

Supporting Information for

Palladium-Catalyzed Enantioselective Carboannulation of 1,3-Dienes with Aryl Iodides Enables Access to Chiral Indanes

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General Information

NMR spectra were recorded on a Bruker-400 MHz spectrometer. Chemical shifts (δ) are given in ppm relative to TMS. The residual solvent signals were used as references and the chemical shifts are converted to the TMS scale (CDCl_3 : $\delta_{\text{H}} = 7.26$ ppm, $\delta_{\text{C}} = 77.16$ ppm). The high resolution mass spectra were recorded on a Thermo LTQ Orbitrap XL (ESI+) or a P-SIMS-Gly of Bruker Daltonics Inc (EI+). Infrared spectra were recorded on a Nicolet MX-1E FT-IR spectrometer. Enantiomeric excesses were determined by chiral HPLC analysis performed on Waters-Breeze (2487 Dual λ Absorbance Detector and 1525 Binary HPLC Pump, UV detection monitored at 254 nm or 230 nm). Chiralcel OD-H, Chiralpak AD-H, and Chiralpak IC columns were purchased from Daicel Chemical Industries, LTD. The absolute configuration of **5** was assigned by the X-ray analysis. Optical rotations were determined at 589 nm (sodium D line) by using a Perkin-Elmer-343 polarimeter.

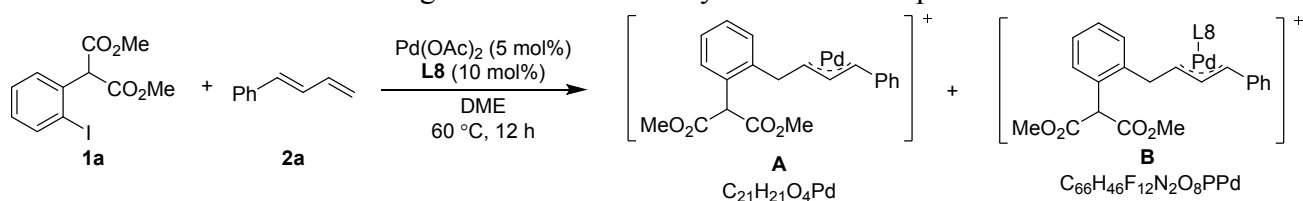
Materials: All starting materials, reagents and solvents were purchased from commercial suppliers (Aldrich, Alfa, TCI, Acros, etc.) and used as supplied unless otherwise stated. $\text{Pd}(\text{OAc})_2$ was purchased from Aldrich. Arylbutadienes were prepared by following the literature report.¹ Aryliodides were prepared by following the literature report.² All solvents were purified and dried according to standard methods prior to use, unless stated otherwise.

General Experimental Procedures

To a flame-dried and Ar-purged Schlenk tube (10 mL) were added $\text{Pd}(\text{OAc})_2$ (0.05 equiv.), phosphoramidite **L8** (0.10 equiv.), aryl iodide **1** (1.0 equiv.), arylbutadiene **2** (1.5 equiv.) and a stirring bar. The Schlenk tube was then evacuated and filled with argon. This cycle was repeated three times and followed by the addition of DIPEA (1.2 equiv.) and DME (1.0 mL) via syringe. The mixture was stirred at 60 °C for 72 h, and then cooled down to room temperature. The reaction mixture was concentrated in vacuo. The product was purified by column chromatography on silica gel (Eluent, PE/AcOEt, 50:1 to 10:1).

High-Resolution Mass Spectrometry Experiments of the Reaction Mixture

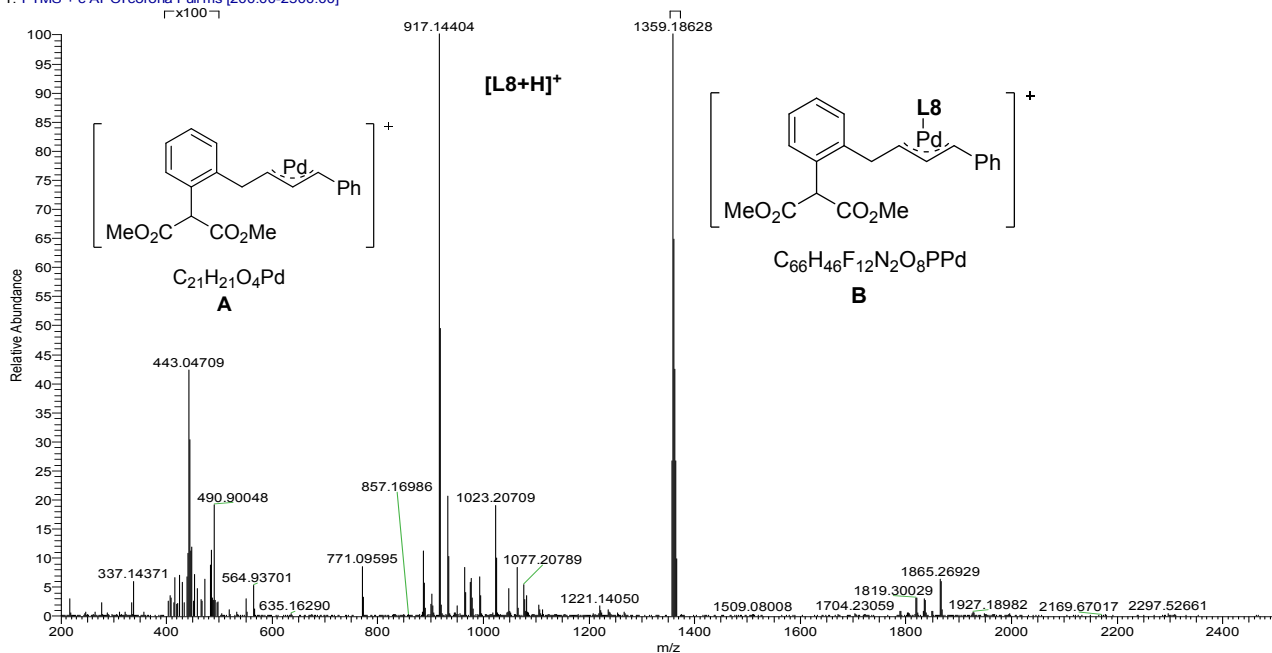
High-resolution mass spectrometry (HRMS) analysis of a reaction mixture of the palladium complex with **1a** and **2a** in the absence of DIPEA was conducted, in which the ratio of ligand/Pd was 2/1 (Figure S1). According to the observations, there were two intermediates **A** and **B** in this reaction, and one molecule of the chiral ligand **L8** was favorably coordinated to palladium.



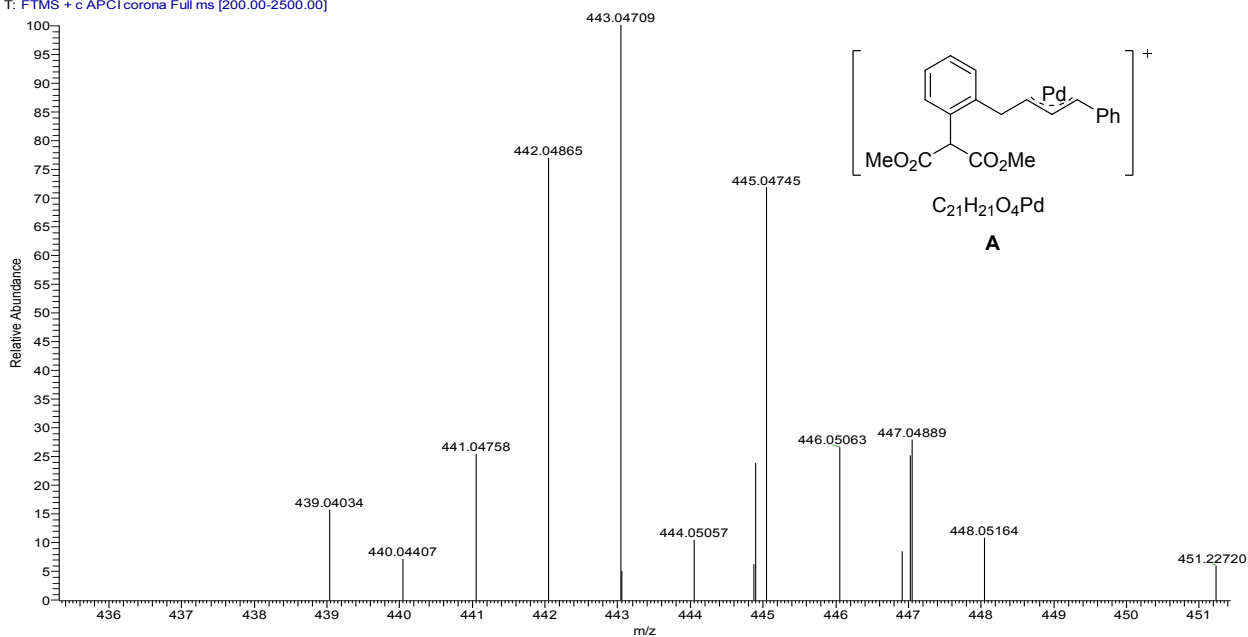
(1) (a) Burks, H. E.; Kliman, L. T.; Morken, J. P. *J. Am. Chem. Soc.* **2009**, *131*, 9134; (b) Stokes, B. J., Liao, L.-Y., Andrade, A. M., Wang, Q.-F., Sigman, M. S. *Org. Lett.* **2014**, *16*, 4066; (c) Röse, P.; Emge, S.; Yoshida, J.; Hilt, G. *Beilstein J. Org. Chem.* **2015**, *11*, 174.

(2) (a) Mei, T. S.; Wang, D. H.; Yu, J. Q. *Org. Lett.* **2010**, *12*, 3140; (b) Yang, W.; Liu, Y.; Zhang, S.; Cai, Q. *Angew. Chem. Int. Ed.* **2015**, *54*, 8805.

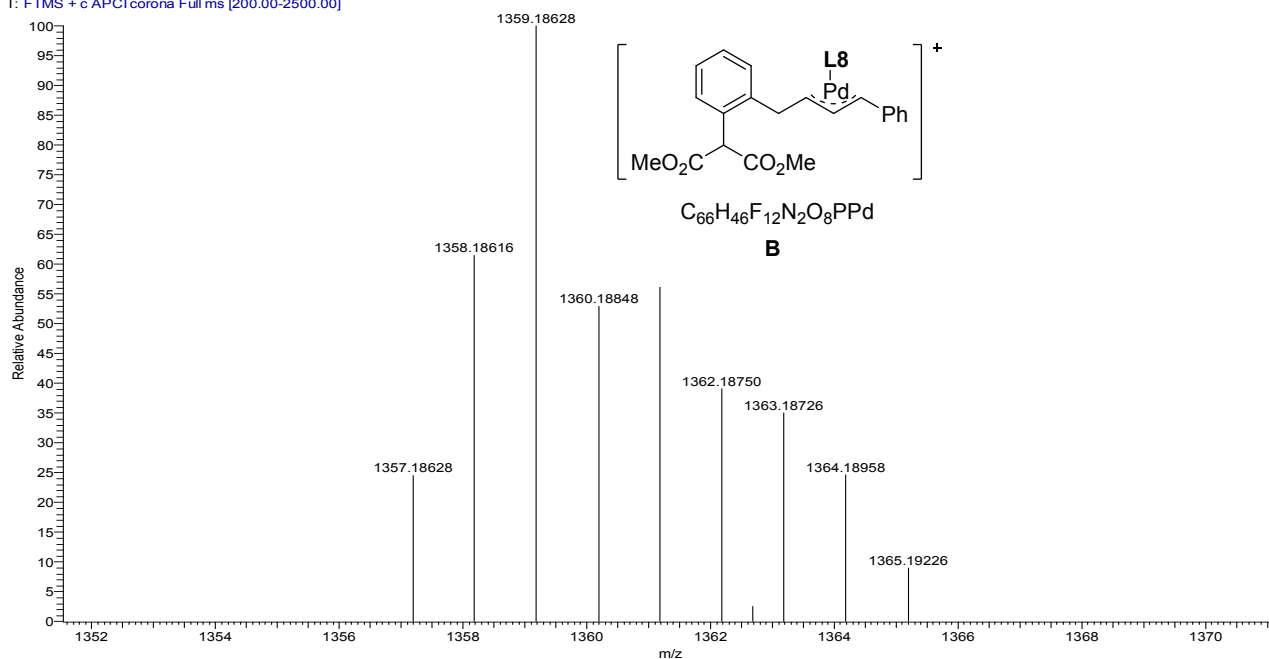
20170908_APCI+WX-107 #17 RT: 0.23 AV: 1 NL: 2.21E9
T: FTMS + c APCI corona Full ms [200.00-2500.00]



20170908_APCI+WX-107 #17 RT: 0.23 AV: 1 NL: 9.31E6
T: FTMS + c APCI corona Full ms [200.00-2500.00]



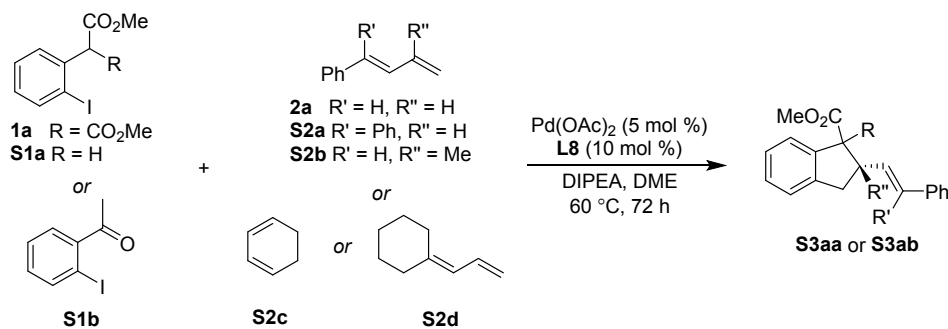
m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
442.0487	7158487	76.88	442.0485	0.13	C21 H21 O4 [105]Pd
443.0471	9311840	100	443.0469	0.17	C21 H21 O4 Pd
445.0475	6681850	71.76	445.0473	0.13	C21 H21 O4 [108]Pd



m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
1358.186	14712349	61.35	1358.185	1.61	C66 H46 O8 N2 F12 P [105]Pd
1359.186	23979614	100	1359.183	3.33	C66 H46 O8 N2 F12 P Pd
1361.186	14281759	59.56	1361.183	2.8	C66 H46 O8 N2 F12 P [108]Pd

Figure S1. High-Resolution Mass Spectra and related data

Investigation of Additional Substrates

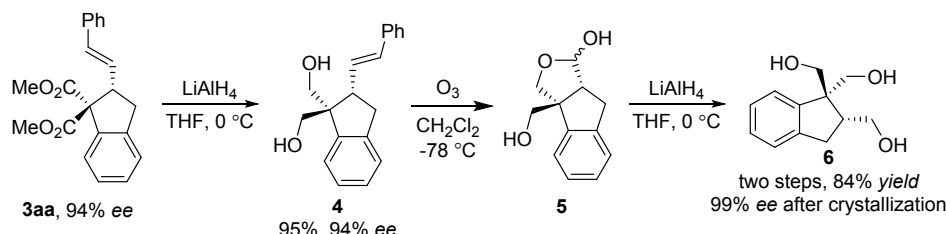


Entry	1	2	3	Yield (%)	ee (%)
1	1a	S2a	S3aa	66	55
2	1a	S2b	S3ab	46	32
3	S1a	2a	NR	-	-
4	S1b	2a	NR	-	-
5	1a	S2c	NR	-	-
6	1a	S2d	NR	-	-

Scheme S1 ^aReaction conditions: **1a**, **S1a** or **S1b** (0.10 mmol), **2a** or **S2a-S2d** (0.15 mmol), Pd(OAc)₂ (0.005 mmol), **L8** (0.010 mmol) and DIPEA (0.12 mmol) were carried out in DME (1 mL) at 60 °C for 72 h. NR = No Reaction.

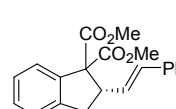
Synthetic transformations of 3aa

To demonstrate the practicability, a reaction of **1a** with **2a** on 1 mmol scale was performed, giving **3aa** in 85% yield and 94% ee, which were almost identical to those in a much smaller scale (entry 13, Table 1). The reduction of **3aa** with LiAlH₄ in THF furnished the corresponding diol **4** in 95% yield and with the retention of stereochemistry (Scheme 2). The ozonolysis of the alkene with a dimethyl sulfide workup provided a hemiacetal **5**, which was then reduced again with LiAlH₄ to give the triol **6** in an overall 84% yield for two steps and with 99% ee after crystallization. The absolute configuration of **6** was assigned by single-crystal X-ray diffraction analysis, and the configuration of **3aa** was assigned to be (*S*).³

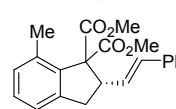


Characterization Data for the Products

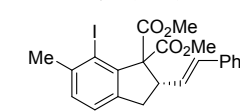
Dimethyl (*S,E*)-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (**3aa**)

 Colorless oil. Yield: 86%; ¹H NMR (400 MHz, CDCl₃) δ 7.58 (d, *J* = 8.9 Hz, 1H), 7.31 – 7.24 (m, 7H), 7.19 (t, *J* = 7.1 Hz, 1H), 6.58 (d, *J* = 15.8 Hz, 1H), 6.16 (dd, *J* = 15.8, 9.0 Hz, 1H), 3.97 (dd, *J* = 13.7, 7.9 Hz, 1H), 3.76 (s, 3H), 3.61 (s, 3H), 3.38 (dd, *J* = 15.7, 7.3 Hz, 1H), 3.00 (dd, *J* = 15.7, 5.3 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 170.14, 169.68, 143.44, 138.50, 137.14, 132.34, 128.93, 128.60, 128.56, 127.56, 127.03, 127.00, 126.41, 124.93, 69.90, 52.98, 52.54, 50.23, 37.35; **HRMS** (ESI) *m/z* (*M*+*H*)⁺ calculated for C₂₁H₂₁O₄: 337.1440, observed: 337.1434; [*α*]_D²⁰ = -107.9 (*c* = 0.7, CHCl₃); The product was analyzed by HPLC to determine the enantiomeric excess: 96% ee (CHIRALCEL OD-H, hexane/*i*-PrOH = 99/1, flow rate: 1.0 mL/min, *T* = 30 °C, 254 nm), *t_R* (major) = 13.14 min, *t_R* (minor) = 16.64 min.

Dimethyl (*S,E*)-7-methyl-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (**3ba**)

 Colorless oil. Yield: 37%; ¹H NMR (400 MHz, CDCl₃) δ 7.30 (t, *J* = 8.9 Hz, 3H), 7.25 – 7.17 (m, 3H), 7.12 – 7.06 (m, 2H), 6.49 (d, *J* = 15.7 Hz, 1H), 6.25 (dd, *J* = 15.8, 10.0 Hz, 1H), 3.89 – 3.81 (m, 1H), 3.75 (s, 3H), 3.61 (s, 3H), 3.40 (dd, *J* = 15.6, 7.3 Hz, 1H), 2.98 (dd, *J* = 15.3, 4.1 Hz, 1H), 2.36 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 170.67, 169.40, 144.15, 137.33, 137.25, 137.20, 131.91, 129.93, 129.31, 128.97, 128.62, 127.56, 126.47, 122.58, 70.47, 52.78, 52.48, 52.39, 38.27, 19.89; **HRMS** (ESI) *m/z* (*M*+*H*)⁺ calculated for C₂₂H₂₃O₄: 351.1596, observed: 351.1606; [*α*]_D²⁰ = -120.5 (*c* = 0.2, CHCl₃); The product was analyzed by HPLC to determine the enantiomeric excess: 88% ee (CHIRALCEL OD-H, hexane/*i*-PrOH = 99/1, flow rate: 1.0 mL/min, *T* = 30 °C, 254 nm), *t_R* (major) = 11.92 min, *t_R* (minor) = 12.67 min.

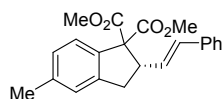
Dimethyl (*S,E*)-7-iodo-6-methyl-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (**3ca**)

 Colorless oil. Yield: 63%; ¹H NMR (400 MHz, CDCl₃) δ 7.36 (s, 1H), 7.27 – 7.20 (m, 3H), 7.19 – 7.06 (m, 3H), 6.54 (d, *J* = 15.8 Hz, 1H), 6.12 (dd, *J* = 15.8, 9.1 Hz, 1H), 3.93 (dd, *J* = 13.6, 7.8 Hz, 1H), 3.74 (s, 3H), 3.59 (s, 3H), 3.31 (dd, *J* = 15.5, 7.3 Hz, 1H), 2.91 (dd, *J* = 15.5, 5.2 Hz, 1H), 2.35 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 170.26, 169.85, 140.45, 138.54, 137.22, 136.73, 132.27, 129.94, 128.77, 128.62, 127.56, 127.45, 126.44, 124.65, 69.88, 53.01, 52.56, 50.52, 37.02, 21.58; **HRMS** (ESI) *m/z* (*M*+*H*)⁺ calculated for C₂₂H₂₂IO₄: 477.0563, observed: 477.0536; [*α*]_D²⁰ = -343.1 (*c* = 0.7, CHCl₃); The

³ CCDC 1817480 (**6**) contains the ESI crystallographic data for this paper.

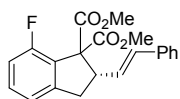
product was analyzed by HPLC to determine the enantiomeric excess: 94% ee (CHIRALCEL OD-H, hexane/i-PrOH = 99/1, flow rate: 1.0 mL/min, T = 30 °C, 254 nm), t_R (major) = 9.91 min, t_R (minor) = 13.10 min.

Dimethyl (*S,E*)-5-methyl-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (**3da**)



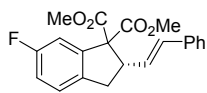
Colorless oil. Yield: 71%; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.46 (d, J = 8.4 Hz, 1H), 7.34 – 7.23 (m, 4H), 7.20 (d, J = 7.3 Hz, 1H), 7.09 (s, 2H), 6.57 (d, J = 15.8 Hz, 1H), 6.16 (dd, J = 15.8, 9.0 Hz, 1H), 3.96 (dd, J = 14.3, 7.4 Hz, 1H), 3.76 (s, 3H), 3.61 (s, 3H), 3.34 (dd, J = 15.6, 7.4 Hz, 1H), 2.95 (dd, J = 15.6, 5.4 Hz, 1H), 2.36 (s, 3H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 170.21, 169.77, 143.47, 138.84, 137.10, 135.56, 132.16, 128.62, 128.50, 127.88, 127.45, 126.55, 126.32, 125.50, 52.87, 52.45, 50.28, 37.16, 21.43; **HRMS** (ESI) m/z ($\text{M}+\text{H}$) $^+$ calculated for $\text{C}_{22}\text{H}_{23}\text{O}_4$: 351.1596, observed: 351.1594; $[\alpha]^{20}_{\text{D}} = -93.7$ (c = 0.4, CHCl_3); The product was analyzed by HPLC to determine the enantiomeric excess: 90% ee (CHIRALCEL OD-H, hexane/i-PrOH = 99/1, flow rate: 1.0 mL/min, T = 30 °C, 254 nm), t_R (major) = 12.10 min, t_R (minor) = 14.34 min.

Dimethyl (*S,E*)-7-fluoro-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (**3ea**)



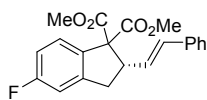
Colorless oil. Yield: 52%; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.34 – 7.24 (m, 5H), 7.21 (d, J = 6.9 Hz, 1H), 7.05 (d, J = 7.5 Hz, 1H), 6.97 (t, J = 9.0 Hz, 1H), 6.53 (d, J = 15.8 Hz, 1H), 6.17 (dd, J = 15.7, 9.7 Hz, 1H), 4.04 – 3.89 (m, 1H), 3.76 (s, 3H), 3.63 (s, 3H), 3.43 (dd, J = 16.1, 7.2 Hz, 1H), 2.97 (dd, J = 15.9, 3.1 Hz, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 169.72, 168.34, 160.11 (d, J = 253.8 Hz), 146.59 (d, J = 3.9 Hz), 137.00, 132.41, 131.09 (d, J = 7.7 Hz), 129.12, 128.66, 128.40, 127.71, 126.49, 120.76 (d, J = 3.5 Hz), 114.75 (d, J = 21.3 Hz), 68.98, 53.21, 52.75, 51.66, 38.42; **HRMS** (ESI) m/z ($\text{M}+\text{H}$) $^+$ calculated for $\text{C}_{21}\text{H}_{20}\text{FO}_4$: 355.1346, observed: 355.1344; $[\alpha]^{20}_{\text{D}} = -24.1$ (c = 0.08, CHCl_3); The product was analyzed by HPLC to determine the enantiomeric excess: >99% ee (CHIRALCEL OD-H, hexane/i-PrOH = 99/1, flow rate: 1.0 mL/min, T = 30 °C, 254 nm), t_R (major) = 16.50 min, t_R (minor) = 20.23 min.

Dimethyl (*S,E*)-6-fluoro-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (**3fa**)



Colorless oil. Yield: 24%; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.30 (m, 5H), 7.24 – 7.15 (m, 2H), 7.01 (t, J = 7.5 Hz, 1H), 6.58 (d, J = 15.8 Hz, 1H), 6.14 (dd, J = 15.8, 8.9 Hz, 1H), 3.99 (dd, J = 14.3, 7.4 Hz, 1H), 3.79 (s, 3H), 3.63 (s, 3H), 3.32 (dd, J = 15.6, 7.2 Hz, 1H), 2.95 (dd, J = 15.3, 5.0 Hz, 1H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 169.69, 169.24, 162.22 (d, J = 243.5 Hz), 140.39 (d, J = 8.6 Hz), 138.88 (d, J = 2.6 Hz), 137.10, 132.63, 128.67, 128.17, 127.70, 126.47, 125.83 (d, J = 8.6 Hz), 116.19 (d, J = 22.5 Hz), 114.22 (d, J = 23.6 Hz), 69.86, 53.16, 52.70, 50.74, 36.63; **HRMS** (ESI) m/z ($\text{M}+\text{H}$) $^+$ calculated for $\text{C}_{21}\text{H}_{20}\text{FO}_4$: 355.1346, observed: 355.1344; $[\alpha]^{20}_{\text{D}} = -134.5$ (c = 0.04, CHCl_3); The product was analyzed by HPLC to determine the enantiomeric excess: 94% ee (CHIRALCEL OD-H, hexane/i-PrOH = 99/1, flow rate: 1.0 mL/min, T = 30 °C, 254 nm), t_R (major) = 10.72 min, t_R (minor) = 13.04 min.

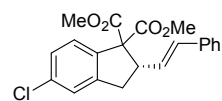
Dimethyl (*S,E*)-5-fluoro-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (**3ga**)



Colorless oil. Yield: 68%; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.53 (dd, J = 8.4, 5.6 Hz, 1H), 7.34 – 7.26 (m, 4H), 7.24 – 7.18 (m, 1H), 7.05 – 6.81 (m, 2H), 6.57 (d, J = 15.7 Hz, 1H), 6.13 (dd, J = 15.8, 9.1 Hz, 1H), 3.99 (dd, J = 14.1, 7.4 Hz, 1H), 3.77 (s, 3H), 3.62 (s, 3H), 3.37 (dd, J = 15.9, 7.4 Hz, 1H), 2.97 (dd, J = 15.8, 5.1 Hz, 1H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 170.02, 169.55, 163.59 (d, J = 246.9 Hz), 145.79 (d, J = 8.5 Hz), 137.07, 134.19 (d, J = 2.5 Hz), 132.65, 128.67, 128.41 (d, J = 9.1 Hz), 128.16, 127.71, 126.47, 114.34 (d, J = 22.8 Hz), 111.92 (d, J = 22.4 Hz), 69.14, 53.07, 52.65, 50.60, 37.39; **HRMS** (ESI) m/z ($\text{M}+\text{H}$) $^+$ calculated for $\text{C}_{21}\text{H}_{20}\text{FO}_4$: 355.1346, observed: 355.1340; $[\alpha]^{20}_{\text{D}} = -84.3$ (c = 0.3, CHCl_3); The product

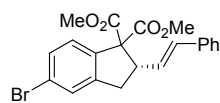
was analyzed by HPLC to determine the enantiomeric excess: 99% ee (CHIRALCEL OD-H, hexane/i-PrOH = 99/1, flow rate: 1.0 mL/min, T = 30 °C, 254 nm), t_R (major) = 11.52 min, t_R (minor) = 14.45 min.

Dimethyl (*S,E*)-5-chloro-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ha)



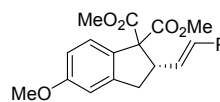
Colorless oil. Yield: 59%; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.49 (d, J = 8.3 Hz, 1H), 7.30 – 7.25 (m, 3H), 7.25 – 7.16 (m, 4H), 6.55 (d, J = 15.8 Hz, 1H), 6.10 (dd, J = 15.8, 9.0 Hz, 1H), 3.95 (dd, J = 13.9, 7.3 Hz, 1H), 3.75 (s, 3H), 3.60 (s, 3H), 3.34 (dd, J = 15.9, 7.3 Hz, 1H), 2.95 (dd, J = 15.9, 5.2 Hz, 1H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 169.79, 169.33, 145.38, 137.09, 137.00, 134.95, 132.72, 128.67, 128.22, 127.98, 127.74, 127.45, 126.46, 125.18, 69.35, 53.15, 52.71, 50.37, 37.23; **HRMS** (ESI) m/z ($M+H$) $^+$ calculated for $\text{C}_{21}\text{H}_{20}\text{ClO}_4$: 371.1050, observed: 371.1040; $[\alpha]^{20}_D$ = -51.9 (c = 0.2, CHCl_3); The product was analyzed by HPLC to determine the enantiomeric excess: 90% ee (CHIRALCEL OD-H, hexane/i-PrOH = 99/1, flow rate: 1.0 mL/min, T = 30 °C, 254 nm), t_R (major) = 13.07 min, t_R (minor) = 15.64 min.

Dimethyl (*S,E*)-5-bromo-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ia)



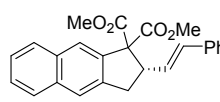
Colorless oil. Yield: 52%; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.48 – 7.36 (m, 3H), 7.32 – 7.25 (m, 4H), 7.22 – 7.16 (m, 1H), 6.55 (d, J = 15.7 Hz, 1H), 6.10 (dd, J = 15.7, 9.0 Hz, 1H), 3.95 (dd, J = 14.2, 7.3 Hz, 1H), 3.75 (s, 3H), 3.60 (s, 3H), 3.35 (dd, J = 15.8, 7.2 Hz, 1H), 2.96 (dd, J = 15.9, 5.1 Hz, 1H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 169.70, 169.23, 145.74, 137.62, 136.99, 132.74, 130.33, 128.67, 128.61, 128.16, 127.84 (d, J = 19.3 Hz), 126.46, 123.16, 69.44, 53.16, 52.72, 50.30, 37.20; **HRMS** (ESI) m/z ($M+H$) $^+$ calculated for $\text{C}_{21}\text{H}_{20}\text{BrO}_4$: 415.0545, observed: 415.0543; $[\alpha]^{20}_D$ = -38.3 (c = 0.2, CHCl_3); The product was analyzed by HPLC to determine the enantiomeric excess: 85% ee (CHIRALCEL OD-H, hexane/i-PrOH = 99/1, flow rate: 1.0 mL/min, T = 30 °C, 254 nm), t_R (major) = 11.68 min, t_R (minor) = 13.81 min.

Dimethyl (*S,E*)-5-methoxy-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ja)

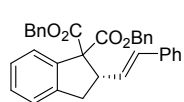


Colorless oil. Yield: 40%; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.47 (d, J = 8.4 Hz, 1H), 7.34 – 7.23 (m, 4H), 7.20 (t, J = 7.0 Hz, 1H), 6.81 (d, J = 12.4 Hz, 2H), 6.57 (d, J = 15.8 Hz, 1H), 6.15 (dd, J = 15.8, 9.0 Hz, 1H), 3.96 (dd, J = 14.0, 7.6 Hz, 1H), 3.81 (s, 3H), 3.76 (s, 3H), 3.61 (s, 3H), 3.35 (dd, J = 15.7, 7.2 Hz, 1H), 2.96 (dd, J = 15.7, 5.1 Hz, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 170.29, 169.89, 160.47, 144.98, 137.06, 132.21, 130.50, 128.56, 128.51, 127.64, 127.47, 126.33, 113.21, 109.81, 69.04, 55.42, 52.85, 52.45, 50.41, 37.44; **HRMS** (ESI) m/z ($M+H$) $^+$ calculated for $\text{C}_{22}\text{H}_{23}\text{O}_5$: 367.1545, observed: 367.1546; $[\alpha]^{20}_D$ = -37.1 (c = 0.5, CHCl_3); The product was analyzed by HPLC to determine the enantiomeric excess: 86% ee (CHIRALCEL OD-H, hexane/i-PrOH = 99/1, flow rate: 1.0 mL/min, T = 30 °C, 254 nm), t_R (major) = 21.12 min, t_R (minor) = 25.90 min.

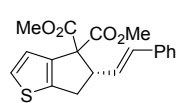
Dimethyl (*S,E*)-2-styryl-2,3-dihydro-1*H*-cyclopenta[*b*]naphthalene-1,1-dicarboxylate (3ka)



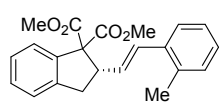
Colorless oil. Yield: 88%; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.07 (s, 1H), 7.86 (d, J = 7.7 Hz, 1H), 7.78 (d, J = 7.5 Hz, 1H), 7.71 (s, 1H), 7.49 – 7.38 (m, 2H), 7.30 (d, J = 7.5 Hz, 2H), 7.26 – 7.21 (m, 2H), 7.18 (t, J = 7.1 Hz, 1H), 6.60 (d, J = 15.8 Hz, 1H), 6.16 (dd, J = 15.9, 8.8 Hz, 1H), 4.02 (dd, J = 14.6, 7.0 Hz, 1H), 3.79 (s, 3H), 3.63 (s, 3H), 3.52 (dd, J = 15.9, 7.2 Hz, 1H), 3.16 (dd, J = 15.8, 5.5 Hz, 1H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 170.07, 169.65, 141.22, 137.30, 137.13, 134.12, 132.98, 132.43, 128.64, 128.39, 127.63, 127.56, 126.45, 126.32, 125.49, 123.15, 69.38, 53.17, 52.68, 50.71, 36.87; **HRMS** (ESI) m/z ($M+H$) $^+$ calculated for $\text{C}_{25}\text{H}_{23}\text{O}_4$: 387.1596, observed: 387.1596; $[\alpha]^{20}_D$ = -34.1 (c = 0.7, CHCl_3); The product was analyzed by HPLC to determine the enantiomeric excess: 84% ee (CHIRALPAK IC, hexane/i-PrOH = 99/1, flow rate: 1.0 mL/min, T = 30 °C, 254 nm), t_R (minor) = 21.66 min, t_R (major) = 27.79 min.

Dibenzyl (*S,E*)-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3la)

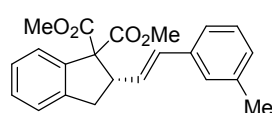
Colorless oil. Yield: 85%; ¹H NMR (400 MHz, CDCl₃) δ 7.59 (d, *J* = 7.4 Hz, 1H), 7.34 – 7.27 (m, 5H), 7.26 – 7.16 (m, 11H), 7.11 (d, *J* = 7.1 Hz, 2H), 6.48 (d, *J* = 15.8 Hz, 1H), 6.16 (dd, *J* = 15.8, 9.1 Hz, 1H), 5.20 (d, *J* = 12.4 Hz, 1H), 5.10 (d, *J* = 12.4 Hz, 1H), 4.99 (q, *J* = 12.3 Hz, 2H), 3.97 (dd, *J* = 15.2, 6.8 Hz, 1H), 3.37 (dd, *J* = 15.6, 7.4 Hz, 1H), 3.01 (dd, *J* = 15.6, 5.6 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 170.05, 169.65, 144.35, 141.51, 137.04, 132.78, 128.67, 128.46, 128.17, 127.72, 126.49, 123.25, 66.79, 55.14, 53.01, 52.69, 34.13; HRMS (ESI) *m/z* (M+H)⁺ calculated for C₃₃H₂₉O₄: 489.2066, observed: 489.2069; [α]_D²⁰ = -86.8 (c = 0.5, CHCl₃); The product was analyzed by HPLC to determine the enantiomeric excess: 86% ee (CHIRALPAK IC, hexane/*i*-PrOH = 99/1, flow rate: 1.0 mL/min, T = 30 °C, 254 nm), *t*_R (major) = 14.62 min, *t*_R (minor) = 16.05 min.

Dimethyl (*S,E*)-5-styryl-5,6-dihydro-4*H*-cyclopenta[*b*]thiophene-4,4-dicarboxylate (3ma)

Colorless oil. Yield: 36%; ¹H NMR (400 MHz, CDCl₃) δ 7.56 (d, *J* = 7.5 Hz, 1H), 7.27 – 7.21 (m, 4H), 6.40 – 6.34 (m, 1H), 6.31 (s, 1H), 6.17 (d, *J* = 2.9 Hz, 1H), 6.10 (dd, *J* = 15.7, 9.0 Hz, 1H), 3.90 (dd, *J* = 15.0, 7.2 Hz, 1H), 3.76 (s, 3H), 3.62 (s, 3H), 3.31 (dd, *J* = 15.5, 7.4 Hz, 1H), 2.98 (dd, *J* = 15.7, 6.0 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 169.44, 169.03, 143.50, 138.57, 137.06, 135.47, 135.33, 132.64, 128.98, 128.64, 128.55, 128.54, 128.37 (d, *J* = 1.5 Hz), 128.27, 128.19, 127.54, 127.06, 126.51, 124.95, 69.79, 67.60, 67.32, 50.45, 37.58; HRMS (ESI) *m/z* (M+H)⁺ calculated for C₁₉H₁₈O₄S: 343.1004, observed: 343.1007; [α]_D²⁰ = -41.0 (c = 0.2, CHCl₃); The product was analyzed by HPLC to determine the enantiomeric excess: 95% ee (CHIRALPAK AD-H, hexane/*i*-PrOH = 95/5, flow rate: 1.0 mL/min, T = 30 °C, 254 nm), *t*_R (major) = 10.30 min, *t*_R (minor) = 11.69 min.

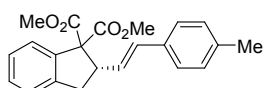
Dimethyl (*S,E*)-2-(2-methylstyryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ab)

Colorless oil. Yield: 42%; ¹H NMR (400 MHz, CDCl₃) δ 7.56 (d, *J* = 7.4 Hz, 1H), 7.30 – 7.23 (m, 4H), 7.14 – 6.99 (m, 3H), 6.76 (d, *J* = 15.5 Hz, 1H), 6.00 (dd, *J* = 15.5, 9.1 Hz, 1H), 3.97 (dd, *J* = 14.0, 7.7 Hz, 1H), 3.75 (s, 3H), 3.62 (s, 3H), 3.38 (dd, *J* = 15.5, 7.2 Hz, 1H), 2.98 (dd, *J* = 15.7, 5.0 Hz, 1H), 2.31 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 170.22, 169.75, 143.49, 138.55, 136.36, 135.35, 130.36, 130.25, 130.00, 128.95, 127.53, 127.10, 127.06, 126.20, 125.96, 124.94, 69.96, 53.00, 52.60, 50.53, 37.58, 19.89; HRMS (ESI) *m/z* (M+H)⁺ calculated for C₂₂H₂₃O₄: 351.1596, observed: 351.1593; [α]_D²⁰ = -33.2 (c = 0.4, CHCl₃); The product was analyzed by HPLC to determine the enantiomeric excess: 93% ee (CHIRALPAK AD-H, hexane/*i*-PrOH = 95/5, flow rate: 1.0 mL/min, T = 30 °C, 254 nm), *t*_R (major) = 6.13 min, *t*_R (minor) = 8.05 min.

Dimethyl (*S,E*)-2-(3-methylstyryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ac)

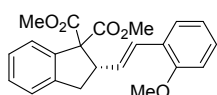
Colorless oil. Yield: 74%; ¹H NMR (400 MHz, CDCl₃) δ 7.59 – 7.51 (m, 1H), 7.28 – 7.21 (m, 3H), 7.15 – 7.04 (m, 3H), 6.98 (d, *J* = 7.2 Hz, 1H), 6.51 (d, *J* = 15.8 Hz, 1H), 6.10 (dd, *J* = 15.8, 9.1 Hz, 1H), 3.97 – 3.85 (m, 1H), 3.73 (s, 3H), 3.58 (s, 3H), 3.35 (dd, *J* = 15.7, 7.3 Hz, 1H), 2.95 (dd, *J* = 15.7, 5.2 Hz, 1H), 2.27 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 170.18, 169.71, 143.49, 138.52, 138.18, 137.10, 132.46, 128.94, 128.51, 128.40, 128.31, 127.06, 127.05, 127.02, 124.96, 123.70, 69.94, 53.00, 52.58, 50.29, 37.44, 21.47; HRMS (ESI) *m/z* (M+Na)⁺ calculated for C₂₂H₂₂O₄Na: 373.1416, observed: 373.1428; [α]_D²⁰ = (c = 0.4, CHCl₃); The product was analyzed by HPLC to determine the enantiomeric excess: 84% ee (CHIRALPAK AD-H, hexane/*i*-PrOH = 95/5, flow rate: 1.0 mL/min, T = 30 °C, 254 nm), *t*_R (major) = 7.43 min, *t*_R (minor) = 8.62 min.

Dimethyl (*S,E*)-2-(4-methylstyryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ad)



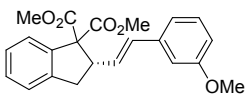
Colorless oil. Yield: 37%; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.57 (d, $J = 7.4$ Hz, 1H), 7.35 – 7.26 (m, 3H), 7.20 (d, $J = 7.7$ Hz, 2H), 7.07 (d, $J = 7.7$ Hz, 2H), 6.54 (d, $J = 15.9$ Hz, 1H), 6.09 (dd, $J = 15.8, 8.9$ Hz, 1H), 3.95 (dd, $J = 14.4, 7.4$ Hz, 1H), 3.76 (s, 3H), 3.61 (s, 3H), 3.37 (dd, $J = 15.9, 7.2$ Hz, 1H), 2.98 (dd, $J = 15.6, 5.2$ Hz, 1H), 2.30 (s, 3H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 170.22, 169.75, 143.55, 138.55, 137.41, 134.40, 132.22, 129.32, 128.94, 127.51, 127.05, 126.35, 124.96, 69.99, 53.00, 52.57, 50.28, 37.44, 21.30; **HRMS** (ESI) m/z ($\text{M}+\text{H}$) $^+$ calculated for $\text{C}_{22}\text{H}_{23}\text{O}_4$: 351.1596, observed: 351.1599; $[\alpha]^{20}_{\text{D}} = -47.9$ ($c = 0.4$, CHCl_3); The product was analyzed by HPLC to determine the enantiomeric excess: 90% ee (CHIRALCEL OD-H, hexane/*i*-PrOH = 99/1, flow rate: 1.0 mL/min, $T = 30^\circ\text{C}$, 254 nm), t_{R} (major) = 9.70 min, t_{R} (minor) = 11.07 min.

Dimethyl (*S,E*)-2-(2-methoxystyryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ae)



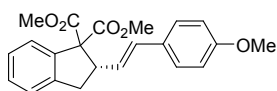
Colorless oil. Yield: 46%; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.56 (d, $J = 7.7$ Hz, 1H), 7.33 – 7.24 (m, 4H), 7.17 (t, $J = 7.8$ Hz, 1H), 6.90 (d, $J = 16.0$ Hz, 1H), 6.83 (dd, $J = 12.3, 7.8$ Hz, 2H), 6.09 (dd, $J = 15.9, 9.1$ Hz, 1H), 3.98 (dd, $J = 14.4, 7.0$ Hz, 1H), 3.81 (s, 3H), 3.75 (s, 3H), 3.62 (s, 3H), 3.37 (dd, $J = 15.8, 7.2$ Hz, 1H), 2.99 (dd, $J = 15.8, 5.0$ Hz, 1H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 170.24, 169.78, 156.60, 143.64, 138.59, 129.03, 128.89, 128.64, 127.12, 127.05, 126.99, 126.81, 126.33, 124.96, 120.74, 110.77, 70.00, 55.53, 52.97, 52.56, 50.60, 37.47; **HRMS** (ESI) m/z ($\text{M}+\text{H}$) $^+$ calculated for $\text{C}_{22}\text{H}_{23}\text{O}_5$: 367.1545, observed: 367.1547; $[\alpha]^{20}_{\text{D}} = -97.4$ ($c = 0.3$, CHCl_3); The product was analyzed by HPLC to determine the enantiomeric excess: 95% ee (CHIRALPAK AD-H, hexane/*i*-PrOH = 95/5, flow rate: 1.0 mL/min, $T = 30^\circ\text{C}$, 254 nm), t_{R} (major) = 8.55 min, t_{R} (minor) = 16.81 min.

Dimethyl (*S,E*)-2-(3-methoxystyryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3af)



Colorless oil. Yield: 96%; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.58 – 7.52 (m, 1H), 7.28 – 7.22 (m, 3H), 7.15 (t, $J = 7.9$ Hz, 1H), 6.88 (d, $J = 7.7$ Hz, 1H), 6.83 – 6.77 (m, 1H), 6.73 (dd, $J = 8.1, 2.3$ Hz, 1H), 6.52 (d, $J = 15.8$ Hz, 1H), 6.12 (dd, $J = 15.8, 9.0$ Hz, 1H), 3.94 (dd, $J = 13.4, 8.0$ Hz, 1H), 3.76 (s, 3H), 3.74 (s, 3H), 3.59 (s, 3H), 3.35 (dd, $J = 15.7, 7.3$ Hz, 1H), 2.97 (dd, $J = 15.7, 5.3$ Hz, 1H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 170.17, 169.69, 159.88, 143.46, 138.63, 138.51, 132.32, 129.61, 128.97, 128.88, 127.08, 127.03, 124.97, 119.13, 113.28, 111.70, 69.92, 55.36, 53.03, 52.60, 50.22, 37.36; **HRMS** (ESI) m/z ($\text{M}+\text{H}$) $^+$ calculated for $\text{C}_{22}\text{H}_{23}\text{O}_5$: 367.1545, observed: 367.1552; $[\alpha]^{20}_{\text{D}} = -87.7$ ($c = 0.7$, CHCl_3); The product was analyzed by HPLC to determine the enantiomeric excess: 85% ee (CHIRALPAK IC, hexane/*i*-PrOH = 99/1, flow rate: 1.0 mL/min, $T = 30^\circ\text{C}$, 254 nm), t_{R} (major) = 25.98 min, t_{R} (minor) = 24.18 min.

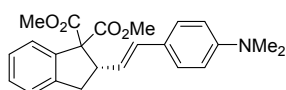
Dimethyl (*S,E*)-2-(4-methoxystyryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ag)



Colorless oil. Yield: 68%; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.56 (d, $J = 7.5$ Hz, 1H), 7.29 – 7.21 (m, 5H), 6.79 (d, $J = 8.4$ Hz, 2H), 6.50 (d, $J = 15.8$ Hz, 1H), 5.99 (dd, $J = 15.8, 9.1$ Hz, 1H), 3.93 (dd, $J = 14.0, 7.6$ Hz, 1H), 3.77 (s, 3H), 3.75 (s, 3H), 3.60 (s, 3H), 3.35

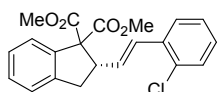
(dd, $J = 15.6, 7.4$ Hz, 1H), 2.97 (dd, $J = 15.6, 5.1$ Hz, 1H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 170.23, 169.77, 159.23, 143.58, 138.55, 131.76, 129.98, 128.92, 127.60, 127.04, 127.02, 126.33, 124.95, 114.02, 70.00, 55.41, 53.00, 52.56, 50.31, 37.50; **HRMS** (ESI) m/z ($\text{M}+\text{H}$) $^+$ calculated for $\text{C}_{22}\text{H}_{23}\text{O}_5$: 367.1545, observed: 367.1549; $[\alpha]^{20}_{\text{D}} = -92.7$ ($c = 0.2$, CHCl_3); The product was analyzed by HPLC to determine the enantiomeric excess: 90% ee (CHIRALPAK AD-H, hexane/*i*-PrOH = 95/5, flow rate: 1.0 mL/min, $T = 30^\circ\text{C}$, 254 nm), t_{R} (major) = 11.21 min, t_{R} (minor) = 17.95 min.

Dimethyl (*S,E*)-2-(4-(dimethylamino)styryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ah)



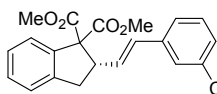
Colorless oil. Yield: 66%; ^1H NMR (400 MHz, CDCl_3) δ 7.57 (d, J = 7.5 Hz, 1H), 7.31 – 7.25 (m, 3H), 7.18 (d, J = 8.1 Hz, 2H), 6.62 (d, J = 8.4 Hz, 2H), 6.47 (d, J = 15.6 Hz, 1H), 5.91 (dd, J = 15.8, 8.9 Hz, 1H), 3.93 (dd, J = 13.4, 7.9 Hz, 1H), 3.75 (s, 3H), 3.60 (s, 3H), 3.36 (dd, J = 15.4, 7.4 Hz, 1H), 3.02 – 2.84 (m, 7H). ^{13}C NMR (100 MHz, CDCl_3) δ 170.32, 169.82, 143.75, 138.63, 132.20, 128.86, 127.39, 127.06, 126.95, 124.94, 124.11, 112.51, 70.10, 52.96, 52.54, 50.44, 40.69, 37.68; **HRMS** (ESI) m/z ($\text{M}+\text{H}$) $^+$ calculated for $\text{C}_{23}\text{H}_{26}\text{NO}_4$: 380.1862, observed: 380.1860; $[\alpha]_D^{20}$ = -52.2 (c = 0.1, CHCl_3); The product was analyzed by HPLC to determine the enantiomeric excess: >99% ee (CHIRALCEL OD-H, hexane/*i*-PrOH = 99/1, flow rate: 1.0 mL/min, T = 30 $^\circ\text{C}$, 254 nm), t_R (major) = 22.38 min, t_R (minor) = 26.08 min.

Dimethyl (*S,E*)-2-(2-chlorostyryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ai)



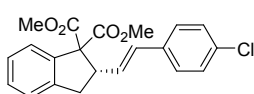
Colorless oil. Yield: 93%; ^1H NMR (400 MHz, CDCl_3) δ 7.56 (d, J = 7.8 Hz, 1H), 7.42 – 7.33 (m, 1H), 7.30 – 7.22 (m, 4H), 7.18 – 7.06 (m, 2H), 6.92 (d, J = 15.7 Hz, 1H), 6.11 (dd, J = 15.8, 9.0 Hz, 1H), 3.98 (dd, J = 14.1, 7.2 Hz, 1H), 3.74 (s, 3H), 3.61 (s, 3H), 3.38 (dd, J = 15.6, 7.2 Hz, 1H), 2.99 (dd, J = 15.7, 5.1 Hz, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 170.07, 169.65, 143.31, 138.38, 135.31, 132.93, 131.55, 129.64, 128.99, 128.68, 128.65, 127.14, 127.11, 126.96, 124.98, 69.82, 53.05, 52.68, 50.33, 37.23; **HRMS** (ESI) m/z ($\text{M}+\text{H}$) $^+$ calculated for $\text{C}_{21}\text{H}_{20}\text{ClO}_4$: 371.1050, observed: 371.1047; $[\alpha]_D^{20}$ = -78.4 (c = 0.2, CHCl_3); The product was analyzed by HPLC to determine the enantiomeric excess: 94% ee CHIRALCEL OD-H, hexane/*i*-PrOH = 95/5, flow rate: 1.0 mL/min, T = 30 $^\circ\text{C}$, 254 nm), t_R (major) = 7.68 min, t_R (minor) = 9.31 min.

Dimethyl (*S,E*)-2-(3-chlorostyryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3aj)



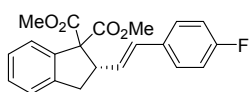
Colorless oil. Yield: 63%; ^1H NMR (400 MHz, CDCl_3) δ 7.59 (d, J = 7.5 Hz, 1H), 7.33 – 7.26 (m, 5H), 7.20 – 7.17 (m, 2H), 6.53 (d, J = 15.8 Hz, 1H), 6.20 (dd, J = 16.0, 8.9 Hz, 1H), 3.97 (dd, J = 14.0, 7.8 Hz, 1H), 3.79 (s, 3H), 3.66 (s, 3H), 3.39 (dd, J = 15.8, 7.5 Hz, 1H), 3.01 (dd, J = 15.8, 5.5 Hz, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 170.09, 169.64, 143.28, 139.02, 138.41, 134.61, 131.08, 130.22, 129.88, 129.04, 127.57, 127.15, 127.02, 126.31, 124.99, 124.68, 69.84, 53.08, 52.66, 50.18, 37.24; **HRMS** (ESI) m/z ($\text{M}+\text{H}$) $^+$ calculated for $\text{C}_{21}\text{H}_{20}\text{ClO}_4$: 371.1050, observed: 371.1055; $[\alpha]_D^{20}$ = -81.1 (c = 0.5, CHCl_3); The product was analyzed by HPLC to determine the enantiomeric excess: 90% ee CHIRALPAK AD-H, hexane/*i*-PrOH = 95/5, flow rate: 1.0 mL/min, T = 30 $^\circ\text{C}$, 254 nm), t_R (major) = 8.56 min, t_R (minor) = 9.92 min.

Dimethyl (*S,E*)-2-(4-chlorostyryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ak)



Colorless oil. Yield: 81%; ^1H NMR (400 MHz, CDCl_3) δ 7.54 (d, J = 7.1 Hz, 1H), 7.29 – 7.18 (m, 7H), 6.49 (d, J = 15.8 Hz, 1H), 6.11 (dd, J = 15.8, 8.9 Hz, 1H), 3.92 (q, J = 7.6 Hz, 1H), 3.73 (d, J = 1.8 Hz, 3H), 3.57 (d, J = 2.0 Hz, 3H), 3.34 (dd, J = 15.7, 7.4 Hz, 1H), 2.96 (dd, J = 15.7, 5.5 Hz, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 170.08, 169.65, 143.31, 138.41, 135.63, 133.19, 131.11, 129.32, 129.00, 128.77, 127.62, 127.11, 127.00, 124.96, 77.48, 77.16, 76.84, 69.87, 53.05, 52.59, 50.19, 37.26; **HRMS** (ESI) m/z ($\text{M}+\text{H}$) $^+$ calculated for $\text{C}_{21}\text{H}_{20}\text{ClO}_4$: 371.1050, observed: 371.1043; $[\alpha]_D^{20}$ = -91.0 (c = 0.3, CHCl_3); The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee CHIRALPAK IC, hexane/*i*-PrOH = 99/1, flow rate: 1.0 mL/min, T = 30 $^\circ\text{C}$, 254 nm), t_R (major) = 13.15 min, t_R (minor) = 14.73 min.

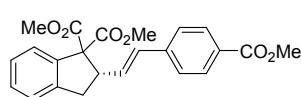
Dimethyl (*S,E*)-2-(4-fluorostyryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3al)



Colorless oil. Yield: 32%; ^1H NMR (400 MHz, CDCl_3) δ 7.57 (d, J = 7.9 Hz, 1H), 7.34 – 7.25 (m, 5H), 6.95 (t, J = 8.7 Hz, 2H), 6.54 (d, J = 15.8 Hz, 1H), 6.08 (dd, J = 15.7, 8.9 Hz, 1H), 3.95 (dd, J = 13.6, 7.1 Hz, 1H), 3.77 (s, 3H), 3.62 (s, 3H), 3.37 (dd, J = 15.7, 7.2 Hz, 1H), 2.99 (dd, J = 15.6, 5.4 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.16, 169.73, 162.35 (d, J = 237.3 Hz),

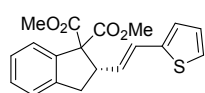
143.41, 138.50, 133.35 (d, $J = 3.3$ Hz), 131.18, 129.00, 128.39 (d, $J = 2.2$ Hz), 127.93 (d, $J = 8.0$ Hz), 127.07 (d, $J = 7.2$ Hz), 124.97, 115.54 (d, $J = 21.6$ Hz), 69.94, 53.04, 52.58, 50.22, 37.37; **HRMS** (ESI) m/z (M+H)⁺ calculated for C₂₁H₂₀FO₄: 355.1346, observed: 355.1343; $[\alpha]^{20}_D = -83.8$ (c = 0.1, CHCl₃); The product was analyzed by HPLC to determine the enantiomeric excess: 93% ee CHIRALCEL OD-H, hexane/i-PrOH = 99/1, flow rate: 0.5 mL/min, T = 30 °C, 254 nm), t_R (major) = 27.78 min, t_R (minor) = 32.27 min.

Dimethyl (S,E)-2-(4-(methoxycarbonyl)styryl)-2,3-dihydro-1H-indene-1,1-dicarboxylate (3am)



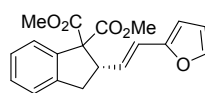
Colorless oil. Yield: 84%; **¹H NMR** (400 MHz, CDCl₃) δ 7.94 (d, $J = 8.2$ Hz, 2H), 7.58 (d, $J = 7.3$ Hz, 1H), 7.37 (d, $J = 8.2$ Hz, 2H), 7.34 – 7.26 (m, 3H), 6.61 (d, $J = 15.8$ Hz, 1H), 6.30 (dd, $J = 15.8, 8.9$ Hz, 1H), 3.99 (dd, $J = 14.0, 7.3$ Hz, 1H), 3.90 (s, 3H), 3.78 (s, 3H), 3.61 (s, 3H), 3.39 (dd, $J = 15.6, 7.3$ Hz, 1H), 3.02 (dd, $J = 15.7, 5.5$ Hz, 1H). **¹³C NMR** (100 MHz, CDCl₃) δ 170.06, 169.63, 167.00, 143.24, 141.62, 138.39, 131.50, 131.48, 130.02, 129.05, 127.16, 127.00, 126.31, 124.99, 69.85, 53.09, 52.63, 52.20, 50.26, 37.18; **HRMS** (ESI) m/z (M+H)⁺ calculated for C₂₃H₂₃O₆: 395.1495, observed: 395.1492; $[\alpha]^{20}_D = -93.6$ (c = 0.2, CHCl₃); The product was analyzed by HPLC to determine the enantiomeric excess: 82% ee CHIRALPAK IC, hexane/i-PrOH = 90/0, flow rate: 1.0 mL/min, T = 30 °C, 254 nm), t_R (major) = 14.65 min, t_R (minor) = 20.96 min.

Dimethyl (S,E)-2-(2-(thiophen-2-yl)vinyl)-2,3-dihydro-1H-indene-1,1-dicarboxylate (3an)



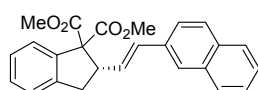
Colorless oil. Yield: 85%; **¹H NMR** (400 MHz, CDCl₃) δ 7.57 (d, $J = 7.6$ Hz, 1H), 7.31 – 7.25 (m, 3H), 7.10 (d, $J = 4.7$ Hz, 1H), 6.91 (d, $J = 5.1$ Hz, 2H), 6.70 (d, $J = 15.6$ Hz, 1H), 6.00 (dd, $J = 15.6, 8.9$ Hz, 1H), 3.94 (dd, $J = 14.8, 7.3$ Hz, 1H), 3.77 (s, 3H), 3.64 (s, 3H), 3.34 (dd, $J = 15.7, 7.4$ Hz, 1H), 3.00 (dd, $J = 15.6, 5.9$ Hz, 1H). **¹³C NMR** (100 MHz, CDCl₃) δ 170.13, 169.65, 143.37, 142.21, 138.49, 128.96, 128.12, 127.39, 127.06, 126.86, 125.58, 124.93, 124.18, 77.48, 69.89, 53.03, 52.62, 50.11, 37.23; **HRMS** (ESI) m/z (M+H)⁺ calculated for C₁₉H₁₉O₄S: 343.1004, observed: 343.0999; $[\alpha]^{20}_D = -83.7$ (c = 0.6, CHCl₃); The product was analyzed by HPLC to determine the enantiomeric excess: >99% ee CHIRALPAK IC, hexane/i-PrOH = 99/1, flow rate: 1.0 mL/min, T = 30 °C, 254 nm), t_R (major) = 16.48 min, t_R (minor) = 18.20 min.

Dimethyl (S,E)-2-(2-(furan-2-yl)vinyl)-2,3-dihydro-1H-indene-1,1-dicarboxylate (3ao)



Colorless oil. Yield: 79%; **¹H NMR** (400 MHz, CDCl₃) δ 7.57 (d, $J = 7.6$ Hz, 1H), 7.31 – 7.26 (m, 4H), 6.38 (dd, $J = 21.6, 11.7$ Hz, 2H), 6.19 (d, $J = 2.7$ Hz, 1H), 6.12 (dd, $J = 15.8, 9.0$ Hz, 1H), 3.92 (dd, $J = 15.0, 7.4$ Hz, 1H), 3.78 (s, 3H), 3.64 (s, 3H), 3.33 (dd, $J = 15.5, 7.4$ Hz, 1H), 3.00 (dd, $J = 15.6, 6.1$ Hz, 1H). **¹³C NMR** (100 MHz, CDCl₃) δ 170.17, 169.62, 152.62, 143.40, 141.92, 138.56, 128.92, 127.18, 127.02, 126.85, 124.90, 120.86, 111.27, 107.64, 69.83, 52.99, 52.52, 50.18, 37.33; **HRMS** (ESI) m/z (M+H)⁺ calculated for C₁₉H₁₉O₅: 327.1232, observed: 327.1236; $[\alpha]^{20}_D = -55.5$ (c = 0.6, CHCl₃); The product was analyzed by HPLC to determine the enantiomeric excess: 87% ee CHIRALPAK AD-H, hexane/i-PrOH = 95/5, flow rate: 1.0 mL/min, T = 30 °C, 254 nm), t_R (major) = 10.28 min, t_R (minor) = 11.31 min.

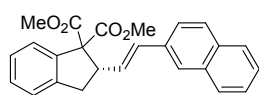
Dimethyl (S,E)-2-(2-(naphthalen-2-yl)vinyl)-2,3-dihydro-1H-indene-1,1-dicarboxylate (from (Z)-1-phenylbutadiene) (3ap)



Colorless oil. Yield: 51%; **¹H NMR** (400 MHz, CDCl₃) δ 7.79 – 7.67 (m, 4H), 7.60 (d, $J = 7.4$ Hz, 1H), 7.51 (d, $J = 8.6$ Hz, 1H), 7.46 – 7.28 (m, 5H), 6.74 (d, $J = 15.7$ Hz, 1H), 6.29 (dd, $J = 15.8, 8.9$ Hz, 1H), 4.03 (dd, $J = 14.1, 7.6$ Hz, 1H), 3.78 (s, 3H), 3.61 (s, 3H), 3.42 (dd, $J = 15.7, 7.5$ Hz, 1H), 3.05 (dd, $J = 15.7, 5.2$ Hz, 1H). **¹³C NMR** (100 MHz, CDCl₃) δ 170.20, 169.75, 143.49, 138.54, 134.63, 133.69, 133.07, 132.47, 129.01, 129.00, 128.27, 128.05, 127.76, 127.11, 127.09, 126.36, 126.18, 125.92, 125.01, 123.77, 70.05, 53.05, 52.60, 50.39, 37.43; **HRMS** (ESI) m/z (M+H)⁺ calculated for

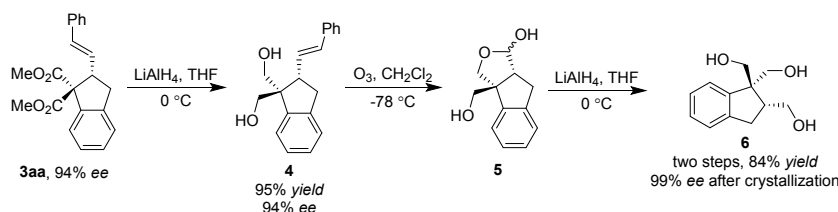
C₂₅H₂₃O₄: 387.1596, observed: 387.1591; [α]_D²⁰ = -57.9 (c = 0.8, CHCl₃); The product was analyzed by HPLC to determine the enantiomeric excess: 47% ee CHIRALCEL OD-H, hexane/i-PrOH = 95/5, flow rate: 1.0 mL/min, T = 30 °C, 254 nm, t_R (minor) = 8.32 min, t_R (major) = 9.63 min.

Dimethyl (*S,E*)-2-(2-(naphthalen-2-yl)vinyl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (from (*E*)-1-phenylbutadiene) (3ap**)**



Colorless oil. Yield: 98%; ¹H NMR (400 MHz, CDCl₃) δ 7.79 – 7.67 (m, 4H), 7.60 (d, *J* = 7.4 Hz, 1H), 7.51 (d, *J* = 8.6 Hz, 1H), 7.46 – 7.28 (m, 5H), 6.74 (d, *J* = 15.7 Hz, 1H), 6.29 (dd, *J* = 15.8, 8.9 Hz, 1H), 4.03 (dd, *J* = 14.1, 7.6 Hz, 1H), 3.78 (s, 3H), 3.61 (s, 3H), 3.42 (dd, *J* = 15.7, 7.5 Hz, 1H), 3.05 (dd, *J* = 15.7, 5.2 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 170.20, 169.75, 143.49, 138.54, 134.63, 133.69, 133.07, 132.47, 129.01, 129.00, 128.27, 128.05, 127.76, 127.11, 127.09, 126.36, 126.18, 125.92, 125.01, 123.77, 70.05, 53.05, 52.60, 50.39, 37.43; HRMS (ESI) *m/z* (M+H)⁺ calculated for C₂₅H₂₃O₄: 387.1596, observed: 387.1591; [α]_D²⁰ = -83.6 (c = 0.4, CHCl₃); The product was analyzed by HPLC to determine the enantiomeric excess: 93% ee CHIRALCEL OD-H, hexane/i-PrOH = 95/5, flow rate: 1.0 mL/min, T = 30 °C, 254 nm, t_R (minor) = 8.07 min, t_R (major) = 9.36 min.

Synthesis of Triol **6**

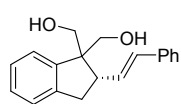


To a flame-dried and Ar-purged flask (25 mL) were added **3aa** (672 mg, 2.0 mmol), THF (10 mL) and a stirring bar. The flask was cooled down to 0 °C and then LiAlH₄ (152 mg, 4.0 mmol) was added. After the resulting reaction mixture was stirred for 5 h at 0 °C, the reaction was quenched by the addition of 4.0 g Na₂SO₄·10H₂O. The reaction mixture was diluted with Et₂O, and then filtered through celite with the aid of Et₂O. The solution was concentrated under the reduced pressure to yield **4** (532 mg, 95% yield) as a colorless oil that was employed in the next step without further purification.

Ozone bubbled through the solution of **4** (532 mg, 1.95 mmol) in CH₂Cl₂ (10 mL) at -78 °C. Ozone addition stopped when the solution turned blue. Nitrogen passed through the solution until the blue color disappeared. Then, Me₂S (248 mg, 4 mmol) was added to the solution and the resultant mixture was stirred for additional 4 h. The solution was concentrated under reduced pressure and the crude product was purified by silica gel column chromatography on silica gel eluting with petroleum ether-EtOAc (2 : 1) to yield **5** (362 mg, 1.76 mmol, 90% yield).

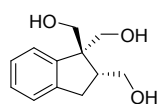
To a flame-dried and Ar-purged flask (25 mL) were added **5** (362 mg, 1.76 mmol), THF (10 mL) and a stirring bar. The flask was cooled down to 0 °C and then LiAlH₄ (133 mg, 3.52 mmol) was added. After the resulting reaction mixture was stirred for 5 h at 0 °C, the reaction was quenched by the addition of 3.5 g Na₂SO₄·10H₂O. The reaction was diluted with Et₂O, and then filtered through celite. The solution was concentrated under reduced pressure and the crude product was purified by silica gel column chromatography on silica gel eluting with petroleum ether-EtOAc (1 : 1) to yield **6** (white solid, 340 mg, 1.64 mmol, 93% yield).

(*S,E*)-(2-styryl-2,3-dihydro-1*H*-indene-1,1-diyl)dimethanol (4)

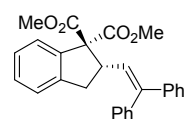


¹H NMR (400 MHz, CDCl₃) δ 7.38 (d, *J* = 7.5 Hz, 2H), 7.33 – 7.20 (m, 7H), 6.59 (d, *J* = 15.8 Hz, 1H), 6.42 (dd, *J* = 15.8, 8.9 Hz, 1H), 3.99 – 3.77 (m, 4H), 3.30 (q, *J* = 8.2 Hz, 1H), 3.15 (dd, *J* = 15.9, 7.9 Hz, 1H), 3.00 (dd, *J* = 15.9, 8.4 Hz, 1H), 2.13 (brs, 1H), 1.80 (brs, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 143.80, 143.51, 137.18, 131.87, 130.09, 128.74, 128.02, 127.57, 126.95, 126.35, 125.20, 124.16, 66.87, 65.65, 57.77, 48.34, 37.23. HRMS (ESI) *m/z* (M+H)⁺ calculated for C₁₉H₂₁O₂: 281.1542, observed: 281.1536; [α]_D²⁰ = -9.7 (c = 0.1, CHCl₃); The product was analyzed by HPLC to determine the enantiomeric excess: 93% ee CHIRALPAK AD-H, hexane/*i*-PrOH = 90/10, flow rate: 1.0 mL/min, T = 30 °C, 254 nm), *t*_R (major) = 12.27 min, *t*_R (minor) = 13.13 min.

