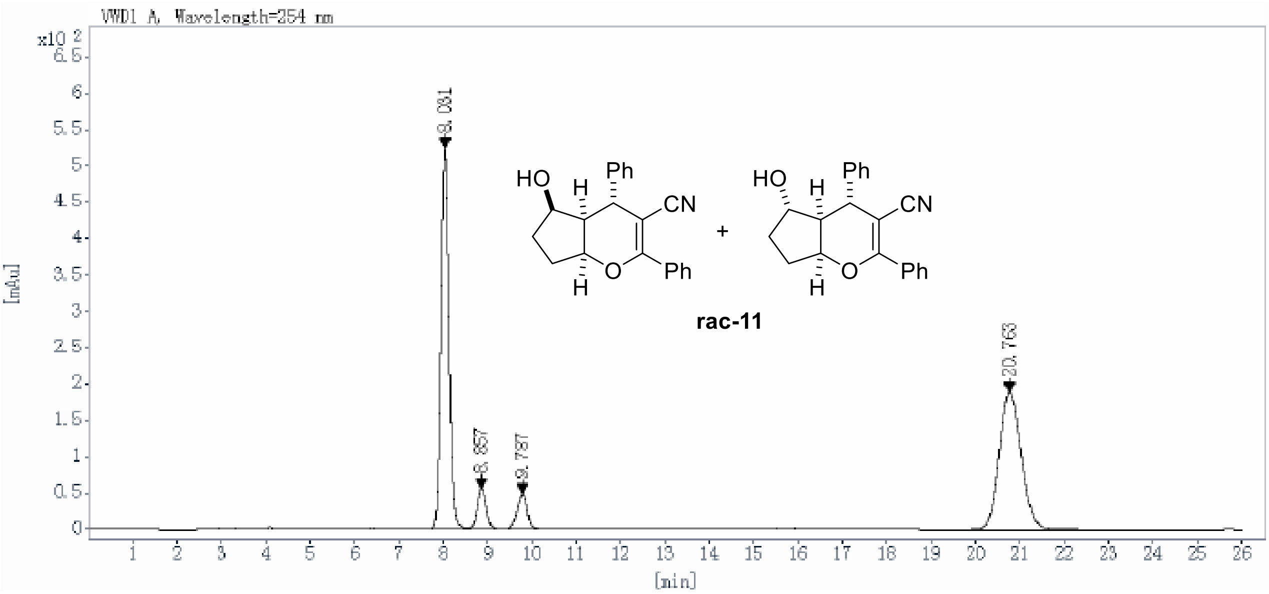


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
11.211	BV R	0.26	265.0678	4573.3223	98.0644
11.885	VB E	0.26	5.0527	90.2708	1.9356
			Totals:	4663.5931	100.0000

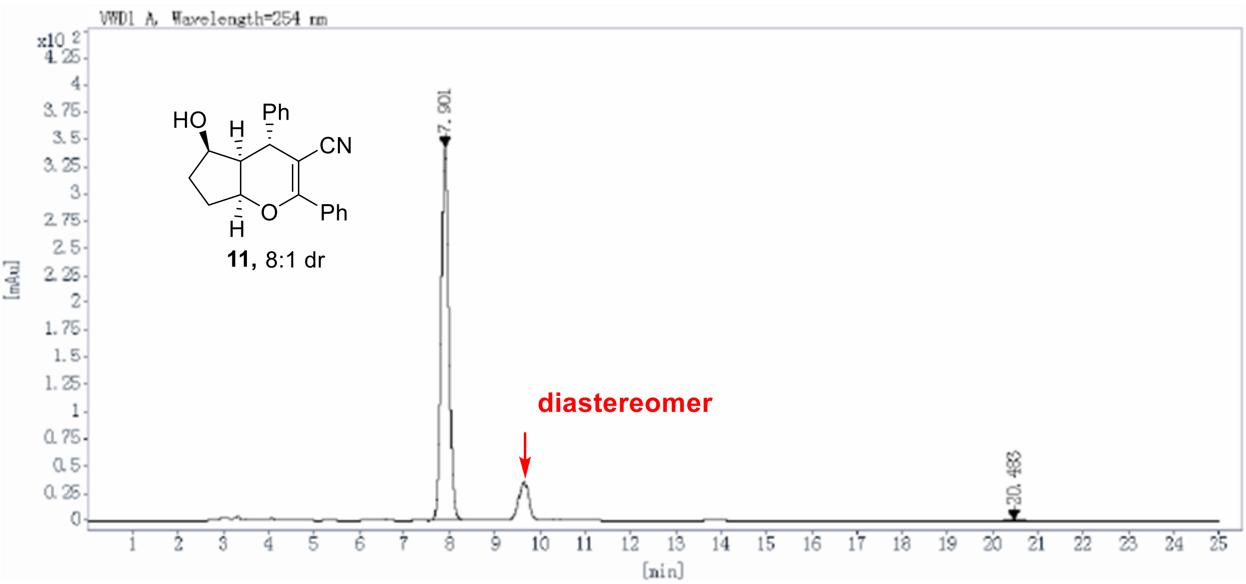

(UTC+08:00)
+ESI Scan (rt: 0.606 min) Frag=175.0V cyc-20200614-5.d
x10^4
O
H
H
O
Ph
10
(ESI-TOF) m/z: [M +Na]+
Calcd for C14H12O2Na+ 235.0730
235.0728
Counts vs. Mass-to-Charge (m/z)


7.810
7.806
7.801
7.797
7.792
7.786
7.460
7.451
7.444
7.439
7.431
7.428
7.412
7.386
7.381
7.367
7.354
7.349
7.341
7.329
7.325
7.308
7.295
7.291
7.273
7.244
4.553
4.543
4.533
4.428
4.417
4.403
3.936
2.309
2.299
2.288
2.277
2.257
2.213
2.196
2.189
2.179
2.172
2.163
2.154
2.059
2.057
2.045
2.033
1.868
1.862
1.853
1.848
1.842
1.829
1.820
1.807
1.796
1.739
HO
H
Ph
CN
O
Ph
H
11, 8:1 dr
^{1}H NMR (400 MHz, $CDCl_3$)
diast
ereo
mer
2.30
3.31
2.01
3.49
1.00
1.09
1.00
1.18
1.31
1.26
2.28
1.07
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

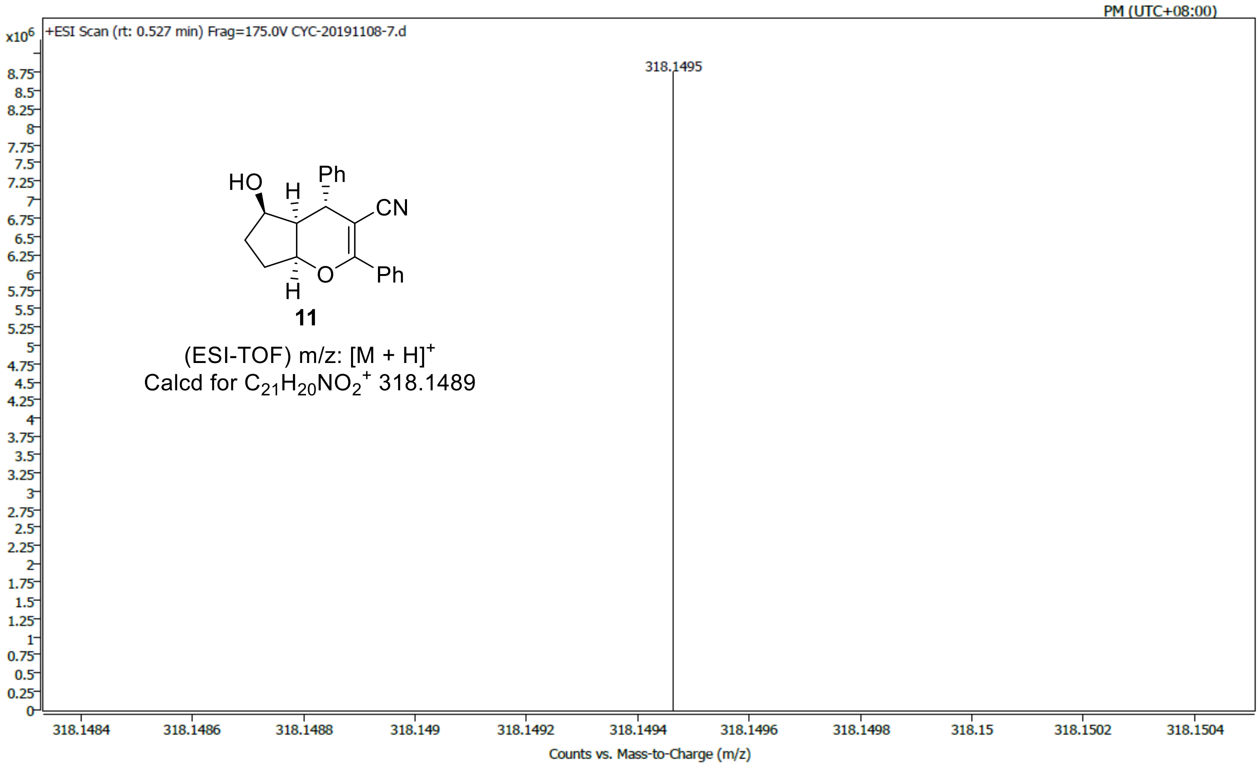

165.909
143.831
133.535
130.703
129.088
128.382
128.184
127.603
127.280
120.383
86.726
77.886
77.397
77.080
76.762
74.121
50.462
38.860
33.293
30.750
HO
H
Ph
CN
O
Ph
H
11, 8:1 dr
^{13}C NMR (100 MHz, $CDCl_3$)
diastereomer
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
8.031	BV	0.19	523.6131	6536.8081	44.8062
8.857	VV	0.22	54.9818	782.4445	5.3632
9.787	VB	0.24	48.0154	755.8801	5.1811
20.763	BB	0.53	189.5540	6513.9346	44.6494
			Totals:	14589.0672	100.0000



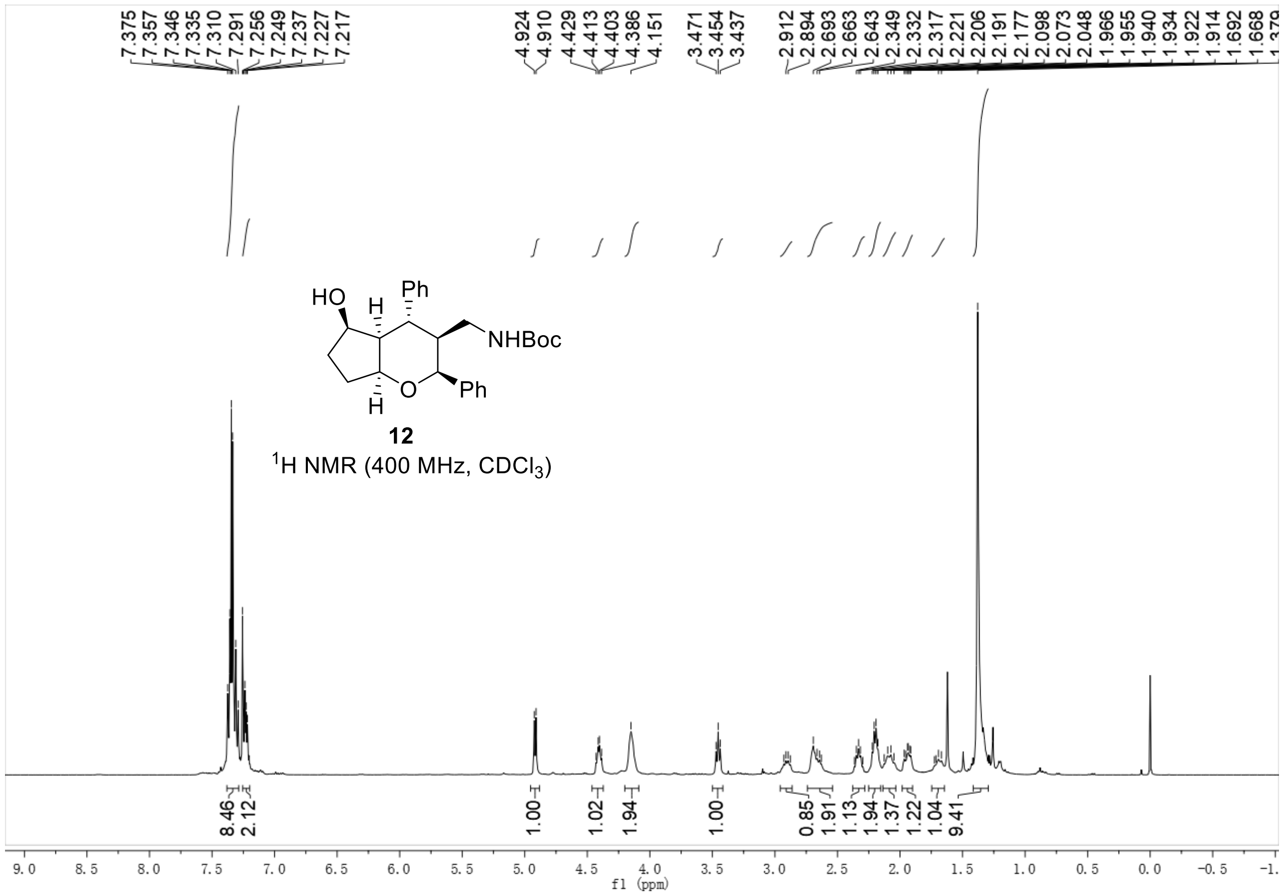
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
7.901	BB	0.19	342.2342	4148.7358	99.8031
20.483	BB	0.45	0.2516	8.1847	0.1969
			Totals:	4156.9205	100.0000



11

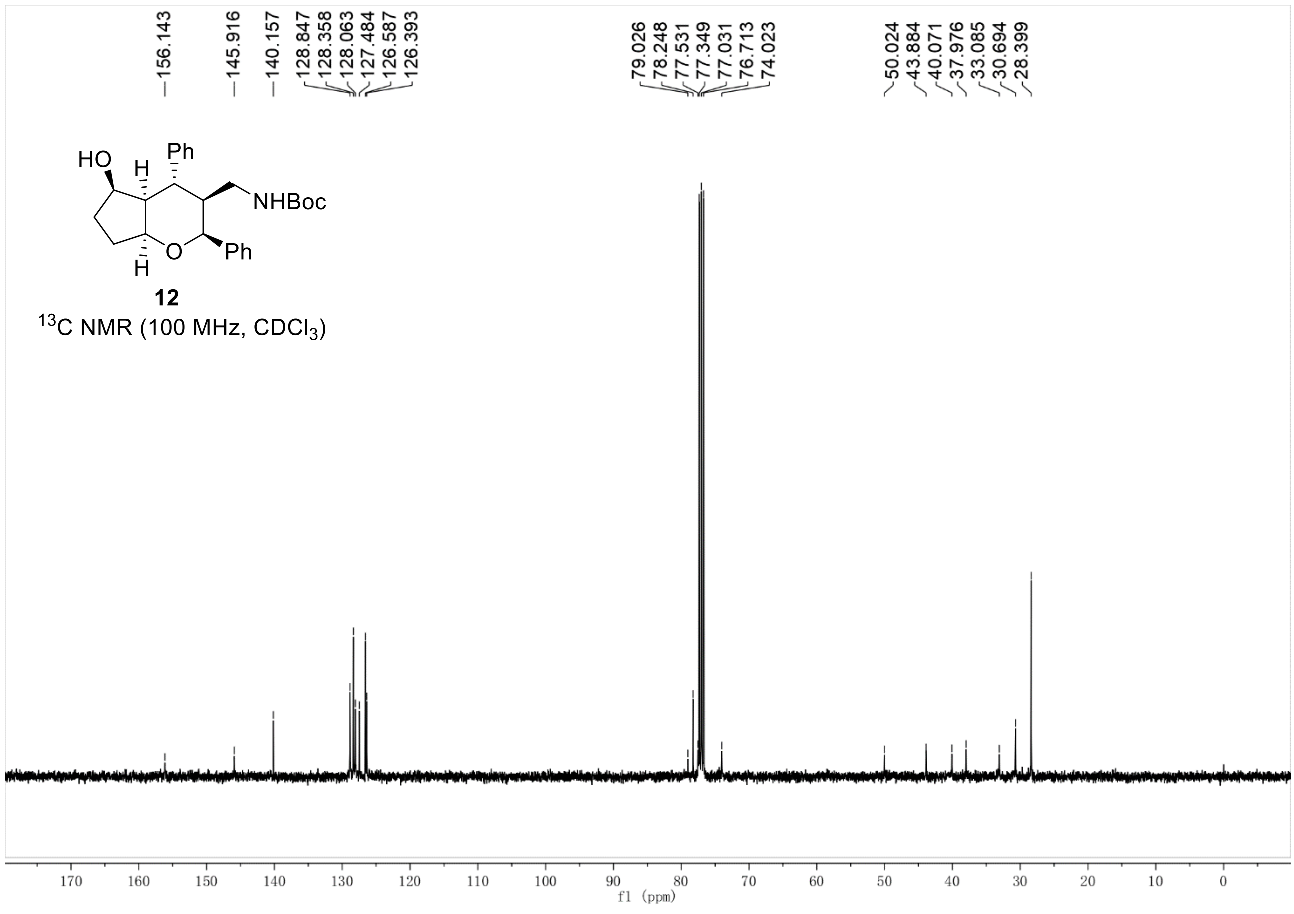
(ESI-TOF) m/z: $[M + H]^+$

Calcd for $C_{21}H_{20}NO_2^+$ 318.1489



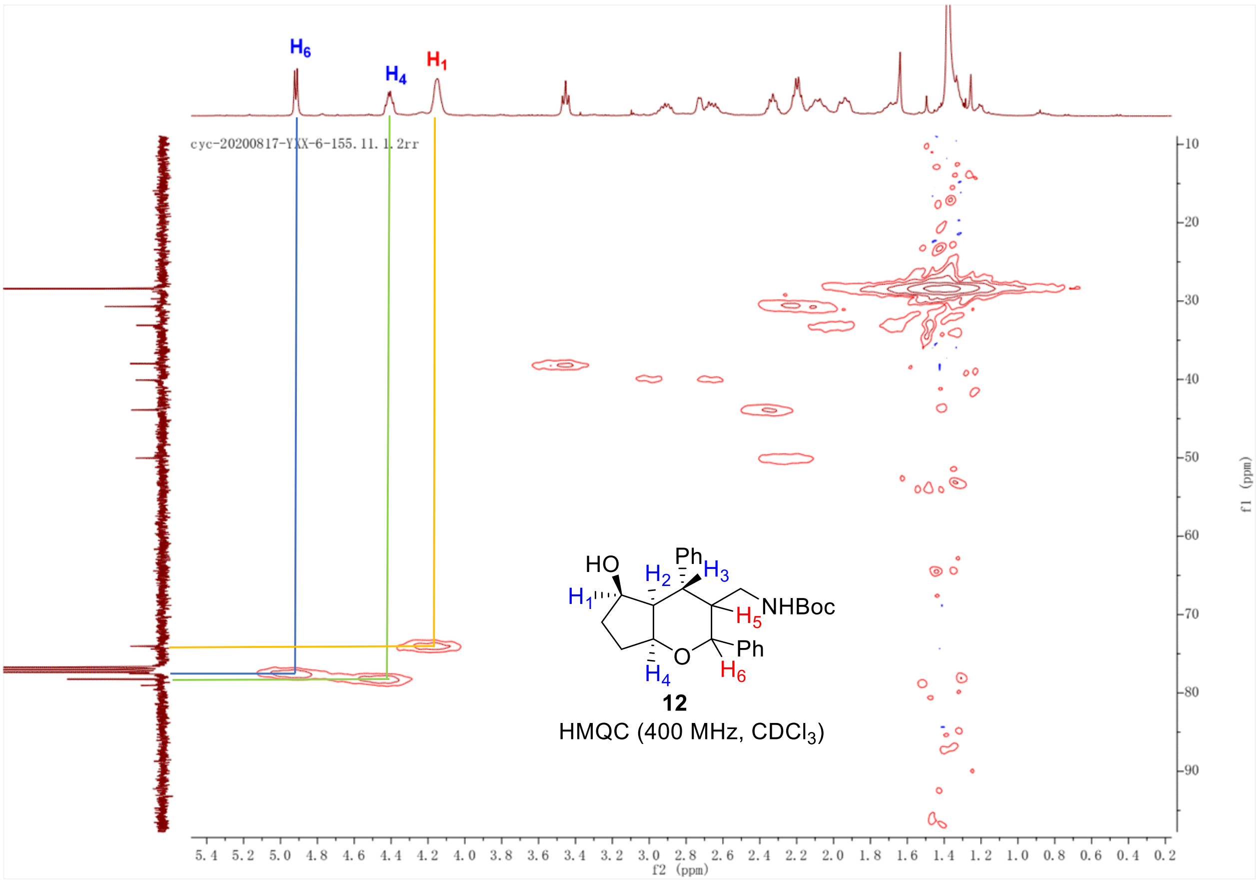
12

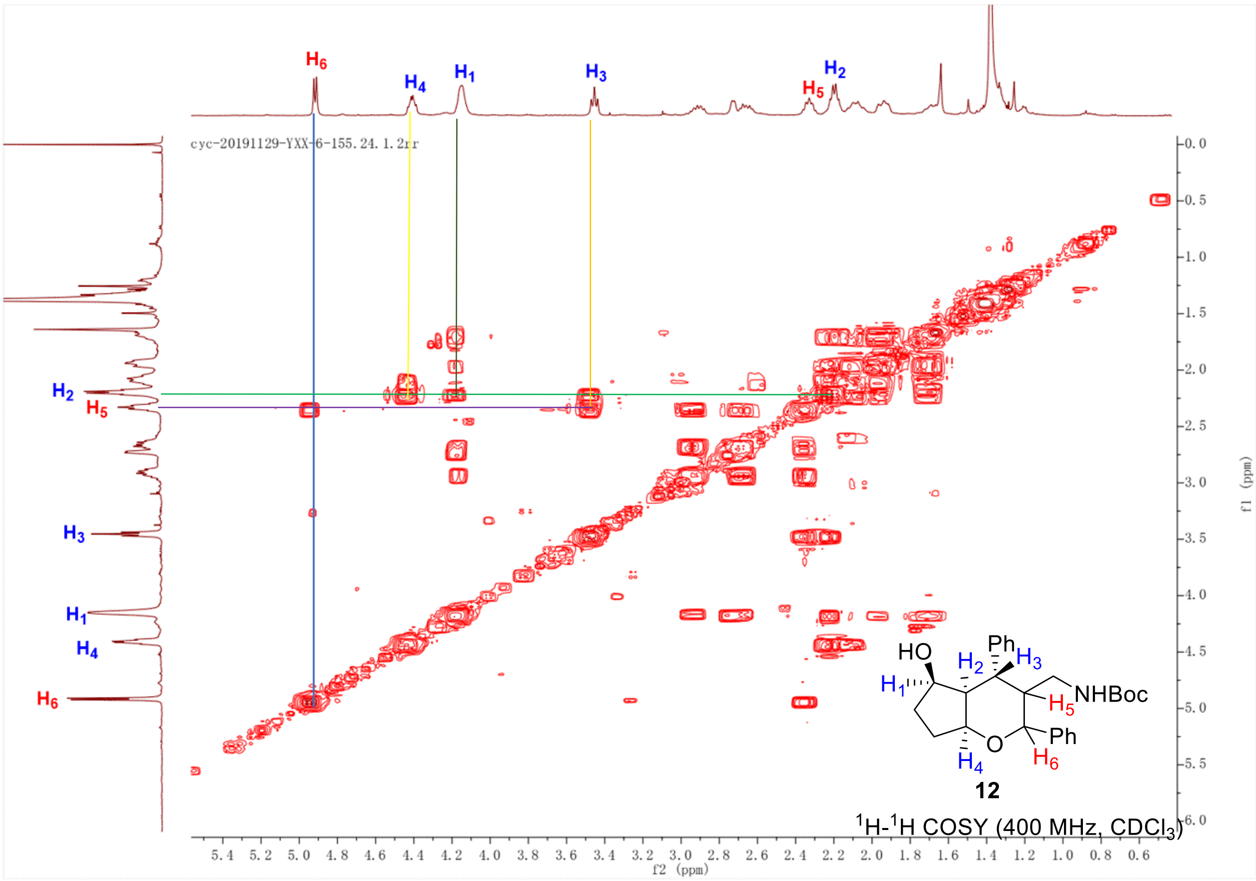
^1H NMR (400 MHz, $CDCl_3$)

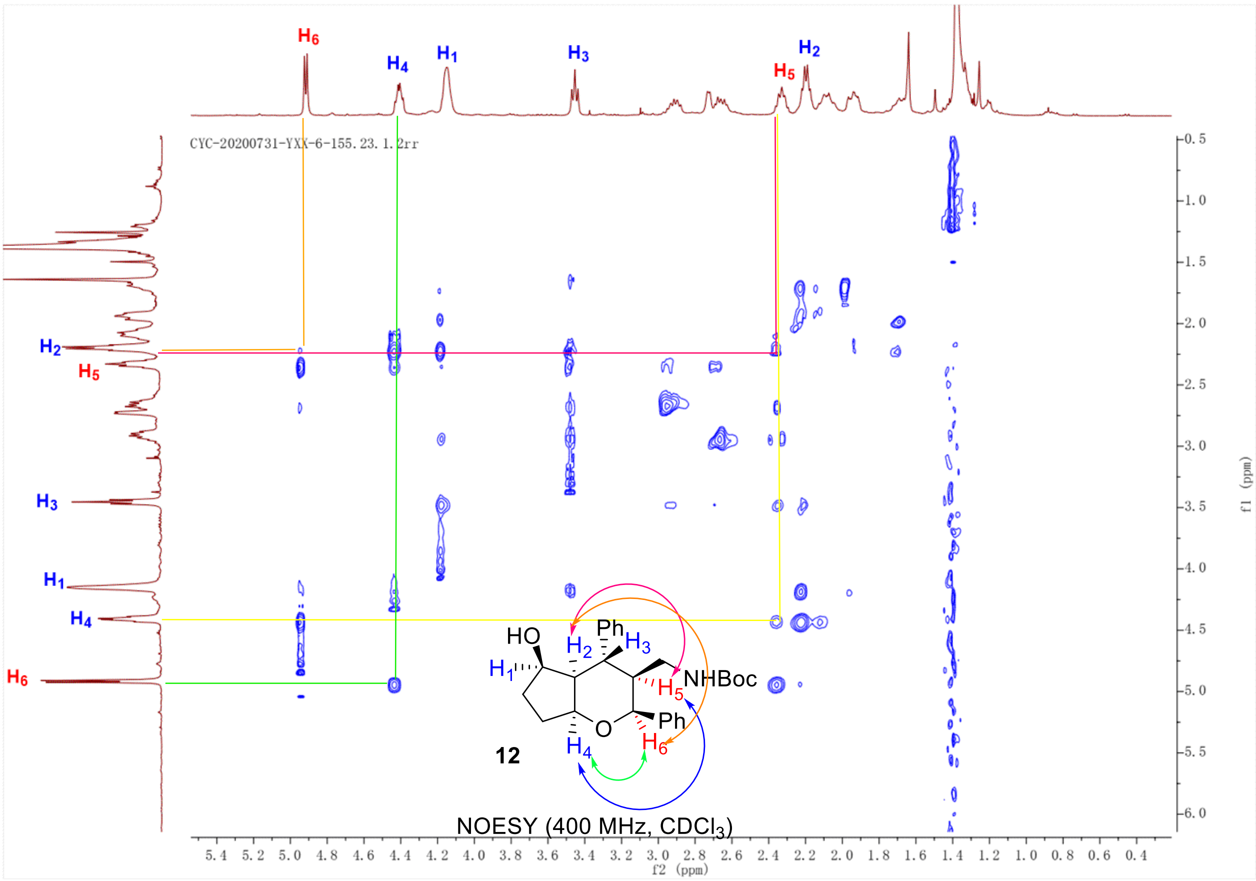


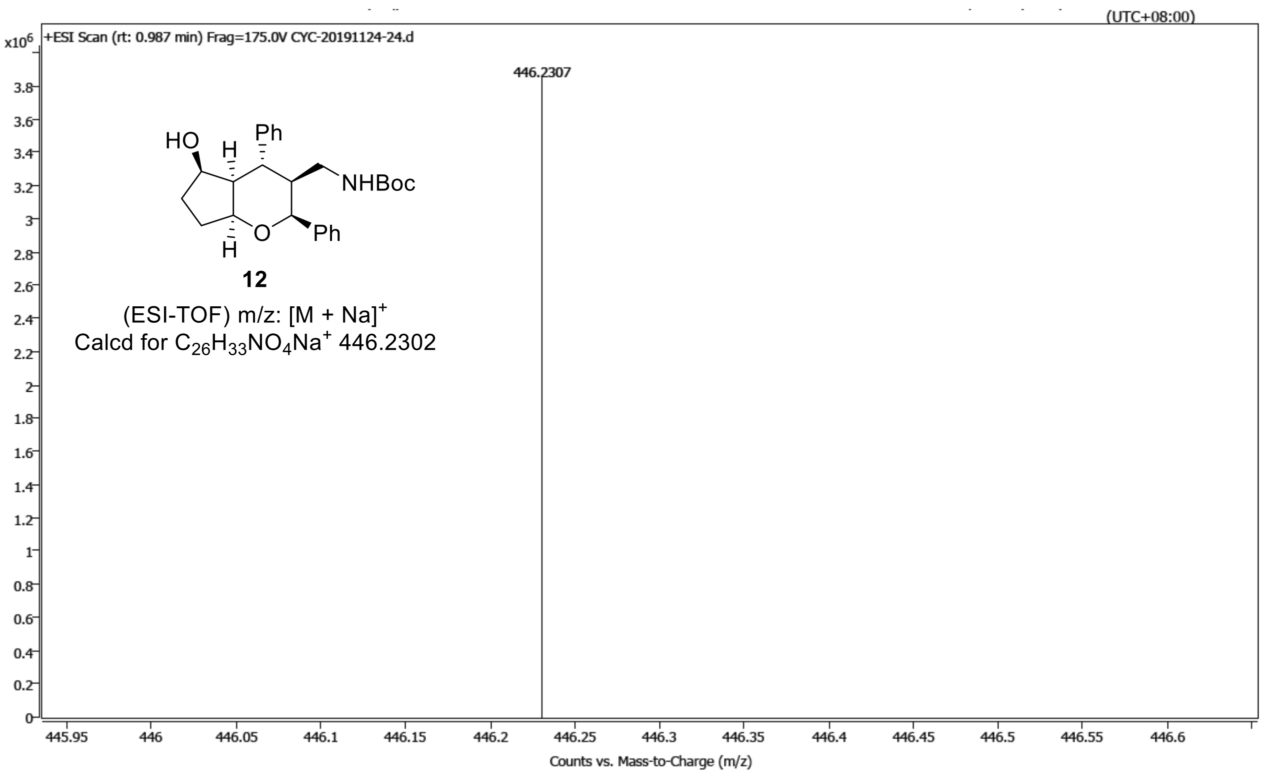
12

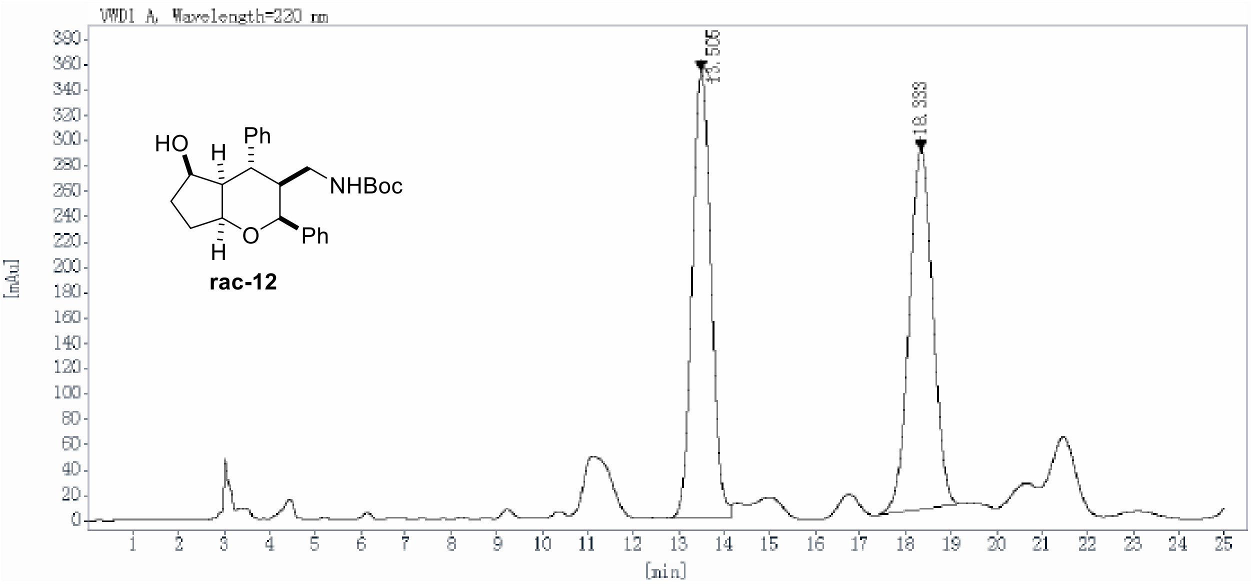
^{13}C NMR (100 MHz, $CDCl_3$)


H6
H4
H1
cyc-20200817-YXX-6-155.11.1.2rr
12
HMQC (400 MHz, CDCl3)
f2 (ppm)
f1 (ppm)

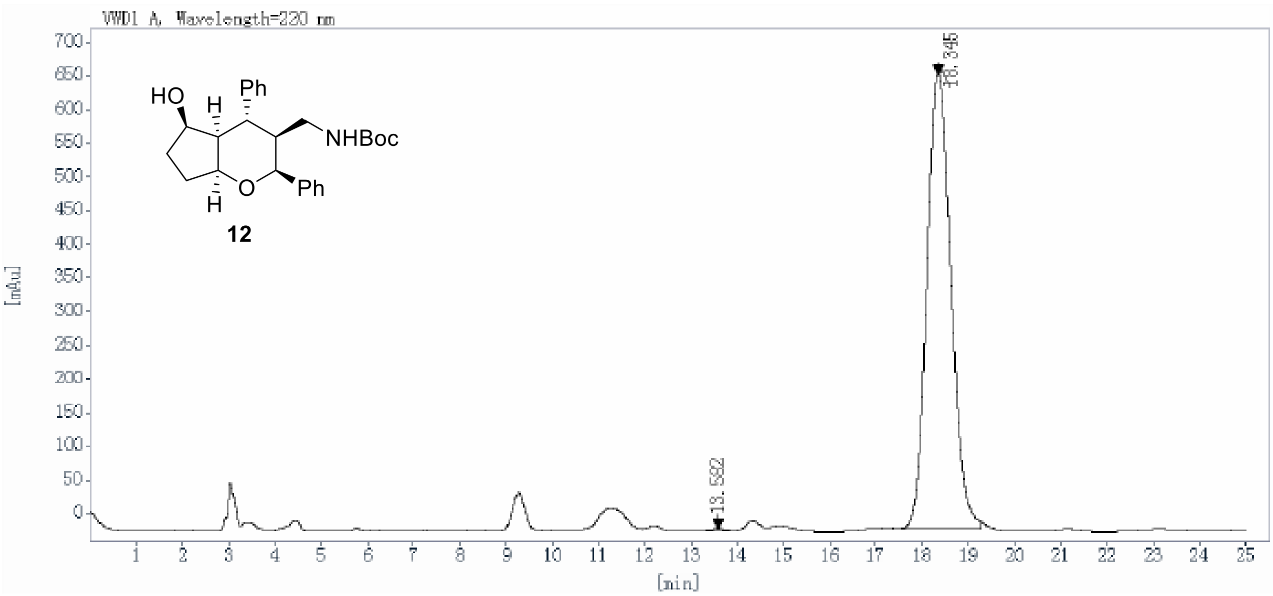

H6
H4
H1
H3
H5
H2
cyc-20191129-YXX-6-155.24.1.2rr
12
1H-1H COSY (400 MHz, CDCl3)
f2 (ppm)
f1 (ppm)


CYC-20200731-YXX-6-155.23.1.2rr
HO
Ph
NHBoc
Ph
O
12
NOESY (400 MHz, CDCl3)
f2 (ppm)
f1 (ppm)


(UTC+08:00)
+ESI Scan (rt: 0.987 min) Frag=175.0V CYC-20191124-24.d
x10^6
446.2307
HO
Ph
NHBoc
Ph
12
(ESI-TOF) m/z: [M + Na]+
Calcd for C26H33NO4Na+ 446.2302
Counts vs. Mass-to-Charge (m/z)



Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
13.505	VV	0.45	352.6948	10076.5938	49.4677
18.333	BB	0.57	283.3948	10293.4678	50.5323
			Totals:	20370.0615	100.0000



Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
13.582	BB	0.38	2.8673	68.8163	0.2819
18.345	BBAS	0.57	674.3080	24343.0645	99.7181
			Totals:	24411.8807	100.0000

13. Computational data

A-INT2'

Zero-pointCorrection= 0.578359 (Hartree/Particle)

ThermalCorrection to Energy= 0.618233

ThermalCorrection to Enthalpy= 0.619177

ThermalCorrection to Gibbs Free Energy= 0.499970

E(solv) = -2179.40769146 A.U.

