Regio- and Diastereodivergent [4 + 2] Cycloadditions with Cyclic 2,4-Dienones

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Supporting Information

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1. General methods

NMR data were obtained for ^{1}H at 400 MHz or 600 MHz and for ^{13}C at 100 MHz or 150 MHz. Chemical shifts were given in parts per million (δ) from tetramethylsilane with the solvent resonance as the internal standard in $CDCl_3$ solution. ESI HRMS was recorded on a Waters SYNAPT G2. In each case, enantiomeric ratio was determined by HPLC analysis on chiral column in comparison with authentic racemate, using a Daicel Chiralpak ID Column (250 × 4.6 mm), Chiralpak IE Column (250 × 4.6 mm), Chiralpak OD-H Column (250 × 4.6 mm) or Chiralpak AD-H Column (250 × 4.6 mm). Two enantiomeric peaks of compounds **7** and **9** were assigned by mixing the products catalyzed by **C2** and **C6**, and **C1** and **C3**, respectively. Racemates of compounds **13** were obtained by using racemic **C4** as the catalyst. UV detection was monitored at 220 nm or 254 nm. Optical rotation data were examined in $CHCl_3$ solution at 20 °C. Column chromatography was performed on silica gel (200-300 mesh) eluting with ethyl acetate and petroleum ether. TLC was performed on glass-backed silica plates. UV light and I_2 were used to visualize products. All chemicals were used without purification as commercially available unless otherwise noted. THF, ethyl acetate, petroleum ether, methylene chloride (CH_2Cl_2), toluene, and MeCN were freshly distilled before use. Cyclic 2,4-dienones **1**,[1] α-cyano-α,β-unsaturated ketones **6**,[2] Meldrum's acid-based alkenes **8**[3] and 4-alkylideneisoxazol-5*(4H)*-ones **12**[4] were prepared according to the literature procedures.

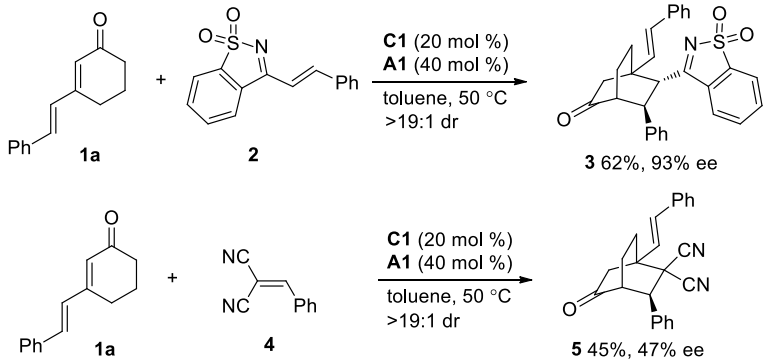
(1) Dieskau, A. P.; Holzwarth, M. S.; Plietker, B. *J. Am. Chem. Soc.* **2012**, *134*, 5048.

(2) Fu, X.; Zhang, S.; Yin, J.; McAllister, T. L.; Jiang, S. A.; Tann, C.-H.; Thiruvengadam, T. K.; Zhang, F. *Tetrahedron Lett.* **2002**, *43*, 573.

(3) Chen, X.; Tan, Y.; Berionni, G.; Ofial, A. R.; Mayr, H. *Chem. - Eur. J.* **2014**, *20*, 11069.

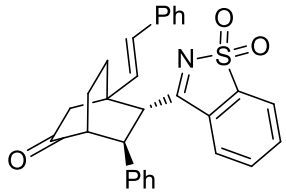
(4) Saikh, F.; Das, J.; Ghosh, S. *Tetrahedron Lett.* **2013**, *54*, 4679.

2. General procedure for amine-catalyzed α',β-[4 + 2] cycloadditions with 2 and 4

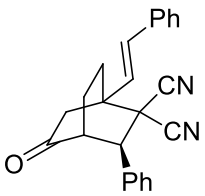


A solution of cyclic 2,4-dienone **1** (0.15 mmol), activated alkene **2** or **4**, salicylic acid **A1** (0.04

mmol) and amine **C1** (0.02 mmol) in dry toluene (1.0 ml) was stirred at 50 °C for 48 h. Purification by flash chromatography on silica gel (EtOAc/petroleum ether) gave the product **3** or **5**.



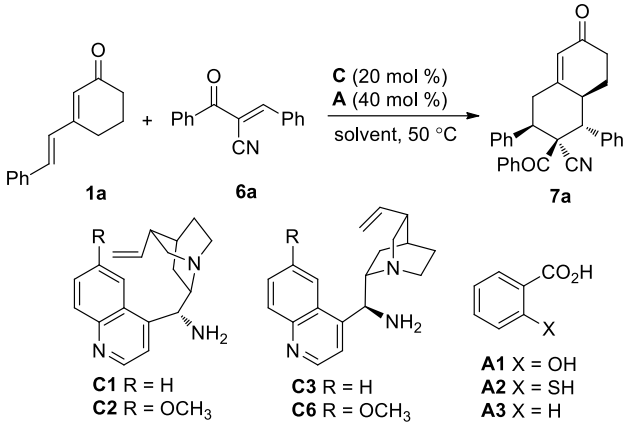
Synthesis of 3: (*E*)-3-styrylbenzo[d]isothiazole 1,1-dioxide (26.9 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (29.7 mg, 0.15 mmol), catalyst **C1** (6.5 mg, 0.02 mmol) and salicyclic acid **A1** (5.5 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 48 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/4) gave product ***(1R,4R,6R)*-5-(1,1-dioxidobenzo[d]isothiazol-3-yl)-6-phenyl-4-((*E*)-styryl) bicyclo[2.2.2]octan-2-one 3**: 29.0 mg, 62% yield, white solid; $[\alpha]_D^{20}$ = +22.2 (*c* = 0.66 in $CHCl_3$); 93% ee, determined by HPLC analysis：[Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 70/30, 1.0 mL/min, λ = 254 nm, t (major) = 10.75 min, t (minor) = 7.78 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.75 (d, *J* = 6.4 Hz, 1H), 7.58-7.51 (m, 3H), 7.37-7.25 (m, 5H), 7.11 (d, *J* = 2.8 Hz, 3H), 6.92-6.89 (m, 2H), 6.29 (d, *J* = 16.4 Hz, 1H), 5.86 (d, *J* = 16.4 Hz, 1H), 4.02 (d, *J* = 8.0 Hz, 1H), 3.89 (d, *J* = 8.4 Hz, 1H), 3.48 (dd, *J* = 19.2 Hz, 2.4 Hz, 1H), 2.64 (s, 1H), 2.28-2.19 (m, 3H), 1,94-1.90 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 212.0, 178.2, 139.5, 139.4, 135.9, 133.5, 133.3, 131.8, 131.8, 130.6, 129.1, 128.3, 127.7, 127.5, 127.4, 125.9, 124.2, 122.6, 49.1, 46.7, 44.1, 43.6, 42.6, 32.5, 18.1; ESI-HRMS: calcd. for $C_{29}H_{25}NNaO_3S^+$ 490.1447, found 490.1444.



Synthesis of 5: 2-benzylidenemalononitrile **4** (15.4 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (29.7 mg, 0.15 mmol), catalyst **C1** (6.5 mg, 0.02 mmol) and salicyclic acid **A1** (5.5 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 48 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/7) gave product ***(1R,3R,4R)*-5-oxo-3-phenyl-1-((*E*)-styryl)bicyclo[2.2.2]octane-2,2-dicarbonitrile 5**, 15.8 mg, 45% yield, white solid; $[\alpha]_D^{20}$ = +9.63 (*c* = 0.49 in $CHCl_3$); 47% ee, determined by HPLC analysis：[Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 7.83 min, t (minor) = 8.64 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.49-7.44 (m, 7H), 7.38-7.32 (m, 3H), 6.65 (d, *J* = 16.4 Hz, 1H), 6.34 (d, *J* = 16.4 Hz, 1H), 3.85 (s, 1H), 3.12 (dd, *J* = 19.2 Hz, 3.6 Hz, 1H), 3.01 (d, *J* = 3.6 Hz, 1H), 2.68-2.61 (m, 1H), 2.58 (d, *J* = 18.8 Hz, 1H), 2.22-2.15 (m, 1H), 2.18 (td, *J* = 12.0 Hz, 2.0 Hz, 1H), 1.90-1.82 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 207.2,

135.3,134.9, 134.0, 129.5, 129.2, 128.8, 127.6, 126.9, 126.7, 116.0, 113.1, 46.8, 46.6, 46.3, 44.0, 43.9, 27.3, 18.4; ESI-HRMS: calcd. for $C_{24}H_{20}N_2NaO^+$ 375.1468, found 375.1467

3. Condition optimizations for amine-catalyzed γ',δ-[4+2] cycloaddition reaction with α-cyano-α,β-unsaturated ketone 6a[a]



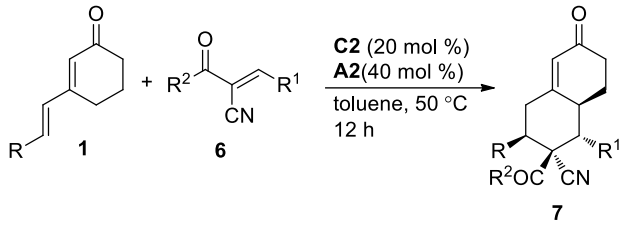
entry	cat	acid	solvent	*t* (h)	yield[b] (%)	ee[c] (%)
1	**C1**	**A1**	toluene	48	52	97
2	**C2**	**A1**	toluene	24	64	98
3	**C3**	**A1**	toluene	48	36	–93
4	**C6**	**A1**	toluene	24	58	–95
5	**C2**	**A3**	toluene	24	38	90
6	**C2**	**A2**	toluene	12	72	98
7	**C2**	**A2**	THF	12	trace	/
8	**C2**	**A2**	$CHCl_3$	12	68	95
9[d]	**C2**	**A2**	toluene	12	75	97
10[d]	**C2**	**A2**	toluene	24	75	97

[a]Unless noted otherwise, reactions were performed with cyclic dienone **1a** (0.075 mmol), **6a** (0.05 mmol), amine **C** (20 mol %) and acid **A** (40 mol %) in solvent (0.5 mL) at 50 °C. [b]Yield of isolated yield. [c]Determined by HPLC analysis on chiral stationary phase; dr >19:1 by ^{1}H-NMR analysis. [d]**6a** (0.1 mmol) was added

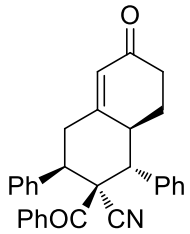
As a result, the optimizations of the conditions for the γ',δ-[4 + 2] cycloaddition of **1a** and **6a** were further screened. First, different primary amines derived from cinchona alkaloids were tested in the presence of acid **A1** in toluene at 50 °C (entries 1–4). Excellent enantioselectivity was observed, and amine **C2** gave a better yield. The combination of **C2** and benzoic acid **A3** gave a low yield (entry 5), while using 2-mercaptobenzoic acid **A2** exhibited higher catalytic efficacy (entry 6). Inferior results were obtained using THF or $CHCl_3$ as the solvent (entries 7 and 8). In addition, it was found that cycloadduct **7a** was obtained in a slightly improved yield with similar

enantioselectivity by using 2.0 equivalent of **6a** (entry 9). However, extending reaction time to 24 h could not improve the yield (entry 10).

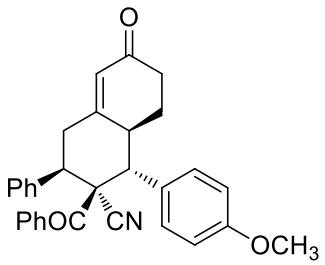
4. General procedure for amine-catalyzed [4 + 2] cycloaddition reactions with α-cyano-α,β-unsaturated ketones



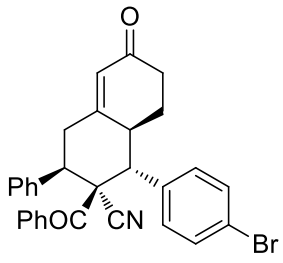
2,4-Dienone **1** (0.20 mmol), α-cyano-α,β-unsaturated ketone **7** (0.10 mmol), 2-mercaptobenzoic acid **A2** (0.04 mmol) and catalyst **C2** (0.02 mmol) were added into a vial equipped with a magnetic stir bar. Toluene (1.0 mL) was added. The mixture was stirred at 50 °C for 12 h. Purification by flash chromatography on silica gel (EtOAc/petroleum ether) gave the product **7**.



Synthesis of 7a: (*E*)-2-benzoyl-3-phenylacrylonitrile (23.3 mg, 0.1 mmol), (E)-3-styrylcyclohex-2-enone (39.6 mg, 0.20 mmol), catalyst **C2** (6.5 mg, 0.02 mmol) and 2-mercaptobenzoic acid **A2** (6.2 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 12 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/8) gave product **(*1R,2S,3R,8aS*)-2-benzoyl-6-oxo-1,3-diphenyl-1,2,3,4,6,7,8,8a-octahydronaphthalene-2-carbonitrile 7a**: 32.3 mg, 75% yield, white solid; $[\alpha]_D^{20}$ = +38.2 (*c* = 0.57 in $CHCl_3$); 97% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 20.10 min, t (minor) = 9.43 min]; ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.57 (d, *J* = 8.4 Hz, 2H), 7.50 (t, *J* = 7.8 Hz, 1H), 7.34 (t, *J* = 7.8 Hz, 2H), 7.30-7.23 (m, 8H), 7.06 (d, *J* = 7.8 Hz, 2H), 6.12 (s, 1H), 4.09 (t, *J* = 4.2 Hz, 1H), 3.67 (d, *J* = 12.6 Hz, 1H), 3.57 (dd, *J* = 16.2 Hz, 5.4 Hz, 1H), 3.33 (t, *J* = 7.6 Hz, 1H), 3.13 (dd, *J* = 16.2 Hz, 4.2 Hz, 1H), 2.50 (d, *J* = 17.2 Hz, 1H), 2.38 (td, *J* = 15.0 Hz, 4.2 Hz, 1H), 1.83-1.80 (m, 1H), 1.70-1.58 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 198.6, 192.1, 161.3, 137.6, 136.7, 136.4, 133.2, 129.2, 128.6, 128.5, 128.4, 128.4, 128.2, 128.0, 127.5, 121.3, 58.8, 48.5, 47.7, 38.9, 37.5, 36.3, 27.9; ESI-HRMS: calcd. for $C_{30}H_{25}NNaO_2^+$ 454.1778, found 454.1777.

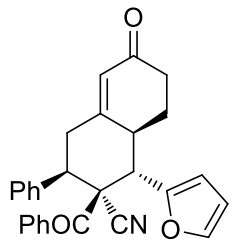


Synthesis of 7b: (*E*)-2-benzoyl-3-(4-methoxyphenyl)acrylonitrile (26.3 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (39.6 mg, 0.20 mmol), catalyst **C2** (6.5 mg, 0.02 mmol) and 2-mercaptobenzoic acid **A2** (6.2 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 12 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/6) gave product ***(1R,2S,3R,8aS)*-2-benzoyl-1-(4-methoxyphenyl)-6-oxo-3-phenyl-1,2,3,4,6,7,8,8a-octahydronaphthalene-2-carb onitrile 7b**: 35.4 mg, 77% yield, white solid; $[\alpha]_D^{20}$ = +42.5 (*c* = 0.74 in $CHCl_3$); 98% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 16.62 min, t (minor) = 8.70 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.60 (d, *J* = 7.6 Hz, 2H), 7.52 (t, *J* = 7.6 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 3H), 7.30-7.21 (m, 4H), 7.05 (d, *J* = 7.2 Hz, 2H), 6.80 (d, *J* = 7.2 Hz, 2H), 6.11 (s, 1H), 4.08 (t, *J* = 4.0 Hz, 1H), 3.75 (s, 3H), 3.64 (d, *J* = 12.4 Hz, 1H), 3.56 (dd, *J* = 16.4 Hz, 6.0 Hz, 1H), 3.29 (t, *J* = 10.8 Hz, 1H), 3.11 (dd, *J* = 16.4 Hz, 4.0 Hz, 1H), 2.52-2.49 (m, 1H), 2.43-2.34 (m, 1H), 1.87-1.83 (m, 1H), 1.70-1.63 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 198.6, 192.3, 161.5, 159.1, 137.6, 136.4, 133.1, 129.2, 128.6, 128.5, 128.4, 128.3, 128.2, 127.4, 121.4, 113.8, 59.0, 55.1, 48.4, 47.0, 39.0, 37.5, 36.3, 27.9; ESI-HRMS: calcd. for $C_{31}H_{27}NNaO_3^+$ 484.1883, found 484.1882.

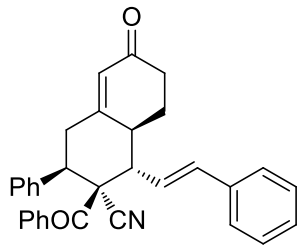


Synthesis of 7c: (*E*)-2-benzoyl-3-(4-bromophenyl)acrylonitrile (31.0 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (39.6 mg, 0.20 mmol), catalyst **C2** (6.5 mg, 0.02 mmol) and 2-mercaptobenzoic acid **A2** (6.2 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 12 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/7) gave product ***(1R,2S,3R,8aS)*-2-benzoyl-1-(4-bromophenyl)-6-oxo-3-phenyl-1,2,3,4,6,7,8,8a-octahydronaphthalene-2-carbonitrile 7c**: 35.6 mg, 70% yield, white solid; $[\alpha]_D^{20}$ = +32.1 (*c* = 0.48 in $CHCl_3$); 98% ee, determined by HPLC analysis: [Daicel chiralpak ID, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 12.42 min, t (minor) = 18.28 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.74 (d, *J* = 8.4 Hz, 2H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.40 (t, *J* = 7.2 Hz, 4H), 7.31-7.20 (m, 5H), 7.01 (d, *J* = 7.6 Hz, 2H), 6.13 (s, 1H), 4.13 (dd, *J* = 6.0 Hz, 2.8 Hz, 1H), 3.65-3.60 (m, 2H), 3.28 (t, *J* = 10.0 Hz, 1H), 3.07 (dd, *J* = 16.8 Hz, 2.8Hz, 1H), 2.53-2.49 (m, 1H), 2.37 (td, *J* = 14.8 Hz, 4.8 Hz, 1H), 1.82-1.78 (m, 1H),

1.72-1.62 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 198.3, 191.2, 160.5, 137.4, 136.0, 135.8, 133.6, 129.2, 128.7, 128.6, 128.6, 128.5, 127.7, 122.1, 121.0, 58.3, 48.4, 46.9, 39.0, 37.3, 36.4, 27.9; ESI-HRMS: calcd. for $C_{30}H_{24}Br^{79}NNaO_2^+$ 532.0888, found 532.0882; $C_{30}H_{24}Br^{81}NNaO_2^+$ 534.0868, found 534.0860.

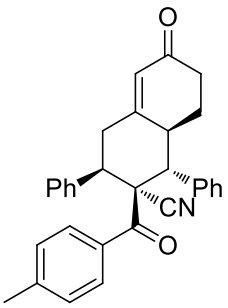


Synthesis of 7d: (*E*)-2-benzoyl-3-(furan-2-yl)acrylonitrile (22.3 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (39.6 mg, 0.20 mmol), catalyst **C2** (6.5 mg, 0.02 mmol) and 2-mercaptobenzoic acid **A2** (6.2 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 12 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/7) gave product ***(1S,2S,3R,8aS)*-2-benzoyl-1-(furan-2-yl)-6-oxo-3-phenyl-1,2,3,4,6,7,8,8a-octahydronaphthalene-2-carbonitrile 7d**: 32.8 mg, 78% yield, white solid; $[\alpha]_D^{20}$ = +28.4 (*c* = 0.60 in $CHCl_3$); 95% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 14.40 min, t (minor) = 7.73 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.91 (d, *J* = 7.6 Hz, 2H), 7.60 (t, *J* = 7.2 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.34 (s, 1H), 7.28-7.25 (m, 1H), 7.20 (t, *J* = 7.6 Hz, 2H), 6.94 (d, *J* = 7.6 Hz, 2H), 6.33 (d, *J* = 3.2 Hz, 1H), 6.27-6.26 (m, 1H), 6.10 (s, 1H), 4.14 (dd, *J* = 6.0 Hz, 2.4 Hz, 1H), 3.81 (d, *J* = 12.0 Hz, 1H), 3.62 (dd, *J* = 16.4 Hz, 6.4 Hz, 1H), 3.40 (bs, 1H), 2.98 (d, *J* = 16.0 Hz, 1H), 2.59-2.55 (m, 1H), 2.48-2.39 (m, 1H), 1.86-1.80 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 198.5, 190.7, 160.1, 151.2, 142.1, 137.2, 135.4, 133.7, 129.0, 128.8, 128.7, 128.6, 128.5, 127.6, 120.4, 110.4, 109.7, 56.9, 47.8, 41.7, 38.6, 37.3, 36.5, 27.6; ESI-HRMS: calcd. for $C_{28}H_{23}NNaO_3^+$ 444.1570, found 444.1571.



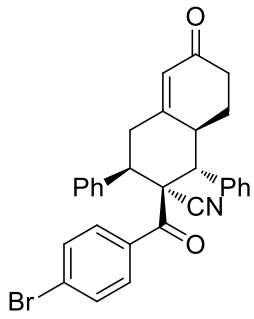
Synthesis of 7e: (2*E*,4*E*)-2-benzoyl-5-phenylpenta-2,4-dienenitrile (25.9 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (39.6 mg, 0.20 mmol), catalyst **C2** (6.5 mg, 0.02 mmol) and 2-mercaptobenzoic acid **A2** (6.2 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 12 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/7) gave product ***(1S,2R,3R,8aS)*-2-benzoyl-6-oxo-3-phenyl-1-((E)-styryl)-1,2,3,4,6,7,8,8a-octahydronaphthalene-2-carbonitrile 7e**: 30.1 mg, 66% yield, white solid; $[\alpha]_D^{20}$ = +47.2 (*c* = 0.52 in $CHCl_3$); 96% ee,

determined by HPLC analysis: [Daicel chiralpak IE, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 11.76 min, t (minor) = 14.61 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.88 (d, *J* = 7.6 Hz, 2H), 7.57 (t, *J* = 7.6 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.39-7.16 (m, 8H), 6.98 (d, *J* = 7.2 Hz, 2H), 6.56 (d, *J* = 15.6 Hz, 1H), 6.08-6.02 (m, 2H), 4.08 (dd, *J* = 6.0 Hz, 3.6 Hz, 1H), 3.49 (dd, *J* = 16.4 Hz, 6.0 Hz, 1H), 3.33 (dd, *J* = 11.2 Hz, 9.2 Hz, 1H), 3.01 (dd, *J* = 16.4 Hz, 2.8 Hz, 1H), 2.96 (t, *J* = 10.8 Hz, 1H), 2.64-2.59 (m, 1H), 2.50-2.40 (m, 2H), 1.88-1.77 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 198.6, 191.3, 160.3, 137.4, 137.2, 136.1, 135.9, 133.5, 129.0, 128.7, 128.6, 128.5, 128.4, 128.1, 127.6, 126.5, 125.3, 120.3, 57.2, 47.4, 45.7, 38.0, 37.5, 36.3, 27.9; ESI-HRMS: calcd. for $C_{32}H_{27}NNaO_2^+$ 480.1934, found 480.1936.

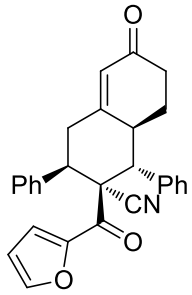


Synthesis of 7f: (*E*)-2-(4-methylbenzoyl)-3-phenylacrylonitrile (24.7 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (39.6 mg, 0.20 mmol), catalyst **C2** (6.5 mg, 0.02 mmol) and 2-mercaptobenzoic acid **A2** (6.2 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 12 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/7) gave product ***(1R,2S,3R,8aS)*-2-(4-methylbenzoyl)-6-oxo-1,3-diphenyl-1,2,3,4,6,7,8,8a-octahydronaphthalene-2-carbonitrile 7f**: 28.9 mg, 65% yield, white solid; $[\alpha]_D^{20}$ = +32.2 (*c* = 0.32 in $CHCl_3$); 96% ee, determined by HPLC analysis: [Daicel chiralpak ID, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 15.43 min, t (minor) = 19.52 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.58 (d, *J* = 8.0 Hz, 2H), 7.33-7.20 (m, 8H), 7.15 (d, *J* = 8.4 Hz, 2H), 7.04 (d, *J* = 7.2 Hz, 2H), 6.12 (s, 1H), 4.10 (dd, *J* = 6.0 Hz, 3.6 Hz, 1H), 3.65 (d, *J* = 12.4 Hz, 1H), 3.61 (dd, *J* = 16.4 Hz, 6.0 Hz, 1H), 3.32 (t, *J* = 11.2 Hz, 1H), 3.10 (dd, *J* = 16.4 Hz, 3.2 Hz, 1H), 2.52-2.48 (m, 1H), 2.43-2.33 (m, 4H), 1.82-1.78 (m, 1H), 1.72-1.61 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 198.7, 191.2, 161.5, 144.3, 137.7, 136.9, 133.7, 130.2, 130.2, 129.2, 129.1, 128.8, 128.5, 128.5, 128.5, 128.5, 128.4, 127.9, 127.4, 121.5, 58.4, 48.5, 47.5, 39.0, 37.5, 36.4, 27.9, 21.6; ESI-HRMS: calcd. for $C_{31}H_{27}NNaO_2^+$ 468.1934, found 468.1932.

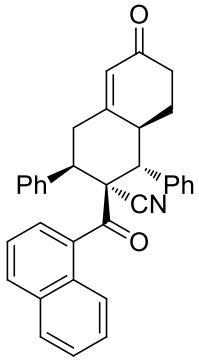
Synthesis of 7g: (*E*)-2-(4-bromobenzoyl)-3-phenylacrylonitrile (31.0 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (39.6 mg, 0.20 mmol), catalyst **C2** (6.5 mg, 0.02 mmol) and 2-mercaptobenzoic acid **A2** (6.2 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 12 h. After completion, purification by flash chromatography on



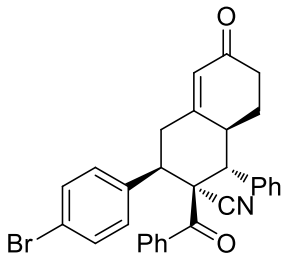
silica gel (EtOAc/petroleum ether = 1/7) gave product ***(1R,2S,3R,8aS)*-2-(4-bromobenzoyl)-6-oxo-1,3-diphenyl-1,2,3,4,6,7,8,8a-octahydronaphthalene-2-carbonitrile 7g**: 36.6 mg, 72% yield, white solid; $[\alpha]_D^{20}$ = +27.1 (*c* = 0.80 in $CHCl_3$); 96% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 38.98 min, t (minor) = 15.14 min]; ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.46 (d, *J* = 9.0 Hz, 2H), 7.37 (d, *J* = 8.4 Hz, 2H), 7.31-7.20 (m, 8H), 7.06 (d, *J* = 7.2 Hz, 2H), 6.11 (s, 1H), 4.03 (t, *J* = 5.4 Hz, 1H), 3.67 (d, *J* = 13.2 Hz, 1H), 3.51 (dd, *J* = 16.2 Hz, 5.4 Hz, 1H), 3.32 (t, *J* = 5.4 Hz, 1H), 3.16 (dd, *J* = 16.2 Hz, 3.6 Hz, 1H), 2.52-2.49 (m, 1H), 2.39 (td, *J* = 16.8 Hz, 5.4 Hz, 1H), 1.85-1.80 (m, 1H), 1.69-1.61 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 198.5, 191.7, 161.1, 137.3, 136.4, 135.0, 131.7, 129.6, 129.1, 128.7, 128.5, 128.5, 128.1, 127.5, 121.2, 58.9, 48.6, 47.9, 38.7, 37.5, 36.0, 27.9; ESI-HRMS: calcd. for $C_{30}H_{24}Br^{79}NNaO_2^+$ 532.0888, found 532.0884; $C_{30}H_{24}Br^{81}NNaO_2^+$ 534.0868, found 534.0863.



Synthesis of 7h: (*E*)-2-(furan-2-carbonyl)-3-phenylacrylonitrile (22.3 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (39.6 mg, 0.20 mmol), catalyst **C2** (6.5 mg, 0.02 mmol) and 2-mercaptobenzoic acid **A2** (6.2 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 12 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/7) gave product ***(1R,2S,3R,8aS)*-2-(furan-2-carbonyl)-6-oxo-1,3-diphenyl-1,2,3,4,6,7,8,8a-octahydronaphthalene-2-carbonitrile 7h**: 26.9 mg, 64% yield, white solid; $[\alpha]_D^{20}$ = +33.6 (*c* = 0.62 in $CHCl_3$); 96% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 10.00 min, t (minor) = 7.92 min]; ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.63 (s, 1H), 7.35 (d, *J* = 3.0 Hz, 1H), 7.27-7.20 (m, 8H), 6.93 (d, *J* = 7.2 Hz, 2H), 6.53 (d, *J* = 2.4 Hz, 1H), 6.11 (s, 1H), 4.13 (dd, *J* = 6.0 Hz, 2.4 Hz, 1H), 3.65-3.60 (m, 2H), 3.30 (t, *J* = 5.4 Hz, 1H), 2.99 (dd, *J* = 15.6 Hz, 2.4 Hz, 1H), 2.49 (dt, *J* = 16.8 Hz, 3.0 Hz, 1H), 2.36 (dt, *J* = 14.4 Hz, 5.4 Hz, 1H), 1.78-1.74 (m, 1H), 1.71-1.66 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 198.7, 161.0, 150.7, 147.2, 137.4, 137.0, 129.0, 128.6, 128.5, 128.5, 127.9, 127.5, 120.5, 120.2, 112.8, 48.0, 45.9, 39.3, 37.4, 36.6, 27.9; ESI-HRMS: calcd. for $C_{28}H_{23}NNaO_3^+$ 444.1570, found 444.1573.

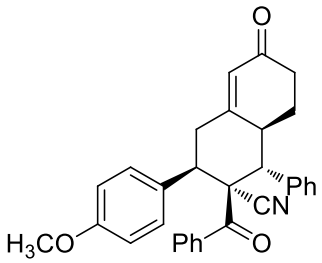


Synthesis of 7i: (*E*)-2-(1-naphthoyl)-3-phenylacrylonitrile (28.3 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (39.6 mg, 0.20 mmol), catalyst **C2** (6.5 mg, 0.02 mmol) and 2-mercaptobenzoic acid **A2** (6.2 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 12 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/7) gave product ***(1R,2S,3R,8aS)*-2-(1-naphthoyl)-6-oxo-1,3-diphenyl-1,2,3,4,6,7,8,8a-octahydronaphthalene-2-carbonitrile 7i**: 32.2 mg, 67% yield, white solid; $[\alpha]_D^{20}$ = +41.1 (*c* = 0.82 in $CHCl_3$); 95% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 6.70 min, t (minor) = 8.97 min]; ^{1}H NMR (600 MHz, $CDCl_3$): *δ* (ppm) 7.92 (d, *J* = 8.4 Hz, 1H), 7.79 (d, *J* = 7.8 Hz, 1H), 7.73 (d, *J* = 7.8 Hz, 1H), 7.44 (t, *J* = 8.4 Hz, 1H), 7.39-7.27 (m, 11H), 7.06 (d, *J* = 7.8 Hz, 1H), 6.56 (d, *J* = 8.4 Hz, 1H), 6.16 (s, 1H), 4.25 (dd, *J* = 6.0 Hz, 1.8 Hz, 1H), 3.71-3.67 (m, 2H), 3.34 (t, *J* = 5.4 Hz, 1H), 3.12 (dd, *J* = 16.8 Hz, 1.8 Hz, 1H), 2.53-2.50 (m, 1H), 2.37 (dd, *J* = 14.4 Hz, 4.8 Hz, 1H), 1.84-1.80 (m, 1H), 1.76-1.61 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): *δ* (ppm) 198.6, 195.1, 161.0, 138.0, 136.7, 135.3, 133.7, 132.6, 129.8, 129.5, 128.7, 128.4, 128.2, 128.1, 127.6, 127.4, 126.4, 124.5, 124.5, 123.4, 121.3, 61.0, 48.8, 48.4, 39.8, 37.4, 37.0, 27.8; ESI-HRMS: calcd. for $C_{34}H_{27}NNaO_2^+$ 504.1934, found 504.1935.

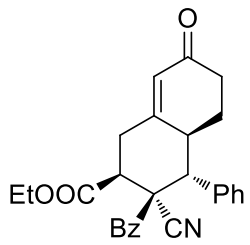


Synthesis of 7j: (*E*)-2-benzoyl-3-phenylacrylonitrile (23.3 mg, 0.1 mmol), (*E*)-3-(4-bromostyryl)cyclohex-2-enone (55.2 mg, 0.20 mmol), catalyst **C2** (6.5 mg, 0.02 mmol) and 2-mercaptobenzoic acid **A2** (6.2 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 12 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/7) gave product ***(1R,2S,3R,8aS)*-2-benzoyl-3-(4-bromophenyl)-6-oxo-1-phenyl-1,2,3,4,6,7,8,8a-octahydronaphthalene-2-carbonitrile 7j**: 36.2 mg, 71% yield, white solid; $[\alpha]_D^{20}$ = +31.2 (*c* = 0.65 in $CHCl_3$); 97% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 21.96 min, t (minor) = 9.68 min]; ^{1}H NMR (400 MHz, $CDCl_3$): *δ* (ppm) 7.60 (d, *J* = 7.6 Hz, 2H), 7.52 (t, *J* = 7.6 Hz, 1H), 7.38-7.35 (m, 5H), 7.28-7.26 (m, 4H), 6.93 (d, *J* = 8.4 Hz, 2H), 6.11 (s, 1H), 4.05 (dd, *J* = 5.6 Hz, 3.6 Hz, 1H), 3.61-3.56 (m, 2H), 3.32 (t, *J* = 3.2 Hz, 1H), 3.07 (dd, *J* = 16.4 Hz, 3.6 Hz, 1H), 2.52-2.48 (m, 1H), 2.38 (td, *J* = 14.4 Hz, 4.8 Hz, 1H), 1.84-1.78 (m, 1H), 1.70-1.58 (m,

1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 198.4, 192.0, 160.6, 136.6, 136.4, 136.1, 133.4, 131.8, 130.7, 128.5, 128.2, 128.2, 128.1, 127.7, 122.7, 121.1, 58.5, 47.9, 47.7, 38.9, 37.4, 36.2, 27.9; ESI-HRMS: calcd. for $C_{30}H_{24}Br^{79}NNaO_2^+$ 532.0888, found 532.0883; $C_{30}H_{24}Br^{81}NNaO_2^+$ 534.0868, found 534.0864.



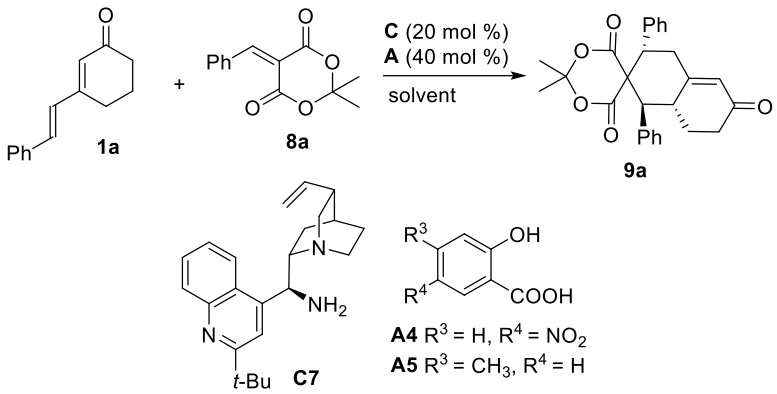
Synthesis of 7k: (*E*)-2-benzoyl-3-phenylacrylonitrile (23.3 mg, 0.1 mmol), (*E*)-3-(4-methoxystyryl)cyclohex-2-enone (45.6 mg, 0.20 mmol), catalyst **C2** (6.5 mg, 0.02 mmol) and 2-mercaptobenzoic acid **A2** (6.2 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 12 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/7) gave product ***(1R,2S,3R,8aS)*-2-benzoyl-3-(4-methoxyphenyl)-6-oxo-1-phenyl-1,2,3,4,6,7,8,8a-octahydronaphthalene-2-carbonitrile 7k**: 29.0 mg, 63% yield, white solid; $[\alpha]_D^{20}$ = +24.1 (*c* = 0.66 in $CHCl_3$); 98% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 33.46 min, t (minor) = 10.74 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.65 (d, *J* = 7.6 Hz, 2H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 3H), 7.26-7.23 (m, 4H), 6.96 (d, *J* = 8.4 Hz, 2H), 6.75 (d, *J* = 8.4 Hz, 2H), 6.11 (s, 1H), 4.08 (dd, *J* = 6.0 Hz, 3.6 Hz, 1H), 3.76 (s, 3H), 3.64-3.57 (m, 2H), 3.31 (t, *J* = 10.8 Hz, 1H), 3.06 (dd, *J* = 16.4 Hz, 3.2 Hz, 1H), 2.51-2.47 (m, 1H), 2.37 (td, *J* = 14.4 Hz, 4.8 Hz, 1H), 1.82-1.78 (m, 1H), 1.71-1.61 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 198.6, 192.0, 161.4, 159.4, 136.9, 136.2, 133.2, 130.3, 129.4, 128.4, 128.3, 127.9, 127.5, 121.4, 113.9, 58.7, 55.2, 47.9, 47.5, 39.1, 37.4, 36.7, 27.9; ESI-HRMS: calcd. for $C_{31}H_{27}NNaO_3^+$ 484.1883, found 484.1884.



Synthesis of 7l: (*E*)-2-benzoyl-3-phenylacrylonitrile (23.3 mg, 0.1 mmol), (*E*)-ethyl 3-(3-oxocyclohex-1-en-1-yl)acrylate (38.8 mg, 0.20 mmol), catalyst **C2** (6.5 mg, 0.02 mmol) and 2-mercaptobenzoic acid **A2** (6.2 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 12 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/6) gave product ***(2S,3R,4R,4aS)*-ethyl 3-benzoyl-3-cyano-7-oxo-4-phenyl-1,2,3,4,4a,5,6,7- octahydronaphthalene-2-carboxylate**: 22.2 mg, 52% yield, white solid; $[\alpha]_D^{20}$ = +33.2 (*c* = 0.52 in $CHCl_3$); 98% ee, determined by HPLC analysis: [Daicel chiralpak AD,

n-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 6.65 min, t (minor) = 5.66 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.50-7.44 (m, 2H), 7.43-3.46 (m, 2H), 7.37-7.23 (m, 6H), 6.03 (s, 1H), 4.19 (qd, *J* = 7.2 Hz, 1.6 Hz, 2H), 3.89 (d, *J* = 11.6 Hz, 1H), 3.47-3.39 (m, 1H), 3.32-3.11 (m, 2H), 2.84 (dd, *J* = 16.4 Hz, 2.4 Hz, 1H), 2.42 (dt, *J* = 16.8 Hz, 3.2 Hz,1H), 2.35-2.26 (m, 1H), 1.87-1.73 (m, 1H), 1.72-1.62 (m, 1H), 1.24 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 198.4, 194.1, 169.6, 167.7, 158.8, 136.2, 136.1, 133.0, 139.0, 128.5, 128.2, 127.9, 127.5, 61.8, 57.0, 49.3, 47.0, 38.8, 37.2, 33.9, 27.2, 13.9; ESI-HRMS: calcd. for $C_{27}H_{25}NNaO_4^+$ 450.1676, found 450.1677.

5. Condition optimizations for amine-catalyzed [4 + 2] cycloaddition reaction with Meldrum's acid-based alkene 8a[a]



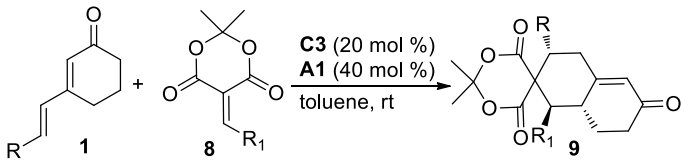
entry	catalyst	acid	solvent	*T* (°C)	*t* (h)	yield (%)[b]	ee (%)[c]	dr[d]
1	**C3**	**A1**	toluene	50	24	73	87	3:1
2	**C3**	**A1**	toluene	35	36	72	92	6:1
3	**C3**	**A1**	toluene	rt	48	70	86	8:1
4	**C6**	**A1**	toluene	rt	48	72	90	5:1
5	**C7**	**A1**	toluene	rt	48	69	80	7:1
6	**C3**	**A1**	MeCN	rt	48	trace	/	/
7	**C3**	**A1**	THF	rt	48	trace	/	/
8	**C3**	**A1**	$CHCl_3$	rt	48	trace	/	/
9	**C3**	**A1**	$PhCF_3$	rt	48	52	86	6:1
10	**C3**	**A1**	PhCl	rt	48	55	80	6:1
11	**C3**	**A1**	mesitylene	rt	48	62	87	8:1
12	**C3**	**A1**	o-xylene	rt	48	66	86	8:1

13	**C3**	**A1**	p-xylene	rt	48	63	85	7:1
14	**C3**	**A2**	toluene	rt	48	69	78	8:1
15	**C3**	**A4**	toluene	rt	48	58	82	6:1
16	**C3**	**A5**	toluene	rt	48	67	85	8:1
17[e]	**C3**	**A1**	**toluene**	**rt**	**48**	**72**	**90**	**10:1**

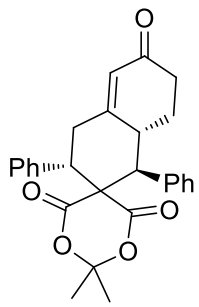
[a]Unless noted otherwise, reactions were performed with **1a** (0.075 mmol), **8a** (0.05 mmol), amine **C** (20 mol %), acid **A** (40 mol %) in toluene (0.5 mL) at room temperature. [b]Yield of the isolated pure diastereomer. [c]Determined by HPLC analysis on a chiral stationary phase. [d]Determined by ^{1}H NMR analysis of the crude product. [e]Toluene (1.0 mL) was used.

As outlined in the above table, the impact of temperature was studied at first. The optimal results were obtained at room temperature (entries 1–3). Then, cinchona-derived catalysts **C6** and **C7** were investigated, which provided inferior results (entries 4 and 5). Solvent effects were also investigated. Tetrahydrofuran and other aromatic solvents didn't give the satisfactory results (entries 6–13). In addition, some acids were also tested, and salicylic acids with various substitutions didn't afford better results (entries 14–16). Finally, when the concentration was diluted to 0.05 M, the desired product was obtained with good yield, enantio- and diastereoselectivity (entry 17).

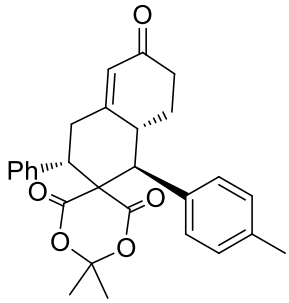
6. General procedure for amine-catalyzed [4 + 2] cycloaddition reactions with Meldrum's acid-based alkenes



2,4-Dienone **1** (0.15 mmol), Meldrum's acid-based alkene **8** (0.10 mmol), salicylic acid **A1** (0.04 mmol) and catalyst **C3** (0.02 mmol) were added into a vial equipped with a magnetic stir bar. Toluene (2.0 mL) was added. The mixture was stirred at room temperature for the indicated time and monitored by TLC. After completion, the resulting crude residue was purified by column chromatography on silica gel eluting with (EtOAc/petroleum) to afford product **9**.

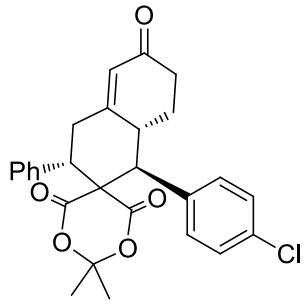


Synthesis of 9a: 5-benzylidene-2,2-dimethyl-1,3-dioxane-4,6-dione (23.2 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (29.7 mg, 0.15 mmol), catalyst **C3** (5.9 mg, 0.02 mmol) and salicylic acid **A1** (4.9 mg, 0.04 mmol) were dissolved in toluene (2.0 mL). Then the mixture was stirred at room temperature for 48 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/10) gave product ***(1'S,3'S,8a'R)*-2,2-dimethyl-1',3'-diphenyl-3',4',8',8a'-tetrahydro-1'H-spiro[[1,3]dioxane-5,2'-naphthalene]-4,6,6'(7'H)-trione 9a**: 10:1 dr, 31.0 mg, 72% yield, white solid; $[\alpha]_D^{20}$ = +28.2 (*c* = 0.41 in $CHCl_3$); 90% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 5.68 min, t (minor) = 7.04 min]; ^{1}H NMR (400 MHz, $CDCl_3$): *δ* (ppm) 7.38-7.27 (m, 7H), 7.21 (d, *J* = 7.2 Hz, 2H), 7.10 (d, *J* = 4.0 Hz, 1H), 6.02 (s, 1H), 4.10 (d, *J* = 14.0 Hz, 1H), 3.90-3.81 (m, 3H), 2.74 (d, *J* = 16.4 Hz, 1H), 2.51-2.45 (m, 2H), 1.96-1.92 (m, 1H), 1.41-1.31 (m, 1H), 0.85 (s, 3H), 0.61 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): *δ* (ppm) 198.6, 169.1, 168.2, 165.6, 137.3, 135.4, 131.6, 129.3, 128.9, 128.7, 128.4, 128.4, 126.0, 106.2, 61.9, 52.1, 47.1, 38.0, 35.7, 32.9, 28.6, 28.5; ESI-HRMS: calcd. for $C_{27}H_{26}NaO_5^+$ 453.1672, found 453.1676.

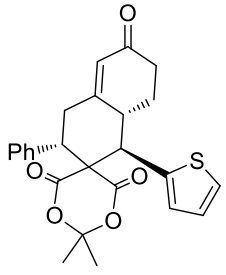


Synthesis of 9b: 2,2-dimethyl-5-(4-methylbenzylidene)-1,3-dioxane-4,6-dione (24.6 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (29.7 mg, 0.15 mmol), amine catalyst **C3** (5.9 mg, 0.02 mmol) and salicylic acid **A1** (4.9 mg, 0.04 mmol) were dissolved in toluene (2.0 mL). Then the mixture was stirred at room temperature for 55 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/10) gave product ***(1'S,3'S,8a'R)*-2,2-dimethyl-3'-phenyl-1'-(p-tolyl)-3',4',8',8a'-tetrahydro-1'H-spiro[[1,3]dioxane-5,2'-naphthalene]-4,6,6'(7'H)-trione 9b**: 8:1 dr, 32.4 mg, 73% yield, white solid; $[\alpha]_D^{20}$ = +21.2 (*c* = 0.61 in $CHCl_3$); 92% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 5.67 min, t (minor) = 11.30 min]; ^{1}H NMR (400 MHz, $CDCl_3$): *δ* (ppm) 7.34-7.20 (m, 7H), 7.07 (d, *J* = 7.2 Hz, 1H), 6.97 (d, *J* = 7.2 Hz, 1H), 6.01 (s, 1H), 4.09 (dd, *J* = 14.0 Hz, 2.0 Hz, 1H), 3.85 (t, *J* = 14.0 Hz, 1H), 3.78-3.77 (m, 2H), 2.73 (d, *J* = 16.0 Hz, 1H), 2.48-2.44 (m, 2H), 2.30 (s, 3H), 1.95-1.91 (m, 1H), 1.38-1.31 (m, 1H), 0.86 (s, 3H), 0.65 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): *δ* (ppm) 198.7, 169.1, 168.3, 165.8, 138.3, 137.4, 132.2, 131.4, 130.0, 129.4, 129.0, 128.9, 128.7, 128.4, 126.0, 106.1, 61.9, 51.7, 47.1,

38.0, 35.7, 32.9, 28.6, 28.5, 28.4, 21.0; ESI-HRMS: calcd. for $C_{28}H_{28}NaO_5^+$ 467.1829, found 467.1825.

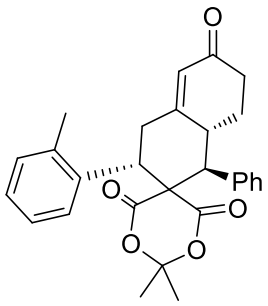


Synthesis of 9c: 5-(4-chlorobenzylidene)-2,2-dimethyl-1,3-dioxane-4,6-dione (26.6 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (29.7 mg, 0.15 mmol), catalyst **C3** (5.9 mg, 0.02 mmol) and salicylic acid **A1** (4.9 mg, 0.04 mmol) were dissolved in toluene (2.0 mL). Then the mixture was stirred at room temperature for 53 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/10) gave product ***(1'S,3'S,8a'R)*-1'-(4-chlorophenyl)-2,2-dimethyl-3'-phenyl-3',4',8',8a'-tetrahydro-1'H-spiro[[1,3]dioxane-5,2'-naphthalene]-4,6,6'(7'H)-trione 9c**: 10:1 dr, 30.2 mg, 65% yield, white solid; $[\alpha]_D^{20}$ = +29.1 (*c* = 0.58 in $CHCl_3$); 92% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 6.51 min, t (minor) = 14.22 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.40-7.27 (m, 6H), 7.20 (d, *J* = 6.4 Hz, 2H), 7.05 (d, *J* = 7.2 Hz, 1H), 6.02 (s, 1H), 4.07 (dd, *J* = 14.0 Hz, 2.4 Hz, 1H), 3.86-3.76 (m, 3H), 2.75 (d, *J* = 12.0 Hz, 1H), 2.51-2.44 (m, 2H), 1.91-1.87 (m, 1H), 1.37-1.33 (m, 1H), 0.85 (s, 3H), 0.74 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 198.3, 168.9, 168.0, 164.9, 137.1, 134.5, 133.9, 132.8, 130.3, 129.5, 129.0, 128.7, 128.5, 126.2, 106.2, 61.7, 51.4, 47.1, 37.8, 35.6, 32.9, 28.9, 28.4, 28.4; ESI-HRMS: calcd. for $C_{27}H_{25}Cl^{35}NaO_5^+$ 487.1288, found 487.1283; $C_{27}H_{25}Cl^{37}NaO_5^+$ 489.1259, found 489.1265.

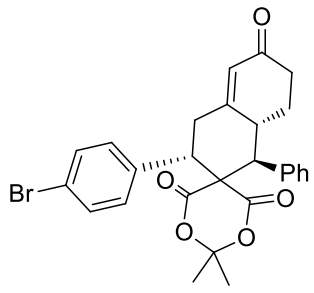


Synthesis of 9d: 2,2-dimethyl-5-(thiophen-2-ylmethylene)-1,3-dioxane-4,6-dione (23.8 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (29.7 mg, 0.15 mmol), catalyst **C3** (5.9 mg, 0.02 mmol) and salicylic acid **A1** (4.9 mg, 0.04 mmol) were dissolved in toluene (2.0 mL). Then the mixture was stirred at room temperature for 57 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/10) gave product ***(1'R,3'S,8a'R)*-2,2-dimethyl-3'-phenyl-1'-(thiophen-2-yl)-3',4',8',8a'-tetrahydro-1'H-spiro[[1,3]dioxane-5,2'-naphthalene]-4,6,6'(7'H)-trione 9d**: 7:1 dr, 27.0 mg, 62% yield, white solid; $[\alpha]_D^{20}$ = +22.8 (*c* = 0.54 in $CHCl_3$); 87% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 6.74 min, t (minor) = 7.78 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm)

7.36-7.30 (m, 3H), 7.23 (d, *J* = 4.8 Hz, 1H), 7.19 (d, *J* = 6.8 Hz, 2H), 6.98-6.96 (m, 2H), 6.00 (s, 1H), 4.12 (d, *J* = 12.4 Hz, 1H), 4.03 (dd, *J* = 13.2 Hz, 2.8 Hz, 1H), 3.81-3.68 (m, 2H), 2.76 (d, *J* = 16.0 Hz, 1H), 2.54-2.40 (m, 2H), 1.99-1.94 (m, 1H), 1.49-1.41 (m, 1H), 0.96 (s, 3H), 0.73 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 198.6, 169.6, 167.9, 164.5, 137.0, 128.9, 128.5, 126.1, 106.3, 62.1, 48.0, 46.5, 37.9, 37.5, 33.0, 29.2, 28.3, 28.1; ESI-HRMS: calcd. for $C_{25}H_{24}NaO_5S^+$ 459.1237, found 459.1232.



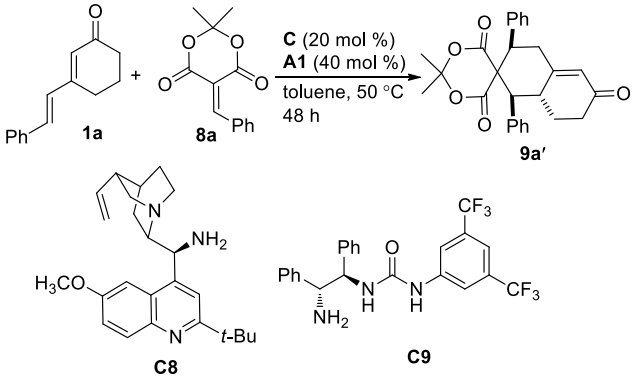
Synthesis of 9e: 5-benzylidene-2,2-dimethyl-1,3-dioxane-4,6-dione (23.2 mg, 0.1 mmol), (*E*)-3-(2-methylstyryl)cyclohex-2-enone (31.8 mg, 0.15 mmol), catalyst **C3** (5.9 mg, 0.02 mmol) and salicylic acid **A1** (4.9 mg, 0.04 mmol) were dissolved in toluene (2.0 mL). Then the mixture was stirred at room temperature for 39 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/10) gave product ***(1'S,3'S,8a'R)*-2,2-dimethyl-1'-phenyl-3'-(o-tolyl)-3',4',8',8a'-tetrahydro-1'H-spiro[[1,3]dioxane-5,2'-naphthalene]-4,6,6'(7'H)-trione 9e**: 8:1 dr, 30.1 mg, 68% yield, white solid; $[\alpha]_D^{20}$ = +18.6 (*c* = 0.32 in $CHCl_3$); 90% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 4.67 min, t (minor) = 7.38 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.37-7.36 (m, 2H), 7.31-7.27 (m, 3H), 7.23 (t, *J* = 2.0 Hz, 1H), 7.20-7.12 (m, 3H), 5.99 (s, 1H), 4.30 (dd, *J* = 13.2 Hz, 2.8 Hz, 1H), 3.96 (t, *J* = 12.8 Hz, 1H), 3.87 (t, *J* = 10.4 Hz, 1H), 3.82-3.74 (m, 1H), 2.65 (dd, *J* = 13.2 Hz, 2.0 Hz, 1H), 2.51-2.48 (m, 2H), 2.32 (s, 3H), 2.04-1.99 (m, 1H), 1.43-1.37 (m, 1H), 0.84 (s, 3H), 0.67 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 198.7, 169.1, 168.0, 165.9, 136.4, 135.8, 135.3, 131.6, 130.9, 129.3, 129.0, 128.8, 128.6, 128.3, 128.0, 126.9, 125.8, 106.0, 60.8, 51.5, 42.4, 38.0, 35.6, 34.8, 28.8, 28.6, 28.0, 19.6; ESI-HRMS: calcd. for $C_{28}H_{28}NaO_5^+$ 467.1829, found 467.1827.



Synthesis of 9f: 5-benzylidene-2,2-dimethyl-1,3-dioxane-4,6-dione (23.2 mg, 0.1 mmol), (*E*)-3-(4-bromostyryl)cyclohex-2-enone (41.4 mg, 0.15 mmol), catalyst **C3** (5.9 mg, 0.02 mmol) and salicylic acid **A1** (4.9 mg, 0.04 mmol) were dissolved in toluene (2.0 mL). Then the mixture was stirred at room temperature for 56 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/10) gave product

***(1'S,3'S,8a'R)*-3'-(4-bromophenyl)-2,2-dimethyl-1'-phenyl-3',4',8',8a'-tetrahydro-1'H-spiro [[1,3]dioxane-5,2'-naphthalene]-4,6,6'(7'H)-trione 9f**: 12:1 dr, 32.5 mg, 64% yield, white solid; $[\alpha]_D^{20}$ = +28.5 (*c* = 0.54 in $CHCl_3$); 91% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 6.86 min, t (minor) = 12.08 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.47 (d, *J* = 8.0 Hz, 2H), 7.40-7.34 (m, 2H), 7.31-7.27 (m, 2H), 7.09 (d, *J* = 8.8 Hz, 3H), 6.01 (s, 1H), 4.07 (dd, *J* = 14.0 Hz, 2.0 Hz, 1H), 3.84-3.78 (m, 3H), 2.70 (d, *J* = 16.0 Hz, 1H), 2.48-2.44 (m, 2H), 1.93-1.90 (m, 1H), 1.38-1.25 (m, 1H), 0.95 (s, 3H), 0.60 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 198.5, 168.9, 168.0, 164.9, 136.3, 135.2, 132.0, 131.6, 130.4, 129.3, 129.0, 128.8, 128.6, 126.2, 122.5, 106.3, 61.6, 52.0, 46.6, 37.9, 35.6, 32.8, 28.8, 28.5, 28.4; ESI-HRMS: calcd. for $C_{27}H_{25}Br^{79}NaO_5^+$ 531.0783, found 531.0779; $C_{27}H_{25}Br^{81}NaO_5^+$ 533.0763, found 533.0771.

7. Attempts of condition optimizations for the diastereomer 9a′[a]

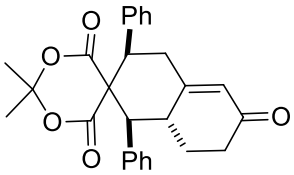


entry	catalyst	concentration	dr (**9a′**:**9a**)[b]	yield (%)[c]	ee (%)[d]
1	**C1**	0.1 M	1:1	47	72
2	**C4**	0.1 M	3:1	66	67
3	**C8**	0.1 M	1:1	45	80
4	**C9**	0.1 M	3:1	50	71
5	**C8**	**0.25 M**	**3:1**	**70**	**71**

[a]Unless noted otherwise, reactions were performed with **1a** (0.075 mmol), **8a** (0.05 mmol), amine **C** (20 mol %), acid **A1** (40 mol %) in toluene at 50 °C for 48 h. [b]Determined by ^{1}H NMR analysis of the crude product. [c]Yield of the isolated pure diastereomer. [d] Determined by HPLC analysis on a chiral stationary phase.

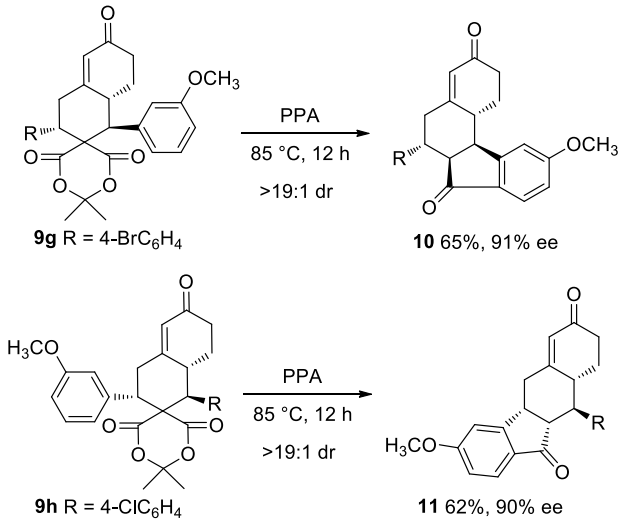
As shown in the above table, it was pleasing to find that the diastereomer **9a′** could be

smoothly obtained as the main product when bifunctional catalyst **C4**, **C9** and cinchona-derived catalyst **C1**, **C8** were employed, and **C8** gave **9a′** with moderate yield and selectivity (entries 1–4). Better results were obtained at a higher concentration (entry 5). In the presence of **C8** and **A1** in toluene at 50 °C, the diastereomer **9a′** was produced in 70% yield, 71% ee and 3:1 dr.

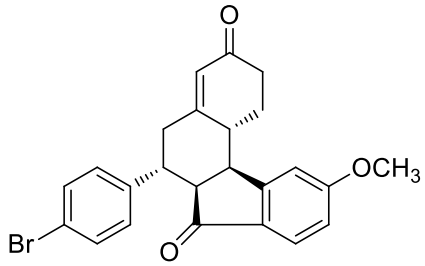


Synthesis of 9a′: 5-benzylidene-2,2-dimethyl-1,3-dioxane-4,6-dione (23.2 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (29.7 mg, 0.15 mmol), catalyst **C8** (7.6 mg, 0.02 mmol) and salicylic acid **A1** (4.9 mg, 0.04 mmol) were dissolved in toluene (0.4 mL). Then the mixture was stirred at room temperature for 48 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/10) gave product ***(1'S,3'R,8a'R)*-2,2-dimethyl-1',3'-diphenyl-3',4',8',8a'-tetrahydro-1'H-spiro[[1,3]dioxane-5,2'-naphthalene]-4,6,6'(7'H)-trione 9a′**: 3:1 dr, 30.1 mg, 70% yield, white solid; $[\alpha]_D^{20}$ = +10.2 (*c* = 0.63 in $CHCl_3$); 71% ee, determined by HPLC analysis: [Daicel chiralpak OD, *n*-hexane/*i*-PrOH = 70/30, 1.0 mL/min, λ = 254 nm, t (major) = 19.00 min, t (minor) = 37.49 min]; ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.39-7.28 (m, 7H), 7.24 (d, *J* = 6.6 Hz, 2H), 7.14 (d, *J* = 7.2 Hz, 1H), 6.02 (s, 1H), 3.81-3.75 (m, 2H), 3.71-3.68 (m, 1H), 3.46 (d, *J* = 12.6 Hz, 1H), 2.66 (d, *J* = 10.8 Hz, 1H), 2.42-2.32 (m, 2H), 1.86-1.82 (m, 1H), 1.50-1.42 (m, 1H), 0.53 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 199.1, 168.2, 165.6, 162.3, 137.8, 136.8, 131.9, 129.4, 129.3, 129.1, 128.6, 128.5, 126.4, 126.4, 106.2, 61.8, 56.0, 50.0, 37.2, 36.8, 36.4, 28.5, 28.1, 27.5; ESI-HRMS: calcd. for $C_{27}H_{26}NaO_5^+$ 453.1672, found 453.1673.

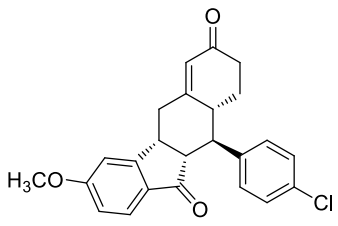
8. Synthetic transformations of [4 + 2] cycloaddition products 9



Cycloaddition product **9g** or **9h** (0.10 mmol) was added into a vial equipped with a magnetic stir bar and PPA (1.0 mL) was added as solvent. The mixture was stirred at 85 °C for 12 h. After completion, water was added at 0 °C, and the resulting solution was extracted with ethyl actetate. The combined organic layer was washed with saturated $NaHCO_3$ solution, dried over anhydrous Na_2SO_4, filtered, concentrated in vacuum and purified by column chromatography on silica gel eluting with (EtOAc/petroleum) to afford product **10** or **11**.



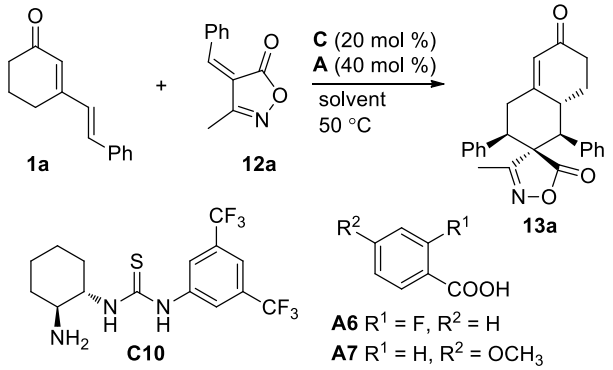
Synthesis of 10: (*1'S,3'S,8a'R*)-3'-(4-bromophenyl)-1'-(3-methoxyphenyl)-2,2-dimethyl-3',4',8',8a'-tetrahydro-1'H-spiro[[1,3]dioxane-5,2'-naphthalene]-4,6,6'(7'*H*)-trione (26.9 mg, 0.05 mmol) was added to PPA (0.5 mL). Then the mixture was stirred at 85 °C for 12 h. After completion, water was added at 0 °C, and the resulting solution was extracted with ethyl actetate. The combined organic layers were washed with saturated $NaHCO_3$ solution, dried over anhydrous Na_2SO_4, filtered, concentrated in vacuum and purified by column chromatography on silica gel eluting with (EtOAc/petroleum = 4:1) to afford product ***(6R,6aS,11bR,11cR)*-6-(4-bromophenyl)-10-methoxy-6,6a,11b,11c-tetrahydro-1*H*-benzo[c]fluorene-3,7(2*H*,5*H*)-dione 10**: 14.2 mg, 65% yield, white solid; $[\alpha]_D^{20}$ = +23.8 (*c* = 0.42 in $CHCl_3$); 91% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 11.82 min, t (minor) = 26.08 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.73 (d, *J* = 8.4 Hz, 1H), 7.48 (d, *J* = 8.4 Hz, 2H), 7.26 (d, *J* = 8.4 Hz, 2H), 7.00-6.97 (m, 2H), 5.96 (s, 1H), 3.92 (s, 3H), 3.39-3.31 (m, 2H), 3.22 (d, *J* = 8.4 Hz, 1H), 2.86-2.80 (m, 1H), 2.67 (dd, *J* = 16.8 Hz, 3.6 Hz, 1H), 2.58 (dt, *J* = 10.0 Hz, 3.6 Hz, 1H), 2.51-2.40 (m, 1H), 2.33-2.20 (m, 2H), 2.05-1.95 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 203.1, 198.4, 164.8, 163.5, 142.9, 131.8, 129.4, 129.2, 126.4, 126.2, 120.7, 115.3, 111.8, 100.0, 55.9, 55.6, 43.7, 41.7, 38.8, 38.2, 37.2, 28.3; ESI-HRMS: calcd. for $C_{24}H_{21}Br^{79}NaO_3^+$ 459.0572, found 459.0564; $C_{24}H_{21}Br^{81}NaO_3^+$ 461.0551, found 461.0549.



Synthesis of 11: (*1'S,3'S,8a'R*)-1'-(4-chlorophenyl)-3'-(3-methoxyphenyl)-2,2-dimethyl-3',4',8',8a'-tetrahydro-1'*H*-spiro[[1,3]dioxane-5,2'-naphthalene]-4,6,6'(7'*H*)-trione (24.7 mg, 0.05 mmol) was

added to PPA (0.5 mL). Then the mixture was stirred at 85 °C for 12 h. After completion, water was added at 0 °C, and the resulting solution was extracted with ethyl actetate. The combined organic layer was washed with saturated $NaHCO_3$ solution, dried over anhydrous Na_2SO_4, filtered, concentrated in vacuo and purified by column chromatography on silica gel eluting with (EtOAc/petroleum = 3:1) to afford product ***(4bR,9aR,10R,10aR)*-10-(4-chlorophenyl)-3-methoxy-9,9a,10,10a-tetrahydro-4b*H*-benzo[b]fluorene-7,11(5*H*,8*H*)- dione 11**: 12.2 mg, 62% yield, white solid; $[\alpha]_D^{20}$ = –23.5 (*c* = 0.51 in $CHCl_3$); 90% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 10.28 min, t (minor) = 21.73 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.66 (d, *J* = 9.2 Hz, 1H), 7.37 (d, *J* = 7.6 Hz, 2H), 7.26 (d, *J* = 8.4 Hz, 2H), 6.95-6.93 (m, 2H), 5.96 (s, 1H), 3.92 (s, 3H), 3.74-3.68 (m, 1H), 3.22 (dd, *J* = 10.8 Hz, 8.0 Hz, 1H), 2.99 (dd, *J* = 16.4 Hz, 4.8 Hz, 1H), 2.81 (t, *J* = 10.4 Hz, 1H), 2.71 (t, *J* = 7.2 Hz, 1H), 2.47-2.40 (m, 2H), 2.30-2.20 (m, 1H), 1.69-1.59 (m, 1H), 1.47-1.39 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 203.2, 198.9, 165.6, 164.4, 158.5, 143.9, 140.5, 132.7, 131.3, 129.5, 128.9, 126.0, 126.0, 116.0, 108.9, 55.7, 54.1, 44.9, 42.2, 37.9, 37.8, 37.1, 28.1; ESI-HRMS: calcd. for $C_{24}H_{21}Cl^{35}NaO_3^+$ 415.1077, found 415.1087; $C_{24}H_{21}Cl^{37}NaO_3^+$ 417.1047, found 417.1049.

9. Condition optimizations for amine-catalyzed [4 + 2] cycloaddition reaction with benzylidene isoxazol-5(*4H*)-one 12a[a]



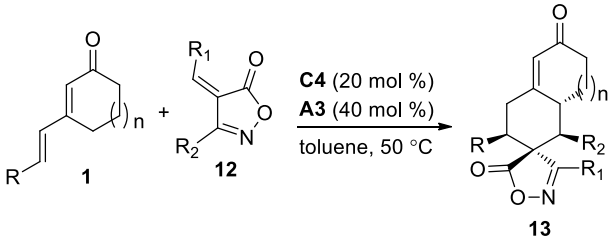
entry	catalyst	acid	solvent	yield (%)[b]	ee (%)[c]
1	**C1**	**A1**	toluene	55	68
2	**C3**	**A1**	toluene	66	-77
3	**C6**	**A1**	toluene	57	-72
4	**C7**	**A1**	toluene	70	-83

5	**C4**	**A1**	toluene	74	88
6	**C4**	**A1**	$CHCl_3$	42	90
7	**C4**	**A1**	*o*-xylene	69	86
8	**C4**	**A1**	$PhCF_3$	67	87
9	**C4**	**A1**	PhCl	72	87
10	**C4**	**A3**	**toluene**	**78**	**90**
11	**C4**	**A6**	toluene	70	86
12	**C4**	**A7**	toluene	63	86
13	**C10**	**A2**	toluene	77	-90

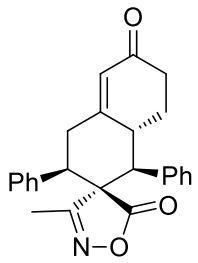
[a]Unless noted otherwise, reactions were performed with **1a** (0.075 mmol), **12a** (0.05 mmol), amine **C** (20 mol %), acid **A** (40 mol %) in solvent (0.5 mL) at 50 °C for 36 h. [b]Yield of isolated product. [c]Determined by HPLC analysis on a chiral stationary phase; dr >19:1 determined by ^{1}H NMR analysis.

First, a variety of primary amine catalysts were tested, and bifunctional catalyst **C4** was proved to be the optimal one (entries 1–5). Then the solvent effect was investigated, and $CHCl_3$ gave a better ee value but with lower yield, while other aromatic solvents gave inferior results (entries 6–9). In addition, some acids were texted, and benzoic acid provided the best results (entries 10–12). Thiourea catalyst **C10** was also employed, affording comparable results (entry 13). As summarized in the above table, the cycloadduct **13a** could be afforded smoothly in the presence of **C4** and **A3**.

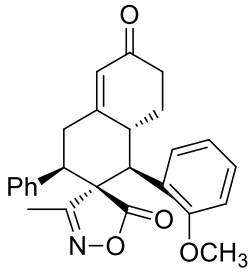
9. General procedure for amine-catalyzed [4 + 2] cycloaddition reactions with alkylidene isoxazol-5(*4H*)-ones



2,4-Dienone **1** (0.15 mmol), alkylidene isoxazol-5(*4H*)-one **12** (0.10 mmol), benzoic acid **A3** (0.04 mmol) and catalyst **C4** (0.02 mmol) were added into a vial equipped with a magnetic stir bar. Toluene (1.0 mL) was added. The mixture was stirred at 50 °C for the indicated time and monitored by TLC. After completion, the resulting crude residue was purified by column chromatography on silica gel eluting with (EtOAc/petroleum) to afford product **13**.

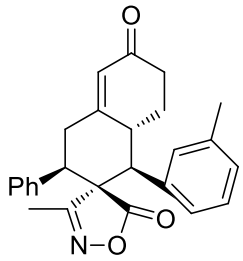


Synthesis of 13a: (*Z*)-4-benzylidene-3-methylisoxazol-5(4*H*)-one (18.7 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (29.7 mg, 0.15 mmol), catalyst **C4** (9.7 mg, 0.02 mmol) and benzoic acid **A3** (4.9 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 36 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/3) gave product ***(1'S,2'S,3'R,8a'R)*-3-methyl-1',3'-diphenyl-3',4',8',8a'-tetrahydro-1'H,5H-spiro[isoxazole-4,2'-naphthalene]-5,6'*(7'H)*-dione 13a**: 30.0 mg, 78% yield, white solid; $[\alpha]_D^{20}$ = +20.1 (*c* = 0.53 in $CHCl_3$); 90% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 5.44 min, t (minor) = 4.78 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.40-7.26 (m, 7H), 7.21-7.20 (m, 2H), 7.02 (d, *J* = 6.8 Hz, 1H), 6.03 (s, 1H), 3.80 (t, *J* = 14.0 Hz, 1H), 3.70-3.66 (m, 1H), 3.27 (dd, *J* = 13.6 Hz, 3.6 Hz, 1H), 2.87 (d, *J* = 12.0 Hz, 1H), 2.60 (dd, *J* = 15.2 Hz, 3.6 Hz, 1H), 2.41-2.28 (m, 2H), 1.69-1.64 (m, 1H), 1.47-1.41 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 199.0, 178.9, 166.7, 161.2, 137.3, 135.8, 130.2, 130.0, 129.3, 128.8, 128.7, 127.1, 126.4, 125.1, 60.3, 54.6, 48.2, 36.7, 35.9, 35.5, 27.5, 12.2; ESI-HRMS: calcd. for $C_{25}H_{23}NNaO_3^+$ 408.1570, found 408.1572.

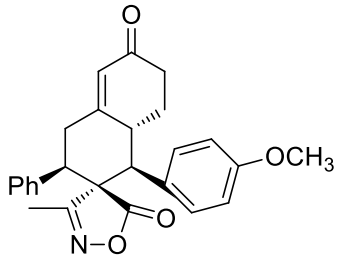


Synthesis of 13b: (*Z*)-4-(2-methoxybenzylidene)-3-methylisoxazol-5(4*H*)-one (21.7 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (29.7 mg, 0.15 mmol), catalyst **C4** (9.7 mg, 0.02 mmol) and benzoic acid **A3** (4.9 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 38 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/3) gave product ***(1'S,2'S,3'R,8a'R)*-1'- (2-methoxyphenyl)-3-methyl-3'-phenyl-3',4',8',8a'-tetrahydro-1'H,5H-spiro[isoxazole-4,2'-naphthalene]-5,6'(7'*H*)-dione 13b**: 29.9 mg, 72% yield, white solid; $[\alpha]_D^{20}$ = +21.1 (*c* = 0.56 in $CHCl_3$); 90% ee, determined by HPLC analysis: [Daicel chiralpak ID, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 15.61 min, t (minor) = 13.71 min]; ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.35-7.24 (m, 5H), 7.21 (d, *J* = 6.6 Hz, 2H), 6.98 (t, *J* = 7.2 Hz, 1H), 6.87 (d, *J* = 7.8 Hz, 1H), 6.02 (s, 1H), 3.83-3.75 (m, 5H), 3.57 (td, *J* = 12.0 Hz, 4.2 Hz, 1H), 3.33 (dd, *J* = 13.8 Hz, 4.2 Hz, 1H), 2.59 (dd, *J* = 15.0 Hz, 4.2 Hz, 1H), 2.38-2.26 (m, 2H), 1.95 (s, 3H), 1.67-1.63 (m, 1H), 1.50-1.44 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 199.2, 179.5, 167.5, 161.9, 156.5, 137.5, 129.3, 129.3, 128.6, 127.2, 126.7, 126.1, 124.6, 122.0, 110.8, 60.3, 55.4, 48.5, 43.4, 36.6, 36.5, 35.8, 26.2, 11.5;

ESI-HRMS: calcd. for $C_{26}H_{25}NNaO_4^+$ 438.1676, found 438.1676.

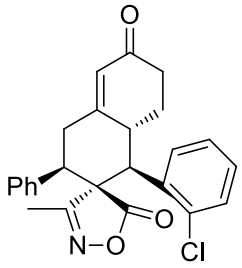


Synthesis of 13c: (*Z*)-3-methyl-4-(3-methylbenzylidene)isoxazol-5(4*H*)-one (20.1 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (29.7 mg, 0.15 mmol), catalyst **C4** (9.7 mg, 0.02 mmol) and benzoic acid **A3** (4.9 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 28 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/3) gave product ***(1'S,2'S,3'R,8a'R)*-3-methyl-3'-phenyl-1'-(*m*-tolyl)-3',4',8',8a'-tetrahydro-1'H,5H-spiro[isoxazole-4,2'-naphthalene]-5,6'(7'*H*)-dione 13c** which contained two rotamers: 31.5 mg, 79% yield, white solid; $[\alpha]_D^{20}$ = +14.3 (*c* = 0.38 in $CHCl_3$); 87% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 5.27 min, t (minor) = 4.65 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.35-7.26 (m, 4H), 7.21-7.10 (m, 4H), 6.82 (s, 1H), 6.02 (s, 1H), 3.80 (t, *J* = 14.0 Hz, 1H), 3.68-3.64 (m, 1H), 3.26 (dd, *J* = 13.6 Hz, 2.8 Hz, 1H), 2.83 (t, *J* = 12.0 Hz, 1H), 2.59 (dd, *J* = 15.2 Hz, 3.6 Hz, 1H), 2.41-2.29 (m, 5H), 1.98-1.96 (m, 3H), 1.71-1.63 (m, 1H), 1.47-1.38 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 199.1, 178.6, 166.8, 161.3, 139.8, 138.5, 137.2, 135.6, 130.7, 130.0, 129.7, 129.5, 129.3, 128.7, 128.6, 127.2, 127.1, 126.3, 125.5, 122.2, 60.3, 54.6, 54.4, 48.2, 36.7, 35.9, 35.5, 27.5, 21.7, 21.3, 12.2; ESI-HRMS: calcd. for $C_{26}H_{25}NNaO_3^+$ 422.1727, found 422.1724.

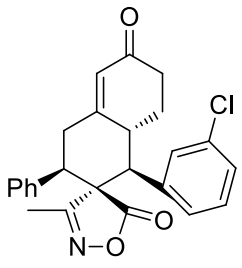


Synthesis of 13d: (*Z*)-4-(2-methoxybenzylidene)-3-methylisoxazol-5(4*H*)-one (21.7 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (29.7 mg, 0.15 mmol), catalyst **C4** (9.7 mg, 0.02 mmol) and benzoic acid **A3** (4.9 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 29 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/2.5) gave product ***(1'S,2'S,3'R,8a'R)*-1'-(4-methoxyphenyl)-3-methyl-3'-phenyl-3',4',8',8a'-tetrahydro-1'H,5H-spiro[isoxazole-4,2'-naphthalene]-5,6'(7'*H*)-dione 13d**: 30.0 mg, 82% yield, white solid; $[\alpha]_D^{20}$ = +24.5 (*c* = 0.40 in $CHCl_3$); 87% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 8.83 min, t (minor) = 5.61 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.34-7.26 (m, 4H), 7.21-7.19 (m, 2H), 6.95-6.91 (m, 2H), 6.80-6.77 (m, 1H), 6.02 (s, 1H),

3.81-3.74 (m, 4H), 3.65-3.60 (m, 1H), 3.25 (dd, *J* = 13.6 Hz, 3.6 Hz, 1H), 2.82 (d, *J* = 12.0 Hz, 1H), 2.59 (dd, *J* = 15.2 Hz, 3.6 Hz, 1H), 2.41-2.28 (m, 2H), 1.97 (s, 3H), 1.72-1.67 (m, 1H), 1.45-1.39 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 199.0, 179.0, 166.9, 161.4, 159.6, 137.4, 131.1, 129.3, 128.7, 127.6, 127.1, 126.3, 126.2, 115.4, 114.1, 60.5, 55.2, 53.8, 48.1, 36.7, 36.1, 35.5, 27.4, 12.2; ESI-HRMS: calcd. for $C_{26}H_{25}NNaO_4^+$ 438.1676, found 438.1678.

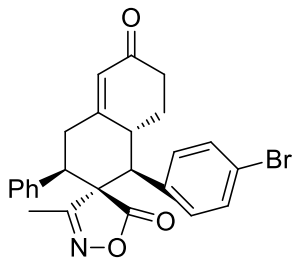


Synthesis of 13e: (*Z*)-4-(2-chlorobenzylidene)-3-methylisoxazol-5(4*H*)-one (22.1 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (29.7 mg, 0.15 mmol), catalyst **C4** (9.7 mg, 0.02 mmol) and benzoic acid **A3** (4.9 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 31 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/3) gave product ***(1'R,2'S,3'R,8a'R)*-1'-(2-chlorophenyl)-3-methyl-3'-phenyl-3',4',8',8a'-tetrahydro-1'H,5H-spiro[isoxazole-4,2'-naphthalene]-5,6'(7'*H*)-dione 13e**: 35.1 mg, 84% yield, white solid; $[\alpha]_D^{20}$ = +24.2 (*c* = 0.19 in $CHCl_3$); 80% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 6.86 min, t (minor) = 5.41 min]; ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.45 (d, *J* = 7.8 Hz, 1H), 7.40 (d, *J* = 7.8 Hz, 1H), 7.34-7.30 (m, 4H), 7.25-7.21 (m, 3H), 6.04 (s, 1H), 3.83-3.80 (m, 2H), 3.63-3.58 (m, 1H), 3.37 (dd, *J* = 13.8 Hz, 3.6 Hz, 1H), 2.63 (dd, *J* = 15.0 Hz, 3.6 Hz, 1H), 2.41 (dt, *J* = 16.8 Hz, 3.6 Hz, 1H), 2.32-2.26 (m, 1H), 2.01 (s, 3H), 1.67-1.58 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 198.8, 179.2, 167.1, 160.6, 137.0, 134.3, 133.9, 130.4, 129.7, 129.3, 128.8, 128.7, 127.2, 127.1, 126.5, 60.0, 48.6, 48.1, 37.1, 36.6, 35.4, 26.0, 12.1; ESI-HRMS: calcd. for $C_{25}H_{22}Cl^{35}NNaO_3^+$ 442.1186, found 442.1177; $C_{25}H_{22}Cl^{37}NNaO_3^+$ 444.1156, found 444.1158.



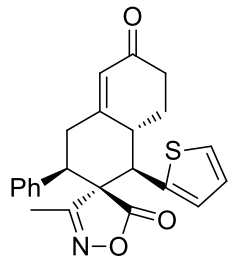
Synthesis of 13f: (*Z*)-4-(3-chlorobenzylidene)-3-methylisoxazol-5(4*H*)-one (22.1 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (29.7 mg, 0.15 mmol), catalyst **C4** (9.7 mg, 0.02 mmol) and benzoic acid **A3** (4.9 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 42 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/3) gave product ***(1'S,2'S,3'R,8a'R)*-1'-(3-chlorophenyl)-3-methyl-3'-phenyl-3',4',8',8a'-tetrahydro-1'H,5H-spiro[isoxazole-4,2'-naphthalene]-5,6'(7'*H*)-dione 13f** which contains two rotamers: 28.5 mg, 68% yield, white solid; $[\alpha]_D^{20}$ = +18.3 (*c* = 0.44 in $CHCl_3$);

88% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 6.00 min, t (minor) = 4.85 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.37-7.29 (m, 5H), 7.25-7.19 (m, 3H), 7.03-6.91 (m, 1H), 6.04 (s, 1H), 3.78 (t, *J* = 14.8 Hz, 1H), 3.65 (bs, 1H), 3.25 (dd, *J* = 14.0 Hz, 4.0 Hz, 1H), 2.86 (dd, *J* = 17.2 Hz, 4.0 Hz, 1H), 2.60 (dd, *J* = 15.2 Hz, 3.2 Hz, 1H), 2.44-2.33 (m, 2H), 1.99-1.97 (m, 3H), 1.72-1.66 (m, 1H), 1.46-1.40 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 198.6, 178.7, 166.5, 166.4, 160.5, 160.5, 138.0, 138.0, 137.0, 137.0, 136.9, 134.5, 131.6, 130.0, 129.9, 129.4, 129.3, 129.0, 128.9, 128.2, 127.1, 126.6, 126.6, 125.5, 123.5, 60.2, 54.1, 54.0, 48.2, 48.2, 36.6, 35.8, 35.7, 35.4, 27.6, 12.2; ESI-HRMS: calcd. for $C_{25}H_{22}Cl^{35}NNaO_3^+$ 442.1186, found 442.1185; $C_{25}H_{22}Cl^{37}NNaO_3^+$ 444.1156, found 444.1165.

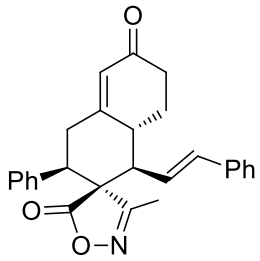


Synthesis of 13g: (*Z*)-4-(4-bromobenzylidene)-3-methylisoxazol-5(4*H*)-one (26.4 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (29.7 mg, 0.15 mmol), catalyst **C4** (9.7 mg, 0.02 mmol) and benzoic acid **A3** (4.9 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 47 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/3) gave product ***(1'S,2'S,3'R,8a'R)*-1'-(4-bromophenyl)-3-methyl-3'-phenyl-3',4',8',8a'-tetrahydro-1'H,5H-spiro[isoxazole-4,2'-naphthalene]-5,6'(7'*H*)-dione 13g**: 29.1 mg, 63% yield, white solid; $[\alpha]_D^{20}$ = +22.5 (*c* = 0.38 in $CHCl_3$); 93% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 6.68 min, t (minor) = 5.64 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.55 (d, *J* = 8.4 Hz, 1H), 7.44 (d, *J* = 8,4 Hz, 1H), 7.38-7.34 (m, 3H), 7.31-7.27 (m, 1H), 7.23-7.21 (m, 2H), 6.94 (d, *J* = 6.8 Hz, 1H), 6.06 (s, 1H), 3.80 (t, *J* = 13.2 Hz, 1H), 3.68-3.64 (m, 1H), 3.28 (dd, *J* = 14.0 Hz, 4.0 Hz, 1H), 2.87 (d, *J* = 4.0 Hz, 1H), 2.63 (dd, *J* = 15.6 Hz, 4.0 Hz, 1H), 2.45-2.31 (m, 2H), 1.99 (s, 3H), 1.72-1.67 (m, 1H), 1.48-1.41 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 198.6, 178.7, 166.5, 160.6, 137.0, 134.9, 133.4, 132.0, 131.5, 129.4, 128.8, 127.0, 126.9, 126.5, 122.9, 60.2, 53.9, 48.1, 36.6, 35.8, 35.4, 27.5, 12.2; $C_{25}H_{22}Br^{79}NNaO_3^+$ 486.0681, found 486.0679; $C_{25}H_{22}Br^{81}NNaO_3^+$ 488.0660, found 488.0663.

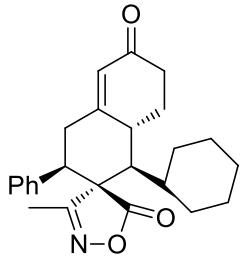
Synthesis of 13h: (*Z*)-3-methyl-4-(thiophen-2-ylmethylene)isoxazol-5(4*H*)-one (19.3 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (29.7 mg, 0.15 mmol), catalyst **C4** (9.7 mg, 0.02 mmol) and



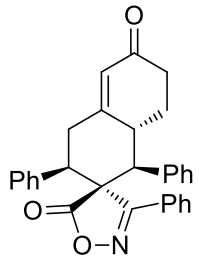
benzoic acid **A3** (4.9 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 30 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/3) gave product ***(1'R,2'S,3'R,8a'R)*-3-methyl-3'-phenyl-1'-(thiophen-2-yl)-3',4',8',8a'-tetrahydro-1'H,5H-spiro [isoxazole-4,2'-naphthalene]-5,6'(7'*H*)-dione 13h**: 33.6 mg, 86% yield, white solid; $[\alpha]_D^{20}$ = +26.2 (*c* = 0.12 in $CHCl_3$); 88% ee, determined by HPLC analysis: [Daicel chiralpak ID, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 5.78 min, t (minor) = 5.04 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.35-7.31 (m, 3H), 7.22-7.19 (m, 3H), 6.99-6.97 (m, 2H), 6.02 (s, 1H), 3.74 (t, *J* = 14.8 Hz, 1H), 3.62-3.59 (m, 1H), 3.22 (dd, *J* = 10.0 Hz, 3.2 Hz, 1H), 3.17 (d, *J* = 11.6 Hz, 1H), 2.58 (dd, *J* = 15.2 Hz, 3.2 Hz, 1H), 2.46-2.31 (m, 2H), 2.04 (s, 3H), 1.89-1.84 (m, 1H), 1.58-1.45 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 198.8, 178.4, 166.6, 160.3, 137.9, 137.0, 129.3, 128.8, 127.7, 127.0, 126.5, 125.7, 125.2, 60.9, 48.8, 47.8, 37.5, 36.7, 35.3, 27.4, 12.2; ESI-HRMS: calcd. for $C_{23}H_{21}NNaO_3S^+$ 414.1134, found 414.1138.



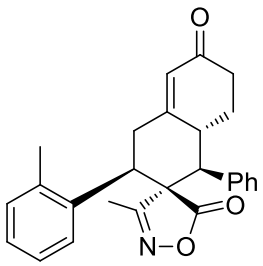
Synthesis of 13i: (*Z*)-3-methyl-4-((*E*)-3-phenylallylidene)isoxazol-5(4*H*)-one (21.3 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (29.7 mg, 0.15 mmol), catalyst **C4** (9.7 mg, 0.02 mmol) and benzoic acid **A3** (4.9 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 28 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/3) gave product ***(1'R,2'R,3'R,8a'R)*-3-methyl-3'-phenyl-1'-((*E*)-styryl)-3',4',8',8a'-tetrahydro-1'H,5H-spiro[isoxazole-4,2'-naphthalene]-5,6'(7'*H*)-dione 13i**: 29.2 mg, 71% yield, white solid; $[\alpha]_D^{20}$ = +23.2 (*c* = 0.19 in $CHCl_3$); 84% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 80/20, 1.0 mL/min, λ = 254 nm, t (major) = 11.57 min, t (minor) = 7.58 min]; ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.34-7.26 (m, 8H), 7.19 (d, *J* = 6.6 Hz, 2H), 6.50 (d, *J* = 15.6 Hz, 1H), 6.01 (s, 1H), 5.77 (dd, *J* = 15.6 Hz, 9.6 Hz, 1H), 3.64 (t, *J* = 14.0 Hz, 3.6 Hz, 1H), 3.31 (td, *J* = 10.2 Hz, 4.2 Hz, 1H), 3.18 (dd, *J* = 13.8 Hz, 4.2 Hz, 1H), 2.55 (dd, *J* = 15.0 4.0 Hz, 1H), 2.52-2.47 (m, 2H), 2.43-2.37 (m, 1H), 2.27-2.23 (m, 1H), 2.01 (s, 3H), 1.63-1.56 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 198.9, 178.3, 167.1, 160.7, 137.3, 136.0, 135.2, 129.4, 128.8, 128.7, 128.6, 127.0, 126.6, 126.5, 123.8, 59.1, 52.1, 47.1, 36.6, 35.5, 34.9, 27.6, 11.9; ESI-HRMS: calcd. for $C_{27}H_{25}NNaO_3^+$ 434.1727, found 434.1726.



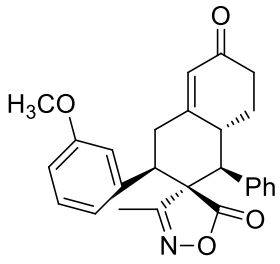
Synthesis of 13j: (*Z*)-4-(cyclohexylmethylene)-3-methylisoxazol-5(4*H*)-one (19.3 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (29.7 mg, 0.15 mmol), catalyst **C4** (9.7 mg, 0.02 mmol) and benzoic acid **A3** (4.9 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 52 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/4) gave product ***(1'R,2'R,3'R,8a'R)*-1'-cyclohexyl-3-methyl-3'-phenyl-3',4',8',8a'-tetrahydro-1'H,5H-spiro[isoxazole-4,2'-naphthalene]-5,6'(7'*H*)-dione 13j**: 20.3 mg, 52% yield, colorless oil; $[\alpha]_D^{20}$ = +21.2 (*c* = 0.32 in $CHCl_3$); 80% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 80/20, 1.0 mL/min, λ = 254 nm, t (major) = 7.83 min, t (minor) = 5.60 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.32-7.30 (m, 3H), 7.14-7.12 (m, 2H), 5.95 (s, 1H), 3.59 (t, *J* = 14.4 Hz, 1H), 3.32-3.27 (m, 1H), 3.04 (dd, *J* = 13.6 Hz, 3.6 Hz, 1H), 2.54-2.41 (m, 4H), 2.00 (s, 3H), 1.79-1.73 (m, 4H), 1.66 (d, *J* = 11.6 Hz, 2H), 1.51-1.46 (m, 2H), 1.35-1.07 (m, 5H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 198.8, 178.9, 168.5, 162.8, 137.4, 129.2, 128.7, 127.0, 126.4, 59.9, 50.9, 48.3, 40.2, 36.6, 35.5, 35.4, 34.0, 29.6, 27.6, 27.5, 26.7, 26.1, 12.1; ESI-HRMS: calcd. for $C_{25}H_{29}NNaO_3^+$ 414.2040, found 414.2045.



Synthesis of 13k: (*Z*)-4-benzylidene-3-phenylisoxazol-5(4*H*)-one (24.9 mg, 0.1 mmol), (*E*)-3-styrylcyclohex-2-enone (29.7 mg, 0.15 mmol), catalyst **C4** (9.7 mg, 0.02 mmol) and benzoic acid **A3** (4.9 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 24 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/6) gave product ***(1'S,2'S,3'R,8a'R)*-1',3,3'-triphenyl-3',4',8',8a'-tetrahydro-1'H,5H-spiro[isoxazole-4,2'-naphthalene]-5,6'(7'*H*)-dione 13k**: 36.7 mg, 82% yield, white solid; $[\alpha]_D^{20}$ = +19.5 (*c* = 0.59 in $CHCl_3$); 84% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 80/20, 1.0 mL/min, λ = 254 nm, t (major) = 11.81 min, t (minor) = 6.07 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.75 (d, *J* = 7.6 Hz, 2H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 2H), 7.41-7.35 (m, 2H), 7.23-7.16 (m, 4H), 7.06-6.95 (m, 3H), 6.47 (d, *J* = 7.2 Hz, 1H), 6.11 (s, 1H), 4.01-3.79 (m, 3H), 3.43 (d, *J* = 12.0 Hz, 1H), 2.66 (d, *J* = 12.0 Hz, 1H), 2.43-2.32 (m, 2H), 1.81-1.74 (m, 1H), 1.52-1.41 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 199.0, 178.5, 165.2, 161.8, 136.9, 135.5, 131.7, 130.6, 129.8, 129.2, 128.9, 128.5, 128.5, 128.4, 128.3, 127.3, 127.1, 126.6, 125.2, 61.4, 54.5, 47.9, 36.6, 35.7, 35.1, 27.4; ESI-HRMS: calcd. for $C_{30}H_{25}NNaO_3^+$ 470.1727, found 470.1723.

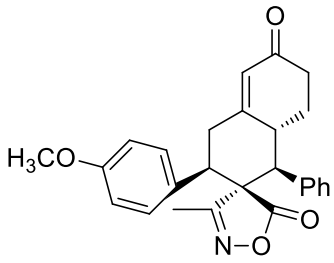


Synthesis of 13l: (*Z*)-4-benzylidene-3-methylisoxazol-5(4*H*)-one (18.7 mg, 0.1 mmol), (*E*)-3-(2-methylstyryl)cyclohex-2-enone (31.8 mg, 0.15 mmol), catalyst **C4** (9.7 mg, 0.02 mmol) and benzoic acid **A3** (4.9 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 24 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/3) gave product ***(1'S,2'S,3'R,8a'R)*-3-methyl-1'-phenyl-3'-(*o*-tolyl)-3',4',8',8a'-tetrahydro-1'H,5H-spiro[isoxazole-4,2'-naphthalene]-5,6'(7'*H*)-dione 13l**: 33.1 mg, 83% yield, white solid; $[\alpha]_D^{20}$ = –20.9 (*c* = 0.58 in $CHCl_3$); 88% ee, determined by HPLC analysis: [Daicel chiralpak ID, *n*-hexane/*i*-PrOH = 80/20, 1.0 mL/min, λ = 254 nm, t (major) = 7.49 min, t (minor) = 6.41 min]; ^{1}H NMR (400 MHz, $CDCl_3$): *δ* (ppm) 7.43-7.27 (m, 4H), 7.21-7.17 (m, 4H), 7.02 (d, *J* = 7.2 Hz, 1H), 6.03 (s, 1H), 3.73-3.56 (m, 3H), 2.93 (d, *J* = 11.6 Hz, 1H), 2.50 (d, *J* = 13.2 Hz, 1H), 2.43-2.34 (m, 5H), 1.82 (s, 3H), 1.71-1.65 (m, 1H), 1.49-1.26 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): *δ* (ppm) 199.1, 179.6, 166.8, 161.3, 136.3, 135.5, 134.3, 131.3, 130.1, 130.0, 128.9, 128.8, 128.0, 127.6, 127.6, 126.3, 125.1, 125.0, 59.2, 55.8, 43.5, 36.9, 36.4, 35.9, 27.8, 19.8, 11.8; ESI-HRMS: calcd. for $C_{26}H_{25}NNaO_3^+$ 422.1727, found 422.1725.

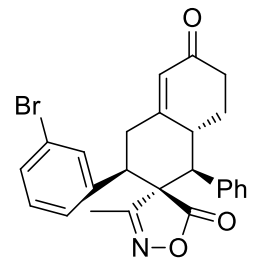


Synthesis of 13m: (*Z*)-4-benzylidene-3-methylisoxazol-5(4*H*)-one (18.7 mg, 0.1 mmol), (*E*)-3-(3-methoxystyryl)cyclohex-2-enone (34.2 mg, 0.15 mmol), catalyst **C4** (9.7 mg, 0.02 mmol) and benzoic acid **A3** (4.9 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 33 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/3) gave product ***(1'S,2'S,3'R,8a'R)*-3'-(3-methoxyphenyl)-3-methyl-1'-phenyl-3',4',8',8a'-tetrahydro-1'H,5H-spiro[isoxazole-4,2'-naphthalene]-5,6'(7'*H*)-dione 13m**: 32.3 mg, 78% yield, white solid; $[\alpha]_D^{20}$ = –15.2 (*c* = 0.12 in $CHCl_3$); 92% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 80/20, 1.0 mL/min, λ = 254 nm, t (major) = 12.41 min, t (minor) = 10.47 min]; ^{1}H NMR (400 MHz, $CDCl_3$): *δ* (ppm) 7.41-7.38 (m, 2H), 7.33-7.21 (m, 3H), 7.02 (d, *J* = 7.2 Hz, 1H), 6.82 (dd, *J* = 8.4 Hz, 3.6 Hz, 1H), 6.78 (d, *J* = 7.6 Hz, 1H), 6.74-6.73 (m, 1H), 6.03 (s, 1H), 3.81-3.74 (m, 4H), 3.67-3.65 (m, 1H), 3.24 (dd, *J* = 14.0 Hz, 4.0 Hz, 1H), 2.86 (d, *J* = 12.0 Hz, 1H), 2.60 (dd, *J* = 15.6 Hz, 4.0 Hz, 1H), 2.41-2.28 (m, 2H), 1.98 (s, 3H), 1.70-1.60 (m, 1H), 1.47-1.39 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): *δ* (ppm) 198.9, 178.9, 166.7, 161.2, 160.0, 138.8, 135.8, 130.4, 130.2, 130.0, 128.8, 126.4,

125.1, 119.2, 113.6, 113.2, 60.2, 55.2, 54.6, 48.2, 36.7, 35.9, 35.5, 27.5, 12.2; ESI-HRMS: calcd. for $C_{26}H_{25}NNaO_4^+$ 438.1676, found 438.1677.

