Iron-catalyzed remote functionalization of inert C(sp^3)-H bonds of alkenes *via* 1,n-hydrogen-atom-transfer by C-centered radical relay

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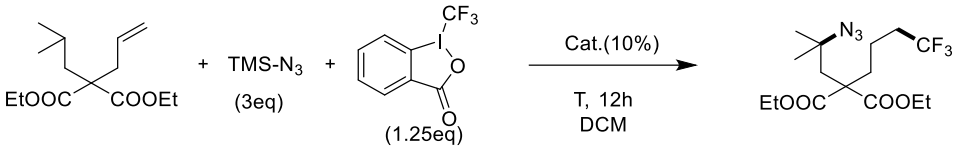
Contents

I. General Information

NMR spectra were recorded on Bruker-400 (400 MHz for ^{1}H; 101 MHz for ^{13}C and 376 MHz for ^{19}F instruments internally referenced to $SiMe_4$ signal for ^{1}H, and $CDCl_3$ for ^{13}C (note: some of the NMR spectra were recorded on Bruker-500 (500 MHz for ^{1}H; 126 MHz for ^{13}C and 471 MHz for ^{19}F). High resolution mass spectra were recorded on P-SIMS-Gly of Bruker Daltonics Inc. using ESI-TOF (electrospray ionization-time of flight) or Micromass GCT using EI (electron impact). Cu salts, Fe salts, $TMSN_3$, and superdry solvent were obtained from J&K, STREM (high quality>99%) and used as received. Togni-II reagent[1] and BIOH[2] was synthesized according to reported method.

II. Optimization of Conditions

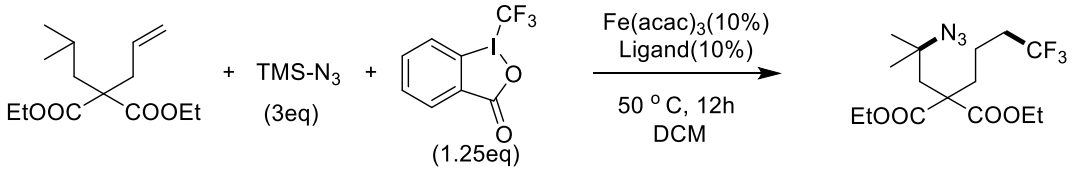
Optimization of Reaction Condition (Catalyst)

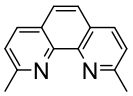
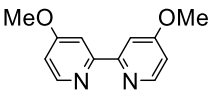
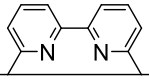


Entry	Cat.	T	solvent	Yield (%)[a]	Entry	Cat.	T	solvent	Yield (%)[a]
1	$FeCl_2$	50	DCM	42	9	$Fe(acac)_3$	60	DCM	71
2	$Fe(OTf)_2$	50	DCM	18	10	FeF_2	50	DCM	72
3	$FeCp_2$	50	DCM	27	11	$CoCl_2$	50	DCM	21
4	$Fe(BF_4)_2$ $6H_2O$	50	DCM	20	12	NiI_2	50	DCM	20
5	$Fe(OAc)_2$	50	DCM	50	13	$MnBr_2$	50	DCM	trace
6	$Fe_2(SO_4)_3$ xH_2O	50	DCM	57	14[d]	CuTc	30	DCM/1,4-dioxane	30
7	$Fe(acac)_3$	50	DCM	84[b] (82)[c]	15[e]	CuI	45	DCE	45
8	$Fe(acac)_3$	40	DCM	73	16[f]	CuI	80	DCM/1,4-dioxane	40

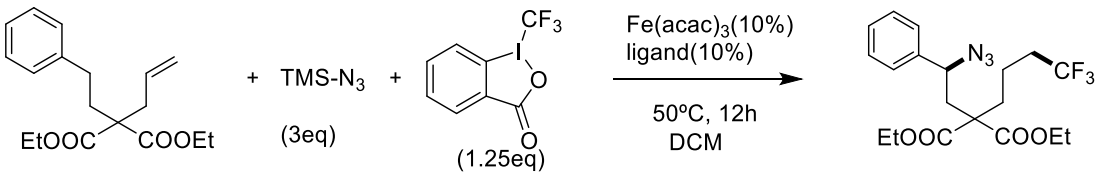
[a] yield was determined by ^1H NMR with CH_2Br_2 as internal standard. [b] 1,6: 1,2> 139:1. [c] the isolated yield. [d] 1,6: 1,2> 5:1. [e] Liu's conditions: 1,6:1,2 = 4.5:1. [f] Sodeoka's conditions: 1,6:1,2 = 4:1.

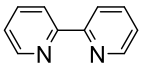
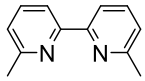
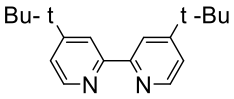
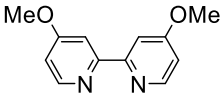
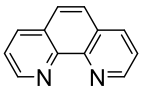
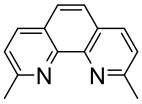
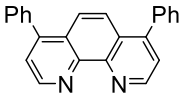
Optimization of Reaction Condition (Ligand)



Entry	Ligand(10%)	T	Conc. (M)	Yield (%)[a]
1		50	0.1	75 (1,6:1,2= 9:1)
2		50	0.1	79 (1,6: 1,2= 10:1)
3		50	0.1	72 (1,6: 1,2= 8:1)

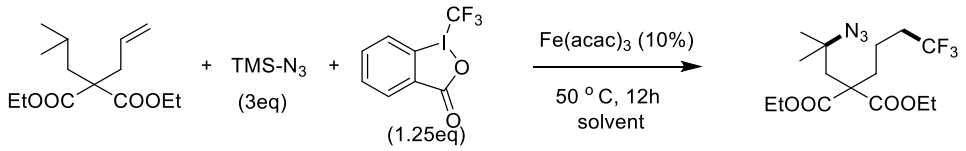
[a] yield was determined by ^1H NMR with CH_2Br_2 as internal standard.



Entry	Ligand(10%)	T	Conc. (M)	Yield (%)[a]
4		50	0.1	76
5		50	0.1	72
6		50	0.1	64
7		50	0.1	68
8		50	0.1	72
9		50	0.1	68
10		50	0.1	68

[a] yield was determined by ^{1}H NMR with CH_2Br_2 as internal standard.

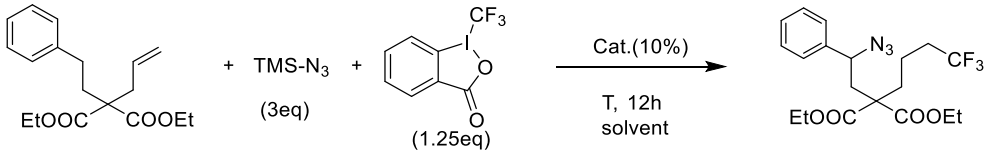
Optimization of Reaction Condition (Solvent)



Entry	Cat.	T	solvent	Yield (%)[a]	Entry	Cat.	T	solvent	Yield (%)[a]
1	$Fe(acac)_3$	50	DCM	84 (82)[b]	5	$Fe(acac)_3$	50	DCE	82
2	$Fe(acac)_3$	50	CH_3CN	73	6	$Fe(acac)_3$	50	DMA	57
3	$Fe(acac)_3$	50	1,4-Dioxane	59	7	$Fe(acac)_3$	50	Toluene	55
4	$Fe(acac)_3$	50	THF	28	8	$Fe(acac)_3$	50	MeOH	trace

[a]yield was determined by ^{1}H NMR with CH_2Br_2 as internal standard. [b]the isolated yield.

Optimization of Reaction Condition for **S13**



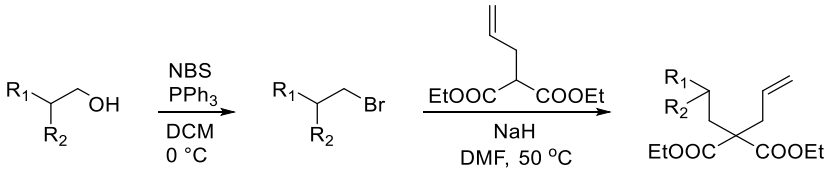
Entry	Cat.	T	solvent	Yield (%)[a]	Entry	Cat.	T	solvent	Yield (%)[a]
1[b]	CuI	45	DCE	52	12	$FeCl_2$	50	DCM	72
2	CuI	40	MeCN	45	13	$FeCl_3$	50	DCM	trace
3	CuI	40	1,4-Dioxane	44	14	$FeBr_3$	50	DCM	12
4	CuTc	40	DCM	64	15	$Fe(acac)_3$	50	DCM	80 (85)[c]
5	CuTc	30	DCM	60	16	$Fe(acac)_3$	50	1,4-Dioxane	44
6	CuTc	30	DCM/dioxane=1:1	68	17	$Fe(acac)_3$	50	CH_3CN	47
7	$Fe(OAc)_2$	30	DCM	48	18	$Fe(acac)_3$	50	Toluene	trace
8	$Fe(OAc)_2$	40	DCM	64	19	$Fe(acac)_3$	50	MeOH	48
9	$Fe(OAc)_2$	50	DCM	77	20	$Fe(acac)_3$	50	Acetone	70
10	$Fe(OTf)_2$	50	DCM	65	21	$Fe(acac)_3$	50	EA	64
11	$Fe(acac)_2$	50	DCM	76	22	$Fe(acac)_3$	50	DMF	40

[a]yield was determined by ^1H NMR with CH_2Br_2 as internal standard. [b]Liu's conditions. [c]the isolated yield.

III. Synthesis and Characterization of New Molecules

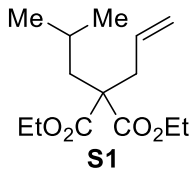
All Substrates were synthesized through the known method.[3,4]

General procedure A for substrates synthesis



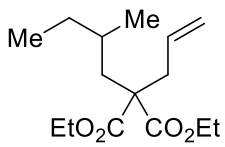
To a solution of alcohol (10 mmol) in dichloromethane (20 mL) was added triphenylphosphine (15 mmol, 1.5 equiv) and N-Bromosuccinimide (15 mmol, 1.5 equiv) in one patch in an ice bath. After reaction reached completion, monitored by TLC, it was quenched with saturated aqueous $NaHCO_3$. The aqueous layer was extracted with dichloromethane three times, and the combined organic phase was washed with brine (20 mL), dried over anhydrous Na_2SO_4, filtered and concentrated under vacuum. The residue was then purified by flash column chromatography to give the alkyl bromide.

To a solution of diethyl allylmalonate (1.0 equiv) in DMF (0.5 M) was added NaH (1.5 equiv) slowly in an ice bath. After 20 mins when solution stopped bubbling at room temperature, the afforded alkyl bromide (1.2 equiv) was added into the mixture dropwise. The resulting solution was stirred at 50 ^oC under air and monitored by TLC. Upon completion, the reaction was quenched with saturated aqueous NH_4Cl, and the aqueous layer was extracted with EtOAc three times. The combined organic phase was washed with brine (20 mL), dried over anhydrous Na_2SO_4, filtered and concentrated under vacuum. The residue was then purified by flash column chromatography to give the target substrate.



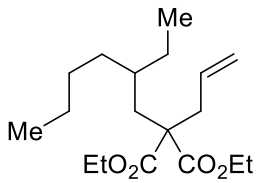
S1

Prepared according to general procedure A and obtained as colorless oil. ^1H NMR (400 MHz, $CDCl_3$) δ 5.73 – 5.56 (m, 1H), 5.14 – 5.03 (m, 2H), 4.17 (qd, *J* = 7.1, 2.9 Hz, 4H), 2.69 (d, *J* = 7.4 Hz, 2H), 1.87 (d, *J* = 6.3 Hz, 2H), 1.74 – 1.62 (m, 1H), 1.25 (t, *J* = 7.1 Hz, 6H), 0.88 (d, *J* = 6.6 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.83, 132.91, 118.90, 61.23, 57.07, 40.63, 37.28, 24.06, 23.78, 14.20. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{14}H_{24}NaO_4$: 279.1572, found: 279.1569.



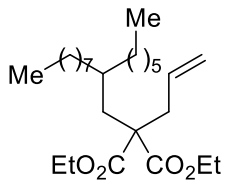
S2

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.74 – 5.58 (m, 1H), 5.16 – 5.04 (m, 2H), 4.26 – 4.08 (m, 4H), 2.78 – 2.59 (m, 2H), 1.97 (dd, *J* = 14.6, 4.5 Hz, 1H), 1.77 (dd, *J* = 14.6, 7.6 Hz, 1H), 1.51 – 1.27 (m, 2H), 1.24 (td, *J* = 7.1, 2.4 Hz, 6H), 1.21 – 1.06 (m, 1H), 0.85 (t, *J* = 7.0 Hz, 3H), 0.84 (d, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.00, 171.76, 132.90, 118.91, 61.23, 61.19, 57.08, 38.76, 37.31, 30.82, 30.22, 20.04, 14.21, 14.17, 11.40. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{15}H_{26}NaO_4$: 293.1729, found: 293.1726.



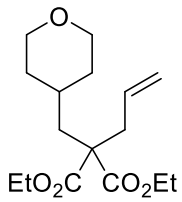
S3

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.75 – 5.57 (m, 1H), 5.17 – 5.00 (m, 2H), 4.26 – 4.02 (m, 4H), 2.67 (d, *J* = 7.3 Hz, 2H), 1.93 – 1.80 (m, 2H), 1.40 – 1.32 (m, 1H), 1.30 – 1.15 (m, 5H), 1.24 (t, *J* = 7.0 Hz, 9H), 0.88 (t, *J* = 6.8 Hz, 3H), 0.81 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.97, 171.92, 132.85, 118.99, 61.22, 57.15, 37.22, 35.76, 34.23, 33.41, 28.54, 26.33, 23.23, 14.30, 14.18, 10.42. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{18}H_{32}NaO_4$: 335.2198, found: 335.2205.



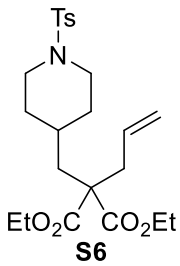
S4

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.73 – 5.59 (m, 1H), 5.16 – 5.00 (m, 2H), 4.24 – 4.06 (m, 4H), 2.67 (d, *J* = 7.3 Hz, 2H), 1.87 (d, *J* = 5.7 Hz, 2H), 1.44 – 1.14 (m, 31H), 0.88 (t, *J* = 6.7 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.90, 132.91, 118.91, 61.19, 57.22, 37.25, 36.36, 34.27, 33.15, 32.05, 30.23, 29.90, 29.79, 29.49, 26.31, 26.28, 22.82, 14.26, 14.18. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{26}H_{48}NaO_4$: 447.3450, found: 447.3443.



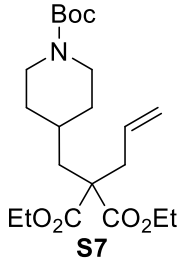
S5

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.70 – 5.59 (m, 1H), 5.17 – 5.04 (m, 2H), 4.23 – 4.13 (m, 4H), 3.89 (dd, *J* = 11.0, 3.1 Hz, 2H), 3.34 (td, *J* = 11.8, 2.0 Hz, 2H), 2.69 (d, *J* = 7.4 Hz, 2H), 1.89 (d, *J* = 6.1 Hz, 2H), 1.66 – 1.55 (m, 1H), 1.54 – 1.46 (m, 2H), 1.38 – 1.27 (m, 2H), 1.25 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.61, 132.59, 119.14, 68.00, 61.35, 56.54, 39.01, 37.58, 33.81, 30.98, 14.18. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{16}H_{26}NaO_5$: 321.1678, found: 321.1678.



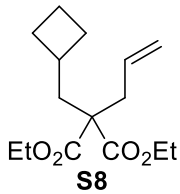
S6

Prepared according to general procedure A and obtained as yellowish solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.8 Hz, 2H), 7.32 (d, *J* = 7.8 Hz, 2H), 5.63 – 5.51 (m, 1H), 5.10 – 5.01 (m, 2H), 4.21 – 4.08 (m, 4H), 3.69 (d, *J* = 11.5 Hz, 2H), 2.60 (d, *J* = 7.3 Hz, 2H), 2.44 (s, 3H), 2.16 (t, *J* = 11.5 Hz, 2H), 1.84 (d, *J* = 5.5 Hz, 2H), 1.62 (d, *J* = 12.5 Hz, 2H), 1.40 – 1.26 (m, 3H), 1.23 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.51, 143.65, 132.36, 129.76, 127.87, 119.36, 61.48, 56.49, 46.49, 38.11, 37.45, 32.21, 31.05, 21.69, 14.19. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{23}H_{33}NO_6SNa$: 474.1926, found: 474.1935



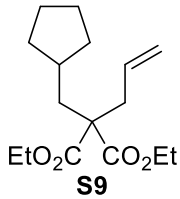
S7

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.71 – 5.55 (m, 1H), 5.16 – 5.05 (m, 2H), 4.18 (q, *J* = 7.1 Hz, 4H), 4.13 – 3.95 (m, 2H), 2.75 – 2.59 (m, 2H), 2.63 (d, *J* = 7.4 Hz, 2H), 1.95 – 1.84 (m, 2H), 1.66 (d, *J* = 12.5 Hz, 2H), 1.45 (s, 9H), 1.24 (t, *J* = 7.1 Hz, 6H), 1.12 – 1.03 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.35, 154.95, 132.49, 119.05, 79.33, 61.30, 57.28, 36.76, 36.36, 32.17, 30.55, 29.34, 28.58, 14.26. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{21}H_{35}NaO_6$: 420.2362, found: 420.2356.



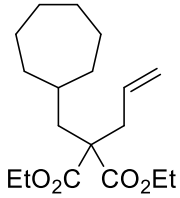
S8

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.69 – 5.57 (m, 1H), 5.17 – 5.00 (m, 2H), 4.22 – 4.08 (m, 4H), 2.62 (d, *J* = 7.3 Hz, 2H), 2.37 – 2.24 (m, 1H), 1.98 (dd, *J* = 17.5, 4.7 Hz, 4H), 1.88 – 1.77 (m, 1H), 1.74 – 1.60 (m, 3H), 1.24 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.51, 132.85, 118.89, 61.17, 56.94, 39.17, 37.05, 31.96, 29.53, 19.09, 14.20. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{15}H_{24}NaO_4$: 291.1572, found: 291.1573.



S9

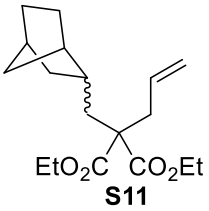
Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.73 – 5.59 (m, 1H), 5.15 – 5.03 (m, 2H), 4.24 – 4.11 (m, 4H), 2.70 (d, *J* = 7.4 Hz, 2H), 2.01 (d, *J* = 5.6 Hz, 2H), 1.79 – 1.68 (m, 3H), 1.66 – 1.54 (m, 2H), 1.53 – 1.42 (m, 2H), 1.24 (t, *J* = 7.1 Hz, 6H), 1.12 – 1.00 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.84, 132.90, 118.90, 61.20, 57.41, 38.00, 37.20, 36.02, 33.64, 24.95, 14.21. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{16}H_{26}NaO_4$: 305.1729, found: 305.1720.



S10

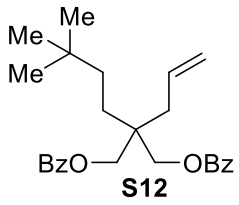
Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.73 – 5.58 (m, 1H), 5.15 – 5.01 (m, 2H), 4.23 – 4.10 (m, 4H), 2.67 (d, *J* = 7.4 Hz, 2H), 1.87 (d, *J* = 5.5 Hz, 2H), 1.65 – 1.51 (m, 7H), 1.51 – 1.31 (m, 4H), 1.29 – 1.13 (m, 2H),

1.24 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.84, 132.96, 118.89, 61.19, 57.25, 40.13, 37.55, 35.81, 34.99, 28.51, 26.18, 14.20. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{18}H_{30}NaO_4$: 333.2042, found: 333.2037.



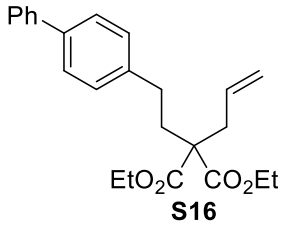
S11

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.72 – 5.56 (m, 1H), 5.15 – 5.00 (m, 2H), 4.28 – 4.00 (m, 4H), 2.84 – 1.67 (m, 6H), 1.60 – 1.52 (m, 1H), 1.51 – 1.39 (m, 2H), 1.34 – 1.20 (m, 9H), 1.15 – 0.98 (m, 2H), 0.67 – 0.53 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.93, 171.74, 132.89, 118.95, 61.24, 61.18, 57.48, 42.58, 41.56, 40.27, 40.03, 37.74, 37.56, 37.35, 37.19, 36.68, 35.71, 35.52, 35.38, 30.39, 30.13, 28.64, 22.57, 14.23, 14.20. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{18}H_{28}NaO_4$: 331.1885, found: 331.1896.



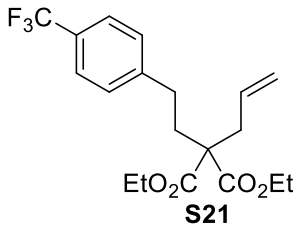
S12

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 – 7.99 (m, 4H), 7.59 – 7.53 (m, 2H), 7.46 – 7.40 (m, 4H), 5.93 – 5.75 (m, 1H), 5.18 – 5.07 (m, 2H), 4.30 (s, 4H), 2.30 (d, *J* = 7.5 Hz, 2H), 1.53 – 1.46 (m, 2H), 1.31 – 1.23 (m, 2H), 0.88 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.47, 133.17, 132.60, 130.21, 129.68, 128.58, 119.25, 66.84, 40.36, 36.40, 36.36, 30.34, 29.39, 26.28. ESI (m/z): $[M+Na]^+$ calcd. for $C_{26}H_{32}NaO_4$: 431.2198, found: 431.2202.



S16

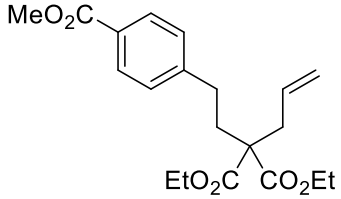
Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.3 Hz, 2H), 7.51 (d, *J* = 8.1 Hz, 2H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 7.3 Hz, 1H), 7.25 (d, *J* = 9.5 Hz, 2H), 5.76 – 5.65 (m, 1H), 5.21 – 5.12 (m, 2H), 4.21 (q, *J* = 7.1 Hz, 4H), 2.76 (d, *J* = 7.4 Hz, 2H), 2.61 – 2.54 (m, 2H), 2.25 – 2.18 (m, 2H), 1.28 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.24, 141.13, 140.66, 139.17, 132.53, 128.93, 128.86, 127.29, 127.20, 127.14, 119.26, 61.44, 57.38, 37.31, 34.32, 30.21, 14.32. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{24}H_{28}NaO_4$: 403.1885, found: 403.1885.



S21

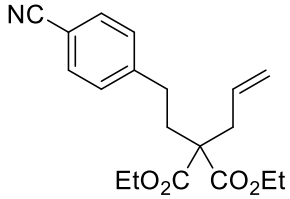
Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.9 Hz, 2H), 7.28 (d, *J* = 8.3 Hz, 2H), 5.76 – 5.61 (m, 1H), 5.23 – 5.11 (m, 2H), 4.21 (q, *J* = 7.1 Hz, 4H), 2.75 (d, *J* = 7.4 Hz, 2H), 2.63 – 2.54 (m, 2H), 2.19 – 2.11 (m, 2H), 1.27 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.95, 145.56, 132.23, 128.70, 128.44 (q, *J*

= 32.2 Hz), 125.35 (q, *J* = 3.8 Hz), 124.23 (q, *J* = 2.7 Hz), 119.26, 61.40, 57.09, 37.26, 34.02, 30.38, 14.16. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{23}F_3NaO_4$: 395.1446, found: 395.1446.



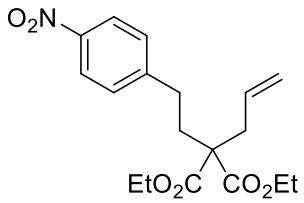
S22

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.4 Hz, 2H), 7.23 (d, *J* = 8.4 Hz, 2H), 5.78 – 5.62 (m, 1H), 5.25 – 5.06 (m, 2H), 4.21 (q, *J* = 7.1 Hz, 4H), 3.90 (s, 3H), 2.75 (d, *J* = 7.4 Hz, 2H), 2.64 – 2.54 (m, 2H), 2.23 – 2.12 (m, 2H), 1.27 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.03, 167.11, 147.01, 132.36, 129.86, 128.50, 128.14, 119.30, 61.44, 57.23, 52.10, 37.30, 34.00, 30.65, 14.25. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{20}H_{26}NaO_6$: 385.1627, found: 385.1824.



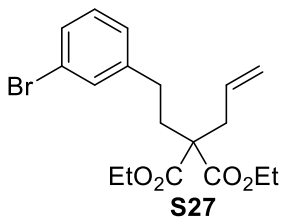
S23

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.1 Hz, 2H), 7.27 (d, *J* = 8.1 Hz, 2H), 5.74 – 5.59 (m, 1H), 5.22 – 5.10 (m, 2H), 4.21 (q, *J* = 7.1 Hz, 4H), 2.74 (d, *J* = 7.4 Hz, 2H), 2.67 – 2.55 (m, 2H), 2.20 – 2.10 (m, 2H), 1.27 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.95, 147.23, 132.39, 132.27, 129.32, 119.44, 119.10, 110.13, 61.56, 57.14, 37.43, 33.96, 30.85, 14.27. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{23}NNaO_4$: 352.1525, found: 352.1521.



S24

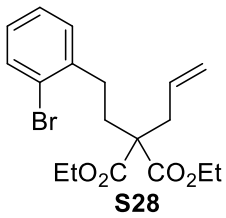
Prepared according to general procedure A and obtained as white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.7 Hz, 2H), 7.33 (d, *J* = 8.6 Hz, 2H), 5.75 – 5.60 (m, 1H), 5.23 – 5.13 (m, 2H), 4.22 (q, *J* = 7.1 Hz, 4H), 2.75 (d, *J* = 7.4 Hz, 2H), 2.70 – 2.62 (m, 2H), 2.21 – 2.12 (m, 2H), 1.28 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.93, 149.41, 146.59, 132.23, 129.33, 123.85, 119.50, 61.60, 57.12, 37.46, 33.98, 30.63, 14.27. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{18}H_{23}NNaO_6$: 372.1423, found: 372.1423.



S27

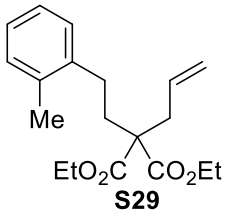
Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, *J* = 6.8 Hz, 2H), 7.14 (t, *J* = 8.0 Hz, 1H), 7.09 (d, *J* = 7.6 Hz, 1H), 5.75 – 5.61 (m, 1H), 5.22 – 5.10 (m, 2H), 4.20 (q, *J* = 7.1 Hz, 4H), 2.73 (d, *J* = 7.3 Hz, 2H), 2.58 – 2.42 (m, 2H), 2.20 – 2.08 (m, 2H), 1.27 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.09, 143.89, 132.39, 131.54, 130.11, 129.31, 127.20, 122.54, 119.35, 61.50, 57.25, 37.35, 34.19, 30.31, 14.29. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{18}H_{23}BrNaO_4$: 405.0677, found:

405.0677.



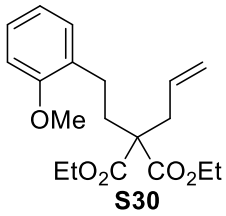
S28

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.9 Hz, 1H), 7.27 – 7.17 (m, 2H), 7.13 – 7.00 (m, 1H), 5.82 – 5.65 (m, 1H), 5.25 – 5.09 (m, 2H), 4.22 (q, *J* = 7.1 Hz, 4H), 2.77 (d, *J* = 7.4 Hz, 2H), 2.72 – 2.62 (m, 2H), 2.19 – 2.11 (m, 2H), 1.28 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.07, 140.84, 132.89, 132.46, 130.52, 127.93, 127.70, 124.32, 119.27, 61.42, 57.34, 37.13, 32.74, 30.99, 14.28. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{18}H_{23}BrNaO_4$: 455.0677, found: 455.0668.



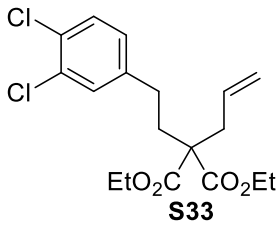
S29

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 – 7.02 (m, 4H), 5.77 – 5.65 (m, 1H), 5.24 – 5.10 (m, 2H), 4.22 (q, *J* = 7.1 Hz, 4H), 2.77 (d, *J* = 7.4 Hz, 2H), 2.55 – 2.45 (m, 2H), 2.29 (s, 3H), 2.14 – 2.04 (m, 2H), 1.32 – 1.24 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.26, 139.73, 135.96, 132.55, 130.35, 129.10, 126.35, 126.23, 119.24, 61.43, 57.47, 37.33, 33.25, 28.02, 19.24, 14.31. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{26}NaO_4$: 341.1729, found: 341.1729.



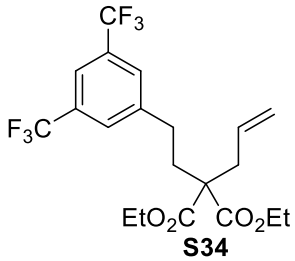
S30

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (td, *J* = 8.0, 1.7 Hz, 1H), 7.10 (dd, *J* = 7.4, 1.6 Hz, 1H), 6.87 (td, *J* = 7.4, 1.1 Hz, 1H), 6.83 (d, *J* = 8.2 Hz, 1H), 5.81 – 5.65 (m, 1H), 5.24 – 5.07 (m, 2H), 4.20 (q, *J* = 7.1 Hz, 4H), 3.80 (s, 3H), 2.76 (d, *J* = 7.4 Hz, 2H), 2.56 – 2.47 (m, 2H), 2.20 – 2.09 (m, 2H), 1.26 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.38, 157.45, 132.69, 129.92, 129.87, 127.42, 120.52, 119.03, 110.27, 61.29, 57.56, 55.28, 36.81, 32.31, 24.97, 14.30. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{26}NaO_5$: 357.1678, found: 357.1678.



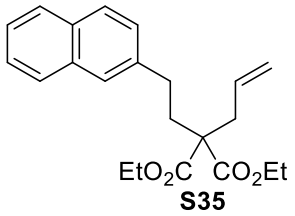
S33

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, *J* = 8.2 Hz, 1H), 7.25 (d, *J* = 1.9 Hz, 1H), 6.99 (dd, *J* = 8.2, 2.0 Hz, 1H), 5.73 – 5.62 (m, 1H), 5.20 – 5.08 (m, 2H), 4.20 (q, *J* = 7.1 Hz, 4H), 2.72 (d, *J* = 7.4 Hz, 2H), 2.56 – 2.43 (m, 2H), 2.19 – 2.07 (m, 2H), 1.27 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.02, 141.81, 132.40, 132.35, 130.45, 130.15, 128.00, 119.42, 61.55, 57.19, 37.46, 34.17, 29.87, 14.30. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{18}H_{22}Cl_2NaO_4$: 395.0793, found: 385.0787.



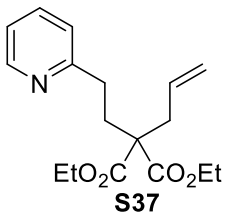
S34

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (s, 1H), 7.61 (s, 2H), 5.76 – 5.60 (m, 1H), 5.28 – 5.08 (m, 2H), 4.37 – 4.07 (m, 4H), 2.76 (d, *J* = 7.3 Hz, 2H), 2.69 (dd, *J* = 10.5, 6.4 Hz, 2H), 2.22 – 2.07 (m, 2H), 1.29 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.91, 144.00, 132.29, 132.23, 131.97, 131.64, 131.35, 128.68, 124.83, 122.12, 120.38, 119.58, 61.67, 57.14, 37.60, 34.17, 30.50, 14.27. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{20}H_{22}F_6NaO_4$: 463.1320, found: 463.1320.



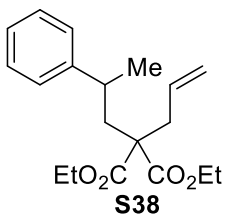
S35

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.4 Hz, 1H), 7.77 (d, *J* = 8.1 Hz, 2H), 7.60 (s, 1H), 7.47 – 7.39 (m, 2H), 7.31 (dd, *J* = 8.4, 1.5 Hz, 1H), 5.79 – 5.65 (m, 1H), 5.23 – 5.11 (m, 2H), 4.21 (q, *J* = 7.1 Hz, 4H), 2.78 (d, *J* = 7.4 Hz, 2H), 2.73 – 2.66 (m, 2H), 2.31 – 2.22 (m, 2H), 1.28 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.27, 139.05, 133.71, 132.55, 132.17, 128.12, 127.74, 127.54, 127.32, 126.47, 126.10, 125.39, 119.28, 61.45, 57.45, 37.40, 34.29, 30.76, 14.32. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{22}H_{26}NaO_4$: 377.1729, found: 377.1729.



S37

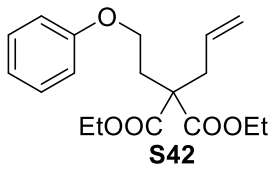
Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, *J* = 4.3 Hz, 1H), 7.59 (td, *J* = 7.7, 1.8 Hz, 1H), 7.15 (d, *J* = 7.8 Hz, 1H), 7.11 (dd, *J* = 7.3, 5.5 Hz, 1H), 5.78 – 5.66 (m, 1H), 5.21 – 5.07 (m, 2H), 4.20 (qd, *J* = 7.1, 2.3 Hz, 4H), 2.79 – 2.69 (m, 4H), 2.36 – 2.25 (m, 2H), 1.26 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.18, 161.25, 149.36, 136.53, 132.52, 122.83, 121.35, 119.22, 61.42, 57.37, 37.43, 33.11, 32.48, 14.26. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{17}H_{23}NNaO_4$: 328.1525, found: 328.1525.



S38

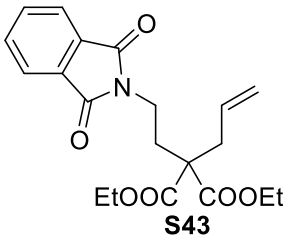
Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.23 (m, 2H), 7.20 – 7.10 (m, 3H), 5.66 – 5.50 (m, 1H), 5.12 – 4.98 (m, 2H), 4.10 (qd, *J* = 7.1, 1.4 Hz, 2H), 3.82 (dq, *J* = 10.8, 7.1 Hz, 1H), 3.58 (dq, *J* = 10.8, 7.1 Hz, 1H), 2.83 – 2.75 (m, 1H), 2.70 (dd, *J* = 14.4, 7.7 Hz, 1H), 2.60 (dd, *J* = 14.4, 7.2 Hz, 1H), 2.37 (dd, *J* = 14.6, 8.9 Hz, 1H), 2.21 (dd, *J* = 14.6, 4.2 Hz, 1H), 1.23 (d, *J* = 7.0 Hz, 3H), 1.21 (t, *J* = 7.1 Hz, 3H), 1.06 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.50, 170.83, 146.66, 132.67, 128.31, 127.53,

126.30, 119.08, 61.27, 61.00, 57.00, 39.53, 36.94, 35.84, 25.02, 14.19, 13.93. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{26}NaO_4$: 341.1729, found: 341.1723.



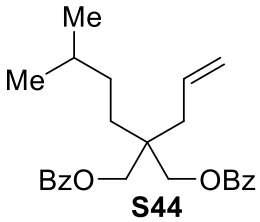
S42

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 – 7.24 (m, 2H), 6.93 (t, *J* = 7.3 Hz, 1H), 6.85 (d, *J* = 8.0 Hz, 2H), 5.73 – 5.64 (m, 1H), 5.23 – 5.05 (m, 2H), 4.19 (qq, *J* = 10.8, 7.1 Hz, 4H), 4.04 (t, *J* = 6.4 Hz, 2H), 2.75 (d, *J* = 7.4 Hz, 2H), 2.41 (t, *J* = 6.4 Hz, 2H), 1.23 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.08, 158.67, 132.45, 129.56, 120.92, 119.49, 114.49, 63.76, 61.54, 55.81, 37.65, 31.99, 14.17. ESI (m/z): $[M+Na]^+$ calcd. for $C_{18}H_{24}NaO_5$: 343.1516, found: 343.1520.



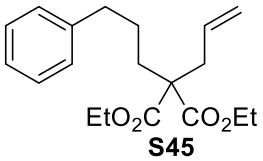
S43

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.71 (dd, *J* = 5.4, 3.0 Hz, 1H), 5.72 (ddt, *J* = 17.4, 10.1, 7.4 Hz, 1H), 5.23 (dd, *J* = 17.0, 1.5 Hz, 2H), 5.17 (dd, *J* = 10.1, 1.4 Hz, 2H), 4.19 (2*q, *J* = 7.1Hz, 4H), 3.79 – 3.65 (m, 2H), 2.76 (d, *J* = 7.4 Hz, 2H), 2.30 – 2.21 (m, 2H), 1.28 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.65, 168.05, 134.10, 132.27, 131.98, 123.34, 119.89, 61.73, 56.14, 37.01, 33.68, 30.66, 14.20. ESI (m/z): $[M+Na]^+$ calcd. for $C_{20}H_{23}NaO_6$: 396.1418, found: 396.1425.



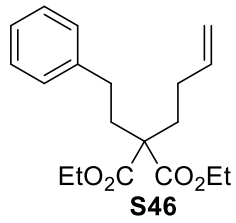
S44

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 7.2 Hz, 4H), 7.56 (t, *J* = 7.4 Hz, 2H), 7.43 (t, *J* = 7.7 Hz, 4H), 5.93 – 5.77 (m, 1H), 5.20 – 5.07 (m, 2H), 4.30 (s, 4H), 2.31 (d, *J* = 7.5 Hz, 2H), 1.57 – 1.45 (m, 3H), 1.36 – 1.19 (m, 2H), 0.89 (d, *J* = 6.6 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.48, 133.17, 132.67, 130.20, 129.68, 128.58, 119.20, 66.94, 40.46, 36.54, 31.78, 29.61, 28.76, 22.71. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{25}H_{30}NaO_4$: 417.2042, found: 417.2043.



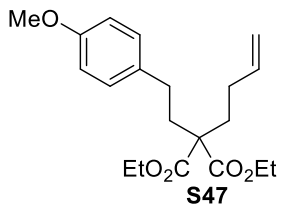
S45

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.24 (m, 2H), 7.20 – 7.13 (m, 3H), 5.66 – 5.53 (m, 1H), 5.10 – 5.01 (m, 2H), 4.15 (q, *J* = 7.1 Hz, 4H), 2.66 – 2.58 (m, 4H), 1.95 – 1.87 (m, 2H), 1.58 – 1.48 (m, 2H), 1.21 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.36, 141.92, 132.54, 128.48, 128.43, 125.96, 118.99, 61.28, 57.39, 36.94, 36.04, 31.74, 25.78, 14.23. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{26}NaO_4$: 341.1729, found: 341.1725.



S46

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.26 (m, *J* = 6.4 Hz, 3H), 7.22-7.16 (m, 2H), 5.93 – 5.70 (m, 1H), 5.07-4.93 (m, 2H), 4.20 (q, *J* = 7.1Hz, 4H), 2.64 – 2.47 (m, 2H), 2.27-2.17 (m, 2H), 2.17 – 1.92 (m, 4H), 1.27 (t, *J* = 7.0 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) 171.58, 141.56, 137.69, 128.57, 128.48, 126.19, 115.24, 61.34, 57.40, 34.55, 32.00, 30.78, 28.59, 14.28. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{26}NaO_4$: 341.1729, found: 341.1725.

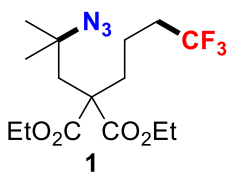


S47

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.09 (d, *J* = 8.6 Hz, 2H), 6.83 (d, *J* = 8.6 Hz, 2H), 5.87 – 5.74 (m, 1H), 5.04 (dd, *J* = 17.1, 1.5 Hz, 1H), 5.01 – 4.94 (m, 1H), 4.20 (q, *J* = 7.1 Hz, 4H), 3.79 (s, 3H), 2.50 – 2.41 (m, 2H), 2.21 – 2.13 (m, 2H), 2.10 – 1.93 (m, 4H), 1.27 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.62, 158.06, 137.72, 133.62, 129.37, 115.22, 113.98, 61.32, 57.37, 55.43, 34.78, 31.99, 29.84, 28.59, 14.28. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{20}H_{28}NaO_5$: 371.1834, found: 371.1828.

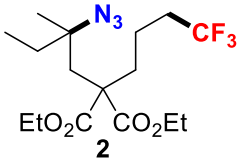
General procedure B for remote azidotrifluoromethylation

Fe salt (0.01 mmol, 10 mol %), Togni-II (0.125mmol, 1.25 equiv) were combined in a 25 mL oven-dried sealed tube. The vessel was evacuated and backfilled with N_2 (repeated for 3 times), after that, alkenes (0.1 mmol), $TMSN_3$ (0.3 mmol, 3.0 equiv) and DCM (1.0 mL) were then added via syringe under N_2. The tube was sealed with a Teflon lined cap and moved into a preheated oil bath at 50 ºC for 12 h. The reaction mixture was then cooled to room temperature, diluted with EtOAc (10 mL) and filtered through a pad of celite. The filtrate was concentrated, and the residue was then purified by flash column chromatography to give the difunctional products.



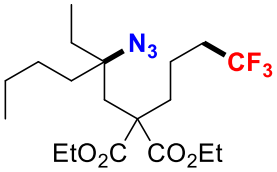
1

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.29 – 4.11 (m, 4H), 2.22 (s, 2H), 2.18 – 2.00 (m, 4H), 1.56 – 1.40 (m, 2H), 1.32 (s, 6H), 1.26 (t, *J* = 7.1 Hz, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.38 (t, *J* = 10.6 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.24, 126.98 (q, *J* = 276.5 Hz), 61.70, 60.32, 56.34, 42.00, 33.98 (q, *J* = 28.8 Hz), 32.33, 27.27, 17.46 (q, *J* = *2.9* Hz), 14.05. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{15}H_{24}F_3N_3O_4Na$: 390.1617, found: 390.1611.



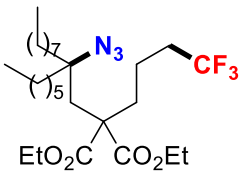
2

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.29 – 4.12 (m, 4H), 2.19 (s, 2H), 2.17 – 2.02 (m, 4H), 1.71 – 1.35 (m, 4H), 1.27 (t, *J* = 7.1 Hz, 3H), 1.26 (t, *J* = 7.1 Hz, 3H), 1.25 (s, 3H), 0.96 (t, *J* = 7.4 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.38 (t, *J* = 10.8 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.47, 171.17, 126.98 (q, *J* = 276.3 Hz), 63.04, 61.70, 56.27, 40.25, 34.80, 34.02 (q, *J* =28.7 Hz), 32.51, 22.43, 17.53 (q, *J* = 3.0 Hz), 14.08, 14.05, 8.46. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{16}H_{26}F_3N_3O_4Na$: 404.1773, found: 404.1770.



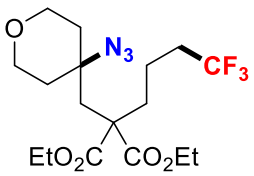
3

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.25 – 4.15 (m, 4H), 2.24 (s, 2H), 2.16 – 2.07 (m, 4H), 1.70 – 1.42 (m, 6H), 1.35 – 1.23 (m, 4H), 1.26 (t, *J* = 7.1 Hz, 6H), 0.93 (t, *J* = 6.7 Hz, 3H), 0.91 (t, *J* = 6.9 Hz, 3H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -66.40 (t, *J* = 10.5 Hz). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.41, 171.39, 126.96 (q, *J* = 276.4 Hz), 65.48, 61.68, 56.24, 38.28, 36.22, 34.00 (q, *J* = 28.8 Hz), 32.39, 29.59, 25.83, 23.09, 17.61 (q, *J* = 3.2 Hz), 14.10, 14.05, 8.27. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{32}F_3N_3O_4Na$: 446.2243, found: 446.2256.



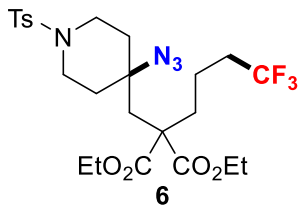
4

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.31 – 4.09 (m, 4H), 2.24 (s, 2H), 2.20 – 2.02 (m, 4H), 1.60 – 1.40 (m, 6H), 1.40 – 1.08 (m, 26H), 0.98 – 0.80 (m, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.41 (t, *J* = 10.8 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.37, 126.96 (q, *J* = 276.4 Hz), 65.30, 61.68, 56.33, 38.83, 37.16, 34.06 (q, *J* = 28.7 Hz), 32.43, 31.96, 31.83, 30.01, 29.68, 29.59, 29.37, 23.79, 23.78, 22.78, 22.74, 17.67 (q, *J* = 2.9 Hz), 14.22, 14.16, 14.07. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{27}H_{48}F_3N_3O_4Na$: 558.3495, found: 558.3499.



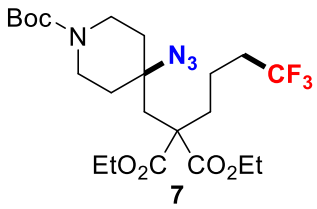
5

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.29 – 4.13 (m, 4H), 3.82 – 3.74 (m, 2H), 3.68 – 3.58 (m, 2H), 2.31 (s, 2H), 2.19 – 2.04 (m, 4H), 1.76 – 1.66 (m, 4H), 1.52 – 1.44 (m, 2H), 1.27 (t, *J* = 7.1 Hz, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.34 (t, *J* = 10.7 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.12, 126.89 (q, *J* = 276.5 Hz), 63.68, 61.93, 60.65, 55.85, 42.14, 35.45, 34.00 (q, *J* = 29.0 Hz), 33.19, 17.60 (q, *J* = 2.9 Hz), 14.08. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{17}H_{26}F_3N_3O_5Na$: 432.1722, found: 432.1719.



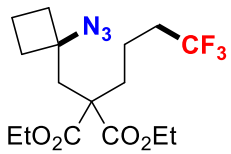
6

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.2 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 4.26 – 4.11 (m, 4H), 3.60 (d, *J* = 12.0 Hz, 2H), 2.50 – 2.37 (m, 2H), 2.45 (s, 3H), 2.27 (s, 2H), 2.14 – 2.05 (m, 4H), 1.85 – 1.66 (m, 4H), 1.47 – 1.38 (m, 2H), 1.25 (t, *J* = 7.1 Hz, 6H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -66.28 (t, *J* = 10.7 Hz). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.84, 143.92, 132.73, 129.90, 127.67, 126.77 (q, *J* = 277.8 Hz), 61.91, 60.51, 55.61, 42.10, 41.40, 34.02, 33.80 (q, *J* = 29.1 Hz), 33.22, 21.62, 17.42 (q, *J* = 2.6 Hz), 13.95. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{24}H_{33}F_3N_4O_6SNa$: 585.1971, found: 585.1979.



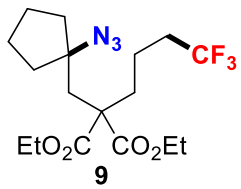
7

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.19 (q, *J* = 7.1 Hz, 4H), 4.07 (s, 2H), 2.66 (s, 2H), 2.13 – 2.02 (m, 2H), 1.99 – 1.83 (m, 4H), 1.67 (d, *J* = 12.5 Hz, 2H), 1.51 – 1.39 (m, 1H), 1.45 (s, 9H), 1.25 (t, *J* = 7.1 Hz, 6H), 1.16 – 0.96 (m, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.33 (t, *J* = 10.8 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.41, 154.96, 126.96 (q, *J* = 276.3 Hz), 79.39, 61.45, 57.29, 36.35, 34.02 (q, *J* = 28.7 Hz), 32.15, 31.49, 30.76, 29.74, 28.59, 17.13 (q, *J* = 2.9 Hz), 14.22. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{22}H_{35}F_3N_4O_6Na$: 531.2407, found: 531.2404.



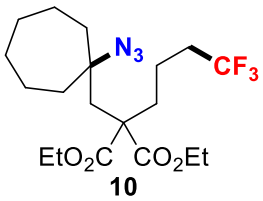
8

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.26 – 4.15 (m, 4H), 2.38 (s, 2H), 2.28 – 2.20 (m, 2H), 2.15 – 2.02 (m, 4H), 2.02 – 1.94 (m, 3H), 1.91 – 1.81 (m, 1H), 1.54 – 1.42 (m, 2H), 1.27 (d, *J* = 7.1 Hz, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.39 (t, *J* = 10.8 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.13, 126.93 (q, *J* = 276.3 Hz), 64.29, 61.72, 56.27, 40.36, 34.01 (q, *J* = 28.7 Hz), 33.41, 31.95, 17.63 (q, *J* = 3.0 Hz), 15.06, 14.07. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{16}H_{24}F_3N_3O_4Na$: 402.1617, found: 402.1613.



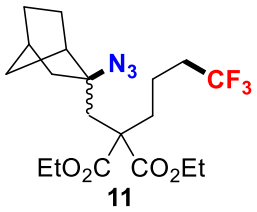
9

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.32 – 4.10 (m, 4H), 2.41 (s, 2H), 2.19 – 2.03 (m, 4H), 1.96 – 1.87 (m, 2H), 1.78 – 1.69 (m, 4H), 1.60 – 1.52 (m, 2H), 1.50 – 1.42 (m, 2H), 1.27 (t, *J* = 7.1 Hz, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.40 (t, *J* = 10.8 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.30, 126.93 (q, *J* = 276.4 Hz), 71.62, 61.72, 56.60, 40.54, 38.03, 34.02 (q, *J* = 28.8 Hz), 32.34, 23.04, 17.62 (q, *J* = 3.0 Hz), 14.06. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{17}H_{26}F_3N_3O_4Na$: 416.1773, found: 416.1768.



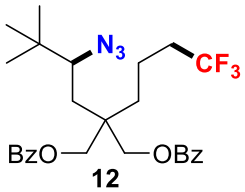
10

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.28 – 4.12 (m, 4H), 2.27 (s, 2H), 2.19 – 2.04 (m, 4H), 1.86 (dd, *J* = 13.5, 9.0 Hz, 2H), 1.66 – 1.41 (m, 12H), 1.26 (t, *J* = 7.1 Hz, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.38 (t, *J* = 10.8 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.36, 126.97 (q, *J* = 276.3 Hz), 66.60, 61.71, 56.31, 41.83, 38.97, 34.04 (q, *J* = 28.8 Hz), 32.69, 30.08, 22.52, 17.57 (q, *J* = 3.0 Hz), 14.09. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{30}F_3N_3O_4Na$: 444.2086, found: 444.2086.



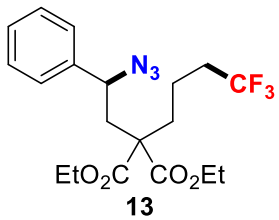
11

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.30 – 4.14 (m, 4H), 2.47 (d, *J* = 15.2 Hz, 1H), 2.38 (d, *J* = 15.2 Hz, 1H), 2.33 – 2.25 (m, 2H), 2.18 – 2.02 (m, 3H), 2.02 – 1.93 (m, 1H), 1.85 – 1.77 (m, 1H), 1.70 (d, *J* = 10.2 Hz, 1H), 1.61 – 1.43 (m, 5H), 1.30 – 1.12 (m, 3H), 1.27 (td, *J* = 7.1, 2.9 Hz, 6H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -66.35 (t, *J* = 10.8 Hz). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.44, 171.38, 126.92 (q, *J* = 276.6 Hz), 69.65, 61.76, 56.79, 47.42, 44.34, 39.28, 37.53, 36.45, 34.02 (q, *J* = 28.8 Hz), 32.26, 28.84, 23.20, 17.88 (q, *J* = 3.3 Hz), 14.09. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{28}F_3N_3O_4Na$: 442.1930, found: 442.1941.



12

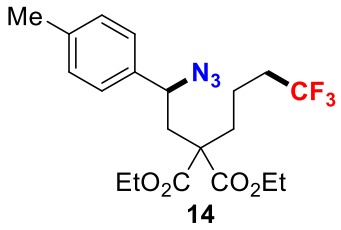
Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.3 Hz, 4H), 7.56 (t, *J* = 7.4 Hz, 2H), 7.43 (t, *J* = 7.6 Hz, 4H), 4.30 (s, 4H), 2.17 – 2.01 (m, 2H), 1.72 – 1.61 (m, 2H), 1.57 – 1.53 (m, 1H), 1.53 – 1.46 (m, 2H), 1.28 – 1.18 (m, 2H), 0.88 (s, 9H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.14 (t, *J* = 10.8 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.44, 133.26, 130.05, 129.65, 128.61, 127.0 8 (q, *J* = 277.6 Hz), 66.68, 40.05, 36.34, 34.44 (q, *J* = 28.7 Hz), 30.97, 30.29, 29.33, 25.98, 15.90 (q, *J* = 2.7Hz). HRMS ESI (m/z): $[M+H]^+$ calcd. for $C_{27}H_{33}N_3O_4F_3$: 520.2423, found: 520.2417.



13

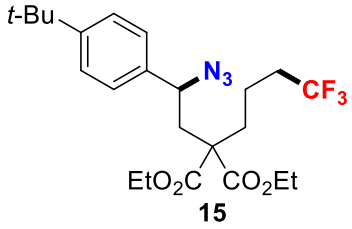
Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.30 (m, 5H), 4.52 (dd, *J* = 8.8, 4.6 Hz, 1H), 4.27 – 4.11 (m, 4H), 2.44 – 2.30 (m, 2H), 2.14 – 1.93 (m, 4H), 1.57 – 1.43 (m, 1H), 1.43 – 1.32 (m, 1H), 1.28 (t, *J* = 7.1 Hz, 3H), 1.24 (t, *J* = 7.3 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.30 (t, *J* = 10.8 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.84, 170.74, 139.57, 129.09, 128.74, 126.97, 126.90 (q, *J* = 276.4 Hz), 62.63, 61.84, 61.77, 56.22, 38.98, 33.91 (q, *J* = 29.1 Hz), 32.09, 17.21 (q, *J* = 2.9 Hz), 14.12, 14.10.

HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{24}F_3N_3NaO_4$: 438.1617, found: 438.1617.



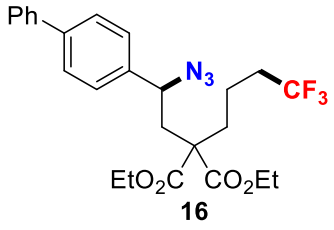
14

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 (s, 4H), 4.47 (dd, *J* = 9.1, 4.3 Hz, 1H), 4.27 – 4.07 (m, 4H), 2.40 – 2.29 (m, 2H), 2.36 (s, 3H), 2.13 – 1.95 (m, 4H), 1.54 – 1.43 (m, 1H), 1.41 – 1.33 (m, 1H), 1.28 (t, *J* = 7.0 Hz, 3H), 1.24 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ-66.31 (t, *J* = 10.8 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.88, 170.78, 138.60, 136.49, 129.71, 126.91, 126.89 (q, *J* = 276.6 Hz), 62.36, 61.82, 61.75, 56.21, 38.86, 33.91 (q, *J* = 28.9 Hz), 32.01, 21.28, 17.19 (q, *J* = 2.9 Hz), 14.13, 14.10. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{20}H_{26}F_3N_3NaO_4$: 452.1773, found: 452.1773.



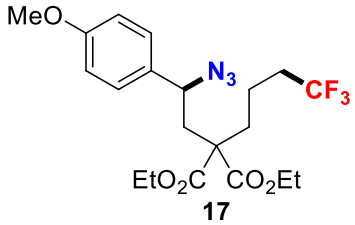
15

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.3 Hz, 2H), 7.25 (d, *J* = 8.4 Hz, 2H), 4.47 (dd, *J* = 8.5, 4.9 Hz, 1H), 4.25 – 4.08 (m, 4H), 2.44 – 2.30 (m, 2H), 2.13 – 1.92 (m, 4H), 1.52 – 1.35 (m, 2H), 1.32 (s, 9H), 1.28 (t, *J* = 7.1 Hz, 3H), 1.24 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.31 (t, *J* = 10.8 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 170.89, 170.77, 151.74, 136.48, 126.88 (q, *J* = 276.5 Hz), 126.71, 125.96, 62.32, 61.82, 61.76, 56.21, 38.77, 34.76, 33.92 (q, *J* = 28.9 Hz), 31.98, 31.39, 17.18, 17.15, 14.14, 14.12. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{23}H_{32}F_3N_3NaO_4$: 494.2243 found: 494.2243.



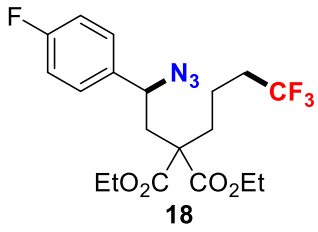
16

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 12.3, 8.0 Hz, 4H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.38 (dd, *J* = 16.4, 7.4 Hz, 3H), 4.58 (dd, *J* = 8.4, 4.8 Hz, 1H), 4.28 – 4.09 (m, 4H), 2.50 – 2.29 (m, 2H), 2.19 – 1.95 (m, 4H), 1.60 – 1.47 (m, 1H), 1.46 – 1.34 (m, 1H), 1.29 (d, *J* = 7.1 Hz, 3H), 1.26 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.26 (t, *J* = 10.7 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.88, 170.77, 141.70, 140.51, 138.54, 128.98, 127.81, 127.71, 127.43, 127.24, 126.90 (q, *J* = 276.5 Hz), 62.38, 61.90, 61.82, 56.23, 39.05, 33.94 (q, *J* = 28.9 Hz), 32.17, 17.25 (q, *J* = 2.9 Hz), 14.16, 14.14. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{25}H_{28}F_3N_3NaO_4$: 514.1930, found: 514.1930.



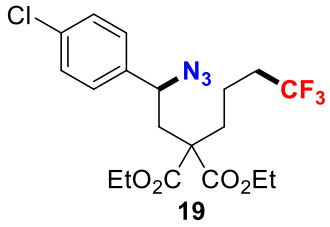
17

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (d, *J* = 9.3 Hz, 2H), 6.91 (d, *J* = 7.7 Hz, 2H), 4.46 (dd, *J* = 8.9, 4.1 Hz, 1H), 4.33 – 4.04 (m, 4H), 3.82 (s, 3H), 2.49 – 2.28 (m, 2H), 2.23 – 1.90 (m, 4H), 1.51 – 1.45 (m, 1H), 1.39 – 1.35 (m, 1H), 1.31 – 1.19 (m, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.28 (t, *J* = 10.7 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.89, 170.78, 159.83, 131.49, 128.31, 126.90 (q, *J*= 277.4Hz), 114.35, 62.09, 61.84, 61.77, 56.19, 55.47, 38.82, 33.93 (q, *J*= 28.8Hz), 31.98, 17.21 (q, *J*= 3.0Hz), 14.14, 14.12. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{20}H_{26}F_3N_3NaO_5$: 468.1722, found: 468.1722.



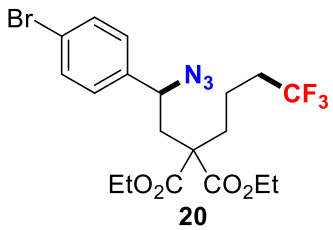
18

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (dd, *J* = 8.7, 5.2 Hz, 2H), 7.09 (t, *J* = 8.6 Hz, 2H), 4.53 (dd, *J* = 8.9, 4.5 Hz, 1H), 4.25 – 4.11 (m, 4H), 2.36 – 2.25 (m, 2H), 2.14 – 1.99 (m, 4H), 1.56 – 1.47 (m, 1H), 1.41 – 1.32 (m, 1H), 1.28 (t, *J* = 7.1 Hz, 3H), 1.25 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.27 (t, *J* = 11.0 Hz, 3F), -113.00 (tt, *J* = 8.8, 5.4 Hz, 1F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.80, 170.70, 162.76 (d, *J* = 247.7 Hz), 135.49 (d, *J* = 3.3 Hz), 128.72 (d, *J* = 8.2 Hz), 126.88 (q, *J* = 276.5 Hz), 116.05 (d, *J* = 21.6 Hz), 61.94, 61.92, 61.83, 56.15, 39.21, 33.90 (q, *J* = 28.9 Hz), 32.20, 17.23 (q, *J* = 2.9 Hz), 14.13, 14.12. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{23}F_4N_3NaO_4$: 456.1522, found: 456.1522.



19

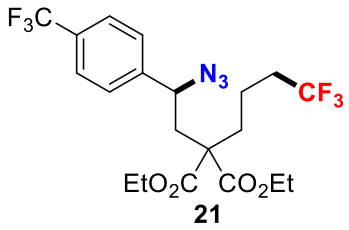
Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 8.5 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 4.53 (dd, *J* = 8.5, 4.8 Hz, 1H), 4.29 – 4.08 (m, 4H), 2.35 – 2.24 (m, 2H), 2.18 – 1.95 (m, 4H), 1.59 – 1.45 (m, 1H), 1.42 – 1.33 (m, 1H), 1.28 (t, *J* = 7.1 Hz, 3H), 1.26 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.26 (t, *J* = 10.7 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.78, 170.67, 138.21, 134.55, 129.30, 128.30, 126.88 (q, *J* = 276.0 Hz), 62.01, 61.95, 61.84, 56.16, 39.24, 33.90 (q, *J* = 28.9Hz), 32.29, 17.24 (q, *J* = 2.9Hz), 14.12, 14.11. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{23}ClF_3N_3NaO_4$: 472.1227, found: 472.1227.



20

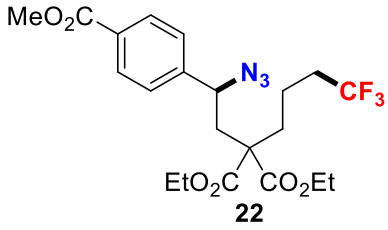
Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.4 Hz, 2H), 7.21 (d, *J* = 8.4 Hz, 2H), 4.52 (dd, *J* = 8.3, 4.9 Hz, 1H), 4.27 – 4.08 (m, 4H), 2.35 – 2.23 (m, 2H), 2.21 –

1.94 (m, 4H), 1.58 – 1.44 (m, 1H), 1.44 – 1.31 (m, 1H), 1.28 (t, *J* = 7.1 Hz, 3H), 1.26 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.26 (t, *J* = 10.8 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.19, 170.76, 170.66, 138.75, 132.26, 128.60, 126.87 (q, *J* = 276.4 Hz), 122.66, 62.07, 61.95, 61.84, 56.15, 39.22, 33.89 (q, *J* = 28.9 Hz), 32.31, 17.23 (q, *J* = 2.9 Hz), 14.12, 14.11. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{23}BrF_3N_3NaO_4$: 516.0722, found: 516.0722.



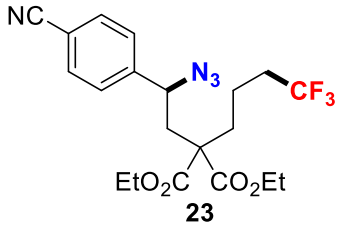
21

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.1 Hz, 2H), 7.47 (d, *J* = 8.1 Hz, 2H), 4.65 (t, *J* = 6.6 Hz, 1H), 4.29 – 4.06 (m, 4H), 2.29 (d, *J* = 6.6 Hz, 2H), 2.17 – 1.97 (m, 4H), 1.61 – 1.47 (m, 1H), 1.43 – 1.33 (m, 1H), 1.29 (t, *J* = 7.1 Hz, 3H), 1.27 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.72 (s, 3F), -66.30 (t, *J* = 10.7 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.75, 170.63, 143.85, 130.88 (q, *J* = 32.6 Hz), 127.29, 126.87 (q, *J* = 277.4 Hz), 126.14 (q, *J* = 3.7 Hz), 123.97 (q, *J* = 272.2 Hz), 62.23, 62.01, 61.89, 56.18, 39.49, 33.88 (q, *J* = 28.8 Hz), 32.48, 17.24 (q, *J* = 3.0 Hz), 14.11, 14.09. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{20}H_{23}F_6N_3NaO_4$: 506.1490, found: 506.1490.



22

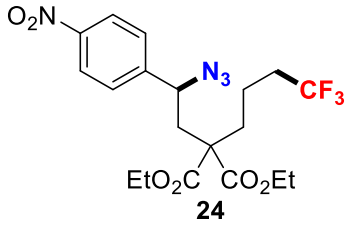
Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.2 Hz, 2H), 7.41 (d, *J* = 8.3 Hz, 2H), 4.62 (dd, *J* = 7.7, 5.5 Hz, 1H), 4.30 – 4.11 (m, 4H), 3.93 (s, 3H), 2.37 – 2.27 (m, 2H), 2.17 – 1.96 (m, 4H), 1.61 – 1.50 (m, 1H), 1.44 – 1.34 (m, 1H), 1.29 (t, *J* = 7.1 Hz, 3H), 1.26 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.27 (t, *J* = 10.7 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.75, 170.65, 166.61, 144.66, 130.48, 130.43, 126.92, 126.88 (q, *J* = 277.5 Hz), 62.34, 61.96, 61.85, 56.19, 52.38, 39.26, 33.90 (q, *J* = 28.8 Hz), 32.38, 17.25 (q, *J* = 3.0 Hz), 14.11, 14.10. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{21}H_{26}F_3N_3NaO_6$: 496.1671, found: 496.1668.



23

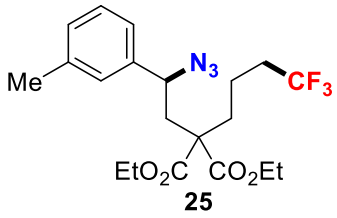
Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.4 Hz, 2H), 7.47 (d, *J* = 8.3 Hz, 2H), 4.67 (dd, *J* = 8.6, 4.4 Hz, 1H), 4.28 – 4.10 (m, 4H), 2.29 – 2.20 (m, 2H), 2.16 – 2.01 (m, 4H), 1.58 – 1.48 (m, 1H), 1.43 – 1.33 (m, 1H), 1.29 (t, *J* = 7.1 Hz, 3H), 1.28 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.24 (t, *J* = 10.7 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.70, 170.56, 145.22, 132.98, 127.61,

126.86 (q, *J* = 277.6 Hz), 118.42, 112.62, 62.31, 62.08, 61.94, 56.18, 39.67, 33.88 (q, *J* = 28.9 Hz), 32.67, 17.27 (q, *J* = 2.9 Hz), 14.12. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{20}H_{23}F_3N_4NaO_4$: 463.1569, found: 463.1566.



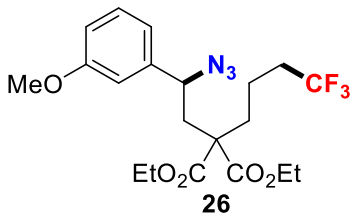
24

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.7 Hz, 2H), 7.54 (d, *J* = 8.7 Hz, 2H), 4.74 (dd, *J* = 9.0, 3.9 Hz, 1H), 4.30 – 4.09 (m, 4H), 2.30 – 2.21 (m, 2H), 2.17 – 1.97 (m, 4H), 1.57 – 1.50 (m, 1H), 1.45 – 1.35 (m, 1H), 1.30 (t, *J* = 7.1 Hz, 3H), 1.29 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.23 (t, *J* = 10.7 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.72, 170.57, 147.97, 147.18, 127.76, 126.85 (q, *J*= 277.4 Hz), 124.44, 62.13, 62.09, 61.98, 56.18, 39.81, 33.87 (q, *J*= 28.7 Hz), 32.75, 17.28 (q, *J*= 3.1 Hz), 14.14. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{23}F_3N_4NaO_6$: 483.1467, found: 483.1467.



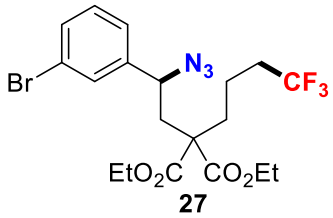
25

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (s, 1H), 7.15 (d, *J* = 7.7 Hz, 1H), 7.12 (s, 1H), 7.11 (d, *J* = 8.4 Hz, 1H), 4.47 (dd, *J* = 9.0, 4.4 Hz, 1H), 4.30 – 4.06 (m, 4H), 2.42 – 2.27 (m, 5H), 2.14 – 1.93 (m, 4H), 1.55 – 1.47 (m, 1H), 1.42 – 1.34 (m, 1H), 1.29 (t, *J* = 7.2 Hz, 3H), 1.25 (t, *J* = 7.2 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.29 (t, *J* = 10.7 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.90, 170.80, 139.51, 138.88, 129.50, 128.96, 127.58, 126.90 (q, *J* = 277.5Hz), 124.04, 62.63, 61.86, 61.78, 56.23, 38.93, 33.93 (q, *J* = 28.9Hz), 32.07, 21.59, 17.21 (q, *J* = 2.9 Hz), 14.15, 14.13. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{20}H_{26}F_3N_3NaO_4$: 452.1773, found: 452.1773.



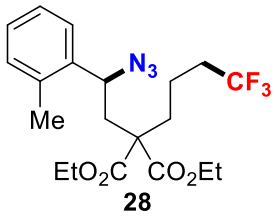
26

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (t, *J* = 7.9 Hz, 1H), 6.94 – 6.82 (m, 3H), 4.49 (dd, *J* = 8.4, 4.9 Hz, 1H), 4.28 – 4.11 (m, 4H), 3.83 (s, 3H), 2.39 – 2.27 (m, 2H), 2.14 – 1.98 (m, 4H), 1.56 – 1.47 (m, 1H), 1.42 – 1.33 (m, 1H), 1.29 (t, *J* = 7.1 Hz, 3H), 1.25 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.29 (t, *J* = 10.8 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.86, 170.78, 160.10, 141.18, 130.15, 126.90 (q, *J* = 276.3 Hz), 119.19, 114.04, 112.52, 62.57, 61.88, 61.78, 56.20, 55.43, 39.01, 33.92 (q, *J* = 28.9 Hz), 32.11, 17.22 (q, *J* = 2.9 Hz), 14.14, 14.13. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{20}H_{26}F_3N_3NaO_5$: 468.1722, found: 468.1722.



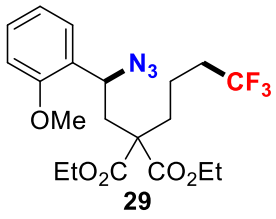
27

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.45 (m, 2H), 7.29 – 7.24 (m, 2H), 4.53 (t, *J* = 6.6 Hz, 1H), 4.26 – 4.10 (m, 4H), 2.28 (d, *J* = 6.7 Hz, 2H), 2.14 – 1.96 (m, 4H), 1.58 – 1.45 (m, 1H), 1.45 – 1.33 (m, 1H), 1.29 (t, *J* = 7.1 Hz, 3H), 1.27 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.24 (t, *J* = 10.7 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.75, 170.65, 142.07, 131.84, 130.69, 129.95, 126.88 (q, *J* = 277.4 Hz), 125.58, 123.14, 62.13, 61.99, 61.87, 56.17, 39.35, 33.91 (q, *J* = 28.9 Hz), 32.39, 17.25 (q, *J* = 2.9 Hz), 14.14, 14.13. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{23}BrF_3N_3NaO_4$: 516.0722, found: 516.0722.



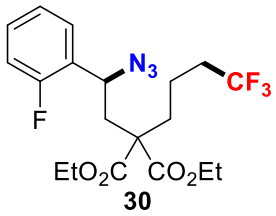
28

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.34 (m, 1H), 7.28 – 7.18 (m, 3H), 4.80 (dd, *J* = 9.8, 3.8 Hz, 1H), 4.26 – 4.08 (m, 4H), 2.40 (dd, *J* = 15.1, 9.8 Hz, 1H), 2.38 (s, 3H), 2.28 (dd, *J* = 15.0, 3.8 Hz, 1H), 2.20 – 1.95 (m, 4H), 1.57 – 1.49 (m, 1H), 1.43 – 1.31 (m, 1H), 1.28 (t, *J* = 7.1 Hz, 3H), 1.25 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.31 (t, *J* = 10.8 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.93, 170.85, 137.62, 135.36, 131.10, 128.45, 126.91 (q, *J* = 277.4 Hz), 126.80, 126.72, 61.89, 61.78, 58.75, 56.28, 38.09, 33.96 (q, *J* = 28.8 Hz), 32.19, 19.36, 17.28 (q, *J* = 3.0 Hz), 14.15, 14.12. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{20}H_{26}F_3N_3NaO_4$: 452.1773, found: 452.1773.



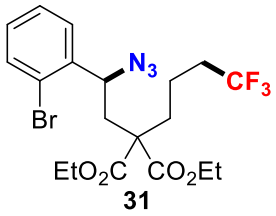
29

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, *J* = 7.6 Hz, 1H), 7.30 (t, *J* = 7.8 Hz, 1H), 7.00 (t, *J* = 7.5 Hz, 1H), 6.90 (d, *J* = 8.2 Hz, 1H), 4.98 (dd, *J* = 10.0, 3.8 Hz, 1H), 4.31 – 4.19 (m, 2H), 4.19 – 4.08 (m, 2H), 3.83 (s, 3H), 2.42 – 2.25 (m, 2H), 2.22 – 2.01 (m, 4H), 1.63 – 1.51 (m, 1H), 1.48 – 1.36 (m, 1H), 1.29 (t, *J* = 7.1 Hz, 3H), 1.23 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.36 (t, *J* = 10.8 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.04, 170.88, 156.12, 129.45, 127.86, 127.19, 126.97 (q, *J* = 276.1 Hz), 121.05, 110.69, 61.73, 61.66, 56.12, 56.03, 55.39, 37.25, 34.11 (q, *J* = 28.9 Hz), 30.95, 16.93 (q, *J* = 2.9 Hz), 14.10. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{20}H_{26}F_3N_3NaO_5$: 468.1722, found: 468.1722.



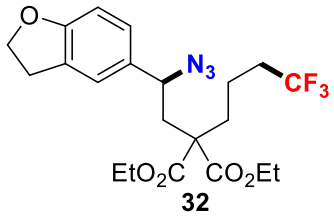
30

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (td, *J* = 7.5, 1.7 Hz, 1H), 7.36 – 7.28 (m, 1H), 7.20 (td, *J* = 7.6, 1.1 Hz, 1H), 7.13 – 7.07 (m, 1H), 4.89 (dd, *J* = 9.7, 3.8 Hz, 1H), 4.27 – 4.08 (m, 4H), 2.42 (dd, *J* = 15.0, 9.7 Hz, 1H), 2.31 (dd, *J* = 15.1, 3.8 Hz, 1H), 2.21 – 1.99 (m, 4H), 1.58 – 1.38 (m, 2H), 1.28 (t, *J* = 7.1 Hz, 3H), 1.24 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.37 (t, *J* = 11.1 Hz, 3F), -118.38 – -118.47 (m, 1F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.75, 170.67, 159.86 (d, *J* = 247.1 Hz), 130.25 (d, *J* = 8.4 Hz), 128.10 (d, *J* = 3.5 Hz), 126.92 (q, *J* = 277.6 Hz), 126.83 (d, *J* = 13.5 Hz), 124.87 (d, *J* = 3.6 Hz), 116.00 (d, *J* = 21.9 Hz), 61.89, 61.80, 56.21, 55.81, 55.78, 37.91, 33.98 (q, *J* = 29.0 Hz), 31.67, 17.13 (q, *J* = 2.9Hz), 14.10, 14.07. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{23}F_4N_3NaO_4$: 456.1522, found: 456.1522.



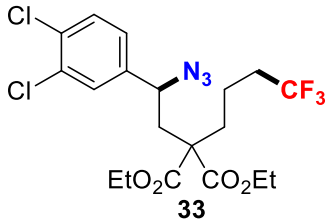
31

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.55 (m, 1H), 7.48 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.43 – 7.35 (m, 1H), 7.20 (td, *J* = 7.9, 1.7 Hz, 1H), 5.08 (dd, *J* = 10.3, 3.3 Hz, 1H), 4.35 – 4.06 (m, 4H), 2.48 – 1.98 (m, 6H), 1.71 – 1.41 (m, 2H), 1.30 (t, *J* = 7.1 Hz, 3H), 1.25 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.29 (t, *J* = 10.7 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.78, 170.67, 139.11, 133.26, 130.05, 128.45, 128.40, 126.93 (q, *J* = 277.8 Hz), 122.79, 61.92, 61.78, 61.12, 56.16, 37.97, 34.05 (q, *J*= 28.9Hz), 31.39, 17.28 (q, *J* = 2.9Hz), 14.13, 14.12. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{23}BrF_3N_3NaO_4$: 516.0721, found: 516.0714.



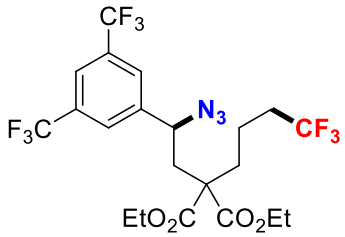
32

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 (s, 1H), 7.04 (d, *J* = 8.2 Hz, 1H), 6.77 (d, *J* = 8.2 Hz, 1H), 4.59 (t, *J* = 8.6 Hz, 2H), 4.50 – 4.36 (m, 1H), 4.29 – 4.09 (m, 4H), 3.22 (t, *J* = 8.5 Hz, 2H), 2.40 – 2.21 (m, 2H), 2.13 – 1.94 (m, 4H), 1.53 – 1.43 (m, 1H), 1.41 – 1.32 (m, 1H), 1.28 (t, *J* = 7.1 Hz, 3H), 1.24 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.30 (t, *J* = 10.3 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.88, 170.78, 160.47, 131.53, 128.01, 127.19, 126.91 (q, *J* = 277.4 Hz), 123.61, 109.46, 71.61, 62.43, 61.80, 61.74, 56.21, 38.95, 33.92 (q, *J* = 28.8 Hz), 31.96, 29.72, 17.20 (q, *J* = 2.9 Hz), 14.12, 14.11. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{21}H_{26}F_3N_3NaO_5$: 480.1722, found: 480.1716.



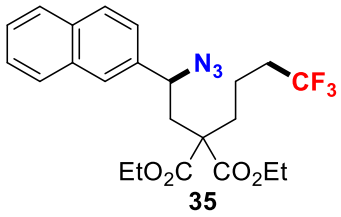
33

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, *J* = 8.3 Hz, 1H), 7.44 (s, 1H), 7.18 (dd, *J* = 8.3, 2.0 Hz, 1H), 4.56 (dd, *J* = 7.4, 5.7 Hz, 1H), 4.31 – 4.07 (m, 4H), 2.30 – 2.19 (m, 2H), 2.16 – 1.99 (m, 4H), 1.59 – 1.47 (m, 1H), 1.44 – 1.33 (m, 1H), 1.28 (q, *J* = 7.0 Hz, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.24 (t, *J* = 10.7 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.71, 170.59, 140.15, 133.30, 132.80, 131.11, 128.86, 126.88 (q, *J* =276.6Hz), 126.19, 62.04, 61.91, 61.70, 56.15, 39.55, 33.90 (q, *J* = 28.90 Hz), 32.57, 17.27 (q, *J* = 3.0 Hz), 14.12, 14.11. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{22}Cl_2F_3N_3NaO_4$: 506.0837, found: 506.0830.



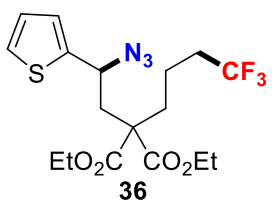
34

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.81 (s, 2H), 4.80 (dd, *J* = 8.9, 3.9 Hz, 1H), 4.33 – 4.12 (m, 4H), 2.35 – 2.22 (m, 2H), 2.22 – 2.00 (m, 4H), 1.64 – 1.50 (m, 1H), 1.46 – 1.34 (m, 1H), 1.30 (t, *J* = 7.1 Hz, 3H), 1.29 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.92 (s), -66.28 (t, *J* = 10.7 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.67, 170.55, 143.13, 132.59 (q, *J* = 33.6 Hz), 127.00, 126.97, 126.87 (d, *J* = 276.4 Hz), 123.16 (d, *J* = 272.8 Hz), 122.77 – 122.53 (m), 56.26, 40.32, 33.89 (q, *J* = 28.9 Hz), 33.02, 17.34 (q, *J* = 2.8 Hz), 14.11, 14.09. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{21}H_{22}F_9N_3NaO_4$: 574.1364, found: 574.1360.



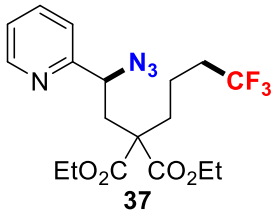
35

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.6 Hz, 1H), 7.88 – 7.82 (m, 2H), 7.77 (s, 1H), 7.56 – 7.49 (m, 2H), 7.46 (dd, *J* = 8.5, 1.7 Hz, 1H), 4.71 (dd, *J* = 8.7, 4.6 Hz, 1H), 4.26 – 4.05 (m, 4H), 2.50 – 2.36 (m, 2H), 2.19 – 1.96 (m, 4H), 1.56 – 1.47 (m, 1H), 1.46 – 1.34 (m, 1H), 1.29 (t, *J* = 7.1 Hz, 3H), 1.24 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.27 (t, *J* = 10.8 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.91, 170.80, 136.91, 133.37, 133.23, 129.21, 128.18, 127.88, 127.07 (q, *J* = 254.6 Hz), 126.76, 126.66, 126.15, 124.41, 62.85, 61.90, 61.82, 56.27, 39.04, 33.93 (q, *J* = 28.9 Hz), 32.24, 17.26 (q, *J* = 2.9 Hz), 14.16, 14.12. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{23}H_{26}F_3N_3NaO_4$: 488.1773, found: 488.1773.



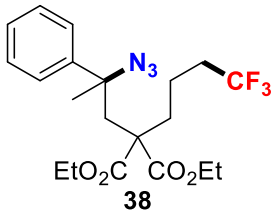
36

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.22 (m, 1H), 7.03 – 6.96 (m, 1H), 6.96 – 6.89 (m, 1H), 4.70 (t, *J* = 6.1 Hz, 1H), 4.24 – 4.03 (m, 4H), 2.44 – 2.37 (m, 2H), 2.18 – 1.83 (m, 4H), 1.49 – 1.39 (m, 1H), 1.37 – 1.28 (m, 1H), 1.20 (t, *J* = 7.1 Hz, 3H), 1.18 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.29 (t, *J* = 10.5 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.71, 170.64, 142.29, 126.99, 126.90 (q, *J* = 277.3 Hz), 125.98, 125.82, 61.97, 61.87, 57.75, 56.18, 39.41, 33.96 (q, *J* = 28.7 Hz), 32.14, 17.29 (q, *J* = 3.1 Hz), 14.12. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{17}H_{22}F_3N_3NaO_4S$: 444.1181, found: 444.1181.



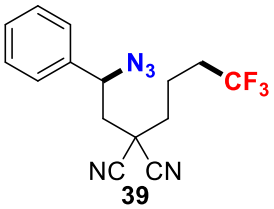
37

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (d, *J* = 4.3 Hz, 1H), 7.74 (td, *J* = 7.7, 1.7 Hz, 1H), 7.34 (d, *J* = 7.8 Hz, 1H), 7.31 – 7.23 (m, 1H), 4.55 (dd, *J* = 9.1, 4.1 Hz, 1H), 4.29 – 4.12 (m, 4H), 2.55 (dd, *J* = 15.0, 4.1 Hz, 1H), 2.47 (dd, *J* = 15.0, 9.2 Hz, 1H), 2.17 – 1.94 (m, 4H), 1.59 – 1.37 (m, 2H), 1.28 (t, *J* = 7.2 Hz, 3H), 1.26 (t, *J* = 7.2 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.29 (t, *J* = 10.8 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.89, 170.80, 158.81, 149.83, 137.27, 126.89 (q, *J* = 276.5 Hz), 123.41, 121.56, 62.88, 61.88, 61.79, 56.13, 37.36, 33.94 (q, *J* = 28.7 Hz), 32.16, 17.17 (q, *J* = 3.0 Hz), 14.10. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{18}H_{23}F_3N_4NaO_4$: 439.1569, found: 439.1569.



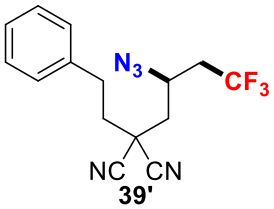
38

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 7.5 Hz, 2H), 7.36 (t, *J* = 7.6 Hz, 2H), 7.31 – 7.25 (m, 1H), 4.31 – 4.15 (m, 2H), 4.10 – 3.965 (m, 2H), 2.68 (d, *J* = 15.4 Hz, 1H), 2.58 (d, *J* = 15.4 Hz, 1H), 1.85 (td, *J* = 13.5, 4.7 Hz, 1H), 1.74 (s, 3H), 1.71 – 1.62 (m, 1H), 1.48 – 1.34 (m, 2H), 1.28 (t, *J* = 7.1 Hz, 3H), 1.18 (t, *J* = 7.1 Hz, 3H), 1.14 – 0.94 (m, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.54 (t, *J* = 10.8 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.09, 170.74, 143.39, 128.70, 127.61, 126.93 (q, *J*= 276.74 Hz), 125.64, 65.04, 61.75, 61.61, 56.43, 42.87, 33.65 (q, *J*= 28.6 Hz), 30.60, 28.57, 17.13 (q, *J*= 3.0Hz), 14.09, 14.02. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{20}H_{26}F_3N_3NaO_4$: 452.1773, found: 452.1776.



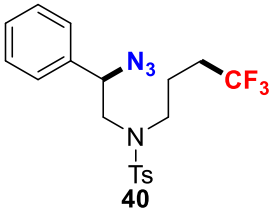
39

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.41 (m, 3H), 7.41 – 7.34 (m, 2H), 4.90 (dd, *J* = 9.9, 4.5 Hz, 1H), 2.40 (dd, *J* = 14.4, 9.9 Hz, 1H), 2.29 – 1.95 (m, 7H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.91 (t, *J* = 10.4 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.99, 129.80, 129.63, 127.04, 126.45 (q, *J* = 277.5 Hz), 114.64, 114.31, 62.86, 43.30, 37.69, 35.47, 32.91 (q, *J* = 29.6 Hz), 18.51 (q, *J* = 3.1 Hz). HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{15}H_{14}F_3N_5Na$: 344.1099, found: 344.1099.



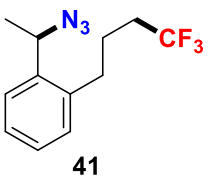
39'

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.31 (m, 2H), 7.30 – 7.20 (m, 4H), 4.17 – 4.04 (m, 1H), 3.12 – 2.93 (m, 2H), 2.63 – 2.48 (m, 1H), 2.46 – 2.36 (m, 1H), 2.34 – 2.23 (m, 2H), 2.23 – 2.07 (m, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.46 (t, *J* = 10.1 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.02, 129.13, 128.54, 127.33, 124.99 (q, *J* = 277.4 Hz), 114.63, 114.43, 54.01 (q, *J* = 2.7 Hz), 41.81, 40.66, 39.05 (q, *J* = 28.9 Hz), 35.27, 31.86. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{15}H_{14}F_3N_5Na$: 344.1099, found: 344.1099.



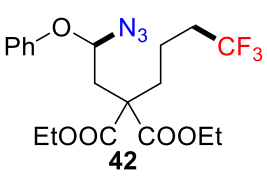
40

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.3 Hz, 2H), 7.44 – 7.35 (m, 3H), 7.35 – 7.30 (m, 4H), 4.94 (dd, *J* = 8.9, 4.9 Hz, 1H), 3.36 – 3.20 (m, 2H), 3.14 – 2.97 (m, 2H), 2.43 (s, 3H), 2.24 – 2.07 (m, 1H), 2.04 – 1.90 (m, 1H), 1.83 – 1.66 (m, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.11 (t, *J* = 10.9 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.10, 137.18, 135.61, 130.05, 129.22, 129.04, 127.40, 127.14, 127.04 (q, *J* = 276.2 Hz), 66.20, 55.09, 49.74, 31.11 (q, *J* = 29.1 Hz), 21.67, 21.26 (q, *J* = 2.8 Hz). HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{21}F_3N_4NaO_2S$: 449.1235, found: 449.1235.



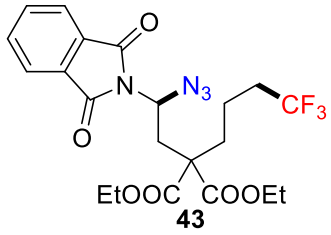
41

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.40 (m, 1H), 7.32 – 7.26 (m, 2H), 7.21 – 7.17 (m, 1H), 4.82 (q, *J* = 6.8 Hz, 1H), 2.81 – 2.70 (m, 2H), 2.23 – 2.09 (m, 2H), 1.88 (dt, *J* = 15.3, 7.7 Hz, 2H), 1.55 (d, *J* = 6.8 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.10 (t, *J* = 10.8 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.44, 138.13, 129.78, 128.37, 127.27, 127.16 (q, *J* = 277.4 Hz), 126.44, 56.73, 33.51 (q, *J* = 28.6 Hz), 31.33, 23.75 (q, *J* = 2.8 Hz), 21.22. HRMS ESI (m/z): $[M-N_2+H]^+$ calcd. for $C_{12}H_{15}F_3N$: 230.1157, found: 230.1157.



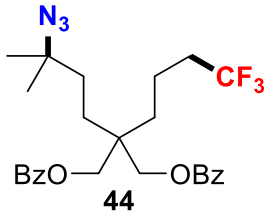
42

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 (dd, *J* = 8.6, 7.5 Hz, 2H), 7.07 (t, *J* = 7.4 Hz, 1H), 7.03 – 6.96 (m, 2H), 5.12 (dd, *J* = 7.8, 4.1 Hz, 1H), 4.24 (q, *J* = 7.2 Hz, 2H), 4.21 – 4.16 (m, 1H), 4.13 – 4.05 (m, 1H), 2.71 – 2.50 (m, 2H), 2.14 – 1.95 (m, 4H), 1.60 – 1.53 (m, 1H), 1.51 – 1.43 (m, 1H), 1.26 (t, *J* = 7.0 Hz, 3H), 1.19 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.50, 156.19, 129.91, 126.89 (q, *J* = 277.2 Hz), 123.29, 116.70, 86.83, 62.07, 61.91, 55.36, 37.64, 33.94 (q, *J* = 28.7 Hz), 32.54, 29.84, 17.32 (q, *J* = 3.1 Hz), 14.11, 13.99. ^{19}F NMR (471 MHz, $CDCl_3$) δ -66.28 (t, *J* = 11.1 Hz). HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{24}F_3N_3NaO_5$: 454.1560, found: 454.1570.