C	-2.793907	-0.225480	0.799293
C	-2.253516	1.166605	0.763502
C	-1.917382	-1.231080	1.106589
C	-3.097947	2.318879	0.348821
C	-4.443061	2.445545	0.722240
C	-2.485306	3.353709	-0.378785
C	-5.164390	3.584161	0.362572
H	-4.926388	1.672970	1.307688
C	-3.213137	4.476497	-0.753104
H	-1.442933	3.245149	-0.659967
C	-4.556752	4.594764	-0.381626
H	-6.203409	3.676801	0.663833
H	-2.736704	5.261027	-1.333887
H	-5.125689	5.473362	-0.671936
O	-1.064463	1.371544	1.090802
C	-4.111950	-0.488022	0.326106
N	-5.185063	-0.714554	-0.066660
C	-2.035166	-2.671183	1.033577
C	-3.244631	-3.386487	0.905069
C	-0.819908	-3.389362	1.052512
C	-3.224835	-4.770548	0.780407
H	-4.192438	-2.864495	0.903987
C	-0.807379	-4.771462	0.912009
H	0.112584	-2.846115	1.144476
C	-2.010517	-5.466528	0.775224
H	-4.161005	-5.312222	0.682985
H	0.139613	-5.302061	0.907034
H	-2.006050	-6.547369	0.666754
H	-0.932382	-0.876706	1.390082
C	-0.351577	-1.824288	-2.593023
C	-0.159479	-0.335833	-2.862813
C	-1.437353	0.258718	-2.764832
C	-2.415590	-0.814005	-2.456982
H	0.671946	0.018039	-3.462603
H	-1.731125	1.203867	-3.207713
H	-3.471406	-0.623530	-2.300897
C	-1.806052	-2.016526	-2.349389
H	-2.243225	-2.964858	-2.067300
O	0.523212	-2.682620	-2.566833
C	1.266612	-0.633618	2.590101
C	2.003208	-0.843596	1.409873
C	2.700058	-2.047936	1.246386
C	2.660391	-3.025388	2.243731
C	1.927361	-2.811930	3.411499
C	1.233438	-1.610729	3.582837
p	1.893272	0.419803	0.081231
C	3.332345	0.067185	-0.998445
C	3.209034	-0.952988	-1.956636
C	4.284072	-1.259784	-2.791105
C	5.479470	-0.544742	-2.694507
C	5.600467	0.477792	-1.752361
C	4.534844	0.781612	-0.904272
C	2.337901	1.971233	0.947361
C	3.218416	2.002338	2.038550
C	3.539506	3.214721	2.648445
C	2.985822	4.406258	2.174294
C	2.108333	4.383011	1.089034
C	1.783582	3.170906	0.480953
Pd	-0.178253	0.547569	-0.947107
H	3.271503	-2.224328	0.341710
H	3.205594	-3.954694	2.104055
H	1.894423	-3.575454	4.183143
H	0.659570	-1.437076	4.488723
H	2.283832	-1.513691	-2.058963
H	4.177191	-2.054625	-3.523836
H	6.311125	-0.779691	-3.353034
H	6.526051	1.041595	-1.674453
H	4.639524	1.576839	-0.174415
H	3.647128	1.077694	2.412208
H	4.220940	3.229193	3.494457
H	3.234179	5.349141	2.653290
H	1.668687	5.306294	0.722684
H	1.088555	3.142516	-0.353471
H	0.716180	0.293190	2.720079

C-TS2

Zero-pointCorrection= 0.579197 (Hartree/Particle)

ThermalCorrection to Energy= 0.617414

ThermalCorrection to Enthalpy= 0.618358

ThermalCorrection to Gibbs Free Energy= 0.505017

E(solv) = -2179.38913717 A.U.

C	2.836076	0.198562	0.011598
C	2.349735	-1.127421	0.202152
C	1.927965	1.314086	0.026745
C	3.257619	-2.310372	0.160601
C	4.559306	-2.294943	0.681162
C	2.751156	-3.508417	-0.369540
C	5.343528	-3.447263	0.649785
H	4.956543	-1.389721	1.124739
C	3.541141	-4.652873	-0.415076
H	1.733537	-3.521284	-0.745533
C	4.841895	-4.625294	0.095239
H	6.347936	-3.422975	1.062316
H	3.143107	-5.568518	-0.843796
H	5.458364	-5.519398	0.065455
O	1.109751	-1.383727	0.430059
C	4.159708	0.393376	-0.470237
N	5.217626	0.594279	-0.921518
C	2.221643	2.685660	0.480260
C	3.510307	3.242628	0.567761
C	1.120101	3.478004	0.858819
C	3.683199	4.546184	1.028309
H	4.377935	2.663631	0.278744
C	1.298659	4.778445	1.317624
H	0.121365	3.066816	0.781297
C	2.582799	5.319472	1.405512
H	4.686054	4.958973	1.093310
H	0.432845	5.367045	1.607274
H	2.726278	6.335021	1.764151
H	0.924679	1.012189	0.302051
C	-0.058980	1.937887	-2.138987
C	-0.611603	0.683032	-2.818947
C	0.523582	0.001193	-3.362762
C	1.700795	0.593996	-2.857668
H	-1.615379	0.656446	-3.225343
H	0.499285	-0.832406	-4.054449
H	2.698601	0.215799	-3.054221
C	1.430682	1.748928	-2.060876
H	2.098710	2.599996	-2.050886
O	-0.720309	2.881892	-1.724479
C	-0.599609	0.513698	2.334739
C	-1.678428	0.784206	1.472184
C	-2.418788	1.961101	1.639862
C	-2.084215	2.857490	2.657165
C	-1.012728	2.588062	3.508373
C	-0.273968	1.413226	3.346060
p	-1.991224	-0.418804	0.129537
C	-3.561238	0.084943	-0.654657
C	-3.606062	1.295633	-1.369773
C	-4.784513	1.683792	-2.005098
C	-5.918629	0.869571	-1.949968
C	-5.872867	-0.336359	-1.250454
C	-4.700853	-0.728930	-0.601900
C	-2.346154	-1.975250	1.011799
C	-3.084568	-1.981135	2.204536
C	-3.353820	-3.185110	2.852356
C	-2.883771	-4.388101	2.318288
C	-2.142800	-4.386492	1.135869
C	-1.872284	-3.183055	0.484323
Pd	-0.165284	-0.622730	-1.218901
H	-3.253532	2.180124	0.984514
H	-2.662797	3.768732	2.778558
H	-0.747446	3.293488	4.290198
H	0.568420	1.204041	3.998482
H	-2.728681	1.934734	-1.430862
H	-4.812048	2.623681	-2.548943
H	-6.832607	1.173634	-2.452118
H	-6.750367	-0.975096	-1.205131
H	-4.674966	-1.666040	-0.056765
H	-3.440265	-1.044850	2.623791
H	-3.924881	-3.185192	3.776292
H	-3.089333	-5.324531	2.828921
H	-1.765857	-5.318933	0.726224
H	-1.278547	-3.171293	-0.425259
H	-0.008551	-0.384717	2.188299

C-INT3

Zero-pointCorrection= 0.581725 (Hartree/Particle)

ThermalCorrection to Energy= 0.619801

ThermalCorrection to Enthalpy= 0.620745

ThermalCorrection to Gibbs Free Energy= 0.507868

E(solv) = -2179.42484699 A.U.

C	-2.726768	-0.040174	-0.409960
C	-2.175144	1.228956	-0.289462
C	-1.862652	-1.303035	-0.458239
C	-3.016088	2.437720	-0.051212
C	-4.150291	2.413574	0.772943
C	-2.621813	3.655006	-0.628520
C	-4.888553	3.575582	0.990222
H	-4.450418	1.487301	1.248931

C	-3.364860	4.813439	-0.416802
H	-1.727191	3.674315	-1.241456
C	-4.502602	4.776787	0.392864
H	-5.764573	3.542222	1.631685
H	-3.055906	5.746601	-0.880264
H	-5.081488	5.680664	0.561973
O	-0.891103	1.509318	-0.360760
C	-4.118996	-0.204359	-0.616243
N	-5.248144	-0.406842	-0.838880
C	-2.420369	-2.483514	0.314807
C	-3.548788	-3.197078	-0.107677
C	-1.772111	-2.883528	1.488550
C	-4.022546	-4.276818	0.637124
H	-4.076531	-2.899850	-1.007695
C	-2.243324	-3.962880	2.234227
H	-0.886897	-2.349347	1.815475
C	-3.373121	-4.663500	1.810918
H	-4.904115	-4.814559	0.299426
H	-1.722589	-4.256640	3.141860
H	-3.744028	-5.506251	2.387942
H	-0.940685	-1.029239	0.061804
C	-0.023007	-2.337869	-1.927422
C	0.850000	-1.433648	-2.755535
C	-0.009237	-0.568532	-3.498280
C	-1.249813	-0.520417	-2.849240
H	1.870361	-1.688568	-3.012584
H	0.289999	0.057512	-4.331443
H	-2.062842	0.136034	-3.133560
C	-1.447012	-1.708382	-1.922076
H	-2.185796	-2.408159	-2.333168
O	0.333297	-3.325483	-1.312890
C	0.275659	0.306308	2.286326
C	1.390215	-0.341765	1.724052
C	1.948475	-1.449679	2.372846
C	1.397494	-1.905629	3.572739
C	0.294486	-1.259233	4.130601
C	-0.263663	-0.152107	3.485277
p	2.023715	0.309489	0.133678
C	3.540021	-0.643054	-0.224204
C	3.409375	-1.997735	-0.579461
C	4.542647	-2.751720	-0.877944
C	5.809957	-2.163501	-0.842298
C	5.941147	-0.817648	-0.500810
C	4.811948	-0.057930	-0.188583
C	2.552742	2.005872	0.534009
C	3.207589	2.297315	1.740081
C	3.606430	3.602900	2.018596
C	3.346885	4.624905	1.100969
C	2.685718	4.341380	-0.094563
C	2.286738	3.034874	-0.378014
Pd	0.363608	0.255152	-1.479210
H	2.807451	-1.957151	1.948804
H	1.833194	-2.768534	4.067911
H	-0.135514	-1.620791	5.060077
H	-1.130943	0.346554	3.907281
H	2.430905	-2.468411	-0.623495
H	4.431858	-3.798846	-1.144090
H	6.690321	-2.752684	-1.082348
H	6.923290	-0.354411	-0.474037
H	4.922011	0.987004	0.080258
H	3.394772	1.504506	2.458213
H	4.112418	3.825416	2.953526
H	3.652287	5.643137	1.323999
H	2.469941	5.137161	-0.801289
H	1.749492	2.810108	-1.294957
H	-0.171625	1.147506	1.767416

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C-TS3

Zero-pointCorrection= 0.580322 (Hartree/Particle)
ThermalCorrection to Energy= 0.618243
ThermalCorrection to Enthalpy= 0.619188
ThermalCorrection to Gibbs Free Energy= 0.505224
E(solv) = -2179.39510301 A.U.

C	2.910113	0.481023	-0.204931
C	2.834402	-0.876473	-0.480494
C	1.701526	1.325538	-0.559340
C	3.827312	-1.885178	-0.012686
C	4.524076	-1.749885	1.198191
C	4.016336	-3.047120	-0.776928
C	5.405459	-2.744749	1.618891
H	4.380708	-0.867807	1.810606
C	4.903074	-4.035720	-0.358499
H	3.454483	-3.159936	-1.697628
C	5.602013	-3.887546	0.841823
H	5.937981	-2.625709	2.558252
H	5.047079	-4.924797	-0.966509
H	6.291451	-4.659926	1.171422
O	1.854996	-1.351771	-1.198966

C	4.044111	1.099026	0.368827
N	4.967904	1.647216	0.828443
C	1.661841	2.675380	0.123325
C	2.421234	3.764698	-0.313626
C	0.857569	2.826812	1.257911
C	2.361360	4.985154	0.356729
H	3.076001	3.662353	-1.174116
C	0.793908	4.046364	1.930936
H	0.284559	1.980584	1.620816
C	1.543028	5.132462	1.478358
H	2.958769	5.821418	0.004947
H	0.160015	4.143312	2.808327
H	1.496249	6.085474	1.997922
H	0.837165	0.760109	-0.195050
C	0.004102	1.874389	-2.407730
C	-0.662705	0.743214	-3.129526
C	0.365056	-0.167842	-3.536283
C	1.569599	0.134899	-2.857635
H	-1.617705	0.880158	-3.623475
H	0.271980	-0.936791	-4.294207
H	2.520913	-0.314390	-3.101229
C	1.462120	1.432048	-2.107867
H	2.177049	2.152644	-2.522398
O	-0.492398	2.940955	-2.106858
C	0.176102	-0.995509	1.749445
C	-1.095553	-0.403941	1.682730
C	-1.559071	0.359517	2.763662
C	-0.754432	0.532446	3.890733
C	0.516215	-0.045924	3.943514
C	0.979781	-0.813920	2.873499
p	-2.045475	-0.597836	0.127644
C	-3.207596	0.810088	0.137648
C	-2.670589	2.104547	0.046379
C	-3.515409	3.211148	0.031096
C	-4.900170	3.037438	0.100380
C	-5.437488	1.752465	0.188146
C	-4.595920	0.638636	0.208427
C	-3.085350	-2.080530	0.373300
C	-3.498157	-2.496441	1.646733
C	-4.314763	-3.618338	1.784510
C	-4.725754	-4.330355	0.655185
C	-4.315504	-3.922410	-0.615472
C	-3.493710	-2.804452	-0.756471
Pd	-0.553507	-0.749136	-1.606370
H	-2.532170	0.837262	2.711705
H	-1.114050	1.132736	4.721567
H	1.148236	0.112207	4.812313
H	1.971263	-1.255419	2.897779
H	-1.599319	2.255554	-0.013786
H	-3.086622	4.205611	-0.044902
H	-5.558273	3.901535	0.083586
H	-6.513503	1.613368	0.243483
H	-5.018139	-0.358083	0.282128
H	-3.175750	-1.946855	2.525427
H	-4.628421	-3.938332	2.773976
H	-5.359617	-5.205365	0.766410
H	-4.627313	-4.478666	-1.494686
H	-3.160422	-2.487356	-1.741442
H	0.555705	-1.566852	0.907269

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C-INT4

Zero-pointCorrection= 0.583049 (Hartree/Particle)

ThermalCorrection to Energy= 0.621124

ThermalCorrection to Enthalpy= 0.622069

ThermalCorrection to Gibbs Free Energy= 0.506882

E(solv) = -2179.42751860 A.U.

C	2.851611	0.514376	0.185315
C	3.248564	-0.623865	-0.450139
C	1.702360	1.332736	-0.386726
C	4.205683	-1.637873	0.034137
C	4.322692	-1.963168	1.394558
C	5.000095	-2.323657	-0.900414
C	5.233156	-2.932165	1.809557
H	3.700516	-1.465524	2.127454
C	5.911975	-3.287576	-0.480606
H	4.896085	-2.090233	-1.954017
C	6.033433	-3.593443	0.876626
H	5.311605	-3.174224	2.865244
H	6.527390	-3.801922	-1.213079
H	6.743245	-4.347583	1.204303
O	2.735212	-0.966623	-1.656610
C	3.408754	0.897234	1.433142
N	3.827984	1.227935	2.469801
C	1.553705	2.708841	0.222505
C	2.600997	3.635950	0.180042
C	0.354918	3.067696	0.841853
C	2.450656	4.899801	0.746461
H	3.544821	3.362600	-0.285458

C	0.201101	4.331337	1.410906
H	-0.459967	2.354218	0.883751
C	1.248143	5.251382	1.364108
H	3.273547	5.608153	0.711525
H	-0.737511	4.592043	1.891971
H	1.131727	6.236137	1.808109
H	0.785170	0.767466	-0.169556
C	0.439931	1.709066	-2.560998
C	-0.029490	0.491574	-3.270175
C	0.950343	-0.499192	-3.209113
C	2.208713	0.037060	-2.556493
H	-0.887932	0.520867	-3.932579
H	1.001626	-1.370500	-3.855705
H	2.998692	0.183304	-3.304633
C	1.814483	1.389643	-1.931424
H	2.526583	2.173805	-2.200347
O	-0.138772	2.777342	-2.477003
C	-0.109932	-0.429862	1.990646
C	-1.417173	-0.067809	1.629101
C	-2.124479	0.834506	2.436055
C	-1.526195	1.375550	3.575241
C	-0.220001	1.023363	3.916608
C	0.485867	0.112446	3.127800
p	-2.101949	-0.725775	0.057333
C	-3.451954	0.455911	-0.325093
C	-3.106950	1.650034	-0.978471
C	-4.083446	2.606843	-1.248409
C	-5.412519	2.375742	-0.884613
C	-5.761591	1.185334	-0.245212
C	-4.785370	0.227917	0.038173
C	-2.973332	-2.260418	0.552521
C	-3.375930	-2.512530	1.870996
C	-4.057651	-3.689459	2.183270
C	-4.345261	-4.620501	1.183435
C	-3.944686	-4.376546	-0.132139
C	-3.256289	-3.205373	-0.445167
Pd	-0.510465	-0.851843	-1.627511
H	-3.130942	1.131713	2.159955
H	-2.076747	2.085504	4.186057
H	0.255823	1.467246	4.785697
H	1.510552	-0.139101	3.378797
H	-2.080677	1.835017	-1.280084
H	-3.802484	3.527539	-1.751271
H	-6.174149	3.118988	-1.103213
H	-6.794591	0.999410	0.035635
H	-5.060974	-0.693753	0.540504
H	-3.152736	-1.791023	2.650569
H	-4.363171	-3.879141	3.208414
H	-4.874388	-5.536674	1.429750
H	-4.159883	-5.101977	-0.911527
H	-2.930817	-3.016276	-1.465241
H	0.453220	-1.111426	1.357616

A-INT2

Zero-pointCorrection= 0.767760 (Hartree/Particle)

ThermalCorrection to Energy= 0.816626

ThermalCorrection to Enthalpy= 0.817570

ThermalCorrection to Gibbs Free Energy= 0.682113

E(solv) = -2703.28595432 A.U.

C	1.284980	-2.545186	-2.771700
C	0.570271	-1.269802	-3.104454
C	-0.812917	-1.493896	-2.868558
C	-0.959914	-2.876460	-2.334412
H	0.991474	-0.572364	-3.819176
H	-1.628064	-1.000629	-3.386864
H	-1.912208	-3.286279	-2.017305
O	2.488831	-2.779809	-2.871414
Pd	-0.107157	-0.311225	-1.227983
p	1.497683	1.055066	-0.173623
p	-2.062750	-0.072615	0.026483
C	1.369274	1.287876	1.641798
C	0.290148	2.004984	2.181973
C	2.258225	0.645765	2.513217
C	0.120595	2.099653	3.561120
H	-0.426419	2.487596	1.525310
C	2.083246	0.736519	3.893724
H	3.075583	0.062763	2.108874
C	1.017681	1.465714	4.421974
H	-0.725276	2.650507	3.961020
H	2.780156	0.229703	4.555756
H	0.878551	1.530025	5.497411
C	3.294538	0.781661	-0.445322
C	4.259993	1.604558	0.155441
C	3.703922	-0.244981	-1.300061
C	5.614646	1.387194	-0.084736
H	3.952528	2.409028	0.816710
C	5.062435	-0.460287	-1.542307
H	2.975868	-0.883831	-1.780791

C	6.018737	0.350930	-0.933035
H	6.355976	2.026285	0.387370
H	5.357822	-1.267887	-2.205426
H	7.076320	0.182859	-1.117873
C	1.297398	2.764050	-0.844410
C	1.491412	3.926845	-0.087492
C	0.930708	2.886752	-2.194263
C	1.303767	5.184618	-0.662889
H	1.769091	3.851804	0.958308
C	0.750417	4.143305	-2.770525
H	0.763845	1.986504	-2.779621
C	0.930573	5.296689	-2.003490
H	1.449224	6.077834	-0.061453
H	0.460326	4.221117	-3.814594
H	0.782324	6.276738	-2.448323
C	-2.974062	1.511145	-0.162482
C	-4.355539	1.624366	0.061064
C	-2.251243	2.652262	-0.534051
C	-4.989041	2.860837	-0.060275
H	-4.936091	0.743005	0.314978
C	-2.884236	3.890119	-0.652106
H	-1.194064	2.568805	-0.748455
C	-4.254352	3.996891	-0.411245
H	-6.058573	2.937167	0.115266
H	-2.302011	4.759731	-0.942890
H	-4.752720	4.957541	-0.506754
C	-1.939853	-0.336895	1.839496
C	-0.866820	-1.106919	2.310328
C	-2.886481	0.155831	2.747497
C	-0.759361	-1.395239	3.670586
H	-0.096954	-1.454902	1.628185
C	-2.767186	-0.126262	4.107723
H	-3.710316	0.768489	2.397643
C	-1.706865	-0.907944	4.571041
H	0.081425	-1.983452	4.025713
H	-3.502608	0.264845	4.805688
H	-1.613926	-1.124531	5.631784
C	-3.328375	-1.315011	-0.460700
C	-3.544039	-2.475101	0.293450
C	-3.991217	-1.168880	-1.689896
C	-4.398065	-3.474558	-0.177958
H	-3.039687	-2.601304	1.245614
C	-4.848199	-2.163631	-2.154834
H	-3.831030	-0.273298	-2.283487
C	-5.050226	-3.324272	-1.402129
H	-4.553904	-4.370778	0.416194
H	-5.355030	-2.036449	-3.107383
H	-5.712791	-4.103279	-1.768079
C	0.241863	-3.491670	-2.272714
H	1.510059	-2.172729	-0.112302
H	0.466860	-4.486471	-1.909705
O	1.854604	-2.052611	0.789333
C	2.465637	-3.281430	1.229971
C	1.381984	-4.359085	1.363068
H	0.902255	-4.539226	0.395095
H	1.804609	-5.306638	1.716360
H	0.609295	-4.036561	2.069599
C	3.070077	-2.950714	2.594799
H	3.508047	-3.845314	3.049769
H	3.855864	-2.195656	2.490116
H	2.302159	-2.554343	3.267410
C	3.555538	-3.700269	0.237895
H	4.042757	-4.627198	0.562731
H	3.143150	-3.856608	-0.764386
H	4.313379	-2.914107	0.162173

A-TS2

Zero-pointCorrection= 0.855976 (Hartree/Particle)

ThermalCorrection to Energy= 0.911901

ThermalCorrection to Enthalpy= 0.912846

ThermalCorrection to Gibbs Free Energy= 0.758982

E(solv) = -3216.05004756 A.U.

C	-0.533596	2.504689	-0.929389
C	-0.037204	1.801914	-2.174218
C	-0.804737	0.645298	-2.372616
H	0.628907	2.273025	-2.885934
H	-0.829408	0.010526	-3.248456
Pd	0.678180	0.114654	-0.765334
p	2.932356	0.685645	-0.451944
p	0.301238	-1.816967	0.502950
C	4.112880	-0.706236	-0.263179
C	4.021141	-1.523445	0.875247
C	5.063906	-1.010708	-1.244552
C	4.868130	-2.616496	1.029565
H	3.287203	-1.304666	1.643557
C	5.903801	-2.115838	-1.092285
H	5.152869	-0.386836	-2.126778
C	5.808292	-2.919945	0.042303

H	4.778031	-3.243749	1.910749
H	6.635906	-2.342524	-1.862303
H	6.459580	-3.781468	0.157562
C	3.597020	1.611745	-1.886593
C	4.490999	2.677993	-1.735374
C	3.207996	1.217213	-3.175839
C	4.983483	3.343771	-2.859201
H	4.794227	2.992416	-0.742329
C	3.712502	1.873609	-4.296717
H	2.499669	0.401200	-3.293084
C	4.598474	2.942742	-4.138894
H	5.667547	4.177898	-2.732520
H	3.405014	1.560910	-5.290489
H	4.981723	3.464229	-5.011144
C	3.283476	1.763974	0.990211
C	4.394930	1.578436	1.823961
C	2.368079	2.790766	1.274540
C	4.577301	2.396388	2.940168
H	5.110364	0.792148	1.611076
C	2.559585	3.606893	2.388602
H	1.508258	2.965229	0.635125
C	3.658339	3.407100	3.228113
H	5.438175	2.240891	3.584392
H	1.841503	4.394164	2.597744
H	3.800211	4.038779	4.100577
C	0.476293	-1.523265	2.306007
C	-0.007402	-2.435830	3.257982
C	1.085592	-0.341733	2.746851
C	0.160792	-2.185579	4.618516
H	-0.542344	-3.323296	2.935687
C	1.254470	-0.091149	4.109144
H	1.412678	0.394572	2.025403
C	0.799056	-1.017716	5.046689
H	-0.218973	-2.896419	5.346710
H	1.731052	0.832236	4.424744
H	0.922072	-0.825356	6.108647
C	1.429912	-3.197351	0.075901
C	2.042420	-3.171438	-1.184312
C	1.684290	-4.271102	0.938804
C	2.895699	-4.201196	-1.577185
H	1.861105	-2.325105	-1.841196
C	2.540308	-5.298761	0.546311
H	1.227948	-4.300534	1.921680
C	3.147184	-5.265545	-0.711020
H	3.376921	-4.161768	-2.549625
H	2.735833	-6.125032	1.224058
H	3.819674	-6.064035	-1.011262
C	-1.363739	-2.573035	0.397650
C	-1.606809	-3.691786	-0.410378
C	-2.436823	-1.964523	1.072376
C	-2.902577	-4.197779	-0.532358
H	-0.786988	-4.171847	-0.935239
C	-3.725694	-2.478939	0.952846
H	-2.277098	-1.086887	1.691480
C	-3.961181	-3.596291	0.148515
H	-3.081286	-5.065208	-1.161835
H	-4.539304	-1.986436	1.472452
H	-4.970706	-3.977383	0.039453
O	-0.144576	3.599034	-0.521635
C	-4.372443	1.284658	-0.252388
C	-4.697231	0.432702	-1.387991
C	-3.496531	2.378777	-0.522609
C	-5.698004	-0.682892	-1.276595
C	-6.729836	-0.728056	-0.328823
C	-5.596536	-1.720617	-2.215602
C	-7.615993	-1.805674	-0.301894
H	-6.851713	0.075684	0.386296
C	-6.481528	-2.793967	-2.191218
H	-4.809909	-1.657208	-2.958929
C	-7.492409	-2.843877	-1.227151
H	-8.410698	-1.827289	0.438602
H	-6.384040	-3.593553	-2.920945
H	-8.185879	-3.680476	-1.204094
O	-4.120868	0.592030	-2.480660
C	-4.653352	0.878011	1.069281
N	-4.828330	0.516002	2.169735
C	-3.330508	3.600098	0.290715
C	-3.429624	3.638965	1.693331
C	-3.024875	4.793009	-0.387261
C	-3.245574	4.835515	2.381189
H	-3.651106	2.736767	2.249015
C	-2.847458	5.989651	0.301186
H	-2.925065	4.772468	-1.468670
C	-2.957439	6.015777	1.691375
H	-3.329999	4.845493	3.464565
H	-2.614729	6.897882	-0.247485
H	-2.816032	6.946313	2.234458
H	-3.415255	2.552174	-1.591956
C	-1.533387	0.406639	-1.161533
H	-2.178329	-0.445148	-1.014384

C	-1.542370	1.591833	-0.330448
H	-1.644899	1.538040	0.746588

A-INT3

Zero-pointCorrection= 0.860720 (Hartree/Particle)
ThermalCorrection to Energy= 0.915819
ThermalCorrection to Enthalpy= 0.916763
ThermalCorrection to Gibbs Free Energy= 0.763949
E(solv) = -3216.08748672 A.U.

C	1.193758	2.344190	0.215500
C	0.738010	1.776735	-1.066416
C	1.272805	0.471670	-1.218069
C	2.259326	0.154025	-0.116391
H	0.332396	2.405784	-1.850697
H	1.395320	-0.036575	-2.168970
H	2.038768	-0.781058	0.406525
Pd	-0.727016	0.268129	-0.499958
p	-2.829432	1.265071	-0.122907
p	-0.841399	-2.019352	-0.056931
C	-3.367642	1.462340	1.621517
C	-2.931905	0.513400	2.556862
C	-4.199098	2.507592	2.047076
C	-3.331302	0.593146	3.889891
H	-2.263601	-0.278561	2.241743
C	-4.596304	2.588715	3.382641
H	-4.527725	3.258874	1.335924
C	-4.166667	1.632072	4.305119
H	-2.976133	-0.147791	4.600836
H	-5.238296	3.404186	3.704046
H	-4.473963	1.702966	5.344718
C	-3.070693	2.948143	-0.819988
C	-4.189805	3.302173	-1.585900
C	-2.077915	3.908448	-0.564194
C	-4.315503	4.599028	-2.088780
H	-4.961820	2.568391	-1.791629
C	-2.214286	5.203243	-1.062170
H	-1.193314	3.654749	0.013524
C	-3.330375	5.551745	-1.826973
H	-5.185120	4.862086	-2.685006
H	-1.438203	5.935123	-0.857080
H	-3.429377	6.559649	-2.220643
C	-4.198492	0.305779	-0.885964
C	-5.495854	0.265119	-0.360210
C	-3.912701	-0.412247	-2.056484
C	-6.490519	-0.476706	-0.999514
H	-5.726738	0.808920	0.550391
C	-4.906812	-1.147775	-2.697079
H	-2.897799	-0.405695	-2.445766
C	-6.198406	-1.182058	-2.167951
H	-7.493620	-0.504946	-0.582497
H	-4.669023	-1.712678	-3.593411
H	-6.971780	-1.766001	-2.658894
C	-2.359294	-2.991446	-0.416233
C	-2.423674	-3.958941	-1.425035
C	-3.519267	-2.691853	0.317550
C	-3.627131	-4.615567	-1.695549
H	-1.535781	-4.208078	-1.996213
C	-4.712076	-3.356914	0.055248
H	-3.490421	-1.932291	1.092174
C	-4.770866	-4.319207	-0.956424
H	-3.663610	-5.365576	-2.480947
H	-5.601321	-3.108075	0.625561
H	-5.705727	-4.830256	-1.168180
C	-0.583292	-2.366798	1.729230
C	0.016763	-1.379497	2.523354
C	-0.968898	-3.577778	2.323366
C	0.236375	-1.596791	3.883691
H	0.278868	-0.427697	2.071927
C	-0.750069	-3.795150	3.683443
H	-1.447731	-4.343872	1.721669
C	-0.146572	-2.806535	4.465245
H	0.695689	-0.819299	4.487178
H	-1.053916	-4.735507	4.134603
H	0.018957	-2.977393	5.525081
C	0.489834	-2.985360	-0.882276
C	1.316828	-3.894583	-0.210735
C	0.701749	-2.758556	-2.252343
C	2.326781	-4.571520	-0.898442
H	1.178077	-4.072974	0.849817
C	1.699755	-3.445063	-2.940924
H	0.083340	-2.032290	-2.773466
C	2.516267	-4.354665	-2.263405
H	2.969171	-5.264333	-0.362528
H	1.849684	-3.261289	-4.000881
H	3.302834	-4.881192	-2.796273
C	2.216165	1.364380	0.833471
H	1.855303	1.055801	1.819583
O	0.871044	3.397831	0.745808
C	4.687386	0.954511	1.039540

C	4.638249	-0.029156	0.100574
C	3.608811	2.032492	1.052877
C	5.614702	-1.096066	-0.169742
C	6.979436	-0.973084	0.140241
C	5.155297	-2.281123	-0.771464
C	7.854313	-2.024396	-0.122479
H	7.359591	-0.057844	0.576504
C	6.034292	-3.328709	-1.027016
H	4.108595	-2.371493	-1.031807
C	7.386829	-3.206151	-0.701716
H	8.907228	-1.915724	0.120403
H	5.660942	-4.241384	-1.483325
H	8.074295	-4.022780	-0.903943
O	3.560424	-0.075303	-0.731435
C	5.714683	1.061327	2.010197
N	6.520573	1.205333	2.841023
C	3.927334	3.169589	0.084133
C	4.176375	2.953830	-1.278043
C	3.959342	4.479681	0.572330
C	4.447968	4.027348	-2.125613
H	4.151883	1.947781	-1.678820
C	4.234277	5.554236	-0.273289
H	3.754858	4.659666	1.623843
C	4.479251	5.331307	-1.627957
H	4.637656	3.841876	-3.179479
H	4.254569	6.563722	0.127876
H	4.692962	6.165334	-2.290699
H	3.588216	2.475091	2.050737

B-TS2

Zero-pointCorrection= 0.856049 (Hartree/Particle)

ThermalCorrection to Energy= 0.911736

ThermalCorrection to Enthalpy= 0.912680

ThermalCorrection to Gibbs Free Energy= 0.759698

E(solv) = -3216.04949681 A.U.

