Supplementary Information

Catalytic Enantioselective α-Alkylation of Azlactones with Unactivated Alkenes via Directed Nucleopalladation

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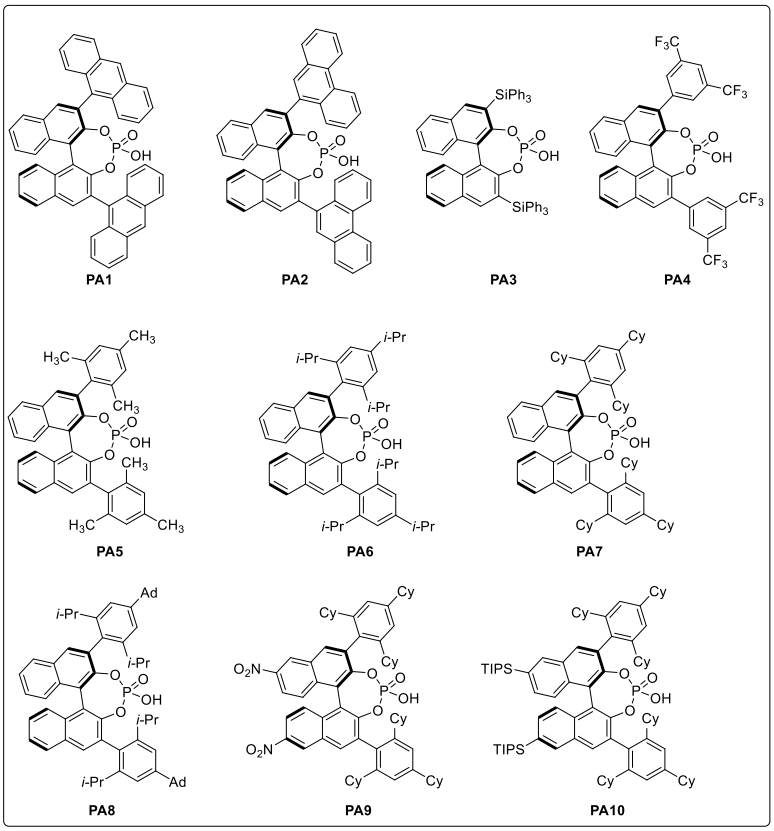
General Information:

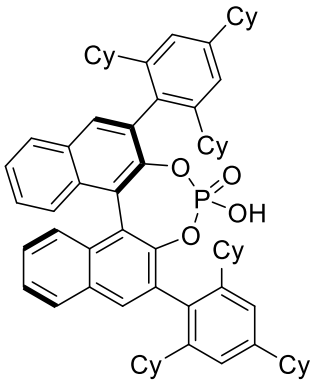
Unless otherwise stated, all reactions were carried out in flame-dried screw-cap reaction tubes with magnetic stirring. All anhydrous solvents were obtained from commercial sources or from a Grubbs-type solvent purification system. NMR spectra were recorded on Bruker AV-400, DRX-500 and AV-600 instruments. ^{1}H NMR spectra were referenced relative to tetramethylsilane (Me_4Si) signal or residual protio solvent signals. The following abbreviations or combinations thereof are used to refer to the ^{1}H NMR peak multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet or unresolved, br = broad. Data for ^{13}C NMR and ^{19}F NMR are reported in terms of chemical shift (δ, ppm). High-resolution mass spectra (HRMS) for new compounds were recorded on an Agilent LC/MSD TOF mass spectrometer.

Preparation of BINOL derived chiral phosphoric acids:

Chiral BINOL-derived phosphoric acids **PA1**–**PA2**,[1a,b] **PA5**–**PA7**,[1a-c] **PA8**,[1d] **PA9**,[1e] and **PA10**[1f] were synthesized according to literature procedures. **PA3** and **PA4** were purchased from MilliporeSigma.

Figure S1: Chiral BINOL phosphoric acids **PA1** – **PA10**.

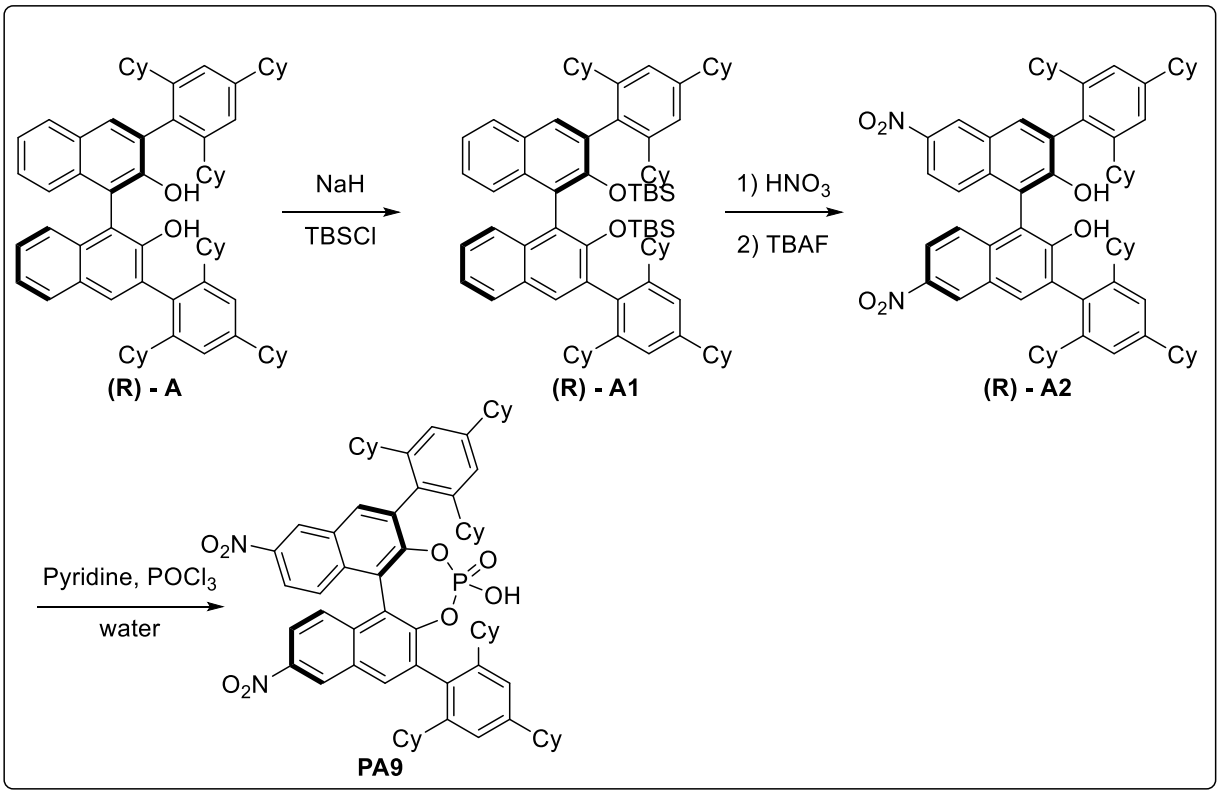


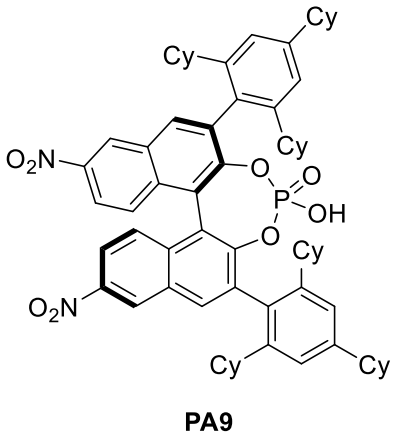

PA7

Chiral phosphoric acid 7 (PA7): The title compound was prepared according to a literature procedure.[1a] Analytical data were in agreement with previously reported values and are included here for convenience.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.2 Hz, 2H), 7.80 (s, 2H), 7.50 (ddd, *J* = 8.1, 6.4, 1.4 Hz, 2H), 7.38–7.25 (m, 4H), 7.04–6.93 (m, 4H), 2.59–2.45 (m, 2H), 2.32–2.13 (m, 4H), 2.02–1.89 (m, 11H), 1.86–1.75 (m, 4H), 1.73–1.66 (m, 2H), 1.62–1.53 (m, 6H), 1.52–1.42 (m, 12H), 1.40–1.32 (m, 6H), 1.27–1.17 (m, 4H), 1.16–1.06 (m, 3H), 1.02–0.57 (m, 12H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 146.62, 146.05, 145.74, 145.68, 145.63, 131.73, 131.72, 131.64, 131.50, 131.11, 130.49, 127.66, 126.23, 125.70, 125.06, 121.85, 121.16, 121.06, 44.33, 41.71, 41.43, 36.69, 34.64, 34.16, 33.85, 32.80, 32.26, 26.89, 26.68, 26.53, 26.36, 25.90, 25.81, 25.56. **^{31}P NMR** (162 MHz, $CDCl_3$) δ 2.04. **HRMS** (ESI-TOF) calcd for $C_{68}H_{82}O_4P$ $[M+H]^+$: 993.5945, Found: 993.5950.

Scheme S1: Synthesis of **PA9**:

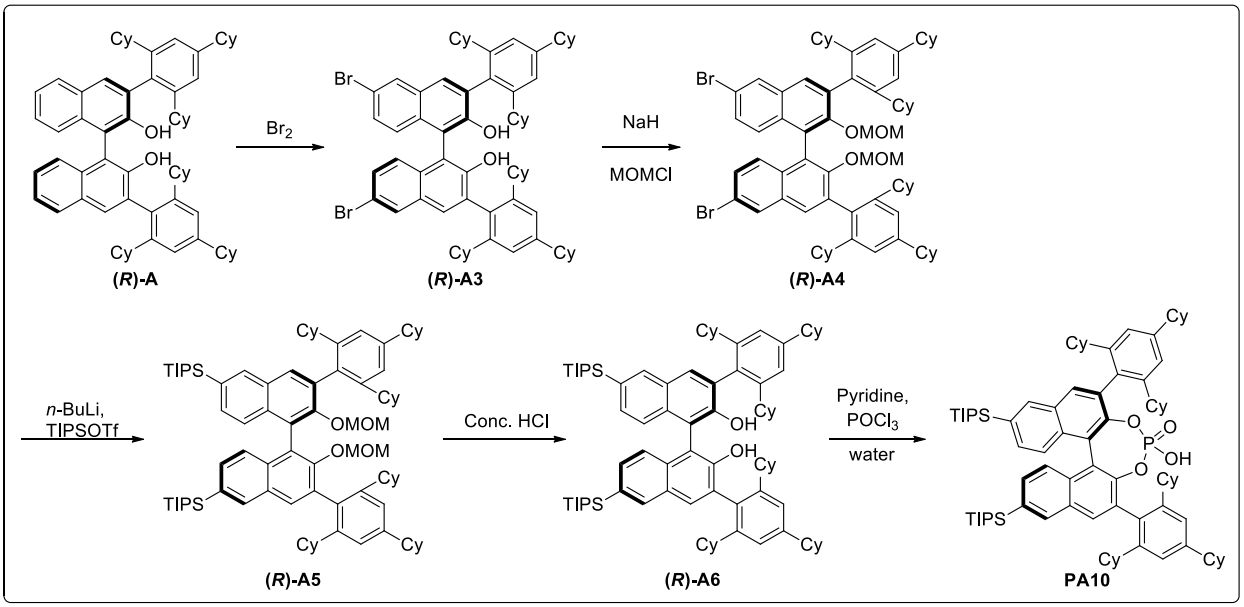




Chiral phosphoric acid 9 (PA9): The title compound was prepared according to a literature procedure, as shown in Scheme **S1**.[1e] Analytical data were in agreement with previously reported values and are included here for convenience. **^{1}H NMR** (600 MHz, CD_2Cl_2) δ 8.88 (d, *J* = 2.4 Hz, 2H), 8.13–8.04 (m, 2H), 7.99 (s, 2H), 7.28 (d, *J* = 9.3 Hz, 2H), 6.96 (s, 4H), 2.55–2.42 (m, 2H), 2.14–1.96 (m, 4H), 1.93–1.75 (m, 14H), 1.67–1.55 (m, 5H), 1.38–1.17 (m, 14H), 1.15–1.04 (m, 3H), 0.91–0.49 (m, 12H). **^{13}C NMR** (150 MHz, CD_2Cl2) δ 149.89, 149.83, 148.70, 146.92, 146.49, 146.09, 135.57, 135.01, 134.85, 130.76, 130.34, 128.15, 125.54, 123.15, 122.43, 121.90, 120.68, 45.36, 43.13, 42.58, 37.39, 35.52, 35.11, 34.82, 33.62, 32.92, 30.25, 27.87, 27.73, 27.60, 27.31, 26.83, 26.60. **^{31}P NMR** (162 MHz, CD_2Cl2) δ -0.49.

Scheme S2: Synthesis of **PA10**.

The title compound was prepared by adapting a literature procedure, as shown in Scheme **S2**.[1f]



(*R*)-A3: To a 100-mL round-bottom flask equipped with a Teflon-coated magnetic stir bar were added **(*R*)-A** (200 mg, 1.0 equiv) and dichloromethane (5 mL). The solution was cooled to –78 °C, and bromine (92.7 mg, 2.7 equiv) was added. The reaction mixture was allowed to warm to room temperature and stir for 1 h. The reaction mixture was quenched with 10% Na_2SO_3 solution (10 mL) and extracted with dichloromethane (3 × 20 mL). The combined organic layers were dried over Na_2SO_3, filtered, and concentrated *in vacuo*. The crude material was purified by column chromatography using 10–12% dichloromethane in hexane as eluent to give product as yellow solid (125 mg, 54% yield). **^{1}H NMR** (600 MHz, CD_2Cl_2) δ 8.05 (d, *J* = 2.0 Hz, 2H), 7.64 (s, 2H), 7.39 (dd, *J* = 9.0, 2.0 Hz, 2H), 7.13 (d, *J* = 1.7 Hz, 2H), 7.11–7.07 (m, 4H), 4.92 (s, 2H), 2.56 (tt, *J* = 11.7, 3.4 Hz, 2H), 2.37 (tt, *J* = 12.0, 3.2 Hz, 2H), 2.19 (tt, *J* = 12.0, 3.3 Hz, 2H), 1.95–1.85 (m, 10H), 1.83–1.73 (m, 9H), 1.71–1.59 (m, 11H), 1.58–1.40 (m, 13H), 1.38–1.21 (m, 6H), 1.12 (ttd, *J* = 16.4, 9.0, 8.4, 3.5 Hz, 5H), 0.96–0.80 (m, 6H). **^{13}C NMR** (150 MHz, CD_2Cl_2) δ 151.55, 149.28, 147.58, 147.40, 132.50, 131.14, 130.97, 130.76, 130.65, 130.29, 126.49, 123.10, 117.93, 113.66, 45.48, 42.53, 35.19, 35.06, 34.70, 34.47, 27.84, 27.57, 27.54, 27.36, 26.80, 26.69, 26.54, 25.81. **HRMS** (ESI-TOF) calcd for $C_{68}H_{81}Br_2O_2$ $[M+H]^+$: 1087.4598, Found: 1087.4602.

(*R*)-A4: To a 50-mL round-bottom flask equipped with a Teflon-coated magnetic stir bar were added **(*R*)-A3** (125 mg, 1.0 equiv) and THF (3 mL). The solution was cooled to 0 °C. NaH (6

mg, 2.2 equiv) was added, and the solution was stirred at room temperature for 30 min. The reaction mixture was again cooled to 0 °C. Chloromethyl methyl ether (37 mg, 4.0 equiv) was added, and the reaction mixture was stirred at room temperature for 5 h. The reaction mixture was quenched with saturated aq. NH_4Cl (10 mL) and extracted with dichloromethane (3 × 10 mL). The combined organic layers were dried over Na_2SO_3, filtered, and concentrated *in vacuo*. The crude material was purified by column chromatography using 4–8% dichloromethane in hexane as eluent to give product as a pale yellow solid (130 mg, 97% yield). **^{1}H NMR** (600 MHz, CD_2Cl_2) δ 8.07 (d, *J* = 2.1 Hz, 2H), 7.71 (s, 2H), 7.42 (dd, *J* = 9.1, 2.0 Hz, 2H), 7.19 (d, *J* = 9.1 Hz, 2H), 7.10 (t, *J* = 1.6 Hz, 4H), 4.39 (d, *J* = 5.5 Hz, 2H), 4.28 (d, *J* = 5.4 Hz, 2H), 2.57 (m, 2H), 2.39–2.33 (m, 4H), 2.31 (s, 6H), 1.95–1.05 (m, 60H). **^{13}C NMR** (150 MHz, CD_2Cl_2) δ 152.96, 148.45, 146.82, 146.78, 136.27, 133.45, 132.65, 132.15, 130.91, 130.89, 130.45, 129.83, 128.32, 126.28, 122.71, 119.49, 97.95, 55.99, 45.51, 42.81, 42.35, 36.61, 36.51, 35.24, 33.62, 33.58, 27.96, 27.78, 27.64, 27.44, 27.21, 26.88, 26.77. **HRMS** (ESI-TOF) calcd for $C_{72}H_{89}Br_2O_4$ $[M+H]^+$: 1175.5122, Found: 1175.5150.

(*R*)-A6: To a 25-mL round-bottom flask equipped with a Teflon-coated magnetic stir bar were added **(*R*)-A4** (130 mg, 1.0 equiv) and THF (3 mL). The solution was cooled to –78 °C, and *n*-butyllithium (2.5 M solution in hexane) (120 μL, 2.54 equiv) was added. After 10 min, riisopropylsilyl triflate (80 μL, 2.6 equiv) was added dropwise to the reaction flask, and the resulting mixture was stirred for an additional 90 min. The reaction mixture was quenched with saturated aq. $NaHCO_3$ (10 mL) and extracted with ethyl acetate (3 × 10 mL). The combined organic layers were dried over Na_2SO_3, filtered, and concentrated *in vacuo* to give **(*R*)-A5**. The crude material was then dissolved in dioxane (4 mL) and transferred to a 10 mL round-bottom flask equipped with a Teflon-coated magnetic stir bar. Conc. HCl (0.5 mL) was added, and the mixture was stirred at 70 °C for 2 h. The solvent was removed *in vacuo*, and the resulting residue was purified by column chromatography using 0–10% dichloromethane in hexane as eluent to give product as a white solid (60 mg, 44% yield). **^{1}H NMR** (600 MHz, CD_2Cl_2) δ 7.95 (s, 2H), 7.69 (s, 2H), 7.41 (dd, *J* = 8.5, 1.2 Hz, 2H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.10 (d, *J* = 1.7 Hz, 2H), 7.05 (d, *J* = 1.7 Hz, 2H), 4.89 (s, 2H), 2.52 (m, 4H), 2.24 (m, 2H), 2.00–1.91 (m, 4H), 1.90–1.72 (m, 16H), 1.56–1.20 (m, 34H), 1.11 (m, 34H), 1.01–0.82 (m, 6H). **^{13}C NMR** (150 MHz, CD_2Cl_2) δ 151.09, 147.90, 146.95, 146.73, 136.30, 133.28, 132.66, 131.25, 130.86, 129.78, 129.05,

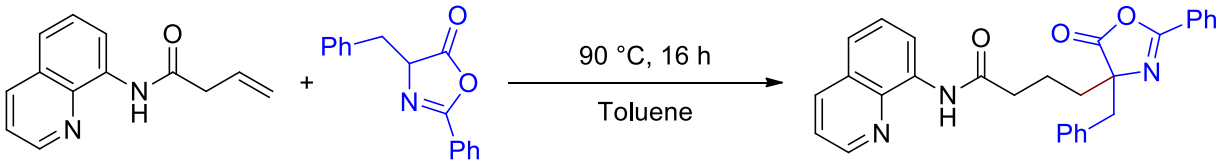
128.79, 122.95, 122.36, 122.35, 112.51, 44.99, 42.06, 41.88, 34.91, 34.69, 34.66, 34.65, 34.46, 34.24, 27.19, 27.12, 27.07, 26.99, 26.86, 26.43, 26.21, 18.85, 18.81, 11.12. **HRMS** (ESI-TOF) calcd for $C_{86}H_{123}O_2Si_2$ $[M+H]^+$: 1243.9056, Found: 1243.9116.

(*R*)-TIPS-TCYP (PA10):

To a flame-dried reaction tube were added **(*R*)-A6** (60 mg, 1.0 equiv) and anhydrous pyridine (1 mL), and the reaction mixture was cooled to 0 °C. Phosphoryl chloride (13.4 µL, 3.0 equiv) was added dropwise, and the reaction tube was heated at 90 °C for 12 h, at which point water (1 mL) was cautiously added. The reaction vessel was heated for an additional 4 h and was then allowed to cool to room temperature. A solution of 6 M aq. HCl (5 mL) was added, and the mixture was extracted with dichloromethane (3 × 10 mL). The combined organic layers were dried over Na_2SO_3, filtered, and concentrated *in vacuo*. The crude material was then purified by column chromatography using 0–2% methanol in dichloromethane as eluent. The resulting product was reacidified by washing with 2 M aq. HCl (10 mL) and extracted in dichloromethane (3 × 10 mL). The combined organic layers were dried over Na_2SO_3, filtered, and concentrated *in vacuo* to give **(*R*)-PA10** as a white solid (38 mg, 60% yield). **^{1}H NMR** (600 MHz, CD_2Cl_2) δ 7.99 (s, 2H), 7.68 (s, 2H), 7.40 (d, *J* = 8.5 Hz, 2H), 7.27 (s, 2H), 6.93 (dd, *J* = 14.1, 1.7 Hz, 4H), 2.51–2.41 (m, 2H), 2.23–1.99 (m, 4H), 1.93–1.82 (m, 10H), 1.80–1.73 (m, 2H), 1.71–1.53 (m, 8H), 1.46–1.35 (m, 14H), 1.33–1.17 (m, 14H), 1.10 (dd, *J* = 7.5, 6.0 Hz, 42H), 0.95–0.56 (m, 12H). **^{13}C NMR** (150 MHz, CD_2Cl2) δ 147.78, 147.36, 146.93, 146.87, 146.77, 136.64, 132.85, 132.75, 132.57, 132.20, 130.94, 125.64, 122.78, 122.15, 45.40, 42.67, 42.54, 37.68, 35.48, 35.10, 34.95, 33.89, 33.03, 27.77, 27.68, 27.45, 27.10, 26.99, 26.65, 18.88, 18.80, 11.41. **^{31}P NMR** (162 MHz, $CDCl_3$) δ 2.26. **HRMS** (ESI-TOF) calcd for $C_{86}H_{122}O_4PSi_2$ $[M+H]^+$: 1305.8614, Found: 1305.8635.

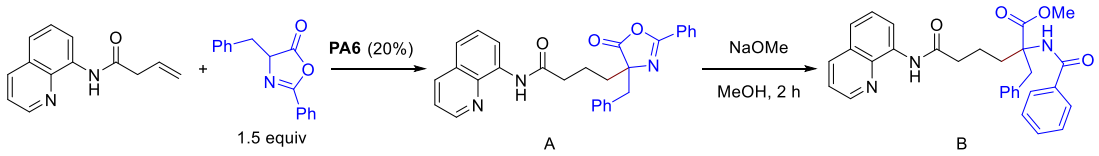
Optimization of reaction conditions:

Table S1: Optimization of palladium precatalyst.



entry	Pd catalyst (10%)	ligand (20%)	yield (%)	entiomeric ratio (*er*)
1	$Pd(OAc)_2$	PA6	30	62:38
2	$PdCl_2$	PA6	32	78:22
3	$PdCl_2(MeCN)_2$	PA6	30	79:21
4	**$PdCl_2(PhCN)_2$**	**PA6**	**34**	**80:20**
5	$Pd(MeCN)_4(BF_4)_2$	PA6	34	63:37
6	$Pd(PhCN)_2Cl_2$	PA1	46	74:26

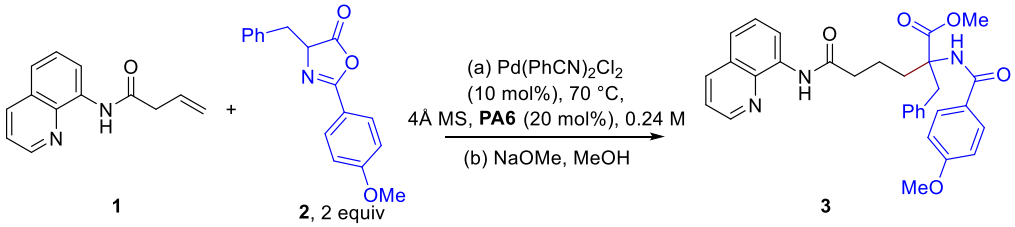
Table S2: Optimization of temperature and concentration.



Entry	Pd source	Solvent (1:1)	Temp. (°C)	Conc. (M)	Yield (%)	er of B (%)
1	$Pd(PhCN)_2Cl_2$	ACN:Toluene	120	2	26	59:41
2	$Pd(PhCN)_2Cl_2$	Toluene	90	0.35	43	82:18
3	$Pd(PhCN)_2Cl_2$	Toluene	65	0.35	39	87:13 (A)
4	$Pd(PhCN)_2Cl_2$	Toluene	65	0.7	36	84:16 (A)
5[a]	**$Pd(PhCN)_2Cl_2$**	**Toluene**	**70**	**0.05**	**35**	**89:11**
6[a]	$Pd(PhCN)_2Cl_2$	ACN:Toluene	70	0.05	31	80:20
7	$Pd(PhCN)_2Cl_2$	Toluene	70	0.015	40	86:14

[a]4Å MS

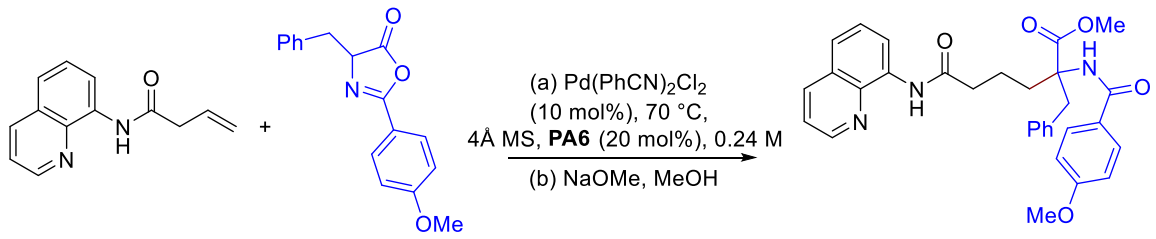
Table S3: Optimization of solvent.



Entry	Solvent	Yield (%)	ee (%)
1	Toluene	N/A	89:11
2	Trifluorotoluene	N/A	89:11
3	p-Xylene	N/A	88:12
4	m-Xylene	N/A	87:13
5	Chlorobenzene	N/A	87:13
6	Ethylbenzene	N/A	85:15
7	Toluene:DCM	36	88:2
8	Toluene + Cyclohexane (1:1), Pd (20%)	65	86:14
9	Benzene	37	93:7
10[a]	**Benzene**	**72**	**86:14**

[a]no 4Å MS, 3 equiv of **2**

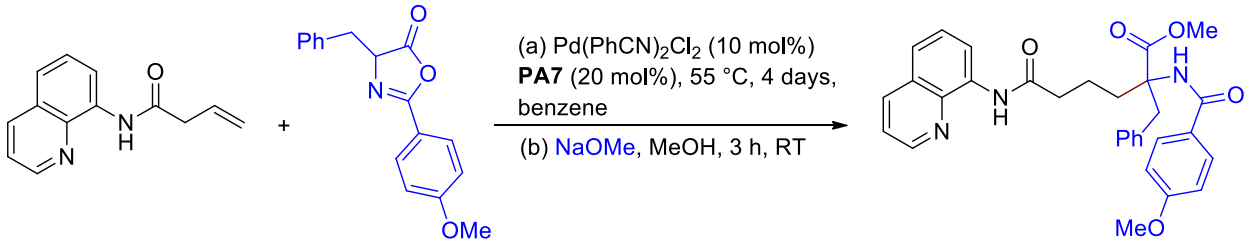
Table S4: Screening of additives.



Entry	Pd source (10%)	Solvent	Time (h)	Additive	Yield (%)	*er*
1	$Pd(PhCN)_2Cl_2$ (20%)	Toluene	24	$AgSbF_6$ (40%)	trace	ND
2	$Pd(PhCN)_2Cl_2$ (20%)	Toluene	24	$NaSbF_6$ (40%)	39	90:10
3	$Pd(PhCN)_2Cl_2$ (20%)	Toluene	24	$NaPF_6$ (40%)	90	67:33
4	$Pd(PhCN)_2Cl_2$	Toluene	24	$NaSbF_6$ (20%)	~25	91:9
5	$Pd(PhCN)_2Cl_2$	Toluene	24	$NaPF_6$ (20%)	~25	86:14
6	$Pd(PhCN)_2Cl_2$	Toluene	24	$NaBF_4$ (20%)	~25	93:7
7	$Pd(PhCN)_2Cl_2$ (20%)	Benzene	36	-	75	89:11
8	$Pd(PhCN)_2Cl_2$ (15%)	Benzene	-	-	63	92:8
9	$Pd(PhCN)_2Cl_2$ (20%)	Benzene	-	-	74	91:9
10	$Pd(PhCN)_2Cl_2$ (20%)	Benzene	36	Conc. 0.1 M	54	91:9
11[a]	$Pd(PhCN)_2Cl_2$ (Filled with O_2)	Benzene	60	Conc. 0.1 M	30	93:7
12[a]	$Pd(PhCN)_2Cl_2$ (Added 5% Pd every 12 h up to 15%)	Benzene	60	Conc. 0.1 M	46	91:9
13	$Pd(PhCN)_2Cl_2$	Benzene	36	3Å MS	~10	ND
14	$Pd(PhCN)_2Cl_2$	Benzene	36	5Å MS	42	90:10

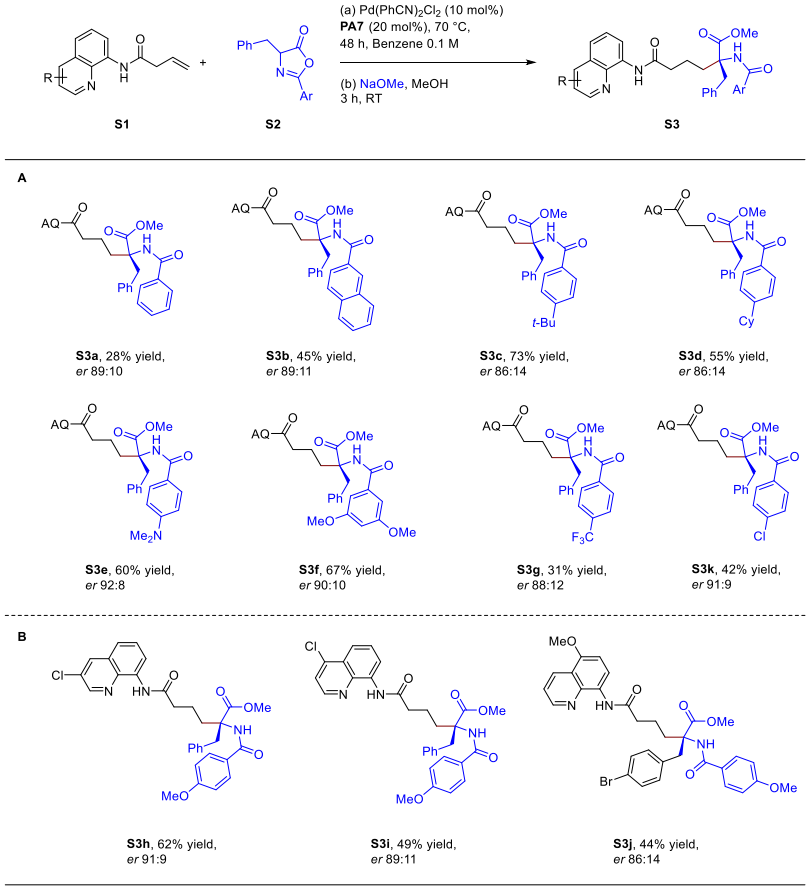
[a]Trace product was observed after 48 h at 50 °C, at which point the temperature was raised to 70 °C for 48 h.

Table S5: Optimization of reaction concentration.



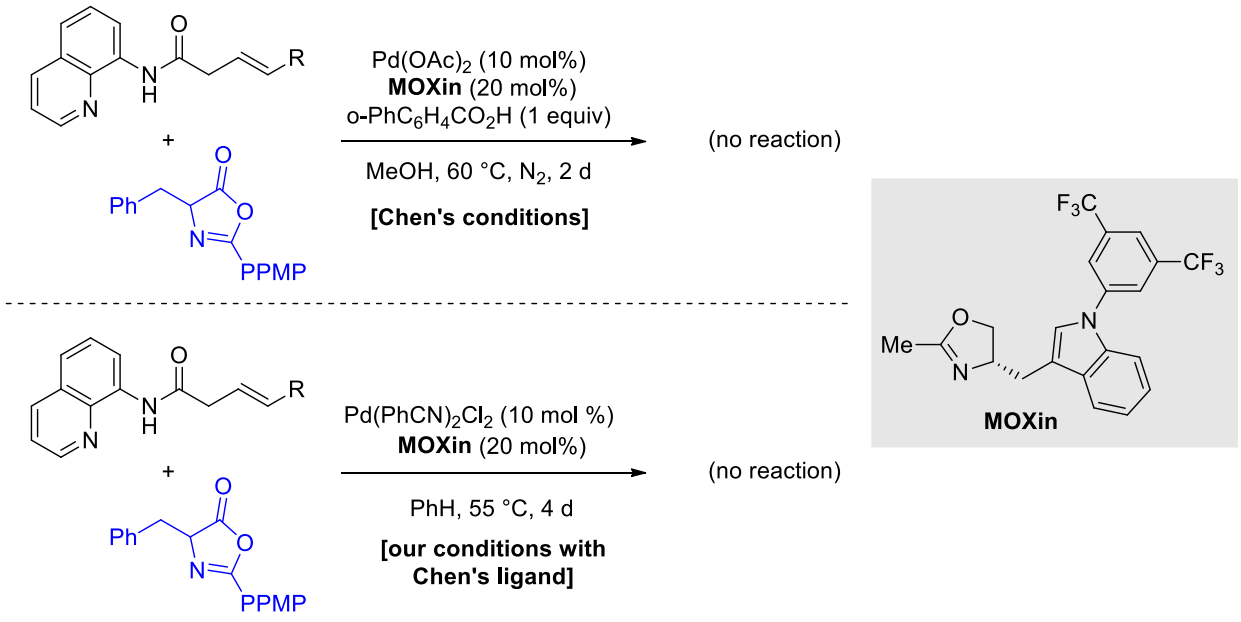
Entry	Conc. (M)	Yield (%)	*er*
1	0.5	N/A	89:11
2	0.1	74	93:7
3	0.05	N/A	93:7

Figure S2: Additional data on optimization of azlactone protecting group.



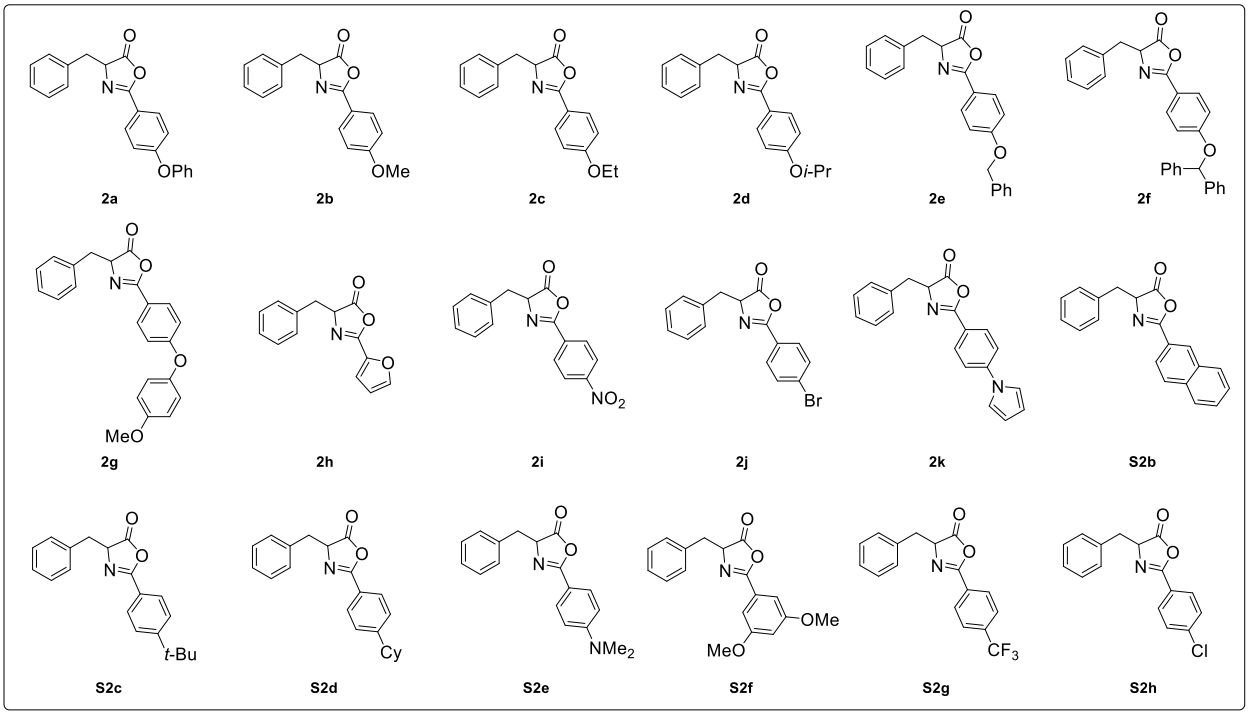
Control experiments with MOXin ligand

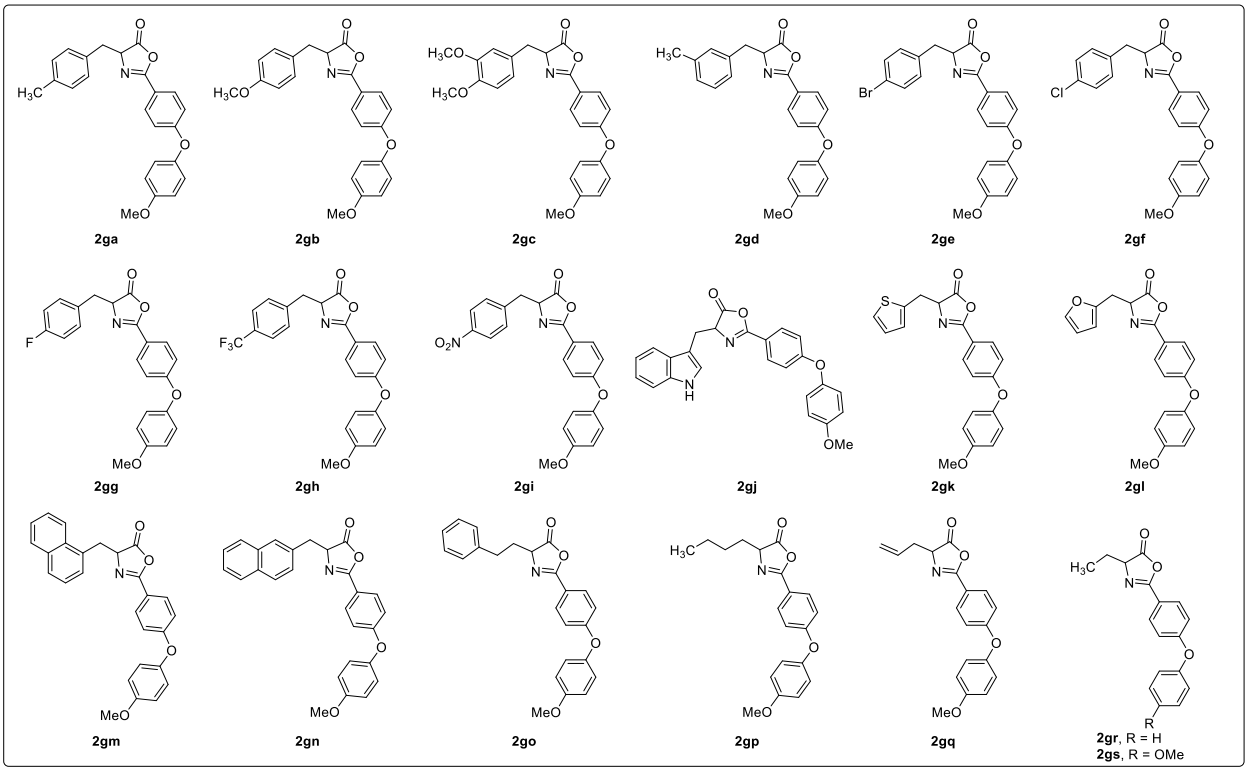
During the course of this study, He, Peng, and Chen described an example of AQ-directed asymmetric hydrocabonation, in which a new chiral center is created on the distal alkenyl carbon atom (γ-position).[2] To test whether this ligand was effective in the present reaction system, with a representative azlactone nucleophile, we found that under Chen's conditions and under optimal conditions from this manuscript, the monodentate chiral oxazoline ligand (**MOXin**) led to no reaction. This result demonstrates that the reactivity and selectivity enabled by the CPA is unique and not readily recapitulated by classical chiral L-type ligands.



General procedure for the synthesis of azlactones:

Figure S3: Azlactone substrates **2a**–**2k**, **2ga**–**2gs**, and **S2b–S2h**:

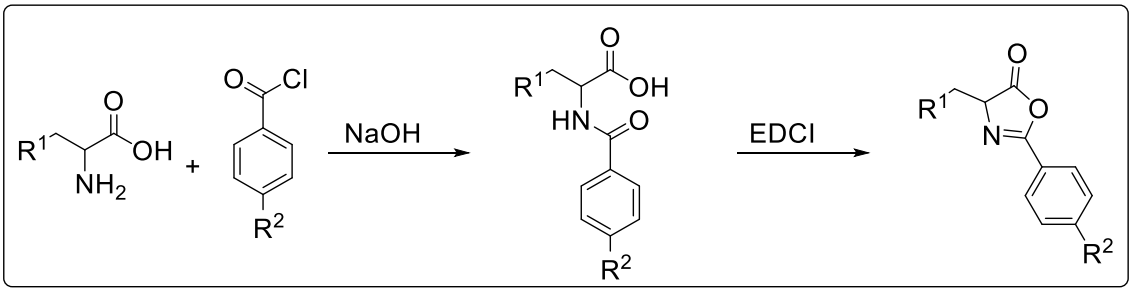


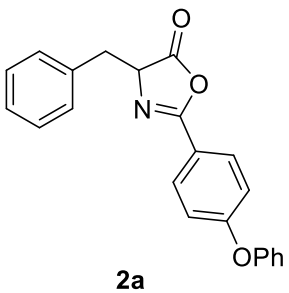


Unless otherwise stated, all the azlactone substrates were synthesized based on previously reported procedures from the corresponding commercially available achiral amino acids.[3] The

amino acid (1 equiv) was dissolved in a 2 M solution of NaOH (4 equiv) in water. The solution was cooled to 0 °C, and the corresponding benzoyl chloride (1.1 equiv) was added. The resulting mixture was allowed to warm to room temperature and stir for 24 h. Aqueous 6 M HCl solution was added to the reaction mixture until pH < 2 (as monitored by pH paper), and the solution was extracted with dichloromethane (×2). The combined organic layers were then dried over Na_2SO_4, filtered, and concentrated to give the acylated intermediate. This intermediate was then dissolved in dichloromethane, EDC•HCl (1 equiv) was added at 0 °C, and the reaction mixture was allowed to warm to room temperature and stir overnight. The reaction mixture was quenched by addition of water, and the two layers of the biphasic mixture were separated. The organic layer was washed with water several times until the aqueous layer became clear. The organic layer was then dried over Na_2SO_4, filtered, and concentrated *in vacuo*. The crude was purified by silica gel column chromatography using ethyl acetate in hexane (10–30%) to afford the desired azlactone.

Scheme S3: General route for the synthesis of azlactones.

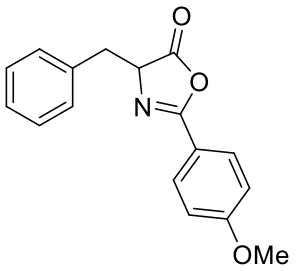




2a

4-benzyl-2-(4-phenoxyphenyl)oxazol-5(4H)-one (2a):

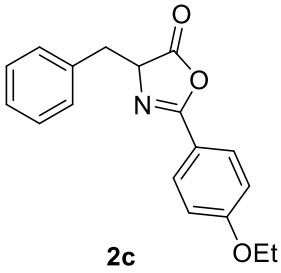
The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a white solid (900 mg, 94% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.91–7.84 (m, 2H), 7.43–7.35 (m, 2H), 7.27 (d, *J* = 4.4 Hz, 4H), 7.24–7.18 (m, 2H), 7.09–7.03 (m, 2H), 7.03–6.97 (m, 2H), 4.67 (dd, *J* = 6.7, 4.9 Hz, 1H), 3.36 (dd, *J* = 14.0, 5.0 Hz, 1H), 3.18 (dd, *J* = 14.0, 6.7 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.67, 161.70, 161.17, 155.41, 135.34, 130.08, 129.84, 129.59, 128.41, 127.18, 124.67, 120.18, 119.93, 117.68, 66.51, 37.39. **HRMS** (ESI-TOF) calcd for $C_{22}H_{18}NO_3$ $[M+H]^+$: 344.1281, Found: 344.1286.



2b

4-benzyl-2-(4-methoxyphenyl)oxazol-5(4H)-one (2b):

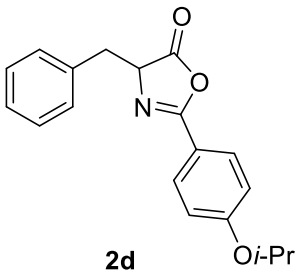
The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a white solid (5.1 g, 91% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.88–7.83 (m, 2H), 7.28–7.23 (m, 4H), 7.22–7.18 (m, 1H), 6.97–6.91 (m, 2H), 4.66 (dd, *J* = 6.7, 5.0 Hz, 1H), 3.86 (s, 3H), 3.35 (dd, *J* = 14.0, 5.0 Hz, 1H), 3.17 (dd, *J* = 14.0, 6.7 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.34, 162.69, 160.94, 134.95, 129.29, 129.12, 127.92, 126.67, 117.61, 113.69, 65.98, 55.01, 36.97. **HRMS** (ESI-TOF) calcd for $C_{17}H_{16}NO_3$ $[M+H]^+$: 282.1125, Found: 282.1129.



2c

4-benzyl-2-(4-ethoxyphenyl)oxazol-5(4H)-one (2c):

The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a white solid (850 mg, 61% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.88–7.81 (m, 2H), 7.29–7.23 (m, 4H), 7.22–7.16 (m, 1H), 6.94–6.88 (m, 2H), 4.65 (dd, *J* = 6.8, 5.0 Hz, 1H), 4.08 (q, *J* = 7.0 Hz, 2H), 3.34 (dd, *J* = 14.0, 5.0 Hz, 1H), 3.16 (dd, *J* = 14.0, 6.8 Hz, 1H), 1.43 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 178.00, 162.71, 161.55, 135.60, 129.87, 129.72, 128.51, 127.25, 117.99, 114.71, 66.58, 63.89, 37.58, 14.80. **HRMS** (ESI-TOF) calcd for $C_{18}H_{18}NO_3$ $[M+H]^+$: 296.1281, Found: 296.1287.

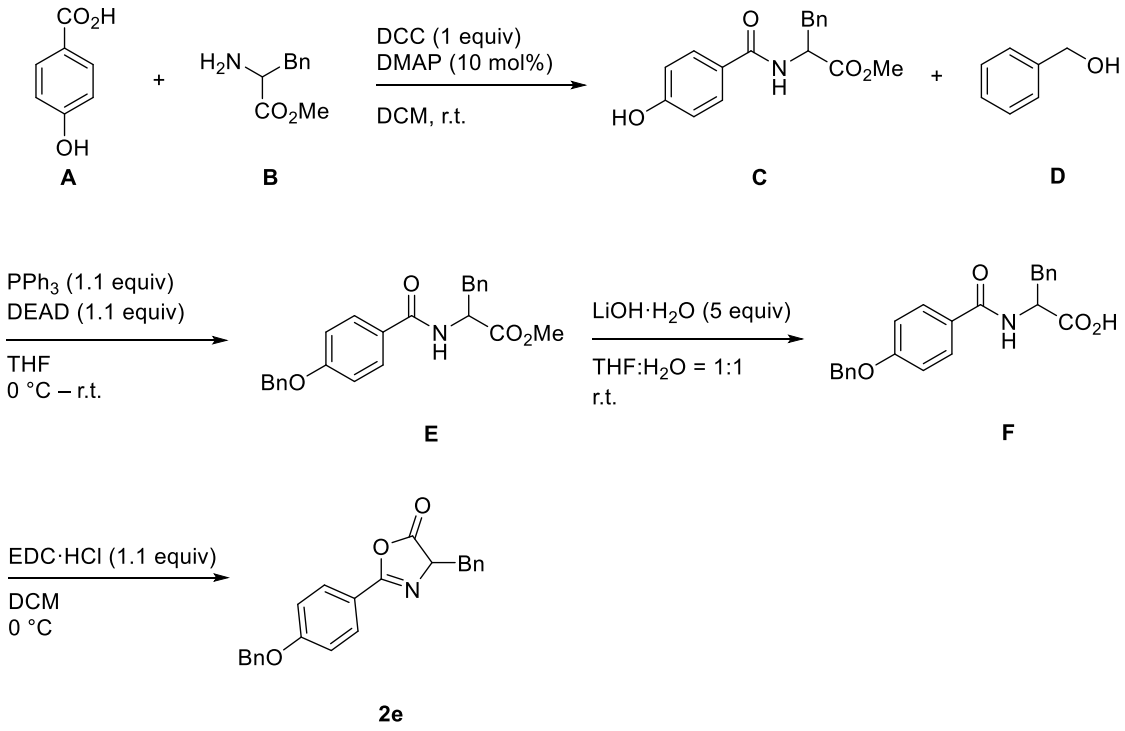


2d

4-benzyl-2-(4-isopropoxyphenyl)oxazol-5(4H)-one (2d):

The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a yellow solid (800 mg, 76% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.86–7.80 (m, 2H), 7.28–7.23 (m, 4H), 7.22–7.18 (m, 1H), 6.93–6.87 (m, 2H), 4.66 (dd, *J* = 6.6, 5.0 Hz, 1H), 4.64–4.58 (m, 1H), 3.34 (dd, *J* = 14.0, 5.0 Hz, 1H), 3.17 (dd, *J* = 14.0, 6.7 Hz, 1H), 1.36 (d, *J* = 6.0 Hz, 6H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.86, 161.84, 161.72, 135.51, 129.94, 129.73, 128.51, 127.26, 117.57, 115.67, 70.28, 66.46, 37.53, 22.04. **HRMS** (ESI-TOF) calcd for $C_{19}H_{20}NO_3$ $[M+H]^+$: 310.1438, Found: 310.1437.

Scheme S4: Synthesis of **2e.**



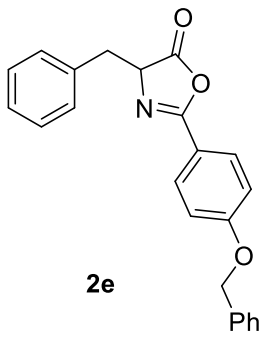
Amide coupling procedure: A 50-mL round-bottom flask equipped with a Teflon-coated magnetic stir bar was charged with methyl phenylalanine (**B**, 941 mg, 5 mmol, 1 equiv), DCC (1.03 g, 1.1 equiv), DMAP (61 mg, 10 mol%) and DCM (20 mL). Then *p*-hydroxybenzoic acid (**A**, 690 mg, 5 mmol, 1 equiv) was added. The mixture was stirred at room temperature for 17 h. After this time, the resulting mixture was filtered through a pad of Celite, which was washed with DCM. The collected organic layer was washed with 2M HCl (×1) and then with saturated $NaHCO_3$ aqueous solution (×1). Finally, the organic layer was washed with brine and dried over Na_2SO_4. The solvent was then removed *in vacuo* and purified via silica gel chromatography with ethyl acetate:hexanes = 3:2 as eluent. The product was obtained as a foamy white solid (1.2 g, 80%), which was carried on to the next step without further purification or analysis.

Mitsunobu procedure: A 50-mL two-neck round-bottom flask was equipped with a Teflon-coated magnetic stir bar. Intermediate **C** (1.2 g, 4 mmol, 1 equiv), benzyl alcohol (**D**, 0.45 mL, 4.4 mmol, 1.1 equiv) and PPh_3 (1.15 g, 4.4 mmol, 1.1 equiv) were added. The flask was evacuated under high vacuum and charged with N_2 on a manifold (×3). The mixture was then dissolved in dry THF (10 mL). DEAD (0.63 mL, 4.4 mmol, 1.1 equiv) was added at 0 °C (ice/water bath), and the reaction mixture was allowed to warm to room temperature gradually

and stir for 16 h. After this time, the reaction mixture was washed with 1 M K_2CO_3 (aq.) followed by brine, and the collected organic layer was dried over Na_2SO_4. The solvent was removed *in vacuo*, and the resulting residue was purified on silica gel chromatography with ethyl acetate:hexanes = 1:2 as eluent. The product was obtained as a white solid (1.54 g, 99%), which was carried on to the next step without further purification or analysis.

Ester deprotection procedure: To a 50-mL round-bottom flask equipped with a Teflon-coated magnetic stir bar were added intermediate **E** (1.54 g, 4 mmol, 1 equiv), LiOH•H_2O (0.84 g, 20 mmol, 5 equiv), THF (5 mL) and water (5 mL). The reaction mixture was stirred at room temperature for 90 min. After this time, the resulting suspension was diluted with water (20 mL) and washed with ethyl acetate. The collected aqueous layer was acidified to pH = 1 (as monitored by pH paper) with 3 M HCl, at which point a white solid precipitated. The resulting suspension was extracted with DCM (×3), and the collected organic layer was dried over Na_2SO_4. The solvent was removed *in vacuo*, and the product was obtained as a white solid (0.98 g, 66%), which was carried on to the next step without further purification or analysis.

Cyclization procedure: To a 50-mL round-bottom flask equipped with a Teflon coated stir bar were added intermediate **F** (0.98 g, 2.6 mmol, 1 equiv), EDC•HCl (0.55 g, 2.9 mmol, 1.1 equiv) and DCM (25 mL). The reaction mixture was stirred at 0 °C (ice/water bath) for 1 h. After this time, the reaction mixture was washed with water (×3) and then brine. The collected organic layer was dried over Na_2SO_4. The solvent was removed *in vacuo*, providing the crude product as a white solid. This material was recrystallized in DCM/hexanes in a refrigerator (4 °C), resulting in a white solid.

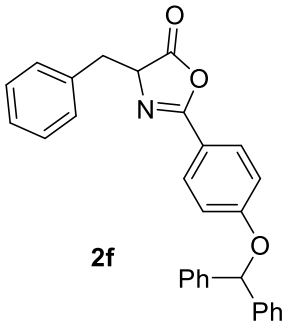


2e

4-benzyl-2-(4-(benzyloxy)phenyl)oxazol-5(4H)-one (2e):

The title compound was prepared according to the sequence depicted in Scheme S2 and was isolated as a white solid (790 mg, 85% yield for the final step). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.88–7.83 (m, 2H), 7.44–7.32 (m, 6H), 7.26–7.18 (m, 4H), 7.03–6.98 (m, 2H), 5.11 (s, 2H), 4.66 (dd, *J* = 6.7, 5.0 Hz, 1H), 3.34 (dd, *J* = 14.0, 5.0 Hz, 1H), 3.16 (dd, *J* = 14.0, 6.7 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.90, 162.45, 161.53, 136.24,

135.54, 129.92, 129.72, 128.85, 128.53, 128.41, 127.62, 127.28, 118.43, 115.14, 70.30, 66.57, 37.56. **HRMS** (ESI-TOF) calcd for $C_{23}H_{20}NO_{32}$ $[M+H]^+$: 358.1438, Found: 358.1439.

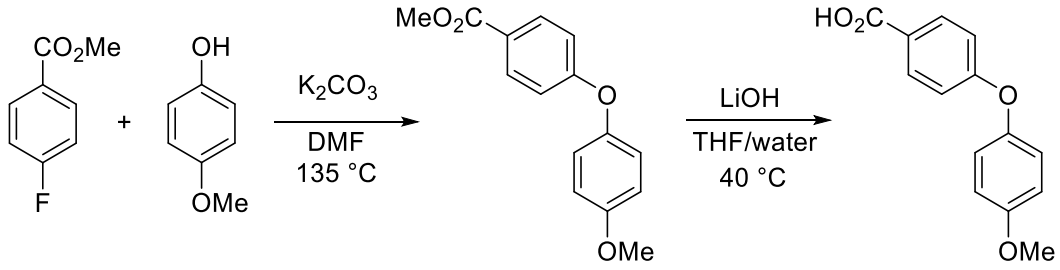


2f

2-(4-(benzhydryloxy)phenyl)-4-benzyloxazol-5(4H)-one (2f):
The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a white solid (380 mg, 47% yield). **^{1}H NMR** (600 MHz, $(CD_3)_2CO$) δ 7.78–7.73 (m, 2H), 7.53–7.48 (m, 5H), 7.31 (m, 4H), 7.25–7.21 (m, 4H), 7.21–7.17 (m, 2H), 7.12 (m, 4H), 6.56 (s, 1H), 4.76 (dd, *J* = 6.9, 4.9 Hz, 1H), 3.29–3.23 (m, 1H), 3.12–3.05 (m, 1H). **^{13}C NMR** (150 MHz, $(CD_3)_2CO$) δ 178.37, 162.20, 161.37, 142.03, 137.10, 130.43, 130.14, 129.45, 129.43, 128.94, 128.63, 119.63, 117.13, 116.45, 81.94, 66.94, 37.73. **HRMS** (ESI-TOF) calcd for $C_{29}H_{24}NO_3$ $[M+H]^+$: 434.1751, Found: 434.1755.

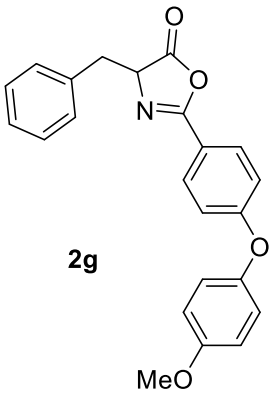
Preparation of 4-(4-methoxyphenoxy)benzoic acid (PPMP–CO_2H)

Scheme S5: Synthesis of PPMP–CO_2H.



Preparation of PPMP–CO_2H was carried out by adapting a procedure from the literature.[4] A suspension of 4-methoxphenol (1.24 g, 10 mmol, 1 equiv), methyl-4-fluorobenzoate (1.79 g, 11.6 mmol, 1.16 equiv), and K_2CO_3 (4.15 g, 30 mmol, 3 equiv) in DMF (20 mL) was heated to 135 °C for 84 h. The reaction mixture was diluted with water (40 mL) and extracted with ethyl acetate (×3). The combined organic layers were washed with 2 M NaOH followed by brine and dried over Na_2SO_4. The mixture was then filtered, and the solvent was removed on rotavap. The crude product was purified on silica gel column (hexane/ethyl acetate = 50/1) to provide the desired compound as a clear oil (1.87 g, 73%). Analytical data were consistent with values from the literature.

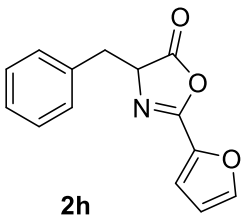
A suspension of methyl 4-(4-methoxyphenoxy)benzoate (3.02 g, 11.7 mmol, 1 equiv) from the previous step and lithium hydroxide monohydrate (2.45 g, 58.5 mmol, 5 equiv) THF/water mixture (1/1 v/v, 20 mL) were heated to 40 °C for 3 h. The reaction mixture was allowed to cool to room temperature and diluted with water (20 mL) and washed with ethyl acetate (20 mL). The organic layer was discarded. The aqueous layer was acidified with 3 M HCl until it reached pH = 1 (pH paper) and then extracted with DCM (×3). The combined organic layers were dried over Na_2SO_4. Finally the solution was filtered, and the solvent was removed on rotavap. The product was thus obtained in pure form as a white solid (2.57 g, 90%). Analytical data were consistent with values from the literature and also with data obtained from an authentic commercial sample.



2g

4-benzyl-2-(4-(4-methoxyphenoxy)phenyl)oxazol-5(4H)-one (2g):

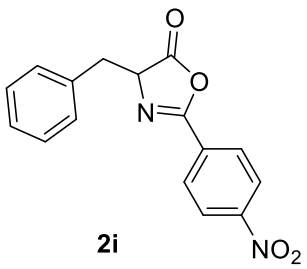
The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a white solid (300 mg, 63% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.87–7.80 (m, 2H), 7.29–7.24 (m, 4H), 7.23–7.18 (m, 1H), 7.04–6.97 (m, 2H), 6.97–6.88 (m, 4H), 4.66 (dd, *J* = 6.7, 5.0 Hz, 1H), 3.82 (s, 3H), 3.35 (dd, *J* = 14.0, 5.0 Hz, 1H), 3.17 (dd, *J* = 14.0, 6.7 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.87, 162.79, 161.35, 156.88, 148.56, 135.50, 129.93, 129.73, 128.54, 127.30, 121.83, 119.50, 116.91, 115.25, 66.64, 55.81, 37.54. **HRMS** (ESI-TOF) calcd for $C_{23}H_{20}NO_4$ $[M+H]^+$: 374.1387, Found: 374.1386.



2h

4-benzyl-2-(furan-2-yl)oxazol-5(4H)-one (2h):

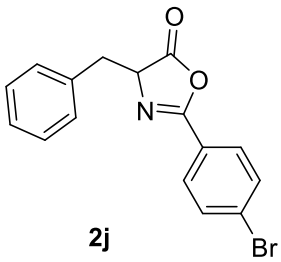
The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a yellow solid (630 mg, 54% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.68–7.60 (m, 1H), 7.32–7.26 (m, 4H), 7.26–7.22 (m, 1H), 7.03 (dt, *J* = 3.5, 0.7 Hz, 1H), 6.55 (dd, *J* = 3.5, 1.8 Hz, 1H), 4.71 (dd, *J* = 6.4, 5.1 Hz, 1H), 3.38 (dd, *J* = 14.1, 5.1 Hz, 1H), 3.23 (dd, *J* = 14.1, 6.5 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 176.45, 154.00, 147.04, 140.73, 135.07, 129.69, 128.59, 127.36, 117.18, 112.14, 65.89, 37.31. **HRMS** (ESI-TOF) calcd for $C_{14}H_{12}NO_3$ $[M+H]^+$: 242.0812, 242.0819.



2i

4-benzyl-2-(4-nitrophenyl)oxazol-5(4H)-one (2i):

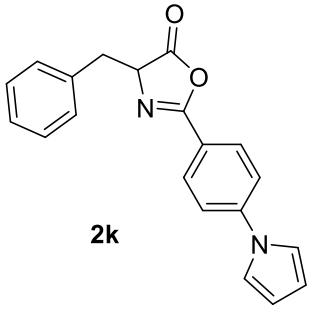
The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a yellow solid (280 mg, 18% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.33–8.28 (m, 2H), 8.12–8.07 (m, 2H), 7.32–7.27 (m, 1H), 7.26–7.19 (m, 4H), 4.76 (dd, *J* = 6.6, 5.0 Hz, 1H), 3.41 (dd, *J* = 14.1, 4.9 Hz, 1H), 3.23 (dd, *J* = 14.1, 6.6 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 176.51, 160.13, 150.28, 134.73, 131.27, 129.51, 128.92, 128.49, 127.42, 123.95, 66.80, 37.19. **HRMS** (ESI-TOF) calcd for $C_{16}H_{13}N_2O_4$ $[M+H]^+$: 297.0870, Found: 297.0870.



2j

4-benzyl-2-(4-bromophenyl)oxazol-5(4H)-one (2j):

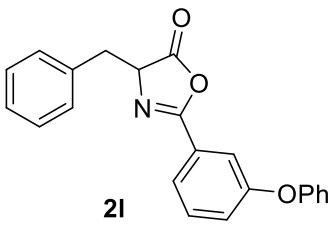
The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a white solid (900 mg, 55% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.79–7.75 (m, 2H), 7.61–7.57 (m, 2H), 7.28–7.18 (m, 5H), 4.67 (dd, *J* = 6.7, 4.9 Hz, 1H), 3.37 (dd, *J* = 14.0, 5.0 Hz, 1H), 3.18 (dd, *J* = 14.0, 6.7 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.33, 161.15, 135.21, 132.26, 129.68, 129.41, 128.57, 127.82, 127.41, 124.80, 66.72, 37.39. **HRMS** (ESI-TOF) calcd for $C_{16}H_{13}BrNO_2$ $[M+H]^+$: 330.0124, Found: 330.0123.



2k

2-(4-(1H-pyrrol-1-yl)phenyl)-4-benzyloxazol-5(4H)-one (2k):

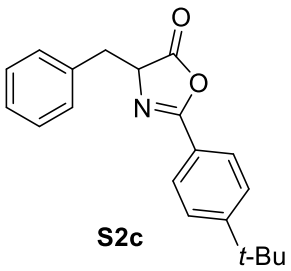
The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a yellow solid (120 mg, 52% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.02–7.91 (m, 2H), 7.46 (d, *J* = 8.7 Hz, 2H), 7.31–7.24 (m, 4H), 7.25–7.19 (m, 1H), 7.15 (t, *J* = 2.2 Hz, 2H), 6.39 (q, *J* = 2.4 Hz, 2H), 4.70 (dd, *J* = 6.7, 5.0 Hz, 1H), 3.38 (dd, *J* = 14.0, 5.0 Hz, 1H), 3.20 (dd, *J* = 14.1, 6.7 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 176.94, 160.62, 143.36, 134.75, 129.12, 129.05, 127.97, 126.78, 121.96, 119.24, 118.50, 111.20, 66.06, 36.91. **HRMS** (ESI-TOF) calcd for $C_{20}H_{17}N_2O_2$ $[M+H]^+$: 317.1285, Found: 317.1288.



2l

4-benzyl-2-(3-phenoxyphenyl)oxazol-5(4H)-one (2l):

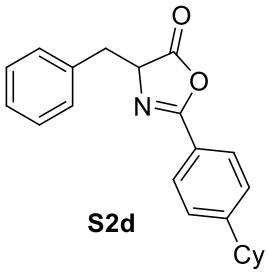
The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a colorless oil (340 mg, 42% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.66–7.62 (m, 1H), 7.56–7.53 (m, 1H), 7.43–7.33 (m, 4H), 7.25–7.20 (m, 4H), 7.19–7.13 (m, 2H), 7.05–6.98 (m, 2H), 4.67 (dd, *J* = 6.7, 5.0 Hz, 1H), 3.35 (dd, *J* = 14.0, 5.0 Hz, 1H), 3.17 (dd, *J* = 14.0, 6.7 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.54, 161.36, 157.92, 156.56, 135.30, 130.33, 130.12, 129.72, 128.56, 127.57, 127.37, 124.13, 123.05, 122.66, 119.35, 117.87, 66.72, 37.42. **HRMS** (ESI-TOF) calcd for $C_{22}H_{18}NO_3$ $[M+H]^+$: 344.1281, Found: 344.1283.



S2c

4-benzyl-2-(4-(tert-butyl)phenyl)oxazol-5(4H)-one (S2c):

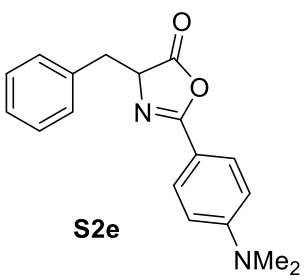
The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a white solid (1.13 g, 74% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.86–7.82 (m, 2H), 7.48–7.44 (m, 2H), 7.29–7.23 (m, 4H), 7.23–7.19 (m, 1H), 4.68 (dd, *J* = 6.6, 5.0 Hz, 1H), 3.36 (dd, *J* = 14.0, 4.9 Hz, 1H), 3.18 (dd, *J* = 14.0, 6.6 Hz, 1H), 1.33 (d, *J* = 1.0 Hz, 9H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.72, 161.76, 156.48, 135.30, 129.59, 128.41, 127.73, 127.16, 125.74, 122.86, 66.46, 37.33, 35.14, 31.07. **HRMS** (ESI-TOF) calcd for $C_{20}H_{22}NO_2$ $[M+H]^+$: 308.1645, Found: 308.1658



S2d

4-benzyl-2-(4-cyclohexylphenyl)oxazol-5(4H)-one (S2d):

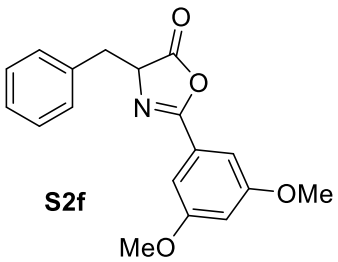
The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a white solid (1.5 g, 61% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.85–7.80 (m, 2H), 7.31–7.23 (m, 6H), 7.20 (ddt, *J* = 8.6, 5.6, 3.0 Hz, 1H), 4.67 (dd, *J* = 6.7, 5.0 Hz, 1H), 3.35 (dd, *J* = 14.0, 5.0 Hz, 1H), 3.17 (dd, *J* = 14.0, 6.7 Hz, 1H), 2.61–2.49 (m, 1H), 1.92–1.80 (m, 4H), 1.76 (m, 1H), 1.40 (m, 4H), 1.26 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.69, 161.83, 153.39, 135.32, 129.58, 128.40, 127.97, 127.27, 127.15, 123.19, 66.43, 44.70, 37.33, 34.10, 26.70, 26.01. **HRMS** (ESI-TOF) calcd for $C_{22}H_{24}NO_2$ $[M+H]^+$: 334.1802, Found: 334.1800.



S2e

4-benzyl-2-(4-(dimethylamino)phenyl)oxazol-5(4H)-one (S2e):

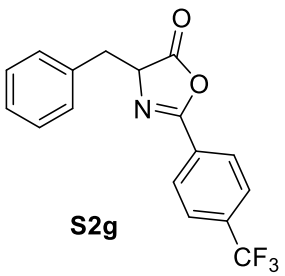
To a round-bottom flask containing a Teflon-coated magnetic stir bar were added phenyl alanine methyl ester (1 g, 1.0 equiv), 4-(dimethylamino)benzoic acid (0.9 g, 1.0 equiv), EDC•HCl (1.6 g, 1.5 equiv), and dichlormethane (15 mL). *N*-Methyl morpholine (1.11 g, 2.0 equiv) was added dropwise, and the resulting mixture was stirred at rt overnight. The reaction mixture was quenched with water, and the coupled product was extracted with dichloromethane. The solvent was removed *in vacuo*, and the crude intermediate was then sapponified to the free carboxylic acid by treatment with aq. NaOH (2 N) in methanol. After 30 min, the reaction mixture was washed with dichloromethane, and the organic layer was discarded. The pH of the aqueous layer was adjusted to pH = 5–6 (as monitored by pH paper), and the hydrolyzed intermediate was extracted with dichloromethane. The resulting carboxylic acid was cyclodehydrated using EDC•HCl and the work-up protocol described in the general procedure to yield the desired product as yellow solid (300 mg, 19% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.76 (dd, *J* = 8.2, 1.4 Hz, 2H), 7.30–7.22 (m, 4H), 7.21–7.16 (m, 1H), 6.69–6.63 (m, 2H), 4.64 (ddd, *J* = 6.4, 5.1, 1.0 Hz, 1H), 3.32 (dd, *J* = 14.0, 5.0 Hz, 1H), 3.16 (dd, *J* = 14.0, 6.6 Hz, 1H), 3.04 (d, *J* = 0.9 Hz, 6H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 178.24, 161.96, 153.03, 135.67, 129.61, 129.39, 128.32, 127.00, 112.24, 111.13, 66.29, 40.03, 37.58. **HRMS** (ESI-TOF) calcd for $C_{18}H_{19}N_2O_2$ $[M+H]^+$: 295.1441, Found: 295.1442.



S2f

4-benzyl-2-(3,5-dimethoxyphenyl)oxazol-5(4H)-one (S2f):

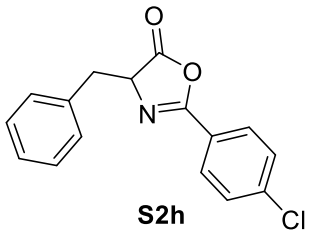
The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a white solid (800 mg, 54% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.28–7.24 (m, 4H), 7.24–7.19 (m, 1H), 7.05 (d, *J* = 2.3 Hz, 2H), 6.62 (t, *J* = 2.3 Hz, 1H), 4.68 (dd, *J* = 6.7, 5.0 Hz, 1H), 3.82 (s, 6H), 3.36 (dd, *J* = 14.1, 5.0 Hz, 1H), 3.19 (dd, *J* = 14.0, 6.7 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.47, 161.60, 160.88, 135.18, 129.56, 128.44, 127.41, 127.23, 105.59, 105.48, 66.61, 55.62, 37.28. **HRMS** (ESI-TOF) calcd for $C_{18}H_{18}NO_4$ $[M+H]^+$: 312.1230, Found: 312.1239.



S2g

4-benzyl-2-(4-(trifluoromethyl)phenyl)oxazol-5(4H)-one (S2g):

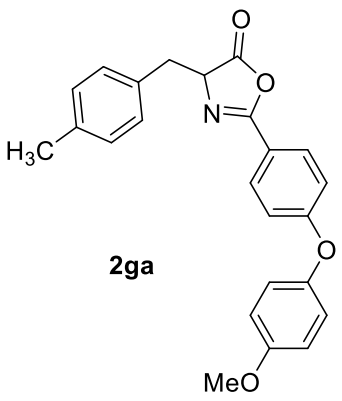
The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a white solid (1.1 g, 69% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.10–8.01 (m, 2H), 7.74 (d, *J* = 8.2 Hz, 2H), 7.33–7.21 (m, 5H), 4.76 (dd, *J* = 6.6, 4.9 Hz, 1H), 3.43 (dd, *J* = 14.0, 5.0 Hz, 1H), 3.24 (dd, *J* = 14.1, 6.6 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 176.90, 160.67, 134.90, 134.25 (q, *J* = 33.0 Hz), 129.54, 129.38, 129.04, 128.78, 128.47, 128.25, 127.35, 125.78 (q, *J* = 3.7 Hz), 123.49 (q, *J* = 272.7 Hz), 66.64, 37.22. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –63.43. **HRMS** (ESI-TOF) calcd for $C_{17}H_{13}F_3NO_2$ $[M+H]^+$: 320.0893, Found: 320.0885.



S2h

4-benzyl-2-(4-(tert-butyl)phenyl)oxazol-5(4H)-one (S2h):

The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a white solid (470 mg, 82% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.6 Hz, 2H), 7.43 (d, *J* = 8.6 Hz, 2H), 7.26 (dd, *J* = 4.8, 1.7 Hz, 5H), 7.22 (ddd, *J* = 8.8, 3.9, 2.3 Hz, 1H), 4.69 (dd, *J* = 6.7, 4.9 Hz, 1H), 3.37 (dd, *J* = 14.0, 4.9 Hz, 1H), 3.19 (dd, *J* = 14.0, 6.7 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.39, 161.02, 139.27, 135.25, 129.69, 129.30, 128.58, 127.41, 124.38, 66.73, 37.44. **HRMS** (ESI-TOF) calcd for $C_{16}H_{13}ClNO_2$ $[M+H]^+$: 286.0629, Found: 286.0631

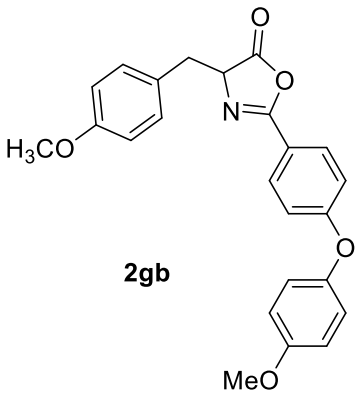


2ga

2-(4-(4-methoxyphenoxy)phenyl)-4-(4-methylbenzyl)oxazol-5(4H)-one (2ga):

The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a white solid (600 mg, 56% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.88–7.81 (m, 2H), 7.16–7.10 (m, 2H), 7.08–7.04 (m, 2H), 7.03–6.98 (m, 2H), 6.97–6.88 (m, 4H), 4.64 (dd, *J* = 6.7, 5.0 Hz, 1H), 3.83 (s, 3H), 3.31 (dd, *J* = 14.0, 5.0 Hz, 1H), 3.13 (dd, *J* = 14.0, 6.7 Hz, 1H), 2.28 (s, 3H).

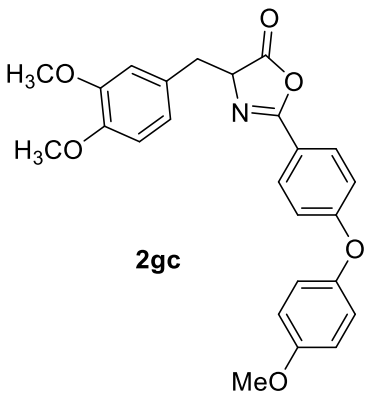
^{13}C NMR (150 MHz, $CDCl_3$) δ 177.28, 162.15, 160.69, 156.27, 147.96, 136.24, 131.78, 129.34, 128.97, 128.64, 121.22, 118.97, 116.28, 114.65, 66.16, 55.20, 36.52, 20.62. **HRMS** (ESI-TOF) calcd for $C_{24}H_{22}NO_4$ $[M+H]^+$: 388.1543, Found: 388.1540.



2gb

4-(4-methoxybenzyl)-2-(4-(4-methoxyphenoxy)phenyl)oxazol-5(4H)-one (2gb):

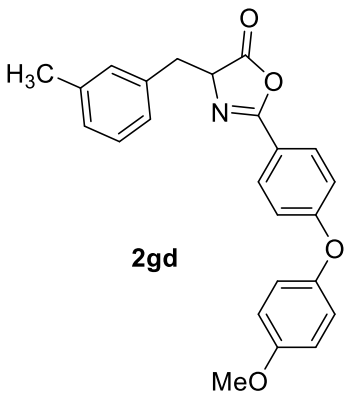
The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a yellow oil (560 mg, 57% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.89–7.83 (m, 2H), 7.21–7.16 (m, 2H), 7.07–7.01 (m, 2H), 6.99–6.91 (m, 4H), 6.84–6.78 (m, 2H), 4.65 (dd, *J* = 6.3, 4.9 Hz, 1H), 3.85 (s, 3H), 3.78 (s, 3H), 3.32 (dd, *J* = 14.1, 5.0 Hz, 1H), 3.16 (dd, *J* = 14.1, 6.4 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.31, 162.16, 160.70, 158.21, 156.27, 147.97, 130.21, 129.32, 126.78, 121.22, 118.93, 116.31, 114.64, 113.32, 66.25, 55.20, 54.71, 36.04. **HRMS** (ESI-TOF) calcd for $C_{24}H_{22}NO_5$ $[M+H]^+$: 404.1492, Found: 404.1495.



2gc

4-(3,4-dimethoxybenzyl)-2-(4-(4-methoxyphenoxy)phenyl)oxazol-5(4H)-one (2gc):

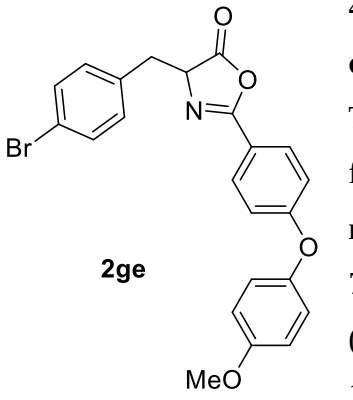
The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a yellow oil (550 mg, 57% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.87–7.80 (m, 2H), 7.03–6.99 (m, 2H), 6.96–6.89 (m, 4H), 6.81–6.72 (m, 3H), 4.66 (dd, *J* = 6.0, 4.8 Hz, 1H), 3.82 (s, 3H), 3.82 (s, 3H), 3.77 (s, 3H), 3.31 (dd, *J* = 14.0, 4.8 Hz, 1H), 3.15 (dd, *J* = 14.0, 6.0 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.85, 162.83, 161.38, 156.88, 148.61, 148.56, 148.23, 129.85, 127.67, 121.93, 121.83, 119.46, 116.96, 115.25, 112.88, 111.12, 66.80, 55.91, 55.86, 55.80, 36.97. **HRMS** (ESI-TOF) calcd for $C_{25}H_{24}NO_6$ $[M+H]^+$: 434.1598, Found: 434.1597.



2gd

2-(4-(4-methoxyphenoxy)phenyl)-4-(3-methylbenzyl)oxazol-5(4H)-one (2gd):

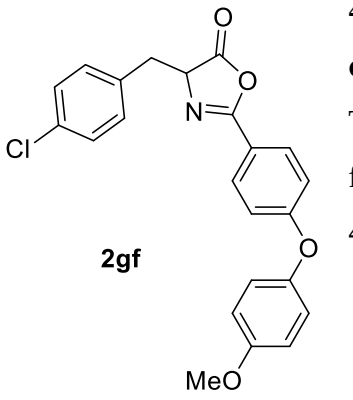
The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a yellow solid (420 mg, 62% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.87–7.79 (m, 2H), 7.15–7.10 (m, 1H), 7.09–7.02 (m, 2H), 7.02–6.95 (m, 3H), 6.95–6.88 (m, 4H), 4.63 (dd, *J* = 6.8, 5.0 Hz, 1H), 3.79 (s, 3H), 3.29 (dd, *J* = 13.9, 5.0 Hz, 1H), 3.09 (dd, *J* = 14.0, 6.8 Hz, 1H), 2.31–2.21 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.73, 162.67, 161.23, 156.78, 148.46, 137.97, 135.38, 130.39, 129.84, 128.31, 127.94, 126.60, 121.72, 119.46, 116.81, 115.16, 66.51, 55.67, 37.41, 21.41. **HRMS** (ESI-TOF) calcd for $C_{24}H_{22}NO_4$ $[M+H]^+$: 388.1543, Found: 388.1542.



2ge

4-(4-bromobenzyl)-2-(4-(4-methoxyphenoxy)phenyl)oxazol-5(4H)-one (2ge):

The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a yellow solid (680 mg, 74% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.85–7.82 (m, 2H), 7.40–7.35 (m, 2H), 7.15–7.10 (m, 2H), 7.04–6.99 (m, 2H), 6.97–6.90 (m, 4H), 4.64 (dd, *J* = 6.5, 4.9 Hz, 1H), 3.83 (s, 3H), 3.31 (dd, *J* = 14.1, 5.0 Hz, 1H), 3.13 (dd, *J* = 14.0, 6.6 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 176.95, 162.34, 160.97, 156.30, 147.90, 133.81, 131.06, 130.88, 129.37, 121.26, 120.84, 118.64, 116.34, 114.66, 65.69, 55.20, 36.18. **HRMS (ESI-TOF)** calcd for $C_{23}H_{19}BrNO_4$ $[M+H]^+$: 452.0492, Found: 452.0485.

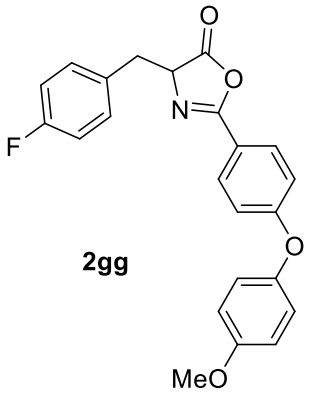


2gf

4-(4-chlorobenzyl)-2-(4-(4-methoxyphenoxy)phenyl)oxazol-5(4H)-one (2gf):

The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a white solid (400 mg, 49% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.90–7.75 (m, 2H), 7.25–

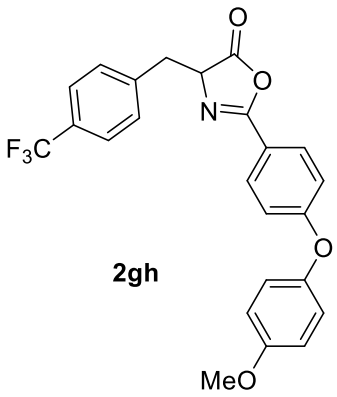
7.13 (m, 4H), 7.02 (m, *J* = 9.0 Hz, 2H), 6.98–6.86 (m, 4H), 4.64 (dd, *J* = 6.5, 4.9 Hz, 1H), 3.82 (s, 3H), 3.32 (dd, *J* = 14.0, 4.9 Hz, 1H), 3.14 (dd, *J* = 14.1, 6.5 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.00, 162.32, 160.93, 156.30, 147.90, 133.29, 132.67, 130.52, 129.35, 128.10, 121.25, 118.68, 116.34, 114.66, 65.79, 55.20, 36.13. **HRMS** (ESI-TOF) calcd for $C_{23}H_{19}ClNO_4$ $[M+H]^+$: 408.0997, Found: 408.0994.



2gg

4-(4-fluorobenzyl)-2-(4-(4-methoxyphenoxy)phenyl)oxazol-5(4H)-one (2gg):

The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a white solid (420 mg, 52% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.88–7.83 (m, 2H), 7.26–7.20 (m, 2H), 7.07–7.01 (m, 2H), 7.01–6.91 (m, 6H), 4.66 (dd, *J* = 6.4, 4.9 Hz, 1H), 3.85 (s, 3H), 3.35 (dd, *J* = 14.1, 4.9 Hz, 1H), 3.19 (dd, *J* = 14.1, 6.4 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.11, 162.28, 161.59 (d, *J* = 245.4 Hz), 160.86, 156.30, 147.91, 130.73 (d, *J* = 8.1 Hz), 130.45 (d, *J* = 3.3 Hz), 129.31, 121.25, 118.72, 116.32, 114.79 (d, *J* = 21.3 Hz), 114.65, 65.96, 55.20, 36.00. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –115.79. **HRMS** (ESI-TOF) calcd for $C_{23}H_{19}FNO_4$ $[M+H]^+$: 392.1293, Found: 392.1286.

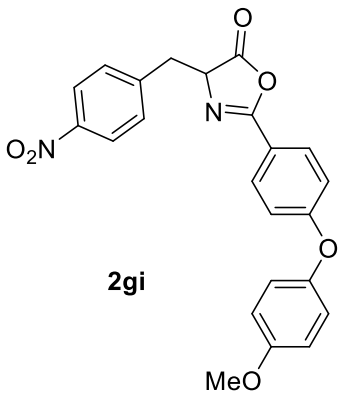


2gh

2-(4-(4-methoxyphenoxy)phenyl)-4-(4-(trifluoromethyl)benzyl)oxazol-5(4H)-one (2gh):

The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a yellow solid (600 mg, 64% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.89–7.80 (m, 2H), 7.57–7.50 (m, 2H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.04–6.98 (m, 2H), 6.97–6.89 (m, 4H), 4.67 (dd, *J* = 6.9, 4.9 Hz, 1H), 3.83 (s, 3H), 3.41 (dd, *J* = 14.1, 4.9 Hz, 1H), 3.21 (dd, *J* = 14.0, 7.0 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.47, 163.00, 161.68, 156.93, 148.47, 139.68, 130.10, 129.99, 129.66 (q, *J* = 32.3 Hz), 125.51 (q, *J* = 3.8 Hz), 124.26 (q, *J* = 272.0 Hz), 121.86, 119.18,

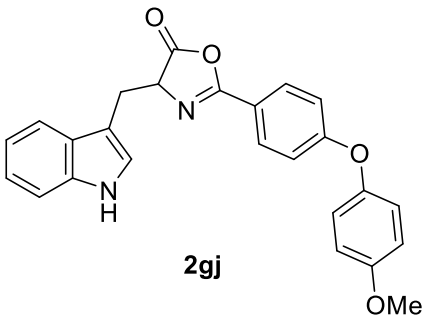
116.95, 115.27, 66.20, 55.80, 37.18. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.77. **HRMS** (ESI-TOF) calcd for $C_{24}H_{19}F_3NO_4$ $[M+H]^+$: 442.1261, Found: 442.1263.



2gi

2-(4-(4-methoxyphenoxy)phenyl)-4-(4-nitrobenzyl)oxazol-5(4H)-one (2gi):

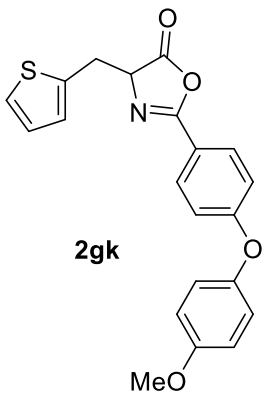
The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a yellow foamy solid (180 mg, 31% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.7 Hz, 2H), 7.83 (d, *J* = 8.9 Hz, 2H), 7.44 (d, *J* = 8.7 Hz, 2H), 7.01 (d, *J* = 9.0 Hz, 2H), 6.96–6.91 (m, 4H), 4.70 (dd, *J* = 6.8, 5.0 Hz, 1H), 3.83 (s, 3H), 3.46 (dd, *J* = 14.0, 5.0 Hz, 1H), 3.27 (dd, *J* = 14.0, 6.7 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.23, 163.15, 161.86, 156.97, 148.40, 147.42, 143.11, 130.71, 130.01, 123.77, 121.89, 118.93, 116.98, 115.28, 65.92, 55.81, 37.08. **HRMS** (ESI-TOF) calcd for $C_{23}H_{19}N_2O_6$ $[M+H]^+$: 419.1238, Found: 419.1237.



2gj

4-((1H-indol-3-yl)methyl)-2-(4-(4-methoxyphenoxy)phenyl)oxazol-5(4H)-one (2gj):

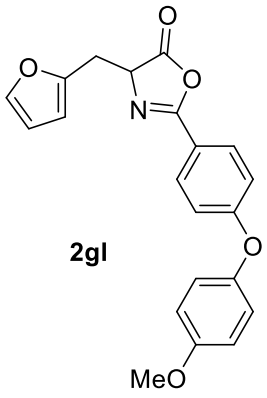
The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a yellow solid (170 mg, 51% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.80 (d, *J* = 9.0 Hz, 2H), 7.73–7.67 (m, 1H), 7.29 (d, *J* = 8.0, 0.9 Hz, 1H), 7.20–7.05 (m, 3H), 7.01–6.96 (m, 2H), 6.94–6.86 (m, 4H), 4.72 (dd, *J* = 6.2, 4.9 Hz, 1H), 3.82 (s, 3H), 3.51 (dd, *J* = 14.9, 5.0, 0.9 Hz, 1H), 3.38 (dd, *J* = 14.8, 6.3, 0.8 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 178.25, 162.68, 161.46, 156.85, 148.59, 136.07, 129.92, 127.59, 123.49, 122.22, 121.81, 119.73, 119.61, 119.36, 116.87, 115.24, 111.11, 109.95, 66.65, 55.81, 27.45. **HRMS** (ESI-TOF) calcd for $C_{25}H_{21}N_2O_4$ $[M+H]^+$: 413.1496, Found: 413.1496.



2gk

2-(4-(4-methoxyphenoxy)phenyl)-4-(thiophen-2-ylmethyl)oxazol-5(4H)-one (2gk):

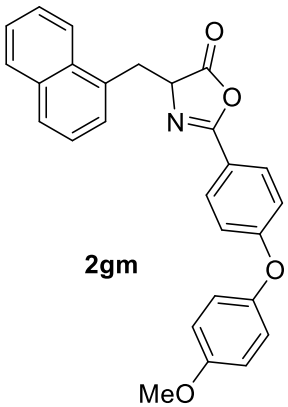
The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a yellow solid (420 mg, 38% yield). ^{1}**H NMR** (600 MHz, $CDCl_3$) δ 7.91–7.84 (m, 2H), 7.12 (dd, *J* = 5.1, 1.3 Hz, 1H), 7.03–7.00 (m, 2H), 6.97–6.88 (m, 6H), 4.66 (dd, *J* = 6.0, 4.7 Hz, 1H), 3.82 (s, 3H), 3.56 (dd, *J* = 15.0, 6.0 Hz, 1H), 3.46 (dd, *J* = 15.0, 6.0 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 176.76, 162.31, 161.47, 156.30, 147.91, 136.03, 129.48, 126.68, 126.36, 124.72, 121.26, 118.84, 116.33, 114.66, 65.75, 55.20, 31.01. **HRMS** (ESI-TOF) calcd for $C_{21}H_{18}NO_4S$ $[M+H]^+$: 380.0951, Found: 380.0951.



2gl

4-(furan-2-ylmethyl)-2-(4-(4-methoxyphenoxy)phenyl)oxazol-5(4H)-one (2gl):

The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a white solid (460 mg, 43% yield). ^{1}**H NMR** (600 MHz, $CDCl_3$) δ 7.93–7.88 (m, 2H), 7.32 (dd, *J* = 1.9, 0.9 Hz, 1H), 7.05–7.02 (m, 2H), 6.99–6.93 (m, 4H), 6.30–6.26 (m, 1H), 6.20–6.17 (m, 1H), 4.70 (dd, *J* = 6.3, 5.4 Hz, 1H), 3.85 (s, 3H), 3.41 (dd, 1H), 3.29 (dd, *J* = 15.4, 6.3, 0.9 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.55, 162.90, 161.90, 156.89, 149.78, 148.53, 142.17, 130.05, 121.84, 119.41, 116.93, 115.26, 110.56, 108.01, 64.52, 55.80, 30.22. **HRMS** (ESI-TOF) calcd for $C_{21}H_{18}NO_5$ $[M+H]^+$: 364.1179, Found: 364.1172.

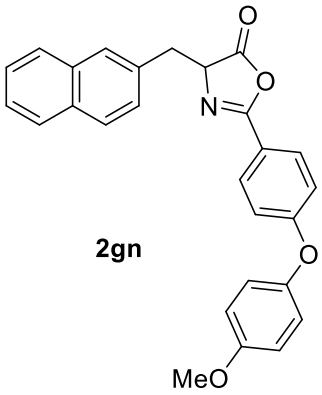


2gm

2-(4-(4-methoxyphenoxy)phenyl)-4-(naphthalen-1-ylmethyl)oxazol-5(4H)-one (2gm):

The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a gummy yellow solid (700 mg, 72% yield). ^{1}**H NMR** (600 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.5, 1H), 7.91–7.77 (m, 4H), 7.61–7.55 (m, 1H), 7.53–7.49 (m, 2H), 7.47–7.41 (m, 1H), 7.06–7.00 (m, 2H), 6.97–6.92 (m, 4H), 4.83 (dd, *J* = 7.8, 5.2

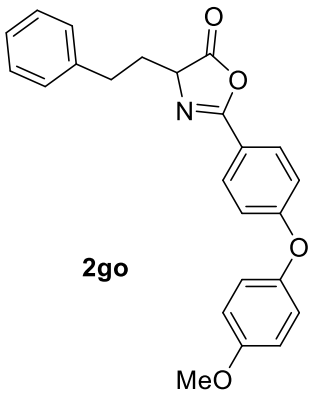
Hz, 1H), 3.89–3.79 (m, 4H), 3.55 (dd, *J* = 14.5, 7.8 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 178.03, 162.77, 161.33, 156.86, 148.55, 134.03, 132.13, 132.02, 129.95, 128.95, 128.24, 128.15, 126.22, 125.79, 125.51, 123.95, 121.81, 119.51, 116.88, 115.24, 66.29, 55.79, 34.95. **HRMS** (ESI-TOF) calcd for $C_{27}H_{22}NO_4$ $[M+H]^+$: 424.1543, Found: 424.1541.



2gn

2-(4-(4-methoxyphenoxy)phenyl)-4-(naphthalen-2-ylmethyl)oxazol-5(4H)-one (2gn):

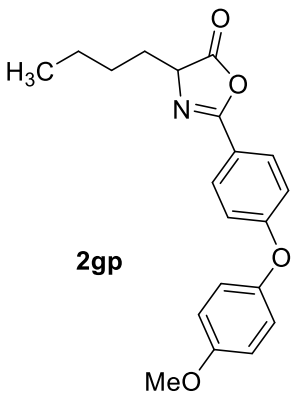
The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a yellow oil (370 mg, 44% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.90–7.85 (m, 2H), 7.81 (ddd, *J* = 7.3, 5.1, 2.0 Hz, 2H), 7.79–7.76 (m, 2H), 7.50–7.42 (m, 3H), 7.06–7.00 (m, 2H), 6.99–6.92 (m, 4H), 4.78 (dd, *J* = 6.8, 5.0 Hz, 1H), 3.84 (s, 3H), 3.56 (dd, *J* = 14.1, 5.0 Hz, 1H), 3.36 (dd, *J* = 14.1, 6.7 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.72, 162.68, 161.35, 156.76, 148.46, 133.42, 133.10, 132.56, 129.88, 128.43, 128.02, 127.84, 127.75, 127.65, 126.06, 125.78, 121.72, 119.37, 116.83, 115.15, 66.58, 55.67, 37.54. **HRMS** (ESI-TOF) calcd for $C_{27}H_{22}NO_4$ $[M+H]^+$: 424.1543, Found: 424.1542.



2go

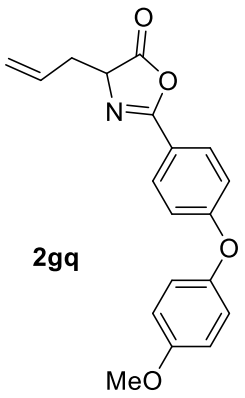
2-(4-(4-methoxyphenoxy)phenyl)-4-phenethyloxazol-5(4H)-one (2go):

The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a white solid (1.11 g, 90% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.96–7.90 (m, 2H), 7.32–7.27 (m, 2H), 7.26–7.18 (m, 3H), 7.06–6.96 (m, 4H), 6.96–6.89 (m, 2H), 4.37 (dd, *J* = 7.5, 5.8 Hz, 1H), 3.83 (s, 3H), 2.90–2.79 (m, 2H), 2.35–2.25 (m, 1H), 2.21–2.10 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 178.02, 162.23, 160.87, 156.28, 148.01, 139.82, 129.40, 128.17, 128.09, 125.88, 121.21, 119.06, 116.43, 114.67, 63.98, 55.21, 32.83, 30.98. **HRMS** (ESI-TOF) calcd for $C_{24}H_{22}NO_4$ $[M+H]^+$: 388.1543, Found: 388.1540.



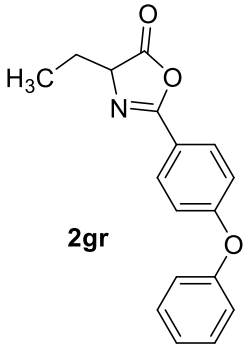
4-butyl-2-(4-(4-methoxyphenoxy)phenyl)oxazol-5(4H)-one (2gp):

The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a white solid (250 mg, 46% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.95–7.89 (m, 2H), 7.04–7.00 (m, 2H), 7.00–6.96 (m, 2H), 6.95–6.91 (m, 2H), 4.38 (dd, *J* = 7.1, 5.5 Hz, 1H), 3.83 (s, 3H), 2.07–1.96 (m, 1H), 1.92–1.78 (m, 1H), 1.54–1.26 (m, 4H), 0.92 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 178.26, 162.15, 160.64, 156.26, 148.02, 129.33, 121.19, 119.11, 116.41, 114.65, 64.89, 55.20, 30.91, 26.85, 21.88, 13.35. **HRMS** (ESI-TOF) calcd for $C_{20}H_{22}NO_4$ $[M+H]^+$: 340.1543, Found: 340.1544.



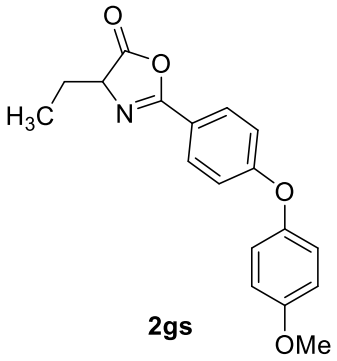
4-allyl-2-(4-(4-methoxyphenoxy)phenyl)oxazol-5(4H)-one (2gq):

The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as an orange solid (200 mg, 32% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.95–7.89 (m, 2H), 7.04–7.00 (m, 2H), 6.99–6.96 (m, 2H), 6.95–6.90 (m, 2H), 5.79 (dddd, *J* = 17.0, 10.2, 7.5, 6.7 Hz, 1H), 5.24 (dq, *J* = 17.1, 1.4 Hz, 1H), 5.16 (ddt, *J* = 10.3, 1.9, 1.0 Hz, 1H), 4.47 (dd, *J* = 6.5, 5.5 Hz, 1H), 3.83 (s, 3H), 2.84–2.74 (m, 1H), 2.68–2.58 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.96, 162.84, 161.48, 156.87, 148.57, 131.62, 130.00, 121.80, 119.82, 119.53, 116.98, 115.25, 65.46, 55.79, 35.56. **HRMS** (ESI-TOF) calcd for $C_{19}H_{18}NO_4$ $[M+H]^+$: 324.1230, Found: 324.1239.



4-ethyl-2-(4-phenoxyphenyl)oxazol-5(4H)-one (2gr):

The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as oil (510 mg, 77% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.98–7.93 (m, 2H), 7.43–7.38 (m, 2H), 7.21 (tt, *J* = 7.3, 1.1 Hz, 1H), 7.10–7.01 (m, 4H), 4.37 (dd, *J* = 6.7, 5.5 Hz, 1H), 2.13–2.00 (m, 1H), 2.00–1.89 (m, 1H), 1.05 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 178.62, 161.81, 161.34, 155.63, 130.23, 130.00, 124.78, 120.27, 120.26, 117.95, 66.52, 25.10, 9.62. **HRMS** (ESI-TOF) calcd for $C_{17}H_{16}NO_3$ $[M+H]^+$: 282.1125, Found: 282.1127.



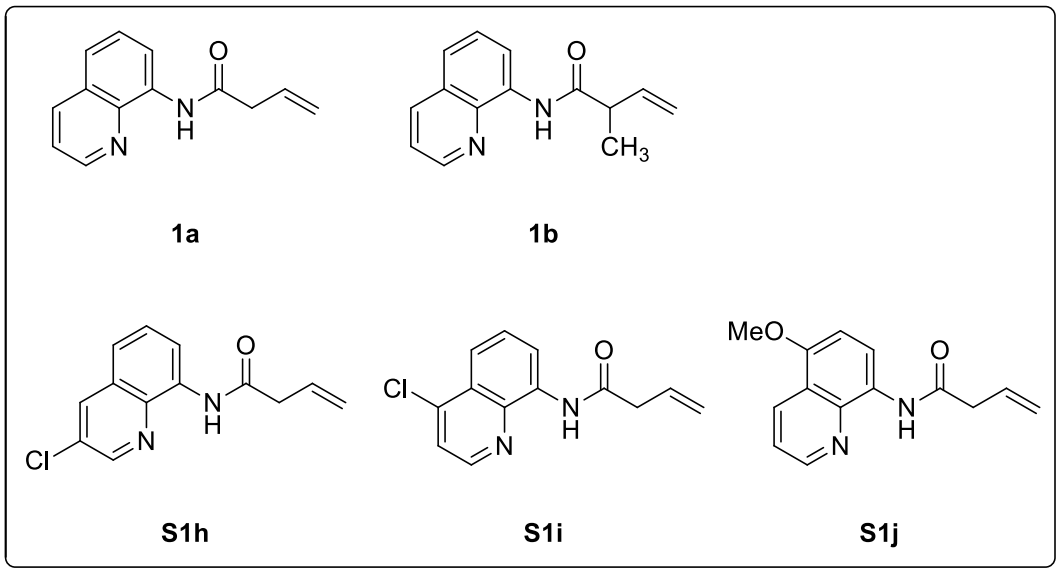
2gs

4-ethyl-2-(4-(4-methoxyphenoxy)phenyl)oxazol-5(4H)-one (2gs): The title compound was prepared according to the general procedure for synthesis of azlactones and was isolated as a white powder (620 mg, 61% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.9 Hz, 2H), 7.02 (d, *J* = 9.1 Hz, 2H), 6.98 (d, *J* = 8.9 Hz, 2H), 6.93 (d, *J* = 9.0 Hz, 2H), 4.37 (dd, *J* = 6.6, 5.6 Hz, 1H), 3.83 (s, 3H), 2.13–2.00 (m, 1H), 1.93 (ddd, *J* = 14.1, 7.6, 6.7 Hz, 1H), 1.04 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 178.63, 162.78, 161.40, 156.86, 148.61, 129.94, 121.79, 119.64, 117.00, 115.25, 66.46, 55.79, 25.08, 9.59. **HRMS** (ESI-TOF) calcd for $C_{18}H_{18}NO_4$ $[M+H]^+$: 312.1230, Found: 312.1227.

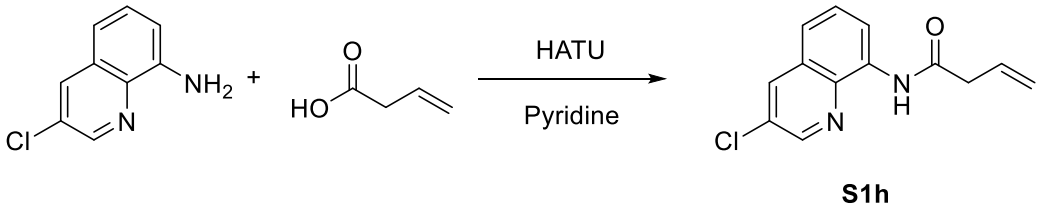
Synthesis of alkene substrates:

All of the alkene substrates were prepared according to modified literature procedure.[3] The synthesis of compounds **1a** and **1b** was previously described.[3a]

Figure S4: Alkene substrates **1a**, **1b**, and **S1h** – **S1j**.



Scheme S6: Synthesis of **S1h**

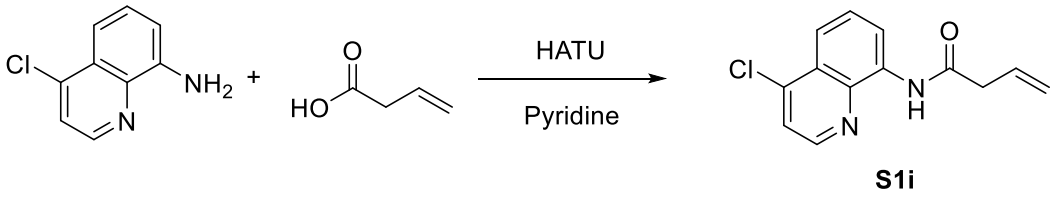


S1h

***N*-(3-chloroquinolin-8-yl)but-3-enamide (S1h):**

To a 25-mL round-bottom flask equipped with a Teflon-coated magnetic stir bar were added vinyl acetic acid (156 mg, 1.3 equiv) and dichloromethane (5 mL) at room temperature. Next, 3-chloroquinolin-8-amine (250 mg, 1.0 equiv), pyridine (0.24 mL, 2.0 equiv), and HATU (684 mg, 1.3 equiv) were added, and the resulting reaction mixture was stirred at room temperature for 16 h. The dark brown reaction mixture was diluted with ethyl acetate (20 mL) and washed with saturated aq. $NaHCO_3$ solution (20 mL). The organic layer was separated, treated with Na_2SO_4, filtered, and concentrated *in vacuo*. The crude product was purified by column chromatography using 0–15% ethyl acetate in hexane as eluent to give **S1h** as a yellow solid (270 mg, 79% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.78 (s, 1H), 8.76 (dd, *J* = 7.7, 1.3 Hz, 1H), 8.69 (d, *J* = 2.4 Hz, 1H), 8.11 (d, *J* = 2.3 Hz, 1H), 7.55 (t, *J* = 8.0 Hz, 1H), 7.42 (dd, *J* = 8.3, 1.2 Hz, 1H), 6.13 (ddt, *J* = 17.2, 10.2, 7.1 Hz, 1H), 5.44–5.34 (m, 2H), 3.35 (dt, *J* = 7.1, 1.3 Hz, 2H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 169.23, 147.44, 136.39, 134.58, 134.25, 130.80, 129.16, 128.83, 128.19, 120.70, 120.28, 116.68, 43.16. **HRMS** (ESI-TOF) calcd for $C_{13}H_{12}ClN_2O$ $[M+H]^+$: 247.0633, Found: 247.0635.

Scheme S7: Synthesis of **S1i**.



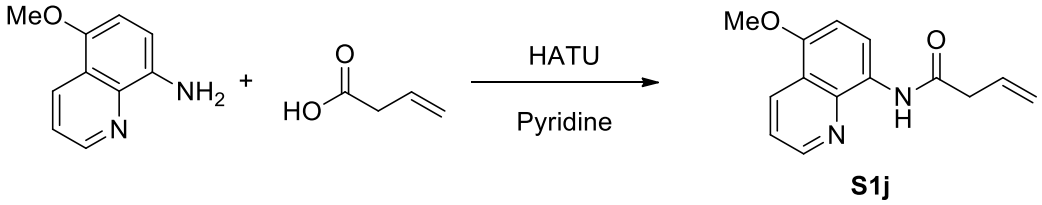
S1i

***N*-(4-chloroquinolin-8-yl)but-3-enamide (S1i):**

To a 25-mL round-bottom flask equipped with a Teflon-coated magnetic stir bar were added vinyl acetic acid (156 mg, 1.3 equiv) and dichloromethane (5 mL) at room temperature. Next, 4-

chloroquinolin-8-amine (250 mg, 1.0 equiv), pyridine (0.24 mL, 2.0 equiv), and HATU (684 mg, 1.3 equiv) were added, and the resulting reaction mixture was stirred at room temperature for 16 h. The dark brown reaction mixture was diluted with ethyl acetate (20 mL) and washed with saturated aq. $NaHCO_3$ solution (20 mL). The organic layer was separated, treated with Na_2SO_4, filtered, and concentrated *in vacuo*. The crude product was purified by column chromatography using 0–15% ethyl acetate in hexane as eluent to give **S1i** as white solid (190 mg, 56% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.94 (s, 1H), 8.84 (dd, *J* = 7.8, 1.2 Hz, 1H), 8.66 (d, *J* = 4.6 Hz, 1H), 7.89 (dd, *J* = 8.5, 1.3 Hz, 1H), 7.67–7.60 (m, 1H), 7.54 (d, *J* = 4.7 Hz, 1H), 6.14 (ddt, *J* = 17.2, 10.1, 7.1 Hz, 1H), 5.43–5.35 (m, 2H), 3.35 (dt, *J* = 7.1, 1.3 Hz, 2H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 169.27, 147.52, 143.14, 139.33, 134.70, 130.82, 128.46, 126.27, 121.81, 120.25, 117.82, 117.27, 43.19. **HRMS** (ESI-TOF) calcd for $C_{13}H_{12}ClN_2O$ $[M+H]^+$: 247.0633, Found: 247.0635.

Scheme S8: Synthesis of **S1j**.



S1j

***N*-(5-methoxyquinolin-8-yl)but-3-enamide (S1j):**

To a 25-mL round-bottom flask equipped with a Teflon-coated magnetic stir bar were added vinyl acetic acid (54.5 mg, 1.3 equiv) and dichloromethane (2 mL) at room temperature. Next, 8-amino-5-methoxyquinoline[3b] (85 mg, 1.0 equiv), pyridine (0.083 mL, 2.0 equiv), and HATU (241 mg, 1.3 equiv) were added, and the resulting reaction mixture was stirred at room temperature for 16 h. The dark brown reaction mixture was diluted with ethyl acetate (20 mL) and washed with saturated aq. $NaHCO_3$ solution (20 mL). The organic layer was separated, treated with Na_2SO_4, filtered, and concentrated *in vacuo*. The crude product was purified by column chromatography using 15–20% ethyl acetate in hexane as eluent to give **S1j** as a pale yellow solid (60 mg, 52% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.71 (s, 1H), 8.81 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.69 (d, *J* = 8.5 Hz, 1H), 8.57 (dd, *J* = 8.4, 1.7 Hz, 1H), 7.43 (dd, *J* = 8.4, 4.2 Hz, 1H), 6.84 (d, *J* = 8.5 Hz, 1H), 6.15 (ddt, *J* = 17.2, 10.2, 7.1 Hz, 1H), 5.43–5.32 (m, 2H), 3.99 (s, 3H), 3.33 (dt, *J* = 7.1, 1.3 Hz, 2H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 168.79, 150.29, 148.68,

139.21, 131.21, 131.18, 127.86, 120.68, 120.42, 119.90, 116.59, 104.30, 55.76, 43.12. **HRMS** (ESI-TOF) calcd for $C_{14}H_{15}N_2O_2$ $[M+H]^+$: 243.1128, Found: 243.1132.

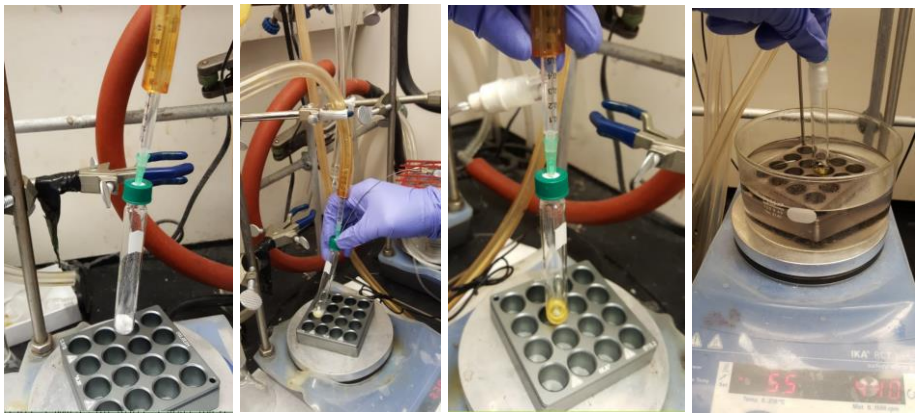
General α-alkylation procedure:

To a flame-dried reaction tube equipped with a Teflon-coated magnetic stir bar were added alkene **1** (1.0 equiv), azlactone **2** (3.0 equiv), **PA** (0.2 equiv), and $PdCl_2(PhCN)_2$ (0.1 equiv). The reaction tube was sealed with a screw-top septum cap. The reaction vessel was evacuated and back-filled with N_2 (×3). Anhydrous benzene (0.1 M) was added, and the reaction tube was placed in a preheated oil bath at 55 °C. The reaction mixture was allowed to stir at 55 °C for 4 d. The reaction mixture was cooled to room temperature. NaOMe in methanol (2 mL, 2 M solution) was added, and the resulting mixture was stirred at room temperature for 2 h. The reaction mixture was quenched with water and extracted with ethyl acetate (×3). The combined organic layers were washed with aq. brine solution. The organic phase was dried over Na_2SO_4, filtered, and concentrated *in vacuo*. The residue was purified by preparative TLC to afford the desired product

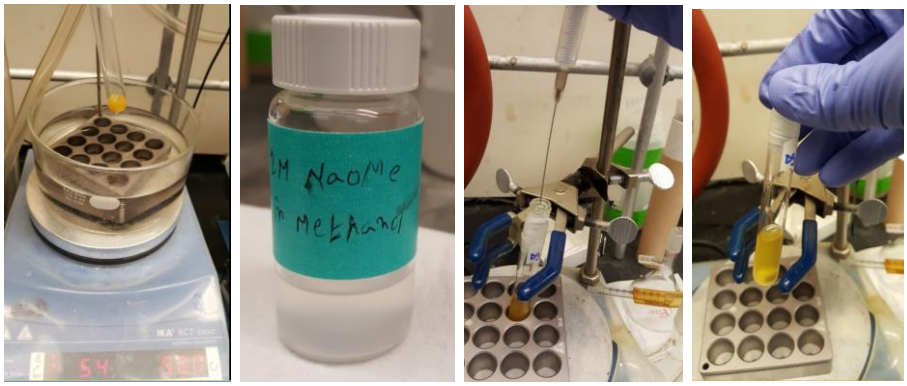
Photographic representation of the general procedure:

(a) Reagents used.

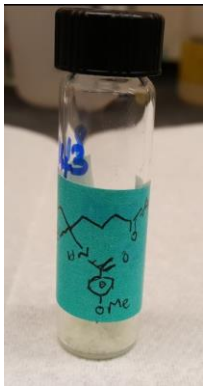
(b) After addition of all reagents, the reaction tube is evacuated and back-filled with nitrogen three times, and anhydrous benzene is added. The reaction mixture becomes homogeneous and turns yellow in color. The reaction vessel is placed in a pre-heated oil bath at 55 °C.



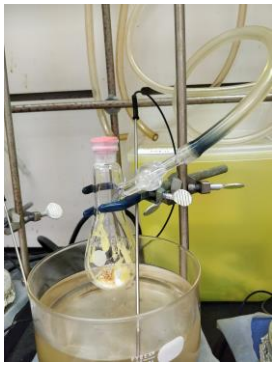
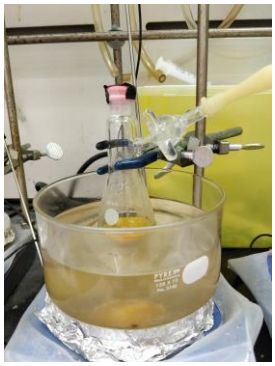
(c) After 4 d, the reaction vessel is allowed to cool to room temperature, and freshly prepared 2 M NaOMe in methanol solution is added. The resulting solution is stirred at room temperature for 2 h.

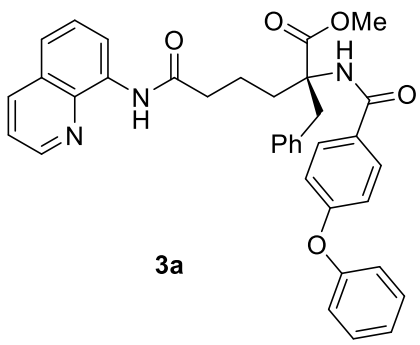


(d) The reaction mixture is quenched with water and extracted in ethyl acetate. After purification by column chromatography using 10–40% ethyl acetate in hexane as eluent, product **3b** is obtained as foamy white solid.



(e) Representative photos from large-scale experiment, following an analogous procedure.

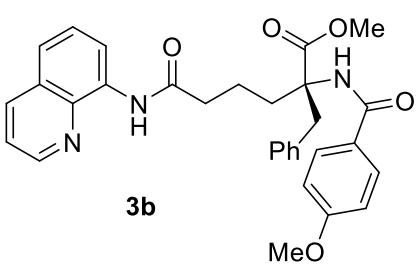






3a

methyl (*S*)-2-benzyl-6-oxo-2-(4-phenoxybenzamido)-6-(quinolin-8-ylamino)hexanoate (3a):

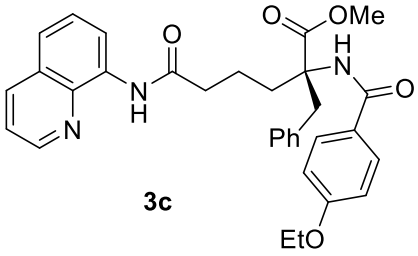
The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2a** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as yellow oil (18 mg, 64% yield, *er* 95:5). **SFC** (chiral column) Compound **3a** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [35% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.81–8.68 (m, 2H), 8.19–8.12 (m, 1H), 7.72–7.65 (m, 2H), 7.56–7.47 (m, 2H), 7.44 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.40–7.33 (m, 2H), 7.22–7.10 (m, 4H), 7.07–7.00 (m, 5H), 7.00–6.93 (m, 2H), 3.91 (d, *J* = 13.6 Hz, 1H), 3.84 (s, 3H), 3.20 (d, *J* = 13.6 Hz, 1H), 2.97–2.84 (m, 1H), 2.68–2.47 (m, 2H), 2.21–2.06 (m, 1H), 1.87–1.76 (m, 1H), 1.69–1.56 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.72, 171.02, 166.14, 160.47, 156.02, 148.11, 138.26, 136.37, 136.26, 134.41, 129.94, 129.65, 129.50, 128.84, 128.23, 127.92, 127.39, 126.90, 124.17, 121.60, 121.44, 119.75, 117.86, 116.44, 66.31, 52.91, 40.73, 37.53, 34.81, 20.52. **HRMS** (ESI-TOF) calcd for $C_{36}H_{34}N_3O_5$ $[M+H]^+$: 588.2493, Found: 588.2490.



3b

methyl (*S*)-2-benzyl-2-(4-methoxybenzamido)-6-oxo-6-(quinolin-8-ylamino)hexanoate (3b):

The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2b** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as white foamy solid (21 mg, 78% yield, *er* 92:8). **SFC** (chiral column) Compound **3b** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [35% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.85–8.64 (m, 2H), 8.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.73–7.64 (m, 2H), 7.58–7.47 (m, 2H), 7.44 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.20–7.12 (m, 3H), 7.06–7.00 (m, 2H), 6.98 (s, 1H), 6.93–6.84 (m, 2H), 3.92 (d, *J* = 13.5 Hz, 1H), 3.83 (s, 6H), 3.18 (d, *J* = 13.6 Hz, 1H), 2.92 (ddd, *J* = 13.6, 12.2, 4.6 Hz, 1H), 2.68–2.46 (m, 2H), 2.15 (ddd, *J* = 13.6, 11.9, 4.7 Hz, 1H), 1.90–1.74 (m, 1H), 1.71–1.55 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.93, 171.17, 166.44, 162.35, 148.26, 138.42, 136.45, 134.58, 129.81, 128.86, 128.33, 128.03, 127.50, 127.49, 126.99, 121.72, 121.53, 116.52, 113.89, 66.38, 55.54, 53.01, 40.87, 37.71, 34.99, 20.68. **HRMS (ESI-TOF)** calcd for $C_{31}H_{32}N_3O_5$ $[M+H]^+$: 526.2336, Found:526.2334.

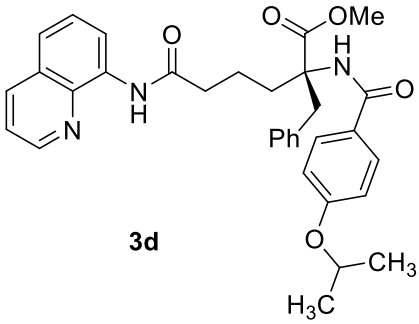


3c

methyl (*S*)-2-benzyl-2-(4-ethoxybenzamido)-6-oxo-6-(quinolin-8-ylamino)hexanoate (3c):

The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2c** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as yellow oil (21 mg, 74% yield, *er* 93:7). **SFC** (chiral column) Compound **3c** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [35% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) 9.77 (s, 1H), 8.80–8.70 (m, 2H), 8.15 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.70–7.63 (m, 2H), 7.56–7.48 (m, 2H), 7.44 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.16 (dd, *J* = 4.3, 2.1 Hz, 3H), 7.01 (dd, *J* = 6.6, 3.0 Hz, 2H), 6.97 (s, 1H), 6.90–6.86 (m, 2H), 4.06 (q, *J* = 7.0 Hz, 2H), 3.92 (d, *J* = 13.5 Hz, 1H), 3.83 (s, 3H), 3.18 (d, *J* = 13.5 Hz, 1H), 2.97–2.85 (m, 1H), 2.67–2.45 (m, 2H), 2.22–2.08 (m, 1H), 1.91–

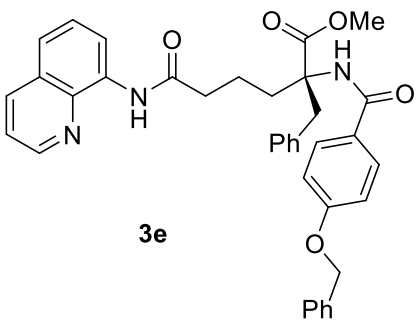
1.73 (m, 1H), 1.69–1.56 (m, 1H), 1.42 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.95, 171.19, 166.49, 161.77, 148.26, 138.43, 136.47, 136.45, 134.59, 129.83, 128.85, 128.33, 128.04, 127.52, 127.29, 126.99, 121.73, 121.54, 116.53, 114.36, 66.39, 63.77, 53.01, 40.89, 37.73, 35.01, 20.69, 14.85. **HRMS** (ESI-TOF) calcd for $C_{32}H_{34}N_3O_5$ $[M+H]^+$: 540.2493, Found: 540.2495.



3d

methyl (*S*)-2-benzyl-2-(4-isopropoxybenzamido)-6-oxo-6-(quinolin-8-ylamino)hexanoate (3d):

The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2d** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as foamy solid (25 mg, 87% yield, *er* 92:8). **SFC** (chiral column) Compound **3d** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [35% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.81–8.69 (m, 2H), 8.14 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.67 (d, *J* = 8.8 Hz, 2H), 7.56–7.47 (m, 2H), 7.44 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.17 (dd, *J* = 4.9, 1.9 Hz, 3H), 7.06–7.00 (m, 2H), 6.97 (s, 1H), 6.91–6.84 (m, 2H), 4.66–4.53 (m, 1H), 3.93 (d, *J* = 13.6 Hz, 1H), 3.83 (s, 3H), 3.18 (d, *J* = 13.5 Hz, 1H), 2.95–2.86 (m, 1H), 2.68–2.46 (m, 2H), 2.21–2.10 (m, 1H), 1.88–1.76 (m, 1H), 1.69–1.59 (m, 1H), 1.34 (d, *J* = 6.1 Hz, 6H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.94, 171.17, 166.48, 160.80, 148.25, 138.41, 136.47, 136.44, 134.58, 129.82, 128.86, 128.32, 128.03, 127.50, 127.06, 126.97, 121.71, 121.52, 116.51, 115.42, 70.11, 66.36, 52.99, 40.88, 37.72, 34.99, 22.07, 20.68. **HRMS** (ESI-TOF) calcd for $C_{33}H_{36}N_3O_5$ $[M+H]^+$: 554.2649, Found: 554.2648.

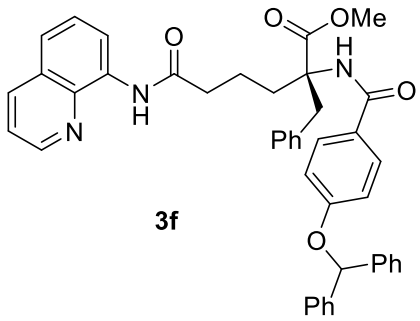


3e

methyl (*S*)-2-benzyl-2-(4-(benzyloxy)benzamido)-6-oxo-6-(quinolin-8-ylamino)hexanoate (3e):

The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2e** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as

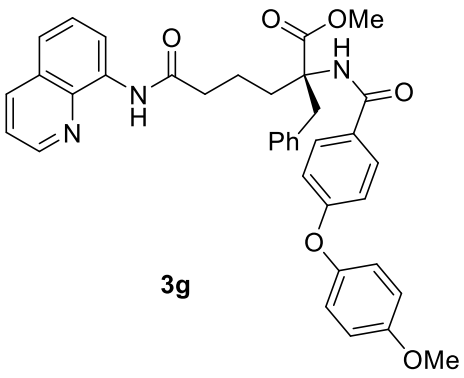
colorless oil (20 mg, 65% yield, *er* 92∶8). **SFC** (chiral column) Compound **3e** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [35% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.80–8.69 (m, 2H), 8.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.73–7.66 (m, 2H), 7.56–7.47 (m, 2H), 7.46–7.36 (m, 5H), 7.36–7.31 (m, 1H), 7.18–7.14 (m, 3H), 7.02 (dd, *J* = 6.7, 2.8 Hz, 2H), 7.00–6.93 (m, 3H), 5.10 (s, 2H), 3.92 (d, *J* = 13.6 Hz, 1H), 3.84 (s, 3H), 3.19 (d, *J* = 13.5 Hz, 1H), 2.98–2.85 (m, 1H), 2.67–2.48 (m, 2H), 2.21–2.10 (m, 1H), 1.87–1.77 (m, 1H), 1.69–1.58 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.91, 171.16, 166.40, 161.50, 148.25, 138.40, 136.51, 136.44, 134.56, 129.80, 128.87, 128.78, 128.33, 128.27, 128.03, 127.72, 127.58, 127.50, 126.98, 121.71, 121.53, 116.52, 114.77, 70.20, 66.38, 53.00, 40.86, 37.69, 34.97, 20.66. **HRMS** (ESI-TOF) calcd for $C_{37}H_{36}N_3O_5$ $[M+H]^+$: 602.2649, Found: 602.2646.



3f

methyl (*S*)-2-(4-(benzhydryloxy)benzamido)-2-benzyl-6-oxo-6-(quinolin-8-ylamino)hexanoate (3f):

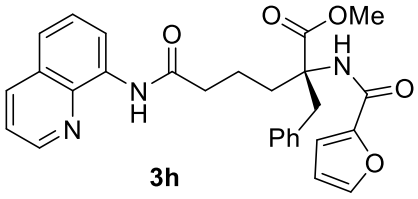
The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2f** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as foamy white solid (25 mg, 72% yield, *er* 91:9). **SFC** (chiral column) Compound **3f** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.78 (s, 1H), 8.83–8.70 (m, 2H), 8.17 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.66–7.61 (m, 2H), 7.57–7.49 (m, 2H), 7.48–7.41 (m, 5H), 7.39–7.34 (m, 4H), 7.33–7.30 (m, 2H), 7.20–7.15 (m, 3H), 7.05–7.00 (m, 2H), 6.99–6.94 (m, 3H), 6.28 (s, 1H), 3.92 (d, *J* = 13.5 Hz, 1H), 3.84 (s, 3H), 3.19 (d, *J* = 13.5 Hz, 1H), 2.96–2.85 (m, 1H), 2.67–2.48 (m, 2H), 2.20–2.12 (m, 1H), 1.85–1.75 (m, 1H), 1.69–1.57 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.86, 171.15, 166.39, 160.78, 148.26, 140.79, 140.78, 138.42, 136.44, 134.58, 129.80, 128.83, 128.76, 128.33, 128.08, 128.04, 127.79, 127.51, 126.97, 126.96, 121.72, 121.53, 116.53, 115.94, 81.94, 66.37, 52.99, 40.88, 37.69, 34.95, 20.65. **HRMS** (ESI-TOF) calcd for $C_{43}H_{40}N_3O_5$ $[M+H]^+$: 678.2962, Found: 678.2961.



3g

methyl (*S*)-2-benzyl-2-(4-(4-methoxyphenoxy)benzamido)-6-oxo-6-(quinolin-8-ylamino)hexanoate (3g):

The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2g** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as colorless oil (23 mg, 81% yield, *er* 93:7). **SFC** (chiral column) Compound **3a** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [35% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.79–8.70 (m, 2H), 8.14 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.67 (d, *J* = 8.6 Hz, 2H), 7.56–7.47 (m, 2H), 7.44 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.17 (dd, *J* = 5.1, 1.8 Hz, 3H), 7.06–6.97 (m, 5H), 6.95–6.86 (m, 4H), 3.91 (d, *J* = 13.5 Hz, 1H), 3.83 (s, 3H), 3.81 (s, 3H), 3.19 (d, *J* = 13.5 Hz, 1H), 2.95–2.85 (m, 1H), 2.66–2.48 (m, 2H), 2.20–2.09 (m, 1H), 1.87–1.73 (m, 1H), 1.69–1.57 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.85, 171.14, 166.30, 161.66, 156.57, 149.09, 148.25, 138.39, 136.46, 136.39, 134.54, 129.78, 128.95, 128.90, 128.34, 128.03, 127.49, 127.01, 121.72, 121.55, 121.54, 116.88, 116.52, 115.14, 66.39, 55.77, 53.02, 40.85, 37.66, 34.94, 20.64. **HRMS** (ESI-TOF) calcd for $C_{37}H_{36}N_3O_6$ $[M+H]^+$: 618.2599, Found: 618.2602.

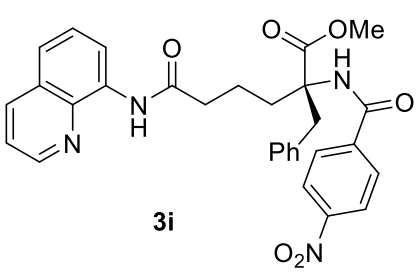


3h

methyl (*S*)-2-benzyl-2-(furan-2-carboxamido)-6-oxo-6-(quinolin-8-ylamino)hexanoate (3h):

The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2h** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as yellow oil (11 mg, 44% yield, *er* 89:11). **SFC** (chiral column) Compound **3a** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [35% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.81–8.69 (m, 2H), 8.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.57–7.47 (m, 2H), 7.45 (dd, *J* =

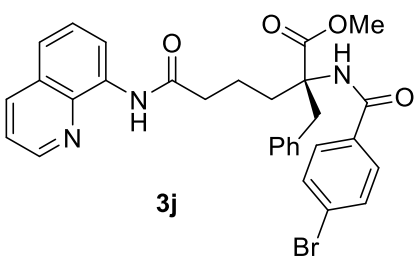
8.2, 4.2 Hz, 1H), 7.39 (dd, *J* = 1.8, 0.9 Hz, 1H), 7.22 (s, 1H), 7.18 (dd, *J* = 5.1, 1.9 Hz, 3H), 7.11 (dd, *J* = 3.5, 0.8 Hz, 1H), 7.06–6.99 (m, 2H), 3.87 (d, *J* = 13.6 Hz, 1H), 3.82 (s, 3H), 3.18 (d, *J* = 13.6 Hz, 1H), 2.91–2.80 (m, 1H), 2.67–2.45 (m, 2H), 2.20–2.11 (m, 1H), 1.88–1.76 (m, 1H), 1.70–1.57 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.35, 171.12, 157.76, 148.27, 148.11, 144.29, 138.43, 136.47, 136.19, 134.58, 129.76, 128.39, 128.05, 127.53, 127.05, 121.74, 121.56, 116.55, 114.29, 112.10, 66.32, 53.03, 41.18, 37.72, 35.12, 20.63. **HRMS** (ESI-TOF) calcd for $C_{28}H_{28}N_3O_5$ $[M+H]^+$: 486.2023, Found: 486.2021.



3i

methyl (*S*)-2-benzyl-2-(4-nitrobenzamido)-6-oxo-6-(quinolin-8-ylamino)hexanoate (3i):

The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2i** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as yellow solid (11 mg, 40% yield, *er* 90:10). **SFC** (chiral column) Compound **3i** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [35% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.79 (s, 1H), 8.79 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.74 (dd, *J* = 7.2, 1.8 Hz, 1H), 8.29–8.22 (m, 2H), 8.19 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.89–7.81 (m, 2H), 7.58–7.51 (m, 2H), 7.48 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.24–7.18 (m, 4H), 7.05–7.00 (m, 2H), 3.91 (s, 3H), 3.89 (d, *J* = 13.7 Hz, 1H), 3.30 (d, *J* = 13.6 Hz, 1H), 2.95–2.83 (m, 1H), 2.71–2.56 (m, 2H), 2.26–2.16 (m, 1H), 1.90–1.78 (m, 1H), 1.74–1.63 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.48, 170.84, 164.71, 149.58, 148.13, 140.50, 138.23, 136.41, 135.93, 134.31, 129.50, 128.36, 128.09, 127.93, 127.39, 127.14, 123.81, 121.65, 121.55, 116.43, 66.59, 53.15, 40.63, 37.29, 34.65, 20.36. **HRMS** (ESI-TOF) calcd for $C_{30}H_{29}N_4O_6$ $[M+H]^+$: 541.2082, Found: 541.2099.

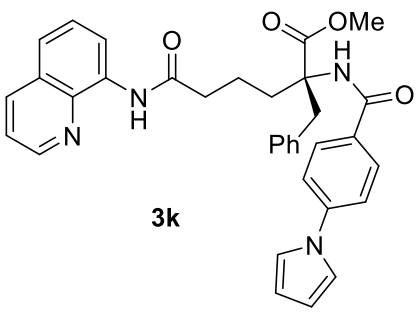


3j

methyl (*S*)-2-benzyl-2-(4-bromobenzamido)-6-oxo-6-(quinolin-8-ylamino)hexanoate (3j):

The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2j** according to the general α-alkylation procedure. Purification using preparative TLC

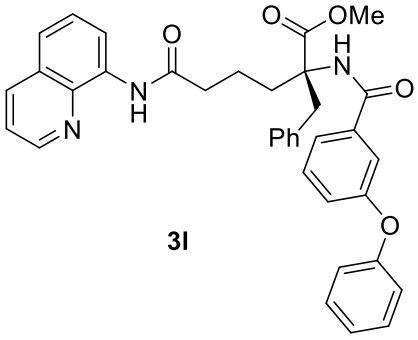
(ethyl acetate/hexanes = 2/5, v/v) gave the product as pale yellow foamy solid (12 mg, 43% yield, *er* 93:7). **SFC** (chiral column) Compound **3j** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [35% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.79–8.69 (m, 2H), 8.15 (dt, *J* = 8.2, 2.3 Hz, 1H), 7.59–7.55 (m, 2H), 7.54–7.48 (m, 4H), 7.45 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.19–7.15 (m, 3H), 7.05 (s, 1H), 7.02–6.97 (m, 2H), 3.92–3.86 (m, 1H), 3.85 (s, 3H), 3.21 (d, *J* = 13.6 Hz, 1H), 2.89 (ddd, *J* = 13.8, 12.1, 4.6 Hz, 1H), 2.65–2.50 (m, 2H), 2.21–2.11 (m, 1H), 1.86–1.75 (m, 1H), 1.70–1.59 (m, 2H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.78, 171.07, 165.92, 148.27, 138.41, 136.50, 136.25, 134.53, 133.98, 131.94, 129.71, 128.68, 128.42, 128.06, 127.52, 127.14, 126.35, 121.76, 121.61, 116.55, 66.55, 53.15, 40.79, 37.60, 34.87, 20.62. **HRMS** (ESI-TOF) calcd for $C_{30}H_{29}N_3O_4$ $[M+H]^+$: 574.1336, Found: 574.1322.



3k

methyl (*S*)-2-(4-(1H-pyrrol-1-yl)benzamido)-2-benzyl-6-oxo-6-(quinolin-8-ylamino)hexanoate (3k):

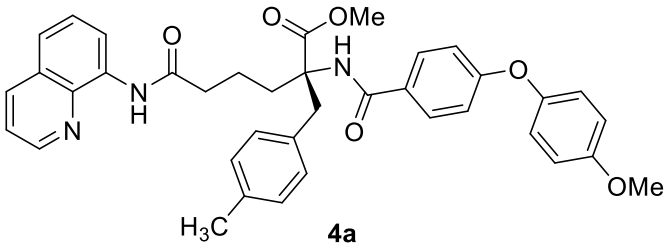
The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2k** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as pale yellow oil (21 mg, 72% yield, *er* 91:9). **SFC** (chiral column) Compound **3k** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.83–8.67 (m, 2H), 8.14 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.82–7.74 (m, 2H), 7.55–7.47 (m, 2H), 7.43 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.42–7.38 (m, 2H), 7.18 (dd, *J* = 5.0, 1.9 Hz, 3H), 7.12 (t, *J* = 2.2 Hz, 2H), 7.08 (s, 1H), 7.05–7.01 (m, 2H), 6.37 (t, *J* = 2.2 Hz, 2H), 3.92 (d, *J* = 13.5 Hz, 1H), 3.86 (s, 3H), 3.22 (d, *J* = 13.6 Hz, 1H), 2.97–2.87 (m, 1H), 2.69–2.51 (m, 2H), 2.23–2.12 (m, 1H), 1.88–1.78 (m, 1H), 1.71–1.61 (m, 2H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.86, 171.12, 165.97, 148.26, 143.14, 138.41, 136.49, 136.35, 134.55, 131.94, 129.77, 128.69, 128.40, 128.05, 127.52, 127.10, 121.75, 121.59, 119.88, 119.22, 116.55, 111.37, 66.53, 53.12, 40.87, 37.65, 34.94, 20.66. **HRMS** (ESI-TOF) calcd for $C_{34}H_{33}N_4O_4$ $[M+H]^+$: 561.2496, Found: 561.2491.



3l

methyl (*S*)-2-benzyl-6-oxo-2-(3-phenoxybenzamido)-6-(quinolin-8-ylamino)hexanoate (3l):

The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2l** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as a colorless oil. (15 mg, 55% yield, *er* 93:7). HPLC: Chiralcel AD-H (Hexane : Isopropanol 90 : 10, 1.0 mL/min), $t_{\text{r-major}}$ 49.94 min, $t_{\text{r-minor}}$ 31.8 min. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.80–8.71 (m, 2H), 8.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.55–7.48 (m, 2H), 7.46–7.41 (m, 2H), 7.38–7.31 (m, 4H), 7.19–7.15 (m, 3H), 7.14–7.09 (m, 2H), 7.05–6.98 (m, 5H), 3.88 (d, *J* = 13.6 Hz, 1H), 3.83 (s, 3H), 3.20 (d, *J* = 13.6 Hz, 1H), 2.88 (ddd, *J* = 13.6, 12.2, 4.5 Hz, 1H), 2.66–2.50 (m, 2H), 2.15 (ddd, *J* = 13.7, 11.9, 4.7 Hz, 1H), 1.87–1.76 (m, 1H), 1.68–1.60 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.71, 171.11, 166.38, 157.93, 156.75, 148.30, 138.44, 137.20, 136.48, 136.29, 134.57, 130.07, 130.04, 129.76, 128.39, 128.06, 127.53, 127.10, 123.89, 121.75, 121.73, 121.58, 121.35, 119.36, 117.57, 116.56, 66.52, 53.09, 40.81, 37.66, 34.91, 20.63. **HRMS** (ESI-TOF) calcd for $C_{36}H_{34}N_3O_5$ $[M+H]^+$: 588.2493, Found: 588.2487.

