Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Organocatalytic Asymmetric Synthesis of Highly Substituted Pyrrolidines Bearing Stereogenic Quaternary Centre at 3-Position

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A. General Information: All the reagents used are of commercial grade and used without purification. Organic solvents that are used for reactions were dried using standard methods. Reactions were monitored by silica gel 60 F254 (0.25mm). NMR spectra were recorded in $CDCl_3$ and tetramethylsilane as the internal standard for ^1H NMR (600 MHz) and $CDCl_3$ solvent as the internal standard for ^{13}C NMR (150 MHz). Chemical shifts are reported in ppm tetramethylsilane ($CDCl_3$: δ 7.26, for ^1H NMR and $CDCl_3$: δ 77.23, for ^{13}C NMR). For ^1H NMR, datareported as follows: chemical shift, multiplicity (s = singlet, d = doublet, dd = double doublet, t =triplet, q = quartet, br = broad, m = multiplet), coupling constants (Hz) and integration. HRMS spectra were recorded using APCI and ESI mode. HPLC data were recorded using Dionex (Ultimate 3000) HPLC Instruments.

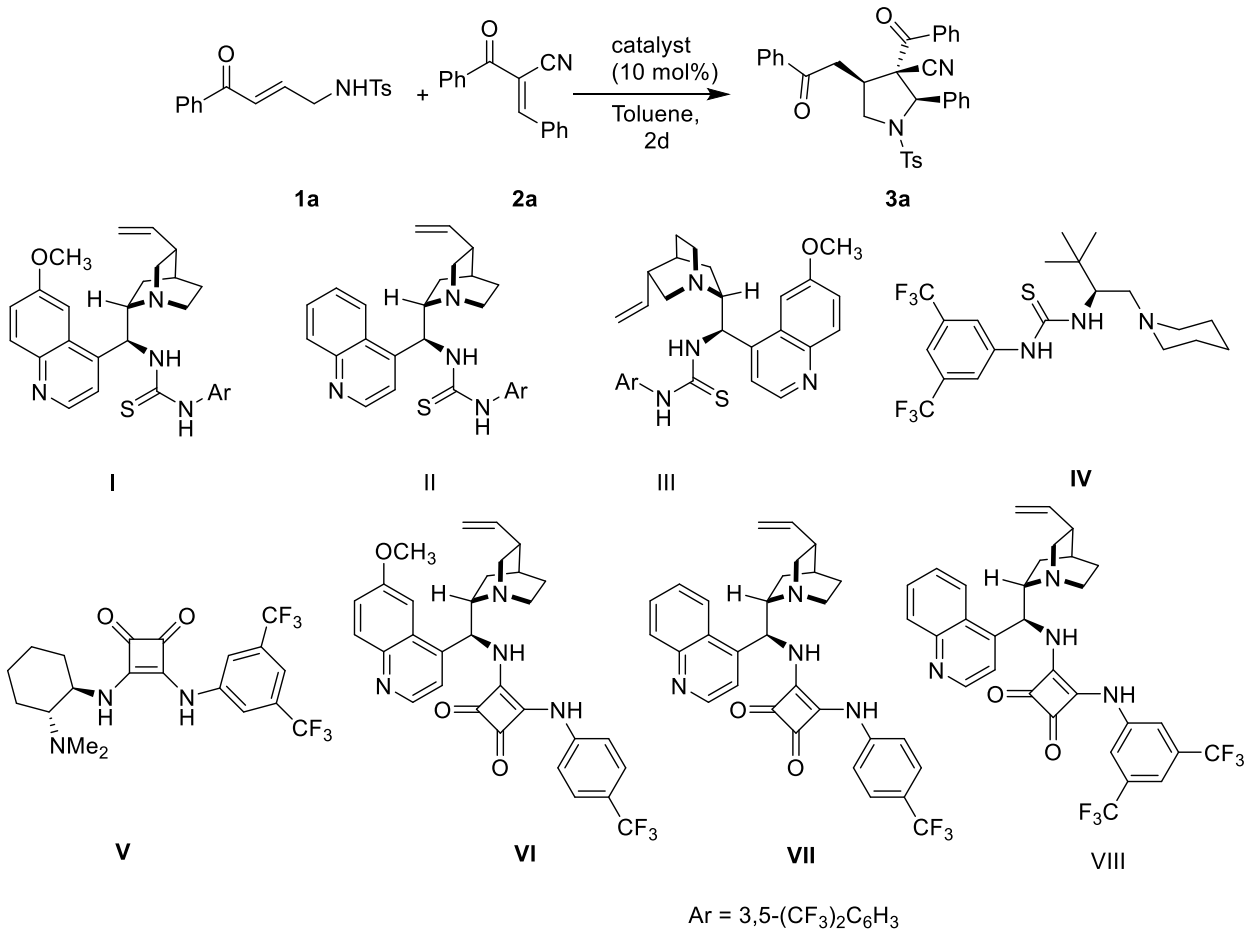
Toluene was distilled over CaH_2 under argon and stored over 4A° molecular sieves. DCM was distilled over CaH_2 under argon and stored over 4A° molecular sieves. Silica gel (60-120 mesh size) was used for the column chromatography. Reactions were monitored by TLC on silica gel 60 F254 (0.25 mm). Thiourea catalysts (I-IV) were prepared according to the reported procedure.[1] Squaramide catalyst was prepared according to the reported procedure.[2] *Trans*-*α*-cyano-*α,β*-unsaturated ketones were prepared following literature procedures.[3] Amino enones were prepared according to literature procedures.[4]

B. General procedure for the synthesis of compound 3:

Under argon atmosphere, compound *N*-tosyl aminomethyl enone **1** (0.05 mmol), *trans*-*α*-cyano-*α,β*-unsaturated ketone **2** (0.075 mmol) and catalyst **VIII**(10 mol %) were added in a round bottom flask. Then methyl tertiary butyl ether (MTBE) 0.2 ml was mixed with the reaction mixture. Next 4 Å MS (For 0.1 mmol of **1a** 100 mg MS was added) was added to the reaction mixture. Then the reaction mixture was stirred at room temperature for 2 days under argon atmosphere. After completion of the reaction as monitored by TLC, the crude product was purified by column chromatography using 15-18 % ethyl acetate in hexane as eluent.

C. Optimization of reaction condition:

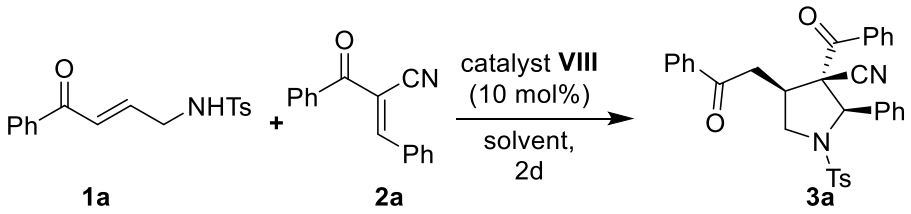
Catalyst screening:



Entry[a]	Catalyst	Yield(%)[b]	dr[c]	ee(%)[d]
1	**I**	60	10:1	30
2	**II**	62	10:1	31
3	**III**	65	10:1	25
4	**IV**	68	10:1	45
5	**V**	70	15:1	45
6	**VI**	72	15:1	50
7	**VII**	75	15:1	55
8	**VIII**	78	15:1	60

[a]Reaction conditions: 0.05 mmol of **1a** and 0.075 mmol**2a** in 0.2 mL solvent using 10 mol% catalyst at RT for 48 h. [b]Isolated yield after silica gel column chromatography. [c]Determined by ^{1}H NMR. [d]Determined by chiral HPLC of the major diastereomer.

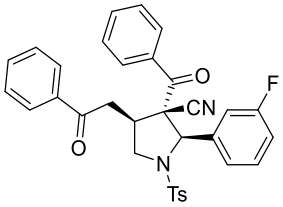
Solvent screening:

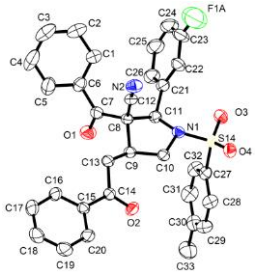


Entry[a]	Solvent	Yield[b]	dr[c]	ee(%)[d]
1	Toluene	78	15:1	60
2	Et_2O	79	15:1	68
3	CH_2Cl_2	75	15:1	43
4	DCE	71	15:1	50
5	$CHCl_3$	76	15:1	63
6	TFT	78	15:1	61
7	MTBE	80	15:1	89
8[e]	MTBE	80	15:1	91

[a]Reaction conditions: 0.05mmol of **1a** and 0.075mmol**2a** in 0.2 mL solvent using 10 mol% catalyst at RT for 48 h. [b]Isolated yield after silica gel column chromatography. [c]Determined by ^{1}H NMR. [d]Determined by chiral HPLC of the major diastereomer. [e]Reaction was carried out in presence of 4 Å MS (For 0.1 mmol of 1a 100 mg MS was added).

D. Crystal data and structure refinement for chiral compound (CCDC No. 1862234) 3i:

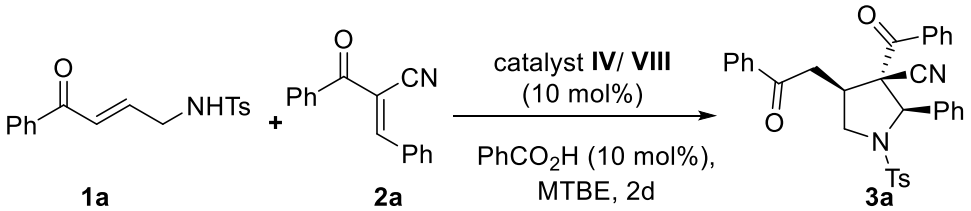


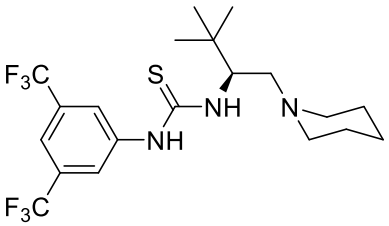


Empirical formula	$C_{33}H_{27}FN_2O_4S$
Formula weight	566.66
CCDC Number	1862234
Crystal habit, colour	Needle, White
Crystal size, mm^3	0.25 × 0.18 ×0.18
Temperature, *T*	293(2)
Wavelength, λ(Å)	0.71073
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	*a* = 9.7629(4)Å *b* = 11.7118(6)Å *c* = 13.5050(7)Å α = 90.002(4)°, β= 91.798(4)° γ = 112.093(4)°
Volume, *V* ($Å^3$)	1429.97(13)
Z	2
Calculated density, $Mg·m^{-3}$	1.3159
Absorption coefficient, μ (mm^{-1})	0.161
F(000)	592.5
θ range for data collection	6.04 to 50.00°
Limiting indices	-13 ≤ h ≤ 11, -15 ≤ k ≤ 14, -16 ≤ l ≤ 18
Reflection collected/unique	11400/5030[*R*(int)=0.0239]
Completeness to θ	99.8% (θ = 25.00°)
Max. and min. transmission	0.817/1.000
Refinement method	'SHELXL–97(Sheldrick, 1997)'

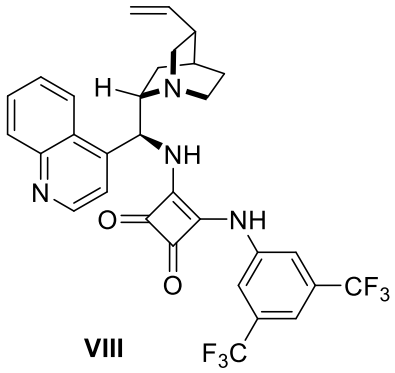
Data/restraints/parameters	5030/0/379
Goodness−of−fit on F^2	1.068
Final *R* indices [*I*>2sigma(*I*)]	R1 = 0.0594, wR2 = 0.1533
R indices (all data)	R1 = 0.0793, wR2 = 0.1689
Largest diff. peak and hole	0.53and -0.58e·Å^{-3}

E. Reaction in presence of benzoic acid:





IV



VIII

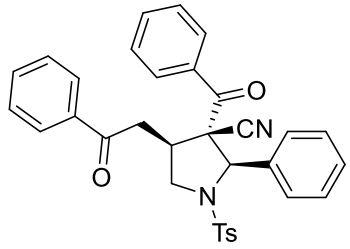
Without acid: 10:1 dr, 45% ee
With acid: 10:1 dr, 39% ee

Without acid: 15:1 dr, 91% ee
With acid: 15:1 dr, 76% ee

We performed the reaction in presence of benzoic acid and absence of benzoic acid using catalyst **IV** and catalyst **VIII**. Product **3a** was isolated with similar diastereomeric ratio with lesser enantioselectivities in presence of acid. This result indicates the bifunctional mode of activation of the catalyst.

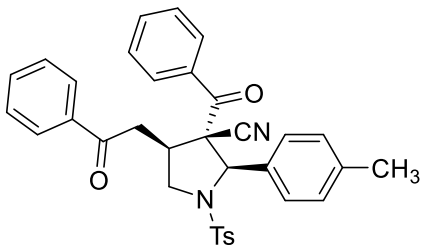
F. Characterization data for compounds (3a-3y):

(2R,3S,4S)-3-benzoyl-4-(2-oxo-2-phenylethyl)-2-phenyl-1-tosylpyrrolidine-3-carbonitrile (3a):



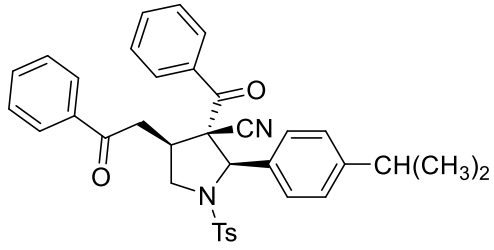
White sticky solid (43.8.4 mg, yield: 80%); **Diastereomeric ratio:** 15:1**; ^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.75 (d, *J* = 7.2 Hz, 2H), 7.60 (d, *J* = 8.3 Hz, 2H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.42 – 7.33 (m, 3H), 7.32 – 7.23 (m, 9H), 7.16 (t, *J* = 7.9 Hz, 2H), 4.88 (s, 1H), 4.32 (dd, *J* = 11.8, 7.3 Hz, 1H), 3.60 – 3.46 (m, 1H), 3.28 – 3.17 (m, 1H), 3.18 – 3.08 (m, 1H), 3.01 (dd, *J* = 17.3, 4.4 Hz, 1H), 2.38 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 196.1, 191.6, 144.6, 136.0, 135.8, 135.3, 134.1, 134.0, 133.6, 130.2, 129.6, 129.5, 129.0, 128.8, 128.5, 128.23, 128.2, 128.1, 117.2, 72.0, 65.0, 53.2, 42.8, 38.2, 21.9; **HRMS (+ESI):** Calc for $C_{33}H_{29}N_2O_4S[M+H]^+$ 549.1843; found 549.1837; The enantiomeric ratio was determined by HPLC analysis using Daicel Chiralpak IB column (80:20 *n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 11.9 min, τ_{major} = 24.9 min); Enantiomeric excess: 91%.

(2R,3S,4S)-3-benzoyl-4-(2-oxo-2-phenylethyl)-2-(p-tolyl)-1-tosylpyrrolidine-3-carbonitrile (3b):



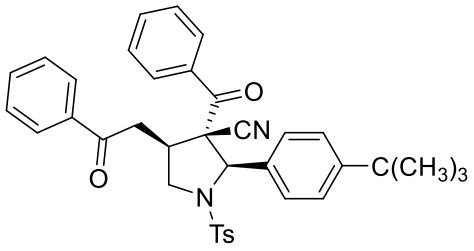
White sticky solid (43.8 mg, yield: 78%); **Diastereomeric ratio:** 12:1; **^{1}H NMR (600 MHz, $CDCl_3$)**: δ 7.84 (d, *J* = 7.2 Hz, 2H), 7.71 (d, *J* = 8.2 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.46 – 7.41 (m, 2H), 7.41 – 7.35 (m, 4H), 7.31 – 7.28 (m, 2H), 7.28 – 7.24 (m, 2H), 7.16 (d, *J* = 7.9 Hz, 2H), 4.93 (s, 1H), 4.39 (dd, *J* = 11.8, 7.3 Hz, 1H), 3.69 – 3.53 (m, 1H), 3.28 (ddd, *J* = 10.3, 9.4, 4.1 Hz, 1H), 3.23 (dd, *J* = 17.3, 9.2 Hz, 1H), 3.11 (dd, *J* = 17.3, 4.2 Hz, 1H), 2.48 (s, 3H), 2.37 (s, 3H); **^{13}C NMR (150 MHz, $CDCl_3$)**:δ 196.2, 191.7, 144.6, 139.5, 135.9, 135.3, 134.0, 133.9, 133.4, 132.7, 130.2, 129.6, 129.5, 129.0, 128.4, 128.2, 128.1, 128.0, 117.3, 71.9, 65.0, 53.2, 42.7, 38.2, 21.9, 21.5; **HRMS (+ESI):** Calc for $C_{34}H_{31}N_2O_4S$ $[M+H]^+$563.1999; found 563.1984; The enantiomeric ratio was determined by HPLC analysis using Daicel Chiralpak IA column (75:25*n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{major} = 21.2 min, τ_{minor}= 24.6 min);Enantiomeric excess: 95%.

(2R,3S,4S)-3-benzoyl-2-(4-isopropylphenyl)-4-(2-oxo-2-phenylethyl)-1-tosylpyrrolidine-3-carbonitrile (3c):



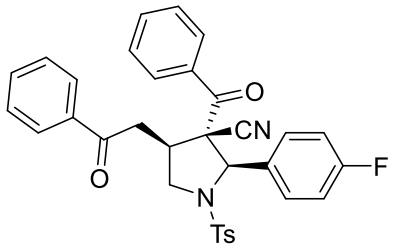
White sticky solid (44.8 mg, yield: 76%); **Diastereomeric ratio:** 15:1; **^{1}H NMR (600 MHz, $CDCl_3$):** δ 7.86 (d, *J* = 8.1 Hz, 2H), 7.66 (d, *J* = 7.9 Hz, 2H), 7.57 (t, *J* = 7.1 Hz, 1H), 7.49 – 7.40 (m, 3H), 7.34 (d, *J* = 7.9 Hz, 2H), 7.28 (t, *J* = 10.8 Hz, 4H), 7.21 (t, *J* = 7.7 Hz, 2H), 7.17 (d, *J* = 7.8 Hz, 2H), 4.85 (s, 1H), 4.44 (dd, *J* = 11.7, 7.7 Hz, 1H), 3.61 (t, *J* = 11.3 Hz, 1H), 3.35 (dt, *J* = 15.7, 11.5 Hz, 1H), 3.22 (dd, *J* = 17.6, 9.3 Hz, 1H), 3.10 (dd, *J* = 17.6, 4.4 Hz, 1H), 2.92 (dt, *J* = 13.7, 6.9 Hz, 1H), 2.46 (s, 3H), 1.26 (d, *J* = 7.1 Hz, 6H); **^{13}C NMR (150MHz, $CDCl_3$)**: δ 196.2, 191.5, 150.5, 144.5, 136.0, 135.2, 134.0, 133.9, 133.6, 132.6, 130.1, 129.7, 129.0, 128.3, 128.3, 128.2, 128.1, 126.8, 117.4, 72.0, 65.0, 53.0, 42.3, 38.3, 34.1, 24.2, 24.1, 21.9; **HRMS (+ESI):** Calc for $C_{36}H_{38}N_3O_4S$ $[M+NH_4]^+$608.2578; found 608.2584; The enantiomeric ratio was determined by HPLC analysis using Daicel Chiralpak IB column (80:20 *n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 7.1 min, τ_{major} = 18.4 min); Enantiomeric excess: 81%.

(2R,3S,4S)-3-benzoyl-2-(4-(tert-butyl)phenyl)-4-(2-oxo-2-phenylethyl)-1-tosylpyrrolidine-3-carbonitrile (3d):



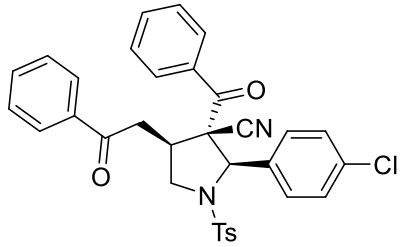
White sticky solid (48.4 mg, yield: 80%); **Diastereomeric ratio:** 15:1; **^{1}H NMR (600 MHz, $CDCl_3$):** δ 7.86 (d, *J* = 7.4 Hz, 2H), 7.65 (d, *J* = 8.2 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.45 (dt, *J* = 15.5, 7.6 Hz, 3H), 7.36 – 7.30 (m, 4H), 7.30 – 7.26 (m, 4H), 7.20 (t, *J*= 7.9 Hz, 2H), 4.83 (s, 1H), 4.45 (dd, *J* = 11.7, 7.7 Hz, 1H), 3.61 (t, *J* = 11.3 Hz, 1H), 3.44 – 3.32 (m, 1H), 3.22 (dd, *J* = 17.6, 9.4 Hz, 1H), 3.11 (dd, *J* = 17.6, 4.5 Hz, 1H), 2.46 (s, 3H), 1.33 (s, 9H); **^{13}C NMR (150 MHz, $CDCl_3$):**δ 196.2, 191.4, 152.7, 144.4, 136.0, 135.2, 134.0, 133.9, 133.6, 132.2, 130.1, 129.7, 129.0, 128.3, 128.2, 128.1, 128.1, 125.7, 117.4, 71.9, 64.9, 53.0, 42.2, 38.3, 34.9, 31.5, 21.9; **HRMS (+ESI):** Calc for $C_{37}H_{38}N_2OS$ $[M+H]^+$605.2469; found 605.2460; The enantiomeric ratio was determined by HPLC analysis using Daicel Chiralpak IB column (90:10 *n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 14.9 min, τ_{major} = 37.7 min); Enantiomeric excess: 95%.

(2R,3S,4S)-3-benzoyl-2-(4-fluorophenyl)-4-(2-oxo-2-phenylethyl)-1-tosylpyrrolidine-3-carbonitrile (3e):



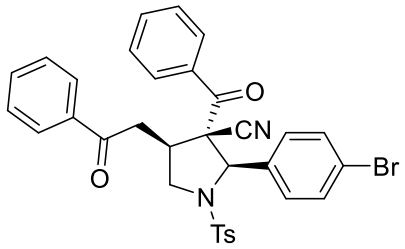
White sticky solid (46.4 mg, yield: 82%); **Diastereomeric ratio:** 16:1; **^{1}H NMR (600 MHz, $CDCl_3$):** δ 7.84 (d, *J* = 7.6 Hz, 2H), 7.70 (d, *J* = 8.2 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.52 (d, *J* = 7.6 Hz, 1H), 7.47 – 7.42 (m, 4H), 7.38 (t, *J* = 7.0 Hz, 4H), 7.30 (t, *J* = 7.9 Hz, 2H), 7.04 (t, *J* = 8.5 Hz, 2H), 4.97 (s, 1H), 4.40 (dd, *J* = 11.8, 7.2 Hz, 1H), 3.65 – 3.55 (m, 1H), 3.31 – 3.26 (m, 1H), 3.26 – 3.20 (m, 1H), 3.12 (dd, *J* = 17.0, 4.0 Hz, 1H), 2.48 (s, 3H); **^{13}C NMR (150 MHz, $CDCl_3$):**δ 196.0, 191.3, 164.2, 162.6, 144.8, 135.9, 135.3, 134.3**,** 134.0, 133.3, 131.7, 131.6, 130.2, 130.1, 130.0, 129.5, 129.0, 128.6, 128.2, 128.1, 117.2, 115.9, 115.8, 71.3, 64.9, 53.1, 42.8, 38.2, 21.9; **HRMS (+ESI):** Calc for $C_{33}H_{28}FN_2O_4S$ $[M+H]^+$567.1748; found 567.1736; The enantiomeric ratio was determined by HPLC analysis using Phenomenex Lux C1 column (75:25*n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 11.3 min, τ_{major} = 42.9 min); Enantiomeric excess: 83%.

(2R,3S,4S)-3-benzoyl-2-(4-chlorophenyl)-4-(2-oxo-2-phenylethyl)-1-tosylpyrrolidine-3-carbonitrile (3f):



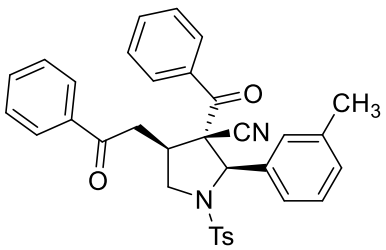
White sticky solid (46.6 mg, yield: 80%); **Diastereomeric ratio:** 15:1; **^{1}H NMR (600 MHz, $CDCl_3$):** δ 7.81 (d, *J* = 8.6 Hz, 2H), 7.70 (d, *J* = 8.2 Hz, 2H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.46 – 7.31 (m, 11H), 7.28 (t, *J* = 3.8 Hz, 2H), 4.96 (s, 1H), 4.42 (dd, *J* = 11.8, 7.5 Hz, 1H), 3.62 (t, *J* = 11.3 Hz, 1H), 3.32 (ddd, *J* = 15.6, 10.0, 4.7 Hz, 1H), 3.20 (dd, *J* = 17.7, 9.1 Hz, 1H), 3.09 (dd, *J* = 17.7, 4.6 Hz, 1H), 2.50 (s, 3H); **^{13}C NMR (150 MHz, $CDCl_3$)**: δ 195.0, 191.4, 144.7, 140.5, 135.6, 135.2, 134.2, 134.1, 133.5, 130.2, 129.7, 129.6, 129.6, 129.3, 128.8, 128.5, 128.3, 128.1, 117.2, 72.0, 64.9, 53.1, 42.7, 38.2, 21.9; **HRMS (+ESI): HRMS (+ESI):** Calc for $C_{33}H_{28}ClN_2O_4S$ $[M+H]^+$583.1453; found 583.1444; The enantiomeric ratio was determined by HPLC analysis using Phenomenex Lux C1 column (70:30 *n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 12.5 min, τ_{major} = 36.5 min); Enantiomeric excess: 82%.

(2R,3S,4S)-3-benzoyl-2-(4-bromophenyl)-4-(2-oxo-2-phenylethyl)-1-tosylpyrrolidine-3-carbonitrile (3g):



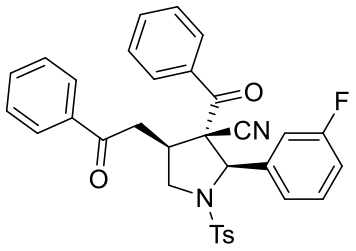
White sticky solid (48.3 mg, yield: 77%); **Diastereomeric ratio:** 15:1; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.72 (d, *J* = 7.3 Hz, 2H), 7.58 (d, *J* = 8.2 Hz, 2H), 7.46 (t, *J* = 7.4 Hz, 1H), 7.40 (d, *J* = 7.4 Hz, 1H), 7.33 (dd, *J* = 18.1, 8.1 Hz, 6H), 7.27 (d, *J* = 8.1 Hz, 2H), 7.20 (t, *J* = 7.9 Hz, 2H), 7.16 (d, *J* = 7.0 Hz, 2H), 4.88 (s, 1H), 4.28 (dd, *J* = 11.8, 6.9 Hz, 1H), 3.56 – 3.42 (m, 1H), 3.21 – 2.95 (m, 3H), 2.37 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):**δ 196.0, 191.2, 144.9, 135.9, 135.3, 135.0, 134.3, 134.0, 133.4, 131.9, 130.3, 129.8, 129.5, 129.0, 128.6, 128.2, 128.1, 123.7, 117.1, 71.2, 64.7, 53.2, 43.0, 38.1, 21.9; **HRMS (+ESI):** Calc for $C_{33}H_{28}BrN_2O_4S$ $[M+H]^+$627.0948; found 627.0944; The enantiomeric ratio was determined by HPLC analysis using Phenomenex column (75:25*n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 15.3 min, τ_{major} = 46.6 min);Enantiomeric excess: 84%.

(2R,3S,4S)-3-benzoyl-4-(2-oxo-2-phenylethyl)-2-(m-tolyl)-1-tosylpyrrolidine-3-carbonitrile (3h):



White sticky solid (44.4 mg, yield: 79%); **Diastereomeric ratio:** 15:1;**^{1}H NMR (600 MHz, $CDCl_3$):** δ 7.85 (d, *J* = 7.3 Hz, 2H), 7.70 (d, *J* = 8.2 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.38 (dd, *J* = 16.5, 7.7 Hz, 4H), 7.28 – 7.22 (m, 3H), 7.18 (d, *J* = 7.1 Hz, 2H), 7.12 (s, 1H), 4.95 (s, 1H), 4.44 (dd, *J* = 11.8, 7.4 Hz, 1H), 3.60 (t, *J* = 11.3 Hz, 1H), 3.30 (ddd, *J* = 11.1, 9.6, 6.9 Hz, 1H), 3.22 (dd, *J* = 17.6, 9.3 Hz, 1H), 3.11 (dd, *J* = 17.5, 4.5 Hz, 1H), 2.47 (s, 3H), 2.27 (s, 3H); **^{13}C NMR (150 MHz, $CDCl_3$)**: δ 196.2, 191.7, 144.5, 138.4, 136.0, 135.6, 135.3, 134.1, 134.0, 133.7, 130.4, 130.1, 129.6, 129.0, 128.8, 128.7, 128.4, 128.2, 128.1, 125.3, 117.2, 72.0, 65.0, 53.1, 42.8, 38.2, 21.9, 21.6.**HRMS (+ESI):** Calc for $C_{34}H_{31}N_2O_4S$ $[M+H]^+$563.1999; found 563.1980; The enantiomeric ratio was determined by HPLC analysis using Daicel Chiralpak IB column (Initially polarity was 92:8 *n*-Hexane/2-PrOH and at 35.798 min polarity was increased to 75:25 *n*- Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 21.3 min, τ_{major} = 48.4 min); Enantiomeric excess: 96%.

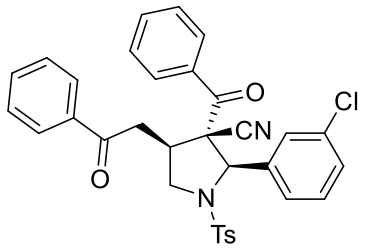
(2R,3S,4S)-3-benzoyl-2-(3-fluorophenyl)-4-(2-oxo-2-phenylethyl)-1-tosylpyrrolidine-3-carbonitrile (3i):



White sticky solid (45.9 mg, yield: 81%); **Diastereomeric ratio:** 15:1; **^{1}H NMR (600 MHz, $CDCl_3$)**: δ 7.84 (d, *J* = 7.3 Hz, 2H), 7.72 (d, *J* = 8.2 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.54 – 7.50 (m, 1H), 7.48 – 7.42 (m, 4H), 7.39 (d, *J* = 8.1 Hz, 2H), 7.31 (t, *J* = 7.9 Hz, 3H), 7.18 – 7.11 (m, 2H), 7.08 (t, *J* = 8.4 Hz, 1H), 5.04 (s, 1H), 4.40 (dd, *J* = 11.9, 6.9 Hz, 1H), 3.62 – 3.55 (m, 1H), 3.25 (dd, *J* = 6.1, 3.4 Hz, 1H), 3.23 (t, *J* = 7.0 Hz, 1H), 3.13 (t, *J* = 10.7 Hz, 1H), 2.49 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 196.0, 191.3, 163.6, 162.0, 144.9, 138.5 (d, *J* = 5 Hz), 135.9, 135.3, 134.3, 134.1, 133.3, 130.3, 129.5, 129.0, 128.6, 128.2 (d, *J* = 5 Hz), 123.8 (d, *J* = 2 Hz), 117.0, 116.7, 116.5, 115.4, 115.2, 71.2, 64.8, 53.2, 43.1, 38.1, 21.9; **HRMS (+ESI):** Calc for $C_{33}H_{28}FN_2O_4S$ $[M+H]^+$567.1748; found 567.1735; The enantiomeric ratio was determined by HPLC analysis using Daicel Chiralpak IB column (Initially the polarity was 93:7 *n*-Hexane/2-

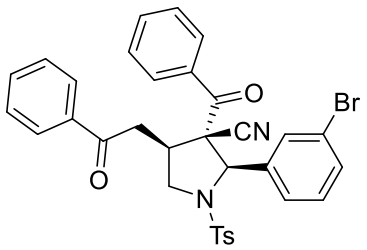
PrOH and at 32.984 min the polarity was increased to 70:30 *n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C 25 °C, 254 nm, τ_{minor} = 26.7 min, τ_{major} = 45.8 min); Enantiomeric excess: 98%.

(2R,3S,4S)-3-benzoyl-2-(3-chlorophenyl)-4-(2-oxo-2-phenylethyl)-1-tosylpyrrolidine-3-carbonitrile (3j):



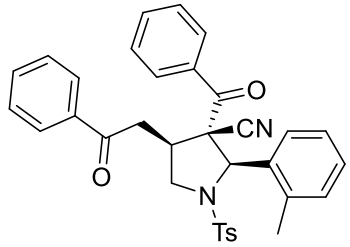
White sticky solid (46.6 mg, yield: 80%); **Diastereomeric ratio:** 15:1; **^{1}H NMR (600 MHz, $CDCl_3$):** δ 7.84 (d, *J* = 7.3 Hz, 2H), 7.70 (d, *J* = 8.2 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.53 (d, *J* = 7.4 Hz, 1H), 7.49 (d, *J* = 7.4 Hz, 2H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.35 (dd, *J* = 8.9, 2.1 Hz, 1H), 7.31 (dd, *J* = 15.9, 7.5 Hz, 5H), 5.03 (s, 1H), 4.42 (dd, *J* = 11.8, 7.1 Hz, 1H), 3.65 – 3.54 (m, 1H), 3.31 – 3.25 (m, 1H), 3.23 (t, *J* = 11.3 Hz, 1H), 3.14 (dd, *J* = 16.7, 3.7 Hz, 1H), 2.48 (s, 3H); **^{13}C NMR (150 MHz, $CDCl_3$):** δ 196.0, 191.1, 144.9, 138.0, 135.9, 135.2, 134.7, 134.3, 134.1, 133.4, 130.3, 130.1, 129.7, 129.5, 129.0, 128.6, 128.3, 128.2, 128.1, 126.4, 116.9, 71.1, 64.7, 53.1, 43.1, 38.1, 21.9; **HRMS (+ESI):** Calc for $C_{33}H_{28}ClN_2O_4S$ $[M+H]^+$583.1453; found 583.1458; The enantiomeric ratio was determined by HPLC analysis using Daicel Chiralpak IB column (Initially the polarity was 93:7 *n*-Hexane/2-PrOH and at 34.039 min the polarity was increased to 70:30 *n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 27.4 min, τ_{major} = 51.4 min); Enantiomeric excess: 95%.

(2R,3S,4S)-3-benzoyl-2-(3-bromophenyl)-4-(2-oxo-2-phenylethyl)-1-tosylpyrrolidine-3-carbonitrile (3k):



White sticky solid (47.7 mg, yield: 76%); **Diastereomeric ratio:** 15:1; **^{1}H NMR (600 MHz, $CDCl_3$):** δ 7.87 – 7.82 (m, 2H), 7.70 (d, *J* = 8.2 Hz, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.53 (d, *J* = 7.4 Hz, 1H), 7.51 – 7.48 (m, 3H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.42 – 7.34 (m, 4H), 7.32 (dd, *J* = 8.3, 7.6 Hz, 2H), 7.23 (t, *J* = 7.8 Hz, 1H), 5.03 (s, 1H), 4.42 (dd, *J* = 11.8, 7.1 Hz, 1H), 3.62 – 3.54 (m, 1H), 3.29 (dd, *J* = 10.1, 5.6 Hz, 1H), 3.22 (d, *J* = 9.0 Hz, 1H), 3.14 (dd, *J* = 17.0, 4.1 Hz, 1H), 2.48 (s, 3H); **^{13}C NMR (150 MHz, $CDCl_3$):**δ 196.0, 191.1, 144.9, 138.2, 135.9, 135.2, 134.4, 134.1, 133.5, 132.6, 131.1, 130.3, 130.2, 129.5, 129.0, 128.7, 128.2, 128.1, 126.9, 122.8, 116.9, 70.9, 64.7, 53.1, 43.1, 38.1, 21.9.**HRMS (+ESI):** Calc for $C_{33}H_{28}BrN_2O_4S$ $[M+H]^+$627.0948; found 627.0948; The enantiomeric ratio was determined by HPLC analysis using Daicel Chiralpak IB column (Initially the polarity was 93:7 *n*-Hexane/2-PrOH and at 35.047 min the polarity was increased to 70:30 *n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 29.0 min, τ_{major} = 54.9 min); Enantiomeric excess: 91%.

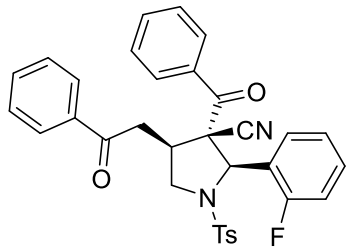
(2R,3S,4S)-3-benzoyl-4-(2-oxo-2-phenylethyl)-2-(o-tolyl)-1-tosylpyrrolidine-3-carbonitrile (3l):



White sticky solid (42.7 mg, yield: 76%); **Diastereomeric ratio:**15:1; **^{1}H NMR (600 MHz, $CDCl_3$)**: δ 7.88 (d, *J* = 7.4 Hz, 2H), 7.81 (d, *J* = 7.6 Hz, 1H), 7.66 (d, *J* = 8.1 Hz, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 2H), 7.38 (d, *J* = 7.6 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 3H), 7.28 (t, *J* = 6.9 Hz, 1H), 7.26 – 7.21 (m, 2H), 7.02 (d, *J* = 7.5 Hz, 1H), 5.30 (d, *J* = 5.7 Hz, 1H), 4.46 (dd, *J* = 11.6, 7.2 Hz, 1H), 3.59 (t, *J* = 11.1 Hz, 1H), 3.46 (td, *J* = 10.8, 4.1 Hz, 1H), 3.24 (dd, *J* = 17.6, 9.6 Hz, 1H), 3.14 (dd, *J* = 17.5, 4.1 Hz, 1H), 2.46 (s, 3H), 1.94 (s, 3H); **^{13}C NMR (150 MHz, $CDCl_3$)**: δ 196.2, 191.3, 144.5, 136.1, 136.0, 134.7, 134.4, 134.2, 134.0, 130.6, 130.1, 129.5, 129.2, 129.0, 128.9, 128.5, 128.3, 128.0, 126.7, 117.4, 66.7, 64.3, 52.8, 43.0, 38.2, 21.9, 19.6; **HRMS (+ESI):** Calc for $C_{34}H_{31}N_2O_4S$ $[M+H]^+$563.1999; found 563.1995; The enantiomeric ratio was determined by HPLC analysis using Daicel Chiralpak IA column (80:20

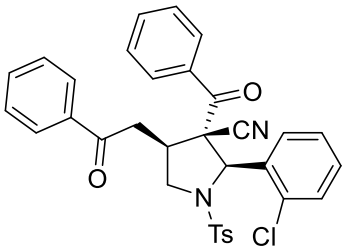
n-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor}= 10.5 min, τ_{major} = 23.6 min); Enantiomeric excess: 87%.

(2S,3S,4S)-3-benzoyl-2-(2-fluorophenyl)-4-(2-oxo-2-phenylethyl)-1-tosylpyrrolidine-3-carbonitrile (3m):



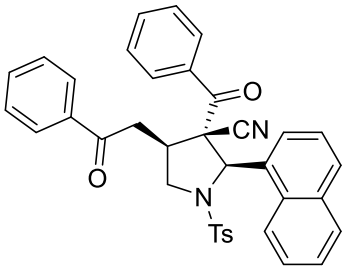
White sticky solid (42.4 mg, yield: 75%); **Diastereomeric ratio:** 15:1; **^{1}H NMR (600 MHz, $CDCl_3$)**: δ 7.85 (d, *J* = 7.3 Hz, 2H), 7.81 (d, *J* = 7.8 Hz, 2H), 7.58 (t, *J* = 6.8 Hz, 3H), 7.53 (t, *J* = 7.4 Hz, 2H), 7.44 (dd, *J* = 13.3, 5.7 Hz, 4H), 7.40 – 7.37 (m, 1H), 7.31 (t, *J* = 7.9 Hz, 3H), 6.94 (t, *J* = 9.2 Hz, 1H), 5.40 (s, 1H), 4.38 (dd, *J* = 12.1, 6.7 Hz, 1H), 3.59 (dd, *J* = 12.0, 10.3 Hz, 1H), 3.24 – 3.08 (m, 3H), 2.49 (s, 3H); **^{13}C NMR (150 MHz, $CDCl_3$)**: δ 196.01, 190.57, 161.00, 159.36, 144.86, 135.92, 134.91, 134.22, 133.99, 131.04, 130.99, 130.34, 129.35, 128.97, 128.56, 128.29, 128.19, 124.96, 124.27, 124.19, 117.07, 77.44, 77.23, 77.02, 63.88, 53.03, 43.49, 38.01, 21.94; **HRMS (+ESI):** Calc for $C_{33}H_{28}FN_2O_4S$ $[M+NH_4]^+$ 584.2014; found 584.2019; The enantiomeric ratio was determined by HPLC analysis using Daicel Chiralpak IA column (85:15*n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 26.5 min, τ_{major} = 31.0 min); Enantiomeric excess: 96%.

(2S,3S,4S)-3-benzoyl-2-(2-chlorophenyl)-4-(2-oxo-2-phenylethyl)-1-tosylpyrrolidine-3-carbonitrile (3n):



White sticky solid (43.1 mg, yield: 74%); **Diastereomeric ratio:** 15:1; **^{1}H NMR (600 MHz, $CDCl_3$)**: δ 8.05 (d, *J* = 9.2 Hz, 1H), 7.85 (dd, *J* = 14.3, 7.7 Hz, 4H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.54 – 7.50 (m, 2H), 7.50 – 7.46 (m, 3H), 7.45 (t, *J* = 8.0 Hz, 3H), 7.37 (t, *J* = 7.7 Hz, 1H), 7.28 (dd, *J* = 10.5, 5.4 Hz, 3H), 5.53 (s, 1H), 4.34 (dd, *J* = 12.1, 6.4 Hz, 1H), 3.62 (dd, *J* = 11.9, 9.6 Hz, 1H), 3.21 (dd, *J* = 18.3, 6.8 Hz, 2H), 3.13 (t, *J* = 10.9 Hz, 1H), 2.50 (s, 3H); **^{13}C NMR (150 MHz, $CDCl_3$):**δ 196.1, 190.3, 144.9, 136.0, 134.8, 134.7, 134.4, 134.0, 133.6, 132.5, 130.7, 130.6, 130.3, 129.5, 129.4, 129.0, 128.52, 128.50, 128.2, 127.7, 117.1, 66.7, 63.6, 53.0, 43.3, 38.1, 22.0; **HRMS (+ESI):** Calc for $C_{33}H_{28}ClN_2O_4S$ $[M+H]^+$ 583.1453; found 583.1453; The enantiomeric ratio was determined by HPLC analysis using Daicel Phenomenex Lux C1 column (85:15*n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 17.9 min, τ_{major} = 39.1 min); Enantiomeric excess: 96%.

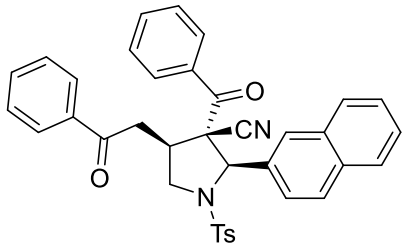
(2R,3S,4S)-3-benzoyl-2-(naphthalen-1-yl)-4-(2-oxo-2-phenylethyl)-1-tosylpyrrolidine-3-carbonitrile (3o):



White sticky solid (47.9 mg, yield: 80%); **Diastereomeric ratio:** 16:1; **^{1}H NMR (600 MHz, $CDCl_3$):** δ 8.17 (d, *J* = 7.2 Hz, 1H), 7.91 (d, *J* = 8.1 Hz, 1H), 7.85 (dd, *J* = 19.8, 8.3 Hz, 3H), 7.74 (d, *J* = 8.2 Hz, 2H), 7.66 (t, *J* = 7.7 Hz, 1H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.46 (dd, *J* = 13.6, 5.8 Hz, 3H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.32 (dd, *J* = 16.0, 8.1 Hz, 2H), 7.24 – 7.19 (m, 1H), 7.18 (d, *J* = 7.5 Hz, 2H), 7.04 (t, *J* = 7.9 Hz, 2H), 5.99 (s, 1H), 4.47 (dd, *J* = 11.9, 7.1 Hz, 1H), 3.70 (dd, *J*

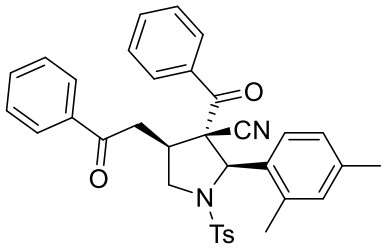
= 11.8, 10.4 Hz, 1H), 3.45 – 3.37 (m, 1H), 3.29 (dd, *J* = 17.7, 9.7 Hz, 1H), 3.14 (dd, *J* = 17.7, 4.0 Hz, 1H), 2.50 (s, 3H); **^{13}C NMR (150 MHz, $CDCl_3$):** δ 196.1, 192.2, 144.7, 136.0, 134.8, 134.0, 133.6, 133.3, 132.1, 131.0, 130.2, 129.9, 129.4, 129.2, 129.0, 128.3, 128.2, 128.1, 127.4, 126.9, 125.8, 125.7, 121.7, 117.3, 66.3, 65.1, 53.2, 44.0, 38.2, 22.0; **HRMS (+ESI):** Calc for $C_{37}H_{31}N_2O_4S$ $[M+H]^+$ 599.1999; found 599.197; The enantiomeric ratio was determined by HPLC analysis using Daicel Chiralpak IB column (85:15*n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 12.9 min, τ_{major} = 25.4 min); Enantiomeric excess: 87%.