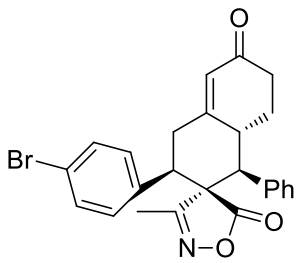


Synthesis of 13n: (*Z*)-4-benzylidene-3-methylisoxazol-5(4*H*)-one (18.7 mg, 0.1 mmol), (*E*)-3-(4-methoxystyryl)cyclohex-2-enone (34.2 mg, 0.15 mmol), catalyst **C4** (9.7 mg, 0.02 mmol) and benzoic acid **A3** (4.9 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 30 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/2.5) gave product ***(1'S,2'S,3'R,8a'R)*-3'-(4-methoxyphenyl)-3-methyl-1'-phenyl-3',4',8',8a'-tetrahydro-1'H,5H-spiro[isoxazole-4,2'-naphthalene]-5,6'(7'*H*)-dione 13n**: 33.2 mg, 80% yield, white solid; $[\alpha]_D^{20}$ = –24.9 (*c* = 0.23 in $CHCl_3$); 87% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 7.31 min, t (minor) = 6.51 min]; ^{1}H NMR (400 MHz, $CDCl_3$): *δ* (ppm) 7.42-7.38 (m, 2H), 7.33-7.27 (m, 2H), 7.12 (d, *J* = 8.4 Hz, 2H), 7.02 (d, *J* = 6.8 Hz, 1H), 6.83 (d, *J* = 8.4 Hz, 2H), 6.03 (s, 1H), 3.80-3.72 (m, 4H), 3.68-3.64 (m, 1H), 3.23 (dd, *J* = 13.6 Hz, 3.6 Hz, 1H), 2.85 (d, *J* = 12.0 Hz, 1H), 2.57 (dd, *J* = 17.2 Hz, 3.6 Hz, 1H), 2.41-2.28 (m, 2H), 1.98 (s, 3H), 1.68-1.64 (m, 1H), 1.47-1.37 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): *δ* (ppm) 199.0, 179.0, 166.7, 161.4, 159.5, 135.9, 130.2, 130.0, 129.2, 128.8, 128.2, 126.3, 125.1, 114.6, 60.6, 55.2, 54.4, 47.4, 36.7, 35.9, 35.7, 27.5, 12.2; ESI-HRMS: calcd. for $C_{26}H_{25}NNaO_4^+$ 438.1676, found 438.1678.

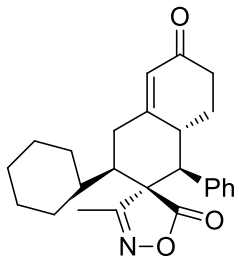


Synthesis of 13o: (*Z*)-4-benzylidene-3-methylisoxazol-5(4*H*)-one (18.7 mg, 0.1 mmol), (*E*)-3-(3-bromostyryl)cyclohex-2-enone (41.4 mg, 0.15 mmol), catalyst **C4** (9.7 mg, 0.02 mmol) and benzoic acid **A3** (4.9 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 32 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/3) gave product ***(1'S,2'S,3'R,8a'R)*-3'-(3-bromophenyl)-3-methyl-1'-phenyl-3',4',8',8a'-tetrahydro-1'H,5H-spiro[isoxazole-4,2'-naphthalene]-5,6'(7'*H*)-dione 13o**: 37.5 mg, 81% yield, white solid; $[\alpha]_D^{20}$ = –20.4 (*c* = 0.64 in $CHCl_3$); 86% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 5.70 min, t (minor) = 4.89 min]; ^{1}H NMR (400 MHz, $CDCl_3$): *δ* (ppm) 7.45-7.27 (m, 6H), 7.23-7.16 (m, 2H), 7.02 (d, *J* = 6.8 Hz, 1H), 6.03 (s, 1H), 3.75 (t, *J* = 13.6 Hz, 1H), 3.68-3.64 (m, 1H), 3.23

(dd, *J* = 13.6 Hz, 3.6 Hz, 1H), 2.85 (d, *J* = 12.0 Hz, 1H), 2.58 (dd, *J* = 15.2 Hz, 3.6 Hz, 1H), 2.41-2.28 (m, 2H), 1.98 (s, 3H), 1.69-1.63 (m, 1H), 1.47-1.38 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 198.8, 178.6, 166.5, 160.5, 139.6, 135.6, 131.9, 131.0, 130.6, 130.2, 130.0, 128.9, 128.8, 126.6, 125.4, 125.1, 123.2, 60.1, 54.5, 47.6, 36.6, 35.8, 35.3, 27.4, 12.2; $C_{25}H_{22}Br^{79}NNaO_3^+$ 486.0681, found 486.0684; $C_{25}H_{22}Br^{81}NNaO_3^+$ 488.0660, found 488.0661.

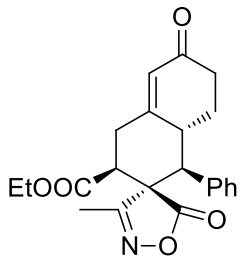


Synthesis of 13p: (*Z*)-4-benzylidene-3-methylisoxazol-5(4*H*)-one (18.7 mg, 0.1 mmol), (*E*)-3-(4-bromostyryl)cyclohex-2-enone (41.4 mg, 0.15 mmol), catalyst **C4** (9.7 mg, 0.02 mmol) and benzoic acid **A3** (4.9 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 40 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/3) gave product ***(1'S,2'S,3'R,8a'R)*-3'-(4-bromophenyl)-3-methyl-1'-phenyl-3',4',8',8a'-tetrahydro-1'H,5H-spiro[isoxazole-4,2'-naphthalene]-5,6'(7'*H*)-dione 13p**: 29.1 mg, 63% yield, white solid; $[\alpha]_D^{20}$ = –24.8 (*c* = 0.17 in $CHCl_3$); 91% ee, determined by HPLC analysis：[Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 7.69 min, t (minor) = 6.38 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.45 (d, *J* = 8.4 Hz, 2H), 7.42-7.26 (m, 4H), 7.08 (d, *J* = 8.4 Hz, 2H), 7.02 (d, *J* = 6.0 Hz, 1H), 6.03 (s, 1H), 3.75 (t, *J* = 14.4 Hz, 1H), 3.71-3.61 (m, 1H), 3.25 (d, *J* = 11.2 Hz, 1H), 2.85 (d, *J* = 11.6 Hz, 1H), 2.57 (dd, *J* = 17.2 Hz, 2.8 Hz, 1H), 2.41-2.29 (m, 2H), 1.97 (s, 3H), 1.69-1.60 (m, 1H), 1.47-1.40 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 198.8, 178.7, 166.5, 160.6, 136.3, 135.6, 132.5, 130.2, 130.0, 128.9, 128.8, 126.6, 125.1, 122.8, 60.2, 54.5, 47.6, 36.6, 35.8, 35.3, 27.4, 12.2; ESI-HRMS: calcd. for $C_{25}H_{22}Br^{79}NNaO_3^+$ 486.0681, found 486.0683; $C_{25}H_{22}Br^{81}NNaO_3^+$ 488.0660, found 488.0658.

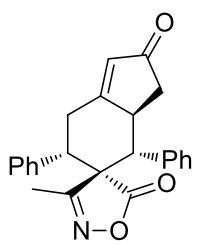


Synthesis of 13q: (*Z*)-4-benzylidene-3-methylisoxazol-5(4*H*)-one (18.7 mg, 0.1 mmol), (*E*)-3-(2-cyclohexylvinyl)cyclohex-2-enone (30.6 mg, 0.15 mmol), catalyst **C4** (9.7 mg, 0.02 mmol) and benzoic acid **A3** (4.9 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 50 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/3) gave product ***(1'S,2'S,3'R,8a'R)*-3'-cyclohexyl-3-methyl-1'-phenyl-3',4',8',8a'-tetrahydro-1'H,5H-spiro[isoxazole-4,2'-naphthalene]-5,6'(7'*H*)-dione 13q**: 21.9 mg,

56% yield, colorless oil; $[\alpha]_D^{20}$ = –20.8 (*c* = 0.61 in $CHCl_3$); 93% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 80/20, 1.0 mL/min, λ = 254 nm, t (major) = 6.92 min, t (minor) = 5.78 min]; ^{1}H NMR (400 MHz, $CDCl_3$): *δ* (ppm) 7.42-7.39 (m, 1H), 7.34-7.26 (m, 3H), 6.98 (d, *J* = 7.2 Hz, 1H), 6.03 (s, 1H), 3.55-3.51 (m, 1H), 3.25 (t, *J* = 14.4 Hz, 1H), 2.72 (d, *J* = 12.0 Hz, 1H), 2.43 (dd, *J* = 14.8 Hz, 3.2Hz, 1H), 2.38-2,24 (m, 2H), 1.99-1.97 (m, 4H), 1.77 (t, *J* = 12.4 Hz, 2H), 1.68-1.58 (m, 3H), 1.44-0.99 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$): *δ* (ppm) 199.0, 179.3, 167.7, 162.5, 135.9, 130.1, 130.0, 128.7, 126.1, 125.1, 58.4, 55.1, 47.8, 39.2, 36.6, 36.1, 33.3, 29.8, 27.6, 27.5, 26.8, 26.2, 25.9, 12.0; ESI-HRMS: calcd. for $C_{25}H_{29}NNaO_3^+$414.2040, found 414.2043.



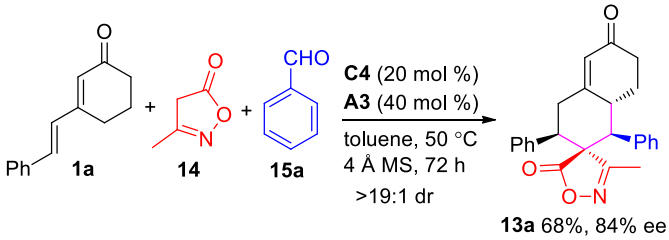
Synthesis of 13r: (*Z*)-4-benzylidene-3-methylisoxazol-5(4*H*)-one (18.7 mg, 0.1 mmol), (*E*)-ethyl 3-(3-oxocyclohex-1-en-1-yl)acrylate (29.1 mg, 0.15 mmol), catalyst **C4** (9.7 mg, 0.02 mmol) and benzoic acid **A3** (4.9 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 36 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/3) gave product ***(1'S,2'R,3'S,8a'R)*-ethyl3-methyl-5,6'-dioxo-1'-phenyl-3',4',6',7',8',8a'-hexahydro-1'H,5H-spiro[isoxazole-4,2'-naphthalene]-3'-carboxylate 13r**: 22.1 mg, 58% yield, colorless oil; $[\alpha]_D^{20}$ = +21.6 (*c* = 0.35 in $CHCl_3$); 87% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 80/40, 1.0 mL/min, λ = 254 nm, t (major) = 5.71 min, t (minor) = 5.02 min]; ^{1}H NMR (400 MHz, $CDCl_3$): *δ* (ppm) 7.42-7.27 (m, 4H), 6.98 (d, *J* = 6.8 Hz, 1H), 6.06 (s, 1H), 4.18 (q, *J* = 7.2 Hz, 2H), 3.62-3.51 (m, 2H), 3.04 (dd, *J* = 14.0 Hz, 4.4Hz, 1H), 2.75 (dd, *J* = 15.6 Hz, 4.4 Hz, 1H), 2.69 (d, *J* = 12.0 Hz, 1H), 2.00 (s, 3H), 1.67-1.60 (m, 1H), 1.41-1.31 (m, 1H), 1.21 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): *δ* (ppm) 198.6, 177.5, 169.5, 166.0, 159.1, 134.7, 130.1, 130.0, 129.0, 128.8, 126.9, 125.2, 62.3, 55.6, 53.6, 46.9, 36.6, 35.6, 31.4, 27.3, 13.9, 11.8; ESI-HRMS: calcd. for $C_{22}H_{23}NNaO_5^+$ 404.1468, found 404.1470.



Synthesis of 13s: (*Z*)-4-benzylidene-3-methylisoxazol-5(4*H*)-one (18.7 mg, 0.1 mmol), (*E*)-3-styrylcyclopent-2-enone (27.6 mg, 0.15 mmol), catalyst **C3** (5.9 mg, 0.02 mmol) and salicyclic acid **A1** (5.5 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 96 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/3) gave product ***(3aS,4R,4'R,6S)*-3'-methyl-4,6-diphenyl-3a,4,6,7-tetrahydro-5'H-spiro[indene-**

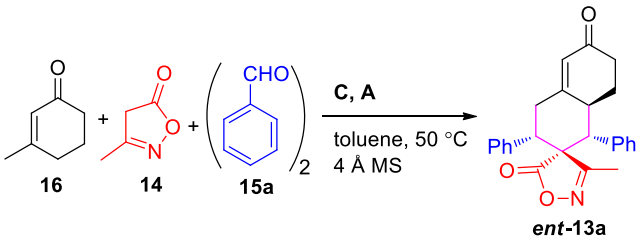
5,4'-isoxazole]-2,5'(3*H*)-dione 13s: 15.2 mg, 41% yield, colorless oil; $[\alpha]_D^{20}$ = –9.3 (*c* = 0.31 in $CHCl_3$); 44% ee, determined by HPLC analysis: [Daicel chiralpak IE, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 17.02 min, t (minor) = 15.16 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.32-7.19 (m, 10H), 6.01 (s, 1H), 4.18-4.13 (m, 1H), 3.77 (t, *J* = 13.6 Hz, 1H), 3.24 (dd, *J* = 13.2 Hz, 3.6 Hz, 1H), 2.98 (dd, *J* = 14.0 Hz, 3.6 Hz, 1H), 2.85 (d, *J* = 12.4 Hz, 1H), 2.37 (dd, *J* = 19.2 Hz, 6.8 Hz, 1H), 1.98 (s, 3H), 1.87 (d, *J* = 19.2 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 207.2, 178.7, 178.7, 166.4, 137.0, 135.9, 129.5, 129.4, 129.0, 129.0, 128.9, 127.5, 127.2, 60.4, 54.8, 49.1, 40.4, 40.1, 31.4, 12.3; ESI-HRMS: calcd. for $C_{24}H_{21}NNaO_3^+$ 394.1414, found 394.1418.

10. General procedure for amine-catalyzed three-component reaction



A mixture of cyclic 2,4-dienone **1a** (0.15 mmol), 3-methylisoxazol-5(*4H*)-one **14** (0.1 mmol), benzaldehyde **15a** (0.15 mmol), benzoic acid **A3** (0.04 mmol), 4 Å molecular sieves (20 mg) and catalyst **C4** (0.02 mmol) in dry toluene (1.0 mL) was stirred at room temperature for 72 h. Purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/3) gave the product **13a** in 68% yield and 84% ee, while providing the product **13a** in 60% yield and 80% ee without 4 Å molecular sieves.

11. Condition optimizations for amine-catalyzed four-component reaction[a]

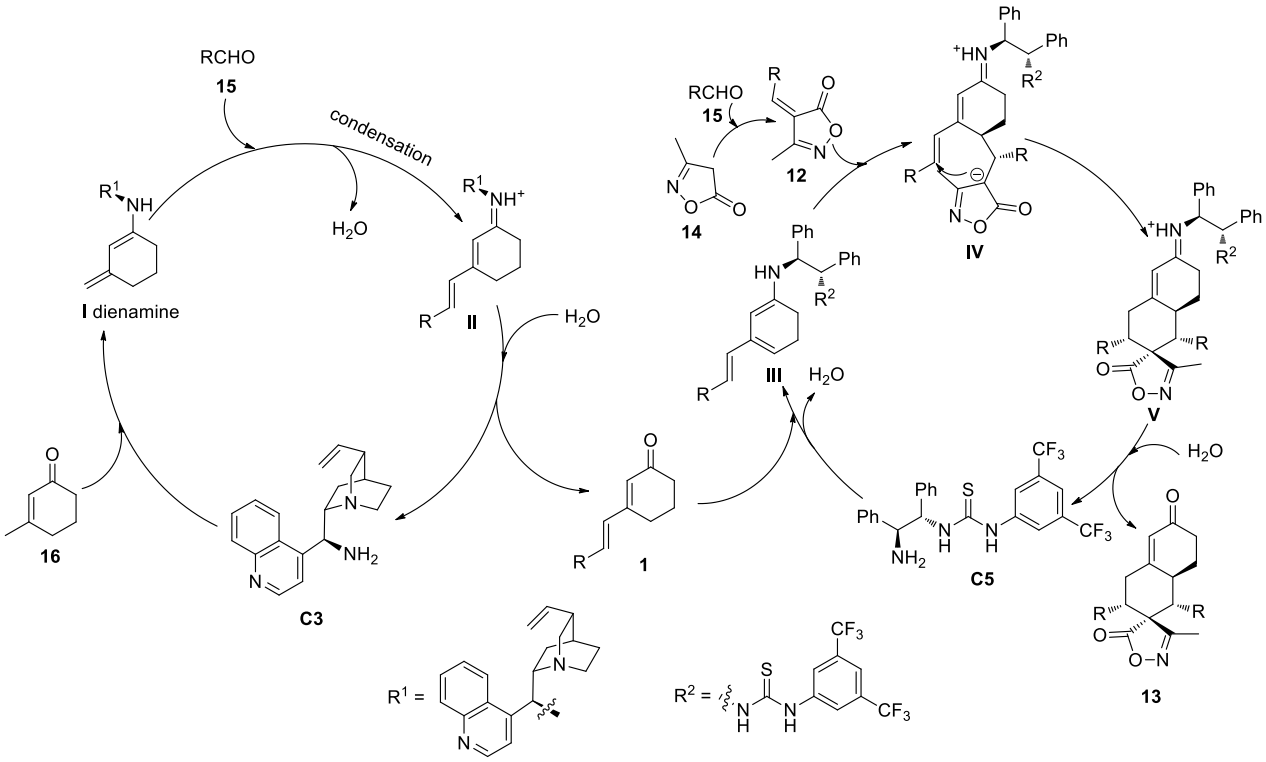


entry	catalyst	acid	yield (%)[b]	ee (%)[c]
1	**C3** (20 mol %)	**A1**	50	60
2	**C4** (20 mol %)	**A1**	trace	
3	**C3** (5 mol %), **C4** (20 mol %)	**A1**	55	46

4	**C3** (5 mol %), **C10** (20 mol %)	**A1**	43	76
5	**C3** (10 mol %), **C10** (20 mol %)	**A1**	48	78
6	**C3** (15 mol %), **C10** (20 mol %)	**A1**	41	68
7	**C3** (10 mol %), **C5** (20 mol %)	**A1**	48	76
8	**C3** (10 mol %), **C10** (20 mol %)	**A3**	46	76
9	**C3** (10 mol %), **C5** (20 mol %)	**A3**	53	82

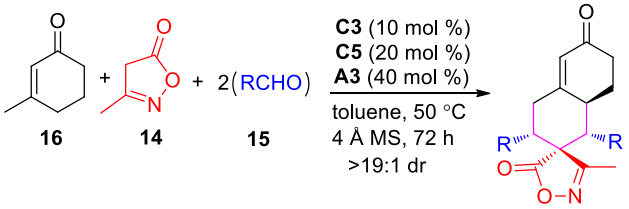
[a]Unless noted otherwise, reactions were performed with **16** (0.075 mmol), **14** (0.05 mmol), **15a** (0.125 mmol) amine **C**, acid **A** (40 mol %) and 4 Å molecular sieves (10 mg) in toluene at 50 °C for 72 h. [b]Yield of isolated product. [c]Determined by HPLC analysis on a chiral stationary phase; dr >19:1 determined by ^{1}H NMR analysis.

In the initial screenings, catalysts **C3** and **C4** were utilized, while **C3** gave the desired product with moderate yield and enantioselectivity, and only trace amount of *ent*-**13a** was observed when **C4** was employed (entries 1 and 2). According to these results, we speculated that amine-thiourea **C4** may not be effective for the condensation steps to form **1a**. As a result, a combination of catalyst **C3** and **C4** were investigated, affording the product with moderate enantioselectivity because that the product catalyzed by **C3** was the enantiomer of **C4 (**entry 3**)**. Therefore, a combination of **C3** and **C10** was applied, which afforded the same enantiomer, giving a significantly improved ee value (entry 4). The ratio of two catalysts was also studied, and the optimal conditions were employing 10 mol% of **C3** and 20 mol% of **C10** (entries 5 and 6). Catalyst **C5** was applied, giving the product with comparable results (entry 7). When the salicylic acid **A1** was replaced by benzoic acid **A3**, the desired product was obtained with 53% yield and 82% ee with catalysts **C3** and **C5**, while the combination **C3** and **C10** gave lower ee value (entries 8 and 9).



The proposed mechanism for four-component reaction was shown in the above scheme. The catalytic cycle started with the condensation of catalyst **C3** and **16**, producing dienamine intermediate **I**. Then, through aldol reaction with aldehyde **15**, the iminium ion intermediate **II** was formed. The substrate **1** was generated along with the release of catalyst **C3**, completing the catalytic cycle for the formation of 2,4-dienone substrate **1**. In contrast, amine-thiourea **C5** might not promote the aldol reaction of **16** and aldehyde **15**. The substrate **1** reacted with catalyst **C5** to provide cross-trienamine intermediate **III**, starting another catalytic cycle. As the cycloaddition was suggested to proceed through a stepwise process, the addition intermediate **IV** was generated with **III** and **12** through cross-trienamine catalysis, while substrate **12** was formed by Knoevenagel condensation with **14** and aldehyde **15**, either catalyzed by **C3** or **C5**. The product **13** was afforded with the recycle of catalyst **C5** through the hydrolysis of the iminium ion intermediate **V**. In conclusion, the reaction was proceeded through relay catalysis of catalyst **C3** and **C5**.

12. General procedure for amine-catalyzed four-component reaction

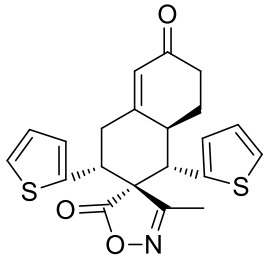


ent-**13a** 53%, 82% *ee*

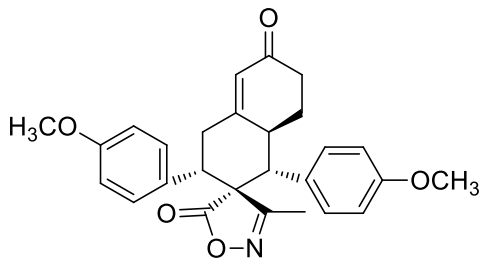
ent-**13t** R = 2-thienyl, 61%, 87% ee

ent-**13u** R = 4-MeOC$_6$H$_4$, 50%, 85% ee

A solution of 3-methyl cyclohexenone **16** (0.15 mmol), 3-methylisoxazol-5(*4H*)-one **14** (0.1 mmol), benzaldehyde **15** (0.25 mmol), benzoic acid **A3** (0.04 mmol), 4 Å molecular sieves (20 mg) and amine catalyst **C3** (0.01 mmol) and **C5** (0.02 mmol) in dry toluene (1.0 mL) was stirred at room temperature for 72 h. Purification by flash chromatography on silica gel (EtOAc/petroleum ether) gave the product ***ent*-13**.



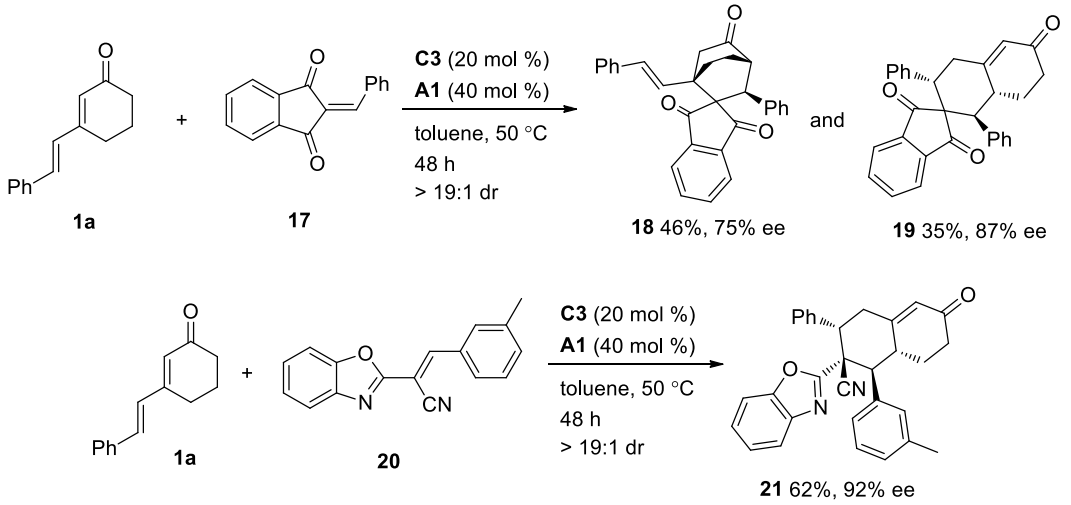
Synthesis of *ent*-13t: 3-methylcyclohex-2-enone (16.5 mg, 0.15 mmol), 3-methylisoxazol-5(*4H*)-one (9.9 mg, 0.1 mmol), thiophene-2-carbaldehyde (28.0 mg, 0.25 mmol), catalyst **C3** (2.9 mg, 0.01 mmol), catalyst **C5** (9.7 mg, 0.02 mmol), benzoic acid **A3** (4.9 mg, 0.04 mmol) and 4 Å molecular sieves (20 mg) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 72 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/3) gave product ***(1'S,2'R,3'R,8a'S)*-3-methyl-1',3'-di(thiophen-2-yl)-3',4',8',8a'-tetrahydro-1'H,5H-spiro[isoxazole-4,2'-naphthalene]-5,6'(7'H)-dione *ent*-13t**: 24.2 mg, 61% yield, white solid; $[\alpha]_D^{20}$ = –29.3 (*c* = 0.30 in $CHCl_3$); 87% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 90/10, 1.0 mL/min, λ = 254 nm, t (major) = 16.09 min, t (minor) = 18.97 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.22 (dd, *J* = 5.2 Hz, 0.8 Hz, 1H), 7.21-7.18 (m, 1H), 7.01-6.94 (m, 4H), 6.02 (s, 1H), 3.79-3.66 (m, 1H), 3.60-3.50 (m, 2H), 3.12 (d, *J* = 11.6 Hz, 1H), 2.71 (dd, *J* = 15.2 Hz, 3.6 Hz, 1H), 2.49-2.26 (m, 2H), 2.11 (s, 3H), 1.89-1.82 (m, 1H), 1.56-1.41 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 198.8, 178.0, 166.5, 159.4, 139.0, 137.8, 127.8, 127.6, 125.8, 125.3, 125.3, 124.9, 61.5, 48.4, 42.0, 37.4, 36.6, 36.5, 27.3, 12.2; ESI-HRMS: calcd. for $C_{21}H_{19}NNaO_3S_2^+$ 420.0699, found 420.0696.



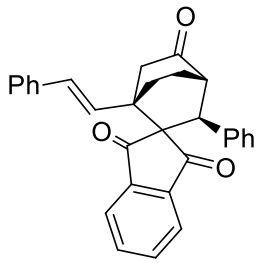
Synthesis of *ent*-13u: 3-methylcyclohex-2-enone (16.5 mg, 0.15 mmol), 3-methylisoxazol-5(*4H*)-one (9.9 mg, 0.1 mmol), 4-methoxybenzaldehyde (28.0 mg, 0.25 mmol), catalyst **C3** (2.9 mg, 0.01 mmol), catalyst **C5** (9.7 mg, 0.02 mmol), benzoic acid **A3** (4.9 mg, 0.04 mmol) and 4 Å molecular sieves (20 mg) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 72 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/3) gave product ***(1'R,2'R,3'S,8a'S)*-1',3'-bis(4-methoxyphenyl)-3-methyl-3',4',8',8a'**

-tetrahydro-1'*H*,5*H*-spiro[isoxazole-4,2'-naphthalene]-5,6'(7'*H*)-dione *ent*-13u: 22.3 mg, 50% yield, white solid; $[\alpha]_D^{20}$ = –20.2 (*c* = 0.37 in $CHCl_3$); 85% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 6.17 min, t (minor) = 9.50 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.29-7.27 (m, 1H), 7.12 (d, *J* = 8.8 Hz, 2H), 6.93 (d, *J* = 6.0 Hz, 2H), 6.82 (d, *J* = 6.4 Hz, 2H), 6.79-6.77 (m, 1H), 6.02 (s, 1H), 3.82-3.71 (m, 7H), 3.61 (m, 1H), 3.21 (dd, *J* = 13.6 Hz, 4.0 Hz, 1H), 2.80 (d, *J* = 12.0 Hz, 1H), 2.56 (dd, *J* = 15.2 Hz, 3.6 Hz, 1H), 2.38-2.32 (m, 2H), 1.98 (s, 3H), 1.72-1.68 (m, 1H), 1.43-1.39 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 199.1, 179.1, 167.0, 161.6, 159.7, 159.6, 131.1, 129.3, 128.2, 127.8, 126.3, 115.5, 114.6, 114.1, 60.8, 55.2, 53.7, 47.4, 36.7, 36.1, 35.8, 27.5, 12.2; ESI-HRMS: calcd. for $C_{27}H_{27}NNaO_5^+$ 468.1781, found 468.1790.

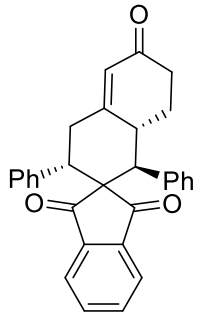
13. More studies for [4 + 2] cycloadditions with other activated alkenes



More activated alkenes were screened with 2,4-dienone **1a**. Interestingly, as outlined in the above scheme, both α′,β-[4 + 2] and γ′,δ-[4 + 2] cycloadducts **18** and **19** were obtained when 2-benzylidene-1*H*-indene-1,3(2*H*)-dione **17** was applied, further verifying that the substitution pattern of the activated alkene has strong effect on the regioselectivity. Moreover, γ′,δ-[4 + 2] cycloadduct **21** was provided smoothly in a moderate yield with excellent enantioselectivity when activated alkene **20** was employed.

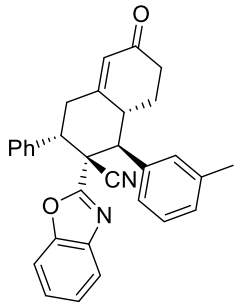


Synthesis of 18: 2-benzylidene-1*H*-indene-1,3(2*H*)-dione (23.4 mg, 0.10 mmol), (*E*)-3-styrylcyclohex-2-enone (29.7 mg, 0.15 mmol), catalyst **C3** (6.5 mg, 0.02 mmol) and salicylic acid **A1** (5.5 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 48 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/12) gave product ***(1S,3S,4S)*-3-phenyl-1-(*(E)*-styryl)spiro[bicycle [2.2.2]octane-2,2'-indene]-1',3',5-trione 18**: 19.9 mg, 46% yield, white solid; $[\alpha]_D^{20}$ = –35.2 (*c* = 0.86 in $CHCl_3$); 75% ee, determined by HPLC analysis: [Daicel chiralpak AD, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 7.52 min, t (minor) = 14.73 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.92-7.90 (m, 1H), 7.74-7.72 (m, 3H), 7.11-7.10 (m, 6H), 6.94-6.92 (m, 2H), 6.77-6.75 (m, 2H), 6.17 (d, *J* = 16.0 Hz, 1H), 5.49 (d, *J* = 16.0 Hz, 1H), 4.08 (s, 1H), 3.64 (dd, *J* = 18.8 Hz, 3.6 Hz, 1H), 3.12-3.09 (m, 2H), 2.37 (t, *J* = 10.8 Hz, 1H), 2.18 (d, *J* = 18.8 Hz, 1H), 2.15-2.10 (m, 1H), 1.50-1.42 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 212.1, 203.4, 199.3, 143.0, 142.1, 138.3, 136.1, 135.8, 135.6, 130.7, 130.4, 128.5, 128.3, 127.8, 126.9, 126.0, 123.0, 122.8, 63.4, 47.0, 45.7, 44.7, 41.7, 28.7, 20.1; ESI-HRMS: calcd. For $C_{30}H_{24}NaO_3^+$ 455.1618, found 455.1619.



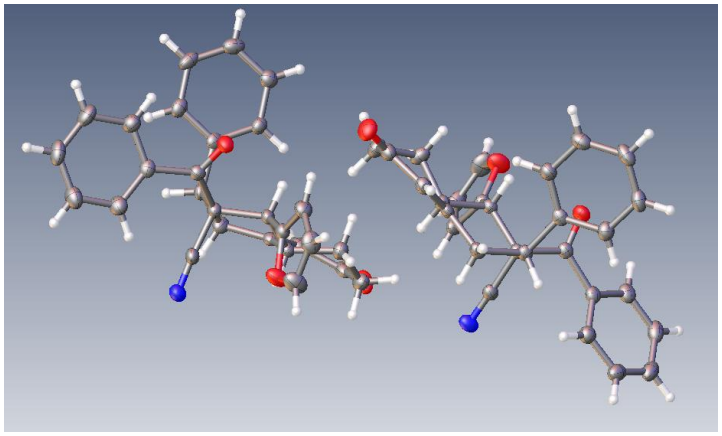
Synthesis of 19: 2-benzylidene-1*H*-indene-1,3(2*H*)-dione (23.4 mg, 0.10 mmol), (*E*)-3-styrylcyclohex-2-enone (29.7 mg, 0.15 mmol), catalyst **C3** (6.5 mg, 0.02 mmol) and salicylic acid **A1** (5.5 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 48 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/9) gave product **1',3'-diphenyl-3',4',8',8a'-tetrahydro-1'*H*-spiro[indene-2,2'-naphthalene]-1,3,6 '(*7'H*)-trione 19:** 15.1 mg, 35% yield, white solid; $[\alpha]_D^{20}$ = –21.7 (*c* = 0.34 in $CHCl_3$); 87% ee, determined by HPLC analysis: [Daicel chiralpak OD, *n*-hexane/*i*-PrOH = 80/20, 1.0 mL/min, λ = 254 nm, t (major) = 14.93 min, t (minor) = 19.72 min]; ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.66 (d, *J* = 7.2 Hz, 1H), 7.56 (t, *J* = 6.6 Hz, 1H), 7.55-7.50 (m, 2H), 7.21 (br, 1H), 7.12-7.05 (m, 4H), 7.04-6.96 (m,3H), 6.91 (br, 1H), 6.79 (br, 1H), 6.08 (s, 1H), 3.74 (t, *J* = 4.8 Hz, 1H), 3.69 (dd, *J* = 10.8 Hz, 3.6 Hz, 1H), 3.54 (d, *J* = 12.0 Hz, 1H), 3.53-3.48 (m, 1H), 3.04 (dd, *J* = 16.8 Hz, 3.6 Hz, 1H), 2.51-2.45 (m, 2H), 1.93-1.89 (m, 1H), 1.48-1.42 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 203.7, 201.8, 199.1, 165.8, 141.9, 141.7, 138.7, 136.1, 135.4, 135.3, 128.9, 128.6, 128.2,

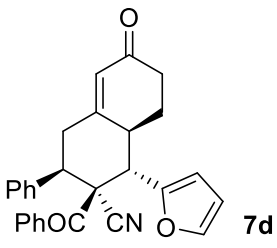
127.9, 127.7, 127.3, 127.3, 126.3, 122.6, 122.5, 62.9, 48.9, 43.8, 37.9, 36.7, 34.4, 28.4; ESI-HRMS: calcd. for $C_{30}H_{24}NaO_3^+$ 455.1618, found 455.1621.



Synthesis of 21: (*E*)-2-(benzo[*d*]oxazol-2-yl)-3-(m-tolyl)acrylonitrile (26.0 mg, 0.10 mmol), (*E*)-3-styrylcyclohex-2-enone (29.7 mg, 0.15 mmol), catalyst **C3** (6.5 mg, 0.02 mmol) and salicylic acid **A1** (5.5 mg, 0.04 mmol) were dissolved in toluene (1.0 mL). Then the mixture was stirred at 50 °C for 48 h. After completion, purification by flash chromatography on silica gel (EtOAc/petroleum ether = 1/7) to give product **2-(benzo[*d*]oxazol-2-yl)-6-oxo-3-phenyl-1-(*m*-tolyl)-1,2,3,4,6,7,8,8a-octahydronaphthalene-2-carbonitrile 21**: 28.4 mg, 62% yield, white solid; $[\alpha]_D^{20}$ = +18.5 (*c* = 0.47 in $CHCl_3$); 92% ee, determined by HPLC analysis: [Daicel chiralpak ID, *n*-hexane/*i*-PrOH = 60/40, 1.0 mL/min, λ = 254 nm, t (major) = 17.34 min, t (minor) = 11.48 min]; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.7 (br, 1H), 7.59-7.57 (m, 1H), 7.38-7.36 (m, 1H), 7.30-7.28 (m, 3H), 7.27-7.23 (m, 2H), 7.19-7.15 (m, 3H), 6.71 (br, 1H), 6.12 (s, 1H), 3.88 (dd, *J* = 14.0 Hz, 3.2 Hz, 1H), 3.56 (d, *J* = 12.4 Hz, 1H), 3.52 (t, *J* = 14.8 Hz, 1H), 2.90 (dd, *J* = 15.2 Hz, 3.2 Hz, 1H), 2.48-2.34 (m, 2H), 1.95-1.88 (m, 1H), 1.63-1.53 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 198.8, 160.3, 160.0, 150.0, 140.1, 138.2, 137.1, 132.4, 128.7, 128.4, 127.7, 126.9, 125.4, 124.7, 120.2, 116.4, 110.5, 57.3, 55.0, 51.1, 38.7, 38.0, 36.5, 27.1, 21.0; ESI-HRMS: calcd. for $C_{31}H_{26}N_2NaO_2^+$ 481.1886, found 481.1888.

14. Crystal data and structure refinement for enantiopure compounds 7d, 9a, and 13n

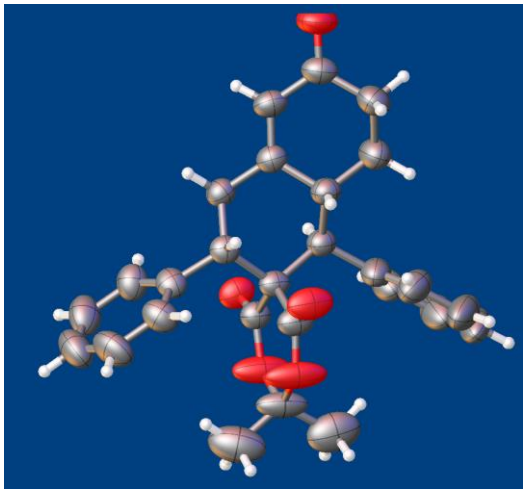


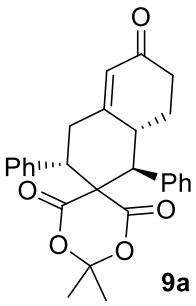


7d

Identification code	**7d**
Empirical formula	$C_{56}H_{46}N_2O_6$
Formula weight	842.95

Temperature/K	294.08(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	10.7180(2)
b/Å	15.6169(3)
c/Å	25.7720(4)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	4313.78(13)
Z	4
ρ_{calc}g/cm^3	1.298
μ/mm^{-1}	0.671
F(000)	1776.0
Crystal size/mm^3	0.7 × 0.6 × 0.35
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.896 to 145.84
Index ranges	-13 ≤ h ≤ 13, -17 ≤ k ≤ 19, -30 ≤ l ≤ 31
Reflections collected	24366
Independent reflections	8418 [R_{int} = 0.0360, R_{sigma} = 0.0340]
Data/restraints/parameters	8418/0/577
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0452, wR_2 = 0.1176
Final R indexes [all data]	R_1 = 0.0468, wR_2 = 0.1195
Largest diff. peak/hole / e Å^{-3}	0.25/-0.27
Flack parameter	0.07(9)

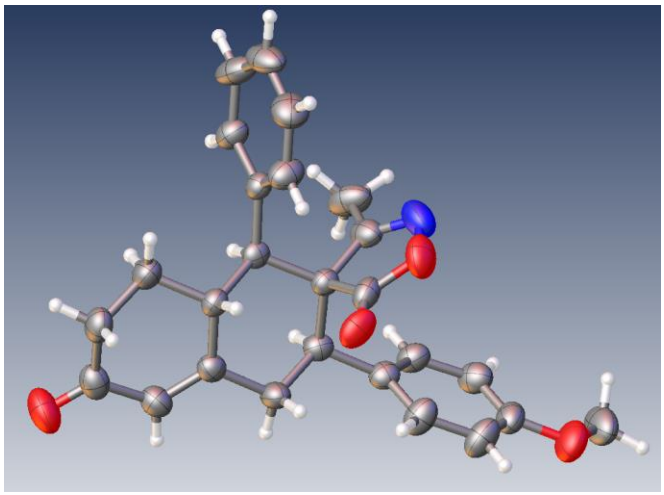


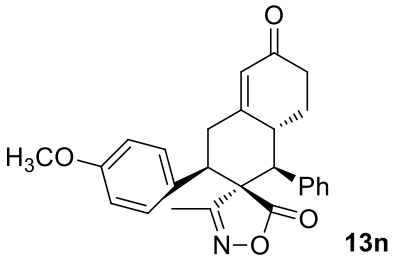


9a

Identification code	**9a**
Empirical formula	$C_{27}H_{26}O_5$
Formula weight	430.48

Temperature/K	293.1(3)
Crystal system	orthorhombic
Space group	$P2_12_12$
a/Å	22.0333(5)
b/Å	13.7082(3)
c/Å	7.53821(15)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2276.82(8)
Z	4
ρ_{calc}g/cm^3	1.256
μ/mm^{-1}	0.696
F(000)	912.0
Crystal size/mm^3	0.7 × 0.3 × 0.3
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	10.302 to 145.536
Index ranges	-25 ≤ h ≤ 27, -11 ≤ k ≤ 16, -9 ≤ l ≤ 8
Reflections collected	12610
Independent reflections	4420 [R_{int} = 0.0400, R_{sigma} = 0.0312]
Data/restraints/parameters	4420/0/291
Goodness-of-fit on F^2	1.056
Final R indexes [I>=2σ (I)]	R_1 = 0.0554, wR_2 = 0.1469
Final R indexes [all data]	R_1 = 0.0601, wR_2 = 0.1549
Largest diff. peak/hole / e Å^{-3}	0.17/-0.32
Flack parameter	0.07(15)





13n

Identification code	**13n**
Empirical formula	$C_{26}H_{26}NO_4$
Formula weight	416.48

Temperature/K	293.3(5)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	11.3294(3)
b/Å	7.7649(2)
c/Å	12.0285(3)
α/°	90
β/°	95.714(2)
γ/°	90
Volume/Å^3	1052.91(5)
Z	2
ρ_{calc}g/cm^3	1.314
μ/mm^{-1}	0.711
F(000)	442.0
Crystal size/mm^3	0.8 × 0.3 × 0.05
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	10.23 to 134.138
Index ranges	$-13 \leq h \leq 13$, $-9 \leq k \leq 9$, $-14 \leq l \leq 14$
Reflections collected	10831
Independent reflections	3613 [R_{int} = 0.0494, R_{sigma} = 0.0481]
Data/restraints/parameters	3613/1/282
Goodness-of-fit on F^2	1.071
Final R indexes [I>=2σ (I)]	R_1 = 0.0528, wR_2 = 0.1362
Final R indexes [all data]	R_1 = 0.0551, wR_2 = 0.1405
Largest diff. peak/hole / e Å^{-3}	0.23/-0.26
Flack parameter	0.0(2)

15. DFT computational calculation studies on regioselective cycloadditions

1) The conformations of 4 and 6a

First, the conformation of alkene **4** and two conformations of **6a** were optimized. As shown in Figure S1, conformation **6a-2** was calculated to have the lowest energy, which was selected for further calculations.

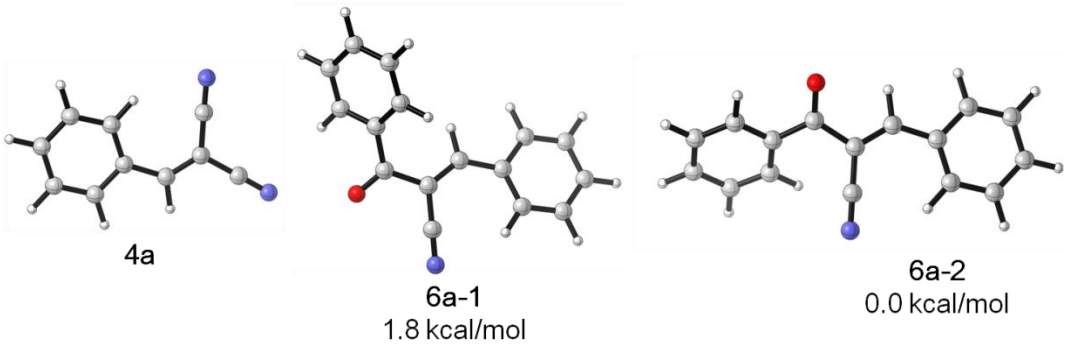
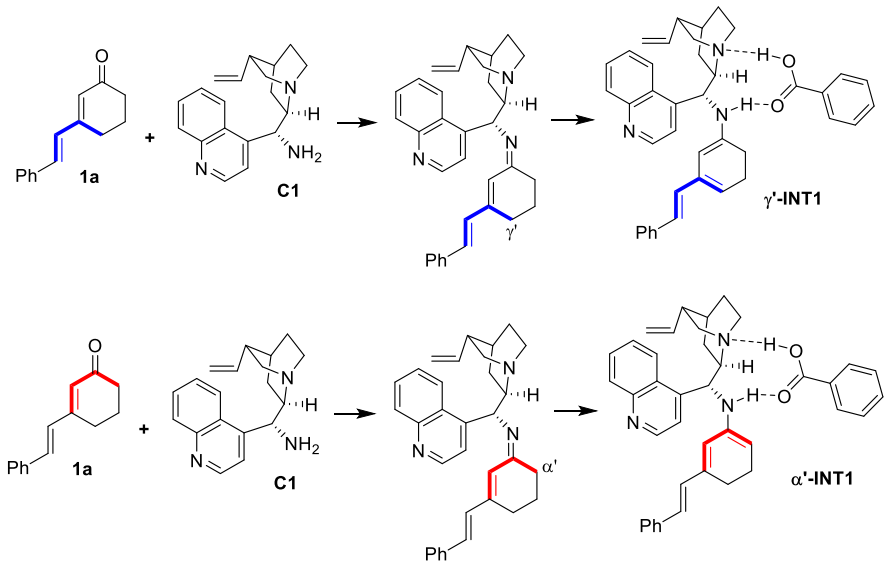


Figure S1. The conformations of **4**, **6a-1**, and **6a-2**

2) The conformations of 1a and the related intermediates



Scheme S1. The process of formation of cross-trienamine intermediates

As previous reported [*Nat. Chem.* **2017**, *8*, 590], the HOMO-activated cross-trienamine intermediates were calculated. When treating 2,4-dienone **1a** with amine **C1**, the imine was produced and then isomerized to **γ'-INT1** by removing a proton at the γ' carbon and the HOMO-activated intermediate was formed. Similarly, the **α'-INT1** was formed by removing the atom at α' carbon. These geometries of intermediates were optimized using M06-2x functional together with the standard 6-31G(d) basis set, and the energy was calculated at 6-31++G(d,p) level (toluene as solvent). The conformations coming from the rotation of C-N bond and the interacted orientation of salicylic acid were also considered. As shown in Figure S2, the energy of **γ'-INT1-B** is lower (2.9 kcal/mol) than **γ'-INT1-A** owing to two hydrogen bonds between salicylic acid and catalyst. For the other conformations resulting from the C-N rotation, both **γ'-INT1-C** and **γ'-INT1-D** had higher energies. The conformation of **γ'-INT1-B** should be considered in the following calculations.

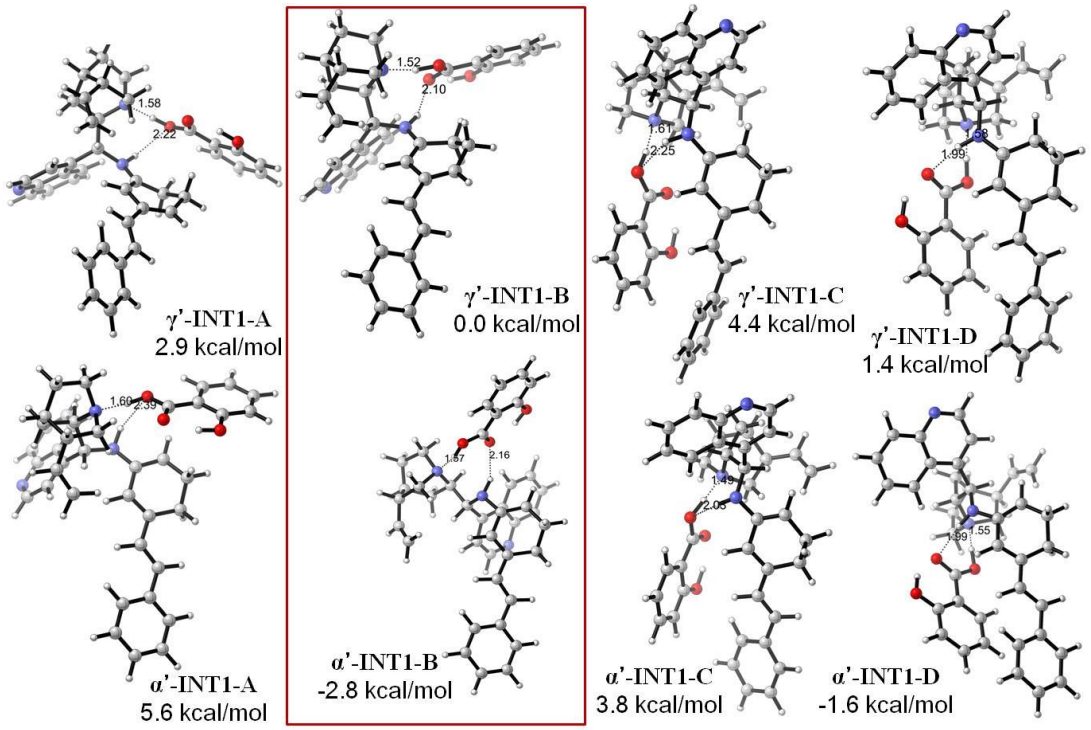
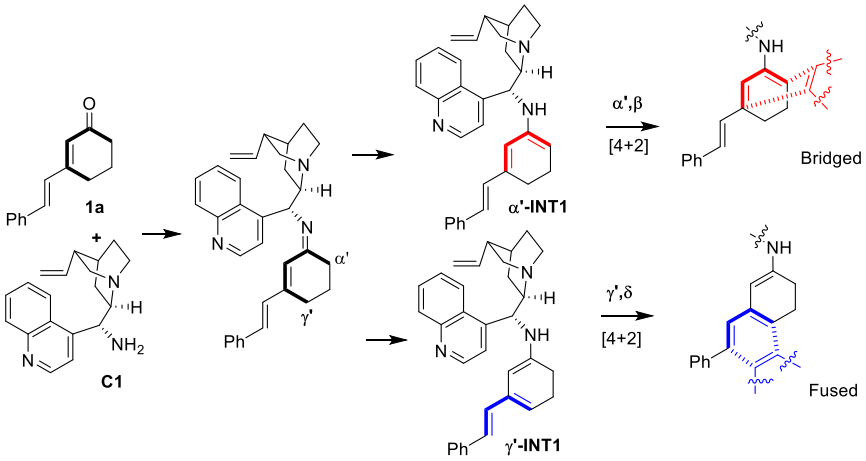


Figure S2. The 3D structures and energies of **γ'-INT1** and **α'-INT1** (energies are related to **γ'-INT1-B**).

Similarly, the conformations of **α'-INT1** were also calculated. The conformation of **α'-INT1-B**, with similar orientation of substrate, salicylic acid, and catalyst as **γ'-INT1-B**, had the lowest energy that was 2.8 kcal/mol lower than that of **γ'-INT1-B**. These results suggested that the hydrogen atom at the α' carbon was easier to be removed than that at the γ' carbon.

3) The regioselectivity of γ′,δ-[4 + 2] cycloaddition reaction



Scheme S2. The regioselectivity of cycloaddition reactions.

As shown in Scheme S2, there were two possible pathways for the cycloadditions of **1a** and **6a**: α′,β-regioselective [4 + 2] cycloaddition and γ′,δ-regioselective [4 + 2] cycloaddition. Density

functional theory (DFT) calculations were performed to clarify the mechanism of the regioselective cycloaddition reaction between **1a** and **6a**. These geometries of intermediates and transition states were optimized using M06-2x functional together with the standard 6-31G(d) basis set, and the energies were calculated at 6-31++G(d,p) level (toluene as solvent). Herein, the reaction process of **1a** and **6a** was studied as stepwise and concerted mechanism. In the stepwise pathway as shown in Figure S3, the γ′-carbon that had more negative charge attacked **A** position in **6a-2** to form γ′-**INT2** via γ′-**TS1**. The reaction positions of the first step were decided by the charge distribution and molecular orbital as shown in Figure S4. Sequentially, the carbanion of **B** position attacked δ-carbon to form γ′,δ-**INT3** via γ′,δ-**TS2** by γ′,δ-regioselective [4 + 2] cycloaddition. Then, γ′,δ-**INT3** would further tack off **C3** to generate the final cyclization product **7a**. On the other hand, the possible α′,β-regioselective [4 + 2] cycloaddition might share the same process as γ′,δ-regioselective [4 + 2] cycloaddition to generate **7a'** via sequentially α′ carbon and β carbon reactions. In the concerted mechanism, the reaction underwent a concerted transition state to form a closed six-membered ring or six-membered bridged product. However, we failed to identify any transition state (TS) in the concerted mechanism. In contrast, the stepwise TSs where the two step additions proceeded sequentially had been identified easily.

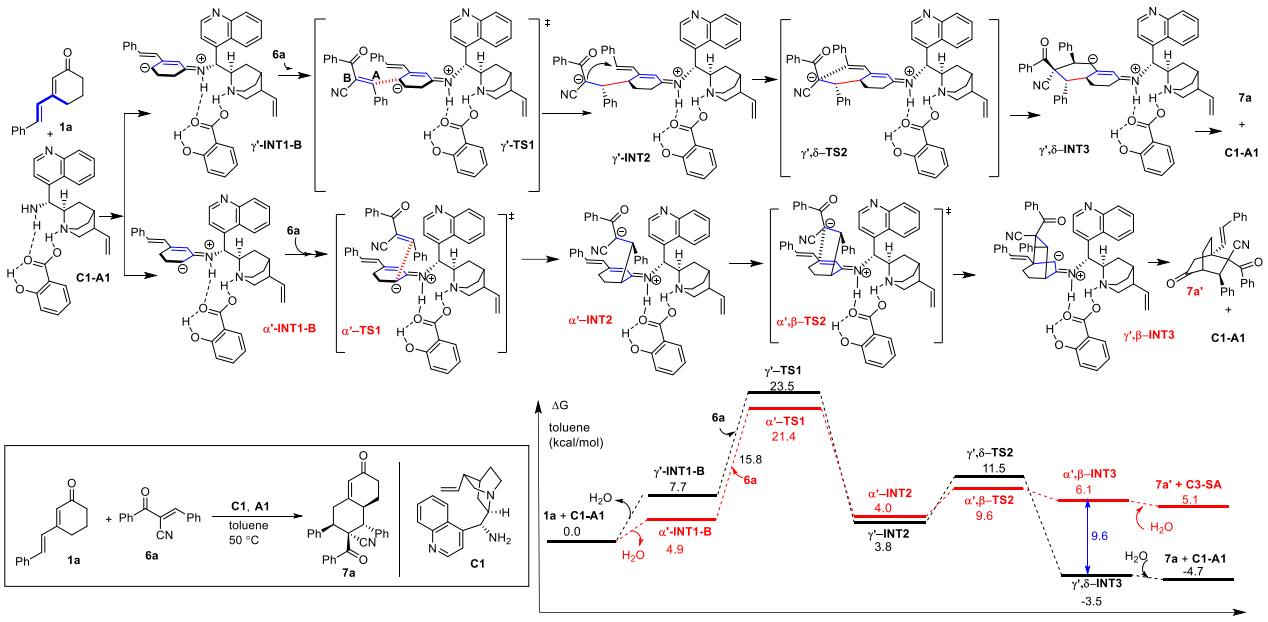


Figure S3. Computed potential energy surface of the reaction of **1a** and **6a**.

For the γ′,δ-regioselective [4 + 2] cycloaddition, the energy barrier of the first addition was 15.8 kcal/mol (γ′-**TS1**), much higher than that of the second step (γ′,δ-**TS2**, 7.7 kcal/mol), suggesting that the first step should be the rate limited step. Similarly, the energy barriers of α′-**TS1** and α′,β-**TS2**

in α′,β-cycloaddition were similar with that of γ′,δ-cycloaddition with values of 16.5 kcal/mol and 5.6 kcal/mol, respectively. Comparing two pathways, the energy of γ′-**TS1** is higher than that of α′-**TS1**, suggesting that α′,β-pathway is kinetically favorable. However, the α′,β-cycloaddition of **1a** and **6a** was theoretically impossible, because the energy of the reaction to form **α′,β-INT3** from **α′-INT1** was 2.1 kcal/mol; in addition, the energy sum of the final products was 9.8 kcal/mol higher than that of the γ′,δ-[4 + 2] pathway, indicating that the α′,β-cycloadduct **7a′** is very thermally unstable, probably due to the crowded structure bearing two vicinal quaternary stereogenic centers.

In brief, the regioselectivity of reaction of 1a and 6a may result from the thermodynamically stable intermediates and the final product.

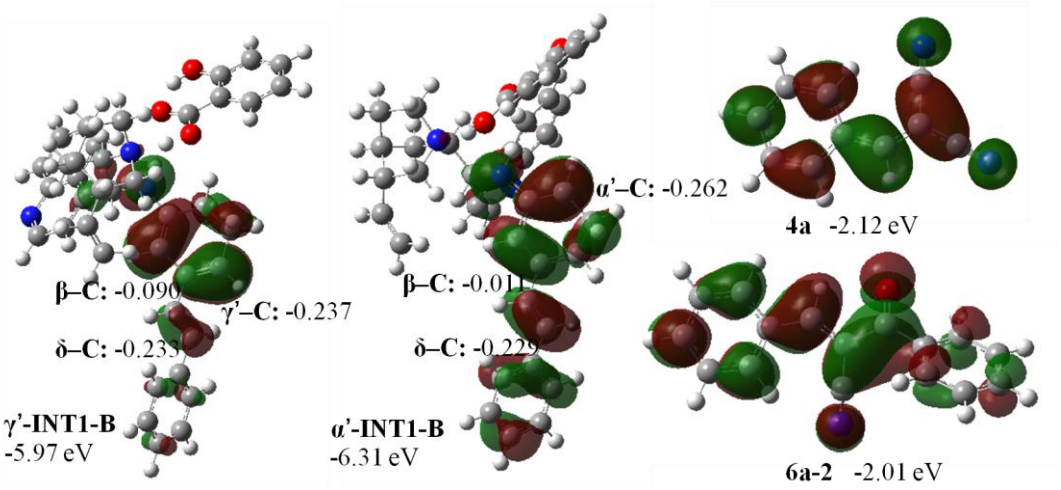


Figure S4. The HOMO of **γ′-INT1-B** and **α′-INT1-B** as well as LUMO of **6a-2** and **4**. The (natural population analysis) NPA charges of different positions at **γ′-INT1-B** and **α′-INT1-B** were labeled. The NPA charges at α'-C in **α′-INT1-B** and γ'-C in **γ′-INT1-B** are more negative than other positions, so they are considered as more favorable positions for the first step addition.

4) The regioselectivity of α′,β-[4 + 2] cycloaddition reaction

When alkene **4** reacted with 2,4-dienone **1a**, α′,β-[4 + 2] cycloaddition product **5** was formed. As showing in Figure S5, the α′,β-[4 + 2] cycloaddition was considered as the favorable pathway due to the energy of **γ′-TS3** is higher than that of **α′-TS3**. Although the intermediate **γ′,δ-INT5** and the product **5a'** were more thermodynamically stable than **α′,β-INT5** and **5a** with energy difference of 7.8 and 8.9 kcal/mol, respectively, the high energy hampered the progress of the γ′,δ-pathway. **Therefore, the α′,β regioselectivity for reaction of 1a and 4 may result from kinetic control**.

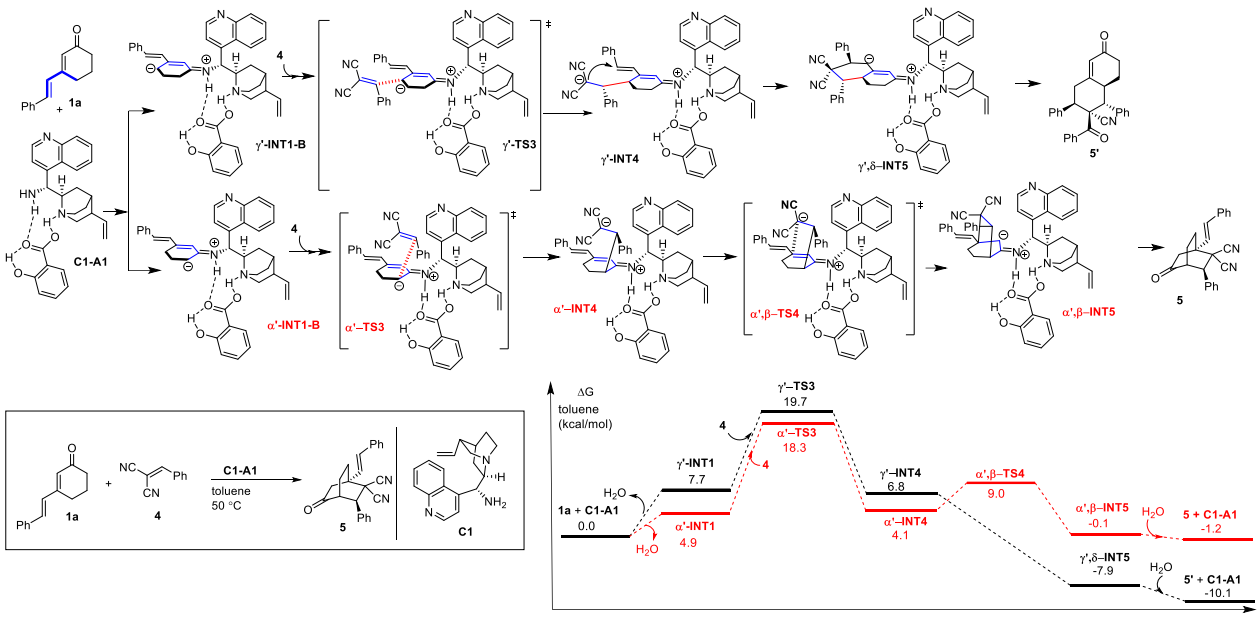


Figure S5. Computed potential energy surface of the reaction of **1a** and **4**.

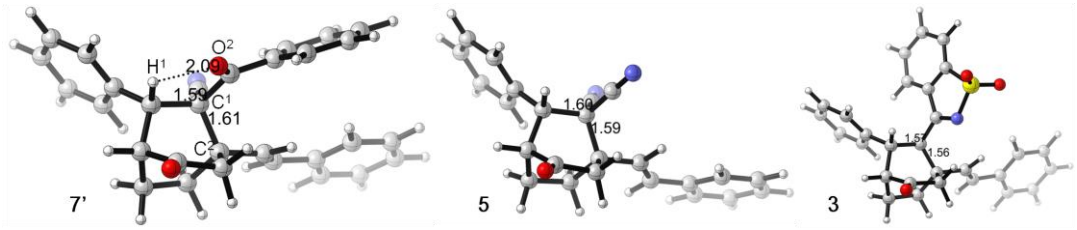
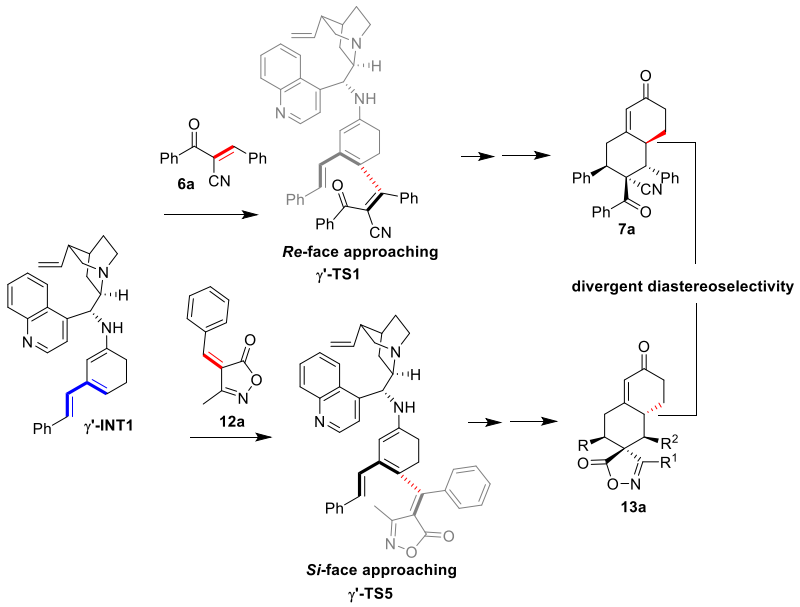


Figure S6. The conformations of **7'**, **5**, and **3**.

Compared with the conformation **5** and **3**, steric hindrance in **7'** may be the reason for its higher energy. For example, the distance between O atom and H atom marked in Figure S6 was 2.09 Å.

5) The diastereoselectivity of γ′,δ-[4 + 2] cycloaddition reaction



Scheme S3. The diastereoselectivity of [4 + 2] cycloaddition reactions.

As shown in Scheme S3, the reactions also showed very interesting divergent diastereoselectivity with different substrates **6a** and **12a**. Opposite enantiocontrol was observed in the γ′-regioselective addition step, while the final δ-regioselective cyclization step exhibited the same face selectivity. Therefore, the first step was calculated as the rate-limiting and key divergent stereoselective step, and the energies of different poses of **γ′-TS1** and **γ′-TS5** were investigated.

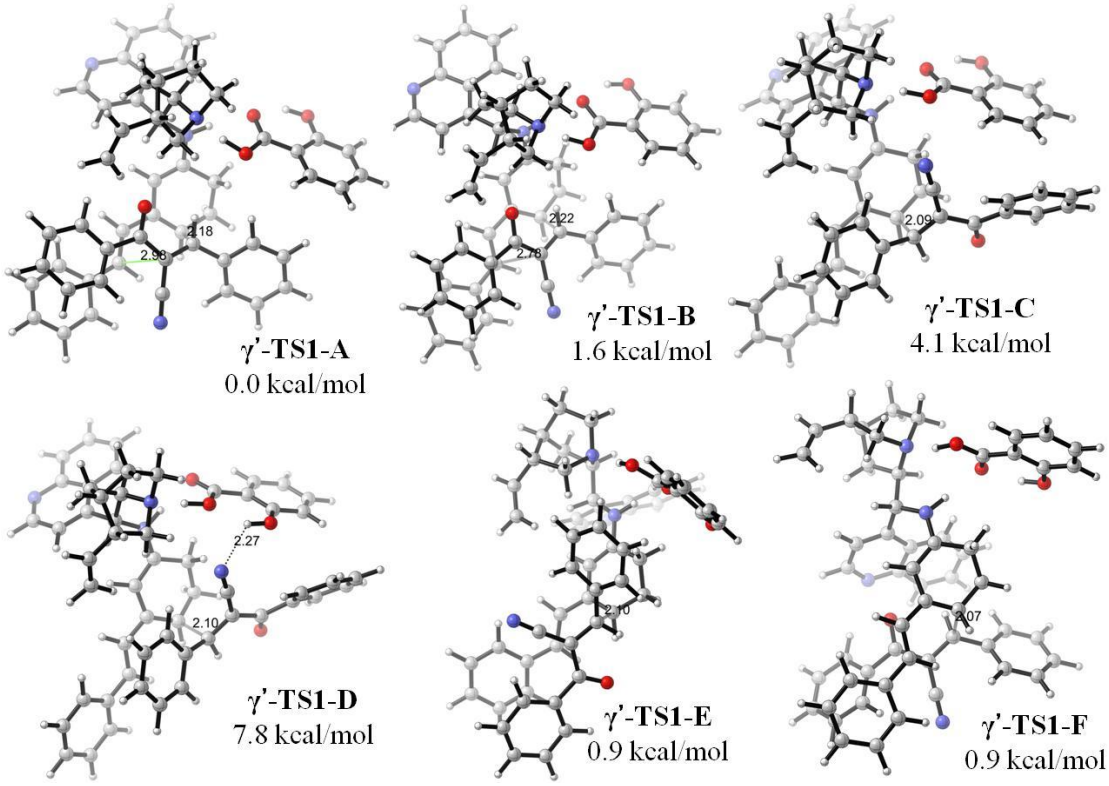


Figure S7. The energies and structures of possible poses of **γ′-TS1**.

Different conformations of **γ′-TS1** were proposed and shown in Figure S7. The **γ′-TS1-A** has the lowest energy, in which there are not obvious hydrogen bonds between **6a** and **γ′-INT-B**, probably because the reaction site is far from the chiral catalyst and the relatively rigid structure of the ring system. We also found similar TS as **γ′-TS1-B** with a higher energy, in which the distance between the reacted atoms had a little difference. Other conformations were also calculated, such as **γ′-TS1-C** and **γ′-TS1-D**. The steric hindrance in these poses increased the energies, even there is a hydrogen bond between SA and **6a**.

In order to understand the stereoselectivity, the TSs to form different isomers were also calculated, in which **6a** approached the **γ′-INT-B** by different orientation (**γ′-TS1-E**) or different side (**γ′-TS1-F**). Their energies also are a little higher than that of **γ′-TS1-A.** As a result, the calculations were consistent with the observed enantioselectivity observed in the γ′-regioselective addition of cross-trienamine intermediate **γ′-INT1** to alkene **6a**.

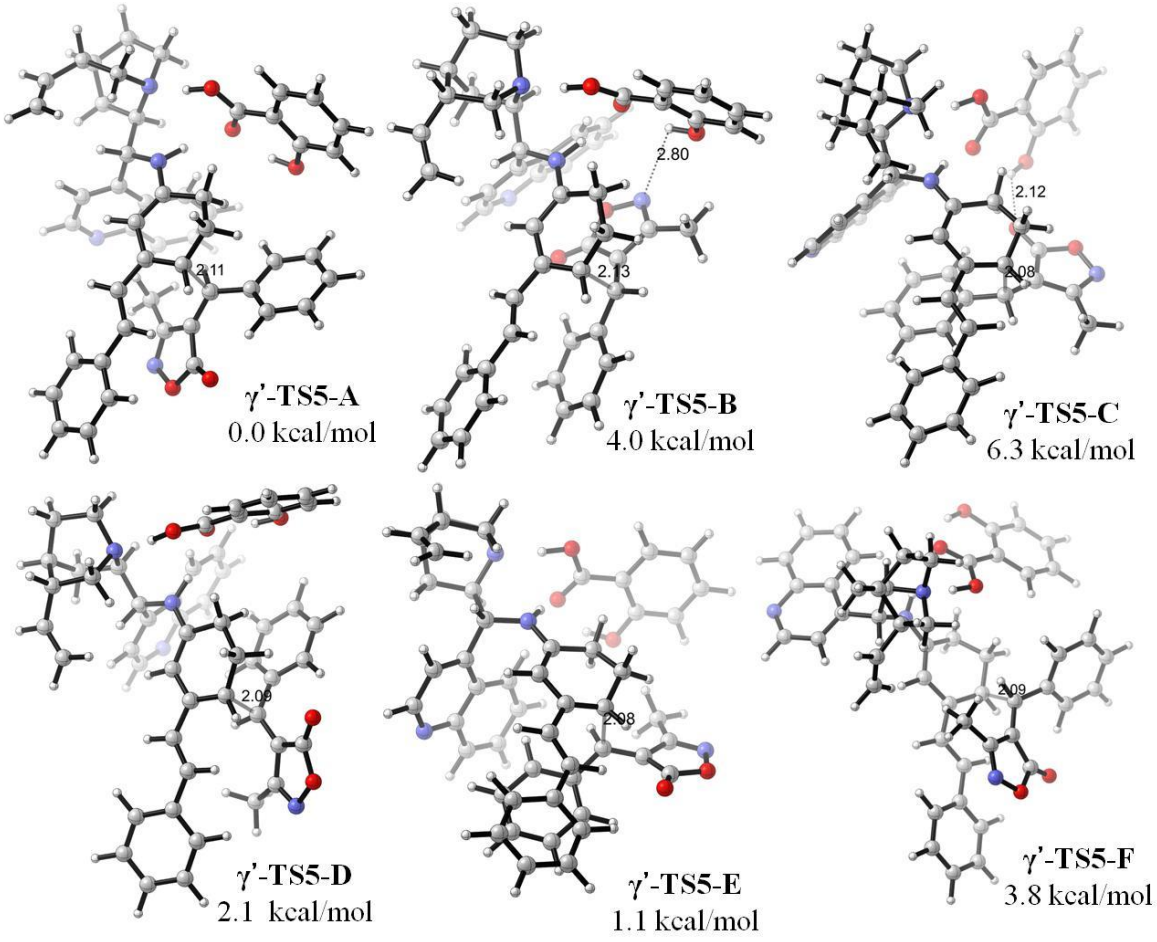


Figure S8. The energies and structures of possible poses of **γ′-TS5**.

In contrast, **γ′-TS5-A**, corresponding to the stereoselectivity observed in chiral **13a**, had the

lowest energy among the calculated poses of **γ′-TS5-A–F**. As previous calculated, the hydrogen bond may not be the key factor for the stereocontrol. Similarly, the TSs to form different isomers were also calculated, in which **12a** approached the **γ′-INT-B** by different orientation (**γ′-TS5-E**) or different side (**γ′-TS5-F**). Their energies were a little higher than that of **γ′-TS5-A**.

To find the TS with the lowest energy, we have calculated more than 10 poses of γ′-TS1 or γ′-TS5. Based on the data we calculated, we did not find obvious hydrogen bond to effect the divergent enantioselectivity observed in the γ′-addition step. Currently, we proposed that the weak interactions and configurations of the substrates might be the main reasons for the switched enantioselectivity. However, because there are much possible conformations of γ′-INT1 and the substrates 6a or 12a also can approach γ′-INT1 by different orientations, much more calculations of the possible poses of γ′-TS1 or γ′-TS5 are necessary to make the more decisive conclusions.

Computational method

All calculations were carried out with the GAUSSIAN 09 packages.[5] The recently developed M06-2x functional,[6] together with the standard 6-31G(d) basis set, were used for optimizing the geometry of all the minima and transition states. All the optimized structures were confirmed by frequency calculations to be either minima or transition states using the same level of theory. For transition states, intrinsic reaction coordinate analysis (IRC) was done to verify that they connect the right reactants.[7] To take solvent effects into account, solution-phase single-point calculations were performed on the gas-phase geometries.[8] The solution-phase single point energy calculations were done using M06-2x method at a larger basis set 6-31++G(d,p). Solvent effect was accounted for using self-consistent reaction field (SCRF) method, using SMD model and UAKS radii.[9] Dichloromethane was used as the solvent. Solution-phase single-point energies corrected by the gas-phase Gibbs free energy corrections were used to describe all the reaction energetics. All of these energies correspond to the reference state of 1 mol/L, 298 K. All energetics reported throughout the text are in kcal/mol, and the bond lengths are in angstroms (Å). Structures were generated using GaussView5.0.8 and CYLview.

(5) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.;

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

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(8) Um, J. M.; DiRocco, D. A.; Noey, E. L.; Rovis, T.; Houk, K. N., *J. Am. Chem. Soc.* **2011,***133*, 11249.

(9) (a)Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**,*113*, 6378. (b)Ribeiro, R. F.; Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2011**,*115*, 14556.

Computational data:

4

Zero-point correction= 0.133264 (Hartree/Particle)
Thermal correction to Energy= 0.142344
Thermal correction to Enthalpy= 0.143288
Thermal correction to Gibbs Free Energy= 0.098397
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6	6	0	0.676950	-0.823999	0.015917
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8	6	0	-0.719097	-0.405112	0.012421
9	6	0	-1.155946	0.930316	0.045311
10	6	0	-1.679566	-1.429791	-0.024956
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15	6	0	-3.455750	0.189965	-0.004175
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6a-1

Zero-point correction= 0.227252 (Hartree/Particle)
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Thermal correction to Enthalpy= 0.242728
Thermal correction to Gibbs Free Energy= 0.183790
E(sov) = -746.017891479 A.U.

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4	6	0	-0.670069	-0.028239	-0.178019
5	1	0	-0.010040	-0.851548	-0.445154
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19	6	0	2.162165	-0.791220	0.958707
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25	6	0	4.243669	-1.835172	0.329802
26	1	0	2.961836	-2.546385	1.906433
27	1	0	5.334358	-0.881714	-1.264697
28	1	0	4.977542	-2.623667	0.465397
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6a-2

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Thermal correction to Gibbs Free Energy= 0.182256
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γ'-INT1-A

Zero-point correction= 0.739739 (Hartree/Particle)
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Thermal correction to Enthalpy= 0.779724
Thermal correction to Gibbs Free Energy= 0.665138
E(sov) = -1938.21806225 A.U.

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26	1	0	4.805429	-1.050845	-1.188061
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28	1	0	1.364107	-3.439226	-1.833591
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30	1	0	4.877679	-2.647465	-2.902960
31	1	0	2.698687	-3.276176	-3.910296
32	1	0	2.323637	0.710617	-3.067027
33	1	0	0.948711	0.147635	-2.164071
34	1	0	2.077778	-0.991878	-4.598599
35	1	0	0.319224	-2.826444	-4.359456
36	1	0	-1.743429	-1.832588	-3.651955
37	1	0	-0.868103	-0.411652	-2.866381
38	1	0	-1.858028	-5.274251	0.135597
39	1	0	-1.037831	-3.177839	-0.927523
40	1	0	3.441986	-2.812651	4.119140
41	1	0	0.268285	-1.402592	-0.974921
42	1	0	3.089696	-1.959862	-0.002139
43	7	0	0.943031	-0.409289	0.706704
44	6	0	-0.133521	0.456280	0.700098
45	1	0	1.831579	0.033524	0.902559
46	6	0	-1.340439	0.211514	0.139776
47	6	0	0.051154	1.724651	1.500344
48	6	0	-2.409387	1.218673	0.221732
49	1	0	-1.579164	-0.748100	-0.308897
50	6	0	-0.697762	2.886644	0.853116
51	1	0	1.113298	1.961780	1.621262
52	1	0	-0.351794	1.542730	2.507180
53	6	0	-2.118537	2.493564	0.549866
54	6	0	-3.773059	0.784702	-0.121356
55	1	0	-0.191746	3.171708	-0.084046
56	1	0	-0.657125	3.765388	1.504801
57	1	0	-2.887266	3.260037	0.512036
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59	1	0	-3.845495	-0.031915	-0.841284
60	6	0	-6.269267	0.902390	0.065944
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62	6	0	-7.312187	1.227025	0.942840
63	6	0	-6.588374	0.219275	-1.116243
64	6	0	-8.625164	0.863422	0.664331
65	1	0	-7.081827	1.765800	1.858589
66	6	0	-7.898543	-0.148005	-1.394812
67	1	0	-5.804023	-0.005636	-1.833095
68	6	0	-8.923720	0.170062	-0.505145
69	1	0	-9.416508	1.122634	1.361375
70	1	0	-8.124596	-0.674702	-2.317255
71	1	0	-9.948098	-0.112155	-0.727969

72	6	0	3.491399	4.872315	2.507653
73	6	0	2.833991	6.046836	2.120589
74	6	0	2.138955	6.113630	0.926256
75	6	0	2.083312	4.998164	0.079467
76	6	0	2.736145	3.808238	0.464880
77	6	0	3.436470	3.766034	1.679804
78	1	0	4.035572	4.830458	3.444689
79	1	0	2.866324	6.920860	2.764537
80	1	0	1.624071	7.015265	0.612633
81	1	0	3.932242	2.840523	1.954010
82	6	0	2.647404	2.617692	-0.404100
83	8	0	2.050830	2.626440	-1.482229
84	8	0	3.232722	1.528782	0.060698
85	1	0	3.026576	0.730712	-0.584169
86	8	0	1.392672	5.120751	-1.062538
87	1	0	1.456883	4.262326	-1.539653

γ'-INT1-B

Zero-point correction= 0.738989 (Hartree/Particle)
Thermal correction to Energy= 0.778348
Thermal correction to Enthalpy= 0.779292
Thermal correction to Gibbs Free Energy= 0.661990
E(sov) = -1938.21951894 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.675885	-2.362717	3.397945
2	6	0	2.188044	-3.351848	4.283352
3	6	0	1.004098	-3.987664	4.015246
4	6	0	0.257122	-3.665756	2.852802
5	6	0	0.747846	-2.674047	1.954394
6	6	0	1.976541	-2.030091	2.264959
7	6	0	0.362657	-1.371915	-0.267600
8	6	0	1.586361	-1.827198	-1.087646
9	7	0	1.956602	-0.791063	-2.087025
10	6	0	3.173309	-1.233223	-2.798851
11	6	0	1.320015	-3.176107	-1.810914
12	6	0	2.892336	-2.507579	-3.630482
13	6	0	1.461522	-2.965484	-3.323506
14	6	0	0.872308	-0.553742	-3.061640
15	6	0	0.477283	-1.866597	-3.788225
16	6	0	-0.958318	-2.307574	-3.625848
17	6	0	-1.989130	-1.602003	-3.164357

18	7	0	-0.914109	-4.340506	2.659904
19	6	0	-1.607898	-4.046022	1.590914
20	6	0	-1.211251	-3.083125	0.631345
21	6	0	-0.036925	-2.390800	0.793464
22	1	0	2.753336	-3.601488	5.175834
23	1	0	0.594646	-4.747711	4.672478
24	1	0	2.373532	-1.262549	1.610877
25	1	0	3.503773	-0.400202	-3.427416
26	1	0	3.944224	-1.396054	-2.039315
27	1	0	2.024464	-3.941444	-1.469400
28	1	0	0.315543	-3.543679	-1.576814
29	1	0	3.001207	-2.305944	-4.701700
30	1	0	3.602624	-3.300827	-3.376597
31	1	0	1.240555	-3.898831	-3.853089
32	1	0	1.246169	0.192010	-3.770056
33	1	0	0.038045	-0.089207	-2.528886
34	1	0	0.639646	-1.733129	-4.867910
35	1	0	-1.146281	-3.326099	-3.971602
36	1	0	-2.984397	-2.035347	-3.133144
37	1	0	-1.902155	-0.577679	-2.810022
38	1	0	-2.543265	-4.586363	1.452644
39	1	0	-1.841182	-2.899036	-0.236471
40	1	0	3.610924	-1.856672	3.618406
41	1	0	-0.479158	-1.335284	-0.966963
42	1	0	2.453241	-1.906426	-0.424377
43	7	0	0.544357	-0.032650	0.233561
44	6	0	-0.444467	0.915106	0.212785
45	1	0	1.477599	0.244827	0.510030
46	6	0	-1.746152	0.684476	-0.091412
47	6	0	-0.024265	2.306663	0.631960
48	6	0	-2.716544	1.785836	-0.090762
49	1	0	-2.123356	-0.323713	-0.233361
50	6	0	-0.824393	3.371301	-0.117928
51	1	0	1.047655	2.452840	0.459318
52	1	0	-0.201900	2.400674	1.712556
53	6	0	-2.298015	3.066957	-0.099585
54	6	0	-4.142478	1.423046	-0.124868
55	1	0	-0.475218	3.408965	-1.163388
56	1	0	-0.619956	4.356228	0.313166
57	1	0	-3.011995	3.880507	-0.187801
58	6	0	-5.127279	2.122835	0.456062
59	1	0	-4.382777	0.491168	-0.638997
60	6	0	-6.560106	1.796782	0.406514
61	1	0	-4.859100	2.993518	1.053656
62	6	0	-7.421885	2.345916	1.364538
63	6	0	-7.108241	0.952789	-0.569809

64	6	0	-8.779610	2.045055	1.365890
65	1	0	-7.013591	3.011280	2.121221
66	6	0	-8.463651	0.649082	-0.568905
67	1	0	-6.467557	0.549248	-1.348512
68	6	0	-9.305997	1.191144	0.400617
69	1	0	-9.428039	2.478371	2.121533
70	1	0	-8.868437	-0.006110	-1.334642
71	1	0	-10.365883	0.956163	0.397010
72	6	0	4.895180	4.934644	-0.270786
73	6	0	5.703600	4.901814	0.872842
74	6	0	5.810385	3.754803	1.638409
75	6	0	5.104337	2.599035	1.278212
76	6	0	4.289222	2.622326	0.126616
77	6	0	4.197379	3.798001	-0.634054
78	1	0	4.819370	5.839525	-0.863526
79	1	0	6.257861	5.788502	1.166588
80	1	0	6.431626	3.715517	2.526465
81	1	0	3.563293	3.788850	-1.514209
82	6	0	3.537158	1.416513	-0.266518
83	8	0	3.573225	0.365383	0.399276
84	8	0	2.806794	1.519974	-1.343901
85	1	0	2.376949	0.569354	-1.554896
86	8	0	5.245594	1.516914	2.056439
87	1	0	4.689209	0.803822	1.670707

γ'-INT1-C

Zero-point correction= 0.740236 (Hartree/Particle)
Thermal correction to Energy= 0.779098
Thermal correction to Enthalpy= 0.780042
Thermal correction to Gibbs Free Energy= 0.667830
E(sov) = -1938.21835745 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.228921	-2.775757	-2.802544
2	6	0	-5.398992	-3.524257	-2.535743
3	6	0	-6.006565	-3.430321	-1.311920
4	6	0	-5.481336	-2.578793	-0.305772
5	6	0	-4.311690	-1.808368	-0.573603
6	6	0	-3.697482	-1.945054	-1.848705
7	6	0	-2.648019	-0.004475	0.312888
8	6	0	-2.974090	1.161395	-0.644562
9	7	0	-1.832165	2.103182	-0.747867

10	6	0	-2.146703	3.119940	-1.771420
11	6	0	-4.259241	1.931221	-0.231402
12	6	0	-3.360782	3.982553	-1.344746
13	6	0	-3.907909	3.409818	-0.032775
14	6	0	-1.558360	2.783242	0.534945
15	6	0	-2.818075	3.524089	1.056064
16	6	0	-3.344473	3.073271	2.398304
17	6	0	-2.719652	2.349152	3.324460
18	7	0	-6.146461	-2.548719	0.885600
19	6	0	-5.671026	-1.764495	1.817973
20	6	0	-4.529165	-0.943778	1.653463
21	6	0	-3.841001	-0.944457	0.464528
22	1	0	-5.805302	-4.179204	-3.300147
23	1	0	-6.898615	-3.995686	-1.063875
24	1	0	-2.782019	-1.408243	-2.062266
25	1	0	-1.245832	3.725198	-1.913640
26	1	0	-2.336207	2.591767	-2.711336
27	1	0	-5.034130	1.820909	-0.997046
28	1	0	-4.672649	1.523792	0.696180
29	1	0	-3.065526	5.027862	-1.203549
30	1	0	-4.138894	3.966224	-2.114718
31	1	0	-4.798837	3.964963	0.281098
32	1	0	-0.727878	3.468647	0.353987
33	1	0	-1.172935	2.039656	1.236159
34	1	0	-2.579141	4.592868	1.159751
35	1	0	-4.352224	3.430056	2.621247
36	1	0	-3.201331	2.122928	4.270668
37	1	0	-1.706649	1.976180	3.200328
38	1	0	-6.206529	-1.755020	2.766138
39	1	0	-4.208664	-0.300225	2.470462
40	1	0	-3.741197	-2.868716	-3.767960
41	1	0	-2.502914	0.442827	1.301909
42	1	0	-3.101732	0.746427	-1.652080
43	7	0	-1.431072	-0.684657	-0.090704
44	6	0	-0.426909	-1.059153	0.791738
45	1	0	-1.082870	-0.457917	-1.014680
46	6	0	0.824514	-1.353634	0.378993
47	6	0	-0.745304	-1.090113	2.269721
48	6	0	1.884281	-1.651882	1.348289
49	1	0	1.086803	-1.289031	-0.674455
50	6	0	0.121135	-2.115827	3.002225
51	1	0	-1.803050	-1.318247	2.434980
52	1	0	-0.557728	-0.085835	2.683983
53	6	0	1.568629	-1.998127	2.610687
54	6	0	3.277786	-1.547710	0.885330
55	1	0	-0.239880	-3.125614	2.748785

56	1	0	-0.008691	-1.999857	4.082680
57	1	0	2.343310	-2.280198	3.317461
58	6	0	4.277648	-1.049068	1.626540
59	1	0	3.477981	-1.848592	-0.145463
60	6	0	5.675729	-0.953623	1.183461
61	1	0	4.045588	-0.624862	2.602860
62	6	0	6.477269	0.101211	1.636333
63	6	0	6.226691	-1.870444	0.278580
64	6	0	7.778083	0.259485	1.169573
65	1	0	6.056655	0.821872	2.332304
66	6	0	7.525281	-1.712856	-0.191068
67	1	0	5.626287	-2.712618	-0.053888
68	6	0	8.304892	-0.643461	0.247273
69	1	0	8.380136	1.092667	1.519858
70	1	0	7.934682	-2.431413	-0.895341
71	1	0	9.319954	-0.521535	-0.118434
72	6	0	3.883311	-0.475742	-3.300525
73	6	0	5.094405	-0.167710	-2.668296
74	6	0	5.128847	0.637622	-1.544244
75	6	0	3.939327	1.150290	-1.008103
76	6	0	2.715198	0.856252	-1.644941
77	6	0	2.707800	0.043821	-2.789063
78	1	0	3.867374	-1.106884	-4.182429
79	1	0	6.026839	-0.570319	-3.054083
80	1	0	6.060820	0.865649	-1.036401
81	1	0	1.754347	-0.166310	-3.262280
82	6	0	1.456826	1.404458	-1.101509
83	8	0	1.410461	2.121460	-0.102424
84	8	0	0.368066	1.083815	-1.783268
85	1	0	-0.455780	1.483312	-1.305490
86	8	0	4.027688	1.897937	0.101133
87	1	0	3.112849	2.155891	0.353429

γ'-INT1-D

Zero-point correction= 0.739633 (Hartree/Particle)
Thermal correction to Energy= 0.778887
Thermal correction to Enthalpy= 0.779831
Thermal correction to Gibbs Free Energy= 0.663527
E(sov) = -1938.21877024 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-3.347700	3.840249	1.013409
2	6	0	-4.379057	4.599049	0.413498
3	6	0	-5.108579	4.065900	-0.615555
4	6	0	-4.844252	2.754118	-1.086737
5	6	0	-3.810225	1.979796	-0.482059
6	6	0	-3.066896	2.569193	0.578867
7	6	0	-2.547627	-0.300561	-0.440800
8	6	0	-2.906656	-0.778122	0.983195
9	7	0	-1.901712	-1.743352	1.491176
10	6	0	-2.196150	-2.028309	2.908280
11	6	0	-4.327703	-1.400308	1.062839
12	6	0	-3.579290	-2.710521	3.056763
13	6	0	-4.216206	-2.805973	1.664508
14	6	0	-1.911729	-3.007068	0.732062
15	6	0	-3.313142	-3.670402	0.752769
16	6	0	-3.958615	-3.891916	-0.593810
17	6	0	-3.425319	-3.746131	-1.804918
18	7	0	-5.619125	2.304576	-2.116992
19	6	0	-5.386196	1.097145	-2.561529
20	6	0	-4.391624	0.239787	-2.032074
21	6	0	-3.598606	0.659317	-0.992491
22	1	0	-4.584204	5.604236	0.768422
23	1	0	-5.904710	4.614710	-1.107653
24	1	0	-2.257027	2.027263	1.053108
25	1	0	-1.387628	-2.661466	3.287483
26	1	0	-2.143329	-1.076588	3.445715
27	1	0	-4.986295	-0.773765	1.672871
28	1	0	-4.778016	-1.459258	0.066867
29	1	0	-3.475699	-3.709820	3.492903
30	1	0	-4.228441	-2.132282	3.722058
31	1	0	-5.209231	-3.263734	1.733489
32	1	0	-1.160492	-3.656778	1.191588
33	1	0	-1.556022	-2.795380	-0.278850
34	1	0	-3.231053	-4.659745	1.226171
35	1	0	-4.993887	-4.232994	-0.531330
36	1	0	-4.006749	-3.965247	-2.694965
37	1	0	-2.398921	-3.429992	-1.972729
38	1	0	-6.008359	0.753277	-3.386552
39	1	0	-4.267321	-0.758099	-2.447692
40	1	0	-2.764724	4.270504	1.821759
41	1	0	-2.588857	-1.183481	-1.086302
42	1	0	-2.834713	0.081301	1.658432
43	7	0	-1.210007	0.234130	-0.457020
44	6	0	-0.236981	0.044558	-1.411849
45	1	0	-0.903215	0.698762	0.390836
46	6	0	1.012731	0.537615	-1.252650

47	6	0	-0.539269	-0.832121	-2.605018
48	6	0	2.096709	0.155996	-2.159174
49	1	0	1.254194	1.139921	-0.380238
50	6	0	0.370424	-0.483272	-3.787591
51	1	0	-1.585854	-0.726897	-2.911765
52	1	0	-0.387650	-1.884289	-2.309683
53	6	0	1.810861	-0.357961	-3.371648
54	6	0	3.470154	0.332767	-1.659074
55	1	0	0.031837	0.477785	-4.207130
56	1	0	0.248402	-1.230293	-4.577818
57	1	0	2.598953	-0.596830	-4.079420
58	6	0	4.502848	-0.462900	-1.973956
59	1	0	3.616532	1.132004	-0.929714
60	6	0	5.873154	-0.316641	-1.464671
61	1	0	4.318509	-1.330087	-2.607806
62	6	0	6.710543	-1.438919	-1.412765
63	6	0	6.374087	0.905733	-0.995029
64	6	0	7.990752	-1.356288	-0.874991
65	1	0	6.339836	-2.390514	-1.786007
66	6	0	7.654163	0.991067	-0.460555
67	1	0	5.753031	1.794999	-1.054632
68	6	0	8.466222	-0.140189	-0.390146
69	1	0	8.618308	-2.241716	-0.836630
70	1	0	8.024314	1.947930	-0.103084
71	1	0	9.466208	-0.069731	0.026634
72	6	0	4.663038	-0.187773	1.738333
73	6	0	5.020915	1.126834	2.065153
74	6	0	4.059689	2.074907	2.368499
75	6	0	2.701591	1.728752	2.355092
76	6	0	2.331829	0.404490	2.038958
77	6	0	3.325558	-0.536644	1.724889
78	1	0	5.427808	-0.910644	1.473583
79	1	0	6.069809	1.409096	2.064006
80	1	0	4.320151	3.098382	2.616006
81	1	0	3.013039	-1.539488	1.454456
82	6	0	0.905287	0.041520	1.967754
83	8	0	-0.003904	0.870180	2.161011
84	8	0	0.646073	-1.199683	1.653553
85	1	0	-0.382409	-1.310792	1.533803
86	8	0	1.811728	2.691773	2.639703
87	1	0	0.916199	2.293456	2.560849

α'-INT1-A

Zero-point correction= 0.739767 (Hartree/Particle)

Thermal correction to Energy= 0.778884
Thermal correction to Enthalpy= 0.779828
Thermal correction to Gibbs Free Energy= 0.664569
E(sov) = -1938.21318192 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.002426	-2.926158	-3.055695
2	6	0	-3.850599	-4.237401	-3.563748
3	6	0	-2.832090	-5.033747	-3.110246
4	6	0	-1.927589	-4.561365	-2.124279
5	6	0	-2.084228	-3.246313	-1.597985
6	6	0	-3.141289	-2.442547	-2.103563
7	6	0	-1.227700	-1.463567	0.098191
8	6	0	-2.440707	-1.348827	1.048387
9	7	0	-2.436094	-0.040962	1.752585
10	6	0	-3.643850	0.047602	2.598604
11	6	0	-2.483315	-2.502647	2.089177
12	6	0	-3.597598	-0.996988	3.741286
13	6	0	-2.387838	-1.906534	3.498227
14	6	0	-1.240376	0.121680	2.609639
15	6	0	-1.103809	-1.057189	3.610113
16	6	0	0.142268	-1.900701	3.467038
17	6	0	1.294322	-1.551851	2.896064
18	7	0	-0.939547	-5.416176	-1.728034
19	6	0	-0.105414	-4.986144	-0.816885
20	6	0	-0.179302	-3.705124	-0.217655
21	6	0	-1.164399	-2.823555	-0.588931
22	1	0	-4.538985	-4.605593	-4.318051
23	1	0	-2.677191	-6.041221	-3.482140
24	1	0	-3.255631	-1.425173	-1.751308
25	1	0	-3.697116	1.070943	2.983270
26	1	0	-4.511358	-0.102896	1.947828
27	1	0	-3.408255	-3.079736	1.985280
28	1	0	-1.657547	-3.201087	1.923272
29	1	0	-3.505211	-0.504210	4.715144
30	1	0	-4.517643	-1.589541	3.762685
31	1	0	-2.361927	-2.711250	4.241582
32	1	0	-1.354995	1.078565	3.121128
33	1	0	-0.369354	0.241275	1.960013
34	1	0	-1.080643	-0.646119	4.630214
35	1	0	0.076690	-2.883887	3.937911
36	1	0	2.143182	-2.229549	2.898338
37	1	0	1.453086	-0.584060	2.425736
38	1	0	0.682116	-5.674779	-0.513856

39	1	0	0.542070	-3.429056	0.548946
40	1	0	-4.801417	-2.293709	-3.430021
41	1	0	-0.352263	-1.431724	0.750762
42	1	0	-3.358297	-1.356495	0.447463
43	7	0	-1.160639	-0.361112	-0.847579
44	6	0	-0.040302	0.488168	-0.928098
45	1	0	-2.020272	0.172928	-0.914900
46	6	0	1.272274	-0.015644	-0.509970
47	6	0	-0.139213	1.738756	-1.419663
48	6	0	2.416620	0.663263	-0.747283
49	1	0	1.347360	-1.002455	-0.060449
50	6	0	1.026472	2.685319	-1.348052
51	1	0	-1.101306	2.116434	-1.753718
52	6	0	3.691767	0.064228	-0.378648
53	1	0	1.002193	3.198242	-0.372107
54	1	0	0.932971	3.471843	-2.103604
55	6	0	4.905440	0.572439	-0.656104
56	1	0	3.619481	-0.892916	0.138406
57	6	0	6.197218	-0.032825	-0.309002
58	1	0	4.971700	1.507164	-1.209892
59	6	0	7.361265	0.462792	-0.911315
60	6	0	6.325555	-1.086529	0.608251
61	6	0	8.607436	-0.084154	-0.627162
62	1	0	7.279692	1.284572	-1.618438
63	6	0	7.569274	-1.633561	0.893651
64	1	0	5.445455	-1.469627	1.116269
65	6	0	8.716672	-1.137958	0.275407
66	1	0	9.494429	0.314520	-1.110161
67	1	0	7.647177	-2.446606	1.609301
68	1	0	9.688028	-1.566628	0.501659
69	6	0	-2.899924	5.489089	-2.134722
70	6	0	-1.955930	6.500594	-1.919555
71	6	0	-1.034399	6.406779	-0.891694
72	6	0	-1.034928	5.291119	-0.043628
73	6	0	-1.975825	4.262638	-0.259039
74	6	0	-2.900228	4.380768	-1.306547
75	1	0	-3.620454	5.572542	-2.940868
76	1	0	-1.943046	7.373336	-2.565925
77	1	0	-0.296443	7.181144	-0.712496
78	1	0	-3.615261	3.577618	-1.452268
79	6	0	-1.946971	3.061661	0.602272
80	8	0	-1.181644	2.956969	1.562349
81	8	0	-2.792319	2.105011	0.269829
82	1	0	-2.594683	1.267790	0.852814
83	8	0	-0.116665	5.253391	0.933461
84	1	0	-0.266186	4.422033	1.440901

85	6	0	2.368528	1.969348	-1.507175
86	1	0	2.554490	1.738988	-2.567196
87	1	0	3.175183	2.633667	-1.183431

α'-INT1-B

Zero-point correction= 0.739135 (Hartree/Particle)
Thermal correction to Energy= 0.778603
Thermal correction to Enthalpy= 0.779547
Thermal correction to Gibbs Free Energy= 0.660051
E(sov) = -1938.22211450 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.208905	0.750066	-3.840750
2	6	0	-1.520036	0.792662	-5.074605
3	6	0	-0.267859	0.246001	-5.175683
4	6	0	0.349848	-0.364632	-4.053488
5	6	0	-0.342332	-0.416108	-2.808028
6	6	0	-1.639183	0.163201	-2.738473
7	6	0	-0.255967	-1.151580	-0.299780
8	6	0	-1.454814	-2.111429	-0.242925
9	7	0	-2.073639	-2.118620	1.105634
10	6	0	-3.267865	-2.984839	1.072569
11	6	0	-1.040999	-3.554685	-0.643131
12	6	0	-2.878876	-4.456020	0.783736
13	6	0	-1.369905	-4.501825	0.516709
14	6	0	-1.135196	-2.609242	2.130569
15	6	0	-0.624448	-4.035311	1.788414
16	6	0	0.870713	-4.176975	1.630387
17	6	0	1.820771	-3.336958	2.035098
18	7	0	1.602190	-0.874862	-4.240467
19	6	0	2.184261	-1.427400	-3.207303
20	6	0	1.590595	-1.528229	-1.926230
21	6	0	0.325590	-1.040605	-1.707048
22	1	0	-1.985415	1.260696	-5.936542
23	1	0	0.297079	0.259246	-6.102018
24	1	0	-2.198870	0.148825	-1.811844
25	1	0	-3.772928	-2.879823	2.038124
26	1	0	-3.936671	-2.577272	0.307752
27	1	0	-1.568258	-3.869663	-1.549422
28	1	0	0.030119	-3.595493	-0.869274
29	1	0	-3.130159	-5.099122	1.634205
30	1	0	-3.424266	-4.839040	-0.084659