(*R*)-(2,3-dihydro-1*H*-indene-1,1,2-triyl)trimethanol (6)

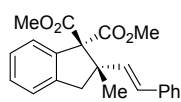


¹H NMR (400 MHz, CDCl₃) δ 7.26 – 7.09 (m, 4H), 4.20 (brs, 1H), 4.10 (d, *J* = 11.0 Hz, 1H), 4.00 – 3.75 (m, 4H), 3.67 (d, *J* = 10.6 Hz, 1H), 3.30 (brs, 1H), 3.00 (q, *J* = 12.1 Hz, 1H), 2.82 – 2.57 (m, 2H), 2.00 (brs, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 144.18, 142.68, 127.95, 126.79, 124.97, 124.03, 77.48, 77.16, 76.84, 68.27, 64.58, 62.34, 56.07, 48.97, 34.14. HRMS (ESI) *m/z* (M+Na)⁺ calculated for C₁₂H₁₆O₃Na: 231.0997, observed: 231.0992; [α]_D²⁰ = 1.5 (c = 0.2, CHCl₃); The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee CHIRALPAK AD-H, hexane/*i*-PrOH = 85/15, flow rate: 1.0 mL/min, T = 30 °C, 254 nm), *t*_R (major) = 15.47 min, *t*_R (minor) = 21.98 min.



Dimethyl (*S*)-2-(2,2-diphenylvinyl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (S3aa)

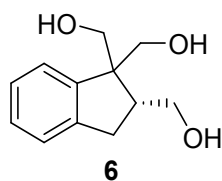
Colorless oil. Yield: 66%. ¹H NMR (400 MHz, CDCl₃) δ 7.60 – 7.53 (m, 1H), 7.46 – 7.36 (m, 3H), 7.36 – 7.29 (m, 1H), 7.29 – 7.26 (m, 1H), 7.25 – 7.18 (m, 6H), 7.17 – 7.12 (m, 2H), 6.03 (d, *J* = 11.2 Hz, 1H), 4.03 – 3.94 (m, 1H), 3.74 (s, 3H), 3.61 (s, 3H), 3.35 (dd, *J* = 15.5, 7.4 Hz, 1H), 3.00 (dd, *J* = 15.6, 4.5 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 170.03, 169.93, 143.88, 143.48, 142.48, 139.78, 138.60, 129.90, 128.92, 128.44, 128.25, 127.65, 127.63, 127.49, 127.45, 127.34, 127.03, 124.93, 69.51, 52.84, 52.61, 46.58, 38.80. HRMS (ESI) *m/z* (M+Na)⁺ calculated for C₂₇H₂₄O₄Na: 435.1572, observed: 435.1572; [α]_D²⁰ = -28.3 (c = 0.54, CHCl₃); The product was analyzed by HPLC to determine the enantiomeric excess: 55% ee CHIRALCEL OD-H, hexane/*i*-PrOH = 99/1, flow rate: 1.0 mL/min, T = 30 °C, 254 nm), *t*_R (minor) = 7.93 min, *t*_R (major) = 9.52 min.



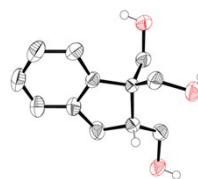
Dimethyl (*S,E*)-2-methyl-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (S3ab)

Colorless oil. Yield: 46%. ¹H NMR (400 MHz, CDCl₃) δ 7.62 – 7.57 (m, 1H), 7.39 – 7.26 (m, 7H), 7.22 – 7.19 (m, 1H), 6.62 (d, *J* = 16.2 Hz, 1H), 6.51 (d, *J* = 16.2 Hz, 1H), 3.77 (s, 3H), 3.61 (s, 3H), 3.43 (d, *J* = 15.1 Hz, 1H), 3.11 (d, *J* = 15.1 Hz, 1H), 1.41 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 169.91, 169.69, 143.26, 139.17, 137.71, 134.46, 128.97, 128.77, 128.62, 127.78, 127.38, 126.83, 126.48, 125.15, 72.34, 52.51, 52.49, 52.46, 45.01, 22.68. HRMS (ESI) *m/z* (M+Na)⁺ calculated for C₂₂H₂₂O₄Na: 373.14167, observed: 373.1416; [α]_D²⁰ = -6.3 (c = 0.32, CHCl₃); The product was analyzed by HPLC to determine the enantiomeric excess: 32% ee CHIRALPAK AD-H, hexane/*i*-PrOH = 98/2, flow rate: 1.0 mL/min, T = 30 °C, 254 nm), *t*_R (major) = 11.81 min, *t*_R (minor) = 16.42 min.

X-ray Single Crystal Data of 6



≡



X-ray structure of 6

Identification code	cu_d8v17262_0m	
Empirical formula	C12 H16 O3	
Formula weight	208.25	
Temperature	296 K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 12.8484(12) Å	$\alpha = 90^\circ$.
	b = 6.1584(6) Å	$\beta = 97.415(4)^\circ$.
	c = 13.6137(13) Å	$\gamma = 90^\circ$.
Volume	1068.18(18) Å ³	
Z	4	
Density (calculated)	1.295 Mg/m ³	
Absorption coefficient	0.749 mm ⁻¹	
F(000)	448	
Crystal size	0.15 x 0.03 x 0.02 mm ³	
Theta range for data collection	3.274 to 70.199°.	
Index ranges	-15 ≤ h ≤ 14, -7 ≤ k ≤ 6, -16 ≤ l ≤ 15	
Reflections collected	14606	
Independent reflections	3905 [R(int) = 0.0408]	
Completeness to theta = 67.679°	98.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7533 and 0.6092	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3905 / 1 / 277	
Goodness-of-fit on F ²	1.106	
Final R indices [I > 2σ(I)]	R1 = 0.0387, wR2 = 0.0911	
R indices (all data)	R1 = 0.0421, wR2 = 0.0942	
Absolute structure parameter	0.10(7)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.158 and -0.194 e.Å ⁻³	

DFT Calculation Details

All the Density Functional Theory (DFT) calculations were carried out in the Gaussian16 software package.⁴ The geometric structures of intermediates and transition states were fully optimized with the B3LYP⁵ functional method. The effective core potential of LANL2DZ⁶ and the associated basis set were used for palladium and Iodine, while the 6-31G(d,p) basis set was used for the other elements. The frequency analysis was also performed based on the optimized structures to verify the energy minima and transition states and to obtain the thermodynamic corrections to Gibbs free energy. Solution-phase single-point energy calculations were conducted based on the gas-phase-optimized structures by using the M06 method⁷ and SMD solvation model⁸ (solvent = tetrahydrofuran). For single-point energy calculations, the basis set SDD⁹ was used for palladium and iodine, and 6-311+ G(d,p) basis set was used for other atoms. Considering the position of ligand and coordinated iodide ion, these are four configurations about transition states and intermediates. Their energies and structures are all listed in Figure S2 and Figure S3. All energies were related to **Int1Rb-Me₃N**. All graphics of optimized structures were generated with CYLview.¹⁰

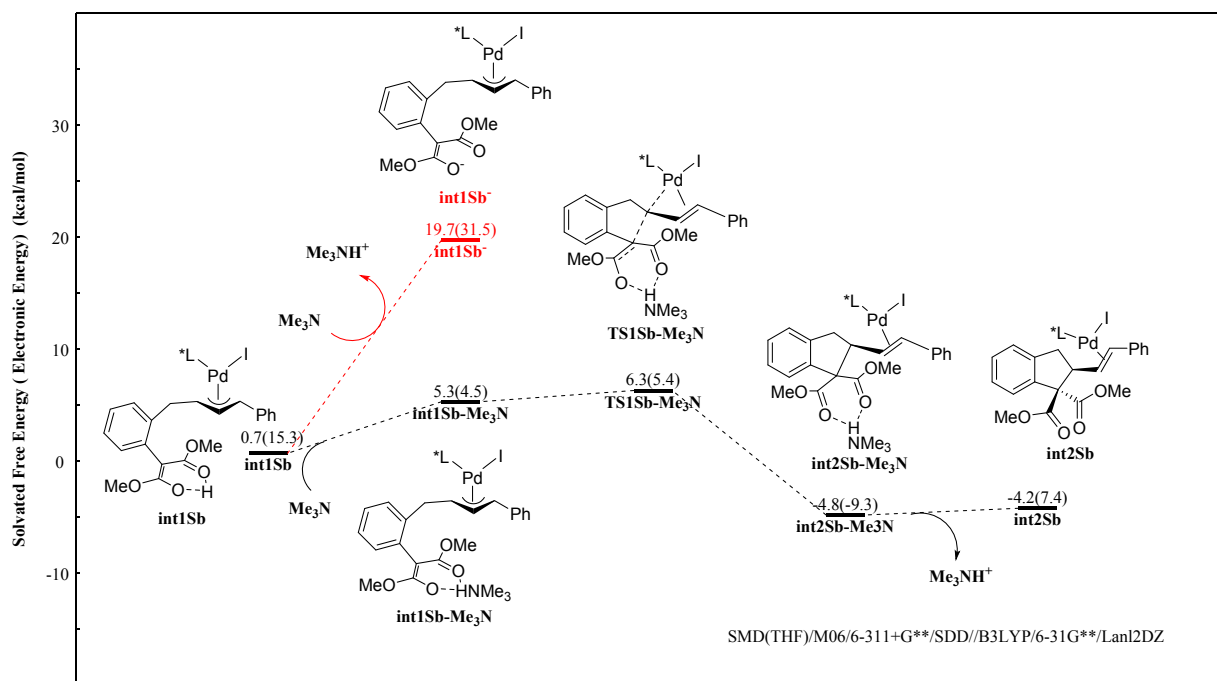


Figure S2

(4) Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

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(8) a) D. Andrae, U. Häussermann, M. Dolg, H. Stoll, H. Preuss, *Theor. Chim. Acta* **1990**, 77, 123–141; b) M. Dolg, U. Wedig, H. Stoll, H. Preuss, *J. Chem. Phys.* **1987**, 86, 866–872.

(9) C. Gonzalez, H. B. Schlegel, *J. Chem. Phys.* **1990**, 94, 5523–5527.

(10) Legault, C. Y. CYLview, 1.0 b; Université de Sherbrooke (<http://www.cylview.org>), 2009.

Initially, we calculated the pathway from **int1Sb** to **int2Sb**. Figure S2 indicates that the overall allylic substitution process (from **int1Sb** to **int2Sb**) is exoergic pathway. The **int1Sb-Me₃N** is obtained when the base Me₃N binding to the proton of **int1Sb**. When allylic alkylation process is complete, **int2Sb-Me₃N** will be generated, which is easily deprotonated by Me₃N and the final intermediate **int2Sb** of this whole process is generated. Energy releases mainly in the allylic alkylation step. Notably, the energy of malonate enolate anion (**int1Sb⁻**) which is generated via deprotonation by Me₃N, is even higher than the reaction barrier of allylic alkylation (5.6 kcal mol⁻¹). Therefore, **int1Sb-Me₃N** should be the most possible intermediate.

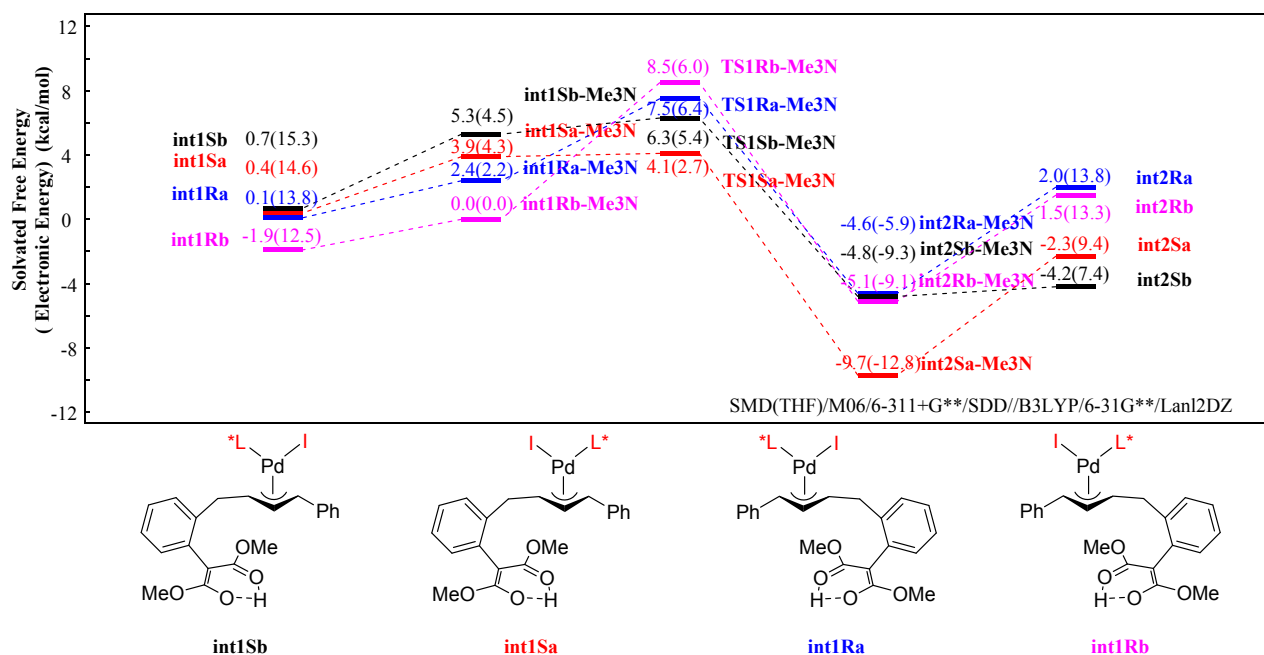


Figure S3

Then, the other three possible pathways from **int1** to **int2** were calculated (Figure S3). Among them, **TS1Sa** is the most stabilized transition state and (*S*)-configuration is favorable. Transition states **TS1Ra** and **TS1Rb** leads to higher barriers by 3.4 kcal mol⁻¹ and 4.4 kcal mol⁻¹ than **TS1Sa** respectively. Moreover, **TS1Sb** also affords the (*S*)-product, which is also less stable than the transition state **TS1Sa** by about 2.2 kcal mol⁻¹. These calculated results indicate that the (*S*)-products should be formed preferentially, which agrees with the experimental observations.

Cartesian Coordinates of Computed Structures

Int1Sa

Thermal correction to Gibbs Free Energy: 0.864788

SCF energy in solution: -4931.561347

Solution-phase Gibbs free energy: -4930.696559

Coordinates:

C	-8.40741900	1.07154000	0.19573100
C	-8.03779400	-0.25809000	0.50770500
C	-6.72076200	-0.58591200	0.74420000
C	-5.69675900	0.39921300	0.67664800
C	-6.07105200	1.73790000	0.32603900
C	-7.44096000	2.04605700	0.10549500
C	-4.30738100	0.10042400	0.89703300
C	-3.36914900	1.09357400	0.66270500
C	-3.72760000	2.44056700	0.35614300
C	-5.06848300	2.73210900	0.20370200
C	-3.84889200	-1.24905100	1.34208700
C	-4.29931500	-1.82614300	2.57943300
C	-3.88245900	-3.15483000	2.91563800
C	-3.02338700	-3.85740100	2.03615600
C	-2.52700800	-3.28631500	0.88058400
C	-2.93735400	-1.95521900	0.57257500
C	-5.11257200	-1.12427000	3.51173700
C	-5.51502900	-1.71545600	4.68914200
C	-5.13263600	-3.04194800	4.99998400
C	-4.33076500	-3.74320300	4.12984400
O	-2.01934900	0.77821500	0.73290800
O	-2.43091300	-1.36845100	-0.58299500
P	-1.31434200	-0.13371400	-0.48785000
N	-1.71373100	0.62250900	-1.95730500
C	-2.91356000	0.31036000	-2.76730300
C	-2.49193900	-0.38486400	-4.06165300
C	-1.58158400	0.53729300	-4.88293500
C	-0.63134400	1.36024600	-4.03681200
C	-0.72508500	1.39463700	-2.62811800
C	0.36186000	2.12459000	-4.66278400
C	1.26620200	2.89723200	-3.94485500
C	1.13949900	2.91766900	-2.55887800
C	0.14673800	2.20506500	-1.89418400
C	-2.70167100	3.51016000	0.23565500
C	-1.61661400	-4.05988100	-0.00335700
C	-1.73807900	3.70069500	1.23636500
C	-0.80941700	4.73805600	1.13723600
C	-0.81382500	5.59595700	0.03877900
C	-1.76800000	5.40782800	-0.96116900
C	-2.70667100	4.38023500	-0.86334300
C	-0.53318300	-4.75569900	0.54421000

C	0.31052600	-5.51565200	-0.26897500
C	0.08432300	-5.60034900	-1.63928200
C	-1.00020800	-4.91419100	-2.18903900
C	-1.84143300	-4.15152500	-1.38498400
N	2.06322200	3.72595000	-1.76421500
O	1.93984200	3.69657300	-0.53391600
O	2.91323300	4.39161300	-2.35363800
C	-1.72573000	6.26900000	-2.19631100
F	-2.93858900	6.36390700	-2.78480400
F	-1.30506800	7.52097700	-1.92029900
F	-0.87714100	5.75944300	-3.11851000
C	0.21030500	4.90673400	2.23337600
F	-0.37080700	4.86323700	3.45531400
F	1.13229200	3.90739200	2.21970200
F	0.88163600	6.06762200	2.13915600
C	-1.28921100	-5.03833800	-3.66166600
F	-2.08317800	-6.10675500	-3.91813600
F	-1.93727500	-3.95157100	-4.14228500
F	-0.16561600	-5.20104100	-4.38520700
C	1.50219500	-6.18592200	0.35954100
F	1.15428700	-6.85333200	1.48617800
F	2.09144100	-7.06905400	-0.47025500
F	2.44358700	-5.28436800	0.72465100
H	-9.45041900	1.31615000	0.01895700
H	-8.80024400	-1.02985300	0.55745900
H	-6.45447800	-1.61053500	0.97433100
H	-7.70879600	3.06862800	-0.14698200
H	-5.37054200	3.75389400	-0.00976400
H	-2.75130900	-4.88057400	2.28023000
H	-5.40648400	-0.10438600	3.29546500
H	-6.12954000	-1.15578200	5.38816600
H	-5.46522400	-3.49818700	5.92754100
H	-4.01788400	-4.75798900	4.36137900
H	-3.58281700	-0.31252500	-2.17961700
H	-3.43206300	1.25418700	-2.98189800
H	-1.96919500	-1.31259500	-3.81051100
H	-3.37921100	-0.65500000	-4.64476200
H	-1.00145200	-0.04666000	-5.60569800
H	-2.19497900	1.23168500	-5.47451500
H	0.43674300	2.09034200	-5.74618500
H	2.04636800	3.47135000	-4.42722200
H	0.05622100	2.30700400	-0.82181700
H	-1.72134600	3.04185100	2.09719200
H	-0.08854100	6.39661200	-0.03470000
H	-3.43799700	4.24662700	-1.65276300

H	-0.33674200	-4.69313800	1.60957100
H	0.75039300	-6.17368400	-2.27169400
H	-2.67103500	-3.61972700	-1.83317200
Pd	0.93306900	-0.53867700	-0.07077500
I	1.48937000	-1.75726600	-2.48201600
C	2.36271200	-0.55380400	1.66267100
C	3.18435500	-0.34193500	0.55488700
H	3.21460400	0.65569500	0.11662800
C	1.27961600	0.31932700	1.96716500
H	1.39266200	1.36570700	1.68742900
C	4.28237300	-1.29609800	0.13951400
H	4.54606500	-1.92774400	0.99749200
C	0.36410300	0.06491800	3.09777500
C	-0.08930900	1.14412600	3.87669000
C	-0.04640700	-1.23300000	3.45355200
C	-0.92232900	0.93287800	4.97511200
H	0.23911700	2.14913900	3.63526900
C	-0.87896400	-1.44220700	4.54970600
H	0.26782400	-2.07814900	2.84756200
C	-1.32259300	-0.35998500	5.31528300
H	-1.25311900	1.78088500	5.56814700
H	-1.19601100	-2.44981500	4.80107500
H	-1.97767100	-0.52593200	6.16526200
C	5.52154400	-0.61026600	-0.40932300
C	6.26171300	0.32046300	0.35170400
C	5.94401800	-0.91600400	-1.70959800
C	7.39701400	0.91394900	-0.21956200
C	7.07633200	-0.31992900	-2.26320400
H	5.36422100	-1.62275600	-2.29695700
C	7.80680400	0.60210800	-1.51433500
H	7.96108300	1.63172000	0.36916900
H	7.38078600	-0.57144800	-3.27525700
H	8.68973100	1.07632400	-1.93365700
C	5.86262600	0.70795700	1.73675700
C	6.03472900	-0.13210700	2.82702700
C	5.31535400	2.00850400	2.04415100
O	5.72465100	0.19899100	4.06066500
O	5.02052700	2.38879000	3.20305700
O	6.52998400	-1.35878900	2.64869000
O	5.11806100	2.80225400	0.98505800
C	4.59994600	4.12166600	1.24622500
H	4.35591800	4.53119900	0.26803000
H	3.70207900	4.07095800	1.86247900
H	5.35705000	4.72689800	1.75272400
C	6.74245800	-2.17069400	3.81509100

H	7.45306800	-1.69497300	4.49547800
H	5.80378200	-2.34981700	4.34490100
H	7.14979700	-3.10814900	3.43749700
H	3.89032700	-1.96593500	-0.63238500
H	2.45748800	-1.49004200	2.21008300
H	5.37381700	1.17111900	3.97644600

Int1Sb

Thermal correction to Gibbs Free Energy: 0.864163

SCF energy in solution: -4931.560200

Solution-phase Gibbs free energy: -4930.696037

Coordinates:

C	3.36422300	6.64371200	-3.16472400
C	1.95680500	6.58847600	-3.30094800
C	1.22177200	5.63359600	-2.63340000
C	1.85527900	4.67465400	-1.79461600
C	3.28448300	4.70801800	-1.69304100
C	4.01135400	5.71935400	-2.37833200
C	1.13088200	3.64950500	-1.09319300
C	1.84783500	2.65696200	-0.43862000
C	3.26921000	2.69162000	-0.30576400
C	3.94985700	3.72422800	-0.92064100
C	-0.36131300	3.60085100	-1.07027400
C	-1.14899100	4.68803500	-0.55248100
C	-2.57796400	4.57716100	-0.56853700
C	-3.18121600	3.39683900	-1.06890700
C	-2.43377500	2.33730300	-1.54015200
C	-1.01352400	2.46012700	-1.51148000
C	-0.57836200	5.86858400	0.00191400
C	-1.37506100	6.89559200	0.46074900
C	-2.78559100	6.79565200	0.40911500
C	-3.37015200	5.65292500	-0.08432900
O	1.16663900	1.57036200	0.09837600
O	-0.26265700	1.39573700	-1.99672600
P	0.57322800	0.39282500	-0.95821300
N	1.85478200	0.01135100	-2.00739100
C	2.14535000	0.74223600	-3.26299800
C	1.85758700	-0.16036200	-4.46140800
C	2.76687400	-1.39342800	-4.41251700
C	2.98492400	-1.92547900	-3.01034900
C	2.54009300	-1.22874700	-1.86509100
C	3.65239100	-3.14486800	-2.83961700
C	3.86347800	-3.70469600	-1.58683600
C	3.41263300	-2.99421800	-0.47803000
C	2.78631300	-1.75760700	-0.59320000
C	4.00791700	1.66184900	0.47187700

C	-3.09253600	1.11911900	-2.08218100
C	3.61446300	1.30698600	1.76993000
C	4.34050900	0.36340700	2.49780600
C	5.46561300	-0.24973900	1.94885100
C	5.86256300	0.10074600	0.65866300
C	5.14510400	1.04803000	-0.07216000
C	-4.03700000	0.42004800	-1.32231400
C	-4.65321300	-0.72158900	-1.84420800
C	-4.35568800	-1.16912700	-3.12839000
C	-3.42527300	-0.46359300	-3.89157500
C	-2.79588900	0.66424500	-3.37475800
N	3.60518800	-3.56100600	0.85699100
O	3.16600600	-2.92693700	1.82425300
O	4.18632100	-4.64122800	0.94943300
C	7.02388100	-0.61469000	0.01929800
F	7.62383900	0.14546500	-0.92378800
F	7.96180200	-0.95767300	0.92655200
F	6.62275100	-1.75471400	-0.58801900
C	3.86648600	-0.01535600	3.87634300
F	3.47291300	1.06822300	4.58124500
F	2.79161900	-0.84483100	3.81548500
F	4.81653900	-0.64760700	4.58899800
C	-3.11642100	-0.89798400	-5.30030300
F	-3.87686100	-0.22266900	-6.19770500
F	-1.82709400	-0.65533200	-5.62798500
F	-3.35253200	-2.20928600	-5.49089300
C	-5.58145500	-1.50978900	-0.96420600
F	-6.44475200	-0.70641300	-0.29682400
F	-6.30997100	-2.41013400	-1.64894700
F	-4.89735700	-2.19848200	-0.00691200
H	3.92932500	7.40740700	-3.69042700
H	1.45078000	7.30409100	-3.94222500
H	0.14567200	5.60038600	-2.75499500
H	5.09336800	5.73897000	-2.27849500
H	5.02955000	3.78701100	-0.81542100
H	-4.26541900	3.33520000	-1.09406400
H	0.49898500	5.95946300	0.06318500
H	-0.91379300	7.78836200	0.87319800
H	-3.40074400	7.61285900	0.77333300
H	-4.45109400	5.54908300	-0.10404700
H	1.54258300	1.64560600	-3.29257500
H	3.20153000	1.04171500	-3.24470600
H	0.80457600	-0.45804000	-4.43391000
H	2.02078700	0.39389900	-5.39227100
H	2.35757600	-2.19487200	-5.03703100

H	3.74915000	-1.14550500	-4.83943100
H	3.98924200	-3.67948000	-3.72355000
H	4.35609000	-4.65898100	-1.45562500
H	2.50683500	-1.22726600	0.30689800
H	2.74640900	1.77729500	2.21666100
H	6.02321500	-0.98318700	2.51799900
H	5.46403500	1.30003900	-1.07738100
H	-4.27963200	0.75439300	-0.31796500
H	-4.82079600	-2.06441400	-3.52063400
H	-2.06017200	1.18759900	-3.97335000
Pd	-0.49743900	-1.39058900	0.08526700
I	-0.80683800	-2.91213100	-2.19678800
C	-0.81039100	-2.03789600	2.20799000
C	-1.13578800	-0.67297900	2.14747500
H	-2.14016500	-0.41523600	1.81486700
C	-1.50654000	-2.97355000	1.41046500
H	-2.51406600	-2.70820200	1.09412000
C	-0.45694400	0.36029800	3.02106900
H	0.61906500	0.17348500	3.03915600
C	-1.17644500	-4.40026900	1.32218300
C	-2.15618500	-5.28968700	0.84636900
C	0.07134500	-4.92086000	1.71594600
C	-1.90654600	-6.65821500	0.78183600
H	-3.11523500	-4.89489100	0.52250400
C	0.31971400	-6.28803800	1.64634400
H	0.86024000	-4.25750200	2.05713800
C	-0.66818300	-7.16262400	1.18298100
H	-2.67586100	-7.32973300	0.41191800
H	1.29140400	-6.66995600	1.94545800
H	-0.46926500	-8.22904100	1.12780000
C	-0.99248800	0.29452500	4.45059700
C	-2.28890500	0.74023700	4.79047800
C	-0.18180400	-0.26076800	5.44989800
C	-2.72873100	0.60172300	6.11484100
C	-0.63421000	-0.39131200	6.76273200
H	0.82114900	-0.58775700	5.19473200
C	-1.91788600	0.03627600	7.09732800
H	-3.72546700	0.95040200	6.37005500
H	0.01617100	-0.82401800	7.51767400
H	-2.28384100	-0.06061500	8.11551100
C	-3.20077000	1.37301400	3.79157400
C	-4.32810300	0.72484900	3.30359400
C	-3.04381500	2.74101400	3.37147300
O	-5.18283500	1.28383500	2.46994600
O	-3.81928000	3.33380100	2.58259500

O	-4.58406600	-0.52680800	3.66924300
O	-1.98763100	3.37276800	3.90555900
C	-1.82546600	4.75647000	3.55610300
H	-0.98515300	5.10645300	4.15598200
H	-1.60704300	4.86631700	2.49299900
H	-2.72851400	5.32330400	3.79399400
C	-5.81865800	-1.12631600	3.22838200
H	-6.67444000	-0.54512700	3.58033700
H	-5.85039400	-1.20282900	2.14183900
H	-5.82321700	-2.11777000	3.67987200
H	-0.60932000	1.35659500	2.59757800
H	0.08632300	-2.33901100	2.74449800
H	-4.81804000	2.24072100	2.34222600

Int1Ra

Thermal correction to Gibbs Free Energy: 0.865662

SCF energy in solution: -4931.562693

Solution-phase Gibbs free energy: -4930.697031

Coordinates:

C	6.91049600	4.74442400	1.02715600
C	5.69070100	5.44780500	1.16767500
C	4.49126000	4.77292000	1.22712600
C	4.44410800	3.35324900	1.14449100
C	5.67835800	2.64760900	0.96576800
C	6.90022300	3.37285200	0.92604100
C	3.21662300	2.60637700	1.18423300
C	3.25630700	1.23936800	0.94615000
C	4.47964300	0.51839100	0.80231700
C	5.65843500	1.23806500	0.82641200
C	1.90206200	3.26406000	1.44551600
C	1.64491800	3.98391400	2.66266100
C	0.37964500	4.63650700	2.82649000
C	-0.59544400	4.53080100	1.80449300
C	-0.38432100	3.78410900	0.66096100
C	0.88138500	3.14215100	0.51583400
C	2.57500000	4.04860300	3.73718500
C	2.28303100	4.74783500	4.88784000
C	1.04744200	5.42354300	5.02999800
C	0.11625600	5.36401000	4.01954600
O	2.06316000	0.53712400	0.84363200
O	1.10716800	2.38928600	-0.63112400
P	1.10883100	0.72176700	-0.52931500
N	2.12007700	0.42712900	-1.85862900
C	2.91244000	1.46330500	-2.55932000
C	2.39867600	1.61473700	-3.99030600
C	2.57130700	0.29291700	-4.74801600

C	2.29926000	-0.93077100	-3.89584200
C	2.08592300	-0.84193800	-2.50270300
C	2.26721200	-2.19278100	-4.50165100
C	2.01334900	-3.35347400	-3.78270600
C	1.80904500	-3.23224500	-2.41136500
C	1.86548100	-2.00628100	-1.75829100
C	4.51898800	-0.96200300	0.65193300
C	-1.45446000	3.66024300	-0.36255700
C	3.87319900	-1.80825800	1.56459100
C	3.99728400	-3.19529200	1.45072600
C	4.74227800	-3.76223000	0.41823900
C	5.37390800	-2.92399400	-0.50039600
C	5.27184600	-1.53842500	-0.38115300
C	-2.76647300	3.37595100	0.03567700
C	-3.79131000	3.26756700	-0.90606800
C	-3.52874500	3.44959900	-2.26143200
C	-2.22476400	3.74427400	-2.66248400
C	-1.19729200	3.84716500	-1.72864700
N	1.55330000	-4.43818800	-1.61877900
O	1.34902900	-4.30218200	-0.40849100
O	1.55932500	-5.52205400	-2.20124600
C	6.10957200	-3.52190800	-1.67081600
F	7.09844800	-2.71043600	-2.10899800
F	6.66484500	-4.71172800	-1.35970000
F	5.27938400	-3.73235200	-2.71745900
C	3.32805800	-4.07729600	2.47441100
F	3.67005400	-3.70209700	3.73456700
F	1.98005900	-4.00301300	2.40924600
F	3.66839100	-5.37156100	2.33549000
C	-1.93020200	4.00773400	-4.11650500
F	-2.04680000	5.32732600	-4.40525500
F	-0.66821400	3.65053200	-4.44676000
F	-2.77411200	3.34950600	-4.93174700
C	-5.16455500	2.86979300	-0.43669300
F	-5.49861200	3.51053800	0.71442800
F	-6.11814600	3.14368700	-1.34505100
F	-5.23371100	1.54497300	-0.16311300
H	7.84858700	5.28982700	0.98910100
H	5.69975900	6.53227900	1.22506500
H	3.56638400	5.32841000	1.32642300
H	7.82793500	2.82034300	0.80276500
H	6.60414600	0.71008800	0.73926500
H	-1.53775700	5.05744600	1.92781000
H	3.52115500	3.52875300	3.65007500
H	3.00772300	4.77796200	5.69616800

H	0.83469500	5.97749600	5.93932300
H	-0.84312100	5.86434100	4.12145400
H	2.83833300	2.39643600	-2.00732100
H	3.96524200	1.15063200	-2.55453400
H	1.34365500	1.90410100	-3.95682700
H	2.94481200	2.41668900	-4.49914900
H	1.91713400	0.26878400	-5.62644800
H	3.59870900	0.21902200	-5.13178600
H	2.42794700	-2.25726100	-5.57438400
H	1.97477100	-4.32755400	-4.25203000
H	1.74905100	-1.98248400	-0.68313800
H	3.28786300	-1.38288800	2.37246400
H	4.83257700	-4.83798900	0.33511000
H	5.77407000	-0.90127100	-1.10062800
H	-2.98829000	3.22403800	1.08681400
H	-4.31949900	3.34757400	-2.99407500
H	-0.19117900	4.06376100	-2.06416300
Pd	-0.95465600	-0.35087300	-0.35576700
I	-1.60479800	-0.32268400	-3.03338400
C	-2.07359000	-1.38861000	1.28925400
C	-2.97277400	-1.24815100	0.21822300
H	-3.50695000	-0.30609800	0.10821900
C	-1.45478300	-0.25939900	1.87227600
H	-1.98433100	0.68785600	1.77111100
C	-3.57295800	-2.44086300	-0.49760000
H	-3.20608700	-2.45031200	-1.52765800
C	-0.48450100	-0.29558400	2.97564600
C	-0.32675200	0.85441500	3.76944200
C	0.26979700	-1.43850900	3.29786000
C	0.54030600	0.86229400	4.85993400
H	-0.89343400	1.74955400	3.52726100
C	1.13200700	-1.43330600	4.39126400
H	0.20146300	-2.32980000	2.68416600
C	1.26989800	-0.28427600	5.17744600
H	0.64663000	1.76340700	5.45621900
H	1.70648200	-2.32433800	4.62174300
H	1.94472100	-0.28485200	6.02859700
C	-5.09383700	-2.42803300	-0.53884500
C	-5.87886700	-2.52368600	0.63025500
C	-5.73471300	-2.32369300	-1.78022700
C	-7.27616300	-2.51426600	0.51480500
C	-7.12551900	-2.31486900	-1.88058200
H	-5.12840700	-2.24146900	-2.67834500
C	-7.90189100	-2.41088100	-0.72636500
H	-7.87372300	-2.58905900	1.41907600

H	-7.59746100	-2.23208400	-2.85562600
H	-8.98642600	-2.40598800	-0.78989200
C	-5.26471300	-2.61126500	1.98824700
C	-5.20003400	-1.47647700	2.87234600
C	-4.72856200	-3.78767900	2.49084400
O	-4.72215500	-1.50643500	4.03099800
O	-4.19545700	-3.89462900	3.68936300
O	-5.68118600	-0.33304300	2.35591100
O	-4.72299300	-4.88730400	1.73890100
C	-4.17122800	-6.08845900	2.30541600
H	-4.27632000	-6.84246200	1.52613200
H	-3.11789000	-5.95195800	2.56130100
H	-4.72438400	-6.38554700	3.19964800
C	-5.63764300	0.82220500	3.20536900
H	-6.34870800	0.72102500	4.03023200
H	-4.63718800	0.96081600	3.62248200
H	-5.90990100	1.66022600	2.56532600
H	-3.21152300	-3.36256100	-0.02532900
H	-1.72885700	-2.38556400	1.55429100
H	-4.29727400	-2.95383000	4.09636900

Int1Rb

Thermal correction to Gibbs Free Energy: 0.864455

SCF energy in solution: -4931.564682

Solution-phase Gibbs free energy: -4930.700227

Coordinates:

C	-3.84768300	-6.58431900	2.96895800
C	-2.49467700	-6.50712400	3.37618400
C	-1.74124300	-5.38557700	3.10746500
C	-2.29966900	-4.27799500	2.41101000
C	-3.65928300	-4.37477800	1.96840500
C	-4.41408100	-5.53904800	2.27743300
C	-1.55109000	-3.09253200	2.09530100
C	-2.13683400	-2.12541100	1.29178600
C	-3.49586500	-2.19609600	0.86035500
C	-4.22555600	-3.31221700	1.22182100
C	-0.15286400	-2.88701400	2.57750900
C	0.16539600	-2.84909700	3.97868800
C	1.53545000	-2.70308600	4.37194100
C	2.53520900	-2.57852600	3.37705800
C	2.23469100	-2.54527600	2.02856300
C	0.86381700	-2.67967900	1.65743500
C	-0.82243200	-2.90844500	5.00087800
C	-0.46968700	-2.85894000	6.33160900
C	0.88781200	-2.75282200	6.71645000
C	1.86698900	-2.67422900	5.75403600
O	-1.37098700	-1.03829300	0.88937000

O	0.53861000	-2.62630900	0.30310200
P	-0.18336800	-1.24540000	-0.28957800
N	-0.96926700	-1.94739900	-1.62136200
C	-1.10446500	-3.40318700	-1.85127800
C	-0.35467300	-3.79267900	-3.12477300
C	-0.96169800	-3.06457800	-4.32941800
C	-1.32587700	-1.62416200	-4.03286700
C	-1.33237800	-1.11557300	-2.71562400
C	-1.67251500	-0.76775800	-5.08599100
C	-1.98876500	0.56987200	-4.88299200
C	-1.98085100	1.04154900	-3.57317600
C	-1.69798900	0.21624500	-2.49106700
C	-4.12881000	-1.11695300	0.05567300
C	3.31893300	-2.38350900	1.02517500
C	-4.03628700	0.23114900	0.43263000
C	-4.67401400	1.22011200	-0.31754300
C	-5.40848400	0.89055200	-1.45660900
C	-5.49944300	-0.44747400	-1.83795200
C	-4.87052800	-1.44244000	-1.08861400
C	4.30891200	-1.41063800	1.21893400
C	5.34954800	-1.26144500	0.30180600
C	5.42483200	-2.08064800	-0.82316300
C	4.44456200	-3.05314200	-1.01726000
C	3.40337300	-3.20760400	-0.10496900
N	-2.27476100	2.45111000	-3.31398000
O	-2.12697900	2.87033300	-2.15813600
O	-2.64258900	3.15008900	-4.25633300
C	-6.20675500	-0.81623600	-3.11553200
F	-6.75555800	-2.05011800	-3.04480900
F	-7.19352400	0.05395300	-3.41397900
F	-5.35323600	-0.82566400	-4.16494700
C	-4.60737500	2.65209100	0.15075700
F	-5.54607000	2.90293400	1.09228200
F	-3.41059300	2.93920300	0.69646900
F	-4.82025700	3.52384600	-0.86076600
C	4.52799300	-3.97969700	-2.20202300
F	5.18272800	-5.12343600	-1.88262800
F	3.30188100	-4.34789800	-2.63971000
F	5.18613000	-3.42402100	-3.23599800
C	6.41596900	-0.22975100	0.55396600
F	7.41589400	-0.72401900	1.32047200
F	6.97551900	0.21770700	-0.58723300
F	5.92462100	0.85029300	1.21548100
H	-4.43080700	-7.47204900	3.19439400
H	-2.04398700	-7.34301200	3.90302900

H	-0.70454400	-5.34629400	3.41975900
H	-5.44757900	-5.59105700	1.94537700
H	-5.26934800	-3.38194700	0.92807400
H	3.57317900	-2.50757400	3.68975200
H	-1.86723000	-2.98374900	4.72459400
H	-1.24243800	-2.89753400	7.09362300
H	1.15078900	-2.72222500	7.76945200
H	2.91218300	-2.57602000	6.03496900
H	-0.71740000	-3.93130300	-0.98345100
H	-2.17331900	-3.63929000	-1.94136800
H	0.70107100	-3.52805800	-3.00739100
H	-0.41044000	-4.87688700	-3.27095500
H	-0.27255200	-3.09223200	-5.18035300
H	-1.87140000	-3.58825900	-4.65671900
H	-1.66274100	-1.16195600	-6.09840400
H	-2.22695000	1.23764000	-5.70045700
H	-1.77849000	0.62301500	-1.49335100
H	-3.46949300	0.51252700	1.31258600
H	-5.89435200	1.66367600	-2.03944500
H	-4.94669900	-2.47713200	-1.40463500
H	4.24882300	-0.74578200	2.07345600
H	6.21350300	-1.94353700	-1.55256900
H	2.64608400	-3.96060000	-0.28288300
Pd	1.02786900	0.70154200	-0.63487900
I	2.34105700	-0.16050300	-2.89754500
C	1.49316000	2.57131300	0.51750000
C	0.25151600	2.08323000	0.97554400
H	-0.65124800	2.37526100	0.43999900
C	1.71413900	2.90162700	-0.83317900
H	0.84091700	3.15840800	-1.43307900
C	0.06306600	1.66289600	2.42572000
H	-0.08094700	0.58110200	2.47408900
C	3.00813200	3.30983300	-1.39146800
C	3.02777500	4.11005200	-2.54650500
C	4.23475300	2.94104800	-0.80964200
C	4.23329500	4.54992800	-3.08920400
H	2.08850900	4.38892600	-3.01659600
C	5.43777400	3.37143500	-1.35745300
H	4.25307400	2.28251200	0.05140100
C	5.44230600	4.18319100	-2.49614000
H	4.22827200	5.17160600	-3.97970500
H	6.37207400	3.05096100	-0.90690300
H	6.38327800	4.51534400	-2.92508000
C	-1.11835300	2.31545600	3.12728200
C	-1.25836400	3.71682700	3.23318300

C	-2.09617400	1.49212700	3.70269400
C	-2.38396200	4.23793600	3.88743300
C	-3.20912800	2.02506400	4.35364100
H	-1.97607500	0.41313300	3.64056000
C	-3.35807100	3.40826100	4.43999300
H	-2.48722400	5.31675400	3.96036900
H	-3.95266800	1.36321400	4.78919300
H	-4.22120000	3.83959100	4.93872000
C	-0.25271000	4.65885000	2.65925000
C	-0.50835100	5.36113900	1.48469200
C	1.02514100	4.90909700	3.26389200
O	0.33882000	6.20565200	0.94067200
O	1.88424900	5.69911100	2.80725100
O	-1.65368000	5.16529500	0.84799900
O	1.26983700	4.21188600	4.39187700
C	2.53058900	4.47182700	5.02698100
H	2.54792400	3.83062400	5.90842000
H	3.36231800	4.23013000	4.36031400
H	2.60902100	5.52236600	5.31768100
C	-1.88408100	5.83868500	-0.40471800
H	-1.99003800	6.91472200	-0.24451200
H	-1.06732400	5.64970900	-1.10296000
H	-2.80599000	5.40489600	-0.78609700
H	0.98686500	1.87919200	2.97754300
H	2.34423900	2.52930800	1.19407300
H	1.15057400	6.19525900	1.56993000

Int1Sa-NMe3

Thermal correction to Gibbs Free Energy: 0.980068

SCF energy in solution: -5105.963857

Solution-phase Gibbs free energy: -5104.983789

Coordinates:

C	-8.06564400	3.10067500	0.69283400
C	-8.02755400	1.72781600	1.03322600
C	-6.82465300	1.07389500	1.18671200
C	-5.59082300	1.75672500	1.00084400
C	-5.63385900	3.13912500	0.62431300
C	-6.89123200	3.78835200	0.49218100
C	-4.31381200	1.10852000	1.12704400
C	-3.17244600	1.81173600	0.77191600
C	-3.19375000	3.20525900	0.45848500
C	-4.42047900	3.83601400	0.39816400
C	-4.17634100	-0.29273600	1.62200900
C	-4.63600000	-0.67454700	2.93050200
C	-4.50311300	-2.04118200	3.33993400
C	-3.89327100	-2.97293000	2.46505500
C	-3.39061700	-2.60135900	1.23491000

C	-3.53120100	-1.23895400	0.84162200
C	-5.18473000	0.25020400	3.86227500
C	-5.60972900	-0.16117300	5.10643300
C	-5.51298300	-1.51918600	5.49135900
C	-4.96640800	-2.43623200	4.62427200
O	-1.95383100	1.14980200	0.72330300
O	-3.03198200	-0.86997600	-0.40085300
P	-1.65681200	0.06689300	-0.53944300
N	-2.10349300	0.87330800	-1.97100200
C	-3.44429800	0.80371000	-2.59521700
C	-3.36442800	-0.00360300	-3.89066200
C	-2.41042800	0.68028700	-4.87889400
C	-1.20803400	1.32110300	-4.21535600
C	-1.08556100	1.40387800	-2.81107600
C	-0.18888100	1.85973300	-5.01145000
C	0.94280600	2.45345500	-4.46655200
C	1.03083500	2.52225900	-3.07910100
C	0.03053700	2.03011400	-2.24748600
C	-1.93539200	3.97033500	0.26066200
C	-2.69897400	-3.59342900	0.37188700
C	-0.88005700	3.85181300	1.17636000
C	0.28781500	4.59690300	1.01657100
C	0.43031700	5.47427200	-0.05721800
C	-0.61660400	5.59735100	-0.97047300
C	-1.78923300	4.85673800	-0.81484500
C	-1.64061300	-4.34055000	0.89649500
C	-0.95984300	-5.26560900	0.10252600
C	-1.34129600	-5.48016600	-1.21846300
C	-2.41134700	-4.74975000	-1.73956200
C	-3.08033500	-3.81115300	-0.95902600
N	2.19502300	3.15686300	-2.46237400
O	2.26291100	3.15360500	-1.22792500
O	3.04147500	3.66266900	-3.19785300
C	-0.43197200	6.46767600	-2.18591300
F	-1.61376100	6.87338900	-2.70012800
F	0.29282300	7.57106700	-1.90530700
F	0.22129300	5.80328700	-3.16659400
C	1.41426800	4.40398600	1.99597700
F	0.95661300	4.31212200	3.27016700
F	2.09455000	3.25033100	1.76233800
F	2.31113300	5.40558700	1.95620700
C	-2.87899500	-4.99724300	-3.14989500
F	-3.90078500	-5.89020400	-3.17368300
F	-3.34258600	-3.86761500	-3.73053300
F	-1.90315600	-5.49516400	-3.93079400

C	0.21439200	-5.98448000	0.70606400
F	-0.15704400	-6.74284400	1.76538400
F	0.83855300	-6.79044600	-0.17062700
F	1.13774100	-5.10447000	1.17945600
H	-9.02113800	3.60441200	0.58197600
H	-8.95665100	1.18265100	1.17118300
H	-6.81182700	0.02050000	1.44046400
H	-6.90639800	4.83993300	0.21799900
H	-4.46283400	4.90019700	0.18214700
H	-3.81479100	-4.01050100	2.77796900
H	-5.25876100	1.29595200	3.59029500
H	-6.02021100	0.56623400	5.80076500
H	-5.86031100	-1.83061500	6.47199400
H	-4.86994300	-3.48003600	4.91142600
H	-4.13917700	0.35692100	-1.88938200
H	-3.77852100	1.83076400	-2.79381700
H	-3.01066200	-1.01219700	-3.65474800
H	-4.36222000	-0.09795200	-4.33339400
H	-2.06120100	-0.03843200	-5.62815600
H	-2.94887800	1.46232200	-5.43290300
H	-0.28202300	1.78796400	-6.09165200
H	1.73736600	2.85588000	-5.08109800
H	0.12680900	2.15876100	-1.17862400
H	-0.97817100	3.17714600	2.01810000
H	1.34180400	6.04492800	-0.18361500
H	-2.58569900	4.95706400	-1.54367000
H	-1.32495600	-4.16895700	1.91983800
H	-0.79841500	-6.17873900	-1.84213400
H	-3.89073800	-3.23559500	-1.38973800
Pd	0.45370200	-0.87229700	-0.48225400
I	0.36047100	-2.14054000	-2.94499400
C	2.22640200	-1.27184600	0.85159900
C	2.95916000	-1.03431100	-0.30561500
H	3.03727100	-0.01555800	-0.68153000
C	1.36129900	-0.28950900	1.42942300
H	1.60190500	0.75371600	1.23100300
C	3.74007500	-2.09641500	-1.02620600
H	3.89544000	-2.94383000	-0.34562400
C	0.63491500	-0.52655500	2.69293600
C	0.24548300	0.57247800	3.48220900
C	0.32922900	-1.81823600	3.16729300
C	-0.42862800	0.39301000	4.68995200
H	0.49170900	1.57511300	3.14733300
C	-0.33949300	-1.99524100	4.37622200
H	0.60625700	-2.69026600	2.58328600

C	-0.72749500	-0.89270700	5.14335100
H	-0.71965600	1.25966400	5.27726500
H	-0.56227900	-3.00088200	4.72251900
H	-1.25766200	-1.03591800	6.08008500
C	5.06927000	-1.63777200	-1.59674100
C	5.96747400	-0.85913500	-0.83620500
C	5.42133100	-2.03476700	-2.89302000
C	7.19571900	-0.50484600	-1.41592500
C	6.64697000	-1.67475800	-3.45095600
H	4.71767300	-2.62673900	-3.47316400
C	7.53913900	-0.90293500	-2.70626000
H	7.88699100	0.09861500	-0.83447000
H	6.89826600	-1.98884700	-4.46036800
H	8.49757200	-0.61122200	-3.12774900
C	5.63209700	-0.39369600	0.54454000
C	5.61193900	-1.30584900	1.62645700
C	5.43151800	1.00641600	0.80003200
O	5.34361000	-1.10035700	2.84024400
O	5.27462900	1.55996400	1.90127500
O	5.90751300	-2.59333900	1.25724500
O	5.40483700	1.74987400	-0.34539900
C	5.28720900	3.16603500	-0.18181700
H	6.22356700	3.58787200	0.20191800
H	5.06938500	3.55979800	-1.17412400
H	4.47494100	3.41963700	0.50017700
C	5.92090000	-3.56337400	2.30077600
H	6.68024200	-3.32879300	3.05390200
H	4.94998700	-3.63302900	2.80107400
H	6.16009700	-4.51135000	1.81592100
H	3.11590200	-2.46717800	-1.84907100
H	2.25515600	-2.27527100	1.26917200
H	5.04031500	0.21079800	3.60707500
N	4.92807000	0.78036900	4.52777300
C	3.75703400	1.69278000	4.40878500
H	2.85355000	1.09130700	4.30075000
H	3.89341300	2.30252100	3.51846600
C	4.73772700	-0.22937800	5.60243000
H	5.58161600	-0.91861600	5.58387500
C	6.20004100	1.53522500	4.69689200
H	7.02460400	0.82084800	4.70979400
H	6.30892600	2.19445700	3.83809000
H	6.17339700	2.09571900	5.63555700
H	3.68352100	2.30751100	5.31070000
H	4.66961500	0.26715700	6.57406800
H	3.82182500	-0.78564500	5.40124000

Int1Sb-NMe3

Thermal correction to Gibbs Free Energy: 0.982109

SCF energy in solution: -5105.963680

Solution-phase Gibbs free energy: -5104.981571

Coordinates:

C	-1.80699100	-3.85044300	5.75520000
C	-2.78536200	-3.38274600	4.88081000
C	-2.48219800	-2.52449900	3.81168100
C	-1.13757800	-2.13136600	3.63172900
C	-0.15895800	-2.60971500	4.51407600
C	-0.48159500	-3.46056300	5.56989500
C	-0.69813600	-1.15818400	2.53632000
C	-1.29907800	-1.40452800	1.17159200
C	-1.01274900	-2.53219400	0.39351200
C	-1.60988700	-2.67060900	-0.88583300
C	-1.30853300	-3.75724700	-1.82680800
C	-2.22005100	-4.03536300	-2.86159400
C	-1.98619400	-5.07341500	-3.76040900
C	-0.82996100	-5.84848900	-3.65016300
C	0.09005600	-5.57799800	-2.63271100
C	-0.14682500	-4.54691600	-1.72818100
C	-3.58620300	-2.09229400	2.89858100
C	-4.12138000	-0.78584800	2.97941300
O	-3.50079900	-0.00919600	3.92762800
C	-4.01687700	1.30547600	4.10222000
Pd	-0.35342300	-0.78498600	-0.85529500
I	-0.61901100	-0.28906100	-3.56494900
P	1.10911000	0.97209700	-0.38729600
N	2.47793900	1.14375600	-1.38021100
C	3.09328600	2.44162600	-1.74063400
C	2.84974500	2.72911900	-3.22143000
C	3.49036000	1.63266700	-4.08247000
C	3.42585700	0.25211500	-3.46012500
C	2.94109000	0.03897800	-2.15110300
C	2.94699700	-1.25129200	-1.60919200
C	3.37462800	-2.31728500	-2.39497700
C	3.84224500	-2.14174200	-3.69458400
C	3.87433300	-0.84930400	-4.19976300
N	3.34935500	-3.66537000	-1.82776600
O	3.67433800	-4.60533600	-2.55245300
O	1.68022000	0.92837600	1.20147300
C	2.54385500	1.91309400	1.65671400
C	2.03939900	3.17655600	1.92488300
C	2.95739600	4.23054600	2.26349000
C	4.34759200	3.91550200	2.41545600
C	4.78493400	2.58180600	2.22079000

C	3.92081800	1.57650000	1.83458300
C	5.26580600	4.94668800	2.75292300
C	4.84339900	6.24671900	2.90552400
C	3.47801100	6.56787900	2.72018900
C	2.55986300	5.58853300	2.41035300
C	0.56912100	3.41095600	1.81584500
C	-0.20328700	3.89905200	2.92579600
C	-1.59410000	4.18347400	2.73149700
C	-2.18093100	3.94950600	1.46350200
C	-1.46362200	3.41453900	0.41187000
C	-0.08343000	3.12453600	0.62584400
C	-2.36179000	4.69117000	3.81503000
C	-1.79682700	4.87722700	5.05537100
C	-0.43463900	4.55452400	5.26244500
C	0.34154300	4.08211900	4.22728900
C	4.41106800	0.18836200	1.63439200
C	3.73538300	-0.90105100	2.19923100
C	4.20508200	-2.20188500	2.01914300
C	5.35965400	-2.44510400	1.27917400
C	6.04295100	-1.36350400	0.72123200
C	5.57645600	-0.06024700	0.89511000
C	-2.11217100	3.19569500	-0.90726400
C	-3.33183800	2.51656700	-0.99493300
C	-3.95950900	2.35277900	-2.23324400
C	-3.38827300	2.85791300	-3.39696700
C	-2.17206200	3.53629600	-3.31066200
C	-1.54014600	3.70478400	-2.08282300
O	0.63549800	2.58061900	-0.42896200
C	3.41889900	-3.33293800	2.62924300
F	3.97548900	-4.53343000	2.40024900
C	7.24030100	-1.61992200	-0.15550200
F	7.95729200	-2.68003900	0.27296400
C	-5.24648600	1.58414000	-2.28702900
F	-5.08089300	0.29678400	-1.88631500
C	-1.55895900	4.13824400	-4.54726400
F	-1.93416400	5.43239400	-4.69946400
O	2.99897100	-3.79237200	-0.64881200
F	6.86895200	-1.88211700	-1.42954700
F	8.07110300	-0.55408800	-0.19768900
F	3.31480600	-3.17981900	3.97411300
F	2.15303000	-3.36233800	2.15037200
F	-0.20738800	4.13332200	-4.49198900
F	-1.92894700	3.48677300	-5.66576300
F	-6.17873700	2.11621400	-1.44444900
F	-5.79504700	1.55526500	-3.51333900

C	-4.13348800	-3.02416700	1.96062500
O	-3.46184600	-4.21871300	1.95002200
C	-3.95312100	-5.20370100	1.04280100
O	-5.09514800	-2.85891500	1.18739100
O	-5.04589500	-0.25907800	2.30440600
H	5.55423100	7.02808600	3.15687400
H	3.15043000	7.59860000	2.81933900
H	1.51973700	5.85397100	2.26430500
H	6.31394700	4.68766900	2.87734800
H	5.83319500	2.34830400	2.38638900
H	-3.22565700	4.20890000	1.31534200
H	1.38054700	3.83293000	4.40563000
H	0.00253600	4.67695100	6.24893000
H	-2.39339000	5.26043000	5.87782200
H	-3.41046100	4.92071700	3.64492700
H	2.67292200	3.22041200	-1.10994300
H	4.16840000	2.37707400	-1.52715300
H	1.77136000	2.77344000	-3.39860100
H	3.26595100	3.70783100	-3.48519600
H	3.01646800	1.59976900	-5.06968600
H	4.54819400	1.87215300	-4.26043400
H	4.23955500	-0.68253900	-5.20947300
H	4.17006600	-2.99603200	-4.27187100
H	2.63636900	-1.43946900	-0.59038100
H	2.83884500	-0.72998600	2.78284500
H	5.71314300	-3.45818200	1.13397500
H	6.11237700	0.76459000	0.43869100
H	-3.77853600	2.09159900	-0.10091200
H	-3.86641200	2.70741300	-4.35628100
H	-0.59231200	4.22654100	-2.03660900
H	-2.19797300	-0.84591500	0.92418500
H	-2.56866600	-2.17775300	-1.03654500
H	0.39077700	-1.20600800	2.45806500
H	-3.11052700	-3.42108900	-2.96104300
H	0.59155000	-4.34374600	-0.95978900
H	-2.70199400	-5.27094400	-4.55332800
H	1.00370000	-6.15891000	-2.54900800
H	-0.64155800	-6.65205800	-4.35643400
H	0.87782100	-2.32438800	4.36576600
H	-3.81975300	-3.68668500	5.01541100
H	0.29985000	-3.82061600	6.23348300
H	-2.07735500	-4.51581700	6.57089600
H	-3.38470200	1.77378000	4.85797400
H	-3.97331600	1.88275000	3.17410800
H	-5.05672200	1.28424600	4.44734200

H	-5.00570300	-5.43443700	1.23573200
H	-3.85272200	-4.87667200	0.00363800
H	-3.33899400	-6.08961600	1.21168800
H	-0.94905100	-0.13722700	2.84492800
H	-0.23263000	-3.21438200	0.72067200
H	-6.14718100	-1.00524800	1.36263200
N	-7.17797300	-1.06360100	1.06207400
C	-7.70154900	0.32951500	1.09577500
H	-7.20303100	0.91141600	0.32160200
H	-7.47054700	0.75475300	2.07174100
C	-7.28702500	-1.67109900	-0.29439800
H	-6.81525200	-2.65030100	-0.26000500
C	-7.81919200	-1.91866200	2.09921700
H	-7.33070900	-2.89107500	2.07071700
H	-8.78059700	0.32208000	0.92145300
H	-8.34230100	-1.74297900	-0.57191000
H	-6.75490600	-1.03766900	-1.00249000
H	-7.65291000	-1.45762700	3.07341000
H	-8.88992700	-2.00304200	1.89619200

Int1Ra-NMe3

Thermal correction to Gibbs Free Energy: 0.981078

SCF energy in solution: -5105.967252

Solution-phase Gibbs free energy: -5105.967252

Coordinates:

C	-7.08465200	-3.17072700	3.63618400
C	-5.89813500	-3.89123600	3.91081500
C	-4.67125000	-3.40455900	3.51643500
C	-4.56206100	-2.16863800	2.81977300
C	-5.76922700	-1.46062500	2.51181400
C	-7.01763300	-1.98168200	2.94825800
C	-3.30689900	-1.62895700	2.37324400
C	-3.31129600	-0.49368400	1.57411700
C	-4.50206400	0.23910400	1.28676600
C	-5.69742300	-0.25568700	1.77048100
C	-2.00579600	-2.27694800	2.71455400
C	-1.57902100	-2.45145400	4.07545200
C	-0.34546500	-3.13462300	4.33102800
C	0.43293300	-3.59725400	3.24158000
C	0.06559300	-3.37598400	1.92770600
C	-1.16195100	-2.68674400	1.69396700
C	-2.30512400	-1.94203900	5.18774700
C	-1.85385700	-2.12888000	6.47611000
C	-0.65391100	-2.83674000	6.72654600
C	0.08366000	-3.32517200	5.67330900
O	-2.11602800	-0.04634100	1.03113700
O	-1.54208200	-2.44767200	0.37904500

P	-1.40502800	-0.89927600	-0.23734000
N	-2.59731200	-1.04509000	-1.43626400
C	-3.55478700	-2.16950800	-1.53976000
C	-3.27199100	-2.96163200	-2.81531700
C	-3.46612000	-2.06089500	-4.04092900
C	-2.98945000	-0.63825600	-3.82538400
C	-2.57539200	-0.17010200	-2.55907700
C	-2.96614600	0.24697400	-4.90995100
C	-2.53330400	1.56046600	-4.78478200
C	-2.13500000	1.99214300	-3.52294100
C	-2.16969600	1.16068300	-2.40922100
C	-4.48713400	1.50922300	0.51056700
C	0.93336400	-3.84656000	0.81663100
C	-3.66599400	2.58361800	0.88062300
C	-3.73337500	3.79527600	0.18823200
C	-4.59660200	3.95047000	-0.89500200
C	-5.40437400	2.87907700	-1.27564200
C	-5.35844800	1.67387000	-0.57553600
C	2.31520000	-3.62730800	0.87189200
C	3.15146700	-4.07884200	-0.15085400
C	2.62632500	-4.76293200	-1.24356700
C	1.25061400	-4.99298100	-1.29872000
C	0.41106000	-4.54163900	-0.28440800
N	-1.69488000	3.37922400	-3.35016600
O	-1.33559600	3.73615000	-2.22383600
O	-1.71386900	4.11640600	-4.33521900
C	-6.27818300	3.00102300	-2.49645400
F	-7.37099500	2.20909200	-2.41118500
F	-6.70511200	4.26751500	-2.68351900
F	-5.61306300	2.63603600	-3.61551700
C	-2.87392800	4.94705800	0.64314800
F	-3.05487900	5.19188800	1.96875700
F	-1.55483800	4.69759600	0.48396100
F	-3.15207400	6.08672200	-0.01480500
C	0.67197800	-5.78527900	-2.44179100
F	0.65416300	-7.11098500	-2.15702300
F	-0.60714700	-5.43053800	-2.70446100
F	1.38338400	-5.63516100	-3.57372900
C	4.61820100	-3.74529900	-0.08409900
F	5.10864100	-3.93801800	1.16862600
F	5.35279900	-4.49583300	-0.92619300
F	4.84800700	-2.44857200	-0.38715100
H	-8.04384000	-3.56380700	3.95932300
H	-5.95565100	-4.84103800	4.43432900
H	-3.77421500	-3.97430200	3.72728800

H	-7.92185100	-1.42504600	2.71648300
H	-6.61501400	0.29475400	1.58109500
H	1.34639500	-4.14680200	3.45133000
H	-3.22078800	-1.39022700	5.01339100
H	-2.42425000	-1.72699000	7.30845300
H	-0.31526400	-2.98433700	7.74767000
H	1.01433500	-3.85794200	5.84990800
H	-3.46418900	-2.79225300	-0.65377200
H	-4.57087100	-1.75277600	-1.55754900
H	-2.24552200	-3.33868400	-2.77436000
H	-3.94013100	-3.82805900	-2.87251900
H	-2.94892800	-2.48273800	-4.90966200
H	-4.53174800	-2.02599500	-4.30853700
H	-3.28063400	-0.11783800	-5.88399800
H	-2.50281100	2.24172800	-5.62472600
H	-1.89230100	1.56663700	-1.44582800
H	-2.98709600	2.47714400	1.71952600
H	-4.64165300	4.89117200	-1.42915700
H	-5.99814600	0.85311600	-0.88056900
H	2.74202400	-3.08676200	1.71026500
H	3.27250200	-5.09572300	-2.04615800
H	-0.65392000	-4.72238100	-0.35330600
Pd	0.73786400	-0.14902800	-0.75560700
I	0.94079400	-1.34388800	-3.22902400
C	2.20677400	1.29075800	0.14744300
C	2.93106100	0.57882700	-0.81961000
H	3.33136400	-0.39776600	-0.55334400
C	1.56323500	0.61812600	1.21192600
H	1.98409900	-0.34520500	1.49871600
C	3.54911700	1.24260400	-2.02742200
H	3.10730800	0.80447300	-2.92719600
C	0.78102900	1.27445300	2.27217500
C	0.67741000	0.64142800	3.52374500
C	0.15896900	2.52617200	2.10633700
C	-0.00466700	1.24045600	4.58189200
H	1.13973400	-0.33164700	3.66556300
C	-0.51829200	3.12895000	3.16567600
H	0.17942000	3.02040400	1.14104300
C	-0.60126600	2.49059200	4.40872100
H	-0.07566500	0.72542700	5.53533300
H	-0.99967900	4.08931000	3.01344300
H	-1.13659300	2.96094200	5.22870100
C	5.06016600	1.07494800	-2.10637300
C	5.91840000	1.56736500	-1.09835700
C	5.60725500	0.42871300	-3.22235000

C	7.30109900	1.39186800	-1.25681600
C	6.98479800	0.26277700	-3.36175200
H	4.93842200	0.04745300	-3.99007000
C	7.83747900	0.74808500	-2.37092900
H	7.96057100	1.77154300	-0.48110500
H	7.38556000	-0.24247900	-4.23637100
H	8.91371600	0.62763700	-2.46418400
C	5.39927800	2.24528500	0.13225300
C	5.36759600	1.53595300	1.37250900
C	4.94220300	3.57954500	0.07399000
O	5.04349500	1.95858100	2.49683700
O	4.45322700	4.30139800	0.98814000
O	5.73093100	0.21733500	1.22986900
O	5.03556200	4.13092500	-1.17696300
C	4.58386700	5.47531800	-1.31565000
H	4.72556600	5.72360300	-2.36874400
H	3.52769300	5.57625500	-1.04737300
H	5.16664200	6.15964800	-0.69033400
C	5.76188300	-0.55661700	2.42348900
H	6.56363700	-0.22690700	3.09414300
H	4.81538000	-0.48916200	2.96990600
H	5.94055200	-1.58389600	2.10438400
H	3.28736900	2.30746300	-2.02754100
H	2.02051700	2.34956500	-0.01434400
H	4.31165800	4.07087100	2.48334600
N	4.20274400	4.42496000	3.51373100
C	3.63654600	5.79499400	3.40245200
H	2.64656600	5.72879900	2.95014400
H	4.28253300	6.38509700	2.75295100
C	3.30566400	3.51372700	4.27572600
H	3.72965300	2.51355000	4.22868800
C	5.58054000	4.43987500	4.07555700
H	5.95968400	3.42009400	4.04096200
H	3.56553700	6.25317300	4.39268300
H	6.20228900	5.07727600	3.44500800
H	5.55990300	4.82801500	5.09789400
H	3.22178900	3.86715400	5.30775600
H	2.32187500	3.51143400	3.80524500

Int1Rb-NMe3

Thermal correction to Gibbs Free Energy: 0.980740

SCF energy in solution: -5105.970783

Solution-phase Gibbs free energy: -5104.990043

Coordinates:

C	7.18450200	2.67702500	3.65320500
C	6.05107400	3.44303600	4.01504900

C	4.78798000	3.06157000	3.61899500
C	4.58860900	1.89271100	2.83321400
C	5.74222900	1.13894700	2.43898700
C	7.02958600	1.55047900	2.87944200
C	3.29305600	1.46283900	2.38387600
C	3.21328700	0.39388000	1.50362800
C	4.34752700	-0.38516000	1.12341400
C	5.58113900	-0.00002300	1.61144500
C	2.03565700	2.14434400	2.81429800
C	1.65493000	2.22037000	4.19858900
C	0.45869200	2.92726400	4.54857100
C	-0.32903900	3.51054700	3.52680400
C	-0.00940000	3.38672100	2.18834500
C	1.17992200	2.67141900	1.85879100
C	2.38821800	1.58836300	5.24105400
C	1.97896200	1.68104200	6.55308300
C	0.81862700	2.41309400	6.89885700
C	0.07486500	3.01981600	5.91413700
O	1.97669100	0.05713600	0.97089700
O	1.50499700	2.52137100	0.51253200
P	1.27404500	1.03383500	-0.20745100
N	2.43571800	1.19610400	-1.43559700
C	3.46621500	2.25695500	-1.48673500
C	3.22869500	3.14294200	-2.70926100
C	3.34338900	2.30703600	-3.98925000
C	2.72031000	0.93159700	-3.86261500
C	2.30451200	0.41454500	-2.61629900
C	2.55617600	0.14073600	-5.00698700
C	1.97195800	-1.11889900	-4.96137300
C	1.57347500	-1.59984600	-3.71741000
C	1.76401200	-0.87432100	-2.54739900
C	4.22428000	-1.57732200	0.24215500
C	-0.88433200	3.99215200	1.15077900
C	3.26890600	-2.57530100	0.48747300
C	3.19525000	-3.70081800	-0.33434300
C	4.06402600	-3.85375400	-1.41438600
C	5.01375300	-2.86353200	-1.66382100
C	5.09708100	-1.73820200	-0.84310000
C	-2.27305500	3.81686000	1.21925500
C	-3.11133400	4.39830400	0.26722900
C	-2.58234900	5.16690800	-0.76801800
C	-1.20148200	5.34762600	-0.83700800
C	-0.35926300	4.77106100	0.11085900
N	0.92943400	-2.91158900	-3.62656000
O	0.49373900	-3.26735800	-2.52519600

