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Support Information

Organocatalytic Enantioselective Ring-Reorganization Domino Sequence of Methyleneindolinones with 2-Aminomalonates

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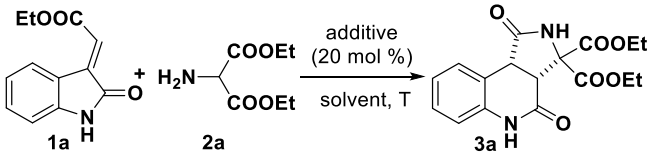
1. General experimental information

Unless otherwise noted, all the reagents were purchased from commercial suppliers and used without further purification. ^{1}H NMR spectra were recorded at 400 MHz. The chemical shifts were recorded in ppm relative to tetramethylsilane and with the solvent resonance as the internal standard. Data were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz), integration. ^{13}C NMR data were collected at 100 MHz with complete proton decoupling. Chemical shifts were reported in ppm from the tetramethylsilane with the solvent resonance as internal standard. Infrared spectra (IR) were measured by FT-IR apparatus. High resolution mass spectroscopy (HRMS) was recorded on TOF MS ES+ mass spectrometer and acetonitrile was used to dissolve the sample. Column chromatography was carried out on aluminum oxide (200-300 mesh). All the substituted methyleneindolinones[1] and aminomalonic acid diesters[2] were prepared according to the reported procedure.

2. Experimental procedures and characterization data

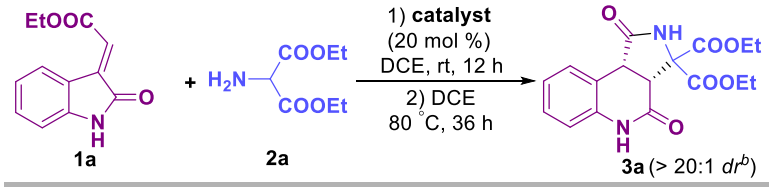
2.1. Optimization of the racemic ring-opening cascade reaction[a]

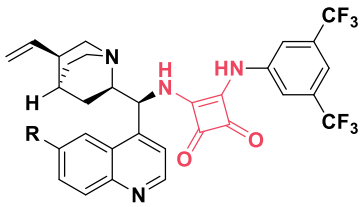


entry	additive	solvent	T (℃)	time (h)	yield[b] (%)
1	-	$CHCl_3$	rt	48	-
2	Et_3N	$CHCl_3$	rt	48	trace
3	Et_3N	$CHCl_3$	40	96	37
4	Et_3N	$CHCl_3$	80	48	69
5	Et_3N	DCE	80	48	69
6	Et_3N	DMF	80	48	63
7	Et_3N	EtOH	80	48	44
8	Et_3N	1,4-dioxane	80	48	65
9	Et_3N	THF	80	48	59
10	Et_3N	toluene	80	48	75
11	Et_3N	toluene	110	24	69
12	-	toluene	80	48	87
13[c]	-	-	**80**	**20**	**95**
14[c,d]	-	-	80	20	82

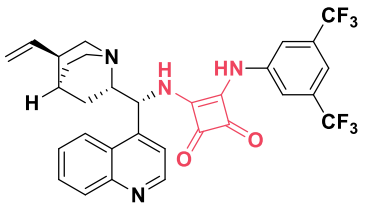
[a]Unless otherwise noted, all reactions were carried out using methyleneindolinone **1a** (0.20 mmol, 1.0 equiv.), diethyl aminomalonate **2a** (0.30 mmol, 1.5 equiv.) and additive (0.04 mmol, 20 mol %) in solvent (1.0 mL). [b]Isolated yields. [c]3.0 equiv. of **2a** was added in this reaction. [d]Recrystallized over dichloromethane/*n*-hexane.

2.2. Screening other chiral bifunctional cinchona alkaloid catalysts[a]

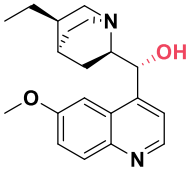




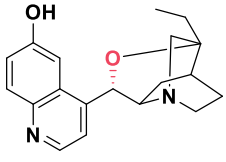
4g R = H, 70% yield[c], 65% *ee*[d]
4h R = OMe, 72% yield, 64% *ee*



4i 71% yield, -25% *ee*



4j 58% yield, -15% *ee*

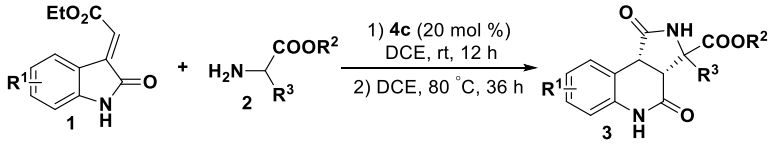


4k 45% yield, 66% *ee*

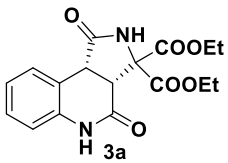
[a]Unless otherwise noted, all reactions were carried out using methyleneindolinone **1a** (0.20

mmol, 1.0 equiv.), diethyl aminomalonate **2a** (0.4 mmol, 2.0 equiv.) and catalyst (0.04 mmol, 20 mol %) in DCE (1.0 mL). After 12 h, the reaction mixture was carried out at 80 ℃ for 36 h. [b]Determined by ^{1}H NMR. [c]Isolated yield. [d]Determined by HPLC on a chiral stationary phase.

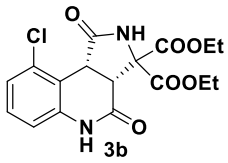
2.3. General procedure for the synthesis of pyrrolo[3,4-*c*]quinolinones 3



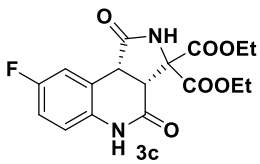
Methyleneindolinones **1** (0.20 mmol, 1.0 equiv.), 2-aminomalonates **2** (0.40 mmol, 2.0 equiv.) and catalyst **4c** (0.04 mmol, 20 mol %) were well mixed in 1,2-dichloroethane (1.0 mL). The resulting mixture was stirred at room temperature until the TLC analysis showed the complete consumption of the starting materials **1**. Subseqently, the reaction mixture was stirred at 80 ℃ (preheated) for 36 h. The reaction mixture was then cooled to room temperature, concentrated under reduced pressure and purified by flash column chromatography on silica gel (EtOAc/PE = 20%-40%) to yield the corresponding products **3**.



(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3a: White solid (58.6 mg, 85% yield, 97% *ee*, >20:1 *dr*); m.p. 247-248 °C; $[\alpha]_D^{20}$ = +68.2 (c = 0.1 in dichloromethane); IR (KBr) *v* 3091, 2998, 1687, 1499, 1388, 1276, 1212, 1077, 1022, 758, 490 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-*d*$_6$) *δ* 10.46 (s, 1H), 9.35 (s, 1H), 7.33 (d, *J* = 7.2 Hz, 1H), 7.18-7.22 (m, 1H), 6.99 (td, *J* = 7.6, 0.8 Hz, 1H), 6.86 (d, *J* = 7.6 Hz, 1H), 4.12-4.32 (m, 4H), 4.04-4.10 (m, 1H), 4.00 (d, *J* = 9.6 Hz, 1H), 1.23 (t, *J* = 7.0 Hz, 3H), 1.16 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-*d*$_6$) *δ* 173.7, 168.2, 167.7, 165.5, 136.8, 129.9, 128.6, 122.7, 117.3, 115.3, 70.3, 62.7, 62.1, 46.1, 43.3, 14.2, 14.1; HRMS (TOF-ES+) m/z: $[M+H]^+$ calcd for $C_{17}H_{19}N_2O_6^+$ 347.1238, found 347.1246; HPLC analysis: (CHIRALCEL OD-H, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 11.91 min (minor), 20.77 min (major).

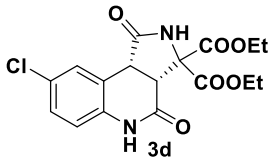


(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3b: White solid (60.1 mg, 79% yield, 91% *ee*, >20:1 *dr*); m.p. 187-188 °C; $[\alpha]_D^{20}$ = +32.1 (c = 0.1 in dichloromethane); IR (KBr) *v* 3281, 1731, 1680, 1488, 1372, 1203, 1002, 749, 692 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-*d*$_6$) *δ* 10.65 (s, 1H), 9.46 (s, 1H), 7.26 (t, *J* = 8.0 Hz, 1H), 7.12 (d, *J* = 8.0 Hz, 1H), 6.87 (d, *J* = 8.0 Hz, 1H), 4.25-4.36 (m, 4H), 4.12-4.23 (m, 2H), 1.21-1.25 (m, 6H); ^{13}C NMR (100 MHz, DMSO-*d*$_6$) *δ* 171.6, 168.1, 167.1, 165.7, 138.5, 134.5, 130.2, 123.6, 116.1, 114.4, 70.3, 62.9, 62.0, 46.4, 42.6, 14.2(3), 14.2(1); HRMS (TOF-ES+) m/z: $[M+Na]^+$ calcd for $C_{17}H_{17}ClN_2NaO_6^+$ 403.0667, found 403.0682; HPLC analysis: (CHIRALCEL IA, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 11.68 min (major), 19.72 min (minor).

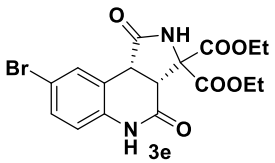


(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3c: White solid (62.6 mg, 86% yield, 99% *ee*, >20:1 *dr*); m.p. 258-259 °C; $[\alpha]_D^{20}$ = +73.6 (c = 0.1 in dichloromethane); IR (KBr) *v* 3346, 3222, 2994, 1726, 1686, 1507, 1386, 1216, 1078, 1024, 828, 721 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-*d*$_6$) *δ* 10.49

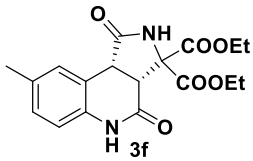
(s, 1H), 9.41 (s, 1H), 7.19 (dd, J = 9.6, 2.8 Hz, 1H), 7.07 (td, J = 8.8, 2.8 Hz, 1H), 6.87 (dd, J = 8.8, 4.8 Hz, 1H), 4.12-4.32 (m, 4H), 4.04-4.10 (m, 2H), 1.23 (t, J = 7.0 Hz, 3H), 1.15 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 173.4, 168.1, 167.6, 165.3, 157.9 (d, $^{1}J_{C\text{-}F}$ = 236 Hz), 133.4 (d, $^{4}J_{C\text{-}F}$ = 2 Hz), 119.3 (d, $^{3}J_{C\text{-}F}$ = 9 Hz), 116.5 (d, $^{3}J_{C\text{-}F}$ = 9 Hz), 116.3 (d, $^{2}J_{C\text{-}F}$ = 24 Hz), 115.3 (d, $^{2}J_{C\text{-}F}$ = 22 Hz), 70.3, 62.8, 62.1, 45.6, 43.2, 14.2, 14.1; HRMS (TOF-ES+) m/z: $[M+H]^+$ calcd for $C_{17}H_{18}FN_2O_6^+$ 365.1143, found 365.1156; HPLC analysis: (CHIRALCEL OD-H, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 10.75 min (minor), 17.59 min (major).



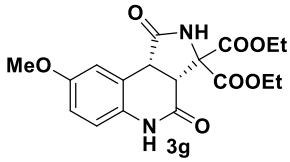
(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3d: White solid (60.9 mg, 80% yield, >99% *ee*, >20:1 *dr*); m.p. 248-249 °C; $[\alpha]_D^{20}$ = +115.9 (c = 0.1 in dichloromethane); IR (KBr) ν 3345, 2981, 1740, 1681, 1499, 1214, 1020, 822, 620, 527 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.57 (s, 1H), 9.42 (s, 1H), 7.40 (d, J = 2.4 Hz, 1H), 7.27 (dd, J = 8.8, 2.4 Hz, 1H), 6.87 (d, J = 8.8 Hz, 1H), 4.12-4.32 (m, 4H), 4.04-4.10 (m, 2H), 1.23 (t, J = 7.2 Hz, 3H), 1.15 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 173.4, 168.1, 167.6, 165.4, 135.9, 129.4, 128.5, 126.3, 119.5, 116.8, 70.4, 62.8, 62.2, 45.6, 43.0, 14.3, 14.1; HRMS (TOF-ES+) m/z: $[M+H]^+$ calcd for $C_{17}H_{18}ClN_2O_6^+$ 381.0848, found 381.0865; HPLC analysis: (CHIRALCEL OD-H, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 11.29 min (minor), 16.48 min (major).



(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3e: White solid (68.7 mg, 81% yield, >99% *ee*, >20:1 *dr*); m.p. 238-239 °C; $[\alpha]_D^{20}$ = +52.4 (c = 0.1 in dichloromethane); IR (KBr) ν 3061, 2974, 1729, 1678, 1498, 1389, 1210, 1079, 851, 493 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.56 (*br* s, 1H), 9.40 (*br* s, 1H), 7.52 (d, J = 2.1 Hz, 1H), 7.39 (dd, J = 8.5, 2.2 Hz, 1H), 6.82 (d, J = 8.5 Hz, 1H), 4.14-4.32 (m, 4H), 4.04-4.13 (m, 2H), 1.23 (t, J = 7.0 Hz, 3H), 1.15 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 173.4, 168.0, 167.6, 165.4, 136.3, 132.2, 131.3, 119.9, 117.3, 114.1, 70.4, 62.8, 62.2, 45.7, 42.9, 14.3, 14.1; HRMS (TOF-ES+) m/z: $[M+H]^+$ calcd for $C_{17}H_{18}BrN_2O_6^+$ 425.0343, found 425.0351; HPLC analysis: (CHIRALCEL OD-H, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 11.24 min (minor), 17.01 min (major).

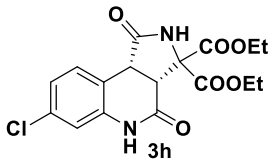


(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3f: White solid (57.7 mg, 80% yield, 98% *ee*, >20:1 *dr*); m.p. 250-251 °C; $[\alpha]_D^{20}$ = +72.2 (c = 0.1 in dichloromethane); IR (KBr) ν 3348, 1736, 1673, 1514, 1394, 1214, 1022, 855 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.36 (s, 1H), 9.30 (s, 1H), 7.13 (s, 1H), 7.01 (d, J = 8.1 Hz, 1H), 6.75 (d, J = 8.0 Hz, 1H), 4.11-4.31 (m, 4H), 4.03-4.09 (m, 1H), 3.93 (d, J = 9.2 Hz, 1H), 2.24 (s, 3H), 1.23 (t, J = 7.0 Hz, 3H), 1.15 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 173.7, 168.2, 167.7, 165.3, 134.4, 131.5, 130.2, 129.1, 117.1, 115.2, 70.3, 62.7, 62.0, 46.1, 43.4, 20.9, 14.3, 14.1; HRMS (TOF-ES+) m/z: $[M+H]^+$ calcd for $C_{18}H_{21}N_2O_6^+$ 361.1394, found 361.1391; HPLC analysis: (CHIRALCEL OD-H, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 13.96 min (minor), 21.96 min (major).

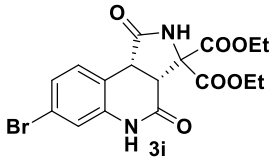


(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3g: White solid (65.4 mg, 87% yield, 90% *ee*, >20:1 *dr*); m.p. 210-211 °C; $[\alpha]_D^{20}$ = +62.4 (c = 0.1 in dichloromethane); IR (KBr) ν 3277, 1774, 1730, 1681, 1467, 1365, 1202, 1102, 1002, 805, 532 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ

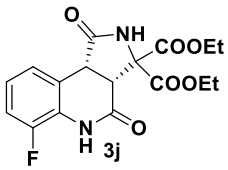
10.29 (s, 1H), 9.31 (s, 1H), 6.94 (s, 1H), 6.80 (s, 2H), 4.12-4.31 (m, 4H), 4.03-4.11 (m, 1H), 3.97 (d, J = 9.2 Hz, 1H), 3.71 (s, 3H), 1.23 (t, J = 7.0 Hz, 3H), 1.15 (t, J = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 173.6, 168.2, 167.7, 165.0, 155.1, 130.3, 118.5, 116.1, 115.3, 114.0, 70.3, 62.7, 62.0, 55.8, 46.0, 43.6, 14.2, 14.1; HRMS (TOF-ES+) m/z: $[M+Na]^+$ calcd for $C_{18}H_{20}N_2NaO_7^+$ 399.1163, found 399.1179; HPLC analysis: (CHIRALCEL OD-H, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 16.09 min (minor), 23.02 min (major).



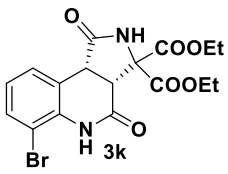
(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3h: White solid (69.9 mg, 92% yield, 95% *ee*, >20:1 *dr*); m.p. 232-233 °C; $[\alpha]_D^{20}$ = +52.2 (c = 0.1 in dichloromethane); IR (KBr) ν 3336, 2983, 1745, 1716, 1594, 1496, 1372, 1212, 1089, 861 cm^{-1}; ^{1}H NMR (400 MHz, acetone-d_6) δ 9.46 (s, 1H), 8.08 (s, 1H), 7.28 (d, J = 8.0 Hz, 1H), 6.93 (dd, J = 8.2, 2.2 Hz, 1H), 6.89 (d, J = 2.0 Hz, 1H), 4.28 (d, J = 9.2 Hz, 1H), 4.00-4.24 (m, 4H), 3.96 (d, J = 9.2 Hz, 1H), 1.15 (t, J = 7.2 Hz, 3H), 1.10 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, acetone-d_6) δ 172.2, 167.7, 166.9, 165.0, 138.0, 133.4, 131.4, 122.2, 116.2, 114.6, 69.9, 62.4, 61.8, 45.8, 43.1, 13.3, 13.2; HRMS (TOF-ES+) m/z: $[M+H]^+$ calcd for $C_{17}H_{18}ClN_2O_6^+$ 381.0848, found 381.0829; HPLC analysis: (CHIRALCEL OD-H, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 11.53 min (minor), 14.85 min (major).



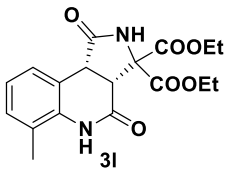
(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3i: White solid (67.8 mg, 80% yield, 98% *ee*, >20:1 *dr*); m.p. 245-246 °C; $[\alpha]_D^{20}$ = +53.8 (c = 0.1 in dichloromethane); IR (KBr) ν 3215, 2983, 1717, 1686, 1590, 1491, 1281, 1218, 1074, 1020, 860 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.55 (s, 1H), 9.39 (s, 1H), 7.30 (d, J = 8.4 Hz, 1H), 7.17 (dd, J = 8.0, 2.0 Hz, 1H), 7.04 (d, J = 1.6 Hz, 1H), 4.15-4.31 (m, 4H), 4.06-4.14 (m, 1H), 4.01 (d, J = 9.6 Hz, 1H), 1.23 (t, J = 7.2 Hz, 3H), 1.16 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 173.4, 168.0, 167.6, 165.6, 138.5, 131.8, 125.3, 121.1, 117.6, 116.9, 70.3, 62.8, 62.2, 45.8, 42.8, 14.3, 14.1; HRMS (TOF-ES+) m/z: $[M+H]^+$ calcd for $C_{17}H_{18}BrN_2O_6^+$ 425.0343, found 425.0353; HPLC analysis: (CHIRALCEL OD-H, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 8.33 min (minor), 11.87 min (major).



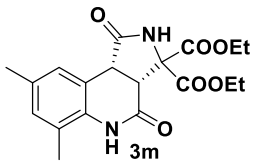
(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3j: White solid (59.7 mg, 82% yield, 99% *ee*, >20:1 *dr*); m.p. 189-190 °C; $[\alpha]_D^{20}$ = +58.5 (c = 0.1 in dichloromethane); IR (KBr) ν 3334, 3217, 1737, 1680, 1506, 1375, 1214, 1023, 759 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.36 (*br* s, 1H), 9.39 (*br* s, 1H), 7.19 (d, J = 7.6 Hz, 1H), 7.12-7.17 (m, 1H), 6.98-7.03 (m, 1H), 4.26-4.32 (m, 2H), 4.15-4.24 (m, 2H), 4.05-4.13 (m, 2H), 1.23 (t, J = 7.2 Hz, 3H), 1.16 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 173.3, 168.0, 167.6, 165.5, 149.3 (d, $^1J_{C\text{-}F}$ = 244 Hz), 125.5 (d, $^3J_{C\text{-}F}$ = 3 Hz), 125.1 (d, $^2J_{C\text{-}F}$ = 13 Hz), 122.9 (d, $^3J_{C\text{-}F}$ = 7 Hz), 120.1 (d, $^4J_{C\text{-}F}$ = 2 Hz), 115.1 (d, $^2J_{C\text{-}F}$ = 18 Hz), 70.3, 62.8, 62.2, 46.1, 43.4, 14.2, 14.1; HRMS (TOF-ES+) m/z: $[M+H]^+$ calcd for $C_{17}H_{18}FN_2O_6^+$ 365.1143, found 365.1150; HPLC analysis: (CHIRALCEL OD-H, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 12.40 min (minor), 19.46 min (major).



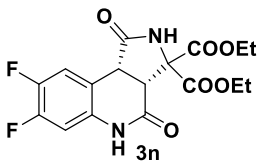
(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3k: White solid (66.9 mg, 79% yield, 90% *ee*, >20:1 *dr*); m.p. 172-173 °C; $[\alpha]_D^{20}$ = +58.5 (c = 0.1 in dichloromethane); IR (KBr) *v* 3297, 1732, 1687, 1489, 1371, 1295, 1216, 1086, 1023 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.94 (s, 1H), 7.49 (d, *J* = 8.1 Hz, 1H), 7.33 (d, *J* = 7.6 Hz, 1H), 7.00 (t, *J* = 7.8 Hz, 1H), 6.53 (s, 1H), 4.41 (d, *J* = 8.4 Hz, 1H), 4.30-4.38 (m, 4H), 4.07 (d, *J* = 8.8 Hz, 1H), 1.32 (t, *J* = 6.8 Hz, 3H), 1.31 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.8, 167.1, 166.6, 164.6, 133.2, 132.4, 129.4, 124.5, 118.1, 109.3, 69.3, 63.3, 63.0, 46.4, 44.5, 13.9, 13.8; HRMS (TOF-ES+) m/z: $[M+H]^+$ calcd for $C_{17}H_{18}BrN_2O_6^+$ 425.0343, found 425.0352; HPLC analysis: (CHIRALCEL OD-H, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 14.23 min (minor), 19.94 min (major).



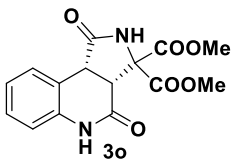
(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3l: White solid (55.0 mg, 76% yield, 80% *ee*, >20:1 *dr*); m.p. 177-178 °C; $[\alpha]_D^{20}$ = +78.2 (c = 0.1 in dichloromethane); IR (KBr) *v* 3225, 1679, 1337, 1209, 1021, 761, 538 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 9.68 (s, 1H), 9.33 (s, 1H), 7.16 (d, *J* = 7.6 Hz, 1H), 7.06 (d, *J* = 7.6 Hz, 1H), 6.91 (t, *J* = 7.6 Hz, 1H), 4.32-4.26 (m, 1H), 4.23-4.10 (m, 4H), 3.98 (d, *J* = 8.8 Hz, 1H), 2.20 (s, 3H), 1.23 (t, *J* = 7.2 Hz, 3H), 1.18 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 173.6, 168.1, 167.6, 166.1, 134.9, 130.4, 127.9, 123.5, 122.6, 117.7, 70.3, 62.8, 62.0, 46.3, 43.9, 17.6, 14.2, 14.1; HRMS (TOF-ES+) m/z: $[M+H]^+$ calcd for $C_{18}H_{20}KN_2O_6^+$ 399.0953, found 399.0928; HPLC analysis: (CHIRALCEL OD-H, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 12.30 min (minor), 16.27 min (major).



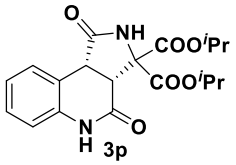
(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3m: Yellow solid (65.2 mg, 87% yield, 99% *ee*, >20:1 *dr*); m.p. 222-223 °C; $[\alpha]_D^{20}$ = +44.7 (c = 0.1 in dichloromethane); IR (KBr) *v* 3364, 3251, 1731, 1666, 1495, 1376, 1287, 1211, 859 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 9.62 (s, 1H), 9.29 (s, 1H), 6.97 (s, 1H), 6.89 (s, 1H), 4.09-4.31 (m, 5H), 3.92 (d, *J* = 8.8 Hz, 1H), 2.22 (s, 3H), 2.17 (s, 3H), 1.24 (t, *J* = 7.0 Hz, 3H), 1.19 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 173.6, 168.1, 167.6, 165.9, 132.5, 131.3, 131.0, 128.2, 123.4, 117.6, 70.2, 62.8, 62.0, 46.4, 43.9, 20.7, 17.5, 14.2, 14.1; HRMS (TOF-ES+) m/z: $[M+H]^+$ calcd for $C_{19}H_{23}N_2O_6^+$ 375.1551, found 375.1542; HPLC analysis: (CHIRALCEL OD-H, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 8.55 min (minor), 13.80 min (major).



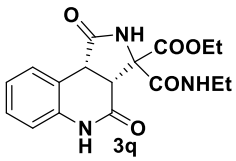
(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3n: White solid (68.2 mg, 89% yield, 99% *ee*, >20:1 *dr*); m.p. 240-241 °C; $[\alpha]_D^{20}$ = +64.0 (c = 0.1 in dichloromethane); IR (KBr) *v* 3347, 1738, 1685, 1532, 1378, 1213, 1024, 857 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 10.55 (s, 1H), 9.45 (s, 1H), 7.43 (t, *J* = 9.8 Hz, 1H), 6.86 (dd, *J* = 11.0, 7.4 Hz, 1H), 4.16-4.33 (m, 4H), 4.04-4.13 (m, 2H), 1.24 (t, *J* = 6.8 Hz, 3H), 1.17 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 173.3, 168.0, 167.5, 165.4, 149.3 (dd, $^{1,2}J_{C\text{-}F}$ = 243, 13 Hz), 145.0 (dd, $^{1,2}J_{C\text{-}F}$ = 238, 13 Hz), 133.9 (dd, $^{3,4}J_{C\text{-}F}$ = 10, 3 Hz), 118.5 (d, $^{2}J_{C\text{-}F}$ = 19 Hz), 114.3 (dd, $^{3,4}J_{C\text{-}F}$ = 7, 4 Hz), 104.1 (d, $^{2}J_{C\text{-}F}$ = 21 Hz), 70.3, 62.8, 62.2, 45.5, 42.7, 14.3, 14.1; HRMS (TOF-ES+) m/z: $[M+H]^+$ calcd for $C_{17}H_{17}F_2N_2O_6^+$ 383.1049, found 383.1033; HPLC analysis: (CHIRALCEL OD-H, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 10.41 min (minor), 14.67 min (major).



(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3o: White solid (52.8 mg, 83% yield, >99% *ee*, >20:1 *dr*); m.p. 264-265 °C; $[\alpha]_D^{20}$ = +67.3 (c = 0.1 in dichloromethane); IR (KBr) *v* 3449, 1761, 1674, 1381, 1287, 1221, 988, 757 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 10.43 (s, 1H), 9.34 (s, 1H), 7.30 (d, *J* = 7.2 Hz, 1H), 7.20 (t, *J* = 7.6 Hz, 1H), 6.99 (t, *J* = 7.4 Hz, 1H), 6.87 (d, *J* = 8.0 Hz, 1H), 4.26 (d, *J* = 9.2 Hz, 1H), 4.01 (d, *J* = 9.2 Hz, 1H), 3.78 (s, 3H), 3.67 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 173.6, 168.8, 168.2, 165.6, 136.7, 130.1, 128.7, 122.8, 117.3, 115.3, 70.2, 54.0, 53.2, 46.3, 43.4; HRMS (TOF-ES+) m/z: $[M+H]^+$ calcd for $C_{15}H_{15}N_2O_6^+$ 319.0925, found 319.0928; HPLC analysis: (CHIRALCEL IA, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 22.48 min (major), 34.76 min (minor).

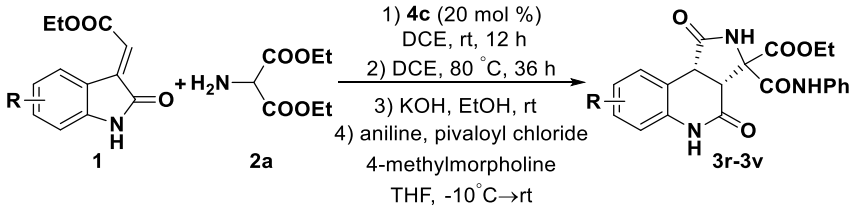


(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3p: White solid (57.6 mg, 77% yield, 97% *ee*, >20:1 *dr*); m.p. 223-224 °C; $[\alpha]_D^{20}$ = +70.0 (c = 0.1 in dichloromethane); IR (KBr) *v* 3260, 2926, 1760, 1712, 1383, 1283, 1236, 1106, 823, 767 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 9.03 (s, 1H), 7.37 (d, *J* = 7.6 Hz, 1H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.08 (t, *J* = 7.6 Hz, 1H), 6.76-6.77 (m, 2H), 5.09-5.21 (m, 2H), 4.35 (d, *J* = 8.8 Hz, 1H), 4.04 (d, *J* = 8.4 Hz, 1H), 1.29-1.32 (m, 9H), 1.25 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.8, 166.8, 166.4, 165.8, 135.4, 129.8, 129.0, 123.9, 116.4, 115.4, 71.2, 70.9, 69.7, 46.2, 44.2, 21.6, 21.5, 21.3(9), 21.3(7); HRMS (TOF-ES+) m/z: $[M+H]^+$ calcd for $C_{19}H_{23}N_2O_6^+$ 375.1551, found 375.1558; HPLC analysis: (CHIRALCEL IA, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 11.31 min (major), 20.70 min (minor).



(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3q: White solid (55.2 mg, 80% yield, >99% *ee*, >20:1 *dr*); m.p. 249-250 °C; $[\alpha]_D^{20}$ = +82.6 (c = 0.1 in dichloromethane); IR (KBr) *v* 3083, 2978, 1714, 1663, 1578, 1388, 1219, 1158, 763, 745, 658 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 10.65 (s, 1H), 8.76 (s, 1H), 8.33 (t, *J* = 5.2 Hz, 1H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.20 (t, *J* = 7.6 Hz, 1H), 7.00 (t, *J* = 7.6 Hz, 1H), 6.89 (d, *J* = 7.6 Hz, 1H), 4.12 (d, *J* = 10.0 Hz, 1H), 3.90-3.97 (m, 3H), 3.18-3.25 (m, 2H), 1.09 (t, *J* = 7.2 Hz, 3H), 0.96 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 173.8, 168.9, 167.3(4), 167.2(6), 136.5, 128.5, 128.4, 123.1, 117.7, 115.7, 70.8, 62.1, 45.6, 42.4, 34.8, 14.8, 13.8; HRMS (TOF-ES+) m/z: $[M+Na]^+$ calcd for $C_{17}H_{19}N_3NaO_5^+$ 368.1217, found 368.1231; HPLC analysis: (CHIRALCEL IA, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 29.61 min (major), 53.41 min (minor).

2.4. Alternative reaction sequence

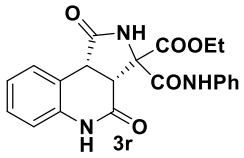


Standard domino sequence: Methyleneindolinones **1** (0.20 mmol, 1.0 equiv.), 2-aminomalonates **2** (0.40 mmol, 2.0 equiv.) and catalyst **4c** (0.04 mmol, 20 mol %) were well mixed in 1,2-dichloroethane (1.0 mL). The resulting mixture was stirred at room temperature until the TLC

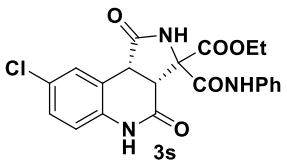
analysis showed the complete consumption of the starting materials **1**. Subseqently, the reaction mixture was stirred at 80 ℃ (preheated) for 36 h. The reaction mixture was then cooled to room temperature, concentrated under reduced pressure and purified by flash column chromatography on silica gel (EtOAc/PE = 20%-40%) to yield the corresponding products.

Hydrolysis: A solution of KOH (1.0 equiv.) in water (1.0 M) was added to a solution of pyrroloquinolinone **3** in ethanol (0.1 M), and the resulting mixture was stirred for 30 min at ambient temperature. Then 3N hydrochloric acid solution was added until pH = 3. Then the mixture was extracted with EtOAc. The organic layer was washed with saturated brine. The organic layer was dried and concentrated *in vacuo* to afford the crude monoacid, which was used for the next step without further purification.

Amidation: The crude monoacid was dissolved in dry tetrahydrofuran, and the solution was cooled in a salt ice bath to -10 ℃. Methylmorpholine (1.0 equiv.) and pivaloyl chloride (1.0 equiv.) were added, and the reaction mixture was stirred for 30 min at -10 ℃. Aniline (1.5 equiv.) was added, and the reaction mixture was stirred an additional 30 min at -10 ℃. The ice bath was removed, and the reaction mixture was stirred overnight at ambient temperature. The reaction mixture was then concentrated under reduced pressure and purified by flash column chromatography on silica gel (EtOAc/PE = 20%-40%) to yield the corresponding products **3**.

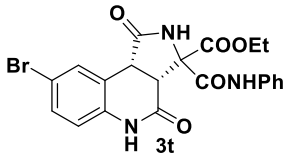


(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3r: White solid (47.1 mg, 60% yield, 94% *ee*, >20:1 *dr*); m.p. 188-189 °C; $[\alpha]_D^{20}$ = +76.4 (c = 0.1 in dichloromethane); IR (KBr) *v* 3281, 1729, 1679, 1486, 1367, 1203, 1103, 1002, 748, 693 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 10.87 (s, 1H), 10.57 (s, 1H), 9.01 (s, 1H), 7.58-7.63 (m, 3H), 7.39 (t, *J* = 8.0 Hz, 2H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.15 (t, *J* = 7.6 Hz, 1H), 7.04 (t, *J* = 7.6 Hz, 1H), 6.94 (d, *J* = 8.0 Hz, 1H), 4.36 (d, *J* = 10.8 Hz, 1H), 4.03 (d, *J* = 10.8 Hz, 1H), 3.96 (q, *J* = 6.8 Hz, 2H), 0.91 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 174.2, 168.9, 167.9, 166.0, 138.8, 136.2, 129.6, 128.4, 128.1, 124.6, 123.4, 119.8, 117.7, 115.9, 71.5, 62.5, 45.1, 41.8, 13.7; HRMS (TOF-ES+) m/z: $[M+Na]^+$ calcd for $C_{21}H_{19}N_3NaO_5^+$ 416.1217, found 416.1235; HPLC analysis: (CHIRALCEL IA, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 19.25 min (major), 36.13 min (minor).

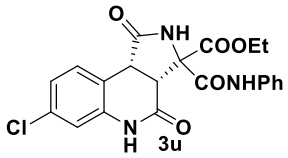


(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3s: White solid (50.3 mg, 59% yield, >99% *ee*, >20:1 *dr*); m.p. 195-196 °C; $[\alpha]_D^{20}$ = +125.8 (c = 0.1 in dichloromethane); IR (KBr) *v* 3062, 1666, 1492, 1394, 1228, 1041, 829, 759, 692 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 11.01 (s, 1H), 10.54 (s, 1H), 9.15 (s, 1H), 7.65 (s, 1H), 7.60 (d, *J* = 8.0 Hz, 2H), 7.40 (t, *J* = 8.0 Hz, 2H), 7.32 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.15 (t, *J* = 7.6 Hz, 1H), 6.97 (d, *J* = 8.8 Hz, 1H), 4.40 (d, *J* = 10.8 Hz, 1H), 4.09 (d, *J* = 11.2 Hz, 1H), 4.00 (q, *J* = 6.8 Hz, 2H), 0.96 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 173.8, 168.8, 167.8, 165.8, 138.7, 135.4, 129.6, 128.3, 127.7, 127.0, 124.6, 119.9, 119.8, 117.5, 71.6, 62.6, 44.6, 41.6, 13.8; HRMS (TOF-ES+) m/z: $[M+Na]^+$ calcd for $C_{21}H_{18}ClN_3NaO_5^+$ 450.0827, found 450.0836; HPLC analysis: (CHIRALCEL IA, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 18.63 min (major), 32.74 min (minor).

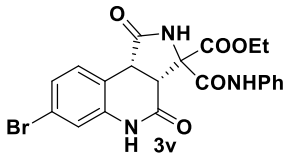
(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3t: White solid (57.4 mg, 61% yield, >99% *ee*, >20:1 *dr*); m.p. 211-212 °C; $[\alpha]_D^{20}$ = +118.4 (c = 0.1 in dichloromethane); IR (KBr) *v* 2919, 1679, 1485, 1374, 1174, 1056, 754 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 11.00 (s, 1H), 10.50 (s, 1H), 9.12 (s,



1H), 7.79 (s, 1H), 7.60 (d, J = 7.6 Hz, 2H), 7.38-7.45 (m, 3H), 7.16 (t, J = 7.6 Hz, 1H), 6.92 (d, J = 8.8 Hz, 1H), 4.39 (d, J = 11.2 Hz, 1H), 4.09 (d, J = 11.2 Hz, 1H), 4.00 (q, J = 6.8 Hz, 2H), 0.96 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 173.8, 168.8, 167.8, 165.8, 138.7, 135.8, 131.2, 130.5, 129.5, 124.6, 120.3, 119.9, 117.9, 114.9, 71.6, 62.6, 44.6, 41.5, 13.8; HRMS (TOF-ES+) m/z: $[M+Na]^+$ calcd for $C_{21}H_{18}BrN_3NaO_5^+$ 494.0322, found 494.0339; HPLC analysis: (CHIRALCEL IA, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 17.47 min (major), 32.22 min (minor).

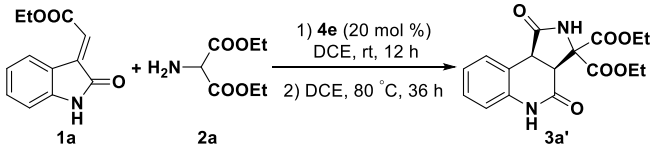


(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3u: White solid (49.4 mg, 58% yield, 99% *ee*, >20:1 *dr*); m.p. 235-236 °C; $[\alpha]_D^{20}$ = +88.9 (c = 0.1 in dichloromethane); IR (KBr) ν 3270, 1695, 1491, 1394, 1236, 749, 571 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.99 (s, 1H), 10.44 (s, 1H), 9.08 (s, 1H), 7.59-7.63 (m, 3H), 7.40 (t, J = 7.6 Hz, 2H), 7.11-7.17 (m, 2H), 6.99 (s, 1H), 4.40 (d, J = 10.8 Hz, 1H), 3.99-4.07 (m, 3H), 0.97 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 173.8, 168.8, 168.0, 165.8, 138.7, 137.8, 132.7, 129.9, 129.5, 124.7, 123.0, 119.9, 116.9, 115.3, 71.5, 62.6, 44.9, 41.5, 13.8; HRMS (TOF-ES+) m/z: $[M+Na]^+$ calcd for $C_{21}H_{18}ClN_3NaO_5^+$ 450.0827, found 450.0843; HPLC analysis: (CHIRALCEL IA, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 15.62 min (major), 28.68 min (minor).



(3*S*, 3a*R*, 9b*R*)-Pyrrolo[3,4-*c*]quinolinone 3v: White solid (59.3 mg, 63% yield, 97% *ee*, >20:1 *dr*); m.p. 263-264 °C; $[\alpha]_D^{20}$ = +120.2 (c = 0.1 in dichloromethane); IR (KBr) ν 3252, 1680, 1485, 1374, 1247, 1172, 789, 756 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.96 (s, 1H), 10.43 (s, 1H), 9.07 (s, 1H), 7.59 (d, J = 8.0 Hz, 2H), 7.55 (d, J = 8.4 Hz, 1H), 7.39 (t, J = 7.6 Hz, 2H), 7.24 (dd, J = 8.4, 1.6 Hz, 1H), 7.15 (t, J = 7.6 Hz, 1H), 7.12 (s, 1H), 4.39 (d, J = 10.8 Hz, 1H), 3.98-4.03 (m, 3H), 0.97 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 173.8, 168.8, 168.0, 165.8, 138.7, 138.0, 130.2, 129.5, 125.9, 124.7, 120.9, 119.9, 118.1, 117.3, 71.5, 62.6, 44.9, 41.5, 13.8; HRMS (TOF-ES+) m/z: $[M+Na]^+$ calcd for $C_{21}H_{18}BrN_3NaO_5^+$ 494.0322, found 494.0337; HPLC analysis: (CHIRALCEL IA, 30% *i*-propanol/*n*-hexane, 0.8 mL/min, UV: 254 nm), t_R = 20.48 min (major), 27.72 min (minor).

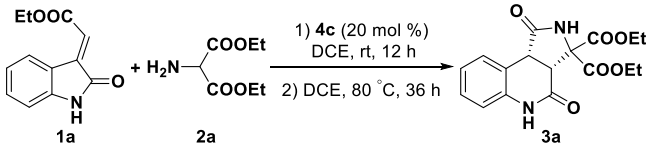
2.5. Synthesis of the enantiomer 3a'



Methyleneindolinone **1a** (0.20 mmol, 1.0 equiv.), amino acid ester **2a** (0.40 mmol, 2.0 equiv.) and catalyst **4e** (0.04 mmol, 20 mol %) were well mixed in 1,2-dichloroethane (1.0 mL). The resulting mixture was stirred at room temperature until the TLC analysis showed the complete consumption of the starting materials **1a**. Subseqently, the reaction mixture was stirred at 80 ℃ (preheated) for 36 h. The reaction mixture was then cooled to room temperature, concentrated under reduced pressure and purified by flash column chromatography on silica gel (EtOAc/PE = 20%-40%) to yield the corresponding product **3a'** as a white solid (58.1 mg, 84% yield, >99% *ee*, >20:1 *dr*); $[\alpha]_D^{20}$ = -70.0 (c = 0.1 in dichloromethane); HPLC analysis: (CHIRALCEL OD-H, 30% *i*-propanol/*n*-

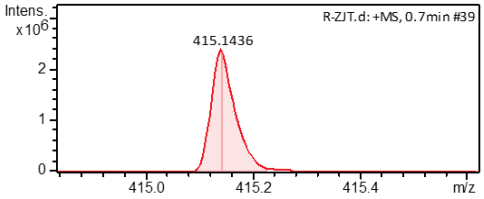
hexane, 0.8 mL/min, UV: 254 nm), t_R = 12.93 min (major), 28.70 min (minor).

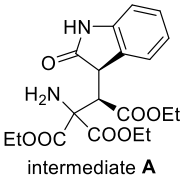
2.6. Synthetic procedure of 5 mmol scale model reaction



Methyleneindolinone **1a** (1.085 g, 5.0 mmol, 1.0 equiv.), amino acid ester **2a** (1.750 g, 10.0 mmol, 2.0 equiv.) and catalyst **4c** (0.595 g, 1.0 mmol, 20 mol %) were well mixed in 1,2-dichloroethane (25.0 mL). The resulting mixture was stirred at room temperature until the TLC analysis showed the complete consumption of the starting materials **1a**. Subseqently, the reaction mixture was stirred at 80 ℃ (preheated) for 36 h. The reaction mixture was then cooled to room temperature, concentrated under reduced pressure and purified by flash column chromatography on silica gel (EtOAc/PE = 20%-40%) to yield the corresponding product **3a** in 85% yield with 97% *ee* and >20:1 *dr*.

2.7. High-resolution mass spectrometry of the intermediate A



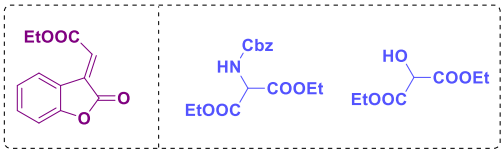


intermediate **A**

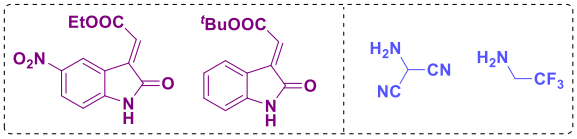
Methyleneindolinone **1a** (0.20 mmol, 1.0 equiv.), amino acid ester **2a** (0.40 mmol, 2.0 equiv.) and catalyst **4c** (0.04 mmol, 20 mol %) were well mixed in 1,2-dichloroethane (1.0 mL). The resulting mixture was stirred at room temperature until the TLC analysis showed the complete consumption of the starting materials **1a**. Subseqently, the reaction mixture was directly characterized by high-resolution mass spectrometry. HRMS (TOF-ES+) m/z: $[M+Na]^+$ calcd for $C_{19}H_{24}N_2NaO_7^+$ 415.1476, found 415.1436.