31	1	0	-1.060126	-5.522891	0.267413
32	1	0	-1.672284	-2.599729	3.084274
33	1	0	-0.331410	-1.873801	2.212806
34	1	0	-0.917923	-4.719759	2.598205
35	1	0	1.180369	-5.107912	1.151128
36	1	0	2.870429	-3.570985	1.888166
37	1	0	1.604258	-2.400709	2.542947
38	1	0	3.185901	-1.824146	-3.366235
39	1	0	2.147038	-1.988049	-1.112606
40	1	0	-3.199164	1.188785	-3.760139
41	1	0	0.541610	-1.608250	0.299592
42	1	0	-2.237899	-1.740059	-0.910841
43	7	0	-0.596838	0.125676	0.327254
44	6	0	0.373235	1.143239	0.197572
45	1	0	-1.513173	0.451432	0.027452
46	6	0	1.713852	0.836148	0.704733
47	6	0	0.114995	2.358713	-0.313233
48	6	0	2.784380	1.595007	0.390736
49	1	0	1.829486	-0.041814	1.339124
50	6	0	1.192356	3.410578	-0.308194
51	1	0	-0.878295	2.598873	-0.685887
52	6	0	4.110138	1.217236	0.858509
53	1	0	1.184539	3.952590	0.650455
54	1	0	1.003065	4.154036	-1.088051
55	6	0	5.265428	1.817734	0.522995
56	1	0	4.133849	0.344503	1.510881
57	6	0	6.606422	1.425135	0.974568
58	1	0	5.242600	2.661854	-0.163813
59	6	0	7.725606	1.960853	0.323500
60	6	0	6.824459	0.539031	2.040189
61	6	0	9.016310	1.612200	0.705573
62	1	0	7.574338	2.657124	-0.497701
63	6	0	8.112605	0.189965	2.423146
64	1	0	5.978603	0.133071	2.586965
65	6	0	9.215739	0.721903	1.756591
66	1	0	9.867073	2.039036	0.182978
67	1	0	8.258662	-0.496082	3.252202
68	1	0	10.221677	0.449374	2.060189
69	6	0	-5.984740	2.913719	3.198750
70	6	0	-6.672886	3.633455	2.213962
71	6	0	-6.465752	3.379313	0.869861
72	6	0	-5.556240	2.390468	0.472084
73	6	0	-4.859175	1.660109	1.457424
74	6	0	-5.086490	1.935790	2.813692
75	1	0	-6.153565	3.121727	4.249527
76	1	0	-7.380445	4.404541	2.505212

77	1	0	-6.990410	3.927623	0.095018
78	1	0	-4.534807	1.361820	3.550475
79	6	0	-3.895460	0.617541	1.055580
80	8	0	-3.662451	0.358495	-0.138217
81	8	0	-3.296305	-0.014592	2.027607
82	1	0	-2.687717	-0.763129	1.615866
83	8	0	-5.395019	2.187354	-0.843810
84	1	0	-4.734729	1.465772	-0.946934
85	6	0	2.572445	2.783301	-0.522842
86	1	0	2.663968	2.436669	-1.563333
87	1	0	3.346332	3.539531	-0.364633

α'-INT1-C

Zero-point correction= 0.739363 (Hartree/Particle)
Thermal correction to Energy= 0.778376
Thermal correction to Enthalpy= 0.779320
Thermal correction to Gibbs Free Energy= 0.665450
E(sov) = -1938.21687301 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.253936	3.624402	-0.784943
2	6	0	-5.490056	3.814347	-1.445954
3	6	0	-6.168245	2.737561	-1.953532
4	6	0	-5.647683	1.424787	-1.815671
5	6	0	-4.410083	1.226122	-1.138767
6	6	0	-3.725111	2.367026	-0.637603
7	6	0	-2.671147	-0.478159	-0.243890
8	6	0	-2.894202	-0.282516	1.277839
9	7	0	-1.626713	-0.410196	2.040616
10	6	0	-1.883977	-0.160966	3.476188
11	6	0	-3.928971	-1.308459	1.818705
12	6	0	-2.838991	-1.226989	4.061946
13	6	0	-3.267612	-2.151352	2.917535
14	6	0	-1.028307	-1.752769	1.872668
15	6	0	-2.008832	-2.854822	2.356822
16	6	0	-2.379551	-3.913010	1.346085
17	6	0	-1.875968	-4.114189	0.130128
18	7	0	-6.381778	0.405833	-2.351697
19	6	0	-5.907830	-0.806875	-2.226114
20	6	0	-4.697685	-1.118369	-1.559211
21	6	0	-3.940550	-0.117547	-1.003588

22	1	0	-5.893955	4.816053	-1.554984
23	1	0	-7.115139	2.842541	-2.472885
24	1	0	-2.761793	2.246884	-0.155794
25	1	0	-0.907167	-0.157924	3.969940
26	1	0	-2.300752	0.847985	3.560160
27	1	0	-4.809943	-0.795697	2.218259
28	1	0	-4.279328	-1.957880	1.009722
29	1	0	-2.340190	-1.805417	4.846544
30	1	0	-3.717893	-0.755881	4.513546
31	1	0	-3.974441	-2.904604	3.282802
32	1	0	-0.099313	-1.751136	2.447714
33	1	0	-0.749635	-1.865559	0.821467
34	1	0	-1.546616	-3.385645	3.202060
35	1	0	-3.148470	-4.601771	1.702249
36	1	0	-2.227426	-4.940624	-0.480343
37	1	0	-1.106347	-3.486971	-0.313371
38	1	0	-6.499404	-1.608562	-2.665921
39	1	0	-4.372761	-2.154442	-1.488757
40	1	0	-3.714667	4.483735	-0.398394
41	1	0	-2.523719	-1.554921	-0.400953
42	1	0	-3.244929	0.740232	1.459238
43	7	0	-1.486172	0.194512	-0.739490
44	6	0	-0.579842	-0.515357	-1.531520
45	1	0	-1.032911	0.824958	-0.092367
46	6	0	0.828682	-0.127516	-1.374731
47	6	0	-0.913940	-1.519371	-2.368561
48	6	0	1.836114	-0.930022	-1.775253
49	1	0	1.048781	0.805014	-0.856856
50	6	0	0.162043	-2.175242	-3.193559
51	1	0	-1.954306	-1.776495	-2.544892
52	6	0	3.216212	-0.599367	-1.437632
53	1	0	0.309460	-1.610320	-4.127508
54	1	0	-0.140643	-3.184997	-3.489276
55	6	0	4.296375	-1.328830	-1.765752
56	1	0	3.354494	0.312707	-0.853144
57	6	0	5.670994	-1.027820	-1.340355
58	1	0	4.184450	-2.203854	-2.403695
59	6	0	6.748962	-1.388793	-2.159240
60	6	0	5.940190	-0.404204	-0.114796
61	6	0	8.056281	-1.099275	-1.785416
62	1	0	6.553129	-1.889192	-3.104506
63	6	0	7.248160	-0.119023	0.260452
64	1	0	5.124531	-0.182611	0.567406
65	6	0	8.310741	-0.457582	-0.575291
66	1	0	8.878983	-1.377914	-2.437144
67	1	0	7.436680	0.349697	1.222542

68	1	0	9.331898	-0.238224	-0.278486
69	6	0	2.963473	3.926695	-0.054031
70	6	0	4.302317	3.647070	0.244050
71	6	0	4.640784	2.603700	1.088220
72	6	0	3.639712	1.806426	1.658317
73	6	0	2.288835	2.073907	1.357071
74	6	0	1.971045	3.139779	0.501695
75	1	0	2.707280	4.746283	-0.716084
76	1	0	5.091145	4.251148	-0.194244
77	1	0	5.674802	2.371847	1.320320
78	1	0	0.924686	3.327189	0.283430
79	6	0	1.230084	1.197169	1.902364
80	8	0	1.471287	0.241596	2.644283
81	8	0	0.005372	1.493577	1.522094
82	1	0	-0.643726	0.680947	1.771575
83	8	0	4.025490	0.796639	2.454969
84	1	0	3.211141	0.324340	2.747127
85	6	0	1.493108	-2.243984	-2.441587
86	1	0	1.445378	-3.017871	-1.659333
87	1	0	2.284535	-2.548095	-3.132464

α'-INT1-D

Zero-point correction= 0.739796 (Hartree/Particle)
Thermal correction to Energy= 0.778784
Thermal correction to Enthalpy= 0.779729
Thermal correction to Gibbs Free Energy= 0.665394
E(sov) = -1938.22545150 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.357062	4.004835	-0.158889
2	6	0	4.434269	4.626489	0.514371
3	6	0	5.221484	3.897253	1.365837
4	6	0	4.973843	2.515985	1.575764
5	6	0	3.898366	1.880361	0.889334
6	6	0	3.091972	2.670995	0.023866
7	6	0	2.622260	-0.335577	0.428286
8	6	0	2.921896	-0.508184	-1.077172
9	7	0	1.869035	-1.311644	-1.747598
10	6	0	2.138619	-1.322350	-3.200197
11	6	0	4.311090	-1.159569	-1.321037
12	6	0	3.477093	-2.037988	-3.507496
13	6	0	4.127349	-2.420457	-2.173286

14	6	0	1.827624	-2.701760	-1.248806
15	6	0	3.197174	-3.405816	-1.428298
16	6	0	3.844656	-3.918666	-0.164790
17	6	0	3.310945	-4.029492	1.049944
18	7	0	5.801101	1.863633	2.444520
19	6	0	5.579444	0.589882	2.643383
20	6	0	4.549732	-0.142788	2.004068
21	6	0	3.705001	0.482324	1.121534
22	1	0	4.628215	5.683229	0.358629
23	1	0	6.051544	4.339195	1.907167
24	1	0	2.244736	2.230338	-0.488516
25	1	0	1.291711	-1.818552	-3.684757
26	1	0	2.140895	-0.280219	-3.533770
27	1	0	4.983983	-0.455018	-1.820736
28	1	0	4.781787	-1.424921	-0.368772
29	1	0	3.307950	-2.934750	-4.113583
30	1	0	4.145654	-1.384155	-4.076593
31	1	0	5.098135	-2.897625	-2.347437
32	1	0	1.043264	-3.213175	-1.815778
33	1	0	1.488977	-2.673253	-0.210052
34	1	0	3.064283	-4.276793	-2.086891
35	1	0	4.873490	-4.256430	-0.305219
36	1	0	3.888528	-4.445059	1.870094
37	1	0	2.291249	-3.733491	1.283934
38	1	0	6.242386	0.084111	3.344111
39	1	0	4.437943	-1.205057	2.210733
40	1	0	2.727143	4.591344	-0.820446
41	1	0	2.674775	-1.335422	0.873866
42	1	0	2.875420	0.475711	-1.556383
43	7	0	1.294771	0.185342	0.650216
44	6	0	0.375613	-0.462309	1.463350
45	1	0	0.894566	0.701312	-0.126004
46	6	0	-1.008838	0.004657	1.302623
47	6	0	0.648962	-1.422336	2.375782
48	6	0	-2.061966	-0.714582	1.737382
49	1	0	-1.165547	0.950364	0.784542
50	6	0	-0.474941	-1.983530	3.209148
51	1	0	1.670425	-1.698527	2.619360
52	6	0	-3.419973	-0.269473	1.452220
53	1	0	-0.621822	-1.368584	4.111577
54	1	0	-0.224249	-2.990142	3.559921
55	6	0	-4.534386	-0.990002	1.669638
56	1	0	-3.501780	0.705059	0.968463
57	6	0	-5.898636	-0.565945	1.333333
58	1	0	-4.448391	-1.992486	2.085571
59	6	0	-6.898575	-1.535378	1.174645

60	6	0	-6.247370	0.780303	1.152798
61	6	0	-8.194129	-1.179466	0.815927
62	1	0	-6.646943	-2.582587	1.324417
63	6	0	-7.542785	1.137652	0.799358
64	1	0	-5.498328	1.552918	1.299740
65	6	0	-8.521380	0.160166	0.622798
66	1	0	-8.949955	-1.948756	0.689627
67	1	0	-7.792550	2.186850	0.668784
68	1	0	-9.533210	0.442291	0.348715
69	6	0	-4.666858	0.281307	-1.846566
70	6	0	-5.021949	1.636191	-1.807954
71	6	0	-4.057261	2.628079	-1.787335
72	6	0	-2.697442	2.287908	-1.809144
73	6	0	-2.330227	0.926520	-1.859492
74	6	0	-3.327912	-0.061384	-1.873002
75	1	0	-5.434829	-0.484920	-1.828279
76	1	0	-6.072045	1.912394	-1.778302
77	1	0	-4.317042	3.680638	-1.752218
78	1	0	-3.017112	-1.100657	-1.883674
79	6	0	-0.905283	0.553623	-1.824360
80	8	0	0.002832	1.403100	-1.759513
81	8	0	-0.648483	-0.726325	-1.816243
82	1	0	0.387470	-0.866862	-1.708474
83	8	0	-1.805646	3.288543	-1.772774
84	1	0	-0.909491	2.882059	-1.777952
85	6	0	-1.788371	-2.033650	2.425153
86	1	0	-1.732949	-2.820968	1.657816
87	1	0	-2.609291	-2.296244	3.098731

1a

Zero-point correction= 0.245318 (Hartree/Particle)
Thermal correction to Energy= 0.258152
Thermal correction to Enthalpy= 0.259097
Thermal correction to Gibbs Free Energy= 0.203683
E(sov) = -616.914843741 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.860692	-0.798692	-0.164361
2	6	0	-2.409191	-1.048914	-0.051996
3	6	0	-1.487388	-0.064908	0.032795
4	1	0	-2.111831	-2.094616	-0.079140
5	6	0	-3.352121	1.550036	0.562958

6	6	0	-0.068062	-0.410298	0.042494
7	1	0	-3.416338	1.276675	1.623114
8	1	0	-3.656049	2.598136	0.482689
9	6	0	0.941833	0.476026	0.013539
10	1	0	0.148599	-1.477063	0.040155
11	6	0	2.375974	0.162304	0.005515
12	1	0	0.709034	1.538882	-0.030382
13	6	0	3.288622	1.188756	-0.269671
14	6	0	2.877696	-1.120417	0.270270
15	6	0	4.657136	0.944374	-0.297764
16	1	0	2.913254	2.189677	-0.468481
17	6	0	4.243894	-1.365340	0.244487
18	1	0	2.196264	-1.929787	0.513990
19	6	0	5.139724	-0.335543	-0.041938
20	1	0	5.346239	1.754214	-0.516725
21	1	0	4.614522	-2.363881	0.455188
22	1	0	6.207366	-0.530843	-0.058752
23	6	0	-1.905149	1.386544	0.097742
24	1	0	-1.773197	1.838099	-0.896420
25	1	0	-1.236464	1.928579	0.774559
26	8	0	-4.657938	-1.714231	-0.227832
27	6	0	-4.289899	0.655227	-0.244150
28	1	0	-5.329034	0.723550	0.087244
29	1	0	-4.263123	0.947299	-1.303906

C3-SA

Zero-point correction= 0.519350 (Hartree/Particle)
Thermal correction to Energy= 0.546350
Thermal correction to Enthalpy= 0.547294
Thermal correction to Gibbs Free Energy= 0.460456
E(sov) = -1397.71988527 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.582932	-2.984541	0.958808
2	6	0	-1.235859	-4.351234	1.073512
3	6	0	-0.036713	-4.799100	0.585612
4	6	0	0.870615	-3.902772	-0.036375
5	6	0	0.530719	-2.521368	-0.147016
6	6	0	-0.726072	-2.091088	0.365857
7	6	0	1.293827	-0.159630	-0.931104
8	6	0	1.449767	0.539038	0.435842

9	7	0	1.152702	1.996404	0.347328
10	6	0	1.156731	2.562322	1.715083
11	6	0	2.868945	0.328036	1.028334
12	6	0	2.542082	2.396159	2.384828
13	6	0	3.468804	1.689544	1.391451
14	6	0	2.152265	2.704240	-0.472850
15	6	0	3.582298	2.548204	0.110967
16	6	0	4.619027	1.979806	-0.826880
17	6	0	4.526099	1.767157	-2.137342
18	7	0	2.038924	-4.431613	-0.504611
19	6	0	2.876299	-3.614398	-1.089514
20	6	0	2.644149	-2.227803	-1.251780
21	6	0	1.486100	-1.659942	-0.777995
22	1	0	-1.927329	-5.044788	1.542646
23	1	0	0.262701	-5.840226	0.647868
24	1	0	-1.011287	-1.051581	0.258228
25	1	0	0.878063	3.618011	1.625954
26	1	0	0.360586	2.056687	2.266637
27	1	0	2.822853	-0.316920	1.911668
28	1	0	3.518296	-0.174534	0.302903
29	1	0	2.959247	3.369451	2.665578
30	1	0	2.461260	1.801934	3.300837
31	1	0	4.464831	1.557654	1.828803
32	1	0	1.854472	3.756625	-0.509202
33	1	0	2.084129	2.321495	-1.494251
34	1	0	3.948434	3.538130	0.421108
35	1	0	5.563860	1.736621	-0.336934
36	1	0	5.366436	1.365010	-2.694207
37	1	0	3.635986	1.996153	-2.716243
38	1	0	3.801216	-4.049856	-1.465274
39	1	0	3.392588	-1.614960	-1.748358
40	1	0	-2.542008	-2.633555	1.328712
41	1	0	2.129393	0.180313	-1.567067
42	1	0	0.681384	0.138178	1.102694
43	6	0	-5.225753	1.824029	-1.712102
44	6	0	-6.000118	0.824808	-1.110933
45	6	0	-5.507229	0.080100	-0.053492
46	6	0	-4.217588	0.322399	0.435819
47	6	0	-3.429869	1.326143	-0.164824
48	6	0	-3.948459	2.063280	-1.237546
49	1	0	-5.621469	2.401655	-2.540380
50	1	0	-7.003435	0.626774	-1.477122
51	1	0	-6.094141	-0.698489	0.421740
52	1	0	-3.319591	2.826586	-1.683549
53	6	0	-2.062652	1.570530	0.333621
54	8	0	-1.600739	0.968575	1.309241

55	8	0	-1.361348	2.466615	-0.327164
56	1	0	-0.370071	2.321892	-0.061938
57	8	0	-3.786385	-0.428774	1.463056
58	1	0	-2.887527	-0.101317	1.704166
59	7	0	-0.014163	0.135833	-1.510830
60	1	0	-0.070965	1.109555	-1.799185
61	1	0	-0.159263	-0.435704	-2.340011

γ'-TS1 (γ'-TS1-A)

Zero-point correction= 0.968435 (Hartree/Particle)
Thermal correction to Energy= 1.021740
Thermal correction to Enthalpy= 1.022684
Thermal correction to Gibbs Free Energy= 0.879109
E(sov) = -2684.24846977 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.194757	-3.201332	2.513590
2	6	0	5.196240	-4.442223	3.191435
3	6	0	4.096967	-5.257218	3.128510
4	6	0	2.952158	-4.872042	2.383577
5	6	0	2.945874	-3.624040	1.695097
6	6	0	4.101609	-2.799442	1.788467
7	6	0	1.645602	-2.019450	0.119936
8	6	0	2.544863	-2.093299	-1.126806
9	7	0	2.395232	-0.896888	-1.995883
10	6	0	3.552205	-0.860912	-2.922352
11	6	0	2.268899	-3.365367	-1.963623
12	6	0	3.707090	-2.216188	-3.648746
13	6	0	2.405291	-3.003410	-3.447224
14	6	0	1.142361	-0.961586	-2.784732
15	6	0	1.216378	-2.092406	-3.837137
16	6	0	-0.059672	-2.874481	-4.012134
17	6	0	-1.236928	-2.636309	-3.438247
18	7	0	1.900928	-5.742785	2.369162
19	6	0	0.841423	-5.396652	1.684624
20	6	0	0.730535	-4.185058	0.959716
21	6	0	1.771464	-3.291059	0.949731
22	1	0	6.068487	-4.741648	3.764015
23	1	0	4.055722	-6.214626	3.637403
24	1	0	4.121547	-1.832332	1.300345
25	1	0	3.368439	-0.043370	-3.626744
26	1	0	4.438228	-0.600642	-2.334379

27	1	0	2.961536	-4.162842	-1.676658
28	1	0	1.253350	-3.734689	-1.774703
29	1	0	3.903665	-2.058371	-4.713831
30	1	0	4.552190	-2.782479	-3.241608
31	1	0	2.401271	-3.908791	-4.062800
32	1	0	0.999643	0.017269	-3.253720
33	1	0	0.314628	-1.090653	-2.084229
34	1	0	1.460235	-1.653252	-4.816958
35	1	0	0.024919	-3.710366	-4.708926
36	1	0	-2.095196	-3.263773	-3.662008
37	1	0	-1.413154	-1.813576	-2.749138
38	1	0	0.009174	-6.098884	1.686119
39	1	0	-0.183336	-3.969100	0.410418
40	1	0	6.065447	-2.555744	2.572726
41	1	0	0.602997	-1.971276	-0.227971
42	1	0	3.591652	-2.083125	-0.799840
43	7	0	1.903716	-0.806793	0.867472
44	6	0	0.914192	-0.115493	1.492942
45	1	0	2.759772	-0.298937	0.653436
46	6	0	-0.311647	-0.645608	1.777557
47	6	0	-1.441584	0.208789	2.026605
48	1	0	-0.505411	-1.697667	1.597409
49	6	0	0.136288	2.033399	2.564939
50	6	0	-2.761743	-0.372917	1.953287
51	1	0	0.238545	3.119261	2.483145
52	1	0	0.270223	1.775247	3.625393
53	6	0	-3.910234	0.344980	1.934584
54	1	0	-2.798381	-1.448818	1.790583
55	6	0	-5.265542	-0.151643	1.698217
56	1	0	-3.858121	1.419805	2.092371
57	6	0	-6.305216	0.784466	1.594658
58	6	0	-5.567097	-1.510835	1.523800
59	6	0	-7.605547	0.376891	1.319344
60	1	0	-6.079405	1.841611	1.701833
61	6	0	-6.865749	-1.916273	1.254042
62	1	0	-4.779895	-2.255541	1.592128
63	6	0	-7.890024	-0.974463	1.149021
64	1	0	-8.394111	1.117765	1.232180
65	1	0	-7.080541	-2.971483	1.113454
66	1	0	-8.904332	-1.296027	0.932053
67	6	0	3.975108	5.463170	-1.307480
68	6	0	4.987326	5.810694	-0.403353
69	6	0	5.559731	4.861717	0.424167
70	6	0	5.132034	3.527833	0.369283
71	6	0	4.100114	3.172206	-0.524417
72	6	0	3.538521	4.151729	-1.357967

73	1	0	3.541389	6.210899	-1.962968
74	1	0	5.335897	6.838059	-0.352797
75	1	0	6.349606	5.113025	1.123621
76	1	0	2.758176	3.851234	-2.050434
77	6	0	3.633590	1.775128	-0.592840
78	8	0	4.185151	0.860939	0.048185
79	8	0	2.596343	1.554292	-1.354498
80	1	0	2.447923	0.493751	-1.453471
81	8	0	5.732959	2.649748	1.183437
82	1	0	5.357118	1.762509	0.989867
83	6	0	-1.498720	2.204378	0.087579
84	1	0	-0.649575	1.600444	-0.228515
85	6	0	-1.188018	3.638379	0.304062
86	6	0	0.055965	4.110528	-0.136630
87	6	0	-2.046100	4.525714	0.966204
88	6	0	0.429975	5.434635	0.067691
89	1	0	0.734977	3.428341	-0.646556
90	6	0	-1.670769	5.848833	1.169603
91	1	0	-3.008435	4.182476	1.330771
92	6	0	-0.433553	6.308103	0.723230
93	1	0	1.402386	5.775702	-0.274984
94	1	0	-2.347853	6.522775	1.685484
95	1	0	-0.142320	7.340393	0.891784
96	6	0	-2.713401	1.708594	-0.423276
97	6	0	-3.896830	2.492933	-0.344828
98	7	0	-4.845968	3.158020	-0.244956
99	6	0	-2.690453	0.333750	-0.933096
100	6	0	-3.922947	-0.405162	-1.378269
101	6	0	-5.115555	0.185748	-1.806164
102	6	0	-3.840129	-1.804144	-1.338821
103	6	0	-6.198763	-0.610347	-2.171912
104	1	0	-5.214971	1.261725	-1.867263
105	6	0	-4.916878	-2.595732	-1.714204
106	1	0	-2.912109	-2.253289	-0.998456
107	6	0	-6.105249	-1.997499	-2.128421
108	1	0	-7.121165	-0.136816	-2.493625
109	1	0	-4.835032	-3.678217	-1.670969
110	1	0	-6.956526	-2.609670	-2.411575
111	8	0	-1.619954	-0.285577	-0.934417
112	6	0	-1.246298	1.583950	2.159922
113	1	0	-2.067079	2.195454	2.521475
114	6	0	1.225026	1.339754	1.747157
115	1	0	1.347356	1.828919	0.773202
116	1	0	2.195439	1.420991	2.252316

γ'-INT2

Zero-point correction= 0.973698 (Hartree/Particle)
Thermal correction to Energy= 1.026612
Thermal correction to Enthalpy= 1.027556
Thermal correction to Gibbs Free Energy= 0.884551
E(sov) = -2684.28529525 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.710954	-3.762051	-1.922313
2	6	0	-4.573523	-5.038966	-2.515600
3	6	0	-3.358841	-5.672238	-2.506645
4	6	0	-2.229982	-5.061234	-1.902820
5	6	0	-2.364187	-3.775598	-1.299489
6	6	0	-3.638273	-3.142976	-1.330698
7	6	0	-1.182100	-1.885947	0.031164
8	6	0	-1.968467	-2.008381	1.347598
9	7	0	-1.938630	-0.737951	2.152729
10	6	0	-3.062252	-0.785269	3.146145
11	6	0	-1.433788	-3.135018	2.252965
12	6	0	-2.975676	-2.106598	3.931980
13	6	0	-1.575733	-2.696708	3.716216
14	6	0	-0.630365	-0.551382	2.863472
15	6	0	-0.526130	-1.591493	3.999210
16	6	0	0.849372	-2.177036	4.197907
17	6	0	1.886664	-2.114975	3.365605
18	7	0	-1.057172	-5.757702	-1.935022
19	6	0	-0.007584	-5.205053	-1.383527
20	6	0	-0.023872	-3.935998	-0.754879
21	6	0	-1.192263	-3.216624	-0.702533
22	1	0	-5.433330	-5.510731	-2.980592
23	1	0	-3.212223	-6.649654	-2.954021
24	1	0	-3.779613	-2.158383	-0.897078
25	1	0	-2.940293	0.094899	3.781924
26	1	0	-3.985249	-0.676028	2.572967
27	1	0	-1.987353	-4.056362	2.050330
28	1	0	-0.376927	-3.331326	2.036758
29	1	0	-3.157190	-1.919083	4.994010
30	1	0	-3.740507	-2.811165	3.588634
31	1	0	-1.407833	-3.547610	4.382817
32	1	0	-0.629530	0.474130	3.241791
33	1	0	0.166289	-0.618566	2.116720

34	1	0	-0.817292	-1.110129	4.943749
35	1	0	0.954305	-2.726229	5.134405
36	1	0	2.823501	-2.598022	3.629151
37	1	0	1.872090	-1.581130	2.416256
38	1	0	0.920122	-5.773142	-1.421371
39	1	0	0.887948	-3.532937	-0.318045
40	1	0	-5.674068	-3.261478	-1.939587
41	1	0	-0.138159	-1.637836	0.266692
42	1	0	-3.027135	-2.162094	1.118459
43	7	0	-1.702453	-0.761646	-0.751060
44	6	0	-0.946018	-0.031100	-1.550693
45	1	0	-2.651696	-0.430049	-0.510105
46	6	0	0.314785	-0.490080	-1.982954
47	6	0	1.345950	0.408981	-2.139680
48	1	0	0.533699	-1.551402	-1.945141
49	6	0	-0.317333	2.155970	-2.597752
50	6	0	2.677877	-0.107025	-2.303292
51	1	0	-0.551152	3.220552	-2.517794
52	1	0	-0.258603	1.903733	-3.661774
53	6	0	3.802747	0.630529	-2.155437
54	1	0	2.757109	-1.189323	-2.388110
55	6	0	5.152205	0.081565	-2.038118
56	1	0	3.729489	1.705913	-2.017137
57	6	0	6.106890	0.836135	-1.340759
58	6	0	5.496892	-1.193686	-2.509687
59	6	0	7.369088	0.308783	-1.093104
60	1	0	5.834117	1.818542	-0.960602
61	6	0	6.765624	-1.706139	-2.279005
62	1	0	4.774252	-1.775039	-3.075708
63	6	0	7.701604	-0.959370	-1.562145
64	1	0	8.091105	0.889035	-0.527237
65	1	0	7.029321	-2.688913	-2.658145
66	1	0	8.690363	-1.367845	-1.375009
67	6	0	-5.128137	4.717655	-0.216122
68	6	0	-6.355466	4.440108	-0.828614
69	6	0	-6.779354	3.135012	-1.014828
70	6	0	-5.978779	2.066303	-0.590153
71	6	0	-4.746381	2.336240	0.039636
72	6	0	-4.339566	3.664906	0.214012
73	1	0	-4.796068	5.741857	-0.083749
74	1	0	-6.986603	5.256533	-1.168243
75	1	0	-7.725472	2.904738	-1.492910
76	1	0	-3.377443	3.838337	0.684931
77	6	0	-3.856610	1.235486	0.496259
78	8	0	-4.186391	0.025291	0.229127
79	8	0	-2.781789	1.517775	1.091758

80	1	0	-2.151775	0.134692	1.562917
81	8	0	-6.429788	0.819737	-0.804946
82	1	0	-5.725662	0.213016	-0.470909
83	6	0	1.035472	2.227583	-0.400364
84	1	0	0.282283	1.573514	0.059327
85	6	0	0.591778	3.666155	-0.201725
86	6	0	-0.500469	3.943562	0.624847
87	6	0	1.246010	4.734121	-0.826299
88	6	0	-0.921843	5.255743	0.832015
89	1	0	-1.032245	3.123737	1.103964
90	6	0	0.821150	6.043662	-0.624668
91	1	0	2.109087	4.546810	-1.458936
92	6	0	-0.264087	6.310321	0.206469
93	1	0	-1.765768	5.453643	1.488030
94	1	0	1.346015	6.858554	-1.113994
95	1	0	-0.592229	7.332998	0.366284
96	6	0	2.335338	1.886865	0.294272
97	6	0	3.407088	2.799913	0.177140
98	7	0	4.272783	3.560938	-0.006192
99	6	0	2.520673	0.576185	0.755428
100	6	0	3.859809	0.137044	1.280546
101	6	0	4.677991	0.932833	2.085868
102	6	0	4.302445	-1.139618	0.916485
103	6	0	5.923418	0.465921	2.499735
104	1	0	4.340789	1.917904	2.391770
105	6	0	5.551324	-1.599894	1.314672
106	1	0	3.652705	-1.752276	0.296925
107	6	0	6.366586	-0.794692	2.109458
108	1	0	6.548710	1.091975	3.129306
109	1	0	5.896659	-2.578927	0.994873
110	1	0	7.343855	-1.150116	2.423501
111	8	0	1.619131	-0.313495	0.660363
112	6	0	1.044792	1.868312	-1.942930
113	1	0	1.812751	2.478490	-2.429235
114	6	0	-1.430129	1.345753	-1.924945
115	1	0	-1.773266	1.842154	-1.008764
116	1	0	-2.305336	1.251141	-2.579848

γ′,δ-**TS2**

Zero-point correction= 0.971062 (Hartree/Particle)
Thermal correction to Energy= 1.023357
Thermal correction to Enthalpy= 1.024301

Thermal correction to Gibbs Free Energy= 0.883195

E(sov) = -2684.27161981 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.581825	-1.287799	-1.279889
2	6	0	-7.203278	-2.258324	-2.099487
3	6	0	-6.497520	-3.356344	-2.515464
4	6	0	-5.142555	-3.532352	-2.134388
5	6	0	-4.510540	-2.556471	-1.308882
6	6	0	-5.272529	-1.430225	-0.893889
7	6	0	-2.322743	-1.834307	-0.096680
8	6	0	-2.782802	-1.800162	1.376921
9	7	0	-1.941746	-0.858915	2.162209
10	6	0	-2.444745	-0.832399	3.554014
11	6	0	-2.721049	-3.212132	2.020300
12	6	0	-2.219817	-2.197357	4.245023
13	6	0	-1.722573	-3.185905	3.184668
14	6	0	-0.511948	-1.255662	2.162072
15	6	0	-0.344503	-2.714875	2.669813
16	6	0	0.231844	-3.694946	1.670778
17	6	0	1.022108	-3.412015	0.635007
18	7	0	-4.510920	-4.652103	-2.592967
19	6	0	-3.259670	-4.820163	-2.251725
20	6	0	-2.533387	-3.913630	-1.441781
21	6	0	-3.142232	-2.780738	-0.961237
22	1	0	-8.239056	-2.127936	-2.396962
23	1	0	-6.937237	-4.122713	-3.145209
24	1	0	-4.831412	-0.668062	-0.261572
25	1	0	-1.924092	-0.021284	4.071898
26	1	0	-3.504582	-0.562759	3.504366
27	1	0	-3.711014	-3.514814	2.376784
28	1	0	-2.411396	-3.957135	1.279939
29	1	0	-1.481358	-2.108356	5.048985
30	1	0	-3.149140	-2.560310	4.695174
31	1	0	-1.628409	-4.188667	3.615691
32	1	0	0.014462	-0.547290	2.807959
33	1	0	-0.097502	-1.101252	1.163464
34	1	0	0.337017	-2.705961	3.532639
35	1	0	-0.010072	-4.740405	1.875033
36	1	0	1.409445	-4.212465	0.008783
37	1	0	1.346340	-2.396876	0.407628
38	1	0	-2.768256	-5.716495	-2.626879
39	1	0	-1.493949	-4.123453	-1.198280
40	1	0	-7.144439	-0.417757	-0.955164

41	1	0	-1.309967	-2.242492	-0.085833
42	1	0	-3.796973	-1.393706	1.429832
43	7	0	-2.230746	-0.490445	-0.642182
44	6	0	-1.139425	0.015884	-1.255154
45	1	0	-2.963865	0.157842	-0.371653
46	6	0	-0.077896	-0.751285	-1.682461
47	6	0	1.176887	-0.172270	-2.007159
48	1	0	-0.127307	-1.834858	-1.630081
49	6	0	-0.024665	1.975225	-2.349244
50	6	0	2.321572	-0.956308	-2.083821
51	1	0	0.063836	3.063848	-2.318467
52	1	0	-0.301283	1.692640	-3.371655
53	6	0	3.584325	-0.363463	-2.125531
54	1	0	2.231574	-2.024349	-1.902059
55	6	0	4.838292	-1.076033	-1.896835
56	1	0	3.704811	0.592133	-2.625861
57	6	0	6.043201	-0.482927	-2.301605
58	6	0	4.881740	-2.302369	-1.213388
59	6	0	7.258479	-1.109956	-2.050366
60	1	0	6.017988	0.483210	-2.797826
61	6	0	6.095309	-2.923669	-0.960028
62	1	0	3.962860	-2.742858	-0.836017
63	6	0	7.285943	-2.330670	-1.381485
64	1	0	8.183694	-0.640068	-2.368827
65	1	0	6.117639	-3.858763	-0.409367
66	1	0	8.235315	-2.815948	-1.175074
67	6	0	-2.502852	5.630899	0.587386
68	6	0	-3.750253	6.078313	0.133843
69	6	0	-4.827917	5.214891	0.042094
70	6	0	-4.684094	3.867404	0.397809
71	6	0	-3.434852	3.410740	0.869610
72	6	0	-2.359058	4.307123	0.956865
73	1	0	-1.654895	6.305603	0.637302
74	1	0	-3.877905	7.116903	-0.157480
75	1	0	-5.797621	5.546324	-0.312844
76	1	0	-1.405210	3.931320	1.309697
77	6	0	-3.248980	1.988520	1.210518
78	8	0	-4.145779	1.142921	1.018225
79	8	0	-2.078389	1.649218	1.672539
80	1	0	-2.039279	0.576320	1.796797
81	8	0	-5.756669	3.072066	0.269254
82	1	0	-5.479103	2.165415	0.527383
83	6	0	1.903695	1.757586	-0.611121
84	1	0	1.229892	1.315867	0.129178
85	6	0	1.848512	3.263543	-0.437508
86	6	0	1.224643	3.784647	0.697563

87	6	0	2.396563	4.152993	-1.367177
88	6	0	1.146967	5.160076	0.905834
89	1	0	0.802458	3.096992	1.428792
90	6	0	2.315298	5.527203	-1.165902
91	1	0	2.901789	3.770462	-2.250424
92	6	0	1.689443	6.036190	-0.029767
93	1	0	0.665802	5.544215	1.801869
94	1	0	2.748043	6.203542	-1.896635
95	1	0	1.632344	7.109077	0.127422
96	6	0	3.267798	1.172528	-0.287779
97	6	0	4.399829	1.942177	-0.654659
98	7	0	5.287990	2.562122	-1.082808
99	6	0	3.263242	0.088024	0.669631
100	6	0	4.498069	-0.506121	1.296814
101	6	0	5.803166	-0.025684	1.142716
102	6	0	4.296880	-1.671223	2.051091
103	6	0	6.874785	-0.710795	1.709534
104	1	0	6.009290	0.868611	0.570207
105	6	0	5.366559	-2.348471	2.620266
106	1	0	3.282309	-2.039107	2.164943
107	6	0	6.664657	-1.871998	2.446016
108	1	0	7.881544	-0.329694	1.566989
109	1	0	5.188711	-3.251999	3.196453
110	1	0	7.505957	-2.401256	2.884347
111	8	0	2.173229	-0.452181	0.928305
112	6	0	1.317963	1.315550	-2.021575
113	1	0	2.042712	1.617721	-2.785384
114	6	0	-1.112650	1.518024	-1.388038
115	1	0	-0.951316	1.949492	-0.391214
116	1	0	-2.098826	1.869785	-1.718094

γ′,δ-INT3

Zero-point correction= 0.972346 (Hartree/Particle)
Thermal correction to Energy= 1.025096
Thermal correction to Enthalpy= 1.026040
Thermal correction to Gibbs Free Energy= 0.882475
E(sov) = -2684.29476365 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.941599	-0.569381	-0.848620
2	6	0	-7.782652	-1.507735	-1.490444

3	6	0	-7.290452	-2.734857	-1.849167
4	6	0	-5.940200	-3.079375	-1.581634
5	6	0	-5.089629	-2.139031	-0.930681
6	6	0	-5.631022	-0.872543	-0.576965
7	6	0	-2.719830	-1.649520	0.019910
8	6	0	-3.055872	-1.451159	1.516445
9	7	0	-2.079739	-0.543910	2.172558
10	6	0	-2.481571	-0.354861	3.582496
11	6	0	-3.081576	-2.810971	2.268310
12	6	0	-2.367437	-1.681080	4.372383
13	6	0	-2.018405	-2.790798	3.374357
14	6	0	-0.700388	-1.076811	2.122574
15	6	0	-0.632354	-2.491371	2.760614
16	6	0	-0.184062	-3.594089	1.828939
17	6	0	0.568589	-3.453317	0.739161
18	7	0	-5.528354	-4.320518	-1.973291
19	6	0	-4.284455	-4.644866	-1.731446
20	6	0	-3.355717	-3.791234	-1.087704
21	6	0	-3.740419	-2.538667	-0.677968
22	1	0	-8.816293	-1.250203	-1.699830
23	1	0	-7.901653	-3.481222	-2.345849
24	1	0	-5.014442	-0.125811	-0.089575
25	1	0	-1.838781	0.426353	4.000468
26	1	0	-3.504618	0.034307	3.573754
27	1	0	-4.070814	-2.993107	2.700883
28	1	0	-2.885736	-3.634618	1.574121
29	1	0	-1.592204	-1.609143	5.142881
30	1	0	-3.309562	-1.911682	4.879629
31	1	0	-1.989720	-3.762003	3.880820
32	1	0	-0.065950	-0.366049	2.661431
33	1	0	-0.362635	-1.067979	1.082123
34	1	0	0.089032	-2.466355	3.590168
35	1	0	-0.488027	-4.598180	2.131641
36	1	0	0.868936	-4.321672	0.157835
37	1	0	0.938715	-2.487302	0.399825
38	1	0	-3.967875	-5.635752	-2.053654
39	1	0	-2.337776	-4.135499	-0.916985
40	1	0	-7.334246	0.404092	-0.571188
41	1	0	-1.775955	-2.202313	-0.008217
42	1	0	-4.021947	-0.944202	1.603975
43	7	0	-2.489430	-0.392951	-0.659004
44	6	0	-1.331472	-0.110756	-1.341422
45	1	0	-3.050796	0.396392	-0.359479
46	6	0	-0.462797	-1.048471	-1.803339
47	6	0	0.906224	-0.694692	-2.139526
48	1	0	-0.691565	-2.107987	-1.720008

49	6	0	0.023925	1.626257	-2.539125
50	6	0	1.940760	-1.547855	-2.026581
51	1	0	0.283085	2.688795	-2.551212
52	1	0	-0.380784	1.371256	-3.525100
53	6	0	3.324636	-0.976682	-2.025569
54	1	0	1.798420	-2.606215	-1.825984
55	6	0	4.428406	-1.979024	-1.781659
56	1	0	3.530441	-0.493310	-2.989836
57	6	0	5.604778	-1.917618	-2.532979
58	6	0	4.320133	-2.945103	-0.775733
59	6	0	6.659308	-2.790109	-2.275399
60	1	0	5.699724	-1.165542	-3.312636
61	6	0	5.373578	-3.815998	-0.516343
62	1	0	3.414750	-2.998920	-0.174948
63	6	0	6.547404	-3.738206	-1.261873
64	1	0	7.567775	-2.727959	-2.866780
65	1	0	5.278418	-4.553580	0.274561
66	1	0	7.369393	-4.417096	-1.056655
67	6	0	-1.339810	5.777961	0.151199
68	6	0	-2.448384	6.457680	-0.368919
69	6	0	-3.691697	5.852559	-0.432998
70	6	0	-3.859191	4.537571	0.020747
71	6	0	-2.752573	3.852670	0.563897
72	6	0	-1.502126	4.486479	0.616596
73	1	0	-0.362262	6.247513	0.181993
74	1	0	-2.335083	7.473365	-0.737001
75	1	0	-4.556691	6.363295	-0.842078
76	1	0	-0.659369	3.933576	1.018594
77	6	0	-2.896078	2.456289	1.015931
78	8	0	-3.945060	1.807250	0.845941
79	8	0	-1.838229	1.922559	1.562470
80	1	0	-2.005313	0.876831	1.722372
81	8	0	-5.079350	3.990285	-0.086138
82	1	0	-5.010792	3.060559	0.225100
83	6	0	2.054985	1.094252	-1.008868
84	1	0	1.457222	0.668673	-0.198608
85	6	0	2.241921	2.560656	-0.689553
86	6	0	1.953556	3.009319	0.601510
87	6	0	2.682330	3.488930	-1.638657
88	6	0	2.110276	4.350566	0.945824
89	1	0	1.594087	2.295705	1.341364
90	6	0	2.832363	4.829576	-1.301531
91	1	0	2.917801	3.158596	-2.647323
92	6	0	2.549537	5.264211	-0.007641
93	1	0	1.883273	4.679767	1.955997
94	1	0	3.177824	5.536442	-2.049473

95	1	0	2.674353	6.310592	0.255062
96	6	0	3.394412	0.256231	-0.977155
97	6	0	4.525136	1.076927	-1.426332
98	7	0	5.395009	1.685422	-1.886231
99	6	0	3.561539	-0.286812	0.468938
100	6	0	4.856879	-0.265482	1.216886
101	6	0	6.119647	-0.382482	0.626999
102	6	0	4.754320	-0.172519	2.610696
103	6	0	7.257906	-0.401959	1.426878
104	1	0	6.226386	-0.486153	-0.446331
105	6	0	5.894110	-0.168814	3.402685
106	1	0	3.767284	-0.099399	3.055394
107	6	0	7.150018	-0.285428	2.809551
108	1	0	8.232837	-0.508211	0.962237
109	1	0	5.804914	-0.079395	4.480856
110	1	0	8.043856	-0.288219	3.426081
111	8	0	2.566868	-0.723489	1.017753
112	6	0	1.266330	0.767715	-2.304480
113	1	0	1.933380	0.891157	-3.169291
114	6	0	-1.033758	1.362259	-1.478910
115	1	0	-0.700561	1.748995	-0.506500
116	1	0	-1.961552	1.899075	-1.718896

7a

Zero-point correction= 0.478303 (Hartree/Particle)
Thermal correction to Energy= 0.505079
Thermal correction to Enthalpy= 0.506023
Thermal correction to Gibbs Free Energy= 0.419825
E(sov) = -1362.97539141 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.507315	-2.073545	0.913762
2	6	0	-3.156630	-2.660813	0.763372
3	6	0	-2.165454	-2.054466	0.093856
4	1	0	-2.970664	-3.568388	1.334560
5	6	0	-3.854033	-0.411678	-0.832901
6	1	0	-3.958298	0.622163	-1.170282
7	1	0	-4.291931	-1.046285	-1.612867
8	6	0	0.229521	-1.687478	-0.612097
9	6	0	1.673179	-2.139463	-0.541759

10	1	0	-0.086315	-1.825084	-1.651785
11	6	0	2.412302	-2.251543	-1.723101
12	6	0	2.306039	-2.407808	0.676216
13	6	0	3.758546	-2.604607	-1.690456
14	1	0	1.929796	-2.041190	-2.674929
15	6	0	3.651850	-2.760618	0.709795
16	1	0	1.754925	-2.320439	1.608453
17	6	0	4.382731	-2.856341	-0.471592
18	1	0	4.317653	-2.682382	-2.617866
19	1	0	4.130872	-2.956201	1.664095
20	1	0	5.432988	-3.129482	-0.442526
21	6	0	-1.433544	0.245237	-0.030816
22	1	0	-1.532250	0.088412	1.046811
23	6	0	-1.716665	1.708805	-0.287356
24	6	0	-1.692367	2.596138	0.791258
25	6	0	-1.979442	2.211304	-1.566247
26	6	0	-1.924985	3.956166	0.601913
27	1	0	-1.487661	2.211523	1.788369
28	6	0	-2.216737	3.568062	-1.756937
29	1	0	-1.990278	1.538782	-2.420378
30	6	0	-2.189853	4.444022	-0.673509
31	1	0	-1.903102	4.630836	1.452115
32	1	0	-2.418742	3.943027	-2.755423
33	1	0	-2.375136	5.502814	-0.825614
34	6	0	0.072178	-0.133059	-0.336577
35	6	0	0.515156	0.524292	-1.574434
36	7	0	0.829307	0.948469	-2.603601
37	6	0	0.900796	0.279954	0.916213
38	6	0	2.181219	1.043579	0.841952
39	6	0	3.124560	0.904282	-0.180843
40	6	0	2.444255	1.905066	1.914293
41	6	0	4.312235	1.626446	-0.127579
42	1	0	2.957054	0.218694	-1.003187
43	6	0	3.619927	2.642011	1.949430
44	1	0	1.710283	1.988110	2.709327
45	6	0	4.556702	2.501738	0.926742
46	1	0	5.047228	1.503300	-0.916248
47	1	0	3.809163	3.321964	2.773981
48	1	0	5.479346	3.073550	0.954142
49	8	0	0.439620	-0.022692	1.999046
50	6	0	-2.371337	-0.787351	-0.711575
51	1	0	-2.003807	-0.954623	-1.734624
52	6	0	-4.633138	-0.632413	0.460621
53	1	0	-4.232130	0.006166	1.260963
54	1	0	-5.692493	-0.391279	0.346586
55	8	0	-5.416150	-2.679212	1.444060

56	6	0	-0.724955	-2.498181	0.262633
57	1	0	-0.455351	-2.382934	1.319134
58	1	0	-0.612504	-3.561556	0.021888

α′-**TS1**

Zero-point correction= 0.968564 (Hartree/Particle)
Thermal correction to Energy= 1.022306
Thermal correction to Enthalpy= 1.023250
Thermal correction to Gibbs Free Energy= 0.877540
E(sov) = -2684.25017968 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.745970	3.177938	3.851001
2	6	0	-2.186261	4.171888	4.686643
3	6	0	-1.017469	4.787626	4.326042
4	6	0	-0.359580	4.442596	3.116528
5	6	0	-0.919822	3.441910	2.267826
6	6	0	-2.132777	2.818349	2.677631
7	6	0	-0.728160	2.141949	0.019711
8	6	0	-1.949713	2.754467	-0.696059
9	7	0	-2.555004	1.843530	-1.700144
10	6	0	-3.874564	2.394866	-2.086831
11	6	0	-1.590569	4.104805	-1.367129
12	6	0	-3.737086	3.843249	-2.612078
13	6	0	-2.242478	4.155360	-2.750865
14	6	0	-1.703495	1.722664	-2.905196
15	6	0	-1.582968	3.077668	-3.644723
16	6	0	-0.178652	3.473116	-4.027272
17	6	0	0.950902	2.805842	-3.797796
18	7	0	0.795183	5.110950	2.831584
19	6	0	1.409689	4.803413	1.717973
20	6	0	0.942093	3.830572	0.802651
21	6	0	-0.218895	3.143208	1.056500
22	1	0	-2.684472	4.439882	5.613155
23	1	0	-0.552571	5.552971	4.938817
24	1	0	-2.578248	2.038658	2.072007
25	1	0	-4.285137	1.724259	-2.848196
26	1	0	-4.526470	2.333705	-1.209096
27	1	0	-1.921801	4.939499	-0.741298
28	1	0	-0.505103	4.197742	-1.480121
29	1	0	-4.242946	3.952951	-3.576682
30	1	0	-4.199748	4.553687	-1.918598

31	1	0	-2.099454	5.144570	-3.198785
32	1	0	-2.161921	0.961402	-3.544879
33	1	0	-0.743265	1.321414	-2.581866
34	1	0	-2.169584	3.033849	-4.574507
35	1	0	-0.119496	4.428510	-4.552314
36	1	0	1.901474	3.209624	-4.135304
37	1	0	0.990947	1.841361	-3.296794
38	1	0	2.332081	5.341511	1.505233
39	1	0	1.509090	3.630786	-0.104578
40	1	0	-3.668903	2.686999	4.143826
41	1	0	0.072177	2.003228	-0.723969
42	1	0	-2.733069	2.909924	0.055168
43	7	0	-1.071789	0.852410	0.566175
44	6	0	-0.201896	-0.042640	1.109586
45	1	0	-2.057374	0.605102	0.607403
46	6	0	1.206188	0.260222	1.249176
47	6	0	2.095289	-0.670563	1.686359
48	1	0	1.584868	1.190819	0.837957
49	6	0	0.125586	-2.106207	2.461364
50	6	0	3.517956	-0.449567	1.480895
51	1	0	-0.154654	-3.163487	2.407751
52	1	0	-0.191206	-1.757014	3.453969
53	6	0	4.477302	-1.355350	1.747293
54	1	0	3.788868	0.493750	1.007546
55	6	0	5.893480	-1.206186	1.394854
56	1	0	4.214138	-2.286837	2.244732
57	6	0	6.862299	-1.960474	2.068471
58	6	0	6.308226	-0.345349	0.370223
59	6	0	8.210219	-1.833802	1.752524
60	1	0	6.549340	-2.647732	2.850495
61	6	0	7.653628	-0.222868	0.050019
62	1	0	5.565377	0.202119	-0.202307
63	6	0	8.611412	-0.961377	0.743612
64	1	0	8.948576	-2.421298	2.289786
65	1	0	7.953274	0.440467	-0.756598
66	1	0	9.662993	-0.867939	0.489809
67	6	0	-6.172976	-3.656918	-1.305193
68	6	0	-6.699301	-4.057713	-0.069539
69	6	0	-6.389611	-3.374689	1.092876
70	6	0	-5.544727	-2.256352	1.050624
71	6	0	-4.994841	-1.858264	-0.185327
72	6	0	-5.321382	-2.568187	-1.351349
73	1	0	-6.425277	-4.196315	-2.211434
74	1	0	-7.362746	-4.916230	-0.019549
75	1	0	-6.791056	-3.671903	2.055502
76	1	0	-4.886977	-2.238291	-2.289630

77	6	0	-4.080017	-0.702045	-0.246056
78	8	0	-3.891585	0.045247	0.730390
79	8	0	-3.464150	-0.521522	-1.383737
80	1	0	-2.962362	0.422050	-1.380028
81	8	0	-5.296802	-1.622174	2.203992
82	1	0	-4.737420	-0.840800	2.001081
83	6	0	1.649000	-1.960499	2.330377
84	1	0	2.110427	-2.019412	3.323806
85	1	0	2.077248	-2.795402	1.765067
86	6	0	-0.630976	-1.320978	1.428178
87	1	0	-1.691180	-1.544091	1.314512
88	6	0	-0.002875	-2.292423	-0.633971
89	1	0	-0.670729	-1.555518	-1.076251
90	6	0	-0.651815	-3.571489	-0.295802
91	6	0	-2.027902	-3.665251	-0.560457
92	6	0	-0.011257	-4.672342	0.292325
93	6	0	-2.747662	-4.809520	-0.246706
94	1	0	-2.529104	-2.818913	-1.023758
95	6	0	-0.732537	-5.823534	0.596913
96	1	0	1.048020	-4.639515	0.518185
97	6	0	-2.097820	-5.897206	0.334658
98	1	0	-3.813522	-4.846663	-0.454574
99	1	0	-0.220126	-6.666040	1.051307
100	1	0	-2.653590	-6.795484	0.585532
101	6	0	1.342275	-2.058854	-0.937925
102	6	0	2.377749	-2.984491	-0.627285
103	7	0	3.221746	-3.728611	-0.335483
104	6	0	1.677549	-0.774481	-1.553117
105	6	0	3.072004	-0.426046	-1.997106
106	6	0	3.991467	-1.343359	-2.513349
107	6	0	3.411120	0.933608	-1.971575
108	6	0	5.222915	-0.903538	-2.995784
109	1	0	3.750447	-2.398697	-2.561458
110	6	0	4.640701	1.370648	-2.448310
111	1	0	2.683918	1.640978	-1.582322
112	6	0	5.549495	0.448596	-2.968589
113	1	0	5.926841	-1.625183	-3.397492
114	1	0	4.889971	2.427303	-2.418730
115	1	0	6.509479	0.785064	-3.349169
116	8	0	0.803042	0.083281	-1.708388

α′-INT2

Zero-point correction= 0.972811 (Hartree/Particle)
Thermal correction to Energy= 1.025832

Thermal correction to Enthalpy= 1.026776
Thermal correction to Gibbs Free Energy= 0.883354
E(sov) = -2684.28371736 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.008811	3.218927	3.714800
2	6	0	-2.550453	4.270812	4.541777
3	6	0	-1.416344	4.961706	4.205580
4	6	0	-0.693188	4.636988	3.028433
5	6	0	-1.153769	3.580915	2.188232
6	6	0	-2.331669	2.879347	2.570854
7	6	0	-0.802480	2.256066	-0.016090
8	6	0	-2.038565	2.751193	-0.794141
9	7	0	-2.547489	1.763121	-1.777447
10	6	0	-3.862884	2.240396	-2.267016
11	6	0	-1.726403	4.092317	-1.508105
12	6	0	-3.747415	3.647720	-2.899889
13	6	0	-2.263382	4.026902	-2.939883
14	6	0	-1.624981	1.611268	-2.927501
15	6	0	-1.481851	2.939077	-3.713088
16	6	0	-0.060617	3.370132	-3.978054
17	6	0	1.057038	2.714368	-3.670166
18	7	0	0.423141	5.375144	2.762475
19	6	0	1.096333	5.082969	1.679153
20	6	0	0.729228	4.057858	0.774844
21	6	0	-0.392483	3.303128	1.010490
22	1	0	-3.098895	4.524144	5.443526
23	1	0	-1.030594	5.772097	4.815264
24	1	0	-2.699101	2.056557	1.967971
25	1	0	-4.217373	1.500486	-2.990992
26	1	0	-4.555298	2.225511	-1.418637
27	1	0	-2.168889	4.928434	-0.957304
28	1	0	-0.645482	4.263267	-1.541120
29	1	0	-4.170231	3.651284	-3.909678
30	1	0	-4.303507	4.385744	-2.311858
31	1	0	-2.130949	4.996492	-3.431950
32	1	0	-2.041187	0.821467	-3.561441
33	1	0	-0.680100	1.228066	-2.539486
34	1	0	-1.972758	2.831913	-4.691861
35	1	0	0.020877	4.330415	-4.491519
36	1	0	2.025030	3.132893	-3.933401
37	1	0	1.072118	1.745862	-3.174138
38	1	0	1.987071	5.677235	1.482384
39	1	0	1.340292	3.872958	-0.106294

40	1	0	-3.903658	2.669691	3.990162
41	1	0	0.029690	2.126243	-0.725241
42	1	0	-2.855669	2.891595	-0.076644
43	7	0	-1.053821	0.948409	0.565662
44	6	0	-0.112619	0.149261	1.041670
45	1	0	-1.992946	0.556110	0.464089
46	6	0	1.233619	0.532151	1.254559
47	6	0	2.142268	-0.402924	1.700148
48	1	0	1.593277	1.475047	0.857940
49	6	0	0.189902	-1.776103	2.530403
50	6	0	3.553847	-0.192433	1.459867
51	1	0	-0.082697	-2.817919	2.714833
52	1	0	-0.220504	-1.186846	3.358454
53	6	0	4.507864	-1.097517	1.764935
54	1	0	3.821889	0.710932	0.915295
55	6	0	5.915334	-0.997523	1.375822
56	1	0	4.241285	-1.989313	2.327616
57	6	0	6.884266	-1.716075	2.088158
58	6	0	6.318075	-0.222267	0.280329
59	6	0	8.227173	-1.629912	1.741240
60	1	0	6.576582	-2.340588	2.922840
61	6	0	7.658395	-0.145360	-0.072502
62	1	0	5.570530	0.284510	-0.322234
63	6	0	8.618351	-0.841048	0.661390
64	1	0	8.968884	-2.185434	2.306787
65	1	0	7.950458	0.446478	-0.935090
66	1	0	9.666133	-0.782568	0.382471
67	6	0	-6.000493	-3.892336	-1.341436
68	6	0	-6.430055	-4.352773	-0.088778
69	6	0	-6.082631	-3.688532	1.073069
70	6	0	-5.293459	-2.531217	1.014600
71	6	0	-4.842653	-2.071185	-0.239531
72	6	0	-5.206777	-2.762833	-1.406052
73	1	0	-6.281792	-4.419007	-2.246685
74	1	0	-7.046850	-5.244547	-0.026070
75	1	0	-6.408620	-4.032389	2.048410
76	1	0	-4.843517	-2.389058	-2.357772
77	6	0	-3.970259	-0.889020	-0.318138
78	8	0	-3.721344	-0.172794	0.669475
79	8	0	-3.446045	-0.640682	-1.490193
80	1	0	-2.963181	0.293020	-1.466983
81	8	0	-5.001951	-1.921344	2.171481
82	1	0	-4.482688	-1.115565	1.963964
83	6	0	1.708469	-1.617287	2.481227
84	1	0	2.110825	-1.512232	3.497429
85	1	0	2.184955	-2.507994	2.060063

86	6	0	-0.461035	-1.284725	1.239316
87	1	0	-1.549927	-1.387205	1.320708
88	6	0	-0.073362	-2.093925	-0.099587
89	1	0	-0.669224	-1.577599	-0.862606
90	6	0	-0.643696	-3.494388	0.040108
91	6	0	-1.885252	-3.753316	-0.548574
92	6	0	-0.041193	-4.513946	0.785955
93	6	0	-2.524095	-4.978851	-0.385569
94	1	0	-2.354239	-2.978312	-1.150225
95	6	0	-0.669764	-5.747593	0.937547
96	1	0	0.932152	-4.359716	1.240026
97	6	0	-1.914892	-5.982829	0.361162
98	1	0	-3.495736	-5.142041	-0.843639
99	1	0	-0.180000	-6.527619	1.512807
100	1	0	-2.403875	-6.943591	0.491174
101	6	0	1.355845	-1.970425	-0.582408
102	6	0	2.345577	-2.919777	-0.257956
103	7	0	3.167391	-3.672952	0.088188
104	6	0	1.665822	-0.827421	-1.351938
105	6	0	3.033142	-0.578490	-1.936172
106	6	0	3.876762	-1.575065	-2.433975
107	6	0	3.437640	0.758758	-2.043358
108	6	0	5.092782	-1.237177	-3.025022
109	1	0	3.582530	-2.617009	-2.378641
110	6	0	4.648738	1.097602	-2.636743
111	1	0	2.771779	1.527566	-1.660848
112	6	0	5.480907	0.095038	-3.134041
113	1	0	5.735055	-2.022754	-3.410898
114	1	0	4.943580	2.140850	-2.712252
115	1	0	6.425579	0.351201	-3.605276
116	8	0	0.813748	0.087498	-1.512680

α′,β-**TS2**

Zero-point correction= 0.971274 (Hartree/Particle)
Thermal correction to Energy= 1.023904
Thermal correction to Enthalpy= 1.024849
Thermal correction to Gibbs Free Energy= 0.882164
E(sov) = -2684.27358159 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-3.287870	3.414413	3.589832
2	6	0	-2.875019	4.525640	4.361361
3	6	0	-1.740460	5.212774	4.018852
4	6	0	-0.972551	4.825920	2.889526
5	6	0	-1.387682	3.710498	2.104203
6	6	0	-2.566129	3.014137	2.494138
7	6	0	-0.952878	2.255667	-0.005427
8	6	0	-2.172119	2.687538	-0.841967
9	7	0	-2.625300	1.636583	-1.786762
10	6	0	-3.952817	2.027638	-2.313025
11	6	0	-1.875706	3.996714	-1.618280
12	6	0	-3.900473	3.432166	-2.960576
13	6	0	-2.430446	3.860332	-3.038718
14	6	0	-1.678883	1.484489	-2.914272
15	6	0	-1.627401	2.766794	-3.780480
16	6	0	-0.236864	3.236956	-4.126170
17	6	0	0.913764	2.615425	-3.875446
18	7	0	0.141553	5.564564	2.614083
19	6	0	0.855020	5.213790	1.574804
20	6	0	0.531140	4.129158	0.724761
21	6	0	-0.587083	3.372150	0.968457
22	1	0	-3.457206	4.826074	5.226892
23	1	0	-1.388155	6.067337	4.587195
24	1	0	-2.893910	2.144498	1.937274
25	1	0	-4.243931	1.259690	-3.036775
26	1	0	-4.664879	1.982478	-1.482344
27	1	0	-2.317406	4.853901	-1.100327
28	1	0	-0.795558	4.173270	-1.669234
29	1	0	-4.348360	3.411599	-3.959343
30	1	0	-4.466126	4.157015	-2.365153
31	1	0	-2.337926	4.812943	-3.571425
32	1	0	-2.010195	0.620024	-3.498927
33	1	0	-0.711431	1.217542	-2.487907
34	1	0	-2.148268	2.580441	-4.731974
35	1	0	-0.209538	4.189958	-4.658151
36	1	0	1.854564	3.052938	-4.198391
37	1	0	0.979245	1.654703	-3.370247
38	1	0	1.744405	5.807787	1.370438
39	1	0	1.173770	3.900710	-0.122984
40	1	0	-4.181824	2.866808	3.871450
41	1	0	-0.093922	2.126282	-0.685283
42	1	0	-3.015238	2.843388	-0.158170
43	7	0	-1.186944	0.981680	0.630550
44	6	0	-0.186863	0.216714	1.112715
45	1	0	-2.124054	0.583708	0.603941
46	6	0	1.131901	0.583537	1.225096

47	6	0	2.062978	-0.482570	1.459070
48	1	0	1.493341	1.550302	0.892797
49	6	0	0.183001	-1.648562	2.673721
50	6	0	3.485895	-0.199223	1.248948
51	1	0	-0.078919	-2.680544	2.917637
52	1	0	-0.209365	-1.017144	3.476381
53	6	0	4.497984	-0.947860	1.719494
54	1	0	3.708832	0.660379	0.618843
55	6	0	5.914467	-0.730005	1.396823
56	1	0	4.288189	-1.785361	2.381967
57	6	0	6.908941	-1.215618	2.254200
58	6	0	6.302687	-0.069024	0.224198
59	6	0	8.254978	-1.017876	1.966594
60	1	0	6.618563	-1.749695	3.155420
61	6	0	7.646881	0.122944	-0.066690
62	1	0	5.546096	0.266219	-0.479077
63	6	0	8.628486	-0.344989	0.805568
64	1	0	9.013008	-1.395668	2.645932
65	1	0	7.927734	0.628127	-0.986527
66	1	0	9.679294	-0.197151	0.575566
67	6	0	-5.578752	-4.274205	-1.366611
68	6	0	-6.067655	-4.736684	-0.136873
69	6	0	-5.879241	-4.009911	1.024327
70	6	0	-5.193211	-2.787826	0.988000
71	6	0	-4.677039	-2.327174	-0.240452
72	6	0	-4.882652	-3.080520	-1.406393
73	1	0	-5.740500	-4.846617	-2.273602
74	1	0	-6.608018	-5.677766	-0.091219
75	1	0	-6.255108	-4.353462	1.981773
76	1	0	-4.478595	-2.700660	-2.339243
77	6	0	-3.911353	-1.069565	-0.290884
78	8	0	-3.827991	-0.299808	0.682261
79	8	0	-3.305694	-0.816169	-1.422250
80	1	0	-2.918431	0.164471	-1.407287
81	8	0	-5.057131	-2.118007	2.140465
82	1	0	-4.600611	-1.272014	1.942461
83	6	0	1.703964	-1.475325	2.555604
84	1	0	2.119307	-1.077228	3.489052
85	1	0	2.205895	-2.431228	2.378948
86	6	0	-0.482372	-1.226841	1.364095
87	1	0	-1.563800	-1.399234	1.409300
88	6	0	0.057192	-2.038361	0.112691
89	1	0	-0.479722	-1.594745	-0.732840
90	6	0	-0.405398	-3.481551	0.216549
91	6	0	-1.553208	-3.839796	-0.498161
92	6	0	0.180634	-4.442820	1.047676

93	6	0	-2.110111	-5.109912	-0.383561
94	1	0	-2.017359	-3.105108	-1.152851
95	6	0	-0.366000	-5.718889	1.154259
96	1	0	1.078271	-4.210442	1.610628
97	6	0	-1.514902	-6.056137	0.444874
98	1	0	-3.010045	-5.352495	-0.940905
99	1	0	0.109909	-6.450014	1.800777
100	1	0	-1.942794	-7.049666	0.538411
101	6	0	1.541815	-1.773771	-0.174451
102	6	0	2.493414	-2.818496	0.014107
103	7	0	3.295610	-3.622990	0.259230
104	6	0	1.778701	-0.803356	-1.251298
105	6	0	3.117292	-0.600912	-1.909777
106	6	0	3.988433	-1.626155	-2.286492
107	6	0	3.452279	0.724475	-2.222746
108	6	0	5.168589	-1.325192	-2.965444
109	1	0	3.749741	-2.660798	-2.073909
110	6	0	4.633001	1.022812	-2.890765
111	1	0	2.767554	1.514457	-1.926806
112	6	0	5.494582	-0.007376	-3.268977
113	1	0	5.833332	-2.131549	-3.258377
114	1	0	4.881344	2.055530	-3.117782
115	1	0	6.416257	0.218093	-3.797231
116	8	0	0.878170	-0.012018	-1.545744

α′,β-**INT3**

Zero-point correction= 0.971969 (Hartree/Particle)
Thermal correction to Energy= 1.025029
Thermal correction to Enthalpy= 1.025973
Thermal correction to Gibbs Free Energy= 0.881675
E(sov) = -2684.27875875 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.294653	3.626044	-3.569220
2	6	0	2.863628	4.748969	-4.313203
3	6	0	1.703071	5.391444	-3.971136
4	6	0	0.927478	4.947101	-2.868527
5	6	0	1.361553	3.820995	-2.109690
6	6	0	2.565384	3.170320	-2.500549
7	6	0	0.943575	2.286781	-0.059060

8	6	0	2.139743	2.719235	0.807725
9	7	0	2.611168	1.641886	1.713418
10	6	0	3.953103	2.016127	2.212951
11	6	0	1.805785	3.982776	1.641223
12	6	0	3.931192	3.436536	2.825502
13	6	0	2.463482	3.839492	3.018641
14	6	0	1.691876	1.480431	2.860948
15	6	0	1.743105	2.712957	3.793054
16	6	0	0.393957	3.139486	4.313714
17	6	0	-0.734042	2.433278	4.267135
18	7	0	-0.213938	5.643136	-2.592300
19	6	0	-0.934670	5.239021	-1.577752
20	6	0	-0.591448	4.140606	-0.752412
21	6	0	0.553906	3.426042	-0.996797
22	1	0	3.451686	5.092389	-5.158675
23	1	0	1.334490	6.252094	-4.519763
24	1	0	2.902747	2.289084	-1.968790
25	1	0	4.237994	1.261274	2.953235
26	1	0	4.654253	1.937957	1.375472
27	1	0	2.153333	4.881843	1.122794
28	1	0	0.720116	4.081436	1.765642
29	1	0	4.465455	3.450552	3.780858
30	1	0	4.428369	4.154361	2.163735
31	1	0	2.392658	4.780735	3.574233
32	1	0	1.968599	0.558975	3.384002
33	1	0	0.692939	1.318256	2.454189
34	1	0	2.365805	2.477713	4.670152
35	1	0	0.381890	4.116038	4.801174
36	1	0	-1.650374	2.822535	4.701610
37	1	0	-0.794995	1.442066	3.823583
38	1	0	-1.846338	5.798618	-1.373892
39	1	0	-1.241661	3.868198	0.076081
40	1	0	4.207836	3.111971	-3.852626
41	1	0	0.081178	2.123781	0.610522
42	1	0	2.985839	2.929801	0.142524
43	7	0	1.200662	1.043467	-0.736108
44	6	0	0.174159	0.199356	-1.055274
45	1	0	2.141731	0.660497	-0.720366
46	6	0	-1.147691	0.469487	-1.050532
47	6	0	-2.029383	-0.746749	-1.164098
48	1	0	-1.579812	1.445457	-0.856782
49	6	0	-0.181901	-1.641217	-2.651337
50	6	0	-3.487126	-0.391741	-1.052578
51	1	0	0.109388	-2.654207	-2.939145
52	1	0	0.161143	-0.968620	-3.442191
53	6	0	-4.505590	-1.108993	-1.537519

54	1	0	-3.702404	0.526736	-0.509123
55	6	0	-5.928838	-0.780513	-1.349197
56	1	0	-4.306104	-2.015968	-2.106578
57	6	0	-6.887555	-1.363652	-2.185395
58	6	0	-6.364078	0.083474	-0.335600
59	6	0	-8.239818	-1.075692	-2.033431
60	1	0	-6.562656	-2.047793	-2.965374
61	6	0	-7.714411	0.369881	-0.180888
62	1	0	-5.642164	0.509338	0.356029
63	6	0	-8.658270	-0.205077	-1.031035
64	1	0	-8.967438	-1.534194	-2.696280
65	1	0	-8.033323	1.035609	0.616217
66	1	0	-9.713704	0.016387	-0.905084
67	6	0	5.499265	-4.292442	1.296207
68	6	0	6.003223	-4.754659	0.072620
69	6	0	5.842599	-4.019946	-1.087851
70	6	0	5.171431	-2.789586	-1.056333
71	6	0	4.636252	-2.331206	0.164634
72	6	0	4.813681	-3.092365	1.329727
73	1	0	5.640374	-4.870306	2.203309
74	1	0	6.534249	-5.701262	0.031192
75	1	0	6.231623	-4.362442	-2.040450
76	1	0	4.398588	-2.712268	2.257748
77	6	0	3.887082	-1.062784	0.206961
78	8	0	3.859170	-0.273085	-0.751210
79	8	0	3.235420	-0.824216	1.317409
80	1	0	2.867813	0.160456	1.304570
81	8	0	5.066299	-2.109930	-2.206344
82	1	0	4.627692	-1.254160	-2.008959
83	6	0	-1.705735	-1.521355	-2.465396
84	1	0	-2.163058	-0.974901	-3.294421
85	1	0	-2.181217	-2.509182	-2.434592
86	6	0	0.508400	-1.240785	-1.340866
87	1	0	1.591207	-1.393084	-1.408065
88	6	0	-0.032436	-2.074068	-0.138587
89	1	0	0.469885	-1.665940	0.741521
90	6	0	0.402626	-3.525062	-0.243649
91	6	0	1.517543	-3.907441	0.509929
92	6	0	-0.155597	-4.466811	-1.115838
93	6	0	2.067021	-5.180806	0.395340
94	1	0	1.966381	-3.186127	1.189711
95	6	0	0.382620	-5.745618	-1.223568
96	1	0	-1.026486	-4.215746	-1.712010
97	6	0	1.497713	-6.106768	-0.472802
98	1	0	2.942939	-5.440918	0.981756
99	1	0	-0.072148	-6.460142	-1.902887

100	1	0	1.920003	-7.102647	-0.566403
101	6	0	-1.556920	-1.735650	0.064356
102	6	0	-2.411815	-2.921335	0.057203
103	7	0	-3.106257	-3.845393	0.002275
104	6	0	-1.745596	-0.916503	1.372268
105	6	0	-3.102259	-0.594526	1.937853
106	6	0	-4.139837	-1.510488	2.138062
107	6	0	-3.277333	0.736782	2.341619
108	6	0	-5.320014	-1.097182	2.753376
109	1	0	-4.035056	-2.545554	1.840484
110	6	0	-4.465555	1.148663	2.931920
111	1	0	-2.469791	1.444426	2.175236
112	6	0	-5.487841	0.225654	3.149998
113	1	0	-6.114128	-1.819166	2.913564
114	1	0	-4.591182	2.185933	3.227702
115	1	0	-6.415126	0.539740	3.619933
116	8	0	-0.780959	-0.387867	1.887096

7a’

Zero-point correction= 0.478121 (Hartree/Particle)
Thermal correction to Energy= 0.504690
Thermal correction to Enthalpy= 0.505635
Thermal correction to Gibbs Free Energy= 0.420407
E(sov) = -1362.96038492 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.992256	1.134697	2.585333
2	6	0	-0.245406	-0.189801	1.338824
3	6	0	-2.392435	-1.247088	2.205551
4	6	0	1.239290	-0.344573	1.127747
5	1	0	-3.073796	-1.989833	1.784971
6	1	0	-2.482134	-1.326937	3.294297
7	6	0	1.863660	-1.451234	0.713449
8	1	0	1.825768	0.551631	1.323108
9	6	0	3.308536	-1.561145	0.448995
10	1	0	1.288787	-2.358434	0.530511
11	6	0	3.874190	-2.829072	0.270984
12	6	0	4.142304	-0.438605	0.346747
13	6	0	5.233728	-2.977923	0.017590
14	1	0	3.235933	-3.706947	0.333495
15	6	0	5.499362	-0.585765	0.090405

16	1	0	3.724962	0.559605	0.444993
17	6	0	6.052042	-1.855631	-0.071972
18	1	0	5.653266	-3.970581	-0.113921
19	1	0	6.127938	0.296359	0.010330
20	1	0	7.112758	-1.967903	-0.274210
21	6	0	-0.932818	-1.504962	1.764535
22	1	0	-0.348746	-1.941975	2.580636
23	1	0	-0.893255	-2.221306	0.936370
24	6	0	-2.828082	0.162818	1.776648
25	1	0	-3.886419	0.343568	1.980283
26	6	0	-2.541091	0.434931	0.276930
27	1	0	-2.761211	1.492725	0.123473
28	6	0	-3.495296	-0.327761	-0.625579
29	6	0	-4.503200	0.404284	-1.261421
30	6	0	-3.479292	-1.716377	-0.804448
31	6	0	-5.467003	-0.221286	-2.046151
32	1	0	-4.532875	1.483772	-1.135586
33	6	0	-4.439406	-2.345488	-1.590542
34	1	0	-2.698484	-2.320492	-0.353973
35	6	0	-5.438581	-1.601980	-2.212102
36	1	0	-6.237089	0.372355	-2.529134
37	1	0	-4.400247	-3.422524	-1.720745
38	1	0	-6.186363	-2.095919	-2.824772
39	6	0	-0.985138	0.308513	0.001922
40	6	0	-0.709799	-0.670940	-1.051673
41	7	0	-0.498644	-1.487849	-1.842804
42	6	0	-0.407008	1.723925	-0.334674
43	6	0	0.969617	1.944188	-0.899295
44	6	0	1.653036	1.089828	-1.773680
45	6	0	1.589050	3.133207	-0.486122
46	6	0	2.927048	1.428886	-2.222168
47	1	0	1.209491	0.167580	-2.121990
48	6	0	2.869310	3.453978	-0.918015
49	1	0	1.046990	3.796518	0.179758
50	6	0	3.540720	2.601842	-1.792808
51	1	0	3.444798	0.759208	-2.901368
52	1	0	3.339020	4.371593	-0.577848
53	1	0	4.539908	2.851101	-2.137514
54	8	0	-1.047296	2.687685	0.028217
55	8	0	-2.437363	2.005079	3.291939
56	6	0	-0.501484	0.860058	2.436170
57	1	0	0.018379	1.805428	2.248905
58	1	0	-0.121187	0.475092	3.391224

γ′-TS3

Zero-point correction= 0.875039 (Hartree/Particle)
Thermal correction to Energy= 0.924088
Thermal correction to Enthalpy= 0.925032
Thermal correction to Gibbs Free Energy= 0.788848
E(sov) = -2432.18700668 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.946473	-2.167565	-2.999849
2	6	0	-5.127473	-3.450653	-3.567294
3	6	0	-4.304004	-4.483133	-3.202955
4	6	0	-3.269520	-4.283227	-2.252540
5	6	0	-3.084172	-2.992849	-1.675244
6	6	0	-3.951228	-1.941756	-2.082752
7	6	0	-1.755391	-1.554794	0.034290
8	6	0	-2.861532	-1.248788	1.058121
9	7	0	-2.484802	-0.117253	1.947186
10	6	0	-3.729330	0.402205	2.567836
11	6	0	-3.234905	-2.468032	1.930927
12	6	0	-4.538479	-0.752414	3.200154
13	6	0	-3.598988	-1.957713	3.331185
14	6	0	-1.560637	-0.569156	3.018144
15	6	0	-2.296360	-1.485743	4.023633
16	6	0	-1.496950	-2.653213	4.541268
17	6	0	-0.291987	-3.063050	4.151154
18	7	0	-2.499415	-5.364735	-1.936761
19	6	0	-1.545996	-5.189859	-1.057903
20	6	0	-1.275752	-3.954711	-0.419957
21	6	0	-2.036452	-2.850294	-0.713964
22	1	0	-5.916390	-3.610235	-4.295529
23	1	0	-4.408238	-5.479941	-3.618453
24	1	0	-3.815939	-0.943888	-1.682372
25	1	0	-3.424317	1.140435	3.316524
26	1	0	-4.291351	0.927144	1.789089
27	1	0	-4.061223	-3.018378	1.470276
28	1	0	-2.387642	-3.159978	2.008797
29	1	0	-4.925972	-0.454156	4.179353
30	1	0	-5.399725	-1.013959	2.575234
31	1	0	-4.068422	-2.754655	3.916634
32	1	0	-1.160836	0.324802	3.506915
33	1	0	-0.715083	-1.071665	2.543131
34	1	0	-2.595984	-0.886220	4.896112
35	1	0	-2.010431	-3.217650	5.321303
36	1	0	0.155539	-3.938661	4.612115

37	1	0	0.307712	-2.565741	3.393005
38	1	0	-0.938892	-6.060847	-0.817227
39	1	0	-0.463981	-3.885329	0.302146
40	1	0	-5.596348	-1.351203	-3.299189
41	1	0	-0.817045	-1.712881	0.587513
42	1	0	-3.746589	-0.904073	0.508493
43	7	0	-1.555026	-0.403062	-0.829367
44	6	0	-0.352892	-0.107089	-1.376360
45	1	0	-2.238304	0.351141	-0.768600
46	6	0	0.678018	-1.010090	-1.444017
47	6	0	2.027137	-0.581486	-1.641621
48	1	0	0.514009	-2.041116	-1.152354
49	6	0	1.183902	1.591710	-2.467563
50	6	0	3.071074	-1.541037	-1.376233
51	1	0	1.410904	2.661089	-2.425214
52	1	0	1.138431	1.316222	-3.529726
53	6	0	4.357650	-1.215357	-1.116866
54	1	0	2.746580	-2.571966	-1.251519
55	6	0	5.421333	-2.141590	-0.726881
56	1	0	4.662530	-0.172261	-1.174293
57	6	0	6.610566	-1.614904	-0.203777
58	6	0	5.298766	-3.534287	-0.853209
59	6	0	7.642080	-2.456171	0.198527
60	1	0	6.708375	-0.539621	-0.084463
61	6	0	6.333024	-4.371046	-0.460587
62	1	0	4.395843	-3.962749	-1.277434
63	6	0	7.507451	-3.835064	0.069693
64	1	0	8.550660	-2.032124	0.613964
65	1	0	6.227179	-5.446069	-0.570287
66	1	0	8.314263	-4.492982	0.377925
67	6	0	-1.361143	6.271148	0.648953
68	6	0	-1.987798	6.845191	-0.465459
69	6	0	-2.757916	6.080782	-1.323052
70	6	0	-2.926403	4.709429	-1.086253
71	6	0	-2.281352	4.118099	0.020668
72	6	0	-1.508041	4.915405	0.879624
73	1	0	-0.769788	6.881320	1.323275
74	1	0	-1.874743	7.907898	-0.659115
75	1	0	-3.253874	6.512953	-2.185217
76	1	0	-1.033014	4.440455	1.732247
77	6	0	-2.421434	2.670705	0.266174
78	8	0	-3.206510	1.962527	-0.393779
79	8	0	-1.651137	2.169705	1.192559
80	1	0	-1.926203	1.144234	1.378567
81	8	0	-3.696092	4.021989	-1.940891
82	1	0	-3.761088	3.100908	-1.604578

83	6	0	2.356290	1.385217	0.168325
84	1	0	1.277970	1.244912	0.247381
85	6	0	2.764596	2.796111	-0.046528
86	6	0	1.782685	3.789376	0.044407
87	6	0	4.074954	3.168253	-0.367984
88	6	0	2.101065	5.126210	-0.169656
89	1	0	0.760921	3.510067	0.296378
90	6	0	4.392264	4.505297	-0.580118
91	1	0	4.849906	2.412130	-0.451903
92	6	0	3.408654	5.487631	-0.483010
93	1	0	1.320977	5.878463	-0.096414
94	1	0	5.413419	4.779636	-0.825924
95	1	0	3.660619	6.529404	-0.655727
96	6	0	3.066378	0.512907	1.024952
97	6	0	4.405503	0.713160	1.448700
98	7	0	5.509085	0.885226	1.772364
99	6	0	2.374886	-0.652185	1.451715
100	7	0	1.721811	-1.575070	1.728114
101	6	0	2.294271	0.778469	-1.837718
102	1	0	3.300263	1.064718	-2.131291
103	6	0	-0.184133	1.326244	-1.827714
104	1	0	-0.331335	1.972737	-0.954498
105	1	0	-0.989851	1.580422	-2.527213

γ′-INT4

Zero-point correction= 0.877715 (Hartree/Particle)
Thermal correction to Energy= 0.926593
Thermal correction to Enthalpy= 0.927537
Thermal correction to Gibbs Free Energy= 0.791843
E(sov) = -2432.21056620 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.944227	-3.603772	-3.477528
2	6	0	-2.536648	-4.894418	-3.888309
3	6	0	-1.603139	-5.582983	-3.159173
4	6	0	-1.038636	-5.017041	-1.986886
5	6	0	-1.446717	-3.716860	-1.567440
6	6	0	-2.413310	-3.027996	-2.350926
7	6	0	-1.219365	-1.861929	0.241553
8	6	0	-2.636249	-1.897248	0.839252
9	7	0	-2.956067	-0.656806	1.596374
10	6	0	-4.435050	-0.575419	1.713624

11	6	0	-2.868282	-3.118263	1.753481
12	6	0	-5.004890	-1.909670	2.244699
13	6	0	-3.841928	-2.697988	2.861585
14	6	0	-2.362726	-0.701747	2.960472
15	6	0	-3.080448	-1.760020	3.831323
16	6	0	-2.188112	-2.540096	4.761372
17	6	0	-0.857945	-2.529428	4.819742
18	7	0	-0.121228	-5.768983	-1.312842
19	6	0	0.404108	-5.255749	-0.229416
20	6	0	0.074309	-3.975596	0.278921
21	6	0	-0.850384	-3.200394	-0.376441
22	1	0	-2.964696	-5.333422	-4.783902
23	1	0	-1.263975	-6.573660	-3.443067
24	1	0	-2.732594	-2.030606	-2.069531
25	1	0	-4.651449	0.256216	2.391566
26	1	0	-4.832266	-0.316799	0.727003
27	1	0	-3.254022	-3.957227	1.165660
28	1	0	-1.924937	-3.443816	2.209018
29	1	0	-5.781906	-1.720888	2.991858
30	1	0	-5.465548	-2.486959	1.435024
31	1	0	-4.210088	-3.577468	3.399046
32	1	0	-2.456913	0.300324	3.390156
33	1	0	-1.293543	-0.898382	2.855368
34	1	0	-3.837400	-1.257370	4.451982
35	1	0	-2.736366	-3.193210	5.442585
36	1	0	-0.346866	-3.161501	5.540391
37	1	0	-0.224918	-1.909736	4.188782
38	1	0	1.136711	-5.867049	0.294548
39	1	0	0.558756	-3.603620	1.179882
40	1	0	-3.681110	-3.061506	-4.061695
41	1	0	-0.493753	-1.665184	1.044694
42	1	0	-3.352769	-1.922921	0.008231
43	7	0	-1.133479	-0.730828	-0.684755
44	6	0	-0.010246	-0.145939	-1.062259
45	1	0	-2.014805	-0.263611	-0.927577
46	6	0	1.254762	-0.729381	-0.852880
47	6	0	2.394795	0.051886	-0.837764
48	1	0	1.321842	-1.787936	-0.627000
49	6	0	1.202037	1.865323	-2.021162
50	6	0	3.680874	-0.583482	-0.771785
51	1	0	1.054243	2.946954	-2.100213
52	1	0	1.619260	1.516342	-2.971480
53	6	0	4.871751	0.056665	-0.698401
54	1	0	3.666623	-1.671932	-0.746192
55	6	0	6.171782	-0.612599	-0.647278
56	1	0	4.900363	1.139861	-0.637322

57	6	0	7.245026	0.040196	-0.024023
58	6	0	6.378266	-1.882314	-1.205324
59	6	0	8.489211	-0.572343	0.053591
60	1	0	7.070829	1.007355	0.438734
61	6	0	7.625847	-2.488474	-1.132404
62	1	0	5.564136	-2.380989	-1.723541
63	6	0	8.683630	-1.836375	-0.500525
64	1	0	9.308734	-0.065164	0.552972
65	1	0	7.776432	-3.467975	-1.575815
66	1	0	9.658022	-2.311977	-0.442418
67	6	0	-3.323448	5.609851	-0.527744
68	6	0	-3.675123	5.831134	-1.866013
69	6	0	-3.879243	4.774202	-2.734130
70	6	0	-3.738044	3.454865	-2.283316
71	6	0	-3.365714	3.222258	-0.942211
72	6	0	-3.166472	4.312107	-0.078528
73	1	0	-3.180051	6.445543	0.148595
74	1	0	-3.794997	6.846881	-2.231003
75	1	0	-4.156936	4.930363	-3.770807
76	1	0	-2.892238	4.106749	0.951711
77	6	0	-3.168704	1.844055	-0.462140
78	8	0	-3.447677	0.852280	-1.171941
79	8	0	-2.643348	1.713264	0.720911
80	1	0	-2.655929	0.669325	1.022397
81	8	0	-3.958634	2.470953	-3.167231
82	1	0	-3.882689	1.618688	-2.685060
83	6	0	1.658198	1.985274	0.511353
84	1	0	0.614315	1.659778	0.583256
85	6	0	1.638913	3.494060	0.644342
86	6	0	0.416720	4.169441	0.603196
87	6	0	2.816347	4.242687	0.744543
88	6	0	0.363376	5.559551	0.661258
89	1	0	-0.506923	3.595409	0.536310
90	6	0	2.764281	5.631661	0.810916
91	1	0	3.777029	3.736554	0.792461
92	6	0	1.539604	6.295218	0.766356
93	1	0	-0.598412	6.063114	0.619265
94	1	0	3.686433	6.198537	0.898444
95	1	0	1.504440	7.379456	0.814099
96	6	0	2.375052	1.186797	1.600332
97	6	0	3.743957	1.353547	1.822023
98	7	0	4.897413	1.531627	1.908453
99	6	0	1.662631	0.135014	2.170042
100	7	0	0.981603	-0.746861	2.538098
101	6	0	2.187128	1.553396	-0.887838
102	1	0	3.135056	2.065411	-1.078455

103	6	0	-0.148727	1.193242	-1.752608
104	1	0	-0.758342	1.836742	-1.108887
105	1	0	-0.720158	1.052812	-2.678442

γ′,δ-INT5

Zero-point correction= 0.879044 (Hartree/Particle)
Thermal correction to Energy= 0.927044
Thermal correction to Enthalpy= 0.927988
Thermal correction to Gibbs Free Energy= 0.795510
E(sov) = -2432.23761601 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.239933	0.892459	-1.454412
2	6	0	-7.162922	0.244798	-2.307600
3	6	0	-6.919721	-1.034731	-2.731797
4	6	0	-5.748054	-1.722740	-2.322471
5	6	0	-4.818148	-1.078290	-1.455420
6	6	0	-5.098896	0.253035	-1.039429
7	6	0	-2.588400	-1.266936	-0.138070
8	6	0	-3.119811	-1.111106	1.306569
9	7	0	-2.107787	-0.487358	2.195354
10	6	0	-2.692669	-0.333611	3.546365
11	6	0	-3.545329	-2.486186	1.895322
12	6	0	-2.959196	-1.712961	4.193320
13	6	0	-2.689778	-2.786172	3.133308
14	6	0	-0.871609	-1.299722	2.285535
15	6	0	-1.192233	-2.743561	2.757400
16	6	0	-0.829876	-3.841009	1.783437
17	6	0	0.101909	-3.785741	0.833758
18	7	0	-5.577835	-2.990967	-2.797989
19	6	0	-4.498074	-3.631712	-2.431018
20	6	0	-3.512486	-3.090672	-1.569512
21	6	0	-3.658131	-1.820823	-1.069668
22	1	0	-8.059715	0.767212	-2.625951
23	1	0	-7.599268	-1.566104	-3.390004
24	1	0	-4.412888	0.788472	-0.392643
25	1	0	-1.993430	0.267109	4.136068
26	1	0	-3.611675	0.250481	3.433620
27	1	0	-4.606864	-2.479065	2.163702
28	1	0	-3.415749	-3.276715	1.149100
29	1	0	-2.306296	-1.868873	5.058641

30	1	0	-3.992405	-1.780349	4.548201
31	1	0	-2.939360	-3.778212	3.525786
32	1	0	-0.202802	-0.790466	2.985050
33	1	0	-0.375297	-1.274402	1.311257
34	1	0	-0.621721	-2.942256	3.675930
35	1	0	-1.370528	-4.777980	1.931930
36	1	0	0.318549	-4.652026	0.213855
37	1	0	0.703237	-2.896621	0.655723
38	1	0	-4.372651	-4.639304	-2.824276
39	1	0	-2.642108	-3.687151	-1.304887
40	1	0	-6.432381	1.909468	-1.126906
41	1	0	-1.802193	-2.026271	-0.094616
42	1	0	-3.968181	-0.418897	1.302330
43	7	0	-1.980045	-0.052515	-0.633362
44	6	0	-0.704767	0.014704	-1.125486
45	1	0	-2.403973	0.826294	-0.353540
46	6	0	0.047749	-1.055177	-1.499362
47	6	0	1.489883	-0.934114	-1.610870
48	1	0	-0.367436	-2.059199	-1.502035
49	6	0	1.067950	1.500977	-2.090064
50	6	0	2.354661	-1.951621	-1.436725
51	1	0	1.509935	2.501154	-2.055136
52	1	0	0.734852	1.322852	-3.118132
53	6	0	3.793380	-1.621199	-1.146057
54	1	0	2.021681	-2.979983	-1.330485
55	6	0	4.643752	-2.805270	-0.740994
56	1	0	4.282741	-1.126801	-1.997733
57	6	0	5.962317	-2.897939	-1.191046
58	6	0	4.148937	-3.803713	0.104026
59	6	0	6.770310	-3.966480	-0.815596
60	1	0	6.360733	-2.120748	-1.838798
61	6	0	4.957117	-4.871114	0.483358
62	1	0	3.131240	-3.743568	0.480548
63	6	0	6.267902	-4.957501	0.022589
64	1	0	7.792269	-4.022337	-1.177176
65	1	0	4.559762	-5.635578	1.143867
66	1	0	6.895643	-5.792498	0.317942
67	6	0	0.659574	5.554926	1.649199
68	6	0	0.144778	6.487460	0.738235
69	6	0	-1.002197	6.217167	0.013989
70	6	0	-1.670966	4.996507	0.181192
71	6	0	-1.156949	4.048936	1.090615
72	6	0	0.008110	4.345886	1.814535
73	1	0	1.553960	5.779475	2.220892
74	1	0	0.648369	7.439399	0.597080
75	1	0	-1.412034	6.928040	-0.695139

76	1	0	0.382980	3.600690	2.509024
77	6	0	-1.808326	2.730558	1.227262
78	8	0	-2.863374	2.451487	0.628051
79	8	0	-1.176252	1.865153	1.966151
80	1	0	-1.646689	0.897164	1.931702
81	8	0	-2.771296	4.785524	-0.554111
82	1	0	-3.127221	3.903401	-0.304022
83	6	0	2.920698	0.778194	-0.459253
84	1	0	2.201021	0.962684	0.345271
85	6	0	3.715959	2.049400	-0.652677
86	6	0	3.313787	3.212835	0.004824
87	6	0	4.787757	2.118532	-1.547684
88	6	0	3.968026	4.420913	-0.220660
89	1	0	2.466703	3.178489	0.687135
90	6	0	5.452482	3.320117	-1.764157
91	1	0	5.117337	1.223380	-2.071470
92	6	0	5.042723	4.475856	-1.102132
93	1	0	3.630892	5.317175	0.291612
94	1	0	6.291685	3.354548	-2.451716
95	1	0	5.558994	5.414773	-1.276119
96	6	0	3.762173	-0.496557	-0.007144
97	6	0	5.140619	-0.155984	0.383920
98	7	0	6.241502	0.074111	0.647930
99	6	0	3.078503	-1.061903	1.174662
100	7	0	2.483580	-1.471049	2.077963
101	6	0	2.110851	0.439445	-1.740630
102	1	0	2.838782	0.401934	-2.562525
103	6	0	-0.135082	1.414267	-1.161922
104	1	0	0.141309	1.709876	-0.140603
105	1	0	-0.918462	2.113921	-1.481765

5’

Zero-point correction= 0.384729 (Hartree/Particle)
Thermal correction to Energy= 0.406955
Thermal correction to Enthalpy= 0.407900
Thermal correction to Gibbs Free Energy= 0.332292
E(sov) = -1110.91928381 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.860423	3.168627	-0.101267

2	6	0	1.436297	3.054256	-0.497338
3	6	0	0.867730	1.883552	-0.814342
4	1	0	0.862229	3.977795	-0.481744
5	6	0	3.147684	0.779662	-0.836136
6	1	0	3.644223	-0.172936	-0.621108
7	1	0	3.459125	1.081702	-1.842467
8	6	0	-1.155310	0.374138	-0.651534
9	6	0	-2.660629	0.359153	-0.481478
10	1	0	-0.904968	-0.386087	-1.399778
11	6	0	-3.401998	-0.681121	-1.045076
12	6	0	-3.329262	1.341971	0.255084
13	6	0	-4.783416	-0.737176	-0.890437
14	1	0	-2.888664	-1.461346	-1.602248
15	6	0	-4.710383	1.284254	0.414244
16	1	0	-2.776217	2.151180	0.723220
17	6	0	-5.441329	0.248140	-0.160443
18	1	0	-5.342754	-1.553057	-1.337314
19	1	0	-5.215127	2.052926	0.990932
20	1	0	-6.518918	0.207115	-0.036116
21	6	0	1.156188	-0.325041	0.323931
22	1	0	1.691571	-0.013281	1.227582
23	6	0	1.486843	-1.784937	0.082878
24	6	0	2.146365	-2.506847	1.079704
25	6	0	1.129844	-2.446114	-1.096262
26	6	0	2.443252	-3.855386	0.908658
27	1	0	2.422938	-2.006256	2.004452
28	6	0	1.420033	-3.795654	-1.268199
29	1	0	0.620187	-1.914688	-1.895900
30	6	0	2.078544	-4.504149	-0.266830
31	1	0	2.956594	-4.397538	1.696399
32	1	0	1.131479	-4.294615	-2.188089
33	1	0	2.305029	-5.556787	-0.403374
34	6	0	-0.385952	-0.086456	0.637794
35	6	0	-1.000776	-1.314773	1.173610
36	7	0	-1.485390	-2.286111	1.567460
37	6	0	-0.505400	0.962650	1.671507
38	7	0	-0.576484	1.806600	2.457420
39	6	0	1.628094	0.582588	-0.842639
40	1	0	1.356346	0.075223	-1.778533
41	6	0	3.582465	1.858254	0.156582
42	1	0	3.344047	1.558774	1.186925
43	1	0	4.658398	2.042167	0.114863
44	8	0	3.391002	4.247754	0.057898
45	6	0	-0.603574	1.740833	-1.112765
46	1	0	-1.154076	2.557424	-0.637716
47	1	0	-0.780719	1.824290	-2.192802

α′-TS3

Zero-point correction= 0.875670 (Hartree/Particle)
Thermal correction to Energy= 0.924646
Thermal correction to Enthalpy= 0.925590
Thermal correction to Gibbs Free Energy= 0.790440
E(sov) = -2432.19078601 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.719283	-3.286972	3.832270
2	6	0	1.037888	-4.317090	4.521953
3	6	0	-0.074111	-4.893109	3.966887
4	6	0	-0.551407	-4.471428	2.699035
5	6	0	0.135093	-3.437034	1.995794
6	6	0	1.281901	-2.855164	2.605373
7	6	0	0.278780	-2.036628	-0.199045
8	6	0	1.583941	-2.630928	-0.764082
9	7	0	2.281184	-1.709790	-1.700186
10	6	0	3.676881	-2.193870	-1.854724
11	6	0	1.339906	-3.984721	-1.472425
12	6	0	3.699671	-3.692791	-2.226413
13	6	0	2.285507	-4.079146	-2.674646
14	6	0	1.616555	-1.706138	-3.026380
15	6	0	1.813638	-3.062842	-3.744193
16	6	0	0.611619	-3.580699	-4.491059
17	6	0	-0.635274	-3.114787	-4.466442
18	7	0	-1.661761	-5.100374	2.216354
19	6	0	-2.107196	-4.722538	1.045511
20	6	0	-1.502092	-3.713526	0.259312
21	6	0	-0.380785	-3.065026	0.715555
22	1	0	1.398054	-4.645386	5.491884
23	1	0	-0.625735	-5.683380	4.465125
24	1	0	1.814437	-2.053387	2.107080
25	1	0	4.140058	-1.576696	-2.631233
26	1	0	4.199190	-1.994941	-0.913411
27	1	0	1.497776	-4.809514	-0.770571
28	1	0	0.303723	-4.051371	-1.824590
29	1	0	4.424865	-3.876665	-3.025317
30	1	0	3.998714	-4.302837	-1.366935
31	1	0	2.272942	-5.092254	-3.089323