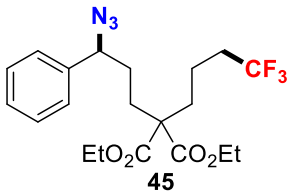
43

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.90 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.79 (dd, *J* = 5.5, 3.0 Hz, 2H), 5.73 (t, *J* = 6.6 Hz, 1H), 4.19 (qd, *J* = 7.1, 2.9 Hz, 2H), 4.17 – 4.09 (m, 1H), 4.08 – 4.00 (m, 1H), 2.84 (qd, *J* = 15.1, 6.6 Hz, 2H), 2.18 – 1.98 (m, 4H), 1.58 – 1.52 (m, 1H), 1.50 – 1.41 (m, 1H), 1.26 – 1.22 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.21, 166.82, 134.72, 131.39, 126.73 (q, *J* = 275.9 Hz), 123.89, 63.35, 61.99, 55.63, 35.01, 33.81 (q, *J* = 28.7 Hz), 32.32, 17.12, 13.93, 13.85. ^{19}F NMR (471 MHz, $CDCl_3$) δ -66.32 (t, *J* = 11.0 Hz). HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{21}H_{23}F_3N_4NaO_6$: 507.1462, found: 507.1465.



44

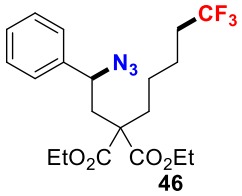
Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 – 7.98 (m, 4H), 7.60 – 7.54 (m, 2H), 7.44 (t, *J* = 7.7 Hz, 4H), 4.30 (s, 4H), 2.18 – 2.05 (m, 2H), 1.73 – 1.49 (m, 8H), 1.27 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.04 (t, *J* = 10.8 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.38, 133.38, 129.91, 129.68, 128.67, 127.04 (q, *J* = 276.5 Hz), 66.40, 61.32, 40.09, 34.53, 34.39 (q, *J* = 28.5 Hz), 31.12, 26.09, 25.85, 15.96 (q, *J* = 3.0 Hz). HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{26}H_{30}N_3O_4F_3Na$: 528.2086, found: 528.2086.



45

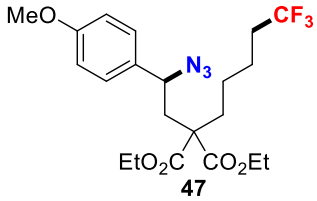
Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.31 (m, 3H), 7.31 – 7.27 (m, 2H), 4.40 (t, *J* = 6.9 Hz, 1H), 4.24 – 4.10 (m, 4H), 2.13 – 1.98 (m, 3H), 1.94 – 1.86 (m, 2H), 1.86 – 1.75 (m, 1H), 1.76 – 1.61 (m, 2H), 1.43 – 1.32 (m, 2H), 1.23 (d, *J* = 7.1 Hz, 3H), 1.21 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.28 (t, *J* = 10.8 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.08, 139.08, 129.05, 128.65 (q, *J* = 277.6

Hz), 126.96, 126.84, 66.18, 61.63, 61.60, 56.94, 33.95 (q, *J* = 28.7 Hz), 31.70, 30.91, 29.17, 17.05 (q, *J* = 2.3 Hz), 14.19, 14.17. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{20}H_{26}N_3O_4F_3Na$: 452.1773, found: 452.1770.



46

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.31 (m, 3H), 7.31 – 7.26 (m, 2H), 4.40 (t, *J* = 6.9 Hz, 1H), 4.28 – 4.08 (m, 4H), 2.14 – 1.96 (m, 3H), 1.97 – 1.86 (m, 2H), 1.86 – 1.75 (m, 1H), 1.75 – 1.58 (m, 3H), 1.48 – 1.29 (m, 2H), 1.24 (t, *J* = 7.1 Hz, 2H), 1.21 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.28 (t, *J* = 10.8 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.07, 139.10, 129.04, 128.64, 126.97, 126.92 (d, *J* = 276.3 Hz), 66.20, 61.62, 61.59, 56.97, 33.97 (q, *J* = 28.7 Hz), 31.74, 30.92, 29.21, 17.07 (d, *J* = 3.0 Hz), 14.19, 14.16. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{20}H_{26}N_3O_4F_3Na$: 452.1773, found: 452.1770.



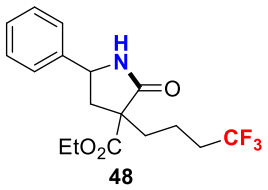
47

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (d, *J* = 8.7 Hz, 2H), 6.91 (d, *J* = 8.6 Hz, 2H), 4.45 (dd, *J* = 8.9, 4.6 Hz, 1H), 4.20 (q, *J* = 7.2 Hz, 2H), 4.16 – 4.04 (m, 2H), 3.81 (s, 3H), 2.38 (dd, *J* = 14.9, 8.9 Hz, 1H), 2.30 (dd, *J* = 14.9, 4.6 Hz, 1H), 2.11 – 1.87 (m, 4H), 1.59 – 1.50 (m, 2H), 1.32 – 1.07 (m, 2H), 1.27 (t, *J* = 7.2 Hz, 3H), 1.23 (t, *J* = 7.2 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.32 (t, *J* = 10.9 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.13, 171.02, 159.84, 131.61, 128.35, 127.16 (q, *J* = 277.5 Hz), 114.33, 62.13, 61.70, 61.65, 56.24, 55.45, 38.79, 33.46 (q, *J* = 28.6 Hz), 32.43, 23.40, 22.20 (q, *J* = 3.0 Hz), 14.15, 14.12. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{21}H_{28}N_3O_5F_3Na$: 482.1879, found: 482.1880.

Derivatization studies

General procedure C for reduction

13 (0.2 mmol) and Pd/C (10%) were combined in a 25 mL oven-dried Schleck tube. The vessel was evacuated and backfilled with H_2. After that, MeOH was added via syringe H_2 stream. The tube was sealed with a rubber cap and inserted with a balloon of H_2. Until completion, the reaction mixture was diluted with EtOAc (10 mL) and filtered through a pad of celite. The filtrate was concentrated, and the residue was then purified by flash column chromatography to give the amide.

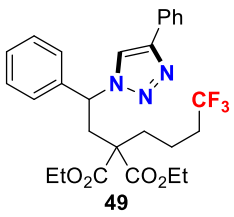


48

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.25 (m, 5H), 6.92 (s, 0.5H), 6.74 (s, 0.5H), 4.87 (t, *J* = 7.8 Hz, 0.5H), 4.71 (t, *J* = 7.4 Hz, 0.5H), 4.34 – 4.20 (m, 1H), 4.16 (q, *J* = 7.1 Hz, 1H), 2.96 (dd, *J* = 13.1, 6.8 Hz, 0.5H), 2.63 – 2.46 (m, 1H), 2.25 – 1.42 (m, 6.5H), 1.31 (t, *J* = 7.1 Hz, 1.5H), 1.22 (t, *J* = 7.1 Hz, 1.5H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.20 (t, *J* = 10.8 Hz, 3F), -66.37 (t, *J* = 10.8 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.49, 174.72, 171.38, 170.83, 141.91, 141.52, 129.12, 128.94, 128.32, 128.19, 126.97 (q, *J* = 277.75 Hz), 126.90 (q, *J* = 277.75 Hz),126.05, 125.80, 62.06, 61.87, 56.37, 56.02, 55.44, 55.38, 41.45, 40.48, 33.98 (q, *J* = 28.3 Hz),33.94 (q, *J* = 28.3 Hz), 33.24, 33.05, 17.66 – 17.45 (m), 14.19, 14.02. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{17}H_{20}F_3NO_3Na$: 366.1293, found: 366.1287.

General procedure D for the synthesis of triazoles

CuI (0.01 mmol) was added in a 25 mL oven-dried sealed tube. The vessel was evacuated and backfilled with N_2 (repeated for 3 times), after that, **13** (0.1 mmol), phenylacetylene (0.3 mmol, 3.0 equiv) and THF (2.0 mL) were then added via syringe under N_2. The tube was sealed with a Teflon lined cap and moved into a preheated oil bath at 60 °C for 16 h. The reaction mixture was then cooled to room temperature, diluted with EtOAc (10 mL) and filtered through a pad of celite. The filtrate was concentrated, and the residue was then purified by flash column chromatography to give the triazoles.

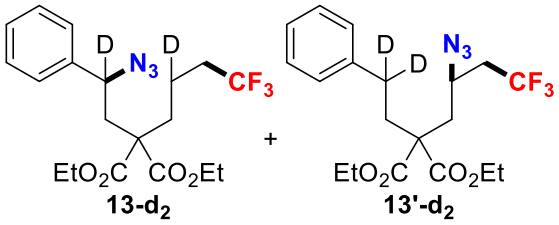


49

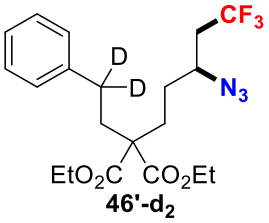
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.2 Hz, 2H), 7.70 (s, 1H), 7.44 – 7.28 (m, 8H), 5.80 (dd, *J* = 8.0, 4.3 Hz, 1H), 4.11 – 4.02 (m, 2H), 4.00 – 3.80 (m, 2H), 3.34 (dd, *J* = 15.1, 8.4 Hz, 1H), 2.91 (dd, *J* = 15.2, 3.9 Hz, 1H), 2.07 – 1.87 (m, 4H), 1.57 – 1.47 (m, 1H), 1.43 – 1.35 (m, 1H), 1.21 (t, *J* = 7.2 Hz, 3H), 1.16 (t, *J* = 7.6 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.24 (t, *J* = 10.8 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.60, 170.39, 147.82, 139.49, 130.50, 129.17, 128.90, 128.83, 128.27, 126.94, 126.82 (q, *J* = 277.4 Hz), 125.73, 119.69, 61.94, 61.90, 56.42, 37.98, 33.77 (q, *J* = 28.9 Hz), 32.46, 17.22 (q, *J* = 2.9 Hz), 13.99, 13.93. HRMS ESI (m/z): $[M+H]^+$ calcd. for $C_{27}H_{31}F_3N_3O_4$: 518.2267, found: 518.2274.

IV. Mechanistic Research

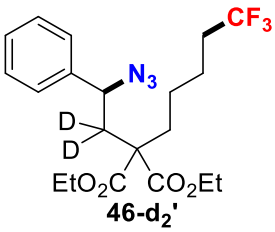
1,5- or 1,6-deuterium shift



Prepared according to General Procedure B and obtained as colorless oil. The product **13-d$_2$** and **13'-d$_2$** was obtained as mixture with the ratio of 1.8: 1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.28 (m, 4H), 7.26 – 7.12 (m, 1H), 4.29 – 4.08 (m, 4H), 3.80 – 3.71 (m, 0.25H), 2.45 – 2.28 (m, 2H), 2.20-1.95 (m, 4H), 1.55 –1.34 (m, 0.75H), 1.31 – 1.22 (m, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.95 (t, *J* = 10.4 Hz, 0.75F), -66.28 (t, *J* = 10.8 Hz, 2.25F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.95, 170.89, 170.87, 170.77, 140.82, 139.50, 129.10, 128.76, 128.72, 128.44, 126.97, 126.91 (q, *J* = 277.3 Hz), 126.45, 125.48 (q, *J* = 278.4 Hz), 62.22 (t, *J* = 21.6 Hz), 62.10, 61.86, 61.78, 56.19, 56.13, 53.64 (q, *J* = 2.7 Hz), 39.63 (q, *J* = 28.4 Hz), 38.87, 38.03, 34.83, 33.83 (q, *J* = 28.8 Hz), 32.03, 29.72, 17.05 – 16.52 (m), 14.17, 14.13, 14.11. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{22}D_2F_3N_3NaO_4$: 440.1742, found: 440.1735.



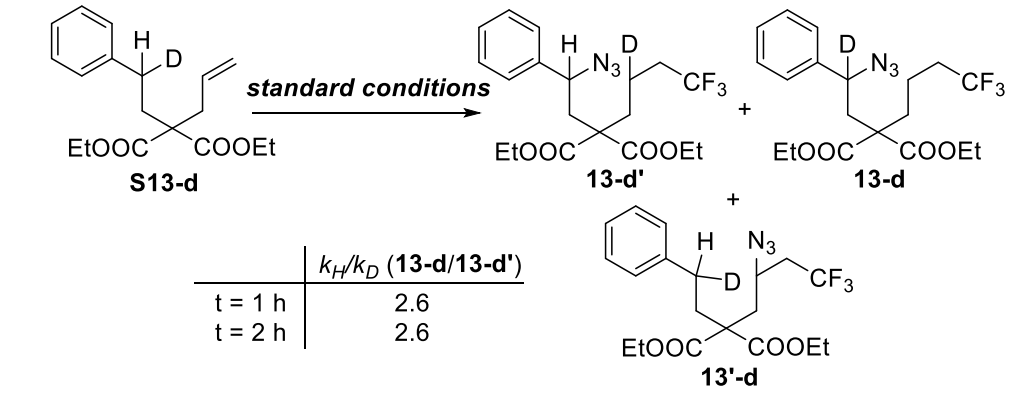
Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, C_6D_6) δ 7.02 (d, *J* = 2.2 Hz, 3H), 6.99 – 6.88 (m, 1H), 3.84 (qd, *J* = 7.1, 1.3 Hz, 4H), 2.99 (dt, *J* = 8.1, 4.0 Hz, 1H), 2.19 (s, 2H), 2.03 (ddd, *J* = 13.9, 11.6, 5.6 Hz, 1H), 1.86 (ddd, *J* = 14.0, 11.5, 5.4 Hz, 1H), 1.64 – 1.47 (m, 1H), 1.46 – 1.30 (m, 1H), 1.24 – 1.09 (m, 2H), 0.81 (t, *J* = 7.1 Hz, 3H), 0.80 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, C_6D_6) δ -63.83 (t, *J* = 10.6 Hz, 3F). ^{13}C NMR (101 MHz, C_6D_6) δ 171.03, 171.01, 141.59, 128.92, 128.70, 128.30, 128.06, 127.82, 126.57, 126.16 (d, *J* = 277.2 Hz), 61.34, 57.39, 56.53 (q, *J* = 2.6 Hz), 37.88 (q, *J* = 28.0 Hz), 35.21, 29.44, 29.01, 14.10. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{22}D_2F_3N_3NaO_4$: 454.1899, found: 454.1903.



Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (400 MHz, C_6D_6) δ 7.20 – 7.13 (m, 2H), 7.10 – 6.99 (m, 3H), 4.57 (s, 1H), 4.03 (q, *J* = 7.1 Hz, 2H), 4.00 – 3.85 (m, 2H), 1.98 (dddd, *J* = 39.7, 14.2, 12.1, 4.9 Hz, 2H), 1.49 (ddd, *J* = 15.4, 8.8, 4.4 Hz, 2H), 1.24 – 1.12 (m, 2H), 1.09 – 0.83 (m, 2H), 0.98 (t, *J* = 7.1 Hz, 3H), 0.92 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, C_6D_6) δ -66.15 (t, *J* = 11.0 Hz, 3F). ^{13}C NMR (101 MHz, C_6D_6) δ 170.96, 170.83, 140.20, 129.20, 128.70, 127.68 (q, *J* = 276.2 Hz), 127.20, 62.94, 61.47, 61.44, 56.37, 33.63, 33.21 (q, *J* = 28.3 Hz), 32.93, 23.48, 22.20 (q, *J* = 2.9 Hz), 14.04, 13.99. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{19}H_{22}D_2F_3N_3NaO_4$: 454.1899, found: 454.1894.

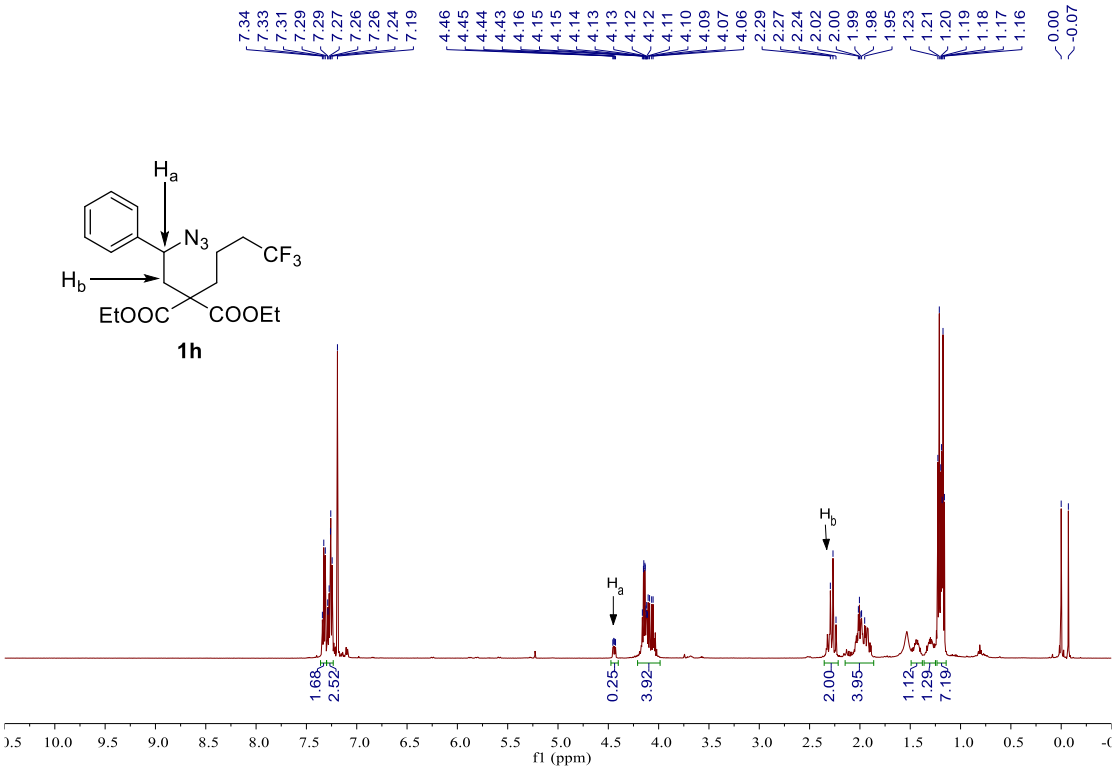
KIE experiments

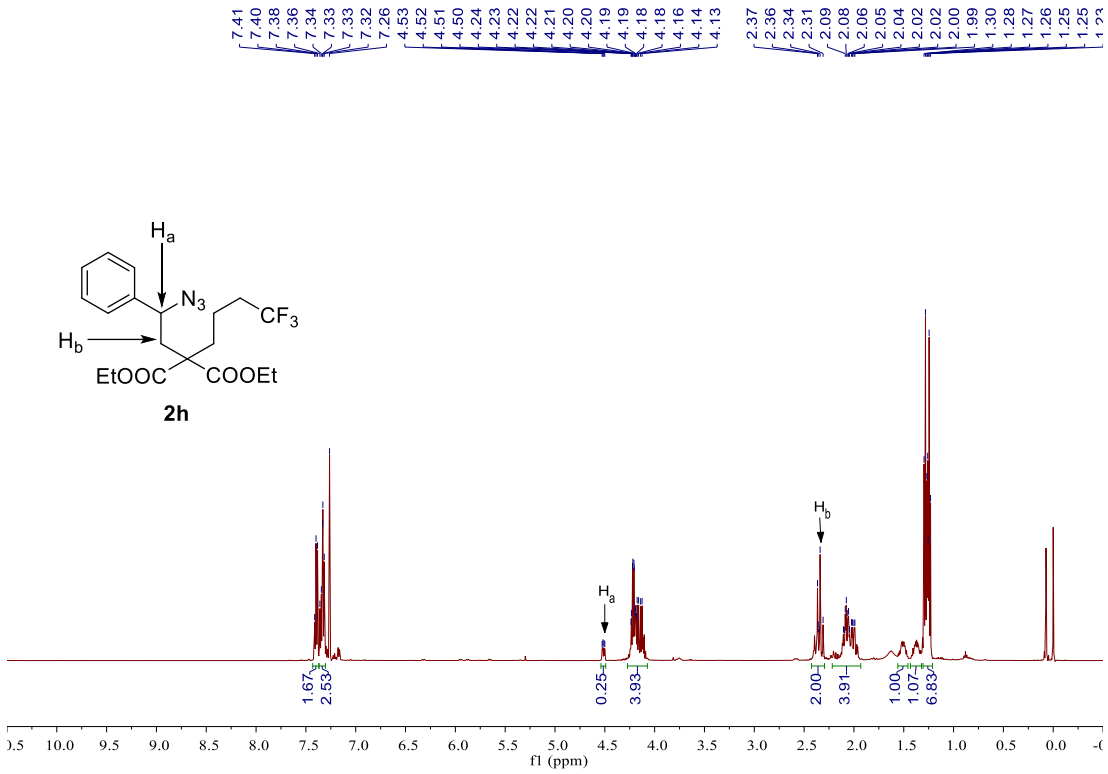
Intramolecular



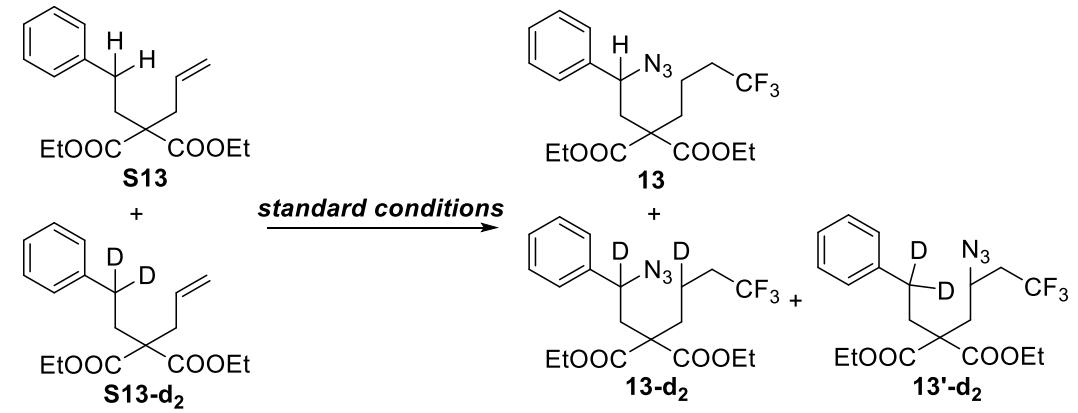
	k_H/k_D (**13-d**/**13-d'**)
t = 1 h	2.6
t = 2 h	2.6

Fe $(acac)_3$ (10 mol%, 0.01 mmol, 3.53 mg), Togni-II (1.25 equiv, 0.125 mmol, 39.5 mg) were combined in a 25 mL oven-dried sealed tube. The vessel was evacuated and backfilled with N_2 (repeated for 3 times), after that, monodeuterated alkene **13-d** (1 equiv, 0.1 mmol), $TMSN_3$ (3.0 equiv, 0.3 mmol) and superdry DCM (1.0 mL) were then added via syringe under N_2. The tube was sealed with a Teflon lined cap and moved into a preheated oil bath at 50 °C for 12 h. The reaction mixture was then cooled to room temperature, diluted with EtOAc (10 mL) and filtered through a pad of celite. The filtrate was concentrated, and the residue was then purified by flash column chromatography. Both recovered substrate and product ratios were determined by ^1H NMR.





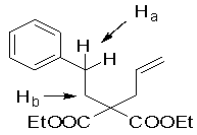
Intermolecular (one-pot)



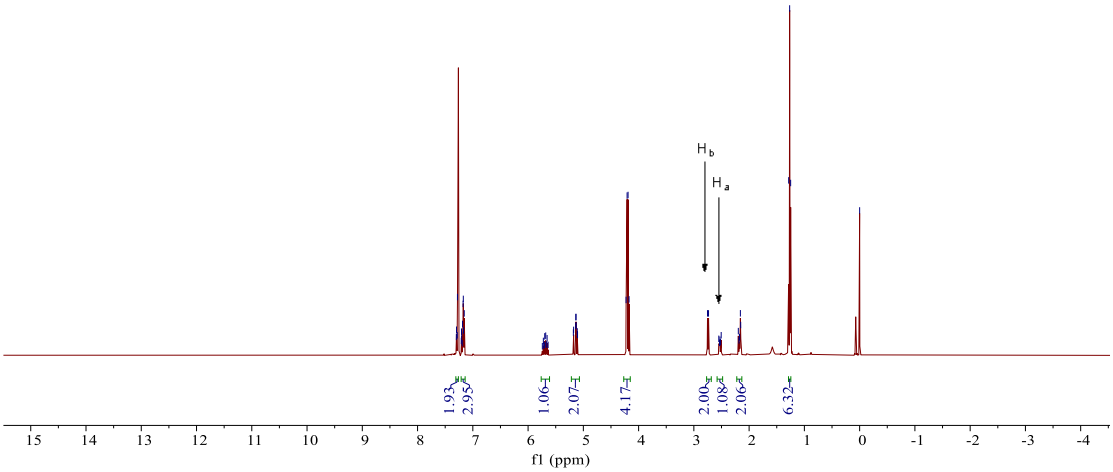
	k_H/k_D (**13**/**13-d$_2$**)	k_H/k_D (**S13**/**S13-d$_2$**)
t = 1 h	1.4	1.0
t = 1.5 h	1.7	1.0

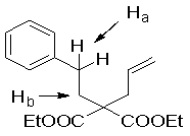
Fe (acac)$_3$ (10 mol%, 0.01 mmol, 3.53 mg), Togni-II (1.25 equiv, 0.125 mmol, 39.5 mg) were combined in a 25 mL oven-dried sealed tube. The vessel was evacuated and backfilled with N_2 (repeated for 3 times), after that, alkene **S13** (0.5 equiv, 0.05mmol), deuterated alkene **S13-d$_2$** (0.5 equiv, 0.05mmol), $TMSN_3$ (3.0 equiv, 0.3 mmol) and superdry DCM (1.0 mL) were then added via syringe under N_2. The tube was sealed with a Teflon lined cap and moved into a preheated oil bath at 50 ^oC for 12 h. The reaction mixture was then cooled to room temperature, diluted with EtOAc (10 mL) and filtered through a pad of celite. The filtrate was concentrated, and the residue was then purified by flash column chromatography. Both recovered substrate and product

ratios were determined by ^{1}H NMR.

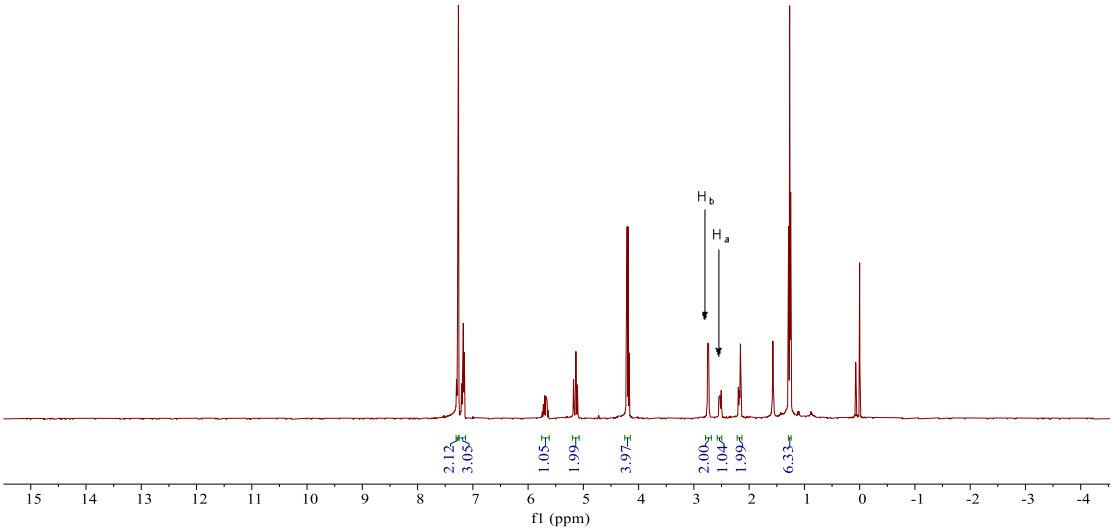


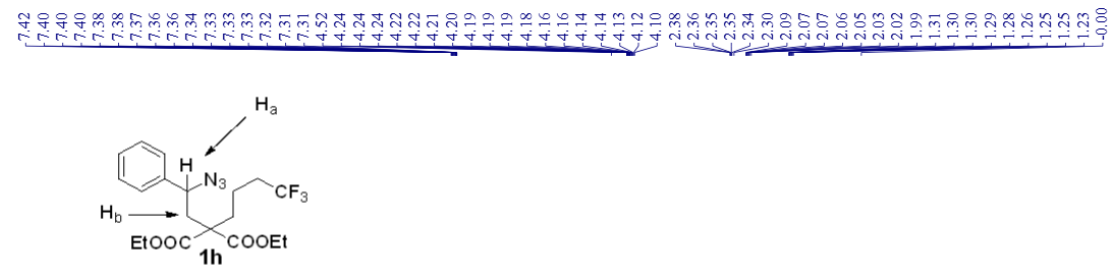
1h





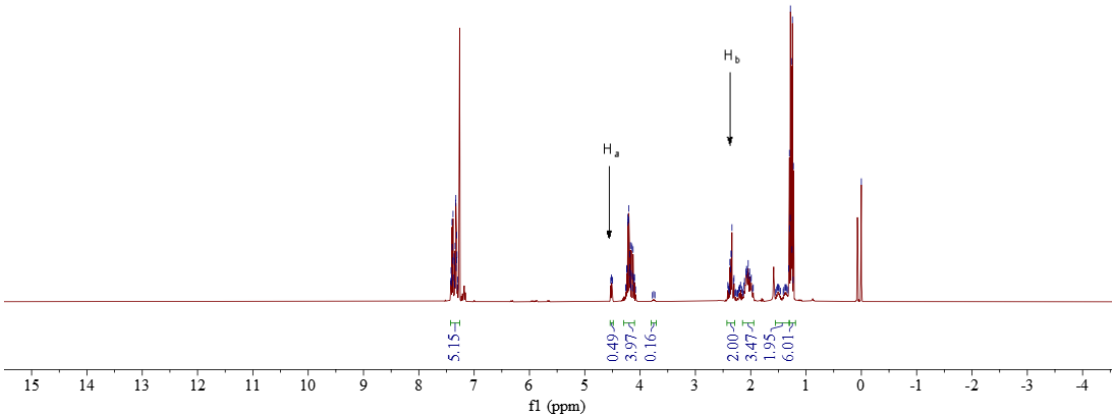
1.5h

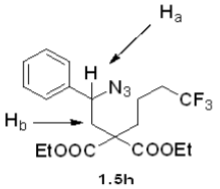




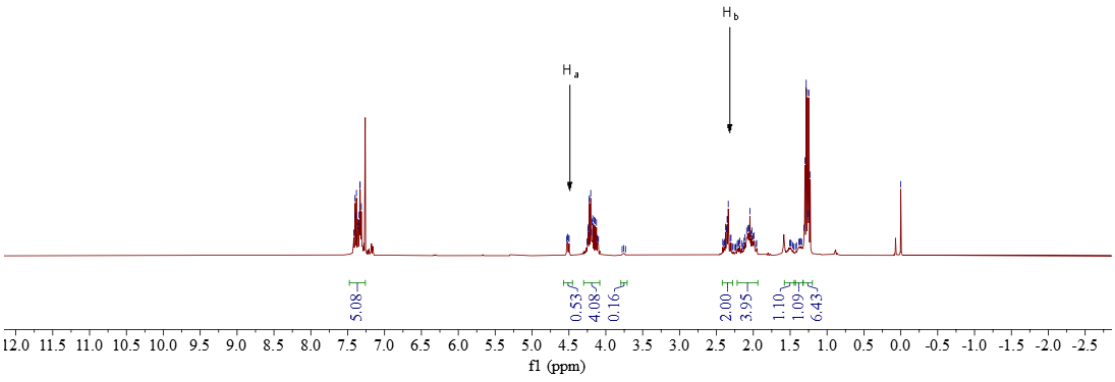
Ha
H
N3
CF3
Hb
EtOOC
COOEt

1h

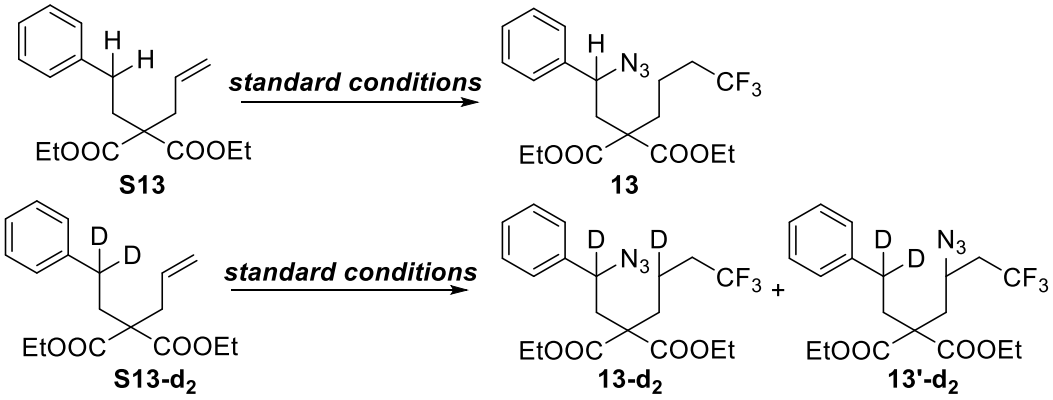

Hb
Ha
5.15
0.49
3.97
0.16
2.00
3.47
1.95
6.01
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


Ha
H
N3
CF3
Hb
EtOOC
COOEt

1.5h

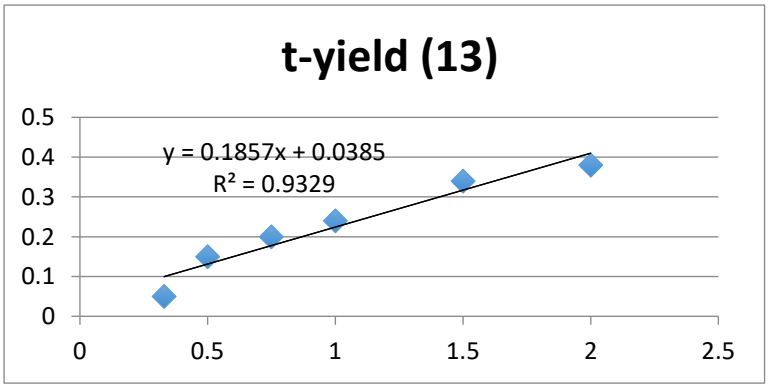

Hb
Ha
5.08
0.53
4.08
0.16
2.00
3.95
1.10
1.09
6.43
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5
f1 (ppm)

Intermolecular (parallel)

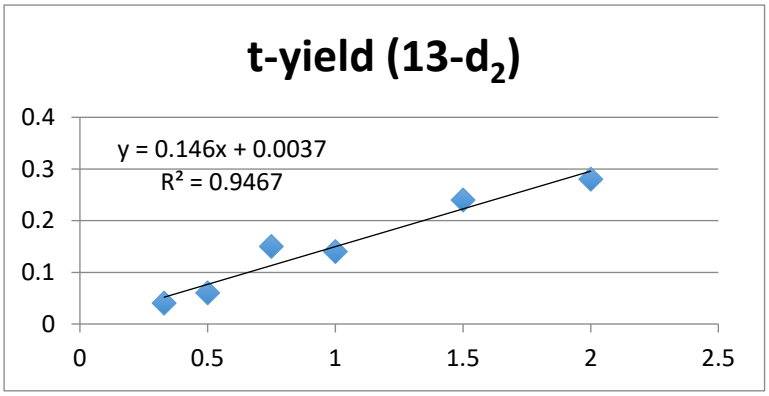


Reaction progress was monitored by ^{19}F NMR. Rate constants were determined by adding the corresponding products with $PhCF_3$ as internal standard over time and extracting the slope after linear fitting of the data (simulating the linear function and slope as the rate constants)

t/h	Reaction of **S13** (yield of product **13**)	t/h	Reaction of **S13-d2** (yield of product **13-d2**)
0.33	0.05	0.33	0.04
0.50	0.15	0.50	0.06
0.75	0.2	0.75	0.15
1.00	0.24	1.00	0.14
1.50	0.34	1.50	0.24
2.00	0.38	2.00	0.28



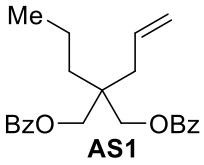
Reaction of **S13**: y = 0.1857 (k_H)x+0.0385, R^2 = 0.9329



Reaction of **S13-d2**: y = 0.0.1460 (k_D)x+0.0037, R^2 = 0.9467

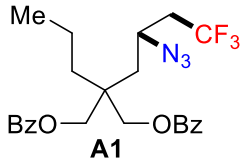
k_H/k_D = 0.1857/0.1460 = 1.272

V. Alternative Testings



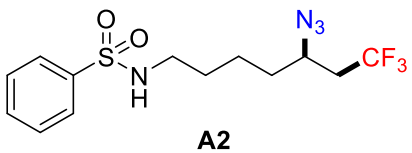
AS1

Prepared according to general procedure A and obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 (d, *J* = 7.3 Hz, 4H), 7.56 (t, *J* = 7.4 Hz, 2H), 7.43 (t, *J* = 7.8 Hz, 4H), 5.92 – 5.79 (m, 1H), 5.20 – 5.07 (m, 2H), 4.31 (d, *J* = 2.7 Hz, 4H), 2.32 (d, *J* = 7.5 Hz, 2H), 1.52 –1.40 (m, 4H), 0.94 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.52, 133.20, 132.76, 130.22, 129.71, 128.60, 119.18, 67.05, 40.65, 36.78, 34.61, 16.34, 15.03. ESI (m/z): $[M+Na]^+$ calcd. for $C_{23}H_{26}NaO_4$: 389.1723, found: 389.1725.



A1

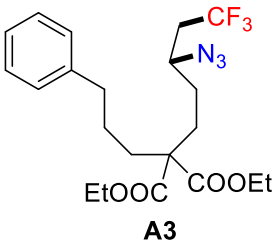
Prepared according to General Procedure B and obtained as colorless oil.^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (ddd, *J* = 7.1, 6.3, 1.3 Hz, 4H), 7.61 – 7.54 (m, 2H), 7.44 (t, *J* = 7.8 Hz, 4H), 4.47 – 4.31 (m, 4H), 3.96 – 3.76 (m, 1H), 2.57 – 2.42 (m, 1H), 2.40 – 2.28 (m, 1H), 1.95 – 1.90 (m, 1H), 1.72 (dd, *J* = 15.1, 2.1 Hz, 1H), 1.68 – 1.61 (m, 1H), 1.59 – 1.53 (m, 1H), 1.50 – 1.42 (m, 1H), 1.40 – 1.33 (m, 1H), 0.97 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.37, 133.42, 133.37, 129.71, 129.70, 128.68, 128.66, 127.63 (q, *J* = 274.7 Hz), 66.93, 66.68, 52.88, 40.44, 40.03 (q, *J* = 28.0 Hz), 36.80, 35.01, 16.48, 14.96. ^{19}F NMR (471 MHz, $CDCl_3$) δ -63.70 (t, *J* = 10.3 Hz). ESI (m/z): $[M+Na]^+$ calcd. for $C_{24}H_{26}F_3N_3NaO_4$: 500.1768, found: 500.1754.



A2

Prepared according to General Procedure B and obtained as colorless oil.^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.2 Hz, 2H), 7.62 – 7.57 (m, 1H), 7.53 (t, *J* = 7.7 Hz, 2H), 5.02 – 4.90 (m, 1H), 3.56 (tt, *J* = 8.9, 4.9 Hz, 1H), 2.97 (q, *J* = 6.5 Hz, 2H), 2.25 (dtdt, *J* = 26.0, 15.2, 10.0, 4.7 Hz, 2H), 1.56 – 1.33 (m, 7H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.95, 132.87, 129.31, 128.89,

127.14,125.72 (q, J = 277.4 Hz), 56.69 (q, J =2.4 Hz), 42.93, 38.58 (q, J = 28.1 Hz), 34.22, 29.25, 22.70. ^{19}F NMR (471 MHz, $CDCl_3$) δ -64.03 (t, J = 10.7 Hz). ESI (m/z): $[M+Na]^+$ calcd. for $C_{13}H_{17}F_3N_4NaO_2S$: 373.0917, found: 373.0917.



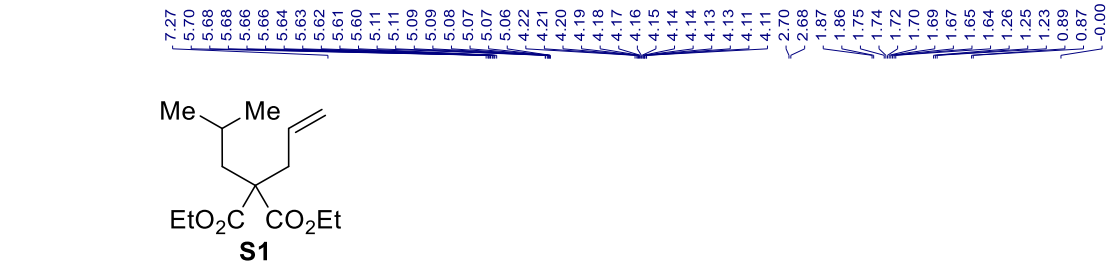
A3

Prepared according to General Procedure B and obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 (d, J = 7.3 Hz, 2H), 7.23 – 7.13 (m, 3H), 4.17 (qd, J = 7.1, 1.4 Hz, 4H), 3.57 (tt, J = 8.4, 4.6 Hz, 1H), 2.68 – 2.58 (m, 2H), 2.35 – 2.16 (m, 2H), 2.09 – 2.00 (m, 1H), 1.96 – 1.85 (m, 3H), 1.55 – 1.47 (m, 2H), 1.45 – 1.35(m, 2H), 1.22 (td, J = 7.1, 1.0 Hz, 7H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.23, 141.58, 128.45, 128.41, 125.99, 125.55 (q, J =277.2 Hz), 61.40, 56.89, 56.63 (q, J = 3.0 Hz), 38.39 (q, J =28.1 Hz), 35.76, 31.86, 29.71, 29.24, 28.31, 25.69, 14.05. ^{19}F NMR (471 MHz, $CDCl_3$) δ -64.06 (t, J = 10.4 Hz). ESI (m/z): $[M+Na]^+$ calcd. for $C_{21}H_{28}F_3N_3NaO_4$: 466.1924, found: 466.1915.

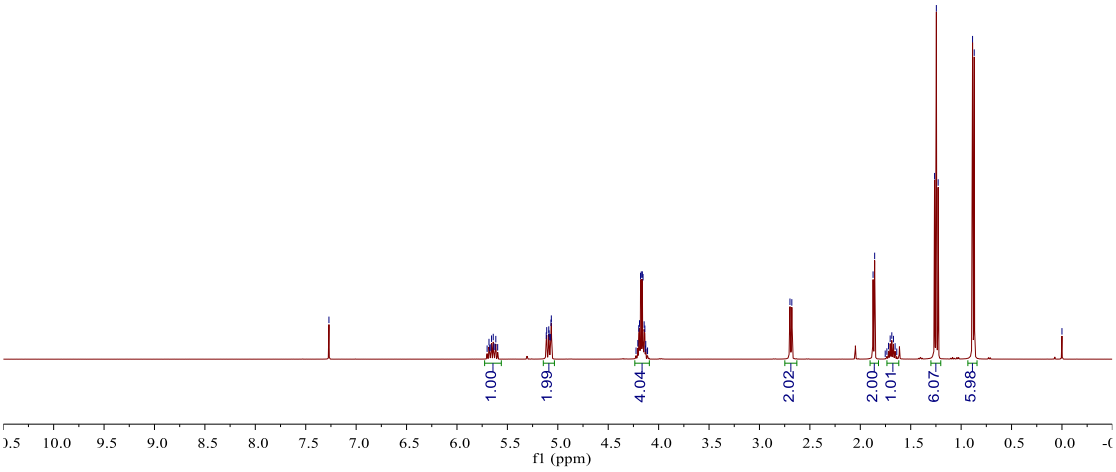
Reference

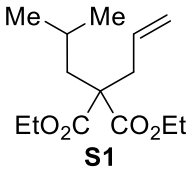
[1] P. Eisenberger, S. GIschig, A. Togni, *Chem. Eur. J.* **2006**, *12*, 2579.
[2] D. F. González, J. P. Brand, J. Waser, *Chem. Eur. J.* **2010**, *16*, 9457.
[3] L. Li, H. Luo, Z. Zhao, Y. Li, Q. Zhou, J. Xu, J. Li, Y.-N. Ma, *Org. Lett.* **2019**, *21*, 9228.
[4] W. Shu, E. Merino, C. Nevado, *ACS Catal.* **2018**, *8*, 6401.

NMR Spectrum Data for New Compounds

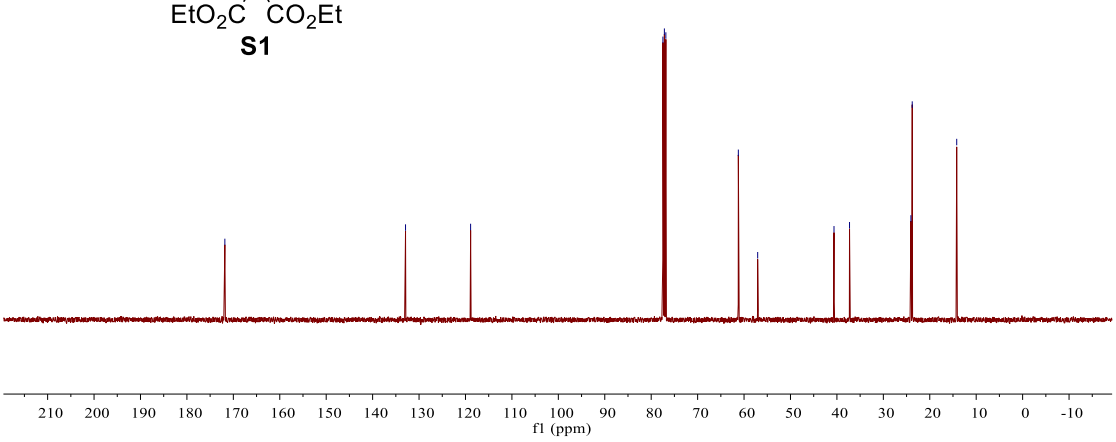


S1





S1




7.27
5.69
5.66
5.64
5.62
5.11
5.09
5.06
4.21
4.20
4.19
4.19
4.18
4.17
4.17
4.16
4.15
4.15
4.14
4.13
4.12
2.72
2.70
2.68
2.66
2.00
1.99
1.96
1.95
1.79
1.77
1.76
1.74
1.46
1.45
1.43
1.42
1.35
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1.33
1.31
1.30
1.28
1.27
1.26
1.25
1.24
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1.22
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1.13
1.11
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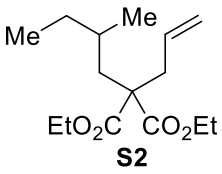
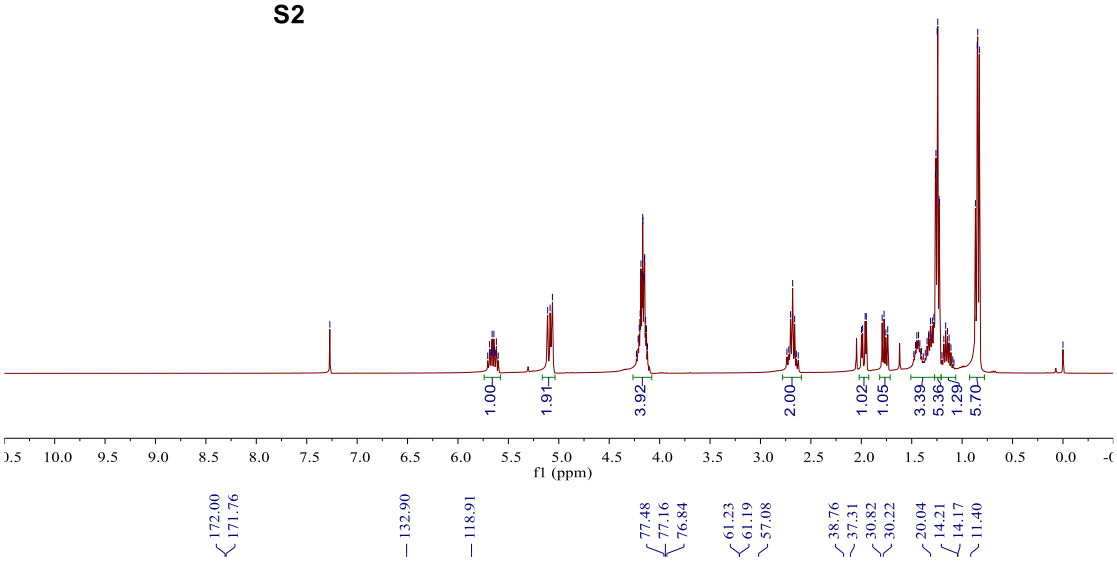
0.85
0.85
0.83
-0.00


Me
Me
EtO2C
CO2Et

S2


1.00
1.91
3.92
2.00
1.02
1.05
3.39
5.36
1.29
5.70
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)

172.00
171.76
132.90
118.91
77.48
77.16
76.84
61.23
61.19
57.08
38.76
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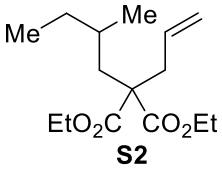
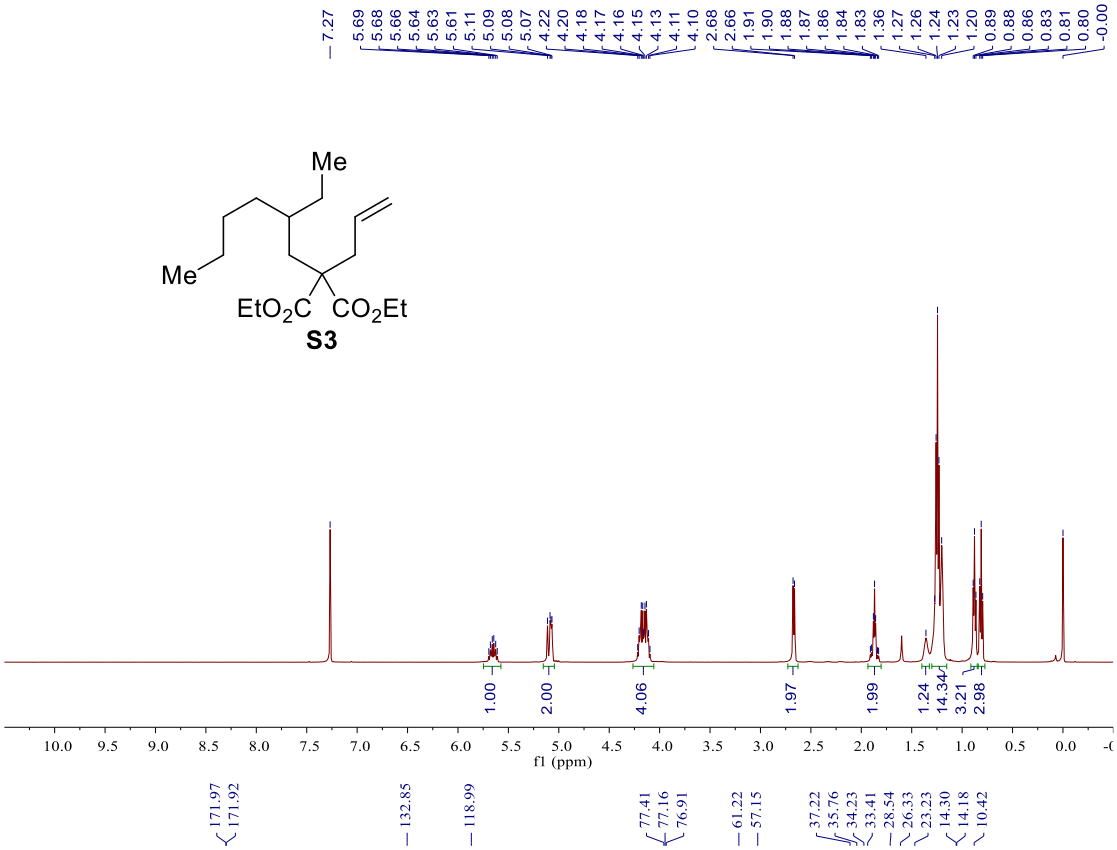
30.82
30.22
20.04
14.21
14.17
11.40


Me
Me
EtO2C
CO2Et

S2

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.27
5.69
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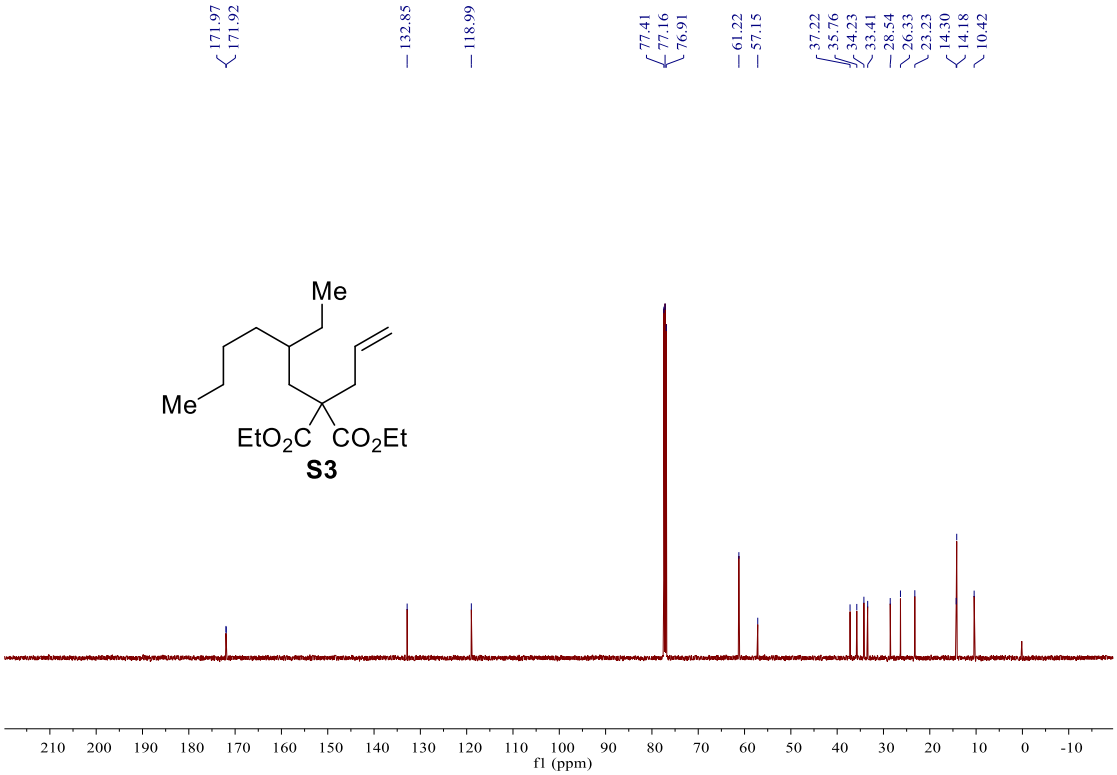
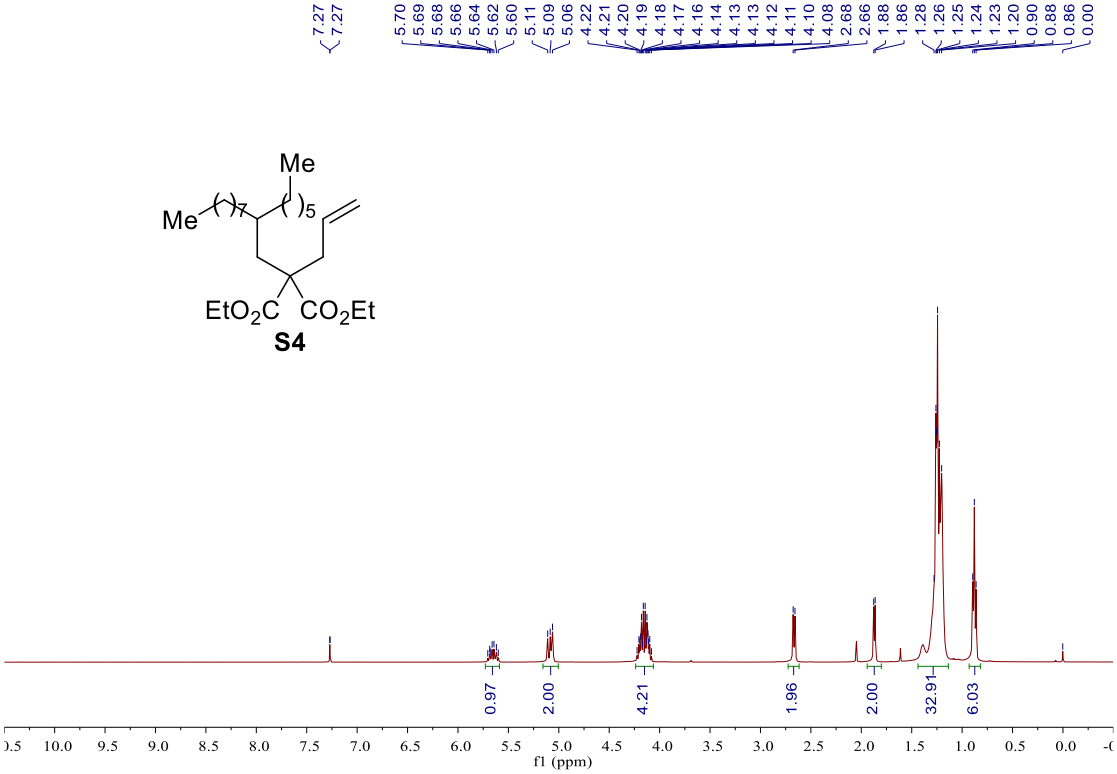
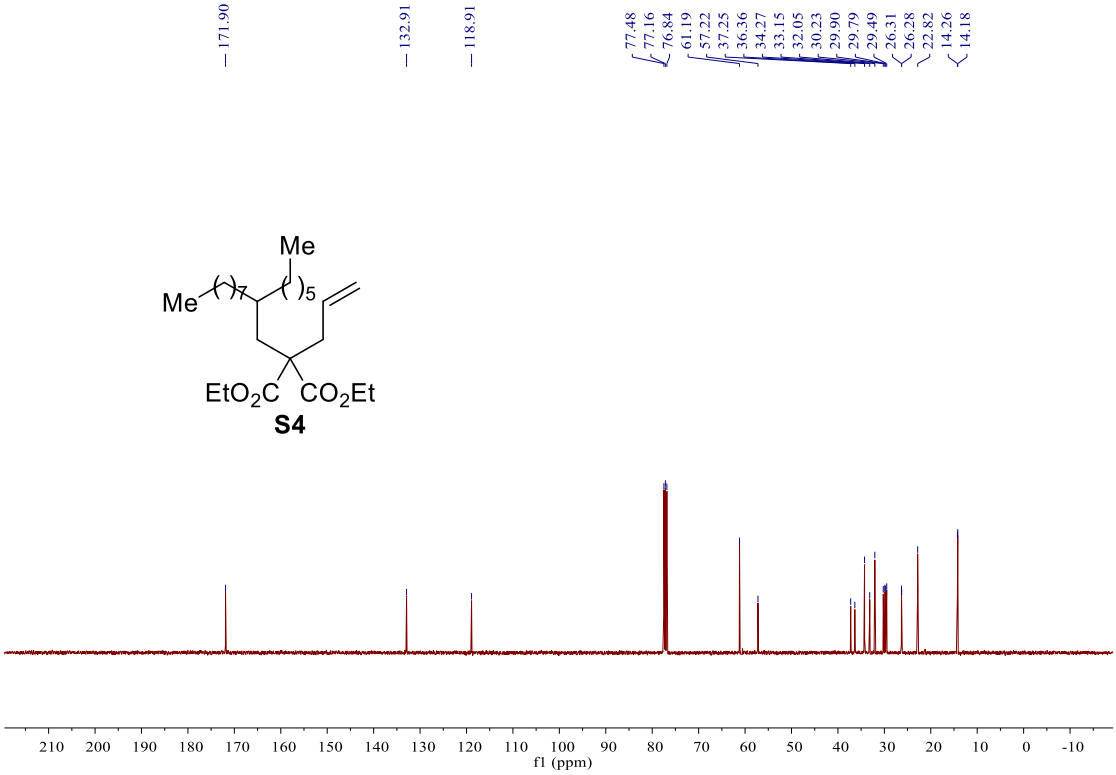
5.64
5.63
5.61
5.11
5.09
5.08
5.07
4.22
4.20
4.18
4.17
4.16
4.15
4.13
4.11
4.10
2.68
2.66
1.91
1.90
1.88
1.87
1.86
1.84
1.83
1.36
1.27
1.26
1.24
1.23
1.20
0.89
0.88
0.86
0.83
0.81
0.80
-0.00
Me
Me
EtO2C CO2Et
S3
1.00
2.00
4.06
1.97
1.99
1.24
14.34
3.21
2.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


171.97
171.92
132.85
118.99
77.41
77.16
76.91
61.22
57.15
37.22
35.76
34.23
33.41
28.54
26.33
23.23
14.30
14.18
10.42
Me
Me
EtO2C CO2Et
S3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.27
7.27
5.70
5.69
5.68
5.66
5.64
5.62
5.60
5.11
5.09
5.06
4.22
4.21
4.20
4.19
4.18
4.17
4.16
4.14
4.13
4.13
4.12
4.11
4.10
4.08
2.68
2.66
1.88
1.86
1.28
1.26
1.25
1.24
1.23
1.20
0.90
0.88
0.86
0.00
Me
Me
5
7
EtO2C
CO2Et
S4
0.97
2.00
4.21
1.96
2.00
32.91
6.03
f1 (ppm)


171.90
132.91
118.91
77.48
77.16
76.84
61.19
57.22
37.25
36.36
34.27
33.15
32.05
30.23
29.90
29.79
29.49
26.31
26.28
22.82
14.26
14.18
Me
Me
5
7
EtO2C
CO2Et
S4
f1 (ppm)


7.28
5.68
5.66
5.65
5.63
5.63
5.62
5.61
5.13
5.12
5.11
5.10
5.08
4.21
4.20
4.20
4.19
4.18
4.17
4.16
4.15
4.14
4.13
3.91
3.90
3.88
3.88
3.37
3.37
3.34
3.34
3.31
3.31
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2.68
1.90
1.89
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1.61
1.60
1.59
1.59
1.58
1.52
1.52
1.49
1.48
1.37
1.36
1.34
1.33
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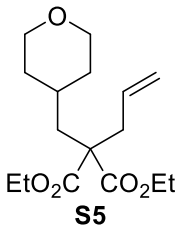
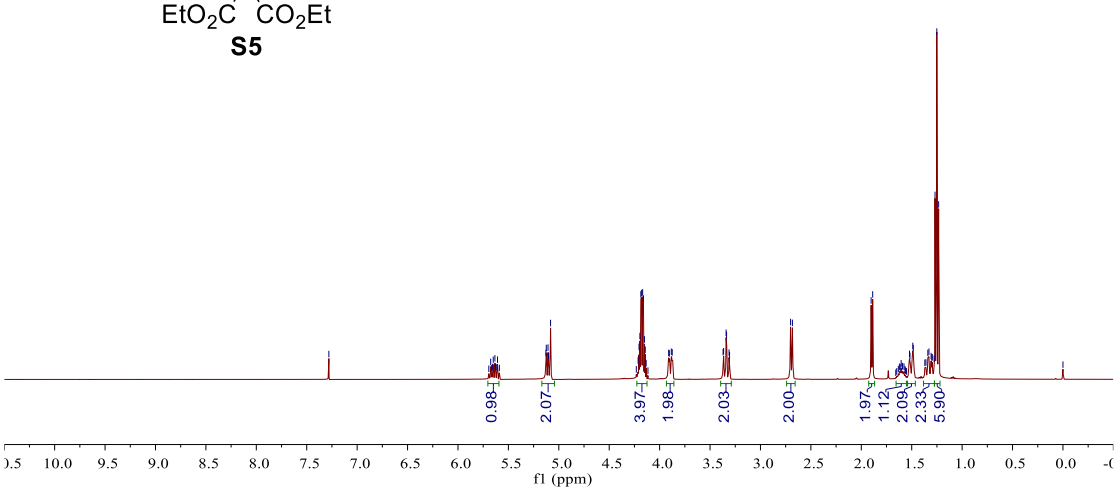
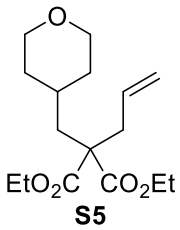
1.30
1.30
1.28
1.27
1.25
1.23
0.00


O
EtO2C
CO2Et

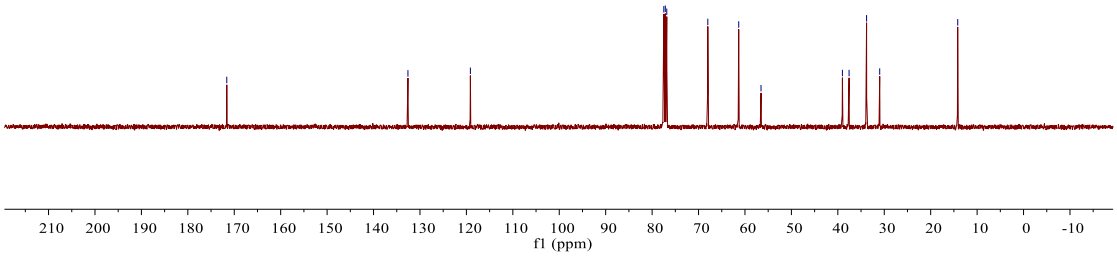
S5

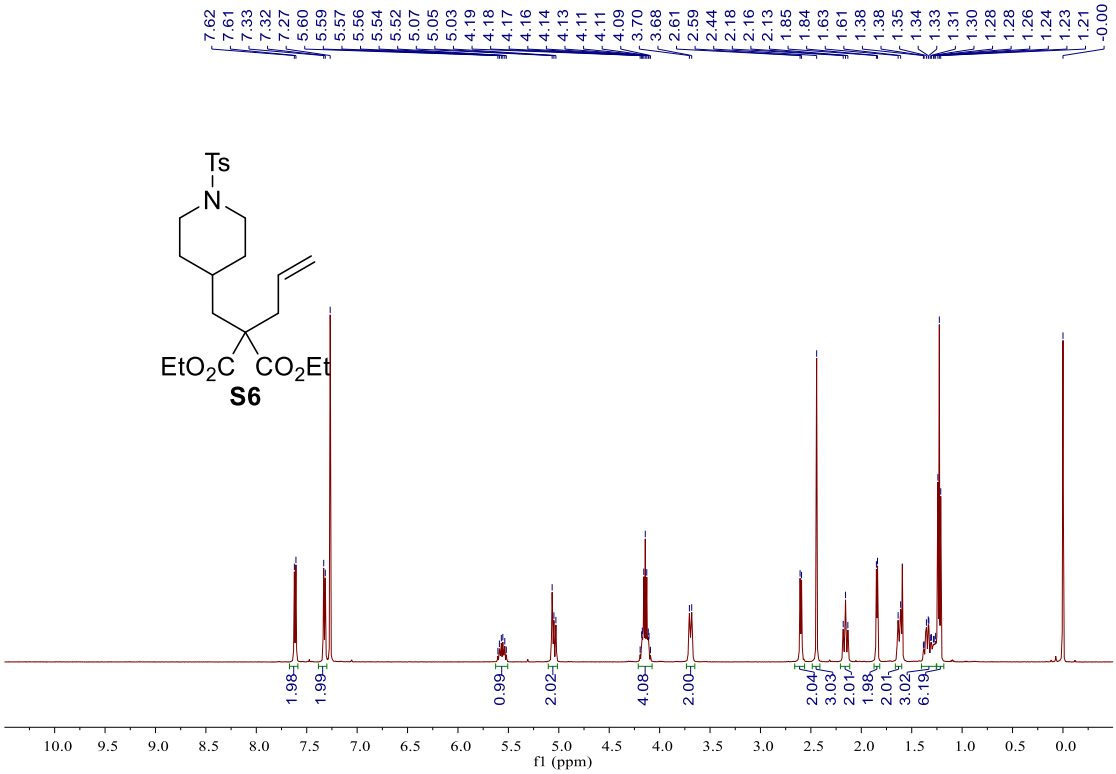

0.98
2.07
3.97
1.98
2.03
2.00
1.97
1.12
2.09
2.33
5.90
f1 (ppm)


171.61
132.59
119.14
77.48
77.16
76.84
68.00
61.35
56.54
39.01
37.58
33.81
30.98
14.18


O
EtO2C
CO2Et

S5


f1 (ppm)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7.61
7.33
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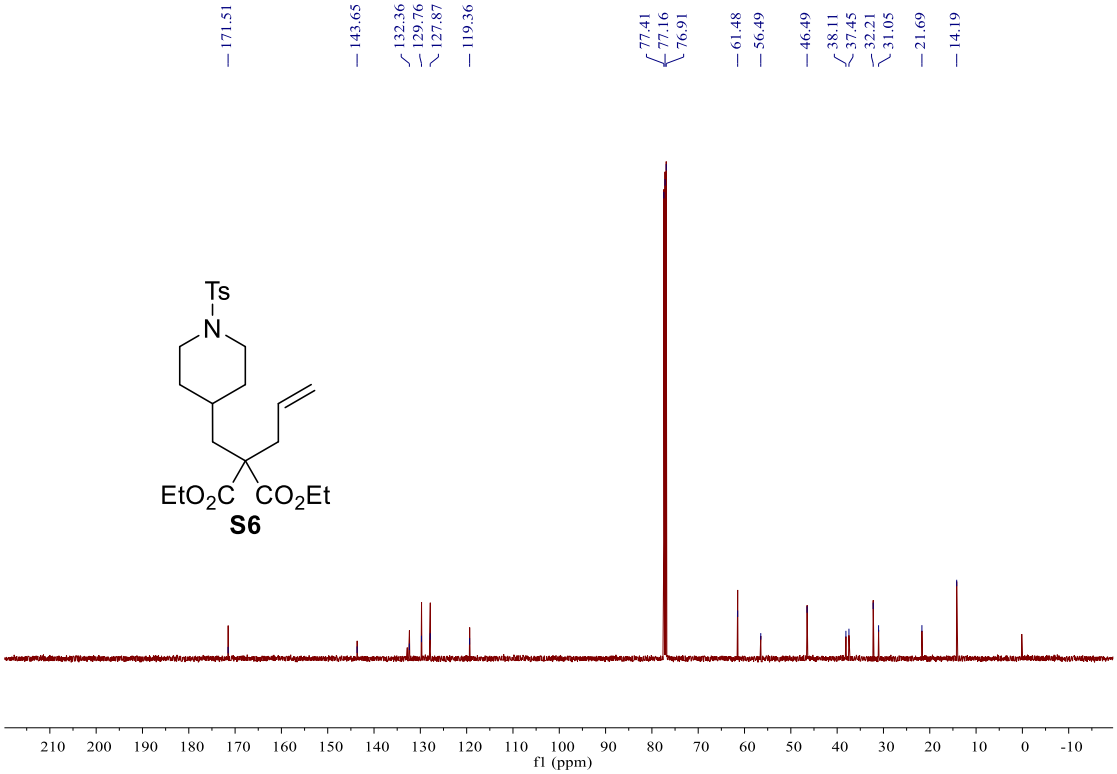
5.57
5.56
5.54
5.52
5.07
5.05
5.03
4.19
4.18
4.17
4.16
4.14
4.13
4.11
4.11
4.09
3.70
3.68
2.61
2.59
2.44
2.18
2.16
2.13
1.85
1.84
1.63
1.61
1.38
1.38
1.35
1.34
1.33
1.31
1.30
1.28
1.28
1.26
1.24
1.23
1.21
-0.00
Ts
N
EtO2C
CO2Et
S6
1.98
1.99
0.99
2.02
4.08
2.00
2.04
3.03
2.01
1.98
2.01
3.02
6.19
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


171.51
143.65
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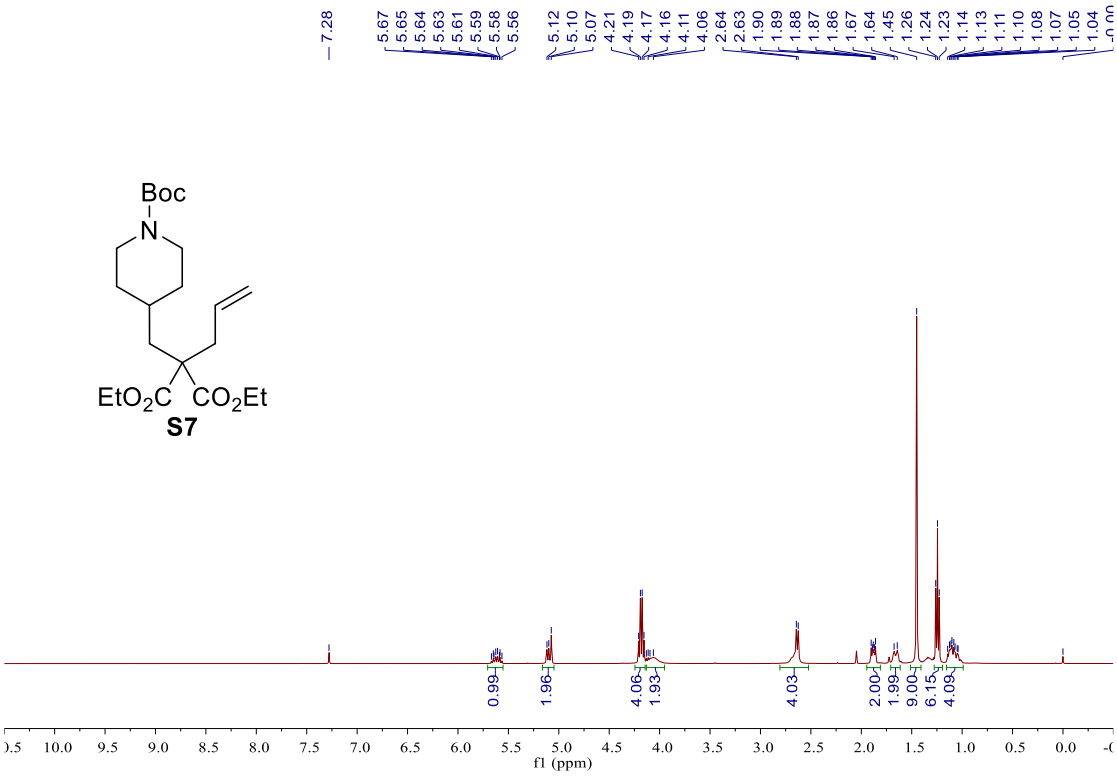
127.87
119.36
77.41
77.16
76.91
61.48
56.49
46.49
38.11
37.45
32.21
31.05
21.69
14.19
Ts
N
EtO2C
CO2Et
S6
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.28
5.67
5.65
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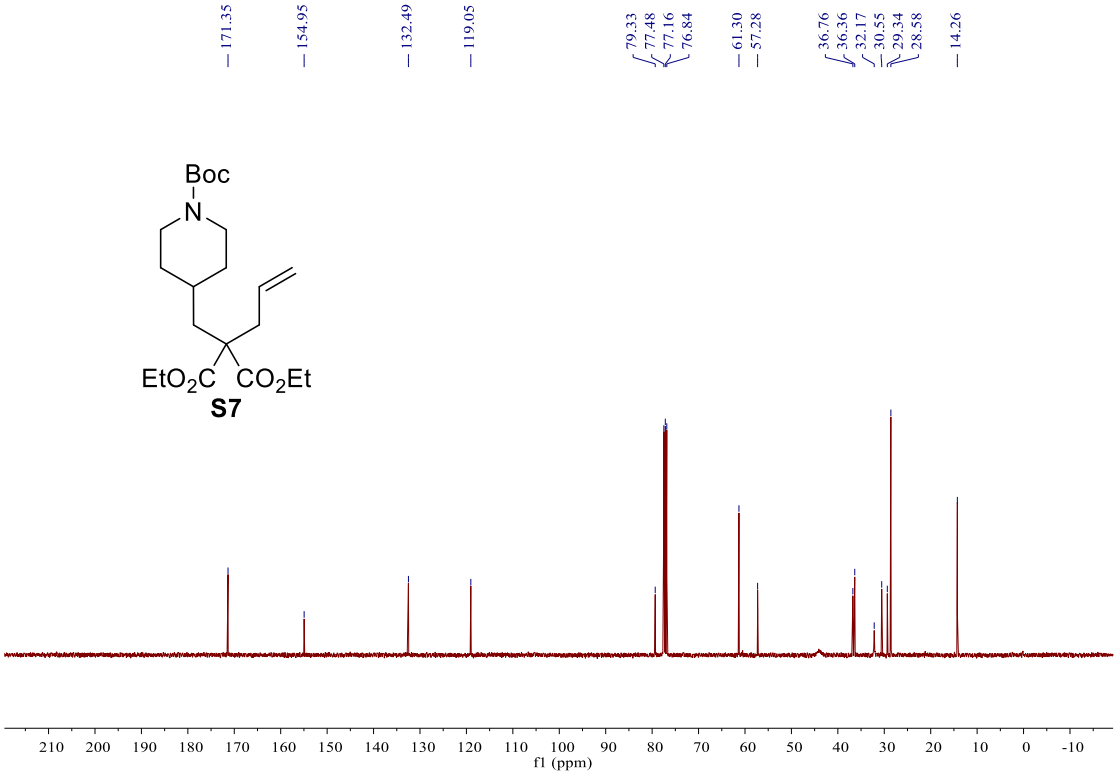
5.63
5.61
5.59
5.58
5.56
5.12
5.10
5.07
4.21
4.19
4.17
4.16
4.11
4.06
2.64
2.63
1.90
1.89
1.88
1.87
1.86
1.67
1.64
1.45
1.26
1.24
1.23
1.14
1.13
1.11
1.10
1.08
1.07
1.05
1.04
Boc
N
EtO2C CO2Et
S7
0.99
1.96
4.06
1.93
4.03
2.00
1.99
9.00
6.15
4.09
f1 (ppm)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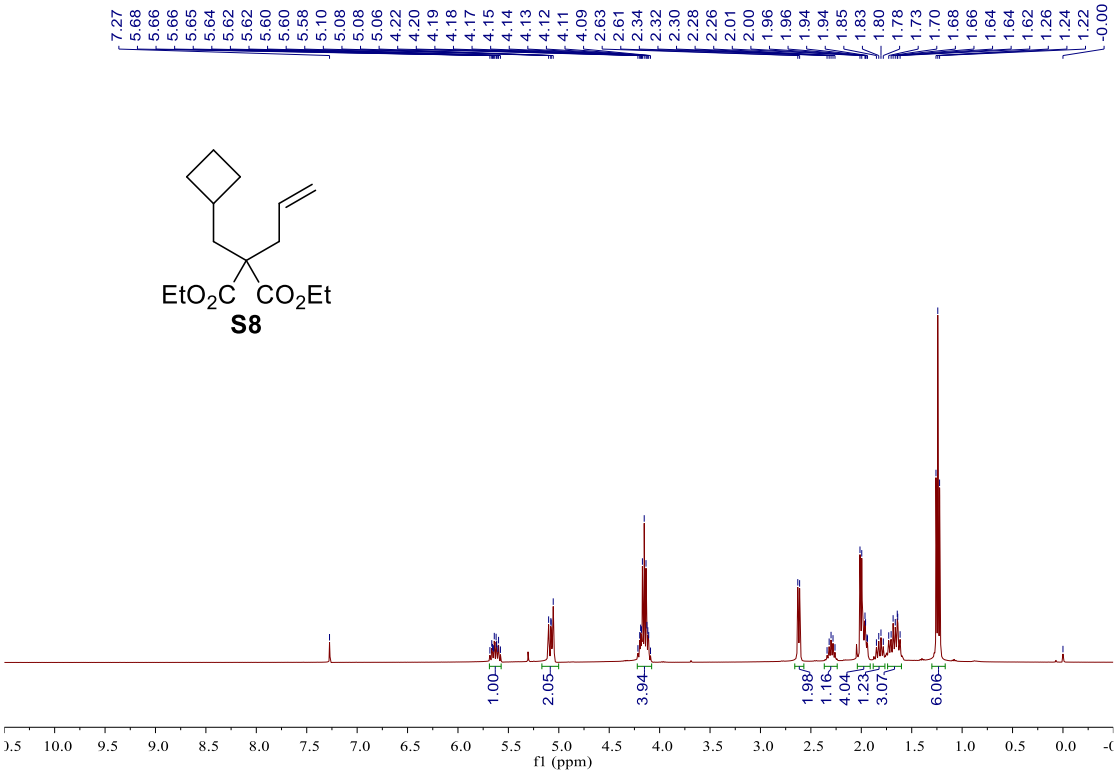
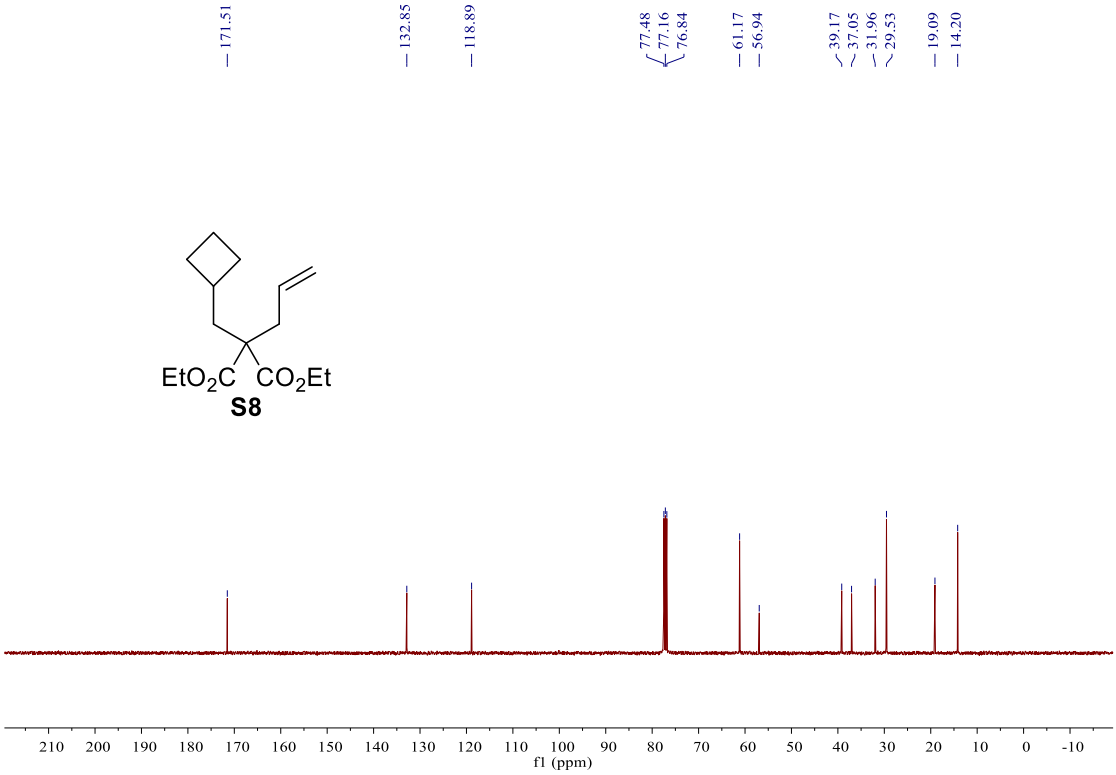
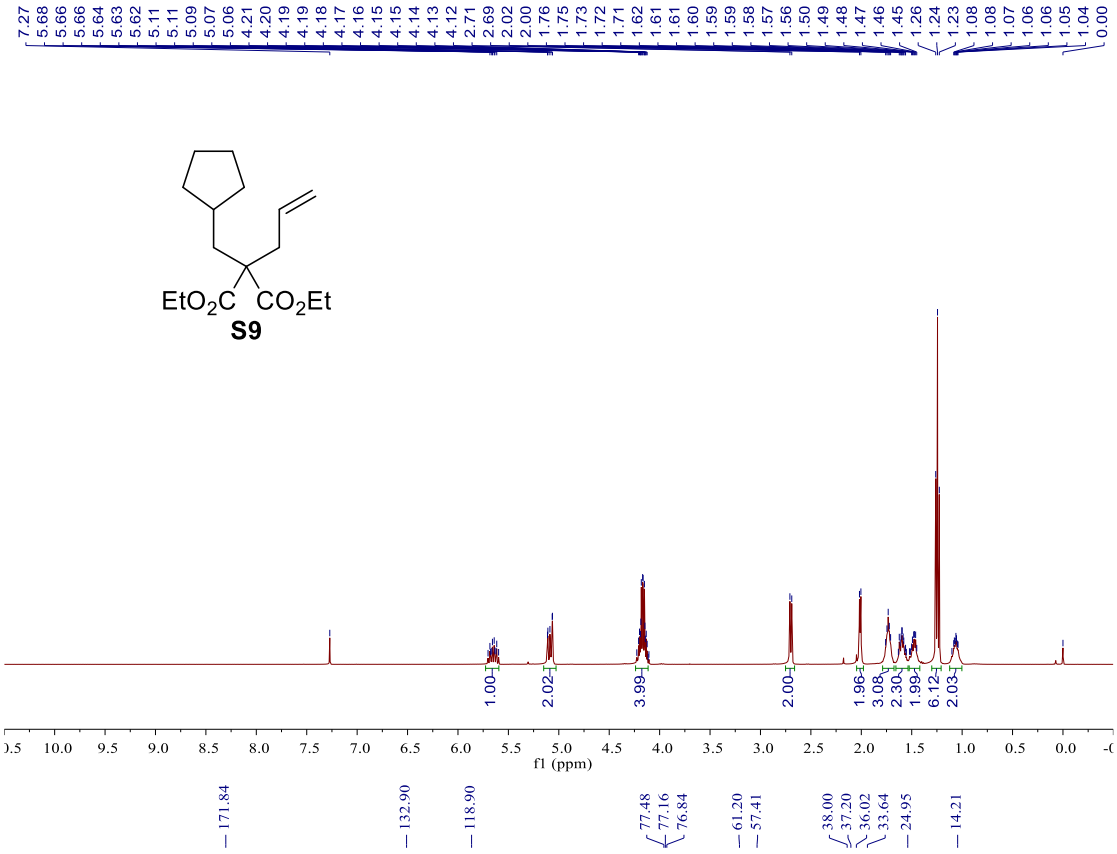
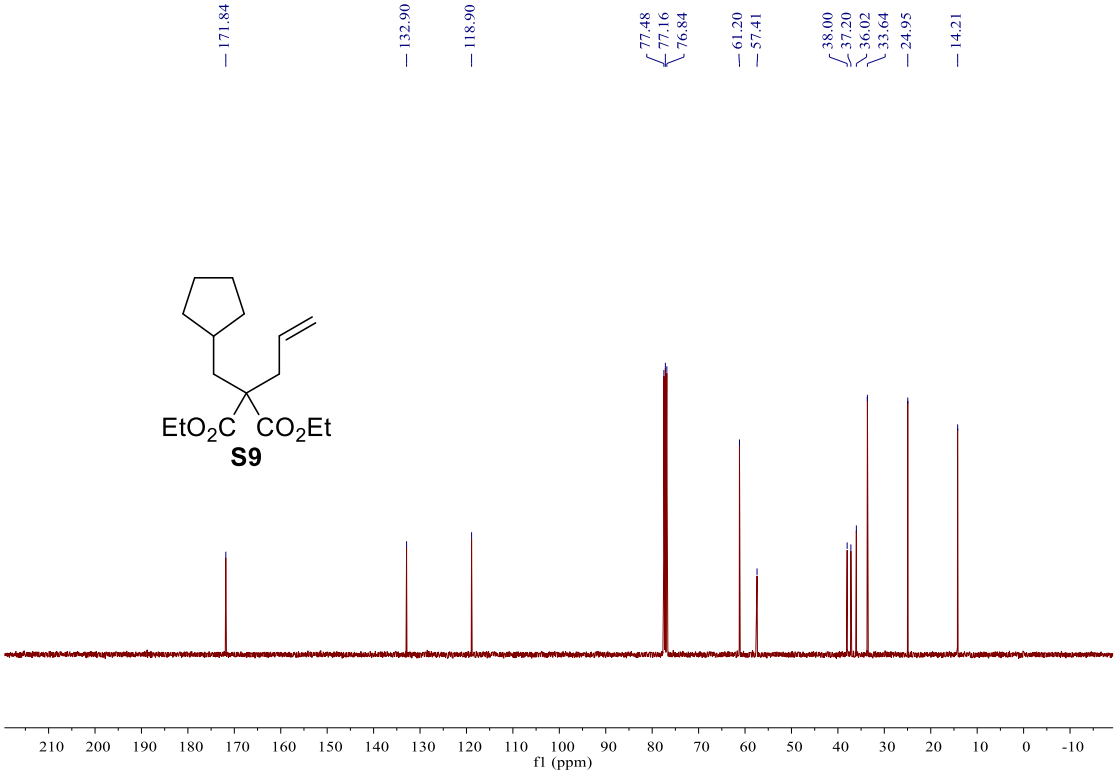
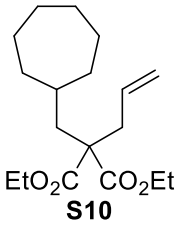
154.95
132.49
119.05
79.33
77.48
77.16
76.84
61.30
57.28
36.76
36.36
32.17
30.55
29.34
28.58
14.26
Boc
N
EtO2C CO2Et
S7
f1 (ppm)