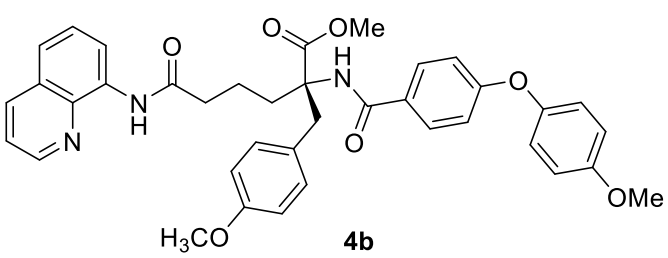


4a

methyl (*S*)-2-(4-(4-methoxyphenoxy)benzamido)-2-(4-methylbenzyl)-6-oxo-6-(quinolin-8-ylamino)hexanoate (4a):

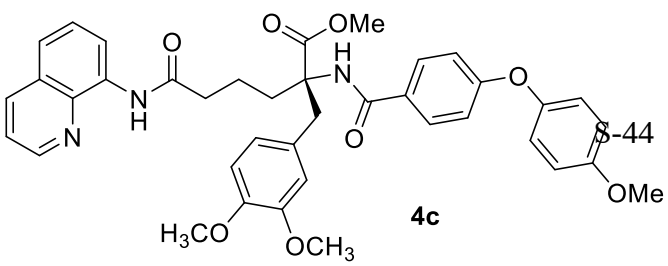
The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2ga** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as foamy white solid (20 mg, 63% yield, *er* 94:6). Larger scale reaction results: 0.30 mmol scale: 69% yield, *er* 95:5. **SFC** (chiral column) Compound **4a** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H),

8.82–8.65 (m, 2H), 8.15 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.73–7.64 (m, 2H), 7.56–7.47 (m, 2H), 7.44 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.06–6.96 (m, 5H), 6.96–6.87 (m, 6H), 3.87 (d, *J* = 13.6 Hz, 1H), 3.83 (s, 3H), 3.82 (s, 3H), 3.14 (d, *J* = 13.6 Hz, 1H), 2.95–2.85 (m, 1H), 2.66–2.51 (m, 2H), 2.25 (s, 3H), 2.19–2.09 (m, 1H), 1.86–1.74 (m, 1H), 1.68–1.57 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.36, 170.57, 165.67, 161.05, 155.99, 148.55, 147.67, 137.83, 135.93, 135.86, 133.99, 132.65, 129.05, 128.48, 128.45, 128.33, 127.45, 126.92, 121.14, 120.95, 116.32, 115.93, 114.56, 65.90, 55.20, 52.40, 39.87, 37.13, 34.30, 20.59, 20.10. **HRMS** (ESI-TOF) calcd for $C_{38}H_{38}N_3O_6$ $[M+H]^+$: 632.2755, Found: 632.2742.



4b

methyl (*S*)-2-(4-methoxybenzyl)-2-(4-(4-methoxyphenoxy)benzamido)-6-oxo-6-(quinolin-8-ylamino)hexanoate (4b): The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2gb** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as foamy white solid (27 mg, 80% yield, *er* 94:6). Larger scale reaction results: 0.32 mmol scale: 91% yield, *er* 94:6; 1.00 mmol scale: 67% yield, *er* 95:5. **SFC** (chiral column) Compound **4a** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.80–8.68 (m, 2H), 8.15 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.73–7.60 (m, 2H), 7.55–7.47 (m, 2H), 7.44 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.05–6.97 (m, 3H), 6.96–6.87 (m, 6H), 6.74–6.68 (m, 2H), 3.85 (d, *J* = 13.8 Hz, 1H), 3.83 (s, 3H), 3.81 (s, 3H), 3.72 (s, 3H), 3.13 (d, *J* = 13.7 Hz, 1H), 2.94–2.81 (m, 1H), 2.65–2.50 (m, 2H), 2.18–2.08 (m, 1H), 1.87–1.74 (m, 1H), 1.69–1.57 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.96, 171.16, 166.23, 161.66, 158.60, 156.58, 149.11, 148.25, 138.40, 136.45, 134.56, 130.75, 128.97, 128.92, 128.40, 128.03, 127.49, 121.72, 121.54, 121.54, 116.90, 116.52, 115.14, 113.76, 66.55, 55.78, 55.24, 53.00, 40.00, 37.69, 34.82, 20.68. **HRMS** (ESI-TOF) calcd for $C_{38}H_{38}N_3O_7$ $[M+H]^+$: 648.2704, Found: 648.2728.

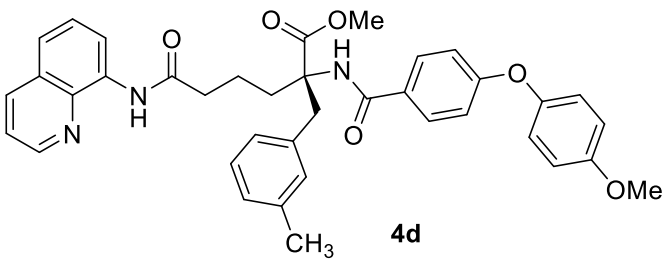


4c

methyl (*S*)-2-(3,4-dimethoxybenzyl)-2-(4-(4-methoxyphenoxy)benzamido)-6-

oxo-6-(quinolin-8-ylamino)hexanoate (4c):

The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2gc** according to the general α-alkylation procedure. Purification using column chromatography with gradient solvent system (ethyl acetate/hexane mixture, 20% to 60%) as eluent gave the product as a foamy white solid (29 mg, 82% yield, *er* 91:9). **SFC** (chiral column) Compound **4c** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.81–8.70 (m, 2H), 8.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.73–7.65 (m, 2H), 7.55–7.47 (m, 2H), 7.44 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.03 (s, 1H), 7.00–6.96 (m, 2H), 6.93–6.88 (m, 4H), 6.70–6.65 (m, 1H), 6.54 (d, *J* = 7.2 Hz, 2H), 3.84 (s, 3H), 3.83 (d, *J* = 3.7 Hz, 1H), 3.81 (s, 3H), 3.79 (s, 3H), 3.56 (s, 3H), 3.14 (d, *J* = 13.6 Hz, 1H), 2.92–2.82 (m, 1H), 2.67–2.49 (m, 2H), 2.18–2.10 (m, 1H), 1.89–1.76 (m, 1H), 1.65–1.58 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.94, 171.14, 166.13, 161.76, 156.60, 149.08, 148.56, 148.26, 147.95, 138.40, 136.46, 134.55, 128.92, 128.90, 128.77, 128.04, 127.50, 121.73, 121.56, 121.51, 116.94, 116.52, 115.19, 115.16, 113.06, 110.95, 66.64, 55.86, 55.79, 55.52, 53.03, 40.32, 37.67, 34.93, 20.67. **HRMS** (ESI-TOF) calcd for $C_{39}H_{40}N_3O_8$ $[M+H]^+$: 678.2810, Found: 678.2802.

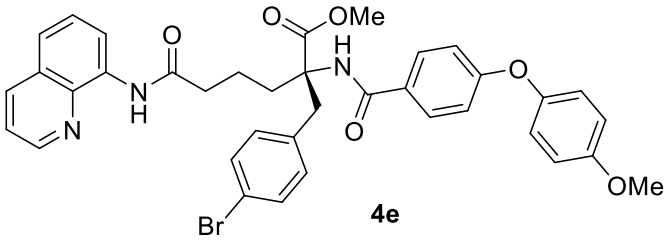


4d

methyl (*S*)-2-(4-(4-methoxyphenoxy)benzamido)-2-(3-methylbenzyl)-6-oxo-6-(quinolin-8-ylamino)hexanoate (4d):

The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2gd** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as colorless oil (21 mg, 65% yield, *er* 92:8). **SFC** (chiral column) Compound **4d** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.80–8.70 (m, 2H), 8.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.70–7.62 (m, 2H), 7.55–7.48 (m, 2H), 7.44 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.06 (t, *J* = 7.5 Hz, 1H), 7.02–6.94 (m, 4H), 6.93–6.88 (m, 4H), 6.85–6.78 (m, 2H), 3.86 (d, *J* = 13.6 Hz, 1H),

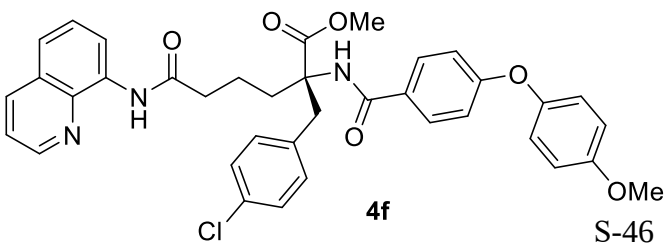
3.83 (s, 3H), 3.82 (s, 3H), 3.15 (d, *J* = 13.4 Hz, 1H), 2.95–2.81 (m, 1H), 2.67–2.49 (m, 2H), 2.18 (s, 3H), 2.17–2.09 (m, 1H), 1.88–1.75 (m, 1H), 1.68–1.58 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.90, 171.18, 166.45, 161.61, 156.57, 149.17, 148.26, 138.42, 137.81, 136.47, 136.28, 134.58, 130.74, 129.17, 128.90, 128.21, 128.05, 127.75, 127.52, 126.72, 121.74, 121.55, 121.51, 116.93, 116.54, 115.15, 66.48, 55.80, 52.97, 40.78, 37.73, 34.97, 21.42, 20.70. **HRMS** (ESI-TOF) calcd for $C_{38}H_{38}N_3O_6$ $[M+H]^+$: 632.2755, Found: 632.2749.



4e

methyl (*S*)-2-(4-bromobenzyl)-2-(4-(4-methoxyphenoxy)benzamido)-6-oxo-6-(quinolin-8-ylamino)hexanoate (4e):

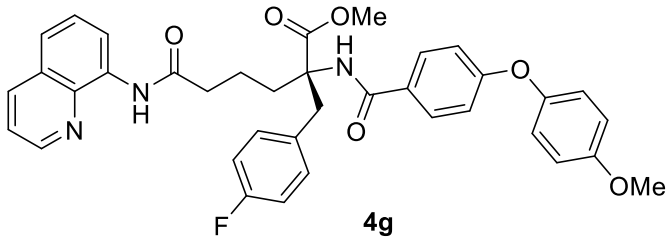
The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2ge** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as pale yellow oil (23 mg, 63% yield, *er* 92:8). Larger scale reaction results: 0.17 mmol scale: 59% yield, *er* 92:8. **SFC** (chiral column) Compound **4e** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.80–8.67 (m, 2H), 8.15 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.70–7.64 (m, 2H), 7.56–7.47 (m, 2H), 7.45 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.31–7.28 (m, 2H), 7.05–6.95 (m, 3H), 6.95–6.86 (m, 6H), 3.89 (d, *J* = 13.6 Hz, 1H), 3.83 (s, 3H), 3.82 (s, 3H), 3.15 (d, *J* = 13.6 Hz, 1H), 2.90–2.82 (m, 1H), 2.66–2.47 (m, 2H), 2.17–2.07 (m, 1H), 1.86–1.72 (m, 1H), 1.68–1.56 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.67, 171.06, 166.30, 161.85, 156.65, 149.05, 148.28, 138.41, 136.50, 135.46, 134.53, 131.50, 131.48, 128.91, 128.64, 128.06, 127.53, 121.76, 121.61, 121.11, 116.95, 116.55, 115.19, 66.20, 55.81, 53.16, 40.16, 37.56, 34.98, 20.56. **HRMS** (ESI-TOF) calcd for $C_{37}H_{35}BrN_3O_6$ $[M+H]^+$: 696.1704, Found: 696.1702.



4f

methyl (*S*)-2-(4-chlorobenzyl)-2-(4-(4-methoxyphenoxy)benzamido)-6-oxo-6-(quinolin-8-ylamino)hexanoate (4f):

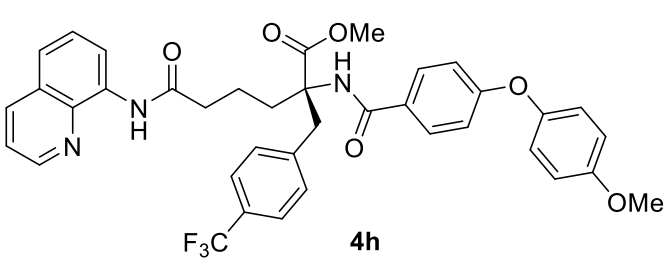
The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2gf** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as foamy solid (28 mg, 79% yield, *er* 89:11). **SFC** (chiral column) Compound **4f** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.81–8.68 (m, 2H), 8.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.71–7.63 (m, 2H), 7.56–7.48 (m, 2H), 7.45 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.17–7.09 (m, 2H), 7.05–6.98 (m, 3H), 6.97–6.86 (m, 6H), 3.90 (d, *J* = 13.6 Hz, 1H), 3.83 (s, 3H), 3.82 (s, 3H), 3.17 (d, *J* = 13.6 Hz, 1H), 2.91–2.80 (m, 1H), 2.65–2.48 (m, 2H), 2.17–2.08 (m, 1H), 1.85–1.73 (m, 1H), 1.68–1.54 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.69, 171.06, 166.28, 161.84, 156.64, 149.05, 148.28, 138.41, 136.49, 134.95, 134.54, 132.94, 131.11, 128.90, 128.67, 128.53, 128.06, 127.52, 121.76, 121.61, 121.60, 116.94, 116.54, 115.18, 66.27, 55.80, 53.15, 40.11, 37.57, 34.97, 20.56. **HRMS** (ESI-TOF) calcd for $C_{37}H_{35}ClN_3O_6$ $[M+H]^+$: 652.2209, Found: 652.2199.



4g

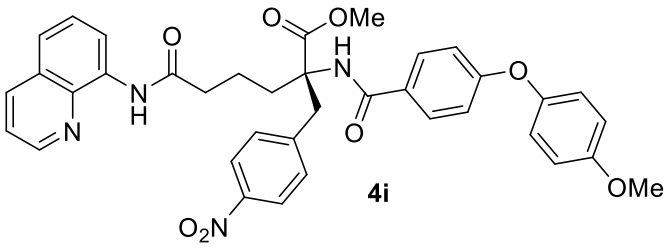
methyl (*S*)-2-(4-fluorobenzyl)-2-(4-(4-methoxyphenoxy)benzamido)-6-oxo-6-(quinolin-8-ylamino)hexanoate (4g): The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2gg** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as oil (25 mg, 75% yield, *er* 90:10). **SFC** (chiral column) Compound **4g** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.83–8.66 (m, 2H), 8.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.73–7.62 (m, 2H), 7.55–7.47 (m, 2H), 7.44 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.03–6.95 (m, 5H), 6.94–6.89 (m, 4H), 6.86 (t, *J* = 8.7 Hz, 2H), 3.90 (d, *J* = 13.7 Hz, 1H), 3.84 (s, 3H), 3.82 (s, 3H), 3.17 (d, *J* = 13.7 Hz, 1H), 2.94–2.81 (m, 1H), 2.68–2.48 (m, 2H), 2.18–2.08 (m, 1H), 1.88–1.74 (m, 1H), 1.71–1.54 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.79, 171.08, 166.26, 162.02 (d, *J* = 245.2 Hz), 161.80, 156.63, 149.05, 148.27, 138.41, 136.48, 134.54, 132.16 (d, *J* = 3.3 Hz), 131.23 (d, *J* = 7.9 Hz), 128.89, 128.74,

128.05, 127.51, 121.75, 121.60, 116.92, 116.53, 115.21 (d, J = 21.1 Hz), 115.17, 115.16, 66.38, 55.79, 53.11, 39.97, 37.59, 34.91, 20.59. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –116.14. **HRMS** (ESI-TOF) calcd for $C_{37}H_{35}FN_3O_6$ $[M+H]^+$: 636.2504, Found: 636.2499.



4h

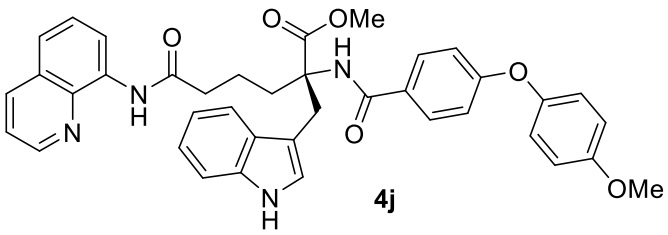
methyl (*S*)-2-(4-(4-methoxyphenoxy)benzamido)-6-oxo-6-(quinolin-8-ylamino)-2-(4-(trifluoromethyl)benzyl)hexanoate (4h): The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2gh** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as yellow oil (14 mg, 40% yield, *er* 89:11). **SFC** (chiral column) Compound **4h** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.82–8.69 (m, 2H), 8.16 (dd, J = 8.3, 1.7 Hz, 1H), 7.73–7.63 (m, 2H), 7.54–7.47 (m, 2H), 7.47–7.40 (m, 3H), 7.14 (d, J = 8.0 Hz, 2H), 7.03 (s, 1H), 7.02–6.98 (m, 2H), 6.95–6.87 (m, 4H), 4.00 (d, J = 13.5 Hz, 1H), 3.85 (s, 3H), 3.82 (s, 3H), 3.27 (d, J = 13.5 Hz, 1H), 2.94–2.81 (m, 1H), 2.69–2.47 (m, 2H), 2.20–2.09 (m, 1H), 1.87–1.73 (m, 1H), 1.68–1.57 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.96, 170.42, 165.75, 161.32, 156.06, 148.40, 147.68, 140.03, 140.02, 137.80, 135.91, 133.91, 129.53, 128.70 (q, J = 32.4 Hz), 128.31, 127.90, 127.46, 126.92, 124.67 (q, J = 3.7 Hz), 123.68 (q, J = 272.0 Hz), 122.78, 121.17, 121.03, 121.02, 116.34, 115.95, 114.58, 65.52, 55.20, 52.62, 39.90, 36.89, 34.46, 19.90. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –62.70. **HRMS** (ESI-TOF) calcd for $C_{38}H_{35}F_3N_3O_6$ $[M+H]^+$: 686.2472, Found: 686.2477.



4i

methyl (*S*)-2-(4-(4-methoxyphenoxy)benzamido)-2-(4-nitrobenzyl)-6-oxo-6-(quinolin-8-ylamino)hexanoate (4i): The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2gi** according to the general α-alkylation procedure.

Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as a foamy yellow solid (20 mg, 59% yield, *er* 83:17). **SFC** (chiral column) Compound **4i** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.77 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.71 (dd, *J* = 6.8, 2.2 Hz, 1H), 8.16 (dd, *J* = 8.2, 1.7 Hz, 1H), 8.06–7.99 (m, 2H), 7.73–7.64 (m, 2H), 7.54–7.48 (m, 2H), 7.45 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.22–7.15 (m, 2H), 7.08 (s, 1H), 7.04–6.98 (m, 2H), 6.97–6.87 (m, 4H), 4.05 (d, *J* = 13.4 Hz, 1H), 3.86 (s, 3H), 3.82 (s, 3H), 3.40–3.30 (m, 1H), 2.89–2.75 (m, 1H), 2.67–2.47 (m, 2H), 2.19–2.09 (m, 1H), 1.87–1.73 (m, 1H), 1.69–1.56 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.37, 170.96, 166.38, 162.07, 156.71, 148.92, 148.30, 147.15, 144.33, 138.38, 136.53, 134.45, 130.68, 128.90, 128.18, 128.07, 127.50, 123.53, 121.79, 121.70, 121.68, 116.94, 116.54, 115.21, 65.90, 55.80, 53.35, 40.48, 37.33, 35.13, 20.35. **HRMS** (ESI-TOF) calcd for $C_{37}H_{35}N_4O_8$ $[M+H]^+$: 663.2449, Found: 663.2440.

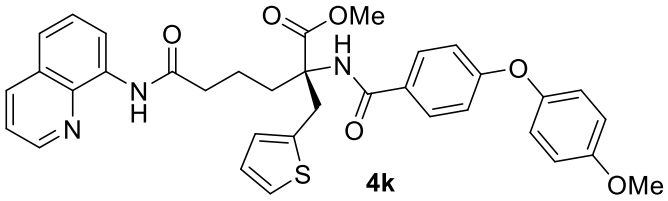


4j

methyl (*S*)-2-((1H-indol-3-yl)methyl)-2-(4-(4-methoxyphenoxy)benzamido)-6-oxo-6-(quinolin-8-ylamino)hexanoatee (4j):

The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2gj** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as a foamy orange solid (22 mg, 65% yield, *er* 90:10). **SFC** (chiral column) Compound **4j** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.81–8.69 (m, 2H), 8.14 (dd, *J* = 8.3, 1.7 Hz, 1H), 8.05 (d, *J* = 2.3 Hz, 1H), 7.70–7.63 (m, 2H), 7.55–7.47 (m, 3H), 7.44 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.29–7.23 (m, 1H), 7.14–7.05 (m, 2H), 7.01–6.96 (m, 3H), 6.92–6.85 (m, 5H), 4.05 (d, *J* = 14.6 Hz, 1H), 3.81 (s, 3H), 3.71 (s, 3H), 3.41 (d, *J* = 14.6 Hz, 1H), 2.98–2.87 (m, 1H), 2.66–2.49 (m, 2H), 2.29–2.17 (m, 1H), 1.91–1.79 (m, 1H), 1.74–1.59 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 174.32, 171.28, 166.26, 161.59, 156.56, 149.14, 148.27, 138.42, 136.47, 135.81, 134.58, 129.07, 128.98, 128.05, 127.95, 127.51, 123.56, 121.96, 121.74, 121.56,

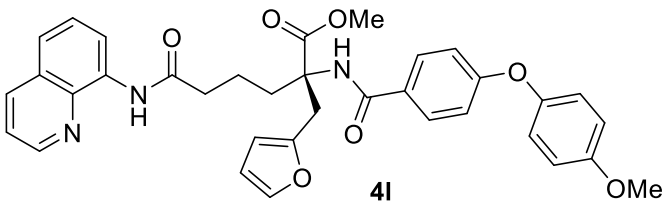
121.50, 119.54, 118.97, 116.90, 116.54, 115.15, 111.14, 110.43, 66.24, 55.79, 53.06, 37.76, 34.77, 31.10, 20.84. **HRMS** (ESI-TOF) calcd for $C_{35}H_{37}N_4O_6$ $[M+H]^+$: 657.2708, Found: 657.2710.



4k

methyl (*S*)-2-(4-(4-methoxyphenoxy)benzamido)-6-oxo-6-(quinolin-8-ylamino)-2-(thiophen-2-ylmethyl)hexanoate (4k):

The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2gk** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as an oil (18 mg, 58% yield, *er* 94:6). **SFC** (chiral column) Compound **4k** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.83–8.67 (m, 2H), 8.15 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.77–7.68 (m, 2H), 7.56–7.48 (m, 2H), 7.44 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.14 (s, 1H), 7.08 (dd, *J* = 5.1, 1.2 Hz, 1H), 7.02–6.99 (m, 2H), 6.95–6.89 (m, 4H), 6.84 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.71 (dd, *J* = 3.5, 1.1 Hz, 1H), 4.19 (d, *J* = 14.7 Hz, 1H), 3.84 (s, 3H), 3.82 (s, 3H), 3.44 (d, *J* = 14.7 Hz, 1H), 2.89–2.77 (m, 1H), 2.67–2.46 (m, 2H), 2.15–2.05 (m, 1H), 1.89–1.77 (m, 1H), 1.71–1.60 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.62, 171.08, 166.22, 161.73, 156.60, 149.11, 148.27, 138.41, 137.83, 136.48, 134.54, 129.72, 129.01, 128.87, 128.05, 127.51, 127.10, 126.78, 124.72, 121.75, 121.58, 116.90, 116.55, 115.16, 66.22, 55.80, 53.22, 37.58, 35.19, 34.75, 20.65. **HRMS** (ESI-TOF) calcd for $C_{35}H_{34}N_3O_6S$ $[M+H]^+$: 624.2163, Found: 624.2154.

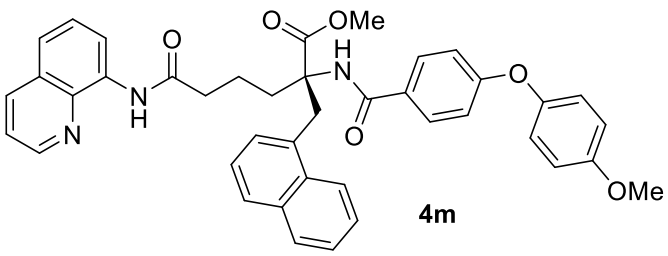


4l

methyl (*S*)-2-(furan-2-ylmethyl)-2-(4-(4-methoxyphenoxy)benzamido)-6-oxo-6-(quinolin-8-ylamino)hexanoate (4l):

The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2gl** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as an oil (19 mg, 61% yield, *er* 86:14). **SFC** (chiral

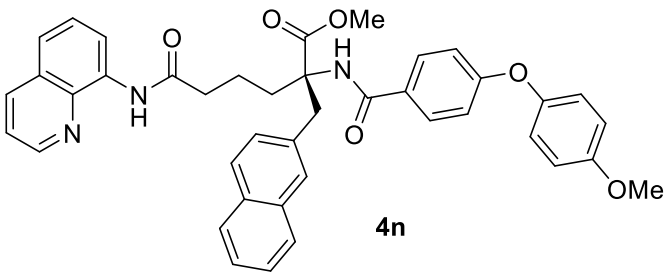
column) Compound **4l** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.81–8.69 (m, 2H), 8.15 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.72–7.62 (m, 2H), 7.54–7.47 (m, 2H), 7.45 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.21 (dd, *J* = 1.8, 0.8 Hz, 1H), 7.10 (s, 1H), 7.02–6.96 (m, 2H), 6.94–6.87 (m, 4H), 6.18 (dd, *J* = 3.2, 1.9 Hz, 1H), 5.99 (d, *J* = 3.1 Hz, 1H), 3.96 (d, *J* = 14.9 Hz, 1H), 3.86 (s, 3H), 3.82 (s, 3H), 3.30 (d, *J* = 14.9 Hz, 1H), 2.79–2.68 (m, 1H), 2.65–2.49 (m, 2H), 2.14–2.06 (m, 1H), 1.87–1.76 (m, 1H), 1.71–1.59 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.88, 171.14, 166.29, 161.65, 156.59, 151.09, 149.14, 148.28, 141.93, 138.42, 136.48, 134.55, 128.96, 128.89, 128.05, 127.52, 121.75, 121.58, 121.55, 116.87, 116.55, 115.15, 110.35, 108.38, 64.65, 55.80, 53.28, 37.61, 34.70, 33.93, 20.49. **HRMS** (ESI-TOF) calcd for $C_{35}H_{34}N_3O_7$ $[M+H]^+$: 608.2391, Found: 608.2384.



4m

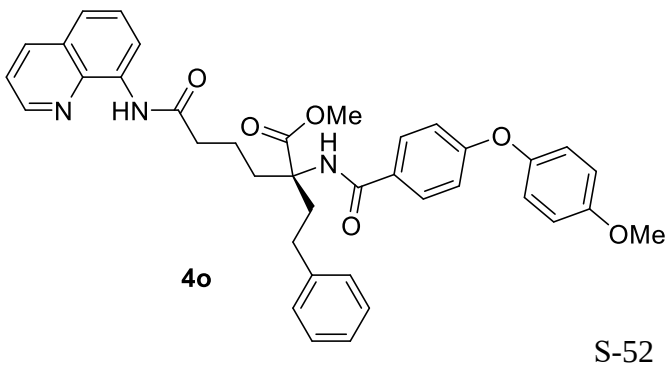
Methyl (*S*)-2-(4-(4-methoxyphenoxy)benzamido)-2-(naphthalen-1-ylmethyl)-6-oxo-6-(quinolin-8-ylamino)hexanoate (4m): The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2gm** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as a foamy yellow solid (22 mg, 65% yield, *er* 85:15). **SFC** (chiral column) Compound **4m** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.78 (s, 1H), 8.81–8.70 (m, 2H), 8.15 (dd, *J* = 8.2, 1.7 Hz, 1H), 8.12–8.06 (m, 1H), 7.80–7.74 (m, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.63–7.58 (m, 2H), 7.55–7.47 (m, 2H), 7.44 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.40–7.34 (m, 2H), 7.29 (dd, *J* = 8.1, 7.1 Hz, 1H), 7.24 (dd, *J* = 7.1, 1.3 Hz, 1H), 7.03–6.95 (m, 3H), 6.93–6.84 (m, 4H), 4.27 (d, *J* = 14.3 Hz, 1H), 3.81 (s, 3H), 3.74 (d, *J* = 14.3 Hz, 1H), 3.64 (s, 3H), 3.15–3.04 (m, 1H), 2.69–2.53 (m, 2H), 2.40–2.27 (m, 1H), 1.88–1.76 (m, 1H), 1.70–1.57 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.75, 171.23, 166.69, 161.60, 156.57, 149.14, 148.27, 138.43, 136.47, 134.59, 133.89, 132.81, 132.73, 129.05, 128.94, 128.75, 128.48, 128.05, 127.86, 127.52, 125.88, 125.51,

125.22, 124.06, 121.74, 121.55, 121.51, 116.86, 116.54, 115.14, 66.37, 55.79, 52.95, 37.74, 37.38, 34.85, 20.71. **HRMS** (ESI-TOF) calcd for $C_{41}H_{38}N_3O_6$ $[M+H]^+$: 668.2755, Found: 668.2750.



4n

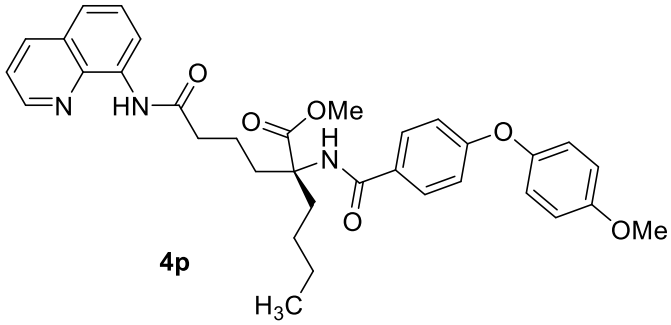
methyl (*S*)-2-(4-(4-methoxyphenoxy)benzamido)-2-(naphthalen-2-ylmethyl)-6-oxo-6-(quinolin-8-ylamino)hexanoate (4n): The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2gn** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as a foamy yellow solid (28 mg, 81% yield, *er* 91:9). **SFC** (chiral column) Compound **4n** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.78 (s, 1H), 8.82–8.68 (m, 2H), 8.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.80–7.72 (m, 1H), 7.71–7.59 (m, 4H), 7.56–7.47 (m, 3H), 7.44 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.42–7.36 (m, 2H), 7.15 (dd, *J* = 8.4, 1.7 Hz, 1H), 7.03–6.97 (m, 3H), 6.90 (d, *J* = 8.2 Hz, 4H), 4.08 (d, *J* = 13.5 Hz, 1H), 3.85 (s, 3H), 3.81 (s, 3H), 3.37 (d, *J* = 13.5 Hz, 1H), 3.01–2.88 (m, 1H), 2.69–2.49 (m, 2H), 2.27–2.13 (m, 1H), 1.90–1.77 (m, 1H), 1.73–1.61 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.80, 171.13, 166.51, 161.65, 156.56, 149.12, 148.25, 138.40, 136.46, 134.55, 133.99, 133.46, 132.50, 129.01, 128.93, 128.69, 128.03, 128.03, 127.86, 127.70, 127.65, 127.50, 126.03, 125.68, 121.72, 121.55, 121.50, 116.95, 116.53, 115.13, 66.53, 55.78, 53.06, 40.90, 37.66, 35.04, 20.65. **HRMS** (ESI-TOF) calcd for $C_{41}H_{38}N_3O_6$ $[M+H]^+$: 668.2755, Found: 668.2756.



4o

methyl (*S*)-2-(4-(4-methoxyphenoxy)benzamido)-6-oxo-2-phenethyl-6-(quinolin-8-ylamino)hexanoate (4o): The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone

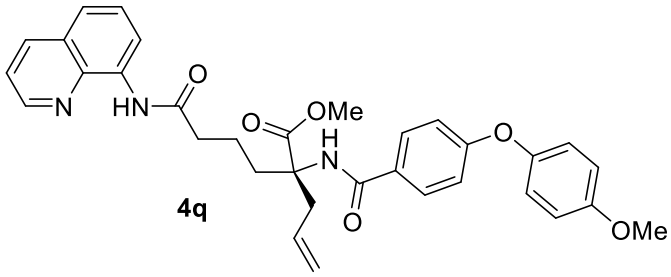
2go according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as an oil (15 mg, 47% yield, *er* 83:17). **SFC** (chiral column) Compound **4o** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.75 (s, 1H), 8.79–8.69 (m, 2H), 8.15 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.83–7.76 (m, 2H), 7.54–7.46 (m, 2H), 7.44 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.31 (s, 1H), 7.24–7.19 (m, 2H), 7.17–7.10 (m, 3H), 7.03–6.99 (m, 2H), 6.98–6.94 (m, 2H), 6.94–6.89 (m, 2H), 3.82 (s, 3H), 3.75 (s, 3H), 3.06–2.96 (m, 1H), 2.80–2.69 (m, 1H), 2.68–2.46 (m, 3H), 2.41–2.32 (m, 1H), 2.26–2.17 (m, 1H), 2.04–1.96 (m, 1H), 1.85–1.73 (m, 1H), 1.65–1.53 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 174.73, 171.18, 165.61, 161.72, 156.59, 149.20, 148.27, 141.08, 138.42, 136.46, 134.56, 128.97, 128.64, 128.55, 128.44, 128.05, 127.51, 126.07, 121.74, 121.56, 121.52, 116.98, 116.51, 115.17, 64.96, 55.81, 53.20, 37.66, 36.88, 35.06, 30.94, 20.47. **HRMS** (ESI-TOF) calcd for $C_{38}H_{38}N_3O_6$ $[M+H]^+$: 632.2755, Found: 632.2750.



4p

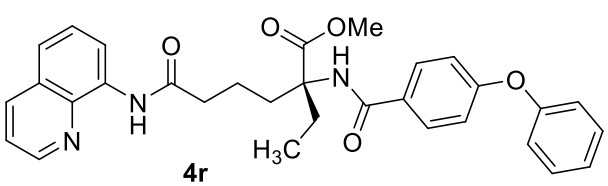
methyl (*S*)-2-butyl-2-(4-(4-methoxyphenoxy)benzamido)-6-oxo-6-(quinolin-8-ylamino)hexanoate (4p): The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2gp** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as an oil (19 mg, 62% yield, *er* 82:18). **SFC** (chiral column) Compound **4p** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.75 (s, 1H), 8.82–8.66 (m, 2H), 8.15 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.83–7.74 (m, 2H), 7.55–7.47 (m, 2H), 7.44 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.25 (s, 1H), 7.02–6.98 (m, 2H), 6.96–6.93 (m, 2H), 6.92–6.89 (m, 2H), 3.83 (s, 3H), 3.82 (s, 3H), 2.79–2.66 (m, 1H), 2.64–2.43 (m, 3H), 2.06–1.93 (m, 1H), 1.90–1.70 (m, 2H), 1.67–1.51 (m, 1H), 1.31–1.18 (m, 3H), 1.04–0.92 (m, 1H), 0.84 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 175.08, 171.27, 165.54, 161.65, 156.58, 149.21, 148.26, 138.42, 136.46, 134.59, 128.94, 128.81,

128.05, 127.51, 121.73, 121.54, 121.51, 116.97, 116.52, 115.16, 65.24, 55.80, 53.17, 37.76, 35.29, 34.91, 26.62, 22.64, 20.58, 14.10. **HRMS** (ESI-TOF) calcd for $C_{34}H_{38}N_3O_6$ $[M+H]^+$: 584.2755, Found: 584.2758.



4q

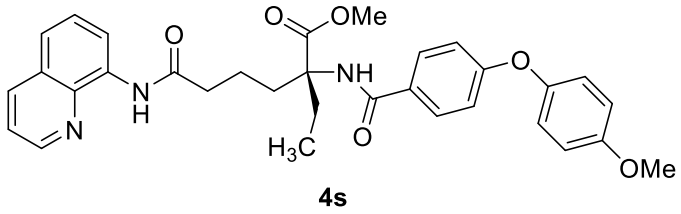
methyl (*S*)-2-allyl-2-(4-(4-methoxyphenoxy)benzamido)-6-oxo-6-(quinolin-8-ylamino)hexanoate (4q): The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2gq** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as an oil (15 mg, 52% yield, *er* 82:18). **SFC** (chiral column) Compound **4q** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.81–8.71 (m, 2H), 8.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.82–7.74 (m, 2H), 7.55–7.47 (m, 2H), 7.44 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.23 (s, 1H), 7.04–6.97 (m, 2H), 6.96–6.88 (m, 4H), 5.63 (ddt, *J* = 17.4, 10.1, 7.4 Hz, 1H), 5.14–4.97 (m, 2H), 3.82 (s, 6H), 3.41–3.29 (m, 1H), 2.75–2.48 (m, 4H), 2.10–1.97 (m, 1H), 1.89–1.75 (m, 1H), 1.70–1.56 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 174.25, 171.22, 165.85, 161.68, 156.58, 149.18, 148.27, 138.41, 136.48, 134.56, 132.48, 128.96, 128.73, 128.05, 127.51, 121.75, 121.58, 121.52, 119.25, 116.94, 116.54, 115.16, 64.89, 55.80, 53.13, 39.66, 37.59, 34.66, 20.42. **HRMS** (ESI-TOF) calcd for $C_{33}H_{34}N_3O_6$ $[M+H]^+$: 568.2442, Found: 568.2436.



4r

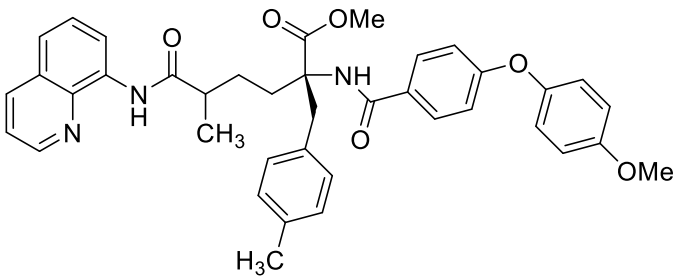
methyl (*S*)-2-ethyl-6-oxo-2-(4-phenoxybenzamido)-6-(quinolin-8-ylamino)hexanoate (4r): The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2gr** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as an oil (13 mg, 48% yield, *er* 83:17). **SFC** (chiral column) Compound **4r** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6×250 mm) under isocratic conditions [35% MeOH / CO_2 (4

mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.80–8.70 (m, 2H), 8.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.85–7.79 (m, 2H), 7.54–7.46 (m, 2H), 7.44 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.40–7.34 (m, 2H), 7.19–7.14 (m, 1H), 7.09–6.97 (m, 5H), 3.83 (s, 3H), 2.79–2.42 (m, 4H), 2.02 (ddd, *J* = 13.7, 11.9, 4.7 Hz, 1H), 1.96–1.87 (m, 1H), 1.85–1.74 (m, 1H), 1.67–1.55 (m, 1H), 0.79 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 174.90, 171.26, 165.58, 160.59, 156.24, 148.26, 138.41, 136.47, 134.57, 130.09, 129.42, 129.01, 128.05, 127.51, 124.28, 121.74, 121.56, 119.82, 118.07, 116.53, 65.86, 53.19, 37.73, 34.70, 28.53, 20.64, 8.67. **HRMS** (ESI-TOF) calcd for $C_{31}H_{32}N_3O_5$ $[M+H]^+$: 526.2336, Found: 526.2339.



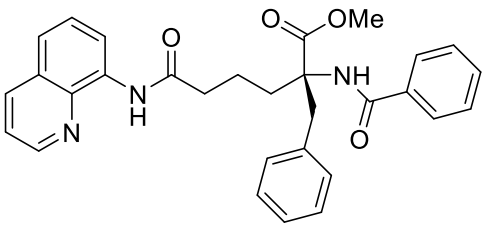
4s

methyl (R)-2-ethyl-2-(4-(4-methoxyphenoxy)benzamido)-6-oxo-6-(quinolin-8-ylamino)hexanoate (4s): The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **2gs** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as a colorless oil (10.8 mg, 39% yield, *er* 82:18). **SFC** (chiral column) Compound **4s** was analyzed by chiral SFC on a Daicel IB column (3 mm, 4.6x250 mm) under isocratic conditions [35% (MeOH containing 0.5% formic acid)/ CO2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (257 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.80–8.75 (m, 1H), 8.75–8.71 (m, 1H), 8.16 (d, *J* = 8.2 Hz, 1H), 7.78 (d, *J* = 8.5 Hz, 2H), 7.58–7.47 (m, 2H), 7.45 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.24 (s, 1H), 7.03–6.97 (m, 2H), 6.94 (d, *J* = 8.4 Hz, 2H), 6.91 (d, *J* = 9.0 Hz, 2H), 3.83 (s, 3H), 3.82 (s, 3H), 2.72 (td, *J* = 13.0, 4.4 Hz, 1H), 2.67–2.46 (m, 3H), 2.05–1.97 (m, 1H), 1.90 (dt, *J* = 14.5, 7.3 Hz, 1H), 1.82–1.76 (m, 1H), 1.63–1.52 (m, 1H), 0.78 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 174.78, 171.19, 165.52, 161.53, 156.44, 149.05, 148.06, 128.80, 128.59, 127.94, 127.43, 121.58, 121.46, 121.38, 116.82, 115.03, 65.70, 55.66, 53.04, 37.58, 34.56, 28.39, 20.49, 8.52. **HRMS** (ESI-TOF) calcd for $C_{32}H_{34}N_3O_6$ $[M+H]^+$: 556.2442, Found: 556.2443.



4t

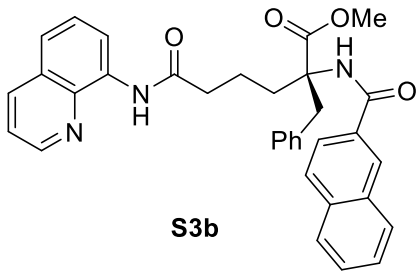
methyl (2*S*)-2-(4-(4-methoxyphenoxy)benzamido)-5-methyl-2-(4-methylbenzyl)-6-oxo-6-(quinolin-8-ylamino)hexanoate (4t): The title compound was prepared on 0.05 mmol scale from alkene **1b** and azlactone **2ga** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as an inseparable 1:1.1 mixture of diastereomers, which were isolated together as an oil (10 mg, 32% yield, *dr* 1:1.4, *er* 74:26 (major), 56:44 (minor)). This reaction was also carried out at 70 °C for two days and the isolated yield was 34%. Interestingly, the *dr* of the product was greater than 20:1 with 82:18 *er* for the major diastereomer. The following analytical data corresponds to the mixture. **SFC** (chiral column) Compound **4t** was analyzed by chiral SFC on a Daicel IBN column (3 μm, 4.6×250 mm) under isocratic conditions [35% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.88 (s, 1H), 9.85 (s, 1H), 8.86–8.80 (m, 2H), 8.78–8.73 (m, 2H), 8.22–8.14 (m, 2H), 7.73–7.64 (m, 4H), 7.62–7.42 (m, 6H), 7.06–6.86 (m, 25H), 3.89–3.82 (m, 12H), 3.81 (s, 3H), 3.19 (d, *J* = 13.6 Hz, 1H), 3.09 (d, *J* = 13.6 Hz, 1H), 2.98 (td, *J* = 13.0, 4.7 Hz, 1H), 2.81 (td, *J* = 13.0, 4.3 Hz, 1H), 2.63 (m, 2H), 2.25 (d, *J* = 10.8 Hz, 6H), 2.21–2.07 (m, 2H), 1.90 (m, 1H), 1.68–1.49 (m, 3H), 1.43 m, 1H), 1.34 (dd, *J* = 22.9, 6.9 Hz, 6H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 174.87, 174.83, 174.01, 173.91, 166.24, 166.18, 161.68, 161.57, 156.61, 156.57, 149.13, 149.10, 148.35, 148.24, 138.56, 138.54, 136.49, 136.48, 136.46, 136.43, 134.69, 134.60, 133.28, 133.22, 129.68, 129.59, 129.05, 129.03, 128.93, 128.89, 128.07, 128.02, 127.52, 127.51, 121.84, 121.77, 121.68, 121.58, 121.56, 121.53, 121.52, 116.89, 116.85, 116.61, 116.58, 115.22, 115.17, 115.14, 66.59, 66.19, 55.80, 52.99, 52.89, 43.04, 42.33, 40.35, 40.32, 33.48, 32.74, 29.27, 28.78, 21.16, 21.15, 18.68, 17.37. **HRMS** (ESI-TOF) calcd for $C_{39}H_{40}N_3O_6$ $[M+H]^+$: 646.2912, Found: 646.2903.



S3a

methyl (S)-2-benzamido-2-benzyl-6-oxo-6-(quinolin-8-ylamino)hexanoate (S3a): The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **S2a** according to the

general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as colorless oil (6.9 mg, 28% yield, *er* 89:11). **SFC** (chiral column) Compound **S3a** was analyzed by chiral SFC on a Daicel IA column (3 μm, 4.6x250 mm) under isocratic conditions [30% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.77 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.74 (dd, *J* = 7.4, 1.6 Hz, 1H), 8.15 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.73–7.69 (m, 2H), 7.55–7.46 (m, 3H), 7.44 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.40 (dd, *J* = 8.4, 7.1 Hz, 2H), 7.17 (dd, *J* = 5.0, 1.8 Hz, 3H), 7.07 (s, 1H), 7.03 (dd, *J* = 6.7, 2.9 Hz, 2H), 3.93 (d, *J* = 13.6 Hz, 1H), 3.84 (s, 3H), 3.20 (d, *J* = 13.6 Hz, 1H), 2.93 (ddd, *J* = 13.7, 12.2, 4.6 Hz, 1H), 2.63 (ddd, *J* = 14.6, 8.6, 5.8 Hz, 1H), 2.55 (ddd, *J* = 15.2, 8.6, 7.0 Hz, 1H), 2.17 (ddd, *J* = 13.6, 11.9, 4.7 Hz, 1H), 1.90–1.76 (m, 1H), 1.70–1.59 (m, 1H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 173.69, 171.00, 166.84, 148.13, 138.28, 136.33, 136.23, 135.08, 134.43, 131.50, 129.64, 128.59, 128.24, 127.91, 127.38, 126.92, 126.90, 121.60, 121.42, 116.41, 66.37, 52.93, 40.70, 37.55, 34.79, 20.53. **HRMS** (ESI-TOF) calcd for $C_{30}H_{30}N_3O_4$ $[M+H]^+$: 496.2236, Found: 496.2240.

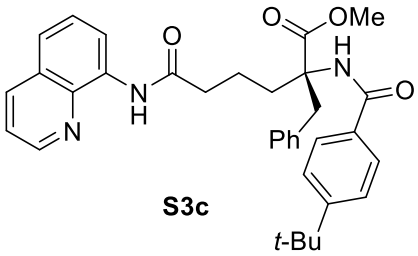


S3b

methyl (*S*)-2-(2-naphthamido)-2-benzyl-6-oxo-6-(quinolin-8-ylamino)hexanoate (S3b):

The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **S2b** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as colorless oil (11 mg, 45% yield, *er* 89:11). **SFC** (chiral column) Compound **S3b** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6x250 mm) under isocratic conditions [35% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.78 (s, 1H), 8.77–8.70 (m, 2H), 8.24–8.15 (m, 1H), 8.13 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.92–7.82 (m, 3H), 7.79 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.59–7.47 (m, 4H), 7.41 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.24 (s, 1H), 7.20–7.12 (m, 3H), 7.10–7.02 (m, 2H), 3.98 (d, *J* = 13.5 Hz, 1H), 3.87 (s, 3H), 3.24 (d, *J* = 13.6 Hz, 1H), 3.03–2.92 (m, 1H), 2.70–2.52 (m, 2H), 2.26–2.15 (m, 1H), 1.94–1.82 (m, 1H), 1.75–1.57 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.34, 170.56, 166.35, 147.65, 137.81, 135.84, 135.80, 134.33, 133.96, 132.16, 131.73, 129.22, 128.55, 128.03, 127.80, 127.43, 127.24, 127.16, 126.93, 126.90, 126.48, 126.22, 123.11, 121.11,

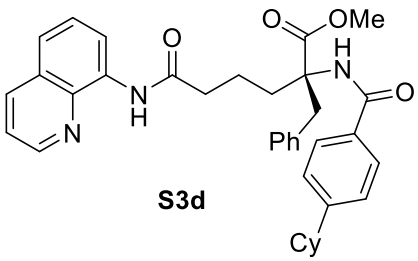
120.96, 115.95, 66.00, 52.51, 40.28, 37.10, 34.38, 20.11. **HRMS** (ESI-TOF) calcd for $C_{34}H_{32}N_3O_4$ $[M+H]^+$: 546.2387, Found: 546.2381.



S3c

methyl (*S*)-2-benzyl-2-(4-(tert-butyl)benzamido)-6-oxo-6-(quinolin-8-ylamino)hexanoate (S3c):

The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **S2c** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as a foamy white solid (19 mg, 73% yield, *er* 86:14). **SFC** (chiral column) Compound **S3c** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6x250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.81–8.70 (m, 2H), 8.15 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.72–7.62 (m, 2H), 7.56–7.47 (m, 2H), 7.46–7.39 (m, 3H), 7.22–7.13 (m, 3H), 7.10–6.98 (m, 3H), 3.94 (d, *J* = 13.6 Hz, 1H), 3.83 (s, 3H), 3.19 (d, *J* = 13.5 Hz, 1H), 2.98–2.88 (m, 1H), 2.66–2.48 (m, 2H), 2.23–2.10 (m, 1H), 1.87–1.74 (m, 1H), 1.67–1.57 (m, 1H), 1.33 (s, 9H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.86, 171.14, 166.88, 155.10, 148.26, 138.42, 136.45, 136.44, 134.58, 132.36, 129.81, 128.36, 128.04, 127.51, 127.00, 126.90, 125.65, 121.71, 121.53, 116.53, 66.43, 53.01, 40.90, 37.71, 35.05, 34.94, 31.30, 20.68. **HRMS** (ESI-TOF) calcd for $C_{34}H_{38}N_3O_4$ $[M+H]^+$: 552.2857, Found: 552.2856.

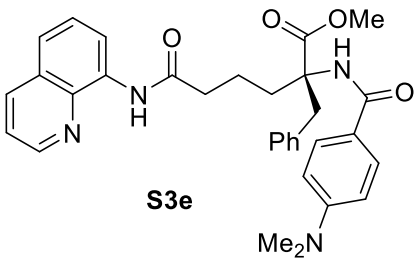


S3d

methyl (*S*)-2-benzyl-2-(4-cyclohexylbenzamido)-6-oxo-6-(quinolin-8-ylamino)hexanoate (S3d):

The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **S2d** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as a foamy white solid (15 mg, 55% yield, *er* 86:14). **SFC** (chiral column) Compound **S3d** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6x250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.81–8.69 (m, 2H), 8.15 (dd, *J* = 8.3, 1.7

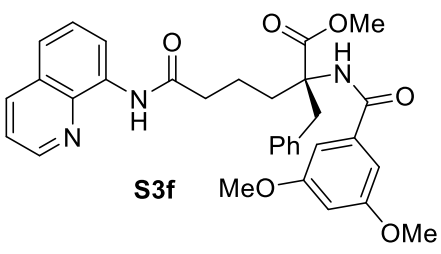
Hz, 1H), 7.68–7.62 (m, 2H), 7.56–7.47 (m, 2H), 7.44 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.25–7.22 (m, 2H), 7.19–7.15 (m, 3H), 7.07–7.00 (m, 3H), 3.93 (d, *J* = 13.6 Hz, 1H), 3.83 (s, 3H), 3.18 (d, *J* = 13.6 Hz, 1H), 2.97–2.88 (m, 1H), 2.68–2.47 (m, 3H), 2.22–2.11 (m, 1H), 1.91–1.71 (m, 6H), 1.70–1.59 (m, 2H), 1.48–1.33 (m, 4H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.28, 170.56, 166.36, 151.44, 147.67, 137.83, 135.85, 133.99, 132.15, 129.22, 127.89, 127.76, 127.44, 126.92, 126.59, 126.54, 126.40, 121.12, 120.94, 115.94, 65.84, 52.42, 44.06, 40.29, 37.12, 34.35, 33.74, 26.31, 25.60, 20.09. **HRMS** (ESI-TOF) calcd for $C_{36}H_{40}N_3O_4$ $[M+H]^+$: 578.3013, Found: 578.3003.



S3e

methyl (*S*)-2-benzyl-2-(4-(dimethylamino)benzamido)-6-oxo-6-(quinolin-8-ylamino)hexanoate (S3e):

The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **S2e** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as an yellow oil (15 mg, 60% yield, *er* 92:8). **SFC** (chiral column) Compound **S3e** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6x250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.81–8.69 (m, 2H), 8.14 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.68–7.59 (m, 2H), 7.55–7.47 (m, 2H), 7.44 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.18–7.14 (m, 3H), 7.06–7.00 (m, 2H), 6.91 (s, 1H), 6.67–6.62 (m, 2H), 3.94 (d, *J* = 13.5 Hz, 1H), 3.81 (s, 3H), 3.15 (d, *J* = 13.5 Hz, 1H), 3.01 (s, 6H), 2.97–2.88 (m, 1H), 2.66–2.48 (m, 2H), 2.19–2.10 (m, 1H), 1.87–1.76 (m, 1H), 1.69–1.61 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.95, 171.15, 166.70, 152.51, 148.12, 138.30, 136.49, 136.28, 134.49, 129.76, 128.43, 128.12, 127.89, 127.36, 126.73, 121.81, 121.56, 121.34, 116.38, 111.08, 66.10, 52.76, 40.83, 40.13, 37.66, 34.96, 20.59. **HRMS** (ESI-TOF) calcd for $C_{32}H_{35}N_4O_4$ $[M+H]^+$: 539.2653, Found: 539.2653.

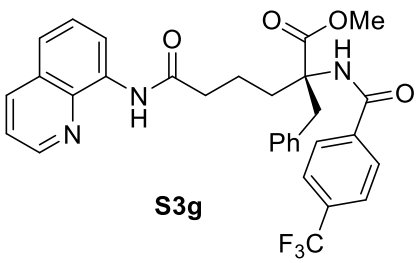


S3f

methyl (*S*)-2-benzyl-2-(3,5-dimethoxybenzamido)-6-oxo-6-(quinolin-8-ylamino)hexanoate (S3f):

The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **S2f** according to the general α-alkylation procedure. Purification using preparative TLC

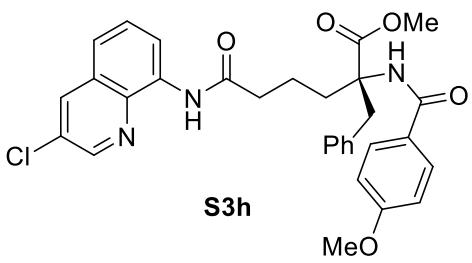
(ethyl acetate/hexanes = 2/5, v/v) gave the product as a white solid (17 mg, 67% yield, *er* 89.5:10.5). **SFC** (chiral column) Compound **S3f** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6x250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.81–8.71 (m, 2H), 8.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.55–7.47 (m, 2H), 7.44 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.21–7.15 (m, 3H), 7.03 (dd, *J* = 7.4, 2.0 Hz, 3H), 6.84 (d, *J* = 2.3 Hz, 2H), 6.56 (t, *J* = 2.3 Hz, 1H), 3.88 (d, *J* = 13.5 Hz, 1H), 3.84 (s, 3H), 3.79 (s, 6H), 3.21 (d, *J* = 13.5 Hz, 1H), 2.92–2.83 (m, 1H), 2.67–2.51 (m, 2H), 2.20–2.11 (m, 1H), 1.87–1.76 (m, 1H), 1.69–1.63 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.57, 170.98, 166.65, 160.87, 148.14, 138.28, 137.27, 136.33, 136.18, 134.42, 129.68, 128.24, 127.91, 127.36, 126.94, 121.59, 121.43, 116.41, 104.74, 103.92, 66.25, 55.54, 52.91, 40.65, 37.51, 34.76, 20.46. **HRMS** (ESI-TOF) calcd for $C_{32}H_{34}N_3O_6$ $[M+H]^+$: 556.2442, Found: 556.2447.



S3g

methyl (*S*)-2-benzyl-6-oxo-6-(quinolin-8-ylamino)-2-(4-(trifluoromethyl)benzamido)hexanoate (S3g):

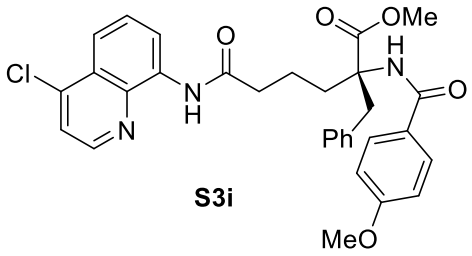
The title compound was prepared on 0.05 mmol scale from alkene **1a** and azlactone **S2g** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as a yellow oil (8 mg, 31% yield, *er* 87.5:12.5). **SFC** (chiral column) Compound **S3g** was analyzed by chiral SFC on a Daicel IC column (3 μm, 4.6x250 mm) under isocratic conditions [30% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.79–8.68 (m, 2H), 8.16 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.85–7.73 (m, 2H), 7.69–7.61 (m, 2H), 7.56–7.48 (m, 2H), 7.45 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.18 (tt, *J* = 3.9, 2.4 Hz, 3H), 7.13 (s, 1H), 7.05–6.96 (m, 2H), 3.89 (d, *J* = 13.7 Hz, 1H), 3.87 (s, 3H), 3.24 (d, *J* = 13.6 Hz, 1H), 2.96–2.84 (m, 1H), 2.68–2.50 (m, 2H), 2.24–2.13 (m, 1H), 1.87–1.74 (m, 1H), 1.71–1.62 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.11, 170.42, 165.00, 147.66, 137.81, 135.91, 135.58, 133.90, 132.75 (q, *J* = 32.7 Hz), 129.08, 127.86, 127.46, 126.92, 126.60, 125.18 (q, *J* = 3.7 Hz), 123.21 (q, *J* = 272.7 Hz), 121.16, 121.03, 115.95, 66.05, 52.61, 40.20, 36.95, 34.24, 19.99. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –63.19. **HRMS** (ESI-TOF) calcd for $C_{31}H_{29}F_3N_3O_4$ $[M+H]^+$: 564.2105, Found: 564.2100.



S3h

methyl (*S*)-2-benzyl-6-((3-chloroquinolin-8-yl)amino)-2-(4-methoxybenzamido)-6-oxohexanoate (S3h):

The title compound was prepared on 0.05 mmol scale from alkene **S1h** and azlactone **2b** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as a foamy solid (14 mg, 62% yield, *er* 91:9). **SFC** (chiral column) Compound **S3h** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6x250 mm) under isocratic conditions [35% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.58 (s, 1H), 8.73 (dd, *J* = 7.8, 1.2 Hz, 1H), 8.64 (d, *J* = 2.3 Hz, 1H), 8.12 (d, *J* = 2.4 Hz, 1H), 7.73–7.64 (m, 2H), 7.55 (t, *J* = 8.0 Hz, 1H), 7.41 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.20–7.11 (m, 3H), 7.01 (dd, *J* = 6.6, 2.9 Hz, 2H), 6.97 (s, 1H), 6.94–6.84 (m, 2H), 3.92 (d, *J* = 13.5 Hz, 1H), 3.84 (d, *J* = 1.5 Hz, 6H), 3.17 (d, *J* = 13.5 Hz, 1H), 2.98–2.87 (m, 1H), 2.66–2.48 (m, 2H), 2.21–2.09 (m, 1H), 1.86–1.75 (m, 1H), 1.67–1.55 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.79, 171.06, 166.29, 162.25, 147.33, 136.27, 136.22, 134.65, 134.28, 129.66, 129.18, 128.85, 128.71, 128.21, 128.19, 127.30, 126.88, 120.53, 116.65, 113.75, 66.28, 55.41, 52.89, 40.80, 37.60, 34.81, 20.54. **HRMS** (ESI-TOF) calcd for $C_{31}H_{31}ClN_3O_5$ $[M+H]^+$: 560.1947, Found: 560.1940.

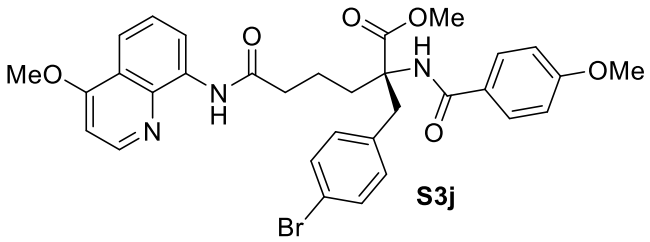


S3i

methyl (*S*)-2-benzyl-6-((4-chloroquinolin-8-yl)amino)-2-(4-methoxybenzamido)-6-oxohexanoate (S3i):

The title compound was prepared on 0.05 mmol scale from alkene **S1i** and azlactone **2b** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as a foamy solid (11 mg, 49% yield, *er* 89:11). **SFC** (chiral column) Compound **S3i** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6x250 mm) under isocratic conditions [35% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.74 (s, 1H), 8.80 (dd, *J* = 7.8, 1.2 Hz, 1H), 8.62 (d, *J* = 4.7 Hz, 1H), 7.88 (dd, *J*

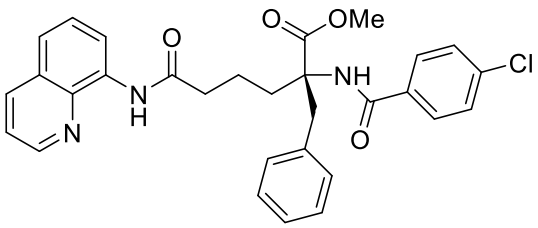
= 8.5, 1.2 Hz, 1H), 7.70–7.66 (m, 2H), 7.65–7.58 (m, 1H), 7.53 (d, *J* = 4.7 Hz, 1H), 7.18–7.13 (m, 3H), 7.04–6.99 (m, 2H), 6.97 (s, 1H), 6.90–6.86 (m, 2H), 3.92 (d, *J* = 13.6 Hz, 1H), 3.84 (s, 6H), 3.17 (d, *J* = 13.6 Hz, 1H), 2.98–2.88 (m, 1H), 2.65–2.49 (m, 2H), 2.20–2.11 (m, 1H), 1.80 (m, *J* = 13.1, 5.2 Hz, 1H), 1.69–1.60 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.33, 170.61, 165.83, 161.77, 146.93, 142.67, 138.64, 135.82, 134.30, 129.20, 128.25, 127.99, 127.74, 126.86, 126.42, 125.78, 121.35, 117.16, 116.74, 113.28, 65.82, 54.95, 52.43, 40.32, 37.14, 34.36, 20.04. **HRMS** (ESI-TOF) calcd for $C_{31}H_{31}ClN_3O_5$ $[M+H]^+$: 560.1947, Found: 560.1949.



S3j

methyl (*S*)-2-(4-bromobenzyl)-2-(4-methoxybenzamido)-6-((4-methoxyquinolin-8-yl)amino)-6-oxohexanoate (S3j):

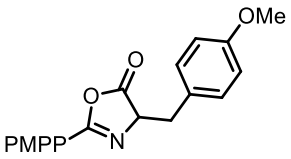
The title compound was prepared on 0.05 mmol scale from alkene **S1j** and azlactone **2b** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as an oil (17 mg, 44% yield, *er* 86.5:13.5). **SFC** (chiral column) Compound **S3j** was analyzed by chiral SFC on a Daicel IB column (3 μm, 4.6x250 mm) under isocratic conditions [40% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.51 (s, 1H), 8.77 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.64 (d, *J* = 8.5 Hz, 1H), 8.57 (dd, *J* = 8.4, 1.7 Hz, 1H), 7.74–7.66 (m, 2H), 7.43 (dd, *J* = 8.4, 4.2 Hz, 1H), 7.30–7.27 (m, 2H), 7.00 (s, 1H), 6.96–6.86 (m, 4H), 6.82 (d, *J* = 8.6 Hz, 1H), 3.98 (s, 3H), 3.89 (d, *J* = 13.6 Hz, 1H), 3.85 (s, 3H), 3.83 (s, 3H), 3.15 (d, *J* = 13.6 Hz, 1H), 2.85 (ddd, *J* = 13.5, 12.1, 4.5 Hz, 1H), 2.64–2.45 (m, 2H), 2.11 (ddd, *J* = 13.6, 11.8, 4.8 Hz, 1H), 1.85–1.73 (m, 1H), 1.69–1.61 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.60, 170.51, 166.29, 162.33, 150.21, 148.59, 139.00, 135.39, 131.39, 131.30, 131.24, 128.72, 127.86, 127.07, 120.92, 120.71, 120.41, 116.55, 113.83, 104.31, 65.99, 55.77, 55.43, 52.97, 40.00, 37.39, 34.90, 20.54. **HRMS** (ESI-TOF) calcd for $C_{32}H_{33}BrN_3O_6$ $[M+H]^+$: 634.1547, Found: 634.1540.



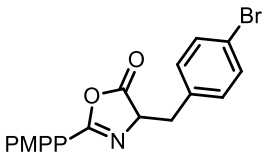
S3k

methyl (S)-2-benzyl-2-(4-chlorobenzamido)-6-oxo-6-(quinolin-8-ylamino)hexanoate (S3k): The title compound was prepared on 0.05 mmol scale from alkene **S1j** and azlactone **S2h** according to the general α-alkylation procedure. Purification using preparative TLC (ethyl acetate/hexanes = 2/5, v/v) gave the product as a white solid (11.2 mg, 42% yield, *er* 91:9). **SFC** (chiral column) Compound **S3k** was analyzed by chiral SFC on a Daicel IB column (3 mm, 4.6x250 mm) under isocratic conditions [40% (MeOH containing 0.5% formic acid) / CO2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.76 (dd, *J* = 4.3, 1.7 Hz, 1H), 8.73 (dd, *J* = 7.3, 1.6 Hz, 1H), 8.16 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.68–7.60 (m, 2H), 7.57–7.47 (m, 2H), 7.45 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.20–7.11 (m, 2H), 7.05 (s, 1H), 7.02–6.97 (m, 2H), 3.89 (d, *J* = 13.4 Hz, 1H), 3.85 (s, 3H), 3.21 (d, *J* = 13.5 Hz, 1H), 2.93–2.82 (m, 1H), 2.67–2.49 (m, 2H), 2.16 (ddd, *J* = 13.7, 11.9, 4.8 Hz, 1H), 1.88–1.74 (m, 1H), 1.64 (ddt, *J* = 18.0, 12.5, 6.4 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.64, 170.94, 165.69, 148.11, 138.25, 137.75, 136.38, 136.12, 134.38, 133.38, 129.58, 128.82, 128.40, 128.35, 128.31, 128.27, 127.92, 127.39, 126.99, 121.61, 121.47, 116.43, 66.40, 53.00, 40.66, 37.46, 34.73, 20.47. **HRMS** (ESI-TOF) calcd for $C_{30}H_{29}ClN_3O_4$ $[M+H]^+$: 530.1841, Found: 530.1843.

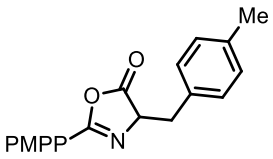
Reaction performance on different scales (representative examples):



80%, 94:6 *er* (0.05 mmol)
91%, 94:6 *er* (0.32 mmol)
67%, 95:5 *er* (1.00 mmol)



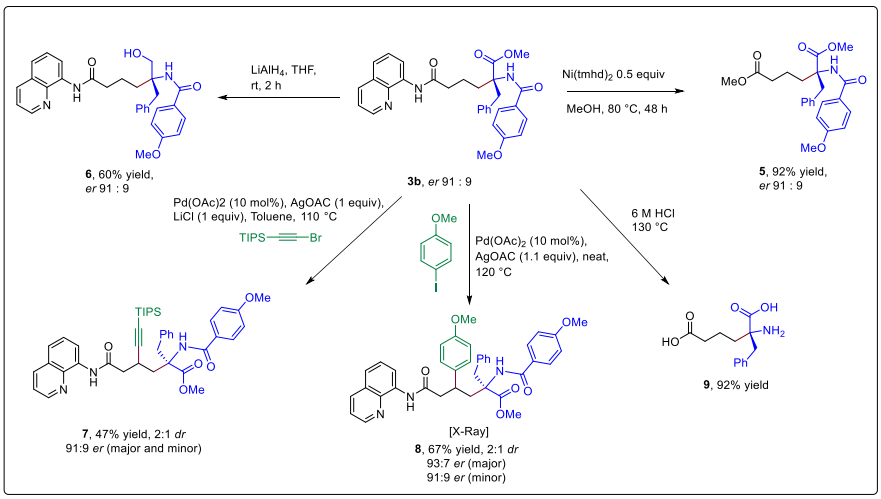
63%, 92:8 *er* (0.05 mmol)
59%, 92:8 *er* (0.17 mmol)

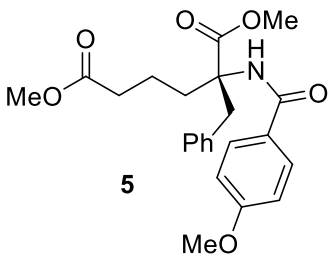


63%, 94:6 *er* (0.05 mmol)
69%, 95:5 *er* (0.30 mmol)

Derivatization reactions of 3b:

Scheme S9:

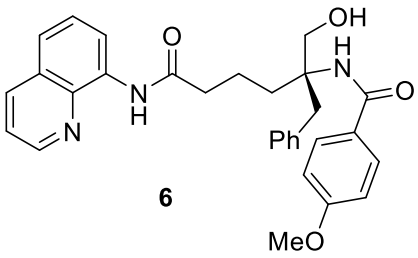




5

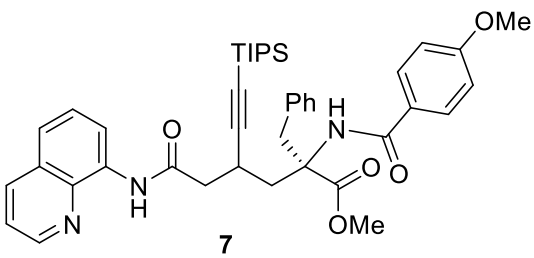
methyl (*S*)-2-ethyl-6-oxo-2-(4-phenoxybenzamido)-6-(quinolin-8-ylamino)hexanoate (5):

The title compound was prepared according to an adapted literature procedure.[4] In a flame-dried reaction vial were added **3b** (25 mg, 1.0 equiv), $Ni(tmhd)_2$ (10 mg, 0.5 equiv), and methanol (0.5 mL). The reaction mixture was heated to 80 °C for 48 h. The reaction mixture was directly loaded onto a silica gel column and purified using 0–30% ethyl acetate in hexane as eluent, affording the product as an oil (18 mg, 92% yield, *er* 91:9). **SFC** (chiral column) Compound **5** was analyzed by chiral SFC on a Daicel IC column (3 μm, 4.6×250 mm) under isocratic conditions [25% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (250 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.4 Hz, 2H), 7.20–7.13 (m, 3H), 7.04–6.96 (m, 2H), 6.94–6.87 (m, 3H), 3.91 (d, *J* = 13.6 Hz, 1H), 3.84 (d, *J* = 4.4 Hz, 6H), 3.64 (s, 3H), 3.14 (d, *J* = 13.5 Hz, 1H), 2.90–2.76 (m, 1H), 2.40–2.25 (m, 2H), 2.08–1.97 (m, 1H), 1.69–1.59 (m, 1H), 1.46–1.34 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.81, 173.56, 166.19, 162.25, 136.26, 129.63, 128.68, 128.21, 127.34, 126.89, 113.78, 66.25, 55.42, 52.84, 51.55, 40.71, 34.76, 33.58, 19.91. **HRMS** (ESI-TOF) calcd for $C_{23}H_{28}NO_6$ $[M+H]^+$: 414.1911, Found: 414.1920



6

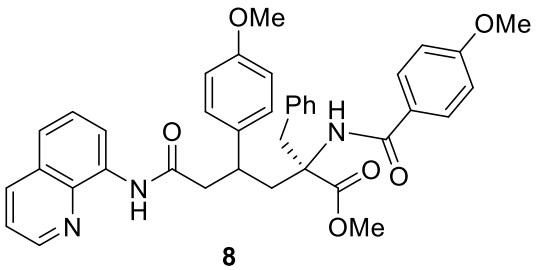
methyl (*S*)-2-ethyl-6-oxo-2-(4-phenoxybenzamido)-6-(quinolin-8-ylamino)hexanoate (6): The title compound was prepared according to an adapted literature procedure.[5] In a flame-dried reaction vial were added **3b** (50 mg, 1.0 equiv) and anhydrous THF (0.5 mL). The reaction vessel was cooled to 0 °C, and $LiAlH_4$ (7.2 mg, 2.0 equiv) was added. The reaction mixture was stirred at 0 °C for 2 h. Quenched with aq. NH_4Cl and extracted in ethyl acetate (3 × 5 mL). The combined organic layers were dried over Na_2SO_4, filtered, and concentrated *in vacuo*. The crude material was purified by using preparative TLC using (ethyl acetate/hexanes = 2/5, v/v) to afford the product as an oil (28 mg, 60% yield, *er* 91:9). **SFC** (chiral column) Compound **6** was analyzed by chiral SFC on a Daicel IA column (3 μm, 4.6×250 mm) under isocratic conditions [30% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.81 (s, 1H), 8.82–8.69 (m, 2H), 8.16 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.85–7.76 (m, 2H), 7.58–7.50 (m, 2H), 7.46 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.29–7.26 (m, 2H), 7.25–7.21 (m, 2H), 7.21–7.17 (m, 1H), 6.97–6.88 (m, 3H), 5.52 (brs, 1H), 3.94 (d, *J* = 11.8 Hz, 1H), 3.85 (s, 3H), 3.72 (d, *J* = 11.9 Hz, 1H), 3.38–3.32 (m, 1H), 3.06 (d, *J* = 13.6 Hz, 1H), 2.67–2.59 (m, 2H), 2.02–1.92 (m, 1H), 1.92–1.84 (m, 1H), 1.84–1.77 (m, 1H), 1.77–1.69 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.73, 171.57, 168.42, 162.29, 148.23, 138.25, 136.79, 136.39, 134.24, 130.69, 129.12, 128.30, 127.94, 127.29, 126.96, 126.63, 121.69, 116.48, 113.68, 67.61, 61.66, 55.41, 39.63, 36.67, 34.82, 18.28. **HRMS** (ESI-TOF) calcd for $C_{30}H_{32}N_3O_4$ $[M+H]^+$: 498.2387, Found: 498.2389.



7

methyl (2*S*)-2-benzyl-2-(4-methoxybenzamido)-4-(2-oxo-2-(quinolin-8-ylamino)ethyl)-6-(triisopropylsilyl)hex-5-ynoate (7): The title compound was prepared according to an adapted literature procedure.[6] In a flame-dried reaction vial were added **3b** (50 mg, 1.0 equiv), (bromoethynyl)triisopropylsilane (32.2 mg, 1.3 equiv), $Pd(OAc)_2$ (2.2 mg, 10 mol%), AgOAc (16 mg, 1.0 equiv) and LiCl (4 mg, 1.0 equiv) under a gentle stream of nitrogen. Anhydrous

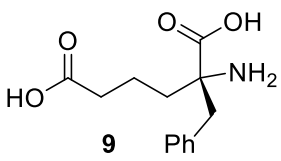
toluene (0.3 mL) was added, and the reaction vessel was placed in a pre-heated oil bath at 110 °C and stirred for 16 h. The reaction vessel was allowed to cool to room temperature, and the reaction mixture was filtered through Celite and purified using column chromatography using 10–60% ethyl acetate in hexane as eluent to give product as inseparable mixture of diastereomers in 2:1 ratio as a pale yellow oil (26 mg, 47% yield, *er* 91:9 (major and minor)). The following analytical data corresponds to the mixture. **SFC** (chiral column) Compound **7** was analyzed by chiral SFC on a Daicel IBN column (3 μm, 4.6×250 mm) under isocratic conditions [20% MeOH / CO_2 (4 mL/min), 1600 psi backpressure] at 30 °C. The enantiomers were detected by UV light (241 nm). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.84 (s, 2H), 9.79 (s, 1H), 8.78 (m, 4H), 8.73 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.66 (t, *J* = 4.5 Hz, 1H), 8.15 (m, 3H), 7.83–7.77 (m, 2H), 7.73–7.65 (m, 4H), 7.57–7.47 (m, 7H), 7.44 (m, 3H), 7.17 (m, 6H), 7.14–7.06 (m, 3H), 7.05–6.99 (m, 8H), 6.92–6.83 (m, 6H), 3.92 (d, *J* = 13.5 Hz, 2H), 3.84 (dd, *J* = 13.0, 3.5 Hz, 18H), 3.75 (d, *J* = 13.4 Hz, 1H), 3.38 (d, *J* = 13.6 Hz, 1H), 3.27 (dd, *J* = 11.2, 5.7 Hz, 3H), 3.21 (m, 2H), 3.09 (dd, *J* = 14.2, 9.2 Hz, 2H), 2.85–2.66 (m, 7H), 2.44 (dd, *J* = 14.2, 9.0 Hz, 1H), 2.29 (dd, *J* = 14.2, 4.3 Hz, 2H), 0.94–0.84 (m, 22H), 0.77 (m, 35H), 0.61 (m, 6H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.25, 172.90, 169.02, 168.64, 166.58, 162.20, 162.17, 148.08, 148.00, 138.30, 138.27, 136.26, 136.24, 136.12, 135.98, 134.35, 134.17, 130.07, 129.92, 129.03, 129.02, 128.17, 128.00, 127.82, 127.78, 127.51, 127.29, 127.26, 127.18, 126.91, 126.73, 121.56, 121.50, 116.69, 116.55, 113.64, 113.55, 109.49, 83.33, 82.88, 65.10, 63.95, 55.40, 52.83, 52.64, 45.11, 44.40, 40.90, 40.62, 39.26, 36.64, 26.37, 25.46, 24.69, 18.49, 18.46, 18.41, 18.38, 11.19, 11.04. **HRMS** (ESI-TOF) calcd for $C_{42}H_{52}N_3O_5Si$ $[M+H]^+$: 706.3671, Found: 706.3657.



8

methyl (2*S*)-2-benzyl-2-(4-methoxybenzamido)-4-(4-methoxyphenyl)-6-oxo-6-(quinolin-8-ylamino)hexanoate (8): The title compound was prepared according to an adapted literature procedure.[7] To a flame-dried reaction vial were added **3b** (50 mg, 1.0 equiv), *p*-iodoanisole (89 mg, 4.0 equiv), $Pd(OAc)_2$ (2.2 mg, 10 mol%), and AgOAc (17.4 mg, 1.1 equiv). The reaction vessel was placed in a pre-heated oil bath at 120 °C and stirred for 1 h. The reaction vessel was allowed to cool to room temperature, and the reaction mixture was loaded directly onto a silica gel

column and purified by using 10–60% ethyl acetate in hexane as eluent. The resulting material consisted mostly of product with trace quantities of starting material **3b**. This material was purified again using preparative TLC with 30% ethyl acetate in hexane. The product was thus obtained as inseparable mixture of diastereomers in 2:1 ratio as pale yellow solid (40 mg, 67% yield, *er* 93:7 (major), 91:9 (minor)). The following analytical data corresponds to the mixture. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.65 (s, 2H), 9.55 (s, 1H), 8.80–8.69 (m, 4H), 8.66–8.55 (m, 2H), 8.12 (dd, *J* = 8.2, 1.7 Hz, 2H), 8.09 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.77–7.71 (m, 2H), 7.54–7.45 (m, 4H), 7.45–7.41 (m, 4H), 7.38 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.21–7.13 (m, 7H), 7.13–7.04 (m, 13H), 6.98–6.92 (m, 6H), 6.91–6.85 (m, 2H), 6.77–6.69 (m, 6H), 6.54–6.48 (m, 4H), 6.38 (s, 2H), 4.01 (d, *J* = 13.4 Hz, 2H), 3.91 (s, 6H), 3.85 (s, 3H), 3.83 (d, *J* = 2.7 Hz, 2H), 3.79 (s, 6H), 3.69 (s, 3H), 3.45 (s, 6H), 3.41–3.33 (m, 3H), 3.21 (s, 4H), 3.16 (t, *J* = 13.6 Hz, 5H), 2.87 (dd, *J* = 14.8, 6.7 Hz, 1H), 2.82–2.68 (m, 4H), 2.57 (dd, *J* = 14.2, 10.0 Hz, 1H), 2.34 (dd, *J* = 14.2, 2.9 Hz, 2H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.71, 172.75, 169.64, 169.52, 166.30, 165.70, 162.11, 161.77, 158.24, 157.92, 148.09, 147.87, 138.21, 138.18, 136.26, 136.25, 136.15, 136.09, 135.10, 134.70, 134.38, 134.26, 129.83, 129.68, 129.26, 128.86, 128.35, 128.28, 128.05, 128.00, 127.85, 127.77, 127.40, 127.28, 127.21, 126.70, 126.69, 121.58, 121.43, 121.40, 121.25, 116.44, 116.32, 113.90, 113.66, 112.98, 66.14, 64.56, 55.39, 55.30, 55.15, 54.75, 52.85, 52.04, 47.09, 46.70, 41.80, 41.23, 40.94, 39.89, 39.53, 37.86. **HRMS** (ESI-TOF) calcd for $C_{38}H_{38}N_3O_6$ $[M+H]^+$: 632.2755, Found: 632.2751. **X-ray** (single-crystal) Colorless needle crystals of X-ray diffraction quality were obtained by vapor diffusion of ethyl acetate into a saturated solution of **8** in hexane. The sample was found to be a 1:1 co-crystal of diastereomers that both had (*S*) configuration at the α-carbon of the amino acid moiety (CCDC 1825332).[8]



9

(*S*)-2-amino-2-benzylhexanedioic acid (9): The title compound was prepared according to an adapted literature procedure.[9]

In a flame-dried reaction vial were added **3b** (50 mg, 1.0 equiv) and 6 M HCl (2.5 mL). The reaction vessel was place in a pre-heated oil bath at 130 °C and stirred for 24 h. After being allowed to cool to room temperature, the reaction mixture was diluted with water (10 mL) and extracted with ethyl acetate (10 mL). To the aqueous layer was added aq. NH_4OH (14.8 M) solution until the pH was adjusted to >10. The resulting aqueous layer was extracted with ethyl acetate (3 × 10 mL). The aqueous layer was

concentrated and dissolved in 1 M HCl. This solution was purified using a column of DOWEX 50WX-8 100 mesh resin. The resin was eluted with water (30 mL), 1 M aq. NH_4OH (50 mL) and 2 M aq. NH_4OH (100 mL). Fractions with pH > 8 were collected and concentrated to afford the product as a white solid (22 mg, 92% yield). **^{1}H NMR** (600 MHz, D_2O) δ 7.45–7.35 (m, 3H), 7.33–7.24 (m, 2H), 3.34 (d, *J* = 14.3 Hz, 1H), 3.02 (d, *J* = 14.4 Hz, 1H), 2.37–2.17 (m, 2H), 2.07–1.97 (m, 1H), 1.80 (ddd, *J* = 14.5, 12.6, 4.3 Hz, 1H), 1.70 (m, 1H), 1.61–1.48 (m, 1H). **^{13}C NMR** (150 MHz, D_2O) δ 184.62, 177.95, 136.90, 132.99, 131.89, 130.75, 68.55, 44.71, 39.53, 38.72, 22.90. **HRMS** (ESI-TOF) calcd for $C_{13}H_{18}NO_4$ $[M+H]^+$: 252.1230, Found: 252.1234.

X – Ray Crystallography:

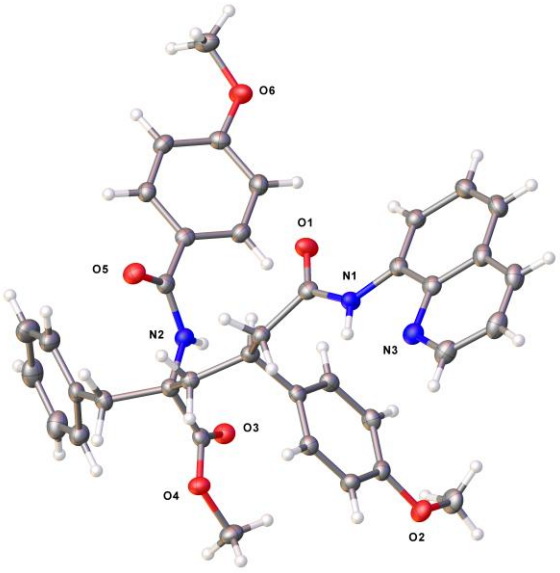


Table S6. Crystal data and structure refinement for **8**.

Report date	2018-02-22
Identification code	SN-E-173F3
Empirical formula	C38 H37 N3 O6
Molecular formula	C38 H37 N3 O6
Formula weight	631.70
Temperature	100 K
Wavelength	1.54178 Å
Crystal system	Triclinic
Space group	P1
Unit cell dimensions	a = 9.5780(2) Å □= 106.2010(10)°.

	b = 13.0993(3) Å □= 102.6500(10)°.
	c = 14.1121(3) Å □ = 95.3300(10)°.
Volume	1636.43(6) Å^3
Z	2
Density (calculated)	1.282 Mg/m^3
Absorption coefficient	0.707 mm^{-1}
F(000)	668
Crystal size	0.176 x 0.031 x 0.027 mm^3
Crystal color, habit	Colorless Needle
Theta range for data collection	3.374 to 65.071°.
Index ranges	-11<=h<=11, -15<=k<=15, -16<=l<=16
Reflections collected	33858
Independent reflections	10625 [R(int) = 0.0307, R(sigma) = 0.0277]
Completeness to theta = 65.071°	98.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.3165 and 0.2302
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10625 / 7 / 869
Goodness-of-fit on F^2	1.051
Final R indices [I>2sigma(I)]	R1 = 0.0252, wR2 = 0.0609
R indices (all data)	R1 = 0.0264, wR2 = 0.0616
Absolute structure parameter	0.04(4)
Extinction coefficient	n/a
Largest diff. peak and hole	0.132 and -0.152 e.Å^{-3}

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **8**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4179(2)	3503(1)	6111(1)	28(1)
O(2)	-2536(2)	1624(1)	7019(1)	26(1)
O(3)	-2155(2)	1386(1)	3363(1)	25(1)
O(4)	-2716(2)	3042(1)	3913(1)	25(1)
O(5)	2118(2)	3138(1)	2818(1)	26(1)
O(6)	5028(2)	-1021(1)	2216(1)	30(1)
N(1)	3777(2)	4602(1)	7556(1)	22(1)
N(2)	311(2)	2081(1)	3072(1)	20(1)
N(3)	4116(2)	5888(1)	9448(1)	25(1)
C(1)	3494(2)	4159(2)	6529(2)	21(1)
C(2)	2257(2)	4535(2)	5909(2)	22(1)
C(3)	1183(2)	3559(2)	5137(2)	20(1)
C(4)	282(2)	3886(2)	4257(2)	20(1)
C(5)	-567(2)	2920(2)	3324(2)	20(1)
C(6)	-1117(2)	3346(2)	2395(2)	23(1)
C(7)	-1595(2)	2464(2)	1380(2)	23(1)
C(8)	-637(3)	2236(2)	764(2)	31(1)
C(9)	-1015(3)	1388(2)	-133(2)	37(1)
C(10)	-2368(3)	747(2)	-440(2)	36(1)
C(11)	-3343(3)	989(2)	147(2)	34(1)
C(12)	-2963(2)	1840(2)	1052(2)	28(1)
C(13)	240(2)	3020(2)	5655(2)	19(1)
C(14)	-629(2)	3604(2)	6209(2)	21(1)
C(15)	-1530(2)	3120(2)	6655(2)	22(1)
C(16)	-1596(2)	2025(2)	6555(2)	22(1)
C(17)	-750(2)	1428(2)	6011(2)	23(1)
C(18)	159(2)	1933(2)	5570(2)	22(1)
C(19)	-1889(2)	2348(2)	3534(2)	21(1)

C(20)	-2688(3)	499(2)	6897(2)	31(1)
C(21)	-3934(2)	2578(2)	4206(2)	29(1)
C(22)	4876(2)	4441(2)	8316(2)	21(1)
C(23)	5746(2)	3664(2)	8155(2)	24(1)
C(24)	6795(2)	3562(2)	8986(2)	28(1)
C(25)	6953(2)	4215(2)	9954(2)	29(1)
C(26)	6063(2)	5012(2)	10148(2)	25(1)
C(27)	5021(2)	5135(2)	9326(2)	22(1)
C(28)	6127(3)	5687(2)	11134(2)	30(1)
C(29)	5212(3)	6422(2)	11258(2)	30(1)
C(30)	4220(3)	6496(2)	10390(2)	28(1)
C(31)	1600(2)	2251(2)	2844(2)	21(1)
C(32)	2382(2)	1320(2)	2631(2)	21(1)
C(33)	3178(2)	1242(2)	1901(2)	22(1)
C(34)	4042(2)	456(2)	1726(2)	24(1)
C(35)	4158(2)	-251(2)	2304(2)	24(1)
C(36)	3362(2)	-196(2)	3029(2)	26(1)
C(37)	2473(2)	579(2)	3179(2)	24(1)
C(38)	6093(2)	-946(2)	1653(2)	30(1)
O(1')	2766(2)	6075(1)	3607(1)	35(1)
O(2')	9119(2)	8487(1)	3266(1)	33(1)
O(3')	6447(2)	8411(1)	7257(1)	25(1)
O(4')	5186(2)	6956(1)	7403(1)	25(1)
O(5')	9812(2)	6081(1)	6174(1)	25(1)
O(6')	13658(2)	9898(1)	5539(1)	31(1)
N(1')	3489(2)	4896(1)	2358(1)	22(1)
N(2')	8457(2)	7374(1)	6635(1)	19(1)
N(3')	3498(2)	3400(1)	642(1)	26(1)
C(1')	3546(2)	5417(2)	3345(2)	24(1)
C(2')	4649(2)	5119(2)	4126(2)	23(1)
C(3')	5585(2)	6126(2)	4966(2)	22(1)
C(4')	6459(2)	5776(2)	5842(2)	21(1)
C(5')	7303(2)	6697(2)	6818(2)	20(1)
C(6')	7920(2)	6211(2)	7683(2)	22(1)
C(7')	8796(2)	7056(2)	8653(2)	22(1)

C(8')	10282(2)	7367(2)	8798(2)	27(1)
C(9')	11077(2)	8195(2)	9651(2)	32(1)
C(10')	10402(3)	8727(2)	10376(2)	33(1)
C(11')	8939(3)	8409(2)	10250(2)	32(1)
C(12')	8141(2)	7577(2)	9401(2)	26(1)
C(13')	6527(2)	6747(2)	4503(2)	21(1)
C(14')	7559(2)	6273(2)	4049(2)	22(1)
C(15')	8448(2)	6820(2)	3632(2)	24(1)
C(16')	8304(2)	7872(2)	3659(2)	25(1)
C(17')	7275(2)	8365(2)	4100(2)	25(1)
C(18')	6400(2)	7804(2)	4517(2)	23(1)
C(19')	6282(2)	7467(2)	7176(2)	19(1)
C(20')	10071(3)	7957(2)	2722(2)	35(1)
C(21')	4212(2)	7635(2)	7815(2)	30(1)
C(22')	2479(2)	4892(2)	1474(2)	23(1)
C(23')	1519(2)	5606(2)	1427(2)	29(1)
C(24')	589(3)	5545(2)	482(2)	35(1)
C(25')	608(3)	4788(2)	-404(2)	33(1)
C(26')	1569(2)	4041(2)	-384(2)	27(1)
C(27')	2516(2)	4085(2)	561(2)	24(1)
C(28')	1680(3)	3245(2)	-1264(2)	32(1)
C(29')	2671(3)	2571(2)	-1173(2)	34(1)
C(30')	3561(3)	2677(2)	-206(2)	31(1)
C(31')	9617(2)	7025(2)	6328(2)	20(1)
C(32')	10669(2)	7840(2)	6175(2)	20(1)
C(33')	11487(2)	7466(2)	5481(2)	22(1)
C(34')	12475(2)	8169(2)	5288(2)	22(1)
C(35')	12673(2)	9271(2)	5795(2)	24(1)
C(36')	11894(2)	9654(2)	6505(2)	28(1)
C(37')	10893(2)	8933(2)	6687(2)	25(1)
C(38')	13934(3)	11030(2)	6051(2)	38(1)

Table S8. Bond lengths [Å] and angles [°] for **8**.

O(1)-C(1)	1.229(3)
O(2)-C(16)	1.370(2)
O(2)-C(20)	1.426(3)
O(3)-C(19)	1.206(3)
O(4)-C(19)	1.337(3)
O(4)-C(21)	1.456(3)
O(5)-C(31)	1.234(3)
O(6)-C(35)	1.363(3)
O(6)-C(38)	1.436(3)
N(1)-H(1)	0.94(2)
N(1)-C(1)	1.357(3)
N(1)-C(22)	1.406(3)
N(2)-H(2)	0.943(19)
N(2)-C(5)	1.458(3)
N(2)-C(31)	1.356(3)
N(3)-C(27)	1.373(3)
N(3)-C(30)	1.322(3)
C(1)-C(2)	1.518(3)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(2)-C(3)	1.538(3)
C(3)-H(3)	1.0000
C(3)-C(4)	1.538(3)
C(3)-C(13)	1.520(3)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(4)-C(5)	1.552(3)
C(5)-C(6)	1.571(3)
C(5)-C(19)	1.537(3)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(6)-C(7)	1.513(3)
C(7)-C(8)	1.394(3)

C(7)-C(12)	1.386(3)
C(8)-H(8)	0.9500
C(8)-C(9)	1.381(3)
C(9)-H(9)	0.9500
C(9)-C(10)	1.387(4)
C(10)-H(10)	0.9500
C(10)-C(11)	1.381(4)
C(11)-H(11)	0.9500
C(11)-C(12)	1.390(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.399(3)
C(13)-C(18)	1.389(3)
C(14)-H(14)	0.9500
C(14)-C(15)	1.378(3)
C(15)-H(15)	0.9500
C(15)-C(16)	1.396(3)
C(16)-C(17)	1.383(3)
C(17)-H(17)	0.9500
C(17)-C(18)	1.394(3)
C(18)-H(18)	0.9500
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.376(3)
C(22)-C(27)	1.429(3)
C(23)-H(23)	0.9500
C(23)-C(24)	1.413(3)
C(24)-H(24)	0.9500
C(24)-C(25)	1.361(3)
C(25)-H(25)	0.9500
C(25)-C(26)	1.413(3)
C(26)-C(27)	1.412(3)

C(26)-C(28)	1.410(3)
C(28)-H(28)	0.9500
C(28)-C(29)	1.362(4)
C(29)-H(29)	0.9500
C(29)-C(30)	1.409(3)
C(30)-H(30)	0.9500
C(31)-C(32)	1.485(3)
C(32)-C(33)	1.397(3)
C(32)-C(37)	1.397(3)
C(33)-H(33)	0.9500
C(33)-C(34)	1.383(3)
C(34)-H(34)	0.9500
C(34)-C(35)	1.391(3)
C(35)-C(36)	1.395(3)
C(36)-H(36)	0.9500
C(36)-C(37)	1.386(3)
C(37)-H(37)	0.9500
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
O(1')-C(1')	1.225(3)
O(2')-C(16')	1.374(3)
O(2')-C(20')	1.425(3)
O(3')-C(19')	1.202(2)
O(4')-C(19')	1.337(2)
O(4')-C(21')	1.449(3)
O(5')-C(31')	1.233(2)
O(6')-C(35')	1.366(3)
O(6')-C(38')	1.428(3)
N(1')-H(1')	0.93(2)
N(1')-C(1')	1.357(3)
N(1')-C(22')	1.399(3)
N(2')-H(2')	0.93(2)
N(2')-C(5')	1.464(3)
N(2')-C(31')	1.352(3)

N(3')-C(27')	1.367(3)
N(3')-C(30')	1.320(3)
C(1')-C(2')	1.513(3)
C(2')-H(2'A)	0.9900
C(2')-H(2'B)	0.9900
C(2')-C(3')	1.546(3)
C(3')-H(3')	1.0000
C(3')-C(4')	1.541(3)
C(3')-C(13')	1.523(3)
C(4')-H(4'A)	0.9900
C(4')-H(4'B)	0.9900
C(4')-C(5')	1.552(3)
C(5')-C(6')	1.560(3)
C(5')-C(19')	1.531(3)
C(6')-H(6'A)	0.9900
C(6')-H(6'B)	0.9900
C(6')-C(7')	1.510(3)
C(7')-C(8')	1.397(3)
C(7')-C(12')	1.394(3)
C(8')-H(8')	0.9500
C(8')-C(9')	1.386(3)
C(9')-H(9')	0.9500
C(9')-C(10')	1.387(4)
C(10')-H(10')	0.9500
C(10')-C(11')	1.382(4)
C(11')-H(11')	0.9500
C(11')-C(12')	1.386(3)
C(12')-H(12')	0.9500
C(13')-C(14')	1.392(3)
C(13')-C(18')	1.396(3)
C(14')-H(14')	0.9500
C(14')-C(15')	1.388(3)
C(15')-H(15')	0.9500
C(15')-C(16')	1.389(3)
C(16')-C(17')	1.392(3)

C(17')-H(17')	0.9500
C(17')-C(18')	1.389(3)
C(18')-H(18')	0.9500
C(20')-H(20D)	0.9800
C(20')-H(20E)	0.9800
C(20')-H(20F)	0.9800
C(21')-H(21D)	0.9800
C(21')-H(21E)	0.9800
C(21')-H(21F)	0.9800
C(22')-C(23')	1.375(3)
C(22')-C(27')	1.431(3)
C(23')-H(23')	0.9500
C(23')-C(24')	1.409(3)
C(24')-H(24')	0.9500
C(24')-C(25')	1.367(4)
C(25')-H(25')	0.9500
C(25')-C(26')	1.406(3)
C(26')-C(27')	1.421(3)
C(26')-C(28')	1.413(3)
C(28')-H(28')	0.9500
C(28')-C(29')	1.364(4)
C(29')-H(29')	0.9500
C(29')-C(30')	1.404(3)
C(30')-H(30')	0.9500
C(31')-C(32')	1.492(3)
C(32')-C(33')	1.398(3)
C(32')-C(37')	1.385(3)
C(33')-H(33')	0.9500
C(33')-C(34')	1.382(3)
C(34')-H(34')	0.9500
C(34')-C(35')	1.395(3)
C(35')-C(36')	1.389(3)
C(36')-H(36')	0.9500
C(36')-C(37')	1.397(3)
C(37')-H(37')	0.9500

C(38')-H(38D)	0.9800
C(38')-H(38E)	0.9800
C(38')-H(38F)	0.9800

C(16)-O(2)-C(20)	117.22(16)
C(19)-O(4)-C(21)	115.61(17)
C(35)-O(6)-C(38)	117.00(17)
C(1)-N(1)-H(1)	117.9(16)
C(1)-N(1)-C(22)	128.21(18)
C(22)-N(1)-H(1)	113.7(16)
C(5)-N(2)-H(2)	118.0(14)
C(31)-N(2)-H(2)	117.6(14)
C(31)-N(2)-C(5)	123.65(17)
C(30)-N(3)-C(27)	117.10(19)
O(1)-C(1)-N(1)	123.50(19)
O(1)-C(1)-C(2)	121.19(19)
N(1)-C(1)-C(2)	115.31(18)
C(1)-C(2)-H(2A)	109.6
C(1)-C(2)-H(2B)	109.6
C(1)-C(2)-C(3)	110.21(17)
H(2A)-C(2)-H(2B)	108.1
C(3)-C(2)-H(2A)	109.6
C(3)-C(2)-H(2B)	109.6
C(2)-C(3)-H(3)	107.4
C(4)-C(3)-C(2)	110.64(16)
C(4)-C(3)-H(3)	107.4
C(13)-C(3)-C(2)	111.43(17)
C(13)-C(3)-H(3)	107.4
C(13)-C(3)-C(4)	112.38(16)
C(3)-C(4)-H(4A)	108.7
C(3)-C(4)-H(4B)	108.7
C(3)-C(4)-C(5)	114.08(16)
H(4A)-C(4)-H(4B)	107.6
C(5)-C(4)-H(4A)	108.7
C(5)-C(4)-H(4B)	108.7

N(2)-C(5)-C(4)	111.83(16)
N(2)-C(5)-C(6)	111.39(16)
N(2)-C(5)-C(19)	104.32(16)
C(4)-C(5)-C(6)	108.75(16)
C(19)-C(5)-C(4)	112.12(16)
C(19)-C(5)-C(6)	108.34(16)
C(5)-C(6)-H(6A)	108.9
C(5)-C(6)-H(6B)	108.9
H(6A)-C(6)-H(6B)	107.7
C(7)-C(6)-C(5)	113.40(17)
C(7)-C(6)-H(6A)	108.9
C(7)-C(6)-H(6B)	108.9
C(8)-C(7)-C(6)	120.08(19)
C(12)-C(7)-C(6)	121.57(19)
C(12)-C(7)-C(8)	118.3(2)
C(7)-C(8)-H(8)	119.5
C(9)-C(8)-C(7)	121.1(2)
C(9)-C(8)-H(8)	119.5
C(8)-C(9)-H(9)	119.9
C(8)-C(9)-C(10)	120.3(2)
C(10)-C(9)-H(9)	119.9
C(9)-C(10)-H(10)	120.5
C(11)-C(10)-C(9)	119.0(2)
C(11)-C(10)-H(10)	120.5
C(10)-C(11)-H(11)	119.6
C(10)-C(11)-C(12)	120.8(2)
C(12)-C(11)-H(11)	119.6
C(7)-C(12)-C(11)	120.5(2)
C(7)-C(12)-H(12)	119.8
C(11)-C(12)-H(12)	119.8
C(14)-C(13)-C(3)	120.52(18)
C(18)-C(13)-C(3)	122.02(18)
C(18)-C(13)-C(14)	117.42(18)
C(13)-C(14)-H(14)	119.3
C(15)-C(14)-C(13)	121.40(19)

C(15)-C(14)-H(14)	119.3
C(14)-C(15)-H(15)	120.0
C(14)-C(15)-C(16)	120.09(19)
C(16)-C(15)-H(15)	120.0
O(2)-C(16)-C(15)	115.30(18)
O(2)-C(16)-C(17)	124.92(18)
C(17)-C(16)-C(15)	119.78(19)
C(16)-C(17)-H(17)	120.4
C(16)-C(17)-C(18)	119.24(19)
C(18)-C(17)-H(17)	120.4
C(13)-C(18)-C(17)	122.07(19)
C(13)-C(18)-H(18)	119.0
C(17)-C(18)-H(18)	119.0
O(3)-C(19)-O(4)	124.20(19)
O(3)-C(19)-C(5)	123.82(19)
O(4)-C(19)-C(5)	111.97(17)
O(2)-C(20)-H(20A)	109.5
O(2)-C(20)-H(20B)	109.5
O(2)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
O(4)-C(21)-H(21A)	109.5
O(4)-C(21)-H(21B)	109.5
O(4)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(1)-C(22)-C(27)	114.92(18)
C(23)-C(22)-N(1)	125.10(19)
C(23)-C(22)-C(27)	119.94(19)
C(22)-C(23)-H(23)	120.0
C(22)-C(23)-C(24)	120.0(2)
C(24)-C(23)-H(23)	120.0
C(23)-C(24)-H(24)	119.5

C(25)-C(24)-C(23)	121.1(2)
C(25)-C(24)-H(24)	119.5
C(24)-C(25)-H(25)	119.8
C(24)-C(25)-C(26)	120.4(2)
C(26)-C(25)-H(25)	119.8
C(27)-C(26)-C(25)	119.4(2)
C(28)-C(26)-C(25)	123.4(2)
C(28)-C(26)-C(27)	117.1(2)
N(3)-C(27)-C(22)	117.70(19)
N(3)-C(27)-C(26)	123.08(19)
C(26)-C(27)-C(22)	119.22(19)
C(26)-C(28)-H(28)	120.1
C(29)-C(28)-C(26)	119.9(2)
C(29)-C(28)-H(28)	120.1
C(28)-C(29)-H(29)	120.5
C(28)-C(29)-C(30)	118.9(2)
C(30)-C(29)-H(29)	120.5
N(3)-C(30)-C(29)	123.9(2)
N(3)-C(30)-H(30)	118.1
C(29)-C(30)-H(30)	118.1
O(5)-C(31)-N(2)	122.2(2)
O(5)-C(31)-C(32)	120.70(18)
N(2)-C(31)-C(32)	117.14(18)
C(33)-C(32)-C(31)	117.54(19)
C(37)-C(32)-C(31)	123.81(18)
C(37)-C(32)-C(33)	118.39(19)
C(32)-C(33)-H(33)	119.5
C(34)-C(33)-C(32)	121.0(2)
C(34)-C(33)-H(33)	119.5
C(33)-C(34)-H(34)	120.1
C(33)-C(34)-C(35)	119.78(19)
C(35)-C(34)-H(34)	120.1
O(6)-C(35)-C(34)	124.01(19)
O(6)-C(35)-C(36)	115.82(19)
C(34)-C(35)-C(36)	120.18(19)

C(35)-C(36)-H(36)	120.3
C(37)-C(36)-C(35)	119.4(2)
C(37)-C(36)-H(36)	120.3
C(32)-C(37)-H(37)	119.4
C(36)-C(37)-C(32)	121.18(19)
C(36)-C(37)-H(37)	119.4
O(6)-C(38)-H(38A)	109.5
O(6)-C(38)-H(38B)	109.5
O(6)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(16')-O(2')-C(20')	116.36(18)
C(19')-O(4')-C(21')	115.31(16)
C(35')-O(6')-C(38')	117.86(18)
C(1')-N(1')-H(1')	115.5(18)
C(1')-N(1')-C(22')	128.51(19)
C(22')-N(1')-H(1')	113.7(18)
C(5')-N(2')-H(2')	115.8(15)
C(31')-N(2')-H(2')	119.1(15)
C(31')-N(2')-C(5')	124.84(17)
C(30')-N(3')-C(27')	117.5(2)
O(1')-C(1')-N(1')	123.8(2)
O(1')-C(1')-C(2')	121.21(19)
N(1')-C(1')-C(2')	115.00(19)
C(1')-C(2')-H(2'A)	109.2
C(1')-C(2')-H(2'B)	109.2
C(1')-C(2')-C(3')	111.89(18)
H(2'A)-C(2')-H(2'B)	107.9
C(3')-C(2')-H(2'A)	109.2
C(3')-C(2')-H(2'B)	109.2
C(2')-C(3')-H(3')	108.1
C(4')-C(3')-C(2')	109.18(17)
C(4')-C(3')-H(3')	108.1
C(13')-C(3')-C(2')	109.75(17)

C(13')-C(3')-H(3')	108.1
C(13')-C(3')-C(4')	113.56(16)
C(3')-C(4')-H(4'A)	108.2
C(3')-C(4')-H(4'B)	108.2
C(3')-C(4')-C(5')	116.19(17)
H(4'A)-C(4')-H(4'B)	107.4
C(5')-C(4')-H(4'A)	108.2
C(5')-C(4')-H(4'B)	108.2
N(2')-C(5')-C(4')	112.70(16)
N(2')-C(5')-C(6')	111.04(16)
N(2')-C(5')-C(19')	104.76(16)
C(4')-C(5')-C(6')	109.56(16)
C(19')-C(5')-C(4')	109.77(16)
C(19')-C(5')-C(6')	108.86(16)
C(5')-C(6')-H(6'A)	109.0
C(5')-C(6')-H(6'B)	109.0
H(6'A)-C(6')-H(6'B)	107.8
C(7')-C(6')-C(5')	112.85(17)
C(7')-C(6')-H(6'A)	109.0
C(7')-C(6')-H(6'B)	109.0
C(8')-C(7')-C(6')	120.34(19)
C(12')-C(7')-C(6')	121.28(19)
C(12')-C(7')-C(8')	118.3(2)
C(7')-C(8')-H(8')	119.6
C(9')-C(8')-C(7')	120.8(2)
C(9')-C(8')-H(8')	119.6
C(8')-C(9')-H(9')	119.9
C(8')-C(9')-C(10')	120.2(2)
C(10')-C(9')-H(9')	119.9
C(9')-C(10')-H(10')	120.3
C(11')-C(10')-C(9')	119.4(2)
C(11')-C(10')-H(10')	120.3
C(10')-C(11')-H(11')	119.7
C(10')-C(11')-C(12')	120.6(2)
C(12')-C(11')-H(11')	119.7

C(7')-C(12')-H(12')	119.7
C(11')-C(12')-C(7')	120.6(2)
C(11')-C(12')-H(12')	119.7
C(14')-C(13')-C(3')	120.69(18)
C(14')-C(13')-C(18')	117.45(19)
C(18')-C(13')-C(3')	121.86(19)
C(13')-C(14')-H(14')	118.9
C(15')-C(14')-C(13')	122.2(2)
C(15')-C(14')-H(14')	118.9
C(14')-C(15')-H(15')	120.4
C(14')-C(15')-C(16')	119.3(2)
C(16')-C(15')-H(15')	120.4
O(2')-C(16')-C(15')	124.2(2)
O(2')-C(16')-C(17')	115.90(19)
C(15')-C(16')-C(17')	119.88(19)
C(16')-C(17')-H(17')	120.1
C(18')-C(17')-C(16')	119.9(2)
C(18')-C(17')-H(17')	120.1
C(13')-C(18')-H(18')	119.3
C(17')-C(18')-C(13')	121.3(2)
C(17')-C(18')-H(18')	119.3
O(3')-C(19')-O(4')	124.04(18)
O(3')-C(19')-C(5')	124.69(17)
O(4')-C(19')-C(5')	111.26(16)
O(2')-C(20')-H(20D)	109.5
O(2')-C(20')-H(20E)	109.5
O(2')-C(20')-H(20F)	109.5
H(20D)-C(20')-H(20E)	109.5
H(20D)-C(20')-H(20F)	109.5
H(20E)-C(20')-H(20F)	109.5
O(4')-C(21')-H(21D)	109.5
O(4')-C(21')-H(21E)	109.5
O(4')-C(21')-H(21F)	109.5
H(21D)-C(21')-H(21E)	109.5
H(21D)-C(21')-H(21F)	109.5

H(21E)-C(21')-H(21F)	109.5
N(1')-C(22')-C(27')	115.10(19)
C(23')-C(22')-N(1')	125.3(2)
C(23')-C(22')-C(27')	119.5(2)
C(22')-C(23')-H(23')	120.0
C(22')-C(23')-C(24')	120.0(2)
C(24')-C(23')-H(23')	120.0
C(23')-C(24')-H(24')	119.1
C(25')-C(24')-C(23')	121.7(2)
C(25')-C(24')-H(24')	119.1
C(24')-C(25')-H(25')	120.1
C(24')-C(25')-C(26')	119.8(2)
C(26')-C(25')-H(25')	120.1
C(25')-C(26')-C(27')	119.5(2)
C(25')-C(26')-C(28')	123.6(2)
C(28')-C(26')-C(27')	116.9(2)
N(3')-C(27')-C(22')	117.57(19)
N(3')-C(27')-C(26')	123.0(2)
C(26')-C(27')-C(22')	119.4(2)
C(26')-C(28')-H(28')	120.2
C(29')-C(28')-C(26')	119.5(2)
C(29')-C(28')-H(28')	120.2
C(28')-C(29')-H(29')	120.3
C(28')-C(29')-C(30')	119.5(2)
C(30')-C(29')-H(29')	120.3
N(3')-C(30')-C(29')	123.6(2)
N(3')-C(30')-H(30')	118.2
C(29')-C(30')-H(30')	118.2
O(5')-C(31')-N(2')	122.52(18)
O(5')-C(31')-C(32')	120.79(18)
N(2')-C(31')-C(32')	116.70(17)
C(33')-C(32')-C(31')	117.44(18)
C(37')-C(32')-C(31')	124.05(19)
C(37')-C(32')-C(33')	118.51(19)
C(32')-C(33')-H(33')	119.5

C(34')-C(33')-C(32')	121.06(19)
C(34')-C(33')-H(33')	119.5
C(33')-C(34')-H(34')	120.0
C(33')-C(34')-C(35')	119.91(19)
C(35')-C(34')-H(34')	120.0
O(6')-C(35')-C(34')	115.27(19)
O(6')-C(35')-C(36')	124.93(19)
C(36')-C(35')-C(34')	119.80(19)
C(35')-C(36')-H(36')	120.2
C(35')-C(36')-C(37')	119.60(19)
C(37')-C(36')-H(36')	120.2
C(32')-C(37')-C(36')	121.1(2)
C(32')-C(37')-H(37')	119.4
C(36')-C(37')-H(37')	119.4
O(6')-C(38')-H(38D)	109.5

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **8**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	26(1)	32(1)	23(1)	3(1)	6(1)	9(1)
O(2)	30(1)	21(1)	32(1)	11(1)	13(1)	2(1)
O(3)	24(1)	22(1)	29(1)	7(1)	6(1)	1(1)
O(4)	21(1)	25(1)	29(1)	7(1)	9(1)	3(1)
O(5)	27(1)	21(1)	31(1)	7(1)	10(1)	1(1)
O(6)	29(1)	26(1)	40(1)	14(1)	15(1)	10(1)
N(1)	21(1)	23(1)	19(1)	4(1)	5(1)	5(1)
N(2)	21(1)	18(1)	20(1)	4(1)	5(1)	1(1)
N(3)	27(1)	20(1)	26(1)	6(1)	8(1)	1(1)
C(1)	19(1)	20(1)	24(1)	6(1)	6(1)	-1(1)
C(2)	20(1)	22(1)	21(1)	6(1)	5(1)	2(1)
C(3)	19(1)	21(1)	20(1)	5(1)	5(1)	4(1)
C(4)	20(1)	19(1)	21(1)	5(1)	5(1)	2(1)
C(5)	20(1)	19(1)	19(1)	5(1)	4(1)	3(1)

C(6)	24(1)	22(1)	23(1)	9(1)	4(1)	4(1)
C(7)	26(1)	25(1)	20(1)	10(1)	4(1)	6(1)
C(8)	28(1)	41(1)	25(1)	12(1)	6(1)	4(1)
C(9)	38(1)	49(2)	25(1)	7(1)	11(1)	12(1)
C(10)	51(2)	30(1)	21(1)	4(1)	6(1)	6(1)
C(11)	41(1)	32(1)	24(1)	8(1)	2(1)	-6(1)
C(12)	27(1)	32(1)	23(1)	9(1)	5(1)	2(1)
C(13)	17(1)	19(1)	18(1)	5(1)	1(1)	1(1)
C(14)	23(1)	18(1)	22(1)	6(1)	4(1)	3(1)
C(15)	23(1)	20(1)	24(1)	6(1)	8(1)	5(1)
C(16)	22(1)	22(1)	19(1)	8(1)	2(1)	1(1)
C(17)	28(1)	18(1)	24(1)	7(1)	4(1)	3(1)
C(18)	23(1)	21(1)	20(1)	4(1)	4(1)	6(1)
C(19)	19(1)	23(1)	16(1)	4(1)	0(1)	2(1)
C(20)	38(1)	21(1)	38(1)	15(1)	13(1)	2(1)
C(21)	22(1)	34(1)	31(1)	8(1)	10(1)	1(1)
C(22)	19(1)	23(1)	22(1)	9(1)	4(1)	1(1)
C(23)	22(1)	24(1)	23(1)	7(1)	6(1)	2(1)
C(24)	24(1)	30(1)	31(1)	12(1)	7(1)	7(1)
C(25)	25(1)	32(1)	29(1)	14(1)	2(1)	2(1)
C(26)	26(1)	25(1)	24(1)	10(1)	4(1)	-3(1)
C(27)	22(1)	21(1)	24(1)	8(1)	6(1)	0(1)
C(28)	34(1)	28(1)	21(1)	8(1)	0(1)	-4(1)
C(29)	41(1)	25(1)	21(1)	2(1)	8(1)	-5(1)
C(30)	36(1)	21(1)	27(1)	4(1)	12(1)	1(1)
C(31)	21(1)	22(1)	17(1)	4(1)	2(1)	1(1)
C(32)	18(1)	21(1)	19(1)	3(1)	2(1)	-1(1)
C(33)	22(1)	22(1)	21(1)	7(1)	5(1)	1(1)
C(34)	23(1)	25(1)	22(1)	5(1)	8(1)	0(1)
C(35)	20(1)	22(1)	27(1)	5(1)	6(1)	3(1)
C(36)	27(1)	27(1)	27(1)	12(1)	7(1)	4(1)
C(37)	23(1)	26(1)	22(1)	7(1)	8(1)	3(1)
C(38)	26(1)	26(1)	40(1)	9(1)	15(1)	6(1)
O(1')	30(1)	41(1)	27(1)	-3(1)	4(1)	14(1)
O(2')	33(1)	35(1)	35(1)	17(1)	13(1)	0(1)

O(3')	26(1)	21(1)	30(1)	8(1)	10(1)	4(1)
O(4')	24(1)	24(1)	28(1)	8(1)	12(1)	3(1)
O(5')	27(1)	18(1)	32(1)	9(1)	11(1)	6(1)
O(6')	29(1)	25(1)	41(1)	11(1)	12(1)	-3(1)
N(1')	24(1)	21(1)	20(1)	6(1)	5(1)	4(1)
N(2')	20(1)	16(1)	21(1)	5(1)	6(1)	1(1)
N(3')	32(1)	23(1)	22(1)	6(1)	8(1)	3(1)
C(1')	20(1)	22(1)	25(1)	2(1)	6(1)	-1(1)
C(2')	23(1)	23(1)	19(1)	4(1)	5(1)	-1(1)
C(3')	20(1)	21(1)	21(1)	3(1)	6(1)	2(1)
C(4')	23(1)	17(1)	20(1)	4(1)	6(1)	0(1)
C(5')	19(1)	18(1)	21(1)	6(1)	6(1)	0(1)
C(6')	24(1)	20(1)	22(1)	7(1)	7(1)	3(1)
C(7')	24(1)	22(1)	22(1)	10(1)	4(1)	5(1)
C(8')	25(1)	34(1)	23(1)	10(1)	7(1)	6(1)
C(9')	23(1)	41(1)	28(1)	13(1)	2(1)	-2(1)
C(10')	36(1)	31(1)	24(1)	5(1)	-1(1)	-1(1)
C(11')	33(1)	38(1)	22(1)	4(1)	6(1)	10(1)
C(12')	22(1)	34(1)	23(1)	10(1)	6(1)	5(1)
C(13')	20(1)	22(1)	15(1)	4(1)	1(1)	0(1)
C(14')	22(1)	22(1)	20(1)	4(1)	3(1)	3(1)
C(15')	21(1)	30(1)	18(1)	6(1)	4(1)	3(1)
C(16')	23(1)	29(1)	21(1)	10(1)	3(1)	-2(1)
C(17')	28(1)	22(1)	24(1)	8(1)	3(1)	2(1)
C(18')	24(1)	23(1)	20(1)	4(1)	3(1)	3(1)
C(19')	19(1)	21(1)	15(1)	4(1)	2(1)	0(1)
C(20')	30(1)	46(2)	31(1)	14(1)	11(1)	-1(1)
C(21')	26(1)	33(1)	36(1)	12(1)	16(1)	10(1)
C(22')	21(1)	23(1)	23(1)	6(1)	5(1)	-2(1)
C(23')	26(1)	32(1)	28(1)	6(1)	7(1)	6(1)
C(24')	26(1)	43(1)	37(1)	14(1)	5(1)	10(1)
C(25')	26(1)	44(1)	27(1)	13(1)	0(1)	2(1)
C(26')	23(1)	32(1)	23(1)	7(1)	3(1)	-5(1)
C(27')	24(1)	24(1)	22(1)	8(1)	5(1)	-2(1)
C(28')	31(1)	35(1)	22(1)	6(1)	3(1)	-6(1)

C(29')	42(1)	28(1)	25(1)	-1(1)	11(1)	-3(1)
C(30')	40(1)	24(1)	26(1)	4(1)	11(1)	5(1)
C(31')	20(1)	21(1)	17(1)	5(1)	2(1)	3(1)
C(32')	18(1)	20(1)	21(1)	6(1)	3(1)	4(1)
C(33')	22(1)	19(1)	22(1)	6(1)	3(1)	2(1)
C(34')	20(1)	26(1)	22(1)	8(1)	5(1)	3(1)
C(35')	18(1)	25(1)	30(1)	12(1)	4(1)	-1(1)
C(36')	25(1)	19(1)	36(1)	2(1)	7(1)	1(1)
C(37')	21(1)	22(1)	28(1)	3(1)	9(1)	3(1)
C(38')	27(1)	23(1)	62(2)	13(1)	12(1)	-1(1)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **8**.

	x	y	z	U(eq)
H(1)	3230(30)	5126(19)	7810(20)	32(7)
H(2)	-100(20)	1362(16)	2961(18)	22(6)
H(2A)	2648	4990	5542	26
H(2B)	1747	4975	6372	26
H(3)	1768	3021	4836	24
H(4A)	938	4341	4029	24
H(4B)	-417	4329	4517	24
H(6A)	-1942	3726	2507	27
H(6B)	-329	3875	2369	27
H(8)	292	2672	964	37
H(9)	-344	1243	-541	45
H(10)	-2621	149	-1046	43
H(11)	-4285	570	-70	41
H(12)	-3644	1995	1449	33
H(14)	-597	4349	6280	26
H(15)	-2107	3533	7030	27
H(17)	-788	682	5939	28
H(18)	740	1520	5199	26
H(20A)	-2976	92	6169	46
H(20B)	-3431	304	7224	46
H(20C)	-1760	327	7216	46
H(21A)	-4754	2271	3603	44
H(21B)	-4219	3141	4714	44
H(21C)	-3648	2010	4500	44
H(23)	5643	3196	7486	28
H(24)	7398	3029	8868	33
H(25)	7665	4136	10502	35
H(28)	6806	5629	11710	35
H(29)	5242	6877	11920	37
H(30)	3590	7012	10488	34

H(33)	3126	1737	1520	27
H(34)	4554	398	1213	28
H(36)	3429	-685	3417	31
H(37)	1915	607	3663	28
H(38A)	5607	-1120	927	45
H(38B)	6759	-1456	1746	45
H(38C)	6640	-212	1903	45
H(1')	4010(30)	4330(20)	2260(20)	43(8)
H(2')	8310(30)	8071(17)	6673(18)	25(6)
H(2'A)	5289	4685	3778	27
H(2'B)	4138	4670	4446	27
H(3')	4917	6603	5243	26
H(4'A)	7162	5339	5580	25
H(4'B)	5782	5303	6038	25
H(6'A)	7105	5818	7834	26
H(6'B)	8541	5685	7440	26
H(8')	10754	7007	8307	32
H(9')	12086	8399	9740	38
H(10')	10941	9305	10954	40
H(11')	8476	8763	10749	38
H(12')	7139	7361	9329	31
H(14')	7657	5552	4025	27
H(15')	9147	6479	3332	28
H(17')	7171	9083	4117	31
H(18')	5701	8146	4817	28
H(20D)	9512	7330	2160	53
H(20E)	10798	7721	3185	53
H(20F)	10559	8457	2448	53
H(21D)	3752	7966	7310	45
H(21E)	4761	8200	8438	45
H(21F)	3463	7196	7974	45
H(23')	1484	6141	2031	35
H(24')	-69	6043	460	42
H(25')	-27	4766	-1033	40
H(28')	1070	3180	-1914	38

H(29')	2759	2035	-1760	40
H(30')	4246	2201	-159	37
H(33')	11362	6716	5136	26
H(34')	13018	7903	4810	27
H(36')	12041	10402	6865	34
H(37')	10357	9198	7170	30
H(38D)	14656	11382	5797	57
H(38E)	14304	11162	6787	57
H(38F)	13032	11325	5922	57

Non-linear effect

Non-linear effect reactions were set up with standard substrates (0.05 mmol), catalyst and TRIP (both enantiomers purchased from Sigma-Aldrich and used as reveived) with variant *ee* following the standard set up procedure as described in previous section, except that the amount of palladium precatalyst and TRIP enantiomers was weighed on analytical balance and that the amount of solvent was measured with volumetric syringe. The reactions ran for four days and followed by ring opening and purification as described in standard procedure. The enantioselectivity excess relationship between ligand and product is listed here.

Table S11. Non-linear effect experiments

Ligand *ee*	*R*-TRIP amount calc. (mg)	*S*-TRIP amount calc. (mg)	*R*-TRIP amount weighed (mg)	*S*-TRIP amount weighed (mg)	Product *ee*
0	3.75	3.75	3.83	3.90	0
20%	4.50	3.00	4.48	3.30	10%
40%	5.25	2.25	5.24	2.38	24%
60%	6.00	1.50	6.16	1.40	43%
80%	6.75	0.75	6.83	0.74	59%
100%	7.50	0	7.49	0	76%

Computational Details

All calculations were performed with Gaussian 09.[10] Unless otherwise mentioned, the B3LYP[11] density functional with Grimme's dispersion correction (D3)[12] and LANL2DZ basis set were used in geometry optimizations. Single-point energies were calculated with M06 and a mixed basis set of SDD for Pd and 6-311+G(d,p) for other atoms. Solvation energy corrections were calculated using the SMD model.[13] In accordance with the experimental conditions, C_6H_6 (ε = 2.3) was used as solvent in the single point calculations. To confirm the nature of the stationary points, vibrational frequency calculations were performed for all optimized structures. All optimized transition state structures have only one imaginary (negative) frequency, and all minima (reactants, products, and intermediates) have no imaginary frequencies. The imaginary frequencies of all transition states are provided in the "Cartesian Coordinates and Energies of the Optimized Structures" section below. The reported Gibbs free energies and enthalpies include zero-point vibrational energies and thermal corrections at 298 K.

The nucleopalladation and protodepalladation pathways resulting in the *S* and *R* products were calculated (Figure 2). The pathway for the *S* product (experimental major product) was determined to be the lowest energy pathway.

The alternative isomeric palladium π-alkene intermediate (**10'**) and the corresponding diastereomeric transition states for nucleopalladation (**TS1_S'** and **TS1_R'**) and protodepalladation (**TS2_S'** and **TS2_R'**) steps were also located computationally (shown in red in Figure S5). The resulting transition states are higher in energy than in the lowest energy pathways reported in the manuscript (**Figure S5**).

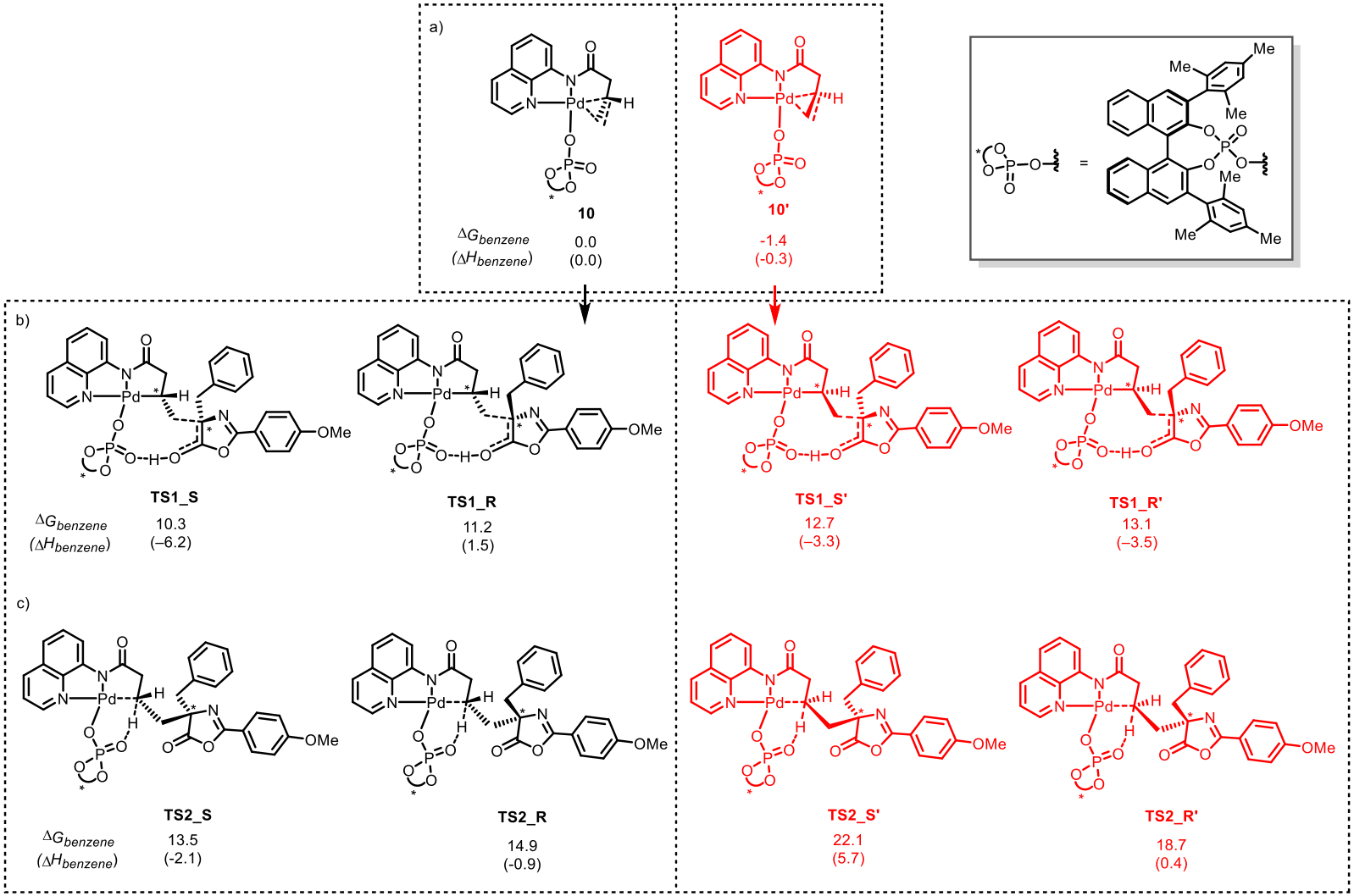


Figure S5: Comparison of a) isomeric palladium π-alkene intermediates (**10** (black) and **10'** (red)) and their corresponding diastereomeric transition states for b) nucleopalladation (**TS1_S** and **TS1_R** (formed from **10**; black), **TS1_S'** and **TS1_R'** (formed from **10'**; red) and c) protodepalladation (**TS2_S** and **TS2_R** (formed from **10**; black), **TS2_S'** and **TS2_R'** (formed from **10'**; red).

Cartesian Coordinates and Energies of the Optimized Structures

2

B3LYP-D3 SCF energy: -937.124474168 a.u.
B3LYP-D3 enthalpy: -936.819463 a.u.
B3LYP-D3 free energy: -936.886698 a.u.
M06 SCF energy in solution: -936.8522516 a.u.
M06 enthalpy in solution: -936.5472406 a.u.
M06 free energy in solution: -936.6144756 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	3.08569300	1.53216800	-0.36807700
O	2.17730100	1.81061800	-0.62130500
C	1.27862700	0.80029400	-0.42597900
C	1.34264500	-0.56467700	-0.24295700
O	-0.05521300	1.20001800	-0.37969900
N	0.02222000	-1.04704800	-0.08246400
C	-0.78110800	-0.00246600	-0.17195500
C	-2.23130700	0.07809600	-0.09298000
C	-2.90610800	1.31878100	-0.21814000
C	-2.98579400	-1.09747800	0.11404200
C	-4.29986900	1.37637800	-0.13756100
H	-2.33035100	2.22530000	-0.37777400
C	-4.38577200	-1.04721900	0.19675800
H	-2.46416400	-2.04563600	0.20905500
C	-5.04585700	0.19540400	0.07054300
H	-4.83516100	2.31602600	-0.23124600
H	-4.94227800	-1.96481500	0.35655900
C	2.52595200	-1.49632700	-0.25441900
H	2.33879800	-2.27294100	0.50050900
H	2.56463500	-2.01600000	-1.22164800
C	3.86268400	-0.81644800	0.02013700
C	4.04035100	-0.01437600	1.17375600
C	4.95347700	-0.98081600	-0.86025100
C	5.27720000	0.60355400	1.43865700
H	3.21186500	0.11248900	1.86793400
C	6.19320500	-0.36560000	-0.59716500
H	4.83157000	-1.58958000	-1.75366200
C	6.35948600	0.43014600	0.55242100
H	5.39566800	1.21436400	2.33032500
H	7.02220000	-0.50392000	-1.28701700
H	7.31496200	0.90735600	0.75503800
O	-6.42815400	0.36510500	0.13660600
C	-7.26763700	-0.80687300	0.35161800

H	-7.03517700	-1.29209600	1.31035000
H	-8.29176300	-0.42876300	0.36917000
H	-7.15455100	-1.53278900	-0.46622300

10

B3LYP-D3 SCF energy: -2588.11234534 a.u.
B3LYP-D3 enthalpy: -2587.237054 a.u.
B3LYP-D3 free energy: -2587.375590 a.u.
M06 SCF energy in solution: -2923.284902 a.u.
M06 enthalpy in solution: -2922.40961 a.u.
M06 free energy in solution: -2922.548146 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	4.17704600	0.67003900	-3.00399400
C	5.08714700	0.64662300	-1.76978100
O	6.30332500	0.32759200	-1.87714800
N	4.47291500	1.00912100	-0.58637600
C	5.12482800	1.03514700	0.66857500
C	4.25087500	1.17463300	1.79515500
C	6.50193400	0.93284600	0.91996600
C	4.73719100	1.21896800	3.13847200
C	6.98977500	0.98209700	2.25803400
H	7.18508300	0.80926400	0.09141700
C	1.99478800	1.35940900	2.52196900
C	3.76941800	1.34746100	4.18184400
C	6.14398800	1.12307900	3.35391200
H	8.06297800	0.90439000	2.41333900
C	2.41306300	1.41832400	3.87869800
H	4.10731800	1.38496100	5.21479400
H	6.53619900	1.15843000	4.36684200
H	1.66228500	1.51281900	4.65563400
N	2.89320200	1.24525600	1.53830900
C	2.68693700	0.73613300	-2.71556800
Pd	2.48106400	1.18146500	-0.46273500
H	0.95454300	1.39567000	2.21290800
H	2.12333500	-0.19332900	-2.79715700
H	4.41226700	-0.22261200	-3.58796100
H	4.48670900	1.53668700	-3.60377000
C	2.01694300	1.94575600	-2.58904700
H	0.93063600	2.01019300	-2.59987300
H	2.56328600	2.88454100	-2.67946300
C	-2.26275400	-1.95717700	0.43092600
C	-0.07784400	-3.70052200	0.94577000
C	0.07535100	-2.69861600	-0.00442400

C	-1.03580400	-1.82426200	-0.22684300
H	0.73700000	-4.40102000	1.11193700
C	-5.61258600	0.65546600	-0.47481600
C	-4.38364600	1.20484000	-0.13796500
C	-3.30882000	0.29854400	0.10793900
C	-3.42599700	-1.08959200	0.06537200
H	-6.45777900	1.31641000	-0.65229100
C	-2.37032300	-2.93967300	1.48334100
C	-1.26416400	-3.82991100	1.72466800
C	-1.36596400	-4.82084500	2.75174000
C	-2.50505700	-4.91554400	3.53797200
C	-3.58781300	-4.00948600	3.32805800
C	-3.52244900	-3.04956000	2.32727900
H	-0.52685500	-5.49460500	2.91261600
H	-2.57457200	-5.66797600	4.31954300
H	-4.46980100	-4.07173700	3.96064100
H	-4.35072400	-2.36435100	2.18523800
C	-5.79097800	-0.75352200	-0.62066400
C	-4.68698500	-1.64555300	-0.36609000
C	-4.88148100	-3.04609300	-0.59119200
C	-6.10921100	-3.53992300	-1.01110500
C	-7.21082300	-2.65863500	-1.22571400
C	-7.04838900	-1.29351000	-1.03736200
H	-4.05114500	-3.72722300	-0.44095000
H	-6.23353600	-4.60624500	-1.18276900
H	-8.16840600	-3.06004900	-1.54775300
H	-7.87575600	-0.61015000	-1.21669500
P	-0.84888900	0.86609500	-0.80400500
O	-0.87747800	-0.83117200	-1.21683900
O	-2.05114000	0.86417600	0.44530900
O	-1.14607300	1.69115900	-2.11807900
O	0.49051900	1.18647000	0.06067200
C	1.35310700	-2.59410900	-0.77947700
C	2.57360600	-2.32534500	-0.10169900
C	1.36887200	-2.87002000	-2.17411300
C	3.78527800	-2.34418700	-0.82170900
C	2.60491000	-2.89639900	-2.85430800
C	3.82689000	-2.65557300	-2.19458300
H	4.71528100	-2.12523000	-0.29958000
H	2.61333700	-3.13634900	-3.91627200
C	-4.17923800	2.68262400	-0.01806200
C	-4.14905300	3.49918600	-1.17805300
C	-4.01204100	3.26002900	1.26705700
C	-3.98174100	4.89063900	-1.02531800
C	-3.84749200	4.65400500	1.37786100
C	-3.82874000	5.48690000	0.24128000

H	-3.95651900	5.51758800	-1.91512200
H	-3.72898400	5.09625100	2.36595300
C	-3.99472600	2.39124400	2.51163900
H	-4.85904700	1.71499300	2.54539700
H	-3.09307000	1.76487100	2.52220100
H	-4.00169400	3.00142000	3.42198100
C	-3.61561500	6.98424300	0.37548800
H	-4.13667900	7.53597700	-0.41674700
H	-3.97508100	7.35660400	1.34273600
H	-2.54747400	7.23629100	0.30204800
C	-4.22381300	2.89797300	-2.57037000
H	-3.31996400	2.30515100	-2.76314900
H	-5.08868700	2.23568200	-2.69304500
H	-4.28509100	3.68318900	-3.33261100
C	0.09020300	-3.17291100	-2.93231500
H	-0.51006600	-3.93157400	-2.41314800
H	-0.53232400	-2.27430800	-3.01337400
H	0.30666200	-3.54157600	-3.94091400
C	5.15261200	-2.77025600	-2.92494300
H	5.62766200	-3.73742700	-2.70704000
H	5.02037000	-2.71221600	-4.01261700
H	5.85441400	-1.98529300	-2.61977100
C	2.60630100	-2.03394200	1.38979500
H	2.52159500	-2.95578500	1.97936800
H	3.54767600	-1.54940000	1.66850200
H	1.77782400	-1.38440900	1.69023100

TS1_S

B3LYP-D3 SCF energy: -3525.26186067 a.u.
B3LYP-D3 enthalpy: -3524.083107 a.u.
B3LYP-D3 free energy: -3524.262678 a.u..
M06 SCF energy in solution: -3860.145426 a.u.
M06 enthalpy in solution: -3858.966673 a.u.
M06 free energy in solution: -3859.146244 a.u.
Imaginary frequency: -445.0604 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	-3.77014600	0.02887200	-0.97463300
C	-4.16875900	-1.37138200	-1.44432500
O	-5.35586100	-1.79723600	-1.34647800
N	-3.11957300	-2.09297900	-1.98619400
C	-3.19754000	-3.39293200	-2.51387300
C	-1.93428700	-3.97601600	-2.88643100
C	-4.35653700	-4.16423700	-2.70405800

C	-1.84500600	-5.29305400	-3.43850400
C	-4.26320500	-5.47162900	-3.25970200
H	-5.31430100	-3.75089100	-2.41827500
C	0.42001700	-3.69926200	-2.96435400
C	-0.54039800	-5.78402500	-3.75663800
C	-3.04585200	-6.03974700	-3.62597200
H	-5.18225300	-6.03716000	-3.39507800
C	0.58304400	-4.99784100	-3.52251200
H	-0.43971900	-6.78156200	-4.17831700
H	-2.99573900	-7.04146900	-4.04522700
H	1.58198900	-5.35371100	-3.75227800
N	-0.79281600	-3.22254300	-2.66784100
C	-2.25377000	0.24623700	-0.84885800
Pd	-1.27585200	-1.39038500	-1.79450700
H	1.25784400	-3.04351000	-2.74851700
H	-1.87064500	0.13475700	0.17033100
H	-4.28419900	0.21389300	-0.02807800
H	-4.19864000	0.74018400	-1.69542400
H	0.71850500	2.34280100	0.11414200
O	-0.04124200	2.79905800	0.81261400
C	-1.25053200	2.96599500	0.38980900
C	-1.82090200	3.18355500	-0.91686000
O	-2.28310800	2.79205700	1.28508500
C	-3.49540500	3.01042900	0.52185200
N	-3.24391100	3.30503800	-0.72682800
C	-4.74568000	2.80243200	1.22711300
C	-4.77071900	2.60266100	2.62396500
C	-5.96044800	2.75455200	0.49549000
C	-5.98111200	2.35922100	3.29038500
H	-3.84116200	2.63681200	3.18360600
C	-7.16700100	2.51178400	1.15090700
H	-5.93519400	2.89482800	-0.58104400
C	-7.18363900	2.31127800	2.55112800
H	-5.97557800	2.20599600	4.36413000
H	-8.10603000	2.45710700	0.60999400
C	-1.11907500	3.97234100	-2.01421900
H	-0.29991200	3.37792000	-2.43511200
H	-1.85880400	4.12607500	-2.80895900
C	-0.56298600	5.30192700	-1.52442800
C	0.82991500	5.48591600	-1.40687500
C	-1.43141500	6.35073700	-1.15135600
C	1.34986800	6.70493000	-0.93117000
H	1.50077900	4.67344800	-1.67861000
C	-0.91375300	7.56883500	-0.67663900
H	-2.50732000	6.20663700	-1.23199100
C	0.48045900	7.75023300	-0.56679400

H	2.42572100	6.83955000	-0.84256100
H	-1.59001700	8.37264200	-0.39458900
H	0.88147900	8.69225300	-0.19999500
C	-1.65152300	1.28357900	-1.65523000
H	-0.57080300	1.35420000	-1.71627300
H	-2.16139300	1.53537000	-2.58702500
C	3.12253500	-1.70125700	1.82226300
C	1.15420200	-3.55275800	2.70477000
C	0.73061300	-2.35923000	2.13027500
C	1.75147800	-1.47018400	1.66880300
H	0.41120100	-4.24002400	3.10003400
C	5.97689300	1.43675600	0.85570800
C	5.04051000	1.05112400	-0.09271900
C	4.14671000	-0.00139700	0.26882000
C	4.11839600	-0.62443400	1.51505700
H	6.69233600	2.21703900	0.60735300
C	3.53562500	-2.99170900	2.31745500
C	2.53039100	-3.91687000	2.77367700
C	2.92936900	-5.19264600	3.28439200
C	4.26699700	-5.55892200	3.31750100
C	5.26233600	-4.65735300	2.83313000
C	4.90573900	-3.40602500	2.34946000
H	2.16109200	-5.87764800	3.63677500
H	4.56207100	-6.53233800	3.70102300
H	6.30743800	-4.95649500	2.84217400
H	5.67094000	-2.73185100	1.97994800
C	5.99559800	0.87227800	2.16604900
C	5.03459700	-0.14148500	2.52469500
C	5.00873000	-0.59576400	3.88252200
C	5.91387100	-0.11212500	4.81740300
C	6.89599700	0.85377300	4.44599700
C	6.92726600	1.33830100	3.14666100
H	4.26410100	-1.32206900	4.18652200
H	5.87228400	-0.46820500	5.84365600
H	7.60410300	1.21642100	5.18671700
H	7.65450000	2.09391800	2.85736200
P	1.60739600	0.05609200	-0.59592300
O	1.31857900	-0.25632300	1.07892000
O	3.23671900	-0.44290800	-0.73673700
O	1.42798500	1.65254600	-0.69835300
O	0.78373500	-0.87549800	-1.59909600
C	-0.72880200	-2.03167700	2.04385400
C	-1.60934400	-2.91769100	1.35848300
C	-1.26047200	-0.88993800	2.70731300
C	-2.99362200	-2.66022900	1.36379200
C	-2.65468900	-0.67286300	2.68591400

C	-3.54233300	-1.55112500	2.03636900
H	-3.65688700	-3.33053700	0.82070700
H	-3.05279100	0.20208400	3.19544500
C	4.90933000	1.74627600	-1.41135000
C	4.39598000	3.07000400	-1.44846900
C	5.25209500	1.07993400	-2.61465300
C	4.24251000	3.70720200	-2.69532900
C	5.08646900	1.75194100	-3.84147100
C	4.58403100	3.06691800	-3.90272700
H	3.84253300	4.71972700	-2.72644100
H	5.34949200	1.23828300	-4.76482400
C	3.95914600	3.78523000	-0.18190000
H	3.58398800	4.78866500	-0.40583100
H	3.15484500	3.22794600	0.31336500
H	4.77717300	3.88723500	0.54017800
C	5.77520200	-0.34415800	-2.59141600
H	6.58105900	-0.46453700	-1.85560400
H	4.97286500	-1.03780800	-2.31020000
H	6.16075300	-0.64179900	-3.57292400
C	4.43426000	3.78322000	-5.23268200
H	3.63520900	4.53360300	-5.19584800
H	5.36321800	4.30530600	-5.50495400
H	4.20392700	3.08037500	-6.04274100
C	-1.10262500	-4.13412000	0.59801700
H	-0.90815400	-4.98214300	1.26770700
H	-1.84583400	-4.45795500	-0.13667800
H	-0.16921800	-3.91953900	0.06643600
C	-0.38656200	0.10073400	3.45534000
H	0.46860800	-0.38728000	3.93776000
H	0.01571500	0.85608800	2.77023200
H	-0.96445400	0.61917900	4.22900500
C	-5.04298500	-1.32673200	2.07063000
H	-5.50591900	-1.57014300	1.10699200
H	-5.51100500	-1.96813500	2.83177000
H	-5.28850000	-0.28736100	2.31812800
O	-8.43623300	2.06953400	3.10190900
C	-8.53643700	1.80318400	4.53300100
H	-8.19463500	2.66606300	5.12163700
H	-9.59748400	1.62693400	4.71866000
H	-7.95712100	0.91124500	4.80979900

11_S

B3LYP-D3 SCF energy: -3525.29517003 a.u.
B3LYP-D3 enthalpy: -3524.111620 a.u.
B3LYP-D3 free energy: -3524.290688 a.u.