32	1	0	2.044264	-0.882743	-3.607258
33	1	0	0.563447	-1.467153	-2.867136
34	1	0	2.630614	-2.963196	-4.474183
35	1	0	0.824597	-4.462753	-5.097142
36	1	0	-1.408380	-3.609915	-5.046700
37	1	0	-0.947841	-2.241330	-3.900226
38	1	0	-2.996514	-5.229911	0.674999
39	1	0	-1.932673	-3.450072	-0.704865
40	1	0	2.595588	-2.829314	4.280660
41	1	0	-0.417391	-1.865356	-1.033634
42	1	0	2.279758	-2.768851	0.072748
43	7	0	0.559677	-0.757008	0.422226
44	6	0	-0.352275	0.124429	0.903340
45	1	0	1.539750	-0.532090	0.585008
46	6	0	-1.759125	-0.180824	0.889946
47	6	0	-2.695700	0.769976	1.159677
48	1	0	-2.087180	-1.138859	0.502961
49	6	0	-0.850185	2.217095	2.145599
50	6	0	-4.086535	0.498050	0.838389
51	1	0	-0.540402	3.266874	2.156178
52	1	0	-0.724574	1.842366	3.170597
53	6	0	-5.037219	1.448254	0.769185
54	1	0	-4.321302	-0.521294	0.535020
55	6	0	-6.419762	1.225925	0.332996
56	1	0	-4.772978	2.482162	0.980473
57	6	0	-7.116294	2.279600	-0.272750
58	6	0	-7.065331	-0.007486	0.492528
59	6	0	-8.417404	2.098898	-0.726980
60	1	0	-6.612263	3.232542	-0.411341
61	6	0	-8.368136	-0.184881	0.044007
62	1	0	-6.548557	-0.821579	0.993169
63	6	0	-9.047520	0.866482	-0.569713
64	1	0	-8.940025	2.920529	-1.207039
65	1	0	-8.858799	-1.143846	0.180538
66	1	0	-10.065641	0.726112	-0.919675
67	6	0	5.804885	3.732282	-0.601270
68	6	0	6.355552	3.912453	0.675584
69	6	0	6.049140	3.050192	1.712333
70	6	0	5.175303	1.974386	1.500990
71	6	0	4.603229	1.794532	0.223880
72	6	0	4.935807	2.678785	-0.815415
73	1	0	6.057022	4.408742	-1.410484
74	1	0	7.038032	4.737697	0.856857
75	1	0	6.471414	3.174132	2.703502
76	1	0	4.487587	2.515098	-1.790351
77	6	0	3.659261	0.686911	-0.011517

78	8	0	3.408803	-0.166570	0.860961
79	8	0	3.082962	0.658112	-1.183975
80	1	0	2.589093	-0.289061	-1.315843
81	8	0	4.925890	1.167166	2.540063
82	1	0	4.324871	0.456122	2.227384
83	6	0	-2.324700	2.112664	1.740671
84	1	0	-2.963886	2.299502	2.611322
85	1	0	-2.588771	2.889963	1.013550
86	6	0	0.043123	1.424670	1.227603
87	1	0	1.114328	1.614078	1.299169
88	6	0	-0.177831	2.274777	-0.772797
89	1	0	0.639776	1.621482	-1.076866
90	6	0	0.277075	3.641350	-0.426751
91	6	0	1.663129	3.842820	-0.370459
92	6	0	-0.566061	4.720196	-0.129234
93	6	0	2.201883	5.074541	-0.026350
94	1	0	2.319848	3.011600	-0.609896
95	6	0	-0.025203	5.957617	0.210310
96	1	0	-1.643593	4.608711	-0.167519
97	6	0	1.353938	6.140618	0.267557
98	1	0	3.281193	5.194761	0.011190
99	1	0	-0.692312	6.784394	0.434343
100	1	0	1.764447	7.108140	0.539929
101	6	0	-1.400436	1.948297	-1.395640
102	6	0	-2.571220	2.749314	-1.413812
103	7	0	-3.539093	3.394320	-1.389264
104	6	0	-1.502475	0.665857	-1.993243
105	7	0	-1.537159	-0.401575	-2.456873

α′-INT4

Zero-point correction= 0.878148 (Hartree/Particle)
Thermal correction to Energy= 0.926894
Thermal correction to Enthalpy= 0.927838
Thermal correction to Gibbs Free Energy= 0.793082
E(sov) = -2432.21615969 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.326971	-3.050196	-3.664043
2	6	0	-1.826609	-4.088172	-4.483797
3	6	0	-0.712396	-4.786146	-4.099695
4	6	0	-0.050732	-4.480931	-2.881752

5	6	0	-0.550609	-3.434991	-2.051406
6	6	0	-1.708718	-2.728369	-2.482272
7	6	0	-0.296454	-2.129466	0.178226
8	6	0	-1.574228	-2.617552	0.888594
9	7	0	-2.113966	-1.638818	1.866896
10	6	0	-3.499775	-2.057316	2.200007
11	6	0	-1.326868	-3.973519	1.594003
12	6	0	-3.539900	-3.534233	2.651233
13	6	0	-2.097533	-3.978329	2.917576
14	6	0	-1.299266	-1.621656	3.106139
15	6	0	-1.431307	-2.959306	3.874769
16	6	0	-0.144413	-3.505663	4.438197
17	6	0	1.091748	-3.044075	4.257907
18	7	0	1.047730	-5.227367	-2.569051
19	6	0	1.665159	-4.953734	-1.448061
20	6	0	1.258439	-3.936950	-0.550687
21	6	0	0.154188	-3.173427	-0.835374
22	1	0	-2.328016	-4.326042	-5.416635
23	1	0	-0.296083	-5.588383	-4.700054
24	1	0	-2.113212	-1.919834	-1.884423
25	1	0	-3.848996	-1.384521	2.989409
26	1	0	-4.119871	-1.880037	1.314748
27	1	0	-1.638678	-4.797772	0.944932
28	1	0	-0.258763	-4.108719	1.800505
29	1	0	-4.150830	-3.640854	3.553149
30	1	0	-3.988181	-4.166762	1.877001
31	1	0	-2.076592	-4.978111	3.363517
32	1	0	-1.646874	-0.779534	3.713098
33	1	0	-0.269693	-1.392819	2.824685
34	1	0	-2.122603	-2.818323	4.718983
35	1	0	-0.282213	-4.398606	5.050799
36	1	0	1.928648	-3.556099	4.724270
37	1	0	1.334696	-2.156257	3.678748
38	1	0	2.541163	-5.555865	-1.213455
39	1	0	1.826778	-3.762590	0.360344
40	1	0	-3.208653	-2.497838	-3.974047
41	1	0	0.504061	-2.015066	0.926167
42	1	0	-2.358695	-2.730573	0.130971
43	7	0	-0.516823	-0.812028	-0.401265
44	6	0	0.430973	-0.019497	-0.886743
45	1	0	-1.477645	-0.460922	-0.403559
46	6	0	1.783671	-0.402965	-0.985519
47	6	0	2.745011	0.548690	-1.261366
48	1	0	2.096814	-1.368432	-0.606583
49	6	0	0.913557	1.969795	-2.256227
50	6	0	4.114494	0.279013	-0.890339

51	1	0	0.652580	3.015949	-2.433654
52	1	0	0.655592	1.414482	-3.165147
53	6	0	5.059982	1.241202	-0.825625
54	1	0	4.330826	-0.717971	-0.510935
55	6	0	6.416660	1.053985	-0.311235
56	1	0	4.800829	2.261916	-1.092992
57	6	0	7.068162	2.147681	0.274947
58	6	0	7.078590	-0.179155	-0.379267
59	6	0	8.348469	2.004491	0.797040
60	1	0	6.540384	3.095543	0.346524
61	6	0	8.362087	-0.316087	0.133220
62	1	0	6.592527	-1.023280	-0.860563
63	6	0	8.998487	0.774372	0.725228
64	1	0	8.839273	2.853320	1.262777
65	1	0	8.871202	-1.272702	0.066215
66	1	0	10.000967	0.664643	1.127441
67	6	0	-5.708834	3.819596	0.915876
68	6	0	-6.282882	4.011090	-0.349236
69	6	0	-5.985668	3.166444	-1.402505
70	6	0	-5.096582	2.098194	-1.220657
71	6	0	-4.504832	1.904348	0.045418
72	6	0	-4.827718	2.771856	1.102542
73	1	0	-5.953632	4.483576	1.737501
74	1	0	-6.975895	4.832081	-0.507854
75	1	0	-6.424017	3.300117	-2.385370
76	1	0	-4.362107	2.600433	2.067897
77	6	0	-3.545603	0.808277	0.248632
78	8	0	-3.279675	-0.018731	-0.646689
79	8	0	-2.965848	0.751081	1.418715
80	1	0	-2.458436	-0.177001	1.509108
81	8	0	-4.854650	1.310676	-2.277147
82	1	0	-4.234289	0.607203	-1.989089
83	6	0	2.409453	1.830166	-1.977166
84	1	0	2.972932	1.839417	-2.918849
85	1	0	2.787781	2.677250	-1.394906
86	6	0	0.080940	1.410045	-1.106309
87	1	0	-0.987874	1.496906	-1.341806
88	6	0	0.252178	2.185637	0.309873
89	1	0	-0.512942	1.697181	0.928105
90	6	0	-0.210357	3.617068	0.114907
91	6	0	-1.542642	3.916424	0.413576
92	6	0	0.597660	4.635390	-0.401321
93	6	0	-2.066674	5.186400	0.197143
94	1	0	-2.174044	3.138881	0.834441
95	6	0	0.079387	5.911583	-0.608799
96	1	0	1.642483	4.447827	-0.626304

97	6	0	-1.253001	6.191683	-0.317391
98	1	0	-3.108977	5.382766	0.433893
99	1	0	0.726181	6.690566	-1.001036
100	1	0	-1.652052	7.187303	-0.486127
101	6	0	1.565273	1.976868	1.024594
102	6	0	2.670512	2.833561	0.986270
103	7	0	3.611194	3.521585	0.880031
104	6	0	1.669544	0.772466	1.728239
105	7	0	1.652039	-0.289684	2.221237

α′,β-TS4

Zero-point correction= 0.877325 (Hartree/Particle)
Thermal correction to Energy= 0.925486
Thermal correction to Enthalpy= 0.926430
Thermal correction to Gibbs Free Energy= 0.792963
E(sov) = -2432.20816021 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.736987	-3.157574	-3.579438
2	6	0	-2.332753	-4.272765	-4.349621
3	6	0	-1.246036	-5.012568	-3.964318
4	6	0	-0.518284	-4.675217	-2.793532
5	6	0	-0.924356	-3.554933	-2.010354
6	6	0	-2.053877	-2.805112	-2.443081
7	6	0	-0.520483	-2.148286	0.138131
8	6	0	-1.802105	-2.512348	0.909177
9	7	0	-2.204754	-1.460982	1.879011
10	6	0	-3.606050	-1.730706	2.285139
11	6	0	-1.653468	-3.865826	1.647788
12	6	0	-3.764816	-3.182776	2.786628
13	6	0	-2.360235	-3.756899	3.002638
14	6	0	-1.334873	-1.484277	3.078654
15	6	0	-1.553656	-2.782010	3.895117
16	6	0	-0.297862	-3.434673	4.413672
17	6	0	0.965162	-3.066356	4.207957
18	7	0	0.549596	-5.464122	-2.477496
19	6	0	1.224365	-5.161826	-1.397987
20	6	0	0.906449	-4.076460	-0.546204
21	6	0	-0.163954	-3.267512	-0.833980
22	1	0	-2.885009	-4.536418	-5.246093
23	1	0	-0.903029	-5.873302	-4.528965
24	1	0	-2.380217	-1.935817	-1.884417

25	1	0	-3.852906	-1.003594	3.065165
26	1	0	-4.245210	-1.520288	1.421128
27	1	0	-2.070941	-4.674827	1.040164
28	1	0	-0.594690	-4.096835	1.813482
29	1	0	-4.339197	-3.204776	3.718067
30	1	0	-4.307431	-3.791373	2.054803
31	1	0	-2.415608	-4.740378	3.480852
32	1	0	-1.571969	-0.595270	3.671398
33	1	0	-0.302633	-1.366150	2.743363
34	1	0	-2.183690	-2.551997	4.767462
35	1	0	-0.488387	-4.322112	5.020007
36	1	0	1.772850	-3.645718	4.645948
37	1	0	1.259513	-2.189802	3.636494
38	1	0	2.076077	-5.797134	-1.160764
39	1	0	1.515509	-3.888775	0.335559
40	1	0	-3.595299	-2.571003	-3.891929
41	1	0	0.309648	-2.071756	0.858915
42	1	0	-2.626580	-2.569811	0.188531
43	7	0	-0.662529	-0.848360	-0.485058
44	6	0	0.373142	-0.124884	-0.943991
45	1	0	-1.598846	-0.448819	-0.545775
46	6	0	1.685444	-0.559003	-0.967495
47	6	0	2.688008	0.429291	-1.110993
48	1	0	1.958433	-1.539798	-0.595542
49	6	0	0.984699	1.787435	-2.377036
50	6	0	4.034810	0.116098	-0.673319
51	1	0	0.784441	2.838685	-2.597920
52	1	0	0.685388	1.208279	-3.255906
53	6	0	5.086301	0.945946	-0.828466
54	1	0	4.152499	-0.802775	-0.100847
55	6	0	6.437433	0.704590	-0.313837
56	1	0	4.943383	1.900054	-1.328755
57	6	0	7.247373	1.805486	-0.005729
58	6	0	6.945095	-0.586578	-0.119032
59	6	0	8.528141	1.620071	0.500981
60	1	0	6.844643	2.806352	-0.137096
61	6	0	8.228865	-0.770043	0.379441
62	1	0	6.338193	-1.447134	-0.385913
63	6	0	9.022894	0.332062	0.693020
64	1	0	9.140151	2.481662	0.749090
65	1	0	8.615881	-1.775061	0.517171
66	1	0	10.025443	0.186344	1.083390
67	6	0	-5.215337	4.324064	1.028040
68	6	0	-5.819741	4.592177	-0.208194
69	6	0	-5.673959	3.725846	-1.275591
70	6	0	-4.912534	2.556811	-1.136631

71	6	0	-4.282292	2.289636	0.096619
72	6	0	-4.452135	3.180836	1.169020
73	1	0	-5.343569	5.005427	1.861989
74	1	0	-6.416191	5.491384	-0.332353
75	1	0	-6.139393	3.916327	-2.236413
76	1	0	-3.964724	2.948563	2.110713
77	6	0	-3.448127	1.086001	0.251424
78	8	0	-3.364955	0.216175	-0.637284
79	8	0	-2.783035	0.984856	1.372203
80	1	0	-2.389869	-0.002288	1.465218
81	8	0	-4.820045	1.749201	-2.201508
82	1	0	-4.288518	0.967429	-1.937677
83	6	0	2.474136	1.566848	-2.083904
84	1	0	3.010601	1.312103	-3.006821
85	1	0	2.947315	2.475880	-1.699949
86	6	0	0.139503	1.327975	-1.190729
87	1	0	-0.924290	1.520122	-1.378348
88	6	0	0.489278	2.108373	0.163553
89	1	0	-0.233030	1.699928	0.881049
90	6	0	0.137494	3.575392	-0.002801
91	6	0	-1.129895	3.983984	0.422714
92	6	0	0.967501	4.519437	-0.615403
93	6	0	-1.568082	5.290765	0.236653
94	1	0	-1.778082	3.261863	0.912215
95	6	0	0.537205	5.832187	-0.790477
96	1	0	1.963761	4.246373	-0.946549
97	6	0	-0.731746	6.222049	-0.371692
98	1	0	-2.562823	5.574286	0.568957
99	1	0	1.201956	6.551960	-1.258308
100	1	0	-1.064346	7.245409	-0.516413
101	6	0	1.873981	1.774423	0.704626
102	6	0	2.950384	2.681977	0.772888
103	7	0	3.892876	3.366163	0.724707
104	6	0	1.877330	0.693063	1.617891
105	7	0	1.775811	-0.275901	2.256940

α′,β-INT5

Zero-point correction= 0.877888 (Hartree/Particle)
Thermal correction to Energy= 0.926532
Thermal correction to Enthalpy= 0.927477
Thermal correction to Gibbs Free Energy= 0.792462
E(sov) = -2432.22214592 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.259713	-3.689253	-3.056856
2	6	0	-2.925927	-4.813928	-3.846939
3	6	0	-1.738619	-5.466064	-3.642593
4	6	0	-0.835840	-5.028061	-2.639771
5	6	0	-1.172481	-3.902919	-1.831476
6	6	0	-2.408300	-3.242872	-2.077271
7	6	0	-0.462894	-2.362596	0.143596
8	6	0	-1.583664	-2.667222	1.158483
9	7	0	-1.784758	-1.518695	2.079314
10	6	0	-2.909540	-1.832725	2.988603
11	6	0	-1.280766	-3.949278	1.981200
12	6	0	-2.559239	-3.021407	3.914150
13	6	0	-1.204073	-3.581300	3.468360
14	6	0	-0.571615	-1.237318	2.881669
15	6	0	-0.123932	-2.496622	3.673222
16	6	0	1.252650	-3.023939	3.337928
17	6	0	2.263324	-2.351844	2.790100
18	7	0	0.329489	-5.727058	-2.509087
19	6	0	1.169854	-5.328321	-1.589838
20	6	0	0.932208	-4.233343	-0.724121
21	6	0	-0.233579	-3.515540	-0.824634
22	1	0	-3.611320	-5.153167	-4.617399
23	1	0	-1.443292	-6.327776	-4.231921
24	1	0	-2.685565	-2.366213	-1.502691
25	1	0	-3.132330	-0.923831	3.555422
26	1	0	-3.780348	-2.047420	2.360549
27	1	0	-2.056571	-4.704091	1.816853
28	1	0	-0.334396	-4.393500	1.657081
29	1	0	-2.506324	-2.697322	4.958966
30	1	0	-3.327841	-3.798282	3.853144
31	1	0	-0.946825	-4.467816	4.058180
32	1	0	-0.821256	-0.410266	3.553215
33	1	0	0.204611	-0.862140	2.209862
34	1	0	-0.113900	-2.249781	4.744540
35	1	0	1.417269	-4.063001	3.630653
36	1	0	3.226367	-2.831195	2.638696
37	1	0	2.191810	-1.303650	2.508768
38	1	0	2.098963	-5.889570	-1.502478
39	1	0	1.674069	-3.971418	0.027448
40	1	0	-4.196863	-3.169707	-3.230821
41	1	0	0.464309	-2.277282	0.721368
42	1	0	-2.530944	-2.775210	0.618757

43	7	0	-0.679453	-1.095163	-0.509549
44	6	0	0.324529	-0.184085	-0.672346
45	1	0	-1.634647	-0.769503	-0.631648
46	6	0	1.644110	-0.323909	-0.420254
47	6	0	2.460245	0.934723	-0.617792
48	1	0	2.128042	-1.239266	-0.098463
49	6	0	0.774898	1.477508	-2.426240
50	6	0	3.891568	0.716591	-0.211233
51	1	0	0.480452	2.435595	-2.861004
52	1	0	0.551893	0.706545	-3.168624
53	6	0	4.967166	1.098571	-0.904169
54	1	0	4.015711	0.216045	0.750147
55	6	0	6.370782	0.881905	-0.510940
56	1	0	4.832258	1.634392	-1.842517
57	6	0	7.373059	1.611646	-1.160097
58	6	0	6.749046	-0.030192	0.482948
59	6	0	8.711369	1.454001	-0.816219
60	1	0	7.092918	2.318272	-1.937340
61	6	0	8.084876	-0.189128	0.827795
62	1	0	5.993582	-0.631382	0.980351
63	6	0	9.071971	0.553837	0.181593
64	1	0	9.472688	2.033924	-1.328875
65	1	0	8.359564	-0.901219	1.600267
66	1	0	10.115691	0.425015	0.450987
67	6	0	-5.376218	3.928527	1.344296
68	6	0	-6.040502	4.216287	0.143897
69	6	0	-5.889553	3.405189	-0.965543
70	6	0	-5.065429	2.272004	-0.905138
71	6	0	-4.371318	1.990509	0.289101
72	6	0	-4.545726	2.825145	1.403941
73	1	0	-5.510029	4.563595	2.213399
74	1	0	-6.688950	5.085406	0.082000
75	1	0	-6.401637	3.610805	-1.899104
76	1	0	-4.009620	2.579272	2.315035
77	6	0	-3.464172	0.828934	0.360771
78	8	0	-3.413311	-0.026527	-0.540578
79	8	0	-2.708594	0.766180	1.425427
80	1	0	-2.246095	-0.195217	1.524569
81	8	0	-4.976088	1.511255	-2.004461
82	1	0	-4.408763	0.739820	-1.788378
83	6	0	2.275480	1.457732	-2.059598
84	1	0	2.829129	0.793817	-2.728769
85	1	0	2.720722	2.456124	-2.154654
86	6	0	-0.059462	1.188003	-1.168851
87	1	0	-1.131605	1.245165	-1.387553
88	6	0	0.257505	2.195064	-0.028399

89	1	0	-0.291783	1.832694	0.846142
90	6	0	-0.283673	3.580309	-0.317047
91	6	0	-1.471582	3.939162	0.325789
92	6	0	0.261757	4.468100	-1.251544
93	6	0	-2.113793	5.139166	0.038954
94	1	0	-1.902384	3.257284	1.054935
95	6	0	-0.370153	5.676862	-1.529050
96	1	0	1.192816	4.234116	-1.758334
97	6	0	-1.560934	6.013819	-0.891118
98	1	0	-3.044897	5.381252	0.542933
99	1	0	0.072687	6.357062	-2.249933
100	1	0	-2.052876	6.954856	-1.117161
101	6	0	1.797161	2.051073	0.335042
102	6	0	2.571344	3.299479	0.236920
103	7	0	3.224710	4.246145	0.127010
104	6	0	1.894074	1.586452	1.730876
105	7	0	1.933122	1.185988	2.815075

5

Zero-point correction= 0.384153 (Hartree/Particle)
Thermal correction to Energy= 0.406498
Thermal correction to Enthalpy= 0.407442
Thermal correction to Gibbs Free Energy= 0.331253
E(sov) = -1110.90412548 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.453862	2.784632	-0.533294
2	6	0	-0.279476	0.959189	-0.351199
3	6	0	1.554753	0.917533	-2.112883
4	6	0	-1.710128	0.671192	0.020645
5	1	0	2.158775	0.095364	-2.502677
6	1	0	1.513254	1.671252	-2.905986
7	6	0	-2.558535	-0.089092	-0.677044
8	1	0	-2.033449	1.126063	0.957590
9	6	0	-3.957884	-0.379059	-0.320292
10	1	0	-2.212884	-0.573445	-1.589259
11	6	0	-4.617387	-1.420915	-0.982257
12	6	0	-4.659304	0.342571	0.654462
13	6	0	-5.931580	-1.750467	-0.668199
14	1	0	-4.085388	-1.984499	-1.744617

15	6	0	-5.971718	0.015426	0.968634
16	1	0	-4.181222	1.174216	1.163191
17	6	0	-6.612729	-1.033821	0.310856
18	1	0	-6.422834	-2.566956	-1.188248
19	1	0	-6.500272	0.584441	1.727220
20	1	0	-7.639262	-1.285872	0.558033
21	6	0	0.127680	0.446138	-1.742533
22	1	0	-0.600293	0.820704	-2.468727
23	1	0	0.053833	-0.647525	-1.762060
24	6	0	2.245598	1.540303	-0.889850
25	1	0	3.280415	1.819520	-1.102719
26	6	0	2.215954	0.609450	0.350220
27	1	0	2.577762	1.209399	1.191135
28	6	0	3.170360	-0.561159	0.223983
29	6	0	4.339228	-0.544433	0.989945
30	6	0	2.972502	-1.623220	-0.665755
31	6	0	5.289074	-1.554615	0.871251
32	1	0	4.506548	0.270722	1.689651
33	6	0	3.919109	-2.635258	-0.784277
34	1	0	2.062429	-1.686930	-1.253703
35	6	0	5.081741	-2.602915	-0.019230
36	1	0	6.187643	-1.522697	1.479270
37	1	0	3.741619	-3.454418	-1.473752
38	1	0	5.818590	-3.394315	-0.113090
39	6	0	0.696262	0.265203	0.696595
40	6	0	0.401542	-1.178977	0.718675
41	7	0	0.126297	-2.300530	0.703775
42	6	0	0.396747	0.785985	2.045099
43	7	0	0.169231	1.252488	3.077503
44	8	0	1.919368	3.894867	-0.459398
45	6	0	-0.018185	2.476304	-0.284478
46	1	0	-0.315032	2.900958	0.681328
47	1	0	-0.618787	2.981410	-1.050794

3

Zero-point correction= 0.480815 (Hartree/Particle)
Thermal correction to Energy= 0.508075
Thermal correction to Enthalpy= 0.509019
Thermal correction to Gibbs Free Energy= 0.421165
E(sov) = -1798.18117381 A.U.

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-1.059094	-2.157592	2.674489
2	6	0	0.529711	-1.649044	0.790800
3	6	0	-1.188801	-3.526503	0.648287
4	6	0	1.915049	-1.159962	0.449517
5	1	0	-1.802331	-3.824706	-0.206300
6	1	0	-1.098924	-4.411901	1.285644
7	6	0	2.722504	-1.657748	-0.491457
8	1	0	2.250266	-0.308965	1.038830
9	6	0	4.051125	-1.117918	-0.836296
10	1	0	2.421829	-2.537618	-1.059256
11	6	0	4.959546	-1.931726	-1.522317
12	6	0	4.436508	0.191317	-0.514899
13	6	0	6.226586	-1.467081	-1.857909
14	1	0	4.667503	-2.945167	-1.787409
15	6	0	5.702717	0.655448	-0.848690
16	1	0	3.735810	0.859706	-0.021265
17	6	0	6.603954	-0.171073	-1.518201
18	1	0	6.918055	-2.116714	-2.386117
19	1	0	5.983056	1.672987	-0.594081
20	1	0	7.590462	0.197565	-1.781916
21	6	0	0.211503	-3.036895	0.197627
22	1	0	0.989304	-3.739482	0.515124
23	1	0	0.266892	-2.983664	-0.896786
24	6	0	-1.906686	-2.424052	1.442853
25	1	0	-2.908350	-2.731238	1.754870
26	6	0	-1.985883	-1.097056	0.642213
27	1	0	-2.351875	-0.336739	1.344535
28	6	0	-2.989955	-1.173489	-0.489525
29	6	0	-4.245121	-0.579087	-0.337604
30	6	0	-2.705685	-1.824158	-1.696085
31	6	0	-5.188967	-0.624907	-1.360052
32	1	0	-4.479013	-0.063007	0.590407
33	6	0	-3.646759	-1.873065	-2.720574
34	1	0	-1.731798	-2.283312	-1.849605
35	6	0	-4.891995	-1.270748	-2.556624
36	1	0	-6.155278	-0.149639	-1.222117
37	1	0	-3.404691	-2.380980	-3.649156
38	1	0	-5.624530	-1.305461	-3.356920
39	6	0	-0.539542	-0.686617	0.186118
40	8	0	-1.461850	-2.274442	3.806789
41	6	0	0.361694	-1.746042	2.321509
42	1	0	0.593225	-0.799320	2.817718
43	1	0	1.051180	-2.499206	2.723837
44	6	0	-0.335476	0.779168	0.462230

45	6	0	-0.930237	1.824184	-0.432657
46	6	0	-0.616697	3.094320	0.034564
47	6	0	-1.690742	1.685010	-1.588860
48	6	0	-1.030842	4.253588	-0.589598
49	6	0	-2.124556	2.844232	-2.234992
50	1	0	-1.952482	0.708457	-1.983788
51	6	0	-1.802689	4.109640	-1.745324
52	1	0	-0.768031	5.231304	-0.199128
53	1	0	-2.723441	2.756445	-3.135638
54	1	0	-2.152589	4.993585	-2.268840
55	1	0	-0.463550	-0.798175	-0.903026
56	7	0	0.325261	1.196996	1.479280
57	16	0	0.381234	2.904219	1.502156
58	8	0	-0.323767	3.389587	2.671096
59	8	0	1.751331	3.306842	1.245824

γ'-TS1-B

Zero-point correction= 0.968073 (Hartree/Particle)
Thermal correction to Energy= 1.021469
Thermal correction to Enthalpy= 1.022414
Thermal correction to Gibbs Free Energy= 0.877926
E(sov) = -2684.24465562 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.314170	-3.093759	-2.512057
2	6	0	-5.356583	-4.349722	-3.160373
3	6	0	-4.274083	-5.187227	-3.101068
4	6	0	-3.106434	-4.811410	-2.387709
5	6	0	-3.059815	-3.549206	-1.726960
6	6	0	-4.197967	-2.700567	-1.817842
7	6	0	-1.702808	-1.950140	-0.193251
8	6	0	-2.586544	-1.986720	1.064881
9	7	0	-2.329308	-0.826434	1.959491
10	6	0	-3.490417	-0.700111	2.875508
11	6	0	-2.414901	-3.290668	1.877126
12	6	0	-3.794076	-2.054746	3.554262
13	6	0	-2.563571	-2.949266	3.364907
14	6	0	-1.096339	-1.034523	2.760440
15	6	0	-1.313159	-2.152191	3.806005
16	6	0	-0.131806	-3.057134	4.027404

17	6	0	1.100146	-2.962554	3.533417
18	7	0	-2.074134	-5.704484	-2.374267
19	6	0	-0.994753	-5.366684	-1.717155
20	6	0	-0.845523	-4.144213	-1.018010
21	6	0	-1.866704	-3.227679	-1.006885
22	1	0	-6.246265	-4.642586	-3.709067
23	1	0	-4.264288	-6.156069	-3.589494
24	1	0	-4.180858	-1.720548	-1.356394
25	1	0	-3.233620	0.071454	3.608590
26	1	0	-4.336713	-0.333165	2.286147
27	1	0	-3.150619	-4.034241	1.554655
28	1	0	-1.421142	-3.722281	1.704119
29	1	0	-4.007862	-1.909377	4.617852
30	1	0	-4.675014	-2.527691	3.106115
31	1	0	-2.654130	-3.864476	3.959187
32	1	0	-0.843737	-0.079387	3.231936
33	1	0	-0.280130	-1.266498	2.072605
34	1	0	-1.551069	-1.694954	4.779083
35	1	0	-0.343837	-3.889903	4.700708
36	1	0	1.841080	-3.707671	3.812845
37	1	0	1.475180	-2.182092	2.874925
38	1	0	-0.177555	-6.086497	-1.719462
39	1	0	0.081357	-3.939055	-0.486552
40	1	0	-6.170811	-2.429602	-2.571079
41	1	0	-0.654215	-1.919666	0.138539
42	1	0	-3.632735	-1.882799	0.750732
43	7	0	-1.953516	-0.740862	-0.950849
44	6	0	-0.949768	-0.072307	-1.587380
45	1	0	-2.763507	-0.188663	-0.676616
46	6	0	0.252771	-0.635405	-1.892644
47	6	0	1.407371	0.193499	-2.141226
48	1	0	0.422307	-1.691509	-1.710912
49	6	0	-0.127296	2.066290	-2.652774
50	6	0	2.712843	-0.402767	-2.023648
51	1	0	-0.190700	3.153461	-2.549183
52	1	0	-0.290674	1.832936	-3.714975
53	6	0	3.855301	0.315576	-1.887423
54	1	0	2.737866	-1.483963	-1.899209
55	6	0	5.199482	-0.207384	-1.631857
56	1	0	3.820297	1.391779	-2.029970
57	6	0	6.260895	0.701938	-1.519530
58	6	0	5.468960	-1.573691	-1.456612
59	6	0	7.548606	0.263885	-1.229959
60	1	0	6.064046	1.763550	-1.634793
61	6	0	6.753812	-2.009962	-1.170217
62	1	0	4.666635	-2.300930	-1.531547

63	6	0	7.799127	-1.092978	-1.052776
64	1	0	8.353451	0.986399	-1.137897
65	1	0	6.941242	-3.070068	-1.027288
66	1	0	8.802698	-1.438285	-0.822901
67	6	0	-3.601094	5.612241	1.471474
68	6	0	-4.615436	6.027983	0.598798
69	6	0	-5.249677	5.126959	-0.237042
70	6	0	-4.884913	3.773530	-0.221851
71	6	0	-3.848529	3.349647	0.636684
72	6	0	-3.223875	4.281447	1.479979
73	1	0	-3.118761	6.323266	2.133751
74	1	0	-4.916526	7.071365	0.580367
75	1	0	-6.042386	5.432000	-0.911359
76	1	0	-2.441960	3.929034	2.145490
77	6	0	-3.444989	1.931413	0.657254
78	8	0	-4.070320	1.057676	0.028437
79	8	0	-2.382621	1.648087	1.362438
80	1	0	-2.280862	0.581138	1.438918
81	8	0	-5.546973	2.943744	-1.039206
82	1	0	-5.215304	2.034436	-0.868751
83	6	0	1.553172	2.138887	-0.163770
84	1	0	0.670131	1.572078	0.126239
85	6	0	1.325023	3.587085	-0.373650
86	6	0	0.104560	4.123033	0.058987
87	6	0	2.236987	4.431249	-1.020484
88	6	0	-0.194685	5.467237	-0.137071
89	1	0	-0.613522	3.473969	0.557781
90	6	0	1.936088	5.774267	-1.216734
91	1	0	3.183552	4.039591	-1.378929
92	6	0	0.721723	6.297153	-0.777268
93	1	0	-1.149592	5.857545	0.202448
94	1	0	2.653594	6.414429	-1.720787
95	1	0	0.489618	7.345254	-0.939587
96	6	0	2.732965	1.563695	0.331456
97	6	0	3.935131	2.323785	0.369900
98	7	0	4.895466	2.978793	0.368336
99	6	0	2.618458	0.197043	0.866476
100	6	0	3.799425	-0.594642	1.359126
101	6	0	4.996042	-0.056087	1.842312
102	6	0	3.660394	-1.988543	1.305014
103	6	0	6.026813	-0.898800	2.251785
104	1	0	5.137838	1.014314	1.915774
105	6	0	4.686096	-2.826885	1.720594
106	1	0	2.730847	-2.396279	0.919196
107	6	0	5.877956	-2.280671	2.192668
108	1	0	6.952175	-0.466647	2.619549

109	1	0	4.561466	-3.904635	1.665387
110	1	0	6.688788	-2.929748	2.510292
111	8	0	1.520676	-0.365058	0.846207
112	6	0	1.245792	1.566232	-2.286500
113	1	0	2.081698	2.162887	-2.636583
114	6	0	-1.221468	1.393965	-1.823942
115	1	0	-1.313332	1.878717	-0.844687
116	1	0	-2.197135	1.508600	-2.311928

γ'-TS1-C

Zero-point correction= 0.969804 (Hartree/Particle)
Thermal correction to Energy= 1.023349
Thermal correction to Enthalpy= 1.024293
Thermal correction to Gibbs Free Energy= 0.878208
E(RM062X) = -2684.24098846 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.302388	4.903423	-2.351147
2	6	0	2.909492	6.052242	-3.075945
3	6	0	1.633287	6.535408	-2.953120
4	6	0	0.696077	5.894034	-2.103119
5	6	0	1.087131	4.734967	-1.370264
6	6	0	2.418697	4.259356	-1.521990
7	6	0	0.365061	2.899787	0.324932
8	6	0	1.317831	3.193573	1.503389
9	7	0	1.638316	1.949097	2.238894
10	6	0	2.600750	2.263258	3.314975
11	6	0	0.701893	4.238257	2.474998
12	6	0	1.968088	3.210061	4.364071
13	6	0	0.572224	3.600461	3.864455
14	6	0	0.431705	1.329422	2.827167
15	6	0	-0.297905	2.324134	3.769185
16	6	0	-1.723073	2.670317	3.409100
17	6	0	-2.505382	2.117659	2.483015
18	7	0	-0.553366	6.440070	-2.034663
19	6	0	-1.426191	5.855098	-1.256151
20	6	0	-1.147325	4.698338	-0.487908
21	6	0	0.100936	4.129279	-0.530670
22	1	0	3.621726	6.545674	-3.729834
23	1	0	1.292441	7.413101	-3.492388
24	1	0	2.758704	3.378979	-0.988876

25	1	0	2.912934	1.312136	3.756378
26	1	0	3.481170	2.708626	2.840365
27	1	0	1.330287	5.133097	2.526257
28	1	0	-0.281411	4.562505	2.117953
29	1	0	1.894218	2.717528	5.339391
30	1	0	2.581430	4.106892	4.498409
31	1	0	0.106321	4.309995	4.557166
32	1	0	0.759423	0.429183	3.354592
33	1	0	-0.200384	0.973583	2.007759
34	1	0	-0.333401	1.889930	4.778964
35	1	0	-2.145220	3.468410	4.023433
36	1	0	-3.530680	2.453815	2.354096
37	1	0	-2.187200	1.303831	1.835716
38	1	0	-2.418728	6.300846	-1.213437
39	1	0	-1.925812	4.268595	0.139111
40	1	0	4.313073	4.520951	-2.454270
41	1	0	-0.596526	2.625329	0.765505
42	1	0	2.272398	3.555187	1.106566
43	7	0	0.830300	1.749941	-0.428600
44	6	0	0.049689	0.757982	-0.881028
45	1	0	1.839755	1.636672	-0.526414
46	6	0	-1.331627	0.780795	-0.848818
47	6	0	-2.108925	-0.319938	-1.300520
48	1	0	-1.856154	1.672175	-0.520129
49	6	0	-0.070528	-1.372249	-2.245428
50	6	0	-3.554510	-0.156656	-1.188841
51	1	0	0.387672	-2.358973	-2.330541
52	1	0	-0.092811	-0.941334	-3.256809
53	6	0	-4.484655	-0.992376	-1.684332
54	1	0	-3.882186	0.729260	-0.646459
55	6	0	-5.932631	-0.857330	-1.502012
56	1	0	-4.169958	-1.846208	-2.282754
57	6	0	-6.798812	-1.534029	-2.369701
58	6	0	-6.486007	-0.091036	-0.465419
59	6	0	-8.178099	-1.426575	-2.229072
60	1	0	-6.380314	-2.143207	-3.167124
61	6	0	-7.862686	0.014566	-0.323171
62	1	0	-5.828642	0.391018	0.252388
63	6	0	-8.714289	-0.648424	-1.206928
64	1	0	-8.833884	-1.953403	-2.915378
65	1	0	-8.276733	0.606526	0.487562
66	1	0	-9.790595	-0.566870	-1.090576
67	6	0	4.765690	-3.380276	-0.323068
68	6	0	5.601525	-3.247940	-1.438596
69	6	0	5.809671	-2.017132	-2.038252
70	6	0	5.179018	-0.875226	-1.530171

71	6	0	4.346060	-0.998046	-0.399181
72	6	0	4.143041	-2.258059	0.188342
73	1	0	4.598590	-4.349812	0.131851
74	1	0	6.090475	-4.127090	-1.849228
75	1	0	6.448802	-1.903147	-2.907225
76	1	0	3.474300	-2.330003	1.041845
77	6	0	3.653154	0.179357	0.141531
78	8	0	3.698762	1.300891	-0.406335
79	8	0	2.942552	-0.038536	1.209988
80	1	0	2.405414	0.806394	1.502451
81	8	0	5.401532	0.293843	-2.154379
82	1	0	4.864046	0.976849	-1.698607
83	6	0	-1.566670	-2.951838	-0.284750
84	1	0	-1.914948	-3.679305	-1.014010
85	6	0	-2.647743	-2.514628	0.631356
86	6	0	-3.906103	-3.107200	0.471493
87	6	0	-2.496287	-1.528331	1.613945
88	6	0	-4.987485	-2.732193	1.262585
89	1	0	-4.036973	-3.870962	-0.291483
90	6	0	-3.576810	-1.153886	2.407792
91	1	0	-1.531293	-1.051663	1.754913
92	6	0	-4.825644	-1.750492	2.234591
93	1	0	-5.957478	-3.195406	1.108112
94	1	0	-3.439463	-0.392588	3.170784
95	1	0	-5.666369	-1.450692	2.853213
96	6	0	-0.256536	-3.298042	0.140556
97	6	0	0.349124	-2.638367	1.236595
98	7	0	0.829954	-2.033566	2.109966
99	6	0	0.424677	-4.320367	-0.650798
100	6	0	1.608293	-5.089074	-0.119135
101	6	0	1.933200	-5.199014	1.236211
102	6	0	2.340674	-5.829112	-1.054951
103	6	0	2.976443	-6.029953	1.641932
104	1	0	1.364582	-4.663828	1.987971
105	6	0	3.378748	-6.658199	-0.650006
106	1	0	2.058116	-5.751297	-2.099228
107	6	0	3.698000	-6.763555	0.703712
108	1	0	3.213051	-6.114464	2.698209
109	1	0	3.935536	-7.228723	-1.387620
110	1	0	4.504438	-7.415969	1.025878
111	8	0	-0.002980	-4.624270	-1.766614
112	6	0	-1.506243	-1.497823	-1.781303
113	1	0	-2.123209	-2.110538	-2.432980
114	6	0	0.785862	-0.469960	-1.353818
115	1	0	1.126190	-0.991256	-0.450087
116	1	0	1.692318	-0.161265	-1.889728

γ'-TS1-D

Zero-point correction= 0.969683 (Hartree/Particle)
Thermal correction to Energy= 1.023073
Thermal correction to Enthalpy= 1.024017
Thermal correction to Gibbs Free Energy= 0.880240
E(sov) = -2684.23876658 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.797333	5.663684	-2.449083
2	6	0	1.103236	6.673274	-3.155287
3	6	0	-0.253068	6.800713	-3.010836
4	6	0	-0.973905	5.927607	-2.156157
5	6	0	-0.278134	4.909216	-1.440032
6	6	0	1.129491	4.803123	-1.614482
7	6	0	-0.462601	2.943292	0.251666
8	6	0	0.384281	3.485360	1.423335
9	7	0	1.047583	2.377387	2.147759
10	6	0	1.888665	2.942960	3.223044
11	6	0	-0.491228	4.309088	2.408034
12	6	0	1.021389	3.664023	4.284039
13	6	0	-0.430221	3.649755	3.792136
14	6	0	0.067720	1.438496	2.734871
15	6	0	-0.904841	2.180037	3.691098
16	6	0	-2.372785	2.106163	3.344945
17	6	0	-2.974195	1.336360	2.438897
18	7	0	-2.322687	6.120164	-2.069659
19	6	0	-2.998394	5.317281	-1.289456
20	6	0	-2.411653	4.272522	-0.534635
21	6	0	-1.057056	4.058724	-0.594414
22	1	0	1.649686	7.342765	-3.812333
23	1	0	-0.822341	7.560286	-3.536288
24	1	0	1.700437	4.037942	-1.101326
25	1	0	2.460005	2.116020	3.655203
26	1	0	2.604404	3.622530	2.749709
27	1	0	-0.135315	5.342597	2.467371
28	1	0	-1.527893	4.352052	2.057656
29	1	0	1.095230	3.161070	5.253986
30	1	0	1.359572	4.695422	4.426006
31	1	0	-1.073873	4.194508	4.491715
32	1	0	0.638093	0.662001	3.251863

33	1	0	-0.445098	0.927924	1.914253
34	1	0	-0.805210	1.746700	4.696987
35	1	0	-2.998068	2.761872	3.954402
36	1	0	-4.053877	1.364511	2.318827
37	1	0	-2.442744	0.636435	1.798242
38	1	0	-4.073477	5.480749	-1.234193
39	1	0	-3.039696	3.645944	0.095112
40	1	0	2.871082	5.560627	-2.570403
41	1	0	-1.309615	2.418211	0.700437
42	1	0	1.195047	4.102168	1.020252
43	7	0	0.289834	1.966639	-0.512647
44	6	0	-0.197168	0.803643	-0.967047
45	1	0	1.292107	2.132231	-0.628655
46	6	0	-1.528759	0.439590	-0.902390
47	6	0	-1.978753	-0.837247	-1.335403
48	1	0	-2.271293	1.146071	-0.546273
49	6	0	0.237332	-1.261326	-2.363018
50	6	0	-3.405558	-1.089867	-1.163503
51	1	0	0.952001	-2.075911	-2.489702
52	1	0	0.052807	-0.838592	-3.361362
53	6	0	-4.081308	-2.166401	-1.604055
54	1	0	-3.947564	-0.321847	-0.613343
55	6	0	-5.496883	-2.445857	-1.344638
56	1	0	-3.564062	-2.910795	-2.207952
57	6	0	-6.166337	-3.390337	-2.132345
58	6	0	-6.202294	-1.822897	-0.303685
59	6	0	-7.507503	-3.684934	-1.910434
60	1	0	-5.626662	-3.891870	-2.931834
61	6	0	-7.540697	-2.115898	-0.082069
62	1	0	-5.684931	-1.133966	0.357655
63	6	0	-8.200463	-3.044890	-0.886585
64	1	0	-8.010414	-4.416457	-2.535349
65	1	0	-8.070542	-1.628081	0.730524
66	1	0	-9.245906	-3.275793	-0.707101
67	6	0	6.077473	-0.235169	-2.249003
68	6	0	6.389847	-1.429914	-1.585849
69	6	0	5.765663	-1.767668	-0.401334
70	6	0	4.797930	-0.924377	0.166246
71	6	0	4.478163	0.281887	-0.495097
72	6	0	5.127281	0.602067	-1.699606
73	1	0	6.569357	0.024416	-3.180053
74	1	0	7.125943	-2.108801	-2.007346
75	1	0	5.982181	-2.695478	0.116825
76	1	0	4.850369	1.534626	-2.181250
77	6	0	3.459588	1.228274	-0.003108
78	8	0	3.137605	2.253008	-0.604629

79	8	0	2.875258	0.866138	1.124284
80	1	0	2.101916	1.513961	1.404259
81	8	0	4.259939	-1.352825	1.315671
82	1	0	3.495094	-0.803460	1.575187
83	6	0	-0.652713	-3.217341	-0.369043
84	1	0	-0.775578	-4.004854	-1.108510
85	6	0	-1.799915	-3.137112	0.565702
86	6	0	-2.816234	-4.087686	0.411945
87	6	0	-1.946587	-2.160129	1.558159
88	6	0	-3.951373	-4.069953	1.216264
89	1	0	-2.712296	-4.850393	-0.356285
90	6	0	-3.083556	-2.139168	2.361233
91	1	0	-1.175222	-1.408627	1.695554
92	6	0	-4.090149	-3.090179	2.193250
93	1	0	-4.732450	-4.809299	1.066363
94	1	0	-3.181212	-1.375737	3.128408
95	1	0	-4.977353	-3.064776	2.818898
96	6	0	0.708255	-3.152533	0.026996
97	6	0	1.109487	-2.340432	1.111716
98	7	0	1.404779	-1.608460	1.970555
99	6	0	1.653544	-3.912109	-0.795289
100	6	0	3.022060	-4.294625	-0.297753
101	6	0	3.378161	-4.347365	1.051966
102	6	0	3.934376	-4.742948	-1.261245
103	6	0	4.623575	-4.845950	1.428499
104	1	0	2.686981	-4.019971	1.820296
105	6	0	5.176415	-5.236228	-0.885955
106	1	0	3.632308	-4.716020	-2.302722
107	6	0	5.521096	-5.296154	0.464814
108	1	0	4.886906	-4.886995	2.480784
109	1	0	5.873239	-5.584718	-1.642710
110	1	0	6.487589	-5.691456	0.764825
111	8	0	1.310058	-4.313690	-1.908664
112	6	0	-1.084226	-1.793432	-1.850828
113	1	0	-1.524242	-2.559536	-2.483639
114	6	0	0.839221	-0.163754	-1.482029
115	1	0	1.344497	-0.574095	-0.598221
116	1	0	1.602494	0.393198	-2.039063

γ'-TS1-E

Zero-point correction= 0.969323 (Hartree/Particle)
Thermal correction to Energy= 1.022562

Thermal correction to Enthalpy= 1.023506
Thermal correction to Gibbs Free Energy= 0.880845
E(sov) = -2684.24879515 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.011348	2.086514	-3.440391
2	6	0	4.960556	3.259266	-4.229214
3	6	0	4.145850	4.296447	-3.859307
4	6	0	3.350886	4.210627	-2.686932
5	6	0	3.402960	3.033855	-1.883496
6	6	0	4.254820	1.973199	-2.301447
7	6	0	2.574413	1.832645	0.264740
8	6	0	3.907100	1.764658	1.040836
9	7	0	4.040220	0.506727	1.812366
10	6	0	5.329644	0.521382	2.535939
11	6	0	4.024591	2.982471	2.003404
12	6	0	5.352262	1.629772	3.616508
13	6	0	4.082206	2.471032	3.448969
14	6	0	2.932770	0.361249	2.779520
15	6	0	2.859333	1.571529	3.744874
16	6	0	1.564263	2.349435	3.728303
17	6	0	0.401558	1.996745	3.182077
18	7	0	2.565571	5.287485	-2.391687
19	6	0	1.826357	5.218225	-1.314932
20	6	0	1.805341	4.102186	-0.443223
21	6	0	2.589425	3.007925	-0.706895
22	1	0	5.564493	3.329377	-5.128468
23	1	0	4.074393	5.211225	-4.438417
24	1	0	4.311399	1.052685	-1.731726
25	1	0	5.470277	-0.473285	2.970657
26	1	0	6.117289	0.665834	1.790059
27	1	0	4.922946	3.566782	1.779325
28	1	0	3.170725	3.655319	1.874326
29	1	0	5.386598	1.194133	4.620883
30	1	0	6.240170	2.260128	3.505440
31	1	0	4.091448	3.317774	4.143946
32	1	0	3.107872	-0.573908	3.322217
33	1	0	2.017609	0.218334	2.200401
34	1	0	2.982517	1.206635	4.775039
35	1	0	1.609770	3.292835	4.275924
36	1	0	-0.473676	2.631936	3.280029
37	1	0	0.256162	1.070341	2.629607
38	1	0	1.199848	6.081363	-1.096335
39	1	0	1.164306	4.118801	0.435638

40	1	0	5.650801	1.262630	-3.741420
41	1	0	1.795140	2.051502	1.002439
42	1	0	4.737661	1.764895	0.327056
43	7	0	2.229398	0.577273	-0.361991
44	6	0	0.969408	0.274025	-0.771317
45	1	0	2.974321	-0.037284	-0.679918
46	6	0	-0.141196	1.012596	-0.472722
47	6	0	-1.461828	0.605738	-0.875016
48	1	0	-0.060531	1.932272	0.097540
49	6	0	-0.448570	-1.142027	-2.331410
50	6	0	-2.571666	1.358233	-0.345239
51	1	0	-0.628970	-2.197067	-2.568616
52	1	0	-0.315506	-0.632513	-3.296367
53	6	0	-3.861039	1.249029	-0.748567
54	1	0	-2.342603	2.032336	0.480151
55	6	0	-5.001554	1.877022	-0.079511
56	1	0	-4.091969	0.701959	-1.661070
57	6	0	-6.183943	2.105279	-0.797558
58	6	0	-4.967634	2.196702	1.285817
59	6	0	-7.296011	2.657446	-0.176664
60	1	0	-6.227501	1.830217	-1.848174
61	6	0	-6.082766	2.747064	1.906067
62	1	0	-4.086404	1.956392	1.871848
63	6	0	-7.246804	2.982507	1.177942
64	1	0	-8.206849	2.819869	-0.744888
65	1	0	-6.049325	2.973974	2.967258
66	1	0	-8.119436	3.404137	1.667983
67	6	0	3.596864	-6.050089	0.540748
68	6	0	3.181057	-6.504344	-0.718577
69	6	0	3.062555	-5.633433	-1.787130
70	6	0	3.363238	-4.273700	-1.625232
71	6	0	3.752612	-3.803449	-0.354694
72	6	0	3.869838	-4.705557	0.713135
73	1	0	3.695913	-6.742876	1.368989
74	1	0	2.951985	-7.555972	-0.864115
75	1	0	2.748747	-5.971463	-2.768659
76	1	0	4.179833	-4.319168	1.678540
77	6	0	3.966101	-2.360208	-0.145962
78	8	0	4.023979	-1.555008	-1.089571
79	8	0	4.062463	-1.981379	1.101228
80	1	0	4.070372	-0.941879	1.181521
81	8	0	3.250141	-3.480709	-2.700950
82	1	0	3.559145	-2.585424	-2.441441
83	6	0	-2.477828	-2.010122	-0.417015
84	1	0	-2.579565	-2.619156	-1.313283
85	6	0	-1.325672	-2.390953	0.429578

86	6	0	-0.639103	-3.572040	0.112265
87	6	0	-0.858861	-1.607613	1.491913
88	6	0	0.500796	-3.950090	0.812896
89	1	0	-0.999165	-4.188767	-0.707791
90	6	0	0.270535	-1.996183	2.205499
91	1	0	-1.377283	-0.691663	1.754865
92	6	0	0.965776	-3.153325	1.858914
93	1	0	1.032895	-4.857468	0.539254
94	1	0	0.603157	-1.392444	3.045502
95	1	0	1.860308	-3.438408	2.404861
96	6	0	-3.732492	-1.573581	0.055387
97	6	0	-3.848621	-1.059646	1.374632
98	7	0	-3.885404	-0.635549	2.457517
99	6	0	-4.825487	-1.600520	-0.922519
100	6	0	-6.246913	-1.231326	-0.589144
101	6	0	-6.763967	-1.071644	0.701025
102	6	0	-7.093161	-1.025462	-1.686498
103	6	0	-8.091631	-0.691593	0.880150
104	1	0	-6.151379	-1.244096	1.576103
105	6	0	-8.417129	-0.648604	-1.505317
106	1	0	-6.681925	-1.167794	-2.680080
107	6	0	-8.919282	-0.474668	-0.217037
108	1	0	-8.477118	-0.563597	1.886914
109	1	0	-9.058221	-0.489426	-2.367579
110	1	0	-9.952773	-0.174460	-0.068797
111	8	0	-4.559029	-1.887546	-2.093349
112	6	0	-1.660011	-0.530257	-1.665646
113	1	0	-2.587604	-0.609010	-2.230801
114	6	0	0.853616	-1.023826	-1.529032
115	1	0	0.955076	-1.837744	-0.800210
116	1	0	1.706239	-1.116468	-2.209427

γ'-TS1-F

Zero-point correction= 0.968531 (Hartree/Particle)
Thermal correction to Energy= 1.022287
Thermal correction to Enthalpy= 1.023231
Thermal correction to Gibbs Free Energy= 0.875975
E(sov) = -2684.24382398 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.957696	0.604118	3.488389
2	6	0	-0.157320	0.187660	4.253520
3	6	0	-0.821760	-0.963833	3.920521
4	6	0	-0.412466	-1.741989	2.806775
5	6	0	0.690990	-1.311365	2.012427
6	6	0	1.371821	-0.123147	2.399890
7	6	0	2.158927	-1.773383	-0.100573
8	6	0	3.512103	-2.167809	0.521936
9	7	0	4.654871	-1.890733	-0.388047
10	6	0	5.899276	-1.917513	0.414526
11	6	0	3.553641	-3.649813	0.964672
12	6	0	6.002864	-3.232455	1.222039
13	6	0	4.951597	-4.204185	0.671024
14	6	0	4.742063	-2.914166	-1.449130
15	6	0	5.121884	-4.297048	-0.865904
16	6	0	4.360238	-5.470711	-1.425450
17	6	0	3.327546	-5.464198	-2.264855
18	7	0	-1.114450	-2.884667	2.562147
19	6	0	-0.773750	-3.585532	1.513300
20	6	0	0.272951	-3.226759	0.632376
21	6	0	1.020398	-2.101011	0.867071
22	1	0	-0.477914	0.778980	5.106092
23	1	0	-1.676764	-1.321061	4.485032
24	1	0	2.229842	0.224768	1.836387
25	1	0	6.732109	-1.808858	-0.288366
26	1	0	5.891661	-1.032064	1.057567
27	1	0	3.304540	-3.733832	2.026770
28	1	0	2.809605	-4.237032	0.414311
29	1	0	7.007131	-3.659203	1.134992
30	1	0	5.816450	-3.051667	2.286203
31	1	0	5.069988	-5.195699	1.120080
32	1	0	5.482842	-2.573363	-2.179393
33	1	0	3.779447	-2.933185	-1.963143
34	1	0	6.187886	-4.484027	-1.061259
35	1	0	4.715120	-6.435414	-1.060190
36	1	0	2.862035	-6.394122	-2.574939
37	1	0	2.908009	-4.557696	-2.691246
38	1	0	-1.352655	-4.486886	1.317149
39	1	0	0.467472	-3.844134	-0.241890
40	1	0	1.492092	1.509063	3.762752
41	1	0	1.989293	-2.404796	-0.986690
42	1	0	3.671887	-1.515244	1.390048
43	7	0	2.227845	-0.385793	-0.513396
44	6	0	1.130459	0.352987	-0.846258
45	1	0	3.001339	0.138485	-0.115651
46	6	0	-0.072601	-0.166237	-1.211910

47	6	0	-1.203511	0.701059	-1.420101
48	1	0	-0.222081	-1.235419	-1.313435
49	6	0	0.063612	2.480424	-0.184719
50	6	0	-2.342964	0.185222	-2.124759
51	1	0	0.101722	3.571097	-0.253861
52	1	0	0.087488	2.234162	0.886262
53	6	0	-3.529402	0.832363	-2.231672
54	1	0	-2.253614	-0.837648	-2.483689
55	6	0	-4.775740	0.295018	-2.775791
56	1	0	-3.597621	1.866901	-1.904302
57	6	0	-5.899783	1.133175	-2.816287
58	6	0	-4.920574	-1.041183	-3.180351
59	6	0	-7.133079	0.651182	-3.242202
60	1	0	-5.808586	2.159269	-2.471096
61	6	0	-6.149004	-1.518506	-3.613120
62	1	0	-4.074941	-1.719584	-3.127401
63	6	0	-7.260901	-0.675599	-3.643409
64	1	0	-7.994889	1.310915	-3.251439
65	1	0	-6.246918	-2.557758	-3.911486
66	1	0	-8.222898	-1.055819	-3.973516
67	6	0	6.344613	4.142536	-2.872676
68	6	0	6.083946	5.257482	-2.065417
69	6	0	5.490213	5.117157	-0.823908
70	6	0	5.141904	3.845260	-0.350471
71	6	0	5.398471	2.717111	-1.157698
72	6	0	5.998539	2.885343	-2.415558
73	1	0	6.808895	4.265312	-3.844828
74	1	0	6.349539	6.250431	-2.416299
75	1	0	5.279268	5.970923	-0.189269
76	1	0	6.181084	2.001666	-3.017669
77	6	0	5.014202	1.377553	-0.685672
78	8	0	4.521085	1.185033	0.442590
79	8	0	5.189582	0.395875	-1.530435
80	1	0	4.847998	-0.488282	-1.091804
81	8	0	4.563657	3.769440	0.857375
82	1	0	4.425539	2.818115	1.060523
83	6	0	-2.415898	1.655172	0.865373
84	1	0	-1.643747	1.013994	1.295434
85	6	0	-2.430960	3.051762	1.382056
86	6	0	-1.709509	3.343632	2.544745
87	6	0	-3.126183	4.087884	0.746901
88	6	0	-1.693988	4.632222	3.069920
89	1	0	-1.167061	2.542436	3.041462
90	6	0	-3.106796	5.376189	1.268201
91	1	0	-3.693328	3.883921	-0.156929
92	6	0	-2.392191	5.653171	2.431935

93	1	0	-1.133993	4.839001	3.977028
94	1	0	-3.653591	6.166947	0.763976
95	1	0	-2.379262	6.660264	2.837297
96	6	0	-3.612976	0.947601	0.613297
97	6	0	-4.858280	1.625756	0.498264
98	7	0	-5.855612	2.207761	0.360010
99	6	0	-3.500434	-0.512818	0.579920
100	6	0	-4.693970	-1.426054	0.613963
101	6	0	-5.928191	-1.160189	0.013437
102	6	0	-4.500837	-2.650432	1.268658
103	6	0	-6.945055	-2.111615	0.059478
104	1	0	-6.107772	-0.228464	-0.508746
105	6	0	-5.525473	-3.585491	1.331076
106	1	0	-3.539310	-2.839330	1.738117
107	6	0	-6.750174	-3.320471	0.718983
108	1	0	-7.891822	-1.898684	-0.427745
109	1	0	-5.369922	-4.524003	1.855184
110	1	0	-7.550016	-4.054519	0.760009
111	8	0	-2.377199	-1.018809	0.572620
112	6	0	-1.227141	1.963086	-0.804311
113	1	0	-1.890115	2.713769	-1.223253
114	6	0	1.301815	1.854731	-0.822527
115	1	0	1.441420	2.214590	-1.850083
116	1	0	2.196378	2.134437	-0.254900

γ'-TS5-A

Zero-point correction= 0.921501 (Hartree/Particle)
Thermal correction to Energy= 0.972026
Thermal correction to Enthalpy= 0.972970
Thermal correction to Gibbs Free Energy= 0.834786
E(sov) = -2567.75008158 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.806608	-0.269386	3.649472
2	6	0	0.018939	-1.078553	4.502013
3	6	0	-0.367418	-2.327630	4.092029
4	6	0	0.012201	-2.820917	2.817138
5	6	0	0.826446	-2.019243	1.961714
6	6	0	1.204188	-0.724456	2.415948

7	6	0	2.170859	-1.921581	-0.279038
8	6	0	3.604399	-1.972475	0.299364
9	7	0	4.569999	-1.219567	-0.543960
10	6	0	5.877721	-1.193983	0.145049
11	6	0	4.100212	-3.429380	0.500738
12	6	0	6.455071	-2.621925	0.302497
13	6	0	5.423640	-3.611418	-0.249926
14	6	0	4.722046	-1.847007	-1.871400
15	6	0	5.198788	-3.318308	-1.751555
16	6	0	4.296994	-4.356407	-2.375034
17	6	0	3.251606	-4.170533	-3.177788
18	7	0	-0.450994	-4.057622	2.474175
19	6	0	-0.118528	-4.519187	1.296473
20	6	0	0.708457	-3.823507	0.382887
21	6	0	1.201960	-2.581609	0.700816
22	1	0	-0.285287	-0.702203	5.473510
23	1	0	-0.985658	-2.972810	4.707462
24	1	0	1.814774	-0.083235	1.792246
25	1	0	6.540419	-0.552269	-0.444547
26	1	0	5.721900	-0.702681	1.110522
27	1	0	4.232380	-3.644839	1.565737
28	1	0	3.359861	-4.141289	0.122689
29	1	0	7.400922	-2.720896	-0.240527
30	1	0	6.660011	-2.844213	1.354398
31	1	0	5.782611	-4.639335	-0.129294
32	1	0	5.442949	-1.241703	-2.429942
33	1	0	3.764157	-1.750919	-2.387526
34	1	0	6.176765	-3.415522	-2.245030
35	1	0	4.578611	-5.382949	-2.132833
36	1	0	2.702508	-5.017985	-3.575831
37	1	0	2.908059	-3.189401	-3.493451
38	1	0	-0.505846	-5.501263	1.029747
39	1	0	0.956857	-4.283049	-0.571662
40	1	0	1.104896	0.722806	3.975048
41	1	0	2.144236	-2.536503	-1.190366
42	1	0	3.586987	-1.438216	1.256808
43	7	0	1.884714	-0.550524	-0.633243
44	6	0	0.673380	-0.064760	-1.041039
45	1	0	2.456995	0.127352	-0.143245
46	6	0	-0.398596	-0.816389	-1.408407
47	6	0	0.612975	1.444082	-1.020440
48	6	0	-1.690086	-0.208762	-1.664708
49	1	0	-0.343386	-1.900450	-1.389746
50	6	0	-0.568123	1.996431	-1.811883
51	1	0	1.548436	1.837536	-1.437283
52	1	0	0.580379	1.777958	0.027051

53	6	0	-1.823034	1.182361	-1.610978
54	6	0	-2.830199	-1.066345	-1.746003
55	1	0	-0.322410	1.959915	-2.883190
56	1	0	-0.730044	3.047294	-1.558148
57	1	0	-2.733401	1.630902	-1.999276
58	6	0	-4.114965	-0.618001	-1.814578
59	1	0	-2.646599	-2.134380	-1.637997
60	6	0	-5.316416	-1.430767	-1.678564
61	1	0	-4.304408	0.431159	-2.028034
62	6	0	-6.552459	-0.867261	-2.029317
63	6	0	-5.292365	-2.727438	-1.144435
64	6	0	-7.725227	-1.597538	-1.899160
65	1	0	-6.581951	0.161695	-2.378418
66	6	0	-6.466131	-3.457123	-1.015621
67	1	0	-4.354622	-3.153157	-0.799364
68	6	0	-7.683189	-2.897797	-1.400028
69	1	0	-8.674864	-1.148024	-2.171552
70	1	0	-6.435642	-4.457011	-0.594106
71	1	0	-8.601360	-3.466904	-1.289470
72	6	0	4.051967	5.432062	-1.712824
73	6	0	3.225543	6.174054	-0.859371
74	6	0	2.619709	5.587920	0.237843
75	6	0	2.830757	4.231758	0.516654
76	6	0	3.658379	3.475426	-0.341042
77	6	0	4.255200	4.090271	-1.452736
78	1	0	4.520410	5.902951	-2.569748
79	1	0	3.052345	7.227390	-1.058901
80	1	0	1.976392	6.154713	0.901699
81	1	0	4.877703	3.482668	-2.100824
82	6	0	3.832049	2.034459	-0.100993
83	8	0	3.387543	1.468483	0.913224
84	8	0	4.427939	1.358903	-1.052112
85	1	0	4.398907	0.342535	-0.820169
86	8	0	2.217242	3.711566	1.592724
87	1	0	2.508603	2.776145	1.672593
88	6	0	-3.799089	-0.496900	1.258328
89	6	0	-3.671002	0.774487	0.593924
90	6	0	-5.048360	1.149456	0.315621
91	8	0	-5.827684	0.174901	0.882292
92	7	0	-5.034277	-0.833253	1.456433
93	6	0	-2.681966	-1.360037	1.742118
94	1	0	-2.020555	-1.646541	0.913988
95	1	0	-2.069094	-0.822795	2.474897
96	1	0	-3.077557	-2.264482	2.210183
97	8	0	-5.550303	2.047447	-0.336527
98	6	0	-2.458256	1.449228	0.388246

99	6	0	-2.283091	2.924691	0.464522
100	6	0	-3.122951	3.843373	-0.177952
101	6	0	-1.194236	3.408532	1.200826
102	6	0	-2.862535	5.207180	-0.084306
103	1	0	-3.985827	3.484017	-0.728172
104	6	0	-0.938171	4.772023	1.294511
105	1	0	-0.542772	2.708264	1.719797
106	6	0	-1.771585	5.677944	0.644322
107	1	0	-3.522502	5.908980	-0.585649
108	1	0	-0.085756	5.109682	1.875935
109	1	0	-1.576917	6.744494	0.708105
110	1	0	-1.609313	0.918255	0.827681

γ'-TS5-B

Zero-point correction= 0.921253 (Hartree/Particle)
Thermal correction to Energy= 0.971629
Thermal correction to Enthalpy= 0.972573
Thermal correction to Gibbs Free Energy= 0.835468
E(sov) = -2567.74443799 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.347367	0.992625	3.809126
2	6	0	-2.873756	1.682904	4.949468
3	6	0	-1.840350	2.572893	4.829507
4	6	0	-1.241137	2.820294	3.566928
5	6	0	-1.733257	2.148648	2.411791
6	6	0	-2.794414	1.217207	2.575574
7	6	0	-1.533964	1.850342	-0.165325
8	6	0	-2.959635	2.315784	-0.538870
9	7	0	-3.472704	1.616259	-1.744835
10	6	0	-4.851604	2.076028	-2.010411
11	6	0	-2.986664	3.853037	-0.769314
12	6	0	-4.878929	3.581527	-2.370583
13	6	0	-3.458351	4.131273	-2.201936
14	6	0	-2.628543	1.890707	-2.925188
15	6	0	-2.527652	3.413157	-3.206855
16	6	0	-1.137714	4.002902	-3.187388
17	6	0	0.033255	3.370104	-3.153129
18	7	0	-0.205943	3.708058	3.537571
19	6	0	0.362730	3.932156	2.382400
20	6	0	-0.051886	3.330598	1.171229

21	6	0	-1.094806	2.439351	1.168345
22	1	0	-3.322151	1.491949	5.919682
23	1	0	-1.435153	3.108729	5.681590
24	1	0	-3.148139	0.630122	1.735634
25	1	0	-5.250766	1.456857	-2.820506
26	1	0	-5.440808	1.859384	-1.113973
27	1	0	-3.657354	4.337350	-0.052388
28	1	0	-1.990883	4.279083	-0.608271
29	1	0	-5.220175	3.729326	-3.400940
30	1	0	-5.570784	4.123796	-1.718448
31	1	0	-3.443048	5.209063	-2.397991
32	1	0	-3.082990	1.362298	-3.769244
33	1	0	-1.653767	1.427806	-2.752177
34	1	0	-2.933619	3.612270	-4.209687
35	1	0	-1.127351	5.093644	-3.233857
36	1	0	0.962961	3.930376	-3.169615
37	1	0	0.131814	2.287910	-3.115849
38	1	0	1.196392	4.632757	2.375473
39	1	0	0.462608	3.580458	0.245475
40	1	0	-4.141159	0.259845	3.914155
41	1	0	-0.859554	2.271728	-0.918118
42	1	0	-3.644798	2.041232	0.268174
43	7	0	-1.428644	0.409879	-0.281722
44	6	0	-0.329981	-0.255504	-0.690391
45	1	0	-2.225001	-0.143306	0.029239
46	6	0	0.904576	0.334819	-0.861689
47	6	0	-0.592619	-1.691368	-1.076122
48	6	0	2.063647	-0.432474	-1.146357
49	1	0	1.042864	1.374251	-0.583986
50	6	0	0.659281	-2.475718	-1.517304
51	1	0	-1.316732	-1.664161	-1.900407
52	1	0	-1.118447	-2.173178	-0.243474
53	6	0	1.981340	-1.826117	-1.178974
54	6	0	3.346539	0.264497	-1.175624
55	1	0	0.631948	-2.591980	-2.608293
56	1	0	0.627218	-3.492564	-1.112458
57	1	0	2.860188	-2.380580	-1.496987
58	6	0	4.484164	-0.226316	-1.698933
59	1	0	3.345830	1.250567	-0.713525
60	6	0	5.807220	0.399076	-1.635017
61	1	0	4.456354	-1.186015	-2.213056
62	6	0	6.862944	-0.178565	-2.352226
63	6	0	6.079480	1.522905	-0.840412
64	6	0	8.147347	0.349678	-2.290893
65	1	0	6.666873	-1.060000	-2.958095
66	6	0	7.361027	2.053242	-0.779932

67	1	0	5.288769	1.966074	-0.242625
68	6	0	8.400809	1.469977	-1.504083
69	1	0	8.951178	-0.115964	-2.853038
70	1	0	7.555380	2.920148	-0.155492
71	1	0	9.402974	1.883717	-1.448015
72	6	0	-4.231996	-5.059898	-2.446020
73	6	0	-4.001201	-5.889467	-1.341134
74	6	0	-3.733258	-5.356309	-0.093626
75	6	0	-3.699238	-3.966002	0.092071
76	6	0	-3.932629	-3.124602	-1.016943
77	6	0	-4.188427	-3.688998	-2.276084
78	1	0	-4.437594	-5.487443	-3.421167
79	1	0	-4.028422	-6.968543	-1.461981
80	1	0	-3.545750	-5.985945	0.769706
81	1	0	-4.353732	-3.016585	-3.111432
82	6	0	-3.859652	-1.663515	-0.850902
83	8	0	-3.759737	-1.133915	0.264865
84	8	0	-3.848979	-0.959057	-1.956972
85	1	0	-3.670059	0.050706	-1.740800
86	8	0	-3.420321	-3.529085	1.326539
87	1	0	-3.391351	-2.547732	1.338684
88	6	0	-0.031946	-2.468402	1.881906
89	6	0	1.176848	-1.747318	1.594420
90	6	0	0.901425	-0.404976	2.084100
91	8	0	-0.393045	-0.438495	2.546437
92	7	0	-0.946962	-1.718235	2.419680
93	6	0	-0.307836	-3.925392	1.670021
94	1	0	-0.495004	-4.158778	0.615263
95	1	0	0.542603	-4.527240	2.004552
96	1	0	-1.198406	-4.207642	2.232759
97	8	0	1.538210	0.631859	2.139848
98	6	0	2.269073	-2.275339	0.882747
99	6	0	3.703598	-1.941083	1.033013
100	6	0	4.172745	-0.801185	1.698221
101	6	0	4.638778	-2.807213	0.449256
102	6	0	5.539240	-0.540489	1.757384
103	1	0	3.462377	-0.114448	2.145428
104	6	0	6.001136	-2.536095	0.497548
105	1	0	4.287246	-3.704100	-0.058831
106	6	0	6.457258	-1.394015	1.151307
107	1	0	5.888408	0.350549	2.271510
108	1	0	6.706224	-3.216377	0.028760
109	1	0	7.518498	-1.164727	1.176871
110	1	0	2.131108	-3.333085	0.642989

γ'-TS5-C

Zero-point correction= 0.922182 (Hartree/Particle)
Thermal correction to Energy= 0.972934
Thermal correction to Enthalpy= 0.973878
Thermal correction to Gibbs Free Energy= 0.834216
E(sov) = -2567.73938089 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.195694	-1.060106	3.867917
2	6	0	1.568171	-1.624479	5.003189
3	6	0	0.544709	-2.522988	4.844786
4	6	0	0.108341	-2.900353	3.548548
5	6	0	0.752008	-2.351179	2.401175
6	6	0	1.801316	-1.411937	2.600721
7	6	0	0.903344	-2.326822	-0.189588
8	6	0	2.317126	-2.936851	-0.331534
9	7	0	3.076372	-2.309629	-1.438310
10	6	0	4.431073	-2.898737	-1.471057
11	6	0	2.234838	-4.475860	-0.533530
12	6	0	4.380126	-4.410608	-1.805067
13	6	0	2.907265	-4.831404	-1.865337
14	6	0	2.412241	-2.543219	-2.735147
15	6	0	2.220936	-4.058408	-3.015932
16	6	0	0.798164	-4.524368	-3.213265
17	6	0	-0.308106	-3.793890	-3.339046
18	7	0	-0.942593	-3.768429	3.478376
19	6	0	-1.371442	-4.100815	2.288360
20	6	0	-0.795834	-3.630860	1.083025
21	6	0	0.266337	-2.762734	1.121829
22	1	0	1.890558	-1.331344	5.997333
23	1	0	0.028157	-2.966616	5.689719
24	1	0	2.280431	-0.925899	1.758771
25	1	0	5.013508	-2.339054	-2.209686
26	1	0	4.888621	-2.716124	-0.493577
27	1	0	2.731057	-4.999830	0.289502
28	1	0	1.190737	-4.807281	-0.537781
29	1	0	4.867724	-4.613802	-2.764621
30	1	0	4.907054	-4.994028	-1.043386
31	1	0	2.826282	-5.908426	-2.048904
32	1	0	3.038368	-2.077001	-3.502369
33	1	0	1.465383	-1.997586	-2.728026
34	1	0	2.762028	-4.318055	-3.937474
35	1	0	0.701251	-5.610049	-3.277863

36	1	0	-1.269208	-4.272003	-3.500586
37	1	0	-0.319013	-2.707387	-3.303664
38	1	0	-2.217573	-4.784909	2.248169
39	1	0	-1.197686	-3.965674	0.128843
40	1	0	2.984000	-0.325263	3.995567
41	1	0	0.280868	-2.744098	-0.990557
42	1	0	2.883881	-2.707851	0.576904
43	7	0	0.959729	-0.897990	-0.400678
44	6	0	-0.035498	-0.136950	-0.870649
45	1	0	1.834904	-0.409179	-0.200956
46	6	0	-1.350076	-0.556894	-1.006959
47	6	0	0.382351	1.262908	-1.213443
48	6	0	-2.365289	0.373197	-1.333139
49	1	0	-1.636829	-1.555978	-0.694275
50	6	0	-0.665790	2.041098	-2.003827
51	1	0	1.320223	1.212304	-1.779298
52	1	0	0.630451	1.769282	-0.269304
53	6	0	-2.064236	1.732862	-1.540048
54	6	0	-3.744573	-0.101616	-1.261460
55	1	0	-0.595600	1.781158	-3.069640
56	1	0	-0.461714	3.114018	-1.923840
57	1	0	-2.839075	2.338554	-2.003635
58	6	0	-4.831770	0.561035	-1.695972
59	1	0	-3.877897	-1.075295	-0.792244
60	6	0	-6.215768	0.118304	-1.494947
61	1	0	-4.710836	1.497814	-2.238736
62	6	0	-7.228186	0.604850	-2.332217
63	6	0	-6.566543	-0.760977	-0.459461
64	6	0	-8.547599	0.201714	-2.163576
65	1	0	-6.969740	1.299124	-3.127943
66	6	0	-7.885569	-1.161016	-0.289030
67	1	0	-5.803217	-1.105794	0.233077
68	6	0	-8.879959	-0.685439	-1.142663
69	1	0	-9.317600	0.583667	-2.826648
70	1	0	-8.142950	-1.834937	0.522351
71	1	0	-9.910919	-0.995633	-1.003708
72	6	0	6.674143	3.429977	-1.534660
73	6	0	6.512195	4.432145	-0.567450
74	6	0	5.496375	4.358850	0.363644
75	6	0	4.599238	3.276343	0.369221
76	6	0	4.773680	2.250108	-0.586341
77	6	0	5.808848	2.355030	-1.534021
78	1	0	7.468504	3.496684	-2.269879
79	1	0	7.186067	5.283853	-0.552656
80	1	0	5.343325	5.133288	1.107013
81	1	0	5.917620	1.558599	-2.261949

82	6	0	3.927388	1.050287	-0.557801
83	8	0	3.095542	0.826215	0.324104
84	8	0	4.124991	0.199250	-1.556897
85	1	0	3.591100	-0.647357	-1.412196
86	8	0	3.656390	3.316560	1.310182
87	1	0	2.909829	2.709532	1.139290
88	6	0	-1.766690	4.993366	-0.198676
89	6	0	-1.417303	3.715446	0.353381
90	6	0	-0.035051	3.886693	0.722111
91	8	0	0.293287	5.177026	0.422156
92	7	0	-0.793491	5.850998	-0.144636
93	6	0	-3.087805	5.403622	-0.765751
94	1	0	-3.353409	4.791453	-1.635279
95	1	0	-3.883679	5.291108	-0.022392
96	1	0	-3.041426	6.448821	-1.077292
97	8	0	0.830071	3.129497	1.168317
98	6	0	-2.287152	2.593019	0.342283
99	6	0	-2.306425	1.503494	1.352062
100	6	0	-1.183638	1.062672	2.063037
101	6	0	-3.545861	0.902114	1.630116
102	6	0	-1.310158	0.063198	3.025689
103	1	0	-0.219066	1.530054	1.895585
104	6	0	-3.659270	-0.122484	2.561926
105	1	0	-4.435822	1.253041	1.113633
106	6	0	-2.534869	-0.551300	3.265395
107	1	0	-0.438487	-0.222533	3.604641
108	1	0	-4.632335	-0.564321	2.759724
109	1	0	-2.614029	-1.343023	4.005503
110	1	0	-3.308855	2.880728	0.087651

γ'-TS5-D

Zero-point correction= 0.921892 (Hartree/Particle)
Thermal correction to Energy= 0.972450
Thermal correction to Enthalpy= 0.973395
Thermal correction to Gibbs Free Energy= 0.834759
E(sov) = -2567.74661918 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.559999	0.041256	3.761777
2	6	0	3.082832	-0.313849	5.044738

3	6	0	2.121293	-1.282442	5.172000
4	6	0	1.598544	-1.939329	4.028019
5	6	0	2.066745	-1.576494	2.731196
6	6	0	3.063301	-0.566049	2.635044
7	6	0	1.838255	-1.937027	0.164852
8	6	0	3.285062	-2.325887	-0.201770
9	7	0	3.642572	-1.837747	-1.556497
10	6	0	5.044251	-2.208554	-1.839378
11	6	0	3.474943	-3.866206	-0.124817
12	6	0	5.207109	-3.746918	-1.914595
13	6	0	3.870625	-4.383228	-1.513324
14	6	0	2.763654	-2.422319	-2.590860
15	6	0	2.798300	-3.973640	-2.549276
16	6	0	1.479899	-4.661740	-2.282897
17	6	0	0.253603	-4.145177	-2.337296
18	7	0	0.655744	-2.902768	4.245205
19	6	0	0.167519	-3.515308	3.198448
20	6	0	0.549014	-3.224757	1.865171
21	6	0	1.489301	-2.257491	1.612798
22	1	0	3.479514	0.182617	5.924693
23	1	0	1.729689	-1.585901	6.137237
24	1	0	3.436401	-0.244344	1.670854
25	1	0	5.327364	-1.721967	-2.778157
26	1	0	5.659406	-1.770326	-1.047125
27	1	0	4.248857	-4.123783	0.605382
28	1	0	2.550347	-4.348646	0.210850
29	1	0	5.482503	-4.060035	-2.927341
30	1	0	6.001946	-4.085938	-1.242925
31	1	0	3.961388	-5.474708	-1.493891
32	1	0	3.119023	-2.045258	-3.554612
33	1	0	1.759579	-2.015509	-2.446818
34	1	0	3.145275	-4.342838	-3.525269
35	1	0	1.578457	-5.725172	-2.056054
36	1	0	-0.616735	-4.769391	-2.158257
37	1	0	0.052001	-3.103008	-2.573170
38	1	0	-0.581288	-4.282827	3.386748
39	1	0	0.086304	-3.768363	1.044128
40	1	0	4.318597	0.811698	3.661952
41	1	0	1.183576	-2.561853	-0.450604
42	1	0	3.978515	-1.823850	0.479130
43	7	0	1.568748	-0.562781	-0.192870
44	6	0	0.357966	-0.080798	-0.550786
45	1	0	2.304251	0.116112	-0.011953
46	6	0	-0.786498	-0.840784	-0.620941
47	6	0	0.382354	1.387074	-0.904815
48	6	0	-2.049426	-0.265287	-0.968376

49	1	0	-0.770041	-1.884884	-0.324888
50	6	0	-0.932042	1.910508	-1.496649
51	1	0	1.193503	1.536781	-1.628687
52	1	0	0.667877	1.943982	-0.003149
53	6	0	-2.164322	1.118820	-1.133772
54	6	0	-3.216824	-1.132630	-1.013892
55	1	0	-0.874108	1.864837	-2.593084
56	1	0	-1.079709	2.963476	-1.246955
57	1	0	-3.052929	1.507043	-1.614589
58	6	0	-4.474573	-0.712867	-1.269592
59	1	0	-3.039703	-2.180510	-0.774013
60	6	0	-5.686952	-1.534711	-1.243956
61	1	0	-4.649132	0.338724	-1.487482
62	6	0	-6.928410	-0.885071	-1.178932
63	6	0	-5.659702	-2.937051	-1.269792
64	6	0	-8.108638	-1.619006	-1.120660
65	1	0	-6.959649	0.202636	-1.144345
66	6	0	-6.839375	-3.666513	-1.221920
67	1	0	-4.709987	-3.458209	-1.350292
68	6	0	-8.068128	-3.010292	-1.143775
69	1	0	-9.060579	-1.100814	-1.059790
70	1	0	-6.803991	-4.751364	-1.251620
71	1	0	-8.989086	-3.584072	-1.107526
72	6	0	3.813022	4.698000	-3.285159
73	6	0	3.770313	5.668762	-2.275546
74	6	0	3.759112	5.310164	-0.940002
75	6	0	3.794094	3.958230	-0.573320
76	6	0	3.837963	2.973442	-1.583994
77	6	0	3.841399	3.362635	-2.933272
78	1	0	3.817912	4.991566	-4.328896
79	1	0	3.742092	6.721304	-2.541554
80	1	0	3.719893	6.050637	-0.148556
81	1	0	3.866360	2.586050	-3.690436
82	6	0	3.830286	1.549597	-1.218560
83	8	0	3.888311	1.167119	-0.035828
84	8	0	3.708235	0.699733	-2.206445
85	1	0	3.644385	-0.275268	-1.836689
86	8	0	3.775295	3.671624	0.736660
87	1	0	3.809321	2.694787	0.828058
88	6	0	-5.408009	1.637013	0.855942
89	6	0	-4.091609	2.117625	0.570808
90	6	0	-4.314858	3.278020	-0.251226
91	8	0	-5.673405	3.422024	-0.357916
92	7	0	-6.333385	2.401359	0.349840
93	6	0	-5.791496	0.472056	1.711941
94	1	0	-5.294460	-0.445454	1.380482

95	1	0	-5.503816	0.656526	2.752062
96	1	0	-6.872034	0.320384	1.665034
97	8	0	-3.542227	3.996772	-0.868818
98	6	0	-2.859882	1.464691	0.807166
99	6	0	-1.636956	2.049642	1.398727
100	6	0	-1.280923	3.399097	1.250398
101	6	0	-0.806233	1.204211	2.149224
102	6	0	-0.088385	3.863567	1.791583
103	1	0	-1.931413	4.057591	0.681330
104	6	0	0.373335	1.680910	2.714022
105	1	0	-1.093075	0.164949	2.294351
106	6	0	0.747748	3.007334	2.514186
107	1	0	0.194638	4.902638	1.652168
108	1	0	0.991933	1.020190	3.313503
109	1	0	1.680216	3.381393	2.926558
110	1	0	-3.006415	0.446386	1.173907

γ'-TS5-E

Zero-point correction= 0.921593 (Hartree/Particle)
Thermal correction to Energy= 0.972246
Thermal correction to Enthalpy= 0.973190
Thermal correction to Gibbs Free Energy= 0.834887
E(sov) = -2567.74842149 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.741787	0.216931	3.400777
2	6	0	-0.132066	-0.463912	4.279585
3	6	0	-0.460994	-1.770753	4.035724
4	6	0	0.044797	-2.444874	2.893871
5	6	0	0.916247	-1.760981	1.994443
6	6	0	1.262069	-0.413056	2.296786
7	6	0	2.262629	-1.887358	-0.237835
8	6	0	3.723191	-1.860306	0.270548
9	7	0	4.627917	-1.154138	-0.675609
10	6	0	5.961903	-1.038962	-0.046973
11	6	0	4.263403	-3.287216	0.557432
12	6	0	6.583576	-2.433411	0.207659
13	6	0	5.564049	-3.491455	-0.226263
14	6	0	4.742677	-1.884964	-1.952137

15	6	0	5.275977	-3.325360	-1.736648
16	6	0	4.389943	-4.439451	-2.239183
17	6	0	3.297731	-4.354314	-2.995348
18	7	0	-0.368139	-3.732471	2.708623
19	6	0	0.053372	-4.353592	1.637320
20	6	0	0.900260	-3.764647	0.668374
21	6	0	1.343996	-2.475126	0.830623
22	1	0	-0.540512	0.052114	5.142429
23	1	0	-1.128059	-2.329817	4.683715
24	1	0	1.942998	0.133799	1.657972
25	1	0	6.583942	-0.435896	-0.716509
26	1	0	5.829637	-0.468130	0.877450
27	1	0	4.436589	-3.422415	1.629592
28	1	0	3.530521	-4.042328	0.256305
29	1	0	7.514271	-2.553169	-0.356871
30	1	0	6.827627	-2.562845	1.266822
31	1	0	5.958266	-4.496374	-0.039804
32	1	0	5.415544	-1.306188	-2.592544
33	1	0	3.760637	-1.863647	-2.430073
34	1	0	6.238787	-3.428973	-2.257627
35	1	0	4.726276	-5.433642	-1.938726
36	1	0	2.765202	-5.249398	-3.300591
37	1	0	2.897820	-3.413507	-3.363265
38	1	0	-0.290743	-5.377256	1.499674
39	1	0	1.180686	-4.333927	-0.215172
40	1	0	1.006911	1.251634	3.599806
41	1	0	2.207695	-2.569818	-1.098263
42	1	0	3.736647	-1.253245	1.183377
43	7	0	1.919827	-0.547208	-0.669095
44	6	0	0.677460	-0.082100	-0.969523
45	1	0	2.553330	0.158595	-0.315840
46	6	0	-0.420446	-0.857962	-1.213505
47	6	0	0.591985	1.425700	-0.948969
48	6	0	-1.716387	-0.270375	-1.422049
49	1	0	-0.342893	-1.940405	-1.180118
50	6	0	-0.655377	1.962153	-1.647416
51	1	0	1.490540	1.840631	-1.422943
52	1	0	0.631930	1.738391	0.107756
53	6	0	-1.879363	1.119772	-1.387749
54	6	0	-2.845484	-1.167598	-1.560932
55	1	0	-0.476064	1.972055	-2.731366
56	1	0	-0.839352	3.001084	-1.353071
57	1	0	-2.803437	1.512724	-1.802563
58	6	0	-4.130849	-0.760409	-1.658054
59	1	0	-2.613007	-2.230499	-1.529676
60	6	0	-5.314408	-1.616955	-1.706908

61	1	0	-4.352937	0.306403	-1.669117
62	6	0	-6.566203	-0.996840	-1.832638
63	6	0	-5.265431	-3.013582	-1.587619
64	6	0	-7.734606	-1.749401	-1.854504
65	1	0	-6.607138	0.088339	-1.899237
66	6	0	-6.432691	-3.764531	-1.609195
67	1	0	-4.310529	-3.514582	-1.461993
68	6	0	-7.670932	-3.136479	-1.744752
69	1	0	-8.695301	-1.253528	-1.953452
70	1	0	-6.380079	-4.844962	-1.513731
71	1	0	-8.581637	-3.727459	-1.757952
72	6	0	3.760294	5.496376	-1.777908
73	6	0	3.013733	6.175295	-0.805589
74	6	0	2.583799	5.534720	0.342883
75	6	0	2.897315	4.186262	0.552896
76	6	0	3.645392	3.493137	-0.423643
77	6	0	4.063281	4.162491	-1.585254
78	1	0	4.087354	6.010106	-2.674940
79	1	0	2.762038	7.221114	-0.953792
80	1	0	2.002592	6.047520	1.101466
81	1	0	4.624883	3.603624	-2.326423
82	6	0	3.906343	2.058977	-0.247570
83	8	0	3.608919	1.447708	0.793517
84	8	0	4.407009	1.422023	-1.280667
85	1	0	4.433562	0.411493	-1.047556
86	8	0	2.444080	3.609339	1.678633
87	1	0	2.794662	2.691728	1.699412
88	6	0	-2.214403	4.178560	0.603526
89	6	0	-2.890300	2.946614	0.338300
90	6	0	-4.016300	3.341793	-0.466214
91	8	0	-3.986666	4.708863	-0.531417
92	7	0	-2.863335	5.208869	0.146040
93	6	0	-0.935494	4.369540	1.354600
94	1	0	-0.992572	3.916839	2.349583
95	1	0	-0.090721	3.905459	0.831659
96	1	0	-0.729558	5.436913	1.460698
97	8	0	-4.838979	2.691586	-1.102121
98	6	0	-2.416094	1.633731	0.553230
99	6	0	-3.240281	0.505710	1.045355
100	6	0	-4.639935	0.517979	1.053043
101	6	0	-2.575914	-0.626874	1.534857
102	6	0	-5.348281	-0.589495	1.513256
103	1	0	-5.171813	1.380896	0.668749
104	6	0	-3.282427	-1.735928	1.983075
105	1	0	-1.487476	-0.637582	1.537246
106	6	0	-4.677399	-1.720728	1.967086

107	1	0	-6.434014	-0.573358	1.492752
108	1	0	-2.745851	-2.607945	2.348927
109	1	0	-5.236937	-2.586674	2.308334
110	1	0	-1.409983	1.594106	0.980977

γ'-TS1-F

Zero-point correction= 0.921322 (Hartree/Particle)
Thermal correction to Energy= 0.971776
Thermal correction to Enthalpy= 0.972720
Thermal correction to Gibbs Free Energy= 0.835152
E(sov) = -2567.74433491 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.332289	-0.489949	1.927810
2	6	0	7.039855	-1.458838	2.675724
3	6	0	6.538163	-2.727808	2.797434
4	6	0	5.309741	-3.082612	2.183499
5	6	0	4.589051	-2.109562	1.430122
6	6	0	5.141417	-0.802927	1.321240
7	6	0	2.465095	-1.602161	0.017081
8	6	0	3.122286	-1.210263	-1.323926
9	7	0	2.240080	-0.324054	-2.121009
10	6	0	3.013365	0.181404	-3.277352
11	6	0	3.505960	-2.463188	-2.154182
12	6	0	3.496907	-0.986875	-4.171454
13	6	0	2.962844	-2.295385	-3.576590
14	6	0	1.036995	-1.025253	-2.614544
15	6	0	1.416136	-2.227445	-3.517994
16	6	0	0.841491	-3.563289	-3.119385
17	6	0	0.069259	-3.863374	-2.077334
18	7	0	4.882437	-4.367292	2.356927
19	6	0	3.748997	-4.706242	1.800534
20	6	0	2.949408	-3.820997	1.037168
21	6	0	3.352034	-2.523883	0.842298
22	1	0	7.978794	-1.192513	3.150757
23	1	0	7.049574	-3.501704	3.360083
24	1	0	4.636407	-0.031094	0.750593
25	1	0	2.360091	0.868044	-3.824977
26	1	0	3.844282	0.768677	-2.874373
27	1	0	4.592550	-2.594548	-2.166568
28	1	0	3.080566	-3.367305	-1.705745

29	1	0	3.137162	-0.863853	-5.198189
30	1	0	4.590502	-1.018386	-4.211901
31	1	0	3.266529	-3.145950	-4.196179
32	1	0	0.447546	-0.288185	-3.169620
33	1	0	0.431200	-1.310473	-1.751666
34	1	0	1.066728	-2.026908	-4.540885
35	1	0	1.124987	-4.375074	-3.791577
36	1	0	-0.269983	-4.881568	-1.915249
37	1	0	-0.282844	-3.124226	-1.363278
38	1	0	3.420033	-5.733479	1.948840
39	1	0	2.016864	-4.178935	0.607182
40	1	0	6.733562	0.514278	1.832389
41	1	0	1.574815	-2.185558	-0.227195
42	1	0	4.008836	-0.605037	-1.115796
43	7	0	2.020645	-0.442638	0.766334
44	6	0	0.733884	-0.164534	1.089017
45	1	0	2.684323	0.316908	0.860709
46	6	0	-0.345196	-0.992565	0.924898
47	6	0	0.497751	1.170256	1.757615
48	6	0	-1.672162	-0.533493	1.266914
49	1	0	-0.224562	-2.034110	0.640173
50	6	0	-0.768429	1.796424	1.187039
51	1	0	1.351789	1.841165	1.619466
52	1	0	0.397754	0.992784	2.836498
53	6	0	-1.949032	0.844843	1.276572
54	6	0	-2.714356	-1.501766	1.406225
55	1	0	-0.561163	2.035446	0.136241
56	1	0	-0.997034	2.743625	1.683785
57	1	0	-2.805145	1.185651	1.851325
58	6	0	-4.024969	-1.188355	1.607763
59	1	0	-2.436982	-2.544304	1.255234
60	6	0	-5.145222	-2.120110	1.572318
61	1	0	-4.293851	-0.169365	1.876844
62	6	0	-6.377675	-1.714644	2.106527
63	6	0	-5.054027	-3.379859	0.961890
64	6	0	-7.474964	-2.563337	2.074483
65	1	0	-6.469258	-0.716995	2.526764
66	6	0	-6.153201	-4.227144	0.930364
67	1	0	-4.127643	-3.682189	0.482326
68	6	0	-7.362945	-3.824679	1.492727
69	1	0	-8.422825	-2.236000	2.489601
70	1	0	-6.072674	-5.196852	0.449166
71	1	0	-8.223591	-4.485770	1.459615
72	6	0	0.886017	5.752901	0.399873
73	6	0	1.923752	6.404163	1.079848
74	6	0	3.163990	5.808251	1.228190

75	6	0	3.400055	4.530886	0.703042
76	6	0	2.364145	3.870612	0.008368
77	6	0	1.116406	4.499467	-0.133909
78	1	0	-0.090220	6.215023	0.296461
79	1	0	1.757139	7.390543	1.502953
80	1	0	3.975335	6.299184	1.754412
81	1	0	0.327640	3.975959	-0.663561
82	6	0	2.579804	2.510312	-0.516470
83	8	0	3.635930	1.880397	-0.319127
84	8	0	1.575992	1.981992	-1.166564
85	1	0	1.834230	0.997407	-1.456757
86	8	0	4.615500	3.995888	0.891235
87	1	0	4.605680	3.099350	0.489920
88	6	0	-3.982832	-0.929365	-1.476399
89	6	0	-4.037428	0.291855	-0.716336
90	6	0	-5.442285	0.393602	-0.348500
91	8	0	-6.068884	-0.668950	-0.950999
92	7	0	-5.145938	-1.476353	-1.631240
93	6	0	-2.763827	-1.548569	-2.076423
94	1	0	-2.361929	-0.924929	-2.883552
95	1	0	-1.982496	-1.648220	-1.314310
96	1	0	-3.002753	-2.534233	-2.481678
97	8	0	-6.058823	1.144450	0.383055
98	6	0	-2.955204	1.166011	-0.527774
99	6	0	-3.094707	2.646621	-0.426803
100	6	0	-3.978113	3.284483	0.452543
101	6	0	-2.273378	3.435692	-1.242833
102	6	0	-4.030461	4.673997	0.505950
103	1	0	-4.640017	2.688349	1.070378
104	6	0	-2.332645	4.825218	-1.192866
105	1	0	-1.579754	2.950805	-1.927818
106	6	0	-3.210510	5.450033	-0.311318
107	1	0	-4.722974	5.152918	1.191434
108	1	0	-1.690812	5.416685	-1.840576
109	1	0	-3.261040	6.533899	-0.265559
110	1	0	-2.074819	0.881846	-1.110129

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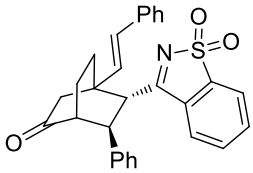
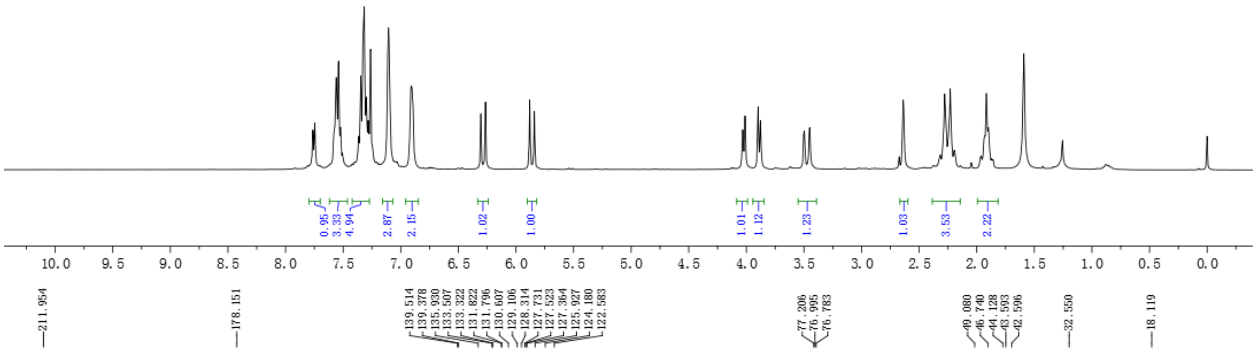
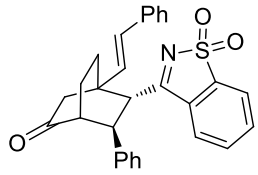
16. NMR spectra and HPLC chromatograms



3

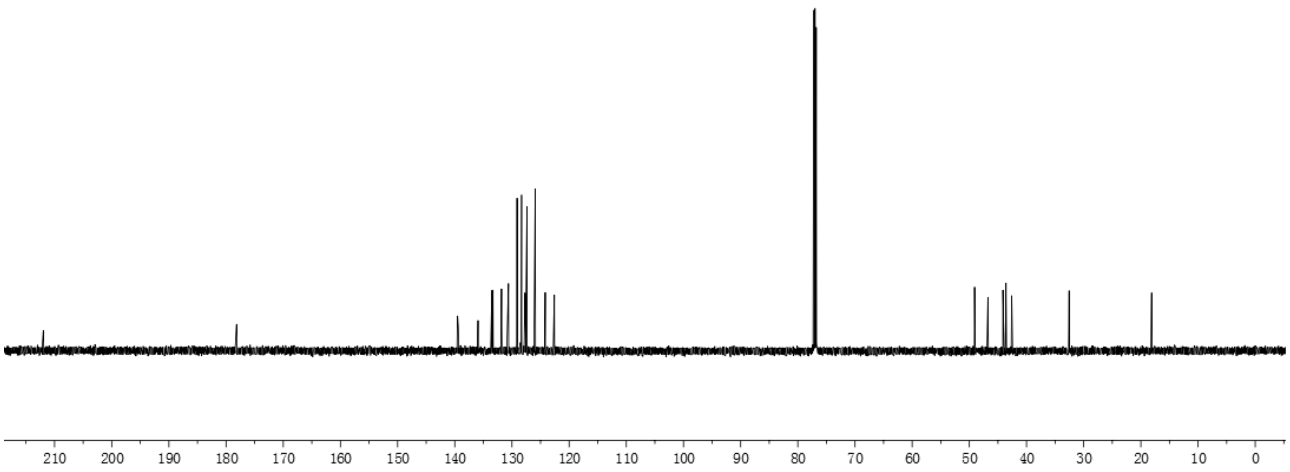
^{1}H NMR (400 MHz, $CDCl_3$)