7.27
5.68
5.66
5.66
5.65
5.64
5.62
5.62
5.60
5.60
5.58
5.10
5.08
5.08
5.06
4.22
4.20
4.19
4.18
4.17
4.15
4.14
4.13
4.12
4.11
4.09
2.63
2.61
2.34
2.32
2.30
2.28
2.26
2.01
2.00
1.96
1.96
1.94
1.94
1.85
1.83
1.80
1.78
1.73
1.70
1.68
1.66
1.64
1.64
1.62
1.26
1.24
1.22
-0.00
EtO2C CO2Et
S8
1.00
2.05
3.94
1.98
1.16
4.04
1.23
3.07
6.06
f1 (ppm)

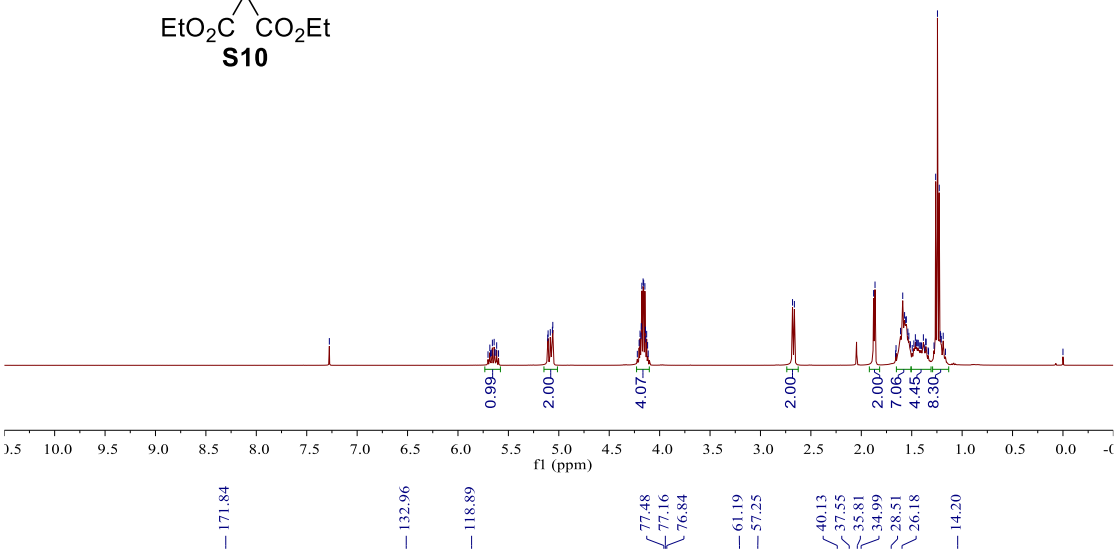

171.51
132.85
118.89
77.48
77.16
76.84
61.17
56.94
39.17
37.05
31.96
29.53
19.09
14.20
EtO2C CO2Et
S8
f1 (ppm)


7.27 5.68 5.66 5.66 5.64 5.63 5.62 5.11 5.11 5.09 5.07 5.06 4.21 4.20 4.19 4.19 4.18 4.17 4.16 4.15 4.15 4.14 4.13 4.12 2.71 2.69 2.02 2.00 1.76 1.75 1.73 1.72 1.71 1.62 1.61 1.61 1.60 1.59 1.59 1.58 1.57 1.56 1.50 1.49 1.48 1.47 1.46 1.45 1.26 1.24 1.23 1.08 1.08 1.07 1.06 1.06 1.05 1.04 0.00
EtO2C CO2Et
S9
1.00 2.02 3.99 2.00 1.96 3.08 2.30 1.99 6.12 2.03
f1 (ppm)


171.84 132.90 118.90 77.48 77.16 76.84 61.20 57.41 38.00 37.20 36.02 33.64 24.95 14.21
EtO2C CO2Et
S9
f1 (ppm)


EtO2C CO2Et

S10


0.99
2.00
4.07
2.00
2.00
7.06
4.45
8.30
f1 (ppm)

171.84
132.96
118.89
77.48
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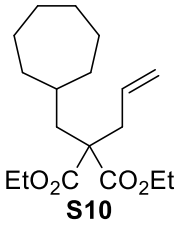
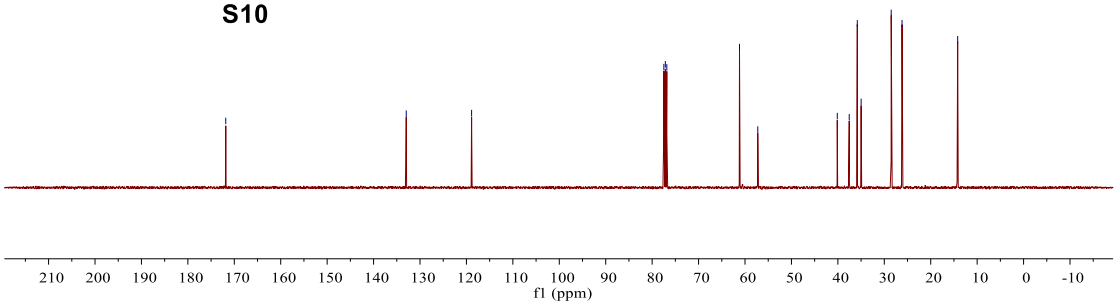
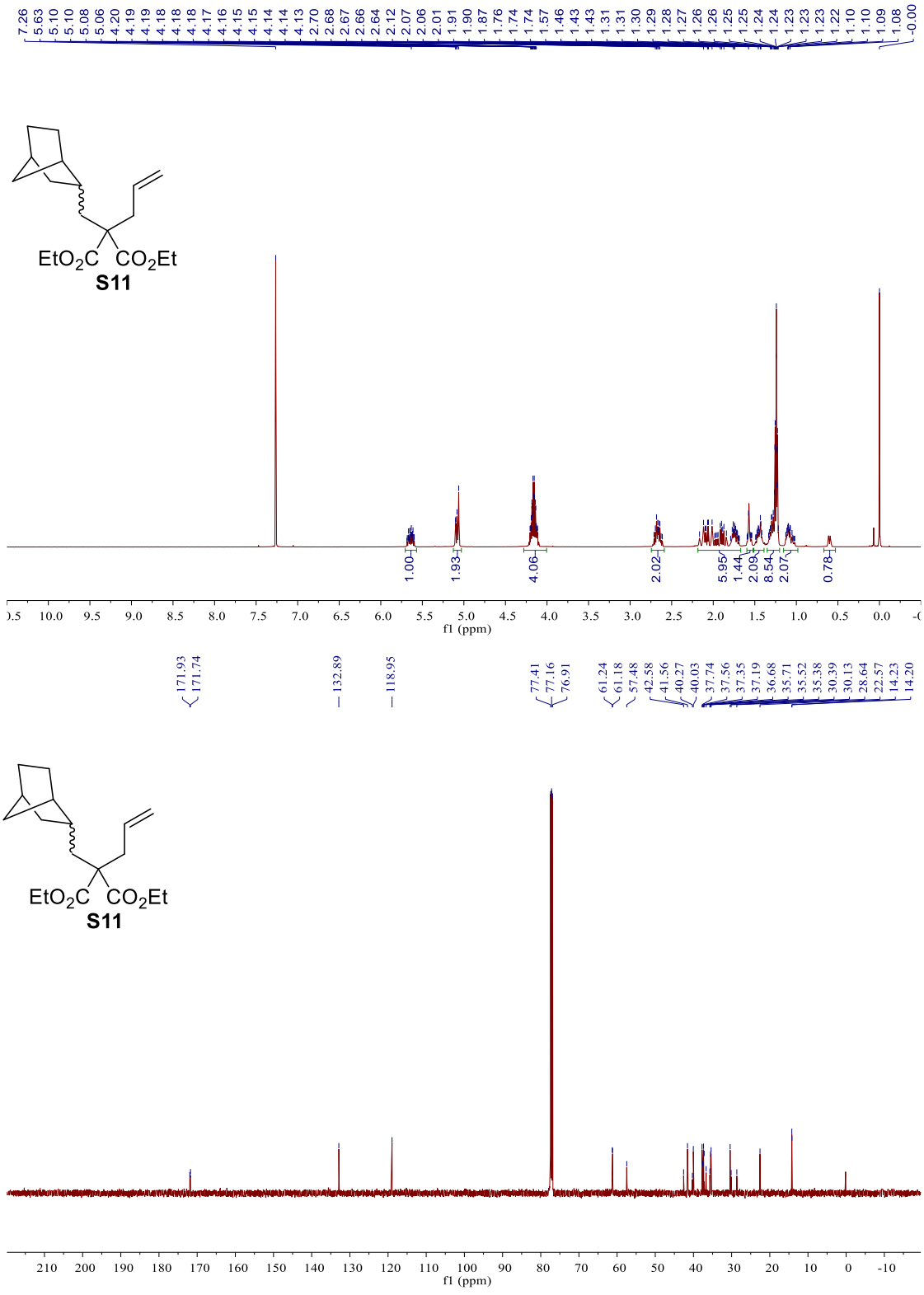
76.84
61.19
57.25
40.13
37.55
35.81
34.99
28.51
26.18
14.20

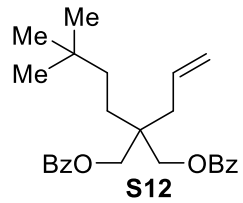

EtO2C CO2Et

S10

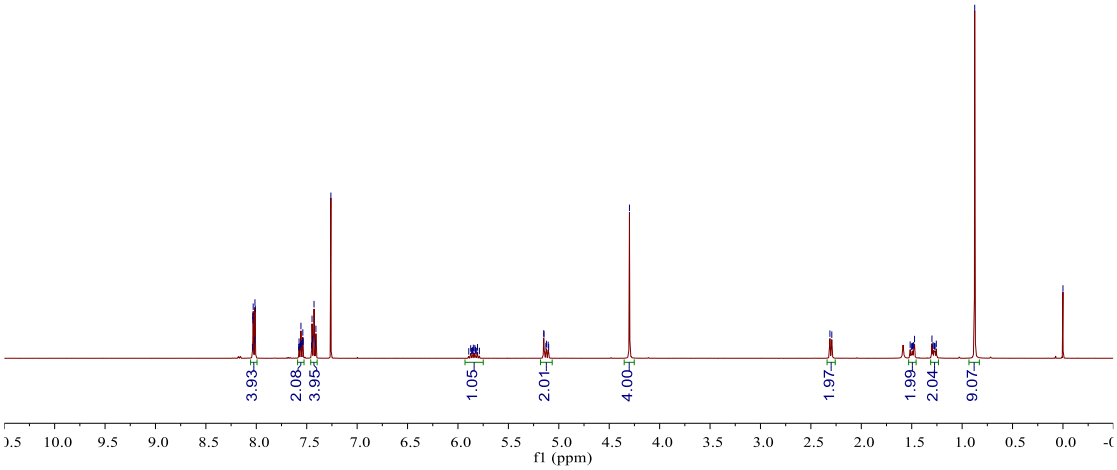

f1 (ppm)


7.26 5.63 5.10 5.10 5.08 5.06 4.20 4.19 4.19 4.18 4.18 4.18 4.17 4.16 4.15 4.15 4.14 4.14 4.13 2.70 2.68 2.67 2.66 2.64 2.12 2.07 2.06 2.01 1.91 1.90 1.87 1.76 1.74 1.74 1.57 1.46 1.43 1.43 1.31 1.31 1.30 1.29 1.28 1.27 1.26 1.26 1.25 1.25 1.24 1.24 1.23 1.23 1.23 1.22 1.10 1.10 1.09 1.08 -0.00
EtO2C CO2Et
S11
1.00 1.93 4.06 2.02 5.95 1.44 2.09 8.54 2.07 0.78
f1 (ppm)
171.93 171.74 132.89 118.95 77.41 77.16 76.91 61.24 61.18 57.48 42.58 41.56 40.27 40.03 37.74 37.56 37.35 37.19 36.68 35.71 35.52 35.38 30.39 30.13 28.64 22.57 14.23 14.20
EtO2C CO2Et
S11
f1 (ppm)

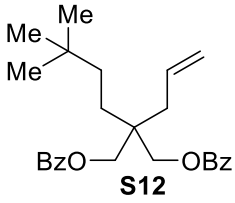

8.04
8.03
8.03
8.03
8.02
8.01
8.01
7.58
7.58
7.57
7.56
7.56
7.55
7.54
7.54
7.54
7.45
7.45
7.44
7.43
7.41
7.41
7.26
5.89
5.87
5.87
5.86
5.85
5.85
5.83
5.83
5.81
5.81
5.79
5.15
5.15
5.13
5.12
5.11
5.10
4.30
2.31
2.29
1.52
1.50
1.50
1.49
1.48
1.47
1.30
1.29
1.28
1.27
1.27
1.26
0.88
0.00


Me
Me
Me
BzO
OBz

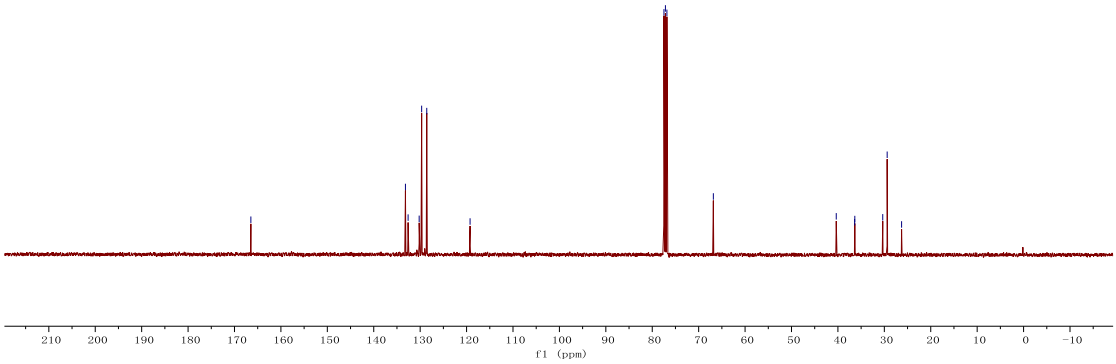
S12

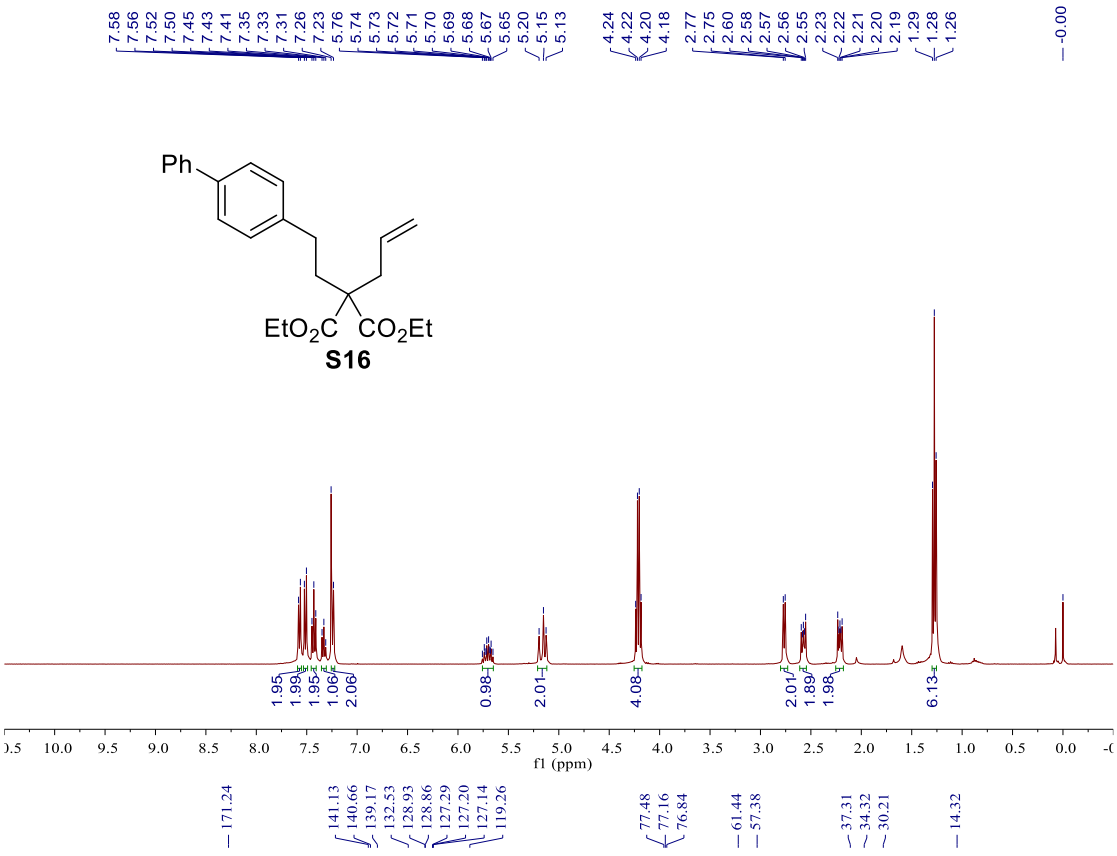

3.93
2.08
3.95
1.05
2.01
4.00
1.97
1.99
2.04
9.07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


166.472
133.172
132.599
130.213
129.678
128.580
119.247
77.478
77.160
76.843
66.837
40.358
36.399
36.360
30.342
29.388
26.282


Me
Me
Me
BzO
OBz

S12


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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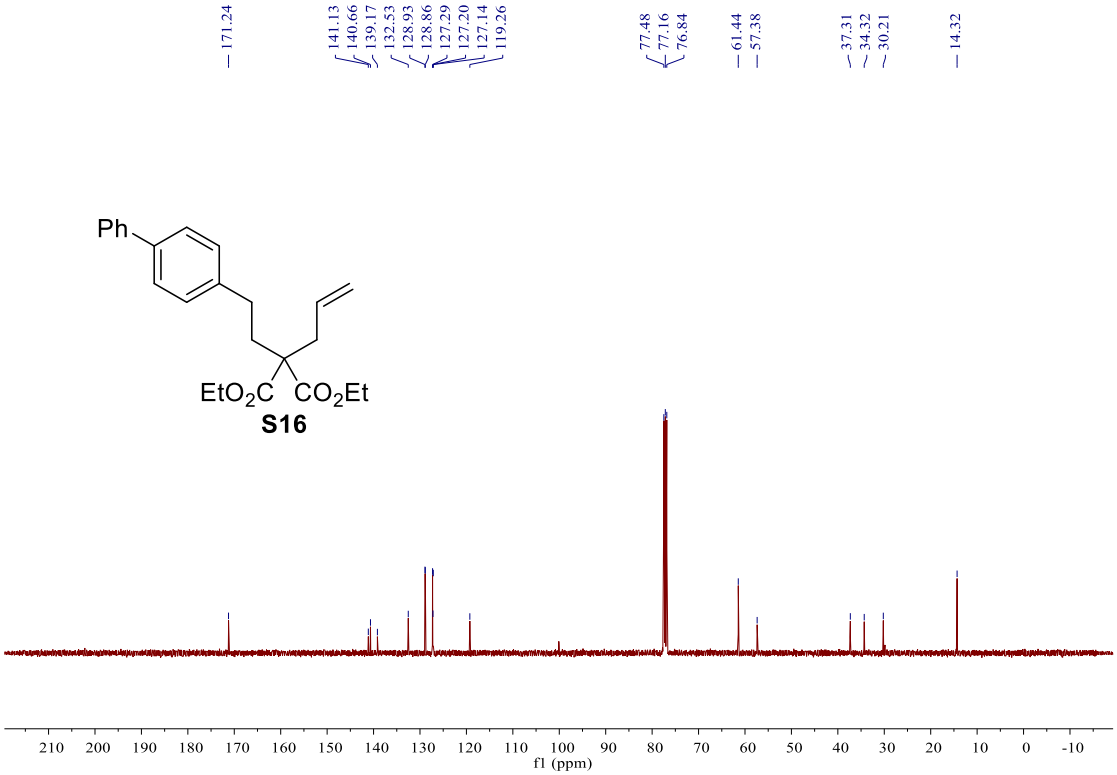
7.35
7.33
7.31
7.26
7.23
5.76
5.74
5.73
5.72
5.71
5.70
5.69
5.68
5.67
5.65
5.20
5.15
5.13
4.24
4.22
4.20
4.18
2.77
2.75
2.60
2.58
2.57
2.56
2.55
2.23
2.22
2.21
2.20
2.19
1.29
1.28
1.26
-0.00
Ph
EtO2C CO2Et
S16
1.95
1.99
1.95
1.06
2.06
0.98
2.01
4.08
2.01
1.89
1.98
6.13
f1 (ppm)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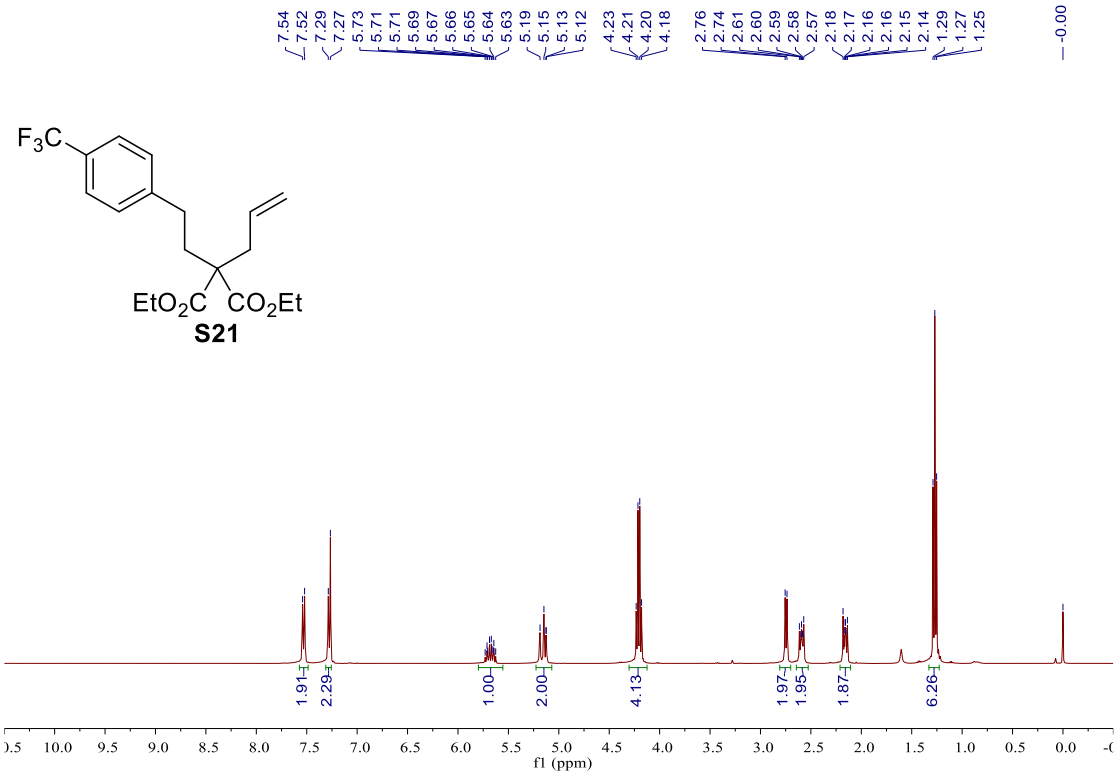
141.13
140.66
139.17
132.53
128.93
128.86
127.29
127.20
127.14
119.26
77.48
77.16
76.84
61.44
57.38
37.31
34.32
30.21
14.32
Ph
EtO2C CO2Et
S16
f1 (ppm)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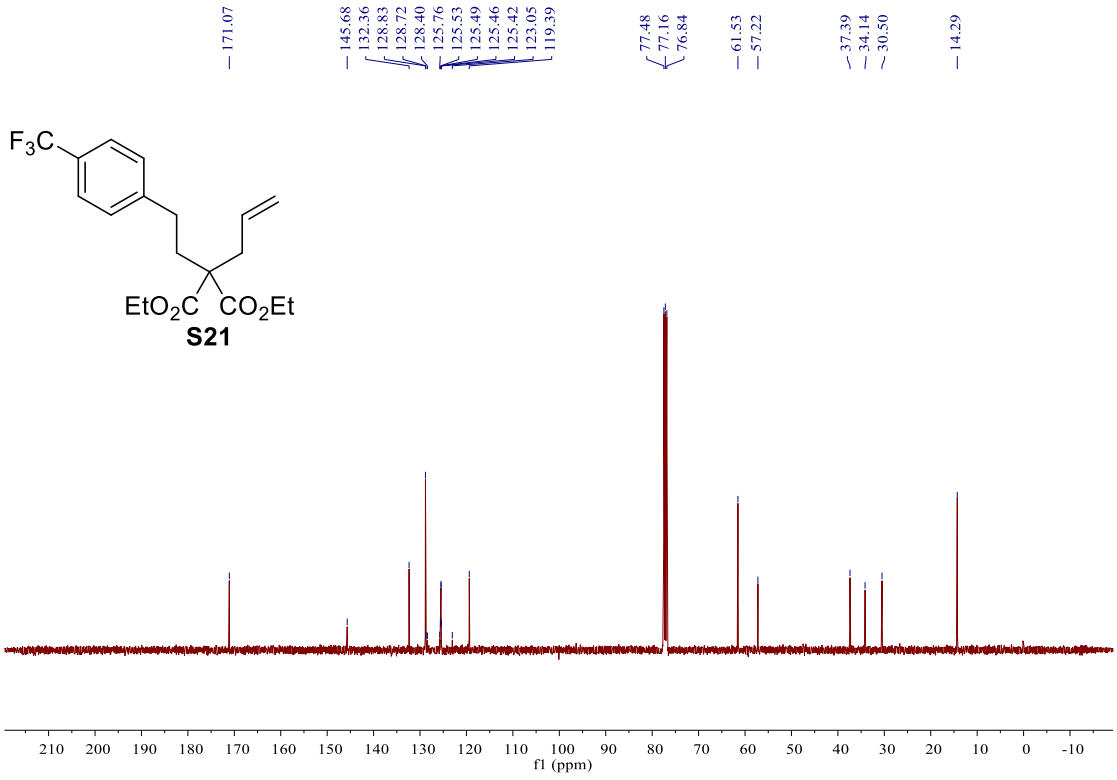
5.71
5.69
5.67
5.66
5.65
5.64
5.63
5.19
5.15
5.13
5.12
4.23
4.21
4.20
4.18
2.76
2.74
2.61
2.60
2.59
2.58
2.57
2.18
2.17
2.16
2.16
2.15
2.14
1.29
1.27
1.25
-0.00
F3C
EtO2C CO2Et
S21
1.91
2.29
1.00
2.00
4.13
1.97
1.95
1.87
6.26
f1 (ppm)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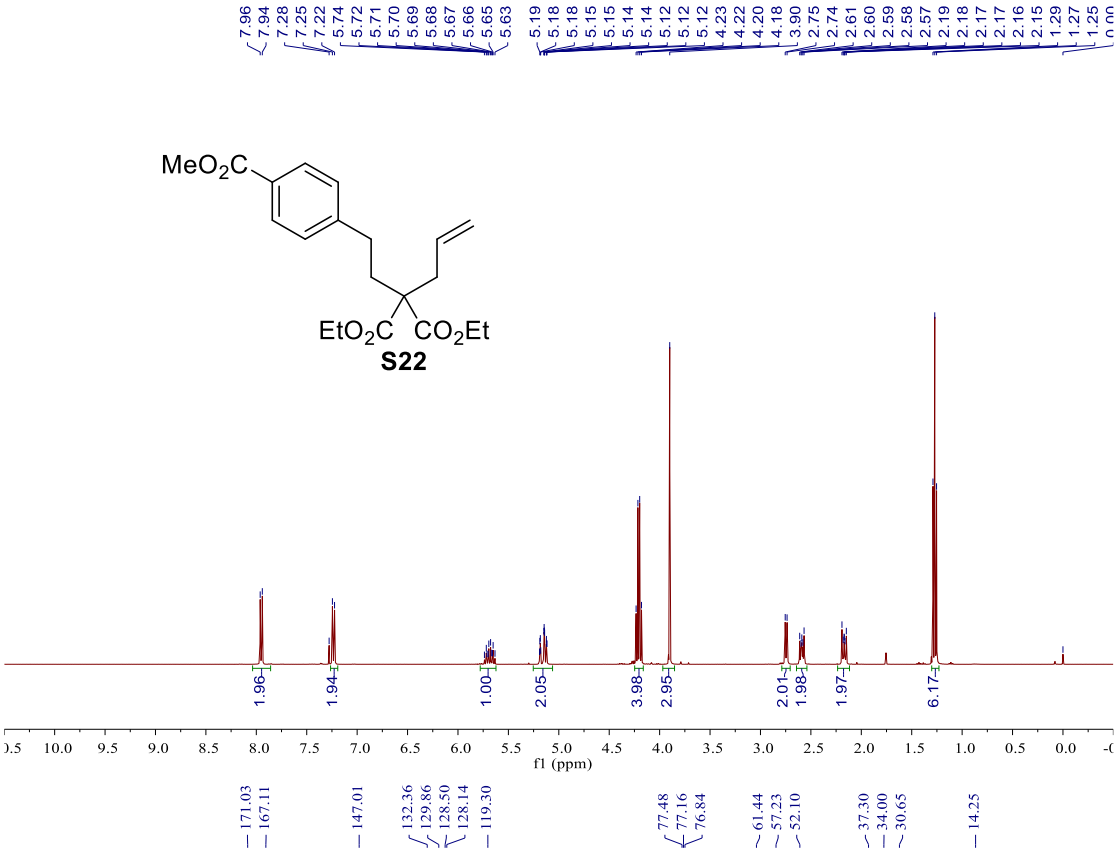
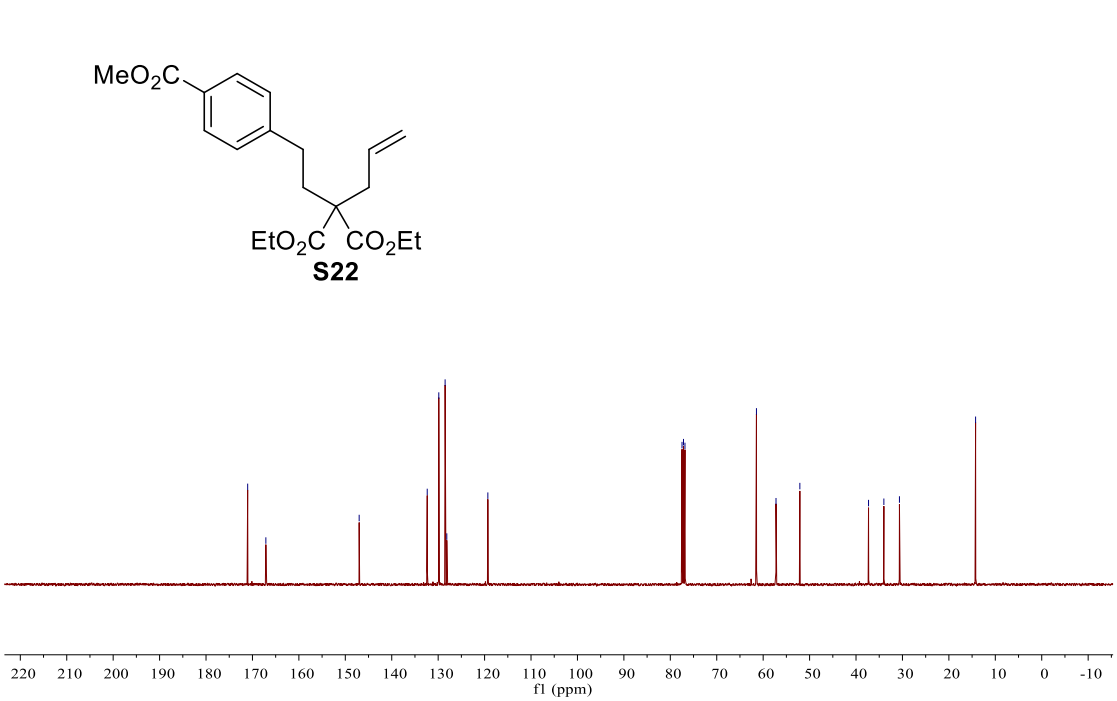
128.40
125.76
125.53
125.49
125.46
125.42
123.05
119.39
77.48
77.16
76.84
61.53
57.22
37.39
34.14
30.50
14.29
F3C
EtO2C CO2Et
S21
f1 (ppm)


7.96
7.94
7.28
7.25
7.22
5.74
5.72
5.71
5.70
5.69
5.68
5.67
5.66
5.65
5.63
5.19
5.18
5.18
5.15
5.15
5.14
5.14
5.12
5.12
5.12
4.23
4.22
4.20
4.18
3.90
2.75
2.74
2.61
2.60
2.59
2.58
2.57
2.19
2.18
2.17
2.17
2.16
2.15
1.29
1.27
1.25
MeO2C
EtO2C CO2Et
S22
1.96
1.94
1.00
2.05
3.98
2.95
2.01
1.98
1.97
6.17
f1 (ppm)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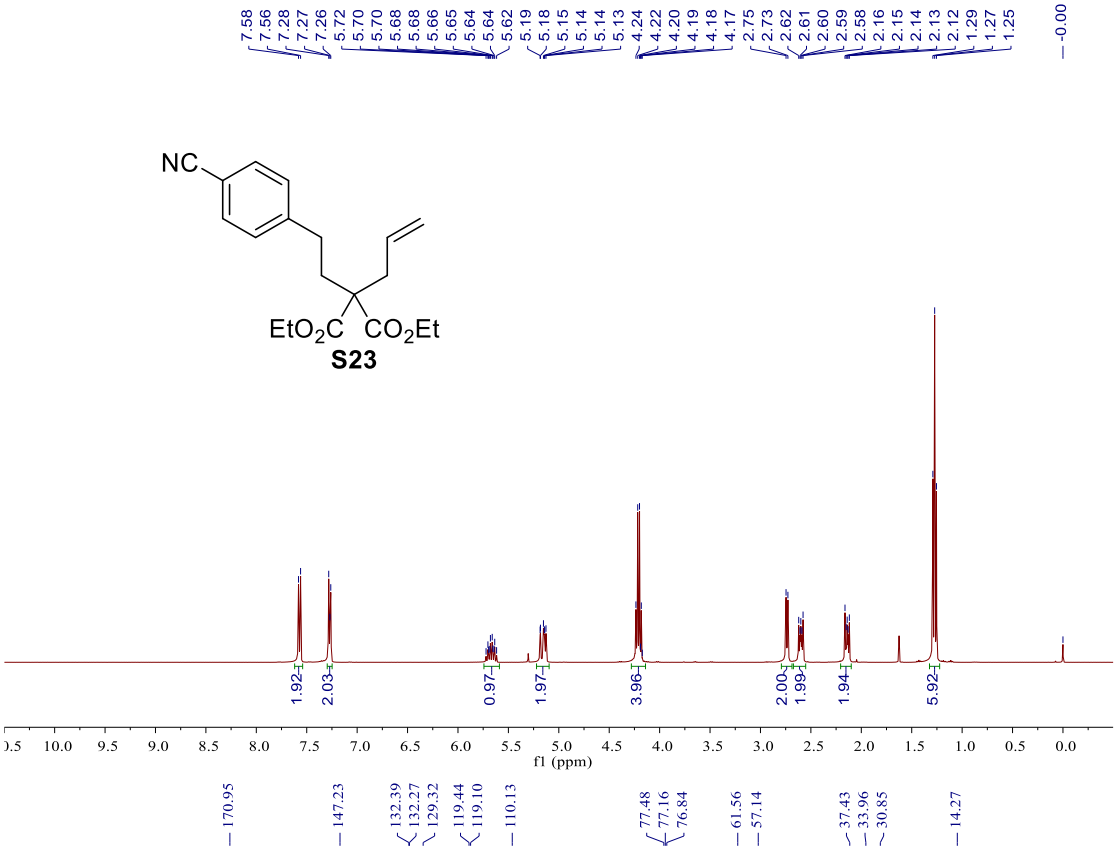
167.11
147.01
132.36
129.86
128.50
128.14
119.30
77.48
77.16
76.84
61.44
57.23
52.10
37.30
34.00
30.65
14.25
MeO2C
EtO2C CO2Et
S22
f1 (ppm)


7.58
7.56
7.28
7.27
7.26
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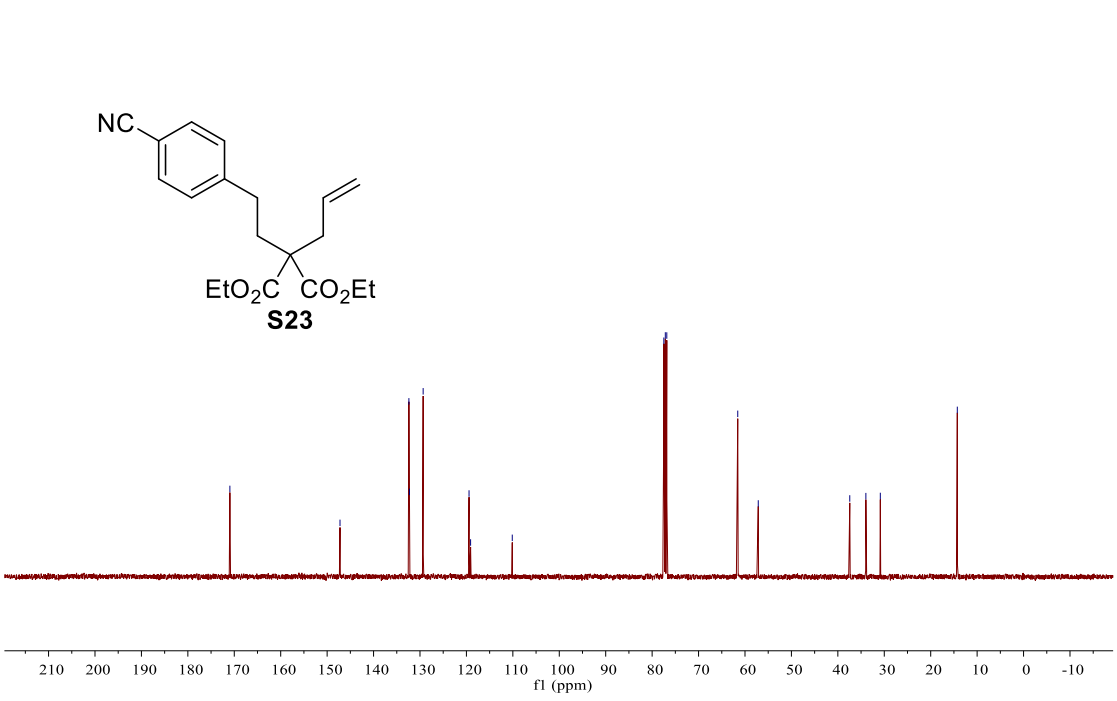
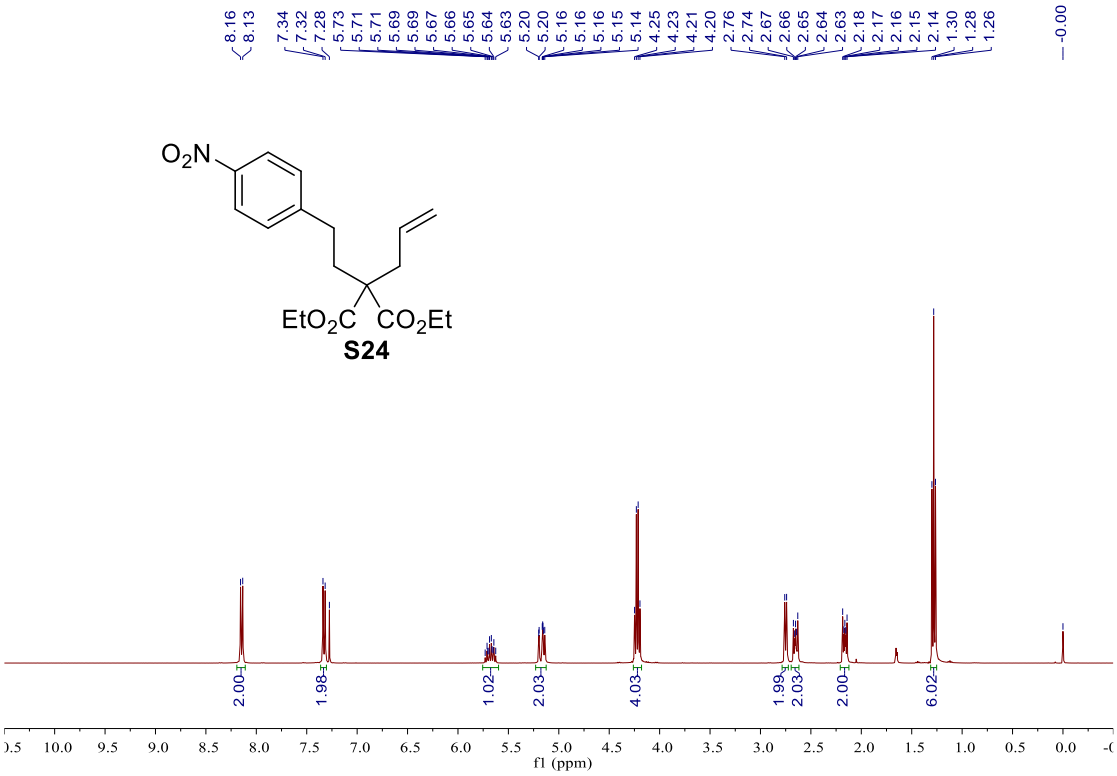
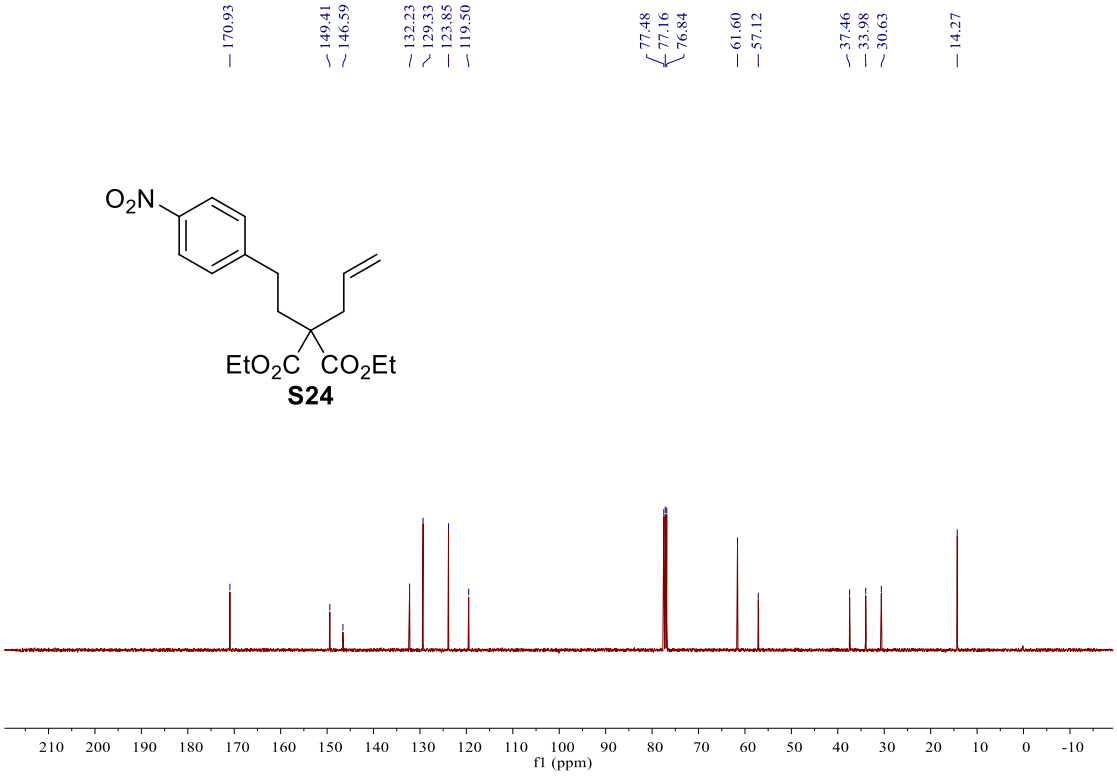
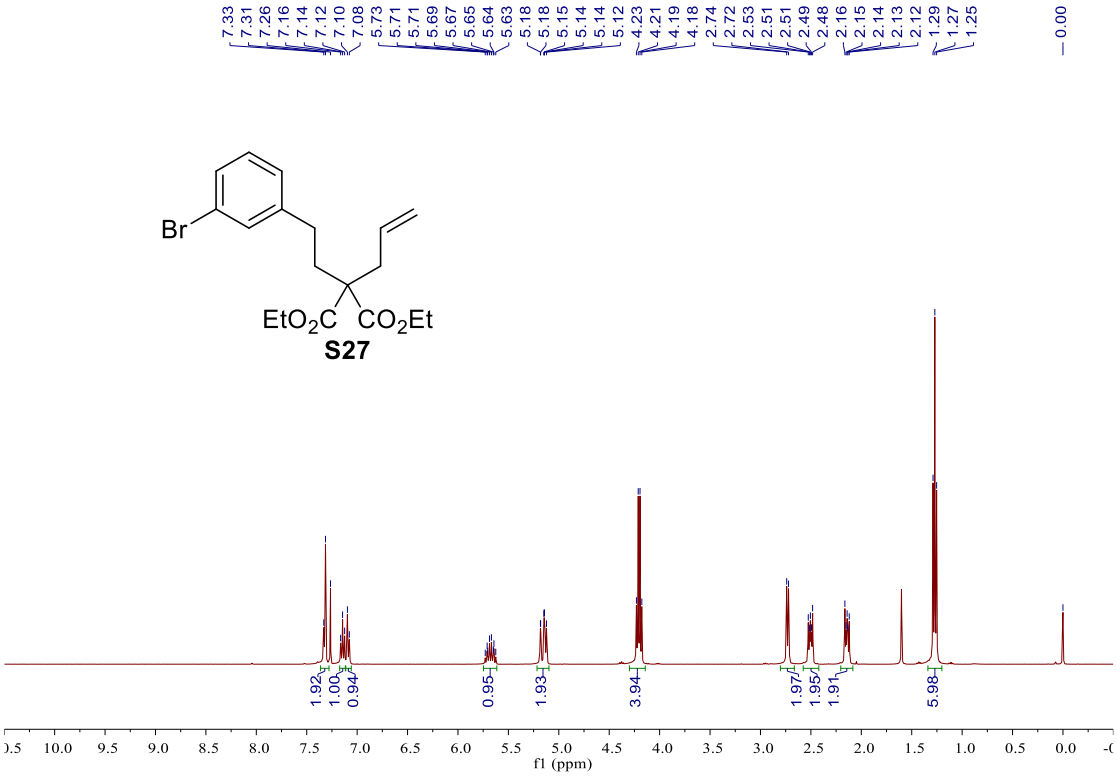
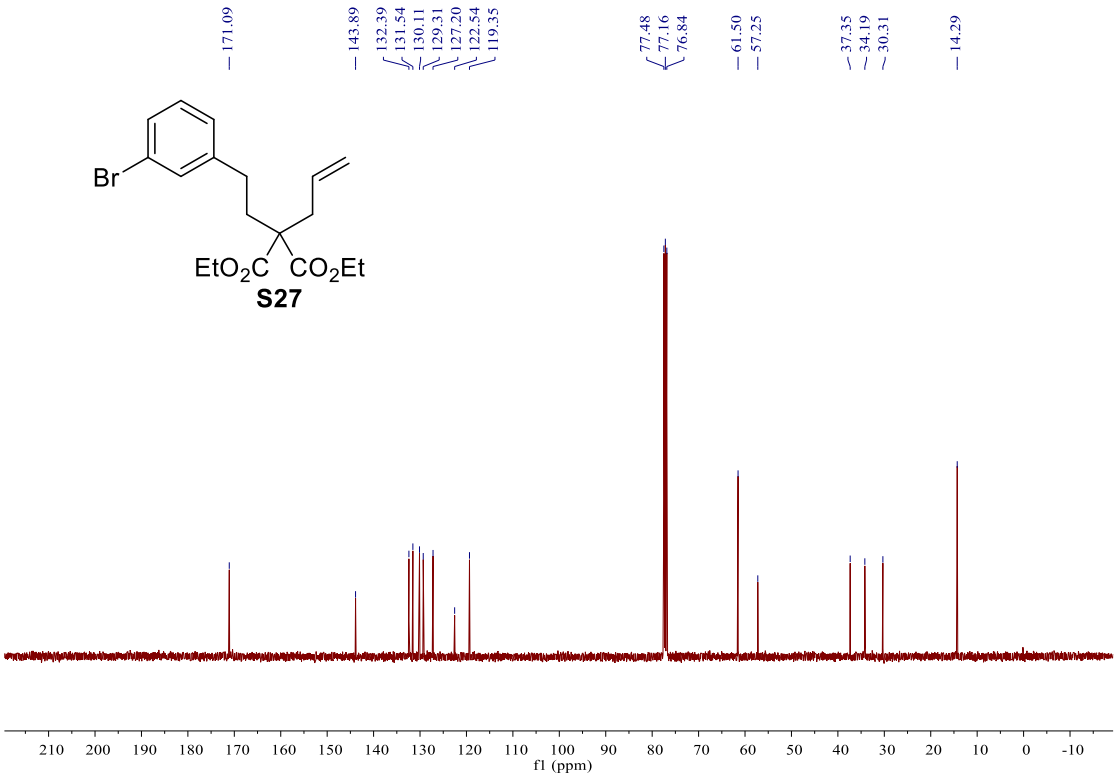
5.70
5.68
5.68
5.66
5.65
5.64
5.64
5.62
5.19
5.18
5.15
5.14
5.14
5.13
4.24
4.22
4.20
4.19
4.18
4.17
2.75
2.73
2.62
2.61
2.60
2.59
2.58
2.16
2.15
2.14
2.13
2.12
1.29
1.27
1.25
-0.00
NC
EtO2C CO2Et
S23
1.92
2.03
0.97
1.97
3.96
2.00
1.99
1.94
5.92
f1 (ppm)

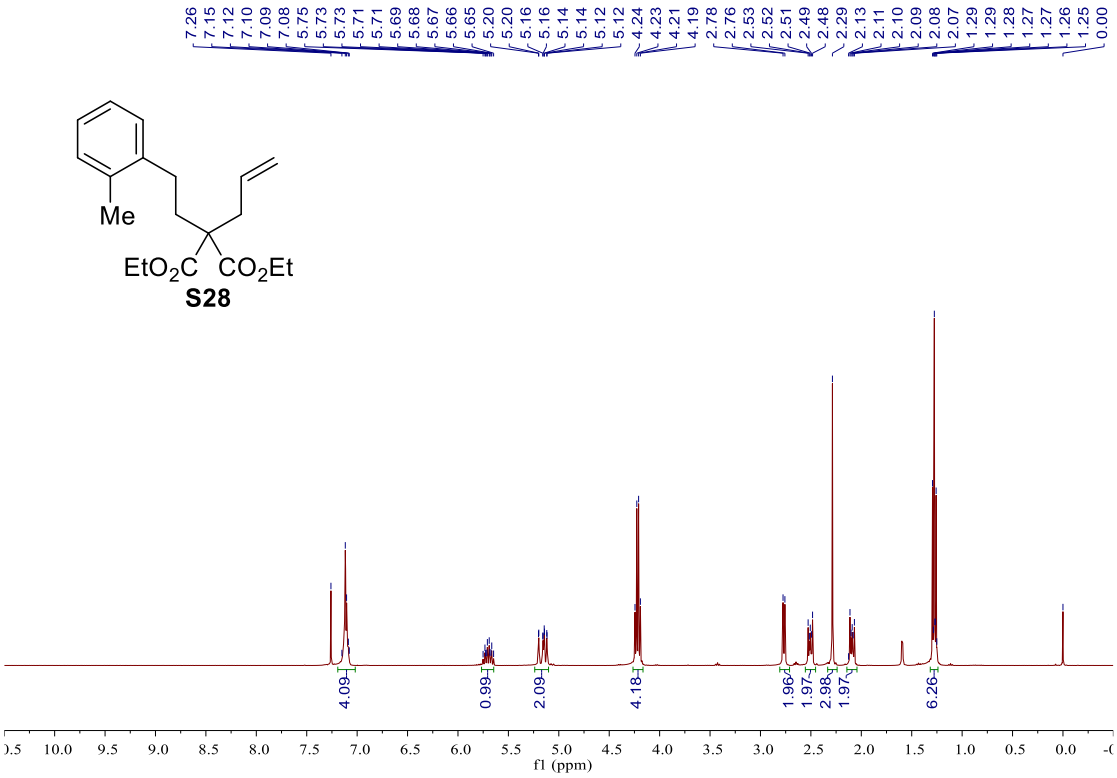

170.95
147.23
132.39
132.27
129.32
119.44
119.10
110.13
77.48
77.16
76.84
61.56
57.14
37.43
33.96
30.85
14.27
NC
EtO2C CO2Et
S23
f1 (ppm)


8.16
8.13
7.34
7.32
7.28
5.73
5.71
5.71
5.69
5.69
5.67
5.66
5.65
5.64
5.63
5.20
5.20
5.16
5.16
5.16
5.15
5.14
4.25
4.23
4.21
4.20
2.76
2.74
2.67
2.66
2.65
2.64
2.63
2.18
2.17
2.16
2.15
2.14
1.30
1.28
1.26
-0.00
O2N
EtO2C CO2Et
S24
2.00
1.98
1.02
2.03
4.03
1.99
2.03
2.00
6.02
f1 (ppm)


170.93
149.41
146.59
132.23
129.33
123.85
119.50
77.48
77.16
76.84
61.60
57.12
37.46
33.98
30.63
14.27
O2N
EtO2C CO2Et
S24
f1 (ppm)


7.33
7.31
7.26
7.16
7.14
7.12
7.10
7.08
5.73
5.71
5.71
5.69
5.67
5.65
5.64
5.63
5.18
5.18
5.15
5.14
5.14
5.12
4.23
4.21
4.19
4.18
2.74
2.72
2.53
2.51
2.51
2.49
2.48
2.16
2.15
2.14
2.13
2.12
1.29
1.27
1.25
0.00
Br
EtO2C CO2Et
S27
1.92
1.00
0.94
0.95
1.93
3.94
1.97
1.95
1.91
5.98
f1 (ppm)


171.09
143.89
132.39
131.54
130.11
129.31
127.20
122.54
119.35
77.48
77.16
76.84
61.50
57.25
37.35
34.19
30.31
14.29
Br
EtO2C CO2Et
S27
f1 (ppm)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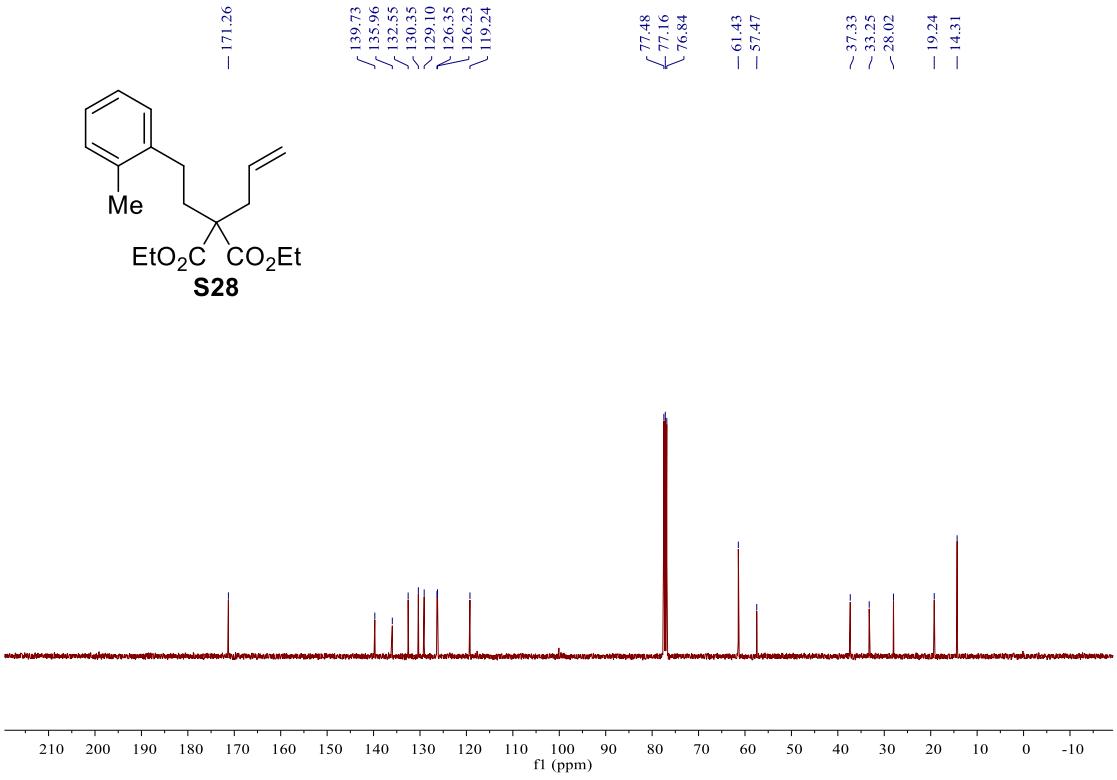
7.15
7.12
7.10
7.09
7.08
5.75
5.73
5.73
5.71
5.71
5.69
5.68
5.67
5.66
5.65
5.20
5.20
5.16
5.16
5.14
5.14
5.12
5.12
4.24
4.23
4.21
4.19
2.78
2.76
2.53
2.52
2.51
2.49
2.48
2.29
2.13
2.11
2.10
2.09
2.08
2.07
1.29
1.29
1.28
1.27
1.27
1.26
1.25
0.00
Me
EtO2C CO2Et
S28
4.09
0.99
2.09
4.18
1.96
1.97
2.98
1.97
6.26
f1 (ppm)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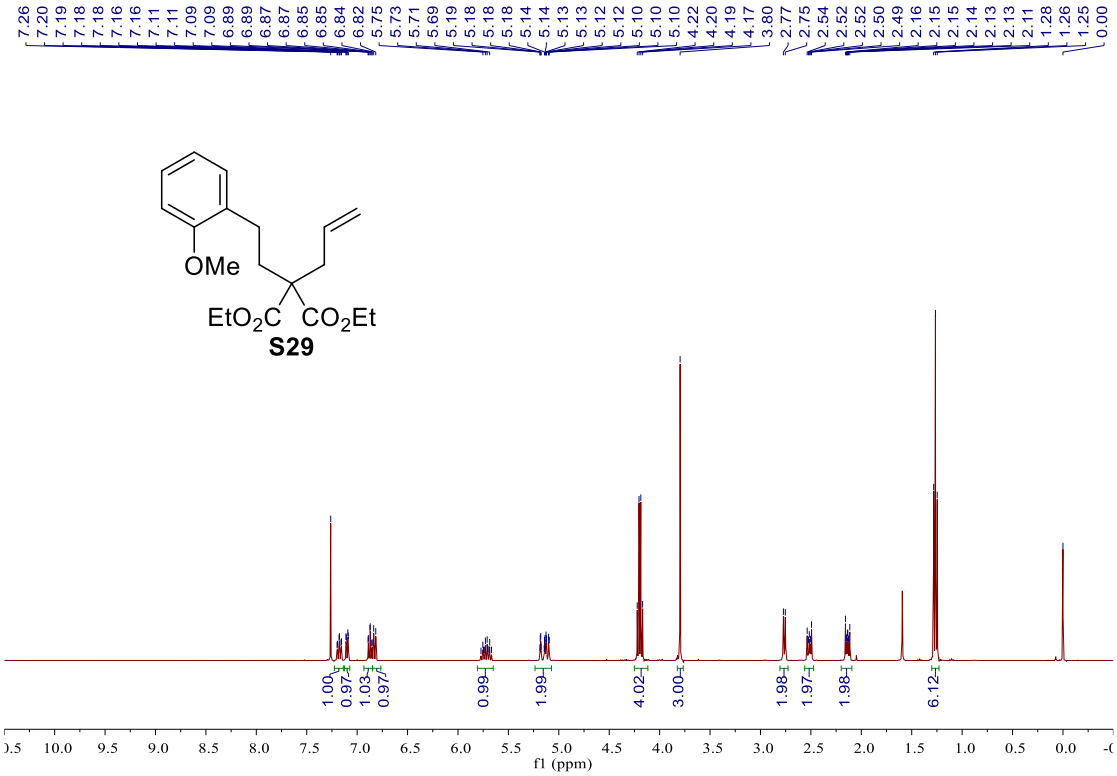
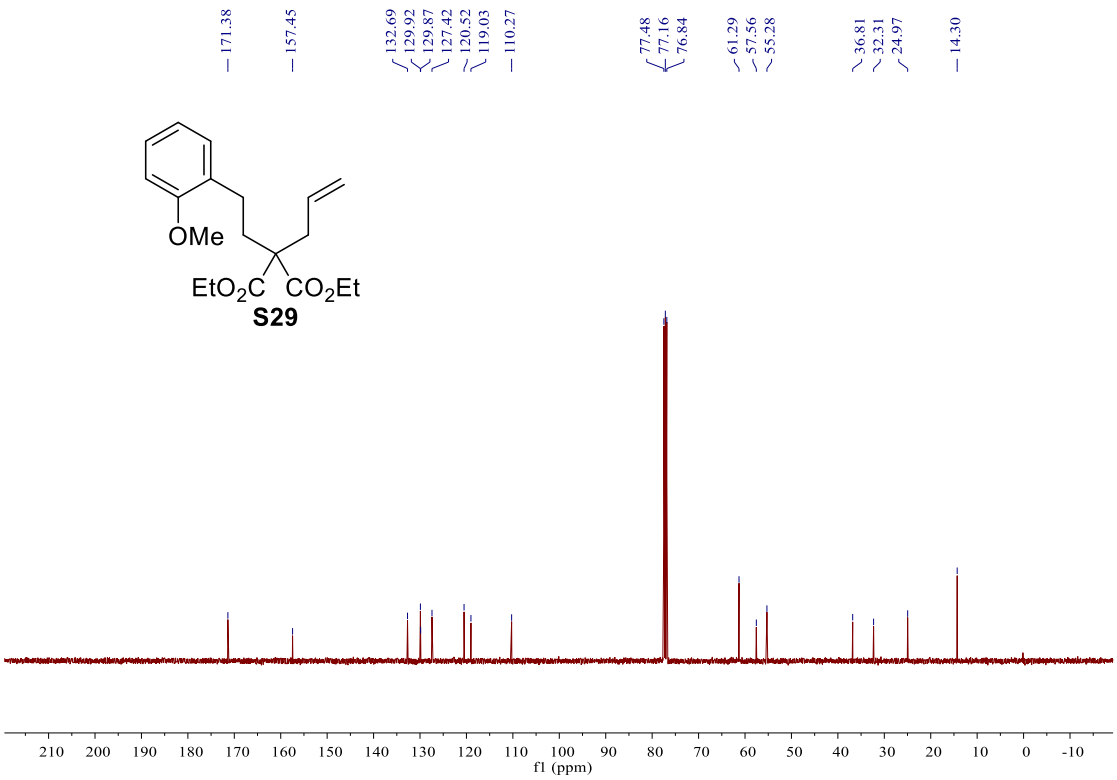
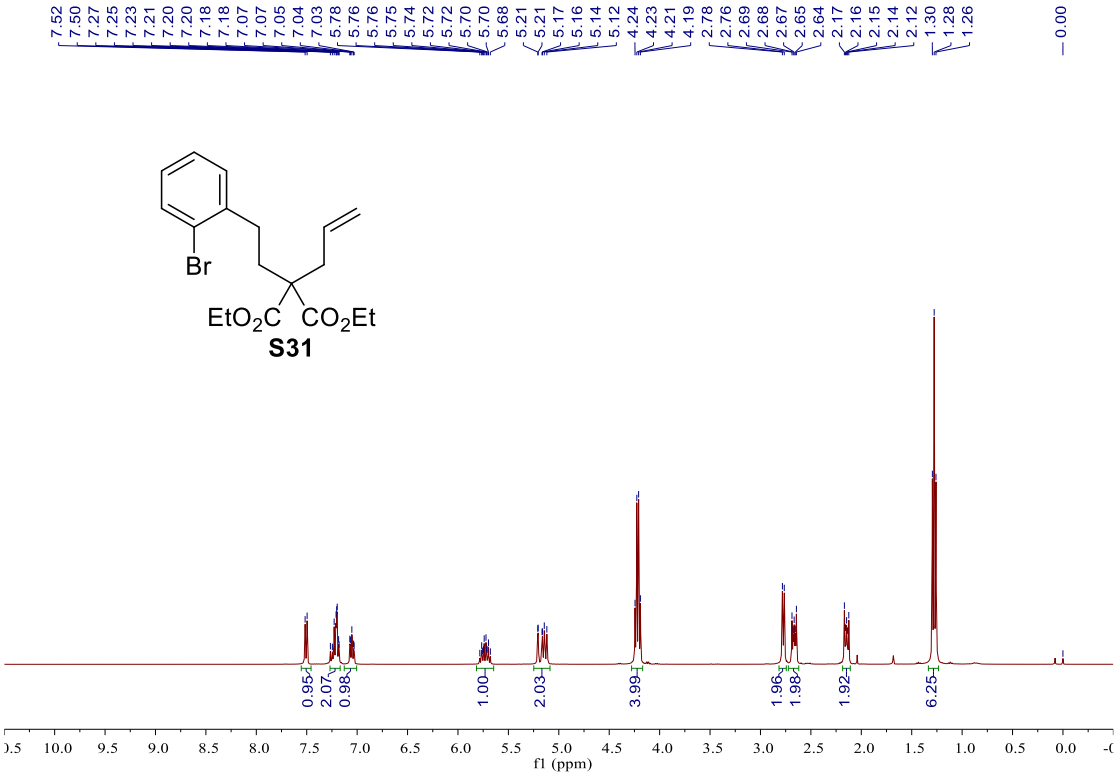
139.73
135.96
132.55
130.35
129.10
126.35
126.23
119.24
77.48
77.16
76.84
61.43
57.47
37.33
33.25
28.02
19.24
14.31
Me
EtO2C CO2Et
S28
f1 (ppm)


OMe
EtO2C CO2Et
S29
f1 (ppm)


OMe
EtO2C CO2Et
S29
f1 (ppm)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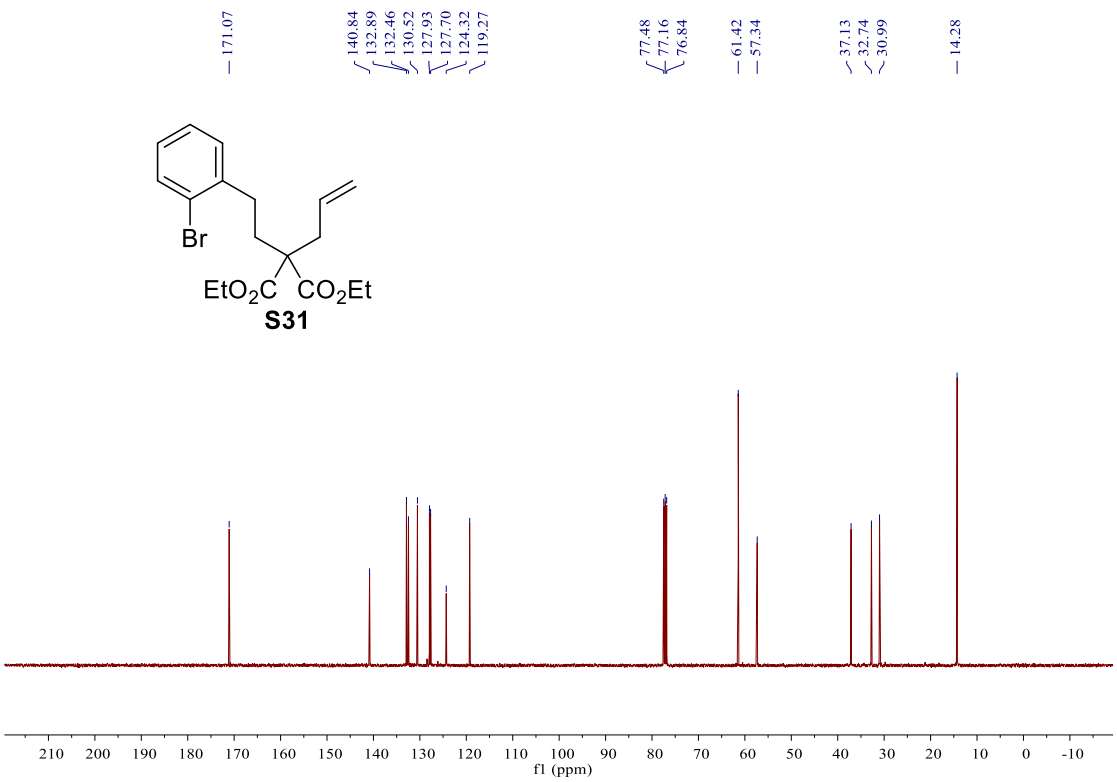
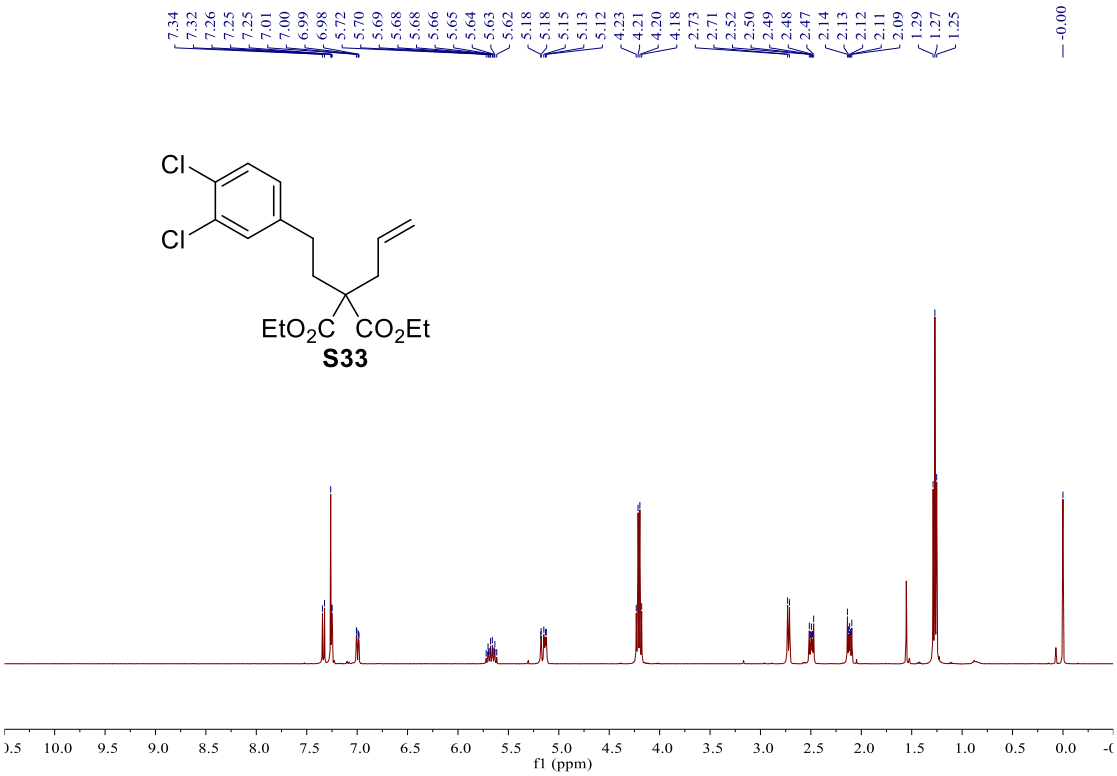
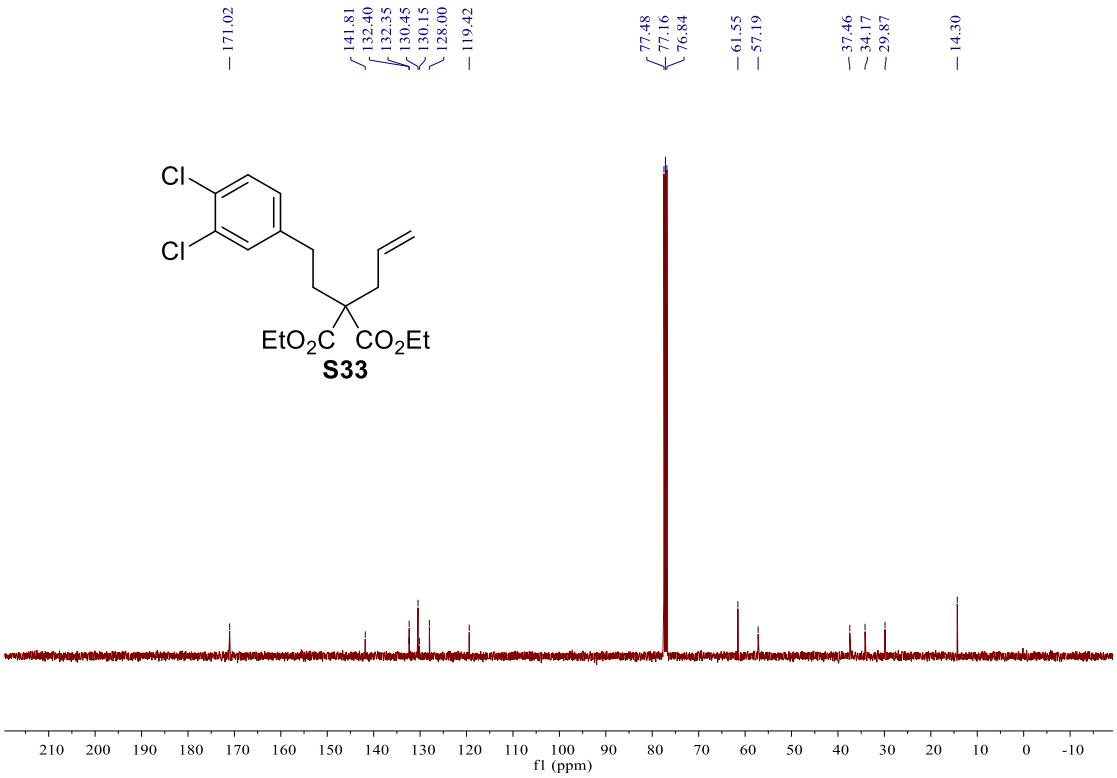
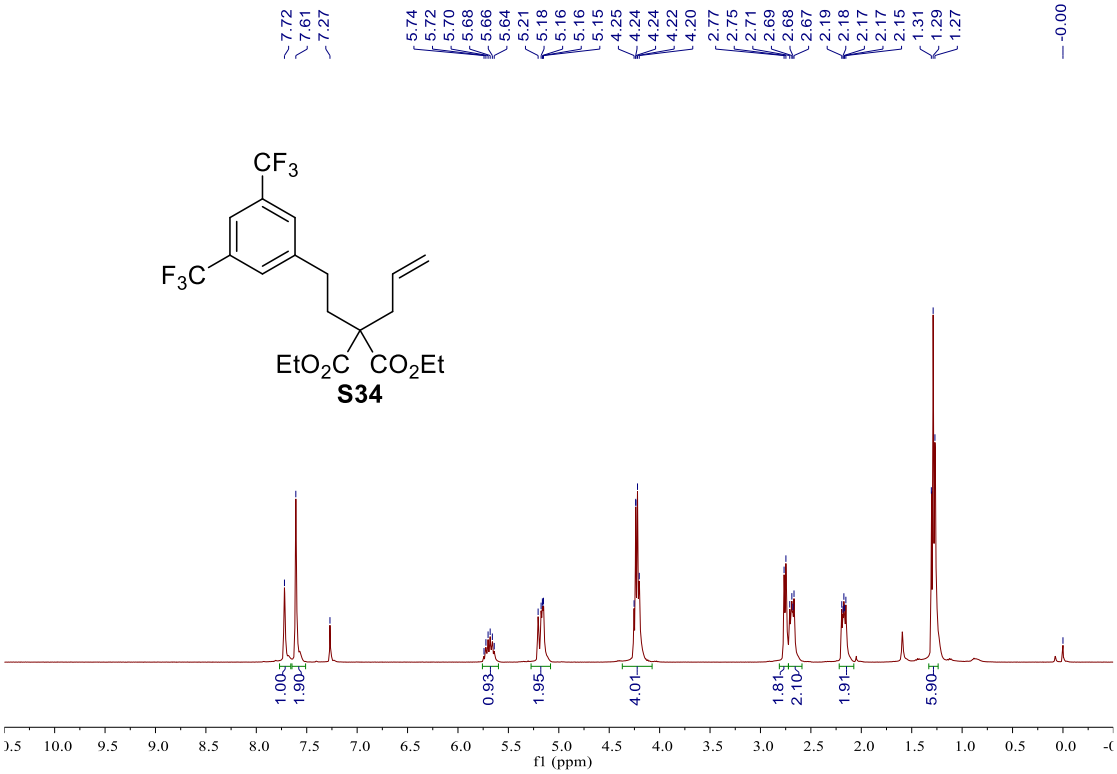
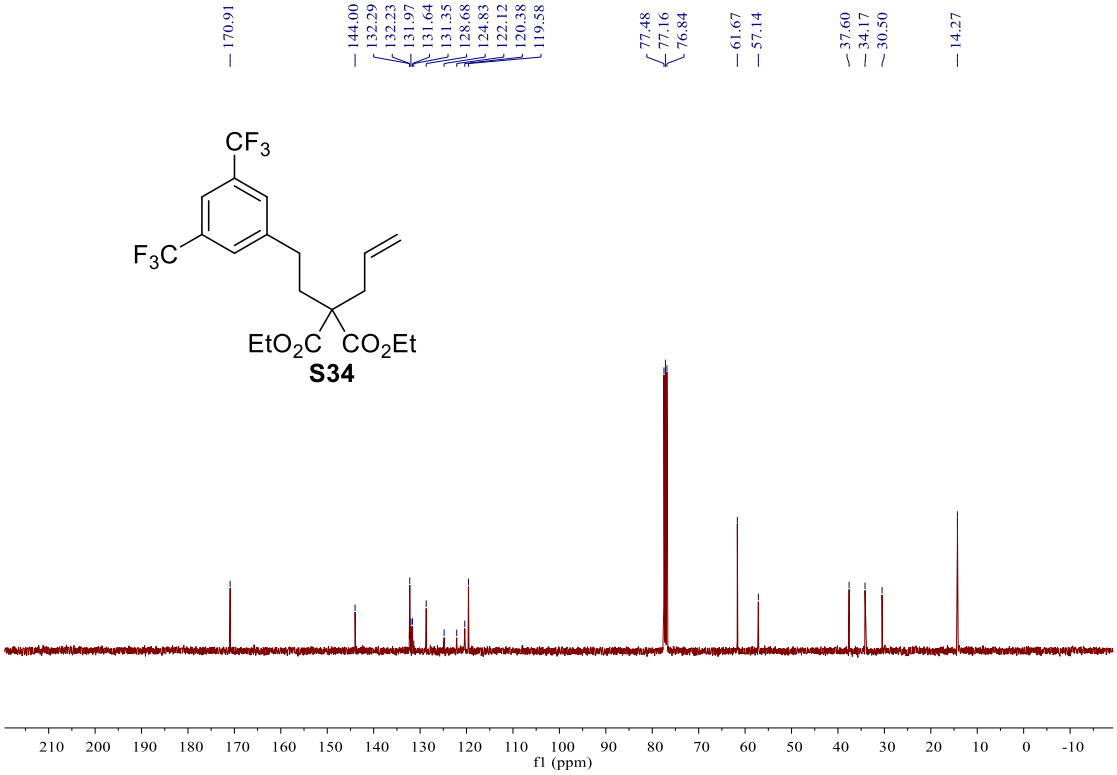
7.50
7.27
7.25
7.23
7.21
7.20
7.20
7.18
7.18
7.07
7.07
7.05
7.04
7.03
5.78
5.76
5.76
5.75
5.74
5.72
5.72
5.70
5.70
5.68
5.21
5.21
5.17
5.16
5.14
5.12
4.24
4.23
4.21
4.19
2.78
2.76
2.69
2.68
2.67
2.65
2.64
2.17
2.16
2.15
2.14
2.12
1.30
1.28
1.26
0.00
Br
EtO2C CO2Et
S31
0.95
2.07
0.98
1.00
2.03
3.99
1.96
1.98
1.92
6.25
f1 (ppm)

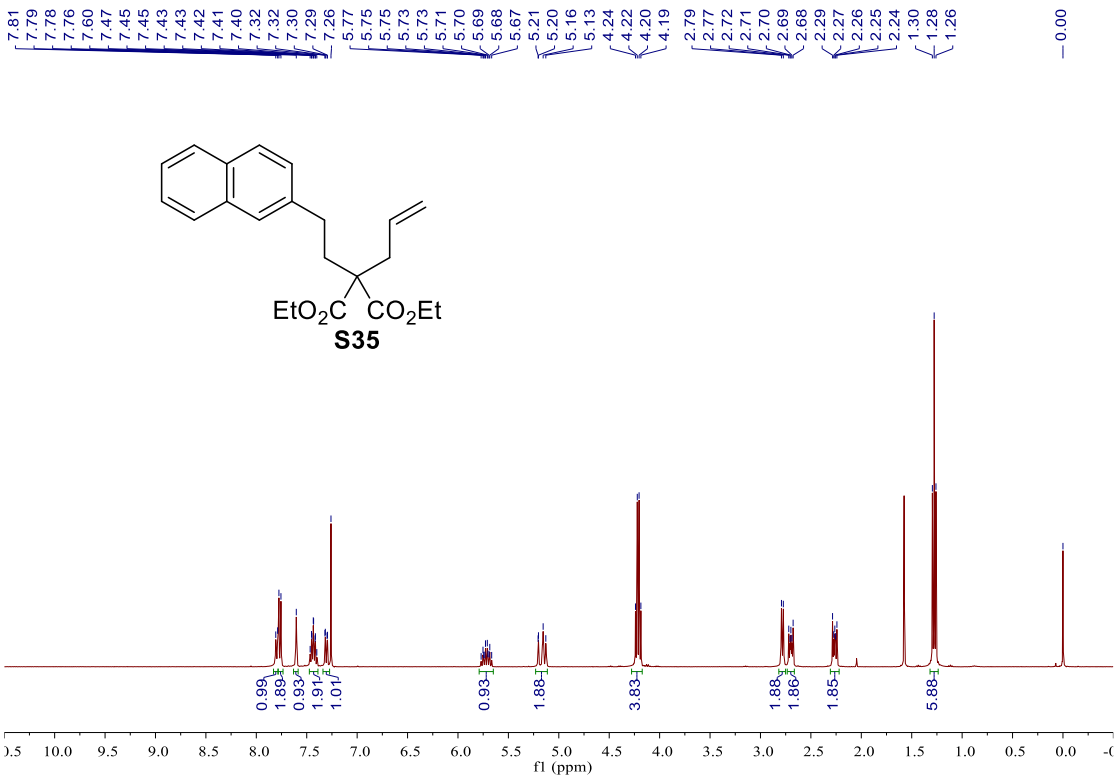

171.07
140.84
132.89
132.46
130.52
127.93
127.70
124.32
119.27
77.48
77.16
76.84
61.42
57.34
37.13
32.74
30.99
14.28
Br
EtO2C CO2Et
S31
f1 (ppm)

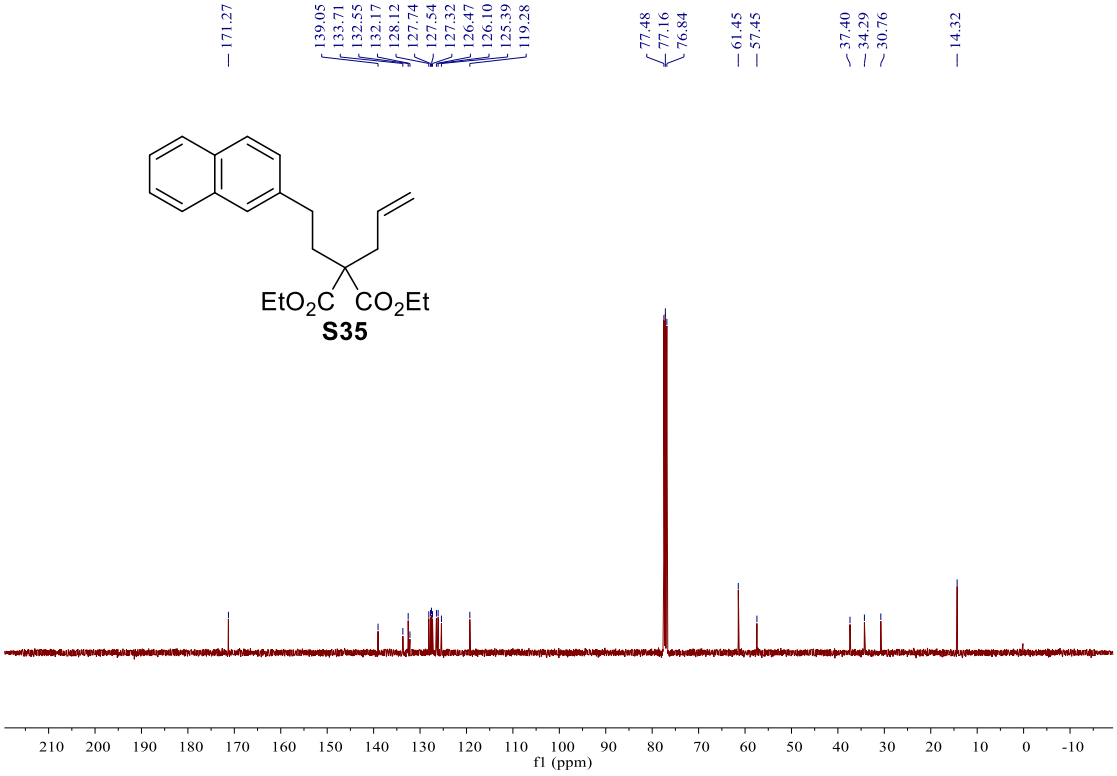

7.34
7.32
7.26
7.25
7.25
7.01
7.00
6.99
6.98
5.72
5.70
5.69
5.68
5.68
5.66
5.65
5.64
5.63
5.62
5.18
5.18
5.15
5.13
5.12
4.23
4.21
4.20
4.18
2.73
2.71
2.52
2.50
2.49
2.48
2.47
2.14
2.13
2.12
2.11
2.09
1.29
1.27
1.25
-0.00
Cl
Cl
EtO2C CO2Et
S33
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


171.02
141.81
132.40
132.35
130.45
130.15
128.00
119.42
77.48
77.16
76.84
61.55
57.19
37.46
34.17
29.87
14.30
Cl
Cl
EtO2C CO2Et
S33
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.72
7.61
7.27
5.74
5.72
5.70
5.68
5.66
5.64
5.21
5.18
5.16
5.15
4.25
4.24
4.22
4.20
2.77
2.75
2.71
2.69
2.68
2.67
2.19
2.18
2.17
2.15
1.31
1.29
1.27
-0.00
CF3
F3C
EtO2C CO2Et
S34
1.00
1.90
0.93
1.95
4.01
1.81
2.10
1.91
5.90
f1 (ppm)


170.91
144.00
132.29
132.23
131.97
131.64
131.35
128.68
124.83
122.12
120.38
119.58
77.48
77.16
76.84
61.67
57.14
37.60
34.17
30.50
14.27
CF3
F3C
EtO2C CO2Et
S34
f1 (ppm)


7.81
7.79
7.78
7.76
7.60
7.47
7.45
7.45
7.43
7.43
7.42
7.41
7.40
7.32
7.30
7.29
7.26
5.77
5.75
5.75
5.73
5.73
5.71
5.70
5.69
5.68
5.67
5.21
5.20
5.16
5.13
4.24
4.22
4.20
4.19
2.79
2.77
2.72
2.71
2.70
2.69
2.68
2.29
2.27
2.26
2.25
2.24
1.30
1.28
1.26
0.00
EtO2C CO2Et
S35
0.99
1.89
0.93
1.91
1.01
0.93
1.88
3.83
1.88
1.86
1.85
5.88
f1 (ppm)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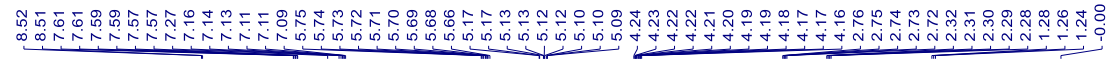
139.05
133.71
132.55
132.17
128.12
127.74
127.54
127.32
126.47
126.10
125.39
119.28
77.48
77.16
76.84
61.45
57.45
37.40
34.29
30.76
14.32
EtO2C CO2Et
S35
f1 (ppm)