(2R,3S,4S)-3-benzoyl-2-(naphthalen-2-yl)-4-(2-oxo-2-phenylethyl)-1-tosylpyrrolidine-3-carbonitrile (3p):



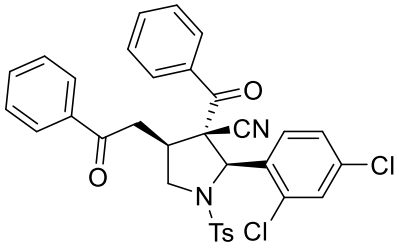
White sticky solid (48.4 mg, yield: 81%); **Diastereomeric ratio:** 16:1; **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.86 (d, *J* = 8.5 Hz, 4H), 7.70 (d, *J* = 8.2 Hz, 4H), 7.58 (dd, *J* = 13.6, 6.4 Hz, 3H), 7.51 – 7.48 (m, 2H), 7.46 – 7.42 (m, 3H), 7.42 – 7.38 (m, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.15 (t, *J* = 7.9 Hz, 2H), 5.20 (s, 1H), 4.49 (dd, *J* = 11.8, 7.4 Hz, 1H), 3.74 – 3.63 (m, 1H), 3.41 – 3.32 (m, 1H), 3.30 – 3.25 (m, 1H), 3.15 (dd, *J* = 17.7, 4.6 Hz, 1H), 2.44 (s, 3H); **^{13}CNMR (150 MHz, $CDCl_3$)**δ 196.2, 191.7, 144.6, 136.0, 135.3, 134.1, 134.0, 133.9, 133.7, 133.2, 133.0, 130.2, 129.5, 129.0, 128.7, 128.5, 128.4, 128.2, 128.1, 128.0, 127.8, 126.9, 126.6, 117.3, 72.0, 65.0, 53.2, 43.0, 38.2, 21.9; **HRMS (+ESI):** Calc for $C_{37}H_{31}N_2O_4S$ $[M+H]^+$599.1999; found 599.199; The enantiomeric ratio was determined by HPLC analysis using Daicel Chiralpak IB column (85:15*n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 14.7 min, τ_{major} = 32.9 min); Enantiomeric excess: 88%.

(2R,3S,4S)-3-benzoyl-2-(2,4-dimethylphenyl)-4-(2-oxo-2-phenylethyl)-1-tosylpyrrolidine-3-carbonitrile (3q):



White sticky solid (44.9 mg, yield: 78%); **Diastereomeric ratio:** 15:1; **^{1}H NMR (600 MHz, $CDCl_3$):** δ 7.88 (d, *J* = 7.4 Hz, 2H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 8.1 Hz, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.51 (d, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 2H), 7.40 (d, *J* = 7.6 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.26 (dd, *J* = 9.1, 6.7 Hz, 2H), 7.15 (d, *J* = 7.7 Hz, 1H), 6.84 (s, 1H), 5.25 (s, 1H), 4.43 (dd, *J* = 11.7, 7.2 Hz, 1H), 3.58 (t, *J* = 11.2 Hz, 1H), 3.43 (dd, *J* = 20.6, 10.7 Hz, 1H), 3.23 (dd, *J* = 17.6, 9.6 Hz, 1H), 3.12 (dd, *J* = 17.5, 4.1 Hz, 1H), 2.47 (s, 3H), 2.34 (s, 3H), 1.89 (s, 3H); **^{13}C NMR (151 MHz, $CDCl_3$):**δ 196.3, 191.5, 144.4, 138.9, 136.0, 135.8, 134.8, 134.4, 134.1, 133.9, 131.3, 130.0, 129.5, 129.0, 128.5, 128.3, 128.1, 127.6, 117.5, 66.7, 64.5, 52.8, 43.0, 38.2, 21.9, 21.4, 19.5.**HRMS (+ESI):** Calc for $C_{35}H_{33}N_2O_4S$ $[M+H]^+$577.2156; found 577.2134; The enantiomeric ratio was determined by HPLC analysis using Merck OD column (85:15*n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 14.4 min, τ_{major} = 49.5 min); Enantiomeric excess: 91%.

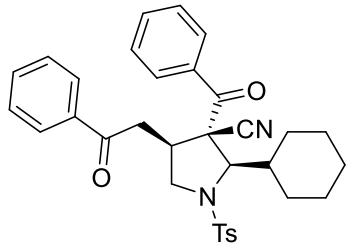
(2S,3S,4S)-3-benzoyl-2-(2,4-dichlorophenyl)-4-(2-oxo-2-phenylethyl)-1-tosylpyrrolidine-3-carbonitrile (3r):



White sticky solid (46.9 mg, yield: 76%); **Diastereomeric ratio:** 7:1; **^{1}H NMR (600 MHz, $CDCl_3$):** δ 7.97 (d, *J* = 8.5 Hz, 1H), 7.86 (d, *J* = 7.3 Hz, 2H), 7.82 (d, *J* = 8.2 Hz, 2H), 7.55 (dd, *J* = 12.9, 8.0 Hz, 4H), 7.50 – 7.44 (m, 5H), 7.33 (dd, *J* = 8.3, 7.5 Hz, 2H), 7.30 (d, *J* = 2.1 Hz, 1H), 5.49 (s, 1H), 4.33 – 4.27 (m, 1H), 3.62 – 3.56 (m, 1H), 3.21 (dd, *J* = 12.1, 7.6 Hz, 2H), 3.14 (t, *J* = 10.9 Hz, 1H), 2.51 (s, 3H); **^{13}C NMR (150 MHz, $CDCl_3$)**:δ 196.0, 190.2, 145.1, 135.9, 135.8,

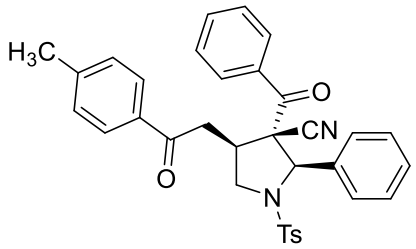
135.0, 134.7, 134.6, 134.2, 134.1, 133.6, 132.3, 131.6, 130.4, 129.4, 129.3, 129.0, 128.7, 128.5, 128.2, 117.0, 66.4, 63.4, 53.0, 43.4, 38.1, 22.0; **HRMS (+ESI):** Calc for $C_{33}H_{27}Cl_2N_2O_4S$ $[M+H]^+$617.1063; found 617.1073; The enantiomeric ratio was determined by HPLC analysis using Daicel Chiralpak IB column (90:10 *n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 15.7 min, τ_{major} = 34.6 min); Enantiomeric excess: 99%.

(2R,3S,4S)-3-benzoyl-2-cyclohexyl-4-(2-oxo-2-phenylethyl)-1-tosylpyrrolidine-3-carbonitrile (3s):



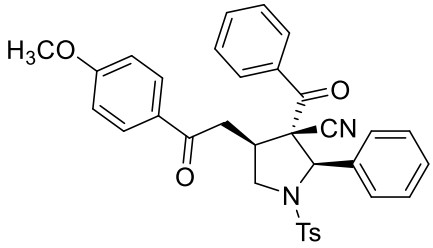
White sticky solid (39.9 mg, yield: 72%); **Diastereomeric ratio:**16:1; **^{1}H NMR (600 MHz, $CDCl_3$):** δ 7.87 (d, *J* = 7.4 Hz, 2H), 7.83 (d, *J* = 7.3 Hz, 2H), 7.77 (d, *J* = 8.3 Hz, 2H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 2H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 4.36 (d, *J* = 6.5 Hz, 1H), 4.19 (dd, *J* = 13.1, 6.7 Hz, 1H), 3.26 (dd, *J* = 17.6, 4.8 Hz, 1H), 3.19 – 3.08 (m, 2H), 2.92 – 2.79 (m, 1H), 2.44 (s, 3H), 2.12 – 2.03 (m, 1H), 2.01 (d, *J* = 12.3 Hz, 1H), 1.85 (d, *J* = 12.6 Hz, 1H), 1.74 (d, *J* = 10.9 Hz, 1H), 1.68 (d, *J* = 12.7 Hz, 1H), 1.43 – 1.27 (m, 5H), 1.19 (d, *J* = 16.0 Hz, 1H); **^{13}C NMR (150 MHz,$CDCl_3$):**δ 196.3, 192.0, 144.4, 136.0, 135.2, 135.0, 133.9, 133.8, 130.1, 129.2, 129.0, 128.9, 128.3, 128.2, 117.8, 71.3, 62.5, 54.0, 43.12, 43.11, 38.6, 31.6, 29.8, 26.5, 26.4, 26.1, 21.9; **HRMS (+ESI):** Calc for $C_{33}H_{35}N_2O_4S$ $[M+H]^+$555.2312; found 555.2322; The enantiomeric ratio was determined by HPLC analysis using Daicel Chiralpak IB column (80:20 *n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 7.1 min, τ_{major} = 18.4 min); Enantiomeric excess: 78%.

(2R,3S,4S)-3-benzoyl-4-(2-oxo-2-(p-tolyl)ethyl)-2-phenyl-1-tosylpyrrolidine-3-carbonitrile (3t):



White sticky solid (45.0 mg, yield: 80%); Diastereomeric ratio: 15:1; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.72 (dd, *J* = 16.1, 8.2 Hz, 4H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.43 – 7.34 (m, 9H), 7.26 (dd, *J* = 8.8, 7.1 Hz, 4H), 4.99 (s, 1H), 4.40 (dd, *J* = 11.8, 7.4 Hz, 1H), 3.67 – 3.56 (m, 1H), 3.30 (dt, *J* = 22.4, 7.6 Hz, 1H), 3.20 (dd, *J* = 17.3, 9.0 Hz, 1H), 3.08 (dd, *J* = 17.3, 4.5 Hz, 1H), 2.47 (s, 3H), 2.39 (s, 3H); **^{13}C NMR (150 MHz, $CDCl_3$)** δ 195.8, 191.7, 145.0, 144.6, 135.8, 135.4, 134.1, 133.5, 133.4, 130.2, 129.7, 129.6, 129.5, 128.8, 128.5, 128.4, 128.2, 128.1, 117.3, 72.1, 65.0, 53.3, 42.9, 38.1, 21.9; **HRMS (+ESI):** Calc for $C_{34}H_{31}N_2O_4S$ $[M+NH4]^+$580.2265; found 580.2276; The enantiomeric ratio was determined by HPLC analysis using Daicel Chiralpak IB column (80:20 *n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 12.0 min, τ_{major} = 16.8 min); Enantiomeric excess: 91%.

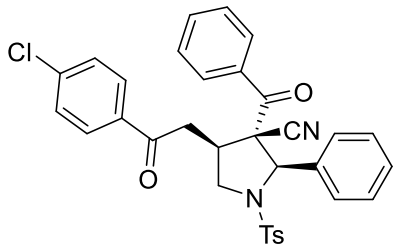
(2R,3S,4S)-3-benzoyl-4-(2-(4-methoxyphenyl)-2-oxoethyl)-2-phenyl-1-tosylpyrrolidine-3-carbonitrile (3u):



White sticky solid (45.7 mg, yield: 79%); **Diastereomeric ratio:** 15:1; **^{1}H NMR (600 MHz, $CDCl_3$):** δ 7.84 (d, *J* = 8.9 Hz, 2H), 7.72 (d, *J* = 8.2 Hz, 2H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.44 – 7.35 (m, 9H), 7.30 – 7.26 (m, 2H), 6.91 (d, *J* = 8.9 Hz, 2H), 5.00 (s, 1H), 4.41 (dd, *J* = 11.8, 7.5 Hz, 1H), 3.87 (s, 3H), 3.63 (t, *J* = 11.3 Hz, 1H), 3.34 – 3.26 (m, 1H), 3.20 (dd, *J* = 17.4, 9.2 Hz, 1H), 3.08 (dd, *J* = 17.4, 4.7 Hz, 1H), 2.49 (s, 3H); **^{13}C NMR (150 MHz,$CDCl_3$):** δ 194.6, 191.6, 164.1, 144.6, 135.8, 135.4, 134.0, 133.4, 130.6, 130.2, 129.9, 129.6, 1295, 129.0, 128.8, 128.4, .128.2, 128.1, 126.6, 117.3, 114.1, 72.0 65.0, 55.7, 53.3, 43.0, 37.8, 21.9; **HRMS (+ESI):** Calc

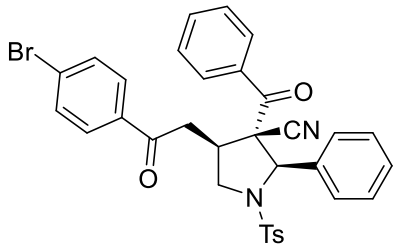
for $C_{34}H_{31}N_2O_5S$ $[M+NH4]^+$ 579.1948; found 579.1955; The enantiomeric ratio was determined by HPLC analysis using Daicel Chiralpak IB column (70:30 *n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 12.8 min, τ_{major} = 13.9 min); Enantiomeric excess: 57%.

(2R,3S,4S)-3-benzoyl-4-(2-(4-chlorophenyl)-2-oxoethyl)-2-phenyl-1-tosylpyrrolidine-3-carbonitrile (3v):



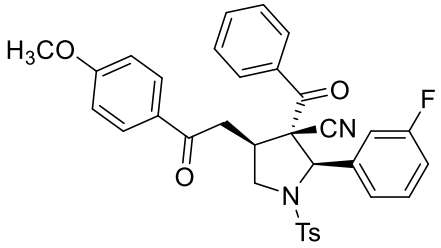
White sticky solid (46.6 mg, yield: 80%); **Diastereomeric ratio:** 15:1; **^{1}H NMR (600 MHz, $CDCl_3$)**: δ 7.81 (d, *J* = 8.6 Hz, 2H), 7.71 (d, *J* = 8.2 Hz, 2H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.46 – 7.34 (m, 11H), 7.31 – 7.26 (m, 2H), 4.96 (s, 1H), 4.42 (dd, *J* = 11.8, 7.5 Hz, 1H), 3.62 (t, *J* = 11.3 Hz, 1H), 3.32 (ddd, *J* = 16.3, 10.5, 4.7 Hz, 1H), 3.20 (dd, *J* = 17.7, 9.1 Hz, 1H), 3.10 (dd, *J* = 17.7, 4.7 Hz, 1H), 2.50 (s, 3H); **^{13}C NMR (150 MHz, $CDCl_3$)**: δ 195.0, 191.4, 144.7, 140.5, 135.6, 135.2, 134.2, 134.1, 133.4, 130.2, 129.7, 129.6, 129.6, 129.3, 128.8, 128.5, 128.2, 128.1, 117.2, 72.0, 64.8, 53.1, 42.7, 38.2, 21.9; **HRMS (+ESI):** Calc for $C_{33}H_{28}ClN_2O_4S$ $[M+H]^+$583.1453; found 583.1456; The enantiomeric ratio was determined by HPLC analysis using Daicel Chiralpak IB column (80:20 *n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 15.5 min, τ_{major} = 16.9 min); Enantiomeric excess: 67%.

(2R,3S,4S)-3-benzoyl-4-(2-(4-bromophenyl)-2-oxoethyl)-2-phenyl-1-tosylpyrrolidine-3-carbonitrile (3w):



White sticky solid (48.9 mg, yield: 78%); **Diastereomeric ratio:** 15:1; **^{1}H NMR (600 MHz, $CDCl_3$):** δ 7.71 (dt, *J* = 16.3, 7.1 Hz, 4H), 7.60 (d, *J* = 8.5 Hz, 2H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.45 – 7.32 (m, 9H), 7.29 – 7.26 (m, 2H), 4.96 (s, 1H), 4.42 (dd, *J* = 11.8, 7.5 Hz, 1H), 3.62 (t, *J* = 11.3 Hz, 1H), 3.36 – 3.28 (m, 1H), 3.19 (dd, *J* = 17.7, 9.1 Hz, 1H), 3.09 (dd, *J* = 17.7, 4.7 Hz, 1H), 2.50 (s, 3H); **^{13}C NMR (150 MHz, $CDCl_3$):** δ 195.2, 191.4, 144.7, 135.6, 135.2, 134.6, 134.2, 133.5, 132.3, 130.2, 129.7, 129.6, 129.6, 129.4, 129.3, 128.8, 128.7, 128.5, 128.2, 128.1, 117.2, 72.0, 64.8, 53.1, 42.7, 38.2, 21.9; **HRMS (+ESI):** Calc for $C_{33}H_{28}BrN_2O_4S$ $[M+H]^+$627.0948; found 627.0949; The enantiomeric ratio was determined by HPLC analysis using Daicel Chiralpak IB column (80:20 *n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 17.4 min, τ_{major} = 18.4 min); Enantiomeric excess: 60%.

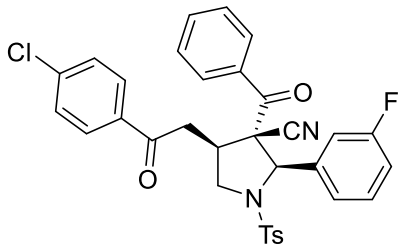
(2R,3S,4S)-3-benzoyl-2-(3-fluorophenyl)-4-(2-(4-methoxyphenyl)-2-oxoethyl)-1-tosylpyrrolidine-3-carbonitrile (3x):



White sticky solid (44.7 mg, yield: 75%); **Diastereomeric ratio:** 7:1; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.81 (d, *J* = 8.9 Hz, 2H), 7.71 (d, *J* = 8.2 Hz, 2H), 7.53 – 7.46 (m, 3H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.30 (t, *J* = 7.9 Hz, 3H), 7.10 (dt, *J* = 17.6, 8.0 Hz, 3H), 6.89 (d, *J* = 8.9 Hz, 2H), 5.07 (s, 1H), 4.37 (dd, *J* = 11.8, 7.1 Hz, 1H), 3.85 (s, 3H), 3.59 (dd, *J* = 11.6, 10.7 Hz, 1H), 3.25 (ddd, *J* = 12.9, 7.3, 3.8 Hz, 1H), 3.21 – 3.03 (m, 2H), 2.48 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 194.4, 191.3, 164.2, 144.8, 138.7 (d, *J* = 7 Hz), 135.4, 134.2, 130.6, 130.2, 129.6, 129.5, 129.2, 128.6, 128.2, 123.8 (d, *J* = 3 Hz), 117.0, 116.6, 116.4, 115.4, 115.2, 114.1, 71.2,

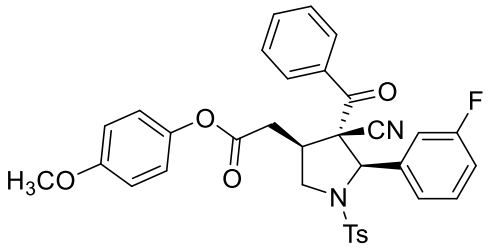
64.9, 55.7, 53.3, 43.4, 37.7, 21.9; **HRMS (+ESI):** Calc for $C_{34}H_{30}FN_2O_5S$ $[M+H]^+$597.1845; found 597.1852; The enantiomeric ratio was determined by HPLC analysis using Daicel Chiralpak IB column (80:20 *n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 19.6 min, τ_{major} = 21.1 min); Enantiomeric excess: 90%.

(2R,3S,4S)-3-benzoyl-4-(2-(4-chlorophenyl)-2-oxoethyl)-2-(3-fluorophenyl)-1-tosylpyrrolidine-3-carbonitrile (3y):



White sticky solid (46.3 mg, yield: 77%); **Diastereomeric ratio:** 10:1; **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.78 (d, *J* = 8.6 Hz, 2H), 7.70 (d, *J* = 8.2 Hz, 2H), 7.51 (d, *J* = 7.4 Hz, 1H), 7.47 (d, *J* = 7.4 Hz, 2H), 7.39 (dd, *J* = 13.4, 8.4 Hz, 4H), 7.30 (t, *J* = 7.9 Hz, 3H), 7.15 – 7.06 (m, 3H), 5.04 (s, 1H), 4.38 (dd, *J* = 11.8, 7.3 Hz, 1H), 3.64 – 3.51 (m, 1H), 3.27 (ddd, *J* = 10.4, 7.7, 4.9 Hz, 1H), 3.22 – 3.06 (m, 2H), 2.48 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 194.9, 191.1, 164.1, 161.6, 144.9, 140.6, 138.5 (d, *J* = 7 Hz), 135.3, 134.3 (d, J = 7 Hz), 133.6, 130.2, 129.6, 129.5, 129.3, 128.6, 128.2, 123.9 (d, *J* = 3 Hz), 117.0, 116.7, 116.5, 115.5, 115.3, 71.2, 64.7, 53.1, 43.0, 38.1, 21.9; **HRMS (+ESI):** Calc for $C_{33}H_{27}ClFN_2O_4S$ $[M+H]^+$ 601.1359; found 601.1361; The enantiomeric ratio was determined by HPLC analysis using Daicel Chiralpak IB column (80:20 *n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 15.2 min, τ_{major} = 16.7 min); Enantiomeric excess: 93%.

G. ***4-methoxyphenyl 2-((3S,4S,5R)-4-benzoyl-4-cyano-5-(3-fluorophenyl)-1-tosylpyrrolidin-3-yl)acetate (4):***



General procedure for the synthesis of compound 4:

To a solution of **3x** (0.1 mmol) in MTBE (4 ml), was added disodium hydrogen phosphate (0.3 mmol) and *m*-CPBA (0.3 mmol). The reaction mixture was stirred at room temperature for 48h. Then the solvent was evaporated and the crude product was purified by column chromatography using 15% ethyl acetate in hexane as the eluent.

White sticky solid (24.5 mg, yield: 40%); **Diastereomeric ratio:** 7:1; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.3 Hz, 2H), 7.53 (t, *J* = 8.1 Hz, 2H), 7.46 (d, *J* = 7.4 Hz, 2H), 7.36 – 7.27 (m, 5H), 7.14 – 7.07 (m, 2H), 6.90 (td, *J* = 9.3, 5.2 Hz, 4H), 5.04 (s, 1H), 4.36 (dd, *J* = 11.8, 7.4 Hz, 1H), 3.80 (s, 3H), 3.68 (t, *J* = 11.4 Hz, 1H), 3.27 – 3.11 (m, 1H), 2.76 (qd, *J* = 16.9, 7.3 Hz, 2H), 2.46 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 191.0, 169.1, 157.8, 144.9, 143.8, 138.3 (d, *J* = 8 Hz), 135.1, 134.5, 133.6, 130.5, 130.4, 130.3, 129.6, 128.7, 128.1, 123.9 (d, *J* = 3 Hz), 122.2, 116.6 (d, *J* = 2 Hz), 115.5, 115.3, 114.8, 71.4, 64.5, 55.8, 52.9, 43.5, 36.9, 21.9; **HRMS (+ESI):** Calc for $C_{34}H_{30}FN_2O_6S$ $[M+H]^+$ 613.1803; found 613.1804; The enantiomeric ratio was determined by HPLC analysis using Phenomenex lux C1 column (88:12 *n*-Hexane/2-PrOH, 1.0 mL/min, 25 °C, 254 nm, τ_{minor} = 77.7min, τ_{major} = 83.8 min); Enantiomeric excess: 90%.

H. References:

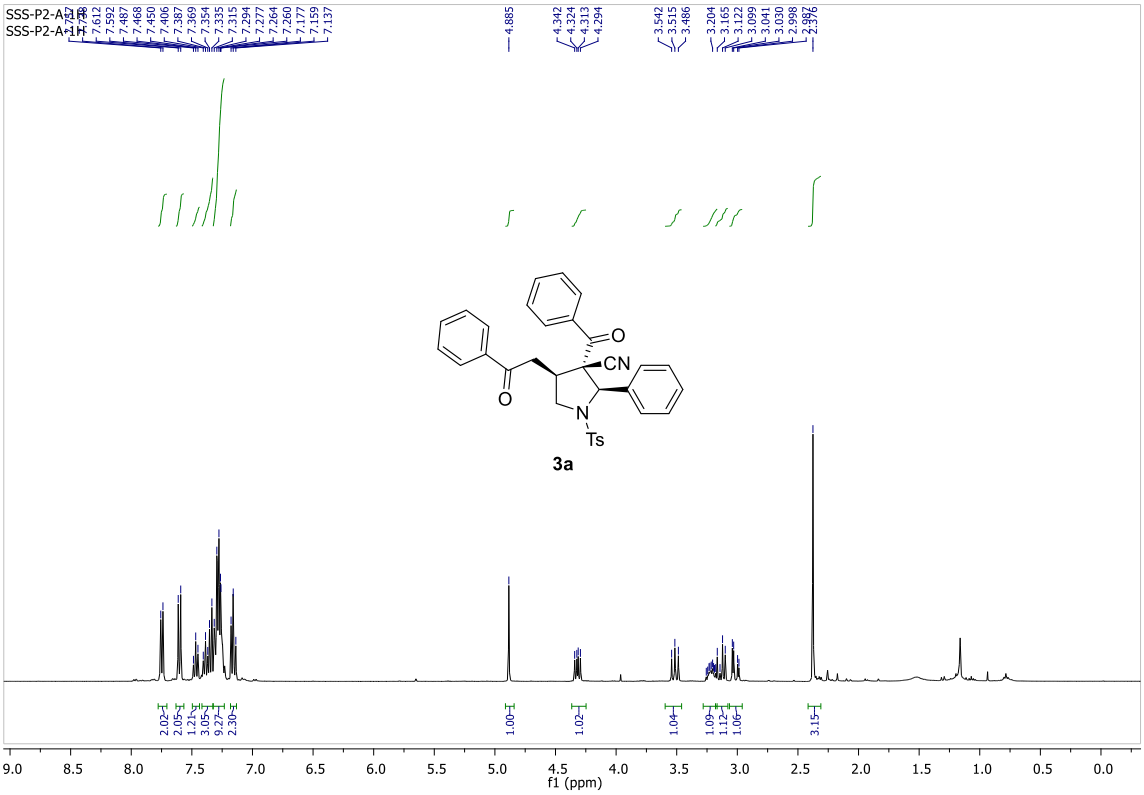
1 (*a*) A. Berkessel, S. Mukherjee, T. N. Muller, F. Cleemann, K. Roland, M. Brandenburg, J.-M. Neudorfl and J. Lex, *Org. Biomol. Chem*., 2006, **4**, 4319; (*b*) B. Vakulya, S. Varga, A. Csámpai and T. Soós, *Org. Lett*., 2005, **7**, 1967; (*c*) M. S. Manna, V. Kumar and S. Mukherjee, *Chem. Commun*., 2012, **48**, 5193; (*d*) C. B. Tripathi, S. Kayal, and S. Mukherjee, *Org. Lett*., 2012, **14**, 3296; (*e*) Y. Gao, Q. Ren, L. Wang and J. Wang, *Chem. Eur. J.*, 2010, **16**, 13068.

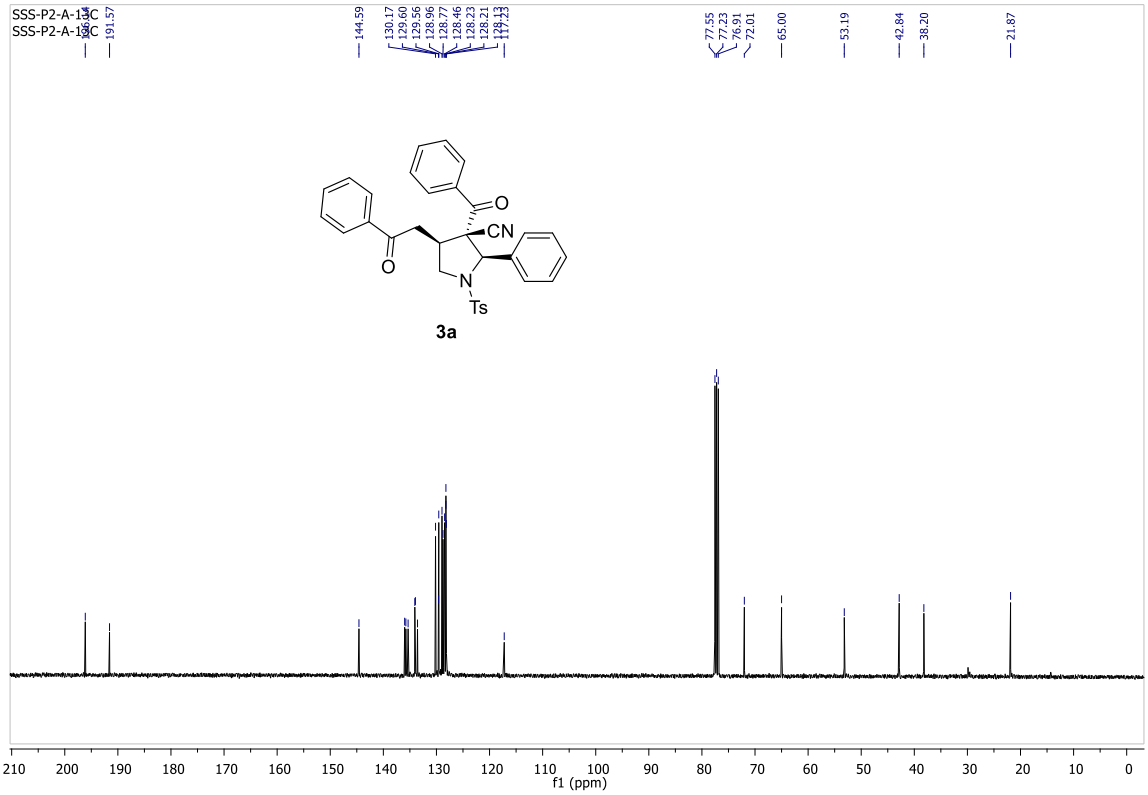
2 (*a*) K. S. Yang, A. E. Nibbs, Y. E. Turkmen and V. H. Rawal, *J. Am. Chem. Soc*., 2013, **135**, 16; (*b*) W. Yang and D. M. Du, *Org. Lett*., 2010, **12**, 5450.

3 S. Meninno, G. Croce and A. Lattanzi, *Org. Lett*., 2013, **15**, 3436.

4 B.-L. Zhao and D.-M. Du, *Asian J. Org. Chem*. 2015, **4**, 1120.

I. NMR Spectra of compounds (3a-3y):

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128.77
128.46
128.23
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77.23
76.91
72.01
65.00
53.19
42.84
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N
Ts
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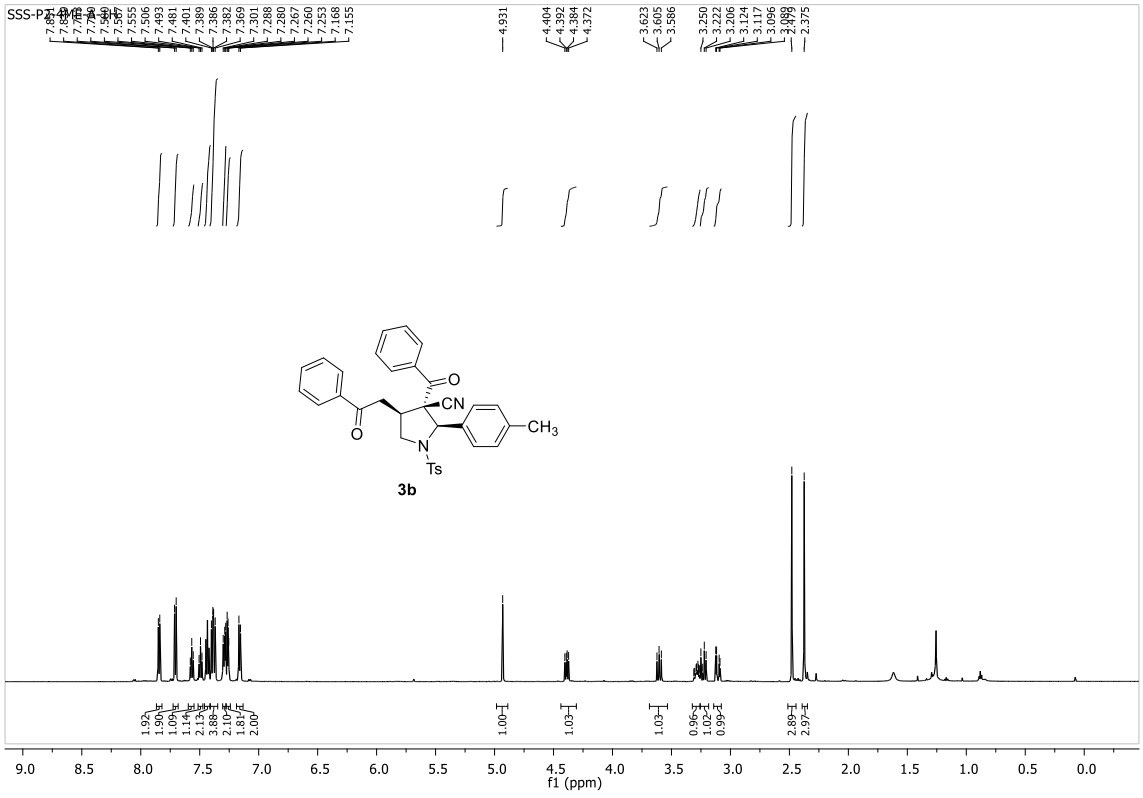
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.506
7.493
7.481
7.401
7.389
7.386
7.382
7.369
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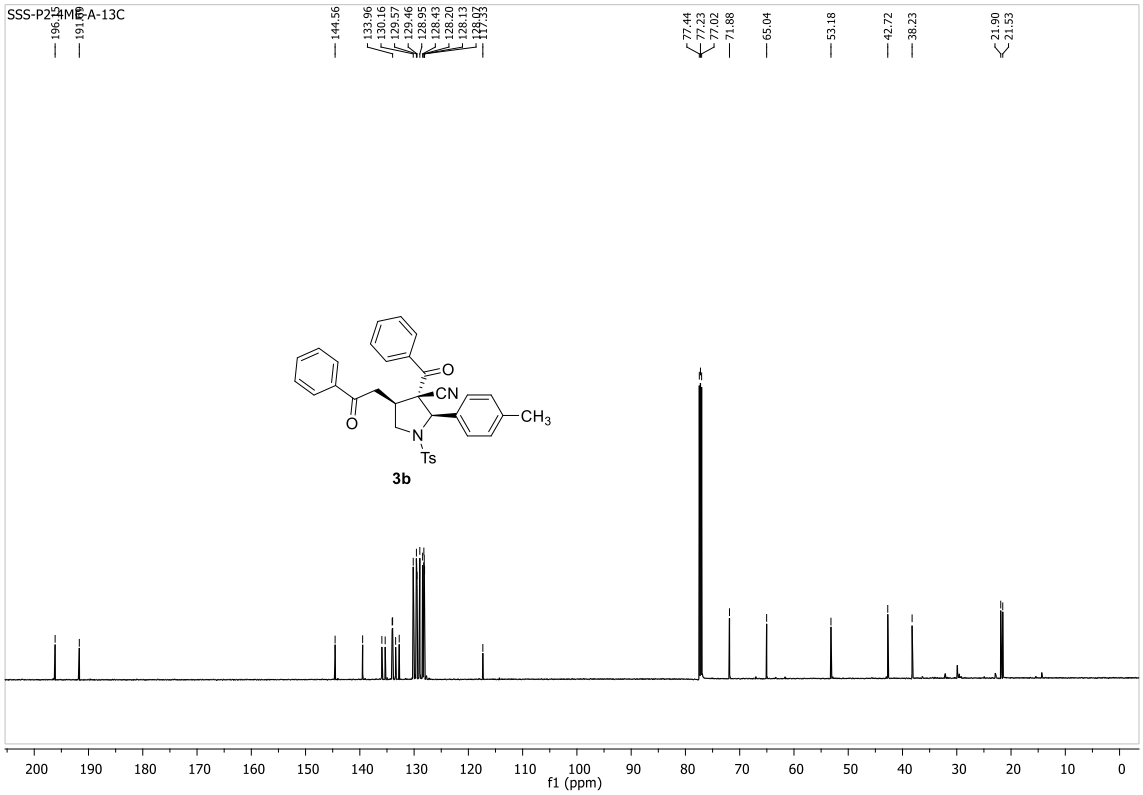
7.280
7.267
7.260
7.253
7.168
7.155
4.931
4.404
4.392
4.384
4.372
3.623
3.605
3.586
3.250
3.222
3.206
3.124
3.117
3.096
2.375
O
CN
O
N
Ts
CH3
3b
1.92
1.90
1.09
1.14
2.13
3.88
2.10
1.81
2.00
1.00
1.03
1.03
0.96
1.02
0.99
2.89
2.97
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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191.69
144.56
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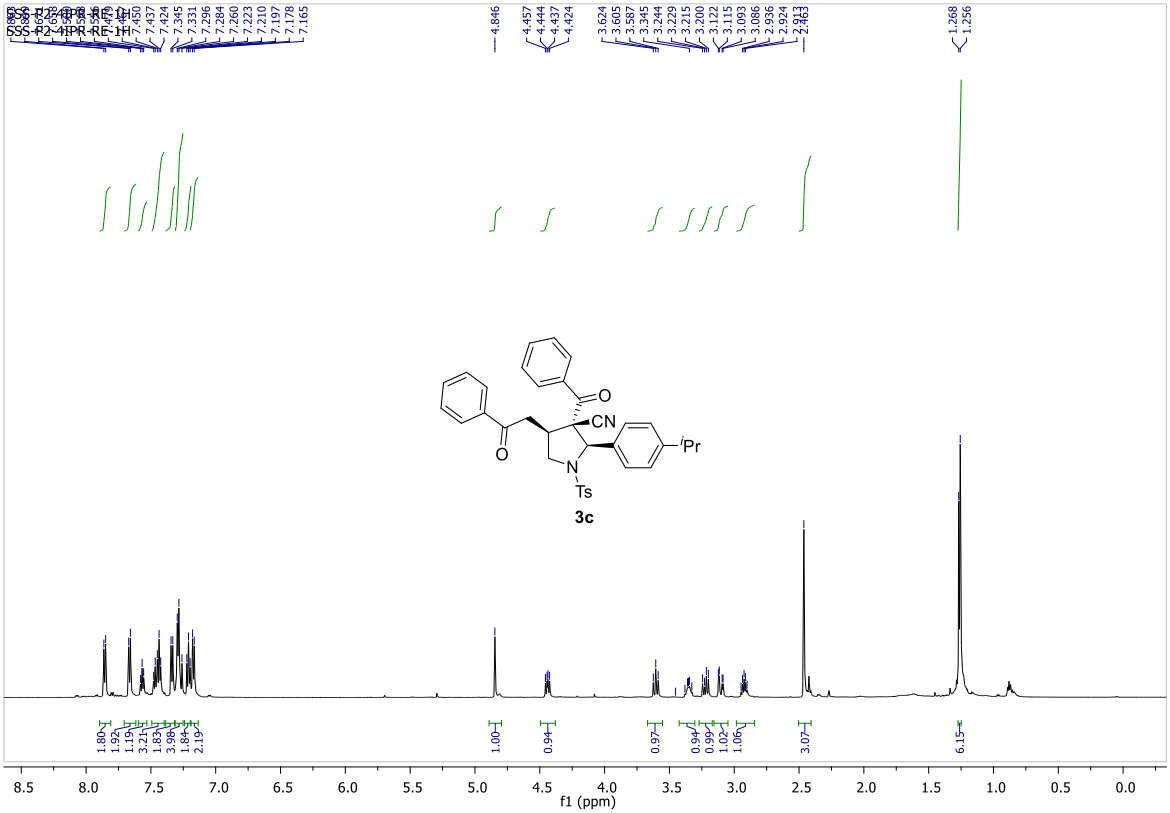
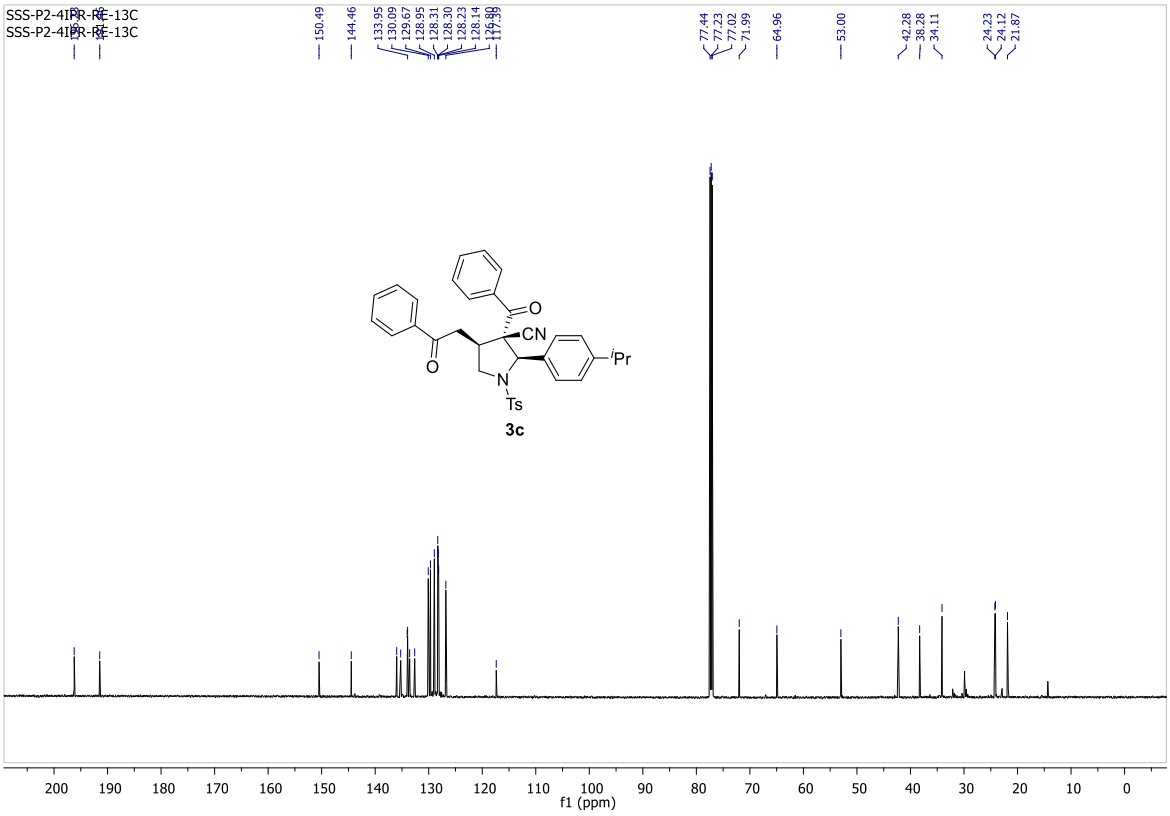
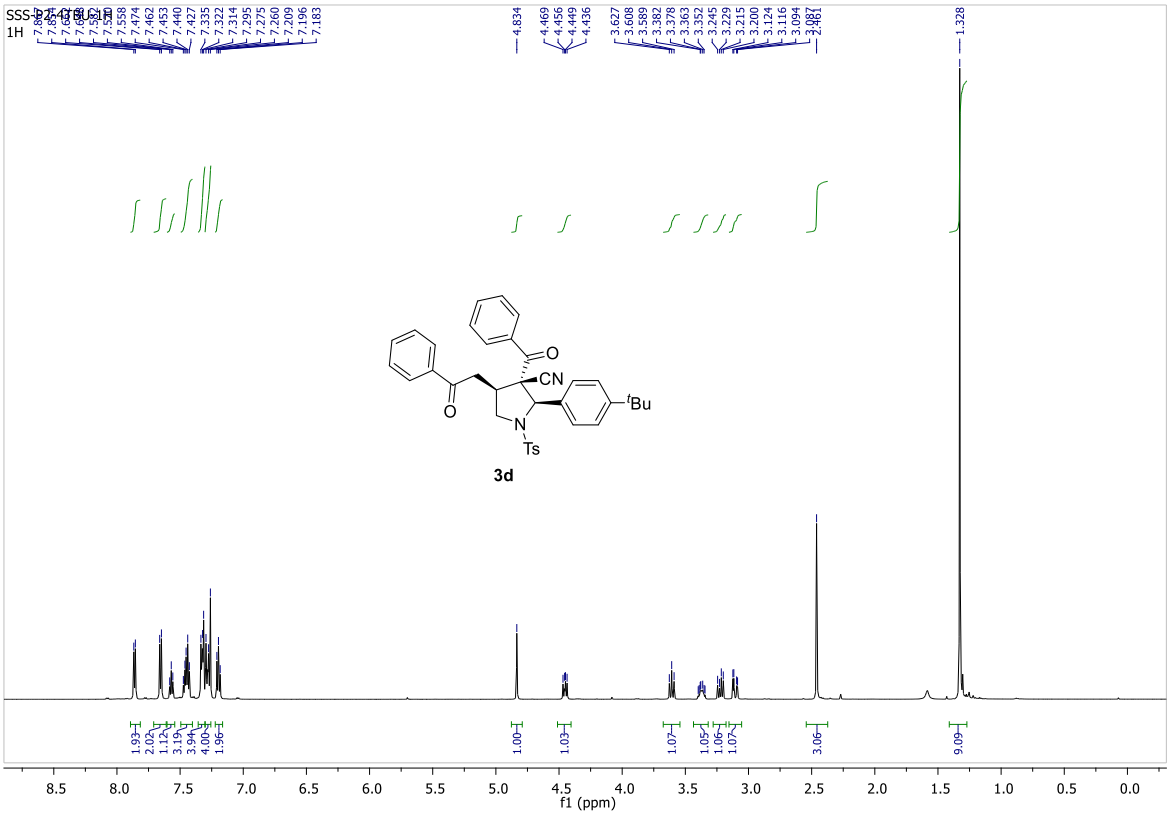
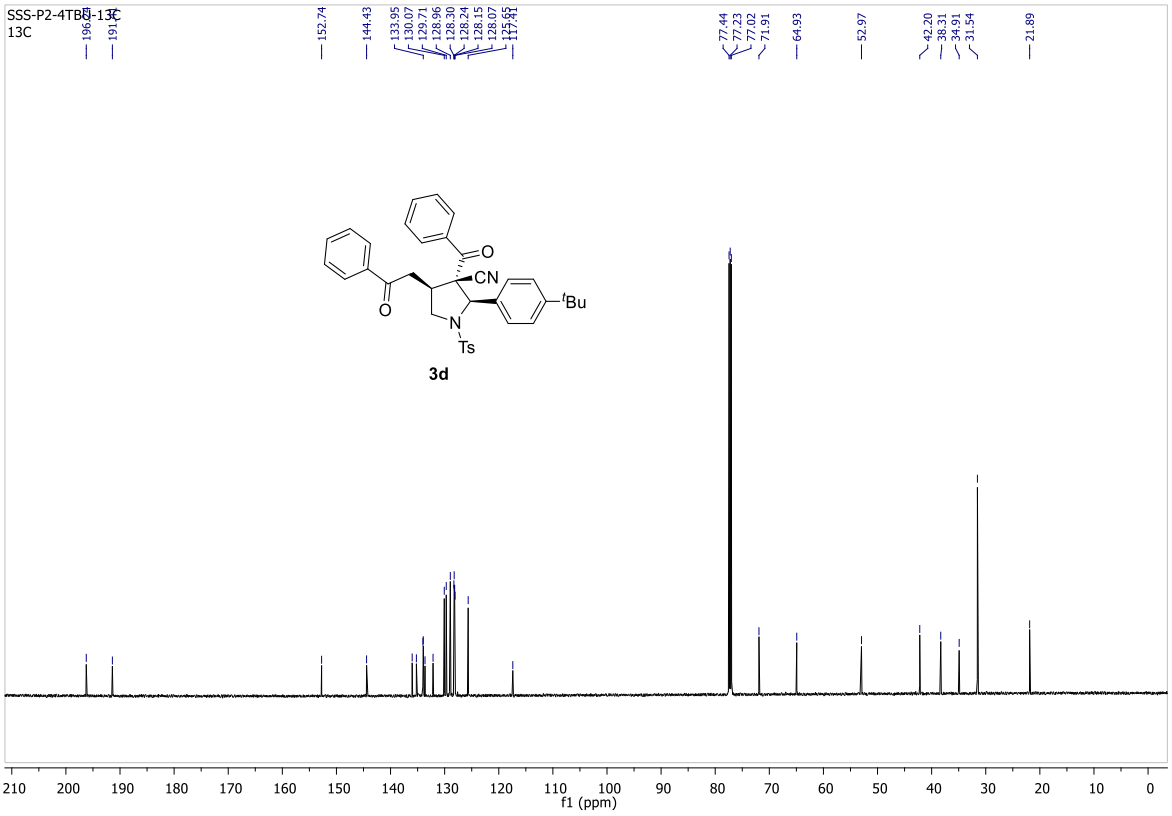
129.46
128.95
128.43
128.20
128.13
77.44
77.23
77.02
71.88
65.04
53.18
42.72
38.23
21.90
21.53
O
CN
CH3
O
N
Ts
3b
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