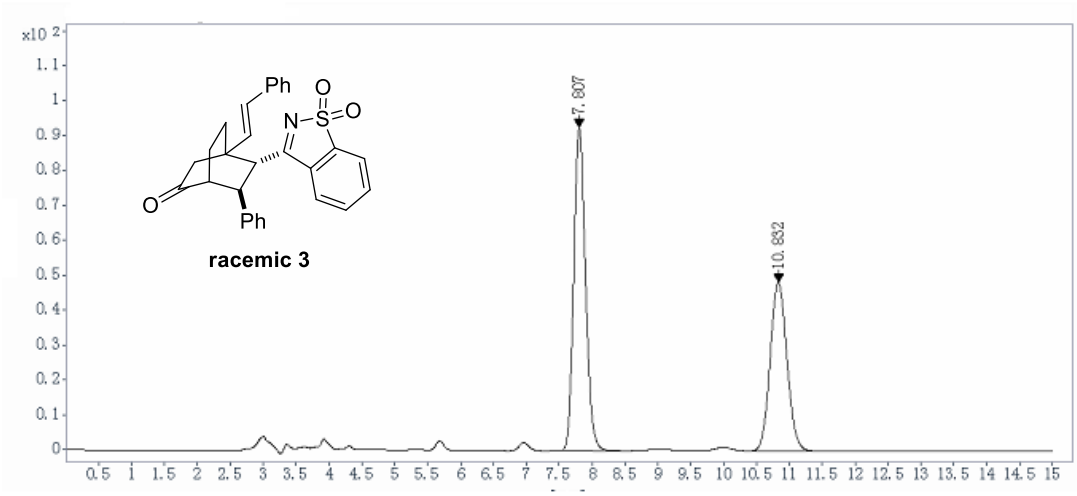




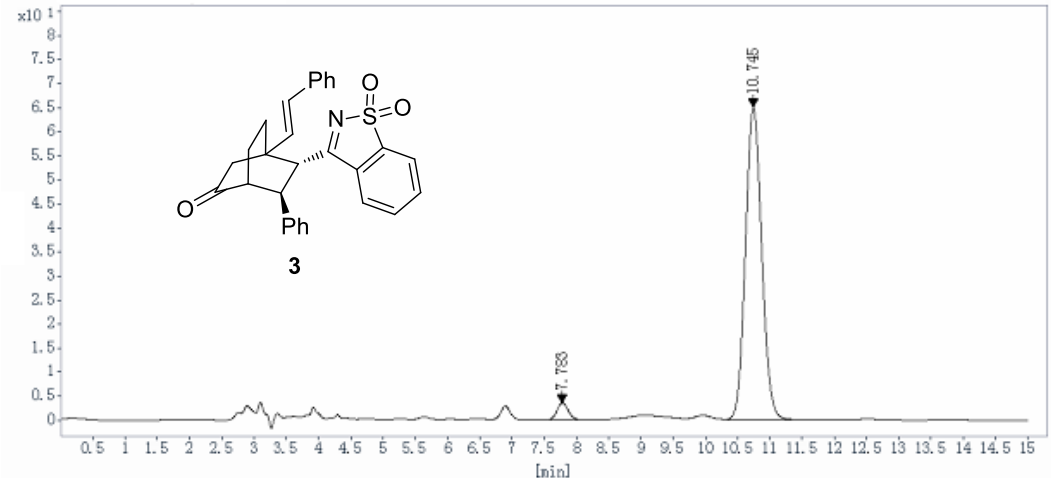
3

^{13}C NMR (150 MHz, $CDCl_3$)

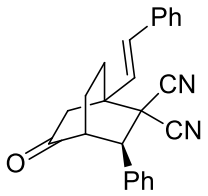




Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
7.807	BB	0.19	92.4965	1147.7917	57.1403
10.832	BB	0.28	48.3600	860.9323	42.8597

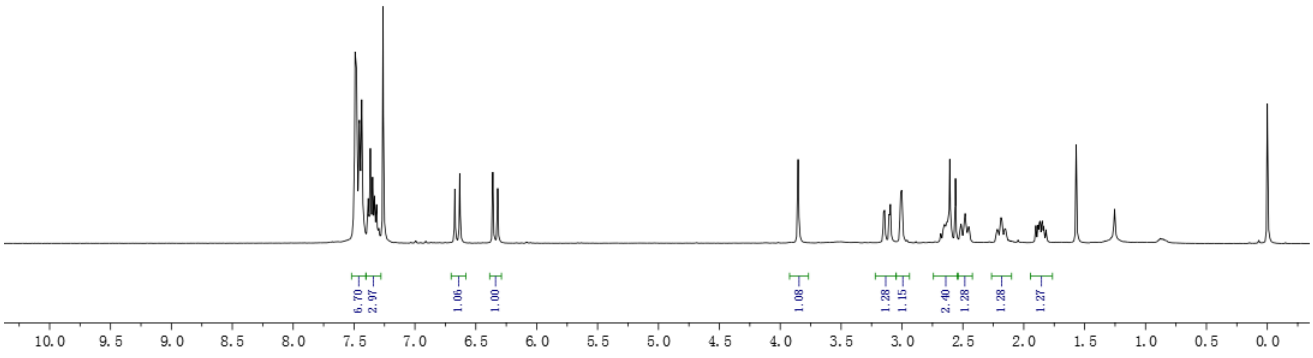


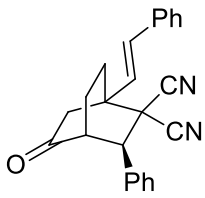
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
7.783	BB	0.19	3.5420	42.6456	3.6237
10.745	BBA	0.27	64.8625	1134.2184	96.3763



5

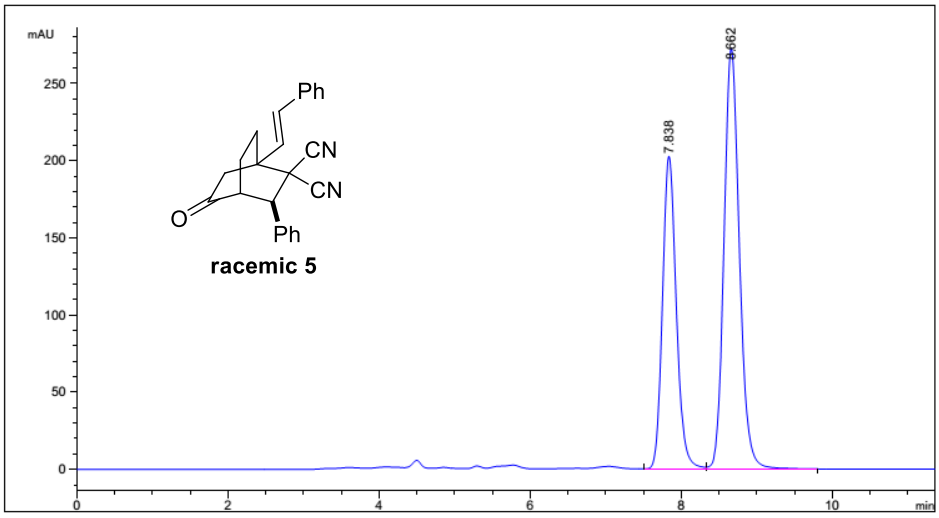
^{1}H NMR (400 MHz, $CDCl_3$)



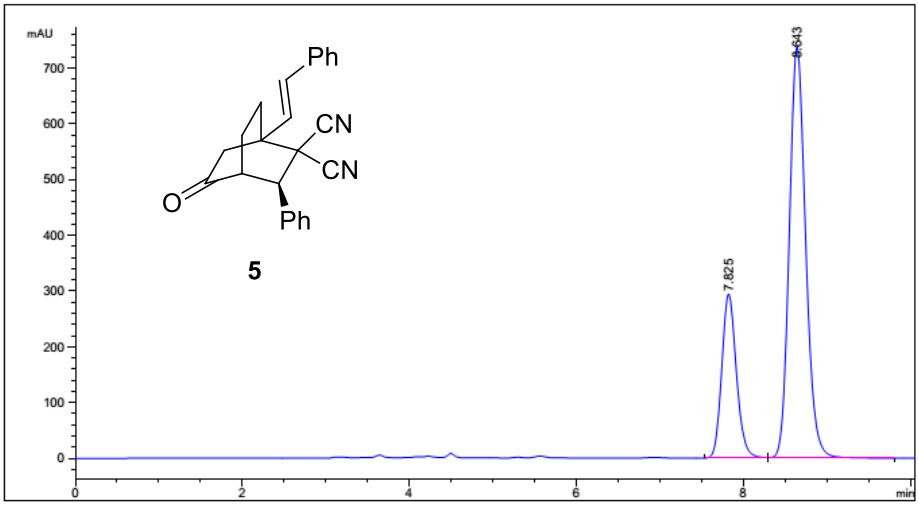


5

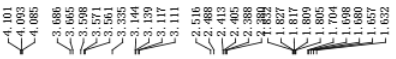
^{13}C NMR (150 MHz, $CDCl_3$)

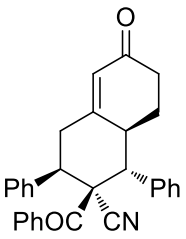


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.838	VV	0.1950	2574.03931	202.35399	40.0492
2	8.662	VB	0.2177	3853.15527	272.01898	59.9508



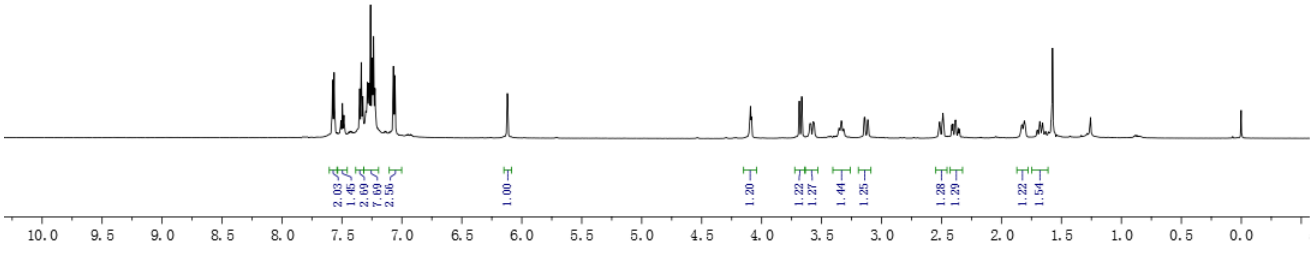
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.825	BV	0.1893	3591.99829	293.74533	26.2951
2	8.643	VB	0.2120	1.00683e4	736.29193	73.7049

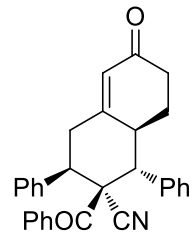




7a

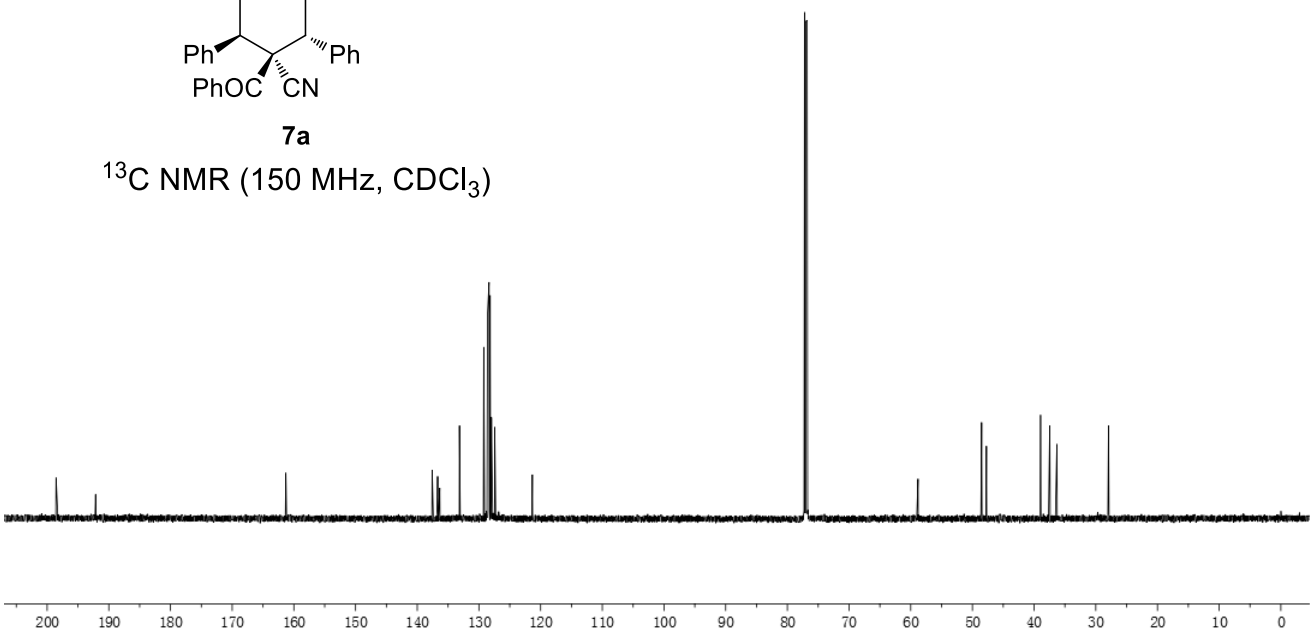
^{1}H NMR (600 MHz, $CDCl_3$)

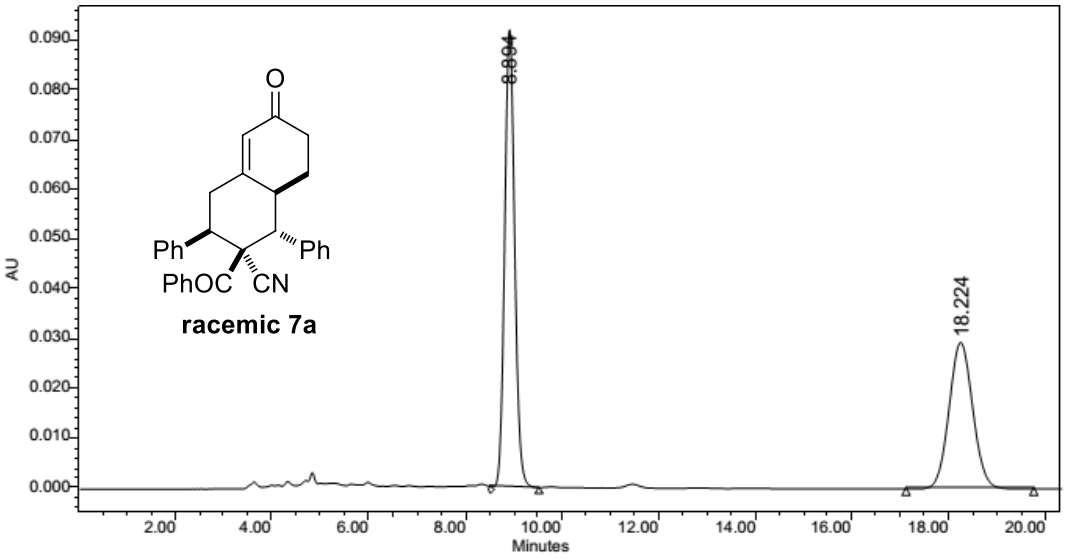




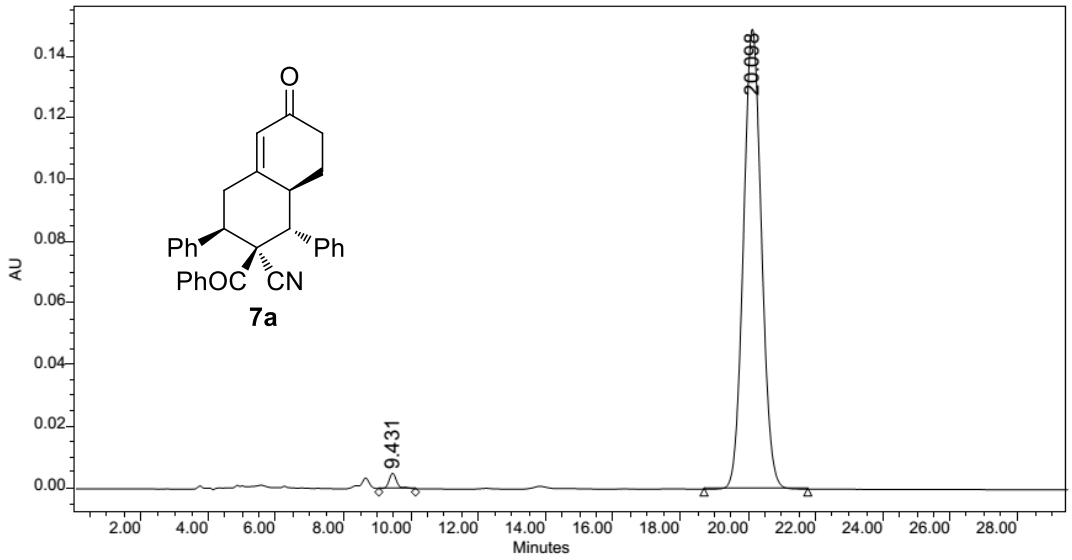
7a

^{13}C NMR (150 MHz, $CDCl_3$)

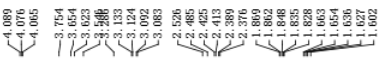


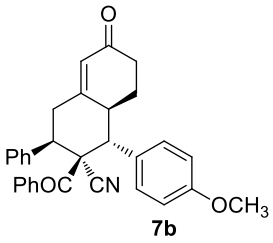


	RT (min)	Area (*sec)	% Area	Height ( )	% Height
1	8.894	1314806	56.73	92107	75.78
2	18.224	1002648	43.27	29431	24.22



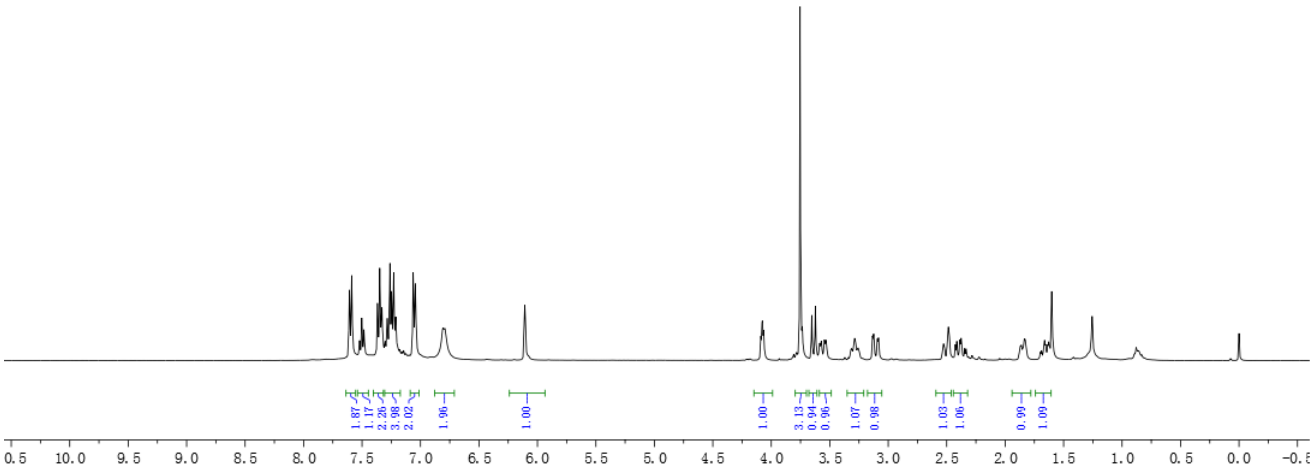
	RT (min)	Area (*sec)	% Area	Height ( )	% Height
1	9.431	86216	1.53	5084	3.30
2	20.098	5538156	98.47	149117	96.70

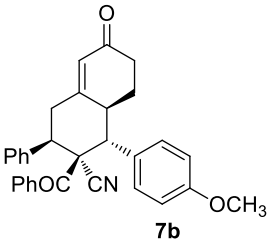




7b

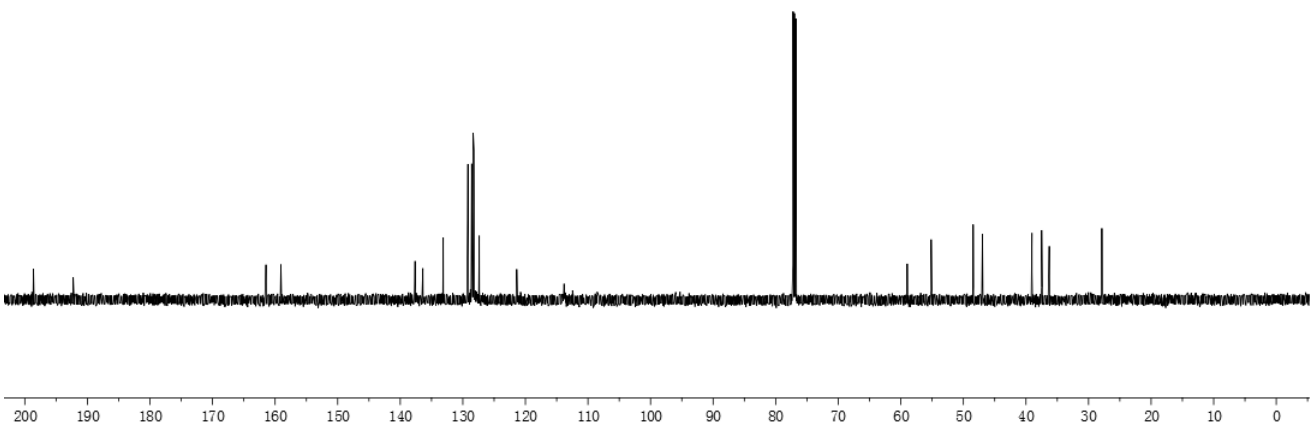
^{1}H NMR (400 MHz, $CDCl_3$)

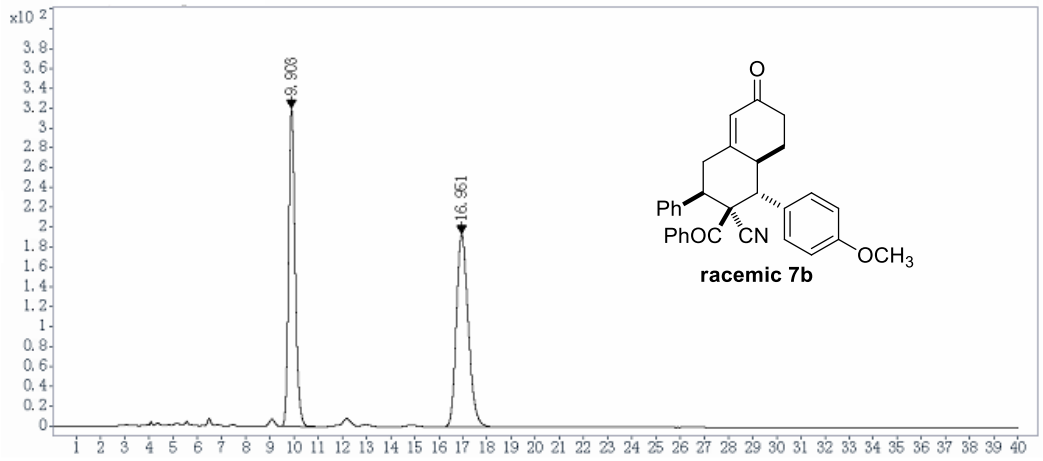




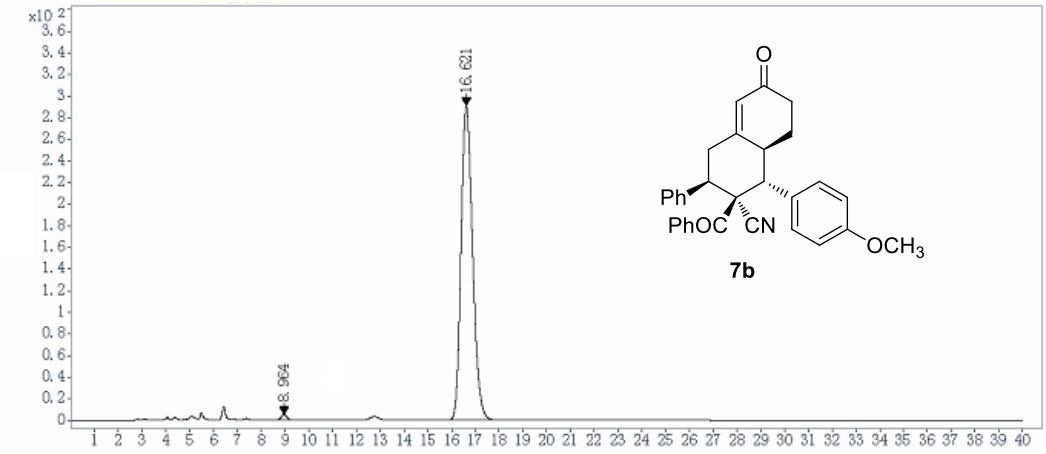
7b

^{13}C NMR (150 MHz, $CDCl_3$)

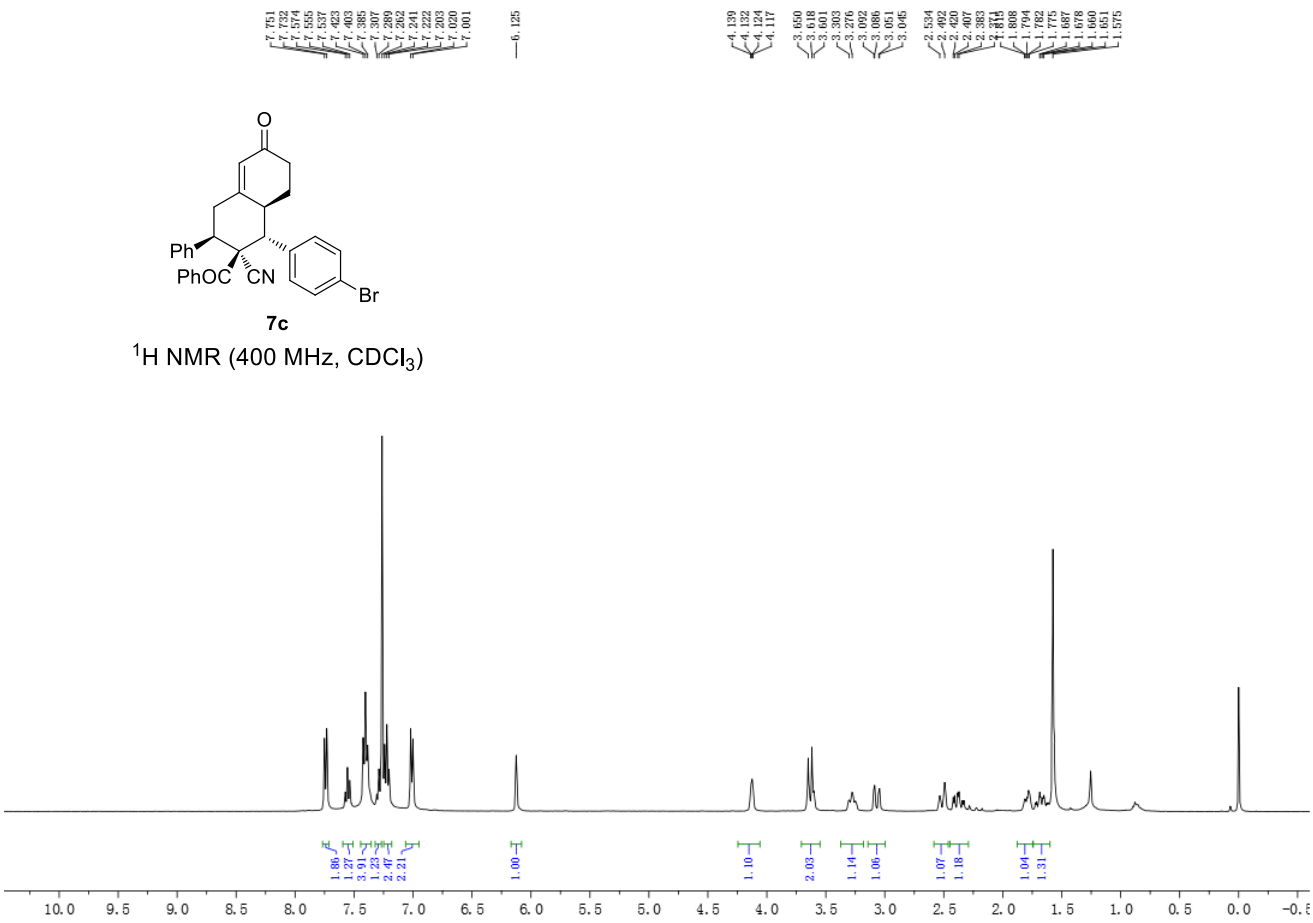




Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
9.903	BB	0.29	320.0838	6020.5420	47.4798
16.951	BB	0.53	194.1192	6659.6685	52.5202

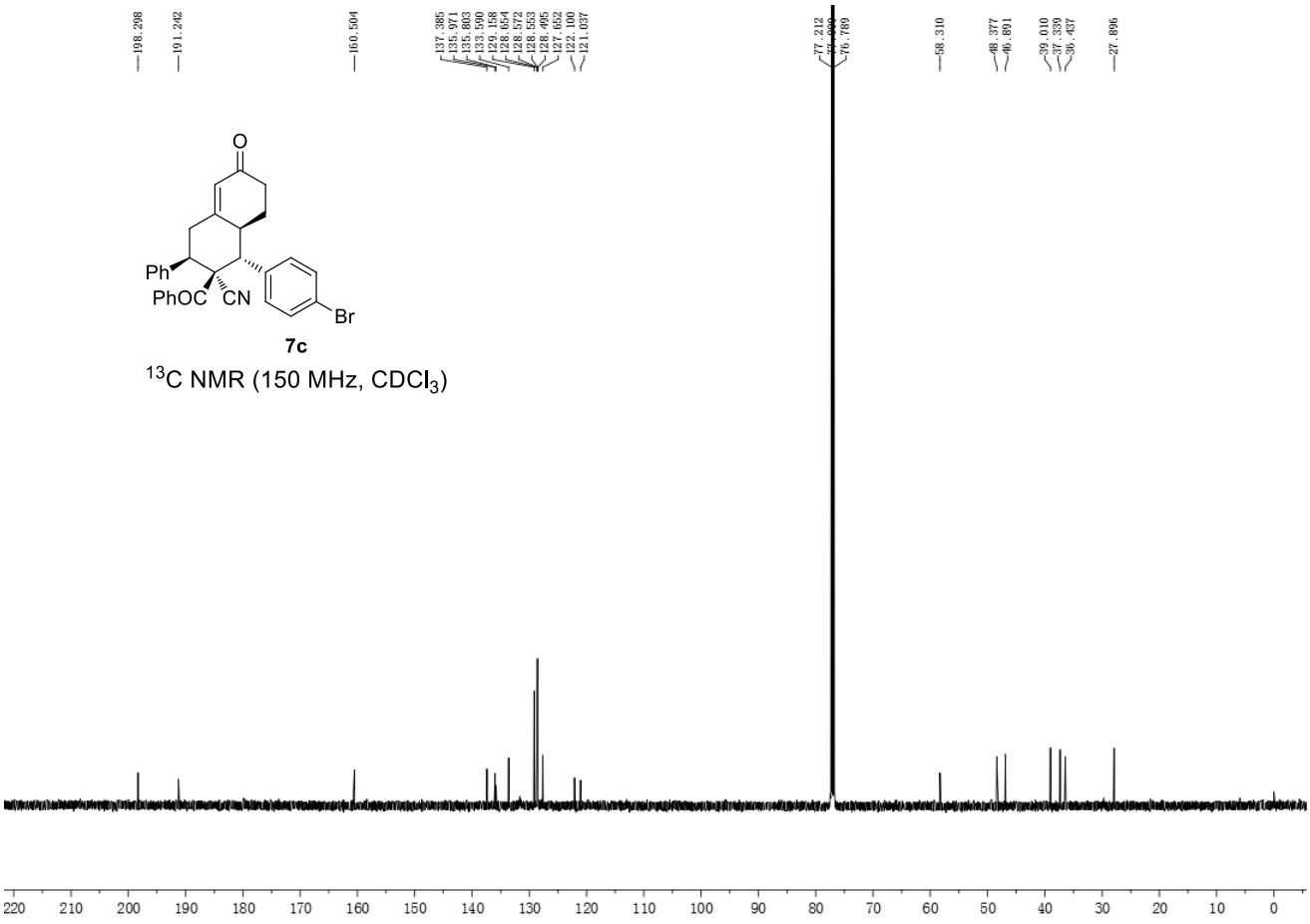


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
8.964	BB	0.24	5.1081	79.7632	0.8098
16.621	BB	0.52	290.5366	9769.5635	99.1902



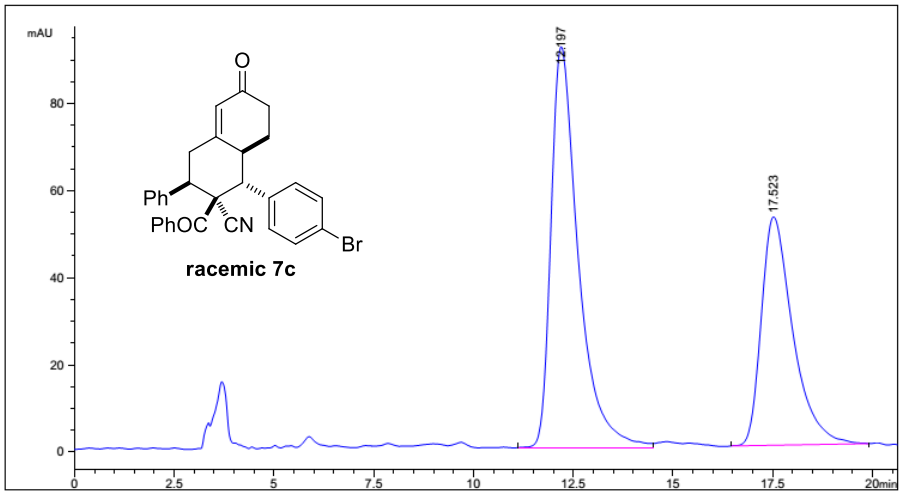
7c

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

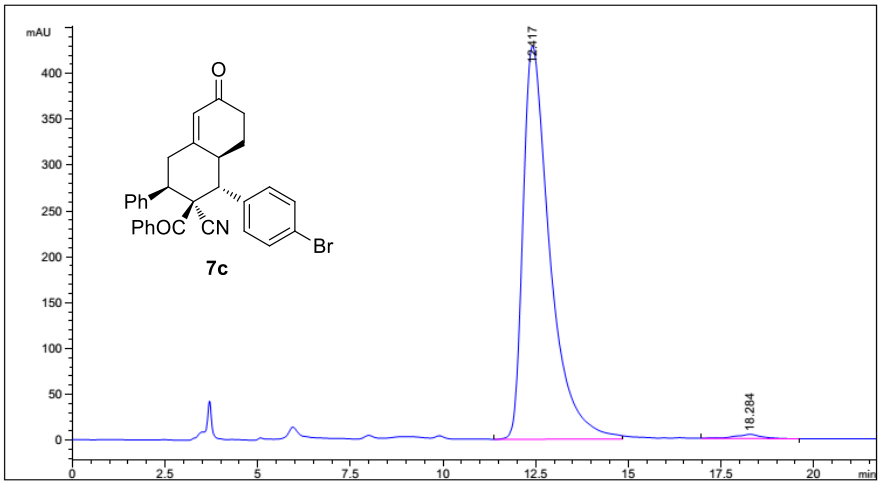


7c

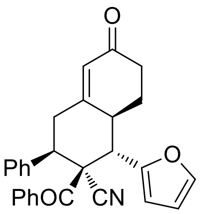
^{13}C NMR (150 MHz, $CDCl_3$)



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	12.197	BB	0.7123	4380.48975	92.07226	60.3574
2	17.523	BB	0.8205	2877.09619	52.44734	39.6426

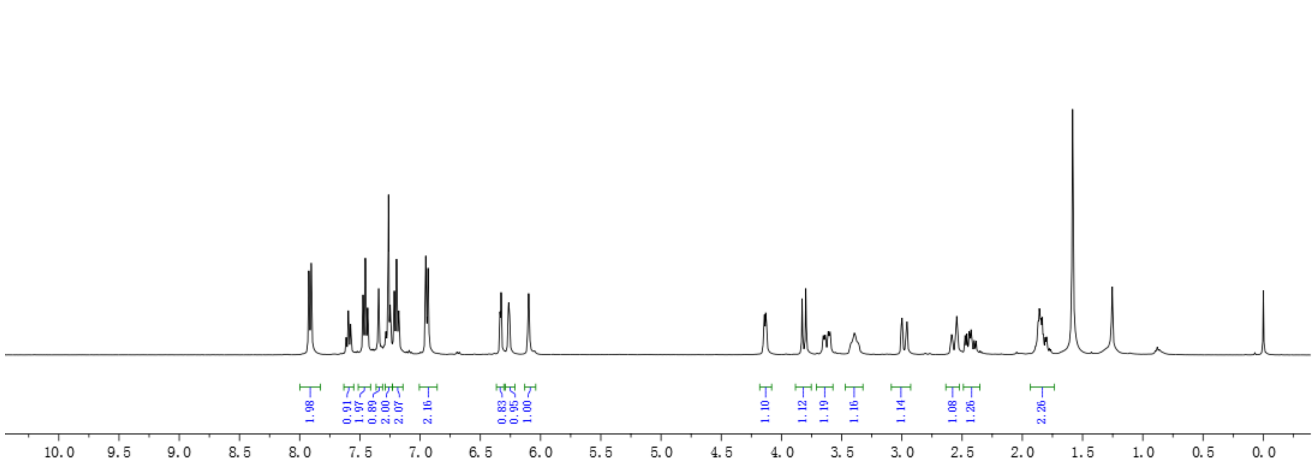


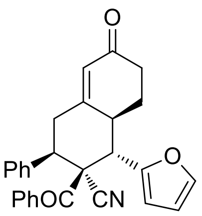
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	12.417	VBA	0.7511	2.16406e4	429.37531	98.9847
2	18.284	BB	0.6462	221.97990	4.63388	1.0153



7d

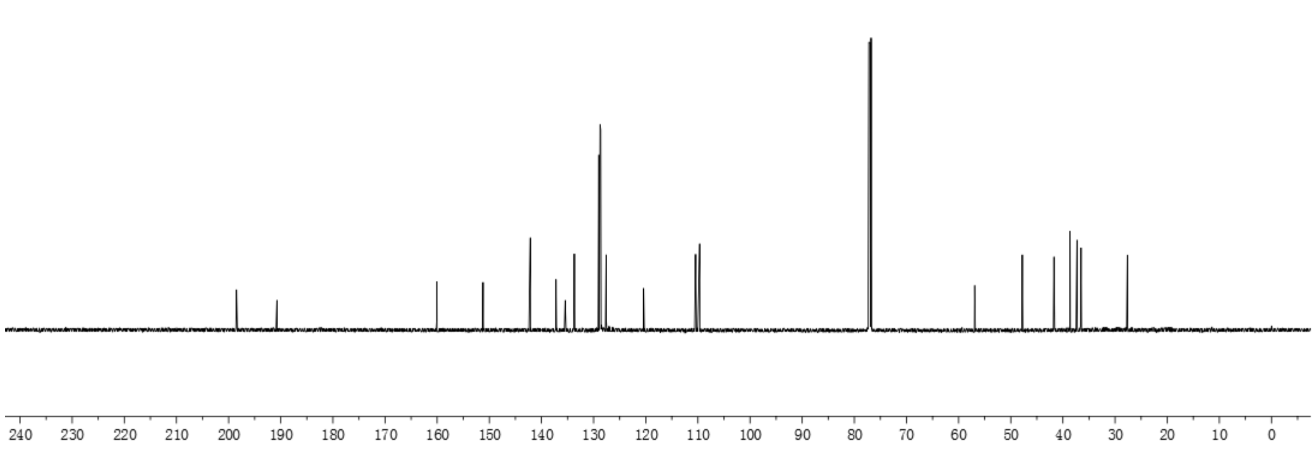
^{1}H NMR (400 MHz, $CDCl_3$)

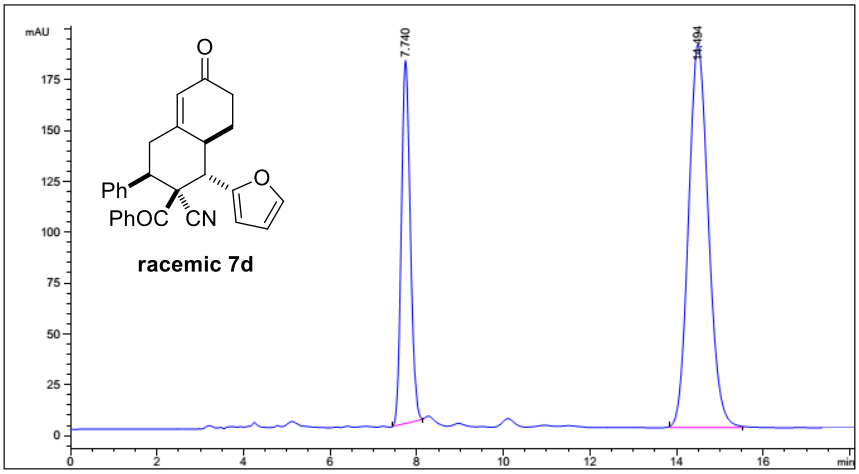




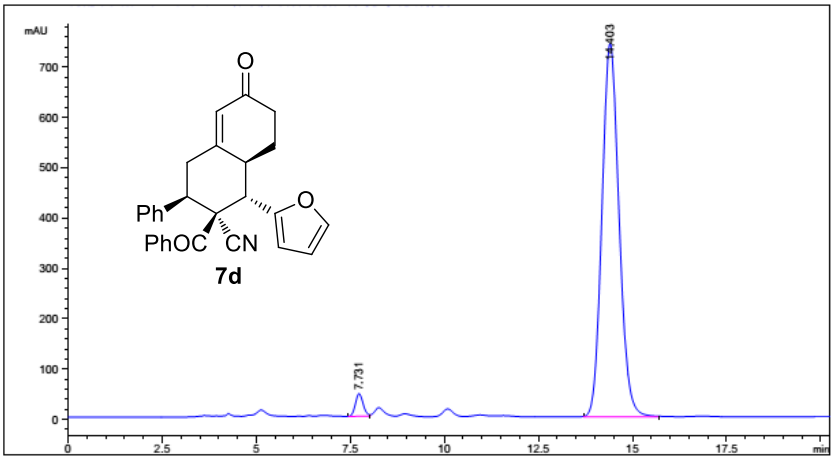
7d

^{13}C NMR (150 MHz, $CDCl_3$)

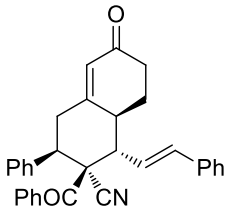




Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.740	BBA	0.2261	2561.54297	178.06241	29.8887
2	14.494	BB	0.4947	6008.71826	188.24652	70.1113

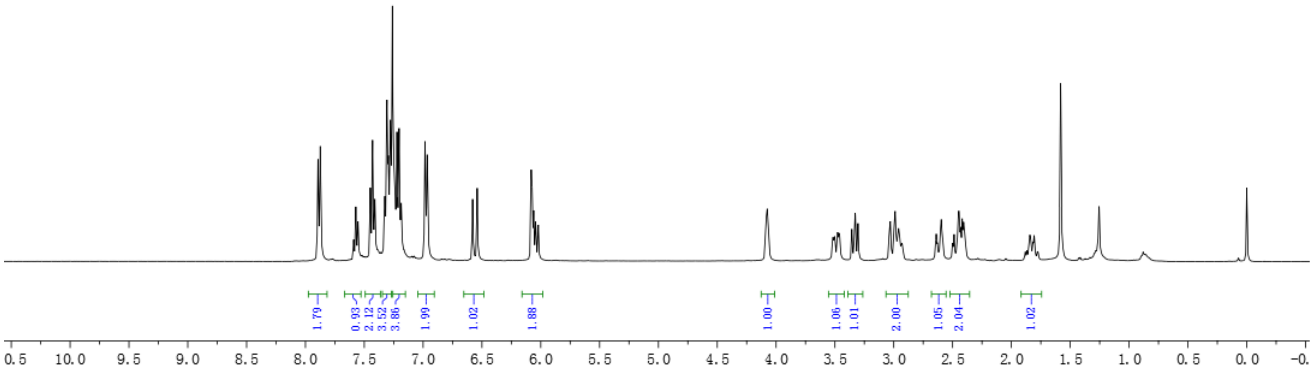


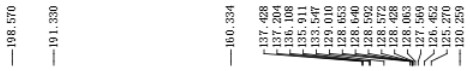
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.731	BV	0.2257	644.60126	44.91129	2.6734
2	14.403	BB	0.4975	2.34666e4	741.26886	97.3266

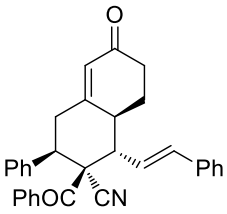


7e

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

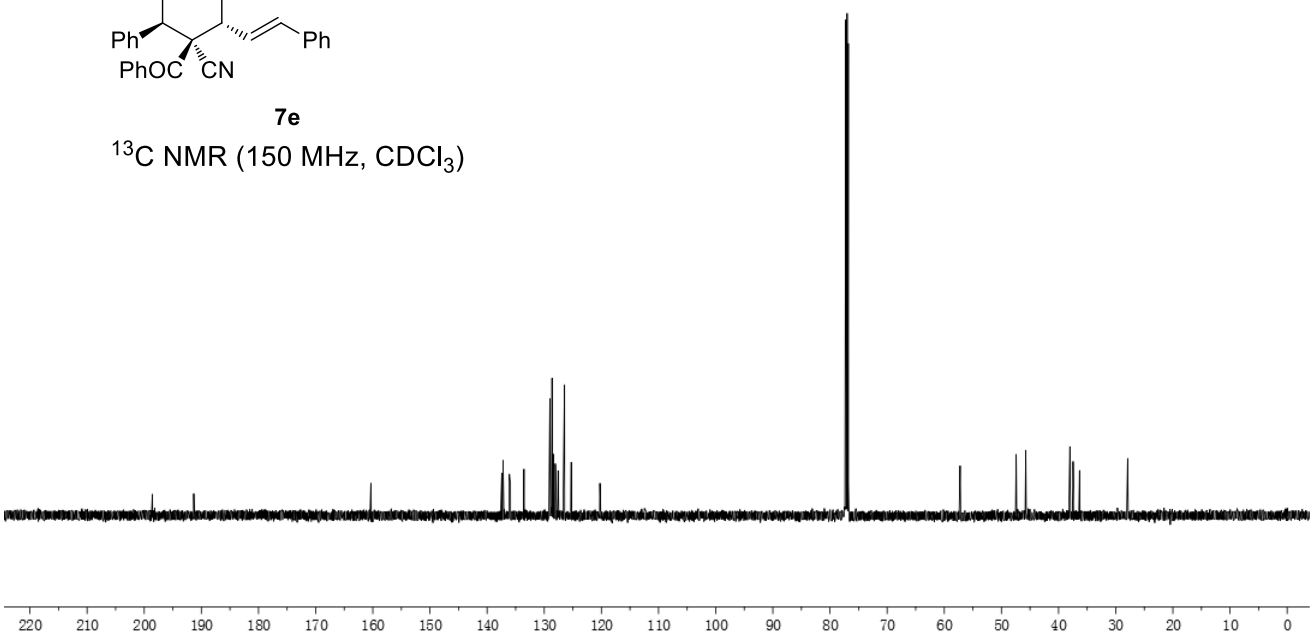


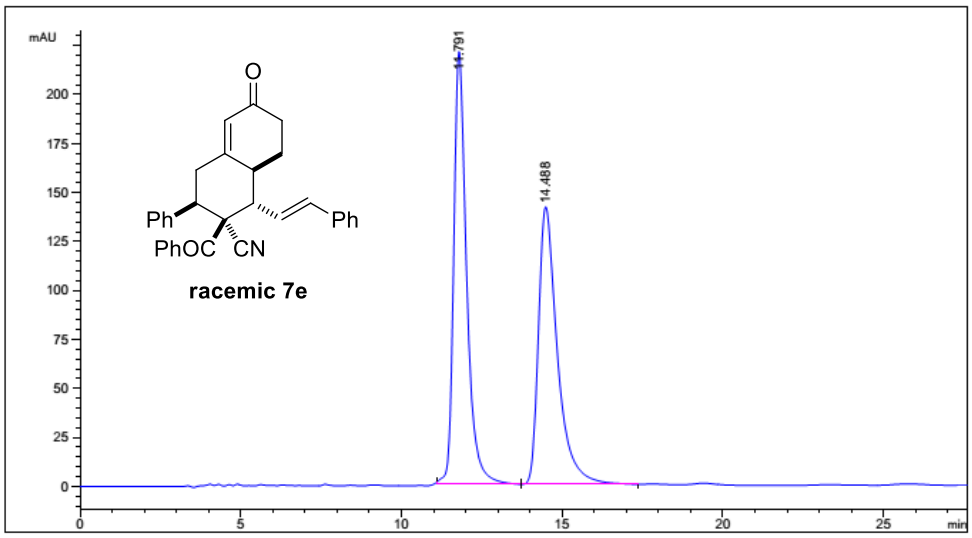




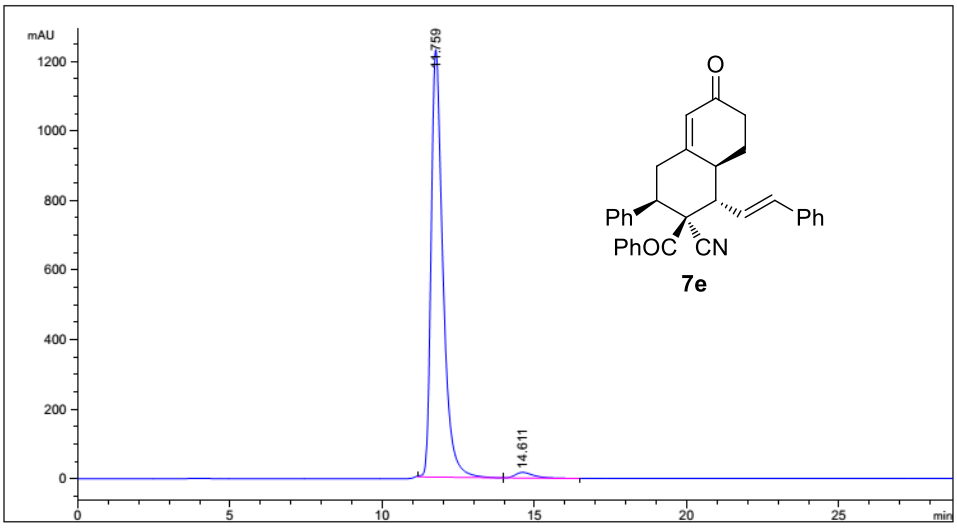
7e

^{13}C NMR (150 MHz, $CDCl_3$)

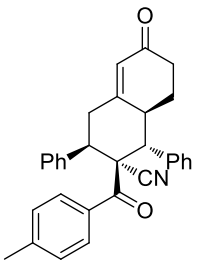




Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.791	BV	0.4254	6178.27637	220.82610	51.6496
2	14.488	VB	0.6105	5783.63281	141.60031	48.3504

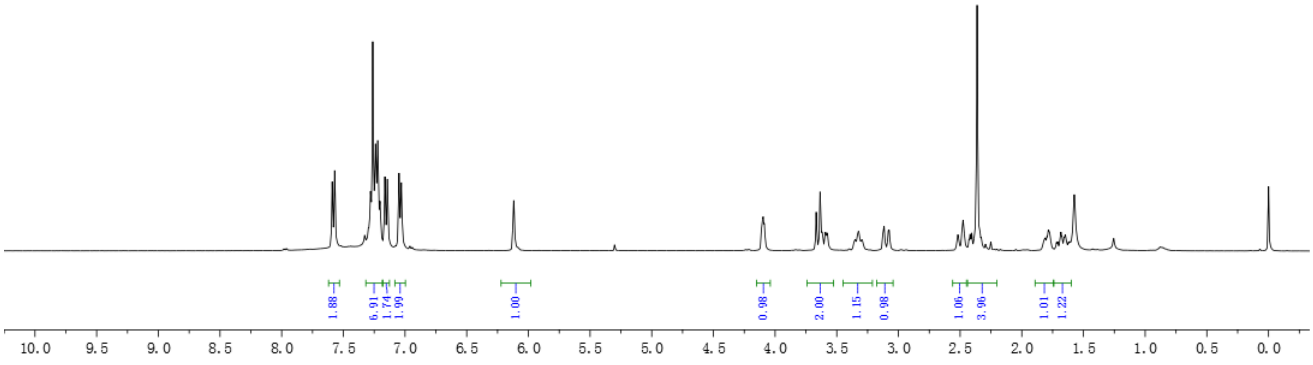


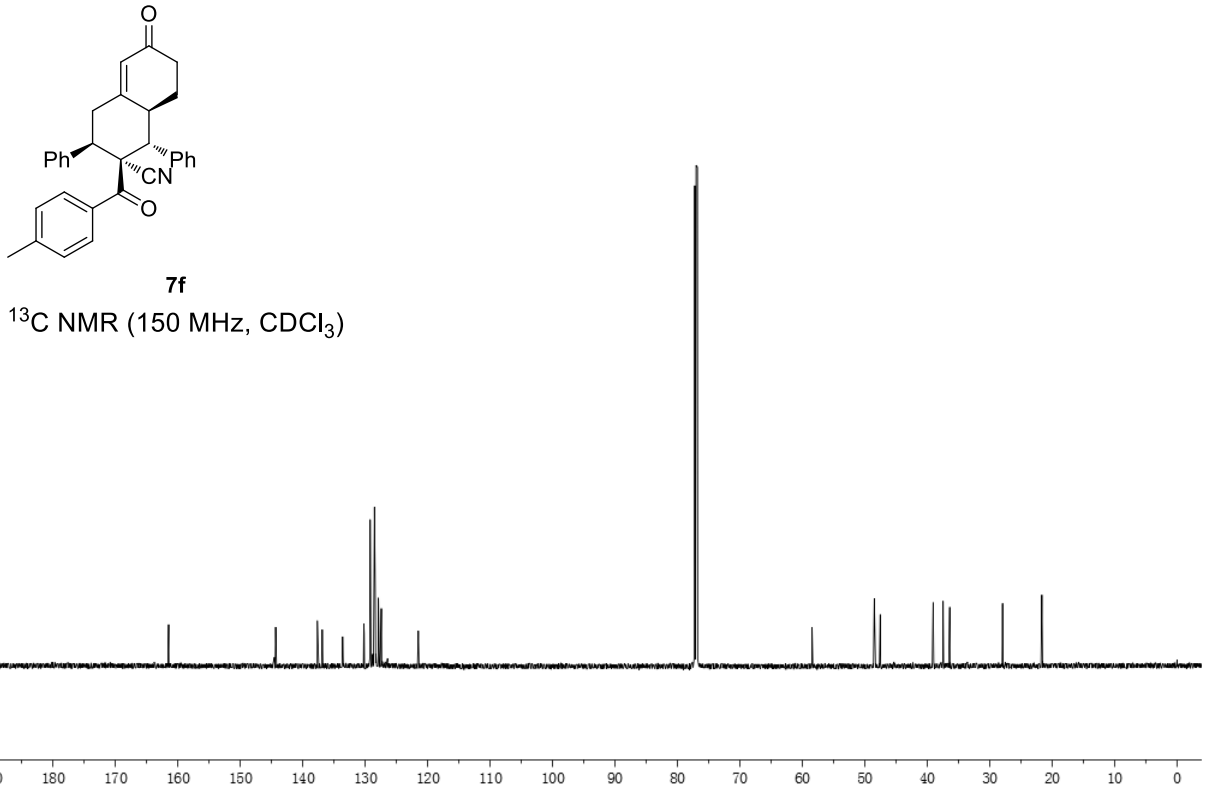
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.759	BV	0.4060	3.29274e4	1228.13416	98.0010
2	14.611	VB	0.6315	671.66034	16.12557	1.9990



7f

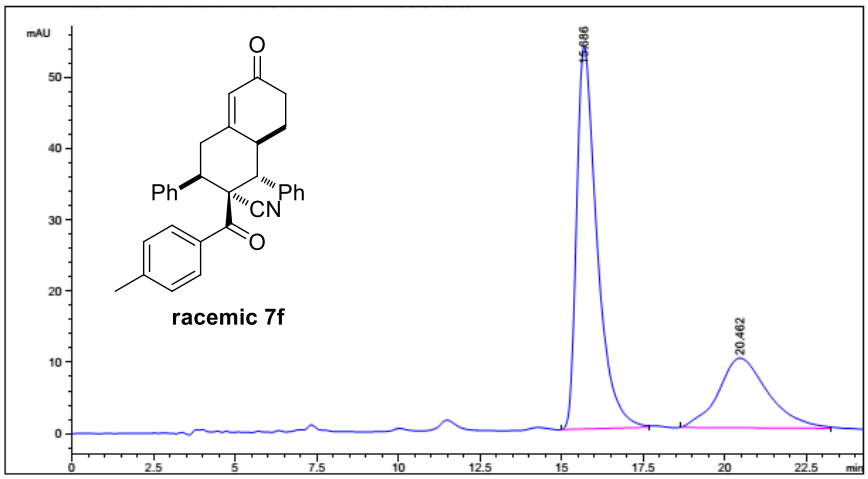
^{1}H NMR (400 MHz, $CDCl_3$)



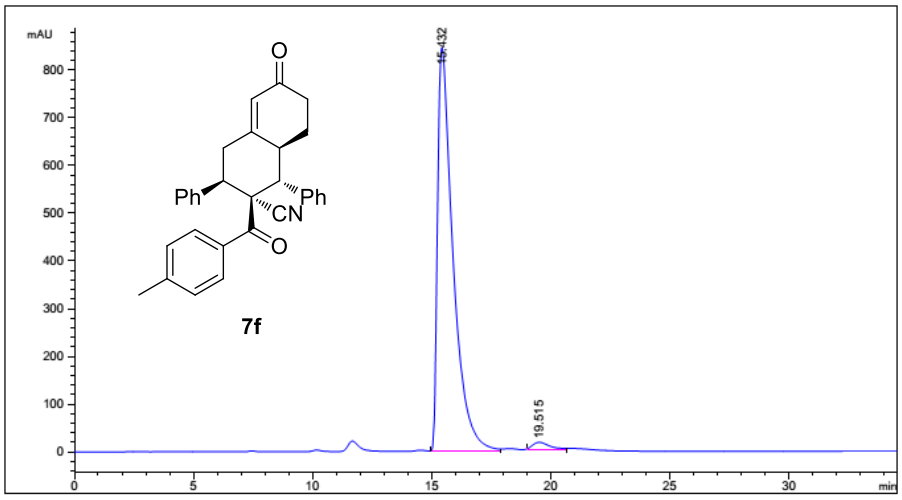


7f

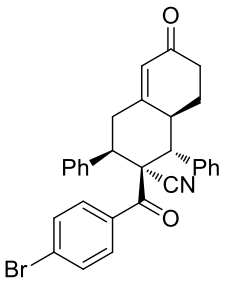
^{13}C NMR (150 MHz, $CDCl_3$)



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	15.686	BB	0.6533	2336.89819	53.69551	69.3054
2	20.462	BB	1.5667	1034.98730	9.77910	30.6946

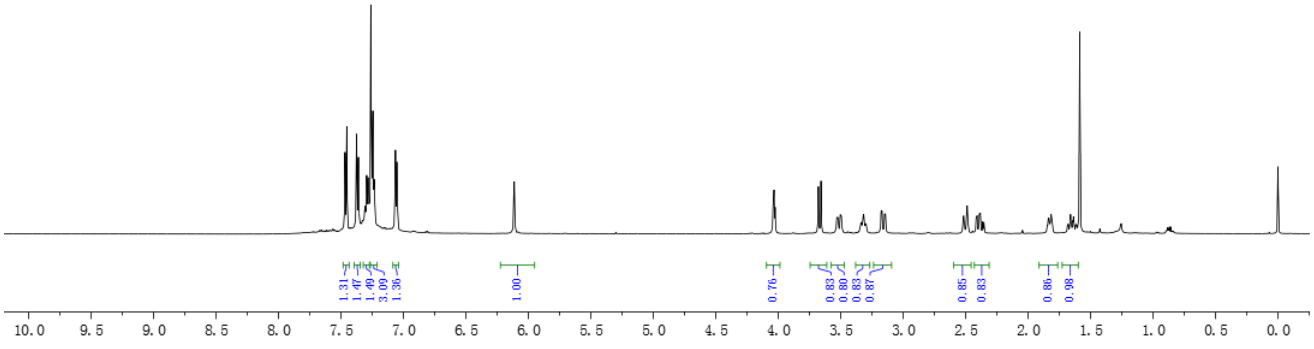


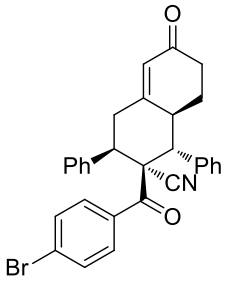
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	15.432	BBA	0.6661	3.81376e4	845.39948	97.9676
2	19.515	BB	0.7745	791.19025	15.39049	2.0324



7g

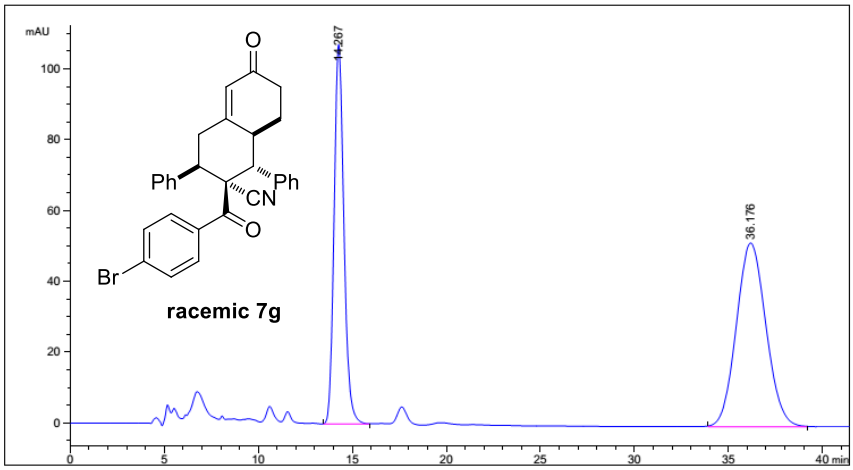
^{1}H NMR (600 MHz, $CDCl_3$)



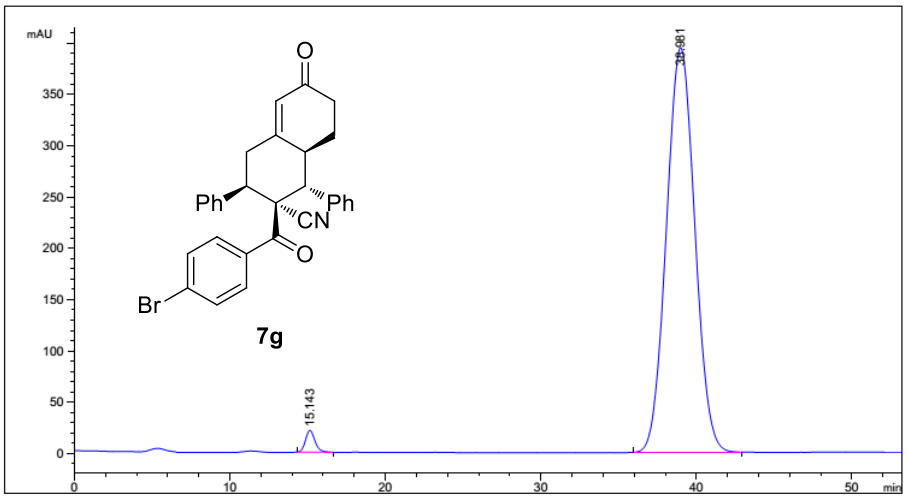


7g

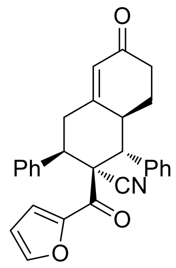
^{13}C NMR (150 MHz, $CDCl_3$)



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.267	BB	0.5630	3886.65332	107.14098	40.6778
2	36.176	BB	1.7052	5668.07959	51.89583	59.3222

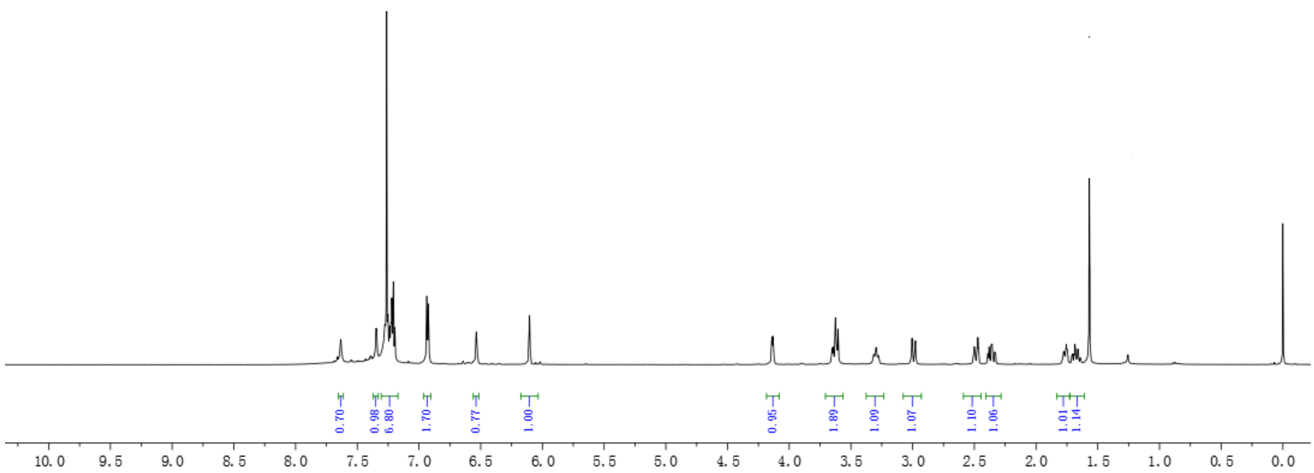


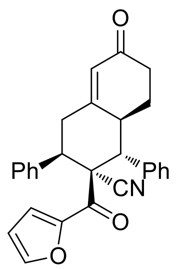
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	15.143	BB	0.6452	899.95099	21.26190	1.7687
2	38.981	BB	1.9908	4.99834e4	394.46841	98.2313



7h

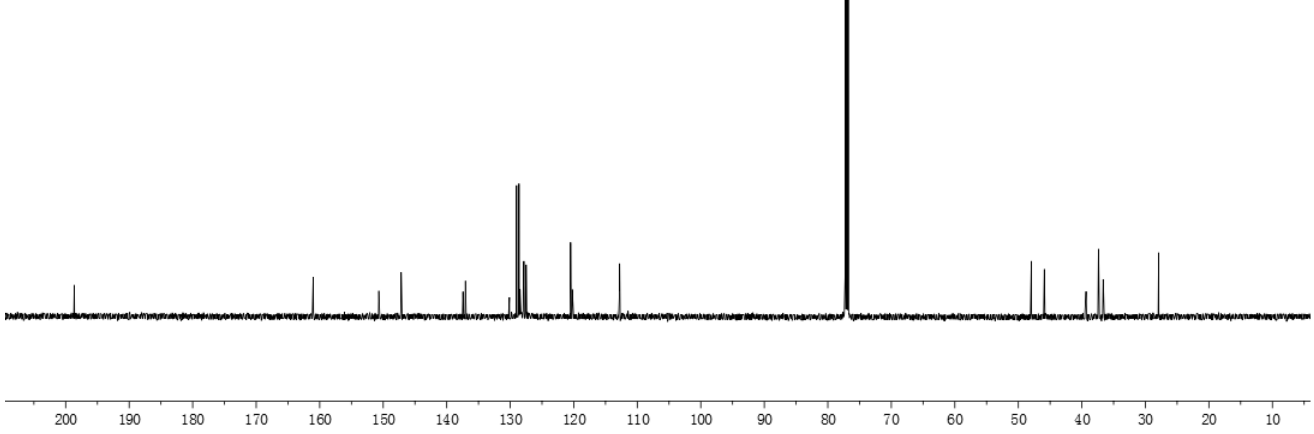
^{1}H NMR (600 MHz, $CDCl_3$)

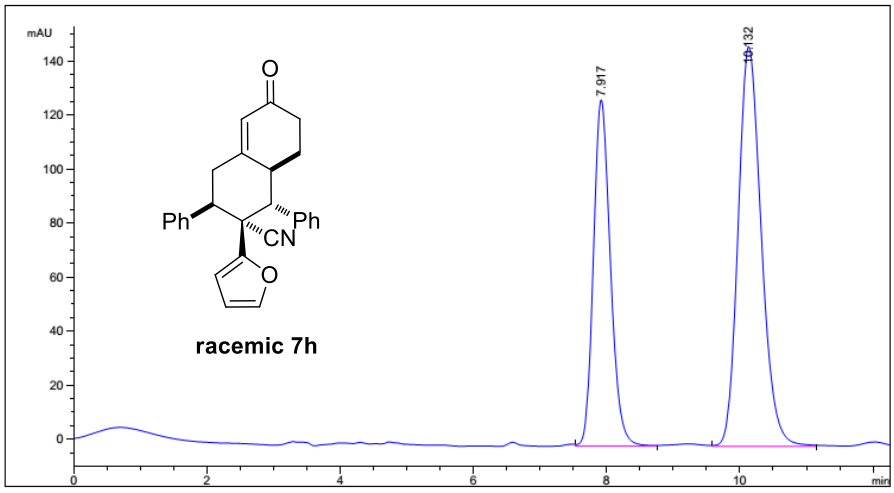




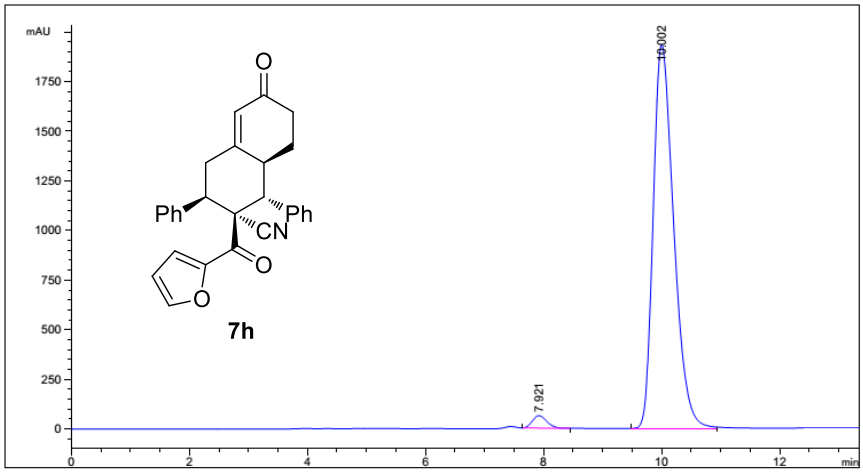
7h

^{13}C NMR (150 MHz, $CDCl_3$)

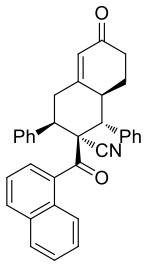




Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.917	VB	0.2762	2264.18335	128.02995	38.8363
2	10.132	VBA	0.3747	3565.88892	147.77191	61.1637

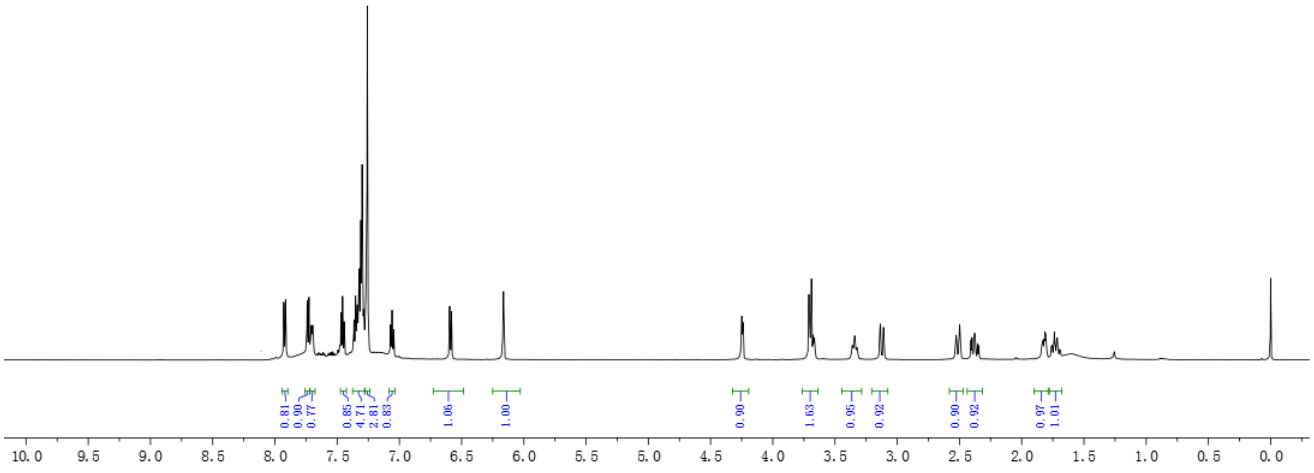


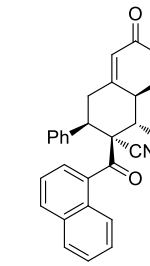
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.921	BV	0.2658	1064.54248	63.40004	2.2299
2	10.002	BBA	0.3690	4.66759e4	1933.40771	97.7701



7i

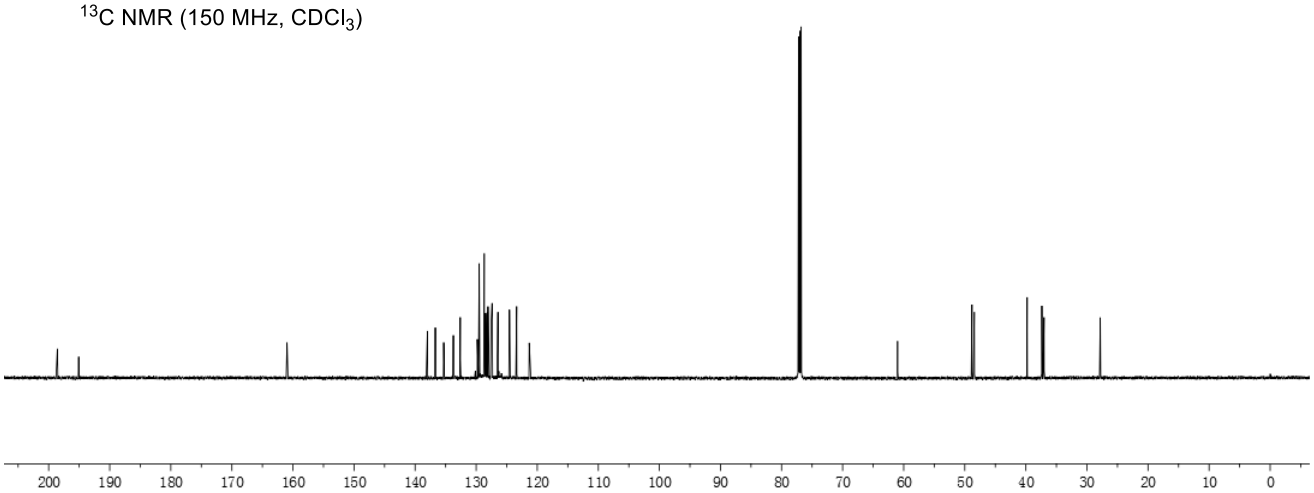
^{1}H NMR (600 MHz, $CDCl_3$)

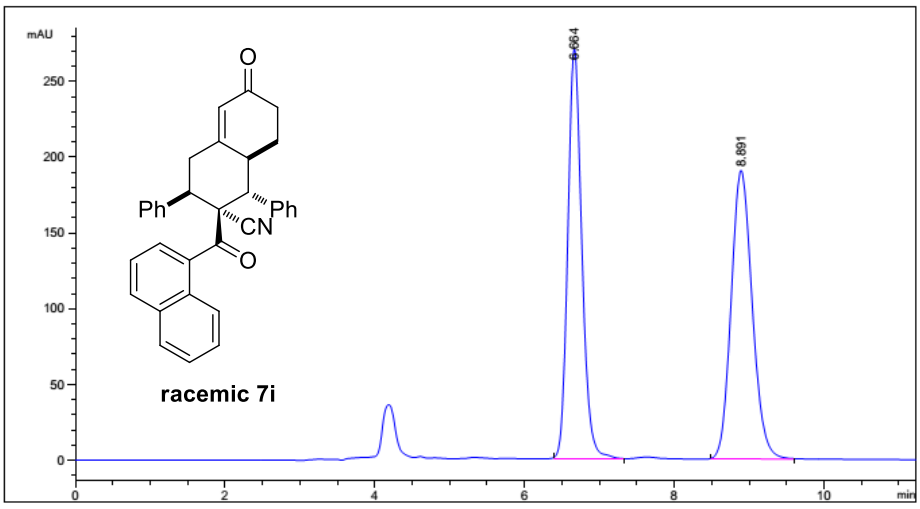




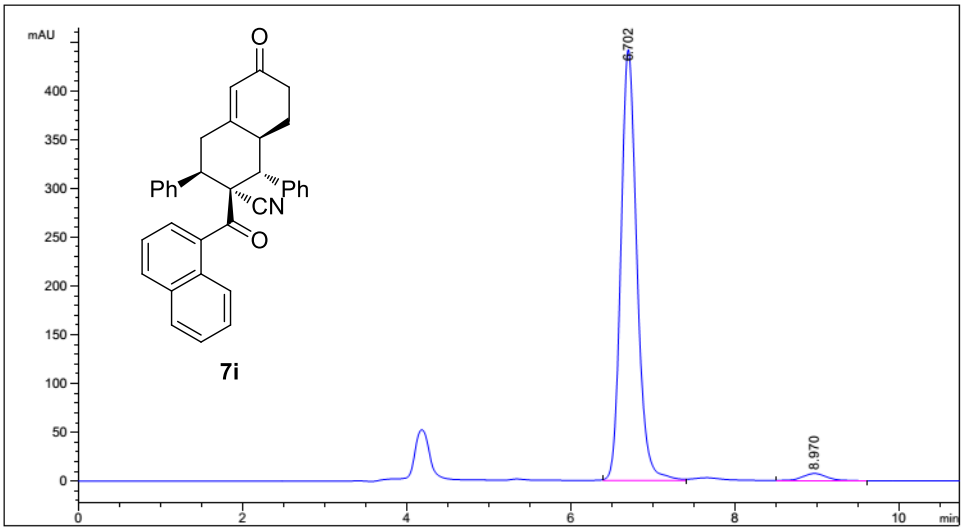
7i

^{13}C NMR (150 MHz, $CDCl_3$)

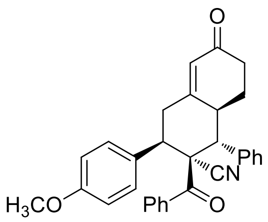




Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.664	BB	0.2045	3521.64014	270.13892	48.7121
2	8.891	BB	0.3032	3707.85522	190.16364	51.2879

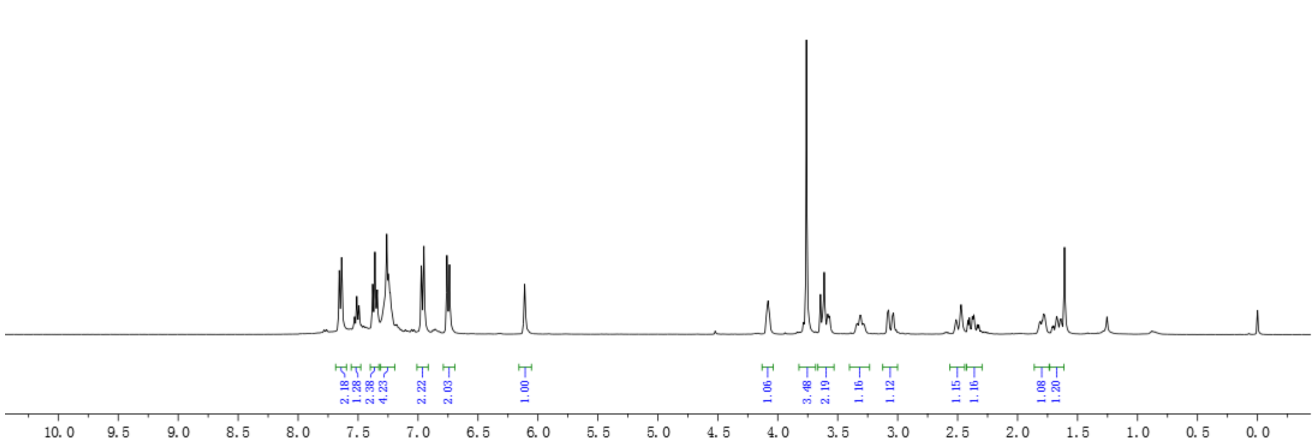


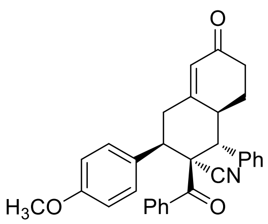
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.702	BB	0.2104	5964.56104	440.53101	97.4283
2	8.970	BB	0.3253	157.44124	7.53524	2.5717



7i

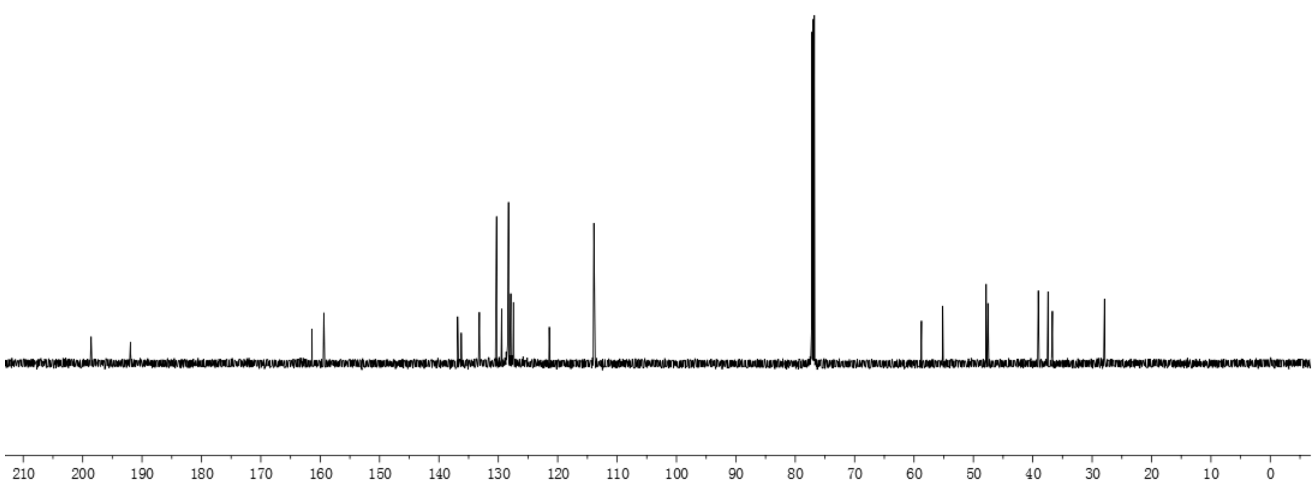
^{1}H NMR (400 MHz, $CDCl_3$)

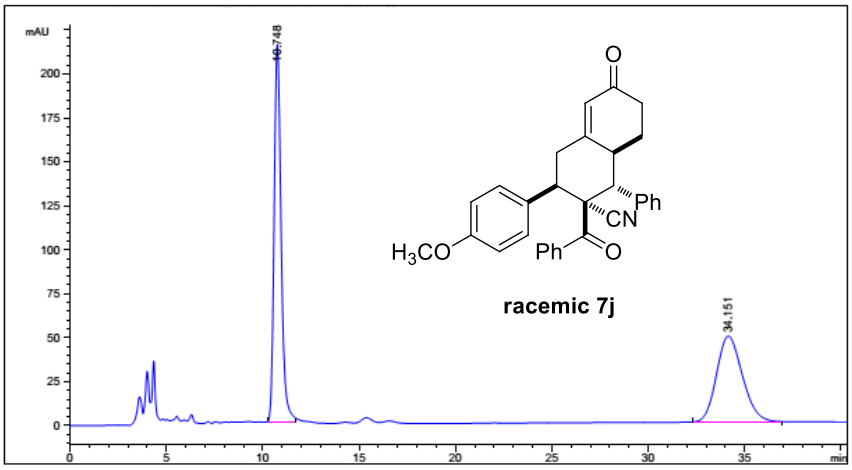




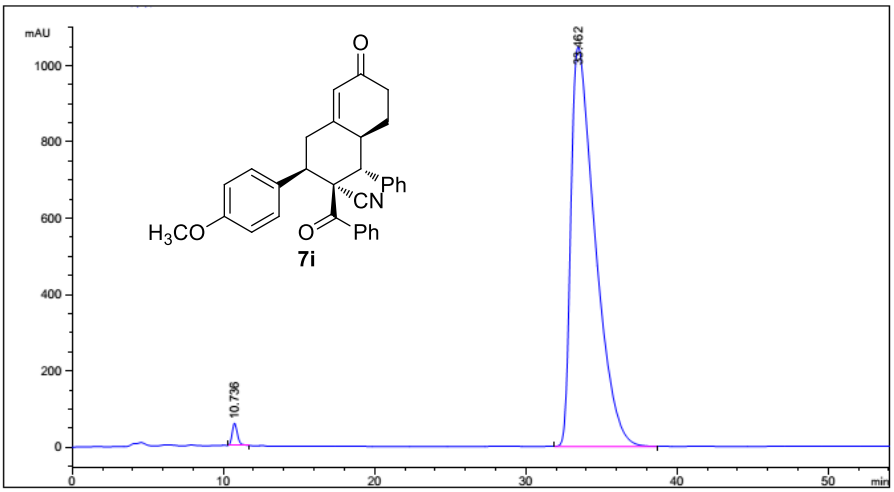
7i

^{13}C NMR (150 MHz, $CDCl_3$)

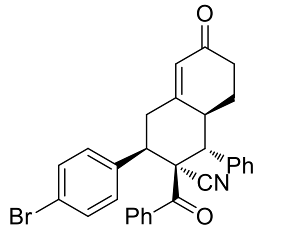




Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	10.748	BBA	0.3851	5364.93750	214.39893	53.9694
2	34.151	BB	1.4483	4575.75928	48.84209	46.0306

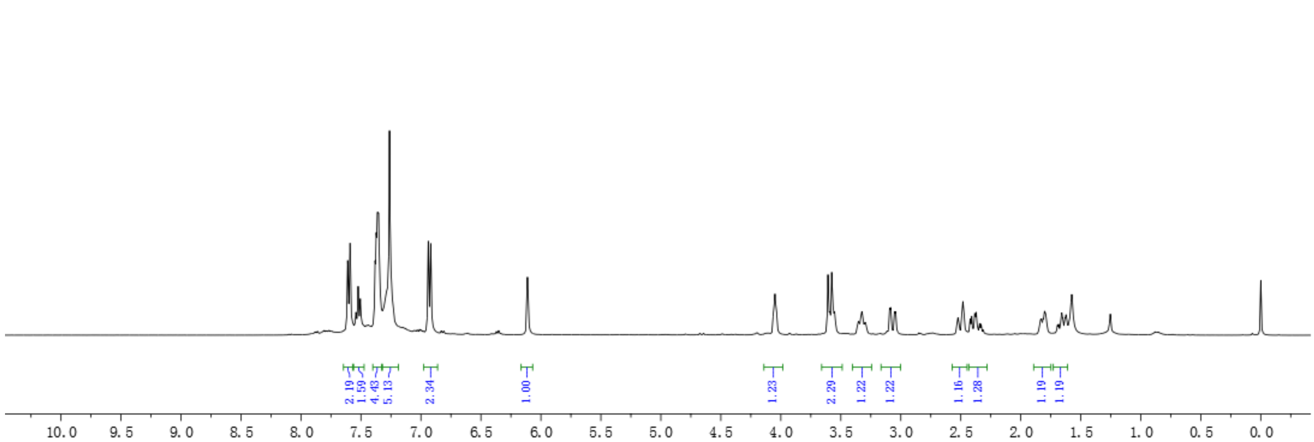


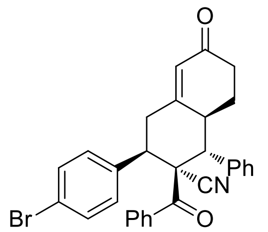
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	10.736	BBA	0.3830	1449.89636	58.37552	1.2363
2	33.462	BB	1.6571	1.15831e5	1047.40466	98.7637



7k

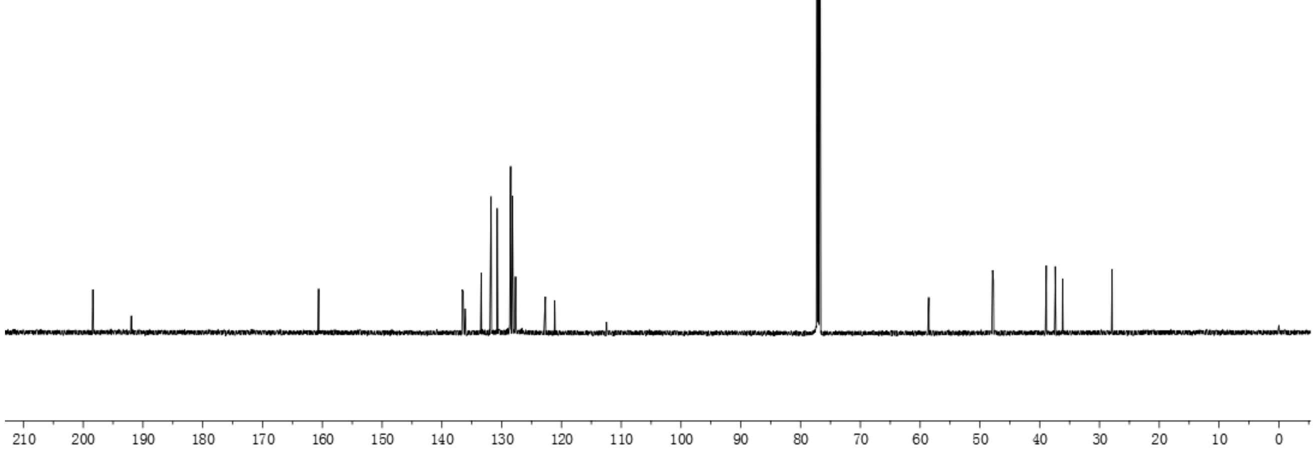
^{1}H NMR (400 MHz, $CDCl_3$)

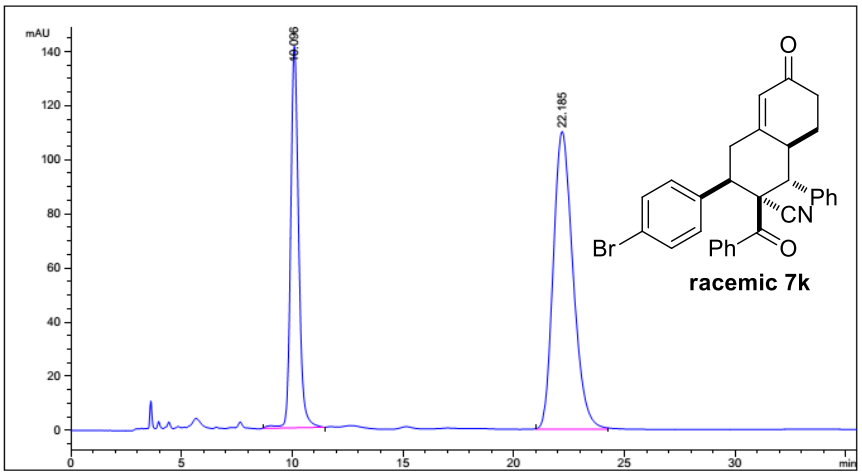




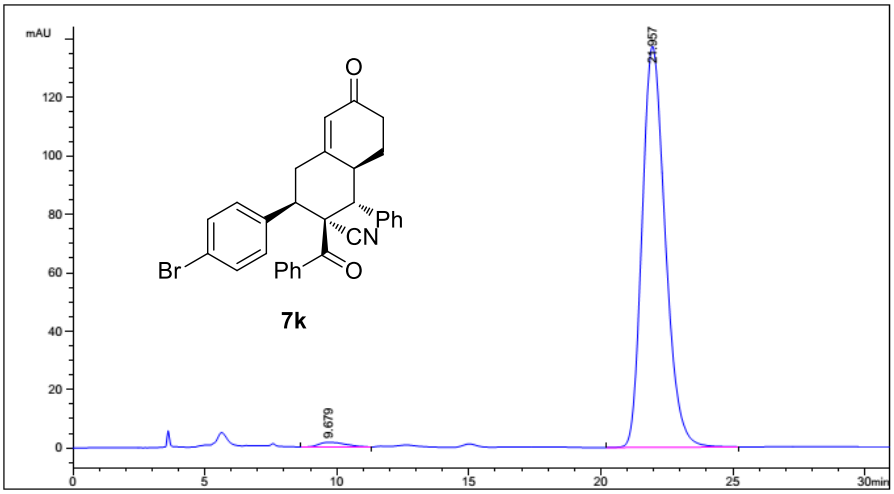
7k

^{13}C NMR (150 MHz, $CDCl_3$)

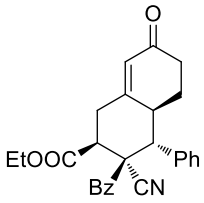




Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	10.096	BB	0.3849	3525.86206	141.01637	34.1972
2	22.185	BB	0.9590	6784.52881	109.89619	65.8028

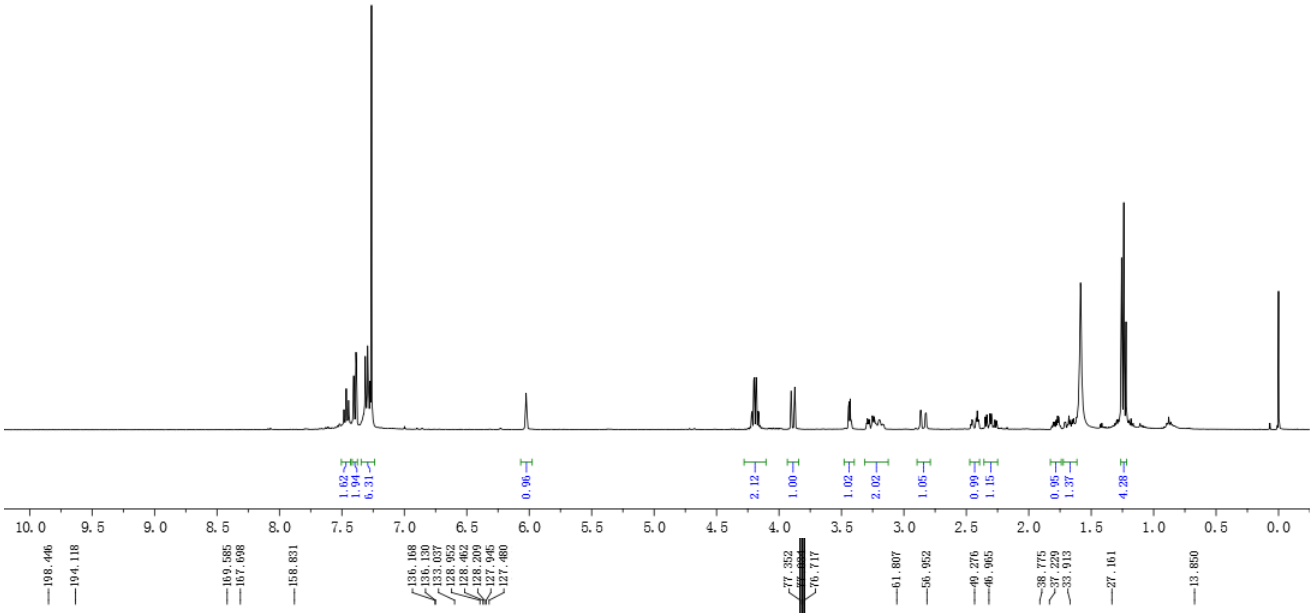


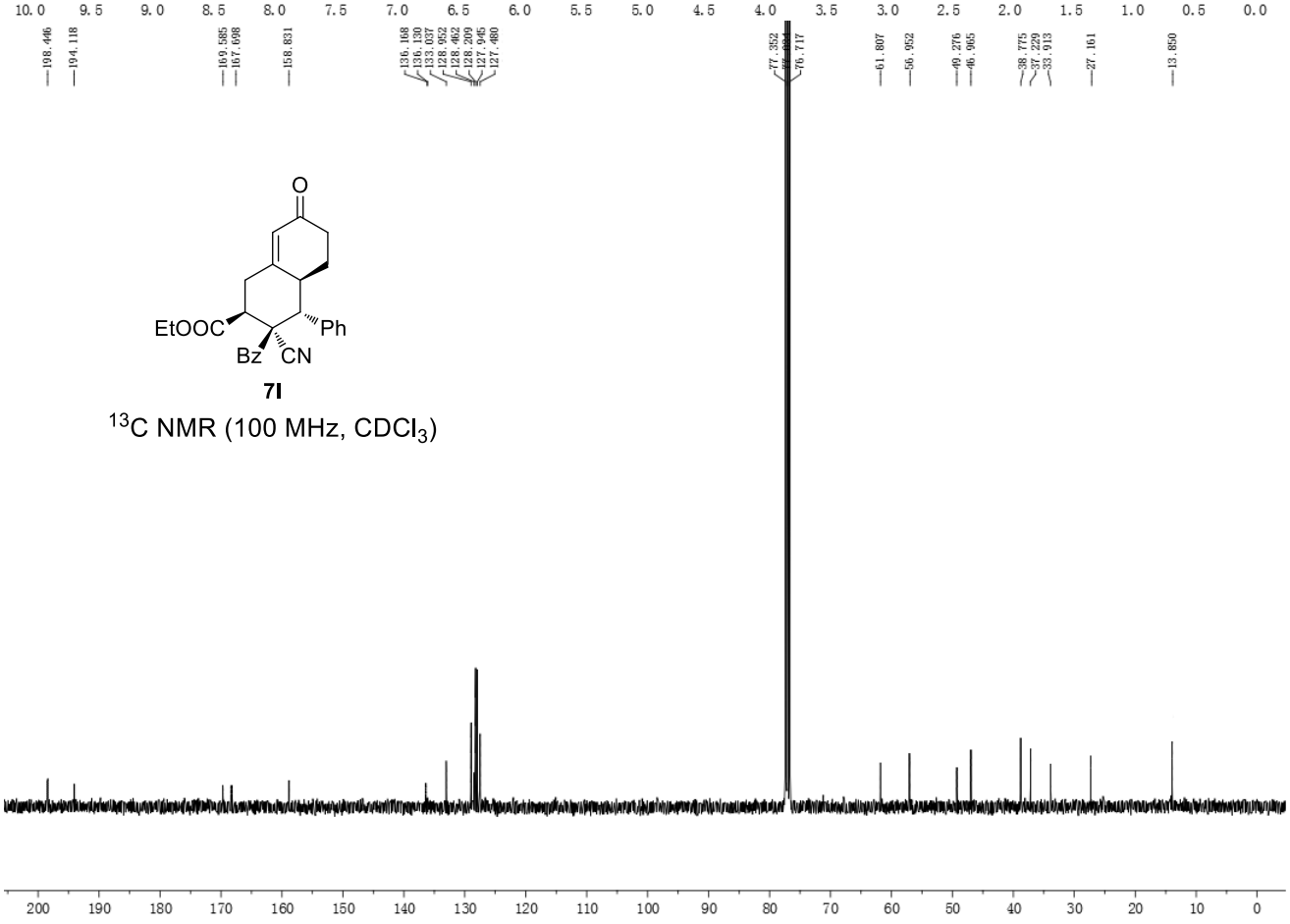
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.679	BV	1.0230	120.49957	1.63489	1.4250
2	21.957	BB	0.9409	8335.76758	137.36533	98.5750