C	1.704939	-0.396865	1.804732
C	1.431640	-1.317992	0.635035
C	1.785191	-0.641620	-0.558203
H	1.311420	-2.385728	0.747313
H	1.832687	-1.064160	-1.551878
Pd	-0.284443	-0.018824	0.046522
p	-1.921556	-1.641136	0.463209
p	-1.384010	1.935458	-0.553435
C	-3.455275	-1.553557	-0.531834
C	-4.311176	-0.454046	-0.356933
C	-3.769478	-2.517211	-1.497417
C	-5.459933	-0.325376	-1.131110
H	-4.077526	0.303361	0.384290
C	-4.917494	-2.378924	-2.280415
H	-3.120291	-3.374681	-1.637170
C	-5.762586	-1.284808	-2.100443
H	-6.106873	0.535156	-0.992781
H	-5.150484	-3.131635	-3.028317
H	-6.652431	-1.176092	-2.713672
C	-1.168783	-3.259270	0.050568
C	-1.183518	-4.337370	0.941188
C	-0.414800	-3.354565	-1.132444
C	-0.433265	-5.483600	0.663529
H	-1.752176	-4.271790	1.862706
C	0.334694	-4.494718	-1.404601
H	-0.373926	-2.506738	-1.811101
C	0.333933	-5.559207	-0.498210
H	-0.434716	-6.308213	1.370458
H	0.956133	-4.537248	-2.293142
H	0.947271	-6.433184	-0.693321
C	-2.496926	-1.789325	2.191318
C	-3.822761	-2.107612	2.518386
C	-1.564825	-1.545265	3.214142
C	-4.216320	-2.169686	3.855309
H	-4.545699	-2.297844	1.732376
C	-1.966227	-1.616740	4.548071
H	-0.528866	-1.302559	2.988090
C	-3.290521	-1.921509	4.871123
H	-5.246087	-2.412553	4.102086
H	-1.237570	-1.426558	5.330359
H	-3.600765	-1.967638	5.911334
C	-2.300896	2.684652	0.845264
C	-2.687347	4.034474	0.840291
C	-2.605673	1.891359	1.960184
C	-3.399758	4.564300	1.914963
H	-2.409514	4.673742	0.007852
C	-3.318200	2.423217	3.035395
H	-2.267581	0.862890	1.998940
C	-3.722350	3.758273	3.010565
H	-3.694961	5.609601	1.902541
H	-3.541097	1.792411	3.890904
H	-4.273107	4.176799	3.848039
C	-2.572272	1.771419	-1.935892
C	-2.388425	0.700500	-2.821937

C	-3.637959	2.656808	-2.140705
C	-3.253496	0.519113	-3.899143
H	-1.576925	0.000417	-2.643671
C	-4.505135	2.471577	-3.216620
H	-3.802088	3.479578	-1.453559
C	-4.314456	1.403980	-4.096265
H	-3.110774	-0.322217	-4.570199
H	-5.332810	3.159251	-3.365888
H	-4.996469	1.257710	-4.928917
C	-0.252686	3.277796	-1.071707
C	-0.076754	3.616026	-2.418277
C	0.572052	3.866198	-0.098409
C	0.916577	4.527220	-2.785984
H	-0.707615	3.166194	-3.178249
C	1.562963	4.770537	-0.469157
H	0.451366	3.596952	0.946639
C	1.738714	5.100452	-1.816208
H	1.049261	4.782061	-3.833503
H	2.215558	5.195302	0.286365
H	2.520312	5.796224	-2.106575
O	1.518222	-0.645594	2.995762
C	4.475038	-0.354616	-0.035340
C	4.303557	-1.756767	0.340222
C	4.270703	0.599915	1.008354
C	4.230907	-2.902630	-0.648235
C	4.107436	-2.788650	-2.042315
C	4.183903	-4.187887	-0.081131
C	3.945440	-3.926194	-2.836524
H	4.136904	-1.821869	-2.524054
C	4.030371	-5.321351	-0.873457
H	4.256096	-4.263881	0.997397
C	3.908230	-5.196080	-2.259674
H	3.855463	-3.813266	-3.913767
H	4.005025	-6.304089	-0.409615
H	3.790045	-6.078573	-2.883367
O	4.117006	-2.039131	1.535911
C	4.768294	0.061874	-1.354014
N	4.992039	0.436252	-2.439680
C	4.664224	2.026625	0.993421
C	4.635769	2.853292	-0.143959
C	5.028485	2.610241	2.221809
C	4.977328	4.201736	-0.051471
H	4.351665	2.449108	-1.105978
C	5.364207	3.958239	2.313775
H	5.042464	1.987783	3.112764
C	5.341997	4.764103	1.172974
H	4.955035	4.815641	-0.947973
H	5.646000	4.378894	3.275276
H	5.608920	5.815431	1.237925
H	4.334224	0.137210	1.988603
C	1.809813	0.753413	-0.225082
H	1.976316	1.539502	-0.950279
C	2.149128	0.870133	1.182160
H	2.102531	1.800194	1.734515

B-INT3

Zero-pointCorrection= 0.858353 (Hartree/Particle)

ThermalCorrection to Energy= 0.913954

ThermalCorrection to Enthalpy= 0.914898

ThermalCorrection to Gibbs Free Energy= 0.761367

E(solv) = -3216.06867086 A.U.

C	-1.688669	0.539197	1.674535
C	-1.415422	1.499345	0.552109
C	-1.736083	0.864143	-0.670139
H	-1.246859	2.556626	0.696927
H	-1.800459	1.345634	-1.637917
Pd	0.301853	0.158183	-0.106085
p	1.997669	1.767278	0.259572
p	1.375820	-1.880629	-0.453664
C	3.545529	1.560221	-0.699587
C	4.365348	0.453281	-0.425506
C	3.898308	2.430367	-1.738016
C	5.516145	0.226476	-1.173782
H	4.103125	-0.232388	0.373735
C	5.048616	2.193463	-2.493567
H	3.278663	3.292978	-1.957053
C	5.857805	1.093083	-2.214861
H	6.134981	-0.638548	-0.956976
H	5.311499	2.874878	-3.297790
H	6.749696	0.907680	-2.806295
C	1.397582	3.429514	-0.224734
C	1.699896	4.578463	0.515564
C	0.588631	3.540569	-1.366597
C	1.192992	5.818205	0.121566
H	2.318754	4.502846	1.403399
C	0.091526	4.780019	-1.763329
H	0.336955	2.647318	-1.932003
C	0.389804	5.921460	-1.014654
H	1.422192	6.702887	0.708489

H	-0.542310	4.852718	-2.642084
H	-0.011375	6.885702	-1.312129
C	2.559849	1.965656	1.989789
C	3.888828	2.276044	2.312930
C	1.618096	1.785568	3.015777
C	4.274699	2.393274	3.648353
H	4.621040	2.416419	1.525068
C	2.012068	1.907843	4.348534
H	0.582497	1.535734	2.796563
C	3.338573	2.205952	4.667848
H	5.306919	2.629547	3.891065
H	1.275629	1.760450	5.132746
H	3.642846	2.292931	5.707171
C	2.294995	-2.476937	1.016769
C	2.736169	-3.805548	1.130469
C	2.540098	-1.586137	2.069335
C	3.448831	-4.213280	2.256594
H	2.498100	-4.524887	0.353214
C	3.252283	-1.994888	3.197420
H	2.157272	-0.575787	2.018554
C	3.715453	-3.307331	3.287816
H	3.787276	-5.242431	2.335555
H	3.427773	-1.285635	4.000868
H	4.267035	-3.632155	4.165366
C	2.567845	-1.832879	-1.843754
C	2.403699	-0.825758	-2.805045
C	3.615139	-2.752020	-1.987146
C	3.270556	-0.738257	-3.892805
H	1.605712	-0.098977	-2.679554
C	4.483617	-2.661557	-3.073716
H	3.764761	-3.528066	-1.245110
C	4.313210	-1.655523	-4.027112
H	3.142810	0.055744	-4.622022
H	5.296533	-3.375172	-3.174077
H	4.996294	-1.582748	-4.868467
C	0.294365	-3.305230	-0.836390
C	0.163631	-3.810283	-2.134963
C	-0.484751	-3.847923	0.198806
C	-0.731975	-4.851817	-2.391312
H	0.763053	-3.399759	-2.941151
C	-1.377216	-4.882073	-0.061676
H	-0.391657	-3.459170	1.208327
C	-1.500391	-5.387351	-1.358855
H	-0.826178	-5.241582	-3.400918
H	-1.997208	-5.273498	0.737491
H	-2.205322	-6.187627	-1.561729
O	-1.353533	0.648310	2.845749
C	-4.486210	0.129422	0.145364
C	-4.350457	1.483710	0.511563
C	-3.811120	-0.868516	1.068310
C	-4.865077	2.637950	-0.301324
C	-5.044430	2.612148	-1.692513
C	-5.085190	3.845187	0.381269
C	-5.452245	3.759475	-2.374833
H	-4.871239	1.700221	-2.249424
C	-5.504187	4.985493	-0.298330
H	-4.908725	3.864270	1.451001
C	-5.689806	4.947355	-1.682679
H	-5.585755	3.720576	-3.452850
H	-5.681959	5.907022	0.250237
H	-6.014408	5.836699	-2.216796
O	-3.695400	1.779827	1.561435
C	-5.250522	-0.292006	-0.959729
N	-5.864276	-0.655875	-1.888264
C	-4.207214	-2.324118	0.916504
C	-4.242879	-2.992989	-0.314872
C	-4.508338	-3.058049	2.072852
C	-4.611847	-4.335913	-0.388448
H	-4.015505	-2.463224	-1.230977
C	-4.854320	-4.407796	2.006496
H	-4.478612	-2.556741	3.037183
C	-4.918336	-5.051518	0.769137
H	-4.655450	-4.822076	-1.358846
H	-5.090727	-4.949563	2.918503
H	-5.208766	-6.097065	0.708567
H	-4.040497	-0.558749	2.094674
C	-1.765185	-0.536387	-0.424661
H	-1.951403	-1.272833	-1.197523
C	-2.221931	-0.741854	1.005115
H	-1.795523	-1.614000	1.503341

B-TS3

Zero-pointCorrection= 0.859040 (Hartree/Particle)
Thermal correction to Energy= 0.913887
Thermal correction to Enthalpy= 0.914831
Thermal correction to Gibbs Free Energy= 0.764696
E(solv) = -3216.06335950 A.U.

C	0.538334	2.519606	0.074344
C	0.071150	2.234522	-1.316014

C	0.884275	1.204177	-1.857544
C	1.678031	0.636430	-0.832643
H	-0.562125	2.912065	-1.874255
H	0.885043	0.870553	-2.887939
H	2.123133	-0.336066	-0.905376
Pd	-0.747320	0.284949	-0.665013
p	-2.945217	0.880676	-0.137095
p	-0.372440	-1.970846	-0.033443
C	-3.220603	1.042476	1.664198
C	-2.316538	0.424835	2.539621
C	-4.298652	1.770005	2.191134
C	-2.505030	0.497851	3.919409
H	-1.452996	-0.097144	2.143844
C	-4.483691	1.844627	3.570924
H	-4.977498	2.290966	1.522750
C	-3.591889	1.204196	4.435981
H	-1.792731	0.013111	4.580365
H	-5.319125	2.410965	3.972467
H	-3.737022	1.270664	5.510364
C	-3.551959	2.477476	-0.803581
C	-4.622726	2.552349	-1.703730
C	-2.888863	3.654701	-0.415249
C	-5.027954	3.789812	-2.209508
H	-5.143132	1.650841	-2.007995
C	-3.302614	4.884910	-0.921426
H	-2.040745	3.614107	0.262810
C	-4.371513	4.956594	-1.819404
H	-5.859524	3.837615	-2.907013
H	-2.782077	5.788077	-0.616446
H	-4.688072	5.917796	-2.214236
C	-4.181119	-0.328730	-0.741056
C	-5.433495	-0.504876	-0.139289
C	-3.844432	-1.097650	-1.864043
C	-6.333119	-1.437575	-0.654859
H	-5.700386	0.074393	0.738412
C	-4.745358	-2.026817	-2.380188
H	-2.861656	-0.979318	-2.312823
C	-5.990520	-2.199505	-1.773913
H	-7.300623	-1.572667	-0.179470
H	-4.467931	-2.628483	-3.240336
H	-6.689517	-2.931911	-2.167218
C	-1.781595	-3.142307	-0.042455
C	-1.768152	-4.304009	-0.824997
C	-2.927751	-2.841334	0.711426
C	-2.877968	-5.150810	-0.846397
H	-0.892848	-4.549991	-1.415686
C	-4.023698	-3.699312	0.705144
H	-2.969649	-1.931166	1.299263
C	-4.003797	-4.854393	-0.078988
H	-2.856138	-6.046964	-1.460039
H	-4.901975	-3.450012	1.291432
H	-4.865130	-5.515888	-0.095503
C	0.345890	-2.089079	1.657909
C	1.646333	-1.598543	1.878042
C	-0.393011	-2.558452	2.752805
C	2.183405	-1.549973	3.163862
H	2.259296	-1.261911	1.050585
C	0.145934	-2.509480	4.040222
H	-1.384520	-2.969787	2.608973
C	1.425777	-1.996316	4.249719
H	3.181150	-1.147422	3.312191
H	-0.439655	-2.880850	4.876900
H	1.839663	-1.950150	5.252684
C	0.883343	-2.774996	-1.098111
C	1.758922	-3.755423	-0.610601
C	0.963913	-2.391803	-2.444838
C	2.704126	-4.334237	-1.456913
H	1.712981	-4.051457	0.431913
C	1.902314	-2.979397	-3.292278
H	0.298438	-1.618094	-2.818860
C	2.775757	-3.949856	-2.797119
H	3.393773	-5.075222	-1.064877
H	1.963447	-2.667907	-4.330732
H	3.520301	-4.394442	-3.450871
C	1.658364	1.503426	0.394860
H	1.368980	0.927877	1.279769
O	0.107825	3.358767	0.848071
C	4.145763	1.176516	0.818246
C	4.485809	0.470109	-0.340495
C	3.024870	2.202768	0.793187
C	5.484140	-0.647510	-0.334469
C	6.632023	-0.665004	0.469588
C	5.245160	-1.728049	-1.197614
C	7.504903	-1.752160	0.428061
H	6.847550	0.171133	1.124068
C	6.109881	-2.818709	-1.227947
H	4.374598	-1.691554	-1.842361
C	7.244551	-2.835547	-0.413152
H	8.392737	-1.750248	1.054413
H	5.902750	-3.653470	-1.893121

H	7.925156	-3.682558	-0.438978
O	3.867689	0.673882	-1.444759
C	4.619253	0.824850	2.098354
N	4.943693	0.550664	3.190908
C	3.264904	3.508512	0.041850
C	3.597227	3.589941	-1.319394
C	3.104087	4.704502	0.756967
C	3.764192	4.832469	-1.933375
H	3.740526	2.675087	-1.878343
C	3.273055	5.945203	0.144107
H	2.831941	4.660520	1.807988
C	3.603175	6.014426	-1.209484
H	4.027592	4.873064	-2.987463
H	3.143986	6.854985	0.724472
H	3.735510	6.978458	-1.693753
H	2.851237	2.498817	1.830552

D-TS2-A

Zero-point correction = 0.579009 (Hartree/Particle)
Thermal correction to Energy = 0.617284
Thermal correction to Enthalpy= 0.618228
Thermal correction to Gibbs Free Energy = 0.504484
E(RB3LYP) = -2179.37965414

C	-1.56114100	1.89012100	0.07874300
C	-0.77375200	2.73366500	-0.81755100
C	-2.73770100	1.16799300	-0.56902000
C	0.45934900	3.45824300	-0.34949900
C	1.20523800	3.09224100	0.78035900
C	0.93403500	4.49616100	-1.16443200
C	2.39119000	3.75434600	1.09036400
H	0.87754900	2.27736100	1.41138100
C	2.11485000	5.16433800	-0.85001700
H	0.36228200	4.75304400	-2.04941500
C	2.84926700	4.79300200	0.27900100
H	2.96457000	3.44566400	1.95952200
H	2.46506000	5.97246500	-1.48671100
H	3.77542300	5.30704700	0.52175800
O	-1.08014300	2.80304200	-2.02308700
C	-1.54672700	2.04336800	1.48970200
N	-1.50772400	2.14168700	2.65513000
C	-3.68596900	0.52200700	0.40365600
C	-3.29185400	-0.51844100	1.25581200
C	-5.00797500	0.97602900	0.46870600
C	-4.19211800	-1.08629200	2.15417600
H	-2.26745700	-0.88590900	1.21858100
C	-5.91052700	0.41522700	1.37128100
H	-5.33146400	1.76637500	-0.20154100
C	-5.50582800	-0.61863700	2.21630900
H	-3.86455300	-1.88821900	2.80981400
H	-6.93187400	0.78287100	1.40846700
H	-6.20901200	-1.05793600	2.91820700
H	-3.26060100	1.87029800	-1.21788300
C	-2.10004900	-2.32027400	-1.77187200
C	-1.37890300	-1.04577900	-1.97834900
C	-2.41257300	0.04842000	-1.98726100
C	-3.73920600	-0.72546800	-2.09988900
H	-0.61185500	-1.03818300	-2.75437800
H	-2.24443800	0.80133600	-2.75245700
C	-3.43792400	-2.14987200	-1.81612400
H	-4.20855200	-2.90116600	-1.69488700
C	0.88043200	-0.59742700	2.73302200
C	1.58225000	-1.41942000	1.83621800
C	2.40975900	-2.43862000	2.32965500
C	2.53900700	-2.62590500	3.70599300
C	1.84403100	-1.80213600	4.59466800
C	1.01514300	-0.78950300	4.10725600
P	1.41561800	-1.08914600	0.04729200
C	1.81070600	-2.67672300	-0.76356400
C	0.98116400	-3.77978100	-0.50133600
C	1.21061100	-4.99710900	-1.13693100
C	2.26243800	-5.12176900	-2.05052900
C	3.08548400	-4.02811900	-2.31752300
C	2.86462100	-2.80736400	-1.67482700
C	2.77190700	0.05738700	-0.38126200
C	3.98249100	0.06041500	0.32561600
C	4.97684800	0.98139500	-0.00191800
C	4.76866600	1.90285600	-1.03061600
C	3.56568500	1.90345700	-1.73740500
C	2.56745600	0.98841900	-1.41137300
Pd	-0.52564500	-0.11044500	-0.38169200
H	2.94347200	-3.08631200	1.64098000
H	3.18006200	-3.41742800	4.08360800
H	1.94487400	-1.95373100	5.66553900
H	0.46307400	-0.14835900	4.78746700
H	0.16215700	-3.67948700	0.20634400
H	0.57007600	-5.84799000	-0.92324900
H	2.43733800	-6.06966000	-2.55089500
H	3.90475500	-4.12231500	-3.02436000
H	3.51118700	-1.95992700	-1.87803000

H	4.13957600	-0.64144000	1.13856900
H	5.90987400	0.98639800	0.55428000
H	5.53807400	2.63101600	-1.27004800
H	3.38400100	2.64099900	-2.51175800
H	1.61303700	1.01982100	-1.92816800
H	0.22005700	0.18614300	2.37249800
H	-1.58026500	-3.26385800	-1.64197500
O	-4.80725900	-0.23501500	-2.40243200

D-TS2-B

Zero-point correction=0.577967 (Hartree/Particle)

Thermal correction to Energy= 0.616835

Thermal correction to Enthalpy= 0.617780

Thermal correction to Gibbs Free Energy= 0.501243

E(RB3LYP) = -2179.37355113

C	3.01158900	1.34646500	-0.20160500
C	1.81729200	1.72300400	-0.87660300
C	3.58887000	0.10407500	-0.56452900
C	1.06104100	2.97988400	-0.60653200
C	0.89945500	3.51756100	0.67931800
C	0.42711500	3.60692100	-1.69260100
C	0.13265700	4.66724400	0.86845500
H	1.35730800	3.03499600	1.53356300
C	-0.32388300	4.76288900	-1.50244800
H	0.53341000	3.17079700	-2.68011300
C	-0.47083700	5.29965300	-0.21984100
H	0.01120200	5.06982800	1.86978600
H	-0.79660200	5.24521700	-2.35320800
H	-1.05314800	6.20484300	-0.07028800
O	1.35864500	0.93539900	-1.78358800
C	3.58648800	2.18627400	0.79234300
N	4.05565400	2.87157700	1.61061600
C	4.93221800	-0.34052900	-0.20014400
C	5.50522000	-0.13504600	1.06830800
C	5.68424900	-1.01938900	-1.17557500
C	6.79679900	-0.57469900	1.33648600
H	4.93861400	0.35933800	1.84772900
C	6.98335500	-1.44046100	-0.91201200
H	5.23826800	-1.21004600	-2.14691100
C	7.54306400	-1.22052000	0.34683700
H	7.22400900	-0.41300200	2.32184200
H	7.55112200	-1.95522500	-1.68140400
H	8.55302000	-1.55874300	0.56105900
H	3.20900500	-0.27382800	-1.50645800
C	0.51621600	-2.71260700	-0.43155600
C	0.88812100	-1.54551400	0.42788400
C	2.31070000	-1.49427000	0.49687200
C	2.81561500	-2.69718000	-0.24163000
H	0.30985900	-1.30007800	1.31333800
H	2.81293000	-1.15641100	1.39359100
C	1.62380800	-3.33166300	-0.88359900
H	1.69271400	-4.17763300	-1.55614900
C	-2.85639200	-2.23943200	-2.05037900
C	-3.18270500	-1.89475900	-0.73022300
C	-4.20139800	-2.59761900	-0.06953600
C	-4.88426600	-3.62330800	-0.72313400
C	-4.55746600	-3.95609800	-2.03957700
C	-3.54328900	-3.26282400	-2.70292400
P	-2.26661400	-0.51196400	0.04543100
C	-2.32252400	-0.89195500	1.83532500
C	-1.93302100	-2.16544500	2.28371200
C	-1.85756800	-2.43974500	3.64840200
C	-2.16342000	-1.44640500	4.58086400
C	-2.54887500	-0.17864700	4.14207300
C	-2.62792600	0.09987800	2.77743800
C	-3.36148400	0.94690800	-0.13997800
C	-4.75220100	0.83110100	-0.27518700
C	-5.54250400	1.97449000	-0.38209800
C	-4.95307800	3.24069000	-0.35118800
C	-3.56929500	3.36262200	-0.21951300
C	-2.77282100	2.22143300	-0.12084000
Pd	-0.22476500	-0.05317500	-0.83965300
H	-4.45158800	-2.34924400	0.95699200
H	-5.66957800	-4.16454000	-0.20325400
H	-5.08790300	-4.75821400	-2.54453200
H	-3.28057000	-3.52365600	-3.72392300
H	-1.69917800	-2.94626800	1.56662800
H	-1.55828600	-3.42915300	3.98178900
H	-2.10201600	-1.66010600	5.64388200
H	-2.79197000	0.59683300	4.86277500
H	-2.92986100	1.08730100	2.44417200
H	-5.21535000	-0.14954400	-0.30461500
H	-6.61893100	1.87662600	-0.49118200
H	-5.57198700	4.12949200	-0.43598900
H	-3.09851700	4.33970000	-0.20399600
H	-1.69474800	2.32096700	-0.03048300
H	-2.05408500	-1.70705200	-2.55556400
O	3.95451000	-3.14352600	-0.25556300
H	-0.50703700	-2.99154900	-0.65399200

L6-RSS-TS1

Zero-pointCorrection= 0.922862 (Hartree/Particle)

ThermalCorrection to Energy= 0.984672

ThermalCorrection to Enthalpy= 0.985617

ThermalCorrection to Gibbs Free Energy= 0.819019

E(solv) = -3744.15623961 A.U.

C	2.216918	-3.891271	-0.764910
C	3.410476	-3.384481	-1.401414
C	0.991403	-3.564037	-1.417915
C	4.778593	-3.575272	-0.825096
C	5.154504	-4.661977	-0.023631
C	5.730335	-2.583591	-1.113732
C	6.442175	-4.730755	0.508597
H	4.450064	-5.456101	0.188094
C	7.011928	-2.648229	-0.575118
H	5.436042	-1.767105	-1.764127
C	7.369847	-3.721362	0.246269
H	6.719641	-5.577572	1.129687
H	7.733051	-1.865804	-0.795601
H	8.368681	-3.774993	0.670522
O	3.292887	-2.651031	-2.412480
C	2.247850	-4.424157	0.546618
N	2.272805	-4.844701	1.636777
C	-0.346346	-4.064751	-1.042859
C	-0.770751	-4.232619	0.287193
C	-1.256036	-4.349924	-2.074482
C	-2.050585	-4.706164	0.565136
H	-0.102230	-3.998635	1.105910
C	-2.535715	-4.823274	-1.795004
H	-0.949363	-4.198446	-3.105622
C	-2.938234	-5.005319	-0.471418
H	-2.353397	-4.848566	1.598826
H	-3.218192	-5.043809	-2.610825
H	-3.937200	-5.366684	-0.246718
H	1.129164	-3.404093	-2.482881
C	1.741978	-0.014080	-2.598136
C	0.365287	0.043060	-2.874481
C	-0.317070	-0.912718	-1.938257
H	2.548667	0.346973	-3.223311
H	-0.106770	0.432723	-3.767750
C	0.739782	-1.498290	-1.050493
H	0.494224	-1.681319	-0.013621
C	-1.145735	3.368831	-1.305944
C	0.093141	3.935250	-1.634113
C	0.461616	4.065518	-2.988461
C	-0.404552	3.652894	-3.997627
C	-1.647290	3.093515	-3.675675
C	-1.995150	2.946739	-2.338131
S	-3.596947	2.258558	-1.914662
O	-4.308490	3.193932	-1.033621
O	-4.213716	1.814889	-3.170023
N	-3.086213	1.000101	-0.948660
C	-3.969157	0.521210	0.122693
C	-3.050711	0.006044	1.251919
O	-2.357044	1.175537	1.773827
C	-1.042662	1.294493	1.560025
C	-0.477327	2.552718	2.123535
O	-0.370998	0.465370	0.966001
C	0.876291	2.921003	1.893075
C	1.318725	4.141286	2.424422
C	0.475241	4.964357	3.170991
C	-0.846214	4.589289	3.401385
C	-1.314385	3.389601	2.875763
C	-3.806141	-0.640922	2.381354
C	-3.807147	-2.033007	2.495682
C	-4.554645	-2.656152	3.494393
C	-5.300897	-1.889542	4.390367
C	-5.299294	-0.496908	4.281625
C	-4.558001	0.125260	3.278349
C	-4.983356	-0.517564	-0.311985
C	-6.341843	-0.286450	-0.081149
C	-7.296063	-1.236889	-0.444419
C	-6.894877	-2.430227	-1.044708
C	-5.538242	-2.665703	-1.277055
C	-4.582987	-1.718951	-0.911321
p	2.011158	1.962202	0.782096
C	2.600363	0.511942	1.738161
C	3.764868	-0.138055	1.292882
C	4.167607	-1.344196	1.863341
C	3.412584	-1.918199	2.888560
C	2.281754	-1.255727	3.365822
C	1.878691	-0.045755	2.799482
C	3.522961	2.997587	0.686670
C	3.782578	3.678777	-0.510049
C	4.921924	4.474998	-0.639461
C	5.816183	4.588485	0.425407
C	5.573331	3.900595	1.618054
C	4.434906	3.107517	1.748520

Pd	0.942115	1.507531	-1.245807
H	-1.473070	3.304082	-0.275554
H	0.717173	4.355102	-0.852719
H	1.420917	4.507418	-3.240779
H	-0.117955	3.765012	-5.038871
H	-2.340013	2.763978	-4.441921
H	-2.650016	0.252669	-1.502513
H	-4.495168	1.396806	0.509914
H	-2.309505	-0.677262	0.835739
H	2.339300	4.459367	2.253622
H	0.857997	5.899334	3.569878
H	-1.509467	5.224753	3.979733
H	-2.340931	3.085550	3.035879
H	-3.234712	-2.626264	1.789772
H	-4.552768	-3.739763	3.572809
H	-5.881986	-2.373681	5.170120
H	-5.879130	0.104004	4.976584
H	-4.559465	1.207882	3.191490
H	-6.652659	0.644926	0.384526
H	-8.349263	-1.042577	-0.262150
H	-7.634950	-3.171595	-1.333316
H	-5.217509	-3.589817	-1.747132
H	-3.532894	-1.918934	-1.099064
H	4.353223	0.293485	0.487124
H	5.055669	-1.844049	1.492477
H	3.693956	-2.882696	3.296306
H	1.698606	-1.688982	4.173178
H	0.995032	0.451662	3.179498
H	3.095498	3.558594	-1.343614
H	5.116131	4.995506	-1.572949
H	6.706497	5.202550	0.324989
H	6.274760	3.978563	2.443766
H	4.253686	2.563572	2.670559
O	-1.524249	-1.147017	-1.891343
C	1.934166	-0.838384	-1.418225
H	2.854298	-0.869759	-0.861522

L6-RSS-TS2

Zero-pointCorrection= 0.921866 (Hartree/Particle)

ThermalCorrection to Energy= 0.984034

ThermalCorrection to Enthalpy= 0.984978

ThermalCorrection to Gibbs Free Energy= 0.814184

E(solv) = -3744.14103385 A.U.

C	2.264685	-1.736689	-1.696033
C	2.167057	-0.655221	-2.711663
C	2.938935	0.448814	-2.266947
H	1.823770	-0.838784	-3.722593
H	3.323350	1.258464	-2.874916
O	1.701942	-2.823960	-1.710488
C	5.908628	-1.681331	-0.052567
C	6.275614	-0.360479	-0.469970
C	4.932915	-2.337993	-0.867488
C	7.200131	0.522358	0.302292
C	8.278933	0.051999	1.063888
C	6.967284	1.906071	0.233673
C	9.090154	0.947820	1.760384
H	8.493237	-1.008507	1.111523
C	7.769396	2.796786	0.941254
H	6.153286	2.263652	-0.387367
C	8.834182	2.318855	1.710120
H	9.925069	0.570619	2.343768
H	7.571663	3.864191	0.884419
H	9.465492	3.011659	2.259709
O	5.686932	0.134229	-1.472560
C	6.304470	-2.210892	1.202679
N	6.623372	-2.650414	2.236054
C	4.452716	-3.718952	-0.655575
C	4.095582	-4.221437	0.606419
C	4.281666	-4.542787	-1.778955
C	3.598375	-5.515158	0.736522
H	4.198861	-3.599961	1.487843
C	3.794988	-5.840449	-1.648248
H	4.527895	-4.153409	-2.762881
C	3.449110	-6.330702	-0.388315
H	3.323962	-5.886937	1.719484
H	3.672580	-6.462634	-2.529957
H	3.060747	-7.339914	-0.282831
H	5.004794	-2.041235	-1.910781
C	3.494845	0.115825	-0.954164
H	3.870650	0.869031	-0.281129
C	3.197252	-1.225488	-0.611921
H	3.044741	-1.542133	0.413210
C	-7.234966	0.497825	1.839720
C	-7.711165	1.761295	1.493925
C	-8.126331	2.018413	0.185093
C	-8.085874	1.009363	-0.779147
C	-7.617349	-0.259352	-0.443801
C	-7.185752	-0.495688	0.861042

S	-6.432500	-2.068013	1.265160
O	-6.587844	-2.276541	2.705193
O	-6.870658	-3.042919	0.264473
N	-4.785450	-1.895214	1.032258
C	-4.223409	-1.732837	-0.308462
C	-2.711572	-2.009718	-0.246717
O	-2.194745	-1.119633	0.806208
C	-1.425602	-0.082743	0.458342
C	-1.011834	0.724392	1.643463
O	-1.130552	0.144509	-0.711748
C	-0.214741	1.893246	1.536839
C	0.092343	2.595006	2.710832
C	-0.357819	2.167704	3.959389
C	-1.123939	1.008859	4.061702
C	-1.444547	0.297550	2.910436
C	-2.232783	-3.405875	0.060876
C	-0.875761	-3.662202	-0.177219
C	-0.331840	-4.917226	0.080787
C	-1.152836	-5.935173	0.572808
C	-2.508939	-5.690476	0.797214
C	-3.053506	-4.428472	0.547504
C	-4.468434	-0.374411	-0.952762
C	-4.708447	-0.304794	-2.327041
C	-4.879577	0.928110	-2.957700
C	-4.805525	2.106505	-2.215154
C	-4.563351	2.045872	-0.841615
C	-4.398559	0.812952	-0.216237
p	0.451336	2.507411	-0.077057
C	1.795128	3.645207	0.426446
C	2.917592	3.090135	1.066507
C	4.026562	3.876923	1.364723
C	4.032623	5.231333	1.015750
C	2.923354	5.790241	0.381874
C	1.805686	5.003674	0.089167
C	-0.900582	3.589857	-0.676658
C	-1.634162	4.421192	0.182453
C	-2.629970	5.253059	-0.327580
C	-2.904090	5.257767	-1.698297
C	-2.187075	4.422606	-2.555727
C	-1.190676	3.588790	-2.047104
H	-6.915909	0.273177	2.851864
H	-7.760483	2.543587	2.245578
H	-8.488117	3.006940	-0.082518
H	-8.411932	1.210807	-1.794588
H	-7.575036	-1.056210	-1.176328
H	-4.333501	-1.368204	1.771491
H	-4.670944	-2.511588	-0.932084
H	-2.270515	-1.670917	-1.183804
H	0.704438	3.487203	2.647932
H	-0.101099	2.737918	4.847402
H	-1.467578	0.655811	5.028865
H	-2.026839	-0.611695	2.984349
H	-0.234397	-2.889803	-0.588240
H	0.721374	-5.087727	-0.120433
H	-0.738933	-6.919958	0.772928
H	-3.151011	-6.482738	1.171775
H	-4.105503	-4.247285	0.732631
H	-4.767974	-1.223360	-2.906312
H	-5.073228	0.965698	-4.026007
H	-4.933563	3.068800	-2.700305
H	-4.496206	2.960027	-0.261096
H	-4.232839	0.779090	0.855734
H	2.915841	2.038009	1.336828
H	4.889616	3.431203	1.849914
H	4.900640	5.845447	1.237367
H	2.923065	6.842459	0.111849
H	0.946979	5.447120	-0.403867
H	-1.425637	4.418974	1.247973
H	-3.190146	5.899142	0.342607
H	-3.679082	5.908224	-2.094066
H	-2.406346	4.413293	-3.619249
H	-0.636825	2.924678	-2.705033
Pd	1.003051	0.752165	-1.467619

L6-RSS-TS3

Zero-pointCorrection= 0.922287 (Hartree/Particle)
ThermalCorrection to Energy= 0.984379
ThermalCorrection to Enthalpy= 0.985323
ThermalCorrection to Gibbs Free Energy= 0.816460
E(solv) = -3744.14119627 A.U.