O	0.84652200	-3.58703000	-4.65151100
C	5.89698800	-2.96370300	-2.87922100
F	7.08795600	-2.35261600	-2.68495500
F	6.14637100	-4.24621400	-3.21655000
F	5.32455600	-2.37446500	-3.95417100
C	2.19518600	-4.78219800	-0.00584200
F	2.65805100	-5.58865000	0.97682900
F	1.02834800	-4.26419500	0.42029500
F	1.93351300	-5.56792600	-1.07348500
C	-0.60956800	6.21139000	-1.91970200
F	-0.46392300	7.49216200	-1.49809100
F	0.62057200	5.78548700	-2.28746500
F	-1.38180100	6.24494000	-3.02163700
C	-4.60046200	4.21839600	0.38323000
F	-5.16082400	5.16866200	1.16683200
F	-5.21900600	4.27805000	-0.81380400
F	-4.92183400	3.02249700	0.94331500
H	8.17308200	2.98618600	3.97898400
H	6.17864900	4.34359600	4.60850400
H	3.93123500	3.66302100	3.89870000
H	7.89277400	0.96074900	2.58234000
H	6.45956200	-0.58733600	1.35822100
H	-1.21398500	4.07345200	3.81023200
H	3.27439700	1.01632700	4.99448200
H	2.55022300	1.18158000	7.32990800
H	0.51223600	2.48224000	7.93822000
H	-0.82866200	3.57006600	6.16292600
H	3.42384200	2.83106700	-0.56465300
H	4.45215700	1.77609000	-1.54055700
H	2.23361800	3.59226100	-2.63126000
H	3.95955400	3.95893500	-2.72394000
H	2.88269600	2.83327700	-4.83231000
H	4.40334800	2.17974400	-4.25217900
H	2.87318600	0.54373500	-5.96497700
H	1.81908100	-1.71761500	-5.84959000
H	1.49684300	-1.32923700	-1.60410800
H	2.58164800	-2.47973900	1.32033000
H	3.99571100	-4.72588800	-2.05314200
H	5.83626100	-0.97420700	-1.05791300
H	-2.69765900	3.19665500	2.00084600
H	-3.22919100	5.59069400	-1.52617400
H	0.71086000	4.91460800	0.03117500
Pd	-0.83822000	0.26154800	-0.77539400
I	-1.19321700	1.87336900	-2.98622500
C	-2.41686700	-0.97838100	0.23210000

C	-1.18080200	-1.38275500	0.77003900
H	-0.61081200	-2.14357700	0.23879000
C	-2.67829500	-1.04682300	-1.14996100
H	-2.10852300	-1.77303700	-1.72938800
C	-0.87666300	-1.23266000	2.24945300
H	-0.03320100	-0.54984900	2.37812900
C	-3.91100600	-0.55867100	-1.78535700
C	-4.34917200	-1.15728900	-2.97985700
C	-4.68125200	0.48510300	-1.24078000
C	-5.53010400	-0.74326200	-3.59714400
H	-3.75194300	-1.94728500	-3.42743300
C	-5.85498900	0.90436300	-1.86133300
H	-4.34060200	1.00157600	-0.35089700
C	-6.28928000	0.28756000	-3.03916700
H	-5.84723400	-1.21478900	-4.52309500
H	-6.41093600	1.73518200	-1.43740100
H	-7.19936900	0.62276500	-3.52825300
C	-0.52798900	-2.54307200	2.93942500
C	-1.42572000	-3.63350100	2.95901900
C	0.71171000	-2.65862300	3.58290700
C	-1.02766700	-4.80911000	3.61243400
C	1.08954400	-3.83667800	4.22785600
H	1.38612800	-1.80459500	3.58489800
C	0.21391000	-4.92157400	4.23680600
H	-1.71681600	-5.64881100	3.62307800
H	2.05670300	-3.90373400	4.71896100
H	0.49259700	-5.84826700	4.73134500
C	-2.77054500	-3.56513400	2.30318800
C	-2.96270100	-4.16666500	1.03499700
C	-3.85465400	-2.90222900	2.94862100
O	-3.99866300	-4.20089200	0.31894200
O	-5.02838000	-2.77229600	2.55623000
O	-1.82995900	-4.75156800	0.54563900
O	-3.48829500	-2.34576500	4.15648600
C	-4.53195400	-1.69876400	4.87632600
H	-4.07323000	-1.33154200	5.79642500
H	-4.95574700	-0.86235900	4.31039200
H	-5.34390800	-2.39304400	5.11638100
C	-1.91429300	-5.36593900	-0.73969800
H	-2.56138000	-6.24957500	-0.71364600
H	-2.30096100	-4.67238300	-1.49080000
H	-0.89328800	-5.64990300	-0.99258300
H	-1.73971600	-0.77006000	2.74409200
H	-3.11638400	-0.45725200	0.88177000
H	-5.40531100	-3.59300900	0.51794300

N	-6.46698900	-3.55684600	0.28265000
C	-6.99809800	-2.17917500	0.47226700
H	-6.47961200	-1.50318700	-0.20887600
H	-6.79803900	-1.88369200	1.49974000
C	-6.57995600	-4.00599400	-1.13142300
H	-6.06613300	-4.96185300	-1.22982500
C	-7.09438500	-4.52404900	1.22404600
H	-6.62702400	-5.49846400	1.07570400
H	-8.07012200	-2.17243800	0.25437100
H	-6.88984800	-4.17709100	2.23548400
H	-8.16870800	-4.58667700	1.02980500
H	-7.63348500	-4.10459600	-1.40679200
H	-6.09417200	-3.26950200	-1.77279300

TS1Sa-NMe3

Thermal correction to Gibbs Free Energy: 0.983001

SCF energy in solution: -5105.966528

Solution-phase Gibbs free energy: -5104.983527

Coordinates:

C	-8.41147100	2.13468300	0.62012900
C	-8.21300100	0.76116500	0.89678600
C	-6.94256200	0.25048700	1.04912700
C	-5.79753000	1.08557000	0.92648200
C	-6.00143200	2.46969800	0.61471500
C	-7.32576000	2.96807100	0.48144900
C	-4.45500400	0.59080100	1.05621600
C	-3.39682800	1.44108800	0.76661800
C	-3.58443900	2.83598900	0.51621300
C	-4.87713500	3.31729400	0.45259200
C	-4.15388100	-0.80450000	1.49125000
C	-4.57422200	-1.30038800	2.77372100
C	-4.25210200	-2.64956800	3.13286200
C	-3.50025400	-3.44692500	2.23611200
C	-3.04260100	-2.95982900	1.02863200
C	-3.37754400	-1.61856700	0.68115800
C	-5.26299800	-0.50255200	3.72990700
C	-5.64309500	-1.02130800	4.94826400
C	-5.35785700	-2.36629700	5.28227600
C	-4.67229000	-3.15894600	4.39157400
O	-2.10961900	0.93643100	0.72854700
O	-2.92699800	-1.12447100	-0.53374000
P	-1.63384300	-0.05507100	-0.57552500
N	-2.12857000	0.79965500	-1.97547500
C	-3.41626400	0.60854900	-2.67627100
C	-3.17205100	-0.05528500	-4.03173700
C	-2.28924300	0.84593800	-4.90351600
C	-1.18923500	1.53896100	-4.12567000

C	-1.13926000	1.49914300	-2.71443600
C	-0.19486100	2.24477500	-4.81666600
C	0.85116800	2.88513000	-4.16475800
C	0.87493700	2.82391100	-2.77327500
C	-0.11006100	2.16828600	-2.04240700
C	-2.42618700	3.75686300	0.38190000
C	-2.20402000	-3.81272900	0.14653000
C	-1.37092000	3.71757900	1.30394500
C	-0.29718300	4.60140200	1.19652100
C	-0.25188500	5.54469900	0.17204700
C	-1.30065400	5.59151300	-0.74691000
C	-2.37741900	4.71015900	-0.64489400
C	-1.05810800	-4.42260500	0.66703100
C	-0.25965400	-5.23781500	-0.13815300
C	-0.59992700	-5.47088600	-1.46768500
C	-1.74878000	-4.87138600	-1.98633400
C	-2.54143600	-4.04637000	-1.19318700
N	1.95342300	3.48106400	-2.04136800
O	1.98672300	3.33763800	-0.81172400
O	2.77495000	4.14407400	-2.67491300
C	-1.21502000	6.54009000	-1.91376900
F	-2.43677500	6.85447700	-2.39799300
F	-0.60005300	7.69394000	-1.57592100
F	-0.51046700	5.99997000	-2.93359300
C	0.80737100	4.51655300	2.21415900
F	0.35330300	4.77332500	3.46485500
F	1.35156300	3.27047500	2.26367400
F	1.81229900	5.37786100	1.96669400
C	-2.17102000	-5.14911400	-3.40509700
F	-3.08058000	-6.15746000	-3.45155900
F	-2.76011600	-4.07512300	-3.97420000
F	-1.13717100	-5.51861400	-4.18289100
C	1.00120700	-5.80487700	0.45049300
F	0.76590700	-6.41887200	1.63576100
F	1.59774400	-6.69961800	-0.35847200
F	1.91658900	-4.83049200	0.71136100
H	-9.41891200	2.52432500	0.50887000
H	-9.07136100	0.10170000	0.98574000
H	-6.80546900	-0.80503200	1.25305800
H	-7.46358200	4.02247400	0.25636400
H	-5.04436600	4.37794800	0.28467500
H	-3.27249900	-4.47238800	2.51378700
H	-5.48322700	0.53192600	3.49650800
H	-6.16479200	-0.38941900	5.66133300
H	-5.67132400	-2.76451100	6.24280000

H	-4.43059200	-4.18912200	4.64001600
H	-4.06886100	0.00615000	-2.04988900
H	-3.88676400	1.59322100	-2.80414100
H	-2.68238500	-1.02049700	-3.86664000
H	-4.12774500	-0.24648300	-4.53240300
H	-1.83837300	0.26606600	-5.71613200
H	-2.90759300	1.61800400	-5.38396900
H	-0.23522800	2.26643700	-5.90232000
H	1.62886100	3.41414100	-4.69976700
H	-0.06790300	2.19939500	-0.96339300
H	-1.39331300	2.99040900	2.10677400
H	0.58837600	6.22185200	0.08504000
H	-3.17375700	4.75157600	-1.37955800
H	-0.77478400	-4.23077300	1.69624800
H	0.02924800	-6.08559200	-2.09838500
H	-3.41716000	-3.57244000	-1.62009200
Pd	0.52476100	-0.81240100	-0.52140200
I	0.66404100	-1.94075800	-3.08951900
C	2.47342600	-1.04690400	0.55848900
C	3.38121200	-0.45402400	-0.35858600
H	3.22765600	0.59444000	-0.60388400
C	1.53296600	-0.29797000	1.32881300
H	1.61748300	0.78695600	1.28711700
C	4.09334500	-1.27708000	-1.39971900
H	4.17386700	-2.31496500	-1.05028400
C	0.87890300	-0.80748200	2.55163200
C	0.13563400	0.08479900	3.35224100
C	0.96896100	-2.14724100	2.98407500
C	-0.49342600	-0.33677400	4.52311800
H	0.05007900	1.11910300	3.03277200
C	0.34233300	-2.56614900	4.15787100
H	1.52050900	-2.87292300	2.39658800
C	-0.39384200	-1.66757900	4.93633000
H	-1.06801700	0.37408100	5.11101700
H	0.43135900	-3.60471600	4.46667700
H	-0.88710300	-2.00079000	5.84449500
C	5.45981000	-0.72059700	-1.70694400
C	6.09670300	-0.02185700	-0.67000400
C	6.10532500	-0.89962300	-2.93263200
C	7.38330100	0.48941300	-0.87690400
C	7.38784600	-0.38660400	-3.13000700
H	5.60062000	-1.43385200	-3.73347300
C	8.02728800	0.30881100	-2.10089900
H	7.87778600	1.03632400	-0.07863800
H	7.88443600	-0.52210400	-4.08687300

H	9.02409600	0.71351700	-2.25336100
C	5.34779300	0.12976600	0.61774600
C	5.41905700	-0.93763500	1.59639900
C	5.02532100	1.47017100	1.09559100
O	4.96932400	-0.93772200	2.75265400
O	4.65553300	1.78707400	2.23362300
O	5.99107100	-2.06309600	1.09667400
O	5.12476400	2.39262700	0.11465400
C	4.82040200	3.75327000	0.45852100
H	5.66187800	4.19772100	1.00094300
H	4.65932500	4.26247800	-0.49022500
H	3.91853000	3.81285500	1.06591300
C	6.01711100	-3.19859600	1.96608100
H	6.59245700	-2.98674400	2.87216500
H	5.00572000	-3.49861300	2.25370300
H	6.49694500	-3.99261000	1.39344300
H	3.46031000	-1.31016100	-2.29705300
H	2.61408700	-2.10503900	0.76312500
H	4.24018100	0.47292700	3.64954900
N	4.09124300	0.72631800	4.66170400
C	3.10477300	1.84321400	4.74215700
H	2.13276000	1.47054300	4.42129400
H	3.43049900	2.63264400	4.06882600
C	3.61887900	-0.49800300	5.37064400
H	4.33821400	-1.29413800	5.18637200
C	5.44353400	1.15115900	5.12421700
H	6.13243100	0.32196800	4.96452600
H	5.75273900	2.00065200	4.51715400
H	5.39992300	1.41852900	6.18248700
H	3.04884100	2.19469600	5.77533100
H	3.53519600	-0.28526700	6.43901600
H	2.64946800	-0.78831700	4.96595400

TS1Sb-NMe3

Thermal correction to Gibbs Free Energy: 0.982172

SCF energy in solution: -5105.962202

Solution-phase Gibbs free energy: -5104.980030

Coordinates:

C	-2.34939000	-0.72965200	6.63644300
C	-3.15703300	-1.07473400	5.55402100
C	-2.80310500	-0.69017300	4.25444700
C	-1.62869900	0.04316700	4.05085600
C	-0.82050100	0.39239300	5.13647200
C	-1.17995900	0.00697300	6.42740500
C	-1.31920400	0.44301500	2.62662300
C	-2.08049200	-0.39239800	1.60500600
C	-1.48545600	-1.54552700	1.00726900

C	-2.02203300	-2.10363100	-0.18848700
C	-1.74076500	-3.45946900	-0.69216500
C	-2.50424800	-3.96238700	-1.76414000
C	-2.28740700	-5.24221400	-2.26715400
C	-1.29068800	-6.05317500	-1.71880100
C	-0.51360400	-5.56587000	-0.66533300
C	-0.73769000	-4.28861200	-0.15234100
C	-3.62582600	-1.01178700	3.04499000
C	-4.68262300	-0.07996500	2.67273400
O	-4.51138000	1.14440000	3.22844600
C	-5.49077500	2.13352800	2.88618100
Pd	-0.53429900	-0.61583800	-0.77844000
I	-1.08494300	-0.62490700	-3.53864900
P	1.24335300	0.84158700	-0.64754100
N	2.54819500	0.63165800	-1.73030500
C	3.30578400	1.73143500	-2.36473800
C	2.91494900	1.83576100	-3.83925400
C	3.25770300	0.52923900	-4.56803400
C	3.07211200	-0.71133000	-3.71676200
C	2.73266800	-0.63835400	-2.34813100
C	2.61517000	-1.81496800	-1.59757600
C	2.78784100	-3.04443400	-2.22678900
C	3.10635900	-3.14794900	-3.57855900
C	3.25752800	-1.97133100	-4.29914100
N	2.66349800	-4.26921900	-1.43577300
O	2.76198900	-5.34883100	-2.01894800
O	1.95324300	0.92508700	0.90654900
C	3.03152500	1.75554600	1.14261800
C	2.82846500	3.12652200	1.21574900
C	3.96976100	3.99426400	1.30755600
C	5.27322900	3.41239900	1.43739100
C	5.40386900	2.00166100	1.47572300
C	4.31906900	1.16060300	1.32333300
C	6.41026600	4.26021700	1.52933200
C	6.27901900	5.62825500	1.46719900
C	4.99686900	6.20489200	1.30658600
C	3.87300100	5.41143500	1.23179100
C	1.42913100	3.64407300	1.19086800
C	0.89445300	4.41890300	2.27799300
C	-0.45179200	4.90262500	2.19019200
C	-1.23239300	4.57779700	1.05383900
C	-0.74668600	3.78200200	0.03550600
C	0.59589600	3.30800300	0.13357400
C	-0.98748600	5.68244600	3.25102800
C	-0.24336500	5.95221800	4.37553900

C	1.07154900	5.44146600	4.48530400
C	1.62572000	4.69755800	3.46685100
C	4.48623300	-0.31426100	1.38485900
C	3.61403000	-1.10824100	2.14308400
C	3.78778400	-2.48991300	2.21295300
C	4.83680400	-3.11058500	1.53894700
C	5.71272900	-2.32602700	0.78810300
C	5.54100000	-0.94385100	0.70864400
C	-1.61465300	3.42237100	-1.11486800
C	-2.88276100	2.88200800	-0.88368100
C	-3.71130900	2.53217400	-1.95230700
C	-3.29912900	2.73044400	-3.26648500
C	-2.04025200	3.28594400	-3.49977500
C	-1.20357200	3.62348200	-2.44027600
O	1.08148400	2.50936600	-0.88510800
C	2.79864500	-3.29289200	3.01588500
F	3.07940800	-4.60805200	3.01690500
C	6.79106400	-2.99522100	-0.02171700
F	7.28481800	-4.08520600	0.60425200
C	-5.01898300	1.86854100	-1.64648500
F	-4.83959800	0.64126000	-1.06927300
C	-1.59109500	3.56340200	-4.91050400
F	-1.87461600	4.84274100	-5.26643000
O	2.46793700	-4.15990100	-0.22075400
F	6.32226400	-3.40738400	-1.22152600
F	7.82767900	-2.16219000	-0.26800900
F	2.76509300	-2.88158600	4.30551500
F	1.53769400	-3.14378300	2.53688500
F	-0.25612900	3.41193700	-5.05224700
F	-2.19865800	2.76341900	-5.80528200
F	-5.75714300	2.57976600	-0.75364500
F	-5.78889900	1.67522000	-2.73276400
C	-3.82600200	-2.41769300	2.68600500
O	-2.93958900	-3.22627300	3.30269500
C	-2.99181100	-4.61677700	2.94873000
O	-4.63909400	-2.86611800	1.87451200
O	-5.63238600	-0.26750900	1.89741200
H	7.15541900	6.26622200	1.53118500
H	4.89811800	7.28431000	1.23729600
H	2.89856200	5.86735300	1.10068500
H	7.39044700	3.80353000	1.63925700
H	6.39017700	1.57558300	1.63870600
H	-2.24399400	4.96912600	0.98593700
H	2.63100900	4.30881500	3.57298300
H	1.64942400	5.63435200	5.38446400

H	-0.66423800	6.54343400	5.18330200
H	-2.00543700	6.05247900	3.15961500
H	3.09998200	2.65603200	-1.83188500
H	4.37689800	1.51201400	-2.26050900
H	1.84122500	2.03670800	-3.90373500
H	3.43623600	2.67797800	-4.30839800
H	2.65144100	0.43060200	-5.47525000
H	4.30473200	0.55521500	-4.90172000
H	3.51009100	-2.02350200	-5.35481700
H	3.23603600	-4.12253900	-4.03006700
H	2.40728800	-1.78905800	-0.53667400
H	2.79142500	-0.64579800	2.67460800
H	4.95687100	-4.18536200	1.58423200
H	6.22042500	-0.35552400	0.10205000
H	-3.20758000	2.70283800	0.13606400
H	-3.92872900	2.43363500	-4.09515600
H	-0.22041000	4.03052400	-2.64205900
H	-2.79115800	0.13091900	0.97222900
H	-2.94615600	-1.66486000	-0.55780200
H	-0.24654100	0.35874700	2.42961400
H	-3.24193000	-3.31621700	-2.23107700
H	-0.10414600	-3.93249600	0.65199900
H	-2.88416200	-5.60066100	-3.10170400
H	0.29189300	-6.16684100	-0.25499000
H	-1.10900800	-7.04654100	-2.11872200
H	0.09049900	0.96228700	4.97096300
H	-4.06401800	-1.65122200	5.71467600
H	-0.54648800	0.27356600	7.26883700
H	-2.62869700	-1.03569300	7.64073100
H	-5.16130100	3.04889900	3.37848400
H	-5.54904000	2.27579900	1.80452500
H	-6.47930700	1.84504800	3.25513700
H	-3.98664300	-5.02843100	3.13910400
H	-2.73518900	-4.75820200	1.89645300
H	-2.25258900	-5.10297300	3.58526700
H	-1.57863000	1.49923100	2.48302400
H	-0.74504900	-2.08566000	1.59041700
H	-6.07887000	-1.61984200	0.96294800
N	-6.74752400	-2.05672800	0.26701400
C	-7.68453300	-0.97632300	-0.15563400
H	-7.10238800	-0.17113800	-0.59900400
H	-8.20321500	-0.60111200	0.72629900
C	-5.93926400	-2.57153300	-0.87934900
H	-5.19695000	-3.26594300	-0.49003900
C	-7.45337500	-3.15969700	0.97963500

H	-6.70516000	-3.86840500	1.32832500
H	-8.39961200	-1.37709800	-0.87753600
H	-6.60364100	-3.06618800	-1.59192200
H	-5.44095800	-1.72845100	-1.35704300
H	-7.98226200	-2.73818300	1.83557900
H	-8.16286000	-3.63427700	0.29779200

TS1Ra-NMe3

Thermal correction to Gibbs Free Energy: 0.982401

SCF energy in solution: -5105.960561

Solution-phase Gibbs free energy: -5104.978160

Coordinates:

C	6.22307700	4.02111400	4.22507300
C	4.90017200	4.45812500	4.47310000
C	3.82271200	3.77140000	3.95840400
C	4.00680900	2.60532800	3.16282000
C	5.34876400	2.18914100	2.88420600
C	6.43848800	2.91082300	3.44261300
C	2.91725000	1.86191700	2.59307000
C	3.18952500	0.81541200	1.71976700
C	4.52344200	0.38364400	1.44998500
C	5.56436800	1.07084900	2.04265900
C	1.49781300	2.23116100	2.86484900
C	0.94602700	2.22580500	4.18999800
C	-0.39786100	2.68463500	4.38081800
C	-1.15000300	3.11464600	3.26037000
C	-0.65431100	3.05432700	1.97095400
C	0.67939800	2.57403500	1.79891700
C	1.66081100	1.74986900	5.32455900
C	1.08909400	1.75773500	6.57799600
C	-0.22564200	2.24650100	6.76895400
C	-0.95117100	2.69741600	5.69072800
O	2.13976400	0.16607400	1.10175000
O	1.19130200	2.46942000	0.51489300
P	1.26320200	0.92076300	-0.14915600
N	2.44324200	1.25920700	-1.33719600
C	3.20266100	2.52051100	-1.45252900
C	2.86526800	3.20824600	-2.77536800
C	3.26486400	2.30442800	-3.94679200
C	2.95093700	0.84194200	-3.70513100
C	2.56234100	0.36487300	-2.43398400
C	3.04967800	-0.06685100	-4.76587300
C	2.75273300	-1.41527800	-4.61784300
C	2.37040200	-1.85562700	-3.35345200
C	2.30282200	-1.00131800	-2.25907000
C	4.83994500	-0.77457100	0.56597800
C	-1.49296100	3.49822000	0.82794700

C	4.42878700	-2.07831400	0.88397600
C	4.86508000	-3.15859400	0.11563500
C	5.67569600	-2.95854200	-1.00458700
C	6.06127300	-1.66379100	-1.33907700
C	5.66081400	-0.58256900	-0.55110600
C	-2.84776200	3.14959300	0.78065900
C	-3.66641100	3.59688500	-0.25768400
C	-3.14823100	4.39507300	-1.27333300
C	-1.79810700	4.74633700	-1.23167400
C	-0.97844400	4.30917700	-0.19511700
N	2.03702400	-3.26850900	-3.15925800
O	1.61130700	-3.61823200	-2.05409000
O	2.19576900	-4.03530900	-4.11026800
C	6.88065800	-1.40665700	-2.57606200
F	7.79788600	-0.43299500	-2.36934900
F	7.54276300	-2.50942800	-2.98408200
F	6.10614400	-0.99972100	-3.60630900
C	4.47829900	-4.56830600	0.48442400
F	4.19023900	-4.68365600	1.80269800
F	3.39591900	-4.99730700	-0.19764900
F	5.47880800	-5.43816700	0.21647500
C	-1.23195400	5.66158500	-2.28529000
F	-1.31828800	6.96020200	-1.90035400
F	0.07741800	5.41620600	-2.51713200
F	-1.88700100	5.55522800	-3.45605900
C	-5.10446600	3.15706000	-0.27826000
F	-5.69268700	3.35376000	0.93541400
F	-5.83644100	3.82512200	-1.18885900
F	-5.22536100	1.83813500	-0.54527800
H	7.06221100	4.56959300	4.64241700
H	4.73226900	5.34882200	5.07162100
H	2.81818200	4.12852100	4.15035100
H	7.44890700	2.57229800	3.22845500
H	6.58516400	0.74641300	1.85879200
H	-2.14788500	3.51061800	3.42720500
H	2.66673900	1.36949200	5.19150800
H	1.65277000	1.38523100	7.42849500
H	-0.65955600	2.25763800	7.76451800
H	-1.96576600	3.06497800	5.82180800
H	2.96178000	3.15249600	-0.60113800
H	4.27608100	2.28823600	-1.40480500
H	1.79139800	3.41643200	-2.80075100
H	3.39070300	4.16762600	-2.84061700
H	2.76655400	2.62941400	-4.86659900
H	4.34451200	2.39783900	-4.13380800

H	3.34383300	0.30755200	-5.74266000
H	2.80513700	-2.11313200	-5.44293700
H	2.05215700	-1.41581400	-1.29207400
H	3.79719400	-2.25001300	1.74806300
H	6.01627000	-3.80123600	-1.59384200
H	5.99371400	0.41802100	-0.80492100
H	-3.26380200	2.51065400	1.55231100
H	-3.77736800	4.72382400	-2.09067200
H	0.06669400	4.58970700	-0.18751900
Pd	-0.68158700	-0.13033800	-0.75077600
I	-1.12432800	1.08091500	-3.25379900
C	-2.18665600	-1.72593600	-0.30023300
C	-3.44580400	-1.16957000	-0.69062300
H	-3.73840200	-0.24758600	-0.19293900
C	-1.48093500	-1.32537800	0.87161300
H	-1.97745900	-0.58376600	1.49852900
C	-3.95039100	-1.28156400	-2.11081900
H	-3.53170400	-0.44695500	-2.68854400
C	-0.50269800	-2.14956300	1.60756000
C	-0.12731900	-1.75893600	2.90945500
C	0.08433200	-3.31746800	1.08111200
C	0.78711100	-2.50134100	3.65732100
H	-0.54158400	-0.84268300	3.32378800
C	0.99664400	-4.06007300	1.82875600
H	-0.14390700	-3.63304000	0.06883600
C	1.35244300	-3.66229000	3.12298100
H	1.06517500	-2.16372500	4.65258200
H	1.45110600	-4.94015200	1.38748500
H	2.07336000	-4.24022500	3.69335400
C	-5.45604700	-1.27554800	-2.11803900
C	-6.05903300	-1.76390100	-0.95002900
C	-6.24459000	-0.84719800	-3.18716300
C	-7.45324400	-1.82410700	-0.86203400
C	-7.63600700	-0.90815500	-3.09350800
H	-5.77183200	-0.45916600	-4.08545400
C	-8.24025800	-1.39557300	-1.93166500
H	-7.92353400	-2.19831100	0.04352300
H	-8.24955800	-0.56838200	-3.92331600
H	-9.32343700	-1.43830000	-1.85803400
C	-5.12061400	-2.21920100	0.12929600
C	-5.20517600	-1.60136600	1.45152400
C	-4.64700900	-3.60180100	0.07285800
O	-4.71455200	-2.01301700	2.50967500
O	-4.01965400	-4.21532200	0.94419500
O	-5.84822800	-0.41170500	1.40786700

O	-4.89362700	-4.18163200	-1.12348600
C	-4.37540600	-5.50465500	-1.30712800
H	-4.64425500	-5.78265700	-2.32600600
H	-3.28973000	-5.52140100	-1.18232400
H	-4.82487600	-6.20192200	-0.59419700
C	-5.91315300	0.33437700	2.62677300
H	-6.59706100	-0.14007700	3.33767200
H	-4.92627000	0.41295500	3.09089900
H	-6.28134800	1.31894000	2.34221900
H	-3.56395200	-2.20044400	-2.57176700
H	-1.86751800	-2.62182600	-0.82859300
H	-3.67302900	-3.65902600	2.69606600
N	-3.46801300	-4.20233700	3.57178100
C	-2.41564100	-5.21175700	3.25043900
H	-1.50037300	-4.69216800	2.96711300
H	-2.76631900	-5.80710700	2.40941100
C	-3.03110700	-3.25071800	4.63391600
H	-3.78883000	-2.47472900	4.72441600
C	-4.77028900	-4.84589300	3.90937200
H	-5.50762200	-4.05801200	4.05915800
H	-2.24164700	-5.83775300	4.12863900
H	-5.06946600	-5.46716500	3.06610800
H	-4.65553300	-5.44804800	4.81333400
H	-2.90970900	-3.79545800	5.57316600
H	-2.08221800	-2.80723800	4.33103900

TS1Rb-NMe3

Thermal correction to Gibbs Free Energy: 0.984735

SCF energy in solution: -5105.961205

Solution-phase Gibbs free energy: -5104.976470

Coordinates:

C	6.95366000	3.99057600	2.90641800
C	5.75303900	4.62276200	3.30817900
C	4.53122500	4.03691600	3.05994400
C	4.44058300	2.78415100	2.39113800
C	5.65675900	2.16610000	1.95308300
C	6.90208400	2.78847500	2.24016400
C	3.18994600	2.13955600	2.09932700
C	3.18795900	0.98980600	1.32049900
C	4.39474000	0.35517200	0.89191500
C	5.59492900	0.94987100	1.23006300
C	1.88859200	2.69516600	2.57456200
C	1.60371700	2.86673200	3.97178900
C	0.36257200	3.47147500	4.35352600
C	-0.55892200	3.85713400	3.35062900
C	-0.32914400	3.62854200	2.00651000
C	0.91172000	3.02120600	1.64496400

C	2.48153000	2.43053200	5.00307500
C	2.16299500	2.61331700	6.33074800
C	0.95307400	3.24597600	6.70333600
C	0.07279800	3.66259500	5.73229700
O	1.97714700	0.43681500	0.94537700
O	1.16664400	2.77556800	0.30318700
P	1.02310200	1.19564800	-0.25736500
N	2.09697000	1.35350300	-1.58261300
C	2.96908200	2.51730900	-1.84109800
C	2.58825300	3.16289800	-3.17349600
C	2.79661700	2.16031300	-4.31335100
C	2.33186400	0.76280300	-3.95992200
C	2.00954900	0.40406600	-2.63207000
C	2.21125400	-0.20145700	-4.96959100
C	1.75080200	-1.48746800	-4.71918600
C	1.43921100	-1.81083500	-3.40050900
C	1.59905300	-0.90612300	-2.35762700
C	4.39322200	-0.90825600	0.10681000
C	-1.35283000	4.01625000	1.00178100
C	3.66244200	-2.03273200	0.51853200
C	3.72316900	-3.22149000	-0.20911100
C	4.50019900	-3.31269500	-1.36445300
C	5.22220500	-2.19655000	-1.78250900
C	5.17488600	-1.00818600	-1.05229500
C	-2.70789700	3.76987800	1.26293400
C	-3.69182800	4.15467600	0.35246500
C	-3.34526000	4.78852900	-0.83950200
C	-1.99898500	5.03764300	-1.10364500
C	-1.01221800	4.66224900	-0.19511000
N	0.91652800	-3.13710600	-3.08804100
O	0.59198800	-3.37078200	-1.91519900
O	0.81009900	-3.95654600	-4.00055000
C	5.99383400	-2.24017200	-3.07477500
F	7.10041200	-1.46383900	-3.02216300
F	6.38943900	-3.49320400	-3.38431900
F	5.24927600	-1.79084200	-4.11045900
C	2.99489700	-4.43915300	0.29976800
F	3.76064800	-5.13514200	1.17403600
F	1.85918200	-4.11107300	0.94182300
F	2.67547900	-5.28973600	-0.70211600
C	-1.60773300	5.77811600	-2.35587600
F	-1.58028900	7.11843100	-2.13624800
F	-0.37340000	5.43433600	-2.78406800
F	-2.47313900	5.56531000	-3.36362200
C	-5.13981900	3.93112000	0.69074800

F	-5.65463800	4.97348700	1.38723000
F	-5.90648200	3.77609100	-0.40658300
F	-5.31597900	2.83101400	1.46903100
H	7.90972300	4.46125000	3.11514000
H	5.79494400	5.58294800	3.81408600
H	3.62178800	4.53923500	3.36697100
H	7.81492700	2.29882600	1.91099800
H	6.52568200	0.47269500	0.93517700
H	-1.47778800	4.35036900	3.65483200
H	3.40889300	1.93861800	4.73494900
H	2.84609300	2.26500100	7.09997200
H	0.71899300	3.39037700	7.75386700
H	-0.86737600	4.13547100	6.00406100
H	2.86749300	3.21844800	-1.01658600
H	4.01340200	2.17520400	-1.86388600
H	1.54040900	3.47605300	-3.12664200
H	3.19722900	4.05835100	-3.34029400
H	2.27510000	2.49330900	-5.21728400
H	3.86394400	2.11508600	-4.57490900
H	2.45648800	0.08436900	-5.98882500
H	1.62425200	-2.21995100	-5.50538200
H	1.39922100	-1.23826300	-1.34949200
H	3.04927400	-1.98354400	1.41039200
H	4.53567900	-4.23536900	-1.93080100
H	5.73996700	-0.14804800	-1.39436600
H	-2.99447000	3.24842100	2.16919200
H	-4.10528100	5.05805700	-1.56250800
H	0.02619200	4.85892500	-0.42676100
Pd	-1.01834300	0.18330500	-0.66388800
I	-1.61993900	1.40550800	-3.11109700
C	-2.15290700	-1.15100700	0.73988200
C	-1.11731700	-1.98342200	1.26279300
H	-0.53225200	-2.55510600	0.54652300
C	-2.66274800	-1.24696900	-0.58314700
H	-2.24388500	-2.03648500	-1.20690700
C	-0.37982900	-1.59069400	2.52829600
H	0.48631700	-0.97835300	2.25673600
C	-3.99062400	-0.77649200	-1.01926100
C	-4.45553600	-1.15148100	-2.29617800
C	-4.83298100	0.02838200	-0.22958700
C	-5.71241800	-0.75904600	-2.75525300
H	-3.79816000	-1.72442400	-2.94459100
C	-6.08620600	0.42837100	-0.69114800
H	-4.50188900	0.36976100	0.74512500
C	-6.53977400	0.02960900	-1.95200600

H	-6.03578700	-1.05128100	-3.75075600
H	-6.70082900	1.07005000	-0.06793100
H	-7.51408500	0.34825600	-2.31111900
C	0.03963400	-2.81475300	3.30219000
C	-0.74611600	-3.95805300	3.10029400
C	1.11671300	-2.84944700	4.19030500
C	-0.43976800	-5.13425900	3.79263700
C	1.41683100	-4.02671500	4.87745000
H	1.72070600	-1.95816200	4.34402800
C	0.63905300	-5.16972600	4.67654800
H	-1.03994500	-6.02543100	3.63180400
H	2.25923000	-4.05524400	5.56304900
H	0.87517700	-6.08867600	5.20579400
C	-1.89504200	-3.81392100	2.14724000
C	-1.95060700	-4.67058600	0.96020800
C	-3.16544500	-3.33827800	2.68403400
O	-2.90277700	-4.79679200	0.17920800
O	-4.26583100	-3.33355400	2.12255900
O	-0.78305900	-5.30060100	0.73759500
O	-3.03002300	-2.79000800	3.91932100
C	-4.21878800	-2.23879000	4.49428000
H	-3.91383500	-1.82856000	5.45729000
H	-4.63583000	-1.45214800	3.85969800
H	-4.97911400	-3.01197300	4.63863400
C	-0.66438100	-6.05943100	-0.47820500
H	-1.47651100	-6.78601200	-0.56114900
H	-0.65849700	-5.39301600	-1.34234400
H	0.29891500	-6.56203300	-0.40335900
H	-1.03185900	-0.95725900	3.14518400
H	-2.69080800	-0.54549000	1.46661400
H	-4.63836200	-4.07184900	0.36347900
N	-5.56062100	-4.38052400	-0.03341200
C	-6.57300200	-3.31377300	0.22416900
H	-6.28358200	-2.41235200	-0.31465500
H	-6.58126600	-3.10981200	1.29311700
C	-5.37240600	-4.64045900	-1.49093800
H	-4.52502600	-5.31369100	-1.60751700
C	-5.87156800	-5.63256300	0.71432600
H	-5.06372200	-6.34171300	0.53746400
H	-7.55046000	-3.66278300	-0.11702100
H	-5.91593700	-5.38984500	1.77532300
H	-6.82545100	-6.03601100	0.36752000
H	-6.28619500	-5.08050000	-1.89694800
H	-5.16158500	-3.69146600	-1.98394300

Thermal correction to Gibbs Free Energy: 0.985558

SCF energy in solution: -5105.991134

Solution-phase Gibbs free energy: -5105.005576

Coordinates:

C	-8.57597600	1.67057100	0.38760600
C	-8.31668200	0.29936300	0.62301600
C	-7.02864200	-0.14997900	0.81532700
C	-5.92545600	0.74733500	0.77581300
C	-6.18917500	2.13032700	0.50619500
C	-7.53122700	2.56388200	0.33026400
C	-4.56660000	0.31778400	0.95068100
C	-3.54068600	1.22985600	0.73709100
C	-3.79276600	2.62294900	0.53117400
C	-5.10531700	3.04033700	0.42851200
C	-4.20571800	-1.06847500	1.36962600
C	-4.64935700	-1.61042700	2.62536400
C	-4.24316800	-2.93544500	2.98884400
C	-3.38095500	-3.65700900	2.12838800
C	-2.90584600	-3.12312400	0.94772300
C	-3.33708800	-1.81304800	0.58433700
C	-5.44291300	-0.88036700	3.55485300
C	-5.84446600	-1.44381000	4.74612700
C	-5.47608700	-2.76834600	5.08057600
C	-4.68676500	-3.49321500	4.21866700
O	-2.23325900	0.79571800	0.73479400
O	-2.88498300	-1.27656500	-0.60824100
P	-1.64472200	-0.13188300	-0.59169800
N	-2.18335000	0.75494600	-1.96879800
C	-3.44224400	0.50530200	-2.69976800
C	-3.13297400	-0.05115300	-4.08976300
C	-2.32923800	0.97701600	-4.89218300
C	-1.27649300	1.68117500	-4.06158700
C	-1.23267300	1.55012500	-2.65436800
C	-0.32191000	2.48628500	-4.69917700
C	0.68259800	3.14332800	-4.00195200
C	0.70404100	2.99283800	-2.61604600
C	-0.24336100	2.23443200	-1.93539500
C	-2.67972100	3.60594000	0.47667200
C	-1.94183900	-3.90172200	0.12350800
C	-1.63733000	3.56802000	1.41471000
C	-0.60968200	4.51119700	1.37650000
C	-0.59831600	5.51363000	0.40858400
C	-1.63296800	5.55847300	-0.52591800
C	-2.66253100	4.61774200	-0.49413200
C	-0.74967900	-4.34500500	0.70894000
C	0.15719100	-5.11341300	-0.02324600

C	-0.11850200	-5.46459300	-1.34348300
C	-1.30685300	-5.02609200	-1.92679800
C	-2.20845200	-4.24424700	-1.20699900
N	1.73842900	3.66261900	-1.83881100
O	1.76821400	3.46234000	-0.61592300
O	2.53804400	4.39543000	-2.42555100
C	-1.57764100	6.57546100	-1.63508600
F	-2.80460600	6.85062900	-2.12944900
F	-1.03518300	7.74077100	-1.21798600
F	-0.82266200	6.13622900	-2.66718000
C	0.48302600	4.43062800	2.40648600
F	0.00406900	4.60827300	3.66113300
F	1.09170000	3.21270900	2.41010300
F	1.45156300	5.34976000	2.21477000
C	-1.65667600	-5.45583800	-3.32702600
F	-2.40155000	-6.59400000	-3.30939400
F	-2.38988300	-4.52719500	-3.97351300
F	-0.56460400	-5.71859300	-4.06876700
C	1.46724900	-5.50111100	0.60220600
F	1.35380000	-5.69935500	1.93931400
F	1.97870400	-6.62905100	0.06914400
F	2.42009100	-4.53641300	0.44887600
H	-9.59693100	2.01153900	0.24382300
H	-9.14162200	-0.40674500	0.64803900
H	-6.84304700	-1.20392900	0.98738200
H	-7.71537600	3.61777400	0.13776000
H	-5.32216700	4.09689500	0.29436800
H	-3.07688200	-4.66005000	2.41498000
H	-5.72848000	0.13810700	3.32262200
H	-6.44780700	-0.86272100	5.43780300
H	-5.80700400	-3.20286900	6.01933700
H	-4.37856400	-4.50514300	4.46883700
H	-4.04749400	-0.18776000	-2.12152700
H	-3.99456100	1.45281800	-2.77478800
H	-2.55383100	-0.97329100	-3.97521900
H	-4.06384700	-0.29778600	-4.61251100
H	-1.84436900	0.49908800	-5.75045800
H	-3.00706700	1.73768800	-5.30682700
H	-0.36101800	2.57466700	-5.78157200
H	1.42917000	3.75033600	-4.49675500
H	-0.20381500	2.19545200	-0.85686000
H	-1.63157500	2.79280000	2.17134600
H	0.20573100	6.23776800	0.37539900
H	-3.44639900	4.65855900	-1.24201300
H	-0.52344300	-4.06540100	1.73123200

H	0.58637700	-6.05249800	-1.91803000
H	-3.11772100	-3.89746500	-1.68359100
Pd	0.55537100	-0.73275300	-0.52490900
I	0.71559100	-1.86694400	-3.13011000
C	2.56650000	-0.81197300	0.32598500
C	3.58708800	-0.02184700	-0.45369000
H	3.17804800	0.96023300	-0.70348600
C	1.69466900	-0.20218300	1.26042000
H	1.67921800	0.88645900	1.29820500
C	4.08964700	-0.69546800	-1.75246000
H	4.06898700	-1.78717700	-1.64959900
C	1.13356900	-0.85395400	2.46241700
C	0.30150800	-0.11242900	3.33070700
C	1.40781000	-2.18996900	2.82437900
C	-0.23390800	-0.67481300	4.48936900
H	0.06012700	0.91316900	3.06629100
C	0.86639400	-2.75410000	3.97994000
H	2.03546600	-2.80111100	2.18713600
C	0.04359600	-2.00318200	4.82598200
H	-0.88132600	-0.07675000	5.12576500
H	1.09000900	-3.79197100	4.21432400
H	-0.38044000	-2.44624600	5.72220400
C	5.50054600	-0.20907200	-1.93090700
C	6.00611500	0.34685800	-0.75293200
C	6.31153300	-0.28259100	-3.06414600
C	7.31542200	0.82039800	-0.68057400
C	7.62226700	0.19709900	-3.00182600
H	5.92470900	-0.70713300	-3.98645100
C	8.12459400	0.74404700	-1.81641000
H	7.70427700	1.25344800	0.23836700
H	8.25653800	0.14806400	-3.88261600
H	9.14457100	1.11598600	-1.77998100
C	4.96802100	0.32696900	0.36589200
C	5.21769300	-0.80526200	1.35903900
C	4.81561500	1.69190600	1.03077800
O	4.99940800	-0.80199500	2.56384900
O	4.70384400	1.92253300	2.22908000
O	5.65802100	-1.89462800	0.72277400
O	4.78505400	2.65239100	0.11090600
C	4.55801200	4.00506200	0.55937800
H	5.45688000	4.38216500	1.05517500
H	4.33565700	4.56643100	-0.34527600
H	3.70632300	4.04622400	1.23737300
C	5.76604800	-3.11285200	1.48231000
H	6.23796500	-2.92676200	2.44837200

H	4.77305700	-3.54584400	1.62834400
H	6.37610100	-3.77937200	0.87393100
H	3.42465500	-0.46540100	-2.58815400
H	2.80659900	-1.86744000	0.44200500
H	4.24994600	0.53659700	3.63288100
N	4.10090600	0.75312600	4.64471300
C	3.05517900	1.81654500	4.75258400
H	2.10726900	1.40434400	4.40845000
H	3.34643200	2.64851300	4.11514900
C	3.68756000	-0.51233500	5.32362000
H	4.45057200	-1.26593800	5.13349400
C	5.42919100	1.23448600	5.12488900
H	6.16296500	0.44687500	4.95287100
H	5.69950600	2.11719800	4.54764800
H	5.36427100	1.46878900	6.18941000
H	2.97530300	2.12652300	5.79691300
H	3.58930400	-0.32381700	6.39484900
H	2.73779400	-0.84497500	4.90641800

Int2Sb-NMe3

Thermal correction to Gibbs Free Energy: 0.987820

SCF energy in solution: -5105.985586

Solution-phase Gibbs free energy: -5104.997766

Coordinates:

C	-2.21871000	-0.88810800	6.57124600
C	-2.95569100	-1.30008200	5.46014700
C	-2.60145100	-0.82274500	4.19758800
C	-1.53565000	0.06446900	4.03914400
C	-0.79930700	0.47583800	5.15180300
C	-1.14419100	-0.00506100	6.41609700
C	-1.36128400	0.48333000	2.60527200
C	-2.23464900	-0.48748400	1.76099100
C	-1.42827800	-1.52741300	1.01659000
C	-1.95807900	-2.15570500	-0.12636800
C	-1.58736000	-3.48677300	-0.65075200
C	-2.26261900	-3.98958900	-1.78110100
C	-1.98129900	-5.25544000	-2.29012600
C	-1.00459900	-6.05434600	-1.69155800
C	-0.30833000	-5.56349400	-0.58451300
C	-0.59759700	-4.30090600	-0.06559500
C	-3.28844400	-1.11624700	2.87036000
C	-4.58580600	-0.32010300	2.72208800
O	-4.45533200	0.91011900	3.23083900
C	-5.58757100	1.78865600	3.07988000
Pd	-0.54147400	-0.60548700	-0.79515800
I	-1.35945100	-0.49131400	-3.53459500
P	1.17776900	0.84957400	-0.64635900

N	2.45765100	0.68470000	-1.78109600
C	3.12688000	1.80703300	-2.47001000
C	2.62124800	1.90186100	-3.91052400
C	2.95035800	0.60893700	-4.66884100
C	2.86592700	-0.63785600	-3.81091600
C	2.62680300	-0.57577600	-2.42061200
C	2.59334100	-1.75843200	-1.66941100
C	2.75778000	-2.98117900	-2.31364900
C	2.98212900	-3.07291900	-3.68562200
C	3.04450900	-1.89119100	-4.41050000
N	2.73028500	-4.20989000	-1.52015400
O	2.83957200	-5.28505700	-2.11078500
O	1.97689200	0.95056700	0.87753500
C	3.05338900	1.79131500	1.05383900
C	2.83981700	3.16042100	1.14094600
C	3.97203500	4.04371600	1.17075200
C	5.28831900	3.47981600	1.22908900
C	5.43851900	2.07097500	1.26187800
C	4.35834300	1.21547000	1.16801800
C	6.41711500	4.34278100	1.25967500
C	6.26462900	5.70910200	1.20647200
C	4.96791500	6.26835200	1.11710700
C	3.85248500	5.45961000	1.10265700
C	1.43530800	3.65925800	1.19819200
C	0.95601900	4.42182900	2.31884500
C	-0.39650700	4.89509900	2.31072500
C	-1.23559100	4.57071300	1.21708200
C	-0.80207300	3.78267200	0.16923300
C	0.54814200	3.31639900	0.18661600
C	-0.87750700	5.66453100	3.40485200
C	-0.07364600	5.93351800	4.48782500
C	1.24926600	5.43228800	4.52009400
C	1.75079400	4.69937300	3.46686100
C	4.55155000	-0.25585900	1.23197600
C	3.72108400	-1.05959300	2.02631500
C	3.92738100	-2.43625800	2.10584700
C	4.96712100	-3.04279200	1.40518500
C	5.79964000	-2.24901800	0.61588300
C	5.59541600	-0.87193300	0.52678300
C	-1.73524400	3.43341600	-0.93212500
C	-2.99631700	2.91165800	-0.63129900
C	-3.89425100	2.58854900	-1.65164800
C	-3.55916000	2.79482000	-2.98630700
C	-2.30634900	3.33037000	-3.28865700
C	-1.40124500	3.64031700	-2.27840900

O	0.98159100	2.52959600	-0.85803100
C	2.98762300	-3.25005600	2.95475400
F	3.27549900	-4.56418300	2.93310500
C	6.86472700	-2.90461500	-0.22168900
F	7.40057700	-3.97839800	0.39896700
C	-5.19874700	1.96303000	-1.27053500
F	-5.02177300	0.74532100	-0.65940500
C	-1.94254500	3.62621600	-4.72035100
F	-2.23332200	4.91692500	-5.03242200
O	2.60132300	-4.11035100	-0.29548700
F	6.36820400	-3.33854700	-1.40212200
F	7.87671600	-2.05388000	-0.50814100
F	3.02218500	-2.84877800	4.24892800
F	1.70113700	-3.10661500	2.54898800
F	-0.62296300	3.46370000	-4.94988700
F	-2.61826500	2.85301900	-5.58901600
F	-5.88179300	2.71267500	-0.36351500
F	-6.02234900	1.74984900	-2.31112400
C	-3.51305700	-2.60235000	2.59666300
O	-2.62237000	-3.35605000	3.23703900
C	-2.65297100	-4.77265000	2.96102500
O	-4.36587900	-3.07659600	1.85914700
O	-5.62102800	-0.67564700	2.17264800
H	7.13469200	6.35872800	1.22297000
H	4.85088300	7.34642900	1.05465300
H	2.86615200	5.90218200	1.02501600
H	7.40788900	3.89910300	1.31522400
H	6.43755500	1.65848800	1.37486900
H	-2.25104800	4.95805300	1.20583100
H	2.76368300	4.31857000	3.51285300
H	1.87588800	5.62494800	5.38615300
H	-0.45254600	6.51762600	5.32127900
H	-1.90150700	6.02813300	3.37240100
H	2.93500600	2.72426400	-1.91943900
H	4.20970500	1.62225100	-2.45049000
H	1.53909500	2.06365000	-3.89293200
H	3.07602400	2.76216300	-4.41512500
H	2.28049900	0.49286800	-5.52797300
H	3.96855000	0.66835000	-5.07925400
H	3.21927600	-1.93371400	-5.48229900
H	3.10840400	-4.04241400	-4.14884800
H	2.45792900	-1.73959800	-0.59701300
H	2.90387900	-0.60862300	2.57543700
H	5.11132800	-4.11418200	1.45747500
H	6.24077000	-0.27700300	-0.10975100

H	-3.26269900	2.72771600	0.40442600
H	-4.24207600	2.51946000	-3.77931500
H	-0.42467100	4.03170100	-2.53504300
H	-2.83873800	0.05551000	1.02996400
H	-2.90357100	-1.77559900	-0.50523800
H	-0.32133900	0.44169200	2.27133000
H	-2.96767100	-3.34517200	-2.29842900
H	-0.02237800	-3.94047100	0.78017600
H	-2.50989500	-5.60891200	-3.17177300
H	0.48744100	-6.15015100	-0.13591600
H	-0.77145800	-7.03549300	-2.09482100
H	0.03283200	1.16469800	5.03401900
H	-3.78240900	-1.99509600	5.58196100
H	-0.57261300	0.30573600	7.28610100
H	-2.47742000	-1.25869100	7.55891900
H	-5.30018700	2.71296300	3.57943700
H	-5.79408700	1.96829700	2.02317200
H	-6.47087100	1.35627400	3.55516000
H	-3.64325900	-5.18010600	3.17668800
H	-2.39046500	-4.95500800	1.91730900
H	-1.90566200	-5.20642000	3.62382100
H	-1.69359100	1.51982600	2.47141900
H	-0.65565400	-2.02133100	1.60077800
H	-5.85761900	-2.07542800	0.95746700
N	-6.49376400	-2.42609500	0.20409100
C	-7.53814400	-1.38311900	-0.02298300
H	-7.04384400	-0.46764600	-0.34149600
H	-8.06463900	-1.20601200	0.91429800
C	-5.66085500	-2.65049100	-1.01994200
H	-4.86398300	-3.35197100	-0.77737000
C	-7.07773500	-3.70340500	0.71015000
H	-6.25963300	-4.38449700	0.93669200
H	-8.23032200	-1.73327100	-0.79138700
H	-6.29785300	-3.04993100	-1.81193100
H	-5.23166600	-1.69793200	-1.32984100
H	-7.64170300	-3.49359400	1.61982500
H	-7.73678900	-4.12292300	-0.05257500

Int2Ra-NMe3

Thermal correction to Gibbs Free Energy: 0.982799

SCF energy in solution: -5105.980197

Solution-phase Gibbs free energy: -5104.997398

Coordinates:

C	6.39085300	4.25407400	3.81634800
C	5.08312000	4.74181500	4.04991400
C	3.98060800	4.03770600	3.61836900
C	4.12230200	2.80220400	2.92522900

C	5.44898400	2.33234100	2.65895100
C	6.56542900	3.07459200	3.13081900
C	3.00531800	2.03743000	2.44436700
C	3.23414600	0.91241100	1.65930000
C	4.55424600	0.42878200	1.40434000
C	5.62222800	1.13998400	1.91502000
C	1.59995800	2.45997100	2.71192700
C	1.07903900	2.58185200	4.04374900
C	-0.25076200	3.08403800	4.22280100
C	-1.02099200	3.42652200	3.08509900
C	-0.55718600	3.24163400	1.79562100
C	0.76558200	2.72539900	1.63538800
C	1.81117900	2.19472200	5.20086600
C	1.27053000	2.32745000	6.46098900
C	-0.02966500	2.85908000	6.63656900
C	-0.77203700	3.22610000	5.53815200
O	2.16117800	0.24006900	1.11923900
O	1.24898700	2.50915200	0.35836500
P	1.27737200	0.90592600	-0.19286100
N	2.47805800	1.14112900	-1.39560200
C	3.26587100	2.37352700	-1.59033300
C	2.94111100	2.98603500	-2.95283900
C	3.32425100	2.00367500	-4.06470600
C	2.98209000	0.56573200	-3.73099000
C	2.57623200	0.17938100	-2.43414000
C	3.06722900	-0.40944300	-4.73232900
C	2.73853900	-1.73864600	-4.50342200
C	2.33737300	-2.08985600	-3.21670200
C	2.28271400	-1.16756400	-2.17798800
C	4.82856400	-0.80737800	0.61763100
C	-1.41956100	3.59529000	0.63894800
C	4.37290800	-2.06750600	1.03678900
C	4.77399100	-3.21936200	0.35885800
C	5.59241800	-3.13698300	-0.77069900
C	6.02054700	-1.88694800	-1.20686100
C	5.65500100	-0.73344800	-0.50953100
C	-2.78385000	3.28133800	0.66660400
C	-3.62594900	3.65220700	-0.38280100
C	-3.12231300	4.33662700	-1.48599600
C	-1.76324300	4.65040700	-1.52046000
C	-0.92016100	4.29000400	-0.47299100
N	1.96986900	-3.47939500	-2.93969000
O	1.54533500	-3.75671700	-1.81345600
O	2.09972500	-4.30427700	-3.84654600
C	6.84892600	-1.75861600	-2.45763400

F	7.78980500	-0.79334700	-2.33267400
F	7.48581500	-2.90905100	-2.76373500
F	6.08868100	-1.42614200	-3.52396500
C	4.34636700	-4.58368500	0.83554700
F	3.99638300	-4.57740400	2.14318500
F	3.29177900	-5.06200500	0.14234200
F	5.34493400	-5.48672700	0.69472900
C	-1.21550200	5.45148500	-2.67246300
F	-1.31383500	6.78375100	-2.42610900
F	0.09281400	5.19683400	-2.89165900
F	-1.88321300	5.21629200	-3.81680300
C	-5.07210100	3.24708300	-0.33080100
F	-5.58460000	3.40217900	0.92367700
F	-5.84146200	3.96937100	-1.16699600
F	-5.25065100	1.94332800	-0.64737600
H	7.25033900	4.81736800	4.16744100
H	4.94691700	5.68542100	4.57046300
H	2.98816200	4.43358600	3.79688900
H	7.56359900	2.69506100	2.92786700
H	6.63180000	0.77670800	1.74172300
H	-2.00732600	3.85580000	3.23823600
H	2.80586000	1.78204600	5.08030500
H	1.84757400	2.02080700	7.32871600
H	-0.43897600	2.96935400	7.63661100
H	-1.77600700	3.62579500	5.65780900
H	3.04233300	3.06259300	-0.77956600
H	4.33456500	2.12147600	-1.53039400
H	1.87056000	3.20940600	-2.99235500
H	3.48345200	3.93022400	-3.07728000
H	2.83155900	2.27857700	-5.00377700
H	4.40549300	2.06572000	-4.25620800
H	3.37529100	-0.10287400	-5.72839700
H	2.78004200	-2.48765500	-5.28292600
H	2.01153900	-1.51365600	-1.19000900
H	3.73389200	-2.14871600	1.90850800
H	5.90560500	-4.03510200	-1.28917600
H	6.01896000	0.23221200	-0.84317100
H	-3.18954000	2.73258700	1.50938700
H	-3.76989200	4.60823300	-2.31021600
H	0.13116600	4.53963000	-0.52535400
Pd	-0.69668000	-0.14902000	-0.69789400
I	-1.09078900	0.90314800	-3.31287700
C	-2.31064500	-1.56126100	-0.26216700
C	-3.71011700	-1.10108000	-0.56578200
H	-3.87085500	-0.10298000	-0.15069700

C	-1.64393000	-1.22492900	0.94319500
H	-2.11636500	-0.46129900	1.56313000
C	-4.10330200	-1.05517700	-2.06058700
H	-3.78599100	-0.10985800	-2.50681200
C	-0.68635500	-2.06340300	1.68992300
C	-0.30330600	-1.67098200	2.99111500
C	-0.12903200	-3.25725800	1.18502900
C	0.58906100	-2.42884300	3.75116100
H	-0.68609600	-0.73373300	3.38955900
C	0.76425800	-4.01194500	1.94306100
H	-0.35663800	-3.57502100	0.17296800
C	1.12674800	-3.61100100	3.23513000
H	0.87529900	-2.08464400	4.74227900
H	1.20167800	-4.90536800	1.51057900
H	1.83411400	-4.19777400	3.81273300
C	-5.58897200	-1.28246300	-2.08079400
C	-6.04804000	-1.81472100	-0.87231100
C	-6.49037900	-1.06043800	-3.12266100
C	-7.38963500	-2.14763400	-0.68996900
C	-7.83838700	-1.38163000	-2.94432800
H	-6.14528500	-0.63869300	-4.06251000
C	-8.28785600	-1.92471800	-1.73613600
H	-7.74106500	-2.56182600	0.25227000
H	-8.54516600	-1.20571900	-3.75051700
H	-9.33850900	-2.16925100	-1.60852800
C	-4.90247100	-2.00456400	0.11946800
C	-5.17206700	-1.41690900	1.49254300
C	-4.48606700	-3.47340500	0.17567300
O	-4.73472100	-1.81129700	2.56895000
O	-4.32223500	-4.16123900	1.17424900
O	-5.89804800	-0.30015200	1.39385300
O	-4.30309100	-3.95814000	-1.05462200
C	-3.84525700	-5.31883900	-1.15538300
H	-3.76692900	-5.51757300	-2.22294300
H	-2.87003500	-5.42778100	-0.67511900
H	-4.56126600	-5.99849300	-0.68765400
C	-6.09235600	0.47388900	2.58935100
H	-6.82744300	-0.01000900	3.23845500
H	-5.15110100	0.58437500	3.13224000
H	-6.45525400	1.44082600	2.24688900
H	-3.58442700	-1.84362200	-2.61816700
H	-2.02333000	-2.48106400	-0.77120200
H	-3.81369500	-3.40288900	2.97935000
N	-3.59536800	-3.95813800	3.83637700
C	-2.54319600	-4.96579600	3.49714000

H	-1.63971700	-4.44506400	3.18044700
H	-2.91611100	-5.57927400	2.67913200
C	-3.13556700	-3.00129300	4.88715400
H	-3.89371100	-2.22756900	4.99954500
C	-4.88809500	-4.60714000	4.20329400
H	-5.62571400	-3.82544300	4.38431700
H	-2.34243100	-5.57468300	4.38126800
H	-5.20893500	-5.22413100	3.36528300
H	-4.74553200	-5.21333900	5.10013000
H	-2.99169000	-3.54384100	5.82394600
H	-2.19545800	-2.55725100	4.55786500

Int2Rb-NMe3

Thermal correction to Gibbs Free Energy: 0.987000

SCF energy in solution: -5105.985246

Solution-phase Gibbs free energy: -5104.998246

Coordinates:

C	-7.13404200	-4.07879000	2.42337900
C	-5.96048400	-4.74864400	2.84376900
C	-4.72278700	-4.16273900	2.69381800
C	-4.58723600	-2.87165700	2.11041700
C	-5.77482900	-2.21375000	1.65260300
C	-7.03831700	-2.83806500	1.83757600
C	-3.31777100	-2.22593500	1.92185400
C	-3.26206100	-1.02938100	1.21693300
C	-4.44391000	-0.35526400	0.77493500
C	-5.66531800	-0.95477500	1.01359500
C	-2.04779700	-2.82838800	2.42315400
C	-1.82957800	-3.09018100	3.81800400
C	-0.61228800	-3.73126300	4.21737100
C	0.35105800	-4.06444800	3.23495500
C	0.18347600	-3.75236800	1.89863700
C	-1.03399300	-3.10943100	1.51857000
C	-2.75113900	-2.71122600	4.83377400
C	-2.49701800	-2.98151600	6.16045400
C	-1.31035200	-3.64870400	6.54748700
C	-0.38879000	-4.01166900	5.59317900
O	-2.03249900	-0.47130800	0.93705300
O	-1.22713900	-2.78154800	0.18796200
P	-1.01935100	-1.16936800	-0.27544700
N	-2.07549200	-1.23014000	-1.63785500
C	-2.92680600	-2.37731100	-2.00916700
C	-2.47940700	-2.94514400	-3.35657700
C	-2.63078100	-1.87730200	-4.44529000
C	-2.19322300	-0.50238800	-3.98601500
C	-1.93622900	-0.22595200	-2.62415200
C	-2.02703600	0.52101000	-4.92978500

C	-1.57962800	1.78826500	-4.58262500
C	-1.33050900	2.03088400	-3.23234800
C	-1.53789100	1.06469000	-2.25400000
C	-4.39629600	0.96197200	0.08610500
C	1.24635400	-4.09227100	0.91776900
C	-3.68124900	2.04480000	0.61840000
C	-3.69997700	3.28776800	-0.01472000
C	-4.42114500	3.47695500	-1.19398200
C	-5.12825800	2.40322400	-1.73177700
C	-5.12098900	1.16019800	-1.09722200
C	2.59025800	-3.87023900	1.24842500
C	3.60962800	-4.21656400	0.36222900
C	3.31020300	-4.78952200	-0.87281300
C	1.97524400	-5.01481000	-1.20578900
C	0.95272700	-4.67403000	-0.32333700
N	-0.82955900	3.33179000	-2.81577400
O	-0.59329900	3.50673000	-1.61005000
O	-0.64938500	4.20126400	-3.67063300
C	-5.83980700	2.55872300	-3.04970100
F	-6.94297600	1.77919800	-3.11730600
F	-6.22907200	3.83433400	-3.26423000
F	-5.04608200	2.20658200	-4.08572500
C	-2.99227600	4.45374700	0.62385800
F	-3.78927700	5.07890000	1.52384400
F	-1.88274300	4.06819400	1.28491400
F	-2.62739900	5.38610600	-0.28581200
C	1.63452500	-5.70196300	-2.50226400
F	1.59730700	-7.05116700	-2.33526100
F	0.41945900	-5.34073700	-2.96654200
F	2.54148100	-5.45486000	-3.46425900
C	5.04386500	-4.02257600	0.76919700
F	5.54184800	-5.12848400	1.37723800
F	5.84608100	-3.76185200	-0.28135600
F	5.18820600	-3.00462300	1.65639600
H	-8.10344600	-4.55046700	2.55395700
H	-6.03584200	-5.73814900	3.28533900
H	-3.83417100	-4.69401600	3.01288100
H	-7.92912900	-2.31803700	1.49463300
H	-6.57585500	-0.44725900	0.70609100
H	1.25128500	-4.58542900	3.54877600
H	-3.66127200	-2.19386500	4.55441500
H	-3.21358000	-2.67680400	6.91781200
H	-1.12688000	-3.86273600	7.59629800
H	0.53394800	-4.51116700	5.87719600
H	-2.86476100	-3.12544500	-1.22300800

H	-3.97078500	-2.03628100	-2.06406200
H	-1.43427100	-3.26058400	-3.27699700
H	-3.07857900	-3.82800800	-3.60636500
H	-2.05588300	-2.15427000	-5.33562400
H	-3.68205900	-1.81878600	-4.76386100
H	-2.22198700	0.29598900	-5.97480600
H	-1.41684000	2.56573800	-5.31721200
H	-1.38449600	1.33169400	-1.21933200
H	-3.11423800	1.91749000	1.53238200
H	-4.42637200	4.44160700	-1.68662500
H	-5.67248700	0.33431600	-1.53280900
H	2.84070200	-3.39746100	2.19113900
H	4.09855400	-5.03035600	-1.57545800
H	-0.07620700	-4.84832200	-0.60889200
Pd	1.02590200	-0.23277400	-0.63085700
I	1.65399900	-1.36617200	-3.16252800
C	1.98060400	1.10817200	0.83991400
C	1.07420000	2.16944800	1.41467000
H	0.42136300	2.56929700	0.63479900
C	2.65224300	1.23104900	-0.39495500
H	2.32340200	2.02596600	-1.06334000
C	0.18979100	1.67316900	2.58555800
H	-0.75032000	1.26121700	2.21135300
C	3.99018400	0.69398200	-0.71485500
C	4.51162700	0.88461800	-2.01324600
C	4.80711300	0.02059500	0.21500200
C	5.78960200	0.44509200	-2.35653100
H	3.87330400	1.33333900	-2.76913700
C	6.08082400	-0.43098100	-0.13235100
H	4.43642700	-0.17327300	1.21684900
C	6.58882300	-0.21085800	-1.41563500
H	6.15090000	0.59110300	-3.37121800
H	6.67167400	-0.97099500	0.60136200
H	7.57894000	-0.56720700	-1.68453100
C	0.01908000	2.86131800	3.49266300
C	0.92695000	3.87860300	3.18658100
C	-0.86760100	3.02200900	4.55806600
C	0.97614200	5.05108700	3.94006600
C	-0.83117000	4.19852900	5.31025900
H	-1.58015000	2.23832200	4.80184400
C	0.08730000	5.20840500	5.00540100
H	1.68195400	5.84093400	3.69623000
H	-1.52286200	4.33166800	6.13738400
H	0.10598900	6.12038200	5.59506500
C	1.82753900	3.49018900	2.01608600

C	1.88299600	4.51785700	0.89097800
C	3.22461000	3.15984900	2.54212000
O	2.77330100	4.60761700	0.04991800
O	4.27680700	3.68588100	2.21134600
O	0.79170700	5.27027700	0.85839600
O	3.16814600	2.20554100	3.47852900
C	4.42249200	1.79815900	4.05311700
H	4.16762300	1.05186500	4.80432500
H	5.06749400	1.36372200	3.28540800
H	4.92768000	2.65015500	4.51362900
C	0.61769700	6.15098100	-0.27579200
H	1.48949900	6.79915800	-0.38794400
H	0.45174400	5.55556200	-1.17421300
H	-0.27320100	6.73071800	-0.04226800
H	0.69589900	0.85974300	3.12104300
H	2.43585800	0.47547800	1.60040500
H	4.52623900	4.09979600	0.10443100
N	5.44714800	4.38042500	-0.30022600
C	6.48723800	3.37830900	0.08928400
H	6.22344900	2.40974200	-0.33368100
H	6.50319600	3.31598100	1.17569800
C	5.26270600	4.45094900	-1.78234800
H	4.40335000	5.08739700	-1.98987700
C	5.72334200	5.72378800	0.28889900
H	4.90958800	6.39342600	0.01194500
H	7.45322600	3.71123900	-0.29670300
H	5.75715700	5.61878200	1.37222300
H	6.67430400	6.09654100	-0.09684600
H	6.16858400	4.85953400	-2.23497200
H	5.07717700	3.44205600	-2.15135100

Int2Sa

Thermal correction to Gibbs Free Energy: 0.853423

SCF energy in solution: -4931.115461

Solution-phase Gibbs free energy: -4930.262038

Coordinates:

C	-8.29017777	2.73754087	0.71736731
C	-8.15248467	1.35561748	0.99024146
C	-6.90577657	0.79136925	1.14972568
C	-5.72373986	1.57619215	1.03918565
C	-5.86670734	2.96867013	0.73154356
C	-7.16760814	3.52314657	0.59043202
C	-4.40633679	1.02530238	1.18164215
C	-3.30249079	1.82396991	0.90290175
C	-3.43400088	3.22850107	0.65138986
C	-4.70478433	3.76545637	0.58189975
C	-4.16920682	-0.38032308	1.61896644

C	-4.61658064	-0.85350046	2.89969380
C	-4.34792938	-2.21145600	3.26781719
C	-3.62567538	-3.03989221	2.37580525
C	-3.14773968	-2.57776369	1.16633767
C	-3.42077531	-1.22329777	0.80843125
C	-5.28060249	-0.02626156	3.84908052
C	-5.68771161	-0.52412098	5.06733732
C	-5.45437317	-1.87699169	5.40993007
C	-4.79301048	-2.69811412	4.52665111
O	-2.05030949	1.26806739	0.88929594
O	-2.94939151	-0.74839972	-0.39689706
P	-1.56051731	0.23821038	-0.42523900
N	-2.03838925	1.16771426	-1.80556925
C	-3.33702528	1.05557420	-2.49552907
C	-3.14778342	0.39032452	-3.85912288
C	-2.22921792	1.25242883	-4.73205331
C	-1.09220377	1.88707174	-3.95643614
C	-1.02135655	1.81718347	-2.54661085
C	-0.08192596	2.56176193	-4.65501157
C	0.99995283	3.14795462	-4.01371867
C	1.04836877	3.06022880	-2.62313900
C	0.05612698	2.42528178	-1.88372062
C	-2.24252799	4.10510471	0.51903885
C	-2.36688470	-3.49158064	0.29097624
C	-1.14812752	3.97349852	1.38718716
C	-0.05301114	4.83031621	1.28536798
C	-0.02116376	5.83714731	0.32243933
C	-1.10524970	5.97305222	-0.54473785
C	-2.20342688	5.11732701	-0.45033847
C	-1.24572828	-4.14843281	0.81146634
C	-0.53372352	-5.05996024	0.02987069
C	-0.93598077	-5.34002285	-1.27424586
C	-2.05238061	-4.68526709	-1.79379465
C	-2.75879126	-3.76279342	-1.02508959
N	2.16176298	3.68888055	-1.91284154
O	2.19648343	3.59079324	-0.68086948
O	3.00726353	4.29331511	-2.57570008
C	-1.04890258	6.99553733	-1.64664836
F	-2.28475134	7.41342995	-2.01136093
F	-0.34616201	8.09216295	-1.28095006
F	-0.45864137	6.50373666	-2.75832864
C	1.08362773	4.66288073	2.25872353
F	0.71950541	5.04868293	3.50770416
F	1.47800040	3.37438960	2.35392309
F	2.16427781	5.39691458	1.91906808

C	-2.54652628	-5.02932856	-3.17204886
F	-3.47489250	-6.02742225	-3.11810804
F	-3.14855843	-3.98510105	-3.77641814
F	-1.56156154	-5.46825285	-3.97868602
C	0.71246638	-5.68795430	0.58764525
F	0.60765198	-5.92423475	1.91823661
F	1.00174255	-6.86731195	-0.00709925
F	1.80444367	-4.89533550	0.42815245
H	-9.27924851	3.17113958	0.59970079
H	-9.03878584	0.73233238	1.07051612
H	-6.81336029	-0.26962697	1.35112077
H	-7.25744996	4.58374535	0.36815200
H	-4.82570507	4.83337925	0.41957091
H	-3.43684904	-4.07181447	2.65891930
H	-5.45597871	1.01564791	3.61055037
H	-6.18655511	0.13188220	5.77545773
H	-5.78377052	-2.25782742	6.37255198
H	-4.58583949	-3.73413592	4.78276901
H	-4.01579100	0.48448967	-1.86752544
H	-3.75661215	2.06558748	-2.61281345
H	-2.69902751	-0.59648334	-3.70586490
H	-4.11824754	0.25075466	-4.35010827
H	-1.80791327	0.65288071	-5.54673731
H	-2.81204382	2.05533586	-5.20779341
H	-0.14270870	2.60316358	-5.73966039
H	1.78699228	3.65843844	-4.55252827
H	0.12839988	2.42054305	-0.80561114
H	-1.14882220	3.18849111	2.13310494
H	0.83868662	6.48969623	0.23975024
H	-3.02669647	5.22656932	-1.14737371
H	-0.91566165	-3.92007213	1.81835705
H	-0.37804505	-6.03799814	-1.88571453
H	-3.61155387	-3.24865762	-1.45204373
Pd	0.49816673	-0.68713402	-0.42523604
I	0.35330944	-1.86460197	-3.06785402
C	2.51932617	-1.17414450	0.36982904
C	3.66763540	-0.60607240	-0.43764307
H	3.46363362	0.44232992	-0.66463320
C	1.83080823	-0.42062620	1.33308568
H	2.04419455	0.64564043	1.37391526
C	3.95793621	-1.34424287	-1.76702287
H	3.76296669	-2.41874813	-1.65962638
C	1.19215142	-0.95358241	2.55732644
C	0.61726330	-0.05563230	3.47772155
C	1.16845727	-2.32269540	2.88807239

C	0.02535872	-0.50270251	4.65712445
H	0.64385735	1.00776257	3.25502907
C	0.57440342	-2.77035390	4.06670776
H	1.62453393	-3.04446789	2.22044880
C	-0.00717577	-1.86599378	4.95977522
H	-0.41131349	0.21772875	5.34465336
H	0.57770868	-3.83498397	4.29011840
H	-0.46840914	-2.21645949	5.87916138
C	5.42248154	-1.10492280	-2.01343685
C	6.07261013	-0.69737533	-0.84254708
C	6.15064729	-1.25972554	-3.19293452
C	7.44438156	-0.44868700	-0.82798283
C	7.52586215	-1.00742386	-3.18818447
H	5.65057465	-1.56939791	-4.10713028
C	8.16908221	-0.60608581	-2.01328683
H	7.92971557	-0.12616054	0.08758809
H	8.09821029	-1.11923563	-4.10593171
H	9.23804827	-0.40863261	-2.02116060
C	5.08064183	-0.59182230	0.31993066
C	5.14844123	-1.79205171	1.27512719
C	5.39143277	0.66927053	1.13603222
O	4.95363645	-1.74938078	2.46864665
O	6.39270524	0.79621597	1.81183975
O	5.37130394	-2.94040956	0.59404146
O	4.49007462	1.64908555	0.96009186
C	4.77831520	2.89926868	1.60779963
H	5.79258563	3.22488312	1.36465890
H	4.03811550	3.59908440	1.22672934
H	4.69156421	2.79003677	2.69221875
C	5.27852696	-4.15202587	1.35709966
H	5.75229962	-4.03147837	2.33314827
H	4.22928878	-4.42966916	1.49362370
H	5.78796163	-4.91477577	0.76661196
H	3.30182313	-0.99856624	-2.56878895
H	2.52924716	-2.25924804	0.46241694

Int2Sb

Thermal correction to Gibbs Free Energy: 0.853648

SCF energy in solution: -4931.118712

Solution-phase Gibbs free energy: -4930.265064

Coordinates:

C	-1.11848700	-2.46213100	6.34564200
C	-1.97657500	-2.88240900	5.32704200
C	-2.05813900	-2.12461700	4.15968000
C	-1.31417400	-0.94904000	4.01411400
C	-0.46220100	-0.52697800	5.03579100
C	-0.36467700	-1.29220600	6.20042700

C	-1.60486600	-0.28546300	2.69172500
C	-2.27779500	-1.39372000	1.83550900
C	-1.28828300	-2.12048100	0.94044900
C	-1.72247900	-2.78100200	-0.21588000
C	-1.04162700	-3.92040400	-0.86555300
C	-1.74417500	-4.67413400	-1.82482100
C	-1.16334500	-5.78044100	-2.44244100
C	0.14218300	-6.16044000	-2.12479700
C	0.85738300	-5.41930500	-1.17954000
C	0.27400400	-4.31898600	-0.55418600
C	-2.94729800	-2.33889700	2.94148400
C	-4.39266600	-1.93678500	3.31954800
O	-4.96724900	-1.08875700	2.44561200
C	-6.34916200	-0.78812000	2.70051800
Pd	-0.72381100	-0.86990400	-0.83179100
I	-1.44431100	-0.71715000	-3.61511800
P	0.57147500	0.93144000	-0.58404000
N	1.81122800	1.25832500	-1.74480600
C	2.06933400	2.57955300	-2.34924300
C	1.46451800	2.63331200	-3.75317000
C	2.11537900	1.56659500	-4.64391900
C	2.47750600	0.29475100	-3.90308800
C	2.30874700	0.16713300	-2.50669800
C	2.66813900	-1.03061700	-1.87340800
C	3.15695700	-2.08685800	-2.63671400
C	3.32908200	-1.98910400	-4.01635300
C	2.99527100	-0.78812100	-4.62474800
N	3.54445800	-3.32763100	-1.96796100
O	3.94230800	-4.26358800	-2.66507400
O	1.40580600	1.14404600	0.93321800
C	2.15622700	2.25957500	1.19189600
C	1.51988200	3.47100500	1.44053300
C	2.30761600	4.66323200	1.57610600
C	3.73648400	4.55517400	1.57328000
C	4.33232100	3.27711400	1.43860700
C	3.58339600	2.13363000	1.23789800
C	4.52652600	5.72836600	1.71196600
C	3.94043300	6.96850700	1.82113800
C	2.53013700	7.08276900	1.79250600
C	1.73616900	5.96276600	1.67630900
C	0.03256600	3.48656000	1.54785500
C	-0.63150300	3.92263500	2.74511100
C	-2.06399700	3.93800800	2.77718200
C	-2.78611600	3.50490900	1.63832000
C	-2.15562200	3.02721500	0.50667600

C	-0.72696500	3.00186000	0.49100900
C	-2.73391500	4.37422900	3.95236000
C	-2.02826200	4.75381200	5.07037900
C	-0.61427300	4.70405800	5.05664700
C	0.06488400	4.30163800	3.92748300
C	4.25384200	0.81239600	1.12837200
C	3.74155500	-0.32148200	1.77808200
C	4.40915900	-1.54336600	1.70862400
C	5.60332800	-1.66591400	1.00127000
C	6.12092200	-0.54287200	0.35605600
C	5.45273700	0.68093500	0.41282100
C	-2.96211000	2.56778500	-0.65296300
C	-4.00646300	1.65756200	-0.46121800
C	-4.79713300	1.24883400	-1.53737400
C	-4.56465000	1.74324000	-2.81662500
C	-3.52503600	2.65401000	-3.00979600
C	-2.72894100	3.06164700	-1.94372600
O	-0.08606400	2.51075400	-0.62292400
C	3.82258200	-2.72310400	2.44019600
F	4.44930700	-3.87679100	2.14072700
C	7.37058700	-0.66800700	-0.47170300
F	8.19654600	-1.62819000	0.00273900
C	-5.88949400	0.25017400	-1.27930200
F	-5.42732100	-0.86627400	-0.68075800
C	-3.28921000	3.24904000	-4.37041800
F	-3.92442000	4.44854900	-4.49449600
O	3.46464200	-3.37922400	-0.73641600
F	7.09732600	-0.98507100	-1.75687400
F	8.07457800	0.48992900	-0.49818400
F	3.91891800	-2.55474800	3.78429400
F	2.51052400	-2.87758500	2.16539700
F	-1.98013900	3.49123200	-4.60194800
F	-3.74881300	2.46642300	-5.36418100
F	-6.83392800	0.76674500	-0.43532700
F	-6.53571500	-0.11965600	-2.40217600
C	-3.08358600	-3.77986700	2.43770100
O	-2.00680000	-4.53153300	2.71685900
C	-2.02540900	-5.86012000	2.16215700
O	-4.05336000	-4.18655100	1.83118600
O	-4.95981900	-2.35652700	4.30546700
H	4.55486700	7.85898900	1.91910100
H	2.06852500	8.06411600	1.85839000
H	0.65763200	6.06564300	1.64763700
H	5.60900800	5.62600800	1.71892600
H	5.41414300	3.20145500	1.50935200

H	-3.87171900	3.54985000	1.66053000
H	1.14733000	4.25944700	3.93842700
H	-0.05775100	4.97944100	5.94818800
H	-2.55123900	5.07615200	5.96619100
H	-3.82098200	4.38712200	3.95354400
H	1.65180000	3.34928900	-1.70537100
H	3.15779600	2.72857800	-2.39097100
H	0.38847800	2.45036100	-3.67812400
H	1.60381400	3.62940000	-4.19031000
H	1.44516700	1.30815600	-5.47118700
H	3.03245100	1.96805000	-5.09952300
H	3.11252900	-0.68600500	-5.70059200
H	3.71381700	-2.83292200	-4.57328900
H	2.58251600	-1.14548000	-0.80203500
H	2.81040300	-0.25195600	2.32603000
H	6.10818300	-2.62147600	0.94185000
H	5.86123500	1.53588400	-0.11436000
H	-4.18047400	1.23943800	0.52494400
H	-5.15772800	1.40140400	-3.65464600
H	-1.91307800	3.75307800	-2.11562900
H	-3.07307200	-0.99536100	1.20769900
H	-2.76321200	-2.65345700	-0.50782900
H	-0.71044900	0.10556800	2.20165700
H	-2.75321600	-4.37258100	-2.09131000
H	0.85837400	-3.75621400	0.16569900
H	-1.73065900	-6.34017900	-3.18214500
H	1.88456300	-5.67975800	-0.94053000
H	0.60191300	-7.01529200	-2.61379300
H	0.11693000	0.38647300	4.92566200
H	-2.56705900	-3.78517700	5.43973100
H	0.30341900	-0.97845700	6.99854800
H	-1.03501900	-3.04920700	7.25642200
H	-6.68000000	-0.19451300	1.85018000
H	-6.92727300	-1.71189400	2.77503800
H	-6.45402600	-0.22999100	3.63521800
H	-2.89070500	-6.41535700	2.53344700
H	-2.06144200	-5.81379300	1.07226300
H	-1.09617700	-6.32405700	2.49219200
H	-2.28968400	0.56140900	2.83647900
H	-0.37286700	-2.44835600	1.42889900

Int2Ra

Thermal correction to Gibbs Free Energy: 0.853255

SCF energy in solution: -4931.108465

Solution-phase Gibbs free energy: -4930.255210

Coordinates:

C	-5.43381000	5.95188000	-2.16331600
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C	-4.05646100	6.26463900	-2.25103500
C	-3.10020200	5.28488700	-2.09843200
C	-3.46409500	3.93070500	-1.84856100
C	-4.85892300	3.62804400	-1.72243400
C	-5.82128600	4.65857700	-1.89981100
C	-2.50279900	2.87737500	-1.67542300
C	-2.93848100	1.60862000	-1.30142600
C	-4.33019100	1.30116900	-1.17996600
C	-5.25068600	2.30531900	-1.40294800
C	-1.03915500	3.13241800	-1.81091000
C	-0.45330100	3.61548100	-3.02845100
C	0.94236200	3.93817400	-3.04334300
C	1.70650400	3.76482900	-1.86368500
C	1.16925400	3.23098900	-0.70716200
C	-0.21768700	2.88441400	-0.71958200
C	-1.18673100	3.75468400	-4.23948200
C	-0.58117200	4.21465400	-5.38810100
C	0.78982200	4.56589700	-5.39024800
C	1.53242200	4.42699100	-4.24066300
O	-2.02381600	0.62174600	-1.06024800
O	-0.77433600	2.31101600	0.40460800
P	-1.01594900	0.62082900	0.34674100
N	-2.18041900	0.58698700	1.62606100
C	-2.79694700	1.77182200	2.24734700
C	-2.41551400	1.84249800	3.72628600
C	-2.96782300	0.61164900	4.44975800
C	-2.81135800	-0.66271900	3.64439500
C	-2.42225500	-0.64327800	2.28505200
C	-3.05878000	-1.89279400	4.26548900
C	-2.91586200	-3.10158200	3.59996700
C	-2.52929500	-3.05540700	2.26241900
C	-2.30607300	-1.85905700	1.59115900
C	-4.82379200	-0.05531100	-0.80945400
C	2.01620000	3.07769000	0.50407300
C	-4.56125800	-1.18790200	-1.59859800
C	-5.16283200	-2.40865100	-1.29037800
C	-5.98614000	-2.54035200	-0.16830300
C	-6.22014400	-1.42852400	0.63368900
C	-5.65837200	-0.19242300	0.30502700
C	3.33803500	2.63129300	0.38598200
C	4.17089700	2.55467500	1.50393100
C	3.69807800	2.90833000	2.76382800
C	2.37973900	3.34800700	2.88955700
C	1.54812600	3.43793000	1.77725300
N	-2.37511000	-4.31460500	1.52902400

O	-1.96926800	-4.26703400	0.36665700
O	-2.66548200	-5.36187700	2.11508600
C	-7.05539200	-1.53684600	1.87952400
F	-7.94248600	-0.51471000	1.97270700
F	-7.76340500	-2.68647500	1.92491600
F	-6.29687700	-1.48881300	2.99705200
C	-4.94983400	-3.61767700	-2.16641800
F	-4.60277300	-3.27575400	-3.42585200
F	-3.99323400	-4.43628300	-1.68867900
F	-6.08550500	-4.35763300	-2.25389800
C	1.87510400	3.80082400	4.23174300
F	2.11264200	5.12759400	4.42340300
F	0.54007800	3.63287700	4.36154900
F	2.47347100	3.15279300	5.24989000
C	5.57767800	2.05235500	1.32563400
F	6.19755700	2.69534800	0.29611600
F	6.33609900	2.25347300	2.42553300
F	5.62138600	0.73810400	1.03902700
H	-6.17758000	6.73317600	-2.29170400
H	-3.74859800	7.29016900	-2.43565300
H	-2.05067800	5.54580100	-2.15915900
H	-6.87458100	4.40351600	-1.81116500
H	-6.31146000	2.07931800	-1.32943000
H	2.74932900	4.06980700	-1.87387500
H	-2.23411300	3.47677200	-4.25418400
H	-1.15988900	4.30106300	-6.30347600
H	1.25453000	4.92988600	-6.30211900
H	2.59079300	4.67541500	-4.23298900
H	-2.47040300	2.65777900	1.70885900
H	-3.89026000	1.70057000	2.14409700
H	-1.32495600	1.87661100	3.80732700
H	-2.81301900	2.76025700	4.17557600
H	-2.47771300	0.48386600	5.42158800
H	-4.03755900	0.75775200	4.66169500
H	-3.35026000	-1.89330900	5.31285400
H	-3.08813500	-4.05443700	4.08203700
H	-2.04326100	-1.89284900	0.54225400
H	-3.91178100	-1.10825100	-2.46320900
H	-6.44811700	-3.49183700	0.06435100
H	-5.86974800	0.67447500	0.92201500
H	3.71398900	2.32029200	-0.58248400
H	4.33675300	2.82645700	3.63389800
H	0.52779600	3.77631100	1.89933700
Pd	0.78686600	-0.73459100	0.28351900
I	1.44191400	-0.85460500	3.08791000

C	2.25696500	-1.97078300	-0.86685900
C	3.70161600	-1.71598600	-0.50420700
H	3.84667200	-0.64717100	-0.31899200
C	1.52595300	-1.17018200	-1.75874500
H	1.99714500	-0.25248900	-2.10728400
C	4.18606200	-2.45717100	0.76543000
H	3.88517600	-1.92182000	1.66962100
C	0.43579500	-1.64010600	-2.64352700
C	0.11791300	-0.88803800	-3.78895900
C	-0.29574500	-2.82189000	-2.41359300
C	-0.88750000	-1.29190000	-4.66695200
H	0.67397900	0.02414200	-3.99010800
C	-1.29901100	-3.22588200	-3.28966900
H	-0.10397500	-3.41127500	-1.52280700
C	-1.60471100	-2.46445000	-4.42378200
H	-1.10763400	-0.68796900	-5.54434400
H	-1.85984000	-4.12932600	-3.07327700
H	-2.39327100	-2.78196300	-5.10032800
C	5.67434700	-2.57950300	0.57982500
C	6.04250400	-2.35039100	-0.75073200
C	6.65243500	-2.90094900	1.52238400
C	7.36888300	-2.46986900	-1.16407300
C	7.98659300	-3.00183800	1.11941700
H	6.37659000	-3.06855600	2.56024400
C	8.34382300	-2.79180200	-0.21714500
H	7.63723700	-2.31258600	-2.20459400
H	8.75373300	-3.24583200	1.85019800
H	9.38419600	-2.87688800	-0.52009500
C	4.81442400	-2.05963700	-1.61566000
C	4.93616400	-0.85922300	-2.55008800
C	4.60384800	-3.31474700	-2.47114500
O	4.29923300	-0.69217700	-3.56666400
O	5.15407000	-3.51363100	-3.53305300
O	5.78213100	0.07367000	-2.04956000
O	3.83273300	-4.23393000	-1.85601200
C	3.67231900	-5.47180300	-2.56388600
H	3.02348000	-6.08479200	-1.93835800
H	3.21139400	-5.29763000	-3.53905900
H	4.64019800	-5.95894300	-2.71087600
C	5.87157400	1.28960100	-2.80136000
H	6.37282300	1.11549100	-3.75822900
H	4.87620100	1.69501900	-3.00350200
H	6.44918300	1.97306100	-2.17998500
H	3.72664800	-3.45268000	0.82097000
H	1.94403500	-3.00369200	-0.73972600

Int2Rb

Thermal correction to Gibbs Free Energy: 0.853332

SCF energy in solution: -4931.109263

Solution-phase Gibbs free energy: -4930.255931

Coordinates:

C	-2.49939500	-7.29374500	2.80009400
C	-1.18758300	-6.97040500	3.22122000
C	-0.66839900	-5.71286700	3.00437200
C	-1.43061100	-4.70395300	2.35001200
C	-2.74488500	-5.04764300	1.89449200
C	-3.25731000	-6.34870900	2.14798100
C	-0.92702700	-3.38439800	2.09181400
C	-1.68072900	-2.50146500	1.32381400
C	-3.00672100	-2.82938900	0.89081200
C	-3.50637300	-4.08078600	1.19392200
C	0.41074600	-2.94615800	2.58542900
C	0.72912900	-2.90630400	3.98420200
C	2.05710200	-2.54343000	4.38035400
C	3.01168500	-2.21936300	3.38650800
C	2.69710300	-2.18795700	2.04077300
C	1.36242400	-2.53417100	1.66203600
C	-0.22373800	-3.17554100	5.00631600
C	0.12579600	-3.11926000	6.33764500
C	1.44813100	-2.79463800	6.72391400
C	2.38977600	-2.51103000	5.76205200
O	-1.15114500	-1.28608200	0.98247400
O	1.01578200	-2.49708300	0.33004400
P	0.10695300	-1.16431100	-0.23545200
N	-0.63143500	-2.02539300	-1.54769500
C	-0.45044400	-3.45853800	-1.84018700
C	0.33913400	-3.63317100	-3.13846300
C	-0.44187600	-3.01749800	-4.30451700
C	-1.12120200	-1.71384700	-3.93817700
C	-1.18583000	-1.26172400	-2.60111600
C	-1.69105100	-0.92835600	-4.94941900
C	-2.29024400	0.29631100	-4.69088300
C	-2.33455600	0.72045000	-3.36364300
C	-1.82146100	-0.04378300	-2.32228600
C	-3.86352500	-1.86166300	0.15539100
C	3.74043400	-1.82984100	1.04577300
C	-4.05585800	-0.55102900	0.61763800
C	-4.92977300	0.31256300	-0.04320700
C	-5.61639200	-0.10284600	-1.18381100
C	-5.41943700	-1.39947500	-1.65609400
C	-4.55626700	-2.27220600	-0.99195400
C	4.62548100	-0.77701000	1.31345300

C	5.64881300	-0.46108300	0.41997000
C	5.80795700	-1.18466100	-0.75994800
C	4.92985900	-2.23335200	-1.03118600
C	3.90886300	-2.55689900	-0.14131100
N	-2.95672800	2.00036500	-3.04198000
O	-2.98758000	2.34932700	-1.85509900
O	-3.42543300	2.67370200	-3.96230700
C	-6.08383700	-1.83939600	-2.93200300
F	-6.34298000	-3.16932800	-2.93144400
F	-7.25967100	-1.20188400	-3.13504100
F	-5.31127400	-1.59335300	-4.01269900
C	-5.19217800	1.68092200	0.53263200
F	-6.15985100	1.62191500	1.48549000
F	-4.09911500	2.19932700	1.11437500
F	-5.62572700	2.55168100	-0.40414300
C	5.13988400	-3.07700200	-2.25964100
F	6.01625400	-4.08989600	-2.00169900
F	4.00063800	-3.66235200	-2.68417000
F	5.65804500	-2.37520200	-3.28304700
C	6.62409300	0.62760700	0.76928000
F	7.67251800	0.13963000	1.48599700
F	7.14579400	1.22392600	-0.31974900
F	6.05985700	1.59185400	1.53675600
H	-2.89863100	-8.28741400	2.98258500
H	-0.58090000	-7.72339700	3.71664000
H	0.34114800	-5.48471900	3.32482300
H	-4.26124400	-6.58579200	1.80415800
H	-4.51954100	-4.33572800	0.89388400
H	4.02699400	-1.99173100	3.69926400
H	-1.24257700	-3.41555400	4.72587000
H	-0.62289700	-3.32024100	7.09888500
H	1.71177000	-2.75815600	7.77711600
H	3.40504400	-2.24310500	6.04395700
H	0.05754500	-3.92470000	-0.99992100
H	-1.44298800	-3.92502000	-1.93047000
H	1.30735500	-3.13426300	-3.03092000
H	0.52514800	-4.69750300	-3.32553700
H	0.22392700	-2.84068100	-5.15644300
H	-1.21017600	-3.72422100	-4.65265800
H	-1.62845300	-1.28237900	-5.97526000
H	-2.70653500	0.91556700	-5.47420700
H	-1.92784500	0.31500000	-1.30934700
H	-3.52535500	-0.20576100	1.49673600
H	-6.28504100	0.57667200	-1.69788000
H	-4.41027800	-3.27582500	-1.37563300

H	4.49662800	-0.18079300	2.20961100
H	6.58100600	-0.91804800	-1.47012500
H	3.23104400	-3.36557800	-0.37962900
Pd	1.00895300	0.83175200	-0.71733600
I	2.36335200	0.16710900	-3.16672400
C	0.82813900	2.61712500	0.64227000
C	-0.55349600	2.77357300	1.24158800
H	-1.30989800	2.51532900	0.49421700
C	1.20509600	3.08332500	-0.61949100
H	0.41412900	3.42173400	-1.28502400
C	-0.78993600	1.87350400	2.48071800
H	-1.10695900	0.86988200	2.18653800
C	2.54847300	3.57618000	-0.99145800
C	2.68017300	4.34763200	-2.15982400
C	3.70578000	3.36226400	-0.21915000
C	3.90633100	4.89137200	-2.53658400
H	1.80158400	4.51977900	-2.77505700
C	4.93272500	3.90261000	-0.59584600
H	3.65301700	2.74870700	0.67480600
C	5.04207300	4.67523700	-1.75542400
H	3.97342200	5.48295700	-3.44637600
H	5.81017600	3.70504000	0.01241100
H	6.00144700	5.09387000	-2.04854300
C	-1.80151500	2.61763300	3.31122900
C	-1.92037600	3.94742200	2.89388800
C	-2.55071700	2.15863000	4.39564100
C	-2.75871000	4.83728100	3.56506200
C	-3.40701700	3.04083100	5.05973300
H	-2.46622100	1.12501900	4.72294900
C	-3.50773300	4.37446300	4.64913200
H	-2.83243300	5.87062400	3.24088400
H	-3.99832400	2.68909400	5.90148800
H	-4.17490700	5.05351600	5.17348300
C	-0.98151200	4.24700300	1.72481400
C	-1.61022100	4.96651200	0.52554900
C	0.12029600	5.14886800	2.29181200
O	-0.97301300	5.48811800	-0.36283000
O	0.07584000	6.35997400	2.29901600
O	-2.95277600	4.87224800	0.52988000
O	1.10029600	4.44414400	2.89784100
C	2.13348000	5.23460700	3.50337000
H	2.81891500	4.52094500	3.96115200
H	2.65161100	5.82844300	2.74653300
H	1.71431300	5.90588000	4.25762600
C	-3.61884400	5.35855300	-0.65068600

H	-3.29389600	6.37574600	-0.88085900
H	-3.41098700	4.69636700	-1.49297700
H	-4.68197700	5.33185200	-0.41038200
H	0.14569300	1.75865800	3.04440300
H	1.61017300	2.51350800	1.39038400

Int1Sb-

Thermal correction to Gibbs Free Energy: 0.853198

SCF energy in solution: -4931.080202

Solution-phase Gibbs free energy: -4930.227004

Coordinates:

C	4.26640900	6.07102500	-3.17479000
C	2.86126600	6.20146300	-3.28392500
C	2.02131100	5.35612500	-2.59315400
C	2.53953300	4.32641000	-1.75876300
C	3.96235900	4.17299500	-1.68196900
C	4.80154000	5.07571900	-2.39041500
C	1.69467600	3.41237900	-1.04031300
C	2.28547000	2.33096300	-0.39814500
C	3.70197500	2.19050700	-0.27371800
C	4.50519000	3.12094700	-0.90390800
C	0.21302300	3.57689400	-0.96730900
C	-0.39252500	4.75538200	-0.40557600
C	-1.81951100	4.80989700	-0.30594000
C	-2.60051300	3.71876900	-0.75808900
C	-2.03119900	2.59459000	-1.32053100
C	-0.60749600	2.53987500	-1.37961900
C	0.35382200	5.86022100	0.09355000
C	-0.28037600	6.97326200	0.60139000
C	-1.69210700	7.03430700	0.66830800
C	-2.44122800	5.96323400	0.24226800
O	1.48541900	1.33628500	0.14172200
O	-0.01074900	1.39759600	-1.91525400
P	0.69721500	0.27100600	-0.91589000
N	1.90319000	-0.24810400	-2.01042000
C	2.22244400	0.44195200	-3.27926300
C	1.78818200	-0.42392200	-4.46052200
C	2.55599600	-1.75064600	-4.43883200
C	2.79531300	-2.28728600	-3.04134600
C	2.46016700	-1.54832700	-1.88430000
C	3.36766700	-3.55608900	-2.89064600
C	3.59653000	-4.12194700	-1.64437100
C	3.25219700	-3.37298100	-0.52218300
C	2.70939300	-2.09588000	-0.61882700
C	4.30615000	1.09542800	0.52930100
C	-2.88065400	1.51968400	-1.90012800
C	3.83507900	0.79090700	1.81526400

C	4.43723200	-0.21569900	2.57095600
C	5.51373900	-0.94088300	2.06399400
C	5.98779800	-0.64132500	0.78677200
C	5.39284100	0.36576100	0.02658700
C	-3.97081200	0.98381600	-1.19521600
C	-4.76841800	0.00816100	-1.80818500
C	-4.50763200	-0.43138800	-3.10481200
C	-3.43025700	0.11170000	-3.80188700
C	-2.62494900	1.07610800	-3.20590600
N	3.50072200	-3.93681900	0.80634900
O	3.16831400	-3.27182900	1.79147600
O	4.03417600	-5.04591300	0.87204500
C	7.09282400	-1.47443800	0.19691700
F	7.77152700	-0.80811500	-0.76622500
F	7.99086400	-1.85467600	1.13338400
F	6.61510600	-2.60559600	-0.37011400
C	3.88048100	-0.53277600	3.93548700
F	3.64295700	0.59343600	4.64371700
F	2.70418600	-1.19525300	3.84956900
F	4.72137200	-1.29958800	4.66116100
C	-3.16376800	-0.29877200	-5.22203600
F	-3.76864300	0.54240300	-6.10473400
F	-1.84414100	-0.27351700	-5.52262400
F	-3.62258500	-1.53671600	-5.49566800
C	-5.88807100	-0.63614500	-1.03526100
F	-6.59033100	0.24023900	-0.30619400
F	-6.76269700	-1.27752700	-1.85161100
F	-5.41360400	-1.58564300	-0.17572200
H	4.91730200	6.75003300	-3.71816100
H	2.44061800	6.97431700	-3.92091600
H	0.94711900	5.46333700	-2.68658400
H	5.87888300	4.95439000	-2.30916800
H	5.58491500	3.04997100	-0.80281300
H	-3.67873900	3.77790900	-0.65987300
H	1.43600200	5.82432200	0.07741000
H	0.31305800	7.80523400	0.97113100
H	-2.17763800	7.91170400	1.08567900
H	-3.52158300	5.96381500	0.34040400
H	1.72232200	1.40615600	-3.28967300
H	3.30587100	0.62294600	-3.30609100
H	0.71135800	-0.60390700	-4.38721700
H	1.97347400	0.10647500	-5.40165000
H	2.02071900	-2.50934300	-5.02059400
H	3.53316000	-1.62233900	-4.92676500
H	3.61772100	-4.12088400	-3.78506400

H	4.02699800	-5.10719500	-1.52523700
H	2.50047800	-1.54504100	0.28831700
H	2.99910500	1.34344300	2.22772700
H	5.97020100	-1.72603700	2.65341900
H	5.76470000	0.57345900	-0.97039400
H	-4.18752100	1.30276600	-0.17342400
H	-5.12391900	-1.19675600	-3.55854000
H	-1.78529300	1.48259600	-3.75602100
Pd	-0.70498700	-1.30103400	0.04318600
I	-1.07141900	-2.83276400	-2.24607000
C	-1.42831500	-1.75257900	2.13007800
C	-1.32998900	-0.35368600	2.04243400
H	-2.15273700	0.19081200	1.58639100
C	-2.25975500	-2.47114800	1.24617900
H	-3.10111900	-1.93607400	0.81009200
C	-0.46548700	0.43478600	3.00077700
H	0.53567200	-0.00432800	3.04517500
C	-2.36608900	-3.93655400	1.20824400
C	-3.51741100	-4.51356500	0.64363100
C	-1.38087100	-4.78988700	1.73897300
C	-3.68863900	-5.89600000	0.62787700
H	-4.27697800	-3.86454800	0.21874000
C	-1.55324900	-6.17055700	1.72068800
H	-0.46606700	-4.37389300	2.15003200
C	-2.70916400	-6.73056500	1.16845500
H	-4.58666100	-6.32135800	0.18830500
H	-0.77938400	-6.81299000	2.13182000
H	-2.83948000	-7.80931600	1.15334300
C	-1.06990500	0.42856600	4.40597400
C	-2.34974800	0.98571500	4.64455400
C	-0.34819800	-0.15371900	5.45542700
C	-2.85542700	0.91816800	5.95194300
C	-0.87341400	-0.20553100	6.74776200
H	0.63748600	-0.56740400	5.25708700
C	-2.13814200	0.32865600	6.99316100
H	-3.83895700	1.33890500	6.13904800
H	-0.29928700	-0.66203500	7.55054400
H	-2.56391800	0.29159200	7.99362600
C	-3.13123200	1.62522100	3.54251300
C	-4.25366800	0.95930300	2.96073000
C	-2.78566700	2.94409900	3.11094600
O	-4.89516400	1.24661000	1.94346100
O	-3.29287900	3.65571700	2.24198200
O	-4.60420900	-0.18382600	3.68204000
O	-1.71277700	3.44038500	3.86790600

C	-1.34228700	4.77940900	3.59185700
H	-0.65573500	5.07424300	4.39160000
H	-0.83452000	4.87514300	2.62634100
H	-2.21169700	5.44443100	3.57919100
C	-5.76658700	-0.85516200	3.21610900
H	-6.64860400	-0.20499800	3.25497600
H	-5.65734200	-1.20396500	2.18663500
H	-5.90613900	-1.70787700	3.88644800
H	-0.36822400	1.46282600	2.64164700
H	-0.74688000	-2.28203300	2.79224500

NMe3

Thermal correction to Gibbs Free Energy: 0.093313

SCF energy in solution: -174.386154

Solution-phase Gibbs free energy: -174.292841

Coordinates:

N	-0.00001200	0.00000500	-0.37158800
C	-0.15509300	-1.38021500	0.06103600
H	-1.09229800	-1.78885600	-0.33159100
H	0.66831600	-1.98656000	-0.33119200
H	-0.16849100	-1.49729400	1.16359300
C	-1.11776600	0.82442300	0.06104300
H	-1.00304200	1.84040500	-0.33154300
H	-2.05458900	0.41454500	-0.33121600
H	-1.21244200	0.89449900	1.16360400
C	1.27285600	0.55579100	0.06103600
H	2.09534000	-0.05161800	-0.33149100
H	1.38635300	1.57199400	-0.33132600
H	1.38095600	0.60286100	1.16359500

NMe3H+

Thermal correction to Gibbs Free Energy: 0.108645

SCF energy in solution: -174.840332

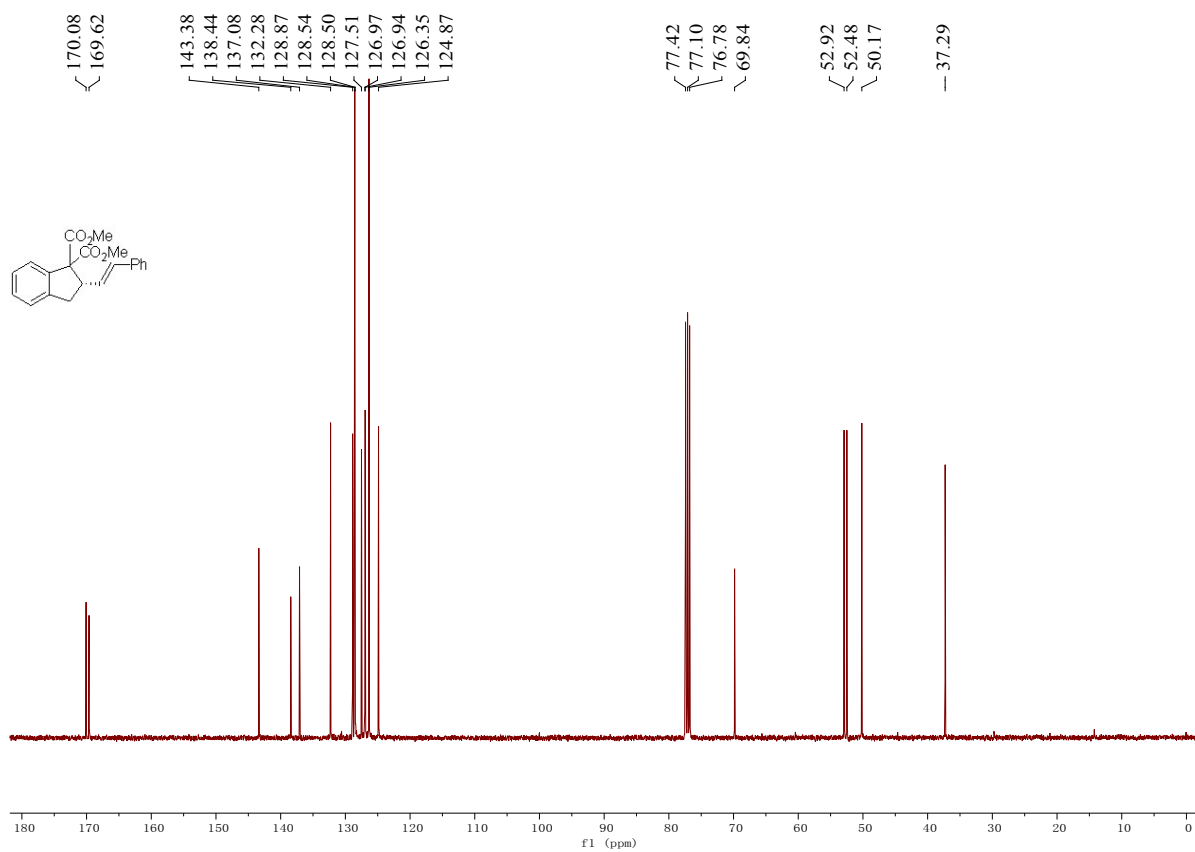
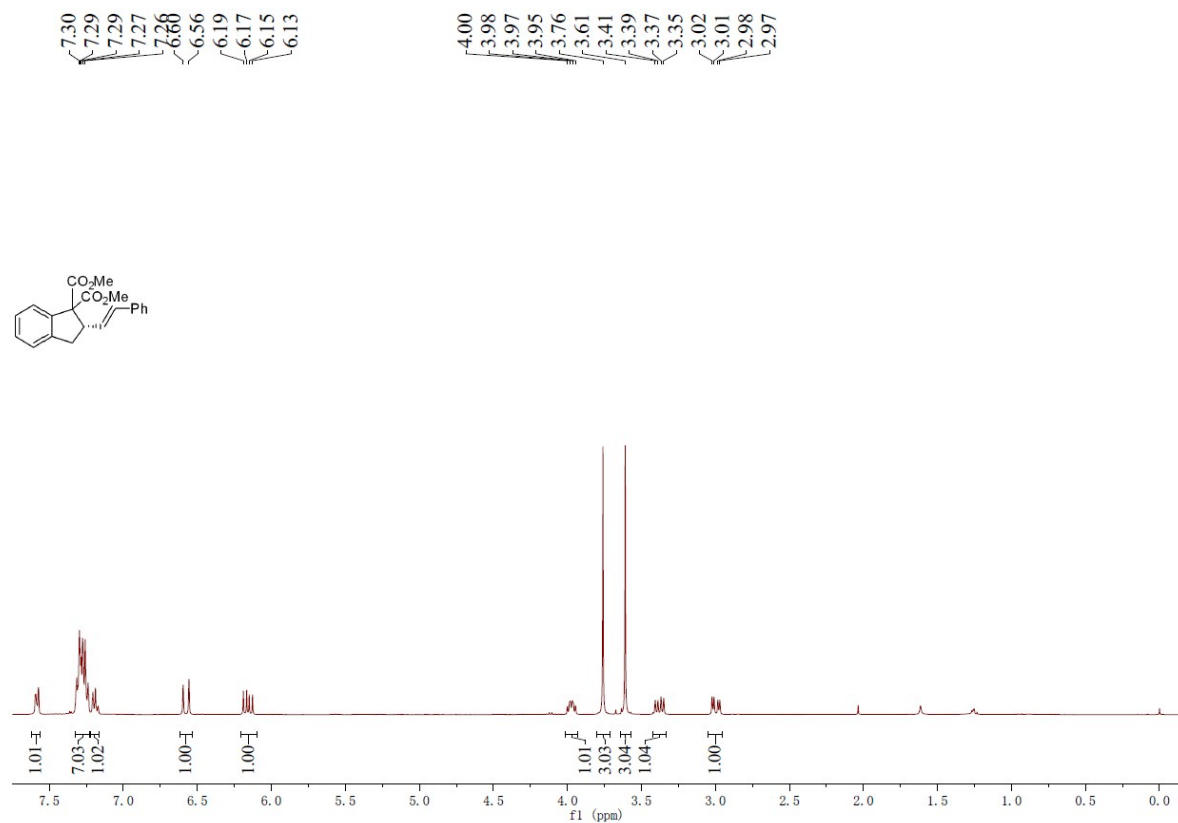
Solution-phase Gibbs free energy: -174.731687

Coordinates:

H	-0.00015400	-0.00016900	-1.36430200
N	-0.00003900	-0.00005100	-0.33926100
C	1.44073600	0.01681000	0.10343200
H	1.91850700	0.91684600	-0.28372000
H	1.93965000	-0.87143200	-0.28426500
C	-0.73489900	1.23929500	0.10344300
H	-1.75370700	1.20247000	-0.28240800
C	-0.70579800	-1.25604700	0.10346600
H	-1.72433600	-1.24436000	-0.28474600
H	1.46551600	0.01679400	1.19358200
H	-0.74590100	1.26153300	1.19358300
H	-0.21587000	2.11538900	-0.28551600
H	-0.16490300	-2.11993300	-0.28305100
H	-0.71876200	-1.27712600	1.19362100

^1H NMR and ^{13}C NMR Spectrum for the Products

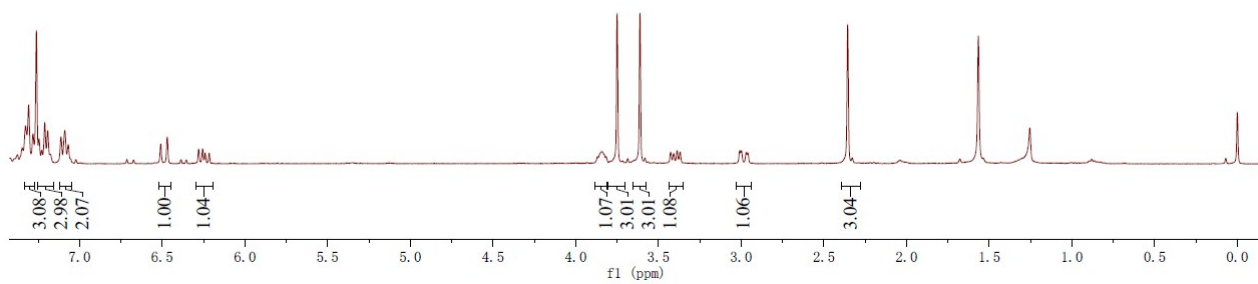
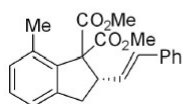
Dimethyl (*S,E*)-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (**3aa**)



Dimethyl (*S,E*)-7-methyl-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ba)

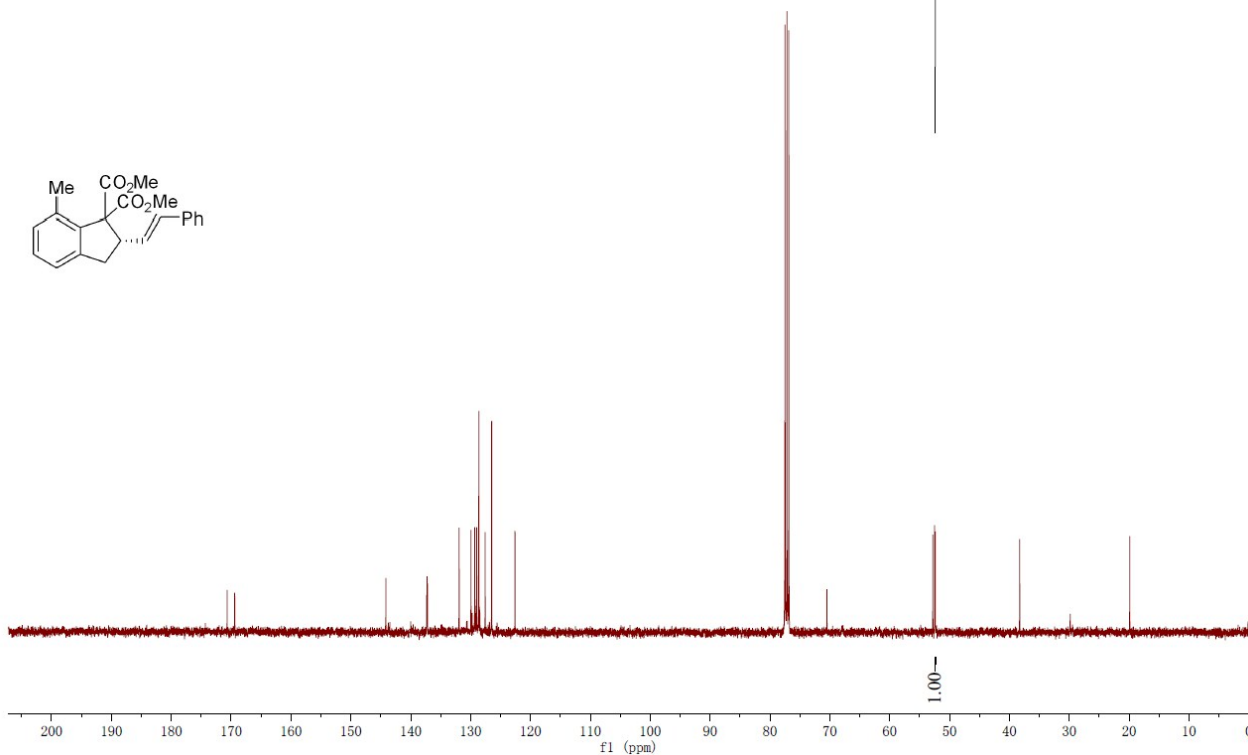
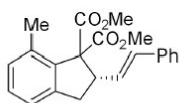
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7.26
7.21
6.47
6.28
6.25
6.24
6.22

3.84
3.75
3.61
3.43
3.41
3.39
3.37
3.01
3.00
2.97
2.96
-2.36



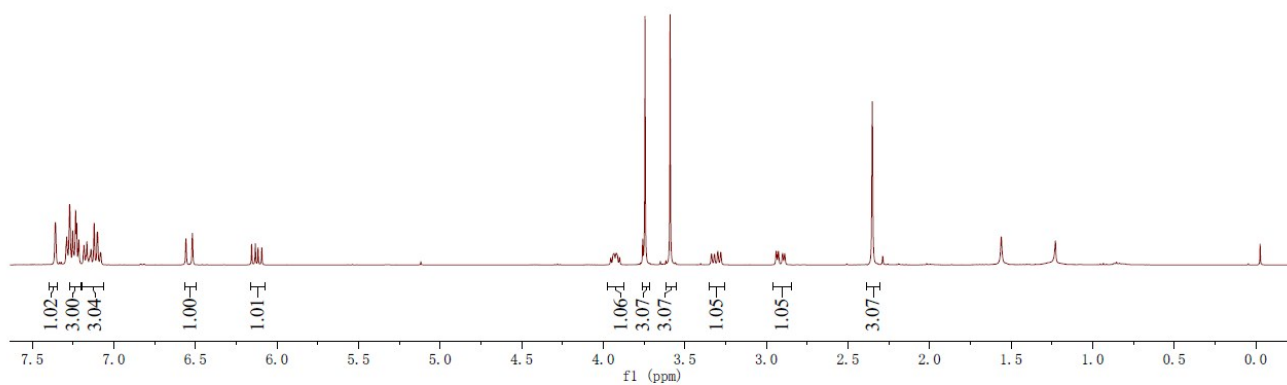
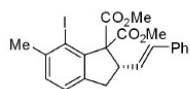
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169.40
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137.33
137.25
137.20
131.91
129.93
129.31
129.12
128.97
128.62
127.56
126.47
122.58

77.48
77.16
76.84
70.47
52.78
52.48
52.39
38.27
19.89

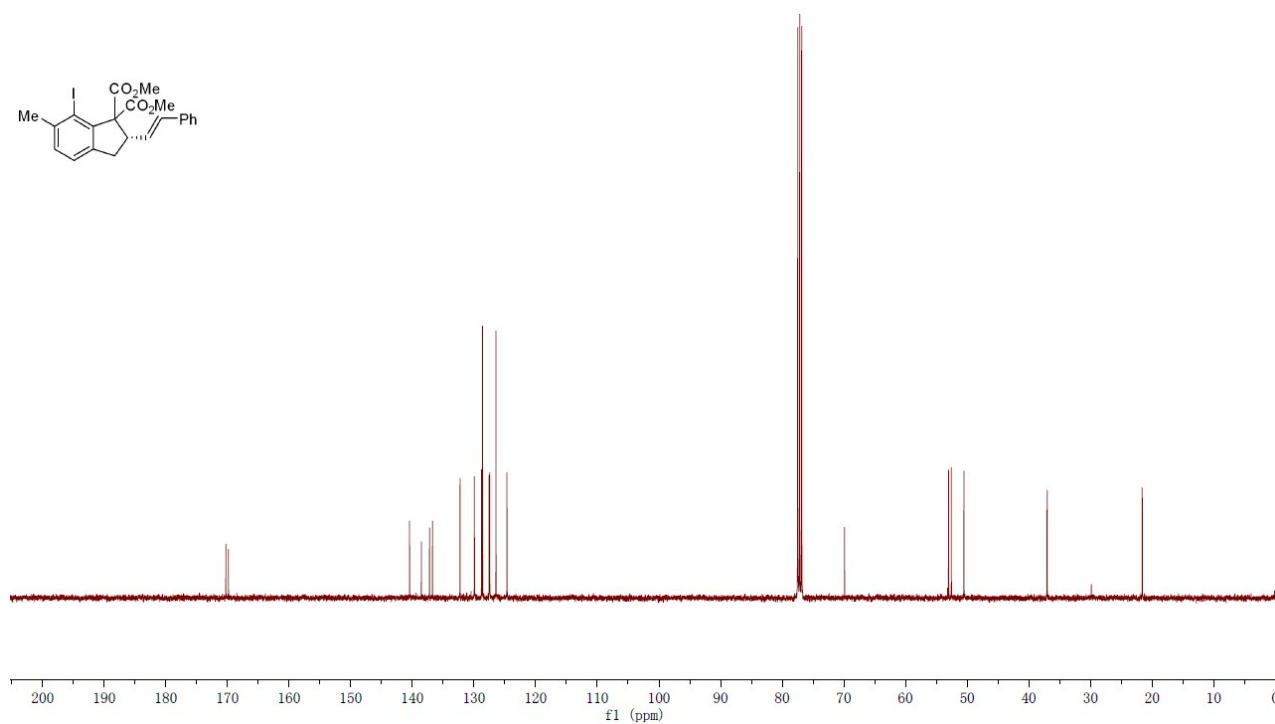
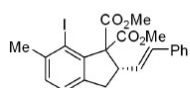


Dimethyl (*S,E*)-7-iodo-6-methyl-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ca)

¹H NMR (CDCl₃) peaks (ppm): 7.36, 7.27, 7.23, 7.23, 7.12, 6.56, 6.52, 6.15, 6.13, 6.12, 6.09, 3.95, 3.93, 3.92, 3.90, 3.74, 3.59, 3.34, 3.32, 3.30, 3.28, 2.94, 2.93, 2.90, 2.89, 2.35

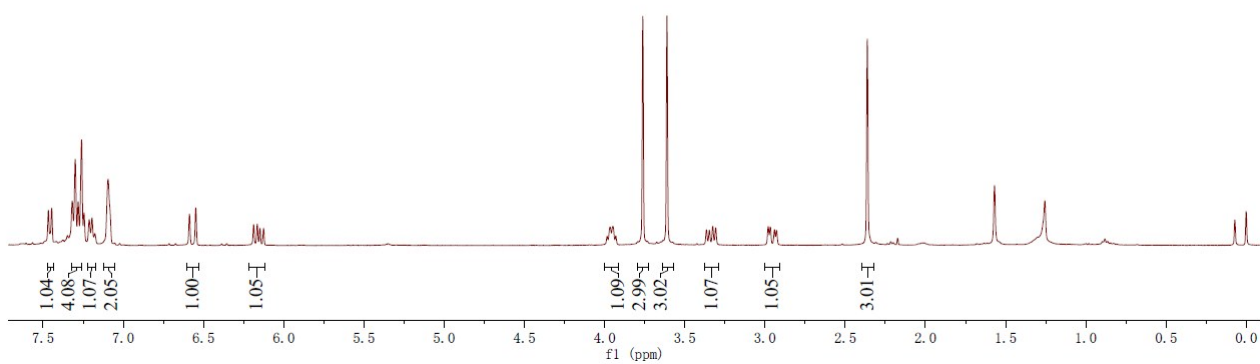
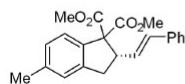


¹³C NMR (CDCl₃) peaks (ppm): 170.26, 169.85, 140.45, 138.54, 137.22, 136.73, 132.27, 129.94, 128.77, 128.62, 127.56, 127.45, 126.44, 124.65, 77.48, 77.16, 76.84, 69.88, 53.01, 52.56, 50.52, 37.02, 21.58

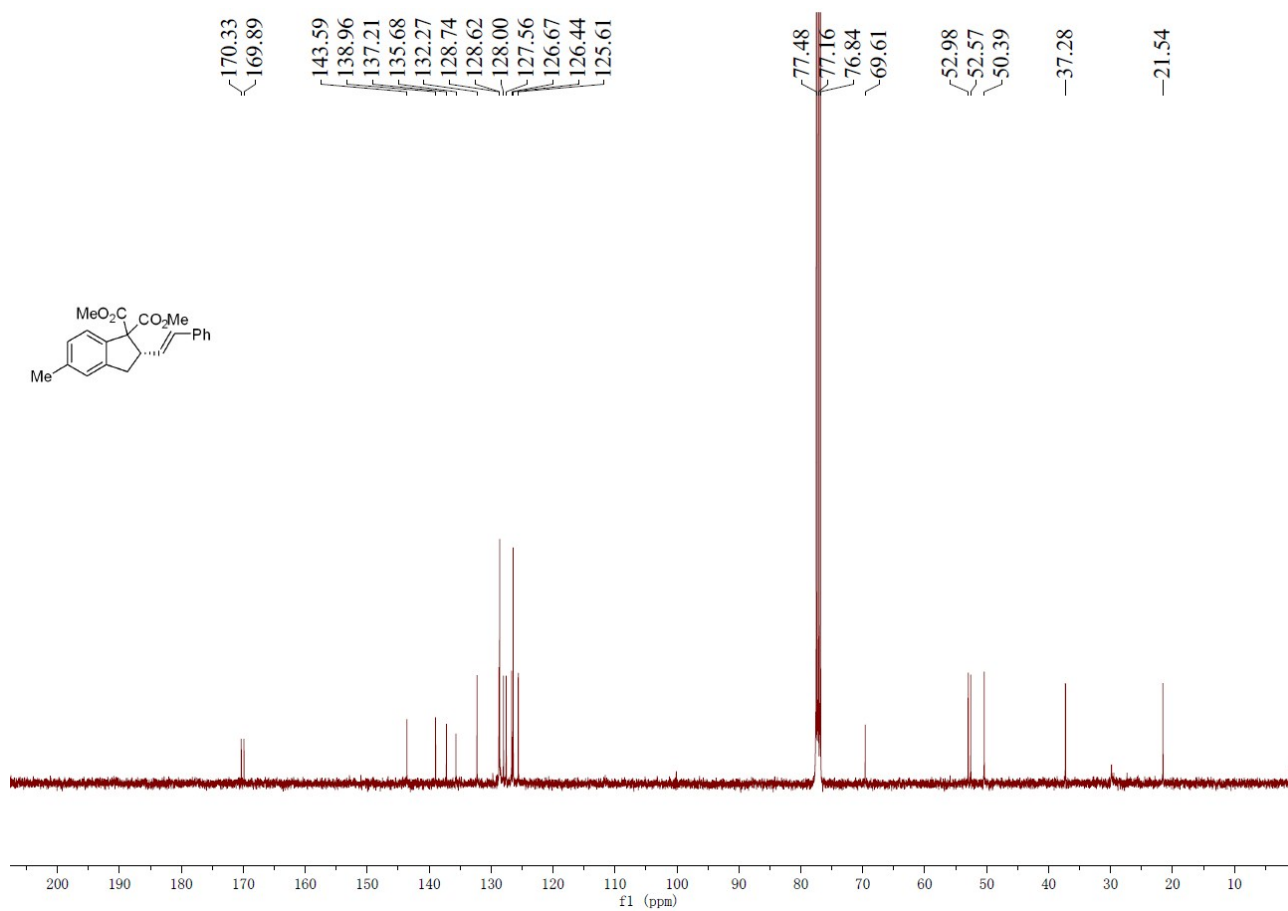
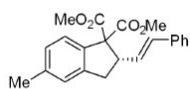


Dimethyl (*S,E*)-5-methyl-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3da)

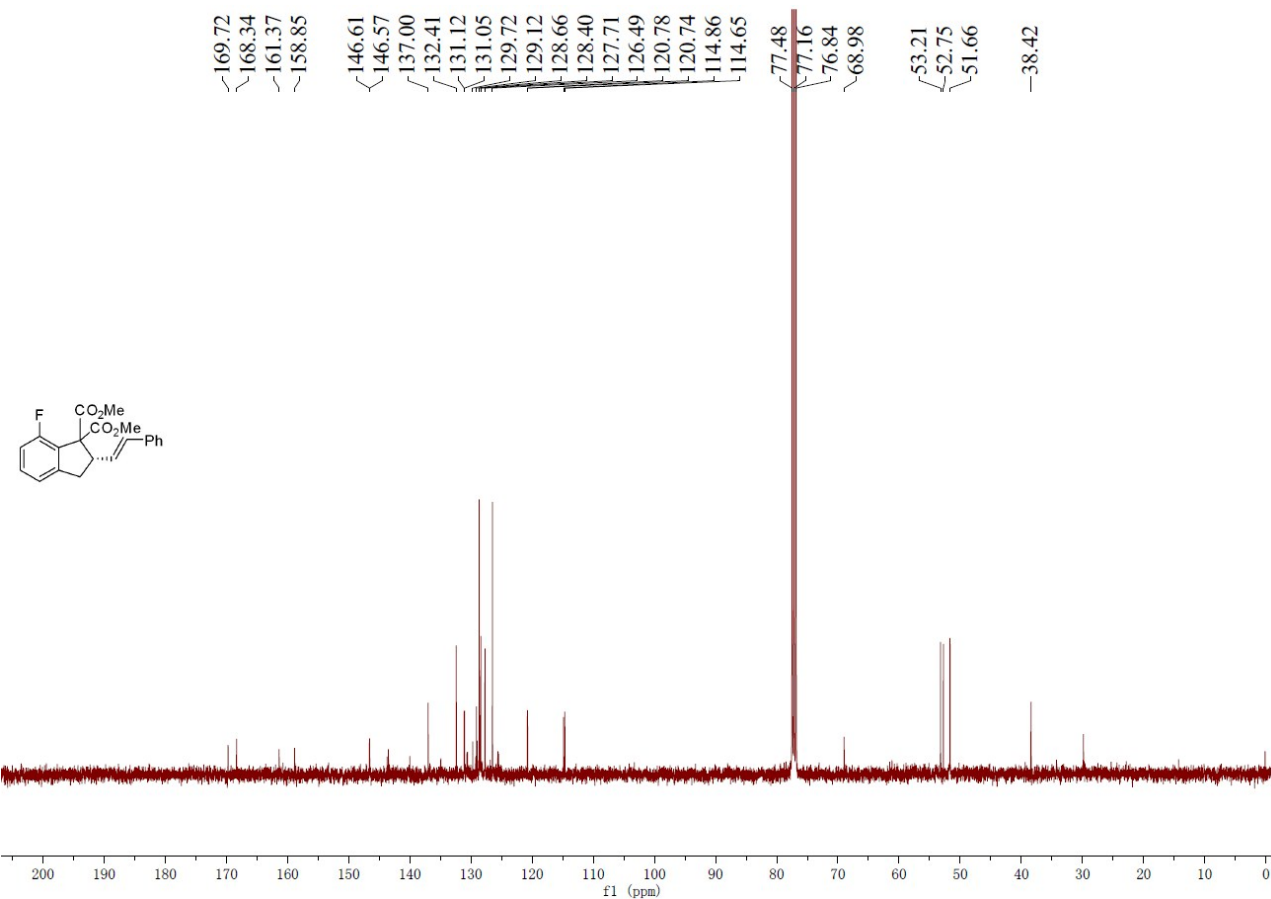
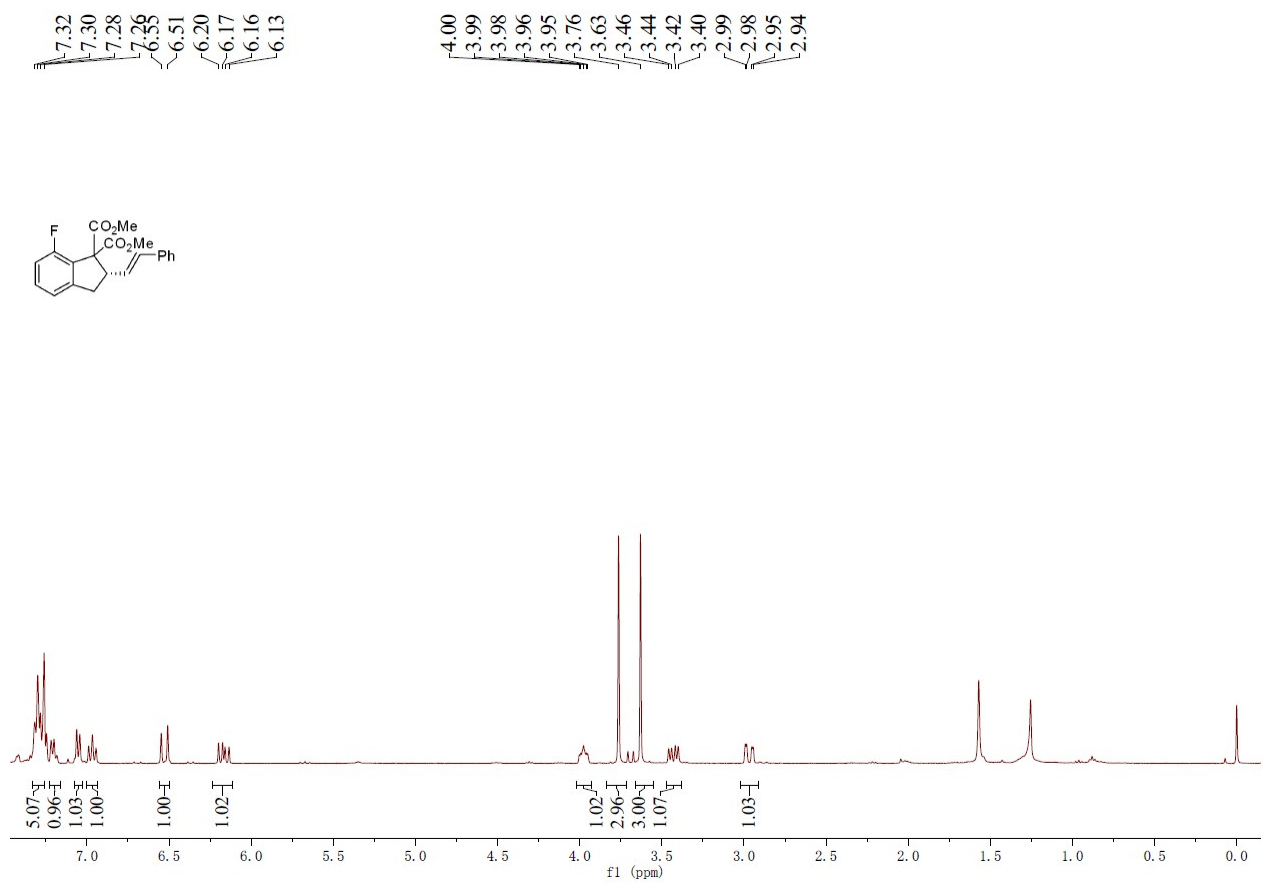
¹H NMR peaks (ppm): 7.45, 7.32, 7.30, 7.28, 7.26, 7.09, 6.55, 6.19, 6.16, 6.15, 6.13, 3.98, 3.96, 3.95, 3.93, 3.76, 3.61, 3.36, 3.35, 3.33, 3.31, 2.98, 2.97, 2.94, 2.93, 2.36