SSS-P2-4IPR-RE-1H
4.846
4.457
4.444
4.437
4.424
3.624
3.605
3.587
3.345
3.244
3.229
3.215
3.200
3.122
3.115
3.093
3.086
2.936
2.924
2.913
2.483
1.268
1.256
O
CN
iPr
O
N
Ts
3c
1.80
1.92
1.19
3.21
1.83
3.98
1.84
2.19
1.00
0.94
0.97
0.94
0.99
1.02
1.06
3.07
6.15
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
f1 (ppm)


SSS-P2-41PR-RE-13C
SSS-P2-41PR-RE-13C
150.49
144.46
133.95
130.09
129.67
128.95
128.31
128.30
128.23
128.14
77.44
77.23
77.02
71.99
64.96
53.00
42.28
38.28
34.11
24.23
24.12
21.87
O
CN
O
N
Ts
iPr
3c
f1 (ppm)


1H
4.834
4.469
4.456
4.449
4.436
3.627
3.608
3.589
3.382
3.378
3.363
3.352
3.245
3.229
3.215
3.200
3.124
3.116
3.094
3.087
2.981
1.328
O
CN
O
N
Ts
tBu
3d
1.93
2.02
1.12
3.19
3.94
4.00
1.96
1.00
1.03
1.07
1.05
1.06
1.07
3.06
9.09
f1 (ppm)


SSS-P2-4TBU-13C
13C
196.11
191.41
152.74
144.43
133.95
130.07
129.71
128.96
128.30
128.24
128.15
128.07
125.65
117.41
77.44
77.23
77.02
71.91
64.93
52.97
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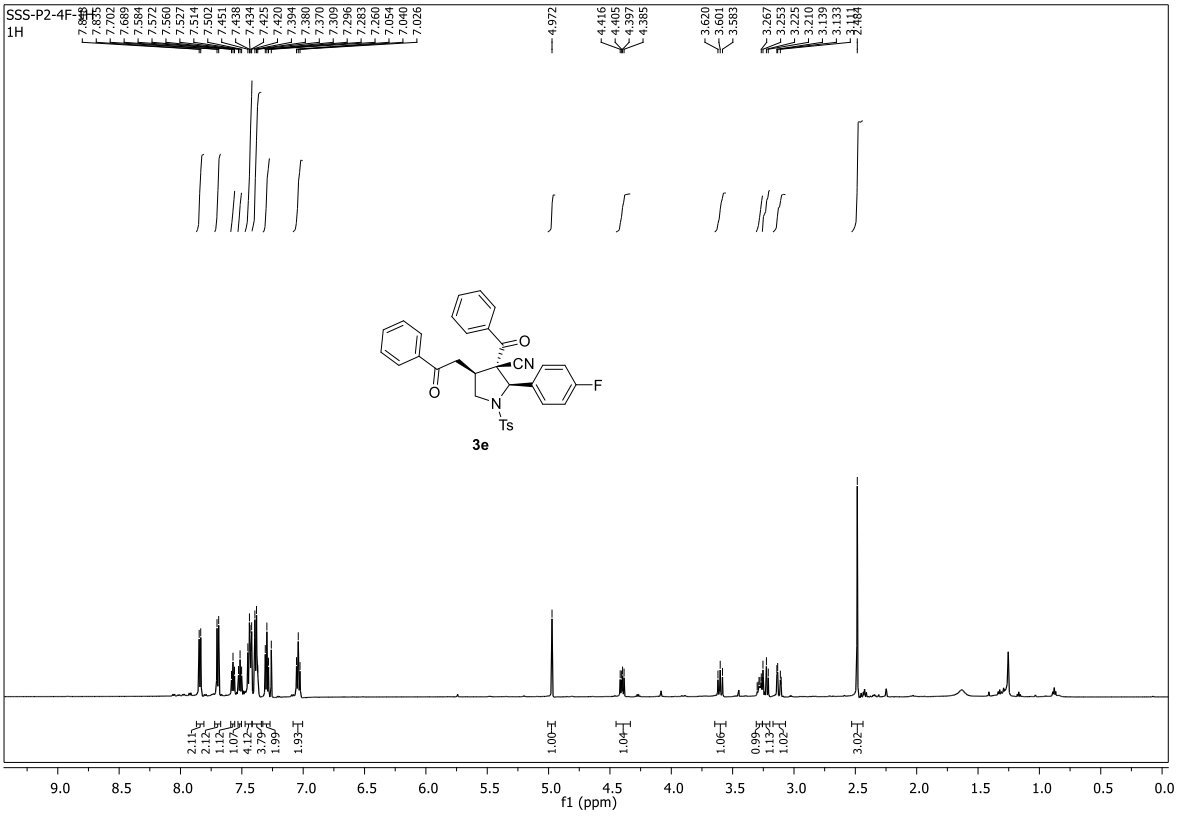
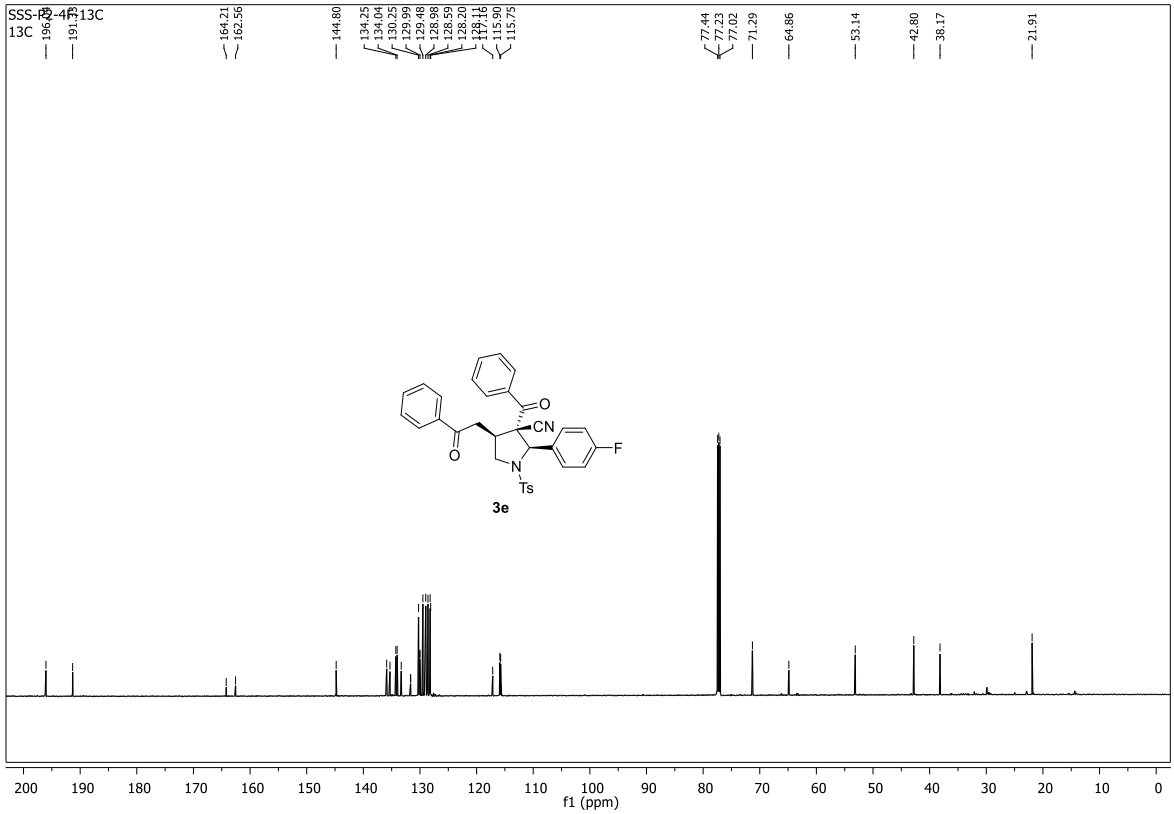
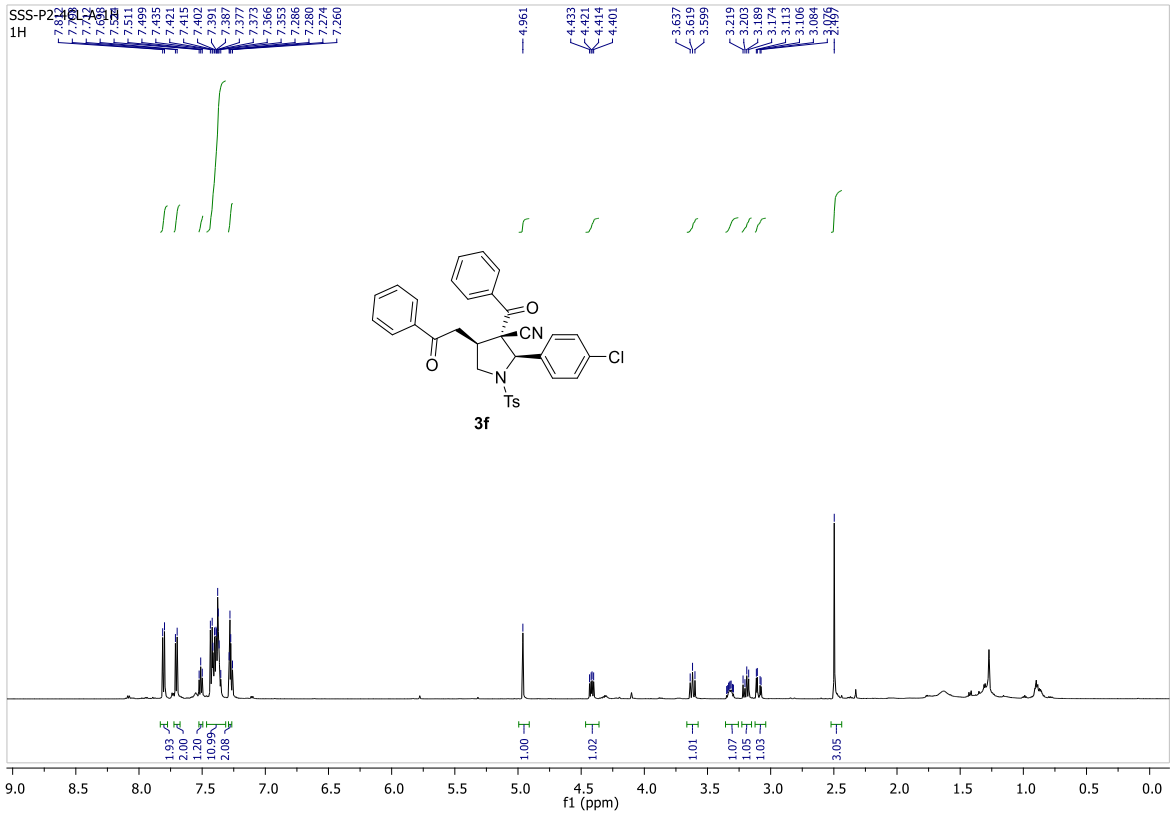
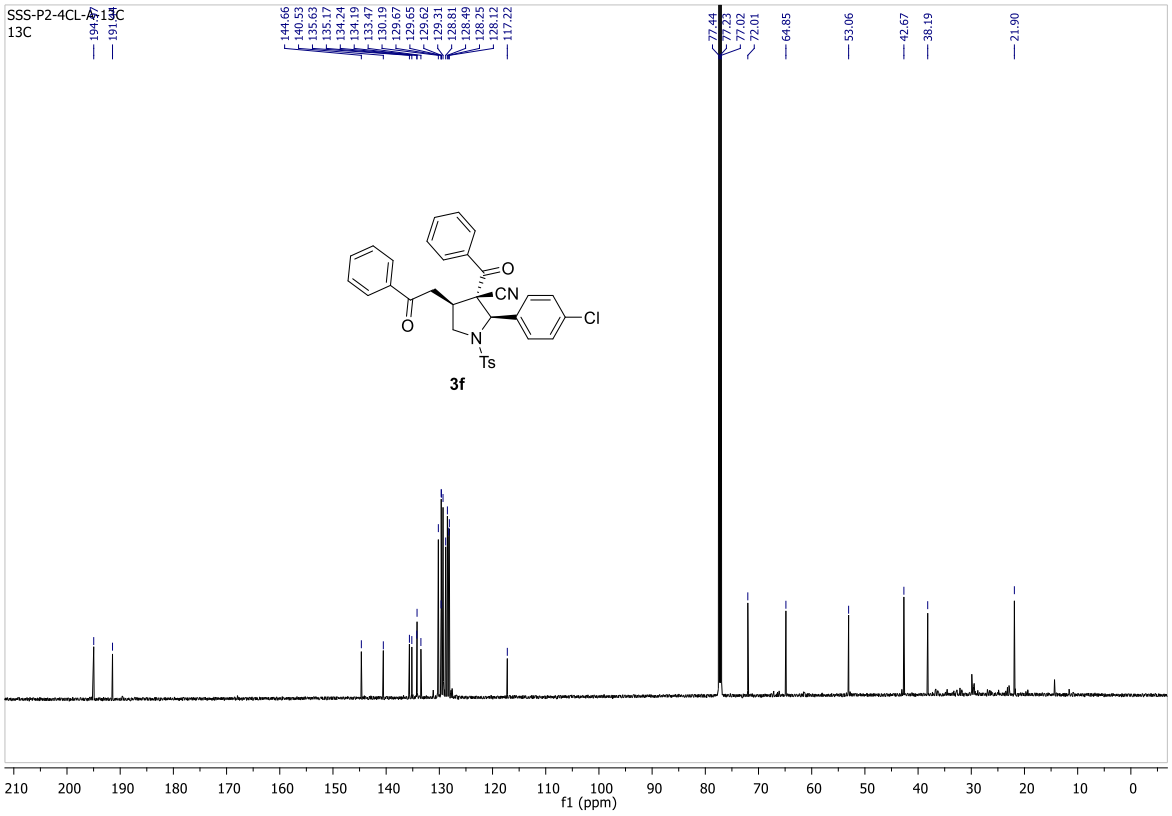
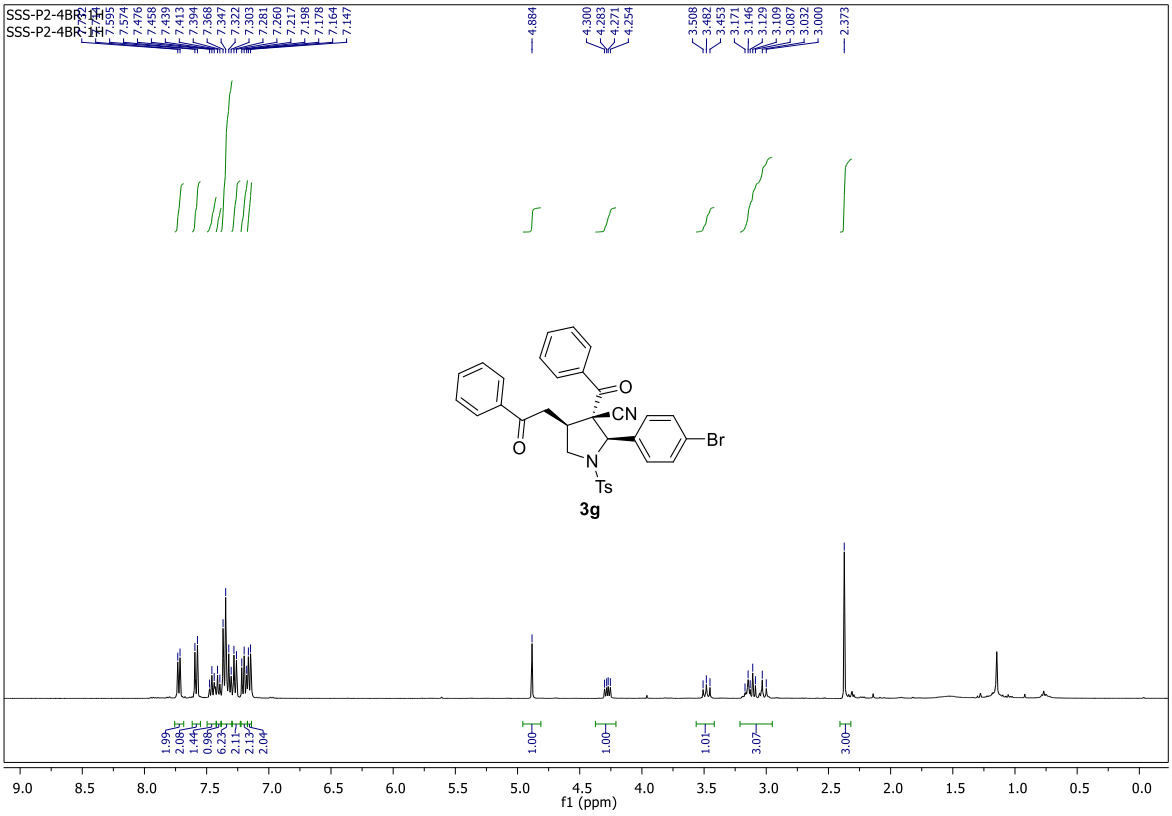
34.91
31.54
21.89
O
CN
O
N
Ts
tBu
3d
f1 (ppm)

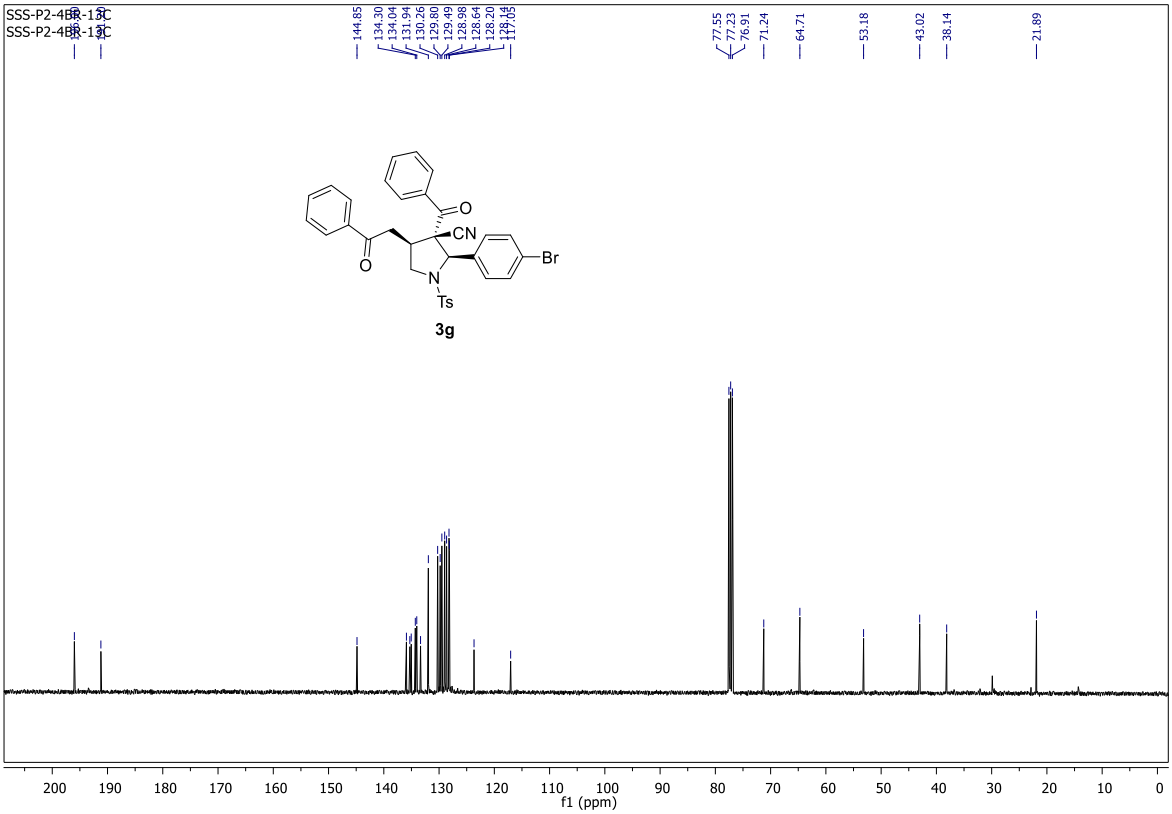

SSS-P2-4F-BU
1H
7.835
7.702
7.689
7.584
7.572
7.560
7.527
7.514
7.502
7.451
7.438
7.434
7.425
7.420
7.394
7.380
7.370
7.309
7.296
7.283
7.260
7.054
7.040
7.026
4.972
4.416
4.405
4.397
4.385
3.620
3.601
3.583
3.267
3.253
3.225
3.210
3.139
3.133
3.111
3.084
2.11
2.12
1.12
1.07
4.12
3.79
1.99
1.93
1.00
1.04
1.06
0.99
1.13
1.02
3.02
O
CN
O
N
Ts
F
3e
f1 (ppm)

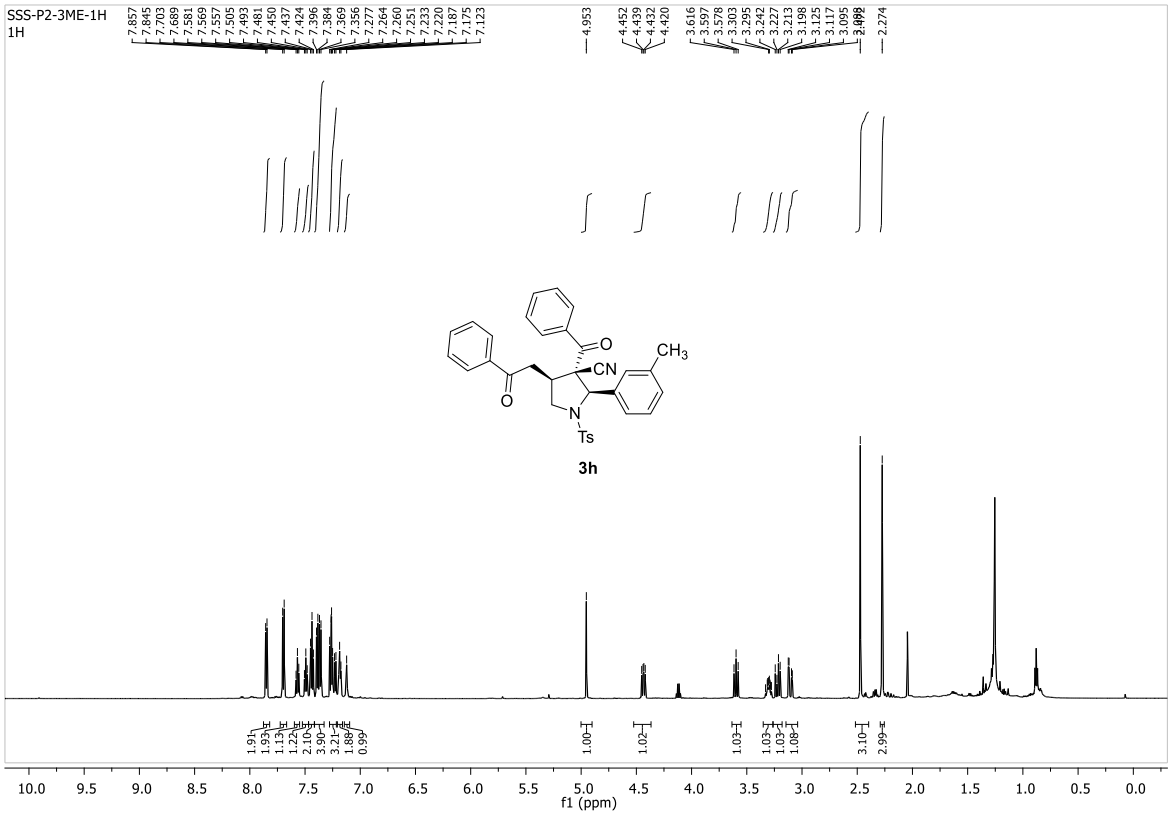

SSS-P2-47-13C
13C
196.22
191.32
164.21
162.56
144.80
134.25
134.04
130.25
129.99
129.48
128.98
128.59
128.20
77.44
77.23
77.02
71.29
64.86
53.14
42.80
38.17
21.91
O
CN
F
N
Ts
O
3e
f1 (ppm)

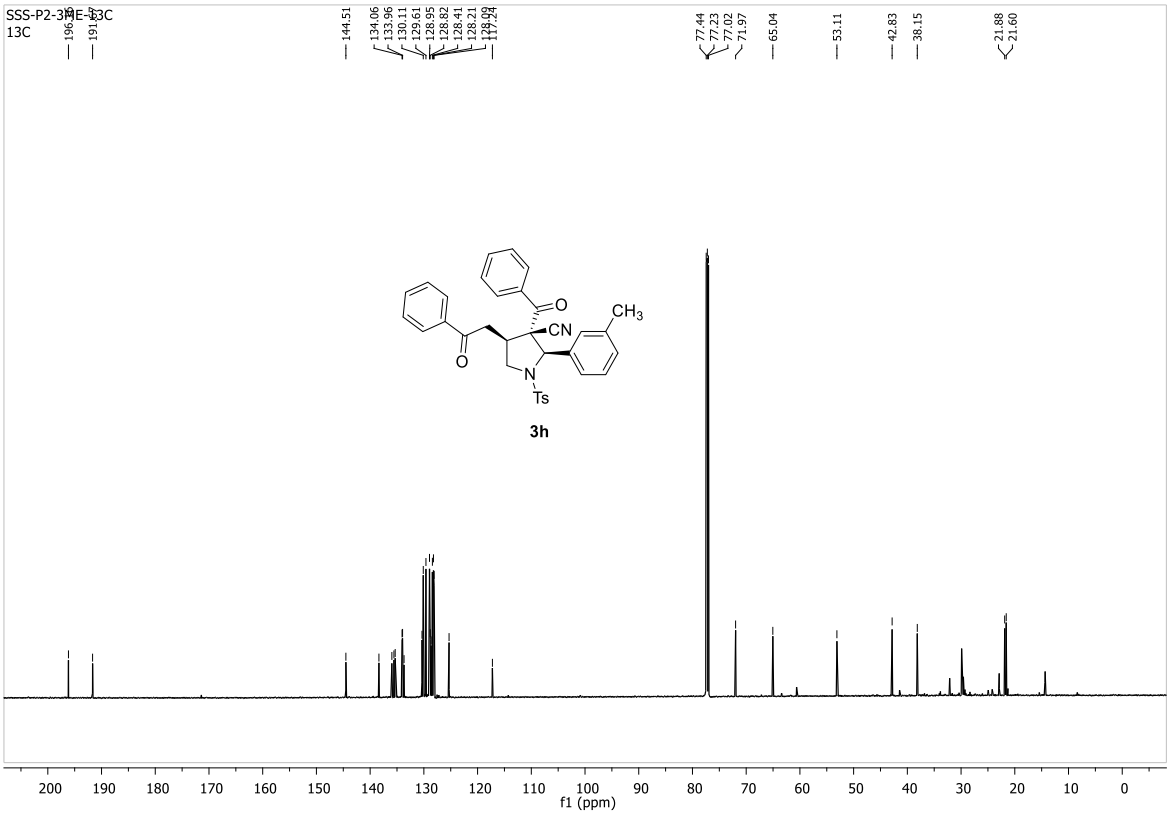

SSS-P2-47-1H
1H
4.961
4.433
4.421
4.414
4.401
3.637
3.619
3.599
3.219
3.203
3.189
3.174
3.113
3.106
3.084
2.997
O
CN
Cl
N
Ts
O
3f
1.93
2.00
1.20
10.99
2.08
1.00
1.02
1.01
1.07
1.05
1.03
3.05
f1 (ppm)

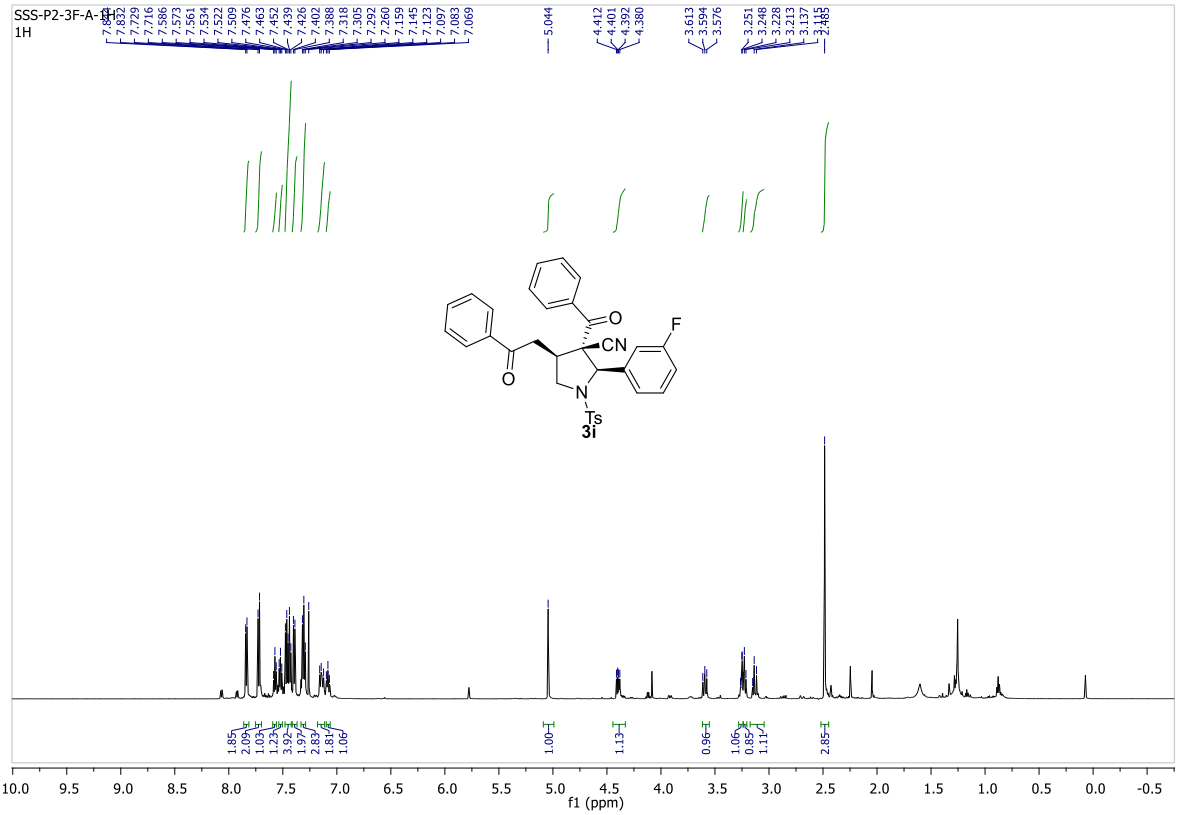

SSS-P2-4CL-A-13C
13C
194.77
191.15
144.66
140.53
135.63
135.17
134.24
134.19
133.47
130.19
129.67
129.65
129.62
129.31
128.81
128.49
128.25
128.12
117.22
77.44
77.23
77.02
72.01
64.85
53.06
42.67
38.19
21.90
O
CN
Cl
O
N
Ts
3f
f1 (ppm)

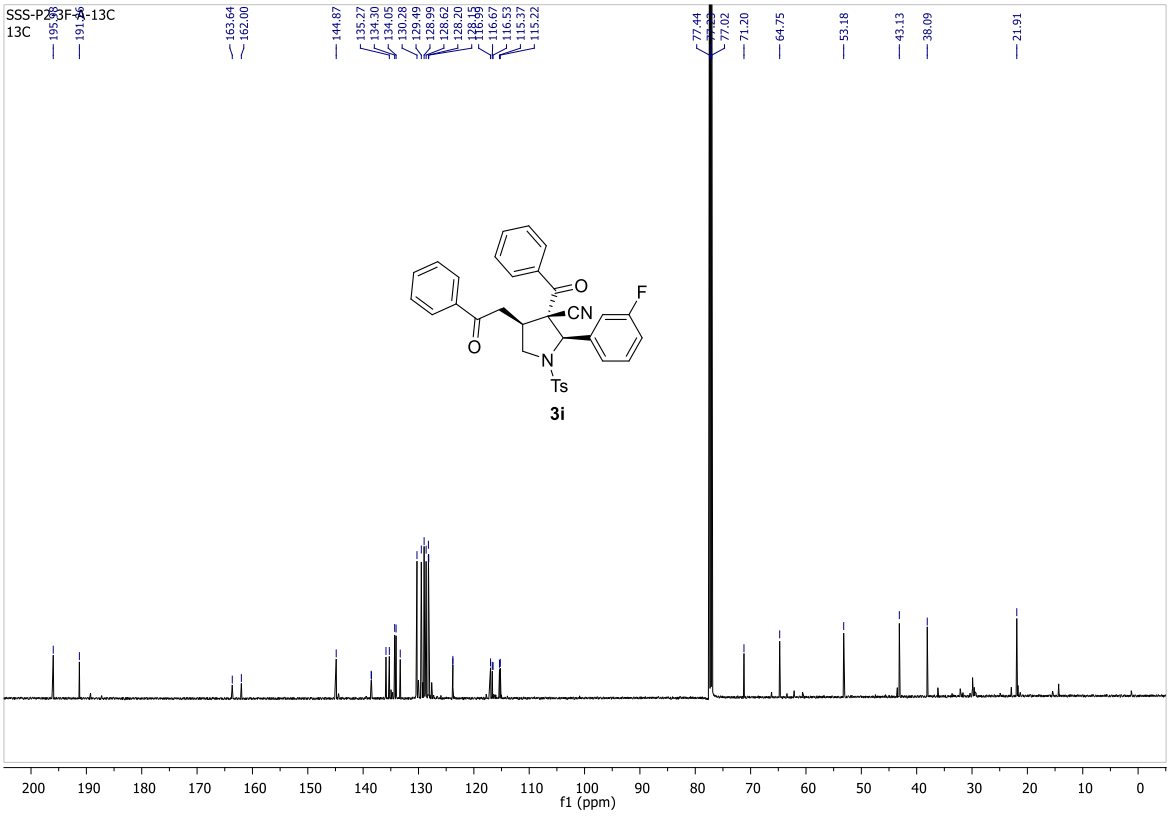

SSS-P2-4BR-1H
SSS-P2-4BR-1H
7.741
7.595
7.574
7.476
7.458
7.439
7.413
7.394
7.368
7.347
7.322
7.303
7.281
7.260
7.217
7.198
7.178
7.164
7.147
4.884
4.300
4.283
4.271
4.254
3.508
3.482
3.453
3.171
3.146
3.129
3.109
3.087
3.032
3.000
2.373
O
CN
Br
O
N
Ts
3g
1.99
2.08
1.44
0.98
6.23
2.11
2.13
2.04
1.00
1.00
1.01
3.07
3.00
f1 (ppm)

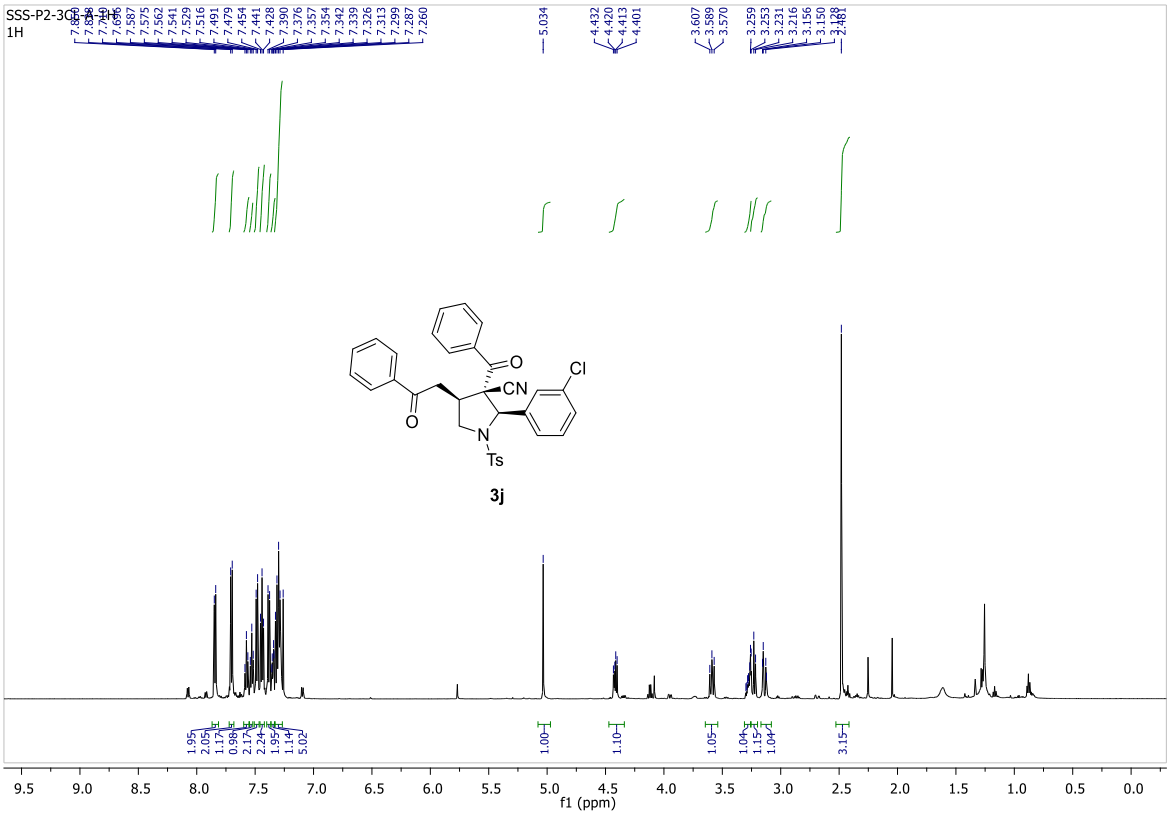

SSS-P2-4BR-13C
SSS-P2-4BR-13C
144.85
134.30
134.04
131.94
130.26
129.80
129.49
128.98
128.64
128.20
77.55
77.23
76.91
71.24
64.71
53.18
43.02
38.14
21.89
O
CN
O
Br
N
Ts
3g
f1 (ppm)