2.8. Unsuccessful substrates

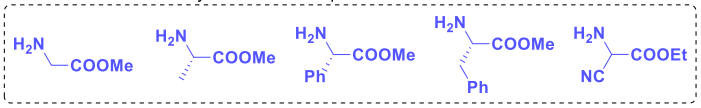
Michael addition products were obtained:



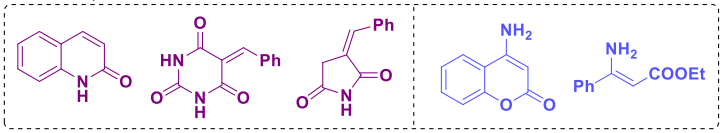
The reactions occurred with a trace yield:



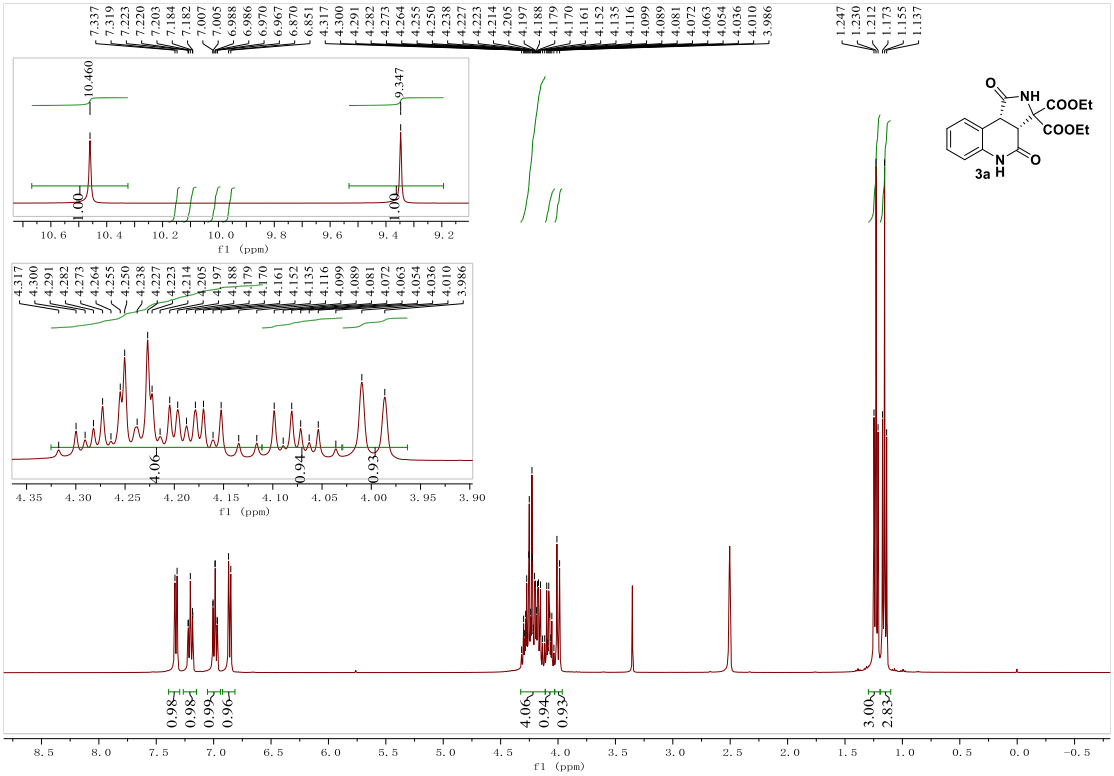
The reactions were messy and no desired products can be isolated:

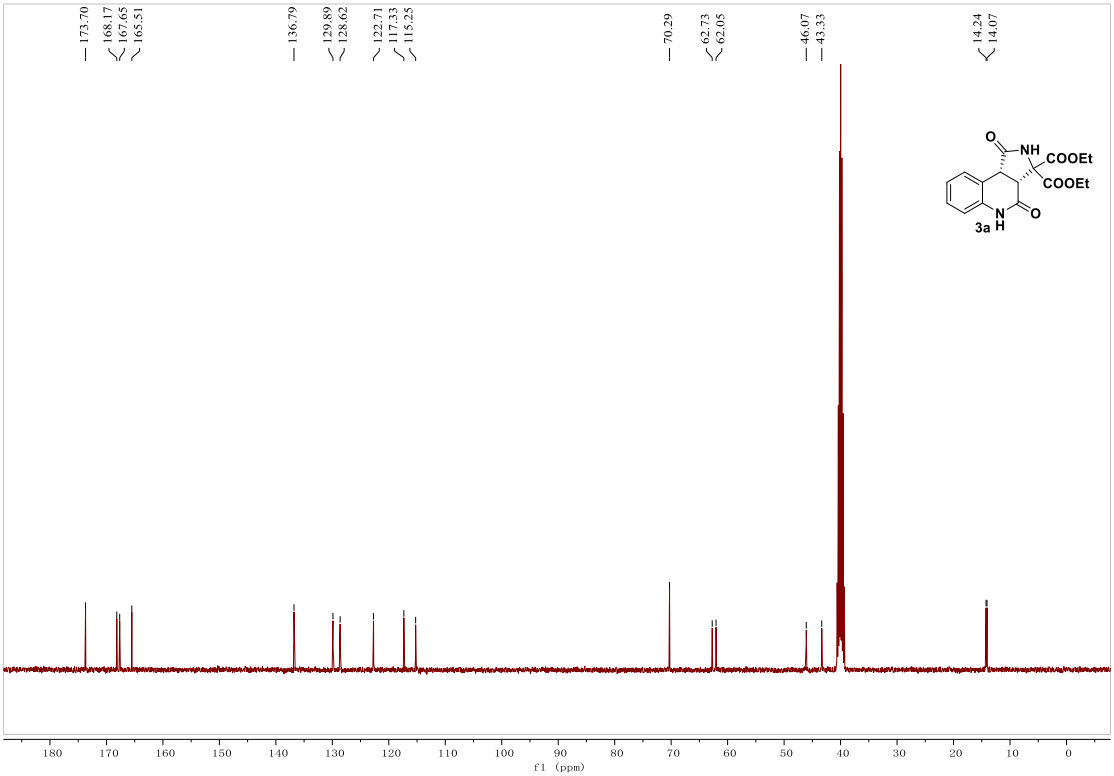


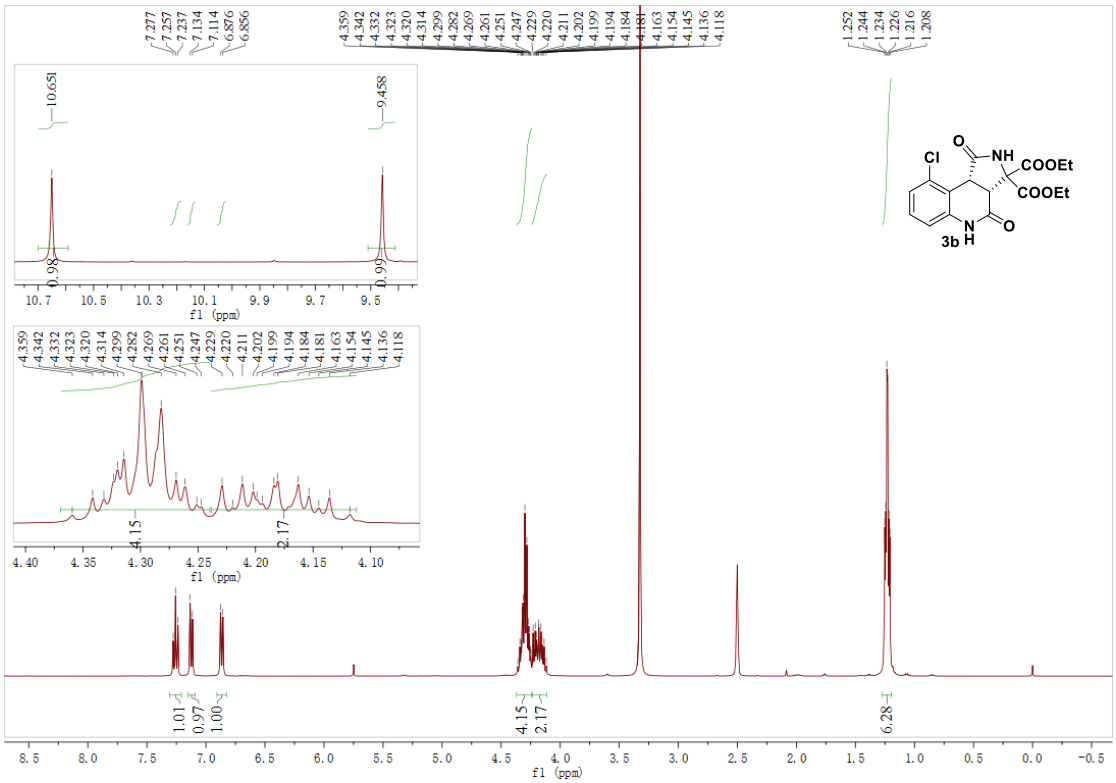
No desired products can be observed:



3. NMR Spectra of 3



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4.314
4.299
4.282
4.269
4.261
4.251
4.247
4.229
4.220
4.211
4.202
4.199
4.194
4.184
4.181
4.163
4.154
4.145
4.136
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1.244
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1.208
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0.99
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1.00
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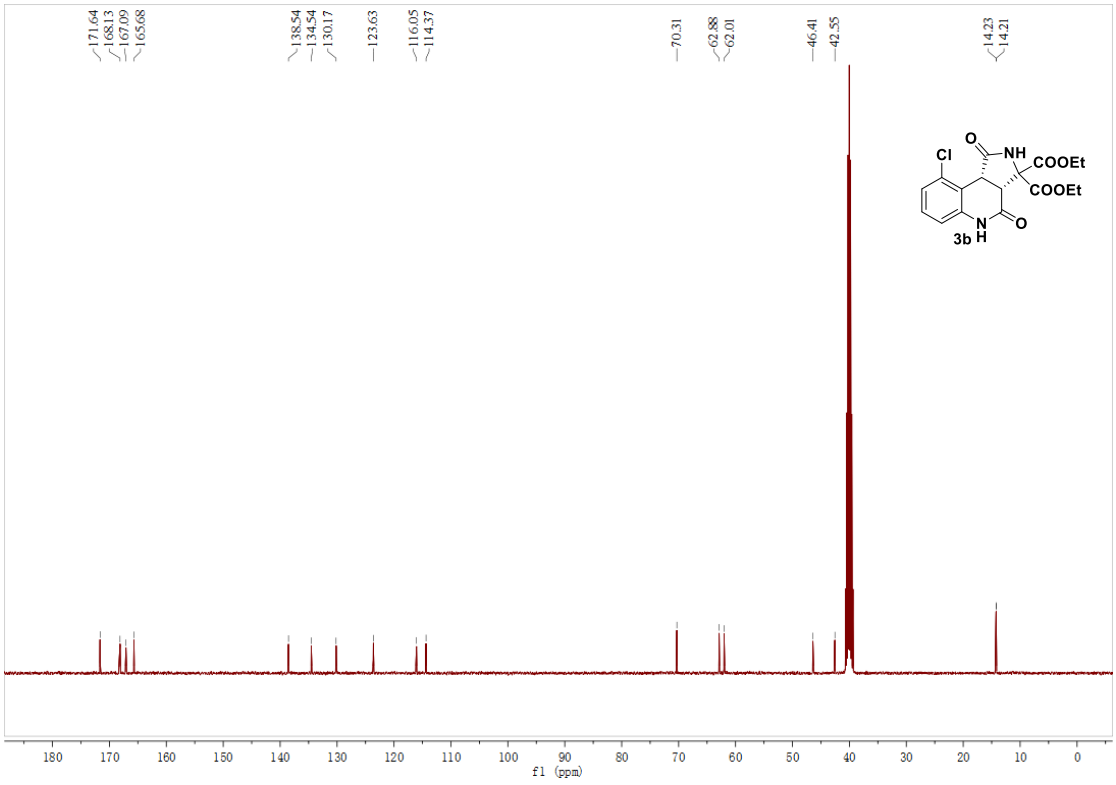
O
N
H
3b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168.13
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134.54
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123.63
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70.31
62.88
62.01
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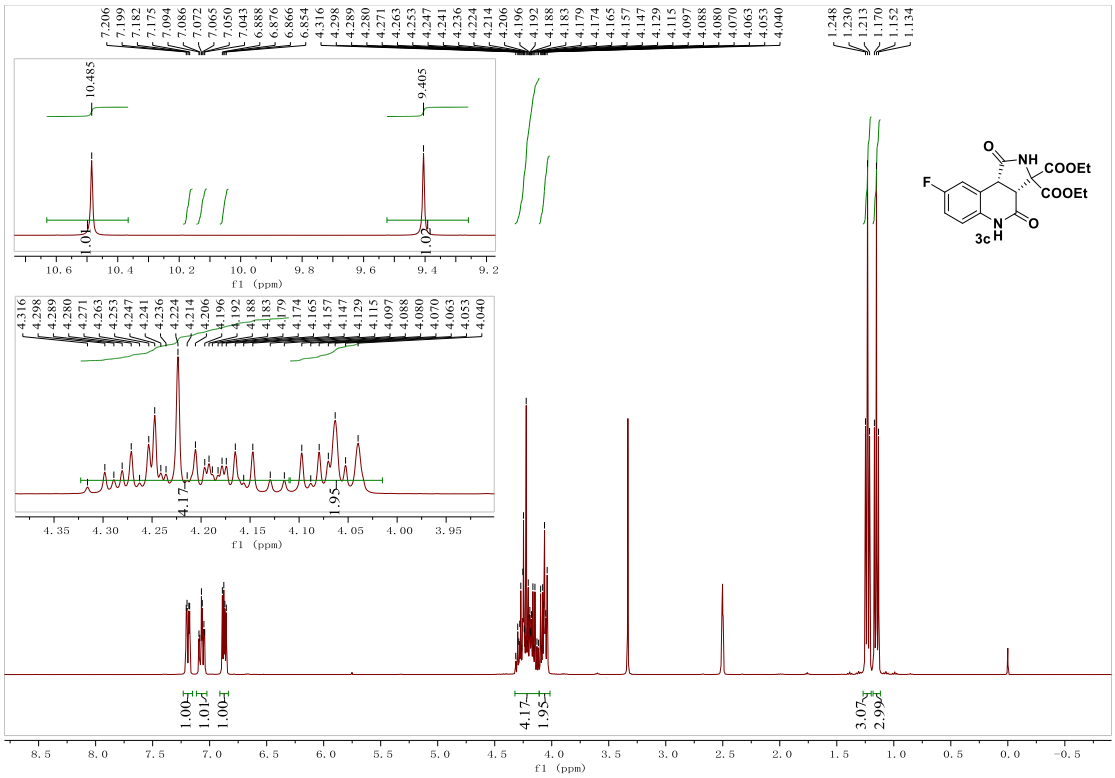
f1 (ppm)
Cl
NH
COOEt
COOEt
O
N
H
3b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4.241
4.236
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4.214
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4.183
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4.157
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4.115
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4.088
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4.070
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1.230
1.213
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1.152
1.134
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1.02
f1 (ppm)
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1.95
1.00
1.01
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f1 (ppm)
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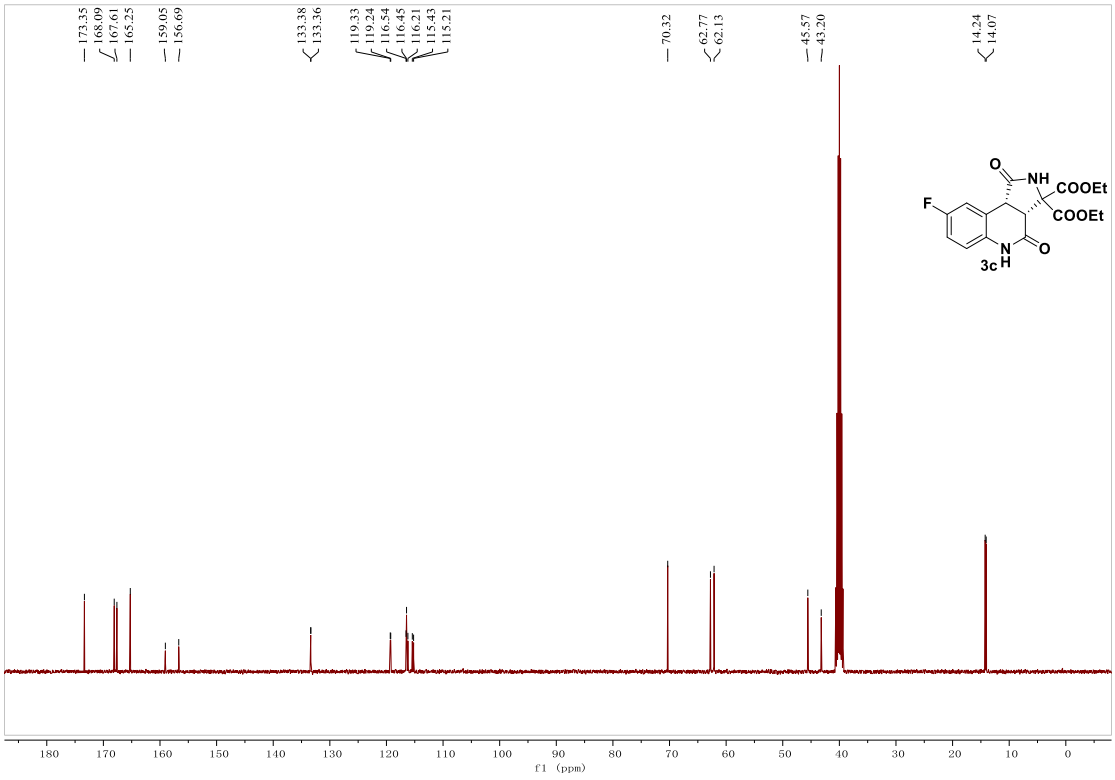
COOEt
F
O
N
H
3c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156.69
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119.24
116.54
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116.21
115.43
115.21
70.32
62.77
62.13
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f1 (ppm)
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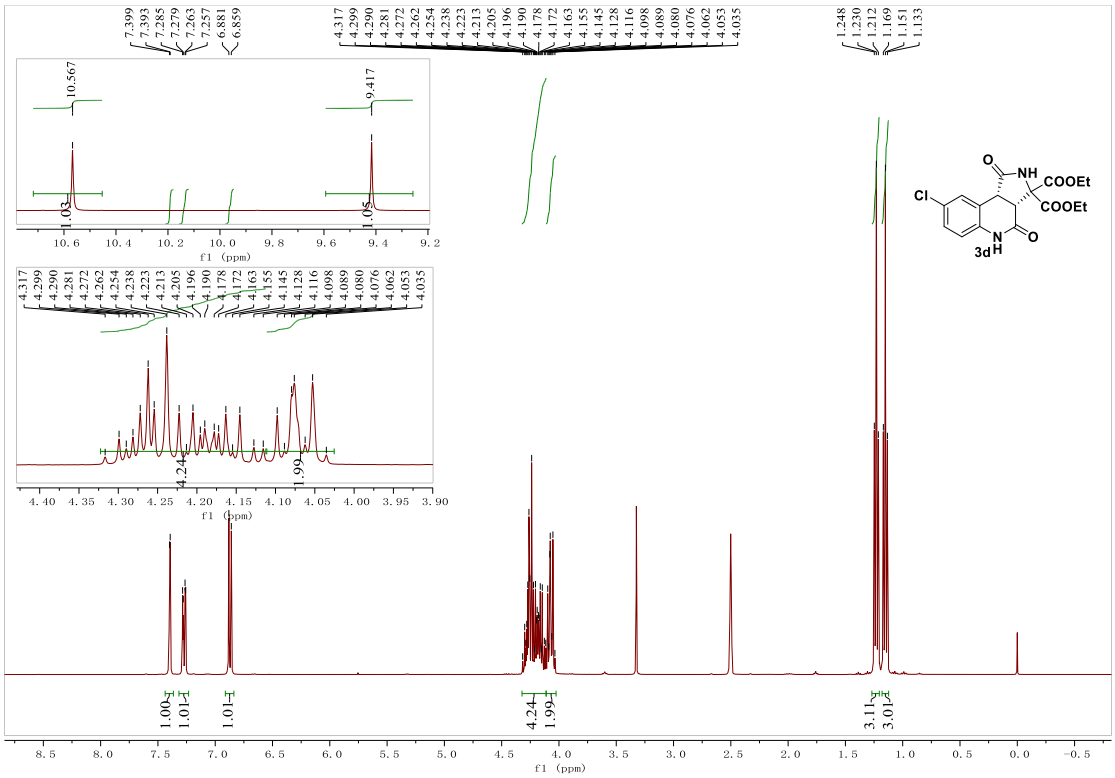
COOEt
F
O
N
H
3c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4.213
4.205
4.196
4.190
4.178
4.172
4.163
4.155
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4.116
4.098
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1.230
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1.151
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Cl
O
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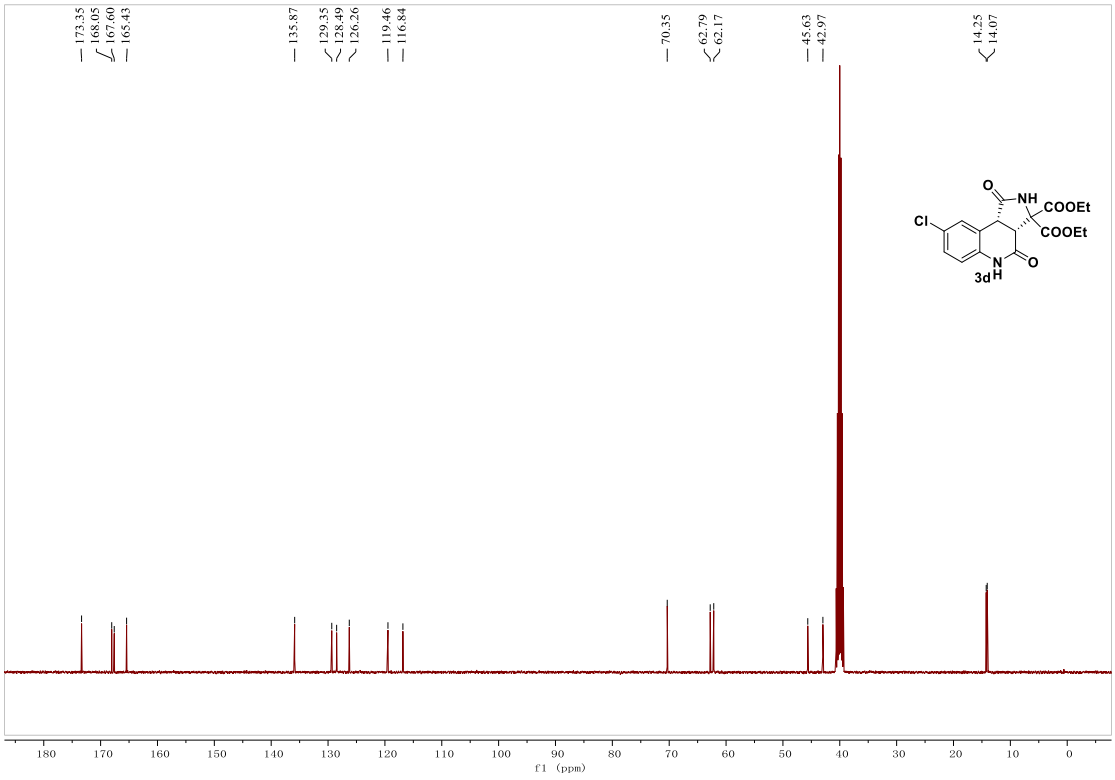
H
3d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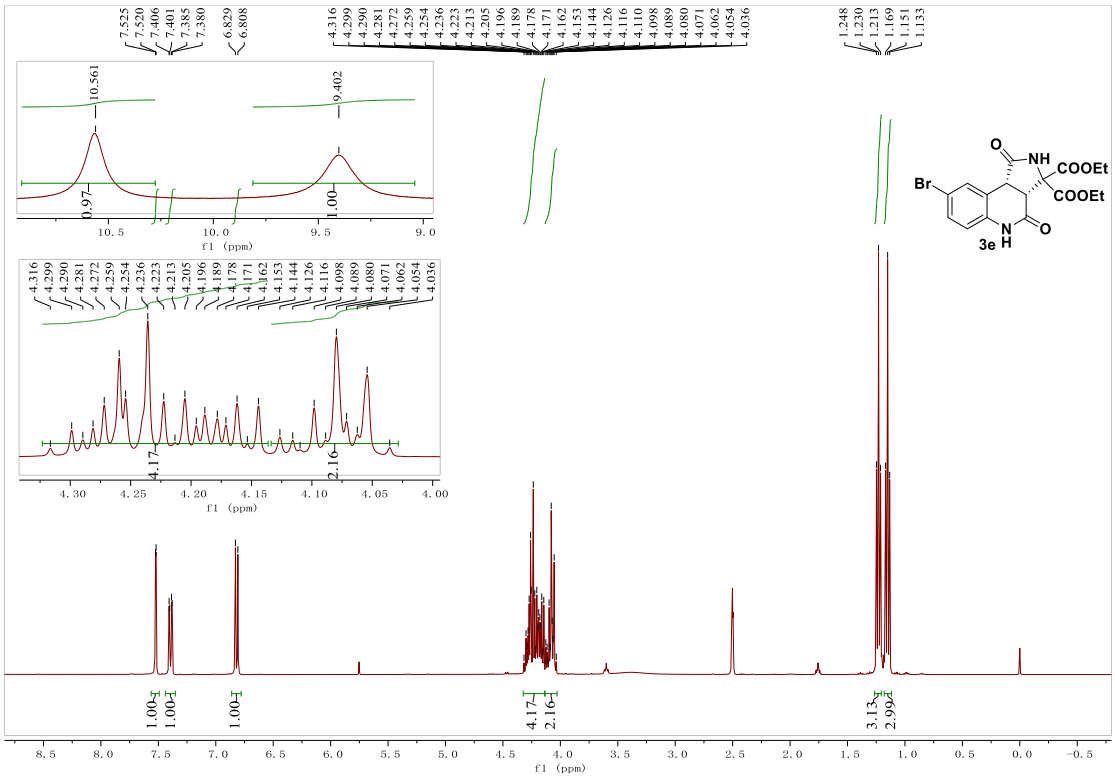
14.07
NH
COOEt
COOEt
Cl
O
N
H
3d
f1 (ppm)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4.110
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4.062
4.054
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1.151
1.133
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2.16
1.00
1.00
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COOEt
COOEt
O
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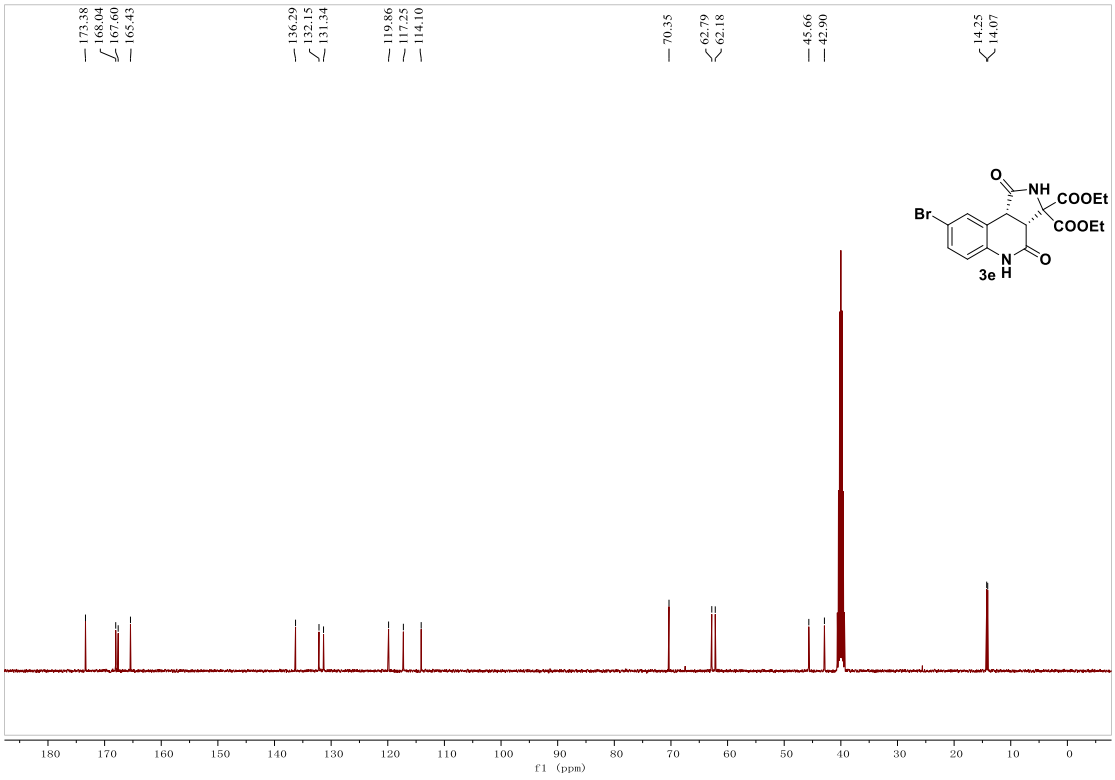
H
3e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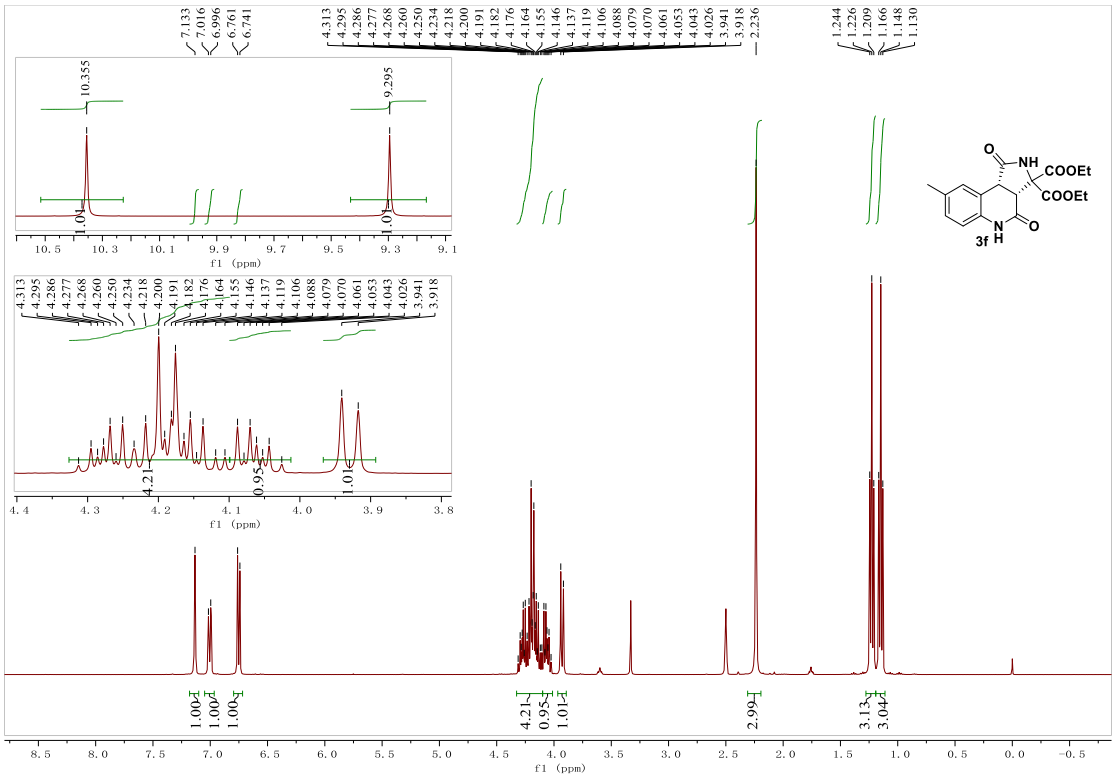
f1 (ppm)
Br
NH
COOEt
COOEt
O
N
H
3e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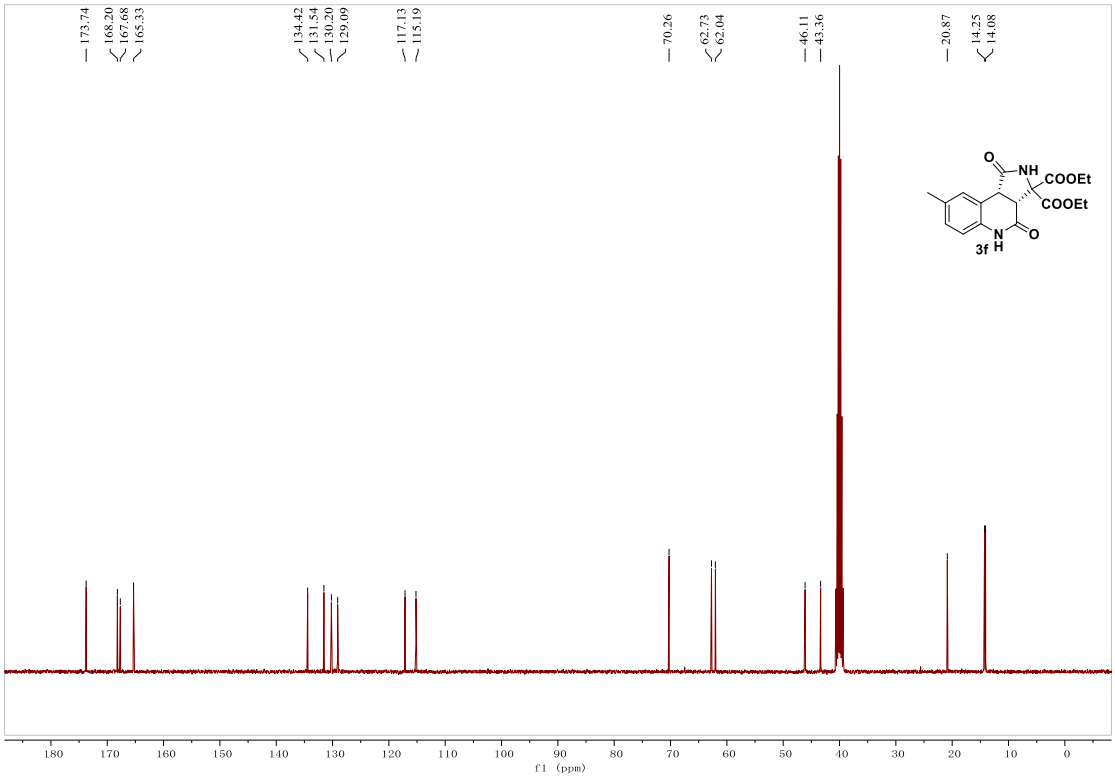
3.13
3.04
NH
COOEt
COOEt
O
N
H
3f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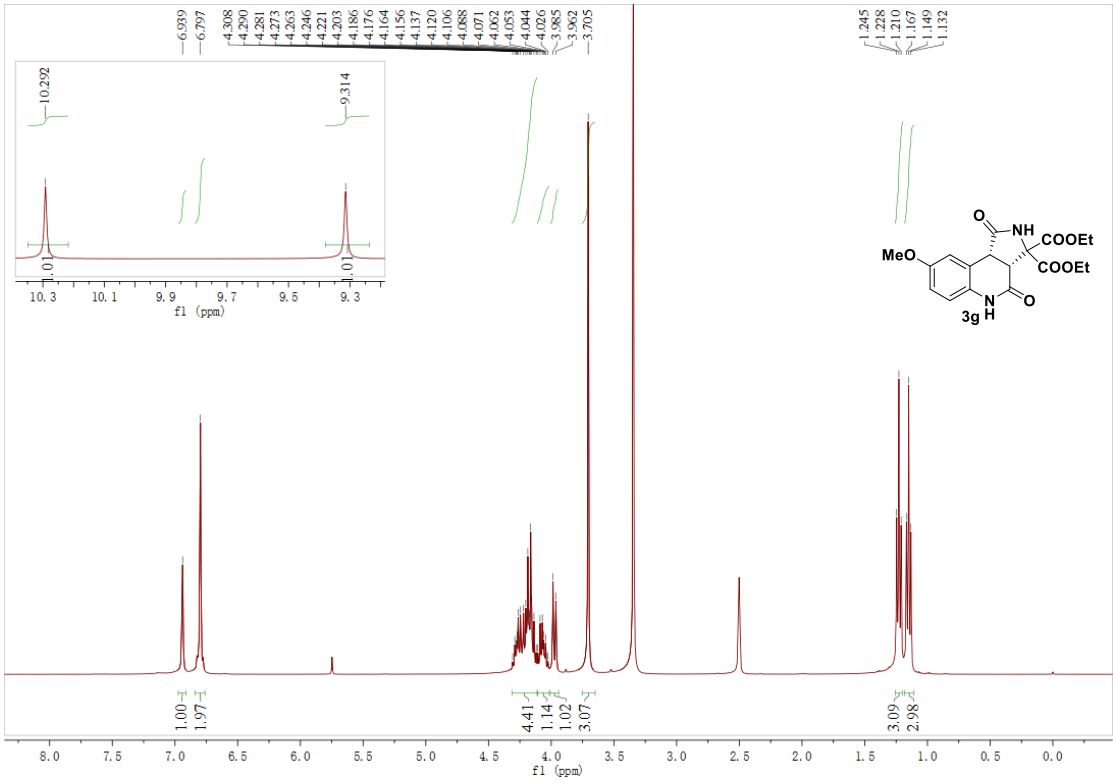
131.54
130.20
129.09
117.13
115.19
70.26
62.73
62.04
46.11
43.36
20.87
14.25
14.08
f1 (ppm)
NH
COOEt
COOEt
O
N
H
3f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4.156
4.137
4.120
4.106
4.088
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4.062
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3.962
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1.132
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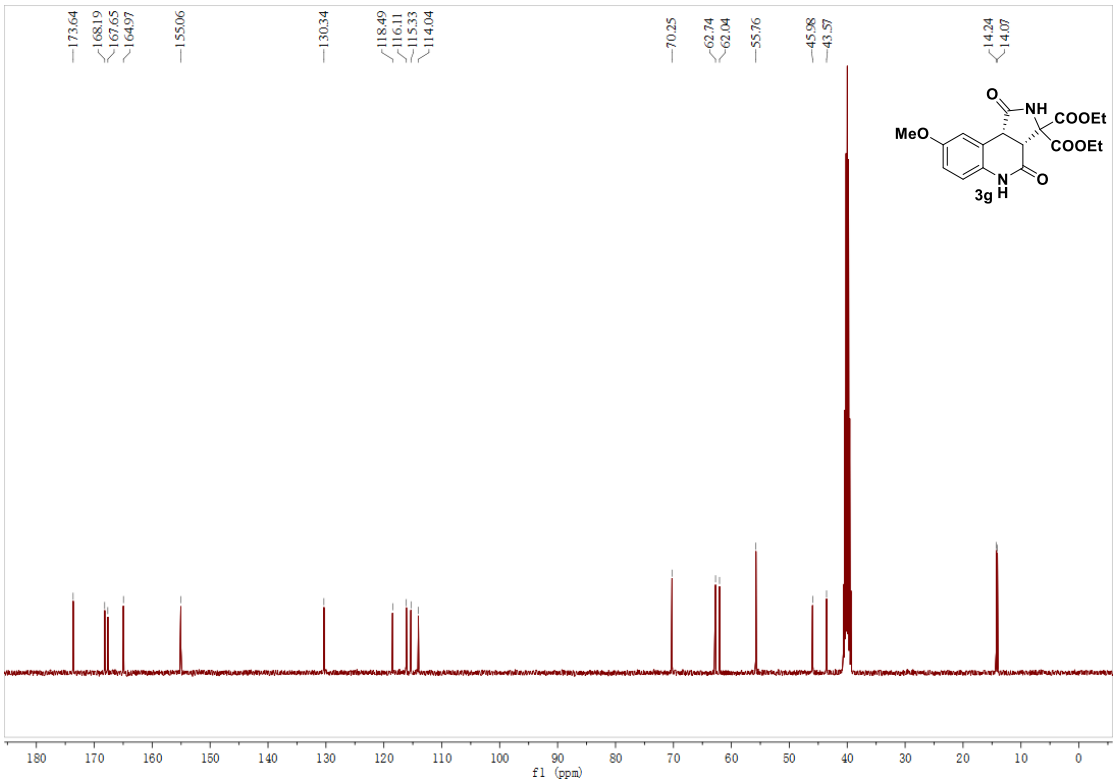
9.314
1.01
1.01
10.3
10.1
9.9
9.7
9.5
9.3
f1 (ppm)
MeO
NH
COOEt
COOEt
O
N
H
3g
1.00
1.97
4.41
1.14
1.02
3.07
3.09
2.98
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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116.11
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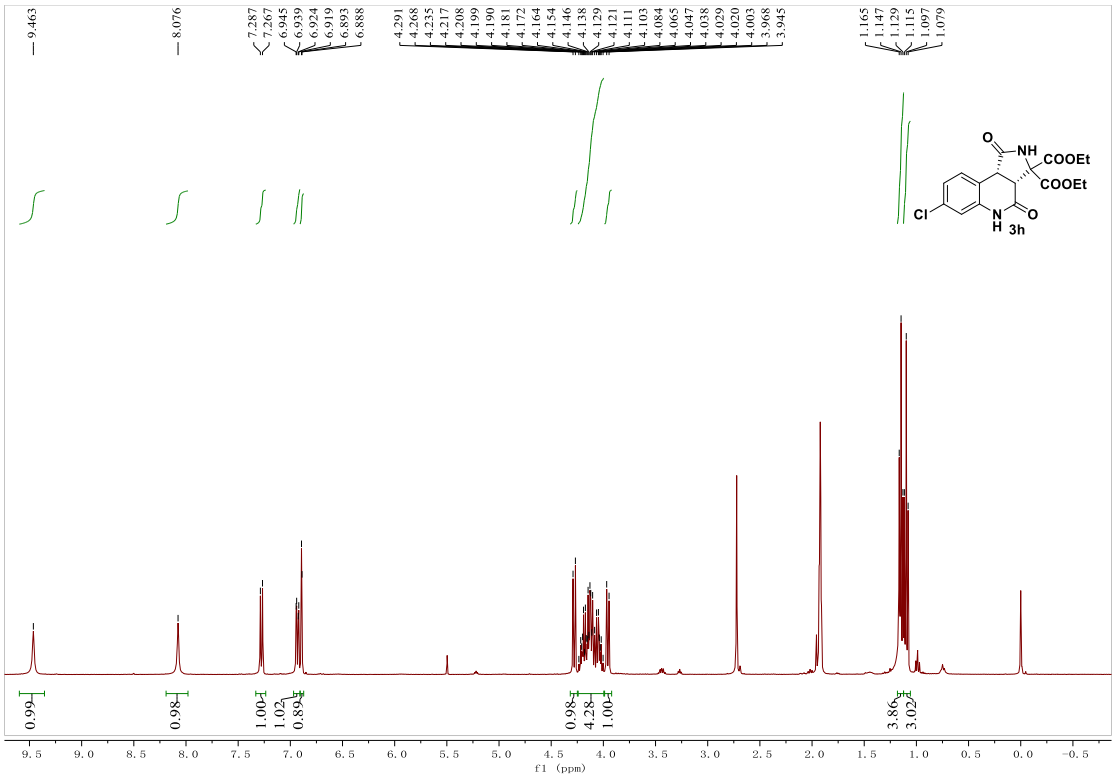
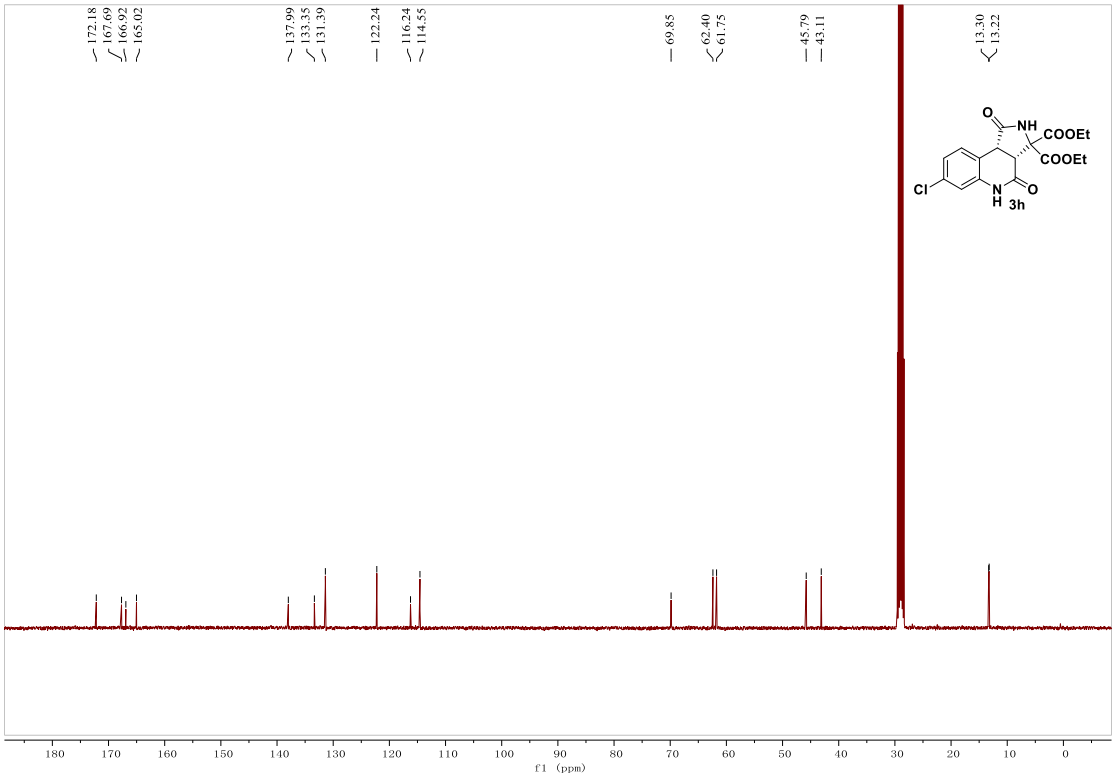
114.04
70.25
62.74
62.04
55.76
45.98
43.57
14.24
14.07
MeO
NH
COOEt
COOEt
O
N
H
3g
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.463
8.076
7.287
7.267
6.945
6.939
6.924
6.919
6.893
6.888
4.291
4.268
4.235
4.217
4.208
4.199
4.190
4.181
4.172
4.164
4.154
4.146
4.138
4.129
4.121
4.111
4.103
4.084
4.065
4.047
4.038
4.029
4.020
4.003
3.968
3.945
1.165
1.147
1.129
1.115
1.097
1.079
NH
COOEt
COOEt
Cl
N
H
O
3h
0.99
0.98
1.00
1.02
0.89
0.98
4.28
1.00
3.86
3.02
f1 (ppm)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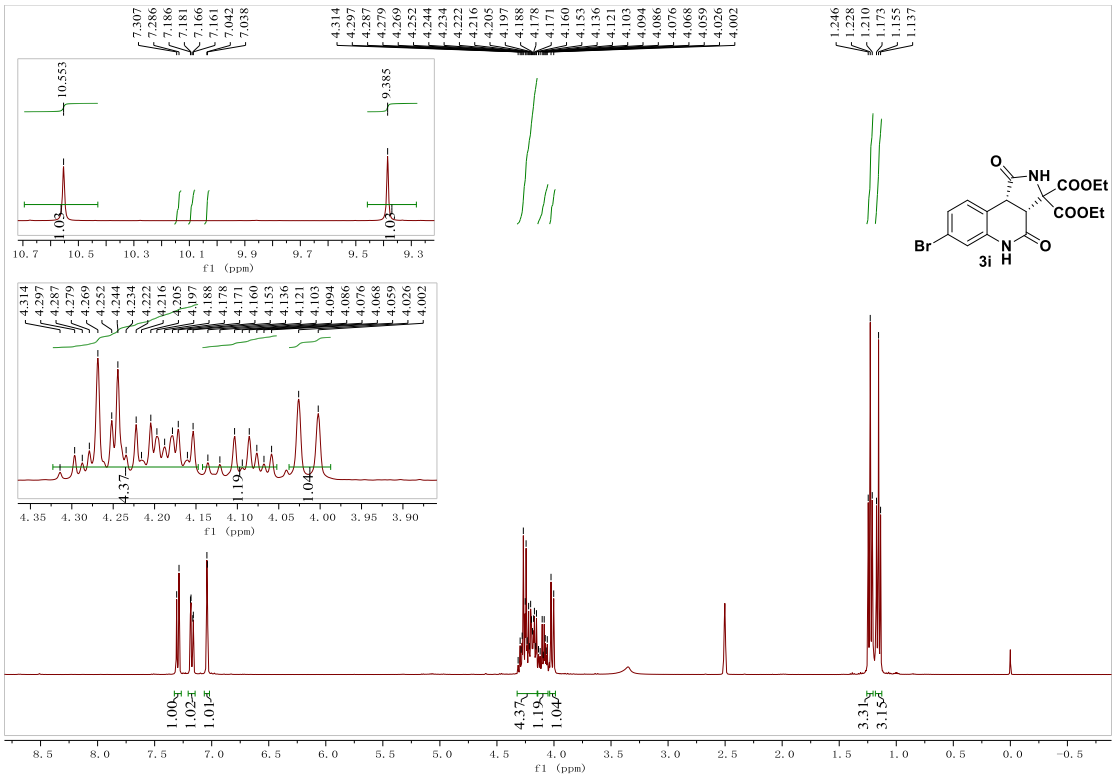
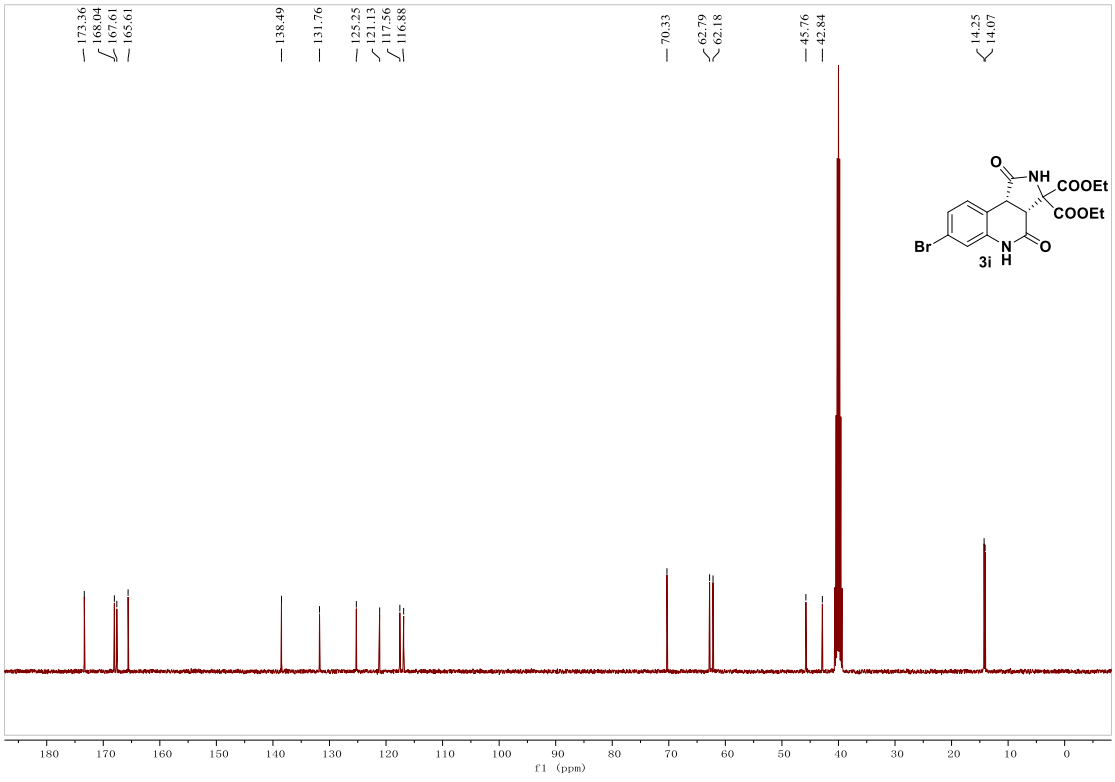
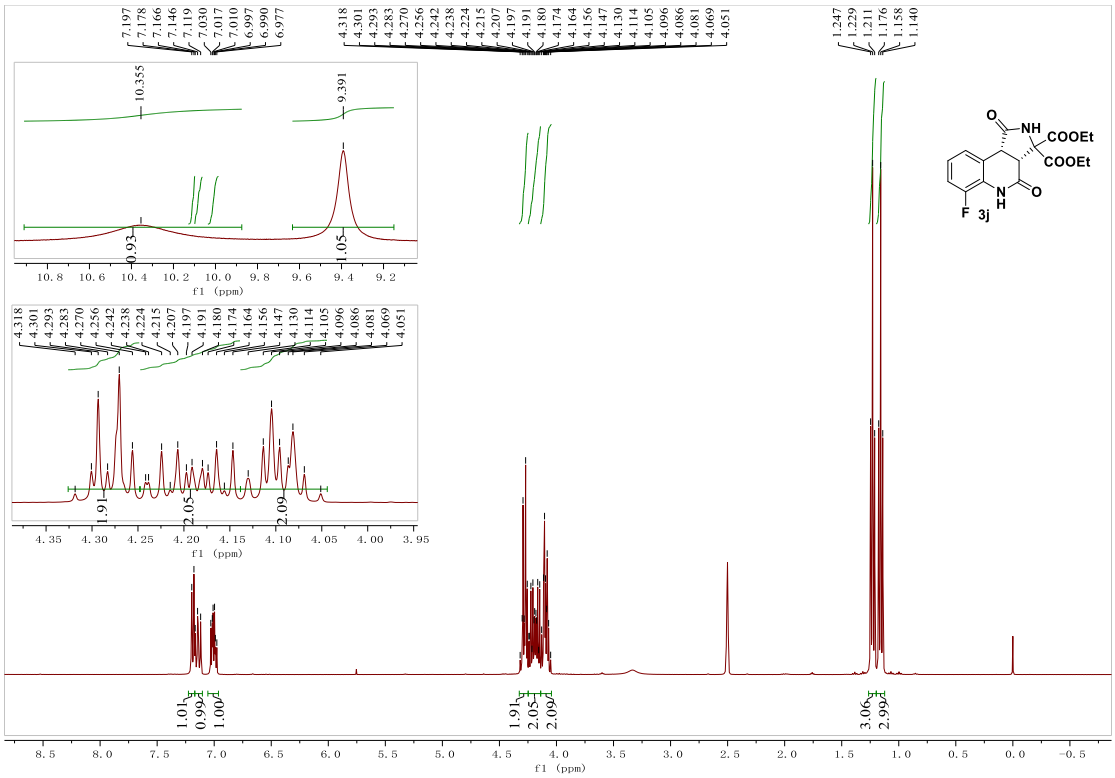
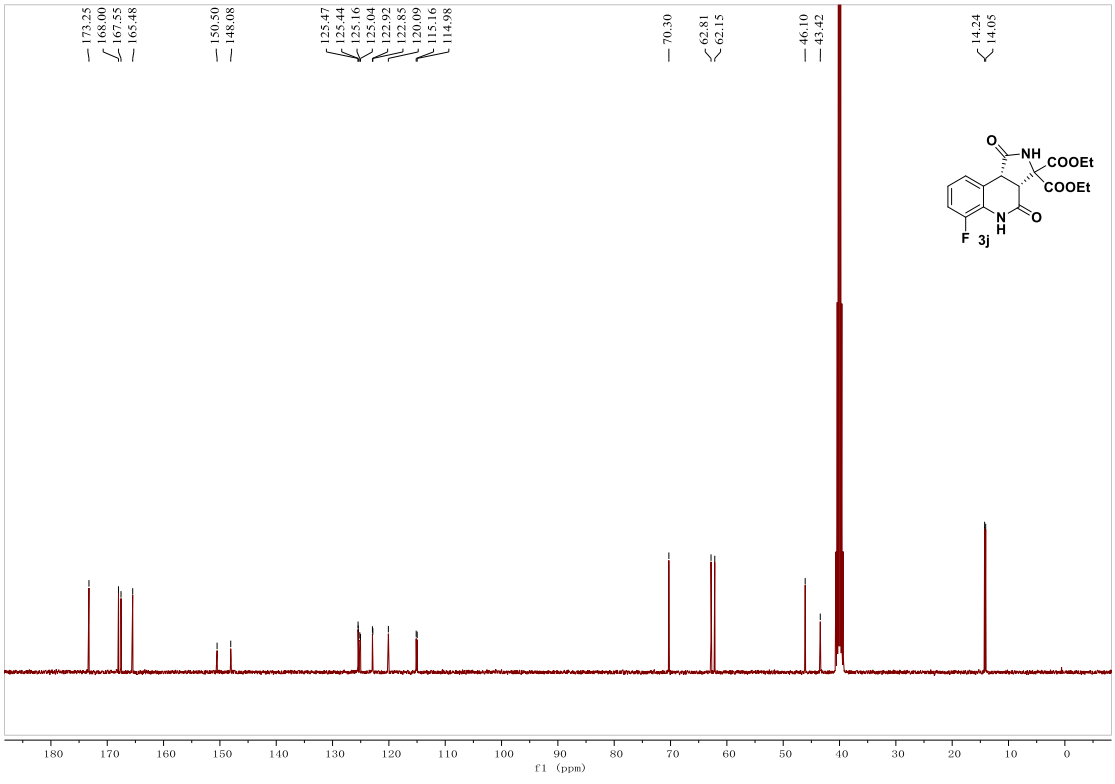
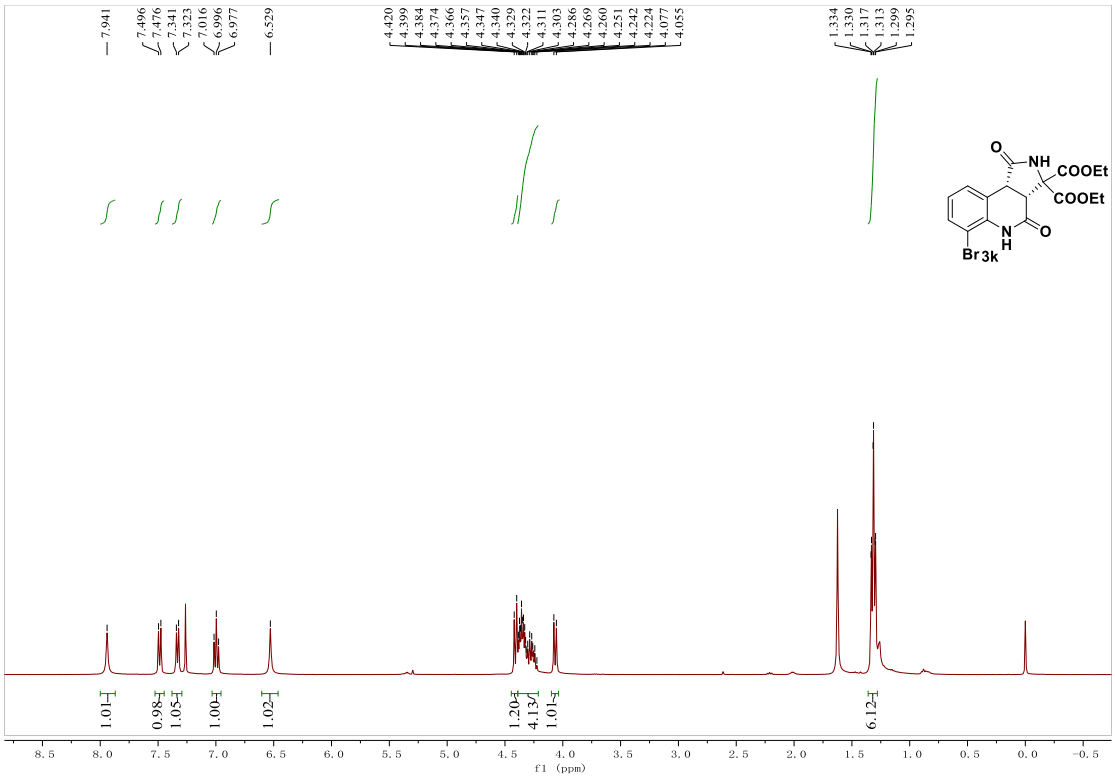
167.69
166.92
165.02
137.99
133.35
131.39
122.24
116.24
114.55
69.85
62.40
61.75
45.79
43.11
13.30
13.22
NH
COOEt
COOEt
Cl
N
H
O
3h
f1 (ppm)