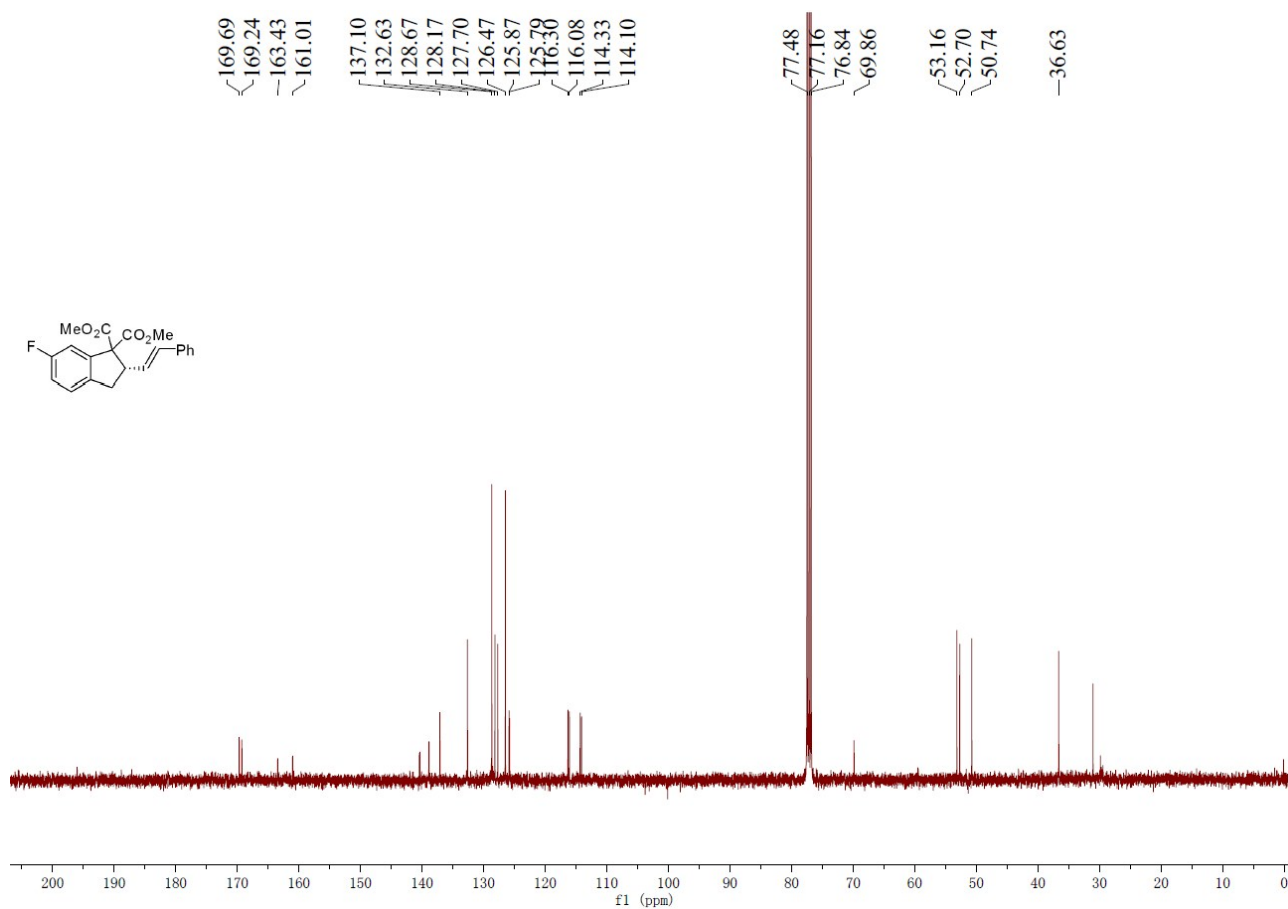
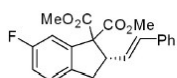
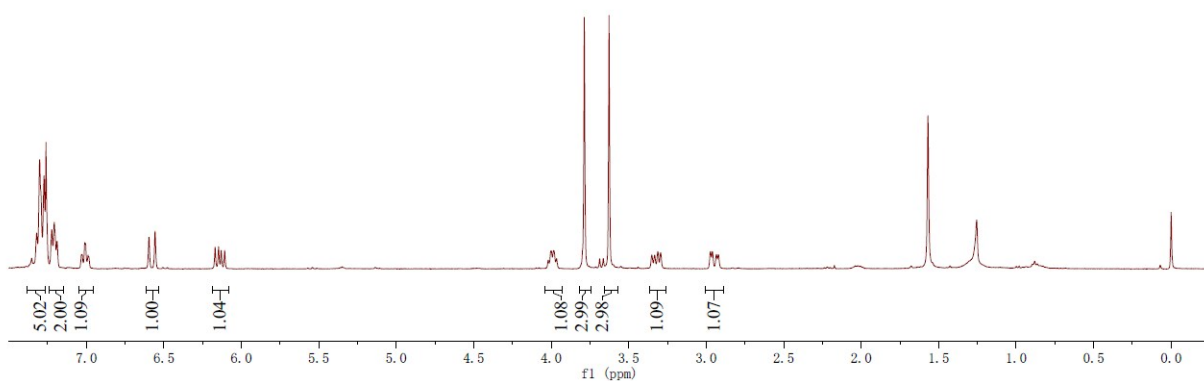
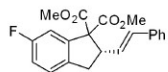
¹³C NMR peaks (ppm): 170.33, 169.89, 143.59, 138.96, 137.21, 135.68, 132.27, 128.74, 128.62, 128.00, 127.56, 126.67, 126.44, 125.61, 77.48, 77.16, 76.84, 69.61, 52.98, 52.57, 50.39, 37.28, 21.54



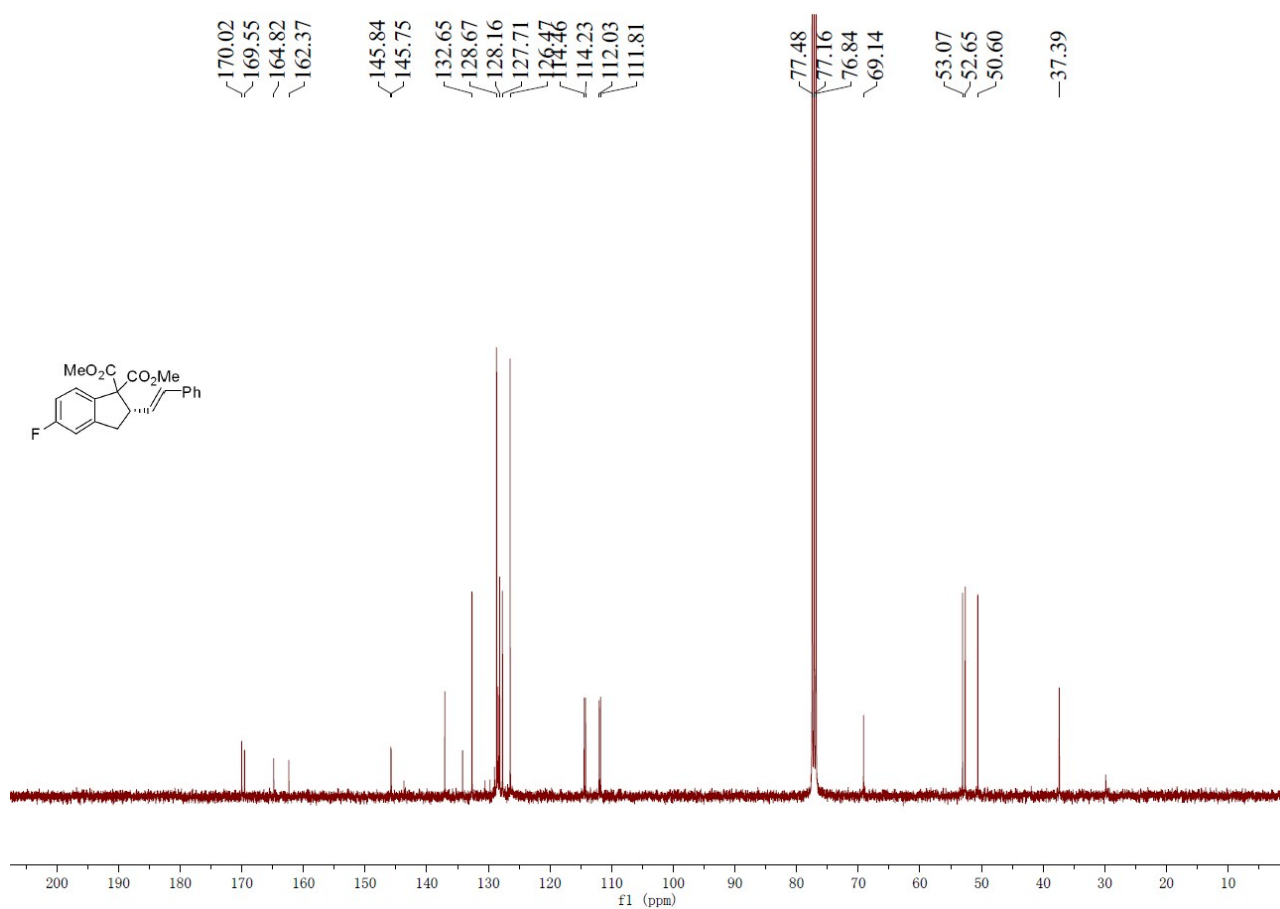
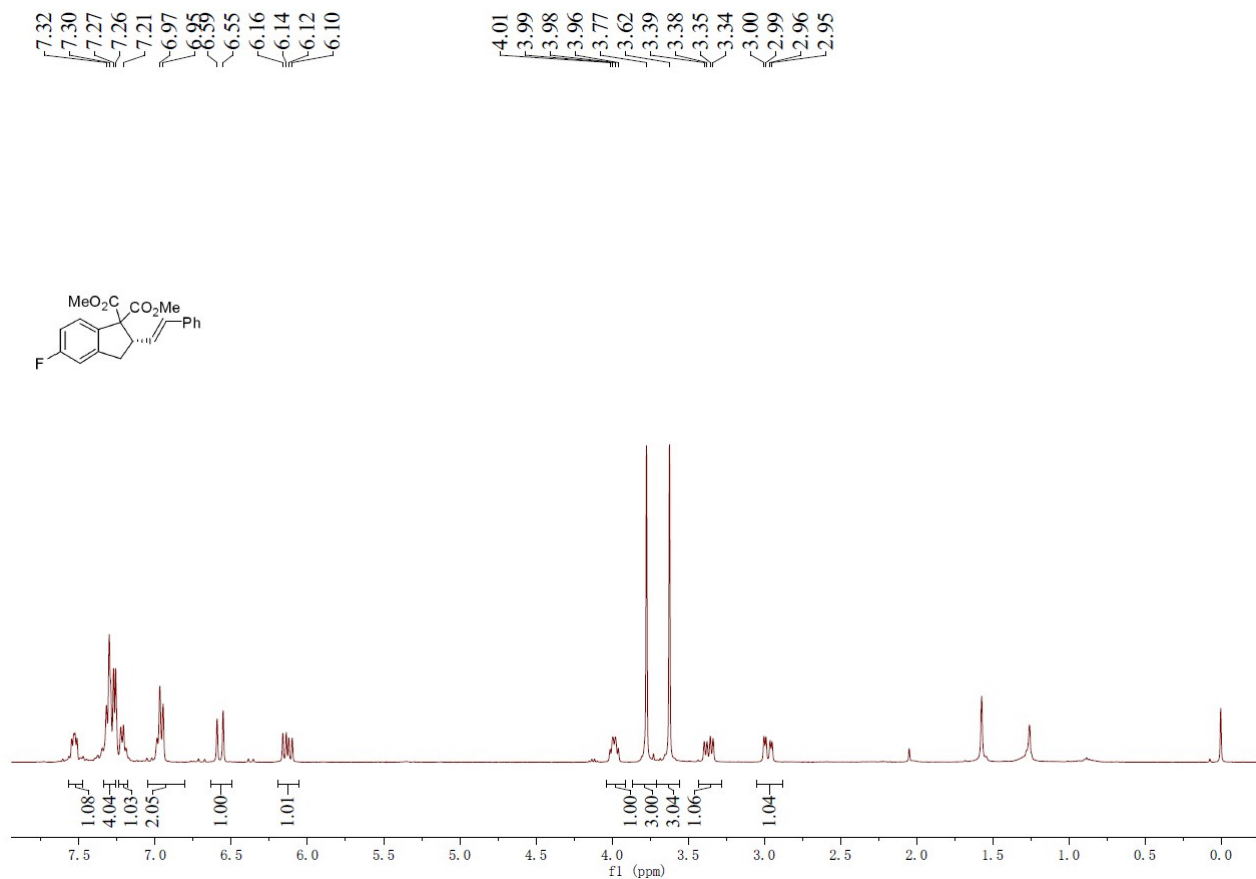
Dimethyl (S,E)-7-fluoro-2-styryl-2,3-dihydro-1H-indene-1,1-dicarboxylate (3ea)



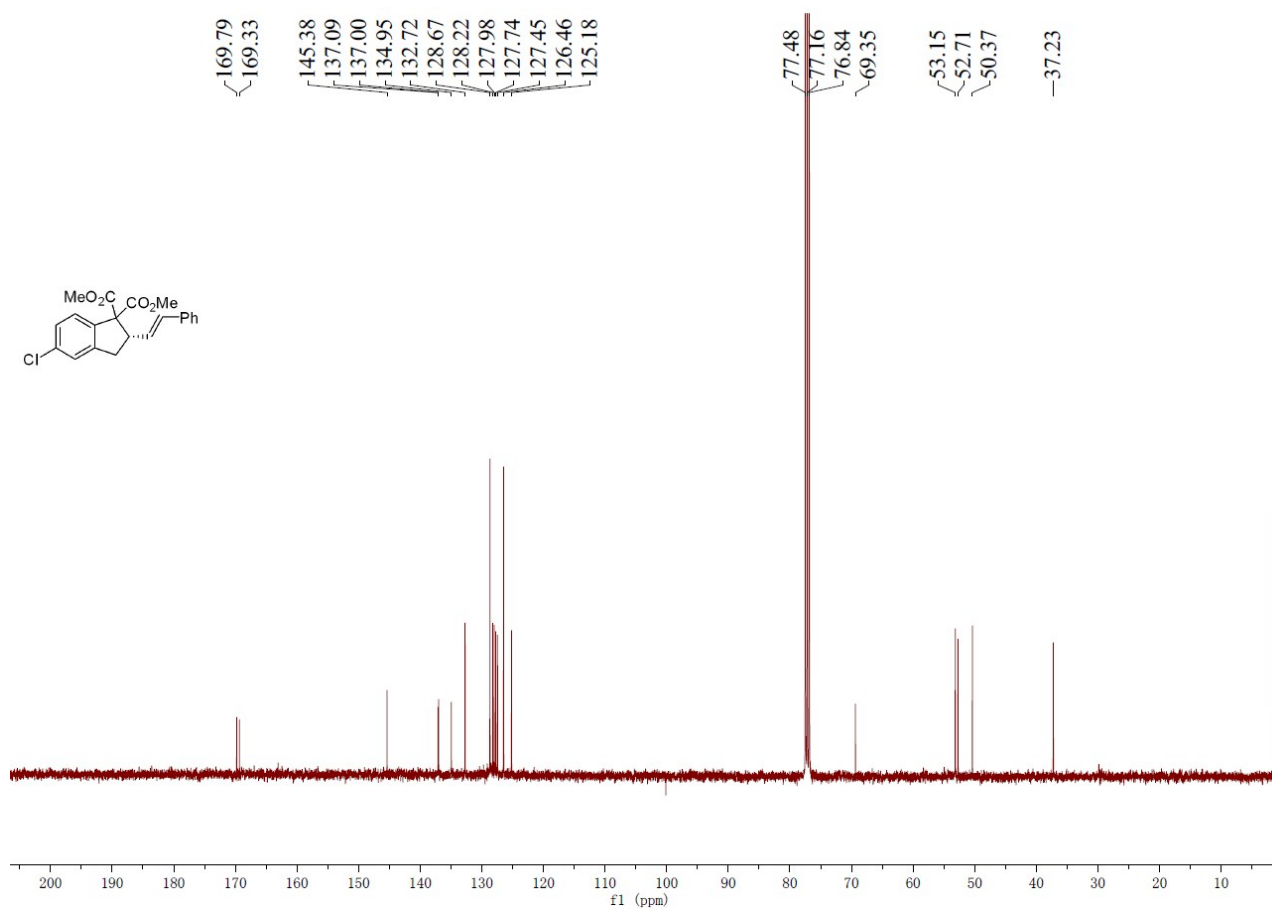
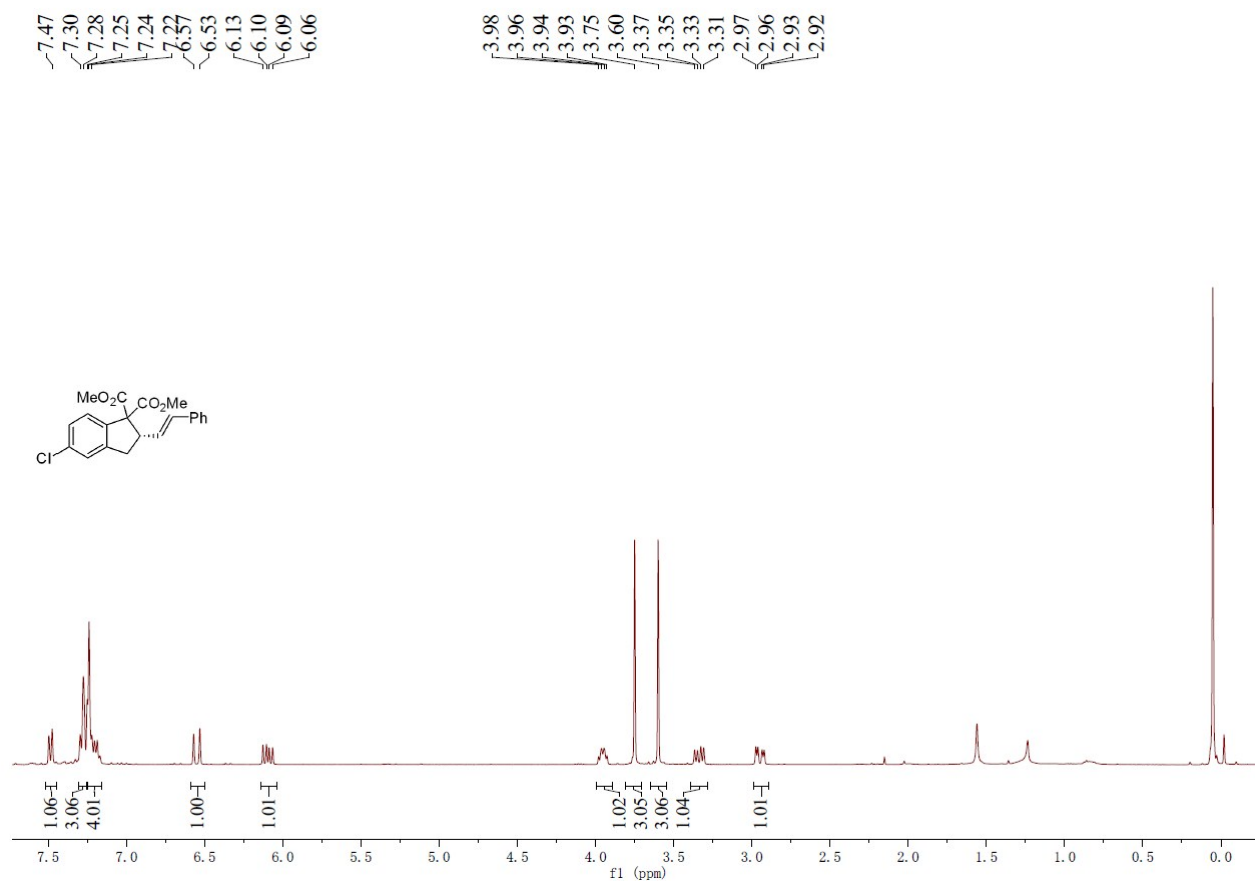
Dimethyl (*S,E*)-6-fluoro-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3fa)



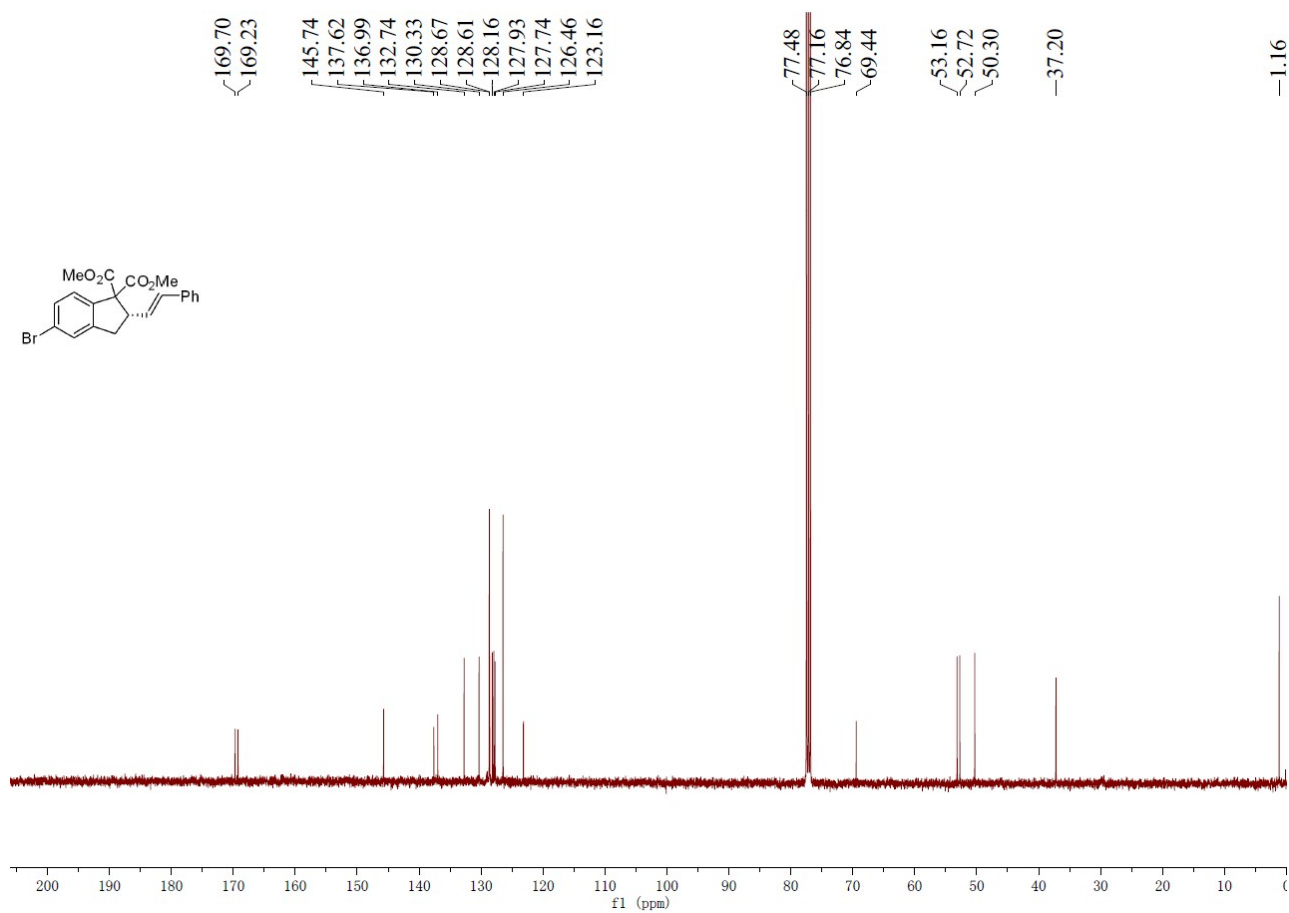
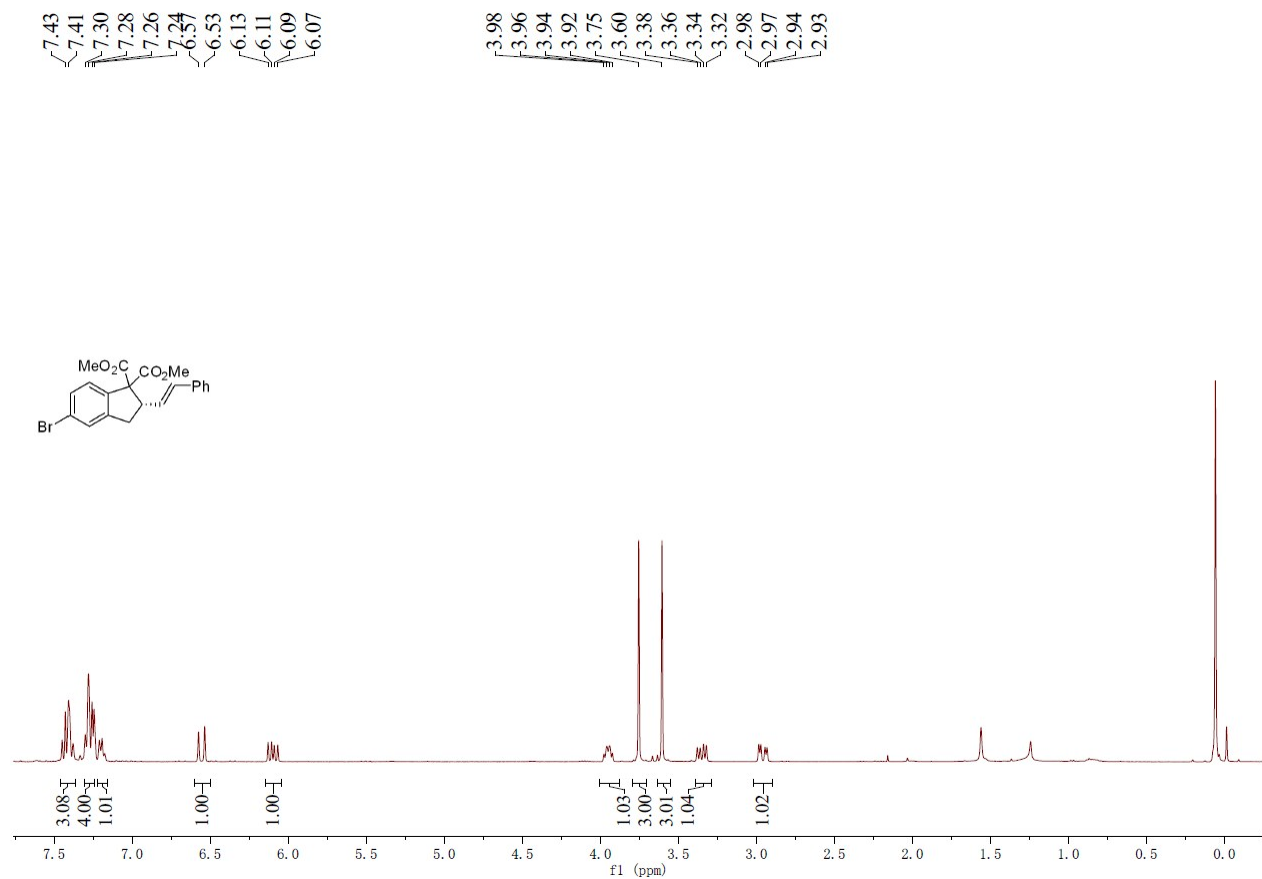
Dimethyl (*S,E*)-5-fluoro-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ga)



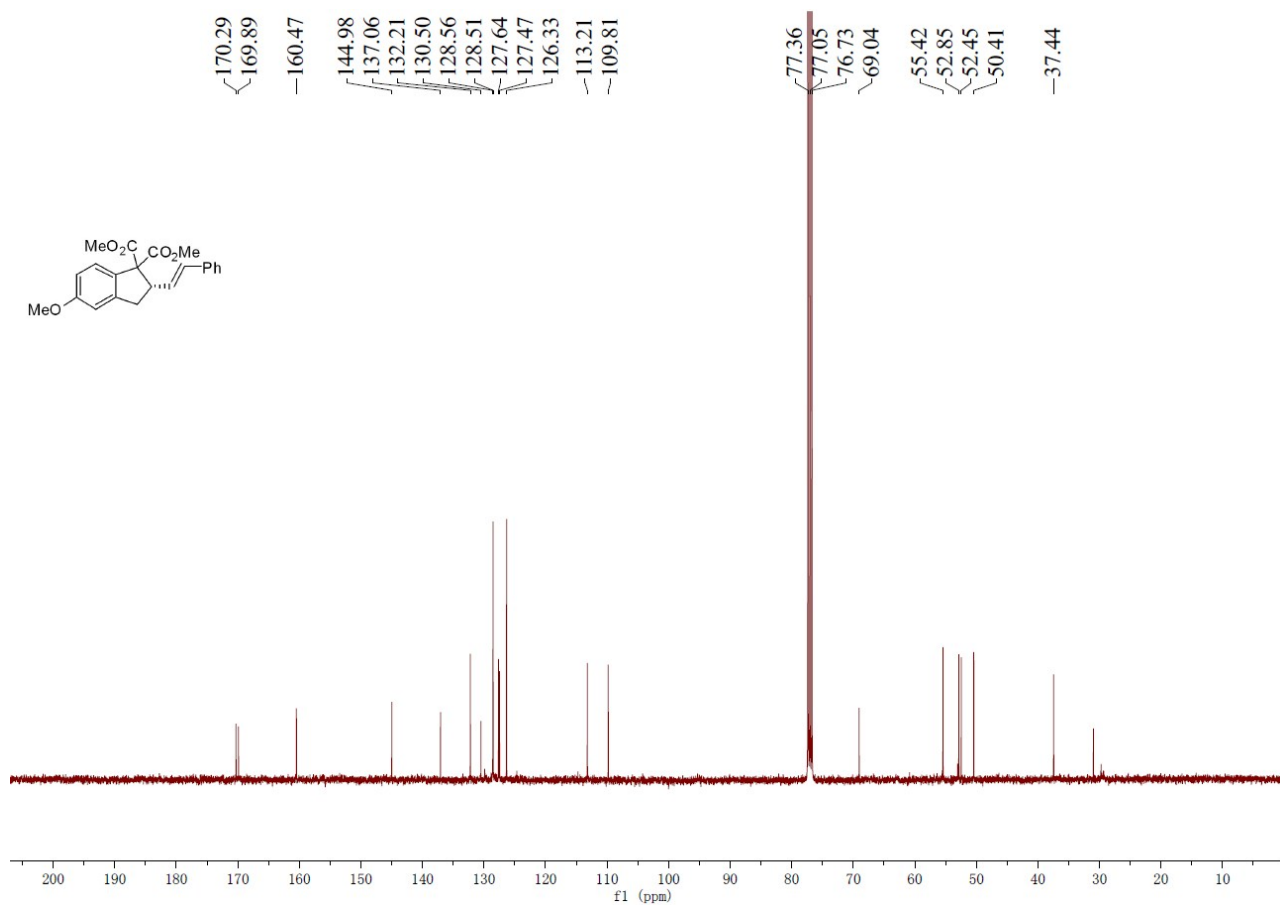
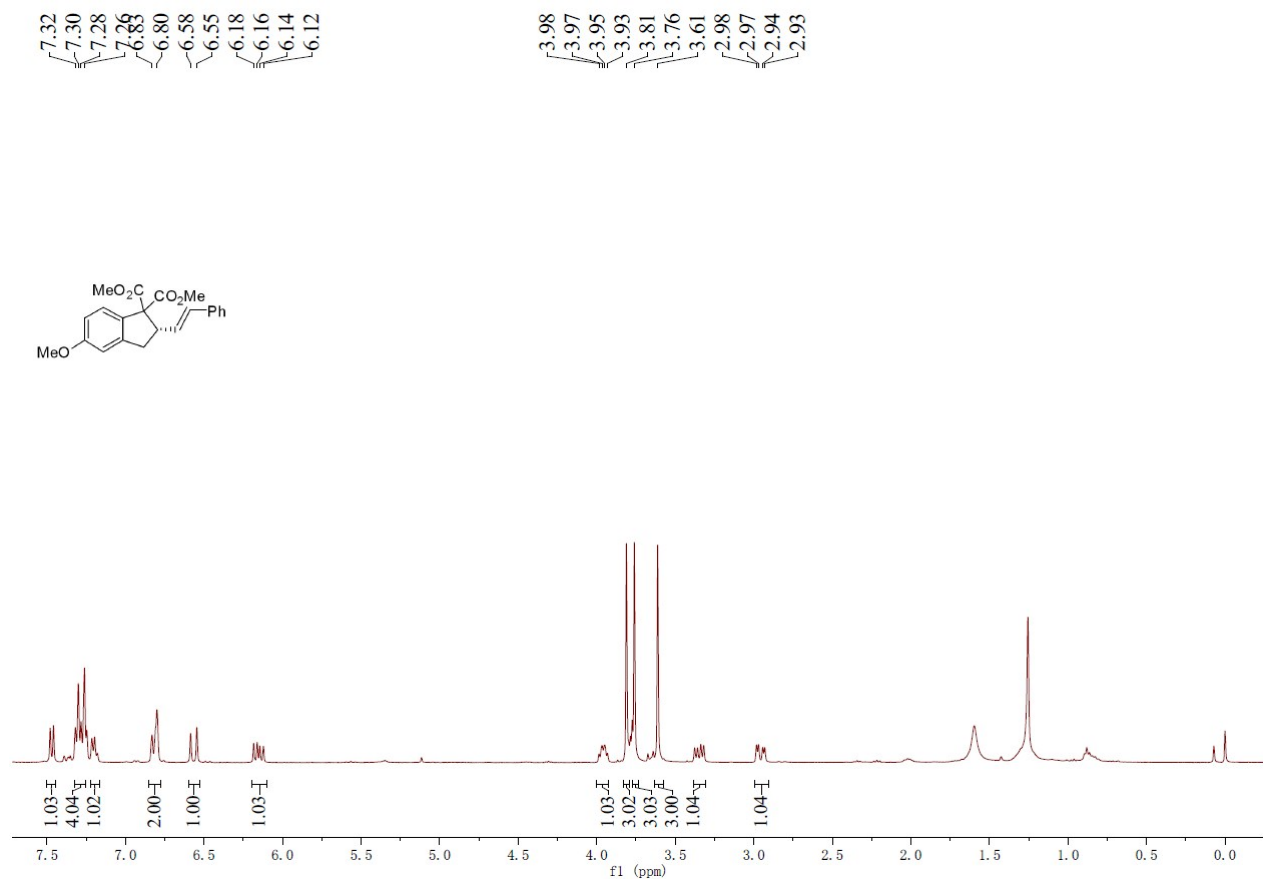
Dimethyl (*S,E*)-5-chloro-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ha)



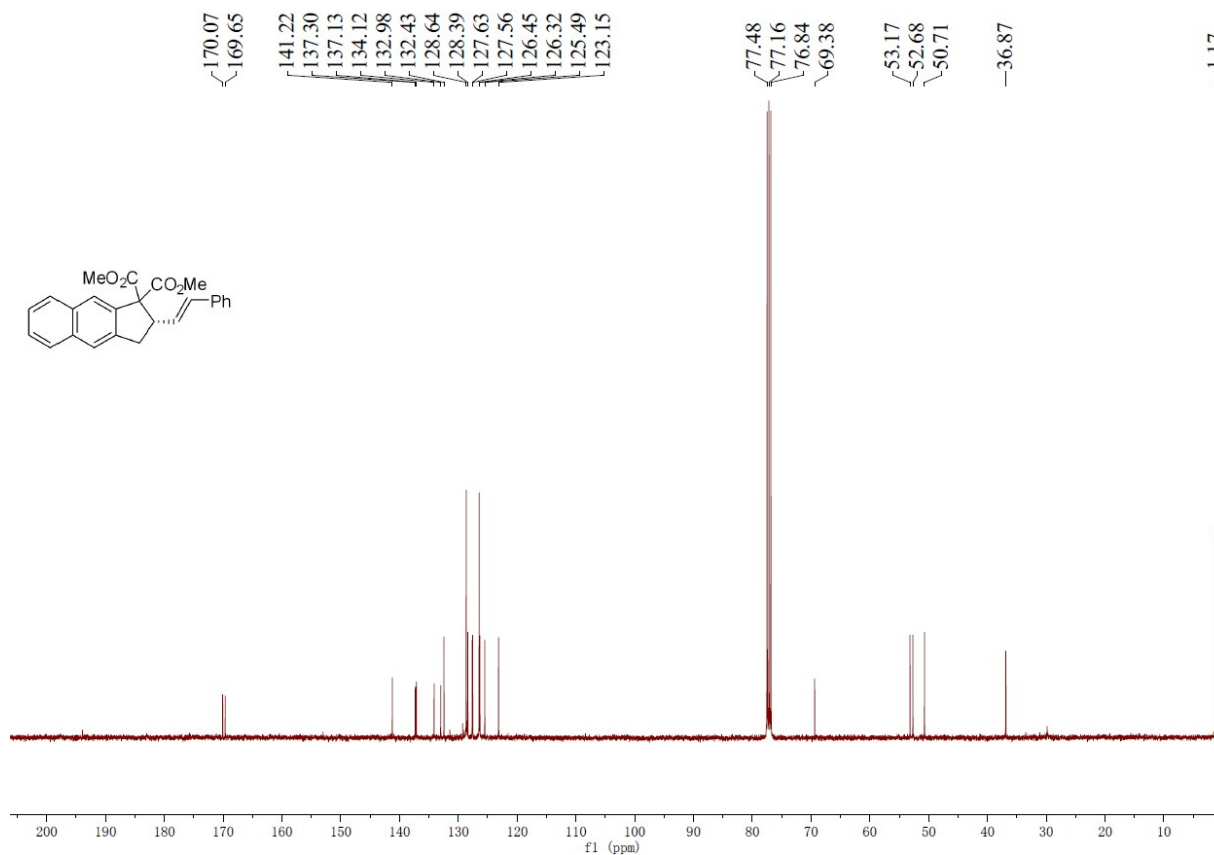
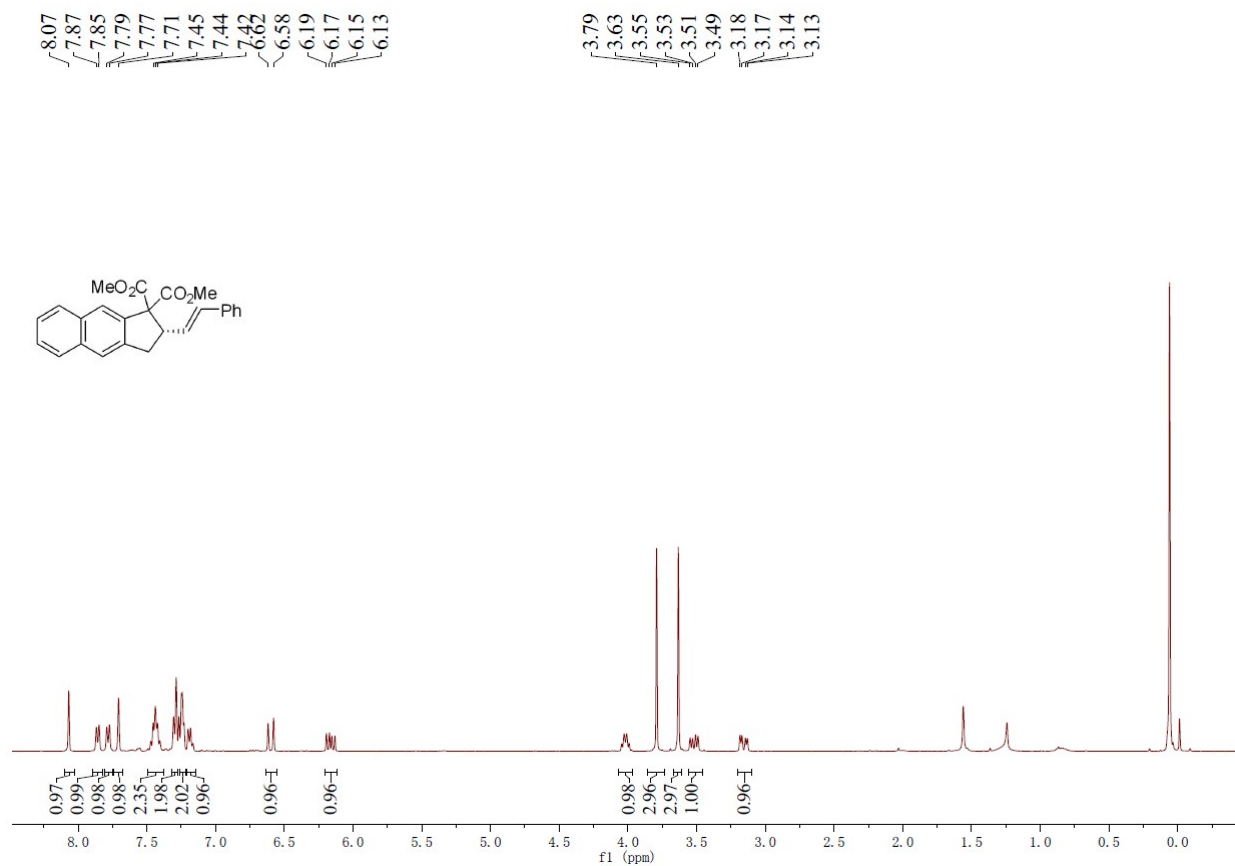
Dimethyl (*S,E*)-5-bromo-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ia)



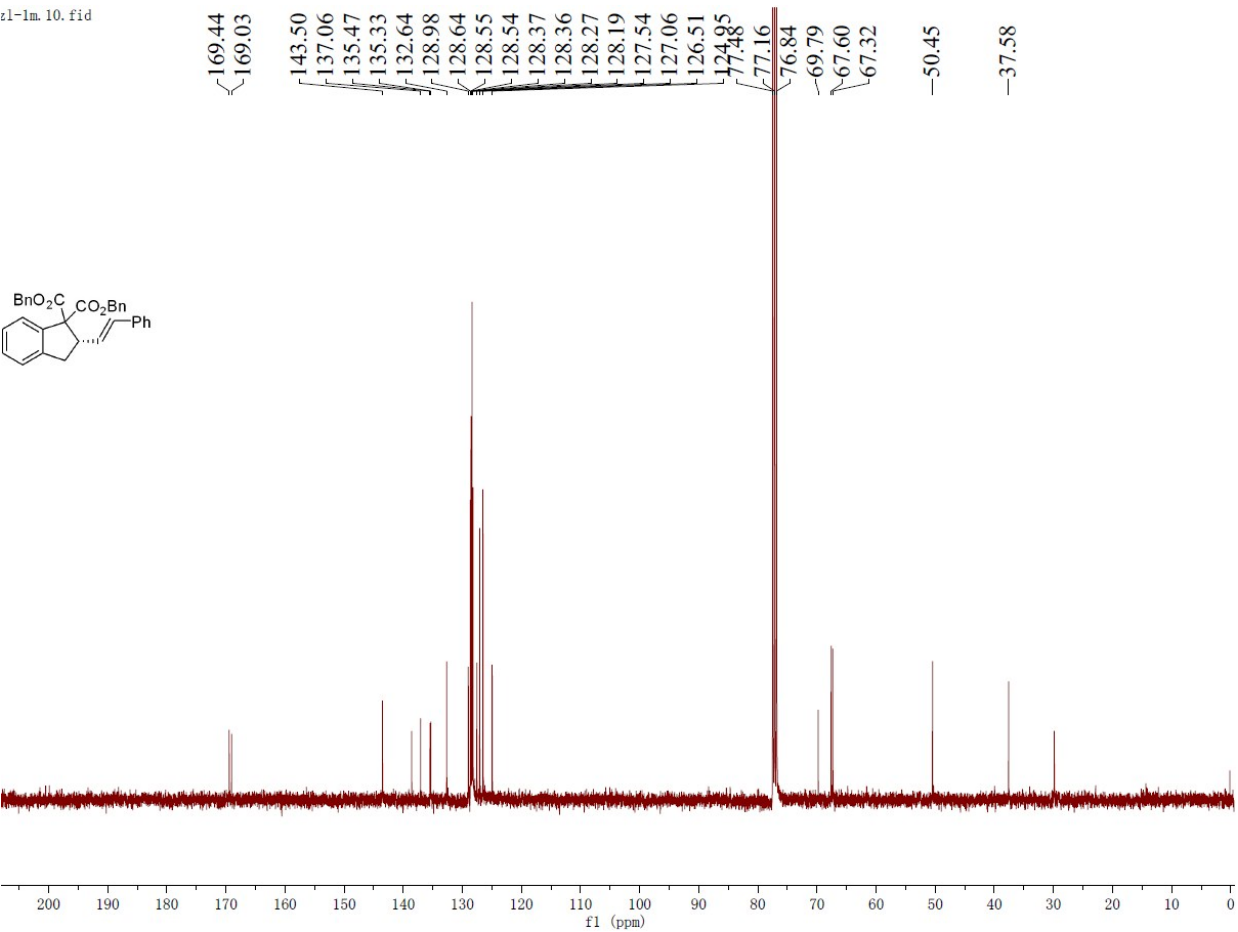
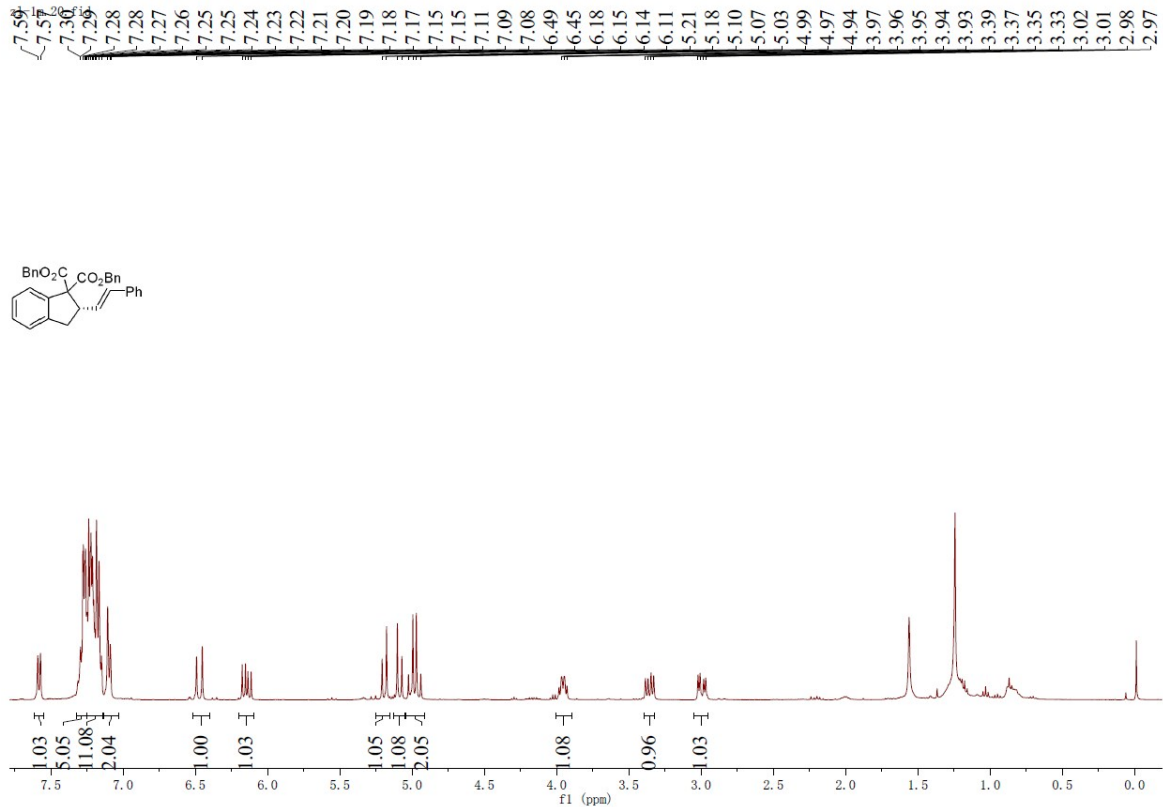
Dimethyl (*S,E*)-5-methoxy-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ja)



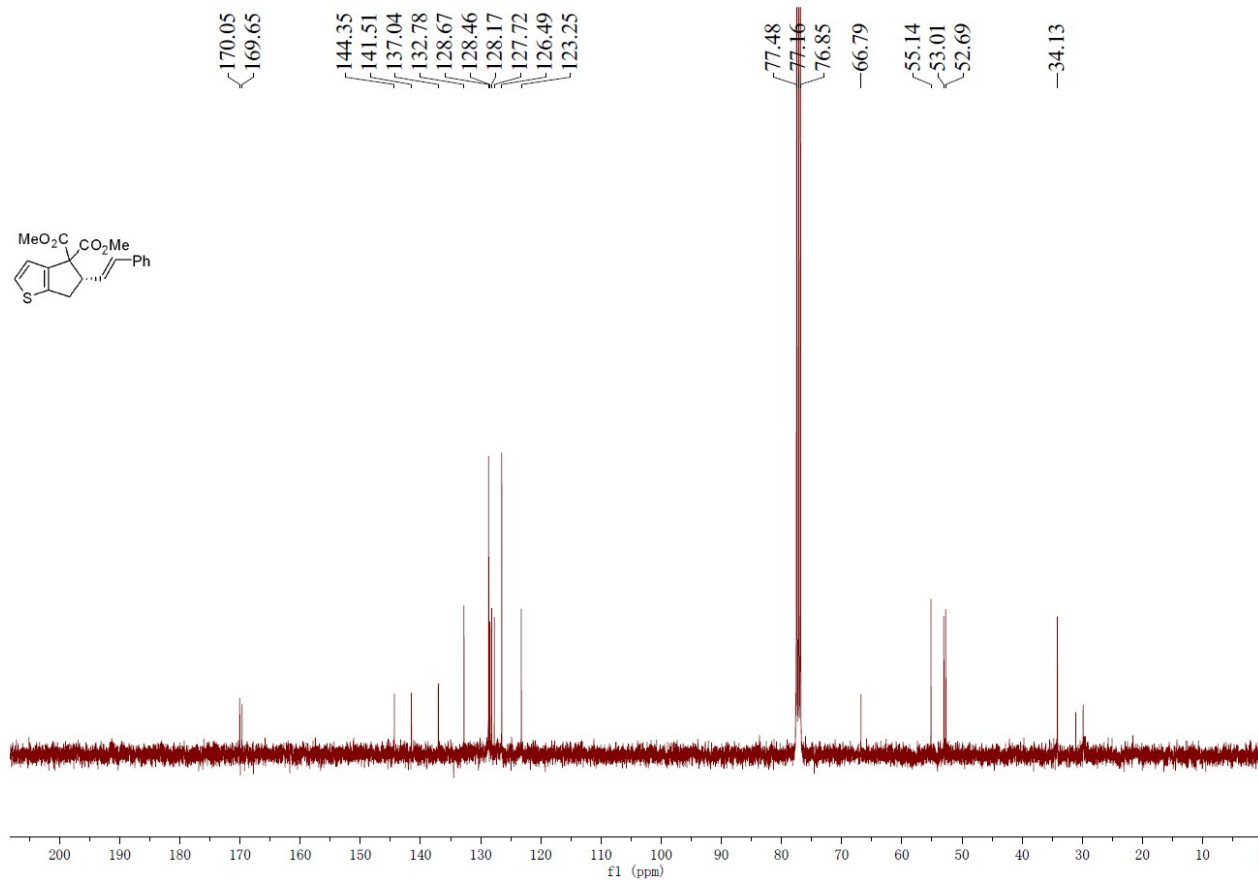
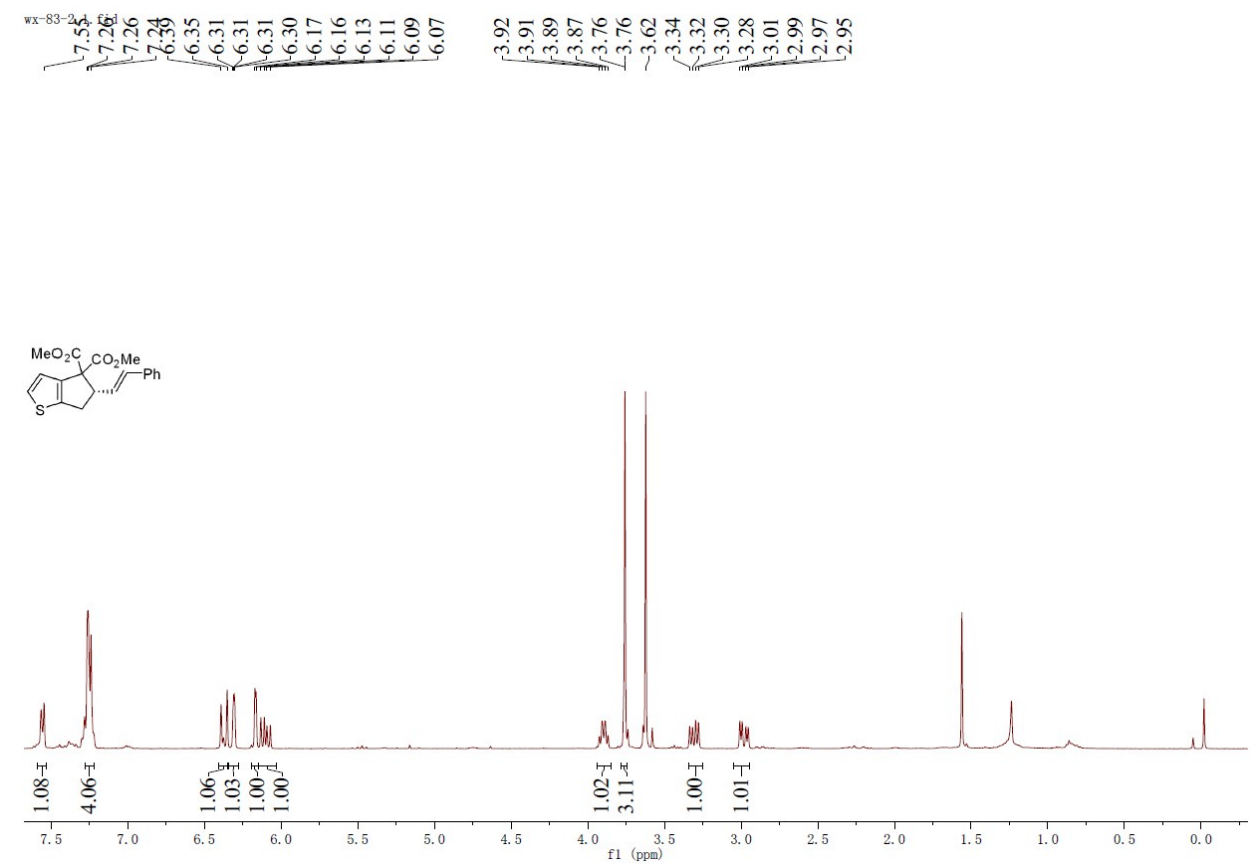
Dimethyl (*S,E*)-2-styryl-2,3-dihydro-1*H*-cyclopenta[*b*]naphthalene-1,1-dicarboxylate (3ka)



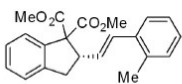
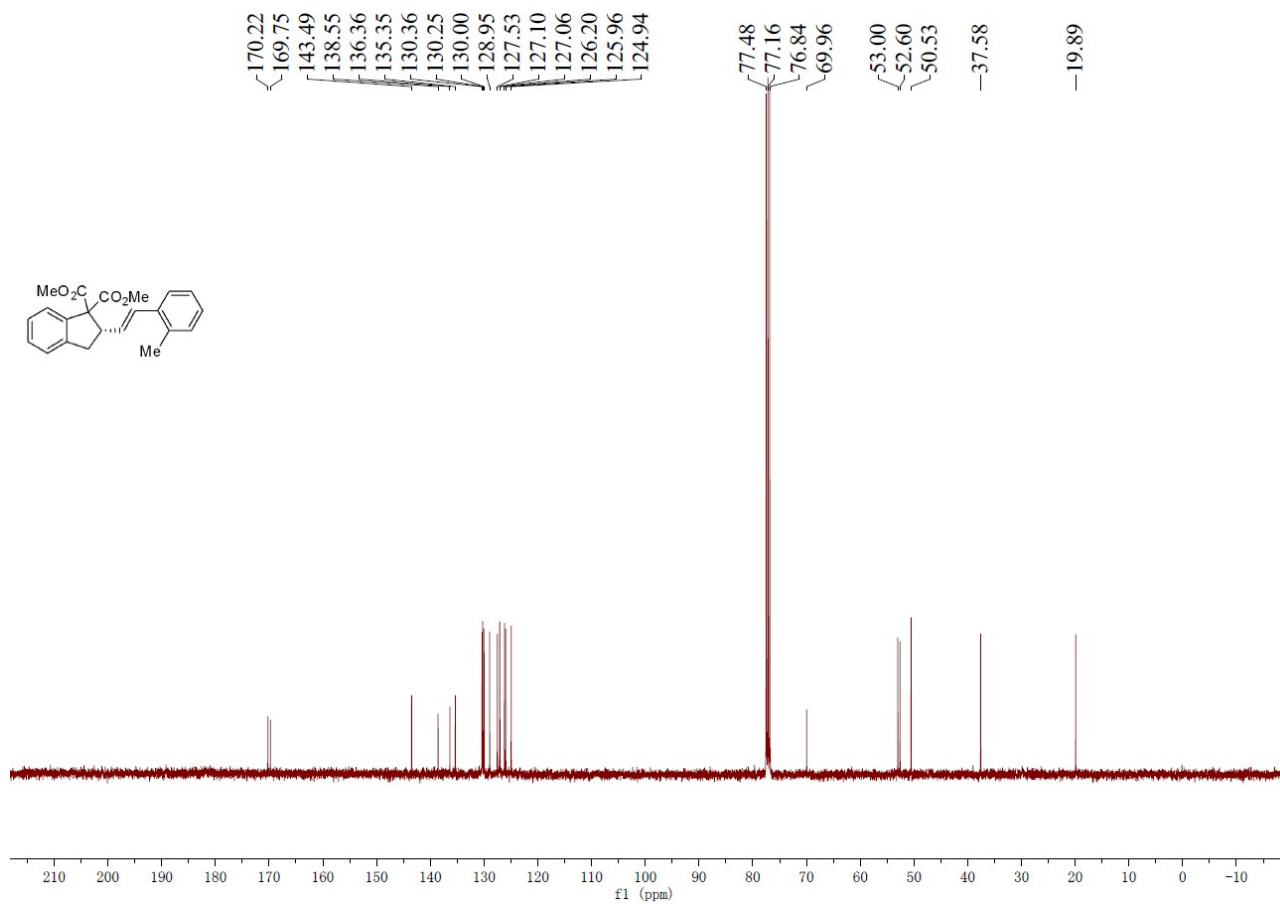
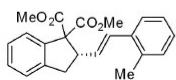
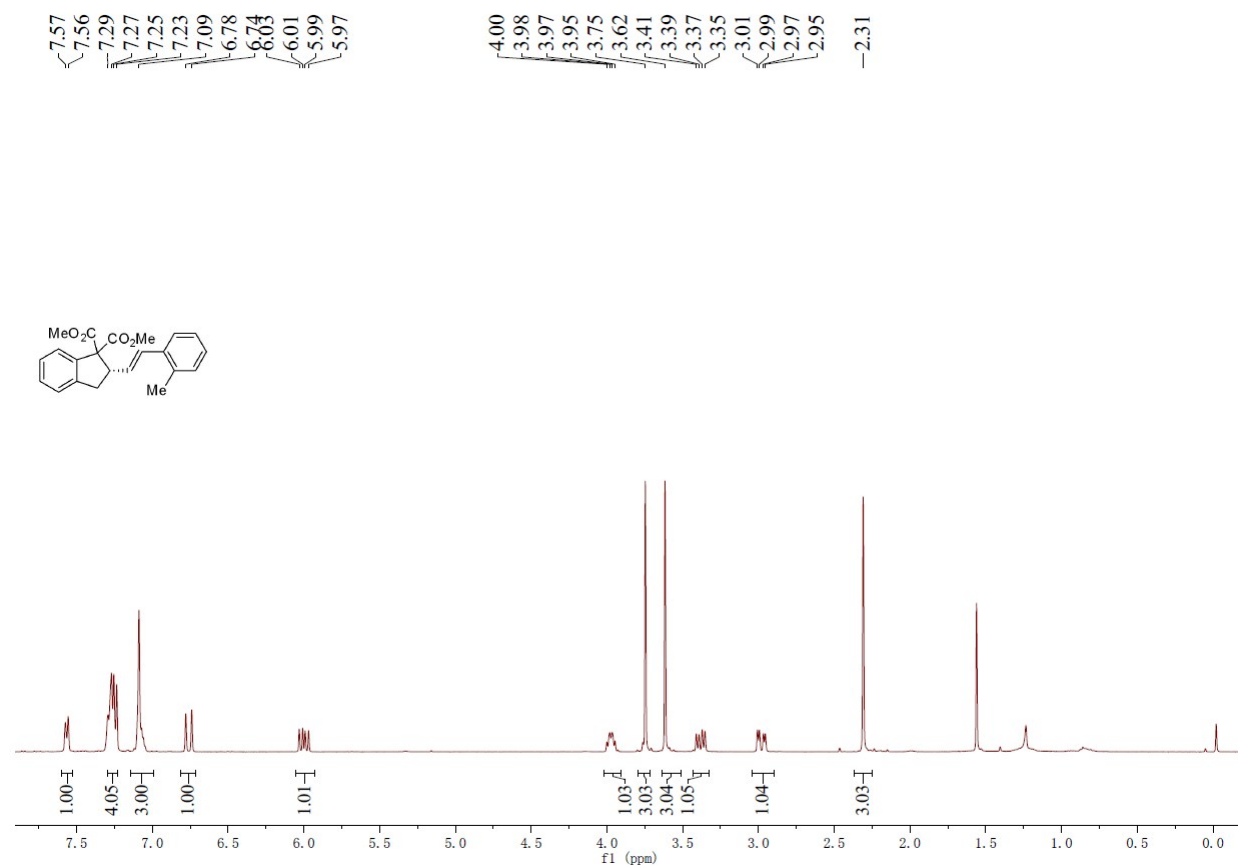
Dibenzyl (S,E)-2-styryl-2,3-dihydro-1H-indene-1,1-dicarboxylate (3la)



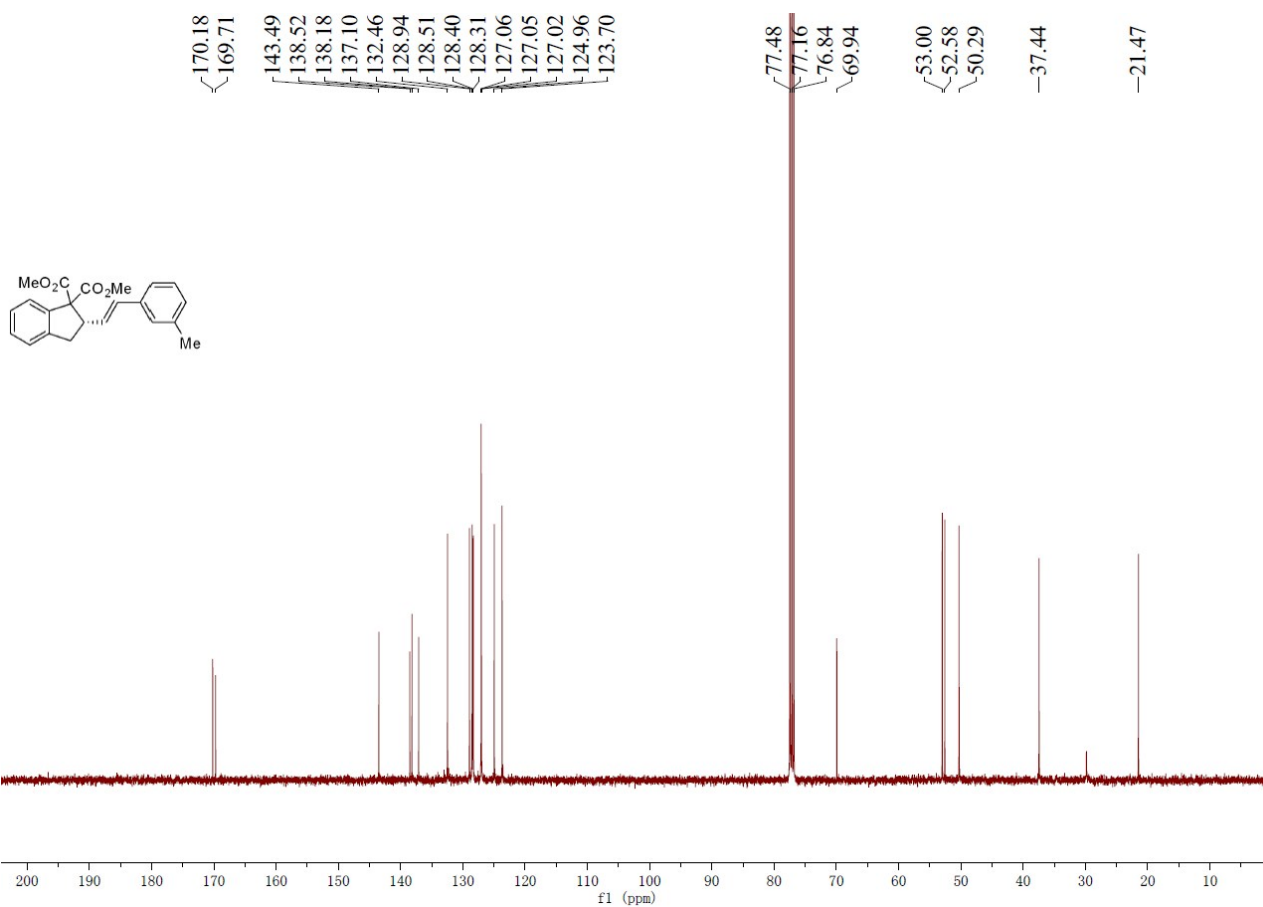
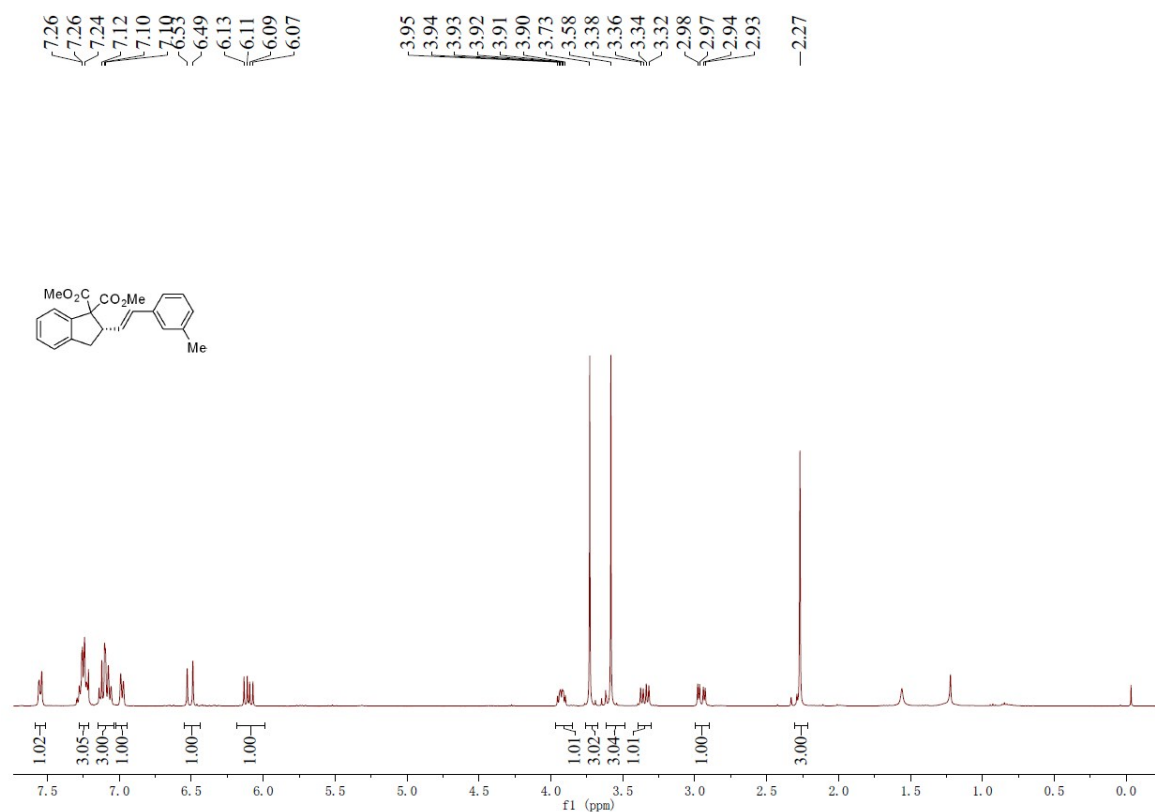
Dimethyl (*S,E*)-5-styryl-5,6-dihydro-4*H*-cyclopenta[*b*]thiophene-4,4-dicarboxylate (3ma)



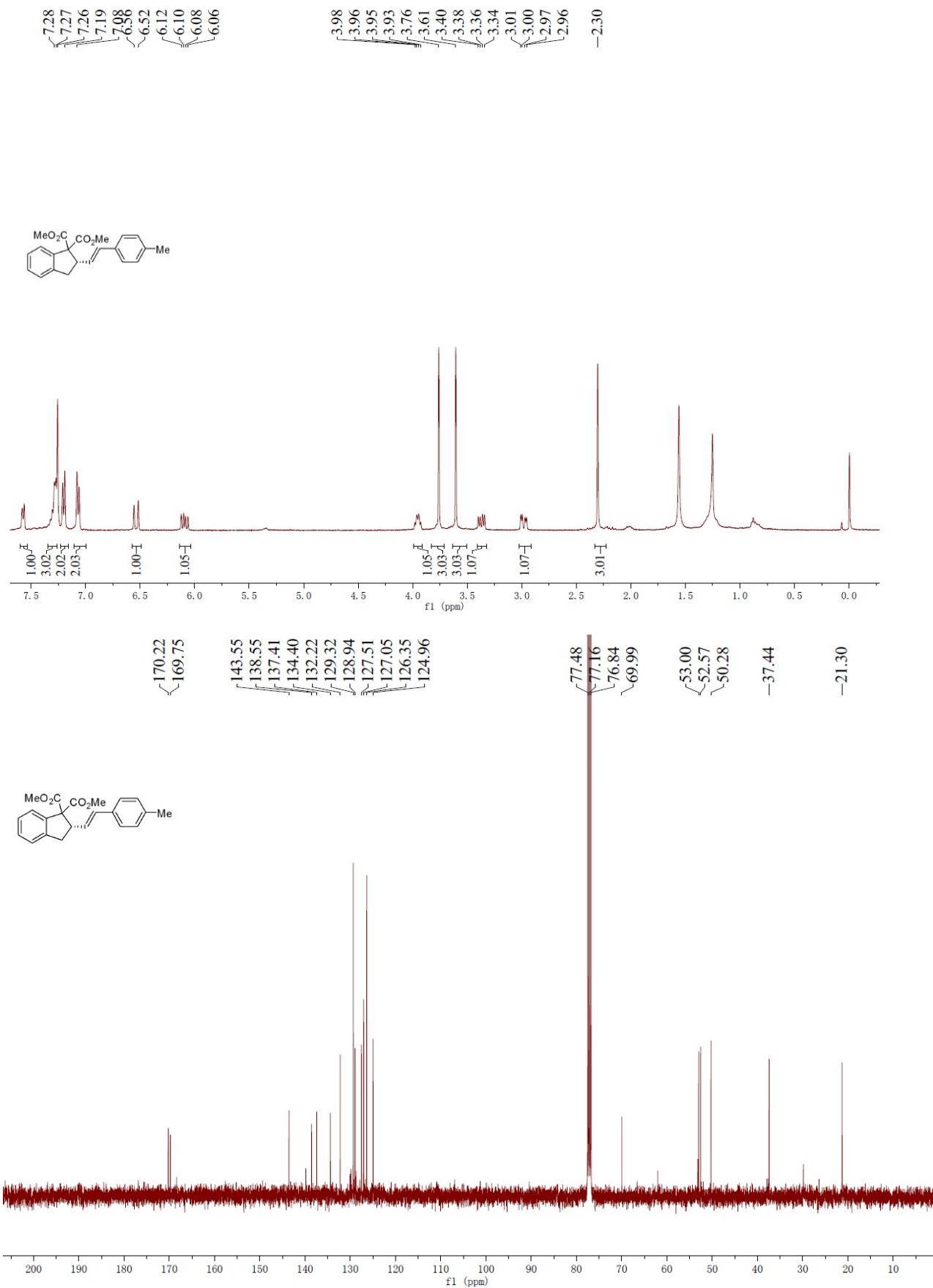
Dimethyl (*S,E*)-2-(2-methylstyryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (**3ab**)