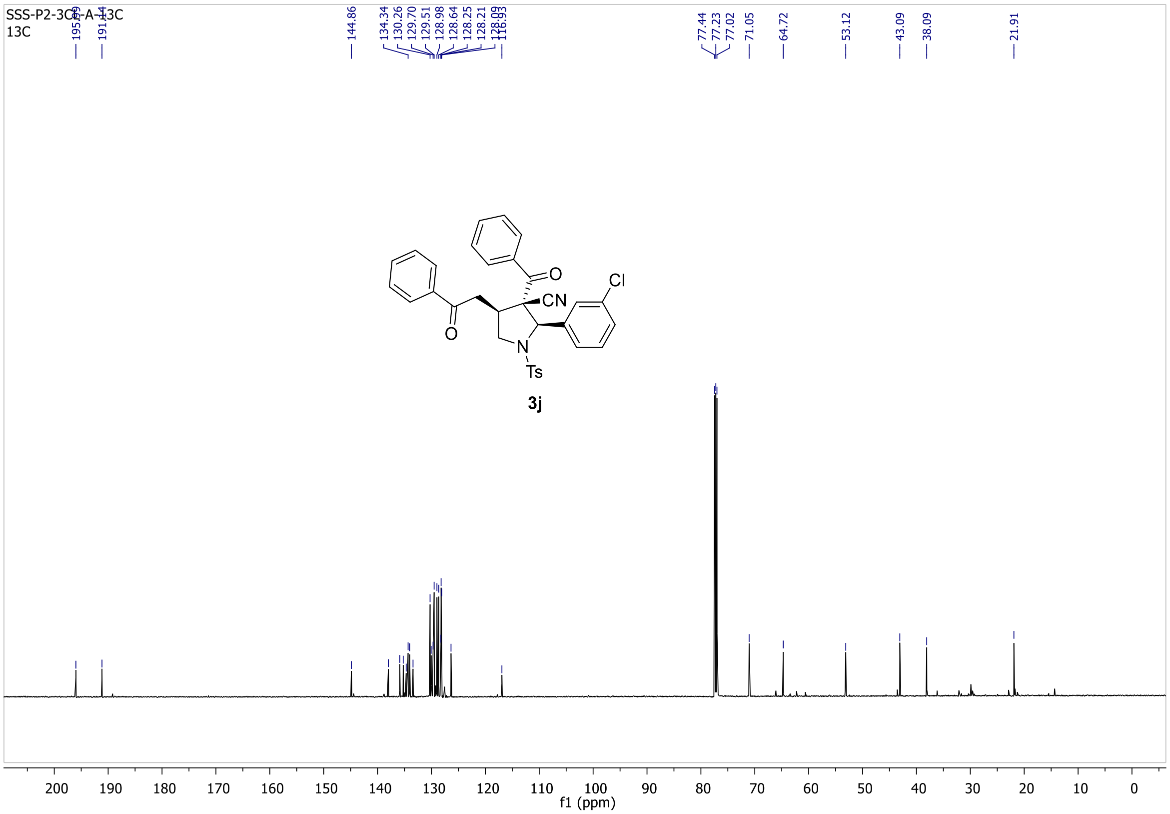

SSS-P2-3ME-1H
1H
4.953
4.452
4.439
4.432
4.420
2.274
O
CN
CH3
O
N
Ts
3h
1.00
1.02
1.03
3.10
2.99
f1 (ppm)

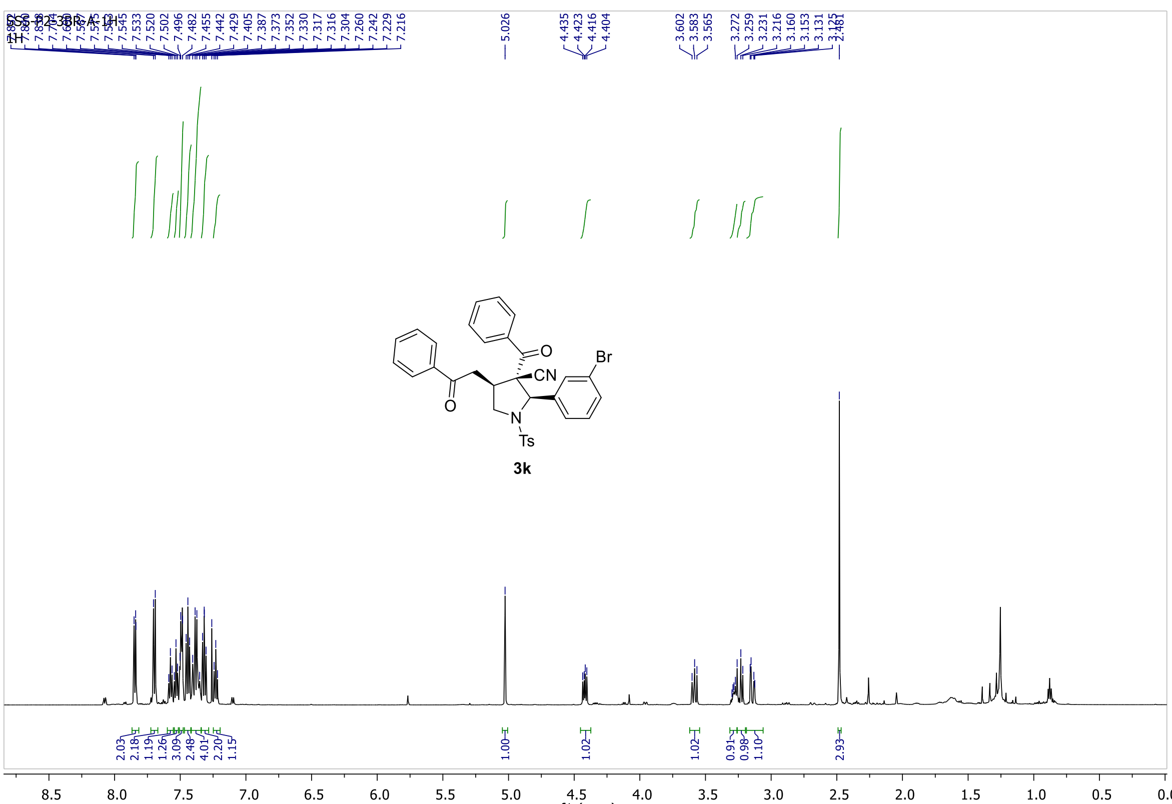

SSS-P2-3ME-13C
13C
196.47
191.63
144.51
134.06
133.96
130.11
129.61
128.95
128.82
128.41
128.21
77.44
77.23
77.02
71.97
65.04
53.11
42.83
38.15
21.88
21.60
O
CN
CH3
O
N
Ts
3h
f1 (ppm)

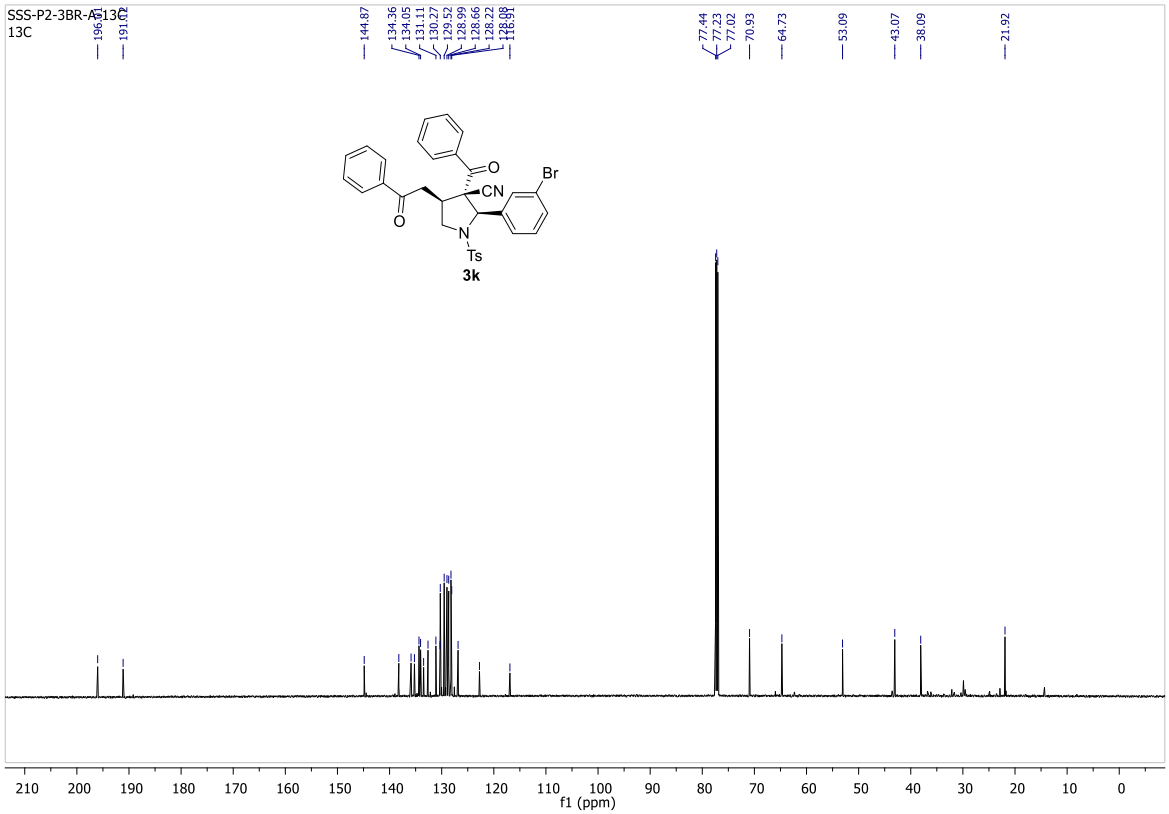

SSS-P2-3F-A-1H
1H
7.832
7.729
7.716
7.586
7.573
7.561
7.534
7.522
7.509
7.476
7.463
7.452
7.439
7.426
7.402
7.388
7.318
7.305
7.292
7.260
7.159
7.145
7.123
7.097
7.083
7.069
5.044
4.412
4.401
4.392
4.380
3.613
3.594
3.576
3.251
3.248
3.228
3.213
3.137
2.485
O
CN
F
O
N
Ts
3i
1.85
2.09
1.03
1.23
3.92
1.97
2.83
1.81
1.06
1.00
1.13
0.96
1.06
0.85
1.17
2.85
f1 (ppm)

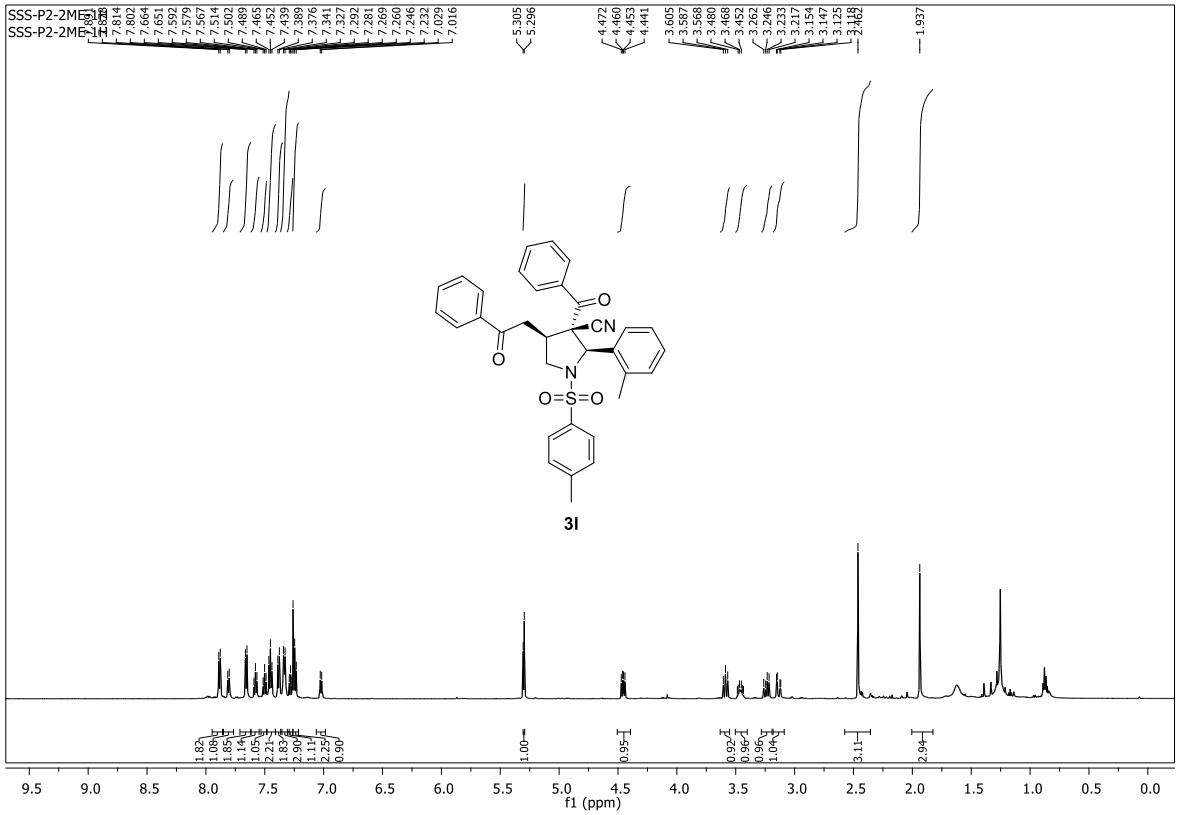

SSS-P2-3F-A-13C
13C
O
CN
F
O
N
Ts
3i
f1 (ppm)

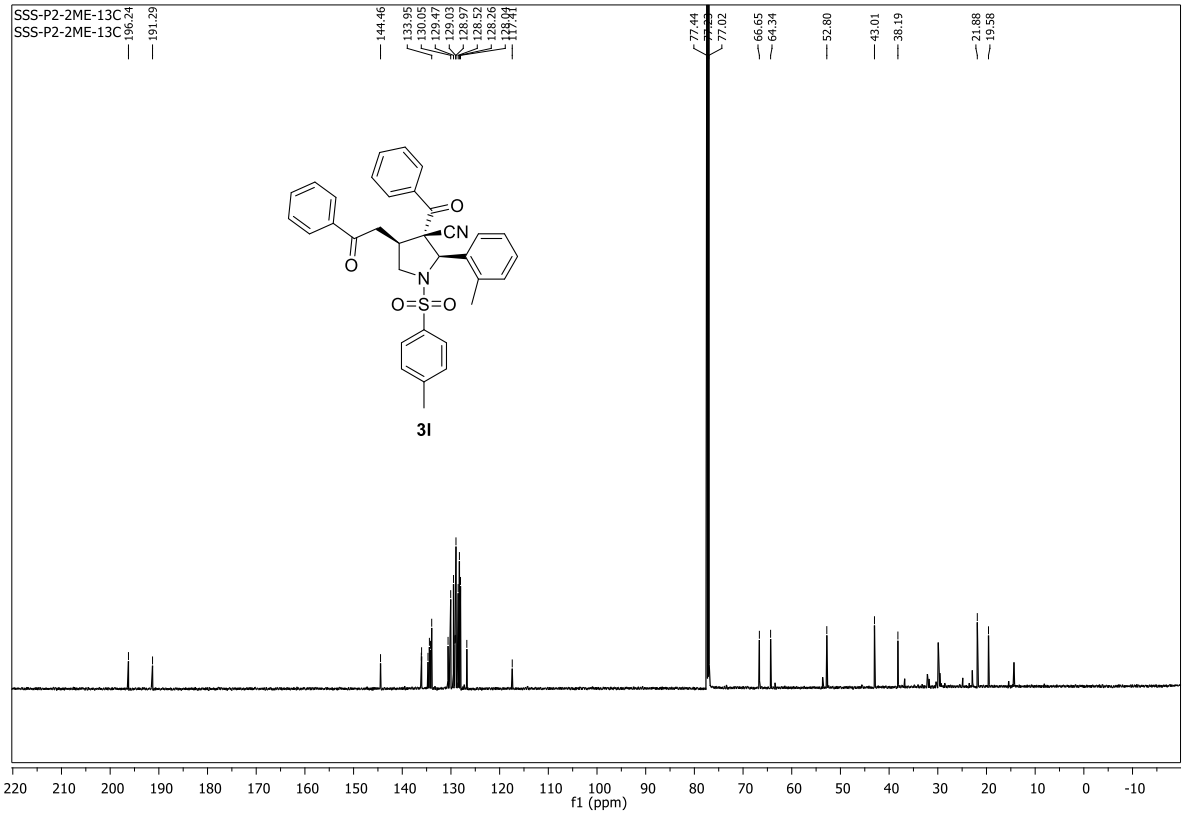

SSS-P2-3Cl-A-1H
1H
O
CN
Cl
O
N
Ts
3j
f1 (ppm)

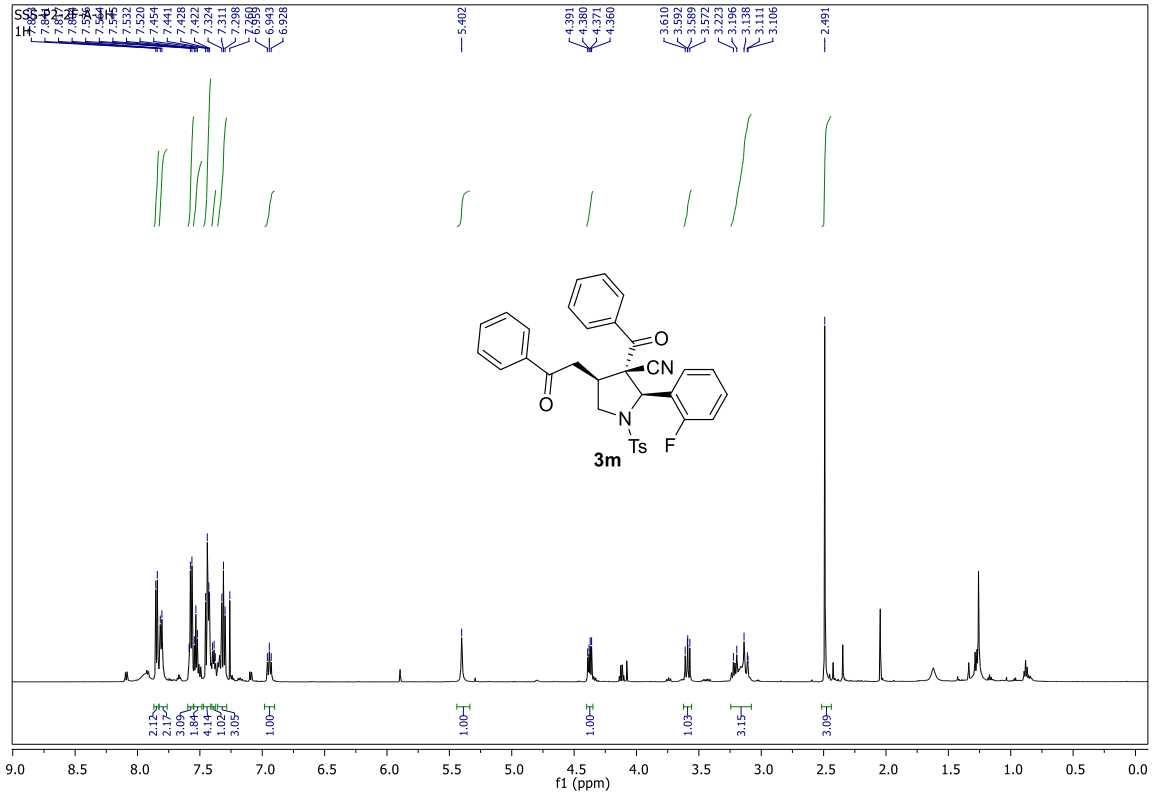

SSS-P2-3Cl-A-13C
13C
195.59
191.44
144.86
134.34
130.26
129.70
129.51
128.98
128.64
128.25
128.21
128.09
116.93
77.44
77.23
77.02
71.05
64.72
53.12
43.09
38.09
21.91
Cl
O
CN
O
N
Ts
3j
f1 (ppm)

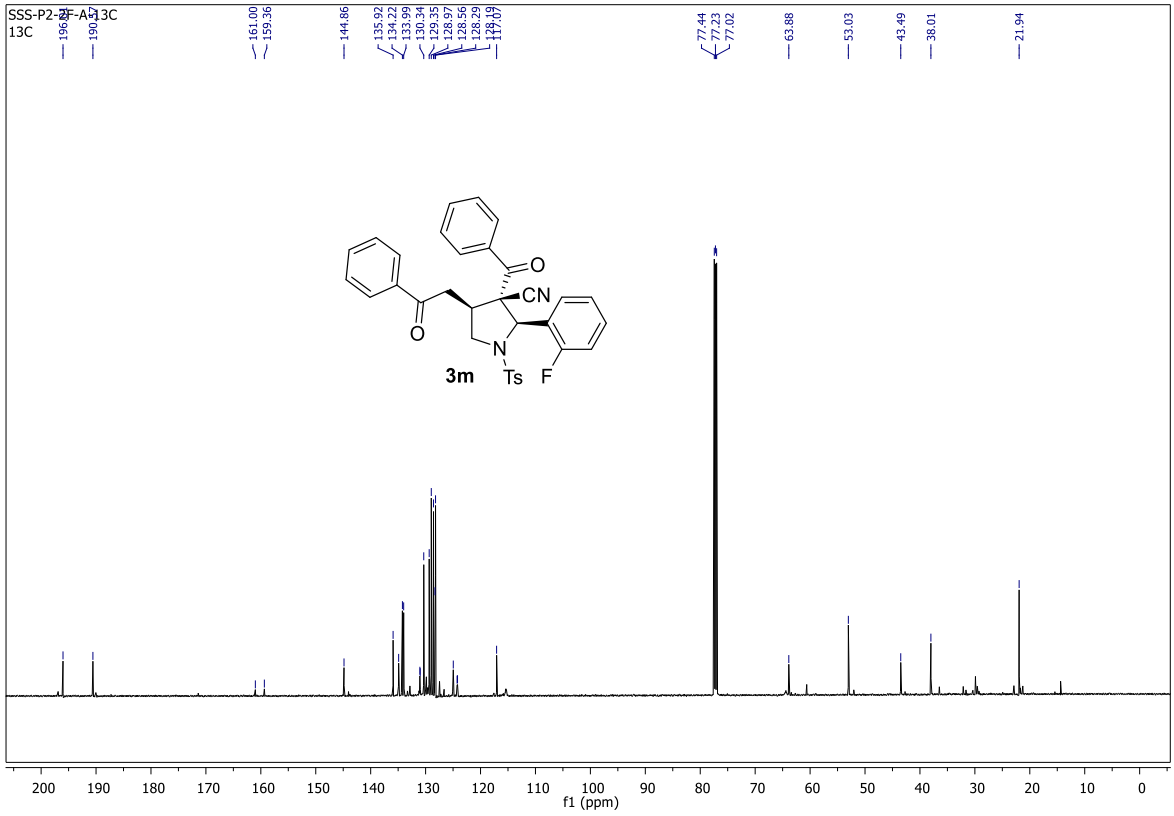

1H
5.026
4.435
4.423
4.416
4.404
3.602
3.583
3.565
3.272
3.259
3.231
3.216
3.160
3.153
3.131
3.125
2.481
Br
O
CN
O
N
Ts
3k
2.03
2.18
1.19
1.26
3.09
2.48
4.01
2.20
1.15
1.00
1.02
1.02
0.91
0.98
1.10
2.93
f1 (ppm)

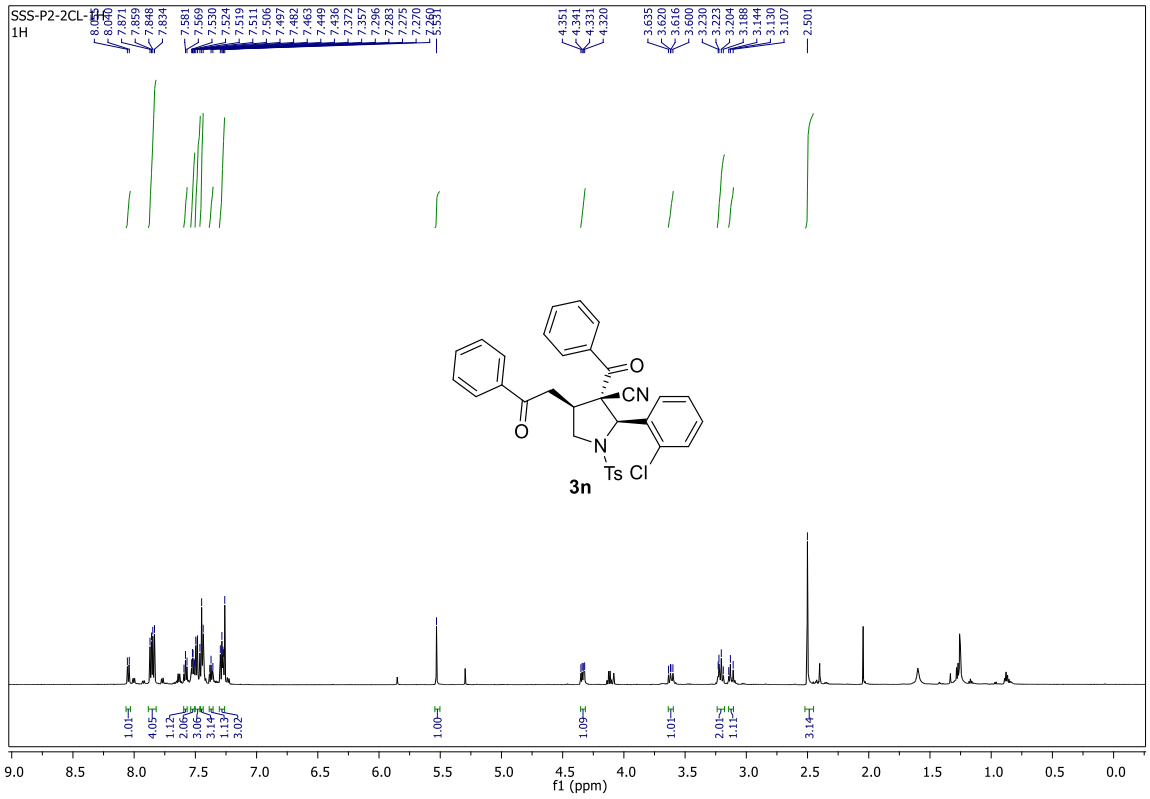

SSS-P2-3BR-A-13C
13C
196.11
191.02
144.87
134.36
134.05
131.11
130.27
129.52
128.99
128.66
128.22
77.44
77.23
77.02
70.93
64.73
53.09
43.07
38.09
21.92
O
CN
Br
O
N
Ts
3k
f1 (ppm)

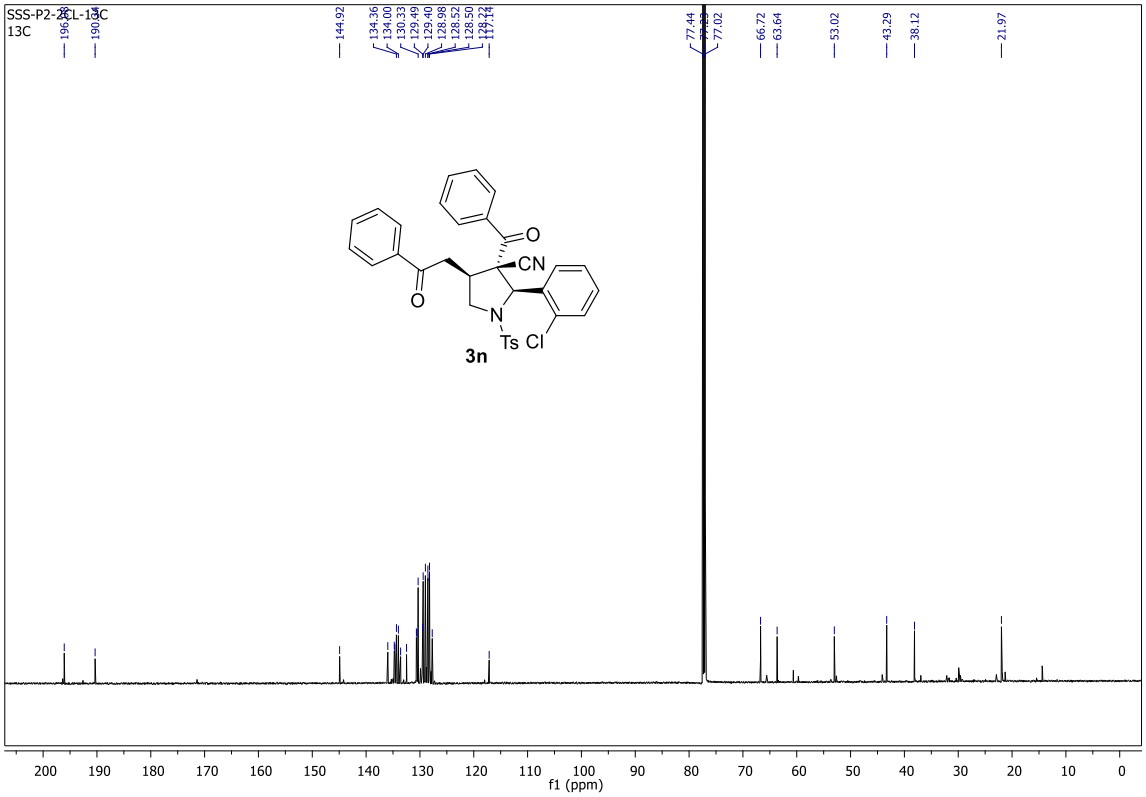

SSS-P2-2ME
SSS-P2-2ME
7.814
7.802
7.664
7.651
7.592
7.579
7.567
7.514
7.502
7.489
7.465
7.452
7.439
7.389
7.376
7.341
7.327
7.292
7.281
7.269
7.260
7.246
7.232
7.029
7.016
5.305
5.296
4.472
4.460
4.453
4.441
3.605
3.587
3.568
3.480
3.468
3.452
3.262
3.246
3.233
3.217
3.154
3.147
3.125
3.118
2.462
1.937
O
CN
O
N
O=S=O
3l
1.82
1.08
1.85
1.14
1.05
2.21
1.83
2.90
1.11
2.25
0.90
1.00
0.95
0.92
0.96
0.96
1.04
3.11
2.94
f1 (ppm)

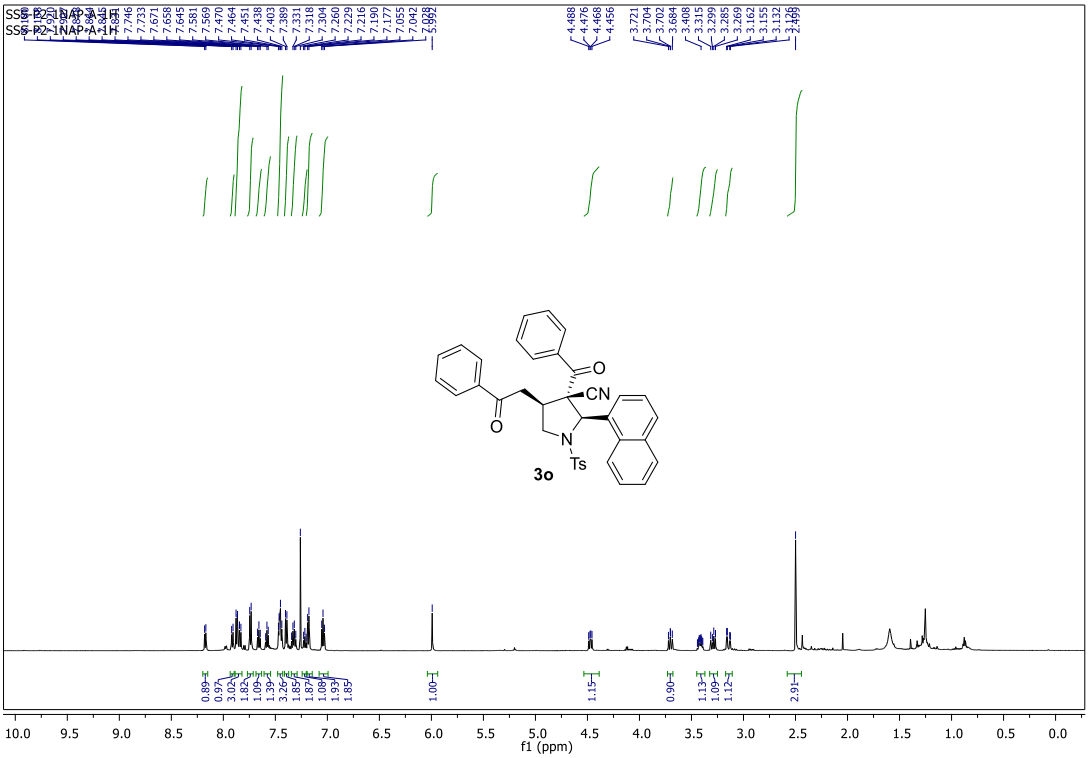

SSS-P2-2ME-13C
SSS-P2-2ME-13C
196.24
191.29
144.46
133.95
130.05
129.47
129.03
128.97
128.52
128.26
128.04
117.41
77.44
77.23
77.02
66.65
64.34
52.80
43.01
38.19
21.88
19.58
O
CN
O
N
O=S=O
3l
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

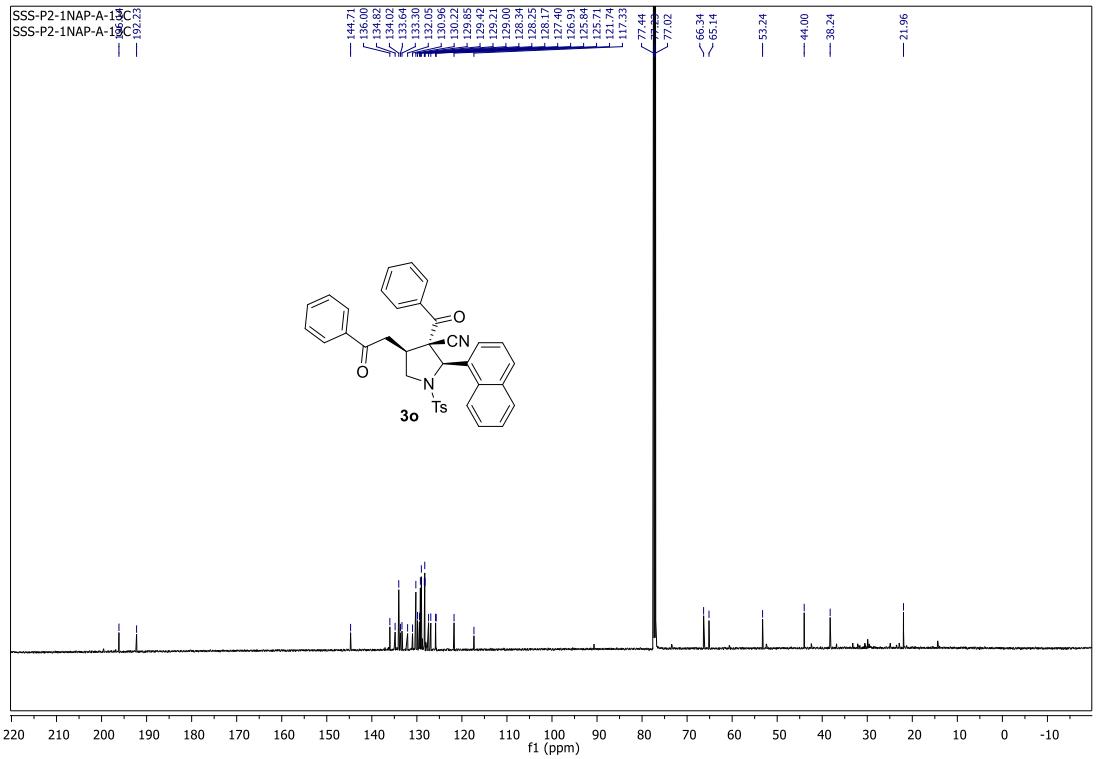

1H
5.402
4.391
4.380
4.371
4.360
3.610
3.592
3.589
3.572
3.223
3.196
3.138
3.111
3.106
2.491
O
CN
O
N
Ts
F
3m
2.12
2.17
3.09
1.84
4.14
1.02
3.05
1.00
1.00
1.00
1.03
3.15
3.09
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

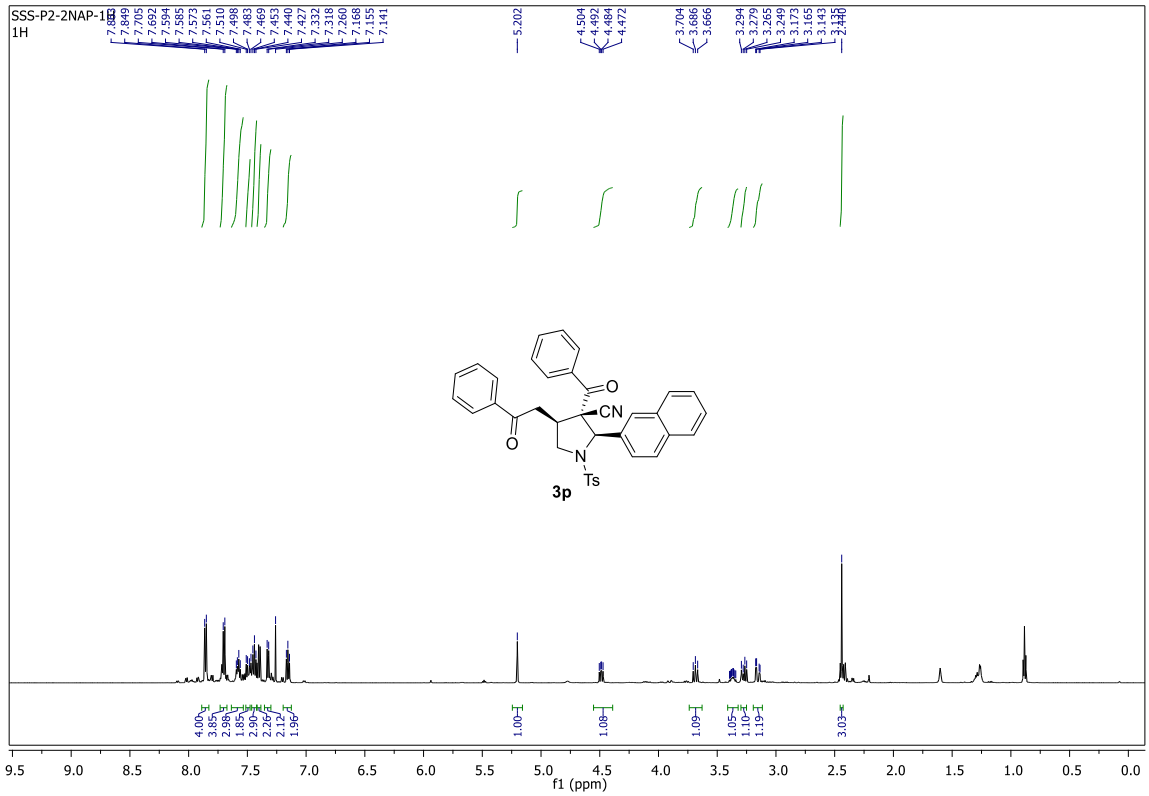

SSS-P2-2F-A-13C
13C
196.62
190.21
161.00
159.36
144.86
135.92
134.22
133.99
130.34
129.35
128.97
128.56
128.29
128.19
127.10
77.44
77.23
77.02
63.88
53.03
43.49
38.01
21.94
O
CN
O
N
Ts
F
3m
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

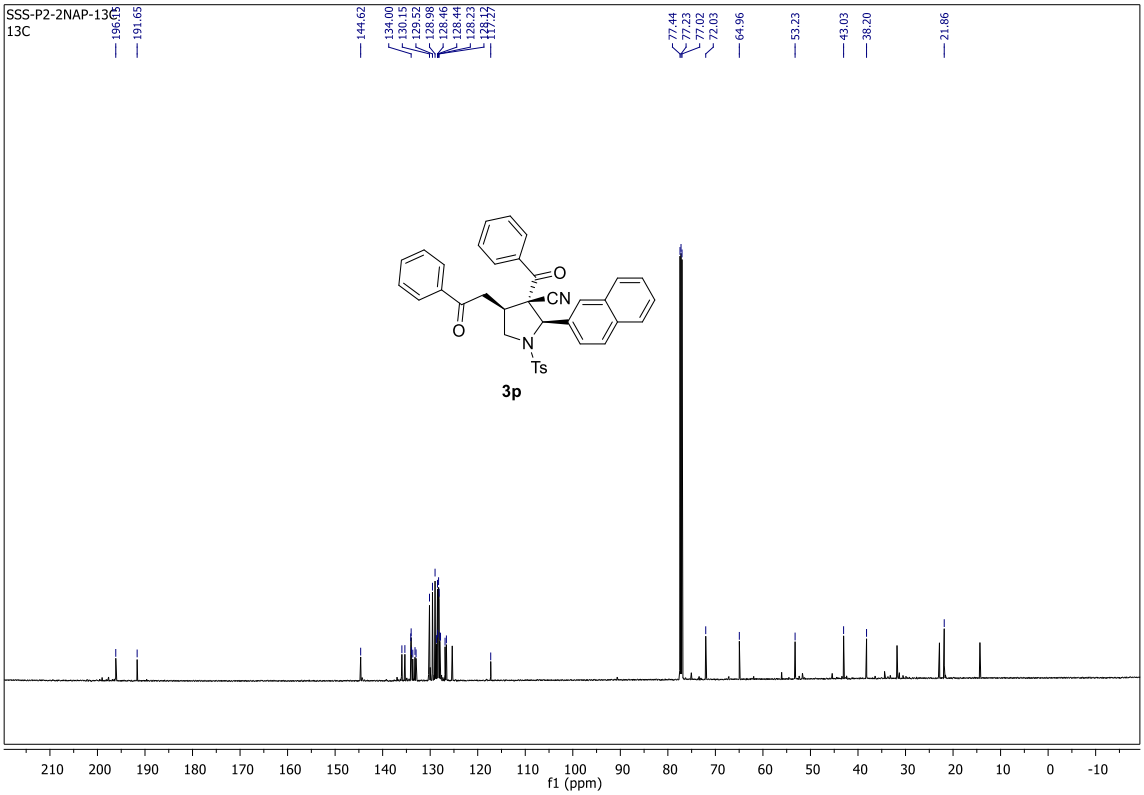

SSS-P2-2CL-1H
1H
8.074
8.070
7.871
7.859
7.848
7.834
7.581
7.569
7.530
7.524
7.519
7.511
7.506
7.497
7.482
7.463
7.449
7.436
7.372
7.357
7.296
7.283
7.275
7.270
7.260
5.531
4.351
4.341
4.331
4.320
3.635
3.620
3.616
3.600
3.230
3.223
3.204
3.188
3.144
3.130
3.107
2.501
O
CN
O
N
Ts
Cl
3n
1.01
4.05
1.12
2.06
3.06
3.14
1.13
3.02
1.00
1.09
1.01
2.01
1.11
3.14
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
f1 (ppm)

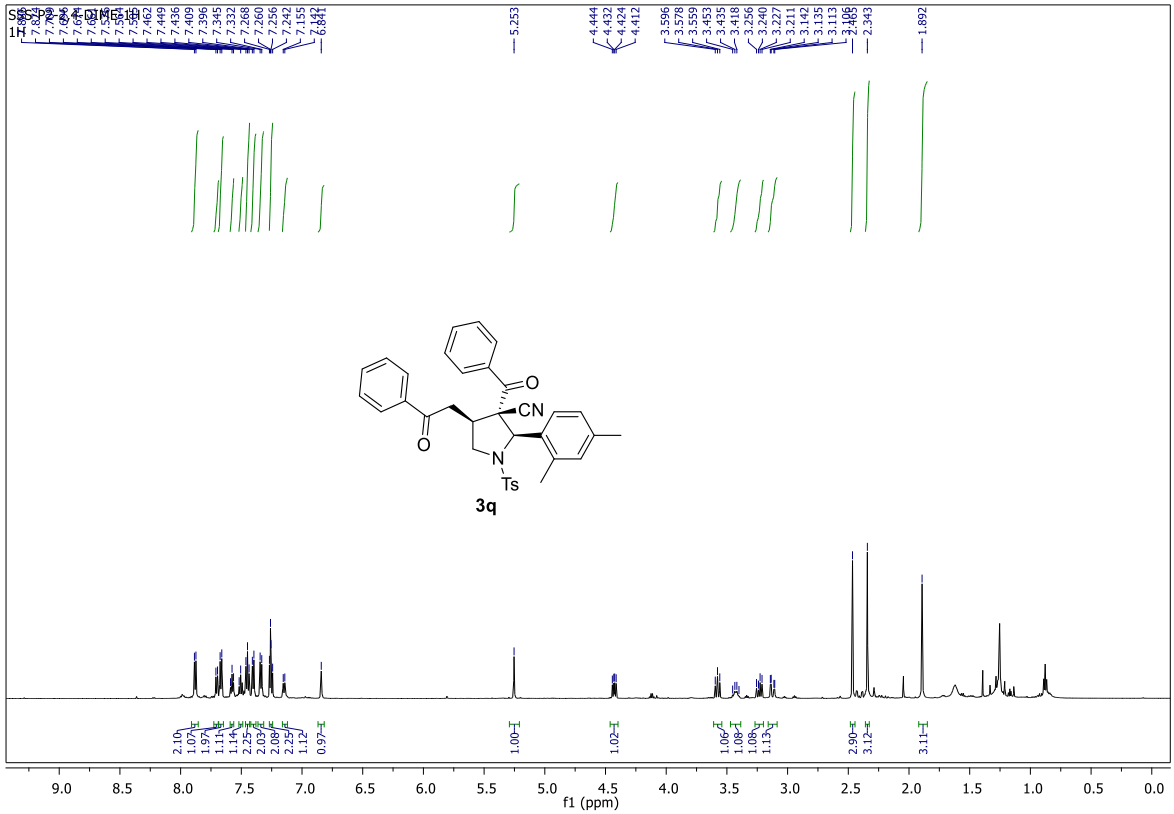

SSS-P2-2CL-13C
13C
144.92
134.36
134.00
130.33
129.40
128.98
128.52
128.50
128.22
117.14
77.44
77.23
77.02
66.72
63.64
53.02
43.29
38.12
21.97
O
CN
O
N
Ts Cl
3n
f1 (ppm)