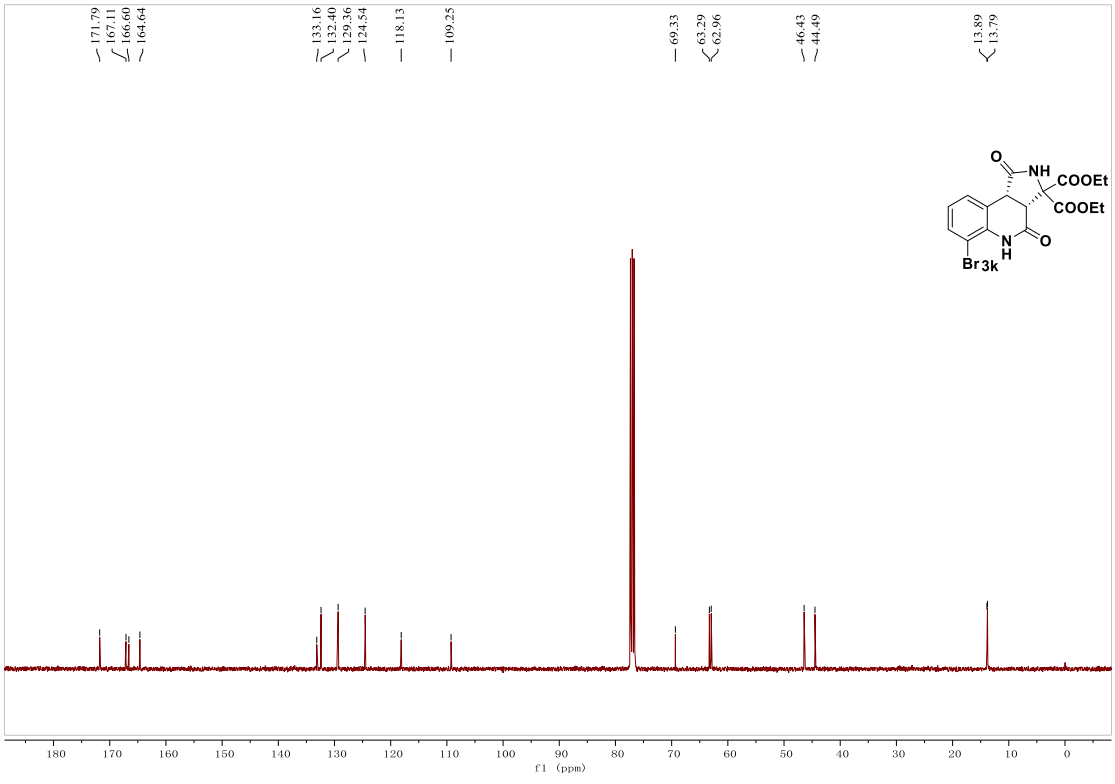

7.307
7.286
7.186
7.181
7.166
7.161
7.042
7.038
4.314
4.297
4.287
4.279
4.269
4.252
4.244
4.234
4.222
4.216
4.205
4.197
4.188
4.178
4.171
4.160
4.153
4.136
4.121
4.103
4.094
4.086
4.076
4.068
4.059
4.026
4.002
1.246
1.228
1.210
1.173
1.155
1.137
10.553
9.385
1.02
1.03
10.7 10.5 10.3 10.1 9.9 9.7 9.5 9.3
f1 (ppm)
4.37
1.19
1.04
4.35 4.30 4.25 4.20 4.15 4.10 4.05 4.00 3.95 3.90
f1 (ppm)
1.00
1.02
1.01
4.37
1.19
1.04
3.31
3.15
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
O
NH
COOEt
COOEt
Br
N
H
O
3i

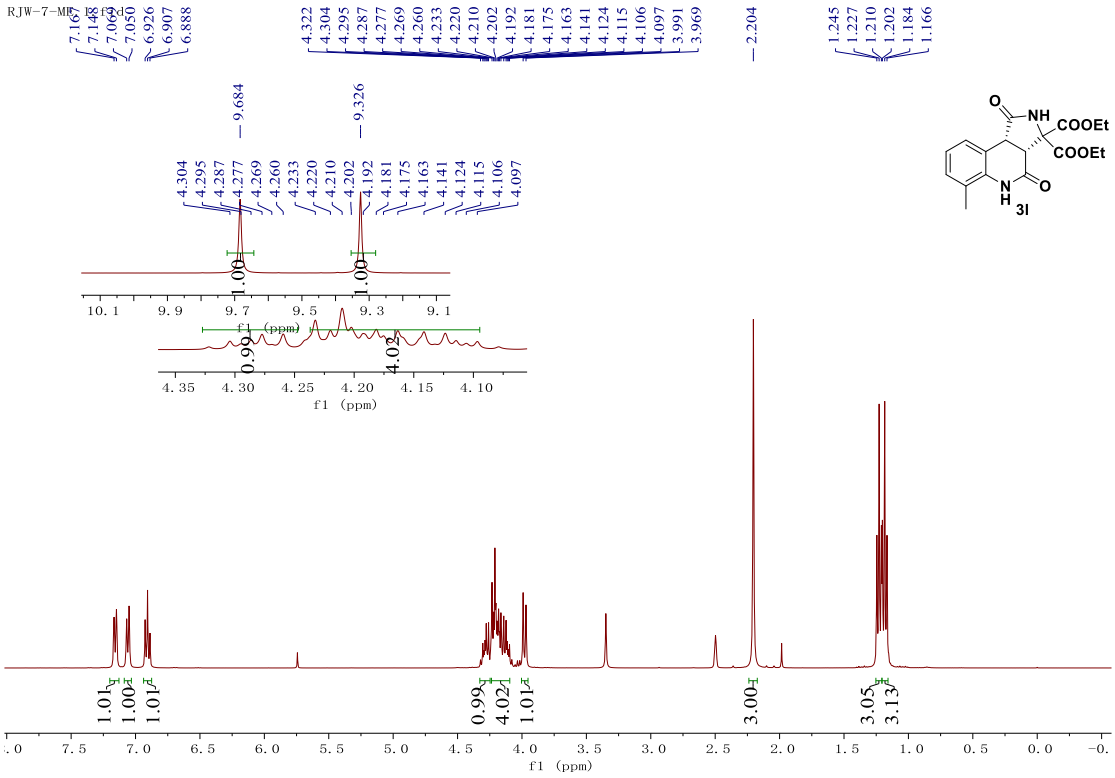

173.36
168.04
167.61
165.61
138.49
131.76
125.25
121.13
117.56
116.88
70.33
62.79
62.18
45.76
42.84
14.25
14.07
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
O
NH
COOEt
COOEt
Br
N
H
O
3i

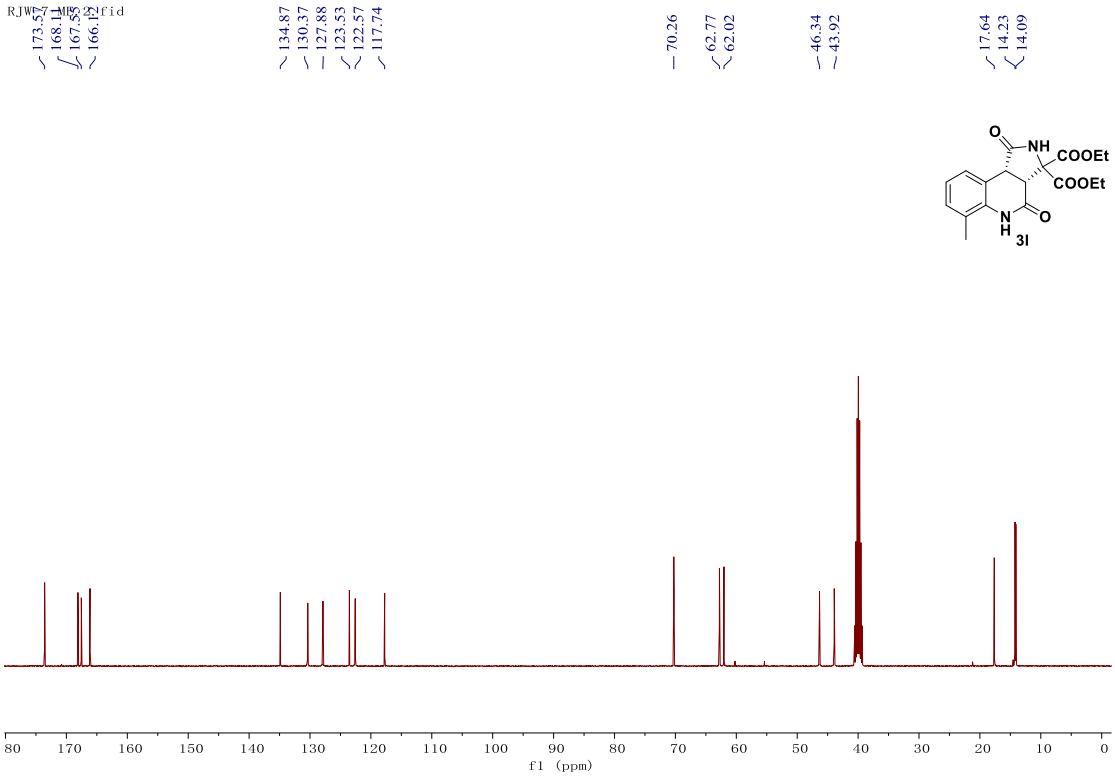

7.197
7.178
7.166
7.146
7.119
7.030
7.017
7.010
6.997
6.990
6.977
4.318
4.301
4.293
4.283
4.270
4.256
4.242
4.238
4.224
4.215
4.207
4.197
4.191
4.180
4.174
4.164
4.156
4.147
4.130
4.114
4.105
4.096
4.086
4.081
4.069
4.051
1.247
1.229
1.211
1.176
1.158
1.140
10.355
9.391
0.93
1.05
f1 (ppm)
1.91
2.05
2.09
1.01
0.99
1.00
3.06
2.99
NH
COOEt
COOEt
O
N
H
F
3j

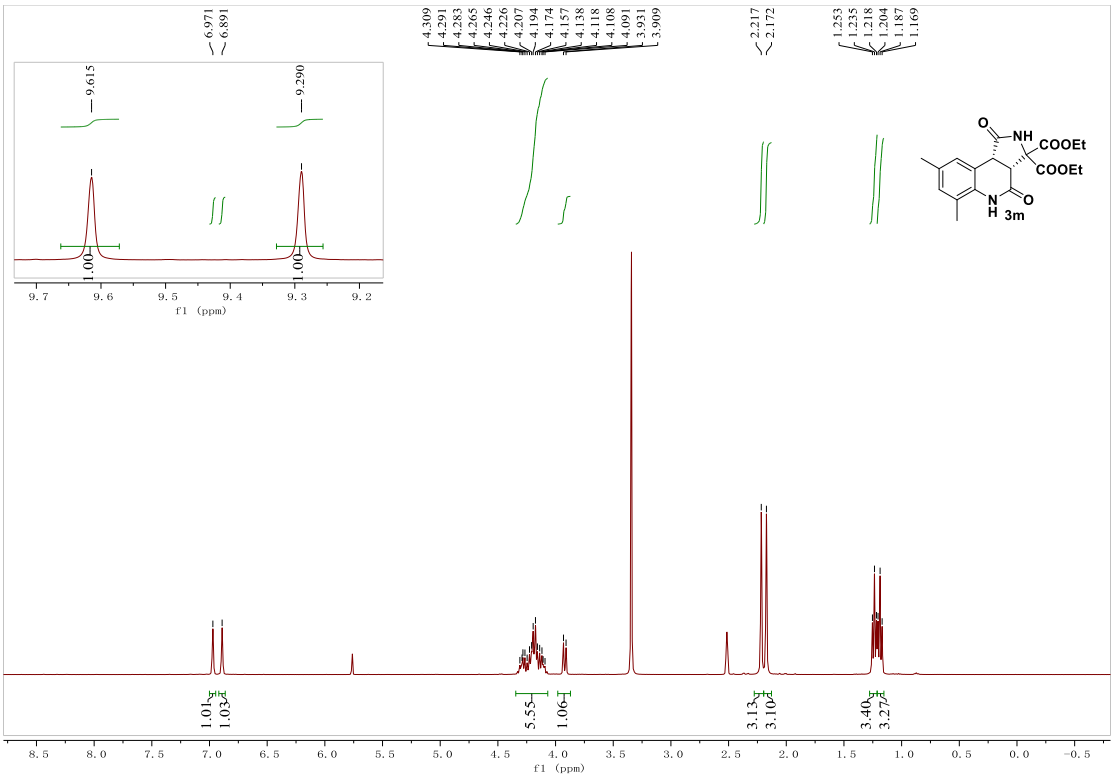

173.25
168.00
167.55
165.48
150.50
148.08
125.47
125.44
125.16
125.04
122.92
122.85
120.09
115.16
114.98
70.30
62.81
62.15
46.10
43.42
14.24
14.05
f1 (ppm)
NH
COOEt
COOEt
O
N
H
F
3j

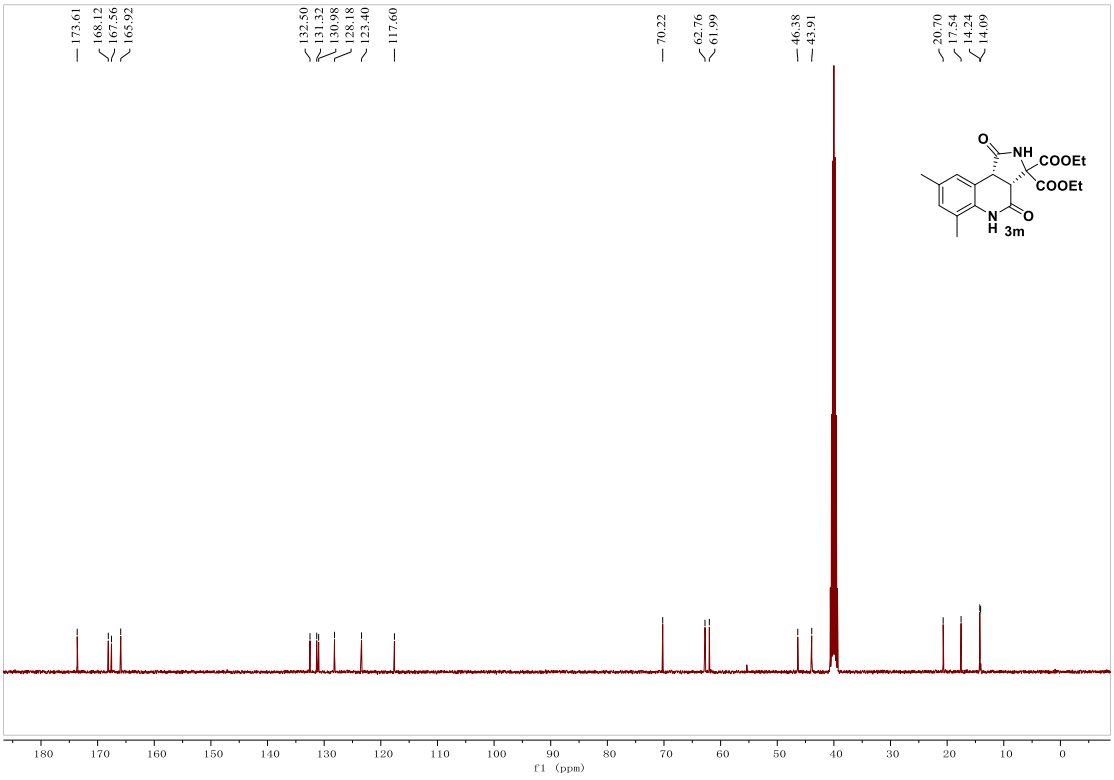

7.941
7.496
7.476
7.341
7.323
7.016
6.996
6.977
6.529
4.420
4.399
4.384
4.374
4.366
4.357
4.347
4.340
4.329
4.322
4.311
4.303
4.286
4.269
4.260
4.251
4.242
4.224
4.077
4.055
1.334
1.330
1.317
1.313
1.299
1.295
1.01
0.98
1.05
1.00
1.02
1.20
4.13
1.01
6.12
f1 (ppm)
O
NH
COOEt
COOEt
N
H
O
Br
3k

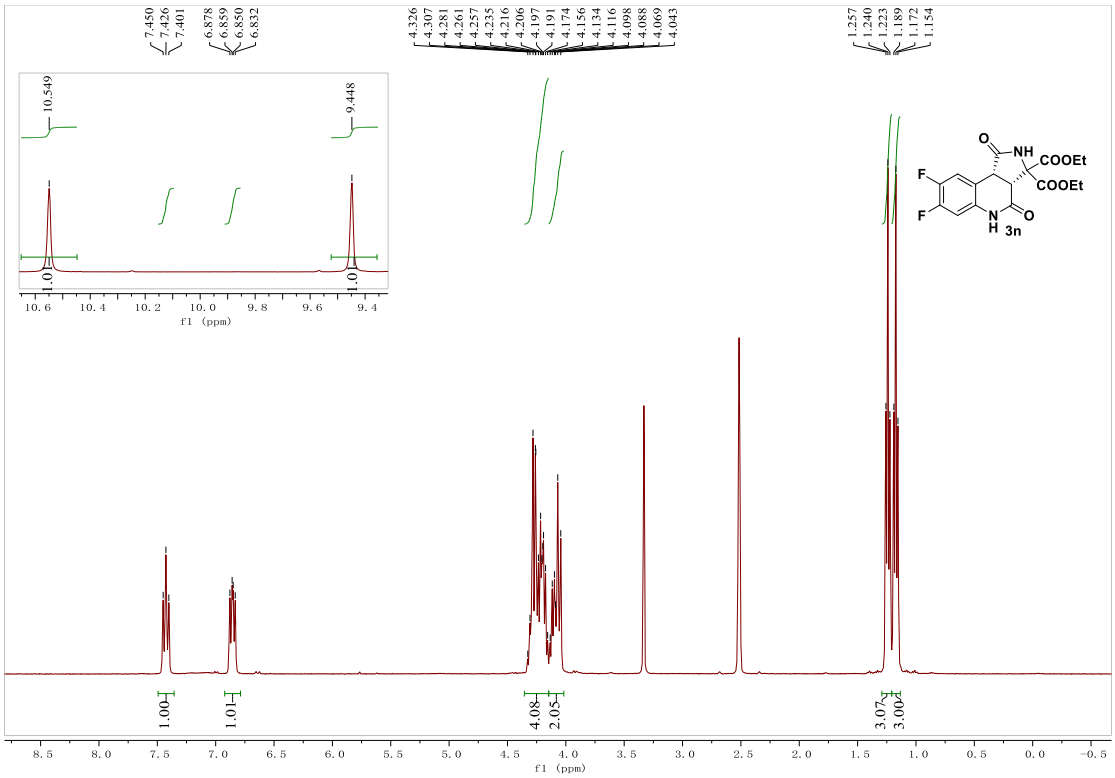

171.79
167.11
166.60
164.64
133.16
132.40
129.36
124.54
118.13
109.25
69.33
63.29
62.96
46.43
44.49
13.89
13.79
f1 (ppm)
O
NH
COOEt
COOEt
N
H
O
Br
3k

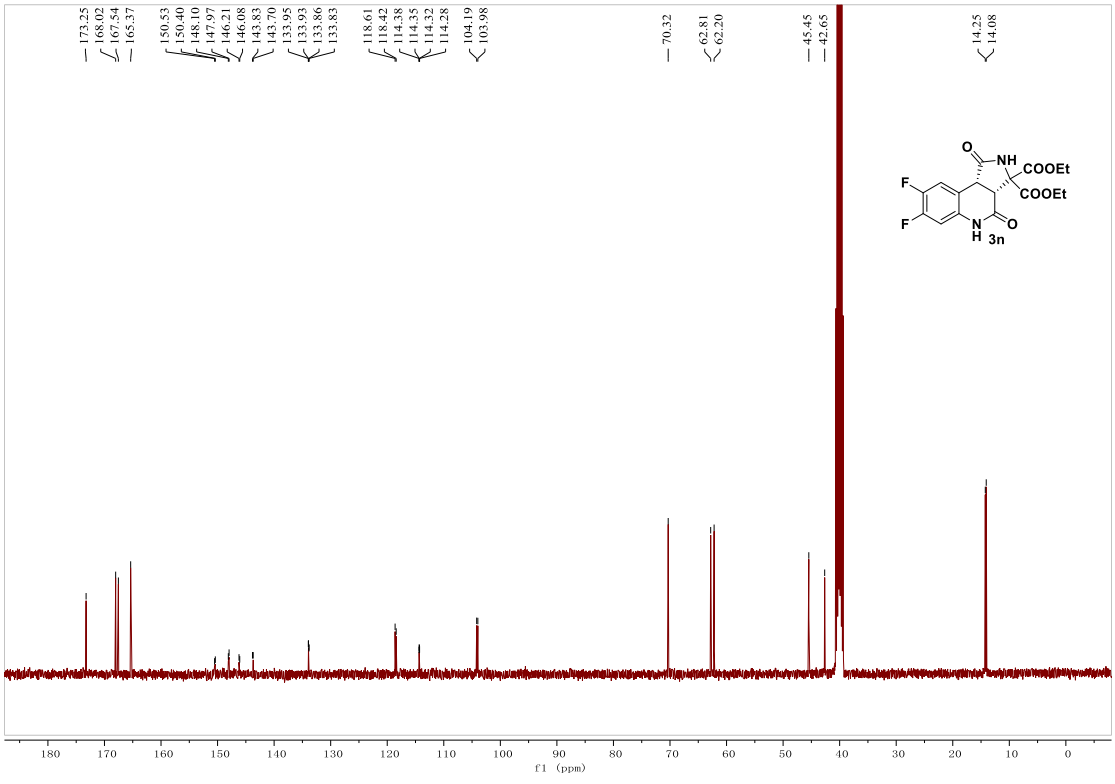

RJW-7-MR.fid
7.167
7.148
7.066
7.050
6.926
6.907
6.888
4.322
4.304
4.295
4.287
4.277
4.269
4.260
4.233
4.220
4.210
4.202
4.192
4.181
4.175
4.163
4.141
4.124
4.115
4.106
4.097
3.991
3.969
2.204
1.245
1.227
1.210
1.202
1.184
1.166
9.684
9.326
1.00
1.00
0.99
4.02
f1 (ppm)
1.01
1.00
1.01
0.99
4.02
1.01
3.00
3.05
3.13
f1 (ppm)
NH
COOEt
COOEt
N
H
O
O
3l

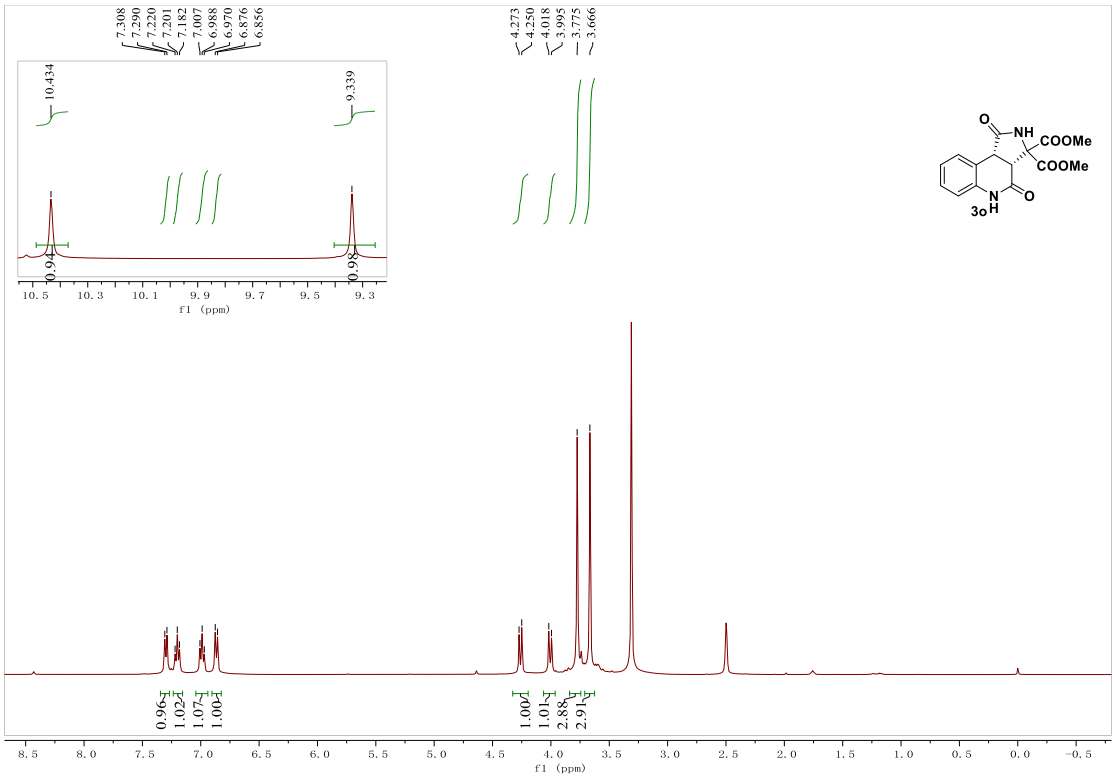

RJW-7-MR.fid
173.57
168.11
167.55
166.12
134.87
130.37
127.88
123.53
122.57
117.74
70.26
62.77
62.02
46.34
43.92
17.64
14.23
14.09
f1 (ppm)
NH
COOEt
COOEt
N
H
O
O
3l

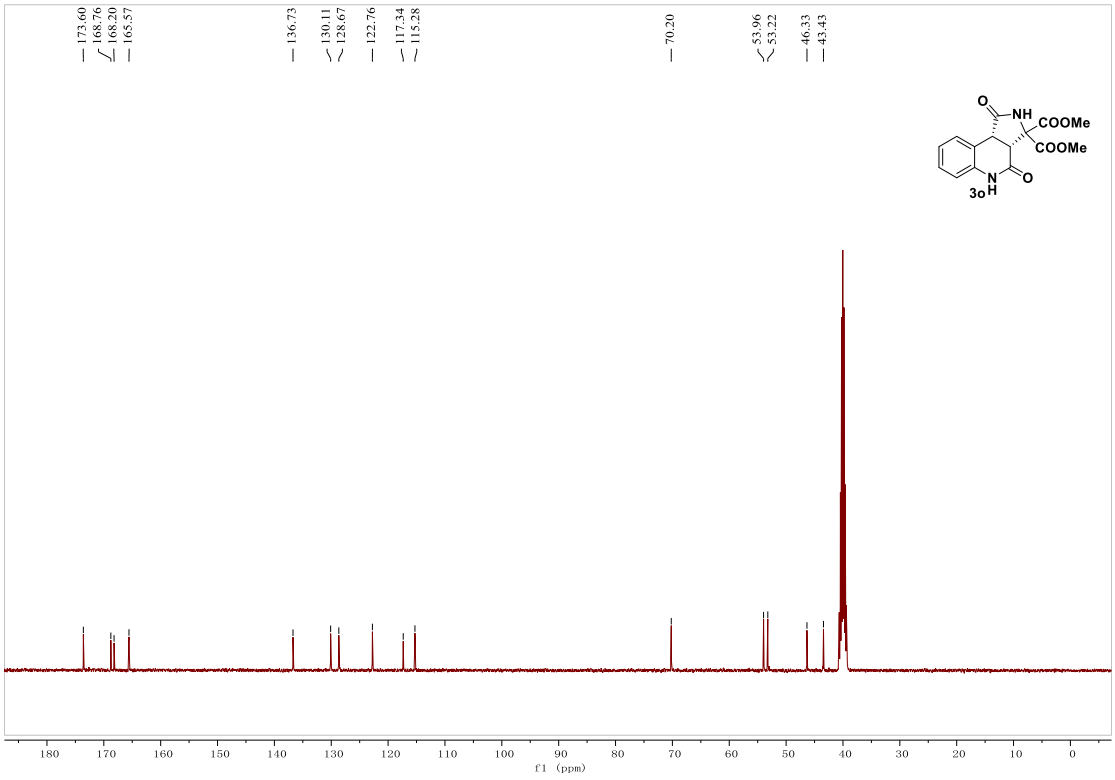

6.971
6.891
4.309
4.291
4.283
4.265
4.246
4.226
4.207
4.194
4.174
4.157
4.138
4.118
4.108
4.091
3.931
3.909
2.217
2.172
1.253
1.235
1.218
1.204
1.187
1.169
9.615
9.290
1.00
1.00
f1 (ppm)
NH
COOEt
COOEt
N
H
O
O
3m
1.01
1.03
5.55
1.06
3.13
3.10
3.40
3.27
f1 (ppm)

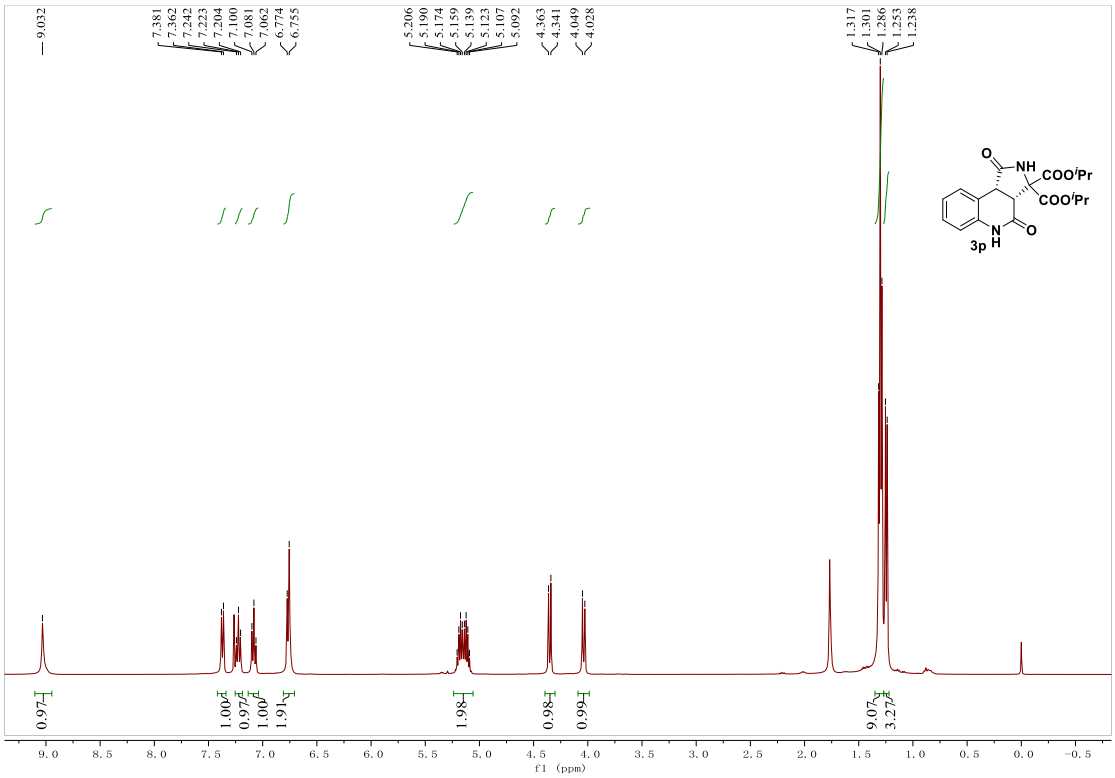

173.61
168.12
167.56
165.92
132.50
131.32
130.98
128.18
123.40
117.60
70.22
62.76
61.99
46.38
43.91
20.70
17.54
14.24
14.09
NH
COOEt
COOEt
N
H
O
O
3m
f1 (ppm)

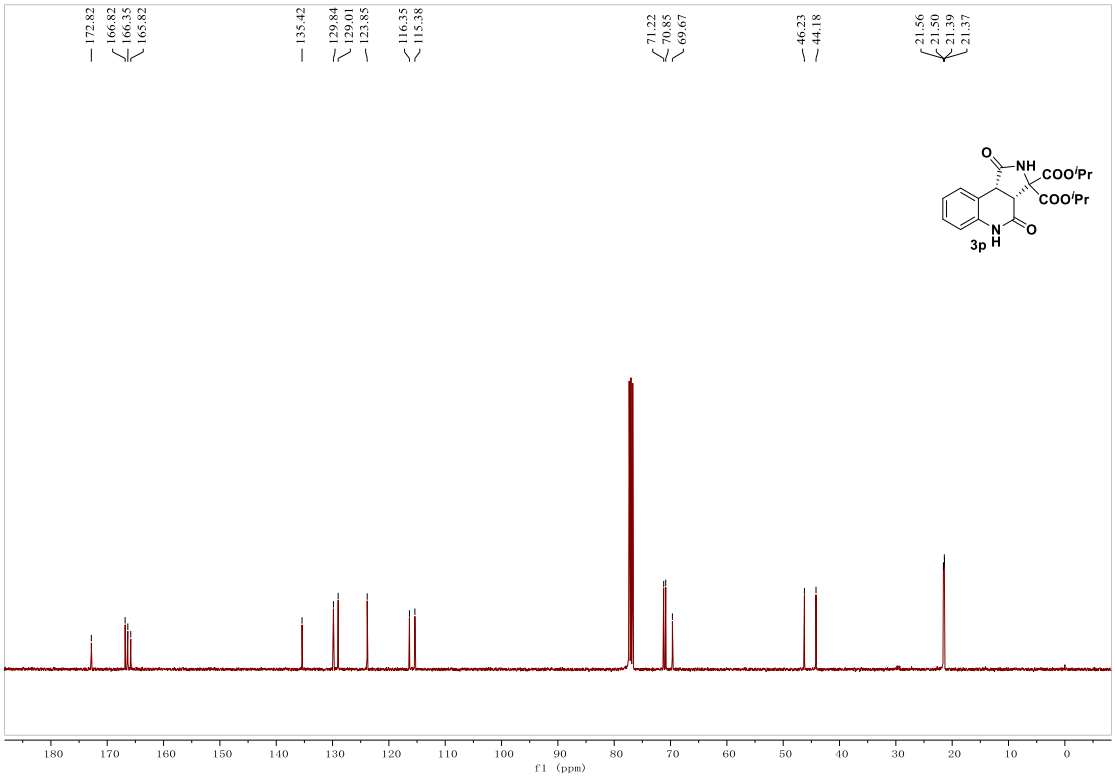

7.450
7.426
7.401
6.878
6.859
6.850
6.832
4.326
4.307
4.281
4.261
4.257
4.235
4.216
4.206
4.197
4.191
4.174
4.156
4.134
4.116
4.098
4.088
4.069
4.043
1.257
1.240
1.223
1.189
1.172
1.154
10.549
9.448
1.00
1.01
4.08
2.05
3.07
3.00
f1 (ppm)
O
NH
COOEt
COOEt
F
F
N
H
O
3n