C	-2.937296	3.813349	0.438042
C	-3.607726	2.650395	-0.062140
C	-1.753558	4.215544	-0.267571
C	-4.874337	2.131866	0.548784
C	-5.852034	1.637626	-0.327193
C	-5.112922	2.080712	1.928928
C	-7.050737	1.123303	0.158482
H	-5.654613	1.681767	-1.392901

C	-6.312426	1.557940	2.416589
H	-4.369882	2.448364	2.625729
C	-7.285391	1.082729	1.535625
H	-7.804564	0.758388	-0.533940
H	-6.484523	1.524412	3.488608
H	-8.220750	0.684478	1.918932
O	-3.133136	2.034535	-1.053690
C	-3.383747	4.505387	1.590224
N	-3.741107	5.074695	2.545524
C	-1.087445	5.518645	-0.050818
C	-0.785414	6.024672	1.222785
C	-0.712256	6.264891	-1.178596
C	-0.147225	7.253766	1.359288
H	-1.046473	5.456580	2.107624
C	-0.081652	7.498738	-1.041771
H	-0.925729	5.871071	-2.168949
C	0.203175	7.996856	0.230013
H	0.079886	7.631960	2.351784
H	0.193264	8.066241	-1.926288
H	0.701463	8.955784	0.341495
H	-1.785438	3.908413	-1.310730
C	0.910114	3.301416	-0.580525
C	0.980189	2.398371	-1.784236
C	-0.093316	1.467665	-1.690779
C	-0.748315	1.655107	-0.417757
H	1.497933	2.691264	-2.690064
H	-0.469827	0.832487	-2.483841
H	-1.425257	0.928247	0.003049
C	-0.318637	2.856553	0.202100
H	-0.331686	2.996865	1.277040
O	1.680001	4.195289	-0.279081
C	-3.611378	-3.494023	-3.230182
C	-4.991414	-3.462471	-3.416214
C	-5.722282	-2.345422	-3.007905
C	-5.074404	-1.251970	-2.430854
C	-3.691604	-1.256998	-2.254665
C	-2.981567	-2.392683	-2.647523
S	-1.213532	-2.495909	-2.419603
O	-0.885376	-3.926023	-2.291007
O	-0.511066	-1.672833	-3.415233
N	-0.952197	-1.685487	-0.986272
C	-1.103616	-2.269075	0.353595
C	-0.226305	-3.516624	0.651800
O	1.084949	-3.518511	-0.012587
C	1.831819	-2.433902	-0.110238

C	3.067796	-2.617697	-0.905499
O	1.512007	-1.362653	0.420811
C	4.066732	-1.606884	-0.955108
C	5.203562	-1.844089	-1.734510
C	5.354520	-3.032474	-2.452804
C	4.364771	-4.012222	-2.409688
C	3.227139	-3.803389	-1.635349
C	-0.083678	-3.757083	2.136584
C	-0.741527	-4.852611	2.705421
C	-0.668761	-5.092620	4.077471
C	0.076505	-4.242447	4.894829
C	0.739561	-3.149136	4.333787
C	0.655539	-2.899221	2.965240
C	-2.573300	-2.523330	0.644987
C	-3.312564	-1.491732	1.233797
C	-4.692619	-1.596839	1.386717
C	-5.350591	-2.749778	0.956106
C	-4.622172	-3.790231	0.380346
C	-3.240354	-3.678522	0.224008
p	3.839942	0.032120	-0.128440
C	5.354392	0.970955	-0.512196
C	5.268202	1.952205	-1.509769
C	6.392865	2.702605	-1.853111
C	7.604096	2.484481	-1.194818
C	7.691998	1.517059	-0.189882
C	6.571691	0.762231	0.153185
C	3.951694	-0.373965	1.655485
C	4.595696	-1.524496	2.128640
C	4.582262	-1.826442	3.491140
C	3.930650	-0.979585	4.389477
C	3.290520	0.171767	3.923493
C	3.296089	0.471426	2.561805
Pd	1.679934	0.657432	-0.744902
H	-3.026032	-4.364583	-3.502857
H	-5.494868	-4.313909	-3.864517
H	-6.801231	-2.328997	-3.133512
H	-5.644543	-0.395476	-2.093413
H	-3.201394	-0.408220	-1.790124
H	-0.161050	-1.055167	-1.097536
H	-0.771924	-1.470112	1.015225
H	-0.675090	-4.387109	0.181736
H	5.979485	-1.089232	-1.787254
H	6.248240	-3.184346	-3.051175
H	4.472169	-4.930571	-2.977992
H	2.438125	-4.544709	-1.601520

H	-1.323625	-5.514338	2.070137
H	-1.189749	-5.944613	4.504539
H	0.139465	-4.430213	5.962983
H	1.325930	-2.482019	4.958607
H	1.168897	-2.041955	2.546612
H	-2.806410	-0.584048	1.553196
H	-5.249879	-0.777253	1.824923
H	-6.428675	-2.830611	1.061786
H	-5.129840	-4.683529	0.028622
H	-2.699222	-4.475132	-0.275156
H	4.314449	2.129954	-1.998871
H	6.318779	3.464994	-2.622818
H	8.477801	3.074625	-1.456086
H	8.632203	1.355193	0.329507
H	6.637641	0.018115	0.941076
H	5.090592	-2.194676	1.432130
H	5.075585	-2.725403	3.849270
H	3.919116	-1.217351	5.449393
H	2.777083	0.830146	4.618199
H	2.774658	1.350412	2.192133

L6-RSS-TS4

Zero-pointCorrection= 0.922872 (Hartree/Particle)

ThermalCorrection to Energy= 0.984635

ThermalCorrection to Enthalpy= 0.985579

ThermalCorrection to Gibbs Free Energy= 0.820092

E(solv) = -3744.14170367 A.U.

C	1.952805	-1.956081	-2.269099
C	2.171101	-1.006715	-3.402269
C	3.075801	-0.010024	-2.984807
H	1.902178	-1.245679	-4.423914
H	3.656951	0.651547	-3.614801
O	1.253307	-2.958620	-2.280391
C	5.034622	-1.948684	0.387446
C	5.733510	-0.761675	-0.038877
C	4.333980	-2.655850	-0.643318
C	6.247441	0.245903	0.945412
C	6.806505	-0.069424	2.191173
C	6.100254	1.596991	0.591275
C	7.170856	0.947409	3.075114
H	6.956671	-1.103024	2.477087
C	6.441655	2.610775	1.481817
H	5.703247	1.834991	-0.388953
C	6.974410	2.286921	2.732699
H	7.604903	0.689415	4.036873
H	6.288764	3.648773	1.199370
H	7.243744	3.073222	3.432513
O	5.750166	-0.461760	-1.256416
C	4.828938	-2.241307	1.756116
N	4.652484	-2.480398	2.886776
C	3.650836	-3.954063	-0.459234
C	2.850482	-4.254173	0.655346
C	3.775725	-4.917324	-1.472875
C	2.229428	-5.494379	0.765692
H	2.705790	-3.517513	1.435484
C	3.154229	-6.158666	-1.362560
H	4.370269	-4.685316	-2.352434
C	2.381373	-6.453211	-0.238370
H	1.612663	-5.706111	1.633496
H	3.269248	-6.892332	-2.155256
H	1.894049	-7.420335	-0.148894
H	4.805369	-2.530850	-1.613608
C	3.280482	-0.176013	-1.550124
H	3.744062	0.570105	-0.930470
C	2.747546	-1.411242	-1.095334
H	2.326588	-1.508915	-0.103188
C	-6.273062	2.139039	-0.671158
C	-7.197398	2.169590	-1.711140
C	-8.418018	1.498136	-1.583868
C	-8.719401	0.797235	-0.416155
C	-7.801932	0.759092	0.634428
C	-6.590565	1.427175	0.487258
S	-5.392702	1.362219	1.808183
O	-4.953670	2.727510	2.124596
O	-5.920251	0.487498	2.862631
N	-4.068920	0.644831	1.035777
C	-3.983679	-0.829460	1.104101
C	-2.666587	-1.234005	0.439763
O	-1.599712	-0.487469	1.133031
C	-0.630293	0.040355	0.371764
C	0.589359	0.356077	1.157770
O	-0.753069	0.190391	-0.841243
C	1.464476	1.407666	0.794617
C	2.664666	1.547543	1.499240
C	3.017423	0.648605	2.508487
C	2.147265	-0.378510	2.869931
C	0.925553	-0.506627	2.210828
C	-2.278755	-2.690216	0.506773

C	-1.346984	-3.155016	-0.431693
C	-0.845042	-4.452020	-0.354687
C	-1.295824	-5.309261	0.650651
C	-2.231696	-4.859213	1.583624
C	-2.711787	-3.550511	1.521825
C	-5.153248	-1.465548	0.376716
C	-6.040465	-2.298108	1.060915
C	-7.131071	-2.864319	0.400037
C	-7.344579	-2.594518	-0.951779
C	-6.464897	-1.755463	-1.639457
C	-5.374998	-1.195208	-0.978579
p	1.132449	2.429090	-0.702069
C	2.400815	3.740616	-0.602300
C	3.531954	3.626088	-1.421989
C	4.573209	4.549515	-1.318472
C	4.482914	5.599969	-0.403425
C	3.349281	5.729133	0.404397
C	2.311544	4.803647	0.307825
C	-0.474911	3.220131	-0.341162
C	-0.963684	3.360836	0.967475
C	-2.241149	3.873774	1.188055
C	-3.035782	4.261663	0.105917
C	-2.547892	4.141778	-1.196239
C	-1.276204	3.612664	-1.420900
H	-5.311115	2.632669	-0.757973
H	-6.966485	2.711811	-2.623304
H	-9.132980	1.519735	-2.401274
H	-9.663740	0.269878	-0.323948
H	-7.998975	0.202305	1.542332
H	-3.224017	1.106224	1.372211
H	-3.988621	-1.156475	2.149213
H	-2.668994	-0.887374	-0.591993
H	3.355393	2.340373	1.240537
H	3.982785	0.743560	2.994583
H	2.439665	-1.094002	3.629610
H	0.240236	-1.305502	2.470375
H	-0.988917	-2.498223	-1.217243
H	-0.091315	-4.767925	-1.066138
H	-0.911597	-6.323563	0.711119
H	-2.582547	-5.522654	2.369162
H	-3.422631	-3.211229	2.267113
H	-5.890147	-2.481238	2.120445
H	-7.816225	-3.508331	0.943772
H	-8.196541	-3.029514	-1.466595
H	-6.634541	-1.528132	-2.687605
H	-4.714355	-0.514475	-1.505985
H	3.589564	2.811846	-2.138253
H	5.449311	4.449430	-1.952355
H	5.290231	6.322398	-0.324648
H	3.275394	6.550835	1.110814
H	1.433587	4.903231	0.938708
H	-0.354961	3.046834	1.809807
H	-2.635247	3.949791	2.195275
H	-4.037556	4.635179	0.289540
H	-3.163402	4.440981	-2.040122
H	-0.909904	3.480832	-2.435735
Pd	1.195615	0.742185	-2.294519

L6-RSS-TS5

Zero-pointCorrection= 0.923281 (Hartree/Particle)

ThermalCorrection to Energy= 0.984864

ThermalCorrection to Enthalpy= 0.985808

ThermalCorrection to Gibbs Free Energy= 0.821590

E(solv) = -3744.14362348 A.U.

C	2.093474	2.142357	-1.588744
C	1.871754	1.224902	-2.758242
C	0.488806	0.874897	-2.781525
H	2.551469	1.197492	-3.601717
H	-0.047445	0.422090	-3.605541
O	3.138592	2.696504	-1.276918
C	-1.281400	4.043432	-0.248697
C	-2.367126	3.447494	-0.988641
C	-0.028797	4.137875	-0.933299
C	-3.748128	3.304754	-0.420958
C	-4.025461	3.013680	0.922391
C	-4.818204	3.436868	-1.321420
C	-5.347037	2.900026	1.357796
H	-3.222347	2.870437	1.633137
C	-6.134981	3.323251	-0.885085
H	-4.592250	3.638648	-2.363113
C	-6.404135	3.061198	0.461363
H	-5.545812	2.681011	2.403052
H	-6.952120	3.449142	-1.590315
H	-7.430913	2.980641	0.807644
O	-2.168278	3.033412	-2.156312
C	-1.401700	4.418581	1.109894
N	-1.464333	4.693363	2.244883
C	1.132179	4.924166	-0.468825
C	1.579296	4.933816	0.863408

C	1.857024	5.655008	-1.422958
C	2.704183	5.668300	1.225282
H	1.052462	4.363294	1.617663
C	2.977986	6.396503	-1.058959
H	1.533184	5.636269	-2.460164
C	3.407017	6.404129	0.268196
H	3.034106	5.667938	2.260692
H	3.521286	6.958880	-1.812817
H	4.285742	6.974677	0.555256
H	-0.156128	4.120215	-2.011651
C	-0.118308	1.369085	-1.575407
H	-1.110422	1.091830	-1.254130
C	0.768197	2.208777	-0.852259
H	0.785813	2.234037	0.229309
C	-4.624494	-2.545067	-2.122026
C	-5.532614	-1.490332	-2.198121
C	-5.077031	-0.179971	-2.366103
C	-3.711946	0.092191	-2.492504
C	-2.796371	-0.958352	-2.427833
C	-3.263845	-2.258369	-2.228329
S	-2.068364	-3.553060	-1.964070
O	-2.529972	-4.830514	-2.510504
O	-0.744813	-3.038584	-2.354575
N	-2.174255	-3.719534	-0.264186
C	-2.233648	-2.478405	0.533730
C	-1.380000	-2.610884	1.813016
O	-0.091965	-3.310214	1.590251
C	0.774882	-2.819589	0.699045
C	2.055921	-3.574416	0.648180
O	0.495224	-1.854454	0.002192
C	3.276344	-2.943436	0.296750
C	4.430550	-3.731208	0.231435
C	4.388757	-5.101595	0.495493
C	3.189255	-5.710746	0.856523
C	2.030720	-4.942815	0.944169
C	-1.207504	-1.296329	2.544643
C	-1.424542	-1.270592	3.926664
C	-1.365696	-0.071282	4.638782
C	-1.092059	1.122601	3.971750
C	-0.857166	1.105697	2.595841
C	-0.910282	-0.091251	1.887672
C	-3.671229	-2.180348	0.933688
C	-4.152503	-0.870032	0.949311
C	-5.481669	-0.614149	1.284951
C	-6.335041	-1.663878	1.624071
C	-5.854582	-2.975181	1.625368
C	-4.529578	-3.230463	1.278221
p	3.362009	-1.140071	-0.088597
C	5.112529	-0.806687	-0.459256
C	5.482375	-0.638330	-1.799806
C	6.812816	-0.381326	-2.131065
C	7.774827	-0.281636	-1.124867
C	7.408432	-0.437712	0.214993
C	6.081111	-0.698047	0.549688
C	3.066919	-0.312219	1.525882
C	2.654244	-0.989828	2.679879
C	2.323389	-0.276837	3.833780
C	2.415719	1.113415	3.850088
C	2.849720	1.793297	2.708885
C	3.169145	1.090001	1.550252
H	-4.954420	-3.564821	-1.960203
H	-6.594775	-1.689293	-2.096924
H	-5.785909	0.642126	-2.380219
H	-3.357530	1.112994	-2.610789
H	-1.729609	-0.790377	-2.512688
H	-1.432372	-4.355711	0.023587
H	-1.845463	-1.642056	-0.043149
H	-1.871067	-3.323474	2.477636
H	5.375559	-3.268064	-0.027209
H	5.300291	-5.687807	0.425298
H	3.152100	-6.774234	1.070115
H	1.092494	-5.402032	1.233436
H	-1.666056	-2.194677	4.445974
H	-1.552221	-0.070786	5.708890
H	-1.066035	2.066363	4.508079
H	-0.645212	2.034158	2.078696
H	-0.718371	-0.082849	0.824188
H	-3.503344	-0.045630	0.673538
H	-5.847065	0.405622	1.259626
H	-7.371750	-1.462390	1.879794
H	-6.514131	-3.799417	1.882922
H	-4.162182	-4.250564	1.228623
H	4.719410	-0.693619	-2.571338
H	7.094568	-0.245823	-3.171047
H	8.809130	-0.072074	-1.382148
H	8.156079	-0.349769	0.997986
H	5.790815	-0.808012	1.590252
H	2.582397	-2.071634	2.689569
H	1.977739	-0.811743	4.712980
H	2.142719	1.666199	4.743883

H	2.925838	2.876439	2.706600
H	3.474539	1.639204	0.665069
Pd	1.644733	-0.529538	-1.496067

L6-RSS-TS6

Zero-pointCorrection= 0.922913 (Hartree/Particle)
ThermalCorrection to Energy= 0.984782
ThermalCorrection to Enthalpy= 0.985726
ThermalCorrection to Gibbs Free Energy= 0.818748
E(solv) = -3744.15495823 A.U.

C	-1.387618	2.388612	-2.256254
C	-1.727665	1.603586	-3.498636
C	-2.771197	0.744673	-3.212946
H	-1.285211	1.800325	-4.467894
H	-3.327436	0.138005	-3.916908
O	-0.534043	3.266397	-2.175910
C	-4.408833	2.577894	0.523018
C	-5.383000	1.517926	0.313322
C	-3.880313	3.204348	-0.646900
C	-5.840329	0.673438	1.468904
C	-6.076421	1.171465	2.757157
C	-6.026402	-0.695880	1.223648
C	-6.458366	0.310260	3.786278
H	-5.967974	2.230324	2.959405
C	-6.391251	-1.556097	2.255061
H	-5.874744	-1.069896	0.216822
C	-6.603428	-1.056277	3.542114
H	-6.642000	0.709587	4.779764
H	-6.511791	-2.616296	2.053601
H	-6.889055	-1.726540	4.348391
O	-5.774555	1.215312	-0.829965
C	-3.789448	2.744909	1.781591
N	-3.241121	2.869090	2.808770
C	-3.160333	4.487752	-0.739311
C	-2.368328	5.035585	0.285237
C	-3.246314	5.186403	-1.957176
C	-1.697860	6.240650	0.092287
H	-2.274459	4.524329	1.233681
C	-2.578466	6.392003	-2.147275
H	-3.846098	4.767618	-2.761445
C	-1.798381	6.925009	-1.120495
H	-1.090613	6.646307	0.896745
H	-2.663466	6.912486	-3.097020
H	-1.270184	7.863245	-1.264948
H	-4.498375	2.989024	-1.513832
C	-2.989927	0.748339	-1.765874
H	-3.829126	0.241533	-1.315096
C	-2.302290	1.884341	-1.188728
H	-1.948586	1.887908	-0.167889
C	8.169696	-0.406518	-1.131973
C	9.027413	0.641171	-1.457813
C	9.415591	1.558917	-0.477054
C	8.956960	1.428395	0.834516
C	8.099615	0.382865	1.174531
C	7.712561	-0.513962	0.181868
S	6.555217	-1.809323	0.584425
O	6.914721	-3.033530	-0.139530
O	6.373526	-1.814882	2.041716
N	5.134941	-1.278790	-0.188348
C	4.256188	-0.392133	0.596307
C	2.908476	-0.306974	-0.127567
O	2.443266	-1.707509	-0.233304
C	1.403565	-1.912965	-1.039830
C	0.851484	-3.294805	-0.931666
O	0.996537	-1.041273	-1.804085
C	-0.536653	-3.560068	-0.853969
C	-0.958652	-4.894479	-0.832018
C	-0.039986	-5.943671	-0.883712
C	1.326770	-5.674914	-0.929663
C	1.768110	-4.353563	-0.941075
C	1.887425	0.512987	0.614229
C	1.383798	1.686874	0.049818
C	0.456605	2.462772	0.748256
C	0.017328	2.058058	2.009428
C	0.512598	0.878131	2.571537
C	1.443299	0.107486	1.880003
C	4.852132	0.994771	0.724430
C	4.891021	1.627160	1.967964
C	5.432271	2.907433	2.089876
C	5.938497	3.560978	0.966064
C	5.897748	2.932670	-0.280914
C	5.354152	1.656457	-0.401326
p	-1.752734	-2.191881	-0.653067
C	-1.727131	-1.854468	1.144900
C	-2.508975	-0.787891	1.614829
C	-2.619395	-0.542832	2.981016
C	-1.928363	-1.350091	3.887654
C	-1.126143	-2.395467	3.426768

C	-1.027046	-2.654076	2.058500
C	-3.398053	-2.944372	-0.908143
C	-4.017433	-2.792950	-2.156435
C	-5.289881	-3.318318	-2.378270
C	-5.950741	-4.000173	-1.354648
C	-5.337541	-4.155744	-0.109347
C	-4.069986	-3.622114	0.119972
H	7.854315	-1.129405	-1.876311
H	9.393215	0.742875	-2.475116
H	10.078846	2.378423	-0.738348
H	9.256800	2.145090	1.592423
H	7.714202	0.269021	2.180065
H	4.646387	-2.125095	-0.479481
H	4.086444	-0.803200	1.597944
H	3.051403	0.069242	-1.141324
H	-2.018083	-5.113941	-0.761433
H	-0.395571	-6.969665	-0.873129
H	2.048169	-6.485405	-0.955738
H	2.830375	-4.137067	-0.977366
H	1.699183	1.994156	-0.942443
H	0.057294	3.353116	0.274444
H	-0.735909	2.631676	2.540211
H	0.157121	0.549124	3.541544
H	1.808553	-0.818768	2.314554
H	4.498511	1.113351	2.840467
H	5.459603	3.391339	3.061868
H	6.364302	4.555885	1.060394
H	6.297791	3.433479	-1.157460
H	5.351106	1.151586	-1.361962
H	-3.040810	-0.151235	0.918123
H	-3.226002	0.286500	3.325453
H	-2.009747	-1.157496	4.953640
H	-0.581665	-3.018471	4.130924
H	-0.417355	-3.480740	1.709745
H	-3.500895	-2.248003	-2.941554
H	-5.769601	-3.184338	-3.343113
H	-6.945935	-4.400681	-1.523239
H	-5.852262	-4.682670	0.688784
H	-3.609439	-3.714947	1.098106
Pd	-1.197456	-0.427036	-1.971425

L6-RSS-TS7

Zero-pointCorrection= 0.921653 (Hartree/Particle)

ThermalCorrection to Energy= 0.984106

ThermalCorrection to Enthalpy= 0.985051

ThermalCorrection to Gibbs Free Energy= 0.812899

E(solv) = -3744.14101696 A.U.

C	-2.821108	1.191166	0.591676
C	-2.540793	1.033319	-0.859480
C	-3.337043	-0.038310	-1.356007
H	-2.038235	1.790867	-1.447422
H	-3.538193	-0.262591	-2.395291
O	-2.255790	1.902031	1.404024
C	-5.282923	2.303876	-0.432981
C	-4.638831	3.612877	-0.277337
C	-5.433306	1.504629	0.752188
C	-4.259318	4.439600	-1.474370
C	-3.908154	3.905654	-2.722320
C	-4.187722	5.828432	-1.287625
C	-3.511274	4.746408	-3.762793
H	-3.937573	2.836653	-2.888548
C	-3.804804	6.667589	-2.329453
H	-4.432565	6.224907	-0.308369
C	-3.464937	6.127749	-3.572874
H	-3.239316	4.318336	-4.723738
H	-3.766090	7.742236	-2.173071
H	-3.162502	6.780547	-4.387386
O	-4.403557	4.066686	0.848983
C	-5.776358	1.833875	-1.666405
N	-6.189495	1.371277	-2.659654
C	-6.632148	0.668567	1.062777
C	-7.264219	-0.182520	0.142585
C	-7.135089	0.725682	2.371863
C	-8.371121	-0.939425	0.523744
H	-6.904183	-0.243691	-0.876813
C	-8.242024	-0.031550	2.752906
H	-6.652975	1.379424	3.094287
C	-8.865401	-0.869368	1.827961
H	-8.851603	-1.585359	-0.206088
H	-8.615941	0.034816	3.770904
H	-9.728278	-1.461748	2.119234
H	-5.119292	2.100639	1.609434
C	-4.057290	-0.610591	-0.251060
H	-4.689619	-1.486066	-0.331226
C	-3.984705	0.246035	0.875552
H	-4.131372	-0.122796	1.885825
C	5.913492	0.364015	-2.381588
C	6.250716	1.294186	-3.360265

C	7.251644	2.239481	-3.112996
C	7.919474	2.256121	-1.888449
C	7.591808	1.328469	-0.899084
C	6.589814	0.399350	-1.160794
S	6.137357	-0.773394	0.105608
O	6.131221	-2.124994	-0.469278
O	6.928437	-0.477444	1.306527
N	4.504830	-0.403313	0.354219
C	4.200788	0.616027	1.380805
C	2.677363	0.683335	1.494973
O	2.243854	-0.684073	1.861328
C	1.104323	-1.115218	1.313681
C	0.610280	-2.374684	1.928642
O	0.549347	-0.494933	0.409710
C	-0.168086	-3.307354	1.199156
C	-0.635032	-4.444872	1.863231
C	-0.354044	-4.656322	3.215573
C	0.418440	-3.739414	3.924973
C	0.907567	-2.606733	3.277047
C	2.105173	1.634507	2.511198
C	0.863774	2.224225	2.241749
C	0.248752	3.043954	3.187355
C	0.880811	3.291365	4.406423
C	2.119956	2.706992	4.682192
C	2.726117	1.873925	3.743520
C	4.754513	1.967884	0.975660
C	5.671911	2.625421	1.796415
C	6.198215	3.861279	1.418808
C	5.811494	4.444834	0.212374
C	4.897646	3.788421	-0.615319
C	4.371601	2.556960	-0.234670
p	-0.561069	-3.013001	-0.579911
C	-1.373145	-4.557591	-1.115200
C	-2.774858	-4.576680	-1.146386
C	-3.453804	-5.736226	-1.519857
C	-2.735743	-6.878243	-1.880029
C	-1.338787	-6.860824	-1.863612
C	-0.657022	-5.706478	-1.480314
C	1.112378	-3.031882	-1.331020
C	2.205490	-3.668809	-0.721494
C	3.480166	-3.567288	-1.277680
C	3.672589	-2.841373	-2.455889
C	2.588015	-2.220725	-3.077488
C	1.314607	-2.305459	-2.512353
H	5.122898	-0.360507	-2.542241
H	5.731269	1.287516	-4.313907
H	7.506232	2.967658	-3.877612
H	8.689019	2.997140	-1.696091
H	8.076917	1.333676	0.069295
H	4.010635	-1.281846	0.509031
H	4.634070	0.324587	2.343739
H	2.260069	0.888958	0.511427
H	-1.219932	-5.177351	1.318560
H	-0.736329	-5.545539	3.708344
H	0.642009	-3.901970	4.974532
H	1.509805	-1.881993	3.812406
H	0.354844	2.027875	1.304418
H	-0.724876	3.466113	2.962495
H	0.408118	3.933538	5.144305
H	2.612771	2.895839	5.631817
H	3.682339	1.415520	3.975044
H	5.990468	2.156532	2.722466
H	6.913783	4.362841	2.063935
H	6.223851	5.404547	-0.085804
H	4.602894	4.230985	-1.561985
H	3.688538	2.032646	-0.895311
H	-3.323750	-3.677054	-0.881150
H	-4.539641	-5.744490	-1.540848
H	-3.263318	-7.778846	-2.180534
H	-0.779923	-7.746831	-2.150870
H	0.428339	-5.693937	-1.470001
H	2.063950	-4.227204	0.198625
H	4.330754	-4.027695	-0.787553
H	4.672304	-2.753280	-2.868239
H	2.733605	-1.652365	-3.991930
H	0.476142	-1.787745	-2.970775
Pd	-1.482743	-0.874951	-0.647993

L6-RSS-TS8

Zero-pointCorrection= 0.921801 (Hartree/Particle)

ThermalCorrection to Energy= 0.984361

ThermalCorrection to Enthalpy= 0.985305

ThermalCorrection to Gibbs Free Energy= 0.813077

E(solv) = -3744.14378303 A.U.

C	0.966733	-1.986188	-0.414630
C	1.399713	-1.547091	-1.782779
C	2.470655	-0.660252	-1.663133
H	1.046318	-2.013577	-2.693616

H	3.082872	-0.261593	-2.460590
O	0.045410	-2.765579	-0.146419
C	4.363381	-2.393489	-0.174428
C	4.061357	-3.274465	-1.299494
C	3.470861	-2.479646	0.934500
C	4.873081	-3.274794	-2.566876
C	5.545277	-2.160324	-3.089831
C	4.882670	-4.472330	-3.299944
C	6.221444	-2.250883	-4.307542
H	5.546774	-1.218061	-2.558204
C	5.570522	-4.565971	-4.505816
H	4.332011	-5.317393	-2.901941
C	6.243631	-3.452491	-5.015400
H	6.732928	-1.376572	-4.700886
H	5.577836	-5.504880	-5.052971
H	6.777645	-3.520802	-5.959426
O	3.106234	-4.066036	-1.223504
C	5.396313	-1.430014	-0.190591
N	6.203779	-0.582844	-0.168740
C	3.712808	-2.004211	2.318483
C	4.354869	-0.796927	2.645276
C	3.169950	-2.768547	3.367215
C	4.438380	-0.372451	3.970218
H	4.791382	-0.185515	1.866516
C	3.262808	-2.348635	4.692330
H	2.664009	-3.700637	3.128784
C	3.892545	-1.140959	5.000121
H	4.929981	0.569641	4.195905
H	2.842289	-2.963689	5.483597
H	3.961849	-0.805635	6.031280
H	2.874484	-3.387060	0.883197
C	2.492627	-0.222503	-0.276532
H	3.244369	0.451794	0.113053
C	1.833212	-1.240408	0.524052
H	1.508472	-1.066452	1.538414
C	-7.136758	0.121825	-2.978106
C	-8.102871	-0.613416	-3.666521
C	-8.472687	-1.880449	-3.213196
C	-7.877989	-2.423822	-2.070199
C	-6.912511	-1.701913	-1.373050
C	-6.555699	-0.434948	-1.840262
S	-5.373960	0.530639	-0.914624
O	-4.853224	1.574882	-1.812897
O	-5.964239	0.906255	0.375879
N	-4.170701	-0.579796	-0.598150

C	-3.729631	-0.836728	0.782447
C	-2.300849	-0.306333	0.976937
O	-2.331921	1.132789	0.675181
C	-1.849949	1.578000	-0.474150
C	-1.757534	3.076369	-0.478910
O	-1.534271	0.845769	-1.422036
C	-0.512609	3.733799	-0.406092
C	-0.485969	5.134064	-0.375020
C	-1.668896	5.867744	-0.429766
C	-2.896011	5.206495	-0.503351
C	-2.945935	3.813820	-0.514829
C	-1.786410	-0.441326	2.386821
C	-0.885150	-1.465934	2.696062
C	-0.395861	-1.590861	3.997518
C	-0.808703	-0.702965	4.992346
C	-1.717180	0.313073	4.685102
C	-2.207015	0.443472	3.386496
C	-3.873240	-2.303226	1.133828
C	-4.910728	-2.695326	1.986156
C	-5.101749	-4.042654	2.296729
C	-4.248572	-5.007532	1.759850
C	-3.208853	-4.619526	0.911734
C	-3.022848	-3.274943	0.593089
p	1.019312	2.740366	-0.248346
C	1.520987	2.867571	1.503336
C	1.215554	1.801907	2.360972
C	1.599191	1.843377	3.701099
C	2.282961	2.955332	4.192376
C	2.574985	4.030097	3.347249
C	2.196021	3.990099	2.006933
C	2.303441	3.612537	-1.202727
C	1.980094	4.305827	-2.378652
C	2.991931	4.821419	-3.188026
C	4.332003	4.637890	-2.842104
C	4.660321	3.936224	-1.680037
C	3.653518	3.424371	-0.863782
H	-6.823717	1.103319	-3.315600
H	-8.561379	-0.197094	-4.558349
H	-9.221845	-2.450750	-3.754594
H	-8.161212	-3.413706	-1.725657
H	-6.427693	-2.119660	-0.496552
H	-3.448797	-0.581815	-1.314762
H	-4.386371	-0.253981	1.431130
H	-1.617915	-0.787861	0.276471
H	0.467652	5.648379	-0.311730

H	-1.632387	6.952900	-0.409710
H	-3.820495	5.773935	-0.547854
H	-3.893306	3.292355	-0.585281
H	-0.567655	-2.154668	1.917907
H	0.321527	-2.371908	4.226148
H	-0.421917	-0.800161	6.003111
H	-2.039810	1.008313	5.454751
H	-2.897150	1.244834	3.141829
H	-5.569537	-1.939922	2.407569
H	-5.910171	-4.334965	2.961076
H	-4.389727	-6.056557	2.004756
H	-2.532665	-5.361916	0.498240
H	-2.193805	-2.999634	-0.050780
H	0.686744	0.936082	1.981864
H	1.373912	1.000119	4.343809
H	2.593564	2.985428	5.232848
H	3.106008	4.896624	3.730680
H	2.444543	4.817549	1.349695
H	0.941191	4.439534	-2.662708
H	2.731117	5.362333	-4.093017
H	5.117700	5.035242	-3.477713
H	5.699884	3.779843	-1.408548
H	3.919999	2.879794	0.036494
Pd	0.707584	0.619600	-1.033519

L6-RSS-TS9

Zero-pointCorrection= 0.923006 (Hartree/Particle)

ThermalCorrection to Energy= 0.985160

ThermalCorrection to Enthalpy= 0.986105

ThermalCorrection to Gibbs Free Energy= 0.816909

E(solv) = -3744.14877387 A.U.