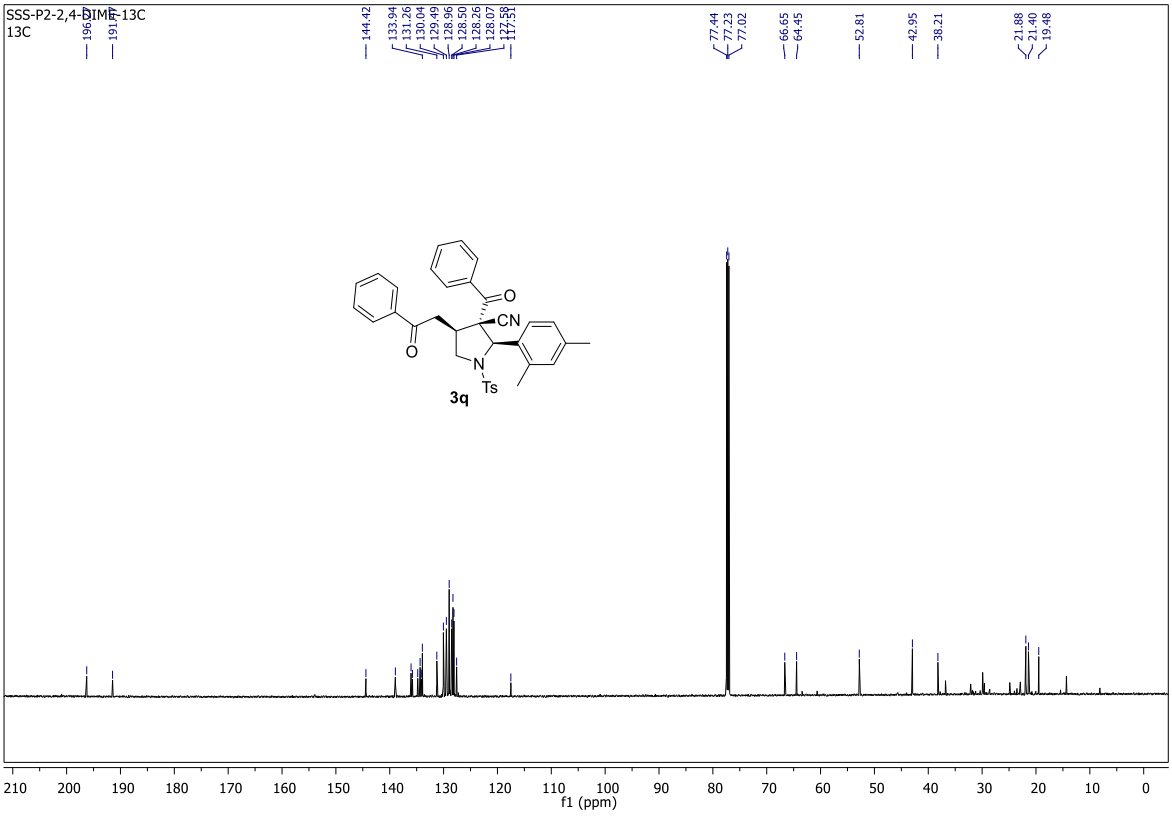

SSS-P2-1NAP-A-1H
4.488
4.476
4.468
4.456
3.721
3.704
3.702
3.684
3.408
3.315
3.299
3.285
3.269
3.162
3.155
3.132
3.126
2.499
O
CN
O
N
Ts
3o
0.89
0.97
3.00
1.82
1.09
1.39
3.26
1.85
1.87
1.08
1.93
1.85
1.00
1.15
0.90
1.13
1.09
1.12
2.91
f1 (ppm)

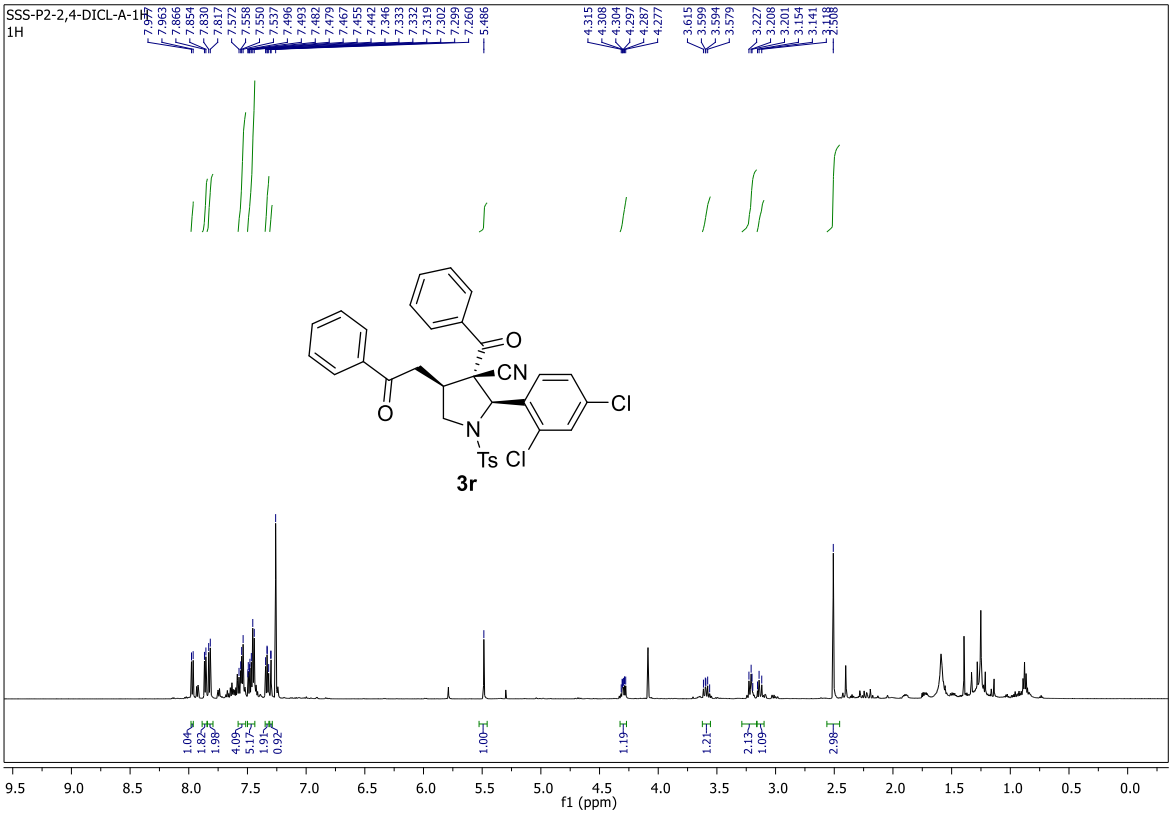

SSS-P2-1NAP-A-13C
SSS-P2-1NAP-A-13C
144.71
136.00
134.82
134.02
133.64
133.30
132.05
130.96
130.22
129.85
129.42
129.21
129.00
128.34
128.25
128.17
127.40
126.91
125.84
125.71
121.74
117.33
77.44
77.23
77.02
66.34
65.14
53.24
44.00
38.24
21.96
192.23
O
CN
O
N
Ts
3o
f1 (ppm)

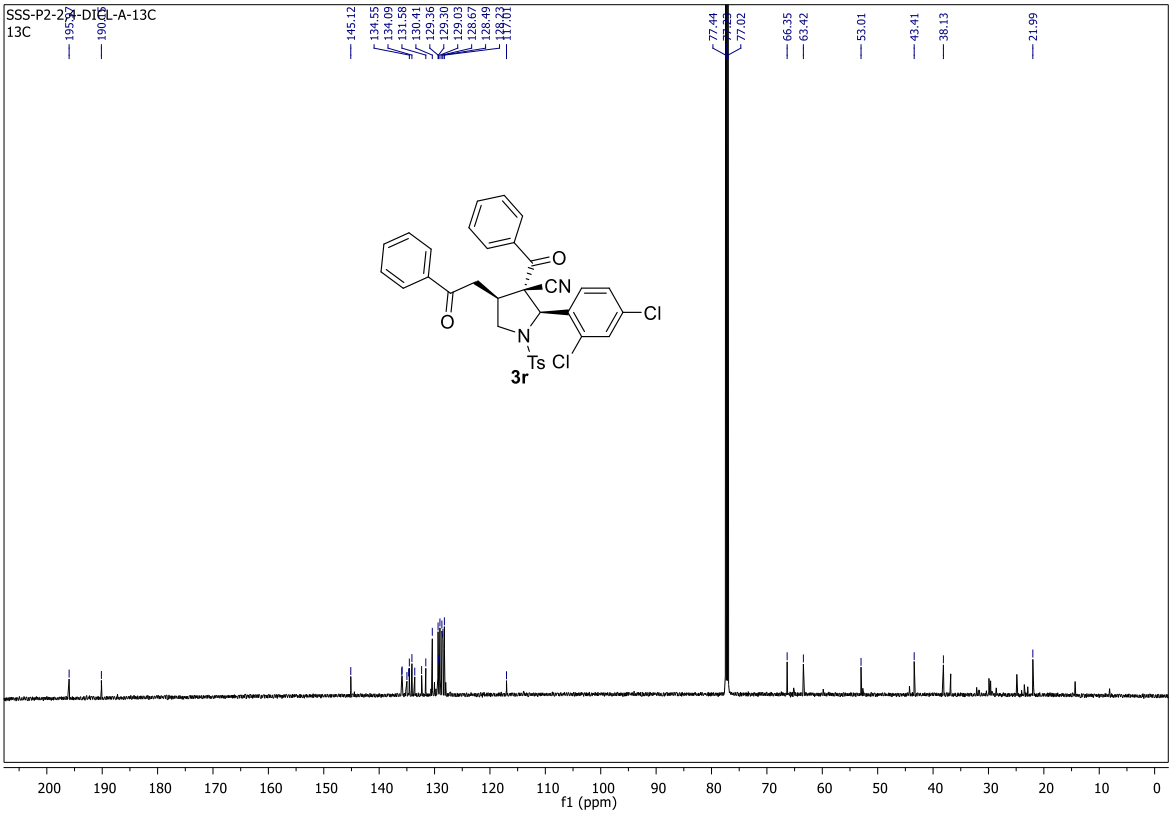

SSS-P2-2NAP-1H
1H
7.849
7.805
7.692
7.594
7.585
7.573
7.561
7.510
7.498
7.483
7.469
7.453
7.440
7.427
7.332
7.318
7.260
7.168
7.155
7.141
5.202
4.504
4.492
4.484
4.472
3.704
3.686
3.666
3.294
3.279
3.265
3.249
3.173
3.165
3.143
3.135
2.440
O
CN
O
N
Ts
3p
4.00
3.85
2.98
1.85
2.90
2.26
2.12
1.96
1.00
1.08
1.09
1.05
1.10
1.19
3.03
f1 (ppm)

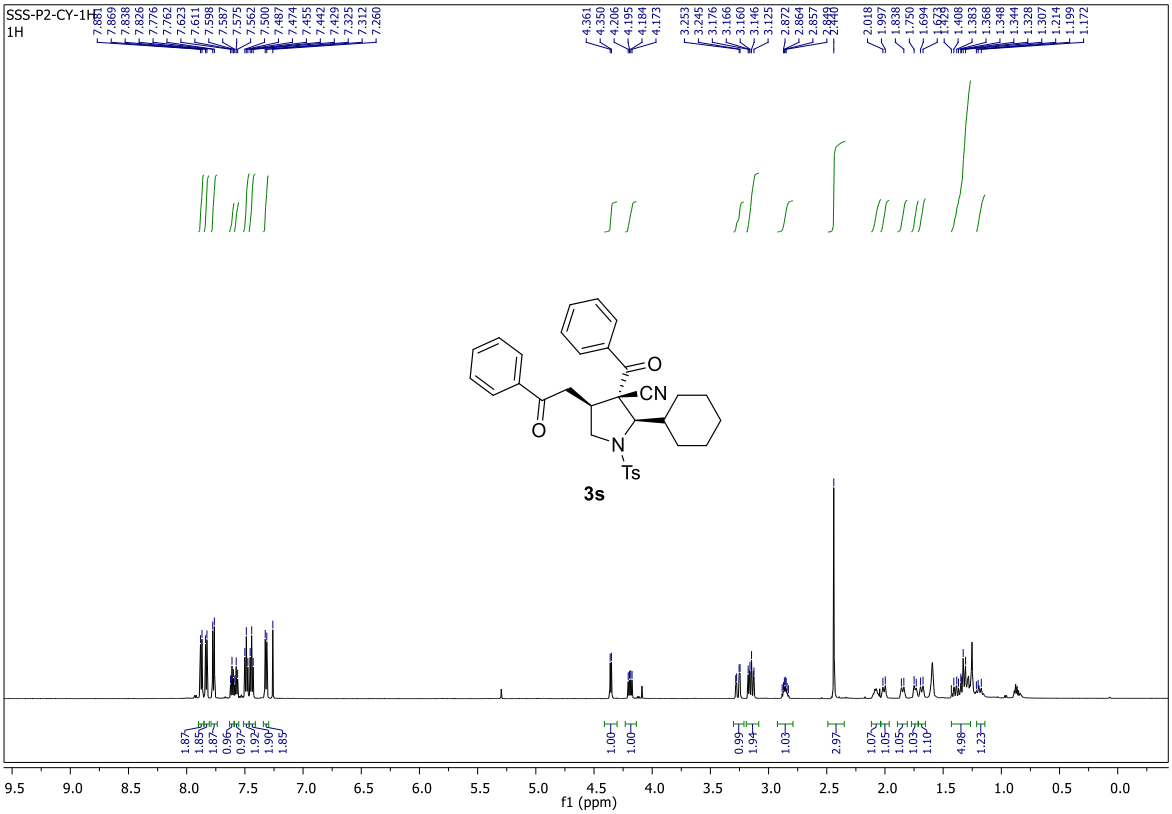

SSS-P2-2NAP-13C
13C
196.03
191.65
144.62
134.00
130.15
129.52
128.98
128.46
128.44
128.23
123.13
117.27
77.44
77.23
77.02
72.03
64.96
53.23
43.03
38.20
21.86
O
CN
O
N
Ts
3p
f1 (ppm)

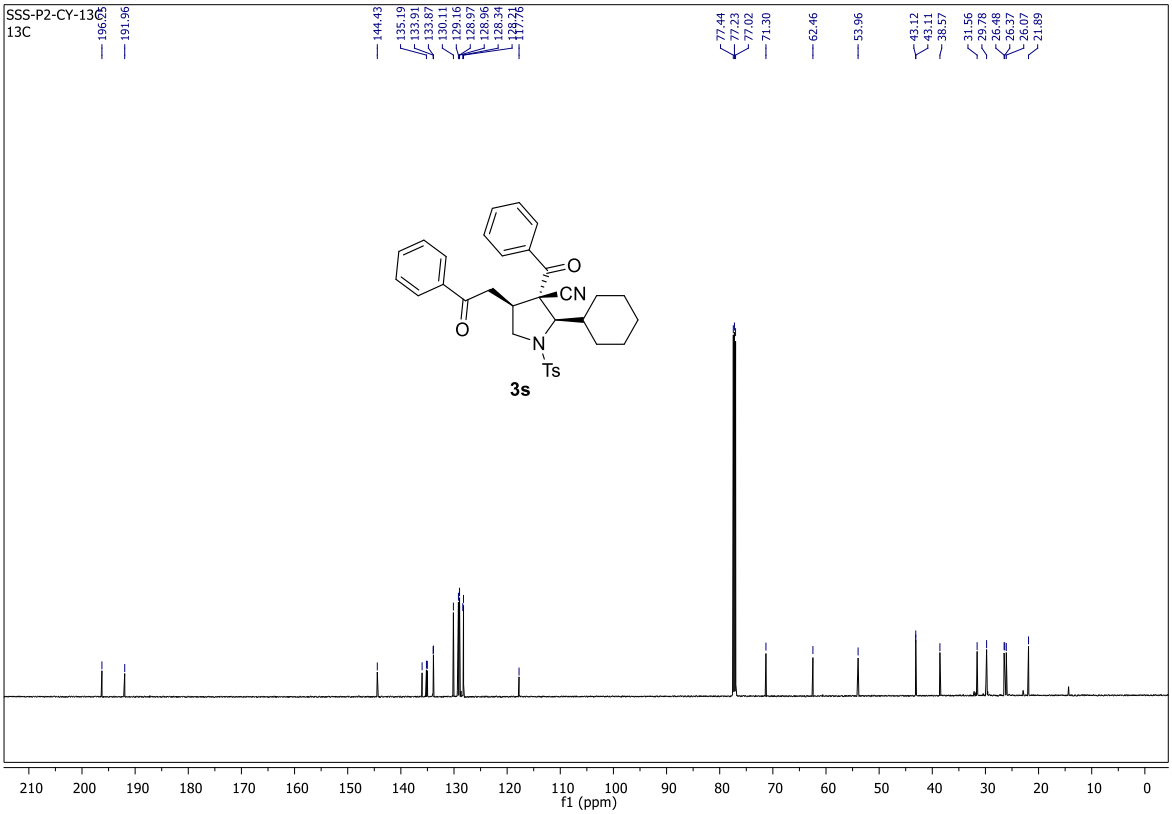

5.253
4.444
4.432
4.424
4.412
3.596
3.578
3.559
3.453
3.435
3.418
3.256
3.240
3.227
3.211
3.142
3.135
3.113
2.343
1.892
O
CN
O
N
Ts
3q
f1 (ppm)

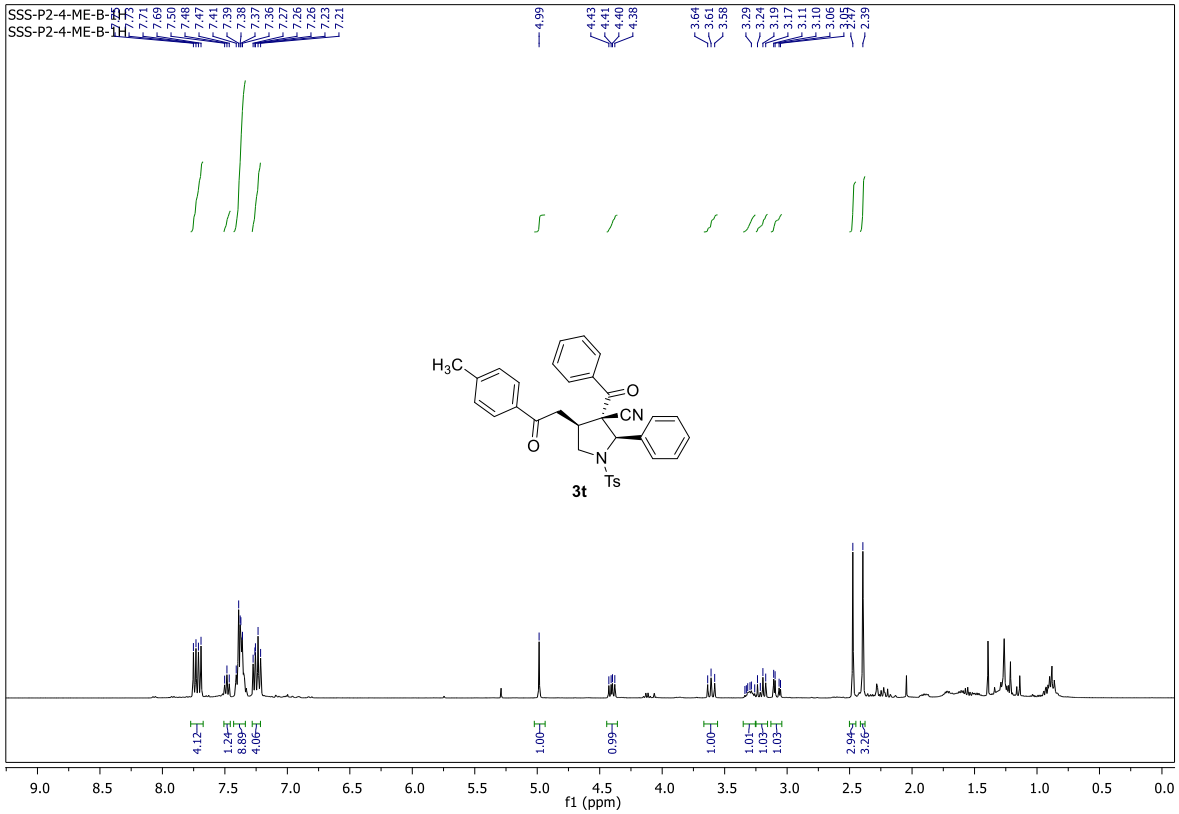

SSS-P2-2,4-DIMET-13C
13C
196.61
191.67
144.42
133.94
131.26
130.04
129.49
128.96
128.50
128.26
128.07
127.58
117.51
77.44
77.23
77.02
66.65
64.45
52.81
42.95
38.21
21.88
21.40
19.48
O
CN
O
N
Ts
3q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

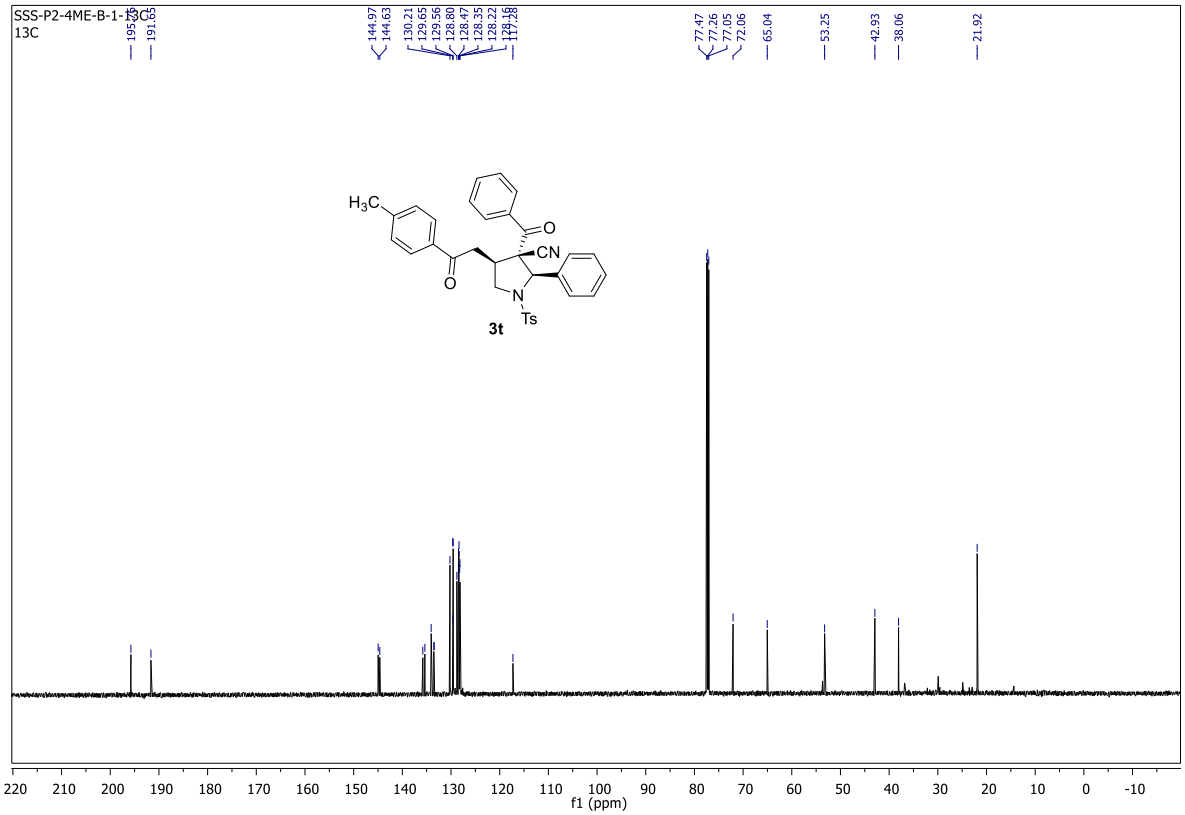

SSS-P2-2,4-DICL-A-1H
1H
7.977
7.963
7.866
7.854
7.830
7.817
7.572
7.558
7.550
7.537
7.496
7.493
7.482
7.479
7.467
7.455
7.442
7.346
7.333
7.319
7.302
7.299
7.260
5.486
4.315
4.308
4.304
4.297
4.287
4.277
3.615
3.599
3.594
3.579
3.227
3.208
3.201
3.154
3.141
3.118
2.508
O
CN
O
N
Ts
Cl
Cl
3r
1.04
1.82
1.98
4.09
5.17
1.91
0.92
1.00
1.19
1.21
2.13
1.09
2.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

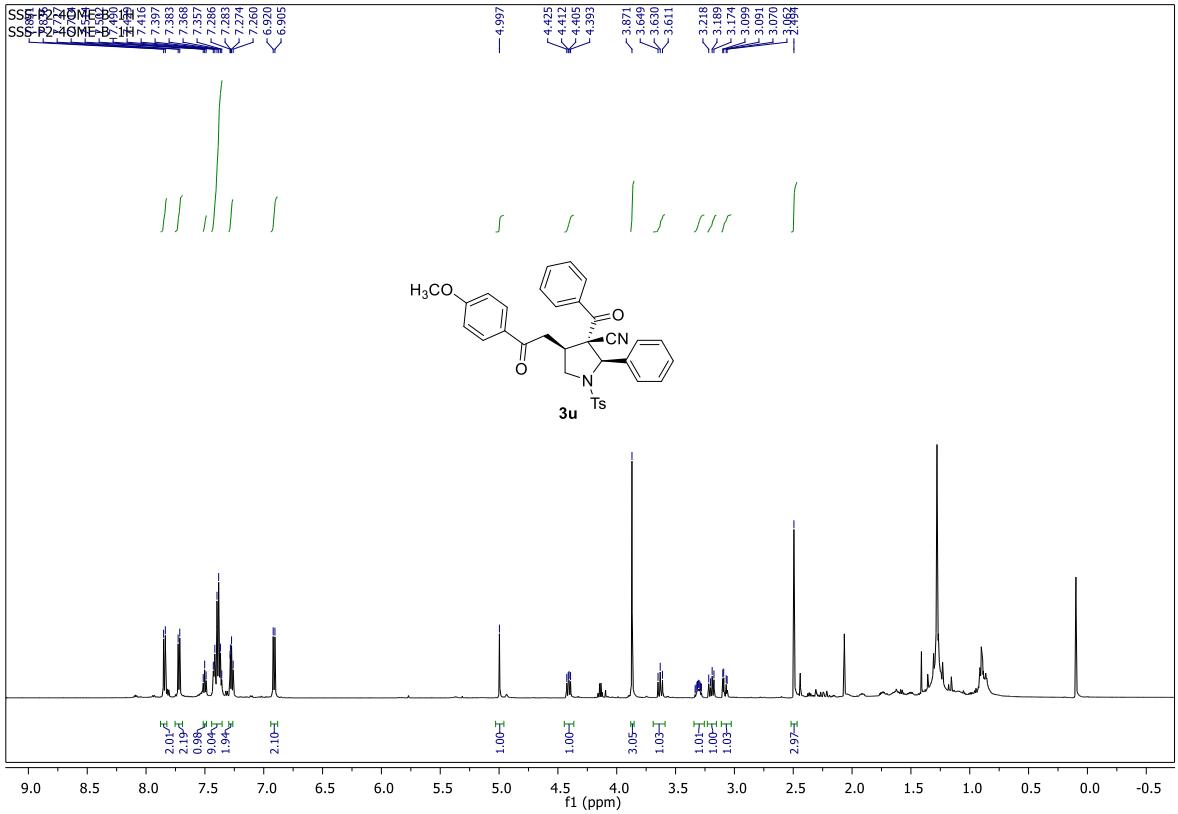

SSS-P2-22-DICL-A-13C
13C
195.47
190.10
145.12
134.55
134.09
131.58
130.41
129.36
129.30
129.03
128.67
128.49
77.44
77.23
77.02
66.35
63.42
53.01
43.41
38.13
21.99
O
CN
O
N
Ts
Cl
Cl
3r
f1 (ppm)

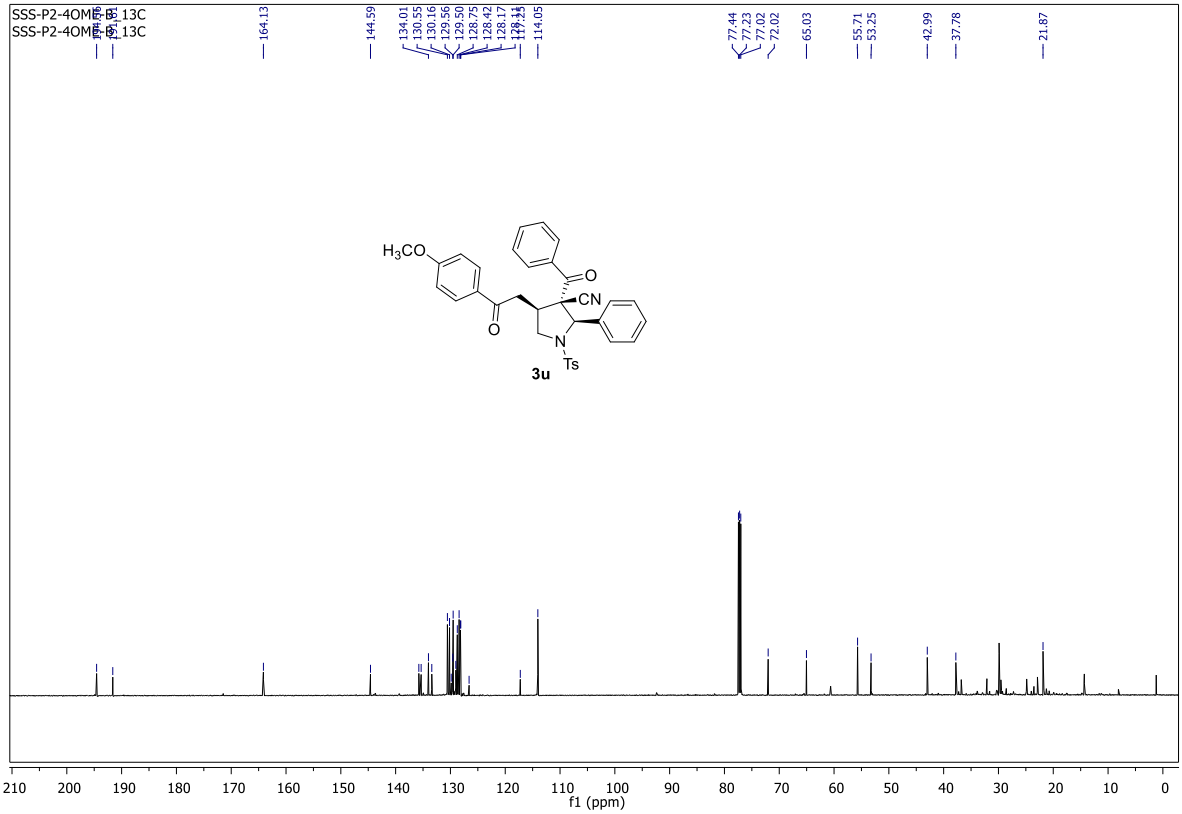

SSS-P2-CY-1H
1H
7.881
7.869
7.838
7.826
7.776
7.762
7.623
7.611
7.598
7.587
7.575
7.562
7.500
7.487
7.474
7.455
7.442
7.429
7.325
7.312
7.260
4.361
4.350
4.206
4.195
4.184
4.173
3.253
3.245
3.176
3.166
3.160
3.146
3.125
2.872
2.864
2.857
2.849
2.840
2.018
1.997
1.838
1.750
1.694
1.623
1.408
1.383
1.368
1.348
1.344
1.328
1.307
1.214
1.199
1.172
O
CN
O
N
Ts
3s
1.87
1.85
1.87
0.96
0.97
1.92
1.90
1.85
1.00
1.00
0.99
1.94
1.03
2.97
1.07
1.05
1.05
1.03
1.10
4.98
1.23
f1 (ppm)

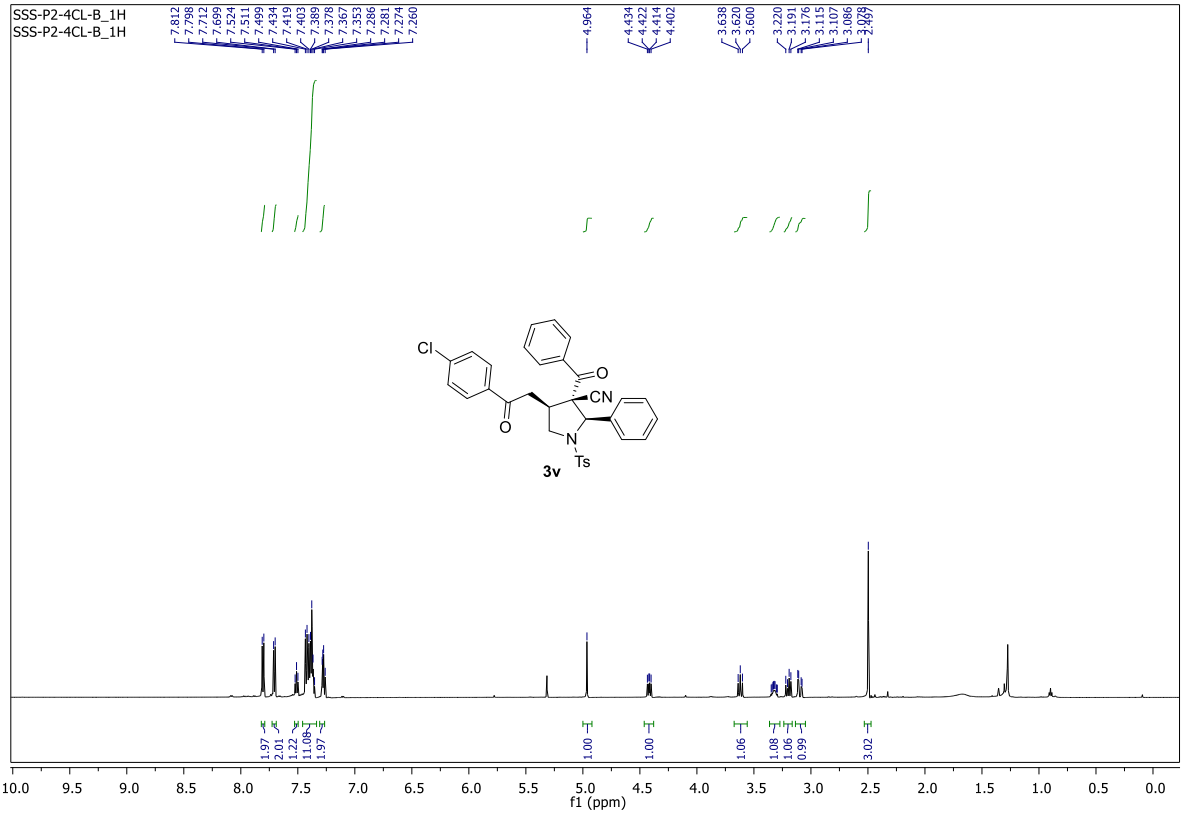

SSS-P2-CY-13C
13C
196.25
191.96
144.43
135.19
133.91
133.87
130.11
129.16
128.97
128.96
128.34
77.44
77.23
77.02
71.30
62.46
53.96
43.12
43.11
38.57
31.56
29.78
26.48
26.37
26.07
21.89
O
CN
O
N
Ts
3s
f1 (ppm)

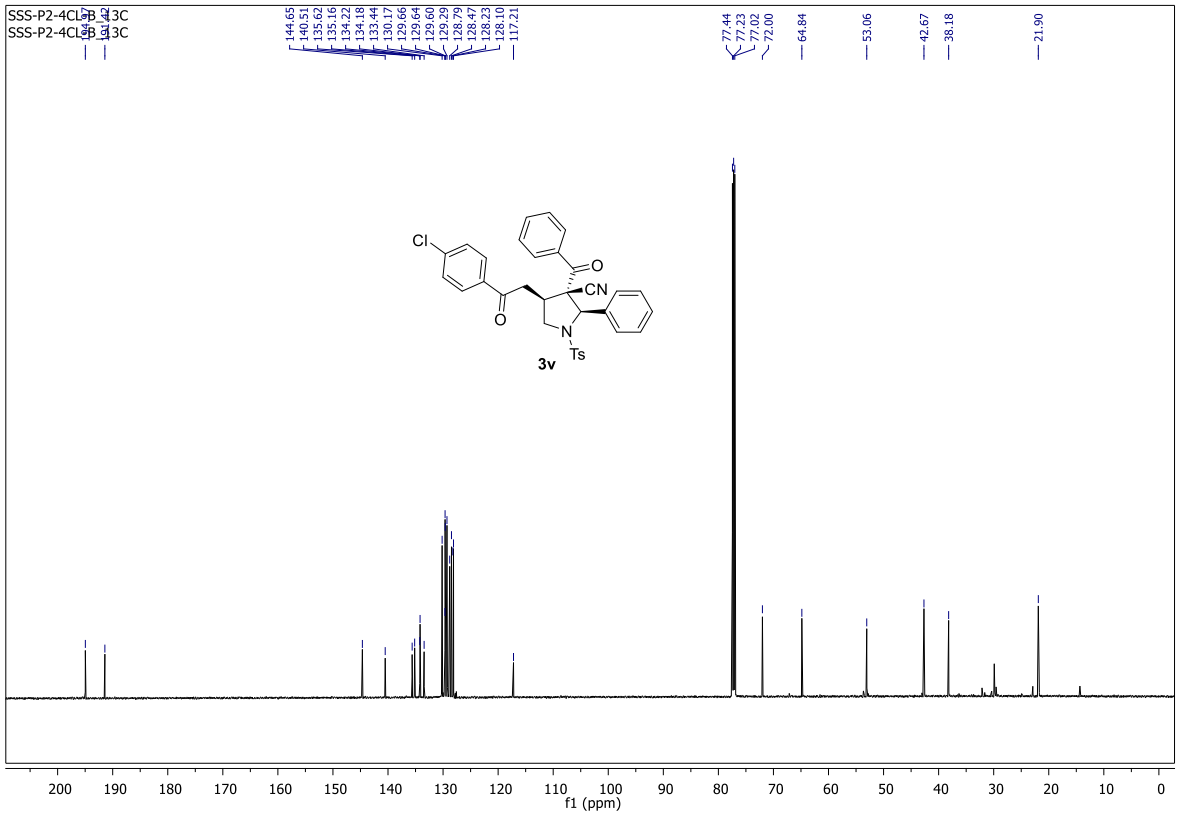

SSS-P2-4-ME-B-1H
SSS-P2-4-ME-B-1H
7.73
7.71
7.69
7.50
7.48
7.47
7.41
7.39
7.38
7.37
7.36
7.27
7.26
7.26
7.23
7.21
4.99
4.43
4.41
4.40
4.38
3.64
3.61
3.58
3.29
3.24
3.19
3.17
3.11
3.10
3.06
2.39
H3C
O
CN
O
N
Ts
3t
4.12
1.24
8.89
4.06
1.00
0.99
1.00
1.01
1.03
1.03
2.94
3.26
f1 (ppm)

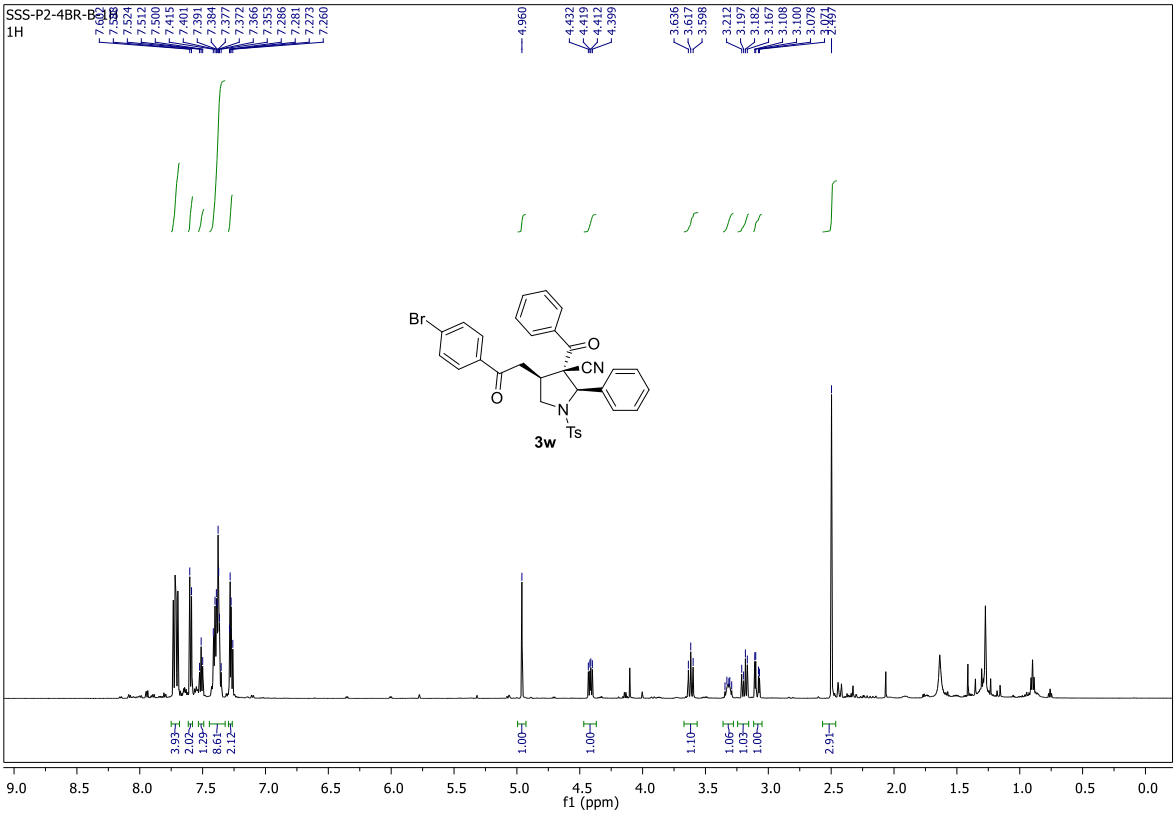

SSS-P2-4ME-B-1-13C
13C
195.19
191.65
144.97
144.63
130.21
129.65
129.56
128.80
128.47
128.35
128.22
128.16
127.28
77.47
77.26
77.05
72.06
65.04
53.25
42.93
38.06
21.92
H3C
O
CN
O
N
Ts
3t
f1 (ppm)