8.52
8.51
7.61
7.61
7.59
7.59
7.57
7.57
7.27
7.16
7.14
7.13
7.11
7.11
7.09
5.75
5.74
5.73
5.72
5.71
5.70
5.69
5.68
5.66
5.17
5.17
5.13
5.13
5.12
5.12
5.10
5.10
5.09
4.24
4.23
4.22
4.22
4.21
4.20
4.19
4.19
4.18
4.17
4.17
4.16
2.76
2.75
2.74
2.73
2.72
2.32
2.31
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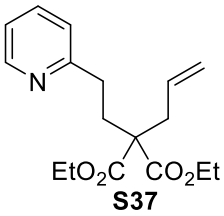
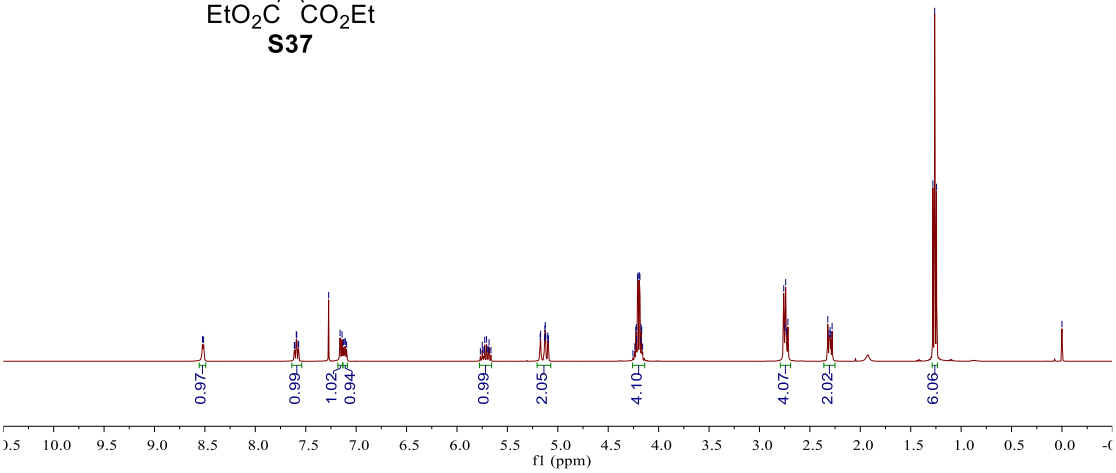
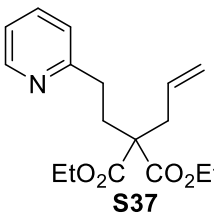
2.28
1.28
1.26
1.24
-0.00


N
EtO2C
CO2Et

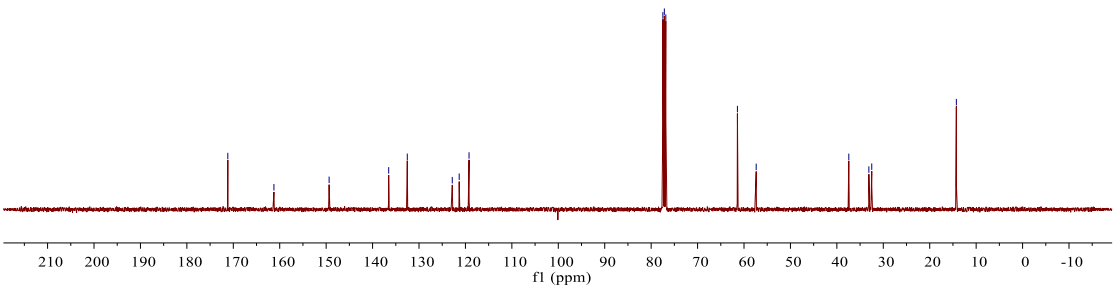
S37

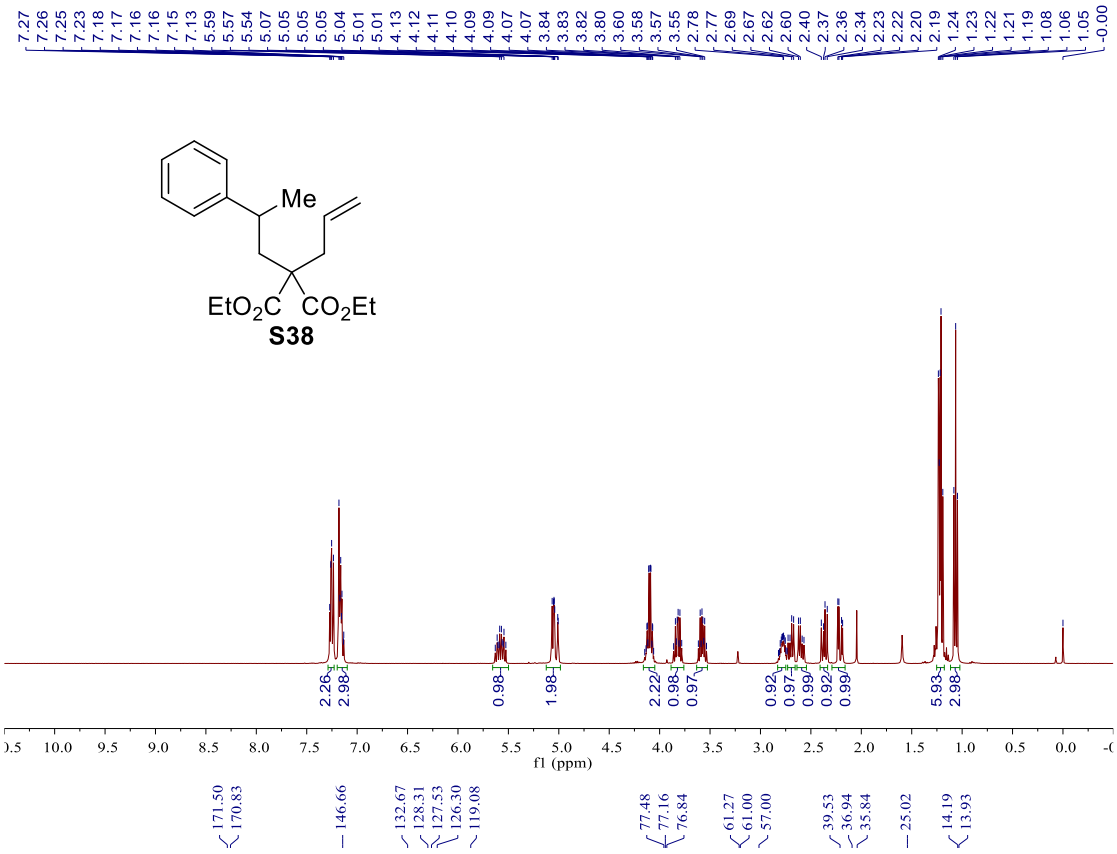

0.97
0.99
1.02
0.94
0.99
2.05
4.10
4.07
2.02
6.06
f1 (ppm)

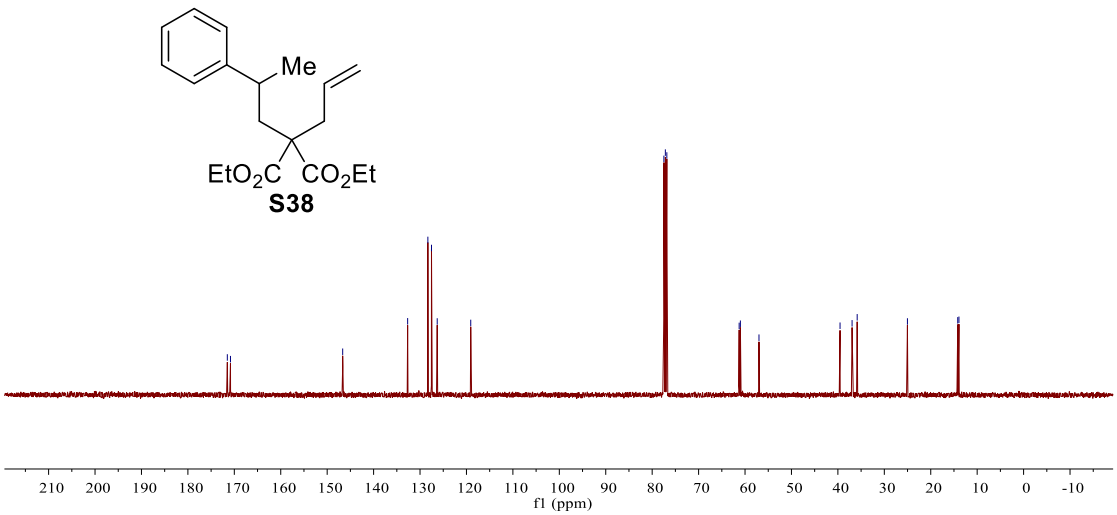

171.18
161.25
149.36
136.53
132.52
122.83
121.35
119.22
77.48
77.16
76.84
61.42
57.37
37.43
33.11
32.48
14.26

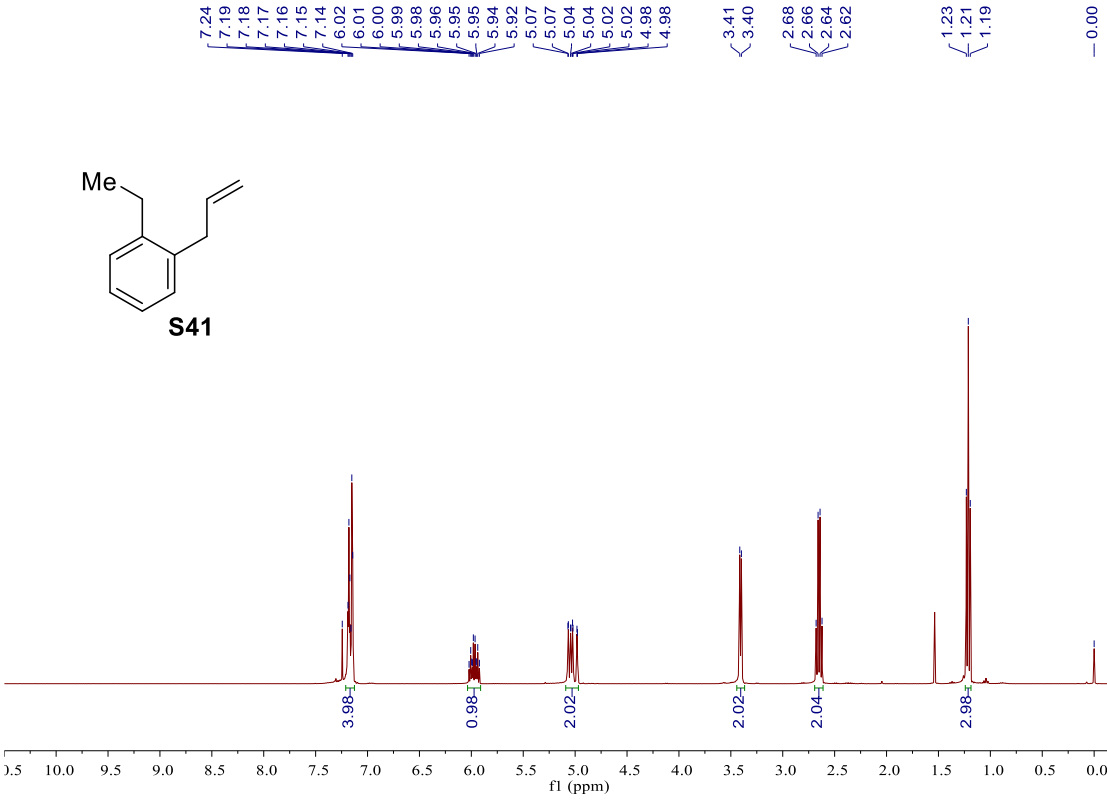

N
EtO2C
CO2Et

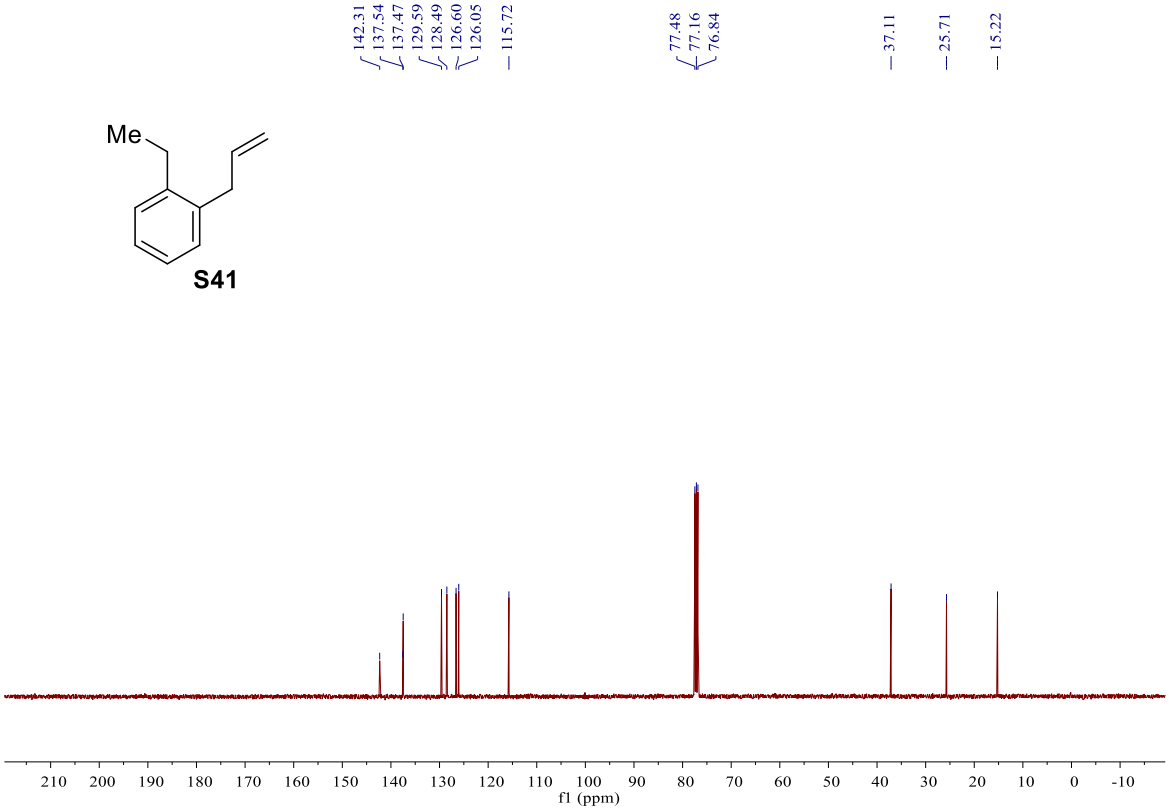
S37

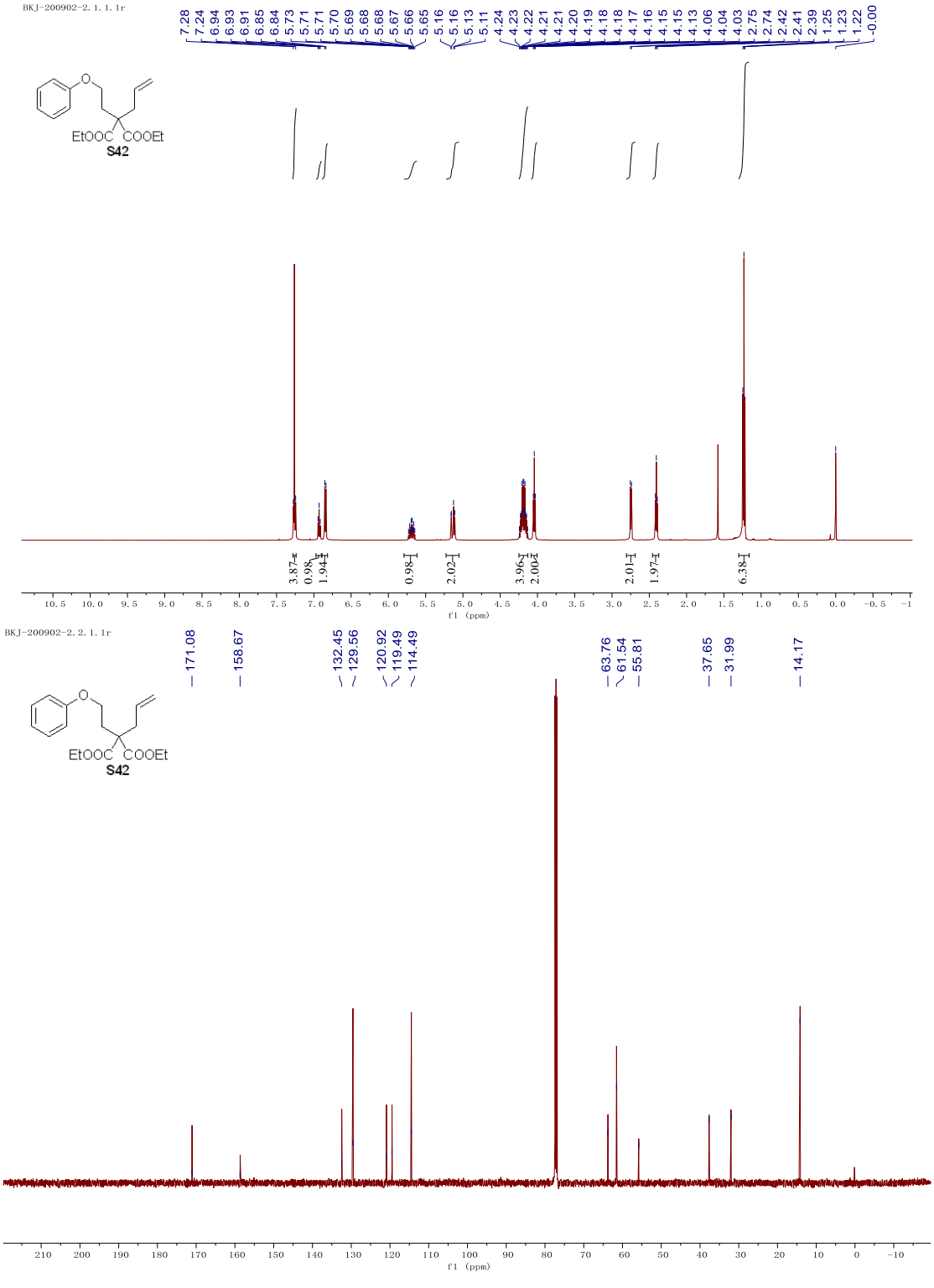

f1 (ppm)

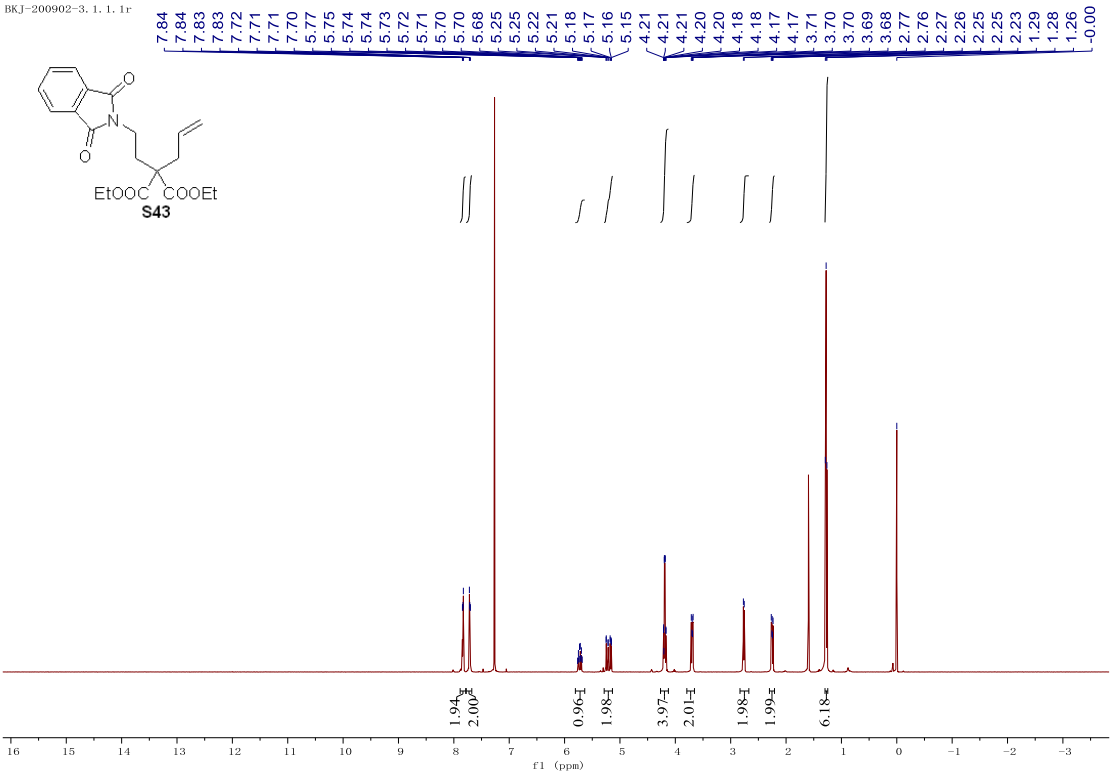

Me
EtO2C CO2Et
S38
f1 (ppm)


Me
EtO2C CO2Et
S38
f1 (ppm)


7.24
7.19
7.18
7.17
7.16
7.15
7.14
6.02
6.01
6.00
5.99
5.98
5.96
5.95
5.95
5.94
5.92
5.07
5.07
5.04
5.04
5.02
5.02
4.98
4.98
3.41
3.40
2.68
2.66
2.64
2.62
1.23
1.21
1.19
0.00
Me
S41
3.98
0.98
2.02
2.02
2.04
2.98
f1 (ppm)


142.31
137.54
137.47
129.59
128.49
126.60
126.05
115.72
77.48
77.16
76.84
37.11
25.71
15.22
Me
S41
f1 (ppm)


BKJ-200902-2.1.1r
7.28
7.24
6.94
6.93
6.91
6.85
6.84
5.73
5.71
5.71
5.70
5.69
5.68
5.68
5.67
5.66
5.65
5.16
5.16
5.13
5.11
4.24
4.23
4.22
4.21
4.21
4.20
4.19
4.18
4.18
4.17
4.16
4.15
4.15
4.13
4.06
4.04
4.03
2.75
2.74
2.42
2.41
2.39
1.25
1.23
1.22
-0.00
EtOOC COOEt
S42
3.87
0.98
1.94
0.98
2.02
3.96
2.00
2.01
1.97
6.38
f1 (ppm)
BKJ-200902-2.2.1.1r
171.08
158.67
132.45
129.56
120.92
119.49
114.49
63.76
61.54
55.81
37.65
31.99
14.17
EtOOC COOEt
S42
f1 (ppm)


BKJ-200902-3.1.1.1r
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7.84
7.83
7.83
7.72
7.71
7.71
7.70
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5.75
5.74
5.74
5.73
5.72
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5.17
5.16
5.15
4.21
4.21
4.21
4.20
4.20
4.18
4.18
4.17
4.17
3.71
3.70
3.70
3.69
3.68
2.77
2.76
2.27
2.26
2.25
2.25
2.23
1.29
1.28
1.26
-0.00
EtOOC COOEt
S43
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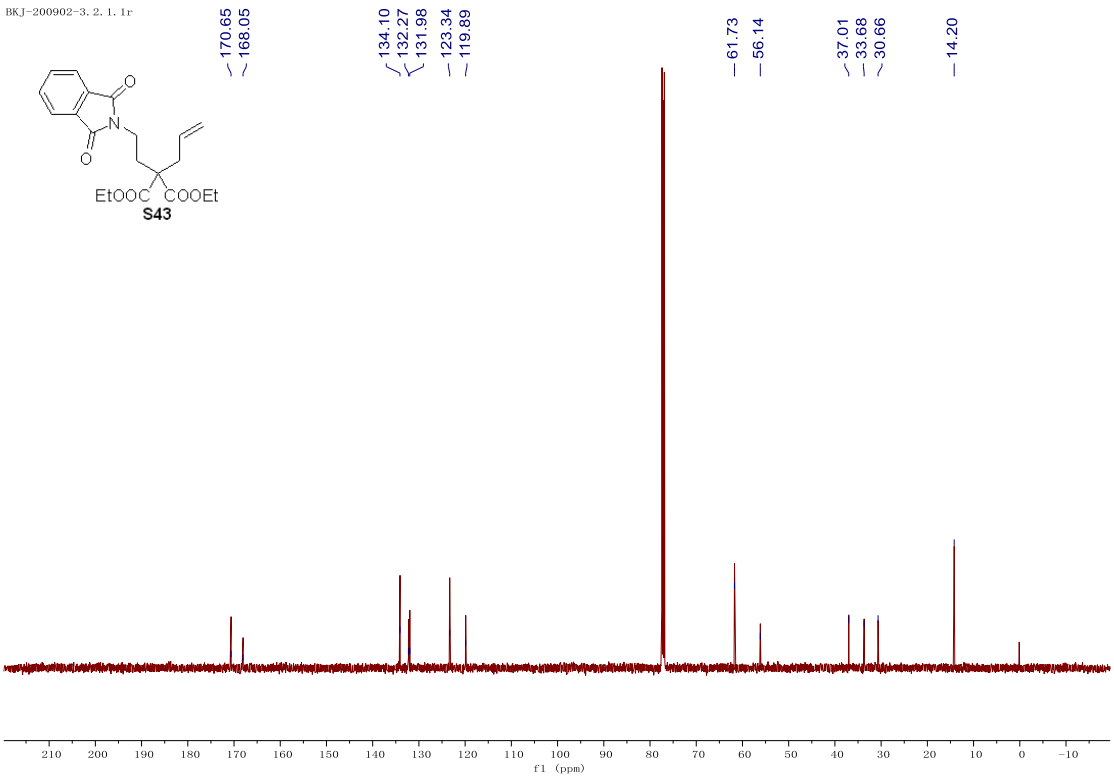
2.00
0.96
1.98
3.97
2.01
1.98
1.99
6.18
f1 (ppm)


BKJ-200902-3.2.1.1r
170.65
168.05
134.10
132.27
131.98
123.34
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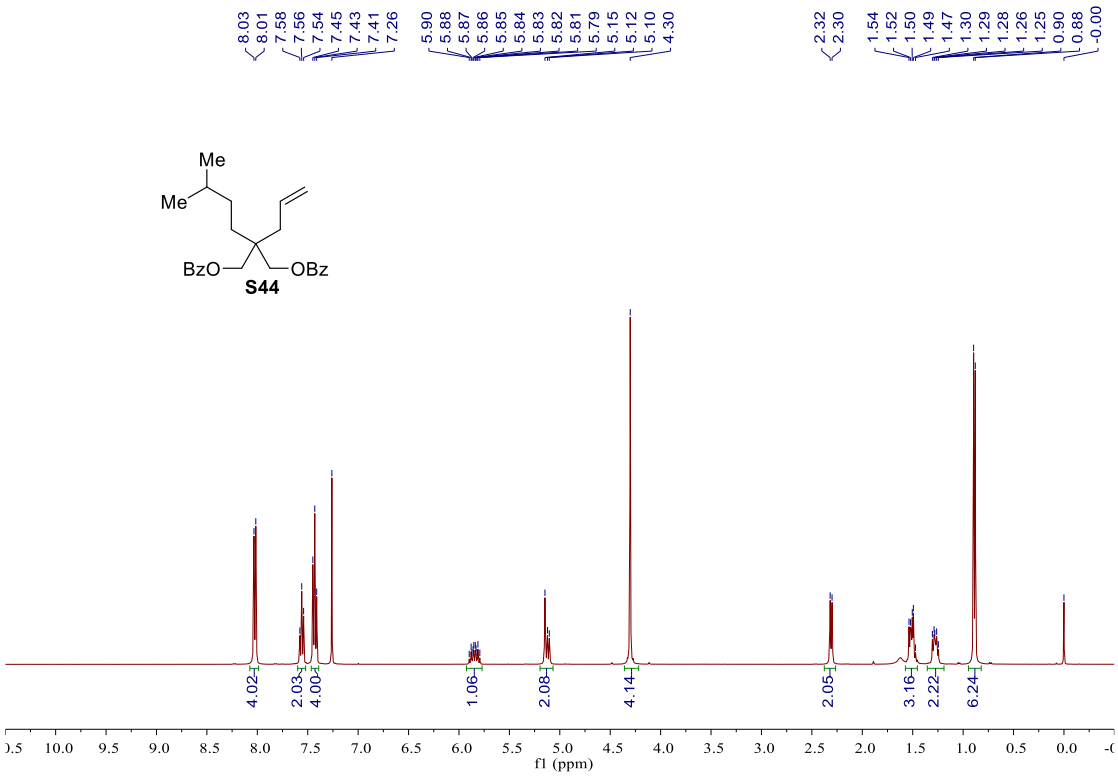
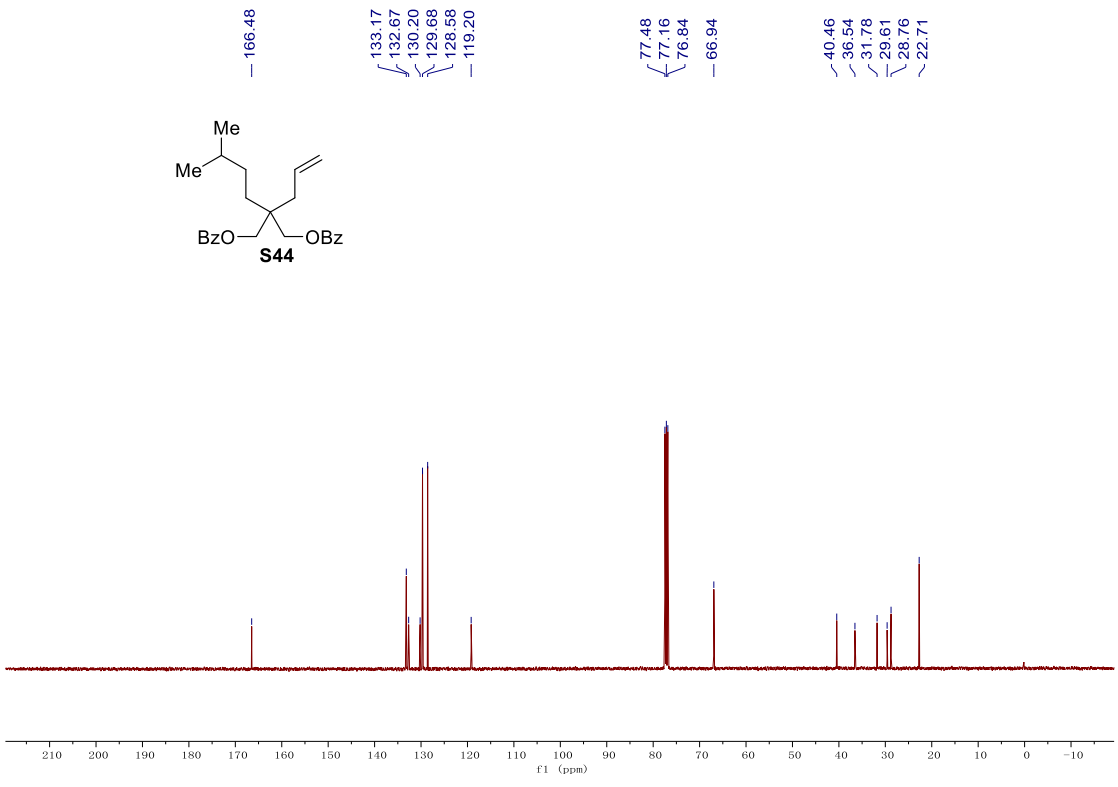
61.73
56.14
37.01
33.68
30.66
14.20
EtOOC COOEt
S43
f1 (ppm)


8.03
8.01
7.58
7.56
7.54
7.45
7.43
7.41
7.26
5.90
5.88
5.87
5.86
5.85
5.84
5.83
5.82
5.81
5.79
5.15
5.12
5.10
4.30
2.32
2.30
1.54
1.52
1.50
1.49
1.47
1.30
1.29
1.28
1.26
1.25
0.90
0.88
-0.00
Me
Me
BzO
OBz
S44
4.02
2.03
4.00
1.06
2.08
4.14
2.05
3.16
2.22
6.24
f1 (ppm)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133.17
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130.20
129.68
128.58
119.20
77.48
77.16
76.84
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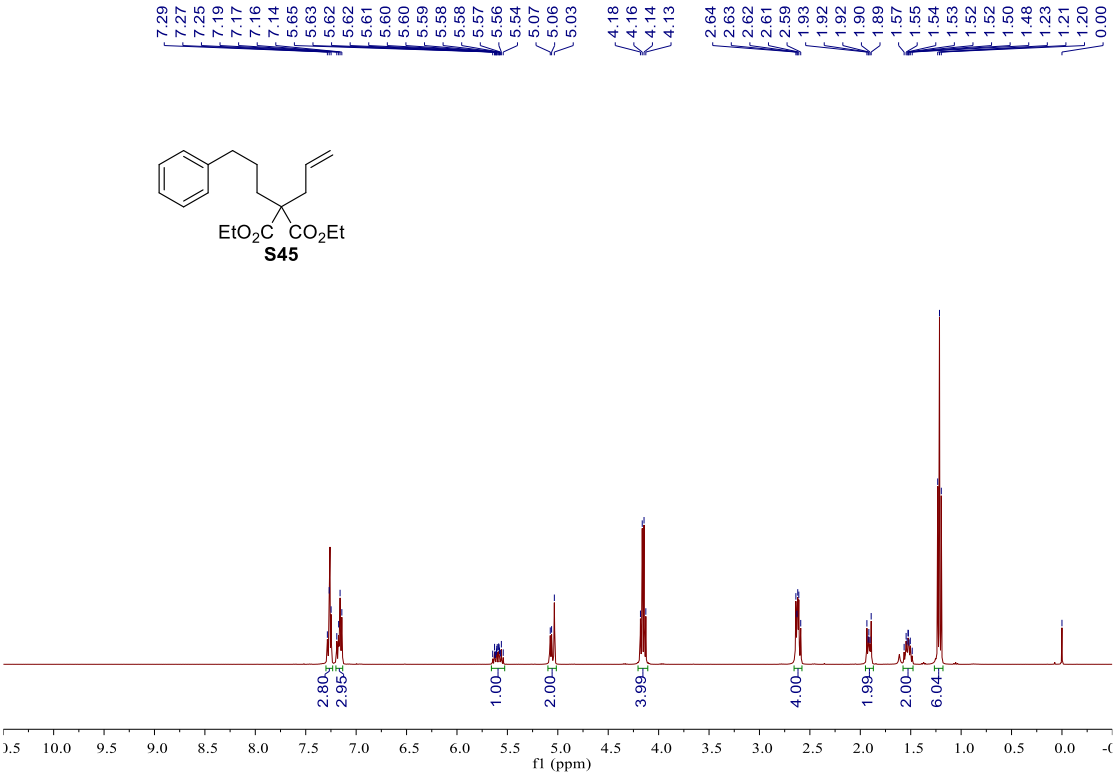
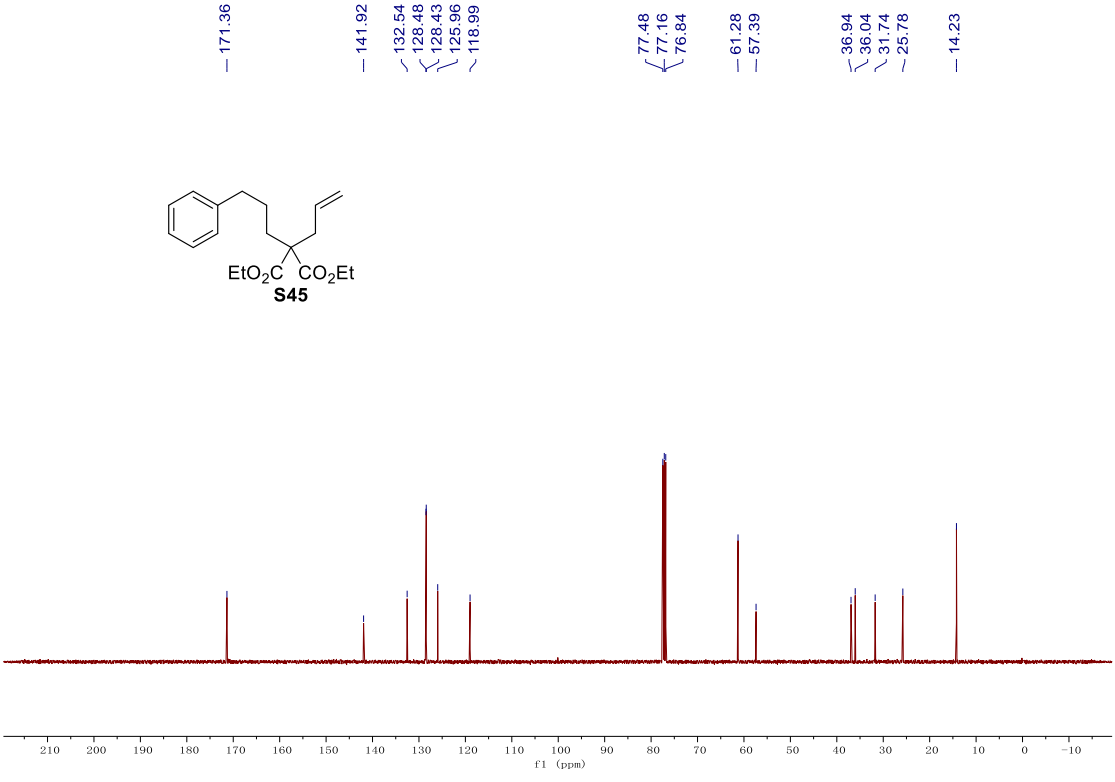
40.46
36.54
31.78
29.61
28.76
22.71
Me
Me
BzO
OBz
S44
f1 (ppm)


7.29
7.27
7.25
7.19
7.17
7.16
7.14
5.65
5.63
5.62
5.62
5.61
5.60
5.60
5.59
5.58
5.58
5.57
5.56
5.54
5.07
5.06
5.03
4.18
4.16
4.14
4.13
2.64
2.63
2.62
2.61
2.59
1.93
1.92
1.92
1.90
1.89
1.57
1.55
1.54
1.53
1.52
1.52
1.50
1.48
1.23
1.21
1.20
0.00
EtO2C CO2Et
S45
2.80
2.95
1.00
2.00
3.99
4.00
1.99
2.00
6.04
f1 (ppm)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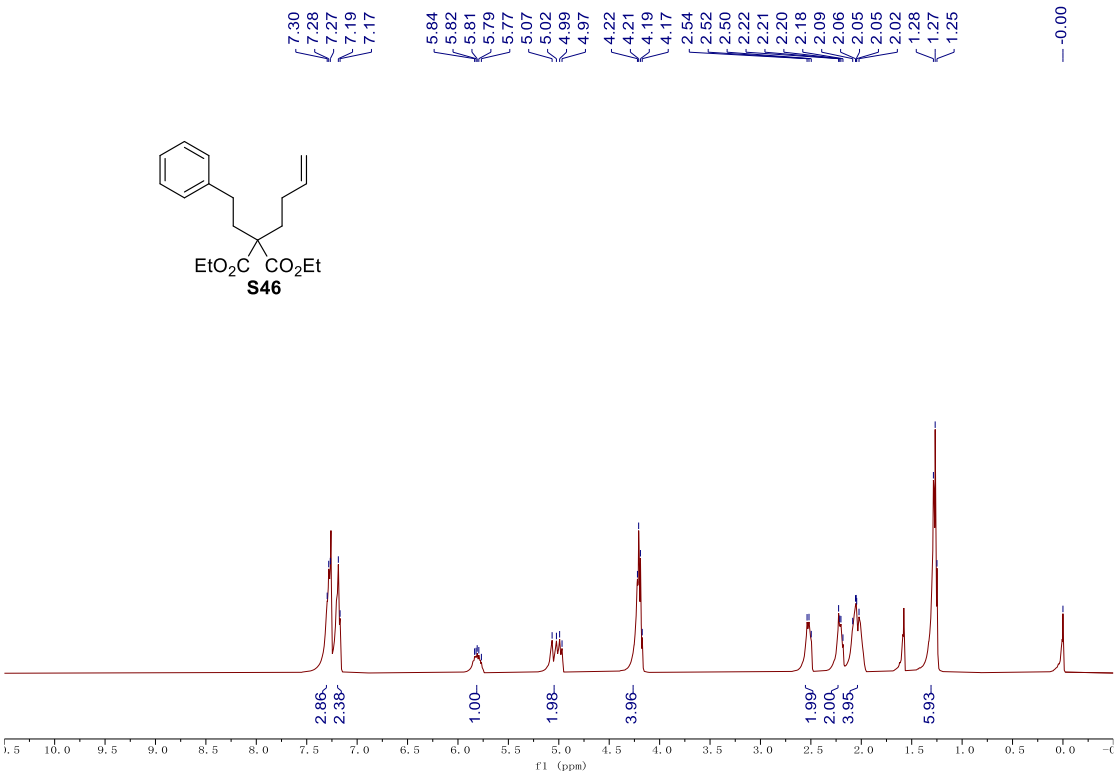
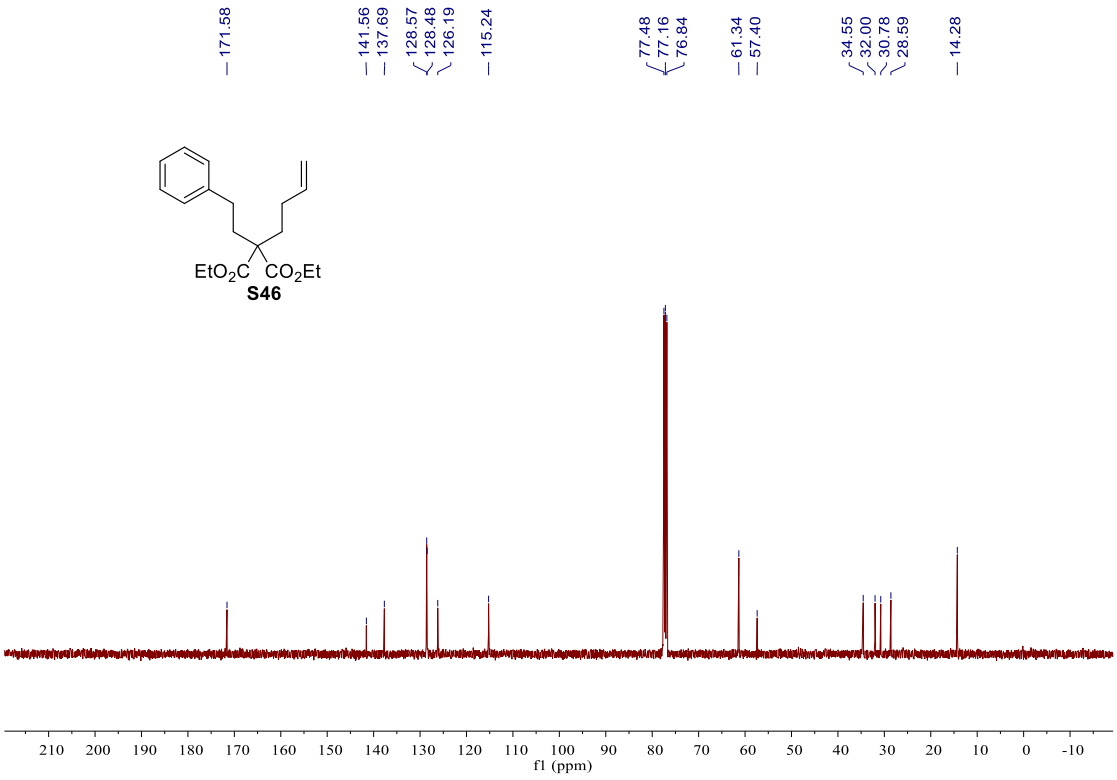
141.92
132.54
128.48
128.43
125.96
118.99
77.48
77.16
76.84
61.28
57.39
36.94
36.04
31.74
25.78
14.23
EtO2C CO2Et
S45
f1 (ppm)


7.30
7.28
7.27
7.19
7.17
5.84
5.82
5.81
5.79
5.77
5.07
5.02
4.99
4.97
4.22
4.21
4.19
4.17
2.54
2.52
2.50
2.22
2.21
2.20
2.18
2.09
2.06
2.05
2.05
2.02
1.28
1.27
1.25
-0.00
EtO2C CO2Et
S46
2.86
2.38
1.00
1.98
3.96
1.99
2.00
3.95
5.93
f1 (ppm)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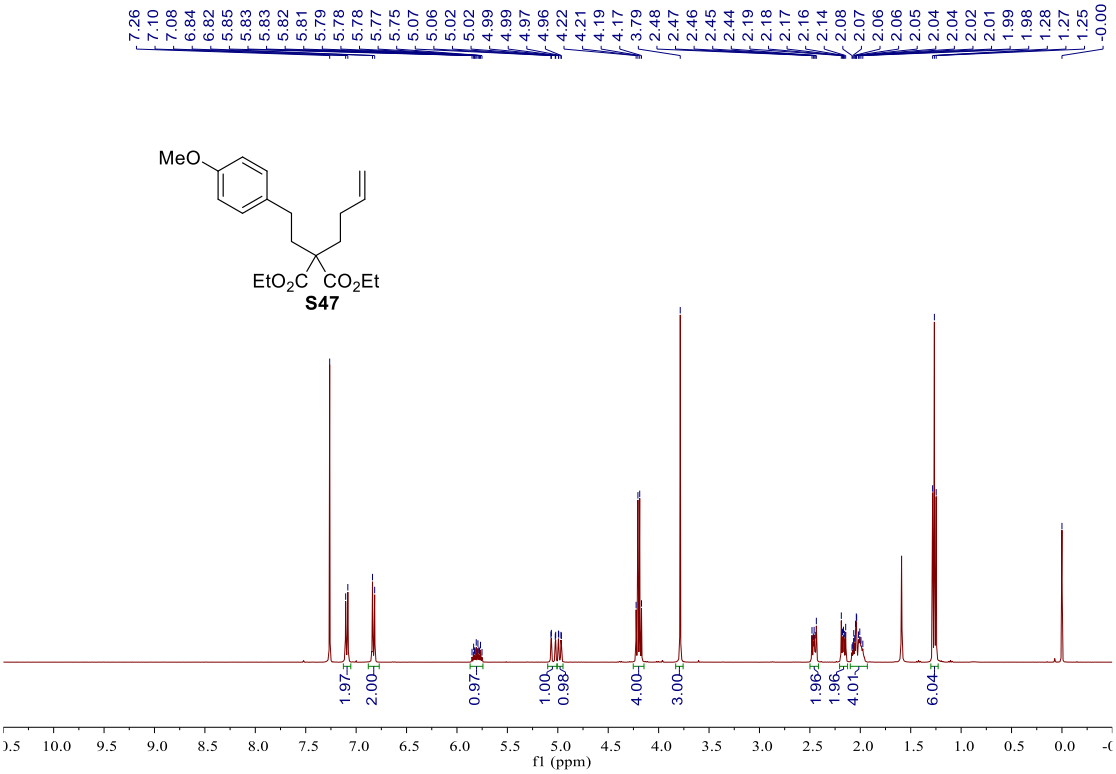
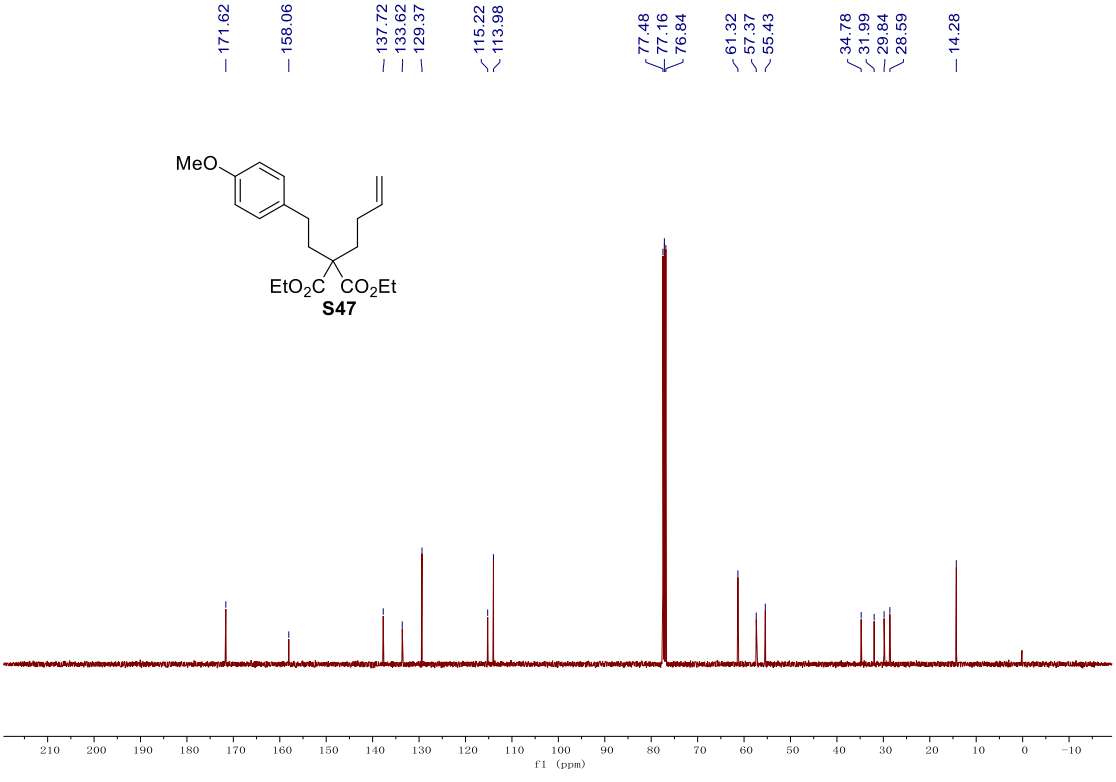
126.19
115.24
77.48
77.16
76.84
61.34
57.40
34.55
32.00
30.78
28.59
14.28
EtO2C CO2Et
S46
f1 (ppm)


7.26
7.10
7.08
6.84
6.82
5.85
5.83
5.83
5.82
5.81
5.79
5.78
5.78
5.77
5.75
5.07
5.06
5.02
5.02
4.99
4.99
4.97
4.96
4.22
4.21
4.19
4.17
3.79
2.48
2.47
2.46
2.45
2.44
2.19
2.18
2.17
2.16
2.14
2.08
2.07
2.06
2.06
2.05
2.04
2.04
2.02
2.01
1.99
1.98
1.28
1.27
1.25
-0.00
MeO
EtO2C CO2Et
S47
1.97
2.00
0.97
1.00
0.98
4.00
3.00
1.96
1.96
4.01
6.04
f1 (ppm)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158.06
137.72
133.62
129.37
115.22
113.98
77.48
77.16
76.84
61.32
57.37
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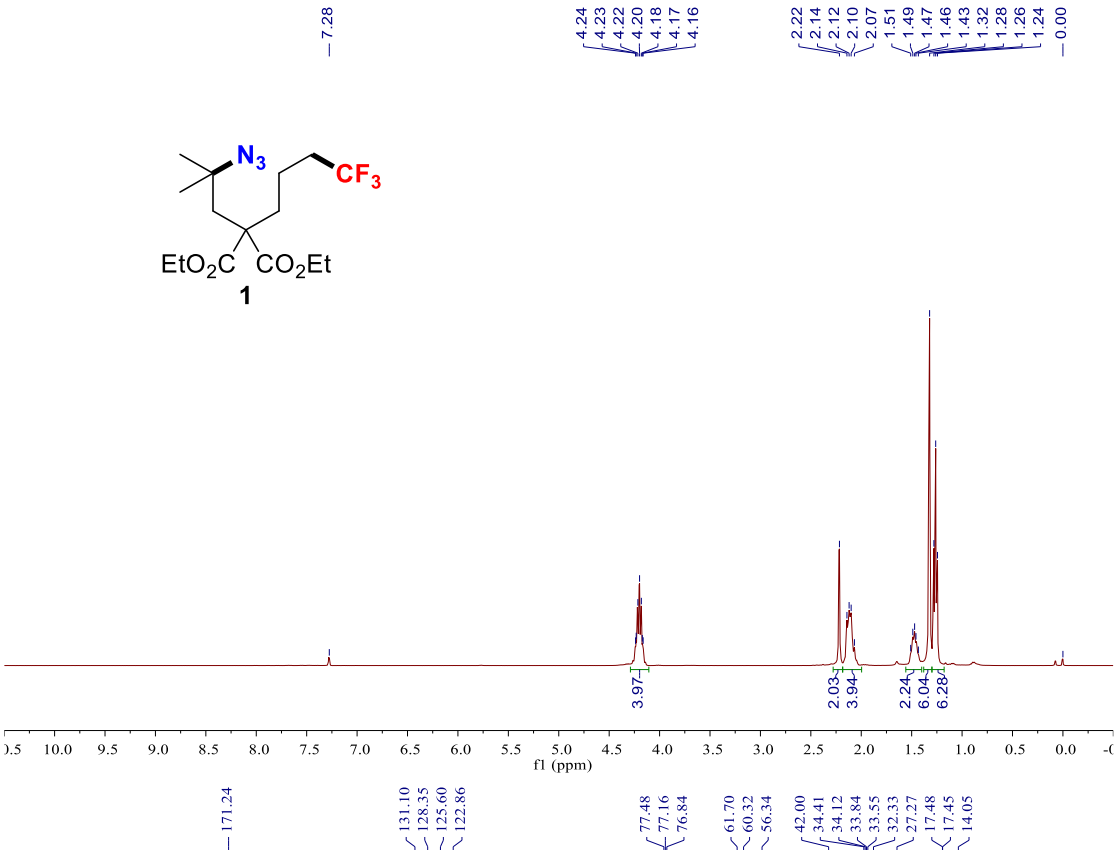
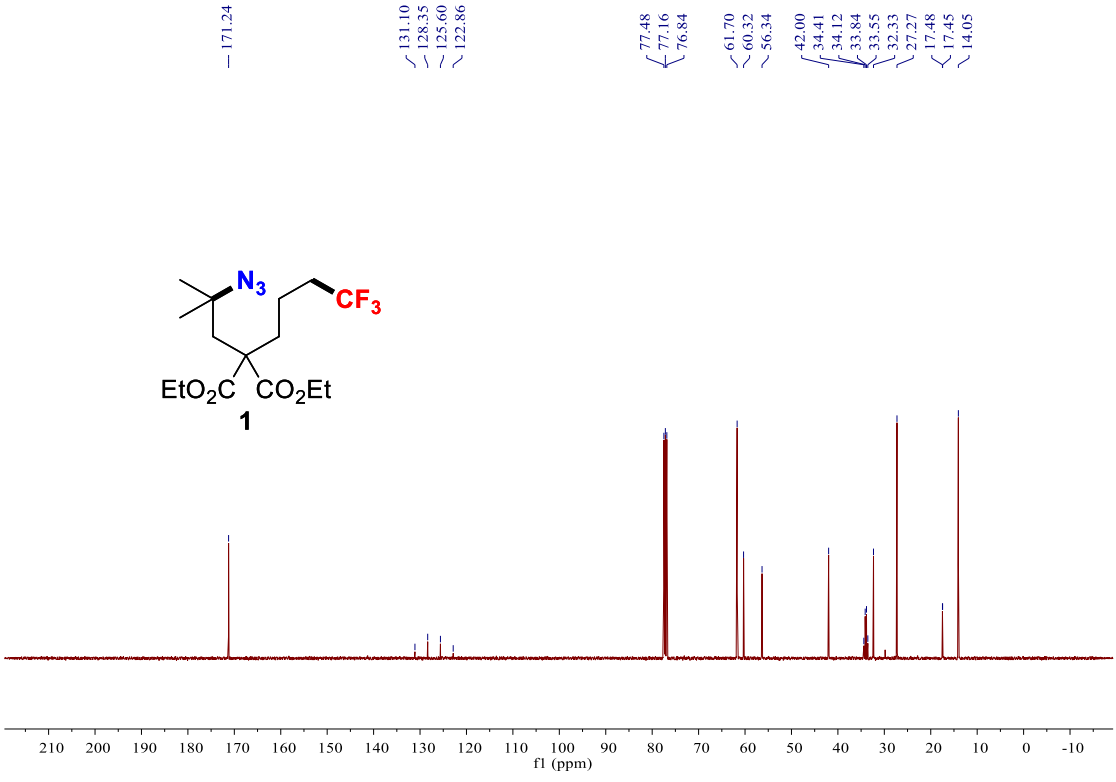
28.59
14.28
MeO
EtO2C CO2Et
S47
f1 (ppm)


7.28
4.24
4.23
4.22
4.20
4.18
4.17
4.16
2.22
2.14
2.12
2.10
2.07
1.51
1.49
1.47
1.46
1.43
1.32
1.28
1.26
1.24
0.00
N3
CF3
EtO2C
CO2Et
1
3.97
2.03
3.94
2.24
6.04
6.28
f1 (ppm)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131.10
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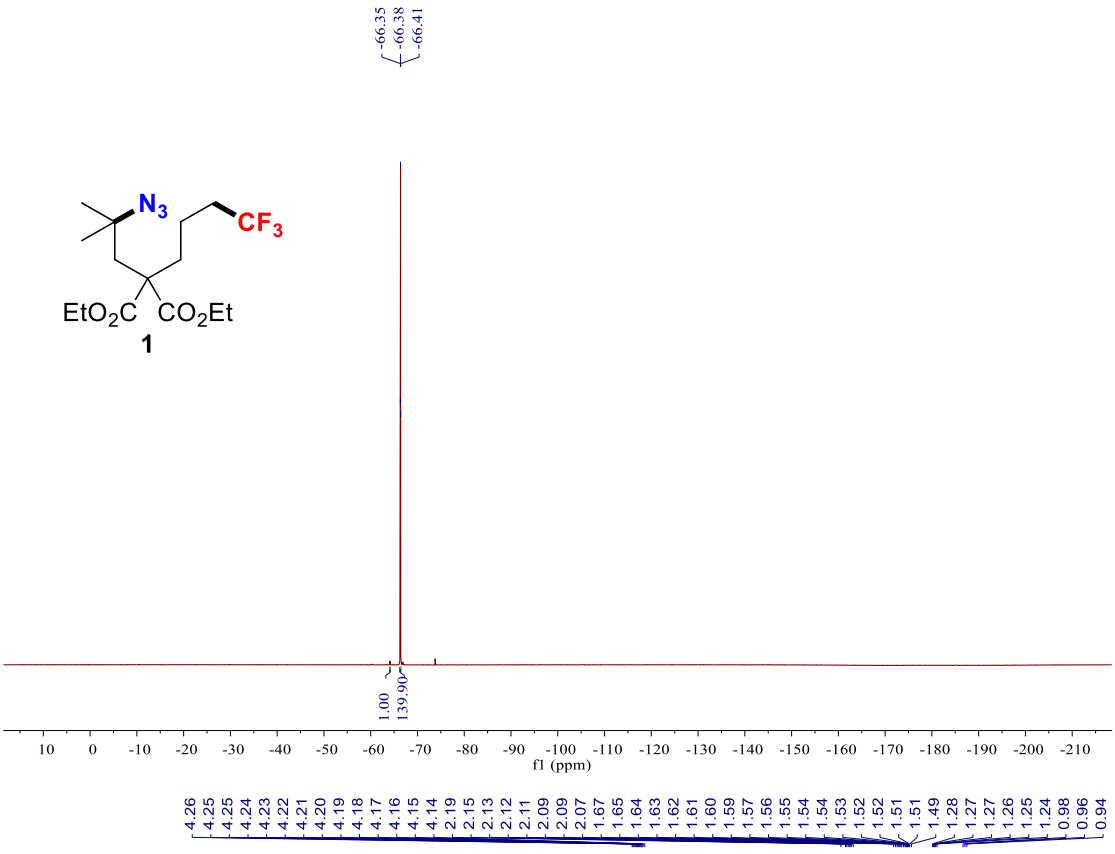
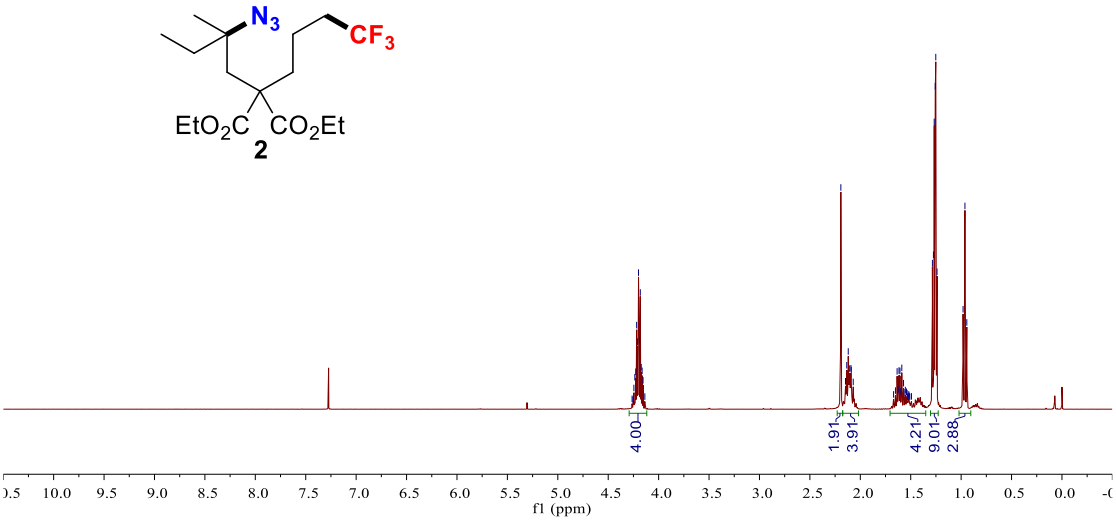
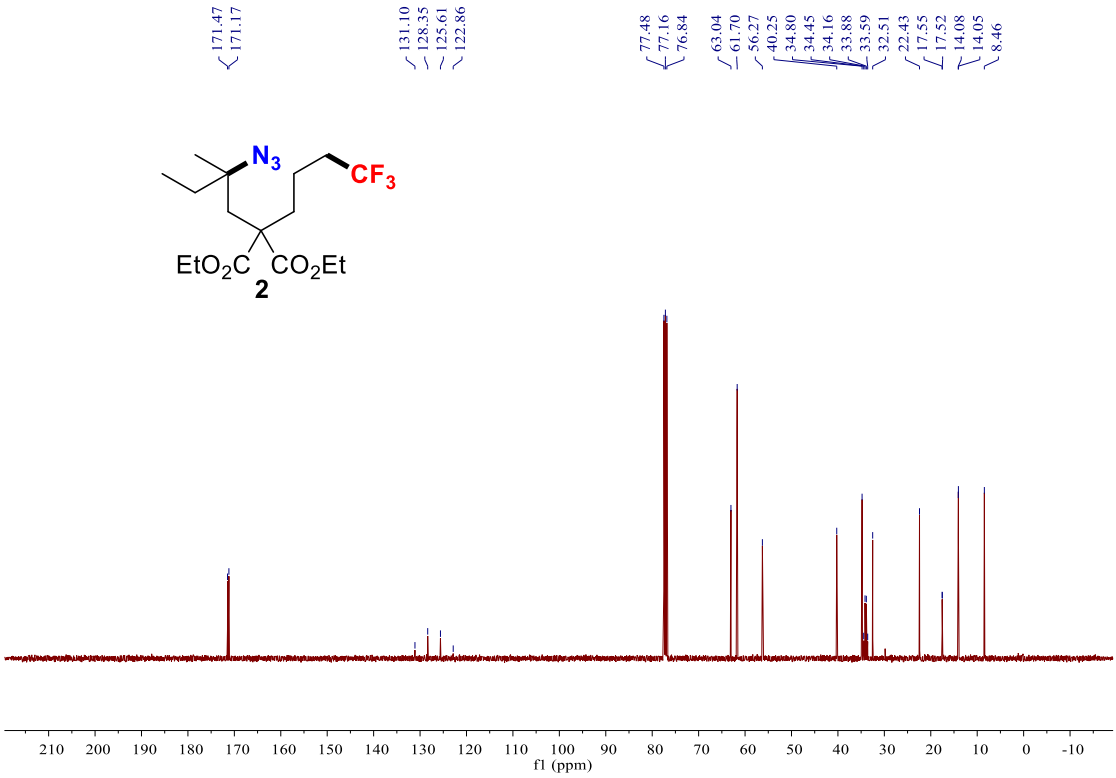
125.60
122.86
77.48
77.16
76.84
61.70
60.32
56.34
42.00
34.41
34.12
33.84
33.55
32.33
27.27
17.48
17.45
14.05
N3
CF3
EtO2C
CO2Et
1
f1 (ppm)


-66.35
-66.38
-66.41
N3
CF3
EtO2C
CO2Et
1
1.00
139.90
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)
4.26 4.25 4.25 4.24 4.23 4.22 4.21 4.20 4.19 4.18 4.17 4.16 4.15 4.14 2.19 2.15 2.13 2.12 2.11 2.09 2.09 2.07 1.67 1.65 1.64 1.63 1.62 1.61 1.60 1.59 1.57 1.56 1.55 1.54 1.54 1.53 1.52 1.52 1.51 1.51 1.49 1.28 1.27 1.27 1.26 1.25 1.24 0.98 0.96 0.94


N3
CF3
EtO2C
CO2Et
2
4.00
1.91
3.91
4.21
9.01
2.88
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)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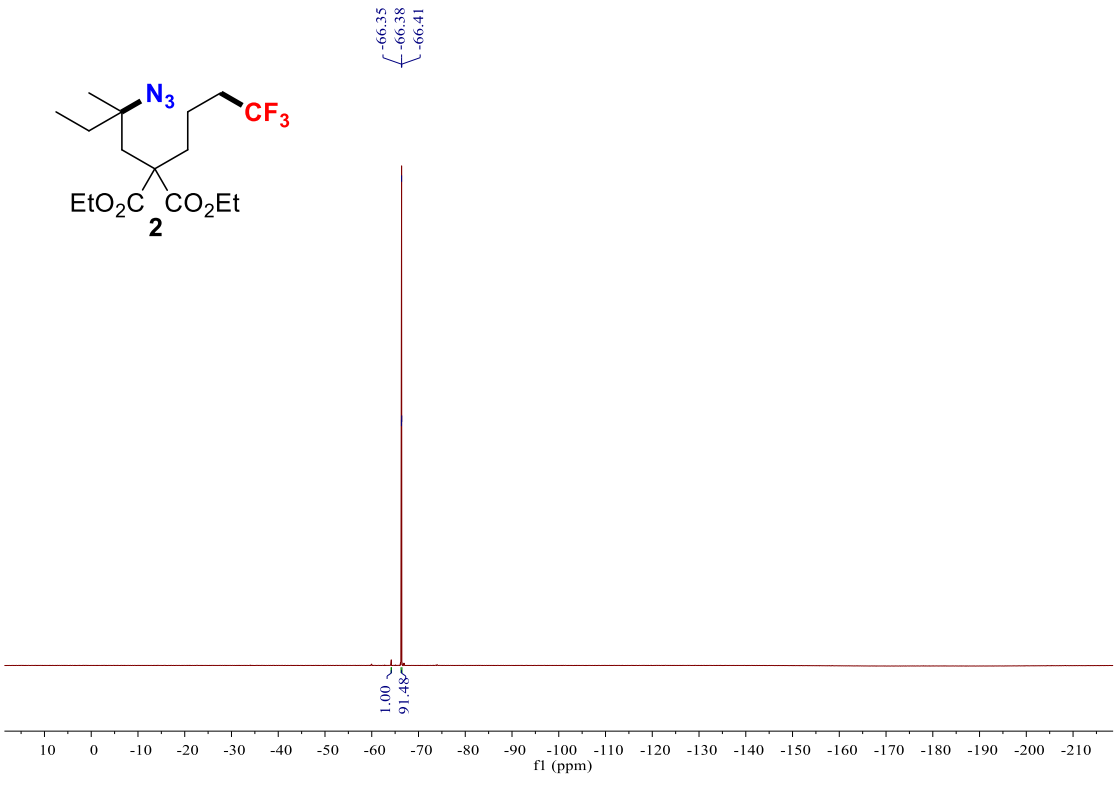
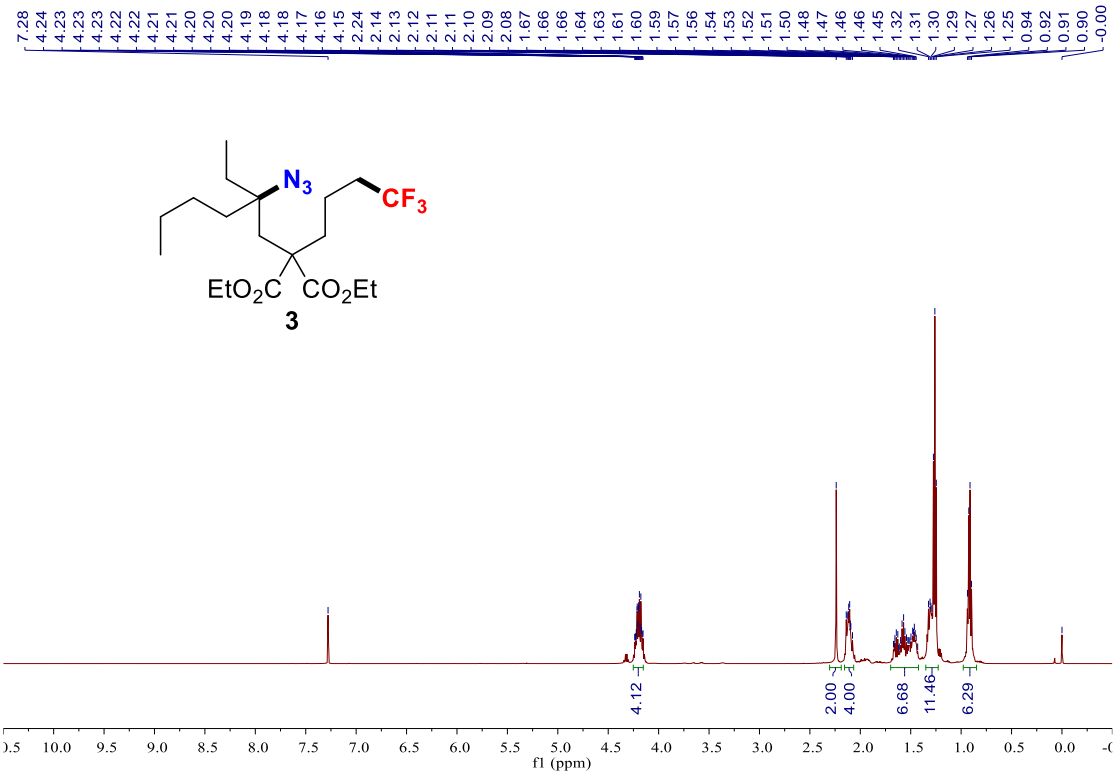
171.17
131.10
128.35
125.61
122.86
77.48
77.16
76.84
63.04
61.70
56.27
40.25
34.80
34.45
34.16
33.88
33.59
32.51
22.43
17.55
17.52
14.08
14.05
8.46
N3
CF3
EtO2C
CO2Et
2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-66.35
-66.38
-66.41
N3
CF3
EtO2C
CO2Et
2
1.00
91.48
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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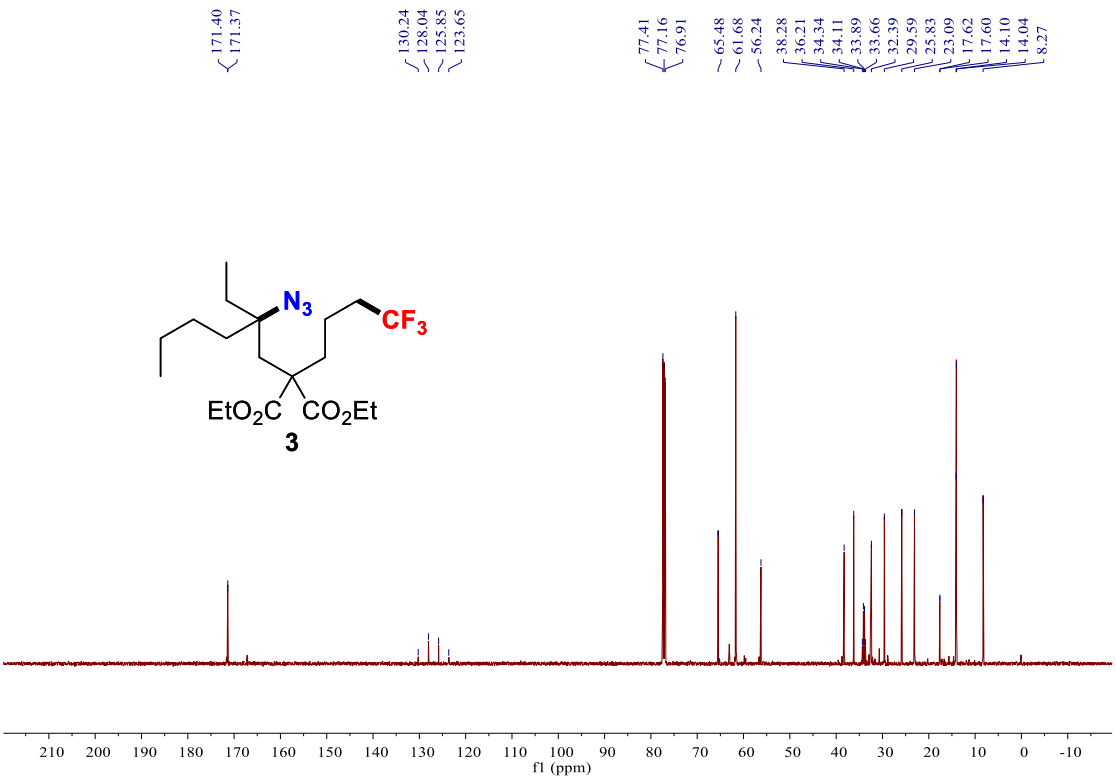
4.24
4.23
4.23
4.23
4.22
4.22
4.21
4.21
4.20
4.20
4.20
4.19
4.18
4.18
4.17
4.16
4.15
2.24
2.14
2.13
2.12
2.11
2.11
2.10
2.09
2.08
1.67
1.66
1.66
1.64
1.63
1.61
1.60
1.59
1.57
1.56
1.54
1.53
1.52
1.51
1.50
1.48
1.47
1.46
1.46
1.45
1.32
1.31
1.30
1.29
1.27
1.26
1.25
0.94
0.92
0.91
0.90
-0.00
N3
CF3
EtO2C
CO2Et
3
4.12
2.00
4.00
6.68
11.46
6.29
f1 (ppm)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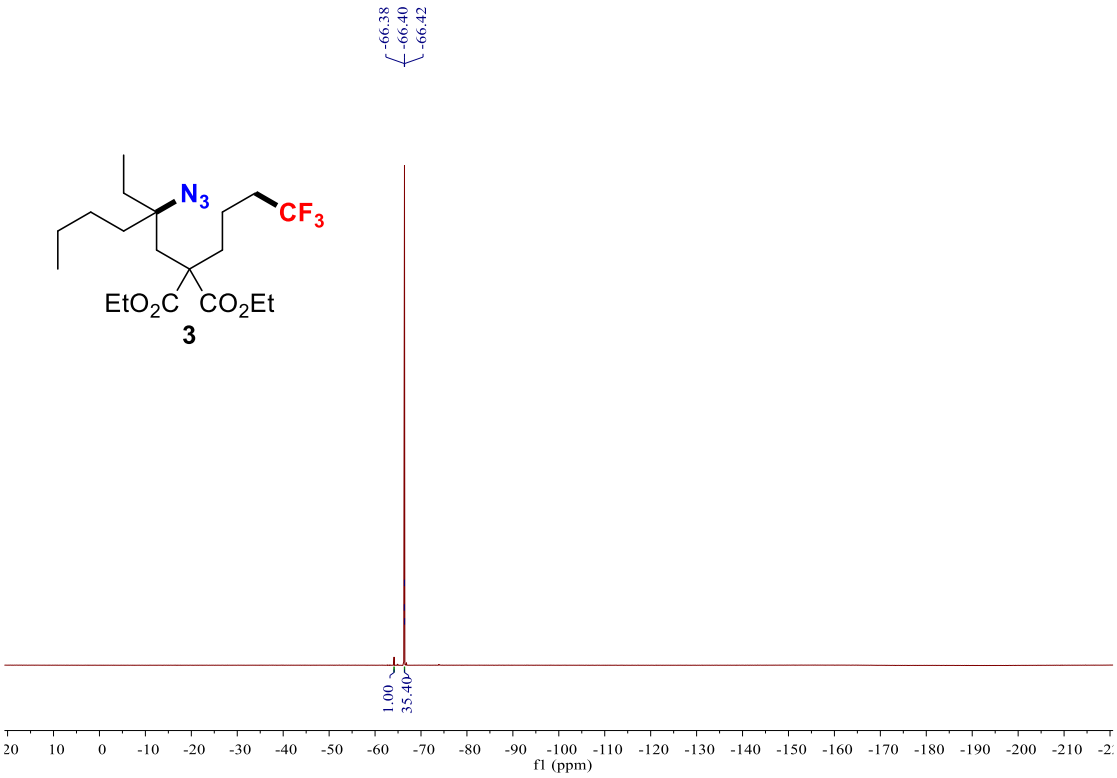
171.37
130.24
128.04
125.85
123.65
77.41
77.16
76.91
65.48
61.68
56.24
38.28
36.21
34.34
34.11
33.89
33.66
32.39
29.59
25.83
23.09
17.62
17.60
14.10
14.04
8.27
N3
CF3
EtO2C
CO2Et
3
f1 (ppm)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-66.42
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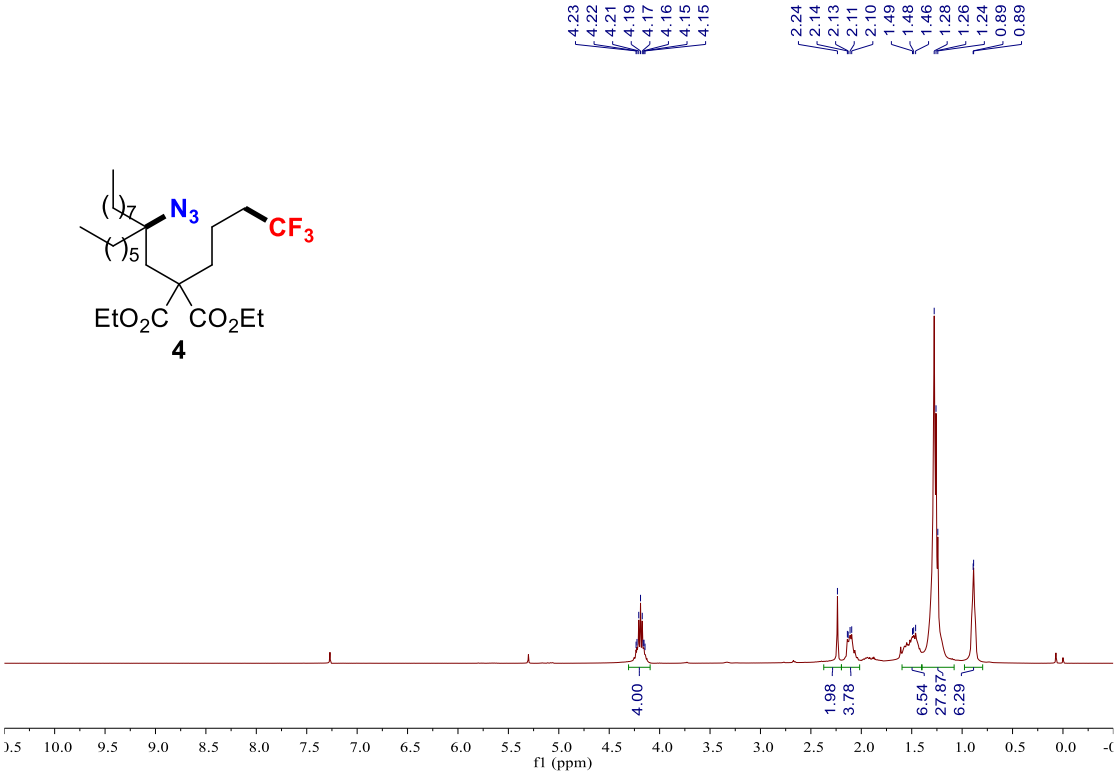
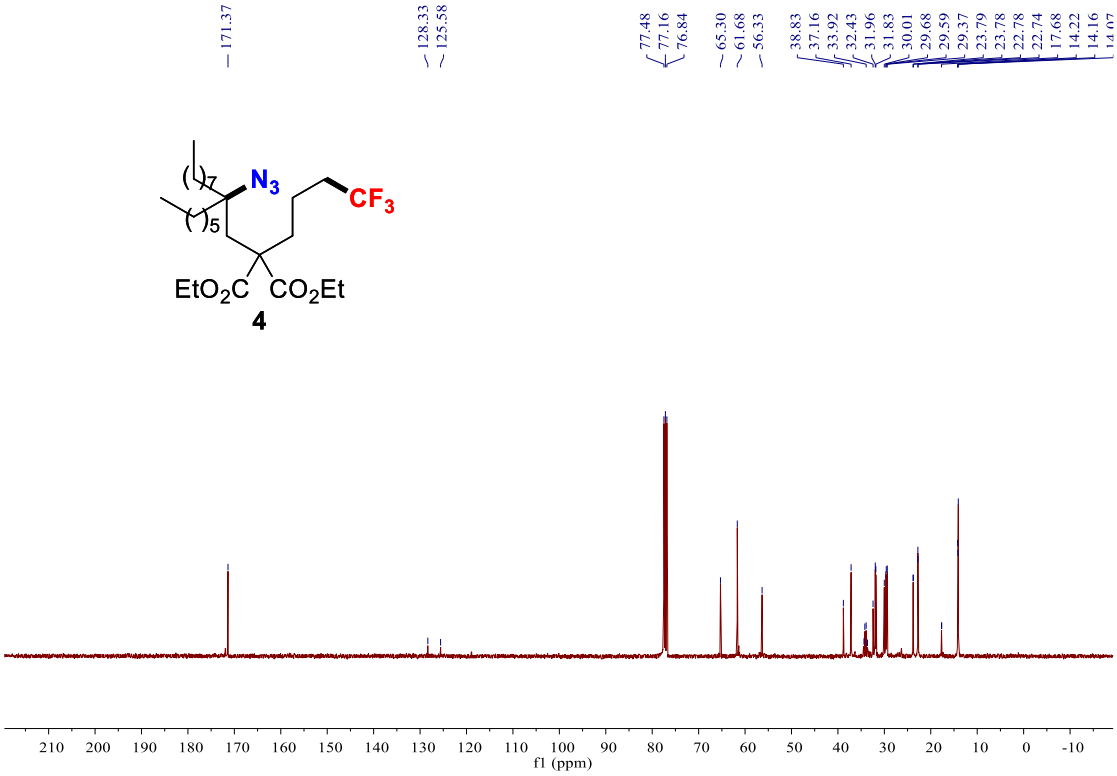
CF3
EtO2C CO2Et
3
1.00
35.40
f1 (ppm)