C	3.934254	-2.001640	1.403962
C	4.026422	-3.446591	1.378865
C	3.038810	-1.465090	2.427141
C	4.857295	-4.171910	0.361865
C	4.955801	-3.781973	-0.980885
C	5.493055	-5.352053	0.776740
C	5.698165	-4.546965	-1.881441
H	4.444715	-2.893364	-1.330040
C	6.247980	-6.103795	-0.118516
H	5.376794	-5.663996	1.809292
C	6.353769	-5.701429	-1.452931
H	5.762321	-4.237581	-2.921046
H	6.749304	-7.006690	0.219886
H	6.939234	-6.288995	-2.155178
O	3.399717	-4.124682	2.220474
C	4.578755	-1.195178	0.452008
N	5.128608	-0.517754	-0.329391
C	3.046724	-0.027197	2.859009
C	3.296017	1.055555	2.001340
C	2.681775	0.258778	4.183799
C	3.193877	2.371896	2.458950
H	3.589214	0.883321	0.977584
C	2.551718	1.571938	4.636866
H	2.489927	-0.565712	4.867139
C	2.800484	2.639180	3.771060
H	3.434353	3.189639	1.784251
H	2.265038	1.759977	5.668083
H	2.691974	3.665010	4.107813
H	3.068106	-2.135070	3.285424
C	-0.173292	-0.275457	2.731396
C	0.048551	0.125165	1.385655
C	1.058768	-0.819901	0.795223
H	-0.675642	0.311662	3.487449
H	-0.134277	1.107805	0.974887
C	1.378102	-1.846882	1.885607
H	1.511879	-2.888784	1.604389
C	-2.612770	3.042549	1.094358
C	-3.634434	2.265018	1.635704
C	-3.569344	1.861406	2.972618
C	-2.486548	2.237668	3.771471
C	-1.449824	3.003595	3.234289
C	-1.528045	3.392712	1.897685
S	-0.180882	4.322675	1.169425
O	-0.742003	5.217705	0.152229
O	0.642469	4.828016	2.273641
N	0.676856	3.119101	0.372539
C	1.007277	3.246802	-1.067690
C	0.480812	2.009721	-1.804438
O	-0.978120	2.073024	-1.655141
C	-1.620370	0.896677	-1.676040
C	-3.099464	1.039046	-1.634645
O	-1.069571	-0.188202	-1.710768
C	-3.885422	-0.020902	-1.131448
C	-5.278881	0.124206	-1.138069
C	-5.878586	1.285199	-1.630364
C	-5.093075	2.329813	-2.117505
C	-3.705604	2.203161	-2.117685
C	0.825868	1.962327	-3.268876

C	1.480280	0.838675	-3.781927
C	1.814012	0.779414	-5.135009
C	1.486529	1.838187	-5.983207
C	0.821498	2.957505	-5.476279
C	0.492067	3.019100	-4.123633
C	2.498310	3.460752	-1.222093
C	2.992433	4.769763	-1.250006
C	4.366526	5.004539	-1.281303
C	5.259019	3.929877	-1.279411
C	4.774584	2.621084	-1.251863
C	3.398563	2.388328	-1.226338
p	-3.108579	-1.513275	-0.371069
C	-2.681202	-2.621155	-1.750408
C	-1.555965	-3.443439	-1.619538
C	-1.211378	-4.323112	-2.644598
C	-1.984405	-4.378959	-3.805989
C	-3.102466	-3.553171	-3.943267
C	-3.451858	-2.673863	-2.918696
C	-4.536153	-2.327437	0.456342
C	-4.972190	-1.777191	1.676457
C	-6.012597	-2.368756	2.388855
C	-6.623143	-3.526903	1.899350
C	-6.190508	-4.083991	0.695473
C	-5.152951	-3.488754	-0.025723
Pd	-1.633377	-1.230999	1.399278
H	-2.647632	3.375366	0.065863
H	-4.478184	1.981355	1.015232
H	-4.372055	1.265305	3.397919
H	-2.449076	1.937333	4.814927
H	-0.594187	3.300450	3.830651
H	1.467958	2.834457	0.948952
H	0.471459	4.122590	-1.438739
H	0.820131	1.097976	-1.314825
H	-5.903418	-0.671998	-0.750041
H	-6.961438	1.369527	-1.630799
H	-5.555889	3.235455	-2.497021
H	-3.075596	3.001162	-2.494374
H	1.723790	0.016971	-3.115174
H	2.327757	-0.094194	-5.525601
H	1.747314	1.792685	-7.036907
H	0.563914	3.782721	-6.134288
H	-0.027227	3.889666	-3.731852
H	2.294626	5.603394	-1.232498
H	4.738830	6.024995	-1.302980
H	6.329850	4.112463	-1.296610
H	5.445549	1.769003	-1.230201
H	3.045876	1.362486	-1.201452
H	-0.942179	-3.372910	-0.725887
H	-0.332745	-4.952769	-2.541097
H	-1.711103	-5.058914	-4.607660
H	-3.699066	-3.589223	-4.850295
H	-4.315218	-2.024256	-3.030632
H	-4.493069	-0.878248	2.058650
H	-6.342165	-1.933114	3.327884
H	-7.429342	-3.994196	2.457153
H	-6.660810	-4.985504	0.313421
H	-4.822012	-3.927823	-0.960581
O	1.588152	-0.744983	-0.298760
C	0.436320	-1.543239	2.931490
H	0.313509	-2.139804	3.829351

L6-RSS-TS10

Zero-pointCorrection= 0.922186 (Hartree/Particle)

ThermalCorrection to Energy= 0.984335

ThermalCorrection to Enthalpy= 0.985279

ThermalCorrection to Gibbs Free Energy= 0.817109

E(solv) = -3744.15195857 A.U.

C	-2.387032	-3.699308	0.387907
C	-3.460340	-2.743115	0.060138
C	-1.820345	-3.601106	1.706710
C	-3.900810	-2.523888	-1.358119
C	-3.992540	-3.528037	-2.333659
C	-4.251241	-1.207312	-1.701409
C	-4.411581	-3.213099	-3.626899
H	-3.757459	-4.556147	-2.091173
C	-4.660545	-0.893523	-2.994973
H	-4.198122	-0.434695	-0.944201
C	-4.739233	-1.897961	-3.963366
H	-4.488964	-4.002167	-4.369765
H	-4.891316	0.136787	-3.243035
H	-5.060384	-1.657681	-4.973455
O	-3.935088	-2.022455	0.946661
C	-1.882555	-4.636494	-0.539597
N	-1.424003	-5.425359	-1.272275
C	-1.299034	-4.736625	2.515178
C	-0.526866	-5.788733	1.996480
C	-1.575863	-4.727346	3.891627
C	-0.059370	-6.800630	2.833167

H	-0.297598	-5.825368	0.939058
C	-1.108711	-5.740275	4.727559
H	-2.170791	-3.916843	4.305128
C	-0.346461	-6.782844	4.199958
H	0.530982	-7.609675	2.412047
H	-1.341208	-5.714132	5.788471
H	0.020452	-7.574882	4.846560
H	-2.425067	-2.912230	2.294800
C	0.604058	-2.895520	-0.512593
C	-0.396859	-1.920964	-0.750297
C	-0.863654	-1.432782	0.572469
H	1.031375	-3.559119	-1.251939
H	-0.934337	-1.752698	-1.672089
C	-0.265808	-2.376118	1.594361
H	-0.170968	-2.062125	2.628227
C	0.772939	0.806954	-2.913314
C	1.563200	-0.250440	-3.379164
C	0.961637	-1.340464	-4.028609
C	-0.419351	-1.375206	-4.214125
C	-1.219000	-0.323839	-3.751754
C	-0.612356	0.746530	-3.100035
S	-1.627925	2.094570	-2.500609
O	-0.979275	3.379761	-2.799841
O	-3.000828	1.862180	-2.969290
N	-1.429124	1.858945	-0.855399
C	-1.970335	2.900729	0.032926
C	-1.059239	2.926922	1.285841
O	0.254517	3.307070	0.797153
C	1.132815	2.336522	0.515308
C	2.224478	2.791101	-0.389629
O	1.049130	1.199569	0.958745
C	3.337895	1.956212	-0.678234
C	4.285109	2.417382	-1.601754
C	4.144930	3.656064	-2.230695
C	3.044902	4.463251	-1.951481
C	2.092777	4.028806	-1.033308
C	-1.511114	3.940269	2.301791
C	-2.304749	3.528106	3.376054
C	-2.807555	4.462975	4.279936
C	-2.513549	5.818037	4.120794
C	-1.716761	6.233740	3.052277
C	-1.221473	5.299474	2.143264
C	-3.442726	2.752122	0.366777
C	-4.296945	3.843843	0.189411
C	-5.654333	3.740386	0.494080

C	-6.173232	2.537029	0.973950
C	-5.325210	1.442966	1.156160
C	-3.965997	1.551626	0.864228
p	3.460063	0.227032	-0.035558
C	3.745210	0.429015	1.760077
C	3.394199	-0.626545	2.610855
C	3.608758	-0.523108	3.984235
C	4.165570	0.640182	4.519948
C	4.508885	1.699069	3.677651
C	4.301086	1.594987	2.301762
C	5.080263	-0.362275	-0.664234
C	5.068466	-1.296287	-1.709734
C	6.264575	-1.778331	-2.243109
C	7.483877	-1.338410	-1.726366
C	7.504914	-0.420059	-0.673014
C	6.310535	0.065463	-0.143090
Pd	1.492899	-0.865429	-0.660453
H	1.221296	1.681748	-2.460304
H	2.642722	-0.190327	-3.293918
H	1.578898	-2.158185	-4.388943
H	-0.886264	-2.221005	-4.709112
H	-2.294369	-0.339914	-3.878527
H	-1.659480	0.907601	-0.545482
H	-1.815424	3.856654	-0.474908
H	-0.998663	1.927668	1.719373
H	5.142799	1.799758	-1.839896
H	4.895648	3.980289	-2.945700
H	2.917986	5.417777	-2.452070
H	1.215162	4.627969	-0.830765
H	-2.544498	2.475059	3.490257
H	-3.428000	4.132290	5.107835
H	-2.903143	6.546959	4.825815
H	-1.483010	7.287036	2.924482
H	-0.600580	5.621738	1.313361
H	-3.896748	4.779477	-0.192118
H	-6.306373	4.596895	0.346759
H	-7.232556	2.451593	1.200062
H	-5.709283	0.492572	1.514718
H	-3.329325	0.690210	1.022258
H	2.933796	-1.516219	2.191746
H	3.329632	-1.344841	4.637693
H	4.323908	0.724454	5.591198
H	4.934771	2.608836	4.091239
H	4.557552	2.426379	1.651758
H	4.113198	-1.652344	-2.087178

H	6.243870	-2.502903	-3.052176
H	8.416330	-1.716463	-2.135600
H	8.453157	-0.085438	-0.261997
H	6.331728	0.771696	0.680912
O	-1.559782	-0.455657	0.808538
C	0.776374	-3.038674	0.902190
H	1.515587	-3.686397	1.357496

L6-RSS-TS10-Second

Zero-pointCorrection= 0.924480 (Hartree/Particle)

ThermalCorrection to Energy= 0.985438

ThermalCorrection to Enthalpy= 0.986382

ThermalCorrection to Gibbs Free Energy= 0.824172

E(solv) = -3744.16591212 A.U.

C	0.048728	1.405277	-2.034048
C	0.074546	0.183314	-2.870885
C	-1.194290	-0.442398	-2.810200
H	0.831343	0.019301	-3.629025
H	-1.581966	-1.196170	-3.484087
O	0.906729	2.277553	-2.016503
C	-3.560405	2.287738	-0.770150
C	-4.277850	1.579097	-1.747589
C	-2.136319	2.646143	-1.166325
C	-5.688895	1.117322	-1.557185
C	-6.610398	1.749237	-0.709329
C	-6.095878	-0.023216	-2.265595
C	-7.893058	1.226218	-0.546226
H	-6.327322	2.647544	-0.174309
C	-7.376914	-0.544456	-2.104607
H	-5.382091	-0.482933	-2.940134
C	-8.280136	0.075201	-1.237123
H	-8.595092	1.725760	0.115961
H	-7.672416	-1.434533	-2.654339
H	-9.281763	-0.327431	-1.109657
O	-3.669283	1.203111	-2.807533
C	-3.970310	2.407005	0.568468
N	-4.277867	2.454138	1.699362
C	-1.556008	3.749447	-0.303425
C	-1.153416	3.531003	1.019928
C	-1.531778	5.059106	-0.797045
C	-0.760964	4.593517	1.832677
H	-1.160342	2.529722	1.435805
C	-1.141447	6.125334	0.012782
H	-1.845605	5.242694	-1.821578
C	-0.761416	5.895794	1.335867
H	-0.455319	4.400100	2.856680
H	-1.138753	7.135276	-0.389319
H	-0.453212	6.722338	1.969351
H	-2.182765	2.987213	-2.204929
C	-1.919759	0.119388	-1.723728
H	-2.824602	-0.300426	-1.321175
C	-1.243176	1.354424	-1.178391
H	-0.930488	1.190351	-0.139976
C	2.962854	4.471927	2.469055
C	3.007612	5.849057	2.246693
C	2.636264	6.367759	1.005707
C	2.199598	5.518698	-0.014647
C	2.142939	4.143384	0.188947
C	2.540162	3.643980	1.430191
S	2.552200	1.880074	1.681991
O	2.870094	1.633031	3.096247
O	1.361654	1.265299	1.074754
N	3.841765	1.412850	0.711543
C	3.781228	0.272894	-0.211191
C	4.088405	-1.057362	0.513289
O	3.121961	-1.228366	1.611193
C	1.859337	-1.490938	1.267417
C	0.909026	-1.522909	2.401583
O	1.586871	-1.697048	0.083358
C	-0.454150	-1.884670	2.238929
C	-1.284798	-1.862873	3.363922
C	-0.800747	-1.481110	4.616236
C	0.533903	-1.114354	4.766794
C	1.382205	-1.138527	3.664534
C	4.189254	-2.326931	-0.312777
C	4.679280	-3.472252	0.322993
C	4.732611	-4.694433	-0.348250
C	4.308214	-4.777796	-1.674442
C	3.832311	-3.633977	-2.321074
C	3.769757	-2.417955	-1.644697
C	4.701681	0.576414	-1.379661
C	4.189910	1.338779	-2.438323
C	5.005850	1.674268	-3.517238
C	6.339212	1.257746	-3.548056
C	6.853929	0.505854	-2.492113
C	6.038184	0.167688	-1.410709
p	-1.160609	-2.420741	0.616121
C	-2.965592	-2.303943	0.799495

C	-3.524324	-1.059538	1.148448
C	-4.905325	-0.881274	1.139427
C	-5.742148	-1.931869	0.755400
C	-5.194576	-3.164001	0.396988
C	-3.811599	-3.355540	0.418665
C	-0.694115	-4.188968	0.583782
C	-1.169129	-5.091074	1.547811
C	-0.728286	-6.412654	1.545036
C	0.205029	-6.838286	0.594925
C	0.691227	-5.942401	-0.357280
C	0.238638	-4.622455	-0.368756
H	3.244569	4.040840	3.422847
H	3.332293	6.512443	3.042836
H	2.671818	7.440375	0.837233
H	1.875234	5.927411	-0.965489
H	1.765941	3.482642	-0.583469
H	4.740031	1.583959	1.154057
H	2.756474	0.245875	-0.578862
H	5.013015	-0.933924	1.082849
H	-2.329700	-2.129959	3.259213
H	-1.475702	-1.462267	5.466818
H	0.914362	-0.797800	5.732561
H	2.410025	-0.818103	3.762538
H	5.001656	-3.410753	1.359602
H	5.109267	-5.575592	0.162948
H	4.355601	-5.724810	-2.204819
H	3.503558	-3.688682	-3.355004
H	3.378044	-1.545664	-2.153406
H	3.155011	1.673481	-2.408391
H	4.599116	2.262720	-4.334805
H	6.973207	1.517796	-4.390937
H	7.889038	0.176881	-2.509210
H	6.451017	-0.433635	-0.605751
H	-2.892159	-0.221044	1.426474
H	-5.310196	0.087152	1.408090
H	-6.814678	-1.775040	0.713490
H	-5.842360	-3.981610	0.093339
H	-3.393656	-4.315942	0.134609
H	-1.880805	-4.757986	2.297421
H	-1.104755	-7.108780	2.289015
H	0.554570	-7.866782	0.602803
H	1.428966	-6.260945	-1.087416
H	0.623601	-3.921980	-1.102895
Pd	-0.186689	-1.192083	-1.083679

L6-RSS-TS11

Zero-pointCorrection= 0.921697 (Hartree/Particle)

ThermalCorrection to Energy= 0.984175

ThermalCorrection to Enthalpy= 0.985119

ThermalCorrection to Gibbs Free Energy= 0.817697

E(solv) = -3744.14113326 A.U.

C	3.161914	-2.082533	-0.829762
C	2.129098	-1.721496	-1.806032
C	3.036584	-3.162683	0.054701
C	1.044285	-2.688964	-2.140170
C	1.332990	-4.042895	-2.376507
C	-0.272019	-2.229716	-2.284914
C	0.316540	-4.926642	-2.733161
H	2.355714	-4.397016	-2.294077
C	-1.289153	-3.123212	-2.614121
H	-0.488407	-1.185748	-2.102278
C	-0.999101	-4.470436	-2.839185
H	0.551786	-5.969452	-2.926064
H	-2.308539	-2.766171	-2.707572
H	-1.795325	-5.161055	-3.103227
O	2.174436	-0.596268	-2.394455
C	4.357904	-1.293033	-0.916639
N	5.333475	-0.663144	-1.015329
C	4.074014	-3.953980	0.705676
C	3.693105	-5.217648	1.208925
C	5.415556	-3.555619	0.879868
C	4.603763	-6.046458	1.853868
H	2.662648	-5.542012	1.083549
C	6.323640	-4.389302	1.527994
H	5.752123	-2.595735	0.512502
C	5.928975	-5.635611	2.019032
H	4.280635	-7.014303	2.227083
H	7.351624	-4.059040	1.649232
H	6.644319	-6.278856	2.523071
H	2.068273	-3.648293	0.020829
C	1.167872	-1.360422	1.966584
C	1.621167	0.090019	1.765704
C	2.985888	0.087576	2.136329
C	3.417430	-1.238983	2.440358
H	0.932958	0.889862	2.019557
H	3.598771	0.971978	2.249365
H	4.433973	-1.496834	2.714389
C	2.387904	-2.146359	2.279372

H	2.366095	-3.181044	2.583690
O	0.014600	-1.772071	1.913331
C	-4.751661	-1.789778	-3.664963
C	-4.171889	-2.178589	-4.873987
C	-3.025515	-1.533078	-5.340641
C	-2.453103	-0.489815	-4.607405
C	-3.023862	-0.088493	-3.402508
C	-4.164189	-0.751260	-2.942241
S	-4.914799	-0.252377	-1.398413
O	-5.046819	1.211096	-1.342127
O	-6.109447	-1.080667	-1.183444
N	-3.653798	-0.626505	-0.345895
C	-3.816221	-0.188559	1.064412
C	-2.502491	0.482855	1.500381
O	-2.270866	1.583195	0.576837
C	-1.371894	1.376882	-0.394266
C	-1.176989	2.599684	-1.229079
O	-0.783860	0.328460	-0.572345
C	0.105740	3.153026	-1.437909
C	0.220871	4.228499	-2.327845
C	-0.899359	4.747307	-2.979398
C	-2.165449	4.222259	-2.727125
C	-2.307166	3.156166	-1.839649
C	-2.539323	1.081785	2.881643
C	-1.712375	0.568722	3.884494
C	-1.715281	1.139295	5.157994
C	-2.544132	2.226763	5.435949
C	-3.372895	2.743084	4.435569
C	-3.370038	2.172966	3.163289
C	-4.228637	-1.331164	1.966196
C	-5.565004	-1.453386	2.358996
C	-5.973494	-2.522848	3.154697
C	-5.046320	-3.483235	3.563001
C	-3.712377	-3.369961	3.168200
C	-3.300969	-2.300434	2.372200
p	1.573499	2.541438	-0.492594
C	1.403453	3.338867	1.150803
C	2.565039	3.535613	1.918080
C	2.472963	3.920772	3.253796
C	1.222030	4.093313	3.852273
C	0.064685	3.901442	3.098869
C	0.153367	3.537041	1.754147
C	3.006019	3.374932	-1.263106
C	3.854438	2.608271	-2.075430
C	4.965048	3.199874	-2.679174
C	5.237621	4.552494	-2.473742
C	4.398459	5.320162	-1.660925
C	3.287233	4.735445	-1.056515
Pd	1.961834	0.239236	-0.325387
H	-5.640657	-2.273670	-3.276369
H	-4.614540	-2.987495	-5.447224
H	-2.571169	-1.847016	-6.275543
H	-1.555491	0.004093	-4.965638
H	-2.583262	0.714036	-2.826759
H	-3.400637	-1.610863	-0.419745
H	-4.590615	0.582895	1.071828
H	-1.672617	-0.217262	1.407388
H	1.193476	4.669130	-2.511838
H	-0.777952	5.573827	-3.673748
H	-3.041663	4.635916	-3.217096
H	-3.285440	2.731955	-1.632295
H	-1.068354	-0.275215	3.659805
H	-1.066431	0.736277	5.930293
H	-2.545962	2.671939	6.427002
H	-4.019871	3.589924	4.646967
H	-3.996794	2.588123	2.379206
H	-6.288555	-0.714336	2.026622
H	-7.014567	-2.606443	3.453274
H	-5.362515	-4.316224	4.184711
H	-2.984692	-4.112851	3.482454
H	-2.257279	-2.225587	2.083052
H	3.541018	3.384011	1.466674
H	3.380486	4.075330	3.830947
H	1.151578	4.372345	4.899563
H	-0.913885	4.017316	3.553738
H	-0.761716	3.395515	1.194044
H	3.656375	1.550905	-2.221508
H	5.622363	2.595018	-3.296256
H	6.107148	5.008888	-2.938384
H	4.612582	6.372165	-1.494374
H	2.642678	5.329132	-0.415314

L6-RSS-TS12

Zero-pointCorrection= 0.922059 (Hartree/Particle)

ThermalCorrection to Energy= 0.984010

ThermalCorrection to Enthalpy= 0.984955

ThermalCorrection to Gibbs Free Energy= 0.819707

E(solv) = -3744.14994028 A.U.

C	2.964091	1.490810	-0.590407
C	2.461402	0.425715	-1.446057
C	4.167657	1.415951	0.143142
C	3.382553	-0.571854	-2.061630
C	4.747893	-0.333789	-2.290103
C	2.825566	-1.789538	-2.483786
C	5.542739	-1.316963	-2.877350
H	5.183705	0.625253	-2.035182
C	3.621468	-2.772778	-3.060299
H	1.764887	-1.944668	-2.347121
C	4.986743	-2.542974	-3.249474
H	6.596551	-1.121023	-3.052342
H	3.174310	-3.715227	-3.362607
H	5.612046	-3.308742	-3.699882
O	1.221178	0.341501	-1.707551
C	2.139971	2.650788	-0.514221
N	1.503615	3.624061	-0.431235
C	5.138912	2.481759	0.408809
C	6.428091	2.084832	0.822941
C	4.885944	3.859199	0.264665
C	7.422913	3.020207	1.085482
H	6.636704	1.024403	0.943383
C	5.885266	4.792581	0.529898
H	3.911225	4.205712	-0.051867
C	7.155540	4.383693	0.941104
H	8.407018	2.685919	1.401619
H	5.667156	5.850427	0.412819
H	7.928487	5.118623	1.146083
H	4.604755	0.422979	0.168439
C	3.138332	-0.224840	2.519861
C	1.609453	-0.262431	2.525901
C	1.199783	1.107063	2.566824
C	2.343511	1.952703	2.531240
H	1.116683	-1.062435	3.069465
H	0.186781	1.458909	2.735486
H	2.286362	3.035348	2.544359
C	3.518814	1.216603	2.423220
H	4.514926	1.564968	2.645394
O	3.892829	-1.182890	2.584334
C	-3.863849	4.874432	0.921700
C	-3.510036	6.097611	0.352469
C	-2.201947	6.311965	-0.085287
C	-1.234627	5.313542	0.054928
C	-1.573119	4.093001	0.632432
C	-2.887526	3.887107	1.053618
S	-3.360808	2.281781	1.677794
O	-2.410731	1.847398	2.715217
O	-4.803403	2.347967	1.954177
N	-3.123974	1.211534	0.447272
C	-3.695708	1.363513	-0.883313
C	-4.015961	0.001142	-1.560130
O	-2.900334	-0.691831	-2.222440
C	-1.903866	-1.184553	-1.477018
C	-1.192484	-2.354269	-2.028520
O	-1.594644	-0.723564	-0.389484
C	-0.246615	-3.031095	-1.213228
C	0.377568	-4.167299	-1.746397
C	0.096147	-4.608196	-3.040358
C	-0.822121	-3.924203	-3.837678
C	-1.471094	-2.805505	-3.323916
C	-4.800606	-1.000083	-0.723008
C	-4.875542	-2.333239	-1.152134
C	-5.666745	-3.257879	-0.473568
C	-6.406035	-2.862084	0.641092
C	-6.334280	-1.539418	1.074712
C	-5.536507	-0.611627	0.403099
C	-2.913655	2.289716	-1.803332
C	-3.574522	3.349800	-2.429934
C	-2.878056	4.235810	-3.252511
C	-1.509751	4.062281	-3.461083
C	-0.843768	3.005761	-2.837918
C	-1.539145	2.127807	-2.009953
p	0.248735	-2.411536	0.463769
C	1.458462	-3.658786	1.040378
C	1.114844	-4.772096	1.820926
C	2.097732	-5.677314	2.221476
C	3.428303	-5.481945	1.845699
C	3.778877	-4.369470	1.079464
C	2.802287	-3.456209	0.689652
C	-1.258156	-2.664926	1.474768
C	-1.675635	-1.654650	2.351697
C	-2.873894	-1.775881	3.050738
C	-3.663791	-2.914247	2.885603
C	-3.257531	-3.924406	2.012733
C	-2.064311	-3.798402	1.301828
Pd	1.063939	-0.247090	0.512939
H	-4.874719	4.672491	1.256186
H	-4.258483	6.877247	0.243537
H	-1.934811	7.260205	-0.543439
H	-0.219295	5.456137	-0.295229

H	-0.824131	3.314692	0.723684
H	-2.261205	0.682972	0.505283
H	-4.687536	1.805634	-0.735084
H	-4.609578	0.271914	-2.437978
H	1.099817	-4.708106	-1.146676
H	0.596511	-5.493667	-3.422422
H	-1.036407	-4.263091	-4.846379
H	-2.197774	-2.263450	-3.918293
H	-4.314695	-2.649945	-2.024793
H	-5.708304	-4.286146	-0.822140
H	-7.026877	-3.580016	1.170017
H	-6.893108	-1.218740	1.949193
H	-5.486027	0.400202	0.783430
H	-4.637205	3.499136	-2.252639
H	-3.402672	5.065772	-3.717653
H	-0.962504	4.755088	-4.094303
H	0.223927	2.869432	-2.968886
H	-0.986158	1.343786	-1.509519
H	0.085167	-4.927583	2.122511
H	1.823259	-6.533899	2.830755
H	4.191564	-6.187008	2.162761
H	4.814988	-4.195324	0.805861
H	3.081876	-2.576311	0.121059
H	-1.098037	-0.742916	2.444823
H	-3.198263	-0.960779	3.689755
H	-4.608320	-3.002137	3.413044
H	-3.883497	-4.798844	1.862956
H	-1.774884	-4.569003	0.592916

L6-RSS-TS13

Zero-pointCorrection= 0.922364 (Hartree/Particle)

ThermalCorrection to Energy= 0.984020

ThermalCorrection to Enthalpy= 0.984964

ThermalCorrection to Gibbs Free Energy= 0.821362

E(solv) = -3744.14750564 A.U.

C	-1.724109	-3.256967	1.068641
C	-0.768238	-2.508964	1.840624
C	-2.722484	-2.556769	0.348977
C	0.572318	-3.067171	2.179126
C	1.228557	-4.002988	1.364924
C	1.236554	-2.567440	3.311230
C	2.509779	-4.443346	1.691732
H	0.746540	-4.380679	0.471442
C	2.520207	-2.998775	3.629051
H	0.730373	-1.835570	3.930237
C	3.159043	-3.943342	2.821928
H	3.006052	-5.164983	1.049726
H	3.024810	-2.597441	4.502708
H	4.161111	-4.282262	3.069838
O	-1.028264	-1.341640	2.256493
C	-1.660927	-4.676780	1.065931
N	-1.630204	-5.843430	1.084227
C	-3.585854	-3.124041	-0.689765
C	-4.185722	-4.394654	-0.604518
C	-3.839274	-2.337494	-1.828060
C	-4.990943	-4.863635	-1.637739
H	-4.024674	-5.012216	0.270482
C	-4.637201	-2.814052	-2.863769
H	-3.404913	-1.348547	-1.891178
C	-5.216653	-4.079813	-2.773423
H	-5.445688	-5.846808	-1.556388
H	-4.812701	-2.189942	-3.735515
H	-5.845144	-4.453396	-3.577200
H	-2.455122	-1.518021	0.166674
C	-4.526974	-0.448719	0.996304
C	-3.780407	0.600442	1.848410
C	-3.606121	-0.034959	3.121425
C	-3.930928	-1.388248	3.015101
H	-4.080646	1.641689	1.756380
H	-3.233516	0.447331	4.017202
H	-3.821592	-2.103640	3.823788
C	-4.401848	-1.723925	1.718959
H	-5.016587	-2.582531	1.489189
O	-5.092352	-0.233628	-0.075478
C	2.229697	3.020480	3.355814
C	1.157334	3.417310	4.156156
C	0.043175	2.584934	4.295636
C	-0.002281	1.349352	3.642932
C	1.055630	0.949514	2.826692
C	2.153331	1.796790	2.690351
S	3.515285	1.291130	1.652830
O	4.645242	2.180921	1.948616
O	3.671011	-0.168321	1.749284
N	2.892886	1.597304	0.114008
C	3.348960	0.816220	-1.059548
C	2.665106	-0.586896	-1.044532
O	1.459548	-0.444601	-1.872532
C	0.307207	-0.139756	-1.282394

C	-0.793156	0.024638	-2.277807
O	0.194983	-0.020458	-0.066388
C	-1.835183	0.969168	-2.099387
C	-2.828911	1.059030	-3.080240
C	-2.812571	0.224397	-4.199241
C	-1.790705	-0.707984	-4.365056
C	-0.774967	-0.791460	-3.414629
C	3.470097	-1.709892	-1.632623
C	4.041394	-2.647140	-0.769147
C	4.833345	-3.676580	-1.277875
C	5.052883	-3.776586	-2.652009
C	4.478581	-2.842098	-3.517673
C	3.691987	-1.810082	-3.010082
C	4.841308	0.847611	-1.348061
C	5.272011	1.570861	-2.465679
C	6.624932	1.644729	-2.798947
C	7.567969	0.988380	-2.009794
C	7.147916	0.264487	-0.891712
C	5.797108	0.191362	-0.560963
p	-1.925896	1.993122	-0.574204
C	-3.265104	3.203008	-0.850728
C	-4.599850	2.768921	-0.768792
C	-5.637622	3.683728	-0.948415
C	-5.361085	5.029823	-1.194315
C	-4.036310	5.463299	-1.269557
C	-2.990236	4.556699	-1.101493
C	-0.402334	3.013025	-0.639565
C	0.290413	3.240734	-1.837290
C	1.406391	4.078913	-1.856761
C	1.825644	4.714757	-0.684166
C	1.138390	4.488486	0.511533
C	0.041533	3.627397	0.539284
Pd	-1.819256	0.455057	1.068393
H	3.117195	3.634275	3.249586
H	1.198941	4.367128	4.681336
H	-0.786071	2.893384	4.926180
H	-0.851185	0.685934	3.761842
H	1.016238	-0.001142	2.313464
H	2.917797	2.599733	-0.061100
H	2.871513	1.343938	-1.889619
H	2.354834	-0.832781	-0.033482
H	-3.628336	1.780861	-2.963949
H	-3.604805	0.305701	-4.937515
H	-1.780376	-1.367439	-5.226766
H	0.033598	-1.503198	-3.535876
H	3.869517	-2.561264	0.298142
H	5.273977	-4.401603	-0.599353
H	5.667251	-4.579515	-3.049418
H	4.647389	-2.916505	-4.588220
H	3.248759	-1.080900	-3.681608
H	4.537712	2.080543	-3.086441
H	6.937922	2.210981	-3.671741
H	8.623209	1.039246	-2.262856
H	7.876600	-0.250076	-0.272083
H	5.485691	-0.374550	0.307206
H	-4.829248	1.722091	-0.577777
H	-6.665660	3.338176	-0.888489
H	-6.173581	5.738889	-1.325628
H	-3.813592	6.508938	-1.462301
H	-1.965558	4.904071	-1.166419
H	-0.047108	2.772896	-2.756381
H	1.936549	4.249906	-2.789515
H	2.684204	5.380078	-0.702030
H	1.466694	4.964312	1.428968
H	-0.463624	3.424440	1.478521

L6-SRR-TS1

Zero-pointCorrection= 0.921949 (Hartree/Particle)
ThermalCorrection to Energy= 0.984149
ThermalCorrection to Enthalpy= 0.985094
ThermalCorrection to Gibbs Free Energy= 0.814848
E(solv) = -3744.14851525 A.U.

C	3.873692	-0.185482	-0.284272
C	3.645887	0.174622	-1.734832
C	2.616231	-0.675784	-2.227684
C	2.124804	-1.477586	-1.140896
H	4.403793	0.679488	-2.322800
H	2.364340	-0.850638	-3.265736
H	1.209352	-2.048226	-1.185659
C	2.923642	-1.320178	0.022575
H	2.503564	-1.412775	1.016954
O	4.661254	0.344614	0.486839
C	-7.477243	1.519479	-0.225204
C	-8.464588	1.050382	-1.088234
C	-9.046820	-0.202091	-0.871096
C	-8.652904	-0.986203	0.214133
C	-7.667168	-0.527328	1.086864
C	-7.088053	0.716369	0.847251

S	-5.771297	1.281708	1.909211
O	-5.895077	2.728188	2.116197
O	-5.681411	0.356138	3.045822
N	-4.404909	1.123185	0.907928
C	-3.728873	-0.186589	0.928969
C	-2.346031	-0.008016	0.271637
O	-1.706283	1.035340	1.056137
C	-0.701716	1.724502	0.487127
C	-0.025495	2.630559	1.450249
O	-0.420973	1.574343	-0.699158
C	1.108149	3.407154	1.091397
C	1.710080	4.197626	2.078017
C	1.209548	4.244971	3.379153
C	0.090479	3.490272	3.725140
C	-0.515845	2.686537	2.765860
C	-1.541150	-1.284252	0.310002
C	-1.625603	-2.181186	-0.760498
C	-1.012485	-3.431280	-0.678926
C	-0.293352	-3.786043	0.464200
C	-0.179641	-2.882183	1.522044
C	-0.809131	-1.638474	1.449566
C	-4.539362	-1.226936	0.186153
C	-4.743715	-2.487445	0.748918
C	-5.471923	-3.457415	0.058923
C	-6.002111	-3.168510	-1.198732
C	-5.799050	-1.907848	-1.766056
C	-5.068422	-0.942689	-1.077662
p	1.835159	3.362768	-0.603609
C	3.389741	4.308709	-0.451355
C	4.547204	3.600416	-0.088745
C	5.757662	4.278413	0.054493
C	5.826976	5.654015	-0.176118
C	4.679673	6.357681	-0.548585
C	3.462420	5.689833	-0.684164
C	0.707810	4.448752	-1.553263
C	-0.064045	5.449590	-0.947583
C	-0.901733	6.254325	-1.720751
C	-0.973358	6.066979	-3.102426
C	-0.207930	5.070275	-3.711406
C	0.625384	4.261088	-2.940422
Pd	1.819180	1.196674	-1.401451
H	-7.011075	2.487275	-0.374191
H	-8.780867	1.660302	-1.929125
H	-9.811704	-0.565992	-1.551057
H	-9.104854	-1.959286	0.378141
H	-7.330987	-1.122319	1.926936
H	-3.771470	1.875516	1.178649
H	-3.565808	-0.525817	1.959080
H	-2.463130	0.354078	-0.751158
H	2.583666	4.786101	1.823689
H	1.697640	4.873016	4.118672
H	-0.306716	3.520006	4.734706
H	-1.377545	2.087927	3.032063
H	-2.198437	-1.911062	-1.642700
H	-1.088331	-4.130626	-1.504945
H	0.181290	-4.757443	0.532948
H	0.394890	-3.161338	2.399733
H	-0.735598	-0.941372	2.278894
H	-4.330116	-2.707869	1.728677
H	-5.625564	-4.435524	0.505307
H	-6.574452	-3.920583	-1.734394
H	-6.219767	-1.673627	-2.739488
H	-4.935209	0.048461	-1.499089
H	4.511684	2.527310	0.082155
H	6.647525	3.724538	0.338965
H	6.773681	6.176596	-0.071340
H	4.731311	7.426707	-0.735087
H	2.572509	6.239497	-0.973305
H	-0.012256	5.598626	0.126549
H	-1.498687	7.026225	-1.243403
H	-1.627928	6.692860	-3.702160
H	-0.266869	4.916405	-4.785015
H	1.208802	3.471330	-3.406387
C	3.284549	-4.133706	0.144312
C	2.701753	-4.461746	-1.132738
C	4.131452	-2.979990	0.161955
C	1.911429	-5.710756	-1.369404
C	2.057029	-6.880308	-0.610126
C	1.007134	-5.706966	-2.443533
C	1.286342	-8.006981	-0.898686
H	2.772270	-6.919858	0.201936
C	0.233959	-6.828926	-2.726164
H	0.935109	-4.807487	-3.045008
C	0.367869	-7.982975	-1.948832
H	1.408715	-8.906215	-0.301814
H	-0.468565	-6.808560	-3.555056
H	-0.233945	-8.860947	-2.167022
O	2.822682	-3.646634	-2.078647
C	2.844318	-4.743791	1.341448
N	2.440149	-5.214308	2.333027

C	5.011780	-2.629291	1.299959
C	4.576512	-2.603912	2.634397
C	6.342607	-2.281812	1.022096
C	5.456426	-2.262234	3.657643
H	3.549394	-2.850170	2.874702
C	7.225515	-1.949684	2.046388
H	6.683230	-2.276305	-0.009736
C	6.784156	-1.938631	3.369728
H	5.103032	-2.248429	4.684794
H	8.253773	-1.690972	1.809978
H	7.467627	-1.673661	4.171659
H	4.578757	-2.803023	-0.813442

L6-SRR-TS2

Zero-pointCorrection= 0.922119 (Hartree/Particle)
ThermalCorrection to Energy= 0.984351
ThermalCorrection to Enthalpy= 0.985295
ThermalCorrection to Gibbs Free Energy= 0.817640
E(solv) = -3744.15040427 A.U.