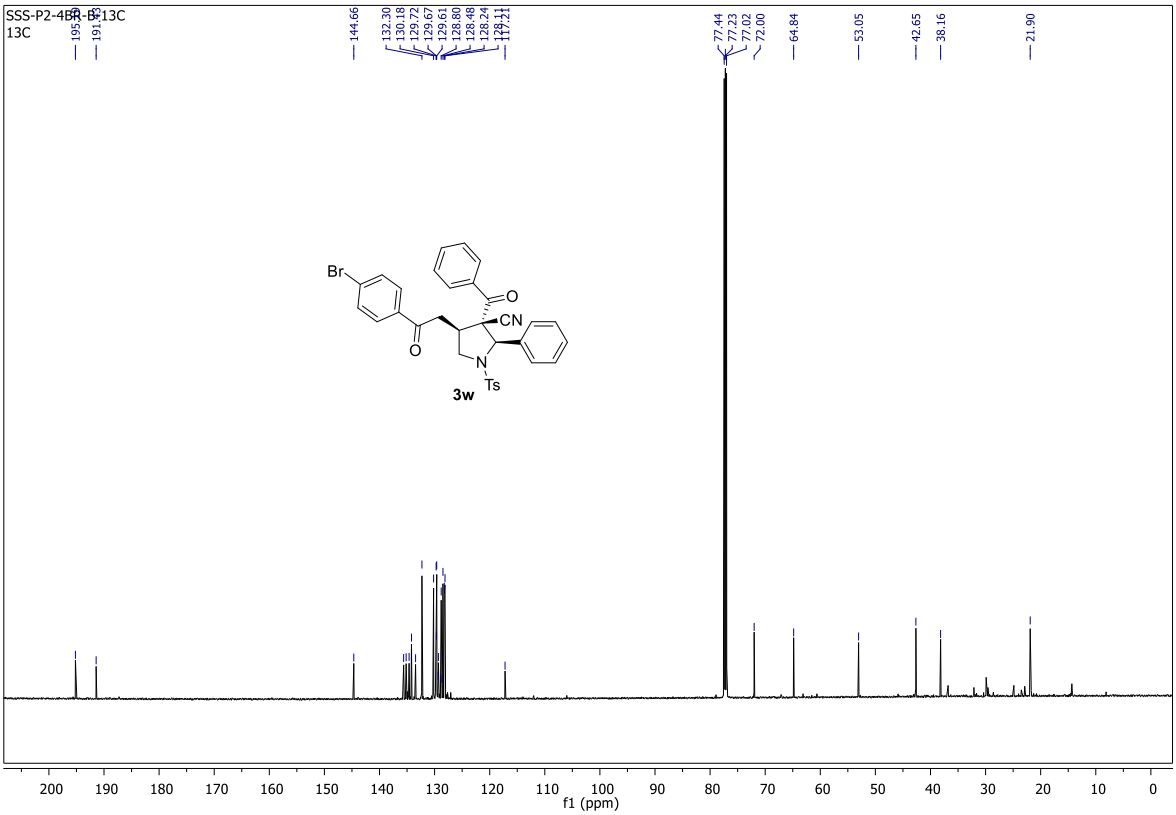

SSS-P2-4OME-B_1H
7.416
7.397
7.383
7.368
7.357
7.286
7.283
7.274
7.260
6.920
6.905
4.997
4.425
4.412
4.405
4.393
3.871
3.649
3.630
3.611
3.218
3.189
3.174
3.099
3.091
3.070
2.494
H3CO
O
CN
O
N
Ts
3u
2.01
2.19
0.98
9.04
1.94
2.10
1.00
1.00
3.05
1.03
1.01
1.00
1.03
2.97
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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)

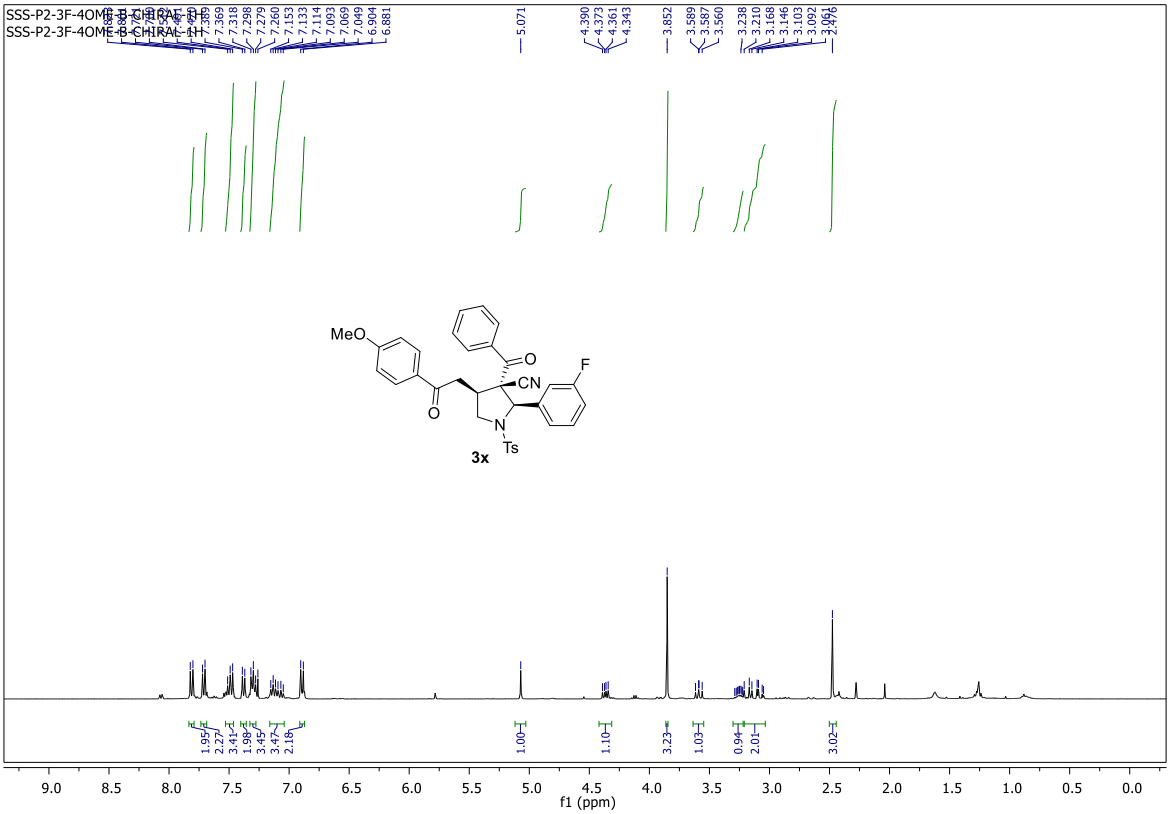

SSS-P2-4OME-B_13C
SSS-P2-4OME-B_13C
164.13
144.59
134.01
130.55
130.16
129.56
129.50
128.75
128.42
128.17
114.05
77.44
77.23
77.02
72.02
65.03
55.71
53.25
42.99
37.78
21.87
H3CO
O
CN
O
N
Ts
3u
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

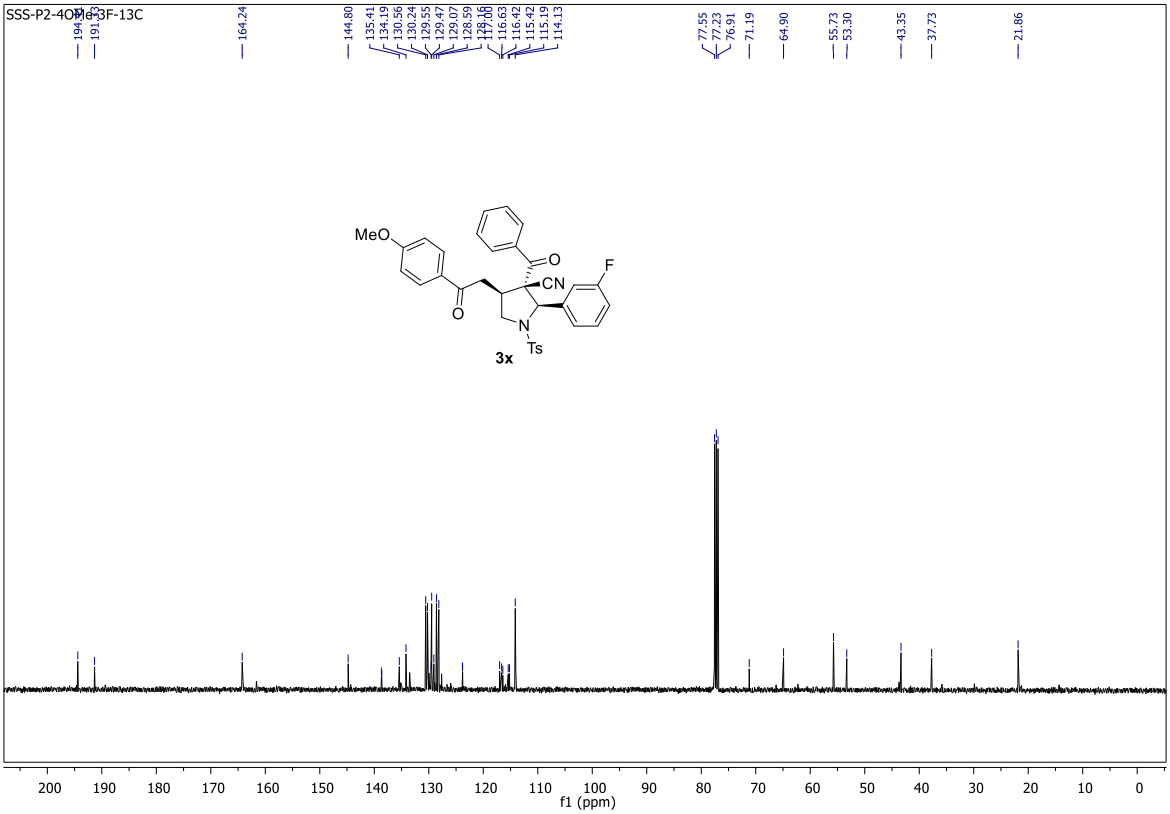

SSS-P2-4CL-B_1H
SSS-P2-4CL-B_1H
7.812
7.798
7.712
7.699
7.524
7.511
7.499
7.434
7.419
7.403
7.389
7.378
7.367
7.353
7.286
7.281
7.274
7.260
4.964
4.434
4.422
4.414
4.402
3.638
3.620
3.600
3.220
3.191
3.176
3.115
3.107
3.086
2.497
Cl
O
CN
O
N
Ts
3v
1.97
2.01
1.22
11.08
1.97
1.00
1.00
1.06
1.08
1.06
0.99
3.02
f1 (ppm)

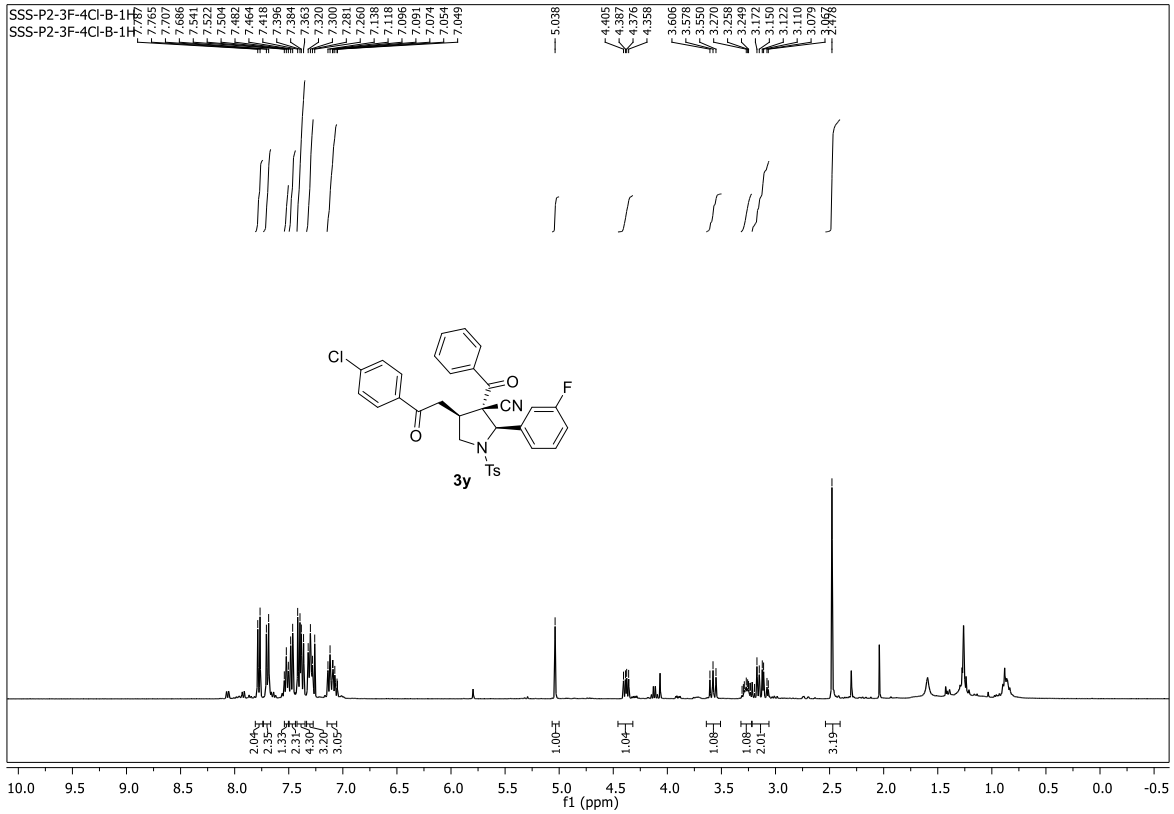

SSS-P2-4CL-B_13C
SSS-P2-4CL-B_13C
144.65
140.51
135.62
135.16
134.22
134.18
133.44
130.17
129.66
129.64
129.60
129.29
128.79
128.47
128.23
128.10
117.21
77.44
77.23
77.02
72.00
64.84
53.06
42.67
38.18
21.90
Cl
O
CN
O
N
Ts
3v
f1 (ppm)

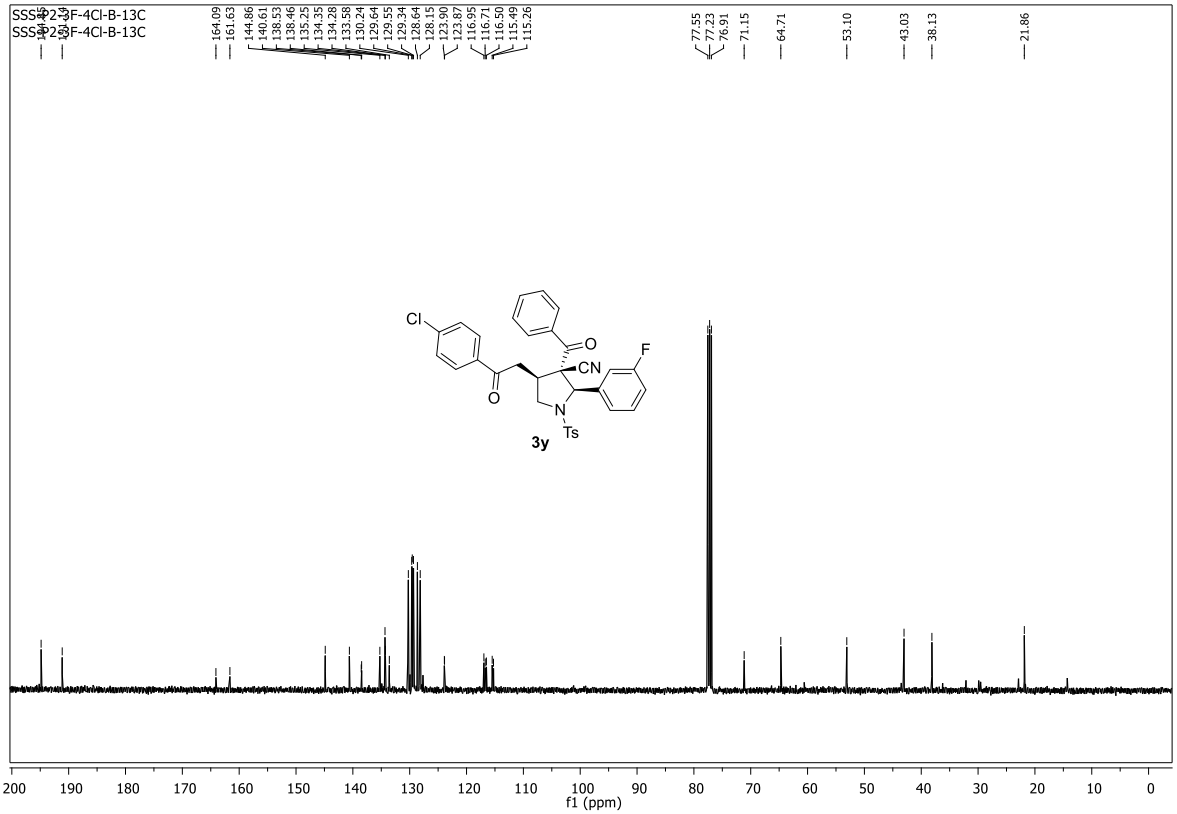

SSS-P2-4BR-B-1H
1H
Br
O
CN
O
N
Ts
3w
f1 (ppm)


SSS-P2-4BR-B-13C
13C
Br
O
CN
O
N
Ts
3w
f1 (ppm)

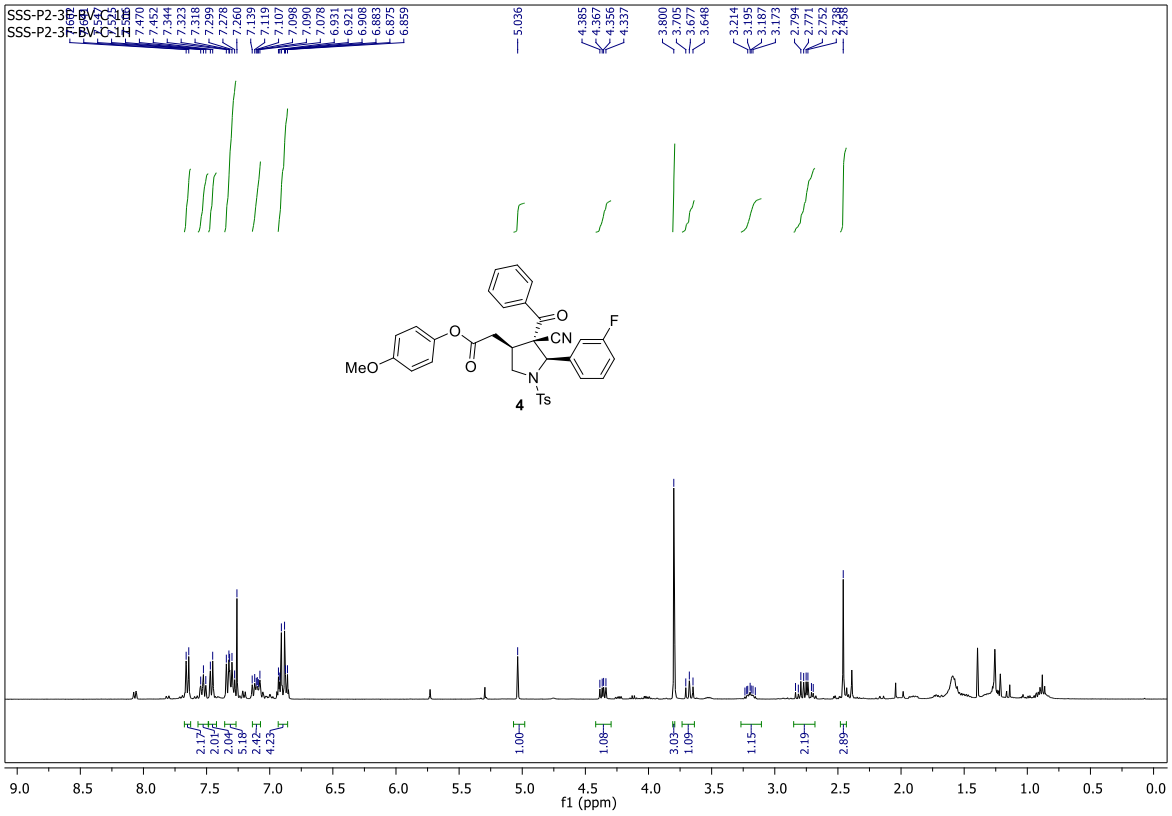

SSS-P2-3F-4OME-B-CHIRAL-1H
MeO
O
CN
F
O
N
Ts
3x
f1 (ppm)

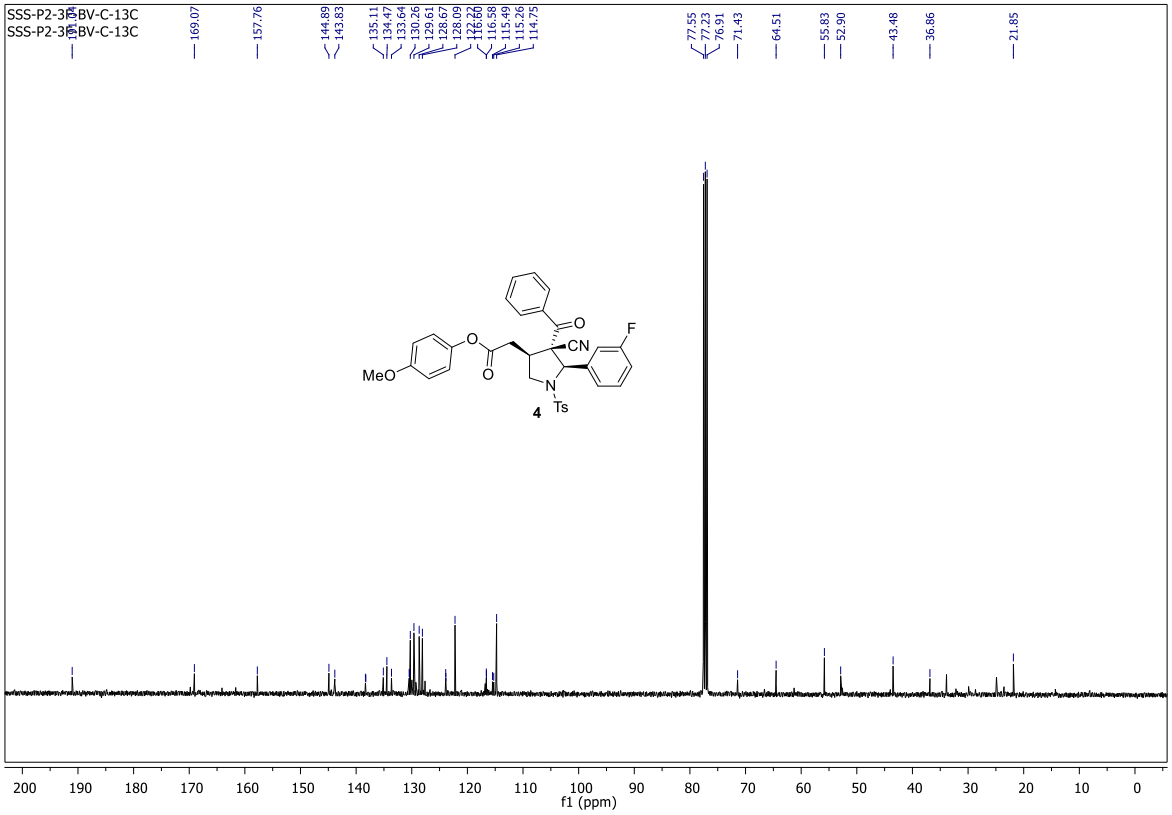

SSS-P2-4OME-3F-13C
MeO
O
CN
F
O
N
Ts
3x
f1 (ppm)


SSS-P2-3F-4Cl-B-1H
SSS-P2-3F-4Cl-B-1H
7.787
7.765
7.707
7.686
7.541
7.522
7.504
7.482
7.464
7.418
7.396
7.384
7.363
7.320
7.300
7.281
7.260
7.138
7.118
7.096
7.091
7.074
7.054
7.049
5.038
4.405
4.387
4.376
4.358
3.606
3.578
3.550
3.270
3.258
3.249
3.172
3.150
3.122
3.110
3.079
3.047
3.028
Cl
O
F
CN
O
N
Ts
3y
2.04
2.35
1.33
2.31
4.30
3.20
3.05
1.00
1.04
1.08
1.08
2.01
3.19
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

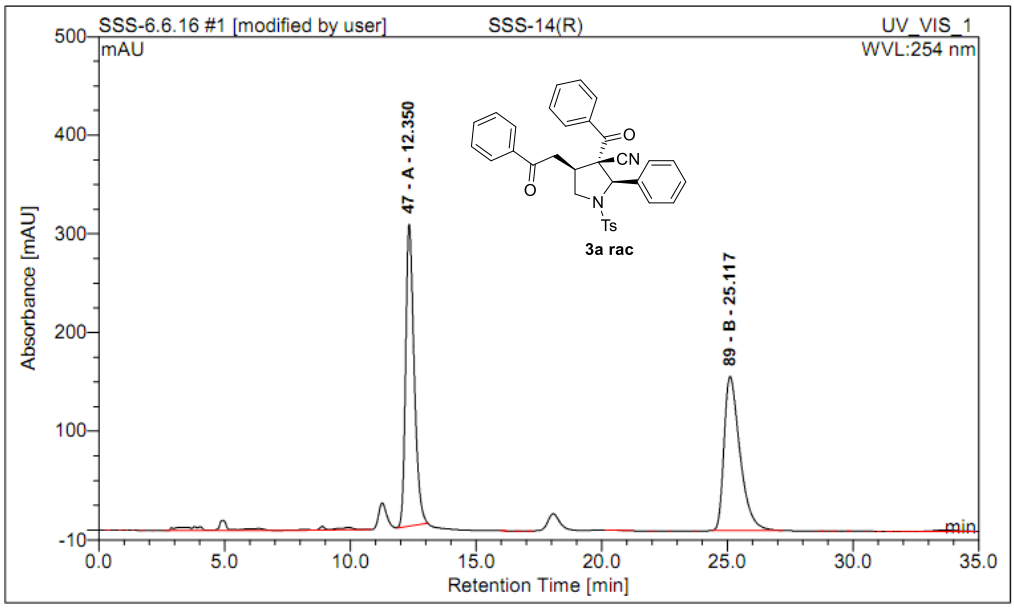

SSS-P2-3F-4Cl-B-13C
SSS-P2-3F-4Cl-B-13C
164.09
161.63
144.86
140.61
138.53
138.46
135.25
134.35
134.28
133.58
130.24
129.64
129.55
129.34
128.64
128.15
123.90
123.87
116.95
116.71
116.50
115.49
115.26
77.55
77.23
76.91
71.15
64.71
53.10
43.03
38.13
21.86
Cl
O
F
CN
O
N
Ts
3y
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

J. NMR Spectra of compounds 4:

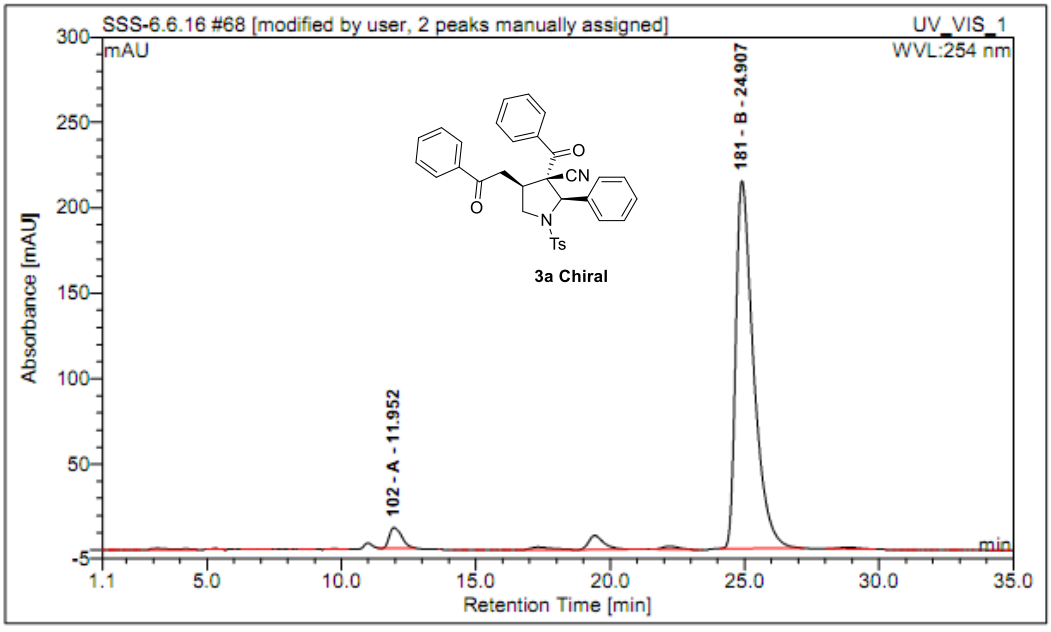




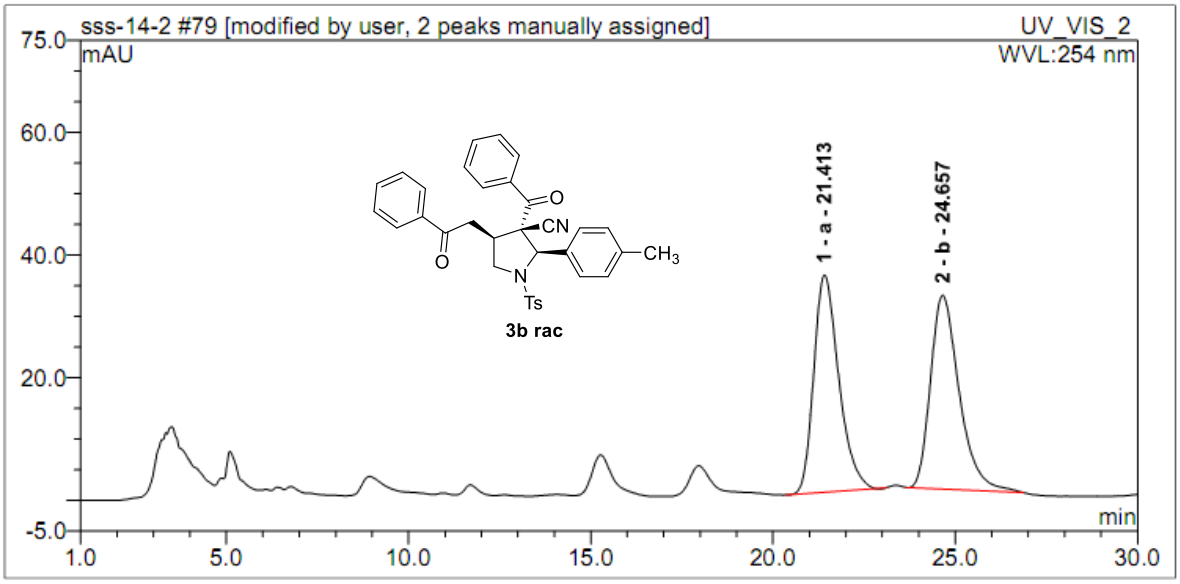
K. HPLC chromatograms of (3a-3y):



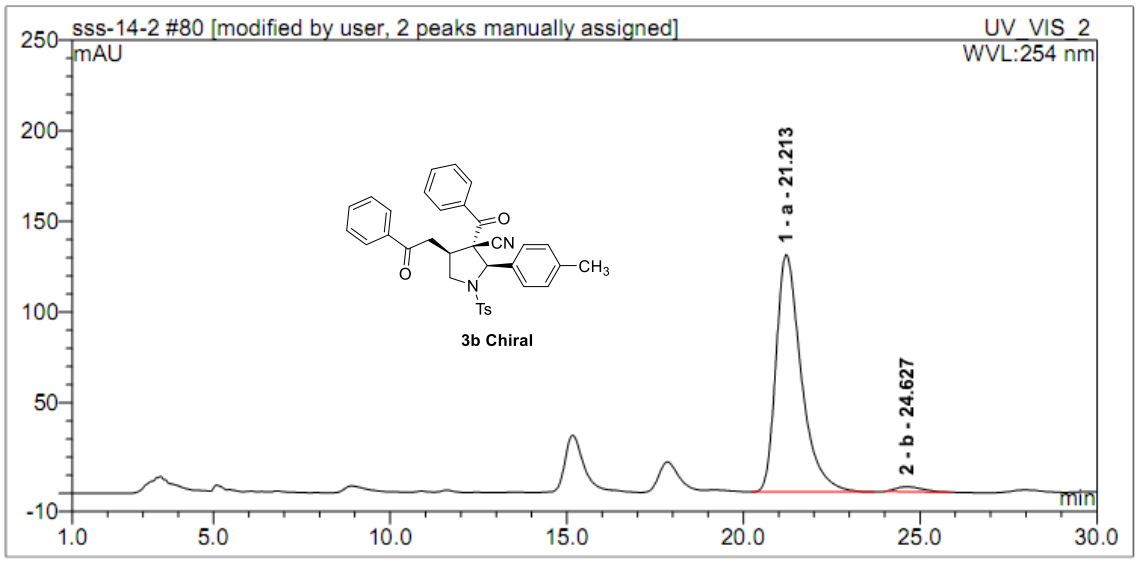
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
47	A	12.35	119.9935	51.18584357	305.9554	n.a.
89	B	25.12	114.434	48.81415643	156.038	n.a.



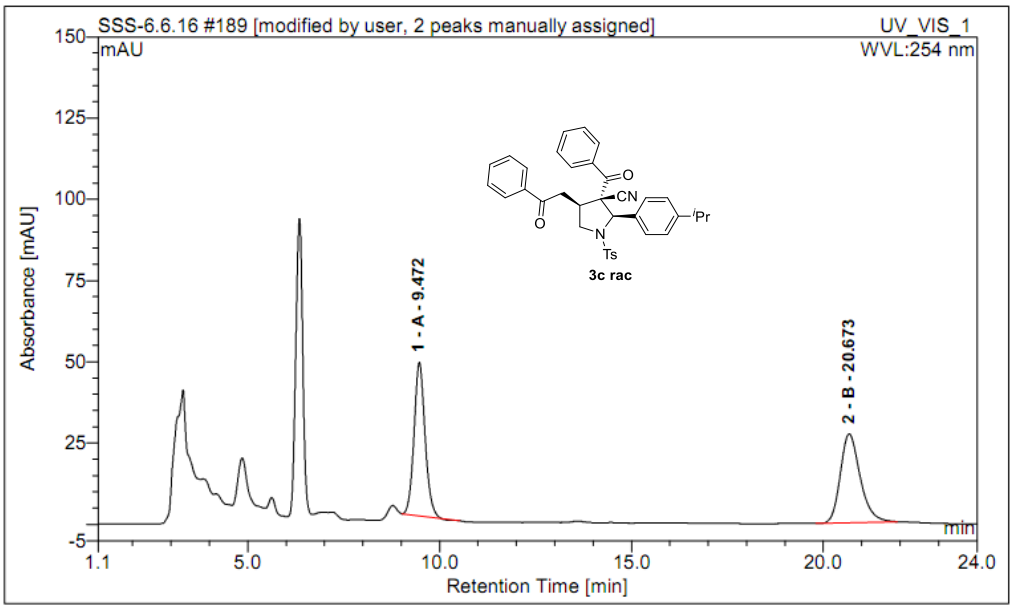
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
102	A	11.95	6.223216	3.647795857	11.84795	n.a.
181	B	24.91	164.379	96.35211932	215.153	n.a.



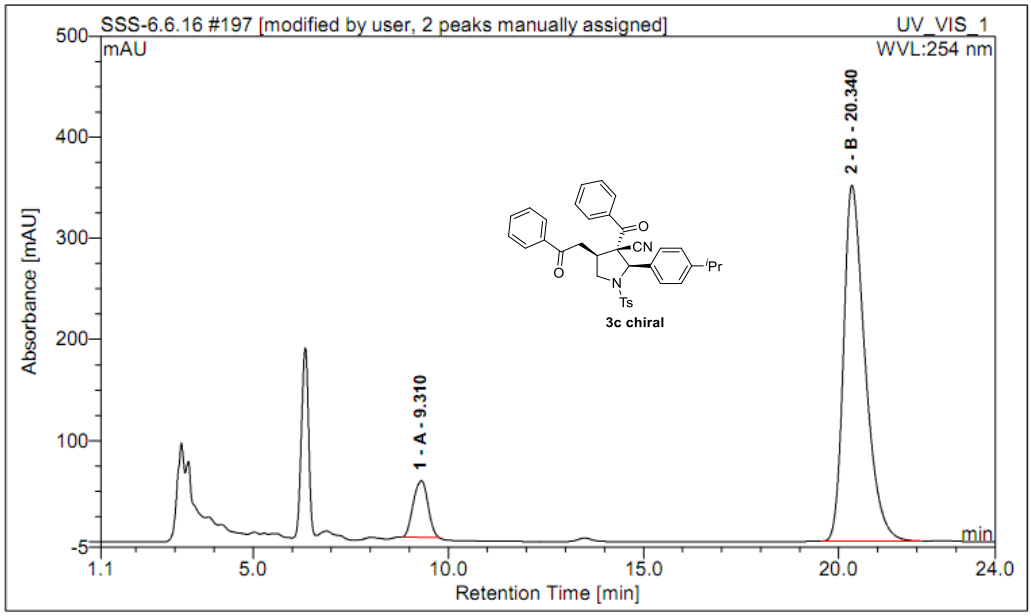
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	21.41	28.15373	49.33569561	35.40188	n.a.
2	b	24.66	28.912	50.66430439	31.609	n.a.



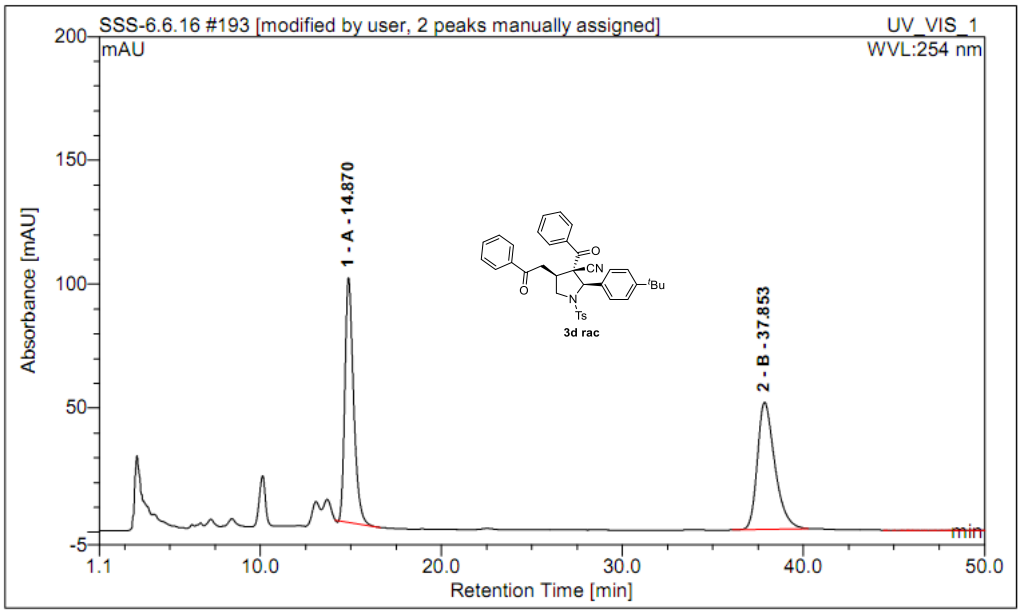
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	21.21	108.6271	97.79521062	130.9079	n.a.
2	b	24.63	2.449	2.204789378	2.780	n.a.



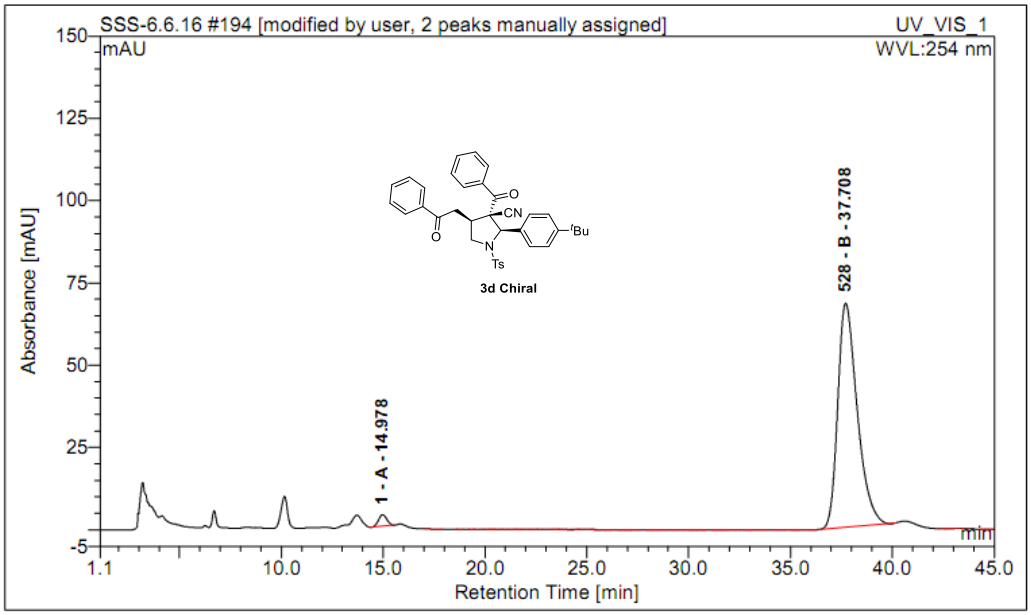
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	A	9.47	15.72327	48.89750634	47.20856	n.a.
2	B	20.67	16.432	51.10249366	27.332	n.a.



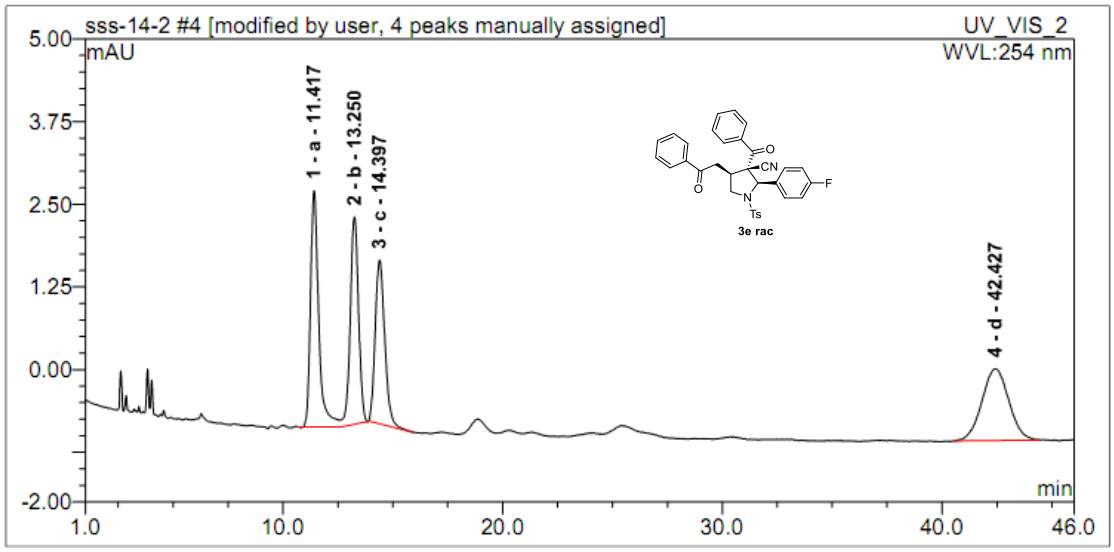
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	A	9.31	24.52906	9.886470601	56.04595	n.a.
2	B	20.34	223.578	90.1135294	351.907	n.a.



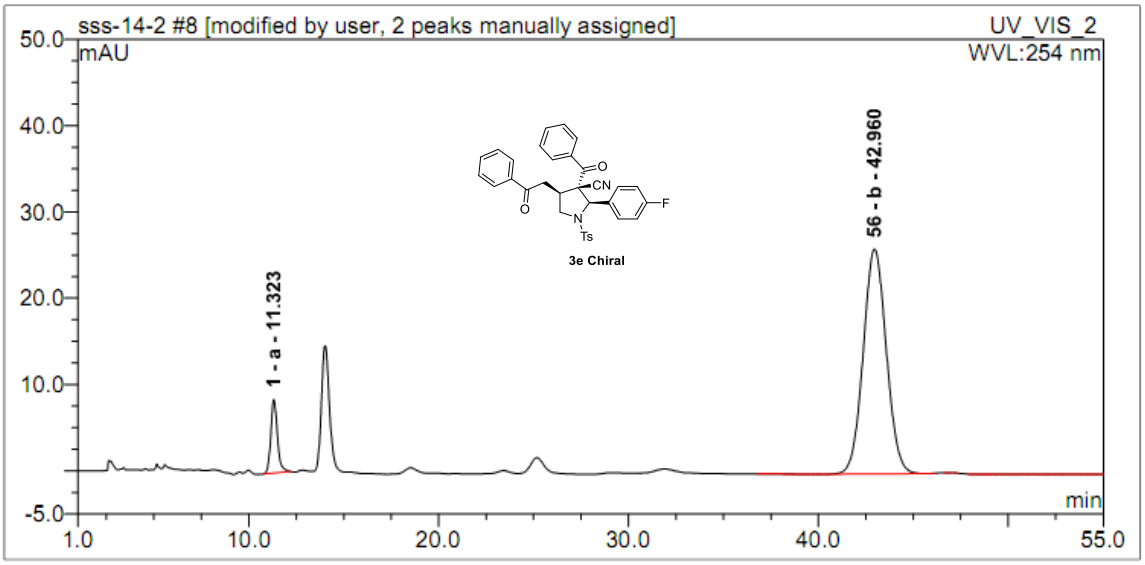
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	A	14.87	54.62341	48.76504742	98.74469	n.a.
2	B	37.85	57.390	51.23495258	51.293	n.a.