4.23
4.22
4.21
4.19
4.17
4.16
4.15
4.15
2.24
2.14
2.13
2.11
2.10
1.49
1.48
1.46
1.28
1.26
1.24
0.89
0.89
N3
CF3
EtO2C CO2Et
4
4.00
1.98
3.78
6.54
27.87
6.29
f1 (ppm)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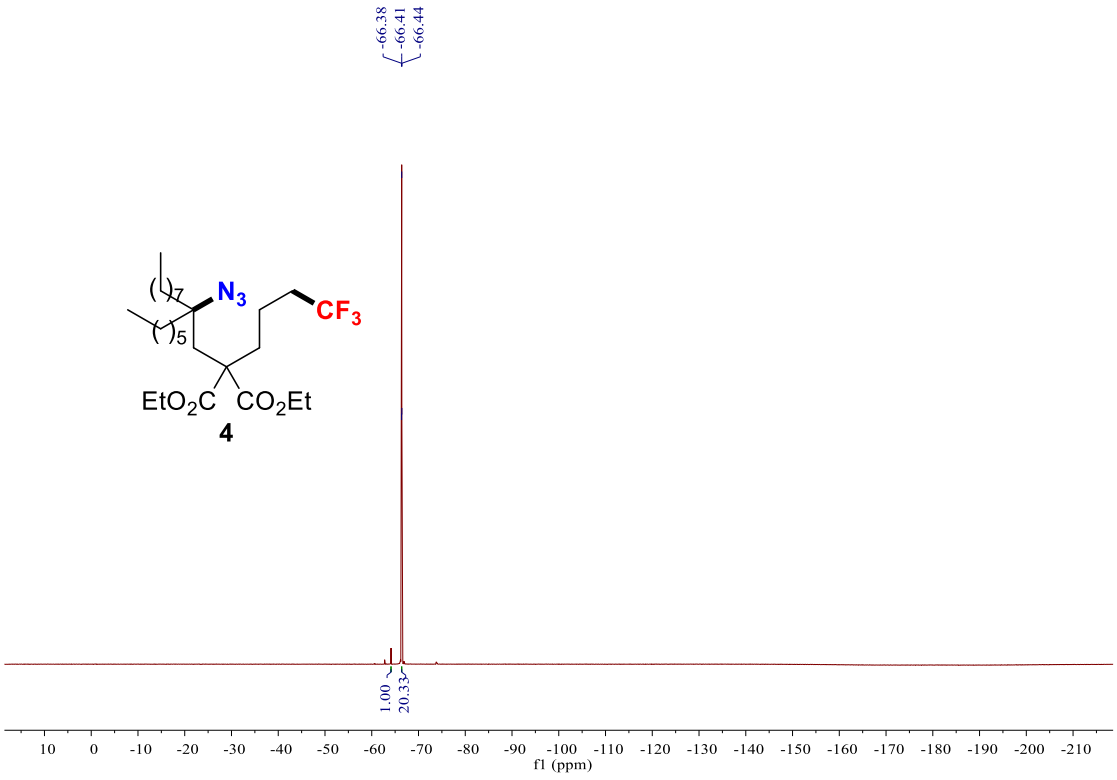
128.33
125.58
77.48
77.16
76.84
65.30
61.68
56.33
38.83
37.16
33.92
32.43
31.96
31.83
30.01
29.68
29.59
29.37
23.79
23.78
22.78
22.74
17.68
14.22
14.16
N3
CF3
EtO2C
CO2Et
4
f1 (ppm)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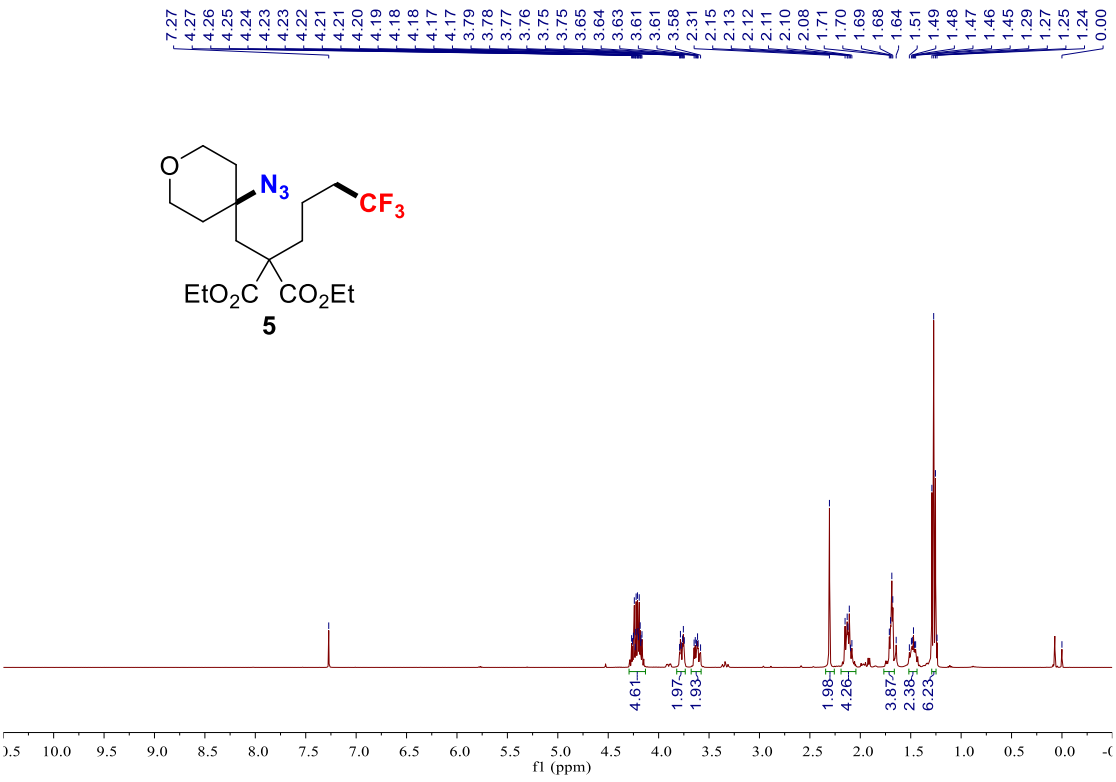
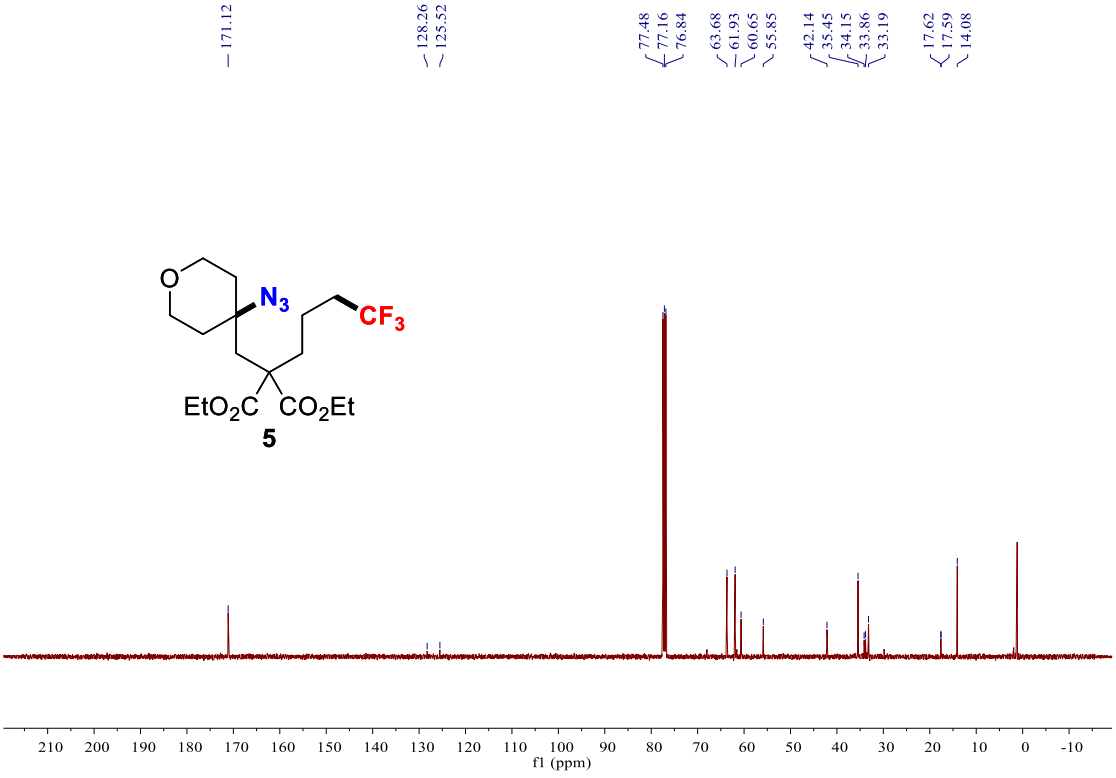
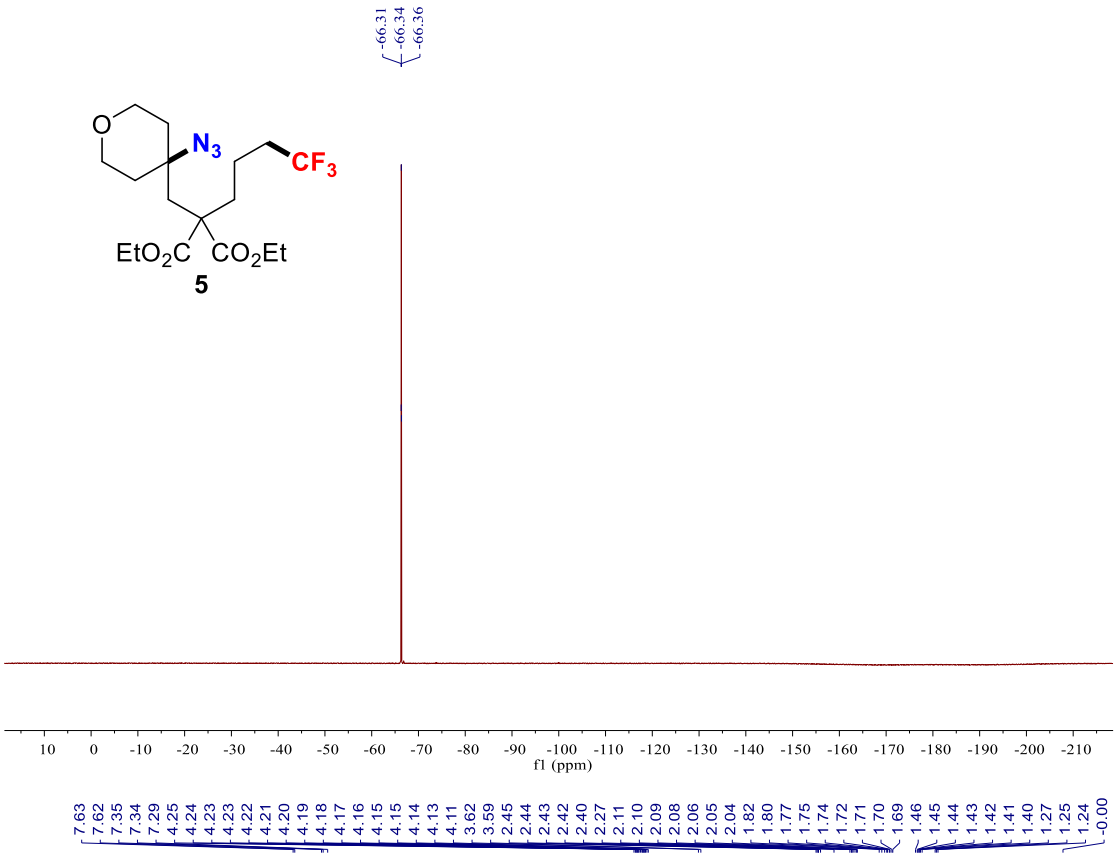
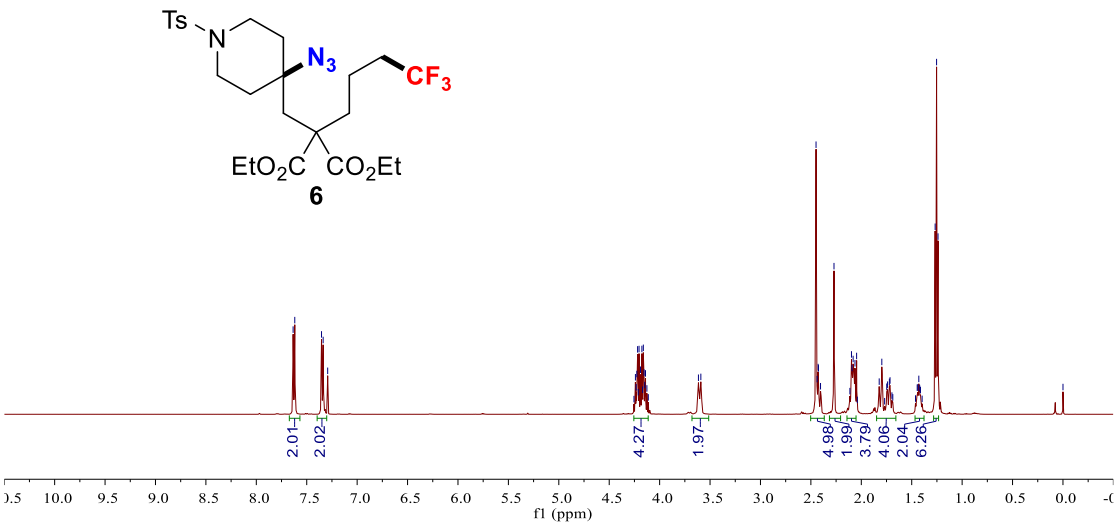
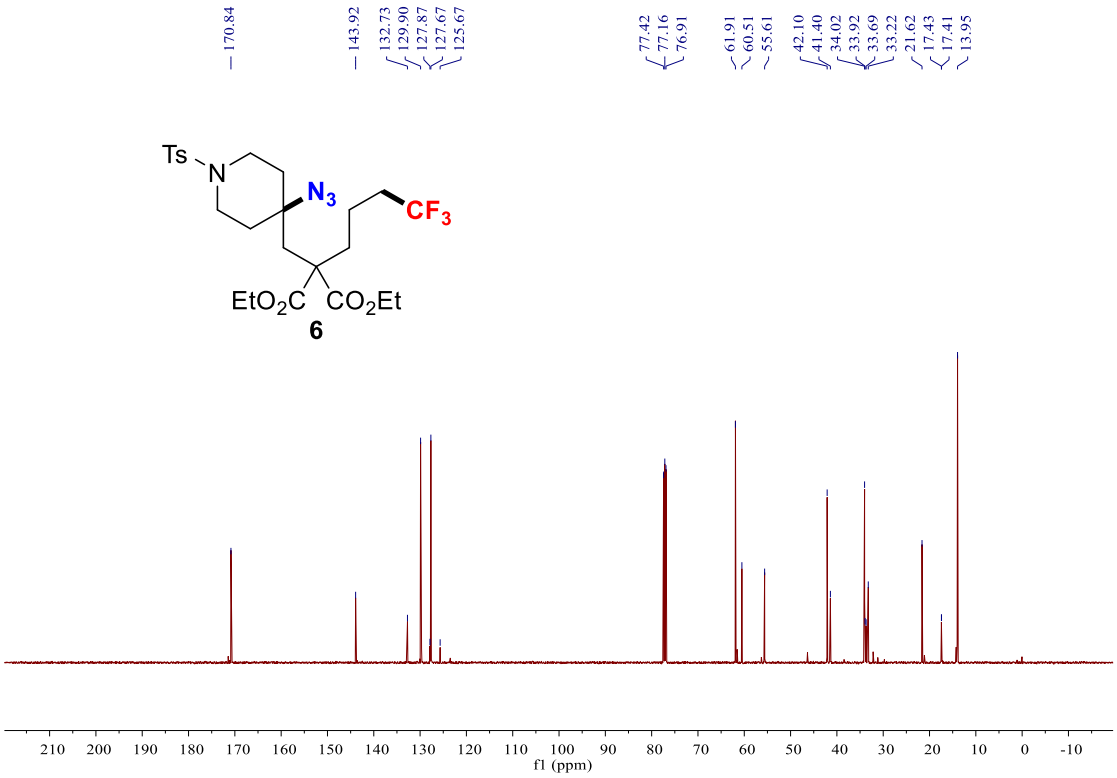
-66.41
-66.44
N3
CF3
EtO2C
CO2Et
4
1.00
20.33
f1 (ppm)


7.27 4.27 4.26 4.25 4.24 4.23 4.23 4.22 4.21 4.21 4.20 4.19 4.18 4.18 4.17 4.17 3.79 3.78 3.77 3.76 3.75 3.75 3.65 3.64 3.63 3.61 3.61 3.58 2.31 2.15 2.13 2.12 2.11 2.10 2.08 1.71 1.70 1.69 1.68 1.64 1.51 1.49 1.48 1.47 1.46 1.45 1.29 1.27 1.25 1.24 0.00
O
N3
CF3
EtO2C CO2Et
5
4.61 1.97 1.93 1.98 4.26 3.87 2.38 6.23
f1 (ppm)


171.12
128.26 125.52
77.48 77.16 76.84 63.68 61.93 60.65 55.85 42.14 35.45 34.15 33.86 33.19 17.62 17.59 14.08
O
N3
CF3
EtO2C CO2Et
5
f1 (ppm)


-66.31
-66.34
-66.36
O
N3
CF3
EtO2C
CO2Et
5
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)
7.63 7.62 7.35 7.34 7.29 4.25 4.24 4.23 4.23 4.22 4.21 4.20 4.19 4.18 4.17 4.16 4.15 4.15 4.14 4.13 4.11 3.62 3.59 2.45 2.44 2.43 2.42 2.40 2.27 2.11 2.10 2.09 2.08 2.06 2.05 2.04 1.82 1.80 1.77 1.75 1.74 1.72 1.71 1.70 1.69 1.46 1.45 1.44 1.43 1.42 1.41 1.40 1.27 1.25 1.24 0.00


Ts
N
N3
CF3
EtO2C
CO2Et
6
2.01 2.02 4.27 1.97 4.98 1.99 3.79 4.06 2.04 6.26
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)


170.84
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132.73
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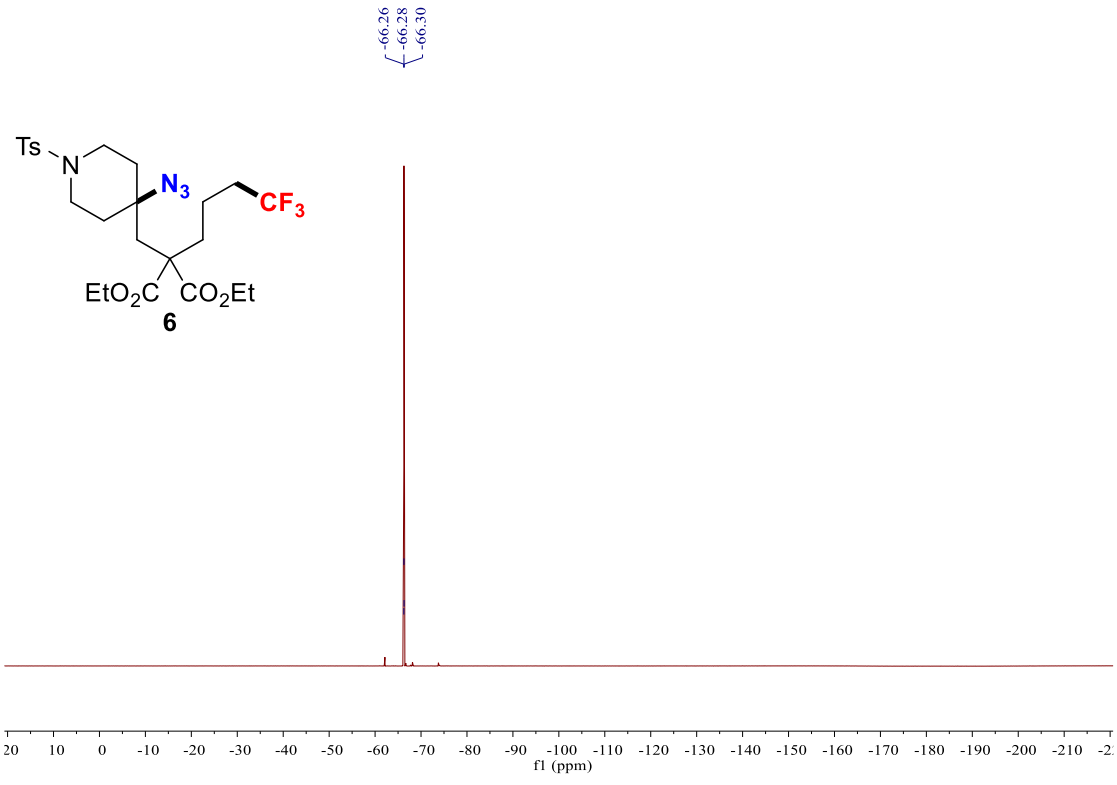
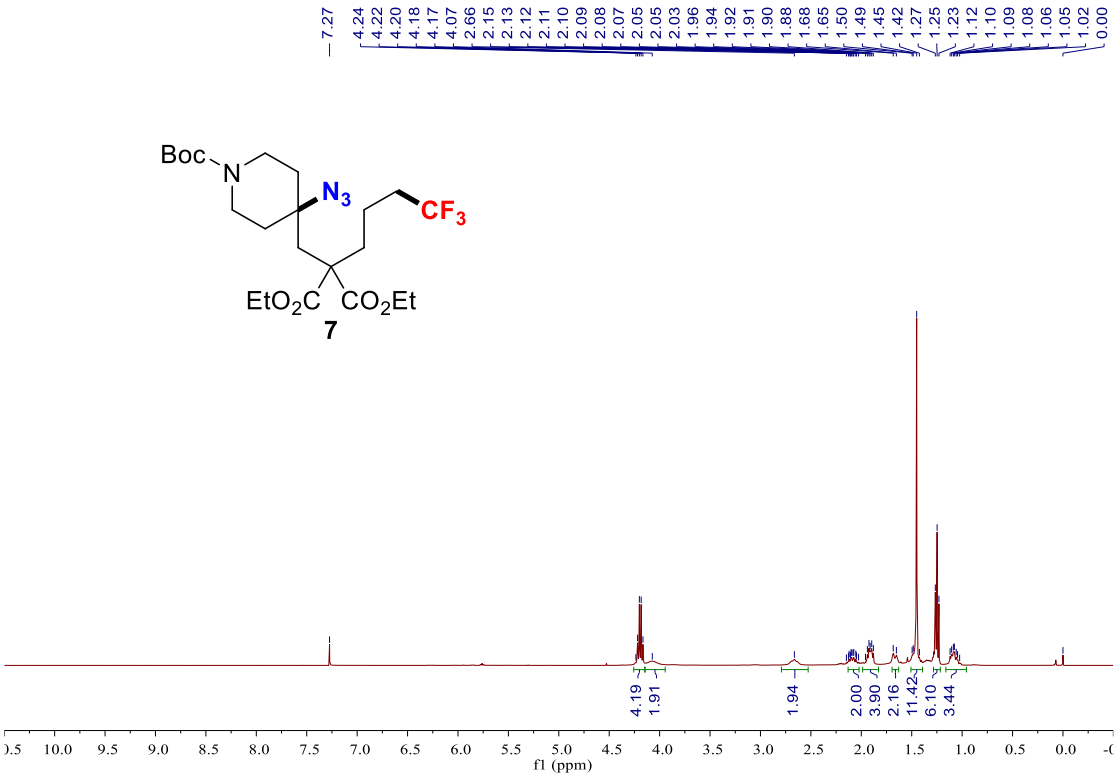
127.87
127.67
125.67
77.42
77.16
76.91
61.91
60.51
55.61
42.10
41.40
34.02
33.92
33.69
33.22
21.62
17.43
17.41
13.95
Ts
N
N3
CF3
EtO2C
CO2Et
6
f1 (ppm)


-66.26
-66.28
-66.30
Ts
N
N3
CF3
EtO2C
CO2Et
6
f1 (ppm)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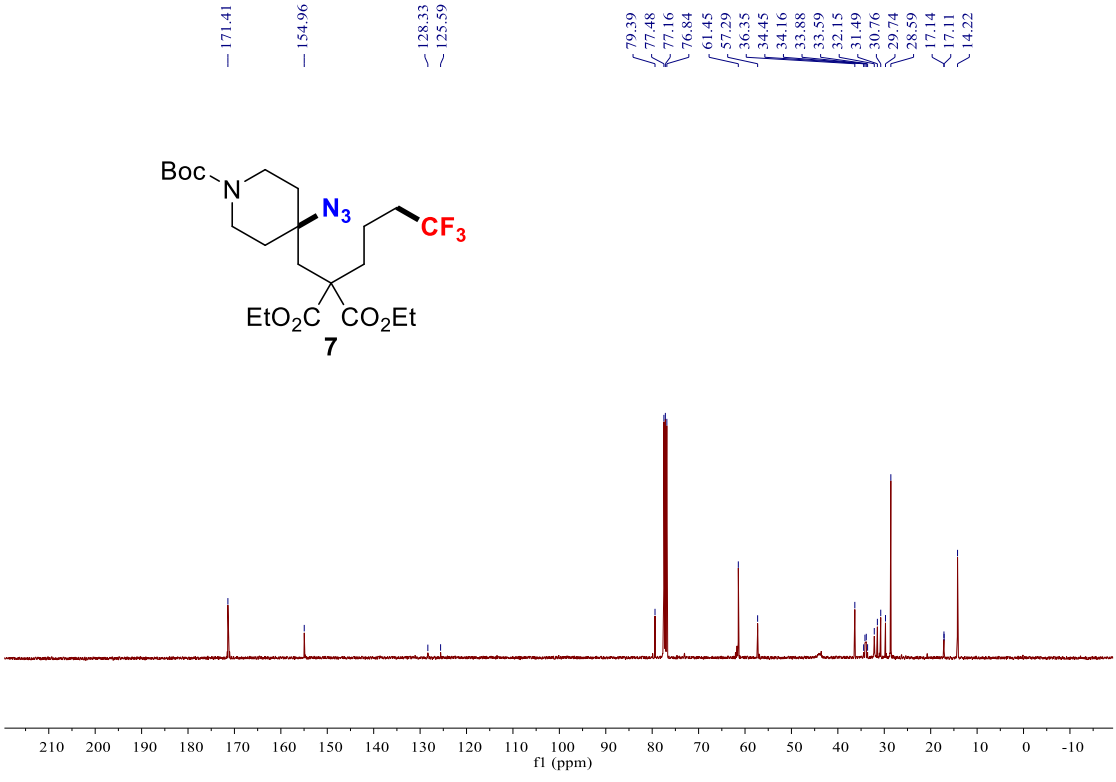
4.22
4.20
4.18
4.17
4.07
2.66
2.15
2.13
2.12
2.11
2.10
2.09
2.08
2.07
2.05
2.05
2.03
1.96
1.94
1.92
1.91
1.90
1.88
1.68
1.65
1.50
1.49
1.45
1.42
1.27
1.25
1.23
1.12
1.10
1.09
1.08
1.06
1.05
1.02
0.00
Boc
N
N3
CF3
EtO2C
CO2Et
7
4.19
1.91
1.94
2.00
3.90
2.16
11.42
6.10
3.44
f1 (ppm)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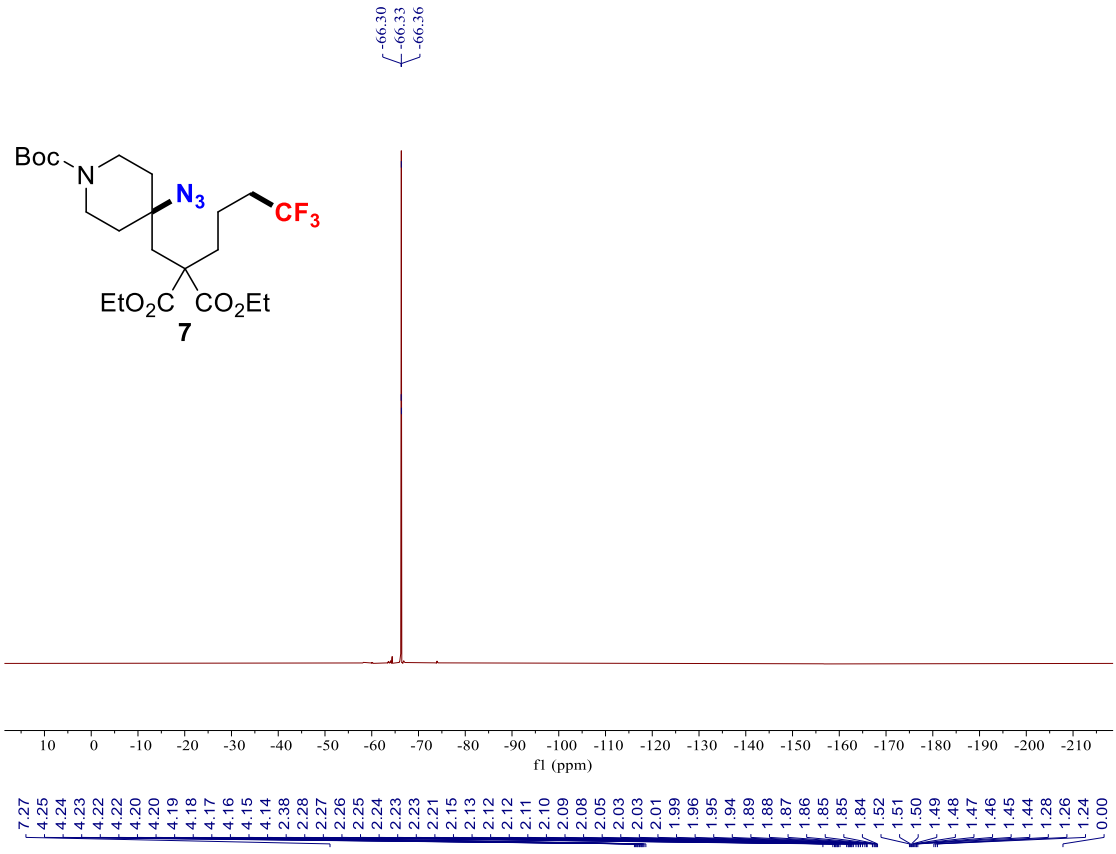
154.96
128.33
125.59
79.39
77.48
77.16
76.84
61.45
57.29
36.35
34.45
34.16
33.88
33.59
32.15
31.49
30.76
29.74
28.59
17.14
17.11
14.22
Boc
N
N3
CF3
EtO2C
CO2Et
7
f1 (ppm)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-66.33
-66.36
Boc
N
N3
CF3
EtO2C
CO2Et
7
f1 (ppm)
7.27
4.25
4.24
4.23
4.22
4.22
4.20
4.20
4.19
4.18
4.17
4.16
4.15
4.14
2.38
2.28
2.27
2.26
2.25
2.24
2.23
2.23
2.21
2.15
2.13
2.12
2.12
2.11
2.10
2.09
2.08
2.05
2.03
2.03
2.01
1.99
1.96
1.95
1.94
1.89
1.88
1.87
1.86
1.85
1.85
1.84
1.52
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1.49
1.48
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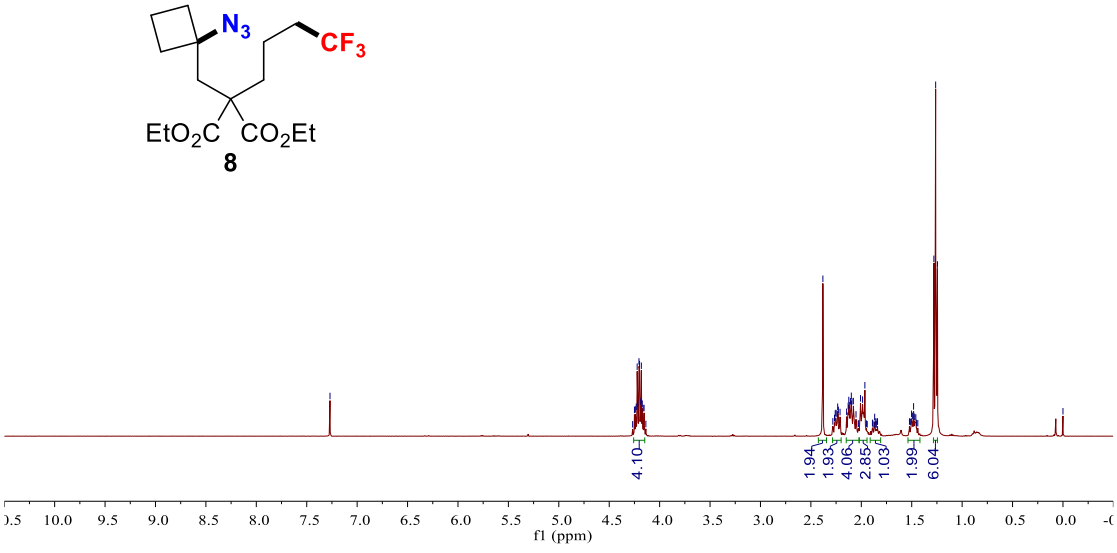
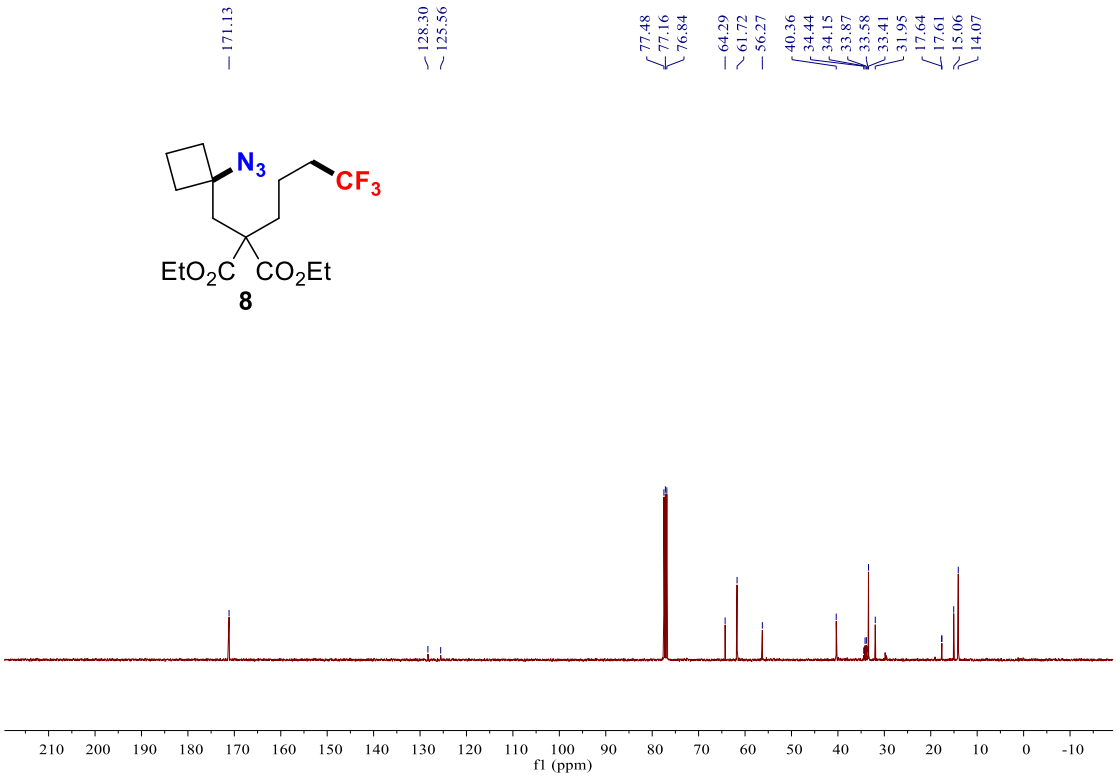
1.46
1.45
1.44
1.28
1.26
1.24
0.00


N3
CF3
EtO2C
CO2Et
8
4.10
1.94
1.93
4.06
2.85
1.03
1.99
6.04
f1 (ppm)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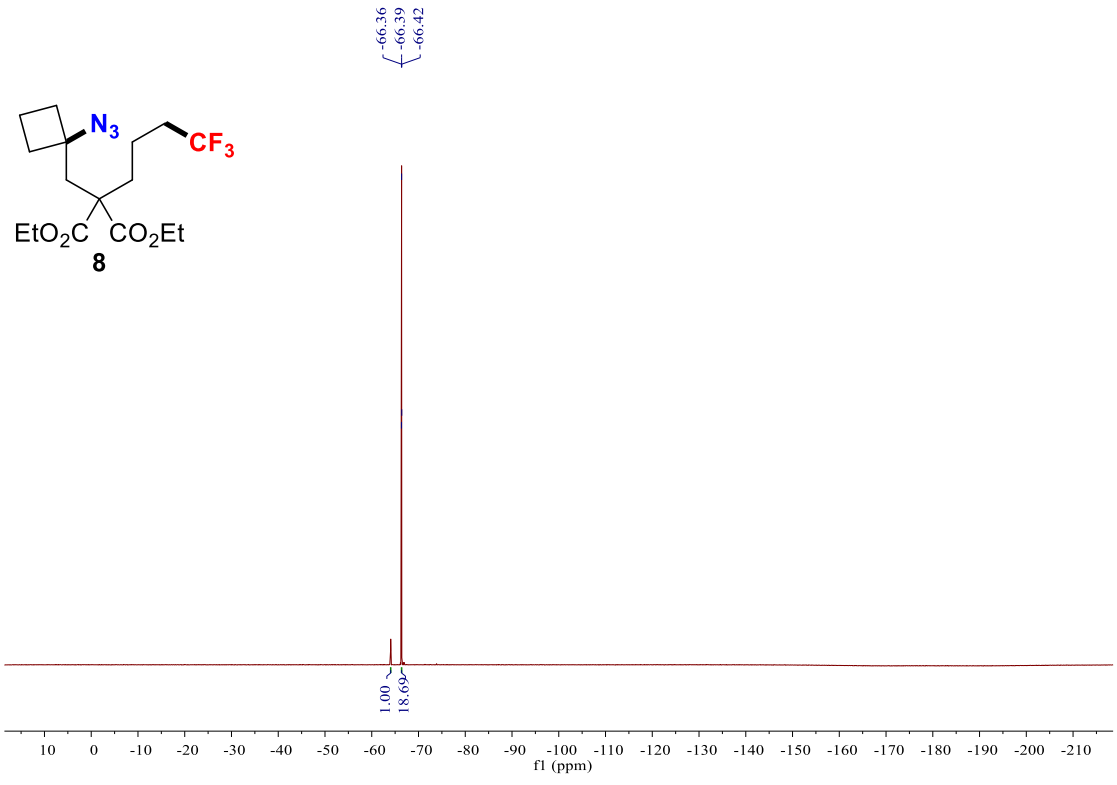
128.30
125.56
77.48
77.16
76.84
64.29
61.72
56.27
40.36
34.44
34.15
33.87
33.58
33.41
31.95
17.64
17.61
15.06
14.07
N3
CF3
EtO2C
CO2Et
8
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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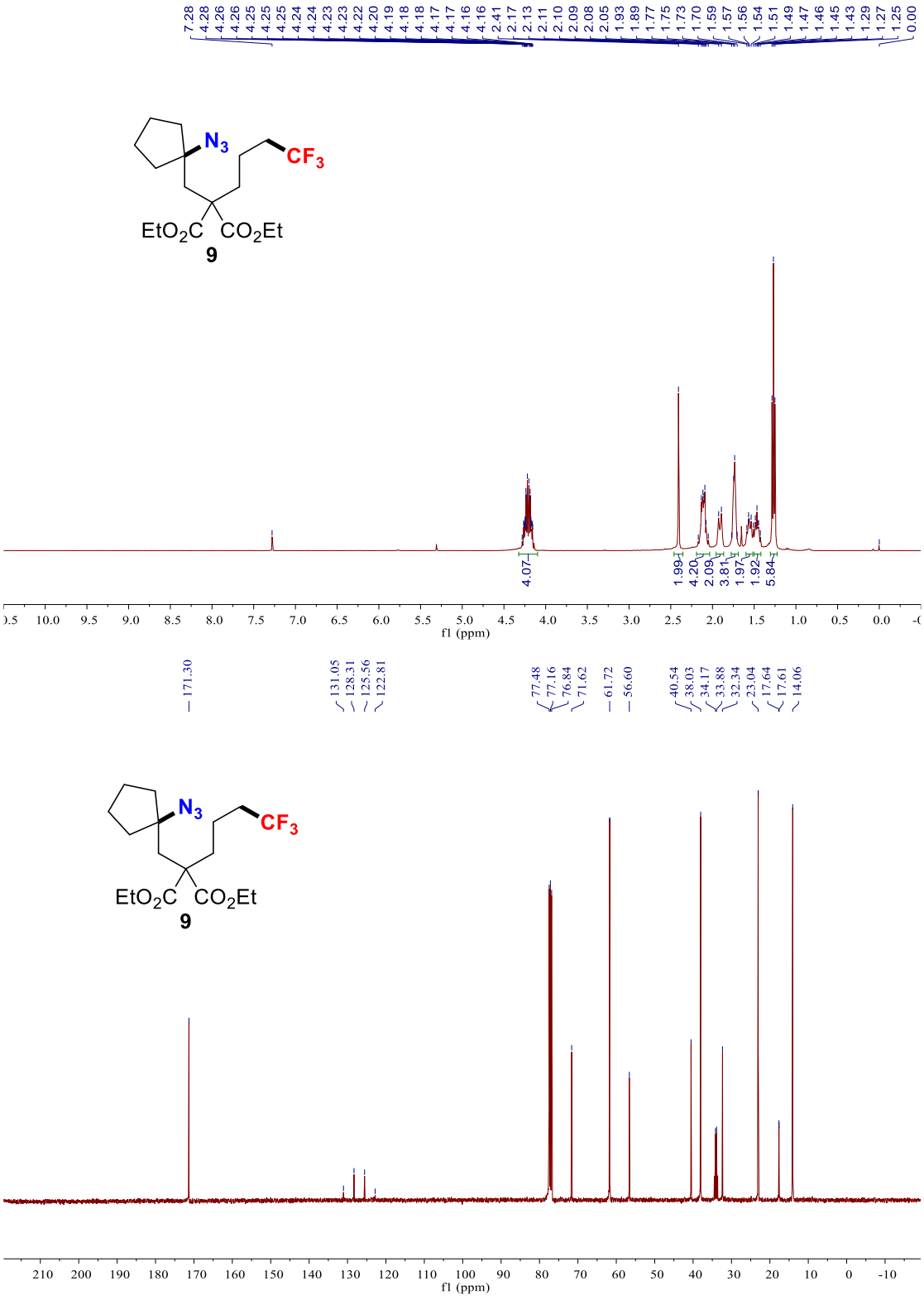
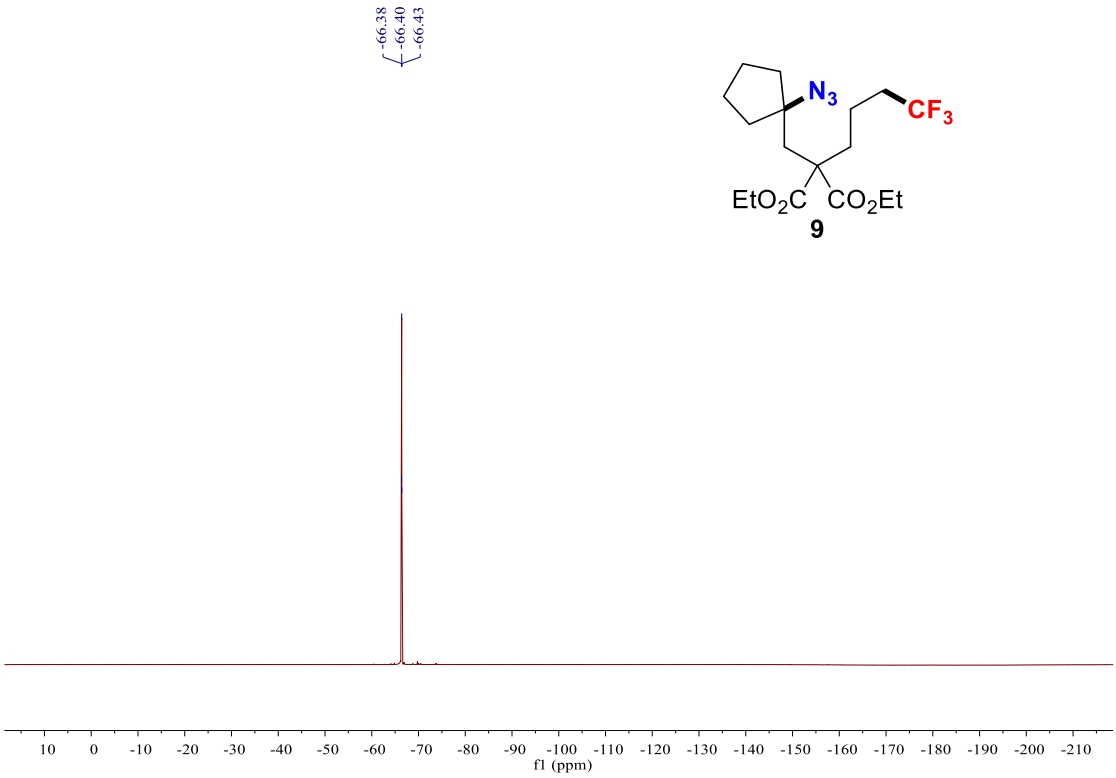
-66.42
N3
CF3
EtO2C
CO2Et
8
1.00
18.69
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


7.28 4.28 4.26 4.26 4.25 4.25 4.25 4.24 4.24 4.23 4.23 4.22 4.20 4.19 4.18 4.18 4.17 4.17 4.16 4.16 2.41 2.17 2.13 2.11 2.10 2.09 2.08 2.05 1.93 1.89 1.77 1.75 1.73 1.70 1.59 1.57 1.56 1.54 1.51 1.49 1.47 1.46 1.45 1.43 1.29 1.27 1.25 0.00
N3
CF3
EtO2C CO2Et
9
4.07
1.99
4.20
2.09
3.81
1.97
1.92
5.84
f1 (ppm)
171.30
131.05
128.31
125.56
122.81
77.48
77.16
76.84
71.62
61.72
56.60
40.54
38.03
34.17
33.88
32.34
23.04
17.64
17.61
14.06
N3
CF3
EtO2C CO2Et
9
f1 (ppm)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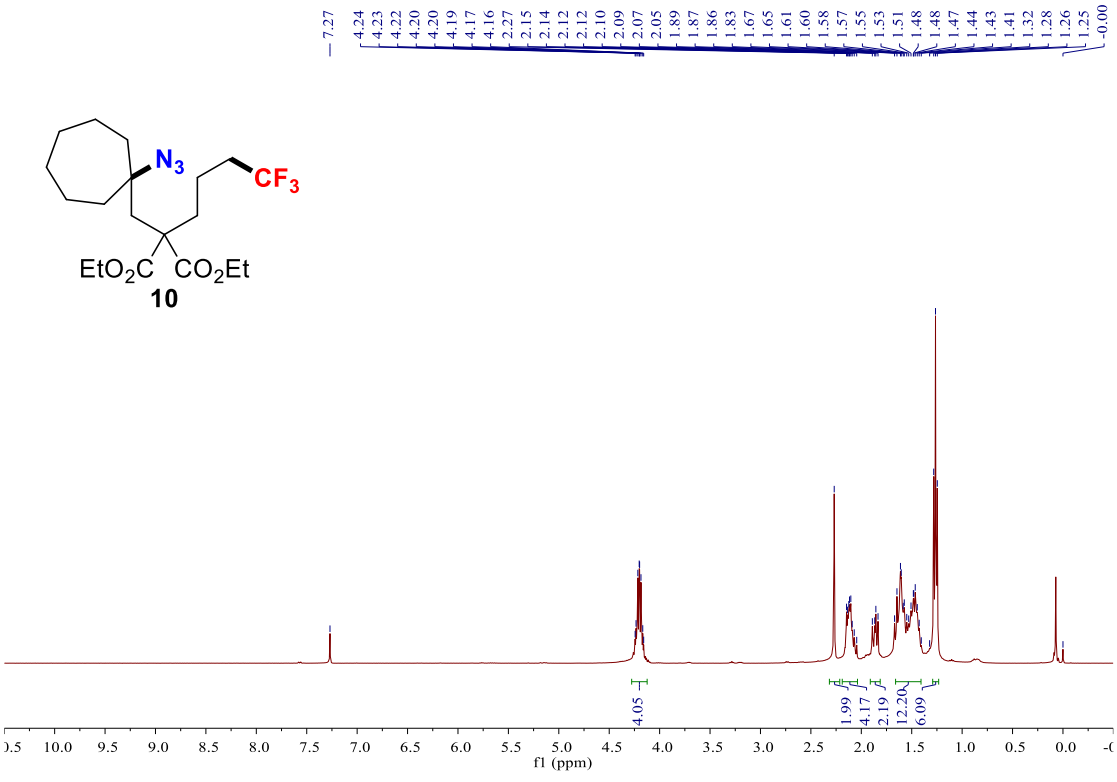
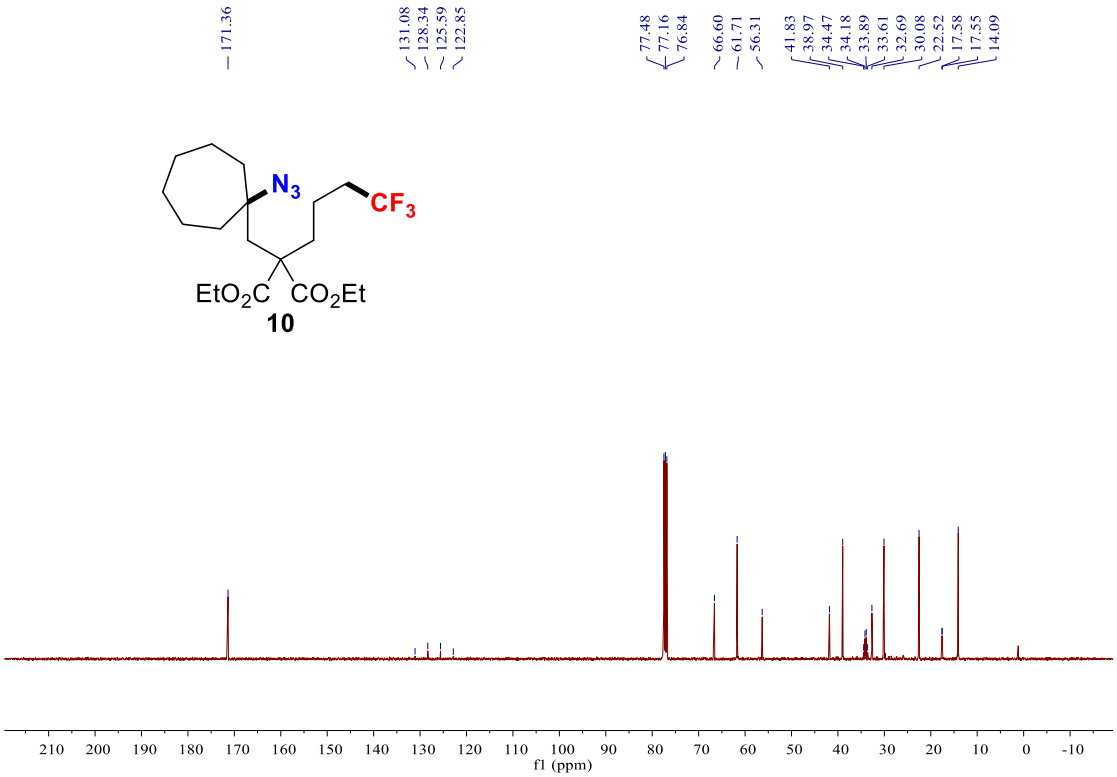
-66.40
-66.43
N3
CF3
EtO2C CO2Et
9
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


7.27
4.24 4.23 4.22 4.20 4.20 4.19 4.17 4.16 2.27 2.15 2.14 2.12 2.12 2.10 2.09 2.07 2.05 1.89 1.87 1.86 1.83 1.67 1.65 1.61 1.60 1.58 1.57 1.55 1.53 1.51 1.48 1.48 1.47 1.44 1.43 1.41 1.32 1.28 1.26 1.25 0.00
N3
CF3
EtO2C CO2Et
10
4.05
1.99
4.17
2.19
12.20
6.09
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)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128.34
125.59
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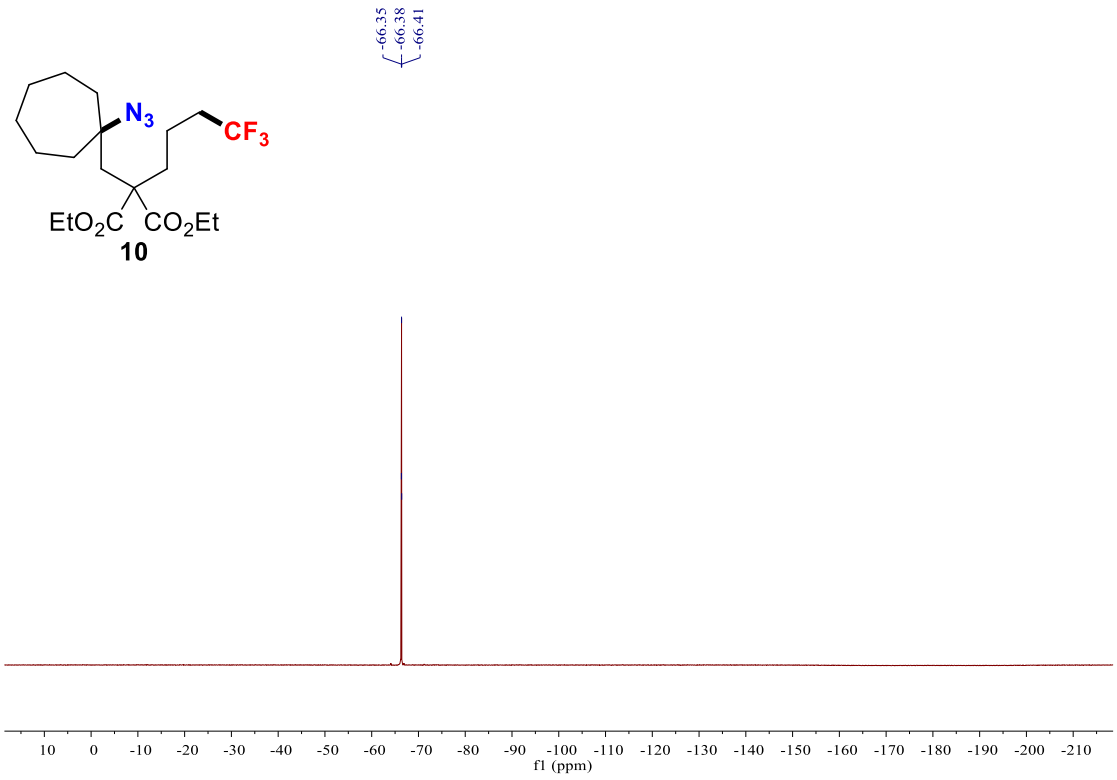
77.48
77.16
76.84
66.60
61.71
56.31
41.83
38.97
34.47
34.18
33.89
33.61
32.69
30.08
22.52
17.58
17.55
14.09
N3
CF3
EtO2C CO2Et
10
f1 (ppm)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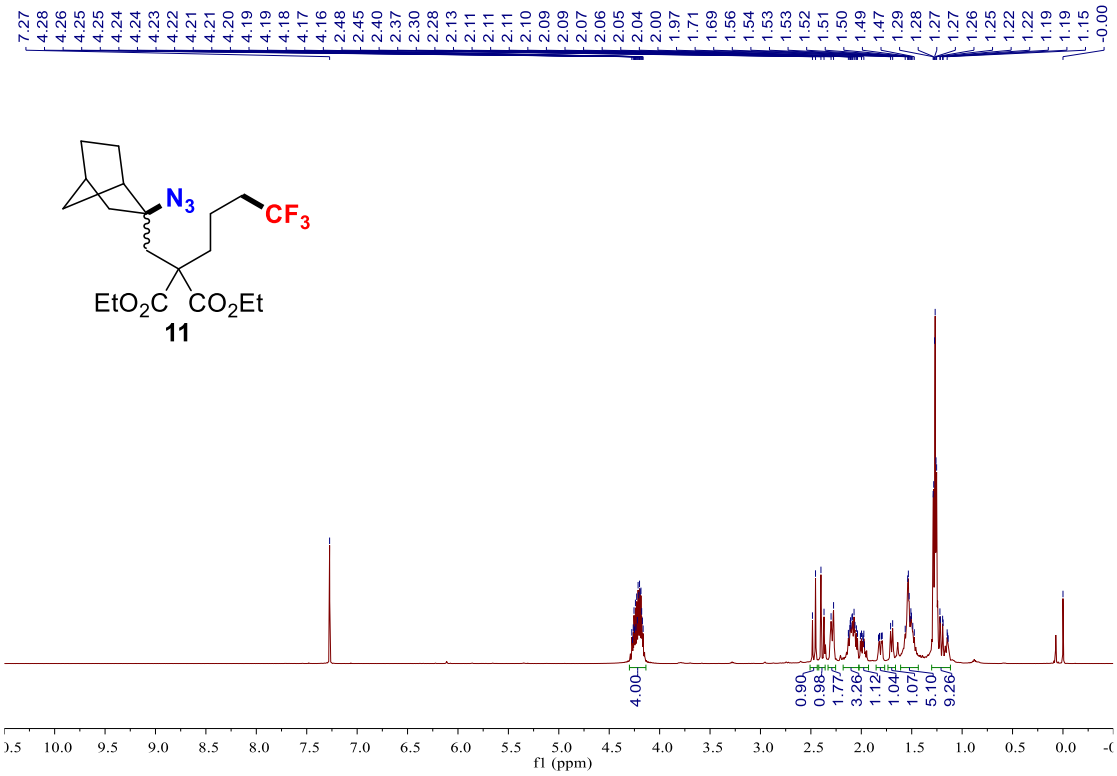
-66.41
N3
CF3
EtO2C CO2Et
10
f1 (ppm)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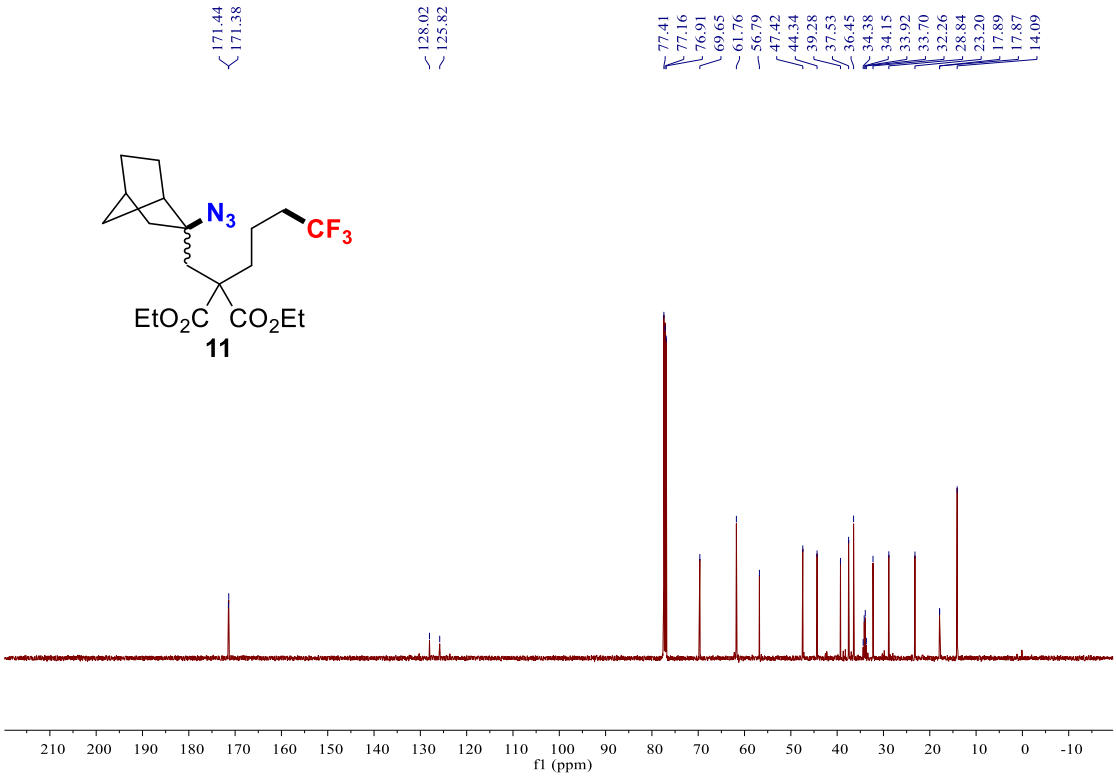
4.28
4.26
4.25
4.25
4.24
4.24
4.23
4.22
4.21
4.21
4.20
4.19
4.19
4.18
4.17
4.16
2.48
2.45
2.40
2.37
2.30
2.28
2.13
2.11
2.11
2.11
2.10
2.09
2.09
2.07
2.06
2.05
2.04
2.00
1.97
1.71
1.69
1.56
1.54
1.53
1.53
1.52
1.51
1.50
1.49
1.47
1.29
1.28
1.27
1.27
1.26
1.25
1.22
1.19
1.19
1.15
-0.00
N3
CF3
EtO2C CO2Et
11
4.00
0.90
0.98
1.77
3.26
1.12
1.04
1.07
5.10
9.26
f1 (ppm)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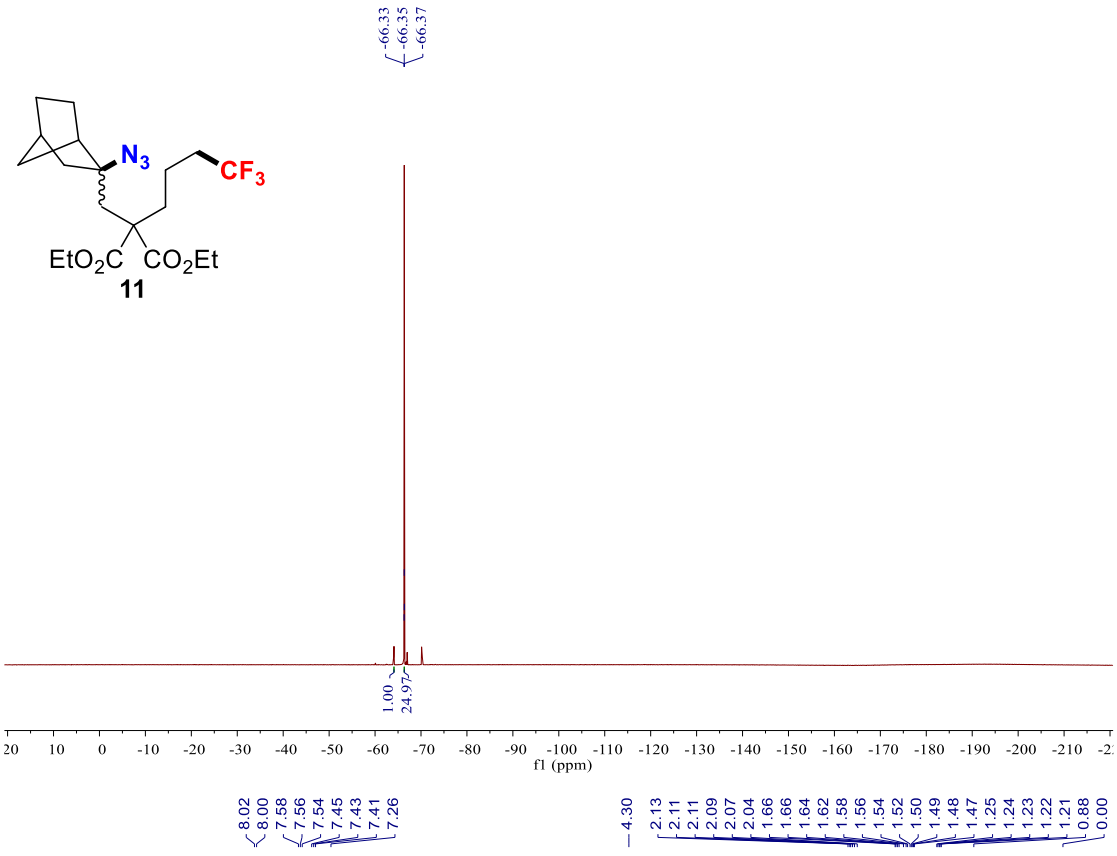
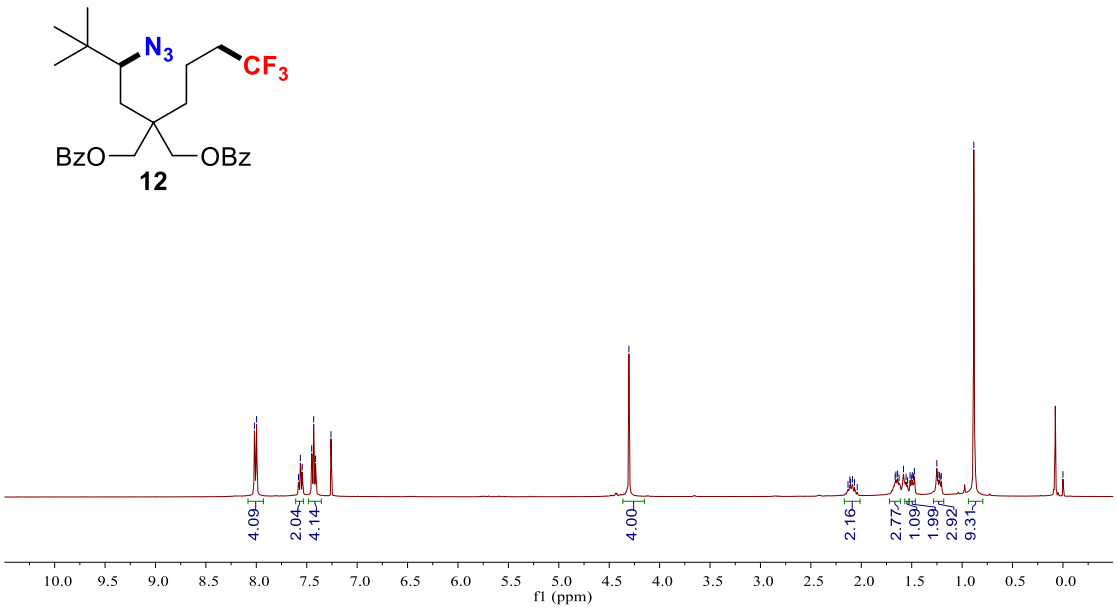
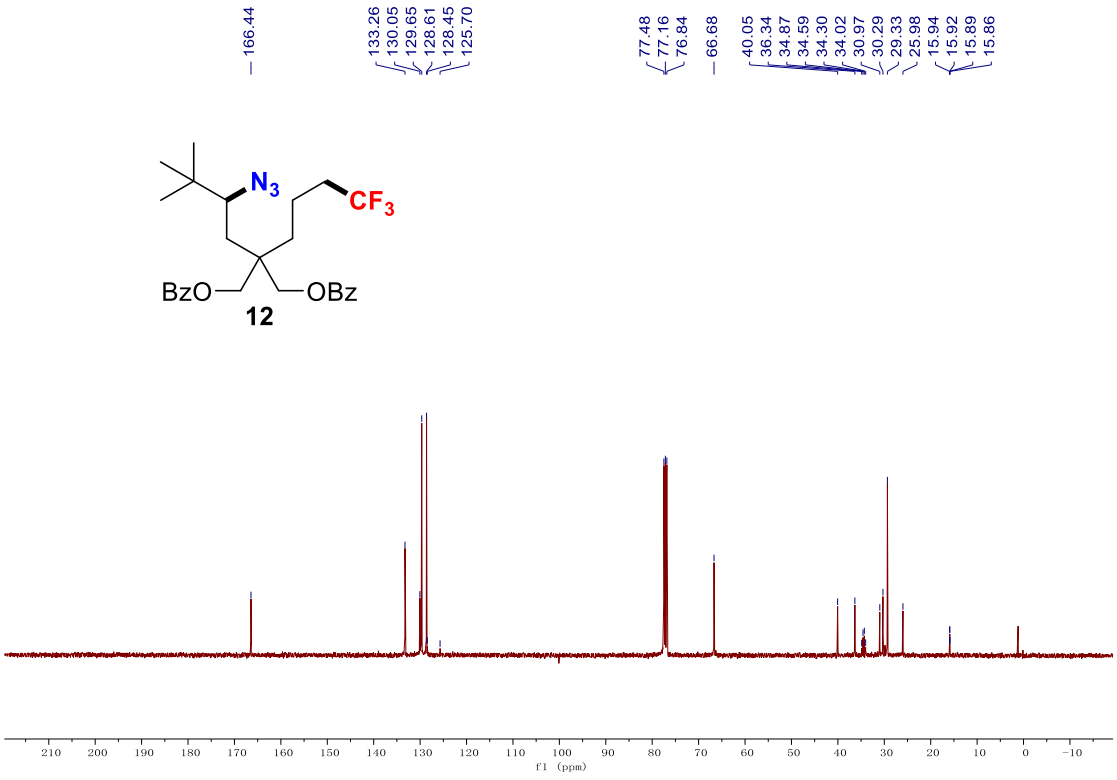
171.38
128.02
125.82
77.41
77.16
76.91
69.65
61.76
56.79
47.42
44.34
39.28
37.53
36.45
34.38
34.15
33.92
33.70
32.26
28.84
23.20
17.89
17.87
14.09
N3
CF3
EtO2C CO2Et
11
f1 (ppm)


-66.33
-66.35
-66.37
N3
CF3
EtO2C
CO2Et
11
1.00
24.97
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)
8.02
8.00
7.58
7.56
7.54
7.45
7.43
7.41
7.26
4.30
2.13
2.11
2.11
2.09
2.07
2.04
1.66
1.66
1.64
1.62
1.58
1.56
1.54
1.52
1.50
1.49
1.48
1.47
1.25
1.24
1.23
1.22
1.21
0.88
0.00


N3
CF3
BzO
OBz
12
4.09
2.04
4.14
4.00
2.16
2.77
1.09
1.99
2.92
9.31
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)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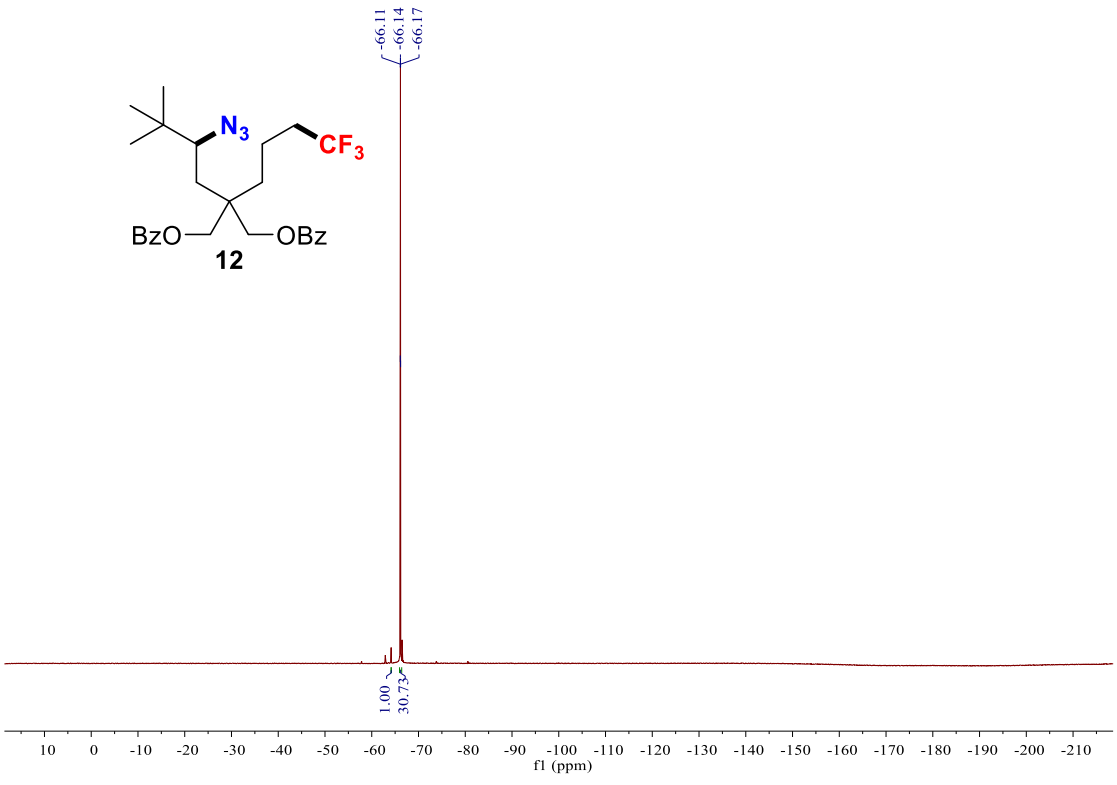
133.26
130.05
129.65
128.61
128.45
125.70
77.48
77.16
76.84
66.68
40.05
36.34
34.87
34.59
34.30
34.02
30.97
30.29
29.33
25.98
15.94
15.92
15.89
15.86
N3
CF3
BzO
OBz
12
f1 (ppm)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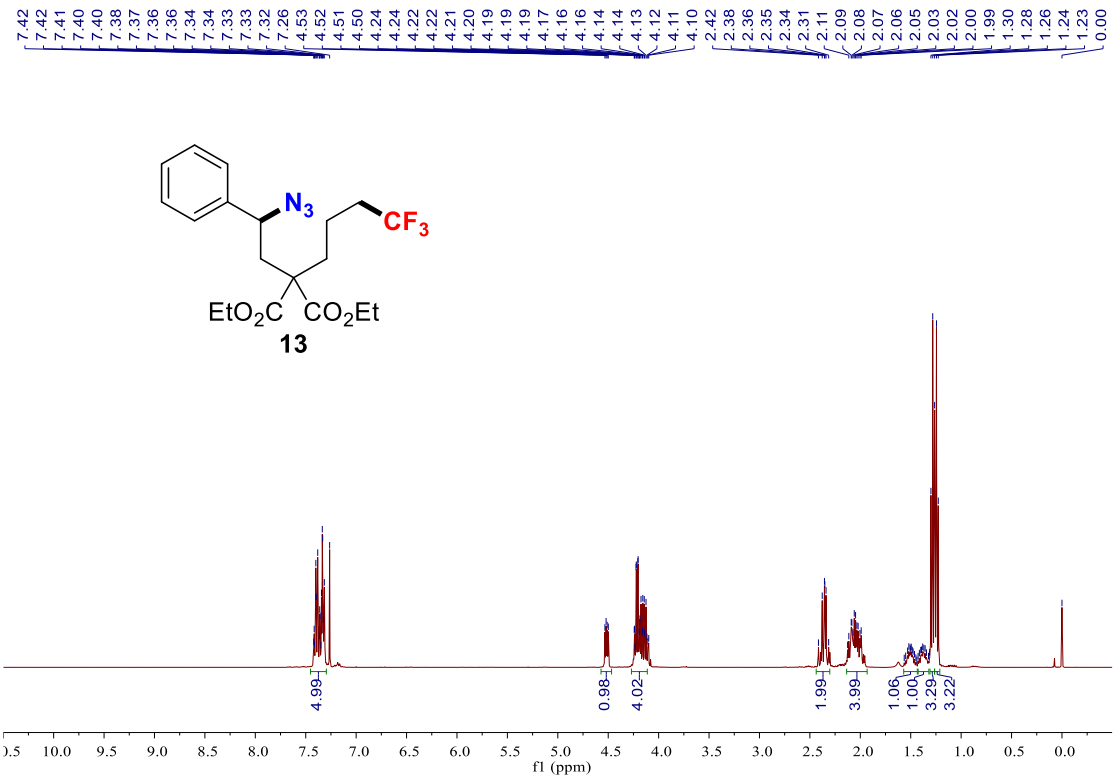
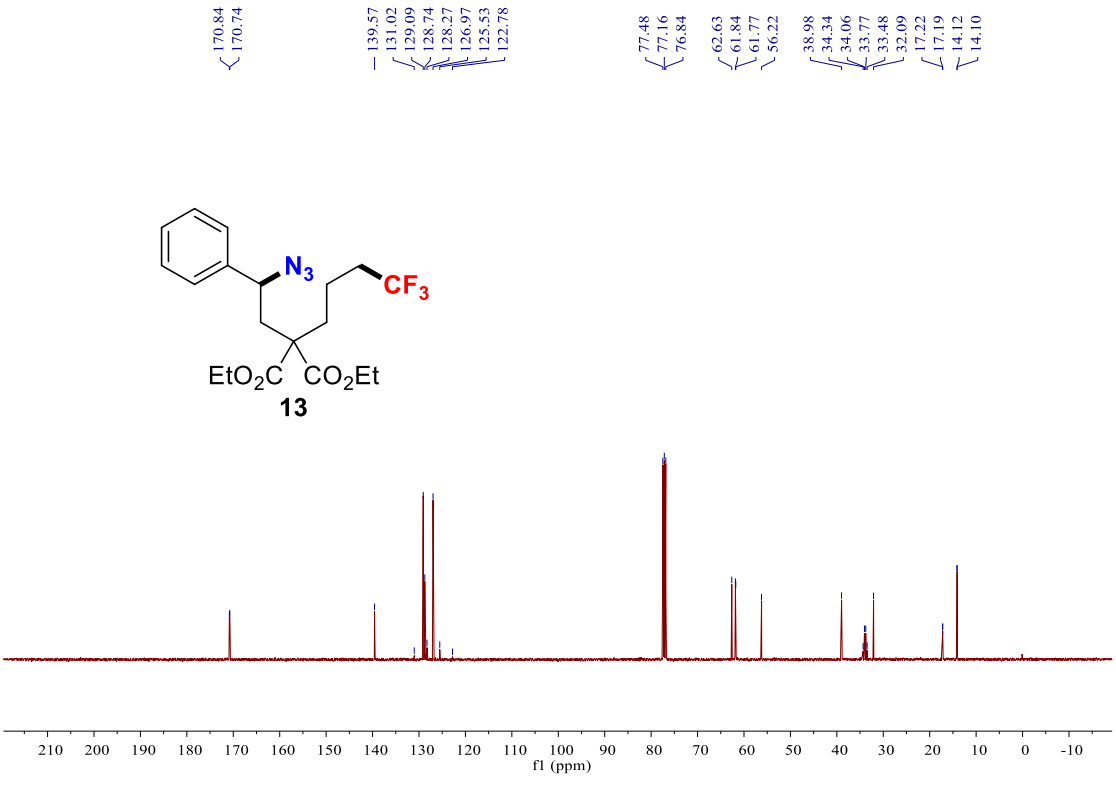
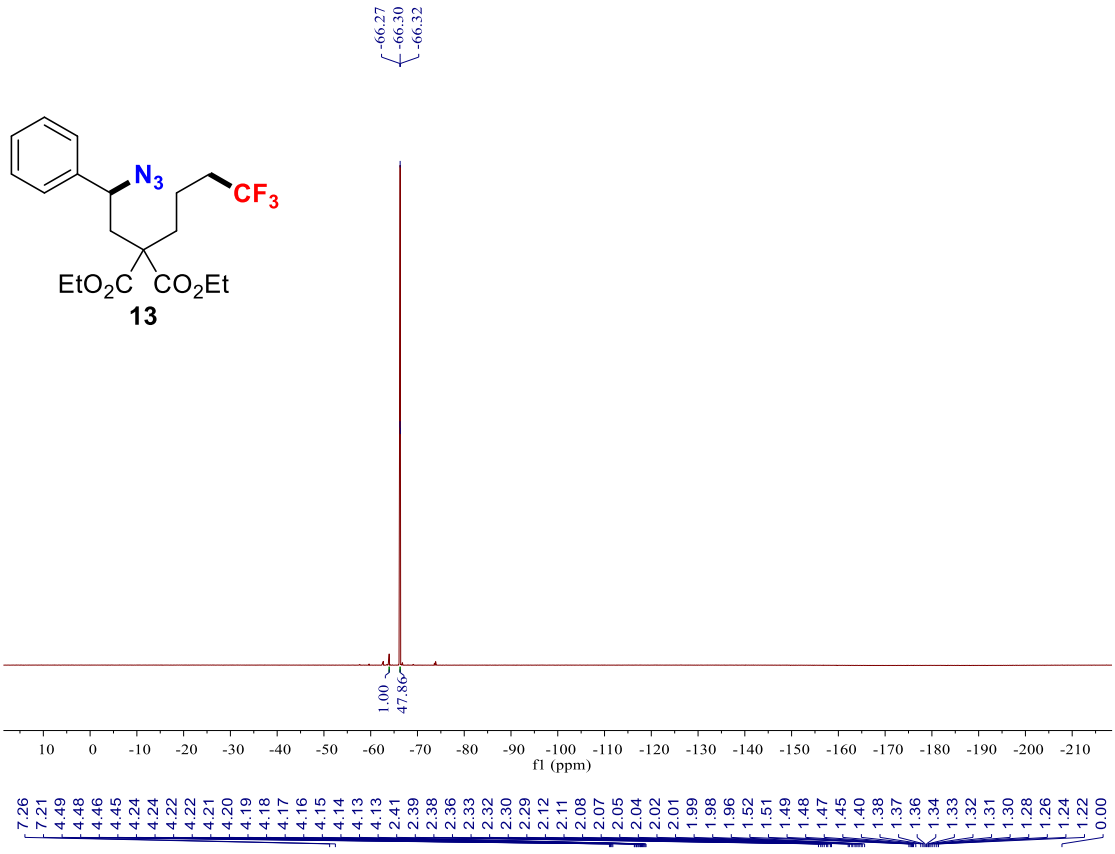
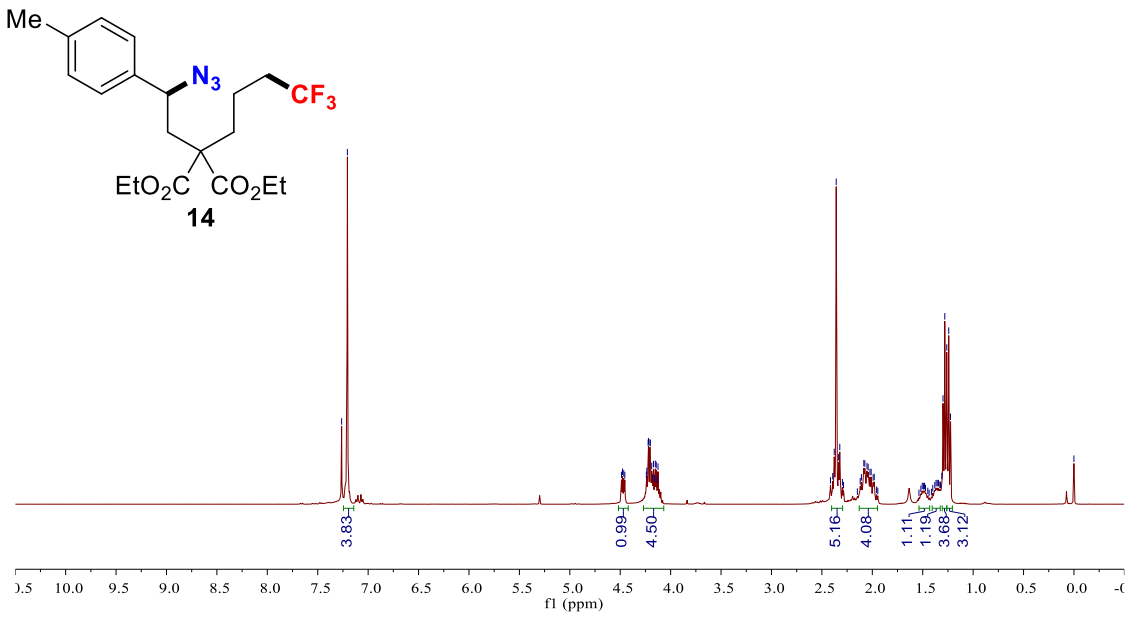
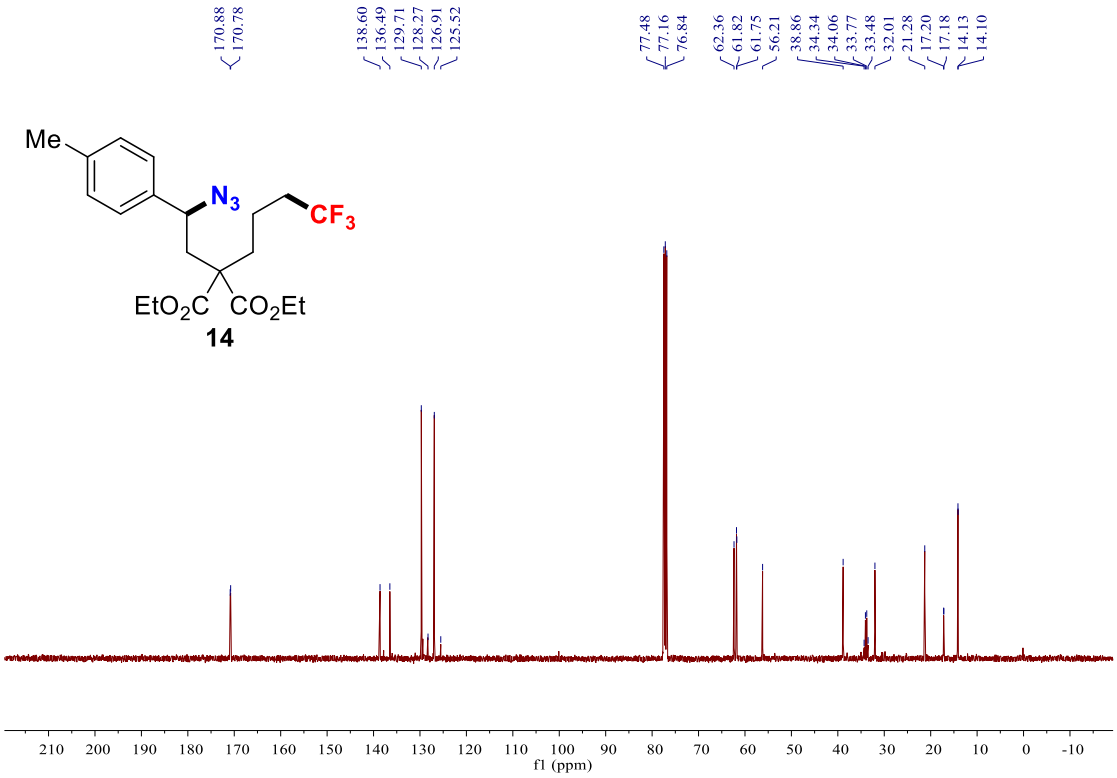
-66.14
-66.17
N3
CF3
BzO
OBz
12
1.00
30.73
f1 (ppm)


7.42 7.42 7.41 7.40 7.40 7.38 7.37 7.36 7.36 7.34 7.34 7.33 7.33 7.32 7.26 4.53 4.52 4.51 4.50 4.24 4.24 4.22 4.22 4.21 4.20 4.19 4.19 4.19 4.17 4.16 4.16 4.14 4.14 4.13 4.12 4.11 4.10 2.42 2.38 2.36 2.35 2.34 2.31 2.11 2.09 2.08 2.07 2.06 2.05 2.03 2.02 2.00 1.99 1.30 1.28 1.26 1.24 1.23 0.00
N3
CF3
EtO2C CO2Et
13
4.99
0.98
4.02
1.99
3.99
1.06
1.00
3.29
3.22
f1 (ppm)


170.84 170.74 139.57 131.02 129.09 128.74 128.27 126.97 125.53 122.78 77.48 77.16 76.84 62.63 61.84 61.77 56.22 38.98 34.34 34.06 33.77 33.48 32.09 17.22 17.19 14.12 14.10
N3
CF3
EtO2C CO2Et
13
f1 (ppm)


-66.27
-66.30
-66.32
N3
CF3
EtO2C CO2Et
13
1.00
47.86
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)
7.26 7.21 4.49 4.48 4.46 4.45 4.24 4.24 4.22 4.21 4.20 4.19 4.18 4.17 4.16 4.15 4.14 4.13 4.13 2.41 2.39 2.38 2.36 2.33 2.32 2.30 2.29 2.12 2.11 2.08 2.07 2.05 2.04 2.02 2.01 1.99 1.98 1.96 1.52 1.51 1.49 1.48 1.47 1.45 1.40 1.38 1.37 1.36 1.34 1.33 1.32 1.31 1.30 1.28 1.26 1.24 1.22 0.00


Me
N3
CF3
EtO2C CO2Et
14
3.83
0.99
4.50
5.16
4.08
1.11
1.19
3.68
3.12
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)


170.88
170.78
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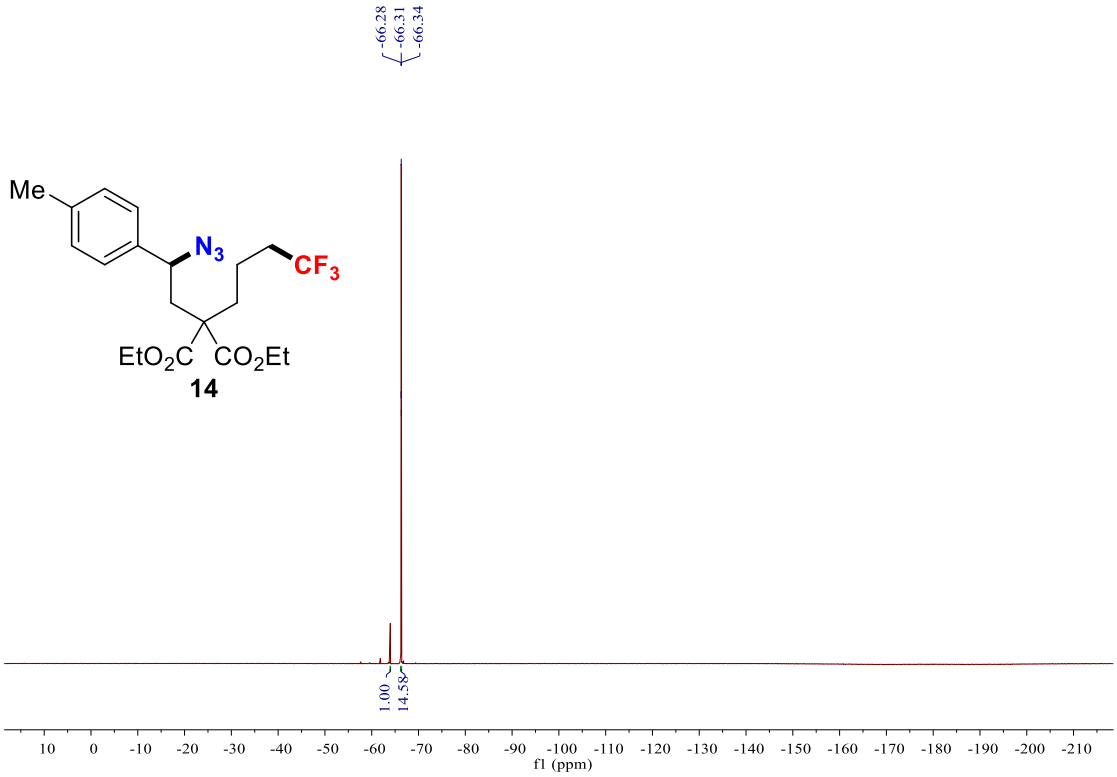
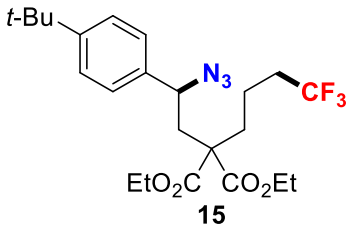
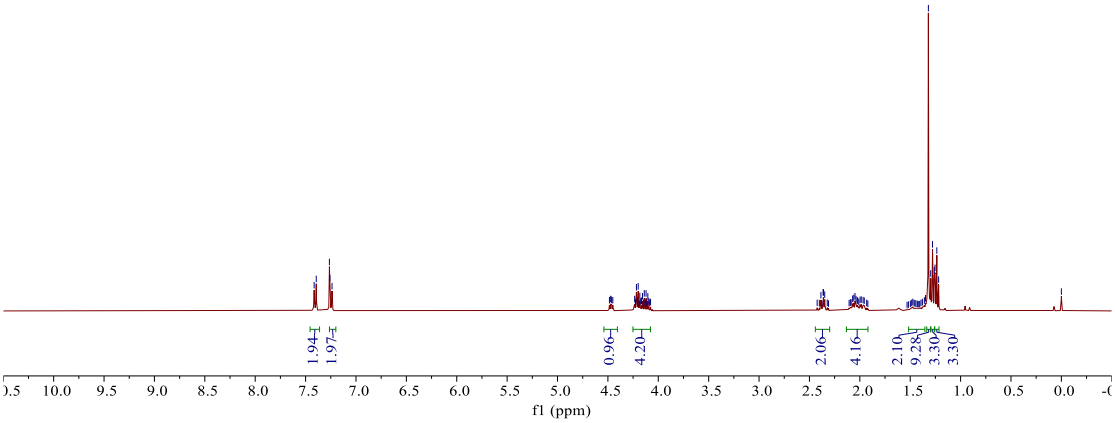
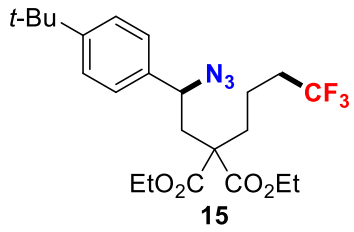
136.49
129.71
128.27
126.91
125.52
77.48
77.16
76.84
62.36
61.82
61.75
56.21
38.86
34.34
34.06
33.77
33.48
32.01
21.28
17.20
17.18
14.13
14.10
Me
N3
CF3
EtO2C
CO2Et
14
f1 (ppm)


-66.28
-66.31
-66.34
Me
N3
CF3
EtO2C
CO2Et
14
1.00
14.58
f1 (ppm)

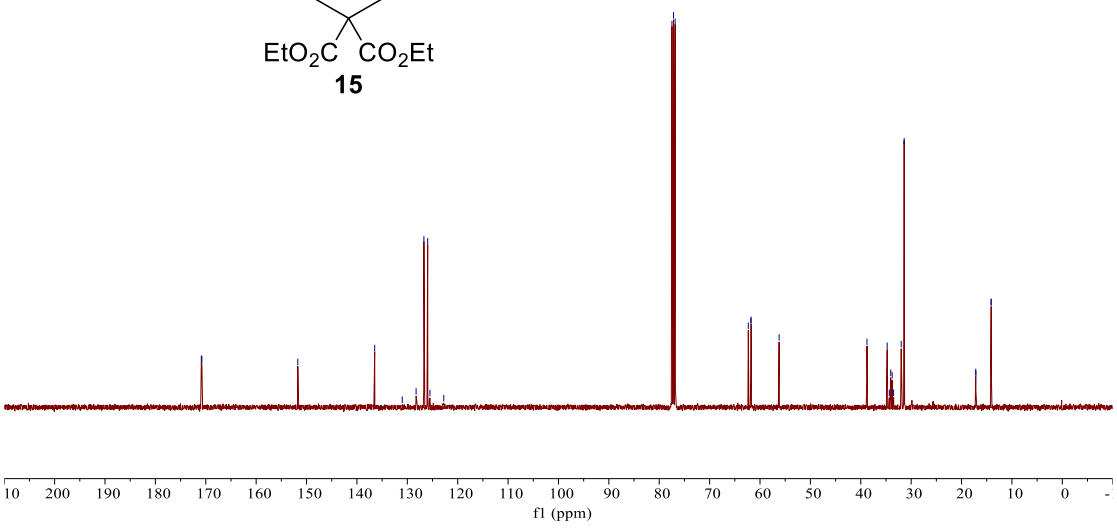

t-Bu
N3
CF3
EtO2C
CO2Et

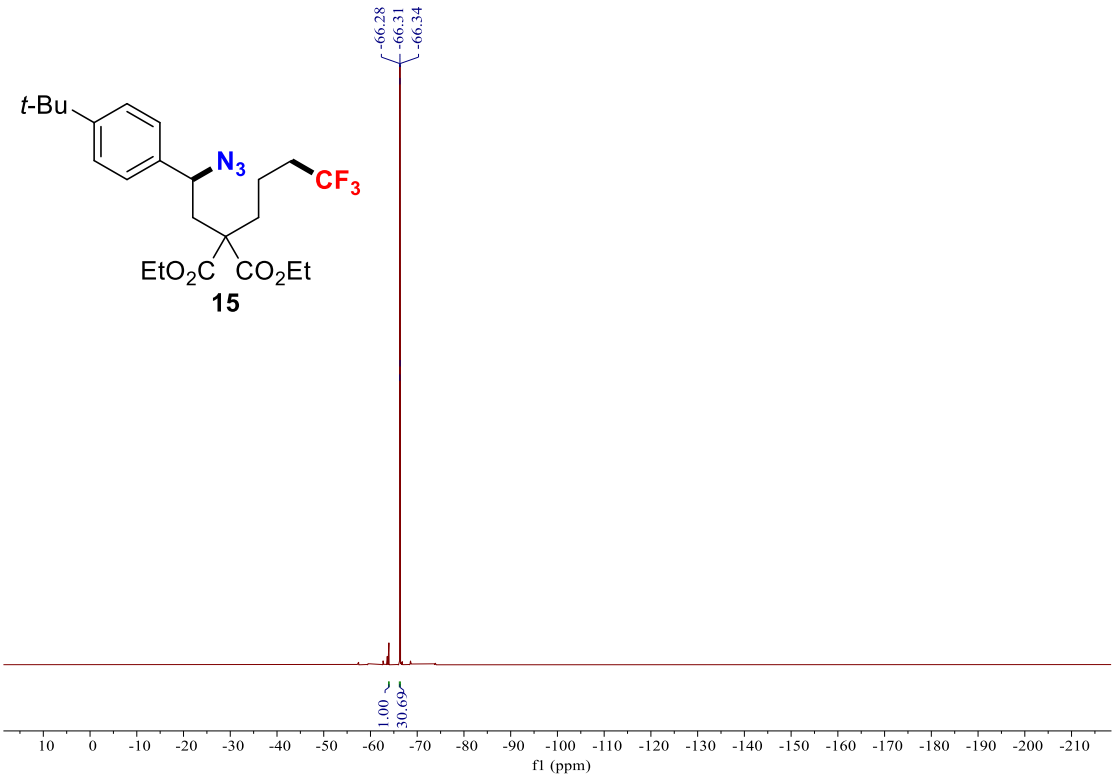
15


1.94
1.97
0.96
4.20
2.06
4.16
2.10
9.28
3.30
3.30
f1 (ppm)


t-Bu
N3
CF3
EtO2C
CO2Et

15


f1 (ppm)


t-Bu
N3
CF3
EtO2C CO2Et
15
-66.28
-66.31
-66.34
1.00
30.69
fl (ppm)