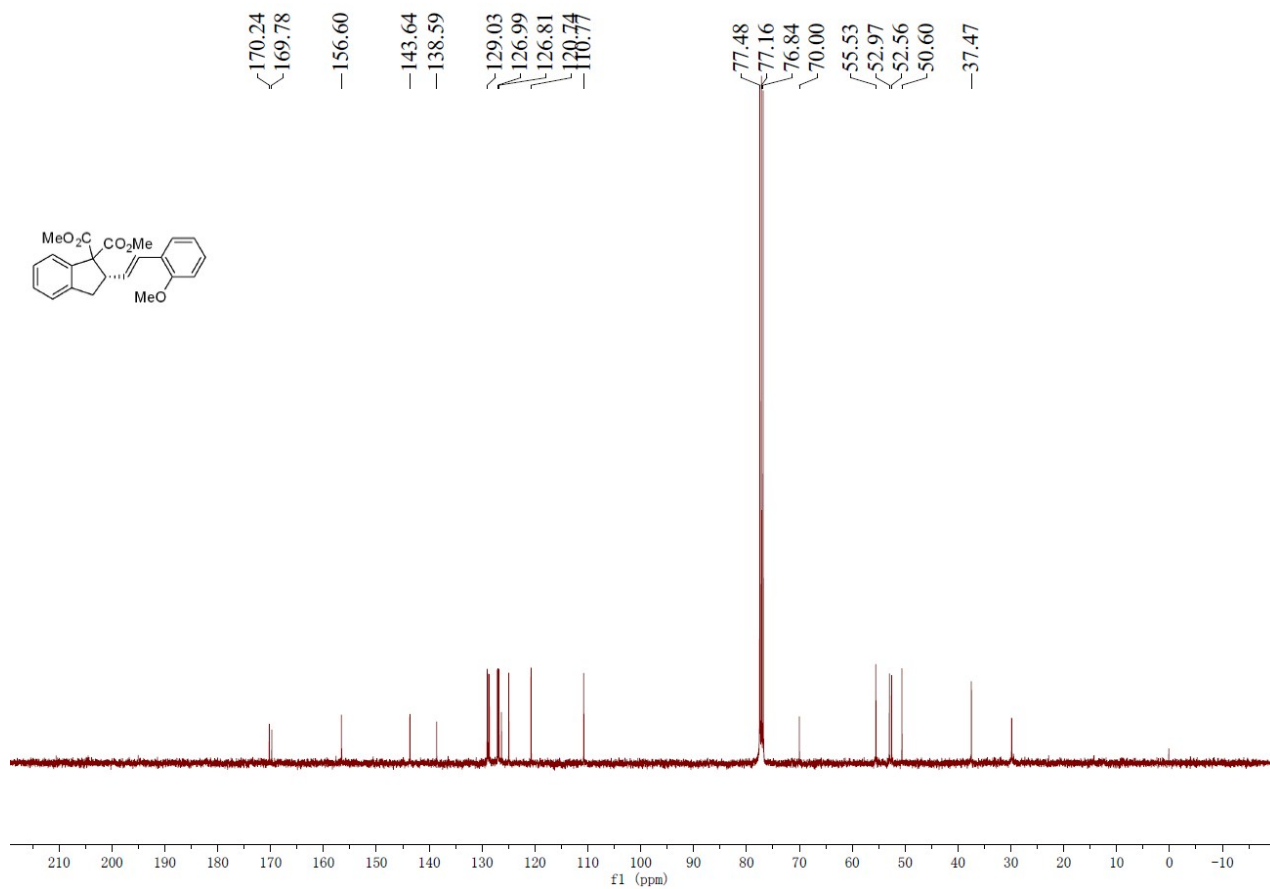
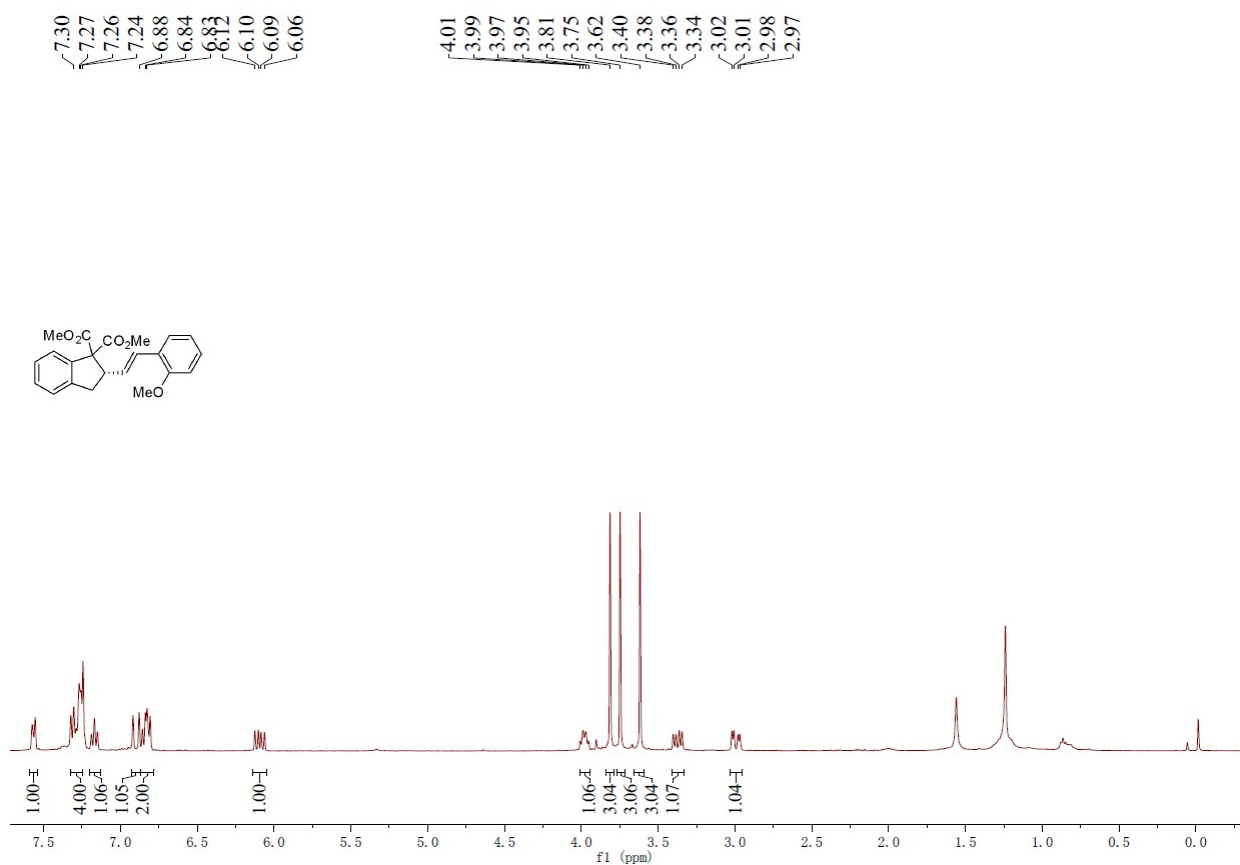
Dimethyl (*S,E*)-2-(3-methylstyryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ac)



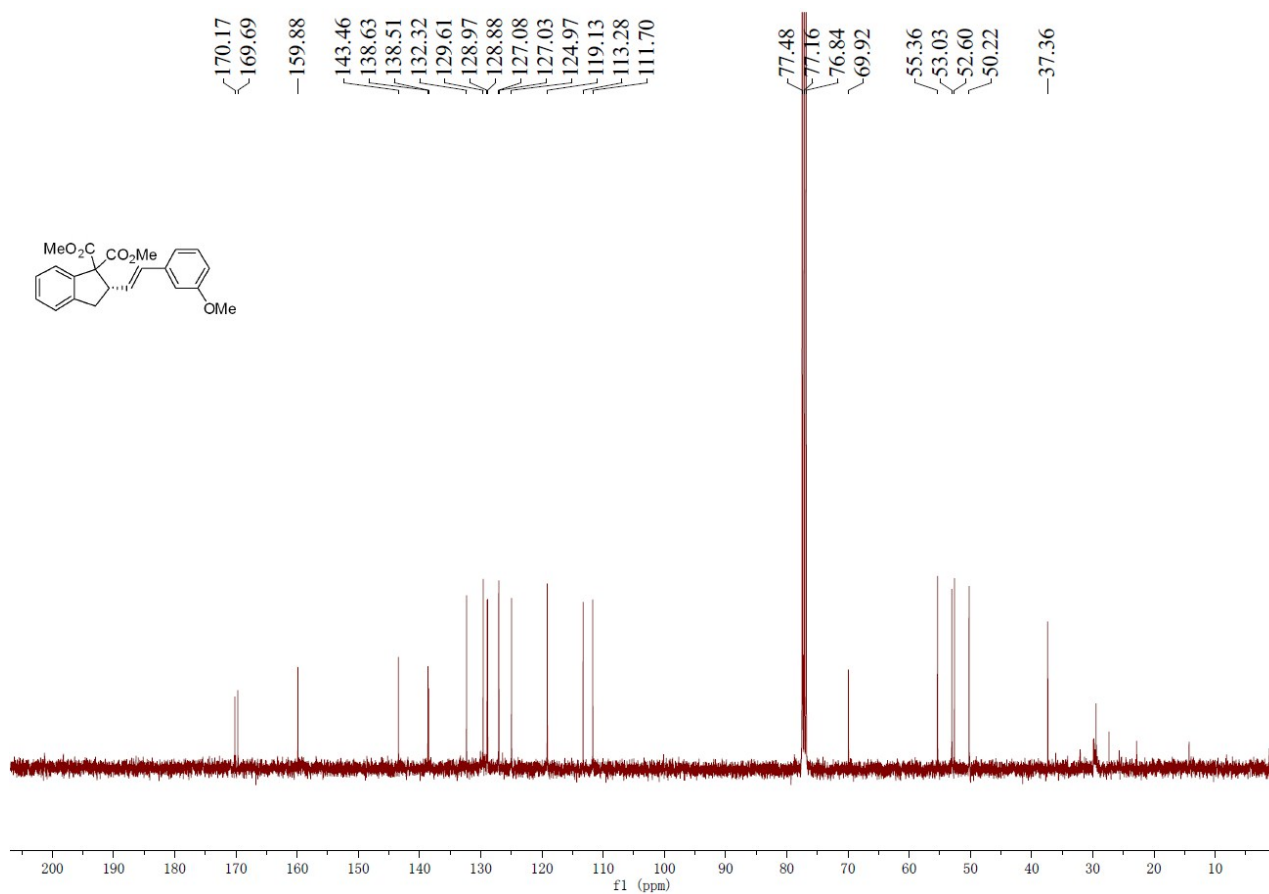
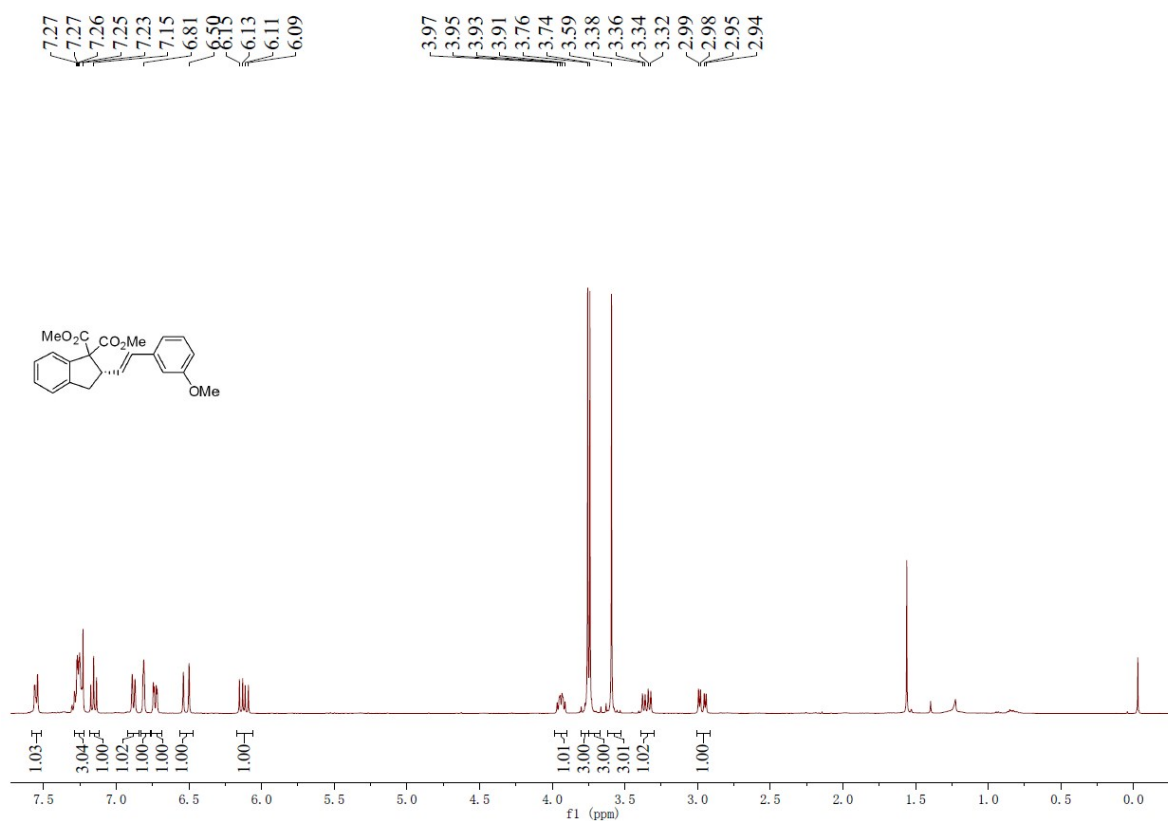
Dimethyl (*S,E*)-2-(4-methylstyryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (**3ad**)



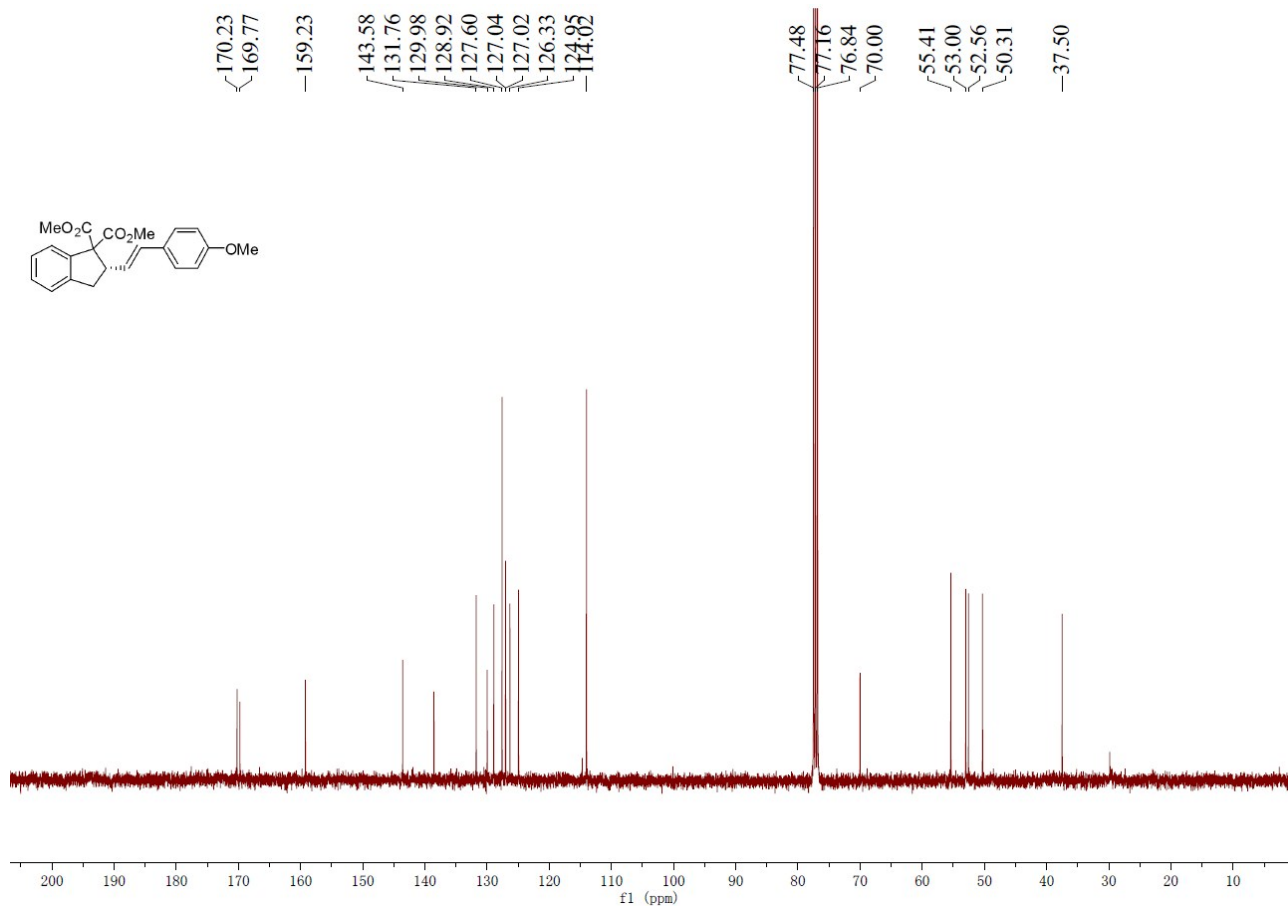
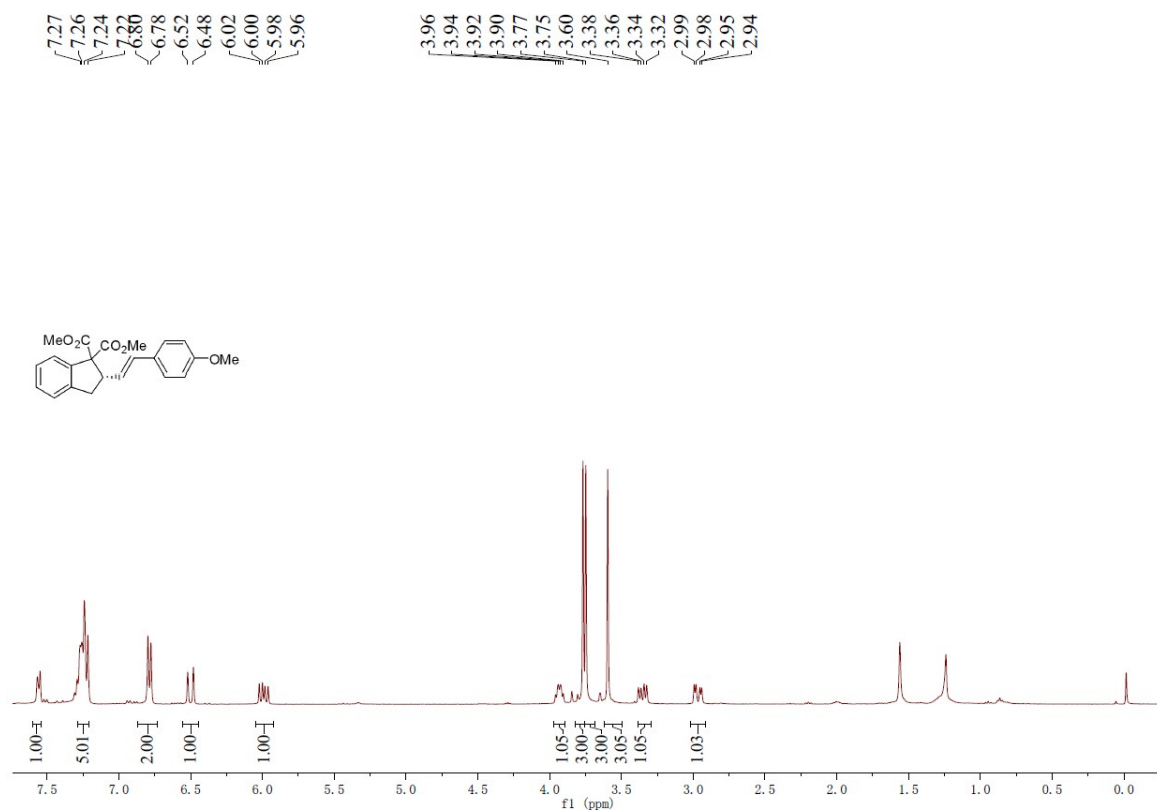
Dimethyl (*S,E*)-2-(2-methoxystyryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (**3ae**)



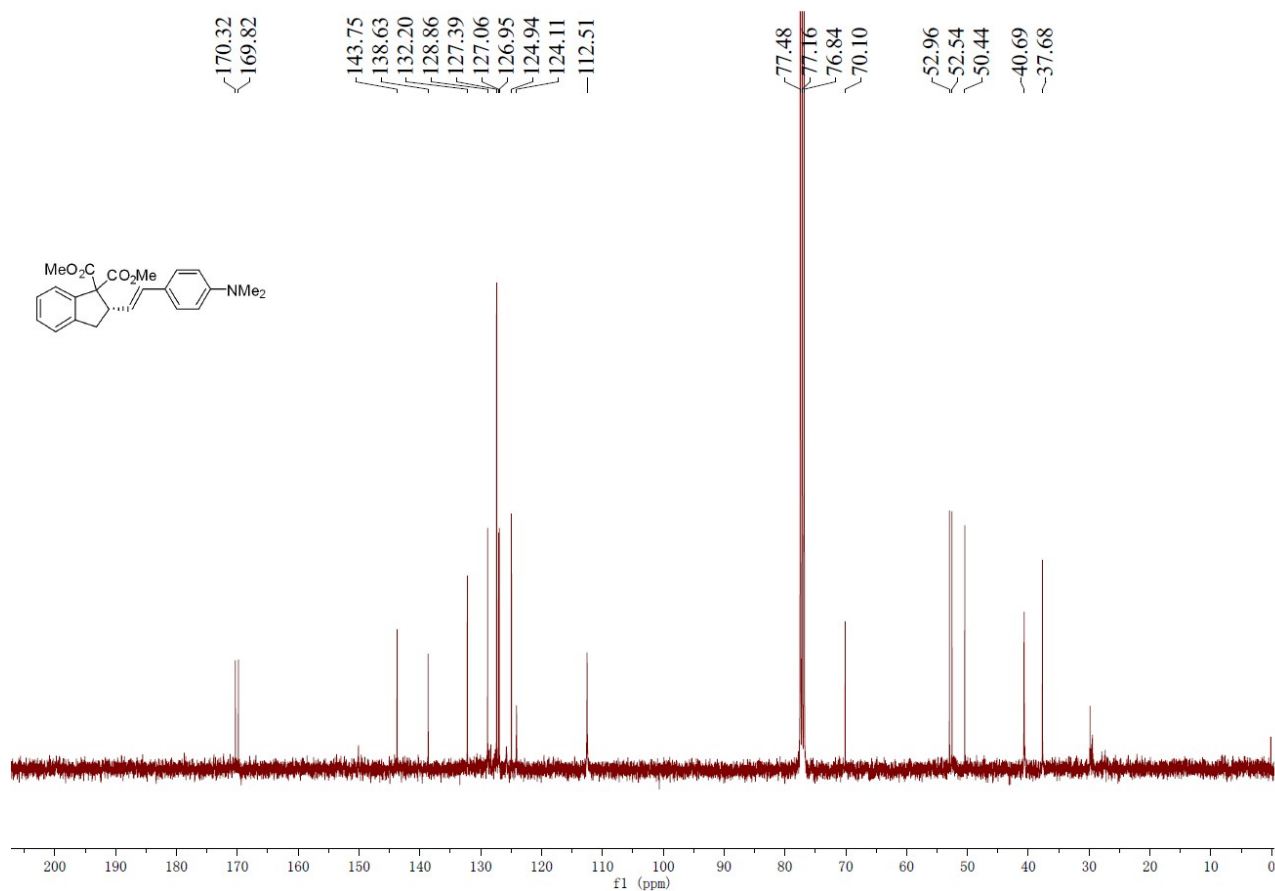
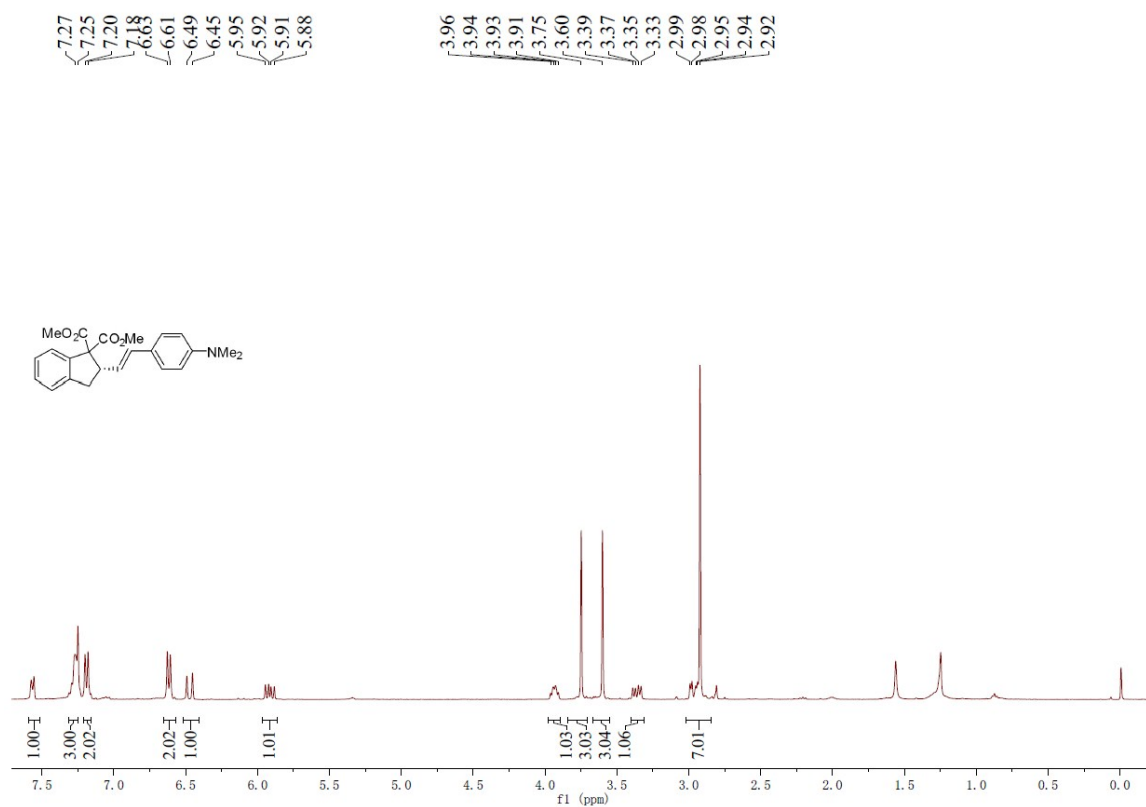
Dimethyl (*S,E*)-2-(3-methoxystyryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3af)



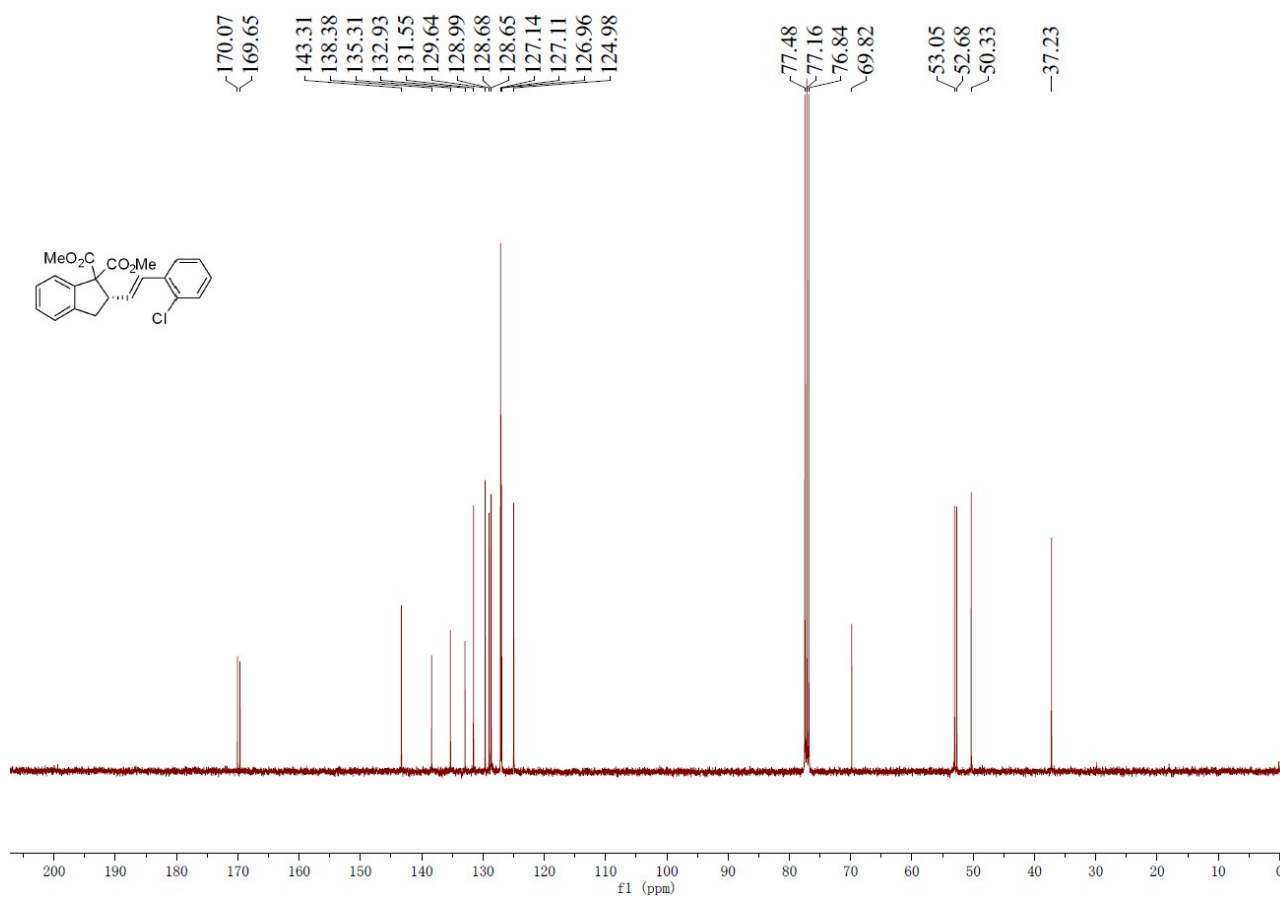
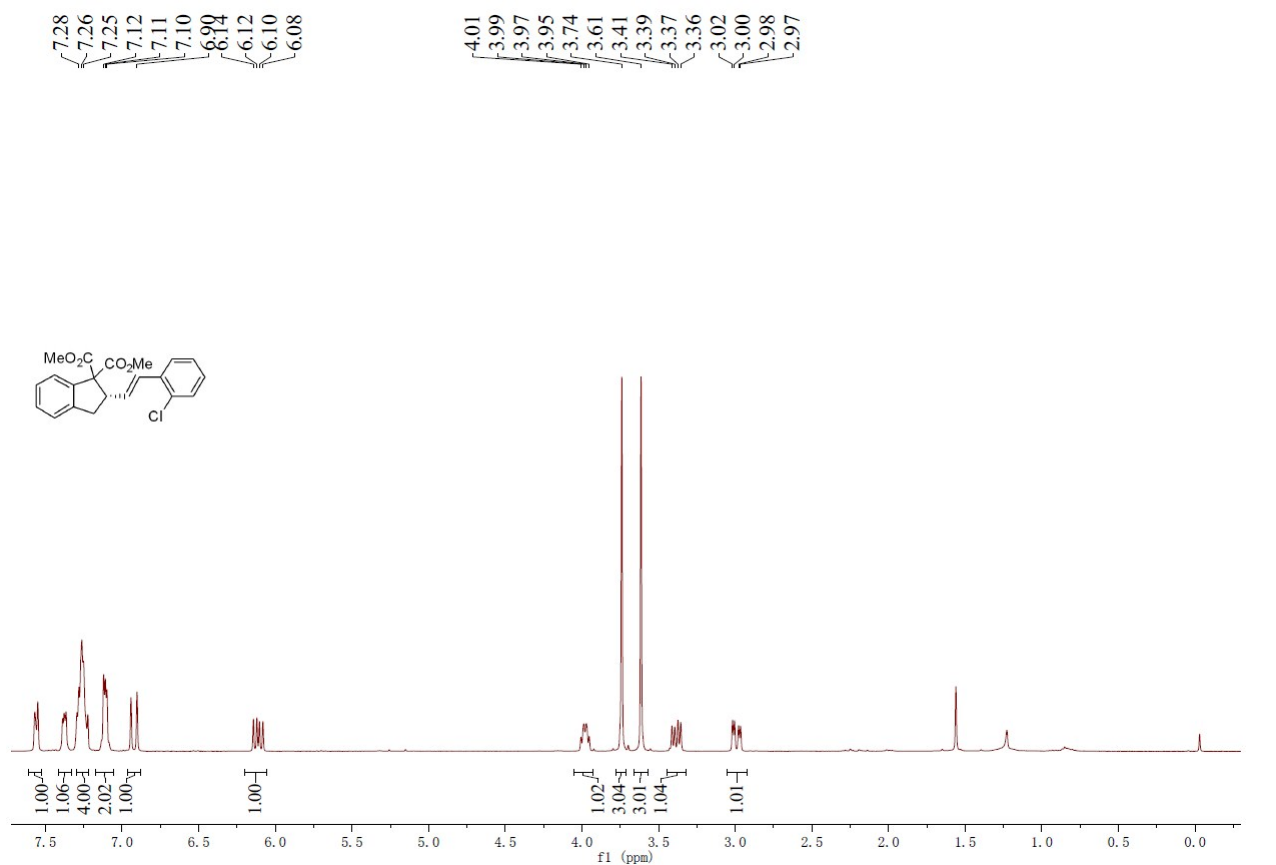
Dimethyl (*S,E*)-2-(4-methoxystyryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ag)



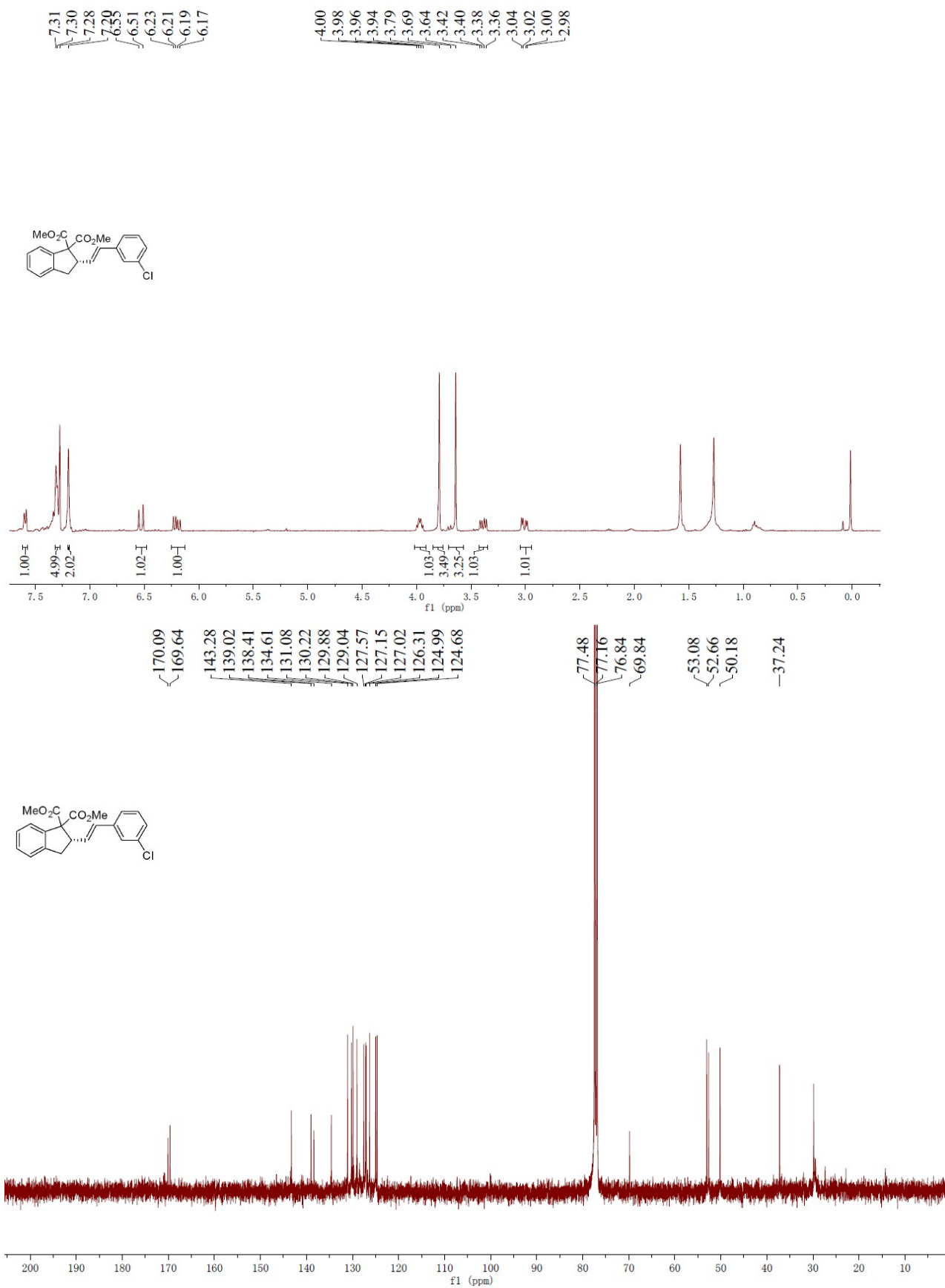
Dimethyl (*S,E*)-2-(4-(dimethylamino)styryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ah)



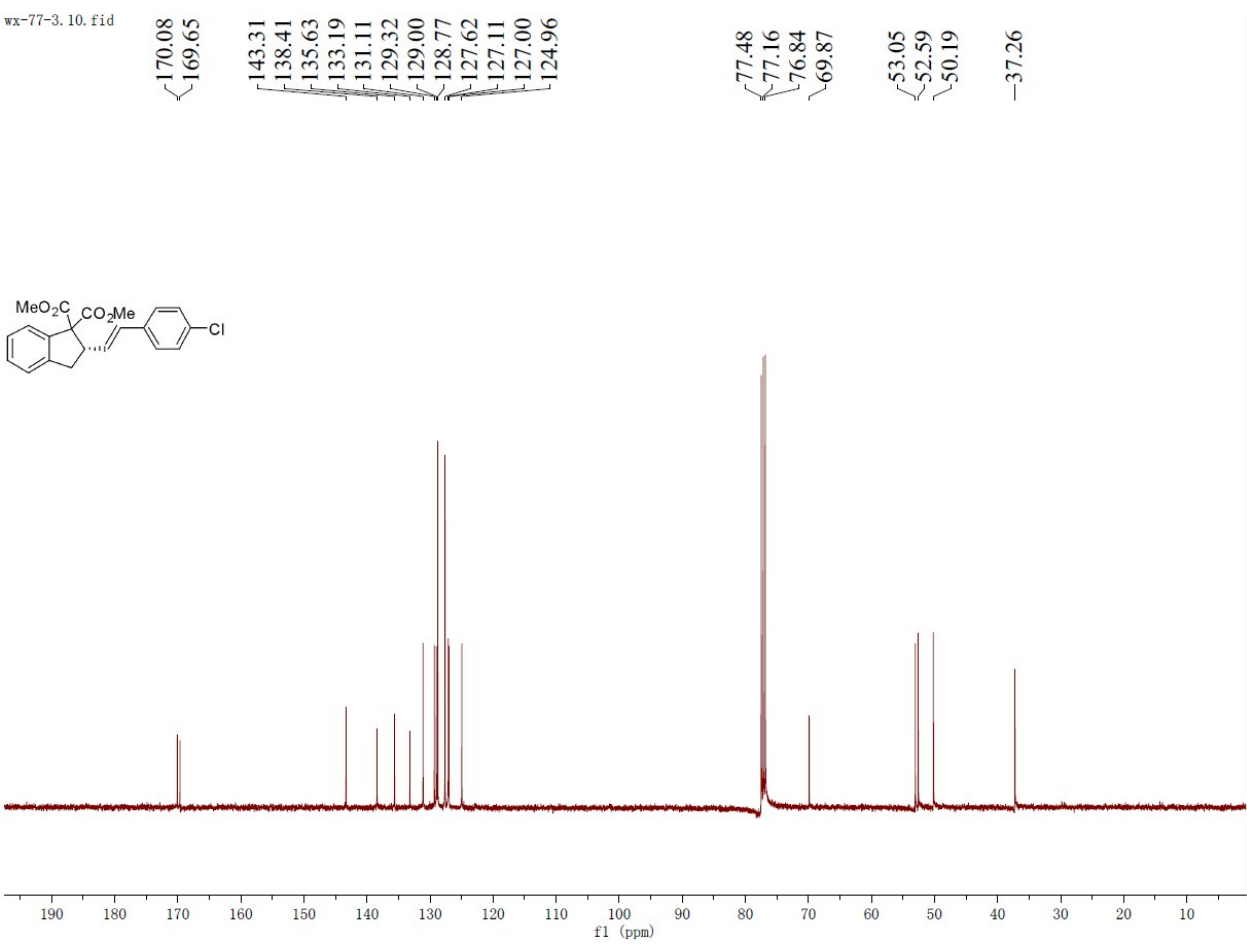
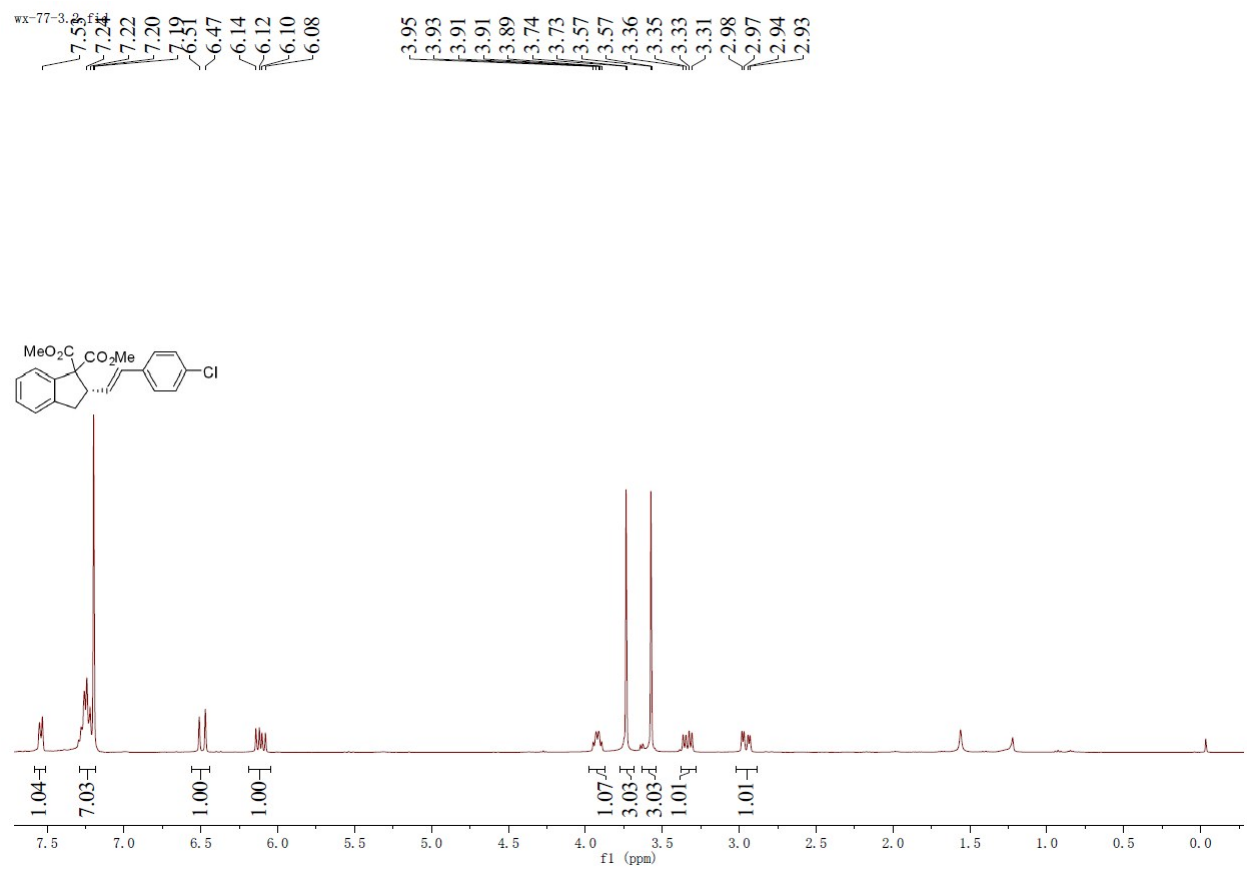
Dimethyl (*S,E*)-2-(2-chlorostyryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ai)



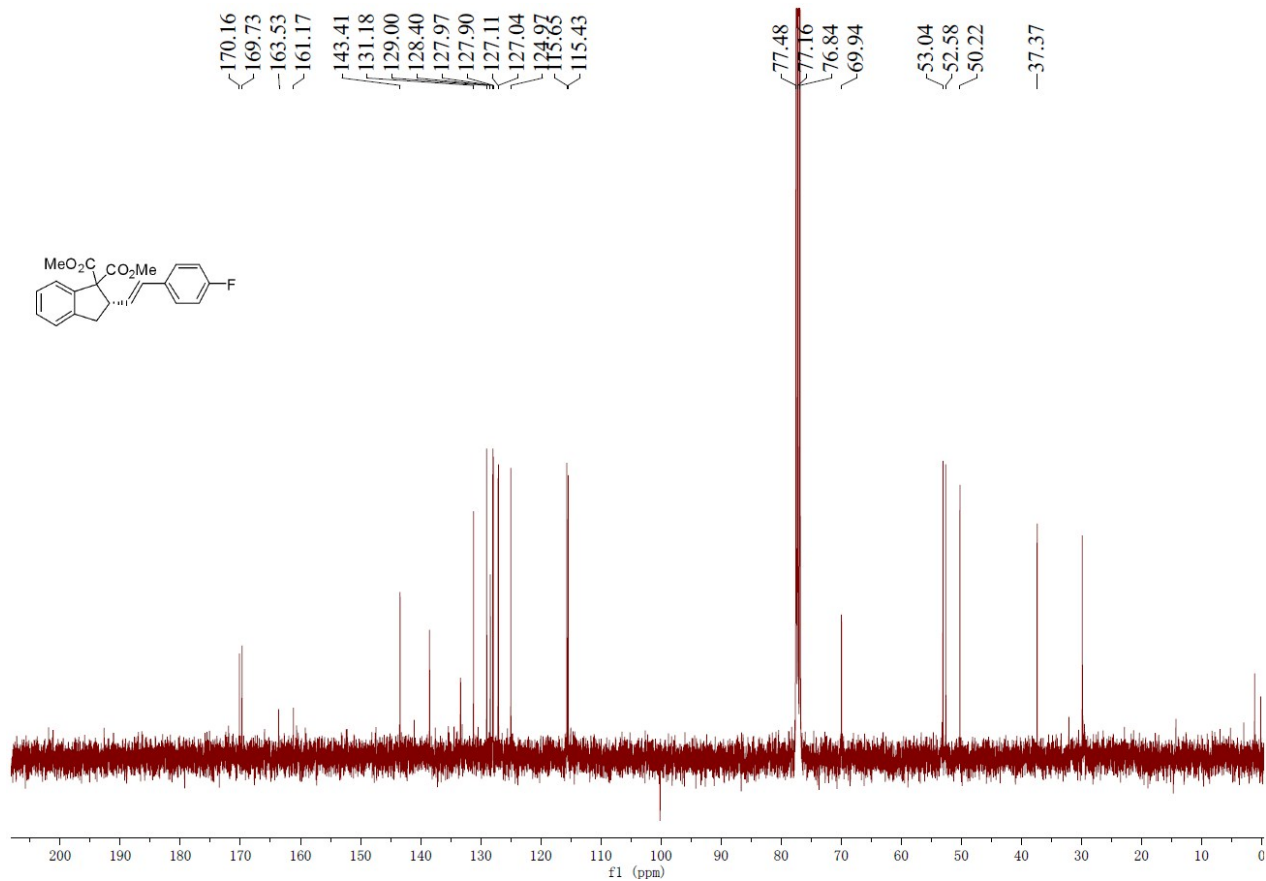
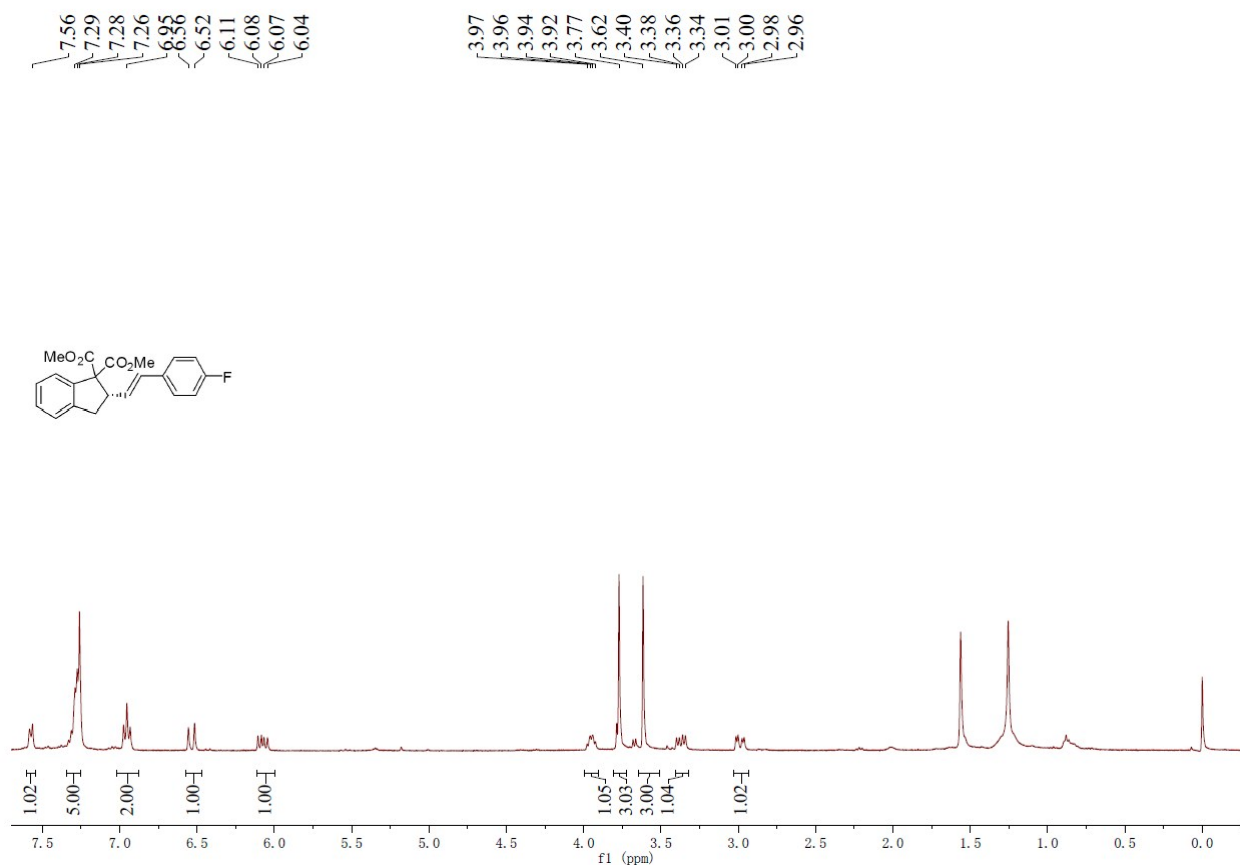
Dimethyl (*S,E*)-2-(3-chlorostyryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3aj)



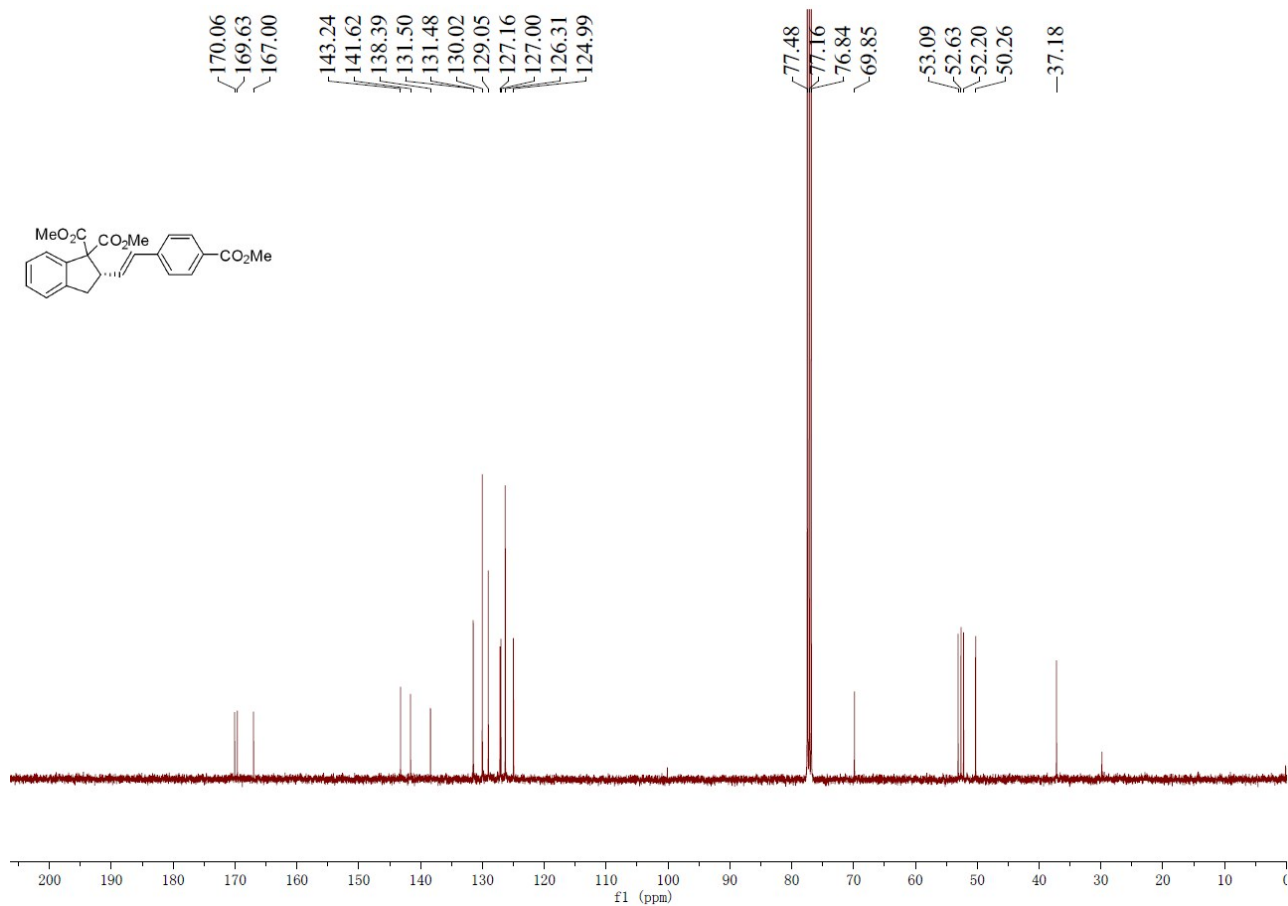
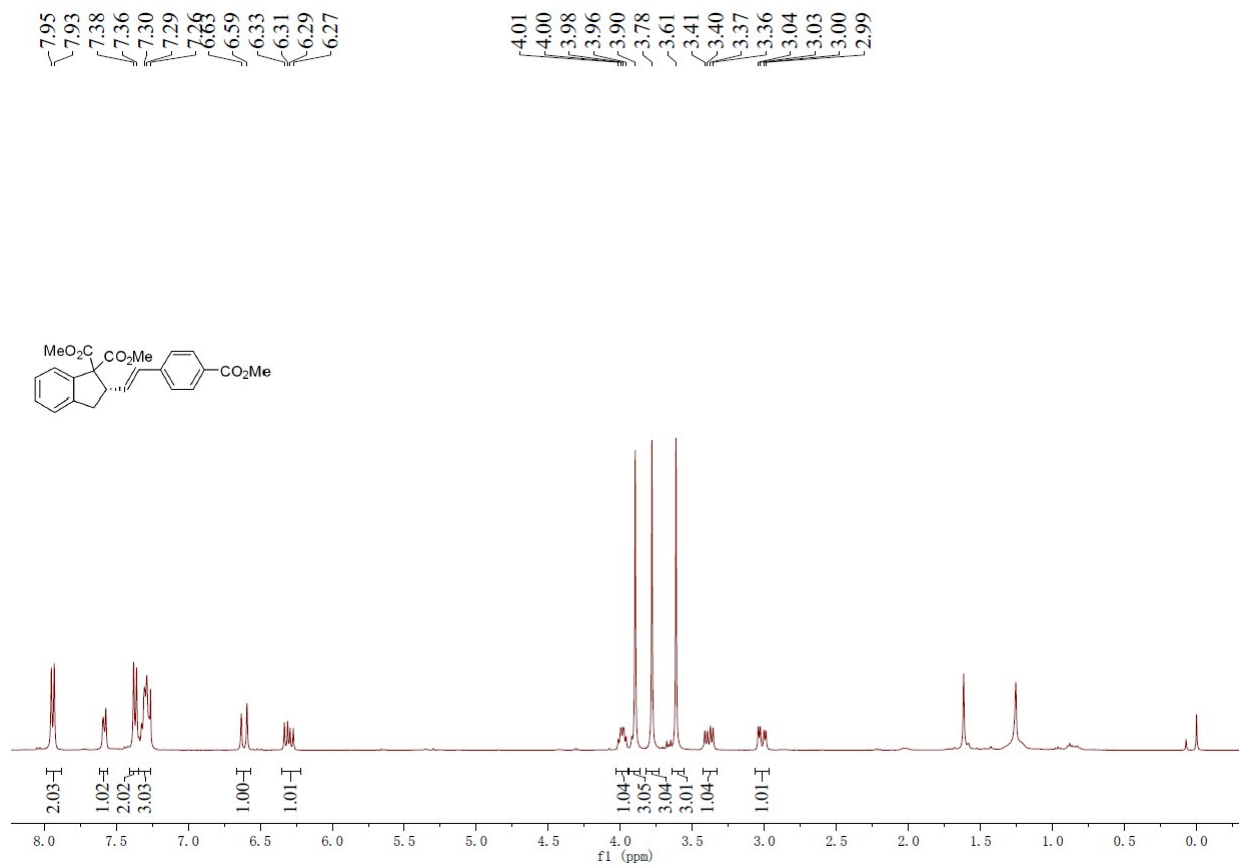
Dimethyl (S,E)-2-(4-chlorostyryl)-2,3-dihydro-1H-indene-1,1-dicarboxylate (3ak)



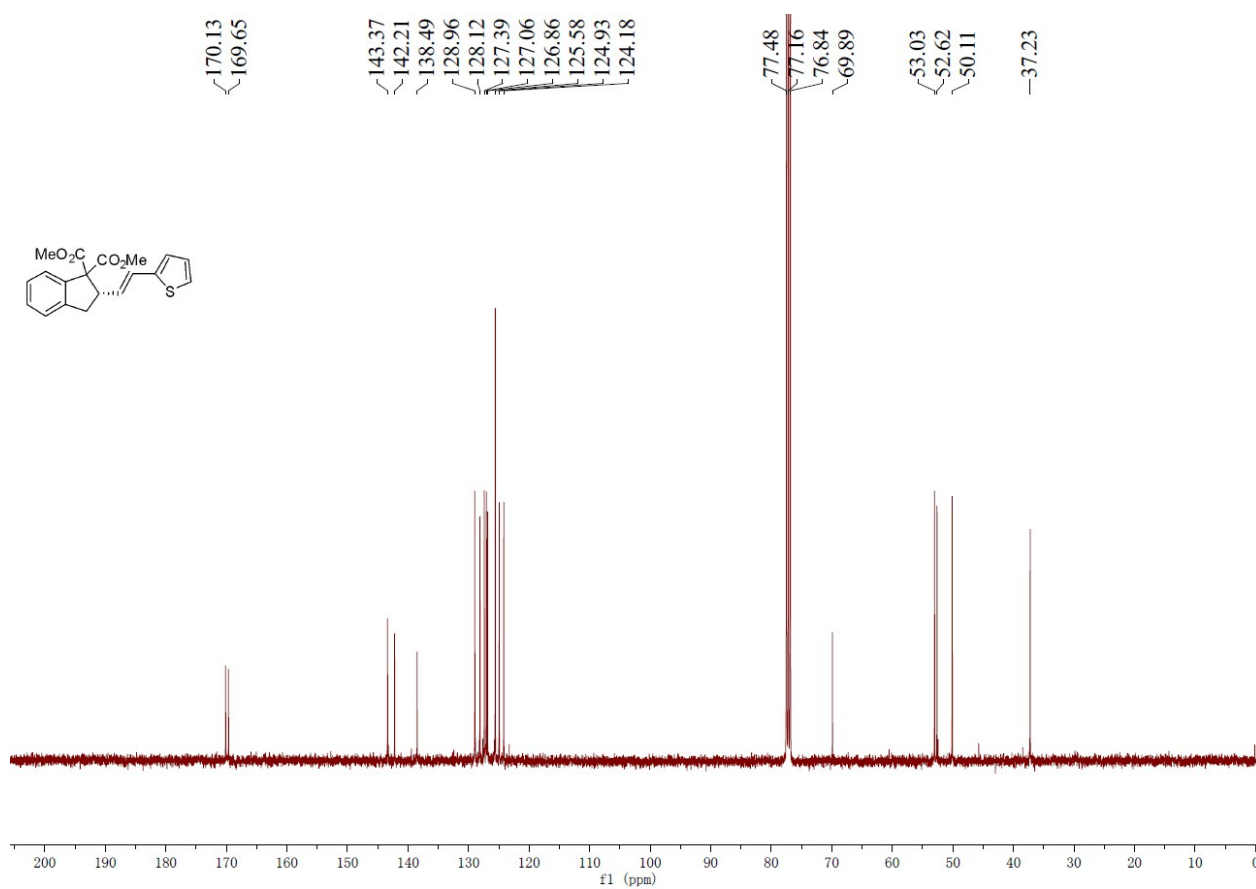
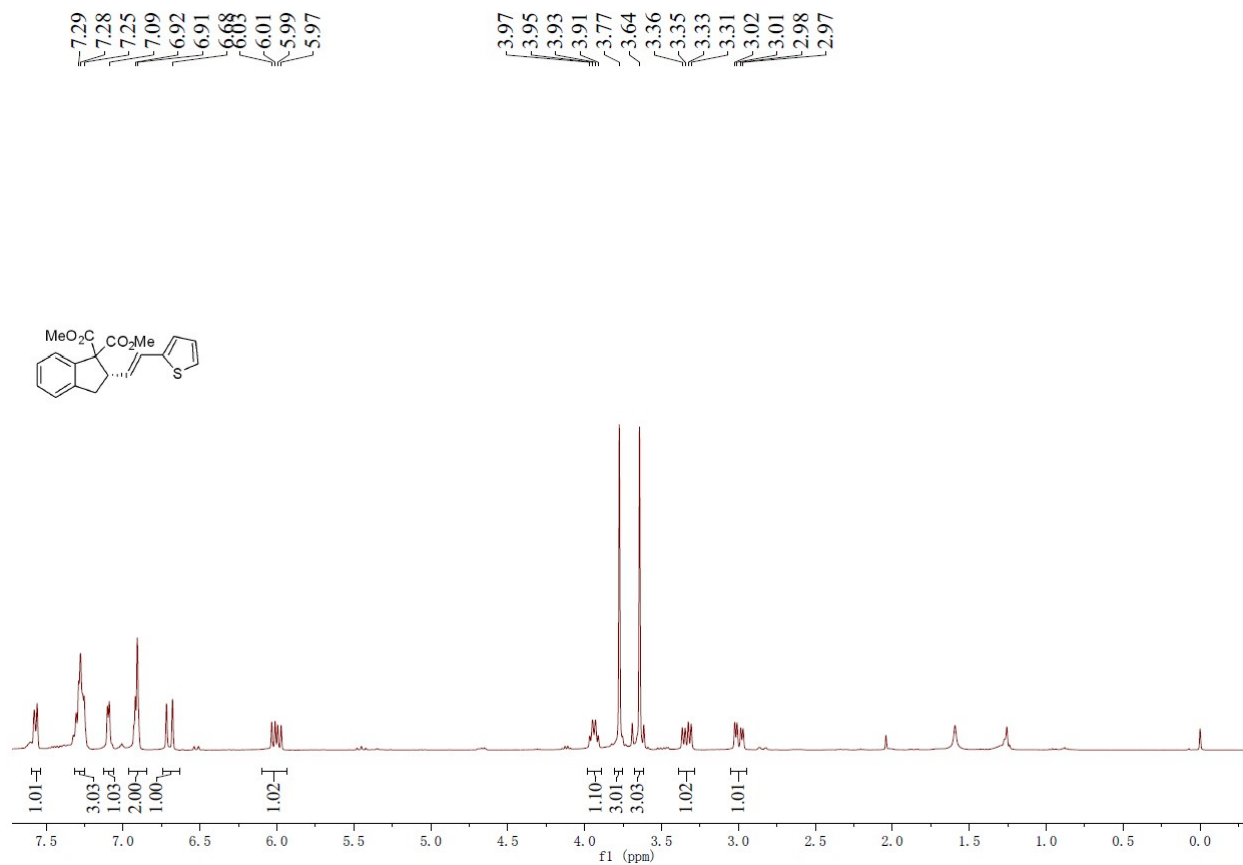
Dimethyl (*S,E*)-2-(4-fluorostyryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3a)