C	-2.634823	-2.853907	1.609098
C	-2.383715	-4.305352	1.565064
C	-2.327824	-2.162932	2.832618
C	-2.266884	-5.005546	0.239148
C	-1.203062	-5.914119	0.119007
C	-3.112149	-4.793507	-0.857620
C	-0.963444	-6.564931	-1.089171
H	-0.567902	-6.079717	0.982801
C	-2.878658	-5.458331	-2.063115
H	-3.958656	-4.122896	-0.779535
C	-1.799316	-6.335034	-2.186541
H	-0.129141	-7.255967	-1.174156
H	-3.544923	-5.290912	-2.904492
H	-1.616238	-6.843617	-3.129028
O	-2.132714	-4.926285	2.598585
C	-3.075697	-2.147030	0.479035
N	-3.444539	-1.530298	-0.444702
C	-3.074289	-0.966001	3.319263
C	-3.379708	0.143242	2.515303
C	-3.485145	-0.947468	4.659938
C	-4.094009	1.223832	3.028511
H	-3.062856	0.163387	1.481246
C	-4.194528	0.136256	5.179016
H	-3.253097	-1.797012	5.296907
C	-4.504200	1.225080	4.364215
H	-4.337508	2.057776	2.376911
H	-4.505702	0.126032	6.219766
H	-5.060167	2.068130	4.764284
H	-2.149940	-2.898587	3.616573
C	0.144131	-2.790617	2.100538
C	0.073054	-2.519691	0.635686
C	-0.276057	-1.161858	0.458612
C	-0.395729	-0.551614	1.758089
H	0.045853	-3.298121	-0.110041
H	-0.577404	-0.694025	-0.470098
H	-0.519250	0.511586	1.910284
C	-0.468311	-1.552447	2.753192
H	-0.265042	-1.340037	3.798262
O	0.599748	-3.761444	2.671577
C	0.908516	-0.542866	-3.156251
C	1.963585	-1.375660	-2.779673
C	1.723919	-2.726494	-2.504101
C	0.429662	-3.246956	-2.601069
C	-0.635236	-2.417005	-2.951802
C	-0.379350	-1.071165	-3.225386
S	-1.742307	0.009601	-3.664851
O	-1.196372	1.169826	-4.379889
O	-2.775037	-0.840818	-4.261486
N	-2.267146	0.555673	-2.178210
C	-2.407776	1.981364	-1.883713
C	-1.365703	2.354674	-0.799131
O	-0.090015	2.220952	-1.476193
C	1.005879	2.078603	-0.712041
C	2.256378	2.139148	-1.515879
O	0.973581	1.916861	0.494134
C	3.448960	1.534573	-1.052236
C	4.599242	1.652890	-1.844349
C	4.578038	2.347507	-3.055005
C	3.395693	2.928199	-3.509660
C	2.240207	2.819302	-2.740281
C	-1.513201	3.741975	-0.233434
C	-2.047312	3.915799	1.045198
C	-2.260267	5.197317	1.551162
C	-1.929115	6.315464	0.784271
C	-1.379734	6.146339	-0.488567
C	-1.173672	4.864388	-0.996025
C	-3.805573	2.394965	-1.463606
C	-4.292691	3.642432	-1.870755
C	-5.526266	4.108347	-1.420107

C	-6.295987	3.326946	-0.556727
C	-5.825829	2.075299	-0.159047
C	-4.587912	1.612080	-0.608446
p	3.472073	0.459468	0.451381
C	3.549844	1.604100	1.870541
C	3.107114	1.139065	3.114908
C	3.172086	1.966592	4.234947
C	3.669578	3.266071	4.116430
C	4.104588	3.735642	2.875589
C	4.047010	2.907492	1.754440
C	5.157897	-0.272673	0.396430
C	5.312535	-1.490684	-0.285107
C	6.561518	-2.103143	-0.370683
C	7.670579	-1.509650	0.236367
C	7.524301	-0.304728	0.926167
C	6.275351	0.313179	1.006182
Pd	1.869672	-1.223092	0.487004
H	1.074913	0.497125	-3.401488
H	2.969485	-0.971718	-2.725280
H	2.547495	-3.376860	-2.222234
H	0.239465	-4.295187	-2.391853
H	-1.644493	-2.806392	-3.019981
H	-2.897130	-0.109678	-1.722323
H	-2.131757	2.529786	-2.787087
H	-1.416020	1.616133	0.002641
H	5.523121	1.191296	-1.516954
H	5.488171	2.425833	-3.642611
H	3.368697	3.457398	-4.456991
H	1.306888	3.246001	-3.087734
H	-2.299031	3.045604	1.644194
H	-2.678231	5.321530	2.546007
H	-2.092611	7.314507	1.178131
H	-1.114245	7.013421	-1.086843
H	-0.749475	4.731782	-1.987239
H	-3.693038	4.259301	-2.533258
H	-5.886246	5.080180	-1.745570
H	-7.258308	3.687381	-0.204431
H	-6.418902	1.450524	0.502567
H	-4.258185	0.626495	-0.301888
H	2.697338	0.135491	3.194703
H	2.824977	1.600887	5.197100
H	3.712126	3.913569	4.987507
H	4.484812	4.748654	2.778878
H	4.376919	3.277751	0.788255
H	4.443908	-1.958695	-0.743826
H	6.667121	-3.046236	-0.899115
H	8.643458	-1.989096	0.178889
H	8.383558	0.155184	1.405973
H	6.167386	1.247707	1.546786

L6-SRR-TS3

Zero-pointCorrection= 0.923244 (Hartree/Particle)
ThermalCorrection to Energy= 0.984753
ThermalCorrection to Enthalpy= 0.985698
ThermalCorrection to Gibbs Free Energy= 0.822322
E(solv) = -3744.15318009 A.U.

C	2.968031	2.252920	-2.061380
C	2.467161	0.923727	-2.572880
C	1.103975	1.118531	-2.949276
H	3.157955	0.234154	-3.048241
H	0.533234	0.500715	-3.626828
O	4.130091	2.548848	-1.846388
C	0.059301	3.687986	0.328492
C	-1.077283	2.943418	-0.115723
C	1.349324	3.093818	0.094460
C	-2.488967	3.360943	0.113194
C	-2.902766	4.077411	1.246502
C	-3.451619	2.961482	-0.829193
C	-4.246967	4.402826	1.417363
H	-2.181755	4.375074	1.998041
C	-4.792218	3.287777	-0.655298
H	-3.149081	2.390345	-1.698614
C	-5.192979	4.013046	0.467620
H	-4.555689	4.956043	2.299858
H	-5.521426	2.954933	-1.387009
H	-6.241071	4.260075	0.610462
O	-0.872642	1.891570	-0.796286
C	-0.076361	5.005028	0.835515
N	-0.172753	6.093639	1.246612
C	2.613768	3.567509	0.703102
C	3.539544	2.591797	1.109046
C	2.962291	4.919771	0.852422
C	4.756544	2.941890	1.684277
H	3.308211	1.546194	0.941980
C	4.182976	5.271814	1.423802
H	2.284812	5.698287	0.525503
C	5.080596	4.288867	1.847944
H	5.453718	2.163253	1.980454

H	4.435258	6.322443	1.535158
H	6.031319	4.573439	2.290178
H	1.278730	2.004000	0.075977
C	0.708850	2.442764	-2.573267
H	-0.231246	2.887370	-2.869525
C	1.746643	3.134896	-1.891921
H	1.853862	4.211598	-1.957282
C	-1.635994	-0.453909	-4.840391
C	-0.556569	-0.741551	-5.680957
C	0.375933	-1.715870	-5.318858
C	0.227187	-2.424090	-4.121116
C	-0.853729	-2.155098	-3.286680
C	-1.764994	-1.161662	-3.647959
S	-3.152318	-0.823402	-2.563080
O	-3.874483	0.321585	-3.138970
O	-3.867917	-2.087514	-2.318070
N	-2.355613	-0.435107	-1.168306
C	-2.835836	-0.717178	0.191535
C	-2.778014	-2.221152	0.540984
O	-1.569663	-2.931077	0.077325
C	-0.355061	-2.401810	0.115753
C	0.720329	-3.364382	-0.259729
O	-0.127954	-1.232655	0.423366
C	2.090045	-3.008646	-0.127687
C	3.058783	-3.928054	-0.544729
C	2.697032	-5.168840	-1.073410
C	1.352474	-5.520281	-1.184039
C	0.371886	-4.620990	-0.771369
C	-2.959869	-2.458204	2.021309
C	-4.117570	-3.100596	2.468592
C	-4.343484	-3.288895	3.831929
C	-3.403566	-2.842681	4.760994
C	-2.241968	-2.205066	4.320153
C	-2.019850	-2.006957	2.958732
C	-4.192307	-0.162390	0.606595
C	-4.237003	0.688393	1.716351
C	-5.449269	1.183687	2.189295
C	-6.639658	0.835642	1.550854
C	-6.605012	-0.010534	0.442029
C	-5.391127	-0.515675	-0.024949
p	2.580843	-1.328833	0.454209
C	4.406865	-1.314866	0.555677
C	5.093041	-0.385792	-0.239896
C	6.481092	-0.267448	-0.143622
C	7.191991	-1.077586	0.741341

C	6.513637	-2.002721	1.541407
C	5.127987	-2.115806	1.456640
C	2.051244	-1.334500	2.213635
C	2.000008	-2.516296	2.965208
C	1.597991	-2.484772	4.300720
C	1.241606	-1.273174	4.895803
C	1.271313	-0.095079	4.146464
C	1.669661	-0.125554	2.810492
H	-2.366694	0.307245	-5.089953
H	-0.440552	-0.196358	-6.612788
H	1.219307	-1.925263	-5.970323
H	0.948416	-3.183986	-3.834879
H	-0.998332	-2.706217	-2.368413
H	-1.884277	0.482056	-1.210390
H	-2.091698	-0.210083	0.800827
H	-3.551809	-2.738515	-0.021974
H	4.108292	-3.670425	-0.457138
H	3.471123	-5.861217	-1.391762
H	1.066214	-6.486676	-1.587007
H	-0.677514	-4.878777	-0.850357
H	-4.854246	-3.435606	1.743871
H	-5.251801	-3.782154	4.165758
H	-3.576034	-2.987947	5.823781
H	-1.504716	-1.853090	5.034363
H	-1.120117	-1.495809	2.633535
H	-3.311580	0.969282	2.210033
H	-5.460356	1.851907	3.044768
H	-7.587714	1.224521	1.912314
H	-7.527137	-0.285501	-0.062604
H	-5.380868	-1.181216	-0.879926
H	4.548661	0.270593	-0.908760
H	6.995245	0.469137	-0.753416
H	8.271490	-0.983702	0.818772
H	7.064449	-2.626853	2.239372
H	4.604916	-2.815906	2.100396
H	2.257928	-3.465184	2.504363
H	1.558415	-3.406661	4.873686
H	0.934143	-1.248375	5.937443
H	0.978509	0.848418	4.597599
H	1.670336	0.789790	2.229747
Pd	1.423920	-0.006549	-1.026354

L6-SSS-TS1

Zero-pointCorrection= 0.923146 (Hartree/Particle)
ThermalCorrection to Energy= 0.985007
ThermalCorrection to Enthalpy= 0.985951
ThermalCorrection to Gibbs Free Energy= 0.819847
E(solv) = -3744.15311645 A.U.

C	-3.219234	-2.081811	1.779553
C	-2.785916	-3.433356	1.507339
C	-2.855877	-1.590894	3.085714
C	-2.993036	-4.143936	0.205337
C	-3.952810	-3.796327	-0.757057
C	-2.152537	-5.242624	-0.047892
C	-4.035804	-4.501671	-1.958368
H	-4.636717	-2.976649	-0.591328
C	-2.240887	-5.948650	-1.243232
H	-1.438282	-5.526144	0.716903
C	-3.178471	-5.572324	-2.209865
H	-4.763149	-4.195590	-2.702929
H	-1.579086	-6.791408	-1.424168
H	-3.239568	-6.110596	-3.151280
O	-2.106790	-4.008204	2.395956
C	-3.788000	-1.253875	0.791064
N	-4.248408	-0.572558	-0.039716
C	-3.435934	-0.399142	3.757044
C	-3.890972	0.755873	3.101884
C	-3.506204	-0.441324	5.161018
C	-4.405739	1.823653	3.834446
H	-3.850388	0.828913	2.025809
C	-4.020127	0.625876	5.891671
H	-3.154542	-1.329896	5.680153
C	-4.472397	1.767245	5.226869
H	-4.751243	2.710093	3.310614
H	-4.070099	0.565867	6.975120
H	-4.873554	2.605223	5.789879
H	-2.735835	-2.427238	3.767419
C	-0.113121	-2.419944	1.178141
C	-0.466627	-1.149363	0.671999
C	-0.884705	-0.295266	1.828249
H	0.012518	-3.317840	0.589436
H	-0.712266	-0.887977	-0.348788
C	-0.921544	-1.223796	3.031301
H	-0.790627	-0.818553	4.028654
C	0.758026	-1.052810	-3.267841
C	1.891235	-1.798532	-2.947493
C	1.752922	-3.056928	-2.355711
C	0.482880	-3.576171	-2.092837
C	-0.658006	-2.832769	-2.397183
C	-0.502021	-1.573198	-2.976401
S	-1.955676	-0.583835	-3.326757
O	-1.620799	0.304606	-4.448147
O	-3.097728	-1.501593	-3.384097
N	-2.129366	0.351468	-1.941837
C	-2.015616	1.825826	-2.023817
C	-0.845412	2.299921	-1.153130
O	0.357680	1.807256	-1.829068
C	1.447253	1.692144	-1.056681
C	2.672425	1.358386	-1.828889
O	1.449341	1.836780	0.152706
C	3.734827	0.679419	-1.193446
C	4.884999	0.398087	-1.942189
C	4.985251	0.785822	-3.279778
C	3.929781	1.456105	-3.898441
C	2.775938	1.738488	-3.170910
C	-0.740314	3.796669	-1.009105
C	-0.681035	4.363727	0.266915
C	-0.585724	5.747236	0.417016
C	-0.540228	6.571623	-0.708255
C	-0.586714	6.008147	-1.985772
C	-0.684936	4.626001	-2.135022
C	-3.329727	2.469350	-1.632196
C	-4.222657	2.864838	-2.631464
C	-5.458882	3.418366	-2.298703
C	-5.811694	3.580595	-0.958520
C	-4.924598	3.184119	0.043570
C	-3.690340	2.629730	-0.289125
p	3.562594	0.061028	0.538732
C	3.984745	1.486235	1.596790
C	3.404951	1.561063	2.868608
C	3.719343	2.619113	3.720226
C	4.606974	3.612774	3.302675
C	5.179627	3.547202	2.030834
C	4.870312	2.487160	1.178535
C	5.019028	-1.055505	0.693274
C	4.879302	-2.362303	0.194001
C	5.930509	-3.272117	0.283041
C	7.132452	-2.892456	0.886443
C	7.275842	-1.601042	1.394992
C	6.226387	-0.684331	1.298242
Pd	1.685822	-1.249808	1.011942
H	0.839882	-0.083111	-3.739489
H	2.876168	-1.397681	-3.163128

H	2.637052	-3.641433	-2.115881
H	0.369618	-4.562781	-1.654589
H	-1.648968	-3.222559	-2.202491
H	-2.952699	0.033923	-1.416767
H	-1.791999	2.078619	-3.062486
H	-0.889807	1.827635	-0.172886
H	5.708699	-0.134079	-1.480647
H	5.890913	0.561416	-3.835968
H	4.003076	1.756386	-4.939141
H	1.942377	2.256261	-3.631882
H	-0.704821	3.712146	1.135042
H	-0.541845	6.180303	1.412408
H	-0.466197	7.649391	-0.592018
H	-0.549841	6.646157	-2.864439
H	-0.720105	4.190055	-3.129745
H	-3.947908	2.727375	-3.674183
H	-6.144291	3.722088	-3.084928
H	-6.773962	4.011136	-0.695890
H	-5.197969	3.302717	1.088114
H	-3.010972	2.317955	0.497104
H	2.691566	0.799927	3.173132
H	3.260983	2.675054	4.703415
H	4.845344	4.441543	3.963221
H	5.862866	4.324181	1.699686
H	5.308490	2.443349	0.185744
H	3.938511	-2.657924	-0.265411
H	5.810157	-4.278388	-0.108449
H	7.950614	-3.602634	0.964343
H	8.206892	-1.303295	1.869054
H	6.346288	0.318171	1.694844
O	-1.195805	0.883483	1.818217
C	-0.278055	-2.417087	2.612474
H	0.081430	-3.201409	3.263297

L6-SSS-TS2

Zero-pointCorrection= 0.922459 (Hartree/Particle)
ThermalCorrection to Energy= 0.984551
ThermalCorrection to Enthalpy= 0.985496
ThermalCorrection to Gibbs Free Energy= 0.818177
E(solv) = -3744.14669373 A.U.

C	-3.320086	2.707060	-0.360195
C	-3.522560	1.937627	0.858672
C	-2.287953	3.713049	-0.327254
C	-4.743187	1.093332	1.015890
C	-5.982429	1.441547	0.460930
C	-4.639930	-0.076055	1.781427
C	-7.094566	0.626244	0.666191
H	-6.081859	2.353014	-0.118037
C	-5.744700	-0.897711	1.971469
H	-3.685940	-0.359321	2.202606
C	-6.976860	-0.545927	1.415863
H	-8.053294	0.906987	0.238957
H	-5.630793	-1.816726	2.537177
H	-7.842718	-1.186561	1.560956
O	-2.681135	1.976206	1.779016
C	-3.939351	2.325876	-1.566712
N	-4.411388	1.994688	-2.585672
C	-2.370103	4.954009	-1.162259
C	-2.596121	4.938243	-2.546553
C	-2.165529	6.188904	-0.530095
C	-2.631666	6.129807	-3.269605
H	-2.756757	3.997236	-3.059830
C	-2.200996	7.381076	-1.253350
H	-1.988371	6.211802	0.542606
C	-2.434711	7.354686	-2.628650
H	-2.814913	6.099005	-4.339929
H	-2.049175	8.327600	-0.741884
H	-2.463271	8.280192	-3.196700
H	-2.060065	3.940296	0.712468
C	0.811177	3.311811	0.974410
C	0.428224	1.948560	1.074231
C	-0.519387	1.670346	-0.060774
H	1.295757	3.897365	1.746502
H	0.458601	1.335310	1.959220
C	-0.662526	2.968423	-0.833963
H	-0.796369	2.890189	-1.909086
C	1.074369	-0.828338	3.574313
C	1.744016	0.255688	4.139318
C	1.024619	1.376057	4.569354
C	-0.363837	1.419198	4.426975
C	-1.047359	0.341158	3.860451
C	-0.314365	-0.768320	3.438487
S	-1.180267	-2.171337	2.737509
O	-0.406641	-3.399233	2.978263
O	-2.573037	-2.118836	3.207992
N	-1.022303	-1.835569	1.104171
C	-1.564893	-2.851390	0.181820
C	-0.623295	-2.936578	-1.046819

O	0.707812	-3.138076	-0.517965
C	1.471449	-2.046588	-0.370455
C	2.561312	-2.236242	0.621360
O	1.313114	-1.008635	-0.989644
C	3.588415	-1.271524	0.739391
C	4.552141	-1.446400	1.740501
C	4.502821	-2.543396	2.603414
C	3.490969	-3.493351	2.475352
C	2.524421	-3.337761	1.484213
C	-0.975756	-4.092132	-1.945543
C	-1.767978	-3.877240	-3.076880
C	-2.161697	-4.950666	-3.875128
C	-1.759485	-6.247579	-3.552503
C	-0.964627	-6.466536	-2.425583
C	-0.578512	-5.394131	-1.622432
C	-3.000623	-2.639965	-0.254612
C	-3.956746	-3.619287	0.027152
C	-5.267098	-3.480485	-0.428901
C	-5.631660	-2.359117	-1.175029
C	-4.685736	-1.372956	-1.456037
C	-3.376651	-1.512114	-0.996355
p	3.682635	0.204320	-0.367351
C	3.870707	-0.490684	-2.046786
C	3.420176	0.264612	-3.135492
C	3.565867	-0.219586	-4.434565
C	4.154896	-1.466290	-4.653618
C	4.599125	-2.227142	-3.570556
C	4.458967	-1.742463	-2.269957
C	5.360767	0.878770	0.000105
C	5.469187	1.840451	1.019966
C	6.705812	2.396672	1.345468
C	7.850052	2.008070	0.645991
C	7.751090	1.061207	-0.375253
C	6.515831	0.497546	-0.696732
Pd	2.265000	2.031707	-0.045245
H	1.611219	-1.711145	3.254747
H	2.823720	0.218623	4.248907
H	1.549314	2.216814	5.014926
H	-0.922765	2.293984	4.742986
H	-2.119645	0.381219	3.722691
H	-1.247908	-0.868158	0.849425
H	-1.482019	-3.812063	0.697512
H	-0.637905	-1.993737	-1.594034
H	5.354512	-0.726670	1.847925
H	5.261300	-2.651032	3.373556
H	3.440667	-4.341656	3.150516
H	1.702025	-4.035502	1.403099
H	-2.094056	-2.870279	-3.318467
H	-2.782506	-4.772380	-4.748407
H	-2.064381	-7.083982	-4.175262
H	-0.647503	-7.473733	-2.169602
H	0.041240	-5.562510	-0.747258
H	-3.670426	-4.495226	0.603220
H	-6.001824	-4.247552	-0.199449
H	-6.653762	-2.245157	-1.524192
H	-4.959579	-0.485505	-2.016990
H	-2.658189	-0.727008	-1.205609
H	2.933228	1.220155	-2.957603
H	3.206118	0.368934	-5.273493
H	4.259351	-1.848243	-5.664923
H	5.050120	-3.201205	-3.736758
H	4.796662	-2.341903	-1.429893
H	4.574745	2.147026	1.558828
H	6.774105	3.137173	2.137315
H	8.813493	2.445034	0.892094
H	8.638151	0.759769	-0.925075
H	6.449721	-0.234331	-1.494148
O	-1.075760	0.621275	-0.328095
C	0.336023	3.824979	-0.274434
H	0.590996	4.804121	-0.664029

L6-SSS-TS3

Zero-pointCorrection= 0.923651 (Hartree/Particle)
ThermalCorrection to Energy= 0.985231
ThermalCorrection to Enthalpy= 0.986175
ThermalCorrection to Gibbs Free Energy= 0.820215
E(solv) = -3744.14979515 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
C			1.513851	3.714161	-0.004546
C			2.197827	4.899840	-0.505570
C			0.137164	3.895134	0.362647
C			3.631069	4.845654	-0.957028
C			4.190893	3.778343	-1.672475
C			4.422249	5.974993	-0.696540

C	5.520384	3.831059	-2.093896
H	3.594075	2.908457	-1.917068
C	5.752932	6.019561	-1.101516
H	3.967565	6.811267	-0.176526
C	6.307790	4.944629	-1.801601
H	5.938232	2.999953	-2.655850
H	6.357397	6.894634	-0.878754
H	7.344905	4.979988	-2.124236
O	1.612311	5.994414	-0.545527
C	2.091174	2.442115	-0.044813
N	2.528599	1.353122	-0.086884
C	-0.643889	3.075764	1.315371
C	-0.237280	1.829792	1.826559
C	-1.822564	3.650705	1.831791
C	-0.966099	1.197754	2.832249
H	0.676055	1.368182	1.487828
C	-2.567892	3.003480	2.811530
H	-2.152230	4.607963	1.443856
C	-2.136914	1.777245	3.322077
H	-0.595113	0.263749	3.238911
H	-3.475210	3.465436	3.190480
H	-2.701495	1.281660	4.105488
H	-0.067436	4.954527	0.480656
C	-2.356672	3.662482	-1.339517
C	-2.627933	2.345073	-2.053210
C	-1.408199	2.010854	-2.749011
C	-0.395055	2.884515	-2.306210
H	-3.631947	2.139770	-2.411206
H	-1.289094	1.287925	-3.547855
H	0.643500	2.800205	-2.608516
C	-0.887790	3.913861	-1.447070
H	-0.518768	4.929085	-1.562454
O	-3.200495	4.355850	-0.785917
C	4.914556	-2.667471	3.009081
C	6.305148	-2.573857	3.024515
C	6.939962	-1.496406	2.403465
C	6.186674	-0.501841	1.775724
C	4.795013	-0.574683	1.763308
C	4.178620	-1.666794	2.375408
S	2.392810	-1.808378	2.362715
O	2.067321	-3.243011	2.451659
O	1.841980	-0.866475	3.343436
N	1.843537	-1.269493	0.894845
C	1.966486	-1.997772	-0.381569
C	1.013117	-3.225695	-0.436983
O	-0.154974	-3.048037	0.407216
C	-0.816522	-1.900559	0.461456
C	-1.723670	-1.851185	1.639341
O	-0.675777	-1.017334	-0.387039
C	-2.950941	-1.147274	1.629640
C	-3.720359	-1.124743	2.795514
C	-3.278380	-1.759583	3.957926
C	-2.064534	-2.443752	3.964944
C	-1.296906	-2.504671	2.803258
C	0.642708	-3.607599	-1.858591
C	1.610024	-4.239232	-2.653055
C	1.331946	-4.579604	-3.975996
C	0.076930	-4.307879	-4.522324
C	-0.897285	-3.700684	-3.730701
C	-0.618954	-3.351765	-2.408375
C	3.398303	-2.334219	-0.762159
C	4.077557	-1.459592	-1.616746
C	5.422456	-1.663969	-1.921319
C	6.105216	-2.750249	-1.372803
C	5.434487	-3.628722	-0.520866
C	4.089098	-3.423775	-0.217413
p	-3.522077	-0.285379	0.115580
C	-5.083767	0.543909	0.535611
C	-5.071286	1.940161	0.656430
C	-6.248604	2.618665	0.974054
C	-7.434879	1.910246	1.168021
C	-7.452068	0.517950	1.035860
C	-6.281640	-0.166128	0.714630
C	-3.989645	-1.684841	-0.978031
C	-4.184489	-2.986944	-0.497467
C	-4.498205	-4.022671	-1.379761
C	-4.630612	-3.766146	-2.744386
C	-4.447489	-2.468181	-3.229326
C	-4.120081	-1.435394	-2.353297
Pd	-1.806715	0.816337	-0.907213
H	4.400425	-3.510655	3.456601
H	6.891929	-3.347332	3.511339
H	8.024346	-1.433084	2.405259
H	6.680588	0.332012	1.286524
H	4.211407	0.189721	1.259732
H	2.026102	-0.268756	0.754430
H	1.595840	-1.269409	-1.102017
H	1.494234	-4.069765	0.054642
H	-4.665201	-0.593709	2.800351
H	-3.886885	-1.714725	4.856636

H	-1.710599	-2.930023	4.868274
H	-0.348184	-3.028126	2.797437
H	2.586435	-4.462669	-2.237346
H	2.096891	-5.064416	-4.575920
H	-0.141715	-4.576121	-5.552112
H	-1.884958	-3.495818	-4.131711
H	-1.397131	-2.885968	-1.819799
H	3.553109	-0.596150	-2.014702
H	5.937306	-0.971733	-2.581529
H	7.154885	-2.909122	-1.602933
H	5.962448	-4.467570	-0.077089
H	3.591290	-4.094009	0.475300
H	-4.157423	2.496965	0.487994
H	-6.232834	3.701320	1.053589
H	-8.351157	2.440879	1.410988
H	-8.378449	-0.031798	1.175584
H	-6.295739	-1.245794	0.596684
H	-4.080261	-3.196263	0.561880
H	-4.635301	-5.030226	-0.998385
H	-4.868996	-4.574466	-3.429340
H	-4.545686	-2.263211	-4.291544
H	-3.948147	-0.432618	-2.732727

L6-RRR-TS1

Zero-pointCorrection= 0.921866 (Hartree/Particle)

ThermalCorrection to Energy= 0.983970

ThermalCorrection to Enthalpy= 0.984914

ThermalCorrection to Gibbs Free Energy= 0.816605

E(solv) = -3744.14876320 A.U.

C	-3.710222	-0.576403	0.494150
C	-2.608444	0.079739	-0.290273
C	-1.924778	0.958800	0.601646
C	-2.537438	0.883855	1.895353
H	-2.650892	0.169540	-1.368809
H	-1.235094	1.729791	0.290579
H	-2.119617	1.323397	2.790095
C	-3.742910	0.133463	1.831958
H	-4.149386	-0.381333	2.696201
O	-4.440004	-1.490009	0.145311
C	1.243995	3.790833	0.631167
C	1.369765	5.056389	1.196005
C	2.165522	6.023968	0.573000
C	2.836515	5.727753	-0.614117
C	2.717002	4.461807	-1.189905
C	1.922832	3.512008	-0.555769
S	1.753426	1.893701	-1.290536
O	0.326702	1.629625	-1.519700
O	2.715445	1.807239	-2.396676
N	2.188153	0.869240	-0.027350
C	3.581286	0.404694	0.046568
C	3.785534	-0.538798	1.260245
O	3.177348	-1.859063	1.059565
C	1.905841	-2.072191	1.382463
C	1.555773	-3.523521	1.401909
O	1.125024	-1.166085	1.669456
C	0.498724	-4.040325	0.620212
C	0.158455	-5.386989	0.766324
C	0.853077	-6.206479	1.660610
C	1.923132	-5.698466	2.395046
C	2.283559	-4.357645	2.253753
C	5.250776	-0.828247	1.472503
C	5.944670	-0.240862	2.531880
C	7.313456	-0.461914	2.684349
C	7.994156	-1.277710	1.780115
C	7.301225	-1.874157	0.723983
C	5.934668	-1.650294	0.568677
C	4.497358	1.607418	0.204409
C	5.541350	1.827456	-0.693390
C	6.375260	2.936185	-0.545288
C	6.167374	3.833034	0.503378
C	5.122298	3.617643	1.404507
C	4.292408	2.509791	1.254240
p	-0.292486	-2.926408	-0.614852
C	-1.419257	-3.990419	-1.573256
C	-2.798220	-3.777756	-1.445382
C	-3.691834	-4.576881	-2.162002
C	-3.215946	-5.579562	-3.006304
C	-1.839356	-5.785459	-3.144184
C	-0.941699	-4.992322	-2.433778
C	1.145796	-2.620488	-1.723752
C	2.241035	-3.495221	-1.804882
C	3.326454	-3.190046	-2.625586
C	3.328556	-2.010837	-3.374585
C	2.238834	-1.140550	-3.307822
C	1.153712	-1.441127	-2.483009
Pd	-0.924614	-0.973820	0.449626
H	0.643261	3.024776	1.108967
H	0.842776	5.290606	2.115750
H	2.260798	7.010479	1.017055

H	3.458550	6.478670	-1.091449
H	3.243618	4.197515	-2.099082
H	1.465205	0.164861	0.107174
H	3.860984	-0.150956	-0.856976
H	3.326598	-0.090932	2.144127
H	-0.642485	-5.800965	0.163426
H	0.566764	-7.248909	1.765159
H	2.478545	-6.339198	3.072806
H	3.119240	-3.949644	2.813803
H	5.417524	0.406451	3.226452
H	7.846135	0.003350	3.508465
H	9.060000	-1.450305	1.898216
H	7.826614	-2.513622	0.020418
H	5.391899	-2.118249	-0.247476
H	5.688448	1.137187	-1.518135
H	7.181403	3.102870	-1.253877
H	6.811655	4.700667	0.613830
H	4.942587	4.320782	2.212269
H	3.457684	2.361435	1.931595
H	-3.181402	-2.983661	-0.812009
H	-4.758533	-4.400248	-2.062651
H	-3.913481	-6.195602	-3.566934
H	-1.467241	-6.557879	-3.811388
H	0.126982	-5.141728	-2.554479
H	2.256673	-4.405877	-1.215378
H	4.170088	-3.873092	-2.677813
H	4.178173	-1.768624	-4.006793
H	2.245061	-0.209608	-3.861865
H	0.328168	-0.740770	-2.403282
C	-4.848662	2.174350	0.319085
C	-3.823882	3.164174	0.540748
C	-5.203278	1.413661	1.489667
C	-3.285106	4.047083	-0.541416
C	-4.013000	4.452545	-1.668734
C	-1.970286	4.510897	-0.384237
C	-3.420347	5.275281	-2.627278
H	-5.039336	4.136193	-1.803700
C	-1.372942	5.317343	-1.346608
H	-1.434108	4.225148	0.511261
C	-2.099464	5.699981	-2.477066
H	-3.995760	5.582009	-3.496198
H	-0.345716	5.644725	-1.214905
H	-1.640196	6.329583	-3.234536
O	-3.300478	3.233443	1.682835
C	-5.346463	1.860585	-0.967686
N	-5.762363	1.588187	-2.025141
C	-6.442372	0.607238	1.644729
C	-7.049485	-0.138031	0.621352
C	-7.029595	0.588839	2.922187
C	-8.215619	-0.858857	0.873379
H	-6.616397	-0.163626	-0.367783
C	-8.193860	-0.131976	3.172823
H	-6.564516	1.157815	3.723921
C	-8.793417	-0.860019	2.143470
H	-8.672118	-1.426608	0.067592
H	-8.632773	-0.123073	4.166737
H	-9.702660	-1.424762	2.330785
H	-4.976902	1.991270	2.380990

L6-RRR-TS2

Zero-pointCorrection= 0.922543 (Hartree/Particle)
ThermalCorrection to Energy= 0.984519
ThermalCorrection to Enthalpy= 0.985463
ThermalCorrection to Gibbs Free Energy= 0.816915
E(solv) = -3744.14922804 A.U.