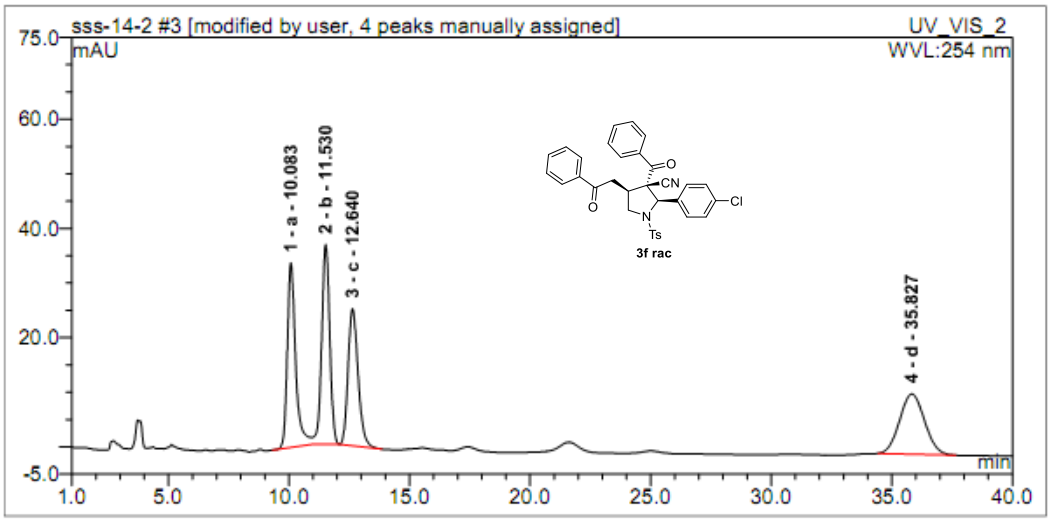
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	A	14.98	1.641753	2.142214333	3.50538	n.a.
528	B	37.71	74.996	97.85778567	68.023	n.a.



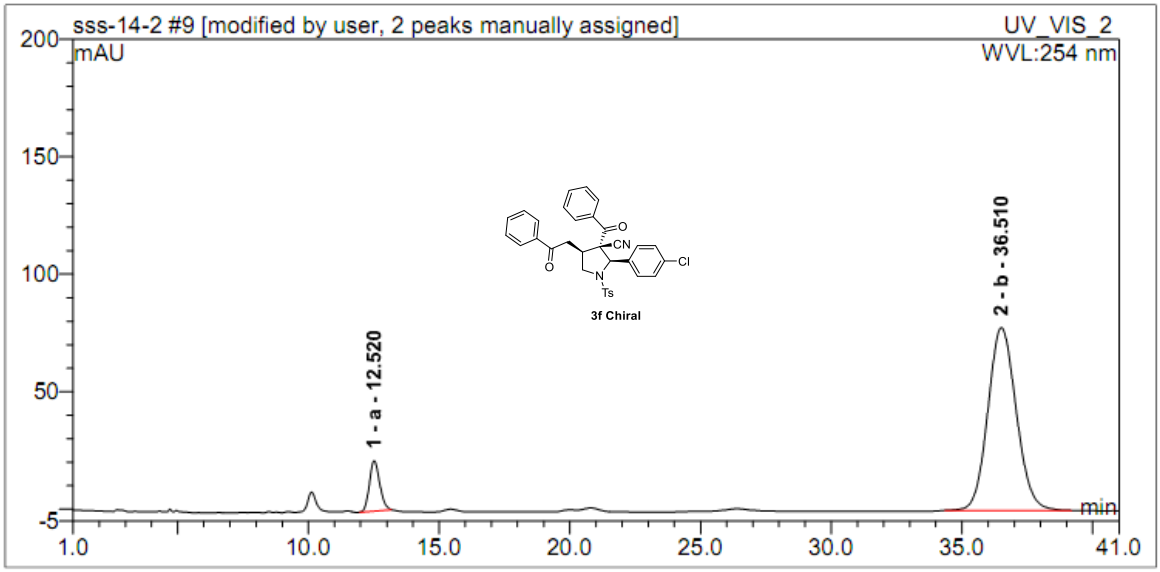
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	11.42	1.553299	27.1965351	3.57601	n.a.
2	b	13.25	1.368065	23.95328276	3.13637	n.a.
3	c	14.40	1.252781	21.93479212	2.4752	n.a.
4	d	42.43	1.537	26.91539003	1.083	n.a.



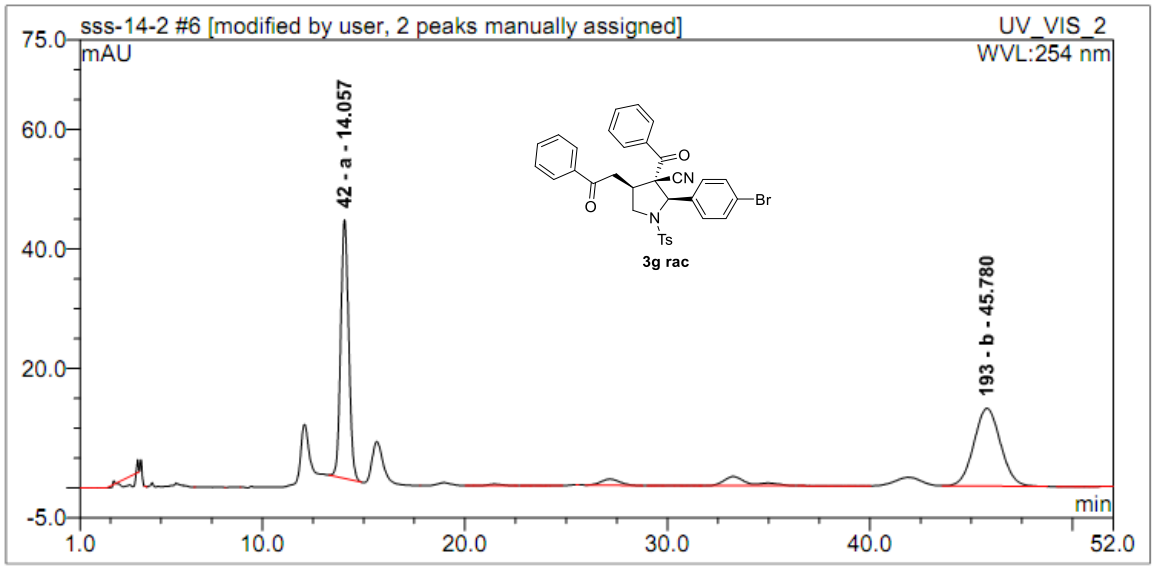
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	11.32	3.423424	8.505946779	8.51202	n.a.
56	b	42.96	36.824	91.49405322	26.060	n.a.



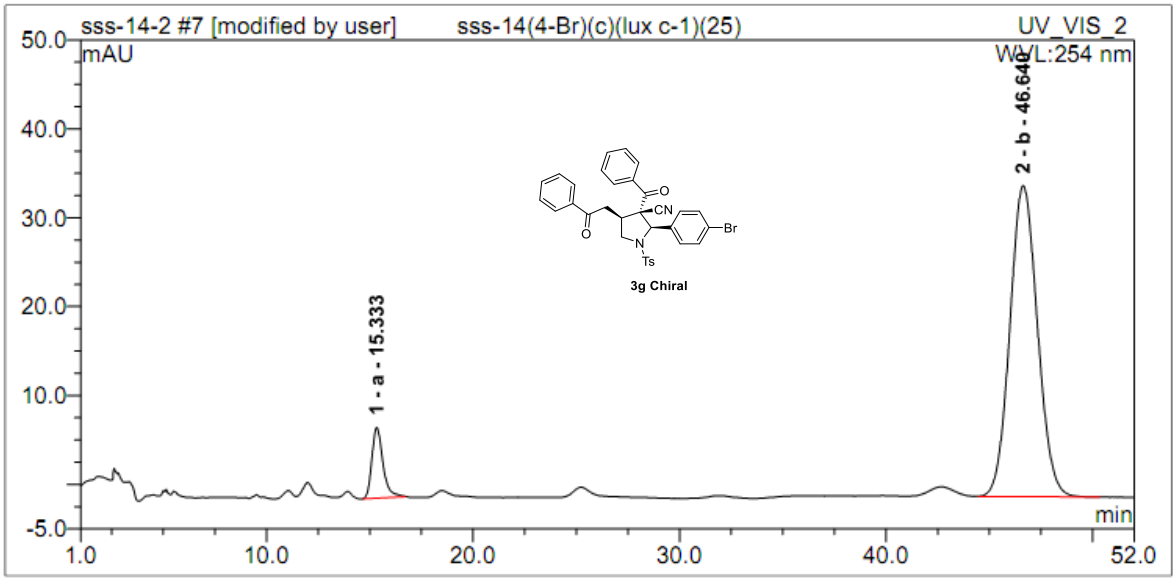
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	10.08	13.51837	25.48475913	33.79812	n.a.
2	b	11.53	14.10603	26.59260893	36.57039	n.a.
3	c	12.64	12.16381	22.93114289	25.10908	n.a.
4	d	35.83	13.257	24.99148905	11.030	n.a.



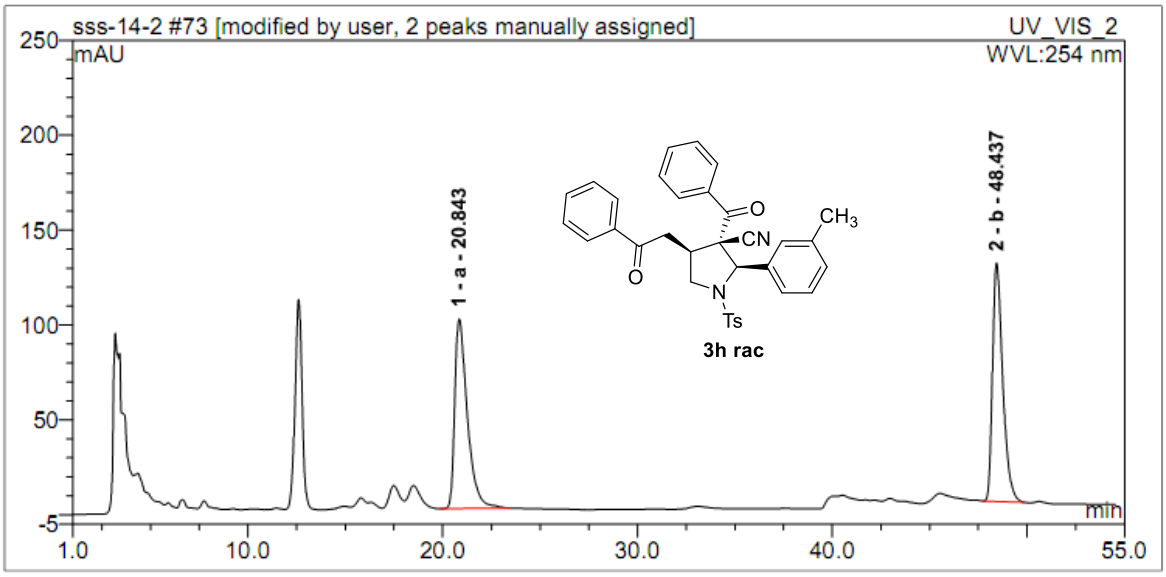
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	12.52	9.789193	9.060136255	21.344	n.a.
2	b	36.51	98.258	90.93986374	77.830	n.a.



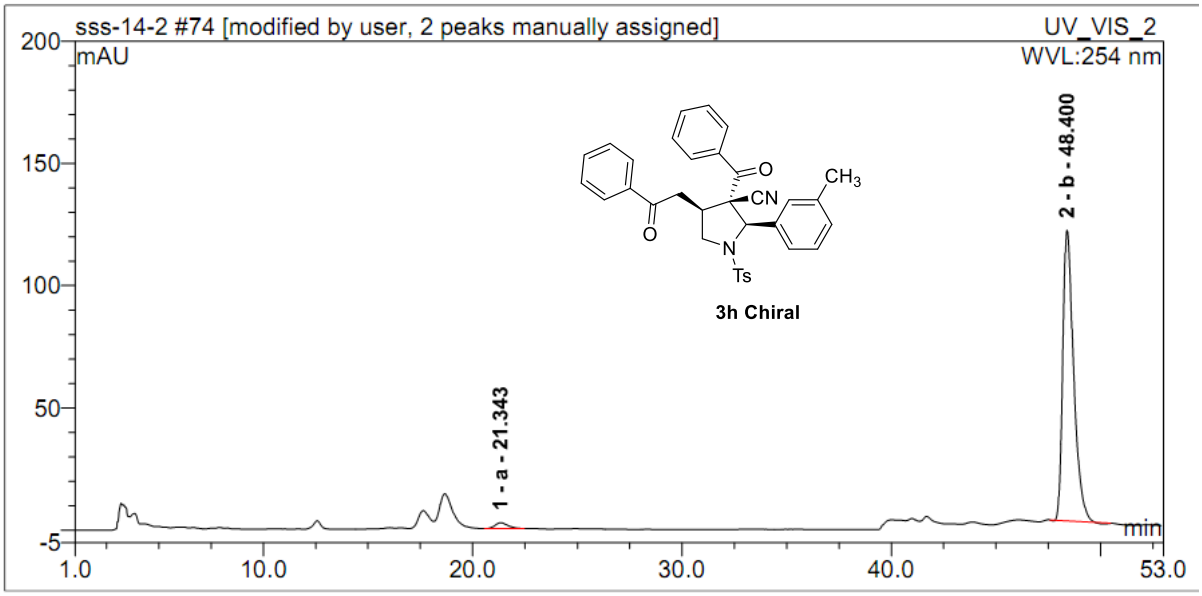
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
42	a	14.06	19.7556	49.84185979	43.28597	n.a.
193	b	45.78	19.881	50.15814021	13.015	n.a.



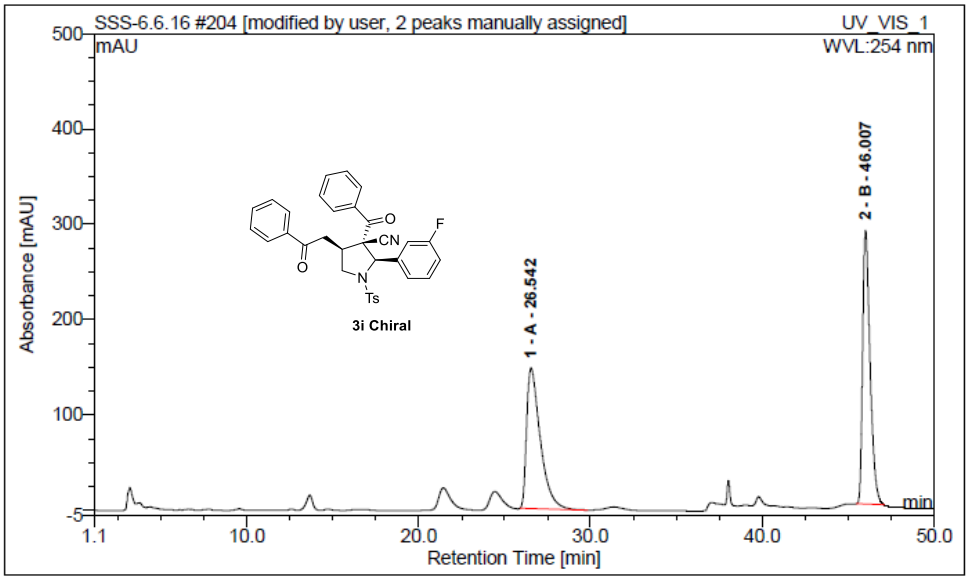
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	15.33	4.935005	8.349526267	7.95797	n.a.
2	b	46.64	54.170	91.65047373	35.007	n.a.



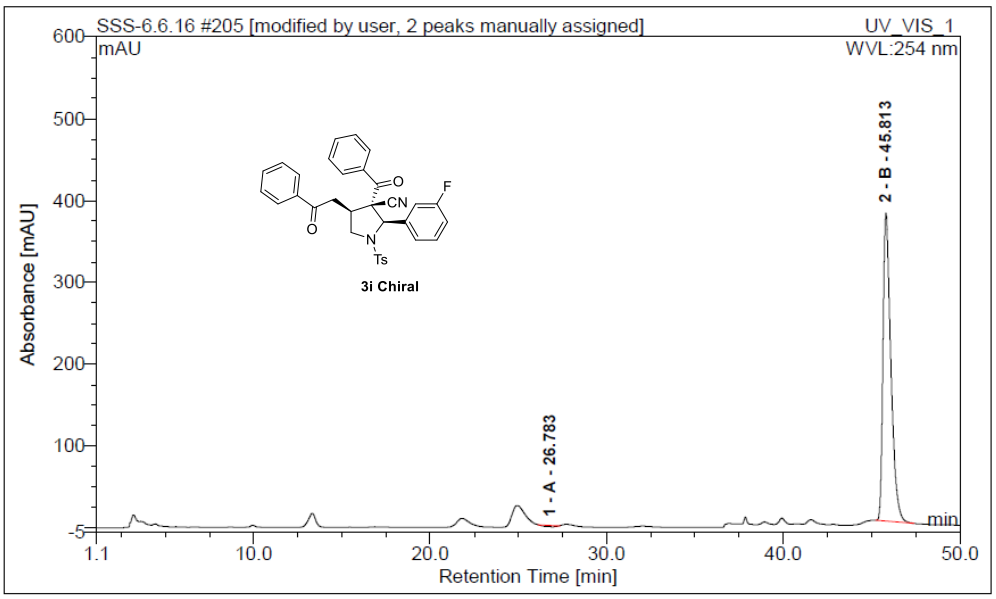
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	20.84	75.01123	49.51442424	99.95133	n.a.
2	b	48.44	76.482	50.48557576	125.751	n.a.



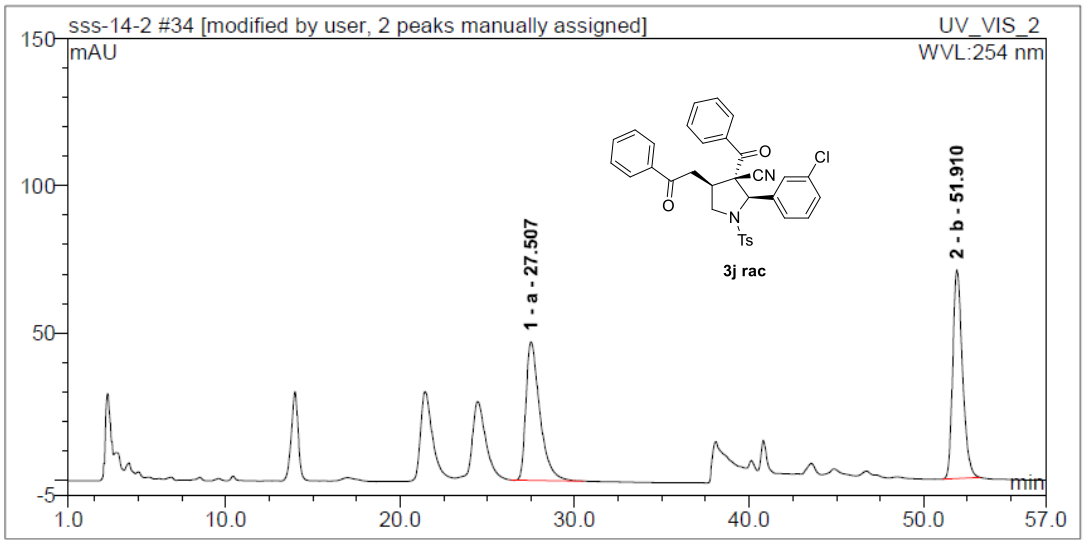
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	21.34	1.722688	2.348071856	2.39917	n.a.
2	b	48.40	71.643	97.65192814	118.840	n.a.



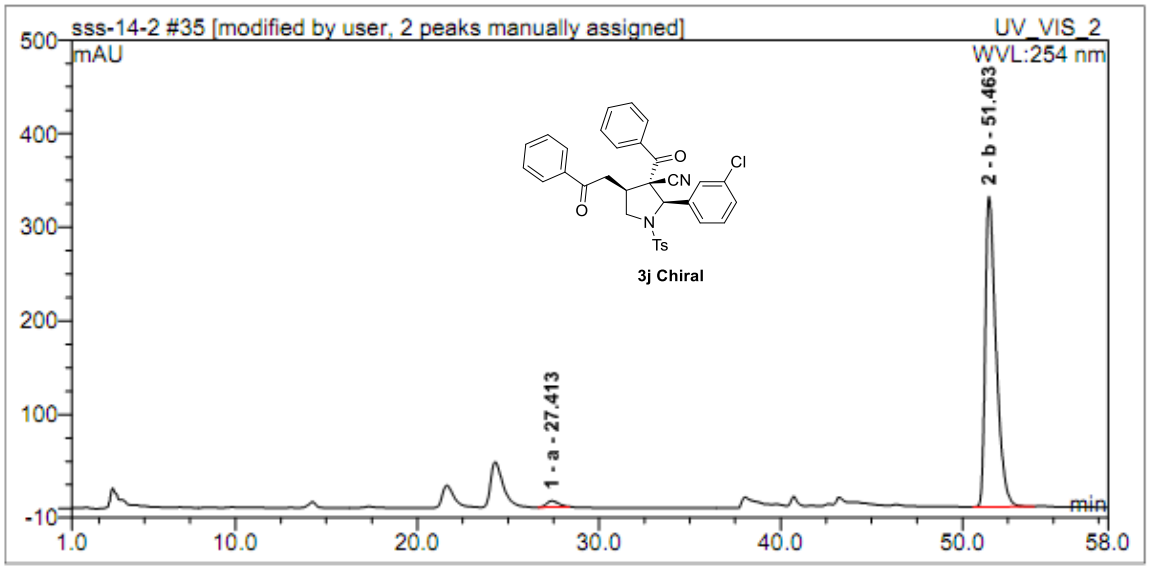
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	A	26.54	135.4358	48.44532586	147.3504	n.a.
2	B	46.01	144.128	51.55467414	287.391	n.a.



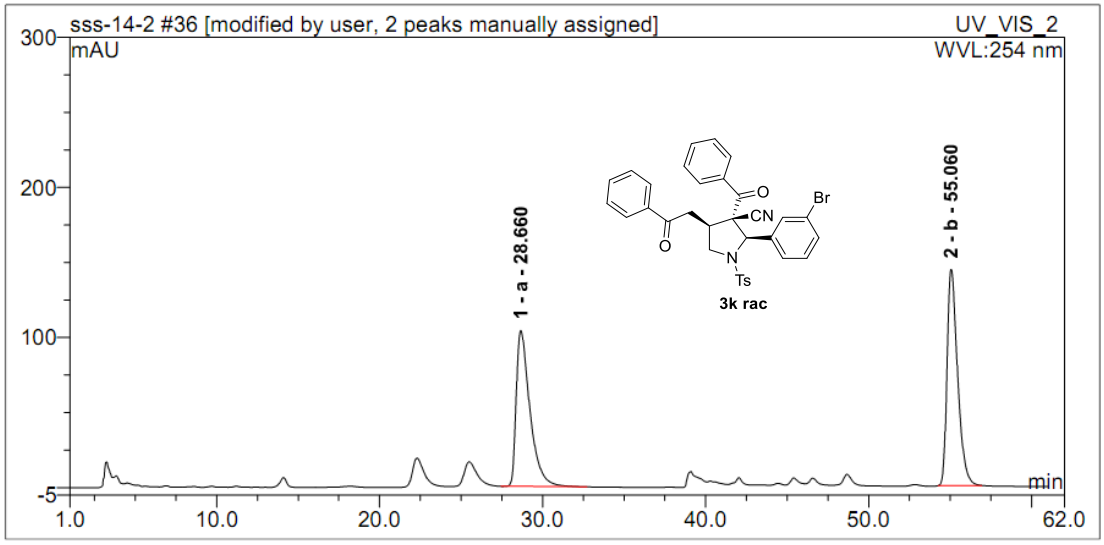
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	A	26.78	1.43681	0.7328803172	1.63607	n.a.
2	B	45.81	194.613	99.26711968	376.433	n.a.



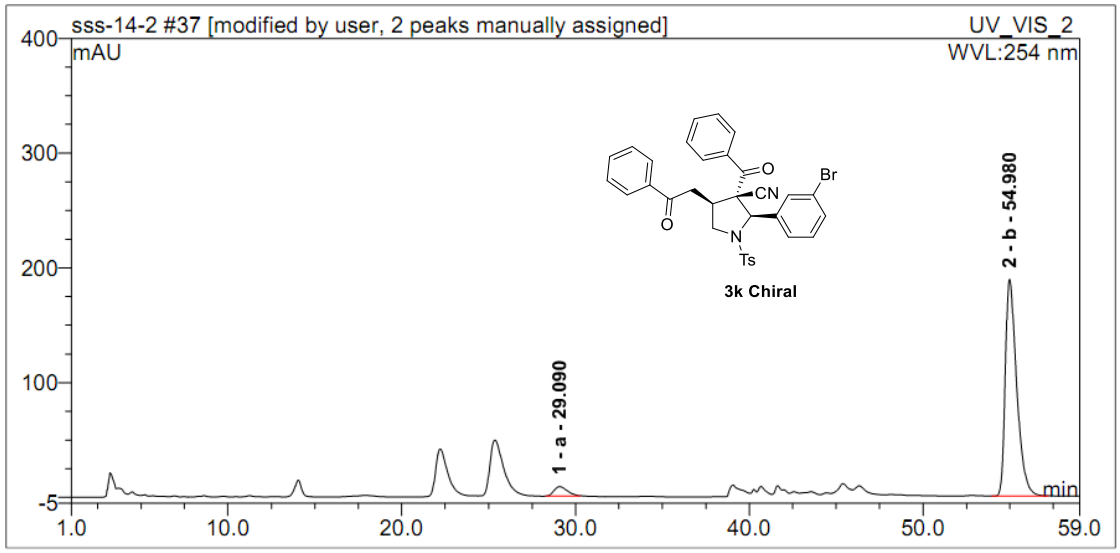
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	27.51	43.58815	48.68511978	46.93932	n.a.
2	b	51.91	45.943	51.31488022	70.888	n.a.



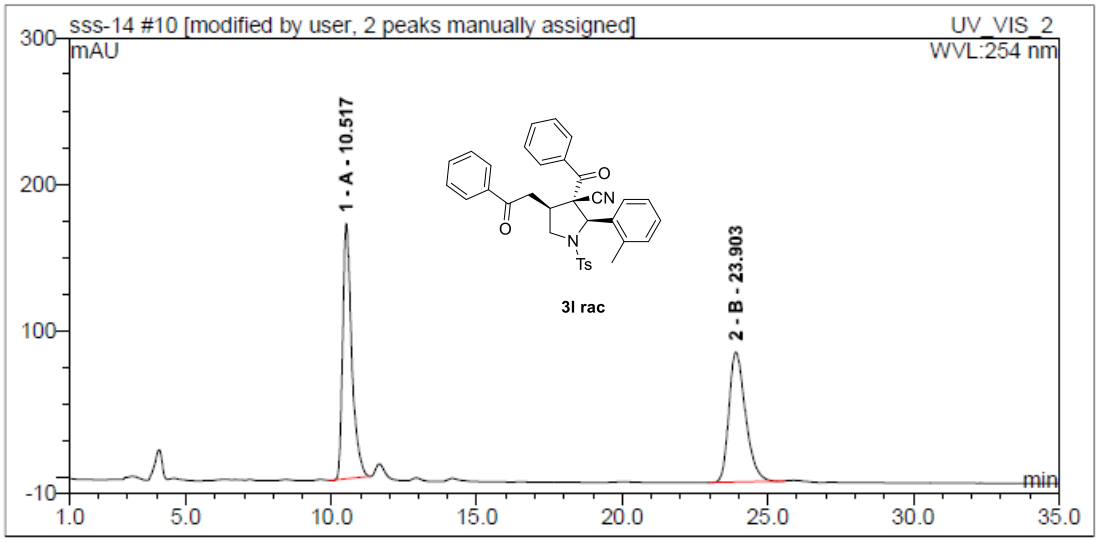
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	27.41	5.039755	2.148483218	6.55197	n.a.
2	b	51.46	229.533	97.85151678	331.460	n.a.



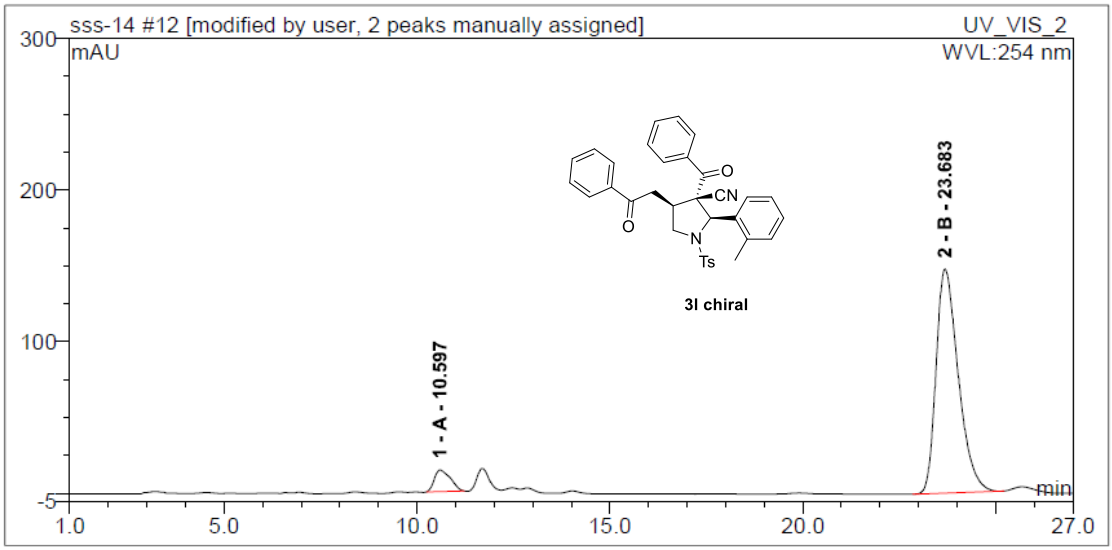
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	28.66	101.5937	48.50237407	103.9172	n.a.
2	b	55.06	107.868	51.49762593	144.130	n.a.



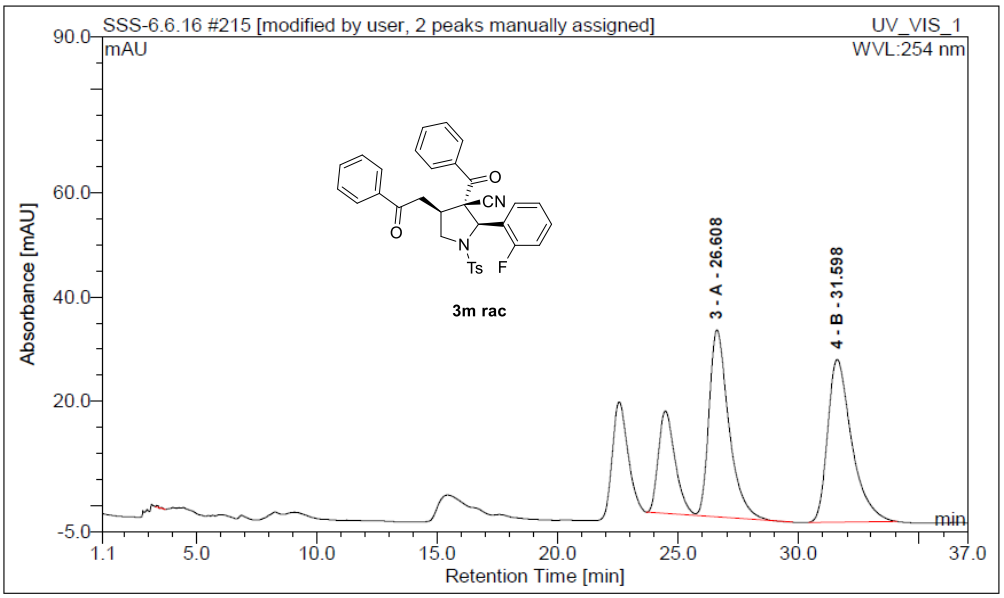
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	29.09	7.255451	4.796204803	8.238	n.a.
2	b	54.98	144.019	95.2037952	188.940	n.a.



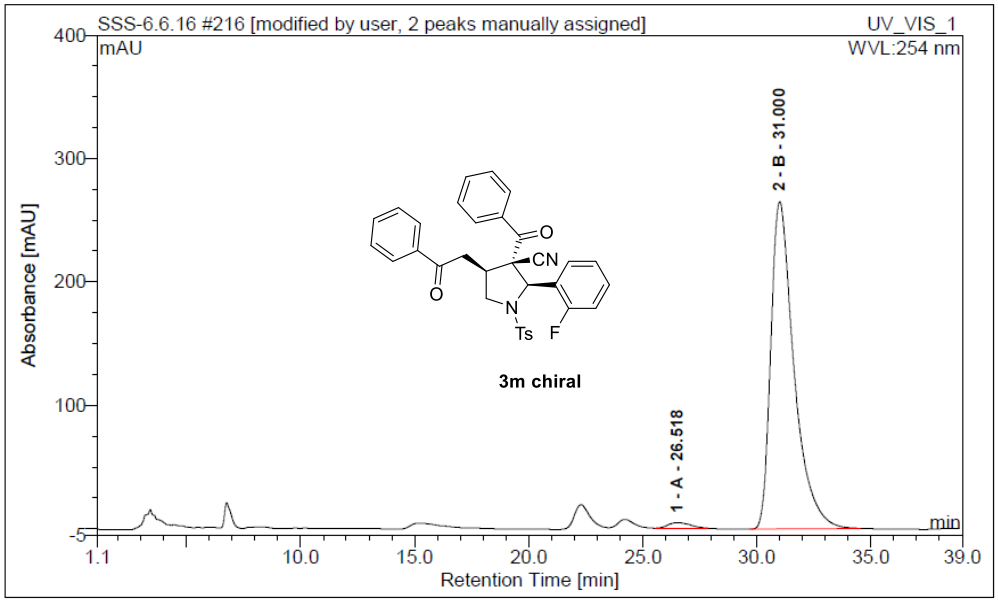
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	A	10.52	62.55318	51.63451523	173.9572	n.a.
2	B	23.90	58.593	48.36548477	88.589	n.a.



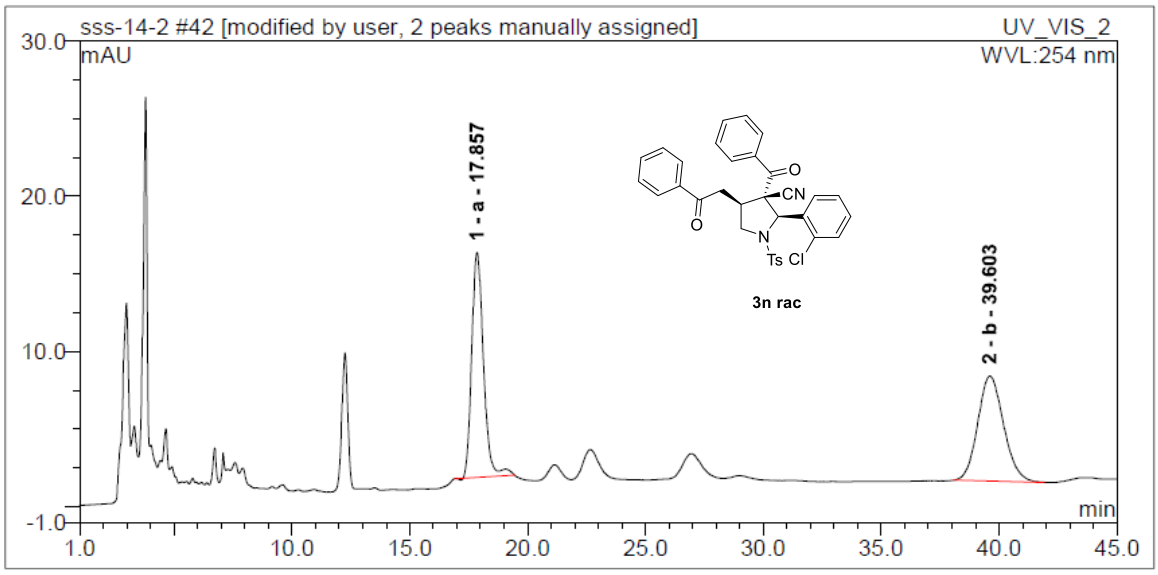
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	A	10.60	6.767471	6.415867329	14.22582	n.a.
2	B	23.68	98.713	93.58413267	147.769	n.a.



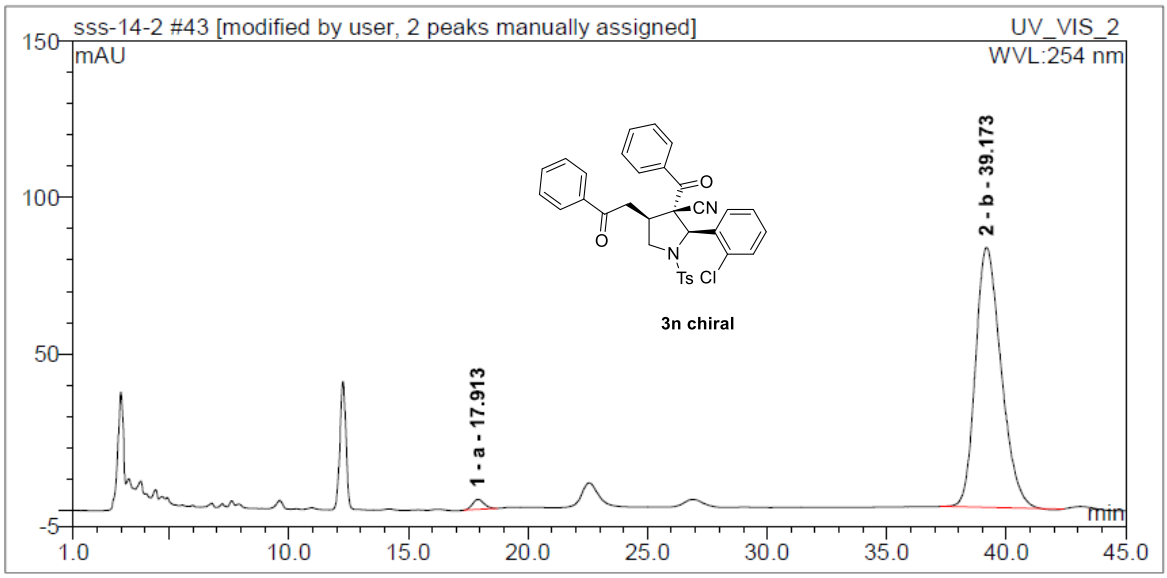
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
3	A	26.61	34.28184	48.66906106	35.92317	n.a.
4	B	31.60	36.157	51.33093894	31.212	n.a.



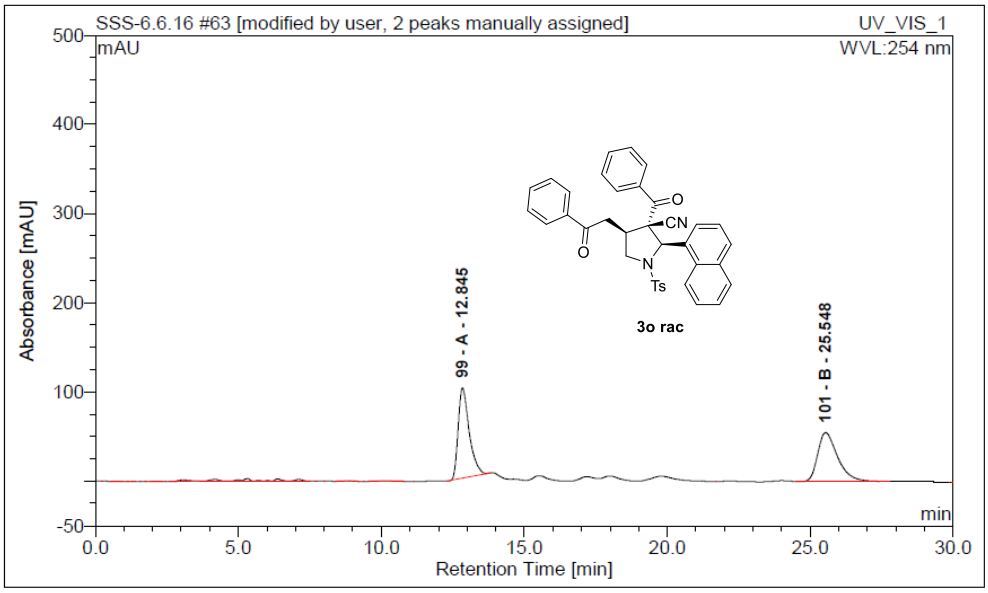
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	A	26.52	5.128334	1.611346803	4.5091	n.a.
2	B	31.00	313.136	98.3886532	265.192	n.a.



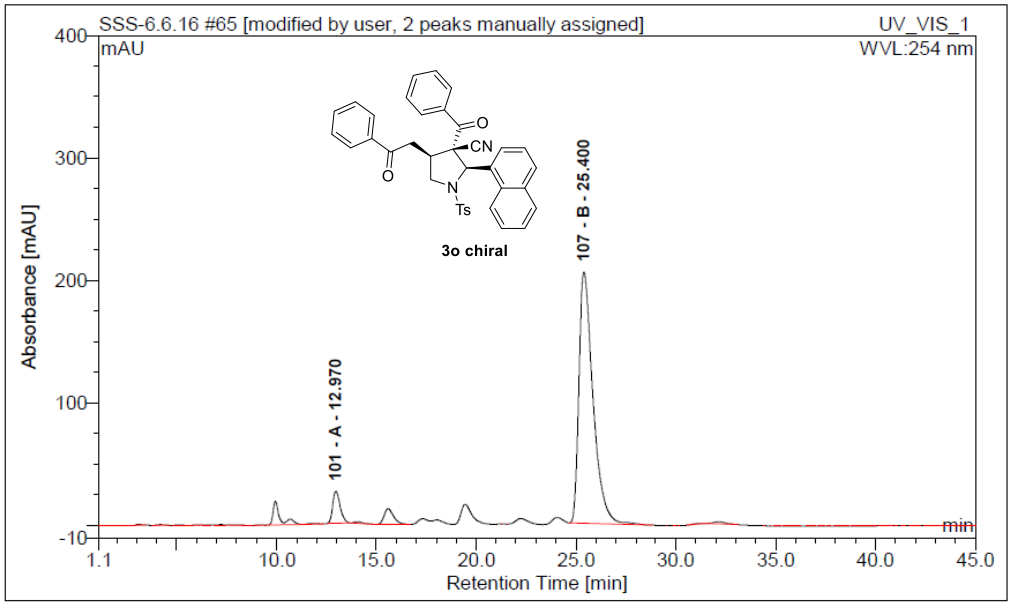
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	17.86	8.40965	49.48251096	14.47981	n.a.
2	b	39.60	8.586	50.51748904	6.764	n.a.



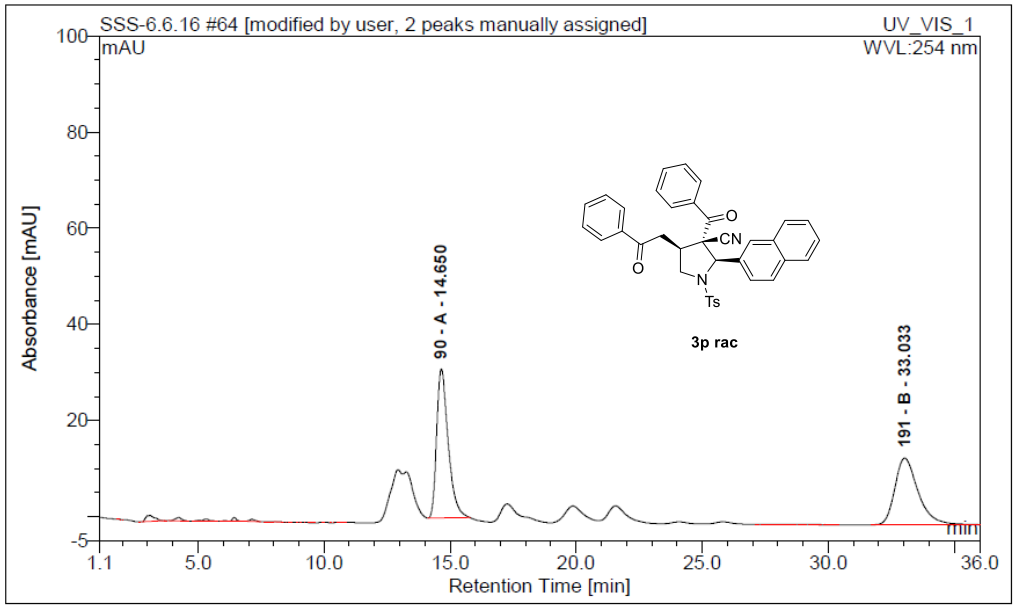
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	17.91	1.780698	1.698704314	3.18792	n.a.
2	b	39.17	103.046	98.30129569	83.036	n.a.