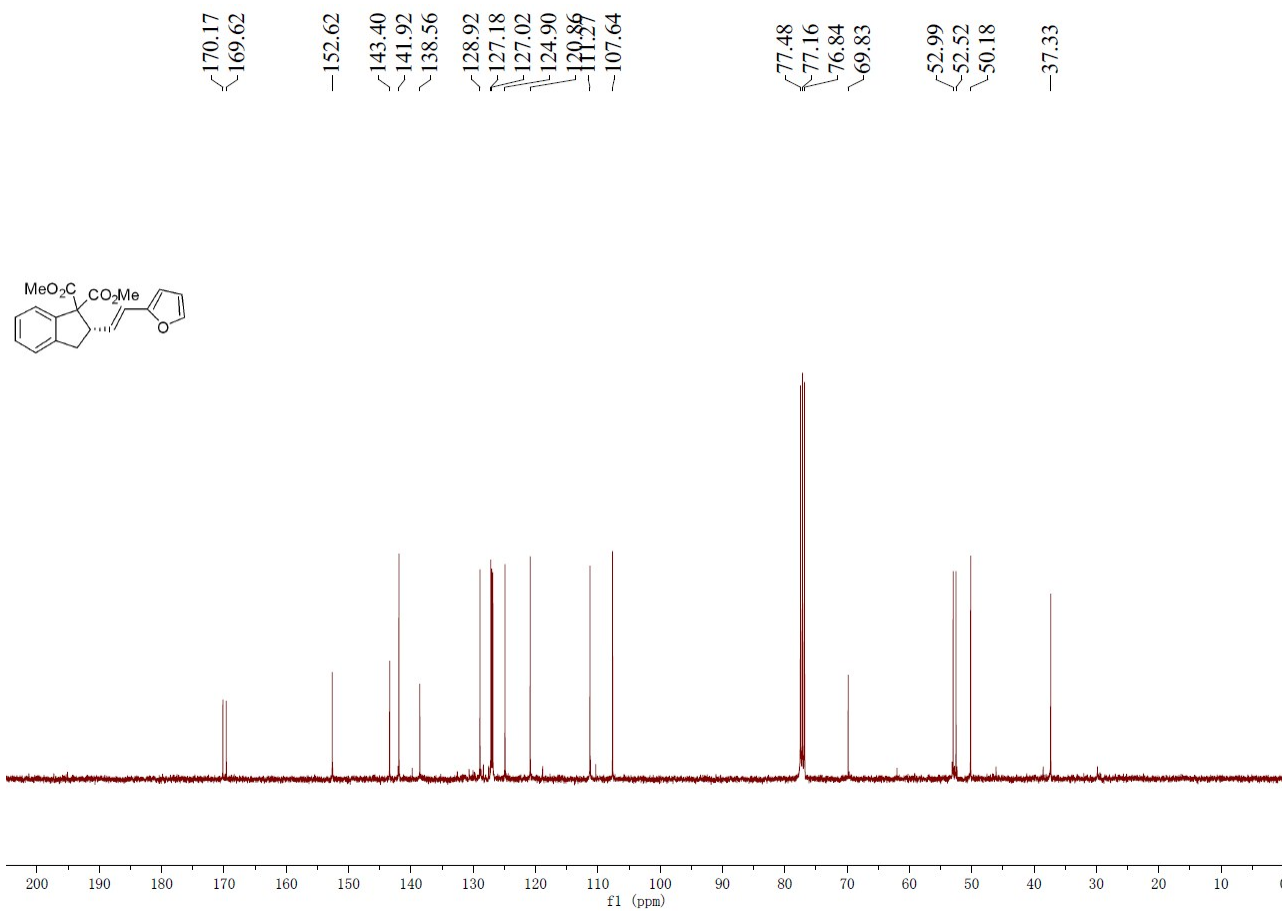
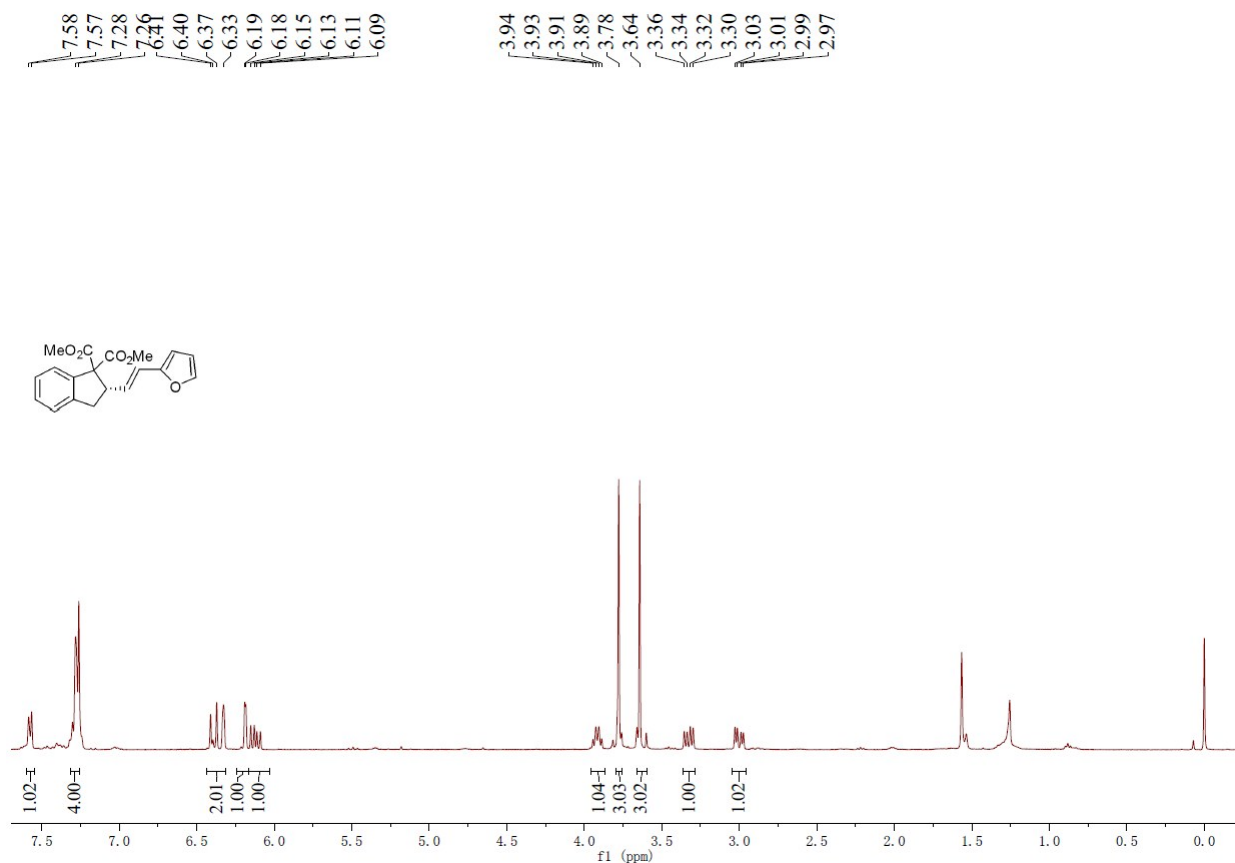
Dimethyl (*S,E*)-2-(4-(methoxycarbonyl)styryl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3am)



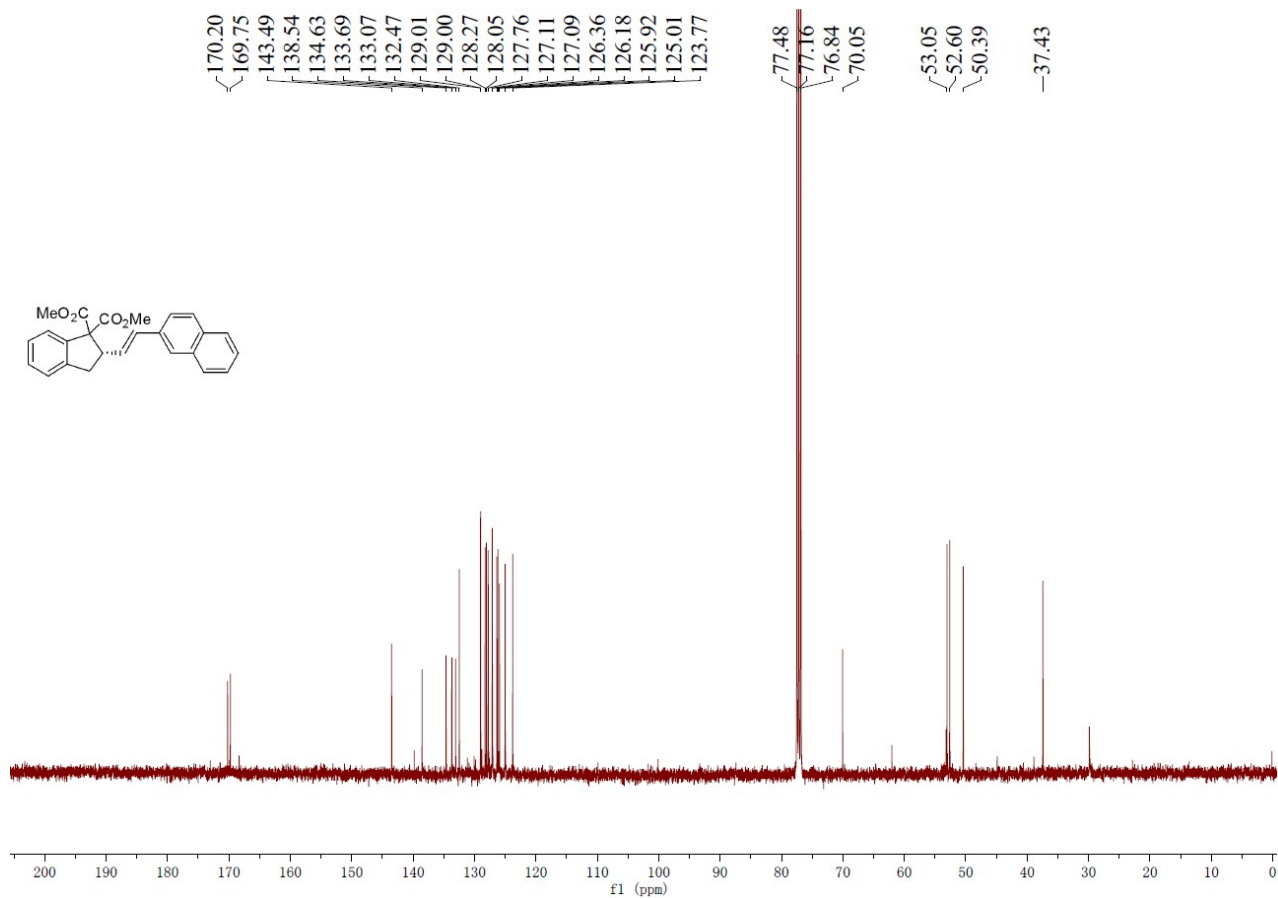
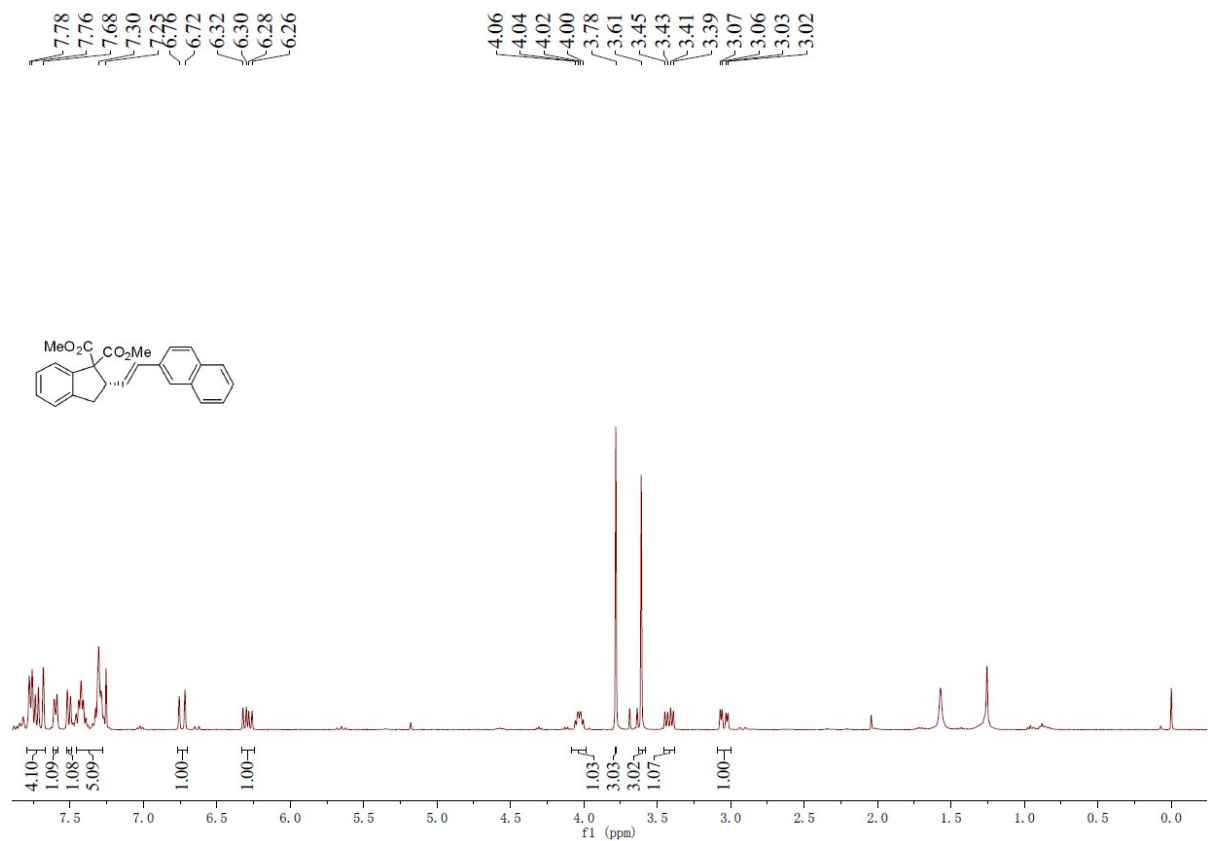
Dimethyl (*S,E*)-2-(2-(thiophen-2-yl)vinyl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3an)



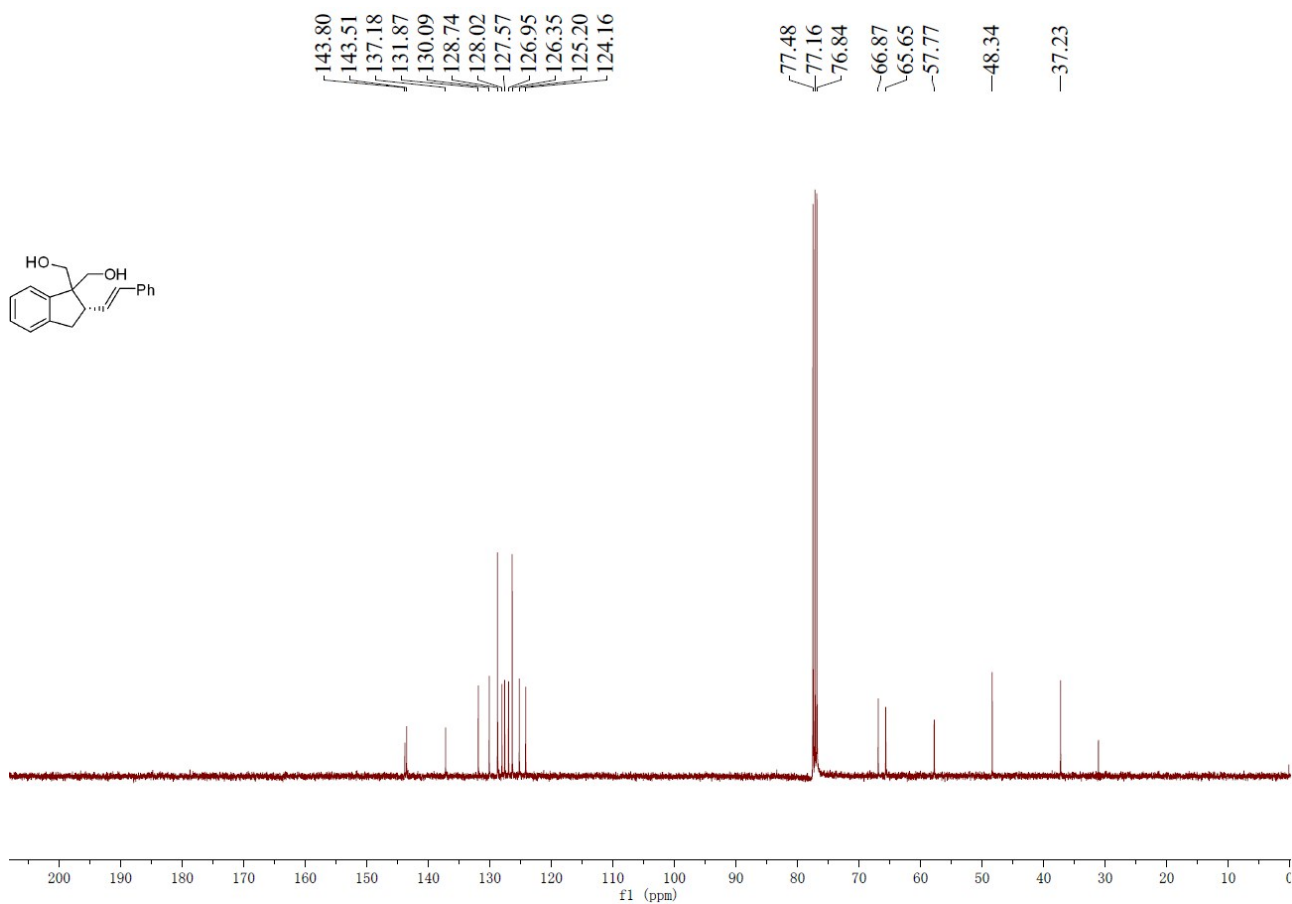
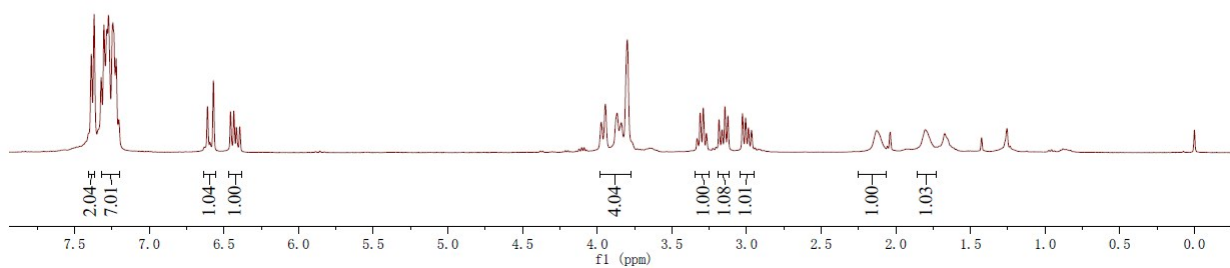
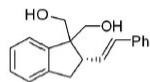
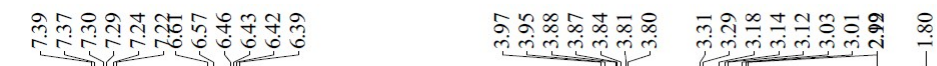
Dimethyl (*S,E*)-2-(2-(furan-2-yl)vinyl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylat (3ao)



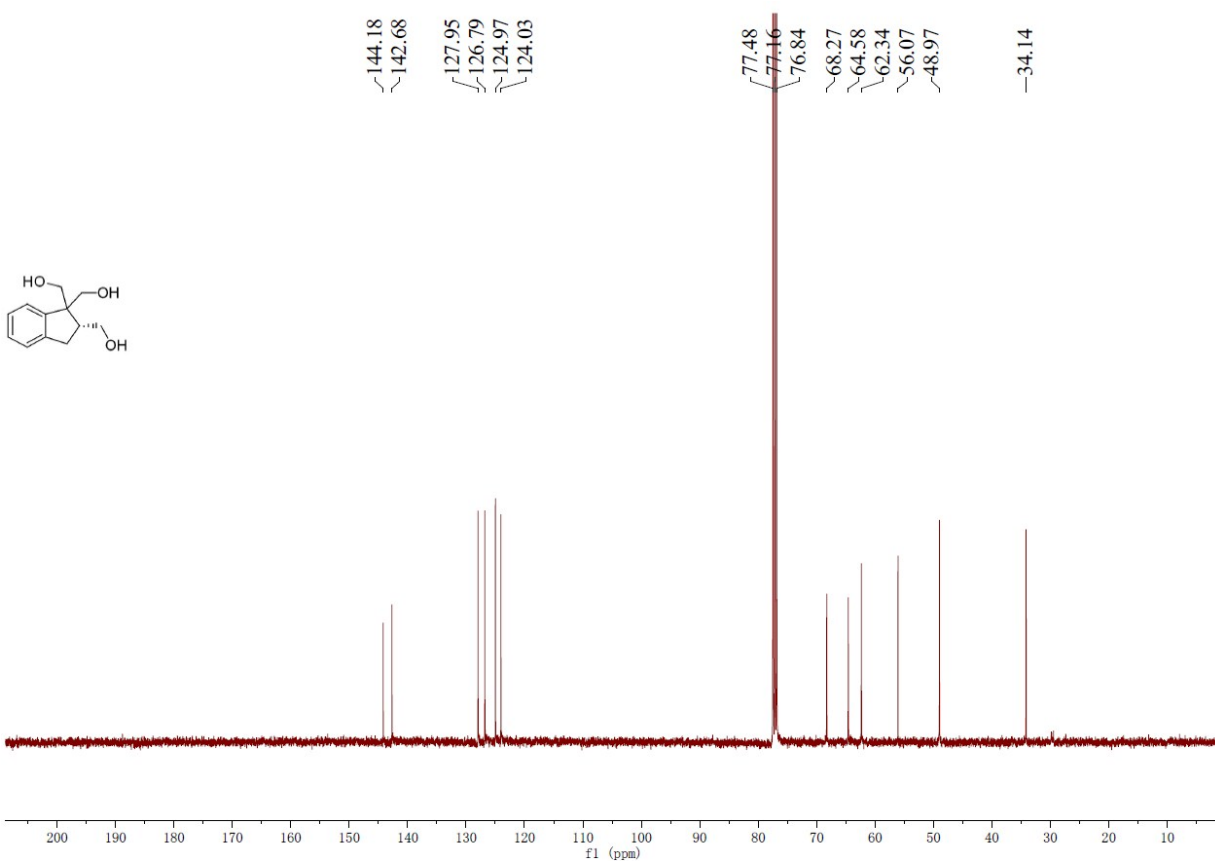
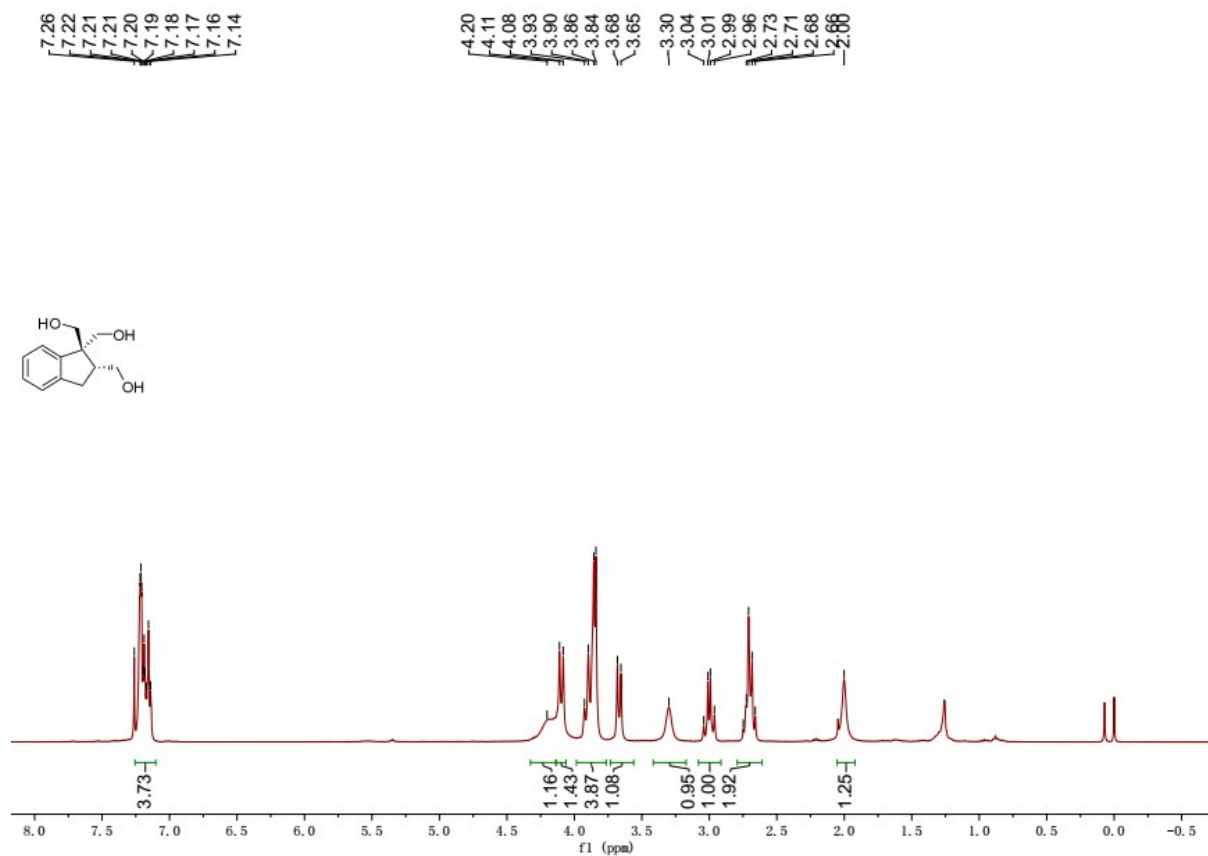
Dimethyl (*S,E*)-2-(2-(naphthalen-2-yl)vinyl)-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (*Z*) (3ap)



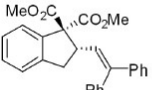
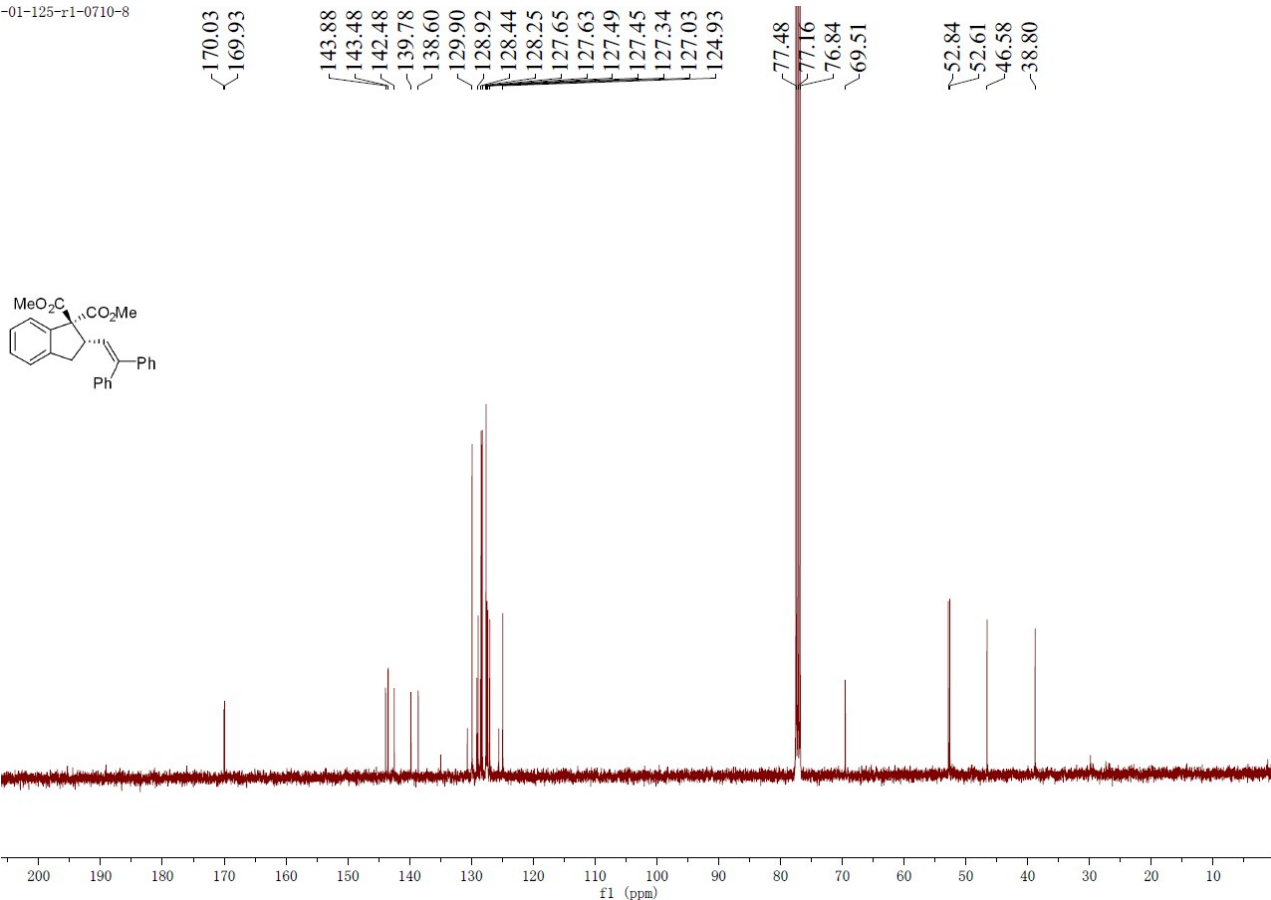
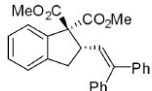
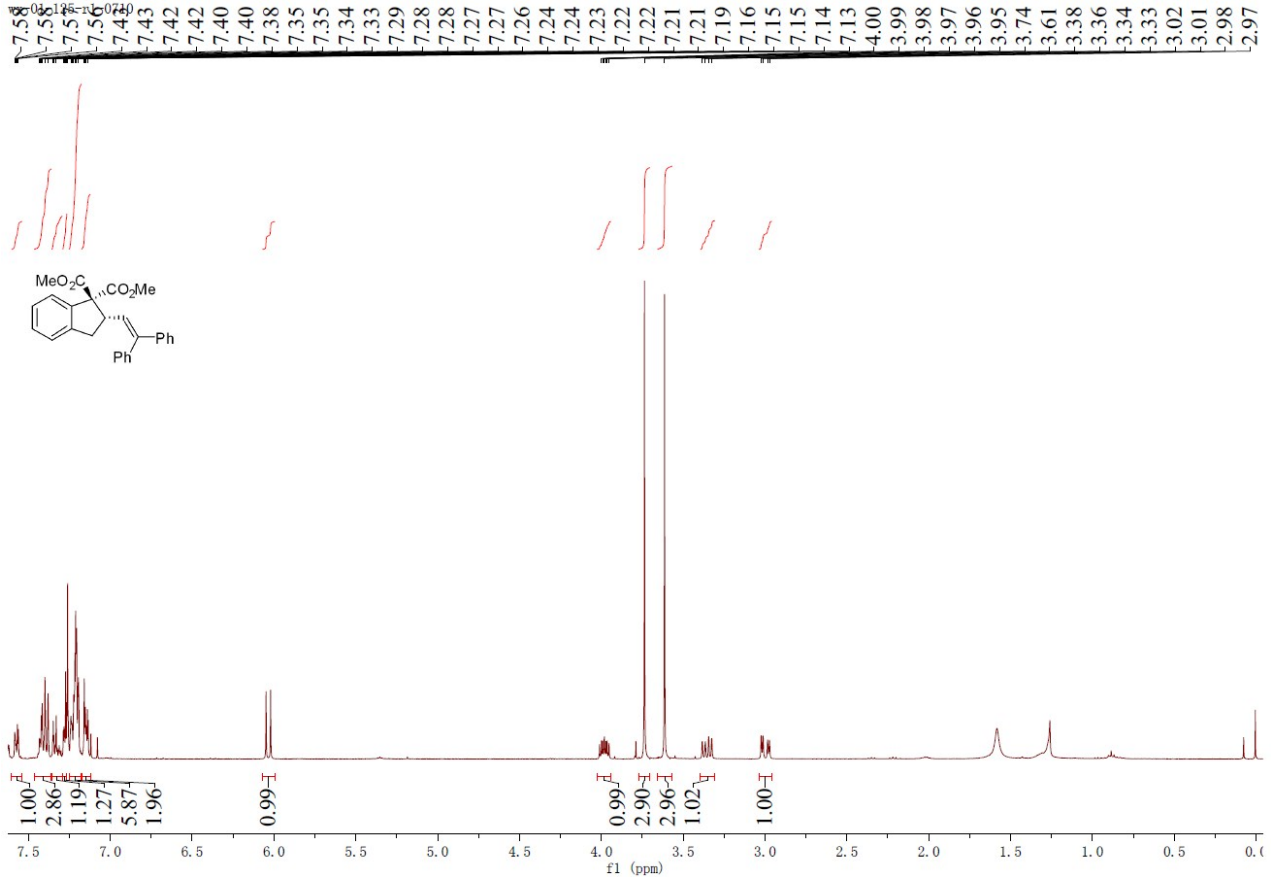
(*S,E*)-(2-styryl-2,3-dihydro-1*H*-indene-1,1-diyl)dimethanol (4)



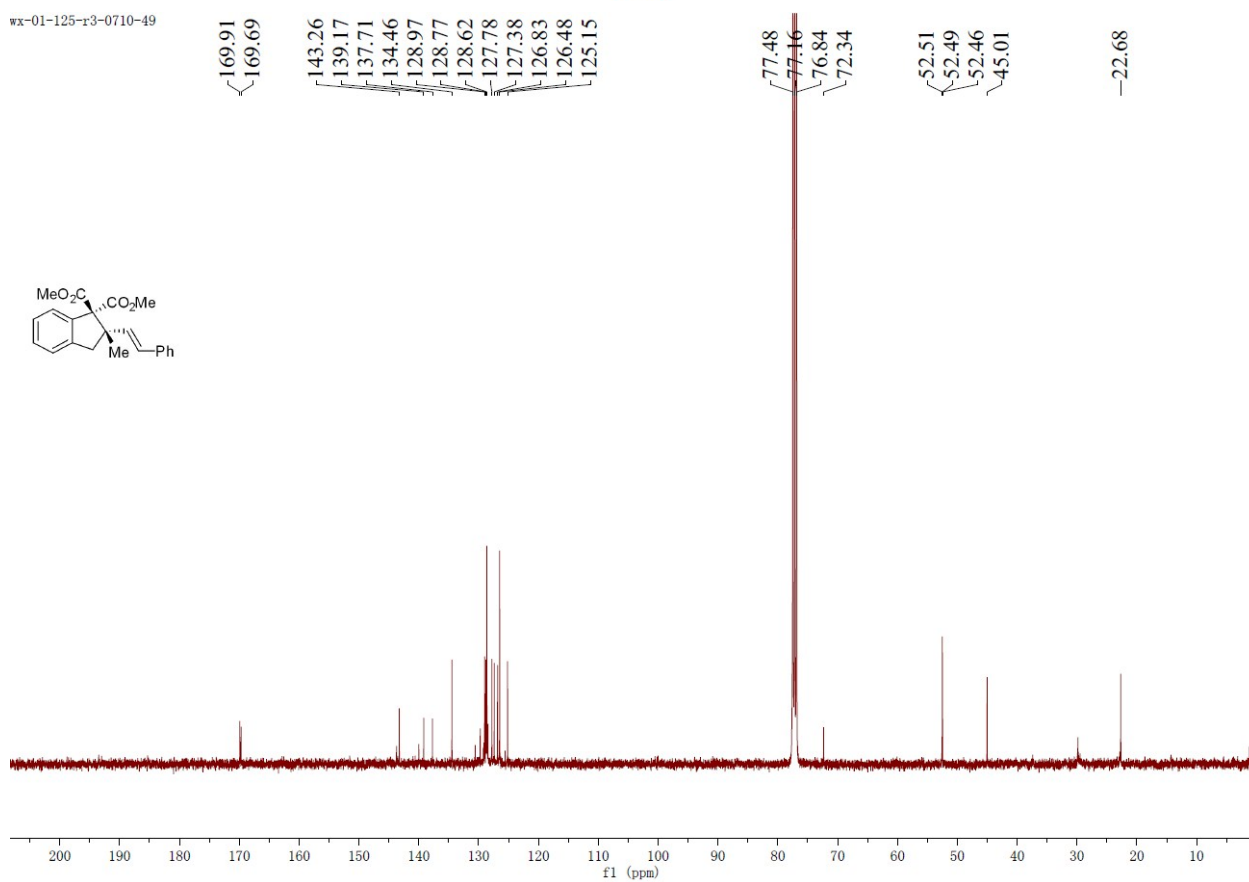
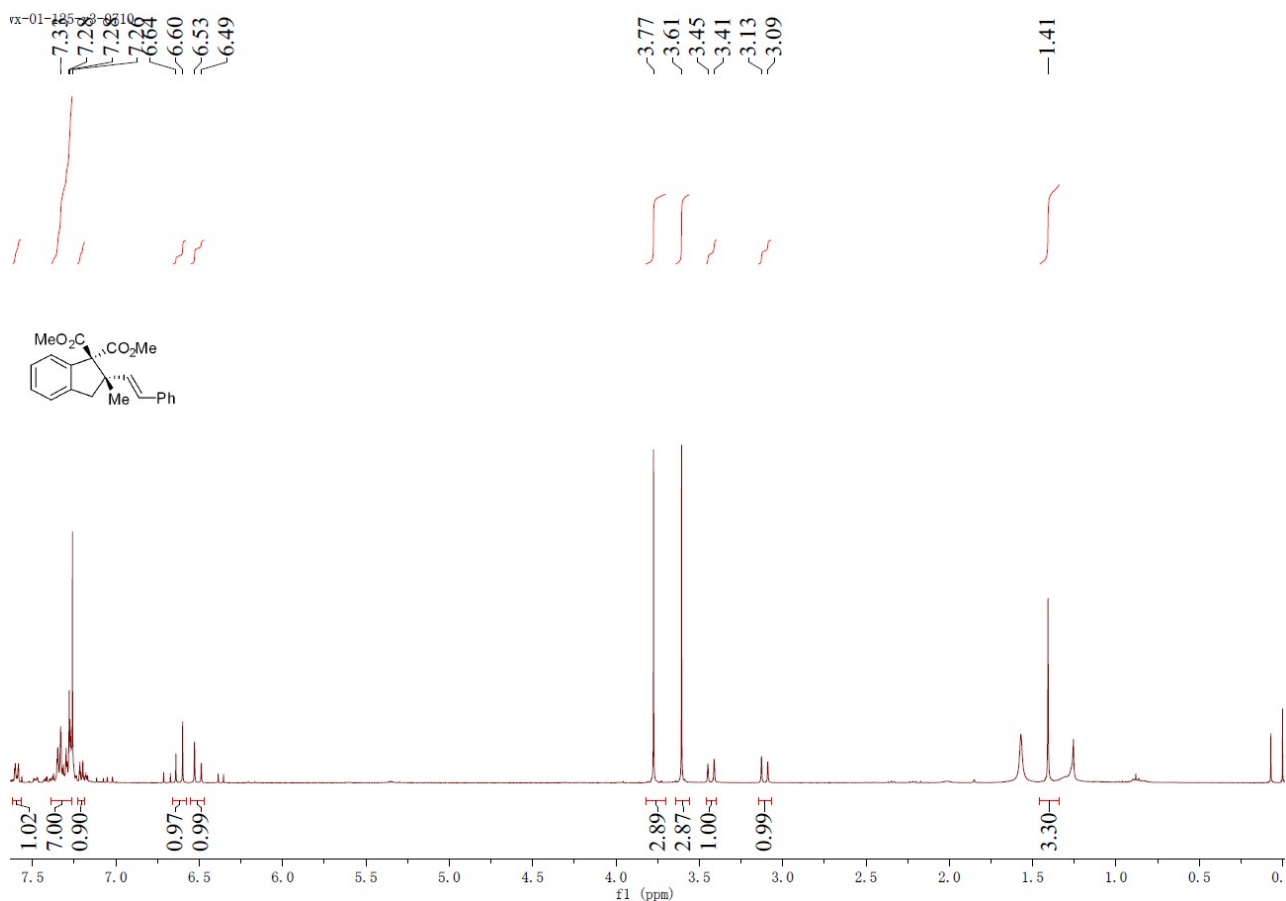
(*R*)-(2,3-dihydro-1*H*-indene-1,1,2-triyl)trimethanol (6)



Dimethyl (S)-2-(2,2-diphenylvinyl)-2,3-dihydro-1H-indene-1,1-dicarboxylate (S3aa)



Dimethyl (*S,E*)-2-methyl-2-styryl-2,3-dihydro-1H-indene-1,1-dicarboxylate (S3ab)



HPLC Analysis of the Products

Dimethyl (*S,E*)-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3aa)

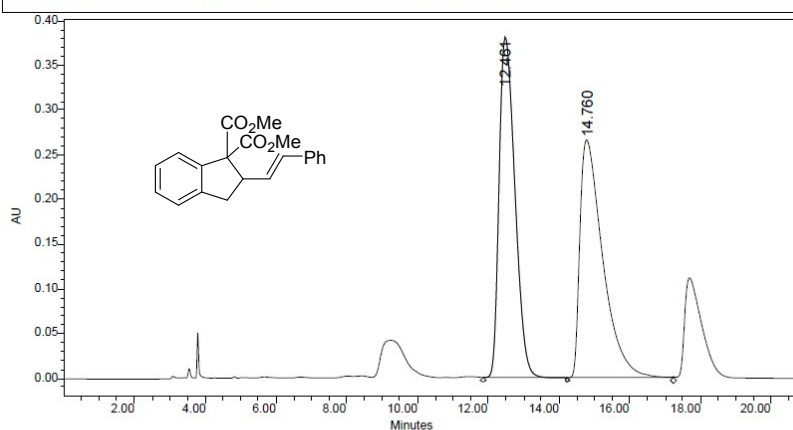
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-sample-rac-1ml-od	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	9/8/2017 7:54:54 PM
Vial:	126	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	9/11/2017 10:09:02 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	12.461	11855395	49.70	380895	58.84
2	14.760	11998103	50.30	266395	41.16

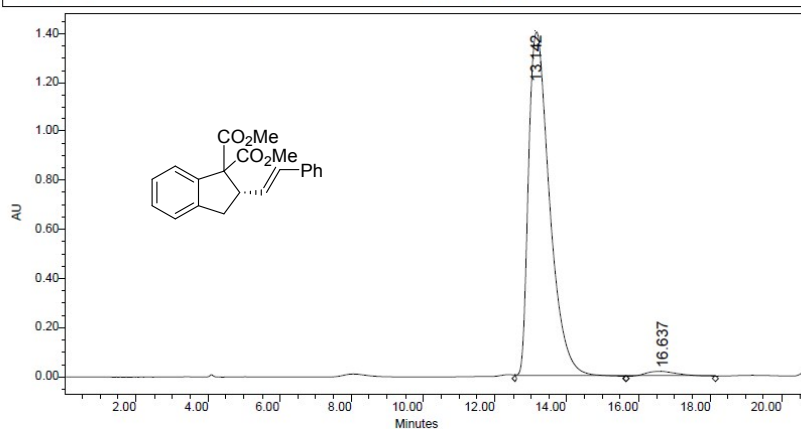
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-K01-054-2-1ml-old-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	3/20/2017 8:35:48 AM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	9/11/2017 10:10:20 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	13.142	57627637	97.74	1408239	98.57
2	16.637	1329973	2.26	20417	1.43

Dimethyl (*S,E*)-7-methyl-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ba)

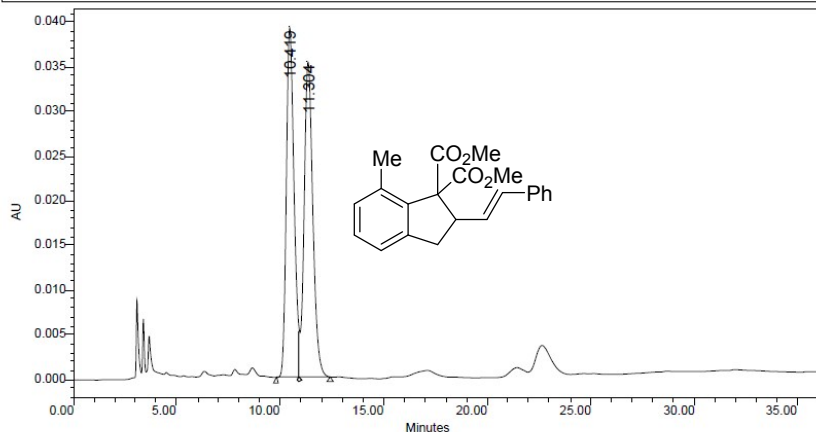
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	z1-2-ME--RAC-1%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/26/2017 11:09:45 AM
Vial:	27	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	8/24/2017 10:20:06 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	10.419	1020202	49.84	39190	52.58
2	11.304	1026884	50.16	35342	47.42

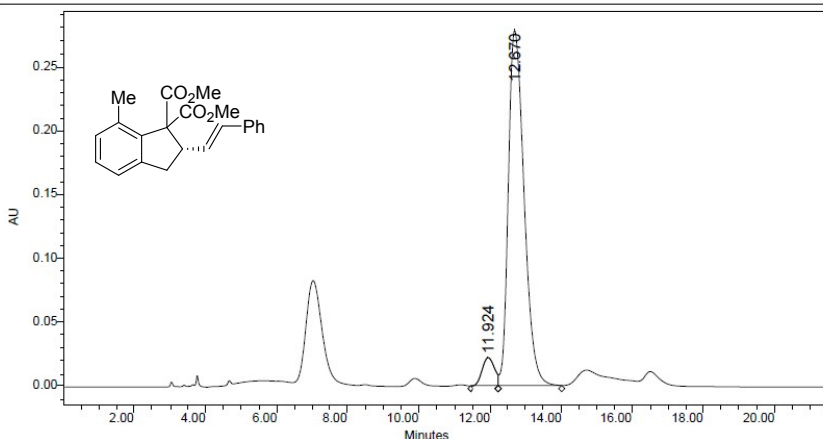
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-69-1-1%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	5/11/2017 3:38:48 PM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	8/27/2017 9:42:16 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	11.924	567581	6.17	22806	7.56
2	12.670	8634407	93.83	278818	92.44

Dimethyl (*S,E*)-7-iodo-6-methyl-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ca)

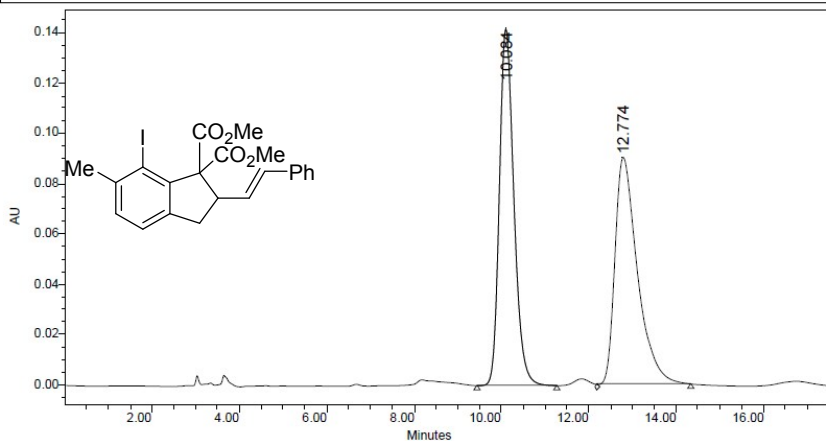
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	zl-p-3me-1%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	4/18/2017 9:38:50 AM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	4/18/2017 10:53:36 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	10.084	3272548	50.17	141844	61.04
2	12.774	3250108	49.83	90534	38.96

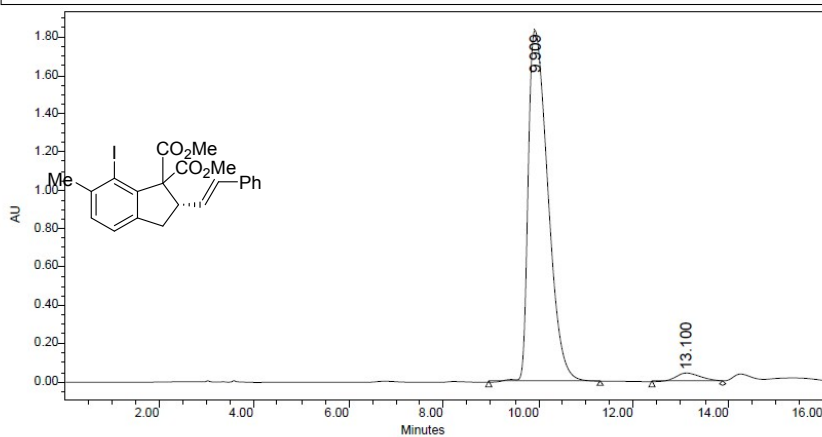
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-71-2-1%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	5/16/2017 7:24:43 PM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	2	Date Processed:	8/23/2017 4:30:43 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	9.909	52878849	97.02	1839168	97.67
2	13.100	1624071	2.98	43961	2.33

Dimethyl (*S,E*)-5-methyl-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3da)

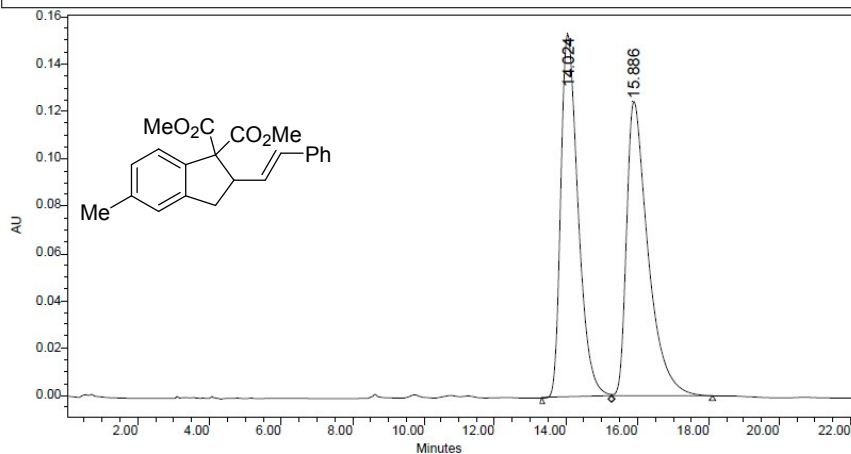
USTC

Project Name: wx
Reported by User: System

'Breeze

SAMPLE INFORMATION

Sample Name:	zL-01-4-me-1%-Rac-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	4/16/2017 1:40:00 PM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	8/24/2017 4:57:09 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	14.024	5221582	49.85	153522	55.16
2	15.886	5253492	50.15	124795	44.84

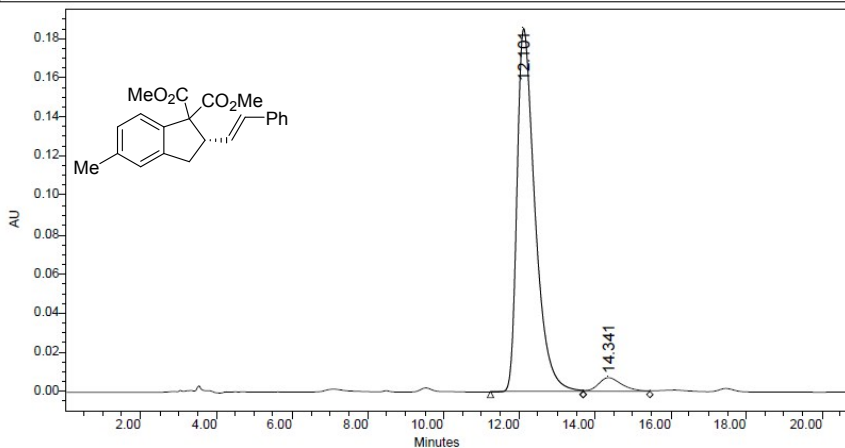
USTC

Project Name: wx
Reported by User: System

'Breeze

SAMPLE INFORMATION

Sample Name:	wx-4me--asy-1%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	4/24/2017 5:07:46 PM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	8/24/2017 4:57:09 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	12.101	6149709	94.77	185470	96.19
2	14.341	339555	5.23	7354	3.81

Dimethyl (S,E)-7-fluoro-2-styryl-2,3-dihydro-1H-indene-1,1-dicarboxylate (3ea)

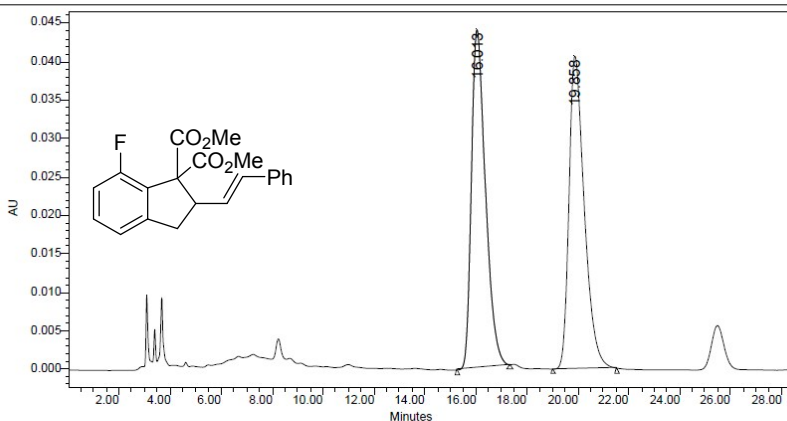
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	zl-2f-rac-1%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	5/22/2017 3:19:49 PM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	2	Date Processed:	8/23/2017 4:16:15 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	16.013	1686364	49.85	43983	51.95
2	19.858	1696835	50.15	40679	48.05

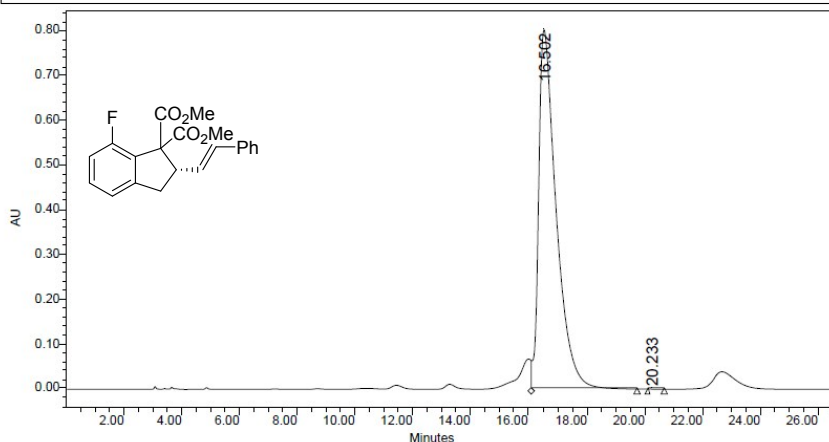
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-71-1-1%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	5/22/2017 10:48:06 AM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	8/23/2017 4:22:38 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	16.502	33673548	100.00	803478	100.00
2	20.233	127	0.00	-8	0.00

Dimethyl (S,E)-6-fluoro-2-styryl-2,3-dihydro-1H-indene-1,1-dicarboxylate (3fa)

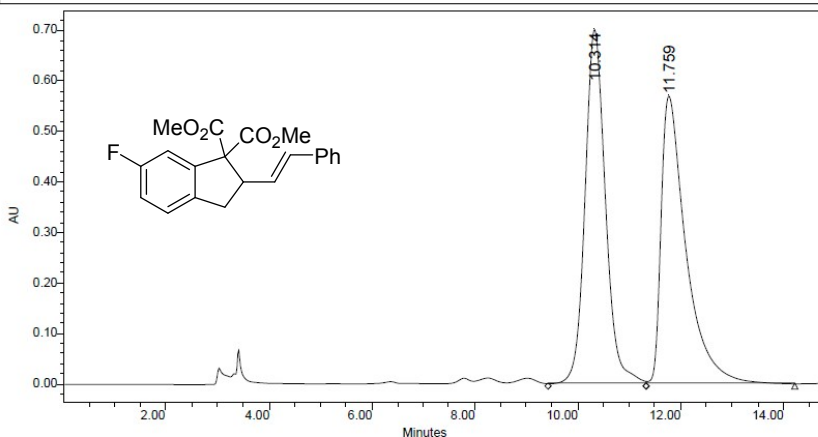
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-3F--RAC-1%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	4/24/2017 6:39:05 PM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	2	Date Processed:	8/23/2017 3:46:38 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	10.314	19466031	50.36	702216	55.15
2	11.759	19189739	49.64	570956	44.85

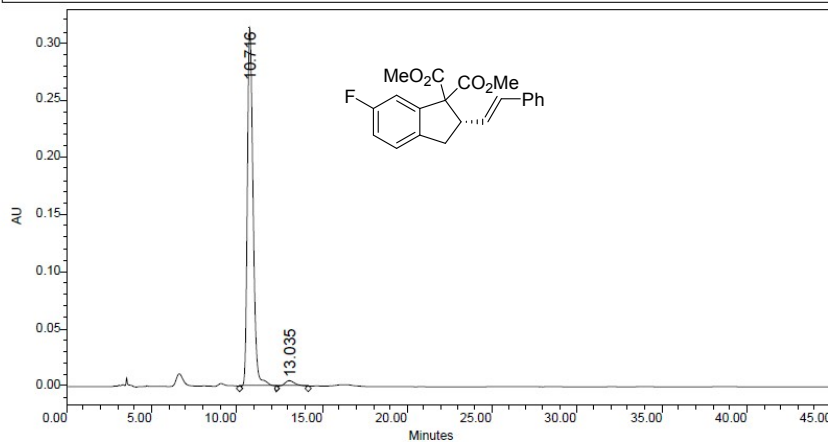
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-3F--asy-1%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	4/24/2017 5:45:21 PM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	8/23/2017 3:49:18 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	10.716	7385122	96.87	313081	98.38
2	13.035	238662	3.13	5153	1.62

Dimethyl (*S,E*)-5-fluoro-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ga)

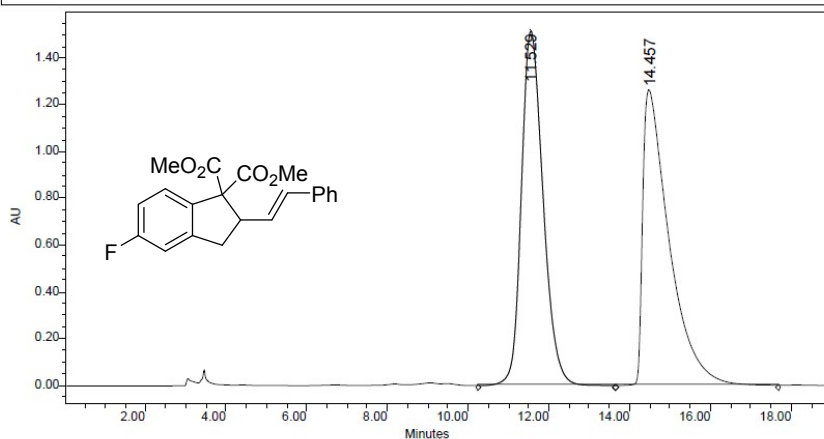
USTC

Project Name: wx
Reported by User: System

1/Breeze

SAMPLE INFORMATION

Sample Name:	wx-4f-rac-1%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	5/11/2017 4:29:10 PM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	2	Date Processed:	8/23/2017 4:09:43 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	11.529	56717939	49.58	1518045	54.53
2	14.457	57670066	50.42	1265905	45.47

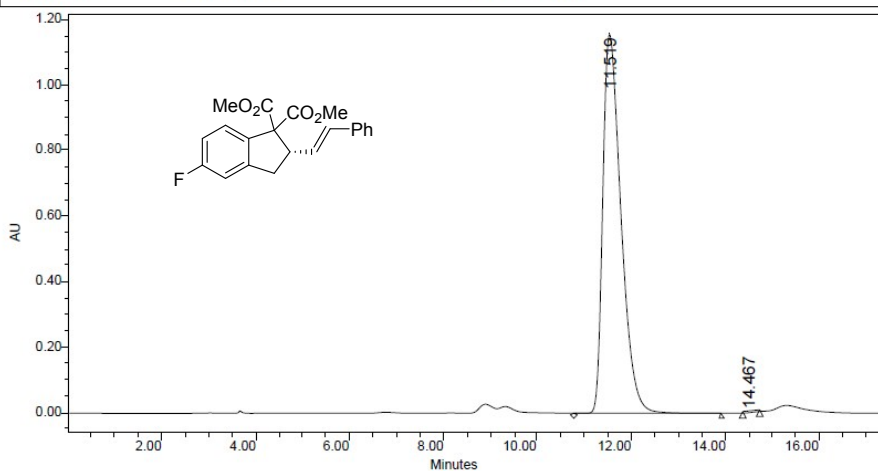
USTC

Project Name: wx
Reported by User: System

1/Breeze

SAMPLE INFORMATION

Sample Name:	WX-4F-ASY-1%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	5/13/2017 4:58:38 PM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	2	Date Processed:	8/23/2017 4:13:39 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	11.519	31098102	99.99	1156856	99.97
2	14.467	4254	0.01	-384	0.03

Dimethyl (S,E)-5-chloro-2-styryl-2,3-dihydro-1H-indene-1,1-dicarboxylate (3ha)

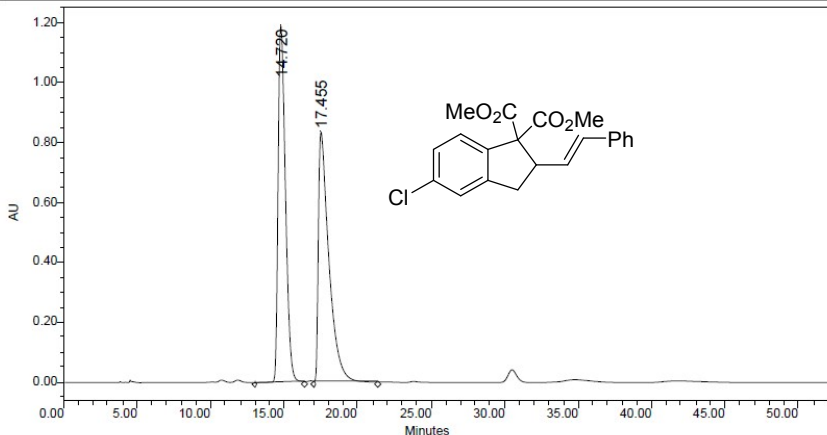
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	zl-01-4cl-1%-Rac-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	4/7/2017 12:25:52 PM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	4/7/2017 2:29:53 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	14.720	41580915	49.75	1192051	58.74
2	17.455	41991127	50.25	837152	41.26

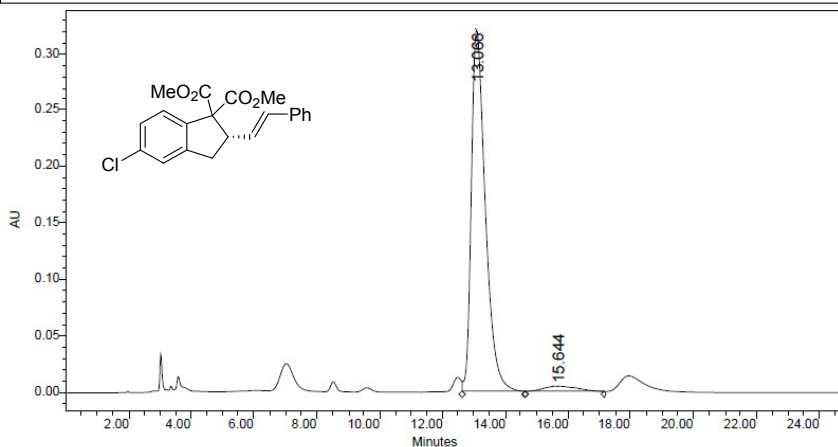
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-4cl-asy-1%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	4/29/2017 9:48:08 AM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	8/23/2017 3:54:04 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	13.066	10065900	95.28	321916	98.25
2	15.644	498320	4.72	5730	1.75

Dimethyl (S,E)-5-bromo-2-styryl-2,3-dihydro-1H-indene-1,1-dicarboxylate (3ia)

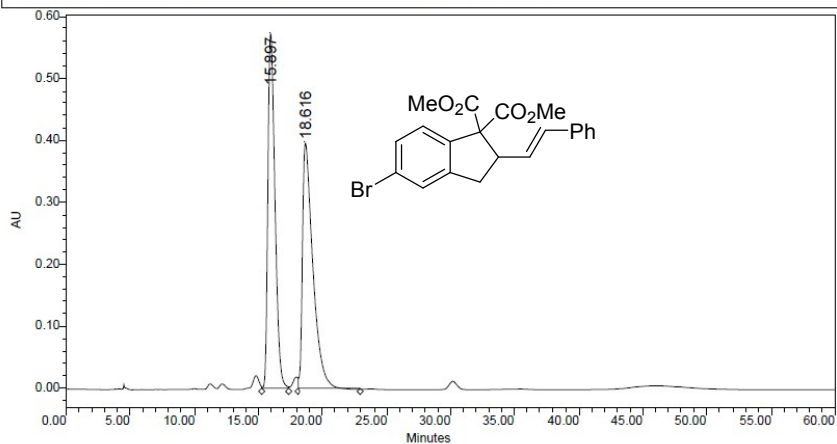
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	zl-01-4br-1%-Rac-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	4/7/2017 1:26:58 PM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	4/7/2017 2:37:14 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	15.897	22211867	49.40	573709	59.07
2	18.616	22752368	50.60	397587	40.93

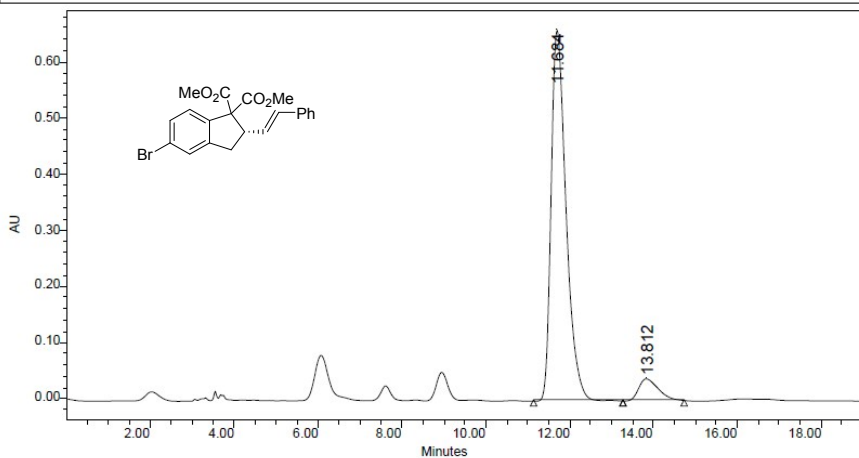
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-80-2-1%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	7/6/2017 2:26:21 PM
Vial:	47	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	8/24/2017 5:17:01 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	11.684	16399646	92.73	660926	94.39
2	13.812	1286510	7.27	39286	5.61

Dimethyl (*S,E*)-5-methoxy-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (3ja)

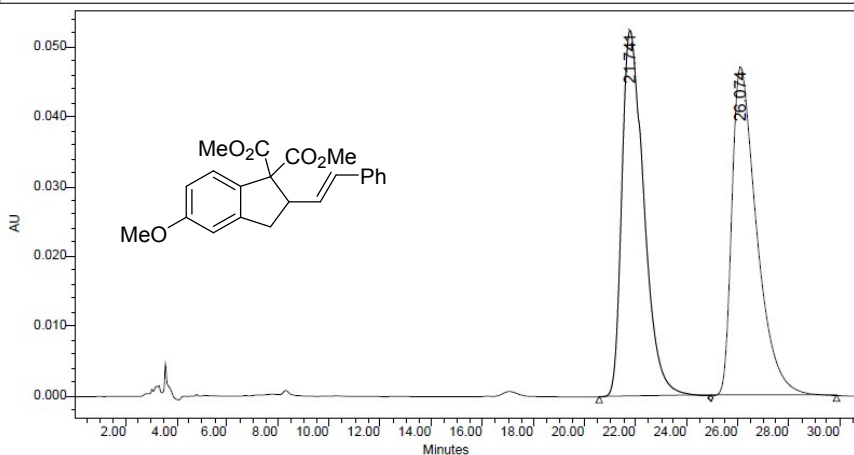
USTC

Project Name: wx
Reported by User: System

'Breeze

SAMPLE INFORMATION

Sample Name:	zl-4-OMe-rac-1%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	4/20/2017 6:13:57 PM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	8/23/2017 3:22:20 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	21.741	3162924	49.66	52541	52.68
2	26.074	3206823	50.34	47188	47.32

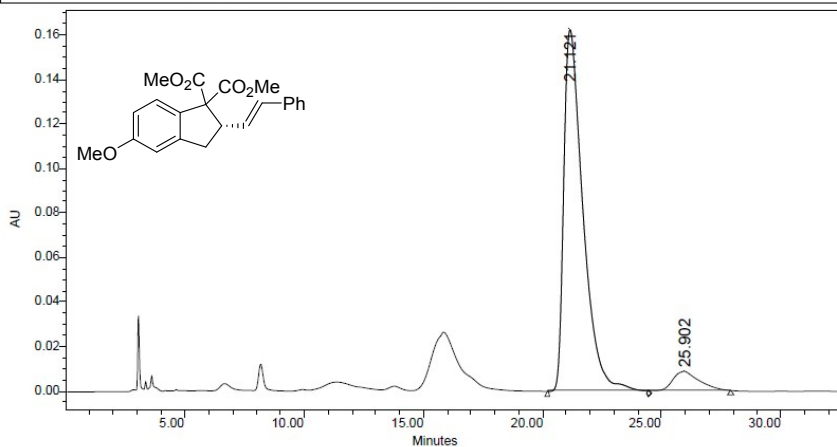
USTC

Project Name: wx
Reported by User: System

'Breeze

SAMPLE INFORMATION

Sample Name:	wx-4ome-asy-1%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	4/29/2017 10:56:29 AM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	2	Date Processed:	8/23/2017 3:57:36 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	21.121	9103516	93.11	162586	94.87
2	25.902	673964	6.89	8788	5.13

Dimethyl (S,E)-2-styryl-2,3-dihydro-1H-cyclopenta[b]naphthalene-1,1-dicarboxylate (3ka)

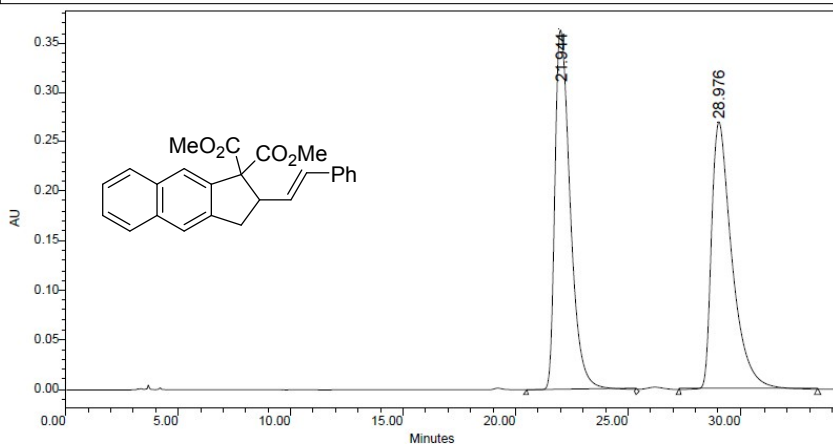
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	zl-01-2na-1%-Rac-1ml-IC	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	4/16/2017 9:44:11 AM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	8/23/2017 3:24:08 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	21.944	17268814	50.23	363523	57.34
2	28.976	17109965	49.77	270401	42.66