7l

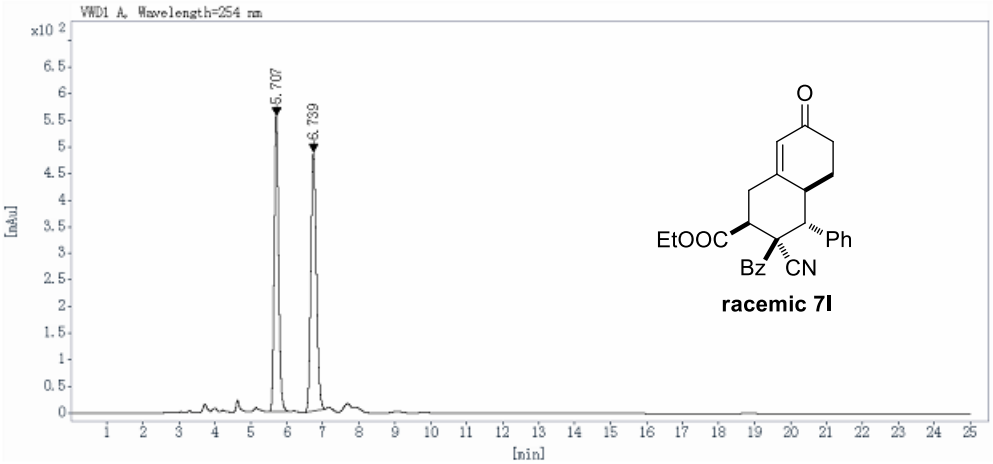
^{1}H NMR (400 MHz, $CDCl_3$)



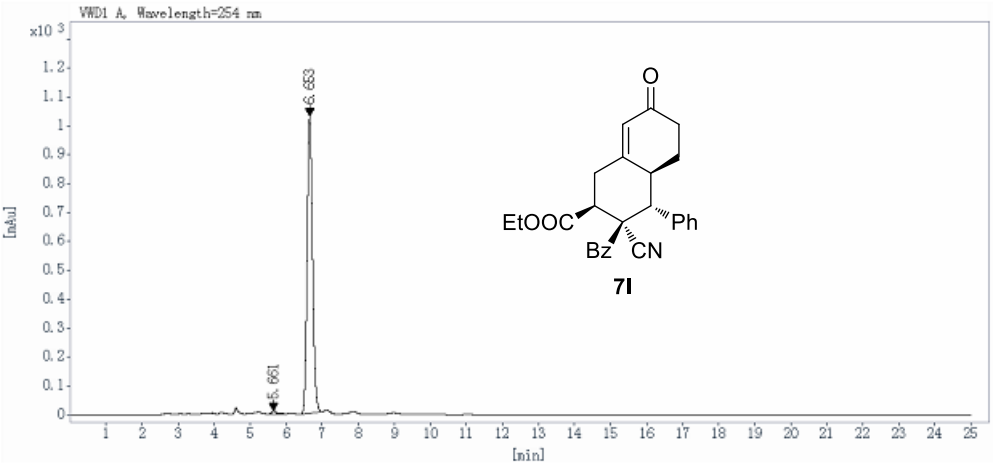


7l

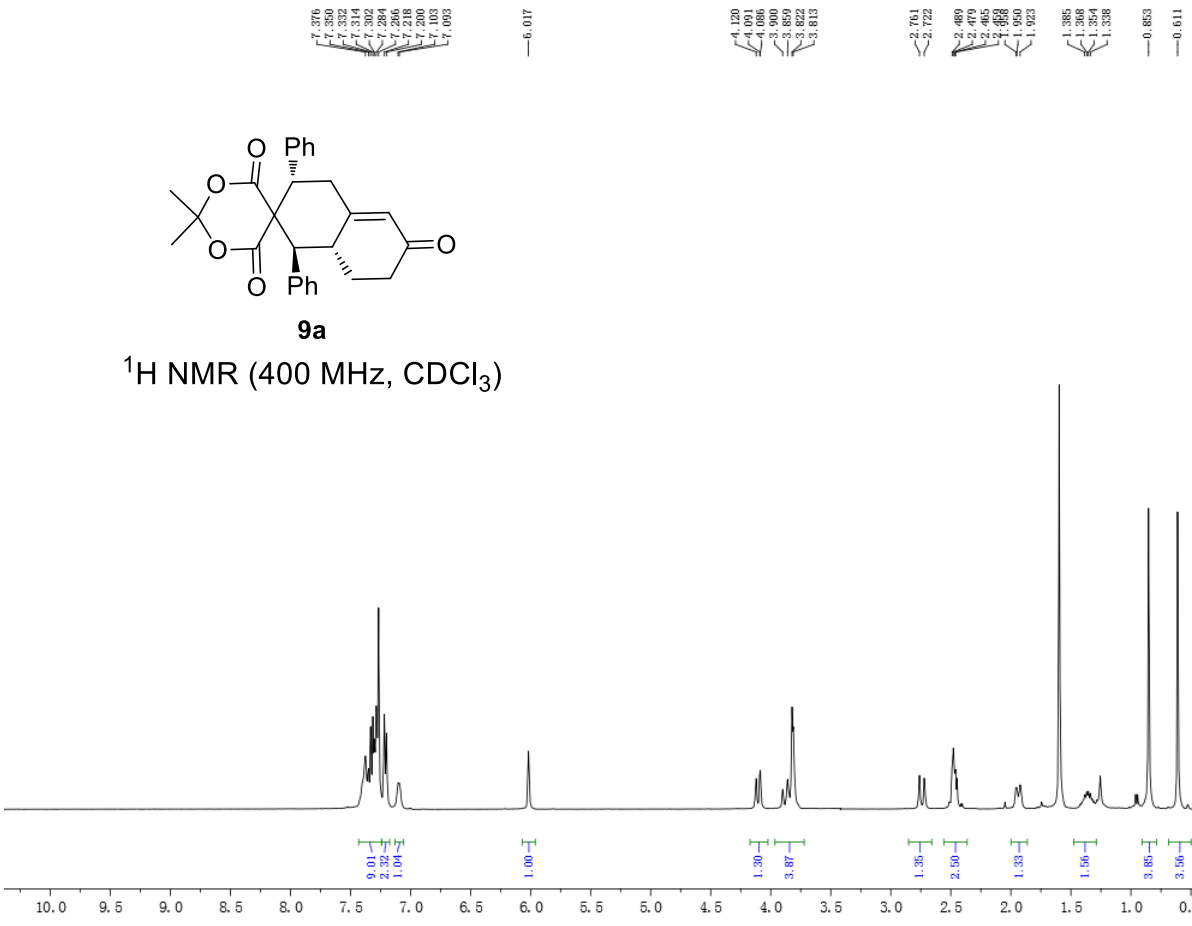
^{13}C NMR (100 MHz, $CDCl_3$)

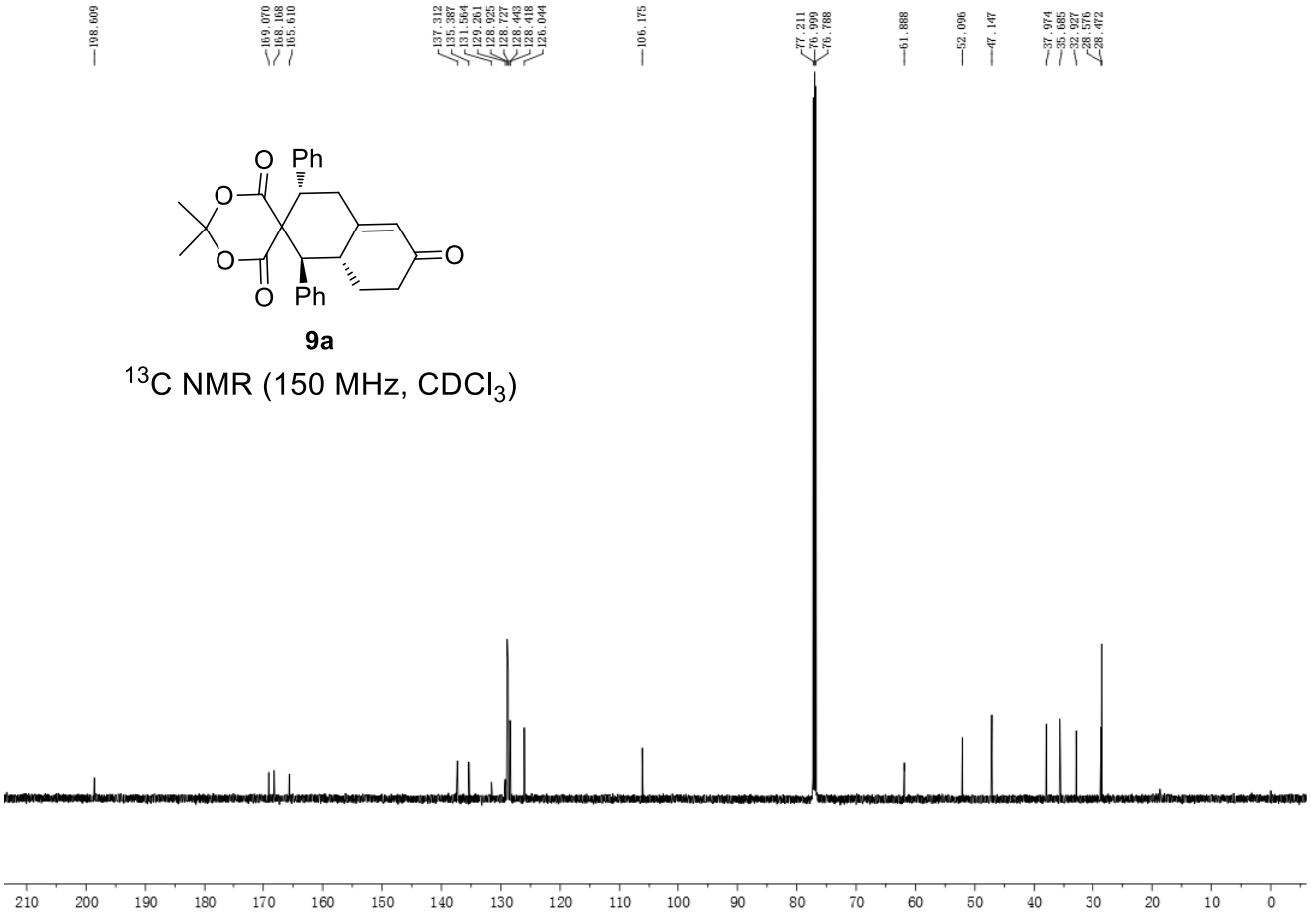


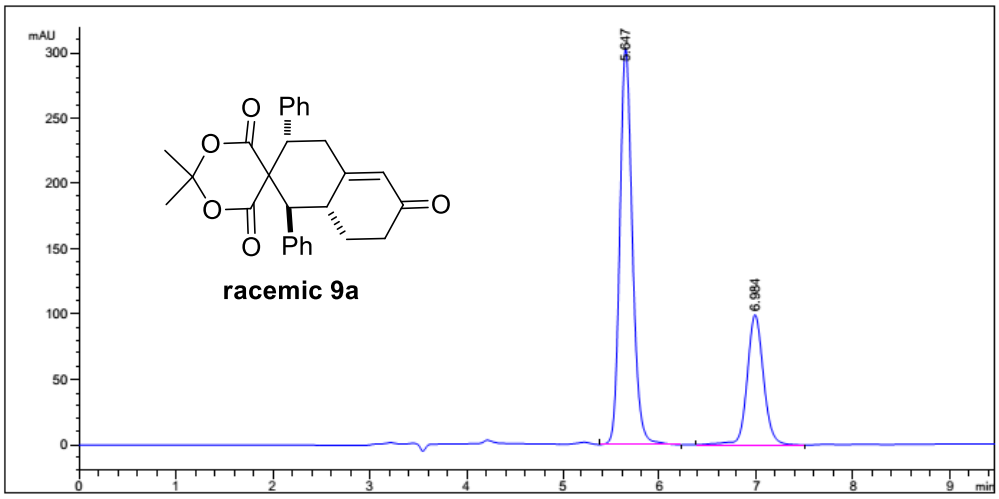
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
5.707	BBA	0.13	555.5540	4717.9414	47.6367
6.739	BB	0.17	485.7625	5186.0654	52.3633



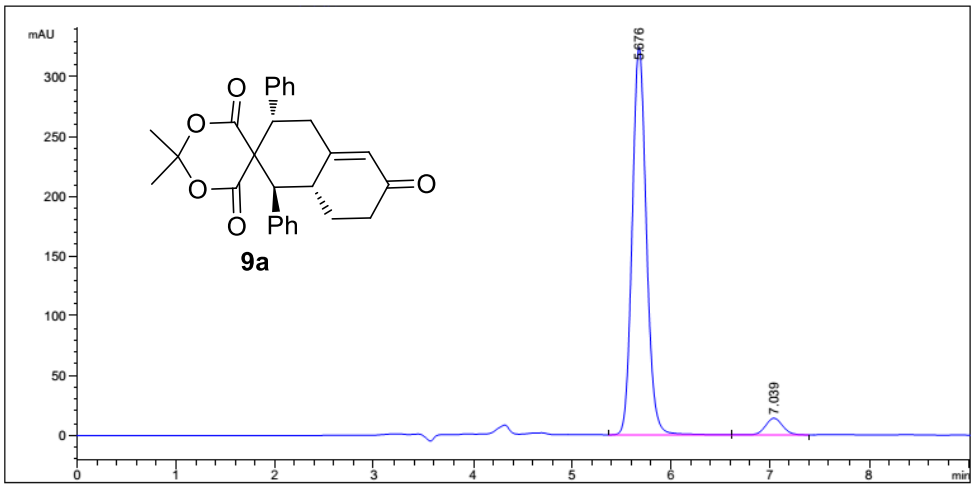
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
5.661	BV R	0.13	10.9090	94.3806	0.8767
6.653	BB	0.16	1026.0026	10670.6846	99.1233
			Totals:	10765.0651	100.0000


7.376
7.350
7.332
7.324
7.314
7.302
7.284
7.266
7.218
7.200
7.103
7.093
6.017
4.120
4.091
4.086
3.900
3.859
3.822
3.813
2.761
2.722
2.499
2.479
2.465
2.459
2.450
2.438
1.950
1.923
1.385
1.368
1.354
1.338
0.853
0.611
O
Ph
O
O
O
Ph
O
9a
1H NMR (400 MHz, CDCl3)
9.01
2.32
1.04
1.00
1.30
3.87
1.35
2.50
1.33
1.56
3.85
3.56
10.0
9.5
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

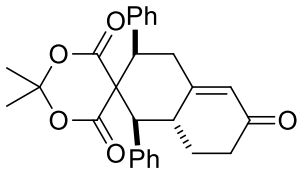

198.609
169.070
168.168
165.610
137.312
135.387
131.564
129.261
128.925
128.727
128.443
128.418
126.044
106.175
77.211
76.999
76.788
61.888
52.096
47.147
37.974
35.685
32.927
28.576
28.472
O
Ph
O
O
O
Ph
O
9a
13C NMR (150 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.647	BB	0.1390	2746.13501	303.55014	70.2001
2	6.984	VB	0.1789	1165.73511	99.53756	29.7999

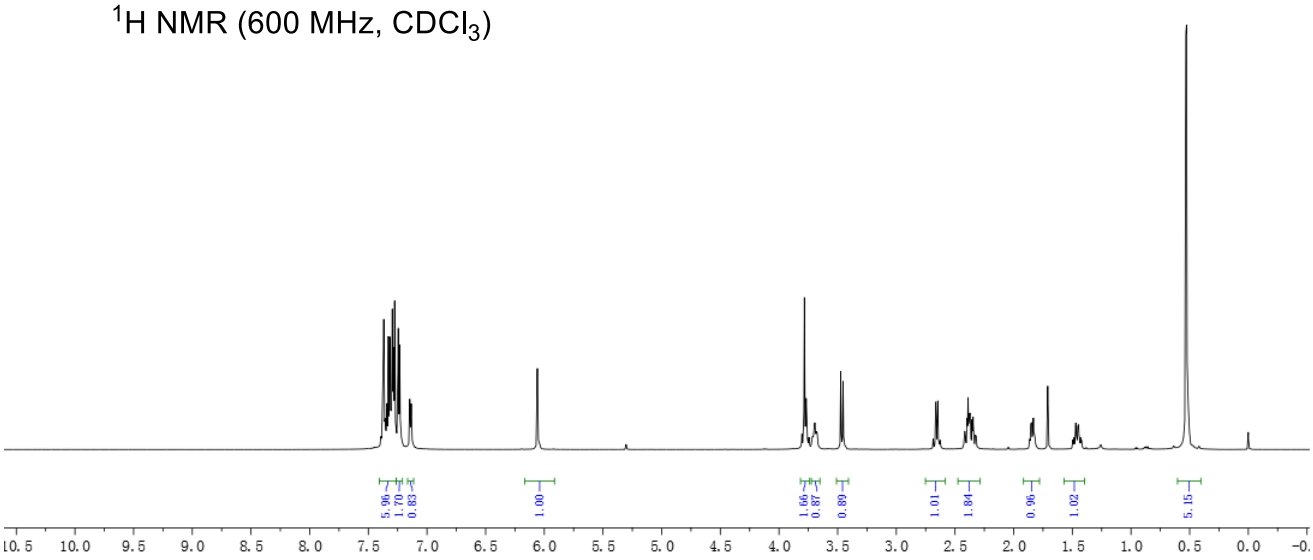


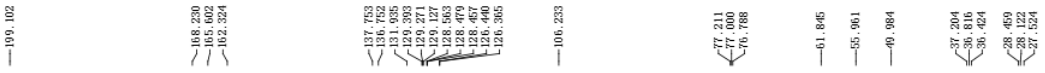
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.676	BB	0.1541	3241.03516	325.18967	95.0646
2	7.039	BB	0.1869	168.26280	13.99102	4.9354

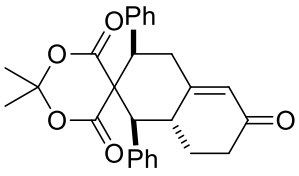


9a′

^{1}H NMR (600 MHz, $CDCl_3$)

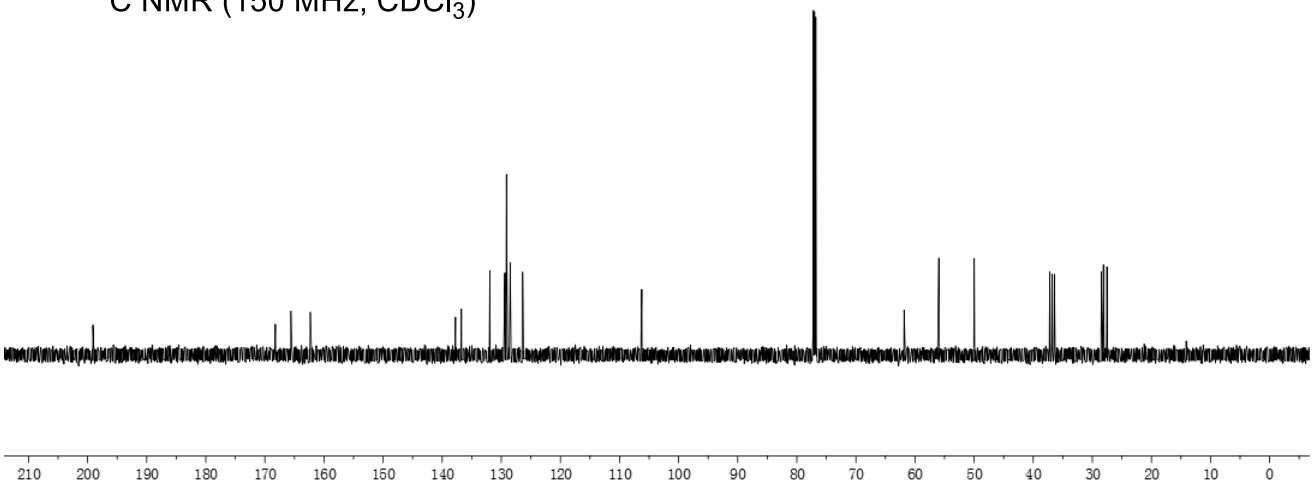


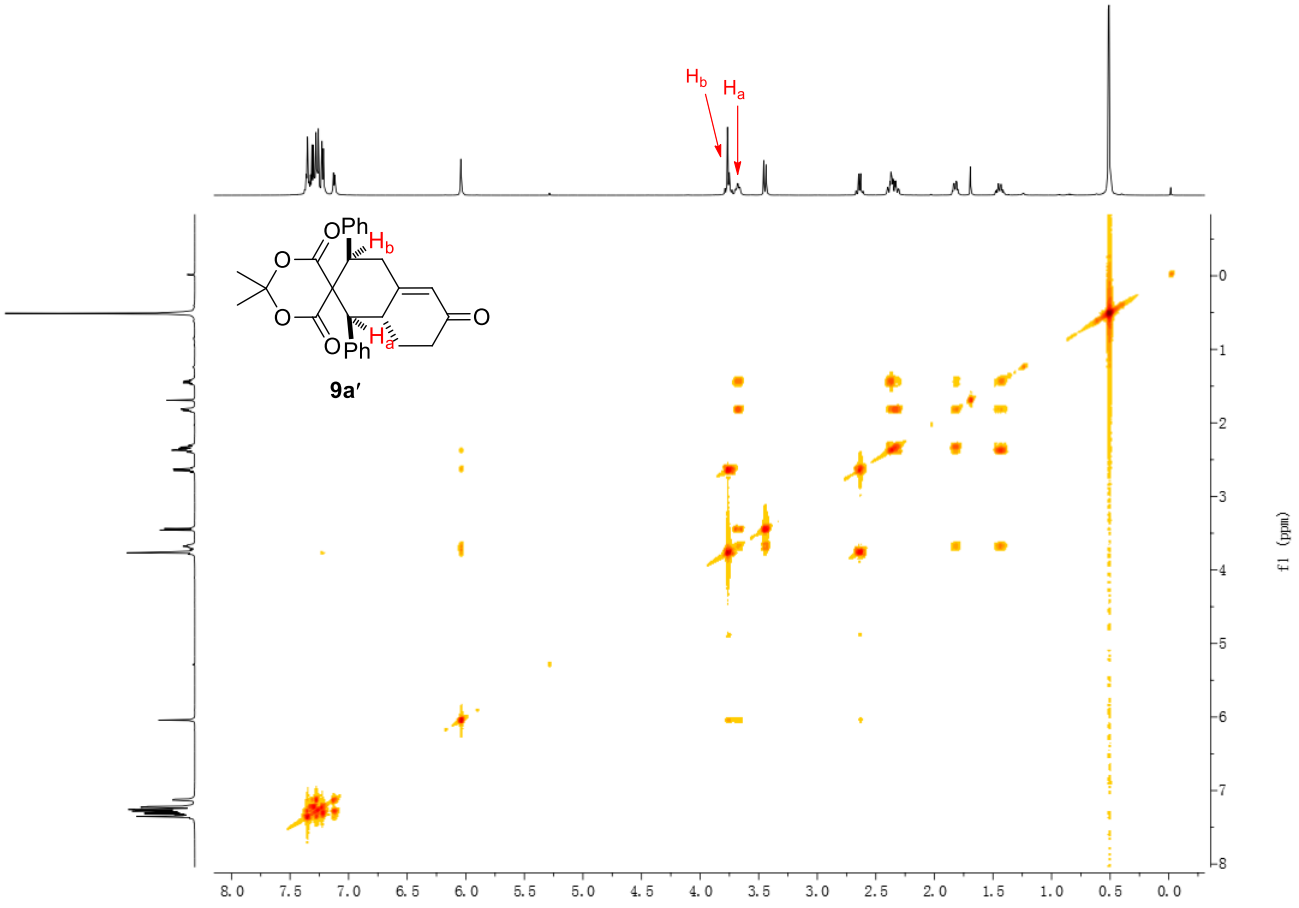


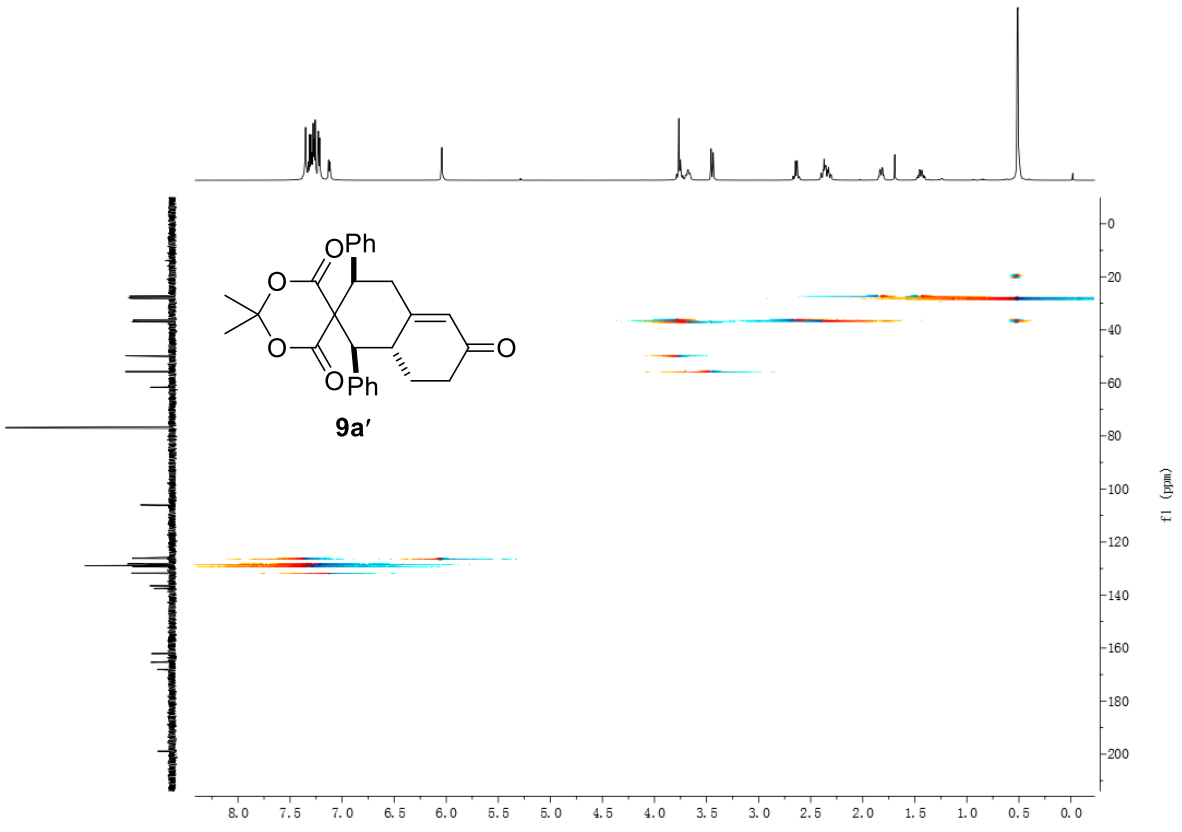


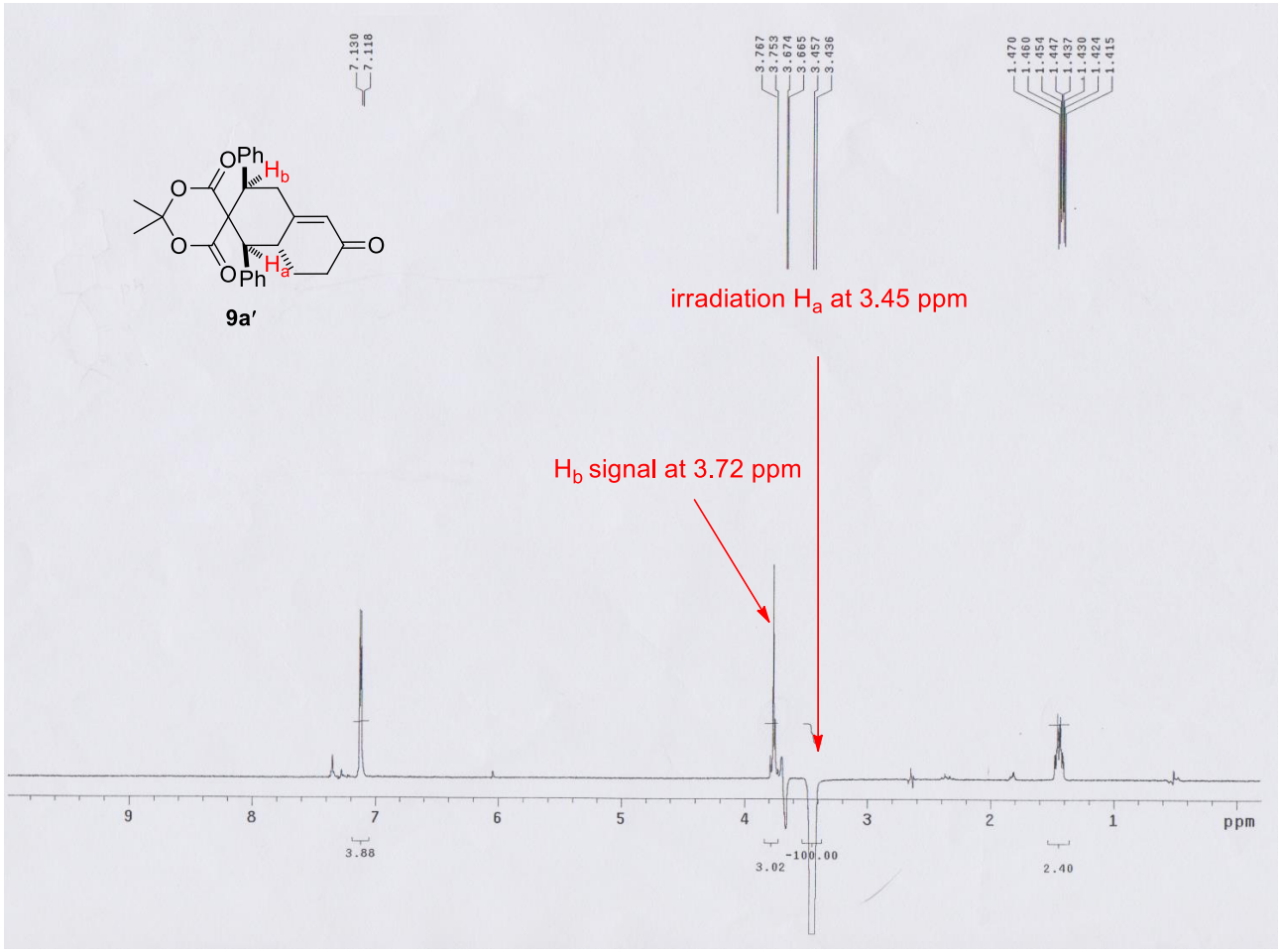
9a′

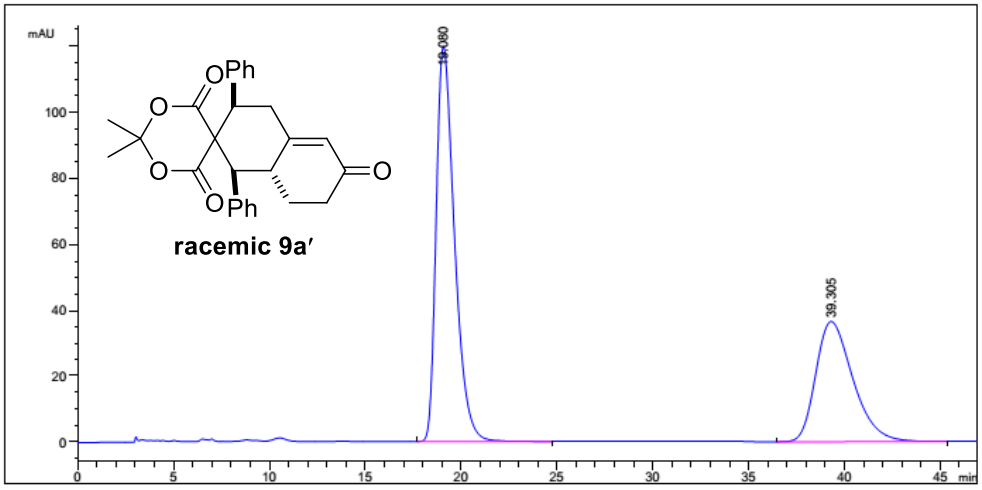
^{13}C NMR (150 MHz, $CDCl_3$)



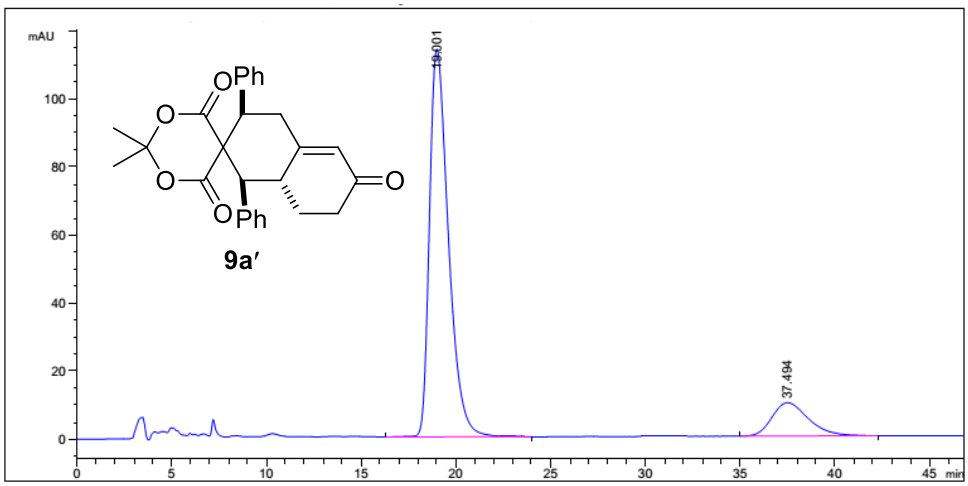

Hb
Ha
OPh
Hb
O
O
O
Ha
OPh
O
9a′
f1 (ppm)


OPh
O
O
O
OPh
9a′
f1 (ppm)

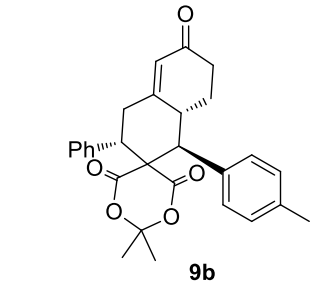

7.130
7.118
3.767
3.753
3.674
3.665
3.457
3.436
1.470
1.460
1.454
1.447
1.437
1.430
1.424
1.415
O
Ph
Hb
O
O
O
Ha
Ph
O
9a′
irradiation Ha at 3.45 ppm
Hb signal at 3.72 ppm
9
8
7
6
5
4
3
2
1
ppm
3.88
3.02
-100.00
2.40



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	19.080	BB	1.0203	7950.53418	119.58485	61.8737
2	39.305	BB	2.0504	4899.08301	36.33877	38.1263

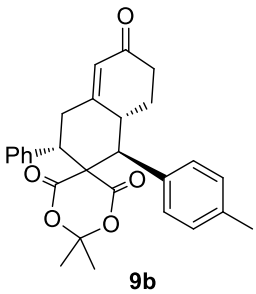


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	19.001	BB	1.0602	7906.10889	113.90681	85.7360
2	37.494	BB	1.9346	1315.34875	9.80685	14.2640



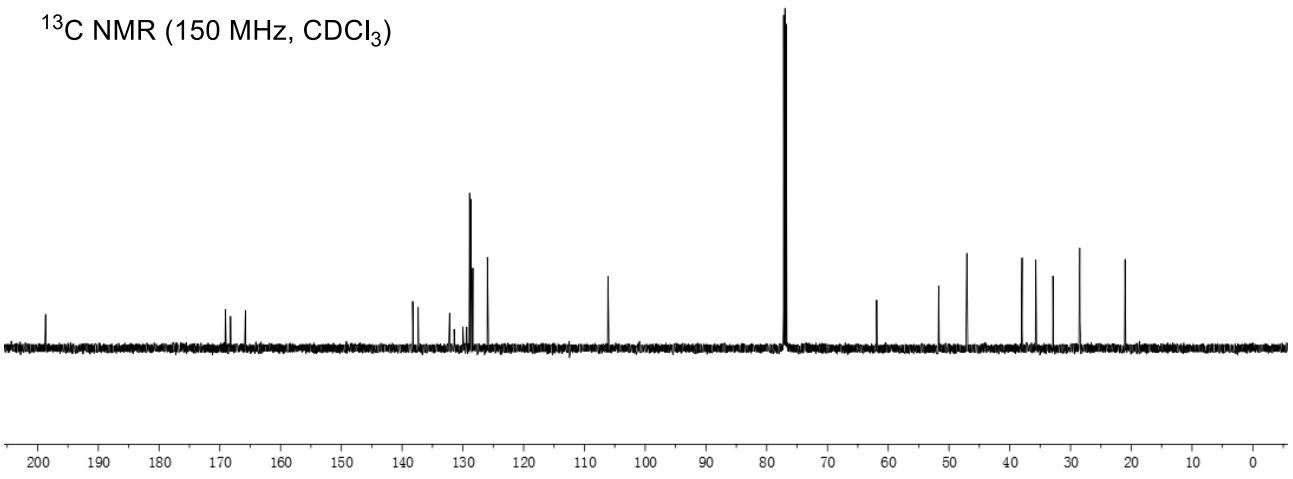
9b

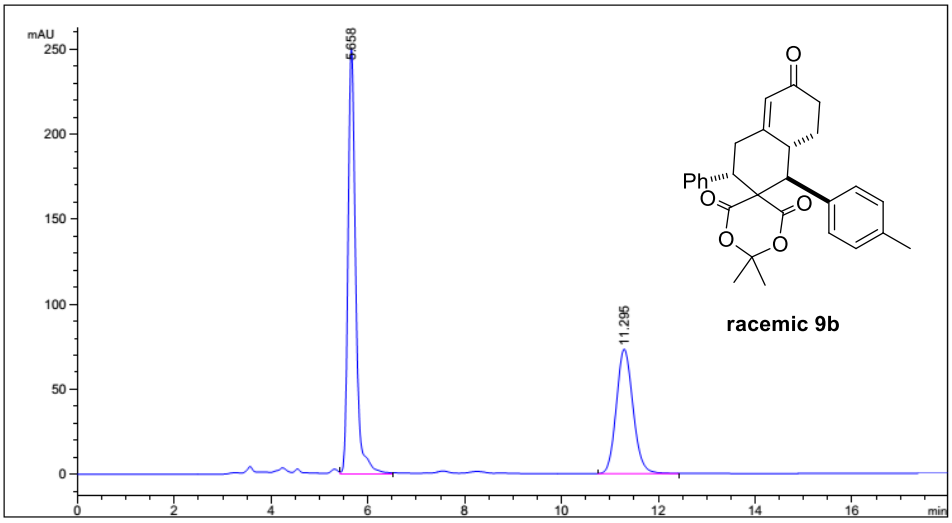
^{1}H NMR (400 MHz, $CDCl_3$)



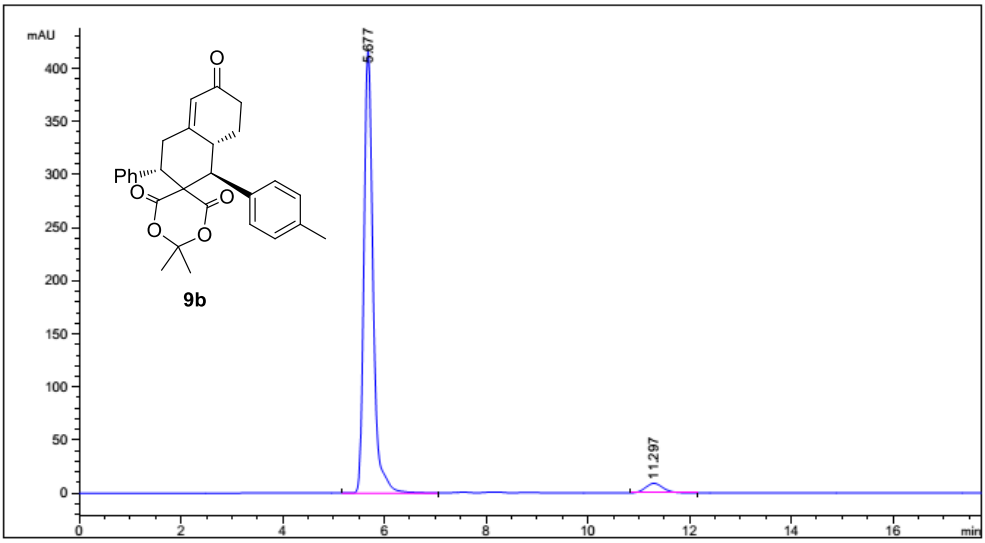
9b

^{13}C NMR (150 MHz, $CDCl_3$)

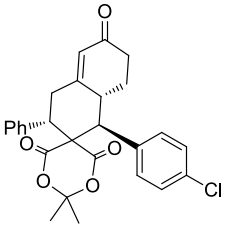




Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.658	VB	0.1693	2746.05273	249.32515	61.0393
2	11.295	BB	0.3727	1752.77698	73.15991	38.9607

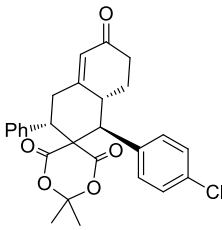


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.677	VV	0.1864	5191.50586	416.02377	95.8501
2	11.297	BB	0.3793	224.76997	9.16524	4.1499



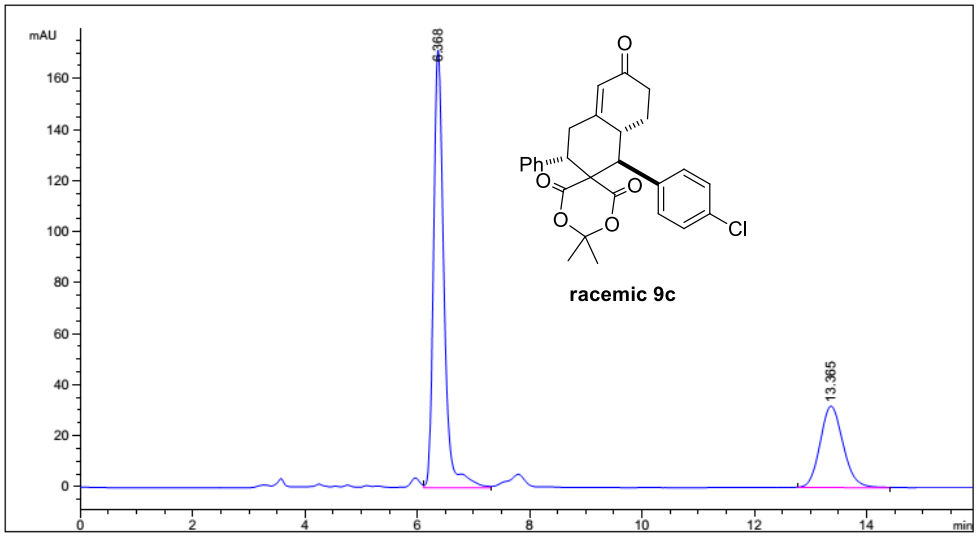
9c

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

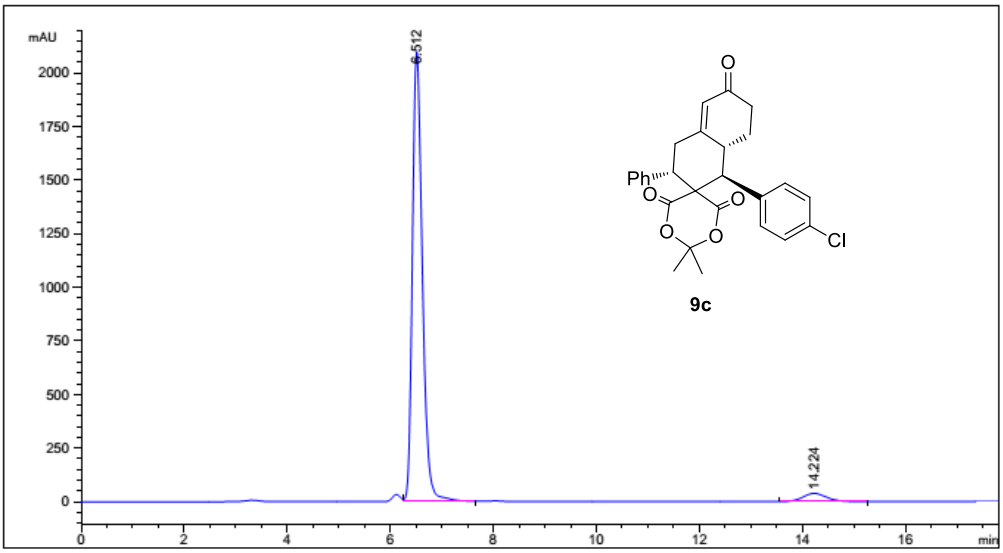


9c

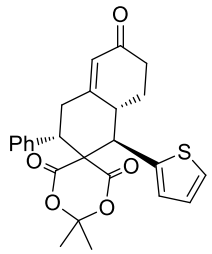
^{13}C NMR (150 MHz, $CDCl_3$)



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.368	VV	0.1969	2201.41406	170.86607	70.8325
2	13.365	BB	0.4420	906.49939	31.92016	29.1675

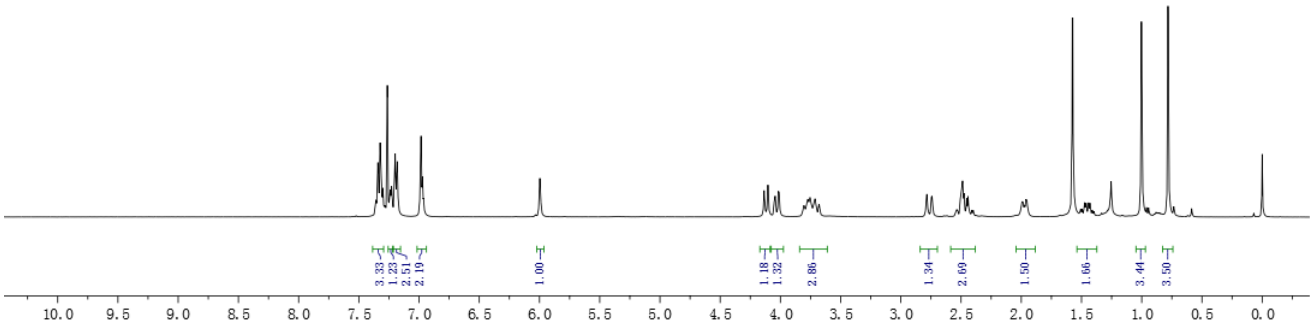


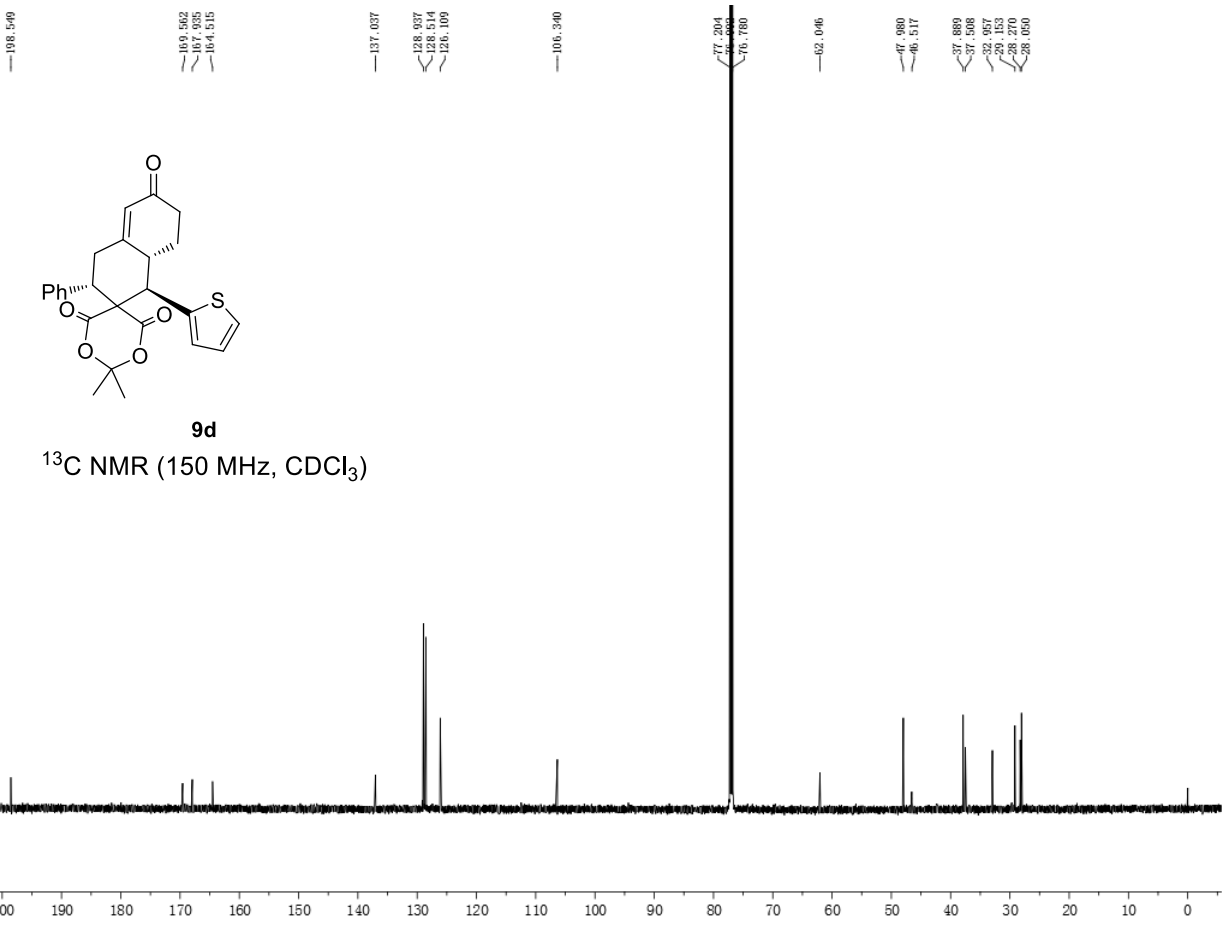
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.512	VV	0.2095	2.82082e4	2094.37256	95.8859
2	14.224	BV	0.4914	1210.29724	38.25651	4.1141



9d

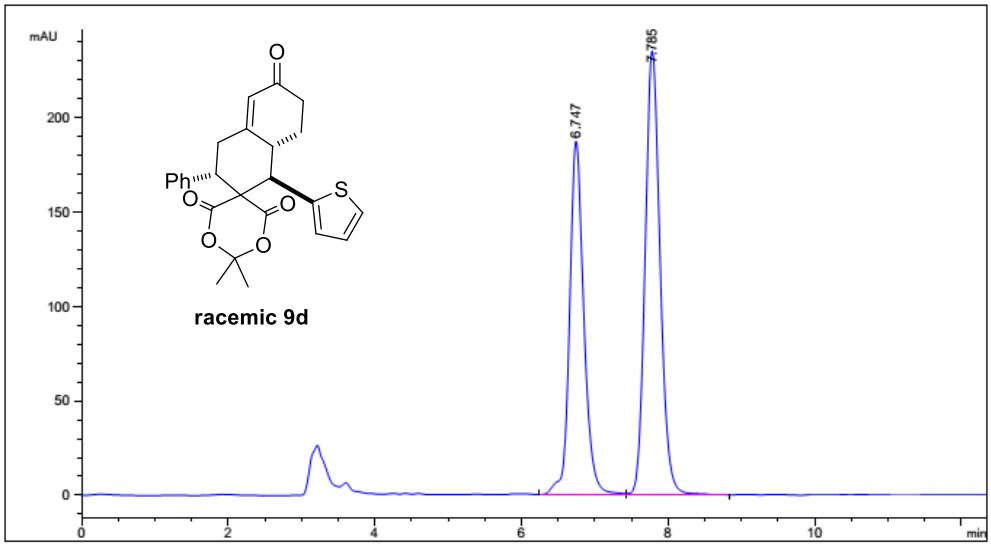
^{1}H NMR (400 MHz, $CDCl_3$)



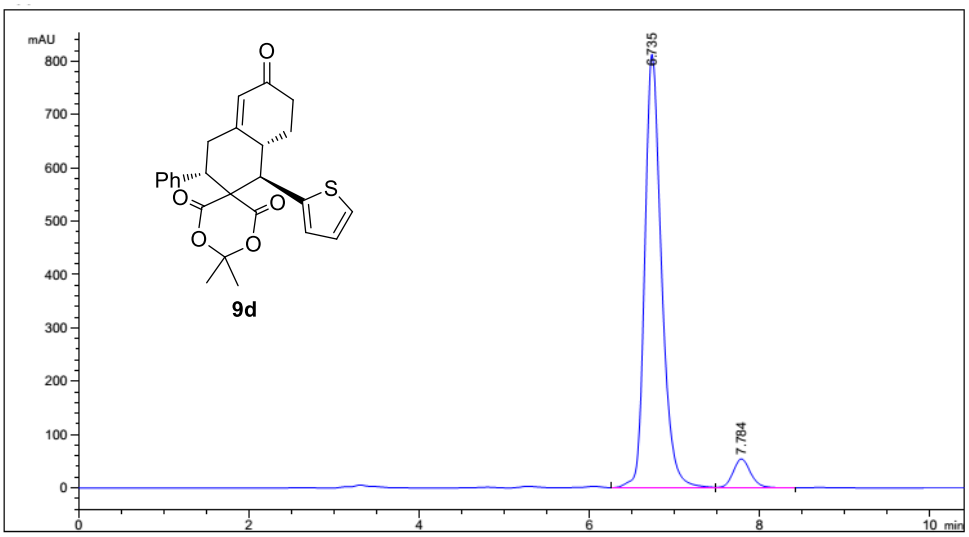


9d

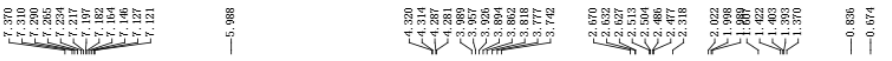
^{13}C NMR (150 MHz, $CDCl_3$)

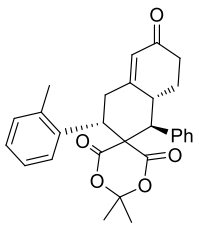


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.747	VV	0.2127	2572.70728	187.29831	43.3563
2	7.785	VB	0.2252	3361.16357	234.91786	56.6437



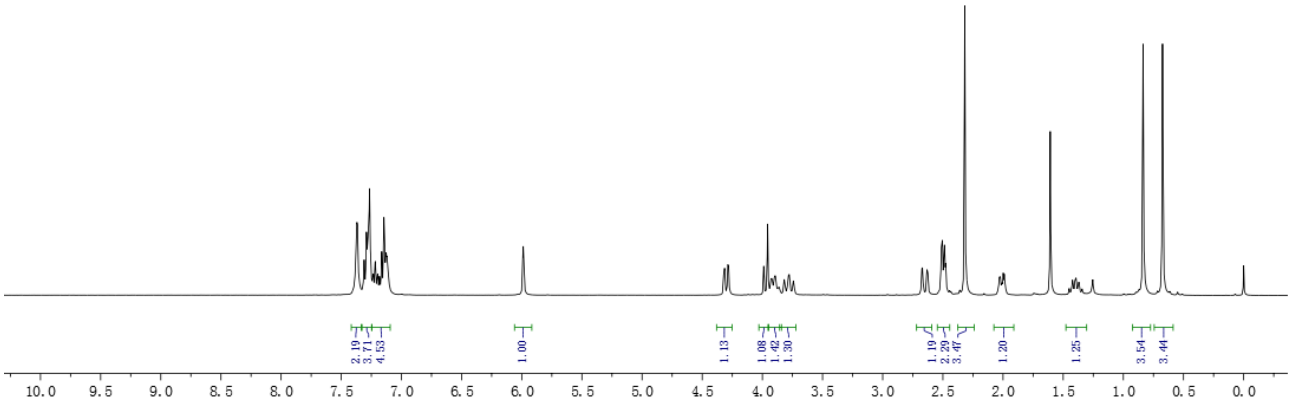
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.735	VV	0.2064	1.11109e4	810.89532	93.2566
2	7.784	VV	0.2295	803.43097	54.71624	6.7434

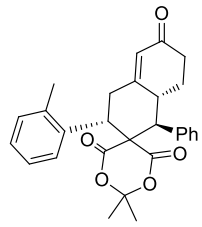




9e

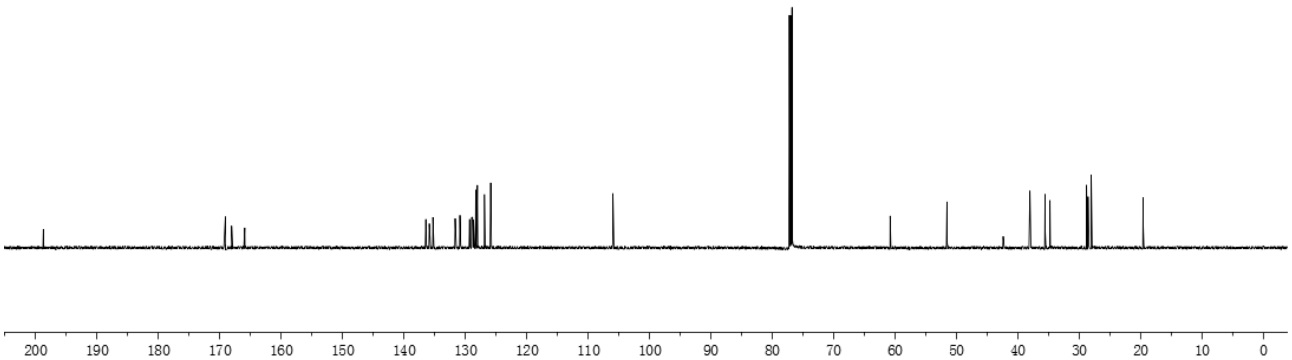
^{1}H NMR (400 MHz, $CDCl_3$)

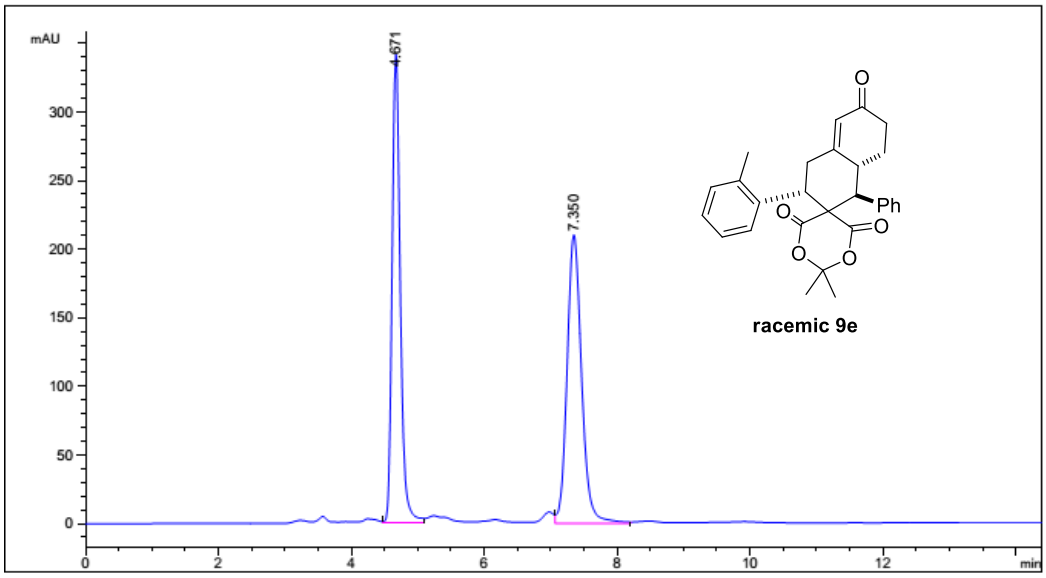




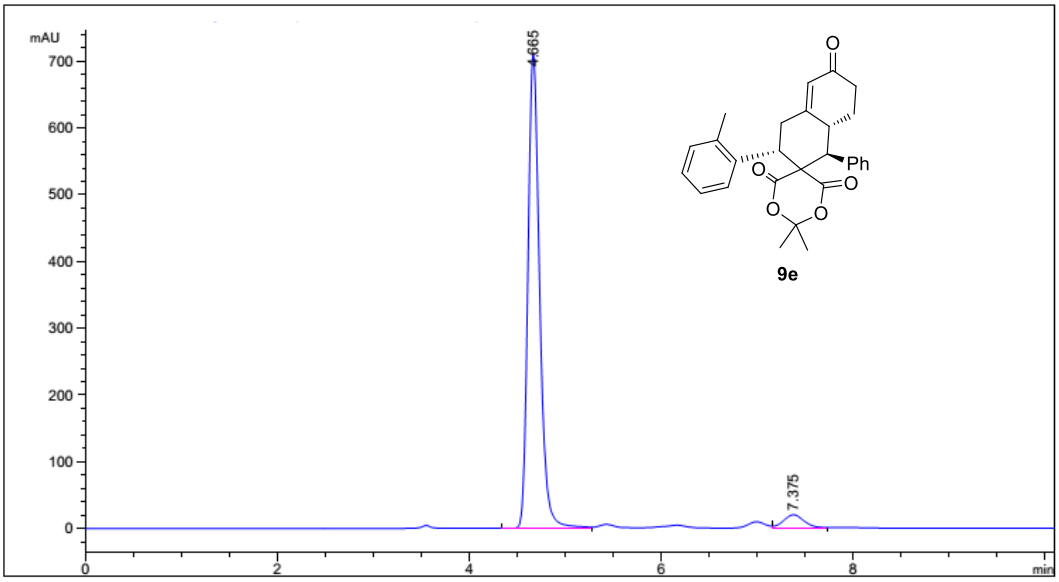
9e

^{13}C NMR (150 MHz, $CDCl_3$)

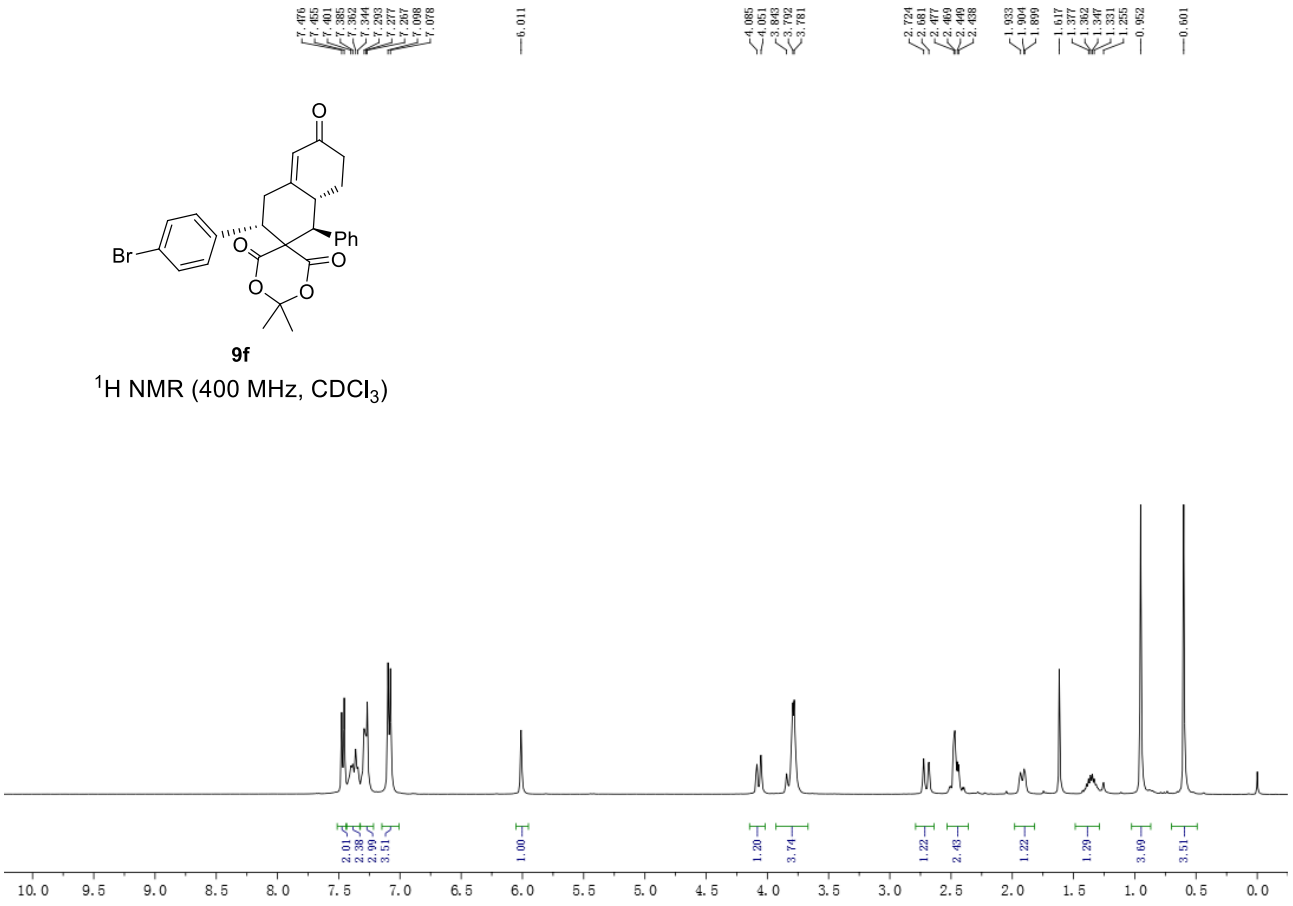




Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.671	VV	0.1356	2940.31421	340.63187	48.0116
2	7.350	VV	0.2351	3183.85913	210.02843	51.9884

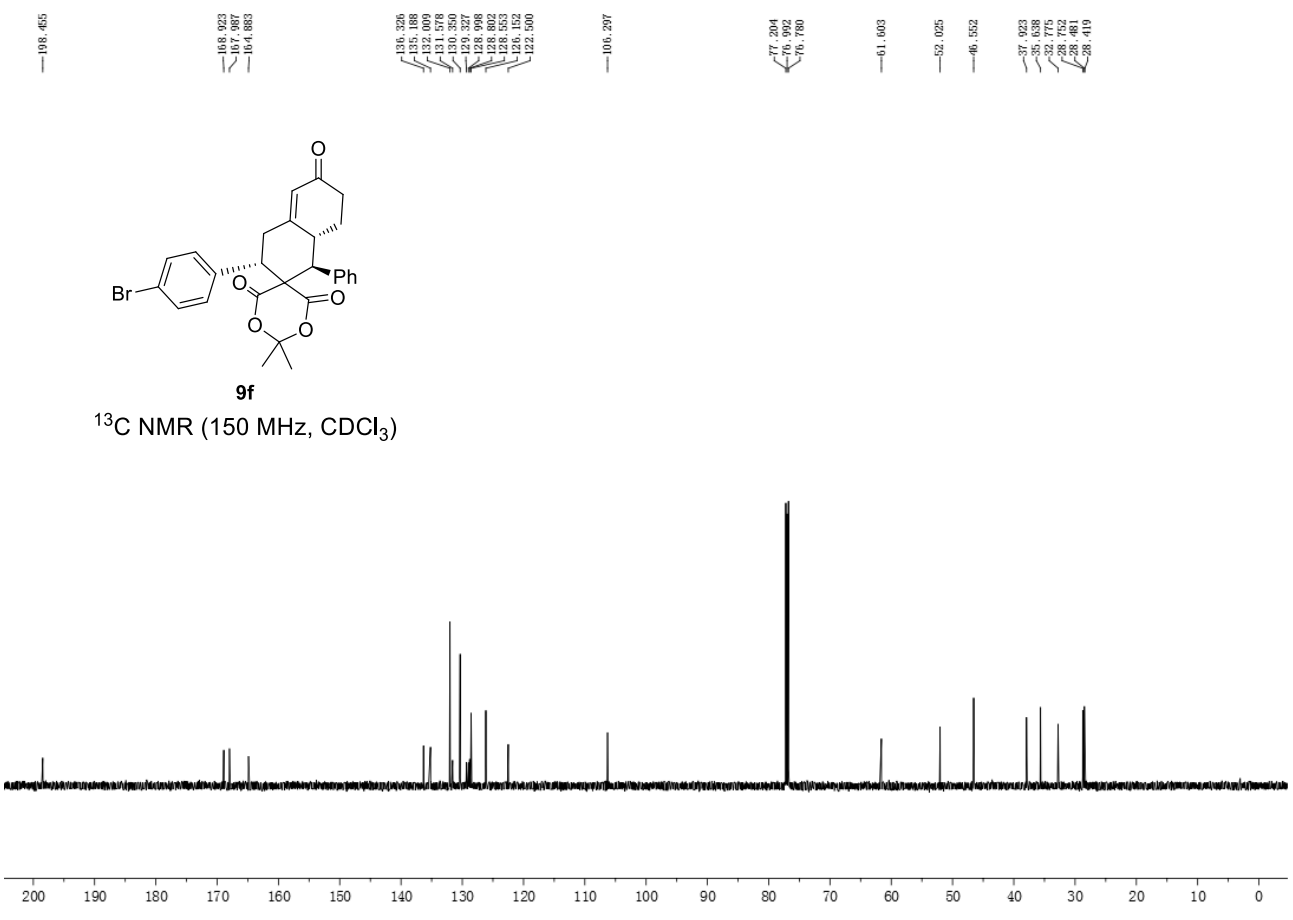


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.665	VV	0.1282	6003.98291	706.70465	95.0484
2	7.375	VV	0.2371	312.78119	20.39864	4.9516



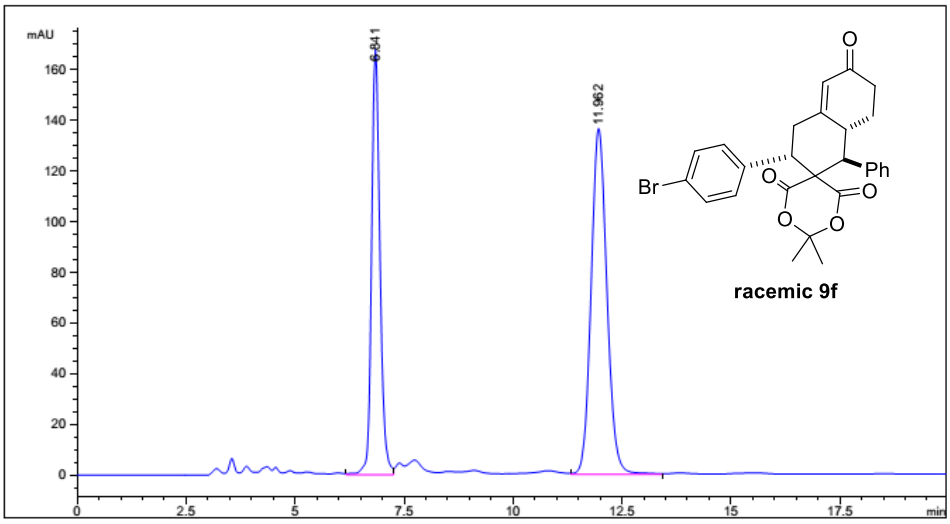
9f

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

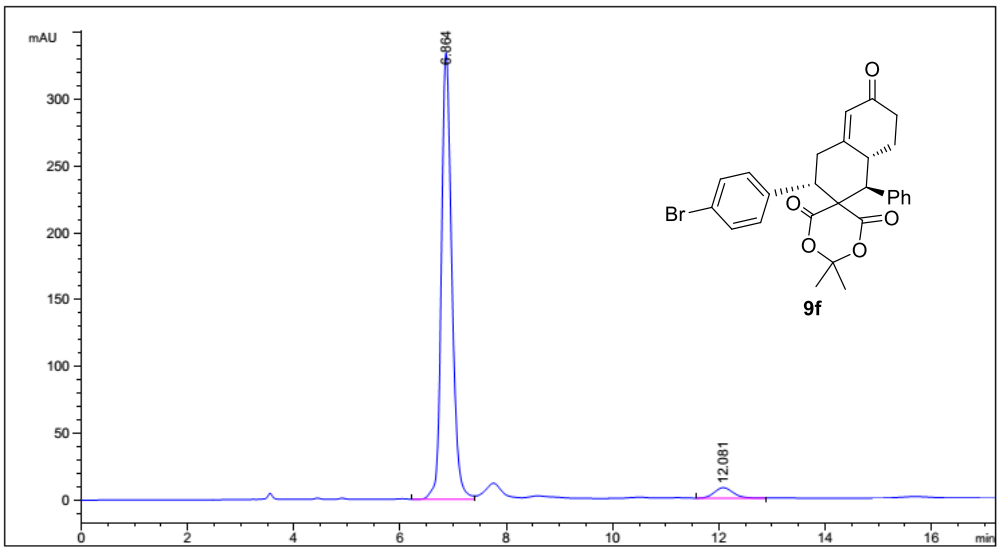


9f

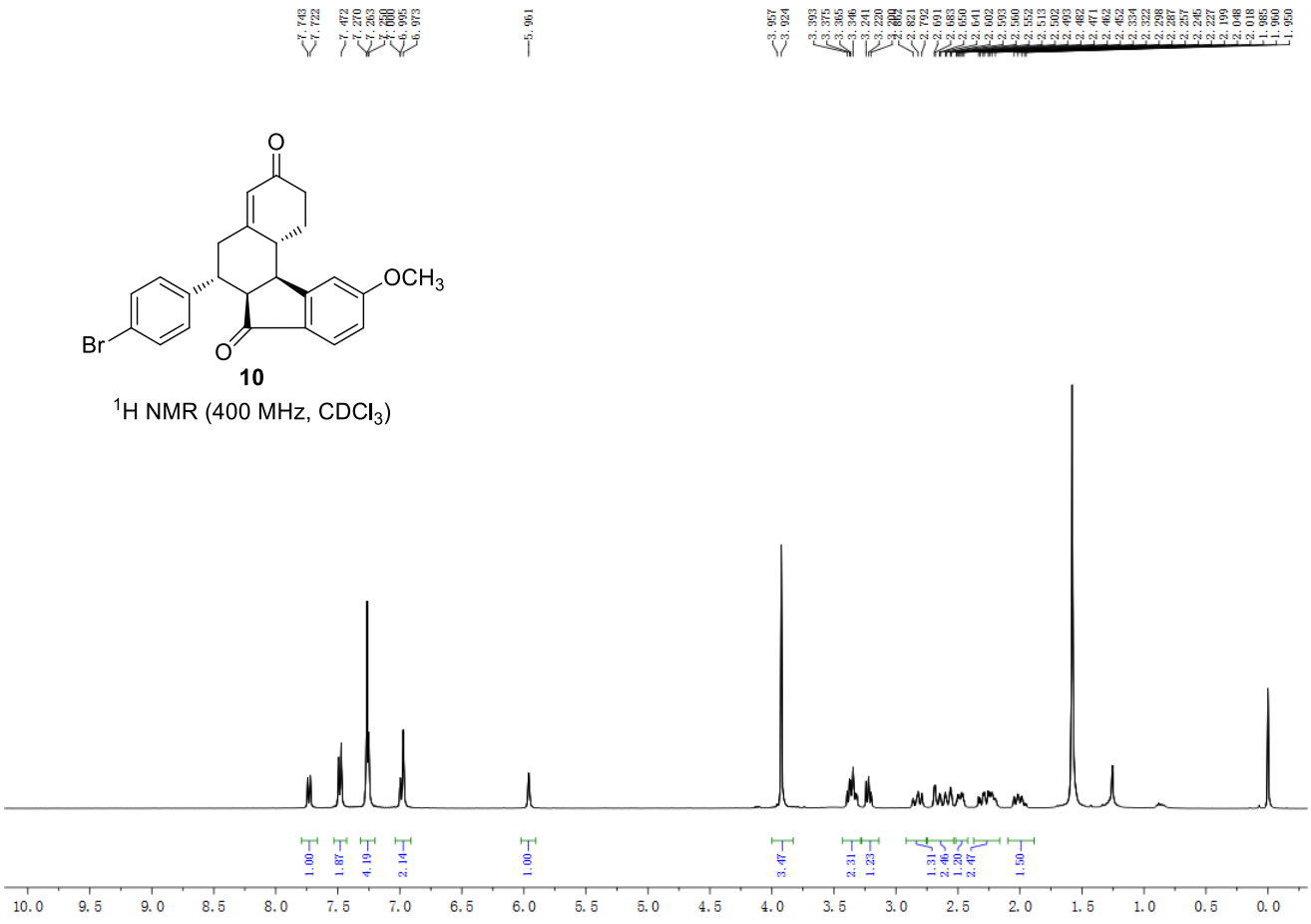
^{13}C NMR (150 MHz, $CDCl_3$)

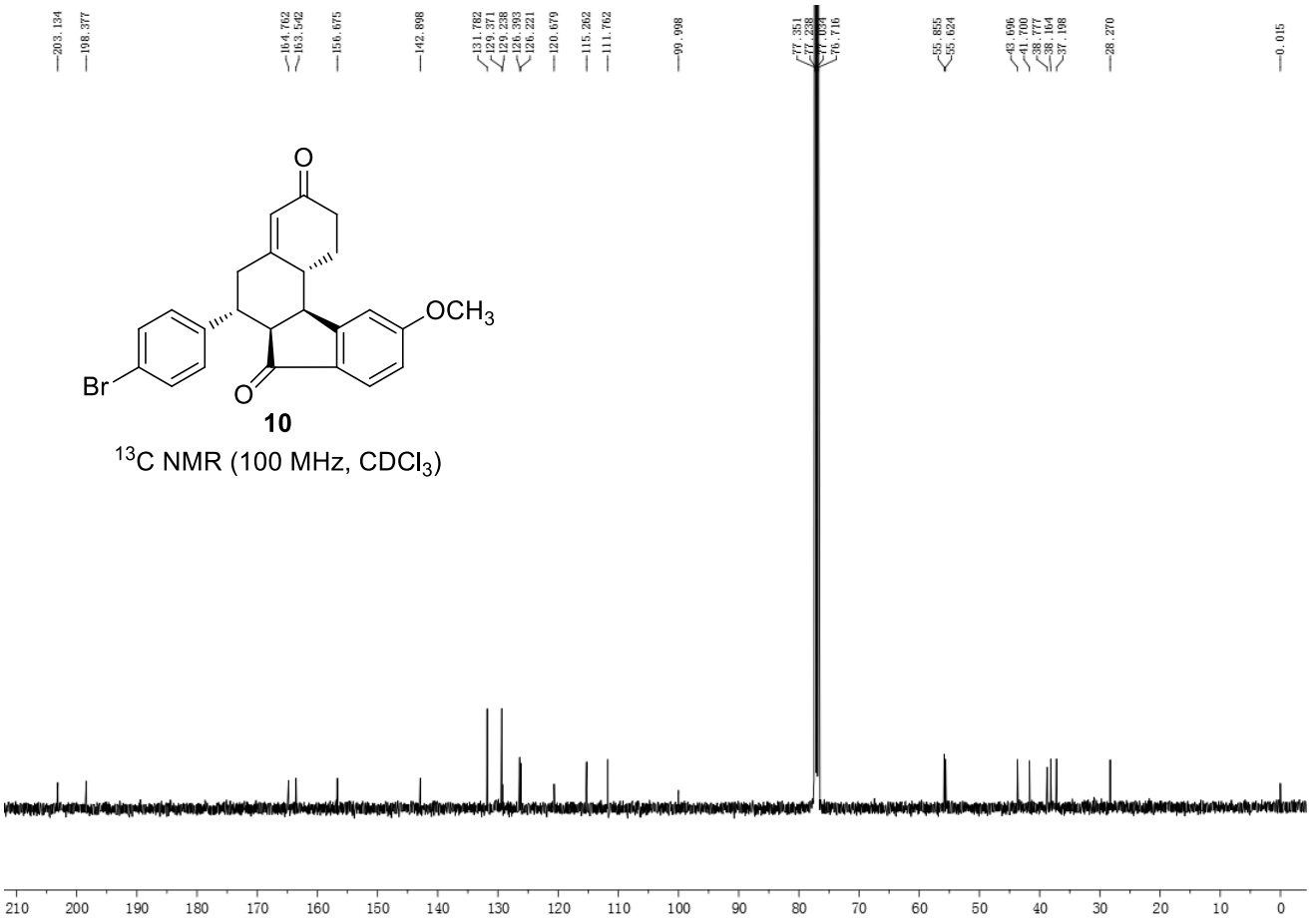


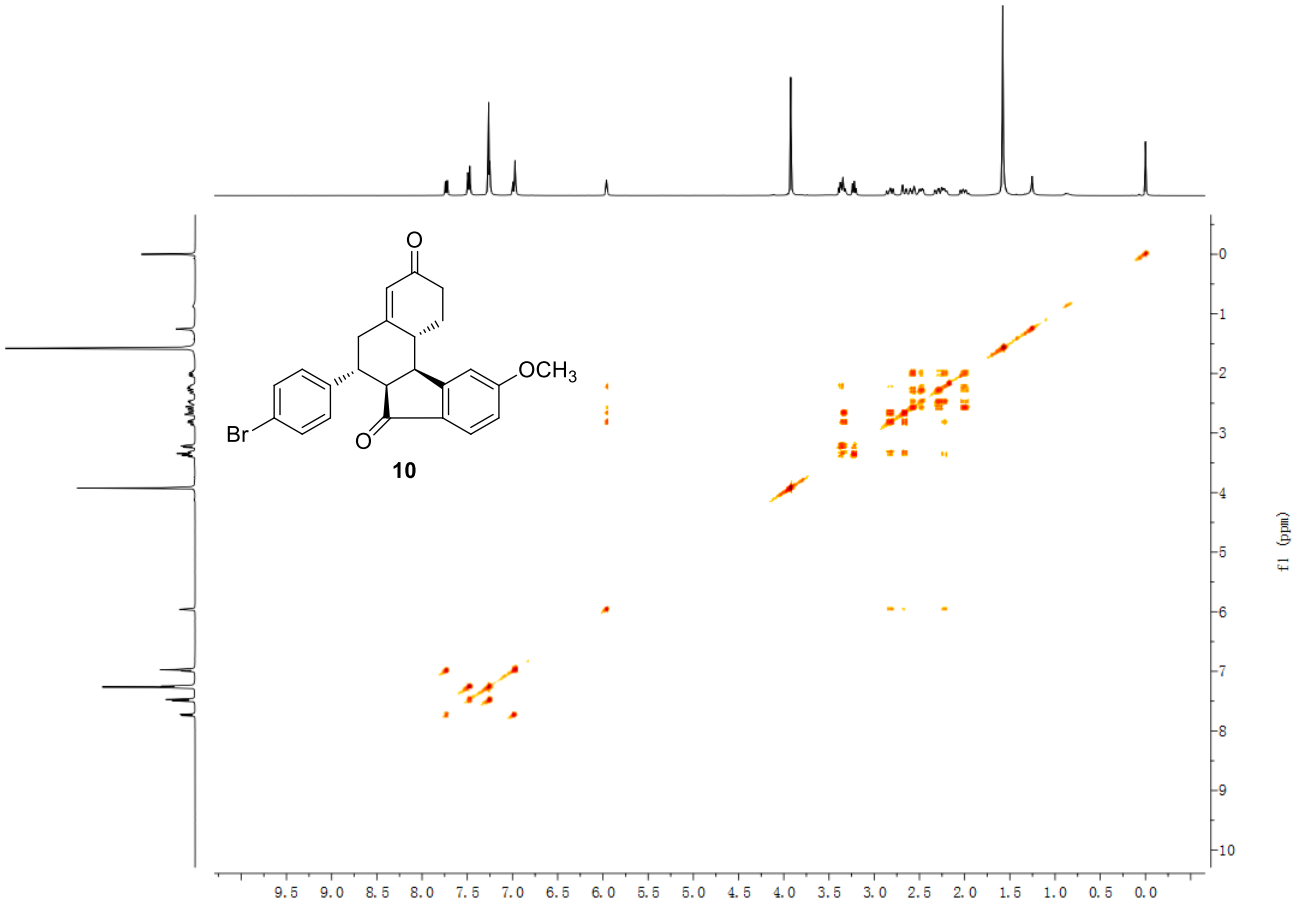
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.841	VV	0.2084	2240.45972	167.62436	39.5158
2	11.962	VB	0.3922	3429.32397	136.46996	60.4842

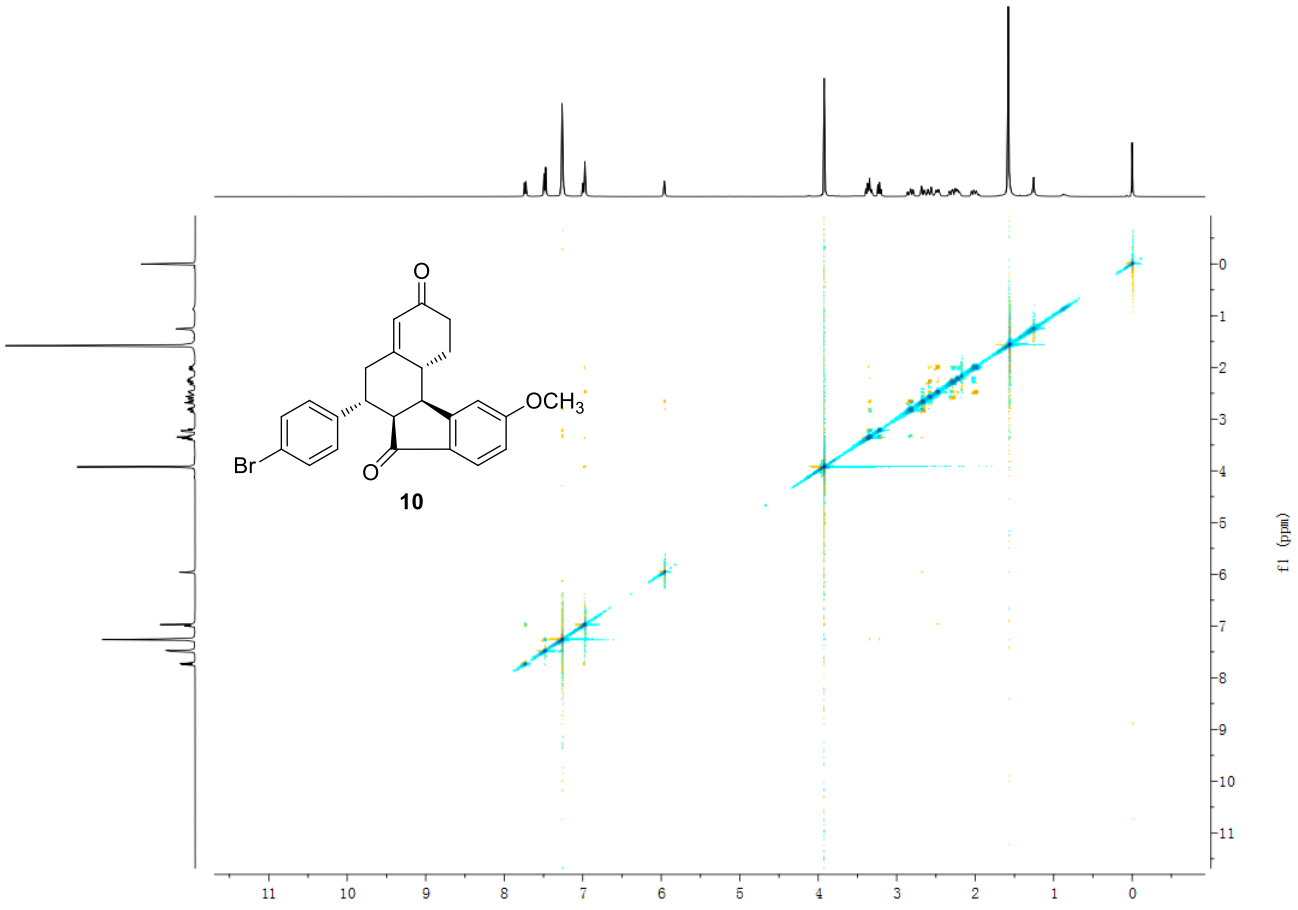


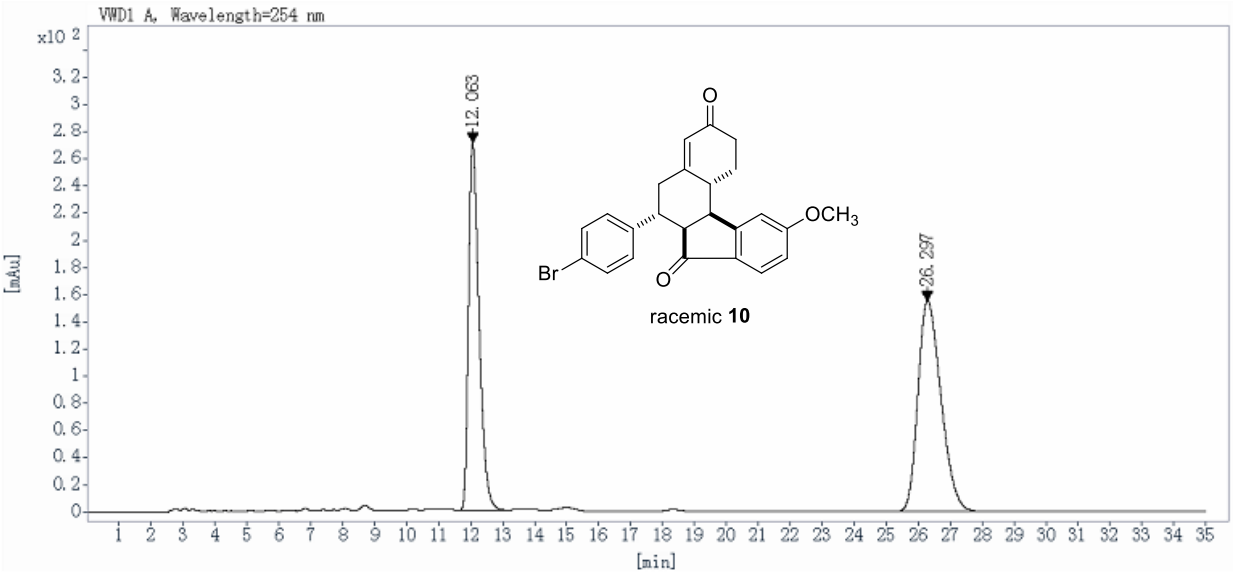
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.864	VV	0.2107	4524.21143	333.45462	95.6211
2	12.081	VB	0.3948	207.18402	8.01437	4.3789


O
OCH3
Br
O
10
1H NMR (400 MHz, CDCl3)

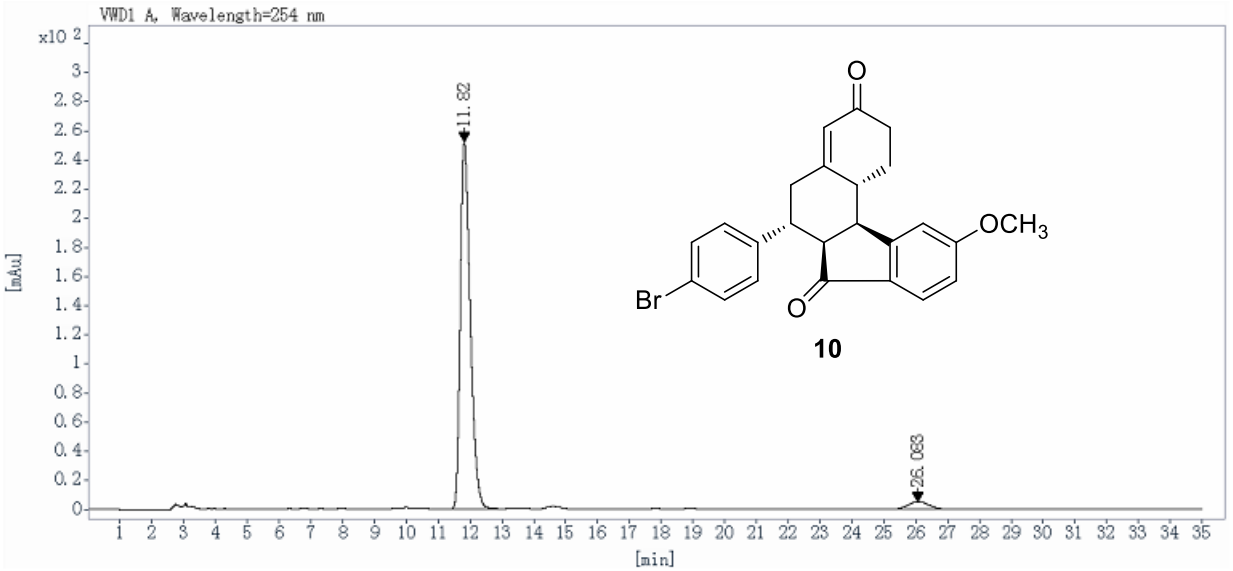

O
OCH3
Br
O
10
13C NMR (100 MHz, CDCl3)


O
OCH3
Br
O
10
f1 (ppm)

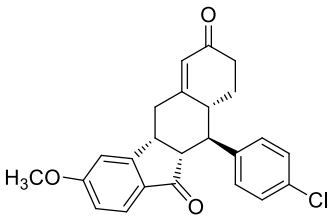

O
OCH3
Br
O
10
f1 (ppm)



Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
12.063	BB	0.35	270.3929	6187.1377	44.3254
26.297	BB	0.78	155.2601	7771.2944	55.6746

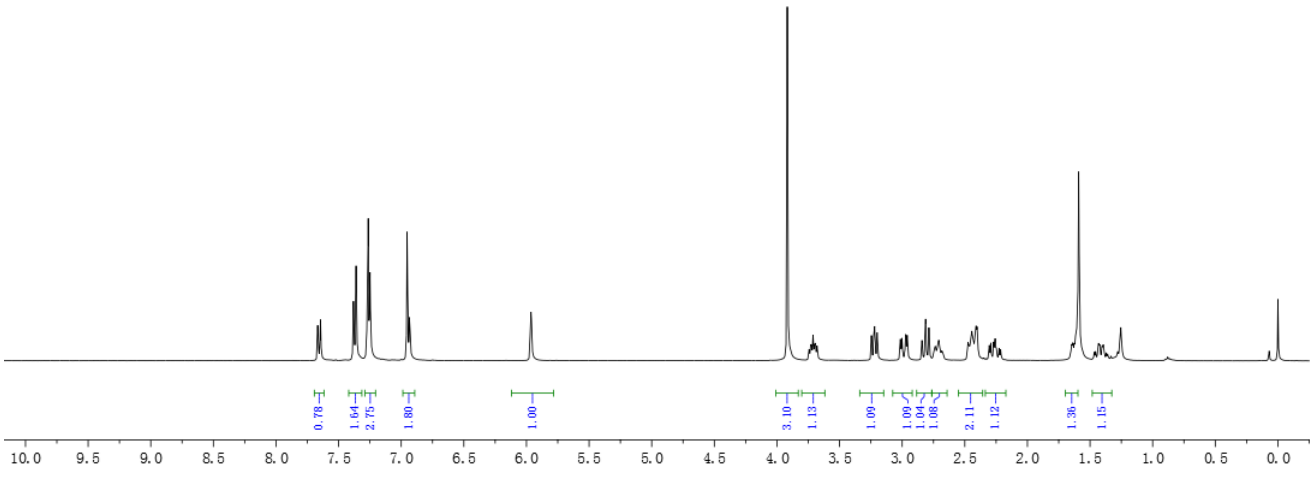


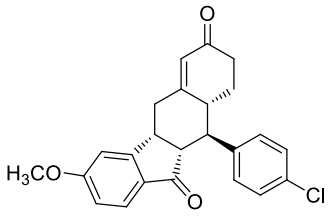
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
11.820	BB	0.34	251.5718	5480.2964	95.5602
26.083	BB	0.71	5.3512	254.6207	4.4398



11

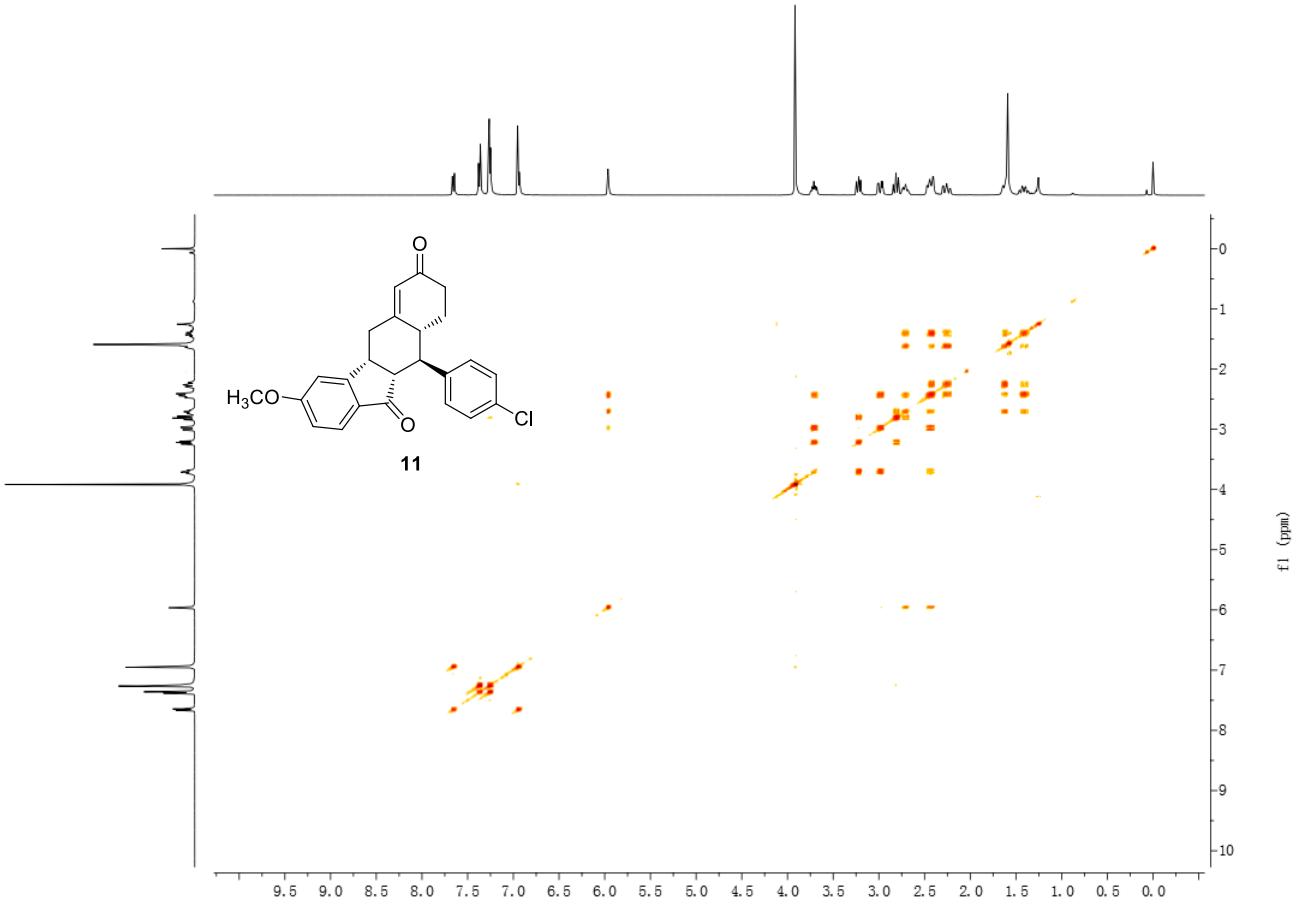
^{1}H NMR (400 MHz, $CDCl_3$)