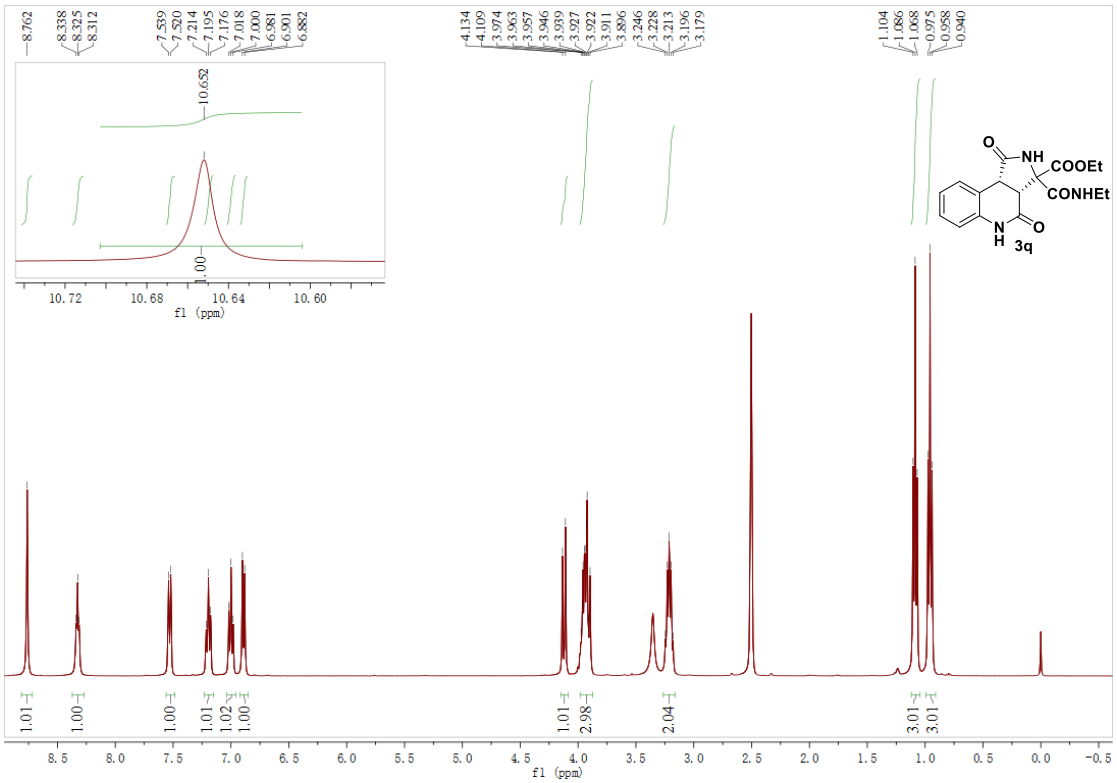

173.25
168.02
167.54
165.37
150.53
150.40
148.10
147.97
146.21
146.08
143.83
143.70
133.95
133.93
133.86
133.83
118.61
118.42
114.38
114.35
114.32
114.28
104.19
103.98
70.32
62.81
62.20
45.45
42.65
14.25
14.08
f1 (ppm)
O
NH
COOEt
COOEt
F
F
N
H
O
3n

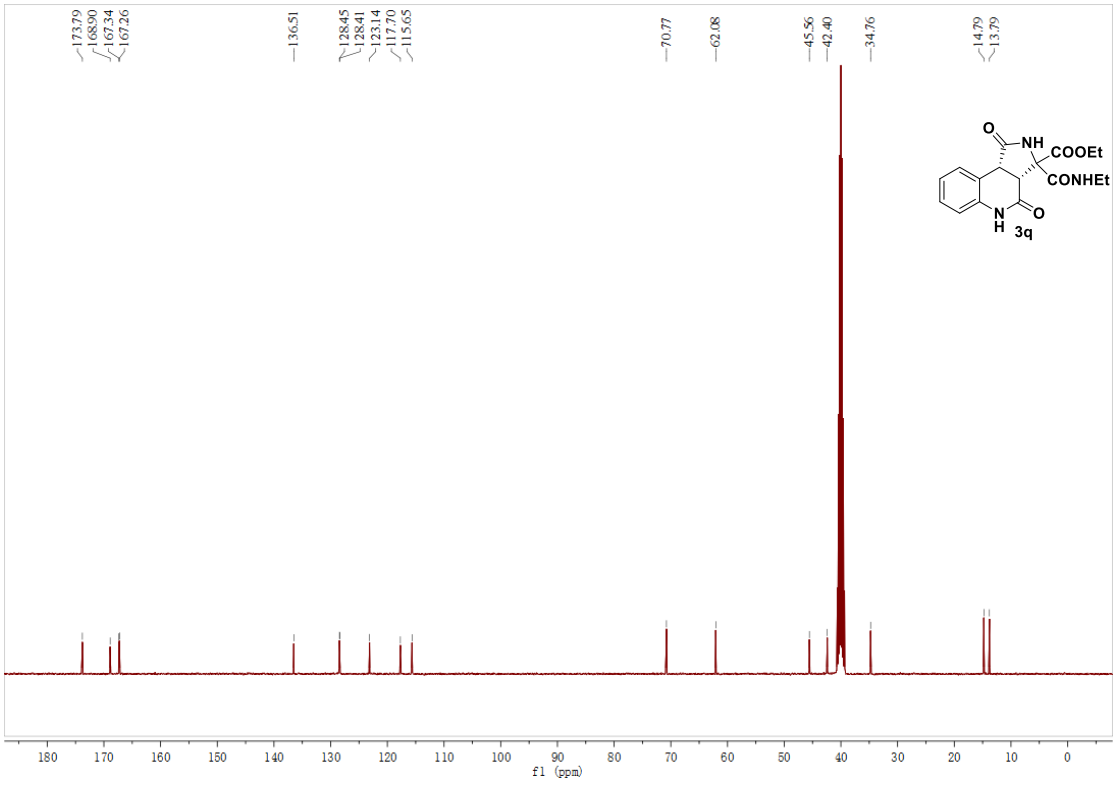

7.308
7.290
7.220
7.201
7.182
7.007
6.988
6.970
6.876
6.856
4.273
4.250
4.018
3.995
3.775
3.666
10.434
9.339
0.94
0.98
f1 (ppm)
NH
COOMe
COOMe
O
N
H
3o
0.96
1.02
1.07
1.00
1.00
1.01
2.88
2.91
f1 (ppm)

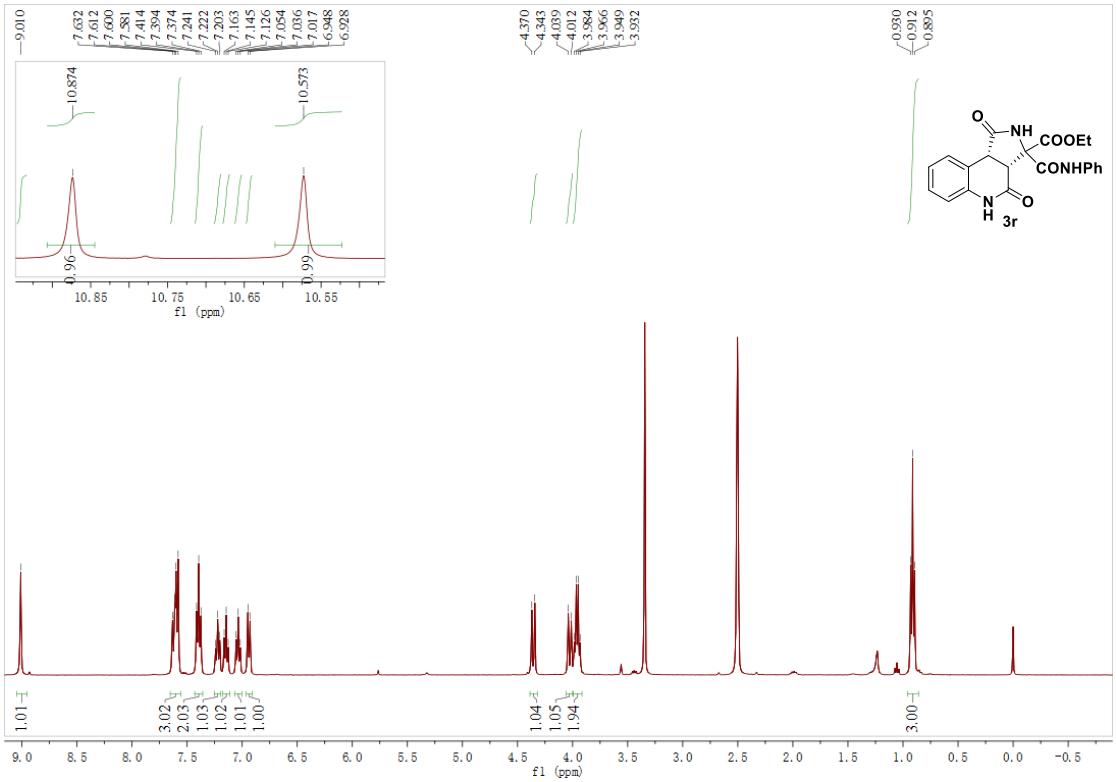

173.60
168.76
168.20
165.57
136.73
130.11
128.67
122.76
117.34
115.28
70.20
53.96
53.22
46.33
43.43
NH
COOMe
COOMe
O
N
H
3o
f1 (ppm)

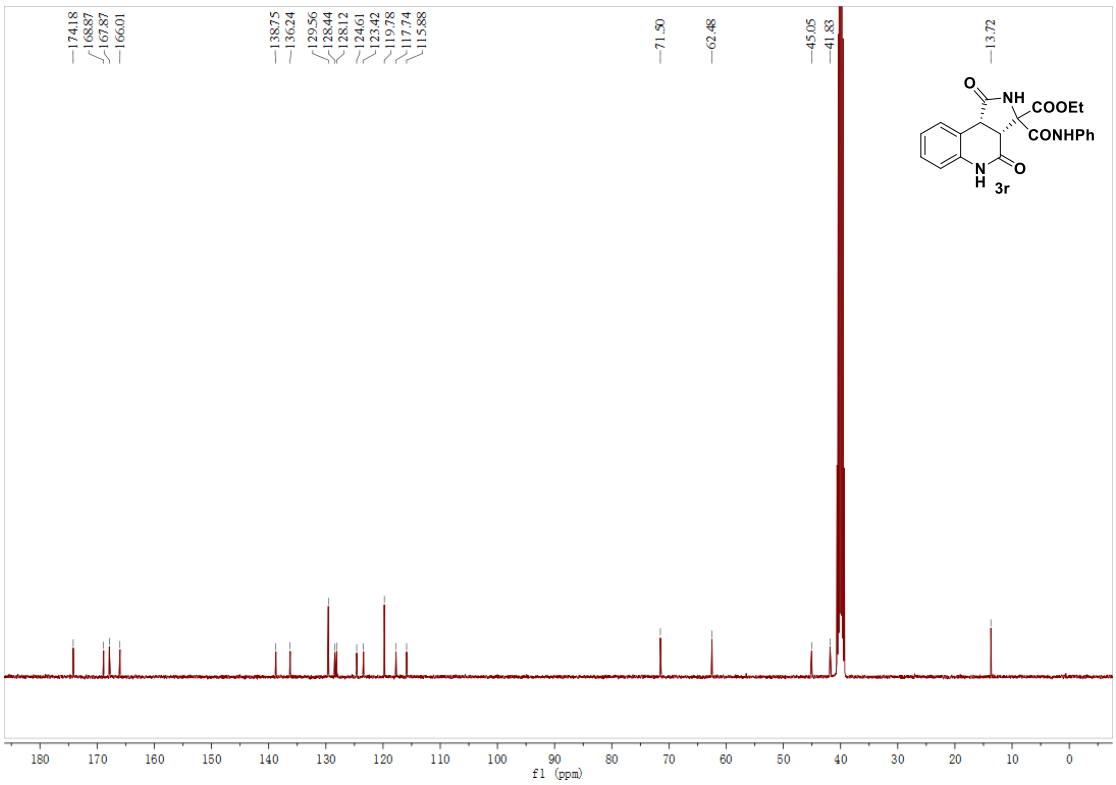

9.032
7.381
7.362
7.242
7.223
7.204
7.100
7.081
7.062
6.774
6.755
5.206
5.190
5.174
5.159
5.139
5.123
5.107
5.092
4.363
4.341
4.049
4.028
1.317
1.301
1.286
1.253
1.238
0.97
1.00
0.97
1.00
1.91
1.98
0.98
0.99
9.07
3.27
f1 (ppm)
NH
COO^{i}Pr
COO^{i}Pr
N
H
3p

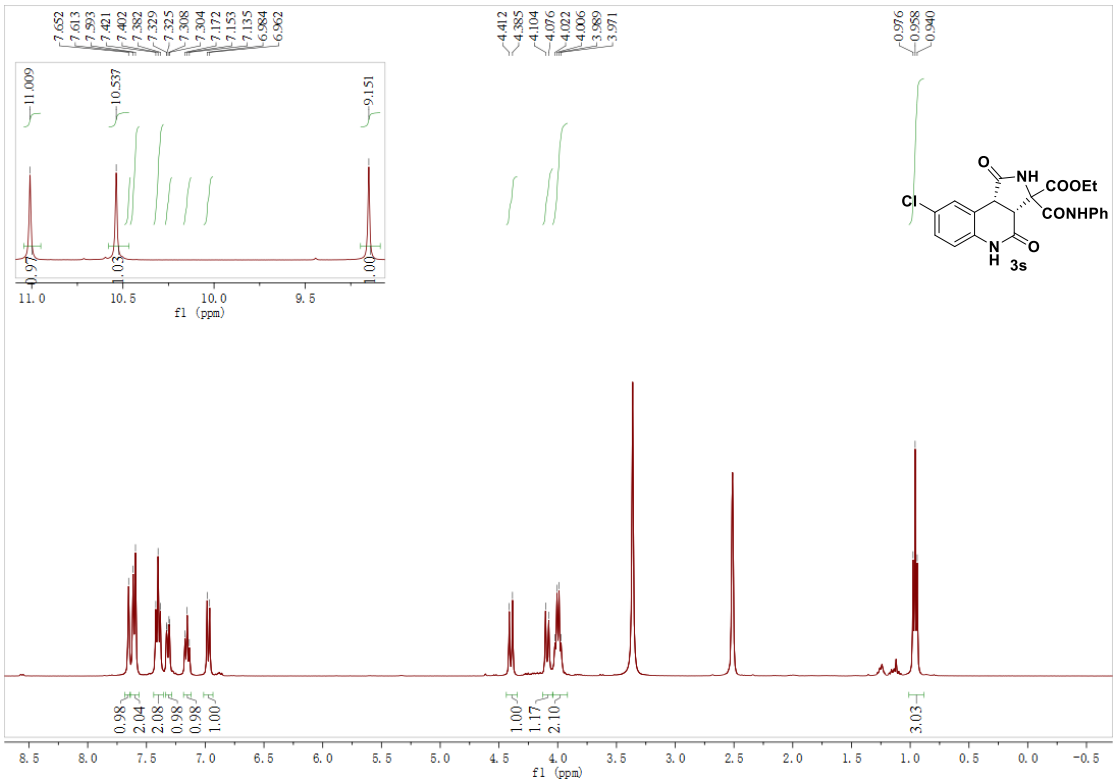

172.82
166.82
166.35
165.82
135.42
129.84
129.01
123.85
116.35
115.38
71.22
70.85
69.67
46.23
44.18
21.56
21.50
21.39
21.37
f1 (ppm)
NH
COO^{i}Pr
COO^{i}Pr
N
H
3p

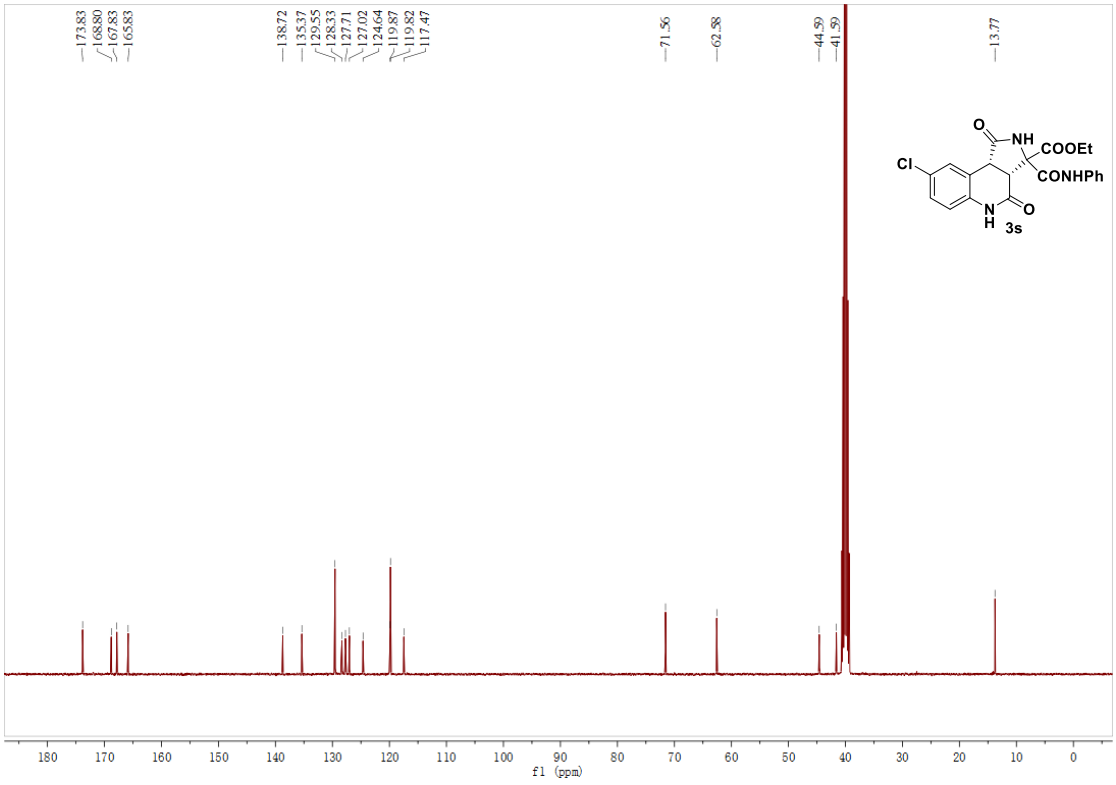

8.762
8.338
8.325
8.312
7.539
7.520
7.214
7.195
7.176
7.018
7.000
6.981
6.901
6.882
4.134
4.109
3.974
3.963
3.957
3.946
3.939
3.927
3.922
3.911
3.896
3.246
3.228
3.213
3.196
3.179
1.104
1.086
1.068
0.975
0.958
0.940
10.652
1.00
10.72
10.68
10.64
10.60
f1 (ppm)
NH
COOEt
CONHEt
N
H
O
3q
1.01
1.00
1.00
1.01
1.02
1.00
1.01
2.98
2.04
3.01
3.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


173.79
168.90
167.34
167.26
136.51
128.45
128.41
123.14
117.70
115.65
70.77
62.08
45.56
42.40
34.76
14.79
13.79
NH
COOEt
CONHEt
N
H
O
3q
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.010
7.632
7.612
7.600
7.581
7.414
7.394
7.374
7.241
7.222
7.203
7.163
7.145
7.126
7.054
7.036
7.017
6.948
6.928
4.370
4.343
4.039
4.012
3.984
3.966
3.949
3.932
0.930
0.912
0.895
10.874
10.573
0.96
0.99
10.85
10.75
10.65
10.55
f1 (ppm)
1.01
3.02
2.03
1.03
1.02
1.01
1.00
1.04
1.05
1.94
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)
O
NH
COOEt
CONHPh
N
H
O
3r


174.18
168.87
167.87
166.01
138.75
136.24
129.56
128.44
128.12
124.61
123.42
119.78
117.74
115.88
71.50
62.48
45.05
41.83
13.72
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
NH
COOEt
CONHPh
N
H
O
3r


7.652
7.613
7.593
7.421
7.402
7.382
7.329
7.325
7.308
7.304
7.172
7.153
7.135
6.584
6.562
4.412
4.385
4.104
4.076
4.022
4.006
3.989
3.971
0.976
0.958
0.940
11.009
10.537
9.151
0.97
1.03
1.00
11.0
10.5
10.0
9.5
f1 (ppm)
O
NH
COOEt
Cl
CONHPh
N
H
O
3s
0.98
2.04
2.08
0.98
0.98
1.00
1.00
1.17
2.10
3.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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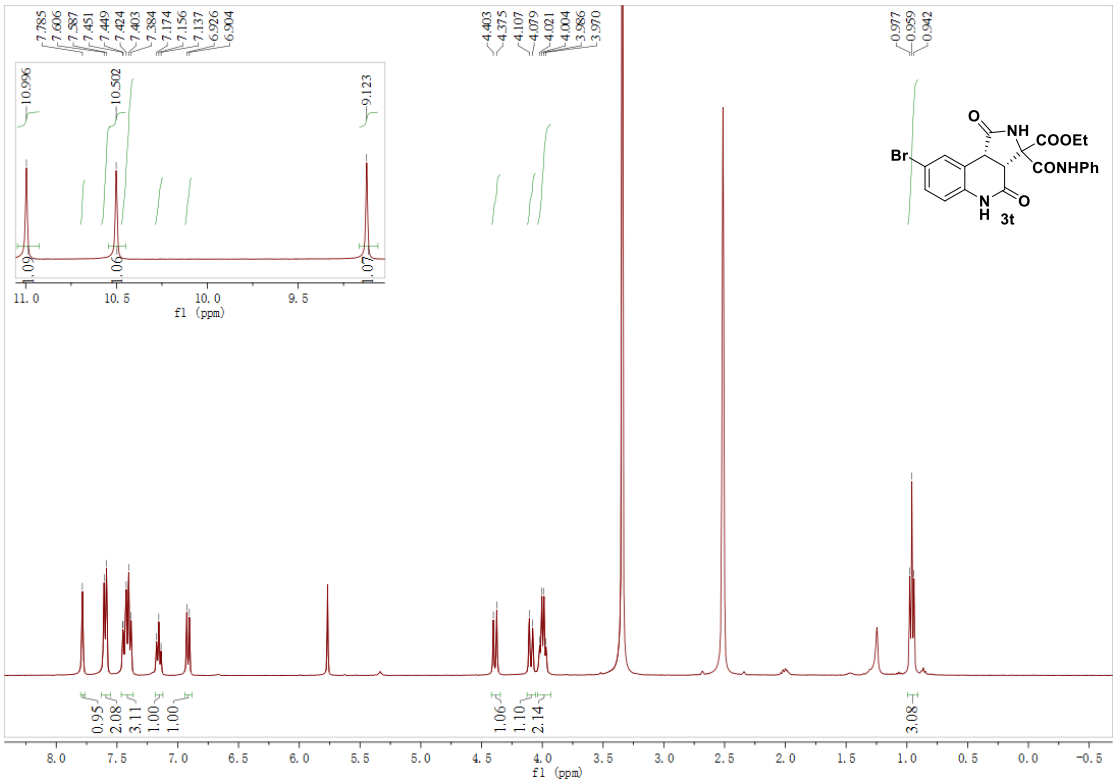
167.83
165.83
138.72
135.37
129.55
128.33
127.71
127.02
124.64
119.87
119.82
117.47
71.56
62.88
44.59
41.59
13.77
O
NH
COOEt
Cl
CONHPh
N
H
O
3s
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.387
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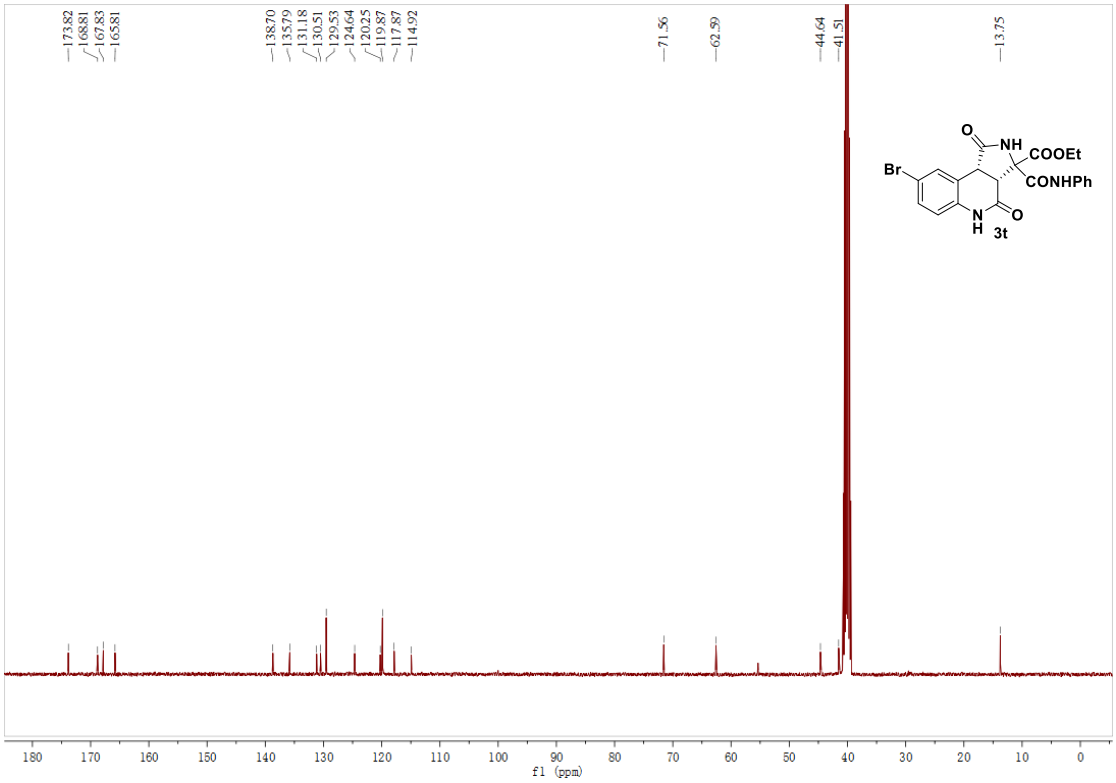
7.449
7.424
7.403
7.384
7.174
7.156
7.137
6.926
6.904
4.403
4.375
4.107
4.079
4.021
4.004
3.586
3.570
0.977
0.959
0.942
10.996
10.502
9.123
1.09
1.06
1.07
11.0
10.5
10.0
9.5
f1 (ppm)
O
NH
COOEt
Br
CONHPh
N
H
O
3t
0.95
2.08
3.11
1.00
1.00
1.06
1.10
2.14
3.08
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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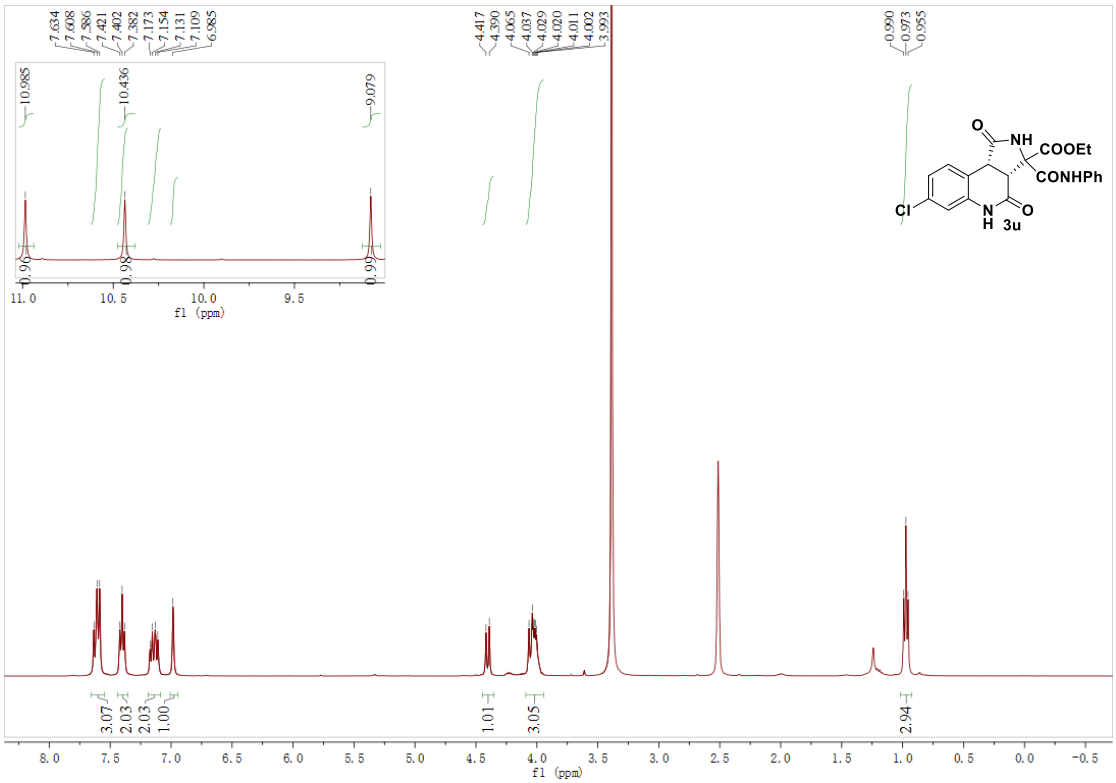
165.81
138.70
135.79
131.18
130.51
129.53
124.64
120.25
119.87
117.87
114.92
71.56
62.99
44.64
41.51
13.75
O
NH
COOEt
Br
CONHPh
N
H
O
3t
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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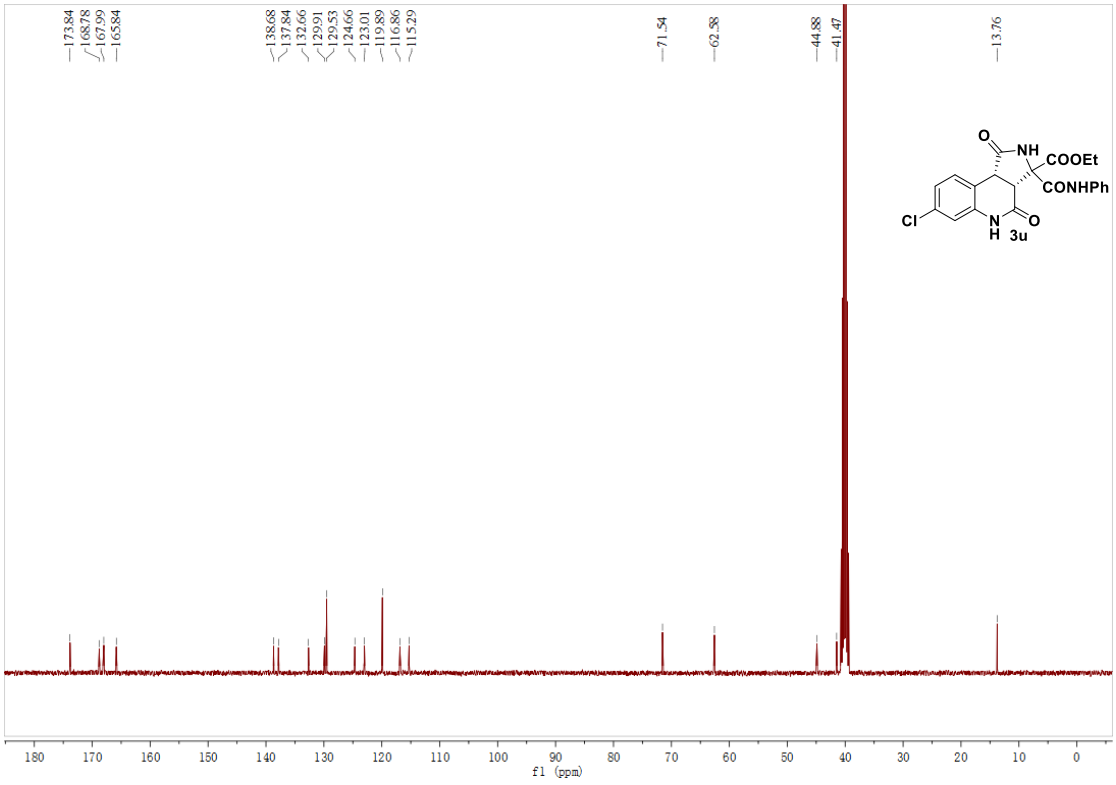
7.402
7.382
7.173
7.154
7.131
7.109
6.985
4.417
4.390
4.065
4.037
4.029
4.020
4.011
4.002
3.992
0.990
0.973
0.955
10.985
10.436
9.079
0.96
0.98
0.99
11.0
10.5
10.0
9.5
f1 (ppm)
3.07
2.03
2.03
1.00
1.01
3.05
2.94
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)
O
NH
COOEt
CONHPh
Cl
N
H
O
3u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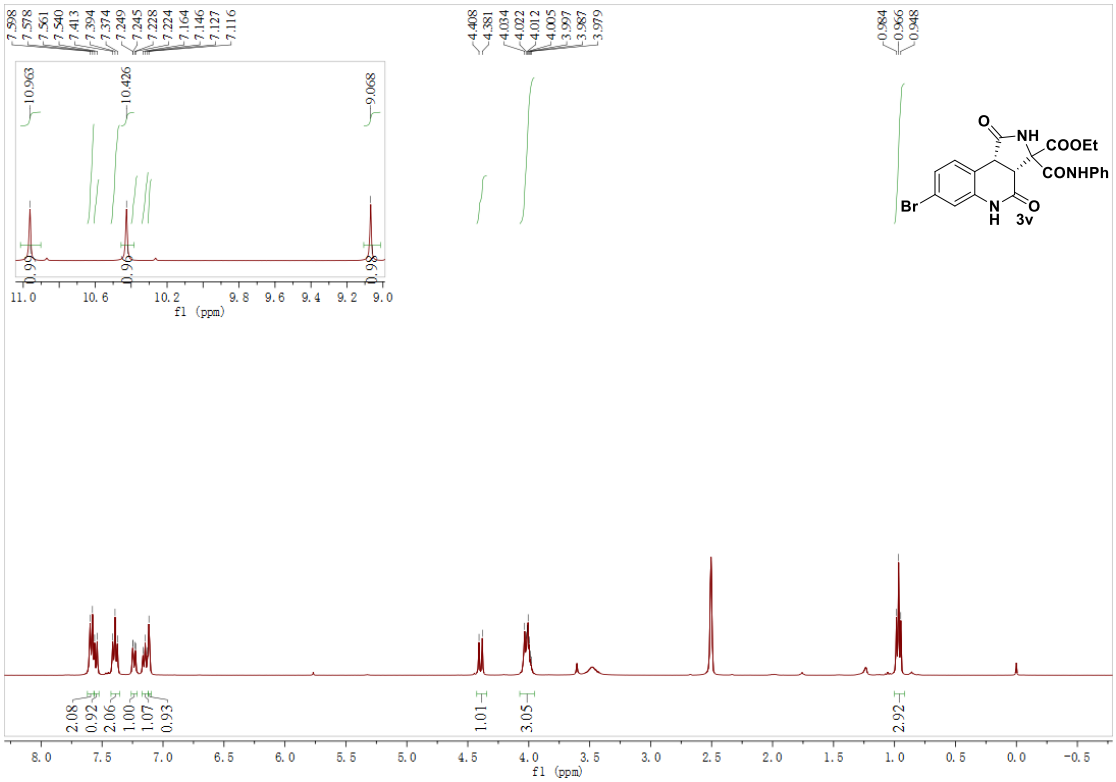
132.66
129.91
129.53
124.66
123.01
119.89
116.86
115.29
71.54
62.58
44.88
41.47
13.76
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
NH
COOEt
CONHPh
Cl
N
H
O
3u


7.598
7.578
7.561
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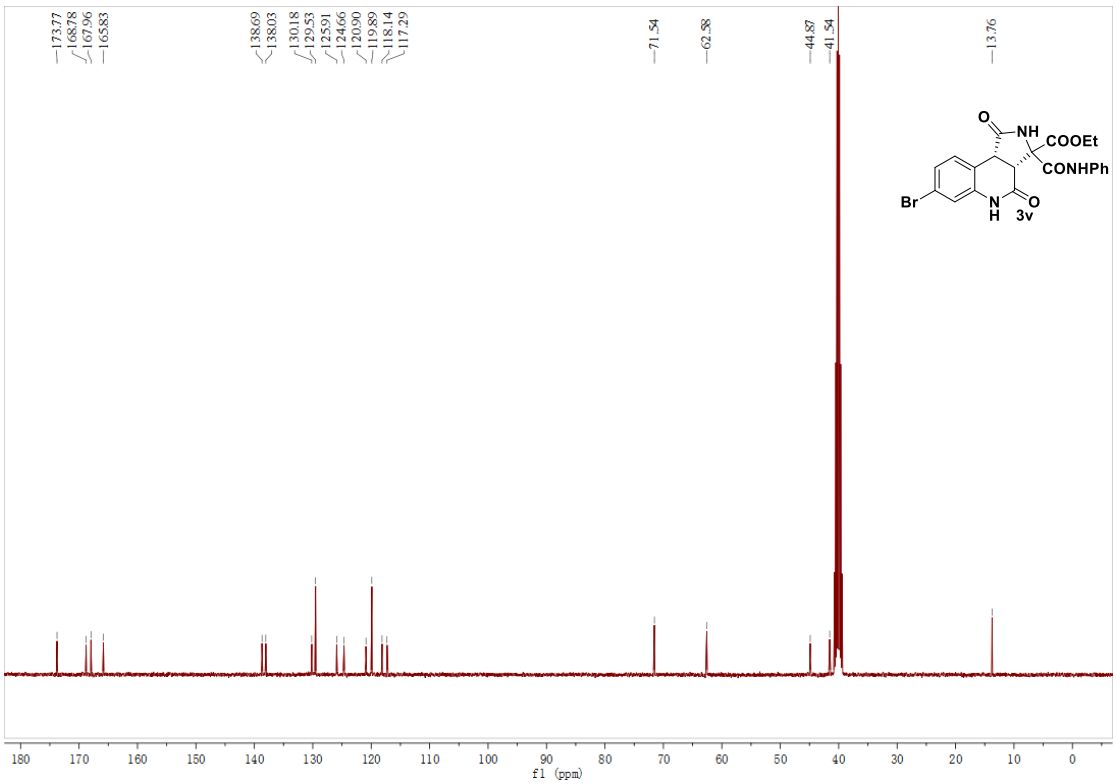
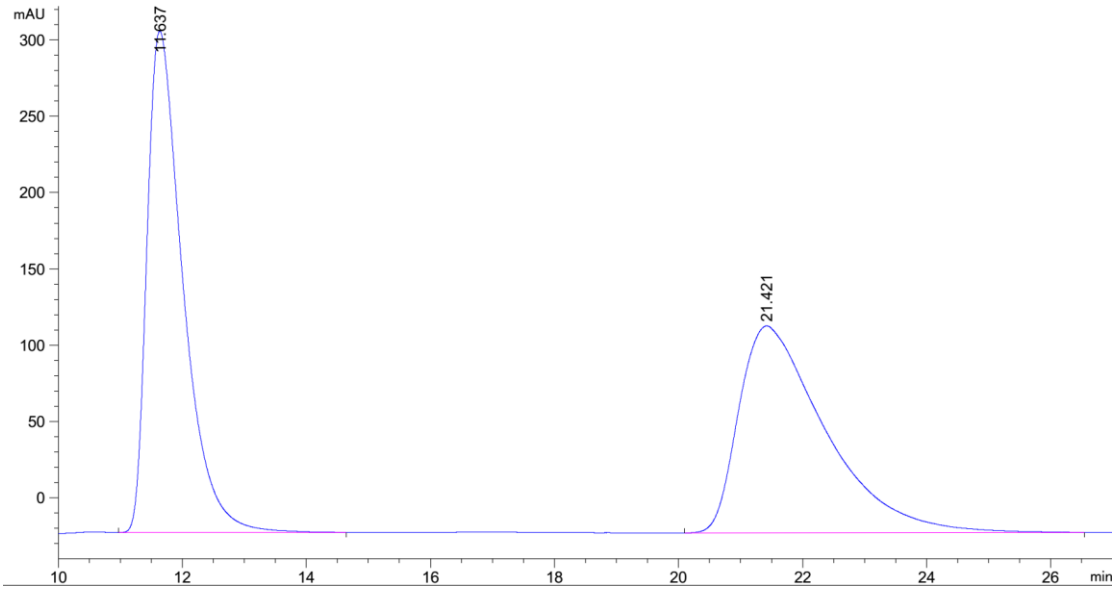
7.413
7.394
7.374
7.249
7.245
7.228
7.224
7.164
7.146
7.127
7.116
4.408
4.381
4.034
4.022
4.012
4.005
3.997
3.987
3.979
0.984
0.966
0.948
10.963
10.426
9.068
0.99
0.96
0.98
11.0
10.6
10.2
9.8
9.6
9.4
9.2
9.0
f1 (ppm)
O
NH
COOEt
CONHPh
Br
N
H
O
3v
2.08
0.92
2.06
1.00
1.07
0.93
1.01
3.05
2.92
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


173.77
168.78
167.96
165.83
138.69
138.03
130.18
129.53
125.91
124.66
120.90
119.89
118.14
117.29
71.54
62.58
44.87
41.54
13.76
O
NH
COOEt
CONHPh
Br
N
H
O
3v
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

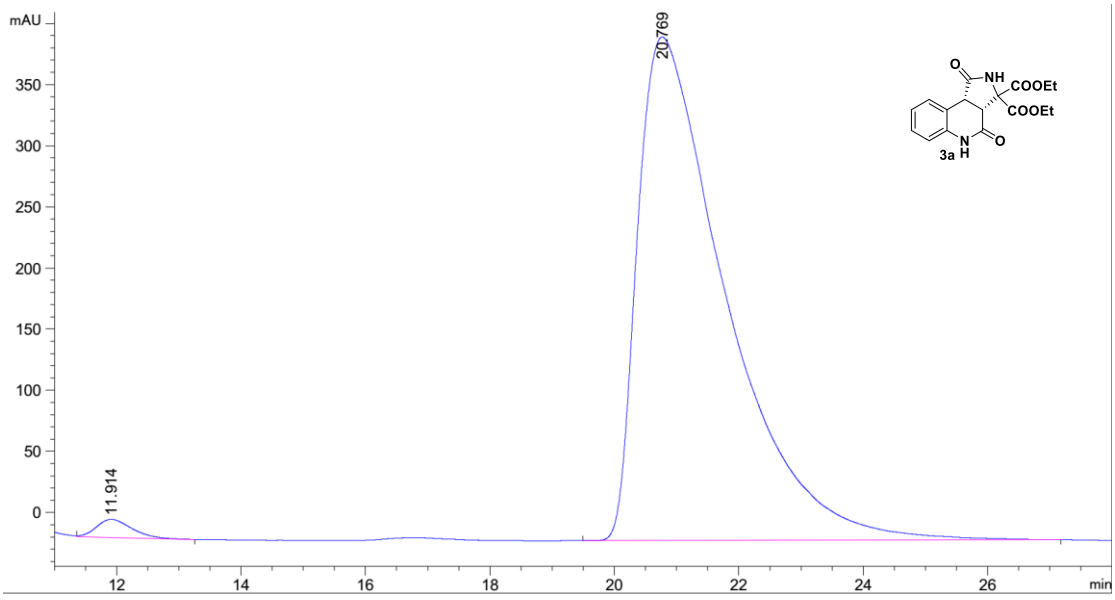
4. Chiral HPLC Spectra of 3

HPLC chromatogram of racemic **3a**



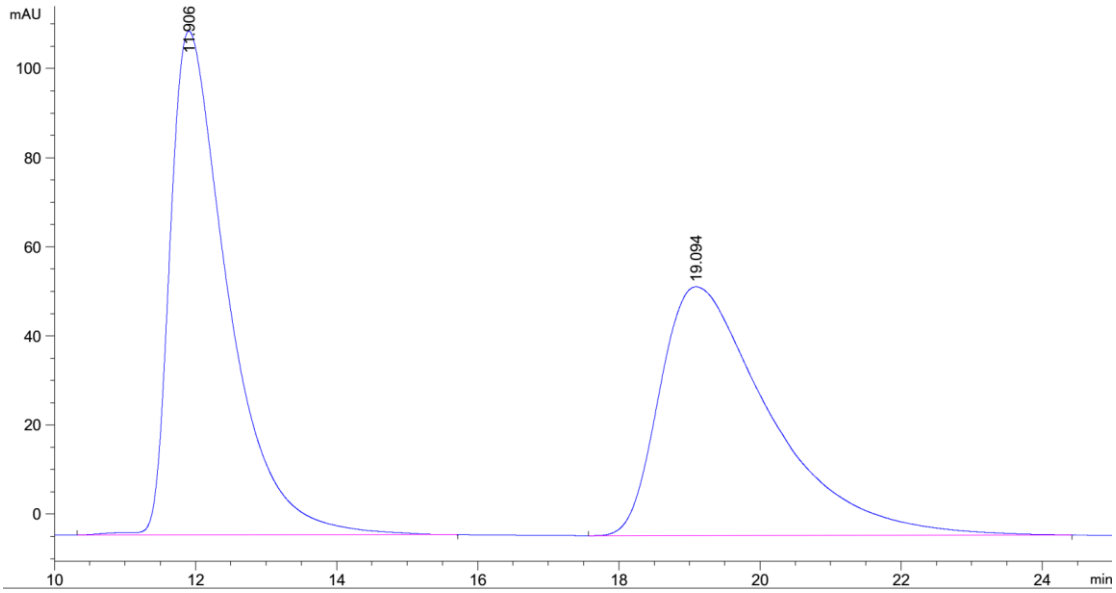
RT [min]	Type	Width [min]	Area	Height	Area%	Name
11.637	BB	0.6047	13221.9512	328.7638	50.1449	
21.421	BB	1.4128	13145.5166	135.6249	49.8551	

HPLC chromatogram of enantiopure **3a**



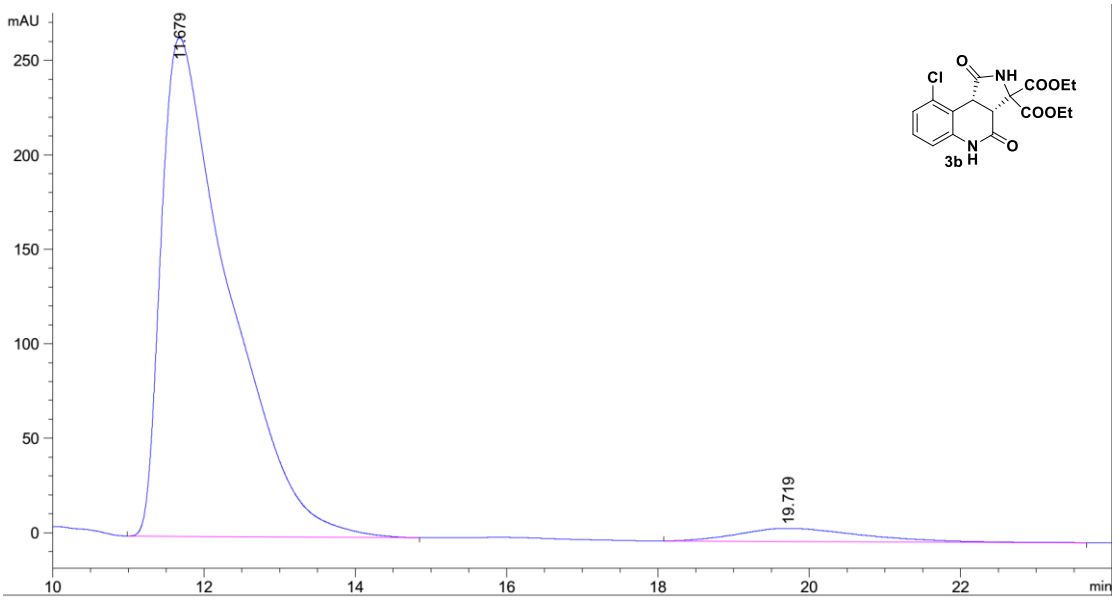
RT [min]	Type	Width [min]	Area	Height	Area%	Name
11.914	VB	0.5936	578.4388	14.6825	1.4079	
20.769	BB	1.3786	40507.0859	411.7857	98.5921	