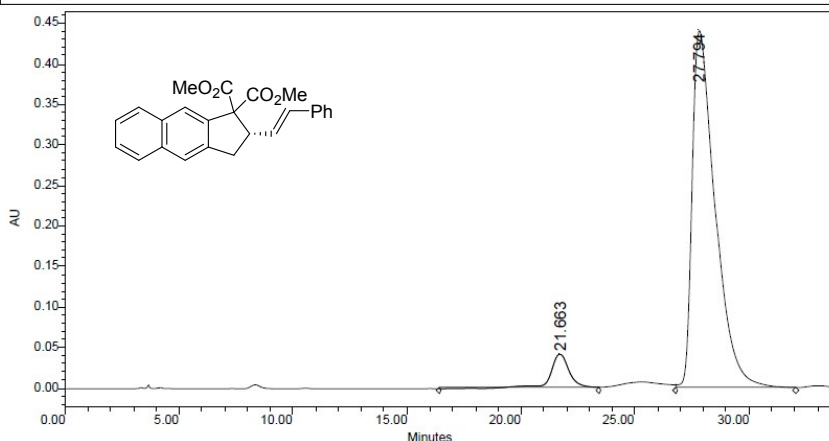
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-2na--asy-1%-1ml-IC	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	4/24/2017 3:36:04 PM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	8/24/2017 5:01:06 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	21.663	2621865	7.79	42043	8.70
2	27.794	31039621	92.21	441016	91.30

Dibenzyl (*S,E*)-2-styryl-2,3-dihydro-1*H*-indene-1,1-dicarboxylate (**3la**)

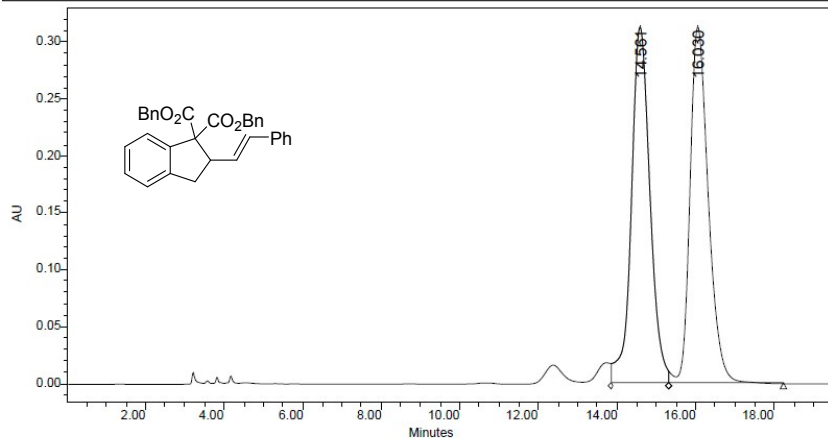
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	zl-bn-rac-1%-1ml-IC	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	5/16/2017 9:03:54 PM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	8/23/2017 4:33:58 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	14.561	10367794	50.36	313611	50.00
2	16.030	10217582	49.64	313550	50.00

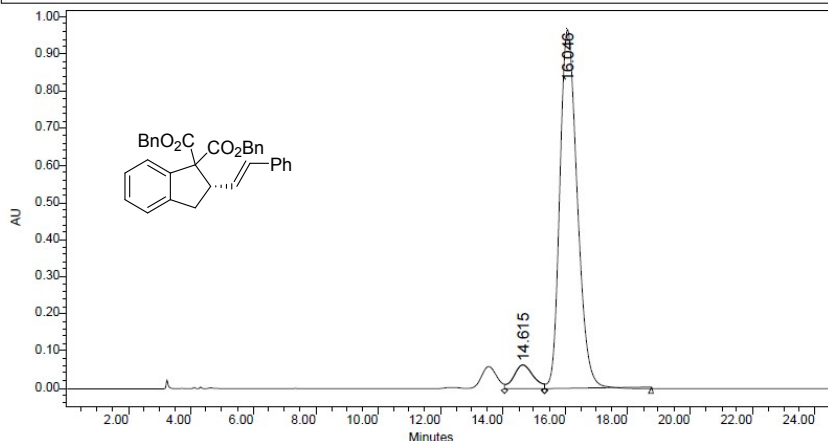
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-71-3-1%-1ml-IC	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	5/22/2017 5:04:35 PM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	8/23/2017 4:39:19 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	14.615	2736359	6.78	63945	6.20
2	16.046	37626312	93.22	967617	93.80

Dimethyl (S,E)-5-styryl-5,6-dihydro-4H-cyclopenta[b]thiophene-4,4-dicarboxylate (3ma)

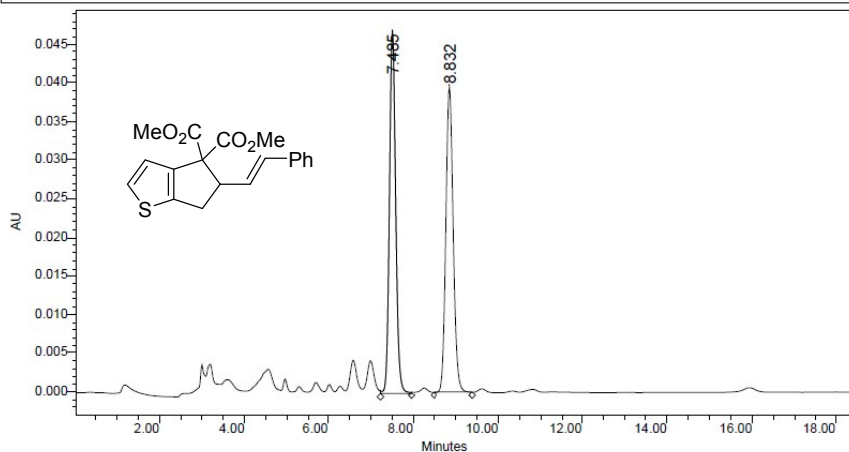
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	zl-4-3-5%-1ml-AD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	7/14/2017 7:51:11 PM
Vial:	59	Acq. Method:	5% 1ML
Injection #:	1	Date Processed:	8/24/2017 8:35:03 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	7.485	483038	50.06	47125	54.29
2	8.832	481916	49.94	39675	45.71

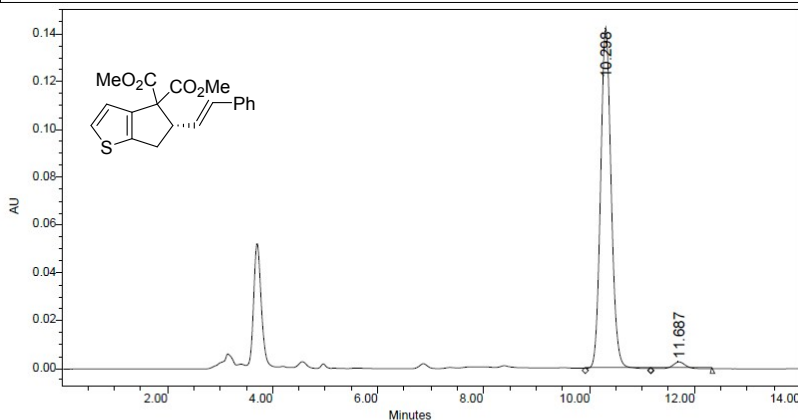
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-84-1-5%-1ml-AD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	7/14/2017 6:54:33 PM
Vial:	57	Acq. Method:	5% 1ML
Injection #:	1	Date Processed:	8/24/2017 8:40:28 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	10.298	1987073	97.68	142684	98.06
2	11.687	47227	2.32	2825	1.94

Dimethyl (S,E)-2-(2-methylstyryl)-2,3-dihydro-1H-indene-1,1-dicarboxylate (3ab)

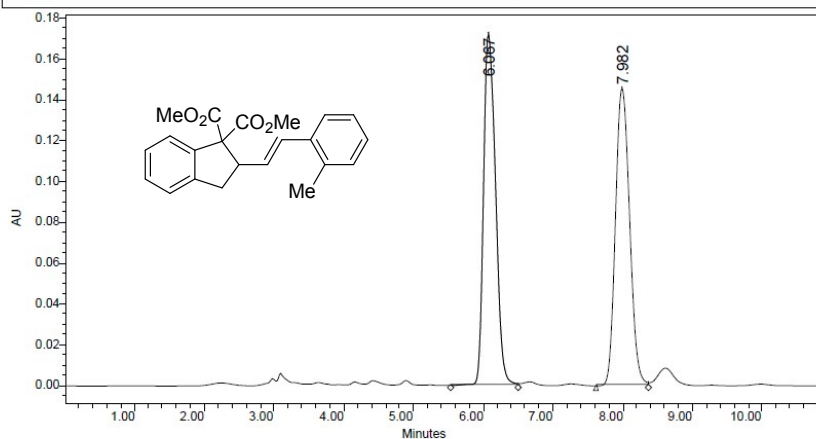
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	zl-11-1-1-5%-1ml-AD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/11/2017 1:10:44 PM
Vial:	1	Acq. Method:	5% 1ML
Injection #:	2	Date Processed:	8/24/2017 10:38:15 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	6.067	2077458	50.13	172720	54.16
2	7.982	2066662	49.87	146196	45.84

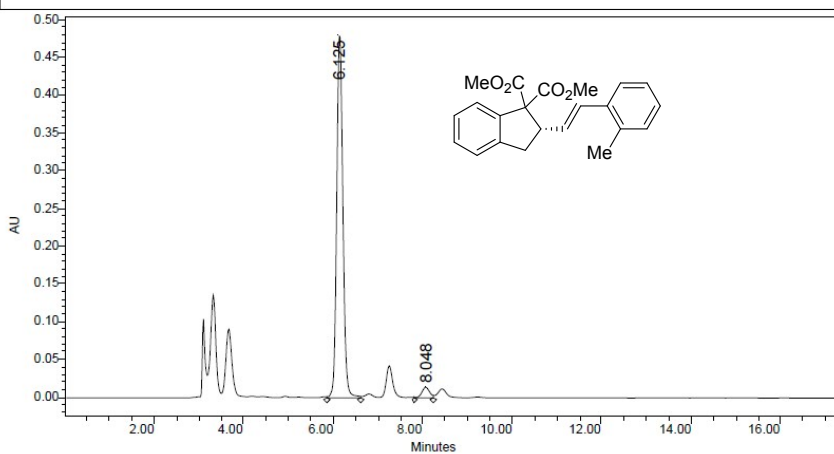
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-70-2-5%-1ml-AD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/11/2017 1:28:52 PM
Vial:	1	Acq. Method:	5% 1ML
Injection #:	3	Date Processed:	8/24/2017 10:42:24 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	6.125	4612594	96.41	482695	97.15
2	8.048	171835	3.59	14140	2.85

Dimethyl (S,E)-2-(3-methylstyryl)-2,3-dihydro-1H-indene-1,1-dicarboxylate (3ac)

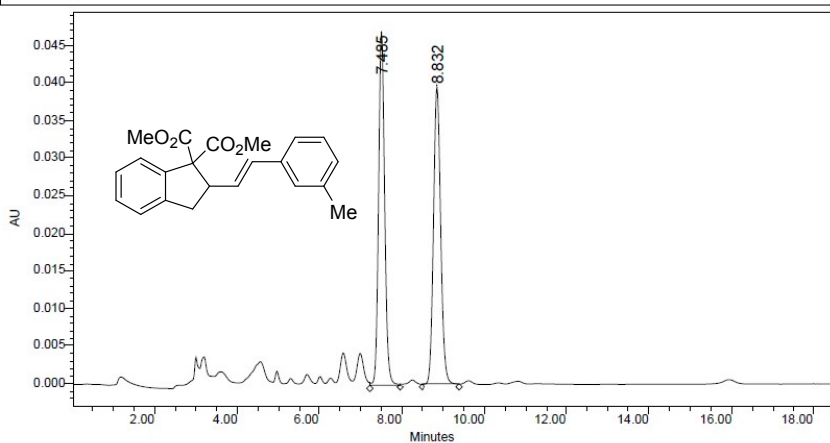
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	zl-4-3-5%-1ml-AD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	7/14/2017 7:51:11 PM
Vial:	59	Acq. Method:	5% 1ML
Injection #:	1	Date Processed:	8/24/2017 9:22:18 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	7.485	483038	50.06	47125	54.29
2	8.832	481916	49.94	39675	45.71

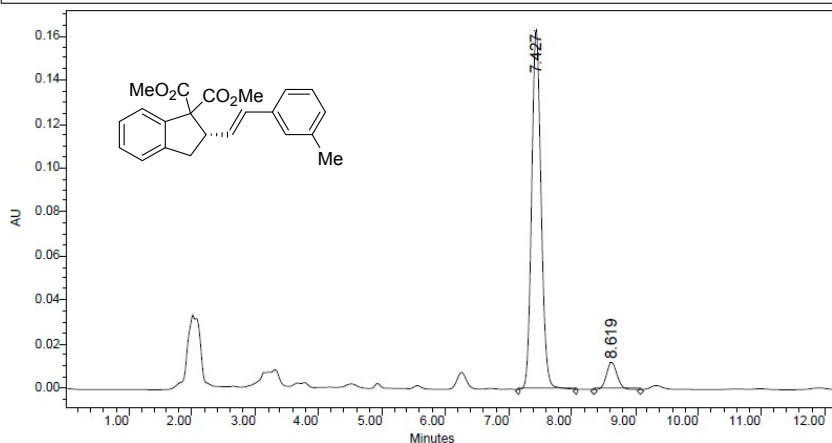
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	zl-62-5%-1ml-AD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	8/11/2017 6:36:40 PM
Vial:	80	Acq. Method:	5% 1ML
Injection #:	1	Date Processed:	8/24/2017 9:22:58 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	7.427	1693311	92.13	164034	92.99
2	8.619	144698	7.87	12361	7.01

Dimethyl (S,E)-2-(4-methylstyryl)-2,3-dihydro-1H-indene-1,1-dicarboxylate (3ad)

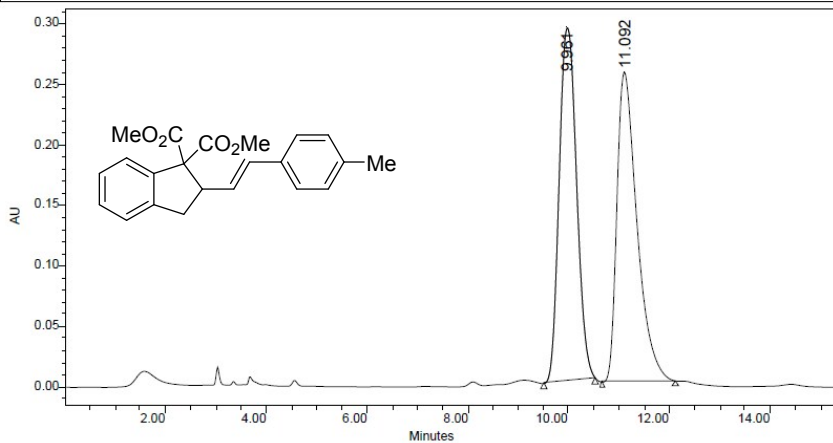
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	zl-4-4-rac-1%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	5/11/2017 9:47:57 PM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	3	Date Processed:	8/24/2017 9:25:30 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	9.961	7050546	49.79	292803	53.32
2	11.092	7110398	50.21	256378	46.68

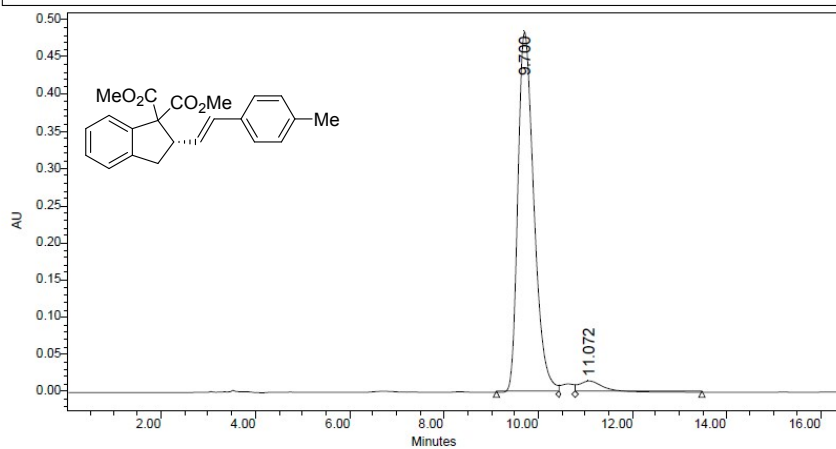
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-72-2-1%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	5/26/2017 4:37:23 PM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	8/24/2017 9:29:25 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	9.700	11437205	95.25	484625	96.96
2	11.072	569776	4.75	15219	3.04

Dimethyl (S,E)-2-(2-methoxystyryl)-2,3-dihydro-1H-indene-1,1-dicarboxylate (3ae)

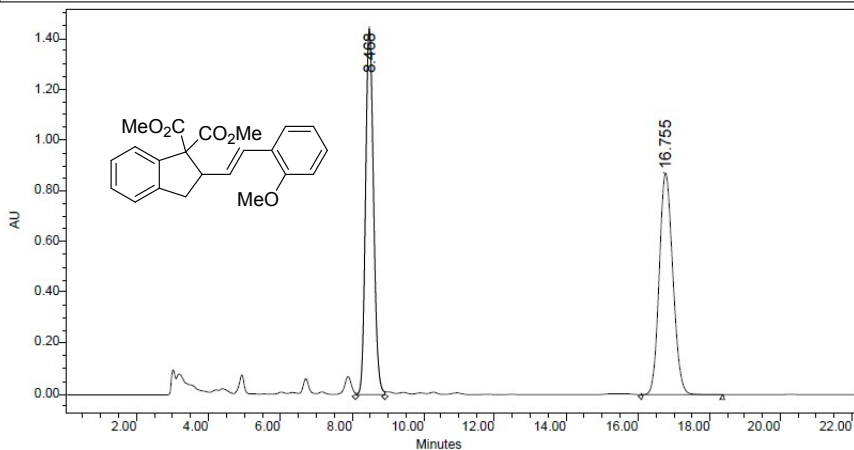
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-4-1-5%-1ml-AD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	5/14/2017 3:51:15 PM
Vial:	1	Acq. Method:	5% 1ML
Injection #:	1	Date Processed:	8/24/2017 8:55:55 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	8.468	22388297	49.32	1440737	62.27
2	16.755	23003719	50.68	872883	37.73

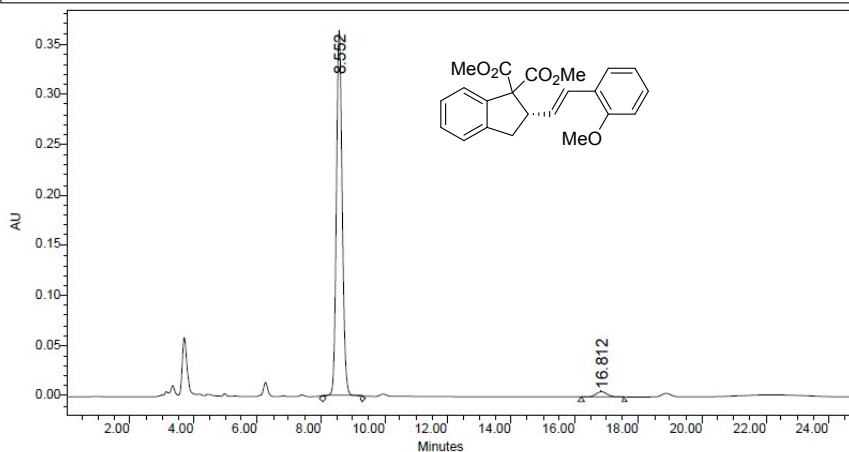
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-78-2-5%-1ml-AD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/25/2017 2:27:28 PM
Vial:	17	Acq. Method:	5% 1ML
Injection #:	1	Date Processed:	8/24/2017 8:58:06 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	8.552	4657611	97.34	364768	98.60
2	16.812	127329	2.66	5191	1.40

Dimethyl (S,E)-2-(3-methoxystyryl)-2,3-dihydro-1H-indene-1,1-dicarboxylate (3af)

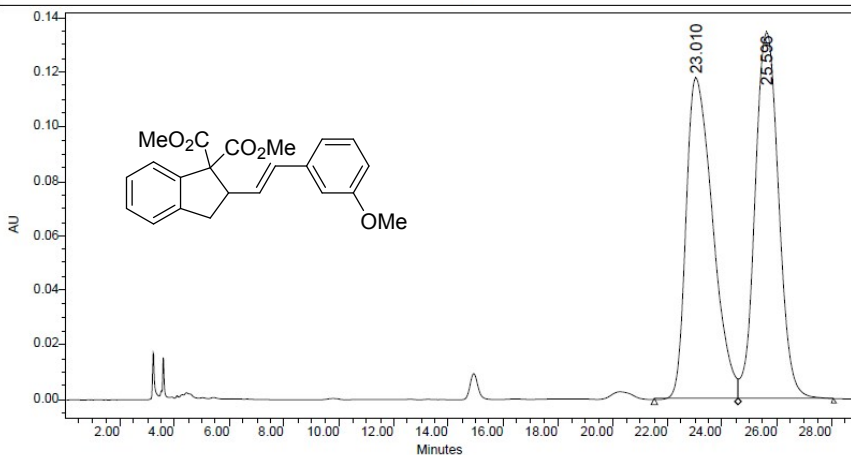
USTC

Project Name: wx
Reported by User: System

'Breeze

SAMPLE INFORMATION

Sample Name:	zl-24-3-1%-1ml-IC	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/26/2017 8:00:33 PM
Vial:	34	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	8/24/2017 11:21:03 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	23.010	7995654	49.82	117990	46.72
2	25.596	8052230	50.18	134550	53.28

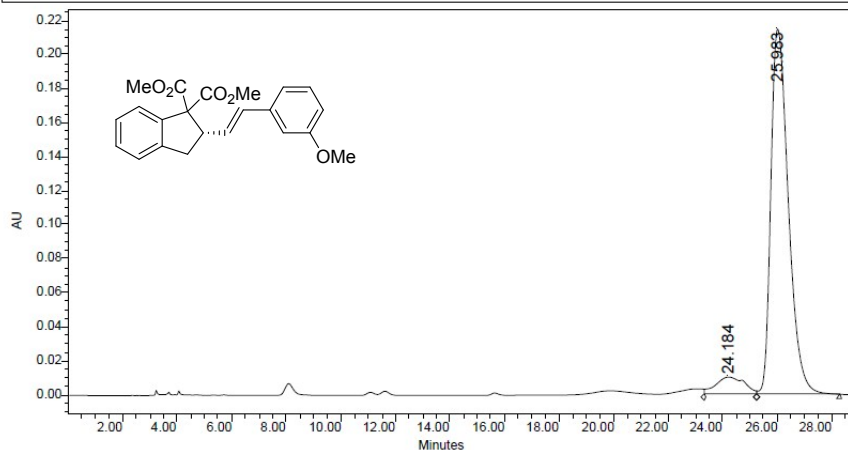
USTC

Project Name: wx
Reported by User: System

'Breeze

SAMPLE INFORMATION

Sample Name:	wx-79-2-1%-1ml-IC	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/30/2017 5:23:04 PM
Vial:	43	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	8/28/2017 9:44:08 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	24.184	766098	7.40	10248	4.55
2	25.983	9581711	92.60	214759	95.45

Dimethyl (S,E)-2-(4-methoxystyryl)-2,3-dihydro-1H-indene-1,1-dicarboxylate (3ag)

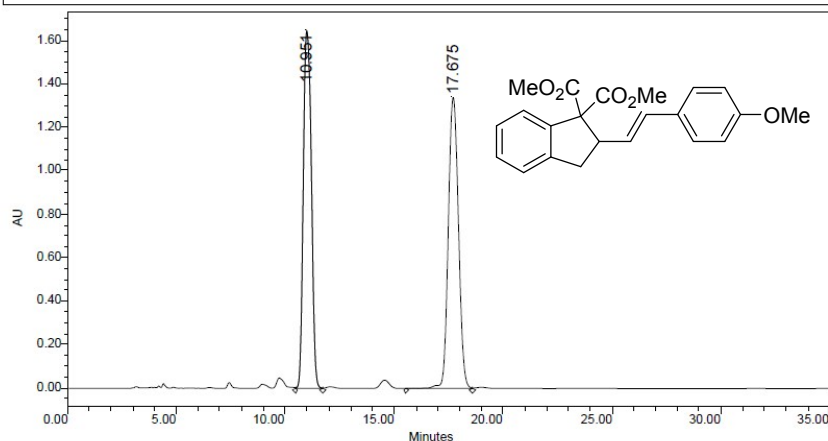
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	ZL-11-2-5%-1ml-AD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/21/2017 8:18:34 PM
Vial:	8	Acq. Method:	5% 1ML
Injection #:	1	Date Processed:	8/24/2017 10:06:18 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	10.951	42357121	49.30	1648319	55.10
2	17.675	43554059	50.70	1342978	44.90

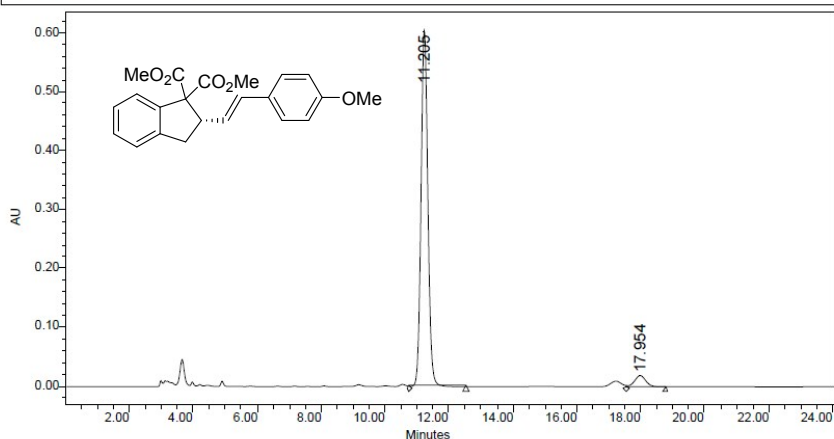
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-72-4-5%-1ml-AD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/20/2017 9:09:10 PM
Vial:	2	Acq. Method:	5% 1ML
Injection #:	1	Date Processed:	8/24/2017 10:08:38 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	11.205	8946875	95.10	604751	96.94
2	17.954	460507	4.90	19094	3.06

Dimethyl (S,E)-2-(4-(dimethylamino)styryl)-2,3-dihydro-1H-indene-1,1-dicarboxylate (3ah)

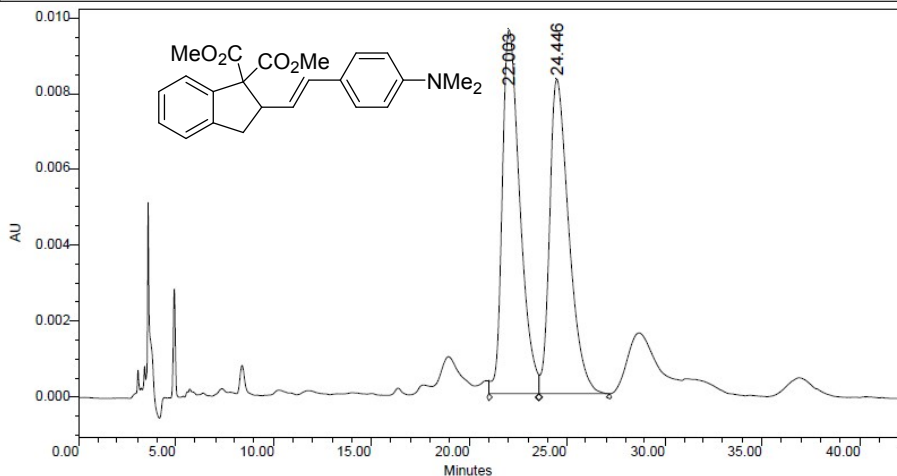
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	zl-4-2-rac-1%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	5/11/2017 8:46:14 PM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	8/24/2017 4:15:52 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	22.003	606339	51.42	9622	53.63
2	24.446	572747	48.58	8320	46.37

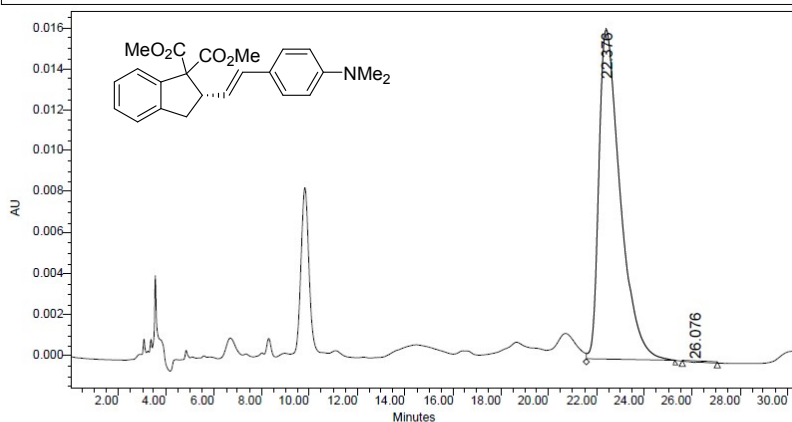
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-72-3-1%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	5/26/2017 4:58:19 PM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	2	Date Processed:	8/24/2017 4:15:52 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	22.376	999355	99.93	16101	99.84
2	26.076	690	0.07	-25	0.16

Dimethyl (S,E)-2-(2-chlorostyryl)-2,3-dihydro-1H-indene-1,1-dicarboxylate (3ai)

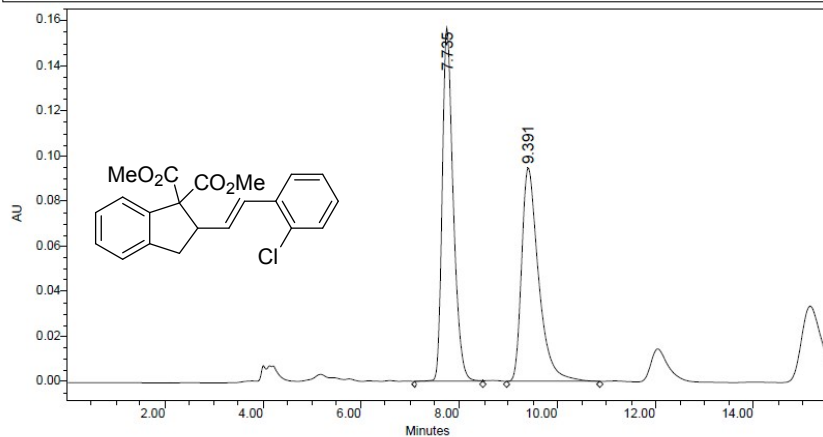
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	zl-24-2-5%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/30/2017 4:53:31 PM
Vial:	42	Acq. Method:	5% 1ML
Injection #:	1	Date Processed:	8/24/2017 11:18:53 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	7.735	2488285	51.70	157122	62.27
2	9.391	2324182	48.30	95207	37.73

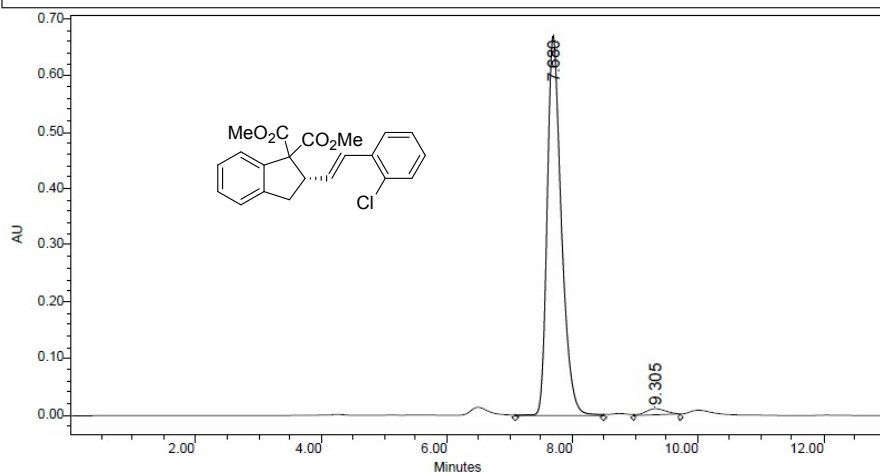
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx--79-1-5%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/30/2017 4:31:20 PM
Vial:	41	Acq. Method:	5% 1ML
Injection #:	1	Date Processed:	8/24/2017 11:17:16 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	7.680	10558154	97.17	671911	98.22
2	9.305	307341	2.83	12145	1.78

Dimethyl (S,E)-2-(3-chlorostyryl)-2,3-dihydro-1H-indene-1,1-dicarboxylate (3aj)

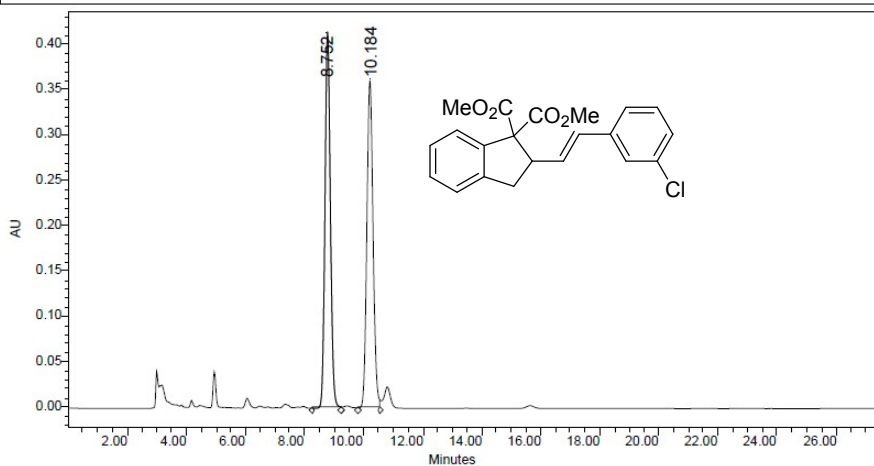
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	zl-15-3-5%-1ml-AD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/10/2017 8:23:23 PM
Vial:	1	Acq. Method:	5% 1ML
Injection #:	2	Date Processed:	8/24/2017 10:34:08 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	8.752	5319956	50.03	415308	53.46
2	10.184	5313235	49.97	361567	46.54

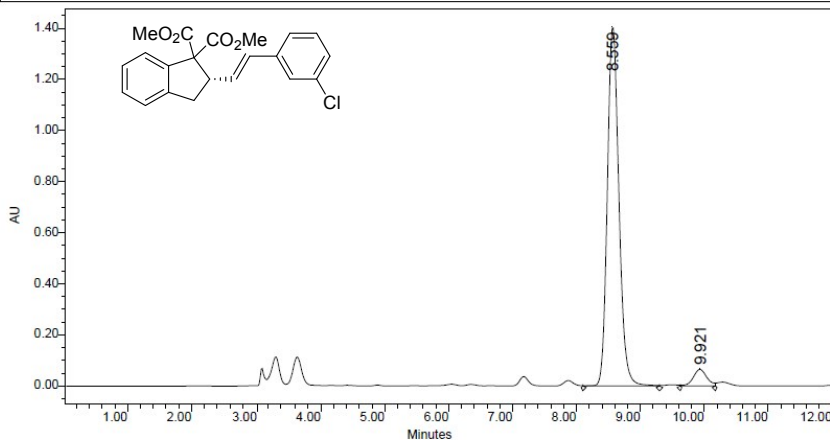
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-73-1-5%-1ml-AD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/11/2017 12:54:48 PM
Vial:	1	Acq. Method:	5% 1ML
Injection #:	1	Date Processed:	8/24/2017 10:35:42 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	8.559	17686416	94.84	1407490	95.56
2	9.921	962901	5.16	65344	4.44

Dimethyl (S,E)-2-(4-chlorostyryl)-2,3-dihydro-1H-indene-1,1-dicarboxylate (3ak)

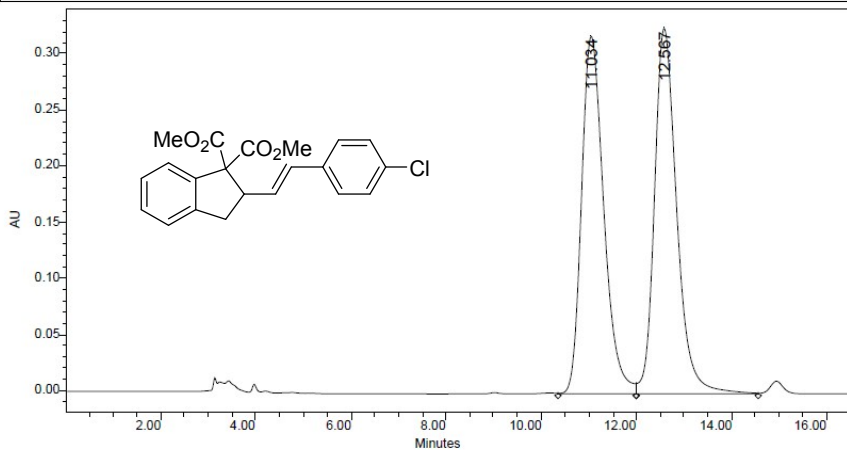
USTC

Project Name: wx
Reported by User: System

'Breeze

SAMPLE INFORMATION

Sample Name:	ZL-22-1-1%-1ml-IC	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/20/2017 10:42:09 AM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	4	Date Processed:	8/24/2017 10:48:21 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	11.034	10341669	49.37	318553	49.45
2	12.567	10604219	50.63	325695	50.55

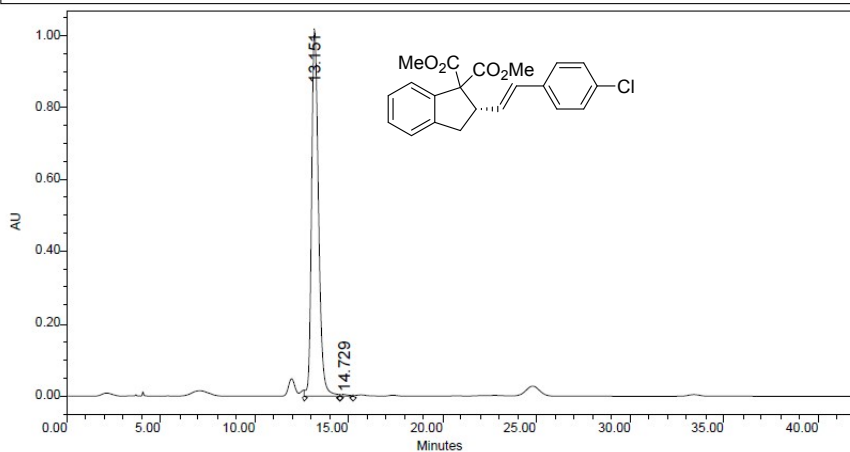
USTC

Project Name: wx
Reported by User: System

'Breeze

SAMPLE INFORMATION

Sample Name:	wx-77-3-1%-1ml-IC	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/20/2017 11:23:55 AM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	6	Date Processed:	8/24/2017 10:49:00 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	13.151	26263647	99.50	1017002	99.54
2	14.729	132609	0.50	4674	0.46

Dimethyl (S,E)-2-(4-fluorostyryl)-2,3-dihydro-1H-indene-1,1-dicarboxylate (3a)

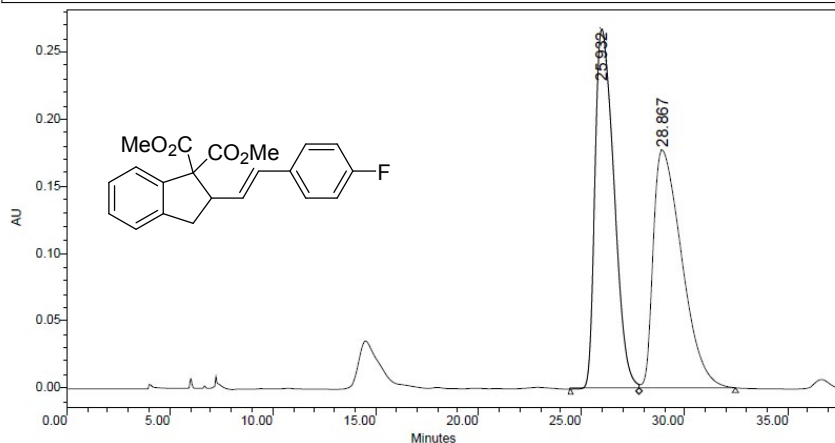
USTC

Project Name: wx
Reported by User: System

1/Breeze

SAMPLE INFORMATION

Sample Name:	ZL-11-3-1%-05ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	5/26/2017 8:17:04 PM
Vial:	1	Acq. Method:	1% 05ML
Injection #:	1	Date Processed:	8/24/2017 11:27:56 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	25.932	17184398	50.13	267587	60.16
2	28.867	17095227	49.87	177203	39.84

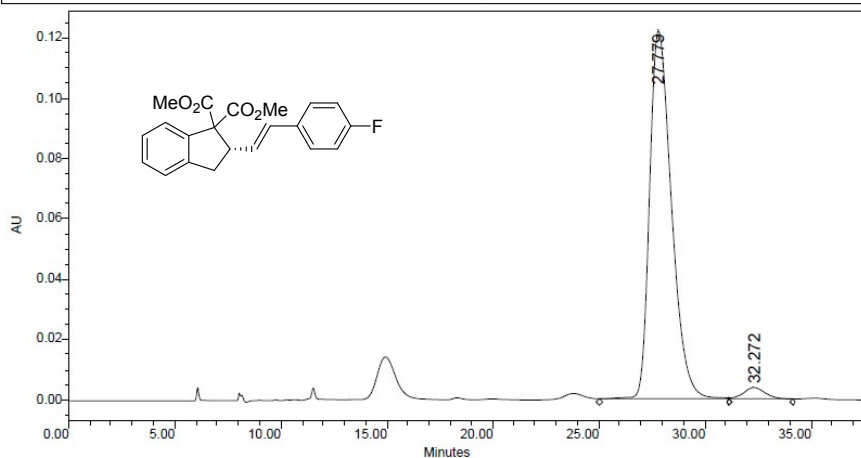
USTC

Project Name: wx
Reported by User: System

1/Breeze

SAMPLE INFORMATION

Sample Name:	wx-73-2-1%-05ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/9/2017 8:02:34 PM
Vial:	1	Acq. Method:	1% 05ML
Injection #:	1	Date Processed:	8/27/2017 9:33:49 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	27.779	8897043	96.48	122365	96.74
2	32.272	324245	3.52	4118	3.26

Dimethyl (S,E)-2-(4-(methoxycarbonyl)styryl)-2,3-dihydro-1H-indene-1,1-dicarboxylate (3am)

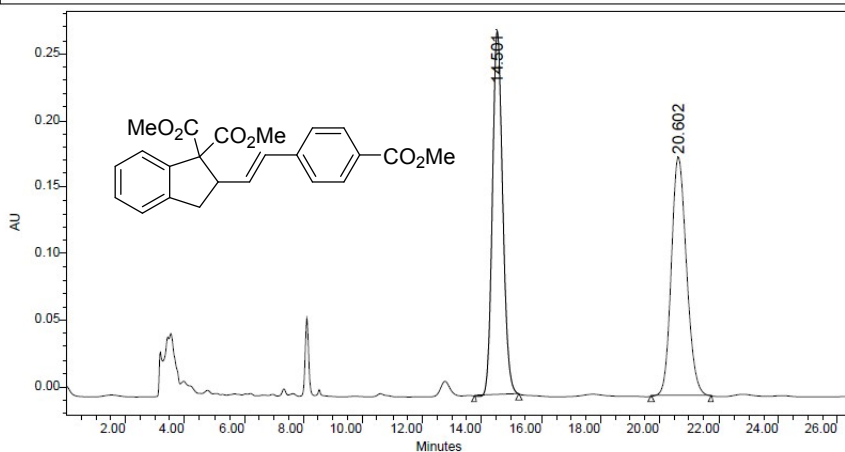
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	zl-4-5-10%-1ml-IC	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/19/2017 8:52:31 PM
Vial:	1	Acq. Method:	10%1ML
Injection #:	1	Date Processed:	8/24/2017 9:32:18 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	14.501	6591156	50.70	273201	60.37
2	20.602	6408550	49.30	179358	39.63

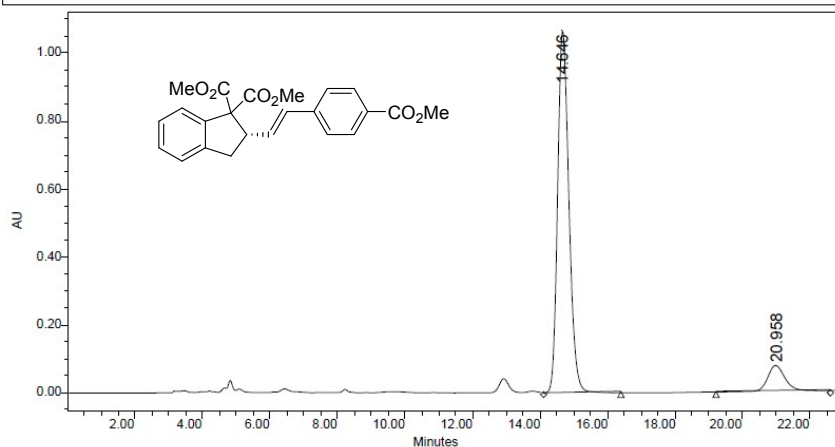
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-77-4-10%-1ml-IC	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/19/2017 9:23:35 PM
Vial:	1	Acq. Method:	10%1ML
Injection #:	2	Date Processed:	8/24/2017 9:33:43 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	14.646	24799071	90.12	1067460	93.33
2	20.958	2719103	9.88	76292	6.67

Dimethyl (S,E)-2-(2-(thiophen-2-yl)vinyl)-2,3-dihydro-1H-indene-1,1-dicarboxylate (3an)

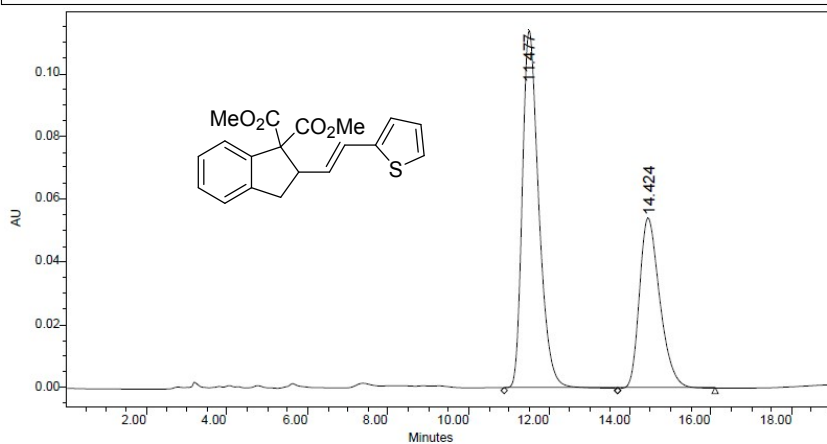
USTC

Project Name: wx
Reported by User: System

'Breeze

SAMPLE INFORMATION

Sample Name:	wx-78-3-5%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/27/2017 10:05:12 PM
Vial:	37	Acq. Method:	5% 1ML
Injection #:	1	Date Processed:	8/24/2017 11:10:49 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	11.477	3249293	63.01	113987	67.76
2	14.424	1907529	36.99	54230	32.24

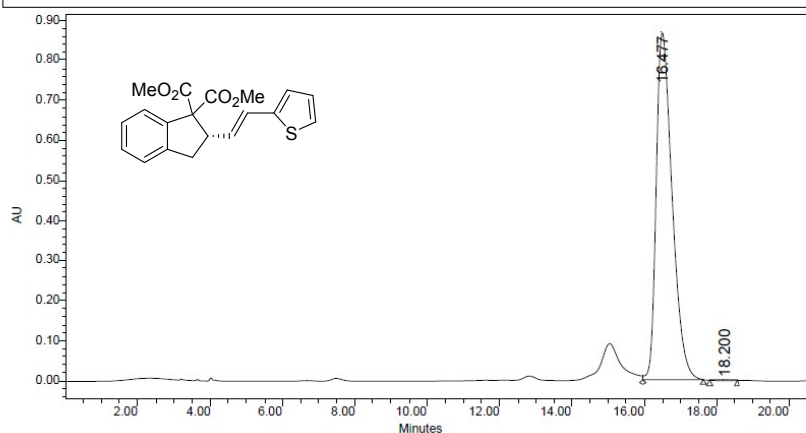
USTC

Project Name: wx
Reported by User: System

'Breeze

SAMPLE INFORMATION

Sample Name:	wx-77-2-1%-1ml-IC	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/20/2017 12:10:40 PM
Vial:	1	Acq. Method:	1% 1ml
Injection #:	7	Date Processed:	8/24/2017 11:06:34 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	16.477	26598820	99.92	867332	99.92
2	18.200	21442	0.08	-698	0.08

Dimethyl (S,E)-2-(2-(furan-2-yl)vinyl)-2,3-dihydro-1H-indene-1,1-dicarboxylat (3ao)

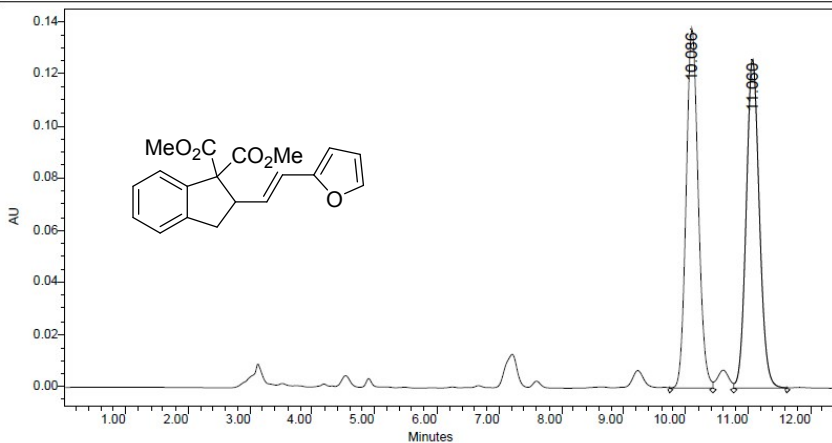
USTC

Project Name: wx
Reported by User: System

'Breeze

SAMPLE INFORMATION

Sample Name:	ZL-43-5-5%-1ml-AD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	7/14/2017 4:17:23 PM
Vial:	54	Acq. Method:	5% 1ML
Injection #:	1	Date Processed:	8/24/2017 11:01:20 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	10.086	1857864	49.92	138093	52.21
2	11.060	1864133	50.08	126388	47.79

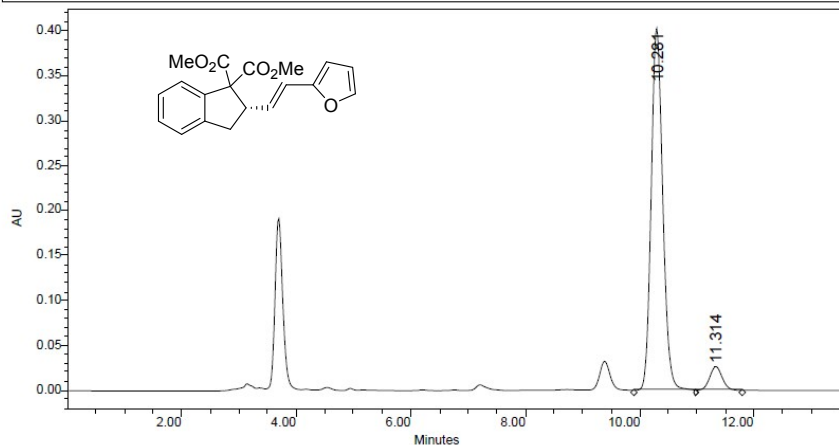
USTC

Project Name: wx
Reported by User: System

'Breeze

SAMPLE INFORMATION

Sample Name:	wx-83-2-5%-1ml-AD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	7/14/2017 4:56:18 PM
Vial:	55	Acq. Method:	5% 1ML
Injection #:	1	Date Processed:	8/24/2017 11:02:01 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	10.281	5687911	93.26	403375	93.80
2	11.314	411298	6.74	26671	6.20

Dimethyl (S,E)-2-(2-(naphthalen-2-yl)vinyl)-2,3-dihydro-1H-indene-1,1-dicarboxylate (Z) (3ap)

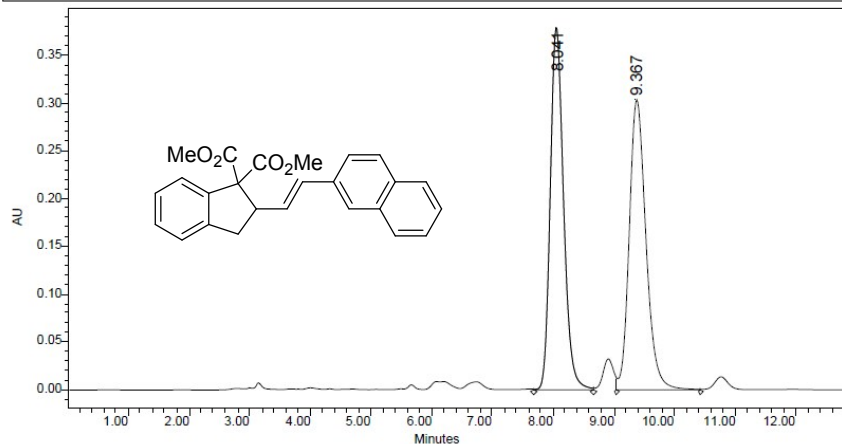
USTC

Project Name: wx
Reported by User: System

'Breeze

SAMPLE INFORMATION

Sample Name:	zl-15-1-5%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/9/2017 7:04:22 PM
Vial:	1	Acq. Method:	5% 1ML
Injection #:	1	Date Processed:	8/24/2017 10:27:12 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	8.041	5788682	49.80	381106	55.59
2	9.367	5834811	50.20	304501	44.41

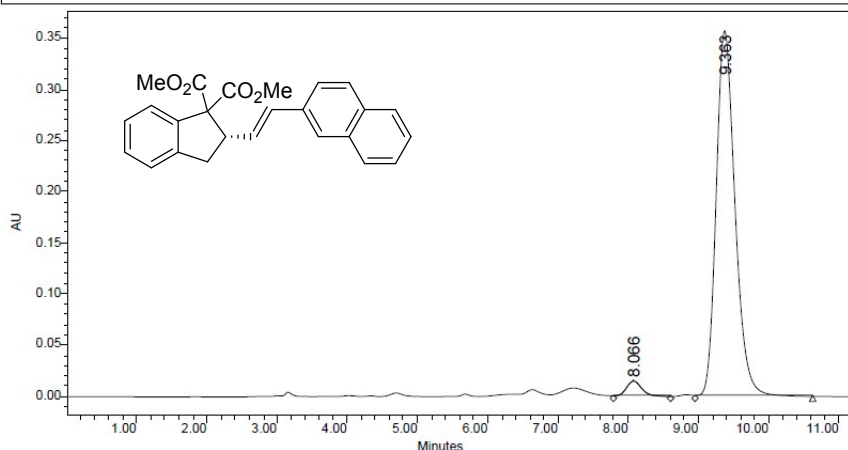
USTC

Project Name: wx
Reported by User: System

'Breeze

SAMPLE INFORMATION

Sample Name:	wx-78-5-5%-1ml-OD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/25/2017 3:57:07 PM
Vial:	20	Acq. Method:	5% 1ML
Injection #:	1	Date Processed:	8/24/2017 10:29:23 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (Δ *sec)	% Area	Height (Δ)	% Height
1	8.066	233268	3.37	15085	4.05
2	9.363	6682259	96.63	357691	95.95

(S,E)-(2-styryl-2,3-dihydro-1H-indene-1,1-diyl)dimethanol (4)

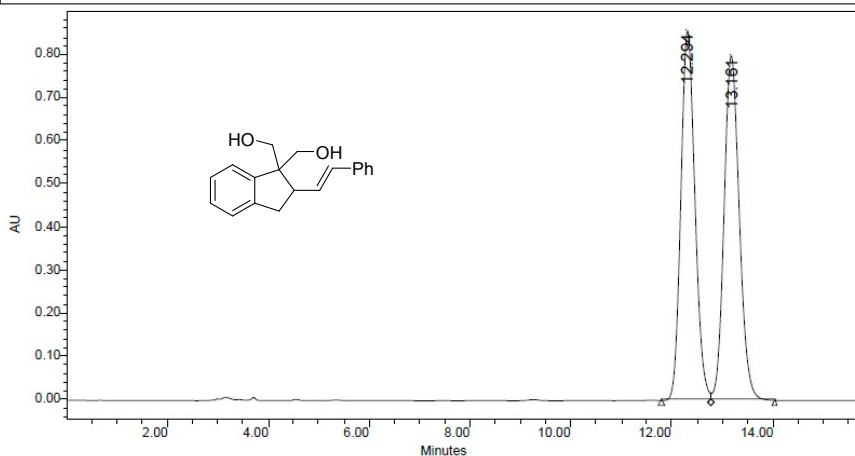
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-2OH-10%-1ml-AD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	8/21/2017 10:59:16 AM
Vial:	83	Acq. Method:	10%1ML
Injection #:	1	Date Processed:	9/11/2017 9:15:09 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	12.294	16640405	49.79	857817	51.75
2	13.161	16780452	50.21	799808	48.25

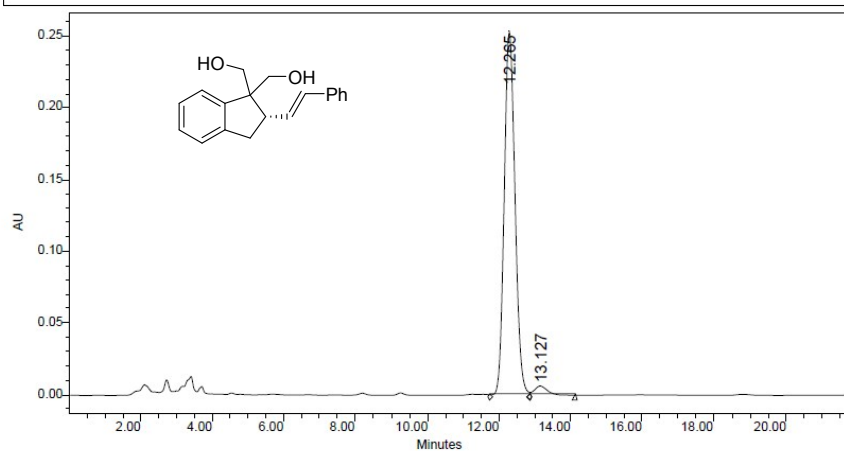
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-72-10%-1ml-AD	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	8/21/2017 11:22:42 AM
Vial:	84	Acq. Method:	10%1ML
Injection #:	1	Date Processed:	9/11/2017 9:15:29 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	12.265	5286131	97.03	253177	97.53
2	13.127	161627	2.97	6415	2.47

(R)-(2,3-dihydro-1H-indene-1,1,2-triyl)trimethanol (6)

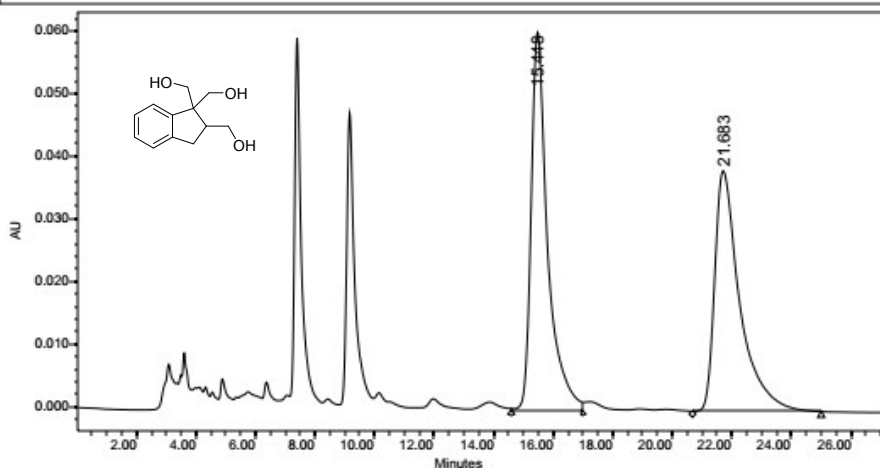
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name: wx-01-105-Rac-AD-15%-1ml
Sample Type: Unknown
Vial: 134
Injection #: 1
Injection Volume: 20.00 ul
Run Time: 60.00 Minutes
Acquired By: System
Date Acquired: 9/14/2017 2:32:33 PM
Acq. Method: 15% 1ml 254
Date Processed: 1/16/2018 10:32:00 AM
Channel Name: 2487Channel 1
Sample Set Name:



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	15.448	2331789	50.91	60428	61.15
2	21.683	2248106	49.09	38397	38.85

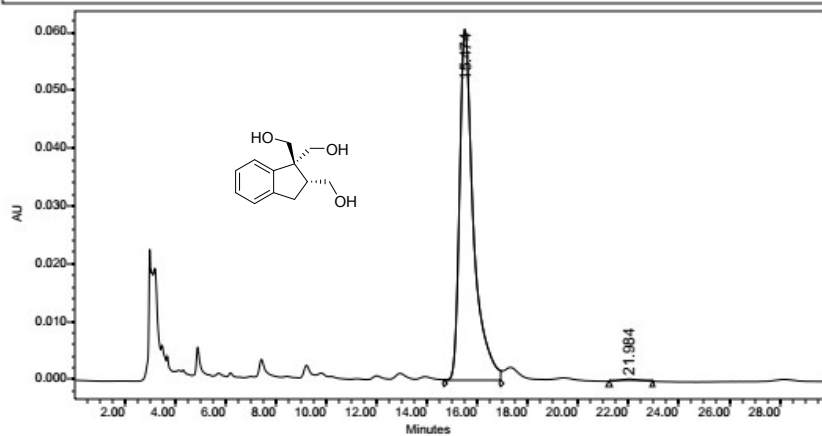
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name: wx-01-105-Asy-AD-15%-1ml
Sample Type: Unknown
Vial: 135
Injection #: 1
Injection Volume: 20.00 ul
Run Time: 60.00 Minutes
Acquired By: System
Date Acquired: 9/14/2017 3:05:39 PM
Acq. Method: 15% 1ml 254
Date Processed: 1/16/2018 10:32:34 AM
Channel Name: 2487Channel 1
Sample Set Name:



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	15.474	2340830	99.25	60765	99.39
2	21.984	17626	0.75	370	0.61

Dimethyl (S)-2-(2,2-diphenylvinyl)-2,3-dihydro-1H-indene-1,1-dicarboxylate (S3aa)

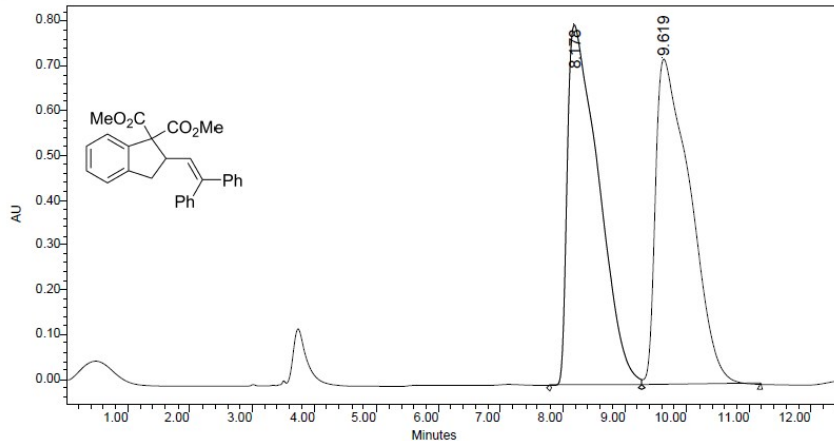
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-01-125-1%-OD-R1	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	7/6/2018 2:29:58 PM
Vial:	142	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	7/13/2018 7:16:25 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1 8.178	28143681	49.87	806039	52.51
2 9.619	28295258	50.13	728893	47.49

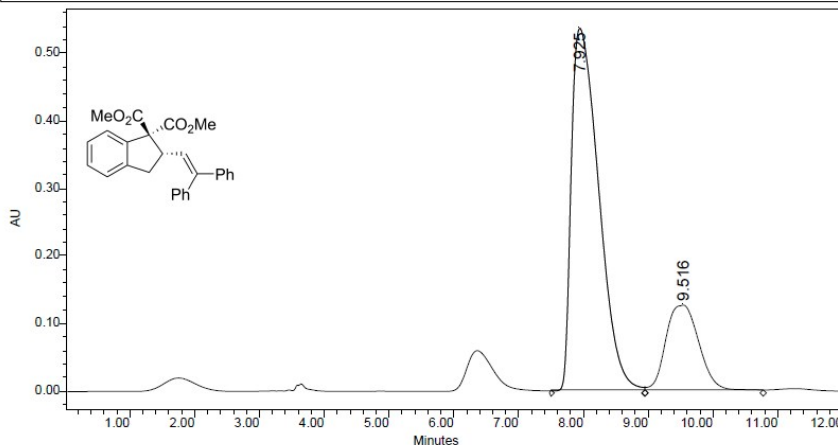
USTC

Project Name: wx
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	wx-01-125-1%-OD-A1	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	7/6/2018 3:09:50 PM
Vial:	144	Acq. Method:	1% 1ml
Injection #:	1	Date Processed:	7/13/2018 7:15:24 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1 7.925	15850424	77.47	538633	80.85
2 9.516	4610722	22.53	127576	19.15

Dimethyl (S,E)-2-methyl-2-styryl-2,3-dihydro-1H-indene-1,1-dicarboxylate (S3ab)

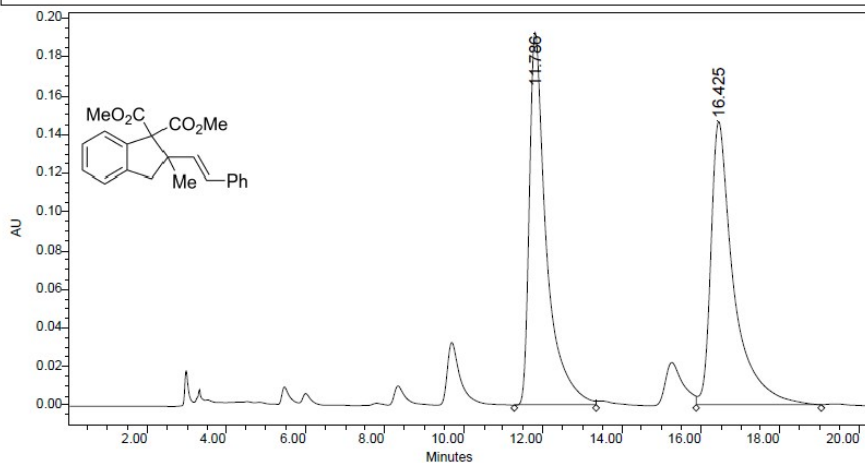
USTC

Project Name: wx
Reported by User: System

'Breeze

SAMPLE INFORMATION

Sample Name:	wx-01-125-2%-AD-R3	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	7/6/2018 8:12:44 PM
Vial:	146	Acq. Method:	2%
Injection #:	1	Date Processed:	7/13/2018 7:13:57 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	11.786	5822844	49.51	192913	56.77
2	16.425	5939021	50.49	146911	43.23

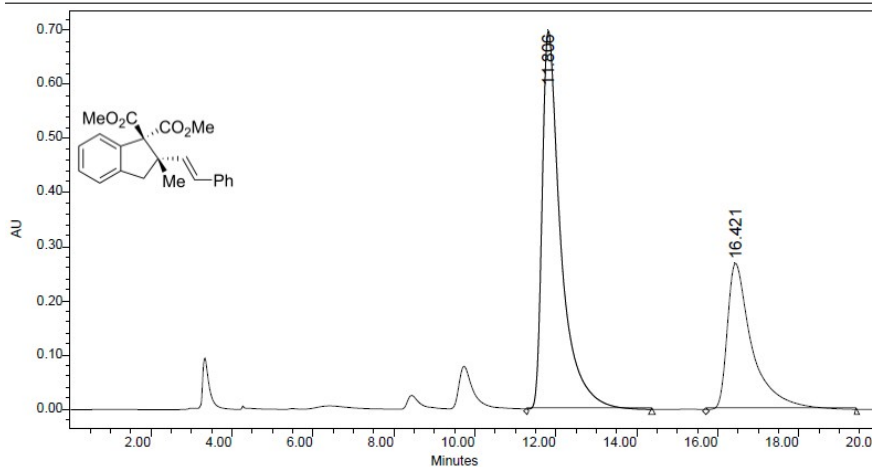
USTC

Project Name: wx
Reported by User: System

'Breeze

SAMPLE INFORMATION

Sample Name:	wx-01-125-2%-AD-A3	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	7/6/2018 8:42:31 PM
Vial:	147	Acq. Method:	2%
Injection #:	1	Date Processed:	7/13/2018 7:12:57 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	11.806	22449989	66.05	700170	72.15
2	16.421	11537602	33.95	270230	27.85