C	4.075078	-0.243506	-0.141035
C	4.122125	0.147282	-1.600967
C	3.150056	-0.647694	-2.279605
C	2.363671	-1.327106	-1.296699
H	4.997464	0.603037	-2.048153
H	3.062585	-0.785186	-3.349824
H	1.482257	-1.911955	-1.531687
C	2.930929	-1.211664	-0.002103
H	2.340396	-1.196259	0.909820
O	4.815135	0.152420	0.751152
C	-7.125034	2.231186	0.076710
C	-8.170935	2.323319	-0.838342
C	-8.907871	1.184229	-1.176201
C	-8.609942	-0.048689	-0.594159
C	-7.566960	-0.153922	0.325061
C	-6.834336	0.987985	0.639220
S	-5.448654	0.853473	1.754719
O	-5.383689	2.049571	2.600278
O	-5.474278	-0.492927	2.341354
N	-4.121739	1.015227	0.702427
C	-3.632614	-0.227991	0.079493
C	-2.251348	0.063734	-0.519918
O	-1.446923	0.539845	0.608740

C	-0.271604	1.108448	0.305655
C	0.622013	1.252721	1.479425
O	-0.008835	1.426164	-0.855618
C	1.756718	2.111418	1.474204
C	2.593457	2.111534	2.591446
C	2.349997	1.266566	3.678034
C	1.249435	0.417347	3.675113
C	0.381449	0.427985	2.586363
C	-1.614404	-1.154634	-1.134714
C	-1.332876	-1.189683	-2.502574
C	-0.775672	-2.334811	-3.075904
C	-0.491063	-3.448282	-2.282131
C	-0.769694	-3.414304	-0.912916
C	-1.325390	-2.272105	-0.341907
C	-4.572815	-0.708027	-1.006641
C	-4.944319	-2.052264	-1.065292
C	-5.802974	-2.502217	-2.068976
C	-6.295962	-1.607110	-3.018851
C	-5.923229	-0.261761	-2.965503
C	-5.062397	0.184622	-1.966061
p	2.250613	3.041749	-0.038598
C	3.706749	4.034238	0.437956
C	4.958456	3.398376	0.503595
C	6.091523	4.132399	0.850282
C	5.993010	5.500870	1.113652
C	4.752680	6.135734	1.040211
C	3.610455	5.406684	0.707462
C	0.906054	4.251585	-0.290974
C	0.130699	4.727287	0.775272
C	-0.898301	5.639566	0.540017
C	-1.155883	6.083925	-0.758601
C	-0.384704	5.613858	-1.823870
C	0.639570	4.696663	-1.592438
Pd	2.272031	1.241565	-1.482978
H	-6.539264	3.100776	0.353847
H	-8.412609	3.281995	-1.287494
H	-9.718289	1.260319	-1.895418
H	-9.181809	-0.931719	-0.861088
H	-7.303677	-1.101199	0.778955
H	-3.387572	1.472618	1.244275
H	-3.521844	-1.018202	0.830952
H	-2.324436	0.875272	-1.245400
H	3.465038	2.754335	2.604992
H	3.040253	1.264489	4.516032
H	1.079557	-0.275264	4.491201
H	-0.471590	-0.237613	2.569059
H	-1.550818	-0.319689	-3.115383
H	-0.558494	-2.352424	-4.140276
H	-0.031726	-4.335334	-2.705867
H	-0.542989	-4.273482	-0.294293
H	-1.525110	-2.256529	0.724615
H	-4.561341	-2.744897	-0.321617
H	-6.088312	-3.549581	-2.105124
H	-6.970463	-1.954673	-3.796305
H	-6.313107	0.441378	-3.695653
H	-4.797990	1.235038	-1.898774
H	5.043835	2.330837	0.321926
H	7.053459	3.631790	0.911361
H	6.880490	6.070210	1.375051
H	4.670616	7.199738	1.243180
H	2.648945	5.905657	0.654438
H	0.329422	4.381176	1.785152
H	-1.498550	6.001505	1.369768
H	-1.959343	6.791920	-0.940236
H	-0.587547	5.953310	-2.835481
H	1.227626	4.310734	-2.420829
C	2.594375	-3.860898	0.755766
C	1.759887	-3.535092	1.895690
C	3.706786	-2.984812	0.518611
C	0.537769	-4.342338	2.227804
C	0.409152	-5.716412	1.984033
C	-0.528047	-3.660631	2.836355
C	-0.775558	-6.380361	2.306493
H	1.229123	-6.271893	1.545743
C	-1.715335	-4.318437	3.144316
H	-0.394848	-2.607696	3.060235
C	-1.843733	-5.683823	2.873451
H	-0.861475	-7.445854	2.113126
H	-2.537751	-3.771883	3.598186
H	-2.767945	-6.202662	3.112499
O	1.994731	-2.518703	2.582883
C	2.189308	-4.798343	-0.218024
N	1.853679	-5.552572	-1.048295
C	4.792079	-3.204232	-0.465717
C	4.584788	-3.700039	-1.764611
C	6.093907	-2.820721	-0.098826
C	5.652674	-3.836539	-2.649392
H	3.590568	-3.985045	-2.083780
C	7.160516	-2.956966	-0.984903
H	6.260172	-2.402992	0.889453

C	6.944040	-3.469814	-2.264640
H	5.472651	-4.230393	-3.645856
H	8.158669	-2.659939	-0.675586
H	7.772890	-3.577623	-2.958774
H	4.057552	-2.535490	1.445070

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L6-RRR-TS3

Zero-pointCorrection= 0.922298 (Hartree/Particle)
ThermalCorrection to Energy= 0.983796
ThermalCorrection to Enthalpy= 0.984741
ThermalCorrection to Gibbs Free Energy= 0.823046
E(solv) = -3744.15746971 A.U.

C	3.031574	2.686449	3.076859
C	4.209301	1.860736	2.647882
C	4.703265	2.438274	1.444889
H	4.788999	1.296191	3.371605
H	5.685929	2.284729	1.014549
O	2.455674	2.669199	4.146803
C	0.313148	1.918783	1.964691
C	0.582306	0.606075	2.499242
C	1.212906	2.491781	1.009869
C	-0.553312	-0.230042	3.008264
C	-1.431825	0.191290	4.013588
C	-0.696716	-1.513571	2.456331
C	-2.453263	-0.657665	4.445606
H	-1.316823	1.170867	4.462501
C	-1.729122	-2.350829	2.877740
H	0.001387	-1.841482	1.696395
C	-2.612189	-1.920865	3.873537
H	-3.124739	-0.327322	5.233009
H	-1.839036	-3.327762	2.417720
H	-3.413626	-2.573262	4.209737
O	1.702712	0.035110	2.488788
C	-0.925412	2.544908	2.246707
N	-1.936329	3.087884	2.467168
C	0.767478	3.393687	-0.081611
C	1.198240	3.085140	-1.382516
C	-0.036225	4.527078	0.108411
C	0.782959	3.843638	-2.473669
H	1.854141	2.234115	-1.533934
C	-0.433725	5.296979	-0.982786
H	-0.366152	4.798740	1.104229
C	-0.041612	4.951681	-2.276893
H	1.099661	3.562353	-3.474017
H	-1.072869	6.159660	-0.822372
H	-0.383157	5.538109	-3.124122
H	1.902891	1.733346	0.634888
C	3.802761	3.462571	1.017695
H	3.943080	4.056851	0.121476
C	2.686483	3.554765	1.880003
H	2.122795	4.471118	2.012801
C	-5.009375	-2.662278	0.825125
C	-6.355901	-2.521120	1.144707
C	-7.324352	-2.568283	0.137642
C	-6.949416	-2.755871	-1.192881
C	-5.600472	-2.884446	-1.527528
C	-4.647983	-2.835634	-0.512377
S	-2.911317	-2.933396	-0.937192
O	-2.275043	-3.900188	-0.035250
O	-2.831951	-3.076976	-2.393231
N	-2.231357	-1.455961	-0.545487
C	-2.885963	-0.227872	-1.017726
C	-1.830975	0.896086	-1.158217
O	-0.795706	0.451311	-2.059651
C	0.352007	-0.013095	-1.544931
C	1.396694	-0.209305	-2.585865
O	0.541560	-0.206593	-0.357812
C	2.687446	-0.682474	-2.240112
C	3.640726	-0.782930	-3.265126
C	3.339971	-0.434891	-4.581308
C	2.066307	0.022994	-4.911657
C	1.104243	0.133535	-3.913862
C	-2.448822	2.146543	-1.740910
C	-2.975127	3.124507	-0.892343
C	-3.624760	4.237109	-1.425498
C	-3.742419	4.390817	-2.806887
C	-3.211914	3.418979	-3.657537
C	-2.575693	2.297790	-3.126013
C	-4.024959	0.239091	-0.129889
C	-5.286321	0.501197	-0.667595
C	-6.323849	0.943230	0.151304
C	-6.102653	1.141624	1.515590
C	-4.840149	0.893040	2.055690
C	-3.809025	0.439548	1.236586
p	3.207667	-1.101171	-0.509442
C	4.865984	-1.862394	-0.783847
C	6.006760	-1.059033	-0.637498
C	7.280876	-1.591425	-0.835878

C	7.428233	-2.937605	-1.174902
C	6.298359	-3.746097	-1.318804
C	5.023997	-3.212996	-1.126231
C	2.218632	-2.562267	-0.031752
C	1.385542	-3.255120	-0.918202
C	0.673459	-4.370668	-0.481895
C	0.797516	-4.808960	0.837727
C	1.637563	-4.130410	1.721498
C	2.341971	-3.005869	1.291767
H	-4.249186	-2.609550	1.596095
H	-6.649151	-2.360366	2.177218
H	-8.373747	-2.453092	0.393014
H	-7.704243	-2.794363	-1.972737
H	-5.277984	-3.017855	-2.553836
H	-1.930842	-1.441215	0.427881
H	-3.258345	-0.441696	-2.023794
H	-1.379234	1.097973	-0.185802
H	4.635199	-1.143512	-3.036320
H	4.105426	-0.529232	-5.346229
H	1.822600	0.292161	-5.934823
H	0.111636	0.495350	-4.147830
H	-2.881719	3.019898	0.182771
H	-4.031059	4.988128	-0.754094
H	-4.244380	5.261651	-3.219842
H	-3.298215	3.529975	-4.735080
H	-2.171414	1.538308	-3.787384
H	-5.456096	0.352658	-1.729925
H	-7.304264	1.132626	-0.276425
H	-6.909252	1.493462	2.152770
H	-4.645147	1.059155	3.110090
H	-2.834699	0.255841	1.674298
H	5.885744	-0.013690	-0.364846
H	8.156195	-0.958889	-0.717609
H	8.419581	-3.356672	-1.322132
H	6.409231	-4.794877	-1.579544
H	4.149526	-3.845824	-1.236612
H	1.274113	-2.916792	-1.943019
H	-0.001848	-4.877887	-1.161134
H	0.223920	-5.666095	1.176789
H	1.726083	-4.456879	2.753623
H	2.965291	-2.455460	1.990247
Pd	3.477753	0.463447	1.205050

L6-INT2

Zero-pointCorrection= 0.696337 (Hartree/Particle)

ThermalCorrection to Energy= 0.742865

ThermalCorrection to Enthalpy= 0.743809

ThermalCorrection to Gibbs Free Energy= 0.613035

E(solv) = -2997.60495548 A.U.

C	-1.316092	-1.072577	-3.079027
C	-0.723187	-2.280303	-2.641358
C	0.736217	-2.014296	-2.478921
H	-2.240854	-0.993828	-3.641006
H	-1.112956	-3.281889	-2.771079
C	0.961185	-0.597064	-2.880006
H	1.920300	-0.101326	-2.809008
C	-0.825886	-2.267207	1.434157
C	-2.064822	-2.768779	1.007549
C	-2.111859	-3.982183	0.290922
C	-0.944108	-4.692928	0.025079
C	0.293306	-4.201663	0.453592
C	0.334264	-2.993908	1.142622
S	1.912192	-2.349241	1.681565
O	1.721638	-1.521991	2.881291
O	2.863447	-3.466818	1.717226
N	2.208111	-1.285321	0.417396
C	3.254641	-0.273301	0.611440
C	2.618523	1.105441	0.269486
O	1.561919	1.279670	1.238586
C	0.291168	1.269035	0.802930
C	-0.693564	1.171141	1.913580
O	-0.022984	1.328773	-0.372130
C	-2.075181	0.991854	1.636989
C	-2.945808	0.850272	2.727111
C	-2.480264	0.891658	4.042470
C	-1.122366	1.061534	4.301580
C	-0.235952	1.196183	3.237044
C	3.582801	2.256638	0.374688
C	4.236081	2.717142	-0.771696
C	5.199225	3.720899	-0.681225
C	5.512790	4.278434	0.559331
C	4.857466	3.827940	1.707187
C	3.898144	2.819781	1.615932
C	4.533825	-0.519847	-0.166137
C	5.744406	-0.061973	0.368713
C	6.933848	-0.188592	-0.344853
C	6.930706	-0.782768	-1.608026

C	5.732084	-1.254285	-2.142404
C	4.538887	-1.124093	-1.428772
p	-2.700032	0.654682	-0.072859
C	-2.638042	2.255932	-0.961146
C	-2.895745	2.245590	-2.337587
C	-2.893147	3.435710	-3.063761
C	-2.628367	4.646910	-2.420628
C	-2.372393	4.661802	-1.048657
C	-2.379615	3.471737	-0.319945
C	-4.520577	0.486347	0.162496
C	-5.107782	-0.766184	-0.060441
C	-6.484585	-0.942849	0.092127
C	-7.288251	0.135326	0.462612
C	-6.714344	1.393001	0.670989
C	-5.340579	1.568939	0.517548
Pd	-1.667971	-1.215449	-0.971441
H	-0.763031	-1.372169	2.038419
H	-2.980998	-2.281868	1.323702
H	-3.071826	-4.370391	-0.036371
H	-0.989729	-5.628663	-0.523157
H	1.213118	-4.738450	0.257097
H	2.240325	-1.800169	-0.467540
H	3.487227	-0.234256	1.679154
H	2.173204	1.057932	-0.724946
H	-4.003139	0.696877	2.550750
H	-3.184858	0.778976	4.861620
H	-0.750925	1.073498	5.321360
H	0.826795	1.287492	3.416539
H	4.003698	2.270871	-1.734586
H	5.704176	4.066495	-1.578655
H	6.262294	5.061491	0.631547
H	5.094711	4.260817	2.675045
H	3.386978	2.469095	2.506910
H	5.750001	0.412863	1.345357
H	7.862192	0.173722	0.087569
H	7.856930	-0.885833	-2.166405
H	5.719738	-1.733395	-3.117334
H	3.630528	-1.534530	-1.858848
H	-3.092227	1.300806	-2.836484
H	-3.092419	3.417256	-4.131680
H	-2.619533	5.573988	-2.986587
H	-2.163226	5.600736	-0.543594
H	-2.170828	3.488076	0.745398
H	-4.477093	-1.592491	-0.378259
H	-6.928325	-1.918190	-0.087223
H	-8.360002	0.001396	0.578838
H	-7.339721	2.237469	0.946828
H	-4.900709	2.550440	0.667487
O	1.596784	-2.789345	-2.044313
C	-0.230422	-0.052316	-3.196656
H	-0.420736	0.987577	-3.435348

N-methyl-L6-INT2

Zero-pointCorrection= 0.723583 (Hartree/Particle)
ThermalCorrection to Energy= 0.772224
ThermalCorrection to Enthalpy= 0.773169
ThermalCorrection to Gibbs Free Energy= 0.632723
E(solv) = -3036.90657889 A.U.

C	-4.342593	3.388042	0.041693
C	-3.845667	3.003979	-1.336700
C	-2.483307	3.374666	-1.407501
C	-2.109508	3.961466	-0.090740
H	-4.533852	2.894841	-2.167350
H	-1.925113	3.579021	-2.314648
H	-1.101110	4.282407	0.143019
C	-3.167887	3.977620	0.750634
H	-3.195910	4.295069	1.785348
O	-5.475064	3.234087	0.484510
C	6.021617	-2.413751	-1.067449
C	7.034267	-2.163047	-1.989527
C	8.018919	-1.211536	-1.706434
C	7.999559	-0.515556	-0.497333
C	6.990639	-0.758279	0.434390
C	6.009082	-1.696929	0.129799
S	4.683028	-1.992287	1.291745
O	4.489153	-3.442344	1.389943
O	4.949507	-1.183222	2.488757
N	3.307228	-1.375603	0.489167
C	3.088731	0.069581	0.752506
C	1.700221	0.544337	0.282689
O	0.741487	-0.044173	1.197614
C	-0.475870	-0.321697	0.697160
C	-1.404061	-0.882838	1.705927
O	-0.736932	-0.127178	-0.486971
C	-2.760990	-1.159278	1.389111
C	-3.584868	-1.657740	2.405608
C	-3.093914	-1.896582	3.689624

C	-1.758190	-1.634683	3.990670
C	-0.922597	-1.125841	3.002143
C	1.565993	2.048733	0.321639
C	1.627838	2.787125	-0.862493
C	1.599205	4.180578	-0.825351
C	1.496642	4.845212	0.398404
C	1.408752	4.109911	1.582690
C	1.443817	2.716381	1.544471
C	4.155732	0.893414	0.052193
C	4.834813	1.898413	0.741582
C	5.780426	2.687663	0.086357
C	6.054652	2.471900	-1.264454
C	5.379768	1.464073	-1.957627
C	4.433775	0.680766	-1.301669
p	-3.461614	-0.808626	-0.287925
C	-5.247174	-1.155765	-0.094987
C	-6.086298	-0.062572	0.171009
C	-7.456207	-0.262066	0.345051
C	-7.998579	-1.544123	0.240555
C	-7.168498	-2.632788	-0.038936
C	-5.797106	-2.441773	-0.205518
C	-2.825075	-2.222045	-1.270177
C	-2.435672	-3.437626	-0.691918
C	-1.951690	-4.474599	-1.491060
C	-1.855771	-4.306820	-2.873633
C	-2.241343	-3.097332	-3.455979
C	-2.717922	-2.057923	-2.658214
Pd	-2.687770	1.260022	-0.960969
H	5.251588	-3.150719	-1.268235
H	7.057782	-2.709906	-2.927424
H	8.803691	-1.015218	-2.431266
H	8.763764	0.224147	-0.280230
H	6.942212	-0.218895	1.371954
H	3.140416	0.264454	1.829582
H	1.492082	0.184796	-0.725195
H	-4.626265	-1.864294	2.188622
H	-3.759754	-2.289774	4.452571
H	-1.369259	-1.820216	4.986968
H	0.114521	-0.908448	3.225523
H	1.716064	2.268605	-1.812250
H	1.653465	4.746184	-1.750799
H	1.473746	5.930710	0.428504
H	1.314118	4.621387	2.536130
H	1.374895	2.143718	2.464246
H	4.623401	2.058372	1.794508
H	6.305574	3.466034	0.632552
H	6.795699	3.081040	-1.774308
H	5.599695	1.281429	-3.005369
H	3.930546	-0.125100	-1.826676
H	-5.679928	0.942819	0.233067
H	-8.095571	0.591264	0.551033
H	-9.066925	-1.695759	0.368273
H	-7.589274	-3.630453	-0.130109
H	-5.155184	-3.288918	-0.426124
H	-2.505837	-3.572967	0.383128
H	-1.650043	-5.412719	-1.033270
H	-1.477676	-5.114208	-3.494476
H	-2.161354	-2.959743	-4.530672
H	-2.995580	-1.105660	-3.102074
C	2.181148	-2.319418	0.399192
H	1.627151	-2.433417	1.337133
H	1.500680	-1.979667	-0.383415
H	2.576071	-3.290919	0.107875

PdL10-RRR-TS1

Zero-pointCorrection= 0.960097 (Hartree/Particle)

ThermalCorrection to Energy= 1.020461

ThermalCorrection to Enthalpy= 1.021405

ThermalCorrection to Gibbs Free Energy= 0.860585

E(solv) = -3426.50695938 A.U.

C	-5.741216	-1.534909	-1.705291
C	-4.615438	-2.195764	-2.194181
C	-3.382559	-1.551466	-2.193980
C	-3.229359	-0.246371	-1.694381
C	-4.370453	0.417935	-1.186249
C	-5.613118	-0.234986	-1.226458
C	-4.469959	1.855935	-0.718171
N	-3.778883	2.313985	0.359796
O	-5.260562	2.590838	-1.314564
C	-2.823861	1.643302	1.261919
C	-2.708513	2.633364	2.426470
C	-2.793452	3.989453	1.718681
C	-3.865016	3.760072	0.645807
C	-3.206130	0.208517	1.663167
p	-1.685484	-0.866118	1.717578
C	-1.201816	-0.724029	3.489183
C	-2.241087	-2.585296	1.408741
C	-3.546700	-2.858410	0.978941

C	-3.952462	-4.157478	0.682126
C	-3.049069	-5.208844	0.813970
C	-1.745032	-4.946147	1.232845
C	-1.311958	-3.648433	1.527887
C	-1.862729	-1.366520	4.563057
C	-1.412764	-1.100483	5.863179
C	-0.362081	-0.220461	6.119156
C	0.267194	0.428676	5.059778
C	-0.153561	0.169007	3.757372
C	0.119307	-3.430646	1.949234
p	-1.524635	0.460293	-1.687195
Pd	-0.133200	-0.060564	0.147332
C	-1.736873	2.196454	-2.196604
C	-2.734246	2.584431	-3.104866
C	-2.857755	3.922069	-3.474499
C	-1.985062	4.877970	-2.949235
C	-0.984050	4.493604	-2.055143
C	-0.858117	3.156970	-1.675656
C	-0.671343	-0.362046	-3.092491
C	-0.484443	0.271943	-4.325875
C	0.295766	-0.334078	-5.313576
C	0.893276	-1.572689	-5.080389
C	0.705150	-2.216257	-3.854192
C	-0.069286	-1.612787	-2.866696
H	-6.713756	-2.018090	-1.711458
H	-4.691209	-3.207382	-2.580802
H	-2.523622	-2.069849	-2.601636
H	-6.485277	0.311794	-0.884127
H	-1.844852	1.623144	0.762543
H	-1.784381	2.482914	2.991126
H	-3.554048	2.498935	3.113127
H	-3.047717	4.813352	2.390533
H	-1.833914	4.222147	1.243217
H	-3.693280	4.324794	-0.273187
H	-4.873263	4.002132	1.001166
H	-3.717481	0.193519	2.629884
H	-3.883604	-0.210966	0.926391
H	-4.271262	-2.061904	0.870178
H	-4.970139	-4.338258	0.349647
H	-3.352332	-6.227687	0.591077
H	-1.037223	-5.764666	1.332740
H	-1.908047	-1.595823	6.694306
H	-0.044034	-0.041100	7.142068
H	1.081470	1.124663	5.238020
H	0.193614	-2.910841	2.910122
H	0.648289	-4.383105	2.037830
H	0.651948	-2.818569	1.214685
H	-3.429151	1.851850	-3.501001
H	-3.644179	4.217215	-4.162113
H	-2.086338	5.920309	-3.237954
H	-0.291719	5.226510	-1.652139
H	-0.058338	2.874652	-1.000470
H	-0.924028	1.246185	-4.508459
H	0.446779	0.173307	-6.261792
H	1.513770	-2.030323	-5.845207
H	1.186954	-3.168573	-3.654900
H	-0.180400	-2.094791	-1.899143
H	0.338832	0.662094	2.927970
C	-3.020517	-2.321094	4.388679
H	-3.490924	-2.521701	5.355503
H	-3.788414	-1.925450	3.717647
H	-2.699318	-3.277765	3.964337
C	2.027640	1.616386	0.013338
C	1.734326	0.467629	-0.921636
C	1.953835	-0.734881	-0.208855
C	1.951581	-0.396794	1.182386
H	1.724397	0.578180	-1.997807
H	1.981225	-1.732602	-0.622679
H	2.020744	-1.129783	1.972831
C	2.391553	0.979388	1.304806
H	2.311901	1.553769	2.220946
O	1.969101	2.813215	-0.253247
C	4.674923	-0.047664	-0.005927
C	4.627561	-1.478528	0.231695
C	4.406869	0.790906	1.130108
C	4.737658	-2.480322	-0.891784
C	4.251161	-2.269536	-2.191207
C	5.262602	-3.740602	-0.567467
C	4.304976	-3.290902	-3.141151
H	3.824789	-1.315195	-2.470560
C	5.331707	-4.753603	-1.520239
H	5.602054	-3.905008	0.449415
C	4.850329	-4.532717	-2.813410
H	3.923679	-3.107215	-4.142331
H	5.754898	-5.718668	-1.254223
H	4.899101	-5.323072	-3.557850
O	4.460063	-1.930298	1.383409
C	4.914813	0.495346	-1.288354
N	5.084922	0.965014	-2.346028
C	4.868922	2.188732	1.319532

C	4.967240	3.144814	0.294989
C	5.202083	2.581173	2.628646
C	5.402226	4.438707	0.577188
H	4.704691	2.885399	-0.720737
C	5.635035	3.874120	2.909393
H	5.127944	1.850214	3.430761
C	5.738254	4.811014	1.879253
H	5.473812	5.161430	-0.230787
H	5.896120	4.148232	3.928141
H	6.076695	5.821836	2.090306
H	4.490648	0.201054	2.039316

L10-RRR-TS2

Zero-pointCorrection= 0.960048 (Hartree/Particle)

ThermalCorrection to Energy= 1.020351

ThermalCorrection to Enthalpy= 1.021295

ThermalCorrection to Gibbs Free Energy= 0.860575

E(solv) = -3426.49969367 A.U.

C	-5.323932	-2.876898	0.446379
C	-4.154408	-3.288715	1.085935
C	-2.918814	-2.917774	0.568352
C	-2.803582	-2.105852	-0.576310
C	-3.991547	-1.667230	-1.205447
C	-5.231358	-2.093016	-0.697944
C	-4.125509	-0.855964	-2.477565
N	-3.676643	0.425279	-2.550575
O	-4.727319	-1.368470	-3.424734
C	-2.974183	1.253979	-1.550812
C	-2.981930	2.645205	-2.198004
C	-2.850254	2.327416	-3.690858
C	-3.739370	1.091364	-3.865184
C	-3.572103	1.200373	-0.134855
p	-2.206229	1.278653	1.128150
C	-1.959247	3.097108	1.297044
C	-2.919989	0.657003	2.696207
C	-4.097962	-0.103890	2.697796
C	-4.582625	-0.680147	3.869984
C	-3.889691	-0.500464	5.065040
C	-2.711395	0.245424	5.070871
C	-2.200772	0.826854	3.904713
C	-2.872399	3.989027	1.905253
C	-2.566258	5.356577	1.891330
C	-1.406339	5.848477	1.293650
C	-0.512393	4.966369	0.690101
C	-0.791925	3.601482	0.702085
C	-0.915047	1.613537	3.973686
p	-1.087219	-1.594631	-1.031395
Pd	-0.295857	0.162598	0.315338
C	-1.050410	-1.494585	-2.851193
C	-1.821296	-2.333136	-3.669999
C	-1.743866	-2.216687	-5.057005
C	-0.888054	-1.276087	-5.634621
C	-0.104129	-0.453568	-4.822723
C	-0.184074	-0.557408	-3.433832
C	-0.039075	-3.052633	-0.625865
C	0.357068	-3.985310	-1.591332
C	1.270570	-4.989824	-1.263143
C	1.798348	-5.071211	0.025191
C	1.402335	-4.151341	0.998799
C	0.491566	-3.150364	0.672787
H	-6.297337	-3.173429	0.825843
H	-4.199434	-3.905295	1.978568
H	-2.020229	-3.273098	1.058594
H	-6.127368	-1.792614	-1.230972
H	-1.928797	0.921774	-1.505831
H	-2.179750	3.274823	-1.804687
H	-3.937362	3.144556	-1.991824
H	-3.154935	3.154639	-4.337644
H	-1.811769	2.071884	-3.928933
H	-3.390899	0.404199	-4.638786
H	-4.778842	1.353966	-4.096635
H	-4.301386	2.001889	0.012900
H	-4.087073	0.255047	0.010385
H	-4.651715	-0.264729	1.781408
H	-5.496227	-1.266773	3.842135
H	-4.257124	-0.941867	5.986998
H	-2.164851	0.379347	6.000950
H	-3.259779	6.049538	2.361057
H	-1.205784	6.916056	1.300494
H	0.394965	5.330951	0.217557
H	-0.423716	1.465816	4.939745
H	-0.219913	1.308513	3.183308
H	-1.088530	2.687594	3.842103
H	-2.501705	-3.054209	-3.230840
H	-2.361016	-2.854042	-5.682660
H	-0.831229	-1.187348	-6.715930
H	0.575933	0.268717	-5.264595
H	0.448677	0.068674	-2.812644

H	-0.021691	-3.914099	-2.604765
H	1.584069	-5.696444	-2.026109
H	2.532459	-5.833560	0.268245
H	1.832886	-4.186923	1.994006
H	0.222302	-2.404967	1.416882
H	-0.092733	2.904904	0.248307
C	-4.140207	3.541689	2.594094
H	-4.786696	4.401040	2.794527
H	-4.710129	2.822122	2.000263
H	-3.924792	3.050954	3.549468
C	2.273147	0.937820	-0.818902
C	1.831295	-0.235217	0.017288
C	1.768063	0.238125	1.362145
C	2.181863	1.596158	1.415468
H	2.031396	-1.251599	-0.292471
H	1.639363	-0.381466	2.239365
H	2.131140	2.213422	2.302013
C	2.732304	1.992224	0.164293
H	2.766108	3.031330	-0.147828
O	2.254178	1.047920	-2.033416
C	4.763810	0.145207	0.468037
C	4.549425	-0.219193	1.849502
C	4.641655	1.558143	0.195163
C	4.504146	-1.645719	2.323470
C	5.163022	-2.717749	1.704953
C	3.756615	-1.897482	3.486196
C	5.049047	-4.009578	2.221357
H	5.771754	-2.555952	0.825770
C	3.637003	-3.186793	3.996933
H	3.290268	-1.053874	3.983315
C	4.282543	-4.252113	3.361533
H	5.569410	-4.826954	1.730117
H	3.050586	-3.361207	4.895282
H	4.196885	-5.259859	3.759337
O	4.293273	0.684758	2.680128
C	4.894946	-0.808936	-0.566358
N	4.989178	-1.592148	-1.429162
C	5.181498	2.245378	-1.009043
C	5.698529	3.539348	-0.821138
C	5.188574	1.706248	-2.305494
C	6.223384	4.269666	-1.883811
H	5.693583	3.968540	0.178111
C	5.714105	2.439030	-3.368809
H	4.784421	0.722070	-2.492259
C	6.233252	3.718224	-3.166419
H	6.626129	5.263858	-1.710750
H	5.713747	2.003215	-4.363827
H	6.641714	4.281683	-4.000865
H	4.833519	2.118341	1.105444

L10-RRR-TS3

Zero-pointCorrection= 0.960245 (Hartree/Particle)

ThermalCorrection to Energy= 1.020630

ThermalCorrection to Enthalpy= 1.021574

ThermalCorrection to Gibbs Free Energy= 0.860324

E(solv) = -3426.49725242 A.U.

C	5.997474	1.477463	-0.922525
C	5.711737	1.131379	0.397293
C	4.408094	1.236767	0.869600
C	3.351572	1.671484	0.049030
C	3.641074	2.009128	-1.293510
C	4.969730	1.926646	-1.744480
C	2.709644	2.598283	-2.335886
N	1.618839	1.927111	-2.788875
Pd	3.027057	3.686806	-2.821666
C	1.050202	0.625629	-2.388427
C	0.004990	0.364095	-3.482506
C	-0.524620	1.767913	-3.788867
C	0.731348	2.643104	-3.727837
C	2.091038	-0.490975	-2.197926
p	1.595519	-1.611762	-0.797906
C	0.605463	-2.862288	-1.722015
C	3.131674	-2.400538	-0.184255
C	4.388694	-1.889618	-0.535457
C	5.560657	-2.430912	-0.011209
C	5.489742	-3.499492	0.878394
C	4.242944	-4.010318	1.239650
C	3.052822	-3.478943	0.731580
C	1.145483	-3.918988	-2.495551
C	0.253995	-4.702762	-3.240806
C	-1.116514	-4.445682	-3.274919
C	-1.637670	-3.379435	-2.547368
C	-0.773853	-2.613116	-1.768522
C	1.737438	-4.073974	1.166387
p	1.668152	1.685129	0.818489
Pd	0.534005	-0.382298	0.906842
C	0.817940	3.118563	0.074259
C	1.499846	4.312451	-0.211570
C	0.809735	5.398931	-0.745319

C	-0.563888	5.308749	-0.984233
C	-1.248358	4.126789	-0.696147
C	-0.558090	3.031520	-0.176683
C	2.008169	2.180795	2.558657
C	1.946548	3.509506	2.992939
C	2.193809	3.823333	4.330952
C	2.510950	2.818446	5.244498
C	2.569830	1.488684	4.819881
C	2.309162	1.171432	3.488666
H	7.011662	1.414596	-1.305670
H	6.496642	0.784335	1.062309
H	4.210496	0.986218	1.904283
H	5.178942	2.240907	-2.761281
H	0.505972	0.766174	-1.445746
H	-0.770342	-0.330345	-3.153887
H	0.496010	-0.067269	-4.364081
H	-1.033455	1.832997	-4.753839
H	-1.232624	2.076278	-3.011932
H	0.546290	3.652441	-3.355039
H	1.227984	2.733463	-4.701003
H	2.212375	-1.077446	-3.113349
H	3.054796	-0.056793	-1.954095
H	4.475974	-1.060566	-1.225118
H	6.519690	-2.012724	-0.301532
H	6.395051	-3.934478	1.291722
H	4.184912	-4.844398	1.934114
H	0.656887	-5.524109	-3.828085
H	-1.767276	-5.066373	-3.884170
H	-2.688759	-3.114961	-2.588529
H	1.170888	-4.482156	0.322475
H	1.896260	-4.878567	1.889618
H	1.104174	-3.314377	1.634272
H	2.569928	4.385779	-0.049812
H	1.349648	6.309688	-0.984902
H	-1.099299	6.160132	-1.394810
H	-2.318937	4.050575	-0.858674
H	-1.106443	2.130164	0.060436
H	1.688241	4.298451	2.296417
H	2.131941	4.857201	4.657767
H	2.700320	3.066941	6.284621
H	2.803903	0.698250	5.527306
H	2.317837	0.133314	3.165436
H	-1.179518	-1.786054	-1.204994
C	2.619317	-4.241174	-2.585396
H	2.795958	-4.953741	-3.396141
H	3.227063	-3.353066	-2.782261
H	3.005634	-4.682673	-1.661135
C	-1.892793	0.392627	1.765211
C	-0.806667	0.031963	2.749376
C	-0.542739	-1.344835	2.649979
C	-1.140390	-1.802878	1.428348
H	-0.480906	0.697548	3.538612
H	0.065654	-1.937638	3.321599
H	-1.080776	-2.821061	1.068903
C	-2.123869	-0.838740	0.963482
H	-2.319298	-0.742887	-0.094698
Pd	-2.443588	1.484004	1.657148
C	-4.745262	-0.548477	0.370720
C	-5.373618	0.679223	0.861153
C	-4.055150	-1.354394	1.326523
C	-5.577819	1.833711	-0.079155
C	-4.631274	2.179881	-1.052375
C	-6.703967	2.647583	0.095398
C	-4.826194	3.302393	-1.857792
H	-3.735180	1.582098	-1.167616
C	-6.904931	3.762664	-0.715005
H	-7.407952	2.390466	0.880195
C	-5.966369	4.092125	-1.696464
H	-4.088363	3.557733	-2.614615
H	-7.789551	4.379269	-0.579869
H	-6.121510	4.961833	-2.329559
Pd	-5.735908	0.792392	2.036501
C	-4.526522	-0.796039	-0.997181
N	-4.230263	-1.066864	-2.100191
C	-3.902812	-2.830627	1.325492
C	-3.984433	-3.632362	0.176347
C	-3.589691	-3.453300	2.547878
C	-3.728024	-5.001145	0.246305
H	-4.243706	-3.185582	-0.773895
C	-3.339694	-4.821716	2.618819
H	-3.540340	-2.846034	3.448146
C	-3.397984	-5.602944	1.462325
H	-3.786488	-5.600084	-0.658426
H	-3.104625	-5.278952	3.576300
H	-3.199735	-6.670054	1.510561
H	-4.193413	-0.952142	2.329282

L10-RRR-TS3-second

Zero-pointCorrection= 0.961363 (Hartree/Particle)

ThermalCorrection to Energy= 1.021254
ThermalCorrection to Enthalpy= 1.022198
ThermalCorrection to Gibbs Free Energy= 0.862740
E(solv) = -3426.52029683 A.U.