HPLC chromatogram of racemic **3b**



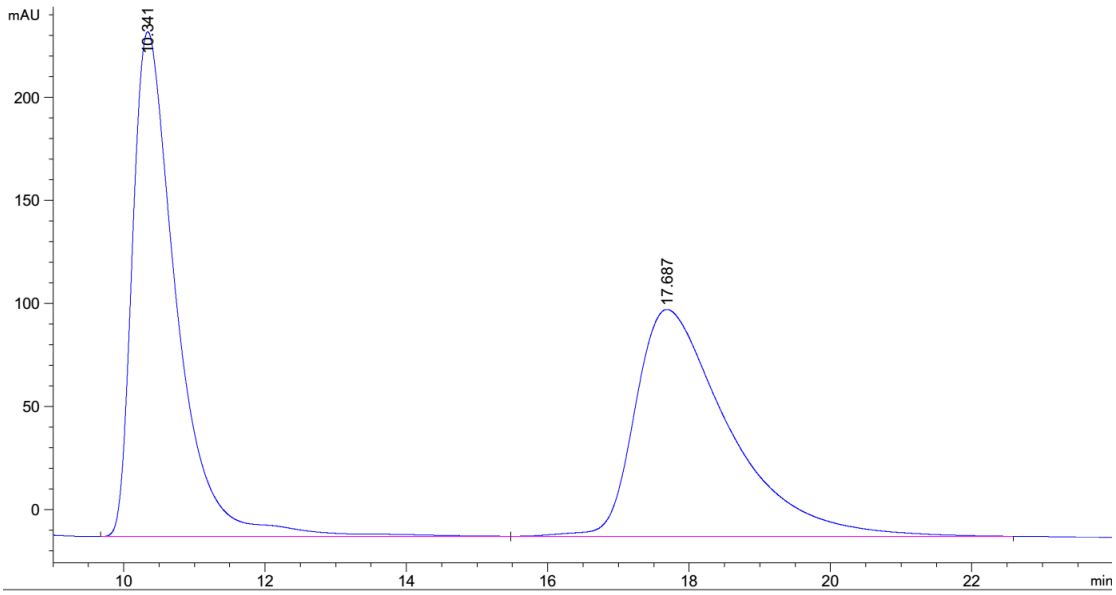
RT [min]	Type	Width [min]	Area	Height	Area%	Name
11.906	BB	0.8422	6432.2114	113.0720	51.4350	
19.094	BB	1.5315	6073.3110	55.8560	48.5650	

HPLC chromatogram of enantiopure **3b**



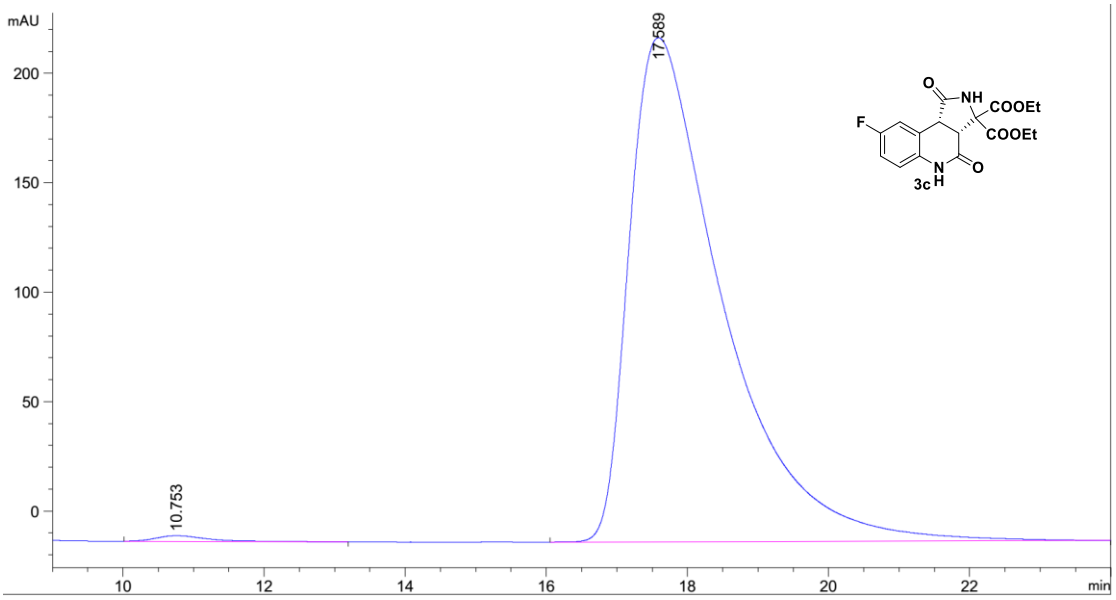
RT [min]	Type	Width [min]	Area	Height	Area%	Name
11.679	BB	0.8887	16382.3447	263.9207	95.4308	
19.719	BB	1.3250	784.3910	6.9352	4.5692	

HPLC chromatogram of racemic **3c**



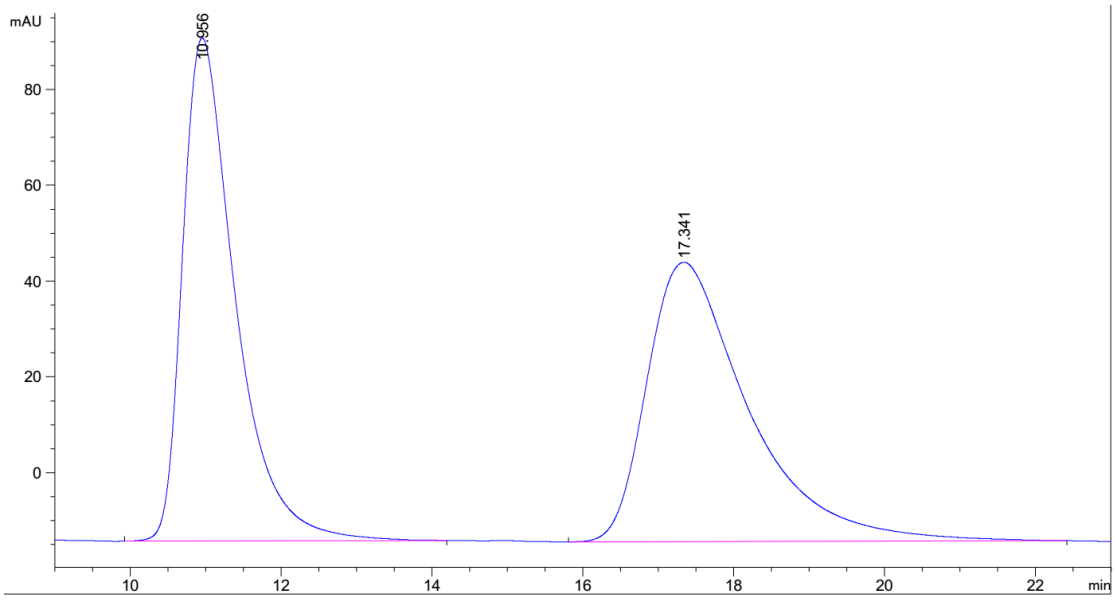
RT [min]	Type	Width [min]	Area	Height	Area%	Name
10.341	BB	0.6494	10564.1250	244.8512	51.0934	
17.687	BB	1.3202	10111.9883	110.0277	48.9066	

HPLC chromatogram of enantiopure **3c**



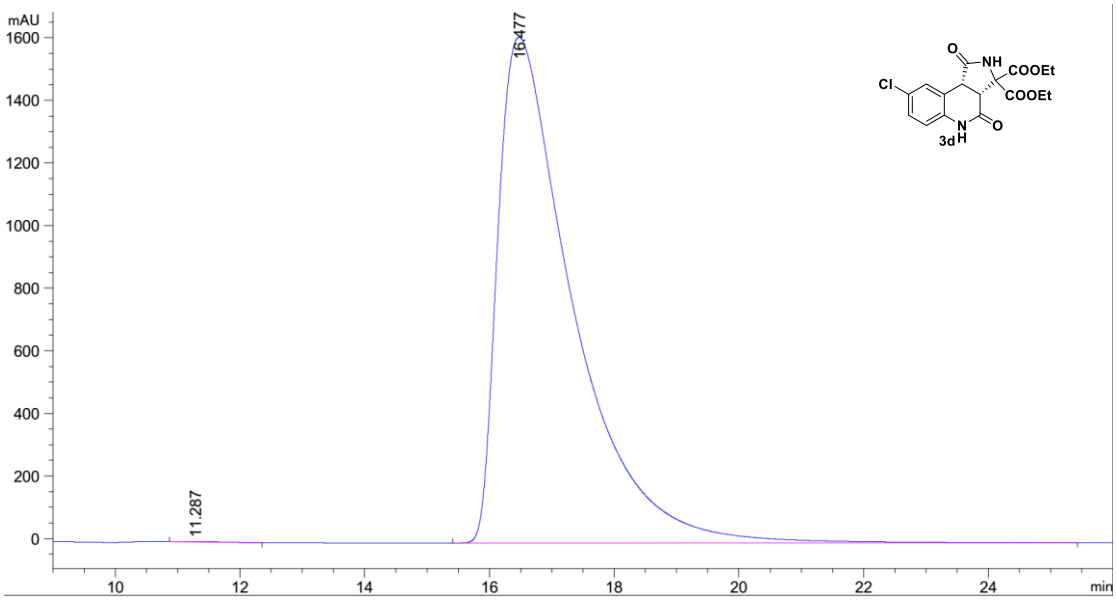
RT [min]	Type	Width [min]	Area	Height	Area%	Name
10.753	BV R	0.6184	133.3428	2.5740	0.6256	
17.589	BB	1.3464	21181.3750	230.2246	99.3744	

HPLC chromatogram of racemic **3d**



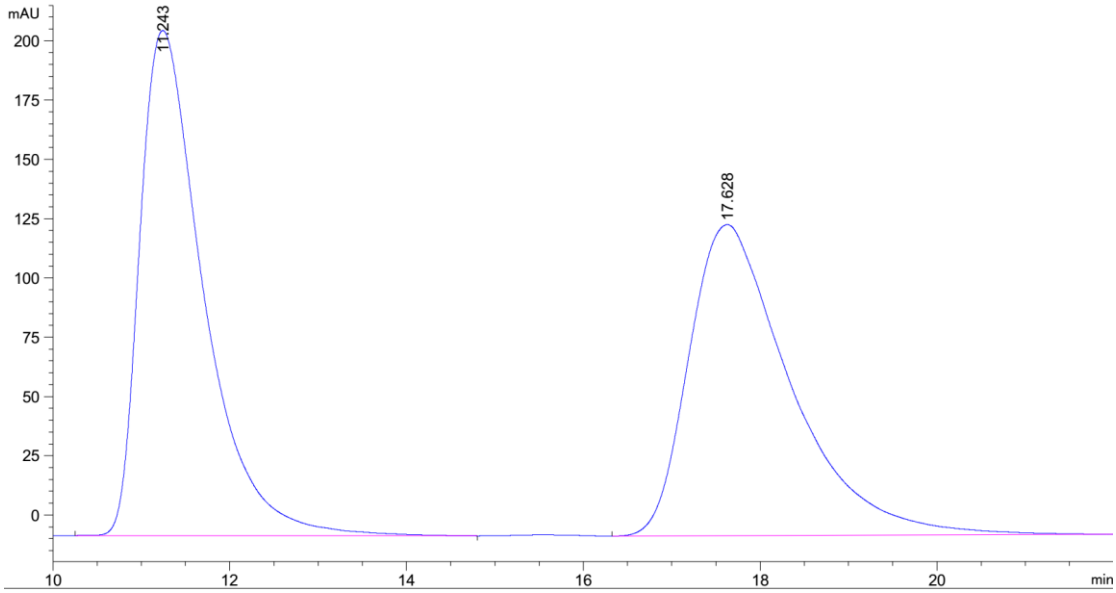
RT [min]	Type	Width [min]	Area	Height	Area%	Name
10.956	BB	0.7298	5106.6748	105.0209	48.3564	
17.341	BB	1.3476	5453.8096	58.3172	51.6436	

HPLC chromatogram of enantiopure **3d**



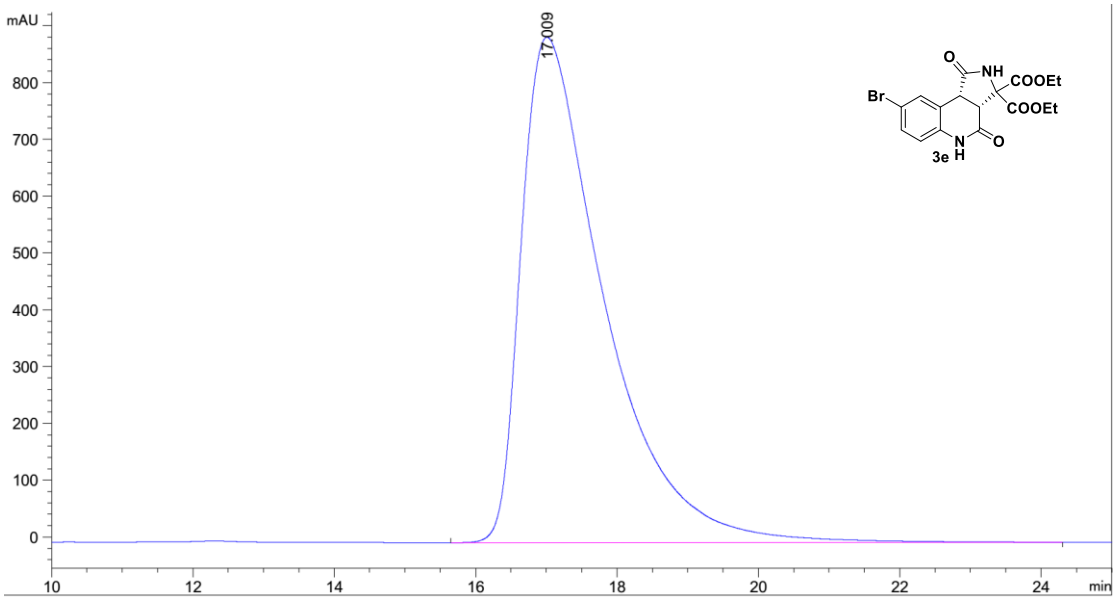
RT [min]	Type	Width [min]	Area	Height	Area%	Name
11.287	BB	0.4926	73.7616	1.7778	0.0547	
16.477	BB	1.2211	134705.3750	1615.8958	99.9453	

HPLC chromatogram of racemic **3e**



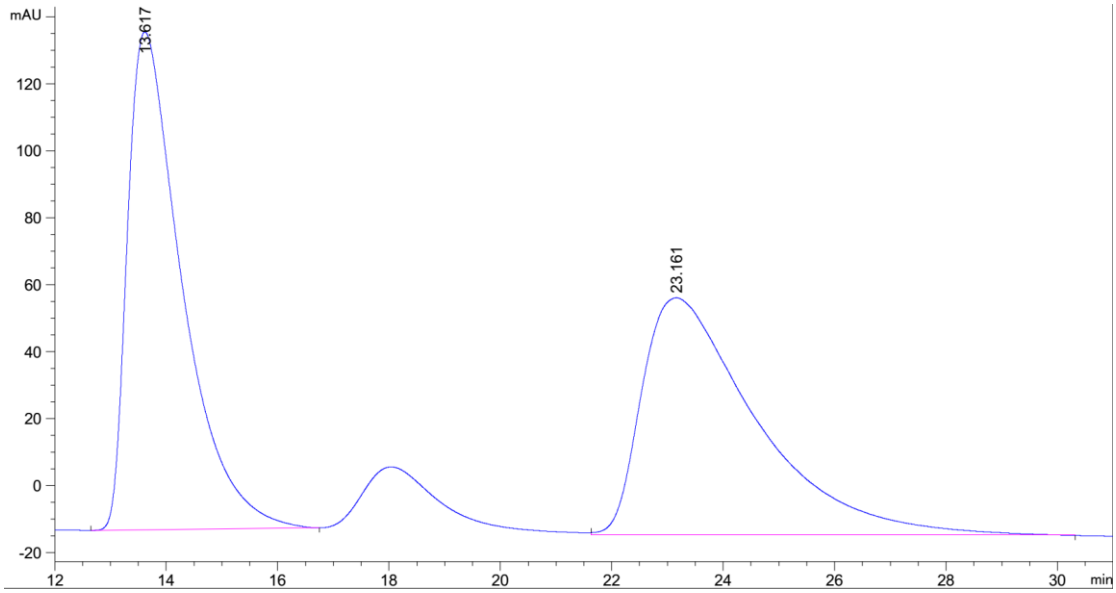
RT [min]	Type	Width [min]	Area	Height	Area%	Name
11.243	BB	0.7604	10668.8838	212.9956	50.4112	
17.628	BBA	1.1949	10494.8447	131.1792	49.5888	

HPLC chromatogram of enantiopure **3e**



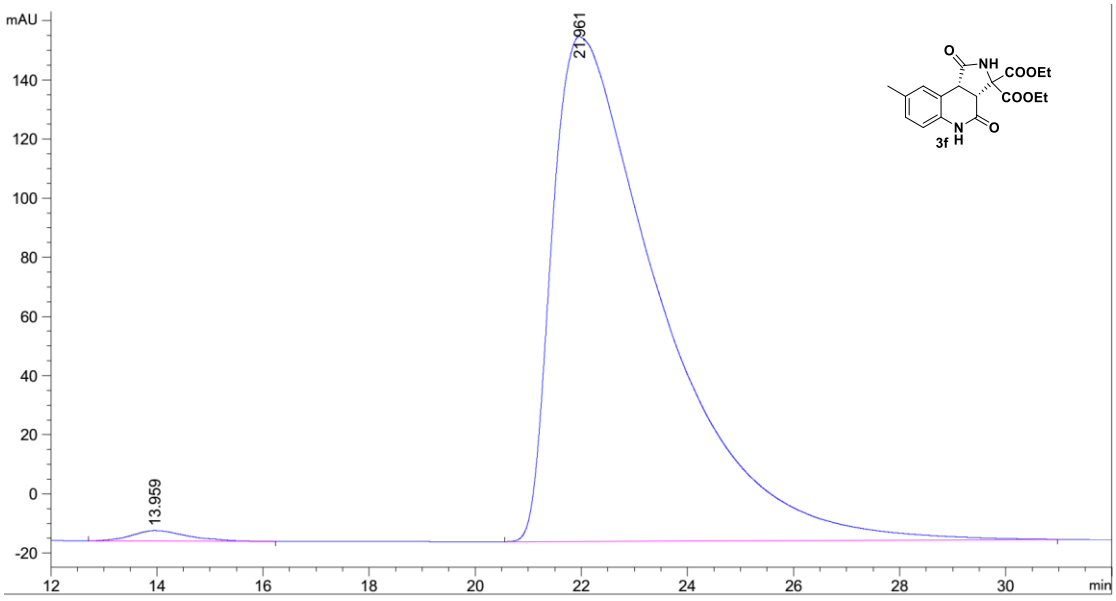
RT [min]	Type	Width [min]	Area	Height	Area%	Name
17.009	BB	1.1901	72689.5703	889.8030	100.0000	

HPLC chromatogram of racemic **3f**



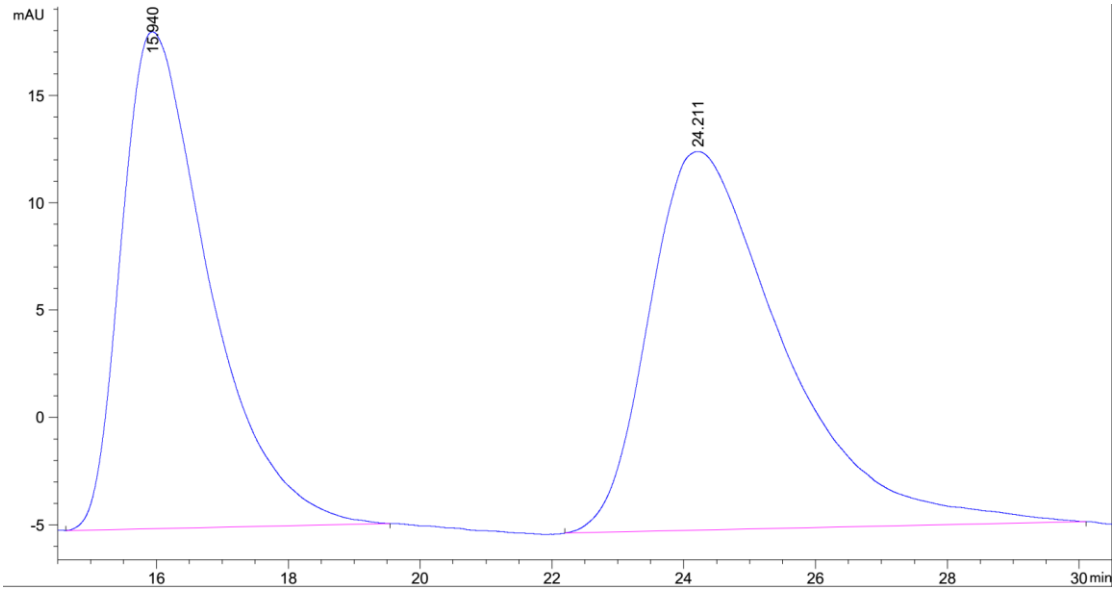
RT [min]	Type	Width [min]	Area	Height	Area%	Name
13.617	BB	1.0141	10129.1514	148.8133	49.9998	
23.161	MM	2.3838	10129.2471	70.8193	50.0002	

HPLC chromatogram of enantiopure **3f**



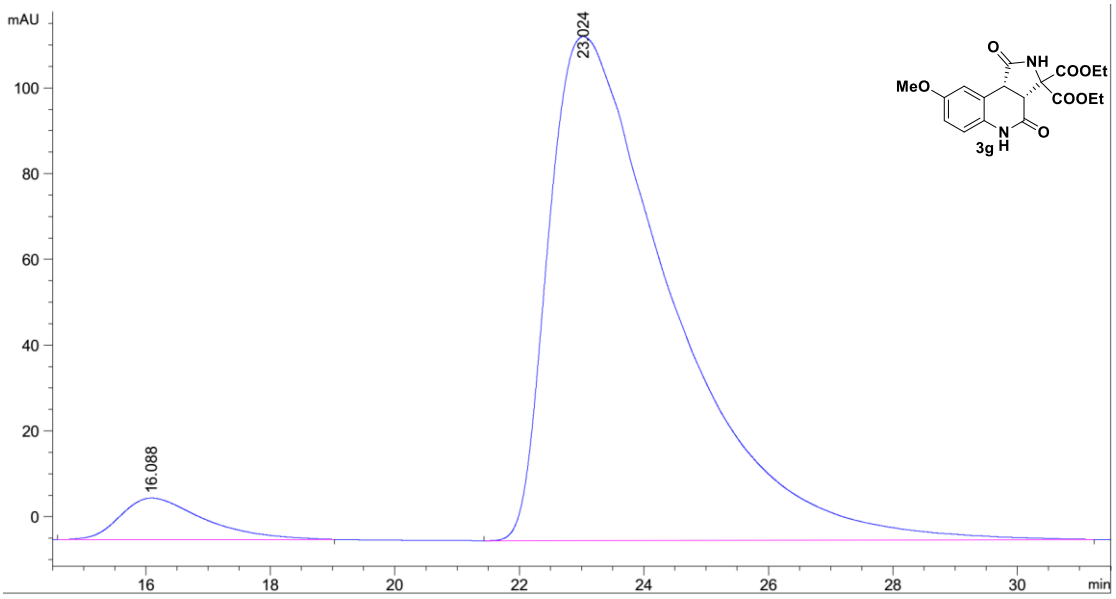
RT [min]	Type	Width [min]	Area	Height	Area%	Name
13.959	BB	0.8804	260.6408	3.5591	1.0642	
21.961	BB	1.8687	24231.2383	170.7459	98.9358	

HPLC chromatogram of racemic **3g**



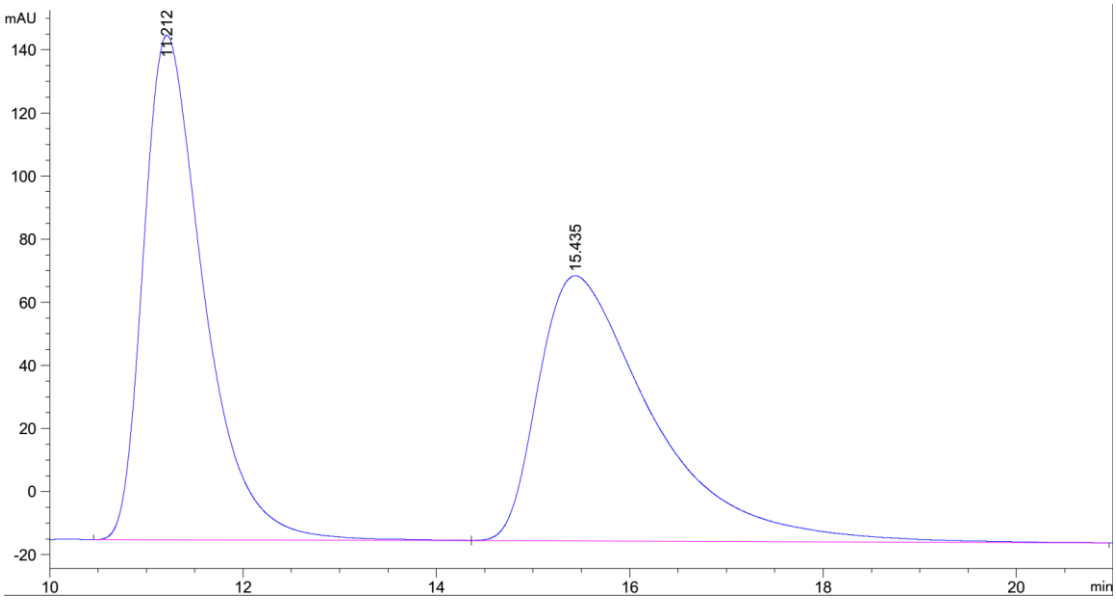
RT [min]	Type	Width [min]	Area	Height	Area%	Name
15.940	BB	1.2095	2131.6145	23.1342	46.0212	
24.211	BB	1.6631	2500.1992	17.6338	53.9788	

HPLC chromatogram of enantiopure **3g**



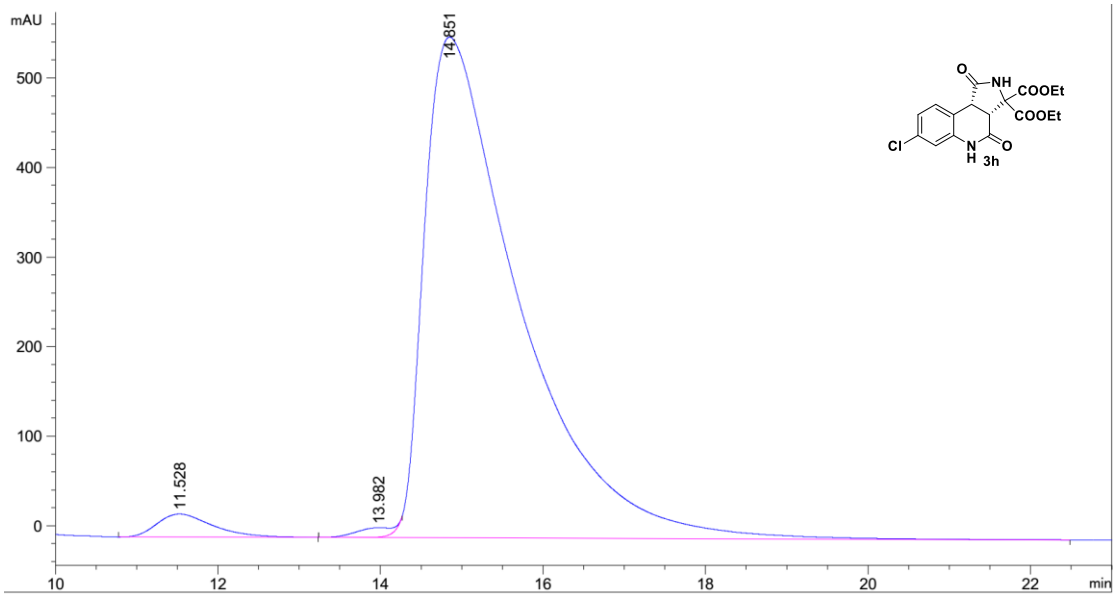
RT [min]	Type	Width [min]	Area	Height	Area%	Name
16.088	BB	1.0952	897.0950	9.6716	5.2438	
23.024	BB	1.8936	16210.6709	117.5317	94.7562	

HPLC chromatogram of racemic **3h**



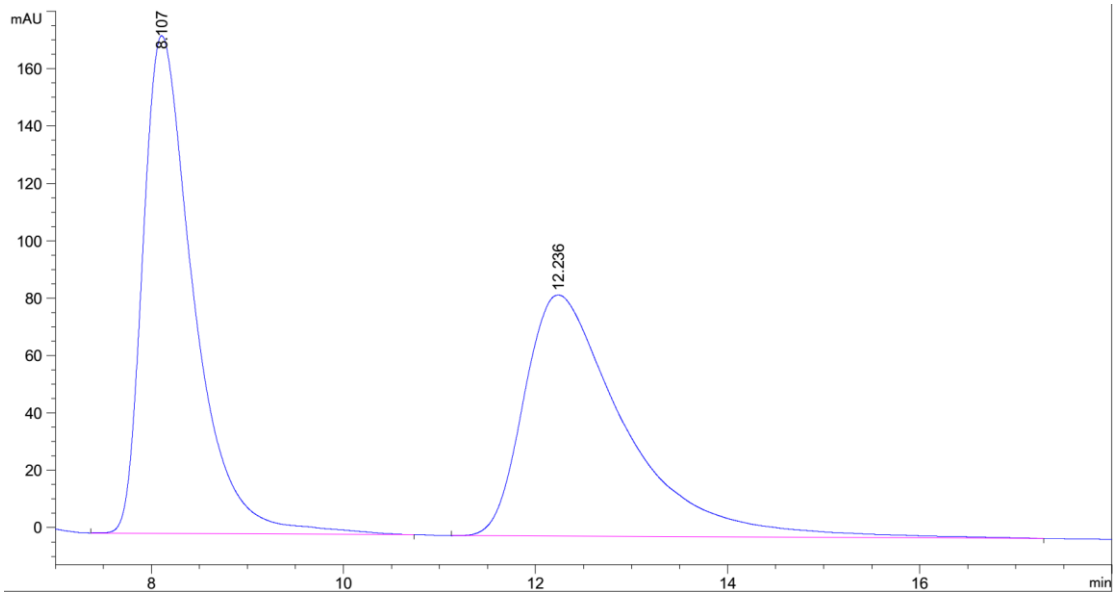
RT [min]	Type	Width [min]	Area	Height	Area%	Name
11.212	BB	0.6565	6927.2202	159.8793	50.1551	
15.435	BBA	1.2167	6884.3799	83.9960	49.8449	

HPLC chromatogram of enantiopure **3h**



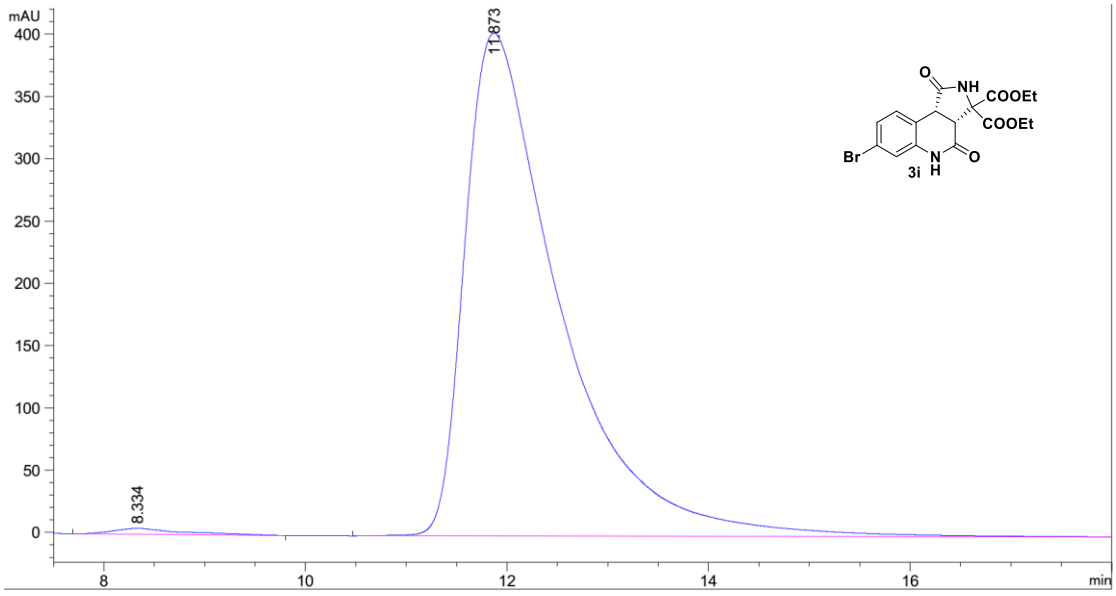
RT [min]	Type	Width [min]	Area	Height	Area%	Name
11.528	BB	0.7133	1228.3304	25.8066	2.6181	
13.982	BV E	0.4416	308.5460	10.4458	0.6577	
14.851	VB R	1.1527	45379.2148	559.2125	96.7242	

HPLC chromatogram of racemic **3i**



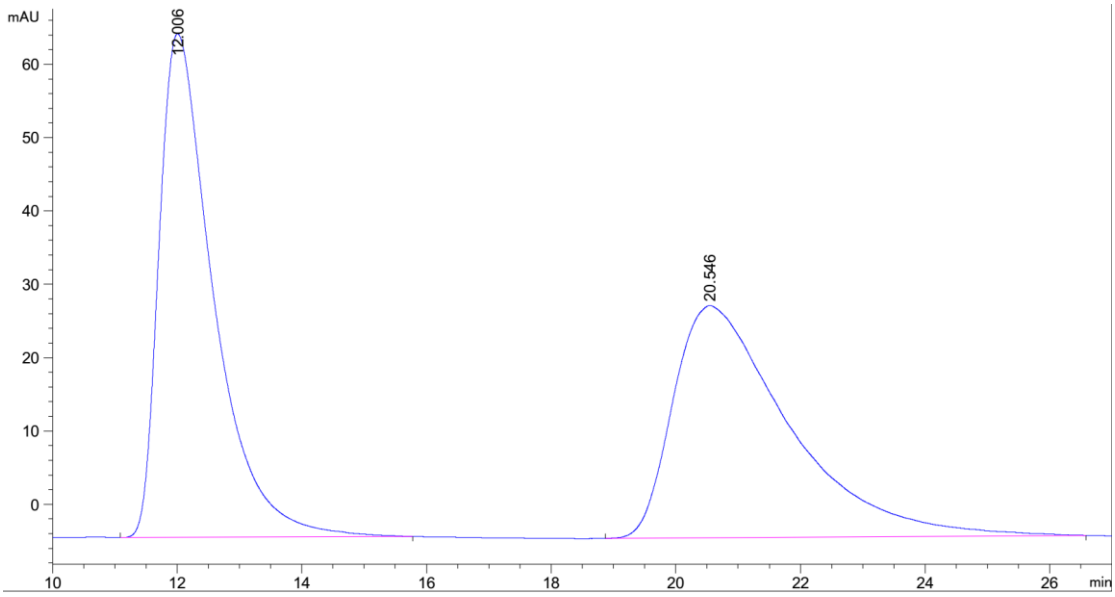
RT [min]	Type	Width [min]	Area	Height	Area%	Name
8.107	BB	0.5518	6361.2964	173.4695	50.8834	
12.236	BB	1.0724	6140.4116	84.0922	49.1166	

HPLC chromatogram of enantiopure **3i**



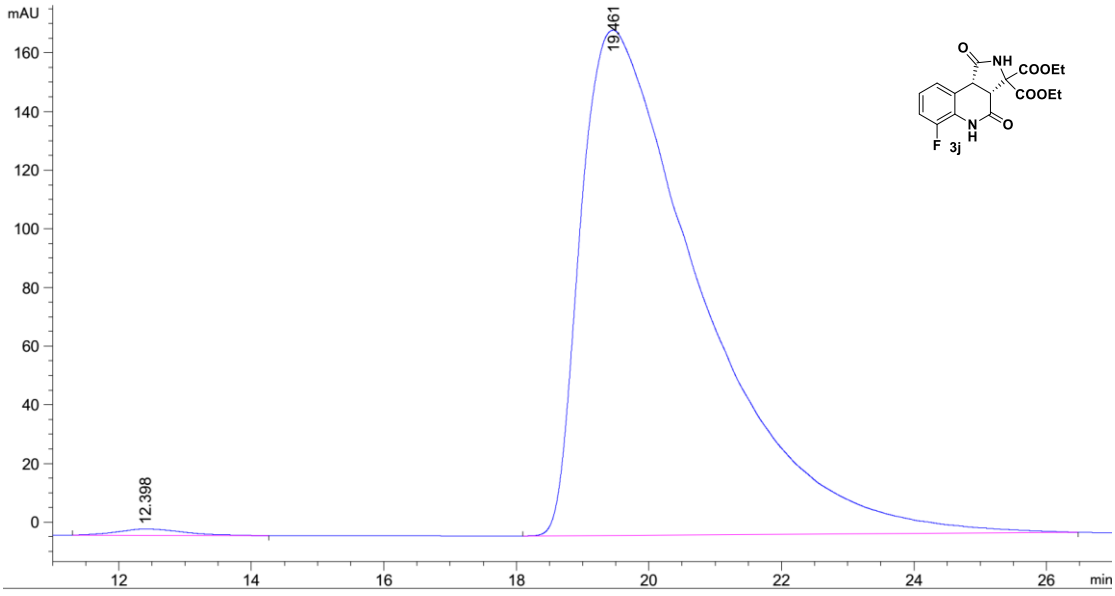
RT [min]	Type	Width [min]	Area	Height	Area%	Name
8.334	BB	0.5998	223.9976	4.7016	0.8410	
11.873	BBA	0.9382	26410.2266	403.7383	99.1590	

HPLC chromatogram of racemic **3j**



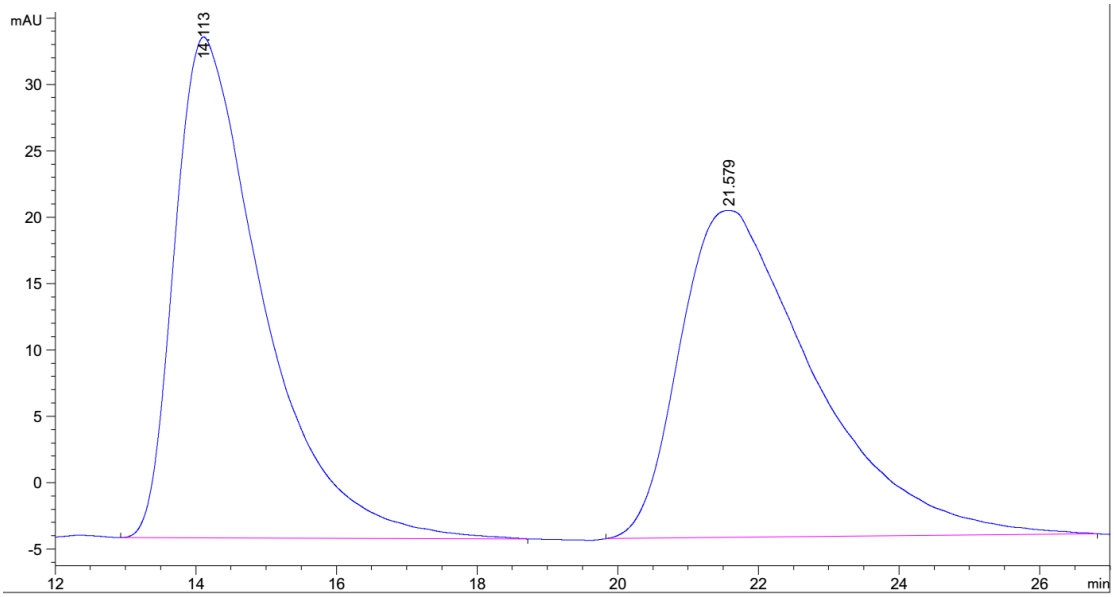
RT [min]	Type	Width [min]	Area	Height	Area%	Name
12.006	BB	0.8896	4158.6475	68.6677	50.4164	
20.546	BB	1.5624	4089.9565	31.6754	49.5836	

HPLC chromatogram of enantiopure **3j**



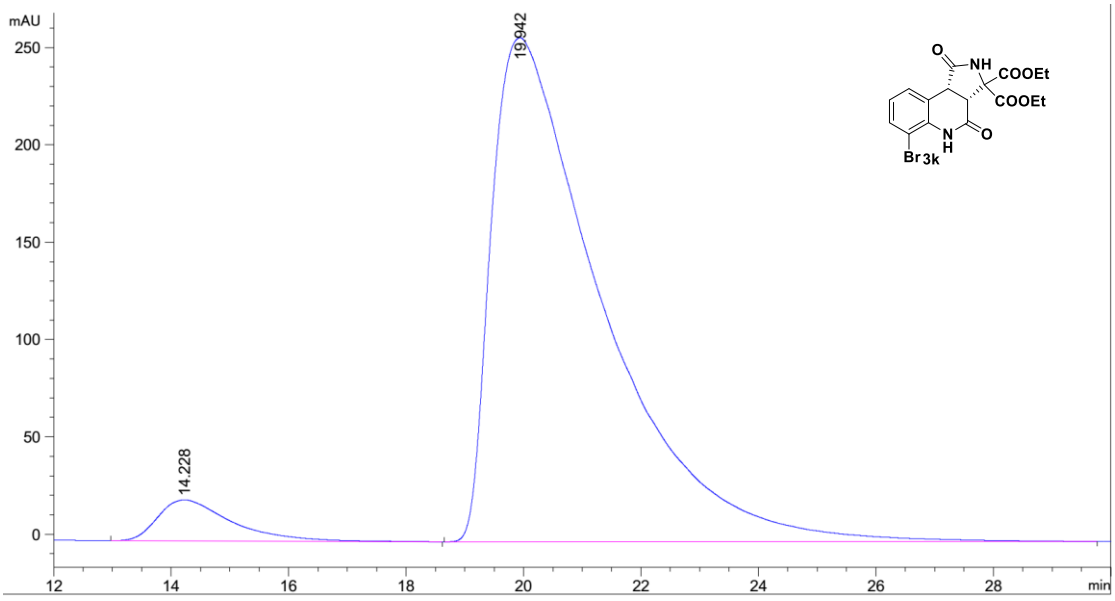
RT [min]	Type	Width [min]	Area	Height	Area%	Name
12.398	BB	0.7930	145.8371	2.1593	0.6632	
19.461	BB	1.7525	21844.5371	172.2010	99.3368	

HPLC chromatogram of racemic **3k**



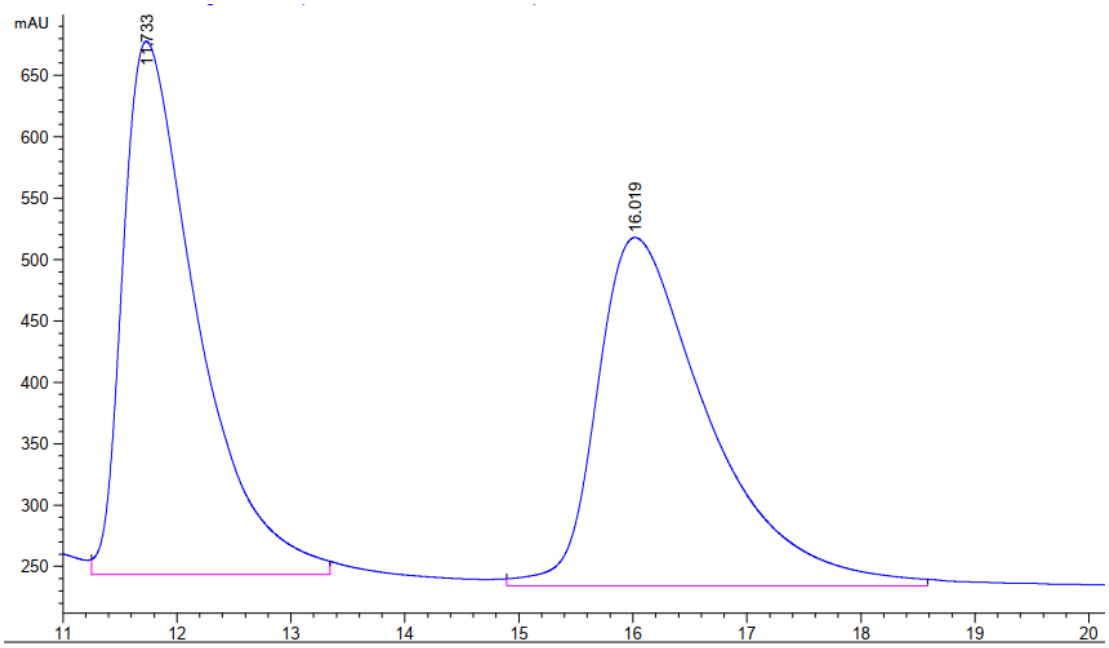
RT [min]	Type	Width [min]	Area	Height	Area%	Name
14.113	BV R	1.1710	3280.2070	37.7398	50.1158	
21.579	BV R	1.5509	3265.0535	24.6332	49.8842	