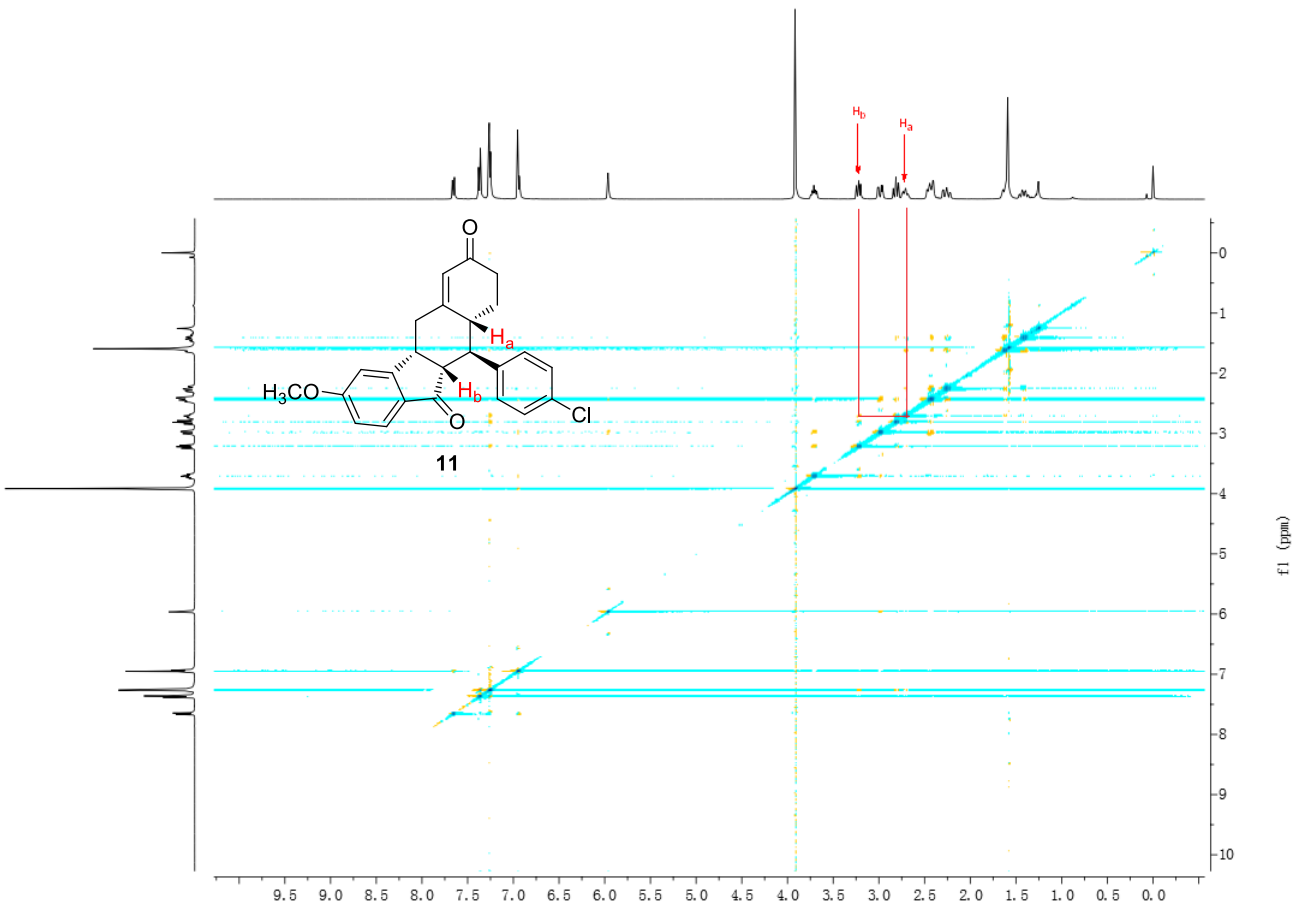


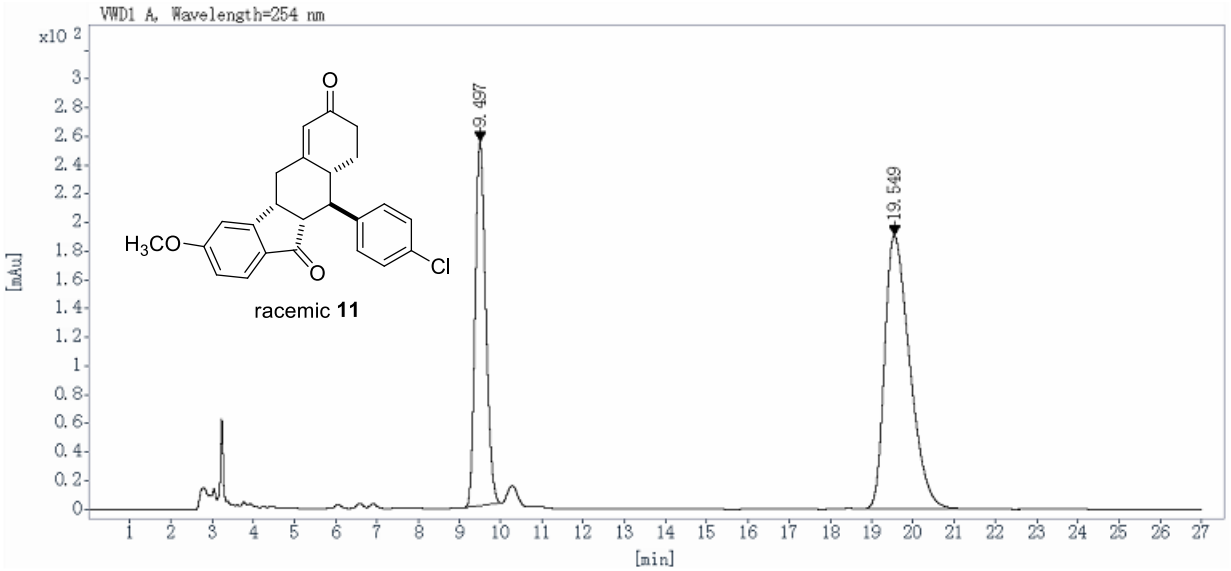


11

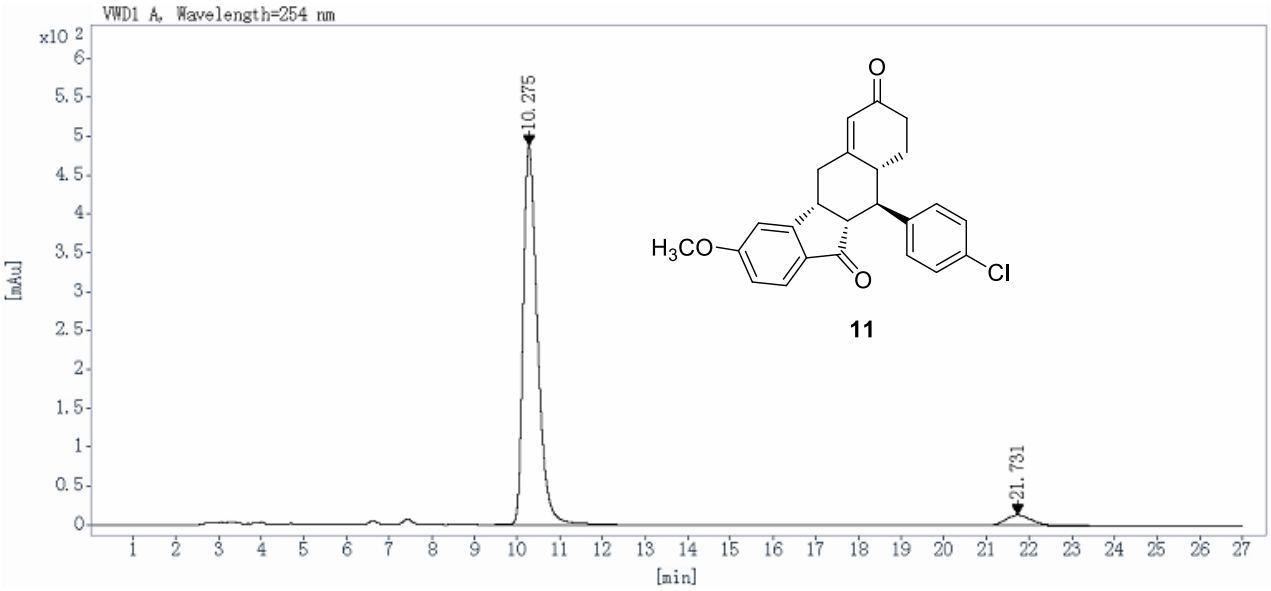
^{13}C NMR (150 MHz, $CDCl_3$)


O
H3CO
O
Cl
11
f1 (ppm)

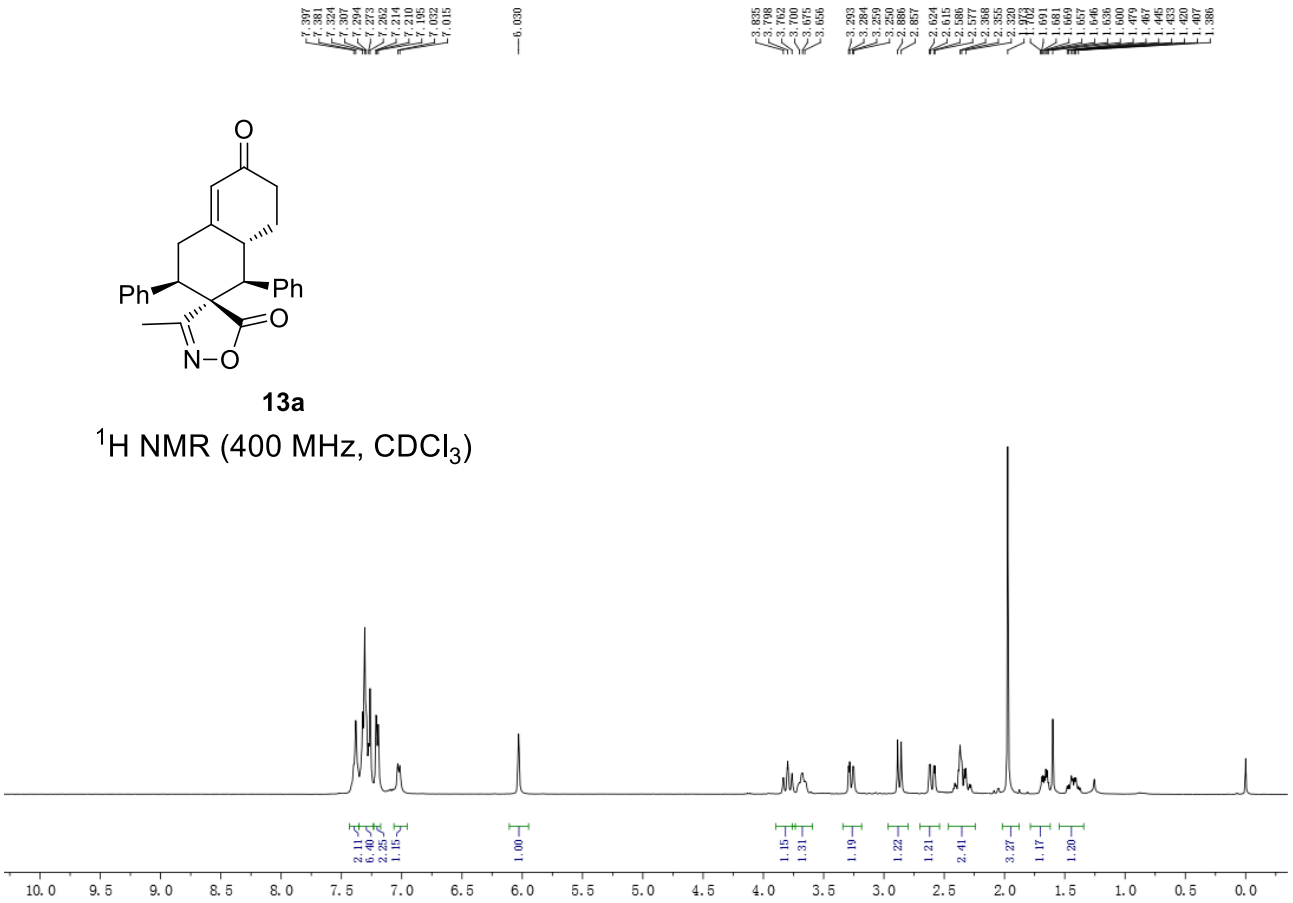

Hb
Ha
O
Ha
H3CO
Hb
O
Cl
11
f1 (ppm)



Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
9.497	BB	0.28	253.9139	4542.3184	36.0857
19.549	BB	0.65	190.6351	8045.2803	63.9143

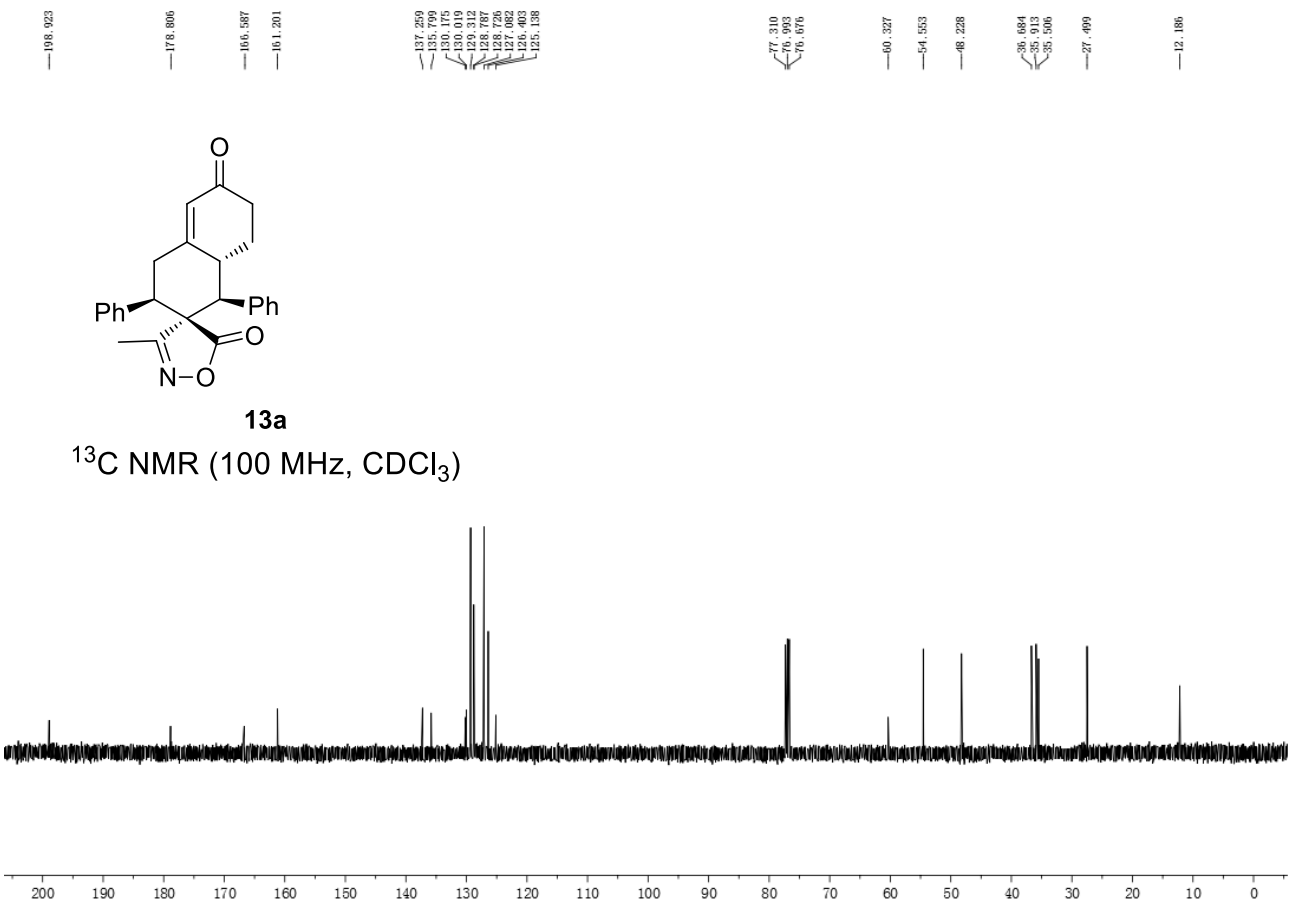


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
10.275	VB R	0.36	487.5642	11372.3848	95.1565
21.731	BB	0.66	13.3807	578.8610	4.8435



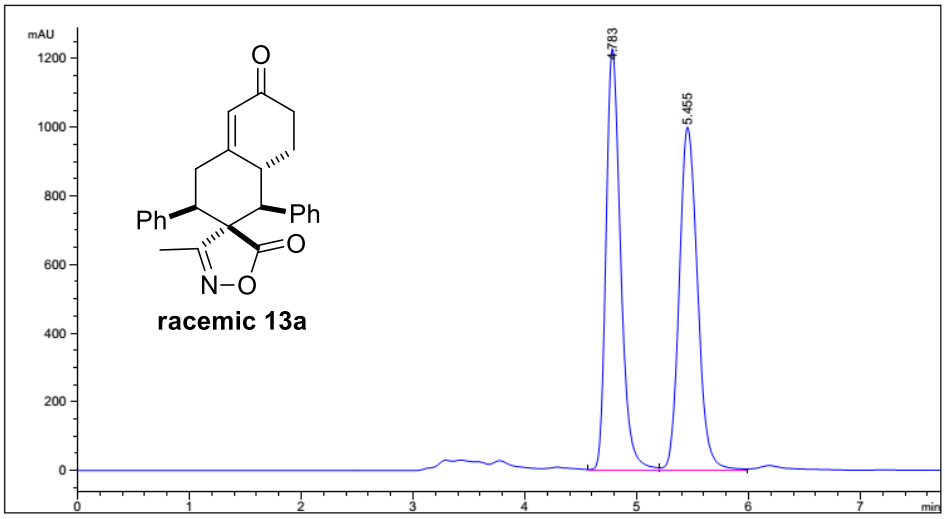
13a

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

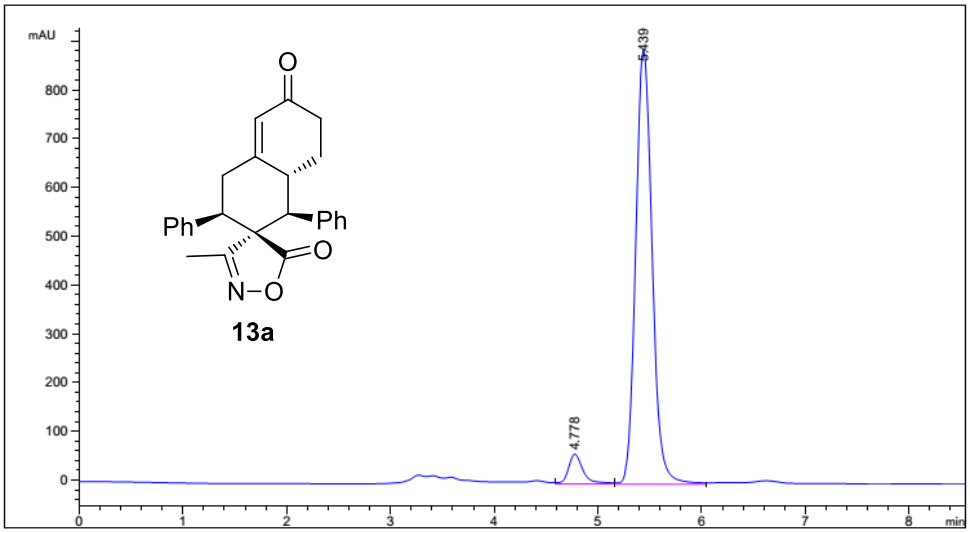


13a

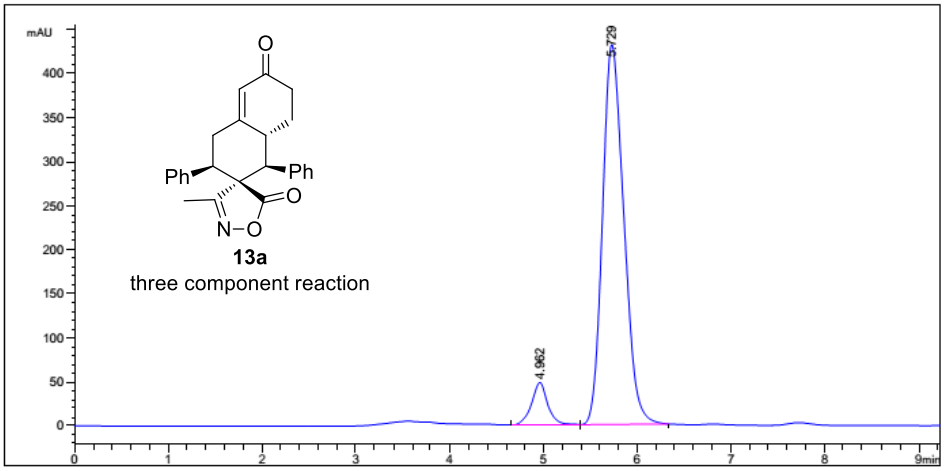
^{13}C NMR (100 MHz, $CDCl_3$)



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.783	VV	0.1352	1.11308e4	1224.12451	49.4623
2	5.455	VV	0.1799	1.13728e4	995.65851	50.5377



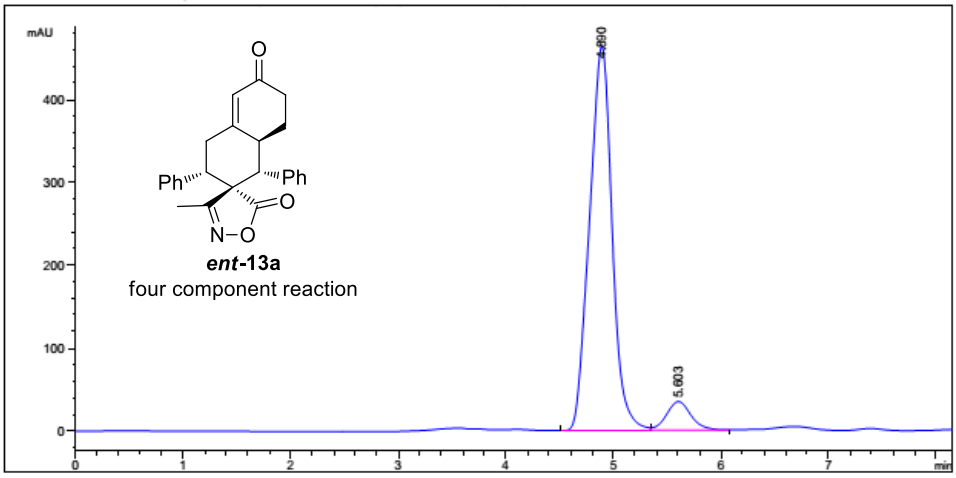
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.778	VV	0.1506	603.46765	60.85759	4.6852
2	5.439	VV	0.1695	9787.82813	887.32831	95.3148



13a

three component reaction

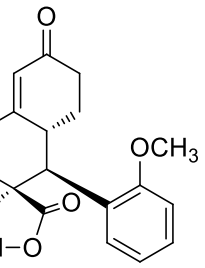
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.962	BB	0.1754	571.49884	47.97073	7.7435
2	5.729	BBA	0.2409	6808.85840	431.39047	92.2565



***ent*-13a**

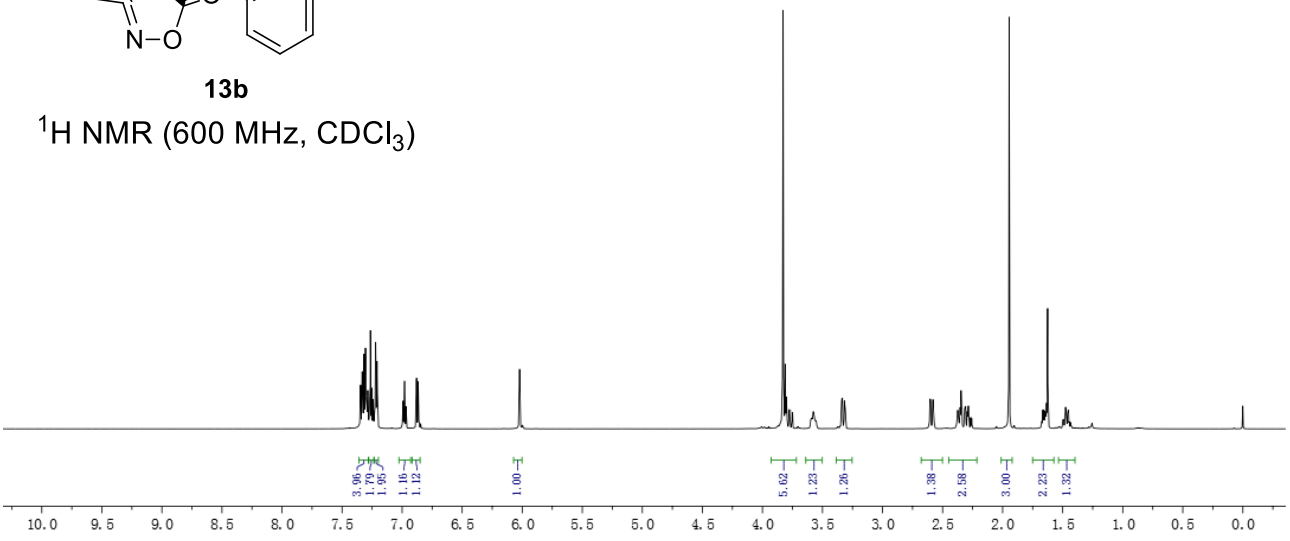
four component reaction

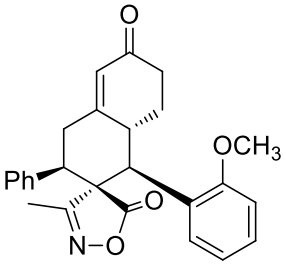
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.890	BV	0.2224	3928.40674	149.06168	91.0186
2	5.603	VBA	0.2418	387.64249	13.84107	8.9814



13b

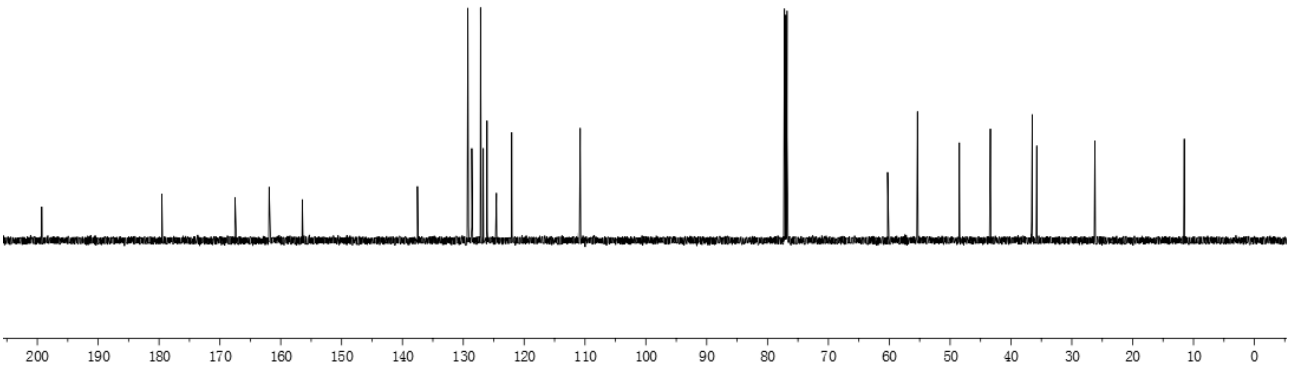
^{1}H NMR (600 MHz, $CDCl_3$)

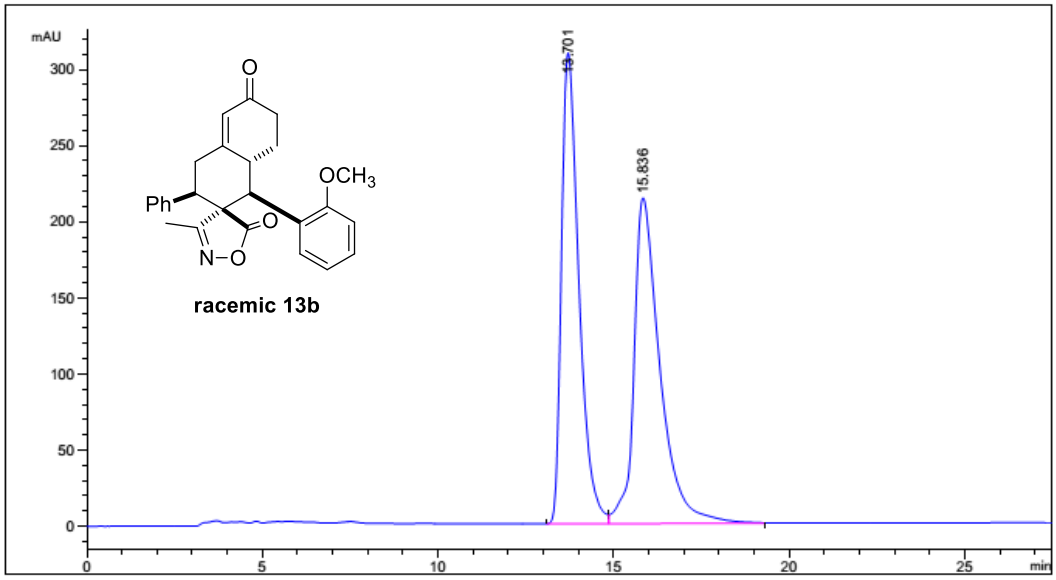




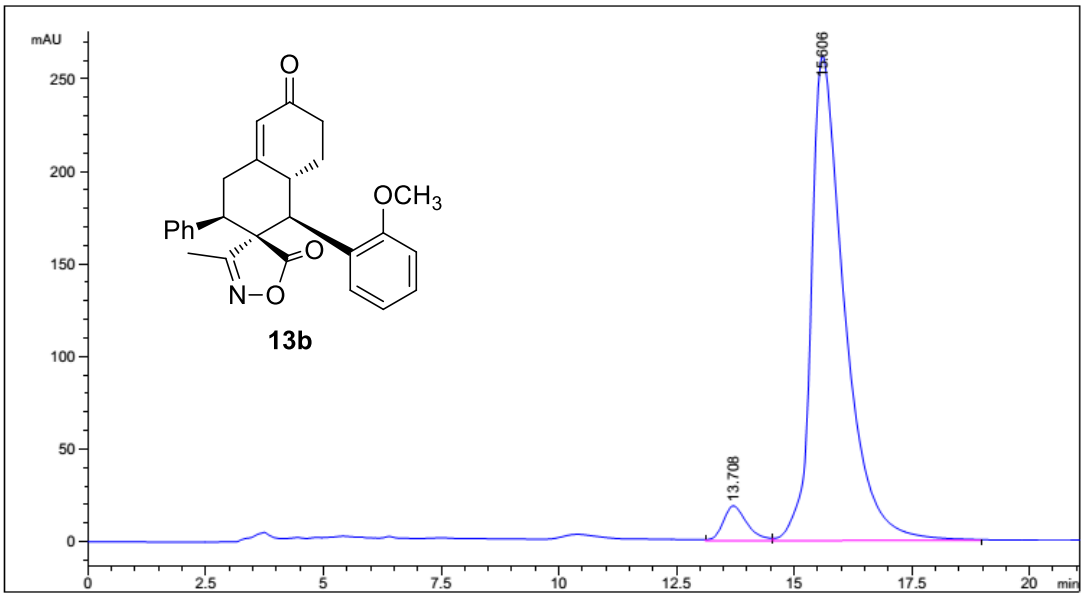
13b

^{13}C NMR (150 MHz, $CDCl_3$)

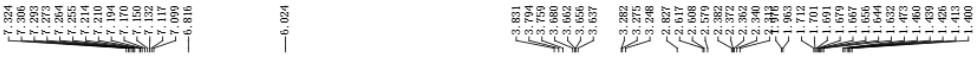


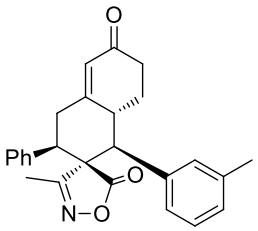


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	13.701	BV	0.5248	1.06660e4	309.15680	49.2718
2	15.836	VB	0.7563	1.09813e4	213.85863	50.7282



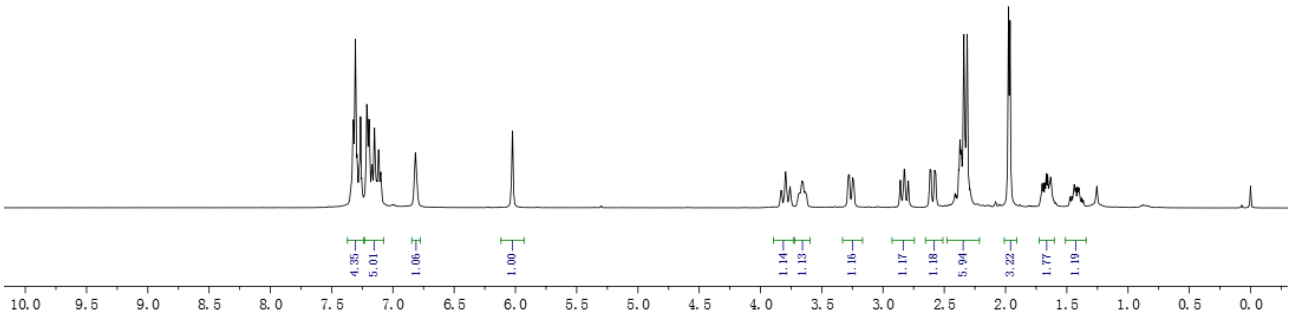
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	13.708	BV	0.5314	661.06262	18.85110	4.8823
2	15.606	VB	0.7251	1.28788e4	261.90662	95.1177

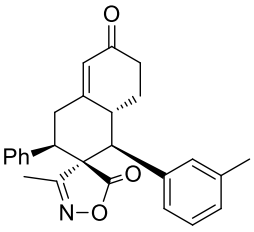




13c

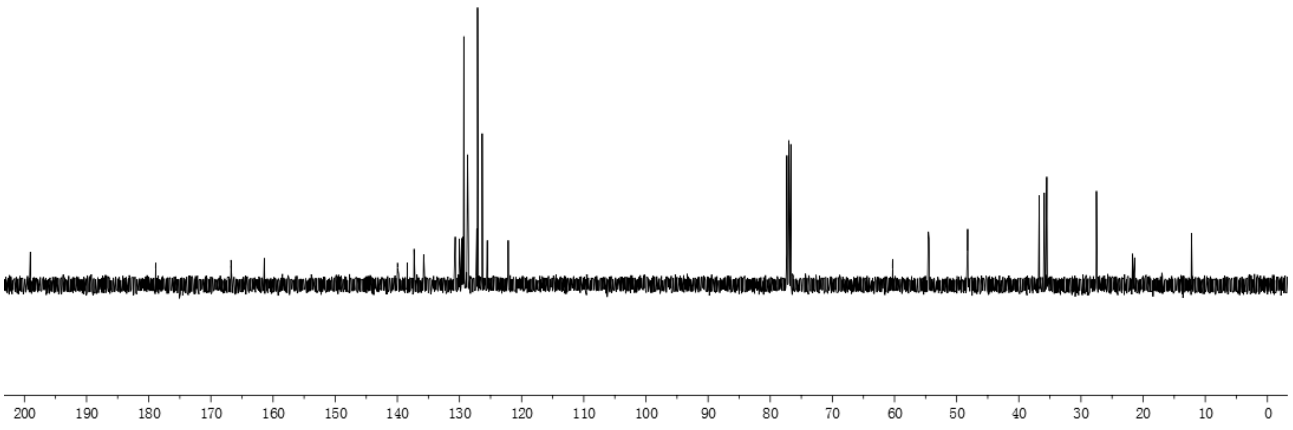
^{1}H NMR (400 MHz, $CDCl_3$)

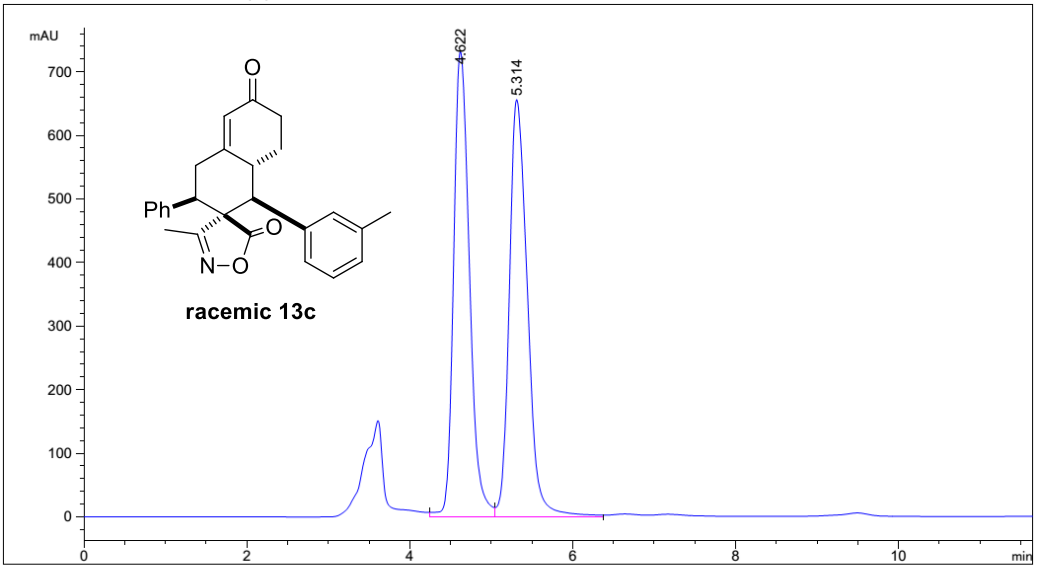




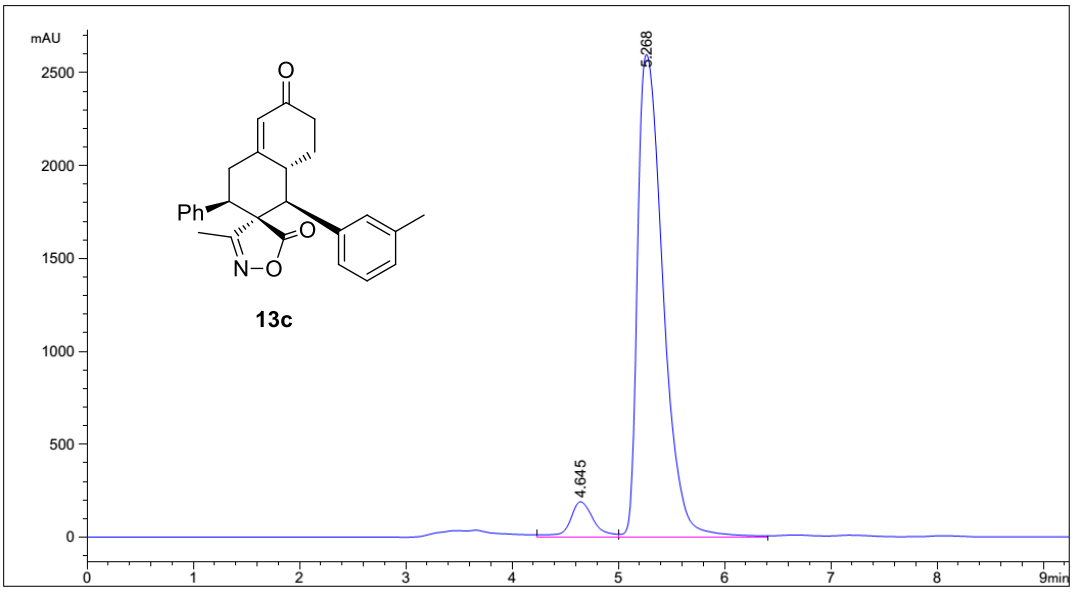
13c

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

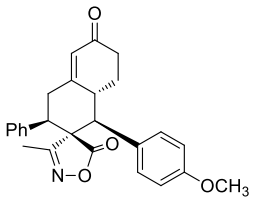




Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.622	VV	0.2109	9913.89844	729.60352	49.3370
2	5.314	VV	0.2450	1.01804e4	656.26086	50.6630

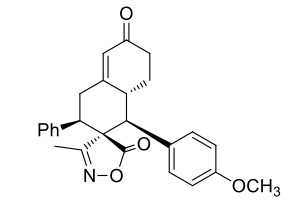


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.645	VV	0.2403	2973.39331	190.55800	6.4384
2	5.268	VV	0.2583	4.32091e4	2595.70166	93.5616



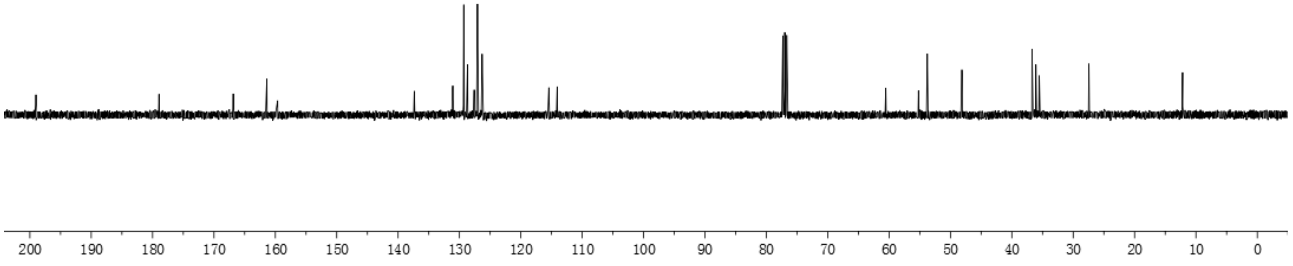
13d

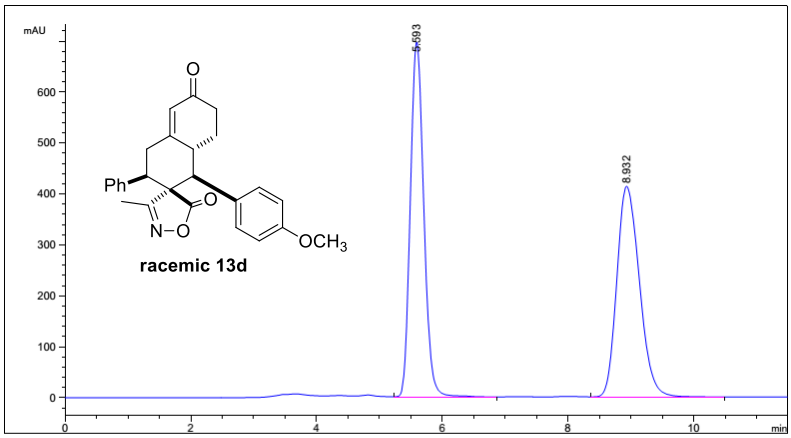
^{1}H NMR (400 MHz, $CDCl_3$)



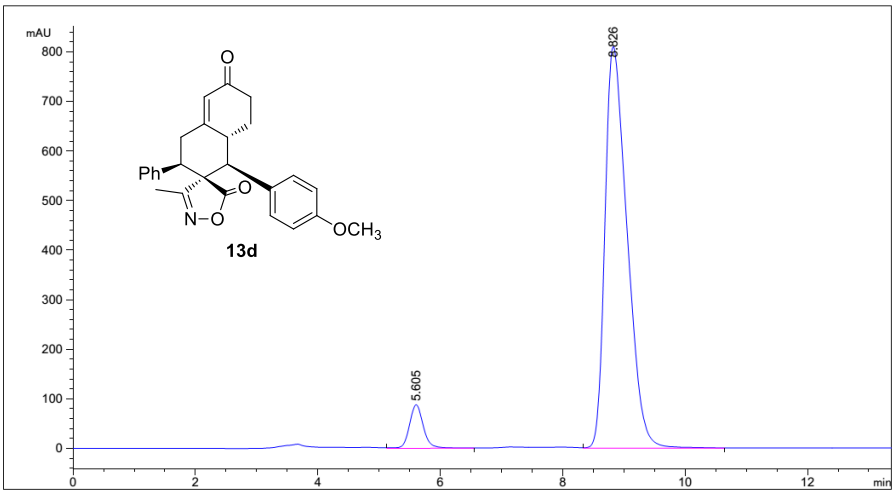
13d

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

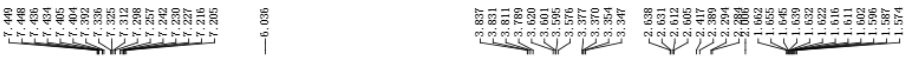


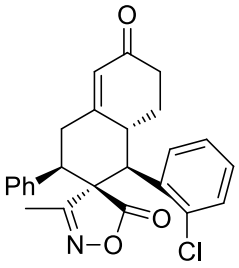


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.593	VV	0.2334	1.04620e4	696.88831	49.9464
2	8.932	VB	0.3997	1.04844e4	414.84833	50.0536



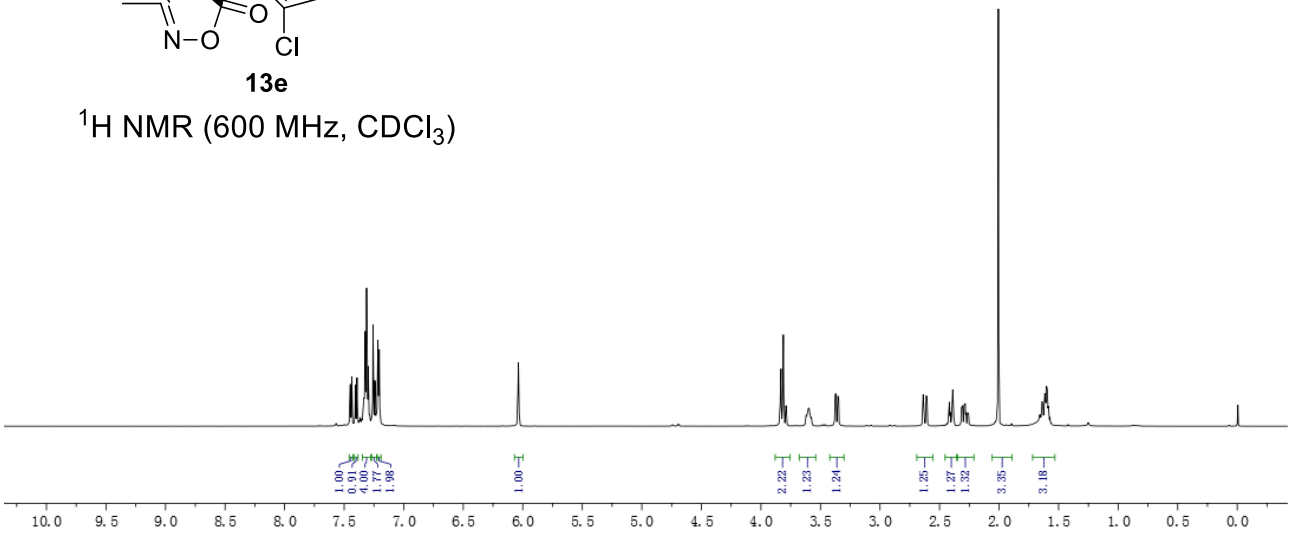
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.605	VB	0.2435	1393.52368	87.75119	6.4234
2	8.826	VB	0.3798	2.03010e4	809.89154	93.5766

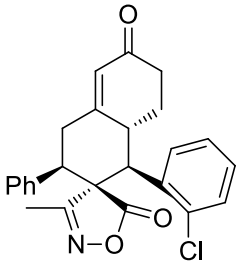




13e

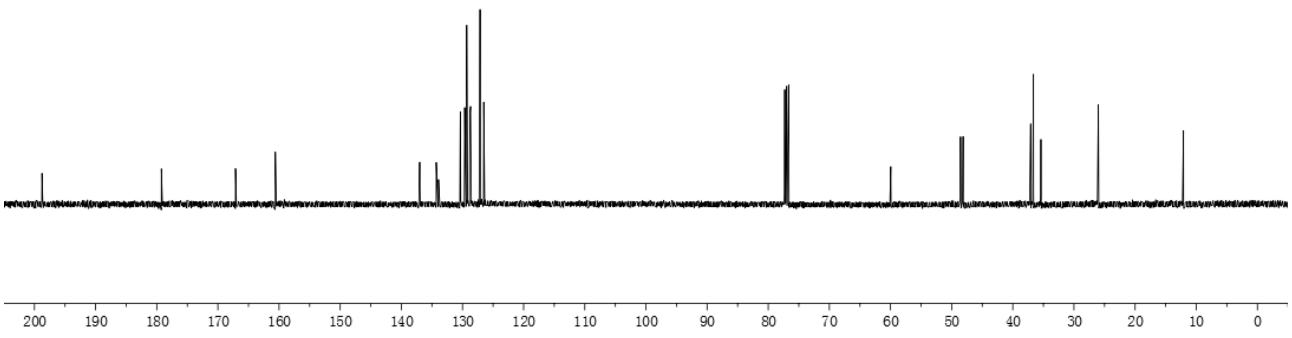
^{1}H NMR (600 MHz, $CDCl_3$)

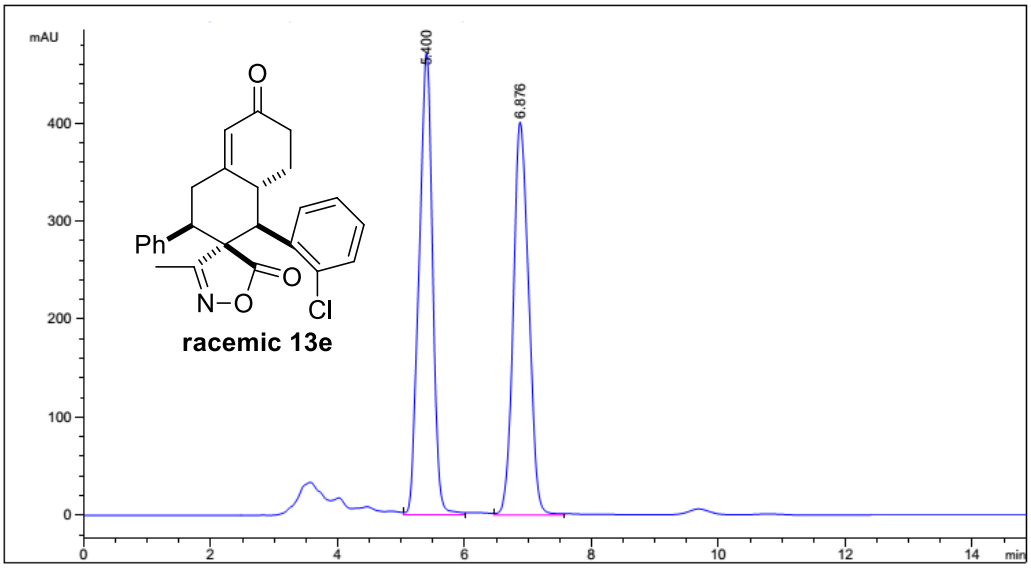




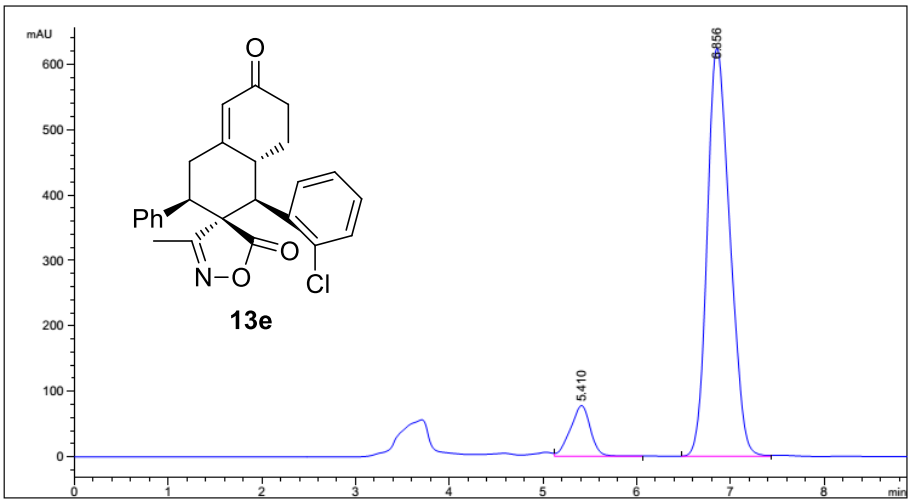
13e

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

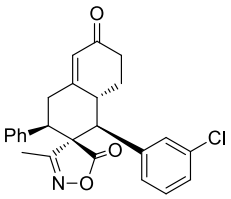




Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.400	VV	0.2251	6969.12500	470.75647	50.7046
2	6.876	VB	0.2732	6775.44580	400.22891	49.2954

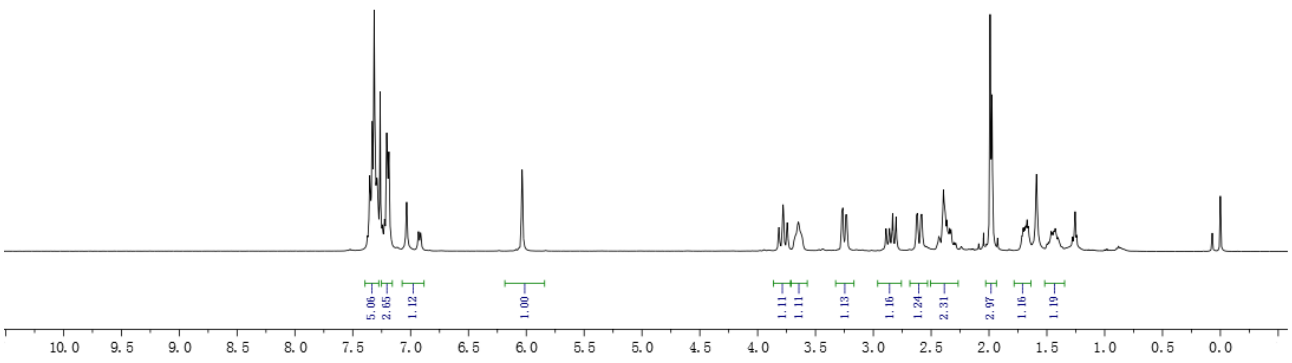


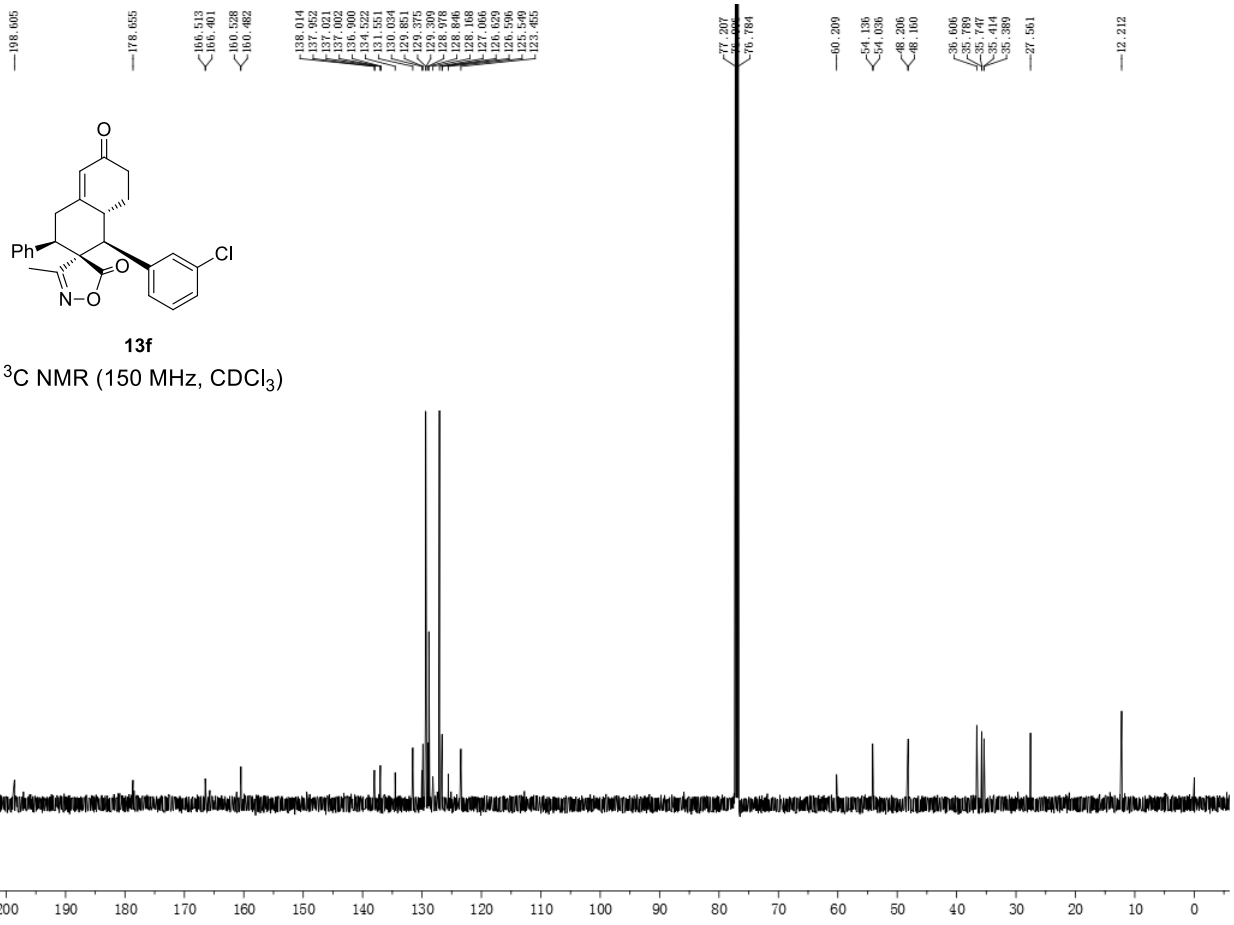
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.410	VB	0.2211	1150.20349	77.56057	9.8944
2	6.856	BV	0.2569	1.04745e4	624.13159	90.1056



13f

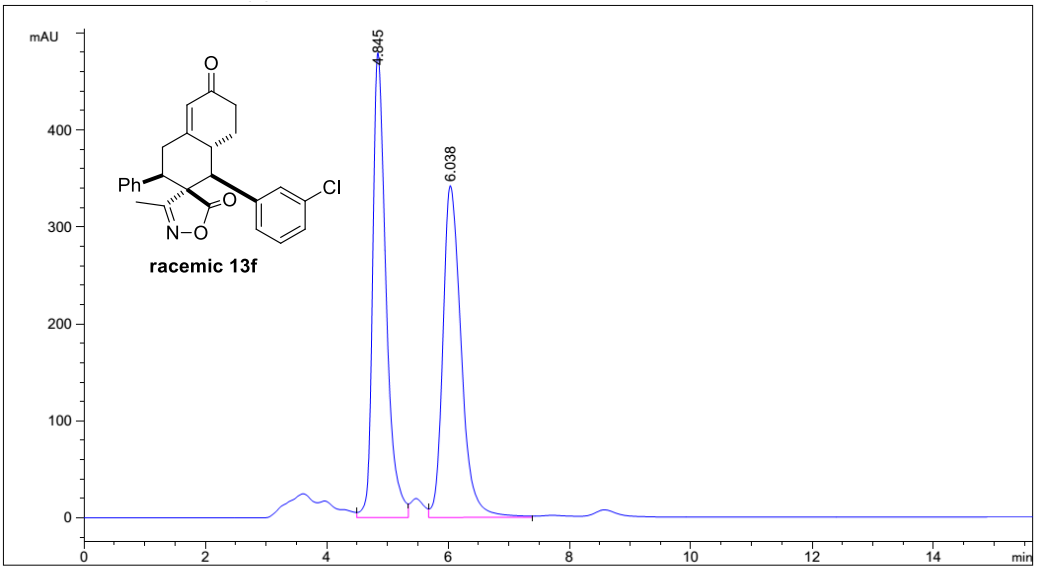
^{1}H NMR (400 MHz, $CDCl_3$)



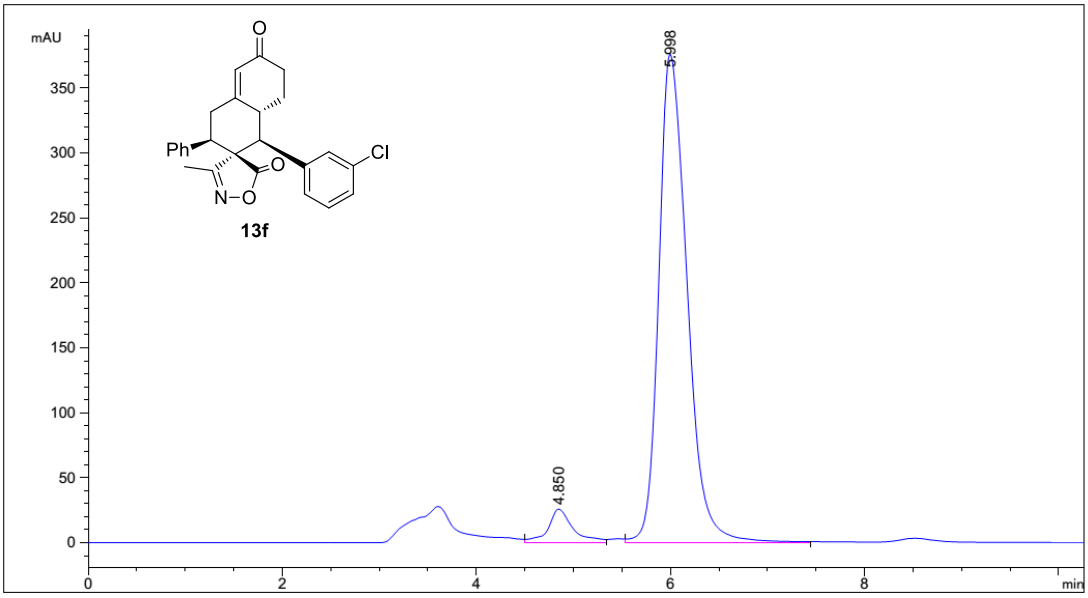


13f

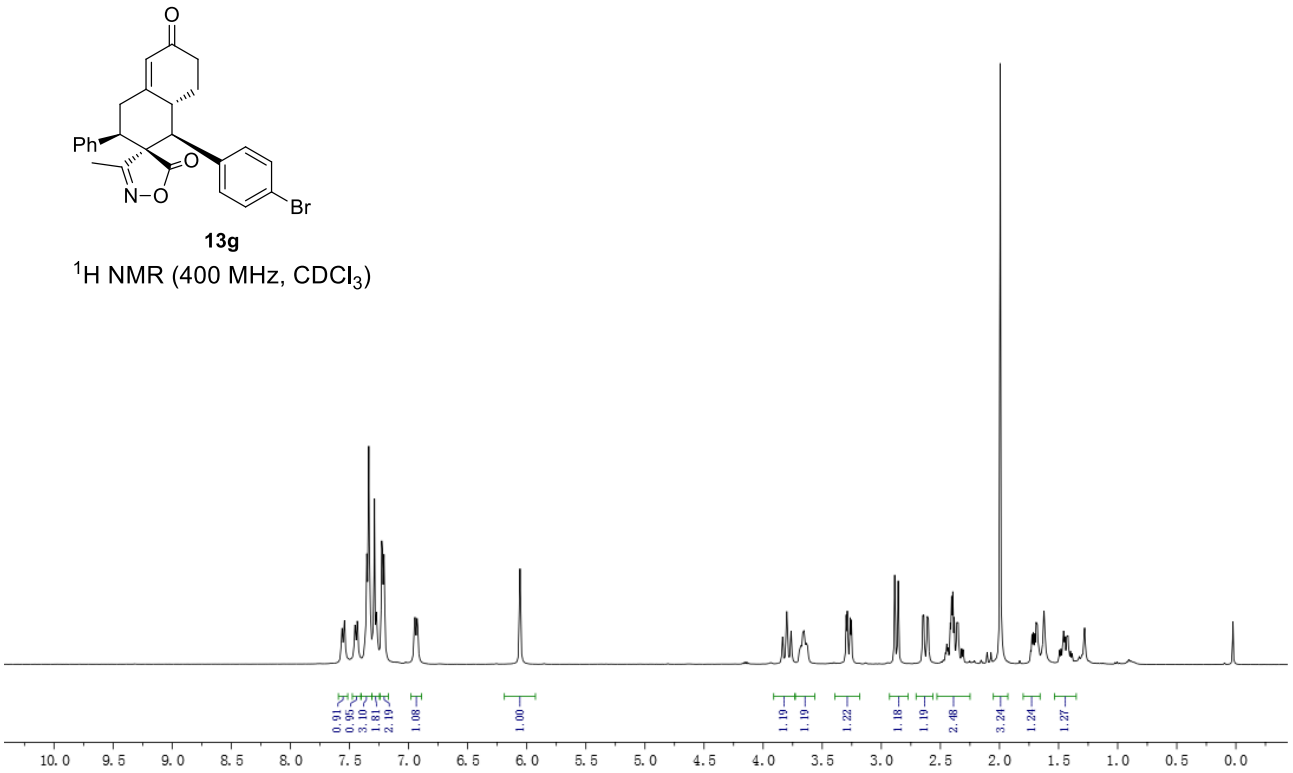
^{13}C NMR (150 MHz, $CDCl_3$)



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.845	VV	0.2365	7319.84814	478.97742	50.5136
2	6.038	VV	0.3264	7171.00342	341.67349	49.4864

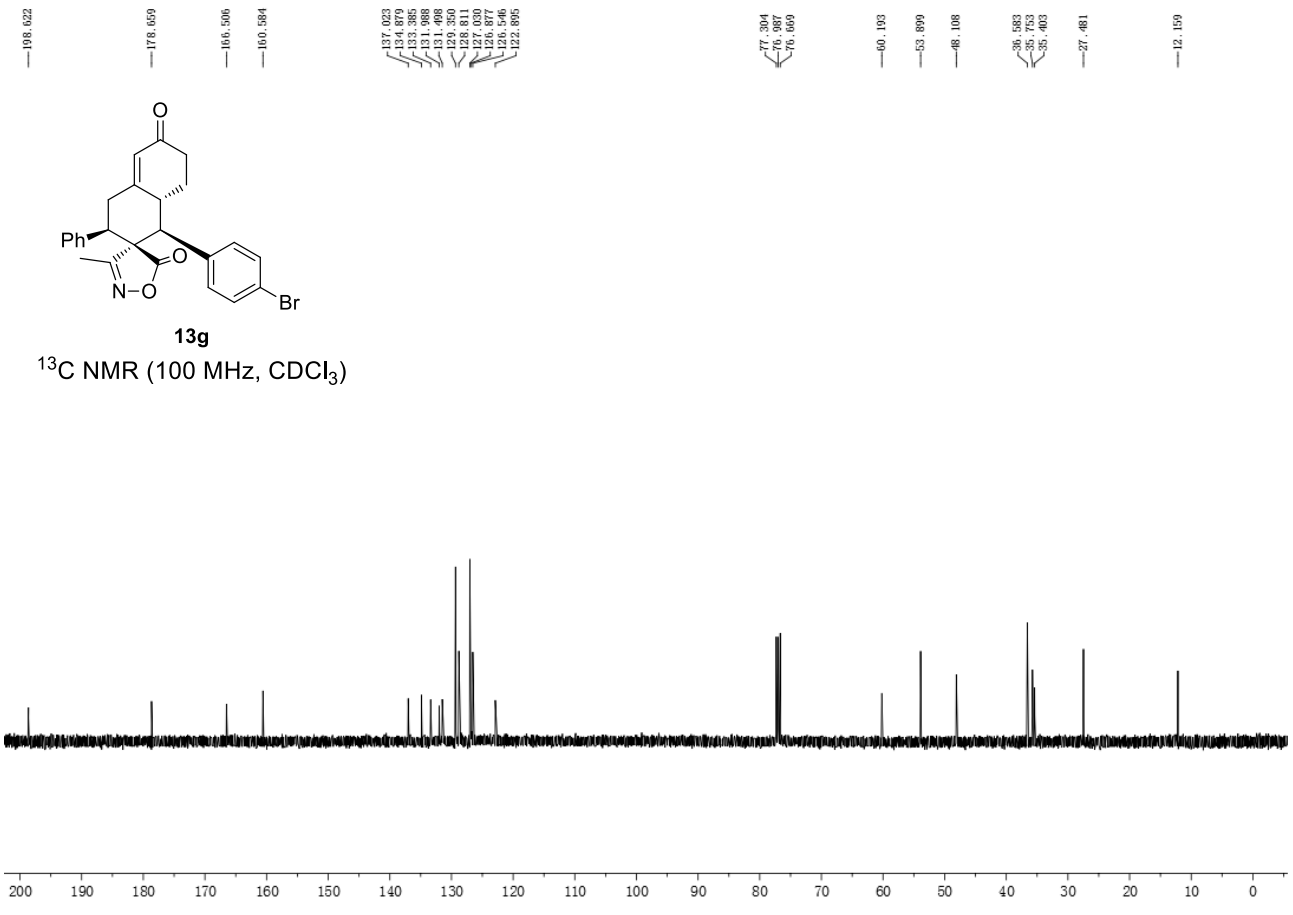


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.850	VV	0.2554	462.70850	25.84717	5.7289
2	5.998	VB	0.3183	7614.07910	375.23184	94.2711



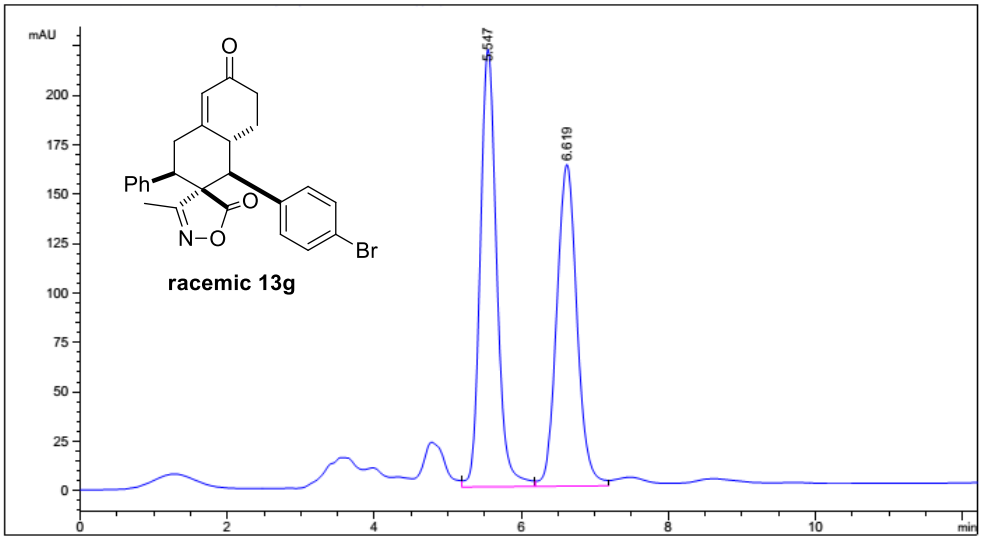
13g

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

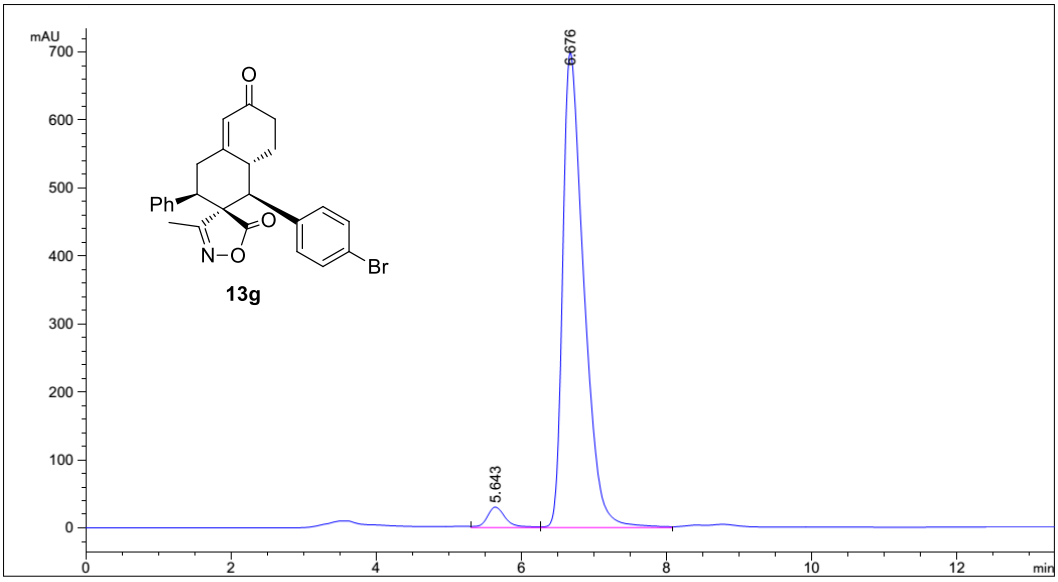


13g

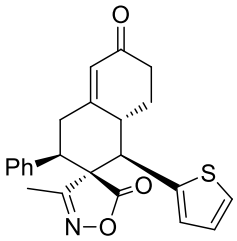
^{13}C NMR (100 MHz, $CDCl_3$)



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.547	VV	0.2392	3425.61206	220.87103	52.3800
2	6.619	VV	0.2993	3114.31152	162.49939	47.6200

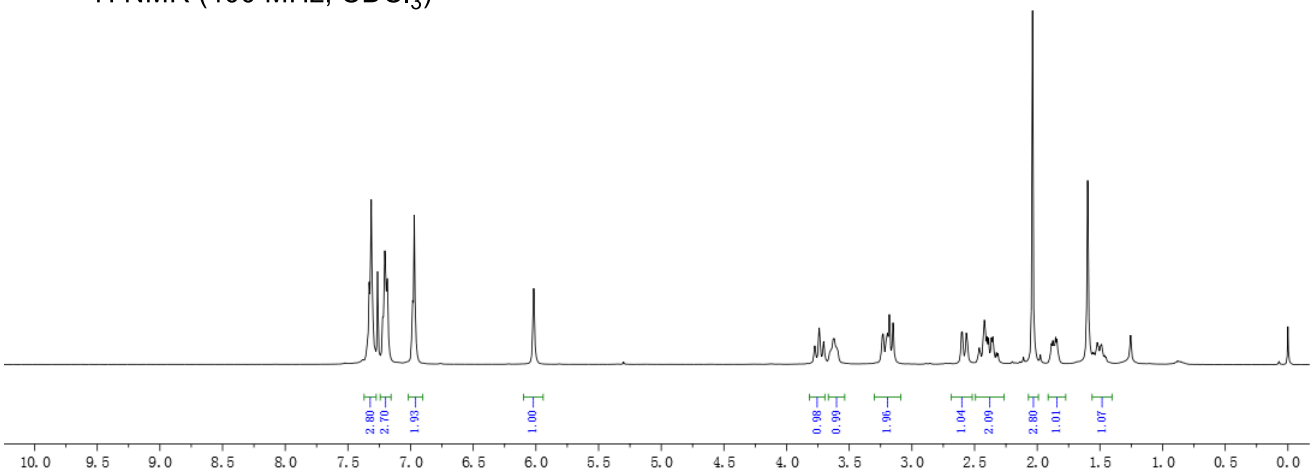


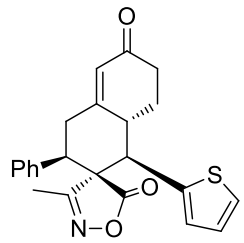
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.643	VV	0.2693	530.15082	30.13525	3.6256
2	6.676	VV	0.2999	1.40922e4	697.07373	96.3744



13h

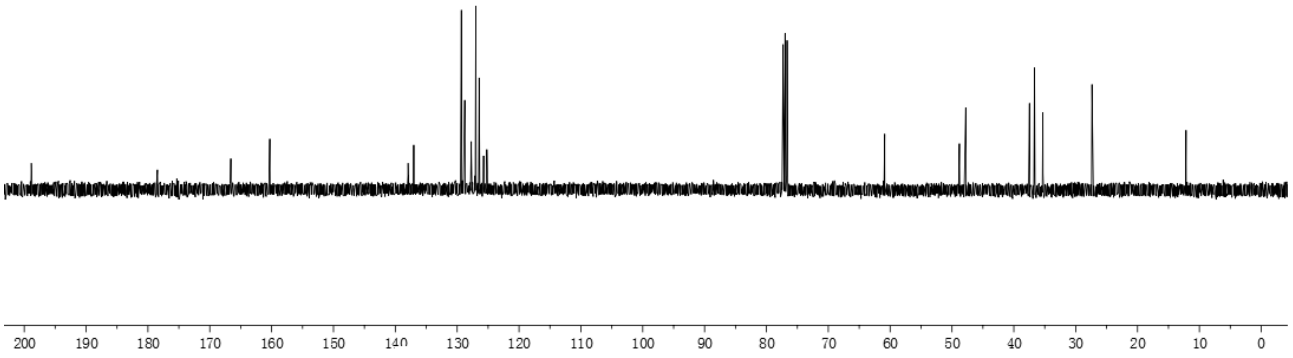
^{1}H NMR (400 MHz, $CDCl_3$)

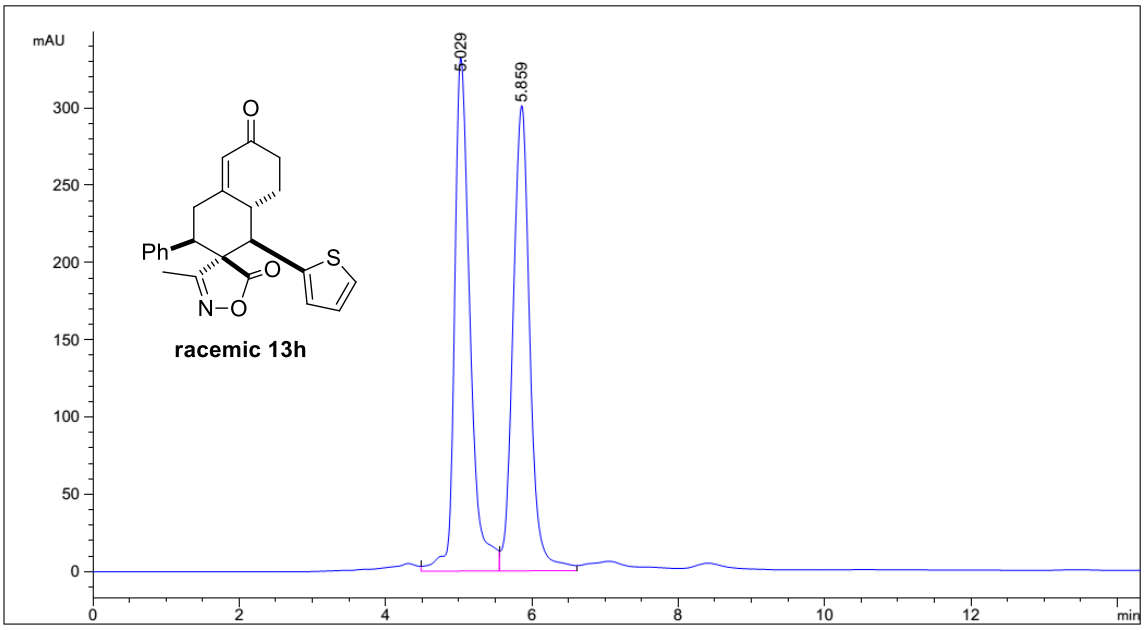




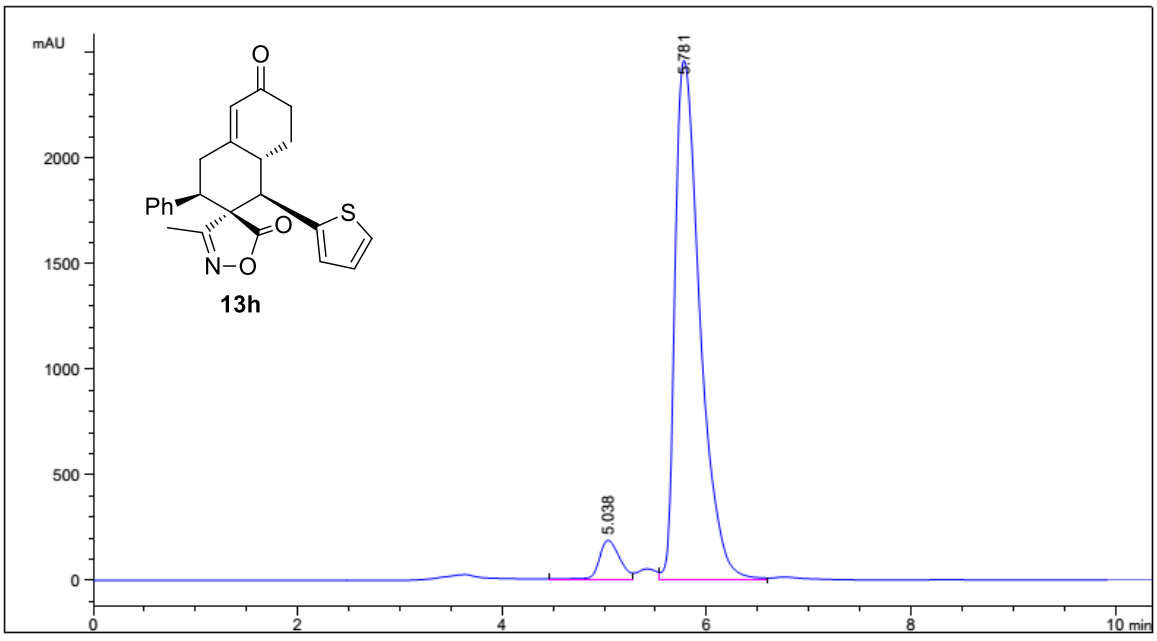
13h

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

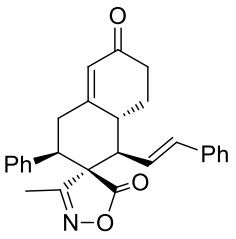




Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.029	VV	0.2251	4896.42041	330.86600	50.3996
2	5.859	VV	0.2512	4818.78613	300.41714	49.6004

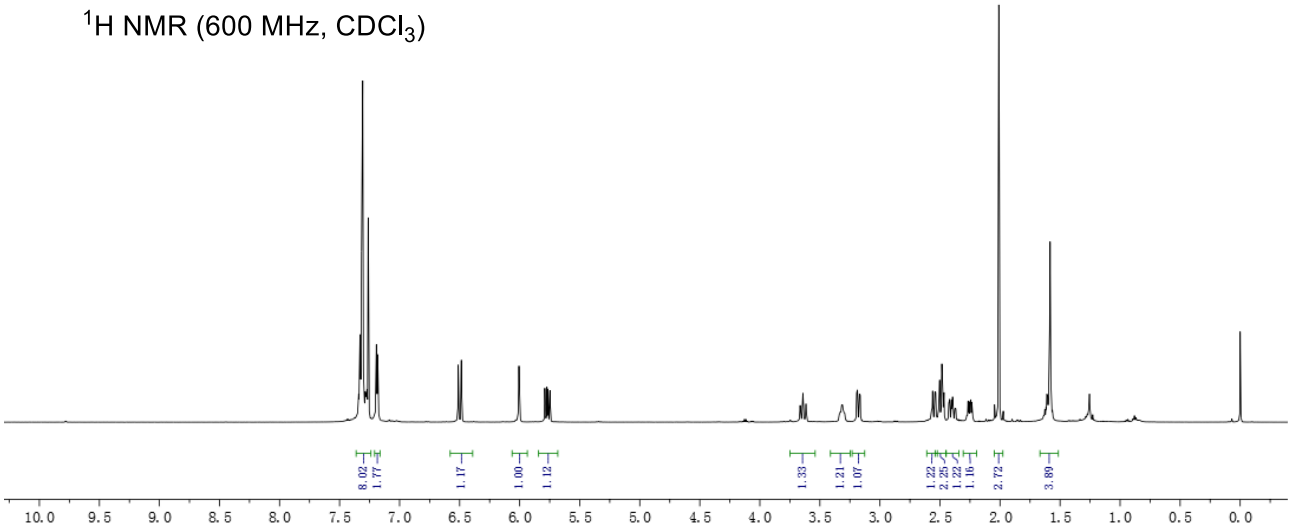


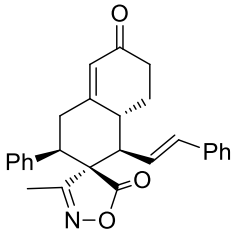
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.038	VV	0.2300	2797.40381	189.99504	6.2508
2	5.781	VV	0.2627	4.19554e4	2464.47192	93.7492



13i

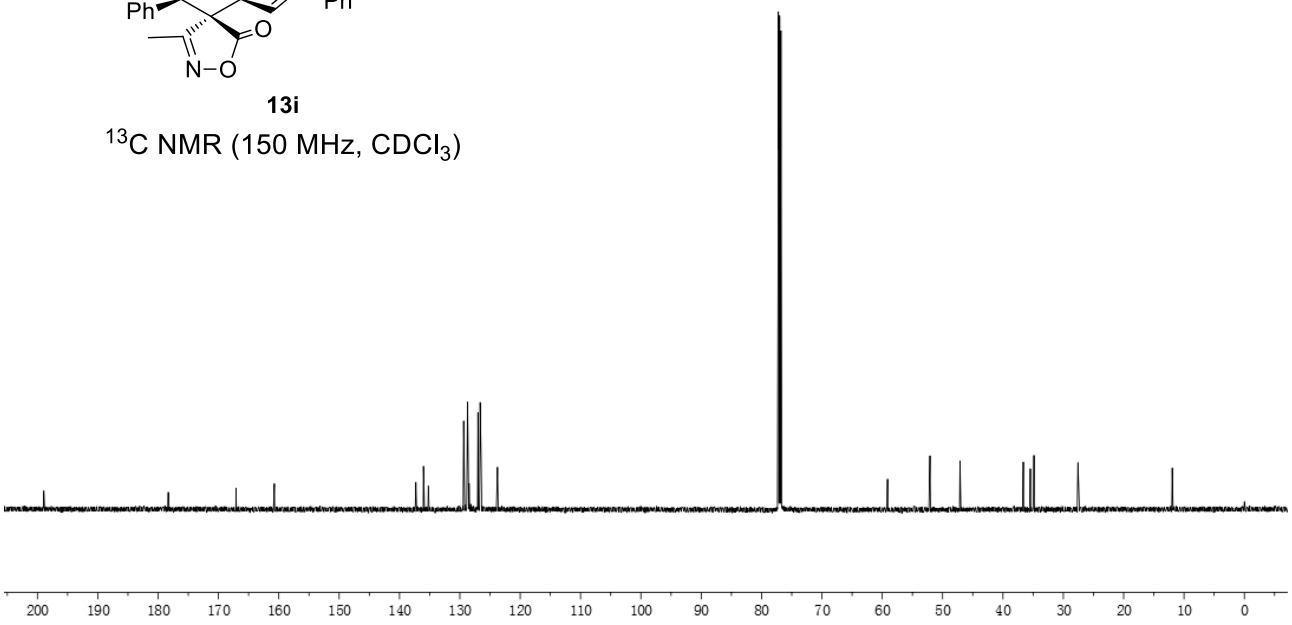
^{1}H NMR (600 MHz, $CDCl_3$)

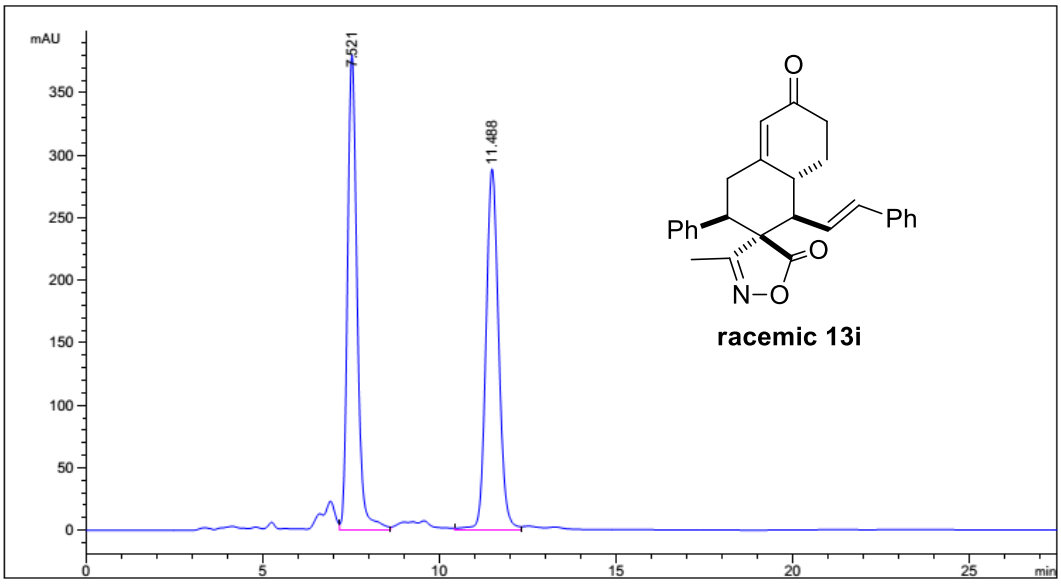




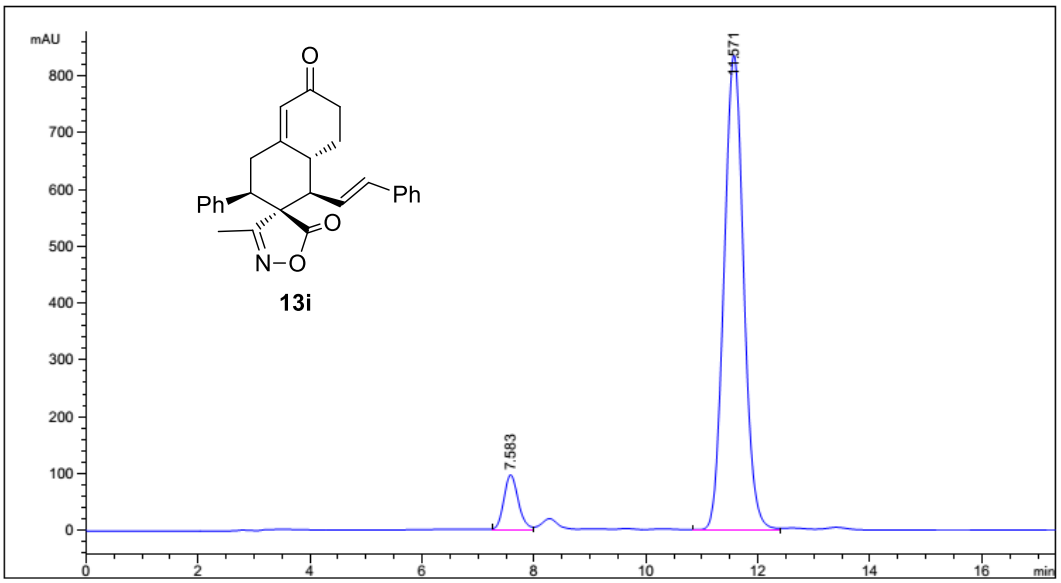
13i

^{13}C NMR (150 MHz, $CDCl_3$)

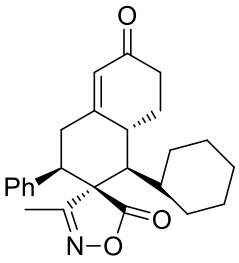




Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.521	VV	0.2895	7153.31934	379.98962	50.0090
2	11.488	VV	0.3822	7150.75342	288.61749	49.9910

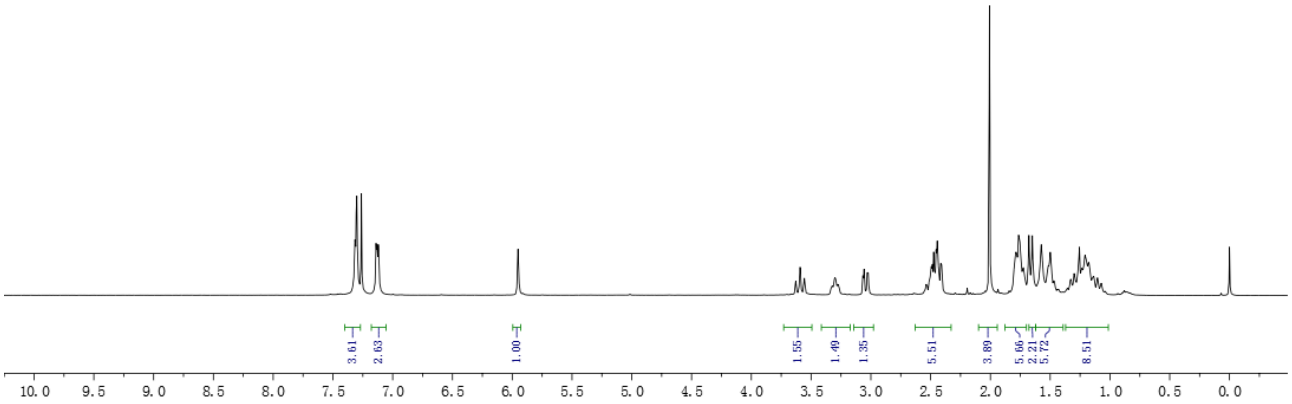


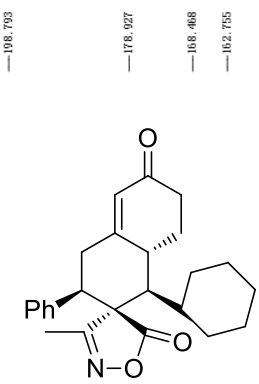
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.583	VV	0.2761	1771.90100	97.48325	8.0083
2	11.571	VV	0.3833	2.03539e4	835.27069	91.9917



13j

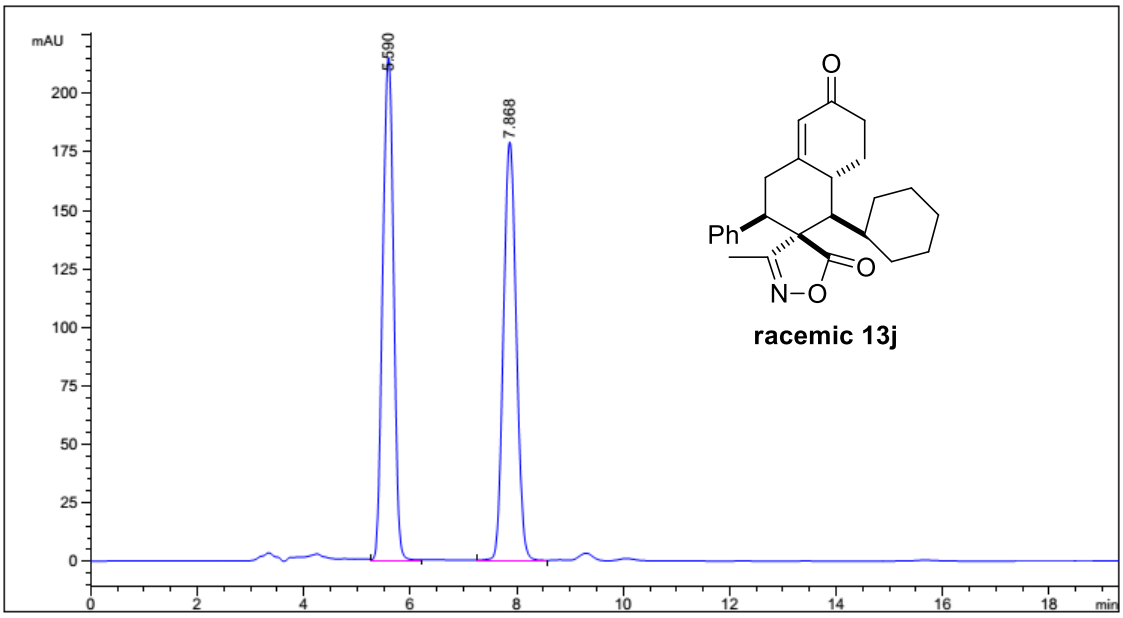
^{1}H NMR (400 MHz, $CDCl_3$)



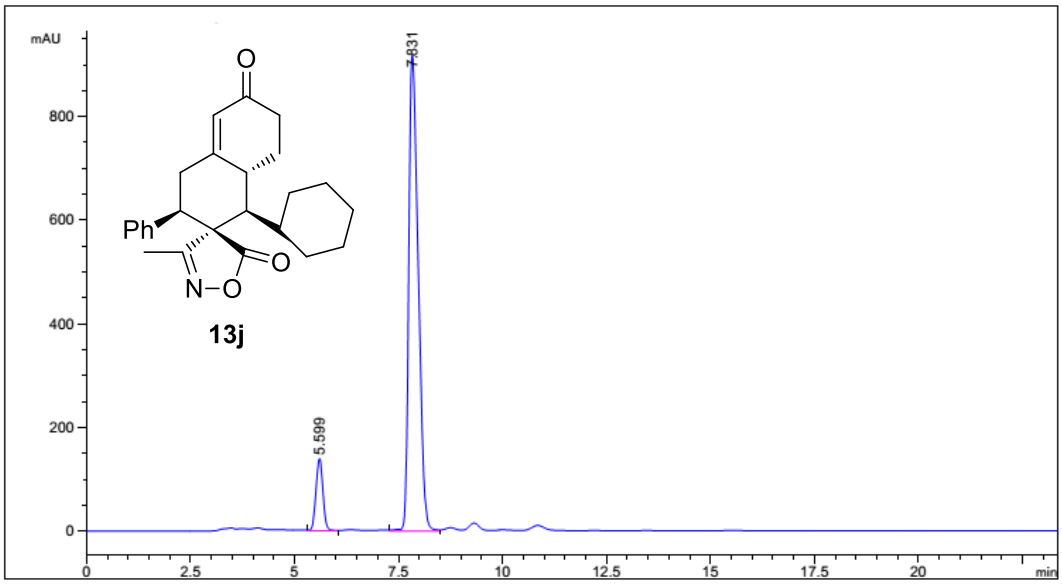


13j

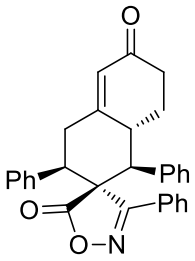
^{13}C NMR (150 MHz, $CDCl_3$)



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.590	VB	0.2312	3081.06299	215.07391	50.5161
2	7.868	VV	0.2665	3018.11255	179.06757	49.4839

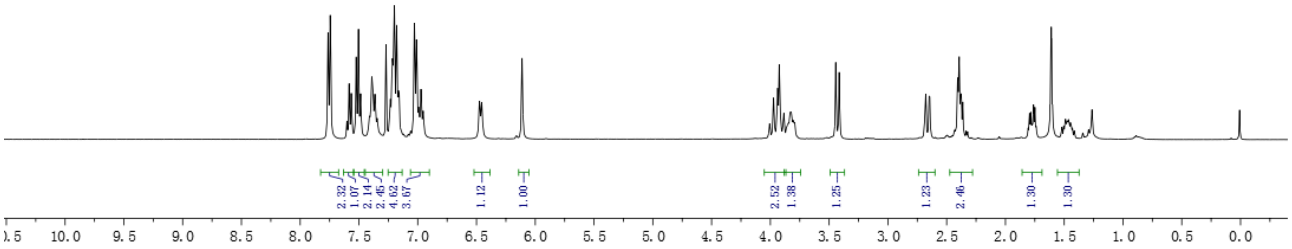


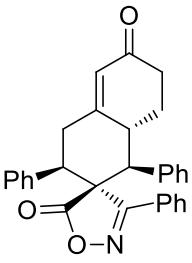
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.599	VV	0.1846	1652.63489	139.66399	10.2504
2	7.831	VV	0.2422	1.44700e4	917.51660	89.7496



13k

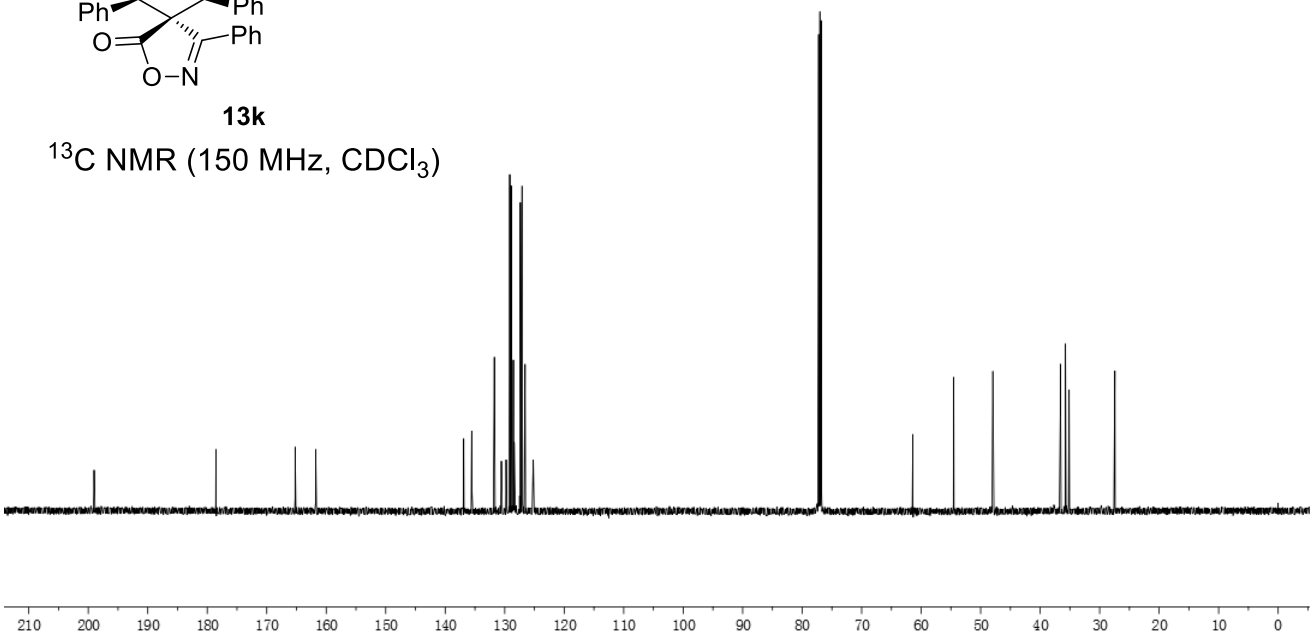
^{1}H NMR (400 MHz, $CDCl_3$)