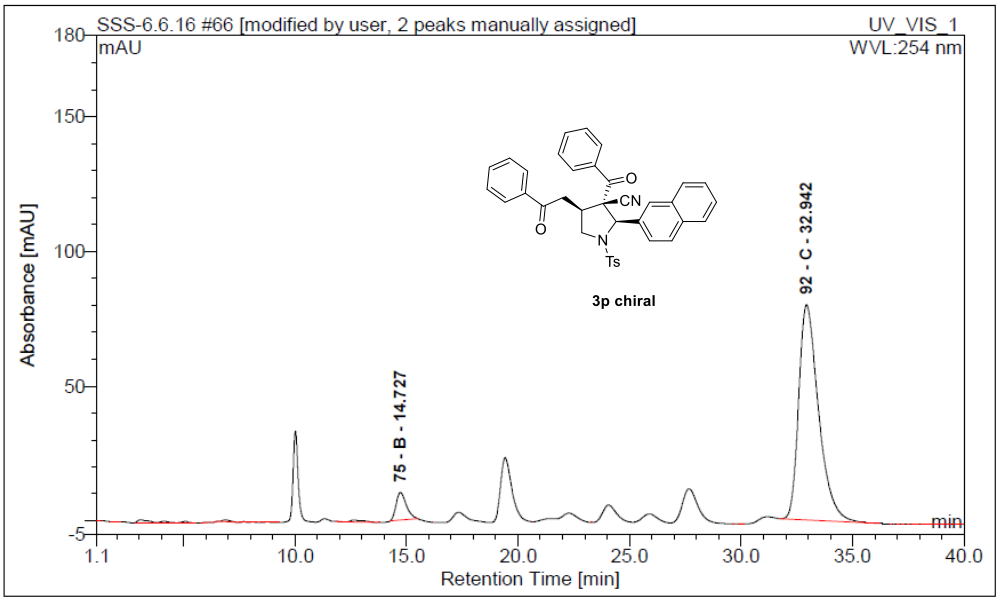
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
99	A	12.85	45.21449	50.59030822	101.1645	n.a.
101	B	25.55	44.159	49.40969178	54.773	n.a.



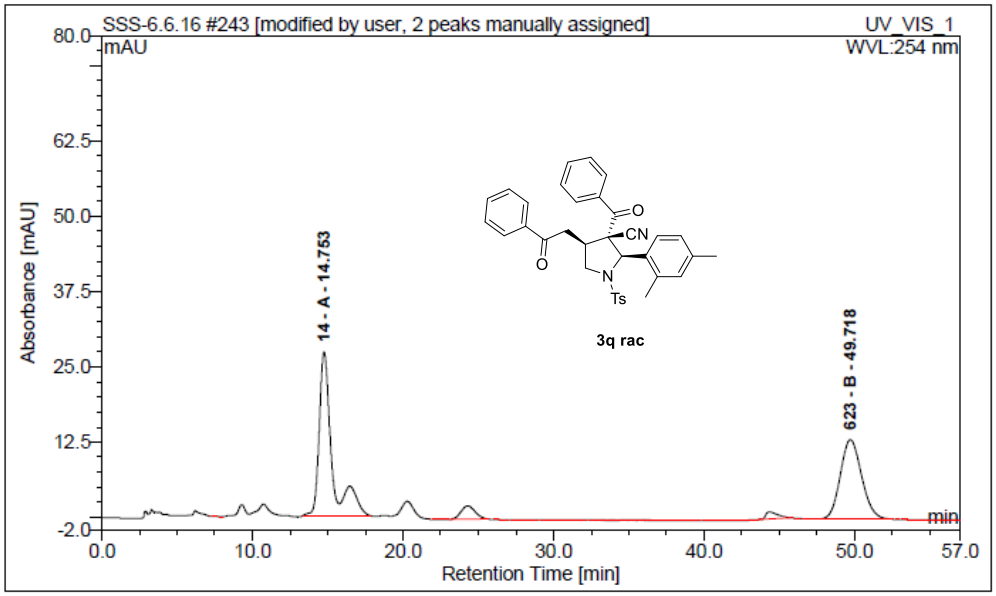
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
101	A	12.97	11.38941	6.405810815	26.26023	n.a.
107	B	25.40	166.409	93.59418918	205.054	n.a.



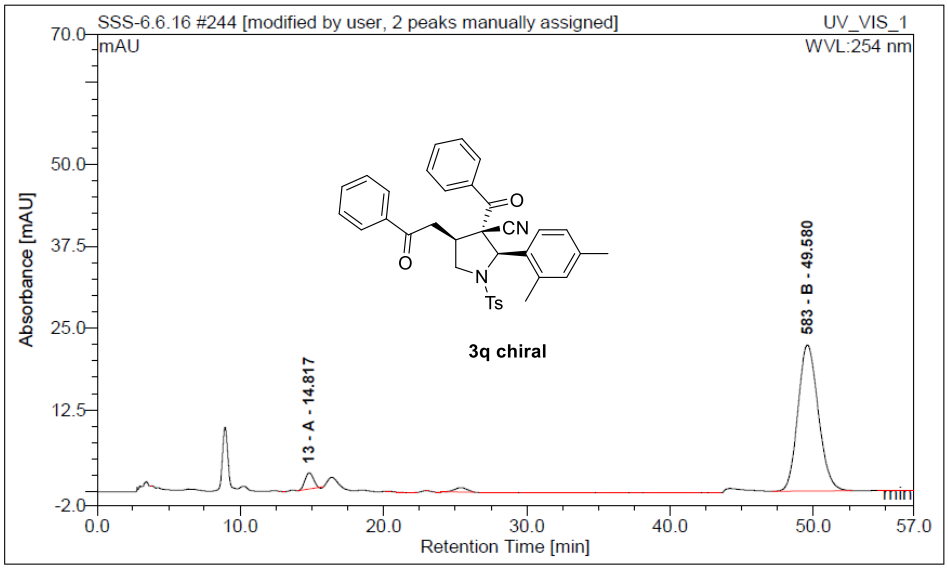
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
90	A	14.65	16.39768	52.33813997	30.9892	n.a.
191	B	33.03	14.933	47.66186003	13.875	n.a.



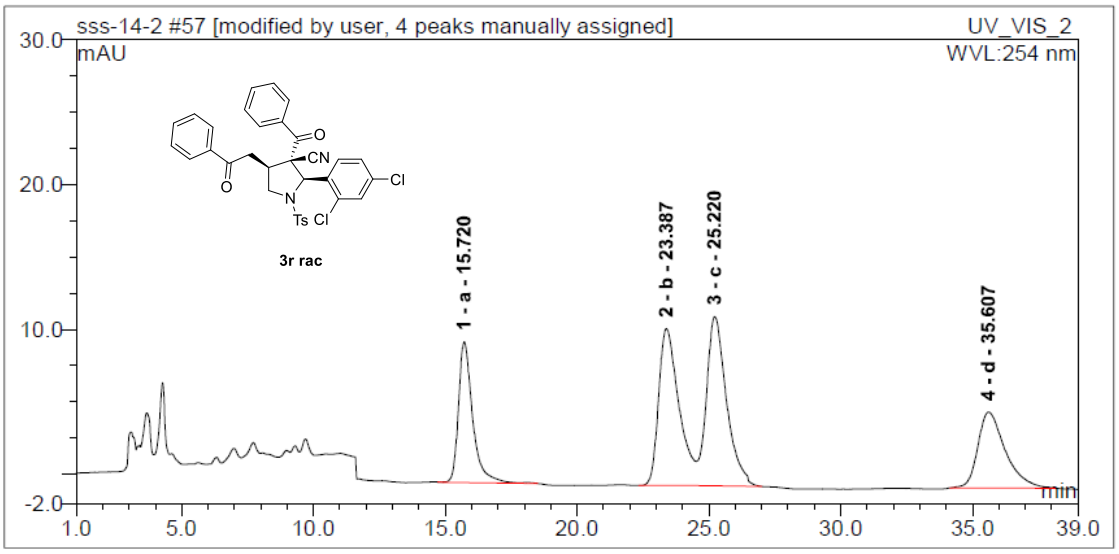
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
75	B	14.73	5.436639	6.171669557	10.2103	n.a.
92	C	32.94	82.654	93.82833044	79.975	n.a.



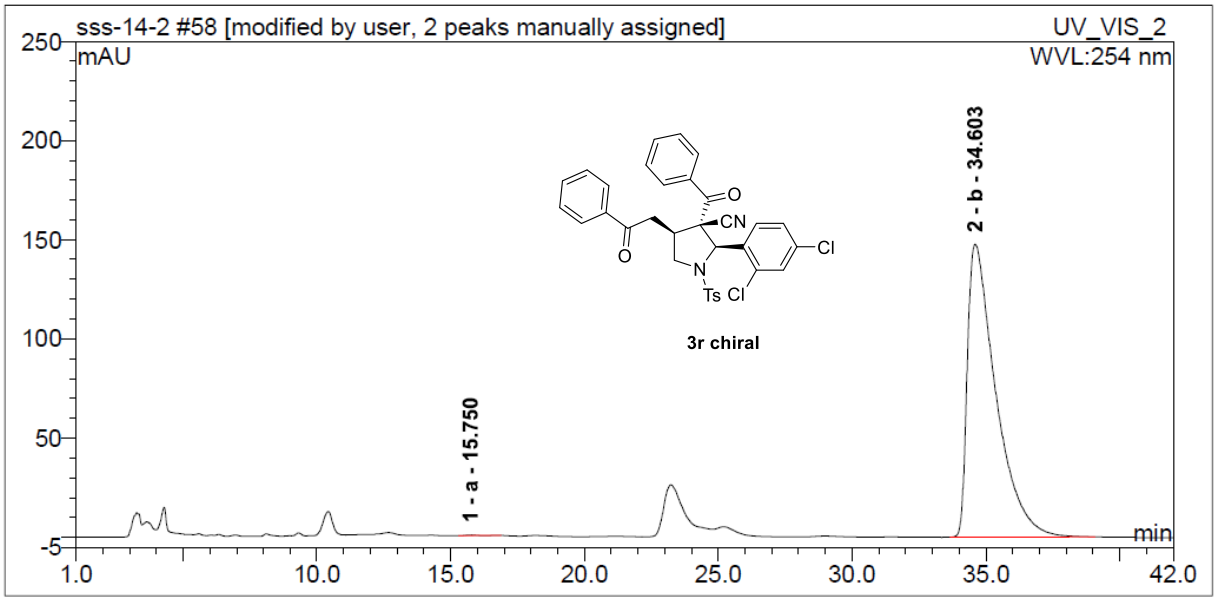
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
14	A	14.75	22.00861	50.69385319	27.15975	n.a.
623	B	49.72	21.406	49.30614681	13.137	n.a.



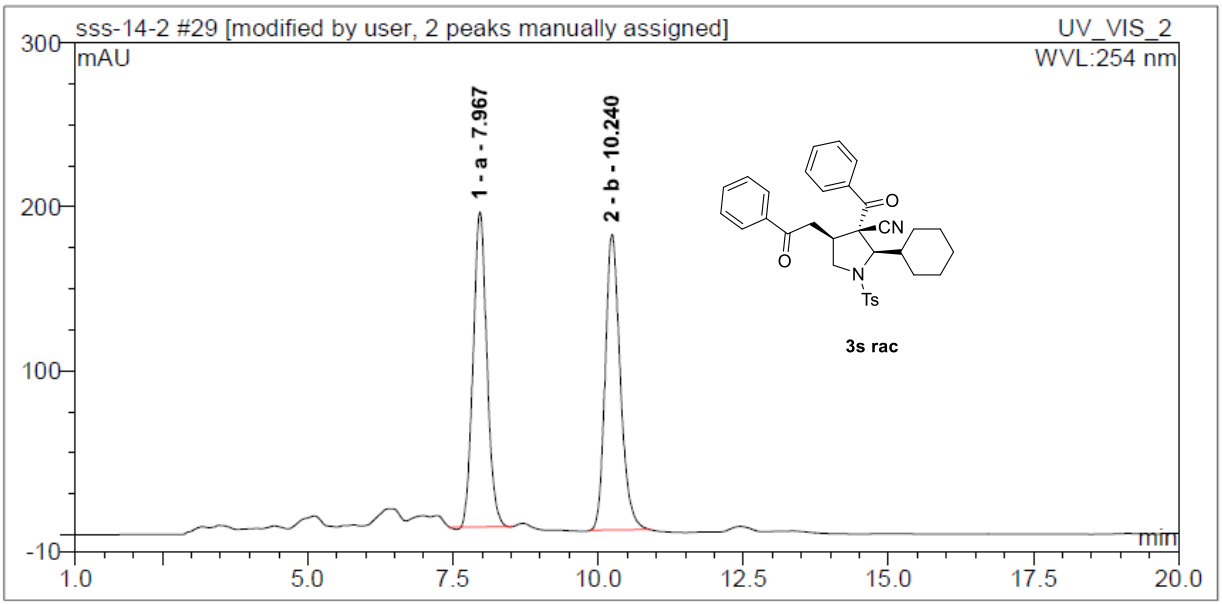
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
13	A	14.82	1.6701	4.350252064	2.49717	n.a.
583	B	49.58	36.721	95.64974794	22.309	n.a.



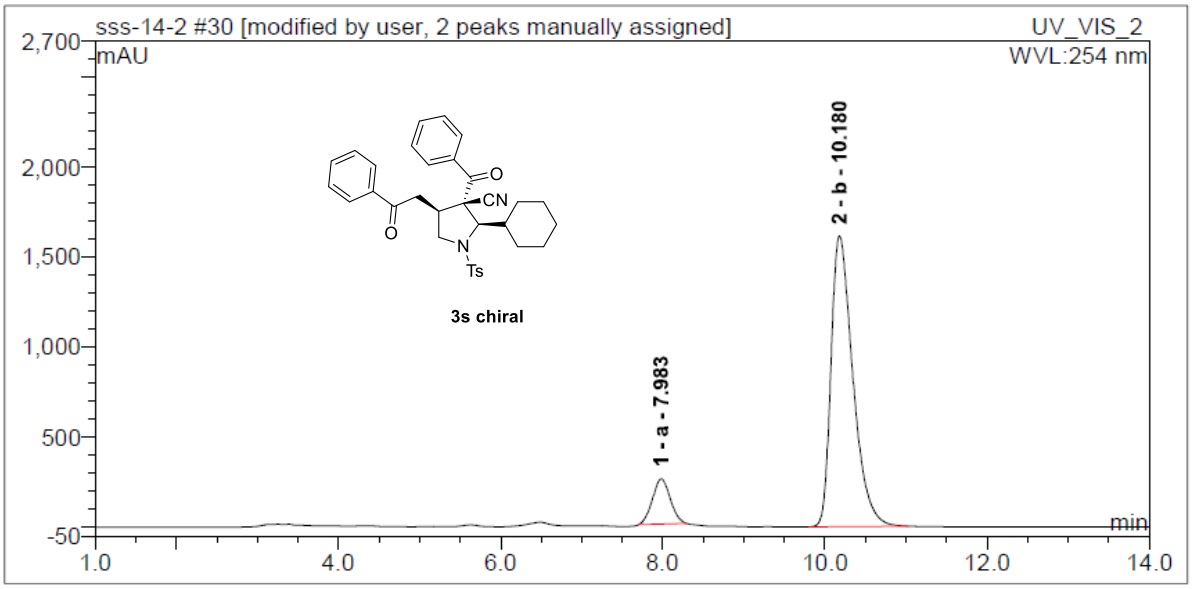
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	15.72	6.039562	18.62199225	9.71281	n.a.
2	b	23.39	9.760187	30.09392563	10.82975	n.a.
3	c	25.22	10.32515	31.8358829	11.68167	n.a.
4	d	35.61	6.308	19.44819922	5.231	n.a.



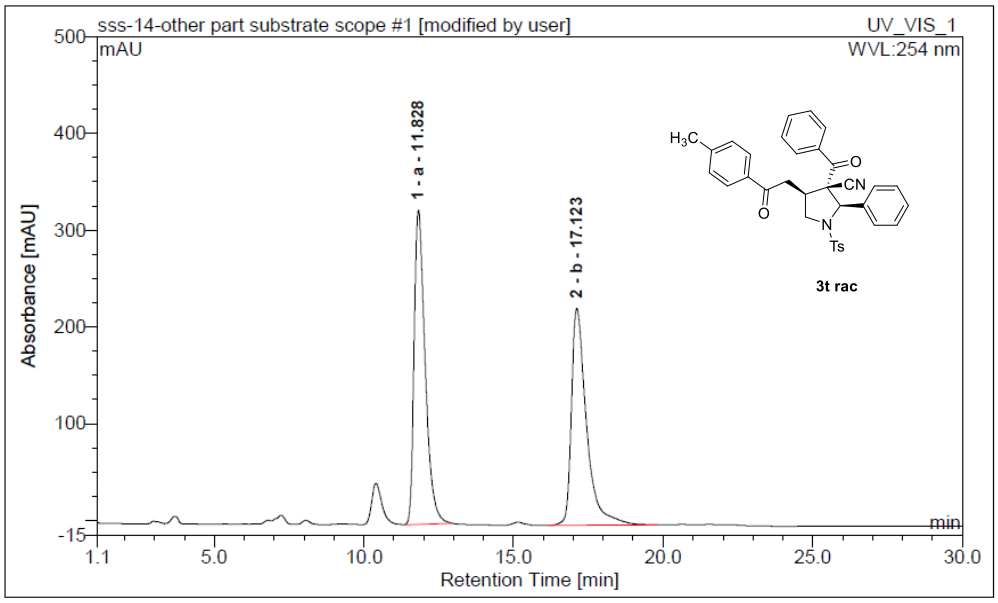
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	15.75	0.150361	0.08259190456	0.37395	n.a.
2	b	34.60	181.902	99.9174081	147.679	n.a.



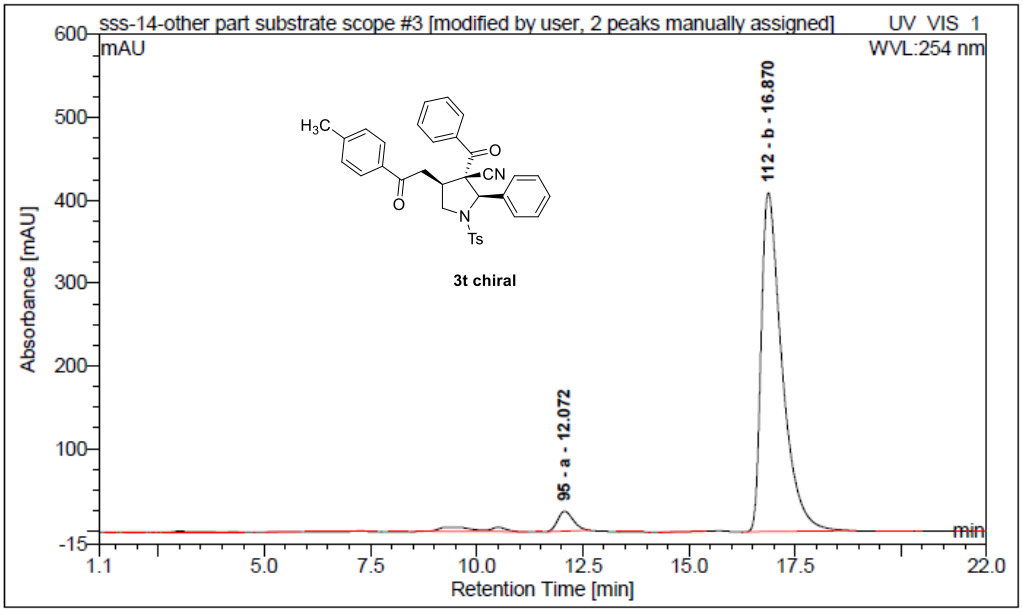
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	7.97	52.6448	49.27488975	192.0112	n.a.
2	b	10.24	54.194	50.72511025	180.209	n.a.



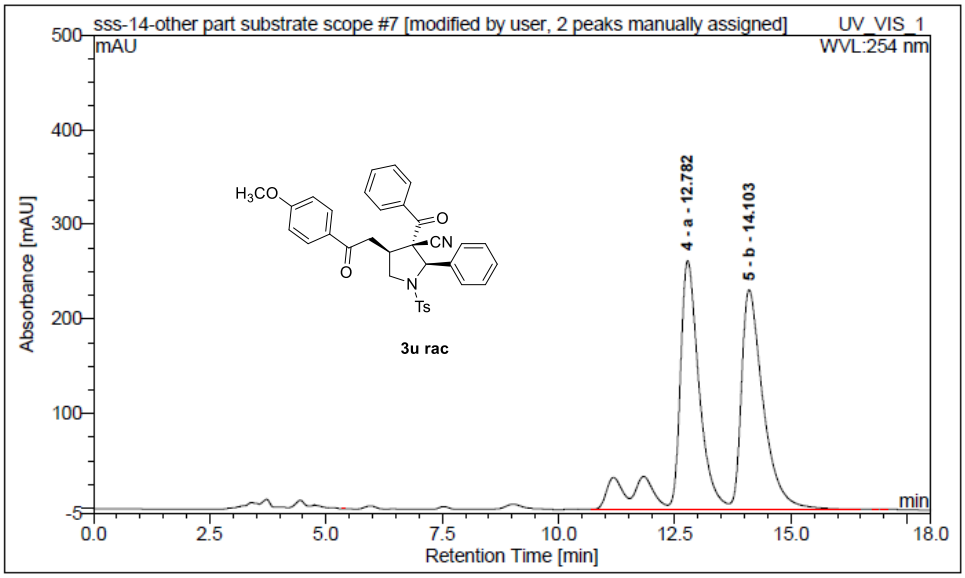
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	7.98	63.75631	11.23725012	250.2983	n.a.
2	b	10.18	503.609	88.76274988	1615.043	n.a.



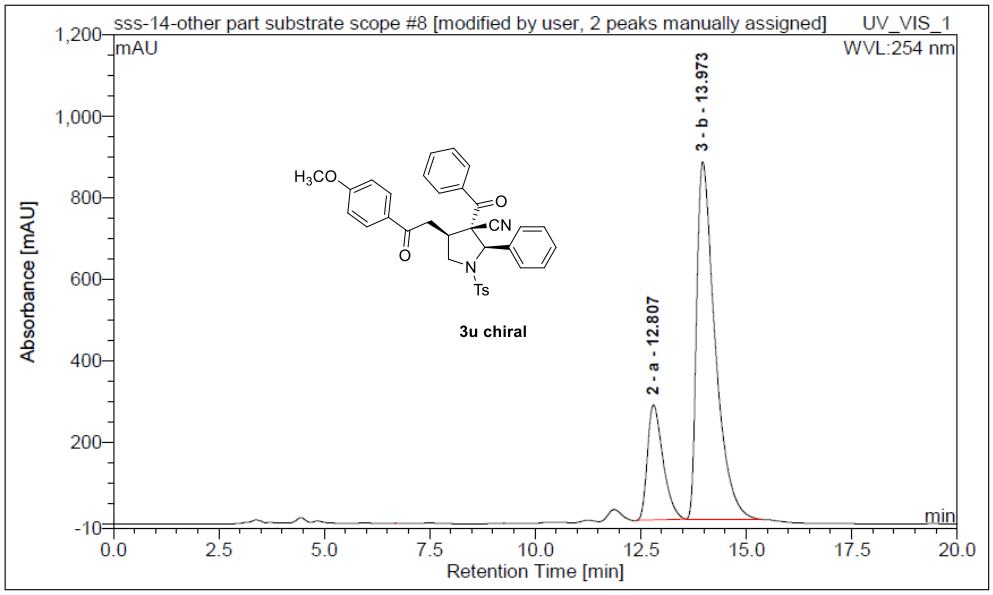
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	11.83	138.9023	51.44223966	324.4802	n.a.
2	b	17.12	131.114	48.55776034	224.110	n.a.



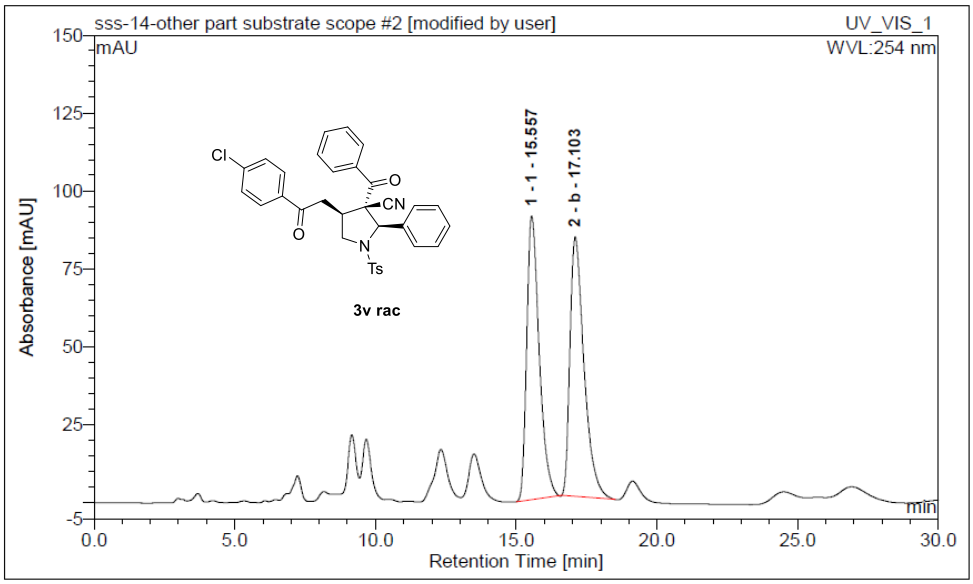
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
95	a	12.07	10.15986	4.181661049	24.03188	n.a.
112	b	16.87	232.802	95.81833895	409.541	n.a.



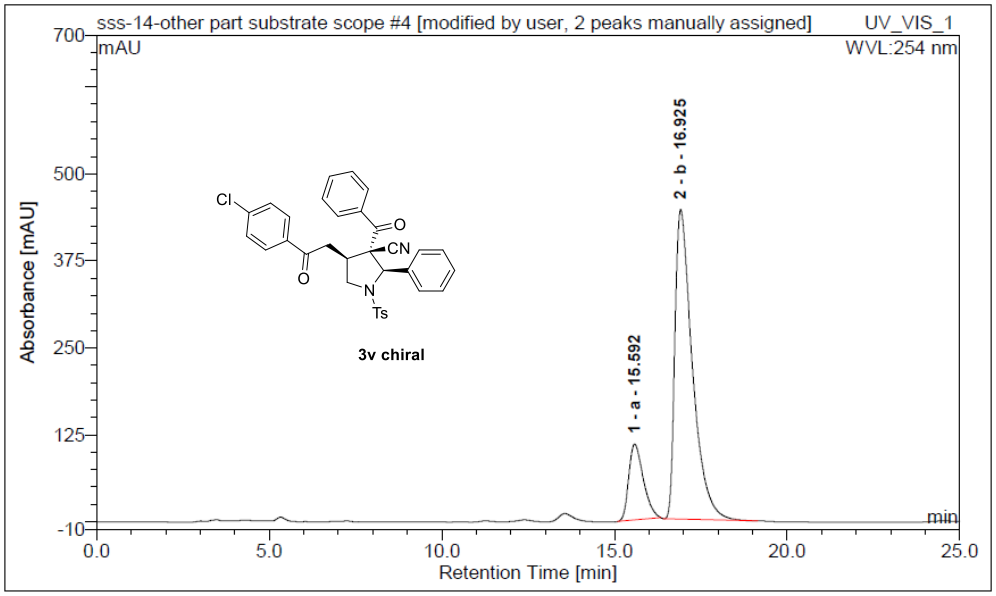
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
4	a	12.78	120.1804	48.89189009	262.7973	n.a.
5	b	14.10	125.628	51.10810991	231.995	n.a.



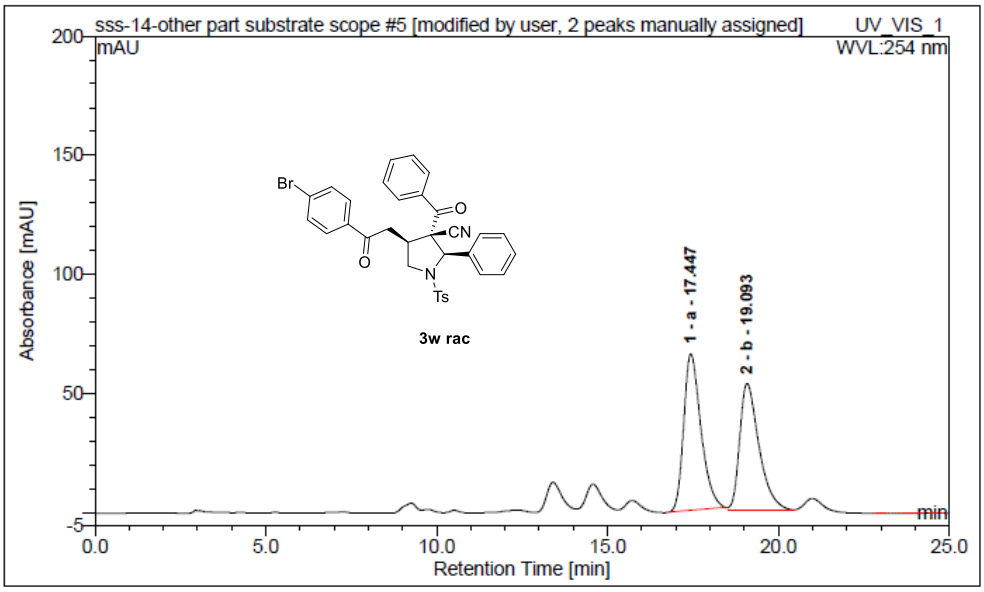
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
2	a	12.81	121.0991	21.43425206	282.5574	n.a.
3	b	13.97	443.880	78.56574794	877.744	n.a.



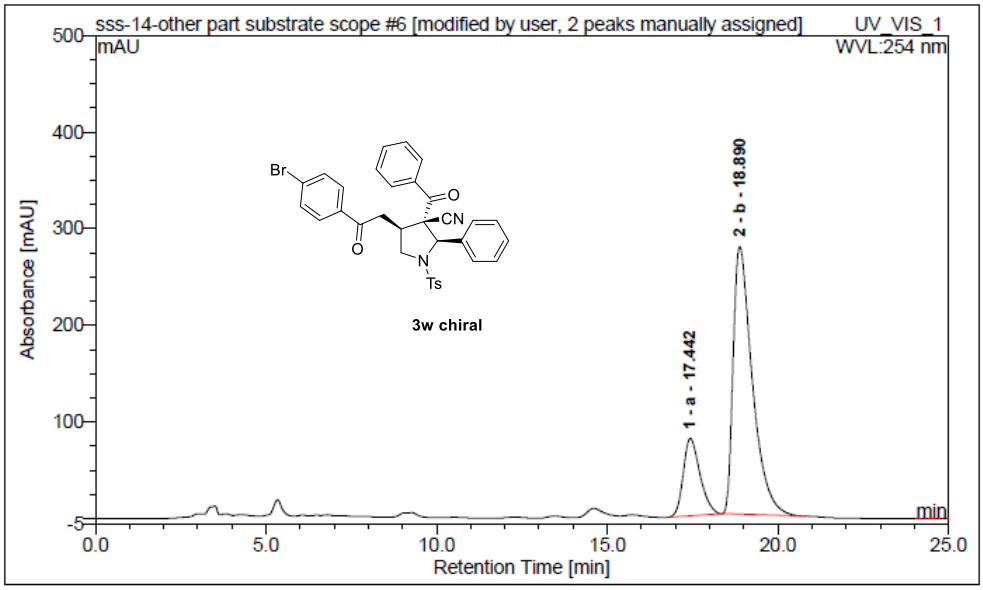
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	15.56	46.76896	49.20027794	90.90852	n.a.
2	b	17.10	48.289	50.79972206	83.231	n.a.



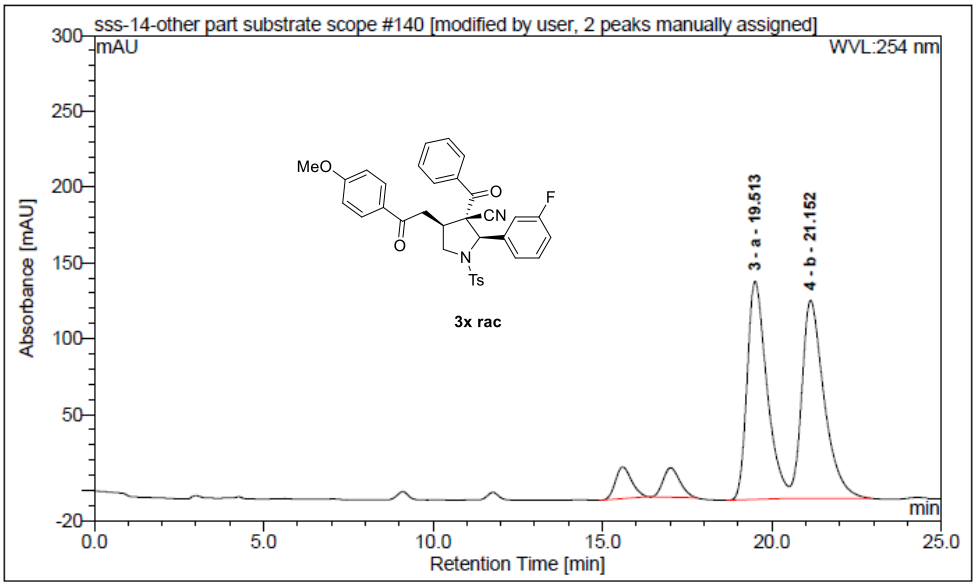
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	15.59	53.20165	16.98930924	109.0134	n.a.
2	b	16.93	259.946	83.01069076	444.916	n.a.



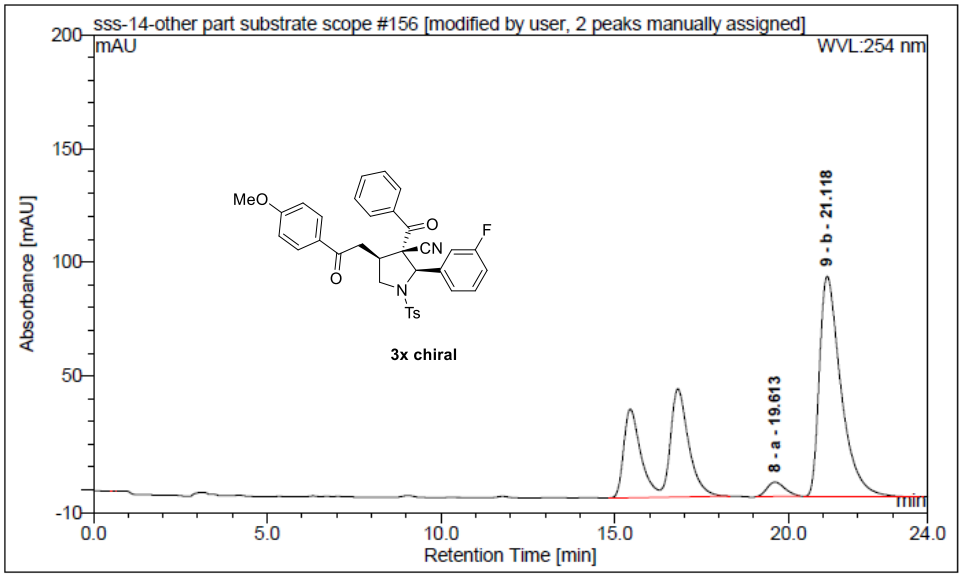
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	17.45	38.21985	52.58956317	65.47385	n.a.
2	b	19.09	34.456	47.41043683	52.904	n.a.



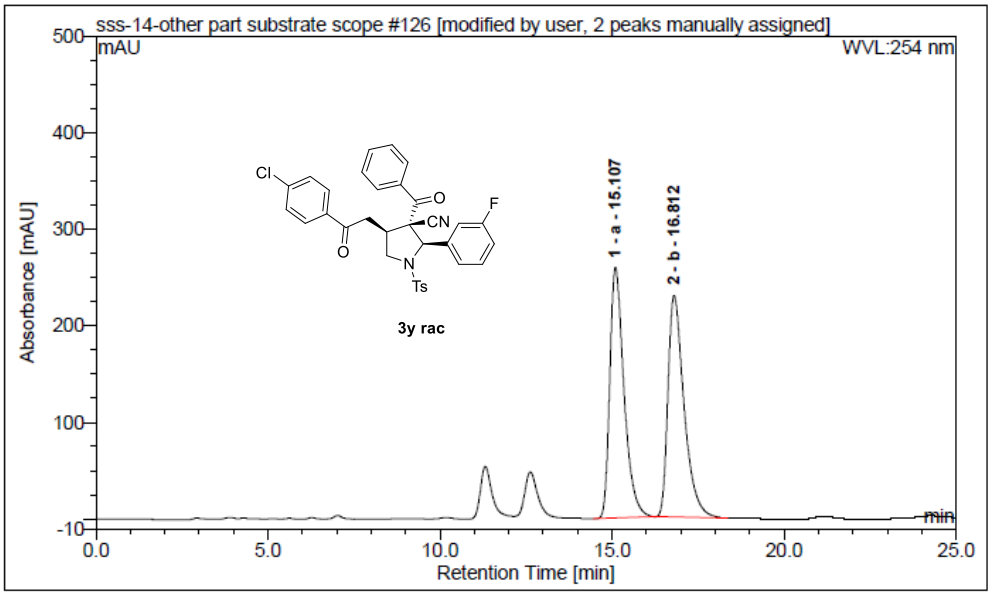
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	17.44	45.01634	20.06051594	79.77786	n.a.
2	b	18.89	179.386	79.93948406	276.408	n.a.



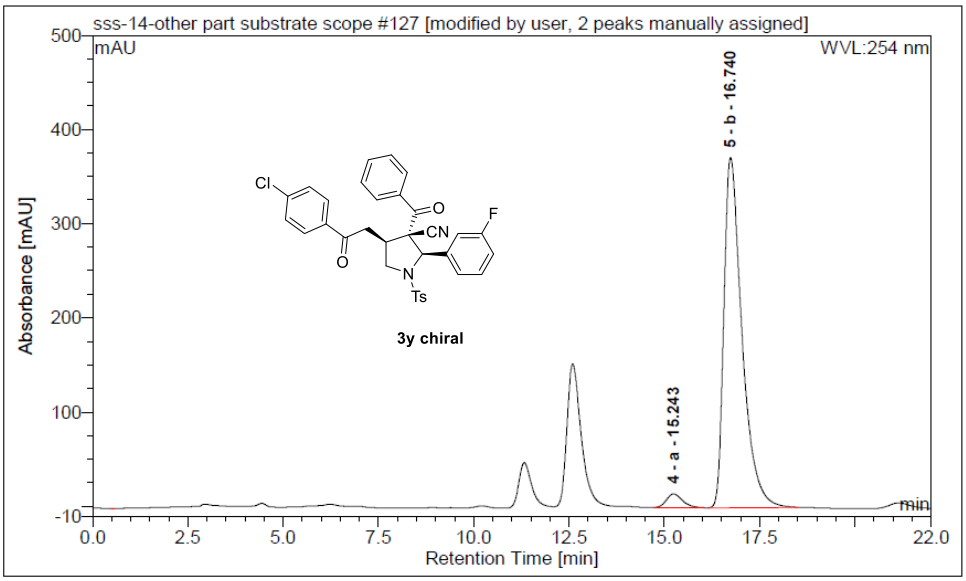
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
3	a	19.51	97.67222	49.50840014	143.8474	n.a.
4	b	21.15	99.612	50.49159986	130.558	n.a.



No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
8	a	19.61	3.688101	5.019105013	6.27596	n.a.
9	b	21.12	69.793	94.98089499	96.793	n.a.

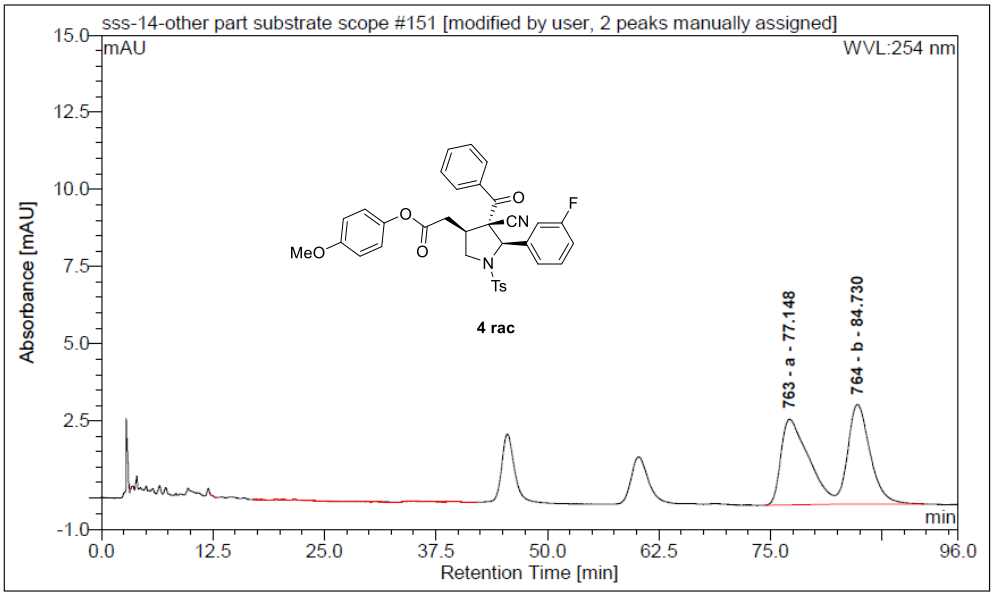


No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	15.11	123.9864	49.95399243	259.234	n.a.
2	b	16.81	124.215	50.04600757	229.266	n.a.

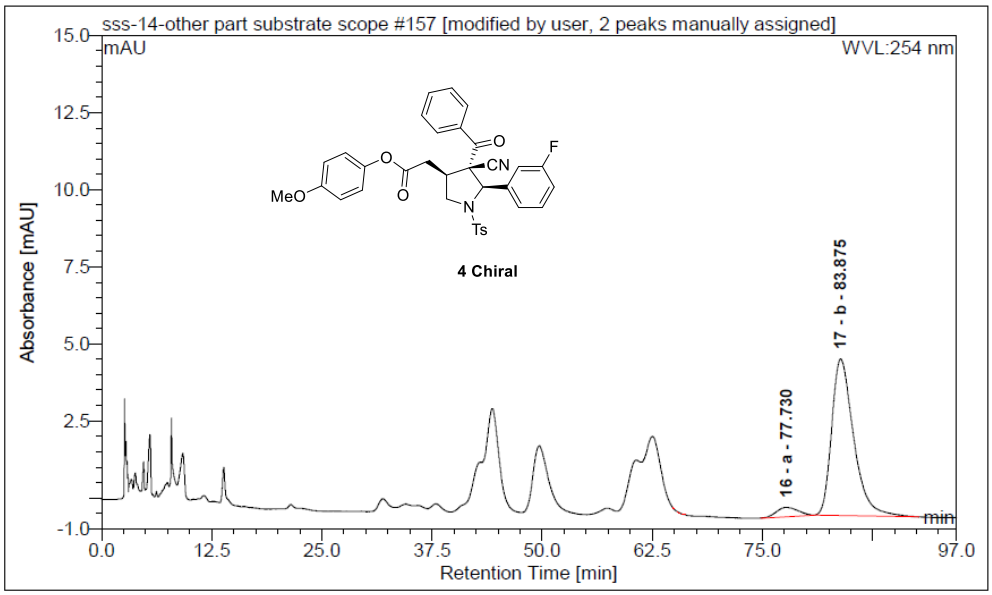


No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
4	a	15.24	7.00885	3.318474881	14.48168	n.a.
5	b	16.74	204.198	96.68152512	371.404	n.a.

L. HPLC chromatograms of 4:



No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
763	a	77.15	9.888247	51.20815972	2.77624	n.a.
764	b	84.73	9.422	48.79184028	3.231	n.a.



No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
16	a	77.73	0.844845	5.444061447	0.30631	n.a.
17	b	83.88	14.674	94.55593855	5.079	n.a.