7.63
7.61
7.60
7.58
7.48
7.46
7.44
7.41
7.39
7.37
7.35
7.26
4.59
4.58
4.57
4.56
4.26
4.24
4.22
4.20
4.19
4.17
4.16
4.14
4.13
4.12
4.12
2.41
2.39
2.38
2.35
2.14
2.13
2.10
2.08
2.06
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2.02
2.00
1.99
1.59
1.57
1.55
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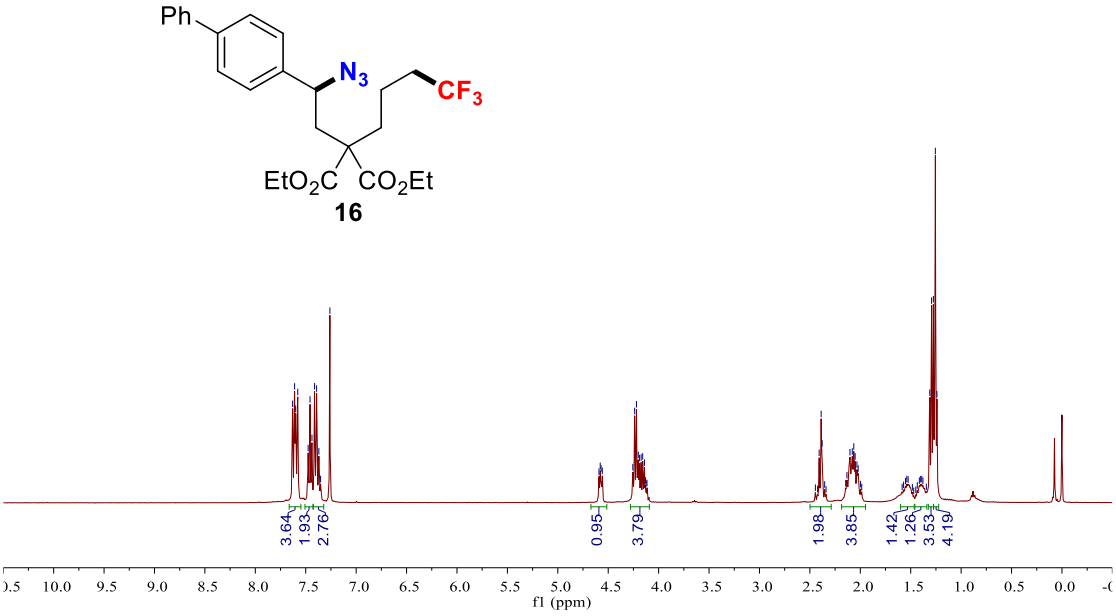
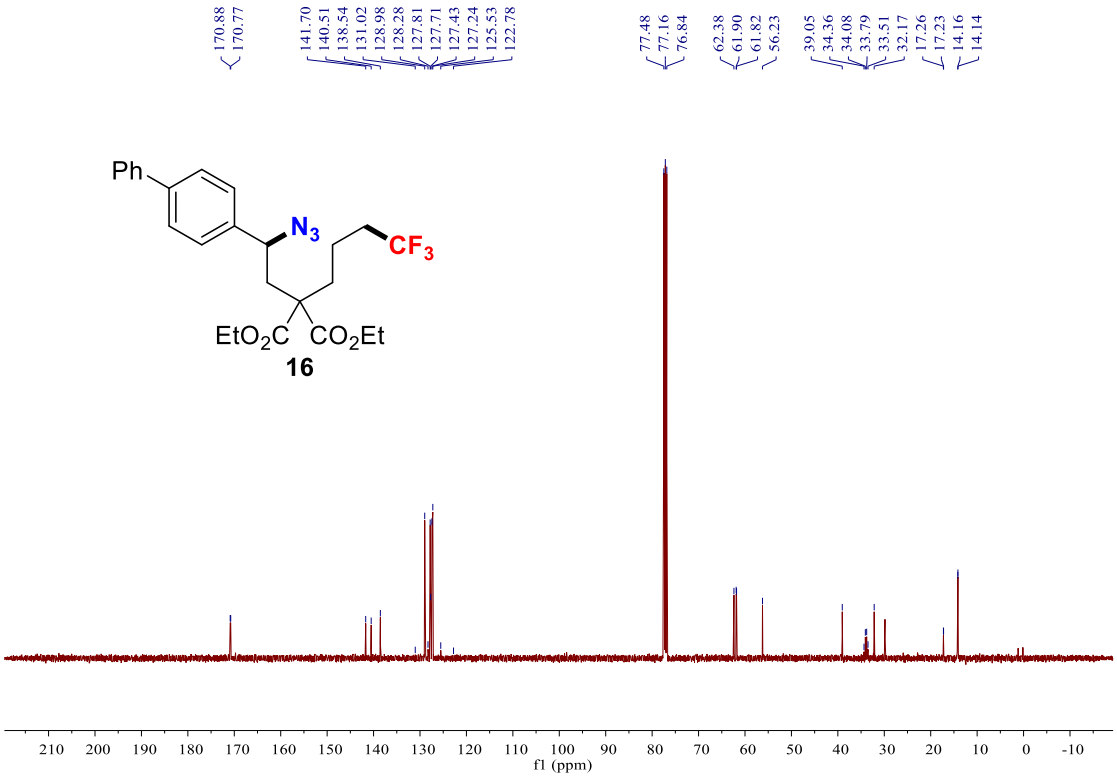
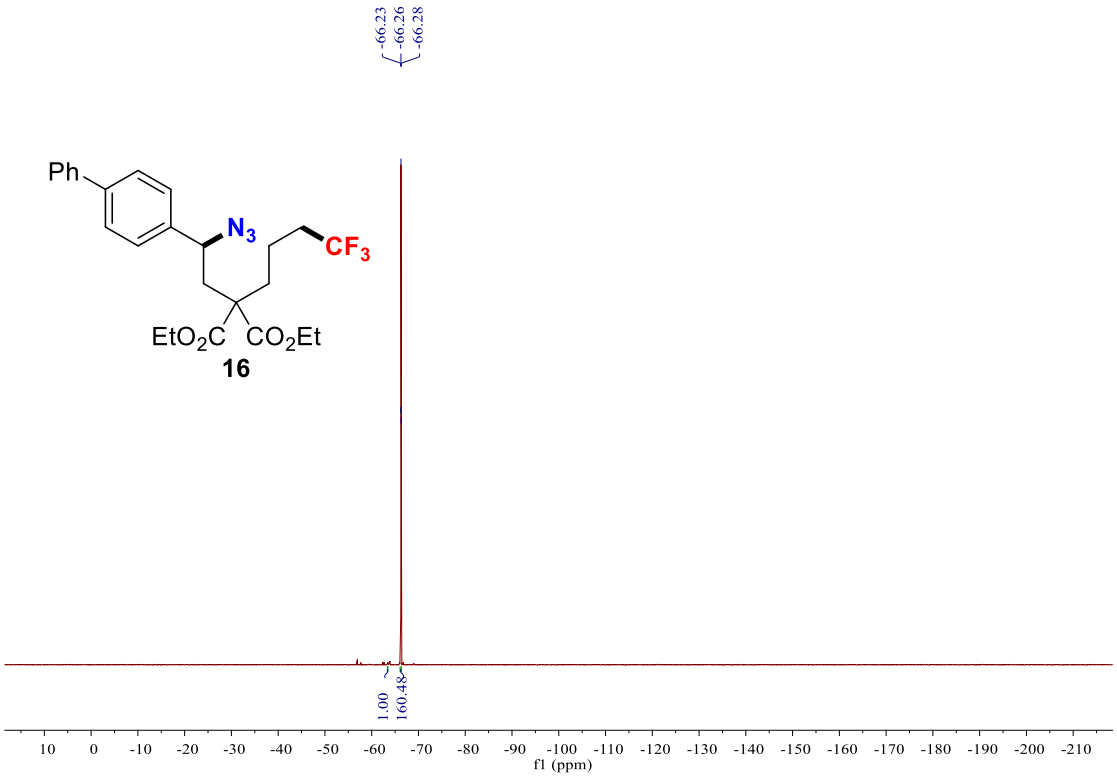
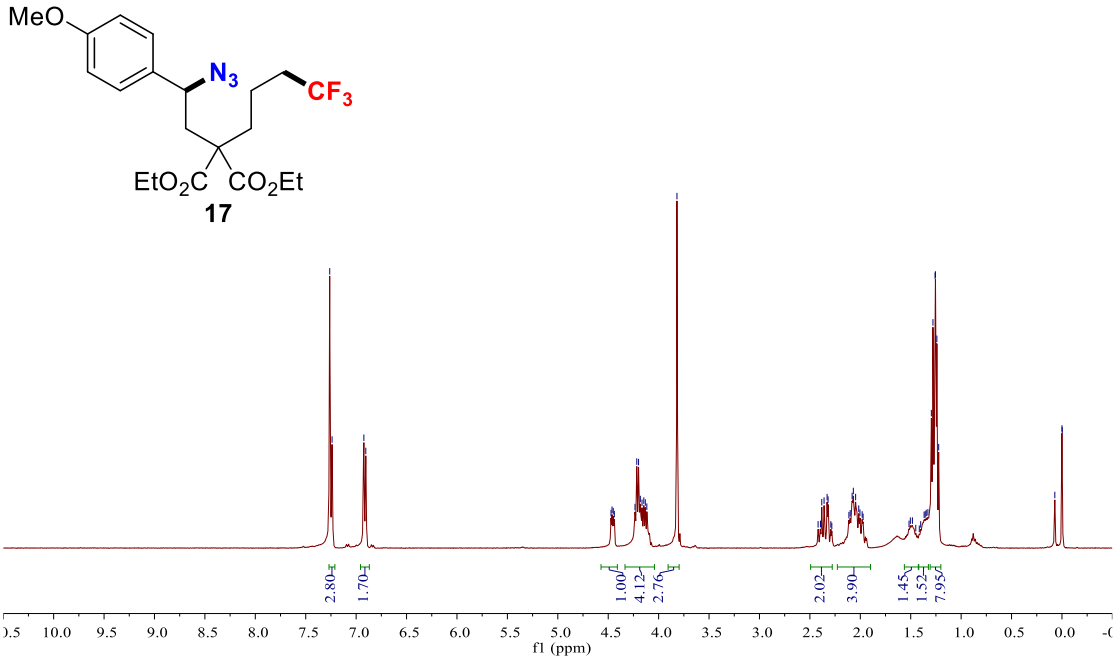
1.53
1.48
1.43
1.41
1.40
1.39
1.38
1.35
1.31
1.29
1.28
1.26
1.24
0.00


Ph
N3
CF3
EtO2C CO2Et
16
3.64
1.93
2.76
0.95
3.79
1.98
3.85
1.42
1.26
3.53
4.19
fl (ppm)


170.88
170.77
141.70
140.51
138.54
131.02
128.98
128.28
127.81
127.71
127.43
127.24
125.53
122.78
77.48
77.16
76.84
62.38
61.90
61.82
56.23
39.05
34.36
34.08
33.79
33.51
32.17
17.26
17.23
14.16
14.14
Ph
N3
CF3
EtO2C CO2Et
16
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-66.23
-66.26
-66.28
Ph
N3
CF3
EtO2C CO2Et
16
1.00
160.48
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


7.26
7.24
6.92
6.90
4.47
4.46
4.45
4.44
4.23
4.22
4.20
4.18
4.16
4.15
4.13
4.12
3.82
2.42
2.40
2.38
2.36
2.33
2.32
2.29
2.28
2.11
2.10
2.08
2.07
2.05
2.02
2.00
1.98
1.97
1.52
1.50
1.48
1.45
1.42
1.40
1.37
1.36
1.35
1.33
1.30
1.28
1.26
1.26
1.24
1.22
0.07
0.00
-0.00


MeO
N3
CF3
EtO2C
CO2Et
17
2.80
1.70
1.00
4.12
2.76
2.02
3.90
1.45
1.52
7.95
f1 (ppm)


170.89
170.78
159.83
131.49
128.31
128.28
125.53
114.35
77.48
77.16
76.84
62.09
61.84
61.77
56.19
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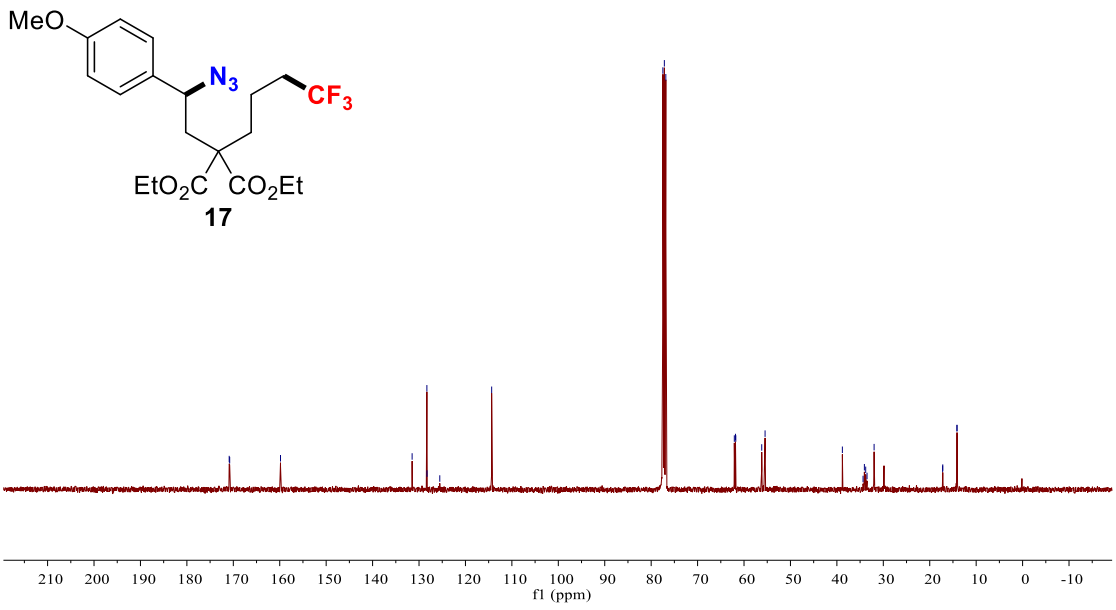
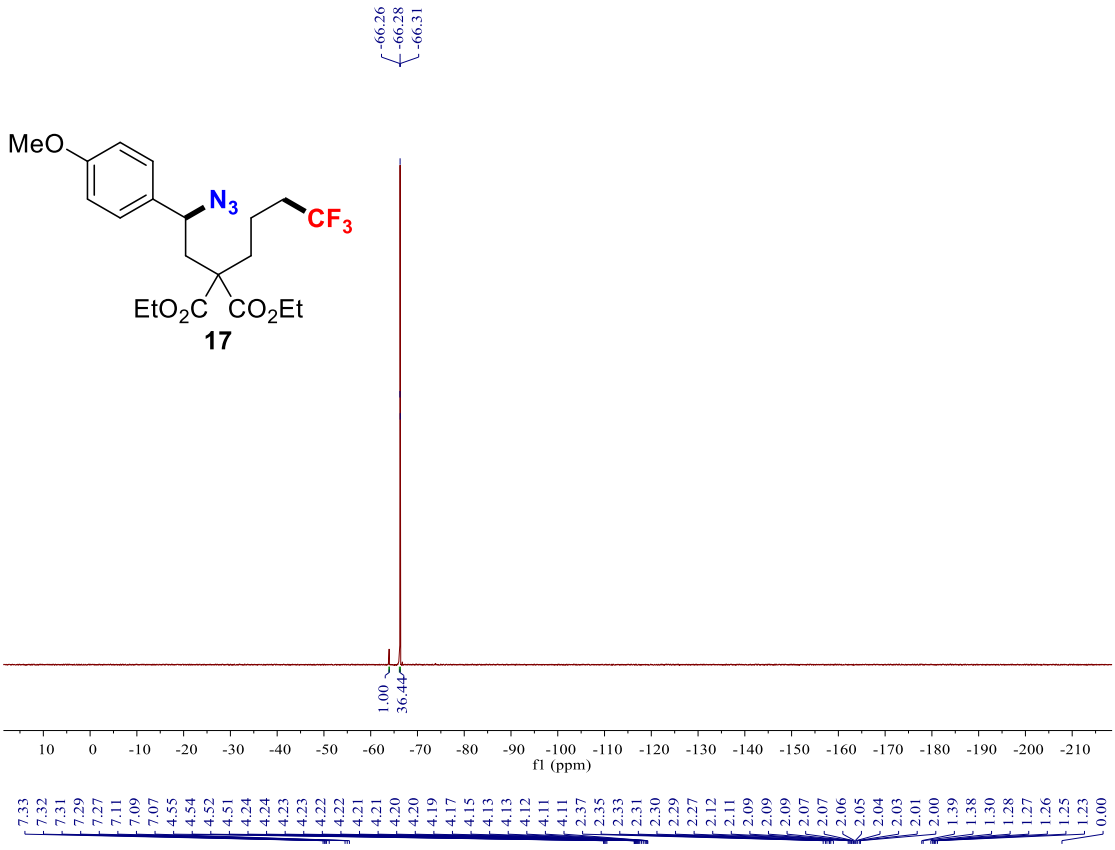
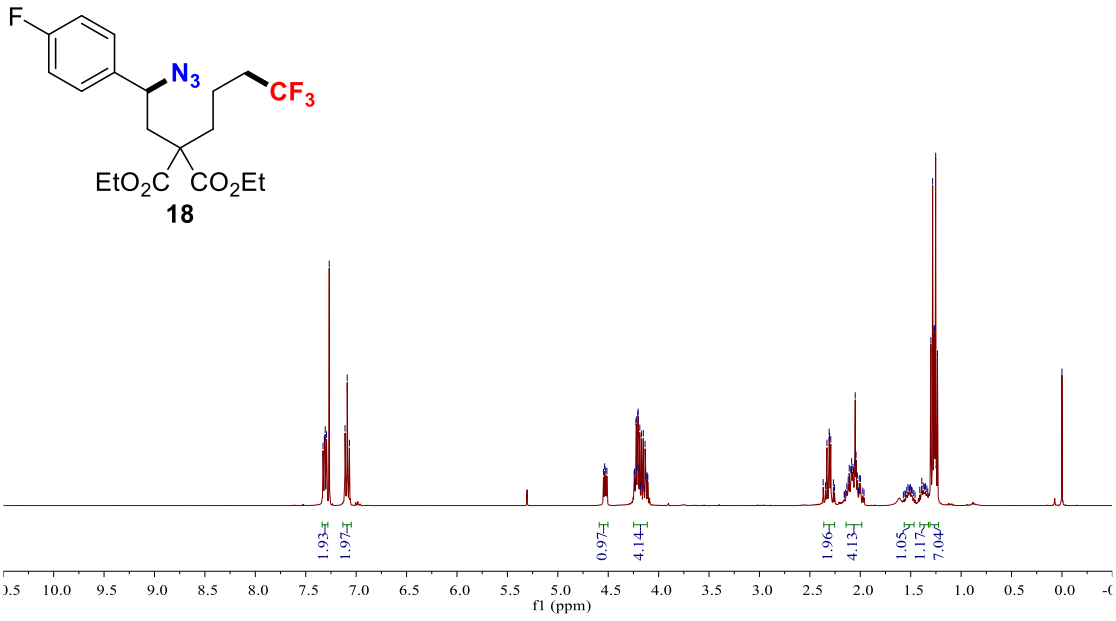
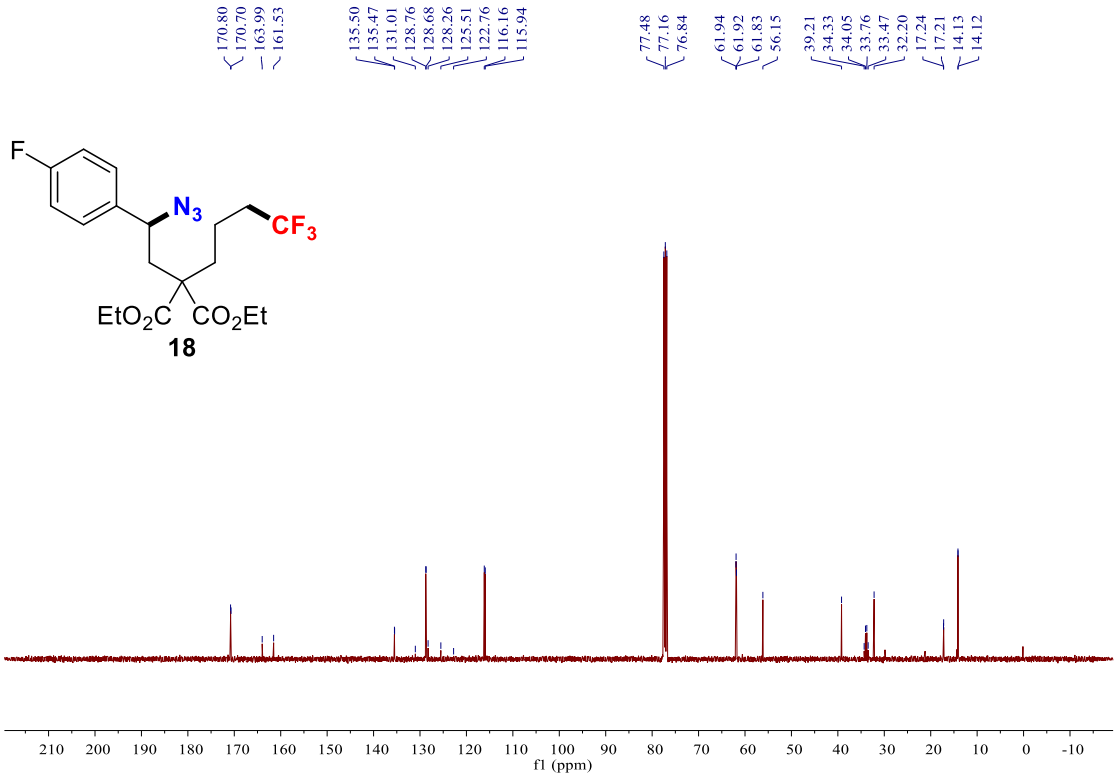
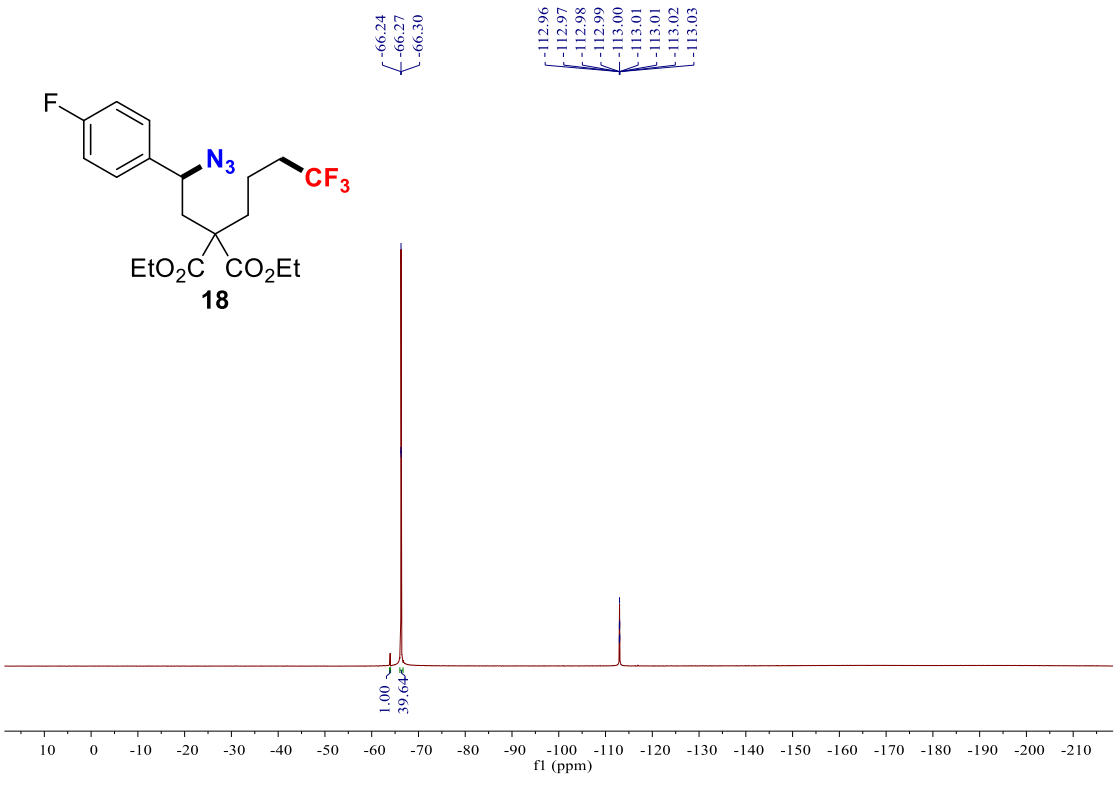
33.50
31.98
17.22
17.19
14.14
14.12

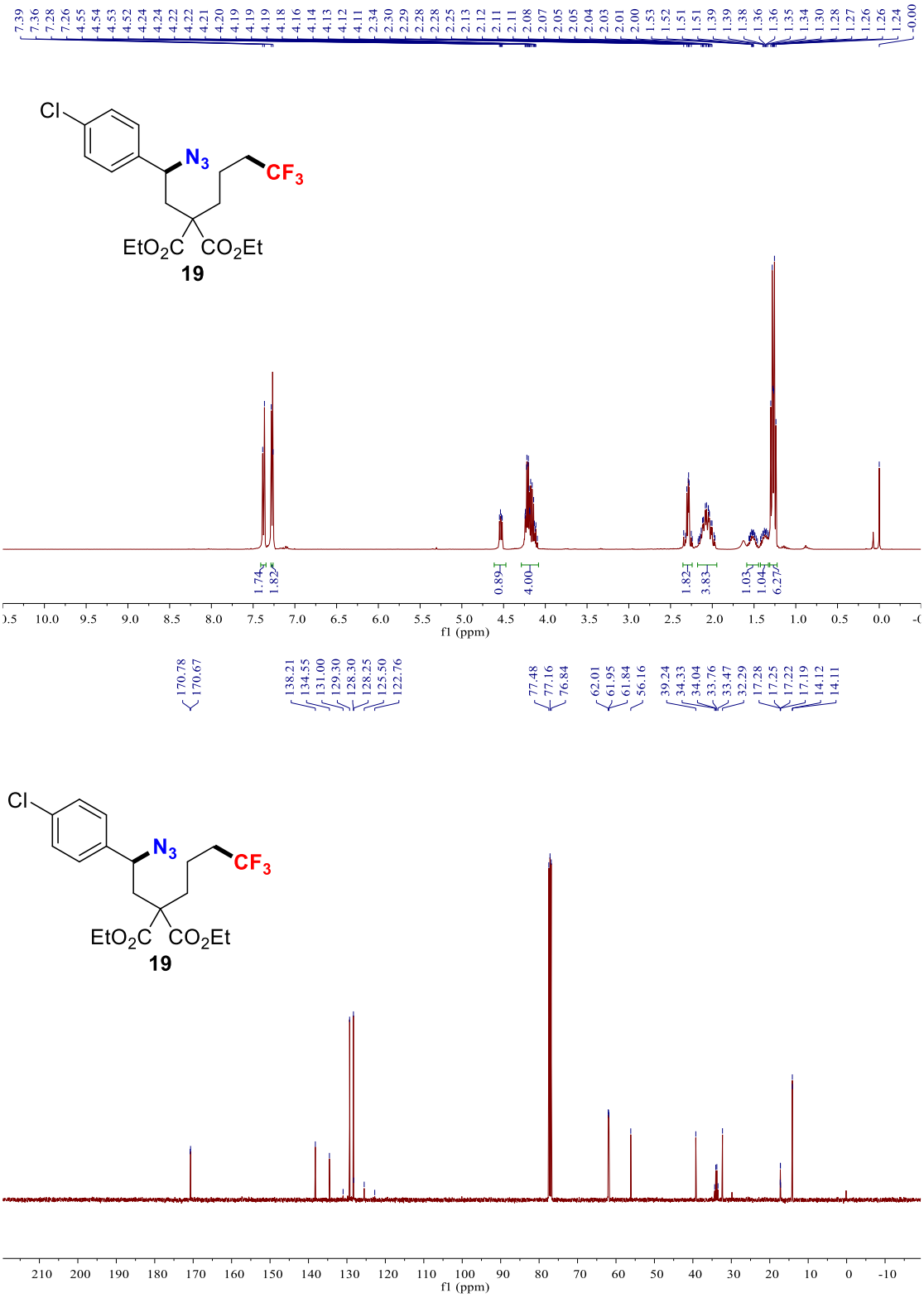

MeO
N3
CF3
EtO2C
CO2Et
17
f1 (ppm)

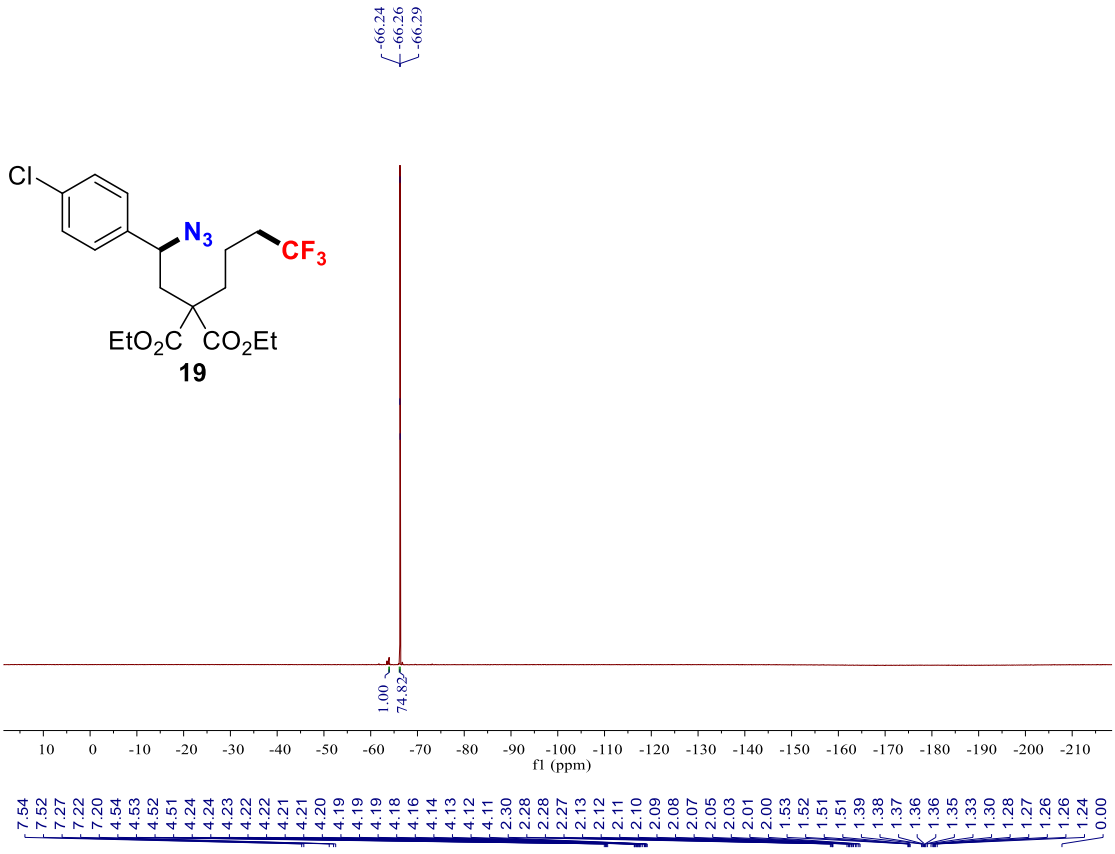

-66.26
-66.28
-66.31
MeO
N3
CF3
EtO2C CO2Et
17
1.00
36.44
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)
7.33 7.32 7.31 7.29 7.27 7.11 7.09 7.07 4.55 4.54 4.52 4.51 4.24 4.24 4.23 4.23 4.22 4.22 4.21 4.21 4.20 4.20 4.19 4.17 4.15 4.13 4.13 4.12 4.11 4.11 2.37 2.35 2.33 2.31 2.30 2.29 2.27 2.12 2.11 2.09 2.09 2.09 2.07 2.07 2.06 2.05 2.04 2.03 2.01 2.00 1.39 1.38 1.30 1.28 1.27 1.26 1.25 1.23 0.00

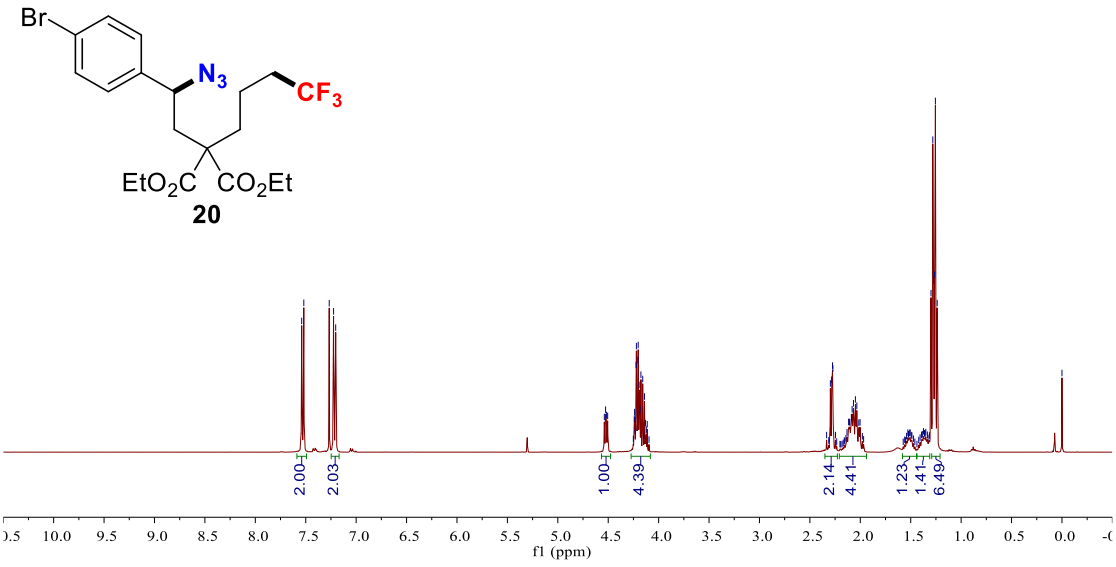

F
N3
CF3
EtO2C CO2Et
18
1.93
1.97
0.97
4.14
1.96
4.13
1.05
1.17
7.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

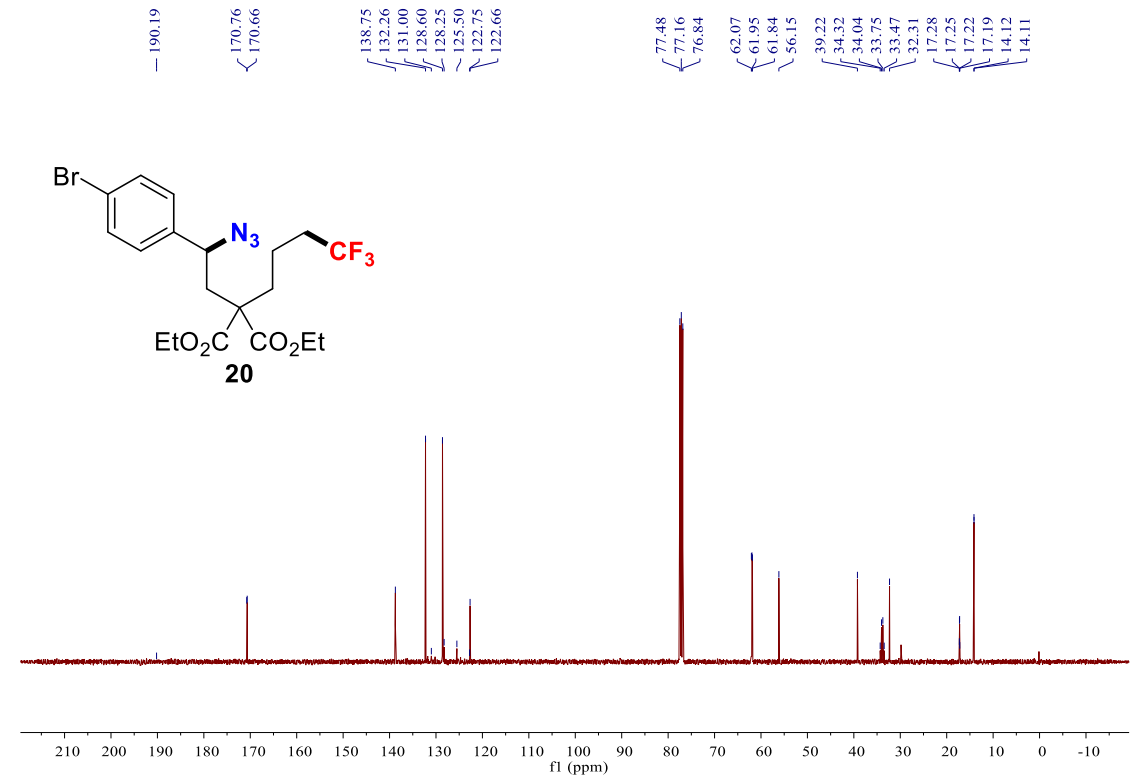

170.80
170.70
163.99
161.53
135.50
135.47
131.01
128.76
128.68
128.26
125.51
122.76
116.16
115.94
77.48
77.16
76.84
61.94
61.92
61.83
56.15
39.21
34.33
34.05
33.76
33.47
32.20
17.24
17.21
14.13
14.12
F
N3
CF3
EtO2C
CO2Et
18
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

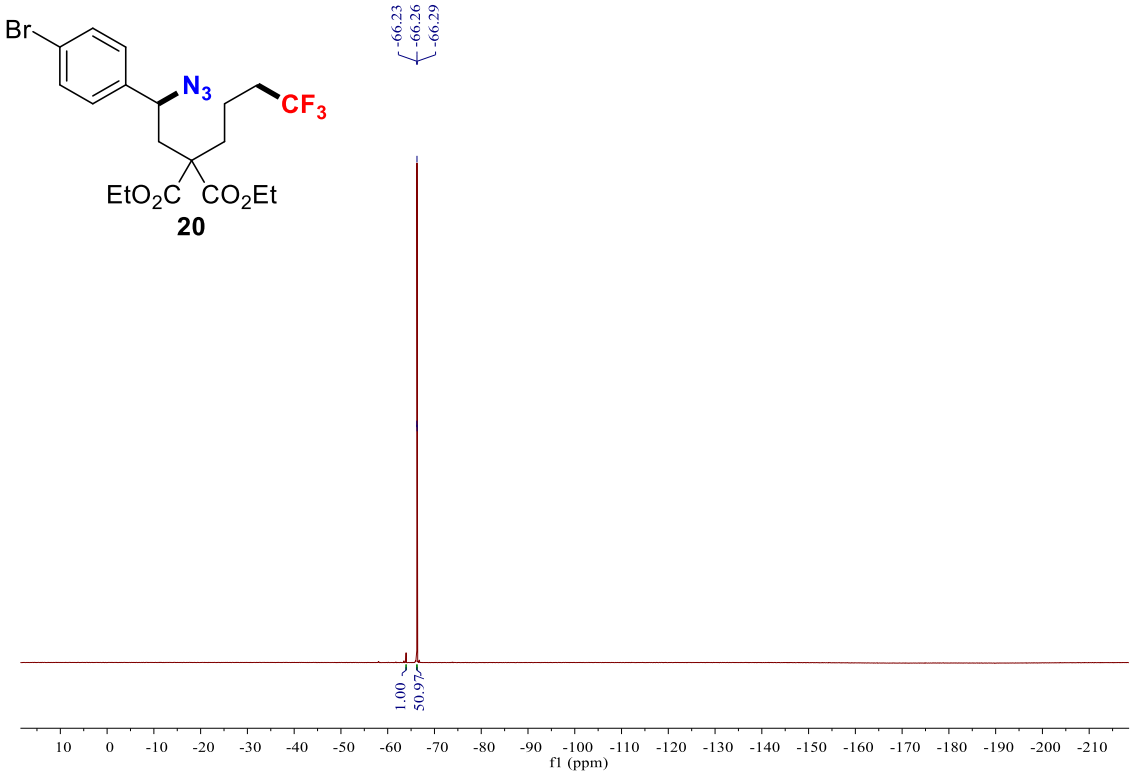

-66.24
-66.27
-66.30
-112.96
-112.97
-112.98
-112.99
-113.00
-113.01
-113.01
-113.02
-113.03
F
N3
CF3
EtO2C
CO2Et
18
1.00
39.64
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

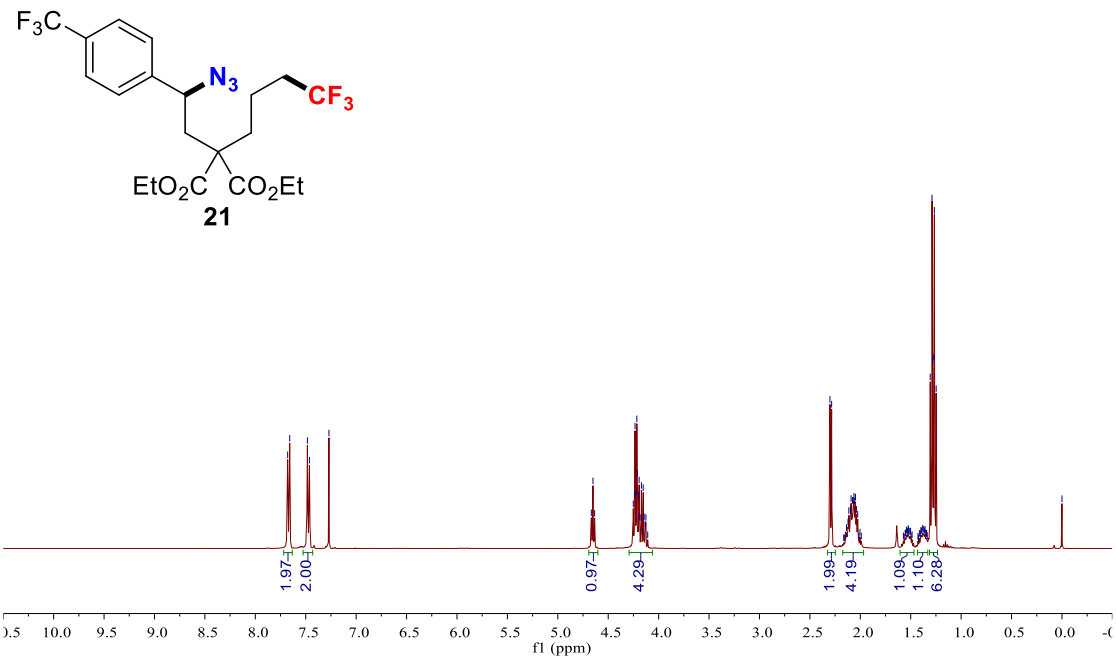

Cl
N3
CF3
EtO2C CO2Et
19
fl (ppm)
Cl
N3
CF3
EtO2C CO2Et
19
fl (ppm)

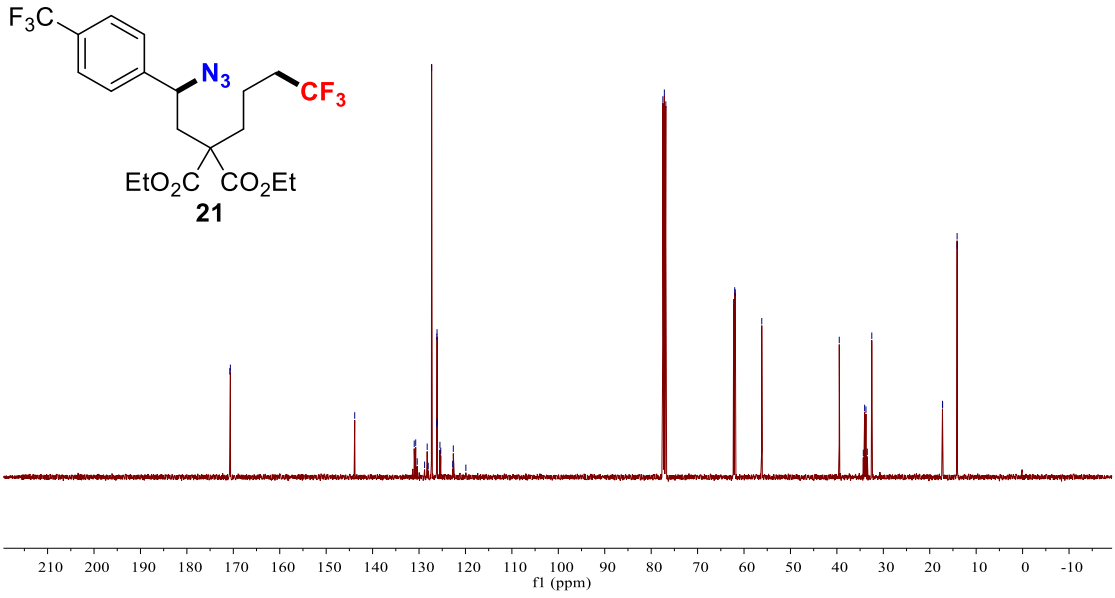

-66.24
-66.26
-66.29
Cl
N3
CF3
EtO2C CO2Et
19
1.00
74.82
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)
7.54 7.52 7.27 7.22 7.20 4.54 4.53 4.52 4.51 4.24 4.24 4.23 4.22 4.22 4.21 4.21 4.20 4.19 4.19 4.19 4.18 4.16 4.14 4.13 4.12 4.11 2.30 2.28 2.28 2.27 2.13 2.12 2.11 2.10 2.09 2.08 2.07 2.05 2.03 2.01 2.00 1.53 1.52 1.51 1.51 1.39 1.38 1.37 1.36 1.36 1.35 1.33 1.30 1.28 1.27 1.26 1.26 1.24 0.00

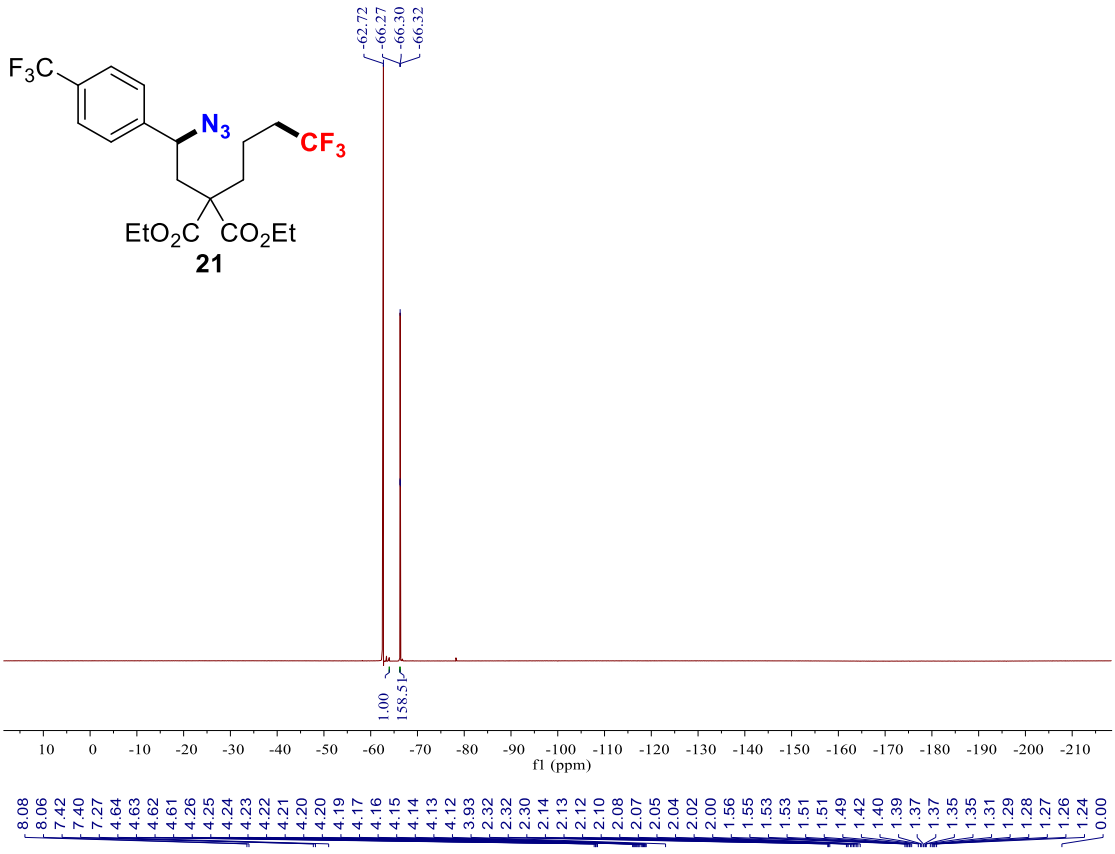

Br
N3
CF3
EtO2C CO2Et
20
2.00
2.03
1.00
4.39
2.14
4.41
1.23
1.41
6.49
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

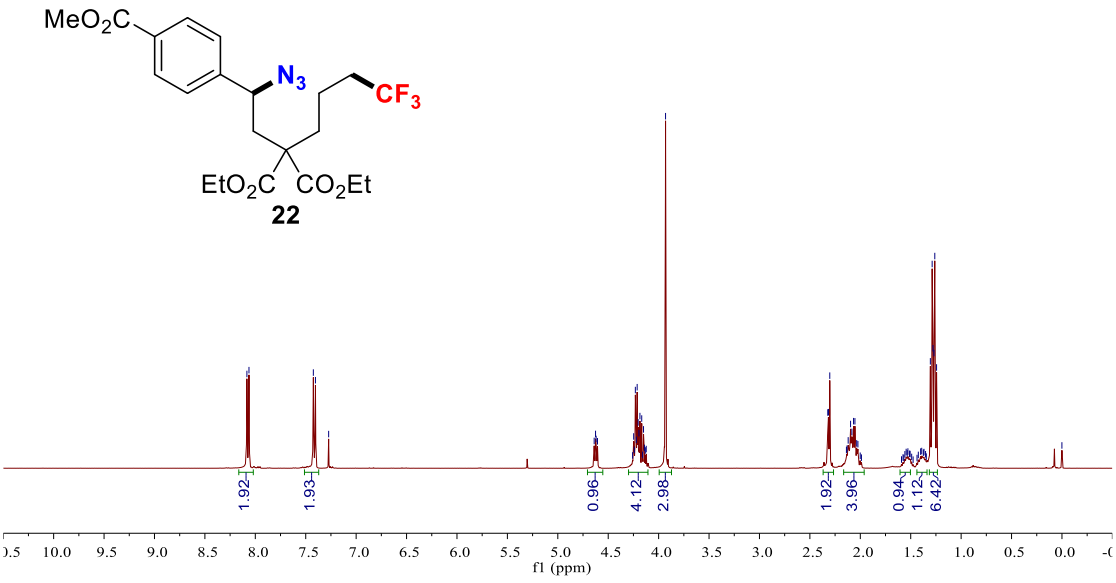

190.19
170.76
170.66
138.75
132.26
131.00
128.60
128.25
125.50
122.75
122.66
77.48
77.16
76.84
62.07
61.95
61.84
56.15
39.22
34.32
34.04
33.75
33.47
32.31
17.28
17.25
17.22
17.19
14.12
14.11
Br
N3
CF3
EtO2C
CO2Et
20
f1 (ppm)

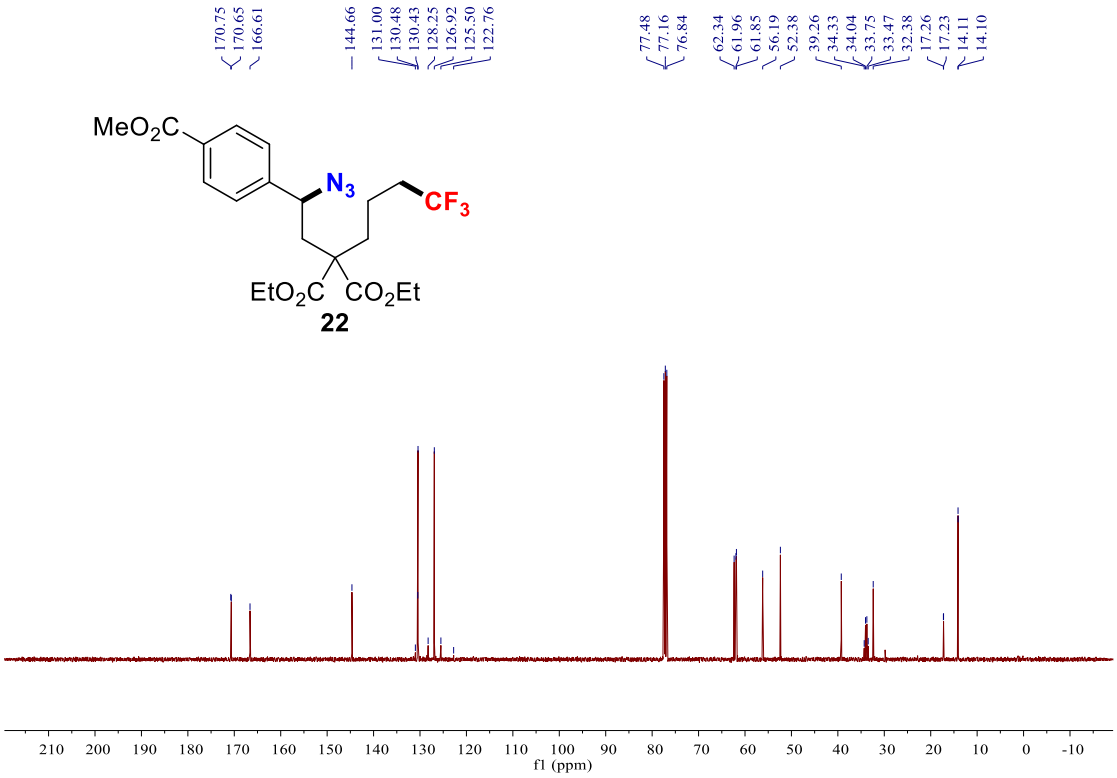

-66.23
-66.26
-66.29
Br
N3
CF3
EtO2C
CO2Et
20
1.00
50.97
f1 (ppm)

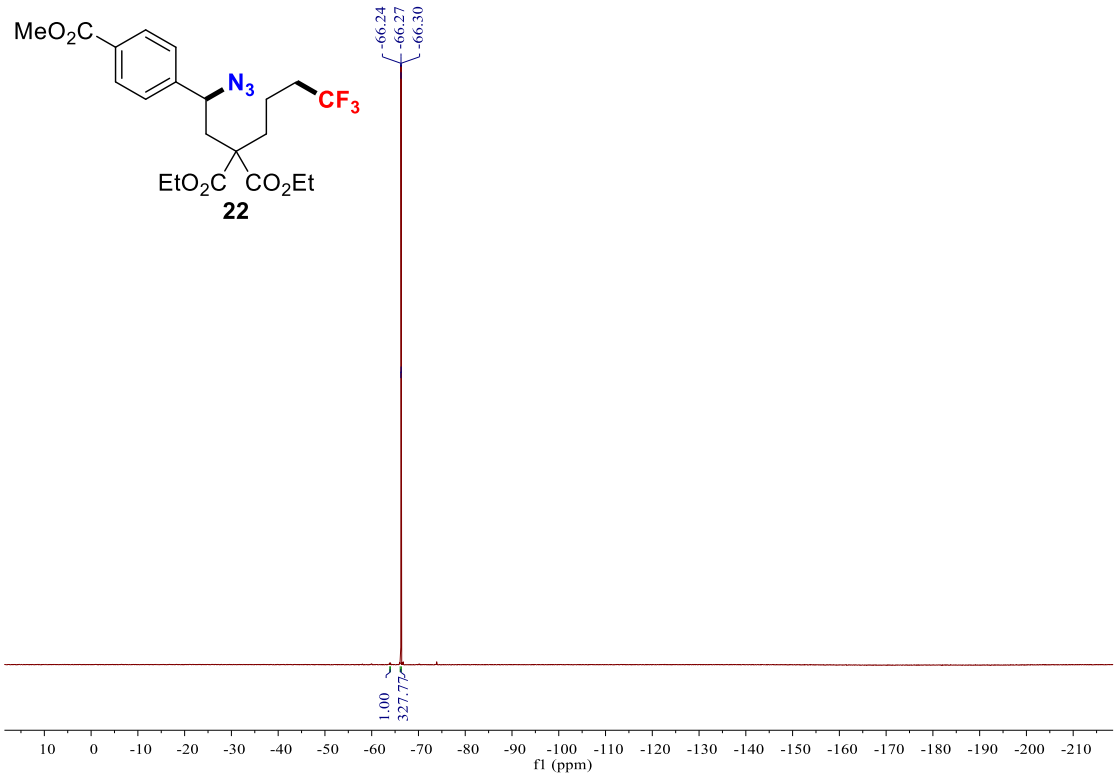

F3C
N3
CF3
EtO2C CO2Et
21
1.97
2.00
0.97
4.29
1.99
4.19
1.09
1.10
6.28
f1 (ppm)

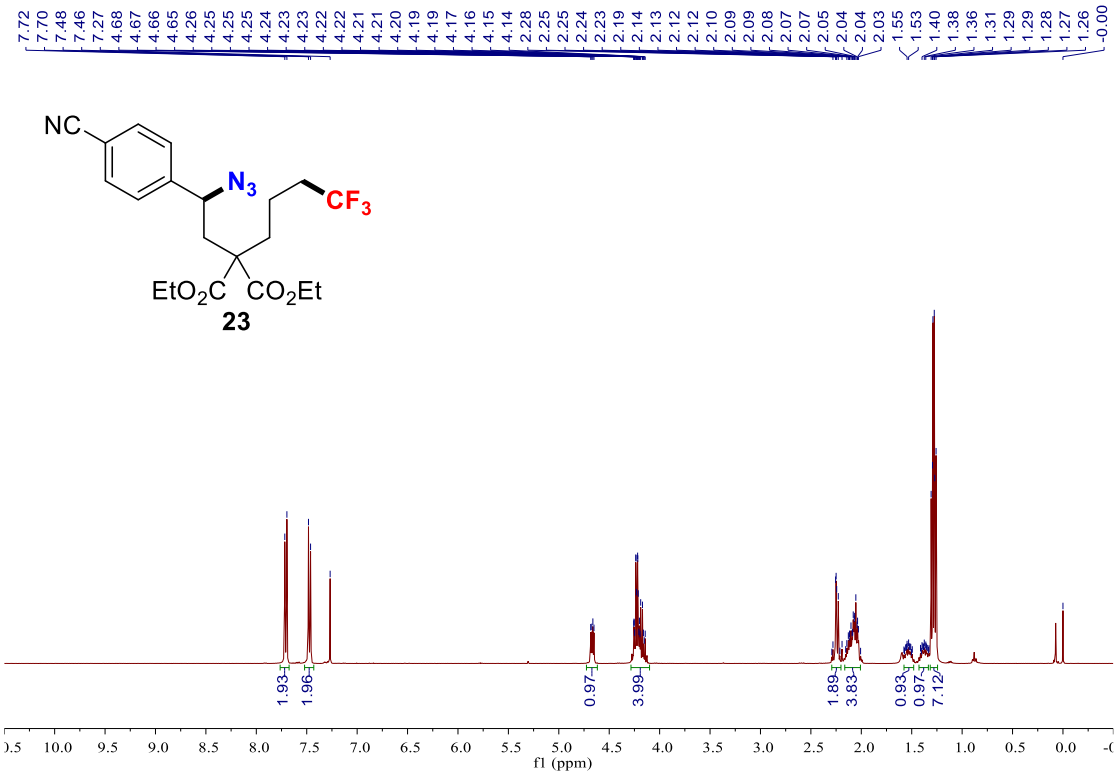

F3C
N3
CF3
EtO2C CO2Et
21
f1 (ppm)

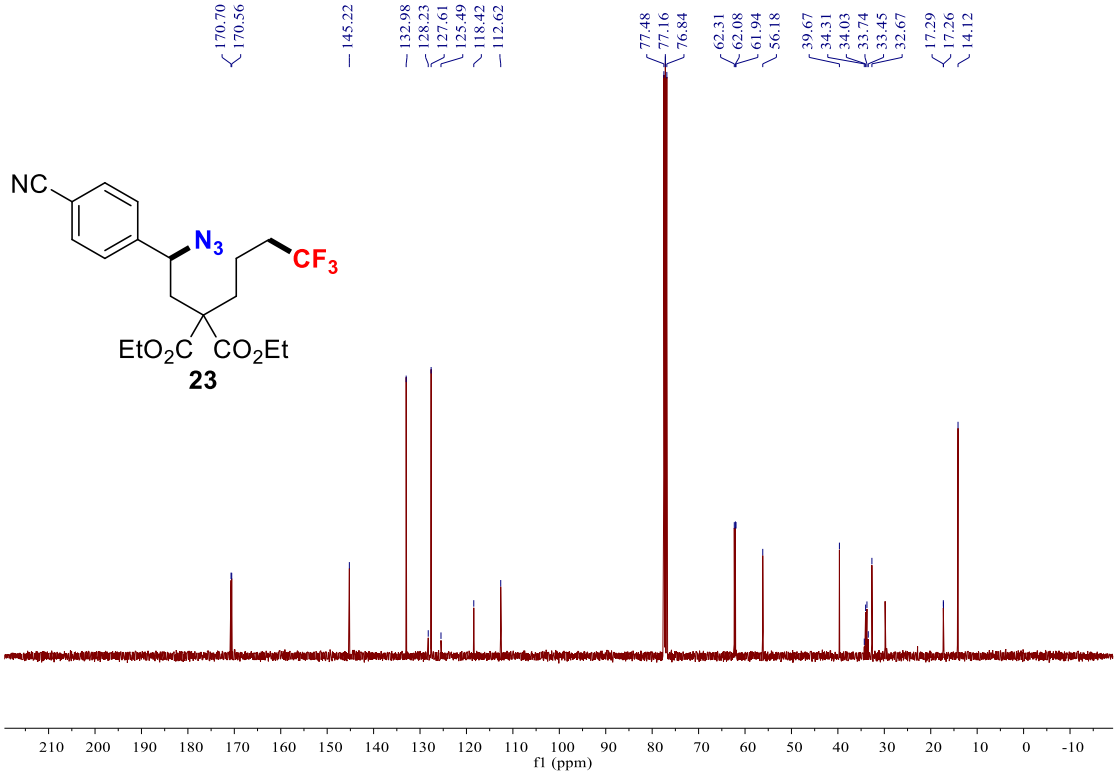

F3C
N3
CF3
EtO2C
CO2Et
21
-62.72
-66.27
-66.30
-66.32
1.00
158.51
f1 (ppm)

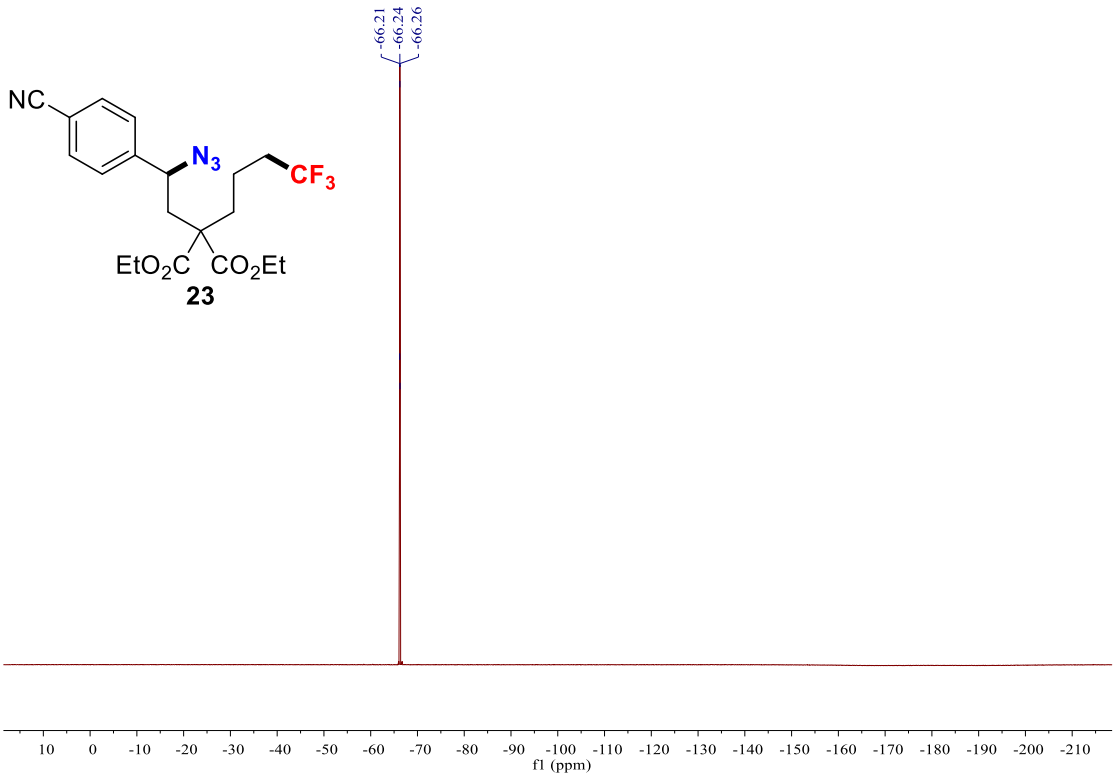

MeO2C
N3
CF3
EtO2C
CO2Et
22
1.92
1.93
0.96
4.12
2.98
1.92
3.96
0.94
1.12
6.42
f1 (ppm)

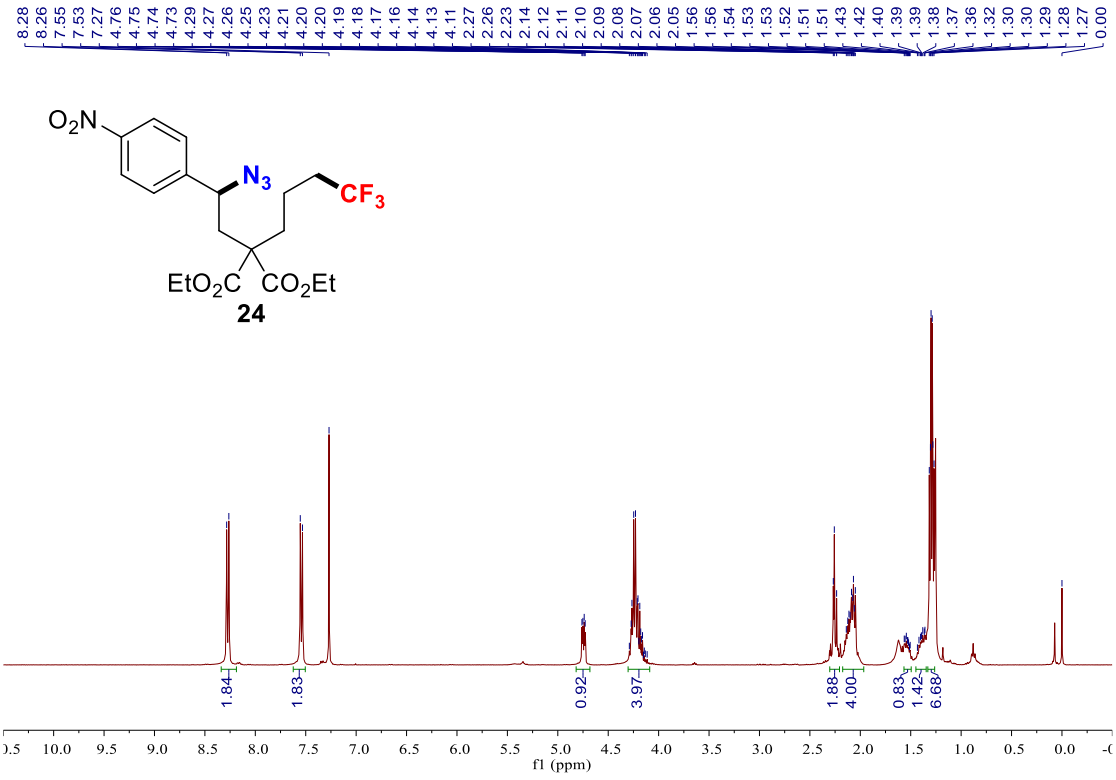

170.75
170.65
166.61
144.66
131.00
130.48
130.43
128.25
126.92
125.50
122.76
77.48
77.16
76.84
62.34
61.96
61.85
56.19
52.38
39.26
34.33
34.04
33.75
33.47
32.38
17.26
17.23
14.11
14.10
MeO2C
N3
CF3
EtO2C CO2Et
22
f1 (ppm)

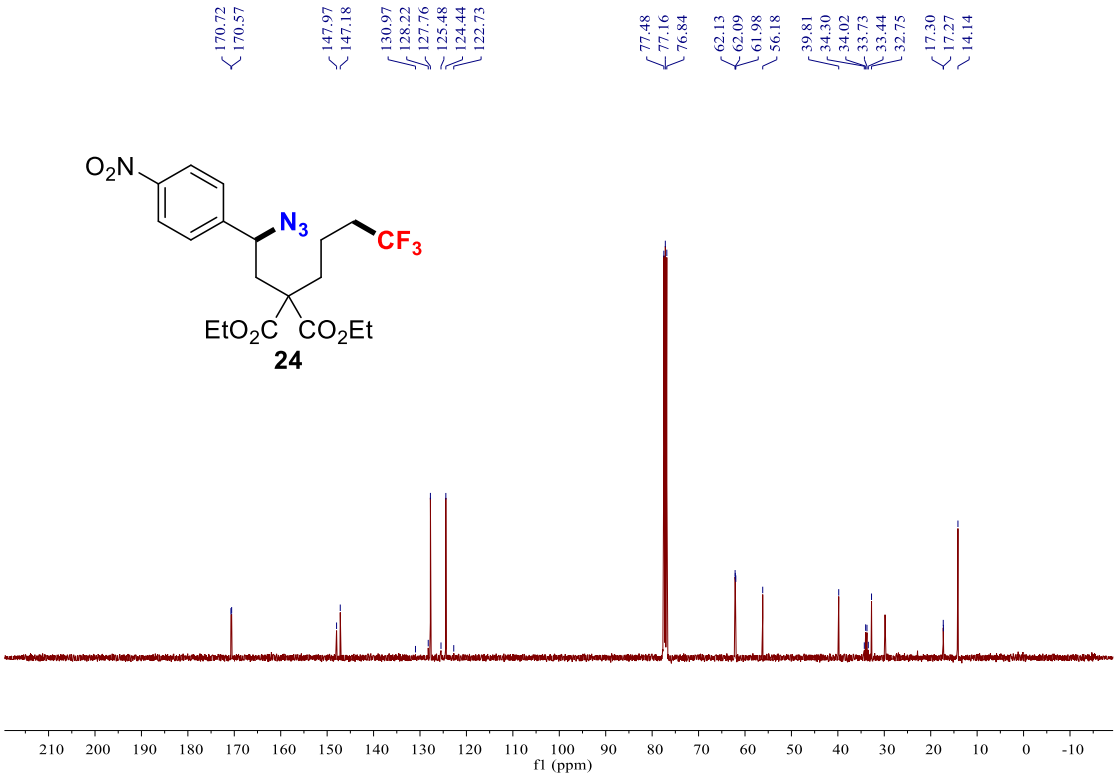

-66.24
-66.27
-66.30
MeO2C
N3
CF3
EtO2C CO2Et
22
1.00
327.77
f1 (ppm)

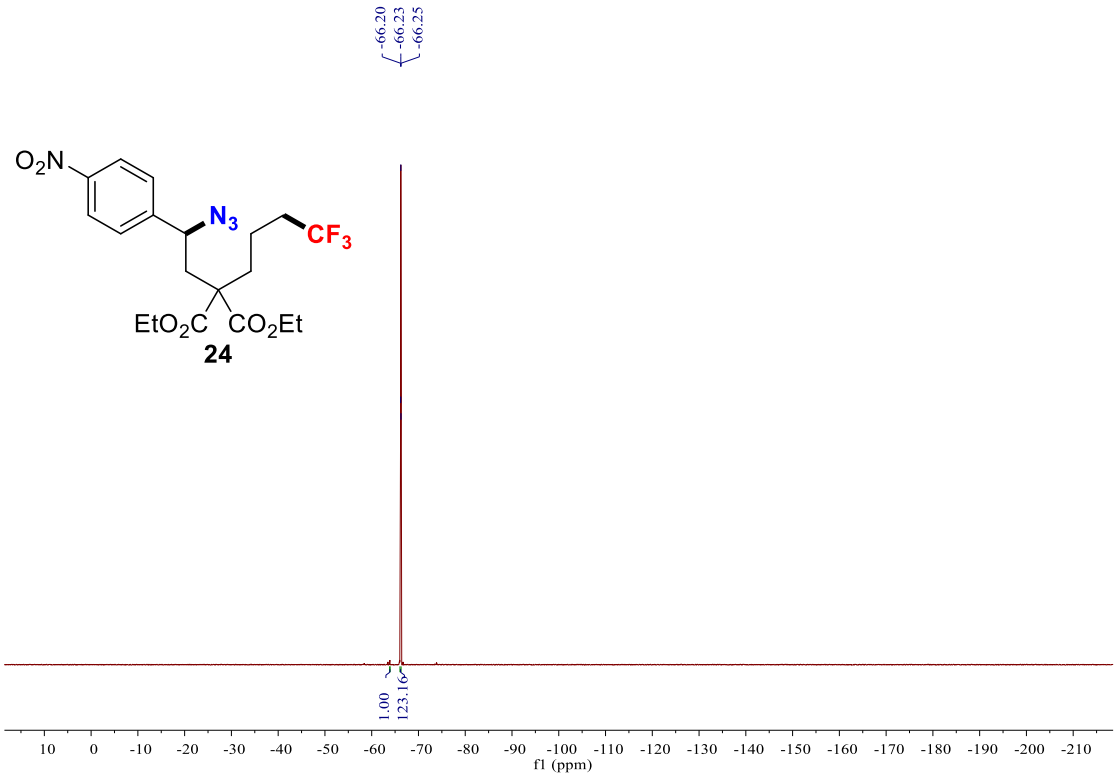

7.72 7.70 7.48 7.46 7.27 4.68 4.67 4.66 4.65 4.26 4.25 4.25 4.25 4.24 4.23 4.23 4.22 4.22 4.21 4.21 4.20 4.19 4.19 4.17 4.16 4.15 4.14 2.28 2.25 2.25 2.24 2.23 2.19 2.14 2.13 2.12 2.12 2.10 2.09 2.09 2.08 2.07 2.07 2.05 2.04 2.04 2.03 1.55 1.53 1.40 1.38 1.36 1.31 1.29 1.29 1.28 1.27 1.26 -0.00
NC
N3
CF3
EtO2C CO2Et
23
1.93 1.96 0.97 3.99 1.89 3.83 0.93 0.97 7.12
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)


170.70 170.56 145.22 132.98 128.23 127.61 125.49 118.42 112.62 77.48 77.16 76.84 62.31 62.08 61.94 56.18 39.67 34.31 34.03 33.74 33.45 32.67 17.29 17.26 14.12
NC
N3
CF3
EtO2C CO2Et
23
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-66.21
-66.24
-66.26
NC
N3
CF3
EtO2C
CO2Et
23
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


8.28 8.26 7.55 7.53 7.27 4.76 4.75 4.74 4.73 4.29 4.27 4.26 4.25 4.23 4.21 4.20 4.20 4.19 4.18 4.17 4.16 4.14 4.13 4.11 2.27 2.26 2.23 2.14 2.12 2.11 2.10 2.09 2.08 2.07 2.06 2.05 1.56 1.54 1.53 1.53 1.52 1.51 1.51 1.43 1.42 1.40 1.39 1.39 1.38 1.37 1.36 1.32 1.30 1.30 1.29 1.28 1.27 0.00
O2N
N3
CF3
EtO2C
CO2Et
24
1.84 1.83 0.92 3.97 1.88 4.00 0.83 1.42 6.68
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)


170.72
170.57
147.97
147.18
130.97
128.22
127.76
125.48
124.44
122.73
77.48
77.16
76.84
62.13
62.09
61.98
56.18
39.81
34.30
34.02
33.73
33.44
32.75
17.30
17.27
14.14
O2N
N3
CF3
EtO2C
CO2Et
24
f1 (ppm)


-66.20
-66.23
-66.25
O2N
N3
CF3
EtO2C
CO2Et
24
1.00
123.16
f1 (ppm)


7.30
7.28
7.26
7.16
7.15
7.12
7.10
4.49
4.47
4.46
4.45
4.25
4.24
4.24
4.23
4.23
4.21
4.21
4.20
4.20
4.19
4.18
4.17
4.16
4.15
4.15
4.14
4.13
4.12
4.11
2.40
2.38
2.37
2.34
2.33
2.32
2.30
2.12
2.11
2.10
2.09
2.08
2.05
2.05
2.04
2.03
2.01
2.00
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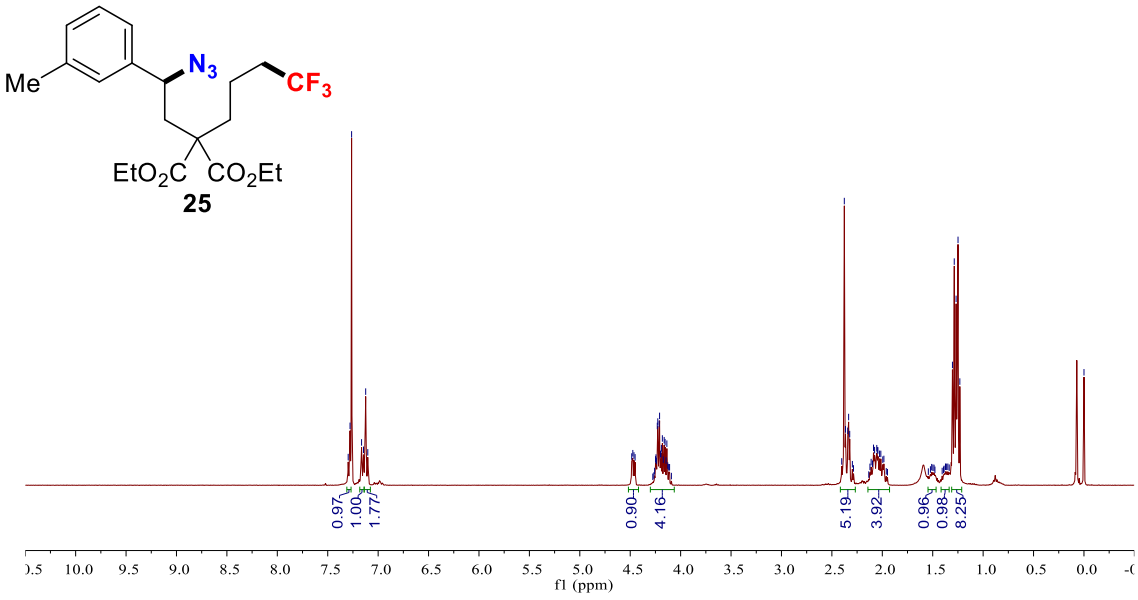
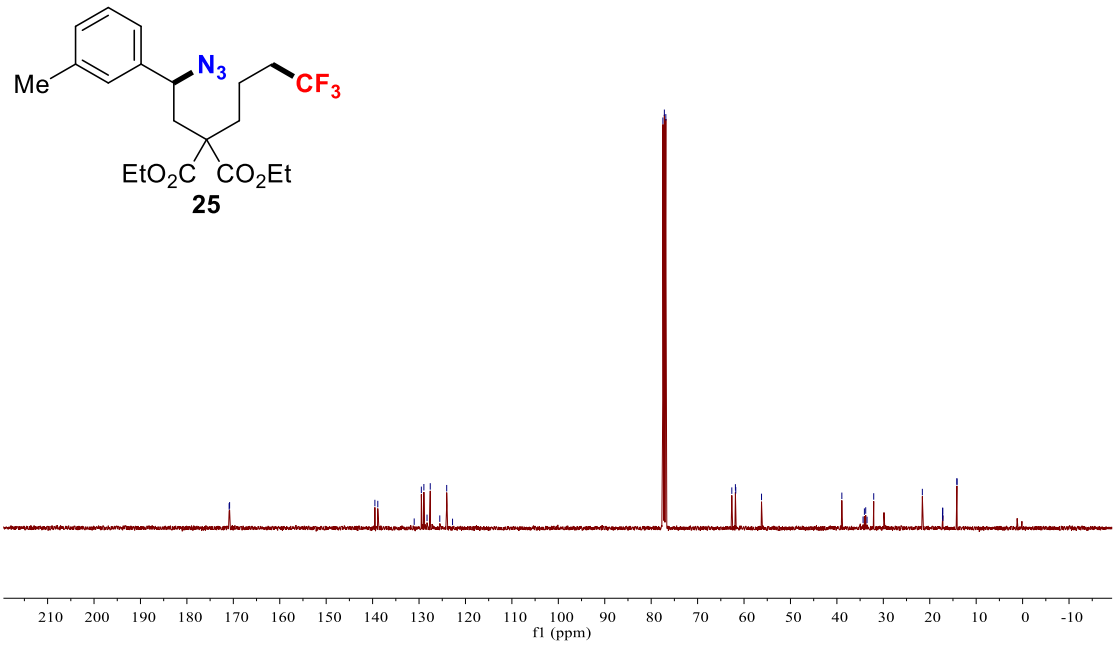
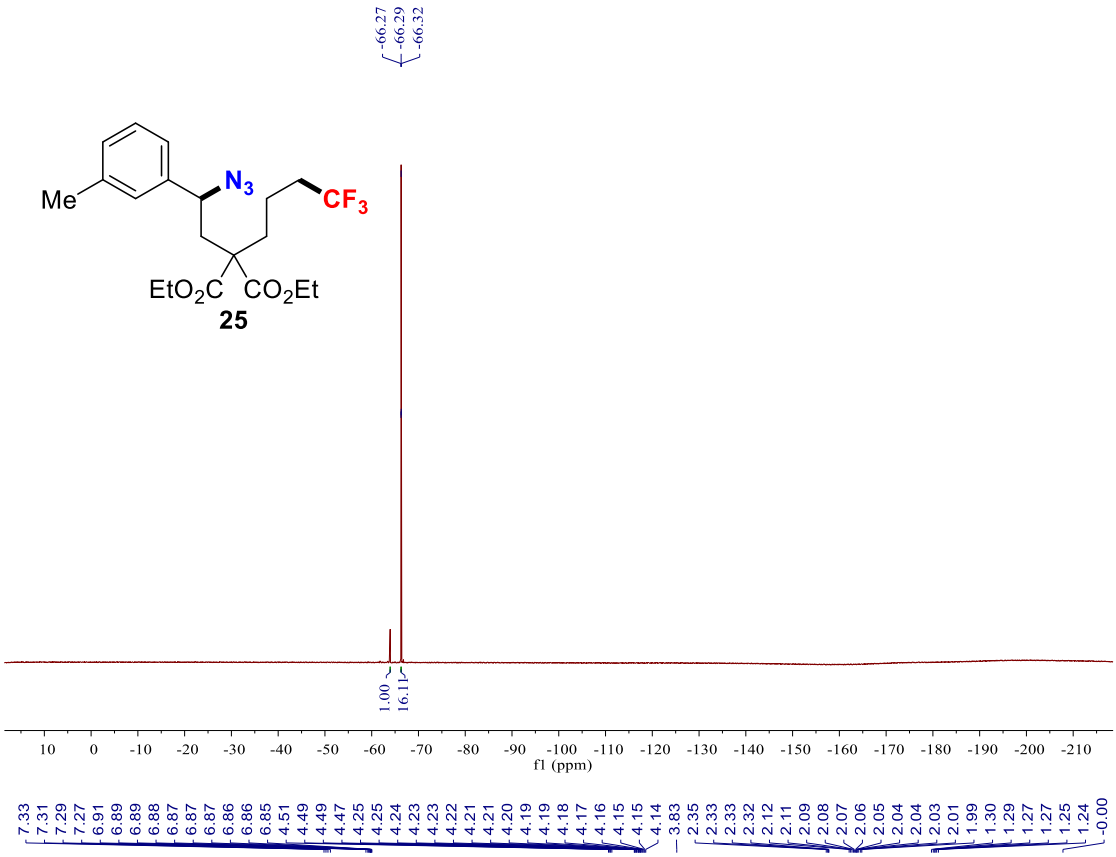
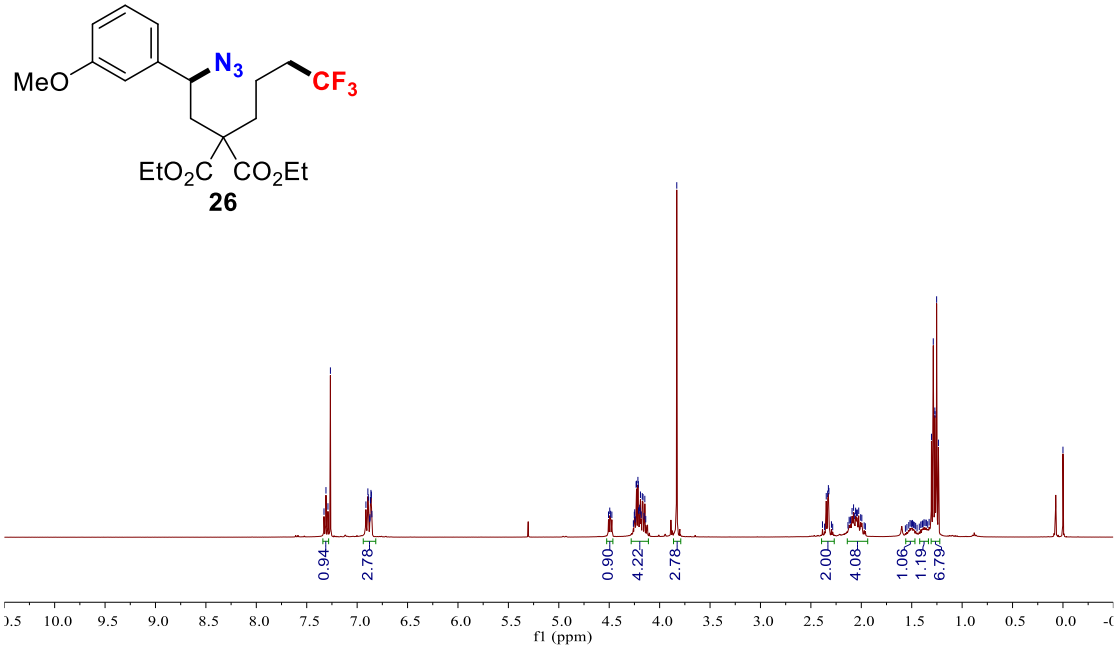
1.30
1.29
1.27
1.25
1.23
-0.00

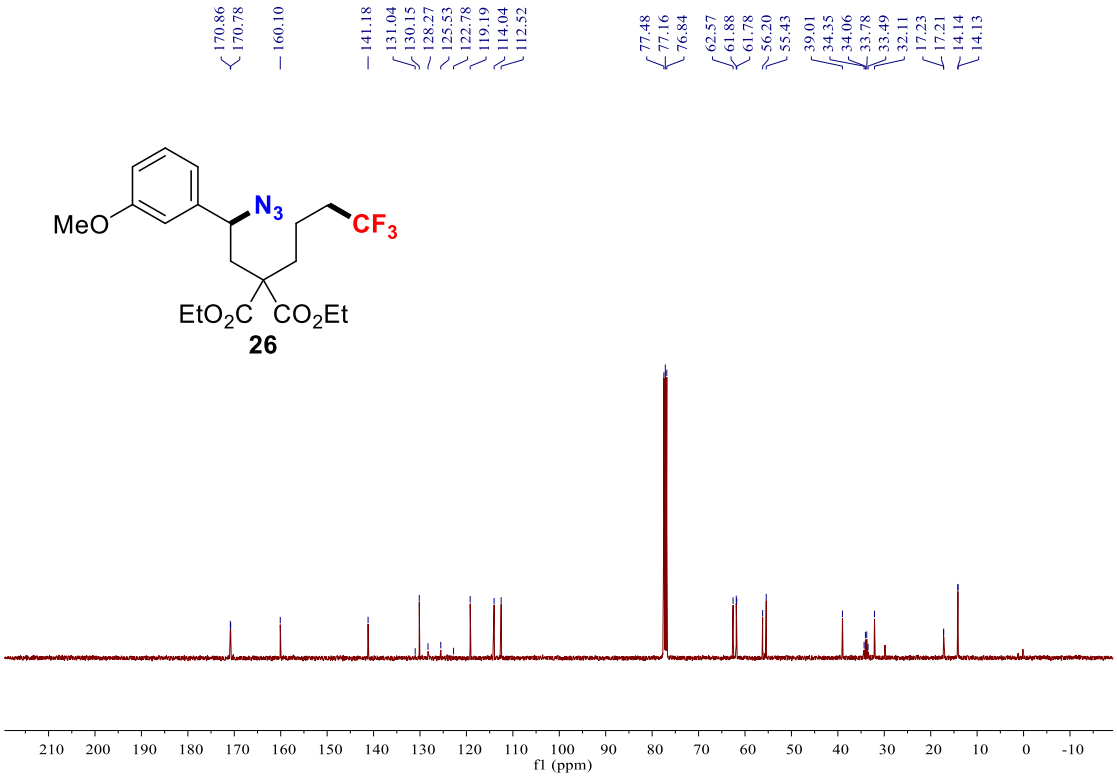

Me
N3
CF3
EtO2C
CO2Et
25
0.97
1.00
1.77
0.90
4.16
5.19
3.92
0.96
0.98
8.25
f1 (ppm)