M06 SCF energy in solution: -3860.177656 a.u.
M06 enthalpy in solution: -3858.994106 a.u.
M06 free energy in solution: -3859.173174 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.49170600	-3.38555100	1.02592300
C	3.77862000	-3.49610700	0.19997700
O	4.71319600	-4.29416400	0.51175800
N	3.81037100	-2.59849300	-0.84954900
C	4.87627900	-2.37053100	-1.72497200
C	4.71396700	-1.23891400	-2.61078300
C	6.07123800	-3.10651300	-1.81037300
C	5.72956500	-0.88109800	-3.55569500
C	7.07110600	-2.74615000	-2.75576400
H	6.21470400	-3.94565900	-1.14226200
C	3.35445900	0.58396700	-3.26944300
C	5.48917700	0.26476000	-4.37756700
C	6.92074300	-1.66380300	-3.61960000
H	7.97997900	-3.34273500	-2.79531000
C	4.31312500	0.99350000	-4.23896600
H	6.24188000	0.55897800	-5.10584800
H	7.69640700	-1.40294100	-4.33554500
H	4.11347400	1.86960300	-4.84784300
N	3.55484800	-0.48669600	-2.49567900
C	1.36366300	-2.61495600	0.29739900
Pd	2.27768300	-1.34117900	-1.01998600
H	2.42431800	1.12172200	-3.11051300
H	0.78121100	-2.01063900	1.00743700
H	2.76373600	-2.84796900	1.94008600
H	2.20817700	-4.40355800	1.33051000
H	-1.64232100	-1.84714700	0.36908300
O	-1.23404000	-6.21073300	-0.86563100
C	-1.57892700	-5.08775300	-0.55892500
C	-0.86234900	-3.96846500	0.19357900
O	-2.91502800	-4.58777300	-0.88491500
C	-2.99629000	-3.28399800	-0.42223900
N	-1.86981400	-2.87856100	0.12511200
C	-4.24766600	-2.58614000	-0.54908700
C	-5.27869200	-3.13596500	-1.34844200
C	-4.47530900	-1.38819500	0.18285000
C	-6.52004900	-2.49976800	-1.43957100
H	-5.09679600	-4.05774500	-1.89222100
C	-5.72296800	-0.78213200	0.12794600
H	-3.68369700	-0.94080300	0.77647000
C	-6.74302700	-1.31945200	-0.69202600

H	-7.29576200	-2.92339400	-2.06758400
H	-5.93210500	0.11547600	0.69160800
C	-0.63778100	-4.42739700	1.67701700
H	-0.00601800	-5.32200700	1.63485700
H	-0.06824700	-3.63840400	2.17487400
C	-1.93651200	-4.69800700	2.41385900
C	-2.50419800	-5.99021900	2.43508800
C	-2.62056400	-3.63949900	3.05249400
C	-3.73490200	-6.22049800	3.07837200
H	-1.98480500	-6.81436200	1.94971900
C	-3.85032800	-3.86620100	3.69535000
H	-2.18737300	-2.64071600	3.04602200
C	-4.41244800	-5.15871400	3.70816400
H	-4.15978000	-7.22119600	3.08972100
H	-4.36513400	-3.04302600	4.18490100
H	-5.36213900	-5.33612300	4.20721400
C	0.45087000	-3.53998700	-0.54044500
H	0.13854200	-3.05884900	-1.47629800
H	0.99648200	-4.45183800	-0.81644800
C	0.96869000	3.55860100	0.81975700
C	3.69945400	3.11837400	1.40848900
C	2.81235000	2.05740100	1.56608500
C	1.44252400	2.30658400	1.21898000
H	4.73410000	2.98377500	1.70914500
C	-3.11843500	4.82171200	0.25510300
C	-2.71384400	3.63593600	-0.34626000
C	-1.38564200	3.17176100	-0.05808700
C	-0.49044800	3.88071700	0.74611300
H	-4.09165400	5.23423700	0.00362500
C	1.93310500	4.59260000	0.51695400
C	3.31536400	4.36345500	0.83761900
C	4.28256100	5.38450300	0.57412700
C	3.90725900	6.58101200	-0.01879400
C	2.54199100	6.79656900	-0.37561700
C	1.58068700	5.83080700	-0.10976000
H	5.32242900	5.19860200	0.83447100
H	4.64689900	7.35089400	-0.22397800
H	2.25475600	7.72562100	-0.86185300
H	0.54909600	6.00926300	-0.39224400
C	-2.31620200	5.50220500	1.21377800
C	-0.99394300	5.01281600	1.49440000
C	-0.23550500	5.66828700	2.51661500
C	-0.74748100	6.76606400	3.19521600
C	-2.04273100	7.27619600	2.88068700
C	-2.81032900	6.65062300	1.90914800
H	0.74922900	5.29221700	2.77038500

H	-0.15830800	7.24163100	3.97532000
H	-2.42521000	8.14376300	3.41249900
H	-3.80763300	7.01603000	1.67265800
P	-0.29656000	0.59624200	-0.02340700
O	0.50922000	1.24766500	1.36974800
O	-0.96190700	2.01370200	-0.73882200
O	-1.40789400	-0.39753600	0.56061900
O	0.69782800	0.07031300	-1.16652700
C	3.32290700	0.76193500	2.11549900
C	2.79240200	0.22070200	3.31986100
C	4.43679800	0.12558200	1.49269700
C	3.36039900	-0.95566900	3.85462100
C	4.96629200	-1.04799300	2.05761900
C	4.44270600	-1.61051300	3.23655300
H	2.95140000	-1.36224400	4.77818500
H	5.78714600	-1.55287900	1.55202000
C	-3.64879900	2.91518800	-1.26668600
C	-4.92820800	2.51520200	-0.78392300
C	-3.31267800	2.68945800	-2.63002700
C	-5.82665500	1.87374000	-1.65612400
C	-4.23430800	2.02112900	-3.46379800
C	-5.48866400	1.59340200	-2.99312000
H	-6.80072300	1.56572200	-1.28242800
H	-3.96452100	1.84118700	-4.50325100
C	5.01728500	-2.90392000	3.78138200
H	4.99337200	-3.68555300	3.00954900
H	6.06702200	-2.77563900	4.07970500
H	4.45923000	-3.25801600	4.65636300
C	1.66482200	0.89936700	4.07796700
H	1.81975800	1.98474400	4.13970500
H	0.70520200	0.74514100	3.57282100
H	1.59208000	0.50906800	5.09939400
C	5.09581400	0.66099500	0.23154400
H	5.60622500	-0.14740000	-0.29756000
H	4.37250300	1.11216000	-0.45286300
H	5.85031500	1.42419200	0.46647400
C	-5.35127900	2.72429300	0.66443500
H	-5.54027000	3.77820100	0.89676100
H	-6.28045300	2.18415000	0.87873000
H	-4.57554700	2.38436500	1.36289800
C	-6.44568100	0.81644400	-3.87871800
H	-6.35121000	-0.26429100	-3.68945900
H	-7.48889100	1.09671400	-3.68198000
H	-6.24241000	0.98291600	-4.94304100
C	-2.00415500	3.17568900	-3.22610000
H	-1.72646800	4.16216300	-2.83399000

H	-1.18712300	2.49136400	-2.97218700
H	-2.07574800	3.24947200	-4.31729300
O	-7.92621700	-0.60654700	-0.69720000
C	-9.02472600	-1.04246900	-1.55988600
H	-9.37381700	-2.04349500	-1.27478200
H	-9.81992900	-0.31308600	-1.39869800
H	-8.71690800	-1.03421700	-2.61351600

TS2_S

B3LYP-D3 SCF energy: -3525.24125010 a.u.
B3LYP-D3 enthalpy: -3524.063588 a.u.
B3LYP-D3 free energy: -3524.244436 a.u.
M06 SCF energy in solution: -3860.137868 a.u.
M06 enthalpy in solution: -3858.960205 a.u.
M06 free energy in solution: -3859.141054 a.u.
Imaginary frequency: -1252.6105 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	2.15144300	2.14046000	1.78714700
C	2.10565800	3.62321400	1.45507300
O	2.91282500	4.46644100	1.94064200
N	1.07186500	3.92869100	0.59063800
C	0.68067000	5.21603900	0.18926700
C	-0.46559500	5.24808900	-0.67120000
C	1.26907800	6.43880100	0.54958500
C	-1.00211600	6.47365200	-1.17500300
C	0.72024000	7.66047500	0.06586500
H	2.13704000	6.43593300	1.19530900
C	-2.07692800	3.96289700	-1.84257900
C	-2.11915900	6.38294400	-2.06195800
C	-0.38657300	7.69792200	-0.77889300
H	1.19633900	8.59025600	0.36794100
C	-2.64418600	5.14071500	-2.40099800
H	-2.54600300	7.29548700	-2.47155200
H	-0.78080400	8.64132700	-1.14764400
H	-3.48397400	5.04710900	-3.08129900
N	-1.03547600	4.03213400	-1.00891900
C	1.70886100	1.22835900	0.62010200
Pd	-0.04856000	2.45054400	-0.15366300
H	-2.46513800	2.97212800	-2.04565700
H	1.87406500	0.21397700	1.02886300
H	1.47388400	1.97797400	2.63860700
H	3.15619000	1.87992100	2.13430700
H	0.47387700	0.42415800	0.55124200

O	4.74051800	0.62838900	-2.85909200
C	4.63145600	0.21507800	-1.71096600
C	4.08222000	0.90095800	-0.44453900
O	5.03021100	-1.09554100	-1.32557500
C	4.72668400	-1.19929900	0.07861800
N	4.21190000	-0.13885200	0.61143200
C	5.00391000	-2.48996900	0.69579000
C	5.57216300	-3.54509700	-0.04680000
C	4.67179400	-2.69460100	2.05866900
C	5.80507100	-4.79399800	0.55018800
H	5.82796000	-3.38493700	-1.08940600
C	4.90020200	-3.93145300	2.66008700
H	4.23106500	-1.87674700	2.62080500
C	5.46670500	-4.98778200	1.90723300
H	6.23978200	-5.59363200	-0.03975700
H	4.65068600	-4.11405500	3.70031700
C	4.96662500	2.15611200	-0.14279400
H	4.86408400	2.82198700	-1.00883700
H	4.55236600	2.67833300	0.72255500
C	6.42563100	1.80630600	0.09175400
C	7.35968300	1.85325900	-0.96581800
C	6.86259200	1.39173200	1.36891200
C	8.70422200	1.49546000	-0.75189400
H	7.03267300	2.16389700	-1.95603000
C	8.20482400	1.03384100	1.58659600
H	6.14578800	1.34510200	2.18513000
C	9.13108100	1.08418400	0.52542200
H	9.41264600	1.53758700	-1.57603600
H	8.52750600	0.71789800	2.57607200
H	10.16991800	0.80853900	0.69277400
C	2.57250800	1.27546200	-0.66635800
H	2.14011100	0.56486700	-1.38401800
H	2.55115200	2.26363100	-1.13867300
C	-4.61632600	-1.86583600	0.15657100
C	-6.39191900	0.28835100	0.76742800
C	-5.03589500	0.45266900	1.00816800
C	-4.18746900	-0.65651900	0.70236000
H	-7.07915000	1.09319100	1.01615200
C	-1.71584800	-5.02568900	-0.60211900
C	-1.47531100	-3.74558000	-1.07931600
C	-2.46361000	-2.75546500	-0.79694100
C	-3.63749800	-2.97688800	-0.07573200
H	-0.99849200	-5.81429700	-0.81541600
C	-6.01477400	-1.97626700	-0.18889100
C	-6.90707100	-0.89686400	0.15830400
C	-8.29860600	-1.01067200	-0.15352600

C	-8.79250200	-2.12615800	-0.81457200
C	-7.90364700	-3.17343600	-1.20067000
C	-6.55152600	-3.10010600	-0.89430500
H	-8.96419200	-0.19656900	0.12540700
H	-9.85043900	-2.20131000	-1.05260800
H	-8.28992100	-4.03328800	-1.74198400
H	-5.88628700	-3.90039000	-1.19894200
C	-2.86222300	-5.32667400	0.19370600
C	-3.82495800	-4.29403100	0.49073900
C	-4.90297800	-4.61095900	1.37831400
C	-5.04693400	-5.88784100	1.90380200
C	-4.12028200	-6.91957300	1.56898400
C	-3.04778000	-6.63758500	0.73560400
H	-5.61065800	-3.83726800	1.65350200
H	-5.86981900	-6.10391400	2.58042000
H	-4.25053300	-7.91702700	1.98084500
H	-2.32053900	-7.40933400	0.49298000
P	-1.64856300	-0.27356900	-0.20181600
O	-2.81659700	-0.49535400	1.02834500
O	-2.19617900	-1.44813400	-1.31643900
O	-0.23765700	-0.58167500	0.53773100
O	-1.59062800	1.15653300	-0.94095800
C	-4.42144900	1.73376500	1.48257300
C	-3.74306800	1.79562300	2.72942400
C	-4.42699800	2.86481000	0.62428000
C	-3.04177400	2.96703200	3.07091900
C	-3.72975500	4.02621500	1.01348600
C	-3.00227500	4.08642300	2.21562400
H	-2.50442700	3.00184200	4.01751300
H	-3.73039300	4.88942300	0.35163300
C	-0.23594800	-3.38243000	-1.83707100
C	1.01437000	-3.32008000	-1.16852300
C	-0.32167100	-3.06918700	-3.21979900
C	2.16189900	-2.95639300	-1.90378800
C	0.84694000	-2.71058500	-3.91645900
C	2.10144000	-2.64428400	-3.27540200
H	3.12026700	-2.92162000	-1.39562200
H	0.77954800	-2.47599400	-4.97764400
C	-2.16508300	5.30152300	2.56574200
H	-1.09686500	5.08190500	2.43273200
H	-2.40387800	6.15774000	1.92397900
H	-2.30856600	5.60480800	3.61063600
C	-3.74838700	0.61775900	3.68626100
H	-4.73718600	0.14502700	3.73776900
H	-3.03777300	-0.14806900	3.35293100
H	-3.46625600	0.93091500	4.69769800

C	-5.11879600	2.83131900	-0.72934100
H	-4.95018800	3.76604500	-1.27389400
H	-4.74284600	2.00174800	-1.34364200
H	-6.20201300	2.69129700	-0.63752100
C	1.13889200	-3.58004700	0.32369100
H	0.75774500	-4.56820000	0.60708200
H	2.18444200	-3.51738600	0.64388600
H	0.56692500	-2.83016700	0.88452600
C	3.34513500	-2.23405300	-4.04194700
H	4.25763200	-2.48042100	-3.48969500
H	3.38599900	-2.72221500	-5.02428500
H	3.36804200	-1.14937400	-4.21201600
C	-1.65428600	-3.10521000	-3.94525100
H	-2.20856700	-4.02798600	-3.72957500
H	-2.28392000	-2.26478200	-3.62595400
H	-1.51628600	-3.03518300	-5.02991000
O	5.64800200	-6.17871700	2.60001200
C	6.22257100	-7.32169800	1.89744600
H	7.23608500	-7.09617100	1.53766700
H	6.26311500	-8.12292600	2.63757800
H	5.58821200	-7.62646100	1.05342600

12_S

B3LYP-D3 SCF energy: -3525.27891347 a.u.
B3LYP-D3 enthalpy: -3524.094706 a.u.
B3LYP-D3 free energy: -3524.279184 a.u.
M06 SCF energy in solution: -3860.171499 a.u.
M06 enthalpy in solution: -3858.987291 a.u.
M06 free energy in solution: -3859.17177 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.97437600	1.80575200	0.80806500
C	1.59233000	3.26559000	0.98241800
O	2.38560400	4.06677800	1.56393700
N	0.37979300	3.68687100	0.43517000
C	-0.05195700	5.03316600	0.47450700
C	-1.27147900	5.29264000	-0.23026700
C	0.55820300	6.13174900	1.10986800
C	-1.86170300	6.59218900	-0.32226500
C	-0.03620300	7.42404000	1.03974600
H	1.48282500	5.98103600	1.64696600
C	-3.00045100	4.33250100	-1.55380000
C	-3.06260000	6.71416500	-1.08519800
C	-1.21587000	7.67325500	0.34364600

H	0.46659700	8.24130500	1.55145200
C	-3.62218400	5.59904500	-1.70286800
H	-3.53227700	7.69040500	-1.17857200
H	-1.64521300	8.67039400	0.29660900
H	-4.53043300	5.67200500	-2.29103800
N	-1.87534700	4.21359200	-0.83911700
Pd	-0.98102600	2.48362200	-0.48338600
H	-3.40601700	3.42216000	-1.98031600
H	1.12953500	1.14683600	1.01879700
H	2.77379300	1.60177100	1.52480400
O	5.27929900	0.11132500	-2.75598600
C	5.17453200	0.13128200	-1.53435000
C	5.08789000	1.31916200	-0.55488200
O	5.07672400	-1.05040700	-0.75658300
C	4.94786900	-0.60701300	0.61510500
N	4.94687300	0.67571800	0.77839400
C	4.82500700	-1.66028900	1.61419700
C	4.89452800	-3.02114400	1.25294500
C	4.62106400	-1.30691200	2.97231800
C	4.76049500	-4.02538200	2.22435000
H	5.05256200	-3.28829300	0.21282600
C	4.48815300	-2.29830400	3.94391000
H	4.56667100	-0.25572200	3.23971700
C	4.55567900	-3.66244600	3.57336100
H	4.81494300	-5.06647700	1.92477200
H	4.32813300	-2.05401200	4.98912400
C	6.40088900	2.16108100	-0.61494500
H	6.43048400	2.64530500	-1.59894600
H	6.29667100	2.94239100	0.14698400
C	7.65599400	1.33849100	-0.38209400
C	8.40827500	0.84776300	-1.47165200
C	8.06754400	1.01707300	0.93048700
C	9.55052700	0.05422100	-1.25535500
H	8.09369100	1.07879900	-2.48730400
C	9.20836900	0.22464500	1.14992700
H	7.48371700	1.38030900	1.77273000
C	9.95455500	-0.25942200	0.05675700
H	10.11918200	-0.31804800	-2.10438700
H	9.51294800	-0.01566800	2.16600300
H	10.83714100	-0.87238600	0.22545000
C	3.85734000	2.19847900	-0.91628900
H	3.95001600	2.44042200	-1.98351200
H	3.93389700	3.13625500	-0.35242800
C	-4.20223500	-2.37336100	0.06566900
C	-6.25498000	-0.65039600	1.05629500
C	-4.93577700	-0.22720800	1.12854200

C	-3.94471300	-1.12441000	0.62638100
H	-7.04233900	-0.01375100	1.45254100
C	-0.82022600	-4.79938000	-1.21362800
C	-0.93422500	-3.49154500	-1.66162900
C	-2.06936500	-2.75043500	-1.22072300
C	-3.05807600	-3.23956800	-0.36433300
H	0.02370200	-5.39921900	-1.54548800
C	-5.58540200	-2.75592400	-0.08919700
C	-6.61132200	-1.89014700	0.44060700
C	-7.98381400	-2.27141300	0.30919100
C	-8.33961500	-3.44151400	-0.34647800
C	-7.32823600	-4.27683800	-0.90820100
C	-5.98669000	-3.94285100	-0.78074700
H	-8.74896600	-1.61799200	0.72294400
H	-9.38563900	-3.71986800	-0.44615400
H	-7.61311600	-5.17956600	-1.44254000
H	-5.22740100	-4.58221600	-1.21787300
C	-1.76063400	-5.36372500	-0.30024800
C	-2.87852400	-4.57570100	0.15846300
C	-3.73805100	-5.14065900	1.15524900
C	-3.53267700	-6.42753000	1.63348700
C	-2.45483500	-7.22197100	1.14089900
C	-1.58523700	-6.69324800	0.19822900
H	-4.55558800	-4.54905900	1.55084900
H	-4.19519500	-6.83330500	2.39382900
H	-2.31235700	-8.23180400	1.51718000
H	-0.74600700	-7.28033700	-0.16854000
P	-1.85581700	-0.09793500	-0.70618500
O	-2.59618500	-0.68712000	0.72747400
O	-2.16892200	-1.42025200	-1.73686300
O	-0.34232000	0.34055300	-0.29281400
O	-2.53434700	1.24548800	-1.34733000
C	2.49170400	1.52620500	-0.63192000
H	1.75027200	1.87813200	-1.35883500
H	2.54440400	0.44016100	-0.77786400
C	-4.51467600	1.11304200	1.64922600
C	-3.71413600	1.20451900	2.81997300
C	-4.83945500	2.28670000	0.92060800
C	-3.23570700	2.46311900	3.22863800
C	-4.35510700	3.53049600	1.37491200
C	-3.53407200	3.63902600	2.51164600
H	-2.60748300	2.52612100	4.11570200
H	-4.60715800	4.42964500	0.81703900
C	0.08775100	-2.86014300	-2.55458800
C	-0.20049300	-2.67936500	-3.93254600
C	1.32785200	-2.42891400	-2.02115800

C	0.77532500	-2.10360100	-4.76579700
C	2.28599800	-1.86666000	-2.89104300
C	2.03153800	-1.69913800	-4.26491500
H	0.55496300	-1.96641400	-5.82354000
H	3.24649900	-1.55947900	-2.48993900
C	3.08109600	-1.10338300	-5.18610700
H	3.91760400	-0.68225400	-4.62021800
H	3.48445300	-1.86810400	-5.86582600
H	2.65164900	-0.30910300	-5.81180400
C	-1.55304400	-3.07635600	-4.49521800
H	-1.81406800	-4.11020300	-4.23247300
H	-2.34004300	-2.42900800	-4.08582600
H	-1.57112600	-2.98632500	-5.58696900
C	1.61929300	-2.48422200	-0.53126600
H	1.03455400	-1.71528000	-0.00690400
H	1.36472500	-3.45239700	-0.08539800
H	2.67672700	-2.28772400	-0.33575300
C	-3.34845600	-0.03236000	3.61907500
H	-4.20285300	-0.71228200	3.72588000
H	-2.54997900	-0.58779700	3.11163300
H	-2.99545200	0.23496800	4.62124400
C	-2.95915100	4.97597500	2.94098100
H	-3.39500400	5.80453800	2.37090200
H	-3.13529900	5.16520300	4.00786400
H	-1.87264100	5.00308000	2.78074400
C	-5.62578700	2.22380400	-0.37806700
H	-6.61415500	1.76889000	-0.24903100
H	-5.77285400	3.22864400	-0.79108900
H	-5.08126900	1.62283000	-1.11834600
O	4.40695900	-4.56861000	4.61754900
C	4.44941200	-5.99652100	4.32134500
H	4.30653600	-6.49381300	5.28253100
H	3.64252100	-6.28142900	3.63178000
H	5.42071800	-6.28381700	3.89487500

TS1_R

B3LYP SCF energy: -3525.04925843 a.u.
B3LYP enthalpy: -3523.872201 a.u.
B3LYP free energy: -3524.062488 a.u.
M06 SCF energy in solution: -3860.131565 a.u.
M06 enthalpy in solution: -3858.954723 a.u.
M06 free energy in solution: -3859.144954 a.u.
Imaginary frequency: -363.9704 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	-2.86346500	2.48932200	-1.62589200
C	-3.05831600	3.74401400	-0.75766600
O	-3.96269800	4.58980700	-1.00277600
N	-2.13012900	3.86186000	0.26681700
C	-2.02292300	4.93787700	1.16656000
C	-0.91685900	4.85584700	2.08542200
C	-2.86375200	6.06061100	1.24712800
C	-0.67356900	5.87648500	3.06023000
C	-2.61513600	7.07301000	2.21628800
H	-3.69758200	6.14166200	0.56236300
C	0.95328500	3.59914100	2.82318900
C	0.44608500	5.69874000	3.93116800
C	-1.55135600	6.99989700	3.11101300
H	-3.28794500	7.92686200	2.24946200
C	1.25264000	4.57152700	3.81761300
H	0.65671500	6.45585700	4.68319300
H	-1.38094000	7.78233500	3.84623200
H	2.10570200	4.41643500	4.46999500
N	-0.08861200	3.74702800	1.99848500
C	-1.85633800	1.48287600	-1.05328200
Pd	-0.77717100	2.43461900	0.50881900
H	1.54758800	2.70014900	2.69306100
H	-1.04853100	1.20214600	-1.73280500
H	-2.52863600	2.84434400	-2.60919200
H	-3.85167700	2.03551200	-1.78231100
H	-0.86493600	-2.19172300	0.29190000
O	-1.85509900	-2.60737400	0.51406900
C	-2.88704200	-2.13543500	-0.11908400
C	-2.34176300	0.44283500	-0.17054300
H	-1.60104600	-0.13041300	0.37515200
H	-3.26240400	0.64222300	0.38052000
C	-3.02703500	-1.22973100	-1.22900900
O	-4.13780400	-2.37803700	0.41148100
N	-4.44193200	-1.03489400	-1.41394600
C	-5.06098900	-1.67126900	-0.45468600
C	-6.47448800	-1.77762500	-0.13569000
C	-6.92758100	-2.56514800	0.94471400
C	-7.42160600	-1.07675500	-0.92793900
C	-8.29767200	-2.66129000	1.23582400
H	-6.20702700	-3.10144200	1.55446800
C	-8.78379500	-1.16697000	-0.64355900
H	-7.07042900	-0.46780000	-1.75572600
C	-9.22931900	-1.96042800	0.43991100
H	-8.62208500	-3.27356300	2.07072800
H	-9.52273800	-0.63686600	-1.23600300

C	-2.12563500	-1.25154400	-2.45556100
H	-2.38358100	-0.37277500	-3.05766700
H	-1.08267200	-1.14455600	-2.14117600
C	-2.27233300	-2.52435500	-3.28586000
C	-3.44614600	-2.77375100	-4.03227700
C	-1.22854100	-3.47431100	-3.31771000
C	-3.57242000	-3.94953800	-4.79354900
H	-4.25641000	-2.04855600	-4.01037600
C	-1.35413100	-4.65291000	-4.07857200
H	-0.31935900	-3.28977600	-2.74851200
C	-2.52677400	-4.89438600	-4.81893500
H	-4.48019200	-4.12868600	-5.36555900
H	-0.54141100	-5.37564700	-4.09419100
H	-2.62461400	-5.80300200	-5.40874900
C	4.59345300	-0.36596500	-0.47028800
C	4.92508200	2.07721100	-1.89686600
C	3.67220900	1.47765100	-1.88351800
C	3.53832100	0.26437700	-1.13543400
H	5.07205500	2.98572700	-2.47617300
C	4.10460900	-4.17159300	1.57521700
C	3.24602200	-3.12274700	1.87641100
C	3.41669300	-1.91051300	1.13640800
C	4.40896100	-1.70682000	0.17581600
H	4.01973400	-5.10294300	2.13017700
C	5.86331800	0.32431400	-0.41580600
C	6.02435100	1.55063100	-1.15534100
C	7.28010900	2.23555600	-1.12198800
C	8.33474700	1.75286900	-0.36109000
C	8.16638300	0.56151600	0.40536900
C	6.96521200	-0.13451600	0.37596200
H	7.38919100	3.15280300	-1.69678200
H	9.28397900	2.28200300	-0.33566200
H	8.98631000	0.19851900	1.02010900
H	6.85279400	-1.03330100	0.97194300
C	5.08026600	-4.07511000	0.53784900
C	5.23280700	-2.83901500	-0.18789300
C	6.16823400	-2.80483900	-1.27192000
C	6.93225000	-3.91827400	-1.59545700
C	6.80711900	-5.12702900	-0.84847700
C	5.89500300	-5.19982600	0.19415600
H	6.26941300	-1.89821200	-1.85795700
H	7.62914300	-3.87200500	-2.42859600
H	7.41758200	-5.98819000	-1.10813700
H	5.77571800	-6.12196200	0.75897200
P	1.31363800	-0.41785500	0.30505700
O	2.26009200	-0.35295600	-1.14292400

O	2.53356300	-0.83935700	1.45007700
O	0.27662700	-1.59438400	-0.01001600
O	0.77689700	1.00120600	0.81519200
C	2.52306100	2.07720800	-2.64006500
C	1.96392400	3.31444900	-2.21921200
C	2.01988500	1.43358200	-3.80344200
C	0.91497800	3.88530700	-2.96882300
C	0.97395400	2.04120100	-4.52755500
C	0.41117900	3.27131700	-4.13202100
H	0.48070200	4.82567100	-2.63332200
H	0.59809000	1.54590800	-5.42147200
C	2.19406000	-3.25274200	2.93843600
C	1.05854800	-4.07702000	2.71843400
C	2.34623600	-2.56966200	4.17523700
C	0.09621300	-4.20426900	3.74142600
C	1.36791900	-2.73332400	5.17523300
C	0.23104500	-3.54228100	4.97658200
H	-0.78032900	-4.82398700	3.56143600
H	1.49446500	-2.21589900	6.12509800
C	0.84158900	-4.80703600	1.40248400
H	1.00466000	-4.14304600	0.54577300
H	1.52710900	-5.65810400	1.28999600
H	-0.18231500	-5.19027900	1.34049900
C	-0.83336900	-3.67034500	6.05184200
H	-1.34982500	-4.63592800	5.99173600
H	-0.40283700	-3.57643600	7.05641400
H	-1.59547200	-2.88427200	5.94672200
C	3.53985200	-1.66783500	4.43543700
H	4.48940100	-2.17610800	4.22198000
H	3.49719900	-0.77605400	3.79661900
H	3.55995600	-1.33772800	5.48019900
C	2.44953400	4.02837200	-0.96749700
H	2.51350800	3.34236200	-0.11478000
H	3.44717800	4.46568200	-1.10658600
H	1.76432000	4.83949600	-0.69843800
C	2.59069800	0.11224200	-4.28733800
H	3.68320700	0.15683700	-4.38883900
H	2.36219800	-0.69452600	-3.58005500
H	2.17126400	-0.15981400	-5.26209100
C	-0.68678400	3.92967800	-4.94862400
H	-1.28819700	3.18844600	-5.48900900
H	-1.36016900	4.52104100	-4.31611700
H	-0.26252200	4.61354800	-5.69821000
O	-10.60569400	-1.98139000	0.63660700
C	-11.15080800	-2.76817500	1.73686700
H	-12.23124000	-2.62274900	1.68469100

H	-10.91384900	-3.83413000	1.61715600
H	-10.77463800	-2.40951600	2.70465000

11_R

B3LYP-D3 SCF energy: -3525.27387237 a.u.
B3LYP-D3 enthalpy: -3524.091768 a.u.
B3LYP-D3 free energy: -3524.273549 a.u.
M06 SCF energy in solution: -3860.168369 a.u.
M06 enthalpy in solution: -3858.986265 a.u.
M06 free energy in solution: -3859.168045 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.65260400	-4.04963000	1.46405000
C	-0.05045700	-5.02674200	0.44863300
O	-0.03923000	-6.28039800	0.63295500
N	0.53064600	-4.37667200	-0.62388500
C	1.29122500	-4.96041600	-1.64124600
C	1.87283900	-4.03509800	-2.58747000
C	1.55360900	-6.33143400	-1.81642700
C	2.67913300	-4.49626600	-3.67945400
C	2.36091900	-6.77708800	-2.89875400
H	1.12652400	-7.03606300	-1.11512800
C	2.14021900	-1.78006700	-3.24933700
C	3.20968100	-3.51032800	-4.56933100
C	2.91768800	-5.89497600	-3.82184700
H	2.53933700	-7.84530500	-3.00090600
C	2.94056000	-2.16241400	-4.36225800
H	3.82494500	-3.83191000	-5.40683100
H	3.52776100	-6.25398100	-4.64714700
H	3.33116800	-1.39708000	-5.02539700
N	1.63739600	-2.68142800	-2.40098900
C	-0.92048200	-2.64427600	0.87078500
Pd	0.41085200	-2.39496700	-0.67572900
H	1.90853400	-0.73992100	-3.04051700
H	-0.71820400	-1.85987100	1.61039600
H	0.08765400	-3.96679100	2.27132200
H	-1.54365300	-4.52332000	1.89859700
H	-1.13929900	1.13906800	1.50458700
C	-3.43357600	-1.85088200	1.17402000
C	-2.32291100	-2.48807700	0.24138100
H	-2.28686600	-1.86091200	-0.66035200
H	-2.71325500	-3.46336100	-0.07697600
C	3.83797600	2.23260300	0.39155900
C	5.58188600	-0.00143200	0.62031400

C	4.24278700	-0.17165400	0.95243700
C	3.39495200	0.97215500	0.80493400
H	6.26591100	-0.83476000	0.75468000
C	1.20518200	5.69725400	0.33643300
C	0.81980300	4.53744800	-0.32034100
C	1.71848700	3.43150900	-0.25008900
C	2.93707800	3.43012600	0.42215900
H	0.56121000	6.57193900	0.29057400
C	5.20540200	2.35011700	-0.05820300
C	6.08434800	1.21801400	0.08143800
C	7.44776700	1.32870900	-0.33839300
C	7.92381100	2.50141400	-0.90605100
C	7.04444000	3.61184700	-1.08270800
C	5.72192100	3.53866600	-0.66741800
H	8.10300800	0.46901500	-0.21604300
H	8.95916100	2.57674200	-1.22844000
H	7.41513000	4.52071300	-1.54993100
H	5.06474500	4.38852400	-0.81508100
C	2.40729400	5.76260800	1.10408600
C	3.27914400	4.61598600	1.17573200
C	4.42676400	4.68978600	2.02816400
C	4.71740000	5.84694000	2.73796200
C	3.87676800	6.99465600	2.63115900
C	2.74288300	6.94675200	1.83331000
H	5.07179300	3.82428100	2.12736600
H	5.59060500	5.87942200	3.38451100
H	4.12171600	7.89647300	3.18637500
H	2.08281700	7.80847600	1.76146900
P	0.73247100	0.98738600	0.09249400
O	2.03487600	0.80218300	1.18779400
O	1.30895300	2.23266900	-0.91875400
O	-0.40147500	1.68875400	1.04932300
O	0.29455500	-0.24883200	-0.79344500
C	3.73781600	-1.49044800	1.45026200
C	3.18649100	-1.60761100	2.75514100
C	3.86801600	-2.64999900	0.63335400
C	2.76774700	-2.87450100	3.21073400
C	3.42262700	-3.89163500	1.12304500
C	2.87825900	-4.02990600	2.41424400
H	2.36171200	-2.96129000	4.21737500
H	3.49379900	-4.76844200	0.48191700
C	-0.48193600	4.42367800	-1.05063000
C	-1.70432900	4.44710600	-0.32731500
C	-0.49259700	4.27981000	-2.46278000
C	-2.91717500	4.32390500	-1.03449400
C	-1.72665300	4.17056800	-3.13274400

C	-2.95025200	4.18375700	-2.43548500
H	-3.85325300	4.33930400	-0.47706200
H	-1.73160200	4.06990800	-4.21678100
N	-4.70056000	-1.77854300	0.39320500
O	-3.93872600	0.39227700	0.64293300
C	-4.92746900	-0.54508200	0.08891300
C	-5.97928200	0.06826900	-0.70544300
C	-5.96387600	1.44861600	-0.99711400
C	-7.03165400	-0.74200700	-1.20523300
C	-6.98142300	2.02235400	-1.77487200
H	-5.15206200	2.06609800	-0.62538500
C	-8.04703400	-0.17742700	-1.97536300
H	-7.03142300	-1.80470200	-0.98133200
C	-8.02683800	1.20867100	-2.26261000
H	-6.94916000	3.08367200	-1.99258700
H	-8.86281300	-0.77480400	-2.36931700
C	-3.05815500	-0.38358000	1.37230800
O	-2.09925900	0.10889500	1.99207100
C	-3.61672000	-2.60692600	2.51231400
H	-3.92901100	-3.62613700	2.25746700
H	-2.63645700	-2.66362700	2.99588100
C	-4.62483500	-1.93680700	3.43068300
C	-4.19114900	-1.06293100	4.45170000
C	-6.01045500	-2.14340900	3.25182100
C	-5.12303100	-0.41181000	5.28192200
H	-3.12596000	-0.89130600	4.59275900
C	-6.94390300	-1.49466300	4.08003800
H	-6.35017900	-2.80521800	2.45880200
C	-6.50281400	-0.62648100	5.09886900
H	-4.77502300	0.25619800	6.06638400
H	-8.00804900	-1.66443700	3.93311300
H	-7.22407800	-0.12626400	5.74108300
C	0.80065800	4.24233200	-3.25619400
H	1.48297100	5.04776000	-2.95523800
H	1.32407200	3.29289100	-3.08726600
H	0.60849300	4.34086600	-4.33031200
C	-4.26823100	4.02352300	-3.17106800
H	-5.07043300	4.58816700	-2.67753700
H	-4.19510200	4.37357100	-4.20770300
H	-4.57641700	2.96915900	-3.19925300
C	-1.73239600	4.58009400	1.18577200
H	-1.02125000	3.88881500	1.64853100
H	-1.46633200	5.59516500	1.50917800
H	-2.73155700	4.35664400	1.57677300
C	3.07797200	-0.41662900	3.69161400
H	3.96928300	0.22186400	3.63890200

H	2.21919000	0.21106300	3.42787400
H	2.95907900	-0.74682200	4.72962700
C	2.45669200	-5.39149100	2.93476300
H	3.33601800	-6.02703500	3.11188400
H	1.91221800	-5.30805700	3.88299200
H	1.81292700	-5.91776300	2.22073300
C	4.48955000	-2.59762800	-0.75324400
H	5.58649500	-2.58976000	-0.69964500
H	4.19796200	-3.47434600	-1.33797100
H	4.18855600	-1.70295500	-1.30729600
O	-9.08063100	1.66879100	-3.04076600
C	-9.12844900	3.08353500	-3.39857400
H	-8.24342000	3.37380400	-3.98188700
H	-10.02617300	3.19440300	-4.00924900
H	-9.20753400	3.71536900	-2.50306300

TS2_R

B3LYP-D3 SCF energy: -3525.24133479 a.u.
B3LYP-D3 enthalpy: -3524.063585 a.u.
B3LYP-D3 free energy: -3524.244232 a.u.
M06 SCF energy in solution: -3860.135975 a.u.
M06 enthalpy in solution: -3858.958225 a.u.
M06 free energy in solution: -3859.138872 a.u.
Imaginary frequency: -1248.1068 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	2.34525700	-0.46635500	-1.93059300
C	3.00201400	-1.73821300	-1.42195100
O	4.08796300	-2.19026800	-1.88609300
N	2.26028800	-2.35512200	-0.43089600
C	2.54226100	-3.59708600	0.16063600
C	1.57215900	-4.03217100	1.12186900
C	3.63751500	-4.43736100	-0.09635100
C	1.70330500	-5.26975000	1.82592700
C	3.75476000	-5.68088000	0.58696600
H	4.38235200	-4.12657400	-0.81633700
C	-0.42710500	-3.49055500	2.27533500
C	0.70303900	-5.57749900	2.79933700
C	2.82163900	-6.10415800	1.53053800
H	4.61269200	-6.30966500	0.36108900
C	-0.34406800	-4.69217300	3.03029500
H	0.77747600	-6.50627500	3.36013000
H	2.93776400	-7.05087800	2.05166800
H	-1.10654300	-4.89814800	3.77391300

N	0.49599700	-3.19301600	1.35713400
C	1.52239700	0.29060200	-0.85768400
Pd	0.57828800	-1.49129800	0.21759000
H	-1.23713800	-2.78069300	2.39181100
H	1.14530100	1.17731100	-1.39868000
H	1.67243800	-0.75375600	-2.75277200
H	3.13459800	0.16437200	-2.34630800
H	0.04276100	0.38588200	-0.78640700
C	3.45703700	1.83520900	0.03564400
C	2.29995100	0.83365600	0.36684500
H	1.60111900	1.36084700	1.03103900
H	2.74301500	0.01047300	0.94030700
C	-5.49850600	-0.05749100	-0.18197900
C	-5.95625400	-2.87221100	-0.34559200
C	-4.71167500	-2.37756200	-0.70739500
C	-4.53202500	-0.96161200	-0.62002900
H	-6.15191500	-3.93806600	-0.43043000
C	-4.61590800	4.20517200	-0.22291400
C	-3.72967300	3.33074300	0.39020100
C	-4.07647400	1.94700900	0.37855800
C	-5.22187300	1.41486000	-0.21607800
H	-4.39962800	5.27057000	-0.21178300
C	-6.74537100	-0.60428300	0.30045200
C	-6.97822800	-2.02272400	0.17865600
C	-8.22299200	-2.56867200	0.62487300
C	-9.18996900	-1.75924300	1.20376900
C	-8.94228700	-0.36354800	1.36744100
C	-7.75228700	0.19844300	0.92515700
H	-8.39322000	-3.63763300	0.51579700
H	-10.13031300	-2.18389000	1.54575200
H	-9.69161600	0.26226900	1.84535400
H	-7.57481000	1.25979600	1.06036600
C	-5.78260700	3.74103900	-0.90060100
C	-6.08262100	2.33061300	-0.93198900
C	-7.19908200	1.89579700	-1.71634700
C	-8.00073100	2.80778100	-2.38914900
C	-7.73068000	4.20668700	-2.31389000
C	-6.63847000	4.65856600	-1.58813000
H	-7.41403200	0.83646500	-1.79513300
H	-8.83941200	2.45417800	-2.98345700
H	-8.37253700	4.90964200	-2.83858000
H	-6.40690600	5.72051600	-1.54412900
P	-2.13306900	0.12226900	0.06337800
O	-3.27857700	-0.46533200	-1.06194900
O	-3.16019600	1.07090000	1.04567500
O	-1.06068100	0.92962600	-0.85062400

O	-1.37141300	-0.95685200	0.98584500
C	-3.55130200	-3.23922600	-1.09950200
C	-2.96238300	-3.12122700	-2.38769900
C	-2.96966900	-4.10287000	-0.13371600
C	-1.77272000	-3.81979300	-2.66364200
C	-1.78361900	-4.79396500	-0.45494100
C	-1.15048400	-4.64016900	-1.70121000
H	-1.31218300	-3.70930800	-3.64439300
H	-1.33176000	-5.44344700	0.29155000
C	-2.45613900	3.80626900	1.01873700
C	-1.39565400	4.27918400	0.20000000
C	-2.31537700	3.79434600	2.42997000
C	-0.22487700	4.76433100	0.81557900
C	-1.12439600	4.28000600	3.00557000
C	-0.06730200	4.77487800	2.21665300
H	0.57531300	5.15561800	0.18863800
H	-1.02187500	4.27630200	4.08917000
N	4.55634500	1.12008500	-0.66263200
O	5.41261200	1.76412300	1.38487200
C	5.58083100	1.07305000	0.12384800
C	6.85347300	0.39545200	-0.08188700
C	7.97493500	0.69144900	0.71944900
C	6.95167100	-0.58817200	-1.10150300
C	9.19800200	0.03692300	0.50265600
H	7.88595400	1.43357100	1.50705600
C	8.16443700	-1.24339800	-1.31764100
H	6.07130000	-0.84705800	-1.68393300
C	9.29164400	-0.93079000	-0.52218700
H	10.05219600	0.28125400	1.12512900
H	8.26496800	-2.00615900	-2.08295400
C	4.09206900	2.27963700	1.36982500
O	3.61495500	2.91906700	2.30105200
C	2.96142700	3.06406600	-0.77609700
H	2.65419800	2.69684200	-1.76180700
H	2.07194900	3.45312800	-0.26781600
C	4.01549000	4.14548000	-0.92819800
C	4.01633500	5.27338900	-0.07898600
C	5.03380400	4.01996600	-1.89884500
C	5.01126800	6.26095100	-0.20058600
H	3.24909100	5.36850500	0.68499100
C	6.03029300	5.00486300	-2.02156400
H	5.04726500	3.14554500	-2.54513800
C	6.02116300	6.13036000	-1.17348500
H	5.00060400	7.12360100	0.46167900
H	6.81000300	4.89497600	-2.77179000
H	6.79094800	6.89290900	-1.26848700

C	-3.42653700	3.26528400	3.31825400
H	-4.39815900	3.70290000	3.05359000
H	-3.51892600	2.17744100	3.20595400
H	-3.22905000	3.48479900	4.37319300
C	1.21284500	5.28665000	2.84984100
H	1.06050200	5.55385300	3.90224900
H	2.00159900	4.52470100	2.81029000
H	1.58383300	6.17848000	2.32698300
C	-1.47667300	4.22316900	-1.31630700
H	-1.58216800	3.18286900	-1.64923400
H	-2.33124100	4.78578000	-1.71049900
H	-0.56626800	4.63312300	-1.76859100
C	-3.58278000	-2.24691600	-3.46212800
H	-4.67771300	-2.31499400	-3.45557800
H	-3.32062300	-1.19496200	-3.29708500
H	-3.22818200	-2.53729700	-4.45746100
C	0.17932000	-5.30697500	-1.99667500
H	0.15440000	-5.85328900	-2.94851300
H	0.97771100	-4.55611100	-2.07129500
H	0.46571700	-6.00985900	-1.20581200
C	-3.56556800	-4.25874700	1.25677100
H	-4.56331400	-4.71197000	1.22945800
H	-2.93071000	-4.89597300	1.87990000
H	-3.67332100	-3.28540900	1.75430000
O	10.44890500	-1.64324500	-0.82438500
C	11.65461600	-1.38820100	-0.04474400
H	11.49691000	-1.62180800	1.01769200
H	12.41266700	-2.05486900	-0.46049100
H	11.98123100	-0.34386500	-0.14896100

12_R

B3LYP-D3 SCF energy: -3525.27682215 a.u.
B3LYP-D3 enthalpy: -3524.092330a.u.
B3LYP-D3 free energy: -3524.276952 a.u.
M06 SCF energy in solution: -3860.171057 a.u.
M06 enthalpy in solution: -3858.986565 a.u.
M06 free energy in solution: -3859.171187 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.59095100	2.30764700	-1.12917200
C	-1.12644200	3.73158900	-0.87068600
O	-1.86452400	4.70462600	-1.21188400
N	0.09547400	3.91906700	-0.22436600
C	0.62575500	5.20630200	0.03426200

C	1.84444600	5.21307500	0.78550700
C	0.12129000	6.45984300	-0.36300500
C	2.54035400	6.41168000	1.14066000
C	0.81924600	7.65548900	-0.02891900
H	-0.80202200	6.50276500	-0.92112800
C	3.45438500	3.86130400	1.90120500
C	3.73206400	6.27339200	1.91508700
C	2.00146100	7.65659800	0.70614500
H	0.39590400	8.59925700	-0.36445800
C	4.18079100	5.01275000	2.29959200
H	4.28175400	7.16636700	2.20284800
H	2.51211100	8.58277200	0.95573500
H	5.07932000	4.88672100	2.89373300
N	2.34055400	3.98604300	1.16961000
Pd	1.30553100	2.44247600	0.48666500
H	3.76645000	2.85273600	2.14612400
H	-0.75605500	1.66138700	-1.41111400
H	-2.28923400	2.36888900	-1.96932100
C	-4.91570600	1.80012900	0.02056600
C	-6.13396100	2.68859100	0.43704700
H	-6.11220300	2.74955100	1.53194800
H	-5.94866600	3.69190500	0.03497400
C	-7.47045600	2.15526700	-0.04823400
C	-8.14707800	1.14551800	0.67128200
C	-8.03947200	2.63397500	-1.24869500
C	-9.36911300	0.62866700	0.20491300
H	-7.70551600	0.76011100	1.58733500
C	-9.26180600	2.11840100	-1.71860600
H	-7.51880400	3.39992200	-1.81926000
C	-9.93137100	1.11471700	-0.99240200
H	-9.87858400	-0.14943200	0.76887100
H	-9.68657800	2.49567000	-2.64592000
H	-10.87640900	0.71576700	-1.35421500
C	-3.59333700	2.43003200	0.53651400
H	-3.67584200	2.43533900	1.63102100
H	-3.56011600	3.47331300	0.19871600
C	4.05446300	-2.72902800	-0.30773000
C	6.31742700	-1.16492300	-1.08863200
C	5.05190900	-0.60875100	-1.19953400
C	3.95082300	-1.43576900	-0.81658800
H	7.18437900	-0.58614700	-1.39754500
C	0.38817500	-4.86469200	0.69369200
C	0.58625300	-3.57727000	1.16616900
C	1.81633500	-2.93814200	0.82985000
C	2.81099200	-3.49644200	0.02384400
H	-0.53193200	-5.38639300	0.94522500

C	5.38553600	-3.24967900	-0.09747000
C	6.51715000	-2.46598600	-0.53158600
C	7.83780300	-2.98604500	-0.35299500
C	8.04503000	-4.21204500	0.26295400
C	6.92989400	-4.96510300	0.73744900
C	5.63517500	-4.49611800	0.55997400
H	8.68273700	-2.39323100	-0.69686000
H	9.05276800	-4.59601500	0.39930300
H	7.09770600	-5.91178400	1.24463900
H	4.79703100	-5.07559900	0.93099300
C	1.33780200	-5.49786500	-0.16471700
C	2.54411700	-4.80145300	-0.54182200
C	3.40478400	-5.41959900	-1.50542700
C	3.11807100	-6.67538100	-2.02312300
C	1.95246600	-7.38406200	-1.60587500
C	1.07932200	-6.79894700	-0.70039000
H	4.28921700	-4.89275400	-1.84439900
H	3.78411700	-7.12174200	-2.75717500
H	1.74609000	-8.37115500	-2.01167600
H	0.17277800	-7.31673900	-0.39459500
P	1.89660700	-0.24655800	0.42774100
O	2.65811300	-0.86620400	-0.98018100
O	1.99972200	-1.64355000	1.40373100
O	0.48252600	0.40726500	-0.04525500
O	2.68469100	0.95831000	1.20388700
C	-2.29741700	1.69197100	0.11220800
H	-1.59175400	1.67556800	0.94950500
H	-2.50298500	0.63780100	-0.10216700
C	4.78824300	0.80966600	-1.60459600
C	4.04363600	1.09812300	-2.77992400
C	5.17706100	1.86524200	-0.73801000
C	3.66620700	2.42761100	-3.04615200
C	4.79970600	3.18572000	-1.05485900
C	4.01702900	3.48554800	-2.18399900
H	3.07414400	2.63923700	-3.93507300
H	5.09997300	3.99266700	-0.38989700
C	-0.44459700	-2.81812800	1.94189000
C	-0.30541400	-2.66774700	3.34710200
C	-1.50477900	-2.17881400	1.25491700
C	-1.25349700	-1.90636700	4.05274300
C	-2.43141300	-1.41685900	1.99717500
C	-2.32472900	-1.26904700	3.38916900
H	-1.14858600	-1.79386000	5.13097400
H	-3.23634000	-0.90753800	1.47990300
C	-3.33548400	-0.43008700	4.15116500
H	-4.07558400	0.00712600	3.47054700

H	-3.87106400	-1.03180100	4.89908600
H	-2.84210100	0.39058000	4.69067400
C	0.87726400	-3.28756200	4.06779800
H	0.98540400	-4.35355200	3.82832400
H	1.80807400	-2.79060600	3.76210200
H	0.77924300	-3.18835900	5.15456400
C	-1.62909600	-2.21614300	-0.25838500
H	-1.05394900	-1.38799300	-0.69597800
H	-1.25200100	-3.14786200	-0.69103300
H	-2.67238600	-2.09940800	-0.56731700
C	3.62499100	-0.00491000	-3.73385900
H	4.43429600	-0.72763700	-3.89687700
H	2.77097500	-0.55624900	-3.32217900
H	3.33101100	0.40543300	-4.70624500
C	3.52972100	4.89793100	-2.44680600
H	4.04057500	5.62724900	-1.80693100
H	3.68534900	5.19197800	-3.49263800
H	2.45306200	4.97942800	-2.24270800
C	5.91053100	1.59843400	0.56559900
H	6.85967200	1.07260900	0.41595300
H	6.12943200	2.53841000	1.08570700
H	5.29007400	0.97652300	1.22432400
N	-5.08212800	0.41780000	0.55253300
C	-4.92655300	1.61713400	-1.51117600
O	-4.84967200	2.42990100	-2.42117800
O	-5.09058500	0.21839100	-1.74819100
C	-5.18658300	-0.39394500	-0.45317500
C	-5.36405000	-1.84067700	-0.44458000
C	-5.49828300	-2.52534800	0.78983300
C	-5.37546000	-2.57353600	-1.64935800
C	-5.62785400	-3.91302300	0.81351700
H	-5.48908100	-1.95681600	1.71426000
C	-5.50518100	-3.97094700	-1.63474200
H	-5.27550200	-2.04529400	-2.59204300
C	-5.62740700	-4.64232100	-0.39850500
H	-5.72155900	-4.45872300	1.74665400
H	-5.50752100	-4.51575200	-2.57277100
O	-5.75376400	-6.02078300	-0.26238600
C	-5.76657900	-6.84738100	-1.46469700
H	-5.87250200	-7.87334700	-1.10714800
H	-6.61590200	-6.59032900	-2.11291300
H	-4.82757800	-6.74372200	-2.02631500

10’

B3LYP-D3 SCF energy: -2588.11121827 a.u.
B3LYP-D3 enthalpy: -2587.236527 a.u.
B3LYP-D3 free energy: -2587.376904 a.u.
M06 SCF energy in solution: -2923.284787 a.u.
M06 enthalpy in solution: -2922.410096 a.u.
M06 free energy in solution: -2922.550473 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	3.66100100	2.08152200	-2.97839200
C	4.80994300	1.43006700	-2.19047400
O	5.98571200	1.38744800	-2.64236200
N	4.43681900	0.99317700	-0.93256100
C	5.31885200	0.65044000	0.11175300
C	4.70227200	0.58364600	1.40516000
C	6.69799500	0.41653200	0.02570500
C	5.45370800	0.32161000	2.59106000
C	7.44421300	0.12884900	1.20543200
H	7.18611500	0.46996200	-0.93825200
C	2.68256000	0.81735200	2.63491600
C	4.74098000	0.32674200	3.83057900
C	6.85491300	0.08093100	2.46583700
H	8.51139200	-0.05251600	1.10453100
C	3.37370600	0.58364800	3.85542500
H	5.28306700	0.13262600	4.75310300
H	7.44440000	-0.13298300	3.35348300
H	2.81694600	0.59851100	4.78602500
N	3.33565100	0.80443500	1.46986900
Pd	2.51630100	0.89494800	-0.41084900
H	1.61251500	0.98829900	2.58150000
H	3.83963000	1.90706500	-4.04655600
H	3.74917900	3.16350900	-2.81474600
C	1.95059700	0.25446400	-2.51946400
H	2.69281700	-0.50940900	-2.72954500
H	0.92185100	-0.08541000	-2.47397700
C	-2.68075900	-1.90057400	0.19767200
C	-0.83011300	-3.99290500	0.73653500
C	-0.41478900	-2.90749100	-0.02209600
C	-1.37080300	-1.87795600	-0.28951100
H	-0.12931800	-4.80187200	0.93086800
C	-5.42710900	1.37604000	-0.56378900
C	-4.17204300	1.63879000	-0.03266200
C	-3.29514400	0.52736000	0.15077800
C	-3.63387100	-0.79579600	-0.13312000
H	-6.12738900	2.19689600	-0.69930900
C	-3.06793500	-2.98622700	1.06800100

C	-2.13573700	-4.05875900	1.30584800
C	-2.51729800	-5.15408900	2.14315900
C	-3.76187200	-5.18175600	2.75547200
C	-4.67081400	-4.09902600	2.55969000
C	-4.33298200	-3.03171300	1.73880500
H	-1.80630900	-5.96228300	2.30217100
H	-4.04408800	-6.01518800	3.39385000
H	-5.63496500	-4.11031500	3.06187200
H	-5.03228700	-2.21381000	1.60782800
C	-5.81428300	0.06130000	-0.96272200
C	-4.90857700	-1.04264400	-0.76412400
C	-5.29909300	-2.33465000	-1.24182300
C	-6.53108400	-2.52977700	-1.85139700
C	-7.44128700	-1.44245500	-2.01258700
C	-7.08362200	-0.17381000	-1.57918000
H	-4.61351700	-3.16819700	-1.13475100
H	-6.80512000	-3.51740800	-2.21395800
H	-8.40539200	-1.61147800	-2.48561000
H	-7.76137400	0.66642700	-1.71438700
P	-0.71373500	0.79403600	-0.48387700
O	-0.95782200	-0.81888200	-1.12793500
O	-2.00090700	0.80611000	0.67399600
O	-0.78576700	1.81887800	-1.68455800
O	0.63165700	0.76197300	0.43924900
C	2.26750900	1.60574500	-2.58835100
H	1.45044100	2.32592400	-2.55121200
C	1.00203800	-2.81620600	-0.49975900
C	2.03001200	-2.52687300	0.43551700
C	1.32656500	-3.05574000	-1.85760900
C	3.36520700	-2.46100500	-0.00886400
C	2.67740300	-3.01000000	-2.26012800
C	3.71029300	-2.69252000	-1.35478500
H	4.15033200	-2.21995200	0.70540900
H	2.92412000	-3.20565400	-3.30257800
C	-3.74649200	3.02187700	0.34981500
C	-3.47858100	3.99214500	-0.65066200
C	-3.60784600	3.35395800	1.72261600
C	-3.09939900	5.29071800	-0.25378000
C	-3.22876200	4.66261500	2.07786700
C	-2.97603400	5.64807500	1.10278900
H	-2.88428600	6.03277000	-1.02091600
H	-3.12668300	4.91605300	3.13204800
C	-3.84241000	2.31291600	2.80220100
H	-4.79557100	1.78769100	2.65741100
H	-3.04798100	1.55584500	2.77670900
H	-3.85160600	2.76942100	3.79841500

C	-2.60068600	7.06328600	1.50476800
H	-3.49718000	7.68979700	1.62240500
H	-2.06212600	7.07964100	2.46041000
H	-1.96526100	7.53963500	0.74807300
C	-3.52304400	3.63974300	-2.12708700
H	-2.74011200	2.90509400	-2.35500000
H	-4.48487700	3.20393100	-2.42180900
H	-3.34913200	4.52780300	-2.74555900
C	0.23107500	-3.33521000	-2.86821900
H	-0.41221800	-4.16339700	-2.54344300
H	-0.41564600	-2.45500000	-2.98055800
H	0.64625200	-3.58791700	-3.85004500
C	5.14556700	-2.54166400	-1.82142900
H	5.85591100	-2.78557100	-1.02247100
H	5.36228200	-3.18410500	-2.68322500
H	5.34876900	-1.50403400	-2.12374000
C	1.70128700	-2.24856200	1.88989100
H	1.21568900	-3.10490900	2.37175400
H	2.60604100	-2.00880200	2.45816900
H	1.00925600	-1.40009000	1.96289100

TS1_S'

B3LYP-D3 SCF energy: -3525.26059020 a.u.
B3LYP-D3 enthalpy: -3524.080803 a.u.
B3LYP-D3 free energy: -3524.261174 a.u.
M06 SCF energy in solution: -3860.141796 a.u.
M06 enthalpy in solution: -3858.962009 a.u.
M06 free energy in solution: -3859.142379 a.u.
Imaginary frequency: -313.2726 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	-2.06544400	-2.30985000	2.23041600
C	-0.93795500	-2.83470500	3.12612900
O	-0.98796800	-3.97704400	3.66597100
N	0.10609900	-1.93540900	3.27040200
C	1.28664800	-2.15561300	4.00246300
C	2.32654400	-1.18135700	3.79588600
C	1.54992500	-3.22596100	4.87212200
C	3.60605600	-1.30822400	4.42504600
C	2.81315500	-3.32958600	5.51982900
H	0.78624900	-3.97599600	5.02808700
C	3.01711000	0.75937300	2.62411700
C	4.59954900	-0.33364000	4.09966300
C	3.83132400	-2.40432800	5.30967600

H	2.97917500	-4.17078700	6.18877900
C	4.31530500	0.68398000	3.19776700
H	5.58509900	-0.41050400	4.55309500
H	4.79672700	-2.50882500	5.79846300
H	5.06122000	1.41739700	2.91508900
N	2.06676200	-0.13267100	2.92502000
Pd	0.15899600	-0.33840000	2.08604900
H	2.75497900	1.53392100	1.91464800
H	-2.84421000	-1.90411500	2.89223800
H	-2.50460800	-3.17302700	1.71792700
H	-1.76538000	0.92628200	-1.91232400
O	-2.76746400	1.36028300	-1.87415900
C	-3.69293600	0.72517700	-1.21838700
C	-3.73911300	-0.57959000	-0.62169000
O	-4.84028400	1.40813500	-0.87545000
C	-5.64151400	0.44768100	-0.13477600
N	-5.03491600	-0.70340700	-0.01041900
C	-6.93817300	0.89956100	0.33561000
C	-7.40730200	2.20157700	0.05840300
C	-7.75294000	0.01128300	1.08588700
C	-8.66663600	2.62057200	0.51621200
H	-6.78570600	2.88187300	-0.51558000
C	-9.00435700	0.42147900	1.54415800
H	-7.38704200	-0.98932200	1.29670900
C	-9.46778500	1.72826400	1.26171800
H	-9.00720500	3.62549900	0.29062000
H	-9.64391700	-0.23999000	2.11974100
C	-3.09093100	-1.79194300	-1.25830800
H	-2.05246700	-1.55748000	-1.50547700
H	-3.07555500	-2.59541600	-0.51825400
C	-3.82918500	-2.23809900	-2.51114000
C	-3.35299200	-1.86935200	-3.78716300
C	-5.00953000	-3.00525800	-2.41417800
C	-4.04212100	-2.26427800	-4.94890700
H	-2.44457200	-1.27646600	-3.86819800
C	-5.69870300	-3.40457300	-3.57381000
H	-5.38808500	-3.27466700	-1.43069400
C	-5.21642900	-3.03563300	-4.84594600
H	-3.66499900	-1.97384300	-5.92686700
H	-6.60598900	-3.99829500	-3.48786900
H	-5.74844300	-3.34443800	-5.74286800
C	-2.42043500	-0.09732000	0.98087600
H	-3.18995700	0.15763000	1.71143200
H	-1.97163600	0.75801000	0.48694100
C	3.96698800	1.18424700	-0.99992700
C	4.21999700	3.71662700	0.29420400

C	3.04242000	3.42341000	-0.37973400
C	2.94933400	2.13908700	-0.99840100
H	4.33560700	4.69352600	0.75701600
C	3.48997700	-2.72038400	-2.85669600
C	2.53850100	-2.26199300	-1.95806800
C	2.71739400	-0.94556100	-1.43983000
C	3.80271900	-0.11837900	-1.72267300
H	3.40004900	-3.72555900	-3.26174800
C	5.14950700	1.47211700	-0.22032700
C	5.27341200	2.76135800	0.41449500
C	6.44231700	3.05685800	1.18481800
C	7.43924700	2.10703600	1.35956600
C	7.29807000	0.81517700	0.77011700
C	6.18550000	0.50872600	-0.00162400
H	6.53100100	4.04006100	1.64170600
H	8.32285400	2.33873500	1.94869200
H	8.06826800	0.06496300	0.92913600
H	6.08995200	-0.47992700	-0.43538800
C	4.58005500	-1.89649300	-3.27649000
C	4.74260100	-0.57578800	-2.71799500
C	5.81437100	0.24005300	-3.20180600
C	6.69537000	-0.23378800	-4.16462800
C	6.55255200	-1.55187400	-4.69206900
C	5.51280300	-2.36114000	-4.25615400
H	5.92813300	1.24789900	-2.81699200
H	7.49818000	0.40443600	-4.52512200
H	7.25307900	-1.91174400	-5.44127300
H	5.38606000	-3.36174900	-4.66379800
P	0.66365600	0.77863400	-0.82597800
O	1.72361400	1.84515700	-1.66424800
O	1.74472800	-0.51895700	-0.51387900
O	-0.53079300	0.38705400	-1.81745500
O	0.29468100	1.28566100	0.66128800
C	-1.58143700	-1.23205400	1.25827600
H	-1.02841300	-1.64219200	0.40691600
C	1.92139400	4.40961400	-0.48936400
C	1.14144500	4.75313800	0.64554400
C	1.64673200	5.00464800	-1.75006800
C	0.10662900	5.70005500	0.49898500
C	0.60609100	5.94597700	-1.85282600
C	-0.18100000	6.30299300	-0.73953500
H	-0.49469900	5.95900500	1.36874600
H	0.40167900	6.40402200	-2.81914400
C	1.36837400	-3.07964900	-1.50543900
C	0.28154000	-3.31457400	-2.38705800
C	1.32695600	-3.57306000	-0.17473600

C	-0.81337600	-4.07699700	-1.93499200
C	0.20788300	-4.31890300	0.24614200
C	-0.86718600	-4.58864500	-0.62308500
H	-1.65038500	-4.24915200	-2.60863900
H	0.17140000	-4.68806700	1.26890500
C	2.44779600	-3.28376700	0.80541700
H	3.43246900	-3.50473500	0.37349500
H	2.44028700	-2.22318200	1.08166300
H	2.33180200	-3.86785600	1.72394200
C	-2.05407000	-5.41296800	-0.15956200
H	-2.99445000	-5.03845100	-0.58575000
H	-1.95195200	-6.45933300	-0.48086300
H	-2.13923600	-5.41386300	0.93346800
C	0.24650600	-2.68938200	-3.77136000
H	0.20883900	-1.59339400	-3.68922100
H	1.13521000	-2.93807600	-4.36258100
H	-0.63758900	-3.01929500	-4.32650700
C	2.45255500	4.63415800	-2.98206100
H	3.53239400	4.67007900	-2.78721000
H	2.21206500	3.61221000	-3.30155900
H	2.23389500	5.31126800	-3.81505300
C	1.33952200	4.07948600	1.99236000
H	0.98508600	3.04325500	1.93306100
H	2.38972200	4.06015300	2.30525200
H	0.76525200	4.59032300	2.77336100
C	-1.32668000	7.28801200	-0.88321100
H	-1.58256100	7.75127500	0.07719700
H	-1.08164500	8.08789800	-1.59324300
H	-2.22893600	6.78303900	-1.25753800
O	-10.72709500	2.03316400	1.76605600
C	-11.27966500	3.36208000	1.52529400
H	-11.40160100	3.55119200	0.44959200
H	-12.25632300	3.35973000	2.01272100
H	-10.64446500	4.14121500	1.96948900

TS1_R’

B3LYP-D3 SCF energy: -3525.25967131 a.u.
B3LYP-D3 enthalpy: -3524.080431 a.u.
B3LYP-D3 free energy: -3524.259844 a.u.
M06 SCF energy in solution: -3860.141582 a.u.
M06 enthalpy in solution: -3858.962342 a.u.
M06 free energy in solution: -3859.141754 a.u.
Imaginary frequency: -369.9956 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	2.79466800	-2.42249700	-0.90375300
C	1.87924200	-3.63394600	-1.14947000
O	2.27456500	-4.82055500	-0.96084600
N	0.61535700	-3.28561900	-1.59613700
C	-0.44450900	-4.16772800	-1.86793700
C	-1.72212200	-3.54059800	-2.10149300
C	-0.38428400	-5.57000600	-1.90224700
C	-2.90408900	-4.31336700	-2.33568200
C	-1.55841600	-6.33215100	-2.16171800
H	0.56225500	-6.05856100	-1.71344700
C	-2.95347900	-1.51627400	-2.15547800
C	-4.13699400	-3.60451000	-2.48464700
C	-2.79824800	-5.73568100	-2.37288000
H	-1.47246400	-7.41612000	-2.18130900
C	-4.16773300	-2.21812900	-2.38547400
H	-5.05165200	-4.16665100	-2.65877100
H	-3.68736400	-6.33467900	-2.55320100
H	-5.09315400	-1.65860600	-2.46972400
N	-1.78650100	-2.15752800	-2.03369800
Pd	0.08310100	-1.37861000	-1.50590000
H	-2.93274600	-0.43800400	-2.05480600
H	3.44166100	-2.33101500	-1.78890500
H	3.44627900	-2.66896800	-0.05833400
H	1.49463400	1.00512900	1.64637600
O	2.51990300	0.66546200	1.86907600
C	3.46072000	0.85663500	1.00661400
C	2.41399600	0.09744600	-1.34885700
H	3.11087100	-0.00021300	-2.18359400
H	1.65165900	0.85451100	-1.48989900
C	3.50433100	1.50008500	-0.28230800
O	4.65654300	0.20326900	1.20895800
N	4.85613000	1.34375400	-0.76342000
C	5.48683000	0.56502500	0.07457800
C	6.82565600	0.00699700	0.04141900
C	7.28714900	-0.85117000	1.06301900
C	7.68484200	0.32213900	-1.04406900
C	8.58152100	-1.39174100	1.01230900
H	6.63102400	-1.09493800	1.89279800
C	8.97211900	-0.21027400	-1.09963400
H	7.32415200	0.97983400	-1.82953100
C	9.42698800	-1.07088800	-0.07223700
H	8.91347700	-2.05170000	1.80655900
H	9.64627300	0.01523600	-1.91968500
C	2.73956600	2.77377300	-0.61862200
H	2.95215800	3.00183800	-1.67059200

H	1.66376800	2.59439500	-0.54238700
C	3.10185700	3.95059800	0.27501100
C	4.40454100	4.49549000	0.26292400
C	2.12674900	4.50820900	1.12886900
C	4.72581800	5.58749700	1.08859200
H	5.15712100	4.05975700	-0.39079400
C	2.44843600	5.60124100	1.95624000
H	1.12568000	4.08223300	1.14902200
C	3.74728900	6.14518300	1.93727300
H	5.73097100	6.00286800	1.07197500
H	1.69078300	6.02259700	2.61297800
H	3.99576000	6.98990500	2.57581000
C	-4.22872400	1.06599700	0.30302500
C	-4.54095900	2.45245200	-2.18244600
C	-3.39377500	2.67293700	-1.43504400
C	-3.28286500	1.95766700	-0.20004900
H	-4.68023100	2.98611400	-3.11906700
C	-3.41546700	-1.21250100	3.93134000
C	-2.48929700	-1.18470600	2.90254000
C	-2.80266600	-0.37997100	1.76637800
C	-3.97980200	0.34655800	1.59562700
H	-3.22347400	-1.82363200	4.80990200
C	-5.37840400	0.78861000	-0.52735800
C	-5.53145200	1.50626700	-1.77112500
C	-6.65831800	1.22453000	-2.60656800
C	-7.58752700	0.25622500	-2.25145200
C	-7.41878900	-0.47772500	-1.03964700
C	-6.34288100	-0.21728800	-0.20131100
H	-6.76846900	1.77748400	-3.53683800
H	-8.43821800	0.04844000	-2.89529200
H	-8.13695200	-1.24892400	-0.77334300
H	-6.21924600	-0.79422200	0.70793500
C	-4.61642000	-0.43564400	3.87027200
C	-4.90534000	0.36455400	2.70303600
C	-6.08528300	1.17404400	2.70728600
C	-6.95187300	1.17032600	3.79222500
C	-6.68319100	0.35328500	4.93040800
C	-5.53640800	-0.42810900	4.96495100
H	-6.29498900	1.80710300	1.85141400
H	-7.83981700	1.79736600	3.77872500
H	-7.37281500	0.35527200	5.77063900
H	-5.31516800	-1.04127500	5.83591500
P	-0.88733700	0.96378300	0.33670500
O	-2.08642600	2.17293400	0.54057100
O	-1.84560300	-0.40812300	0.73094700
O	0.27398300	1.37613700	1.34846700

O	-0.50274600	0.68195400	-1.20127400
C	2.00283000	-1.12680100	-0.68311800
H	1.64915600	-1.02650500	0.35126500
C	-2.24701000	3.54038700	-1.86023500
C	-1.42461400	3.15394300	-2.95203400
C	-1.89235600	4.67021000	-1.07139800
C	-0.24317200	3.88301800	-3.20721800
C	-0.70659100	5.36809200	-1.36015600
C	0.14697100	4.97534900	-2.41165800
H	0.39624800	3.57071700	-4.03102600
H	-0.43049700	6.22112500	-0.74226800
C	-1.19096100	-1.93231800	2.87517200
C	-1.07239000	-3.08394200	2.05469200
C	-0.05048600	-1.39660400	3.52434800
C	0.18557500	-3.69885800	1.91003500
C	1.19274000	-2.03840100	3.35545600
C	1.33098600	-3.19185400	2.55769900
H	0.27983200	-4.57358700	1.26977100
H	2.07321000	-1.61162600	3.83108100
C	-0.14069600	-0.11711500	4.33827400
H	-0.91586400	-0.17991000	5.11199200
H	0.81516000	0.10341100	4.82538600
H	-0.38851800	0.73736400	3.69471200
C	-2.27453800	-3.62388200	1.30259400
H	-3.12223000	-3.80968100	1.97494500
H	-2.61147500	-2.90102100	0.54935600
H	-2.03187300	-4.55729900	0.78441300
C	-2.75517200	5.11718600	0.09476700
H	-3.82343400	5.07864400	-0.15220000
H	-2.59427900	4.46224600	0.96005800
H	-2.51043200	6.14274000	0.39319100
C	-1.72876800	1.93585300	-3.80660600
H	-1.57935900	1.02562200	-3.21579300
H	-2.75617100	1.93099900	-4.18594100
H	-1.05287800	1.88788100	-4.66791000
C	2.67729200	-3.87790700	2.41313900
H	3.49584800	-3.14561900	2.41734600
H	2.85353700	-4.56622100	3.25260100
H	2.73489300	-4.46163800	1.48793300
C	1.45288600	5.70749000	-2.65673800
H	1.96657900	5.32909900	-3.54824800
H	1.28697400	6.78434800	-2.79374500
H	2.13016300	5.59261700	-1.79932400
O	10.72299300	-1.54698900	-0.22852000
C	11.26650100	-2.45615000	0.77583700
H	12.27642600	-2.69027300	0.43441700

H	11.31000500	-1.97487700	1.76280000
H	10.67184800	-3.37812000	0.83752100

TS2_S'

B3LYP-D3 SCF energy: -3525.23226876 a.u.
B3LYP-D3 enthalpy: -3524.054154 a.u.
B3LYP-D3 free energy: -3524.233814 a.u.
M06 SCF energy in solution: -3860.125862 a.u.
M06 enthalpy in solution: -3858.947747 a.u.
M06 free energy in solution: -3859.127407 a.u.
Imaginary frequency: -886.8473 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	3.31766300	-2.67321400	-1.23342400
C	4.21479500	-1.91699900	-2.18492900
O	5.28012800	-2.41105200	-2.65563800
N	3.78539900	-0.62537100	-2.41517200
C	4.50474900	0.35588800	-3.12011200
C	3.86801800	1.63747400	-3.18068900
C	5.76112800	0.21765900	-3.73511900
C	4.47744500	2.76105400	-3.82263600
C	6.36418700	1.33431600	-4.38029000
H	6.25734500	-0.74269800	-3.70794000
C	1.96396300	2.91092100	-2.57105500
C	3.75559400	3.99404100	-3.80676600
C	5.75462800	2.58543500	-4.43210200
H	7.33706300	1.19143000	-4.84486100
C	2.51501800	4.06934600	-3.18361800
H	4.18970500	4.86841100	-4.28621600
H	6.23357900	3.42569200	-4.92820200
H	1.94916500	4.99459500	-3.16021900
N	2.62517600	1.74817100	-2.58005400
C	1.80351500	-2.33482700	-1.26034400
Pd	1.98172400	-0.04487100	-1.77521200
H	1.00235100	2.91112300	-2.07742900
H	1.37205200	-2.58319500	-2.24195600
H	3.69560600	-2.46258000	-0.22527000
H	3.46794400	-3.74535900	-1.42468400
H	0.77985000	-1.35718000	-0.50602800
O	-0.76902200	-3.57493600	2.27610000
C	0.22966900	-2.87847100	2.14338900
C	1.48858900	-3.09217500	1.27273200
O	0.44971300	-1.69429900	2.89359500
C	1.68545100	-1.15525800	2.41031400

N	2.29085900	-1.86252500	1.51356500
C	2.11933300	0.10807600	2.99125400
C	1.53713600	0.60213100	4.17417200
C	3.16924900	0.82908100	2.36952100
C	2.00446300	1.79276000	4.75300100
H	0.72838700	0.04757800	4.63946800
C	3.63127800	2.01792700	2.93188800
H	3.60152200	0.44312900	1.45077400
C	3.05062600	2.50022300	4.12608700
H	1.54852100	2.15513200	5.66828800
H	4.42371200	2.59664600	2.46871600
C	2.25848800	-4.33664000	1.84825700
H	1.62053100	-5.21126100	1.66940800
H	3.16403700	-4.44693300	1.24075200
C	2.60781500	-4.22344400	3.32083900
C	1.76630300	-4.78693100	4.30462400
C	3.76042500	-3.51841300	3.73192900
C	2.07043000	-4.65124700	5.67179700
H	0.86797500	-5.31977000	3.99986900
C	4.06769900	-3.38115700	5.09726000
H	4.40384000	-3.06792800	2.98012600
C	3.22295900	-3.94796800	6.07247400
H	1.41190900	-5.08915100	6.41835700
H	4.95782300	-2.83392200	5.39893400
C	1.14213200	-3.33026100	-0.23692100
H	0.06196300	-3.34629600	-0.35132000
H	1.50022900	-4.33064600	-0.51822900
C	-4.10742500	1.26319800	0.09881500
C	-3.70974900	4.07012600	0.41562100
C	-2.63292900	3.21483900	0.59918500
C	-2.88012300	1.81667200	0.46326400
H	-3.56155800	5.14012400	0.54037300
C	-4.69852800	-2.93819600	-0.78830900
C	-3.61212900	-2.27389500	-1.34339600
C	-3.42820600	-0.91030600	-0.95013400
C	-4.27462200	-0.21210600	-0.08871000
H	-4.89862300	-3.96446400	-1.08262800
C	-5.19244400	2.17693300	-0.19119500
C	-4.99169600	3.58949700	0.01705300
C	-6.06535400	4.50101600	-0.23447500
C	-7.28596400	4.04818700	-0.71243200
C	-7.47077800	2.65778700	-0.97330600
C	-6.45267900	1.74865000	-0.72067500
H	-5.90104300	5.56180900	-0.05803800
H	-8.09614800	4.74657400	-0.90556500
H	-8.41720200	2.30871500	-1.37825300

H	-6.61145200	0.69911300	-0.93692400
C	-5.53974700	-2.32946000	0.18983500
C	-5.32068500	-0.95713700	0.56913600
C	-6.13209700	-0.39859800	1.60682500
C	-7.12987900	-1.14889900	2.21374500
C	-7.37200000	-2.49593100	1.80889500
C	-6.58850300	-3.07148400	0.81926000
H	-5.95162400	0.62148700	1.92851400
H	-7.72925800	-0.71127500	3.00796500
H	-8.16061000	-3.06952300	2.28906500
H	-6.75004700	-4.10464700	0.51972100
P	-0.97900500	0.18209400	-0.55031400
O	-1.77373800	0.95483900	0.74666000
O	-2.32171300	-0.22133500	-1.53150900
O	-0.21351800	-1.10743900	0.07746700
O	0.06586300	1.02154900	-1.43106700
C	-1.25696700	3.74109800	0.85714700
C	-0.65609800	3.60315000	2.13132900
C	-0.55894500	4.39182100	-0.19580700
C	0.62582800	4.14809500	2.34340200
C	0.72768100	4.90405600	0.05225500
C	1.33849900	4.79504700	1.31802400
H	1.07983300	4.05318900	3.32404200
H	1.27000200	5.39533400	-0.75388400
C	-2.64909300	-2.93491200	-2.27795600
C	-1.92181200	-4.08159900	-1.85005200
C	-2.42168100	-2.40163900	-3.57768600
C	-0.92977600	-4.61703000	-2.69628900
C	-1.42126900	-2.97046500	-4.38950600
C	-0.64167500	-4.05971300	-3.95595900
H	-0.35835200	-5.47809700	-2.35345700
H	-1.24284900	-2.54767200	-5.37688400
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TS2_R'

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B3LYP-D3 enthalpy: -3524.062128 a.u.
B3LYP-D3 free energy: -3524.238724 a.u.
M06 SCF energy in solution: -3860.134944 a.u.
M06 enthalpy in solution: -3858.95626 a.u.
M06 free energy in solution: -3859.132857 a.u.
Imaginary frequency: -502.2458 cm^{-1}

Cartesian coordinates

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[8] CCDC 1825332 of **8** contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

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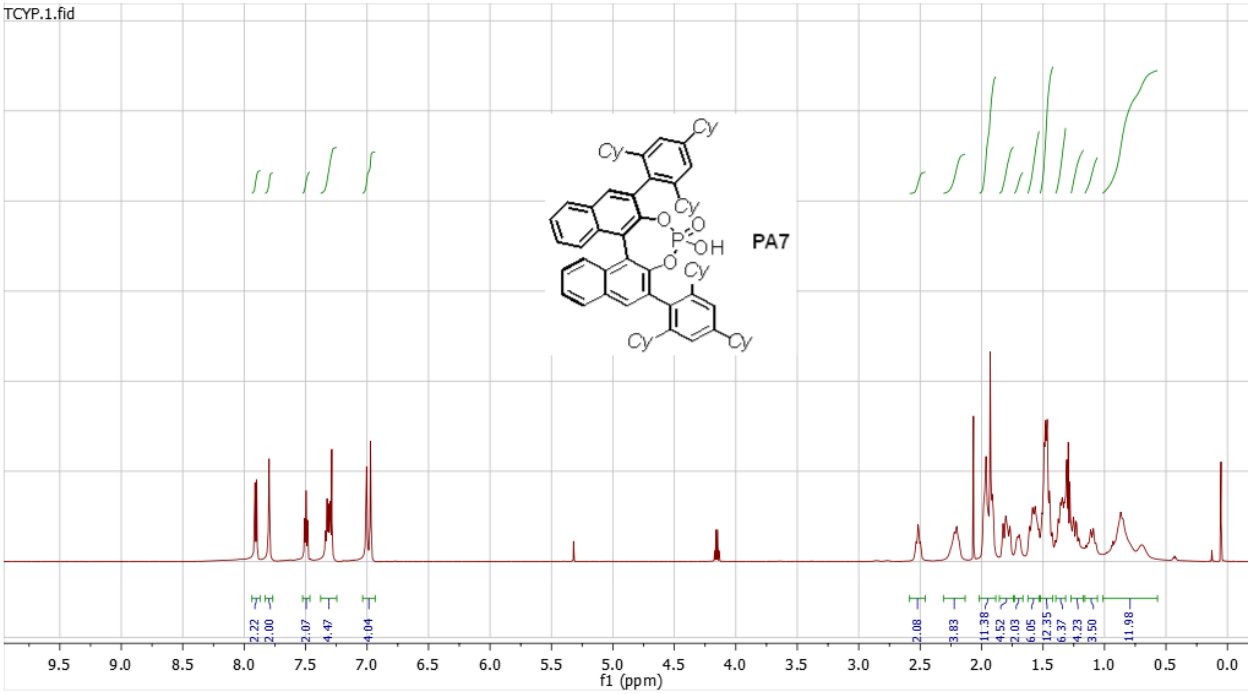

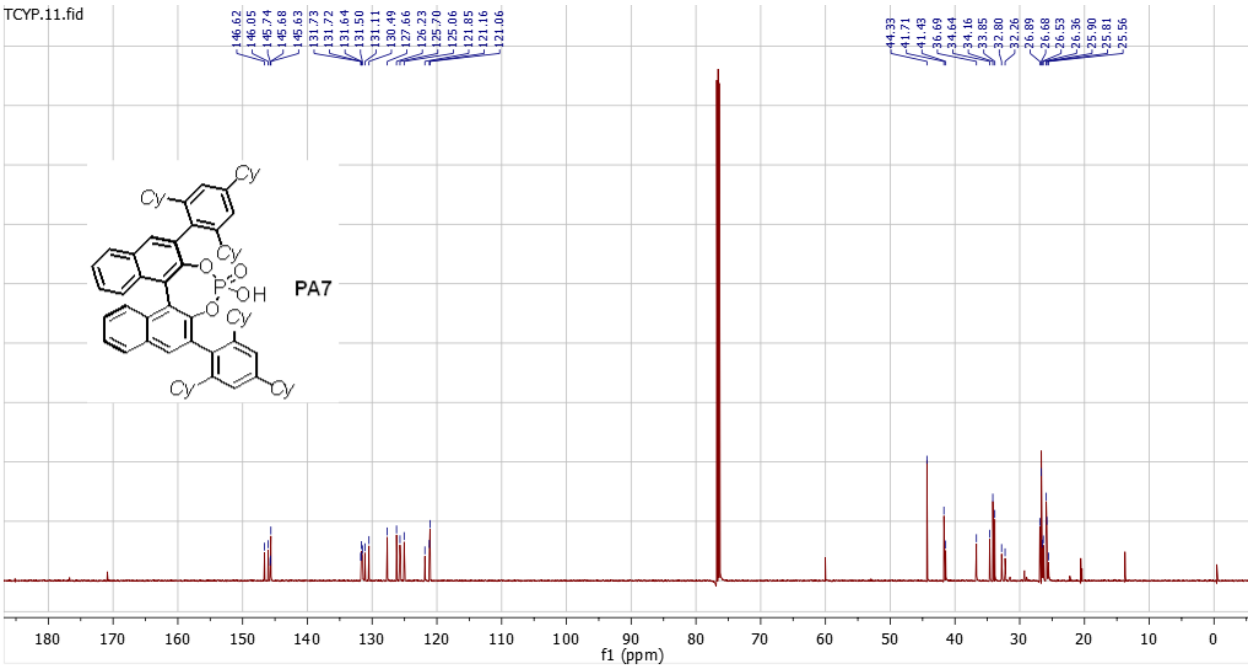

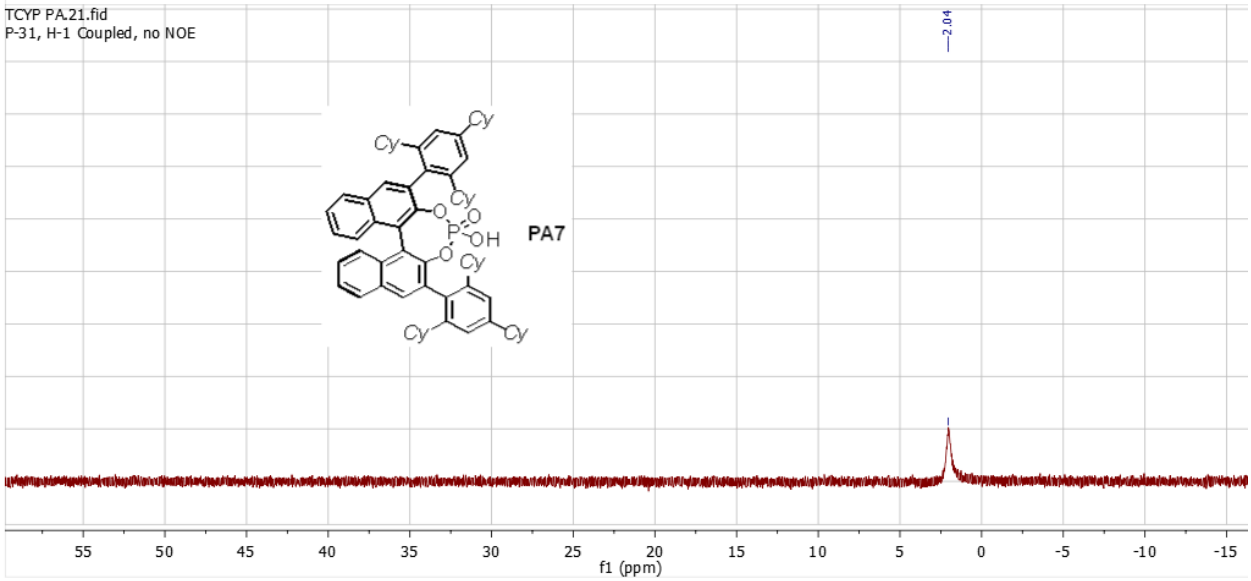
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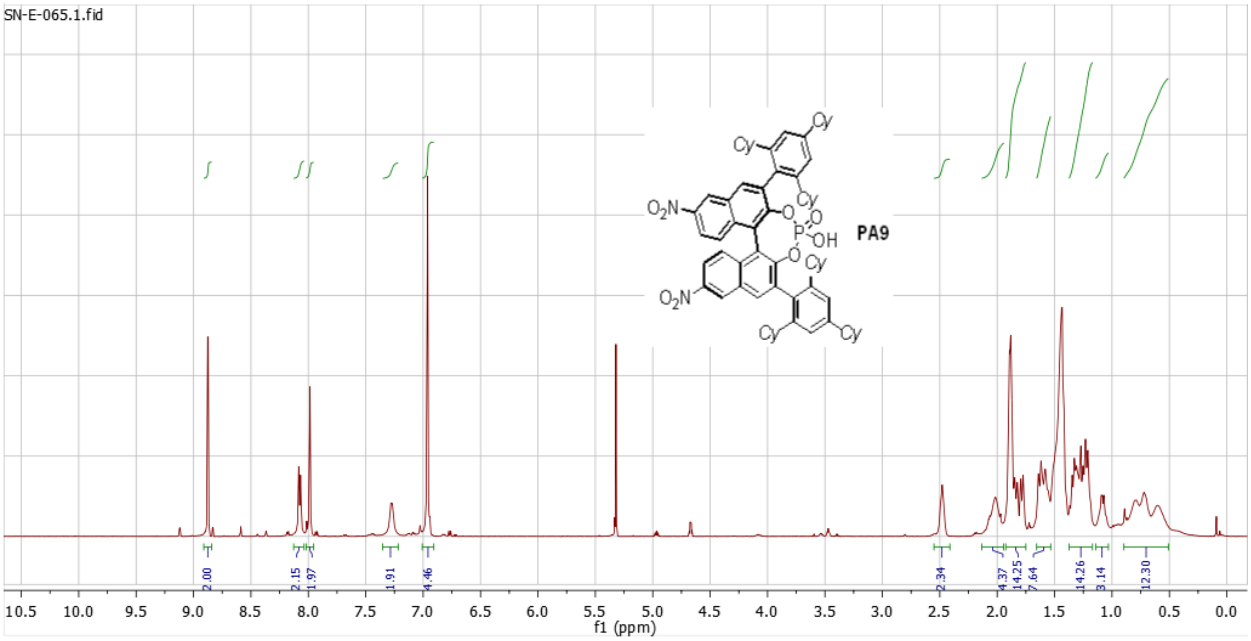
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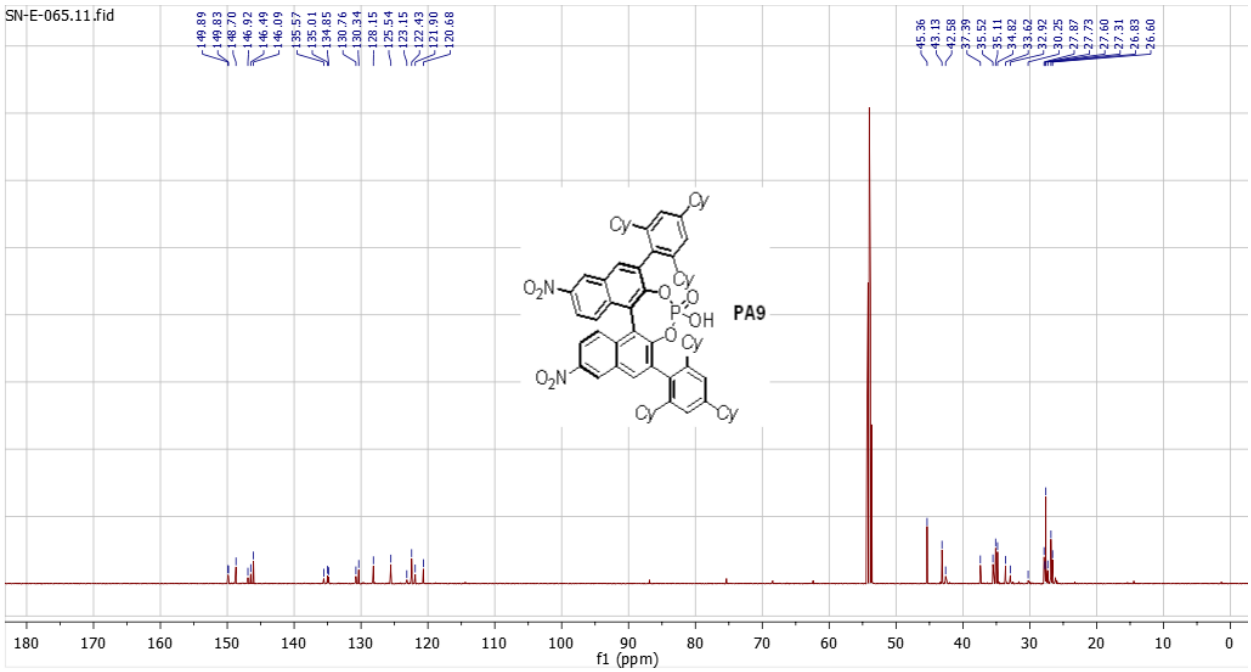
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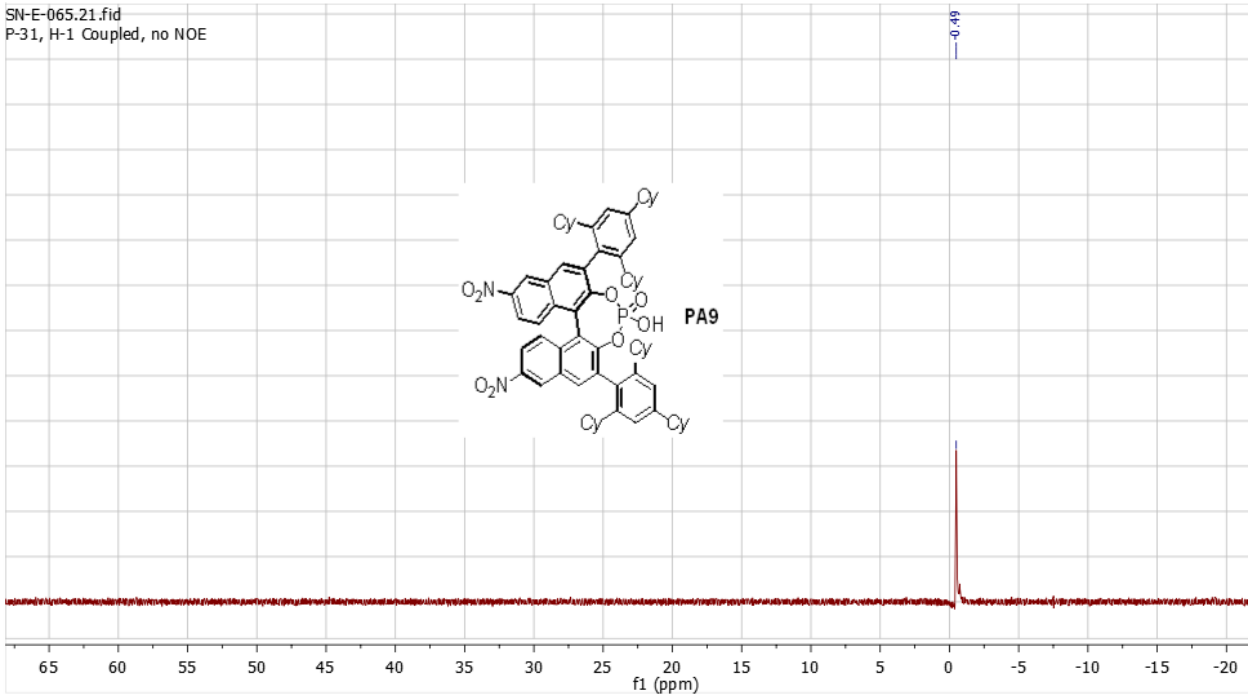
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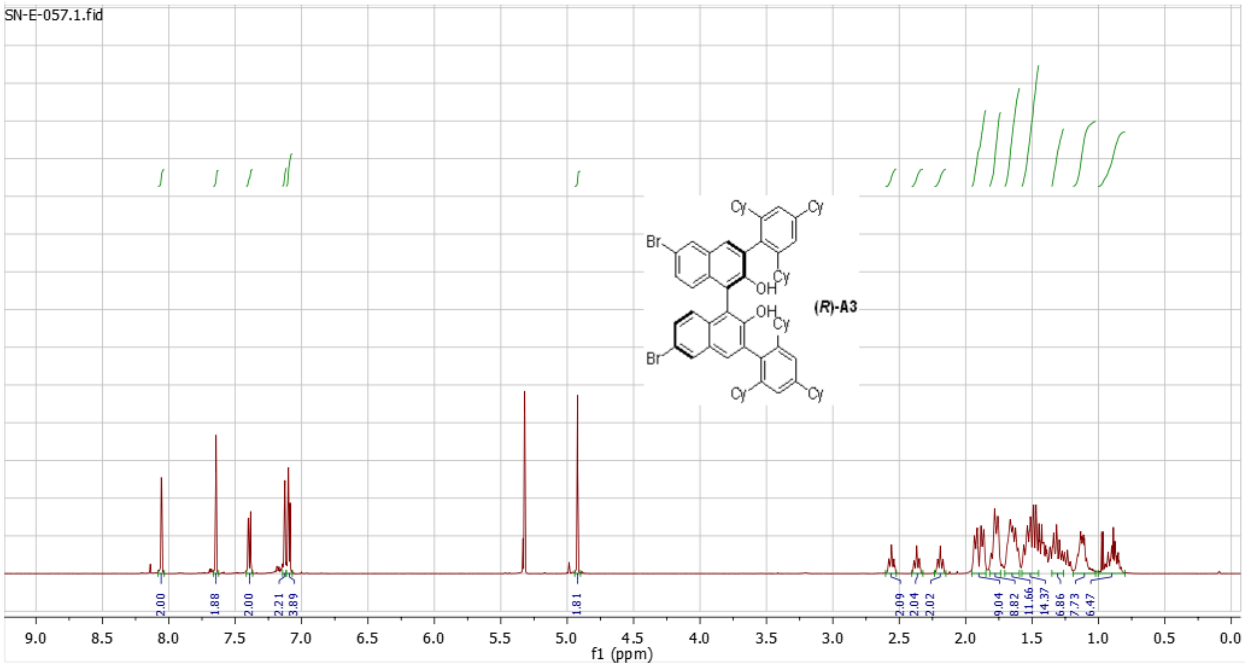
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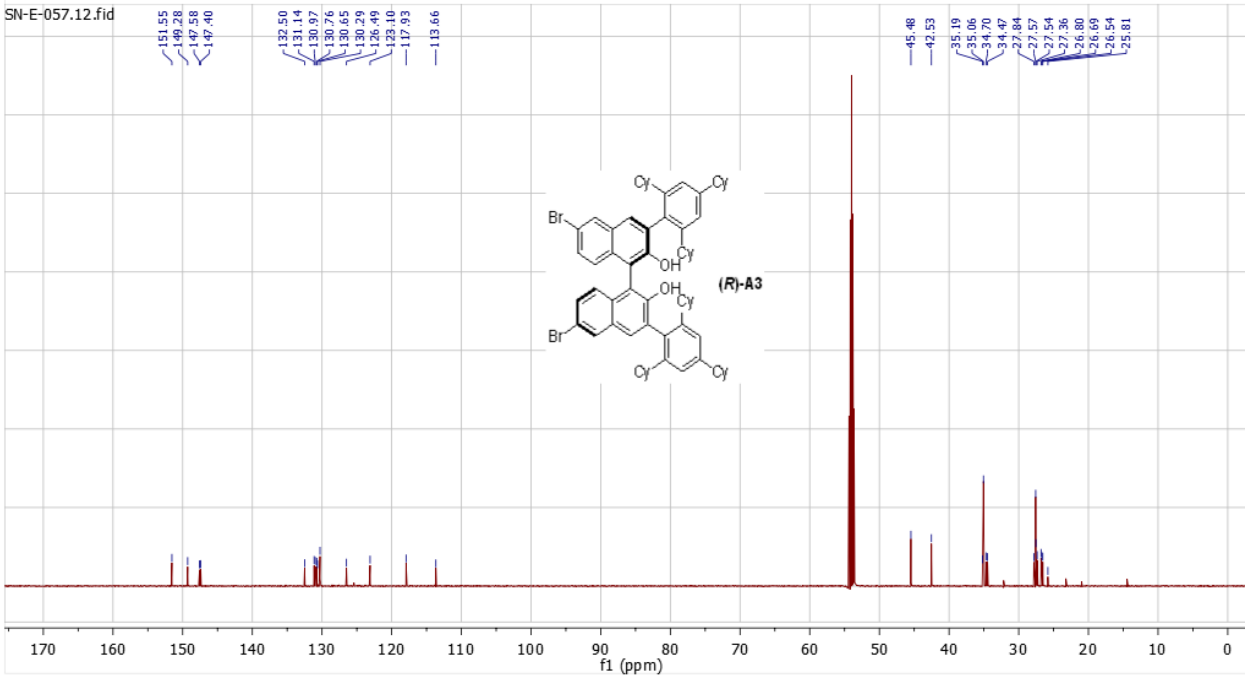
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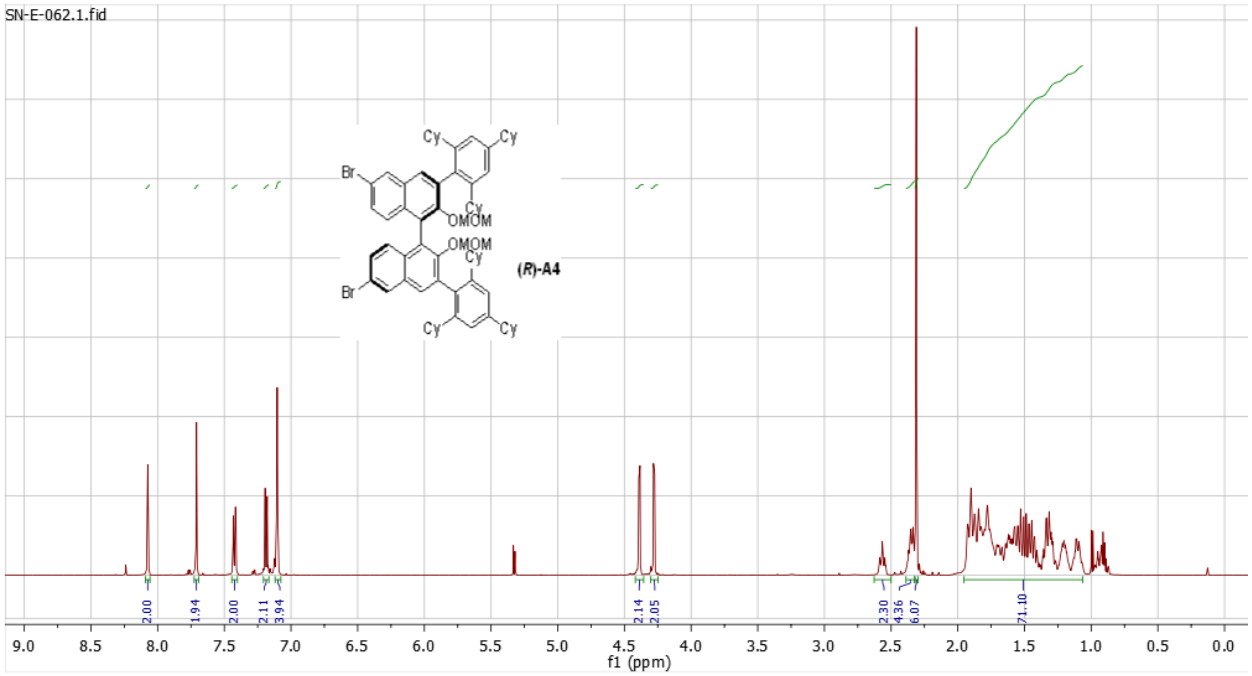
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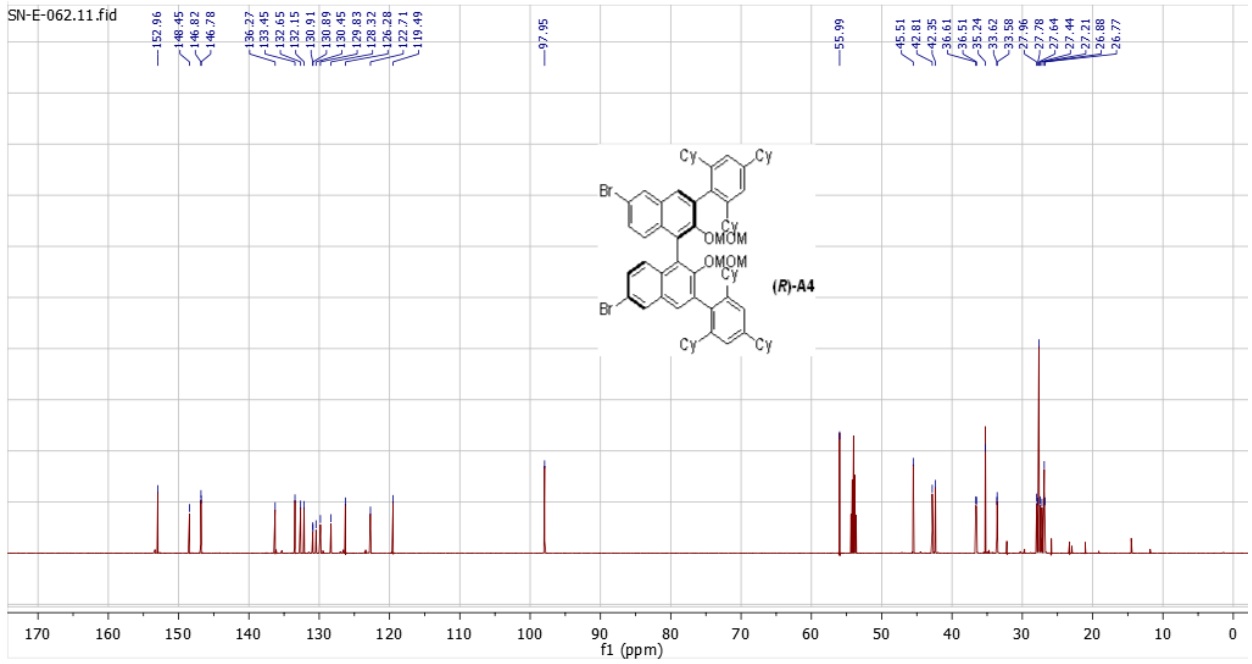
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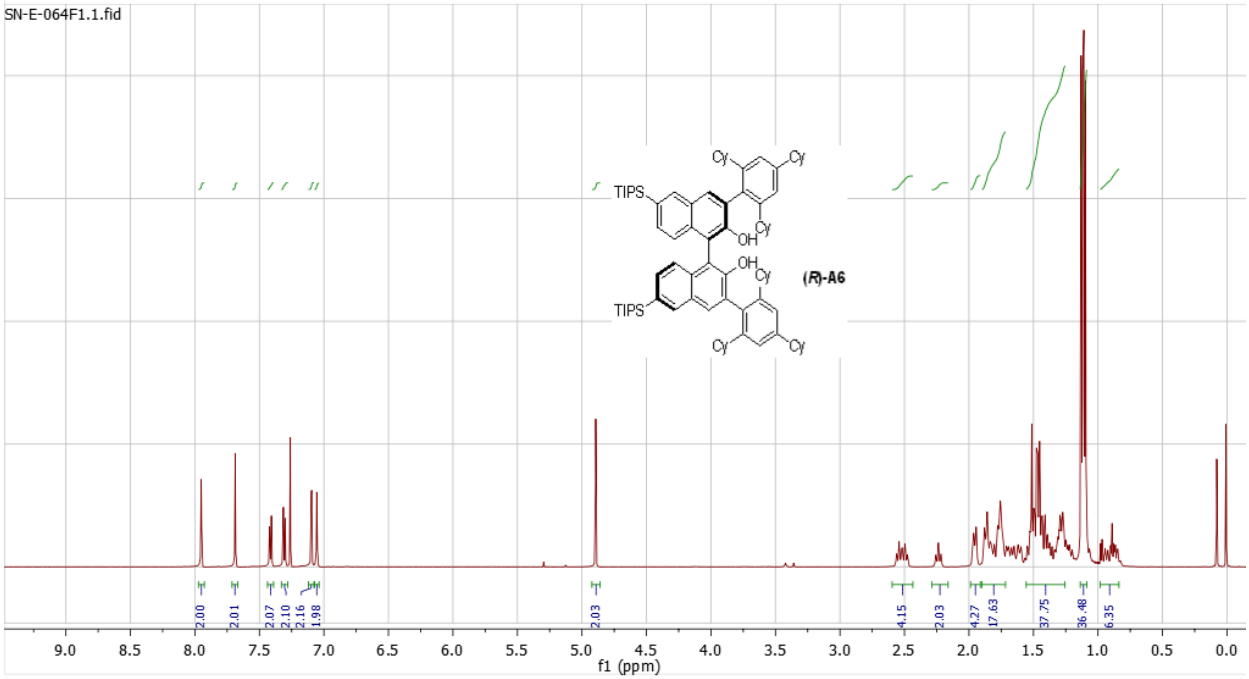
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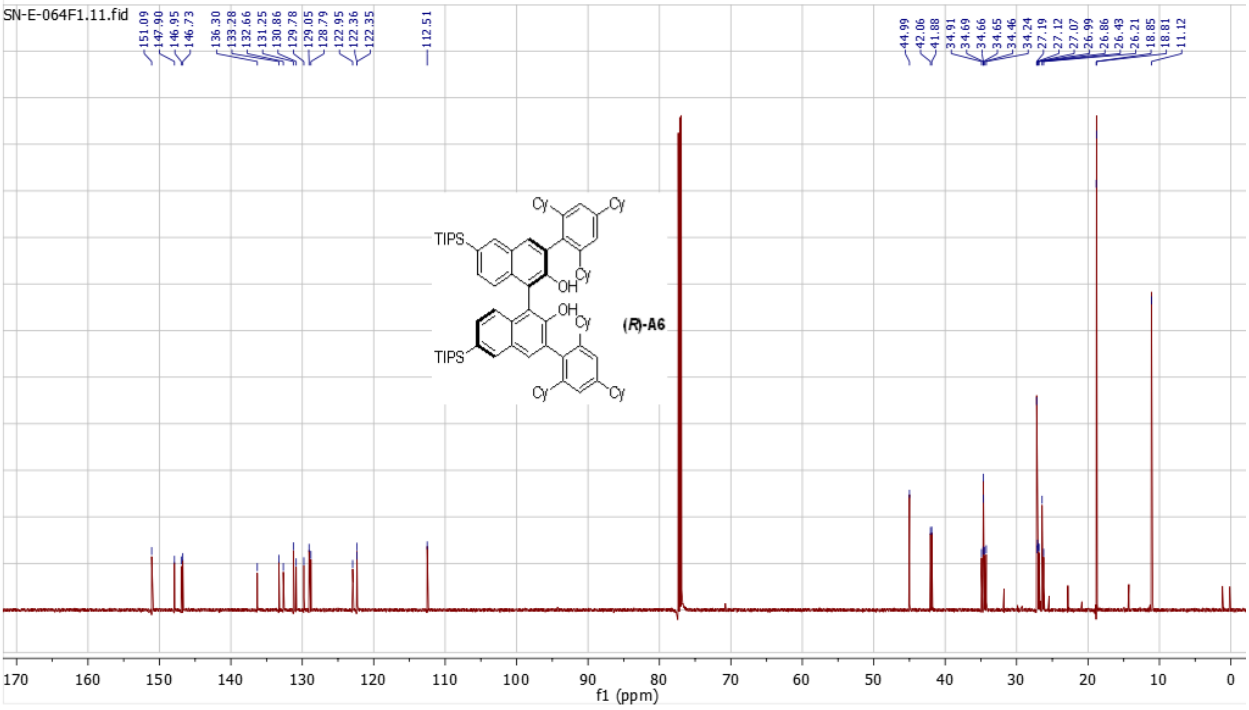
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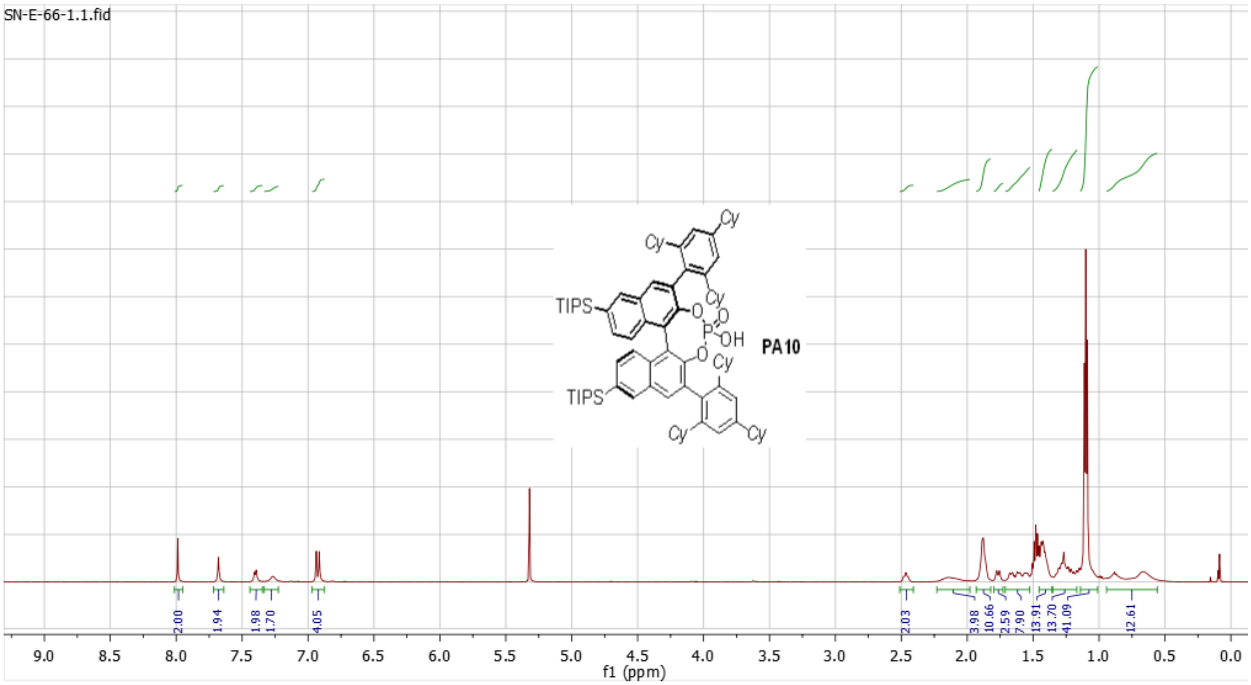
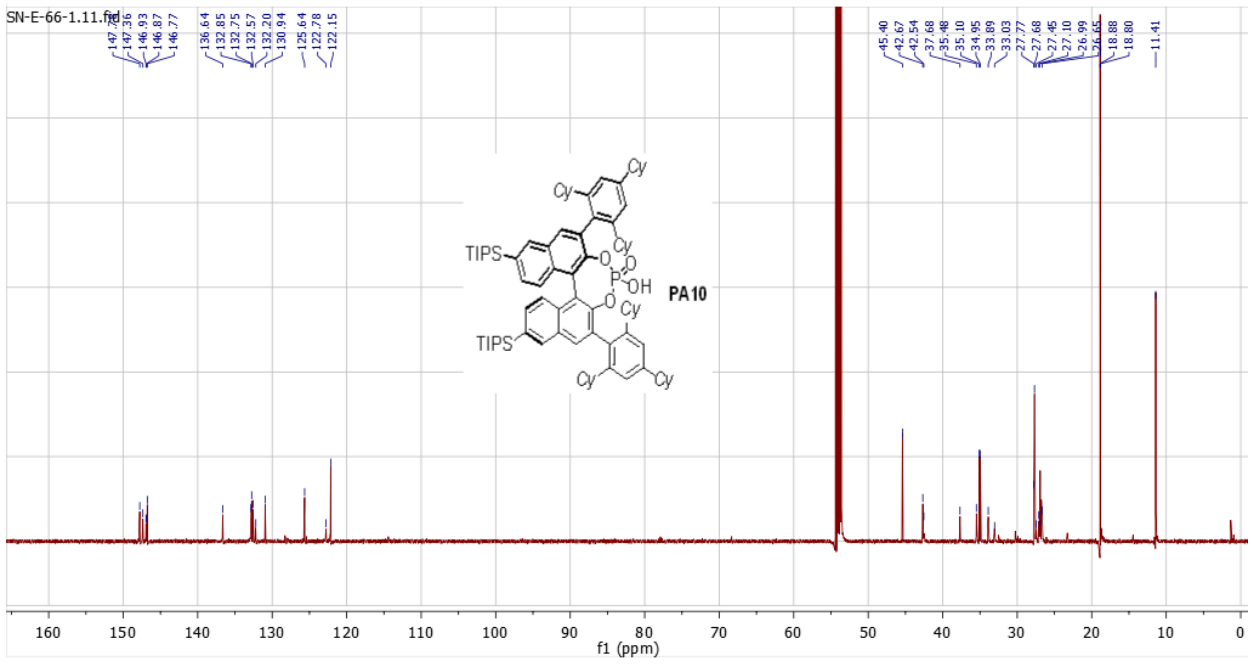
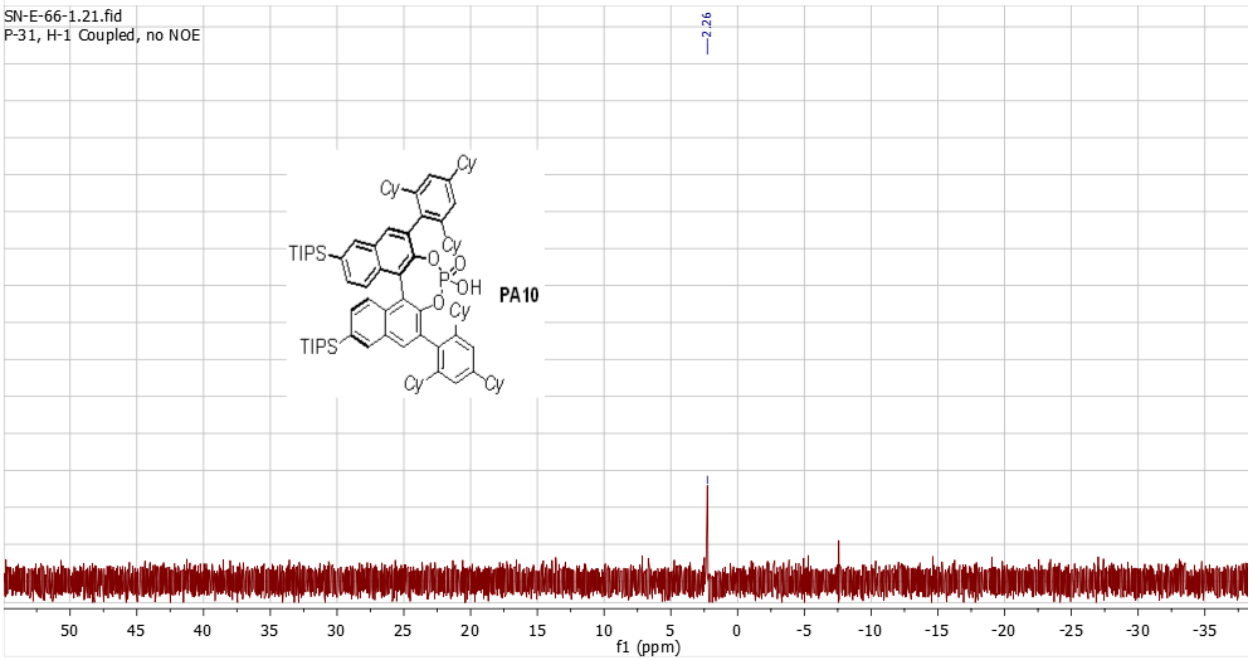
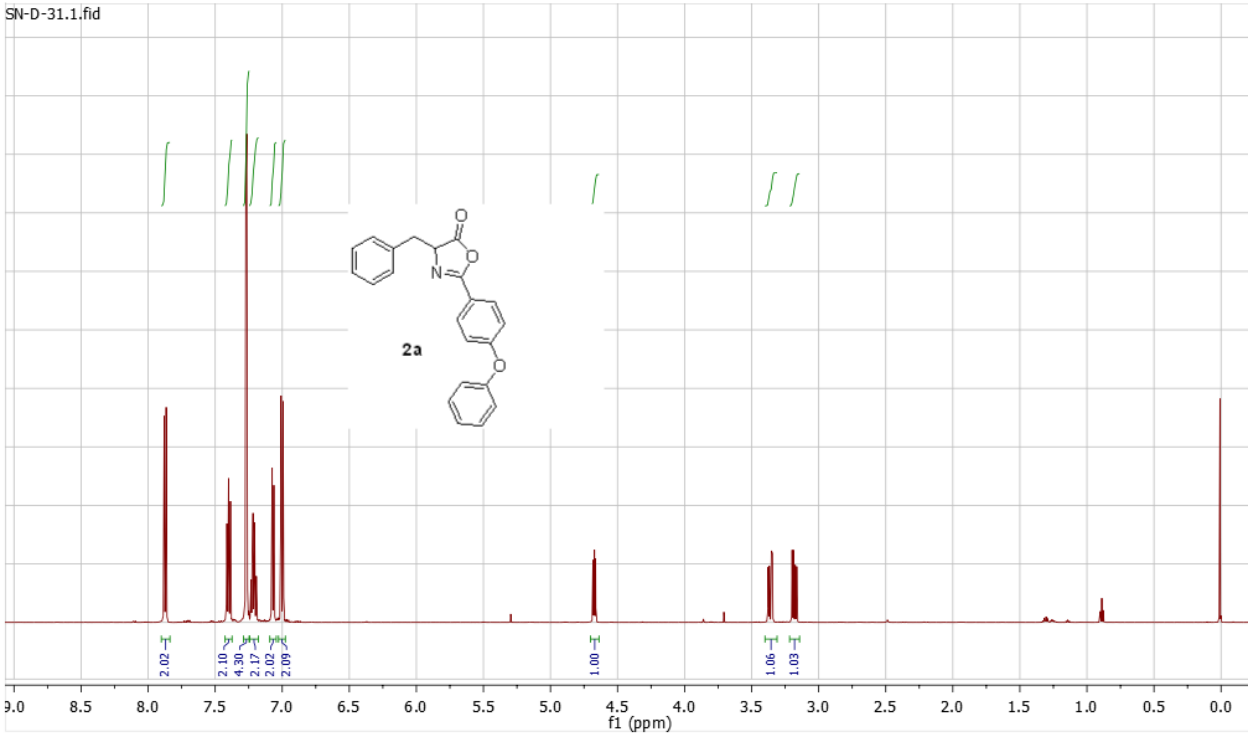
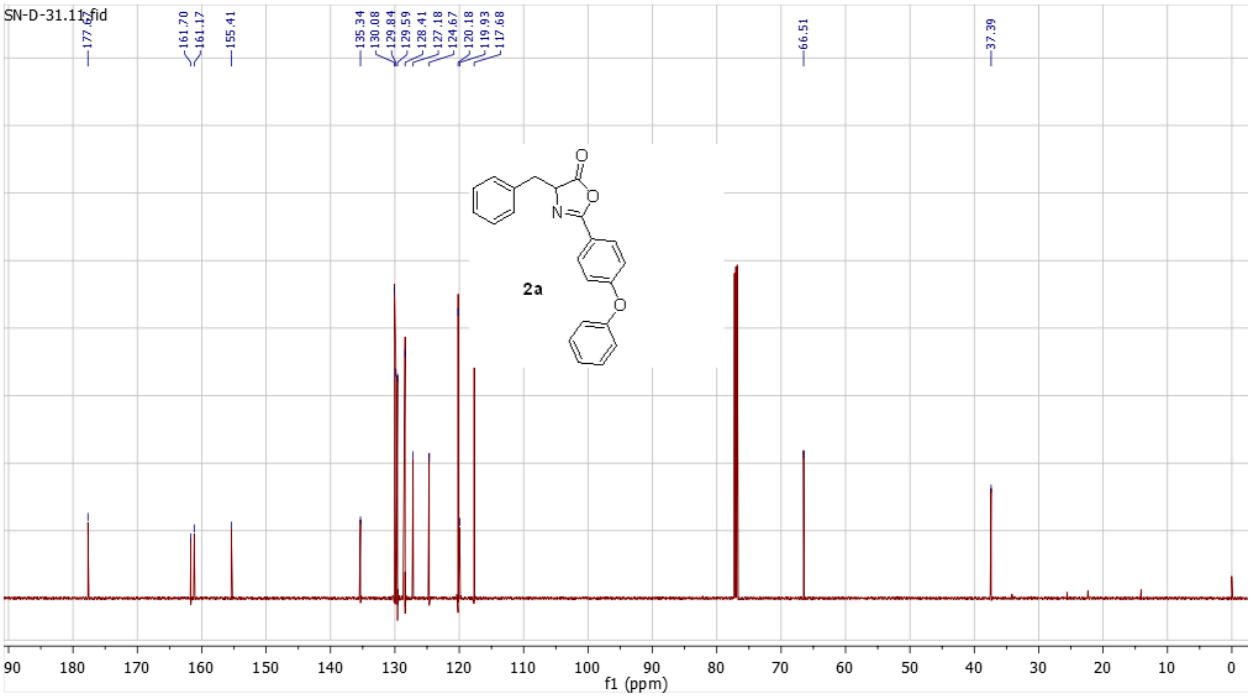
27.07
26.99
26.86
26.43
26.21
18.85
18.81
11.12
TIPS
OH
Cy
(R)-A6
f1 (ppm)

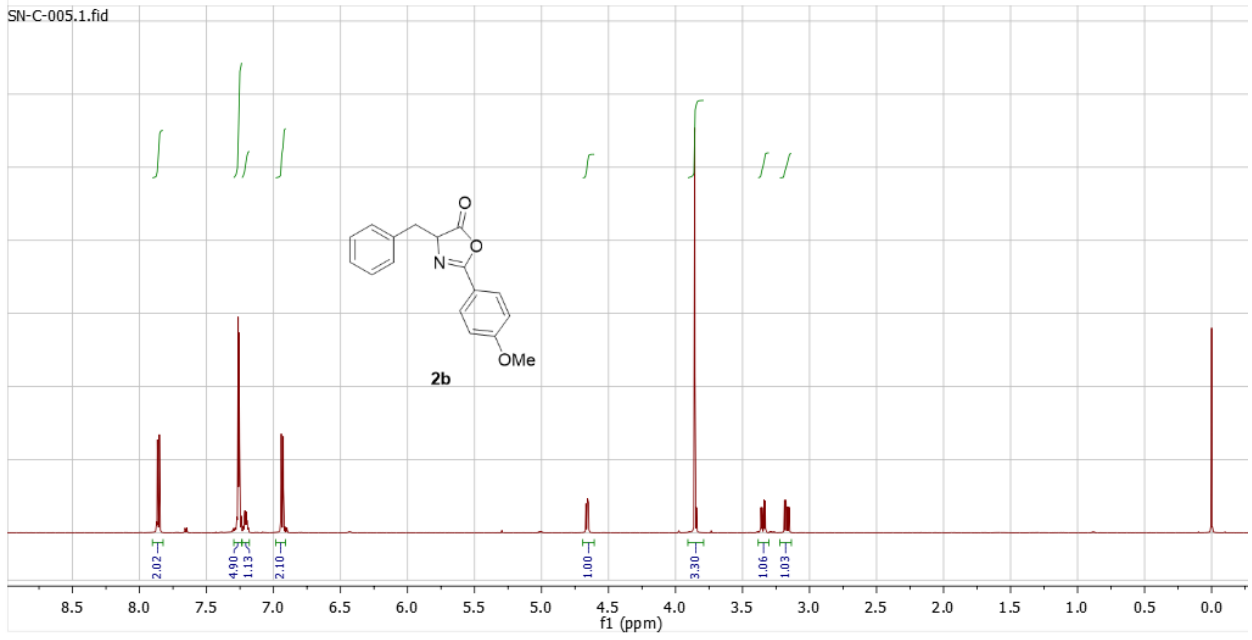

SN-E-66-1.1.fid
TIPS
TIPS
Cy
OH
PA10
2.00
1.94
1.98
1.70
4.05
2.03
3.98
10.66
2.59
7.90
13.91
13.70
41.09
12.61
f1 (ppm)

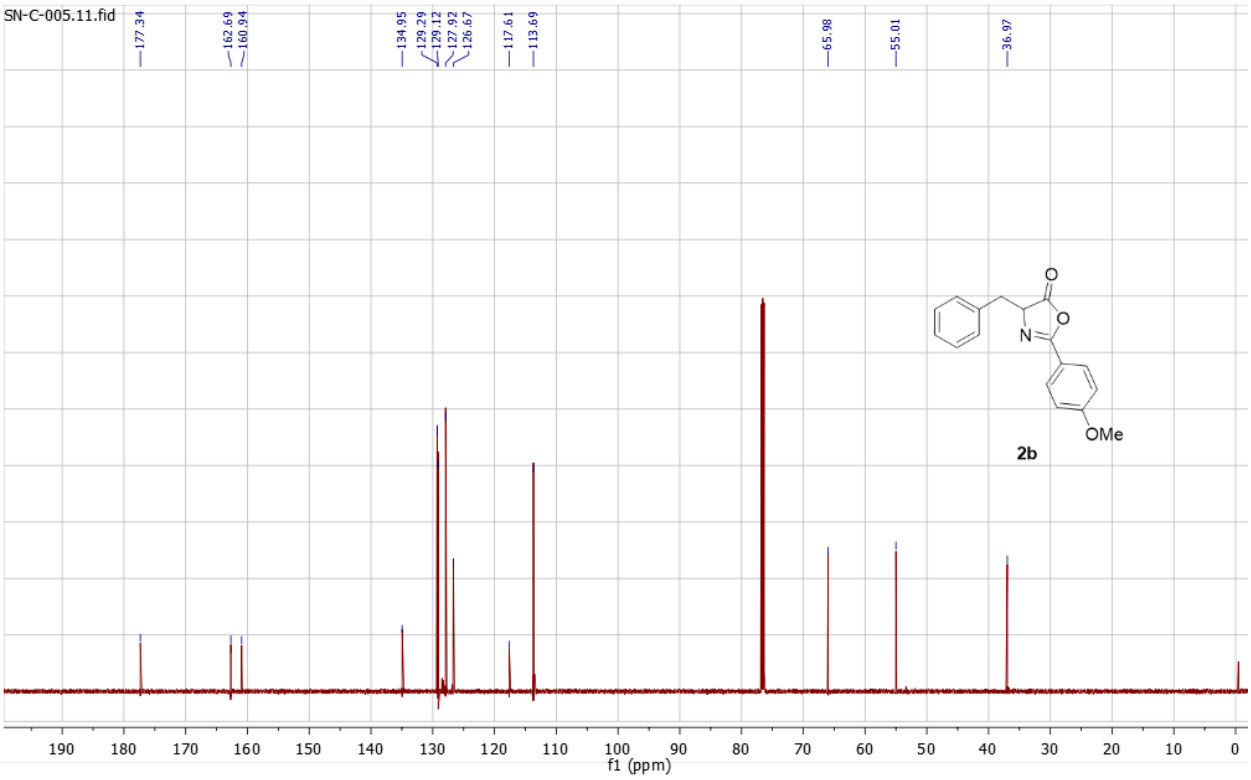

SN-E-66-1.11.fid
TIPS
TIPS
Cy
OH
PA10
f1 (ppm)

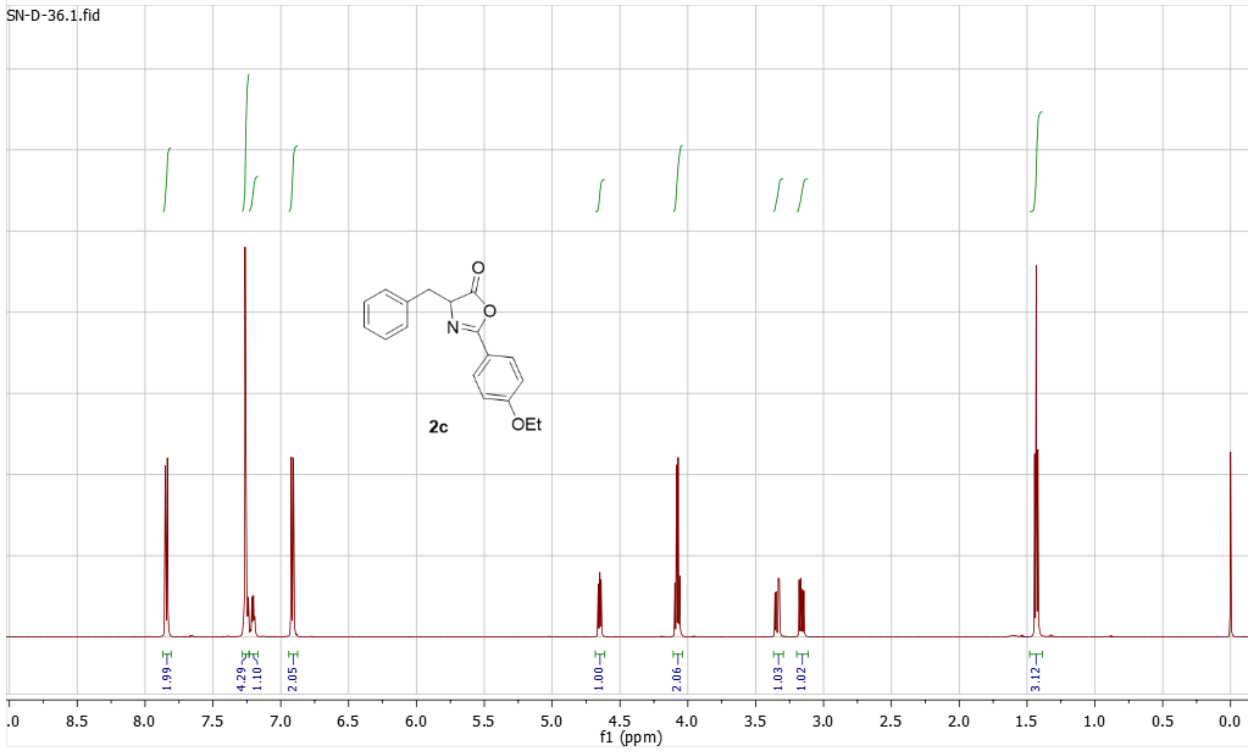

SN-E-66-1.21.fid
P-31, H-1 Coupled, no NOE
2.26
TIPS
TIPS
Cy
OH
PA10
f1 (ppm)

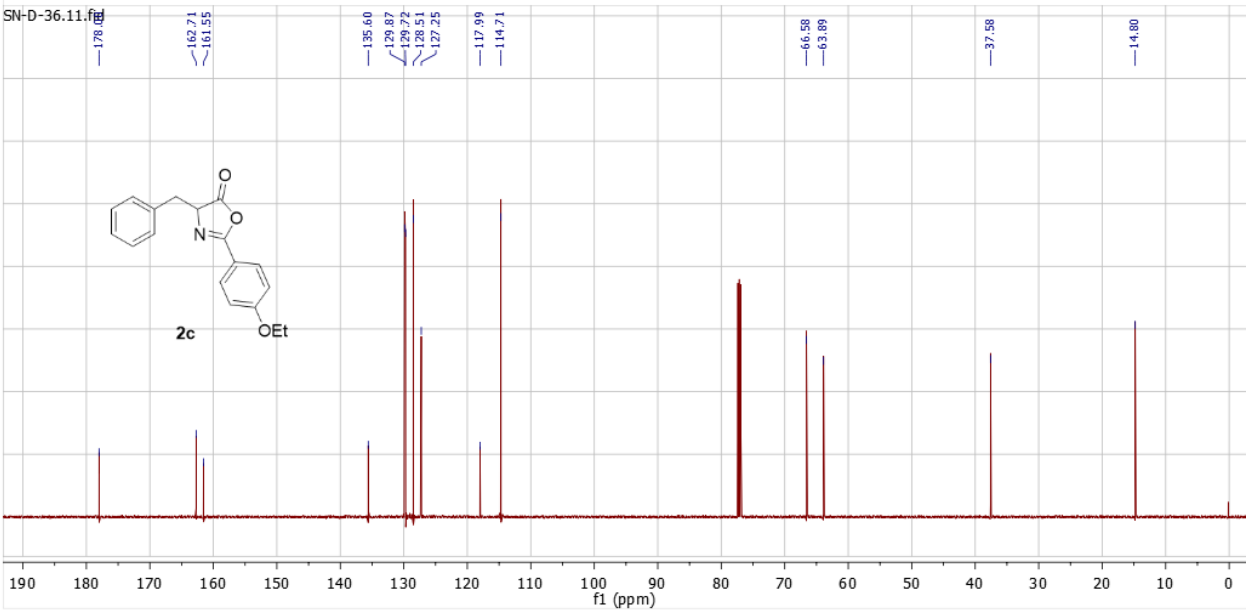

SN-D-31.1.fid
2a
2.02
2.10
4.30
2.17
2.02
2.09
1.00
1.06
1.03
f1 (ppm)