HPLC chromatogram of enantiopure **3k**



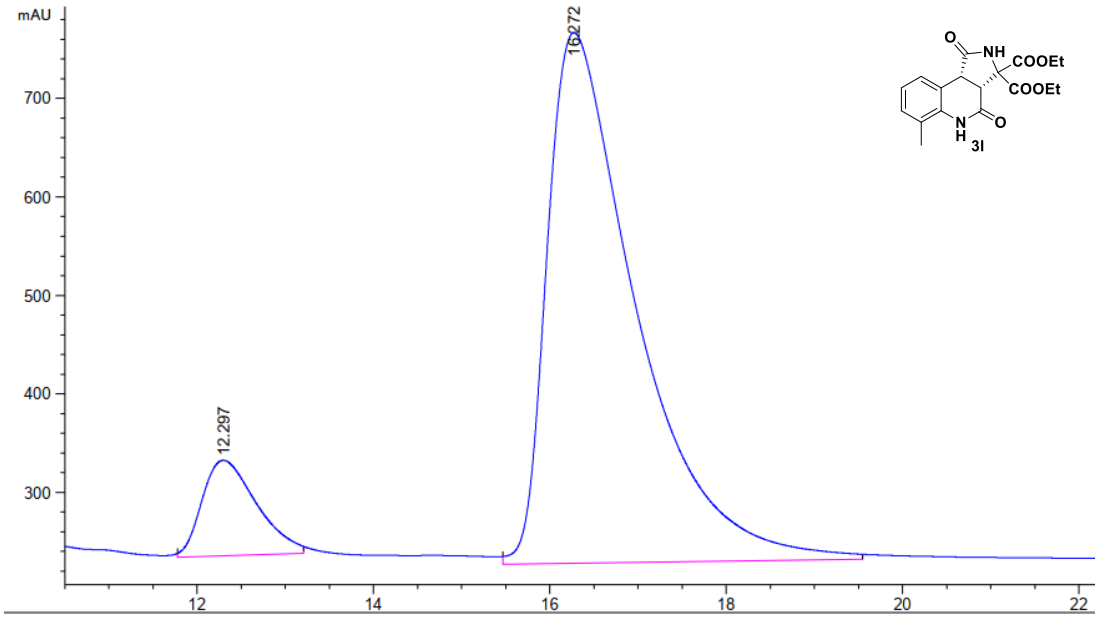
RT [min]	Type	Width [min]	Area	Height	Area%	Name
14.228	BB	1.1976	1836.0479	21.1338	5.1318	
19.942	BB	1.8023	33941.9453	258.9309	94.8682	

HPLC chromatogram of racemic **3l**



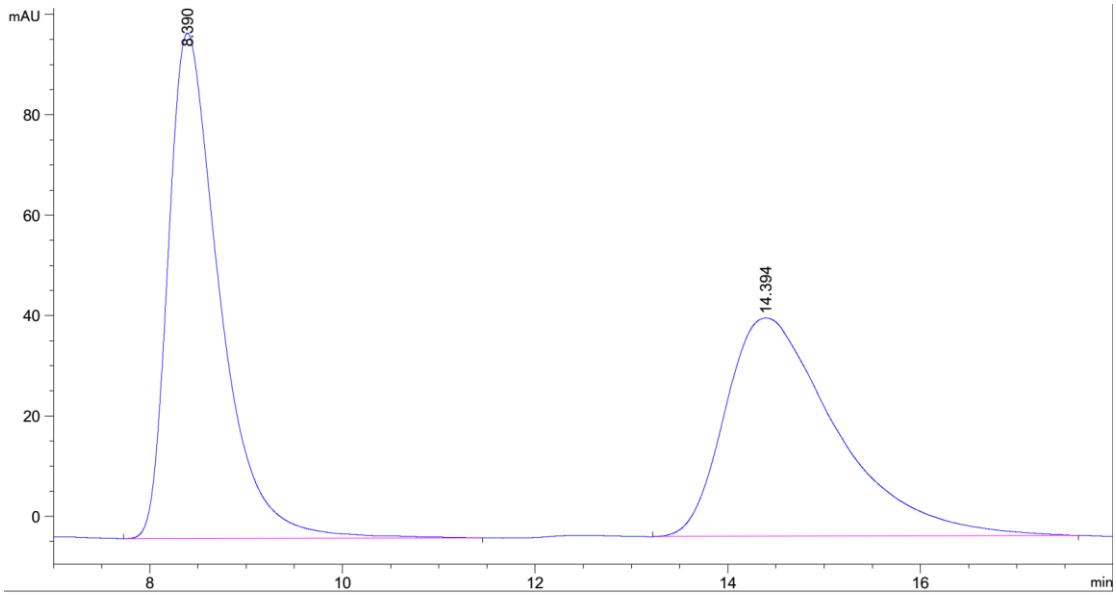
RT [min]	Type	Width [min]	Area	Height	Area%	Name
11.733	MM R	0.7529	1.96114e4	434.13776	50.2739	
16.019	MM R	1.1389	1.93977e4	283.86484	49.7261	

HPLC chromatogram of enantiopure **3l**



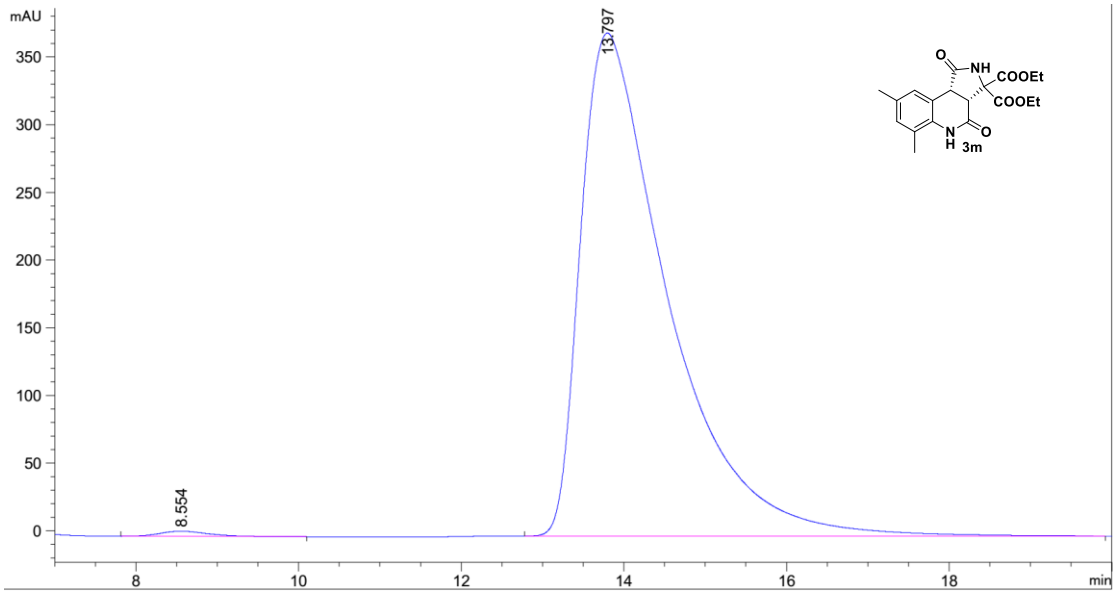
RT [min]	Type	Width [min]	Area	Height	Area%	Name
12.297	MM R	0.7143	4158.68896	97.03934	9.9212	
16.272	MM R	1.1457	3.77584e4	538.92755	90.0788	

HPLC chromatogram of racemic **3m**



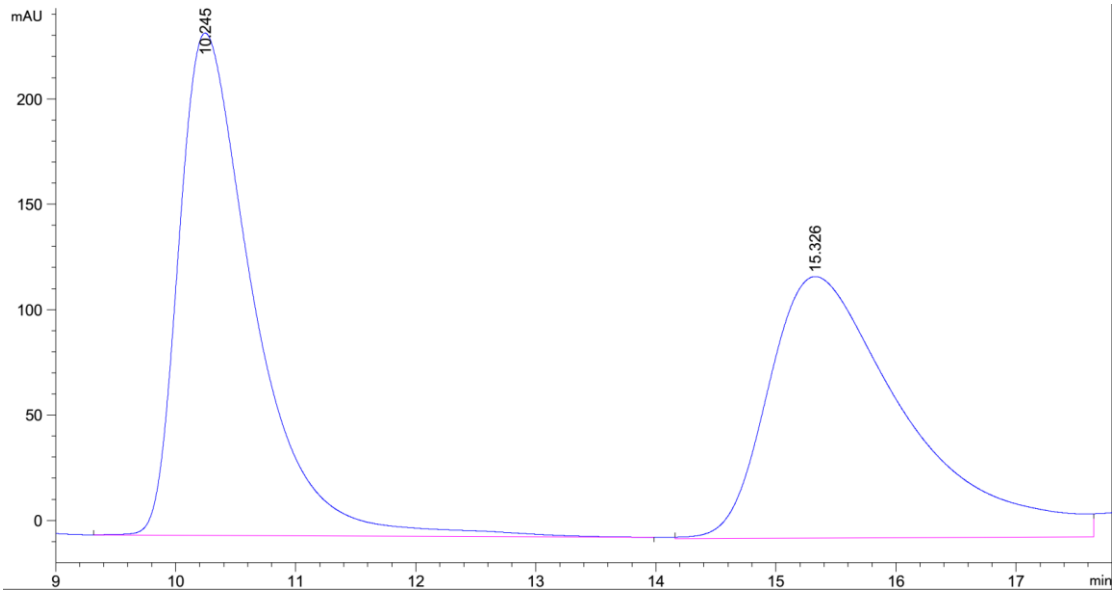
RT [min]	Type	Width [min]	Area	Height	Area%	Name
8.390	BB	0.5603	3731.3003	100.7046	51.7127	
14.394	BB	1.1294	3484.1421	43.5035	48.2873	

HPLC chromatogram of enantiopure **3m**



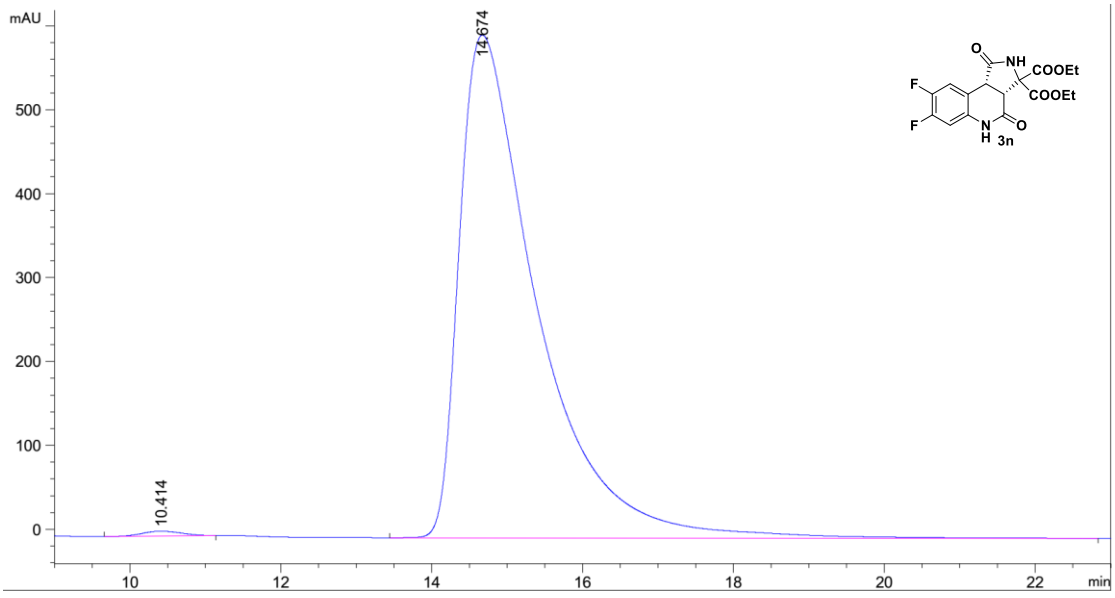
RT [min]	Type	Width [min]	Area	Height	Area%	Name
8.554	BB	0.5745	166.9447	3.8877	0.5992	
13.797	BB	1.0481	27692.9629	371.5115	99.4008	

HPLC chromatogram of racemic **3n**



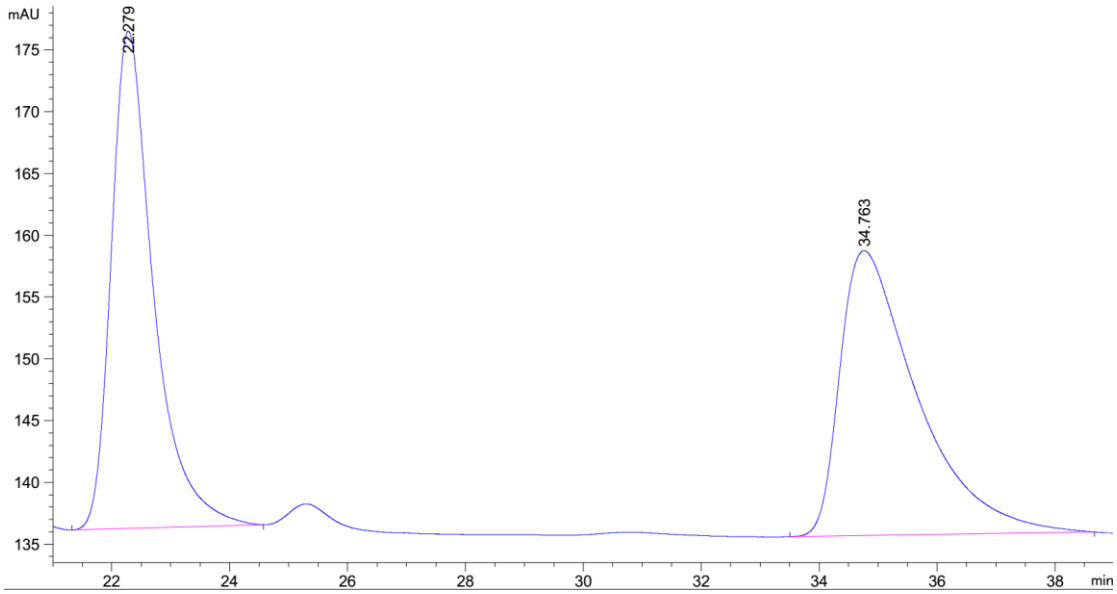
RT [min]	Type	Width [min]	Area	Height	Area%	Name
10.245	BB	0.6469	10317.7441	238.1982	51.2404	
15.326	MM	1.3197	9818.2051	123.9986	48.7596	

HPLC chromatogram of enantiopure **3n**



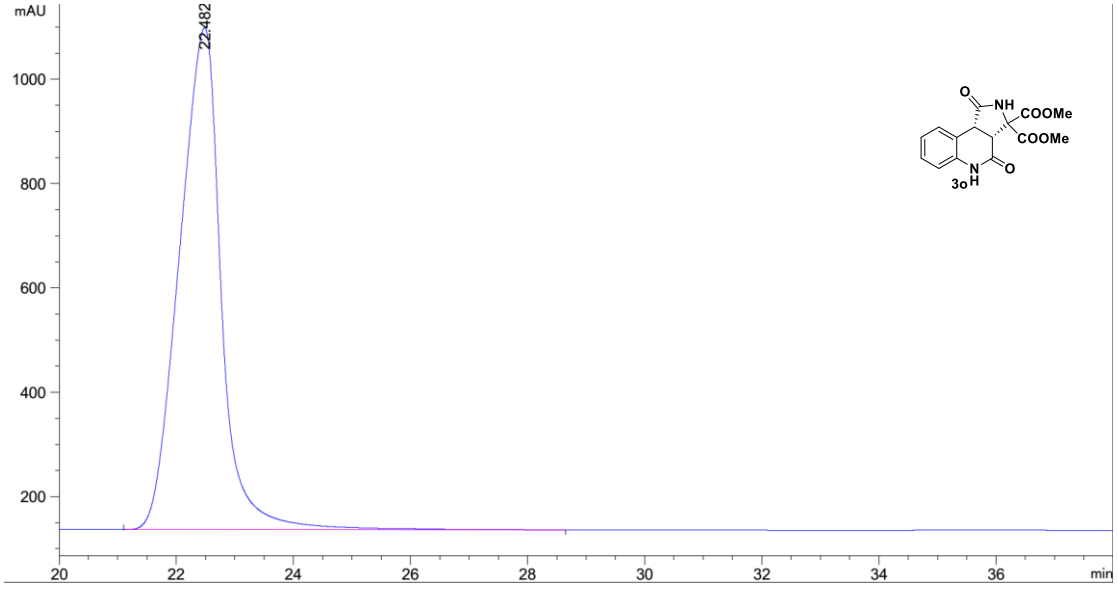
RT [min]	Type	Width [min]	Area	Height	Area%	Name
10.414	BB	0.5251	208.8058	5.8477	0.4839	
14.674	BB	1.0316	42940.8281	599.1741	99.5161	

HPLC chromatogram of racemic **3o**



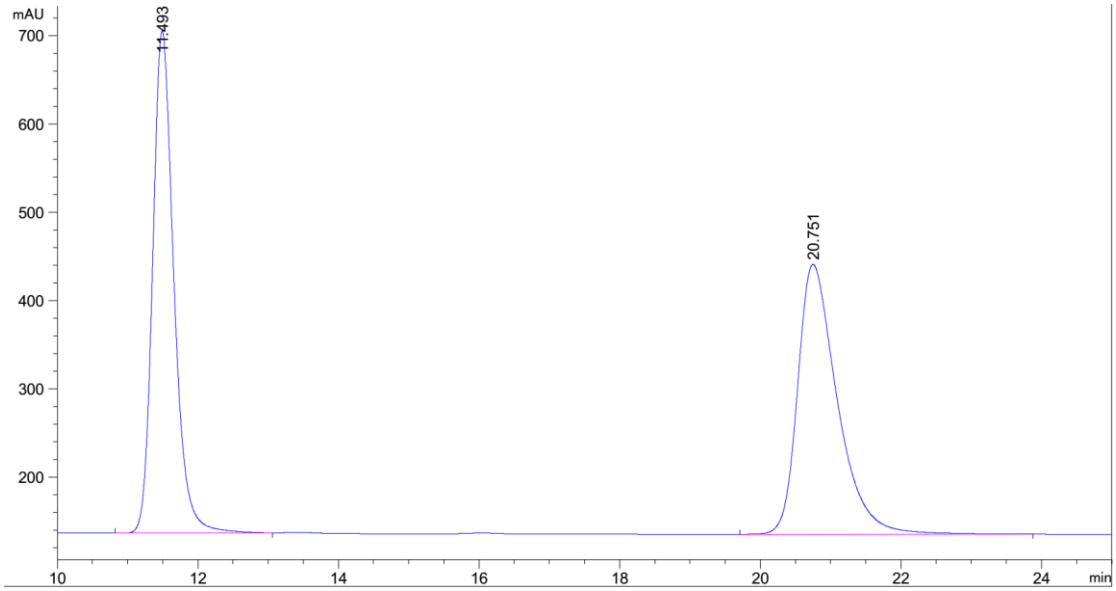
RT [min]	Type	Width [min]	Area	Height	Area%	Name
22.279	BB	0.7394	2005.9098	40.2498	48.8432	
34.763	BB	1.2142	2100.9241	23.0534	51.1568	

HPLC chromatogram of enantiopure **3o**



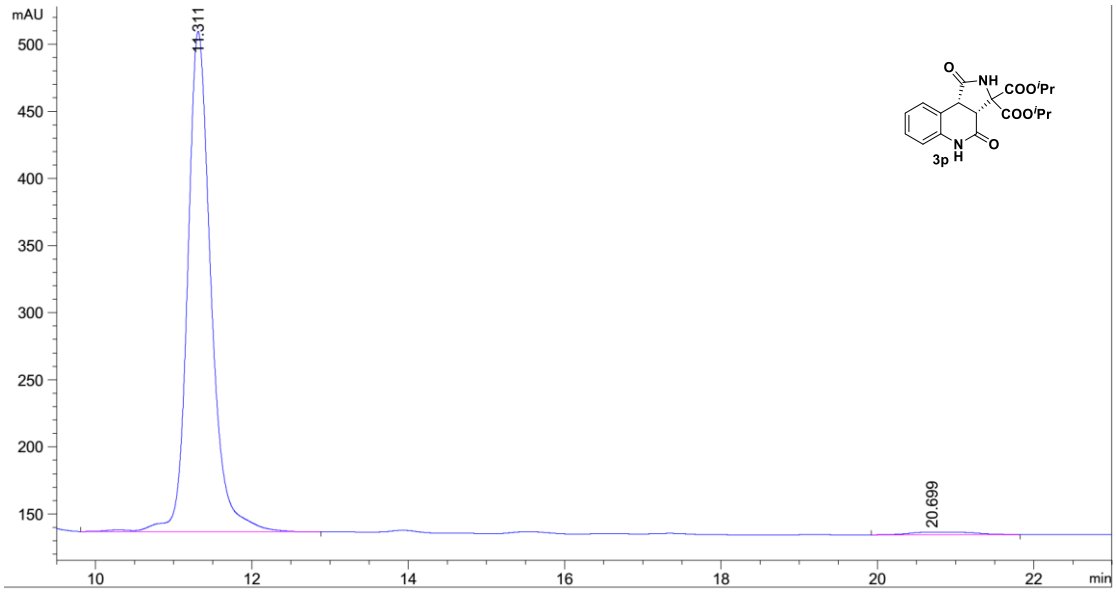
RT [min]	Type	Width [min]	Area	Height	Area%	Name
22.482	BB	0.7486	47807.8633	962.3862	100.0000	

HPLC chromatogram of racemic **3p**



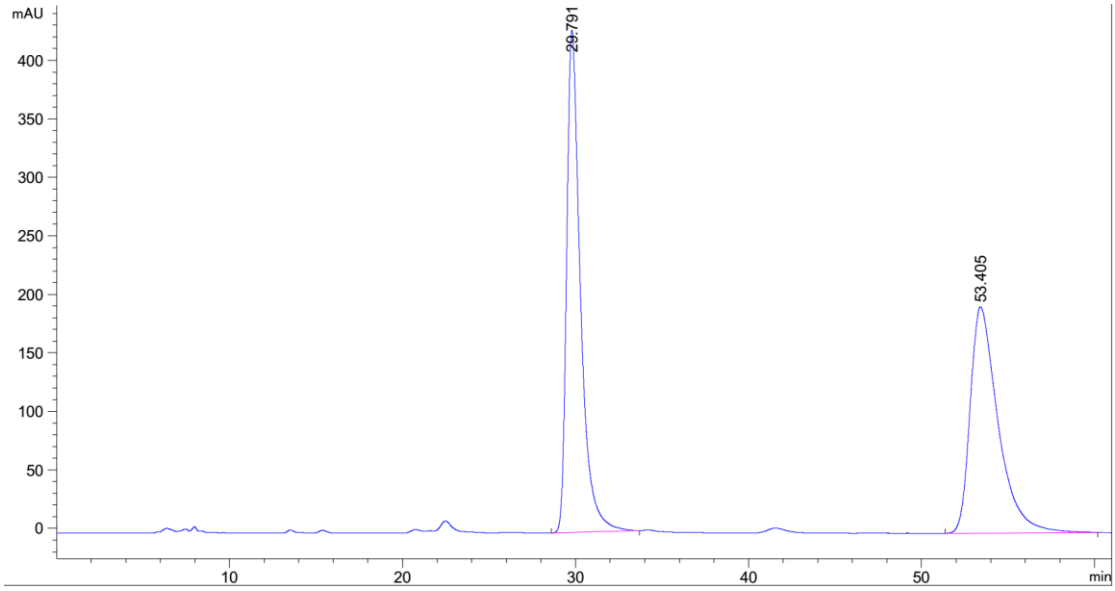
RT [min]	Type	Width [min]	Area	Height	Area%	Name
11.493	BB	0.3186	11900.5693	568.8248	49.9264	
20.751	BB	0.5865	11935.6797	305.7274	50.0736	

HPLC chromatogram of enantiopure **3p**



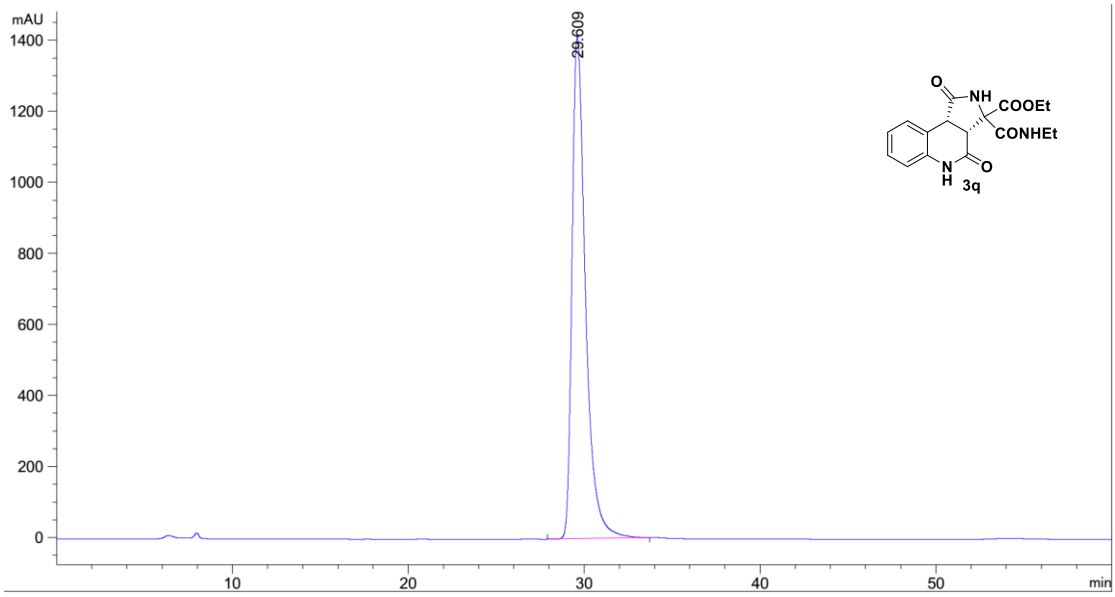
RT [min]	Type	Width [min]	Area	Height	Area%	Name
11.311	VB R	0.3136	7769.1748	372.7758	98.6310	
20.699	BB	0.6676	107.8339	1.8972	1.3690	

HPLC chromatogram of racemic **3q**



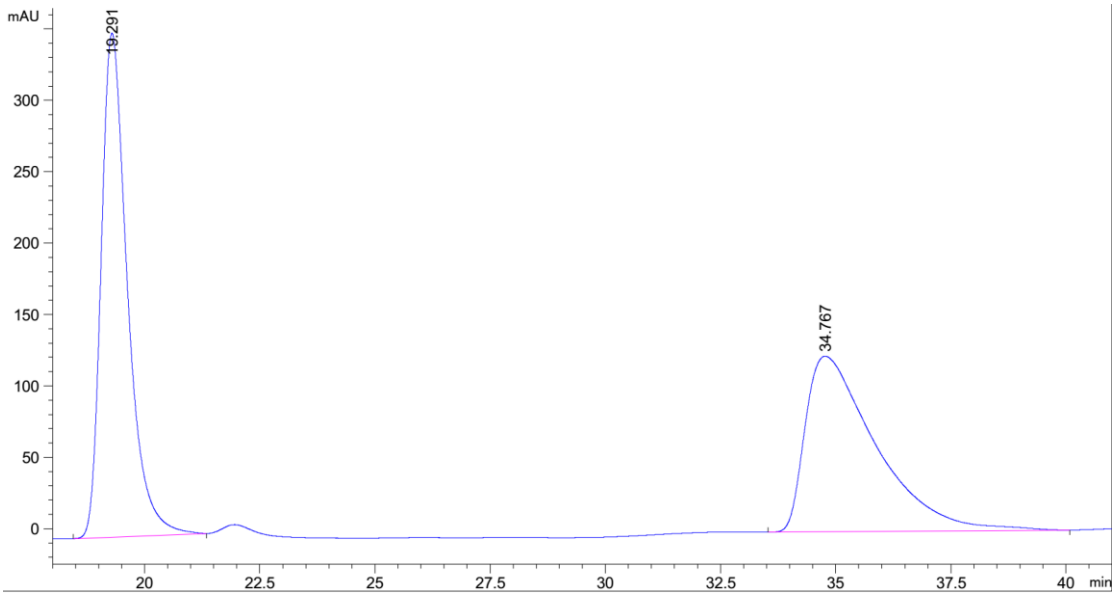
RT [min]	Type	Width [min]	Area	Height	Area%	Name
29.791	BB	0.8235	23757.3320	429.0283	52.3049	
53.405	BB	1.5653	21663.4863	193.4079	47.6951	

HPLC chromatogram of enantiopure **3q**



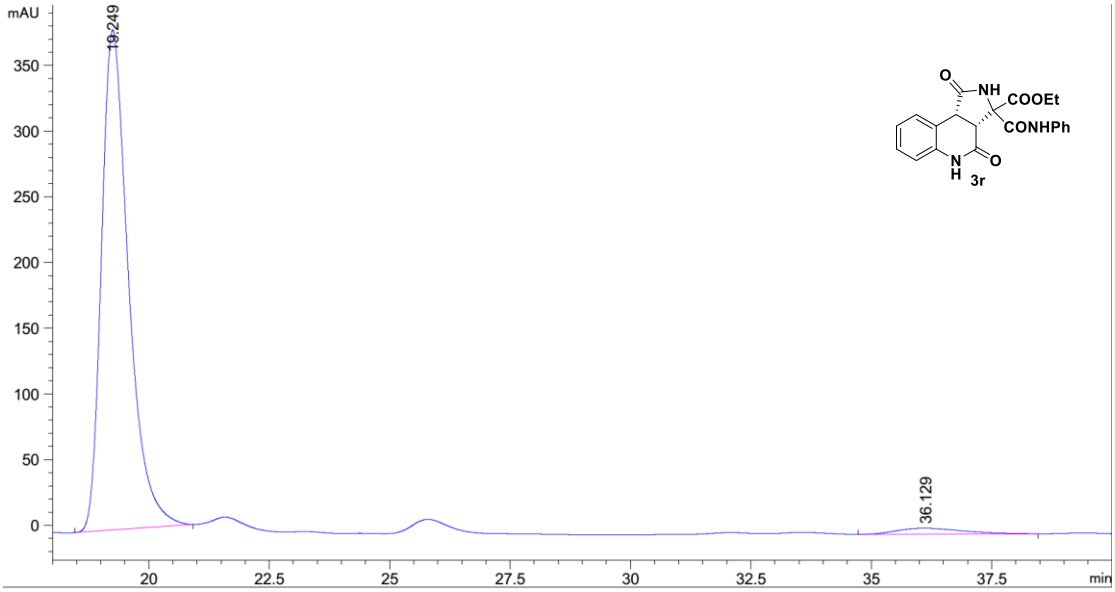
RT [min]	Type	Width [min]	Area	Height	Area%	Name
29.609	BB	0.8146	75392.7031	1413.9264	100.0000	

HPLC chromatogram of racemic **3r**



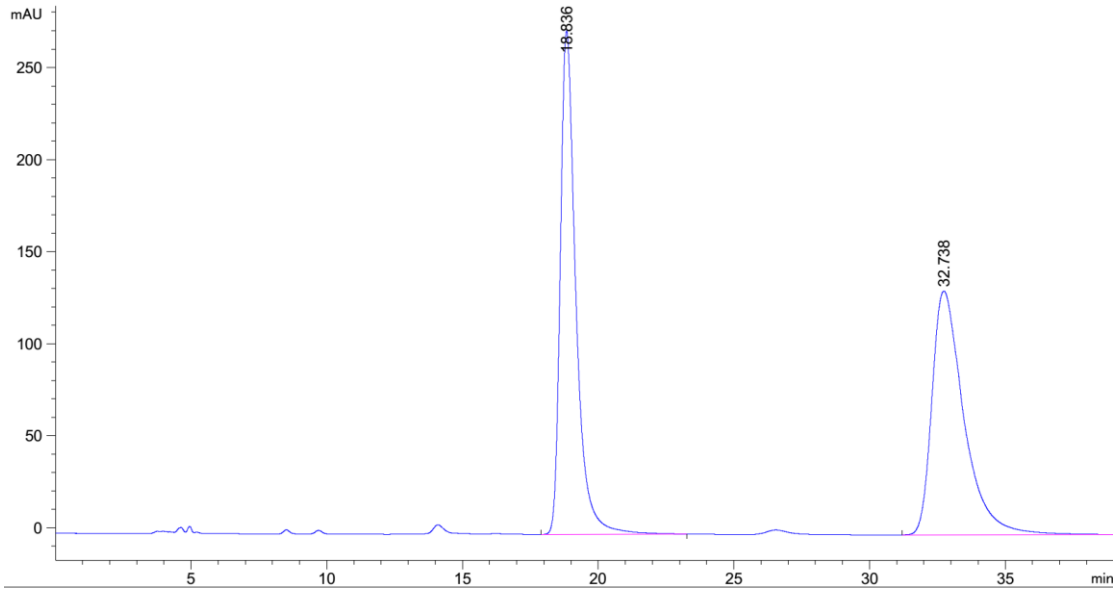
RT [min]	Type	Width [min]	Area	Height	Area%	Name
19.291	BB	0.6020	13979.7900	352.9915	51.6189	
34.767	BB	1.5048	13102.9209	123.0973	48.3811	

HPLC chromatogram of enantiopure **3r**



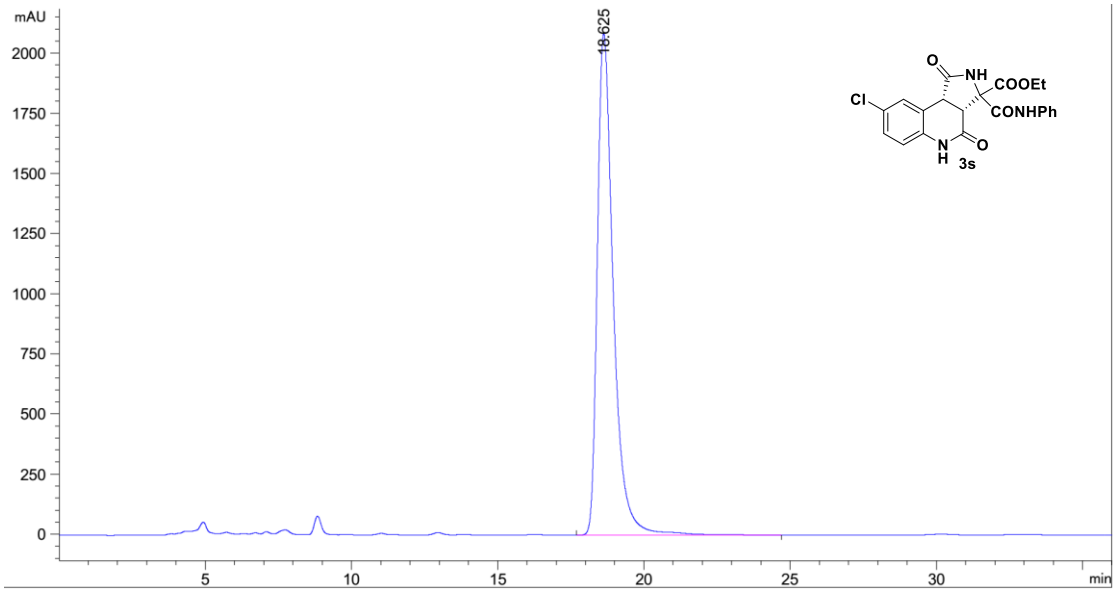
RT [min]	Type	Width [min]	Area	Height	Area%	Name
19.249	BB	0.5938	14823.3320	380.6400	97.1839	
36.129	BB	1.1208	429.5366	4.4893	2.8161	

HPLC chromatogram of racemic **3s**



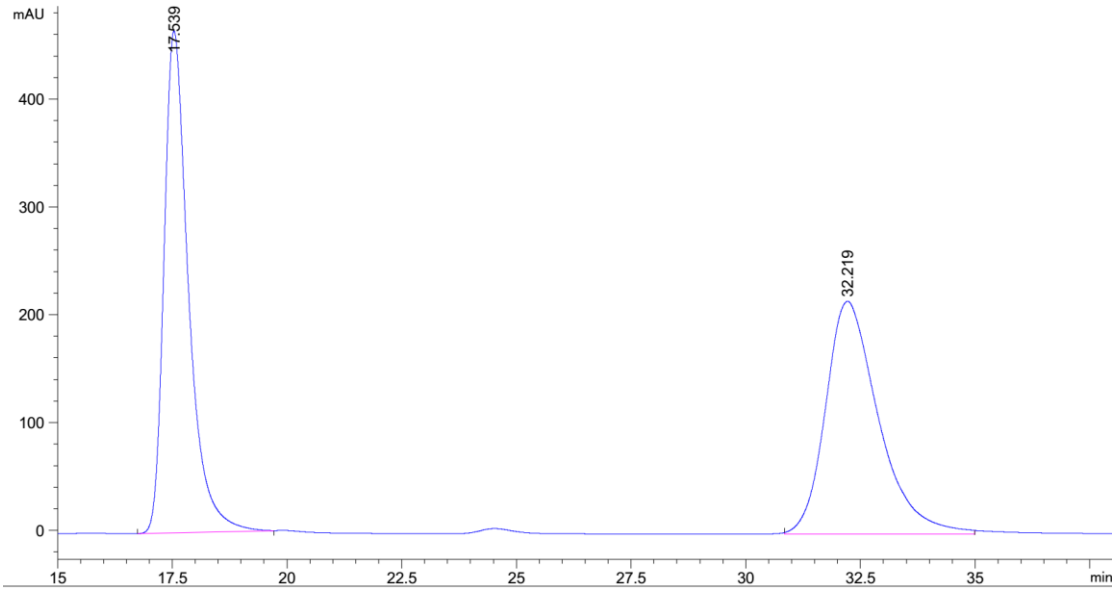
RT [min]	Type	Width [min]	Area	Height	Area%	Name
18.836	BB	0.5998	10921.2676	273.5613	50.2015	
32.738	BBA	1.1701	10833.5977	132.4084	49.7985	

HPLC chromatogram of enantiopure **3s**



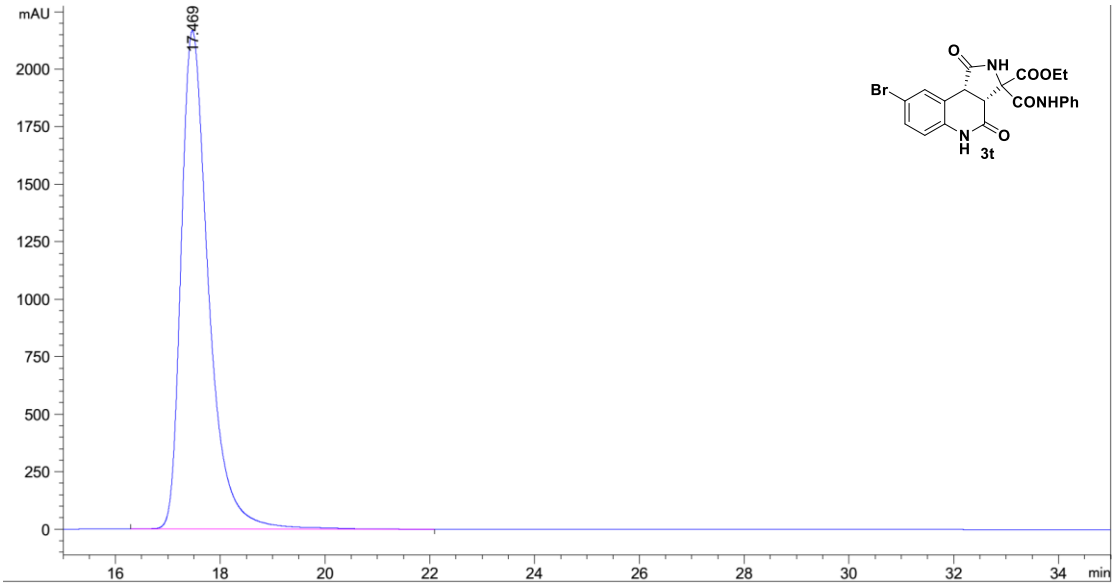
RT [min]	Type	Width [min]	Area	Height	Area%	Name
18.625	BB	0.5804	79411.8125	2084.9924	100.0000	

HPLC chromatogram of racemic **3t**



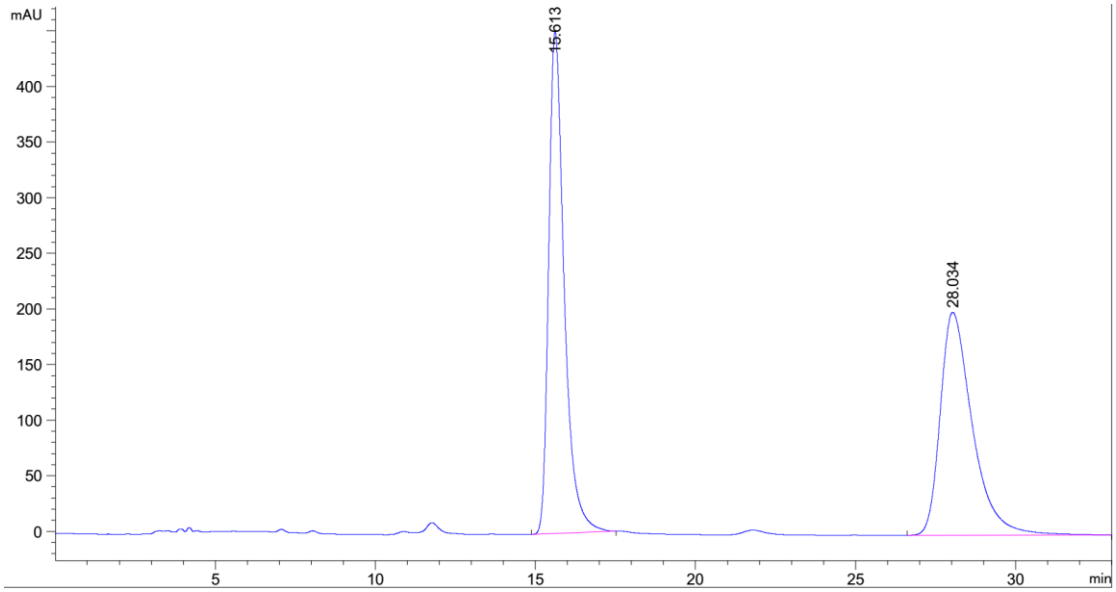
RT [min]	Type	Width [min]	Area	Height	Area%	Name
17.539	BB	0.5603	17248.1504	465.4599	49.8061	
32.219	MM R	1.3400	17382.4473	216.1970	50.1939	

HPLC chromatogram of enantiopure **3t**



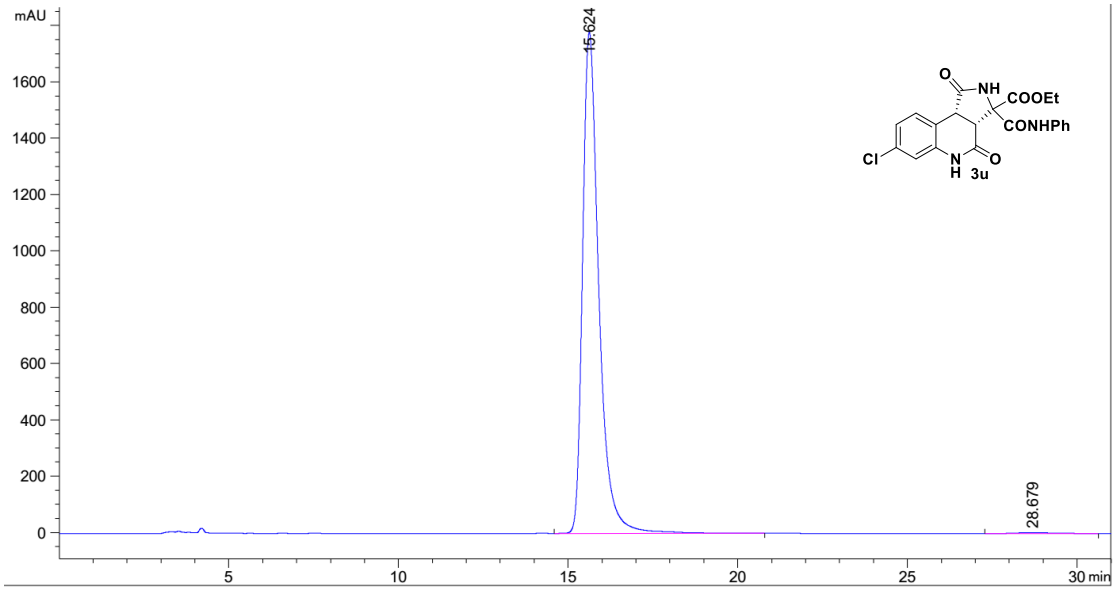
RT [min]	Type	Width [min]	Area	Height	Area%	Name
17.469	BB	0.5533	78909.1953	2167.2500	100.0000	

HPLC chromatogram of racemic **3u**



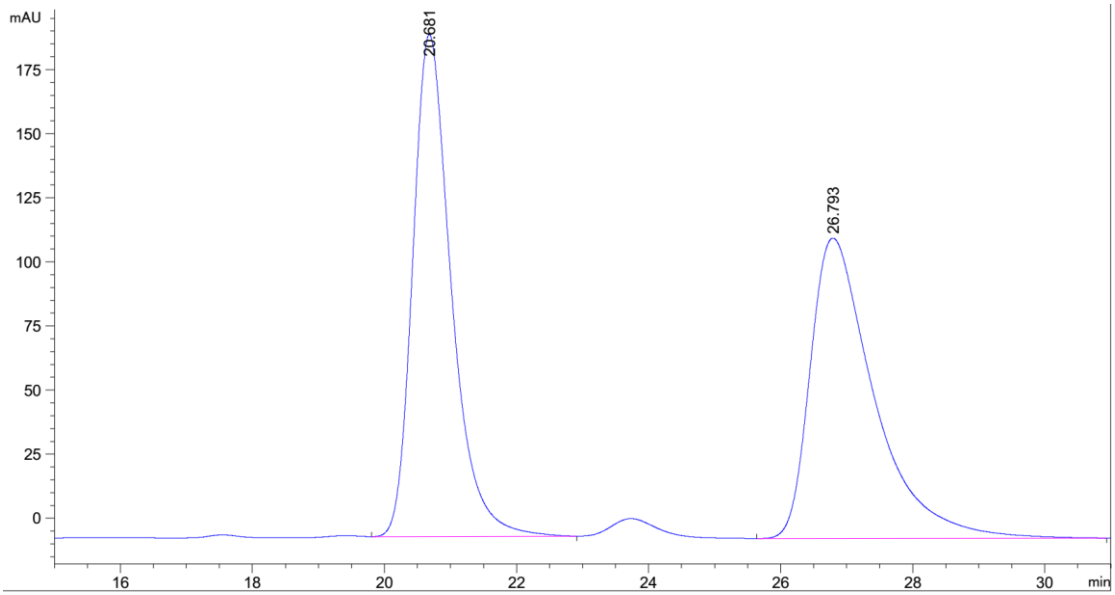
RT [min]	Type	Width [min]	Area	Height	Area%	Name
15.613	BB	0.5092	15227.2061	451.2583	52.1024	
28.034	BBA	1.0383	13998.3447	200.4240	47.8976	