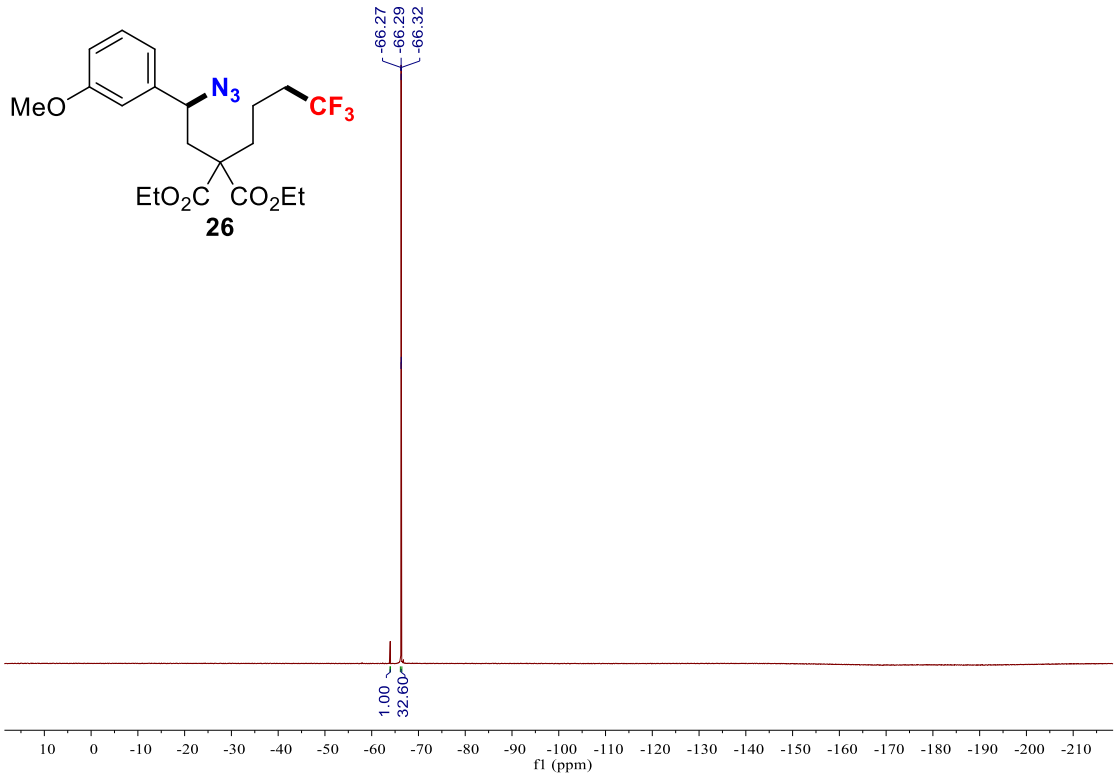

170.90
170.80
139.51
138.88
131.04
129.50
128.96
128.28
127.58
125.53
124.04
122.78
77.48
77.16
76.84
62.63
61.86
61.78
56.23
38.93
34.36
34.08
33.79
33.51
32.07
21.59
17.26
17.23
17.20
17.17
14.15
14.13

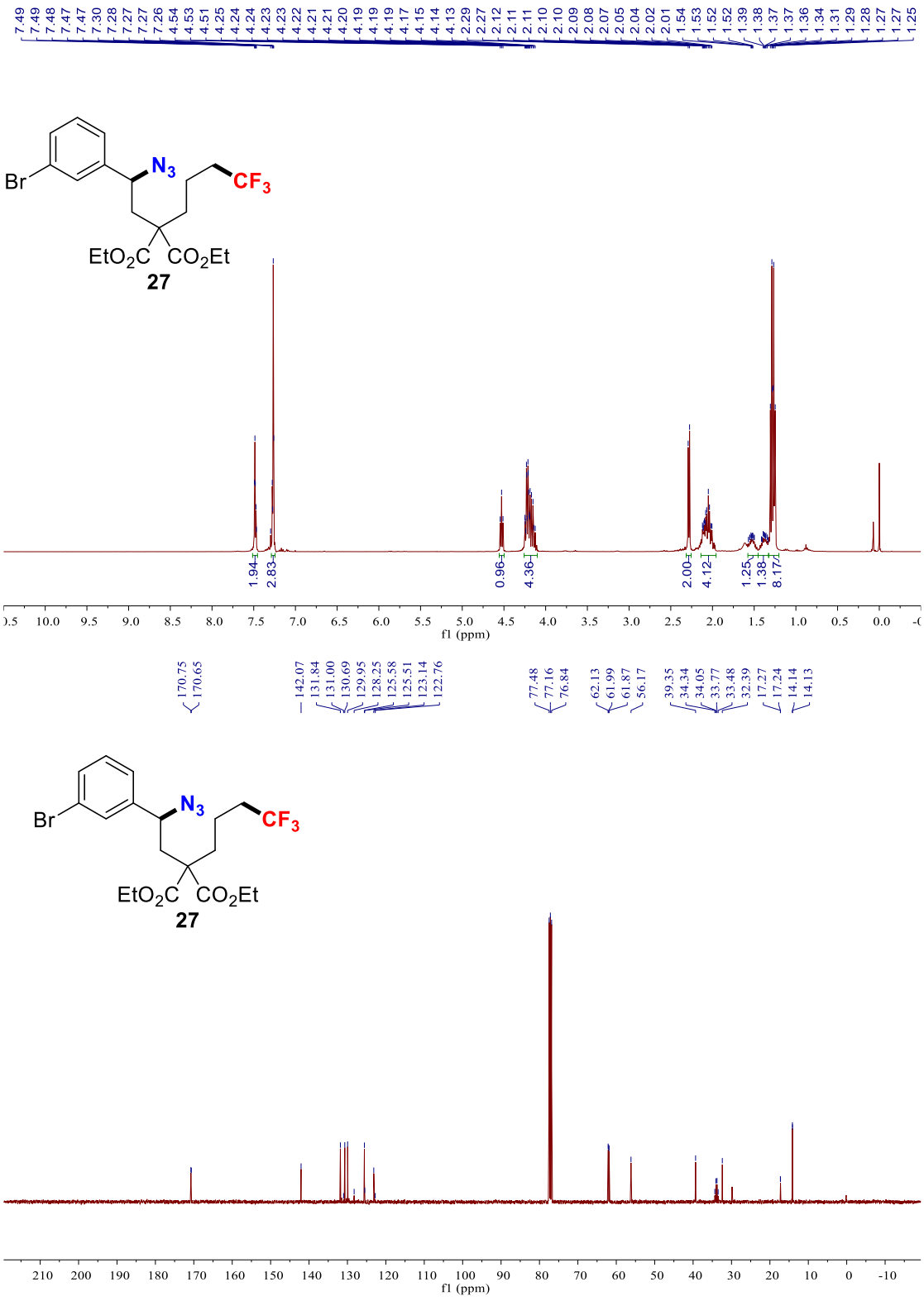

Me
N3
CF3
EtO2C
CO2Et
25
f1 (ppm)

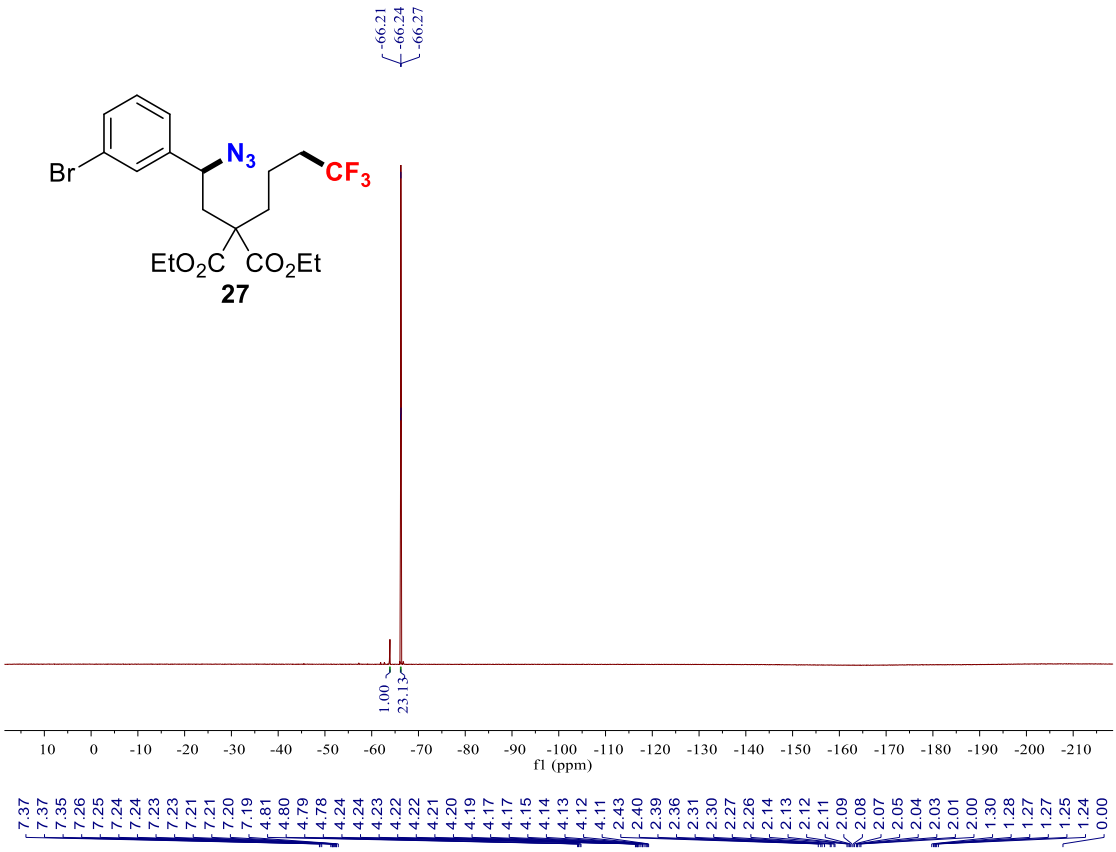

-66.27
-66.29
-66.32
Me
N3
CF3
EtO2C
CO2Et
25
1.00
16.11
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)
7.33
7.31
7.29
7.27
6.91
6.89
6.89
6.88
6.87
6.87
6.87
6.86
6.86
6.85
4.51
4.49
4.49
4.47
4.25
4.25
4.24
4.23
4.23
4.22
4.21
4.21
4.20
4.19
4.19
4.18
4.17
4.16
4.15
4.15
4.14
3.83
2.35
2.33
2.33
2.32
2.12
2.11
2.09
2.08
2.07
2.06
2.05
2.04
2.04
2.03
2.01
1.99
1.30
1.29
1.27
1.27
1.25
1.24
0.00

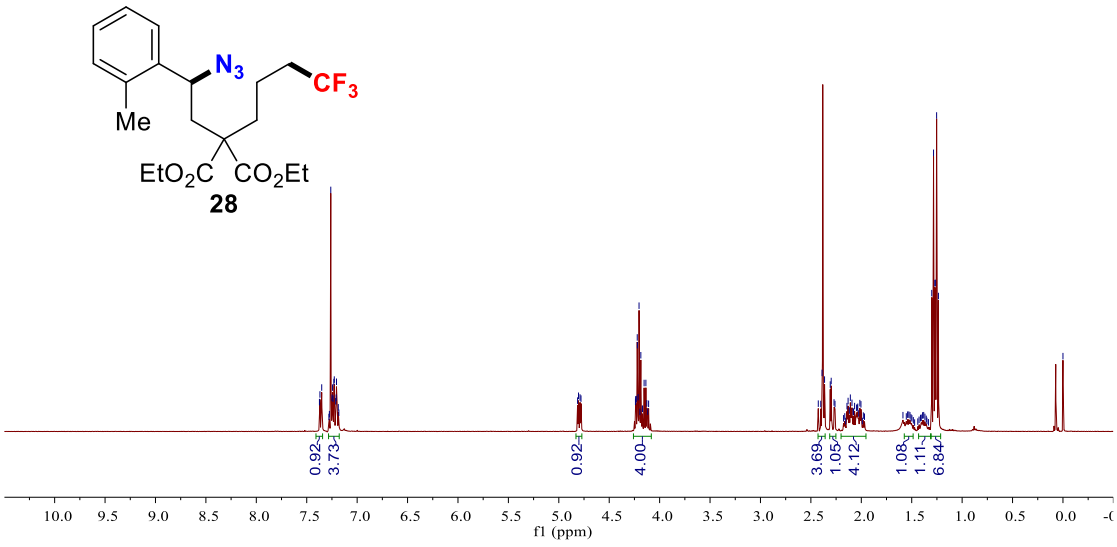

MeO
N3
CF3
EtO2C
CO2Et
26
0.94
2.78
0.90
4.22
2.78
2.00
4.08
1.06
1.19
6.79
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

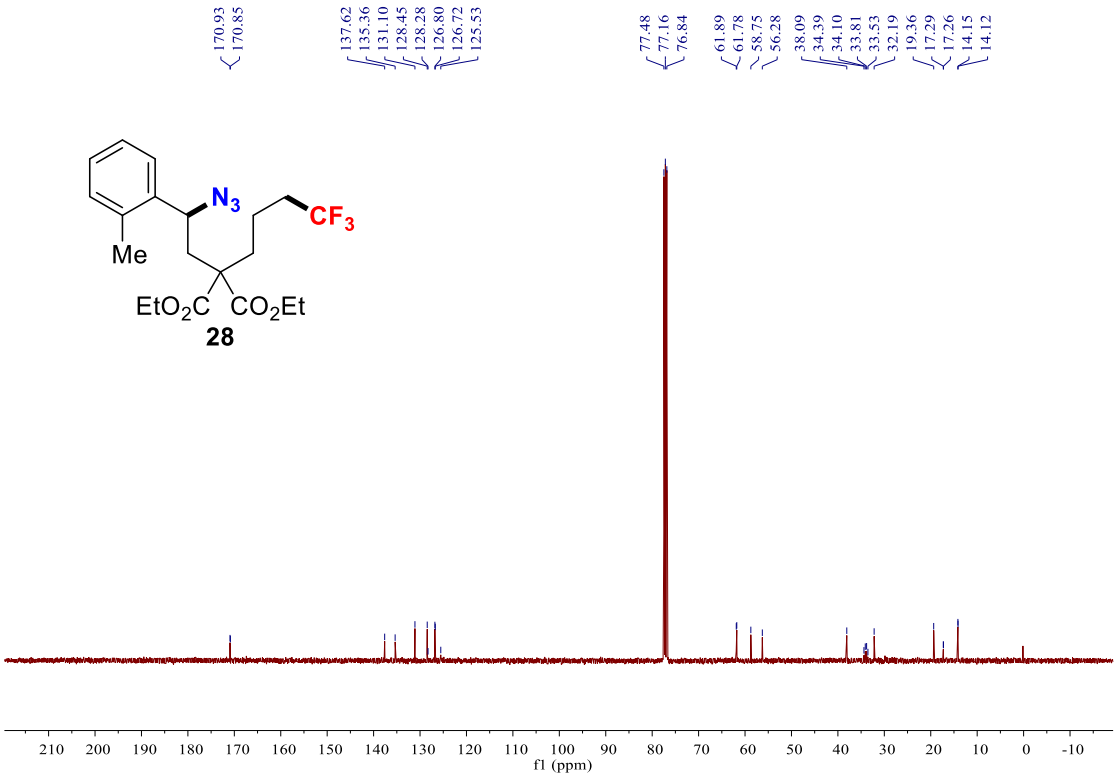

170.86
170.78
160.10
141.18
131.04
130.15
128.27
125.53
122.78
119.19
114.04
112.52
77.48
77.16
76.84
62.57
61.88
61.78
56.20
55.43
39.01
34.35
34.06
33.78
33.49
32.11
17.23
17.21
14.14
14.13
MeO
N3
CF3
EtO2C
CO2Et
26
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

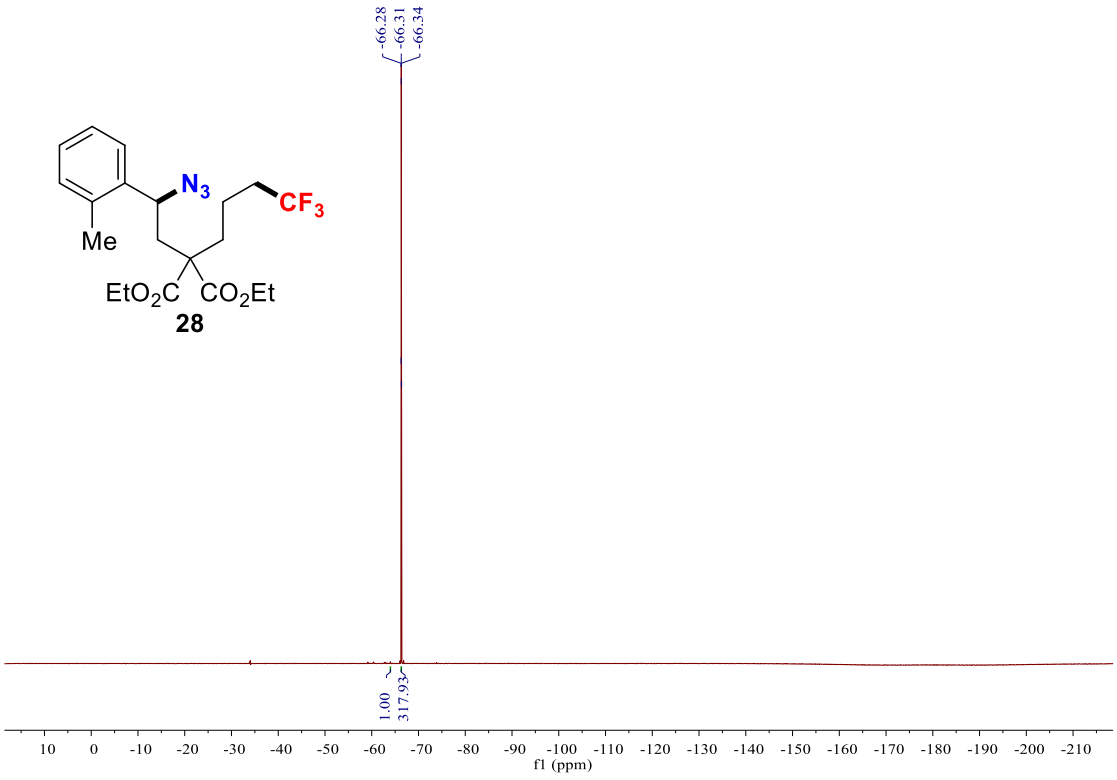

-66.27
-66.29
-66.32
MeO
N3
CF3
EtO2C
CO2Et
26
1.00
32.60
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

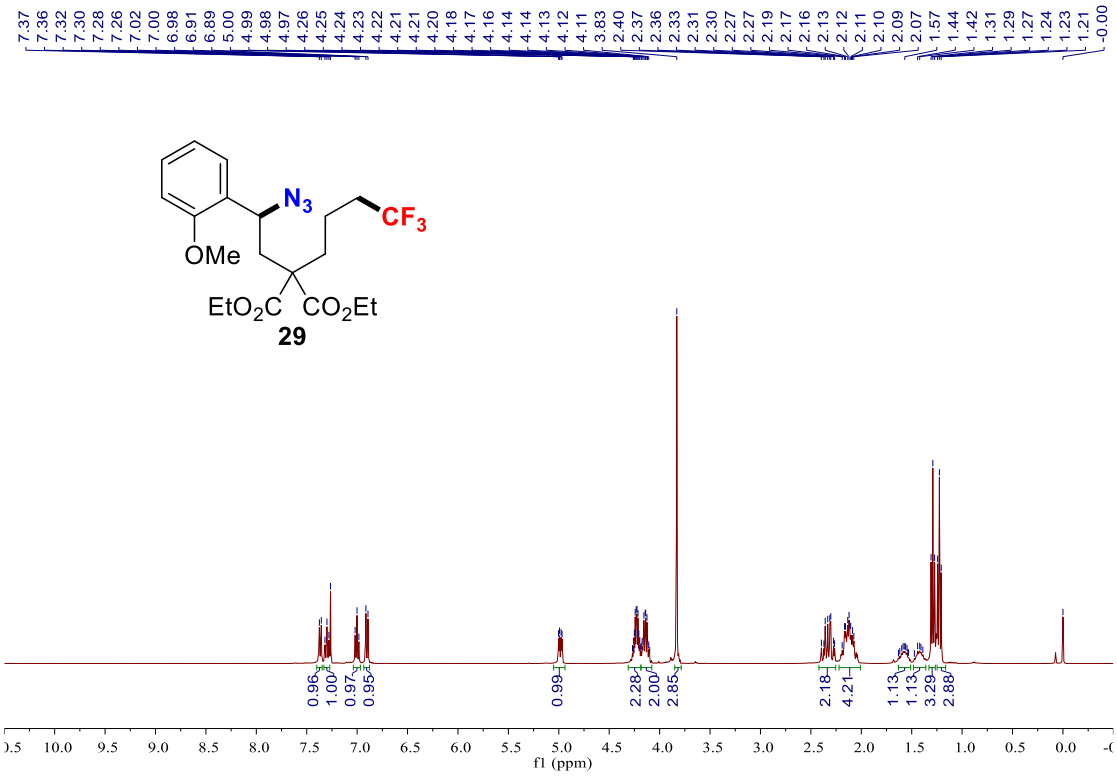

7.49 7.49 7.48 7.47 7.47 7.30 7.28 7.27 7.27 7.26 4.54 4.53 4.51 4.25 4.24 4.24 4.23 4.23 4.22 4.21 4.21 4.20 4.19 4.19 4.19 4.17 4.15 4.14 4.13 2.29 2.27 2.12 2.11 2.11 2.10 2.10 2.09 2.08 2.07 2.05 2.04 2.02 2.01 1.54 1.53 1.52 1.52 1.39 1.38 1.37 1.37 1.36 1.34 1.31 1.29 1.28 1.27 1.27 1.25
Br
N3
CF3
EtO2C CO2Et
27
1.94 2.83 0.96 4.36 2.00 4.12 1.25 1.38 8.17
f1 (ppm)
170.75 170.65 142.07 131.84 131.00 130.69 129.95 128.25 125.58 125.51 123.14 122.76 77.48 77.16 76.84 62.13 61.99 61.87 56.17 39.35 34.34 34.05 33.77 33.48 32.39 17.27 17.24 14.14 14.13
Br
N3
CF3
EtO2C CO2Et
27
f1 (ppm)

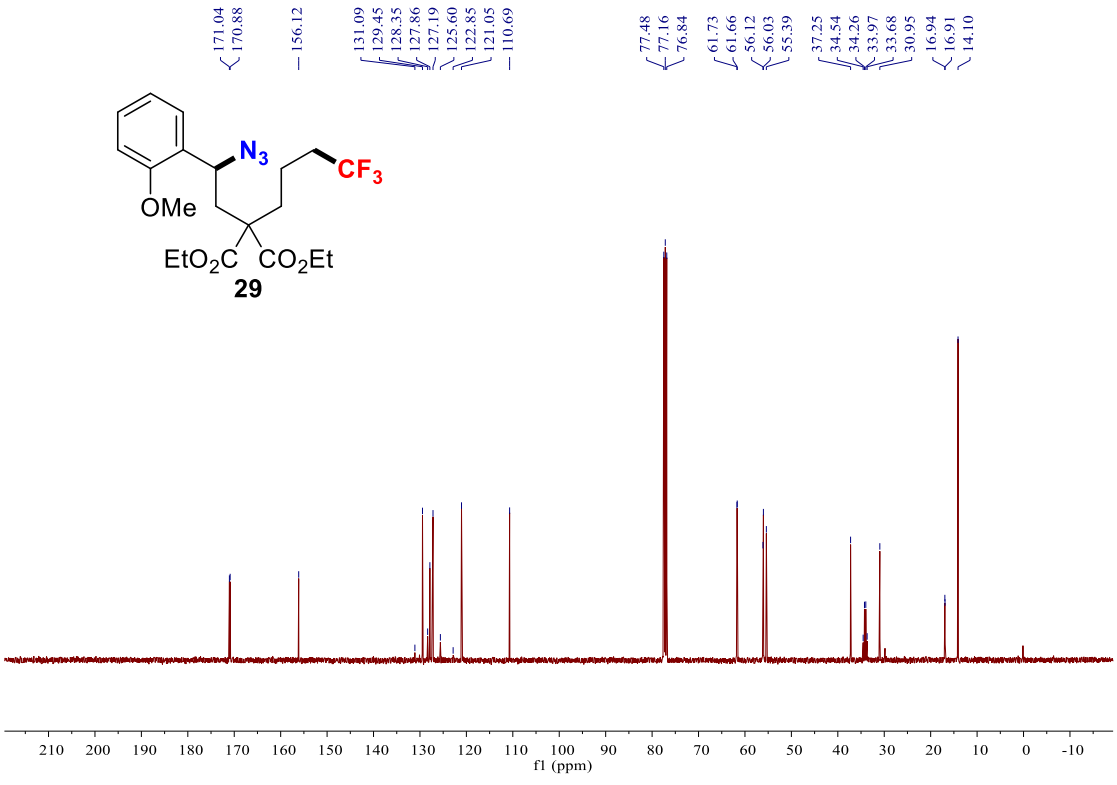

-66.21
-66.24
-66.27
Br
N3
CF3
EtO2C CO2Et
27
1.00
23.13
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)
7.37 7.37 7.35 7.26 7.25 7.24 7.24 7.23 7.23 7.21 7.21 7.20 7.19 4.81 4.80 4.79 4.78 4.24 4.24 4.23 4.22 4.22 4.21 4.20 4.19 4.17 4.17 4.15 4.14 4.13 4.12 4.11 2.43 2.40 2.39 2.36 2.31 2.30 2.27 2.26 2.14 2.13 2.12 2.11 2.09 2.08 2.07 2.05 2.04 2.03 2.01 2.00 1.30 1.28 1.27 1.27 1.25 1.24 0.00

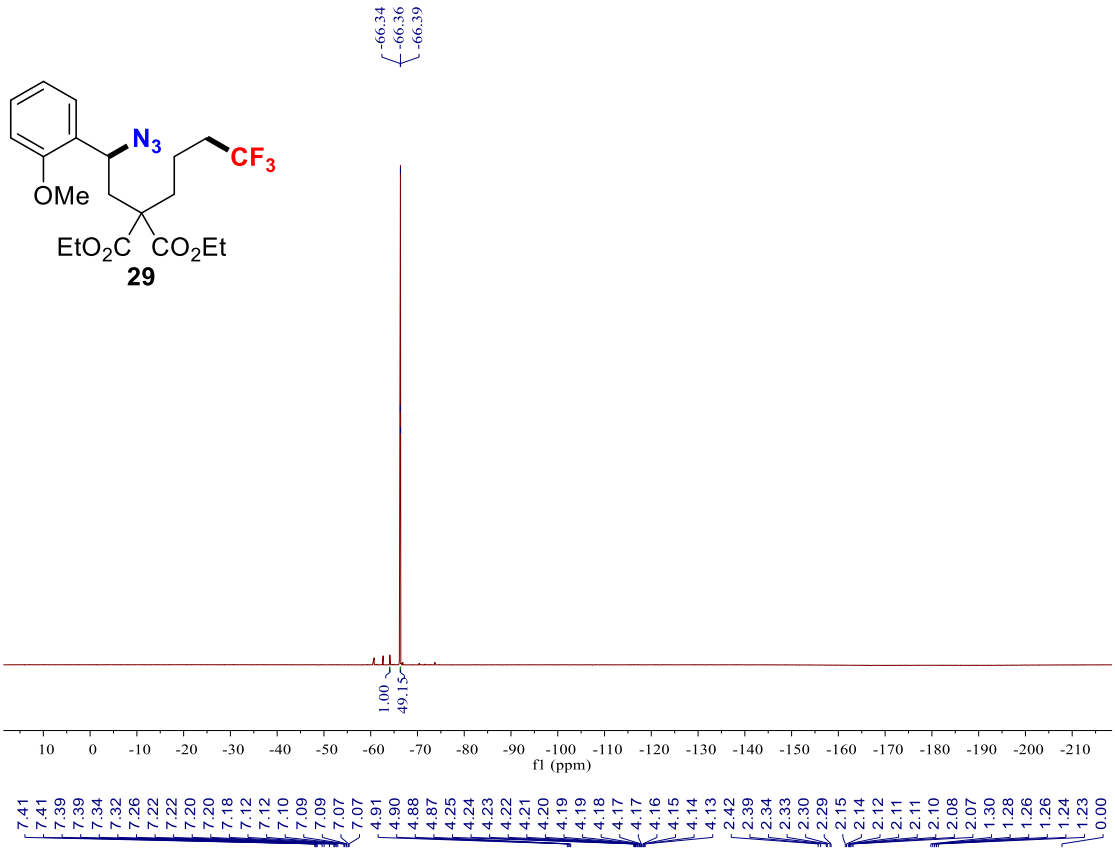

N3
CF3
Me
EtO2C CO2Et
28
0.92
3.73
0.92
4.00
3.69
1.05
4.12
1.08
1.11
6.84
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

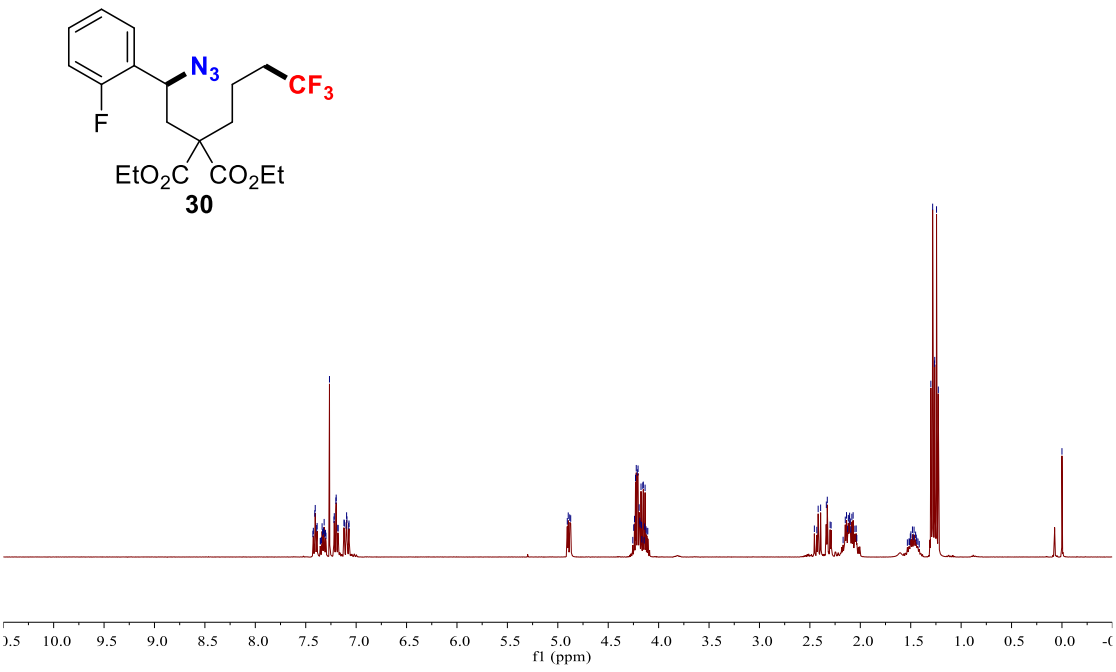

170.93
170.85
137.62
135.36
131.10
128.45
128.28
126.80
126.72
125.53
77.48
77.16
76.84
61.89
61.78
58.75
56.28
38.09
34.39
34.10
33.81
33.53
32.19
19.36
17.29
17.26
14.15
14.12
N3
CF3
Me
EtO2C CO2Et
28
f1 (ppm)

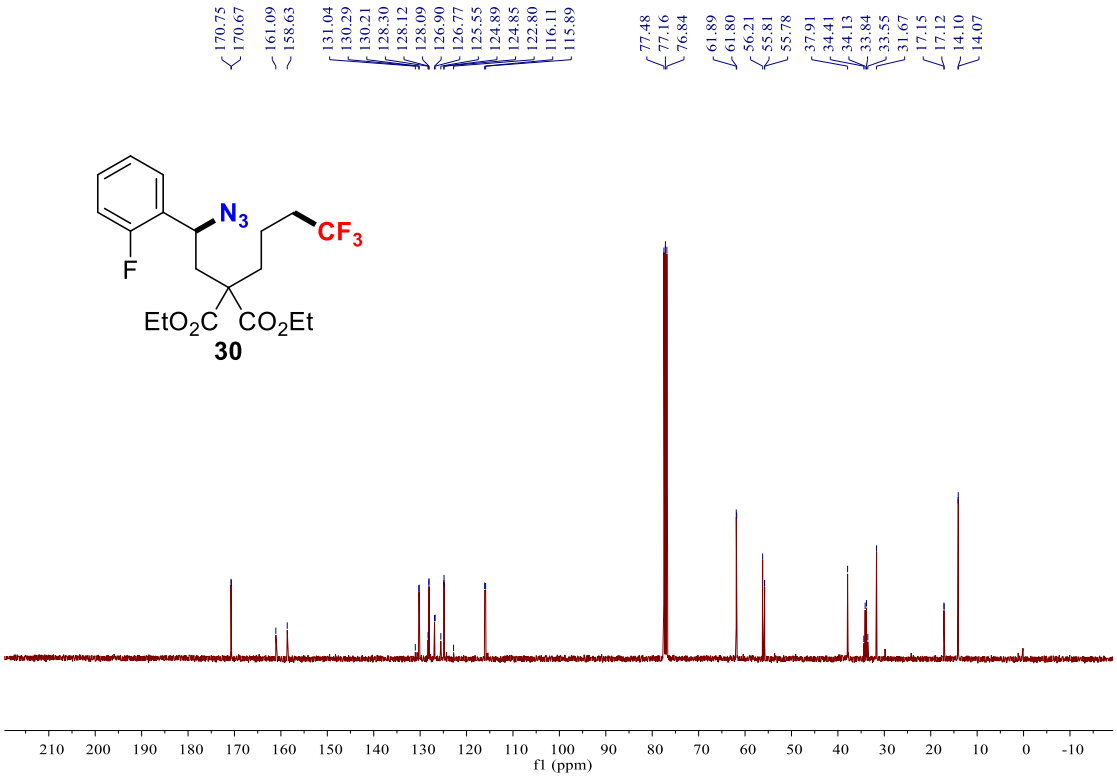

-66.28
-66.31
-66.34
N3
CF3
Me
EtO2C CO2Et
28
1.00
317.93
f1 (ppm)


7.37 7.36 7.32 7.30 7.28 7.26 7.02 7.00 6.98 6.91 6.89 5.00 4.99 4.98 4.97 4.26 4.25 4.24 4.23 4.22 4.21 4.21 4.20 4.18 4.17 4.16 4.14 4.14 4.13 4.12 4.11 3.83 2.40 2.37 2.36 2.33 2.31 2.30 2.27 2.27 2.19 2.17 2.16 2.13 2.12 2.11 2.10 2.09 2.07 1.57 1.44 1.42 1.31 1.29 1.27 1.24 1.23 1.21 -0.00
N3
CF3
OMe
EtO2C CO2Et
29
0.96 1.00 0.97 0.95 0.99 2.28 2.00 2.85 2.18 4.21 1.13 1.13 3.29 2.88
f1 (ppm)


171.04 170.88 156.12 131.09 129.45 128.35 127.86 127.19 125.60 122.85 121.05 110.69 77.48 77.16 76.84 61.73 61.66 56.12 56.03 55.39 37.25 34.54 34.26 33.97 33.68 30.95 16.94 16.91 14.10
N3
CF3
OMe
EtO2C CO2Et
29
f1 (ppm)


N3
CF3
OMe
EtO2C
CO2Et
29
-66.34
-66.36
-66.39
1.00
49.15
f1 (ppm)


N3
CF3
F
EtO2C
CO2Et
30
f1 (ppm)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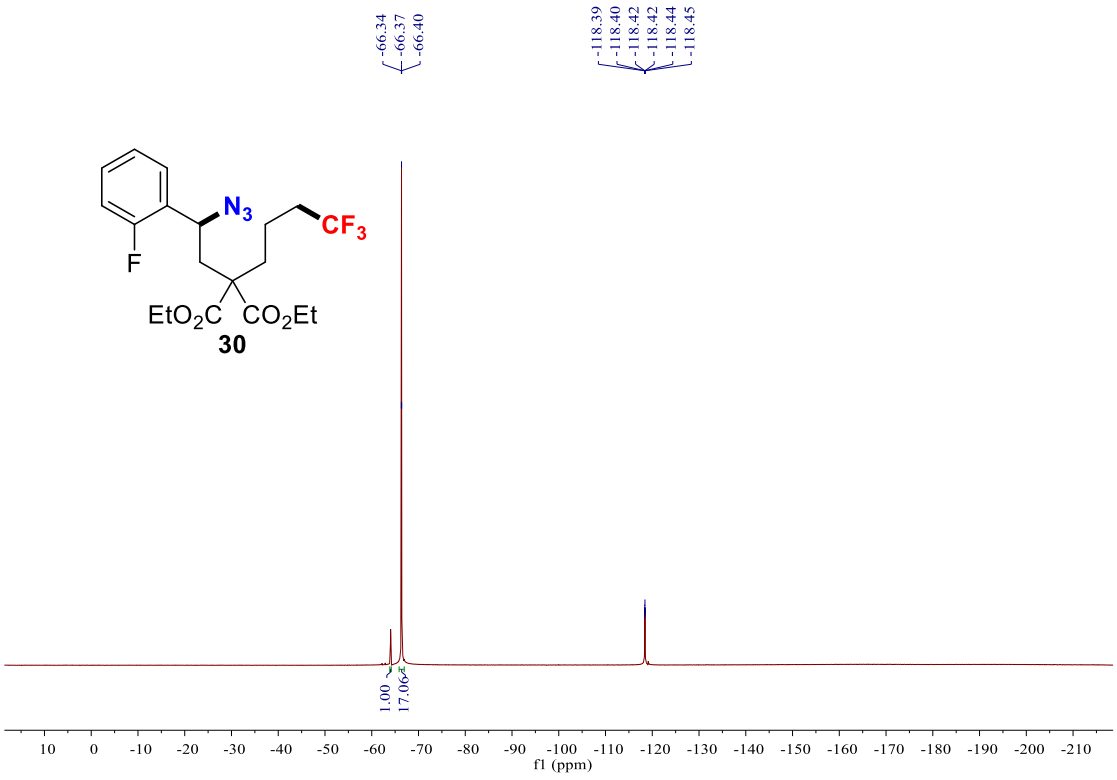
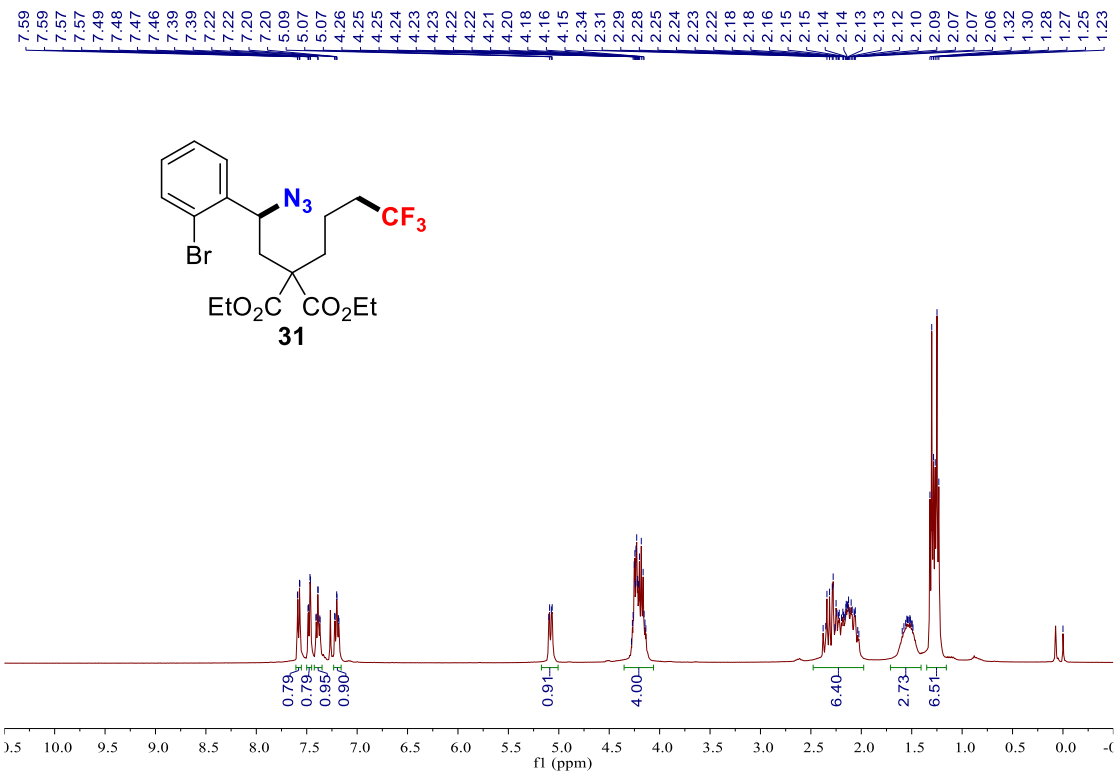
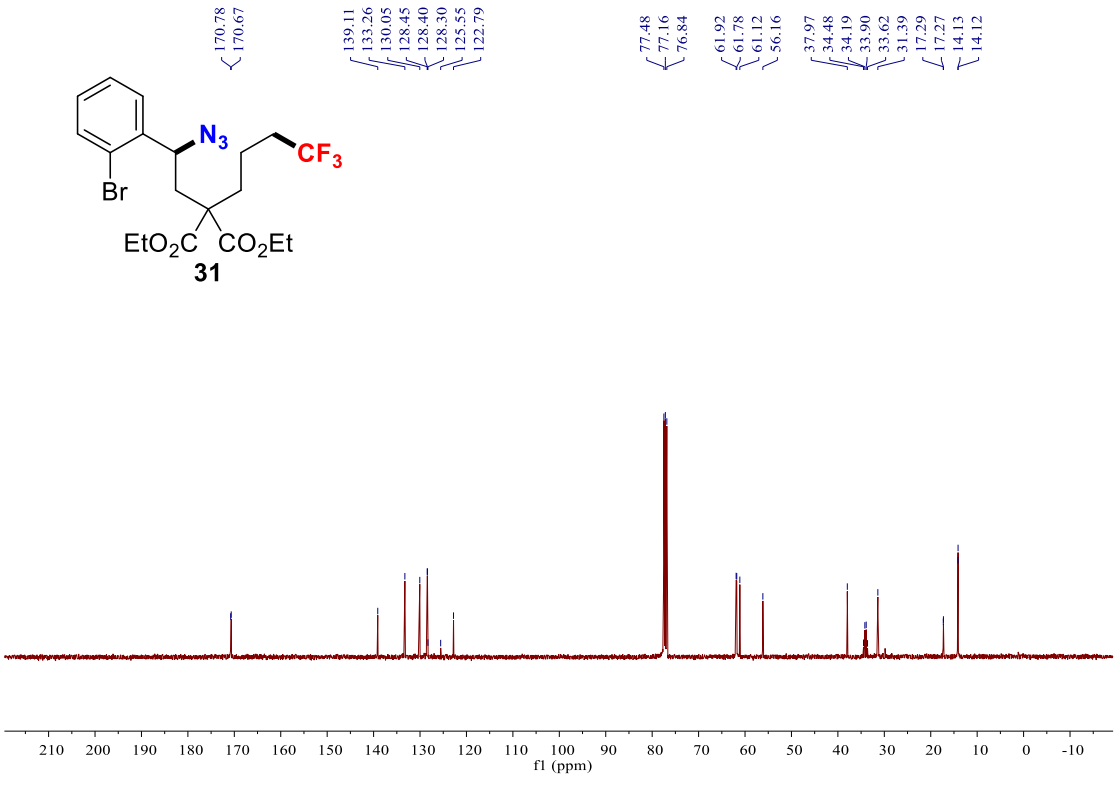
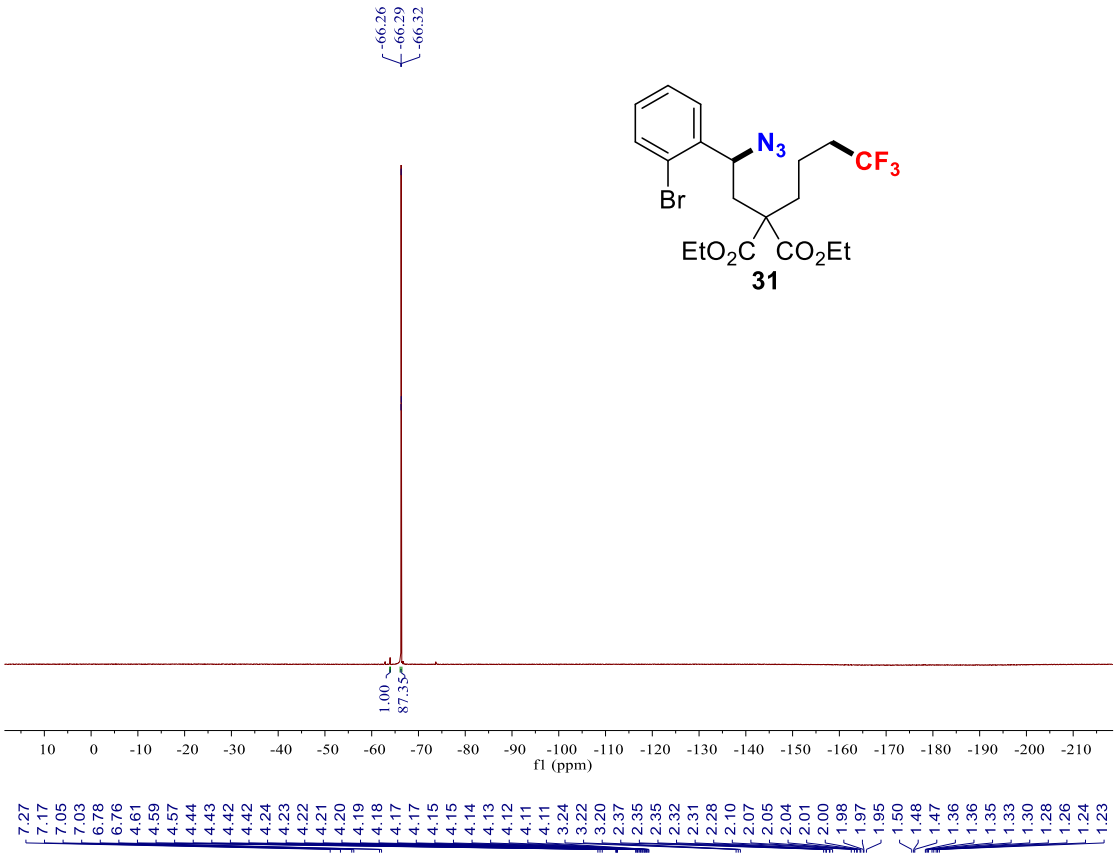
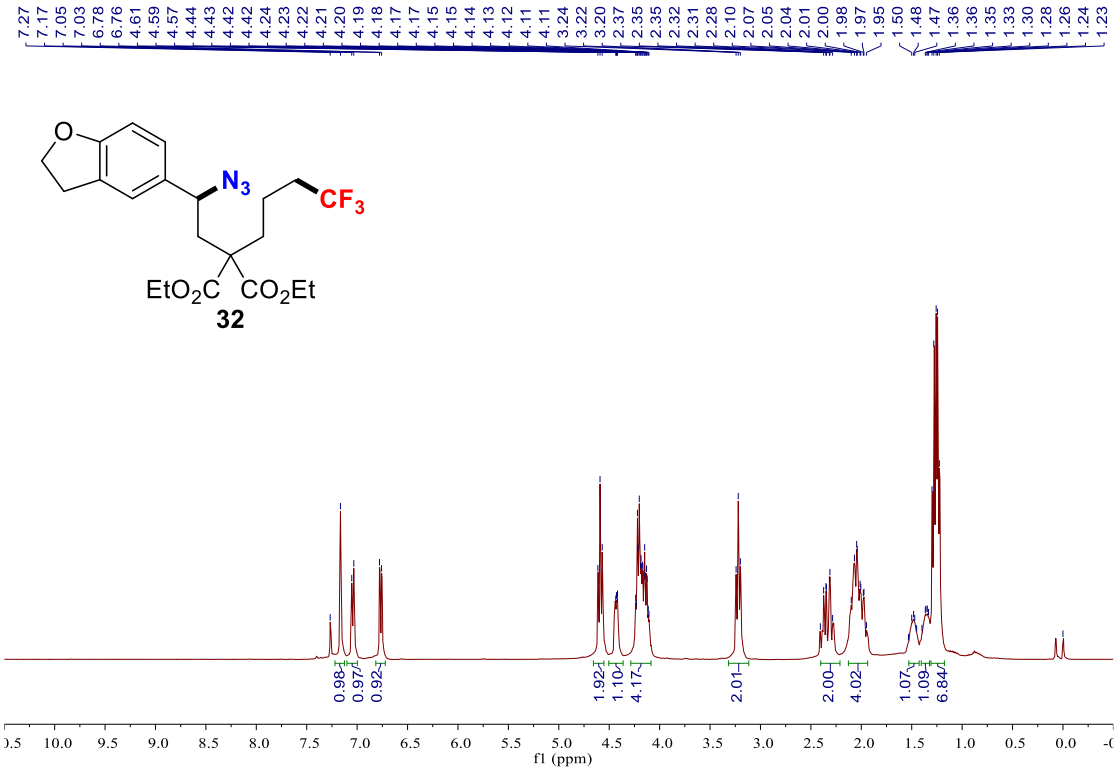
170.67
161.09
158.63
131.04
130.29
130.21
128.30
128.12
128.09
126.90
126.77
125.55
124.89
124.85
122.80
116.11
115.89
77.48
77.16
76.84
61.89
61.80
56.21
55.81
55.78
37.91
34.41
34.13
33.84
33.55
31.67
17.15
17.12
14.10
14.07
N3
CF3
F
EtO2C CO2Et
30
f1 (ppm)

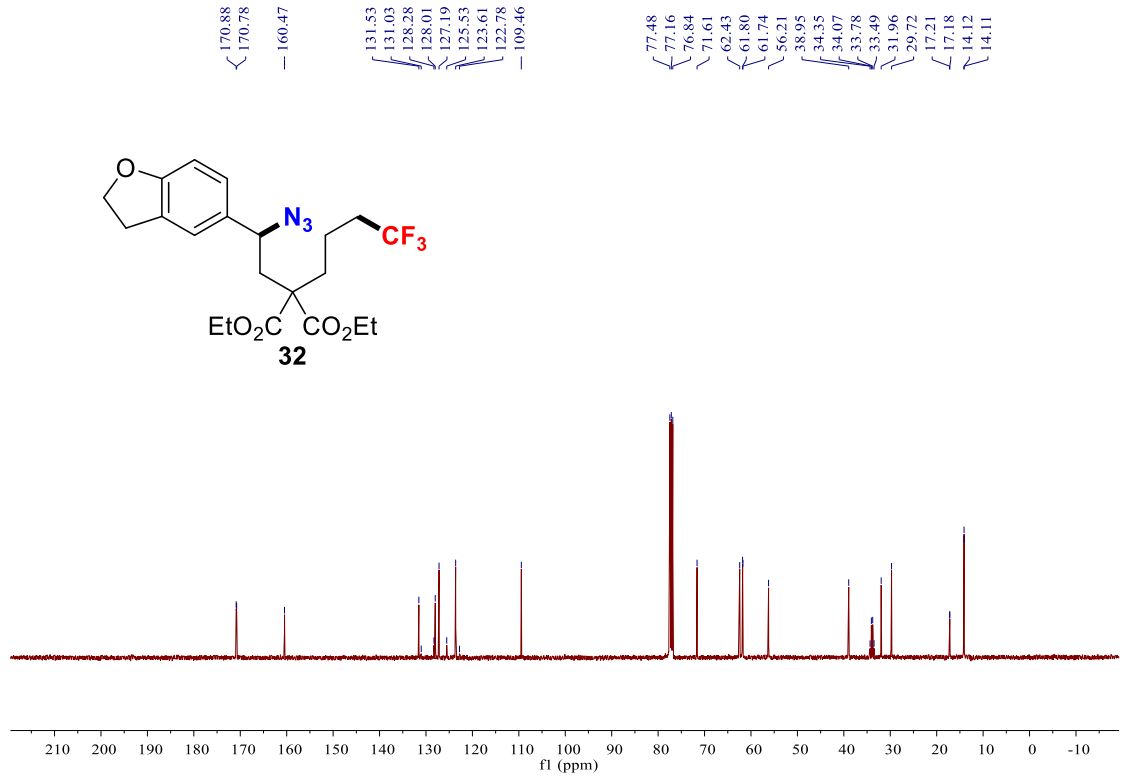

-66.34
-66.37
-66.40
-118.39
-118.40
-118.42
-118.42
-118.44
-118.45
N3
CF3
F
EtO2C CO2Et
30
1.00
17.06
f1 (ppm)


7.59 7.59 7.57 7.57 7.49 7.48 7.47 7.46 7.39 7.39 7.22 7.22 7.20 7.20 5.09 5.07 5.07 4.26 4.25 4.25 4.24 4.23 4.23 4.22 4.22 4.21 4.20 4.18 4.16 4.15 2.34 2.31 2.29 2.28 2.25 2.24 2.23 2.22 2.18 2.18 2.16 2.15 2.15 2.14 2.14 2.13 2.13 2.12 2.10 2.09 2.07 2.07 2.06 1.32 1.30 1.28 1.27 1.25 1.23
N3
CF3
Br
EtO2C CO2Et
31
0.79 0.79 0.95 0.90 0.91 4.00 6.40 2.73 6.51
f1 (ppm)


170.78 170.67 139.11 133.26 130.05 128.45 128.40 128.30 125.55 122.79 77.48 77.16 76.84 61.92 61.78 61.12 56.16 37.97 34.48 34.19 33.90 33.62 31.39 17.29 17.27 14.13 14.12
N3
CF3
Br
EtO2C CO2Et
31
f1 (ppm)


-66.26
-66.29
-66.32
N3
CF3
Br
EtO2C CO2Et
31
1.00
87.35
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


7.27 7.17 7.05 7.03 6.78 6.76 4.61 4.59 4.57 4.44 4.43 4.42 4.42 4.24 4.23 4.22 4.21 4.20 4.19 4.18 4.17 4.17 4.15 4.15 4.14 4.13 4.12 4.11 4.11 3.24 3.22 3.20 2.37 2.35 2.35 2.32 2.31 2.28 2.10 2.07 2.05 2.04 2.01 2.00 1.98 1.97 1.95 1.50 1.48 1.47 1.36 1.36 1.35 1.33 1.30 1.28 1.26 1.24 1.23
O
N3
CF3
EtO2C CO2Et
32
0.98 0.97 0.92 1.92 1.10 4.17 2.01 2.00 4.02 1.07 1.09 6.84
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)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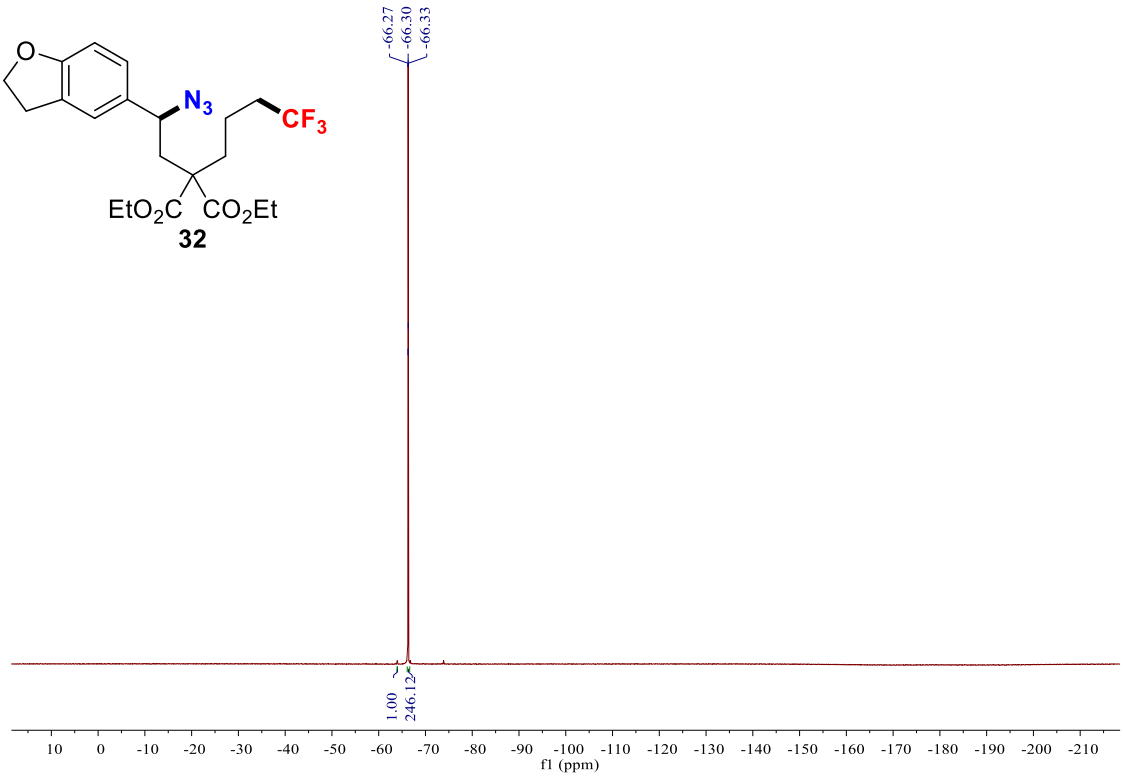
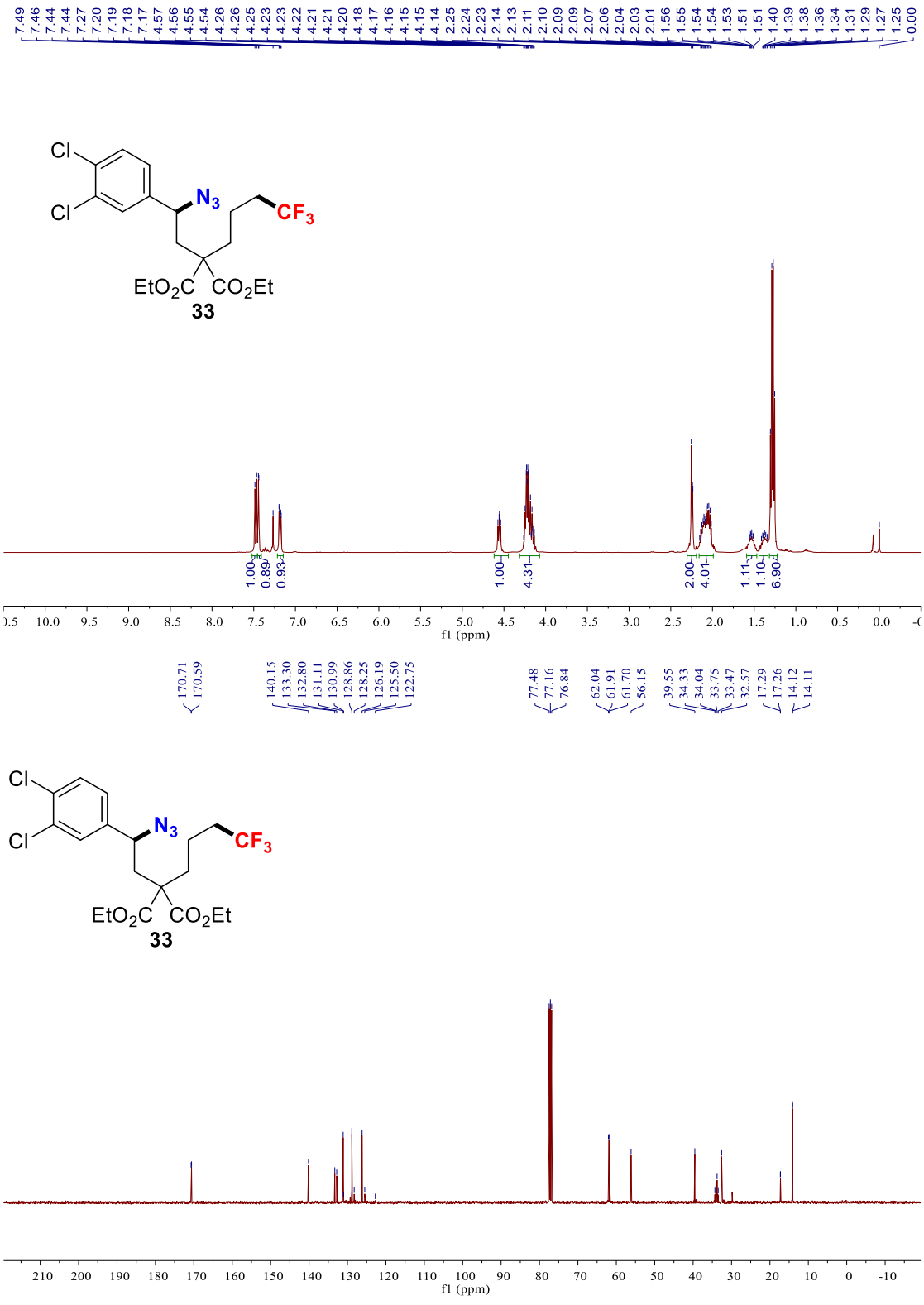
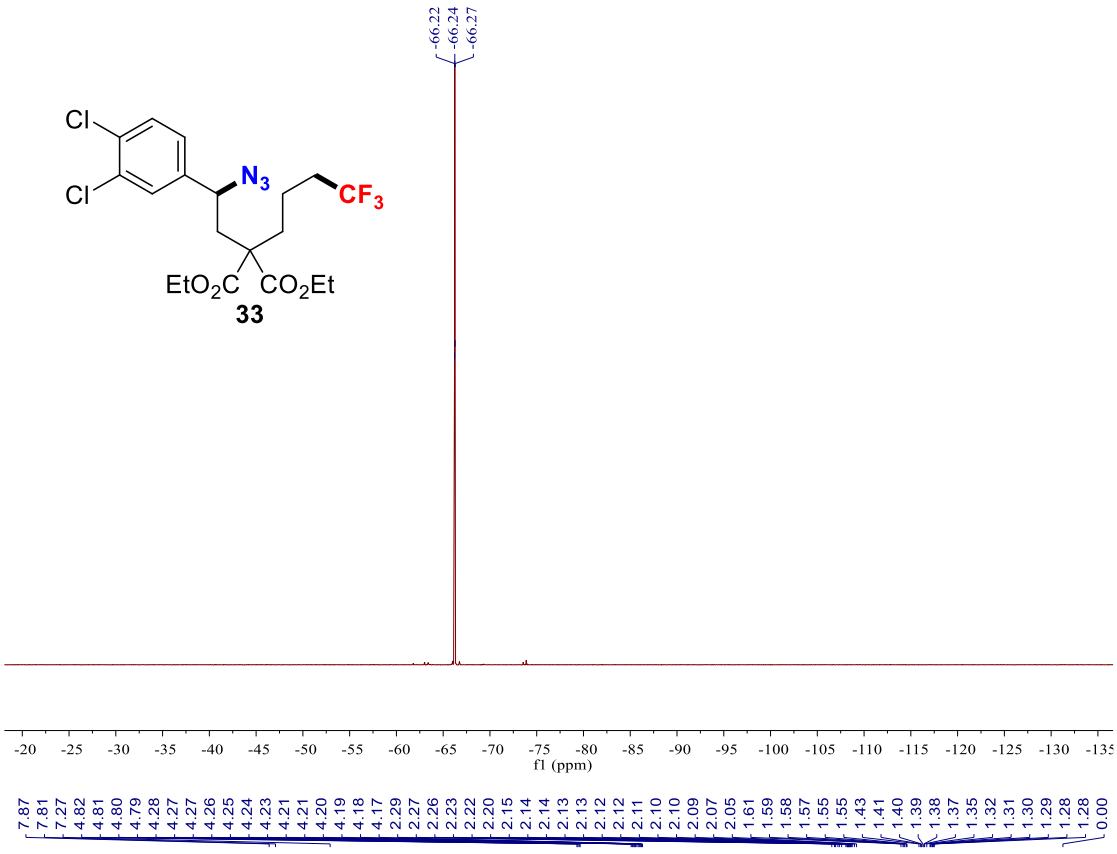
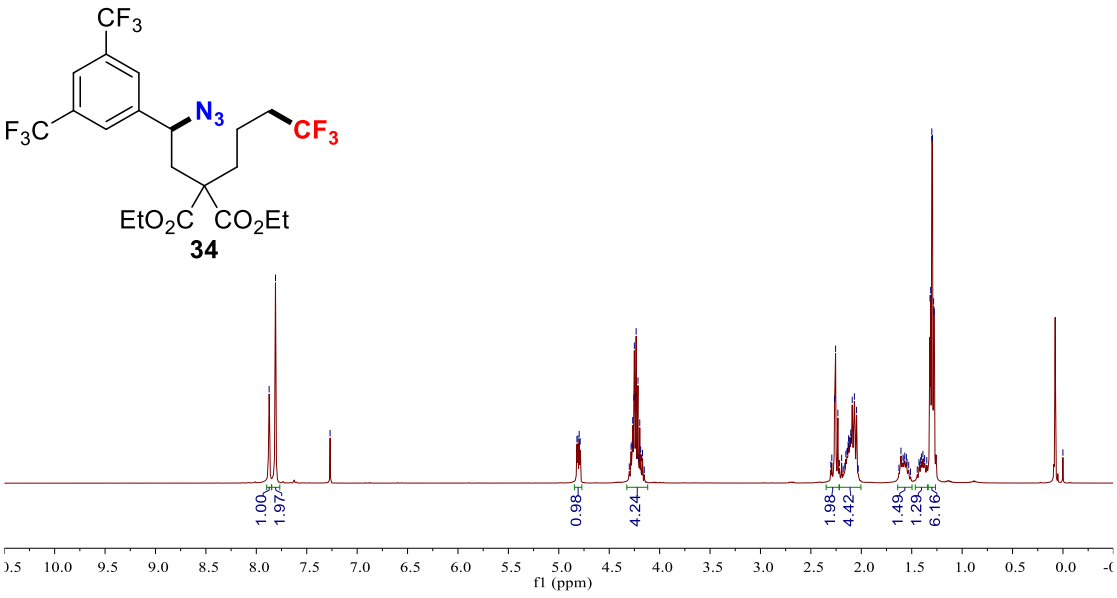
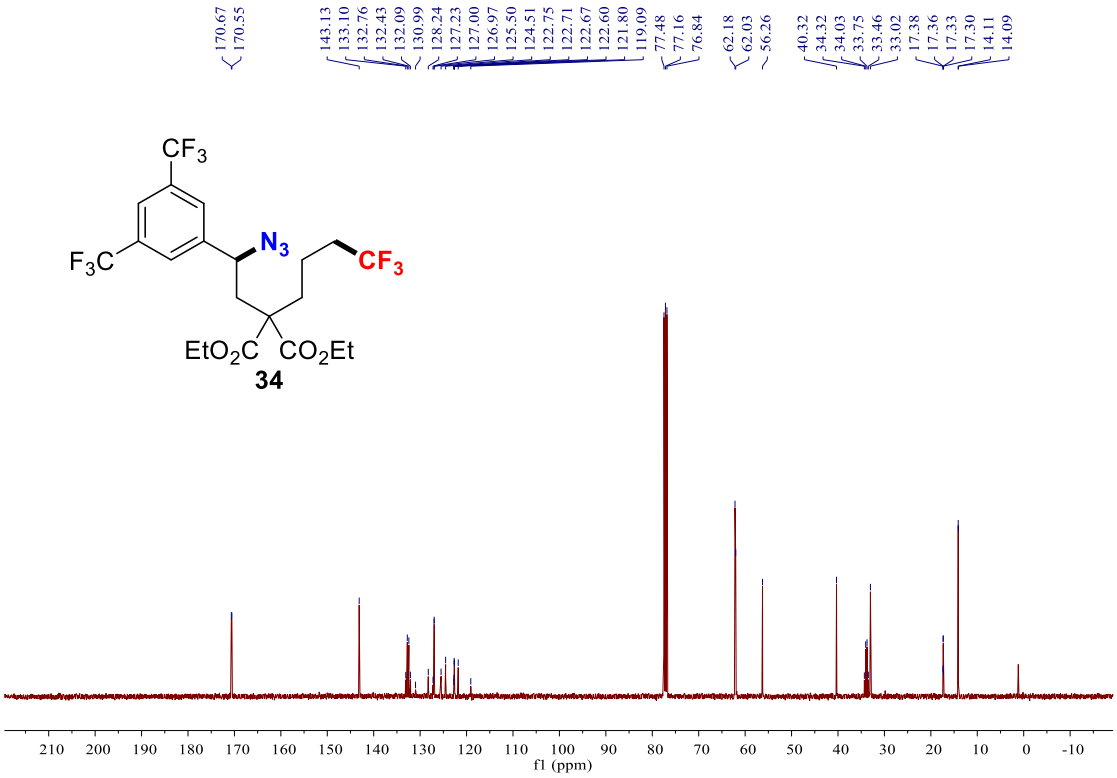
170.78
160.47
131.53
131.03
128.28
128.01
127.19
125.53
123.61
122.78
109.46
77.48
77.16
76.84
71.61
62.43
61.80
61.74
56.21
38.95
34.35
34.07
33.78
33.49
31.96
29.72
17.21
17.18
14.12
14.11
O
N3
CF3
EtO2C
CO2Et
32
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

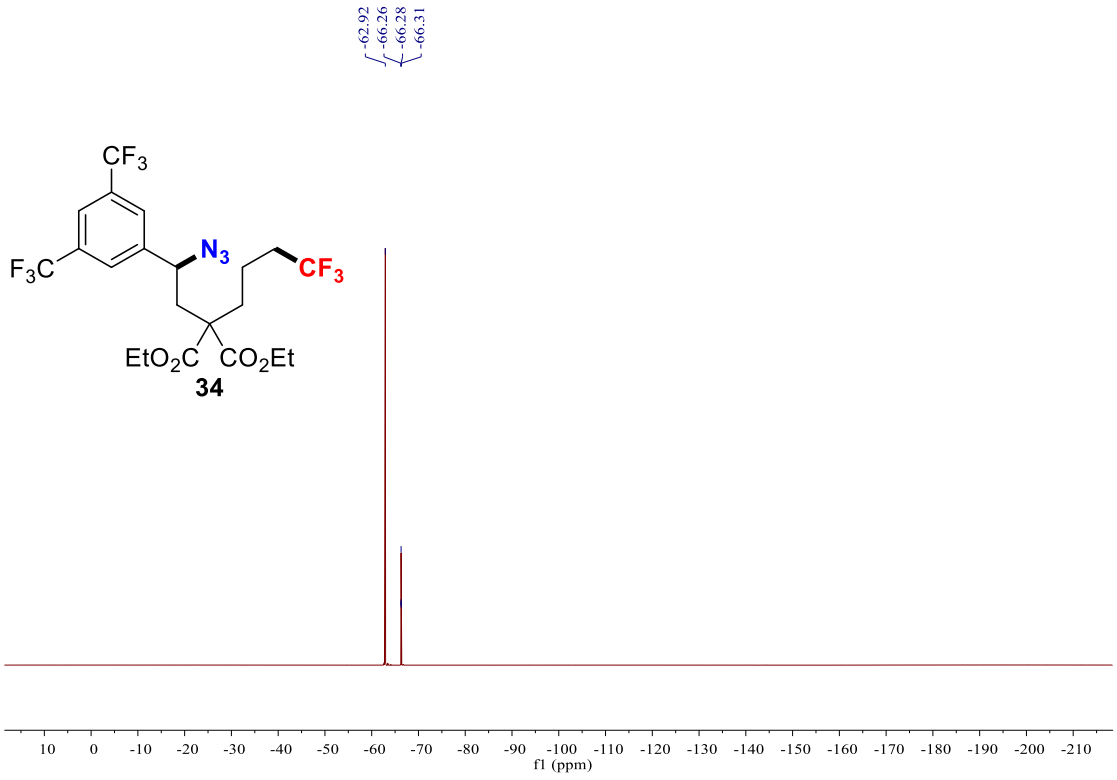

-66.27
-66.30
-66.33
O
N3
CF3
EtO2C
CO2Et
32
1.00
246.12
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

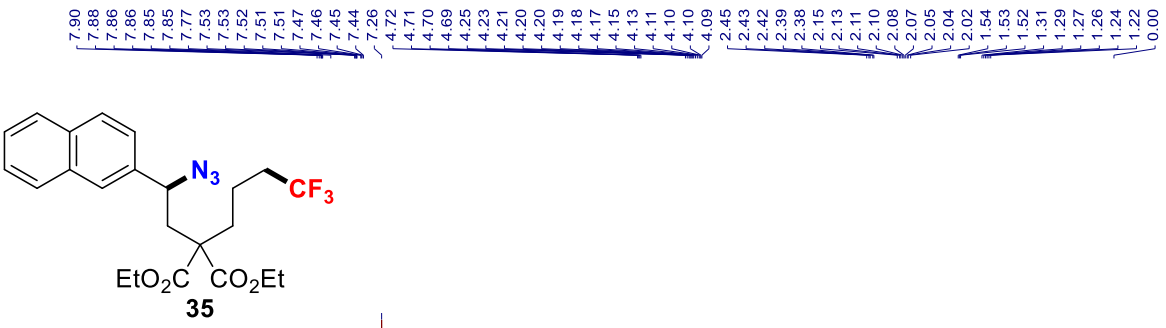

7.49 7.46 7.44 7.44 7.27 7.20 7.19 7.18 7.17 4.57 4.56 4.55 4.54 4.26 4.26 4.25 4.23 4.23 4.22 4.21 4.21 4.20 4.18 4.17 4.16 4.15 4.15 4.14 2.25 2.24 2.23 2.14 2.13 2.11 2.10 2.09 2.09 2.07 2.06 2.04 2.03 2.01 1.56 1.55 1.54 1.54 1.53 1.51 1.51 1.40 1.39 1.38 1.36 1.34 1.31 1.29 1.27 1.25 0.00
Cl
Cl
N3
CF3
EtO2C
CO2Et
33
1.00 0.89 0.93 1.00 4.31 2.00 4.01 1.11 1.10 6.90
f1 (ppm)
170.71 170.59 140.15 133.30 132.80 131.11 130.99 128.86 128.25 126.19 125.50 122.75 77.48 77.16 76.84 62.04 61.91 61.70 56.15 39.55 34.33 34.04 33.75 33.47 32.57 17.29 17.26 14.12 14.11
Cl
Cl
N3
CF3
EtO2C
CO2Et
33
f1 (ppm)


-66.22
-66.24
-66.27
Cl
Cl
N3
CF3
EtO2C
CO2Et
33
fl (ppm)


CF3
F3C
N3
CF3
EtO2C
CO2Et
34
1.00
1.97
0.98
4.24
1.98
4.42
1.49
1.29
6.16
fl (ppm)

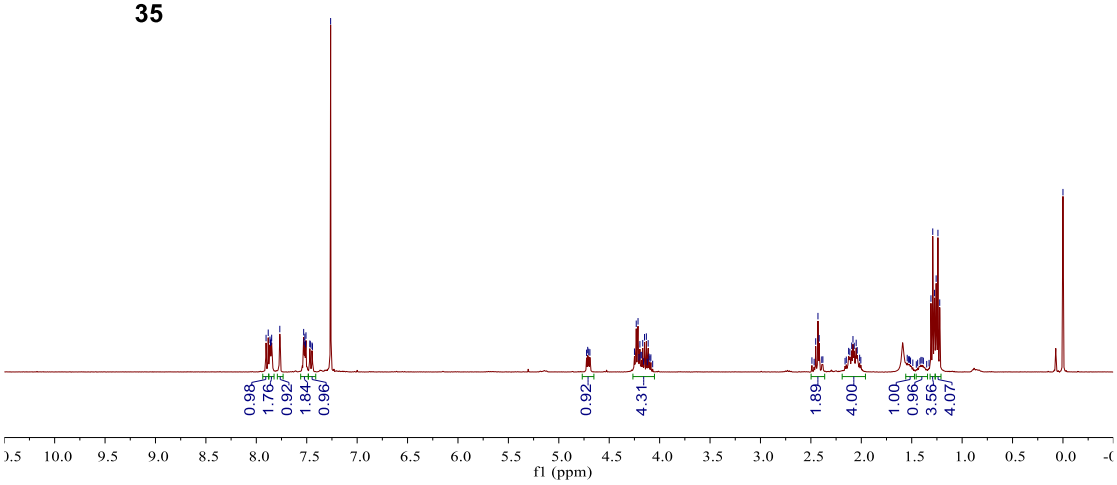

170.67
170.55
143.13
133.10
132.76
132.43
132.09
130.99
128.24
127.23
127.00
126.97
125.50
124.51
122.75
122.71
122.67
122.60
121.80
119.09
77.48
77.16
76.84
62.18
62.03
56.26
40.32
34.32
34.03
33.75
33.46
33.02
17.38
17.36
17.33
17.30
14.11
14.09
CF3
F3C
N3
CF3
EtO2C
CO2Et
34
f1 (ppm)


-62.92
-66.26
-66.28
-66.31
CF3
F3C
N3
CF3
EtO2C
CO2Et
34
f1 (ppm)


7.90
7.88
7.86
7.86
7.85
7.85
7.77
7.53
7.53
7.52
7.51
7.51
7.47
7.46
7.45
7.44
7.26
4.72
4.71
4.70
4.69
4.25
4.23
4.21
4.20
4.20
4.19
4.18
4.17
4.15
4.13
4.11
4.10
4.10
4.09
2.45
2.43
2.42
2.39
2.38
2.15
2.13
2.11
2.10
2.08
2.07
2.05
2.04
2.02
1.54
1.53
1.52
1.31
1.29
1.27
1.26
1.24
1.22
0.00

N3
CF3
EtO2C
CO2Et

35


0.98
1.76
0.92
1.84
0.96
0.92
4.31
1.89
4.00
1.00
0.96
3.56
4.07
f1 (ppm)


170.91
170.80
136.91
133.37
133.23
130.82
129.21
128.28
128.18
127.88
126.76
126.66
126.15
125.86
124.41
123.35
77.48
77.16
76.84
62.85
61.90
61.82
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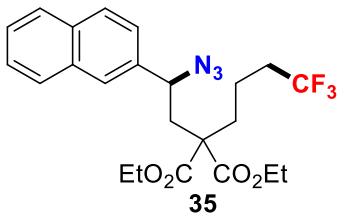
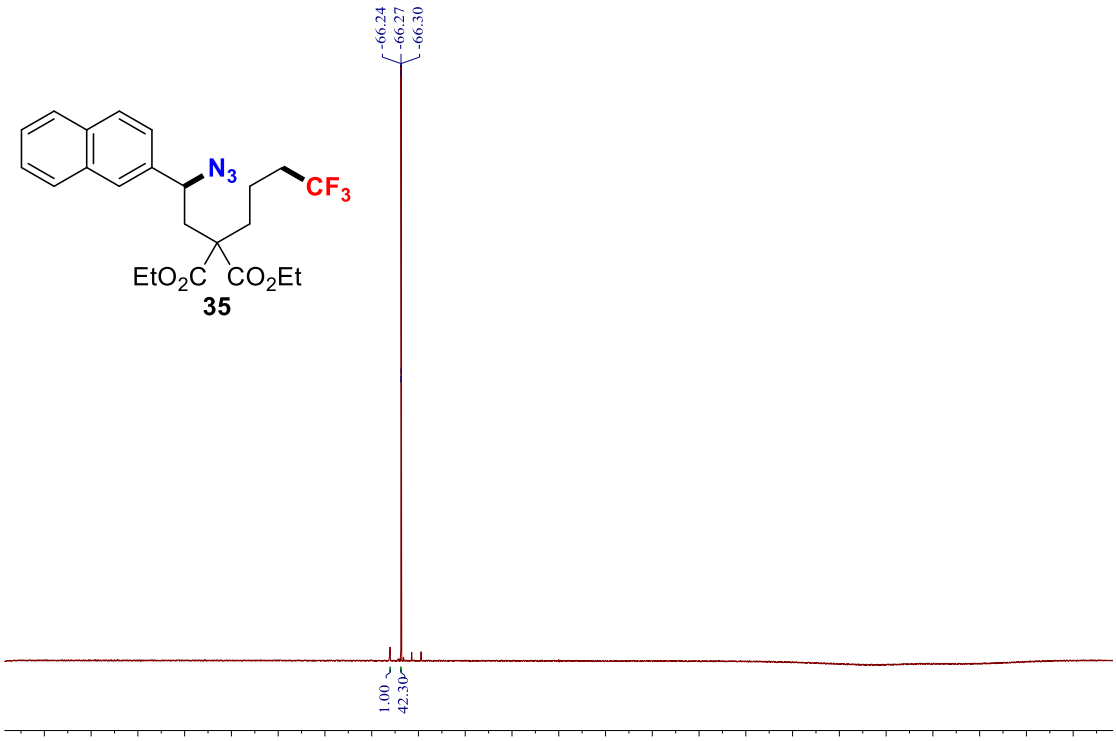
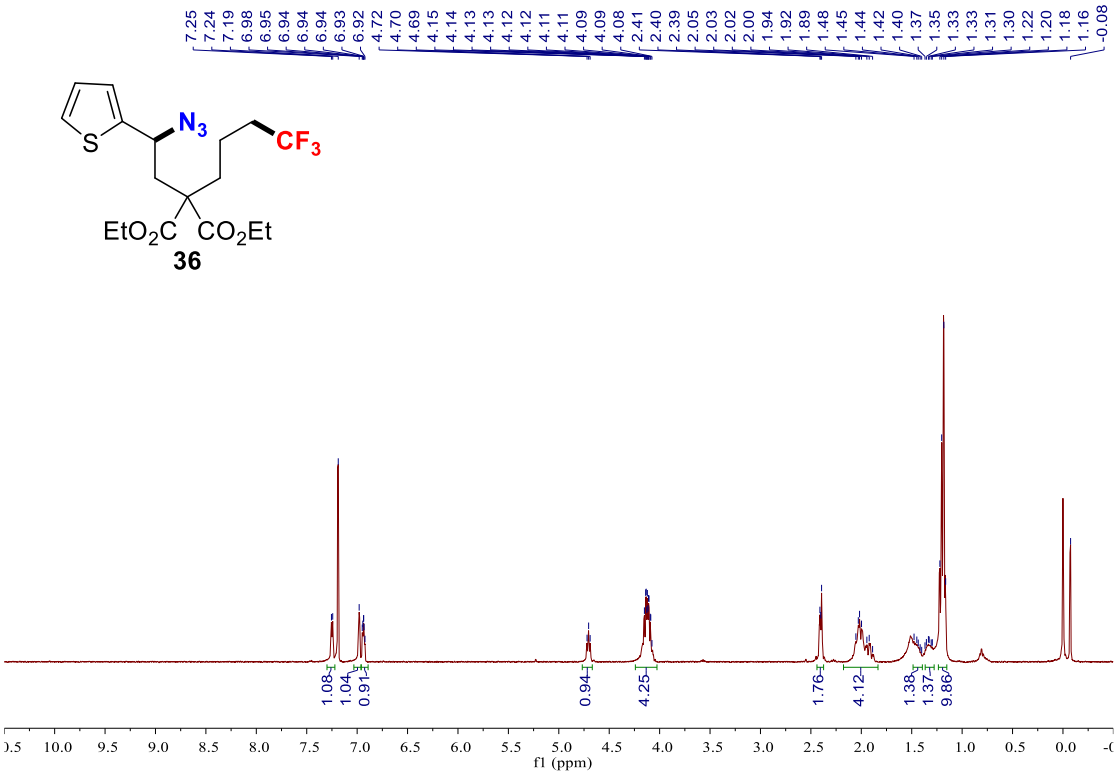
33.79
33.50
32.24
17.28
17.25
14.16
14.12

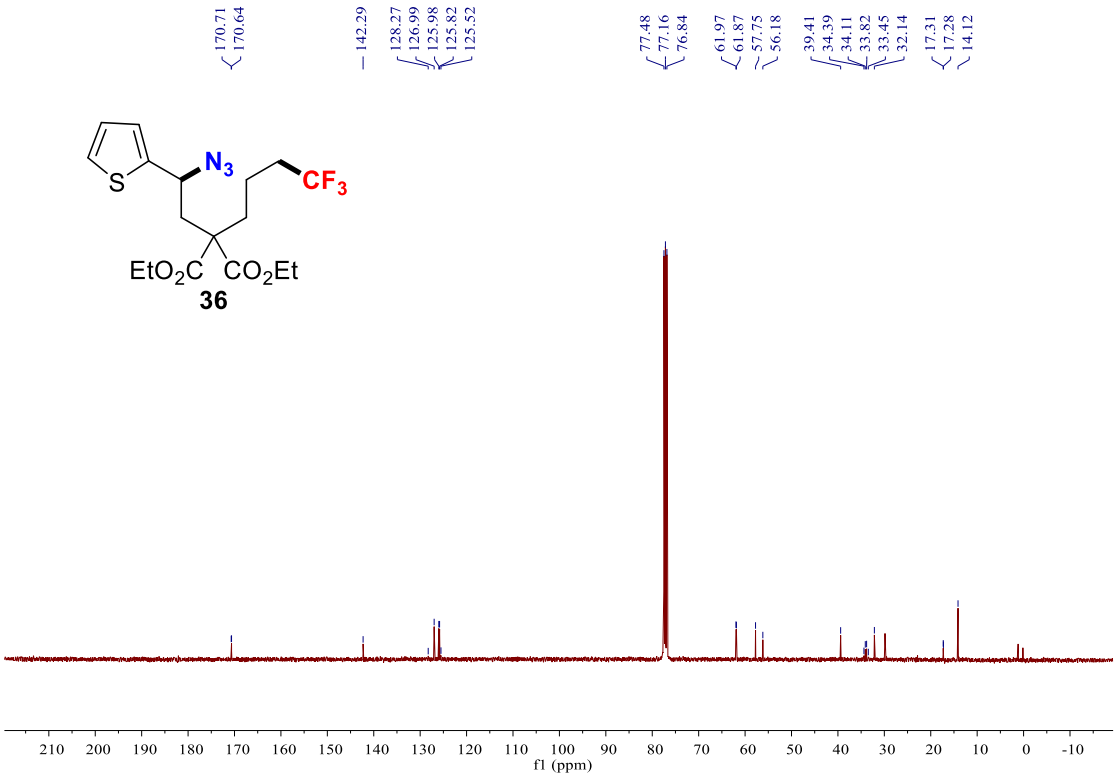

N3
CF3
EtO2C
CO2Et

35

f1 (ppm)


-66.24
-66.27
-66.30
N3
CF3
EtO2C CO2Et
35
1.00
42.30
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


7.25 7.24 7.19 6.98 6.95 6.94 6.94 6.94 6.93 6.92 4.72 4.70 4.69 4.15 4.14 4.13 4.12 4.12 4.11 4.11 4.09 4.09 4.08 2.41 2.40 2.39 2.05 2.03 2.02 2.00 1.94 1.92 1.89 1.48 1.45 1.44 1.42 1.40 1.37 1.35 1.33 1.33 1.31 1.30 1.22 1.20 1.18 1.16 -0.08
N3
CF3
S
EtO2C CO2Et
36
1.08 1.04 0.91 0.94 4.25 1.76 4.12 1.38 1.37 9.86
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)