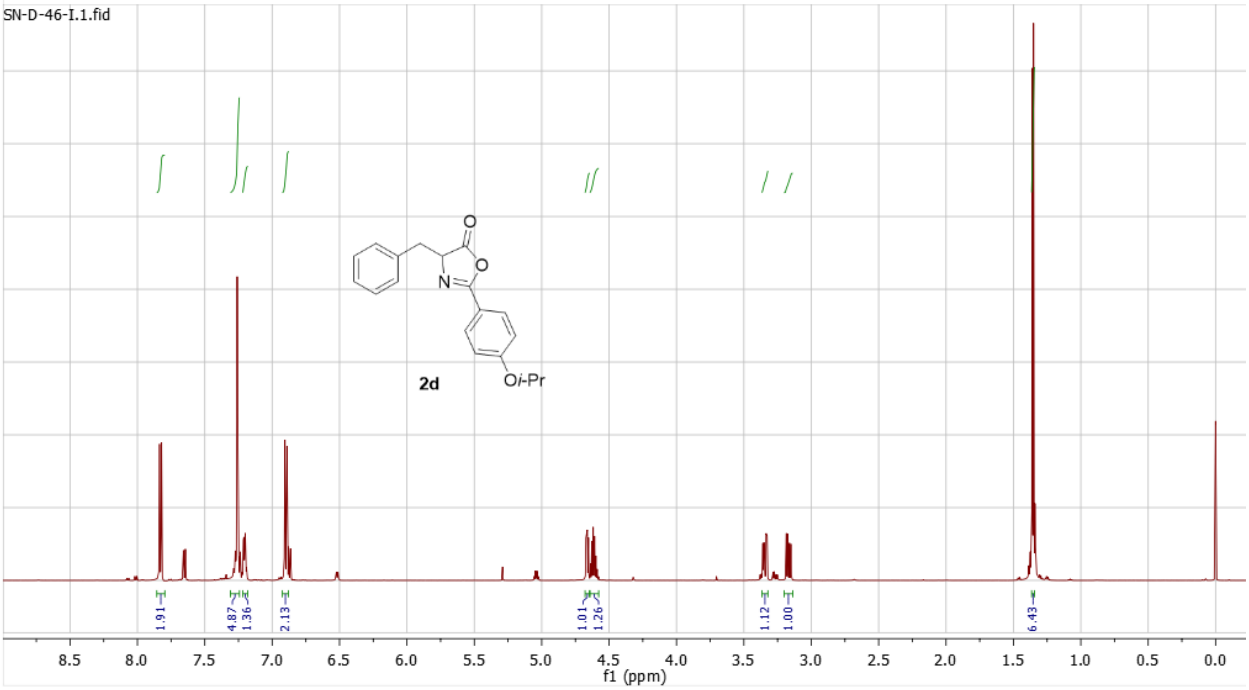

SN-D-31.11.fid
177.62
161.70
161.17
155.41
135.34
130.08
129.84
129.59
128.41
127.18
124.67
120.18
119.93
117.68
66.51
37.39
2a
f1 (ppm)

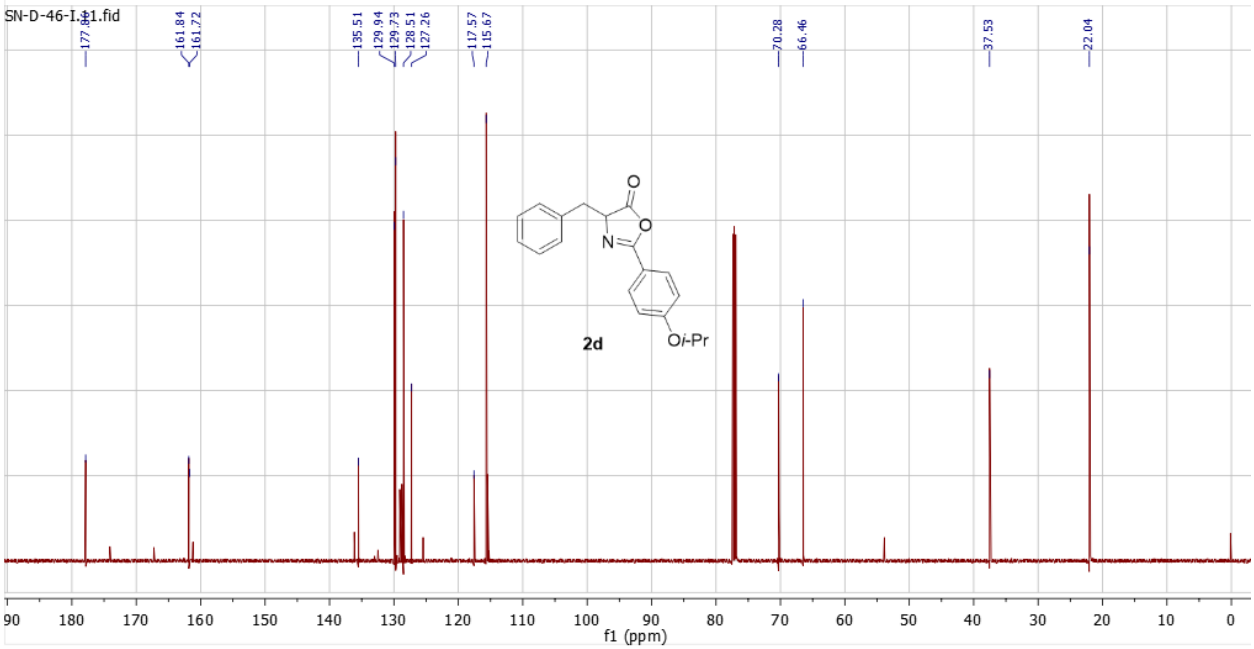

SN-C-005.1.fid
2.02
4.90
1.13
2.10
1.00
3.30
1.06
1.03
OMe
2b
f1 (ppm)

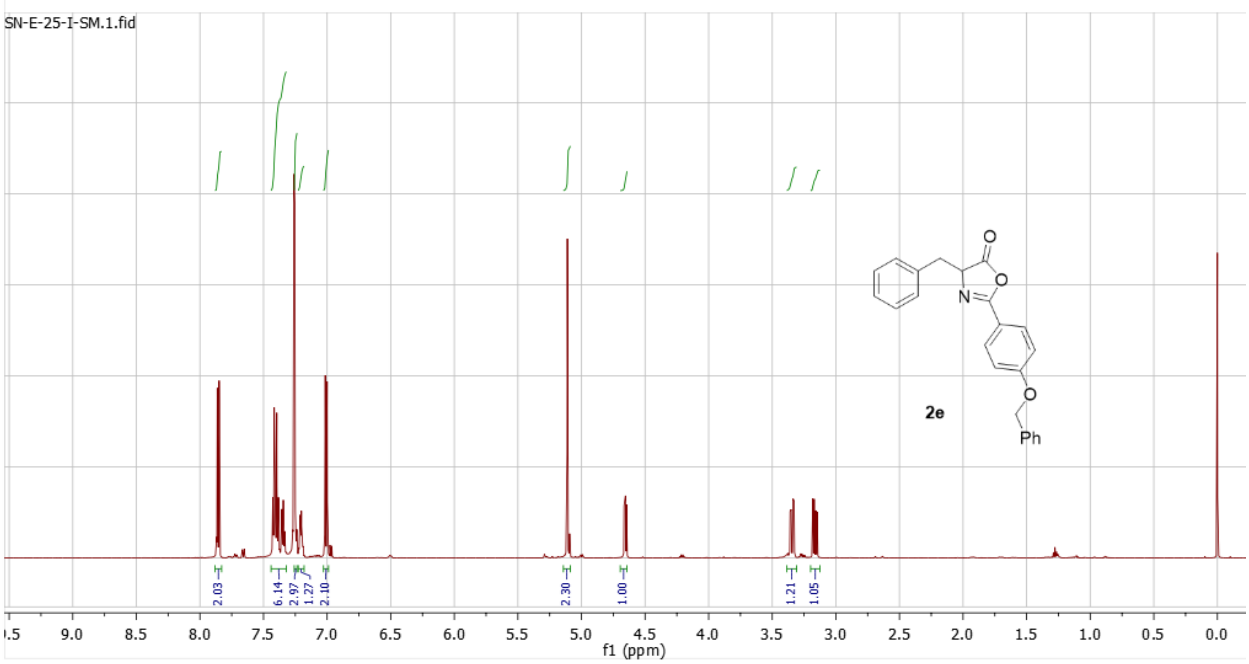

SN-C-005.11.fid
177.34
162.69
160.94
134.95
129.29
129.12
127.92
126.67
117.61
113.69
65.98
55.01
36.97
O
O
N
OMe
2b
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

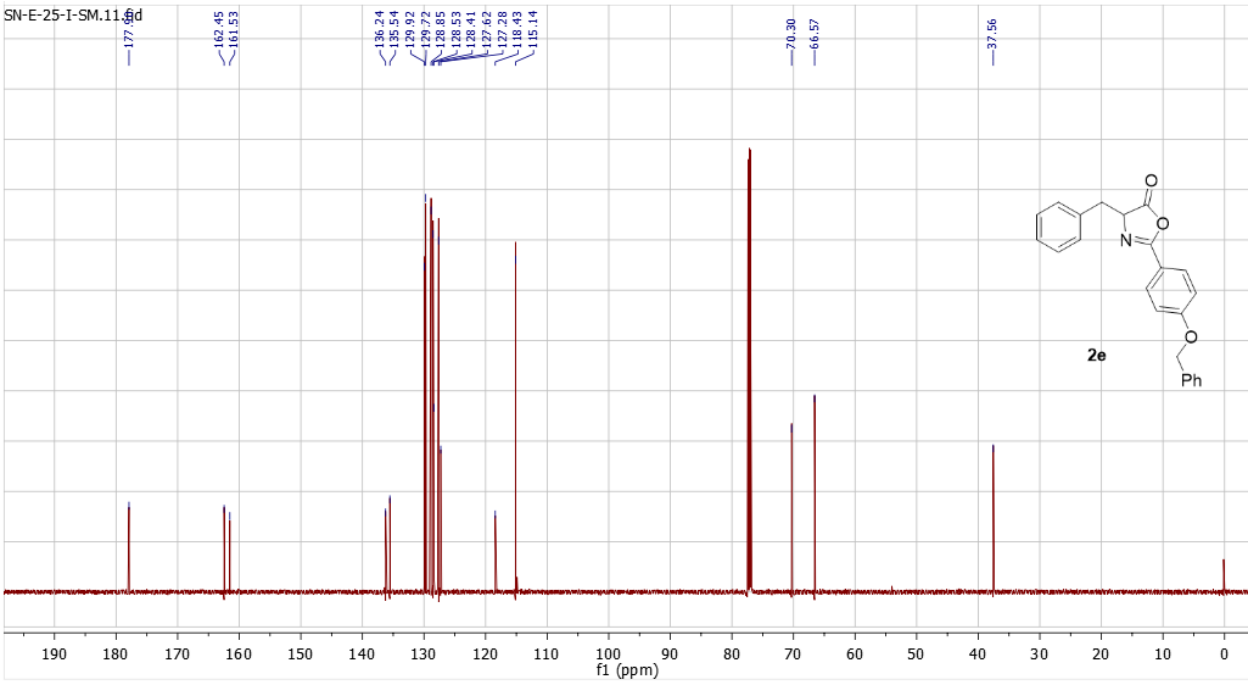

SN-D-36.1.fid
O
O
N
2c
OEt
1.99
4.29
1.10
2.05
1.00
2.06
1.03
1.02
3.12
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

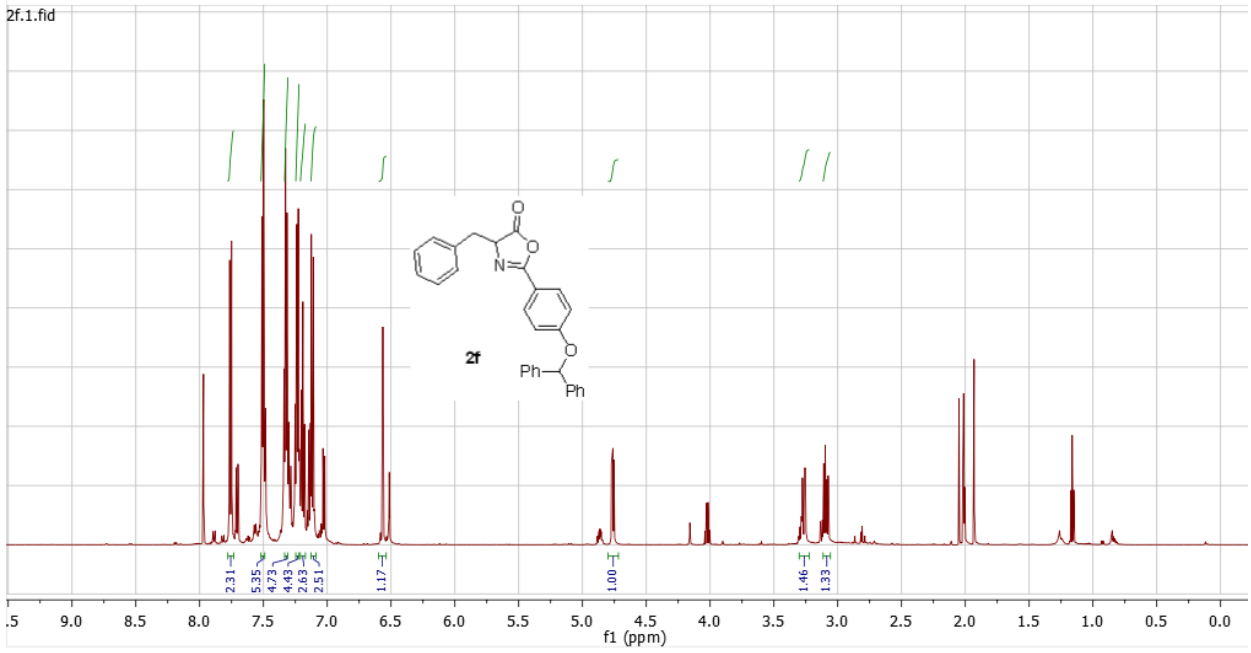

SN-D-36.11.fid
178.18
162.71
161.55
135.60
129.87
129.72
128.51
127.25
117.99
114.71
66.58
63.89
37.58
14.80
2c
OEt
f1 (ppm)

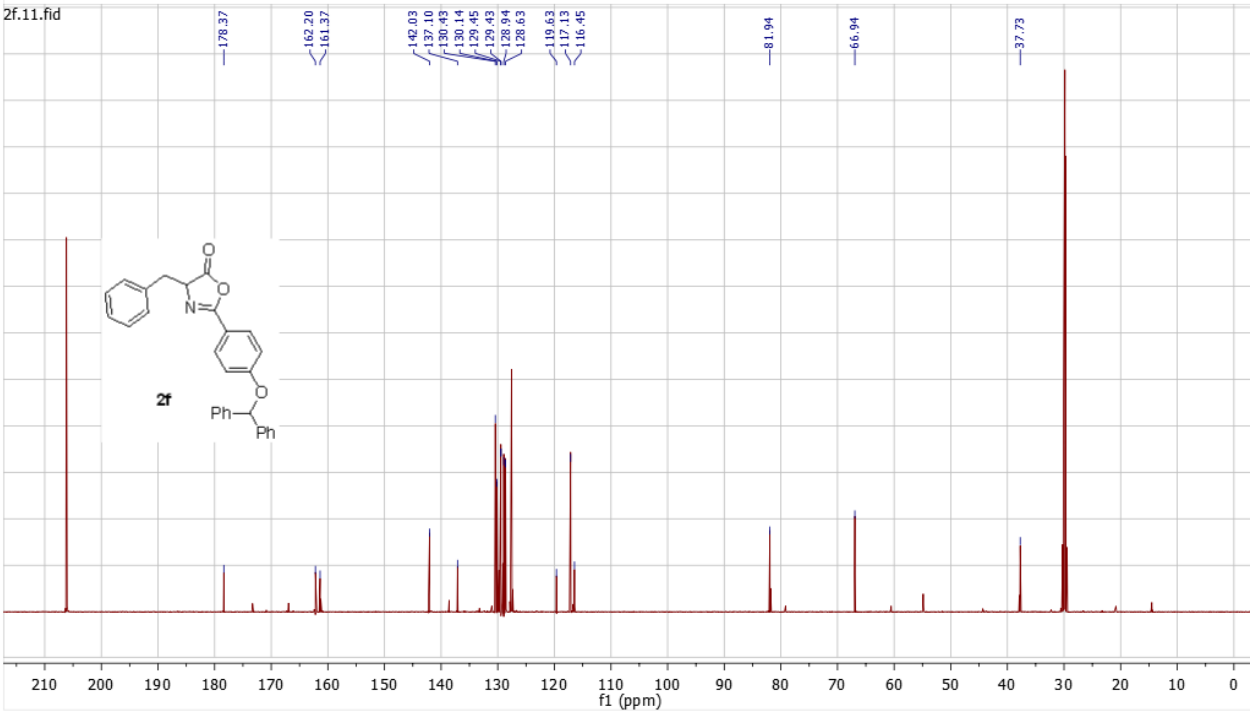

SN-D-46-I.1.fid
2d
Oi-Pr
1.91
4.87
1.36
2.13
1.01
1.26
1.12
1.00
6.43
f1 (ppm)

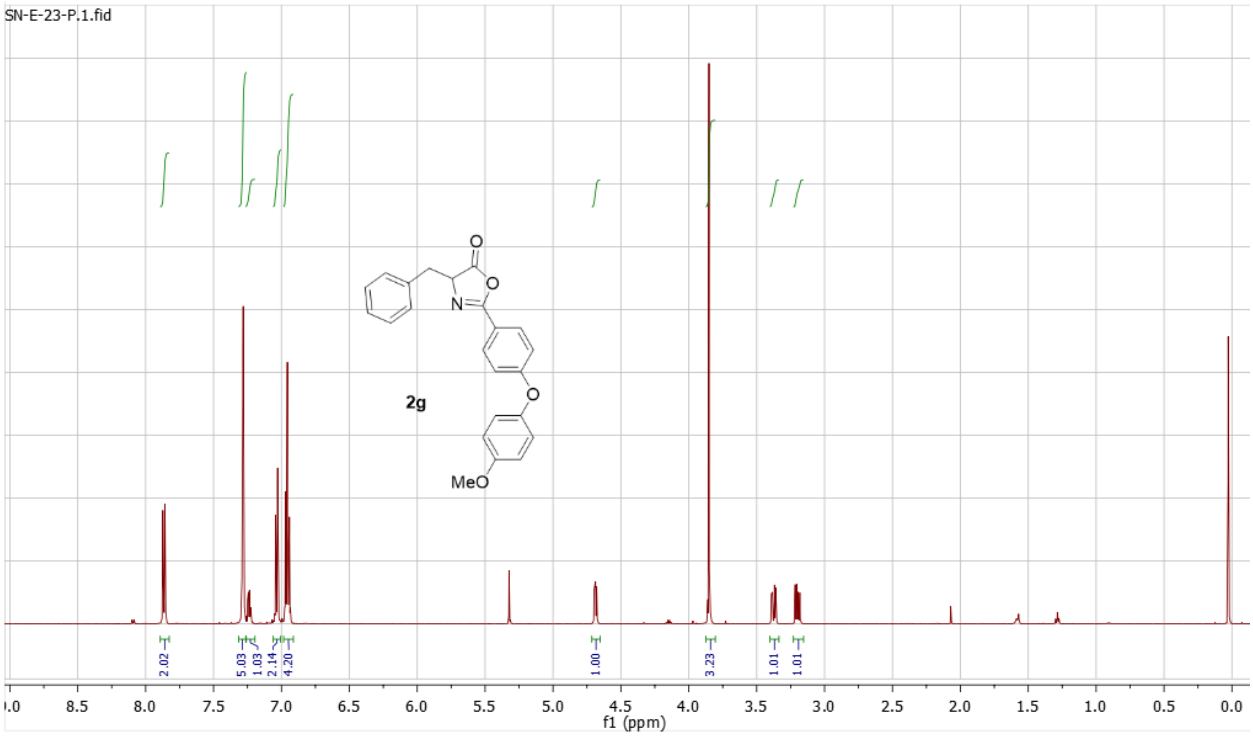

SN-D-46-I.11.fid
177.86
161.84
161.72
135.51
129.94
129.73
128.51
127.26
117.57
115.67
70.28
66.46
37.53
22.04
O
O
N
O
2d
Oi-Pr
f1 (ppm)

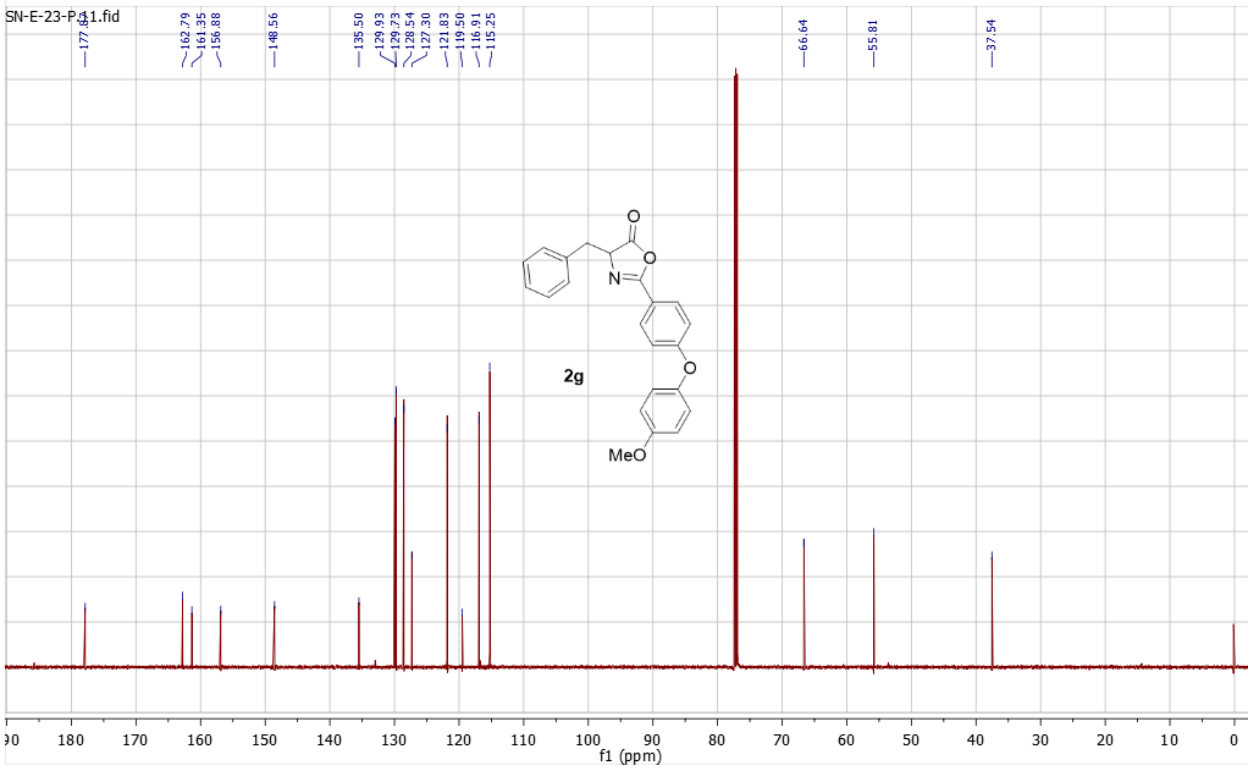

SN-E-25-I-SM.1.fid
2.03
6.14
2.97
1.27
2.10
2.30
1.00
1.21
1.05
O
O
N
O
2e
Ph
f1 (ppm)

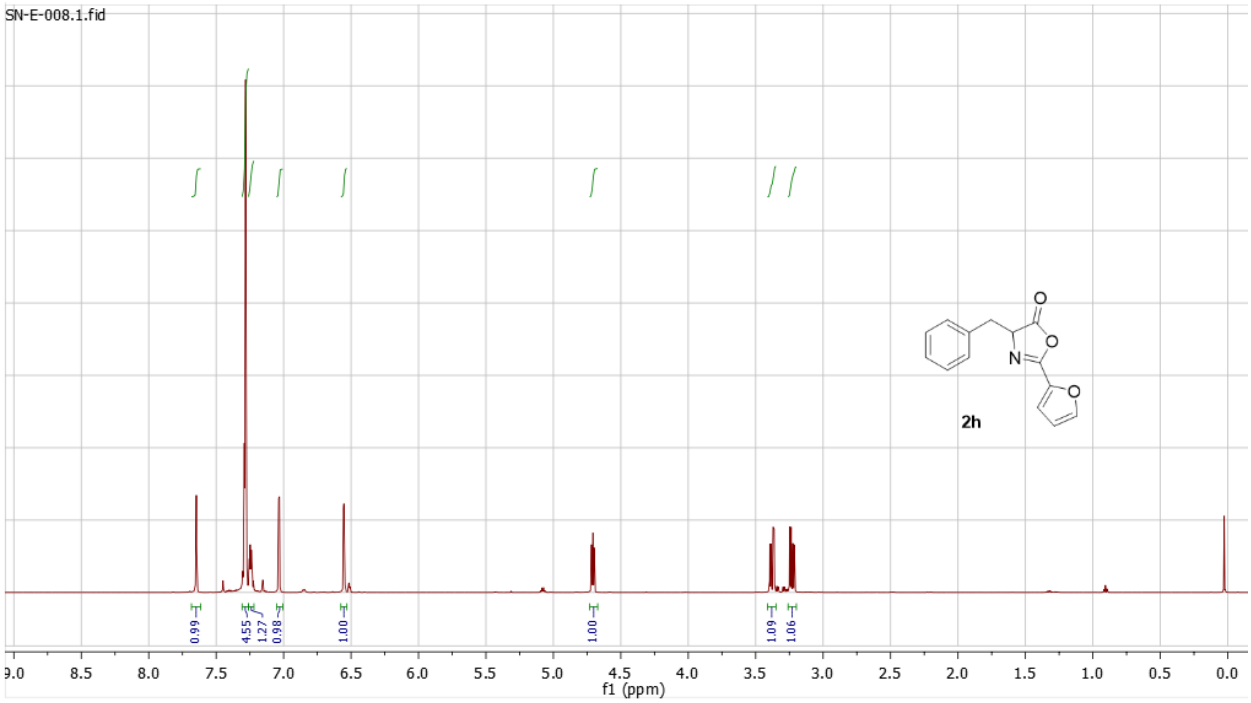

SN-E-25-I-SM.11.fid
177.66
162.45
161.53
136.24
135.54
129.92
129.72
128.85
128.53
128.41
127.62
127.28
118.43
115.14
70.30
66.57
37.56
2e
f1 (ppm)

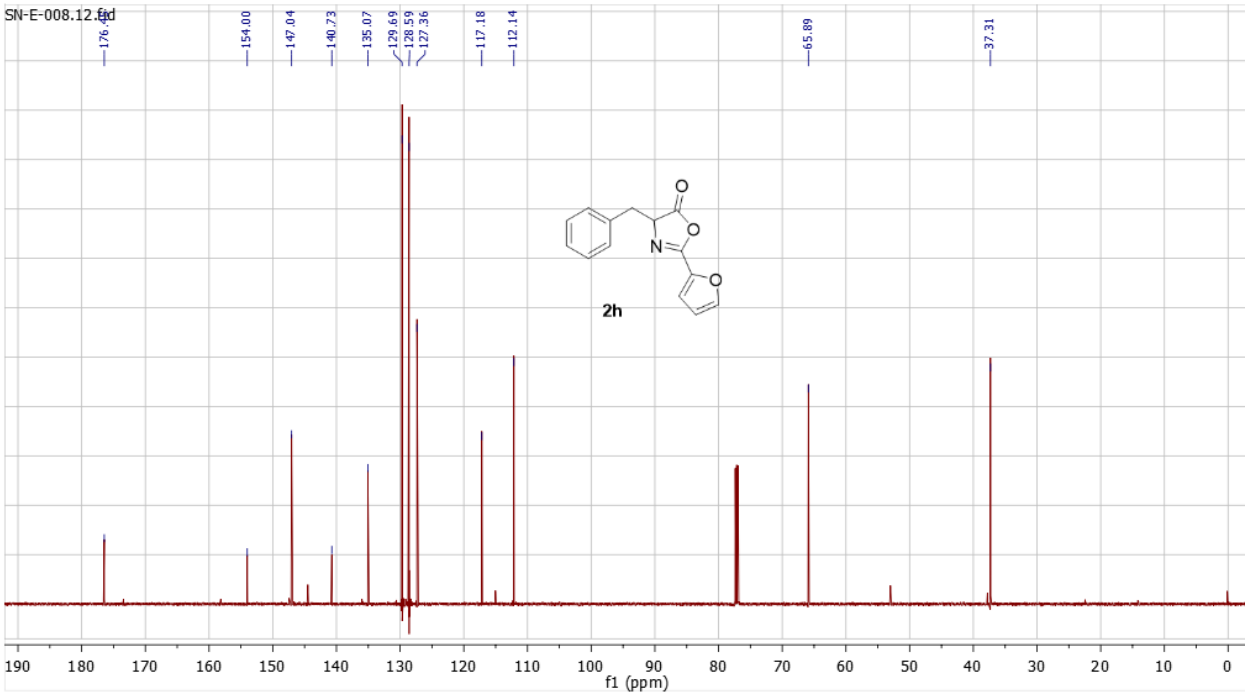

2f.1.fid
2f
2.31
5.35
4.73
4.43
2.63
2.51
1.17
1.00
1.46
1.33
f1 (ppm)

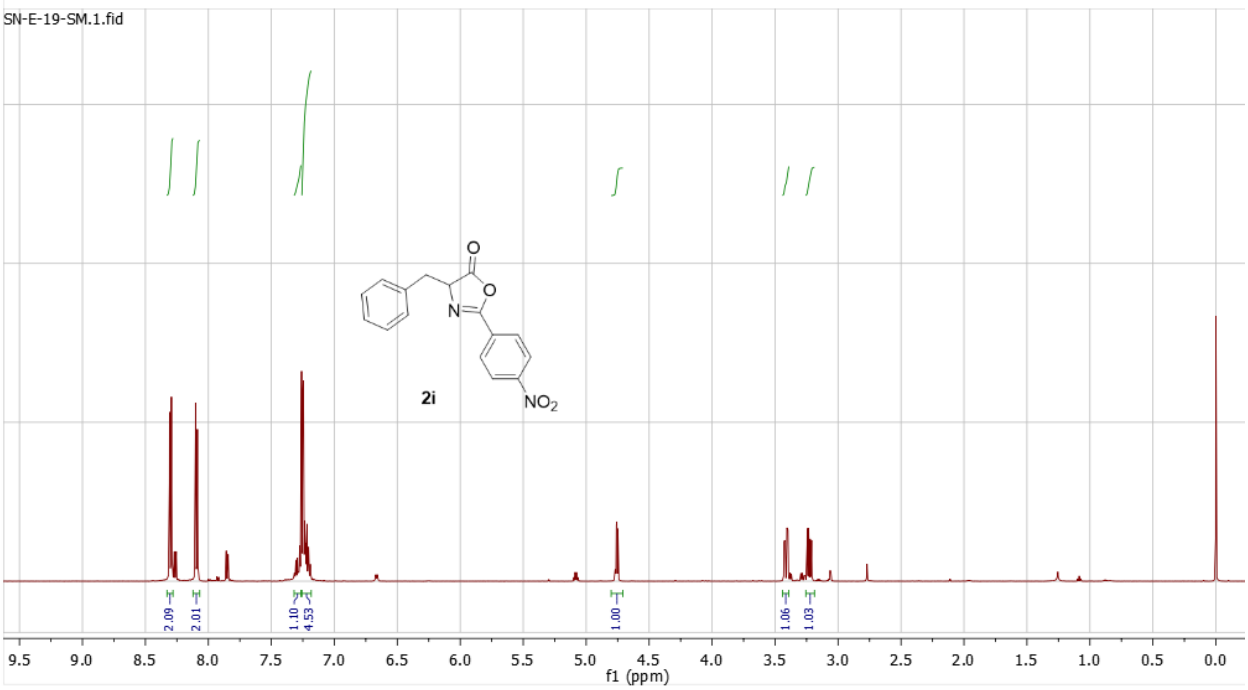

2f.11.fid
178.37
162.20
161.32
142.03
137.10
130.43
130.14
129.45
129.43
128.94
128.63
119.63
117.13
116.45
81.94
66.94
37.73
2f
Ph
Ph
f1 (ppm)

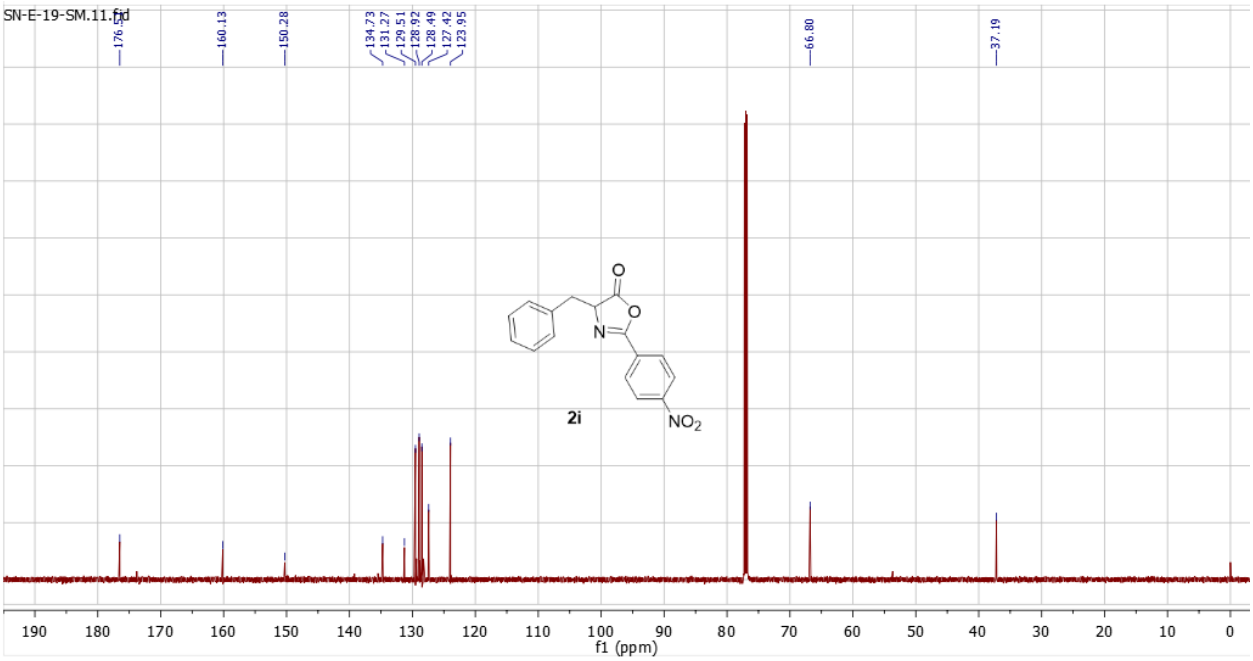

SN-E-23-P.1.fid
2g
MeO
2.02
5.03
1.03
2.14
4.20
1.00
3.23
1.01
1.01
f1 (ppm)

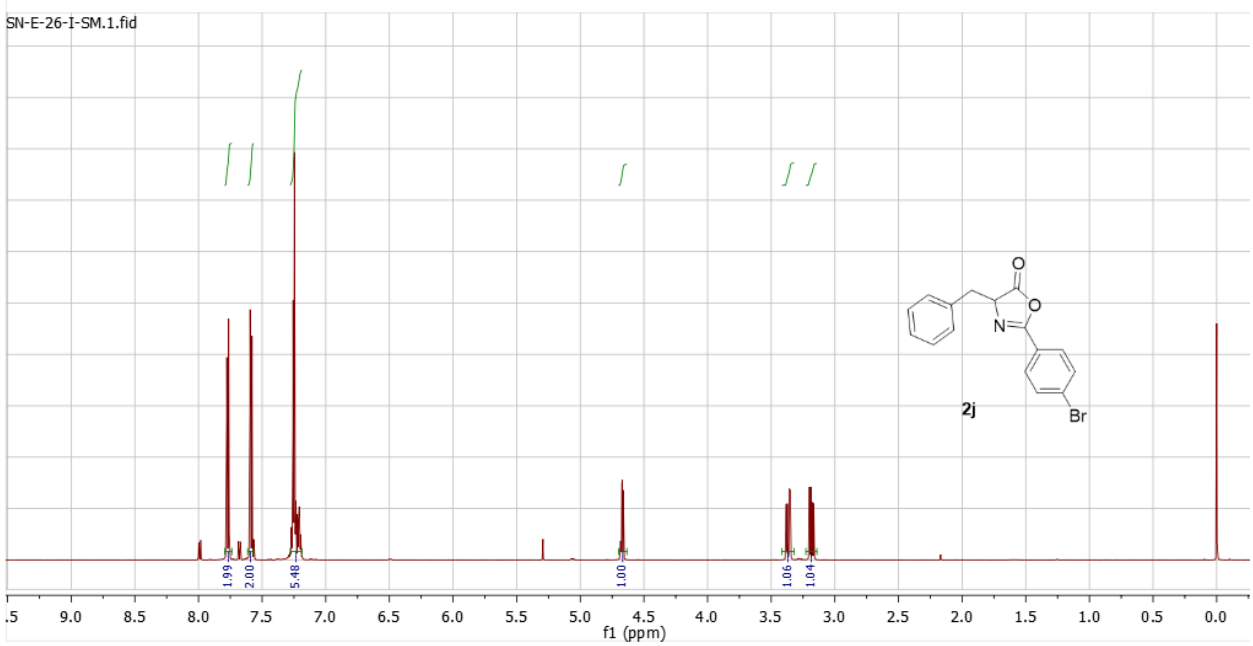

SN-E-23-P11.fid
177.87
162.79
161.35
156.88
148.56
135.50
129.93
129.73
128.54
127.30
121.83
119.50
116.91
115.25
66.64
55.81
37.54
2g
MeO
f1 (ppm)

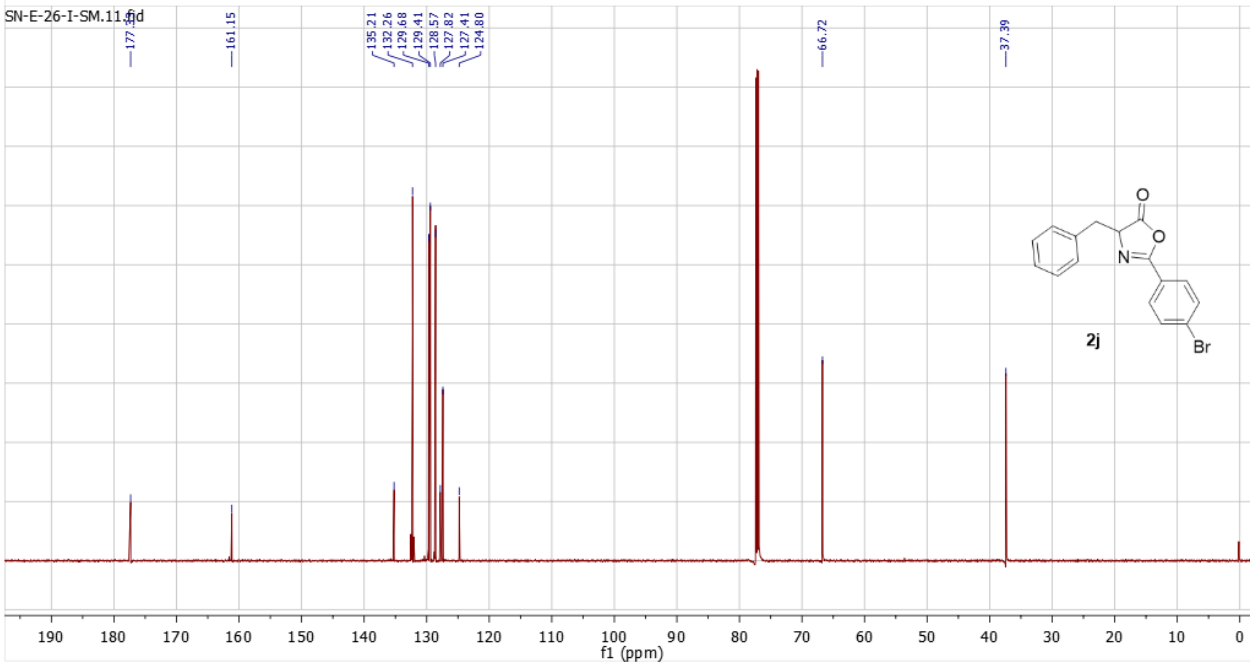

SN-E-008.1.fid
0.99
4.55
1.27
0.98
1.00
1.00
1.09
1.06
2h
f1 (ppm)

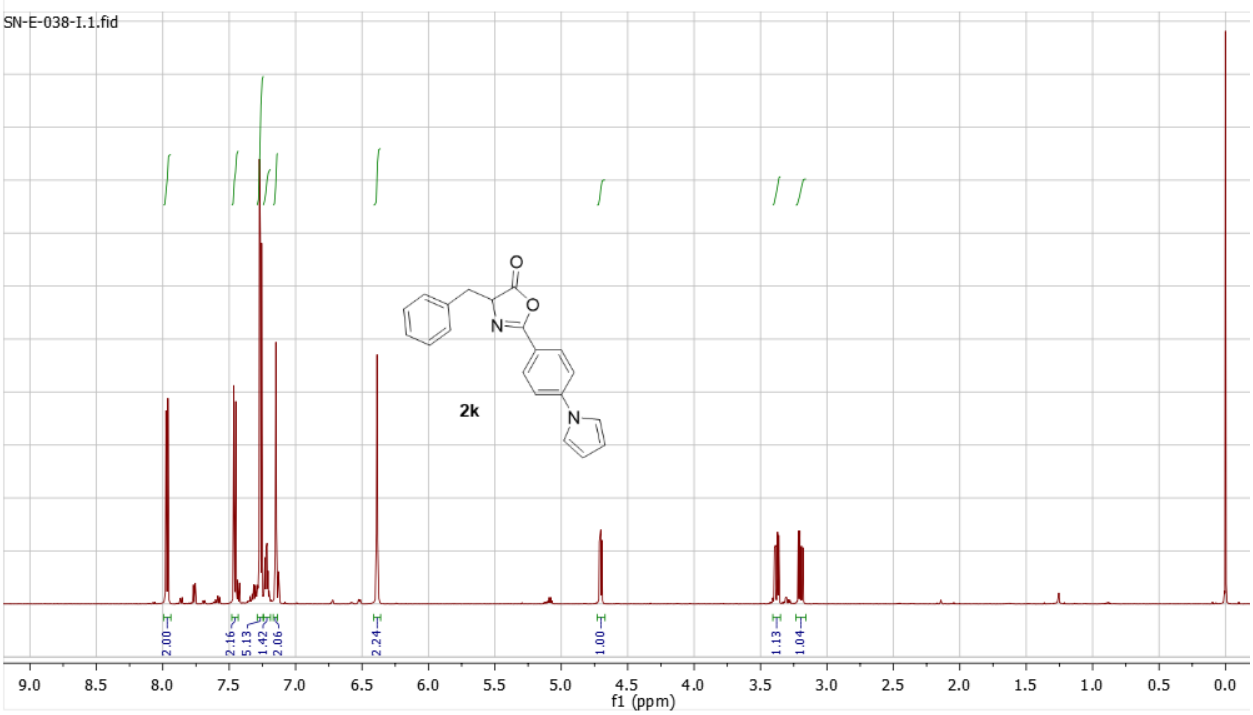

SN-E-008.12.fid
176.44
154.00
147.04
140.73
135.07
129.69
128.59
127.36
117.18
112.14
65.89
37.31
O
O
N
O
2h
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

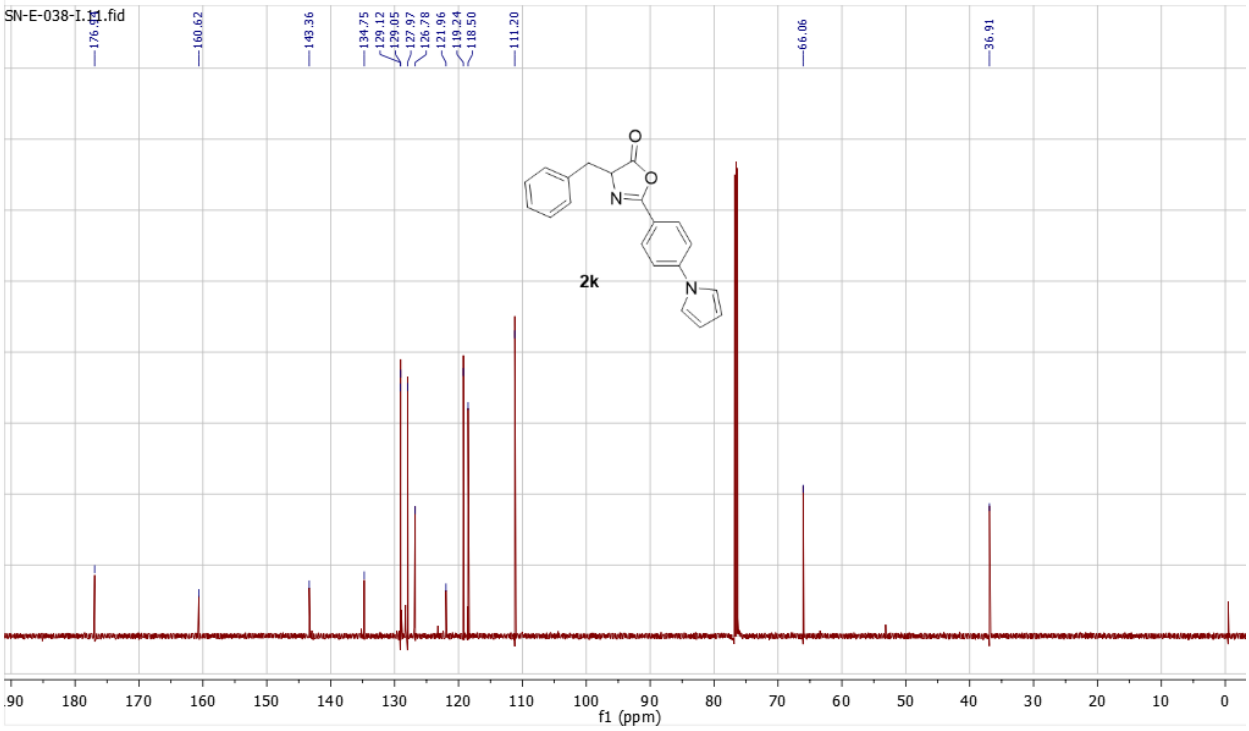

SN-E-19-SM.1.fid
O
O
N
2i
NO2
2.09
2.01
1.10
4.53
1.00
1.06
1.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

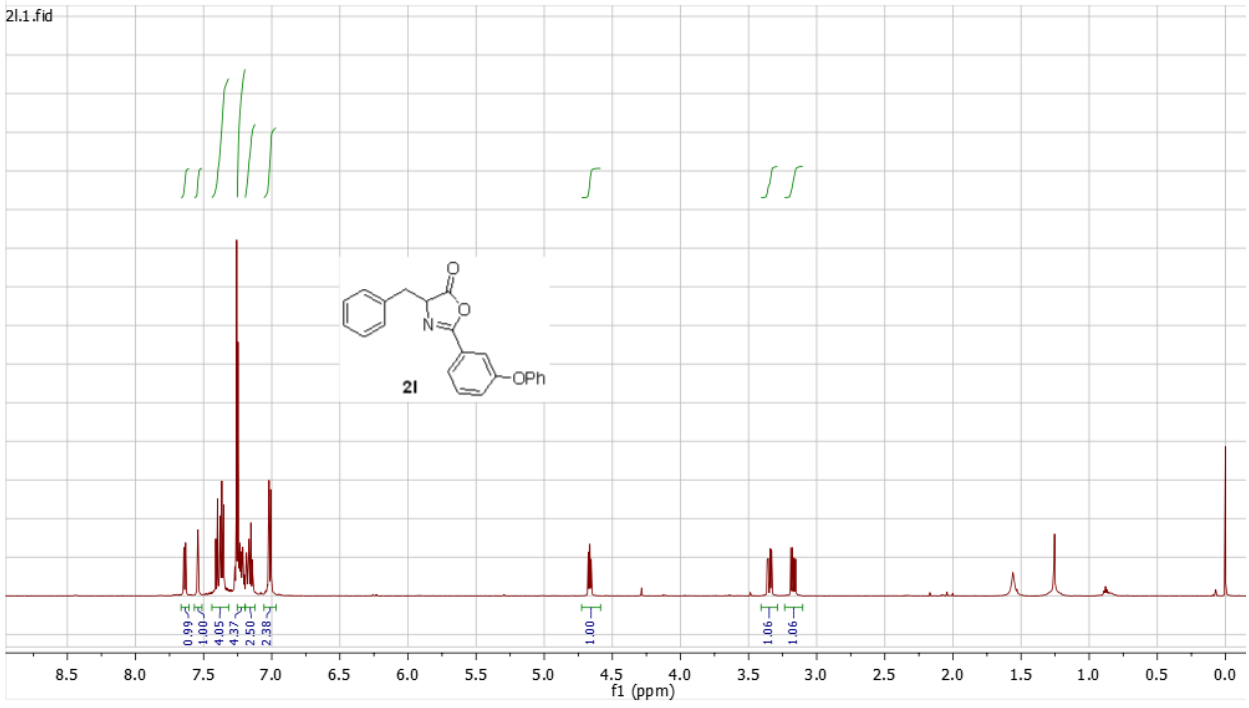

SN-E-19-SM.11.fid
176.73
160.13
150.28
134.73
131.27
129.51
128.92
128.49
127.42
123.95
66.80
37.19
O
O
N
NO2
2i
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

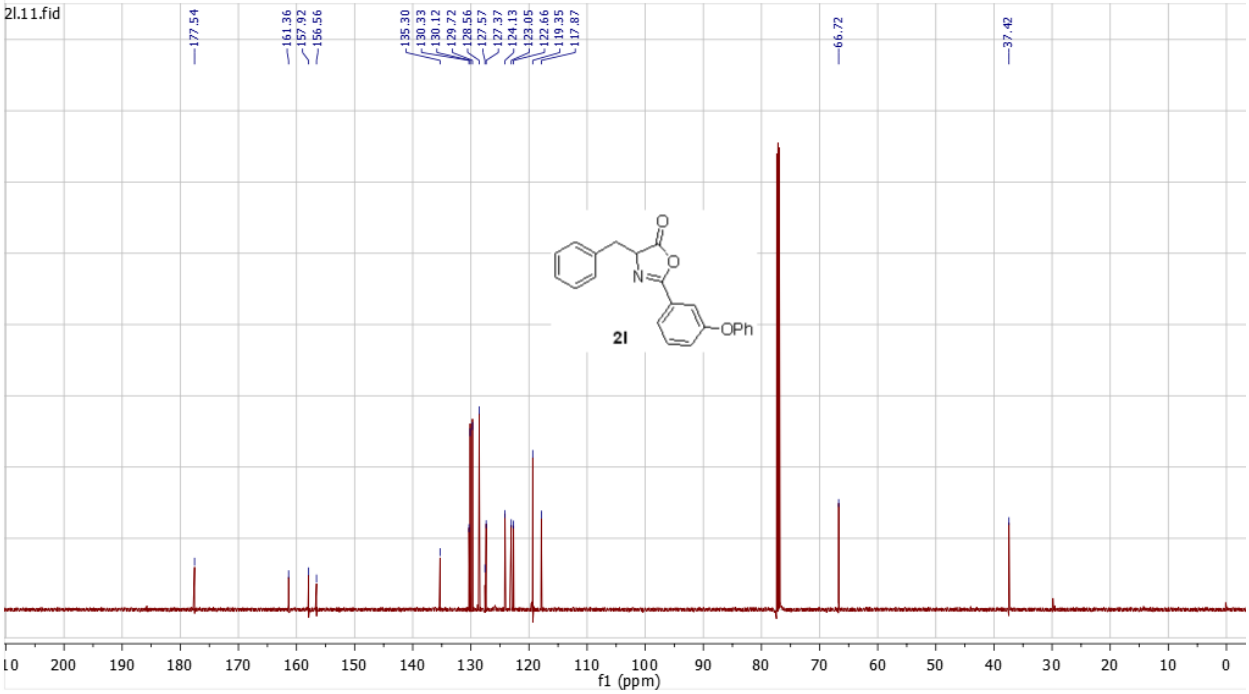

SN-E-26-I-SM.1.fid
1.99
2.00
5.48
1.00
1.06
1.04
O
O
N
Br
2j
.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

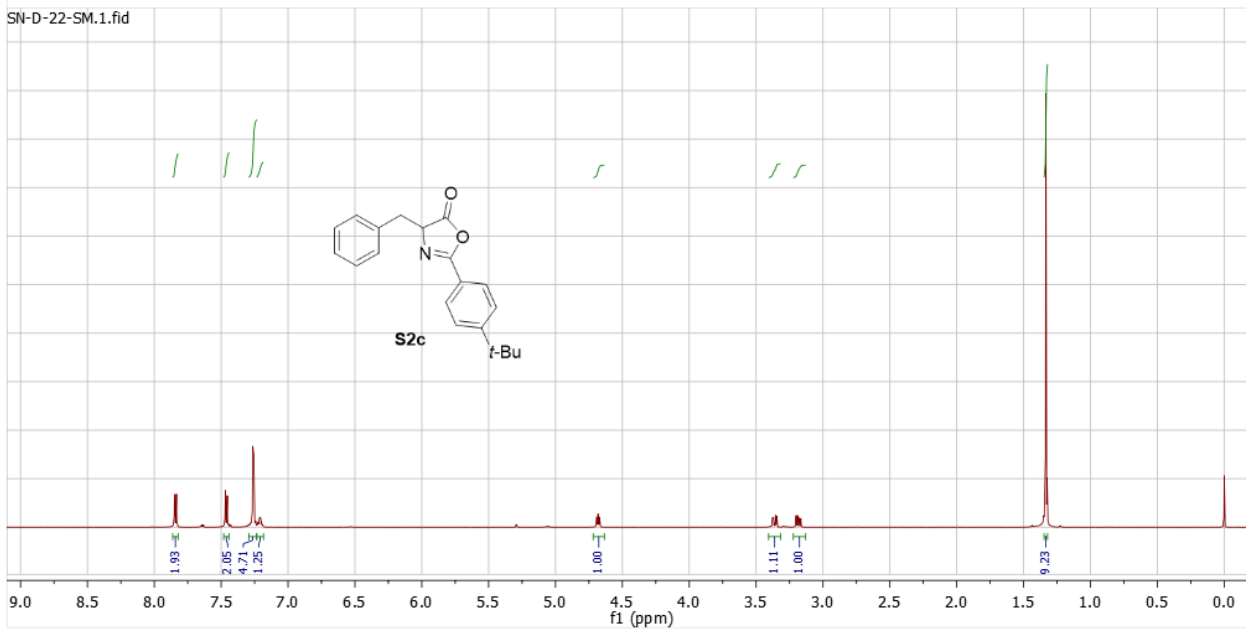

SN-E-26-I-SM.11.fid
177.38
161.15
135.21
132.26
129.68
129.41
128.57
127.82
127.41
124.80
66.72
37.39
2j
Br
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

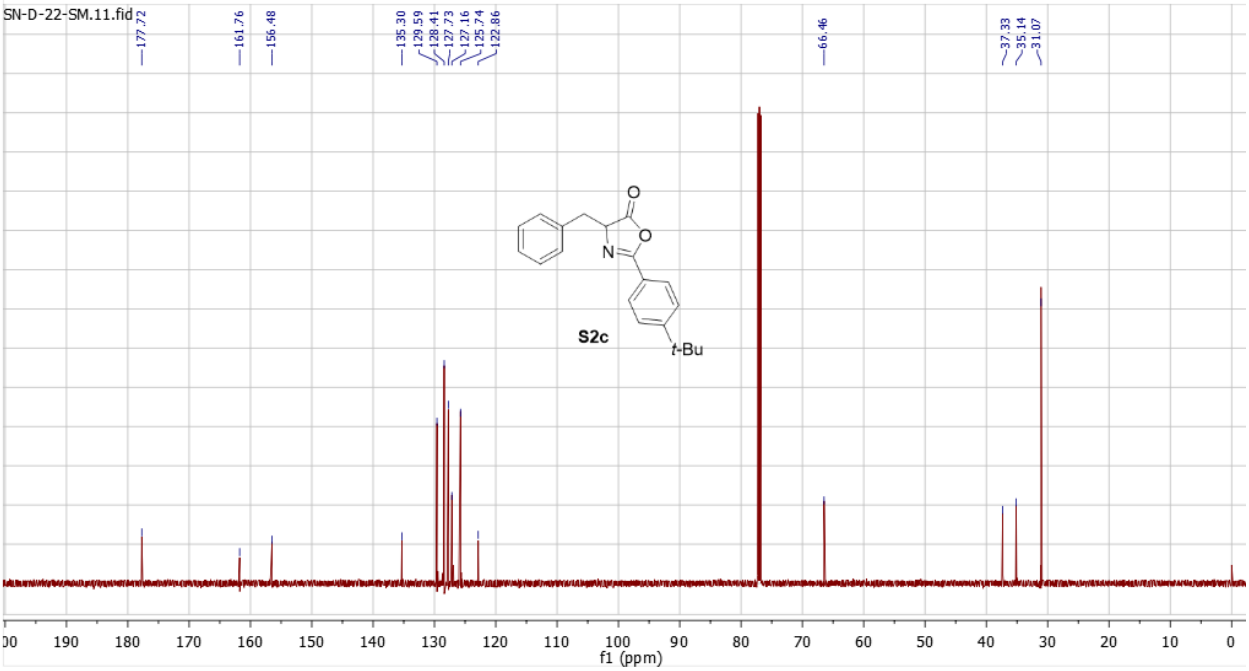

SN-E-038-I.1.fid
2k
2.00
2.16
5.13
1.42
2.06
2.24
1.00
1.13
1.04
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

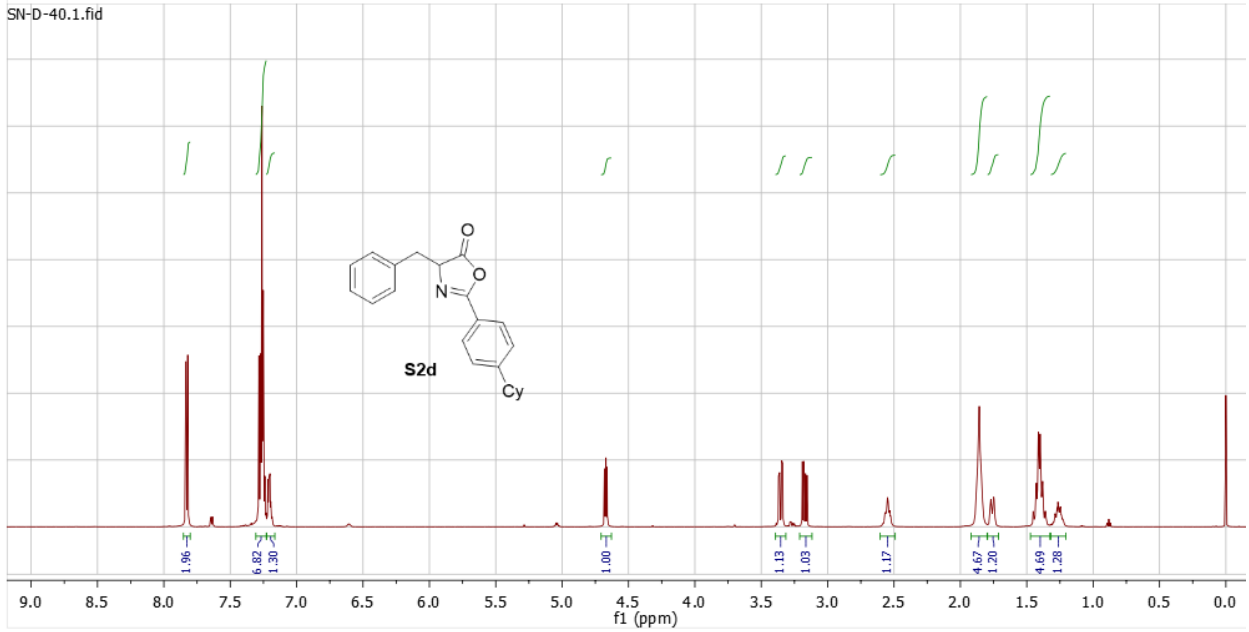

SN-E-038-I.11.fid
176.41
160.62
143.36
134.75
129.12
129.05
127.97
126.78
121.96
119.24
118.50
111.20
66.06
36.91
2k
f1 (ppm)

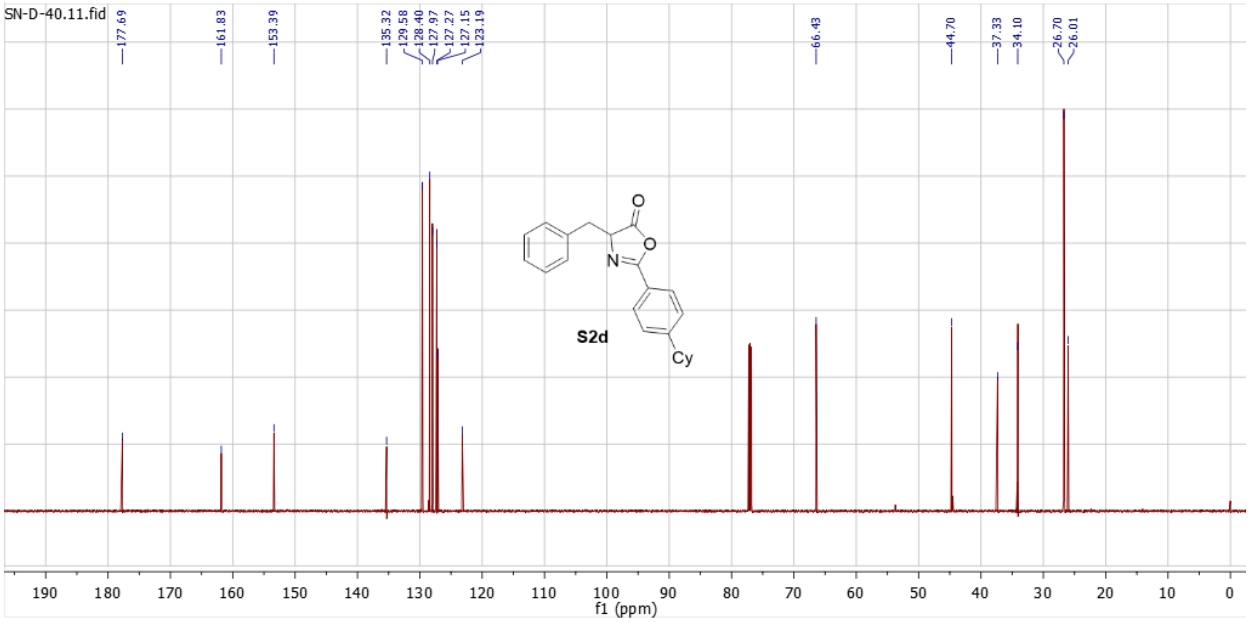

2l.1.fid
2l
OPh
0.99
1.00
4.05
4.37
2.50
2.38
1.00
1.06
1.06
f1 (ppm)

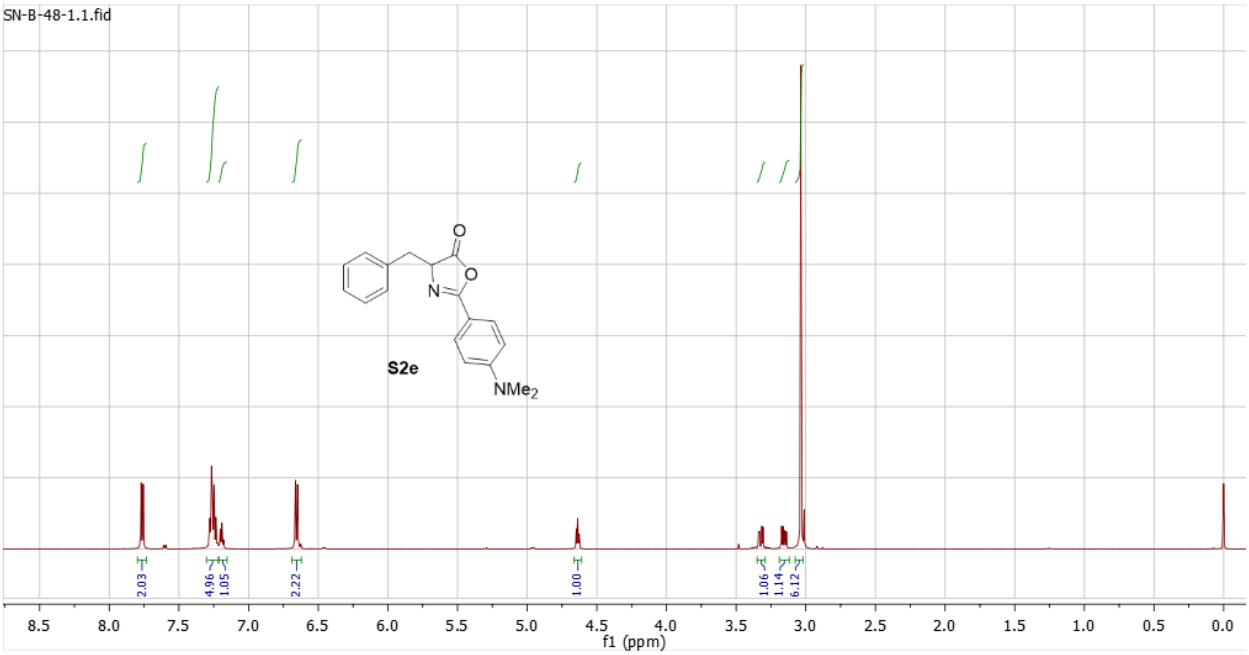

2l.11.fid
177.54
161.36
157.92
156.56
135.30
130.33
130.12
129.72
128.56
127.57
127.37
124.13
123.05
122.66
119.35
117.87
66.72
37.42
2l
OPh
f1 (ppm)

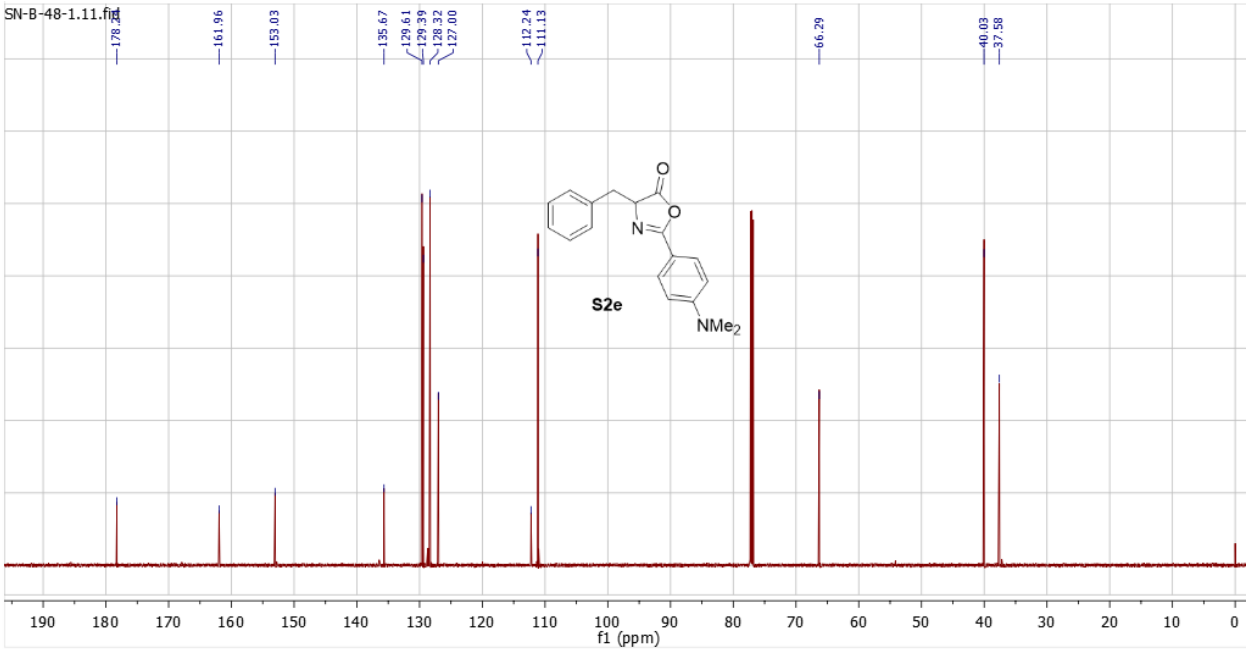

SN-D-22-SM.1.fid
S2c
t-Bu
1.93
2.05
4.71
1.25
1.00
1.11
1.00
9.23
f1 (ppm)

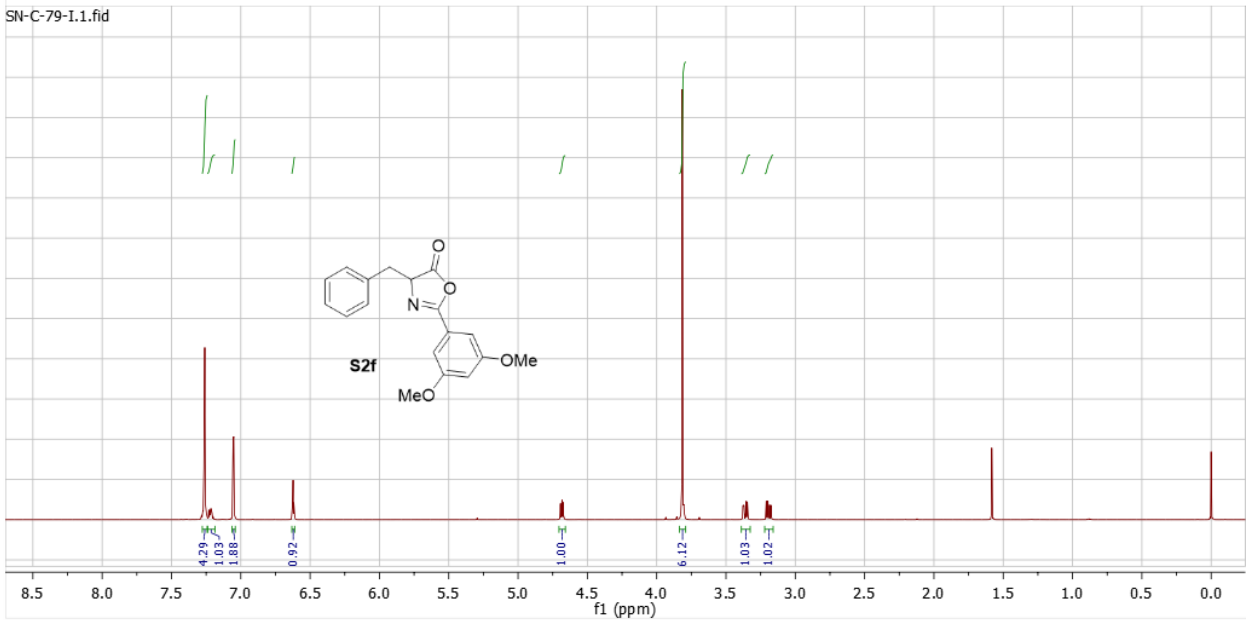

SN-D-22-SM.11.fid
177.72
161.76
156.48
135.30
129.59
128.41
127.73
127.16
125.74
122.86
66.46
37.33
35.14
31.07
S2c
t-Bu
f1 (ppm)

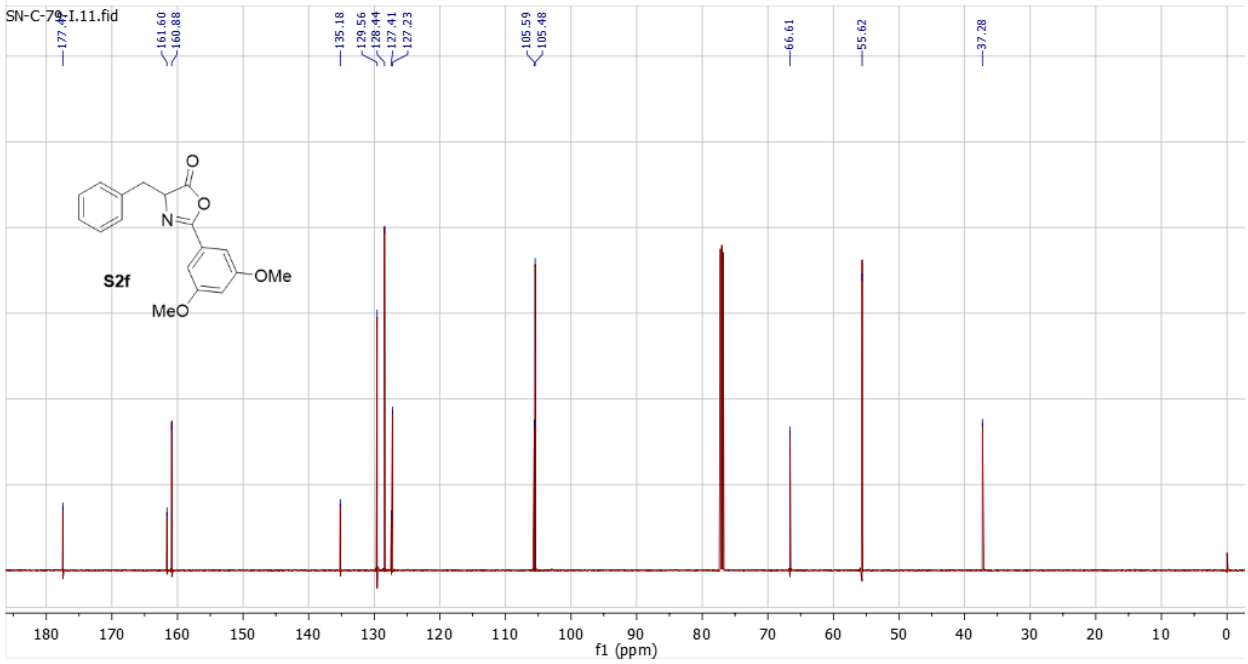

SN-D-40.1.fid
S2d
Cy
1.96
6.82
1.30
1.00
1.13
1.03
1.17
4.67
1.20
4.69
1.28
f1 (ppm)

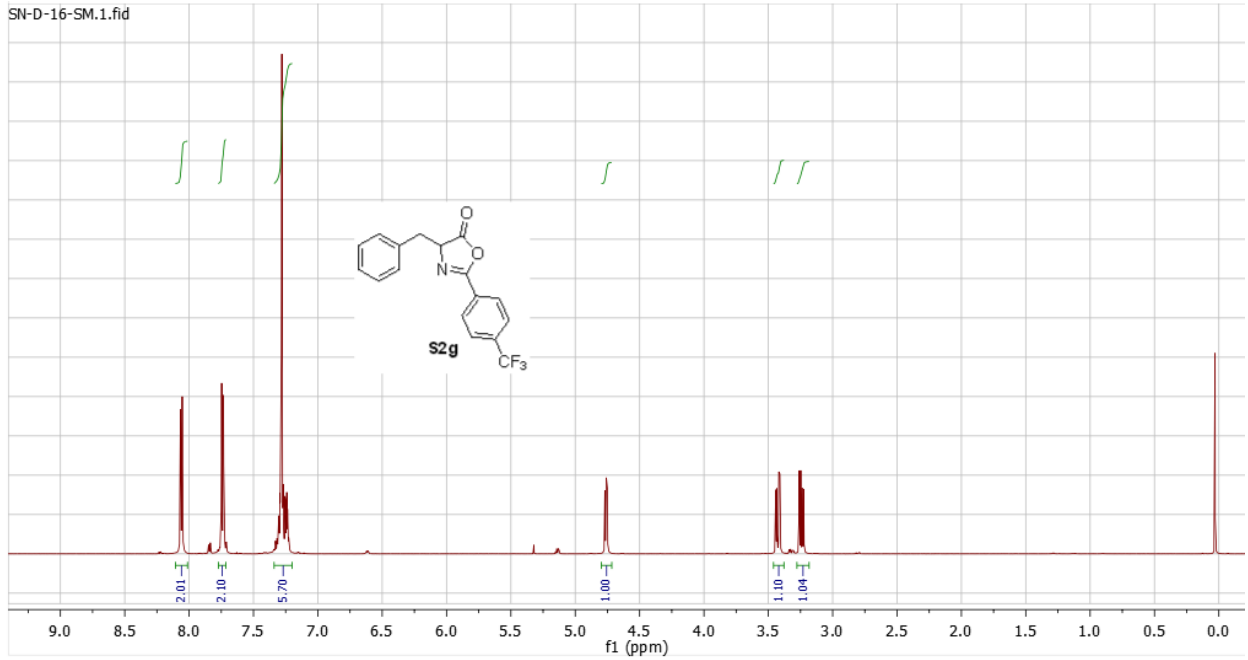

SN-D-40.11.fid
177.69
161.83
153.39
135.32
129.58
128.40
127.97
127.27
127.15
123.19
66.43
44.70
37.33
34.10
26.70
26.01
S2d
Cy
f1 (ppm)

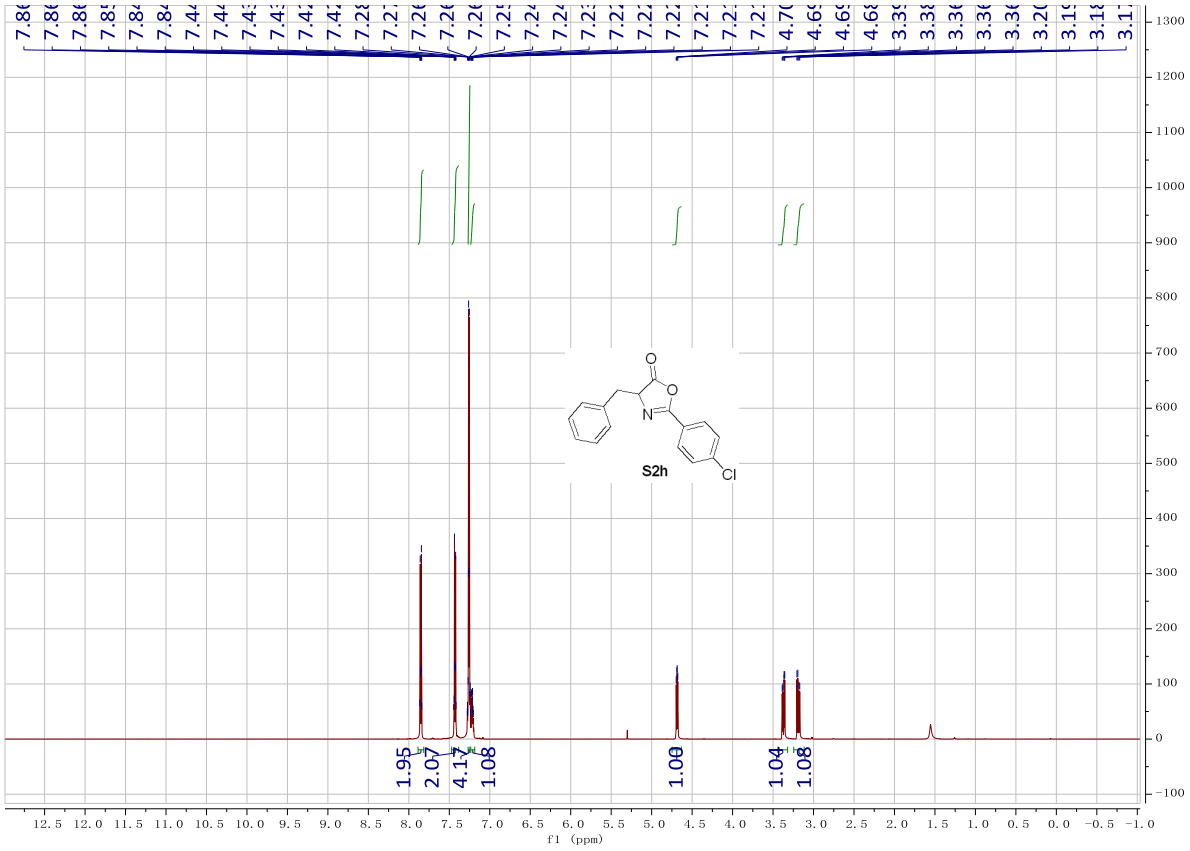

SN-B-48-1.1.fid
S2e
NMe2
2.03
4.96
1.05
2.22
1.00
1.06
1.14
6.12
f1 (ppm)

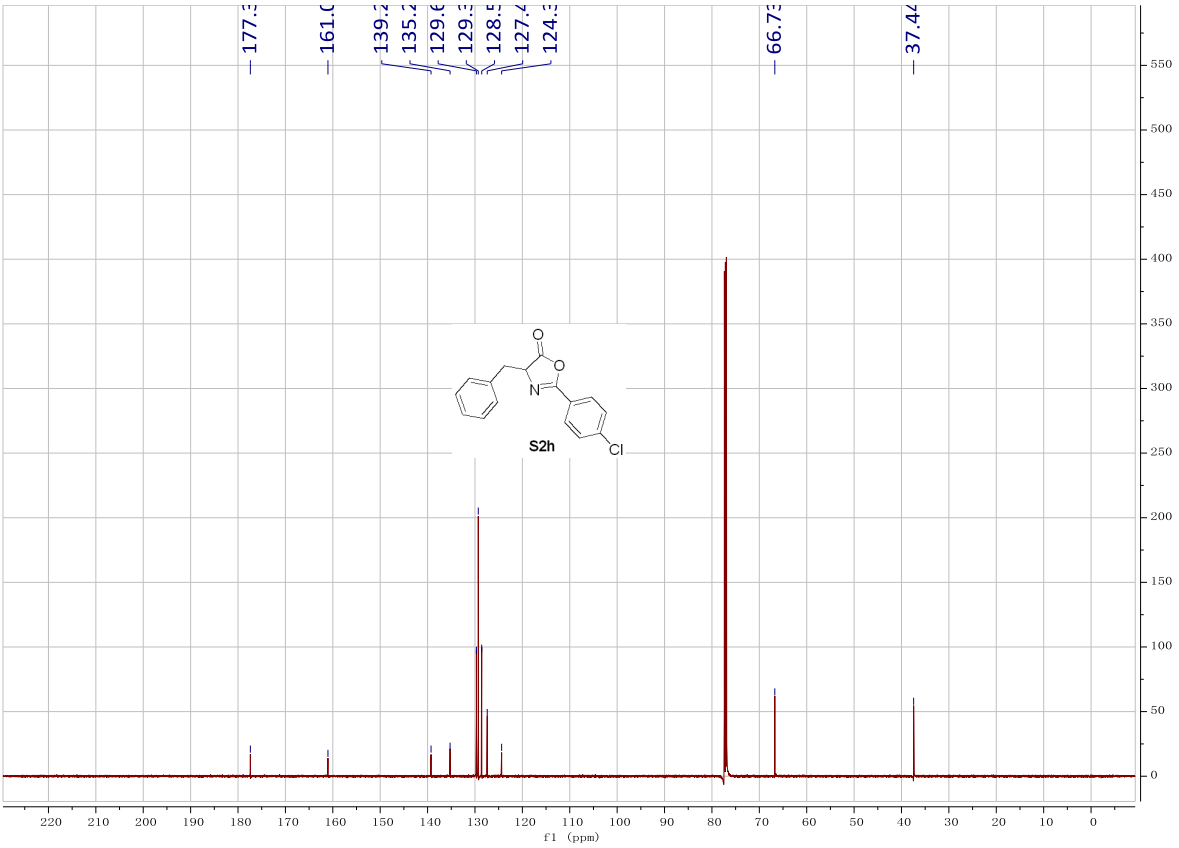

SN-B-48-1.11.fid
178.22
161.96
153.03
135.67
129.61
129.39
128.32
127.00
112.24
111.13
66.29
40.03
37.58
O
O
N
S2e
NMe2
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

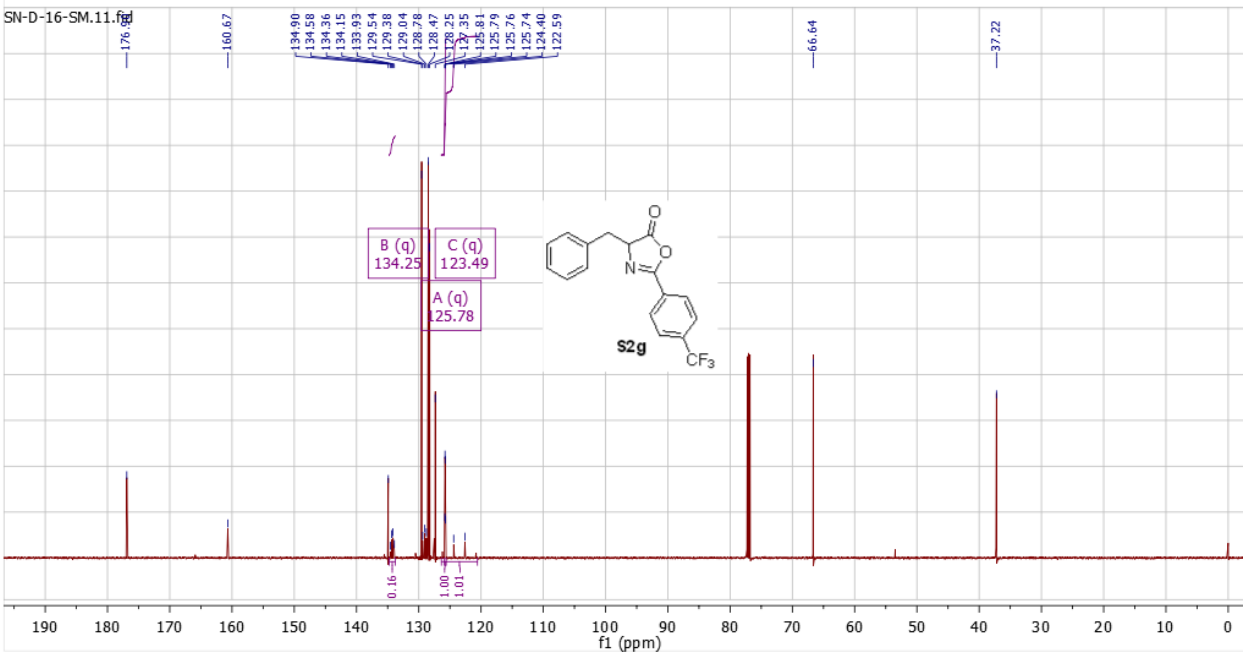

SN-C-79-I.1.fid
O
O
N
S2f
OMe
MeO
4.29
1.03
1.88
0.92
1.00
6.12
1.03
1.02
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

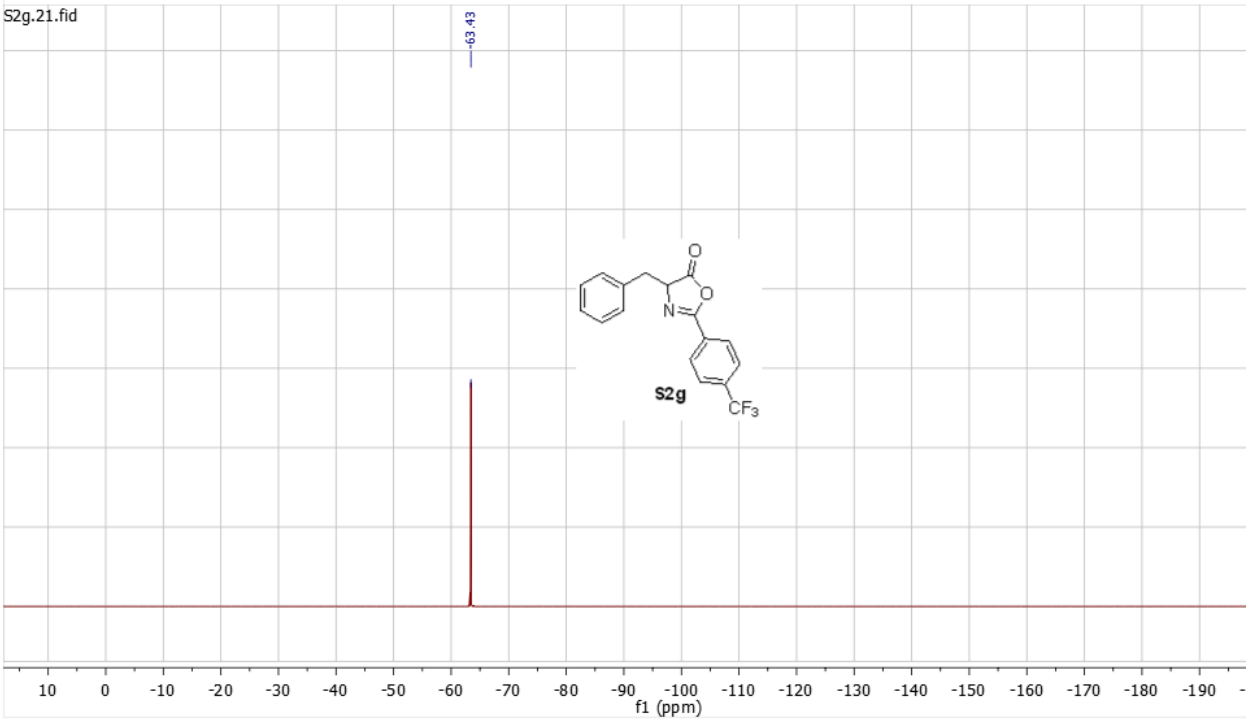

SN-C-79-I.11.fid
177.42
161.60
160.88
135.18
129.56
128.44
127.41
127.23
105.59
105.48
66.61
55.62
37.28
S2f
OMe
MeO
f1 (ppm)

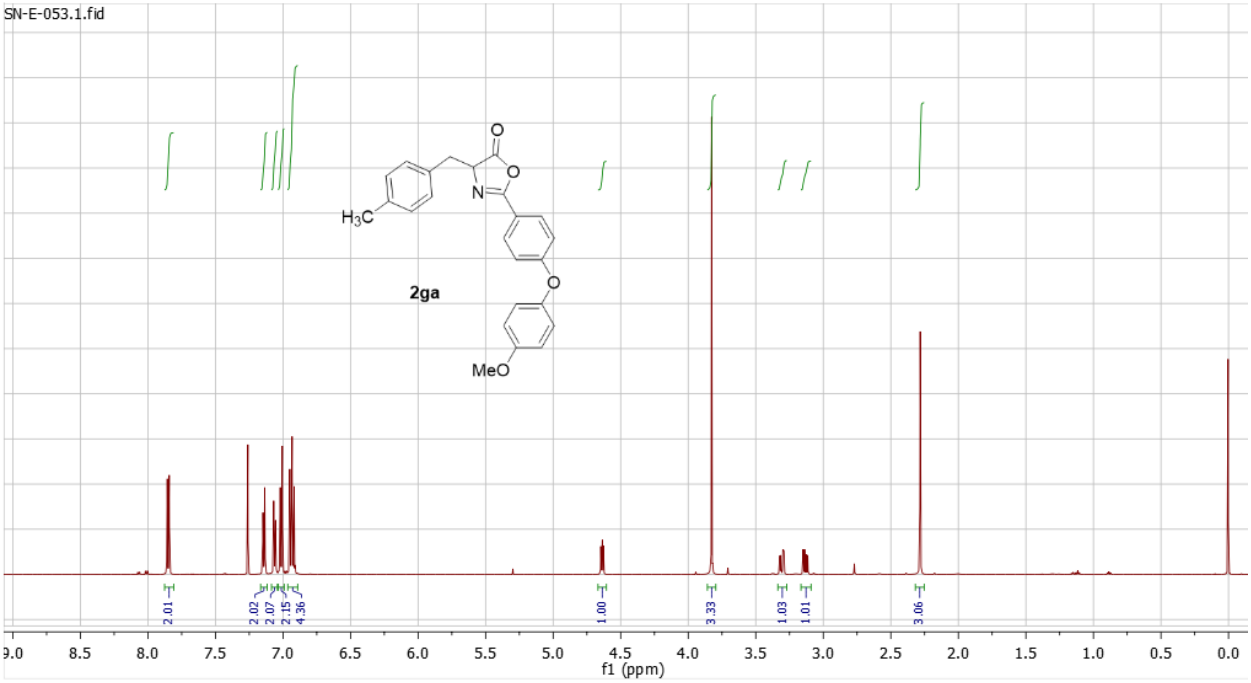

SN-D-16-SM.1.fid
S2g
CF3
2.01
2.10
5.70
1.00
1.10
1.04
f1 (ppm)

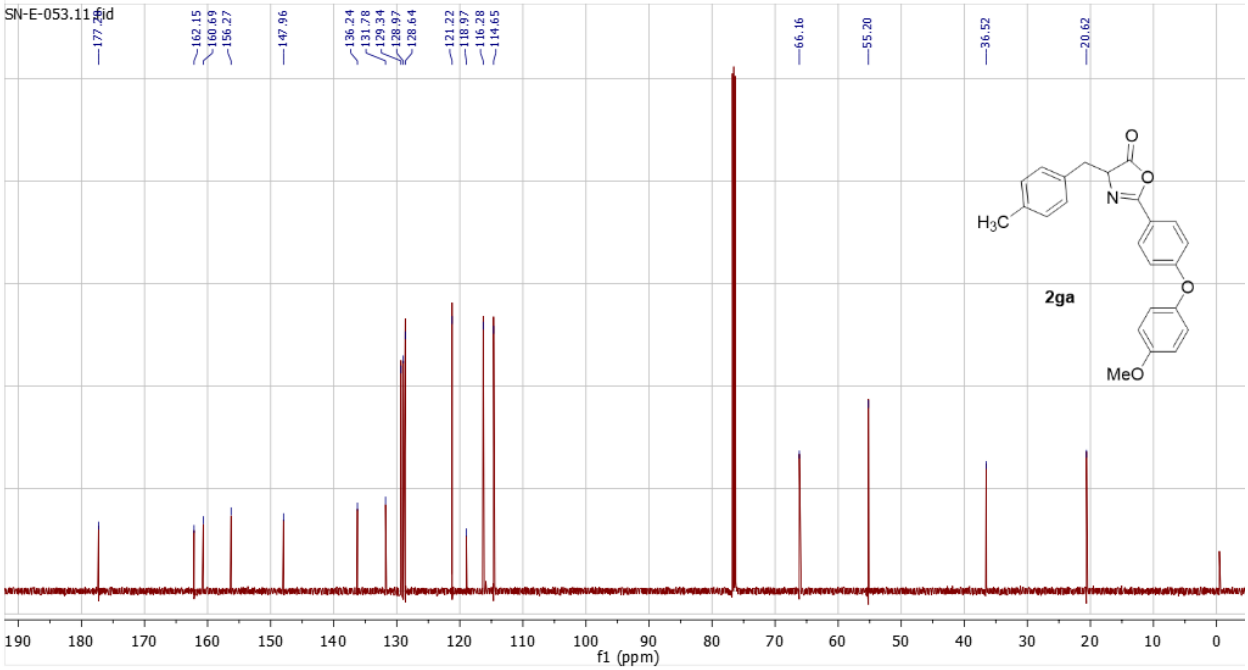

S2h
Cl
1.95
2.07
4.17
1.08
1.00
1.04
1.08
f1 (ppm)

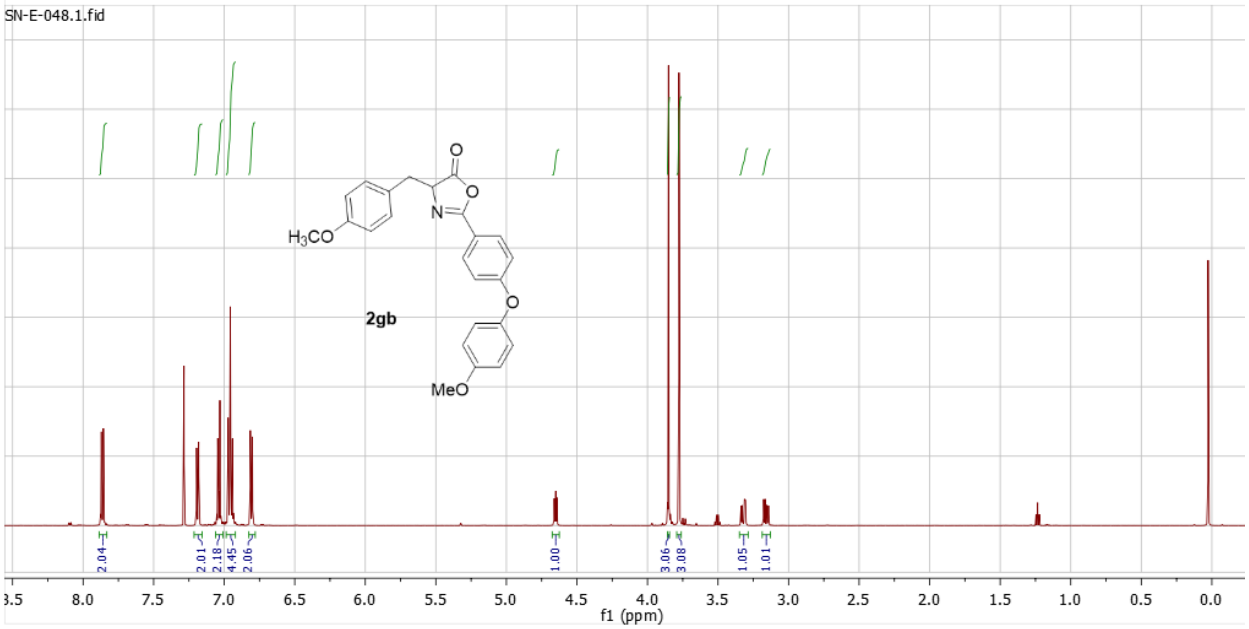

177.3
161.0
139.2
135.2
129.6
129.3
128.5
127.4
124.3
66.73
37.44
S2h
Cl
f1 (ppm)

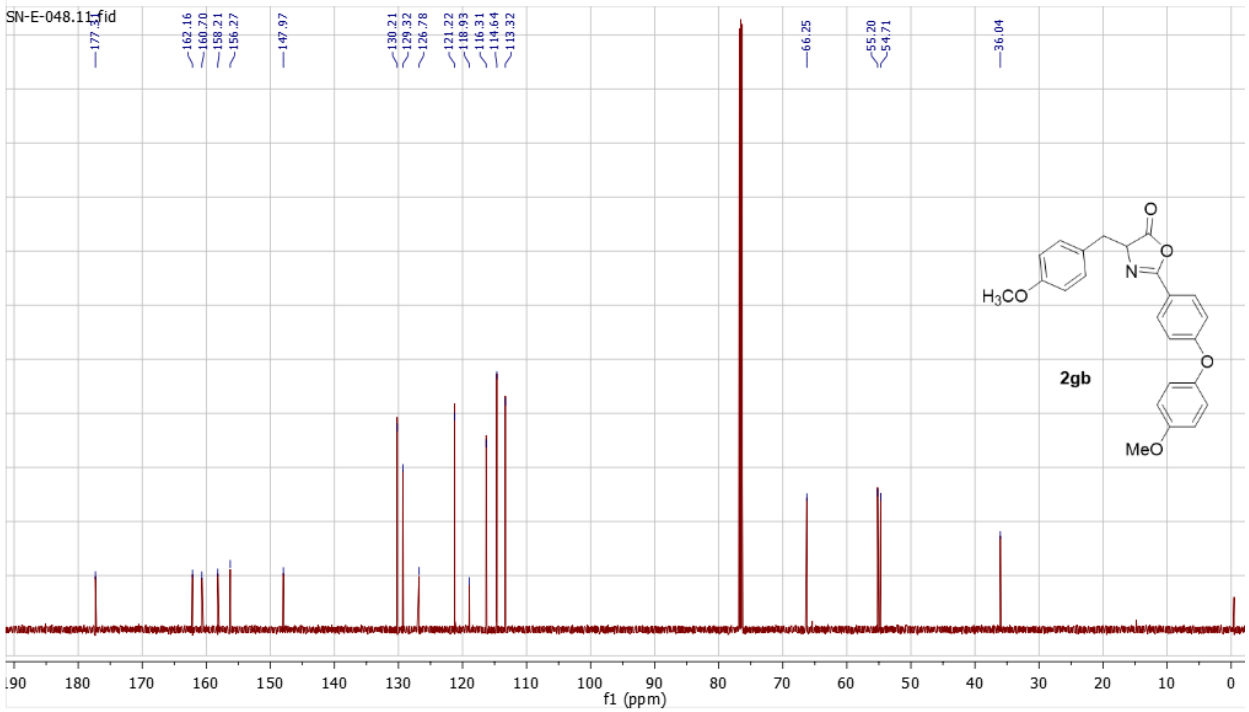

SN-D-16-SM.11.fid
176.4
160.67
134.90
134.58
134.36
134.15
133.93
129.54
129.38
129.04
128.78
128.47
128.25
125.81
125.79
125.76
125.74
124.40
122.59
66.64
37.22
B (q)
134.25
C (q)
123.49
A (q)
125.78
S2g
CF3
0.16
1.00
1.01
f1 (ppm)

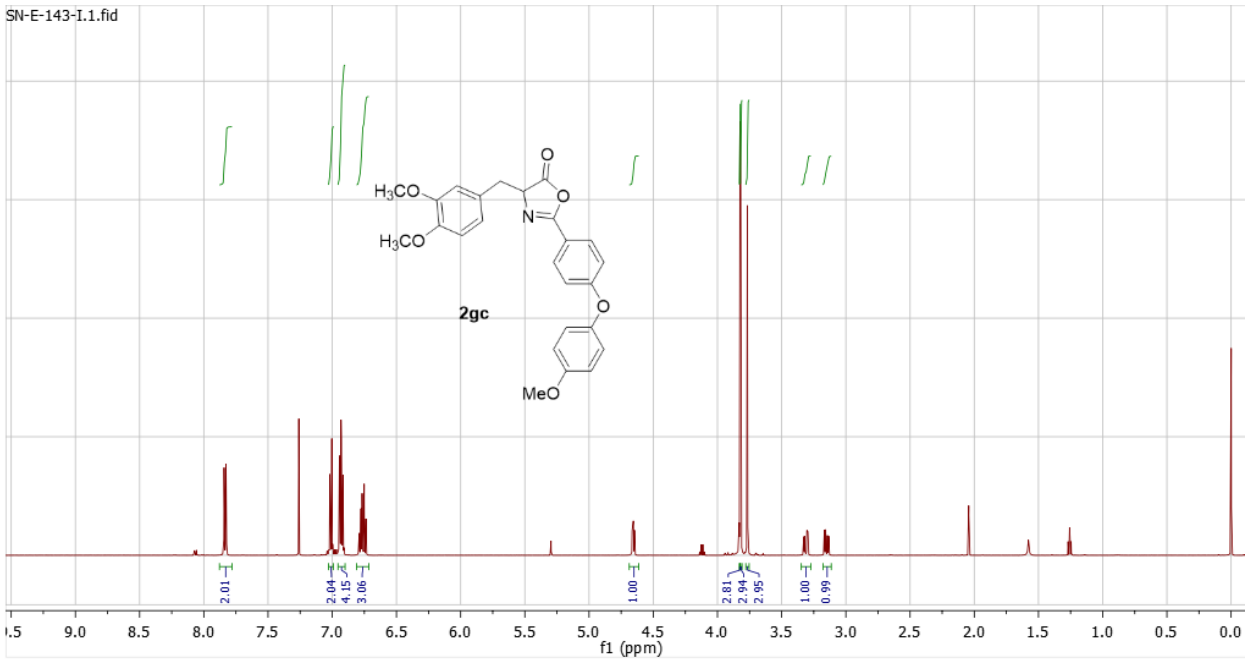

S2g.21.fid
-63.43
O
O
N
S2g
CF3
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

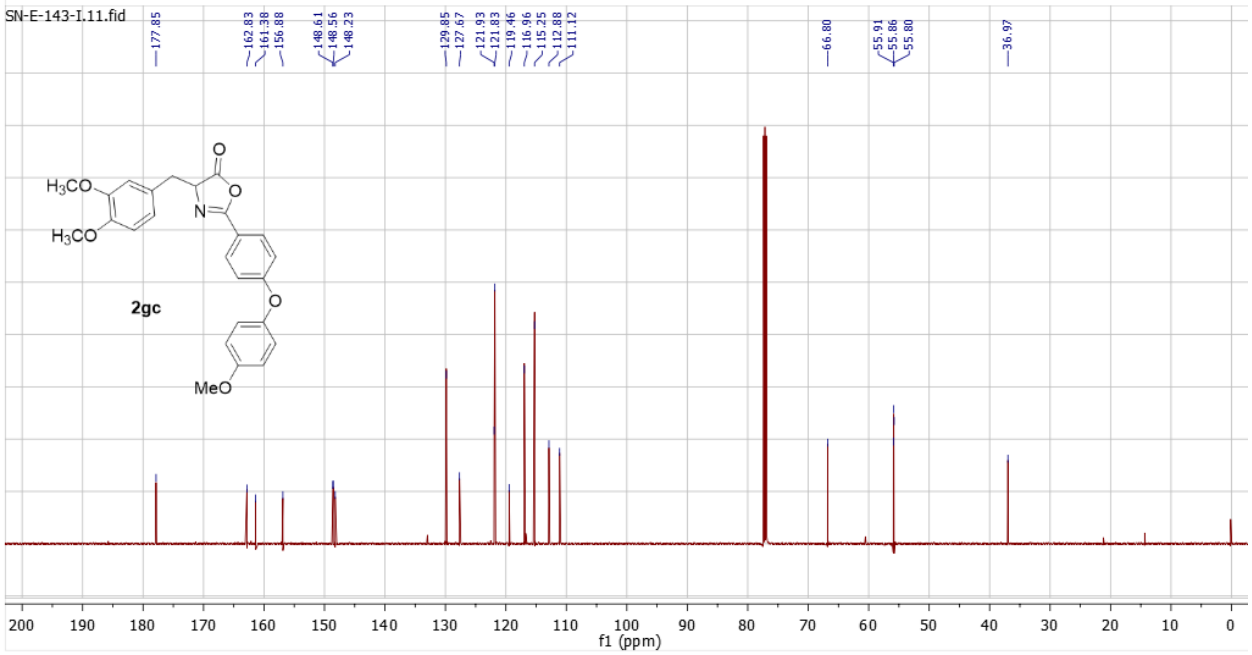

SN-E-053.1.fid
2ga
f1 (ppm)

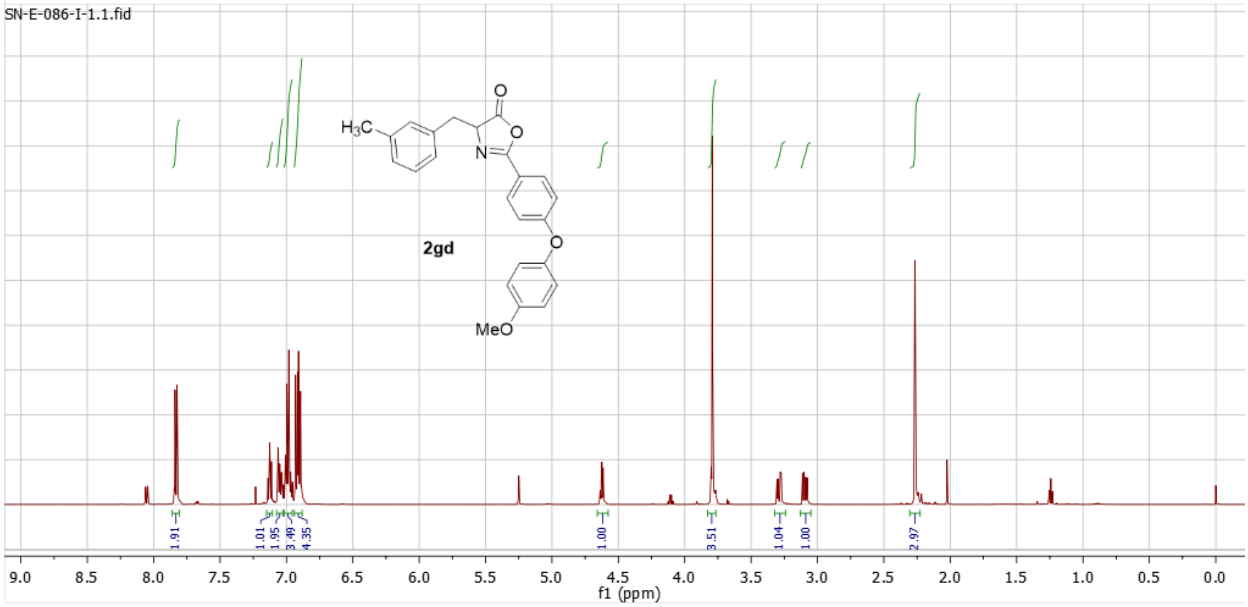

SN-E-053.11.fid
2ga
f1 (ppm)

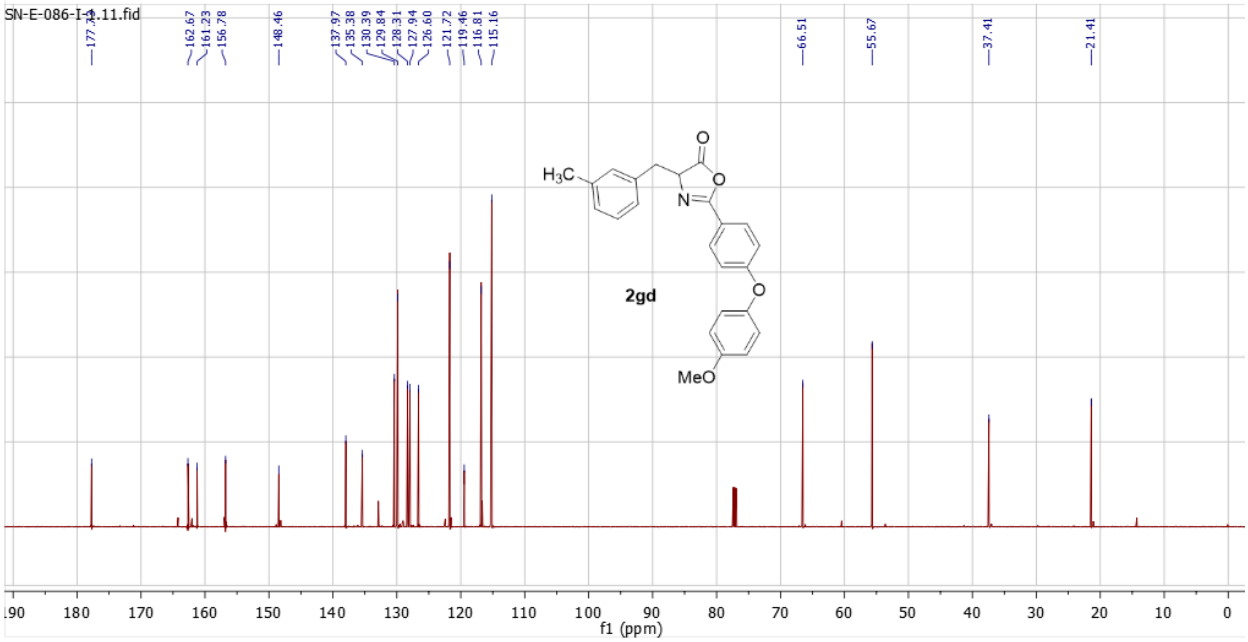

SN-E-048.1.fid
2gb
f1 (ppm)

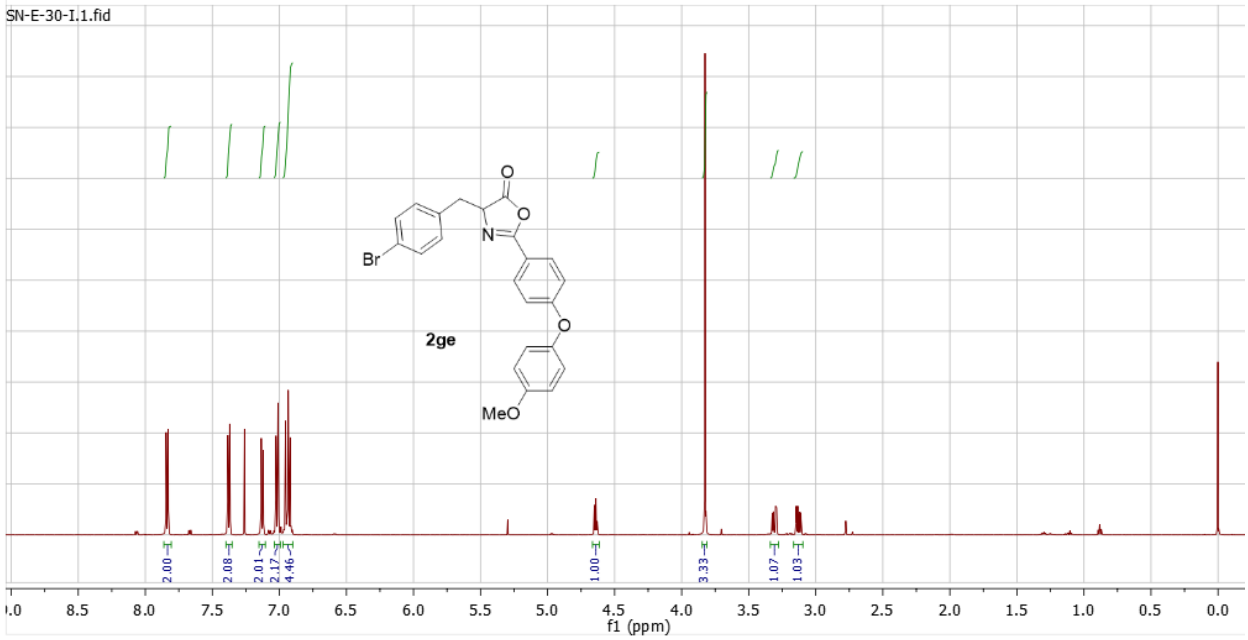

SN-E-048.11.fid
2gb
f1 (ppm)

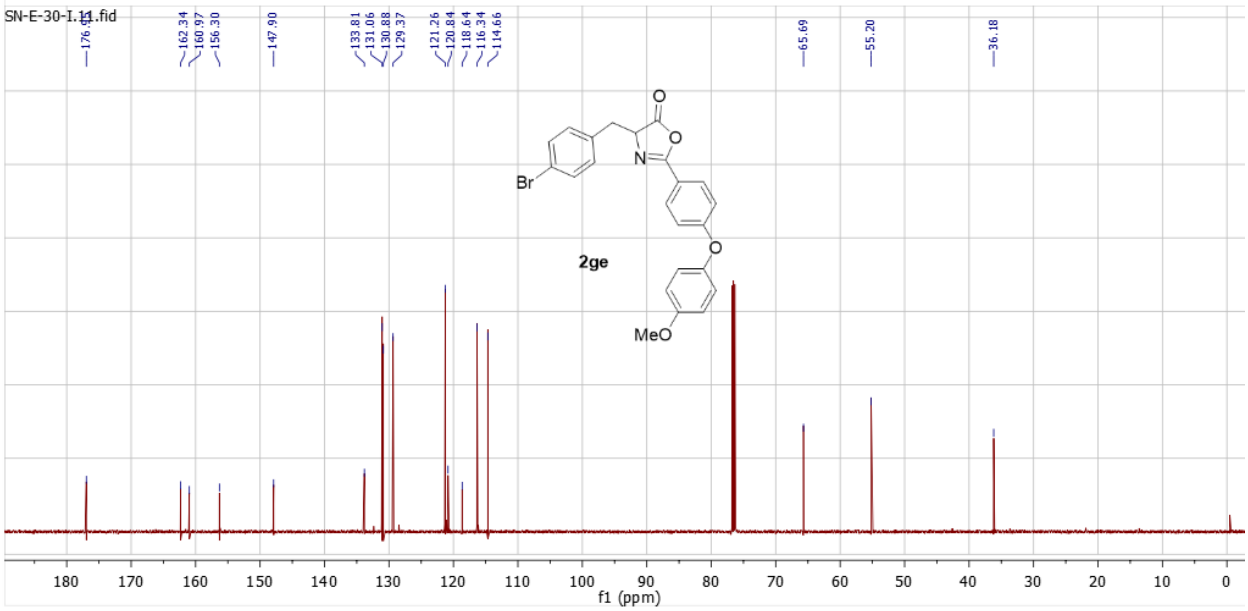

SN-E-143-I.1.fid
H3CO
H3CO
O
O
N
O
2gc
MeO
2.01
2.04
4.15
3.06
1.00
2.81
2.94
2.95
1.00
0.99
f1 (ppm)

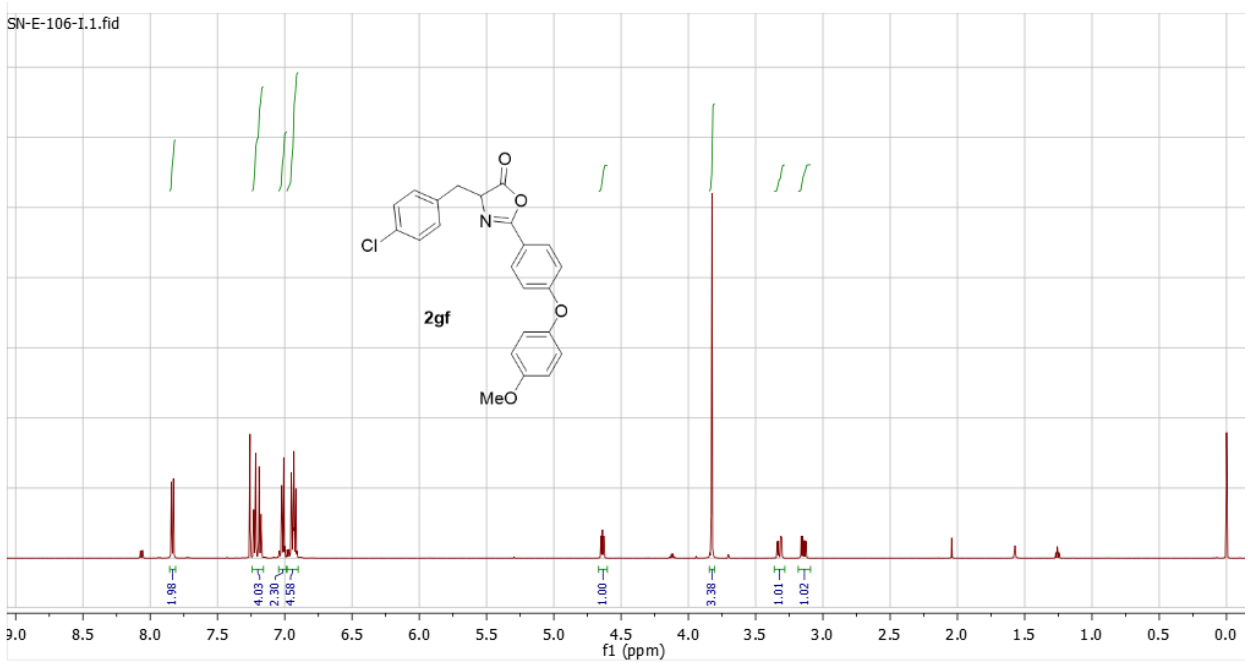

SN-E-143-I.11.fid
177.85
162.83
161.38
156.88
148.61
148.56
148.23
129.85
127.67
121.93
121.83
119.46
116.96
115.25
112.88
111.12
66.80
55.91
55.86
55.80
36.97
H3CO
H3CO
O
O
N
O
2gc
MeO
f1 (ppm)

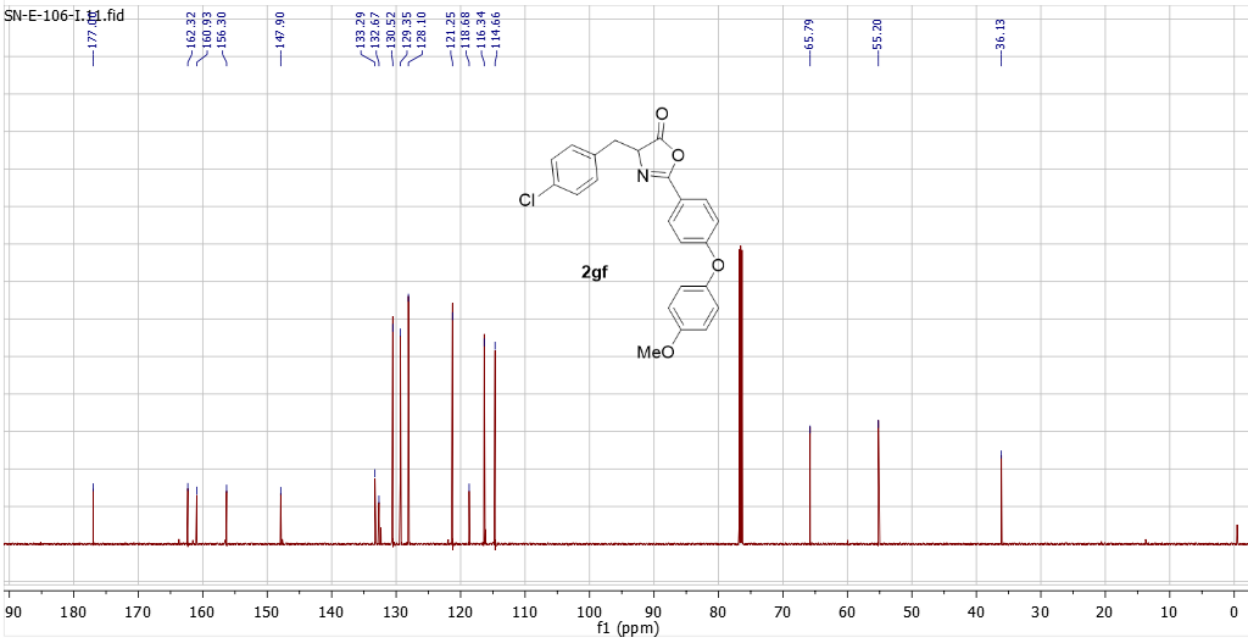

SN-E-086-I-1.1.fid
2gd
MeO
1.91
1.01
1.95
3.49
4.35
1.00
3.51
1.04
1.00
2.97
f1 (ppm)

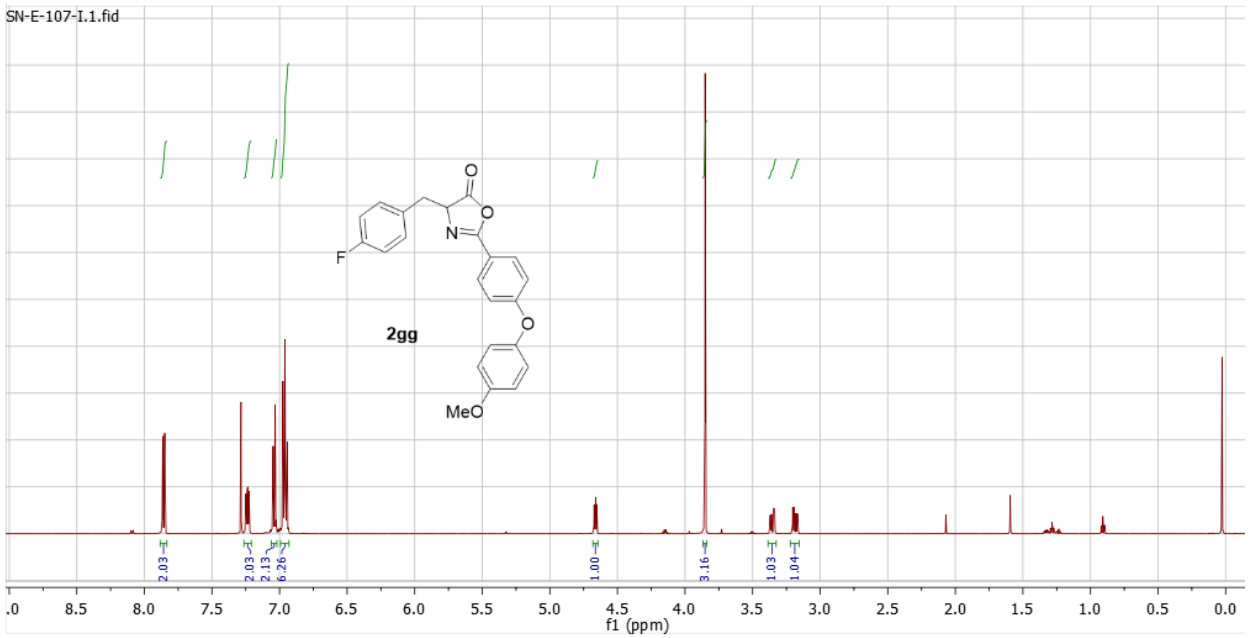

SN-E-086-I-1.11.fid
177.44
162.67
161.23
156.78
148.46
137.97
135.38
130.39
129.84
128.31
127.94
126.60
121.72
119.46
116.81
115.16
66.51
55.67
37.41
21.41
2gd
MeO
f1 (ppm)

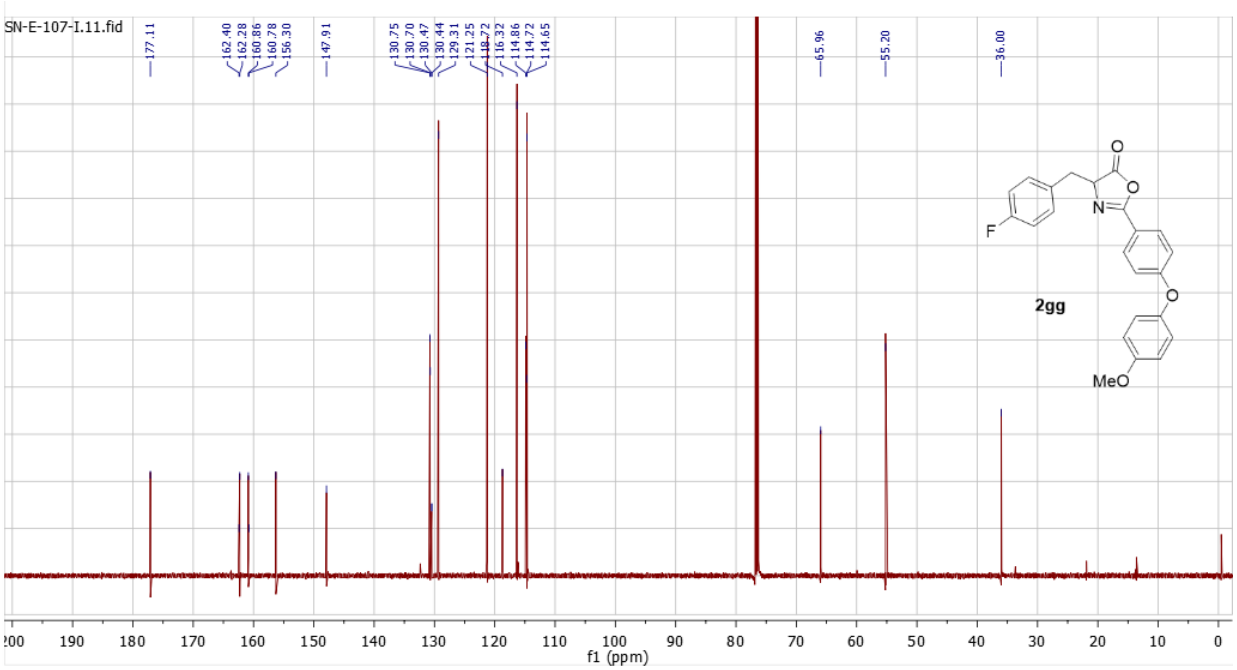

SN-E-30-I.1.fid
2ge
Br
MeO
2.00
2.08
2.01
2.17
4.46
1.00
3.33
1.07
1.03
f1 (ppm)

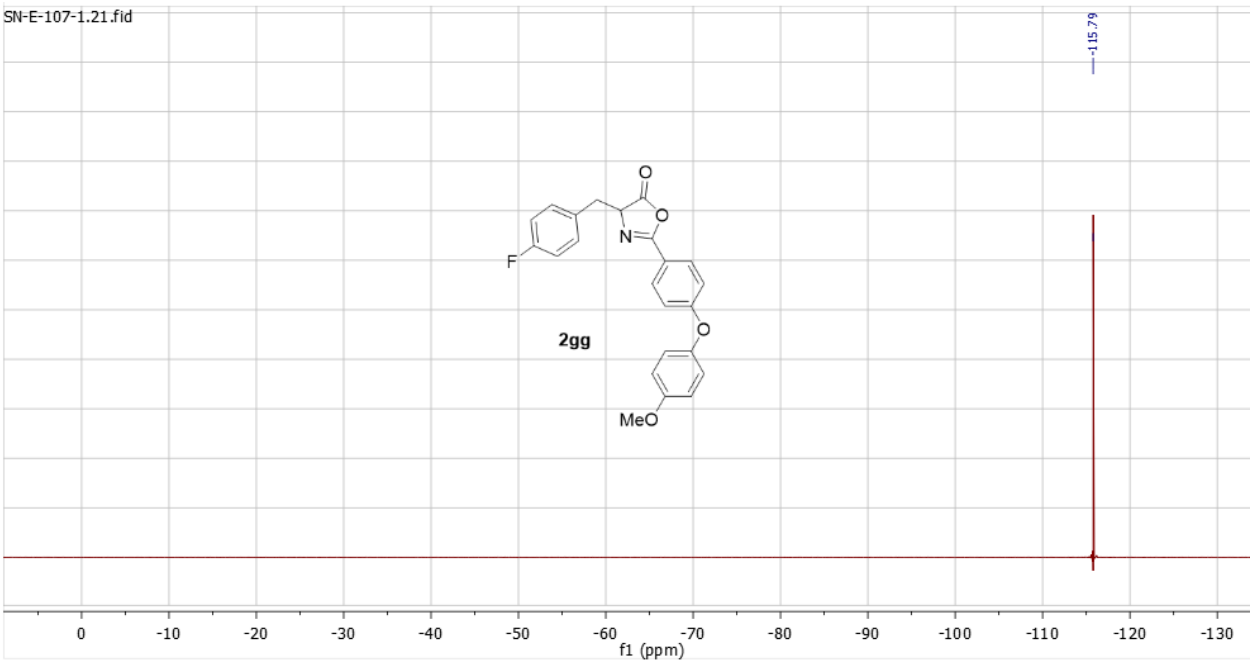

SN-E-30-I.1.fid
176.41
162.34
160.97
156.30
147.90
133.81
131.06
130.88
129.37
121.26
120.84
118.64
116.34
114.66
65.69
55.20
36.18
2ge
Br
MeO
f1 (ppm)

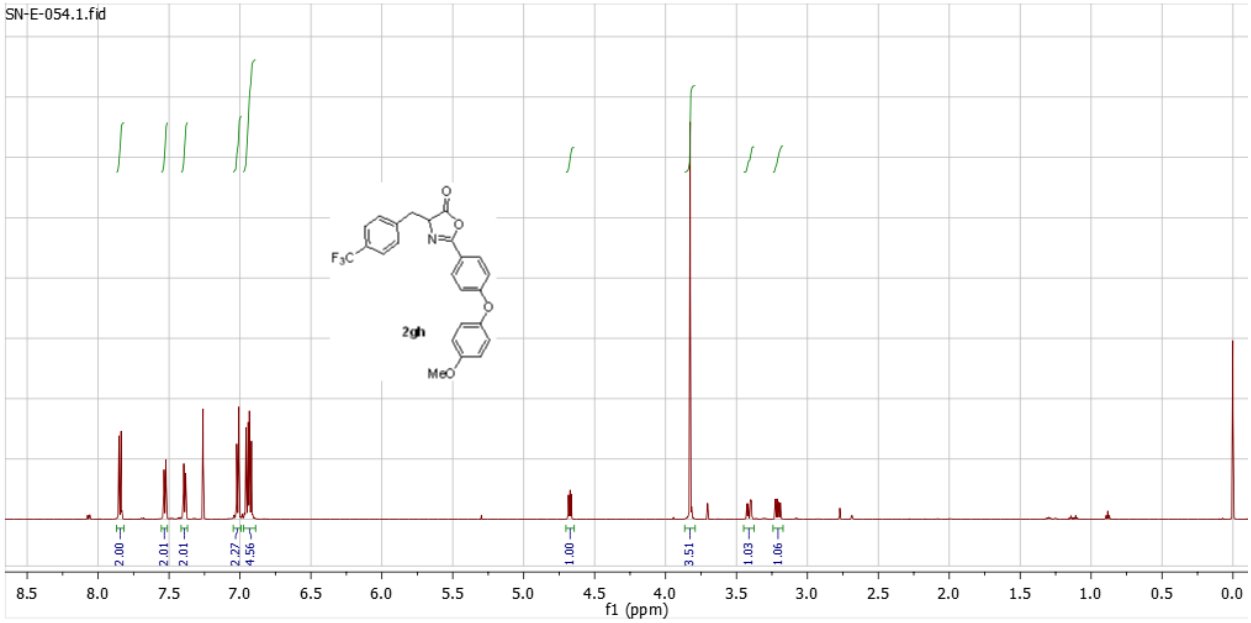

SN-E-106-I.1.fid
Cl
O
O
N
O
2gf
O
MeO
1.98
4.03
2.30
4.58
1.00
3.38
1.01
1.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

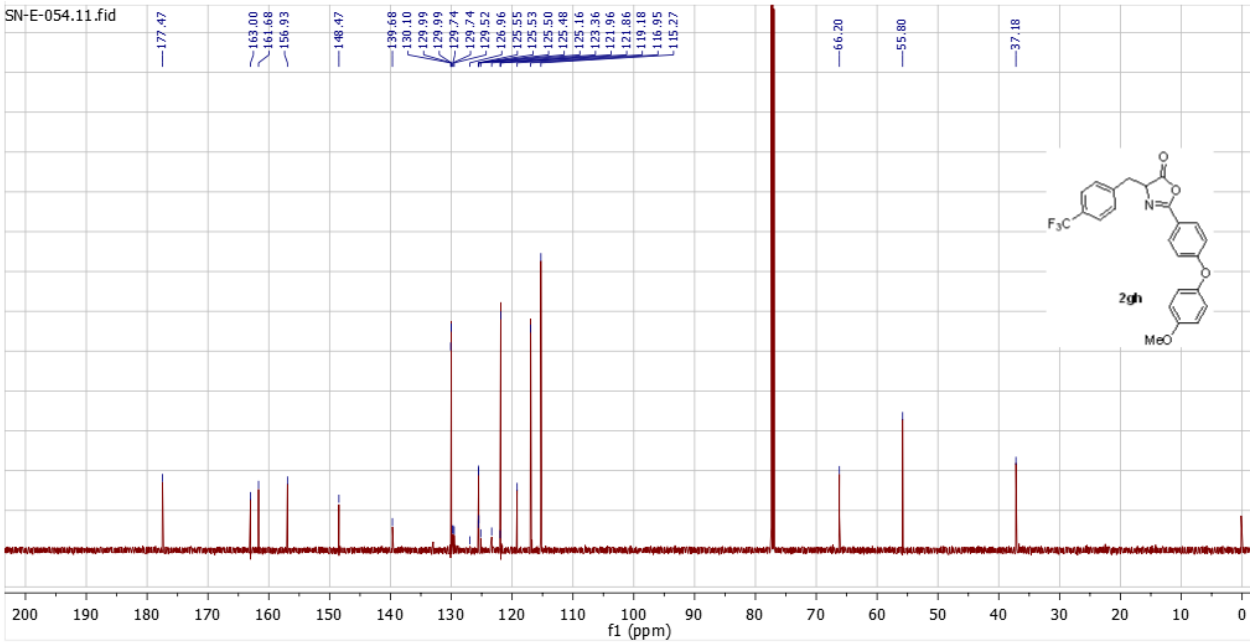

SN-E-106-I.1.fid
177.15
162.32
160.93
156.30
147.90
133.29
132.67
130.52
129.35
128.10
121.25
118.68
116.34
114.66
65.79
55.20
36.13
Cl
O
O
N
O
2gf
O
MeO
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

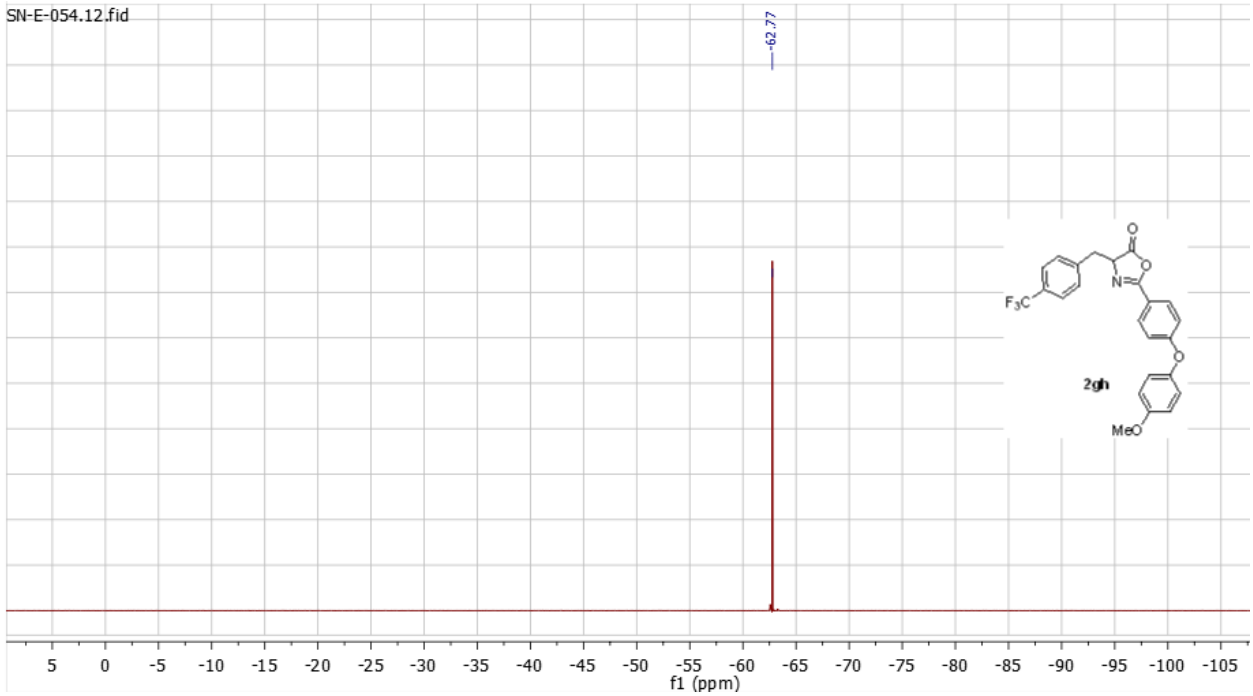

SN-E-107-I.1.fid
2gg
f1 (ppm)