HPLC chromatogram of enantiopure **3u**



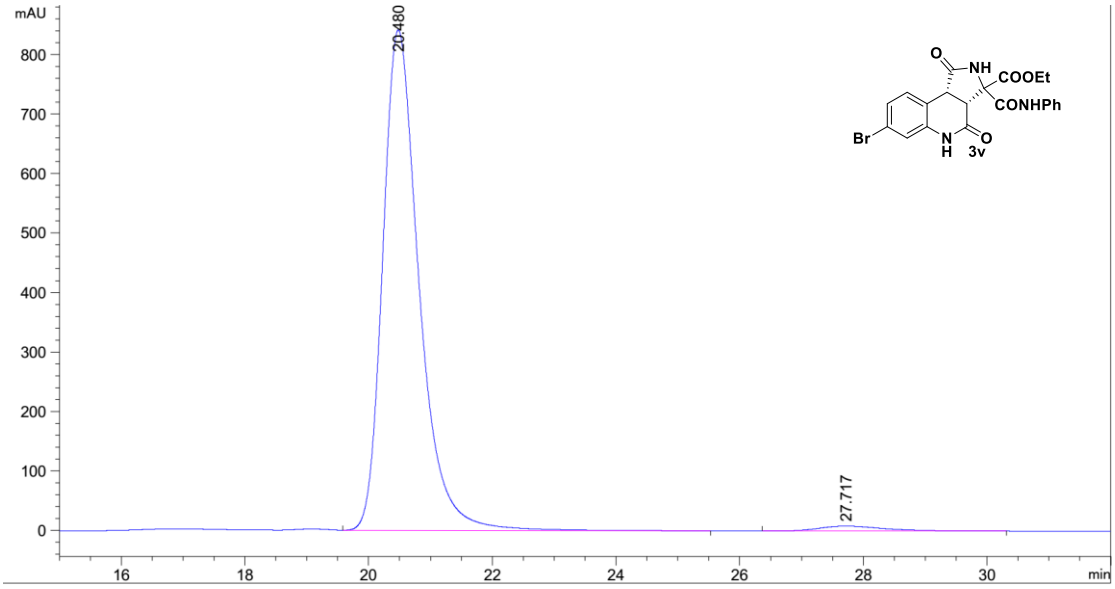
RT [min]	Type	Width [min]	Area	Height	Area%	Name
15.624	BB	0.5045	59429.2578	1780.1254	99.6060	
28.679	BB	0.8634	235.0753	3.1932	0.3940	

HPLC chromatogram of racemic **3v**



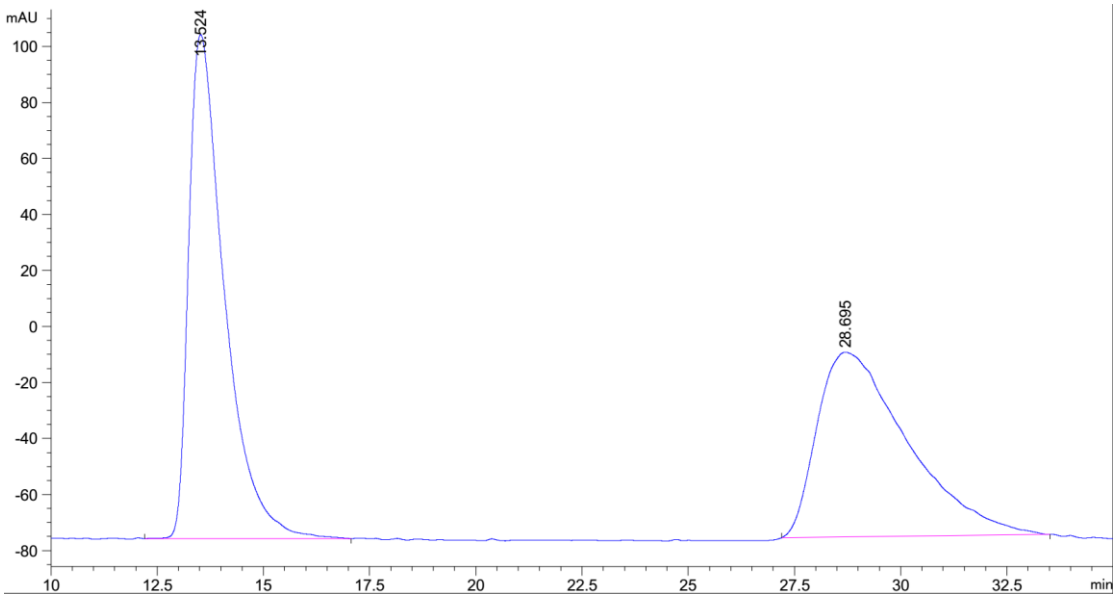
RT [min]	Type	Width [min]	Area	Height	Area%	Name
20.681	BB	0.6147	7934.4492	195.8283	50.2494	
26.793	BB	0.9672	7855.6870	117.0941	49.7506	

HPLC chromatogram of enantiopure **3v**



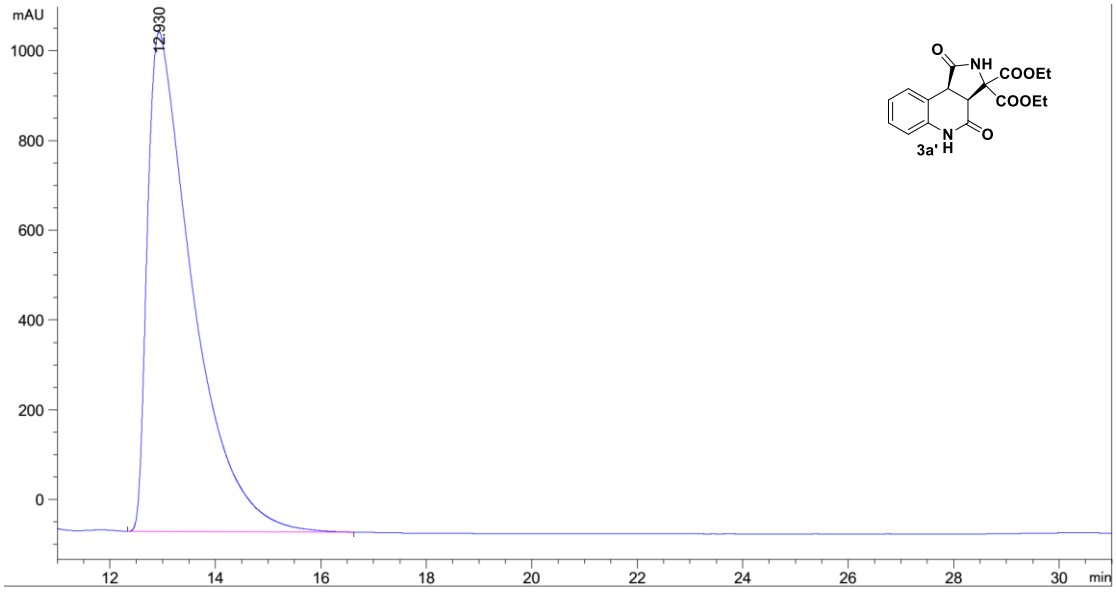
RT [min]	Type	Width [min]	Area	Height	Area%	Name
20.480	BB	0.6189	34270.1797	840.9966	98.2727	
27.717	BB	0.8793	602.3400	8.2942	1.7273	

HPLC chromatogram of racemic **3a'**



RT [min]	Type	Width [min]	Area	Height	Area%	Name
13.524	BB	0.8751	10544.8252	179.9688	52.0232	
28.695	BB	1.8449	9724.6533	65.9651	47.9768	

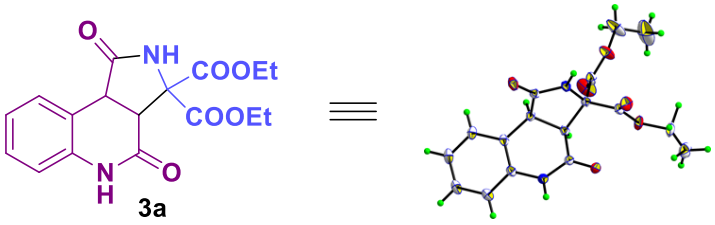
HPLC chromatogram of enantiopure **3a'**



RT [min]	Type	Width [min]	Area	Height	Area%	Name
12.930	BB	0.8672	66338.7578	1114.0272	100.0000	

5. Crystal structure of racemic compound 3a

The relative configurations of compound **3a** (CCDC 1565939) were determined by single crystal X-ray analysis. Ellipsoids are drawn at the 20% probability level.



Datablock: good

```
Bond precision:  C-C = 0.0032 A          Wavelength=0.71073

Cell:          a=8.1209(12)       b=10.5753(16)    c=11.3680(18)
               alpha=113.295(7)   beta=93.648(8)   gamma=107.911(7)
Temperature:   296 K

                 Calculated                Reported
Volume           833.9(2)                  833.9(2)
Space group      P -1                      P-1
Hall group       -P 1                      P-1
Moiety formula   C17 H18 N2 O6             ?
Sum formula      C17 H18 N2 O6             C17 H17 N2 O6
Mr               346.33                    345.32
Dx,g cm-3        1.379                     1.375
Z                2                         2
Mu (mm-1)        0.106                     0.106
F000             364.0                     362.0
F000'            364.21
h,k,lmax         9,12,13                   9,12,13
Nref             2939                      2920
Tmin,Tmax
Tmin'

Correction method= Not given

Data completeness= 0.994          Theta(max)= 25.008

R(reflections)= 0.0508( 2574)     wR2(reflections)= 0.1385( 2920)

S = 1.048                 Npar= 284
```

6. Determination of the absolute configuration of 3r

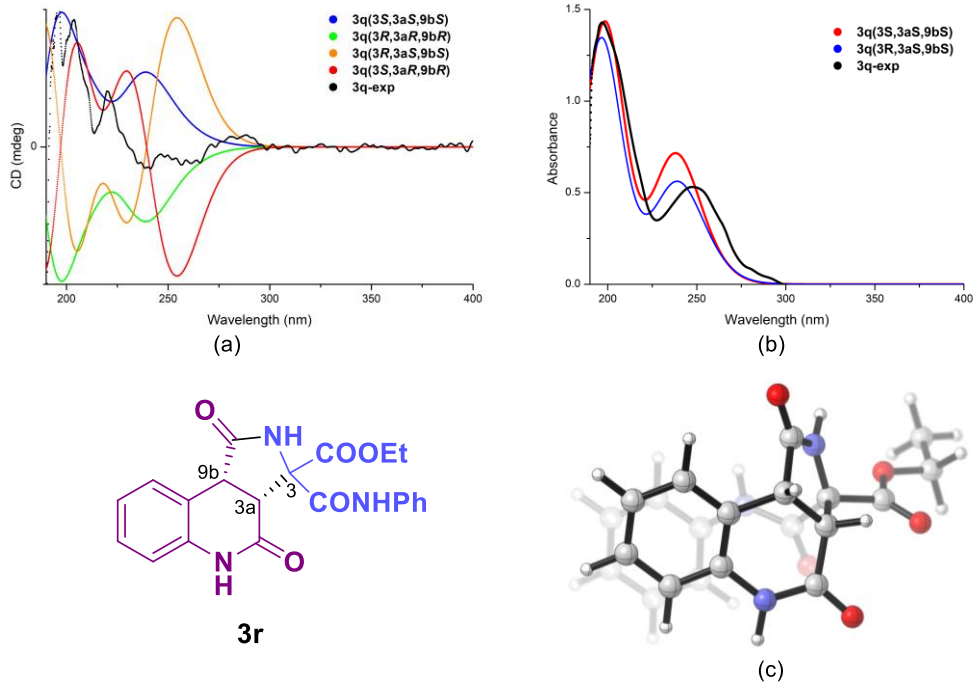


Figure S1. Experimental and calculated ECD spectra (a) and UV spectra (b) of compound **3r**, (c) the assigned configuration of **3r**.

Based on the racemic crystallography data of **3a**, the plausible configurations should be (3a*R*, 9b*R*) or (3a*S*, 9b'*S*). To figure out the dominant enantiomer in this asymmetric reaction, the CD spectrum of **3r** bearing three contiguous chiral centers was determined. As shown in Figure **S1**, the comparison between experimental and predicted CD spectra suggests that the dominant configuration of the product **3r** can be assigned to be (*S*, 3a*R*, 9b*R*) (Figure **S1(c)**).

6.1 Experimental section of circular dichroism spectra

The chiral compound **3r** (0.13 mg) was dissolved in a solution of methanol (1.0 mL, chromatographic grade). the CD spectrum was recorded on JASCO J-815 spectrometer with 0.1 cm cell at room temperature under the following conditions: scanning speed 100 nm/min; time constant 0.5 s; bandwidth 1.00 nm; measure range 190-400 nm; data interval 0.1 nm; noise reduction was carried out with a low-pass filter.

6.2 Computational details of circular dichroism spectra

The ECD spectra of **3r(3*S*,3a*S*,9b*S*)** and **3r(3*R*,3a*S*,9b*S*)** were generated by TDDFT calculations as follows, while **3r(3*R*,3a*R*,9b*R*)** and **3r(3*S*,3a*R*,9b*R*)** were given by mirror inversion of their corresponding enantiomers. Conformational search was carried out to access all the possible stable conformations. The initial conformers were optimized at M06-2X[3]/def2-TZVP[4] theoretical level in methanol with SMD solvent model[5] using Gaussian16 software.[6] Frequency calculations were carried out at the same theoretical level to obtain the thermal corrections. The optimized stable conformers were then used for TDDFT calculation at the CAM-B3LYP[7]/def2-TZVP level in methanol using SMD solvent model. The number of excitation states was chosen to be 25. The overall ECD curves of each configuration were weighted by Boltzmann distribution based on Gibbs free energies. The ECD spectra were generated with the help of SpecDis 1.7 software,[8] with a half-bandwidth of 0.4 eV. The calculated ECD and UV curves were red-shift by 5 nm and scaled to fit better with the experimental curves.

6.3 Table of energies and other thermodynamic parameters

3r(3*S*,3a*S*,9b*S*)	E_{ele}	E_0	E	H	G
conf1	-1352.16571	-1351.78650	-1351.76213	-1351.76119	-1351.84346
conf2	-1352.16423	-1351.78477	-1351.76054	-1351.75960	-1351.84138
conf3	-1352.16632	-1351.78649	-1351.76215	-1351.76121	-1351.84327
conf4	-1352.16371	-1351.78418	-1351.75995	-1351.75901	-1351.84010
conf5	-1352.16546	-1351.78609	-1351.76175	-1351.76081	-1351.84229
conf6	-1352.16774	-1351.78794	-1351.76361	-1351.76267	-1351.84440
conf7	-1352.16673	-1351.78680	-1351.76259	-1351.76165	-1351.84319
conf8	-1352.16762	-1351.78801	-1351.76364	-1351.76269	-1351.84424
conf9	-1352.16588	-1351.78628	-1351.76206	-1351.76111	-1351.84222
conf10	-1352.16735	-1351.78713	-1351.76304	-1351.76209	-1351.84256
conf11	-1352.16661	-1351.78686	-1351.76255	-1351.76161	-1351.84316
conf12	-1352.16640	-1351.78694	-1351.76245	-1351.76150	-1351.84460
conf13	-1352.16453	-1351.78556	-1351.76114	-1351.76020	-1351.84248
conf14	-1352.16644	-1351.78645	-1351.76214	-1351.76119	-1351.84323
conf15	-1352.16778	-1351.78777	-1351.76368	-1351.76274	-1351.84337

3r(3*R*,3a*S*,9b*S*)	E_{ele}	E_0	E	H	G
conf1	-1352.16408	-1351.78472	-1351.76037	-1351.75943	-1351.84121
conf2	-1352.16661	-1351.78679	-1351.76254	-1351.76160	-1351.84201
conf3	-1352.16620	-1351.78652	-1351.76225	-1351.76131	-1351.84179
conf4	-1352.16382	-1351.78436	-1351.75999	-1351.75905	-1351.84095
conf5	-1352.16656	-1351.78635	-1351.76225	-1351.76131	-1351.84117
conf6	-1352.16527	-1351.78543	-1351.76127	-1351.76033	-1351.84099
conf7	-1352.16422	-1351.78480	-1351.76033	-1351.75939	-1351.84145
conf8	-1352.16588	-1351.78580	-1351.76174	-1351.76080	-1351.84045
conf9	-1352.16611	-1351.78636	-1351.76213	-1351.76118	-1351.84178
conf10	-1352.16335	-1351.78380	-1351.75940	-1351.75846	-1351.84081
conf11	-1352.16507	-1351.78551	-1351.76113	-1351.76019	-1351.84239
conf12	-1352.16352	-1351.78395	-1351.75969	-1351.75875	-1351.84031
conf13	-1352.16527	-1351.78562	-1351.76141	-1351.76047	-1351.84147
conf14	-1352.16475	-1351.78522	-1351.76096	-1351.76002	-1351.84107
conf15	-1352.16380	-1351.78412	-1351.75971	-1351.75877	-1351.84154
conf16	-1352.16402	-1351.78448	-1351.76000	-1351.75905	-1351.84203
conf17	-1352.16422	-1351.78464	-1351.76029	-1351.75935	-1351.84170
conf18	-1352.16391	-1351.78419	-1351.75994	-1351.75899	-1351.84079
conf19	-1352.16358	-1351.78381	-1351.75955	-1351.75860	-1351.84030

Notes: E_{ele}, E_0, E, H, and G are the electronic energies, sum of electronic and zero-point energies, sum of electronic and thermal energies, sum of electronic and thermal ethalpies, and sum of electronic and thermal free energies, respectively, which were given at the M06-2X/def2-TZVP theoretical level in methanol with SMD solvent model.

6.4 Coordinates for stable conformations

3r(3S,3aS,9bS) conf1

0 imaginary frequency

C	4.441049	-3.262432	0.130224
C	5.215608	-2.530874	-0.761663
C	4.749636	-1.329651	-1.274241
C	3.502727	-0.859219	-0.882771
C	2.716552	-1.580614	0.009665
C	3.193547	-2.784657	0.508926
N	3.032896	0.368751	-1.374153
C	1.787803	0.865064	-1.238397
C	0.756539	-0.039855	-0.567505
C	1.401876	-1.009009	0.430236
O	1.492764	1.969947	-1.671430
H	4.805151	-4.201132	0.526829
C	-0.186666	0.769946	0.367079
N	0.633814	0.886328	1.545164
C	1.470734	-0.164028	1.706734
O	2.145423	-0.399984	2.689729
C	-0.626211	2.117116	-0.208517
O	-1.374934	2.203322	-1.152884
O	-0.153222	3.135347	0.469496
C	0.186026	5.455096	0.869533
C	-0.486806	4.453495	-0.029274
C	-1.439645	-0.114069	0.701042
O	-1.512837	-0.641408	1.796262
N	-2.327377	-0.262899	-0.294282
C	-3.519886	-1.018638	-0.277294
C	-3.733959	-2.088477	0.588315
C	-4.930379	-2.791330	0.515816
C	-5.907356	-2.447157	-0.407381
C	-5.680881	-1.385775	-1.275859
C	-4.495199	-0.673660	-1.212464
H	6.188211	-2.896855	-1.065266
H	5.344572	-0.753286	-1.972555
H	2.577515	-3.346224	1.201646
H	3.681488	0.948326	-1.896148
H	0.205730	-0.542630	-1.363668
H	0.705013	-1.820551	0.658727
H	0.346699	1.447322	2.337735
H	-0.043145	6.461219	0.517268
H	-0.171851	5.357676	1.894935
H	1.268039	5.321154	0.856157
H	-0.132428	4.518201	-1.058661
H	-1.572056	4.554461	-0.020714
H	-2.195306	0.335270	-1.103099
H	-2.978183	-2.377537	1.301290
H	-5.091768	-3.622419	1.191099
H	-6.835192	-3.002659	-0.453841
H	-6.430859	-1.107300	-2.005491
H	-4.315164	0.156294	-1.885953

3r(3S,3aS,9bS) conf2

0 imaginary frequency

C	4.136963	-3.602116	-0.026164
C	5.201465	-2.746630	-0.282421
C	4.983154	-1.389197	-0.462700
C	3.689850	-0.889198	-0.378649
C	2.614086	-1.734195	-0.121725
C	2.848075	-3.091179	0.050228
N	3.461798	0.487391	-0.531331
C	2.264223	1.090480	-0.668735
C	1.046896	0.181118	-0.758903
C	1.250757	-1.136150	-0.000279
O	2.168314	2.306249	-0.760195
H	4.309068	-4.661575	0.111570
C	-0.172799	0.771095	-0.014303
N	0.097031	0.361949	1.346554
C	0.870341	-0.744605	1.432282
O	1.187341	-1.322478	2.452679
C	-0.372881	2.285805	-0.170591
O	-0.750586	2.778675	-1.201916
O	-0.181266	2.930358	0.960782
C	0.789565	5.093494	0.373142
C	-0.396764	4.364058	0.953810
C	-1.459131	0.121689	-0.613032
O	-1.576914	0.018005	-1.820250
N	-2.372030	-0.266712	0.293734
C	-3.623716	-0.876072	0.055903
C	-4.219828	-1.523331	1.138131
C	-5.455727	-2.129080	0.991728
C	-6.109308	-2.097736	-0.234754
C	-5.515293	-1.446156	-1.305681
C	-4.276859	-0.829759	-1.173266
H	6.209555	-3.136148	-0.346400

H	5.805352	-0.713320	-0.665239
H	2.008413	-3.747532	0.247407
H	4.269832	1.099512	-0.567161
H	0.826854	0.040205	-1.816959
H	0.494108	-1.860868	-0.319752
H	-0.302930	0.816143	2.158437
H	0.923761	4.861153	-0.682676
H	0.621070	6.167002	0.471965
H	1.700841	4.835938	0.913894
H	-1.314380	4.568792	0.403849
H	-0.543586	4.609624	2.002786
H	-2.107628	-0.204444	1.268115
H	-3.705652	-1.546402	2.092220
H	-5.907672	-2.628636	1.839376
H	-7.074136	-2.574208	-0.351876
H	-6.019337	-1.407501	-2.263347
H	-3.834643	-0.316600	-2.011836

3r(3S,3aS,9bS) conf3

0 imaginary frequency

C	-5.397899	-0.910106	-0.909407
C	-5.409685	-1.530247	0.333517
C	-4.216371	-1.820858	0.971852
C	-3.008786	-1.483230	0.369386
C	-2.978901	-0.849564	-0.869826
C	-4.188498	-0.581182	-1.503677
N	-1.815765	-1.800042	1.041790
C	-0.591010	-1.404179	0.685180
C	-0.411583	-0.733830	-0.657580
C	-1.658828	-0.535179	-1.532911
O	0.389140	-1.569858	1.411571
H	-6.326465	-0.689606	-1.419715
C	0.247421	0.679977	-0.495112
N	-0.460949	1.470298	-1.462343
C	-1.553027	0.909771	-2.012000
O	-2.306747	1.464808	-2.790778
C	0.014019	1.284637	0.904509
O	0.879074	1.781752	1.576882
O	-1.259901	1.197869	1.229968
C	-1.881403	3.208087	2.450913
C	-1.667363	1.716551	2.520616
C	1.763623	0.715502	-0.783914
O	2.213263	1.557634	-1.542833
N	2.470073	-0.215231	-0.124438
C	3.863972	-0.417357	-0.114023
C	4.755803	0.261180	-0.942539
C	6.113923	-0.022475	-0.854289
C	6.593491	-0.968083	0.039457
C	5.697096	-1.644171	0.859878
C	4.342454	-1.372635	0.785374
H	-6.347148	-1.794142	0.806163
H	-4.207320	-2.310631	1.938388
H	-4.176592	-0.113843	-2.479223
H	-1.891916	-2.249986	1.948058
H	0.301588	-1.364678	-1.189629
H	-1.576860	-1.149427	-2.432298
H	-0.183396	2.421503	-1.671823
H	-2.239679	3.561642	3.418711
H	-0.953074	3.728752	2.215505
H	-2.629109	3.451288	1.695350
H	-2.591228	1.185014	2.738119
H	-0.910139	1.439956	3.253204
H	1.938355	-0.816425	0.506645
H	4.401703	0.995672	-1.647010
H	6.801401	0.508761	-1.500945
H	7.653625	-1.178746	0.097291
H	6.053174	-2.386809	1.562876
H	3.640246	-1.896738	1.424374

3r(3S,3aS,9bS) conf4

0 imaginary frequency

C	4.640600	-3.112973	0.149462
C	5.597949	-2.151944	-0.151473
C	5.220751	-0.843367	-0.411732
C	3.875972	-0.497450	-0.362995
C	2.906818	-1.449149	-0.061258
C	3.299430	-2.756304	0.190595
N	3.487787	0.829546	-0.605682
C	2.229608	1.277078	-0.788709
C	1.123246	0.230770	-0.796295
C	1.479910	-1.016067	0.022778
O	1.997035	2.460815	-0.990750
H	4.936101	-4.134734	0.348704
C	-0.156522	0.716629	-0.072085
N	0.135835	0.376108	1.302138
C	1.040396	-0.619140	1.435331
O	1.416644	-1.112944	2.479755
C	-0.486511	2.204088	-0.268186

O	-0.967392	2.625019	-1.288245
O	-0.240965	2.912853	0.812799
C	-1.947328	4.643044	0.978620
C	-0.489465	4.338341	0.736062
C	-1.371301	-0.063279	-0.658644
O	-1.461552	-0.229238	-1.861379
N	-2.265697	-0.480734	0.254139
C	-3.474801	-1.174788	0.029363
C	-4.109470	-1.226404	-1.209320
C	-5.309337	-1.917500	-1.327541
C	-5.883564	-2.548316	-0.233639
C	-5.248923	-2.482880	1.001385
C	-4.051327	-1.801603	1.134078
H	6.646037	-2.420638	-0.188718
H	5.958614	-0.087016	-0.651116
H	2.541664	-3.496019	0.421368
H	4.219528	1.525945	-0.697761
H	0.908741	0.010022	-1.841912
H	0.821762	-1.841966	-0.267324
H	-0.310192	0.819039	2.096082
H	-2.260577	4.262140	1.951328
H	-2.090560	5.724511	0.969947
H	-2.577380	4.205635	0.204434
H	0.143660	4.758201	1.514064
H	-0.148676	4.691941	-0.236238
H	-2.021082	-0.355783	1.227771
H	-3.683341	-0.730962	-2.066602
H	-5.799022	-1.954339	-2.292711
H	-6.818730	-3.082969	-0.339580
H	-5.686075	-2.964843	1.866809
H	-3.552887	-1.747354	2.095069

3r(3S,3aS,9bS) conf5

0 imaginary frequency

C	5.029897	-2.673602	-0.538233
C	5.882621	-1.578270	-0.599690
C	5.377308	-0.290049	-0.512158
C	4.009675	-0.102248	-0.355429
C	3.143972	-1.189966	-0.290302
C	3.664431	-2.472995	-0.386196
N	3.493256	1.198140	-0.244144
C	2.193192	1.550664	-0.286264
C	1.188900	0.437541	-0.550693
C	1.687971	-0.933504	-0.075973
O	1.844220	2.717034	-0.165395
H	5.425289	-3.678338	-0.610330
C	-0.094930	0.603687	0.290555
N	0.278011	-0.033904	1.533009
C	1.271455	-0.939708	1.398989
O	1.734593	-1.635128	2.281307
C	-0.560575	2.040832	0.544816
O	-0.559464	2.540875	1.639644
O	-1.028971	2.588321	-0.555952
C	-2.948978	3.950144	0.055545
C	-1.531307	3.943118	-0.462020
C	-1.275130	-0.115786	-0.433221
O	-1.301265	-0.204564	-1.646631
N	-2.230893	-0.567945	0.398369
C	-3.429038	-1.230365	0.047044
C	-4.053439	-1.051787	-1.184208
C	-5.243167	-1.720079	-1.443767
C	-5.816711	-2.551886	-0.492333
C	-5.193668	-2.712967	0.739482
C	-4.004001	-2.057533	1.009927
H	6.948506	-1.724547	-0.720637
H	6.032864	0.571166	-0.561963
H	2.987704	-3.318363	-0.339201
H	4.153872	1.962980	-0.157990
H	0.958531	0.463068	-1.615528
H	1.095325	-1.720433	-0.554037
H	-0.166002	0.171067	2.419887
H	-3.325082	4.974153	0.053807
H	-3.590885	3.345212	-0.586233
H	-3.000207	3.565639	1.074187
H	-0.855085	4.516740	0.170865
H	-1.473606	4.317669	-1.481084
H	-2.037319	-0.528568	1.390813
H	-3.625904	-0.394224	-1.925112
H	-5.726770	-1.578926	-2.402342
H	-6.744340	-3.067220	-0.706015
H	-5.632266	-3.353894	1.493913
H	-3.511005	-2.180965	1.967350

3r(3S,3aS,9bS) conf6

0 imaginary frequency

C	-5.343179	0.667921	-1.026367
C	-5.377623	-0.708702	-1.210183
C	-4.195544	-1.422911	-1.300250

C	-2.976692	-0.760345	-1.197936
C	-2.923745	0.617269	-1.005995
C	-4.122739	1.320575	-0.933720
N	-1.796282	-1.518615	-1.285706
C	-0.564381	-1.074099	-1.020689
C	-0.357819	0.413555	-0.851761
C	-1.590169	1.325646	-0.962530
O	0.399223	-1.833743	-0.919900
H	-6.263040	1.234729	-0.964648
C	0.315007	0.740422	0.524616
N	-0.361381	1.942526	0.926797
C	-1.449919	2.285609	0.214844
O	-2.175834	3.231692	0.461485
C	0.057598	-0.340849	1.592552
O	0.901340	-0.765385	2.338478
O	-1.211177	-0.690385	1.596774
C	-3.054560	-2.042560	2.245809
C	-1.624588	-1.692416	2.557734
C	1.837496	0.984582	0.452027
O	2.315558	1.976235	0.976597
N	2.517813	0.024156	-0.192765
C	3.911444	-0.086606	-0.370233
C	4.388421	-1.331016	-0.785054
C	5.742172	-1.522105	-1.000105
C	6.637119	-0.476352	-0.803604
C	6.157836	0.760490	-0.397969
C	4.800844	0.969092	-0.181278
H	-6.324074	-1.228172	-1.288966
H	-4.203978	-2.496469	-1.447501
H	-4.093871	2.394863	-0.810424
H	-1.891914	-2.522156	-1.402246
H	0.355490	0.684648	-1.631029
H	-1.507710	1.944779	-1.858628
H	-0.057852	2.474195	1.733530
H	-3.133668	-2.505839	1.261610
H	-3.420286	-2.749788	2.990989
H	-3.686368	-1.153310	2.271455
H	-0.959150	-2.550104	2.458229
H	-1.508075	-1.264924	3.553825
H	1.968675	-0.772289	-0.519481
H	3.686704	-2.143776	-0.934852
H	6.098414	-2.493099	-1.320715
H	7.696437	-0.625211	-0.969012
H	6.844341	1.584784	-0.249080
H	4.444120	1.940137	0.121725

3r(3S,3aS,9bS) conf7

0 imaginary frequency

C	-5.703432	0.526261	-0.605803
C	-5.664527	-0.802157	-1.010492
C	-4.448487	-1.409880	-1.271012
C	-3.268924	-0.688914	-1.117540
C	-3.288222	0.637341	-0.696208
C	-4.521258	1.236577	-0.457446
N	-2.052486	-1.331037	-1.406285
C	-0.833230	-0.835674	-1.184415
C	-0.708927	0.600435	-0.729341
C	-2.001440	1.417482	-0.573923
O	0.185851	-1.511807	-1.331905
H	-6.651318	1.011566	-0.412724
C	0.036104	0.682970	0.649768
N	-0.683154	1.721310	1.330854
C	-1.844944	2.109949	0.776888
O	-2.618681	2.913266	1.265850
C	-0.157271	-0.631634	1.438257
O	-1.260619	-1.084398	1.613790
O	0.964185	-1.149882	1.880640
C	0.766239	-3.552178	1.578495
C	0.885133	-2.423204	2.572671
C	1.531667	1.050129	0.553310
O	1.990980	1.900786	1.297352
N	2.217179	0.351552	-0.365233
C	3.603948	0.372022	-0.613687
C	4.120581	-0.699943	-1.343332
C	5.470677	-0.752248	-1.643471
C	6.322061	0.262061	-1.219868
C	5.802859	1.329159	-0.501587
C	4.448810	1.397901	-0.195341
H	-6.581051	-1.365492	-1.130788
H	-4.399378	-2.442628	-1.595453
H	-4.549506	2.275742	-0.157976
H	-2.092433	-2.298522	-1.709866
H	-0.070557	1.078917	-1.472277
H	-2.019083	2.220282	-1.314591
H	-0.365234	2.086139	2.220497
H	-0.164656	-3.486758	1.014436
H	1.606514	-3.538225	0.883126
H	0.777597	-4.500987	2.116729

H	1.813855	-2.474319	3.135019
H	0.044267	-2.387518	3.263458
H	1.698024	-0.384173	-0.846246
H	3.452695	-1.489511	-1.669508
H	5.858439	-1.590462	-2.208769
H	7.378661	0.220904	-1.451261
H	6.454795	2.129203	-0.173185
H	4.059373	2.240609	0.352669

3r(3S,3aS,9bS) conf8

0 imaginary frequency

C	5.298012	-0.094302	0.164947
C	5.132973	1.273039	-0.016026
C	3.949311	1.765003	-0.539741
C	2.930028	0.883932	-0.882990
C	3.078822	-0.490807	-0.706664
C	4.274929	-0.965476	-0.180476
N	1.739302	1.405400	-1.423102
C	0.583948	0.738912	-1.548241
C	0.582909	-0.708554	-1.108344
C	1.946042	-1.410481	-1.117776
O	-0.435725	1.267133	-1.983916
H	6.221385	-0.483636	0.573396
C	0.062068	-0.949590	0.346647
N	0.676576	-2.209531	0.658119
C	1.747846	-2.523236	-0.094587
O	2.436542	-3.520052	0.027975
C	0.553876	0.143005	1.321071
O	1.409078	-0.034736	2.146595
O	-0.072445	1.279695	1.101074
C	-0.402163	3.619152	1.327744
C	0.374582	2.439448	1.845824
C	-1.466428	-1.072853	0.522329
O	-1.878437	-1.769776	1.436595
N	-2.222077	-0.369369	-0.330847
C	-3.628250	-0.230762	-0.297148
C	-4.158085	0.935255	-0.847359
C	-5.529102	1.129689	-0.870867
C	-6.381263	0.165882	-0.344671
C	-5.847919	-0.997057	0.193032
C	-4.475004	-1.208042	0.218091
H	5.925522	1.959987	0.251649
H	3.802523	2.828720	-0.685465
H	4.405728	-2.031238	-0.043554
H	1.722242	2.389690	-1.669809
H	-0.096817	-1.234982	-1.778136
H	2.159062	-1.854491	-2.091020
H	0.397264	-2.747855	1.468693
H	-0.090874	4.517124	1.862096
H	-0.215271	3.765264	0.262775
H	-1.471965	3.475844	1.483581
H	0.192046	2.251294	2.903783
H	1.448197	2.546259	1.683186
H	-1.743498	0.243278	-0.991438
H	-3.485887	1.683385	-1.252425
H	-5.931474	2.039221	-1.298852
H	-7.452748	0.319043	-0.358844
H	-6.504231	-1.759036	0.594712
H	-4.072712	-2.124421	0.621119

3r(3S,3aS,9bS) conf9

0 imaginary frequency

C	4.502098	-3.209371	-0.621427
C	5.484419	-2.228880	-0.687583
C	5.147591	-0.888992	-0.569086
C	3.818373	-0.533690	-0.376439
C	2.823907	-1.504997	-0.309375
C	3.176210	-2.841360	-0.435918
N	3.471402	0.818386	-0.227372
C	2.224683	1.330142	-0.229714
C	1.088001	0.359819	-0.515083
C	1.415960	-1.070228	-0.065608
O	2.023103	2.524039	-0.056049
H	4.766344	-4.254472	-0.716337
C	-0.163033	0.663791	0.337984
N	0.147792	-0.022876	1.570638
C	1.020534	-1.043213	1.415286
O	1.403331	-1.801129	2.284274
C	-0.471426	2.140053	0.620159
O	-0.443822	2.600226	1.732603
O	-0.863025	2.771253	-0.464758
C	-0.050224	5.069030	-0.284609
C	-1.253949	4.159864	-0.326031
C	-1.410604	0.077154	-0.394416
O	-1.506072	0.160296	-1.605316
N	-2.327065	-0.474373	0.419506
C	-3.557277	-1.062884	0.047070
C	-4.246115	-0.700234	-1.106964

C	-5.463317	-1.307209	-1.388838
C	-6.000766	-2.259381	-0.534206
C	-5.312548	-2.605808	0.622494
C	-4.095102	-2.013017	0.913280
H	6.520523	-2.505715	-0.835678
H	5.905095	-0.116016	-0.622035
H	2.399221	-3.595390	-0.385728
H	4.223975	1.491260	-0.128578
H	0.861473	0.434349	-1.578580
H	0.721369	-1.769342	-0.543580
H	-0.262758	0.225573	2.462643
H	0.559902	4.883260	0.598850
H	0.563616	4.935187	-1.175811
H	-0.395671	6.103588	-0.255184
H	-1.869899	4.254085	0.567334
H	-1.866059	4.346641	-1.205086
H	-2.076618	-0.581527	1.393763
H	-3.846888	0.050922	-1.770464
H	-5.996857	-1.022444	-2.287137
H	-6.950415	-2.725283	-0.764041
H	-5.722059	-3.342690	1.301905
H	-3.551793	-2.280968	1.812469

3r(3S,3aS,9bS) conf10

0 imaginary frequency

C	-5.433107	0.665857	-0.867620
C	-5.452756	-0.708083	-1.070014
C	-4.263381	-1.402547	-1.210604
C	-3.052990	-0.721127	-1.141574
C	-3.014073	0.653472	-0.924573
C	-4.220219	1.336366	-0.802004
N	-1.864380	-1.455932	-1.292918
C	-0.633208	-1.004565	-1.037750
C	-0.443331	0.479580	-0.826371
C	-1.688160	1.378353	-0.901982
O	0.340878	-1.755325	-0.979620
H	-6.359073	1.217057	-0.767479
C	0.237435	0.777193	0.553713
N	-0.446166	1.962626	0.989453
C	-1.537197	2.319872	0.288803
O	-2.260445	3.262808	0.555166
C	0.002691	-0.340351	1.590006
O	0.869859	-0.807023	2.281506
O	-1.272934	-0.667968	1.630717
C	-1.375269	-3.079666	1.934964
C	-1.668628	-1.727754	2.537931
C	1.757167	1.040167	0.472307
O	2.226301	2.032080	1.004874
N	2.443246	0.099125	-0.193711
C	3.832217	0.007205	-0.408139
C	4.757852	0.941494	0.052895
C	6.107992	0.749656	-0.218064
C	6.547155	-0.351565	-0.937284
C	5.617627	-1.279416	-1.394252
C	4.270520	-1.103145	-1.133141
H	-6.393289	-1.241228	-1.124317
H	-4.259706	-2.473665	-1.374769
H	-4.204115	2.408521	-0.659359
H	-1.948627	-2.456821	-1.438032
H	0.259660	0.782780	-1.603341
H	-1.631628	2.010667	-1.790694
H	-0.136035	2.482281	1.801405
H	-0.307899	-3.208535	1.753393
H	-1.702783	-3.855295	2.628841
H	-1.915821	-3.208690	0.996406
H	-1.152231	-1.576848	3.484697
H	-2.735144	-1.569516	2.679122
H	1.894535	-0.679337	-0.561611
H	4.436574	1.803808	0.613338
H	6.821721	1.479436	0.143886
H	7.601504	-0.487807	-1.140809
H	5.941542	-2.145919	-1.957114
H	3.542627	-1.824171	-1.487971

3r(3S,3aS,9bS) conf11

0 imaginary frequency

C	5.348975	-0.102981	0.006732
C	5.199241	1.214026	-0.408618
C	4.005519	1.631321	-0.972645
C	2.960428	0.726646	-1.119826
C	3.092754	-0.597454	-0.705877
C	4.299889	-0.998281	-0.144645
N	1.761754	1.171828	-1.708402
C	0.598933	0.506944	-1.713650
C	0.581476	-0.839499	-1.026001
C	1.933878	-1.552952	-0.908990
O	-0.418052	0.963620	-2.229097
H	6.280349	-0.434587	0.446776

C	0.052632	-0.802508	0.446428
N	0.665737	-1.980088	0.993432
C	1.733238	-2.440003	0.314790
O	2.417704	-3.397008	0.629359
C	0.540348	0.454055	1.201927
O	1.444216	0.438196	1.993949
O	-0.143844	1.517961	0.833820
C	-0.359159	2.979360	2.768223
C	0.244316	2.796807	1.397875
C	-1.477164	-0.895319	0.632654
O	-1.892298	-1.400595	1.664161
N	-2.228448	-0.381574	-0.349988
C	-3.634376	-0.253025	-0.376804
C	-4.156900	0.682579	-1.270313
C	-5.526375	0.856788	-1.372177
C	-6.388568	0.101847	-0.585109
C	-5.863907	-0.833254	0.295107
C	-4.491575	-1.022226	0.406196
H	6.011678	1.920099	-0.293744
H	3.871696	2.654935	-1.301928
H	4.417688	-2.025880	0.174304
H	1.754872	2.098240	-2.122702
H	-0.105973	-1.468228	-1.591441
H	2.123256	-2.186312	-1.776604
H	0.387432	-2.350594	1.893581
H	-0.098099	3.970377	3.141992
H	-1.445881	2.903349	2.719507
H	0.019614	2.235235	3.468693
H	1.332734	2.845441	1.413626
H	-0.139638	3.524162	0.686552
H	-1.741477	0.088899	-1.113023
H	-3.479353	1.269808	-1.880304
H	-5.920205	1.587008	-2.067940
H	-7.459469	0.239531	-0.661873
H	-6.526454	-1.433904	0.905903
H	-4.099509	-1.763360	1.084133

3r(3S,3aS,9bS) conf12

0 imaginary frequency

C	5.805396	-0.546815	-0.344220
C	5.761639	0.562479	-1.179419
C	4.545901	1.020016	-1.657545
C	3.370972	0.371576	-1.291508
C	3.394897	-0.732341	-0.444202
C	4.628220	-1.188691	0.011269
N	2.154685	0.855703	-1.803430
C	0.936350	0.443756	-1.446778
C	0.817393	-0.764519	-0.546993
C	2.114901	-1.450917	-0.091492
O	-0.086981	1.016508	-1.823637
H	6.753416	-0.916999	0.023839
C	0.022456	-0.407294	0.757184
N	0.737953	-1.132251	1.768845
C	1.927403	-1.646665	1.410048
O	2.701443	-2.210005	2.162715
C	0.151360	1.100064	1.069784
O	1.231150	1.635525	1.099100
O	-0.995659	1.688383	1.309892
C	-2.378919	3.561013	1.795698
C	-0.957549	3.108942	1.599725
C	-1.459408	-0.836894	0.744662
O	-1.927486	-1.415417	1.710971
N	-2.127917	-0.495906	-0.368862
C	-3.509445	-0.639799	-0.613238
C	-4.078134	0.222334	-1.551041
C	-5.425080	0.125250	-1.857245
C	-6.218640	-0.829160	-1.231437
C	-5.646315	-1.689498	-0.305265
C	-4.295197	-1.607410	0.008244
H	6.674102	1.070160	-1.465047
H	4.493465	1.879232	-2.315979
H	4.660719	-2.062765	0.647949
H	2.191650	1.668615	-2.409786
H	0.214692	-1.476460	-1.111475
H	2.163631	-2.457622	-0.512659
H	0.399868	-1.179365	2.722198
H	-2.386936	4.629673	2.011868
H	-2.968054	3.384665	0.895072
H	-2.840986	3.034762	2.631367
H	-0.348976	3.252644	2.492408
H	-0.476867	3.606102	0.756918
H	-1.615661	0.073790	-1.043305
H	-3.455793	0.967909	-2.033561
H	-5.855704	0.800847	-2.585681
H	-7.272383	-0.903305	-1.467744
H	-6.252846	-2.443709	0.180687
H	-3.859314	-2.293515	0.717352

3r(3S,3aS,9bS) conf13

0 imaginary frequency

C	4.160106	-3.564450	0.218224
C	5.209385	-2.736316	-0.161068
C	4.972766	-1.410713	-0.491505
C	3.676708	-0.913666	-0.433618
C	2.616652	-1.730901	-0.053775
C	2.868483	-3.057395	0.267324
N	3.431623	0.432362	-0.746853
C	2.226615	1.006720	-0.932935
C	1.011465	0.092670	-0.852471
C	1.250197	-1.134554	0.035629
O	2.121462	2.194776	-1.204366
H	4.346001	-4.599879	0.471914
C	-0.188512	0.761314	-0.133636
N	0.103075	0.474214	1.252531
C	0.898330	-0.604641	1.429411
O	1.247525	-1.072358	2.494863
C	-0.351807	2.263224	-0.412698
O	-0.819502	2.684740	-1.438769
O	0.015648	3.001719	0.611742
C	0.461149	5.076220	1.686546
C	-0.047053	4.435529	0.423483
C	-1.491262	0.082787	-0.650421
O	-1.649993	-0.086199	-1.845701
N	-2.373512	-0.261186	0.304105
C	-3.628770	-0.882935	0.110482
C	-4.383192	-0.703455	-1.045390
C	-5.618362	-1.329337	-1.153179
C	-6.109423	-2.119601	-0.123147
C	-5.356628	-2.280414	1.033866
C	-4.120273	-1.667030	1.151983
H	6.219573	-3.123167	-0.205005
H	5.782715	-0.757221	-0.792814
H	2.040158	-3.692571	0.559090
H	4.233690	1.034429	-0.899289
H	0.745488	-0.164960	-1.877665
H	0.495849	-1.896990	-0.186634
H	-0.277488	1.005265	2.026148
H	0.428991	6.160383	1.574847
H	-0.158456	4.797940	2.539653
H	1.491629	4.778873	1.883328
H	0.568258	4.684213	-0.442021
H	-1.081766	4.704873	0.211225
H	-2.071785	-0.182392	1.266285
H	-4.019559	-0.076019	-1.844362
H	-6.202609	-1.187749	-2.053849
H	-7.073401	-2.602711	-0.218327
H	-5.729796	-2.888604	1.848231
H	-3.526354	-1.791189	2.049972