C	5.813156	-2.548259	-0.258287
C	4.739020	-3.166012	-0.896183
C	3.435388	-2.851464	-0.520491
C	3.169074	-1.911323	0.487777
C	4.260187	-1.305129	1.150365
C	5.566853	-1.645153	0.772498
C	4.196345	-0.433375	2.387734
N	3.767922	0.859492	2.350115
O	4.660365	-0.905595	3.426752
C	3.063841	1.647072	1.318634
C	3.257166	3.082548	1.815179
C	3.101454	2.928155	3.331375
C	3.795792	1.591234	3.633976
C	3.481662	1.406101	-0.142010
p	1.958072	1.422279	-1.218604
C	1.844924	3.200245	-1.671977
C	2.336343	0.447282	-2.719009
C	3.439585	-0.417313	-2.754491
C	3.639147	-1.285532	-3.825830
C	2.732149	-1.294927	-4.882734
C	1.639848	-0.427580	-4.861010
C	1.414936	0.452737	-3.796046
C	2.706354	3.850844	-2.585782
C	2.540156	5.228675	-2.777249
C	1.572154	5.959619	-2.089278
C	0.738270	5.316403	-1.177412
C	0.877942	3.944037	-0.980601
C	0.227426	1.379753	-3.841181
p	1.423999	-1.476392	0.896663
Pd	0.272236	0.440929	0.112222
C	1.383734	-1.743670	2.700368
C	1.964673	-2.880228	3.281686
C	1.970420	-3.031197	4.665839
C	1.408806	-2.045286	5.480631
C	0.838638	-0.906352	4.910179
C	0.826866	-0.755865	3.523546
C	0.415653	-2.779978	0.106728
C	-0.378977	-3.660784	0.849837
C	-1.319955	-4.467037	0.204610
C	-1.466187	-4.414683	-1.181454
C	-0.659776	-3.554026	-1.930357
C	0.263942	-2.728313	-1.293211
H	6.834827	-2.784966	-0.539878
H	4.908464	-3.896011	-1.682164
H	2.613466	-3.349117	-1.017930
H	6.392993	-1.200423	1.317724
H	1.990443	1.413621	1.413098
H	2.536650	3.768194	1.361294
H	4.266725	3.427682	1.558491
H	3.534182	3.756263	3.898491
H	2.037272	2.868384	3.589216
H	3.291885	1.002639	4.405452
H	4.836816	1.717702	3.949498
H	4.204249	2.157434	-0.472879
H	3.950687	0.432829	-0.244426
H	4.159514	-0.429392	-1.946606
H	4.497735	-1.950038	-3.823682
H	2.872216	-1.969421	-5.722493
H	0.935765	-0.428419	-5.688618
H	3.191576	5.737465	-3.483109
H	1.474529	7.026891	-2.265322
H	-0.018285	5.870828	-0.630296
H	0.540786	2.427810	-3.905135
H	-0.398617	1.160289	-4.709694
H	-0.412871	1.281712	-2.959729
H	2.426542	-3.633487	2.650849
H	2.426369	-3.910458	5.110491
H	1.423256	-2.161912	6.560200
H	0.404051	-0.136690	5.541140
H	0.396688	0.133112	3.073263
H	-0.288577	-3.693229	1.930599
H	-1.959253	-5.120140	0.790609
H	-2.234523	-5.003149	-1.670841
H	-0.788768	-3.485928	-3.005795
H	0.836444	-2.013378	-1.878864
H	0.229208	3.428871	-0.281166
C	3.778865	3.136383	-3.373400
H	3.349208	2.505751	-4.158881
H	4.445090	3.861458	-3.849499
H	4.389348	2.478784	-2.747554
C	-2.244355	0.417813	-1.029947
C	-1.721295	1.519073	-0.175031
C	-1.597862	1.045830	1.149122
C	-1.763268	-0.351533	1.156096
H	-1.754303	2.553576	-0.488958
H	-1.415815	1.648765	2.029785

H	-1.650651	-0.969199	2.034334
C	-2.369834	-0.838081	-0.123649
H	-1.821538	-1.670741	-0.559672
O	-2.456049	0.482483	-2.230050
C	-4.732182	-0.051466	0.160876
C	-4.628284	0.651912	1.380391
C	-3.868498	-1.295382	0.081109
C	-5.283232	1.979288	1.628116
C	-5.606947	2.895980	0.616593
C	-5.516731	2.340899	2.964371
C	-6.168479	4.132414	0.937912
H	-5.422984	2.650321	-0.421841
C	-6.086302	3.570663	3.283041
H	-5.235725	1.635477	3.738801
C	-6.415660	4.473160	2.268447
H	-6.412899	4.830930	0.141961
H	-6.272215	3.828224	4.322797
H	-6.858895	5.434900	2.513693
O	-3.910995	0.174082	2.318892
C	-5.528450	0.309584	-0.939316
N	-6.169797	0.573186	-1.882640
C	-4.273712	-2.360175	-0.916312
C	-4.071145	-2.229284	-2.296499
C	-4.829165	-3.550346	-0.431074
C	-4.403596	-3.272673	-3.160892
H	-3.642994	-1.313352	-2.687438
C	-5.167055	-4.593720	-1.294031
H	-4.995272	-3.659335	0.637993
C	-4.948851	-4.459721	-2.666355
H	-4.241949	-3.152935	-4.229081
H	-5.598897	-5.507862	-0.894794
H	-5.210347	-5.268018	-3.344269
H	-3.894780	-1.750885	1.074993

L10-SSS-TS1

Zero-pointCorrection= 0.959923 (Hartree/Particle)

ThermalCorrection to Energy= 1.020308

ThermalCorrection to Enthalpy= 1.021252

ThermalCorrection to Gibbs Free Energy= 0.859197

E(solv) = -3426.50260390 A.U.

C	-4.866461	0.271169	0.133258
C	-4.631275	1.686209	0.025246
C	-4.658548	-0.463913	-1.090844
C	-4.749946	2.624364	1.188253
C	-5.631315	2.439578	2.262013
C	-3.944818	3.774675	1.164484
C	-5.680954	3.370647	3.300132
H	-6.283855	1.576219	2.291090
C	-3.985139	4.696378	2.206467
H	-3.303898	3.930219	0.302590
C	-4.853876	4.494233	3.282511
H	-6.371094	3.215205	4.124545
H	-3.348362	5.576863	2.177408
H	-4.891963	5.213058	4.096567
O	-4.226167	2.155202	-1.069542
C	-5.075650	-0.367090	1.377929
N	-5.237875	-0.899046	2.406102
C	-5.183363	-1.827745	-1.368276
C	-5.282608	-2.857383	-0.419327
C	-5.590380	-2.094301	-2.687349
C	-5.791223	-4.103020	-0.783522
H	-4.960674	-2.695823	0.599136
C	-6.096721	-3.339191	-3.050707
H	-5.514237	-1.304830	-3.431710
C	-6.200126	-4.351140	-2.094337
H	-5.862207	-4.885858	-0.033804
H	-6.413398	-3.517196	-4.074806
H	-6.595535	-5.325209	-2.369459
H	-4.797783	0.203338	-1.936756
C	-1.819204	0.923322	0.094989
C	-1.782030	-0.323221	0.783901
C	-2.301158	-1.368062	-0.150688
H	-1.764353	1.899402	0.559062
H	-1.836037	-0.465406	1.855183
C	-2.730599	-0.624166	-1.399735
H	-2.737142	-1.149161	-2.349666
O	-2.388233	-2.567507	0.047547
C	-2.202079	0.694824	-1.266977
H	-2.128934	1.434824	-2.048643
C	5.949771	-1.975535	-0.429414
C	4.902950	-2.747780	-0.930288
C	3.616302	-2.569477	-0.434426
C	3.325460	-1.616631	0.558701
C	4.387704	-0.825652	1.057488
C	5.686748	-1.040028	0.565340
C	4.361465	0.172927	2.199427
N	3.663414	1.338478	2.119634
O	5.078806	-0.061397	3.174678
C	2.724557	1.823573	1.092295

C	2.469576	3.273399	1.519358
C	2.506504	3.188987	3.048604
C	3.643926	2.196785	3.320353
C	3.200979	1.660117	-0.360202
p	1.754191	1.223421	-1.449281
C	1.257793	2.862699	-2.139246
C	2.437097	0.253701	-2.851557
C	3.765938	-0.190026	-2.860902
C	4.259387	-0.975653	-3.900138
C	3.421460	-1.331877	-4.953547
C	2.093973	-0.904784	-4.949009
C	1.575784	-0.120951	-3.912012
C	1.996806	3.599714	-3.095382
C	1.494832	4.844680	-3.497447
C	0.309426	5.368573	-2.982383
C	-0.406530	4.647439	-2.030181
C	0.072417	3.404819	-1.620501
C	0.126733	0.292226	-3.954385
p	1.544618	-1.457289	1.045562
Pd	0.176078	0.051293	-0.123989
C	1.617747	-1.128620	2.844376
C	2.548784	-1.770387	3.674789
C	2.573128	-1.503509	5.042561
C	1.671837	-0.592509	5.595628
C	0.747820	0.058641	4.775606
C	0.722700	-0.207326	3.407256
C	0.904456	-3.162607	0.865277
C	0.920259	-4.104772	1.901458
C	0.417049	-5.387134	1.686358
C	-0.097933	-5.741865	0.438186
C	-0.124402	-4.805488	-0.595038
C	0.361346	-3.518328	-0.378372
H	6.963584	-2.109922	-0.794910
H	5.081398	-3.490286	-1.702054
H	2.818702	-3.192870	-0.819702
H	6.495676	-0.461076	0.998314
H	1.777641	1.279567	1.212575
H	1.525350	3.649763	1.115158
H	3.277426	3.916562	1.147778
H	2.672689	4.155527	3.531695
H	1.561534	2.780118	3.423479
H	3.485099	1.580684	4.207526
H	4.614559	2.694694	3.431199
H	3.701182	2.565950	-0.714114
H	3.915002	0.844358	-0.419805
H	4.442252	0.072210	-2.057664
H	5.293581	-1.305688	-3.877572
H	3.793105	-1.941059	-5.772445
H	1.435717	-1.186412	-5.766741
H	2.054226	5.415866	-4.234064
H	-0.047518	6.335991	-3.323755
H	-1.332061	5.035746	-1.615547
H	-0.374522	-0.139771	-4.825192
H	-0.401956	-0.043477	-3.055792
H	0.011930	1.380826	-4.001448
H	3.277121	-2.452782	3.250002
H	3.309312	-1.994774	5.670927
H	1.695238	-0.383874	6.661280
H	0.046834	0.772314	5.198669
H	0.014530	0.305949	2.766818
H	1.309920	-3.838038	2.877097
H	0.424340	-6.109001	2.498026
H	-0.494450	-6.740185	0.277589
H	-0.555553	-5.062494	-1.557560
H	0.301188	-2.775107	-1.168939
H	-0.479515	2.832999	-0.885924
C	3.286872	3.115811	-3.714658
H	3.784548	3.936856	-4.238922
H	3.984573	2.720268	-2.971339
H	3.111541	2.311127	-4.436081

L10-SSS-TS2

Zero-pointCorrection= 0.960348 (Hartree/Particle)
ThermalCorrection to Energy= 1.020677
ThermalCorrection to Enthalpy= 1.021621
ThermalCorrection to Gibbs Free Energy= 0.861299
E(solv) = -3426.50087204 A.U.

C	4.265344	1.123494	3.674571
C	4.873432	0.048613	3.027450
C	4.113677	-0.793625	2.216487
C	2.739080	-0.585989	2.034446
C	2.132114	0.517456	2.669419
C	2.902311	1.350066	3.492582
C	0.643653	0.797718	2.678178
N	0.180192	1.976756	2.186383
O	-0.083436	0.024908	3.310119
C	0.712173	2.958793	1.222091
C	0.638099	4.261982	2.032922
C	-0.662699	4.096401	2.861819

C	-1.037460	2.593397	2.741180	H	6.864412	-0.418110	-2.606382
C	2.042063	2.670715	0.527828	H	4.944326	-0.449540	-4.166958
p	1.754007	1.553767	-0.943742	H	2.222084	5.458377	-4.100451
C	1.238325	2.841114	-2.168046	H	-0.192364	5.517599	-4.611544
C	3.407683	0.989761	-1.496834	H	-1.729646	3.879780	-3.503527
C	4.498513	0.993362	-0.617963	H	1.508849	-0.044011	-3.284375
C	5.737199	0.484653	-1.003869	H	2.145898	1.324025	-4.185239
C	5.903261	-0.023769	-2.289784	H	2.669169	-0.317832	-4.599412
C	4.820295	-0.038175	-3.168188	H	1.484669	-2.019222	3.857054
C	3.561549	0.443739	-2.793582	H	0.334174	-3.757192	5.183401
C	2.110830	3.791636	-2.757152	H	-0.893814	-5.592421	4.043897
C	1.558952	4.731839	-3.637173	H	-0.940229	-5.690650	1.556621
C	0.195064	4.768623	-3.926484	H	0.229423	-3.962727	0.229978
C	-0.660028	3.854878	-3.318459	H	3.509155	-3.880259	1.751607
C	-0.132817	2.898250	-2.452190	H	5.148607	-5.279052	0.532201
C	2.412947	0.346900	-3.769009	H	5.532442	-4.916481	-1.896644
p	1.757165	-1.634797	0.879217	H	4.261353	-3.148631	-3.100316
Pd	0.383535	-0.320092	-0.488103	H	2.620934	-1.752521	-1.867001
C	0.951205	-2.882545	1.956189	H	-0.806346	2.213473	-1.958543
C	0.977568	-2.831418	3.352473	C	3.602515	3.855402	-2.515030
C	0.315669	-3.809372	4.098529	H	3.869300	3.725964	-1.463427
C	-0.373372	-4.839271	3.459363	H	4.138146	3.075588	-3.066543
C	-0.399147	-4.896568	2.062579	H	3.991341	4.824160	-2.842848
C	0.259621	-3.923848	1.316017	C	-1.871940	-1.374567	0.615926
C	2.987389	-2.692180	0.024234	C	-1.514978	-1.390231	-0.781947
C	3.690847	-3.706425	0.695180	C	-1.654629	-0.075165	-1.305415
C	4.606901	-4.497910	0.006314	C	-2.099270	0.812673	-0.194548
C	4.820241	-4.295170	-1.360953	H	-1.421115	-2.296627	-1.366024
C	4.107655	-3.305983	-2.037108	H	-1.761343	0.185575	-2.350226
C	3.190382	-2.512435	-1.347064	C	-2.331173	-0.092457	0.995523
H	4.845431	1.784207	4.312104	H	-2.174457	0.257505	2.005556
H	5.936875	-0.136219	3.148938	C	-4.773814	-0.456319	-0.281552
H	4.601679	-1.611458	1.700797	C	-4.495496	-1.818188	-0.658143
H	2.418891	2.190041	3.983017	C	-4.343120	-0.111771	1.043166
H	-0.064231	3.025969	0.446334	C	-4.757174	-2.371892	-2.025310
H	0.621598	5.138893	1.378890	C	-5.010042	-3.749925	-2.115208
H	1.517790	4.340979	2.683203	C	-4.689141	-1.618200	-3.206125
H	-0.506122	4.385824	3.904855	C	-5.221927	-4.356003	-3.350065
H	-1.472582	4.714498	2.465740	H	-5.030681	-4.328990	-1.198325
H	-1.870650	2.466879	2.047303	C	-4.888135	-2.230027	-4.444121
H	-1.283469	2.110629	3.686141	H	-4.473442	-0.558362	-3.167486
H	2.433279	3.620851	0.152460	C	-5.161876	-3.596075	-4.521056
H	2.778175	2.261088	1.212160	H	-5.430187	-5.421365	-3.401497
H	4.392962	1.392800	0.382695	H	-4.827953	-1.633976	-5.350529
H	6.564732	0.491394	-0.300415	H	-5.323487	-4.067004	-5.487006

O	-3.965441	-2.580249	0.191454
C	-5.356291	0.483708	-1.162981
N	-5.845259	1.265358	-1.880703
H	-1.713111	-2.201973	1.289677
O	-2.257800	2.030972	-0.228003
C	-4.628703	1.143970	1.776720
C	-4.621670	1.072185	3.182162
C	-4.809708	2.399807	1.175014
C	-4.788989	2.209618	3.965711
H	-4.466332	0.107045	3.658339
C	-4.979037	3.539208	1.961392
H	-4.800428	2.496423	0.099666
C	-4.965939	3.453411	3.354061
H	-4.780371	2.126812	5.048973
H	-5.116149	4.501750	1.476771
H	-5.094907	4.346825	3.959057
H	-4.341474	-0.987734	1.684557

L10-SSS-TS3

Zero-pointCorrection= 0.960320 (Hartree/Particle)
ThermalCorrection to Energy= 1.020704
ThermalCorrection to Enthalpy= 1.021648
ThermalCorrection to Gibbs Free Energy= 0.861643
E(solv) = -3426.49669732 A.U.

C	-4.700507	-3.310268	1.968232
C	-3.483452	-3.627889	2.571320
C	-2.285921	-3.321270	1.925907
C	-2.280964	-2.700352	0.670037
C	-3.509820	-2.367544	0.068980
C	-4.708138	-2.683477	0.722814
C	-3.629641	-1.833100	-1.340378
N	-4.346363	-0.690608	-1.547242
O	-3.269762	-2.541397	-2.280223
C	-4.520850	0.546885	-0.773339
C	-6.013474	0.823958	-0.989750
C	-6.215713	0.432887	-2.477627
C	-4.985904	-0.450733	-2.840908
C	-3.990193	0.586876	0.655670
p	-2.183354	1.077130	0.619377
C	-2.431707	2.894081	0.378926
C	-1.545167	0.813235	2.316253
C	-2.123376	-0.193838	3.103966
C	-1.574665	-0.551135	4.332507
C	-0.433737	0.102504	4.793138
C	0.143127	1.106809	4.019456
C	-0.386723	1.480413	2.778045
C	-2.852281	3.793666	1.387825
C	-3.004237	5.143916	1.041920
C	-2.780629	5.610312	-0.252003
C	-2.417774	4.712811	-1.252872
C	-2.248177	3.368750	-0.929004
C	0.309289	2.579195	2.013619
p	-0.708891	-2.218055	-0.149848
Pd	-0.771812	-0.009054	-0.933872
C	-0.334161	-3.612014	-1.281058
C	-1.251017	-4.637538	-1.537654
C	-0.897950	-5.694396	-2.377689
C	0.365868	-5.733715	-2.966330
C	1.284087	-4.713406	-2.706822
C	0.943331	-3.656172	-1.865230
C	0.595912	-2.413210	1.119915
C	1.029276	-3.688869	1.519670
C	2.043989	-3.816819	2.465420
C	2.651005	-2.677477	3.003218
C	2.243597	-1.407899	2.594349
C	1.218230	-1.282107	1.656966
H	-5.638253	-3.547348	2.462049
H	-3.462807	-4.110049	3.544327
H	-1.343615	-3.547381	2.410575
H	-5.648993	-2.427386	0.244465
H	-3.983488	1.324339	-1.340783
H	-6.268932	1.867372	-0.782287
H	-6.607570	0.186315	-0.325028
H	-7.152152	-0.111336	-2.624956
H	-6.250691	1.320955	-3.115006
H	-4.300172	0.073518	-3.519783
H	-5.238406	-1.407245	-3.299048
H	-4.528270	1.367354	1.201248
H	-4.153513	-0.351035	1.175892
H	-3.001842	-0.723842	2.760244
H	-2.034706	-1.342883	4.916400
H	0.013985	-0.174541	5.742880
H	1.044991	1.604294	4.365286
H	-3.312481	5.843880	1.814364
H	-2.903326	6.665954	-0.475966
H	-2.257656	5.051383	-2.272023
H	0.184117	2.488267	0.935957
H	-0.079569	3.567681	2.288445

H	1.380818	2.565147	2.228118
H	-2.241210	-4.606845	-1.102798
H	-1.617016	-6.485016	-2.572933
H	0.636388	-6.557341	-3.621304
H	2.273999	-4.739717	-3.153312
H	1.674080	-2.879807	-1.654241
H	0.584352	-4.575398	1.078249
H	2.373883	-4.806140	2.769691
H	3.454796	-2.780890	3.726689
H	2.739039	-0.514938	2.961143
H	0.915124	-0.298629	1.325325
H	-1.962497	2.663829	-1.701875
C	-3.147430	3.398038	2.817069
H	-3.691351	2.453578	2.893020
H	-2.231343	3.271225	3.402484
H	-3.748893	4.173315	3.300703
C	0.573414	1.820493	-1.648988
C	0.131887	1.000206	-2.734028
C	0.737129	-0.268894	-2.577965
C	1.836969	-0.141711	-1.547980
H	-0.560002	1.292768	-3.513986
H	0.655400	-1.105891	-3.259867
C	1.710730	1.237409	-0.987970
H	1.839380	1.367209	0.077676
C	4.358591	1.524353	-0.489764
C	5.282413	0.605867	-1.156212
C	3.439504	2.235721	-1.317417
C	5.999663	-0.432822	-0.344895
C	7.354497	-0.671861	-0.607288
C	5.331364	-1.222459	0.599344
C	8.045455	-1.655773	0.096300
H	7.849400	-0.077908	-1.369285
C	6.019014	-2.222033	1.286516
H	4.269394	-1.085634	0.756751
C	7.377939	-2.433145	1.047124
H	9.101011	-1.824121	-0.100832
H	5.485517	-2.842186	2.001889
H	7.914292	-3.207070	1.590464
O	5.502601	0.684462	-2.370508
C	4.162433	1.522077	0.904113
N	3.874517	1.557558	2.041289
H	0.224294	2.826850	-1.466681
O	2.636898	-1.010696	-1.216683
C	2.924111	3.615226	-1.108052
C	2.448234	4.310634	-2.234065
C	2.817190	4.237064	0.145989
C	1.855190	5.565312	-2.113329
H	2.538814	3.846816	-3.213234
C	2.220707	5.492307	0.267507
H	3.194299	3.739397	1.029850
C	1.727673	6.159056	-0.855387
H	1.497356	6.081029	-3.000591
H	2.143632	5.951470	1.249472
H	1.260445	7.134581	-0.753628
H	3.632739	2.015964	-2.366726

L10-RSS-TS1

Zero-pointCorrection= 0.960696 (Hartree/Particle)
ThermalCorrection to Energy= 1.020789
ThermalCorrection to Enthalpy= 1.021733
ThermalCorrection to Gibbs Free Energy= 0.863524
E(solv) = -3426.50544419 A.U.

C	-4.617407	1.079533	-0.533920
C	-4.684625	-0.048334	-1.434610
C	-3.807989	2.193988	-0.972009
C	-5.383841	-1.340585	-1.093372
C	-5.542428	-1.851517	0.202730
C	-5.799557	-2.129992	-2.179023
C	-6.110262	-3.110878	0.403635
H	-5.225815	-1.277279	1.061397
C	-6.383033	-3.377187	-1.977897
H	-5.643425	-1.740130	-3.178694
C	-6.540132	-3.874910	-0.680824
H	-6.217680	-3.491564	1.415752
H	-6.715296	-3.963357	-2.830954
H	-6.993524	-4.849550	-0.519014
O	-4.106190	-0.006854	-2.545069
C	-5.195947	1.075348	0.751317
N	-5.624960	1.084064	1.841354
C	-3.919555	3.581484	-0.461918
C	-4.045530	3.908484	0.898623
C	-3.846215	4.628426	-1.394631
C	-4.118382	5.239296	1.301718
H	-4.090825	3.124110	1.643601
C	-3.924635	5.959249	-0.991809
H	-3.728426	4.388271	-2.448006
C	-4.062116	6.270050	0.360972
H	-4.220221	5.472048	2.358225

H	-3.871053	6.751644	-1.733184
H	-4.119605	7.306761	0.681330
H	-3.652317	2.145227	-2.046739
C	-0.833782	0.688742	-2.293458
C	-0.173313	1.913923	-2.114172
C	-0.896190	2.688512	-1.034984
H	-0.722723	-0.003520	-3.118801
H	0.528173	2.381155	-2.795246
C	-1.900438	1.738577	-0.458928
H	-2.077911	1.774073	0.610130
O	-0.686442	3.852328	-0.724652
C	-1.668997	0.482498	-1.148431
H	-2.280217	-0.392525	-1.022882
C	4.835338	-0.775601	3.628247
C	4.085795	0.399493	3.659862
C	3.512641	0.881822	2.488608
C	3.656595	0.213653	1.258325
C	4.420128	-0.976867	1.227477
C	5.010651	-1.436728	2.417569
C	4.848623	-1.791849	0.021302
N	3.957367	-2.463544	-0.755023
O	6.060783	-1.898637	-0.181864
C	2.483181	-2.468727	-0.738935
C	2.136383	-3.592487	-1.723688
C	3.244547	-3.480360	-2.775205
C	4.490798	-3.161599	-1.941421
C	1.847660	-2.621295	0.650859
p	0.259186	-1.656604	0.722729
C	-0.995106	-2.895673	0.200407
C	-0.042173	-1.253588	2.488902
C	1.036525	-1.238911	3.386064
C	0.874434	-0.829204	4.707002
C	-0.380009	-0.419851	5.152016
C	-1.457309	-0.428817	4.268027
C	-1.322061	-0.839663	2.935476
C	-1.478893	-3.934937	1.029527
C	-2.508276	-4.744712	0.531291
C	-3.049624	-4.559709	-0.739464
C	-2.528926	-3.574201	-1.573839
C	-1.502030	-2.761590	-1.101470
C	-2.557064	-0.863780	2.072595
p	2.726711	0.953544	-0.160090
Pd	0.489349	0.309067	-0.550531
C	3.796017	0.682056	-1.619849
C	5.195067	0.733467	-1.540315
C	5.971796	0.529293	-2.680178
C	5.360856	0.277304	-3.909619
C	3.967774	0.226020	-3.998177
C	3.189654	0.425570	-2.858710
C	2.813554	2.751777	0.177005
C	3.887798	3.553697	-0.234326
C	3.895849	4.914542	0.065655
C	2.836872	5.485995	0.775994
C	1.762282	4.695327	1.180256
C	1.748368	3.334808	0.877607
H	5.296560	-1.164473	4.531108
H	3.945865	0.943799	4.588830
H	2.944289	1.803134	2.528193
H	5.632739	-2.323826	2.365830
H	2.133564	-1.527340	-1.181269
H	1.126020	-3.478746	-2.125067
H	2.187132	-4.560944	-1.210465
H	3.365036	-4.387000	-3.374029
H	3.032779	-2.648468	-3.456200
H	5.208655	-2.517297	-2.452662
H	5.024265	-4.065755	-1.624904
H	1.663925	-3.673254	0.886757
H	2.516185	-2.226393	1.408961
H	2.025069	-1.542641	3.070243
H	1.730681	-0.827473	5.374592
H	-0.522386	-0.092903	6.177969
H	-2.438231	-0.110515	4.610329
H	-2.900599	-5.533337	1.168419
H	-3.878260	-5.174929	-1.072115
H	-2.938746	-3.411425	-2.564592
H	-3.337556	-0.219946	2.485181
H	-2.363672	-0.530942	1.054622
H	-2.967731	-1.876686	1.993077
H	5.682187	0.895705	-0.585244
H	7.054019	0.551065	-2.600507
H	5.968447	0.114361	-4.795022
H	3.487579	0.027288	-4.952059
H	2.107365	0.372812	-2.919670
H	4.709094	3.122863	-0.795578
H	4.728883	5.530831	-0.260379
H	2.843133	6.549192	0.997841
H	0.915648	5.135056	1.696804
H	0.896532	2.728052	1.167689
H	-1.093407	-1.993752	-1.747333
C	-0.968070	-4.209897	2.425368

H	-1.222086	-5.232161	2.720903
H	0.115870	-4.095550	2.508841
H	-1.410146	-3.530181	3.161663

L10-SRR-TS1

Zero-pointCorrection= 0.960432 (Hartree/Particle)
ThermalCorrection to Energy= 1.020742
ThermalCorrection to Enthalpy= 1.021686
ThermalCorrection to Gibbs Free Energy= 0.862259
E(solv) = -3426.50671756 A.U.

C	5.578640	2.957699	0.109552
C	5.196382	2.465836	-1.137736
C	4.378658	1.344027	-1.213928
C	3.901375	0.687257	-0.064181
C	4.279981	1.196822	1.199273
C	5.135512	2.310961	1.257491
C	3.986714	0.625075	2.572171
N	2.721325	0.536504	3.057352
O	4.954073	0.321320	3.275526
C	1.420896	0.836177	2.425802
C	0.450586	0.771908	3.613648
C	1.042167	-0.344592	4.478510
C	2.552083	-0.107279	4.375294
C	1.379001	2.150384	1.630544
p	0.245361	1.973373	0.166328
C	-1.368391	2.430838	0.924724
C	0.729521	3.281411	-1.025370
C	1.998938	3.871676	-0.944068
C	2.430358	4.794647	-1.894375
C	1.589151	5.144096	-2.947304
C	0.326814	4.558225	-3.039794
C	-0.126206	3.623047	-2.102351
C	-1.759694	3.756033	1.235975
C	-2.995297	3.940834	1.870441
C	-3.814754	2.871905	2.228069
C	-3.404600	1.567941	1.966120
C	-2.193272	1.362014	1.308998
C	-1.503955	3.032007	-2.269435
p	2.736395	-0.721221	-0.370054
Pd	0.494377	-0.148191	-0.826143
C	3.031250	-1.919275	0.975011
C	4.303999	-2.129677	1.526715
C	4.477862	-3.064468	2.546060
C	3.388933	-3.805541	3.010420
C	2.123322	-3.611630	2.453271
C	1.941990	-2.669177	1.441766
C	3.451177	-1.516342	-1.869544
C	4.366882	-2.572158	-1.800859
C	4.869397	-3.143982	-2.971280
C	4.470227	-2.664017	-4.218469
C	3.553915	-1.612356	-4.295873
C	3.039873	-1.050431	-3.129204
H	6.227035	3.825085	0.189822
H	5.534120	2.946132	-2.051077
H	4.112703	0.965326	-2.192656
H	5.454928	2.652653	2.236093
H	1.171612	0.007567	1.750516
H	-0.575788	0.586136	3.291628
H	0.466334	1.728208	4.151605
H	0.686319	-0.323207	5.511838
H	0.790060	-1.321810	4.052150
H	3.145413	-1.022931	4.412780
H	2.925644	0.562586	5.158877
H	1.052648	2.982173	2.261510
H	2.369556	2.387812	1.257710
H	2.675226	3.620231	-0.138009
H	3.419979	5.232588	-1.804383
H	1.909278	5.864736	-3.694242
H	-0.331226	4.828648	-3.861471
H	-3.312845	4.955937	2.095901
H	-4.771505	3.055662	2.705452
H	-4.016111	0.720034	2.252055
H	-2.178302	3.318396	-1.455726
H	-1.952318	3.358345	-3.211790
H	-1.468976	1.940220	-2.277171
H	5.151809	-1.543137	1.190383
H	5.461540	-3.200840	2.984299
H	3.527746	-4.533137	3.804987
H	1.274400	-4.194936	2.796668
H	0.960675	-2.541178	1.001552
H	4.676949	-2.962170	-0.838391
H	5.571627	-3.969861	-2.904462
H	4.862217	-3.112751	-5.126500
H	3.228384	-1.239976	-5.262992
H	2.300383	-0.255953	-3.188760
H	-1.876290	0.349291	1.096409
C	-0.929299	4.981513	0.929625
H	-1.311011	5.839275	1.490972
H	0.124253	4.851385	1.192779

H	-0.952699	5.241231	-0.133932
C	-0.659109	-2.614661	-1.073787
C	-0.097411	-1.876326	-2.261077
C	-0.878388	-0.733129	-2.490214
C	-1.696705	-0.531029	-1.327646
H	0.627996	-2.314503	-2.934104
H	-0.850574	-0.084347	-3.356274
H	-2.369183	0.301002	-1.213504
C	-1.745918	-1.741014	-0.536858
H	-1.924589	-1.739765	0.531647
O	-0.278010	-3.698965	-0.646129
C	-4.522932	-1.521359	-0.318720
C	-4.838710	-0.349344	-1.114912
C	-3.651708	-2.484245	-0.924530
C	-5.627520	0.794652	-0.542505
C	-6.635208	0.660400	0.421589
C	-5.317255	2.075994	-1.024127
C	-7.292518	1.788427	0.914714
H	-6.915084	-0.320006	0.786739
C	-5.963564	3.201509	-0.524027
H	-4.560228	2.161631	-1.795979
C	-6.953027	3.061092	0.452817
H	-8.075134	1.669376	1.658847
H	-5.698179	4.188373	-0.893721
H	-7.462699	3.937435	0.844647
O	-4.377046	-0.219103	-2.267069
C	-4.780167	-1.556969	1.068209
N	-4.936980	-1.576971	2.228802
C	-3.474007	-3.894160	-0.518790
C	-3.488920	-4.346596	0.811938
C	-3.237856	-4.832623	-1.538329
C	-3.294597	-5.694627	1.100590
H	-3.651543	-3.648578	1.622945
C	-3.048030	-6.180670	-1.248620
H	-3.206906	-4.491751	-2.570061
C	-3.076580	-6.617821	0.075690
H	-3.312440	-6.025764	2.135345
H	-2.872128	-6.886892	-2.055157
H	-2.924576	-7.668104	0.308651
H	-3.608769	-2.337547	-2.000389