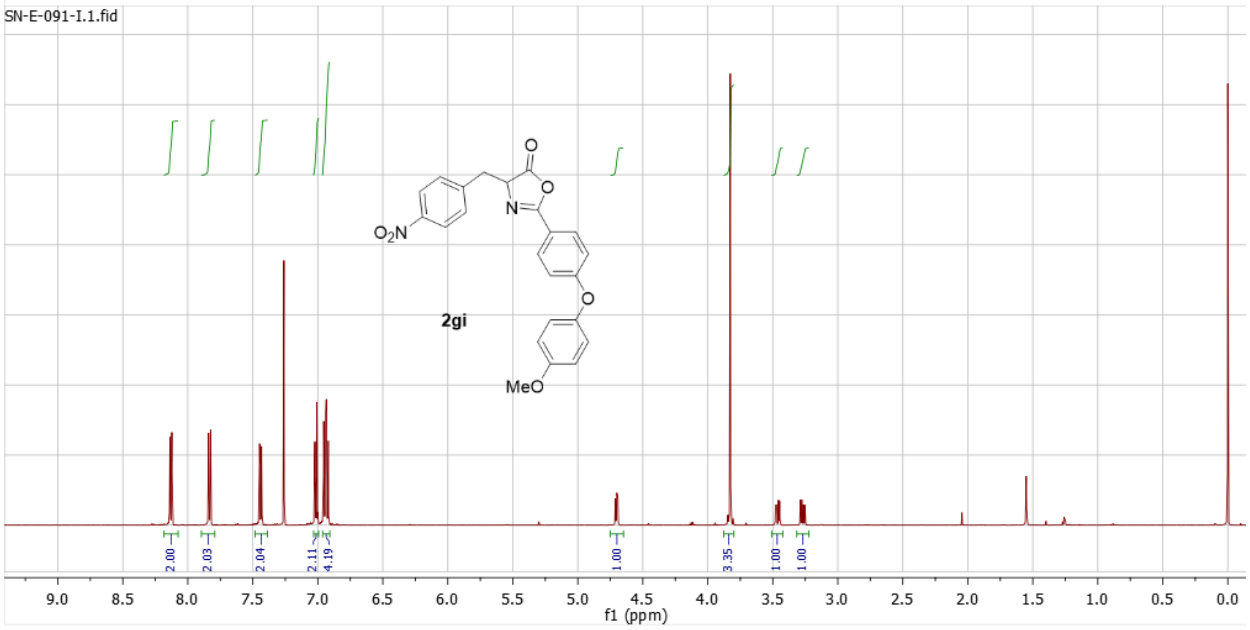

SN-E-107-I.11.fid
2gg
f1 (ppm)

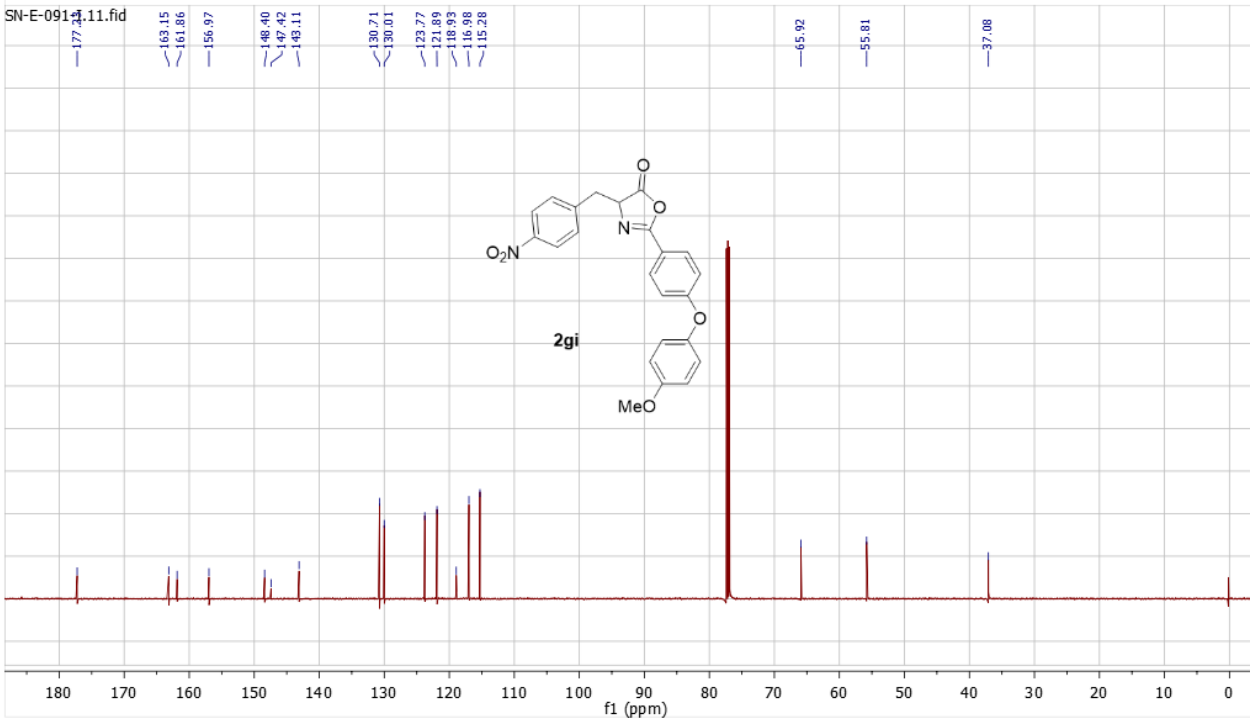

SN-E-107-1.21.fid
-115.79
O
O
N
F
2gg
O
MeO
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
f1 (ppm)

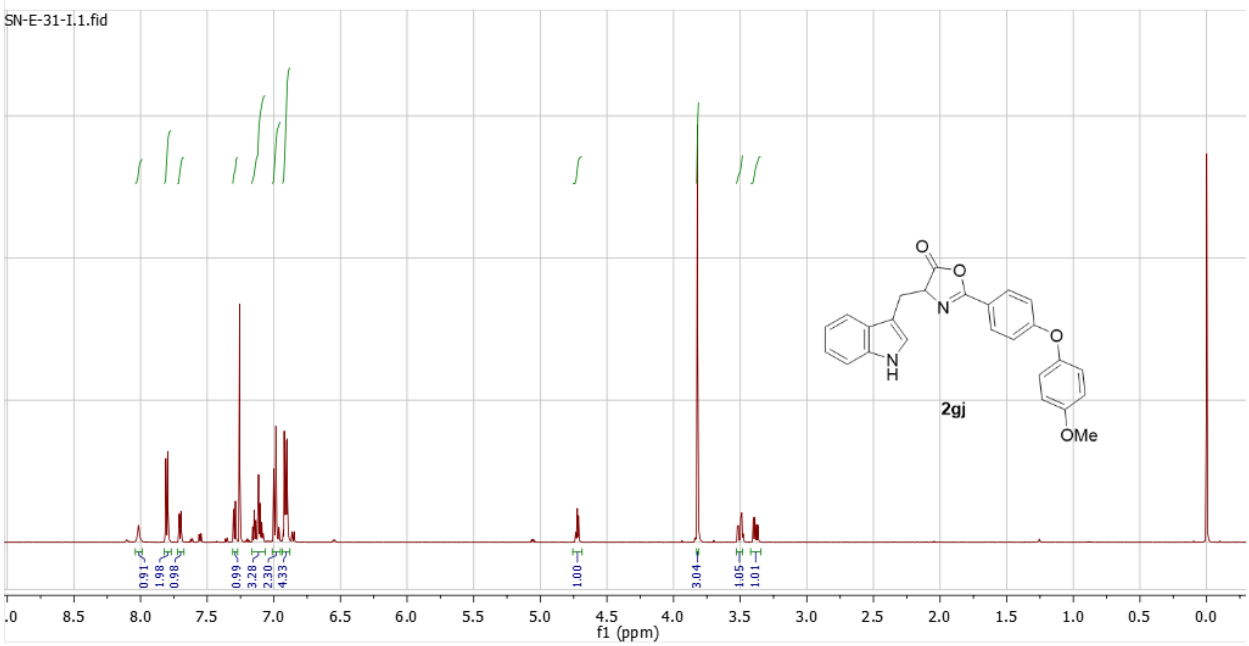

SN-E-054.1.fid
O
O
N
F3C
2gh
O
MeO
2.00
2.01
2.01
2.27
4.56
1.00
3.51
1.03
1.06
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

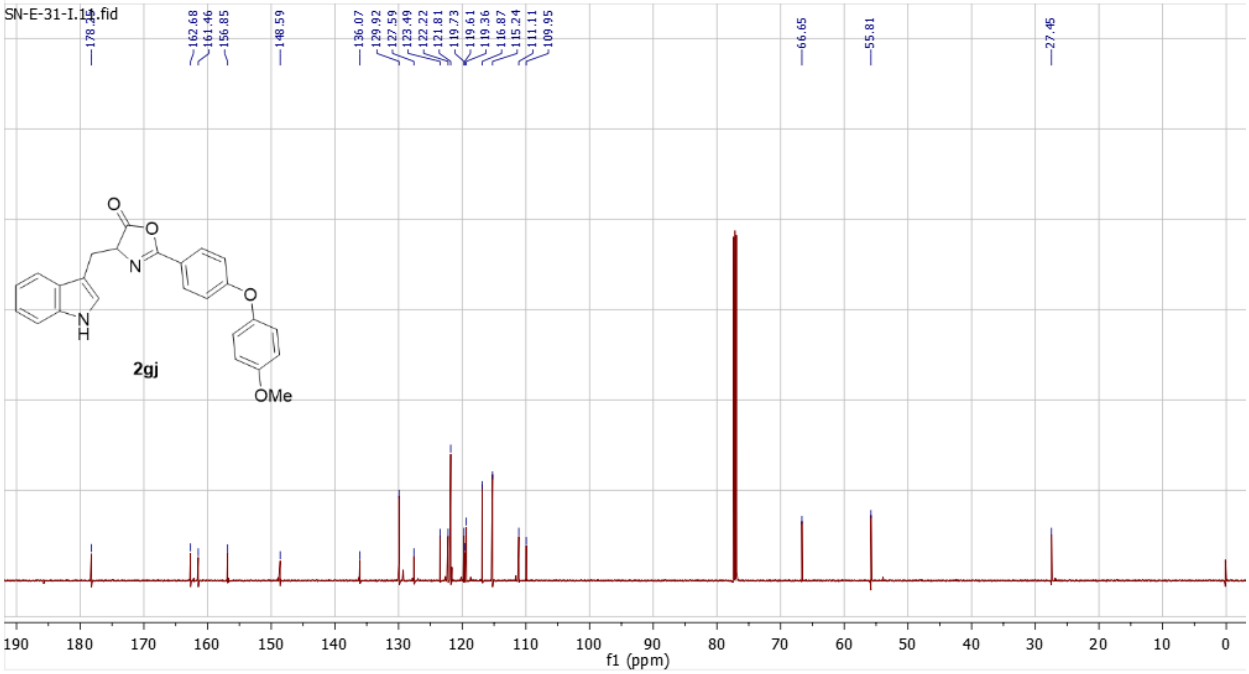

SN-E-054.11.fid
177.47
163.00
161.68
156.93
148.47
139.68
130.10
129.99
129.99
129.74
129.74
129.52
126.96
125.55
125.53
125.50
125.48
125.16
123.36
121.96
121.86
119.18
116.95
115.27
66.20
55.80
37.18
F3C
2gh
MeO
f1 (ppm)

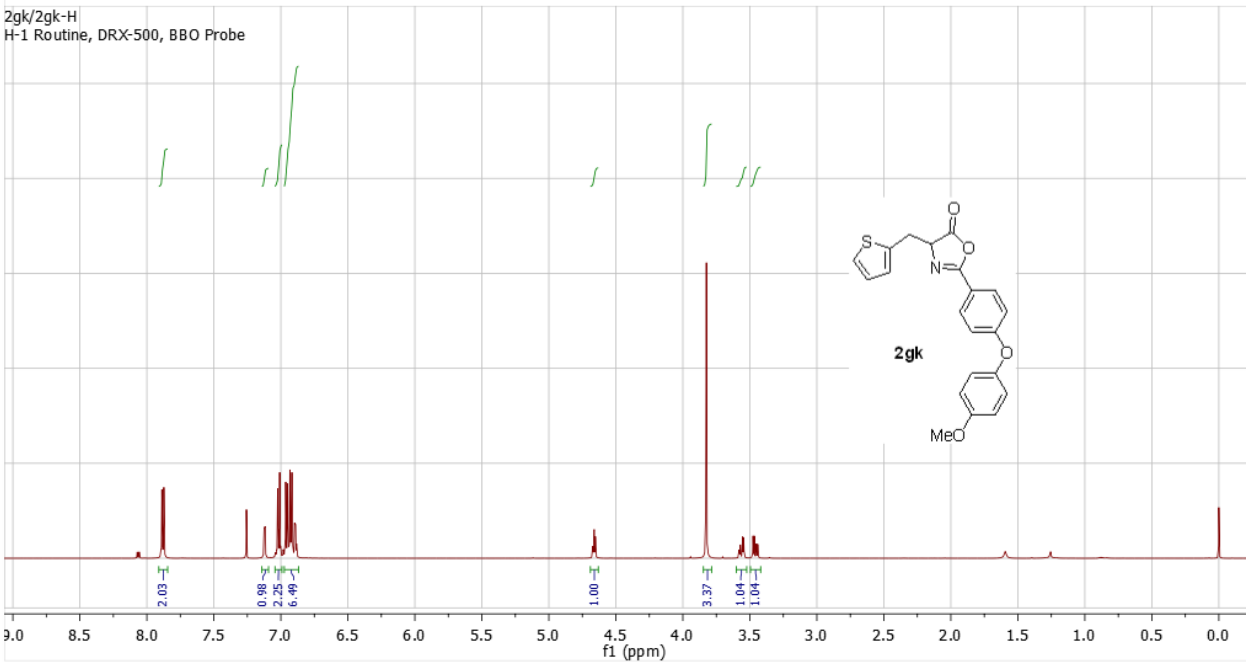

SN-E-054.12.fid
-62.77
F3C
2gh
MeO
f1 (ppm)

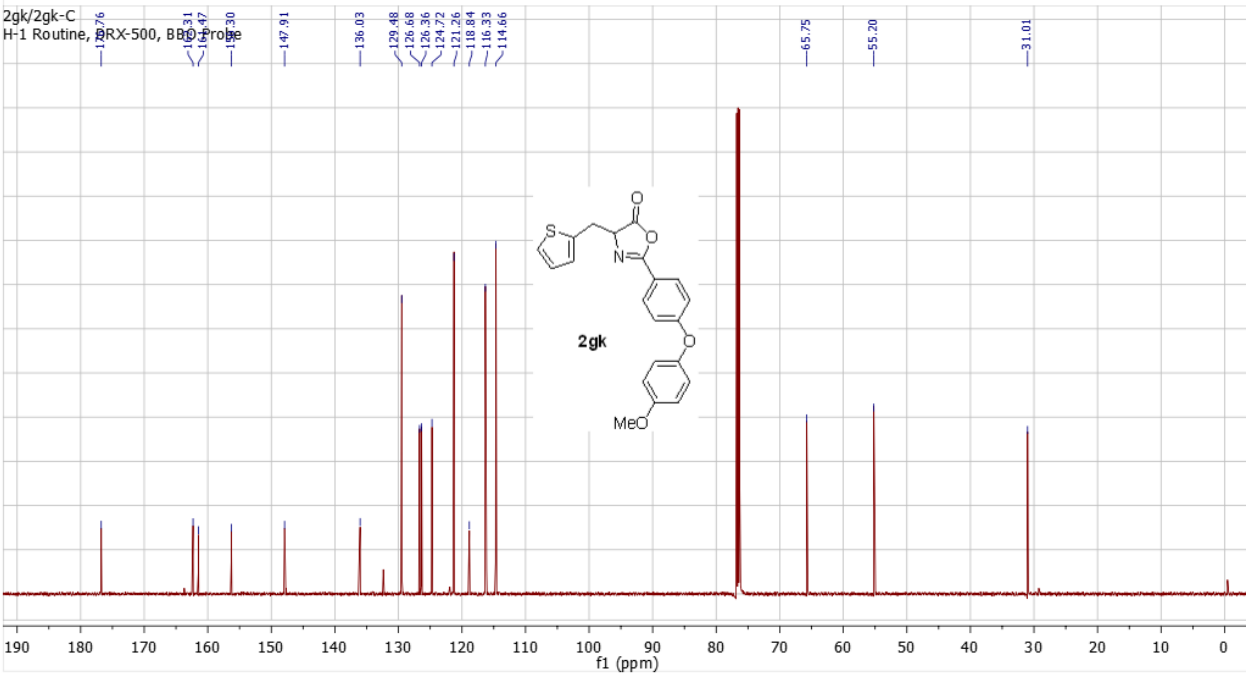

SN-E-091-I.1.fid
2gi
MeO
2.00
2.03
2.04
2.11
4.19
1.00
3.35
1.00
1.00
f1 (ppm)

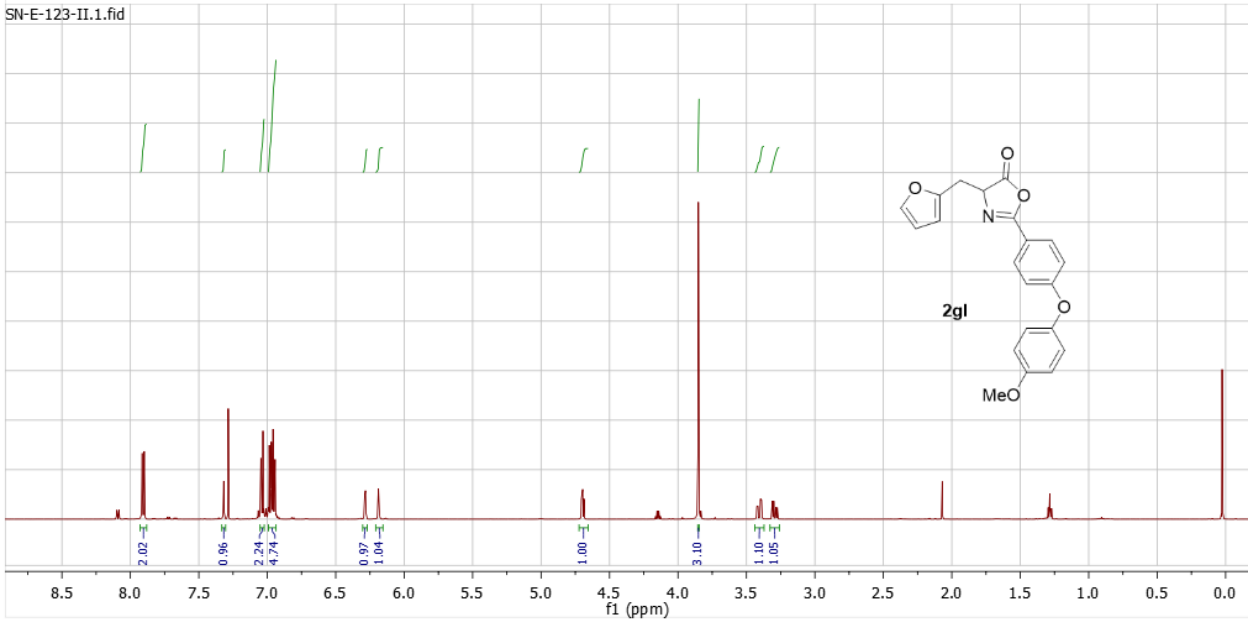

SN-E-091-I.11.fid
177.21
163.15
161.86
156.97
148.40
147.42
143.11
130.71
130.01
123.77
121.89
118.93
116.98
115.28
65.92
55.81
37.08
2gi
MeO
f1 (ppm)

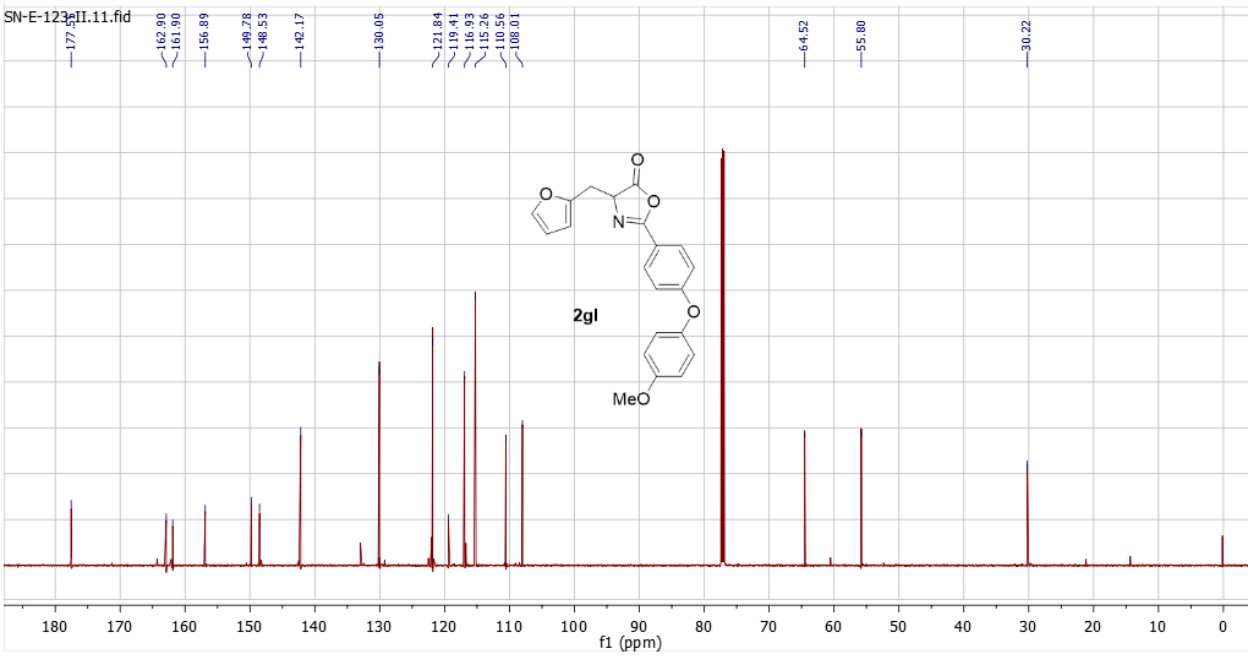

SN-E-31-I.1.fid
0.91
1.98
0.98
0.99
3.28
2.30
4.33
1.00
3.04
1.05
1.01
f1 (ppm)
2gj
OMe

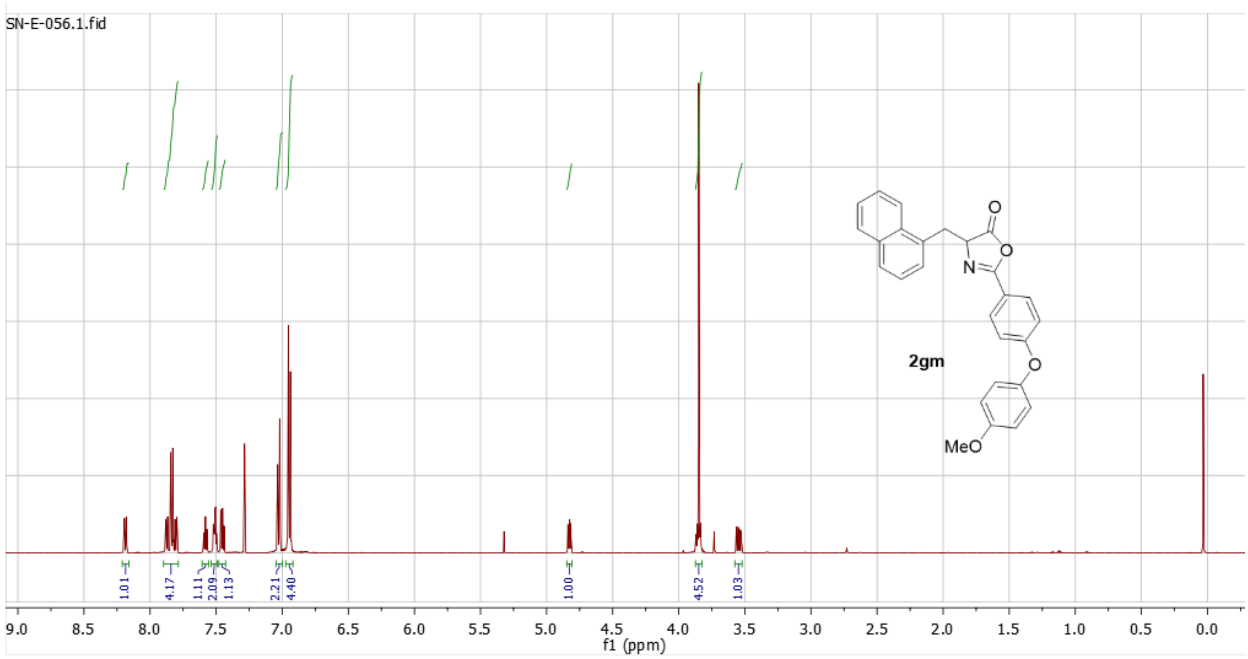

SN-E-31-I.13.fid
178.44
162.68
161.46
156.85
148.59
136.07
129.92
127.59
123.49
122.22
121.81
119.73
119.61
119.36
116.87
115.24
111.11
109.95
66.65
55.81
27.45
f1 (ppm)
2gj
OMe

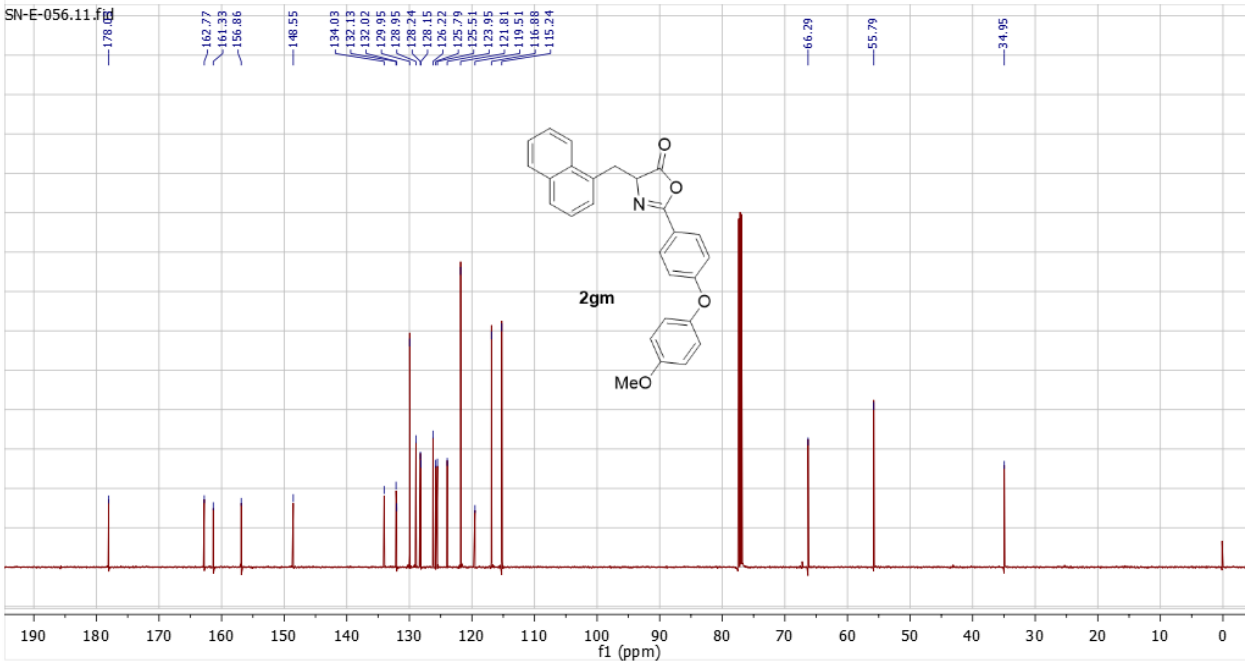

2gk/2gk-H
H-1 Routine, DRX-500, BBO Probe
2gk
MeO
f1 (ppm)

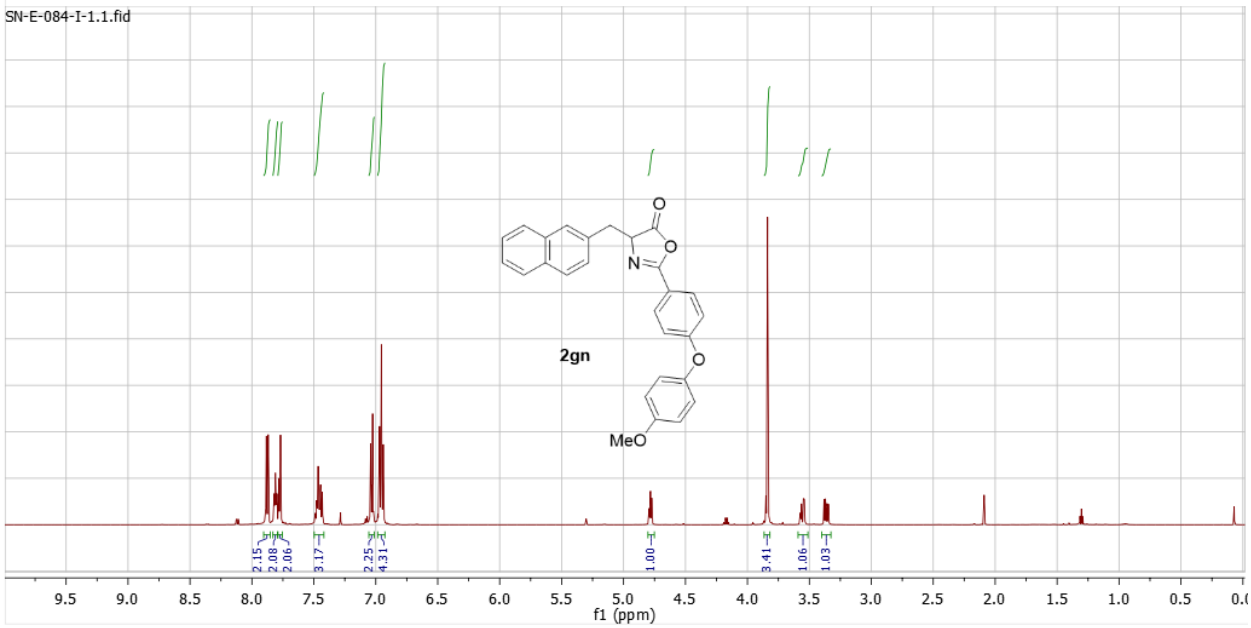

2gk/2gk-C
H-1 Routine, DRX-500, BBO Probe
2gk
MeO
f1 (ppm)

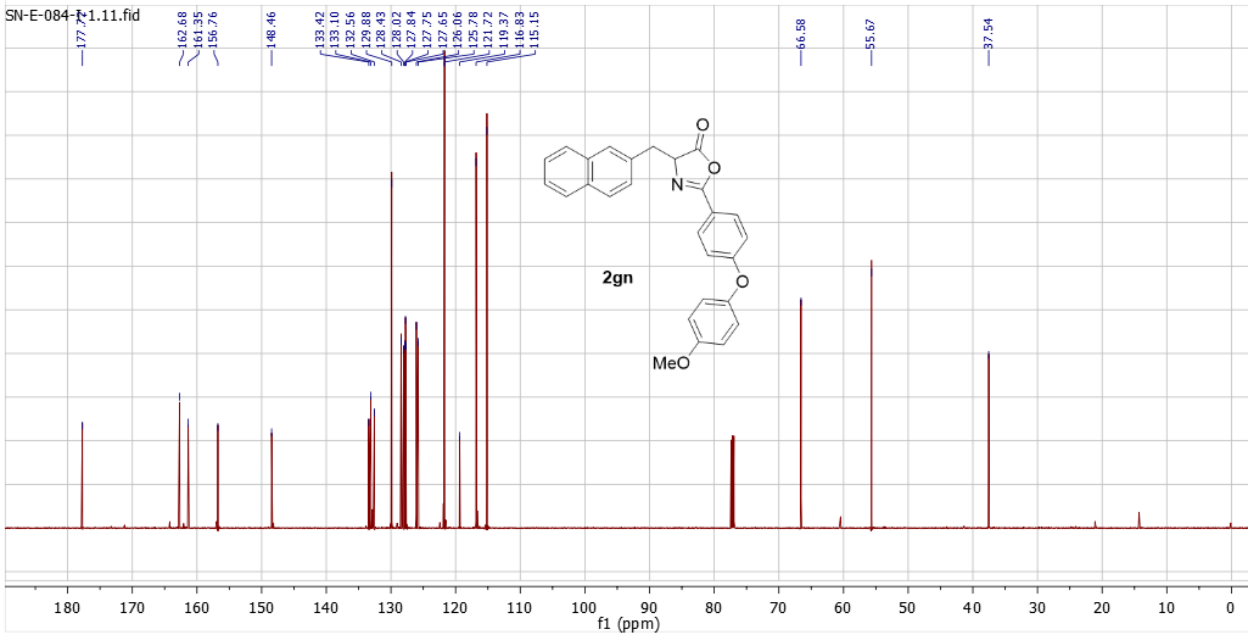

SN-E-123-II.1.fid
2gl
MeO
f1 (ppm)

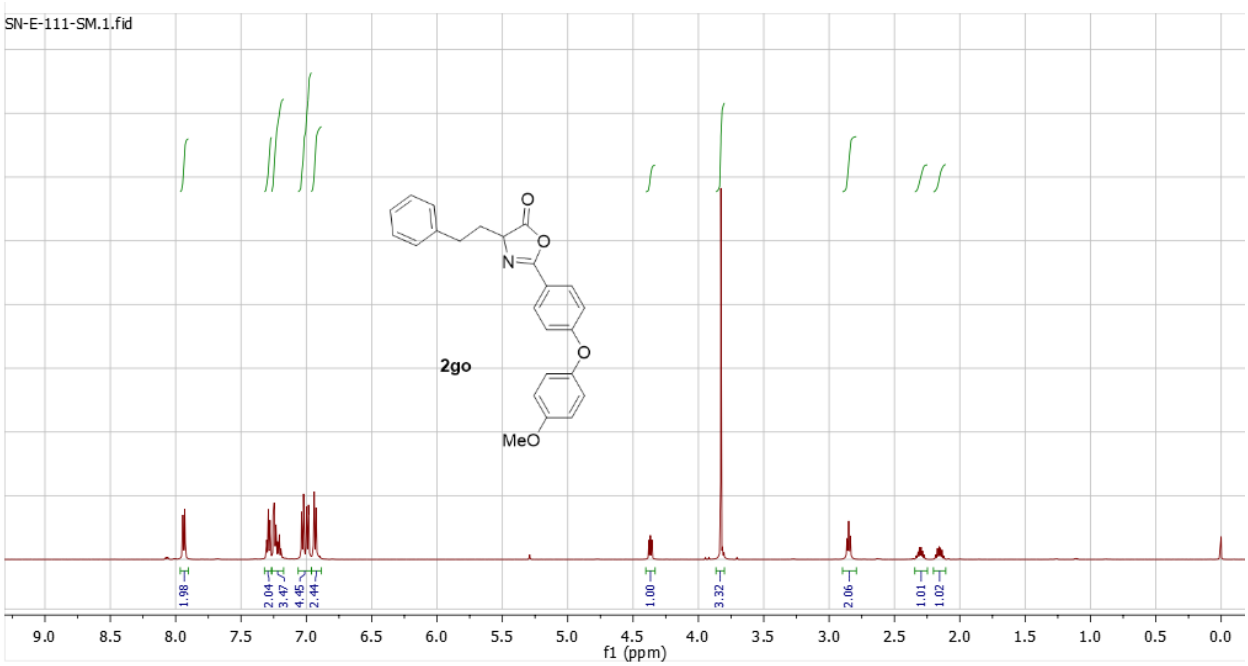

SN-E-123-II.11.fid
2gl
MeO
f1 (ppm)

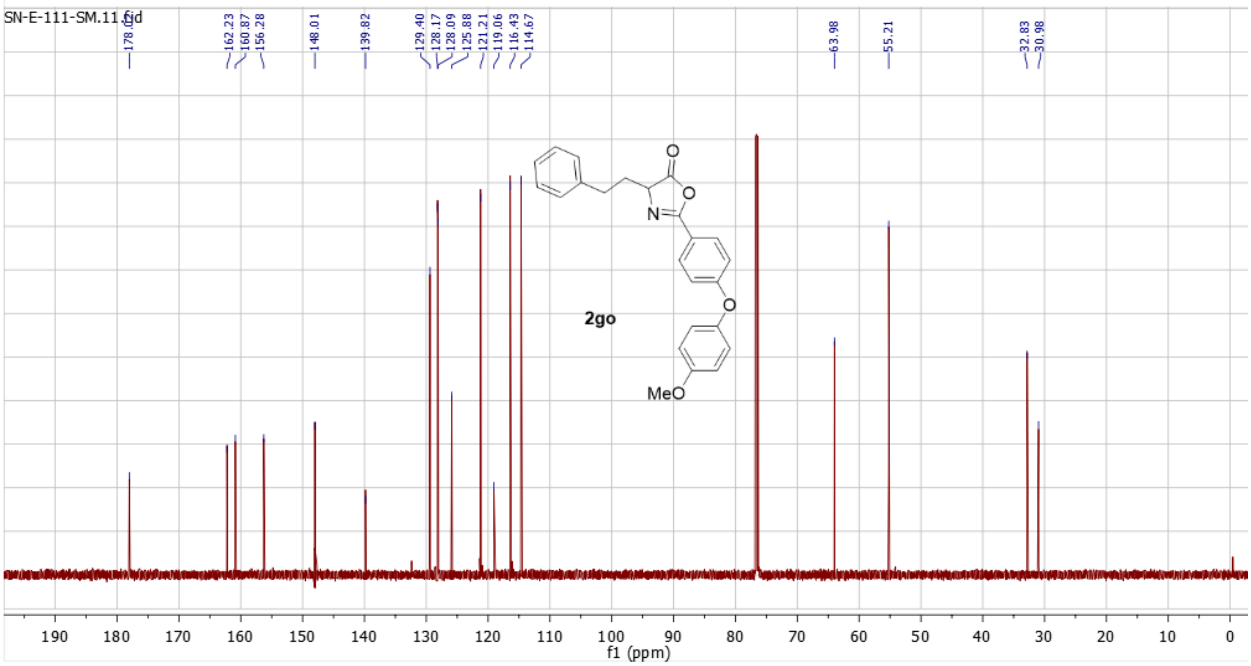

SN-E-056.1.fid
2gm
MeO
1.01
4.17
1.11
2.09
1.13
2.21
4.40
1.00
4.52
1.03
f1 (ppm)

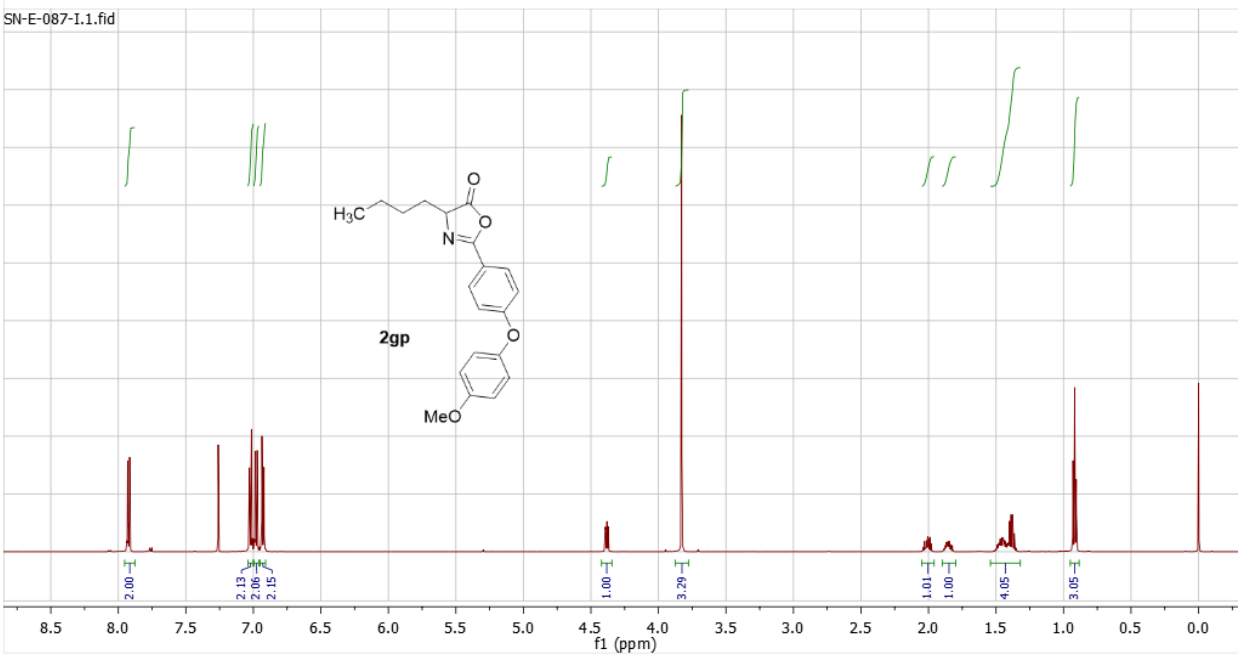

SN-E-056.11.fid
178.68
162.77
161.33
156.86
148.55
134.03
132.13
132.02
129.95
128.95
128.24
128.15
126.22
125.79
125.51
123.95
121.81
119.51
116.88
115.24
66.29
55.79
34.95
2gm
MeO
f1 (ppm)

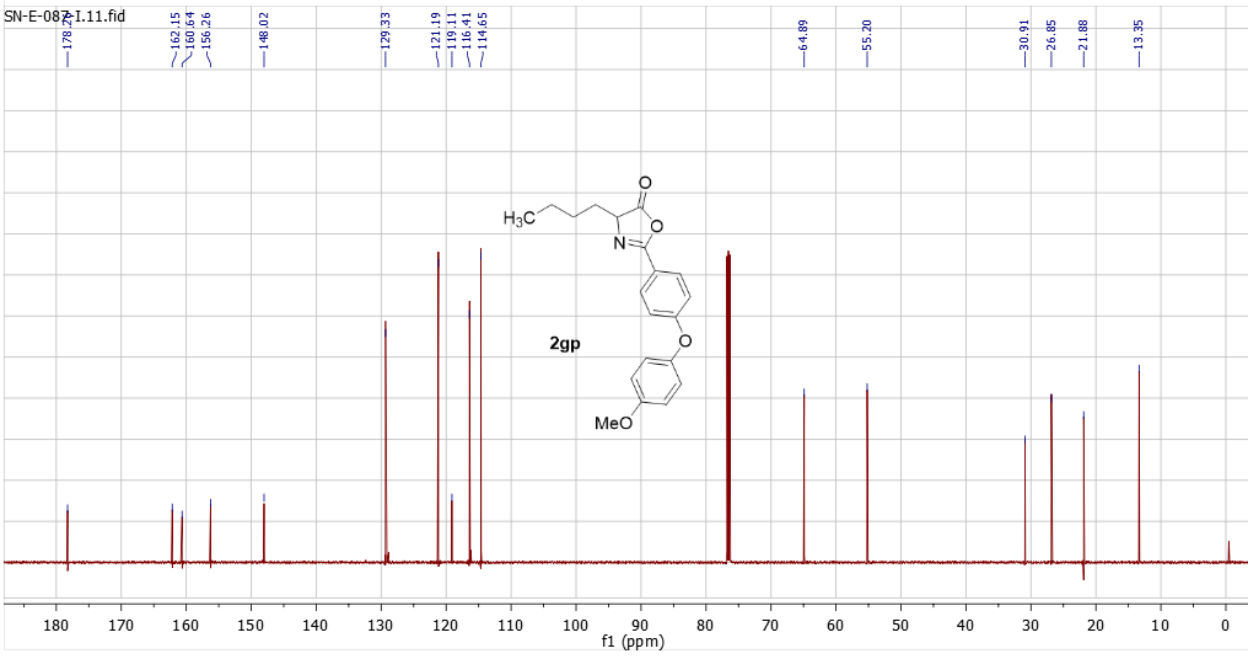

SN-E-084-I-1.1.fid
2gn
MeO
2.15
2.08
2.06
3.17
2.25
4.31
1.00
3.41
1.06
1.03
f1 (ppm)

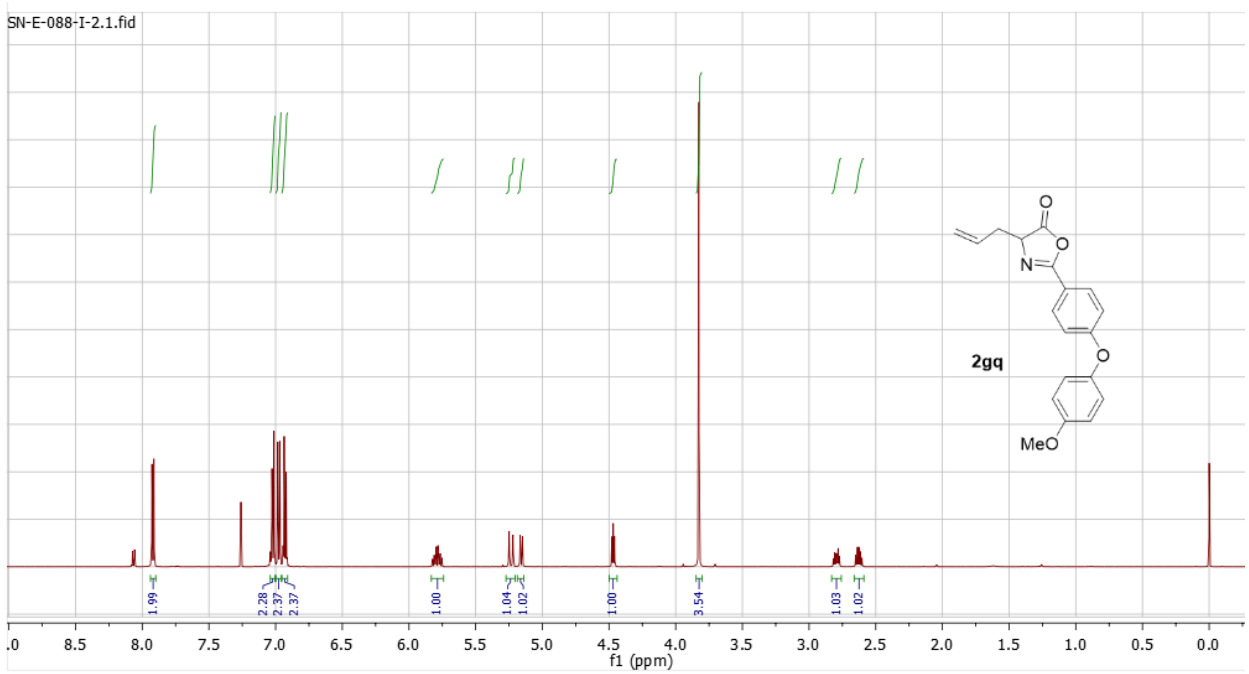

SN-E-084-I-1.11.fid
177.72
162.68
161.35
156.76
148.46
133.42
133.10
132.56
129.88
128.43
128.02
127.84
127.75
127.65
126.06
125.78
121.72
119.37
116.83
115.15
66.58
55.67
37.54
2gn
MeO
f1 (ppm)

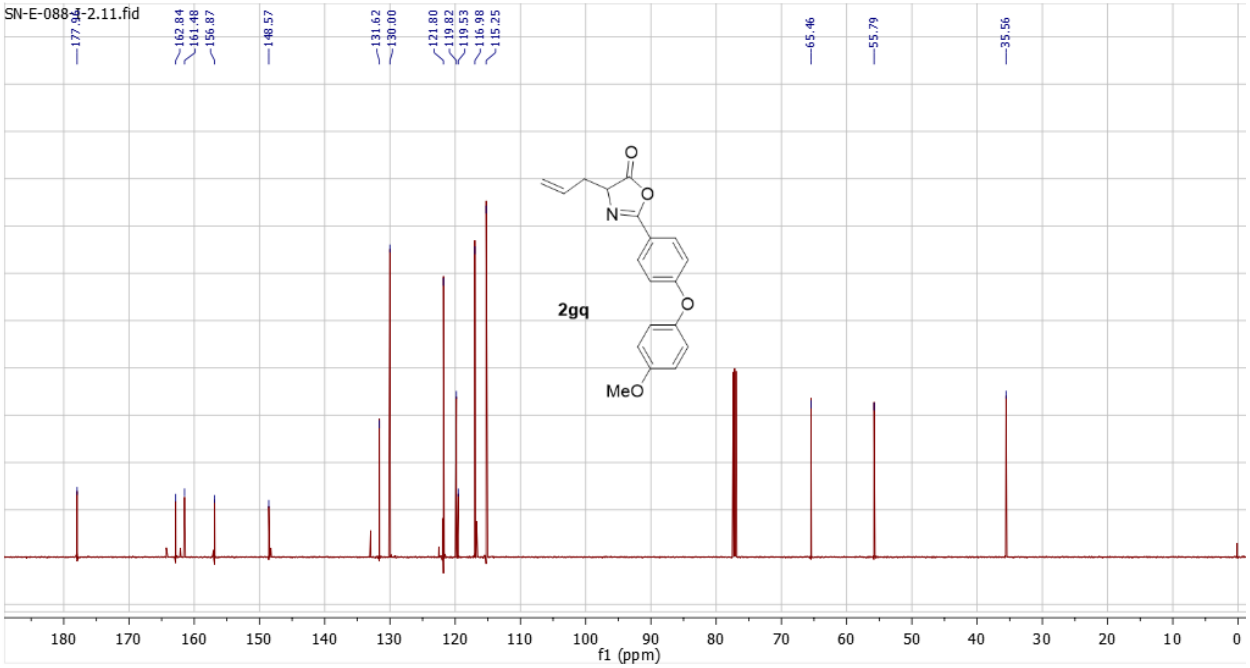

SN-E-111-SM.1.fid
2go
MeO
1.98
2.04
3.47
4.45
2.44
1.00
3.32
2.06
1.01
1.02
f1 (ppm)

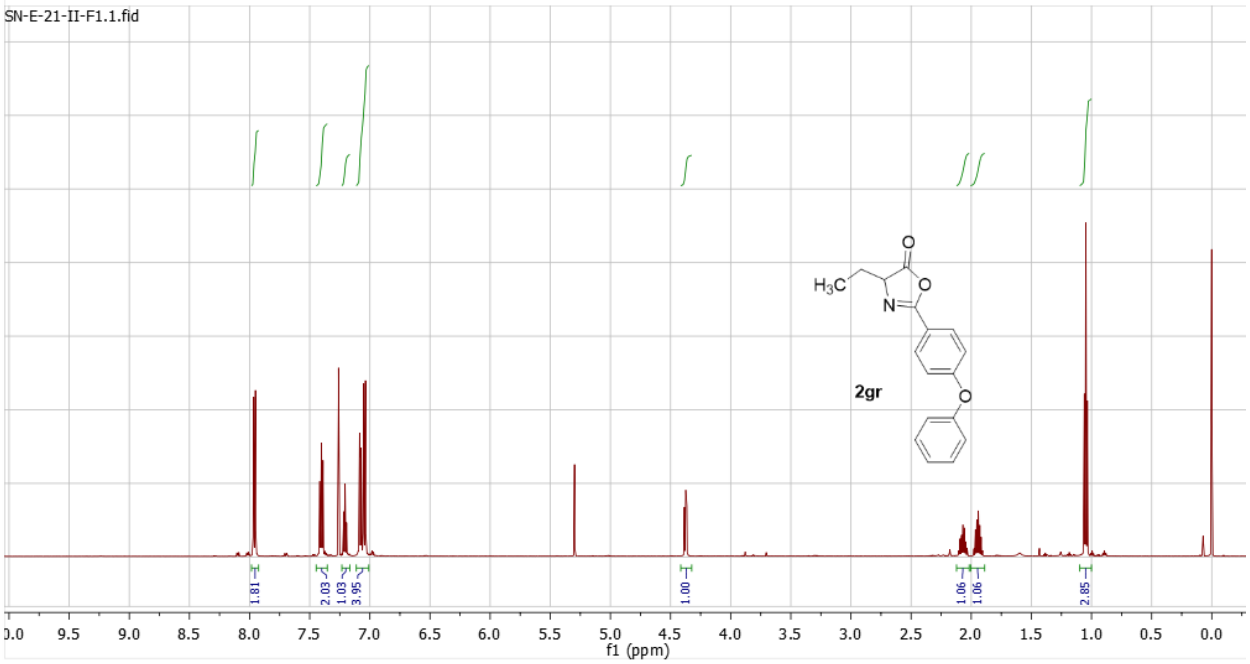

SN-E-111-SM.11.fid
178.01
162.23
160.87
156.28
148.01
139.82
129.40
128.17
128.09
125.88
121.21
119.06
116.43
114.67
63.98
55.21
32.83
30.98
2go
MeO
f1 (ppm)

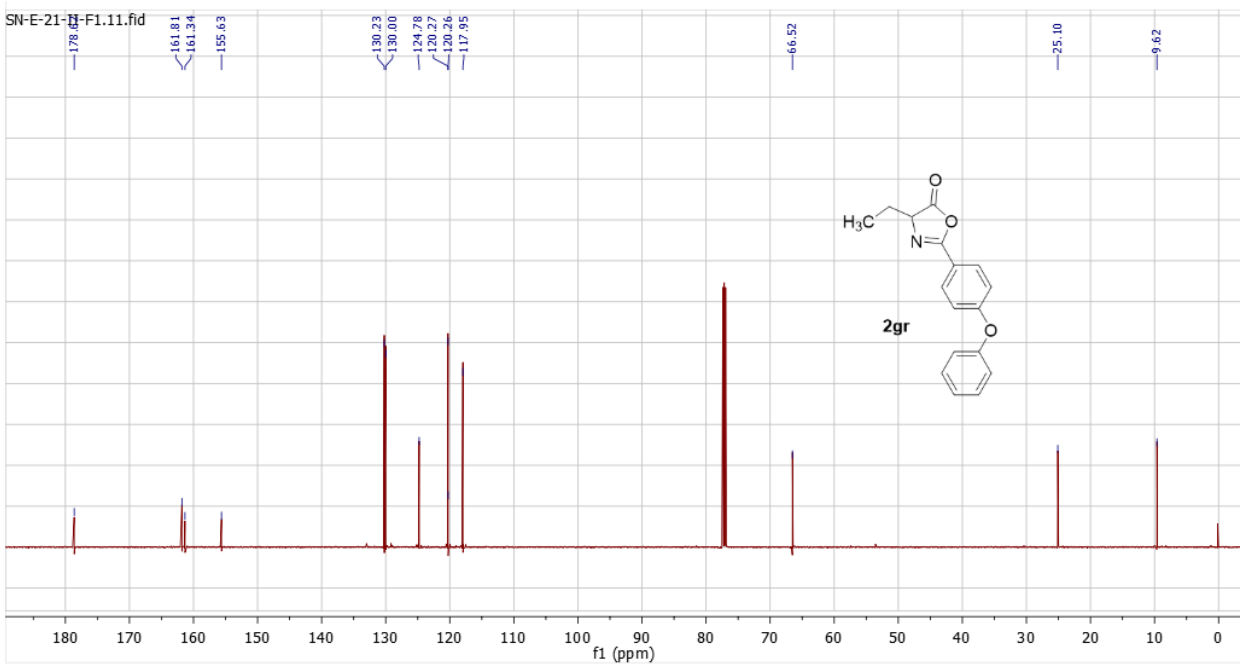

SN-E-087-I.1.fid
2gp
2.00
2.13
2.06
2.15
1.00
3.29
1.01
1.00
4.05
3.05
f1 (ppm)

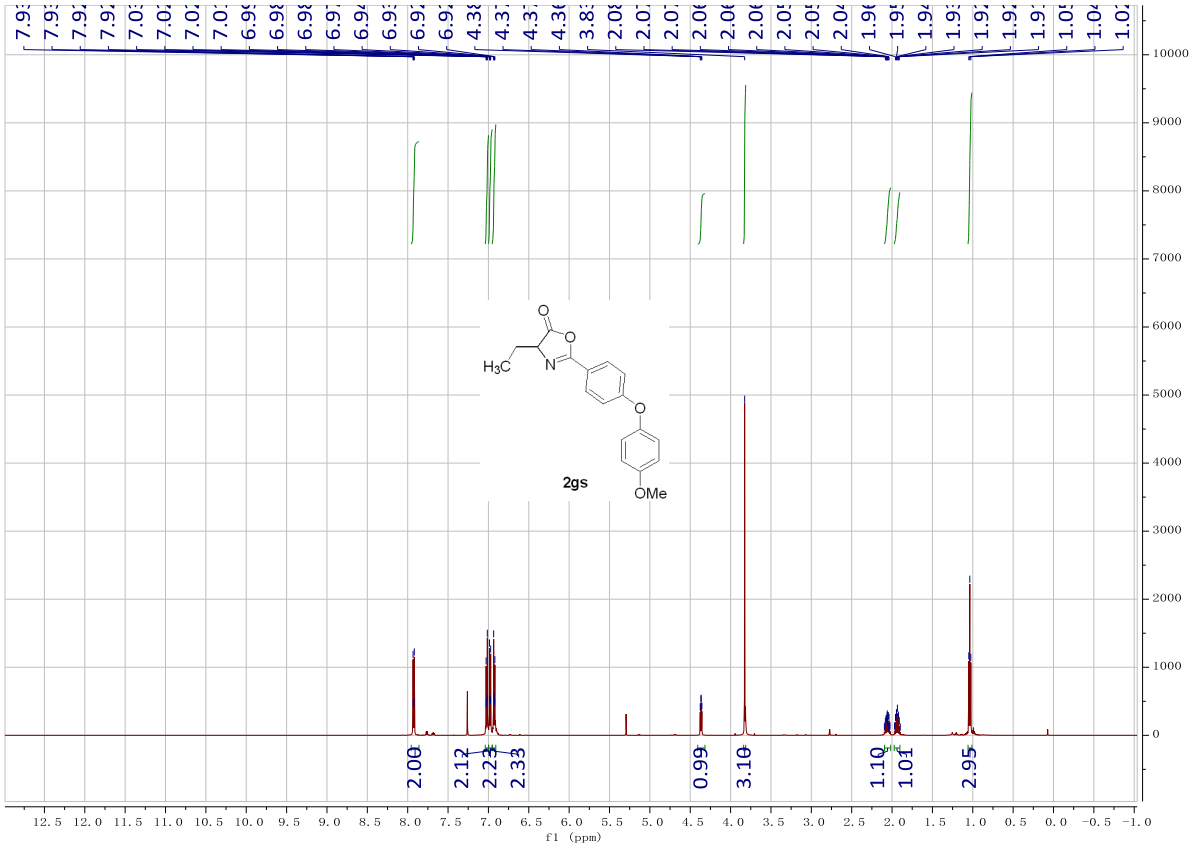

SN-E-087-I.11.fid
178.27
162.15
160.64
156.26
148.02
129.33
121.19
119.11
116.41
114.65
64.89
55.20
30.91
26.85
21.88
13.35
2gp
f1 (ppm)

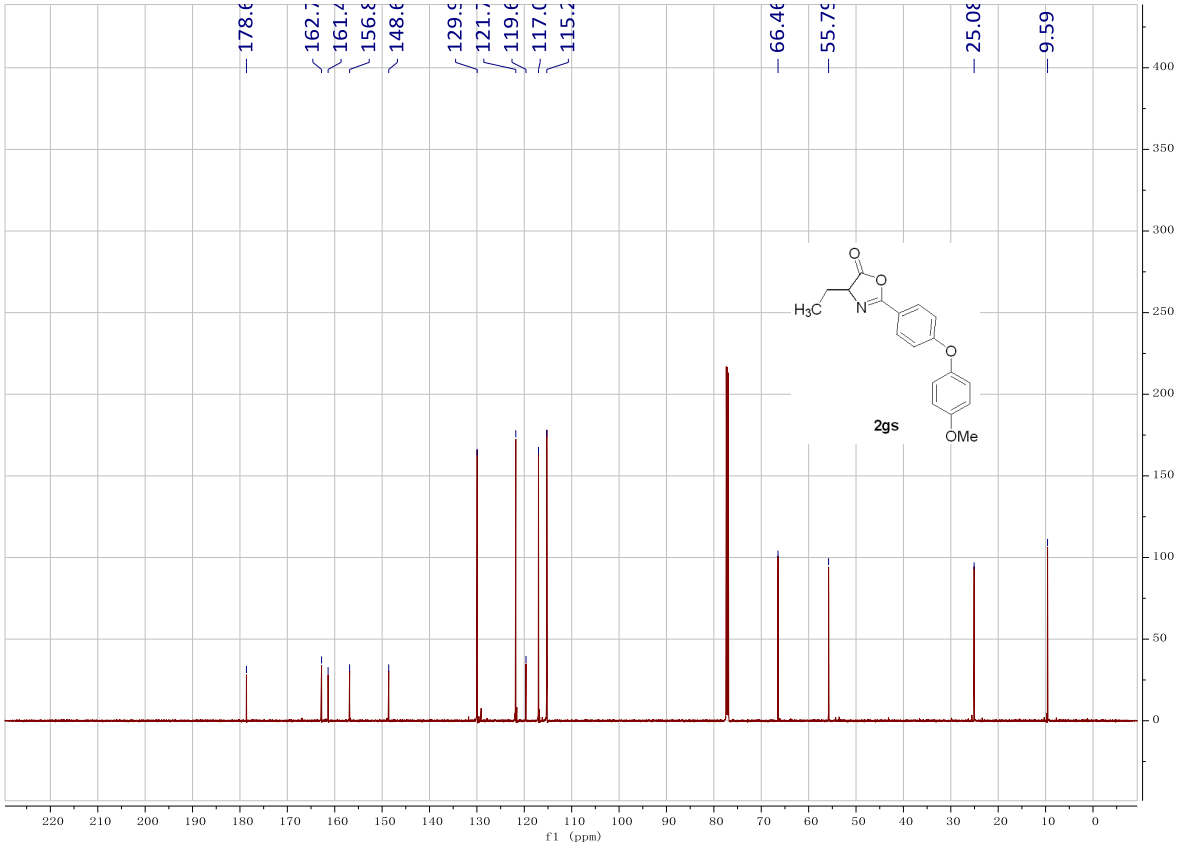

SN-E-088-I-2.1.fid
2gq
MeO
f1 (ppm)

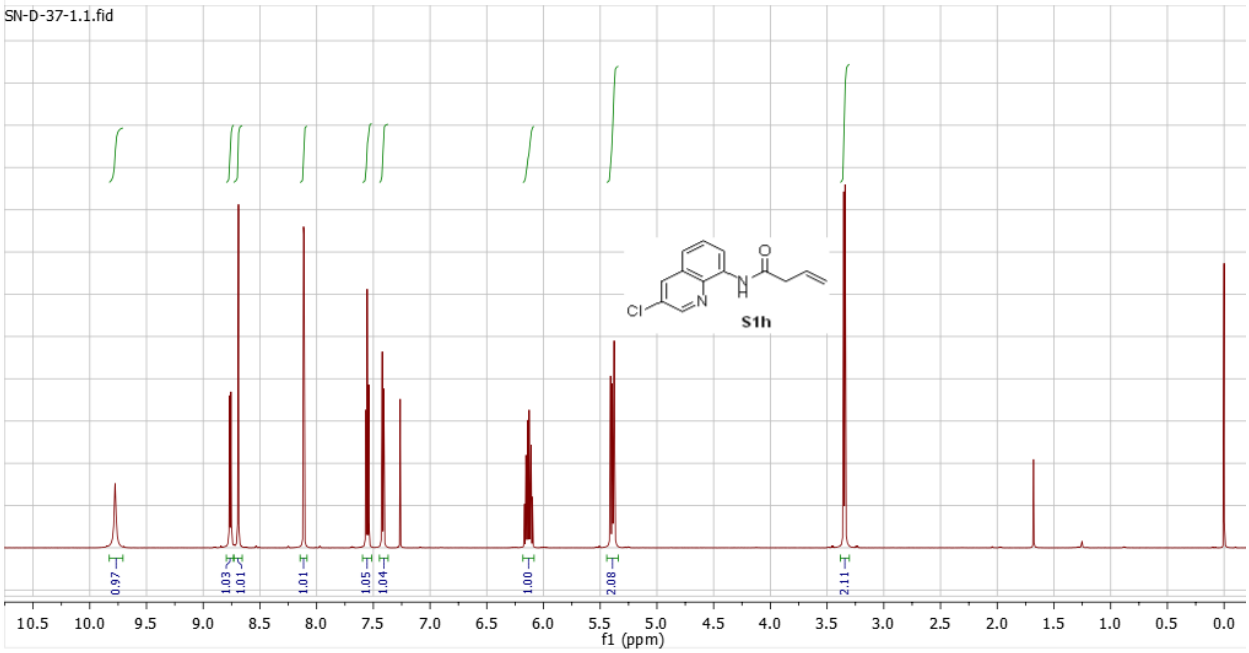

SN-E-088-I-2.11.fid
177.94
162.84
161.48
156.87
148.57
131.62
130.00
121.80
119.82
119.53
116.98
115.25
65.46
55.79
35.56
2gq
MeO
f1 (ppm)

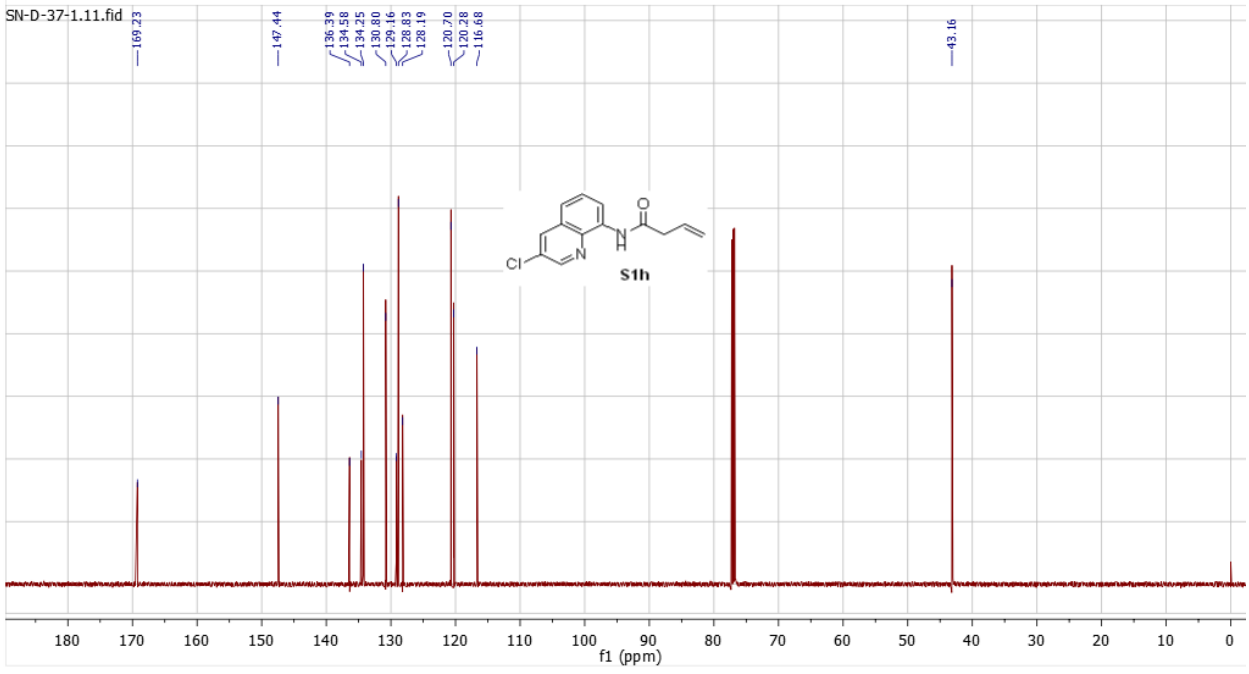

SN-E-21-II-F1.1.fid
2gr
1.81
2.03
1.03
3.95
1.00
1.06
1.06
2.85
f1 (ppm)

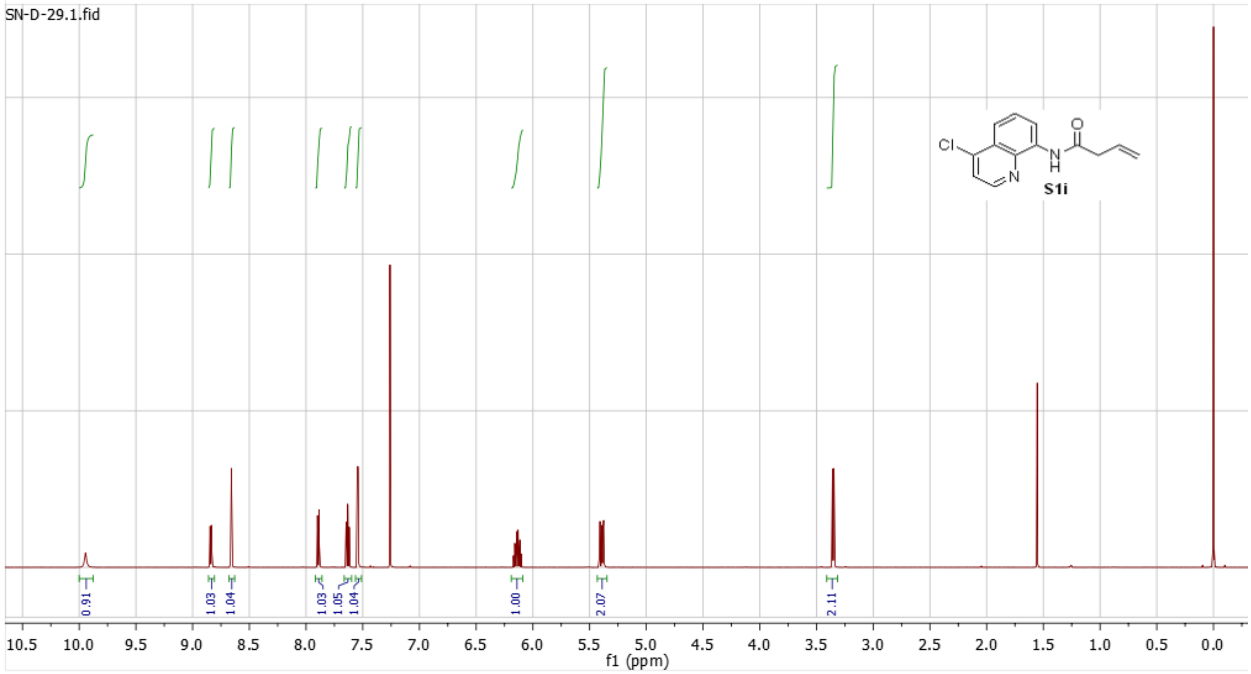

SN-E-21-II-F1.11.fid
178.62
161.81
161.34
155.63
130.23
130.00
124.78
120.27
120.26
117.95
66.52
25.10
9.62
2gr
f1 (ppm)

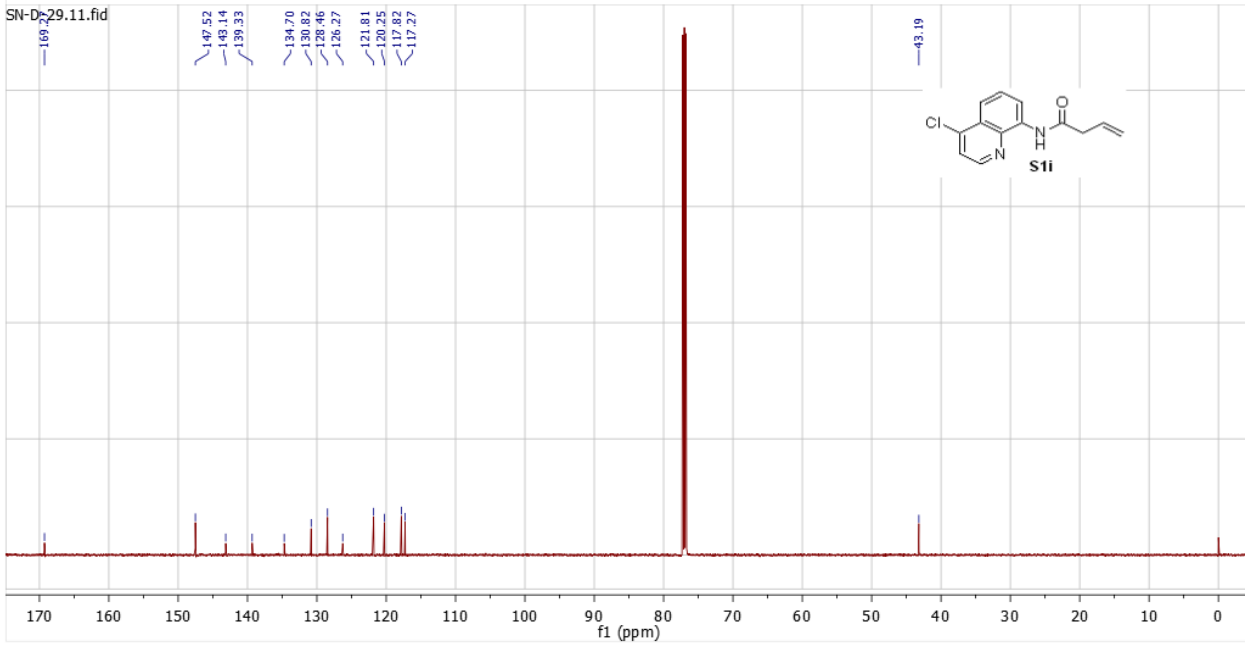

2gs
OMe
2.00
2.12
2.23
2.33
0.99
3.10
1.10
1.01
2.95
f1 (ppm)

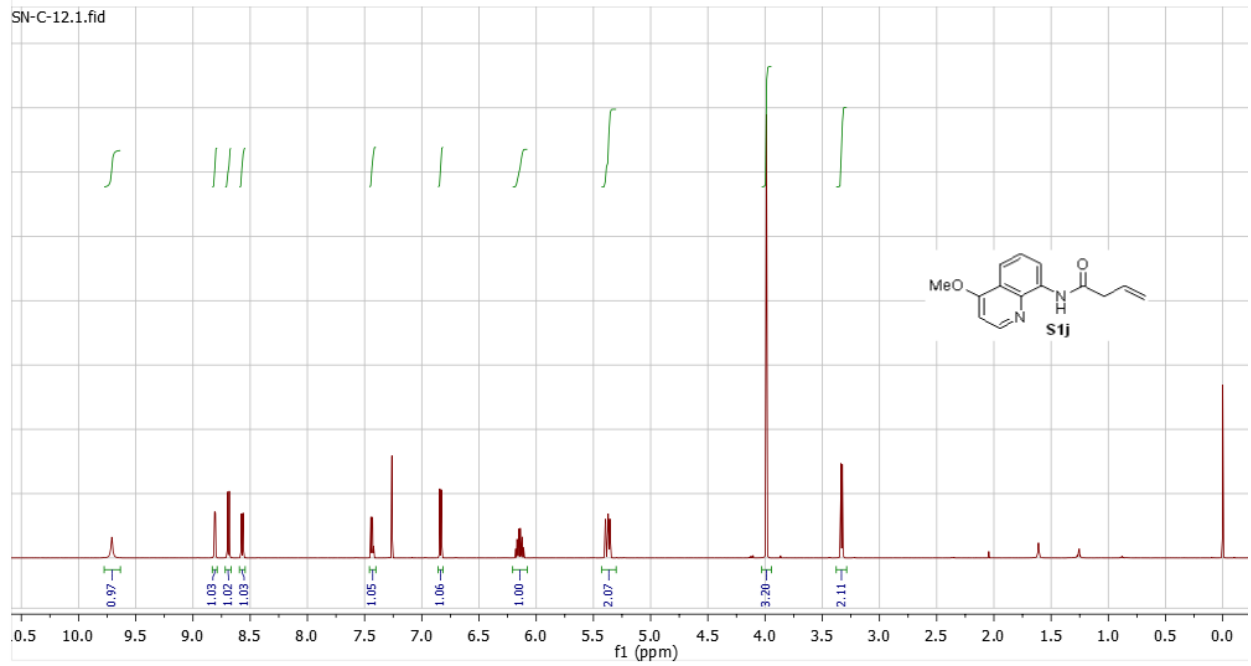

178.6
162.7
161.4
156.8
148.6
129.9
121.7
119.6
117.0
115.2
66.46
55.79
25.08
9.59
2gs
OMe
f1 (ppm)

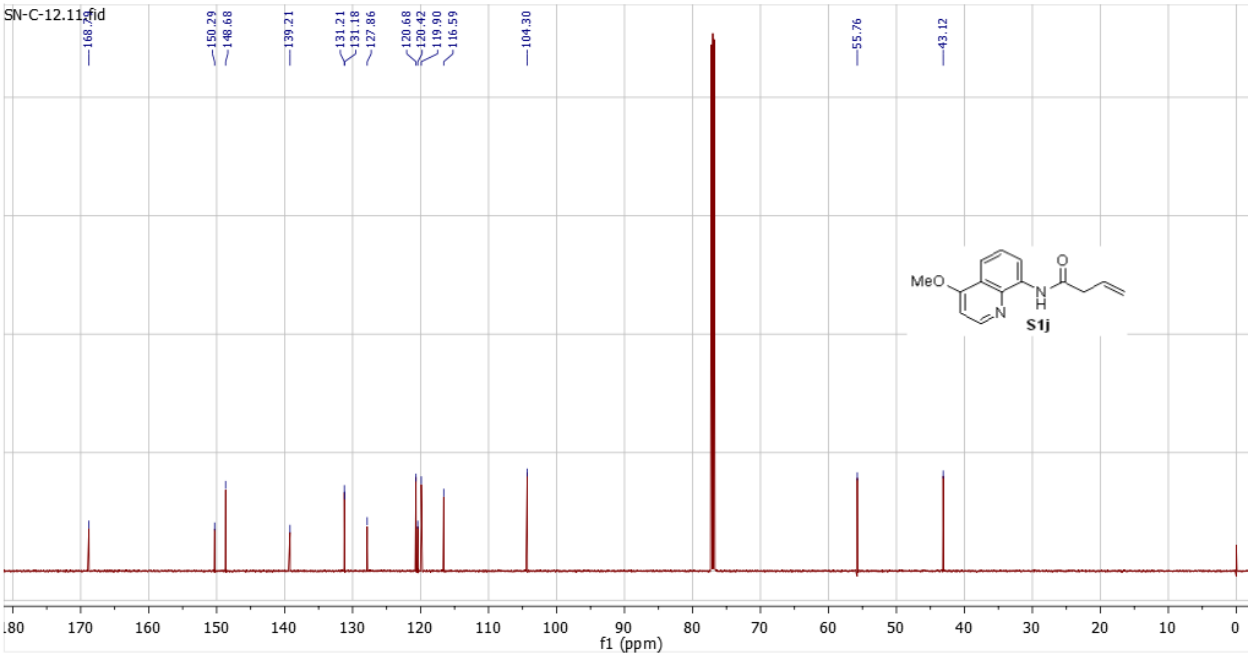

SN-D-37-1.1.fid
S1h
0.97
1.03
1.01
1.01
1.05
1.04
1.00
2.08
2.11
f1 (ppm)


SN-D-37-1.11.fid
169.23
147.44
136.39
134.58
134.25
130.80
129.16
128.83
128.19
120.70
120.28
116.68
43.16
S1h
f1 (ppm)


SN-D-29.1.fid
Cl
N
H
O
S1i
0.91
1.03
1.04
1.03
1.05
1.04
1.00
2.07
2.11
10.5 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
f1 (ppm)


SN-D-29.11.fid
169.72
147.52
143.14
139.33
134.70
130.82
128.46
126.27
121.81
120.25
117.82
117.27
43.19
Cl
N
H
O
S1i
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


SN-C-12.1.fid
MeO
N
H
O
S1j
0.97
1.03
1.02
1.03
1.05
1.06
1.00
2.07
3.20
2.11
f1 (ppm)


SN-C-12.11.fid
168.72
150.29
148.68
139.21
131.21
131.18
127.86
120.68
120.42
119.90
116.59
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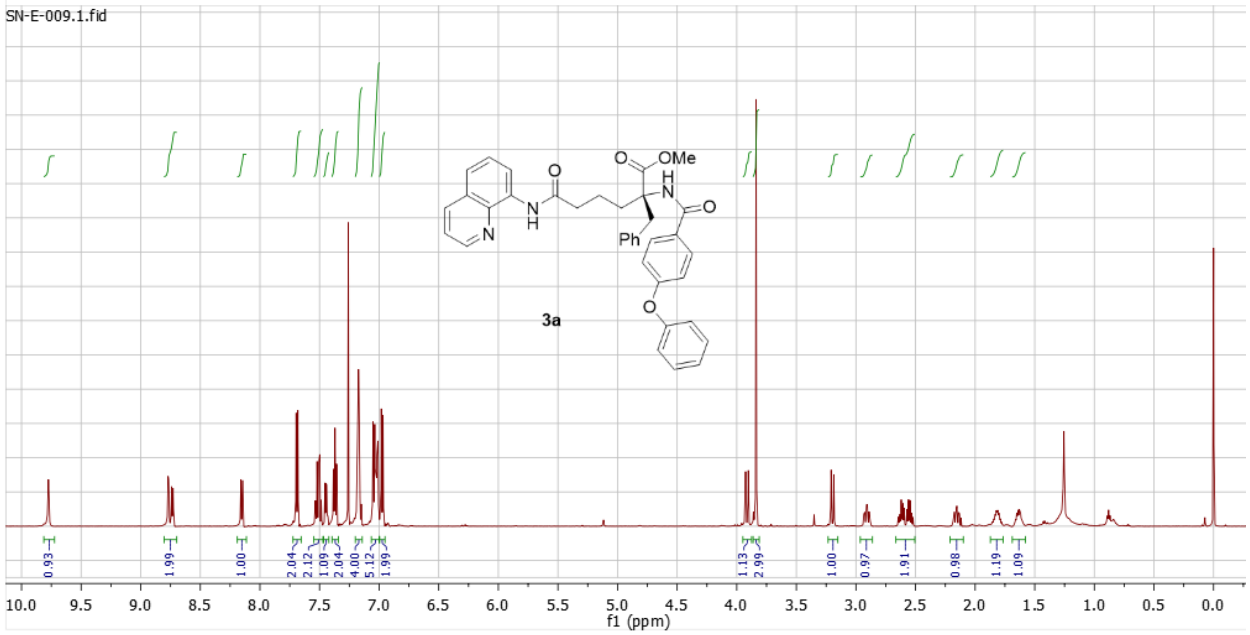
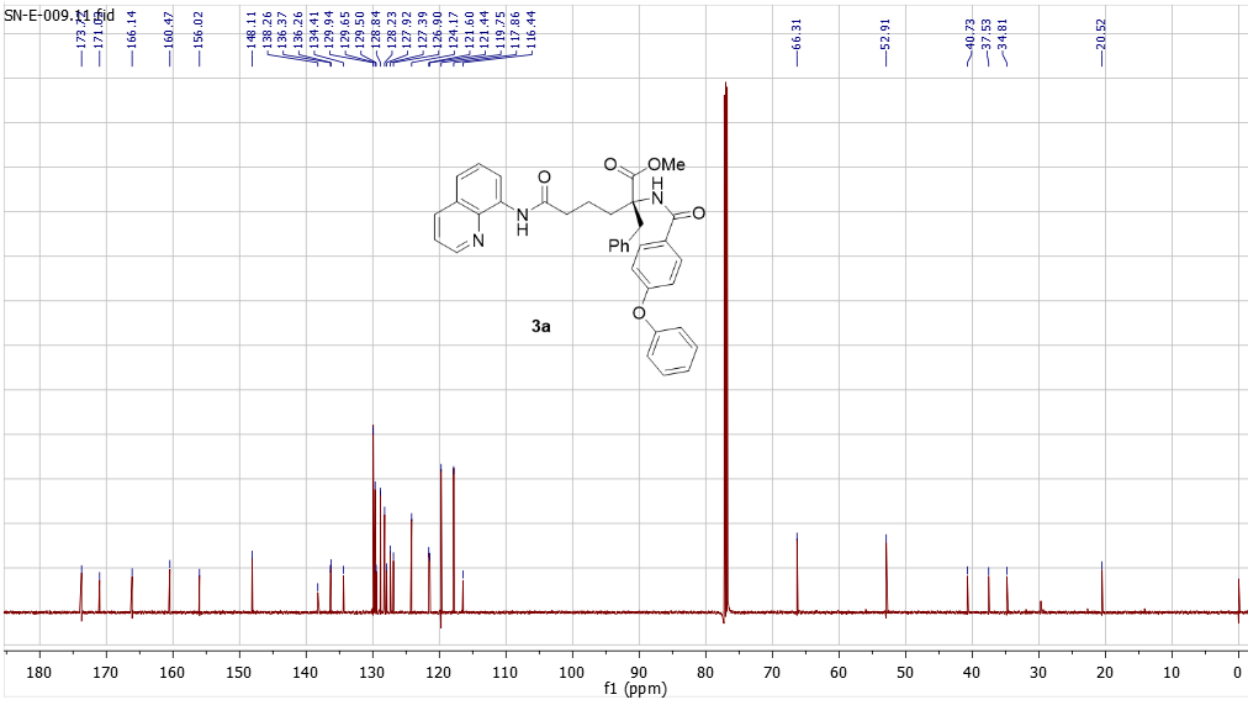
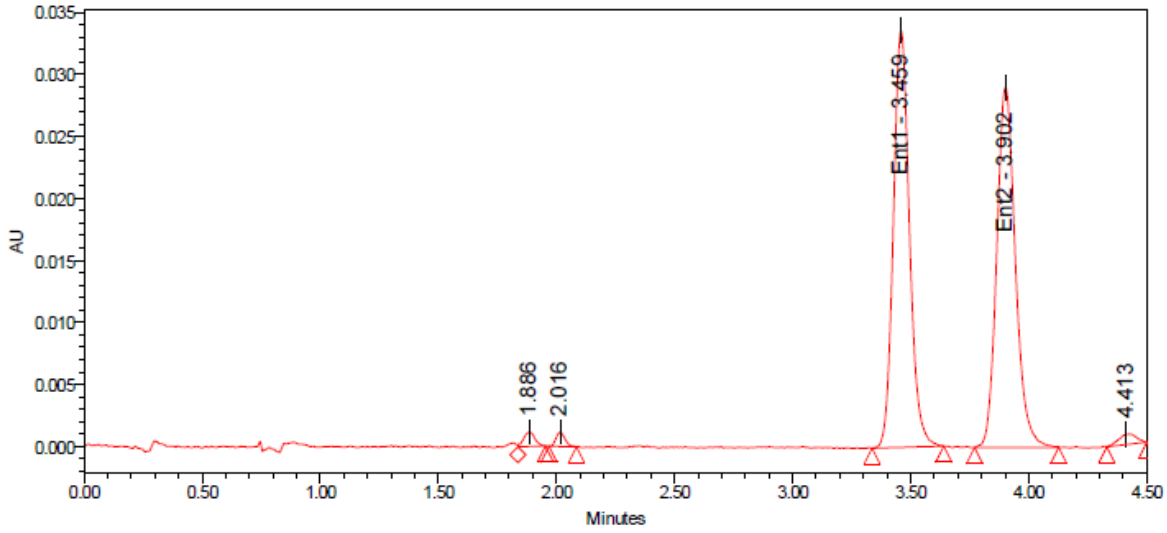
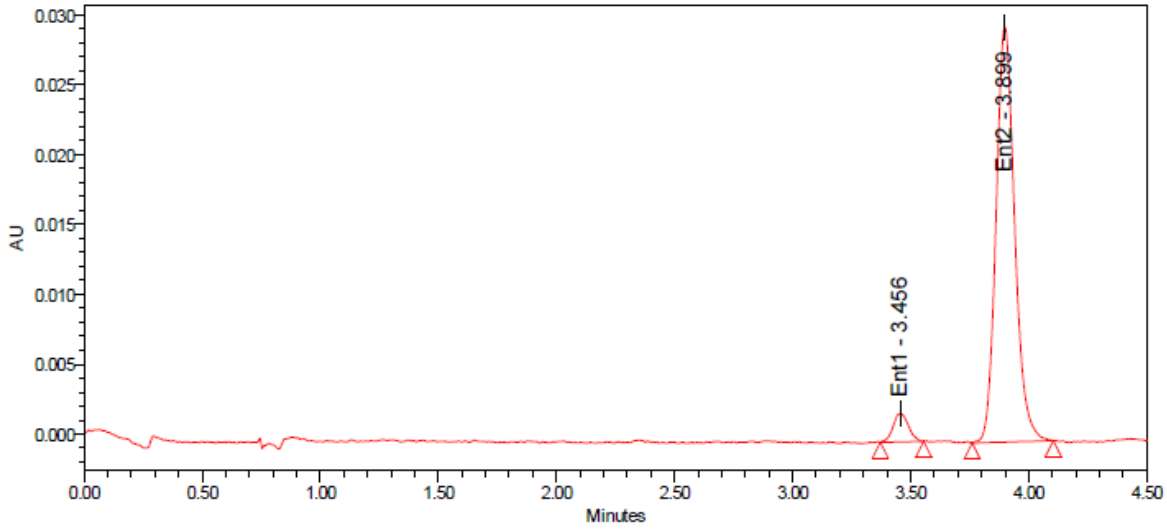
55.76
43.12
MeO
N
H
O
S1j
f1 (ppm)


SN-E-009.1.fid
OMe
Ph
3a
f1 (ppm)

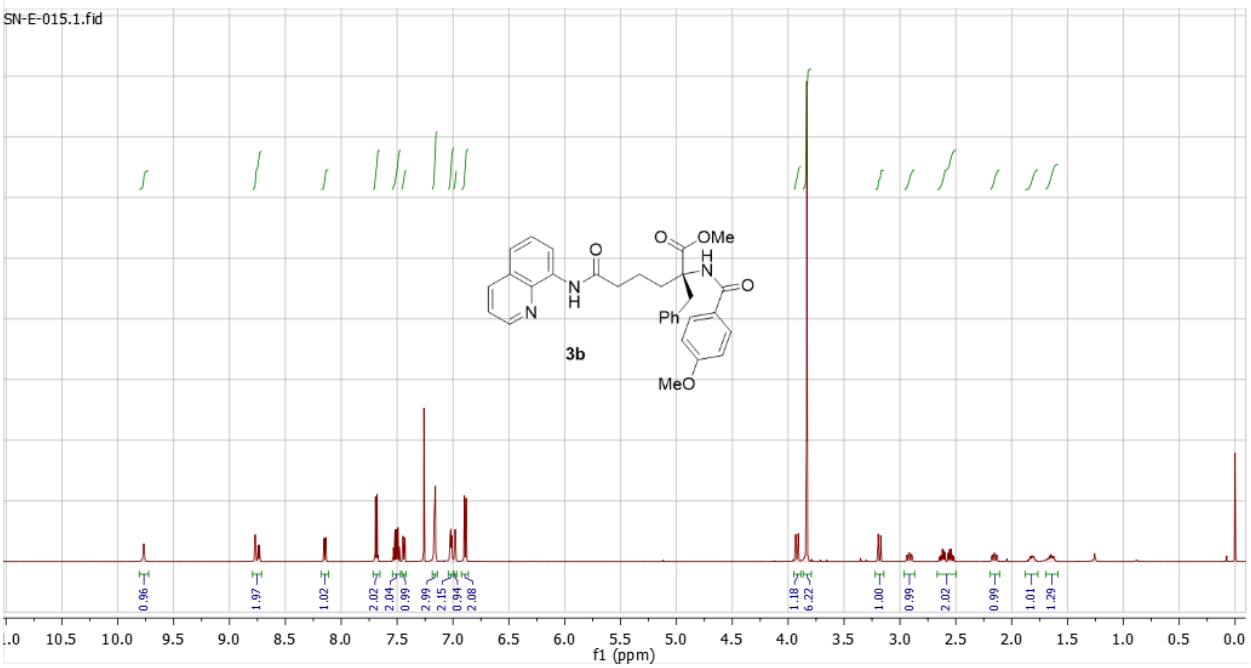

SN-E-009.11.fid
OMe
Ph
3a
f1 (ppm)

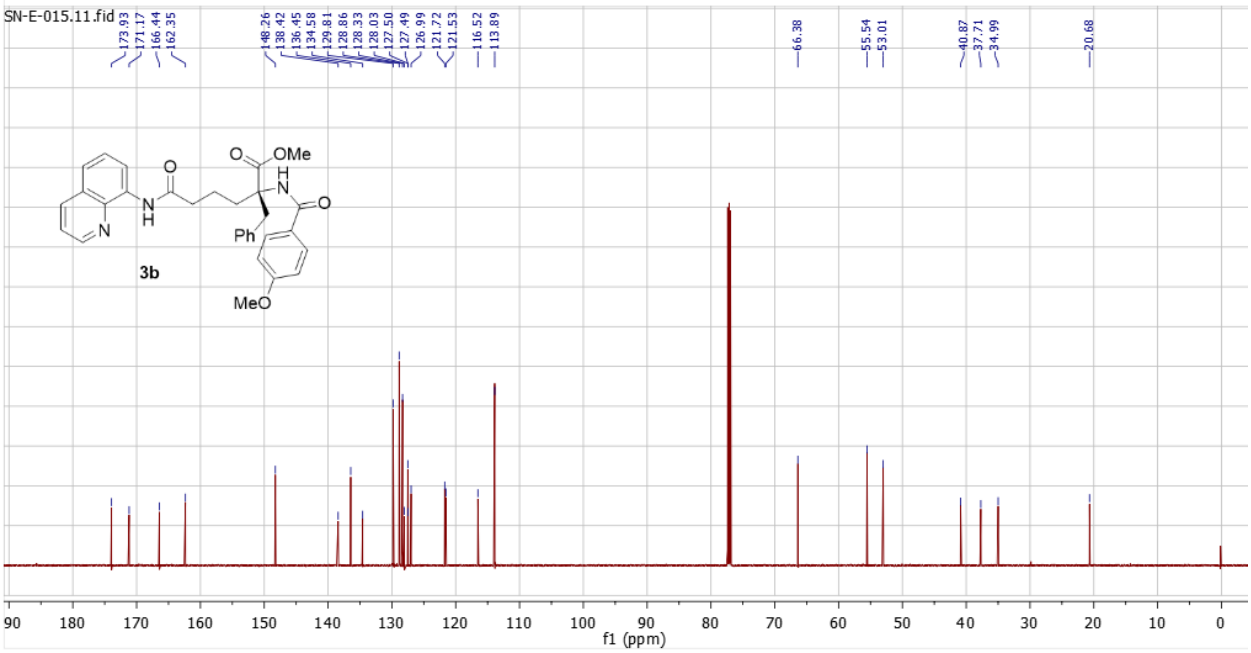


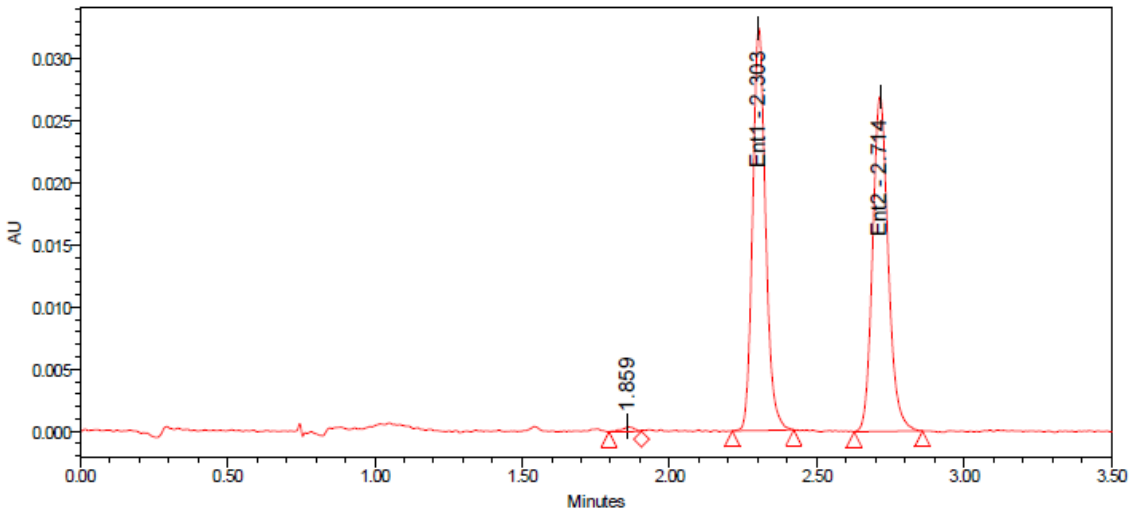


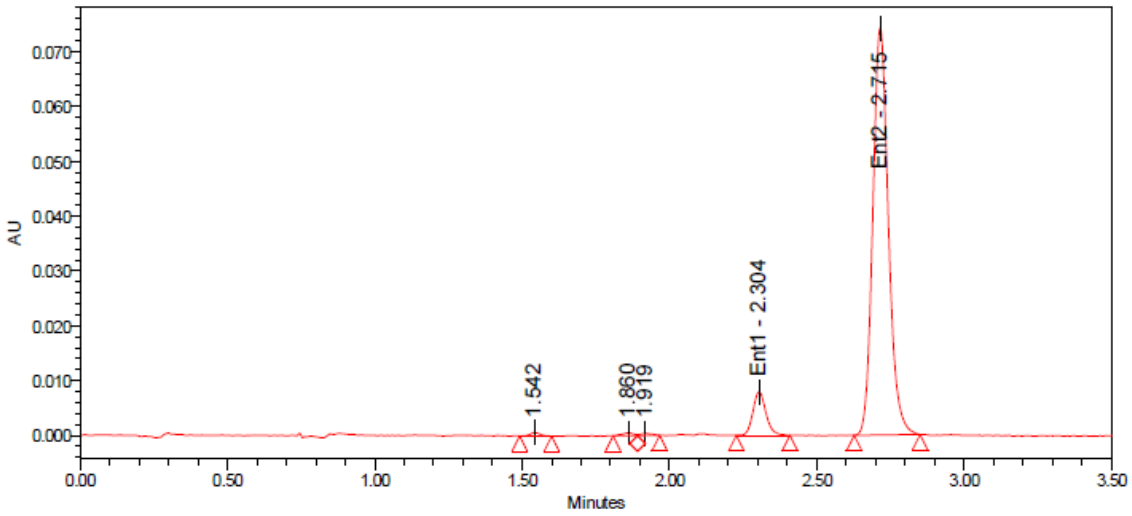
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-D-39I	49.95	50.05	-0.11	158904	159239
2	SN-E-9	5.33	94.67	-89.34	9156	162614


SN-E-015.1.fid
3b
f1 (ppm)

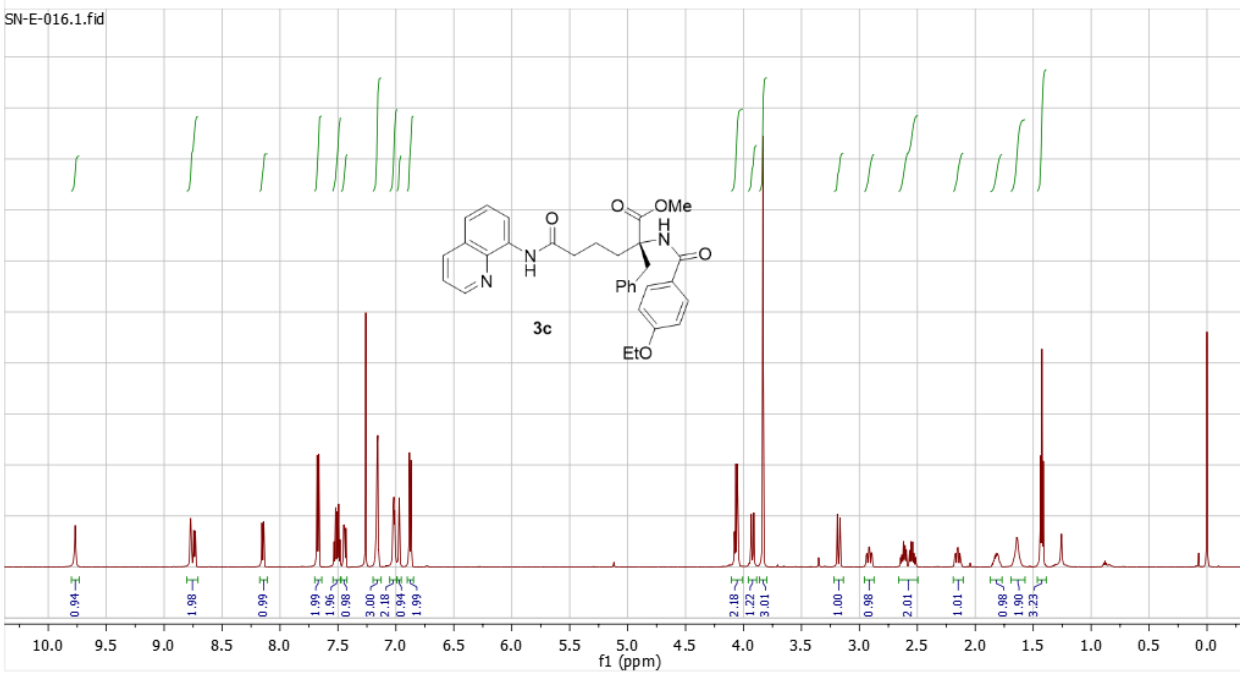

SN-E-015.11.fid
3b
f1 (ppm)

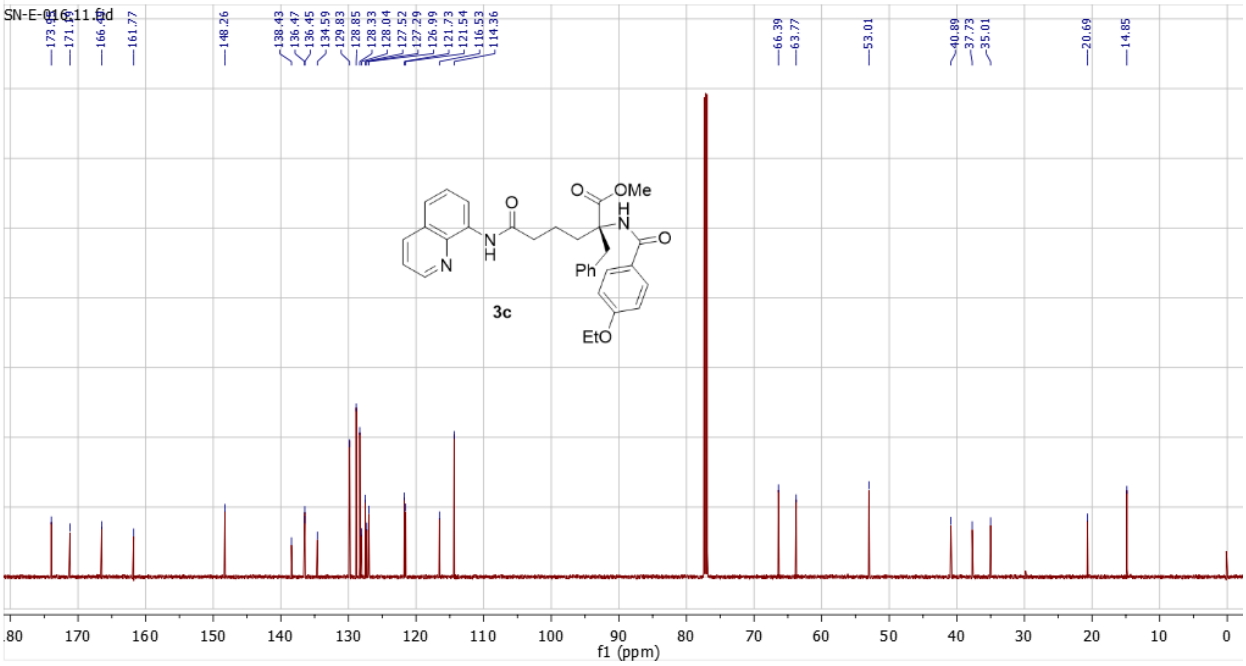


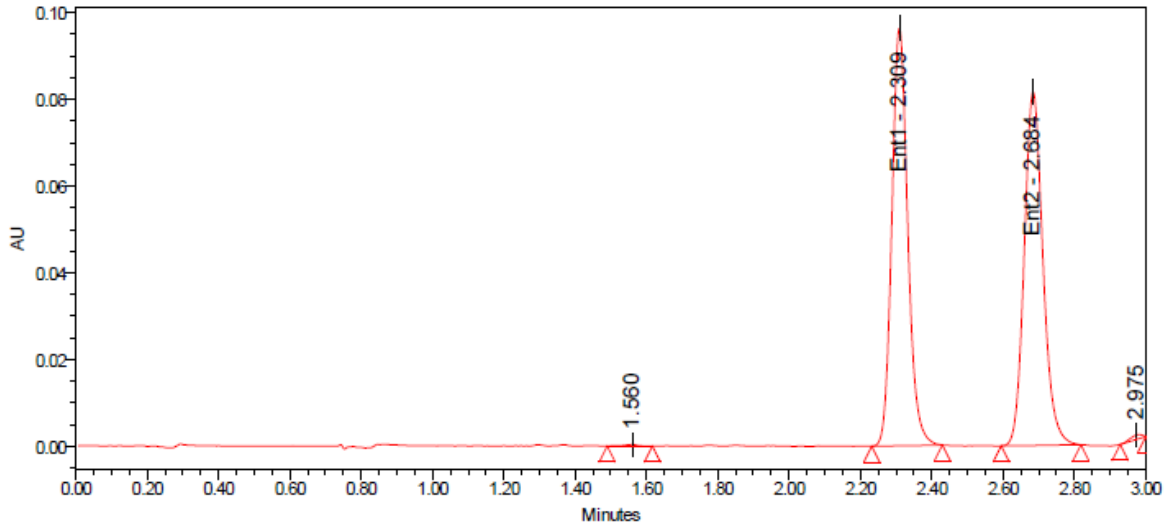


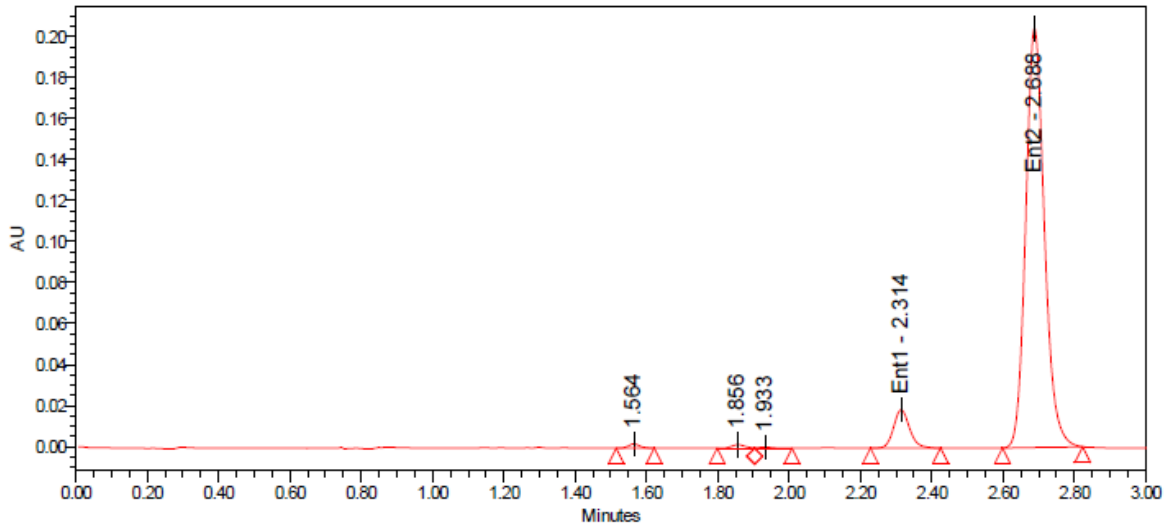
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-003-1	49.94	50.06	-0.12	99458	99705
2	SN-E-015-1	8.16	91.84	-83.68	24207	272499


SN-E-016.1.fid
OMe
Ph
EtO
3c
f1 (ppm)

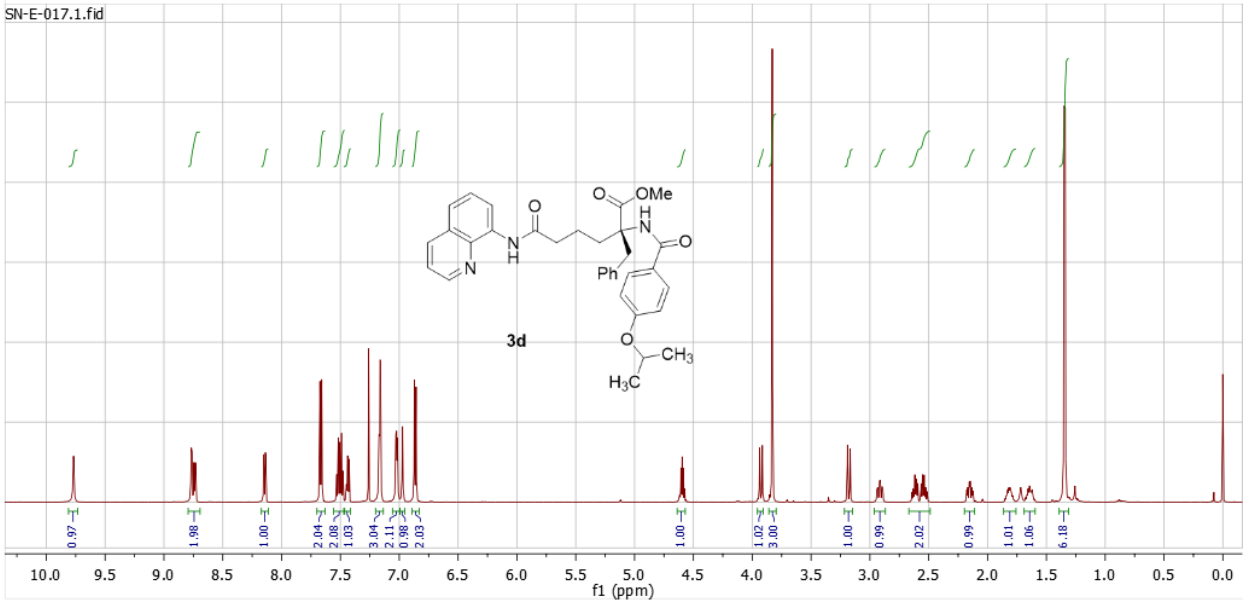

SN-E-016.11.fid
OMe
Ph
EtO
3c
f1 (ppm)

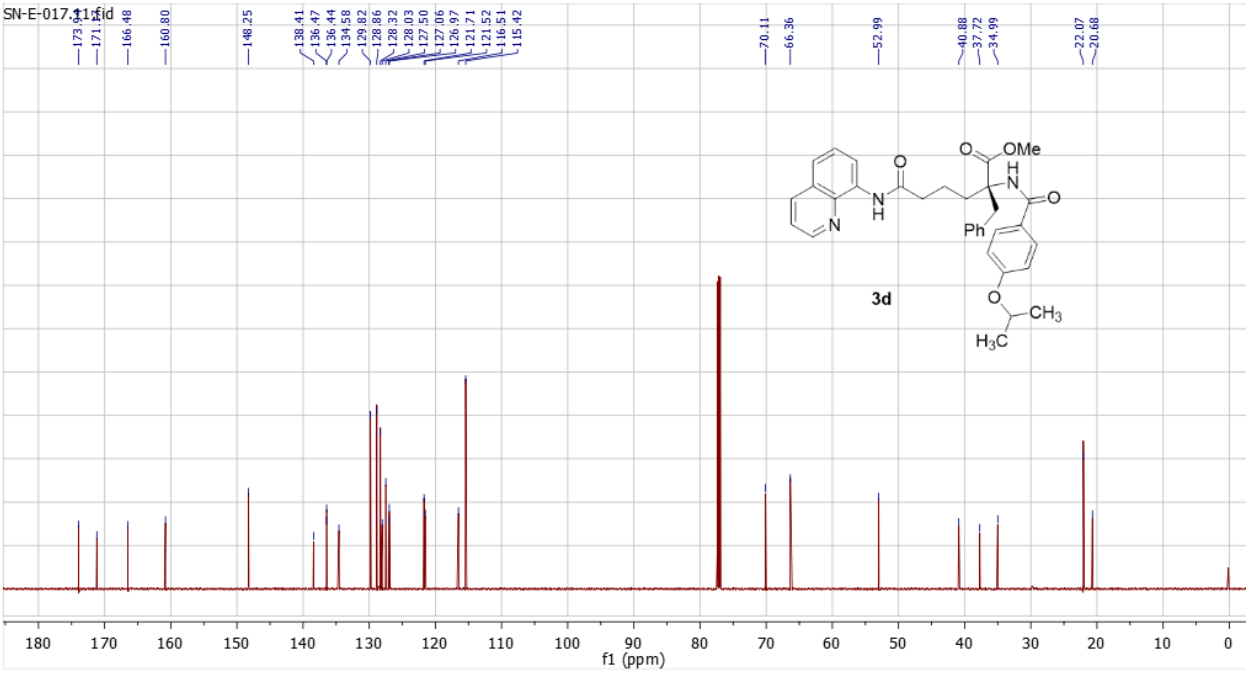


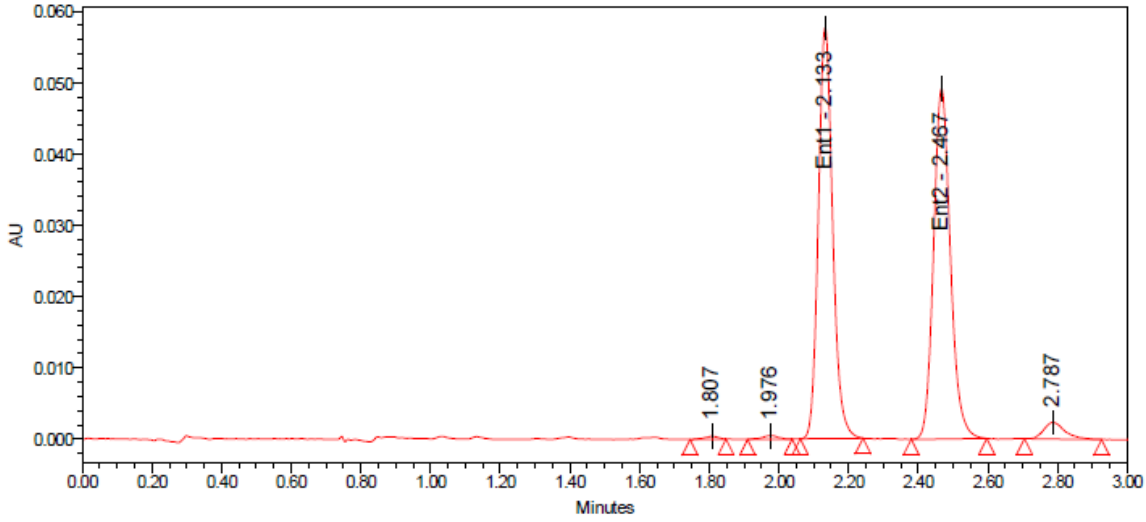


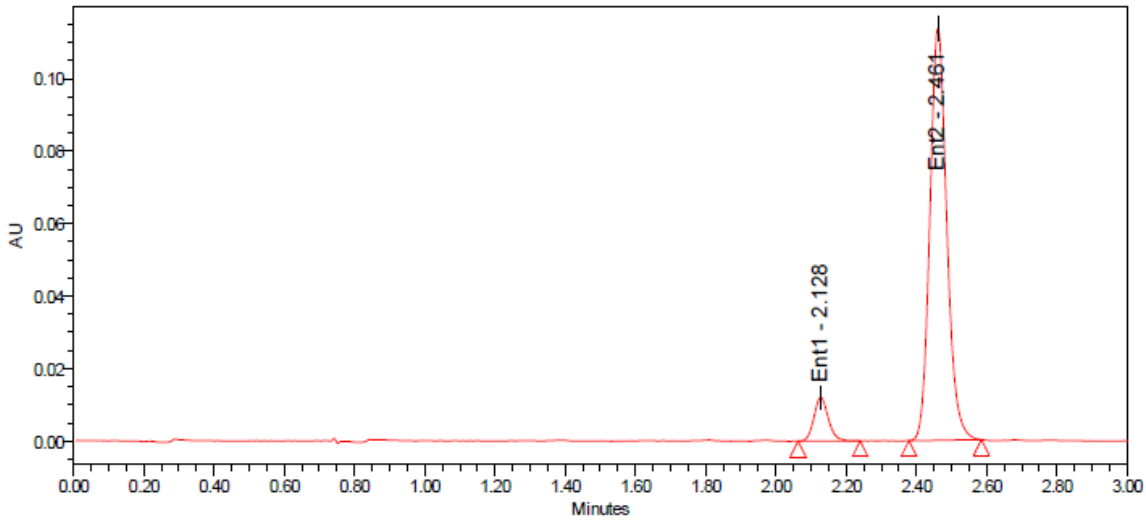
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-D-41I	50.09	49.91	0.18	298475	297381
2	SN-E-16	7.22	92.78	-85.57	57891	744278


SN-E-017.1.fid
3d
f1 (ppm)

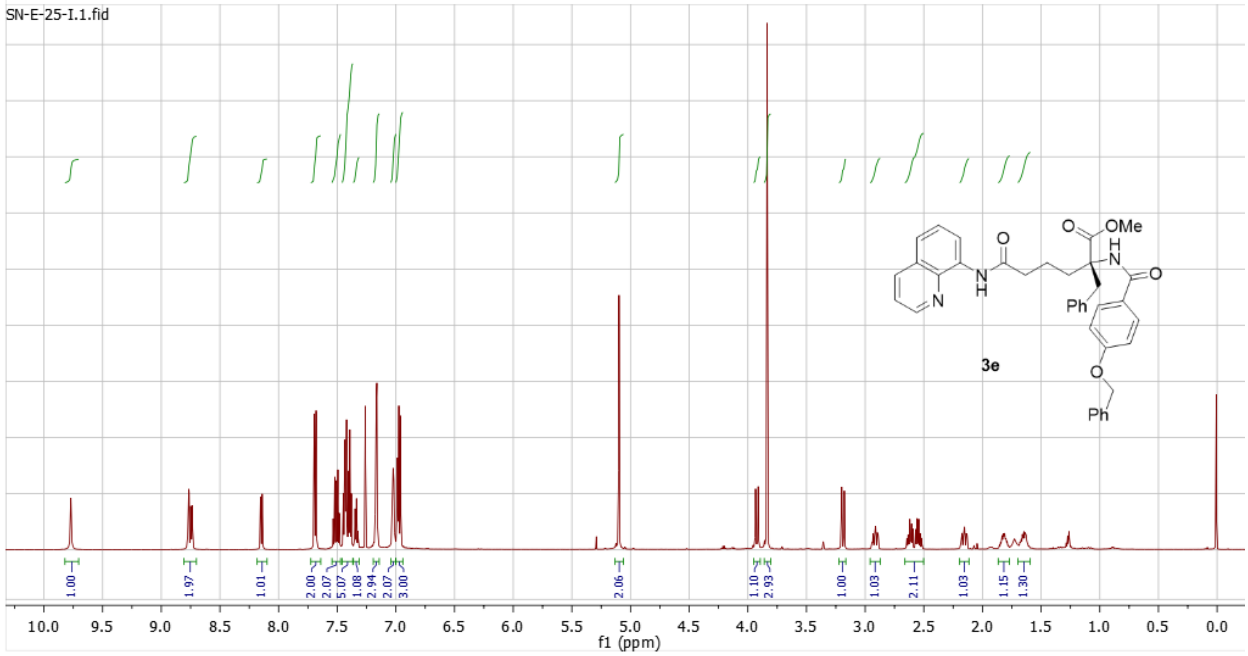

SN-E-017.11.fid
3d
f1 (ppm)

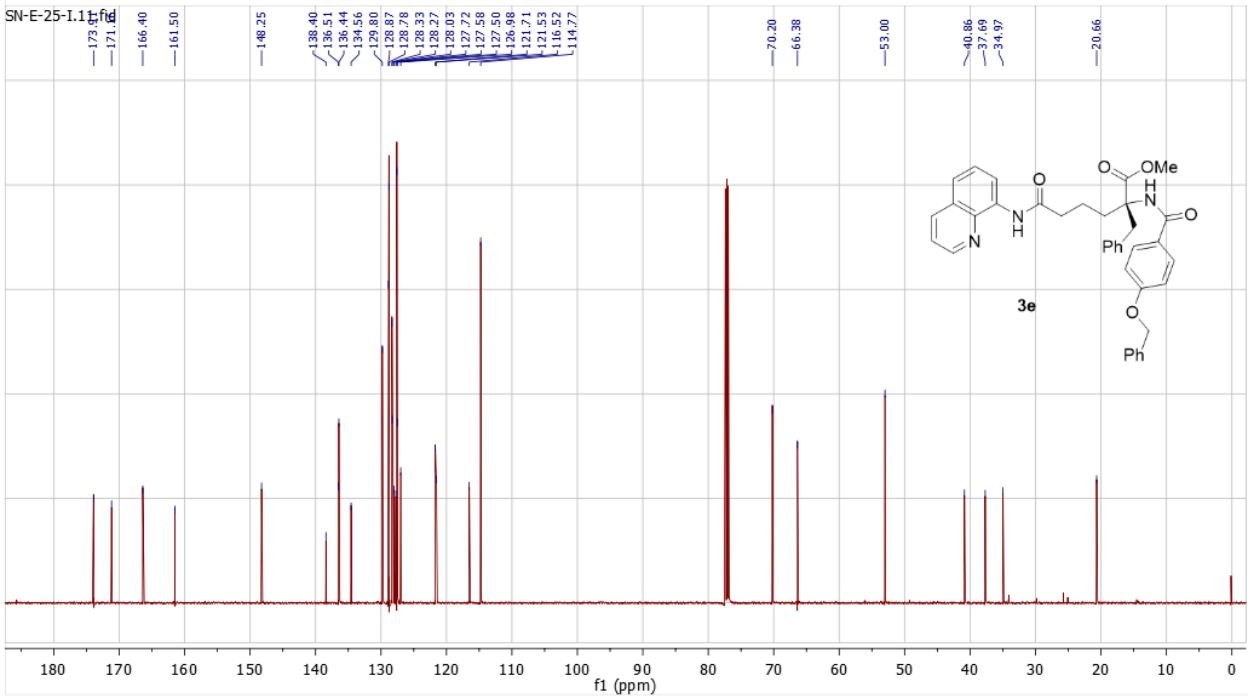


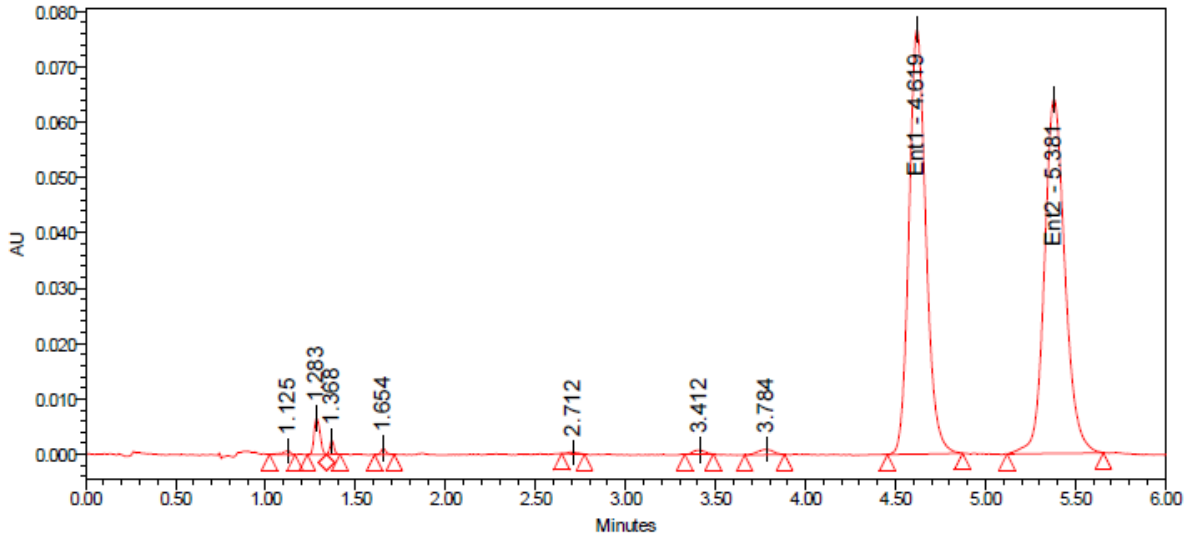


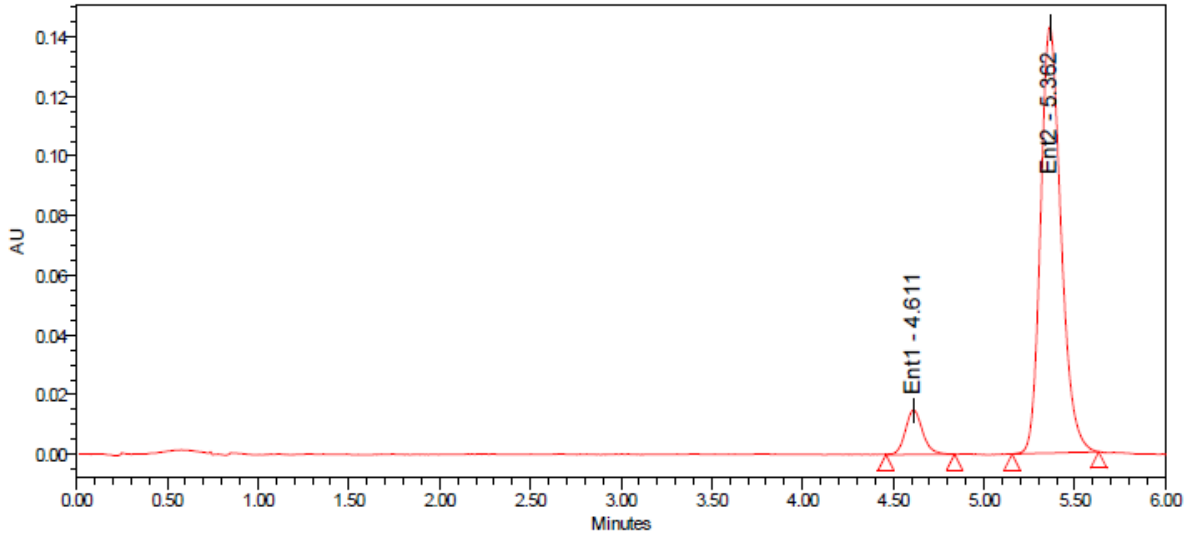
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-D-50l	49.98	50.02	-0.05	164619	164778
2	SN-E-17	8.24	91.76	-83.53	34202	381019


SN-E-25-I.1.fid
3e
f1 (ppm)

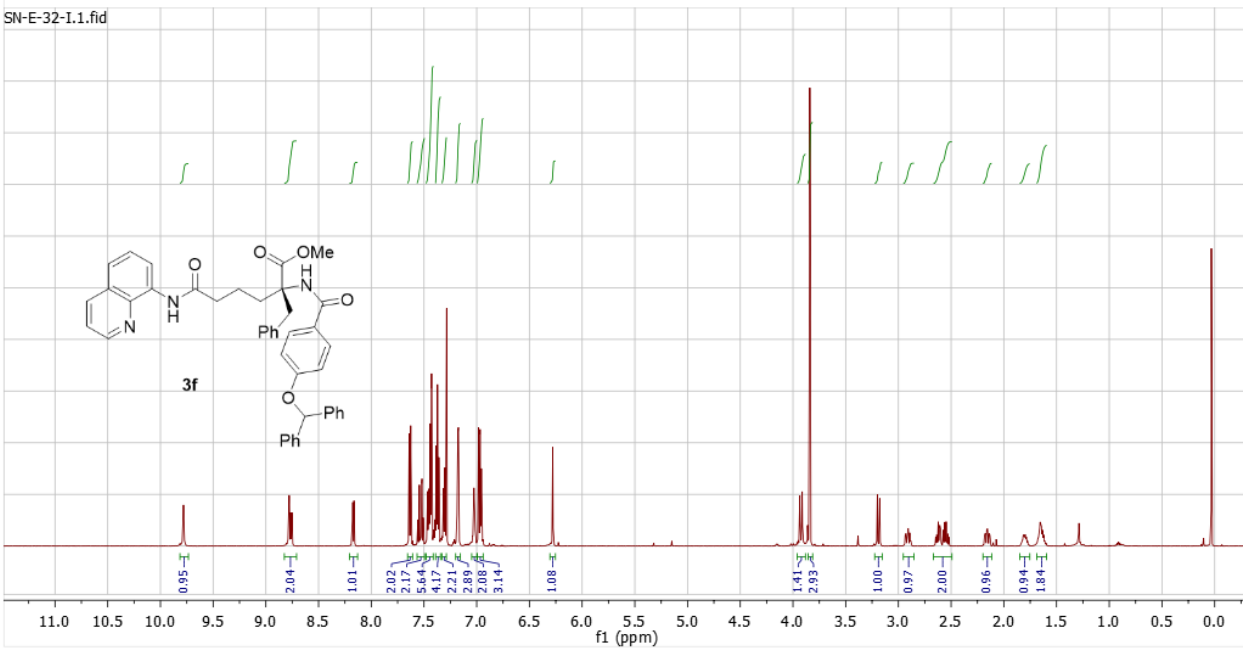

SN-E-25-I.11.fid
3e
f1 (ppm)

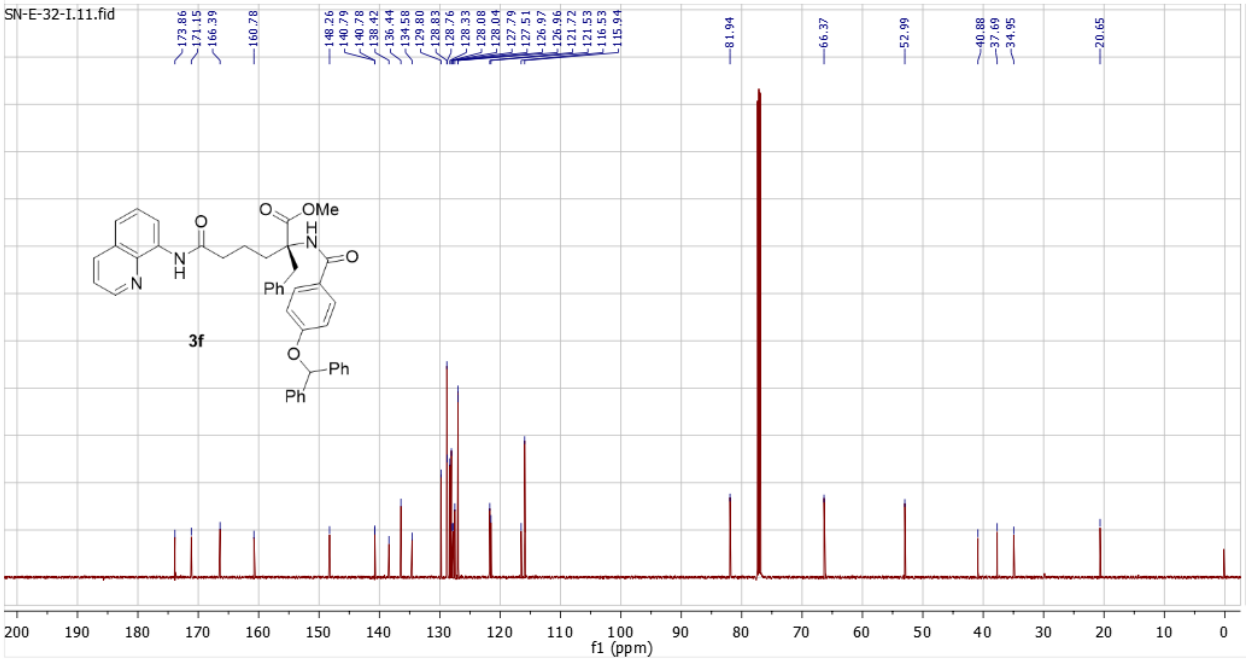


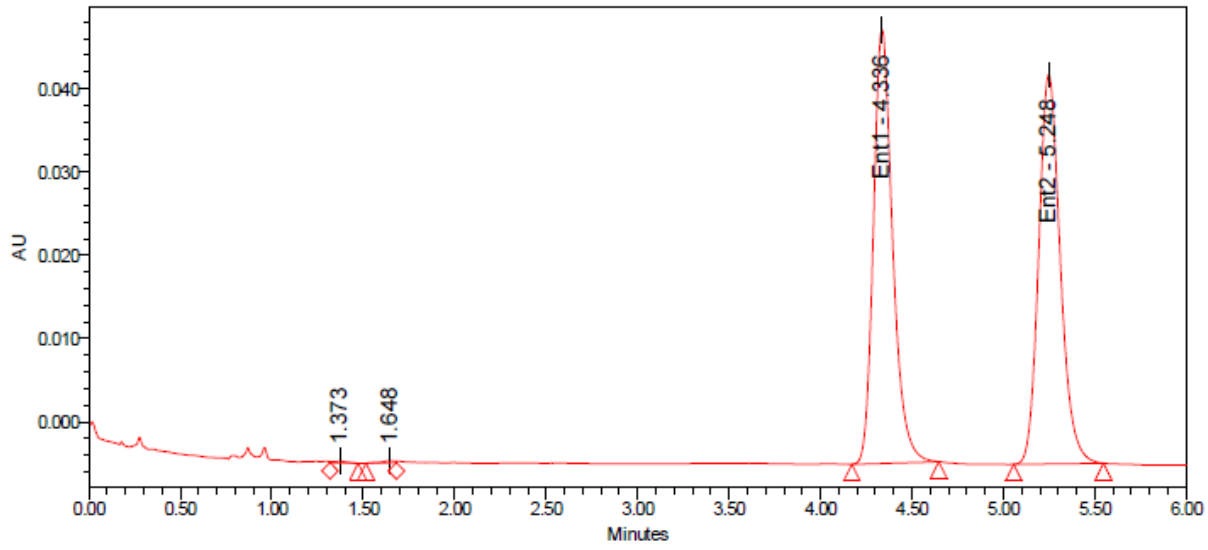


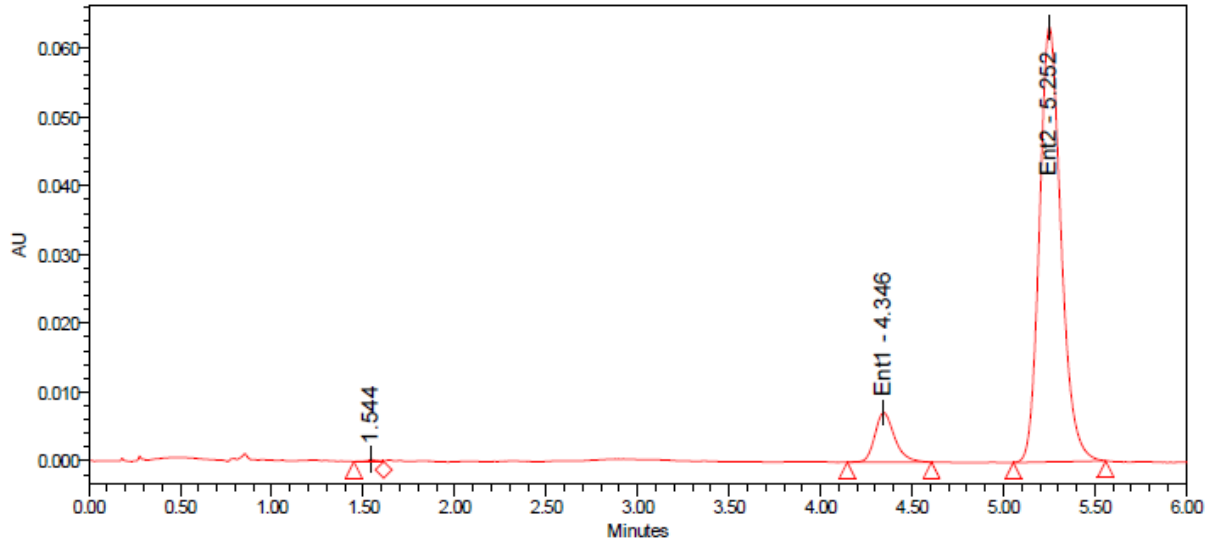
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-D-69I	49.62	50.38	-0.77	500900	508659
2	SN-E-25I	8.09	91.91	-83.82	98357	1117517


SN-E-32-I.1.fid
3f
f1 (ppm)

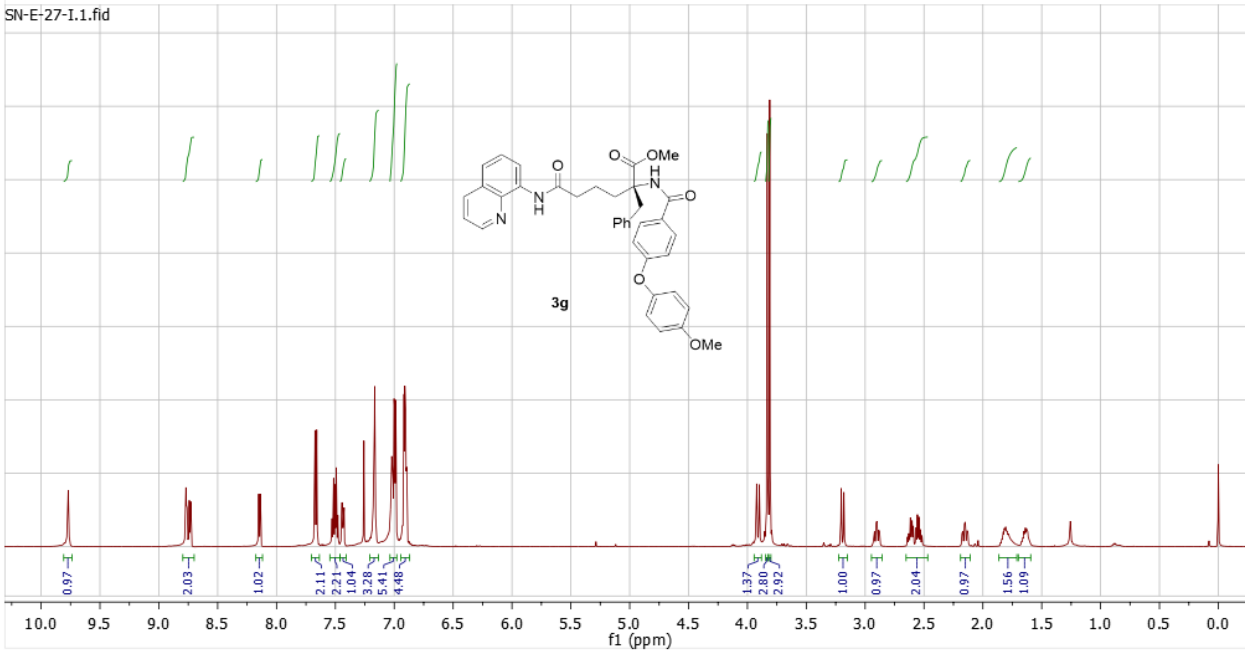

SN-E-32-I.11.fid
3f
f1 (ppm)