3r(3S,3aS,9bS) conf14

0 imaginary frequency

C	5.784733	-0.569474	-0.302020
C	5.738488	0.475801	-1.215893
C	4.522299	0.890090	-1.730806
C	3.349513	0.262931	-1.323423
C	3.375901	-0.775439	-0.397285
C	4.609530	-1.189853	0.095569
N	2.133059	0.698913	-1.876418
C	0.915198	0.312060	-1.491065
C	0.798986	-0.815214	-0.491770
C	2.097359	-1.473265	0.000908
O	-0.109215	0.846383	-1.918035
H	6.733139	-0.906698	0.095538
C	0.025390	-0.344457	0.788987
N	0.741533	-1.003308	1.844765
C	1.914918	-1.569598	1.512487
O	2.681448	-2.100953	2.295602
C	0.181305	1.179492	0.986170
O	1.267840	1.700837	0.953354
O	-0.953265	1.799504	1.205605
C	-2.303175	3.719860	1.588413
C	-0.891711	3.235688	1.397781
C	-1.463793	-0.749797	0.830234
O	-1.924396	-1.236036	1.849925
N	-2.142188	-0.498010	-0.300400
C	-3.518940	-0.667192	-0.547596
C	-4.373295	-1.391589	0.281499
C	-5.715836	-1.505796	-0.060536
C	-6.215776	-0.916202	-1.211965
C	-5.355676	-0.202206	-2.038798
C	-4.017089	-0.077522	-1.711070
H	6.649394	0.966537	-1.534145
H	4.467278	1.698777	-2.450269
H	4.643872	-2.014437	0.795176
H	2.169097	1.459858	-2.546805
H	0.182739	-1.567435	-0.984737

H	2.146307	-2.503836	-0.357235
H	0.408341	-0.982089	2.800755
H	-2.757188	3.254780	2.463868
H	-2.910597	3.495029	0.711077
H	-2.293017	4.800135	1.735855
H	-0.420753	3.668763	0.515072
H	-0.264650	3.430503	2.267755
H	-1.621016	-0.023341	-1.038703
H	-4.000676	-1.864811	1.175067
H	-6.374083	-2.070298	0.588304
H	-7.263489	-1.013033	-1.466043
H	-5.727600	0.261874	-2.943660
H	-3.343211	0.478772	-2.353019

3r(3S,3aS,9bS) conf15

0 imaginary frequency

C	5.127519	-0.110983	0.273440
C	5.003409	-1.394311	-0.244859
C	3.800384	-2.070894	-0.139792
C	2.720869	-1.462245	0.490916
C	2.832802	-0.182066	1.030980
C	4.047394	0.485486	0.907830
N	1.509021	-2.167993	0.589717
C	0.322690	-1.638283	0.918002
C	0.310351	-0.180227	1.324225
C	1.653903	0.391013	1.791765
O	-0.713120	-2.298449	0.908692
H	6.064729	0.423640	0.189707
C	-0.146386	0.823506	0.215050
N	0.466457	2.040691	0.670213
C	1.489433	1.881649	1.528622
O	2.164793	2.776742	2.005755
C	0.337772	0.391585	-1.183451
O	-0.033859	-0.641930	-1.683644
O	1.148221	1.262612	-1.736416
C	2.819851	-0.046628	-2.922061
C	1.682371	0.936709	-3.045391
C	-1.672540	1.047448	0.084721
O	-2.066250	2.174861	-0.168369
N	-2.435084	-0.043720	0.226693
C	-3.834368	-0.158193	0.085374
C	-4.677632	0.902024	-0.240796
C	-6.043611	0.670708	-0.357622
C	-6.578233	-0.592513	-0.154923
C	-5.730296	-1.645511	0.170079
C	-4.368631	-1.432319	0.290026
H	5.842737	-1.869093	-0.736813
H	3.682034	-3.068273	-0.546702
H	4.149900	1.478309	1.326554
H	1.500025	-3.135699	0.284541
H	-0.412537	-0.099072	2.136405
H	1.798630	0.233431	2.861654
H	0.209943	2.939233	0.281756
H	3.582889	0.337731	-2.242619
H	3.272523	-0.192037	-3.904125
H	2.470879	-1.012599	-2.557420
H	2.016598	1.894618	-3.435687
H	0.869669	0.556933	-3.663061
H	-1.958012	-0.918254	0.449838
H	-4.282604	1.891154	-0.402124
H	-6.693142	1.499218	-0.611754
H	-7.643838	-0.757646	-0.248978
H	-6.129311	-2.639197	0.330783
H	-3.704452	-2.251646	0.540747

3r(3*R*,3a*S*,9b*S*) conf1

0 imaginary frequency

C	-5.320033	-1.909938	0.179637
C	-4.884213	-2.919799	-0.669730
C	-3.594614	-2.900131	-1.177572
C	-2.735599	-1.865922	-0.824424
C	-3.156688	-0.851375	0.028369
C	-4.454118	-0.880528	0.522132
N	-1.430496	-1.844092	-1.339027
C	-0.554406	-0.821892	-1.270078
C	-0.983583	0.417552	-0.497813
C	-2.181447	0.205077	0.436737
O	0.516195	-0.861939	-1.859853
H	-6.328719	-1.922764	0.571280
C	0.108256	0.954277	0.474330
N	-0.242155	0.315494	1.722457
C	-1.539414	-0.069255	1.794672
O	-2.092967	-0.518315	2.777000
C	0.048489	2.486291	0.649533
O	0.365840	3.005249	1.690664
O	-0.346589	3.129297	-0.423457
C	-0.828296	5.091266	-1.680492
C	-0.345400	4.577159	-0.351606

C	1.564414	0.674301	0.040138
O	2.125275	1.467804	-0.697953
N	2.113500	-0.428393	0.568897
C	3.388378	-0.962363	0.277974
C	4.042498	-0.721178	-0.926897
C	5.282877	-1.304008	-1.153407
C	5.868575	-2.126397	-0.201087
C	5.200834	-2.374602	0.992335
C	3.966302	-1.794851	1.234317
H	-5.551977	-3.726387	-0.944584
H	-3.246416	-3.678288	-1.846445
H	-4.781408	-0.085818	1.182403
H	-1.150157	-2.616676	-1.933767
H	-1.188824	1.163280	-1.264743
H	-2.701244	1.159988	0.571075
H	0.288991	0.493119	2.568163
H	-0.835716	6.181445	-1.659897
H	-0.168773	4.764229	-2.484739
H	-1.840652	4.742284	-1.886441
H	-0.998815	4.874251	0.468553
H	0.672318	4.898379	-0.128779
H	1.551435	-0.956596	1.224749
H	3.587082	-0.098223	-1.681368
H	5.789556	-1.114559	-2.091540
H	6.835568	-2.575465	-0.388372
H	5.642598	-3.020018	1.741100
H	3.440292	-1.982093	2.163459

3r(3*R*,3a*S*,9b*S*) conf2

0 imaginary frequency

C	-3.395258	-1.755510	-1.186669
C	-3.849691	-1.231478	0.016933
C	-2.980161	-1.097291	1.086621
C	-1.652747	-1.492142	0.953015
C	-1.181554	-2.021073	-0.248274
C	-2.068775	-2.145976	-1.311834
N	-0.790344	-1.348686	2.052501
C	0.552928	-1.458577	2.022906
C	1.168749	-1.706555	0.663977
C	0.276504	-2.431144	-0.350485
O	1.238261	-1.349969	3.028446
H	-4.069462	-1.860757	-2.026673
C	1.605743	-0.404924	-0.080474
N	1.539663	-0.821810	-1.459626
C	0.864336	-1.975675	-1.679906
O	0.735454	-2.520283	-2.758323
C	3.031167	0.024851	0.286588
O	3.707689	-0.495456	1.131768
O	3.402624	1.038293	-0.470320
C	4.929562	2.707264	-1.209874
C	4.731705	1.569904	-0.245185
C	0.685375	0.777557	0.293947
O	0.892481	1.347121	1.354602
N	-0.319181	1.028454	-0.556672
C	-1.493678	1.776040	-0.326285
C	-1.817101	2.335288	0.908065
C	-3.037344	2.983382	1.057716
C	-3.931013	3.081811	0.001243
C	-3.596784	2.526242	-1.228643
C	-2.385060	1.878229	-1.394477
H	-4.881036	-0.919947	0.124121
H	-3.316556	-0.682675	2.029810
H	-1.715455	-2.558138	-2.248791
H	-1.203589	-1.118040	2.949550
H	2.076165	-2.283246	0.834320
H	0.372736	-3.514118	-0.269310
H	1.994432	-0.309372	-2.206583
H	4.190657	3.491149	-1.041403
H	4.851045	2.359733	-2.240469
H	5.923413	3.130878	-1.062538
H	5.447923	0.763842	-0.404802
H	4.789044	1.895003	0.793714
H	-0.309888	0.514834	-1.429936
H	-1.138688	2.259058	1.742512
H	-3.286747	3.412702	2.020148
H	-4.878725	3.588013	0.132499
H	-4.283000	2.593638	-2.063496
H	-2.126745	1.432741	-2.348915

3r(3*R*,3a*S*,9b*S*) conf3

0 imaginary frequency

C	3.237857	-2.038708	-0.333276
C	3.351752	-1.232596	-1.458686
C	2.213725	-0.798296	-2.118904
C	0.958725	-1.174055	-1.651447
C	0.828663	-1.983160	-0.522358
C	1.981221	-2.407397	0.128562
N	-0.186271	-0.732693	-2.332639

C	-1.436004	-0.709487	-1.826499
C	-1.586183	-1.251135	-0.417882
C	-0.567309	-2.335861	-0.041862
O	-2.390541	-0.309824	-2.476142
H	4.123736	-2.376323	0.188915
C	-1.431796	-0.217670	0.750686
N	-1.049783	-1.074249	1.844525
C	-0.619503	-2.304069	1.479171
O	-0.307737	-3.200707	2.238020
C	-2.721864	0.519589	1.112771
O	-2.996528	0.791149	2.255453
O	-3.441648	0.822148	0.063645
C	-5.284030	1.804328	-1.063173
C	-4.656995	1.578580	0.286059
C	-0.384498	0.873035	0.393404
O	-0.665375	1.685881	-0.472267
N	0.776972	0.799636	1.059529
C	1.996224	1.443457	0.762765
C	2.158644	2.352113	-0.280901
C	3.421452	2.877814	-0.529184
C	4.513651	2.517425	0.245689
C	4.339826	1.619524	1.293410
C	3.090078	1.085852	1.552795
H	4.327196	-0.933622	-1.821181
H	2.283853	-0.161700	-2.992987
H	1.894079	-3.034514	1.007528
H	-0.063070	-0.312478	-3.247150
H	-2.594425	-1.657143	-0.347488
H	-0.866629	-3.320903	-0.400517
H	-1.209086	-0.811807	2.810406
H	-4.610453	2.364902	-1.712047
H	-5.525533	0.854097	-1.540443
H	-6.204714	2.375370	-0.940048
H	-5.298323	0.998434	0.949609
H	-4.386038	2.512123	0.779604
H	0.845022	0.071414	1.759960
H	1.322108	2.639756	-0.896327
H	3.543994	3.579501	-1.344935
H	5.491316	2.934066	0.040110
H	5.181283	1.329641	1.910077
H	2.952076	0.375444	2.360511

3r(3*R*,3a*S*,9b*S*) conf4

0 imaginary frequency

C	-4.386154	1.886926	-0.377802
C	-3.622226	2.883040	0.217234
C	-2.476348	2.550423	0.919166
C	-2.093278	1.217470	1.022309
C	-2.840690	0.207552	0.422126
C	-3.993406	0.560558	-0.271500
N	-0.946920	0.902234	1.769985
C	-0.369811	-0.308554	1.870522
C	-0.925087	-1.399438	0.974239
C	-2.396592	-1.235736	0.560317
O	0.574635	-0.511100	2.622068
H	-5.286069	2.140213	-0.922948
C	-0.162545	-1.547645	-0.394210
N	-1.192513	-2.039910	-1.259058
C	-2.449440	-1.926103	-0.796897
O	-3.453744	-2.300149	-1.376170
C	0.987063	-2.560263	-0.374654
O	1.186989	-3.311381	-1.293372
O	1.714937	-2.477921	0.719163
C	4.042772	-2.565979	0.047893
C	2.929486	-3.270222	0.782648
C	0.358933	-0.167227	-0.900790
O	-0.300040	0.466937	-1.701076
N	1.515095	0.241738	-0.344041
C	2.084883	1.532163	-0.449027
C	2.824498	1.986114	0.641202
C	3.423971	3.234256	0.598551
C	3.285944	4.037565	-0.527115
C	2.552575	3.576083	-1.611420
C	1.951814	2.323791	-1.585645
H	-3.918485	3.921242	0.138089
H	-1.870600	3.313534	1.393442
H	-4.589938	-0.216587	-0.731484
H	-0.531673	1.641356	2.327405
H	-0.800419	-2.336871	1.513303
H	-3.059267	-1.762551	1.247841
H	-0.983578	-2.411140	-2.177265
H	3.803482	-2.448569	-1.009763
H	4.227272	-1.582861	0.483492
H	4.956110	-3.156579	0.130572
H	3.133530	-3.354694	1.847012
H	2.718580	-4.256830	0.374342
H	1.917473	-0.345606	0.378448
H	2.918947	1.355423	1.518178

H	3.996391	3.580304	1.449958
H	3.750581	5.014684	-0.559469
H	2.448457	4.191186	-2.496481
H	1.399207	1.966180	-2.440672

3r(3*R*,3a*S*,9b*S*) conf5

0 imaginary frequency

C	-3.516566	-1.950108	-0.627755
C	-3.865848	-1.183684	0.477000
C	-2.902740	-0.831147	1.407719
C	-1.587556	-1.250537	1.235088
C	-1.220674	-2.020568	0.132066
C	-2.201200	-2.362659	-0.793131
N	-0.632597	-0.885238	2.197604
C	0.701874	-1.044489	2.091390
C	1.205542	-1.580748	0.769625
C	0.224933	-2.459419	-0.016556
O	1.466031	-0.750767	2.998137
H	-4.264151	-2.228032	-1.359241
C	1.609470	-0.460626	-0.241874
N	1.412473	-1.121596	-1.507718
C	0.696367	-2.269730	-1.453405
O	0.456009	-2.994179	-2.398829
C	3.067402	-0.017801	-0.073755
O	3.790924	-0.371994	0.816972
O	3.396198	0.801153	-1.054829
C	4.714405	2.575030	-0.055300
C	4.713165	1.404852	-1.007868
C	0.751385	0.806642	-0.028007
O	1.082779	1.582781	0.855175
N	-0.343650	0.898853	-0.795182
C	-1.487165	1.701640	-0.599600
C	-1.669144	2.519106	0.513434
C	-2.868895	3.205685	0.658007
C	-3.879300	3.089743	-0.285631
C	-3.685433	2.276406	-1.396572
C	-2.496352	1.586334	-1.555961
H	-4.887896	-0.853820	0.614058
H	-3.155819	-0.228351	2.272213
H	-1.930061	-2.964565	-1.651519
H	-0.967333	-0.460613	3.055957
H	2.112394	-2.143212	0.984591
H	0.326691	-3.511217	0.252323
H	1.809025	-0.769412	-2.371575
H	3.971109	3.313399	-0.357947
H	5.697945	3.046715	-0.069363
H	4.500283	2.253280	0.964212
H	4.899822	1.715609	-2.032813
H	5.433977	0.639040	-0.725758
H	-0.430975	0.215412	-1.537728
H	-0.897536	2.612761	1.260787
H	-3.009051	3.836422	1.527081
H	-4.809449	3.628643	-0.159063
H	-4.464370	2.174419	-2.141770
H	-2.345725	0.939885	-2.413872

3r(3*R*,3a*S*,9b*S*) conf6

0 imaginary frequency

C	-3.158562	2.150695	0.076451
C	-3.357540	1.550033	-1.160126
C	-2.270501	1.191626	-1.941031
C	-0.980434	1.437856	-1.482650
C	-0.765087	2.036951	-0.241101
C	-1.867550	2.388041	0.529289
N	0.113816	1.082863	-2.286406
C	1.378722	0.916714	-1.850007
C	1.611030	1.198944	-0.378760
C	0.665056	2.248308	0.220705
O	2.288119	0.599568	-2.601780
H	-4.004776	2.428512	0.691381
C	1.447389	-0.010102	0.608357
N	1.164803	0.670929	1.845774
C	0.781015	1.961047	1.710609
O	0.548399	2.731298	2.621534
C	2.725100	-0.838083	0.772767
O	3.138915	-1.153870	1.860268
O	3.271737	-1.150296	-0.375889
C	5.683134	-1.018722	-0.116136
C	4.498530	-1.923210	-0.349805
C	0.312559	-0.963593	0.138407
O	0.467768	-1.603728	-0.887955
N	-0.786155	-0.968441	0.909001
C	-2.057858	-1.498952	0.609164
C	-2.335662	-2.262646	-0.522691
C	-3.640128	-2.688240	-0.747421
C	-4.661223	-2.370672	0.135463
C	-4.372431	-1.619600	1.269866
C	-3.080216	-1.187137	1.507098

H	-4.360467	1.353142	-1.517409
H	-2.408326	0.715543	-2.904773
H	-1.713253	2.853848	1.495085
H	-0.065537	0.834210	-3.252980
H	2.641437	1.541907	-0.288142
H	0.997477	3.265817	0.013930
H	1.365806	0.249848	2.745218
H	5.626960	-0.539542	0.861503
H	6.598314	-1.610842	-0.158203
H	5.732500	-0.250018	-0.888230
H	4.405781	-2.692431	0.415214
H	4.534731	-2.390865	-1.330539
H	-0.762295	-0.371481	1.726590
H	-1.555530	-2.520055	-1.219727
H	-3.852185	-3.278150	-1.630507
H	-5.672231	-2.708229	-0.053075
H	-5.156641	-1.365855	1.972001
H	-2.850586	-0.592136	2.383963

3r(3*R*,3a*S*,9b*S*) conf7

0 imaginary frequency

C	-4.443365	1.699077	-0.000767
C	-3.672533	2.692609	0.589656
C	-2.459453	2.371766	1.174552
C	-2.016620	1.053633	1.165226
C	-2.769599	0.047853	0.564965
C	-3.989733	0.387970	-0.009274
N	-0.801259	0.746946	1.798867
C	-0.168626	-0.439888	1.775224
C	-0.747400	-1.495684	0.852468
C	-2.254274	-1.378189	0.570689
O	0.839609	-0.645481	2.437936
H	-5.395314	1.942505	-0.454337
C	-0.096281	-1.516166	-0.582180
N	-1.172230	-2.008174	-1.388929
C	-2.390108	-1.982966	-0.821427
O	-3.422379	-2.367688	-1.341624
C	1.090486	-2.476063	-0.707902
O	1.215001	-3.231192	-1.636430
O	1.939446	-2.353469	0.288117
C	3.953270	-2.792006	1.461725
C	3.148533	-3.152112	0.242442
C	0.307629	-0.078153	-1.034663
O	-0.453324	0.564170	-1.731749
N	1.480553	0.368671	-0.547239
C	1.945401	1.704461	-0.590718
C	1.681398	2.558495	-1.656946
C	2.180251	3.854643	-1.624890
C	2.941488	4.298857	-0.552587
C	3.211861	3.433808	0.501193
C	2.714719	2.140834	0.486004
H	-4.015492	3.719300	0.598060
H	-1.846578	3.132515	1.643624
H	-4.590457	-0.387260	-0.467066
H	-0.373372	1.469122	2.368885
H	-0.536937	-2.459294	1.313829
H	-2.833069	-1.979734	1.272450
H	-1.026034	-2.309571	-2.344053
H	4.875673	-3.373319	1.467348
H	4.211278	-1.732082	1.454703
H	3.395786	-3.015173	2.371858
H	2.855805	-4.201714	0.231910
H	3.670670	-2.917456	-0.685315
H	1.981750	-0.239049	0.091725
H	1.106775	2.215670	-2.503520
H	1.973820	4.518556	-2.455053
H	3.325785	5.310720	-0.539084
H	3.808060	3.766259	1.341641
H	2.913324	1.460500	1.306770

3r(3*R*,3a*S*,9b*S*) conf8

0 imaginary frequency

C	-3.438614	-2.130021	0.075281
C	-3.685319	-1.188733	1.066867
C	-2.631597	-0.639484	1.778213
C	-1.327763	-1.036560	1.499299
C	-1.063503	-1.980162	0.508172
C	-2.134023	-2.518789	-0.197562
N	-0.275641	-0.475178	2.239781
C	1.040607	-0.602253	1.973564
C	1.393004	-1.324578	0.688404
C	0.374759	-2.380228	0.232484
O	1.895886	-0.153802	2.721428
H	-4.257575	-2.561768	-0.485162
C	1.545886	-0.390860	-0.563269
N	1.196132	-1.277536	-1.642167
C	0.618882	-2.442645	-1.269532
O	0.322047	-3.354466	-2.016328

C	2.955131	0.160201	-0.792569
O	3.338798	0.433689	-1.903036
O	3.636625	0.314123	0.314933
C	4.722459	2.477449	0.159322
C	4.920178	0.982843	0.223017
C	0.629933	0.852378	-0.427385
O	1.010584	1.783930	0.264129
N	-0.556590	0.758312	-1.043370
C	-1.717553	1.529861	-0.827007
C	-2.823334	1.220660	-1.618844
C	-4.027498	1.871541	-1.414059
C	-4.140550	2.838255	-0.421044
C	-3.034674	3.146934	0.357761
C	-1.818595	2.502343	0.165324
H	-4.698534	-0.875847	1.285183
H	-2.805232	0.100812	2.550324
H	-1.942128	-3.255103	-0.968067
H	-0.514677	0.065061	3.064214
H	2.359120	-1.799001	0.850104
H	0.586738	-3.356061	0.670221
H	1.474790	-1.088671	-2.598184
H	4.175547	2.826150	1.035838
H	5.697485	2.966272	0.140343
H	4.174962	2.764846	-0.738860
H	5.440073	0.681214	1.128837
H	5.451107	0.595820	-0.645095
H	-0.688107	-0.046637	-1.644379
H	-2.733034	0.456853	-2.383466
H	-4.881096	1.619135	-2.030542
H	-5.082222	3.346765	-0.258830
H	-3.111559	3.898312	1.133892
H	-0.971377	2.745961	0.786279

3r(3*R*,3a*S*,9b*S*) conf9

0 imaginary frequency

C	-3.269979	-2.078808	-1.000631
C	-3.769436	-1.489792	0.154115
C	-2.914131	-1.176375	1.197441
C	-1.555745	-1.456199	1.087115
C	-1.039199	-2.047043	-0.065569
C	-1.912813	-2.353029	-1.103361
N	-0.709242	-1.133891	2.160996
C	0.638516	-1.125380	2.130319
C	1.274448	-1.440816	0.794628
C	0.450191	-2.328717	-0.145173
O	1.311396	-0.863874	3.116013
H	-3.932546	-2.324508	-1.820328
C	1.595117	-0.177130	-0.065023
N	1.566204	-0.718273	-1.401758
C	0.992573	-1.940352	-1.515032
O	0.906818	-2.584473	-2.541555
C	2.976579	0.407491	0.252463
O	3.691278	0.027098	1.139382
O	3.254325	1.377547	-0.597816
C	5.622371	1.213806	-1.135318
C	4.542313	2.031177	-0.470866
C	0.570647	0.946234	0.205313
O	0.721385	1.630248	1.205980
N	-0.450344	1.020883	-0.659498
C	-1.689794	1.673653	-0.495120
C	-2.064124	2.329819	0.675362
C	-3.341002	2.870791	0.766955
C	-4.240041	2.768237	-0.284640
C	-3.854366	2.117548	-1.451369
C	-2.586073	1.574167	-1.558809
H	-4.825290	-1.267467	0.243242
H	-3.285898	-0.710124	2.102341
H	-1.523658	-2.815884	-2.001702
H	-1.142125	-0.855473	3.035074
H	2.228674	-1.918663	1.008813
H	0.644967	-3.387411	0.028291
H	1.975317	-0.235688	-2.193688
H	5.745763	0.248341	-0.644533
H	5.386683	1.051977	-2.187730
H	6.567289	1.755299	-1.072602
H	4.401130	2.989940	-0.963633
H	4.739233	2.194945	0.587521
H	-0.392855	0.424019	-1.476131
H	-1.380333	2.409394	1.505104
H	-3.630631	3.376253	1.679877
H	-5.232177	3.192336	-0.198634
H	-4.544152	2.028863	-2.281260
H	-2.283646	1.054763	-2.461013

3r(3*R*,3a*S*,9b*S*) conf10

0 imaginary frequency

C	-3.019751	3.480327	0.134595
C	-3.711642	2.449844	-0.489224

C	-3.017362	1.442939	-1.138103
C	-1.627338	1.468155	-1.159786
C	-0.917623	2.486871	-0.528432
C	-1.632520	3.493215	0.111644
N	-0.944144	0.455469	-1.852837
C	0.381050	0.227874	-1.820734
C	1.189925	1.087168	-0.868492
C	0.598283	2.473342	-0.570611
O	0.903076	-0.640364	-2.507336
H	-3.557159	4.272669	0.639075
C	1.404506	0.461932	0.562007
N	1.573024	1.636203	1.364913
C	1.159785	2.788276	0.809780
O	1.216165	3.887770	1.331809
C	2.675690	-0.388238	0.664415
O	3.488752	-0.223071	1.535564
O	2.748218	-1.297778	-0.283696
C	5.073402	-1.495483	-0.962035
C	3.904778	-2.175153	-0.293333
C	0.146551	-0.335014	1.031111
O	-0.643488	0.189364	1.791926
N	0.001695	-1.557279	0.485072
C	-1.177914	-2.339231	0.512600
C	-1.462876	-3.096071	-0.622018
C	-2.598364	-3.889496	-0.655428
C	-3.456638	-3.927688	0.437185
C	-3.162233	-3.175913	1.566315
C	-2.023151	-2.382452	1.616649
H	-4.793862	2.428636	-0.472963
H	-3.539965	0.632002	-1.631679
H	-1.093262	4.296425	0.597074
H	-1.489456	-0.165956	-2.441190
H	2.176726	1.201841	-1.315648
H	0.960695	3.218347	-1.279855
H	1.916529	1.586161	2.315529
H	5.911007	-2.192751	-1.008507
H	4.811473	-1.200536	-1.978725
H	5.389196	-0.613807	-0.404136
H	4.123704	-2.464679	0.733079
H	3.568986	-3.045343	-0.851841
H	0.702770	-1.857160	-0.183078
H	-0.791048	-3.052993	-1.472379
H	-2.814643	-4.474765	-1.540313
H	-4.346394	-4.543630	0.409680
H	-3.819990	-3.208160	2.425915
H	-1.790458	-1.815657	2.505145

3r(3*R*,3a*S*,9b*S*) conf11

0 imaginary frequency

C	-5.747857	-0.728981	0.465172
C	-5.558210	-2.046027	0.064338
C	-4.314206	-2.472886	-0.373411
C	-3.253462	-1.575175	-0.401694
C	-3.427702	-0.255497	0.000562
C	-4.681734	0.159230	0.428917
N	-1.992705	-2.005598	-0.840879
C	-0.926178	-1.228660	-1.119531
C	-1.081460	0.270899	-0.907980
C	-2.246797	0.659959	0.011526
O	0.100298	-1.704821	-1.583134
H	-6.720559	-0.394911	0.801768
C	0.131234	0.932333	-0.202015
N	-0.253853	0.886351	1.193454
C	-1.592255	0.786995	1.385948
O	-2.160124	0.830168	2.457792
C	0.280040	2.395180	-0.671177
O	-0.278310	2.868888	-1.625241
O	1.099631	3.048090	0.128021
C	2.330341	4.960524	0.828799
C	1.362217	4.435244	-0.196014
C	1.500259	0.289313	-0.497670
O	2.087060	0.622654	-1.514365
N	1.950418	-0.564742	0.433330
C	3.104630	-1.373930	0.372838
C	4.189066	-1.100738	-0.457559
C	5.289982	-1.948648	-0.434927
C	5.326005	-3.053789	0.402753
C	4.243326	-3.313667	1.235043
C	3.138022	-2.480414	1.221374
H	-6.383774	-2.746106	0.086432
H	-4.155957	-3.495519	-0.694648
H	-4.816122	1.189743	0.736630
H	-1.889278	-2.986168	-1.079420
H	-1.187606	0.693926	-1.907485
H	-2.564767	1.679116	-0.232468
H	0.352568	1.239914	1.925358
H	3.264408	4.398605	0.802418
H	1.905913	4.898295	1.831293

H	2.549105	6.006089	0.610016
H	0.412891	4.970732	-0.178844
H	1.771303	4.471276	-1.205937
H	1.305405	-0.796738	1.179260
H	4.182233	-0.238424	-1.104434
H	6.130733	-1.731946	-1.082194
H	6.189966	-3.705853	0.410609
H	4.256172	-4.170123	1.897437
H	2.290345	-2.681390	1.866529

3r(3*R*,3a*S*,9b*S*) conf12

0 imaginary frequency

C	-5.237577	-2.045236	0.303067
C	-4.767377	-3.149692	-0.397118
C	-3.471303	-3.168345	-0.888340
C	-2.640670	-2.075394	-0.669230
C	-3.096831	-0.965155	0.033037
C	-4.399852	-0.958392	0.512477
N	-1.327773	-2.092097	-1.163987
C	-0.474274	-1.050065	-1.221349
C	-0.948552	0.274788	-0.641315
C	-2.150455	0.158847	0.304455
O	0.610843	-1.148239	-1.776805
H	-6.251005	-2.029492	0.682160
C	0.110839	0.979015	0.255262
N	-0.226167	0.492563	1.574377
C	-1.513246	0.082344	1.689886
O	-2.062619	-0.250707	2.719444
C	-0.021246	2.517532	0.234193
O	0.265172	3.174834	1.203430
O	-0.437903	2.996533	-0.914571
C	-1.864118	4.909915	-0.441928
C	-0.558807	4.437089	-1.032861
C	1.580464	0.712995	-0.137540
O	2.097433	1.411297	-0.994441
N	2.191756	-0.260146	0.552839
C	3.497495	-0.755189	0.335901
C	4.125696	-0.685723	-0.904450
C	5.399076	-1.220817	-1.050509
C	6.043673	-1.828237	0.018181
C	5.402606	-1.906820	1.248852
C	4.135227	-1.371576	1.410266
H	-5.413264	-4.001618	-0.567781
H	-3.096195	-4.021646	-1.440874
H	-4.753505	-0.089938	1.055995
H	-1.018705	-2.932278	-1.641250
H	-1.166294	0.896268	-1.509008
H	-2.691623	1.111716	0.307629
H	0.287715	0.803178	2.391981
H	-1.907825	4.712636	0.629204
H	-1.956652	5.985531	-0.598558
H	-2.705180	4.416691	-0.930647
H	0.303887	4.894448	-0.551037
H	-0.512326	4.617850	-2.103880
H	1.661074	-0.715512	1.284882
H	3.625268	-0.232137	-1.746308
H	5.885332	-1.165578	-2.016506
H	7.036113	-2.241903	-0.107236
H	5.890766	-2.384011	2.089285
H	3.629685	-1.427490	2.367267

3r(3*R*,3a*S*,9b*S*) conf13

0 imaginary frequency

C	-5.788421	-0.759614	0.367014
C	-5.586064	-2.035176	-0.146140
C	-4.331202	-2.420031	-0.591724
C	-3.272703	-1.522541	-0.514328
C	-3.459722	-0.244456	0.000318
C	-4.724279	0.129154	0.435337
N	-2.000690	-1.910595	-0.960593
C	-0.932850	-1.109340	-1.150098
C	-1.094676	0.363531	-0.802996
C	-2.281294	0.666008	0.121500
O	0.102082	-1.539074	-1.639938
H	-6.769514	-0.457879	0.709758
C	0.102849	0.949418	-0.010046
N	-0.315776	0.776887	1.365344
C	-1.658664	0.664785	1.515824
O	-2.251457	0.611730	2.573665
C	0.280061	2.446839	-0.337312
O	-0.249585	3.013468	-1.256047
O	1.091552	3.003999	0.540874
C	2.555935	4.468310	-0.723820
C	1.468895	4.385272	0.319623
C	1.473539	0.327019	-0.335848
O	2.086800	0.757526	-1.300549
N	1.904727	-0.613836	0.514452
C	3.089226	-1.376258	0.400435

C	3.691011	-1.639521	-0.826694
C	4.839975	-2.419142	-0.864648
C	5.384229	-2.942686	0.299967
C	4.767135	-2.687835	1.518992
C	3.624922	-1.905947	1.572141
H	-6.409870	-2.735115	-0.205966
H	-4.162521	-3.409346	-1.000335
H	-4.868453	1.127710	0.831329
H	-1.890740	-2.864775	-1.286908
H	-1.176879	0.879587	-1.760035
H	-2.595451	1.703574	-0.034044
H	0.269526	1.067762	2.140836
H	3.422455	3.880480	-0.419075
H	2.864660	5.508542	-0.836508
H	2.203967	4.106189	-1.690149
H	1.814842	4.725607	1.292528
H	0.579178	4.946053	0.037460
H	1.311800	-0.833378	1.305131
H	3.263413	-1.252472	-1.739066
H	5.306693	-2.622629	-1.820399
H	6.279738	-3.549450	0.258844
H	5.177295	-3.095824	2.434212
H	3.139508	-1.699749	2.518949

3r(3*R*,3a*S*,9b*S*) conf14

0 imaginary frequency

C	-5.566765	-1.327660	0.471881
C	-5.238267	-2.628437	0.109406
C	-3.952428	-2.936527	-0.306647
C	-2.989456	-1.935178	-0.351156
C	-3.303274	-0.630025	0.011757
C	-4.597670	-0.335207	0.418366
N	-1.685887	-2.243993	-0.767539
C	-0.706988	-1.367366	-1.070497
C	-1.017829	0.113096	-0.898698
C	-2.222344	0.401543	0.006888
O	0.364942	-1.746184	-1.521062
H	-6.572273	-1.086952	0.791327
C	0.117518	0.906860	-0.200860
N	-0.267436	0.843161	1.194246
C	-1.592290	0.620512	1.381338
O	-2.169256	0.631770	2.448957
C	0.114483	2.372239	-0.684884
O	-0.495852	2.775111	-1.639355
O	0.868311	3.108389	0.108129
C	-0.249081	5.250197	0.386765
C	0.951279	4.527389	-0.173030
C	1.541180	0.398616	-0.488944
O	2.086987	0.764092	-1.518432
N	2.085044	-0.377330	0.457909
C	3.343623	-1.017307	0.406914
C	3.958333	-1.358808	-0.794251
C	5.186037	-2.007956	-0.766375
C	5.796756	-2.325677	0.438842
C	5.166992	-1.996243	1.633346
C	3.945823	-1.342674	1.620322
H	-5.987370	-3.409298	0.145058
H	-3.686744	-3.945708	-0.598244
H	-4.840390	0.684028	0.695817
H	-1.479220	-3.215043	-0.976272
H	-1.158061	0.500624	-1.908238
H	-2.641318	1.377570	-0.259541
H	0.290276	1.279997	1.920218
H	-0.328181	5.083327	1.461595
H	-1.169540	4.918825	-0.094231
H	-0.134770	6.320750	0.210994
H	1.048839	4.659053	-1.249619
H	1.872429	4.839748	0.312801
H	1.533250	-0.551923	1.288475
H	3.481254	-1.133147	-1.735761
H	5.662996	-2.272397	-1.701939
H	6.753608	-2.831713	0.448643
H	5.628836	-2.244975	2.580558
H	3.449502	-1.079365	2.547251

3r(3*R*,3a*S*,9b*S*) conf15

0 imaginary frequency

C	-4.488110	1.287996	-0.992811
C	-3.949764	2.436209	-0.425777
C	-2.889667	2.339504	0.459147
C	-2.365131	1.090564	0.774157
C	-2.885416	-0.069670	0.205924
C	-3.956192	0.047122	-0.673895
N	-1.308184	1.017796	1.697450
C	-0.596467	-0.080174	2.005296
C	-0.895353	-1.328786	1.202330
C	-2.297387	-1.415560	0.582399
O	0.279764	-0.065293	2.860567

H	-5.320573	1.356392	-1.680915
C	0.071714	-1.527419	-0.011462
N	-0.744120	-2.280091	-0.922559
C	-2.066122	-2.258568	-0.666266
O	-2.922180	-2.814815	-1.329783
C	1.332210	-2.314496	0.355235
O	1.754036	-2.428155	1.476406
O	1.894745	-2.805648	-0.730216
C	4.288885	-2.487896	-0.473035
C	3.164872	-3.489021	-0.575025
C	0.488607	-0.168046	-0.645505
O	-0.120054	0.268228	-1.602454
N	1.506348	0.453583	-0.016870
C	1.937086	1.783445	-0.243030
C	1.927001	2.365473	-1.506452
C	2.372725	3.672815	-1.652233
C	2.833284	4.393766	-0.559064
C	2.852506	3.798480	0.696543
C	2.403735	2.497626	0.857870
H	-4.355864	3.409614	-0.669482
H	-2.459805	3.224070	0.914067
H	-4.378021	-0.848193	-1.111645
H	-1.057944	1.865893	2.195054
H	-0.734601	-2.171715	1.872184
H	-2.986585	-1.947245	1.239456
H	-0.367971	-2.682249	-1.772338
H	4.187918	-1.869207	0.419179
H	5.237865	-3.022628	-0.414503
H	4.308081	-1.844254	-1.353247
H	3.103670	-4.134663	0.299530
H	3.246637	-4.100395	-1.470054
H	1.857753	0.033799	0.837697
H	1.587365	1.804800	-2.364049
H	2.363992	4.125619	-2.635761
H	3.179724	5.411595	-0.684503
H	3.213668	4.348398	1.556413
H	2.407785	2.026614	1.834523

3r(3*R*,3a*S*,9b*S*) conf16

0 imaginary frequency

C	3.995011	2.247935	-1.190183
C	4.475464	1.039727	-0.701006
C	3.731676	0.320030	0.218471
C	2.502419	0.809809	0.646145
C	2.000082	2.013151	0.156533
C	2.766003	2.726166	-0.759568
N	1.783289	0.077242	1.605149
C	0.532288	0.332790	2.025666
C	-0.211000	1.440401	1.307503
C	0.660063	2.521467	0.651385
O	0.002441	-0.320888	2.915033
H	4.574606	2.817939	-1.904538
C	-1.121039	0.923745	0.142185
N	-1.149008	2.056186	-0.739546
C	-0.193155	2.979942	-0.525086
O	-0.039220	3.999786	-1.172425
C	-2.533929	0.569494	0.612574
O	-2.807452	0.249475	1.740500
O	-3.386652	0.623636	-0.388296
C	-5.541232	0.406064	-1.375308
C	-4.761836	0.268379	-0.096059
C	-0.494541	-0.310168	-0.570238
O	0.154213	-0.159584	-1.586538
N	-0.695367	-1.483227	0.062175
C	-0.036534	-2.702165	-0.231162
C	0.296071	-3.522774	0.843664
C	0.929974	-4.733730	0.615418
C	1.238839	-5.127477	-0.681088
C	0.897720	-4.306144	-1.747165
C	0.255109	-3.093663	-1.533484
H	5.431958	0.656325	-1.032649
H	4.092993	-0.621910	0.613988
H	2.392521	3.669469	-1.136548
H	2.250552	-0.708217	2.046075
H	-0.871610	1.895255	2.043442
H	0.811138	3.366895	1.323567
H	-1.760106	2.093738	-1.545742
H	-5.502522	1.431384	-1.744165
H	-5.149383	-0.263171	-2.141723
H	-6.583030	0.144979	-1.187233
H	-4.768674	-0.753090	0.284624
H	-5.123260	0.940051	0.682494
H	-1.160420	-1.458066	0.964071
H	0.056916	-3.202031	1.851667
H	1.186581	-5.367957	1.454573
H	1.738006	-6.071402	-0.859062
H	1.125247	-4.610756	-2.761030
H	-0.025273	-2.468118	-2.367629

3r(3*R*,3a*S*,9b*S*) conf17

0 imaginary frequency

C	2.294828	3.749809	-0.718599
C	3.239600	3.003266	-0.025851
C	2.831947	2.018646	0.858319
C	1.474915	1.781161	1.048532
C	0.514635	2.521264	0.360445
C	0.942949	3.506561	-0.521530
N	1.084403	0.782988	1.957598
C	-0.145761	0.248036	2.055400
C	-1.198851	0.811750	1.127443
C	-0.951938	2.233933	0.614449
O	-0.407517	-0.650206	2.843925
H	2.607951	4.520863	-1.410375
C	-1.423271	-0.018504	-0.195592
N	-2.006725	0.982792	-1.038729
C	-1.748140	2.256114	-0.684223
O	-2.093974	3.247112	-1.301890
C	-2.383462	-1.174956	0.093878
O	-2.047937	-2.171759	0.688048
O	-3.599034	-0.940659	-0.338590
C	-5.895256	-1.480064	-0.647167
C	-4.592828	-1.962471	-0.069248
C	-0.070093	-0.501187	-0.805976
O	0.400306	0.100284	-1.754413
N	0.514477	-1.532506	-0.173884
C	1.812228	-2.042932	-0.395643
C	2.835983	-1.283390	-0.957261
C	4.098724	-1.845094	-1.097542
C	4.351803	-3.145290	-0.682980
C	3.327420	-3.892228	-0.113462
C	2.062675	-3.346354	0.030311
H	4.296506	3.184992	-0.173736
H	3.555304	1.423441	1.403214
H	0.207037	4.090641	-1.058952
H	1.802969	0.367927	2.541076
H	-2.140043	0.783856	1.676623
H	-1.366268	2.977543	1.296706
H	-2.418770	0.756649	-1.935061
H	-5.809410	-1.328986	-1.723577
H	-6.665480	-2.229612	-0.463313
H	-6.203767	-0.544499	-0.179921
H	-4.253533	-2.889390	-0.531424
H	-4.645246	-2.102411	1.010367
H	-0.053793	-2.031852	0.503848
H	2.655616	-0.266805	-1.272442
H	4.892218	-1.250969	-1.533695
H	5.339666	-3.572489	-0.798426
H	3.511000	-4.905828	0.220190
H	1.259539	-3.922560	0.475131

3r(3*R*,3a*S*,9b*S*) conf18

0 imaginary frequency

C	2.369925	3.712109	-0.347150
C	3.197149	2.932718	0.451737
C	2.656025	1.929587	1.238078
C	1.283317	1.706546	1.224389
C	0.440001	2.480367	0.427863
C	1.001275	3.483500	-0.353602
N	0.755946	0.687291	2.036711
C	-0.475292	0.158034	1.925529
C	-1.377625	0.773378	0.881667
C	-1.050676	2.208390	0.462331
O	-0.854691	-0.774553	2.621277
H	2.787444	4.497492	-0.963599
C	-1.420584	-0.004395	-0.490088
N	-1.904975	1.030902	-1.355773
C	-1.665132	2.287600	-0.930348
O	-1.904783	3.304218	-1.555945
C	-2.405229	-1.167415	-0.344881
O	-2.099006	-2.229665	0.140757
O	-3.611043	-0.847591	-0.753485
C	-5.152010	-1.733557	0.901752
C	-4.666528	-1.816742	-0.524396
C	0.000287	-0.450735	-0.954652
O	0.565160	0.188519	-1.824069
N	0.531053	-1.494755	-0.295895
C	1.851738	-1.982501	-0.406423
C	2.918366	-1.179116	-0.802634
C	4.196795	-1.720513	-0.844652
C	4.422747	-3.044245	-0.493253
C	3.354709	-3.835305	-0.087073
C	2.073874	-3.309541	-0.042909
H	4.266164	3.102896	0.462804
H	3.287097	1.308616	1.863377
H	0.356379	4.093303	-0.973185
H	1.381441	0.239413	2.697990

H	-2.389042	0.736060	1.287690
H	-1.547777	2.932759	1.109262
H	-2.176268	0.843769	-2.313040
H	-5.518329	-0.730357	1.122113
H	-5.971823	-2.439567	1.040876
H	-4.357553	-1.985538	1.604947
H	-5.440807	-1.533369	-1.232742
H	-4.288720	-2.805776	-0.777598
H	-0.103512	-2.038970	0.280317
H	2.757361	-0.144583	-1.065917
H	5.023575	-1.092561	-1.152843
H	5.423204	-3.455783	-0.531289
H	3.516645	-4.867879	0.195681
H	1.236466	-3.920397	0.273865

3r(3*R*,3a*S*,9b*S*) conf19

0 imaginary frequency

C	-2.778193	-3.342789	-0.845603
C	-3.596918	-2.483904	-0.123221
C	-3.045677	-1.623236	0.811119
C	-1.670961	-1.622917	1.021972
C	-0.836090	-2.478700	0.304744
C	-1.407747	-3.336314	-0.627929
N	-1.132749	-0.747581	1.980915
C	0.165434	-0.413527	2.093232
C	1.118409	-1.097053	1.137457
C	0.654255	-2.445914	0.580270
O	0.563656	0.397828	2.917866
H	-3.204014	-4.017267	-1.576992
C	1.467335	-0.273350	-0.161846
N	1.906897	-1.327267	-1.028568
C	1.451186	-2.555233	-0.713465
O	1.646224	-3.570431	-1.357187
C	2.578745	0.727498	0.163768
O	2.376839	1.738572	0.792694
O	3.751176	0.337135	-0.277292
C	4.951426	2.332174	-0.990386
C	4.887111	1.197162	0.001196
C	0.208219	0.420129	-0.773070
O	-0.310639	-0.059067	-1.764789
N	-0.248056	1.489501	-0.099225
C	-1.454155	2.187457	-0.326114
C	-1.534482	3.490299	0.162340
C	-2.705577	4.215290	0.015405
C	-3.804836	3.648809	-0.618962
C	-3.721509	2.348184	-1.096360
C	-2.554485	1.608210	-0.954143
H	-4.666897	-2.480439	-0.287649
H	-3.668786	-0.942440	1.379551
H	-0.770213	-4.007611	-1.188916
H	-1.779968	-0.249334	2.582531
H	2.054213	-1.231415	1.680422
H	0.933176	-3.267089	1.241913
H	2.351139	-1.140051	-1.918417
H	4.079845	2.981171	-0.906970
H	5.844070	2.926382	-0.789991
H	5.014479	1.947286	-2.008646
H	4.807521	1.548453	1.028640
H	5.743713	0.533909	-0.088523
H	0.364300	1.873554	0.613624
H	-0.674292	3.925987	0.657537
H	-2.757171	5.226997	0.397710
H	-4.719360	4.215856	-0.736458
H	-4.575033	1.893818	-1.584136
H	-2.506354	0.593712	-1.319839

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