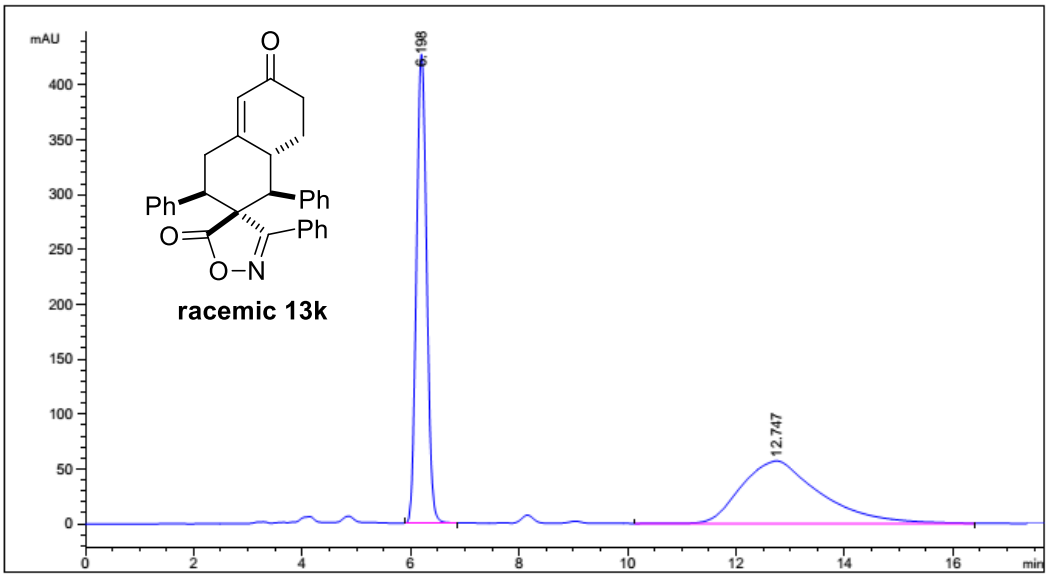




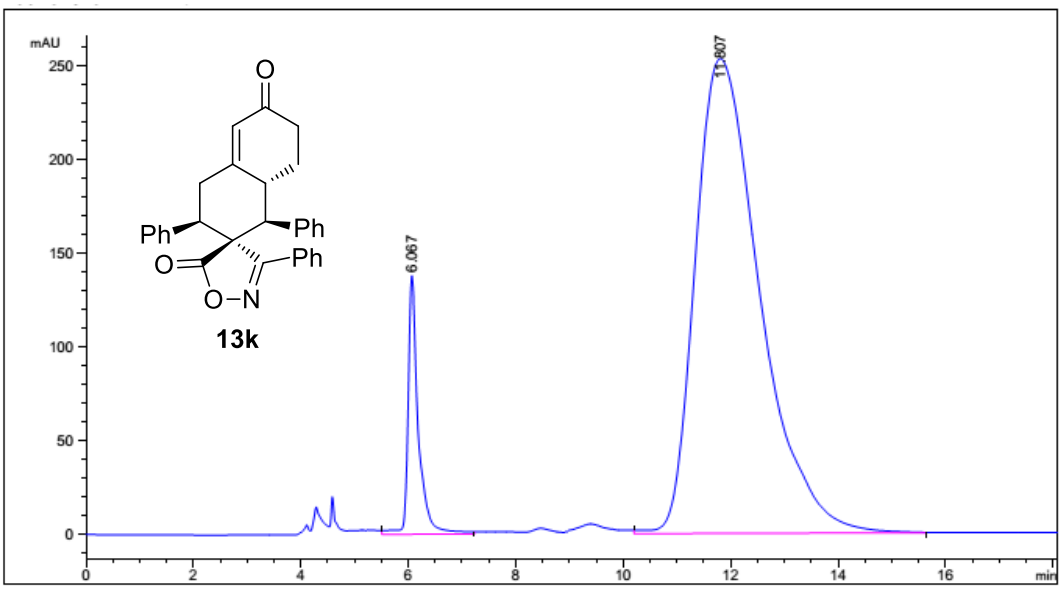
13k

^{13}C NMR (150 MHz, $CDCl_3$)

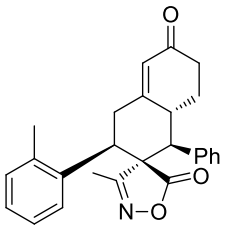




Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.198	BB	0.2056	5611.95313	427.30008	49.2795
2	12.747	VB	1.5192	5776.05811	57.03867	50.7205

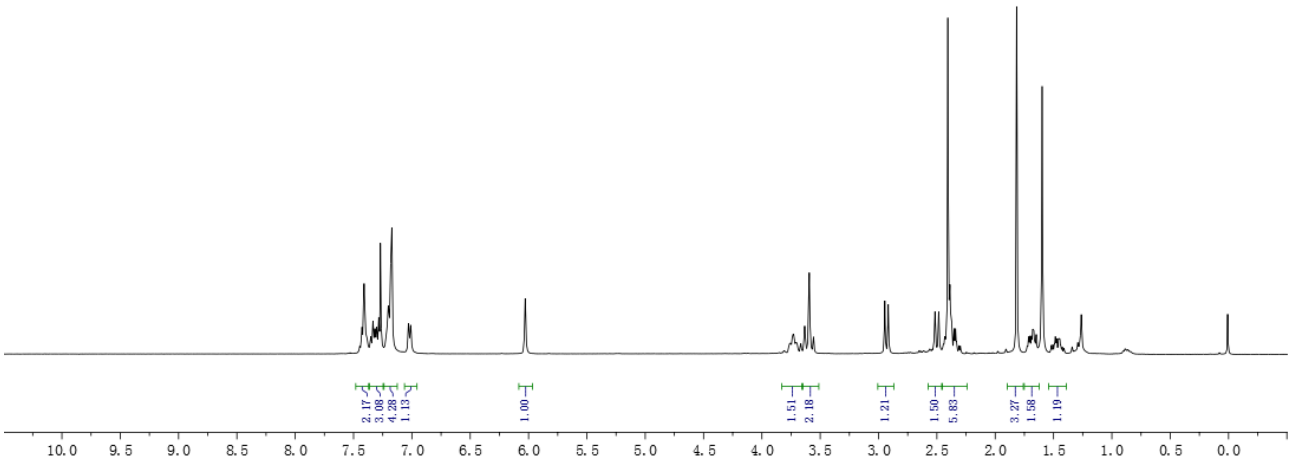


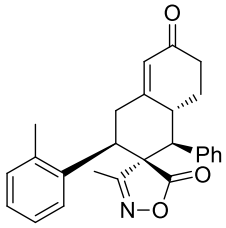
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.067	VB	0.1959	1827.38940	137.45547	7.9843
2	11.807	BB	1.2853	2.10599e4	253.07703	92.0157



13l

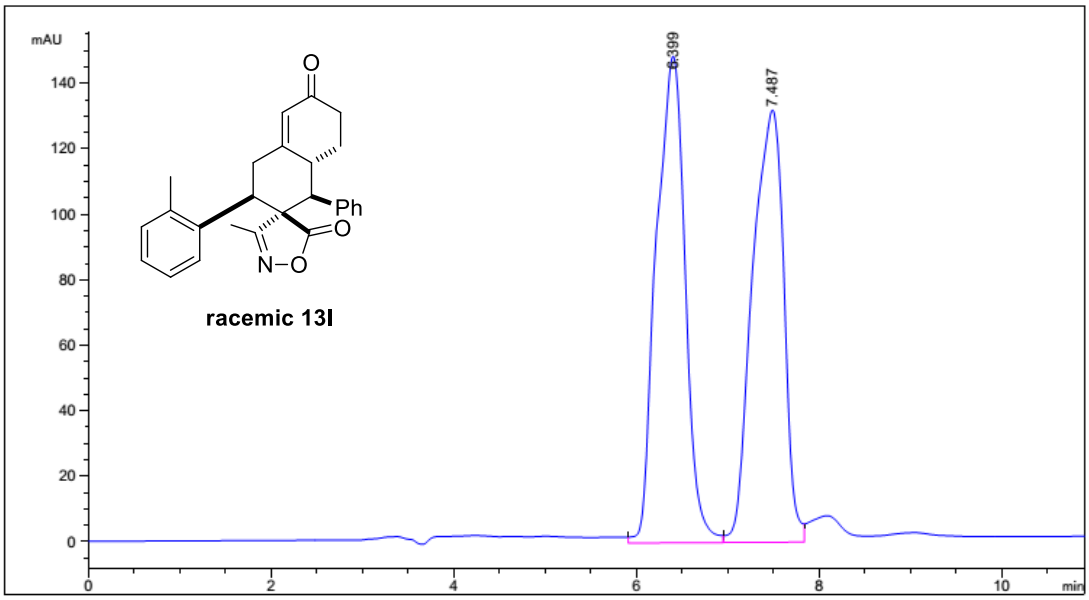
^{1}H NMR (400 MHz, $CDCl_3$)



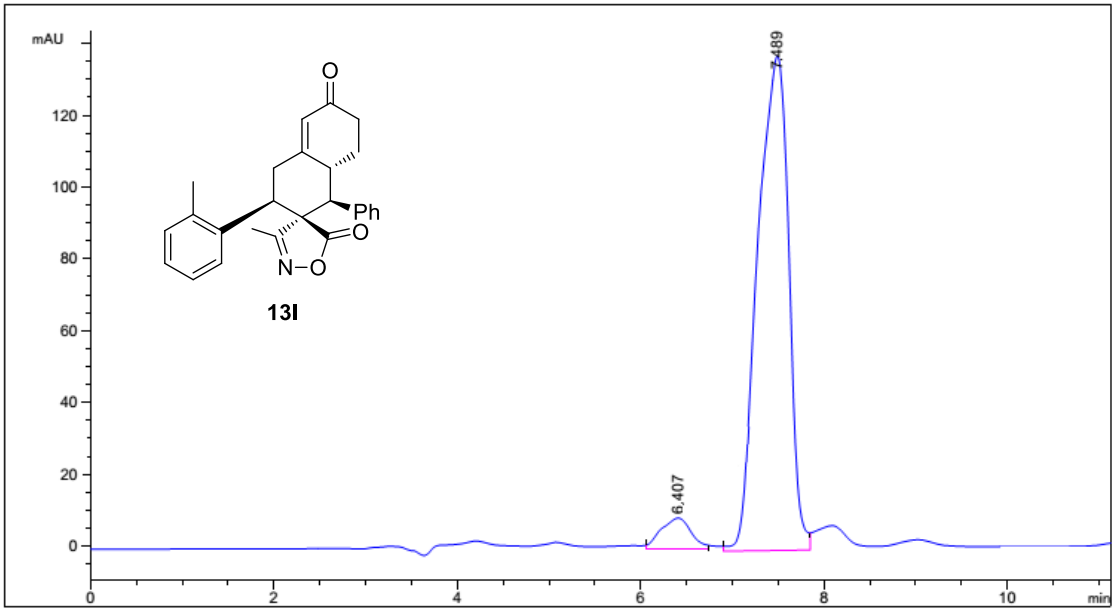


13l

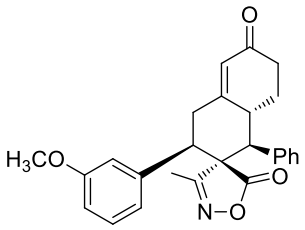
^{13}C NMR (150 MHz, $CDCl_3$)



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.399	BV	0.3152	3270.58423	148.48781	50.9654
2	7.487	VV	0.3426	3146.68579	131.82051	49.0346

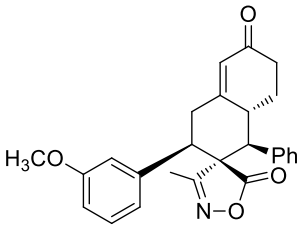


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.407	MM	0.3798	194.75266	8.54584	5.6702
2	7.489	VV	0.3388	3239.89111	137.57536	94.3298



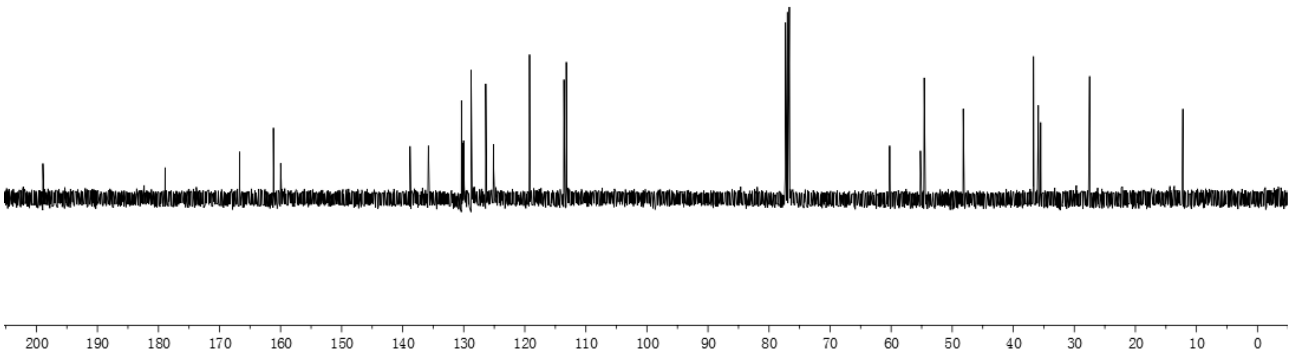
13m

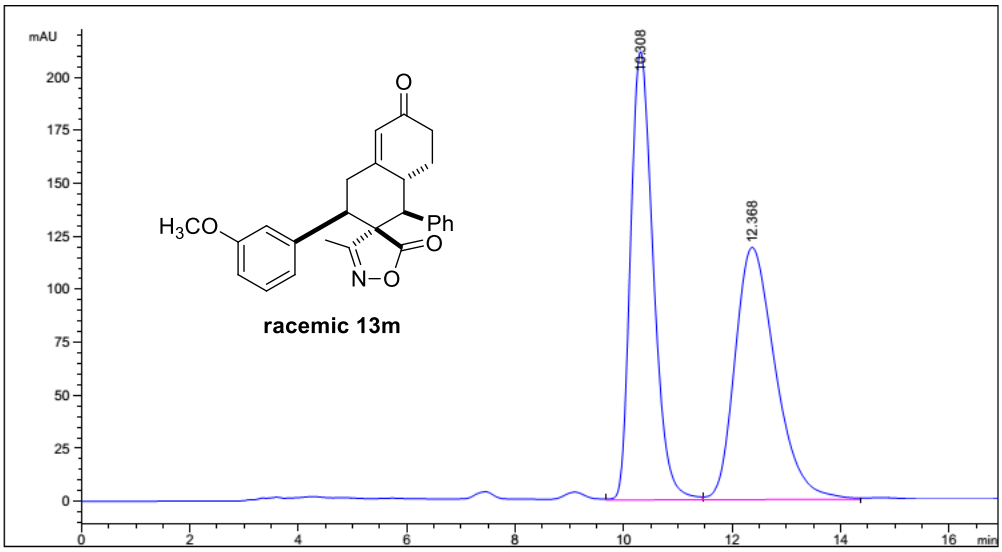
^{1}H NMR (400 MHz, $CDCl_3$)



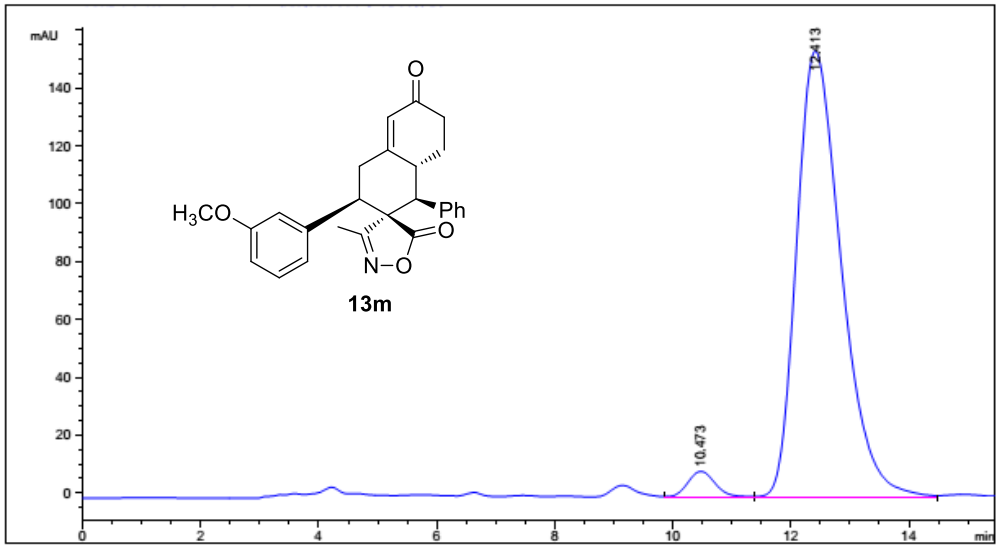
13m

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

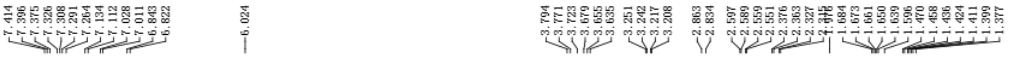


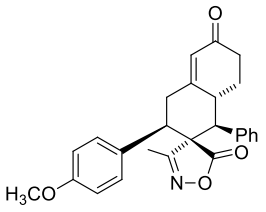


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	10.308	VV	0.4564	6155.14111	211.23463	49.9619
2	12.368	VV	0.7968	6164.52100	118.95893	50.0381



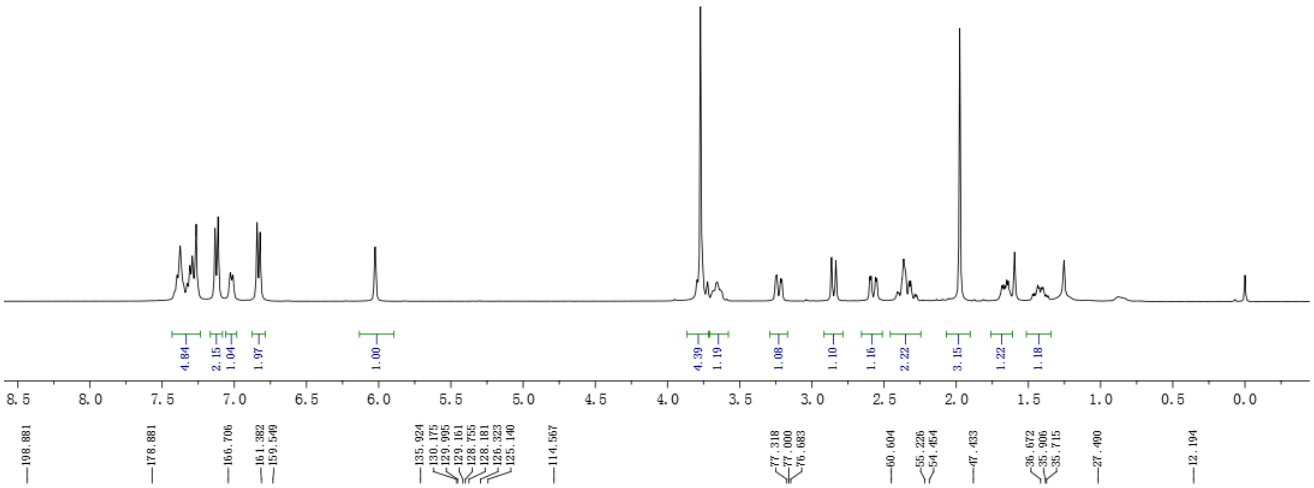
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	10.473	VV	0.5300	320.21506	9.29611	3.7694
2	12.413	VV	0.8144	8174.96094	154.72624	96.2306

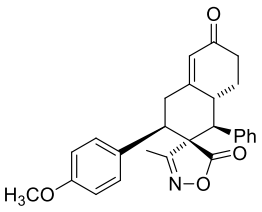




13n

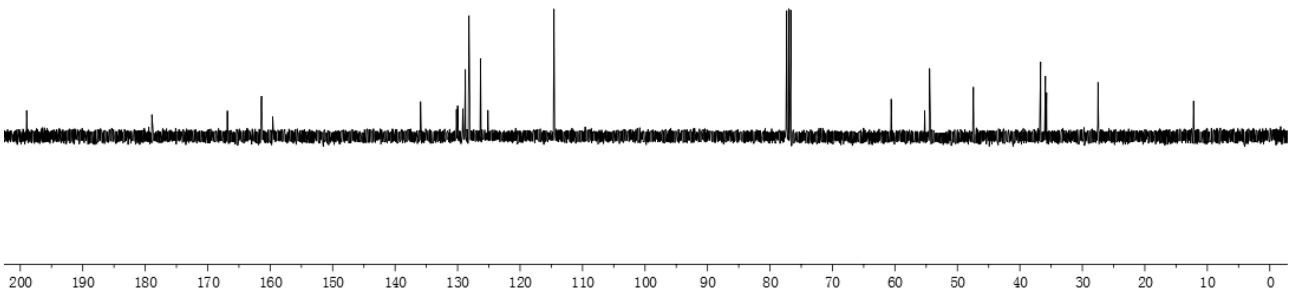
^{1}H NMR (400 MHz, $CDCl_3$)

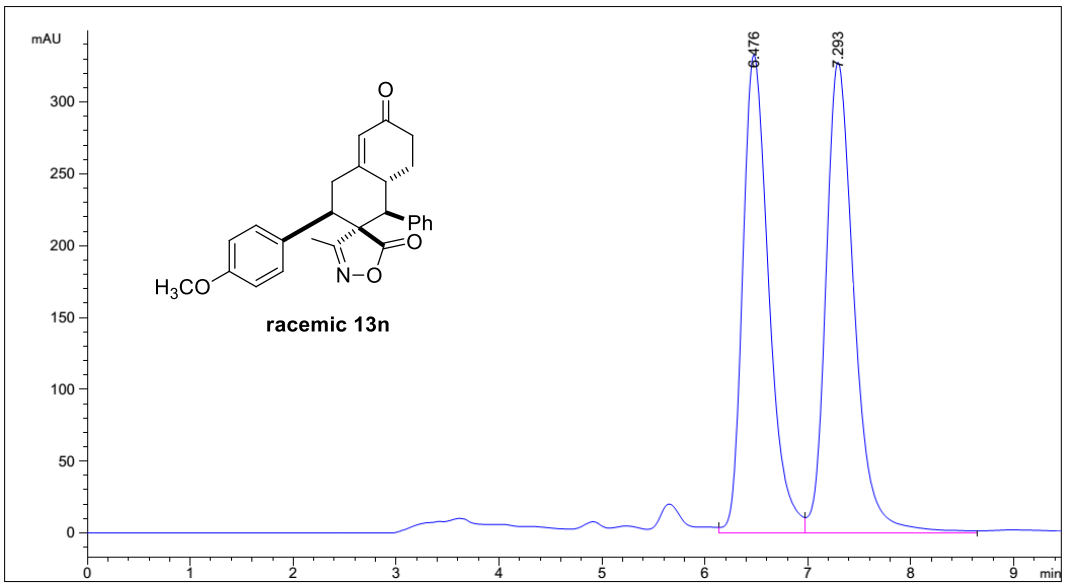




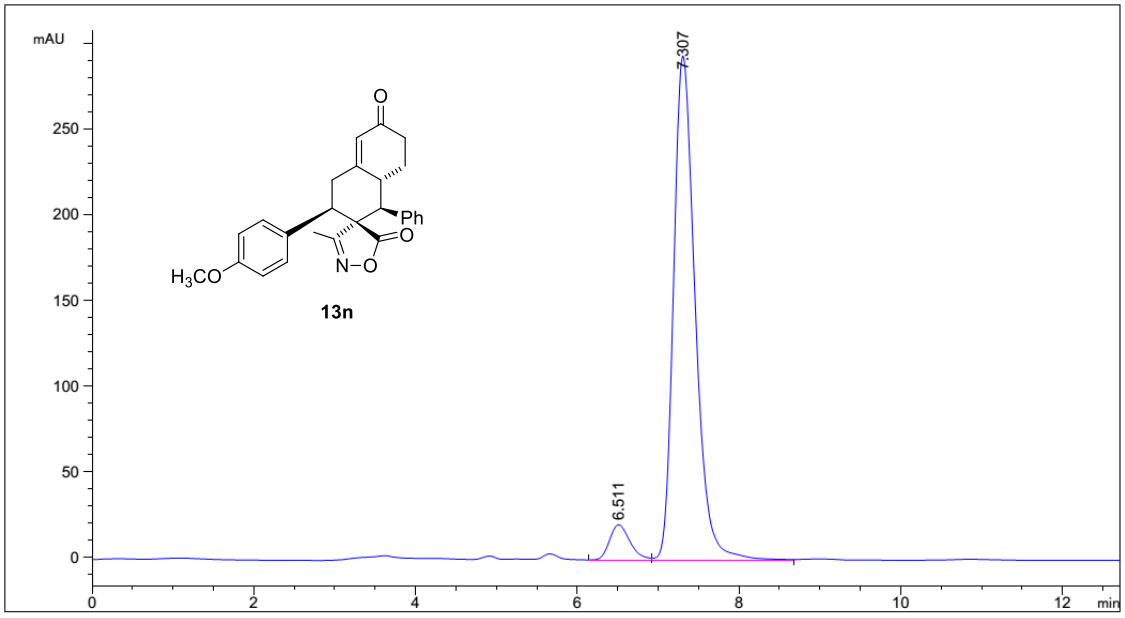
13n

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

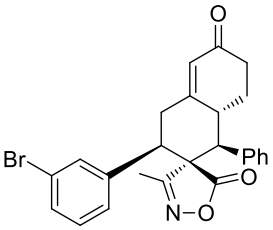




Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.476	VV	0.2691	5841.41650	332.35223	48.3382
2	7.293	VV	0.2925	6243.04785	327.25598	51.6618

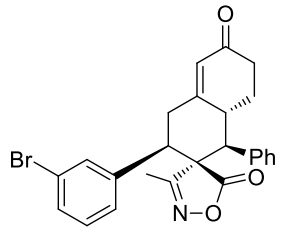


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.511	VV	0.2723	370.69382	20.77178	6.3564
2	7.307	VV	0.2866	5461.08887	294.02106	93.6436



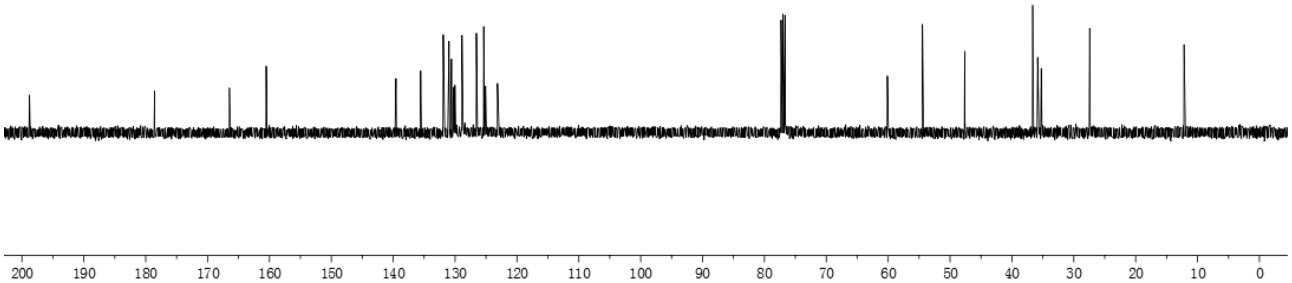
13o

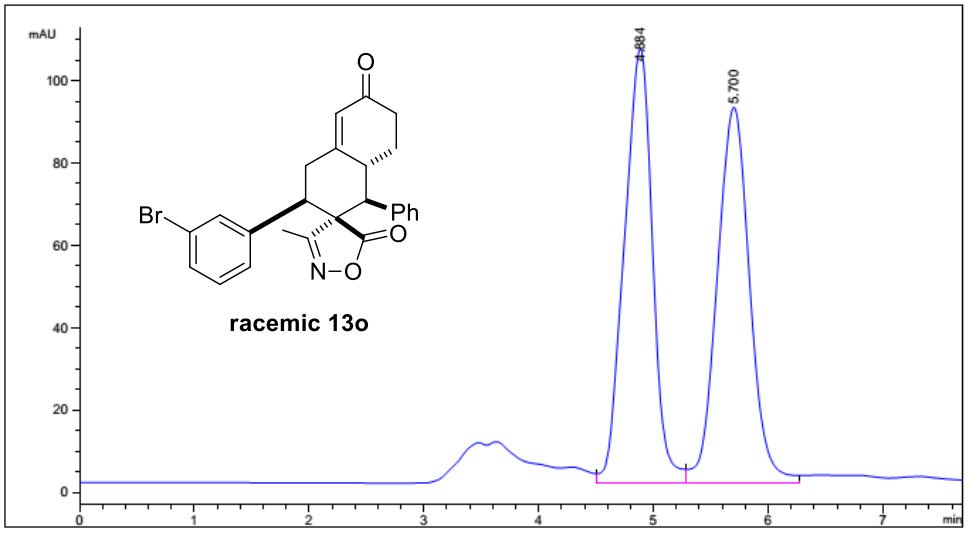
^{1}H NMR (400 MHz, $CDCl_3$)



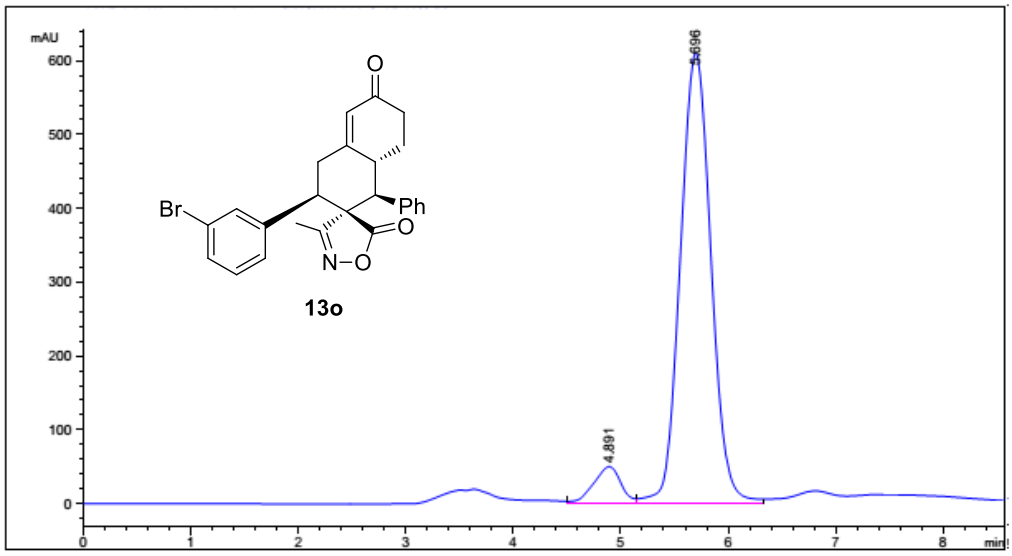
13o

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

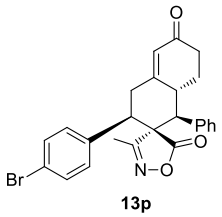




Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.884	VV	0.2582	1802.78931	105.21002	50.0634
2	5.700	VV	0.3118	1798.22437	91.12373	49.9366

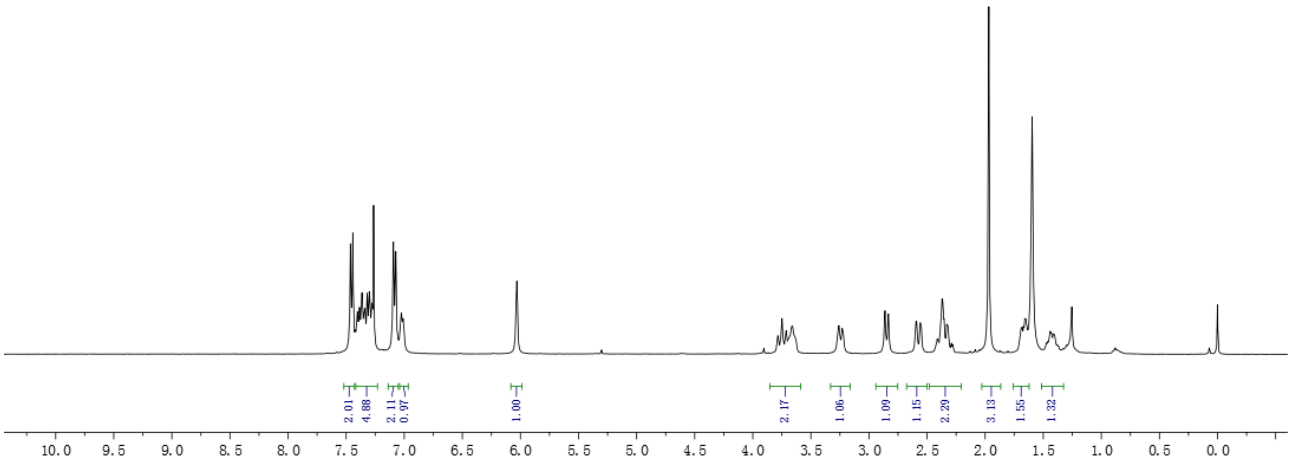


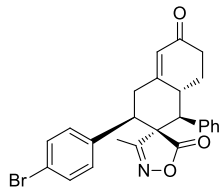
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.891	VV	0.2685	910.40698	50.51965	6.9894
2	5.696	VV	0.3130	1.21152e4	610.63562	93.0106



13p

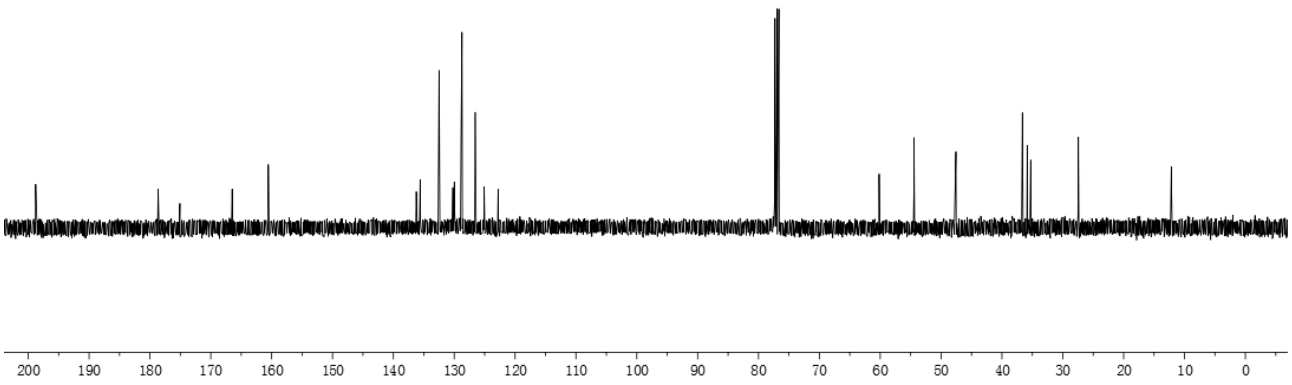
^{1}H NMR (400 MHz, $CDCl_3$)

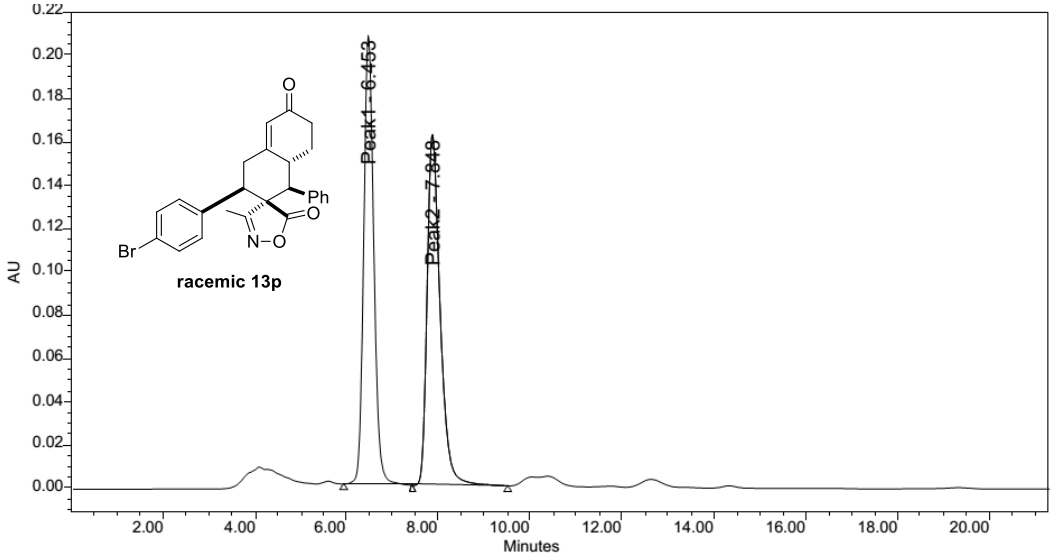




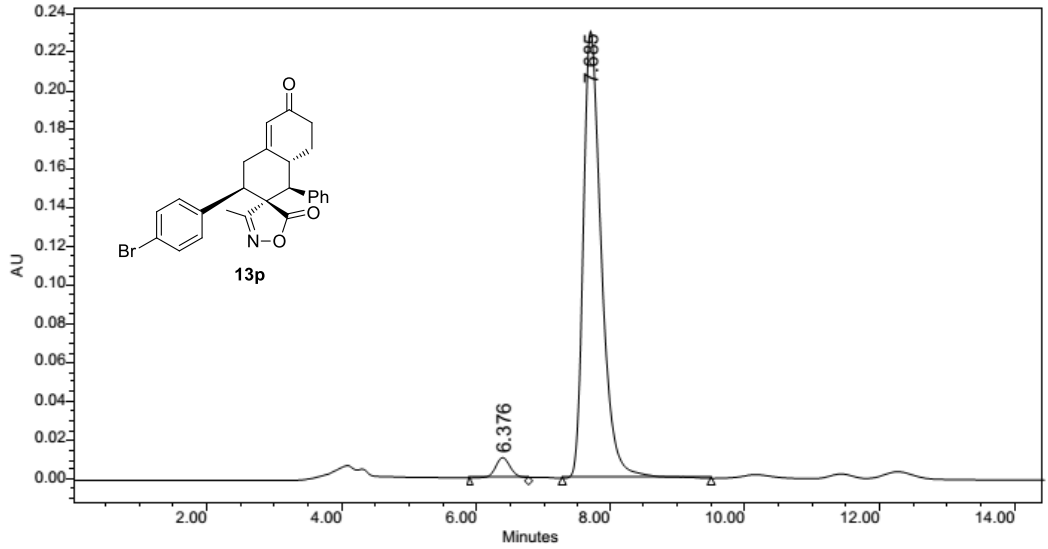
13p

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

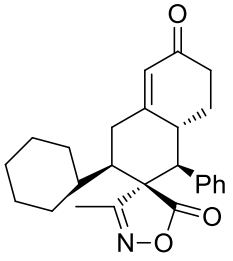




	Peak Name	RT (min)	Area (*sec)	% Area	Height ( )	% Height
1	Peak1	6.453	3168582	49.76	207490	56.13
2	Peak2	7.848	3199698	50.24	162197	43.87

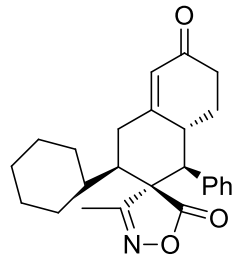


	RT (min)	Area (*sec)	% Area	Height ( )	% Height
1	6.376	164148	3.66	10535	4.37
2	7.685	4319305	96.34	230533	95.63



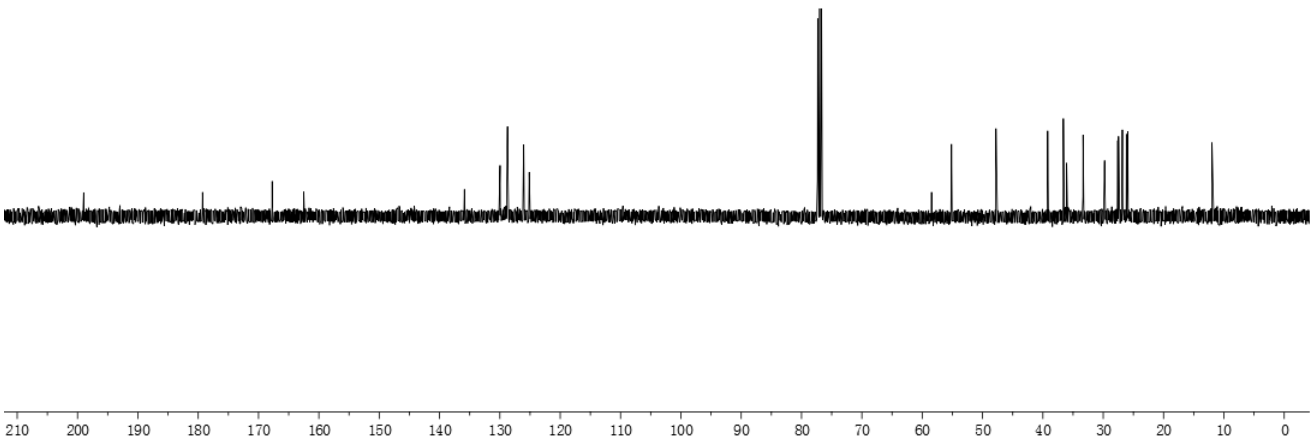
13q

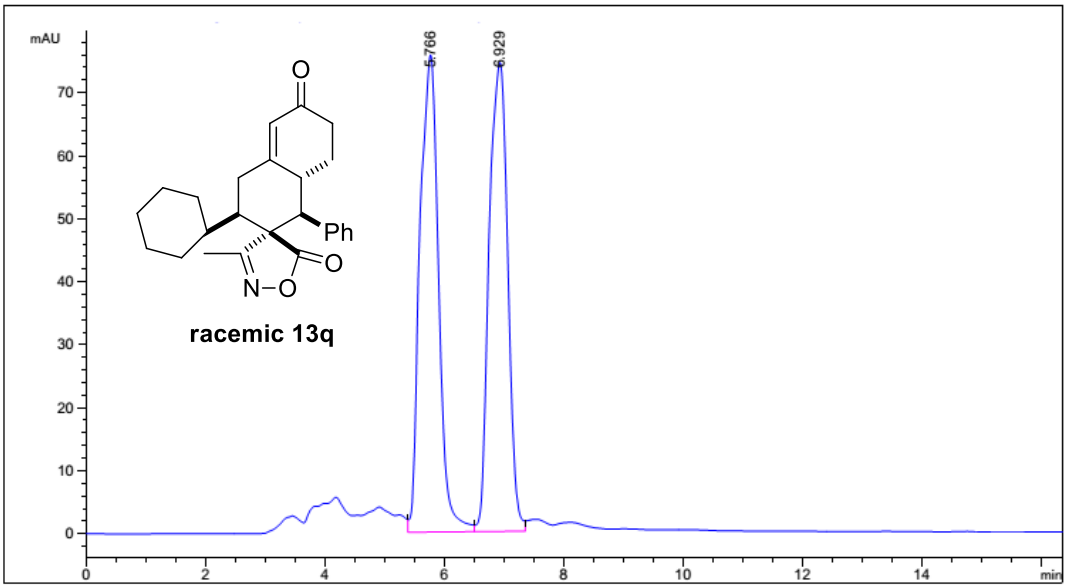
^{1}H NMR (400 MHz, $CDCl_3$)



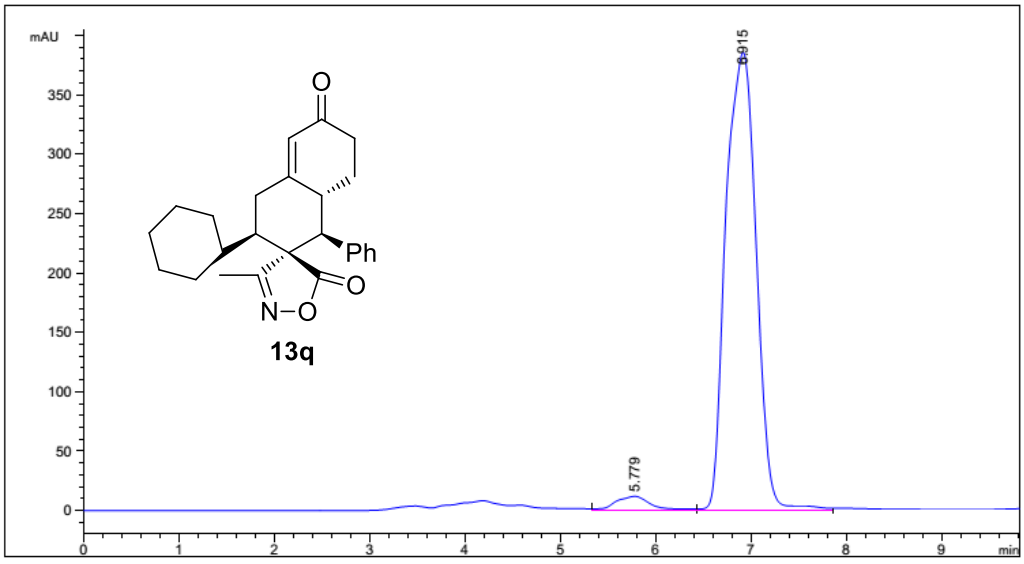
13q

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

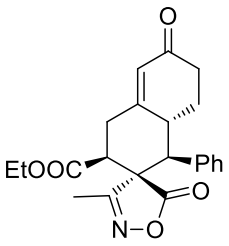




Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.766	VV	0.3047	1637.06909	75.70399	50.4175
2	6.929	VV	0.3572	1609.95483	74.42674	49.5825

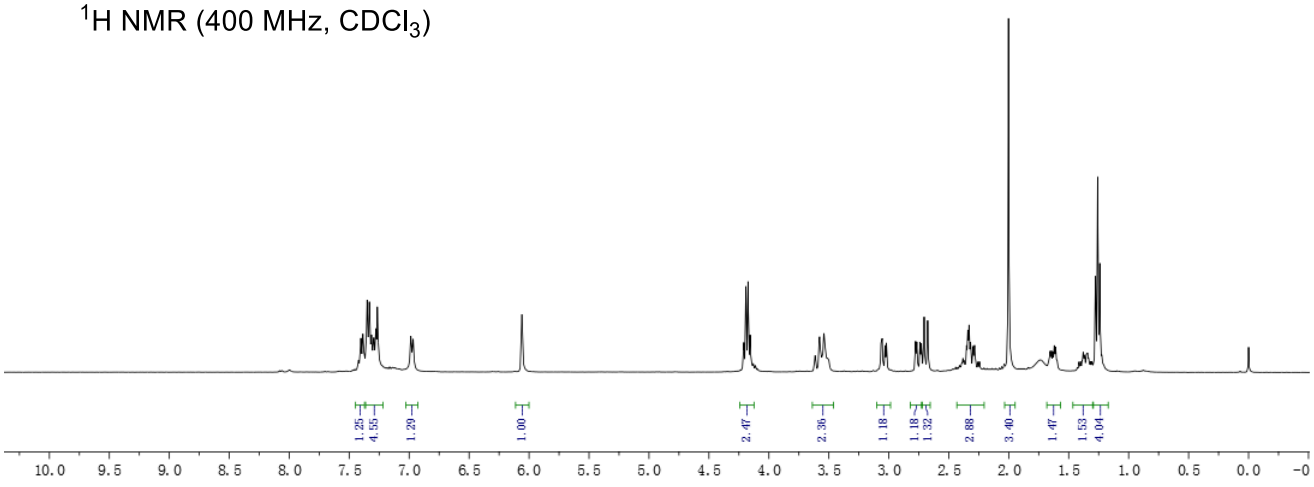


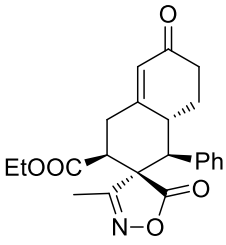
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.779	BV	0.3699	323.21811	12.09911	3.6433
2	6.915	VV	0.3635	8548.28125	385.49197	96.3567



13r

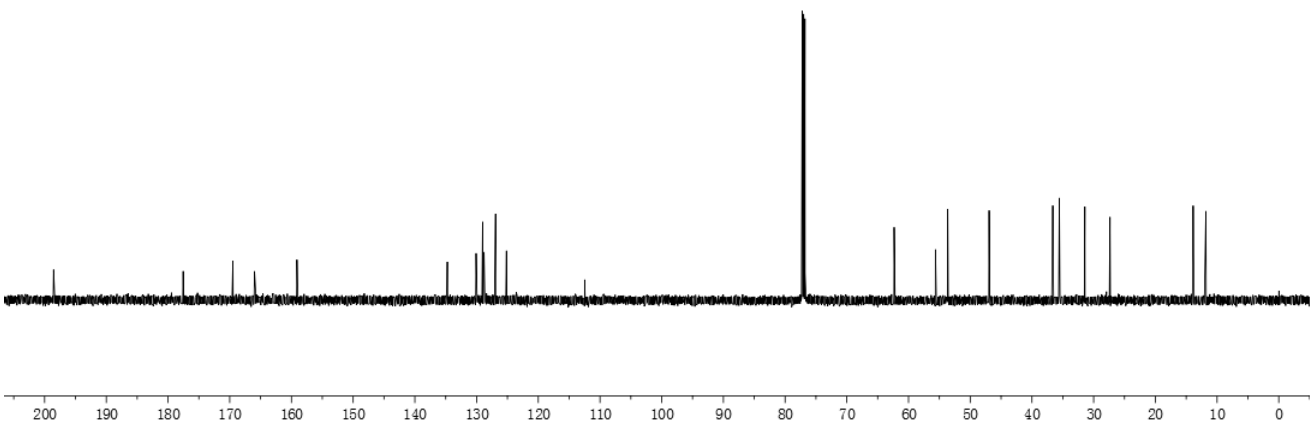
^{1}H NMR (400 MHz, $CDCl_3$)

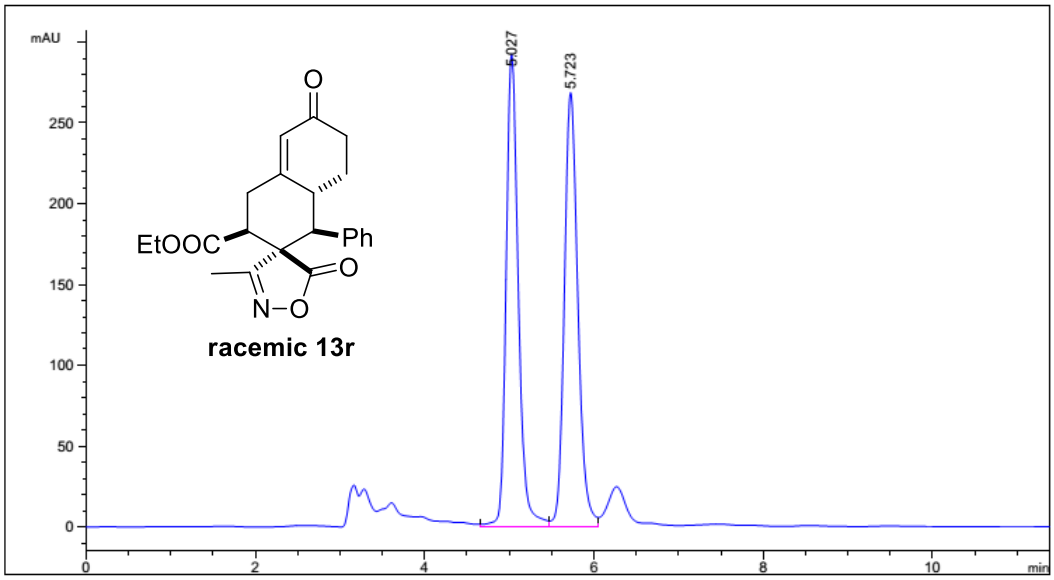




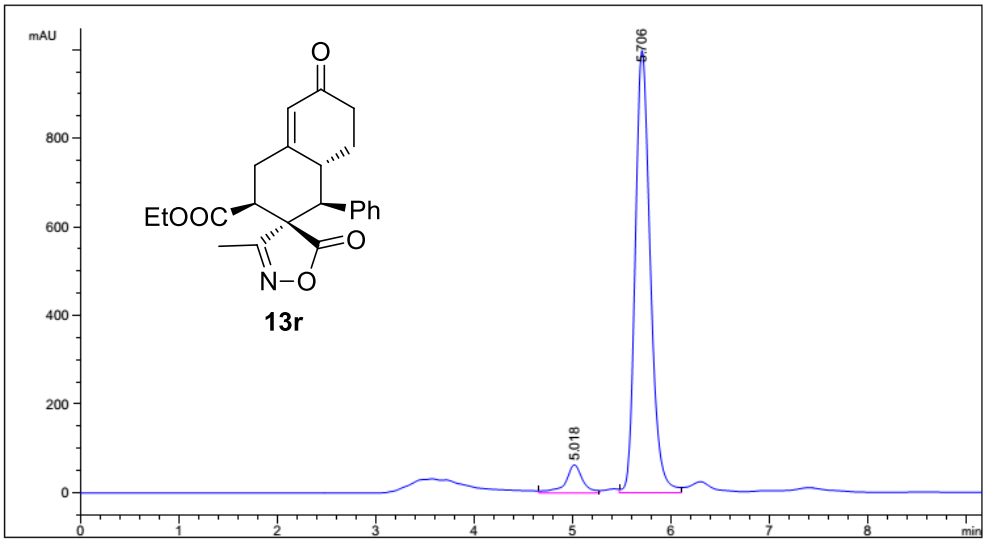
13r

^{13}C NMR (150 MHz, $CDCl_3$)

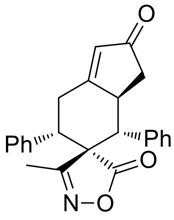




Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.027	VV	0.1529	2941.61108	291.04843	49.5351
2	5.723	VV	0.1769	2996.82837	268.27042	50.4649

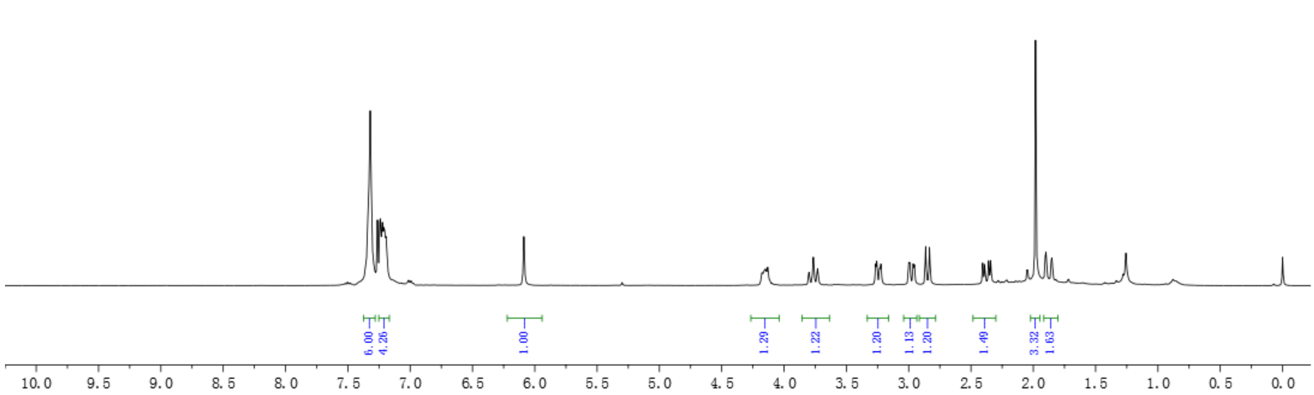


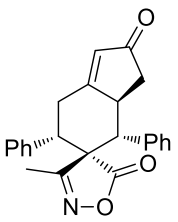
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.018	VV	0.1744	754.66699	63.13018	6.6432
2	5.706	VV	0.1654	1.06054e4	992.87402	93.3568



13s

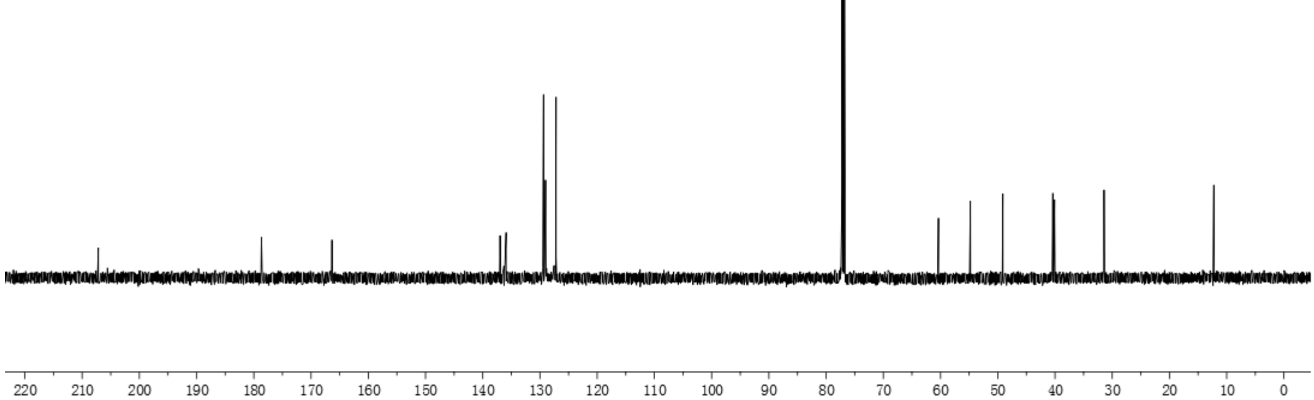
^{1}H NMR (400 MHz, $CDCl_3$)

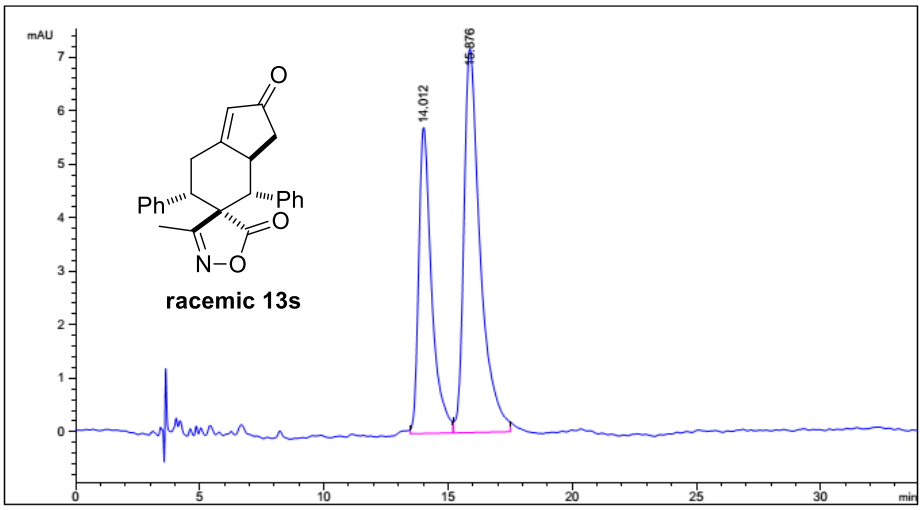




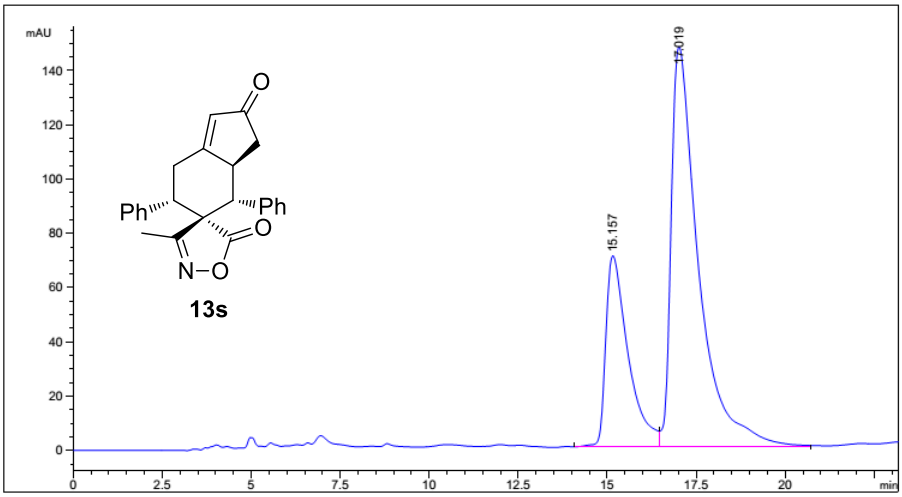
13s

^{13}C NMR (150 MHz, $CDCl_3$)

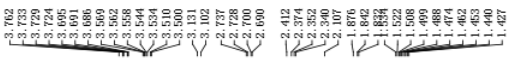


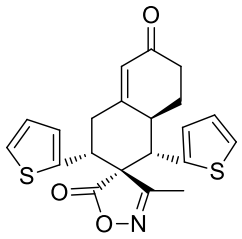


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.012	BB	0.5385	206.83646	5.71809	38.7325
2	15.876	BB	0.6719	327.17630	7.17343	61.2675



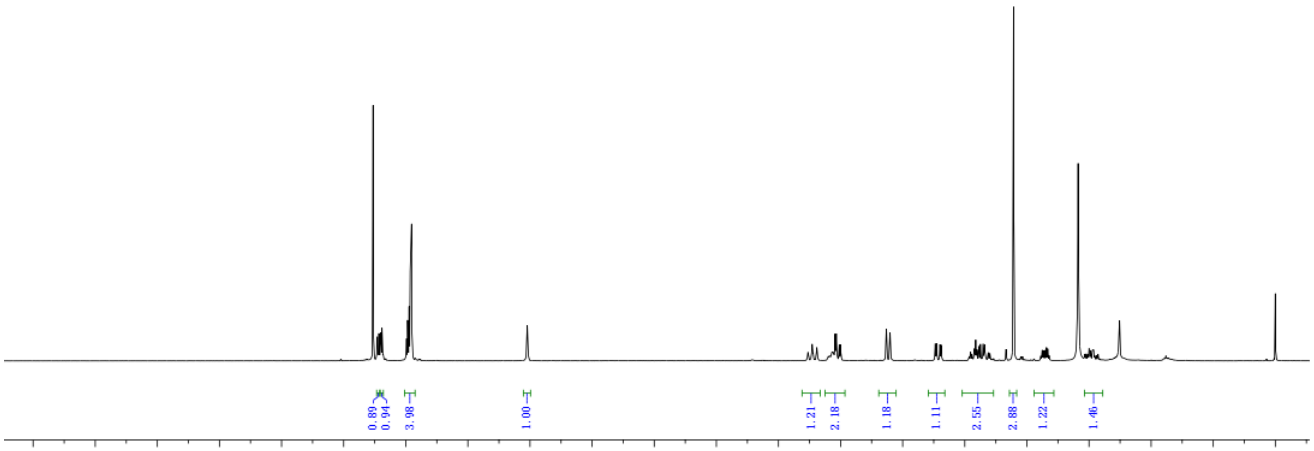
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	15.157	VV	0.6472	3105.21582	70.58112	28.1332
2	17.019	VB	0.7841	7932.33545	147.63524	71.8668

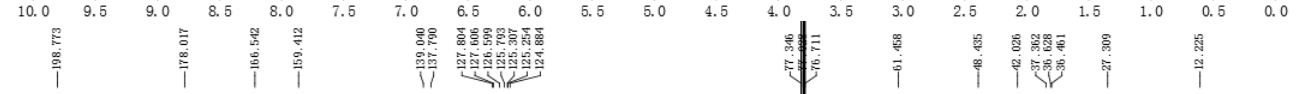


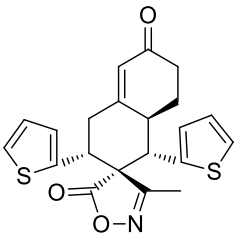


***ent*-13t**

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

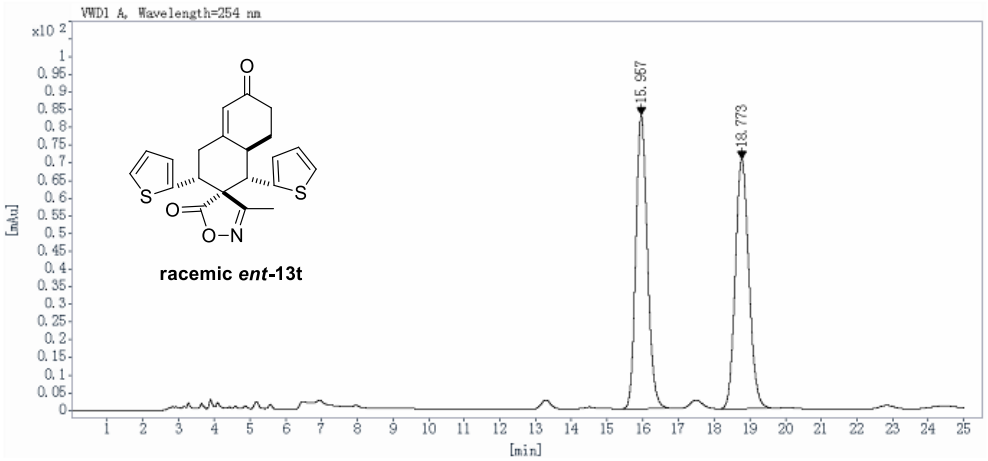




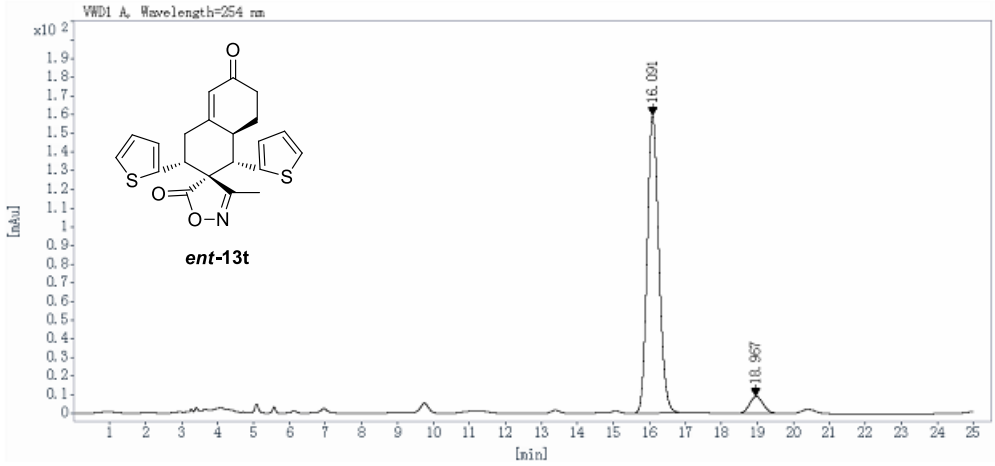


***ent*-13t**

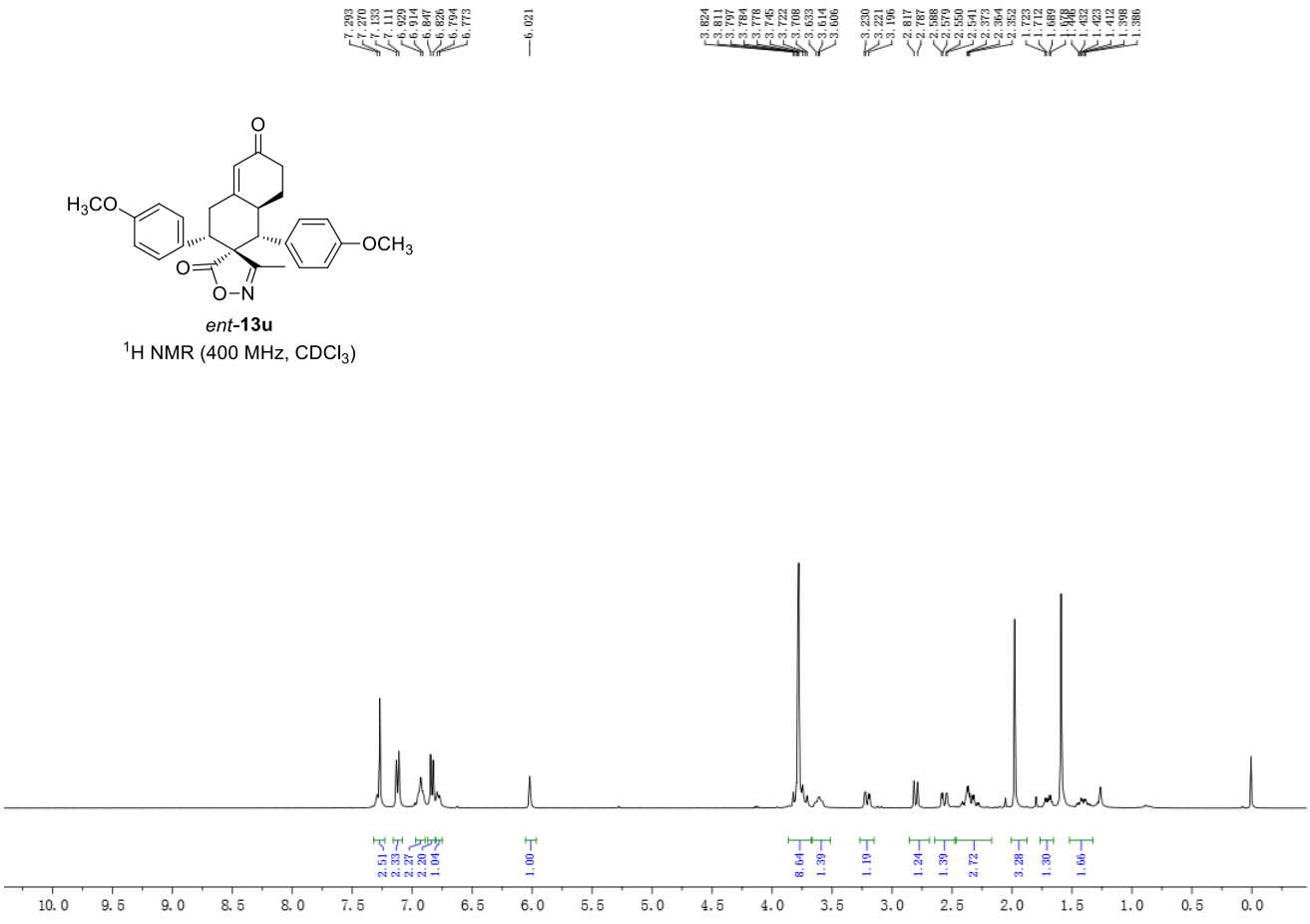
^{13}C NMR (100 MHz, $CDCl_3$)



Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
15.957	BB	0.35	82.8911	1866.9664	50.1372
18.773	BB	0.41	70.5774	1856.7478	49.8628

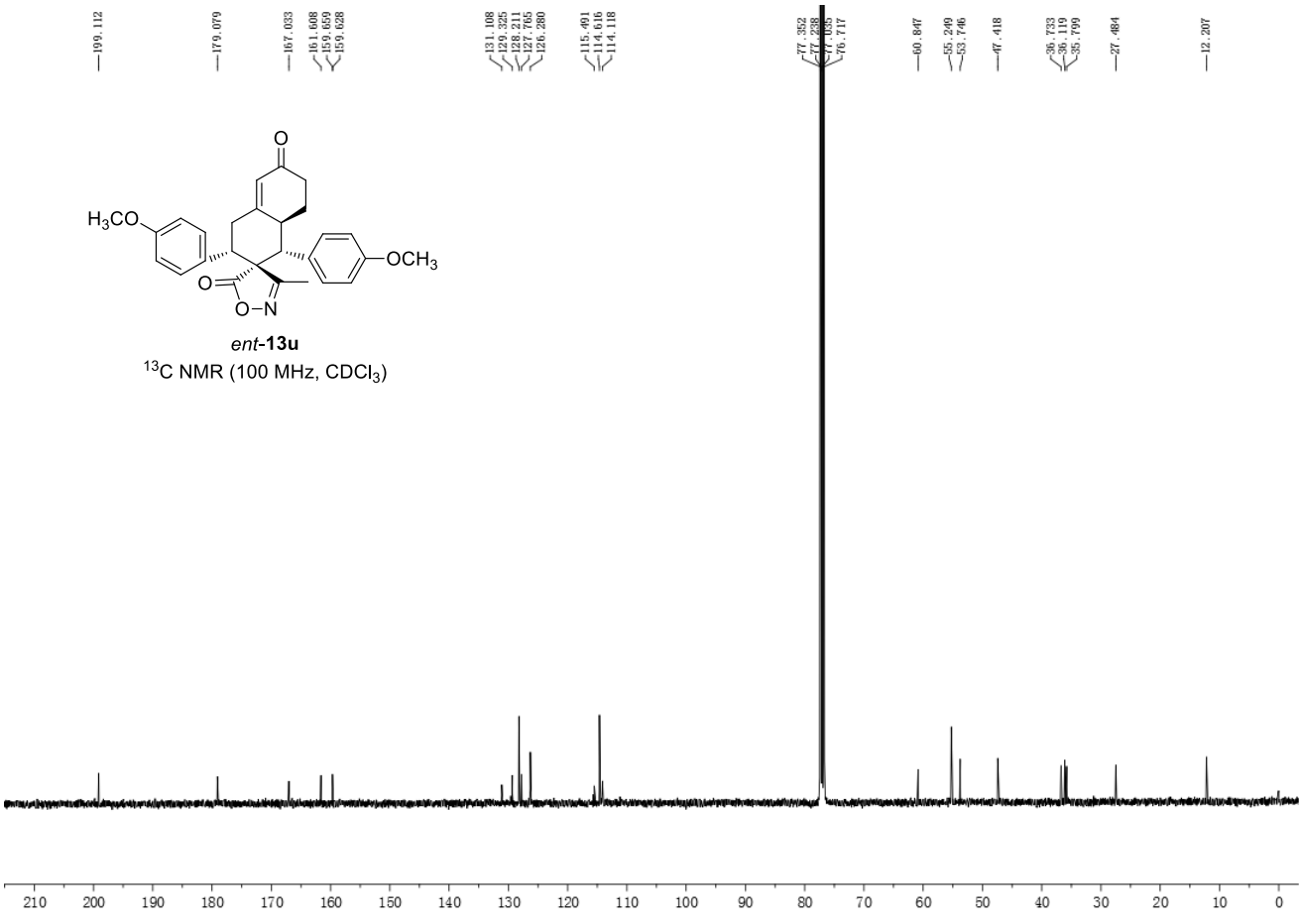


Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
16.091	BB	0.35	159.4962	3594.2729	93.5725
18.967	BB	0.41	9.3125	246.8899	6.4275



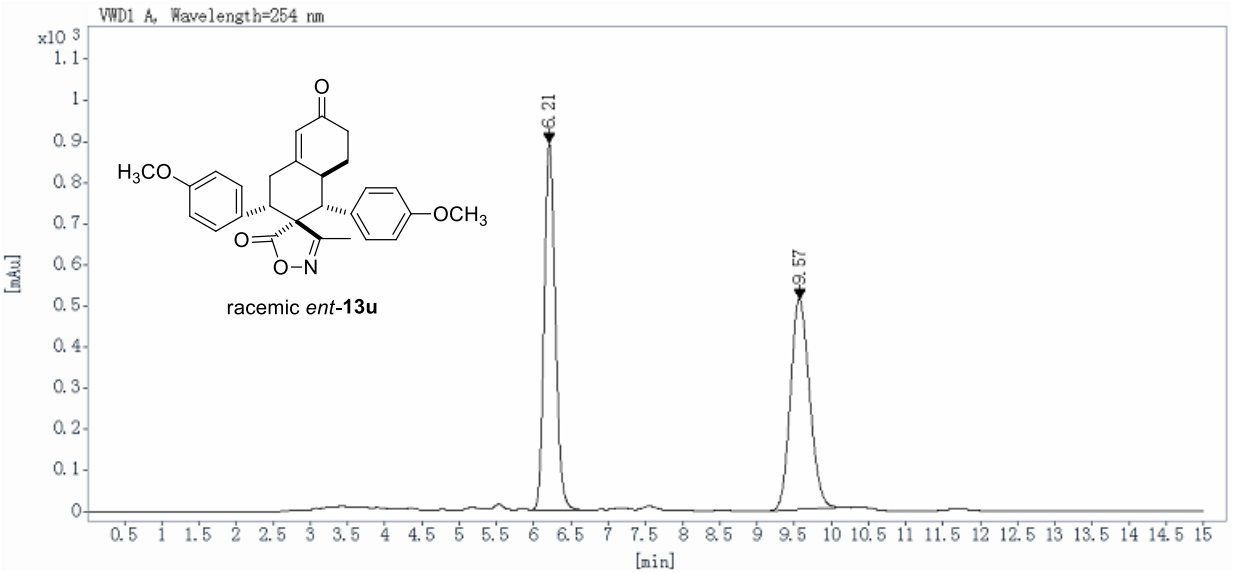
ent-**13u**

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

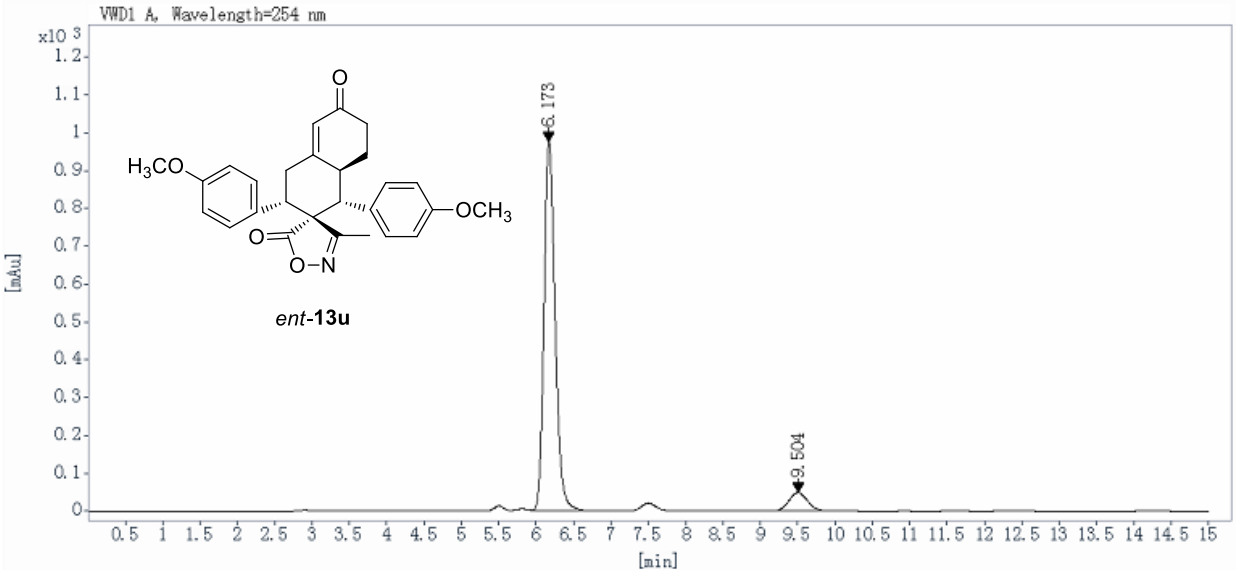


ent-**13u**

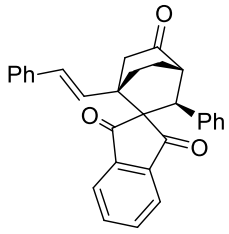
^{13}C NMR (100 MHz, $CDCl_3$)



Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
6.210	BB	0.16	891.4242	9226.4326	50.1358
9.570	BBA	0.28	511.6721	9176.4385	49.8642

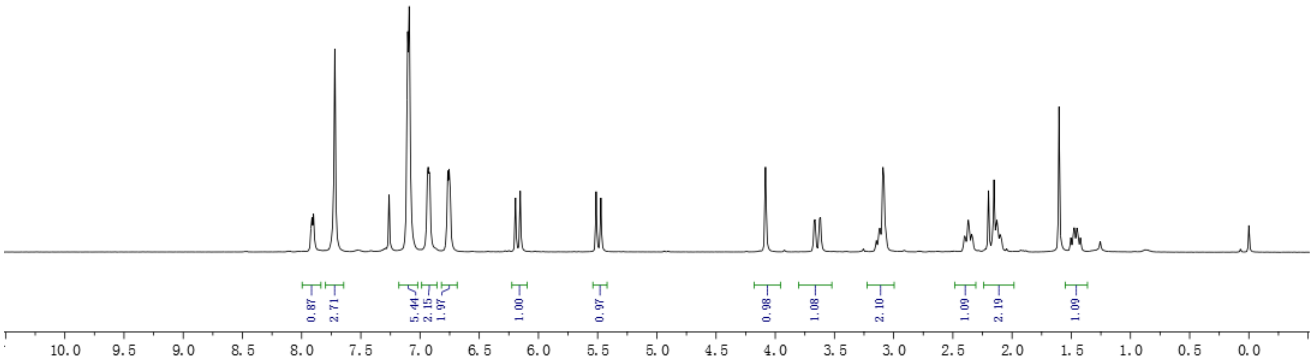


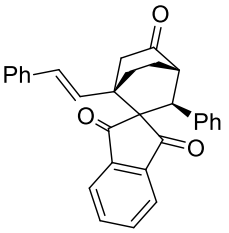
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
6.173	BV R	0.16	973.1561	10137.0020	92.3852
9.504	BBA	0.27	48.2114	835.5417	7.6148



18

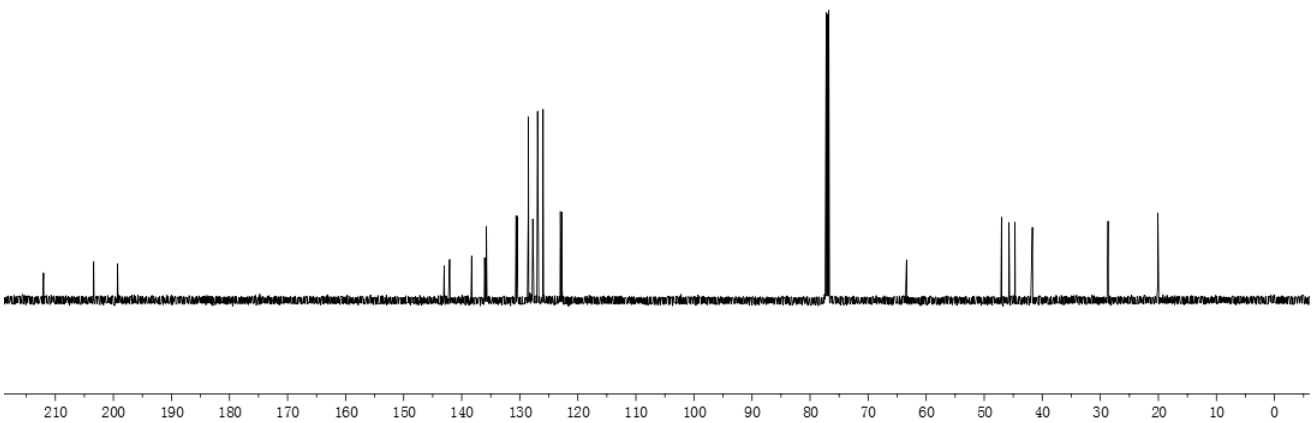
^{1}H NMR (400 MHz, $CDCl_3$)

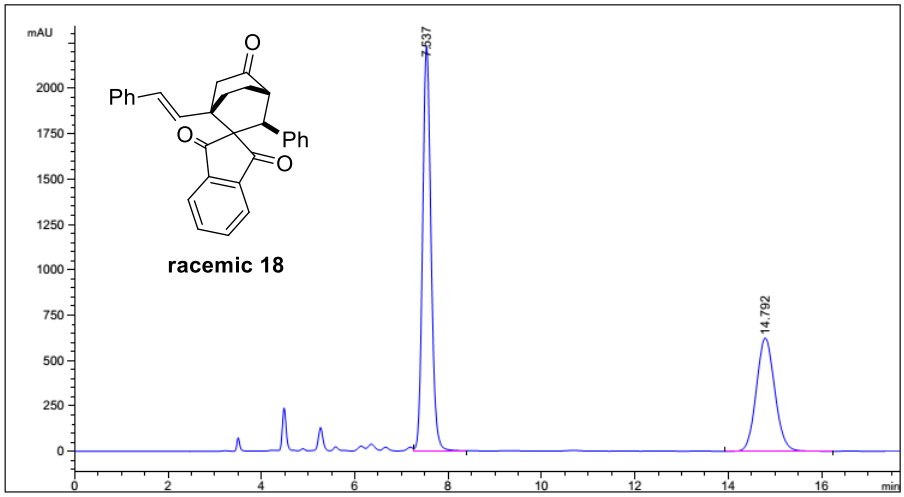




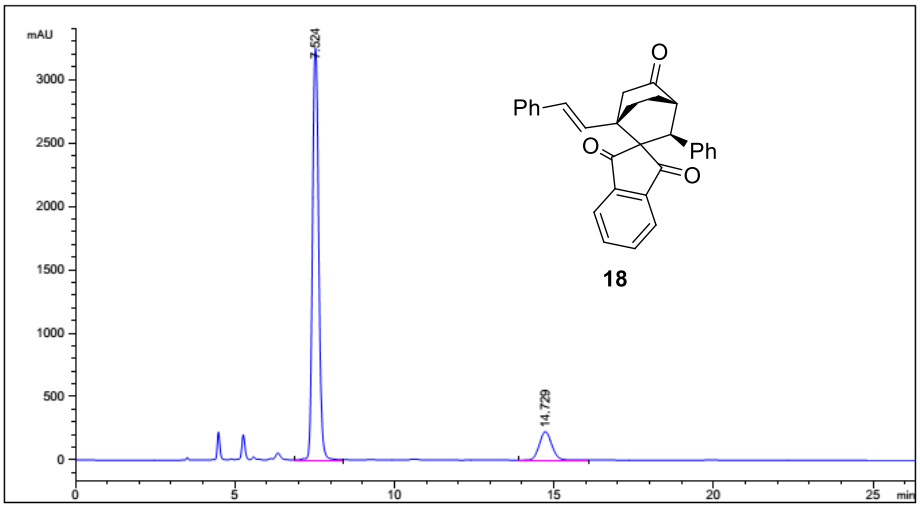
18

^{13}C NMR (150 MHz, $CDCl_3$)

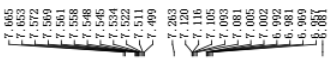


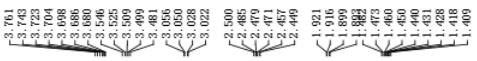


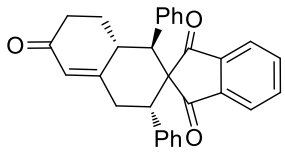
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.537	VV	0.1933	2.79915e4	2225.73975	62.0595
2	14.792	VB	0.4252	1.71128e4	623.28131	37.9405



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.524	VV	0.2096	4.37245e4	3246.36743	87.7242
2	14.729	VB	0.4218	6118.67285	225.22871	12.2758

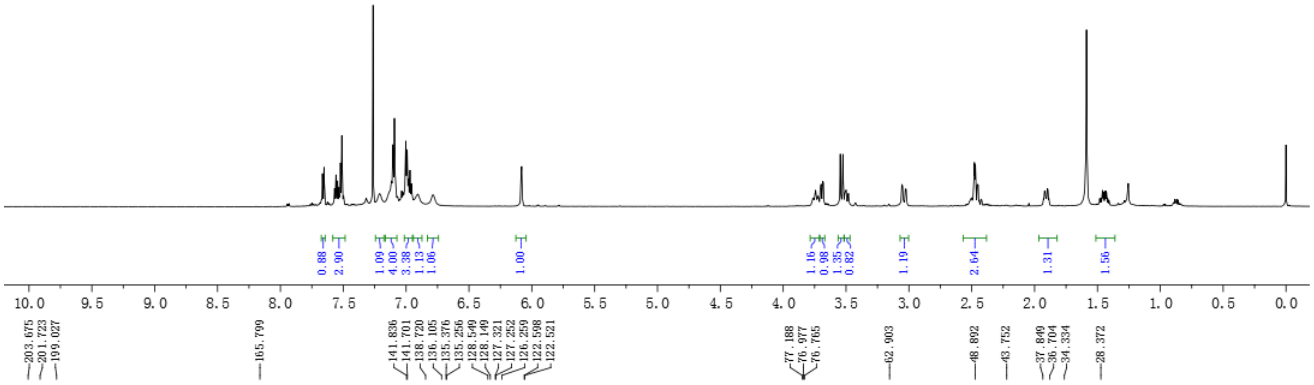


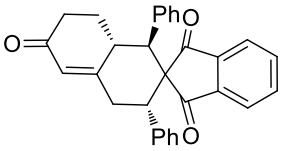




19

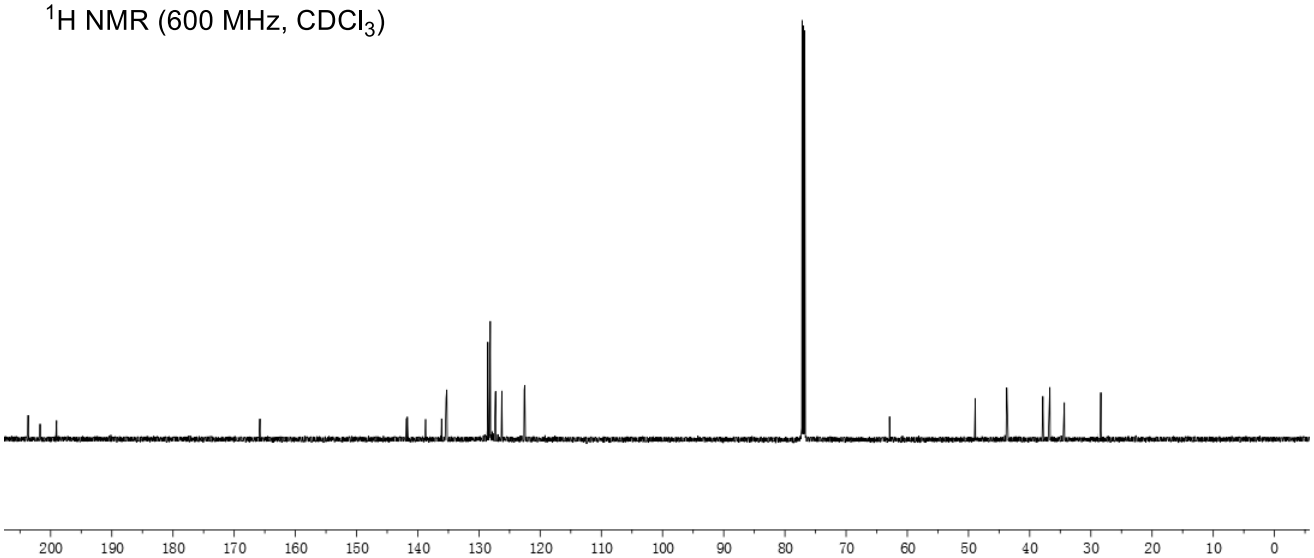
^{1}H NMR (600 MHz, $CDCl_3$)

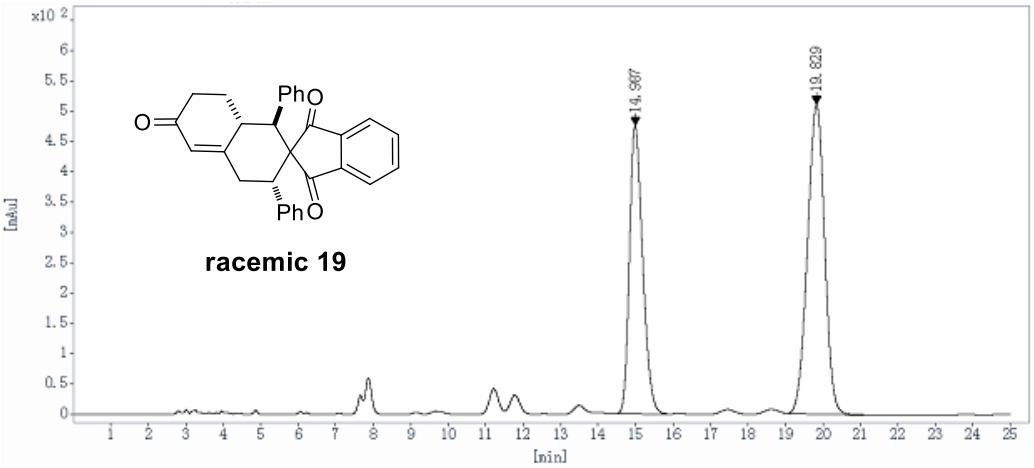




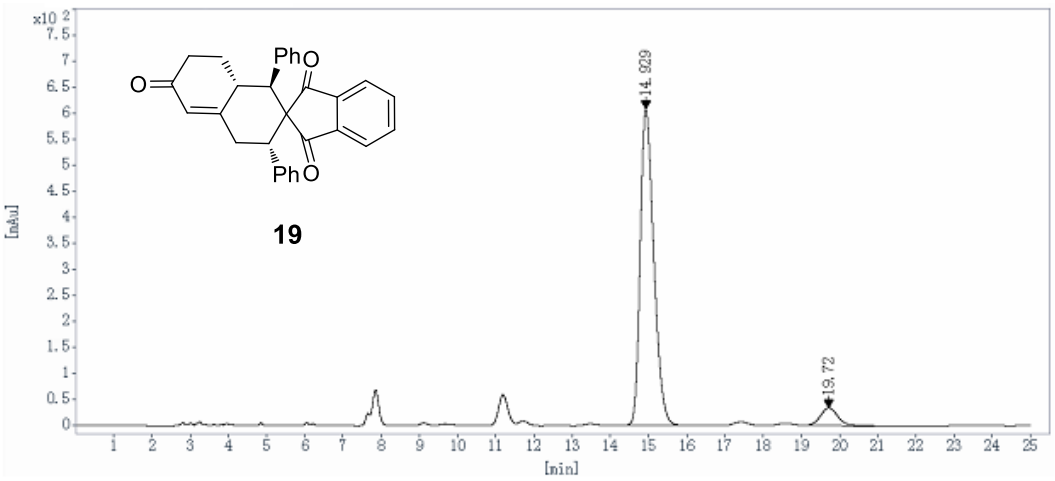
19

^{1}H NMR (600 MHz, $CDCl_3$)

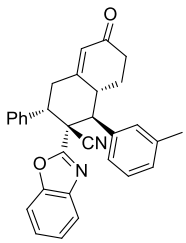




Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
14.987	BBA	0.38	475.0784	11597.4238	41.7237
19.829	BBA	0.50	510.1060	16198.3408	58.2763

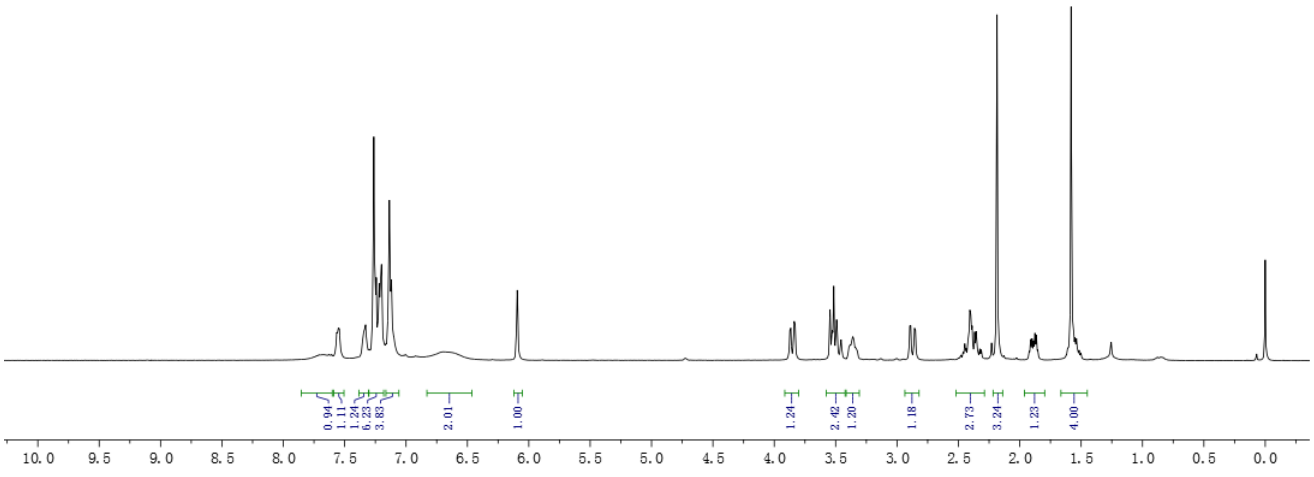


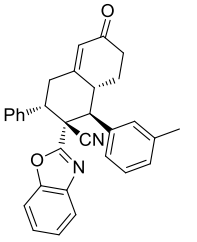
Ret Time [min]	Peak Type	Width [min]	Height [mAU]	Area [mAU*s]	Area [%]
14.929	BBA	0.38	607.2078	14986.6611	93.3873
19.720	BB	0.49	33.4445	1061.1936	6.6127



20

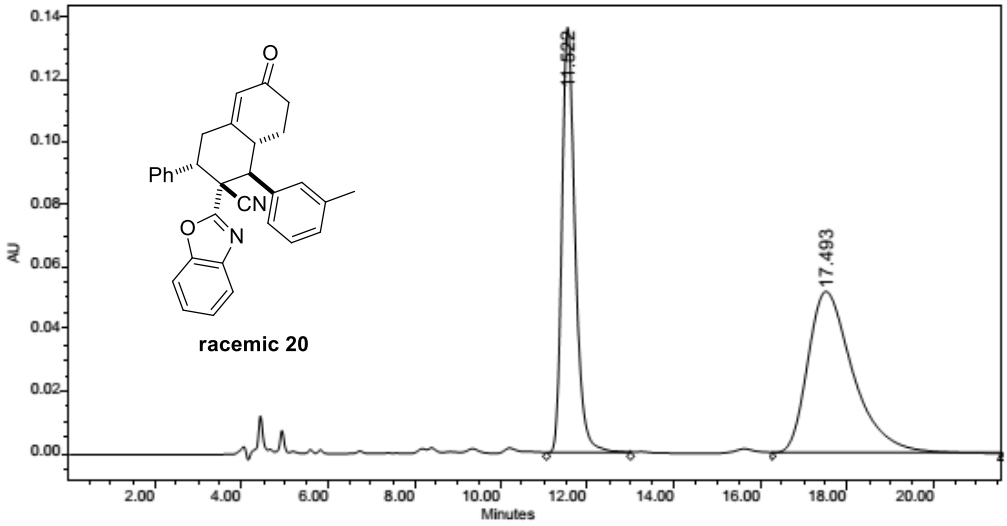
^{1}H NMR (400 MHz, $CDCl_3$)



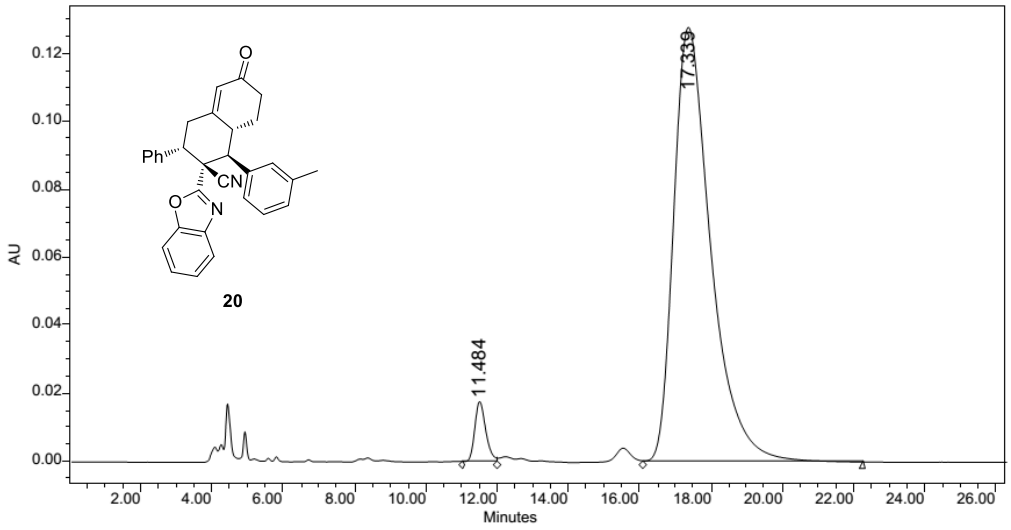


20

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



	RT (min)	Area (*sec)	% Area	Height ( )	% Height
1	11.522	2929800	43.47	137017	72.50
2	17.493	3810292	56.53	51960	27.50



	RT (min)	Area (*sec)	% Area	Height ( )	% Height
1	11.484	393757	4.06	17906	12.26
2	17.339	9294228	95.94	128098	87.74