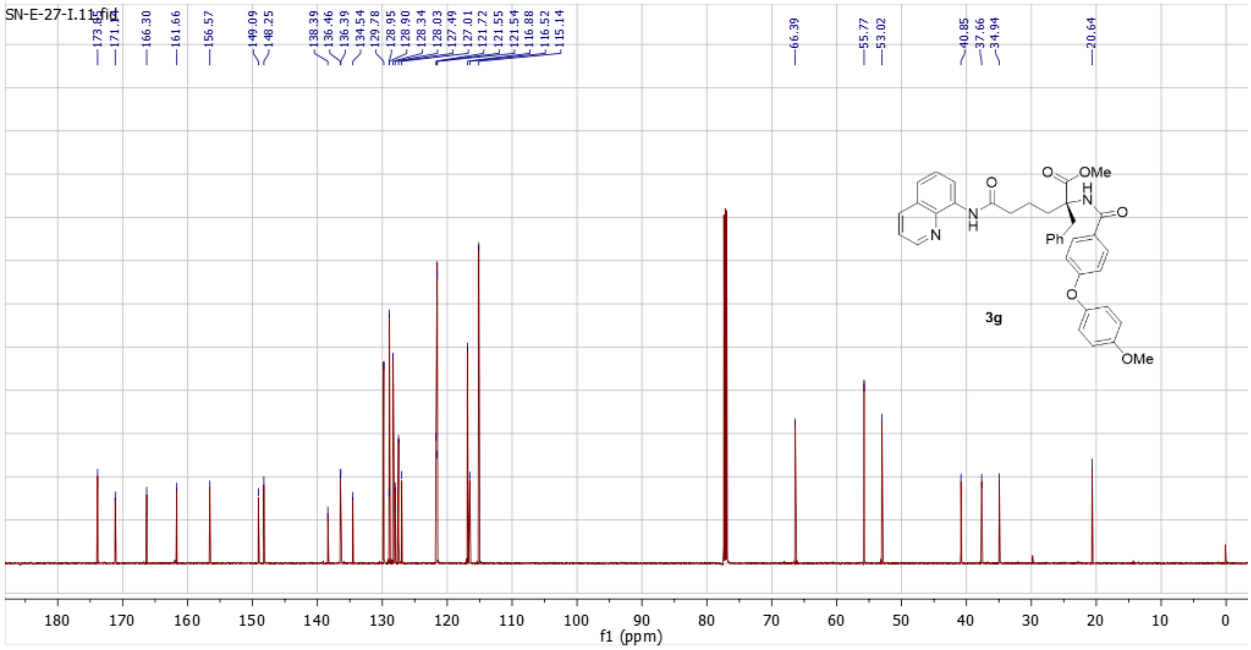


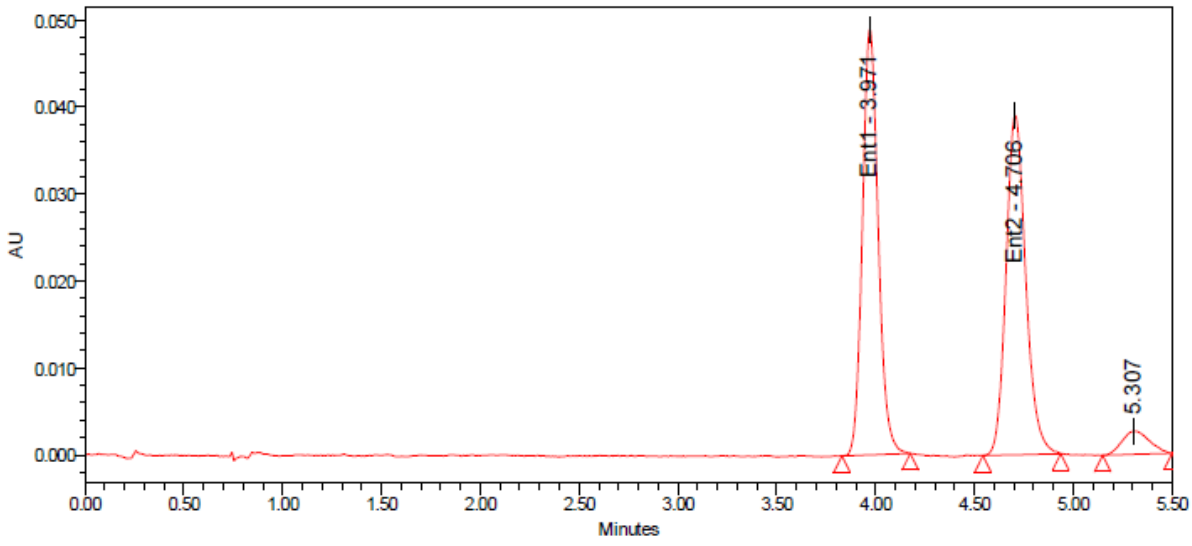


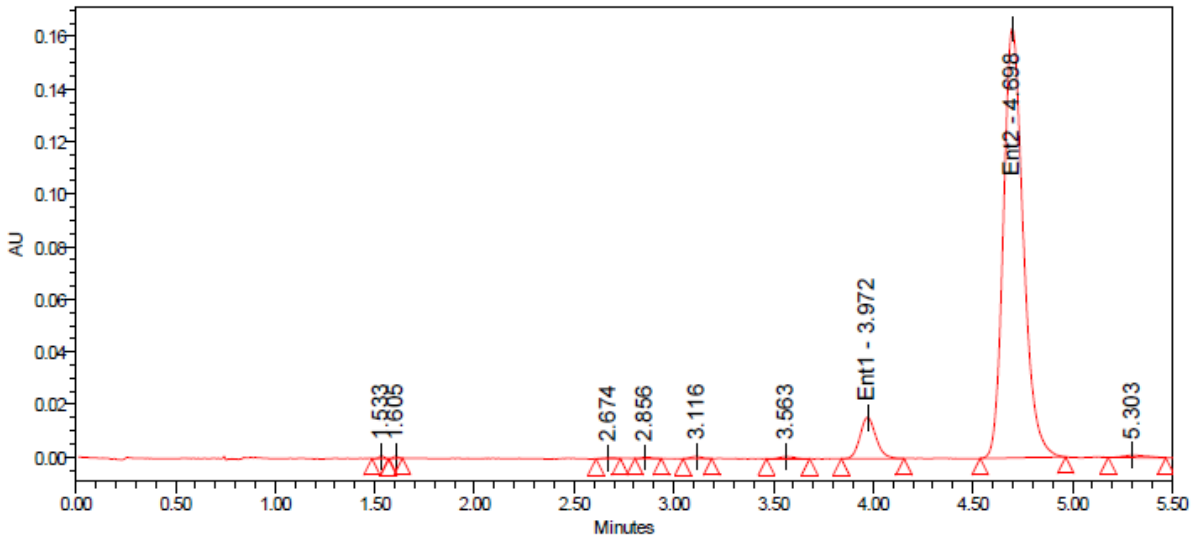
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-32II	49.87	50.13	-0.27	380517	382559
2	SN-E-32I	9.43	90.57	-81.14	54049	519114


SN-E-27-I.1.fid
3g
f1 (ppm)

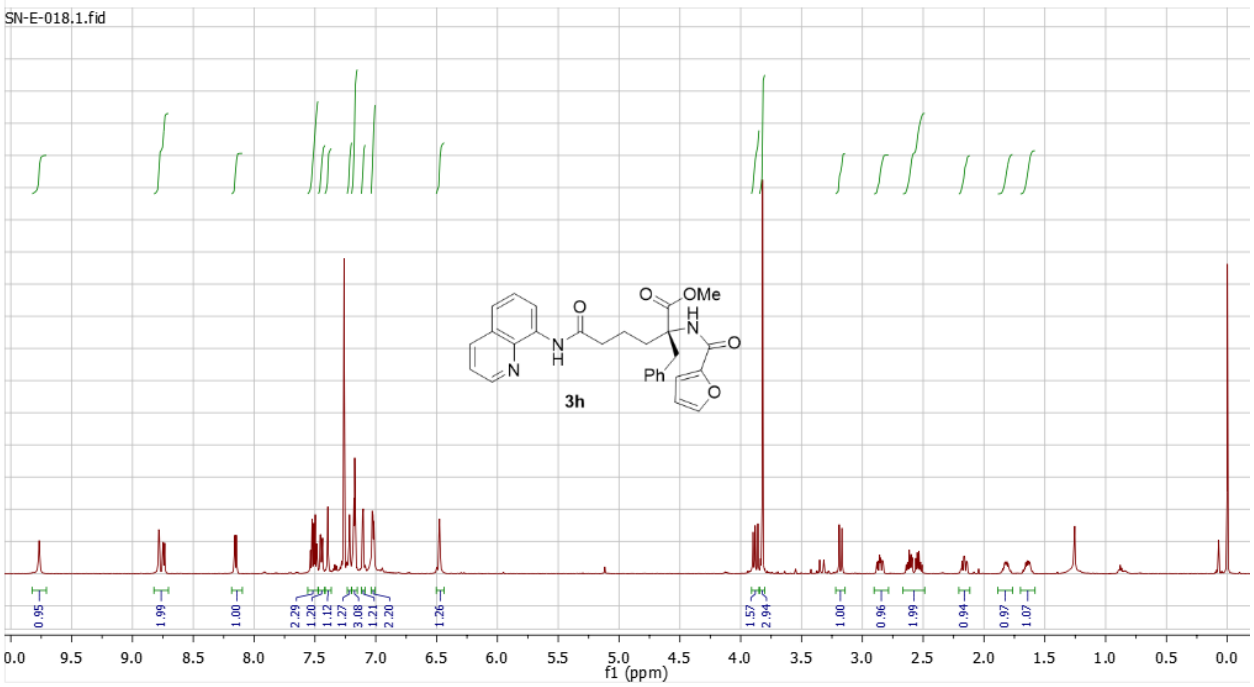

SN-E-27-I.1.fid
3g
f1 (ppm)

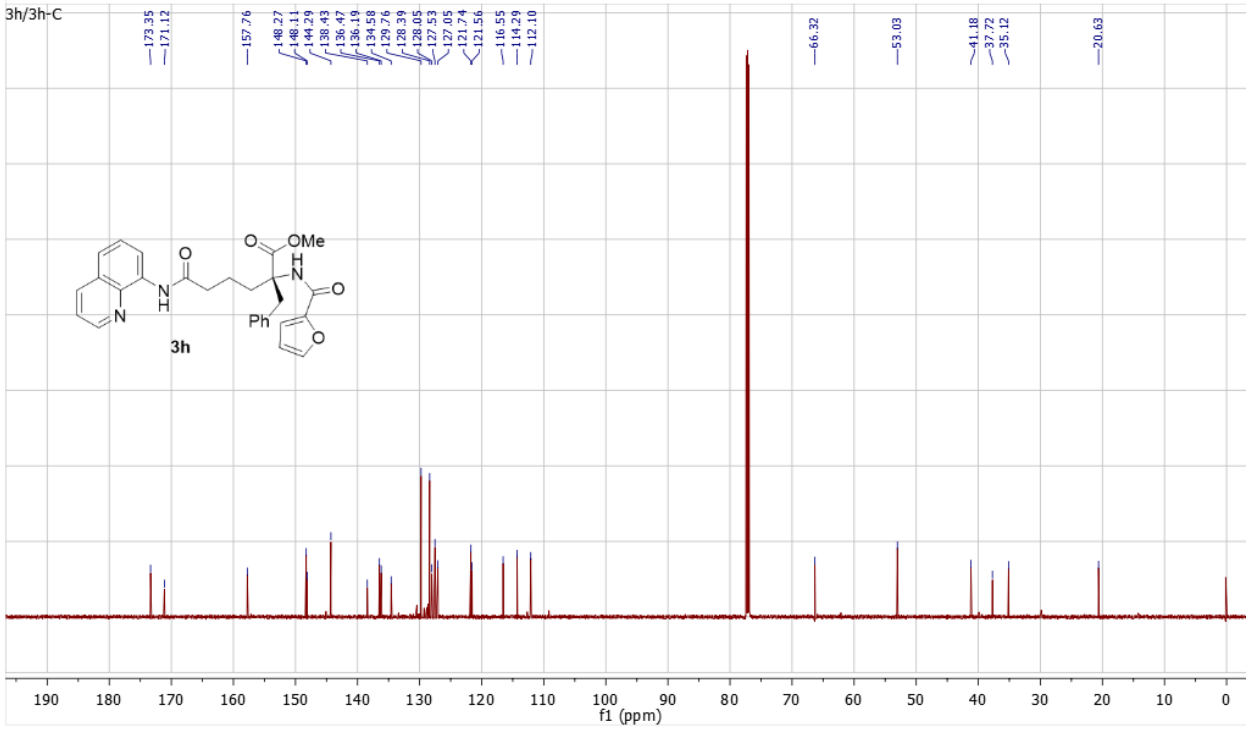


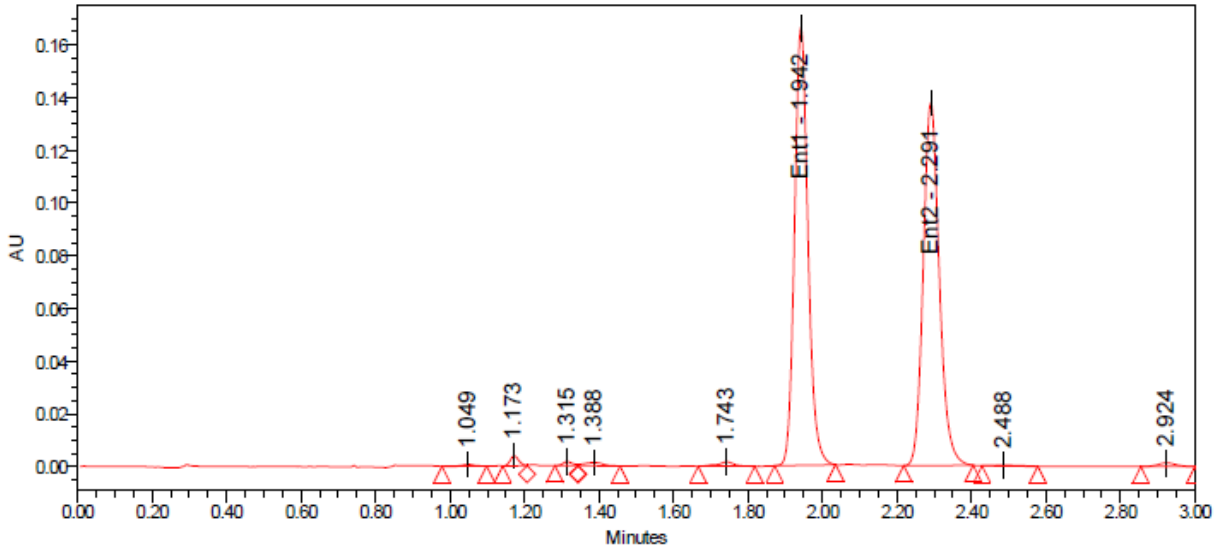


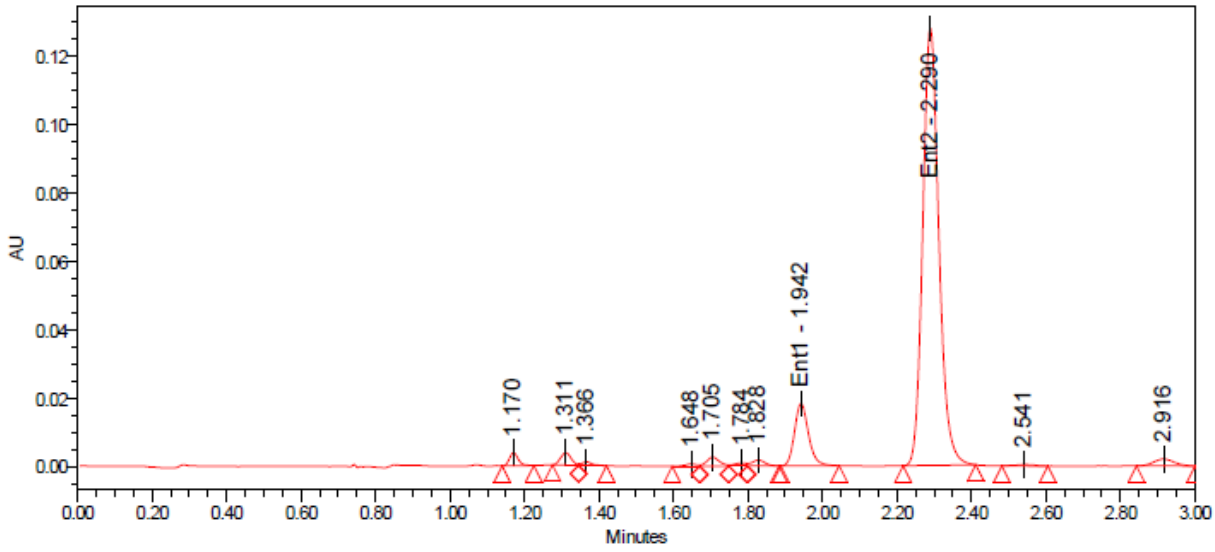
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-27II	50.05	49.95	0.10	271410	270872
2	SN-E-27I	7.18	92.82	-85.64	87658	1133005


SN-E-018.1.fid
OMe
Ph
3h
0.95
1.99
1.00
2.29
1.20
1.12
1.27
3.08
1.21
2.20
1.26
1.57
2.94
1.00
0.96
1.99
0.94
0.97
1.07
f1 (ppm)

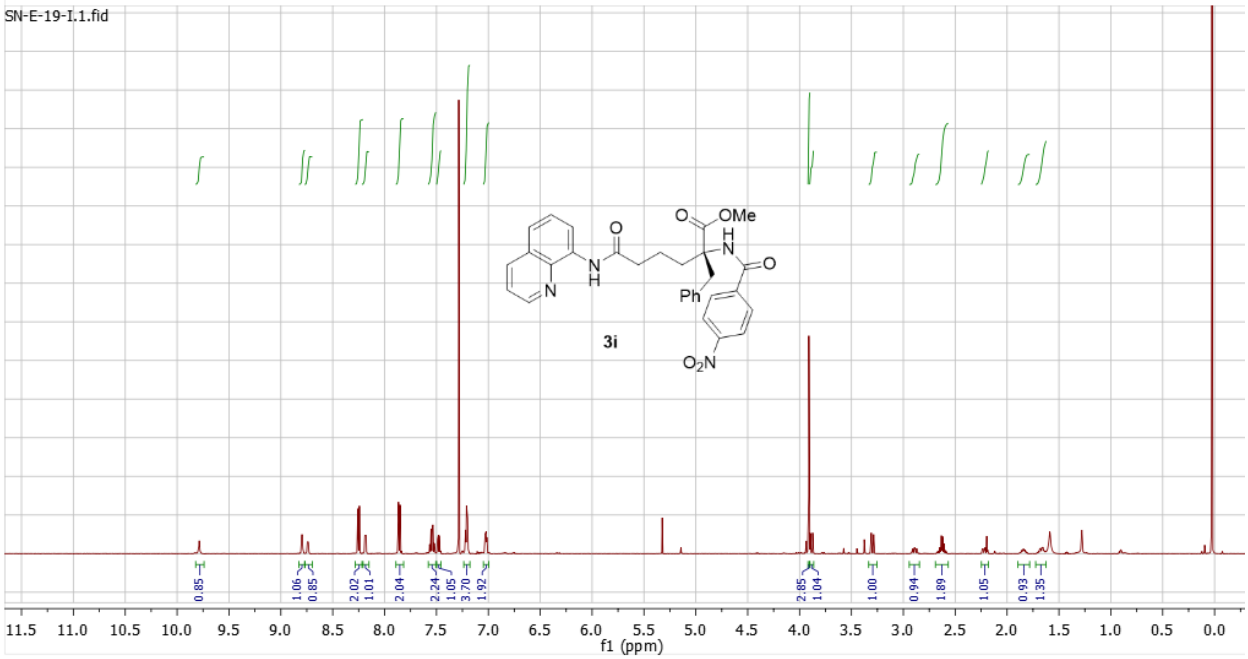

3h/3h-C
173.35
171.12
157.76
148.27
148.11
144.29
138.43
136.47
136.19
134.58
129.76
128.39
128.05
127.53
127.05
121.74
121.56
116.55
114.29
112.10
66.32
53.03
41.18
37.72
35.12
20.63
OMe
Ph
3h
f1 (ppm)

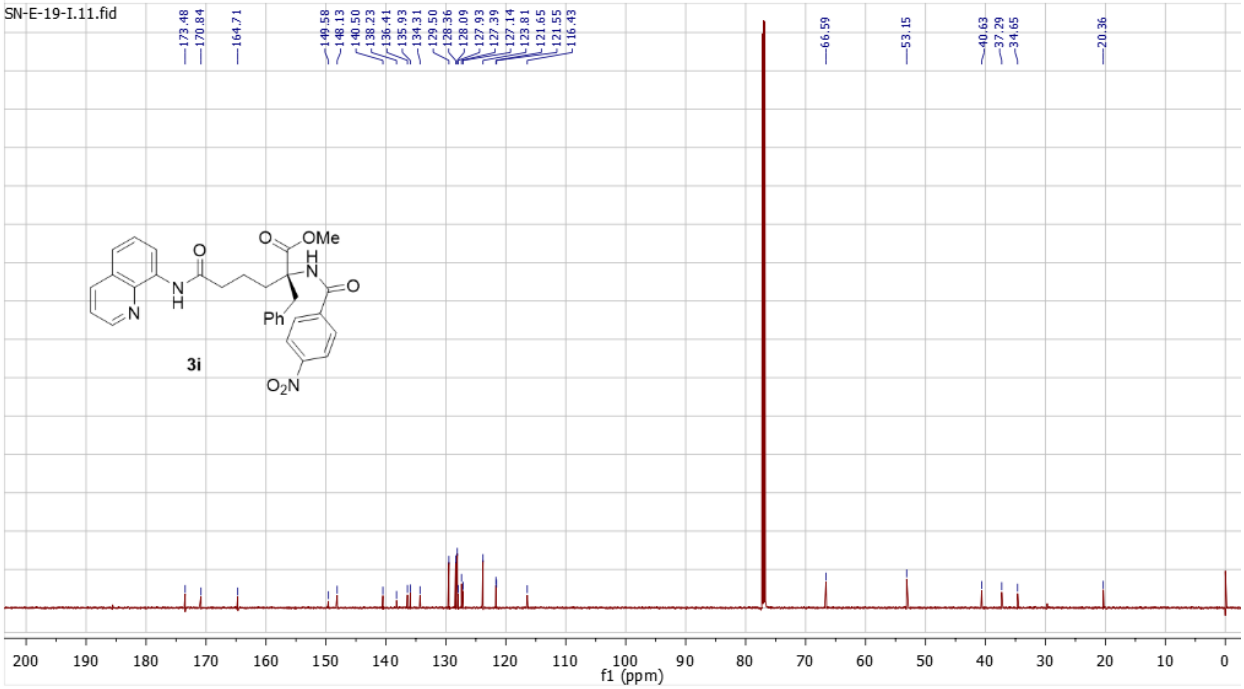


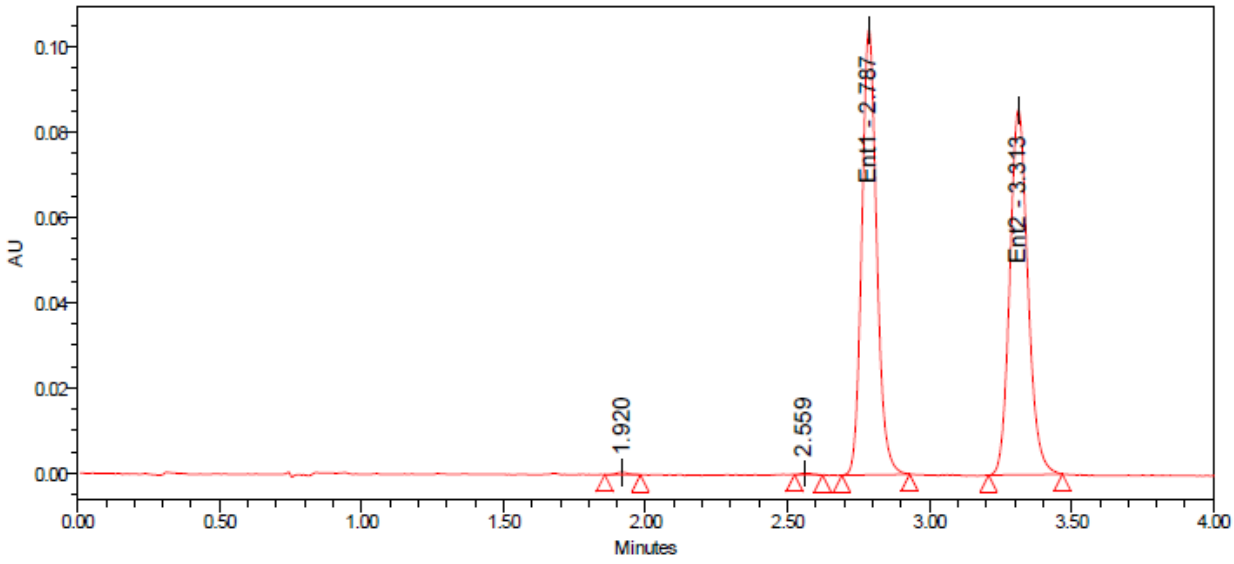


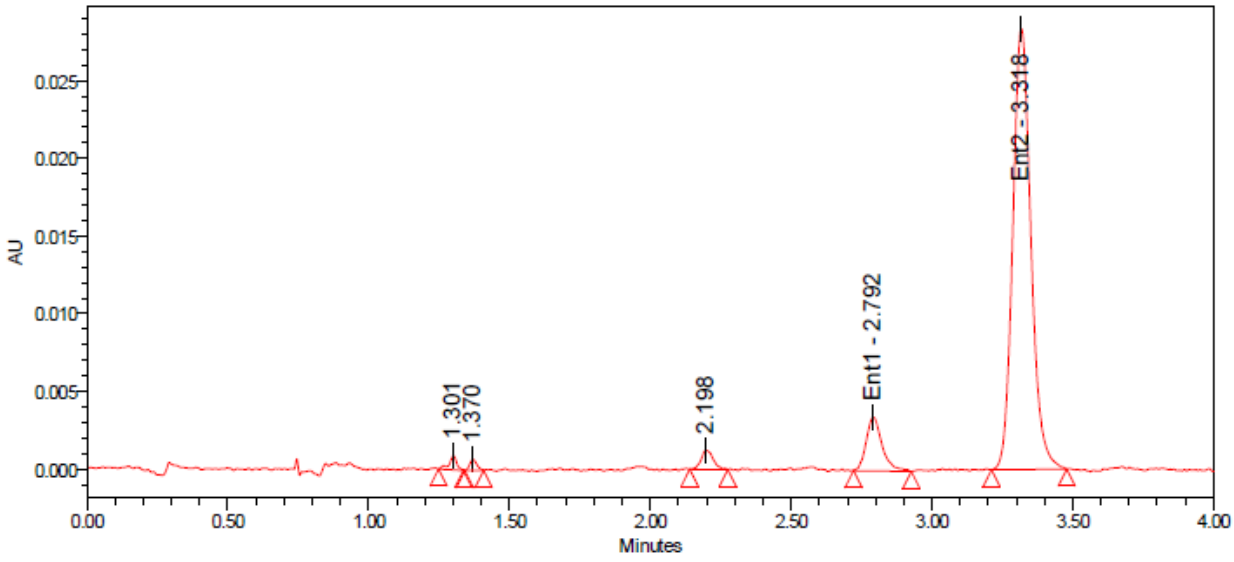
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-18II	50.16	49.84	0.33	416084	413360
2	SN-E-18	10.97	89.03	-78.05	47445	384860


SN-E-19-I.1.fid
3i
f1 (ppm)

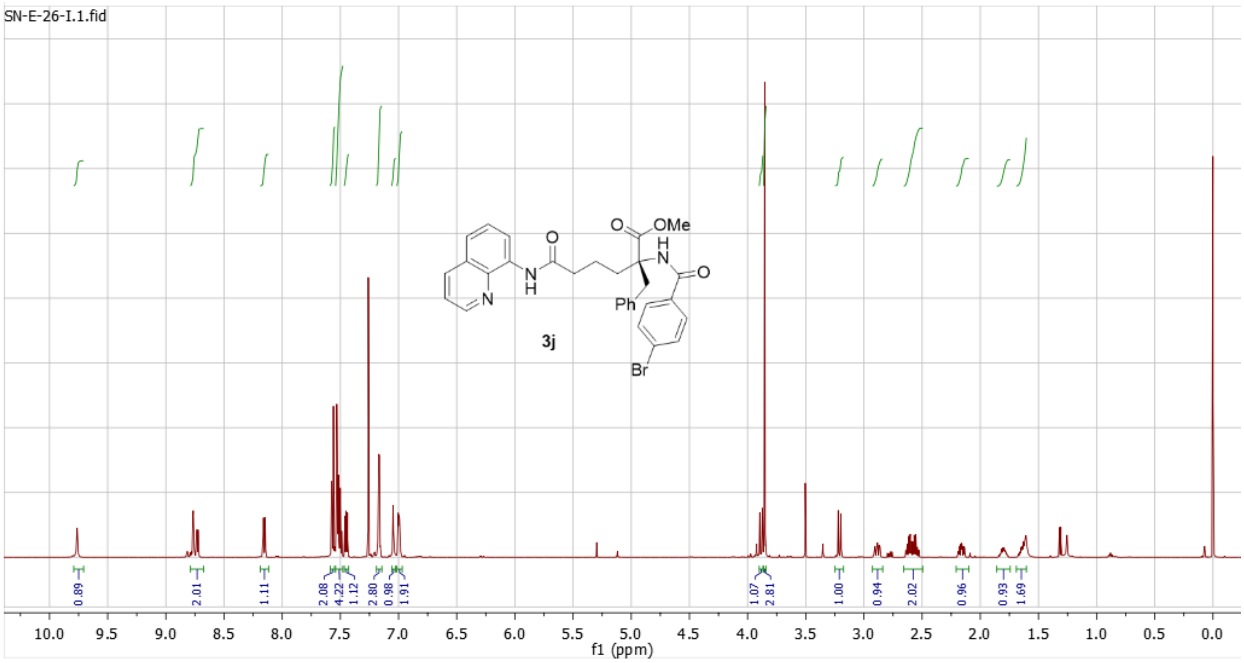

SN-E-19-I.11.fid
3i
f1 (ppm)

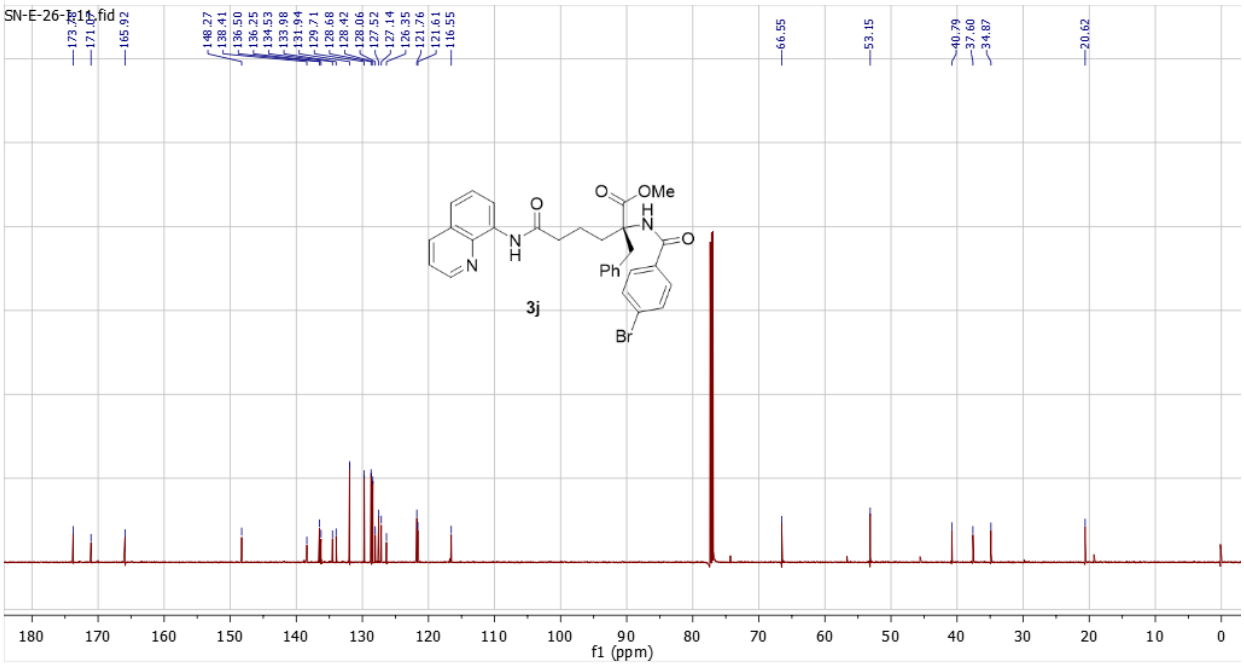




Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-19II	50.12	49.88	0.24	382010	380169
2	SN-E-19	9.69	90.31	-80.61	13639	127060


SN-E-26-I.1.fid
OMe
Ph
Br
3j
0.89
2.01
1.11
2.08
4.22
1.12
2.80
0.98
1.91
1.07
2.81
1.00
0.94
2.02
0.96
0.93
1.69
f1 (ppm)


SN-E-26-I-13.fid
173.78
171.07
165.92
148.27
138.41
136.50
136.25
134.53
133.98
131.94
129.71
128.68
128.42
128.06
127.52
127.14
126.35
121.76
121.61
116.55
66.55
53.15
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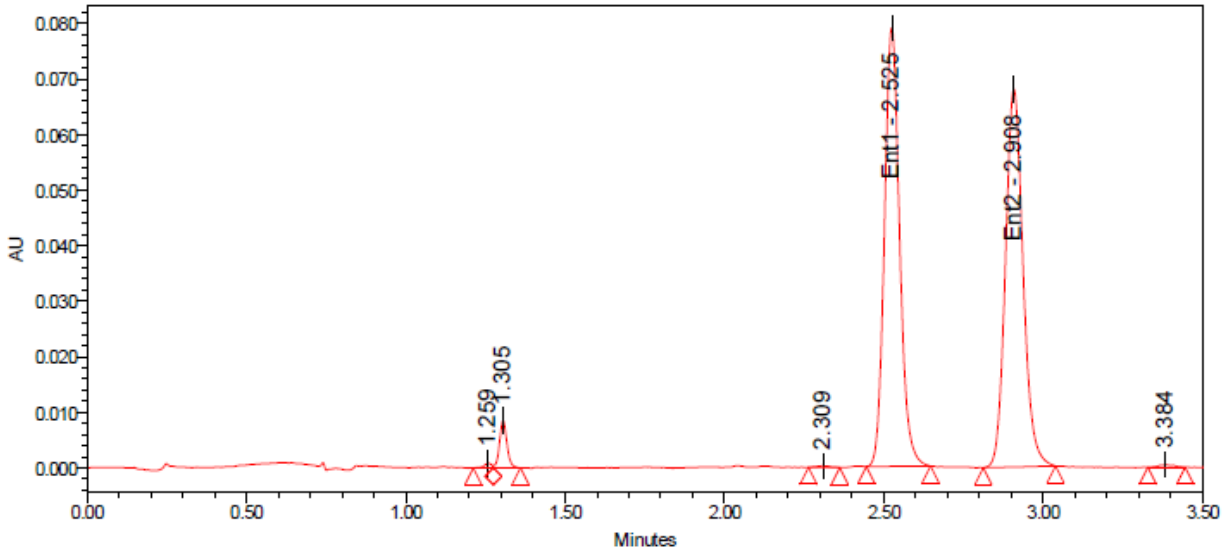
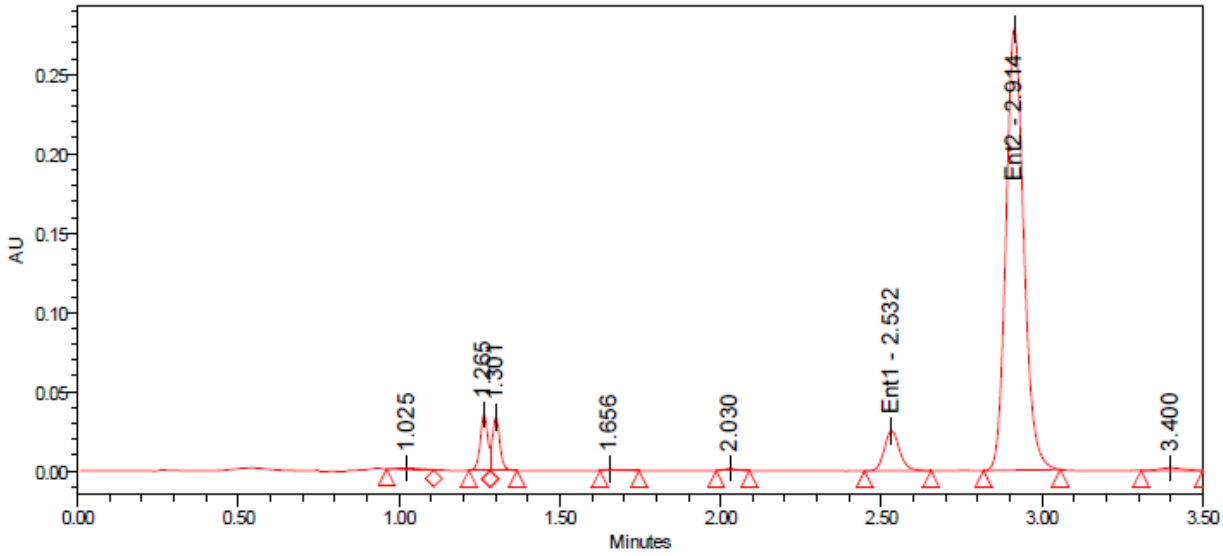
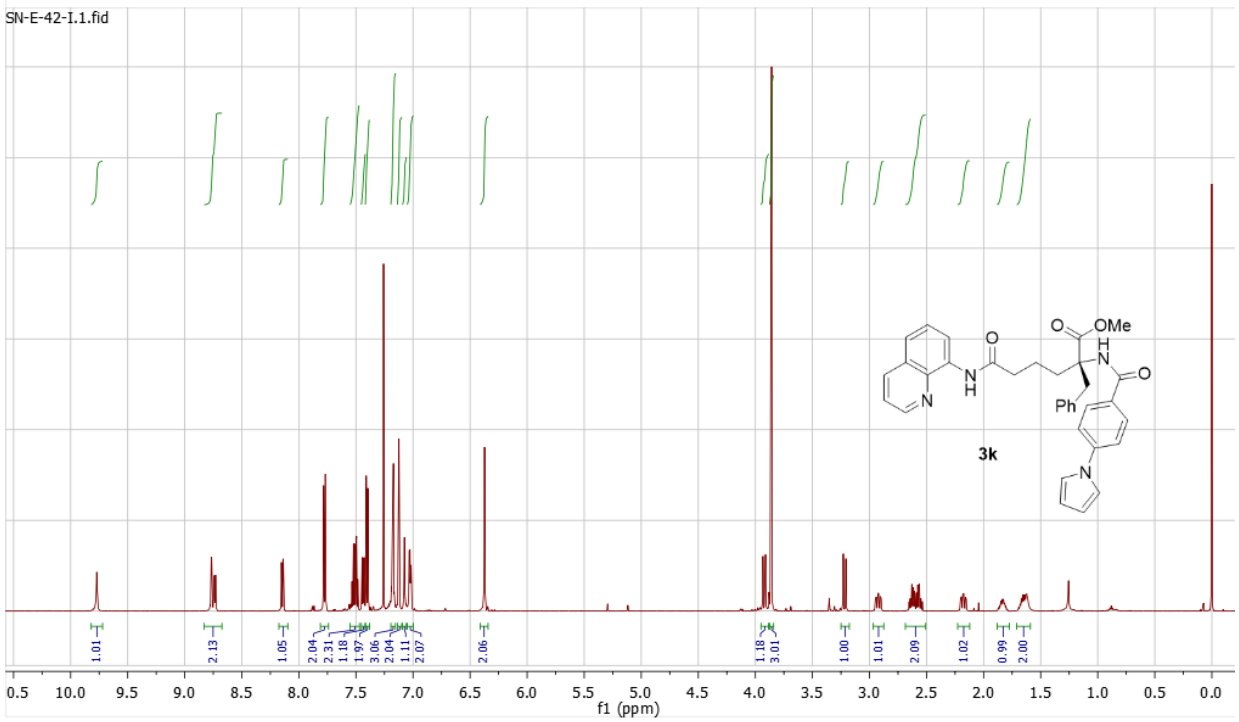
34.87
20.62
OMe
Ph
Br
3j
f1 (ppm)

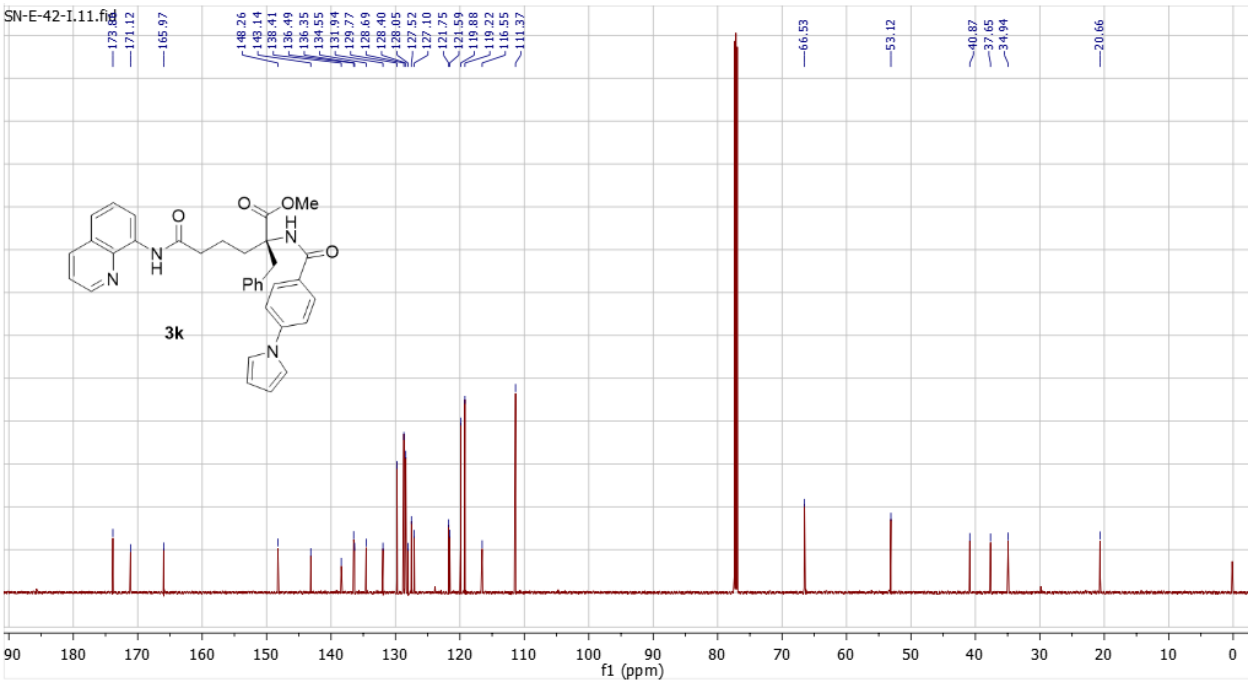


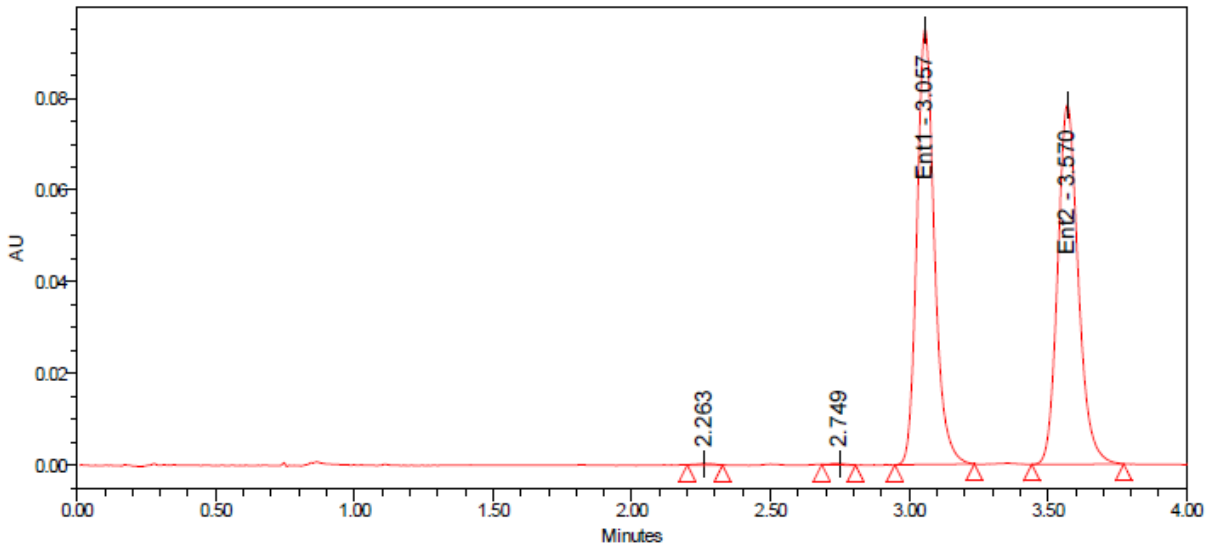


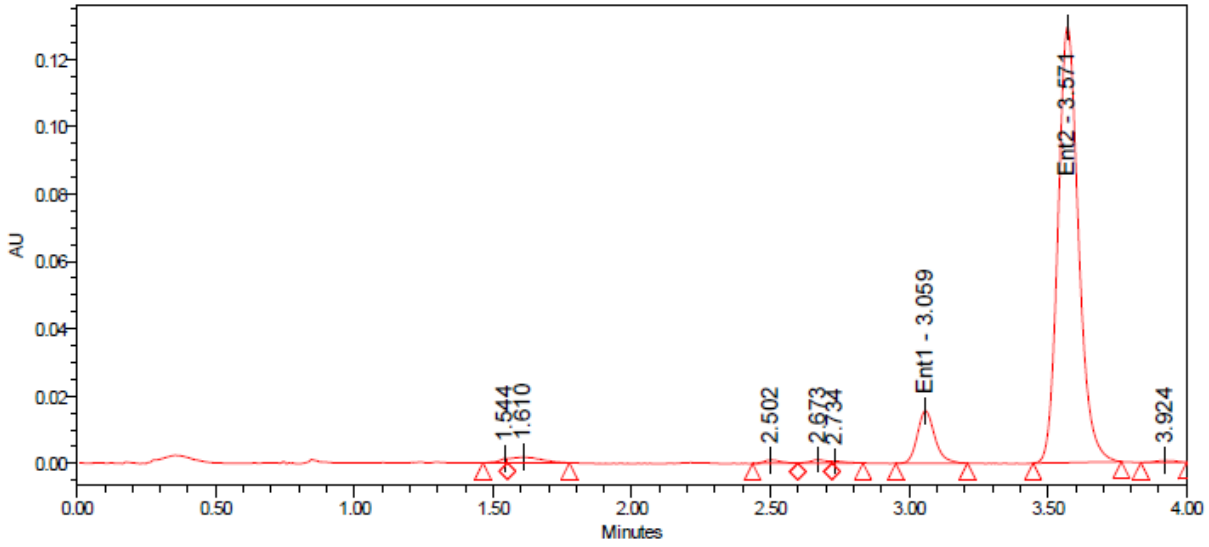
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-26II	49.98	50.02	-0.03	260781	260943
2	SN-E-26I	7.26	92.74	-85.49	83564	1068116


SN-E-42-I.1.fid
3k
f1 (ppm)

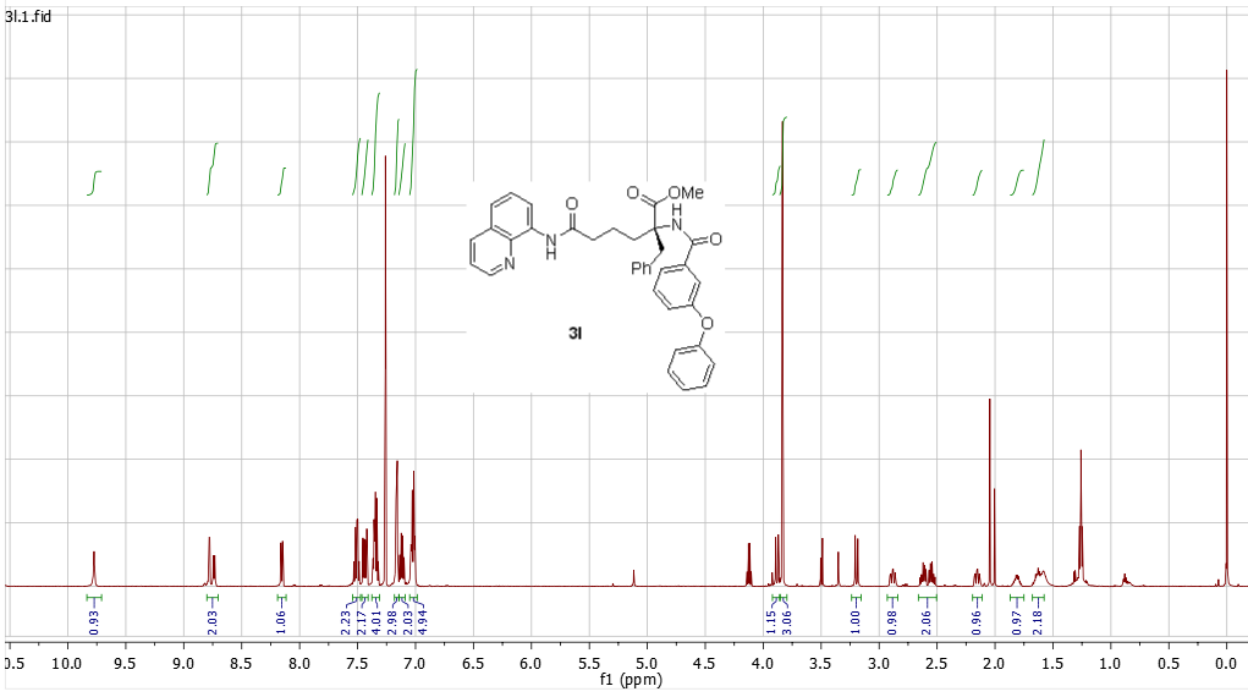

SN-E-42-I.11.fid
3k
f1 (ppm)

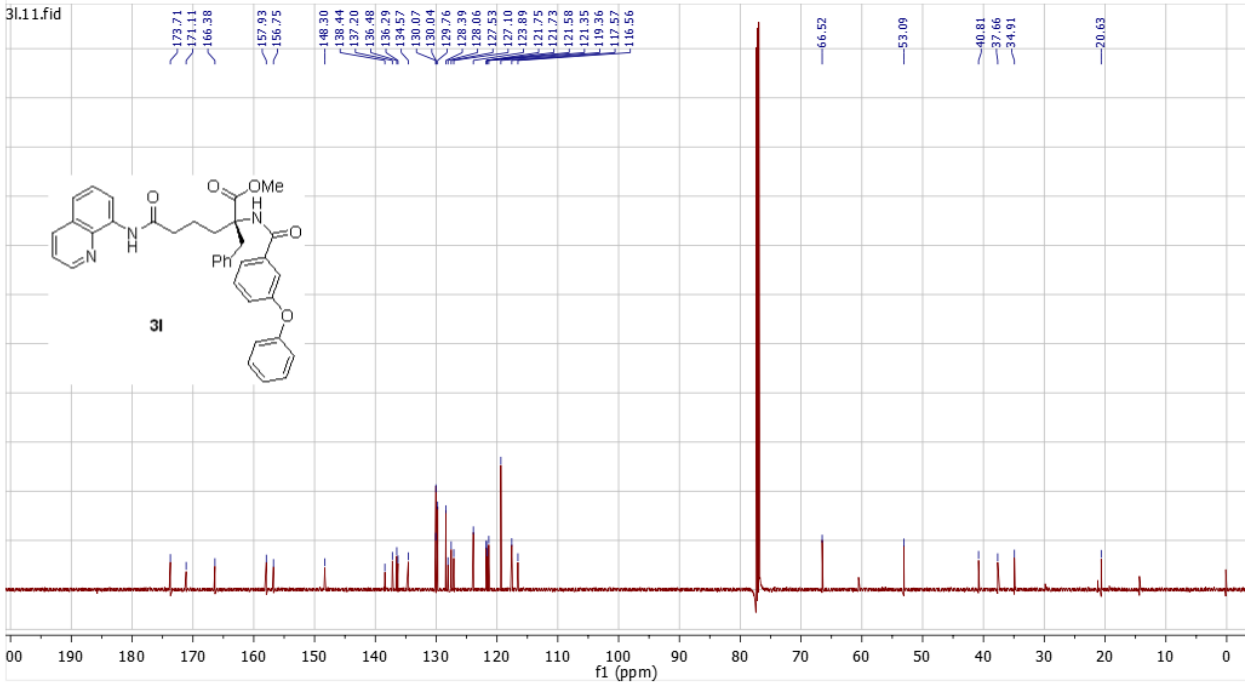




Area Summarized by Name

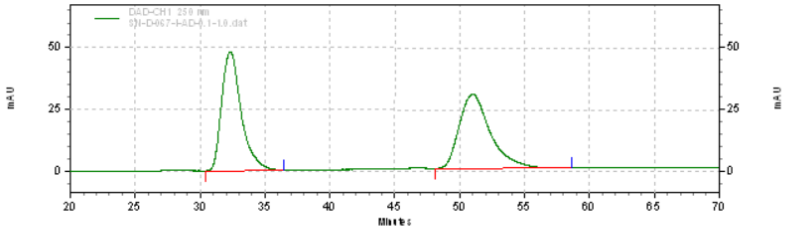
	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-42II	50.63	49.37	1.27	415319	404914
2	SN-E-42I	9.30	90.70	-81.40	68332	666406


3l.1.fid
OMe
Ph
3l
0.93
2.03
1.06
2.23
2.17
4.01
2.98
2.03
4.94
1.15
3.06
1.00
0.98
2.06
0.96
0.97
2.18
f1 (ppm)


3l.11.fid
173.71
171.11
166.38
157.93
156.75
148.30
138.44
137.20
136.48
136.29
134.57
130.07
130.04
129.76
128.39
128.06
127.53
127.10
123.89
121.75
121.73
121.58
121.35
119.36
117.57
116.56
66.52
53.09
40.81
37.66
34.91
20.63
OMe
Ph
3l
f1 (ppm)

Area % Report

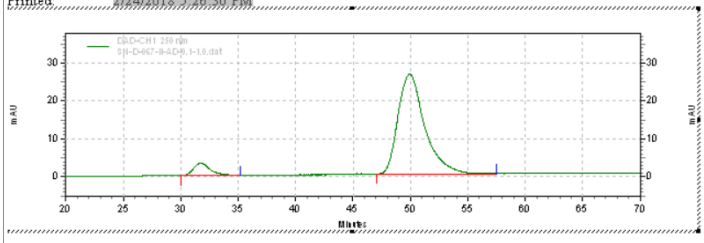
Data File: C:\ENGLE LAB DATA\Sri\SN-D-067-I-AD-0.1-1.0.dat
Method: C:\EZChrom Elite\Enterprise\Projects\engle project 1\Method\untitled.met
Acquired: 9/11/2017 10:45:00 PM
Printed: 2/24/2018 5:18:33 PM



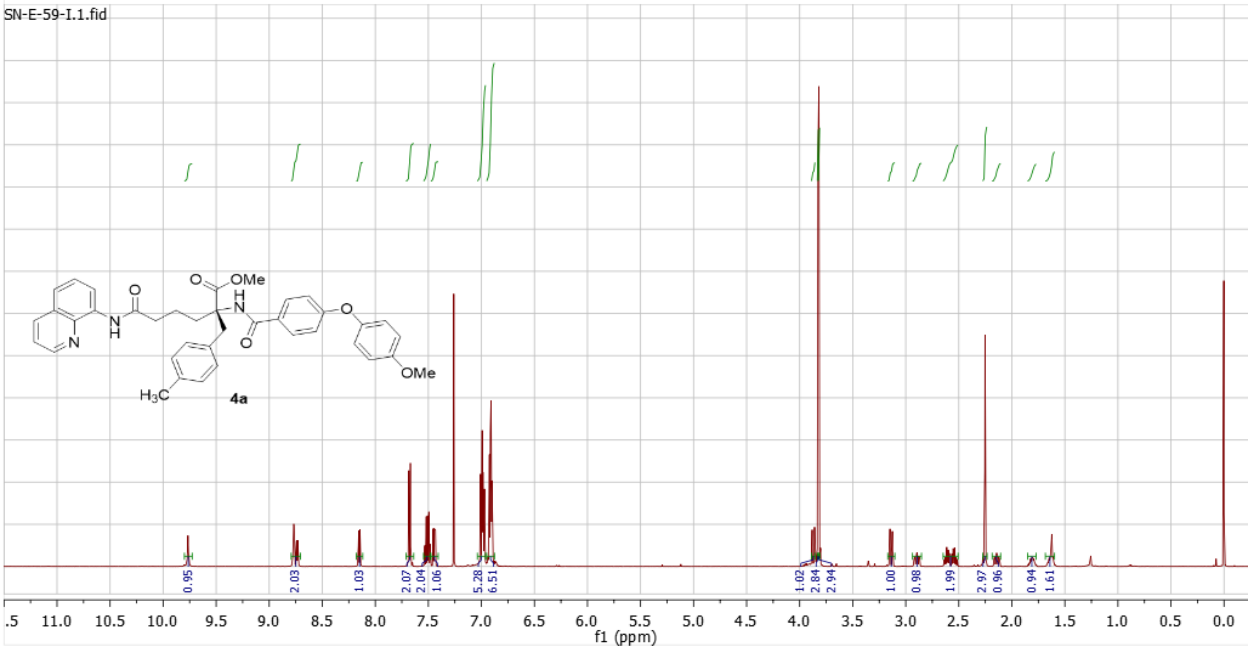
DAD-CH1 250 nm Results				
Retention Time	Area	Area %	Height	Height %
32.320	20028947	50.15	191654	61.60
50.987	19909888	49.85	119457	38.40
Totals				
	39938835	100.00	311111	100.00

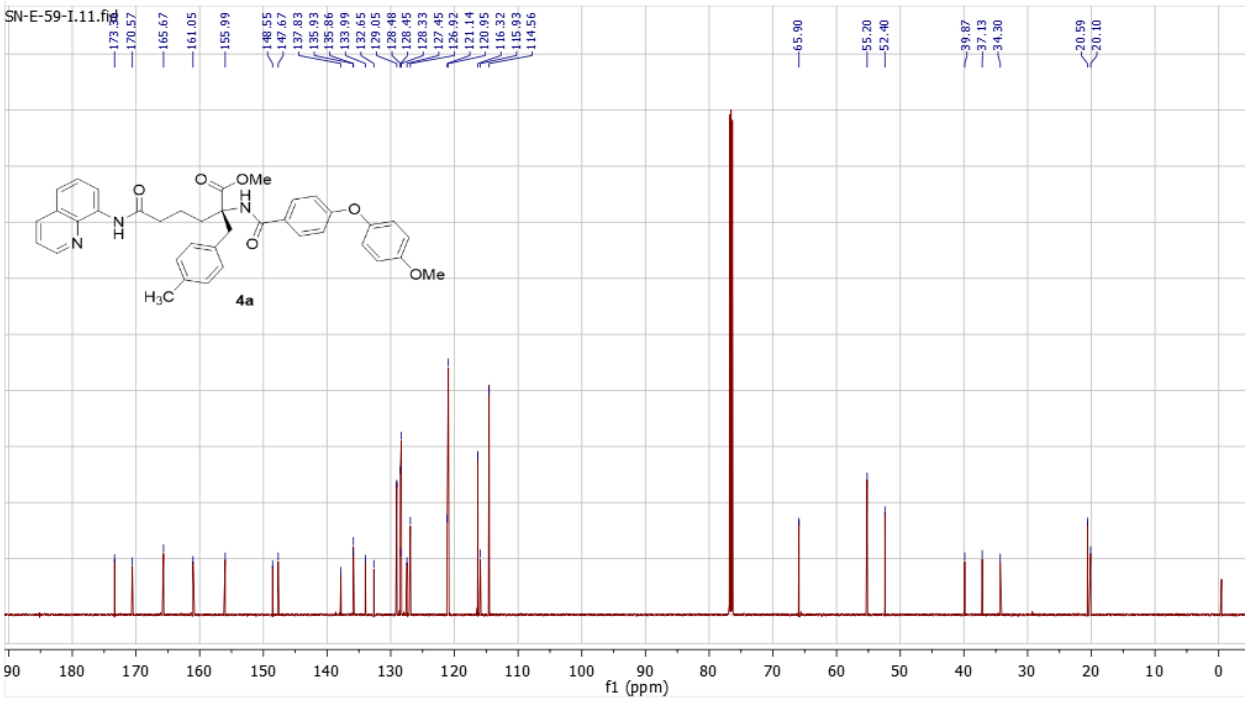
Area % Report

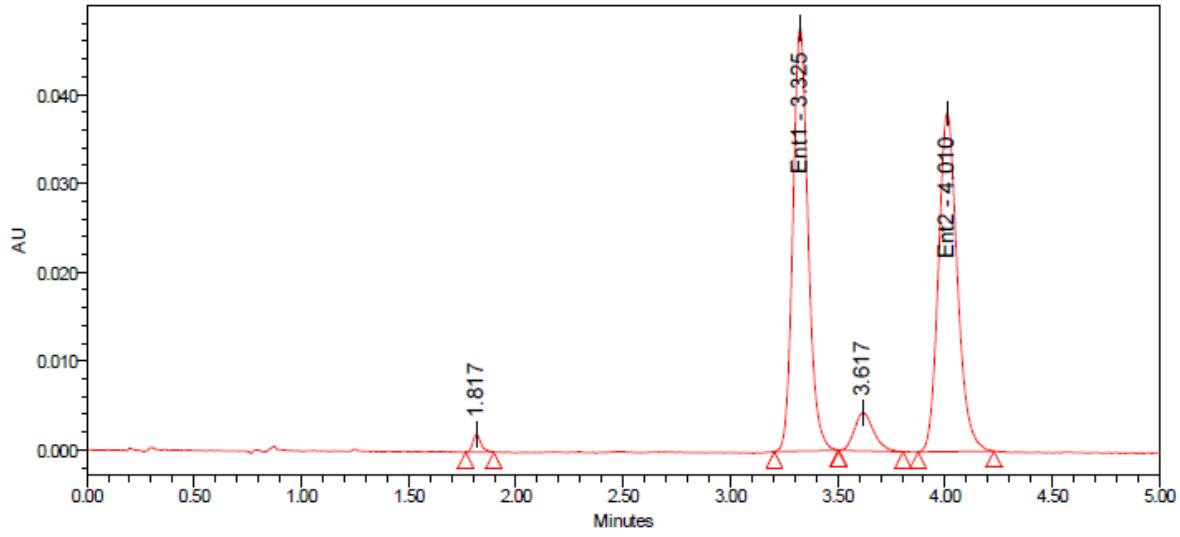
Data File: C:\ENGLE LAB DATA\Sri\SN-D-067-II-AD-0.1-1.0.dat
Method: C:\EZChrom Elite\Enterprise\Projects\engle project 1\Method\untitled.met
Acquired: 9/12/2017 12:47:00 AM
Printed: 2/24/2018 5:26:30 PM

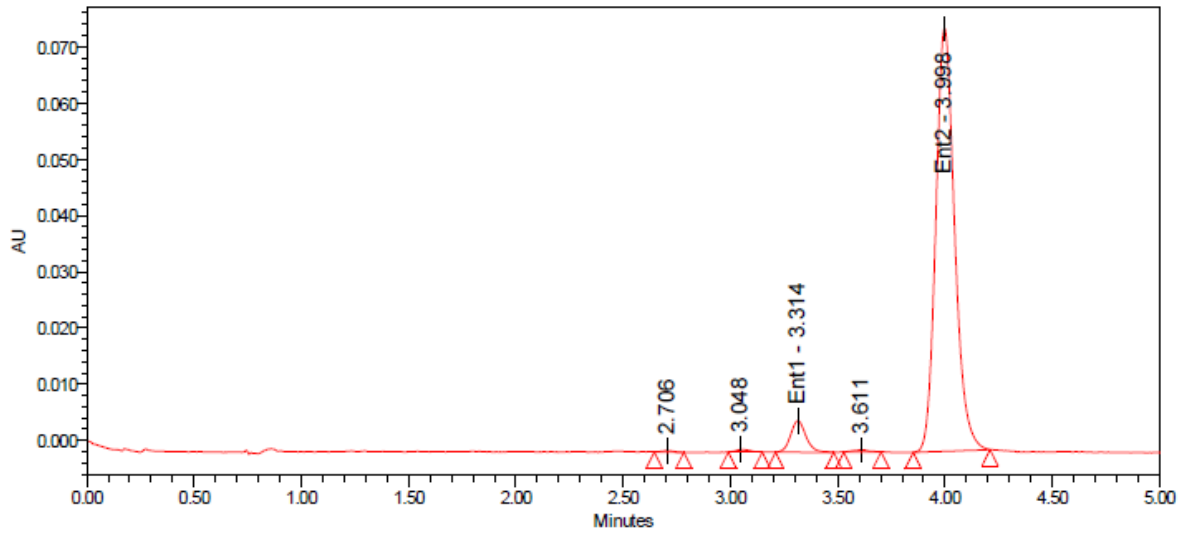


DAD-CH1 250 nm Results				
Retention Time	Area	Area %	Height	Height %
31.807	1359080	7.39	12995	10.99
49.940	17028426	92.61	105265	89.01
Totals				
	18387506	100.00	118260	100.00


SN-E-59-I.1.fid
OMe
OMe
H3C
4a
f1 (ppm)

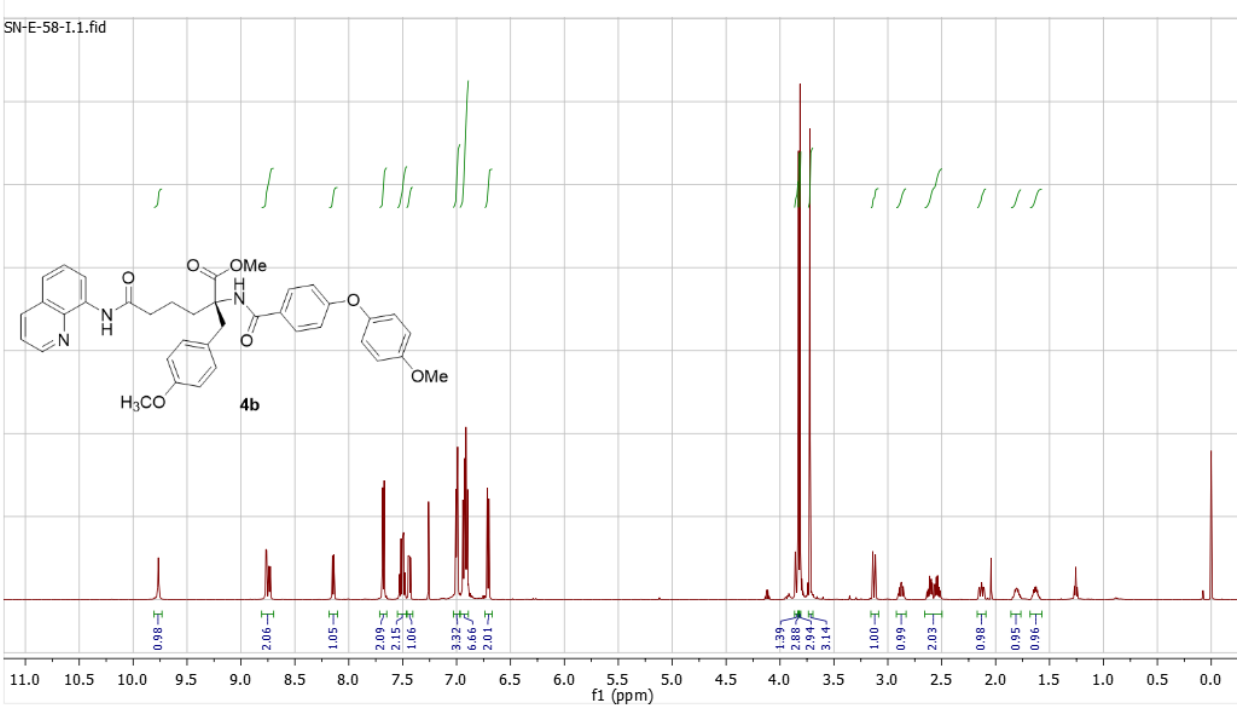

SN-E-59-I.11.fid
OMe
OMe
H3C
4a
f1 (ppm)

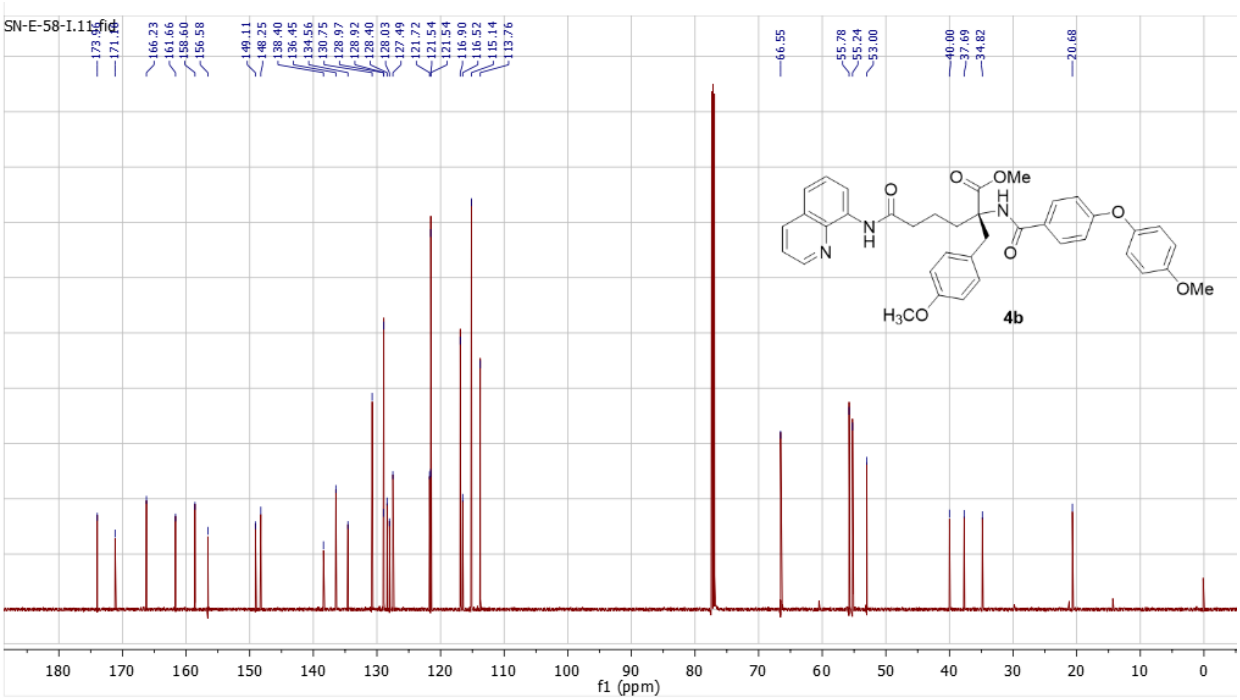


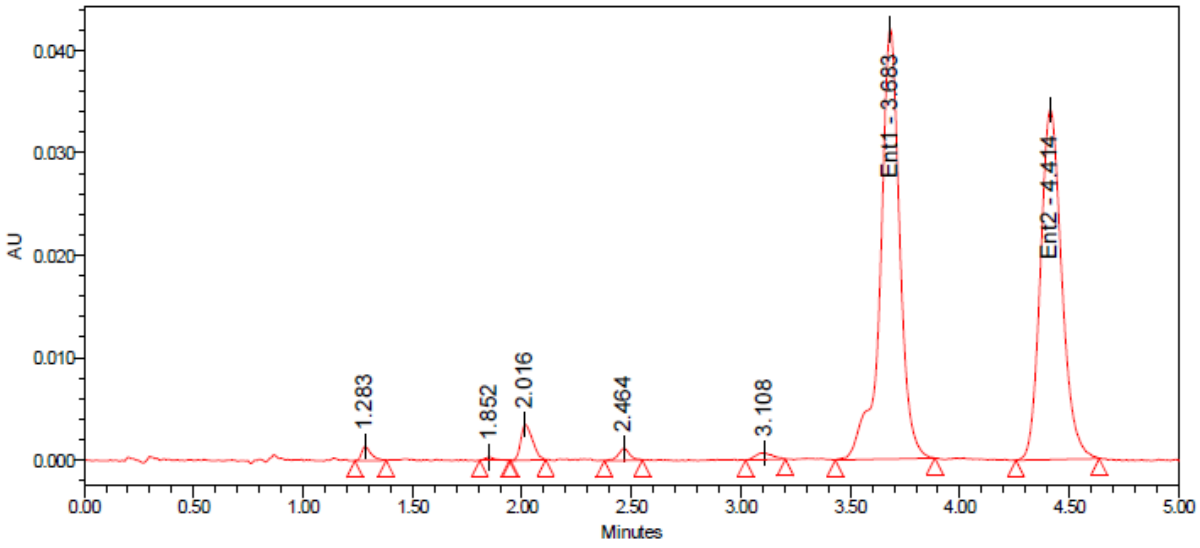


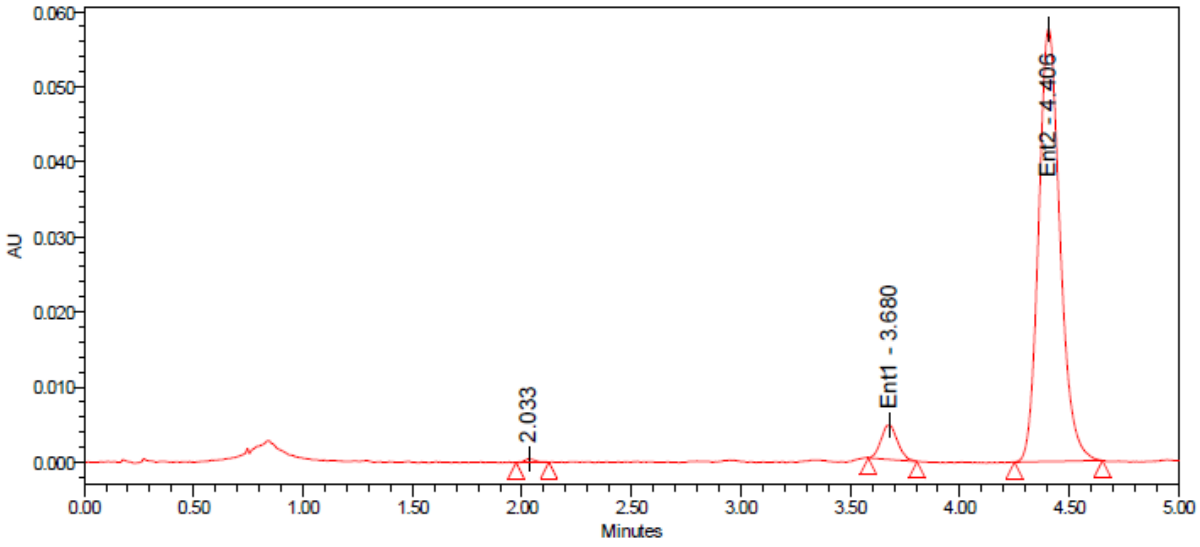
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-59II	50.08	49.92	0.16	233778	233008
2	SN-E-59I	5.71	94.29	-88.58	27791	459004


SN-E-58-I.1.fid
4b
f1 (ppm)

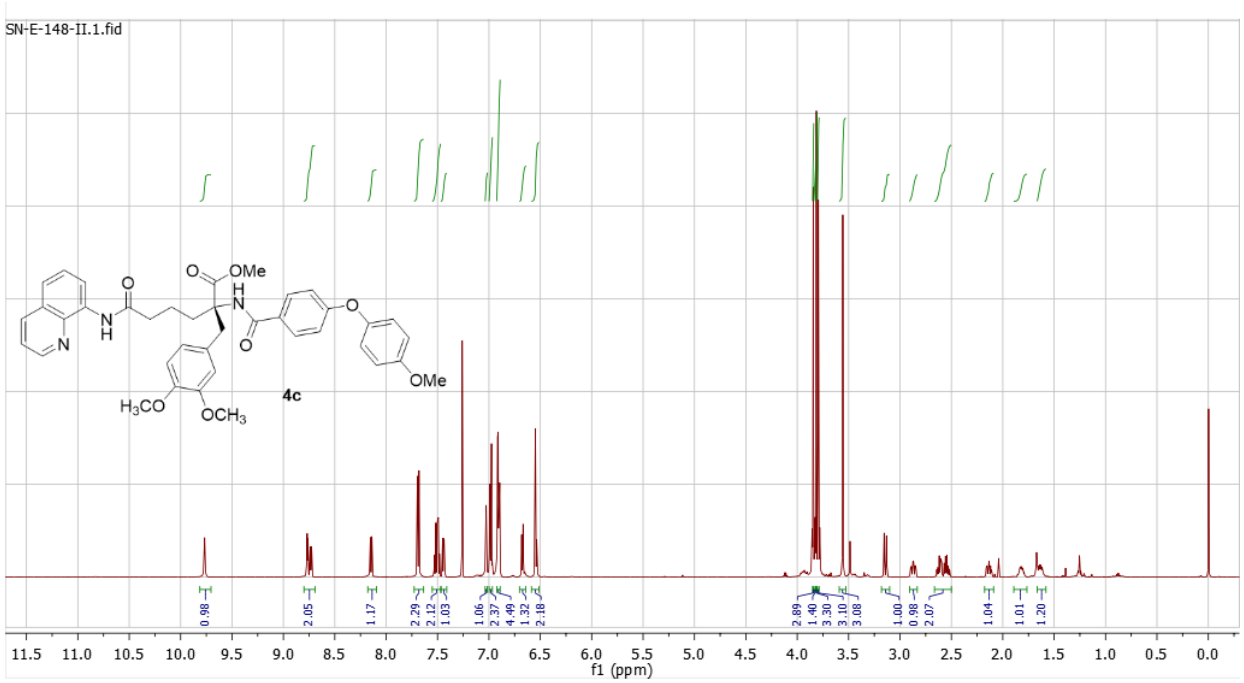

SN-E-58-I.11.fid
4b
f1 (ppm)

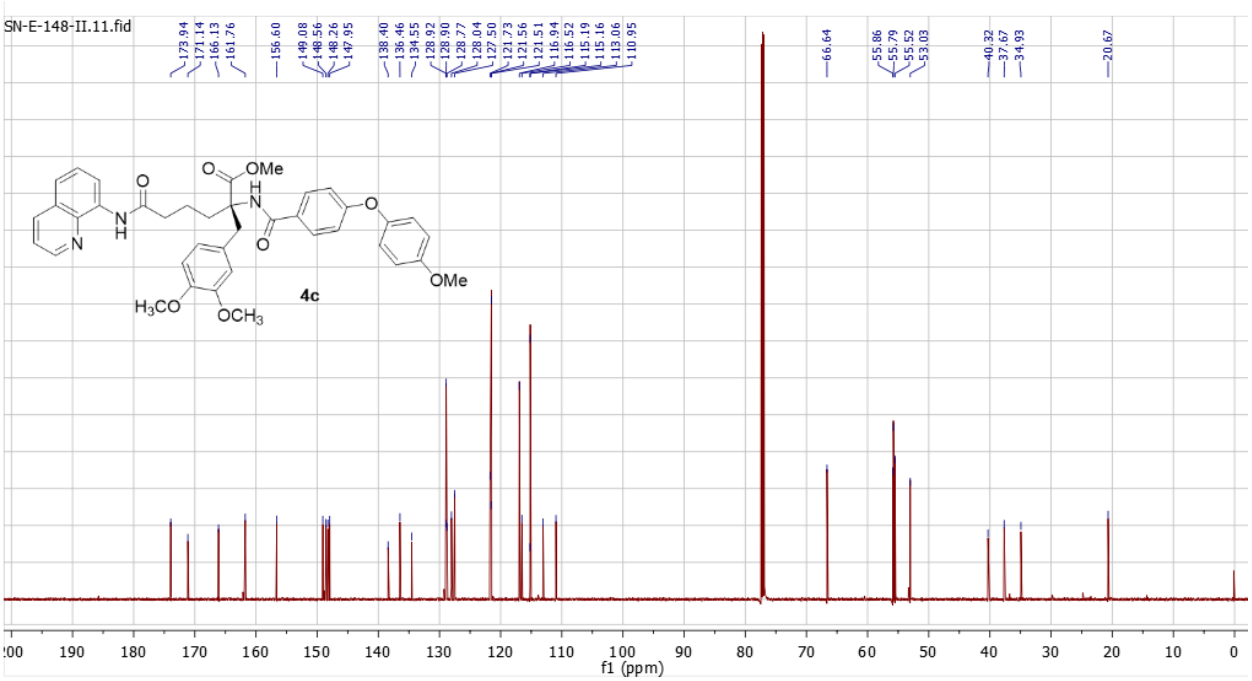


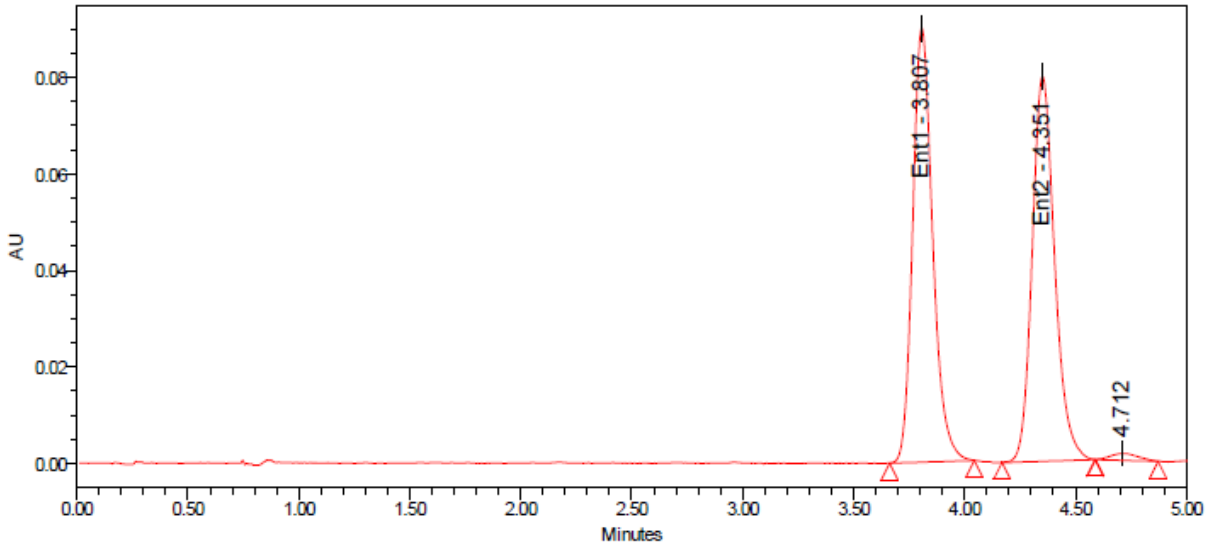


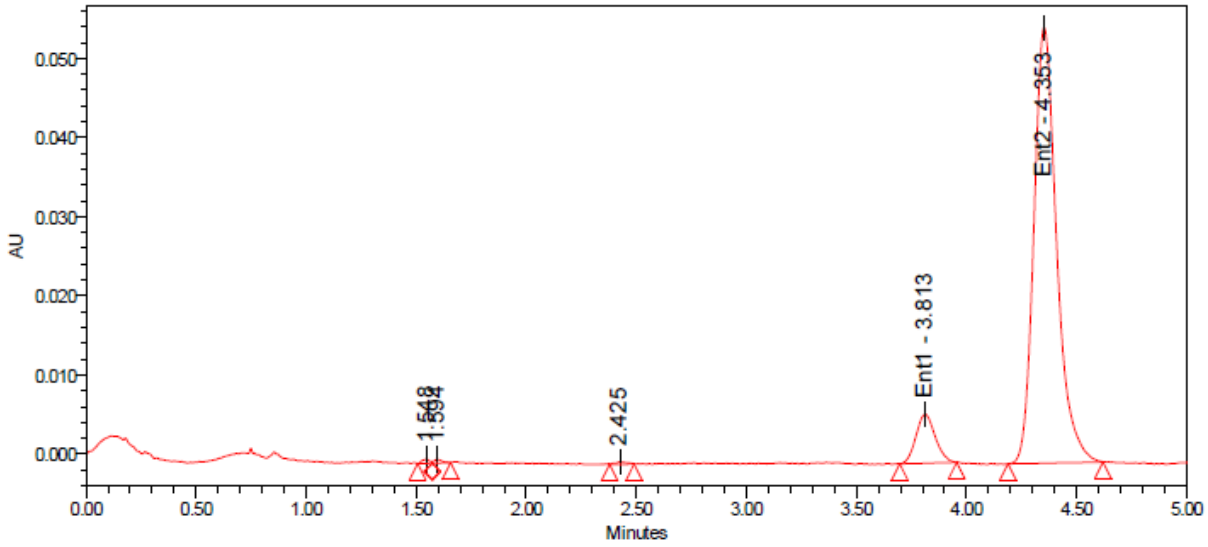
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-58II	52.85	47.15	5.70	259366	231413
2	SN-E-58I	5.82	94.18	-88.37	24184	391701


SN-E-148-II.1.fid
4c
f1 (ppm)

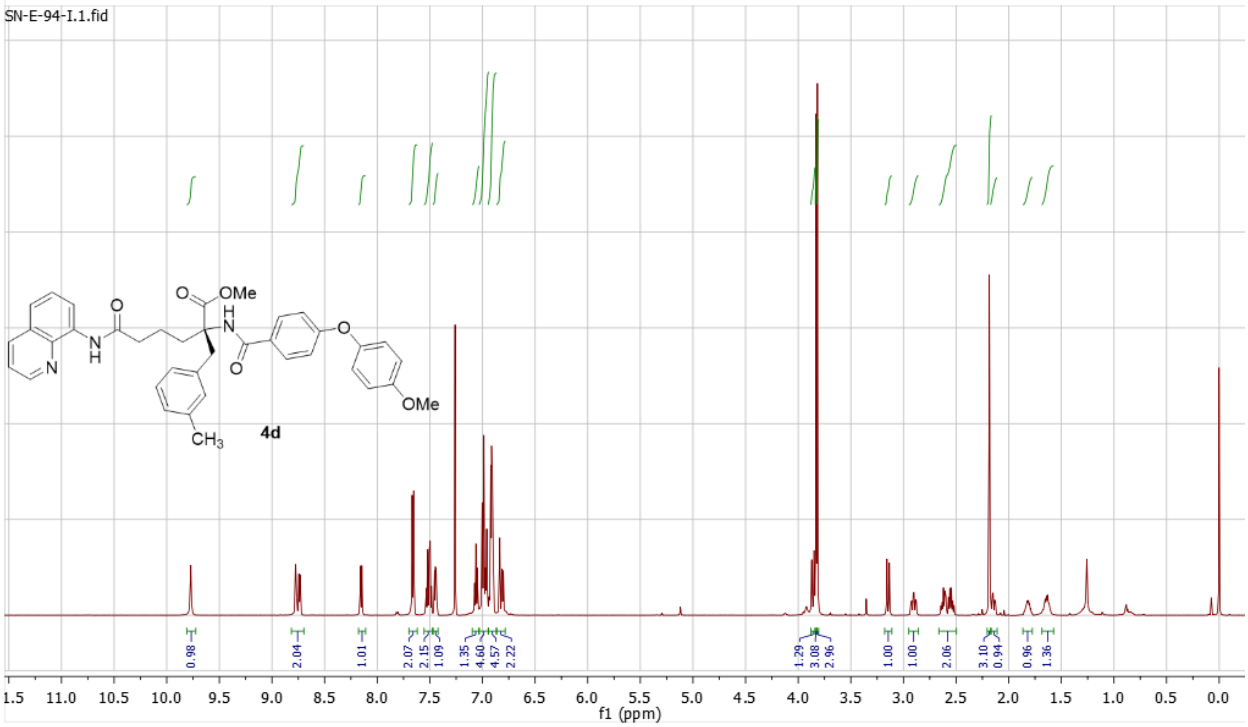

SN-E-148-II.11.fid
4c
f1 (ppm)

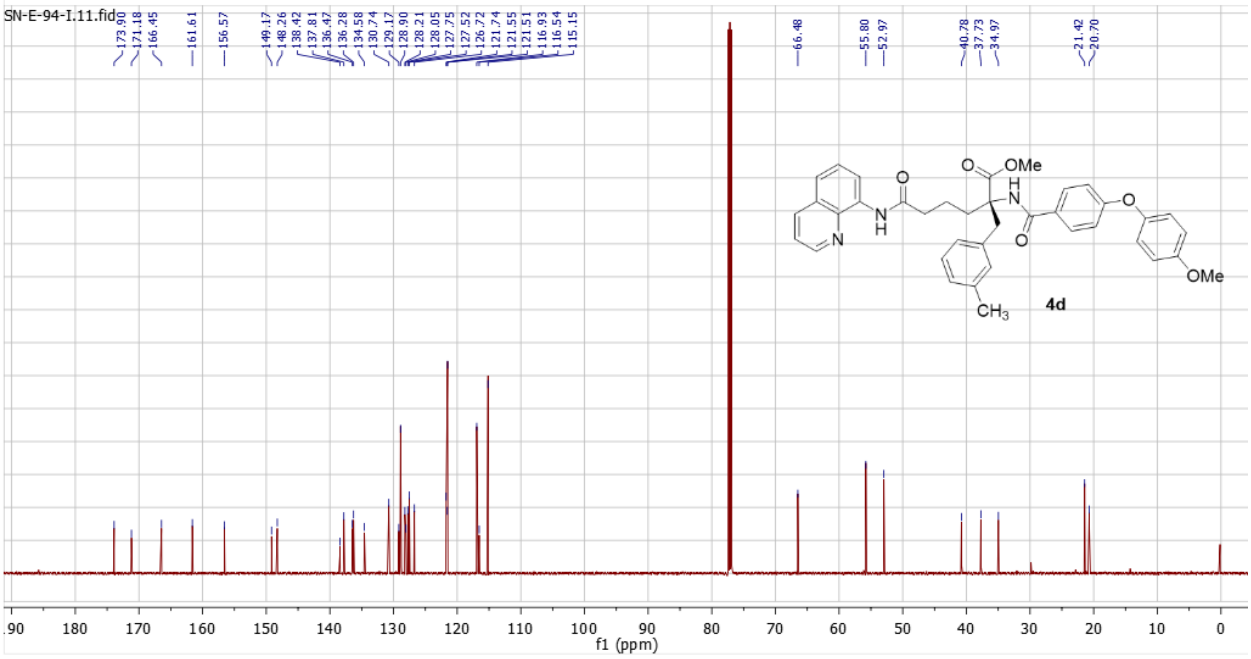


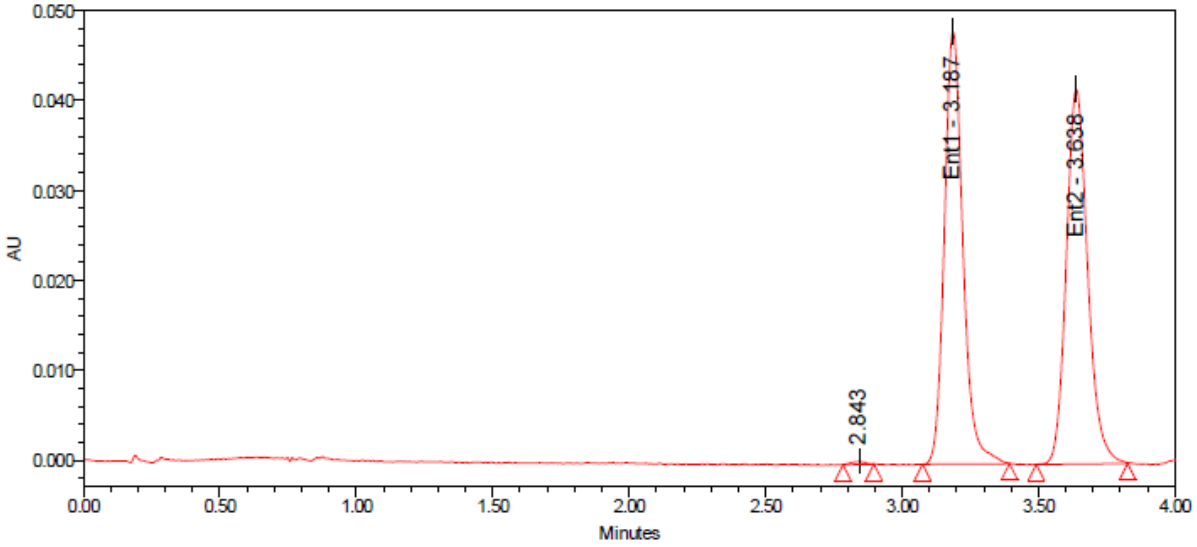


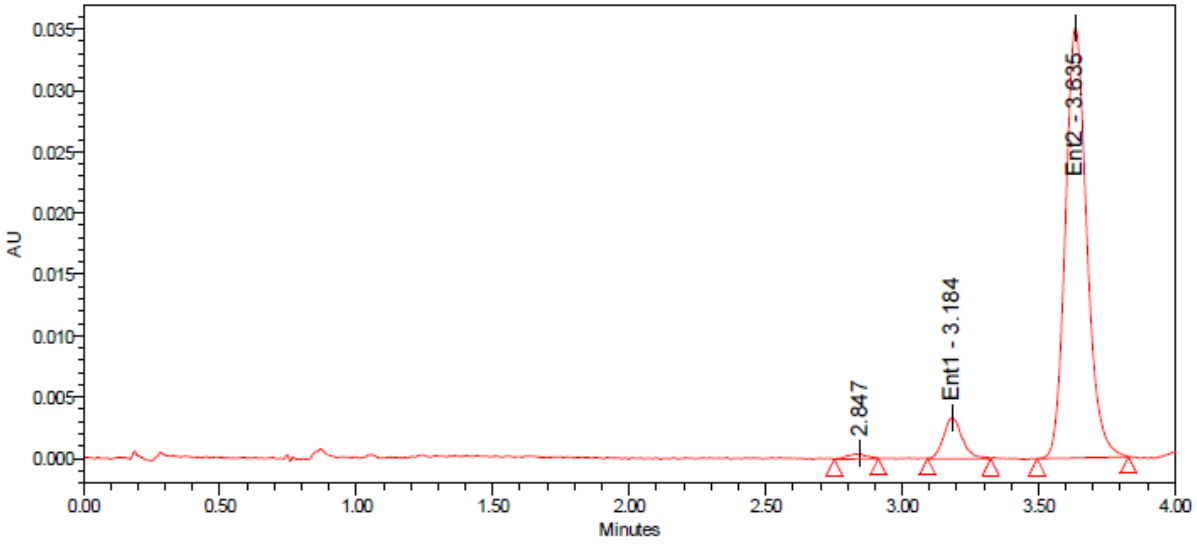
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-148II	50.09	49.91	0.18	563828	561839
2	SN-E-148I	8.68	91.32	-82.64	37540	394894


SN-E-94-I.1.fid
OMe
OMe
CH3
4d
f1 (ppm)

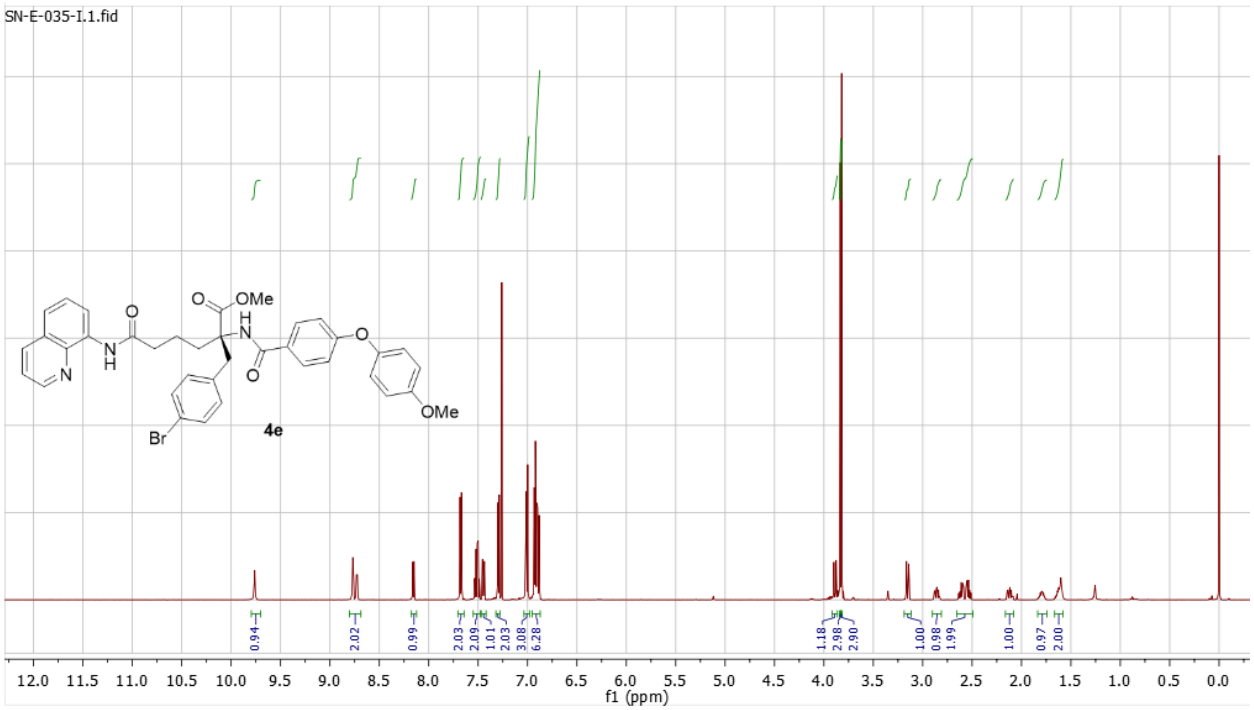

SN-E-94-I.11.fid
OMe
OMe
CH3
4d
f1 (ppm)

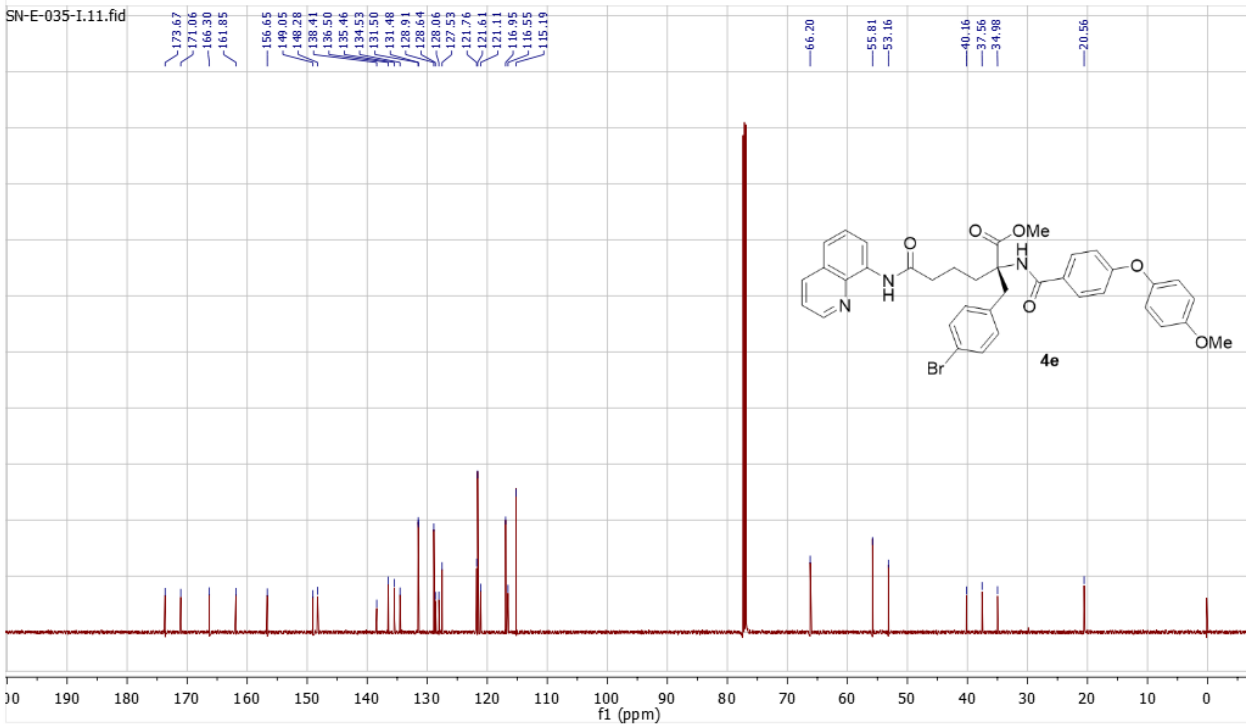


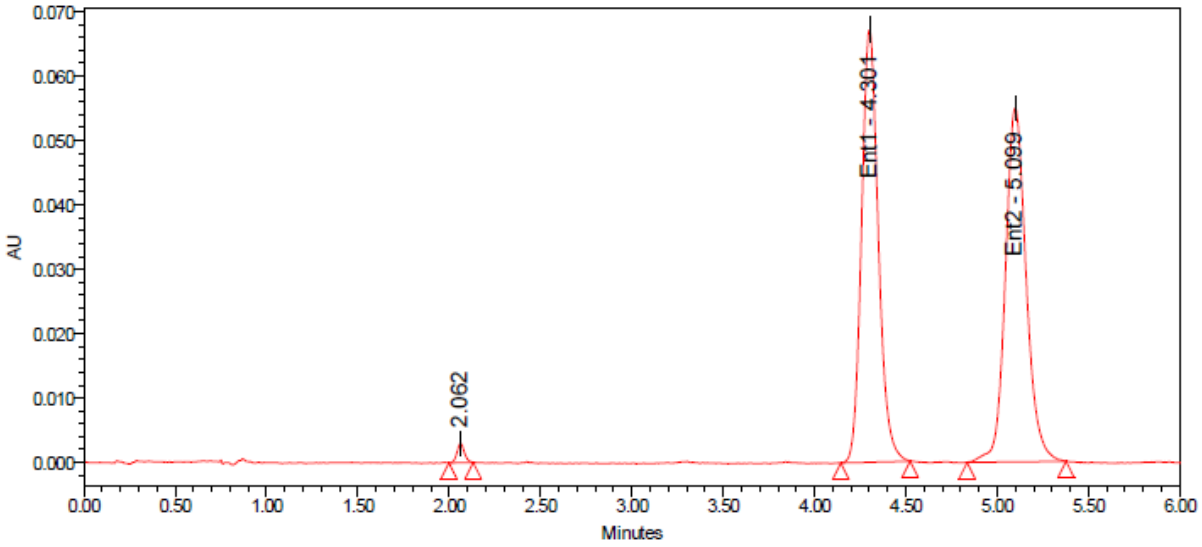


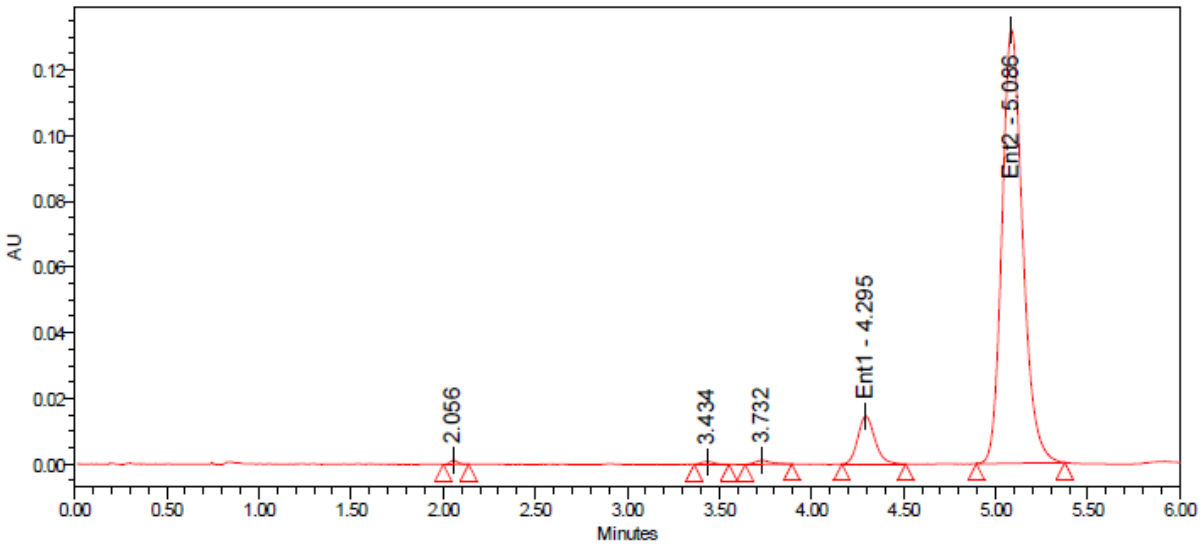
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-94II	49.99	50.01	-0.02	226906	227003
2	SN-E-94I	7.70	92.30	-84.61	15967	191502


SN-E-035-I.1.fid
OMe
O
N
H
N
O
O
OMe
Br
4e
0.94
2.02
0.99
2.03
2.09
1.01
2.03
3.08
6.28
1.18
2.98
2.90
1.00
0.98
1.99
1.00
0.97
2.00
12.0 11.5 11.0 10.5 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
f1 (ppm)

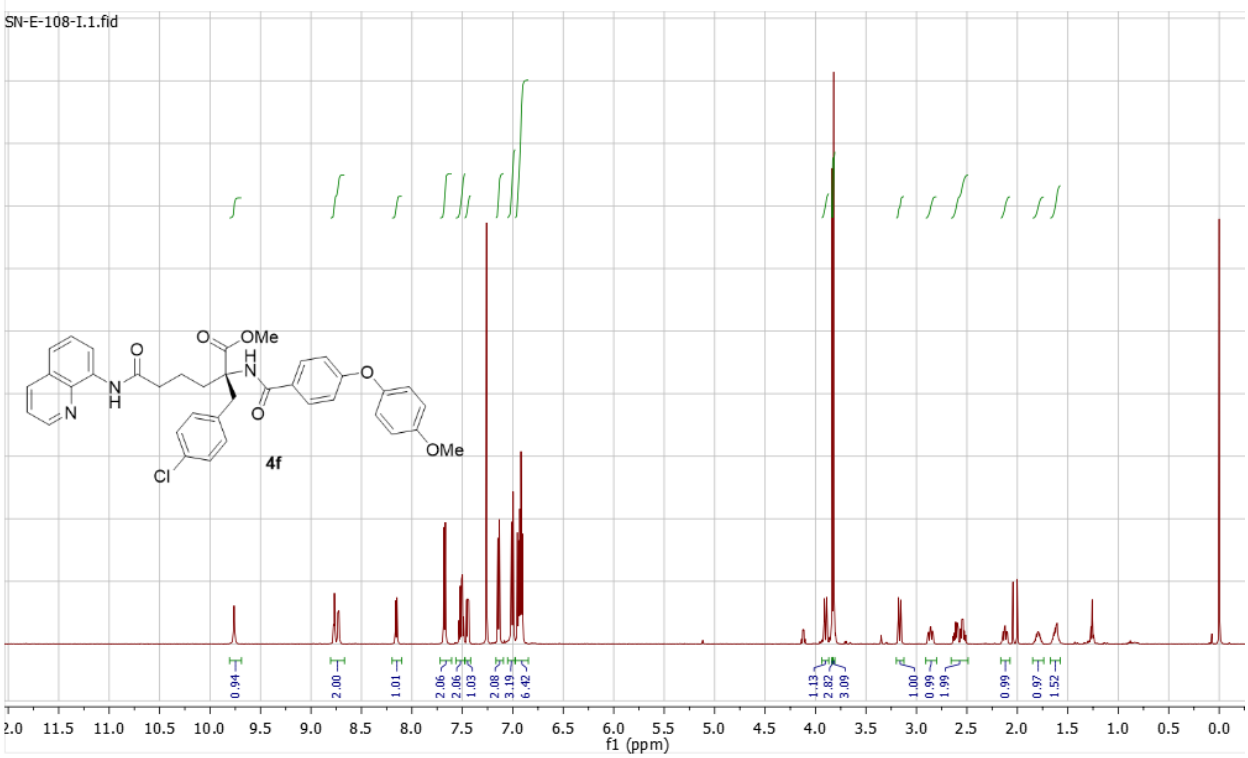

SN-E-035-I.11.fid
173.67
171.06
166.30
161.85
156.65
149.05
148.28
138.41
136.50
135.46
134.53
131.50
131.48
128.91
128.64
128.06
127.53
121.76
121.61
121.11
116.95
116.55
115.19
66.20
55.81
53.16
40.16
37.56
34.98
20.56
OMe
O
N
H
N
O
O
OMe
Br
4e
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

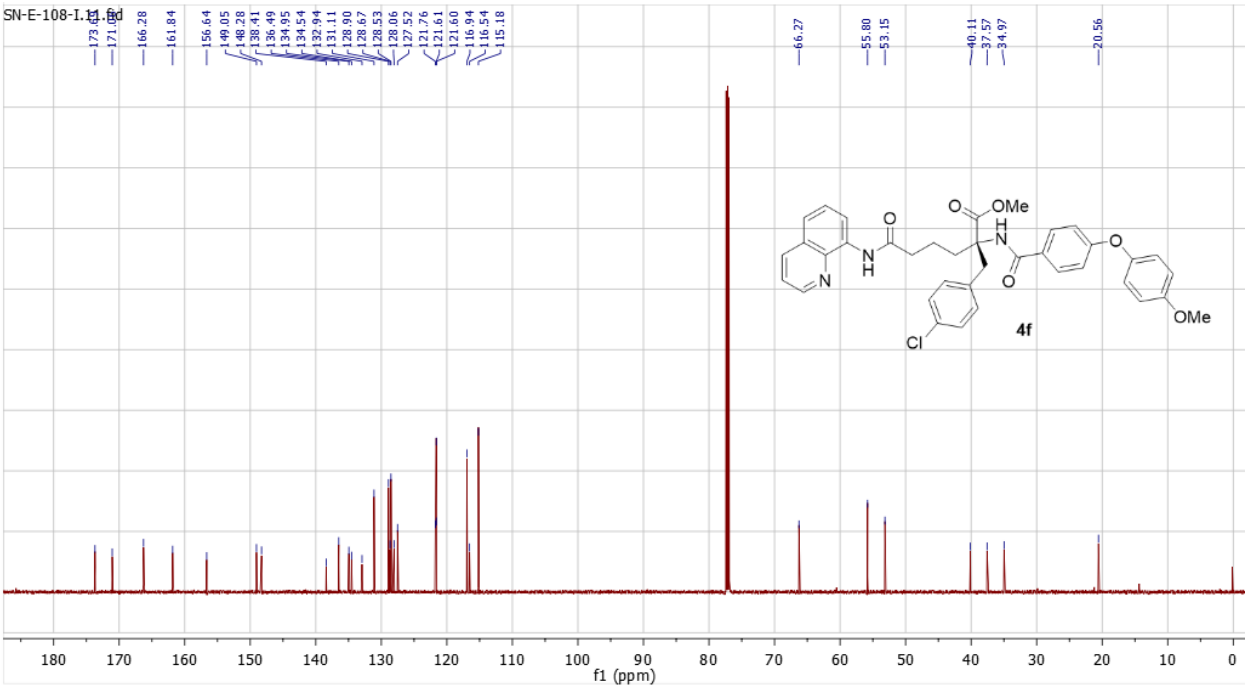


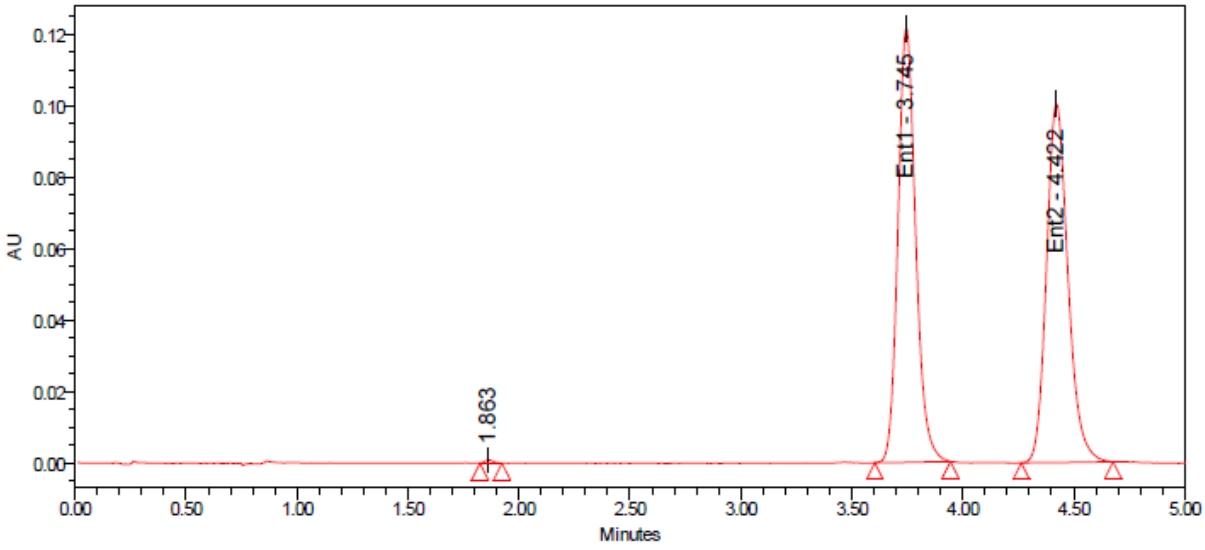


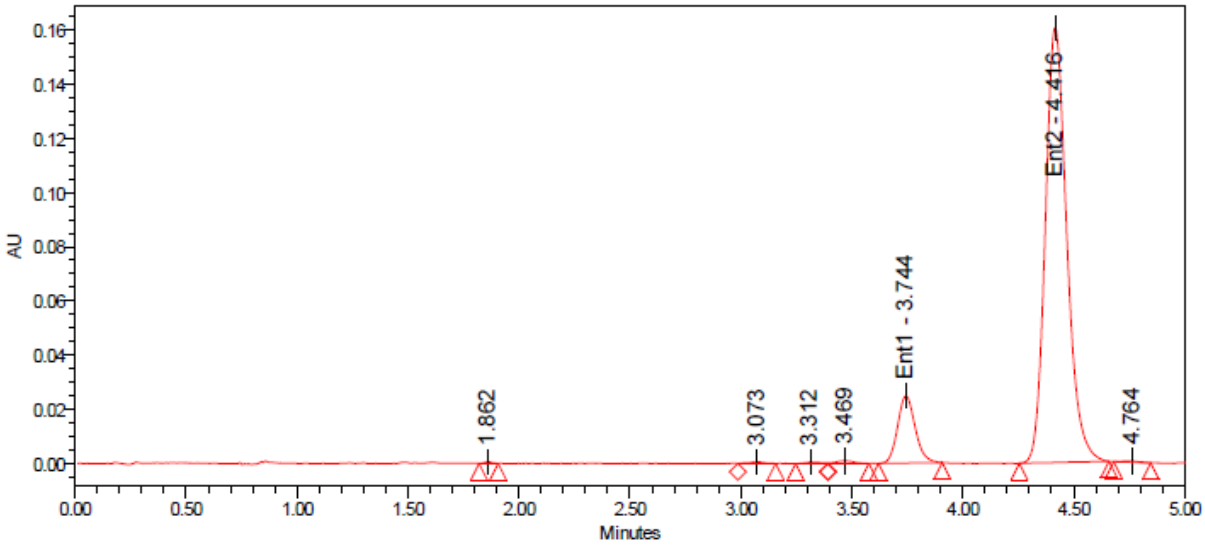
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-35II	49.61	50.39	-0.78	429189	435959
2	SN-E-35III	8.33	91.67	-83.34	93842	1032501


SN-E-108-I.1.fid
OMe
O
H
N
O
N
H
O
O
N
Cl
4f
OMe
0.94
2.00
1.01
2.06
2.06
1.03
2.08
3.19
6.42
1.13
2.82
3.09
1.00
0.99
1.99
0.99
0.97
1.52
f1 (ppm)

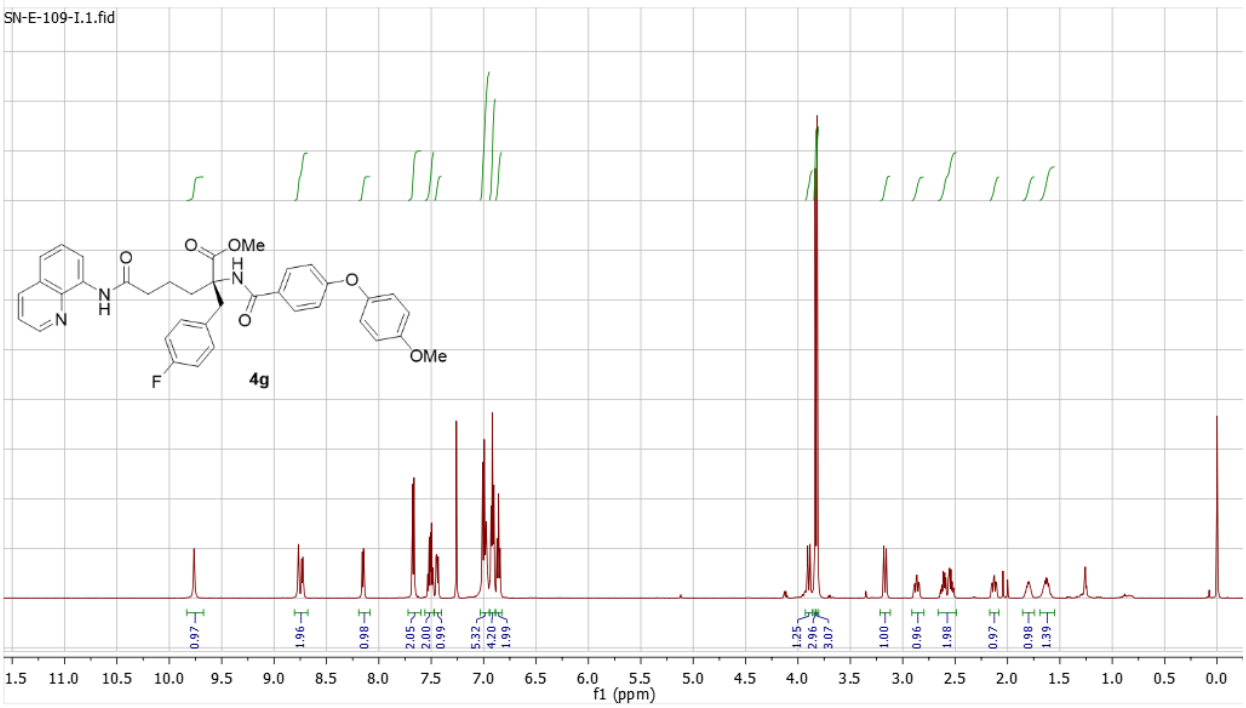

SN-E-108-I.11.fid
173.11
171.45
166.28
161.84
156.64
149.05
148.28
138.41
136.49
134.95
134.54
132.94
131.11
128.90
128.67
128.53
128.06
127.52
121.76
121.61
121.60
116.94
116.54
115.18
66.27
55.80
53.15
40.11
37.57
34.97
20.56
OMe
O
H
N
O
N
H
O
O
N
Cl
4f
OMe
f1 (ppm)

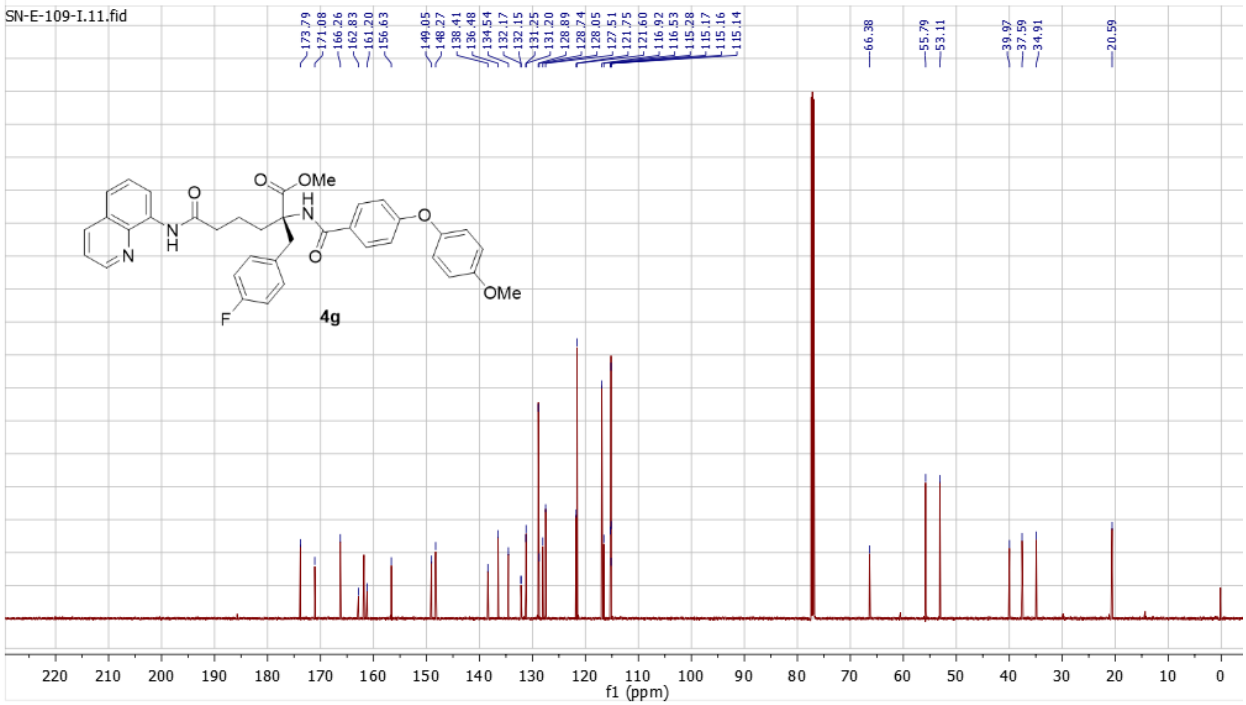


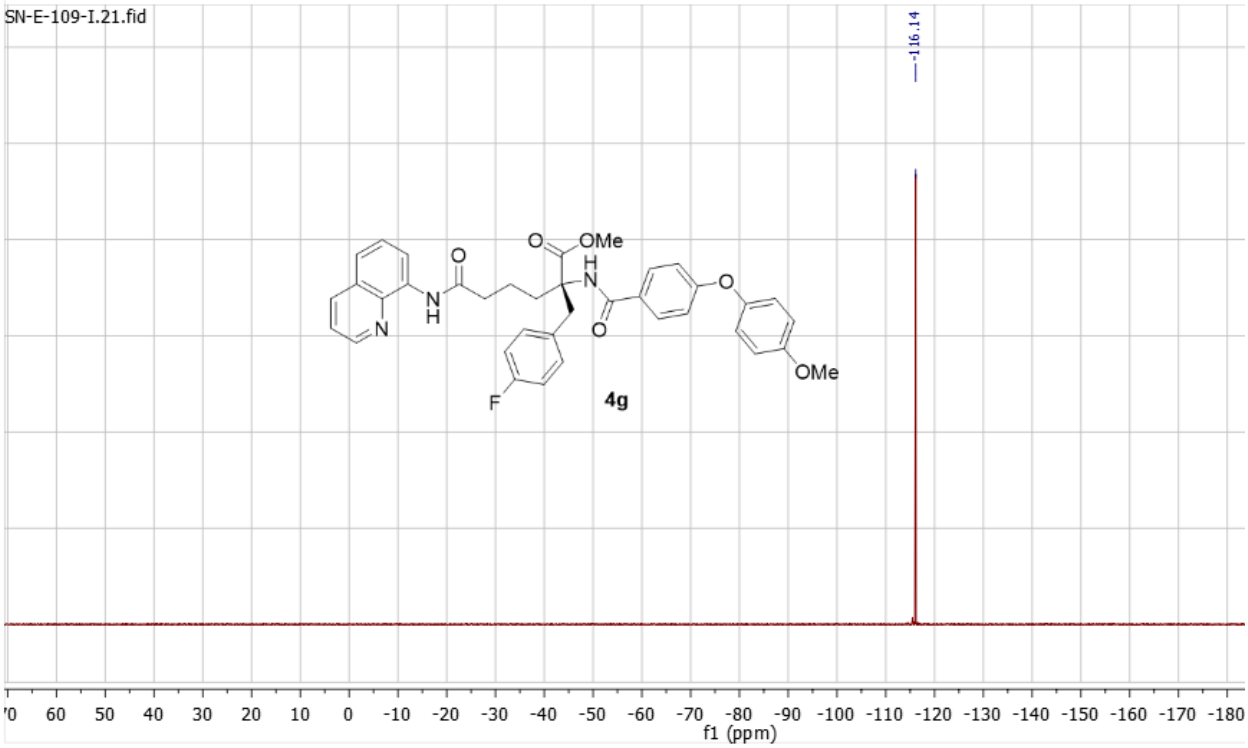


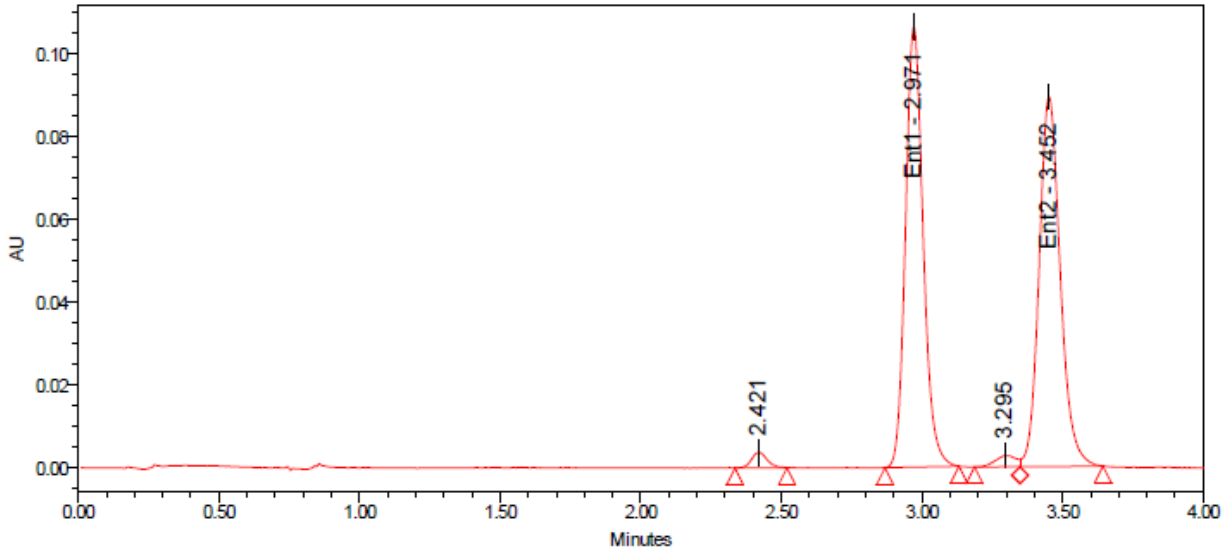
Area Summarized by Name

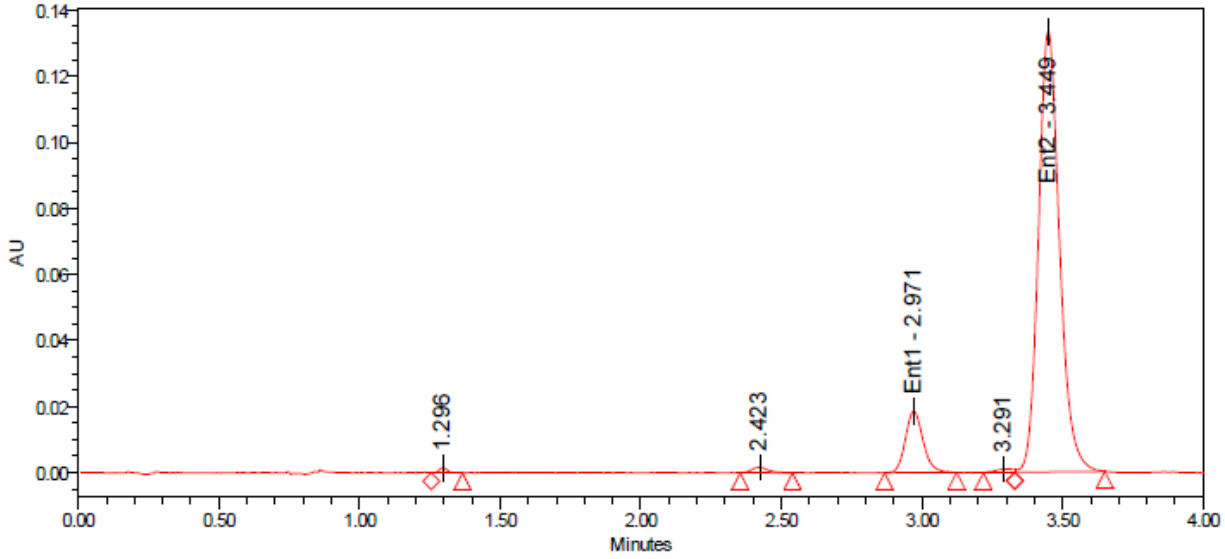
	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-108II	49.95	50.05	-0.10	674669	675998
2	SN-E-108I	11.22	88.78	-77.56	136337	1078739


SN-E-109-I.1.fid
OMe
OMe
F
4g
0.97
1.96
0.98
2.05
2.00
0.99
5.32
4.20
1.99
1.25
2.96
3.07
1.00
0.96
1.98
0.97
0.98
1.39
f1 (ppm)


SN-E-109-I.11.fid
173.79
171.08
166.26
162.83
161.20
156.63
149.05
148.27
138.41
136.48
134.54
132.17
132.15
131.25
131.20
128.89
128.74
128.05
127.51
121.75
121.60
116.92
116.53
115.28
115.17
115.16
115.14
66.38
55.79
53.11
39.97
37.59
34.91
20.59
OMe
OMe
F
4g
f1 (ppm)

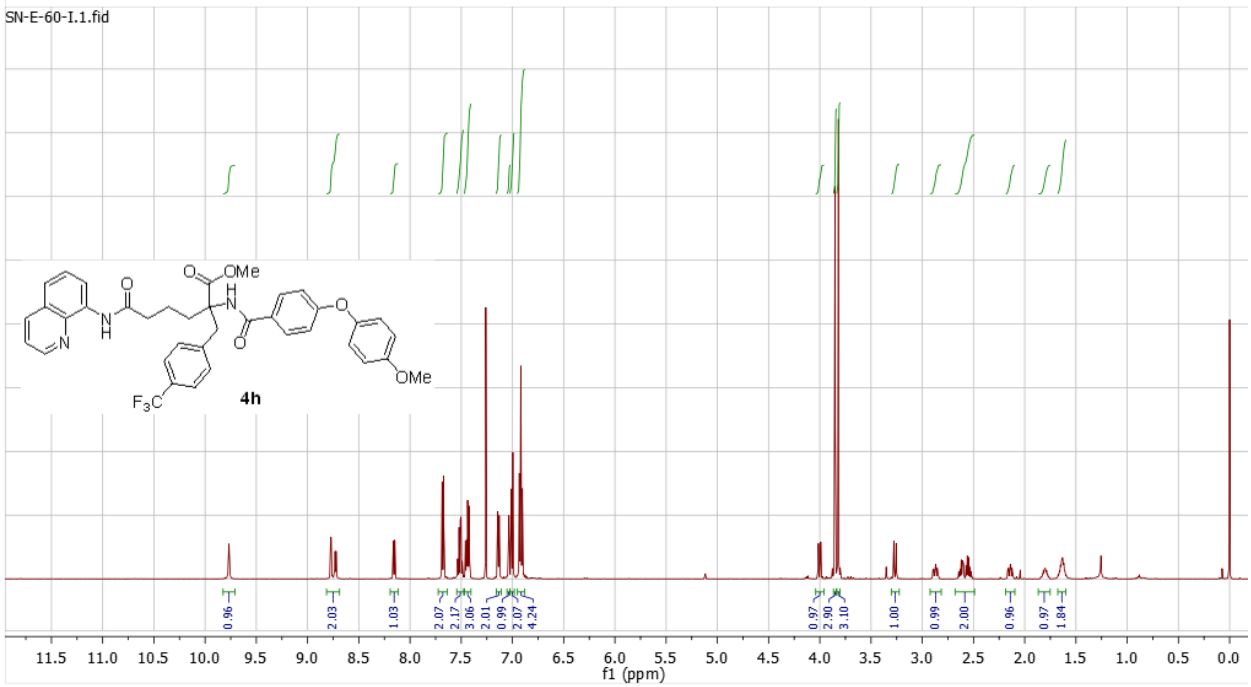

SN-E-109-I.21.fid
-116.14
O
OMe
H
N
O
N
H
N
O
O
OMe
F
4g
'0 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180
f1 (ppm)

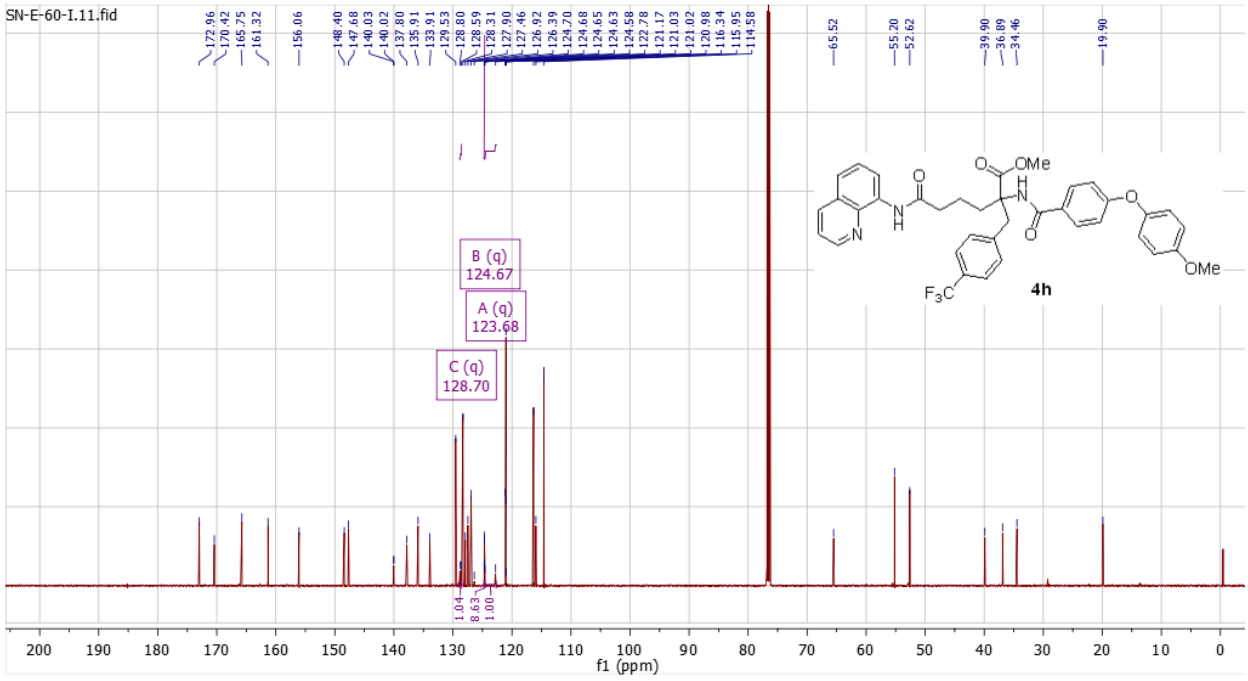


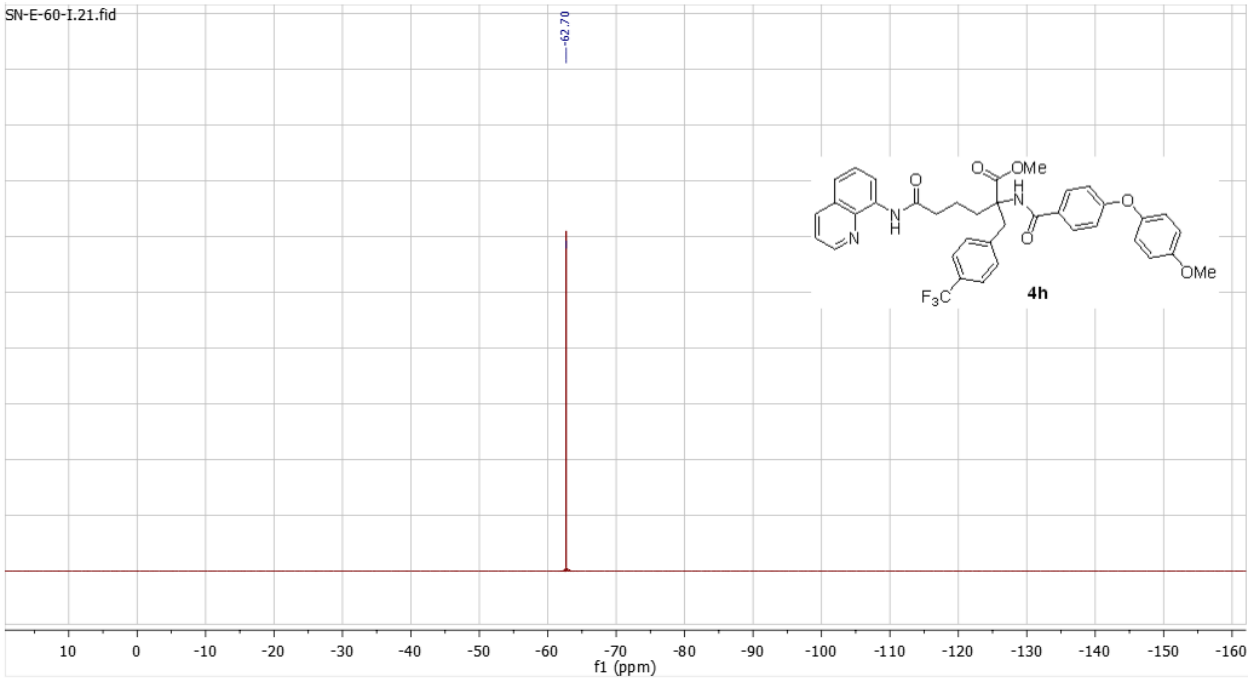


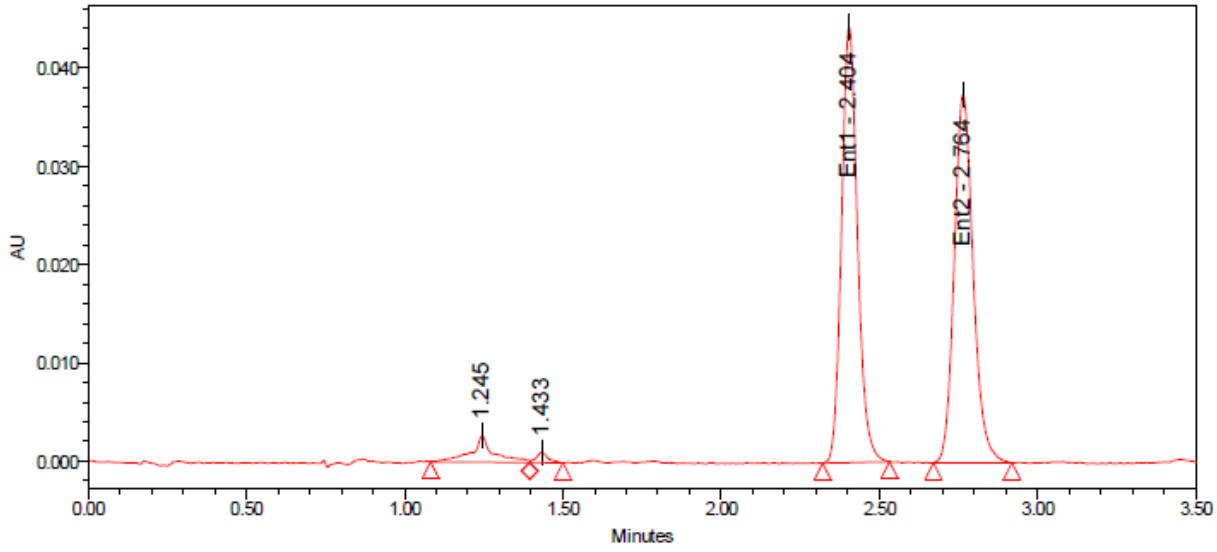
Area Summarized by Name

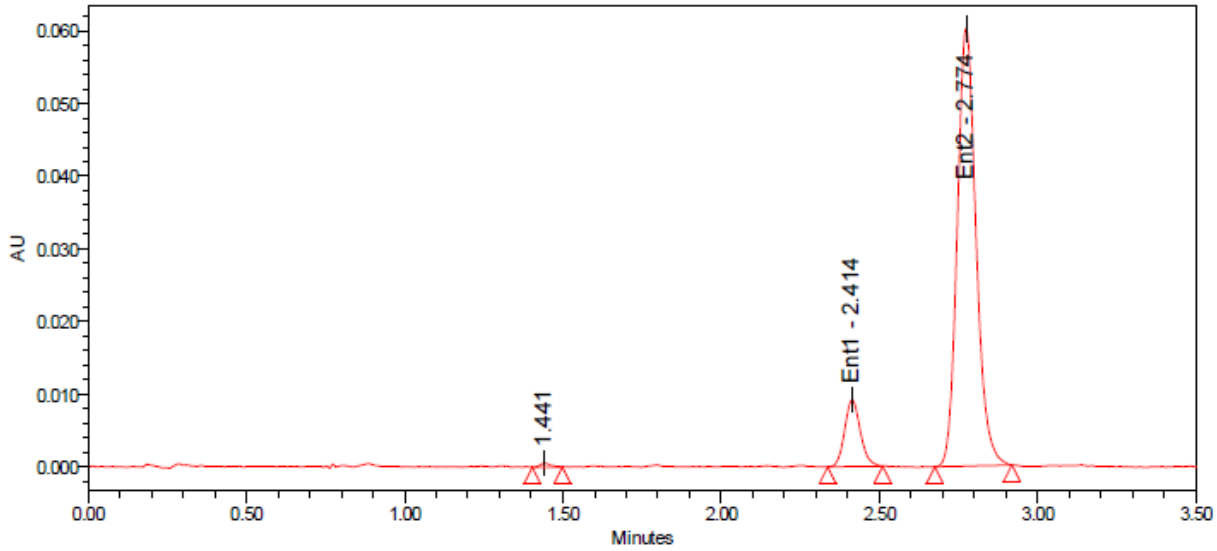
	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-109II	49.79	50.21	-0.42	462454	466309
2	SN-E-109I	10.47	89.53	-79.05	81058	692919


SN-E-60-I.1.fid
4h
f1 (ppm)


SN-E-60-I.11.fid
B (q)
124.67
A (q)
123.68
C (q)
128.70
4h
f1 (ppm)

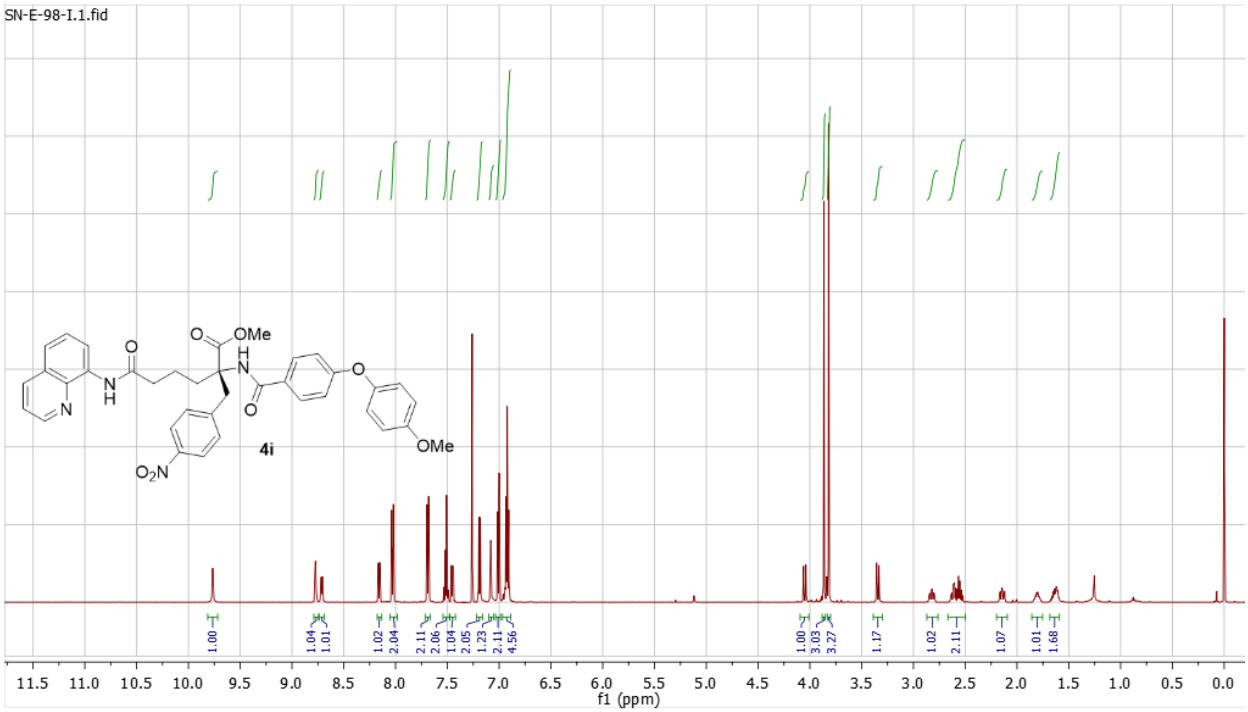

SN-E-60-I.21.fid
-62.70
OMe
O
N
H
N
H
O
O
OMe
F3C
4h
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
f1 (ppm)

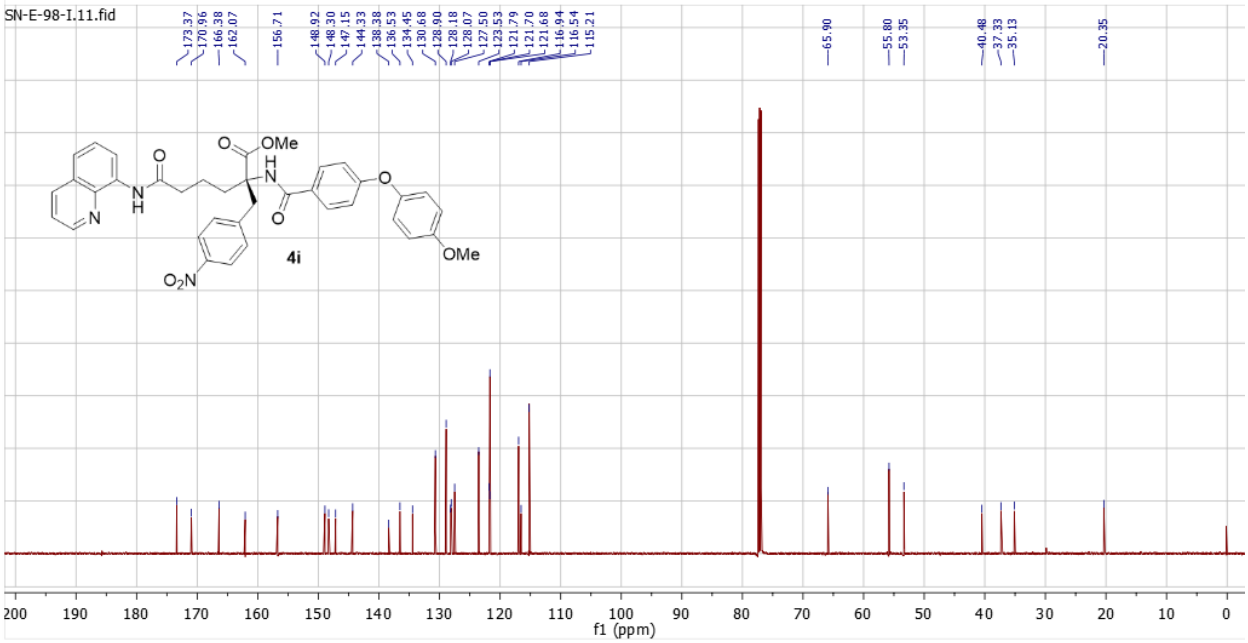


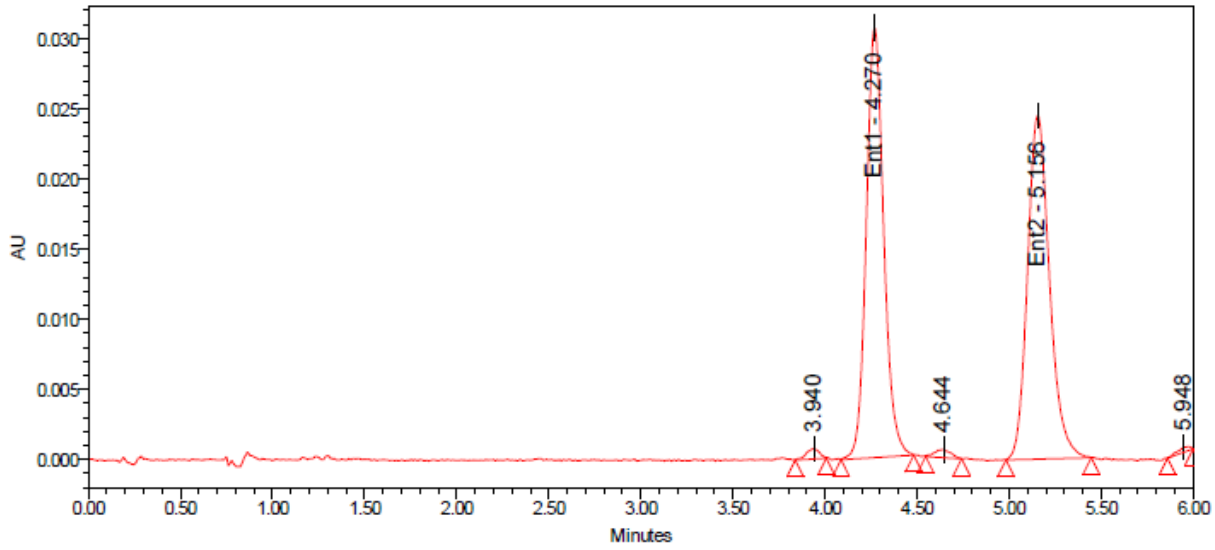


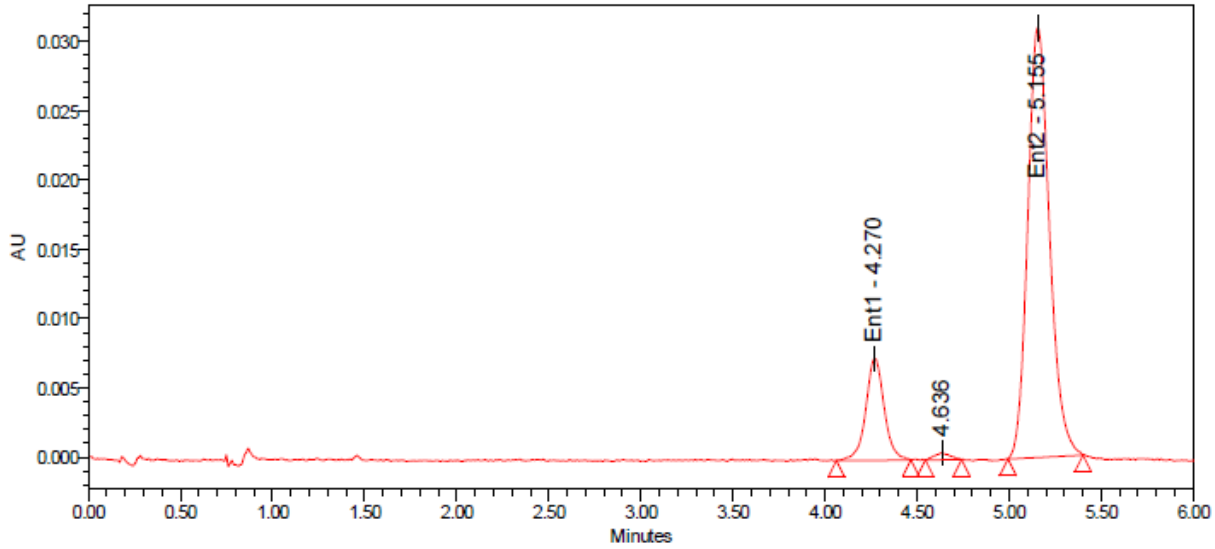
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-60II	49.90	50.10	-0.19	155087	155691
2	SN-E-60I	11.29	88.71	-77.42	31632	248546


SN-E-98-I.1.fid
4i
f1 (ppm)

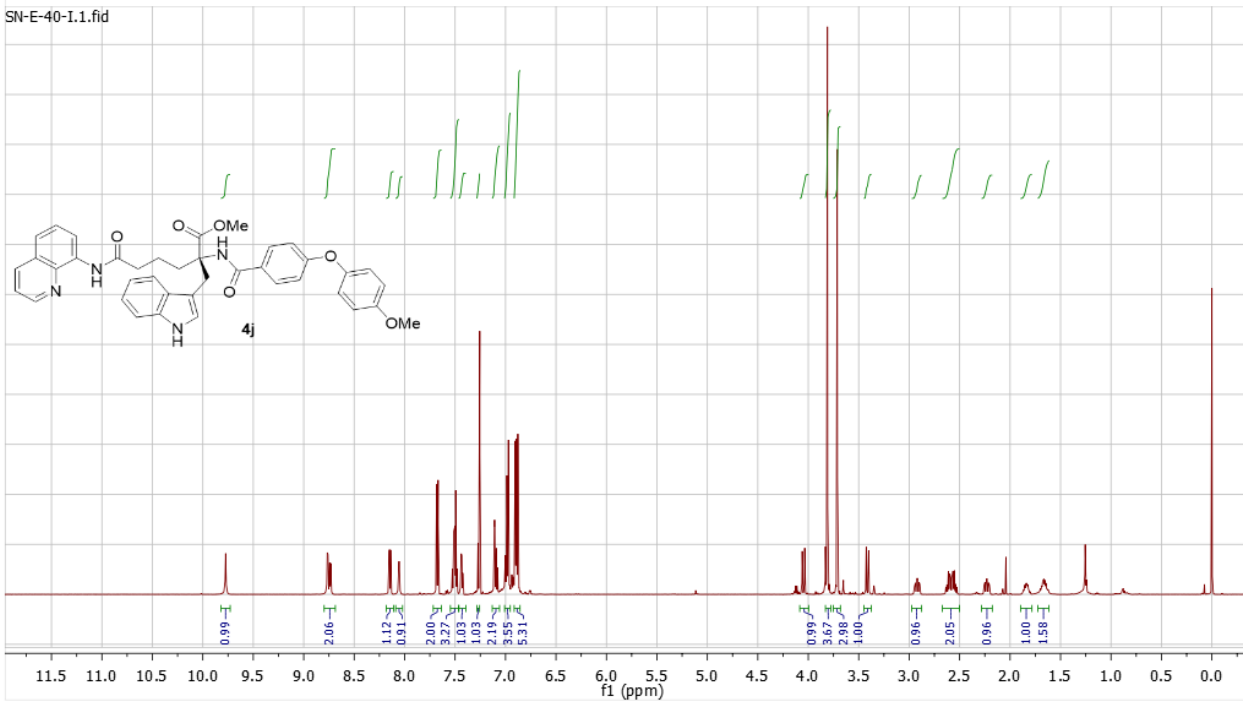

SN-E-98-I.11.fid
4i
f1 (ppm)

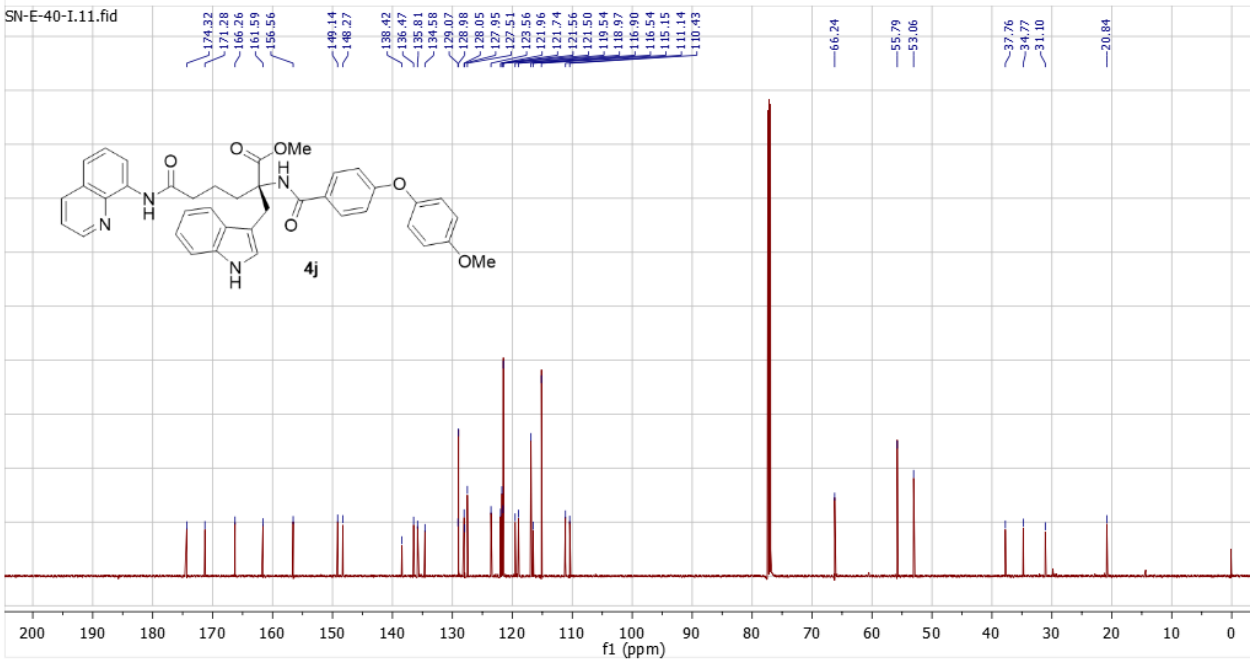


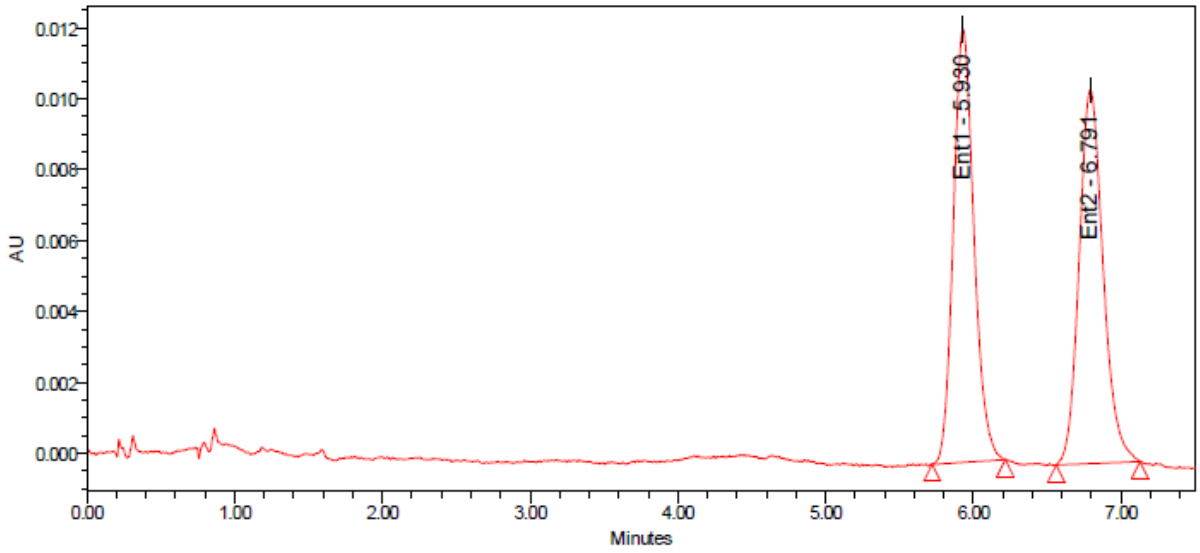


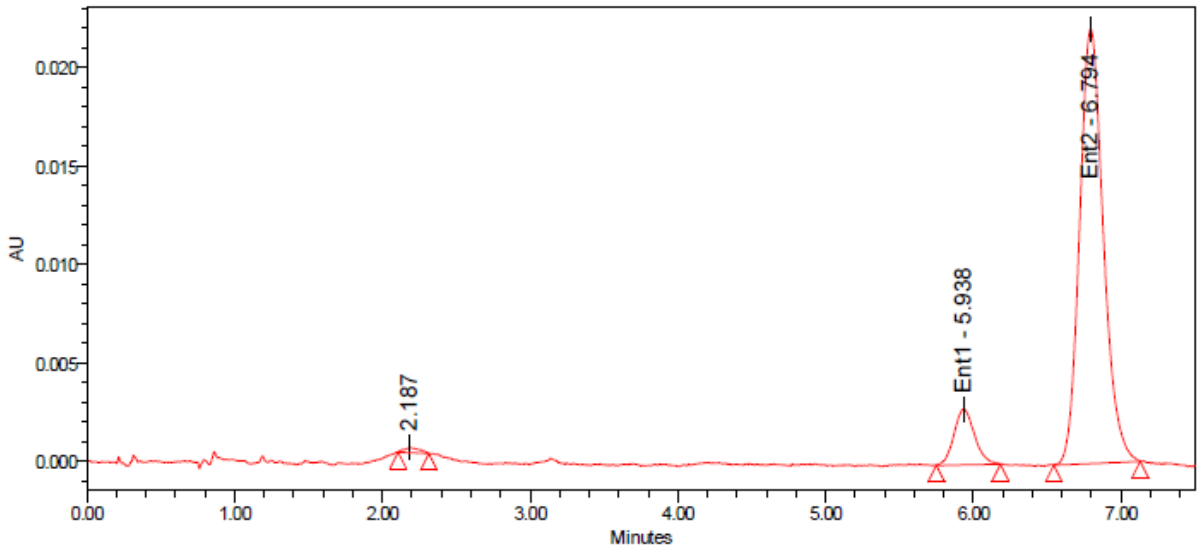
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-98II	49.80	50.20	-0.40	202053	203667
2	SN-E-98I	16.69	83.31	-66.62	51094	255057


SN-E-40-I.1.fid
4j
f1 (ppm)

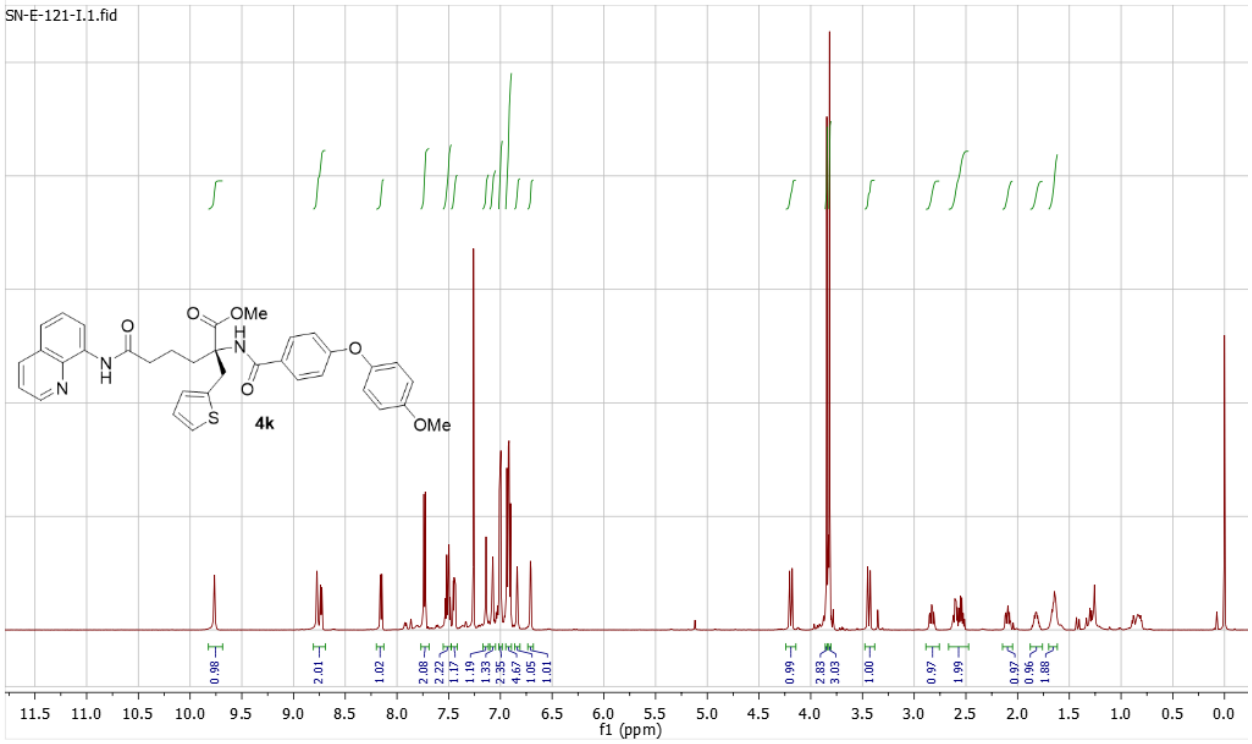

SN-E-40-I.11.fid
4j
f1 (ppm)

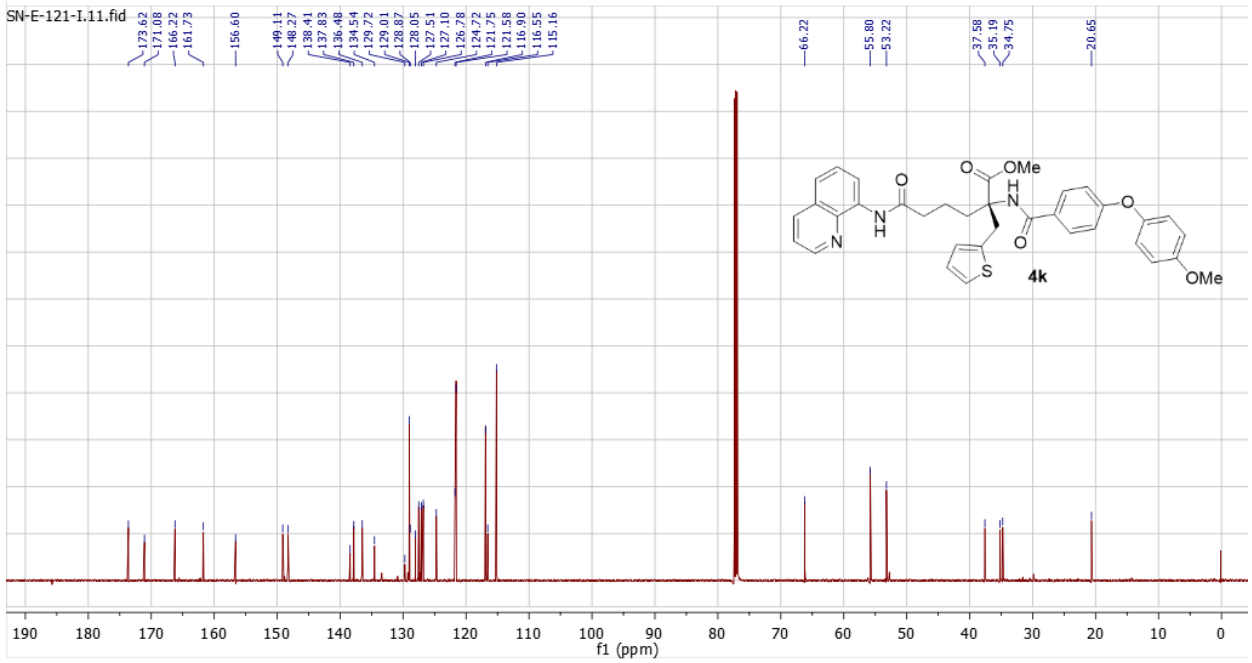


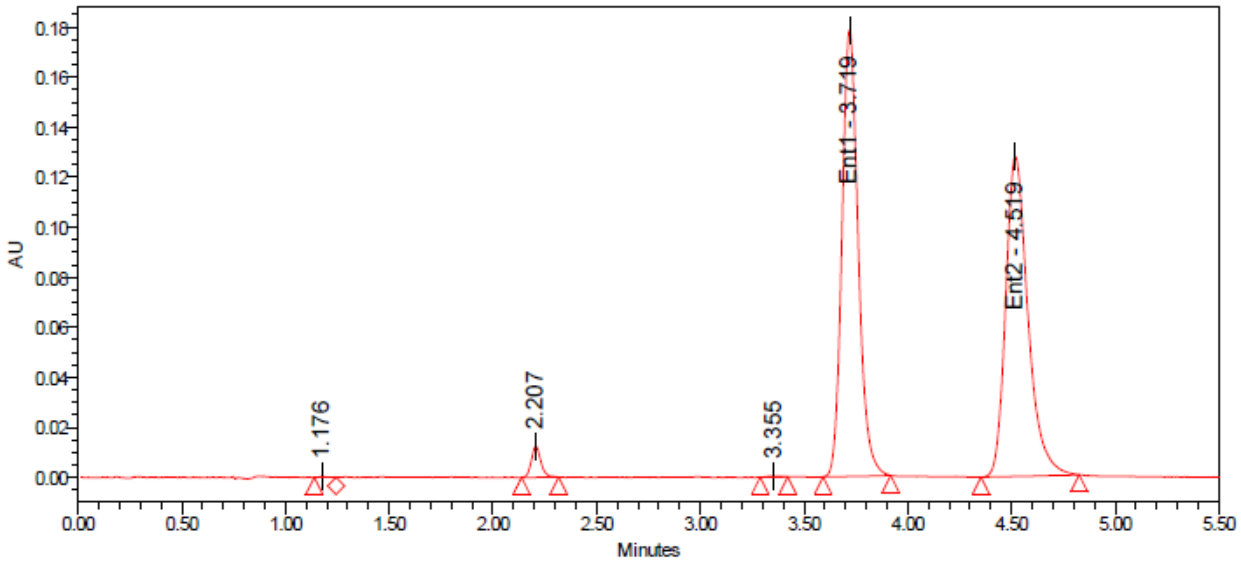


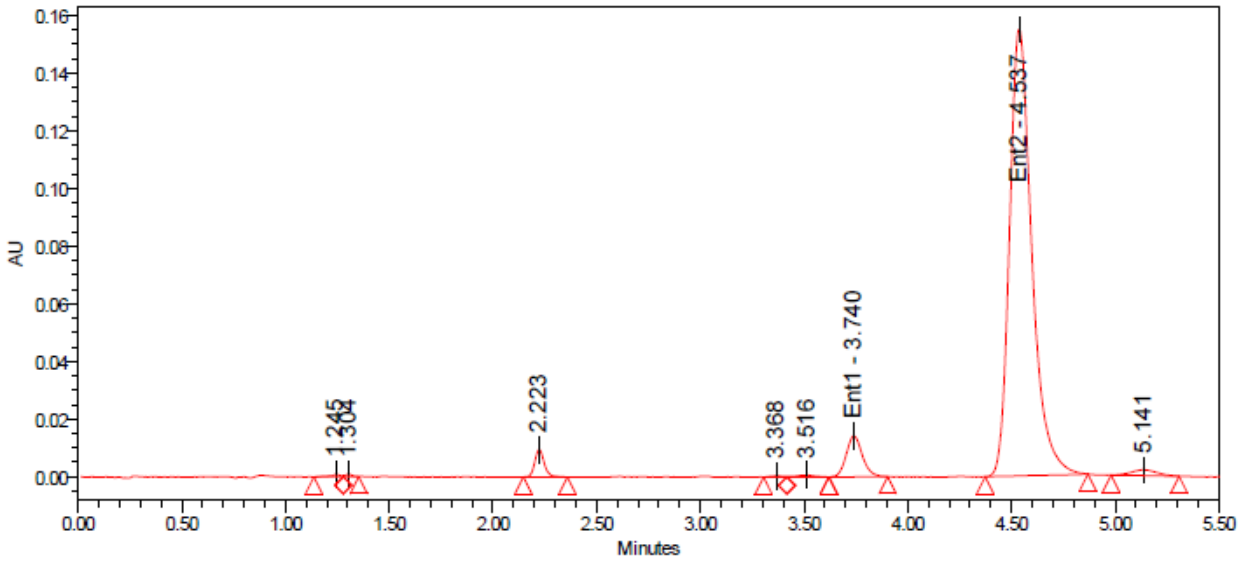
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-40II	49.76	50.24	-0.48	118081	119220
2	SN-E-40I	10.01	89.99	-79.98	27445	246693


SN-E-121-I.1.fid
4k
f1 (ppm)

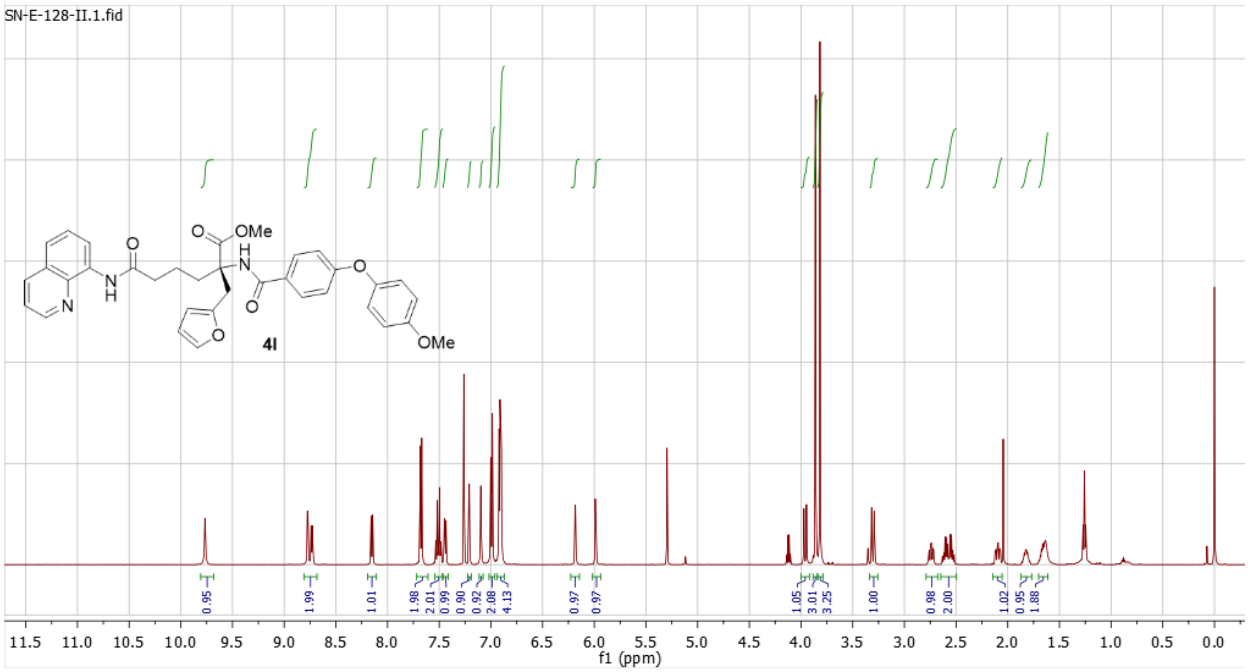

SN-E-121-I.11.fid
4k
f1 (ppm)

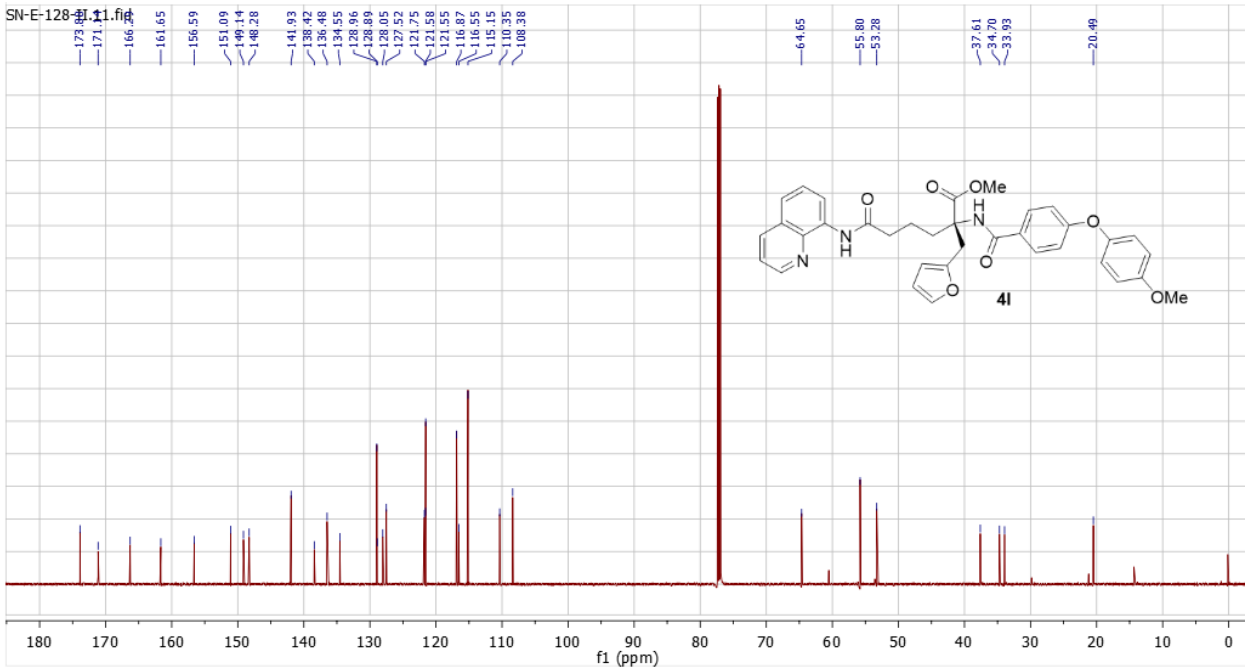


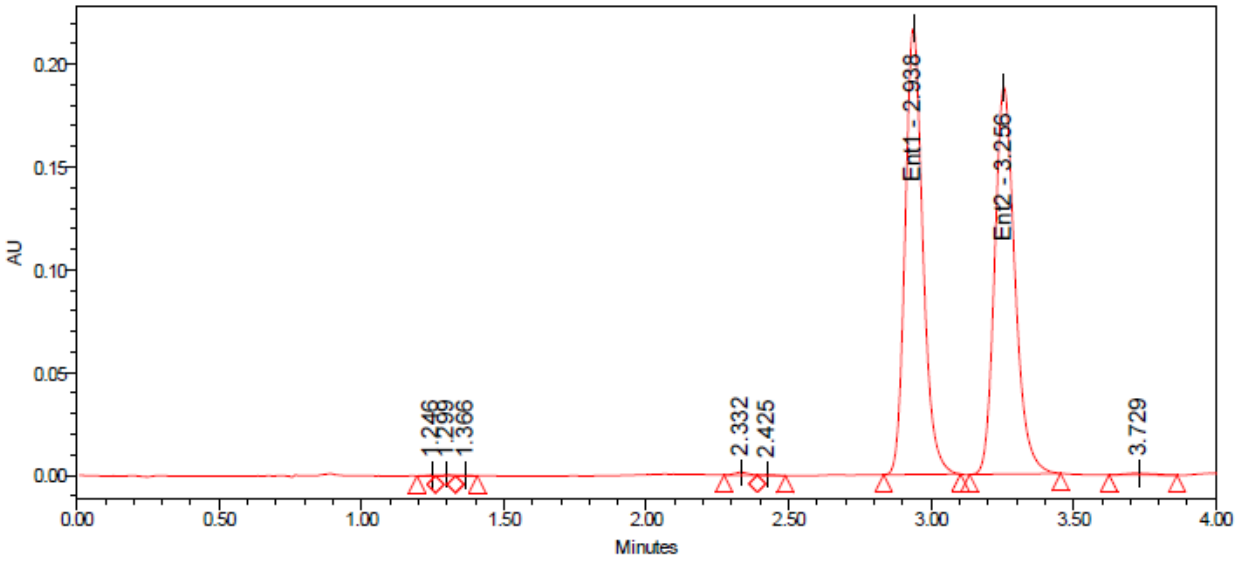


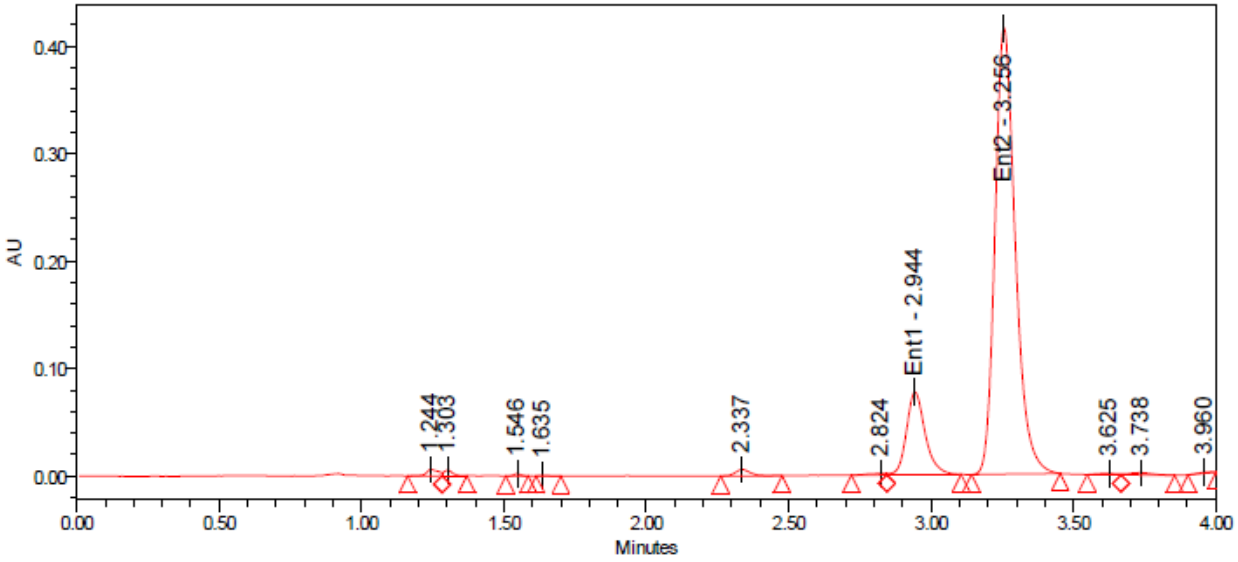
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-121II	50.40	49.60	0.80	970891	955505
2	SN-E-121I	6.22	93.78	-87.56	76720	1156453


SN-E-128-II.1.fid
OMe
O
N
H
O
O
N
O
O
OMe
4l
0.95
1.99
1.01
1.98
2.01
0.99
0.90
0.92
2.08
4.13
0.97
0.97
1.05
3.01
3.25
1.00
0.98
2.00
1.02
0.95
1.88
11.5
11.0
10.5
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
f1 (ppm)

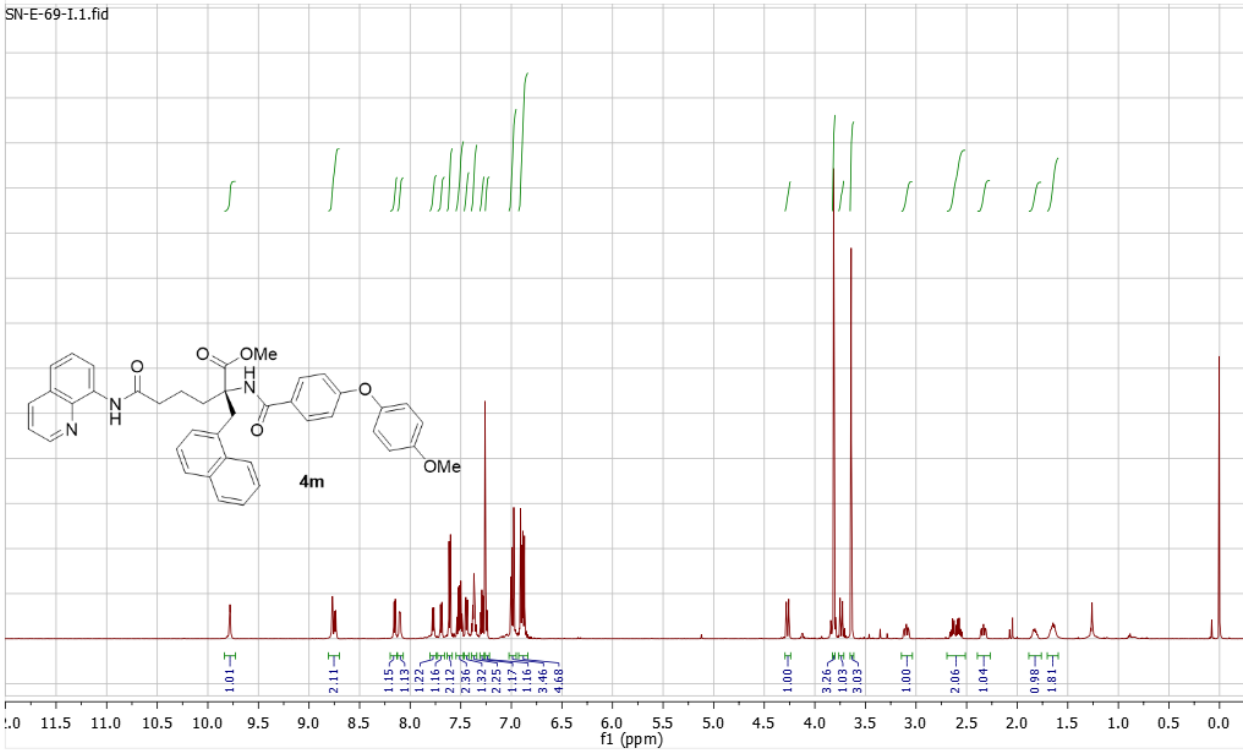

SN-E-128-II.1.fid
173.61
171.11
166.29
161.65
156.59
151.09
149.14
148.28
141.93
138.42
136.48
134.55
128.96
128.89
128.05
127.52
121.75
121.58
121.55
116.87
116.55
115.15
110.35
108.38
64.65
55.80
53.28
37.61
34.70
33.93
20.49
OMe
O
N
H
O
O
N
O
O
OMe
4l
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

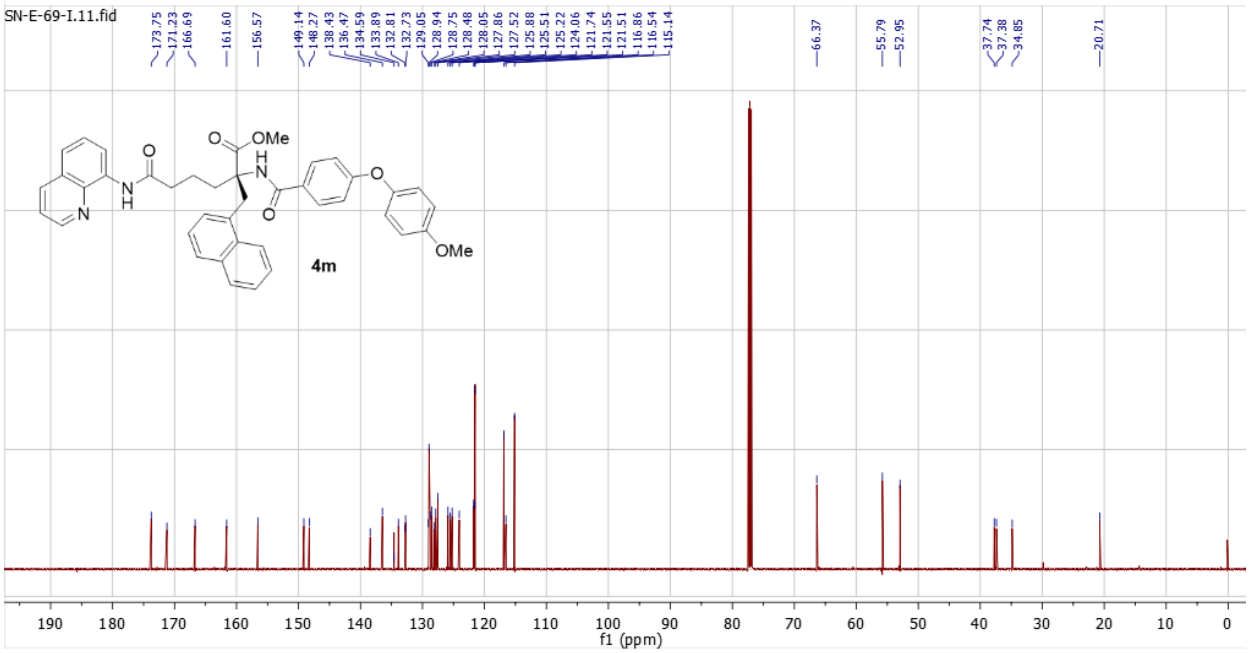


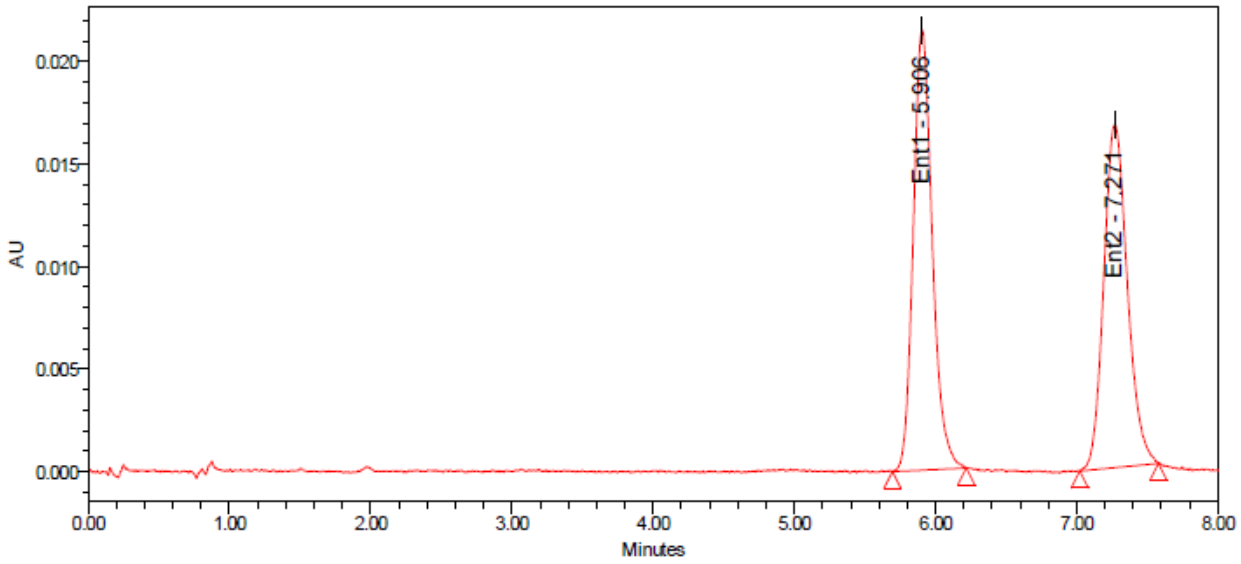


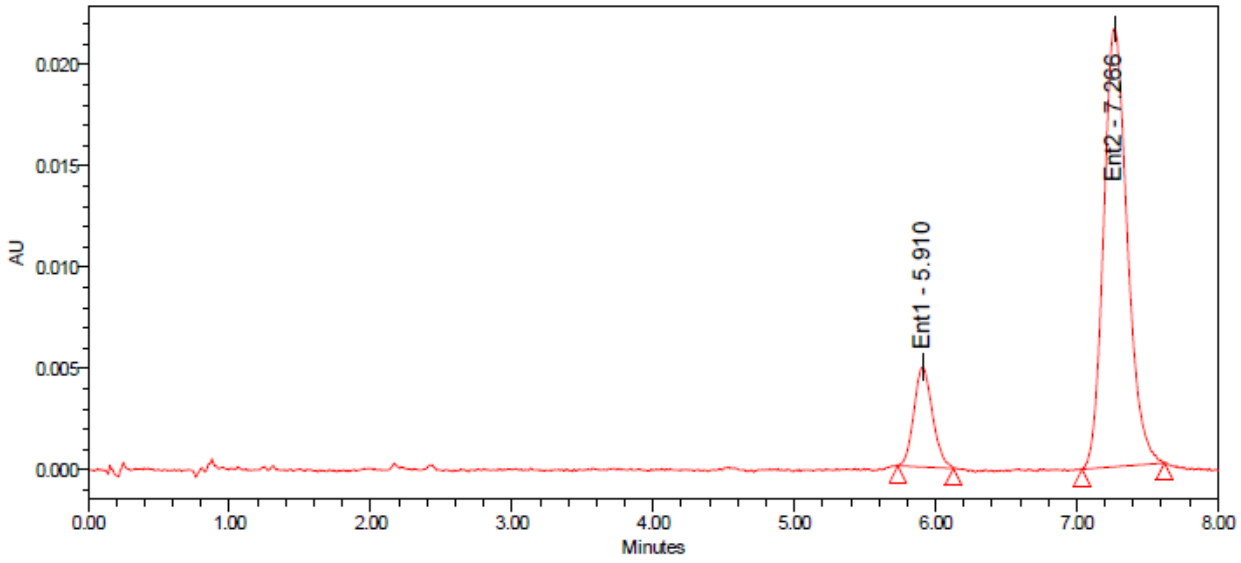
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-128II	50.20	49.80	0.40	940541	932992
2	SN-E-128I	14.59	85.41	-70.81	350756	2052851


SN-E-69-I.1.fid
OMe
OMe
4m
f1 (ppm)

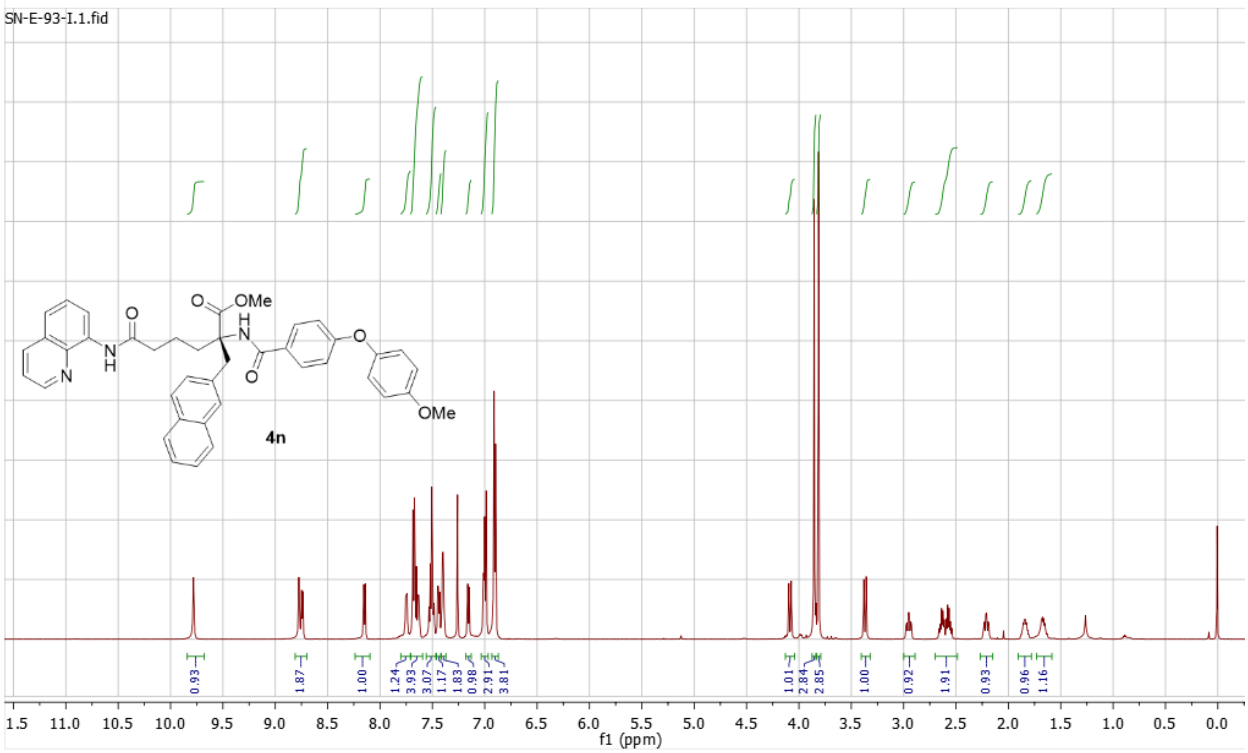

SN-E-69-I.11.fid
OMe
OMe
4m
f1 (ppm)

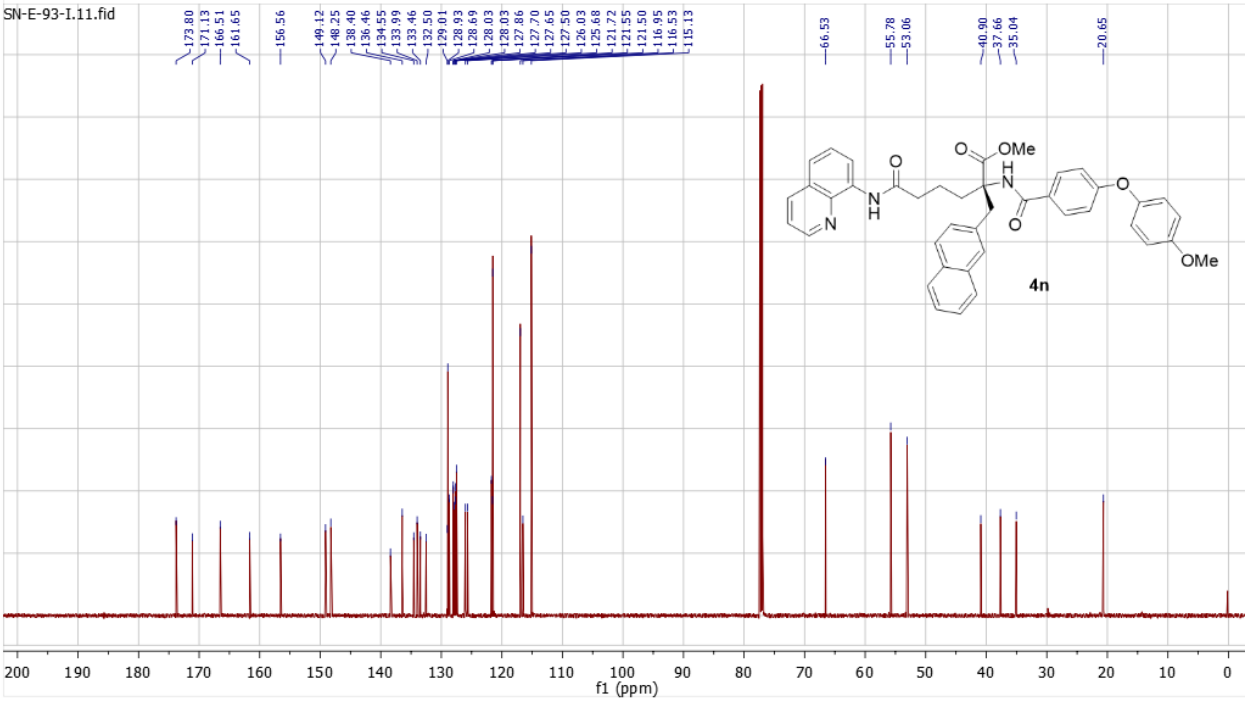


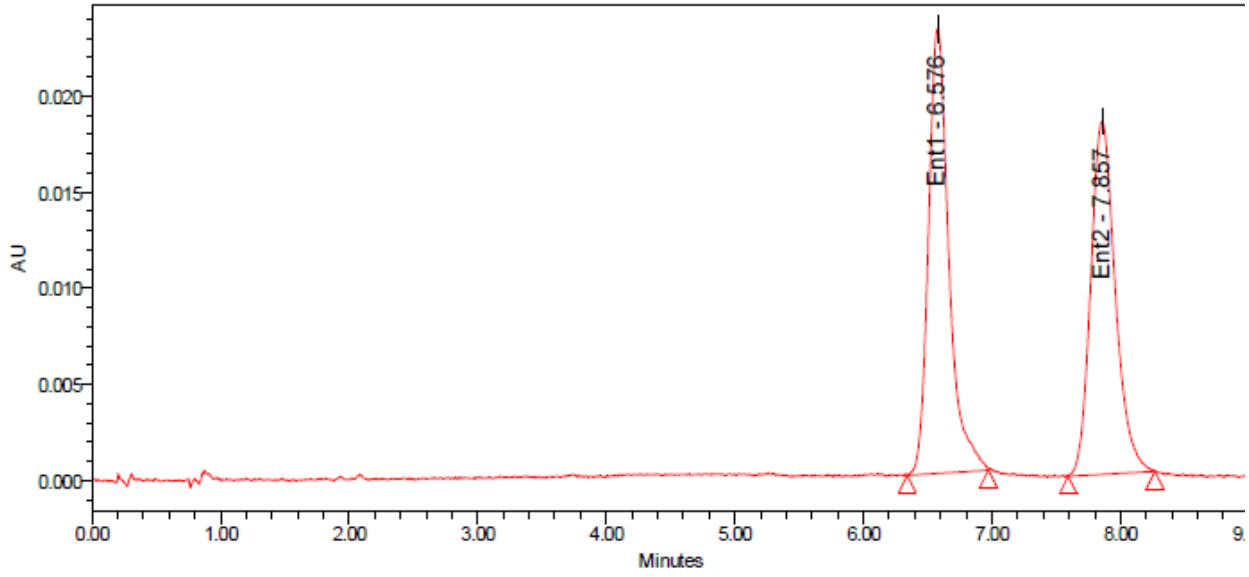


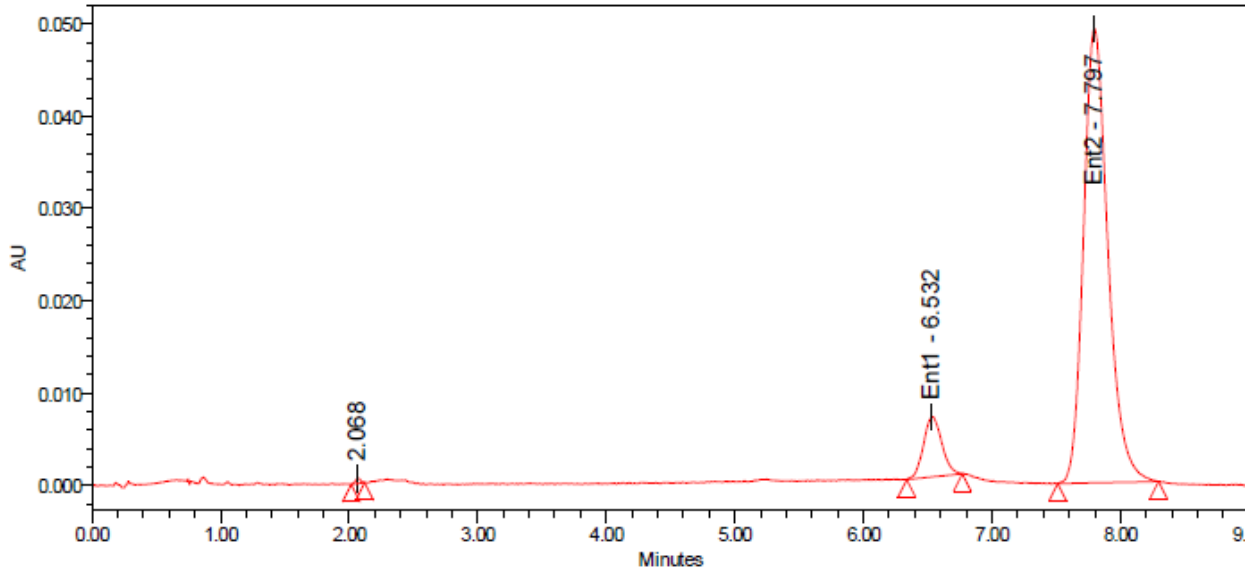
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-69II	50.78	49.22	1.56	200481	194305
2	SN-E-69I	15.22	84.78	-69.56	45180	251640


SN-E-93-I.1.fid
OMe
O
H
N
O
N
H
O
O
OMe
4n
0.93
1.87
1.00
1.24
3.93
3.07
1.17
1.83
0.98
2.91
3.81
1.01
2.84
2.85
1.00
0.92
1.91
0.93
0.96
1.16
1.5 11.0 10.5 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
f1 (ppm)

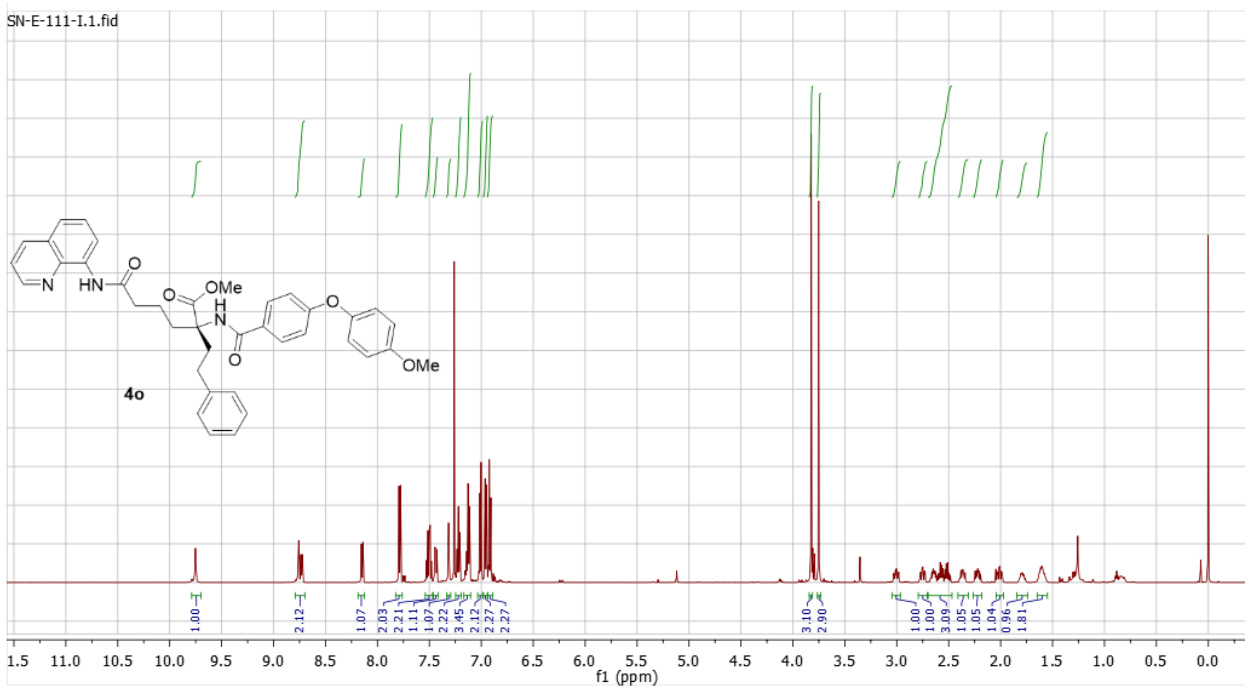

SN-E-93-I.11.fid
173.80
171.13
166.51
161.65
156.56
149.12
148.25
138.40
136.46
134.55
133.99
133.46
132.50
129.01
128.93
128.69
128.03
128.03
127.86
127.70
127.65
127.50
126.03
125.68
121.72
121.55
121.50
116.95
116.53
115.13
66.53
55.78
53.06
40.90
37.66
35.04
20.65
OMe
O
H
N
O
N
H
O
O
OMe
4n
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

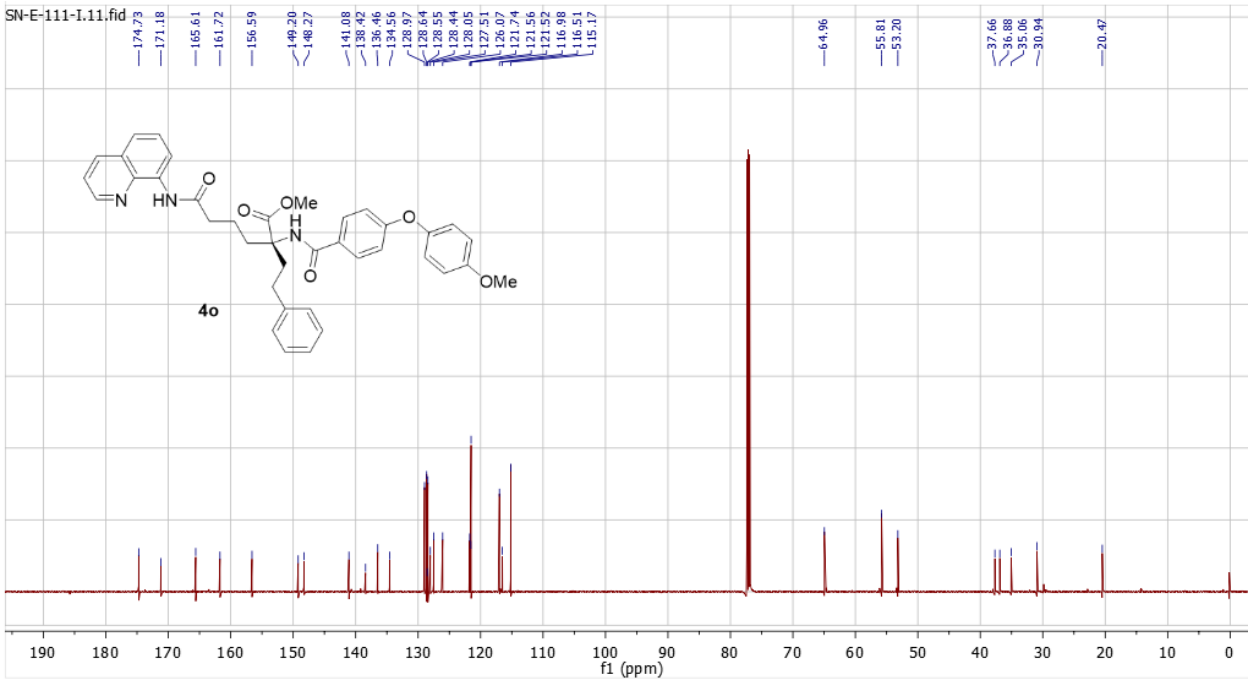


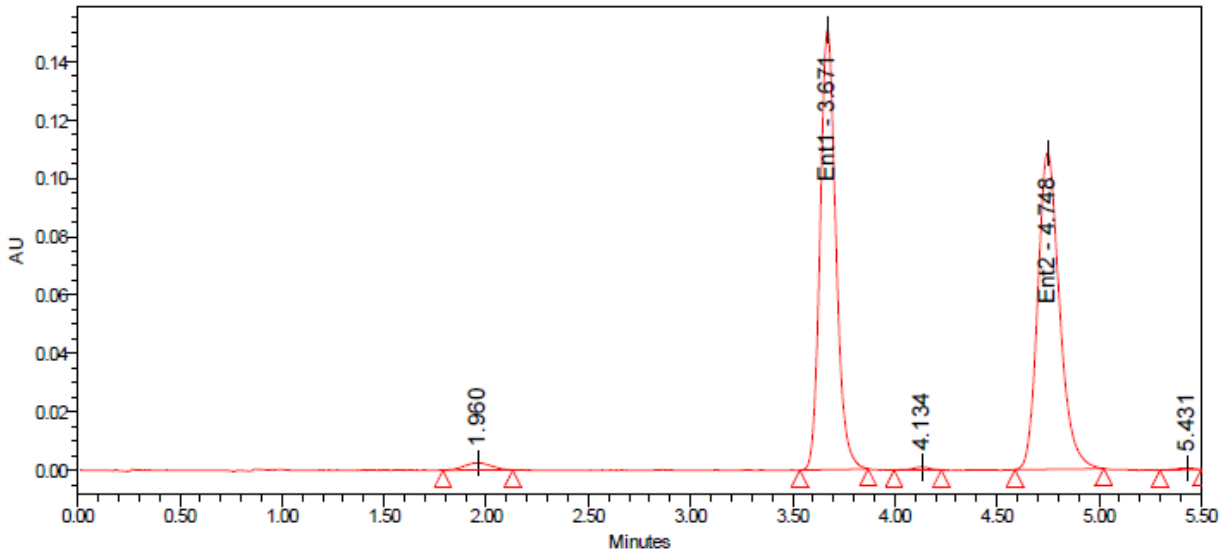


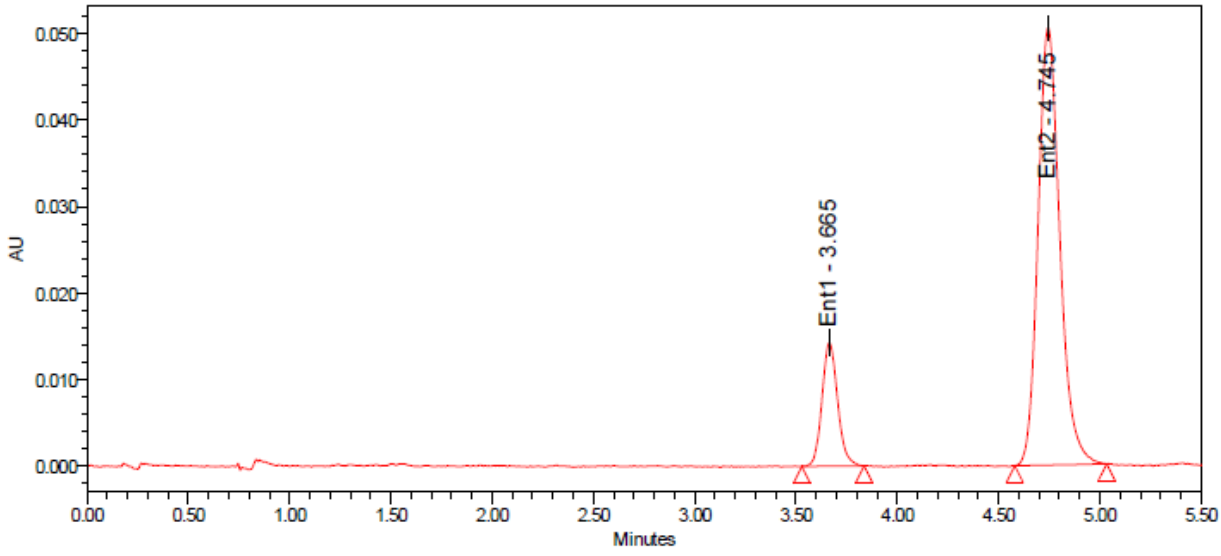
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-93II	51.17	48.83	2.34	255182	243506
2	SN-E-93I	9.05	90.95	-81.89	64706	649958


SN-E-111-I.1.fid
4o
f1 (ppm)

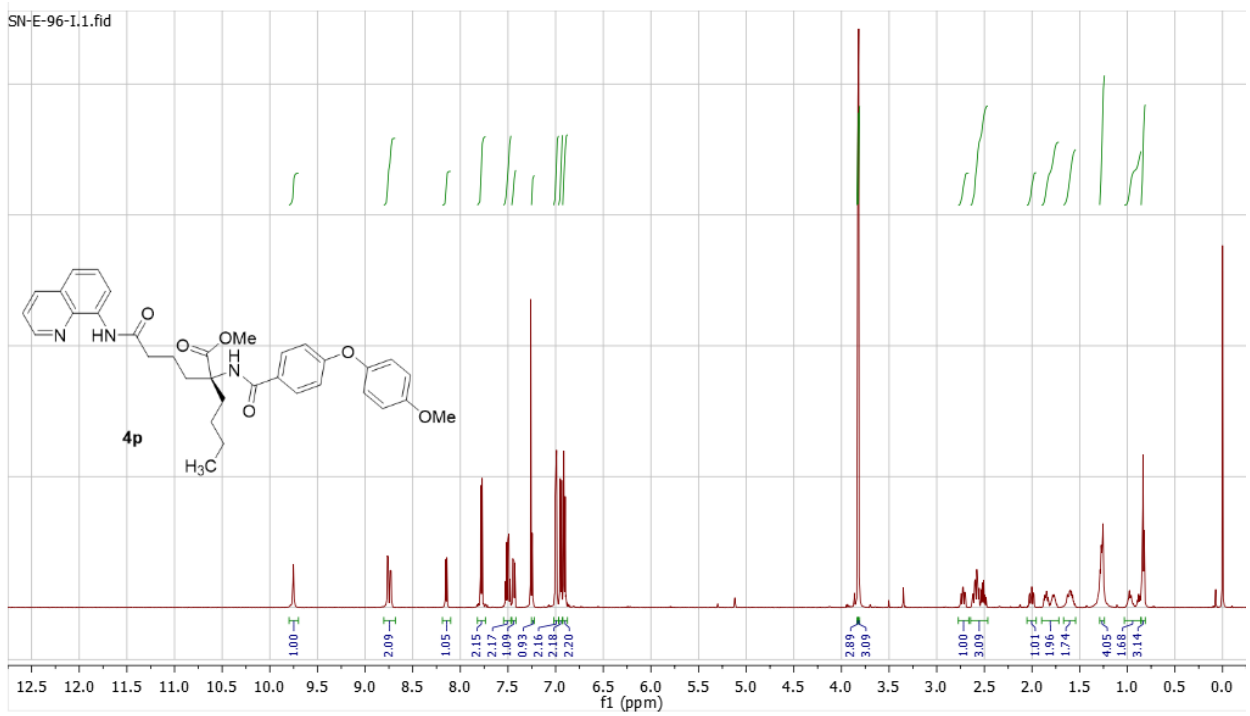

SN-E-111-I.11.fid
4o
f1 (ppm)

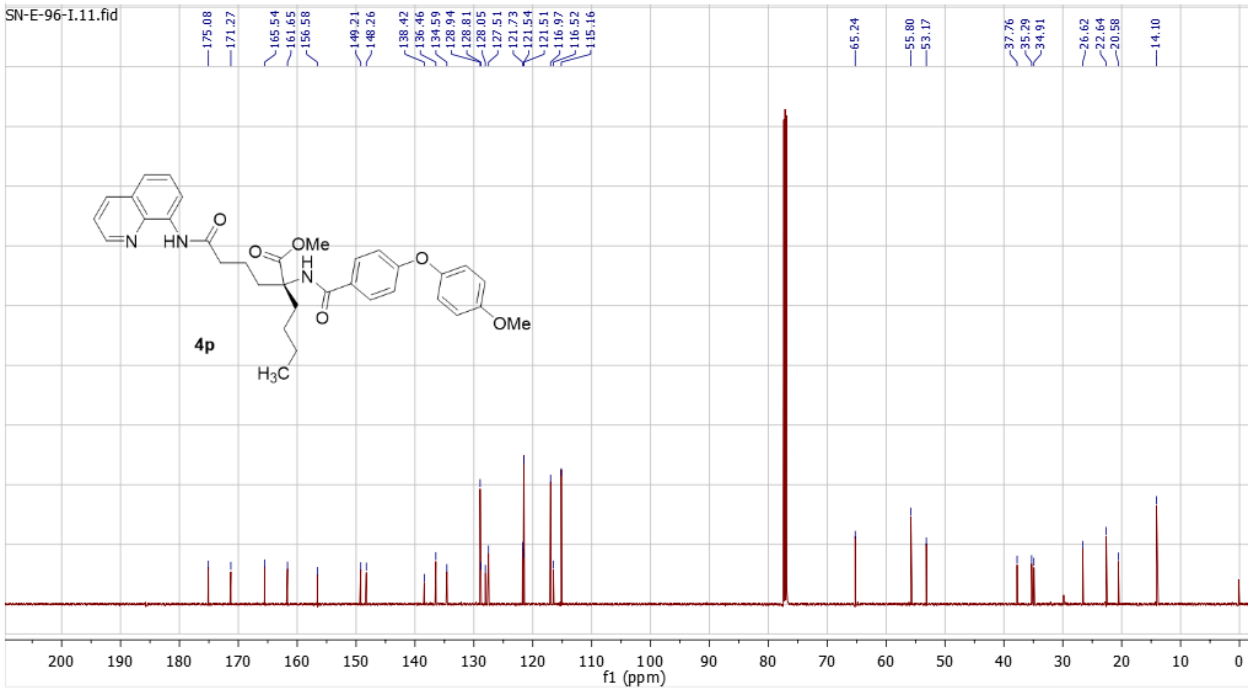


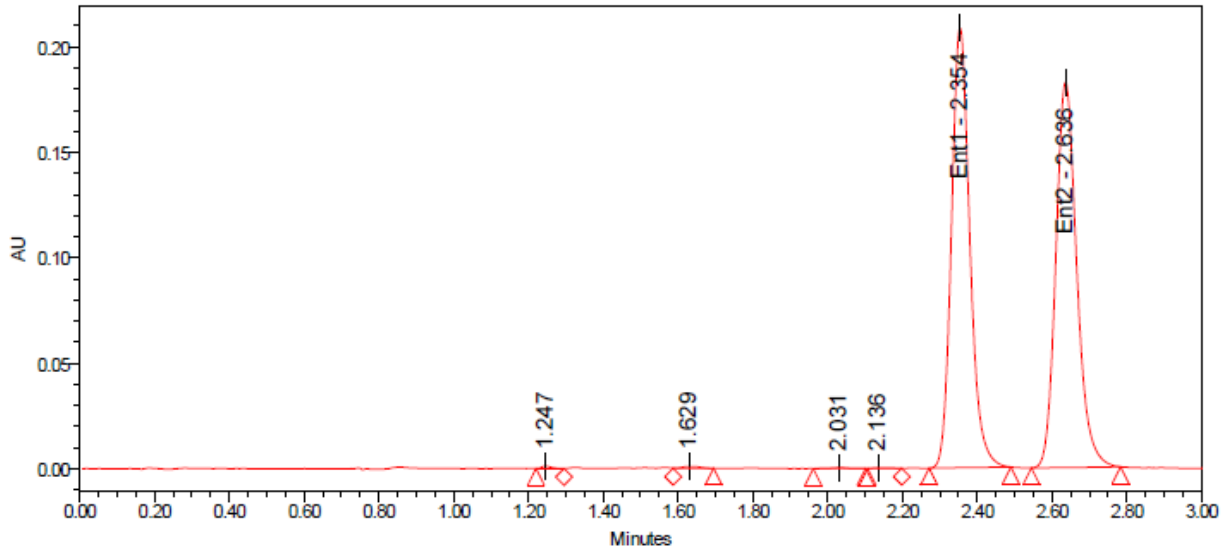


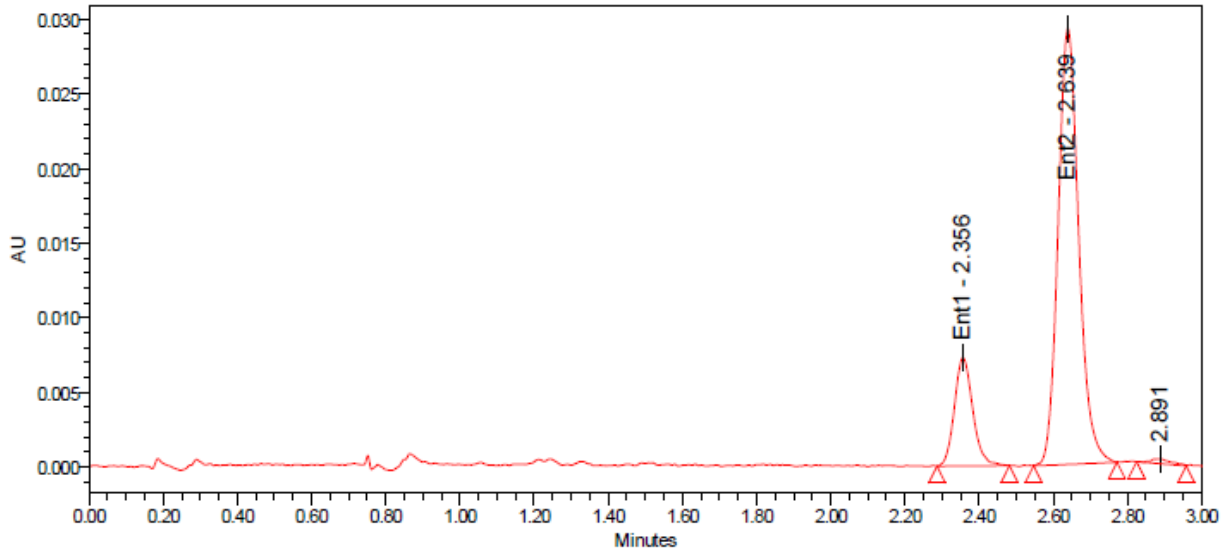
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-111II	50.19	49.81	0.38	808856	802663
2	SN-E-111I	16.89	83.11	-66.21	76747	377537


SN-E-96-I.1.fid
4p
f1 (ppm)

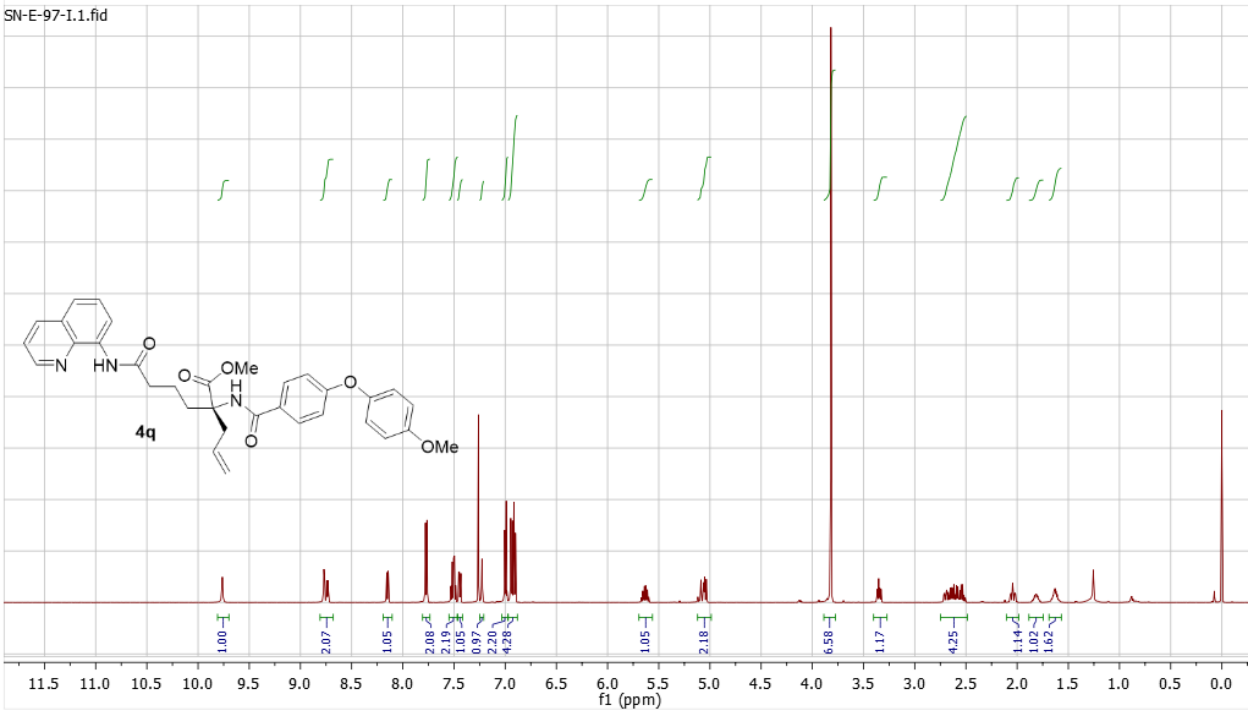

SN-E-96-I.11.fid
4p
f1 (ppm)

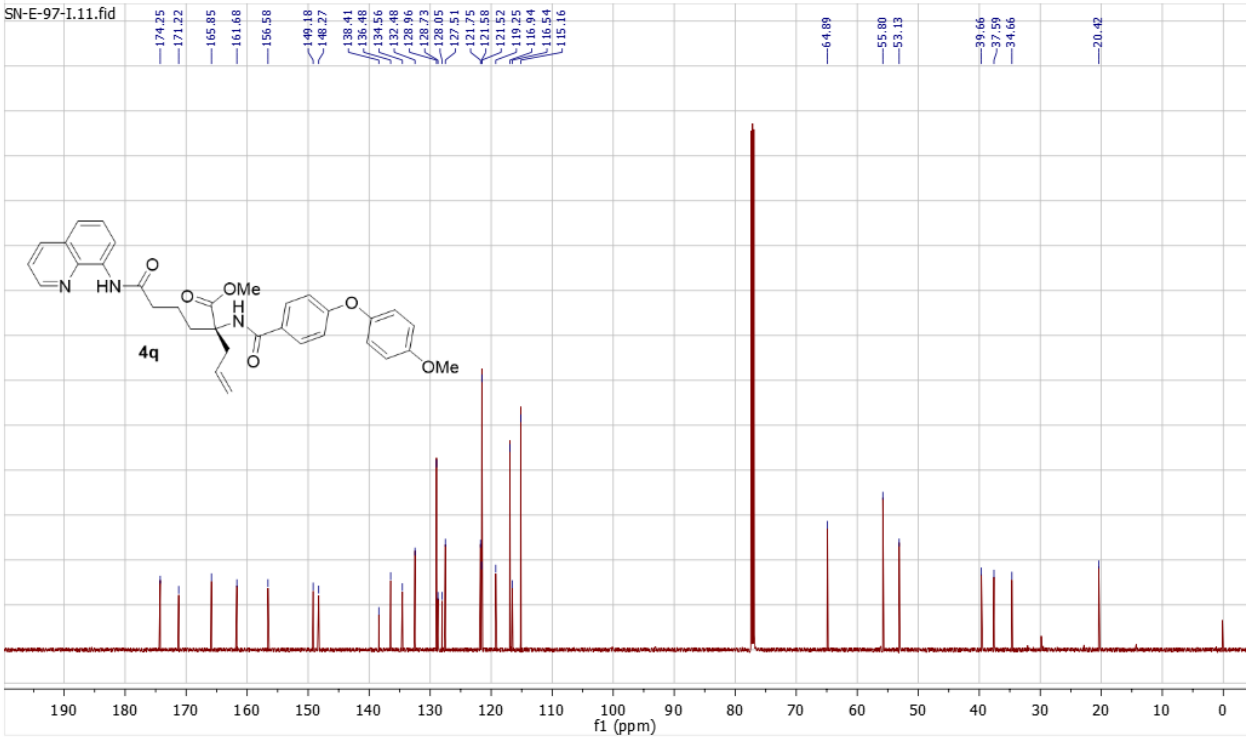


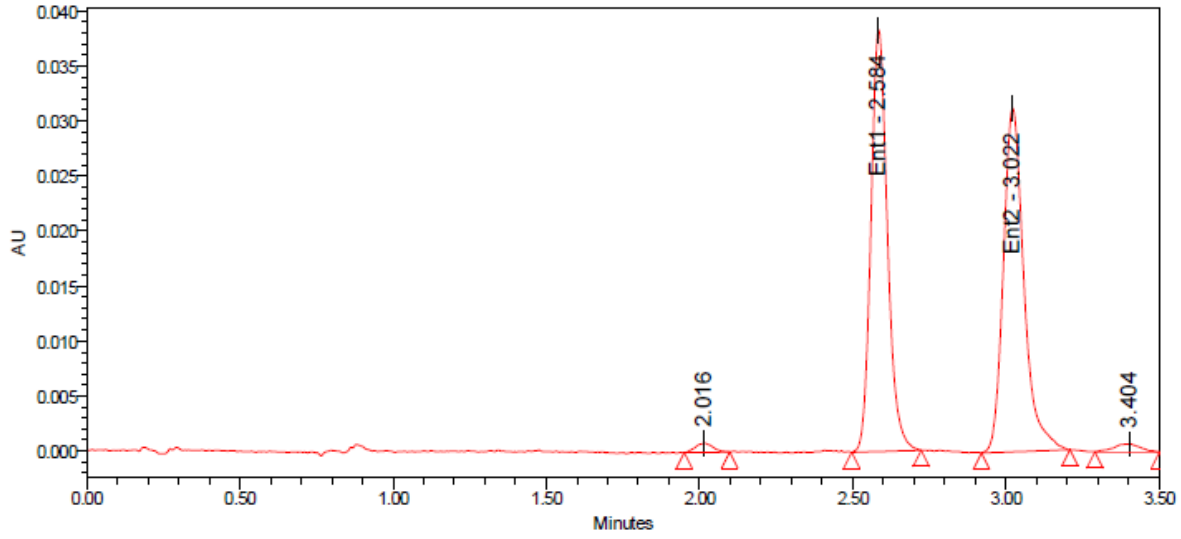


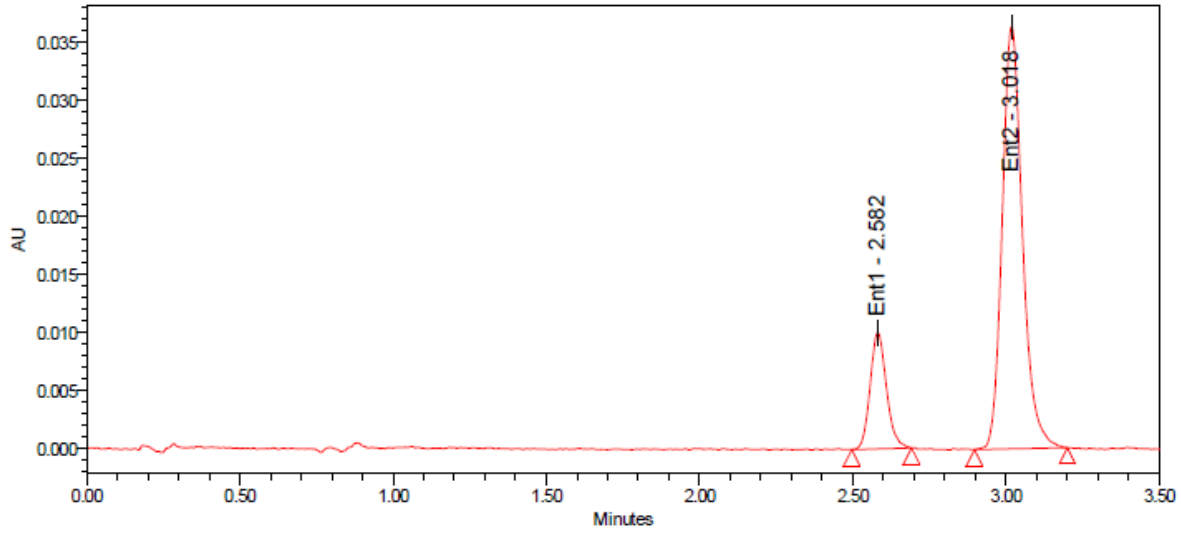
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-96II	50.10	49.90	0.20	711778	708923
2	SN-E-96I	18.13	81.87	-63.74	25032	113055


SN-E-97-I.1.fid
4q
OMe
OMe
f1 (ppm)

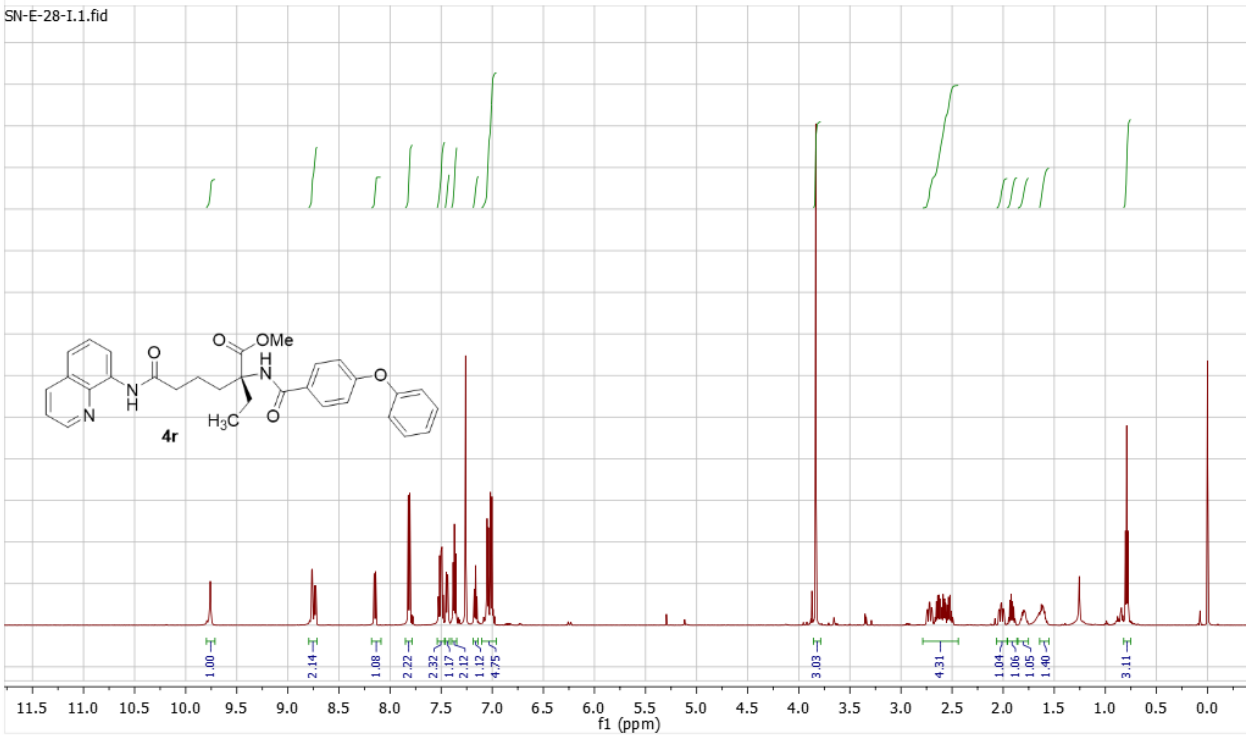

SN-E-97-I.11.fid
4q
OMe
OMe
f1 (ppm)

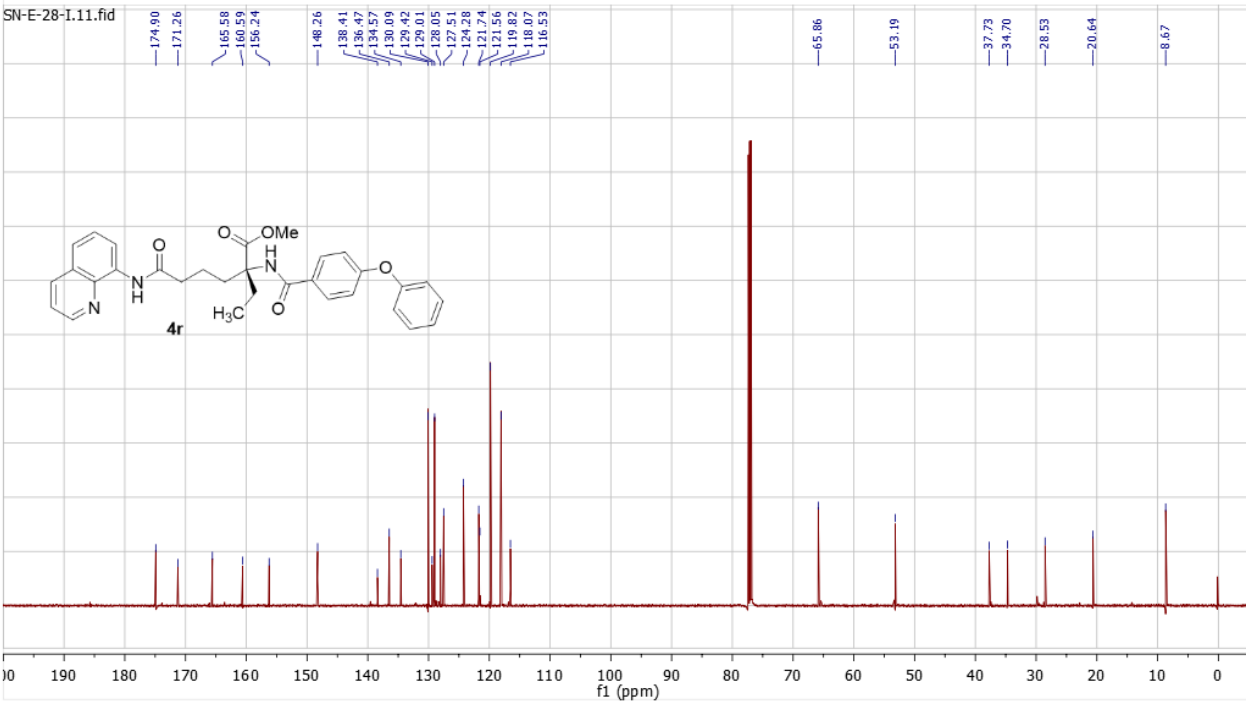


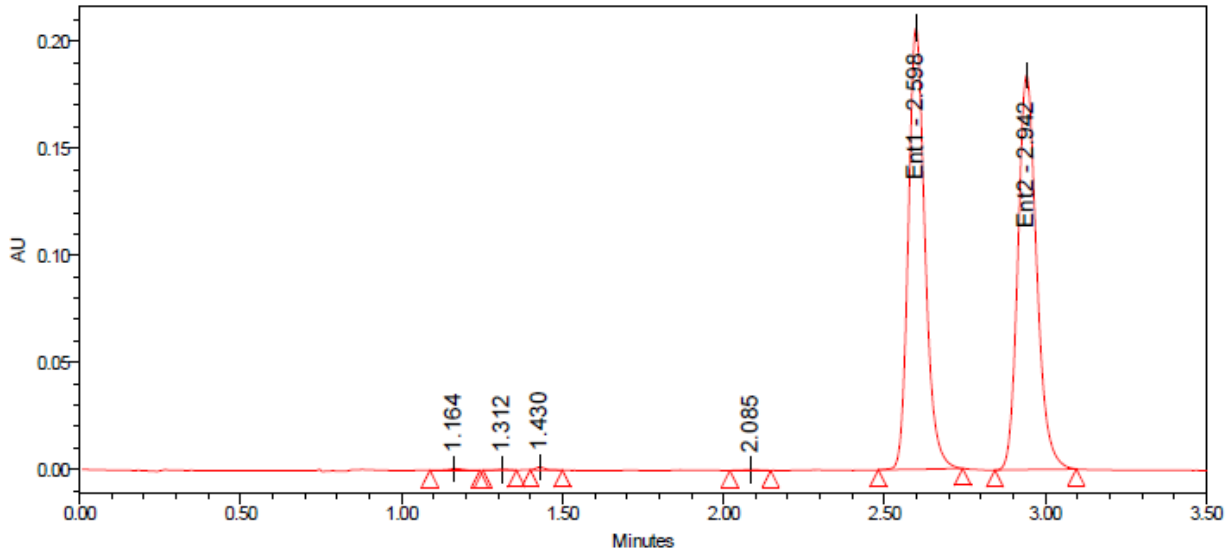


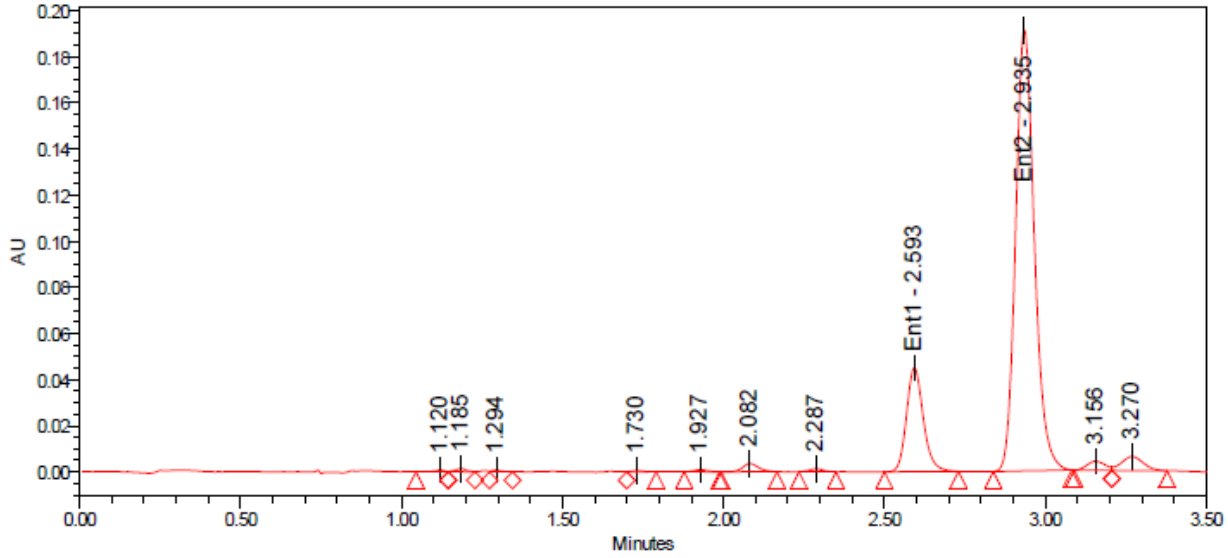
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-97II-2	49.60	50.40	-0.79	143503	145797
2	SN-E-97I	18.18	81.82	-63.63	37151	167157


SN-E-28-I.1.fid
4r
1.00
2.14
1.08
2.22
2.32
1.17
2.12
1.12
4.75
3.03
4.31
1.04
1.06
1.05
1.40
3.11
f1 (ppm)

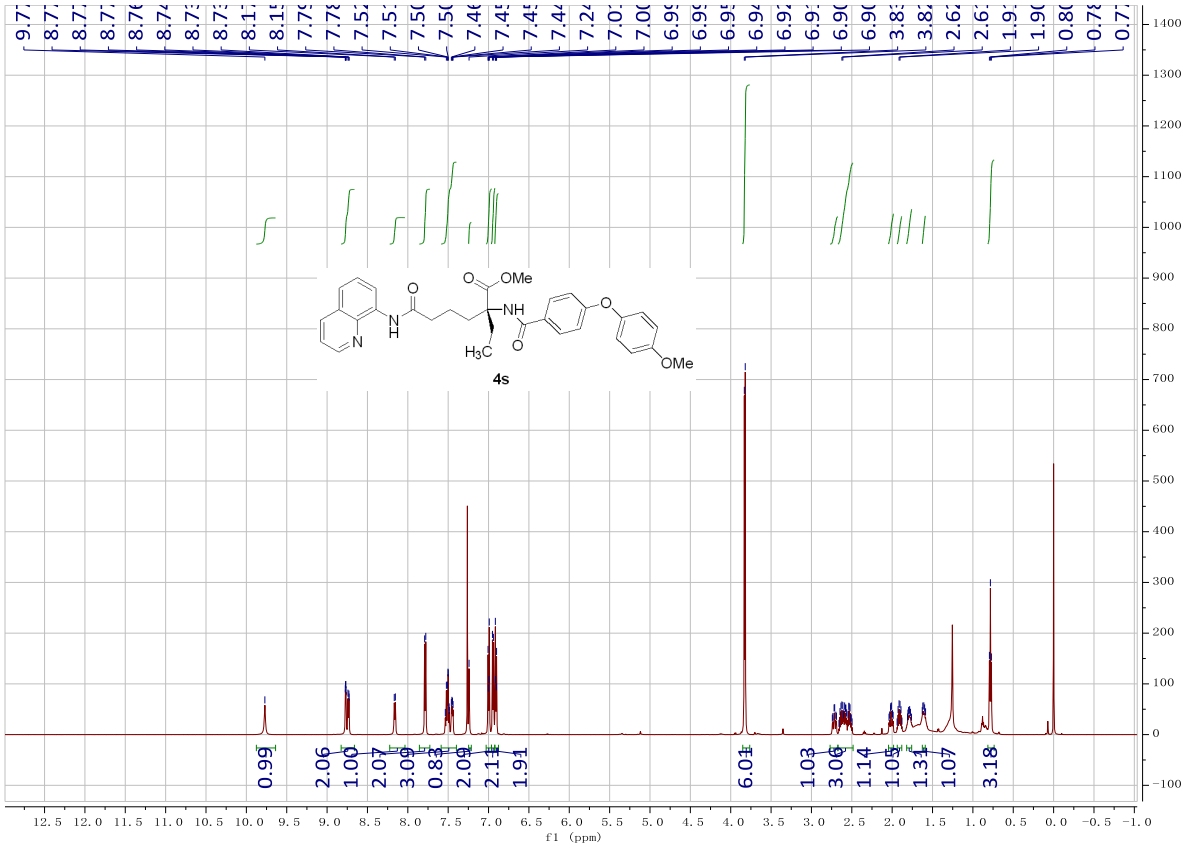

SN-E-28-I.11.fid
174.90
171.26
165.58
160.59
156.24
148.26
138.41
136.47
134.57
130.09
129.42
129.01
128.05
127.51
124.28
121.74
121.56
119.82
118.07
116.53
65.86
53.19
37.73
34.70
28.53
20.64
8.67
4r
f1 (ppm)

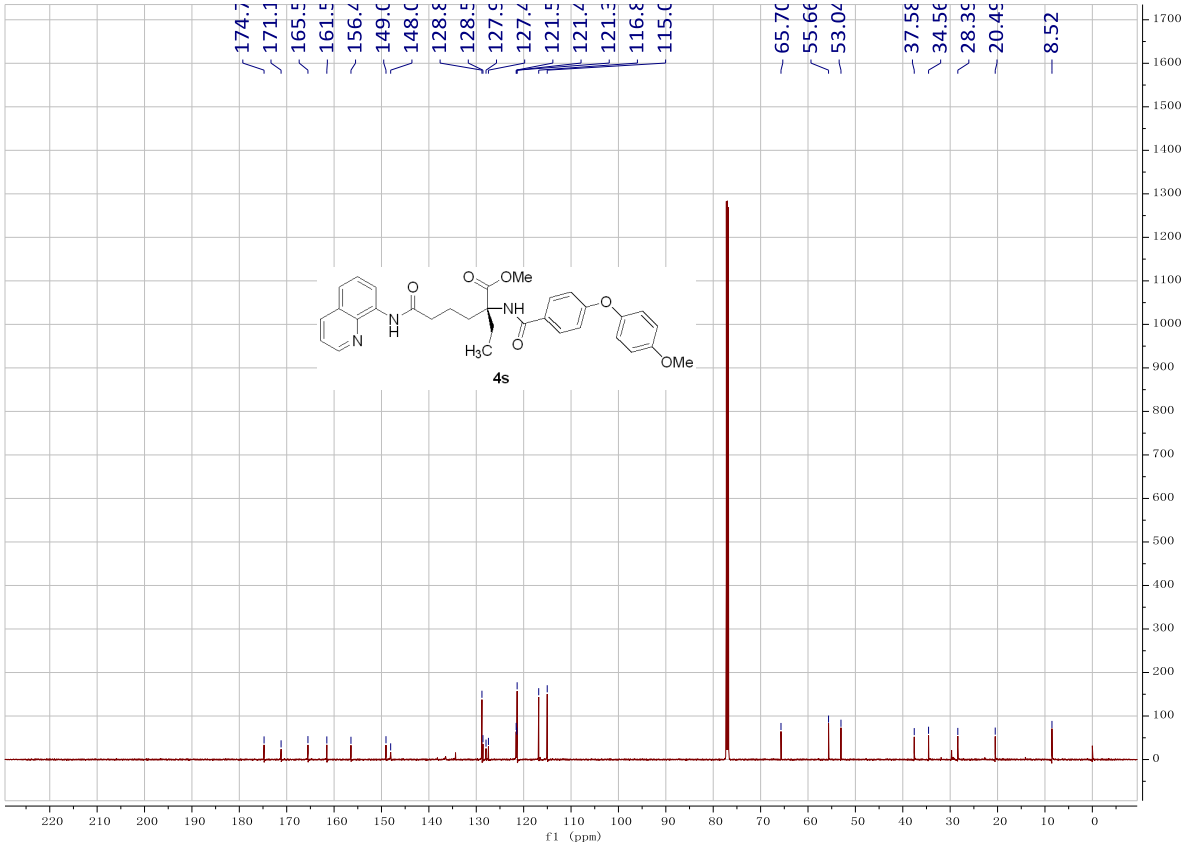


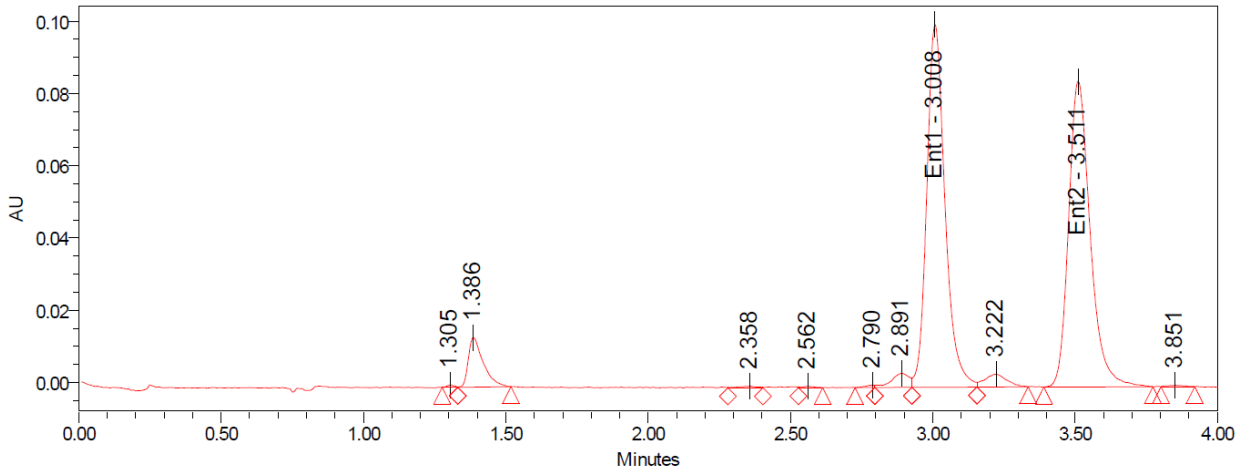


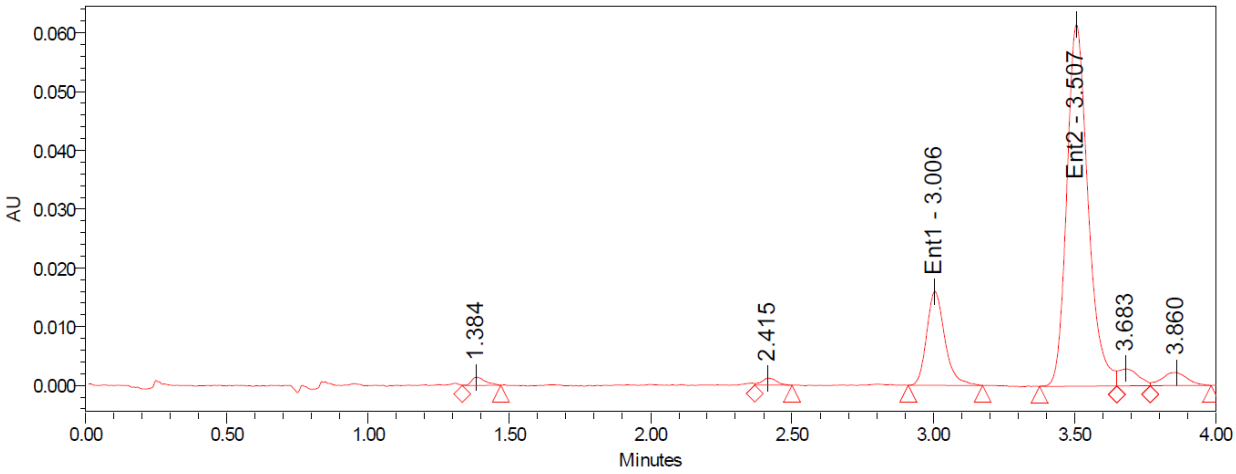
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-28II	49.80	50.20	-0.41	741102	747132
2	SN-E-28I	17.43	82.57	-65.13	163068	772234


4s
f1 (ppm)


4s
f1 (ppm)

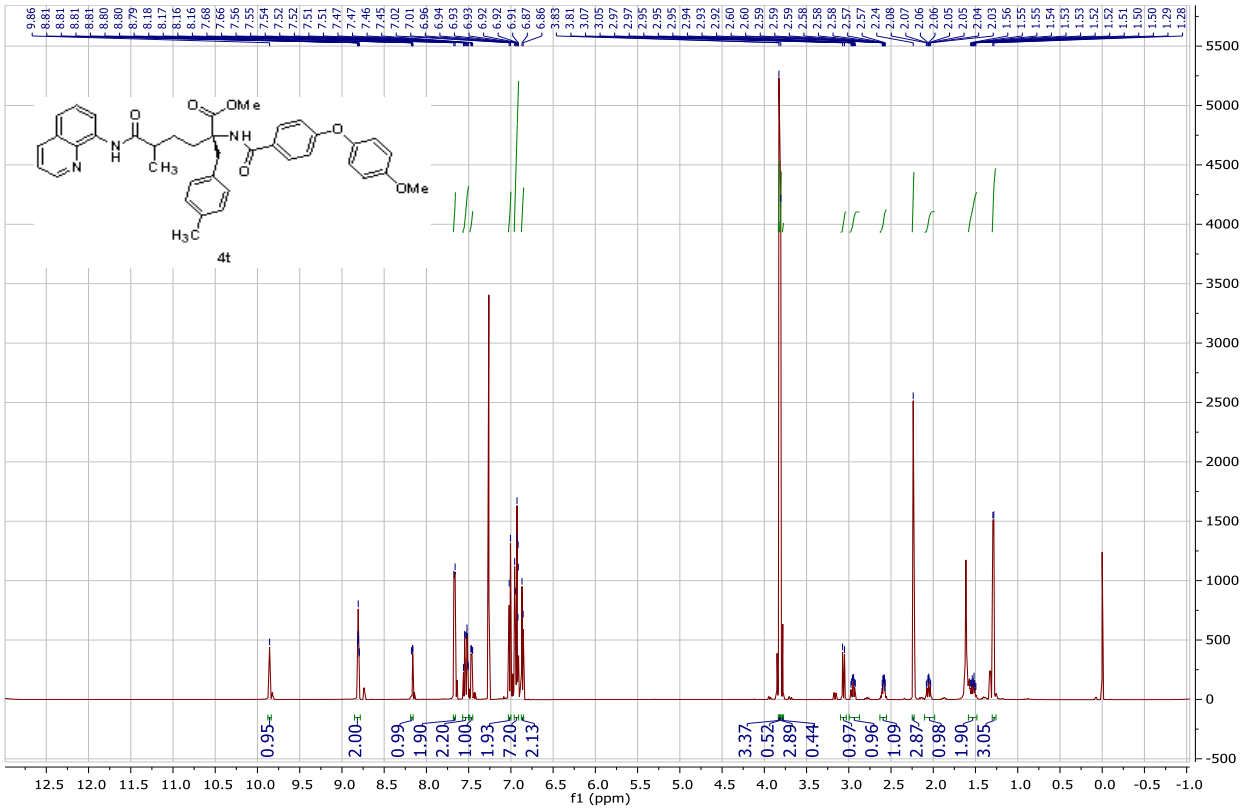


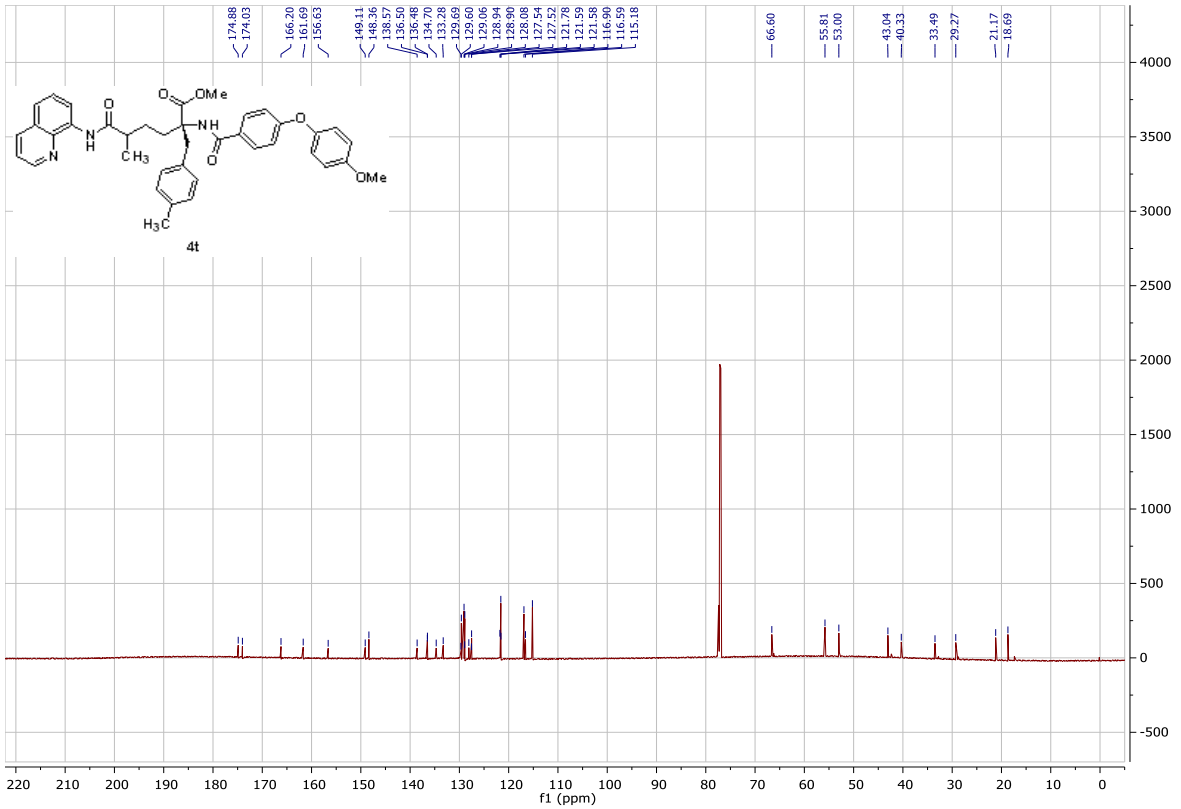


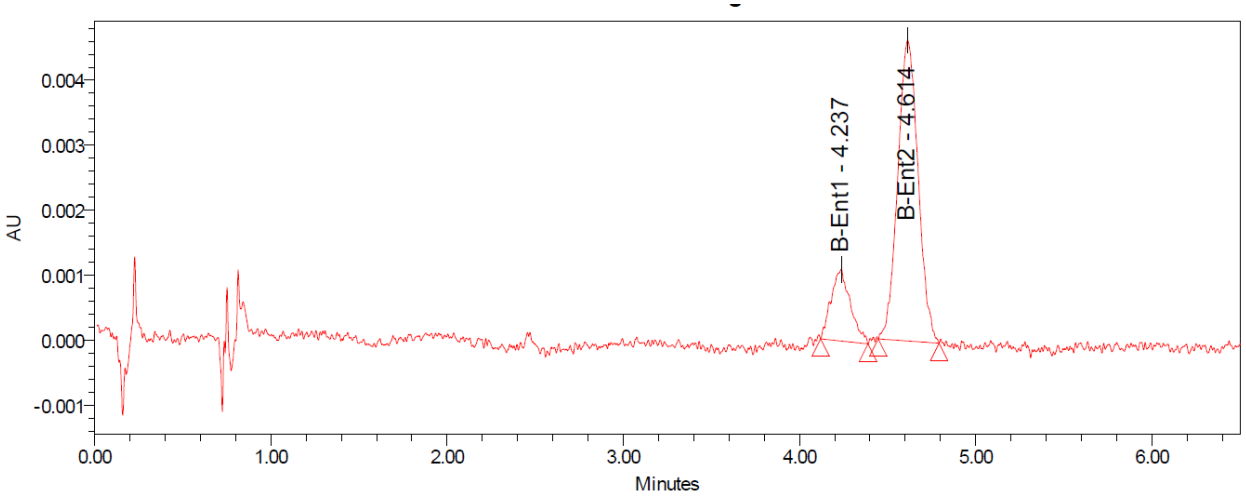
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	MYL-E-263	50.04	49.96	0.08	446310	445597

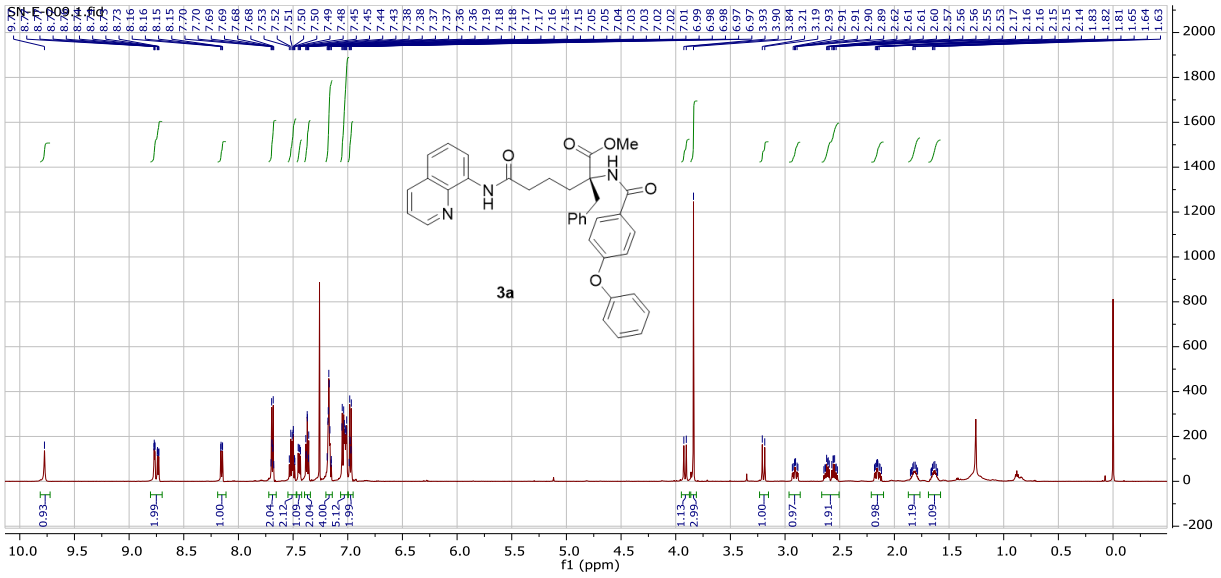
	SampleName	ent1	ent2	ee	Ent1	Ent2
1	MYL-264	18.08	81.92	-63.85	71138	322405

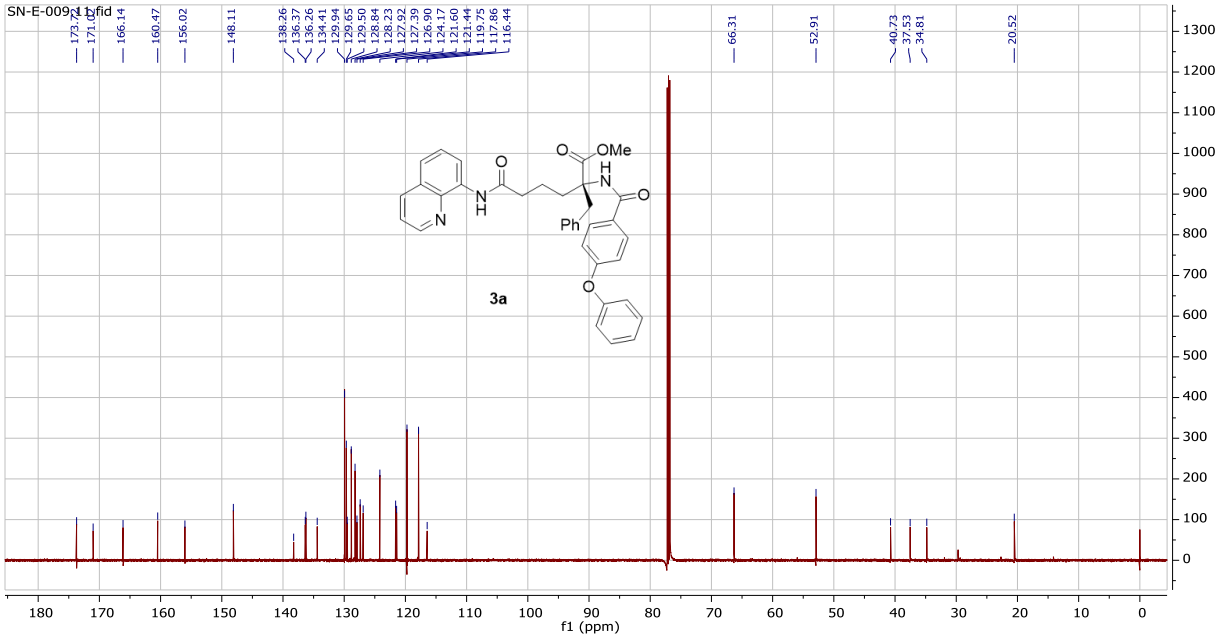

4t
f1 (ppm)

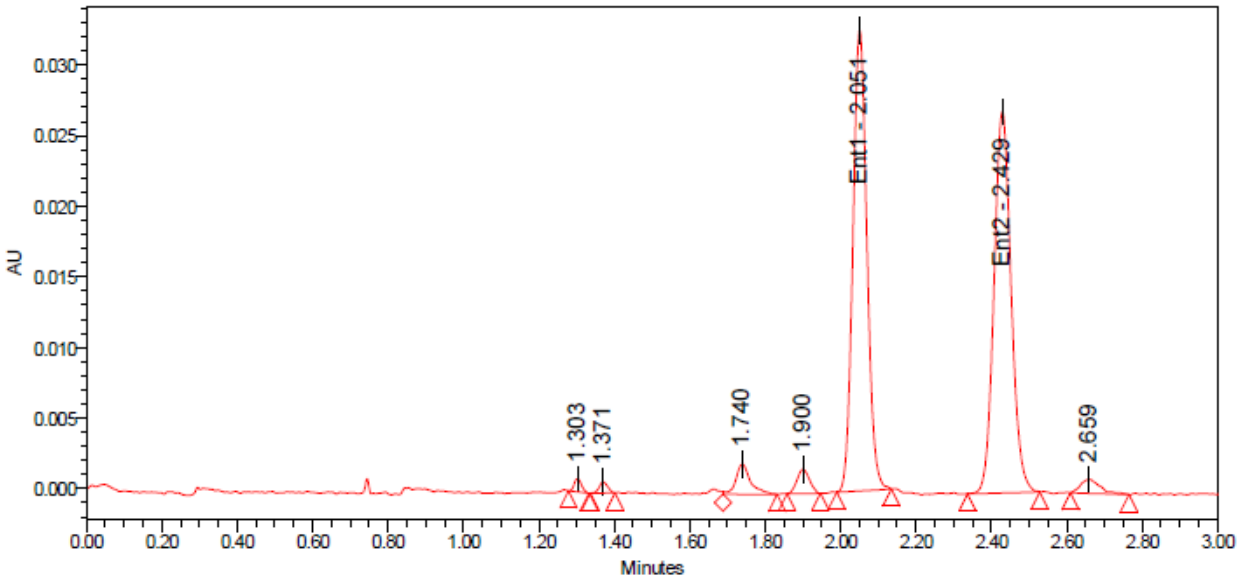

4t
f1 (ppm)



	SampleName	ent1	ent2	ee	A-Ent1	B-Ent1	B-Ent2	A-Ent2
1	MYL-E-275							
2	MYL-E-275	18.34	81.66	-63.32				

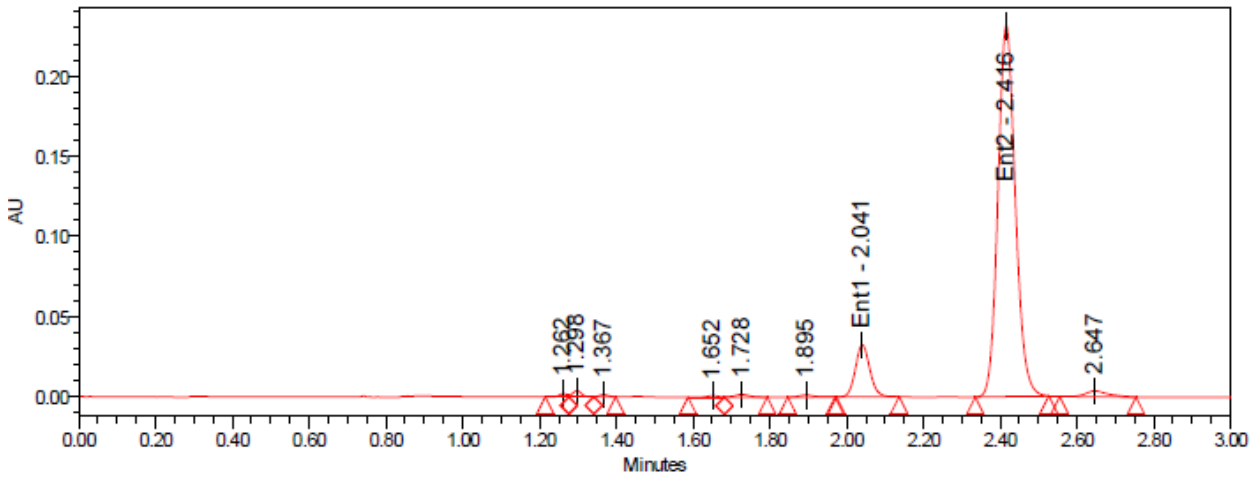

SN-E-009-1.fid
3a
f1 (ppm)


SN-E-009-1.fid
3a
f1 (ppm)

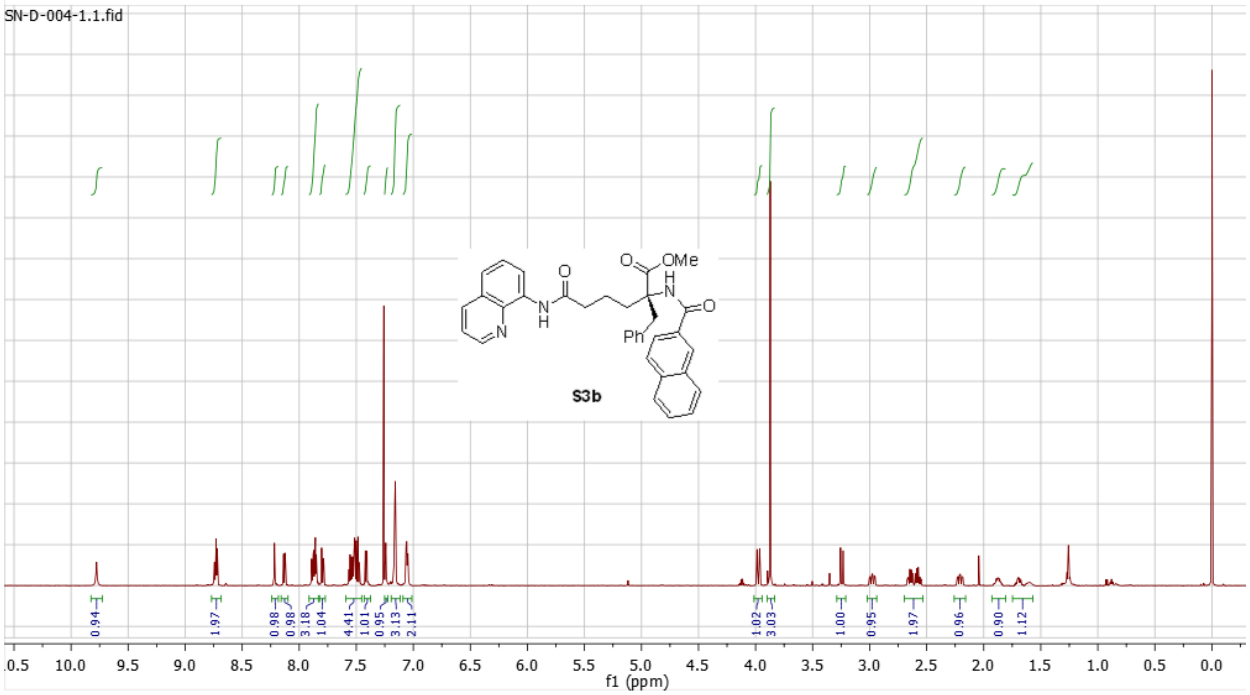


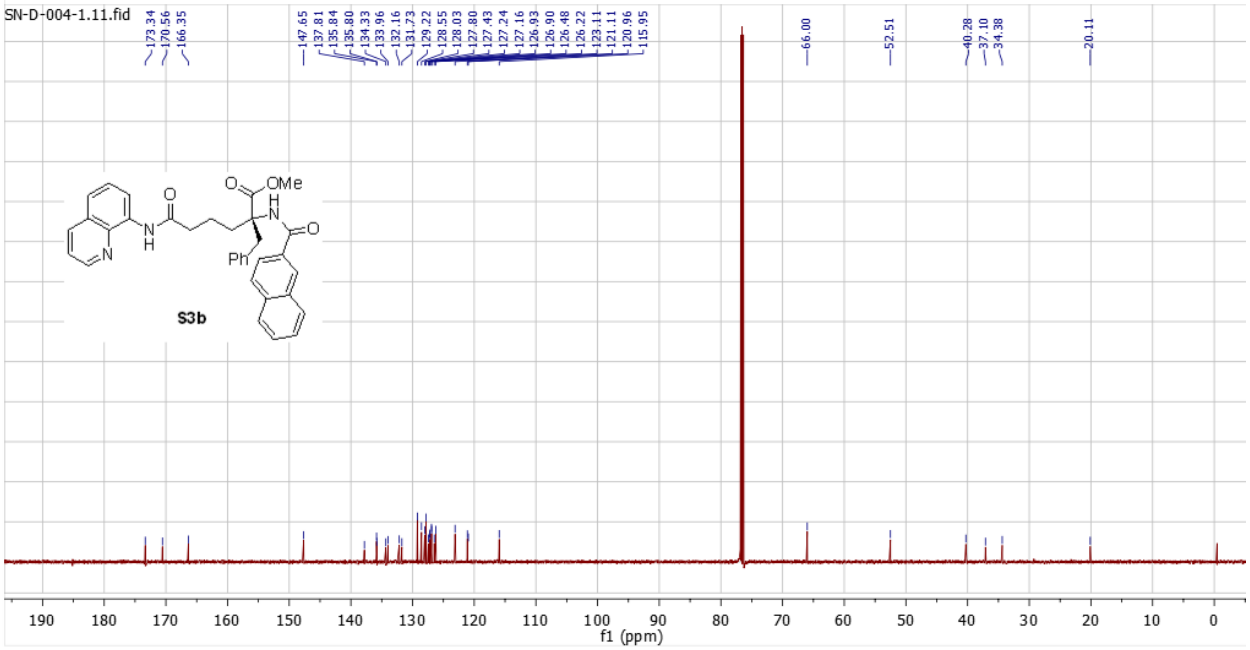
Area Summarized by Name

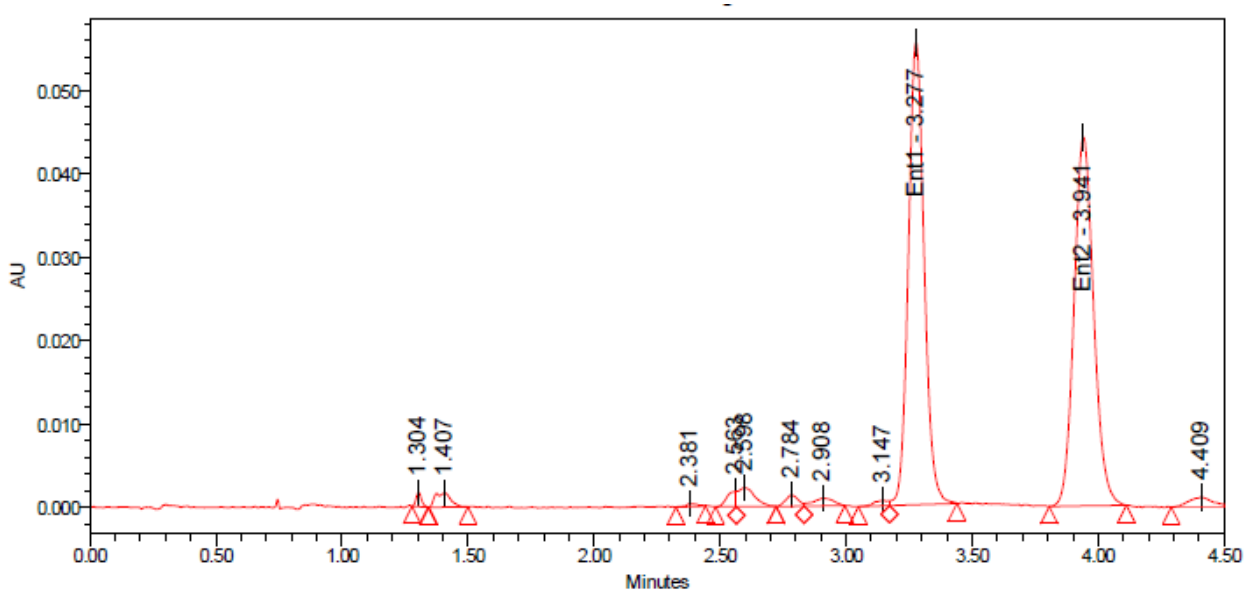
	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-C-92_IB35%	49.63	50.37	-0.75	83981	85244



SampleName	ent1	ent2	ee	Ent1	Ent2
SN-D-002	10.40	89.60	-79.20	84352	726701

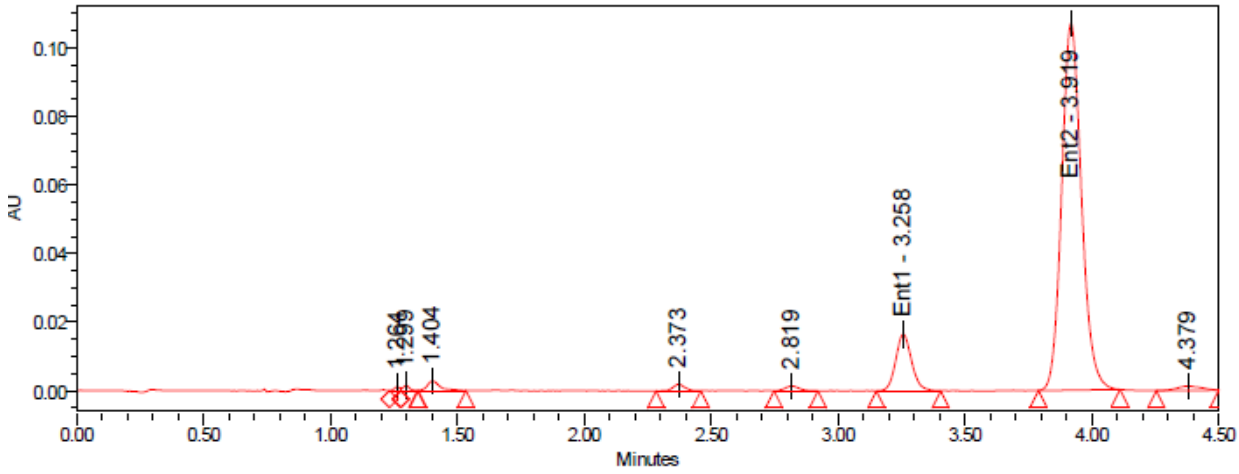

SN-D-004-1.1.fid
S3b
f1 (ppm)


SN-D-004-1.11.fid
S3b
f1 (ppm)

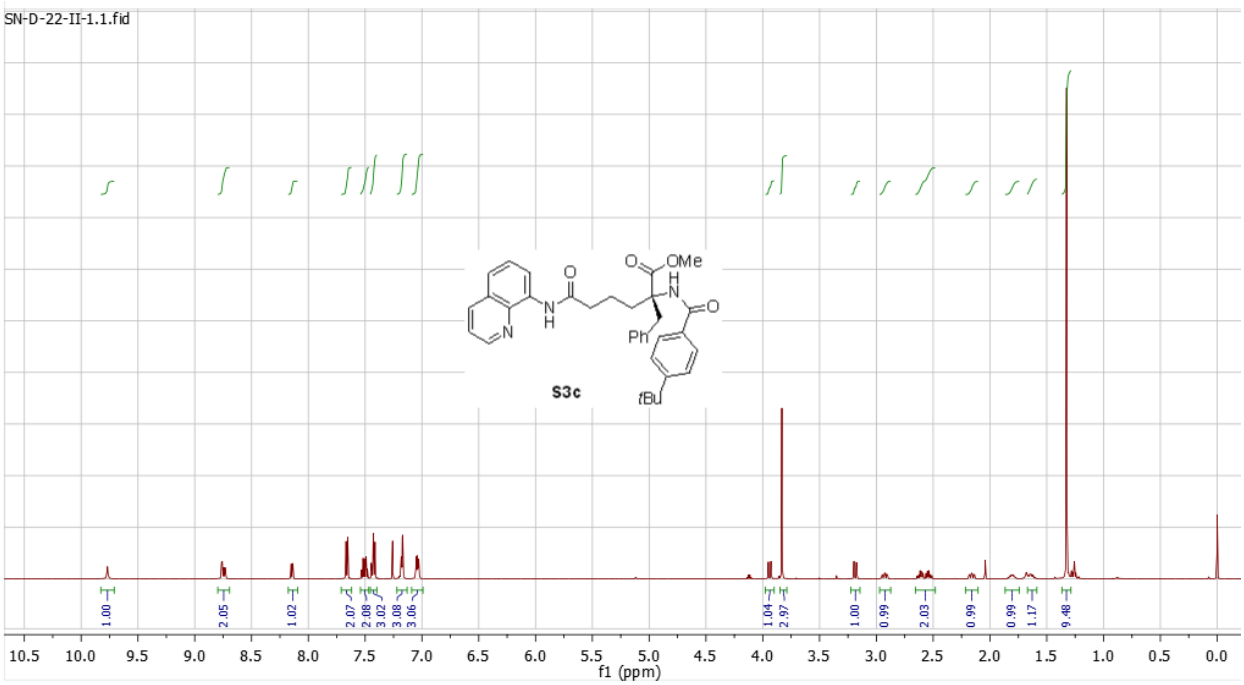


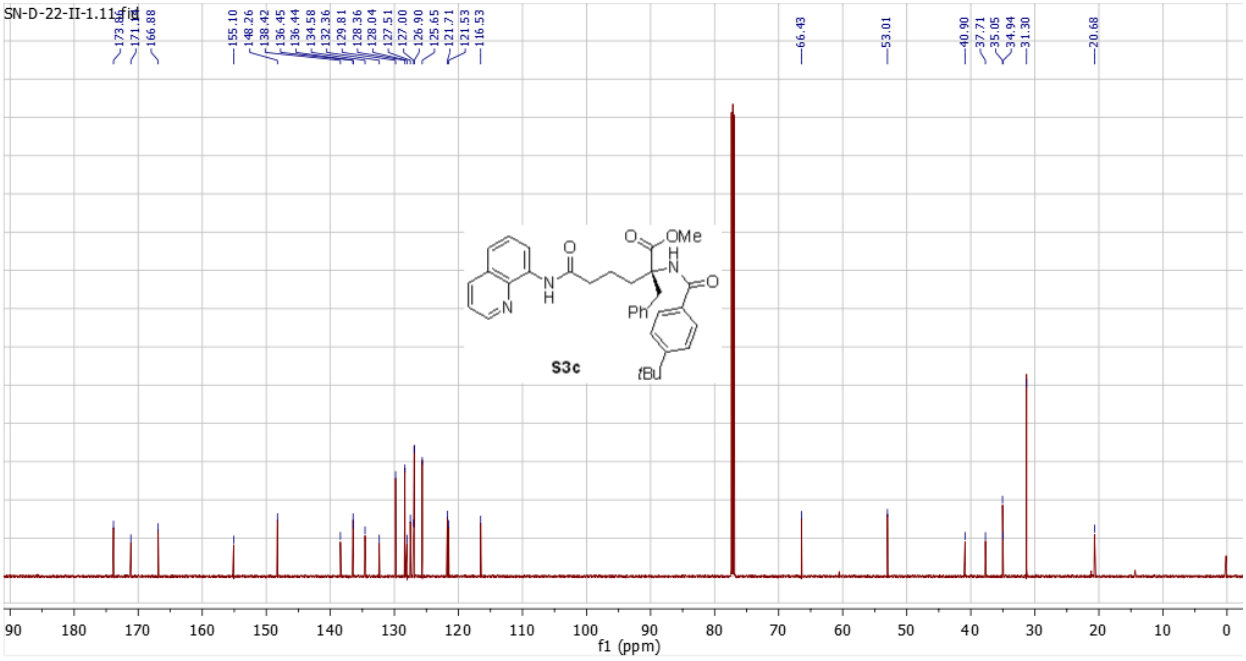
Area Summarized by Name

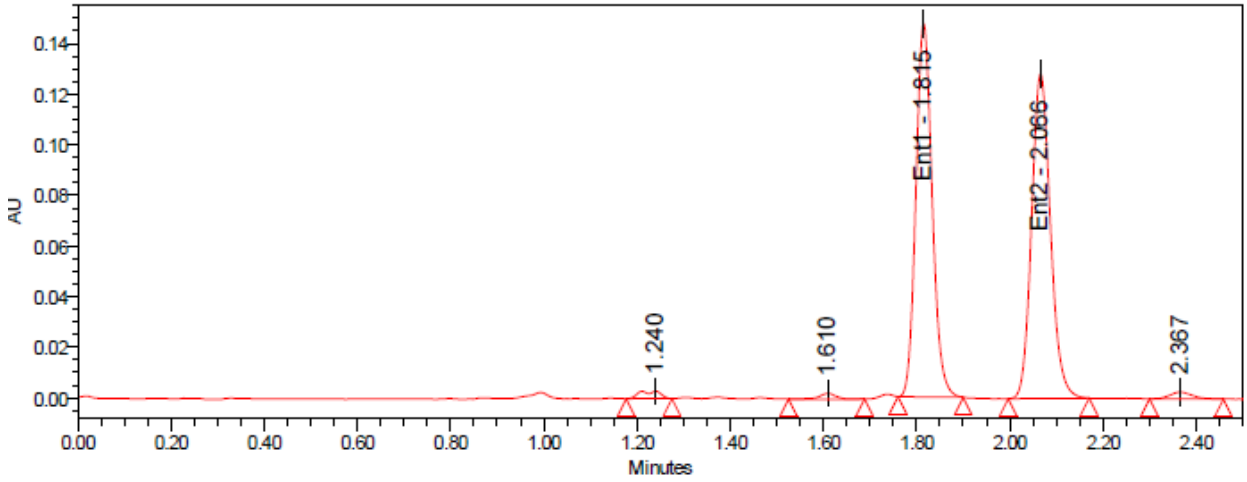
	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-C-94_IB35%	50.28	49.72	0.55	241822	239175

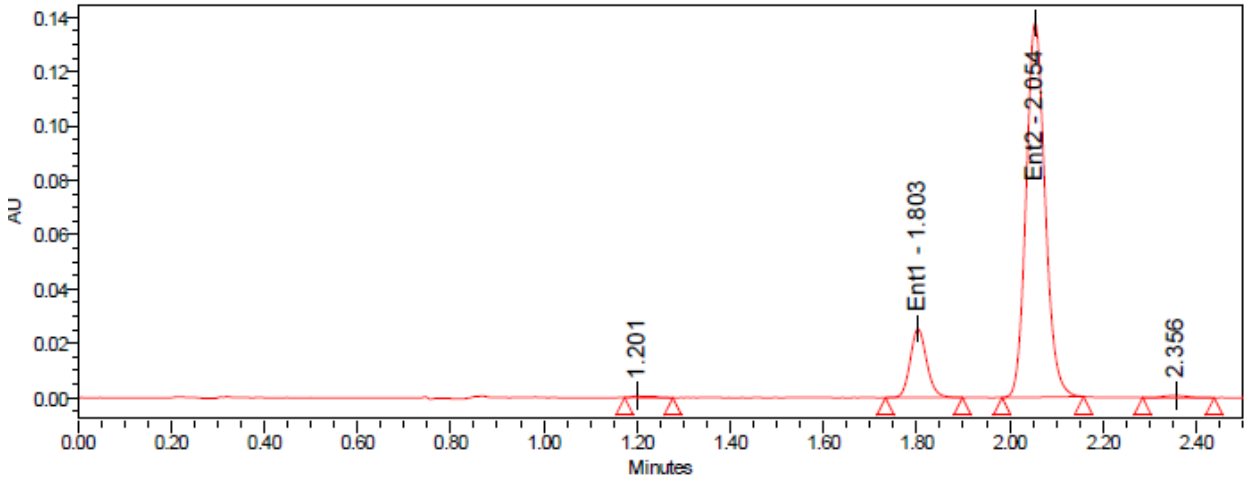


SampleName	ent1	ent2	ee	Ent1	Ent2
SN-D-004	11.05	88.95	-77.90	71897	578881

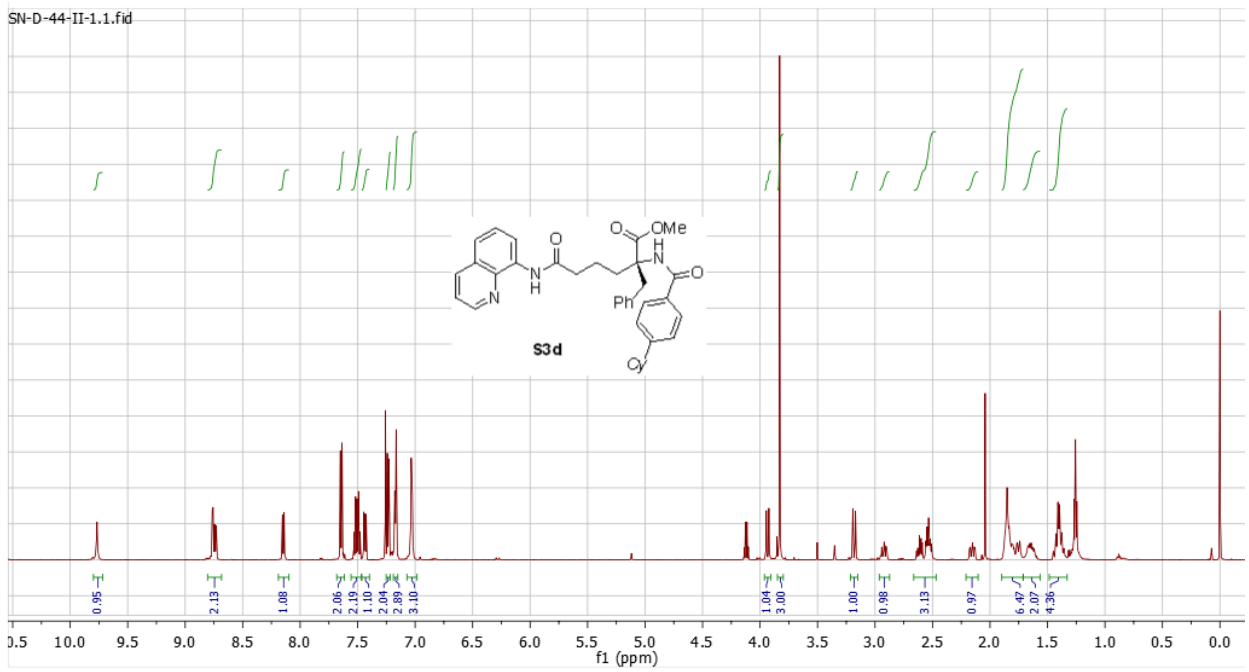

SN-D-22-II-1.1.fid
S3c
f1 (ppm)

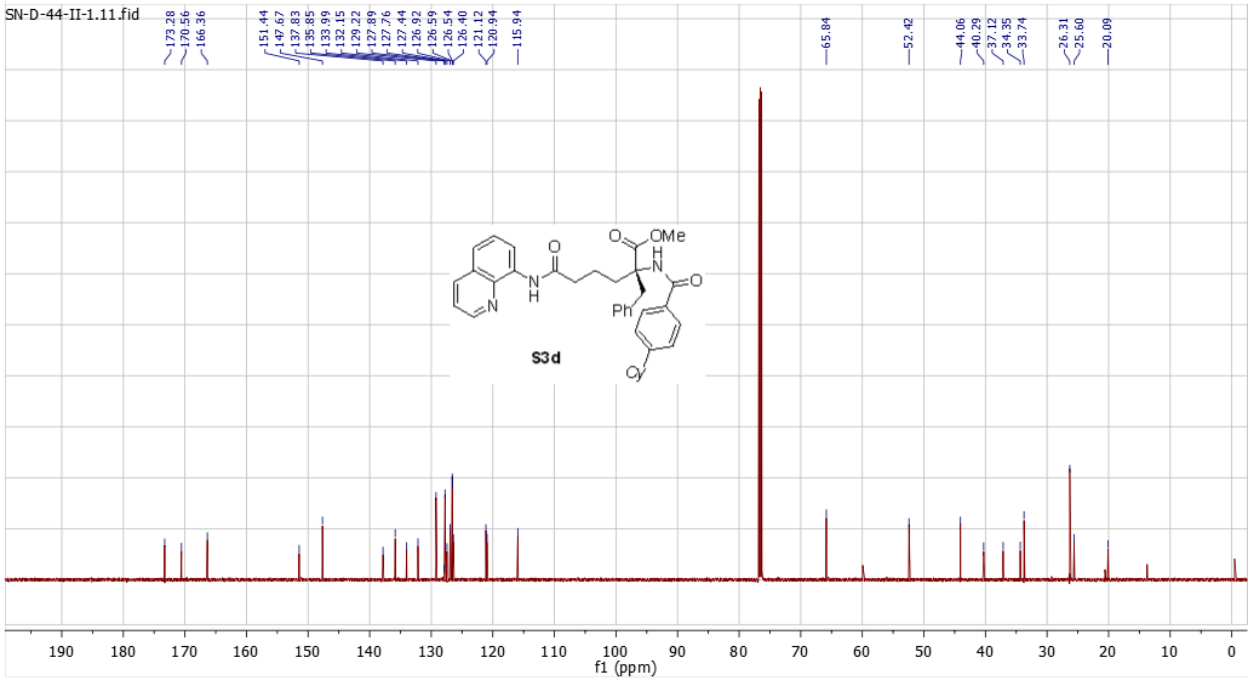

SN-D-22-II-1.11.fid
S3c
f1 (ppm)

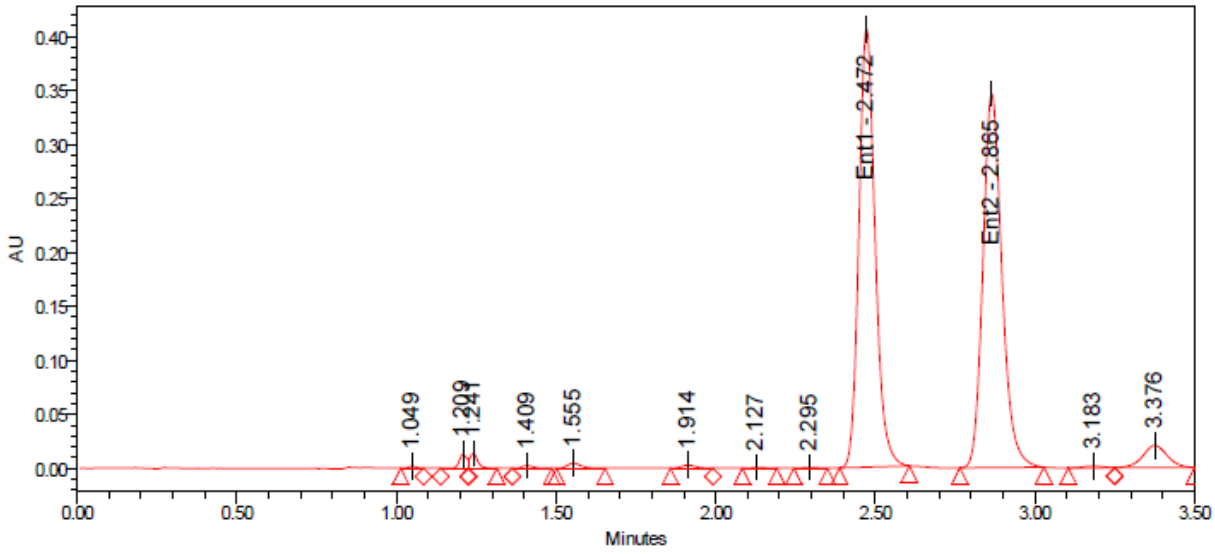


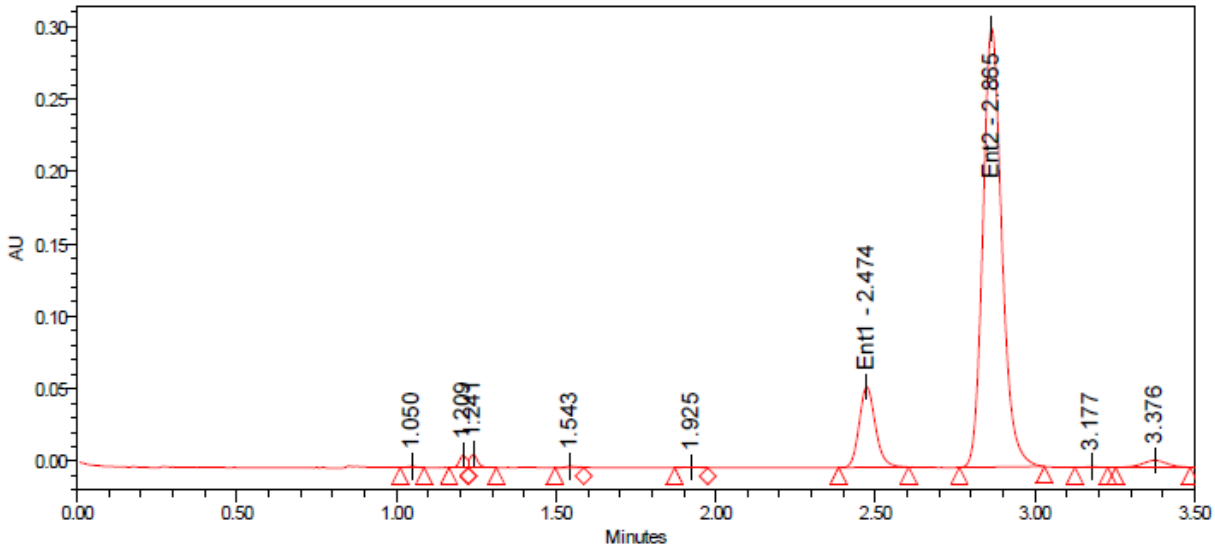


	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-D-22I	49.76	50.24	-0.48	357561	360979
2	SN-D-22II	13.81	86.19	-72.38	62463	389854


SN-D-44-II-1.1.fid
S3d
f1 (ppm)

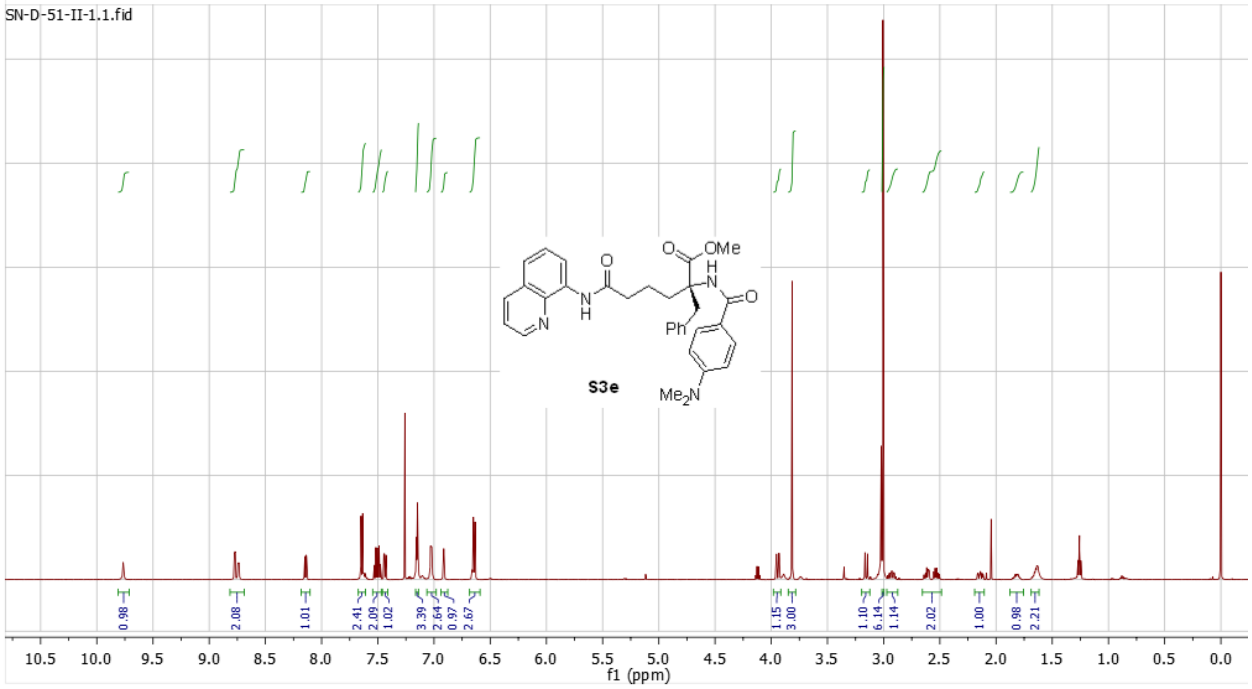

SN-D-44-II-1.11.fid
S3d
f1 (ppm)

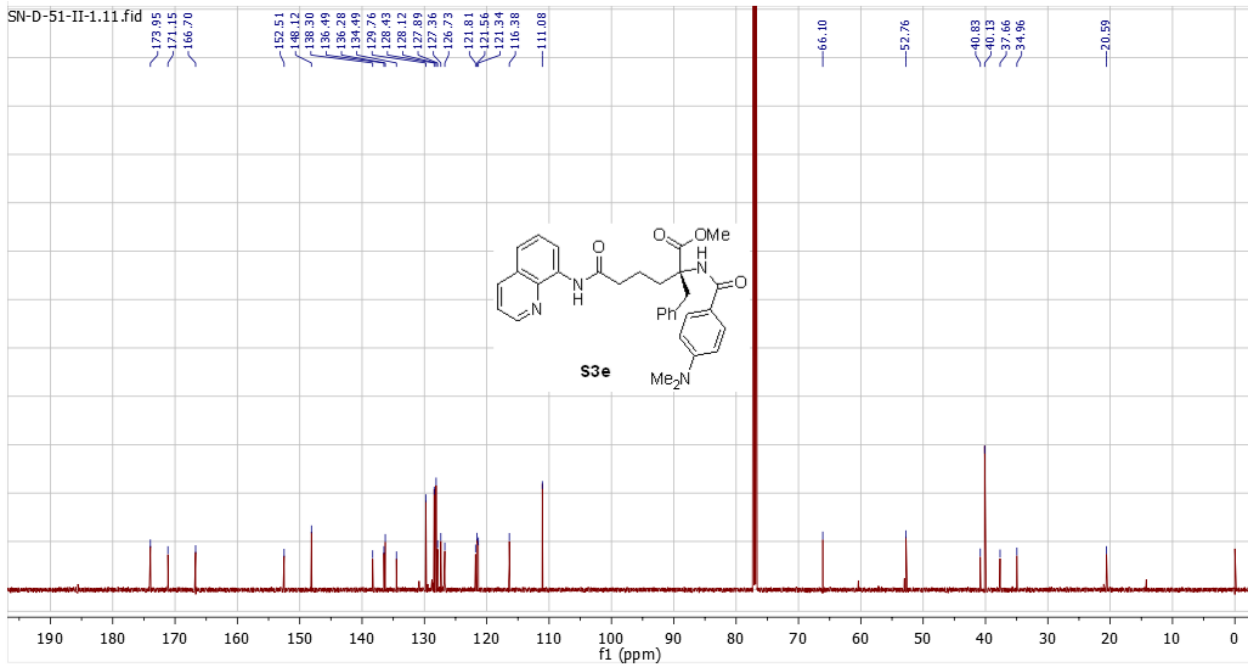


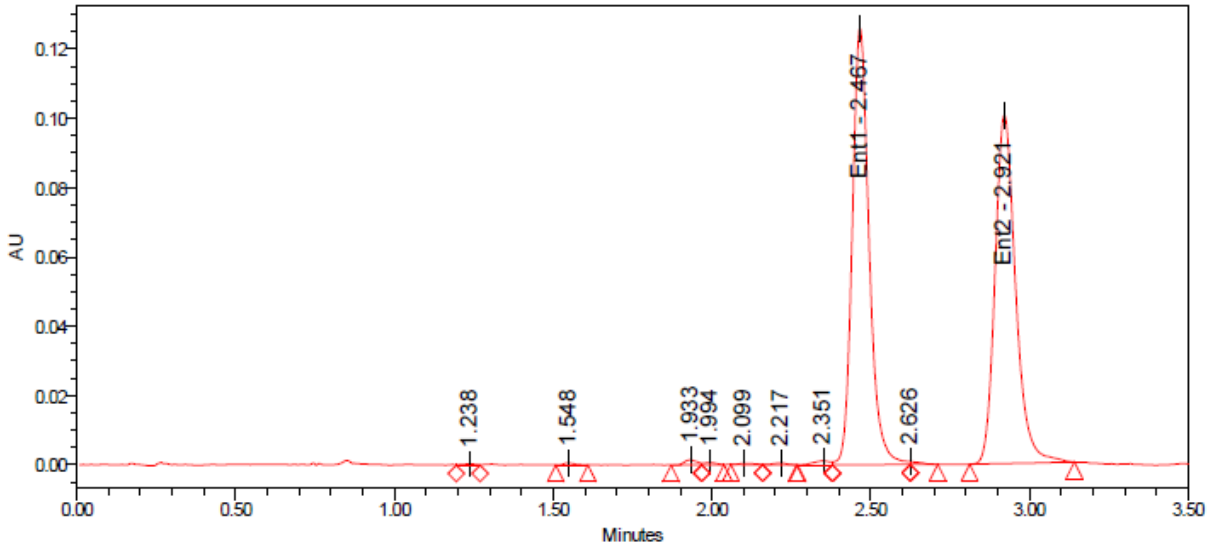


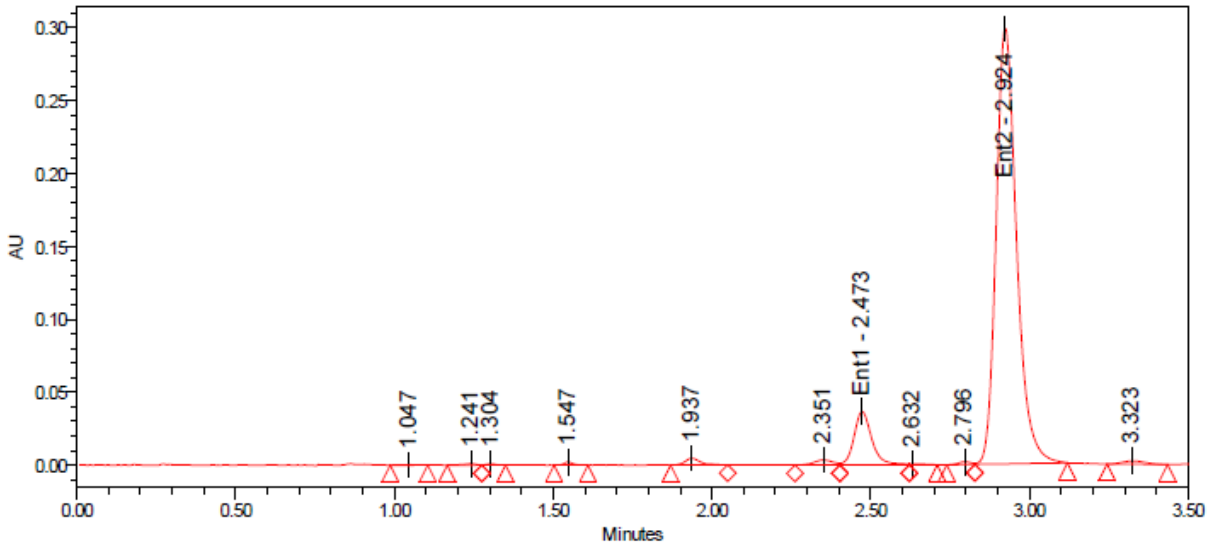
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-D-44I	49.90	50.10	-0.20	1430001	1435753
2	SN-D-44II	13.53	86.47	-72.95	196119	1253742


SN-D-51-II-1.1.fid
S3e
f1 (ppm)

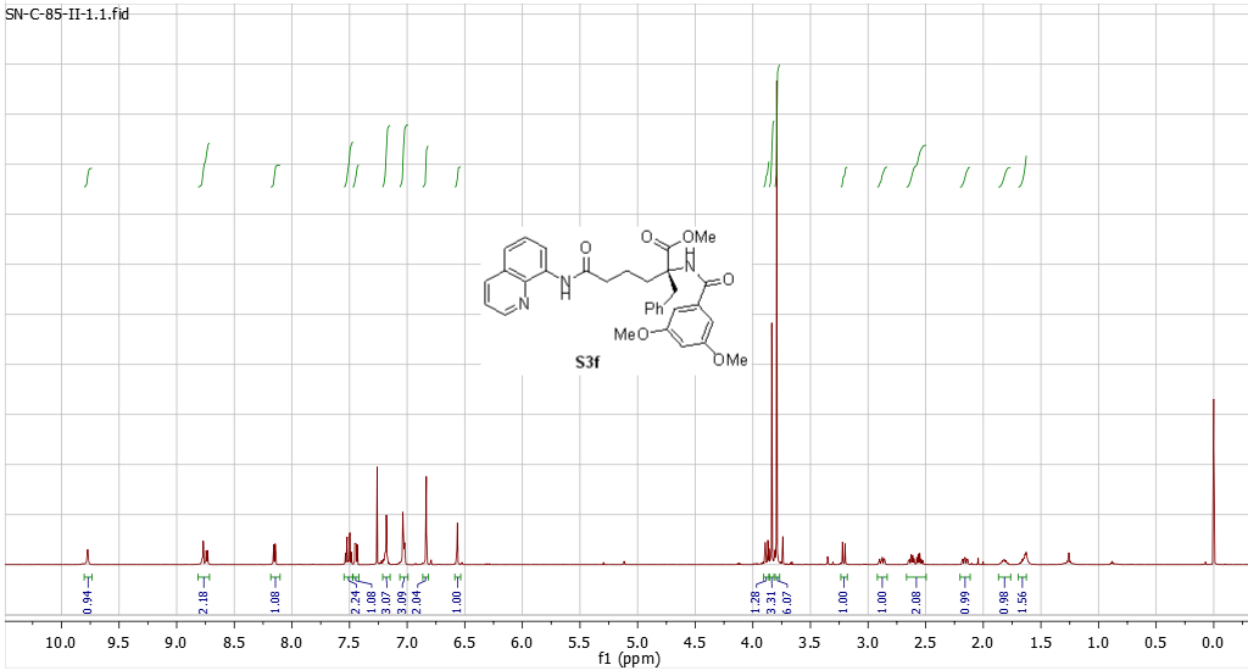

SN-D-51-II-1.11.fid
S3e
f1 (ppm)

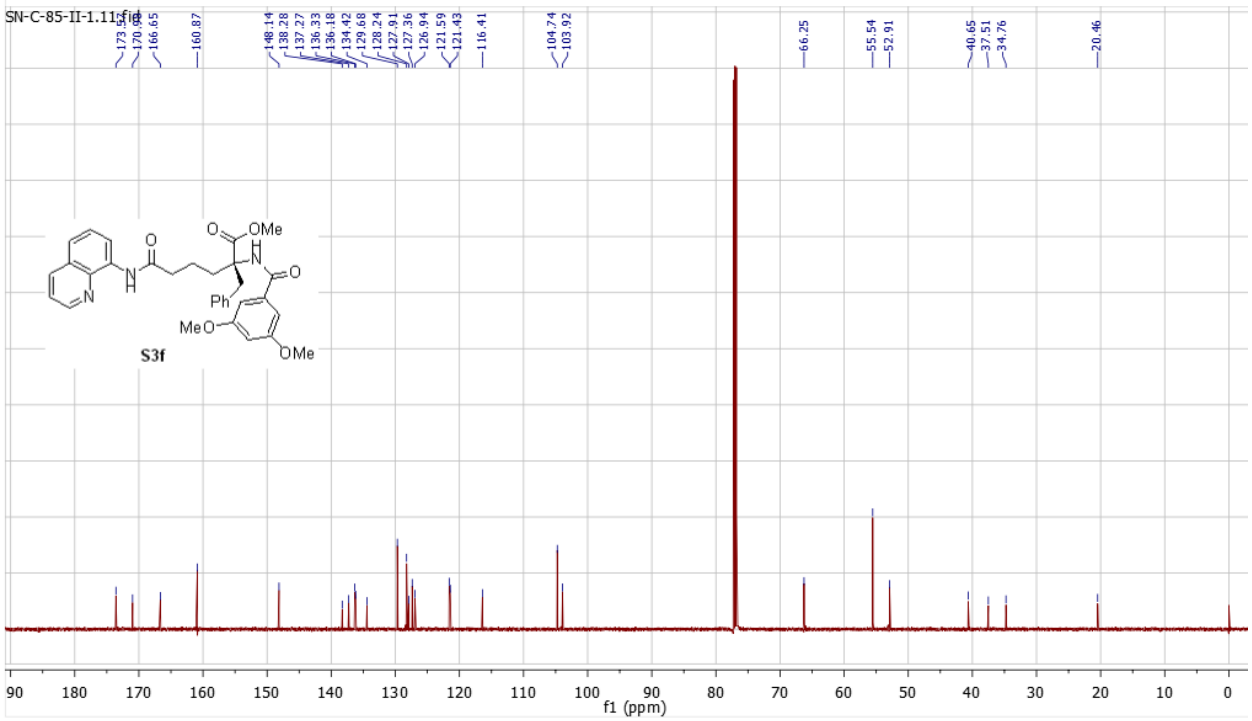


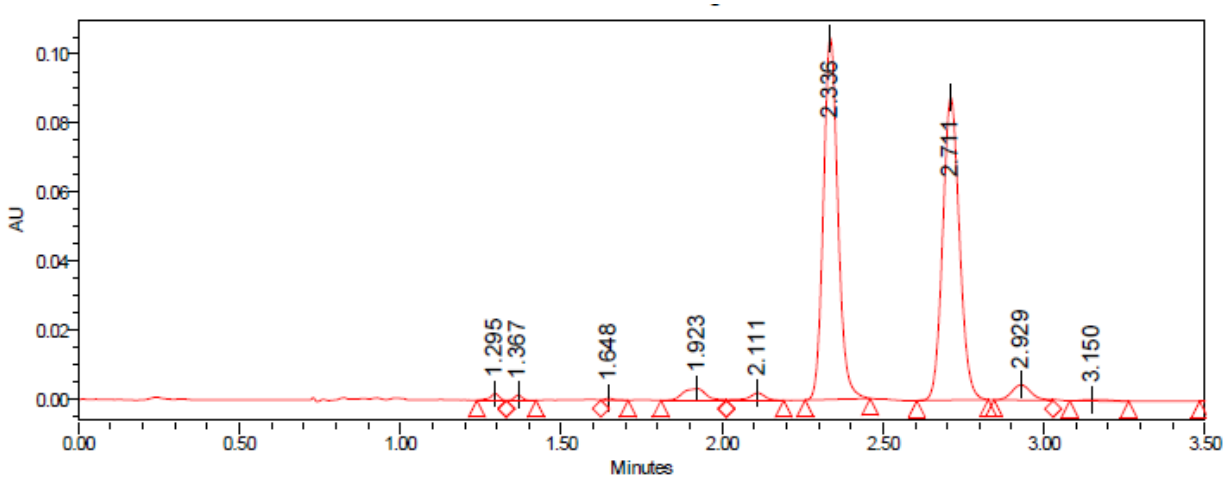


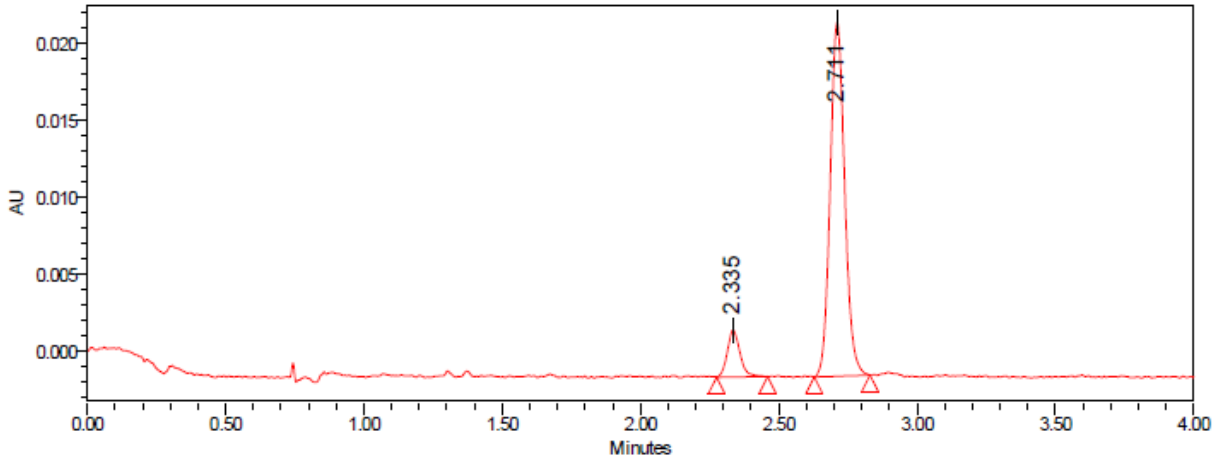
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-D-51I	50.72	49.28	1.44	466363	453090
2	SN-D-51II	9.60	90.40	-80.81	141456	1332561


SN-C-85-II-1.1.fid
S3f
f1 (ppm)

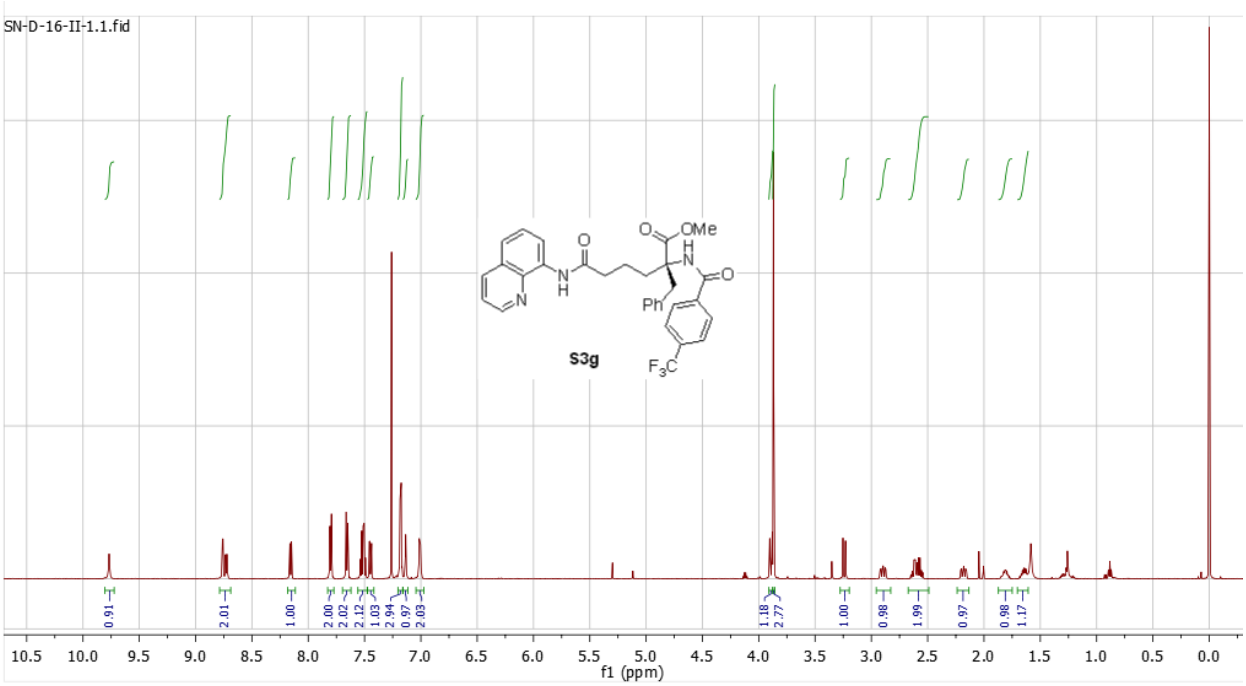

SN-C-85-II-1.11.fid
S3f
f1 (ppm)

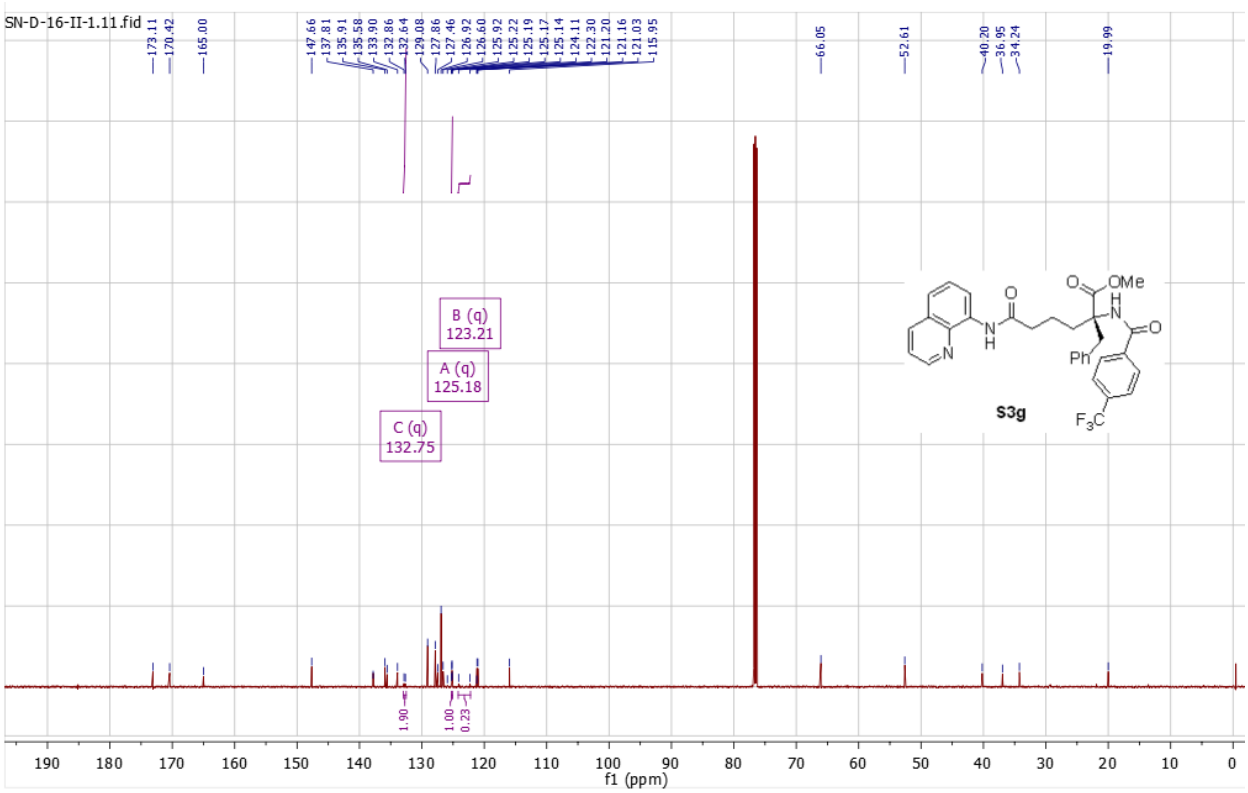


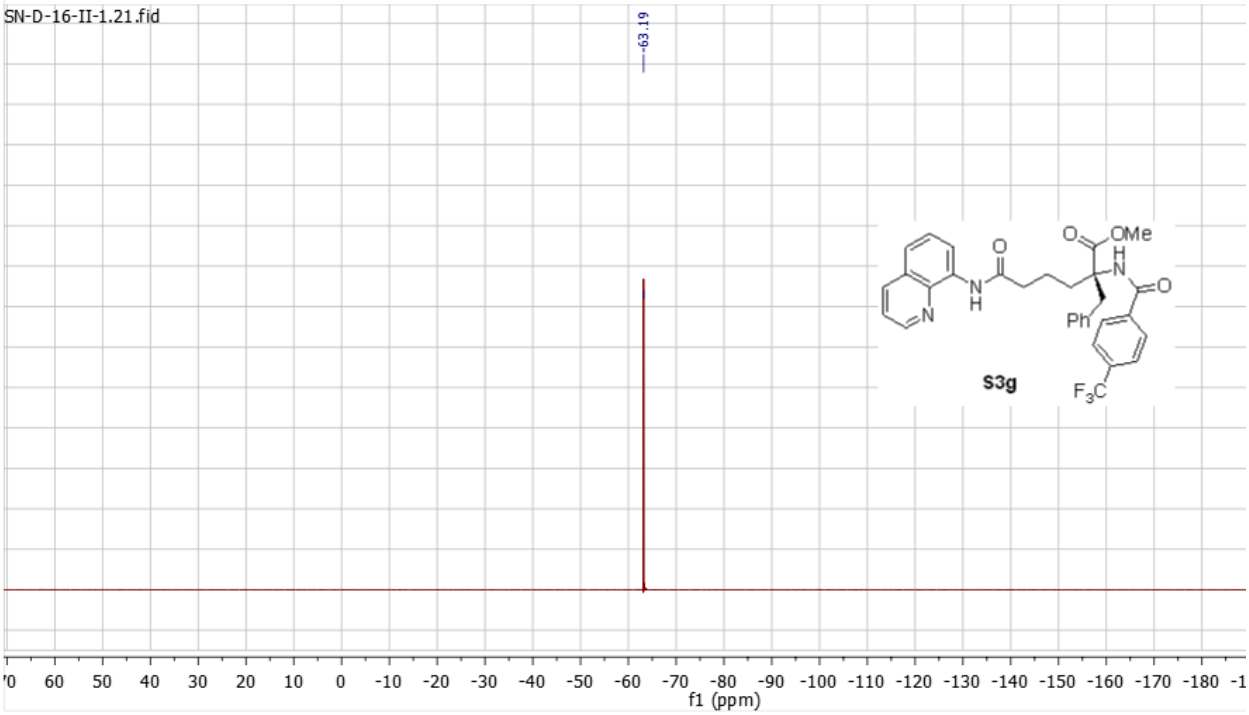


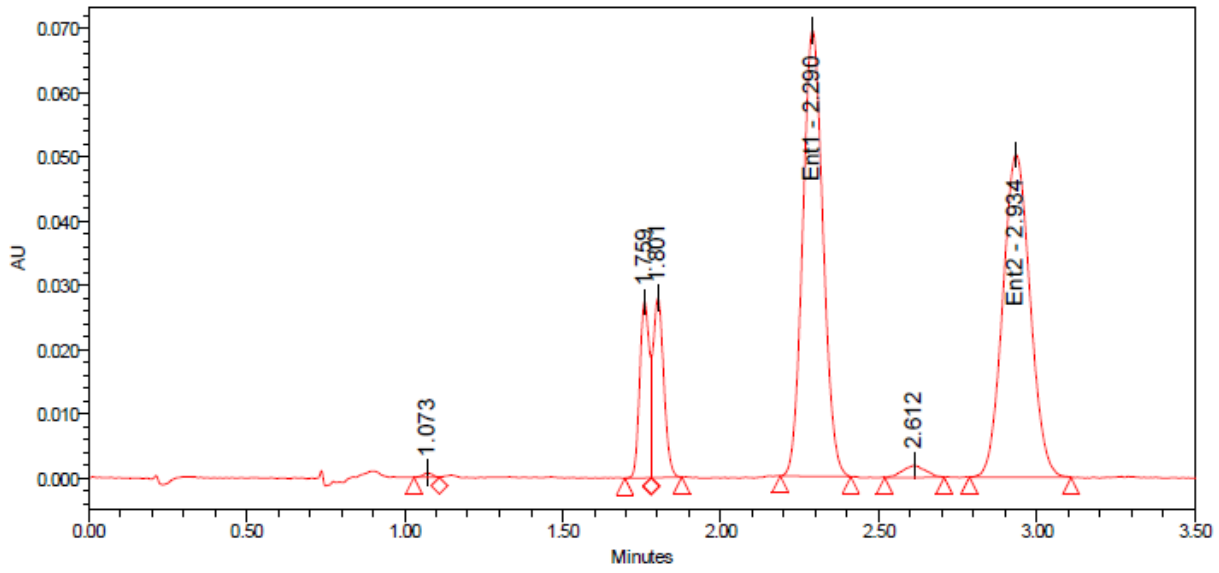
Peak Results

	Name	RT	Area
1		2.335	9677
2		2.711	83723


SN-D-16-II-1.1.fid
S3g
f1 (ppm)

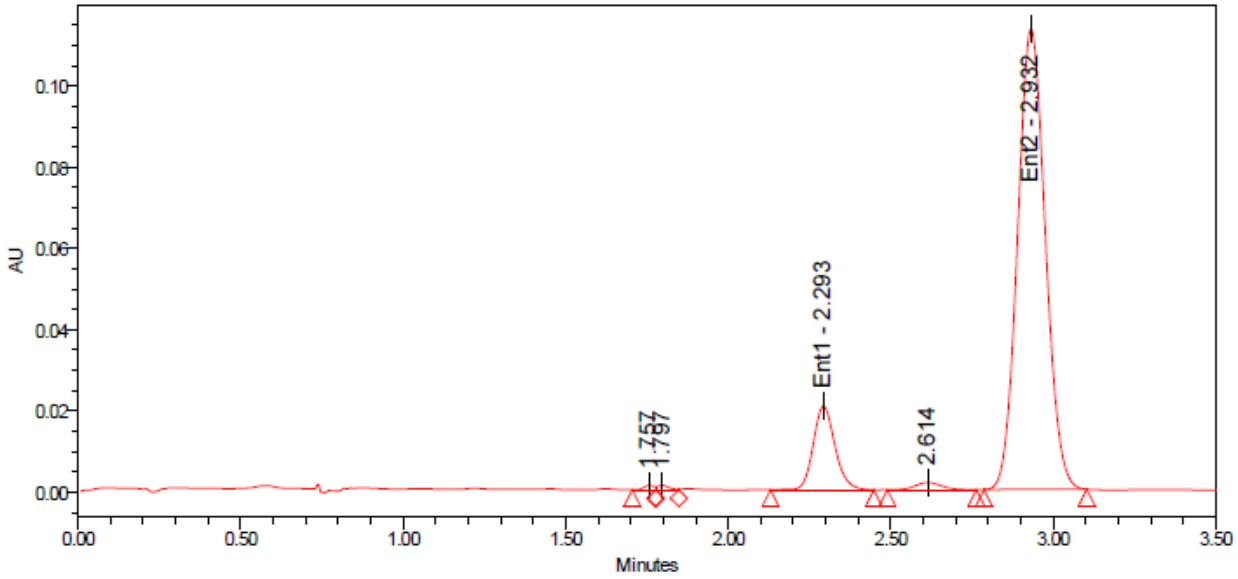

SN-D-16-II-1.11.fid
B (q)
123.21
A (q)
125.18
C (q)
132.75
S3g
f1 (ppm)


SN-D-16-II-1.21.fid
-63.19
S3g
f1 (ppm)



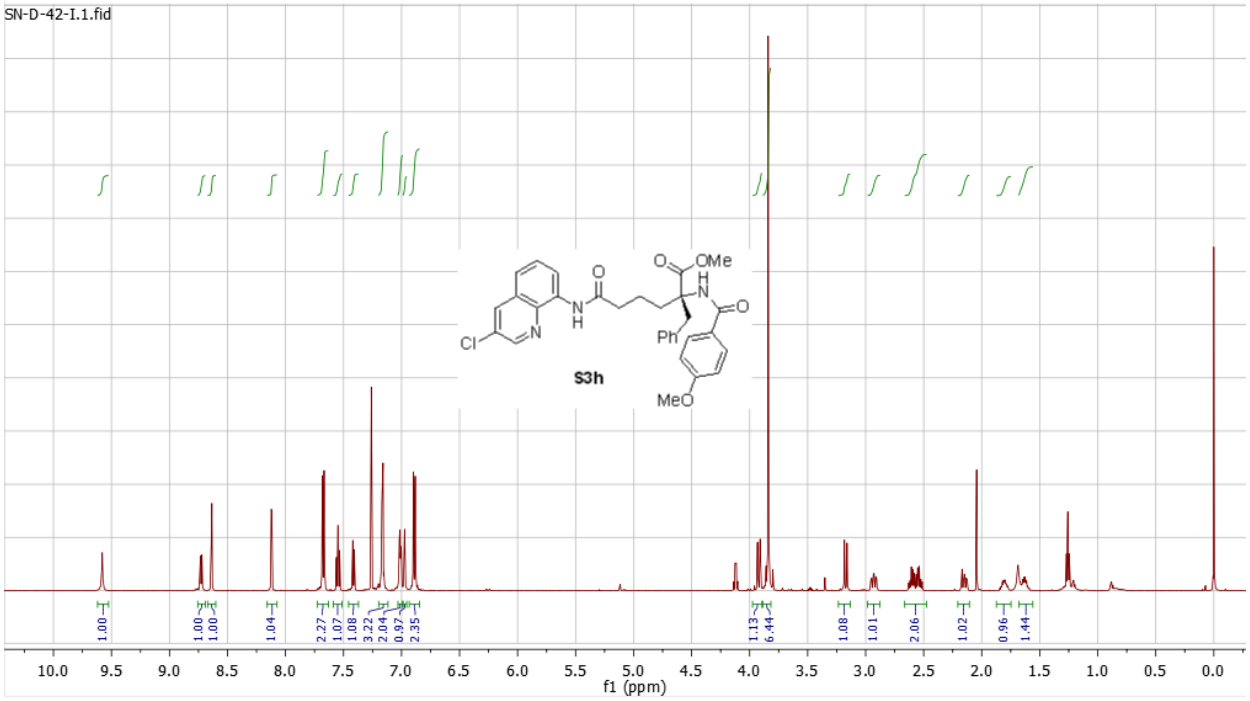
Area Summarized by Name

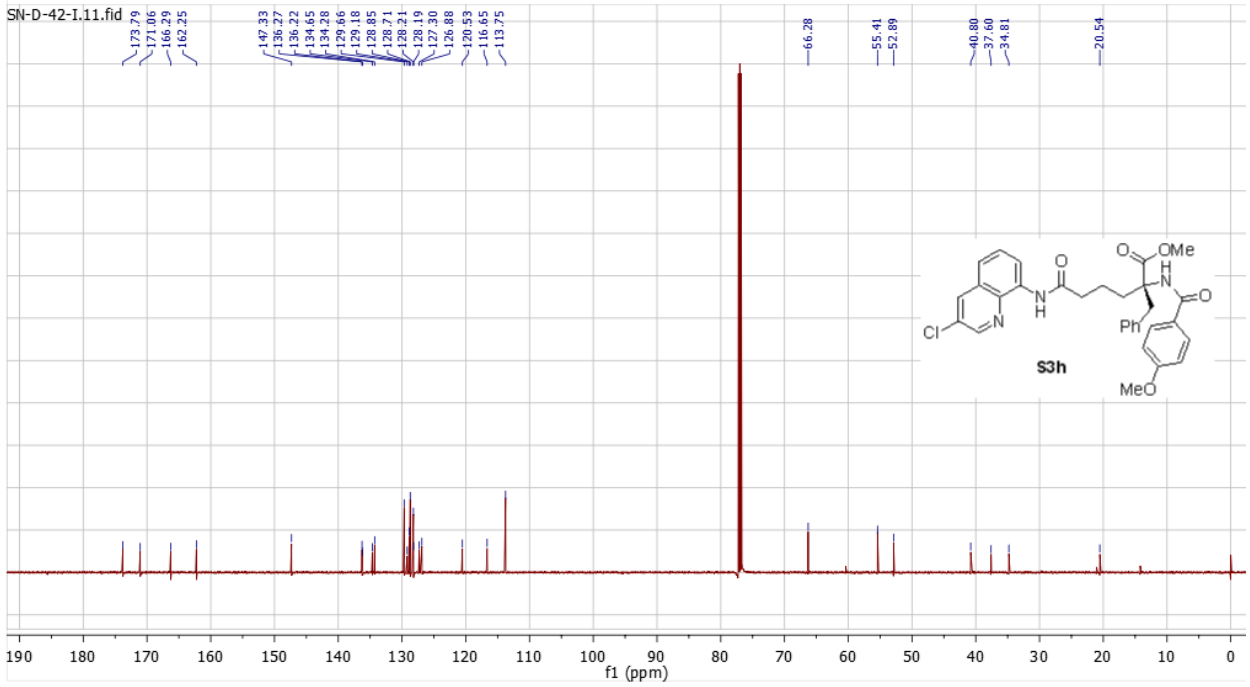
	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-D-16l_IC30%	50.54	49.46	1.08	309425	302819

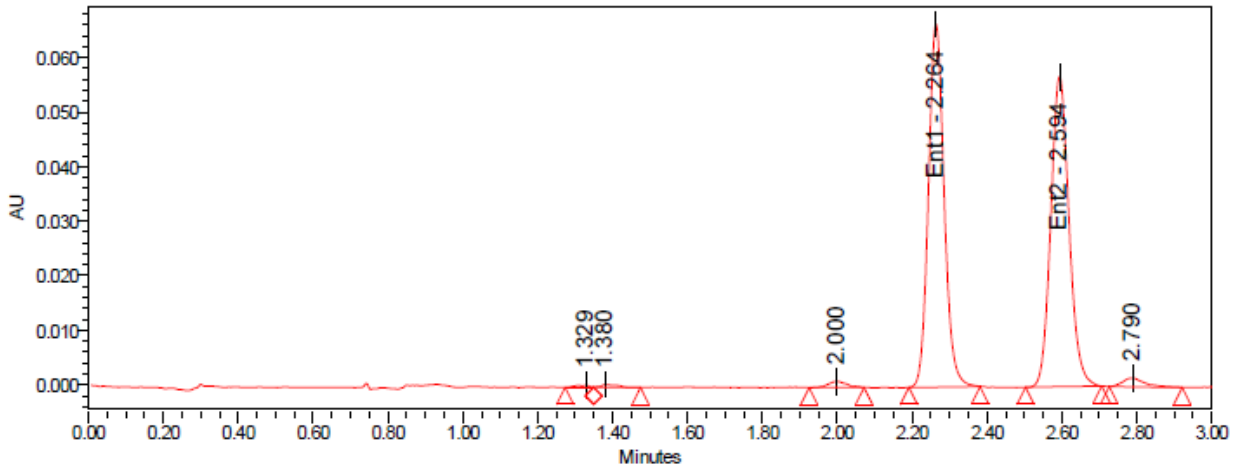


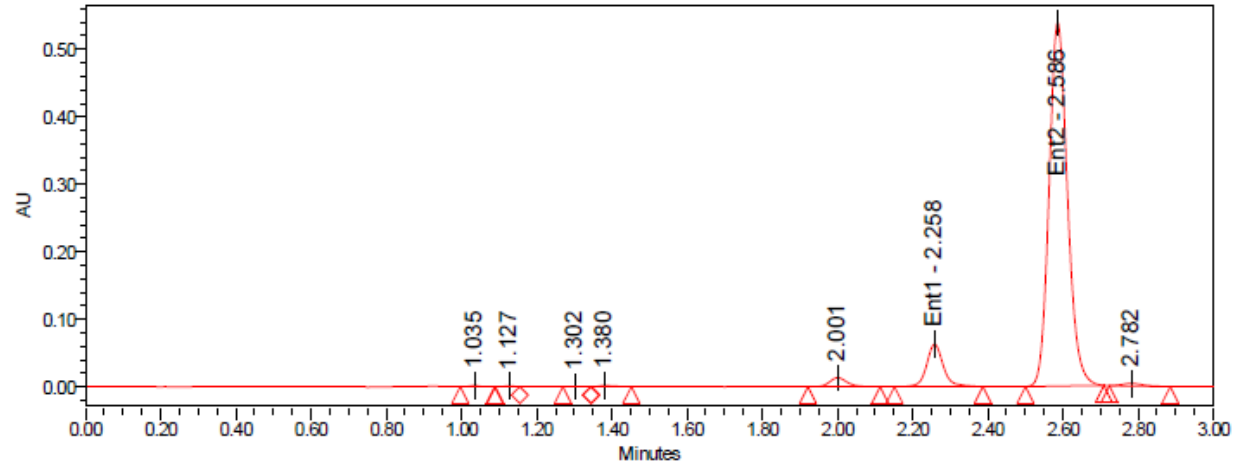
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-D-016II	12.44	87.56	-75.12	95450	671929

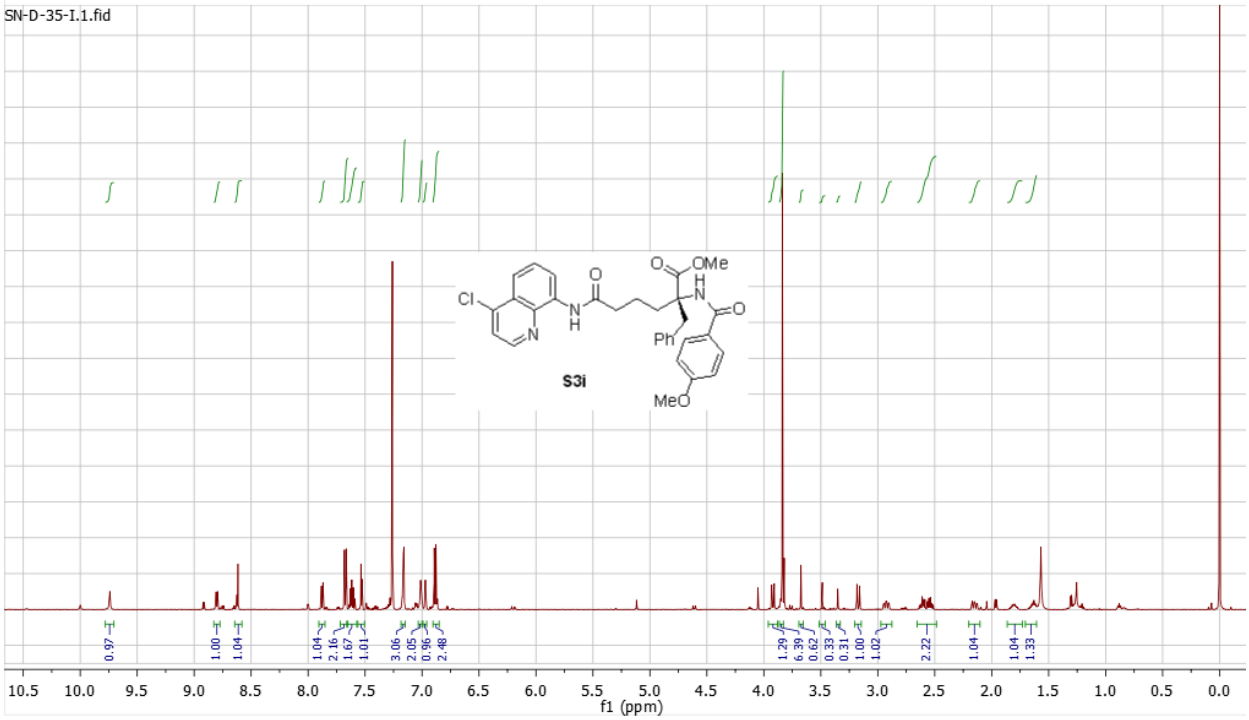

SN-D-42-I.1.fid
S3h
f1 (ppm)

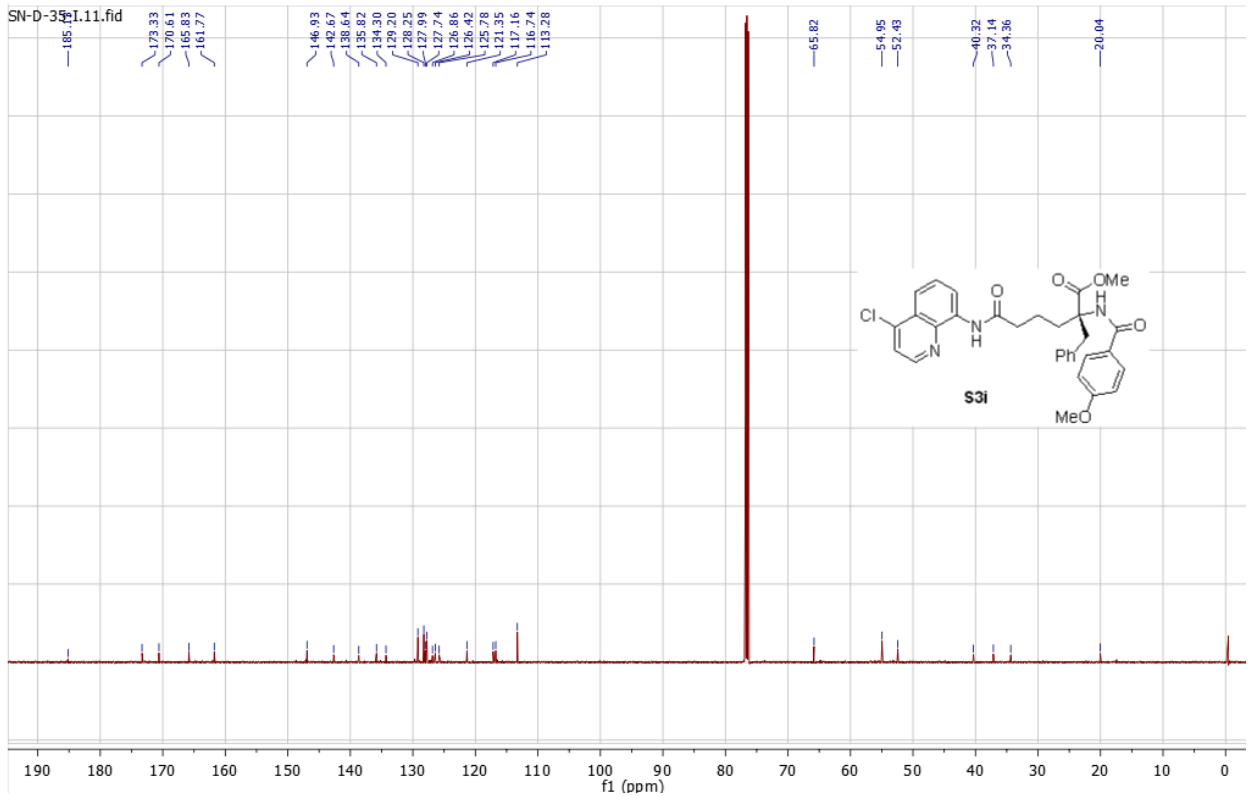

SN-D-42-I.11.fid
S3h
f1 (ppm)

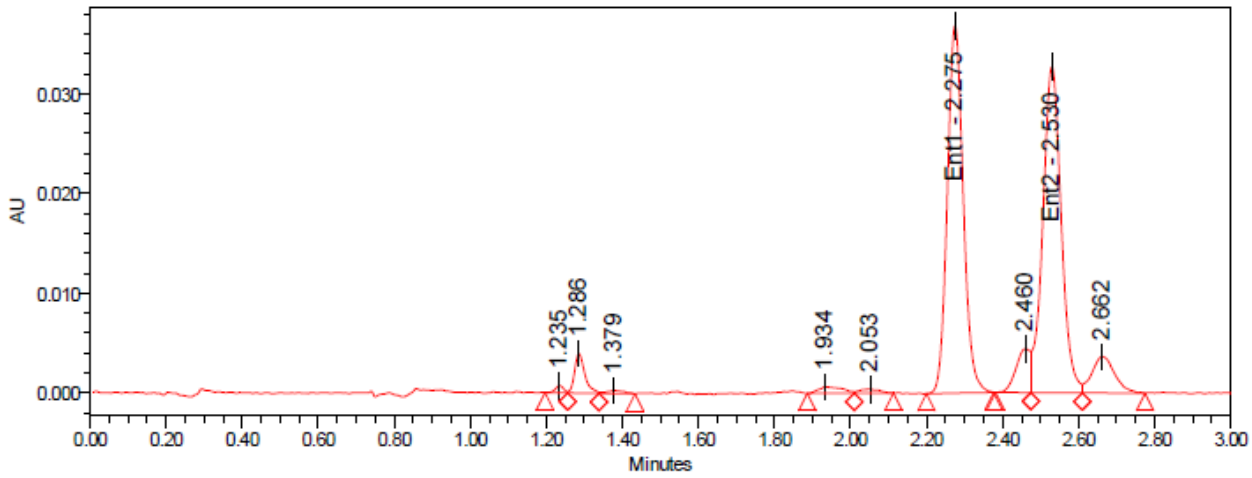


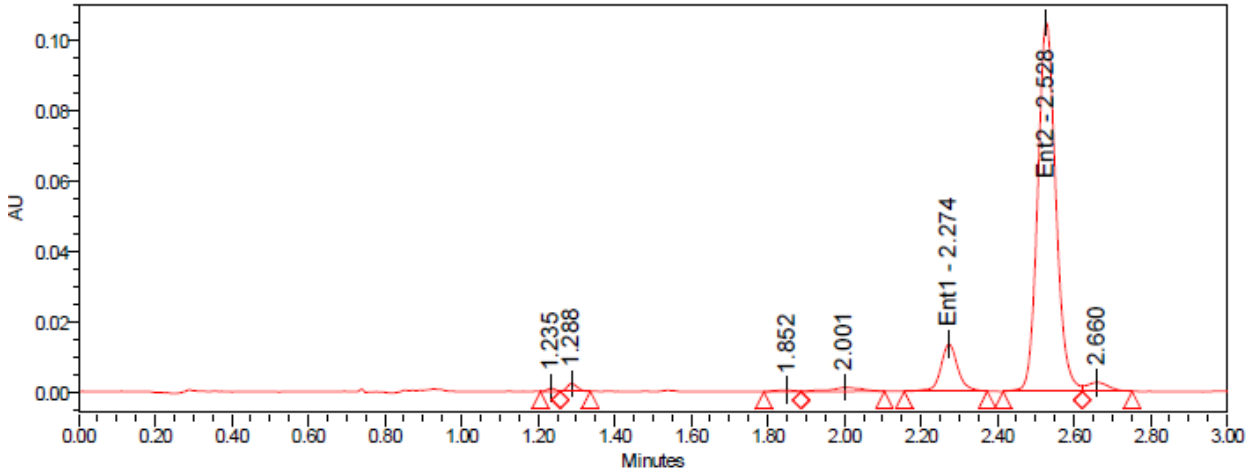


SampleName	ent1	ent2	ee	Ent1	Ent2
SN-D-42I	50.21	49.79	0.42	194124	192512
SN-D-42II	9.49	90.51	-81.02	191657	1828015

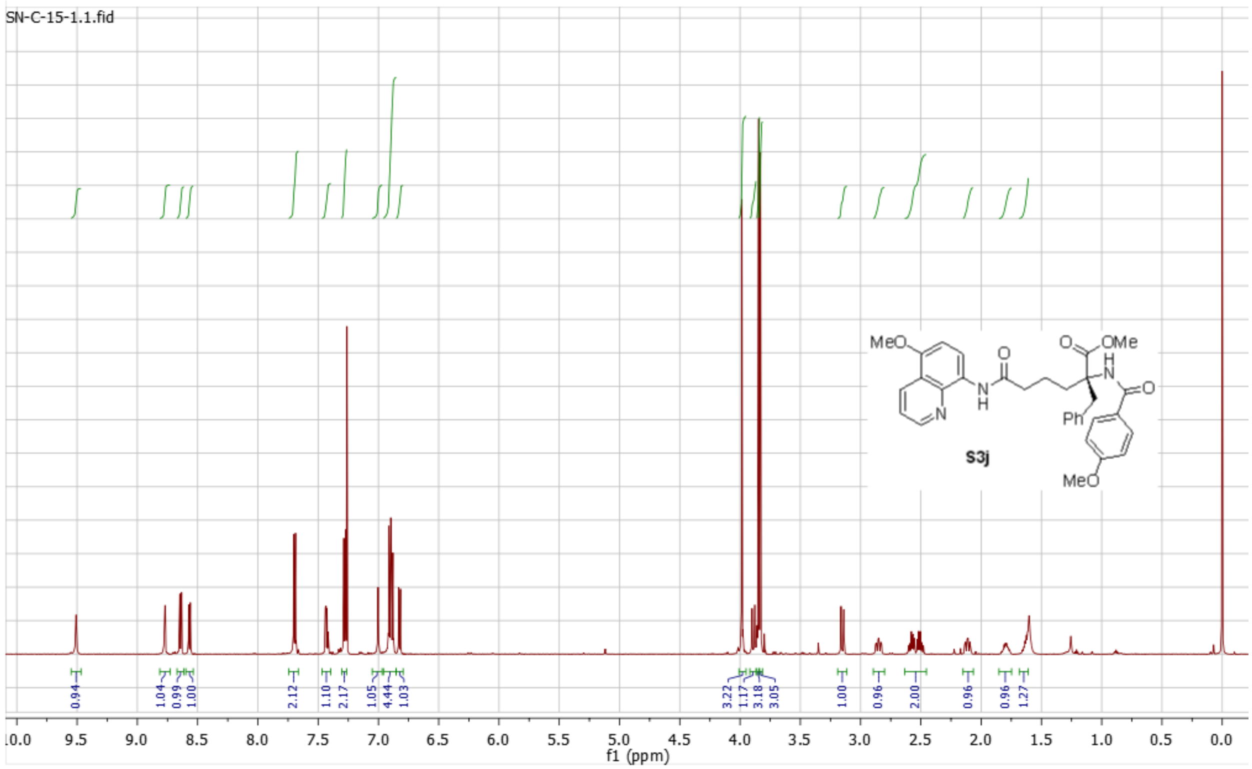

SN-D-35-I.1.fid
S3i
f1 (ppm)

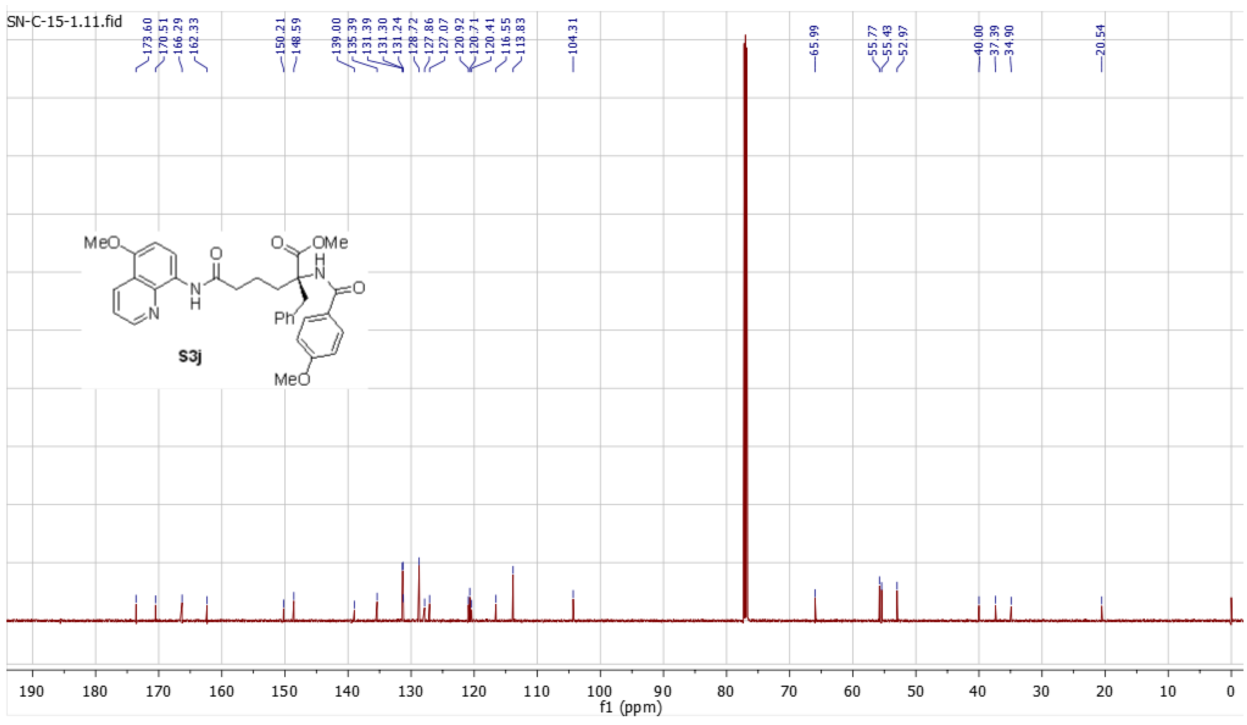

SN-D-35-I.11.fid
S3i
f1 (ppm)

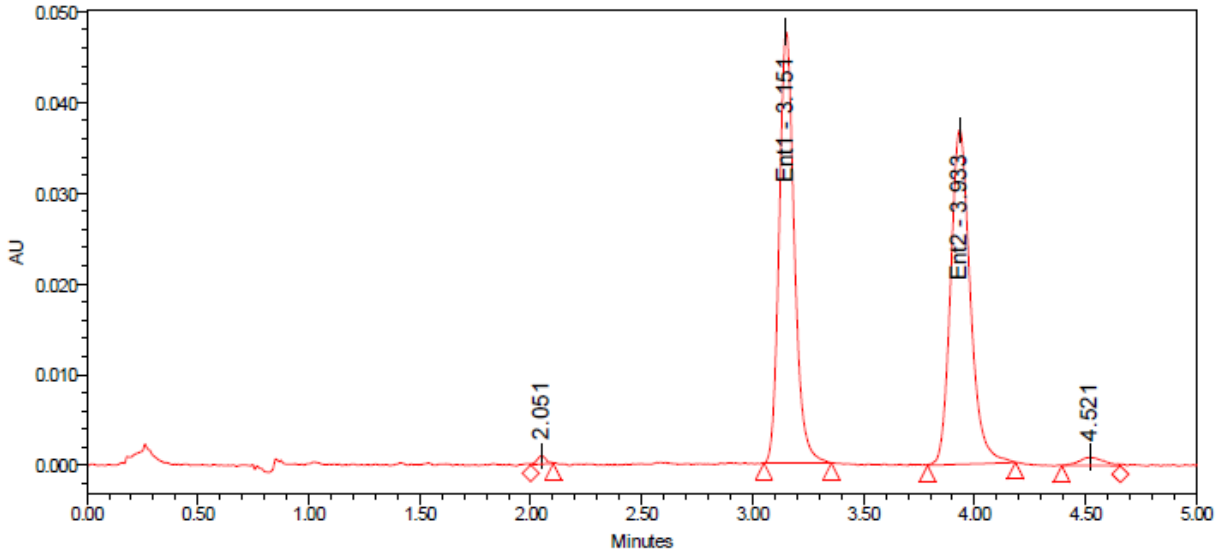


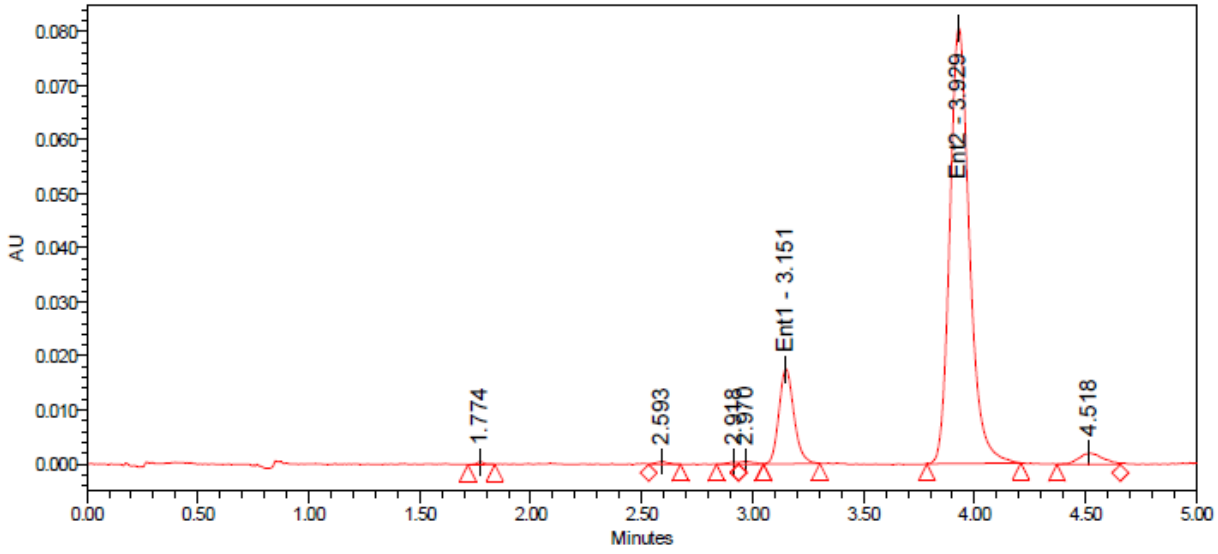


SampleName	ent1	ent2	ee	Ent1	Ent2
SN-D-35I	49.31	50.69	-1.37	107175	110153
SN-D-35II	10.66	89.34	-78.69	41230	345706


SN-C-15-1.1.fid
MeO
N
H
O
O
OMe
H
N
O
Ph
S3j
MeO
0.94
1.04
0.99
1.00
2.12
1.10
2.17
1.05
4.44
1.03
3.22
1.17
3.18
3.05
1.00
0.96
2.00
0.96
0.96
1.27
f1 (ppm)

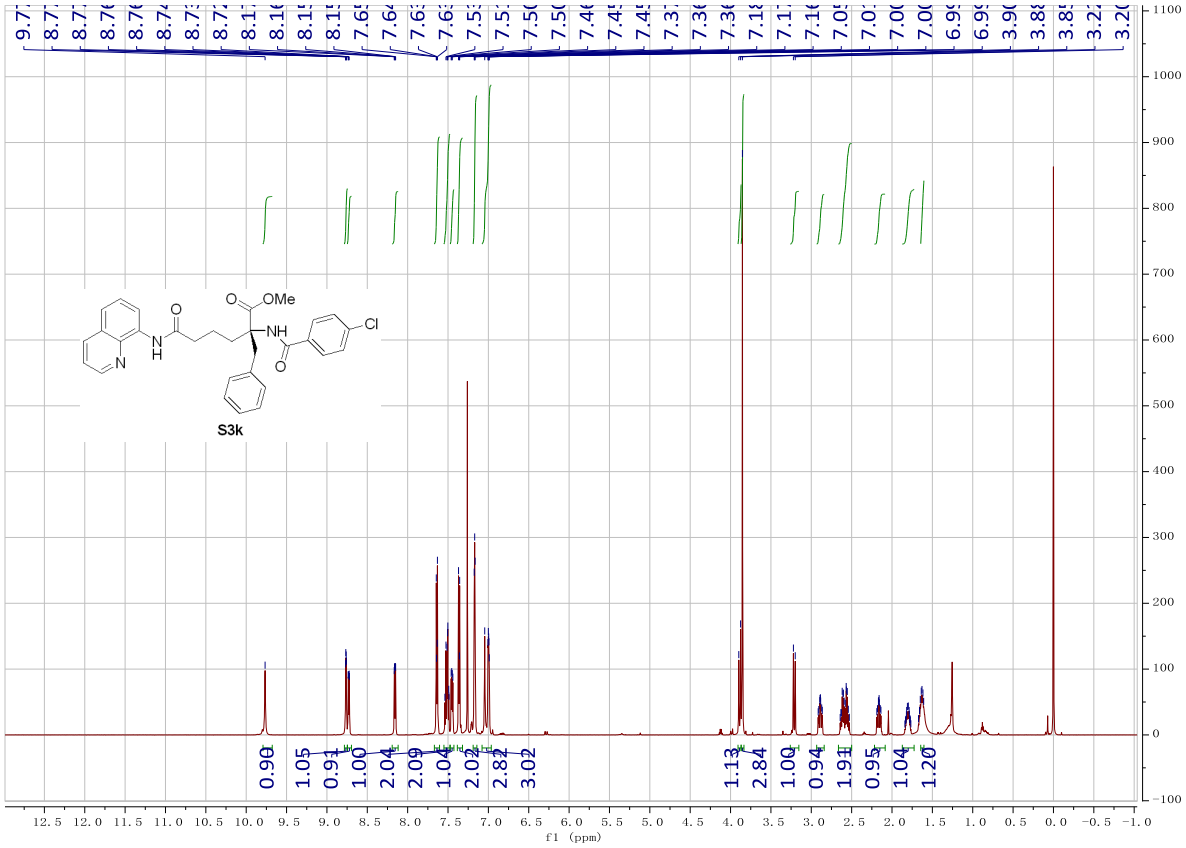

SN-C-15-1.11.fid
173.60
170.51
166.29
162.33
150.21
148.59
139.00
135.39
131.39
131.30
131.24
128.72
127.86
127.07
120.92
120.71
120.41
116.55
113.83
104.31
65.99
55.77
55.43
52.97
40.00
37.39
34.90
20.54
MeO
N
H
O
O
OMe
H
N
O
Ph
S3j
MeO
f1 (ppm)

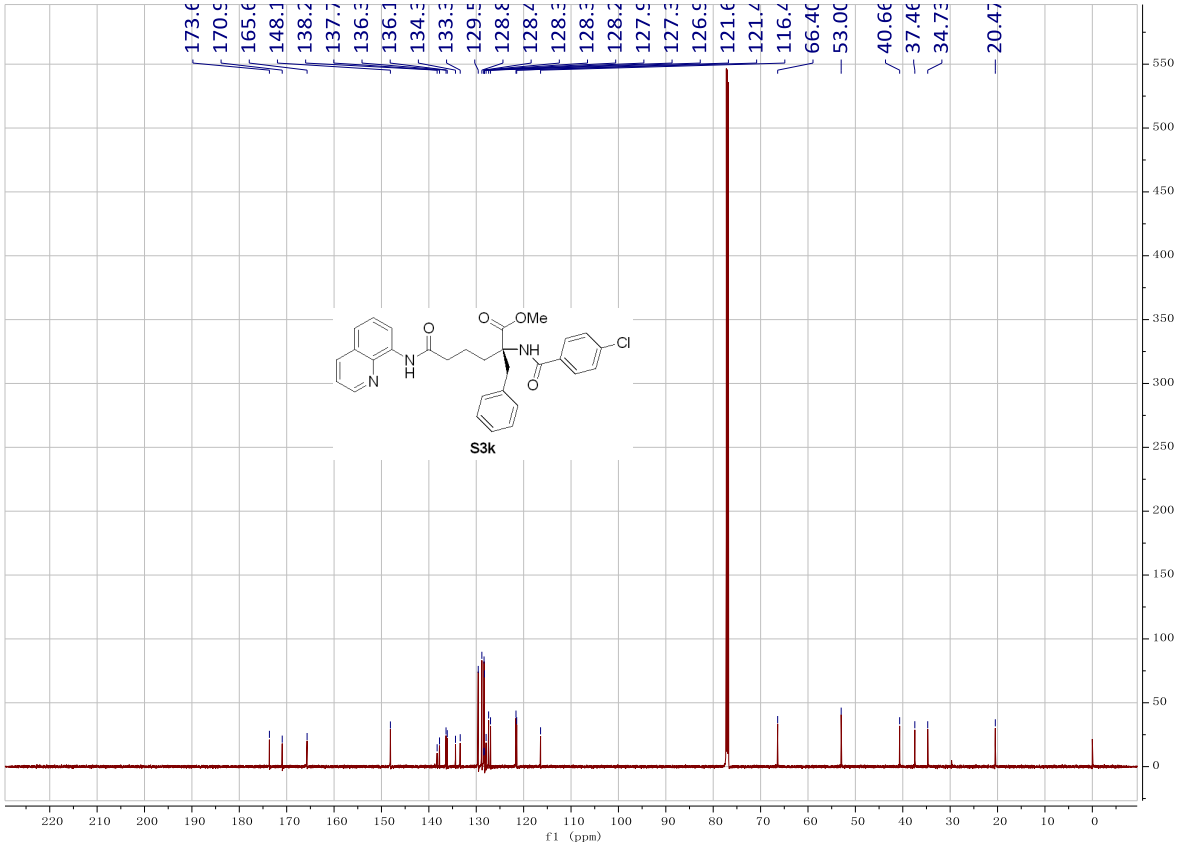


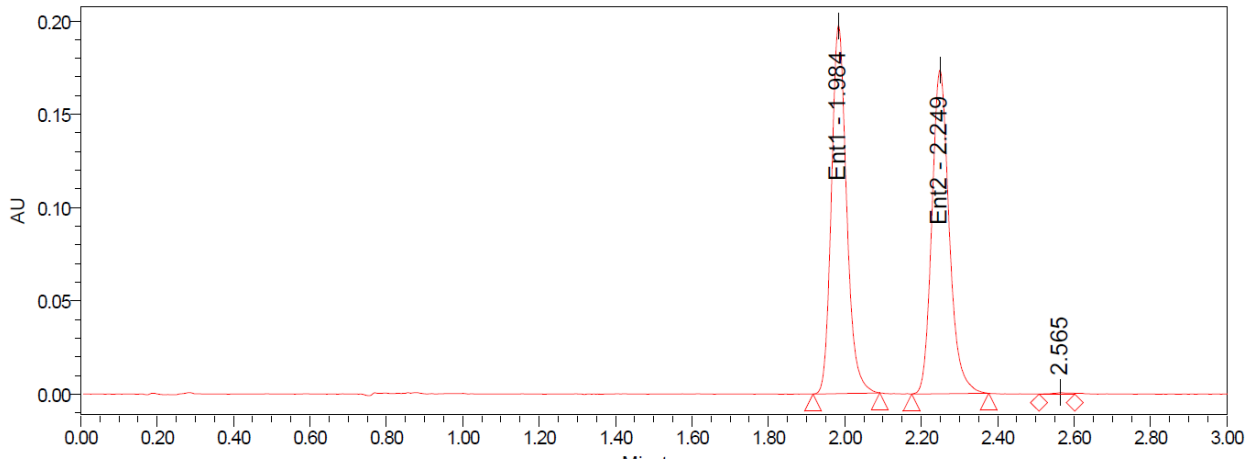


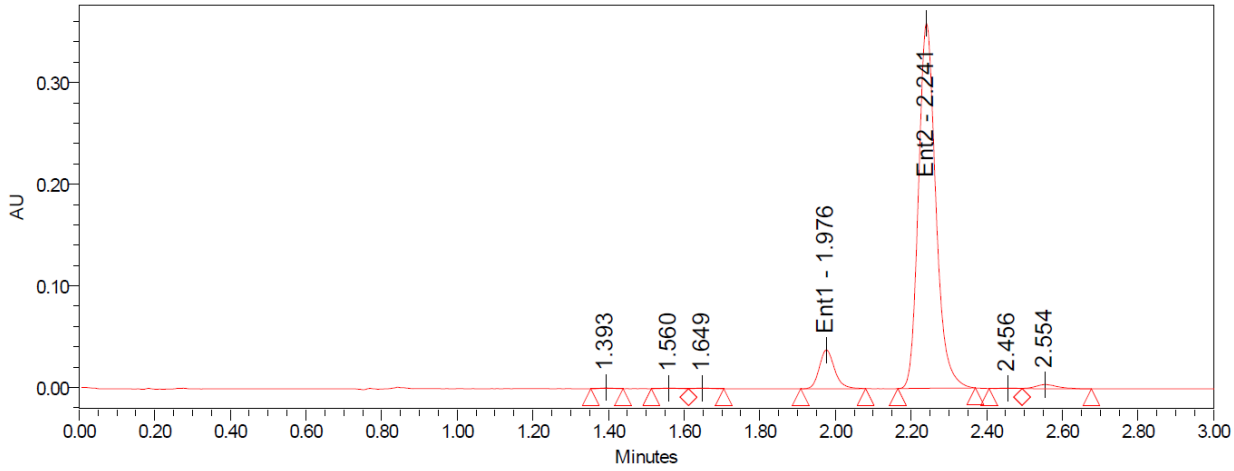
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-C-15I	49.82	50.18	-0.35	225752	227355
2	SN-C-15II	14.28	85.72	-71.43	82641	495905


S3k
f1 (ppm)


S3k
f1 (ppm)

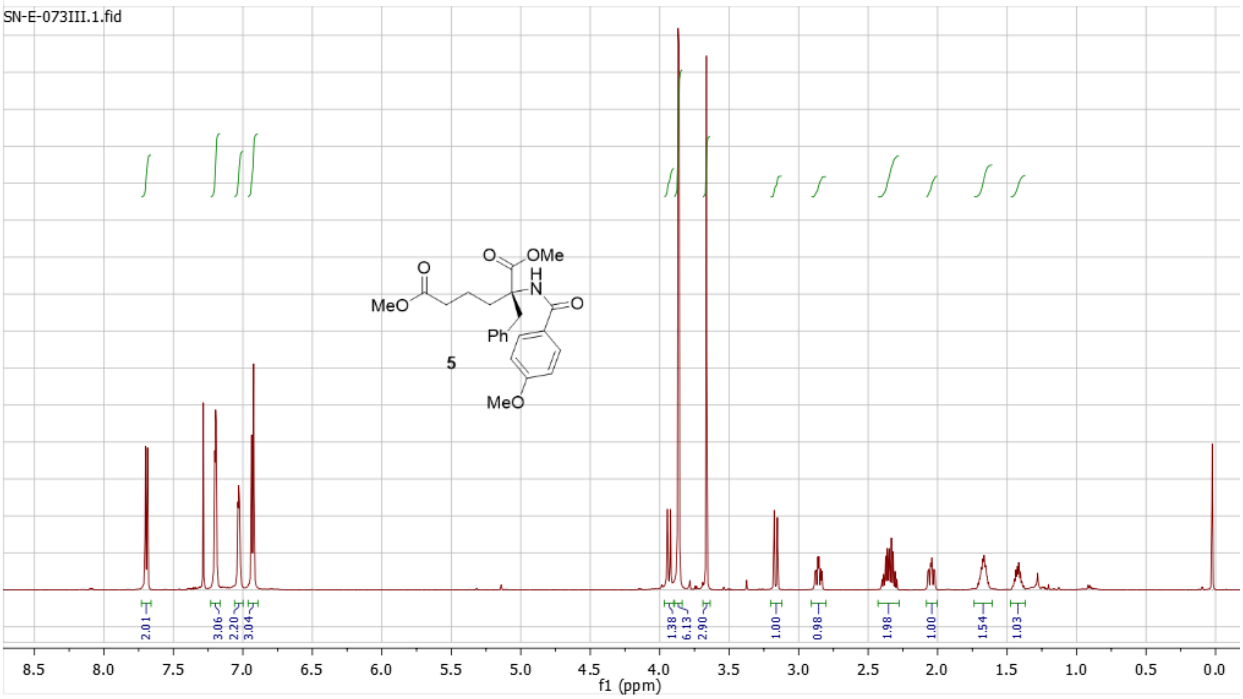


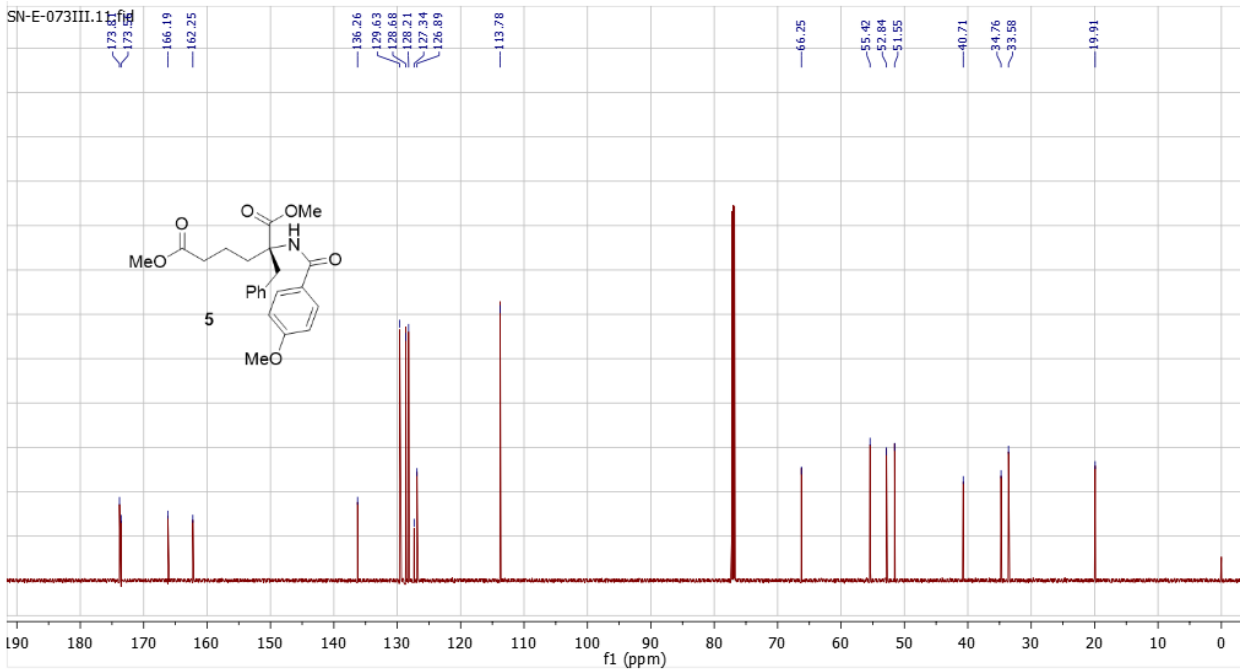


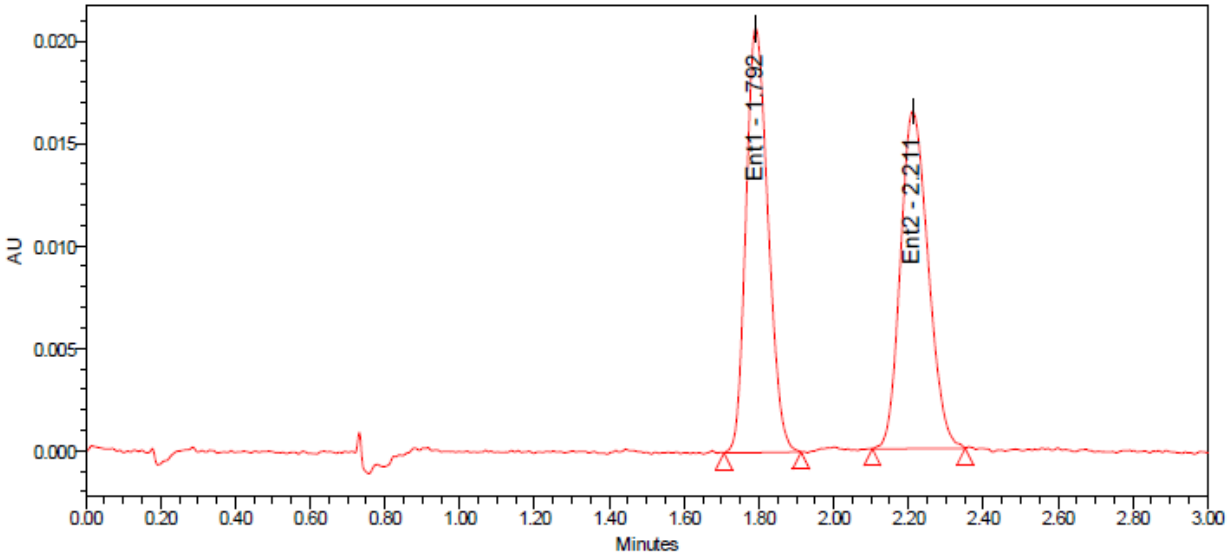
Area Summarized by Name

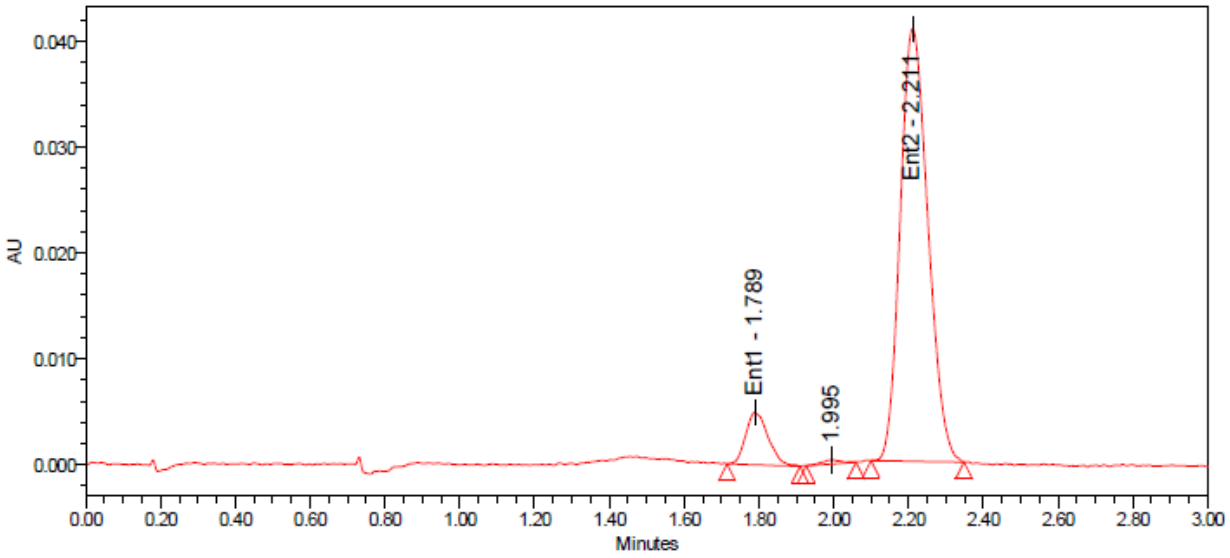
	SampleName	ent1	ent2	ee	Ent1	Ent2
1	MYL-Z-250	49.90	50.10	-0.21	545553	547843

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	MYL-E-257-1	8.53	91.47	-82.93	106577	1142272


SN-E-073III.1.fid
O
OMe
H
N
O
MeO
Ph
5
MeO
2.01
3.06
2.20
3.04
1.38
6.13
2.90
1.00
0.98
1.98
1.00
1.54
1.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

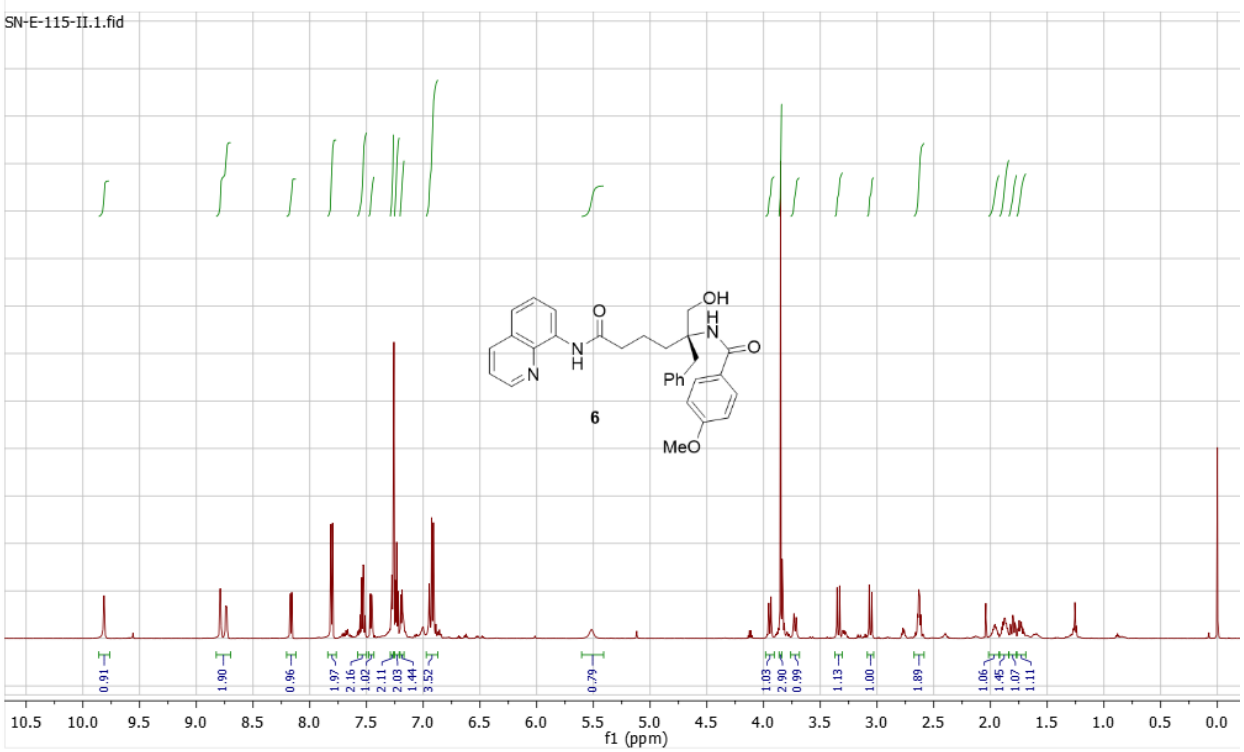

SN-E-073III.11.fid
173.58
166.19
162.25
136.26
129.63
128.68
128.21
127.34
126.89
113.78
66.25
55.42
52.84
51.55
40.71
34.76
33.58
19.91
O
OMe
H
N
O
MeO
Ph
5
MeO
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

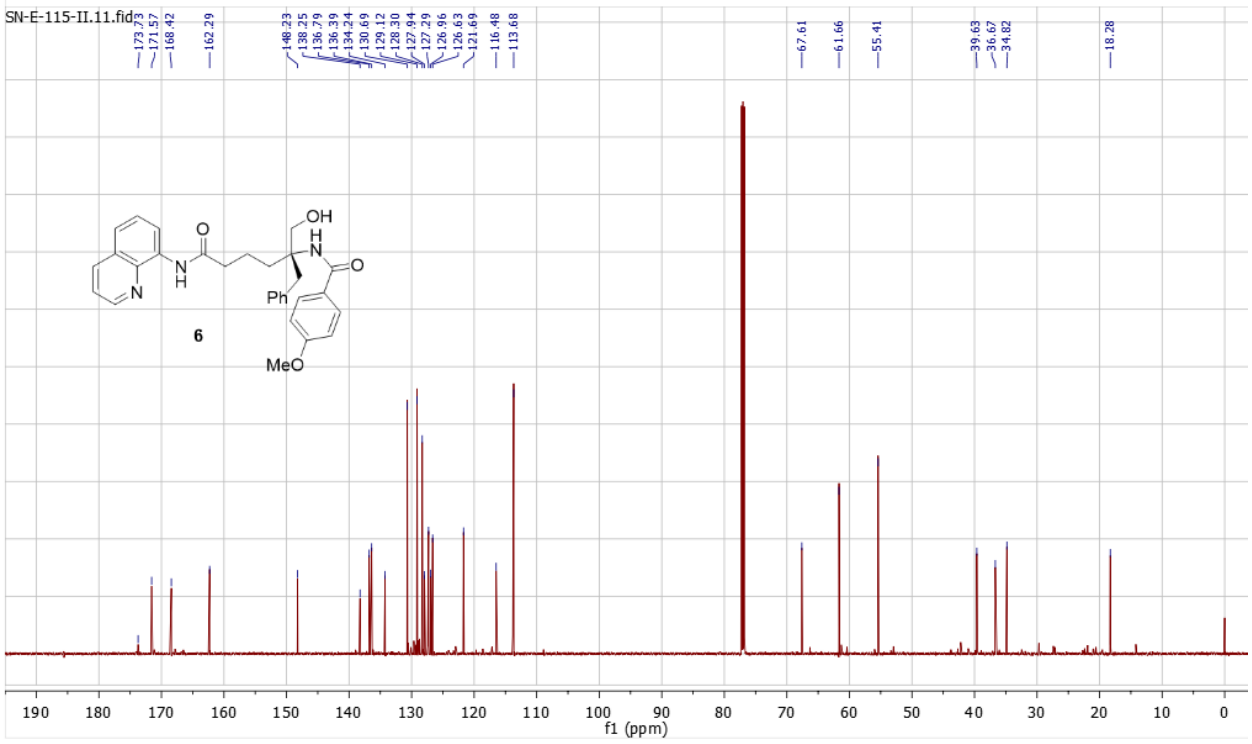


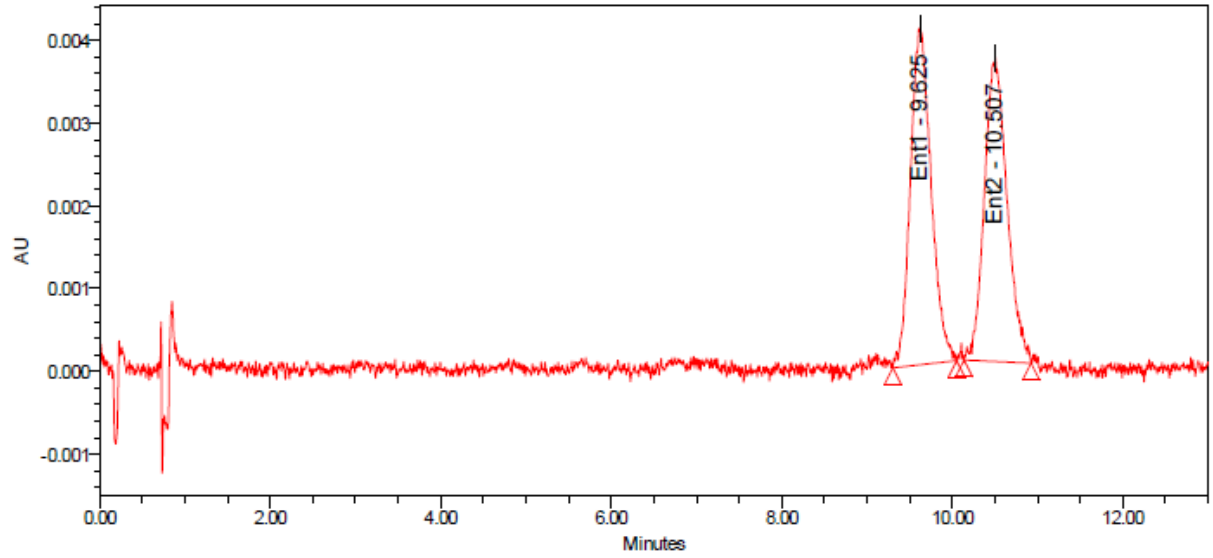


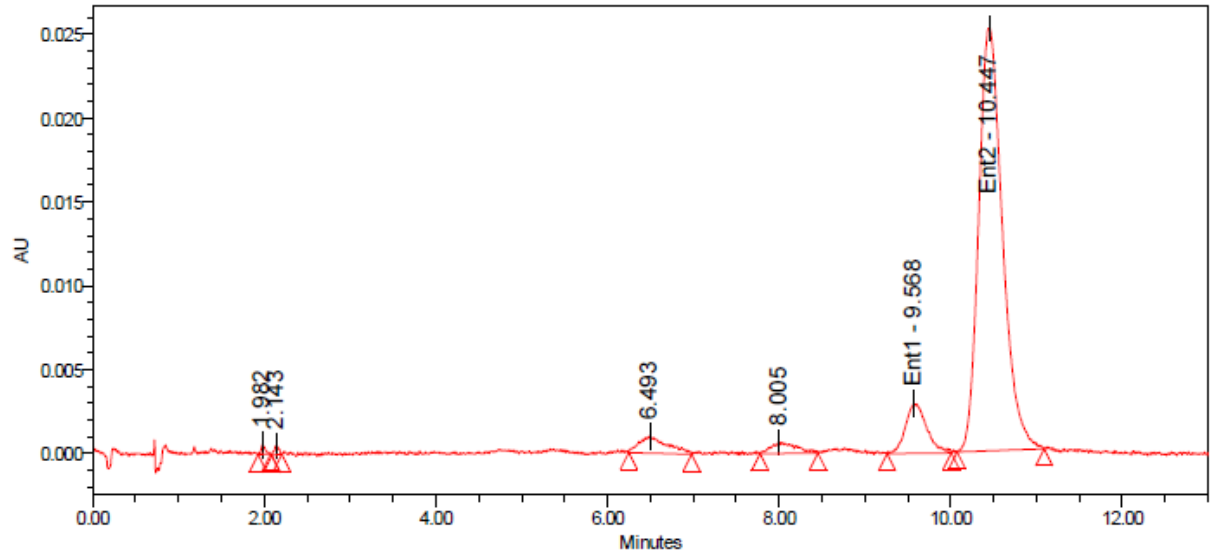
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-73I	50.02	49.98	0.05	85168	85083
2	SN-E-73III	8.92	91.08	-82.16	20637	210769


SN-E-115-II.1.fid
OH
H
N
O
N
H
O
N
Ph
MeO
6
0.91
1.90
0.96
1.97
2.16
1.02
2.11
2.03
1.44
3.52
0.79
1.03
2.90
0.99
1.13
1.00
1.89
1.06
1.45
1.07
1.11
10.5 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
f1 (ppm)

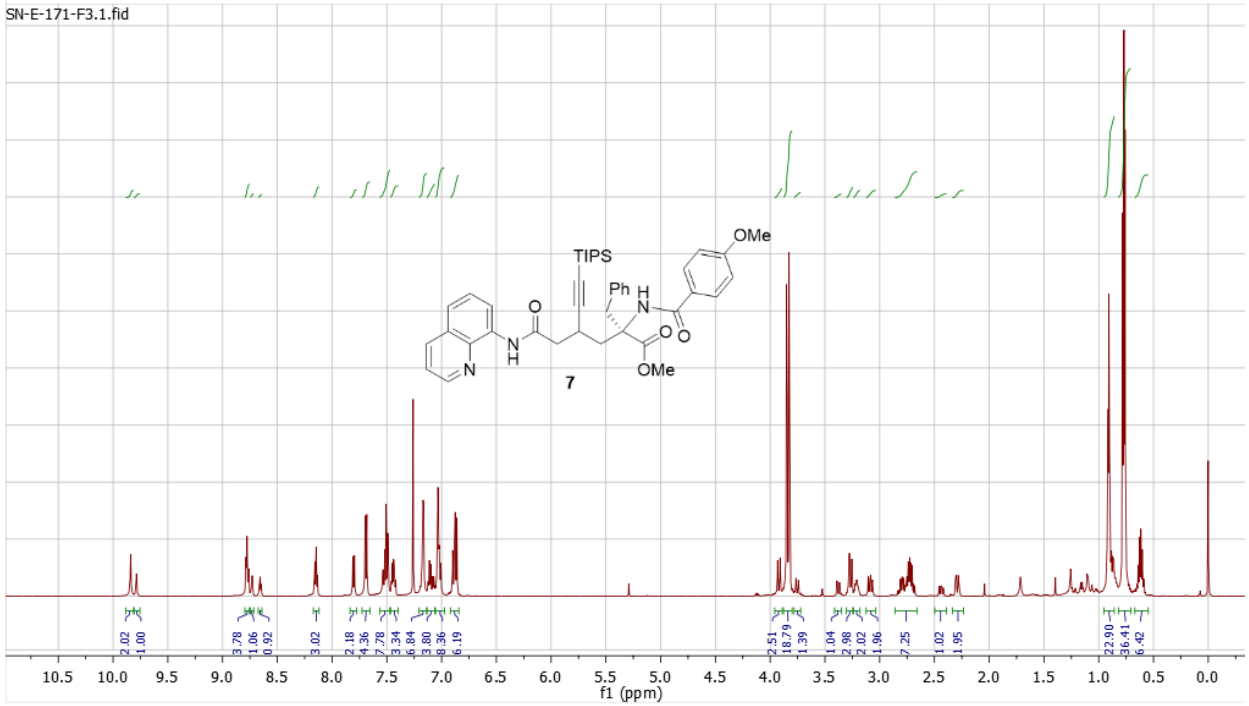

SN-E-115-II.11.fid
173.73
171.57
168.42
162.29
148.23
138.25
136.79
136.39
134.24
130.69
129.12
128.30
127.94
127.29
126.96
126.63
121.69
116.48
113.68
67.61
61.66
55.41
39.63
36.67
34.82
18.28
OH
H
N
O
N
H
O
N
Ph
MeO
6
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

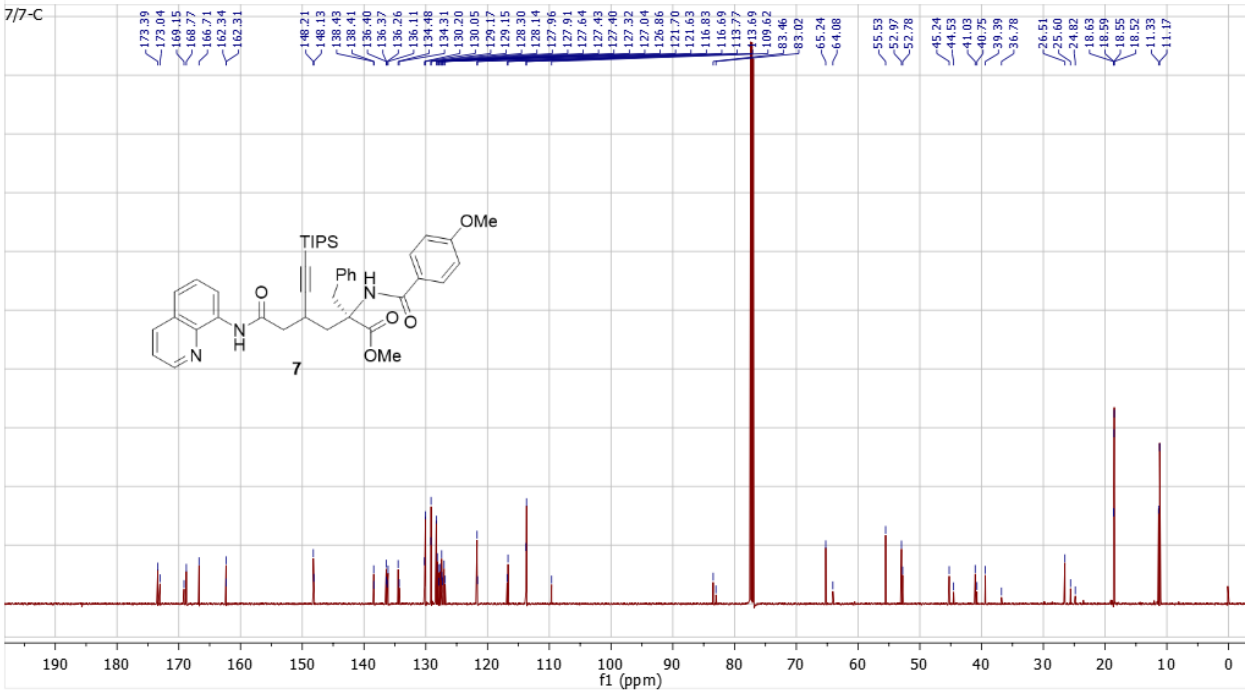


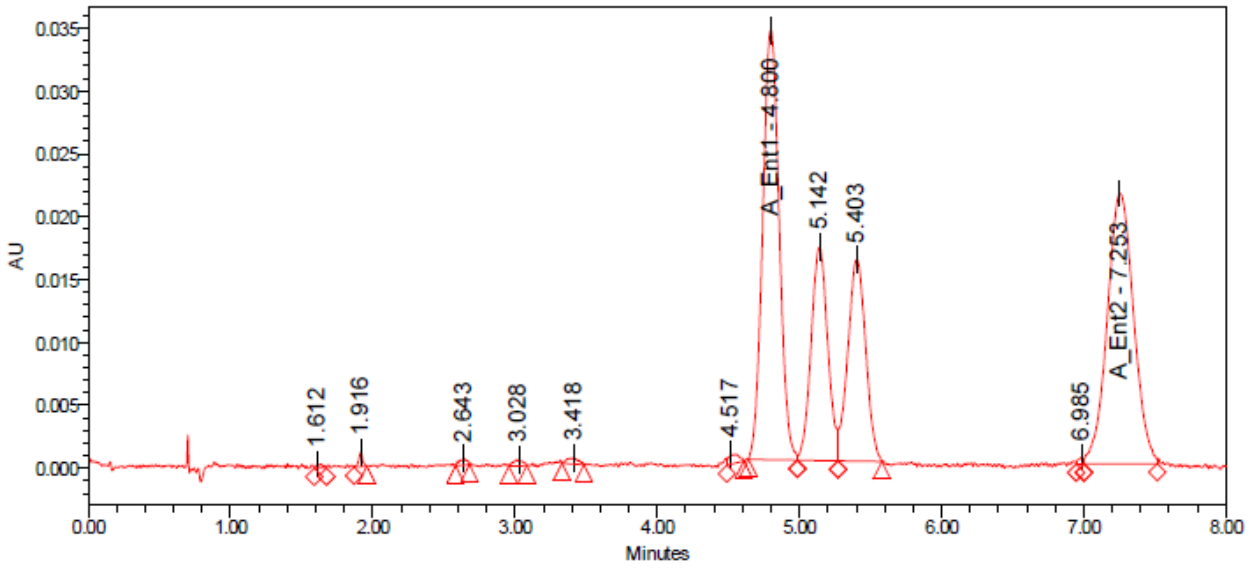


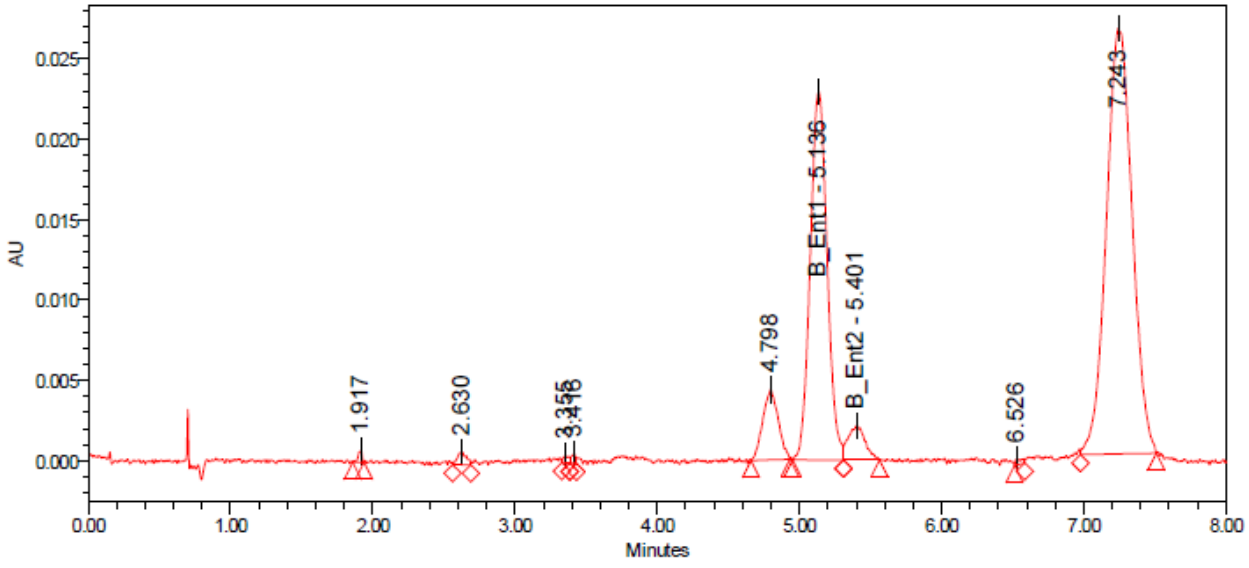
Area Summarized by Name

	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-115I-2	50.36	49.64	0.72	68667	67690
2	SN-E-115II	9.48	90.52	-81.04	50886	485900


SN-E-171-F3.1.fid
TIPS
Ph
H
N
OMe
O
O
N
H
N
O
OMe
7
f1 (ppm)

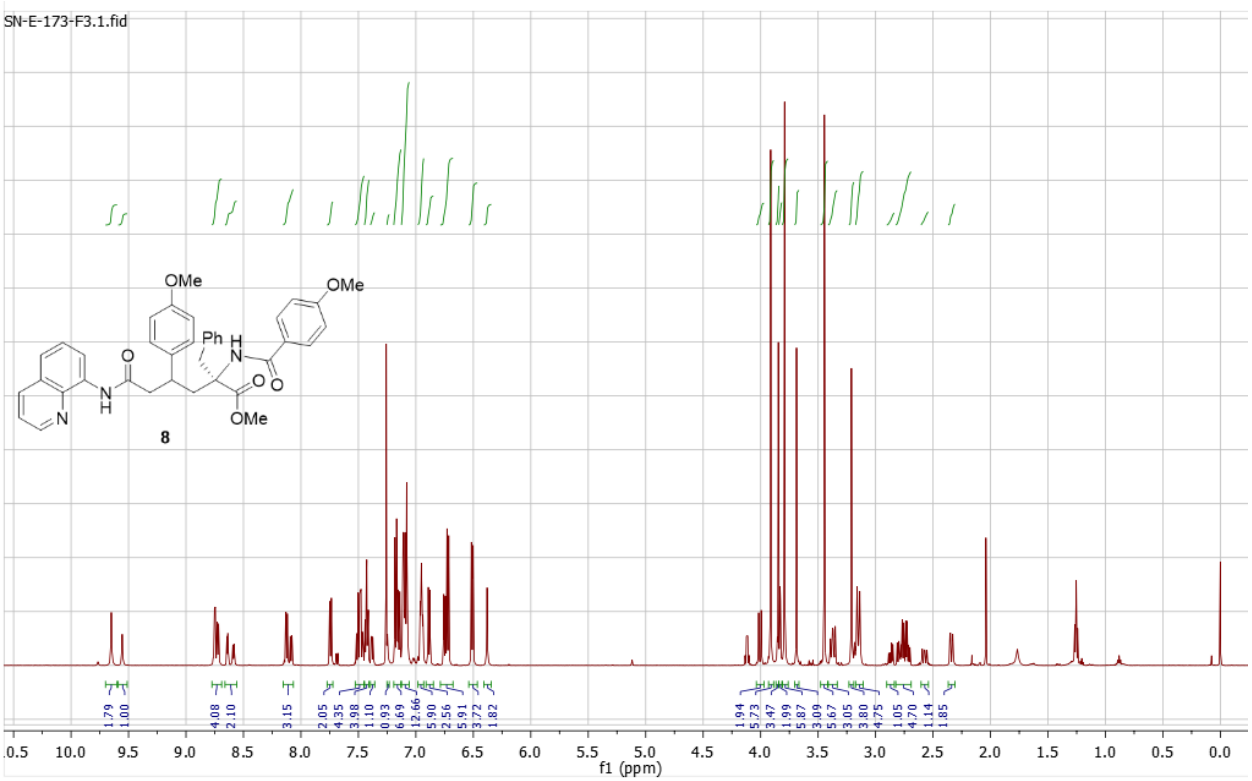

7/7-C
TIPS
Ph
H
N
OMe
O
O
N
H
N
O
OMe
7
f1 (ppm)

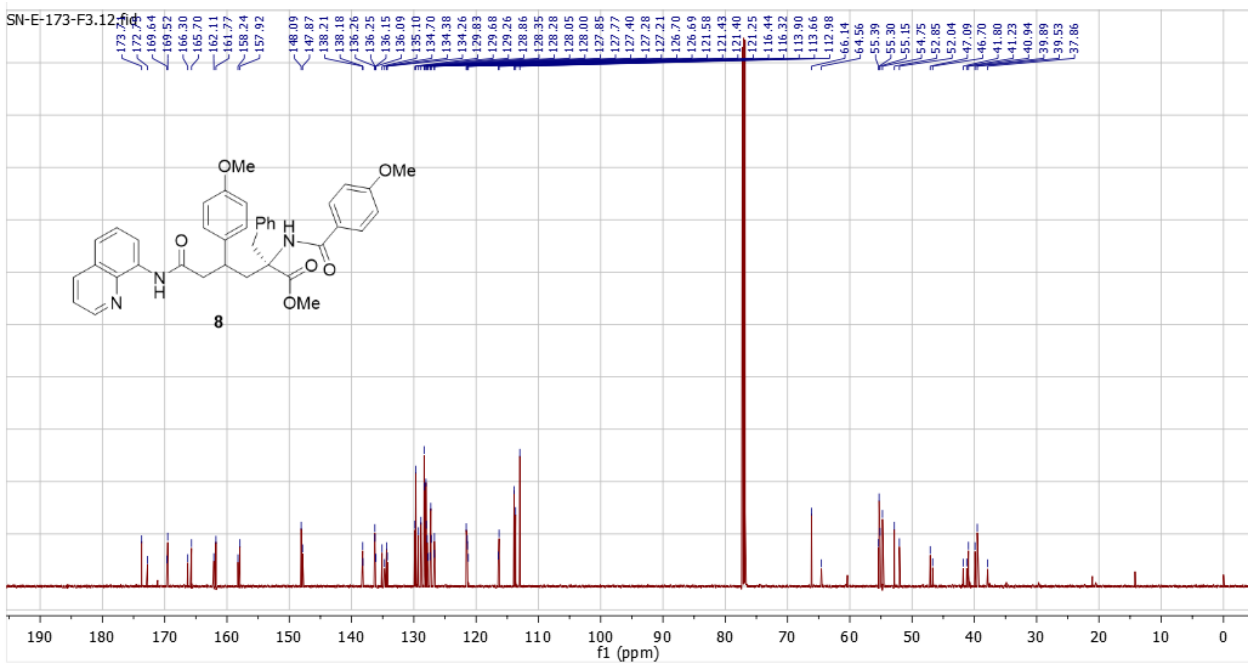


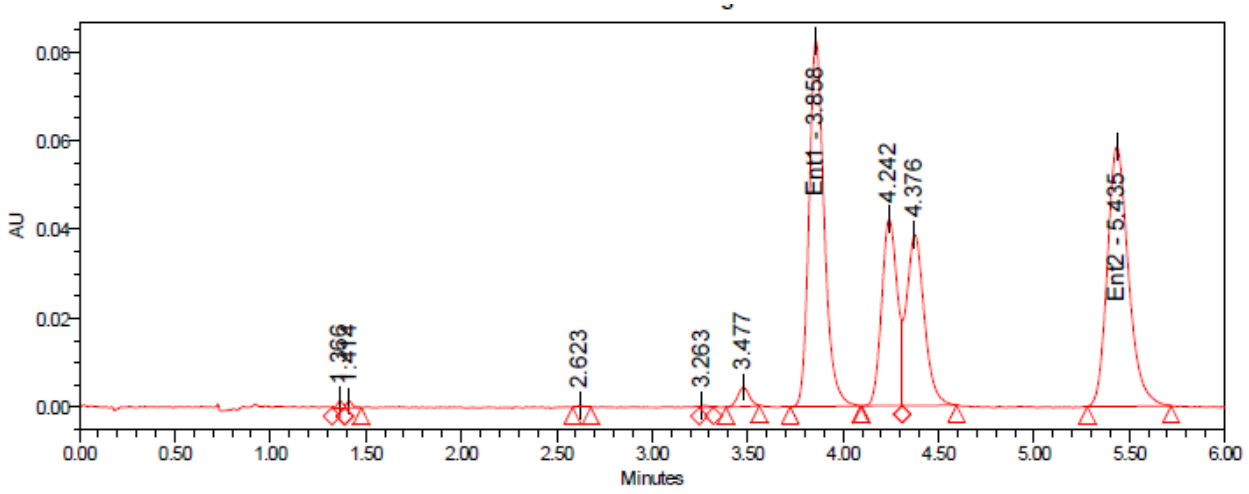


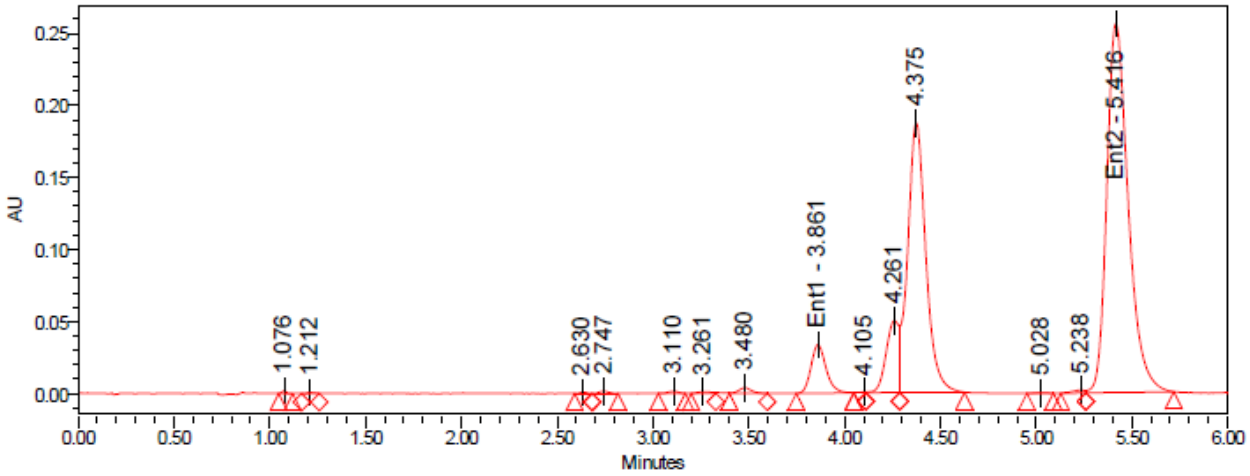
Area Summarized by Name

	SampleName	ent1	ent2	ee	A_Ent1	B_Ent1	B_Ent2	A_Ent2
1	SN-E-170F3	49.83	50.17	-0.35	274706			276619
2	SN-E-171F3	91.47	8.53	82.93		189352	17665	

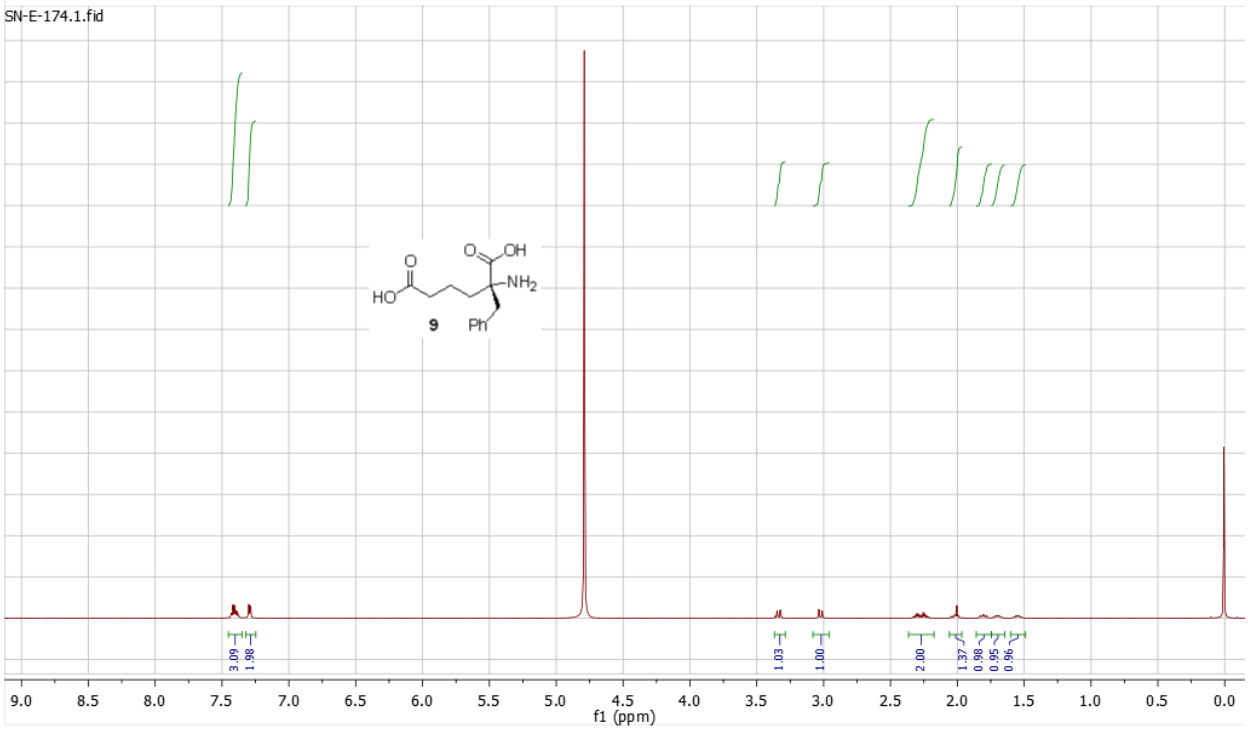

SN-E-173-F3.1.fid
OMe
OMe
Ph
H
N
O
O
O
N
H
N
OMe
8
1.79
1.00
4.08
2.10
3.15
2.05
4.35
3.98
1.10
0.93
6.69
12.66
5.90
2.56
5.91
3.72
1.82
1.94
5.73
3.47
1.99
5.87
3.09
5.67
3.05
3.80
4.75
1.05
4.70
1.14
1.85
f1 (ppm)

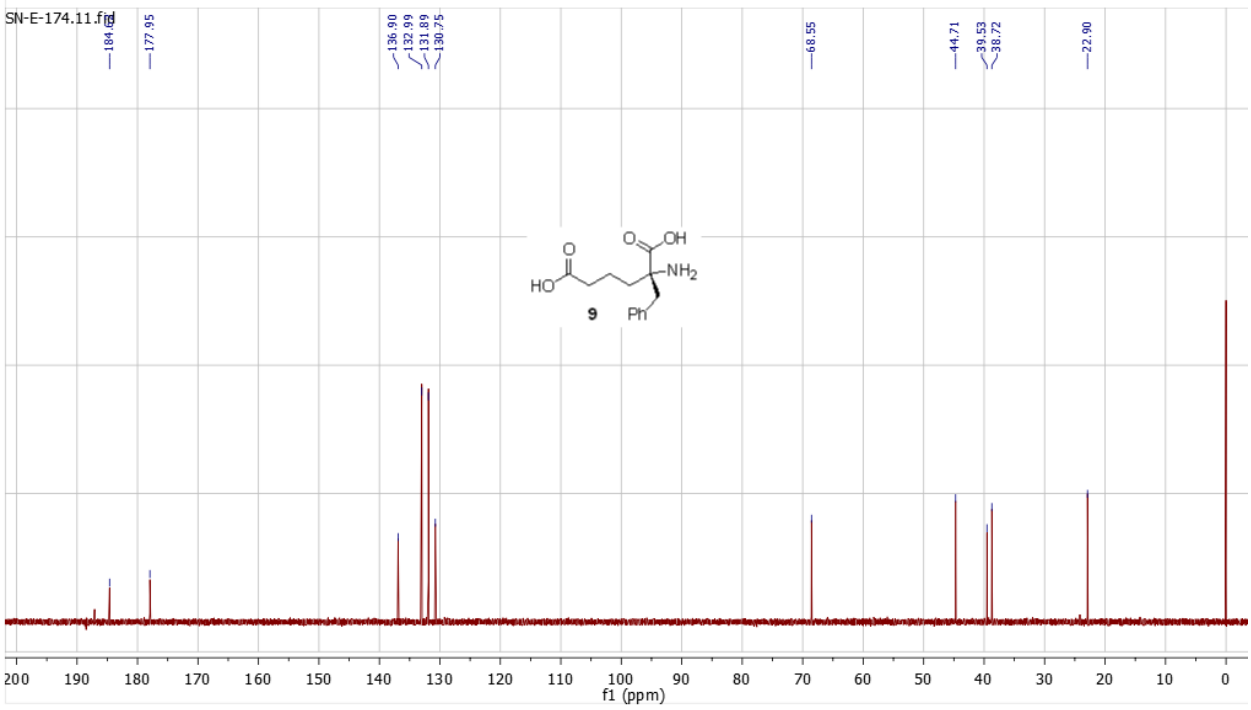

SN-E-173-F3.12.fid
OMe
OMe
Ph
H
N
O
O
O
N
H
N
OMe
8
f1 (ppm)





	SampleName	ent1	ent2	ee	Ent1	Ent2
1	SN-E-172-F3	50.22	49.78	0.45	453768	449723
2	SN-E-173-F3	8.46	91.54	-83.08	183946	1990148


SN-E-174.1.fid
O
OH
HO
NH2
9
Ph
3.09
1.98
1.03
1.00
2.00
1.37
0.98
0.95
0.96
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)


SN-E-174.11.fid
184.03
177.95
136.90
132.99
131.89
130.75
68.55
44.71
39.53
38.72
22.90
O
OH
HO
NH2
9
Ph
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)