170.71
170.64
142.29
128.27
126.99
125.98
125.82
125.52
77.48
77.16
76.84
61.97
61.87
57.75
56.18
39.41
34.39
34.11
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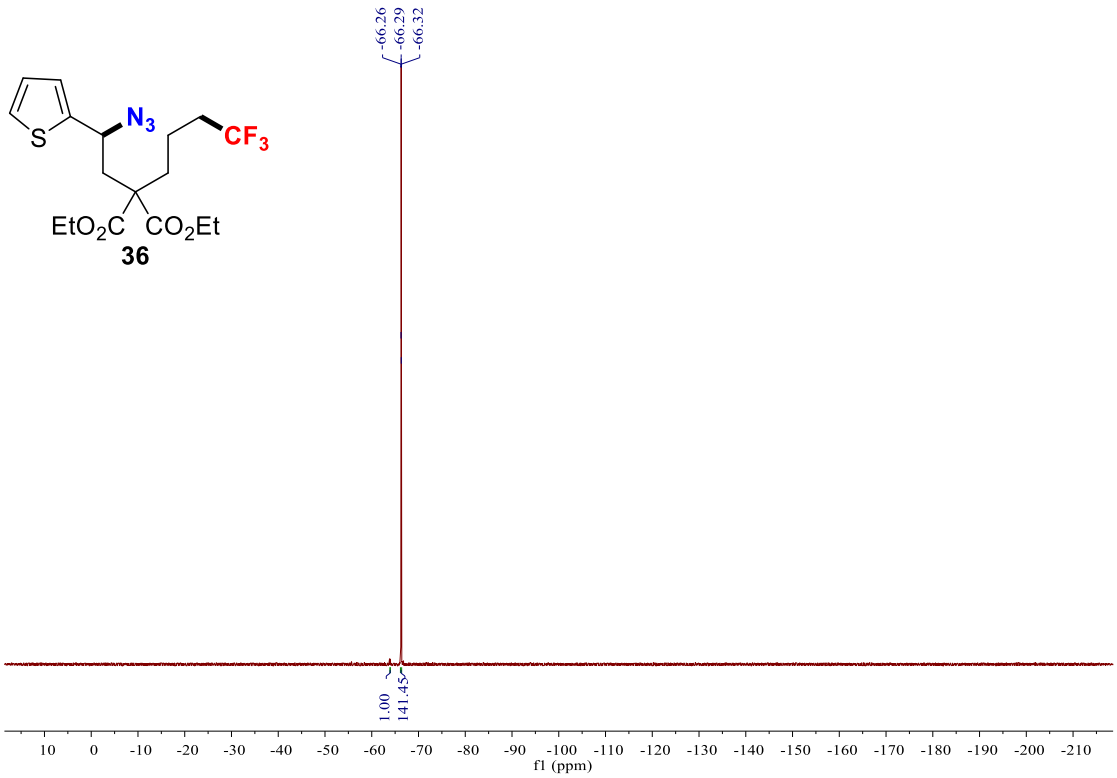
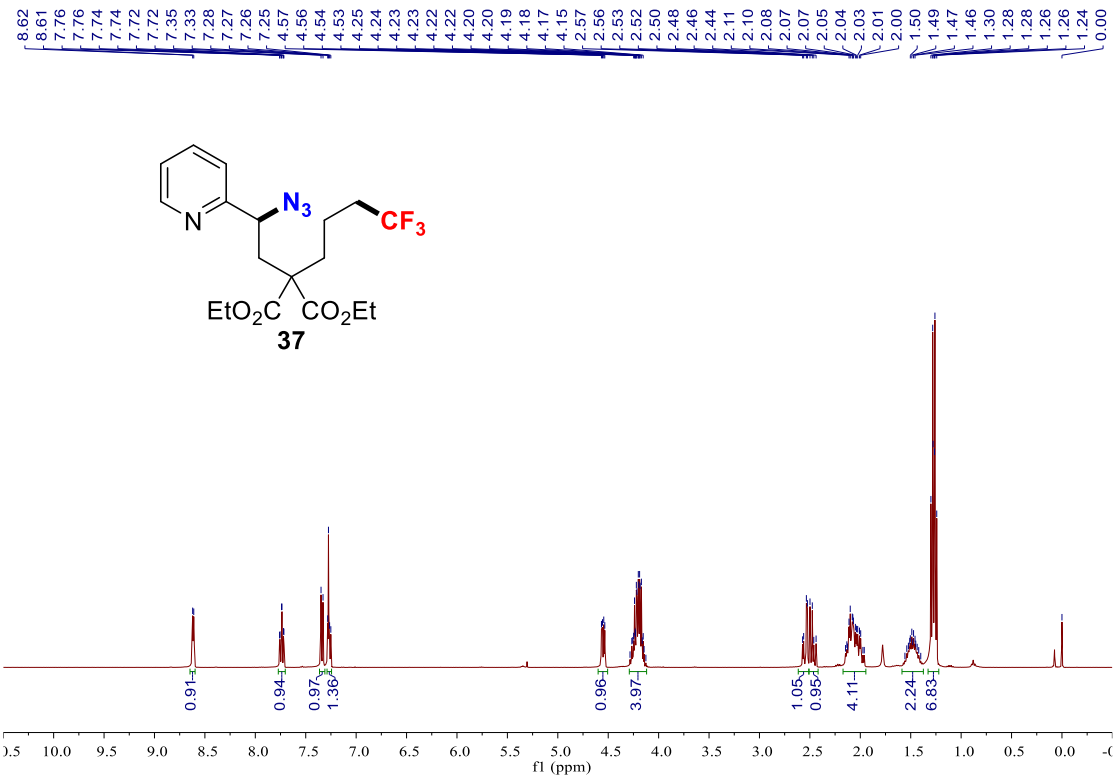
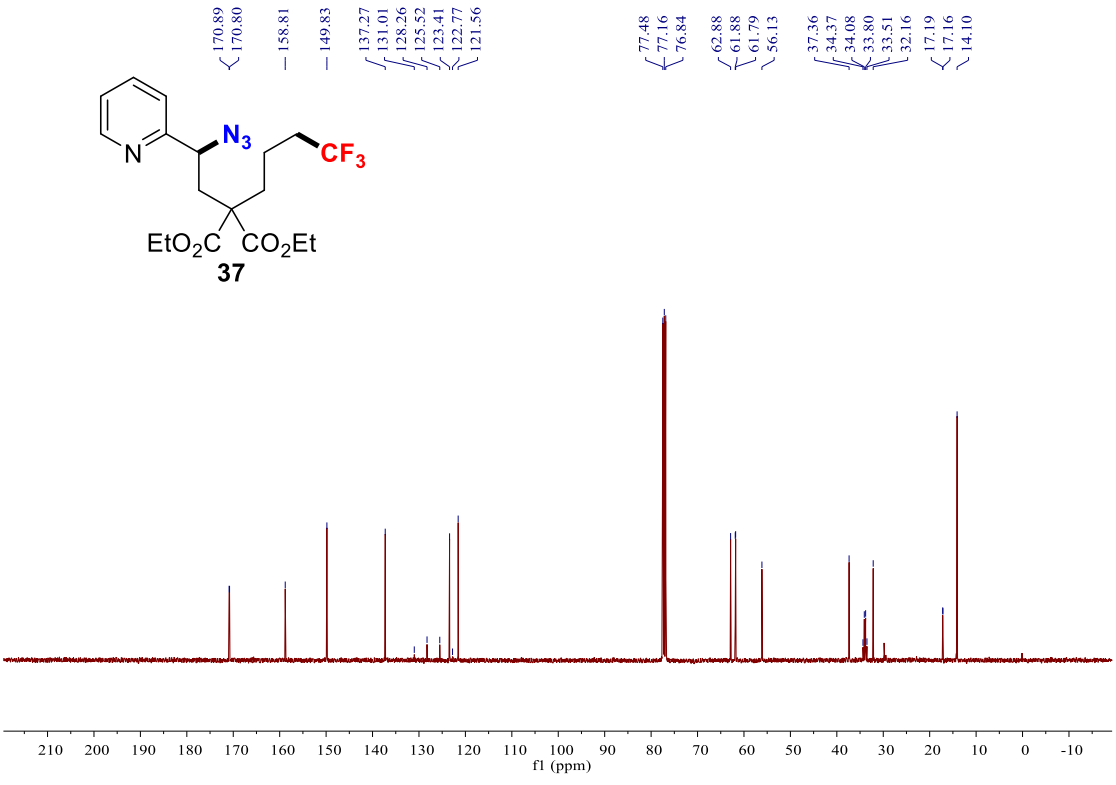
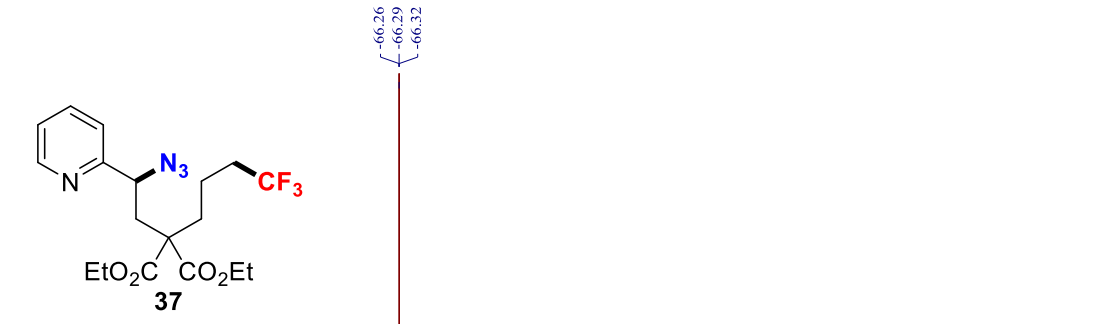
17.31
17.28
14.12
N3
CF3
S
EtO2C
CO2Et
36
f1 (ppm)

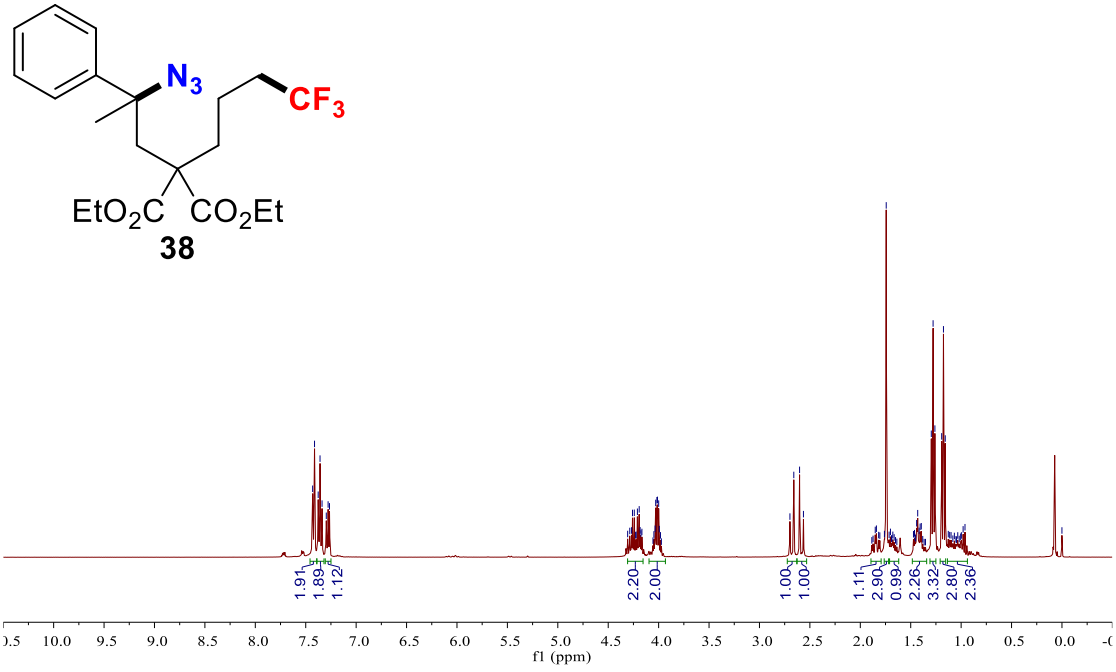

-66.26
-66.29
-66.32
N3
CF3
S
EtO2C
CO2Et
36
1.00
141.45
f1 (ppm)

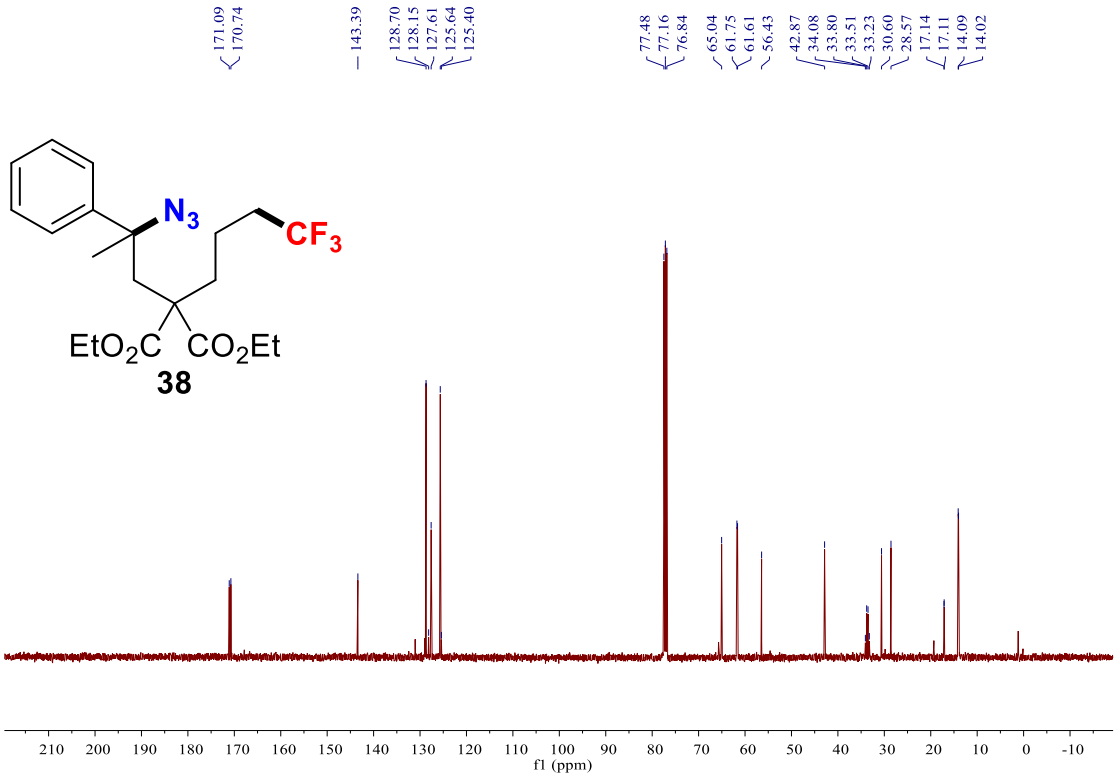

8.62 8.61 7.76 7.76 7.74 7.74 7.72 7.72 7.35 7.33 7.28 7.27 7.26 7.25 4.57 4.56 4.54 4.53 4.25 4.24 4.23 4.23 4.22 4.22 4.20 4.20 4.19 4.18 4.17 4.15 2.57 2.56 2.53 2.52 2.50 2.48 2.46 2.44 2.11 2.10 2.08 2.07 2.07 2.05 2.04 2.03 2.01 2.00 1.50 1.49 1.47 1.46 1.30 1.28 1.28 1.26 1.26 1.24 0.00
N
N3
CF3
EtO2C CO2Et
37
0.91 0.94 0.97 1.36 0.96 3.97 1.05 0.95 4.11 2.24 6.83
f1 (ppm)

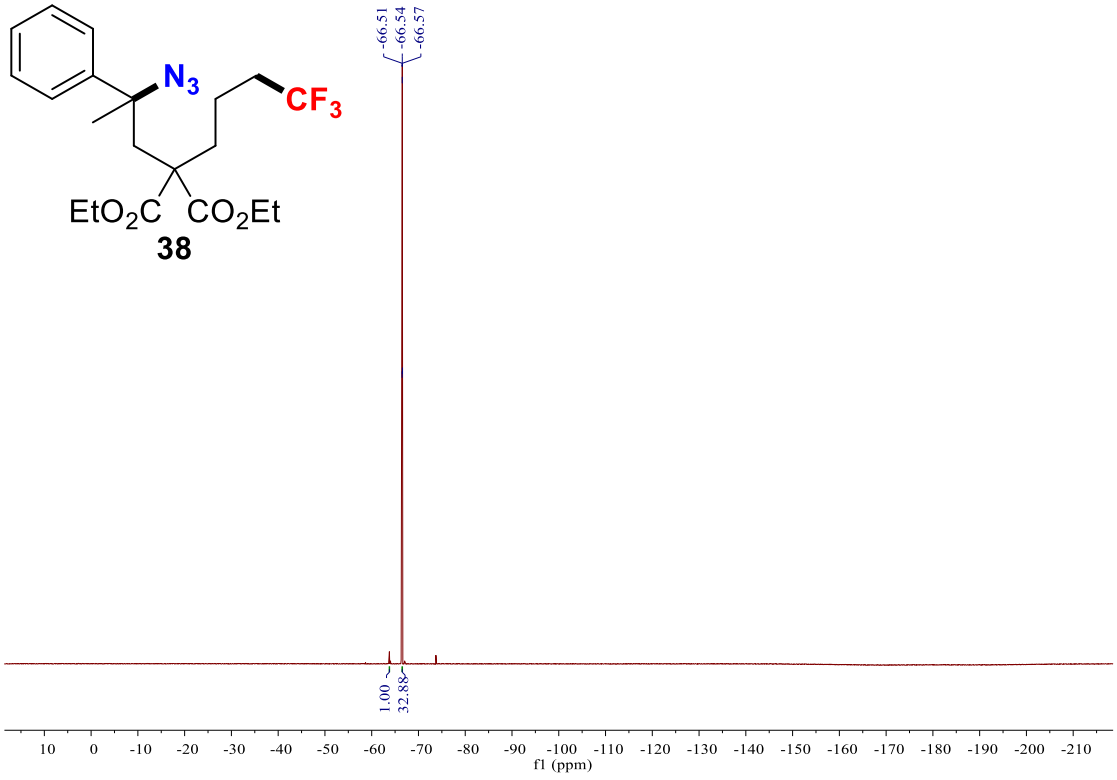

170.89 170.80 158.81 149.83 137.27 131.01 128.26 125.52 123.41 122.77 121.56 77.48 77.16 76.84 62.88 61.88 61.79 56.13 37.36 34.37 34.08 33.80 33.51 32.16 17.19 17.16 14.10
N
N3
CF3
EtO2C CO2Et
37
f1 (ppm)

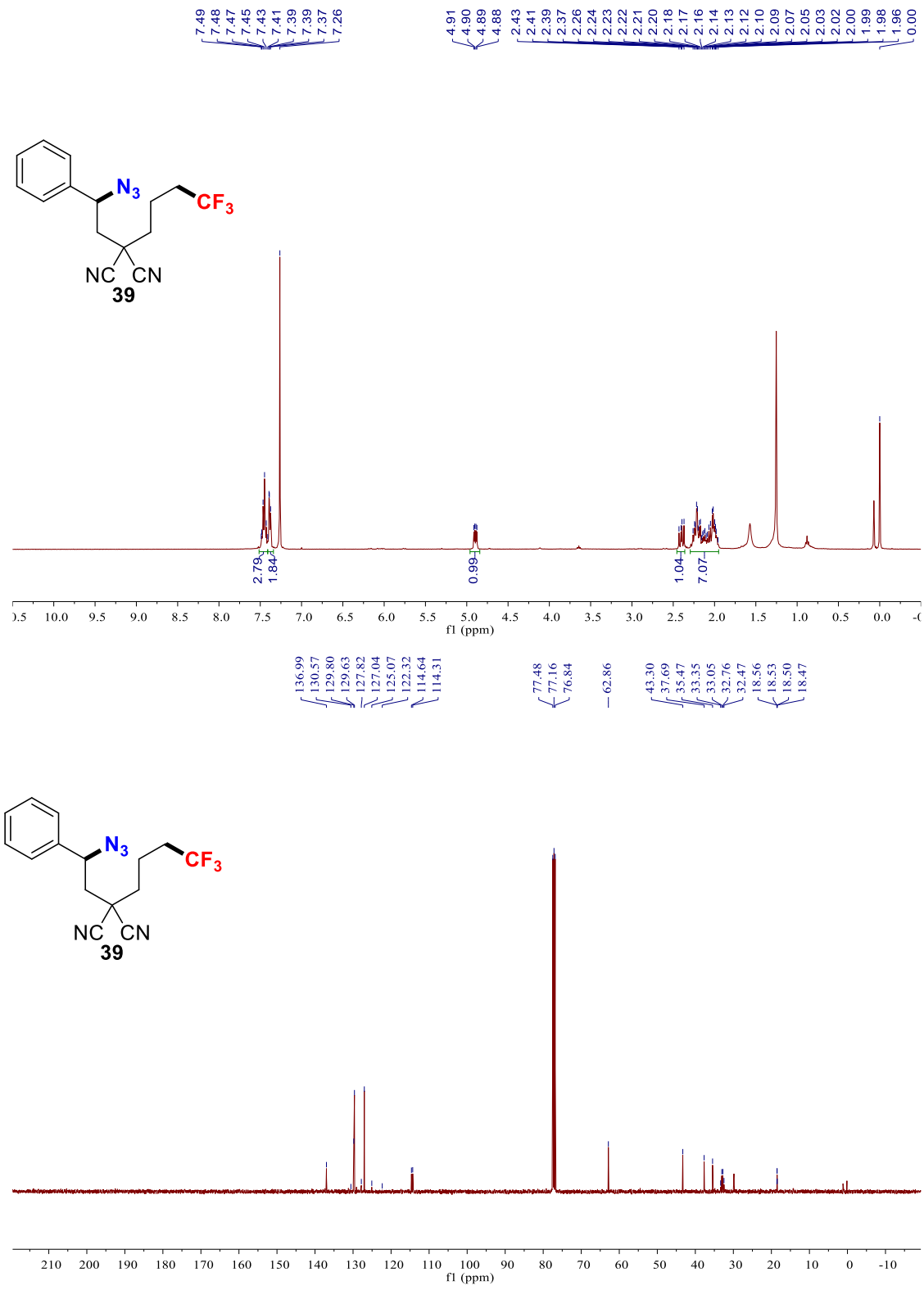

-66.26
-66.29
-66.32
N
N3
CF3
EtO2C
CO2Et
37
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

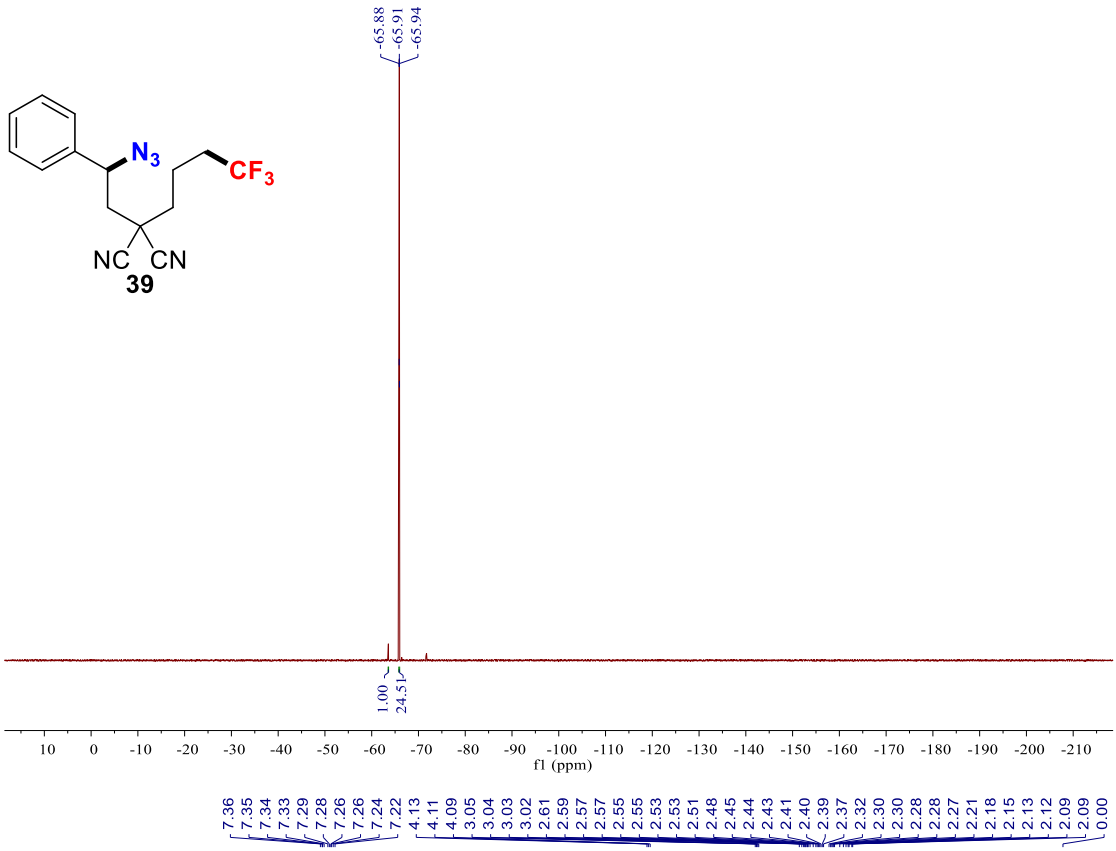

7.43 7.41 7.38 7.36 7.34 7.30 7.28 7.26 4.31 4.29 4.27 4.26 4.24 4.23 4.22 4.21 4.19 4.18 4.18 4.17 4.05 4.03 4.03 4.02 4.01 4.00 3.99 3.98 2.70 2.66 2.60 2.56 1.85 1.84 1.82 1.76 1.74 1.71 1.70 1.68 1.47 1.46 1.44 1.43 1.42 1.41 1.40 1.30 1.28 1.26 1.19 1.18 1.16 1.13 1.11 1.10 0.98 0.96 0.00

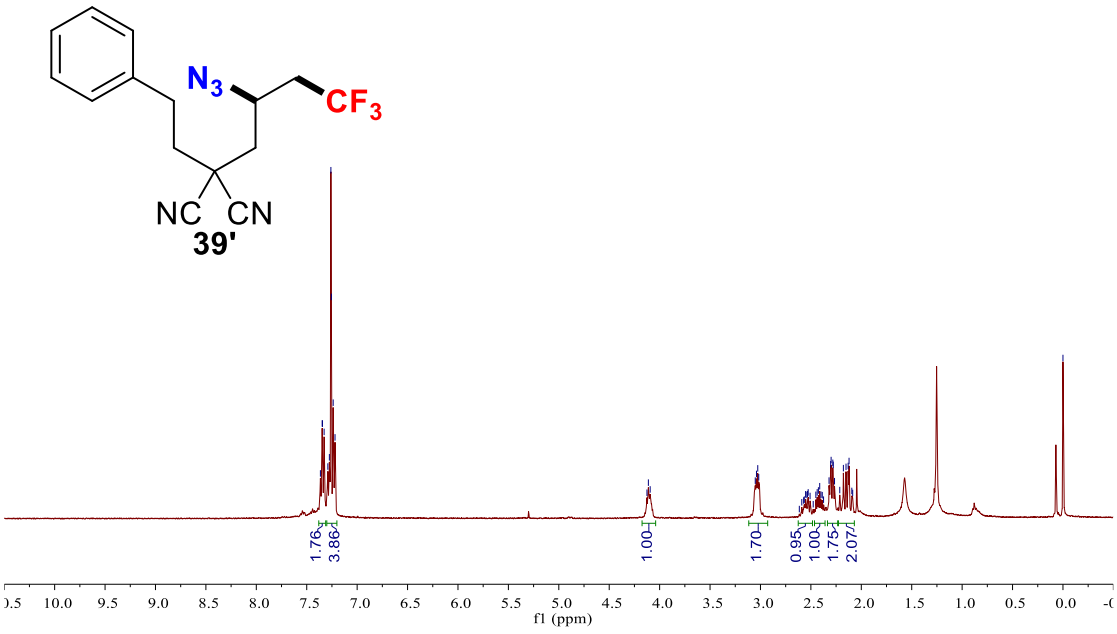

N3
CF3
EtO2C
CO2Et
38
1.91 1.89 1.12 2.20 2.00 1.00 1.00 1.11 2.90 0.99 2.26 3.32 2.80 2.36
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

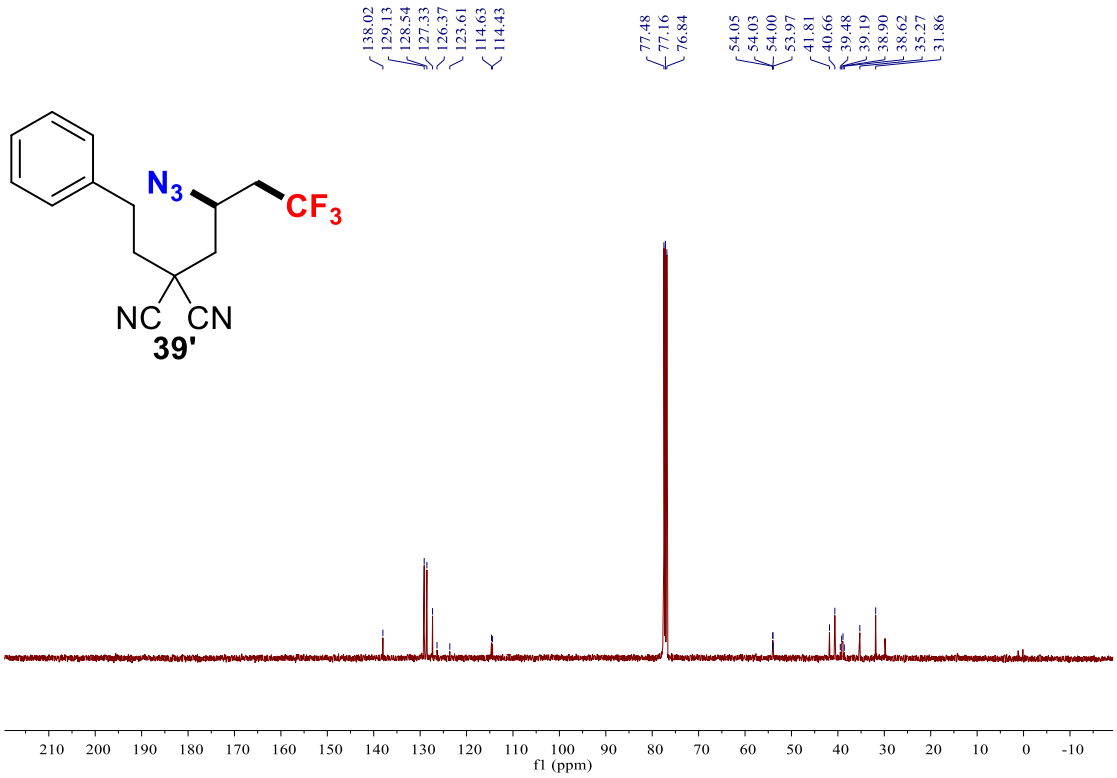

171.09
170.74
143.39
128.70
128.15
127.61
125.64
125.40
77.48
77.16
76.84
65.04
61.75
61.61
56.43
42.87
34.08
33.80
33.51
33.23
30.60
28.57
17.14
17.11
14.09
14.02
N3
CF3
EtO2C CO2Et
38
f1 (ppm)

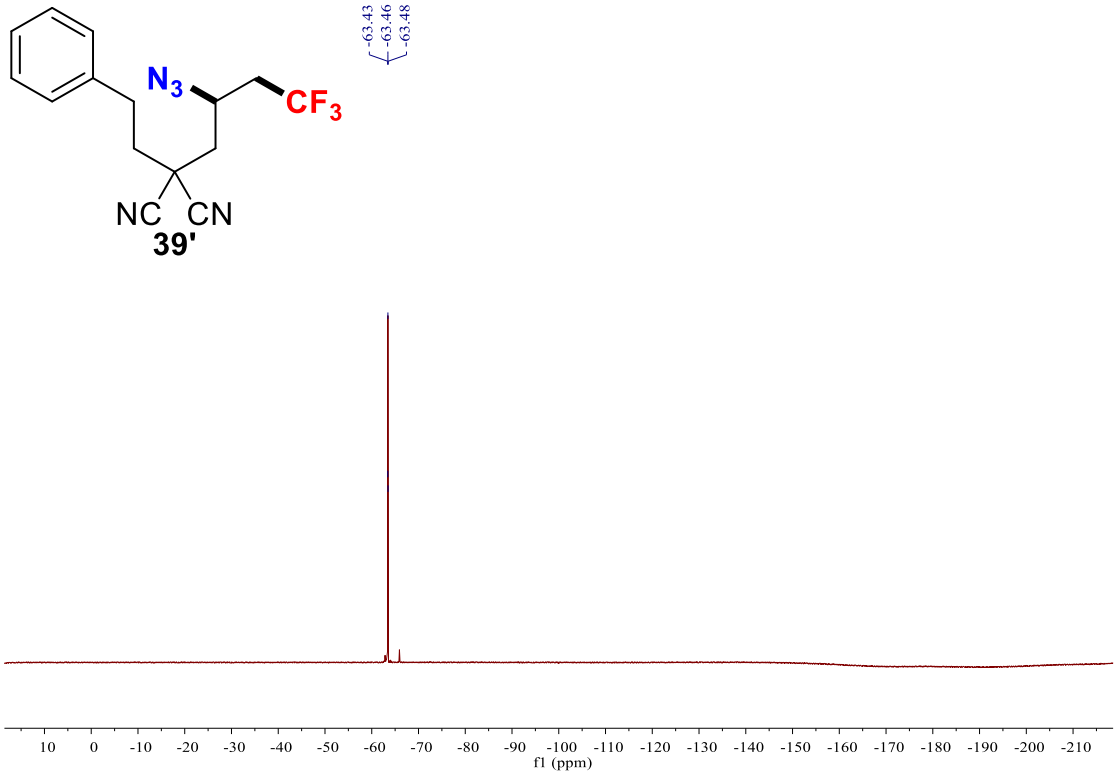

-66.51
-66.54
-66.57
N3
CF3
EtO2C CO2Et
38
1.00
32.88
f1 (ppm)

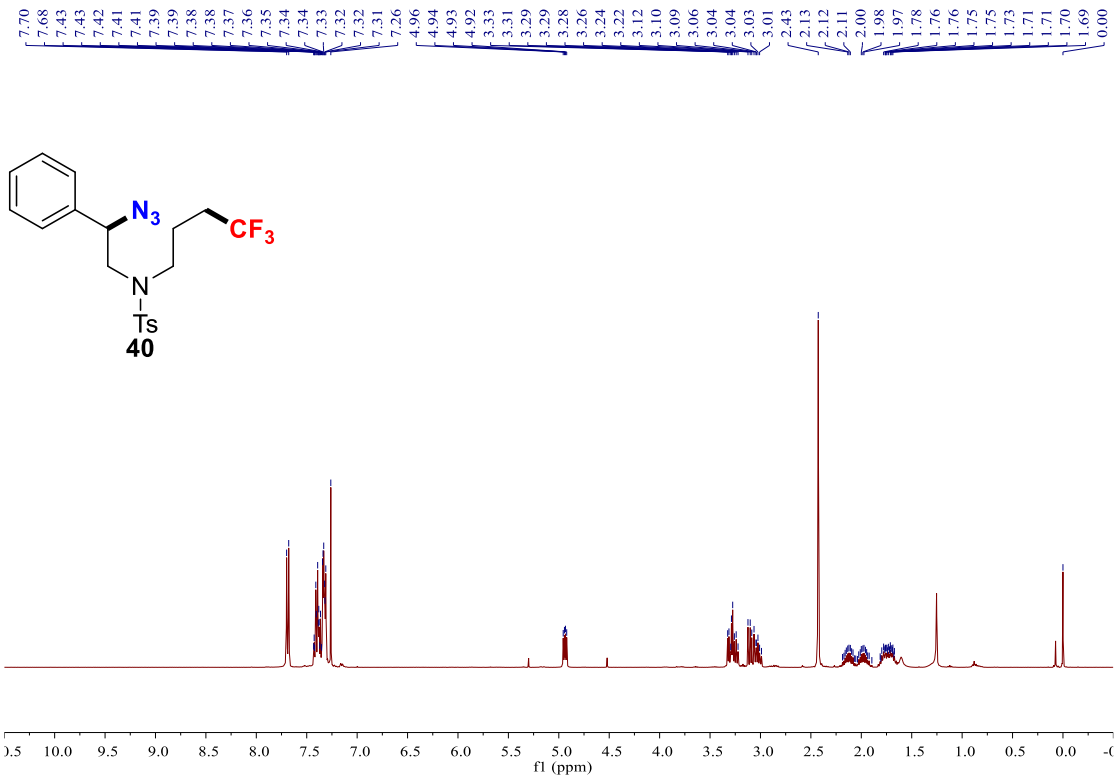

7.49
7.48
7.47
7.45
7.43
7.41
7.39
7.39
7.37
7.26
4.91
4.90
4.89
4.88
2.43
2.41
2.39
2.37
2.26
2.24
2.23
2.22
2.21
2.20
2.18
2.17
2.16
2.14
2.13
2.12
2.10
2.09
2.07
2.05
2.03
2.02
2.00
1.99
1.98
1.96
0.00
N3
CF3
NC CN
39
2.79
1.84
0.99
1.04
7.07
f1 (ppm)
136.99
130.57
129.80
129.63
127.82
127.04
125.07
122.32
114.64
114.31
77.48
77.16
76.84
62.86
43.30
37.69
35.47
33.35
33.05
32.76
32.47
18.56
18.53
18.50
18.47
N3
CF3
NC CN
39
f1 (ppm)

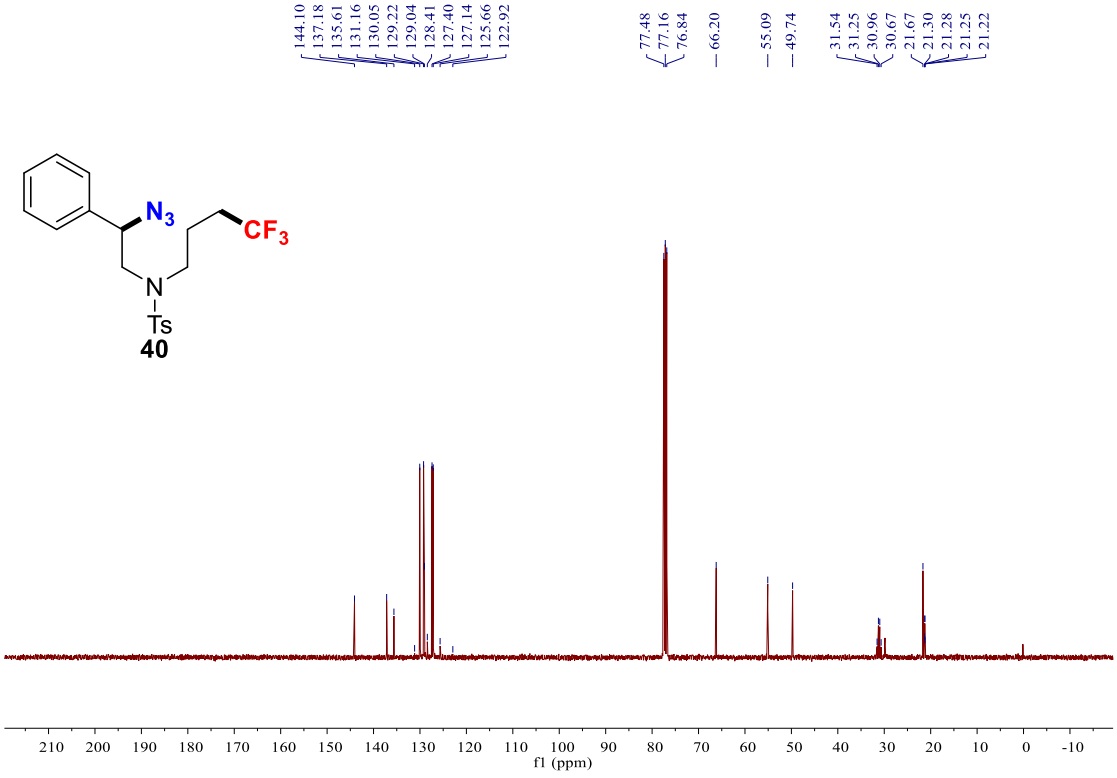

N3
CF3
NC CN
39
-65.88
-65.91
-65.94
1.00
24.51
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)
7.36 7.35 7.34 7.33 7.29 7.28 7.26 7.26 7.24 7.22 4.13 4.11 4.09 3.05 3.04 3.03 3.02 2.61 2.59 2.57 2.57 2.55 2.55 2.53 2.53 2.51 2.48 2.45 2.44 2.43 2.41 2.40 2.39 2.37 2.32 2.30 2.30 2.28 2.28 2.27 2.21 2.18 2.15 2.13 2.12 2.09 2.09 0.00

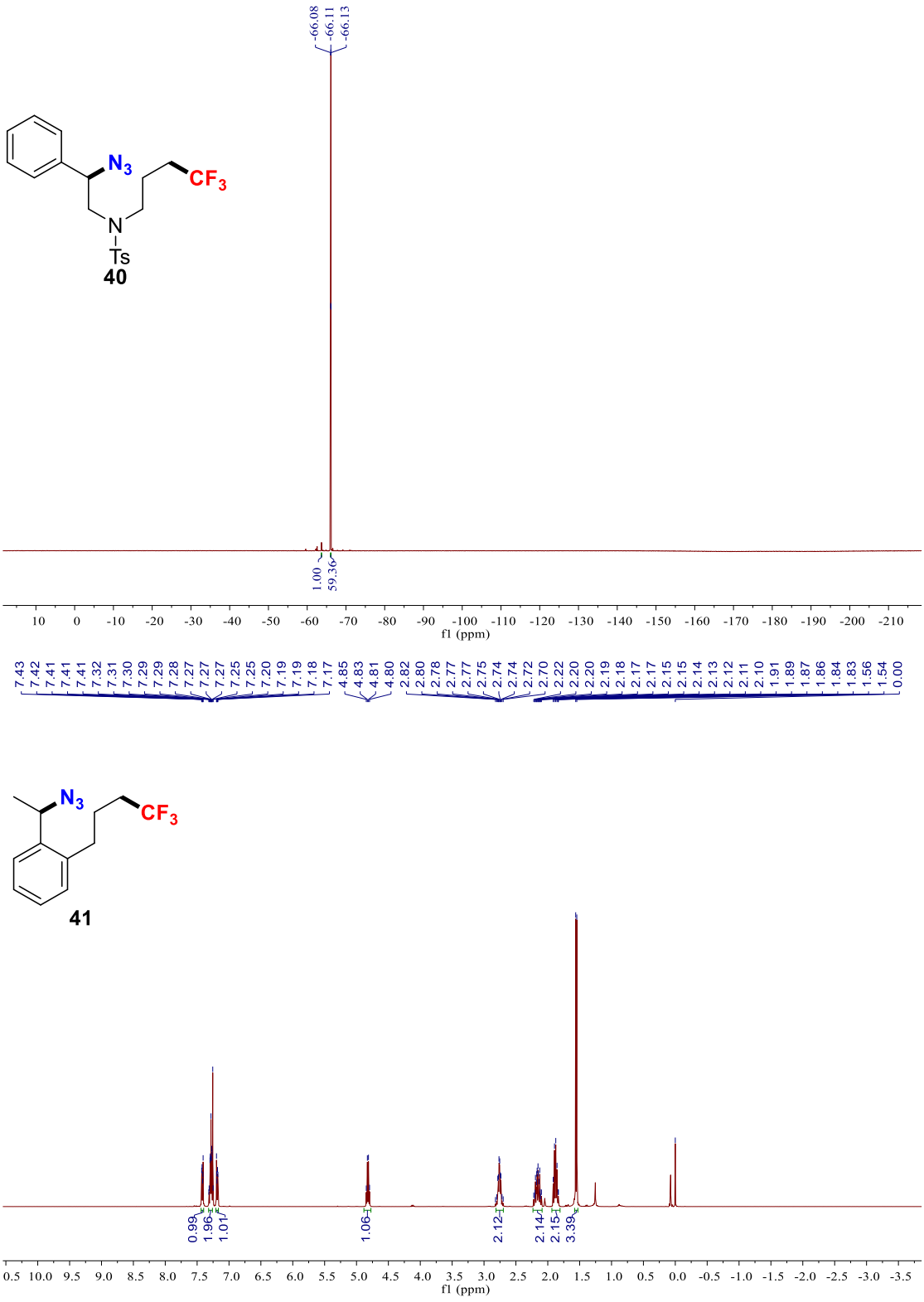

N3
CF3
NC CN
39'
1.76
3.86
1.00
1.70
0.95
1.00
1.75
2.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

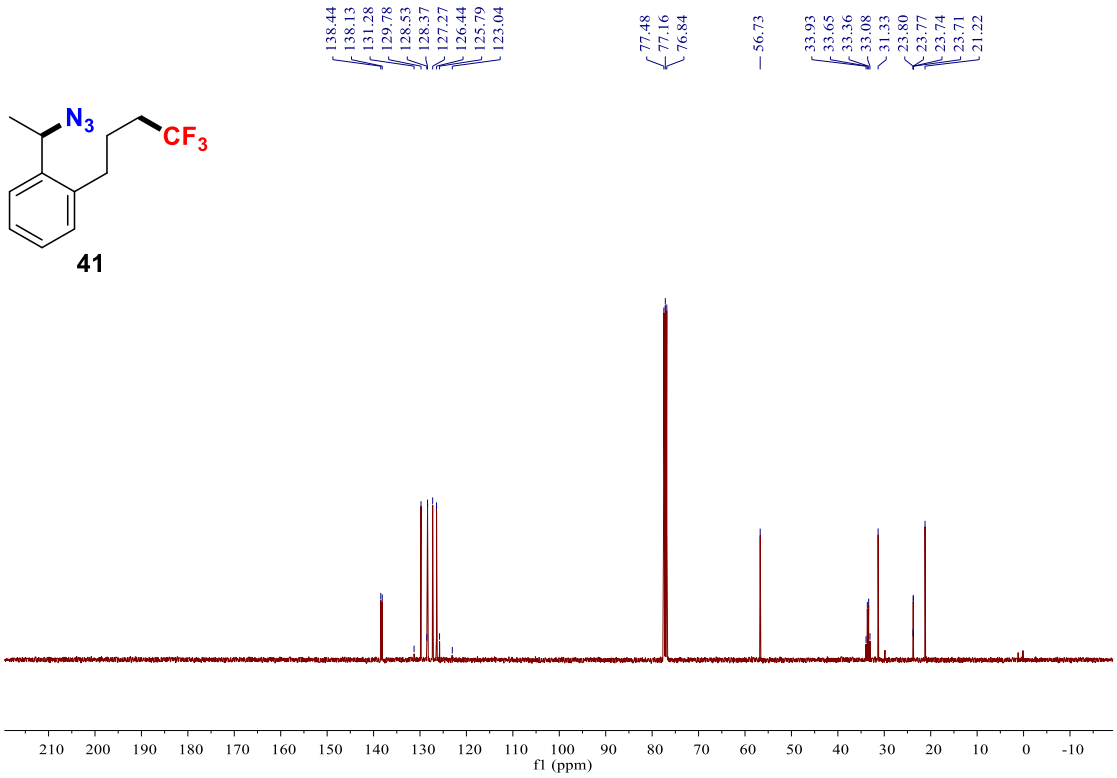

138.02
129.13
128.54
127.33
126.37
123.61
114.63
114.43
77.48
77.16
76.84
54.05
54.03
54.00
53.97
41.81
40.66
39.48
39.19
38.90
38.62
35.27
31.86
N3
CF3
NC CN
39'
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

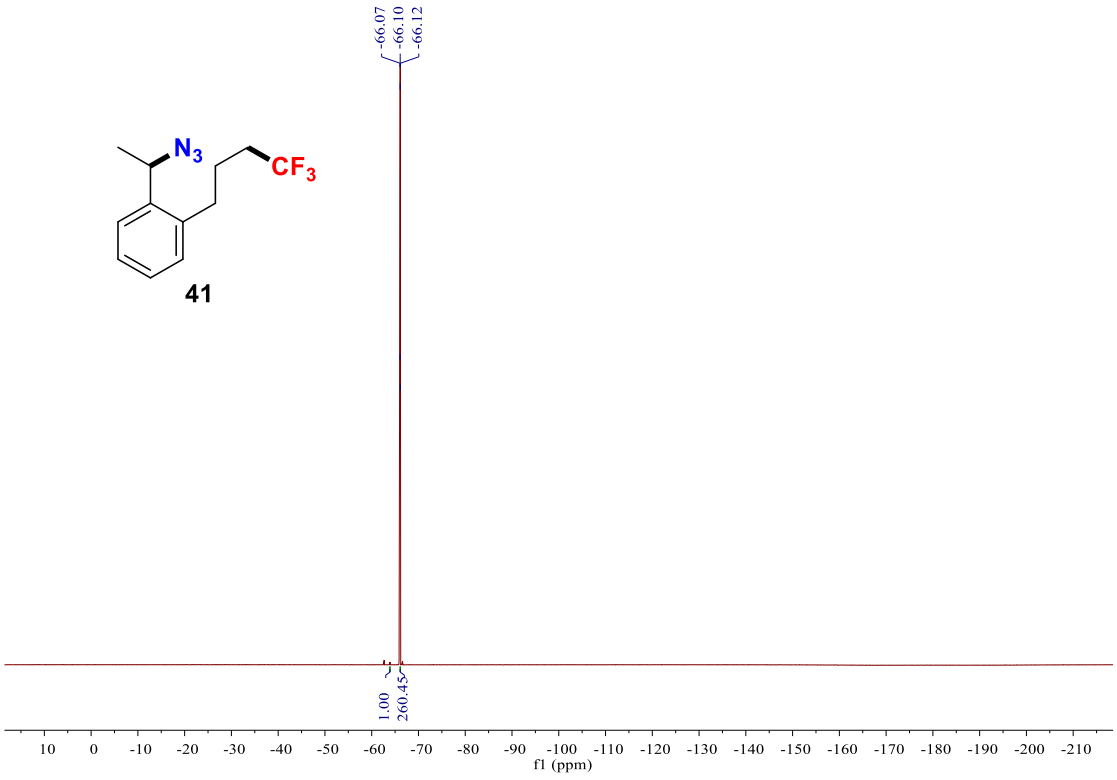

-63.43
-63.46
-63.48
N3
CF3
NC CN
39'
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

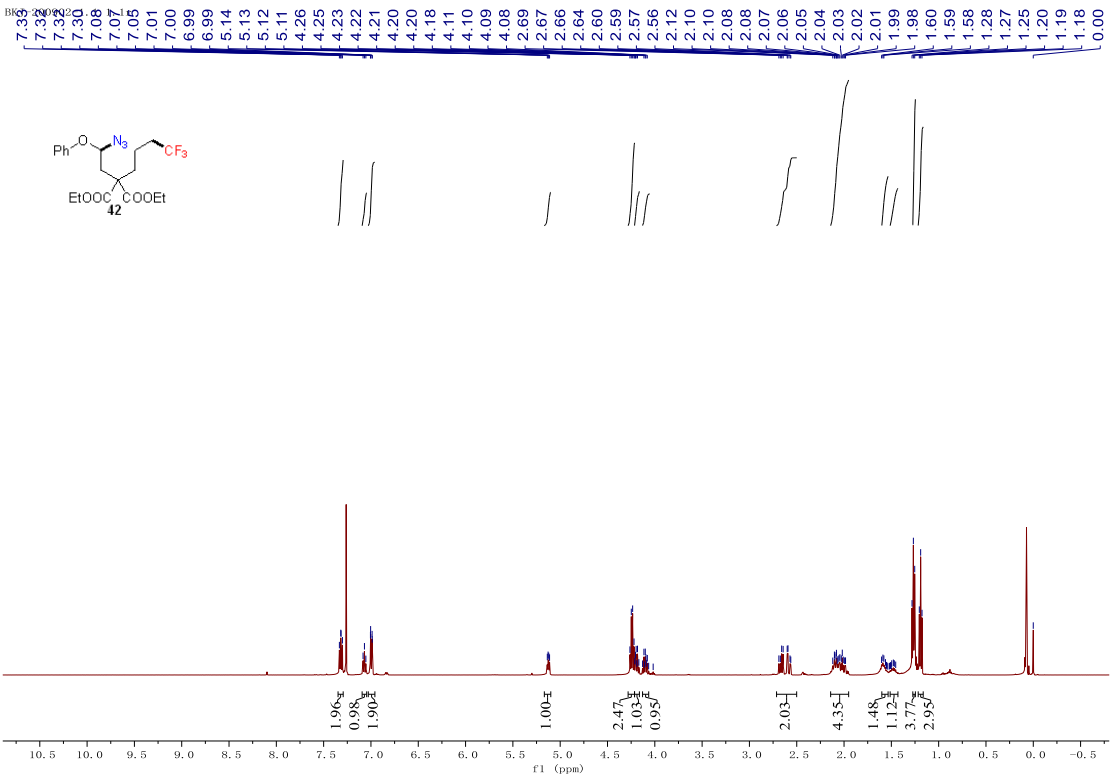

7.70 7.68 7.43 7.43 7.42 7.41 7.41 7.39 7.39 7.38 7.38 7.37 7.36 7.35 7.34 7.34 7.33 7.32 7.32 7.31 7.26
4.96 4.94 4.93 4.92 3.33 3.31 3.29 3.29 3.28 3.26 3.24 3.22 3.12 3.10 3.09 3.06 3.04 3.04 3.03 3.01
2.43 2.13 2.12 2.11 2.00 1.98 1.97 1.78 1.76 1.76 1.75 1.75 1.73 1.71 1.71 1.70 1.69 0.00
N3
CF3
N
Ts
40
f1 (ppm)

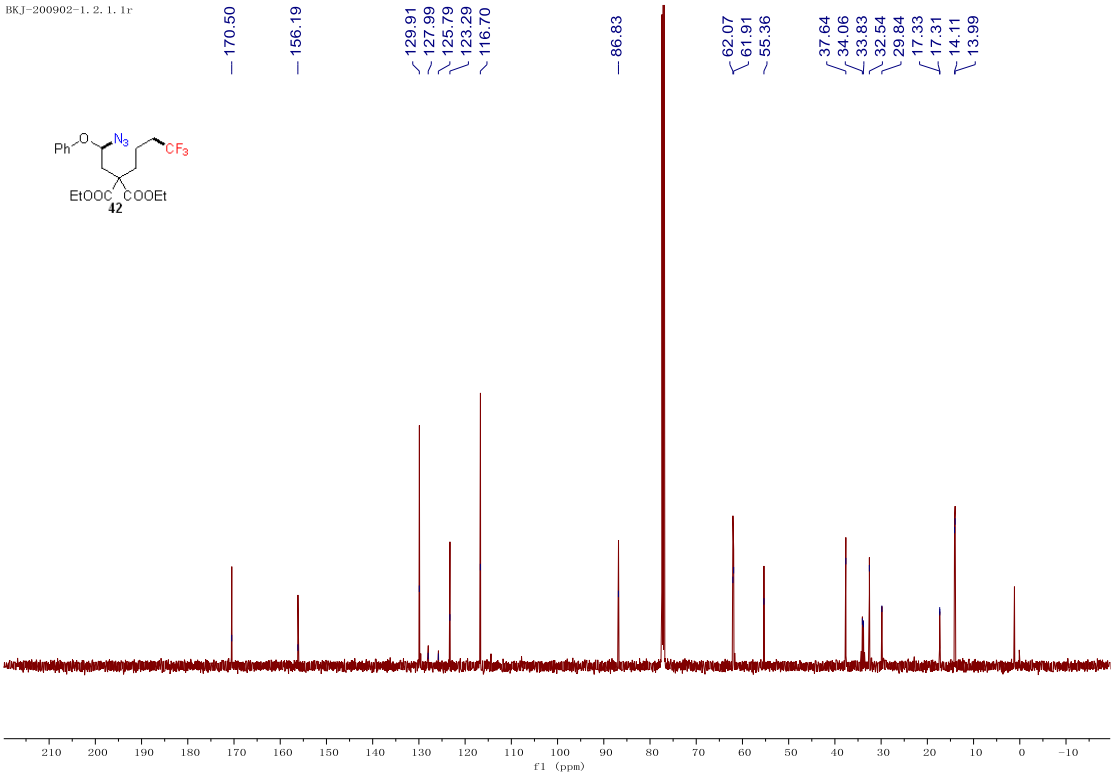

144.10 137.18 135.61 131.16 130.05 129.22 129.04 128.41 127.40 127.14 125.66 122.92
77.48 77.16 76.84 66.20 55.09 49.74
31.54 31.25 30.96 30.67 21.67 21.30 21.28 21.25 21.22
N3
CF3
N
Ts
40
f1 (ppm)

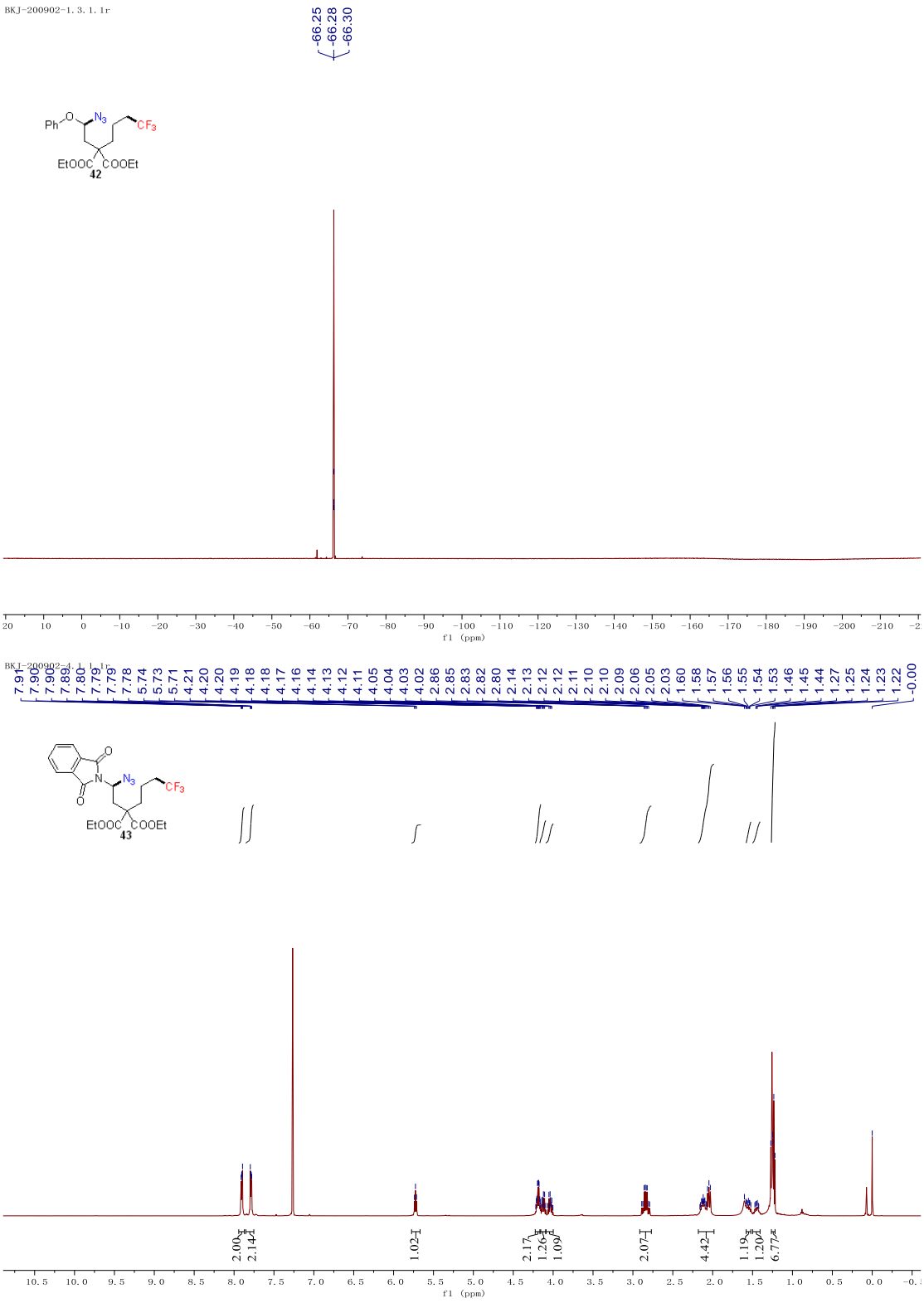

-66.08
-66.11
-66.13
N3
CF3
N
Ts
40
1.00
59.36
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)
7.43 7.42 7.41 7.41 7.41 7.32 7.31 7.30 7.29 7.29 7.28 7.27 7.27 7.27 7.25 7.25 7.20 7.19 7.19 7.18 7.17
4.85 4.83 4.81 4.80
2.82 2.80 2.78 2.77 2.77 2.75 2.74 2.74 2.72 2.70 2.22 2.20 2.20 2.19 2.18 2.17 2.17 2.15 2.15 2.14 2.13 2.12 2.11 2.10 1.91 1.89 1.87 1.86 1.84 1.83 1.56 1.54 0.00
N3
CF3
41
0.99
1.96
1.01
1.06
2.12
2.14
2.15
3.39
0.5 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 -0.5 -1.0 -1.5 -2.0 -2.5 -3.0 -3.5
f1 (ppm)

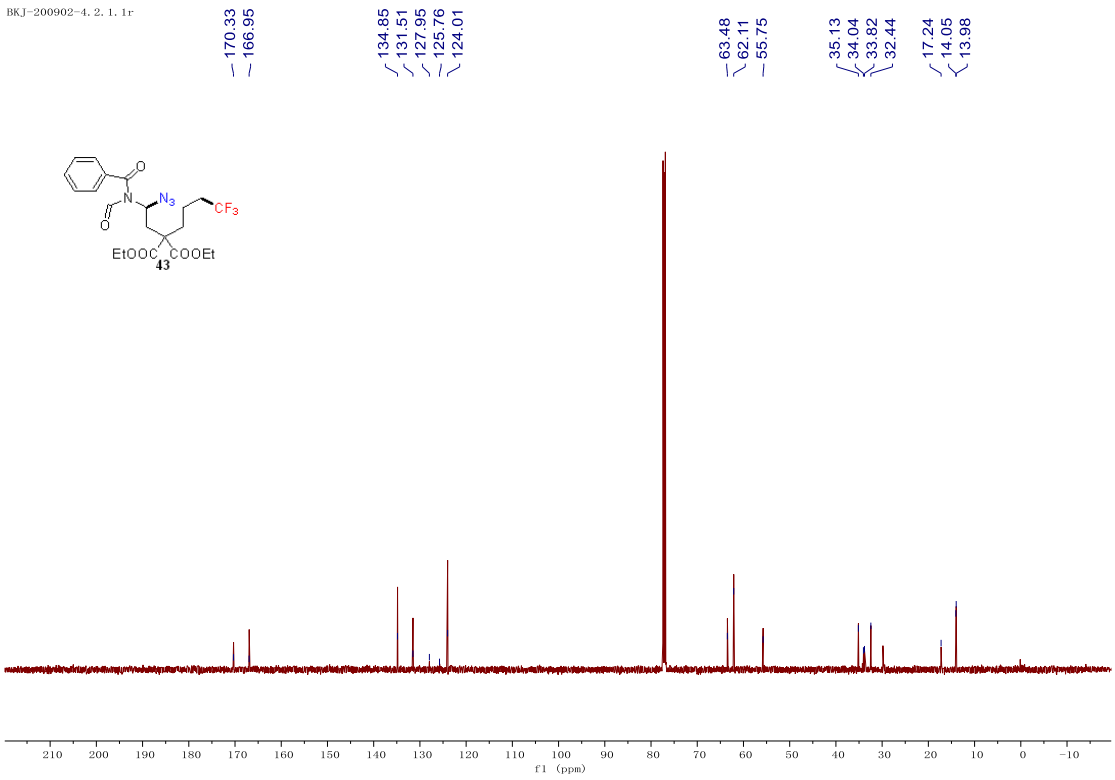

138.44
138.13
131.28
129.78
128.53
128.37
127.27
126.44
125.79
123.04
77.48
77.16
76.84
56.73
33.93
33.65
33.36
33.08
31.33
23.80
23.77
23.74
23.71
21.22
N3
CF3
41
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

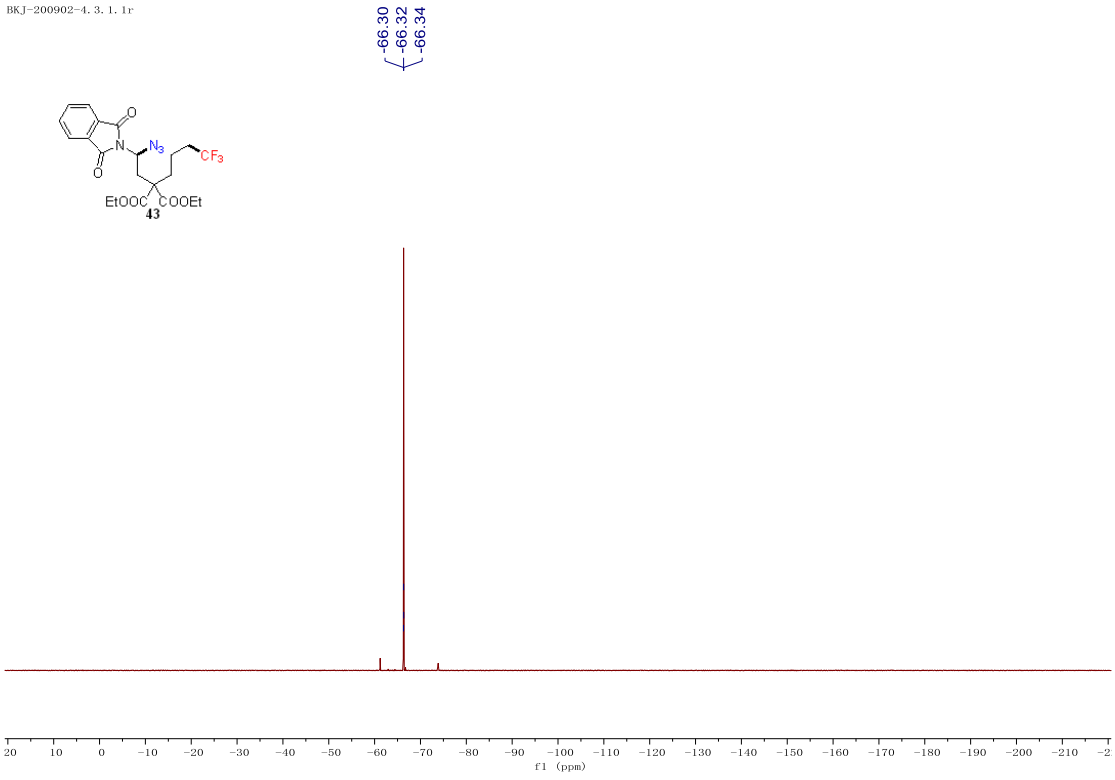

-66.07
-66.10
-66.12
N3
CF3
41
1.00
260.45
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

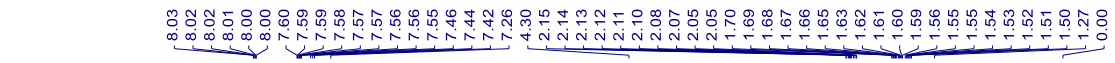

7.33
7.32
7.30
7.08
7.07
7.05
7.01
7.00
6.99
6.99
5.14
5.13
5.12
5.11
4.26
4.25
4.23
4.22
4.21
4.20
4.20
4.18
4.11
4.10
4.09
4.08
2.69
2.67
2.66
2.64
2.60
2.59
2.57
2.56
2.12
2.10
2.10
2.08
2.08
2.07
2.06
2.05
2.04
2.03
2.02
2.01
1.99
1.98
1.60
1.59
1.58
1.28
1.27
1.25
1.20
1.19
1.18
0.00
Ph
O
N3
CF3
EtOOC
COOEt
42
1.96
0.98
1.90
1.00
2.47
1.03
0.95
2.03
4.35
1.48
1.12
3.77
2.95
f1 (ppm)

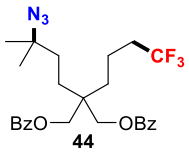

BKJ-200902-1.2.1.1r
170.50
156.19
129.91
127.99
125.79
123.29
116.70
86.83
62.07
61.91
55.36
37.64
34.06
33.83
32.54
29.84
17.33
17.31
14.11
13.99
Ph
O
N3
CF3
EtOOC
COOEt
42
f1 (ppm)


BKJ-200902-1.3.1.1r
-66.25
-66.28
-66.30
Ph
O
N3
CF3
EtOOC
COOEt
42
f1 (ppm)
BKJ-200902-1.1.1r
7.91
7.90
7.90
7.89
7.80
7.79
7.79
7.78
5.74
5.73
5.71
4.21
4.20
4.20
4.19
4.18
4.18
4.17
4.16
4.14
4.13
4.12
4.11
4.05
4.04
4.03
4.02
2.86
2.85
2.83
2.82
2.80
2.14
2.13
2.12
2.12
2.11
2.10
2.10
2.09
2.06
2.05
2.03
1.60
1.58
1.57
1.56
1.55
1.54
1.53
1.46
1.45
1.44
1.27
1.25
1.24
1.23
1.22
-0.00
O
N
O
N3
CF3
EtOOC
COOEt
43
2.00
2.14
1.02
2.17
1.26
1.09
2.07
4.42
1.19
1.20
6.77
f1 (ppm)

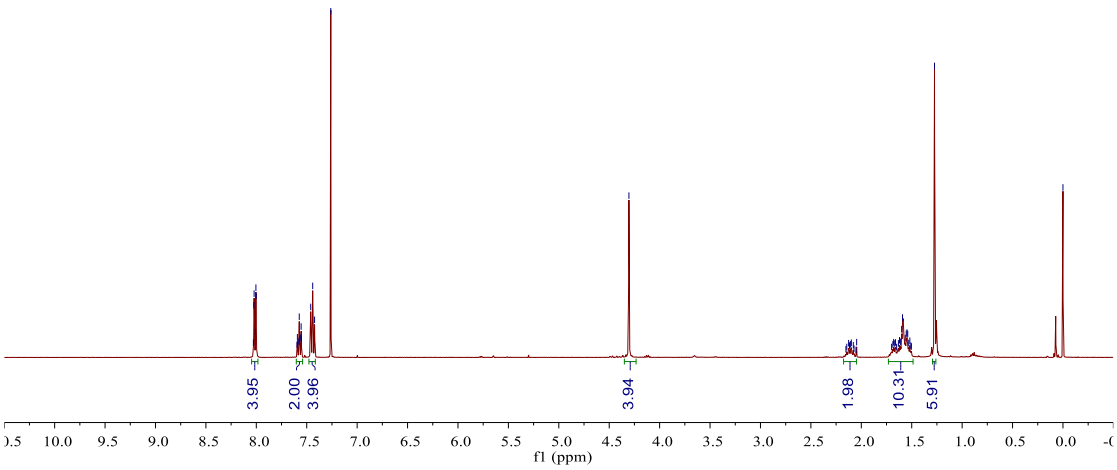

BKJ-200902-4.2.1.1r
170.33
166.95
134.85
131.51
127.95
125.76
124.01
63.48
62.11
55.75
35.13
34.04
33.82
32.44
17.24
14.05
13.98
N3
CF3
EtOOC
COOEt
43
f1 (ppm)


BKJ-200902-4.3.1.1r
-66.30
-66.32
-66.34
N3
CF3
EtOOC
COOEt
43
f1 (ppm)

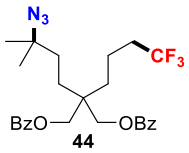

8.03
8.02
8.02
8.01
8.00
8.00
7.60
7.59
7.59
7.58
7.57
7.57
7.56
7.56
7.55
7.46
7.44
7.42
7.26
4.30
2.15
2.14
2.13
2.12
2.11
2.10
2.08
2.07
2.05
2.05
1.70
1.69
1.68
1.67
1.66
1.65
1.63
1.62
1.61
1.60
1.59
1.56
1.55
1.55
1.54
1.53
1.52
1.51
1.50
1.27
0.00


N3
CF3
BzO
OBz

44

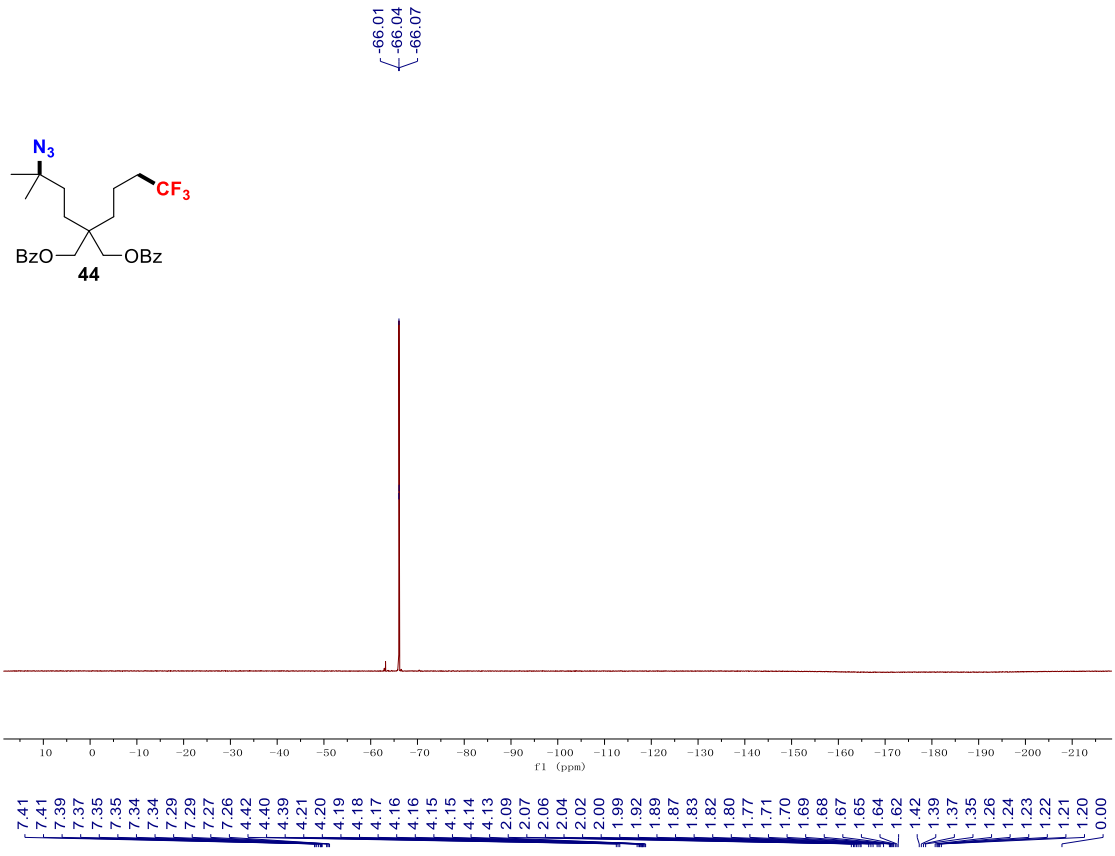

3.95
2.00
3.96
3.94
1.98
10.31
5.91
f1 (ppm)

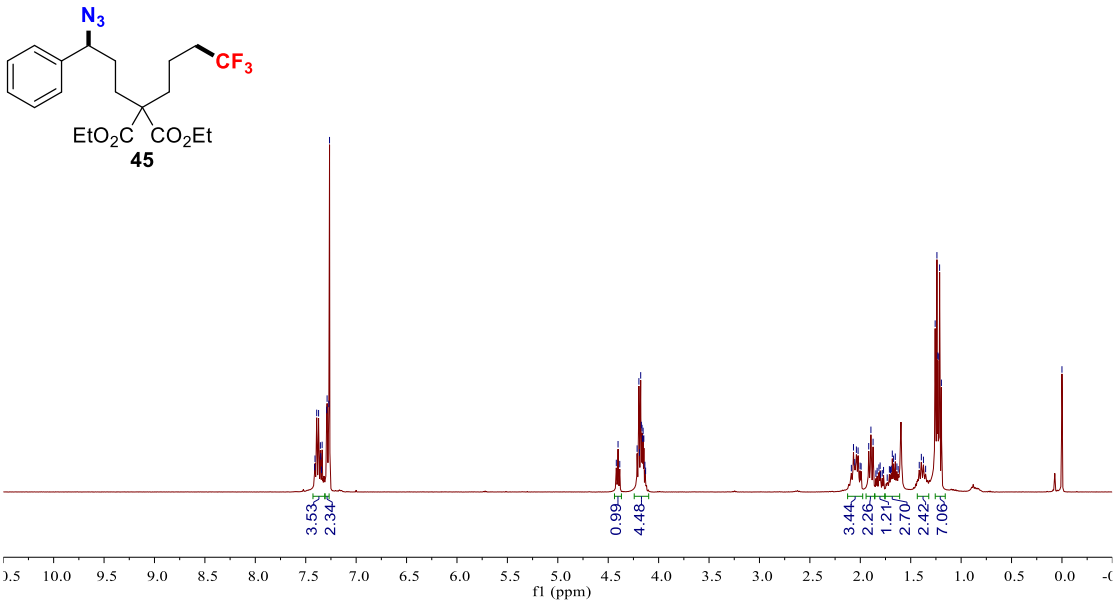

166.384
133.377
129.905
129.679
128.668
128.416
125.668
77.478
77.160
76.843
66.396
61.323
40.088
34.815
34.530
34.247
33.960
31.124
26.092
25.846
16.000
15.971
15.943
15.913

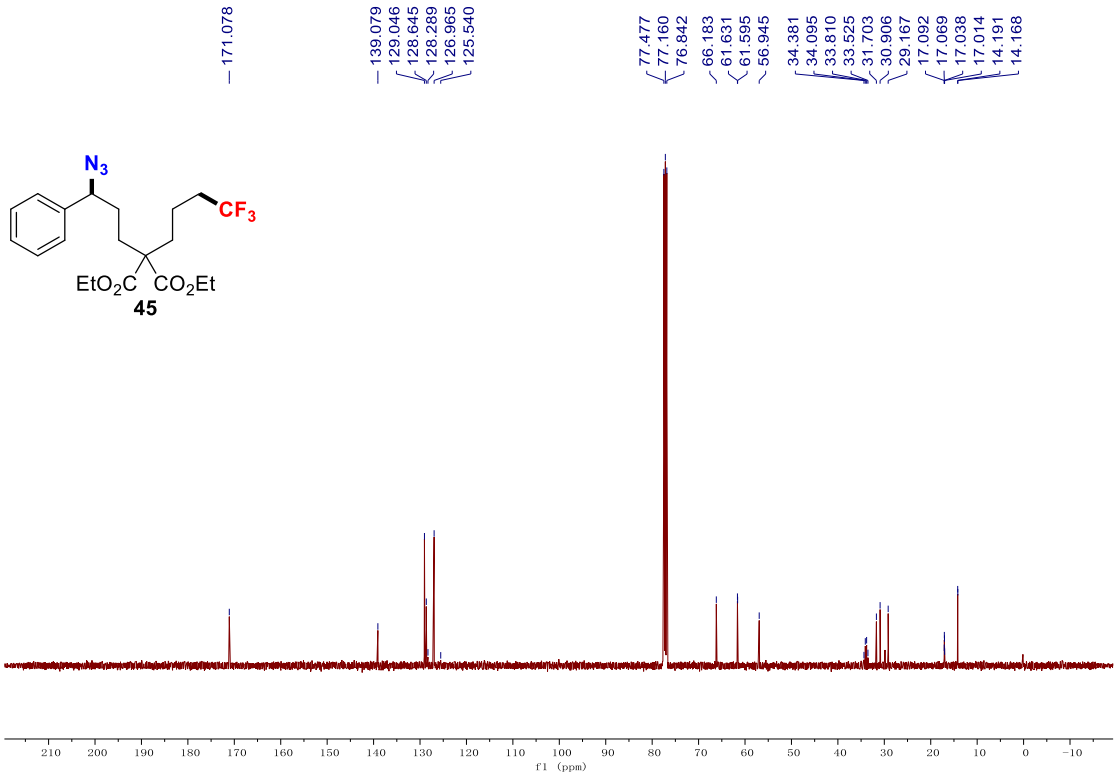

N3
CF3
BzO
OBz

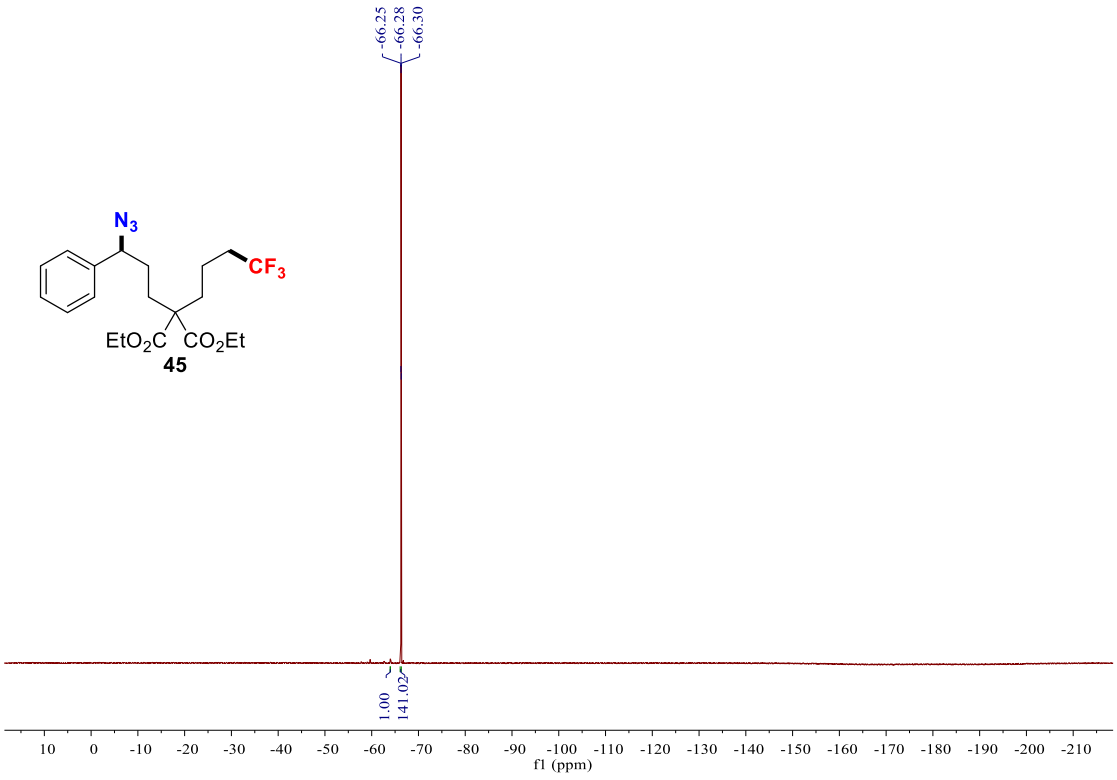
44

f1 (ppm)

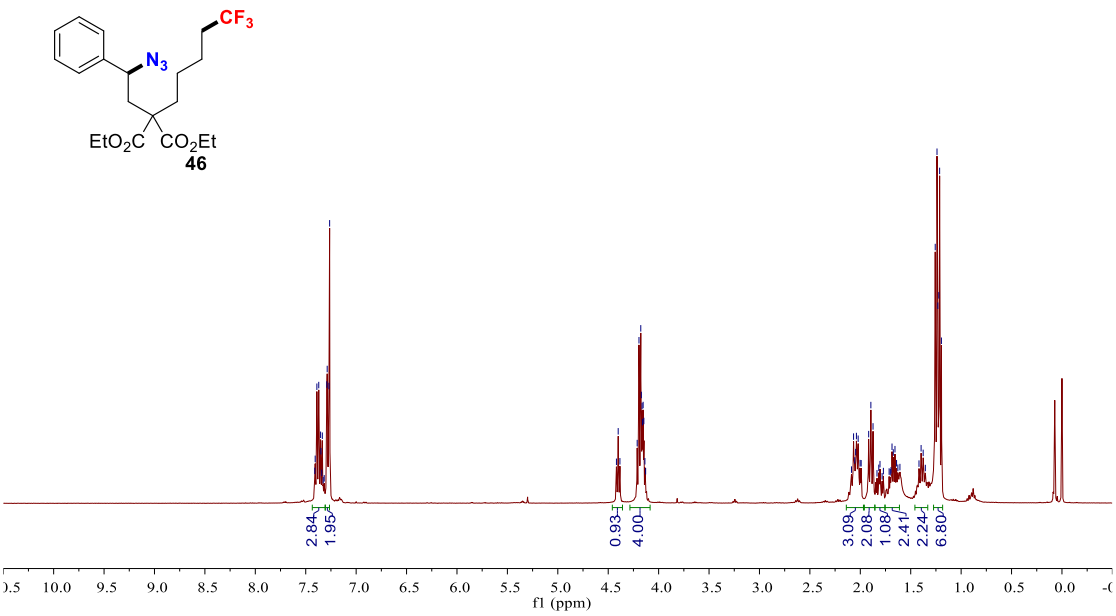

-66.01
-66.04
-66.07
N3
CF3
BzO
OBz
44
f1 (ppm)

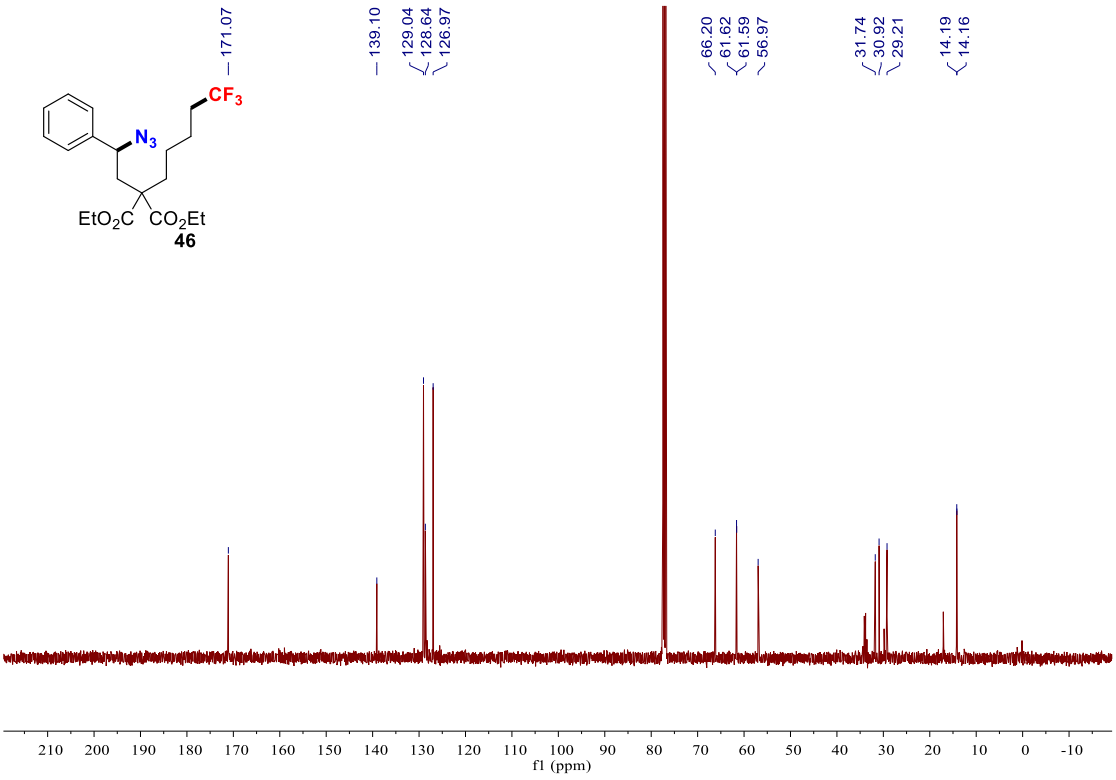

N3
CF3
EtO2C
CO2Et
45
3.53
2.34
0.99
4.48
3.44
2.26
1.21
2.70
2.42
7.06
f1 (ppm)

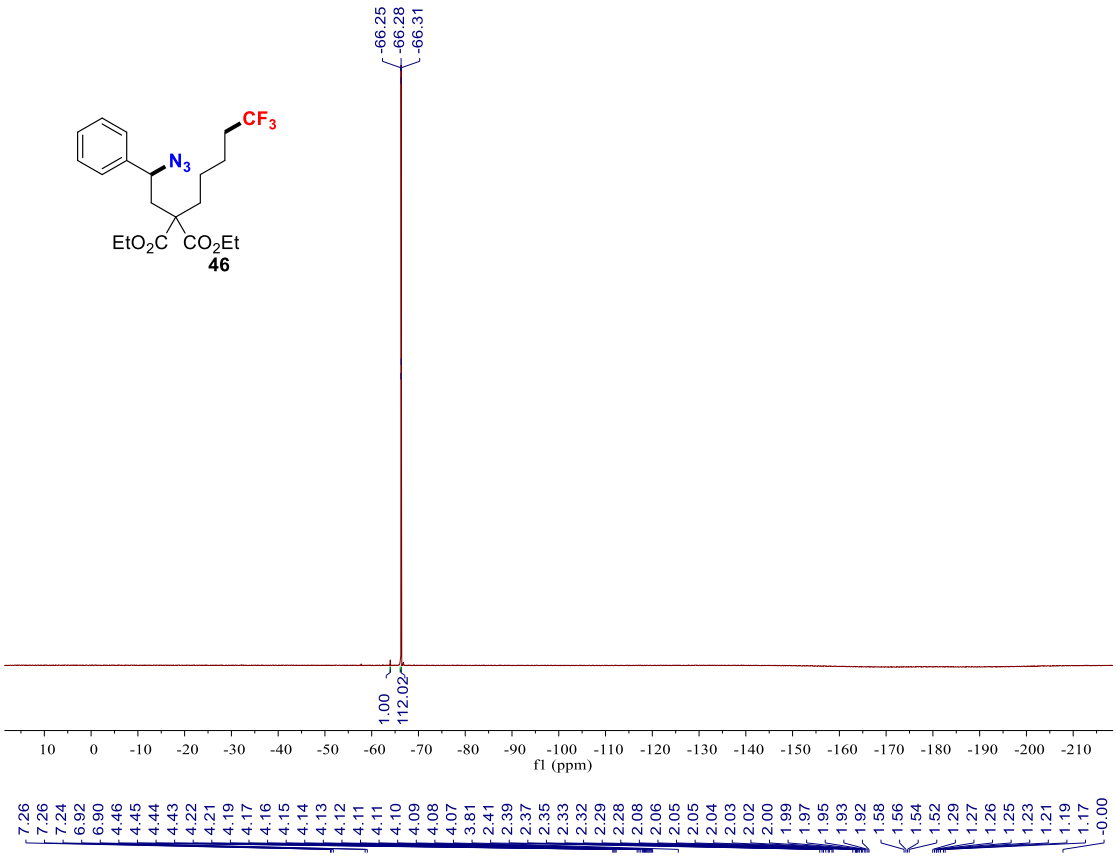

171.078
139.079
129.046
128.645
128.289
126.965
125.540
77.477
77.160
76.842
66.183
61.631
61.595
56.945
34.381
34.095
33.810
33.525
31.703
30.906
29.167
17.092
17.069
17.038
17.014
14.191
14.168
N3
CF3
EtO2C CO2Et
45
f1 (ppm)

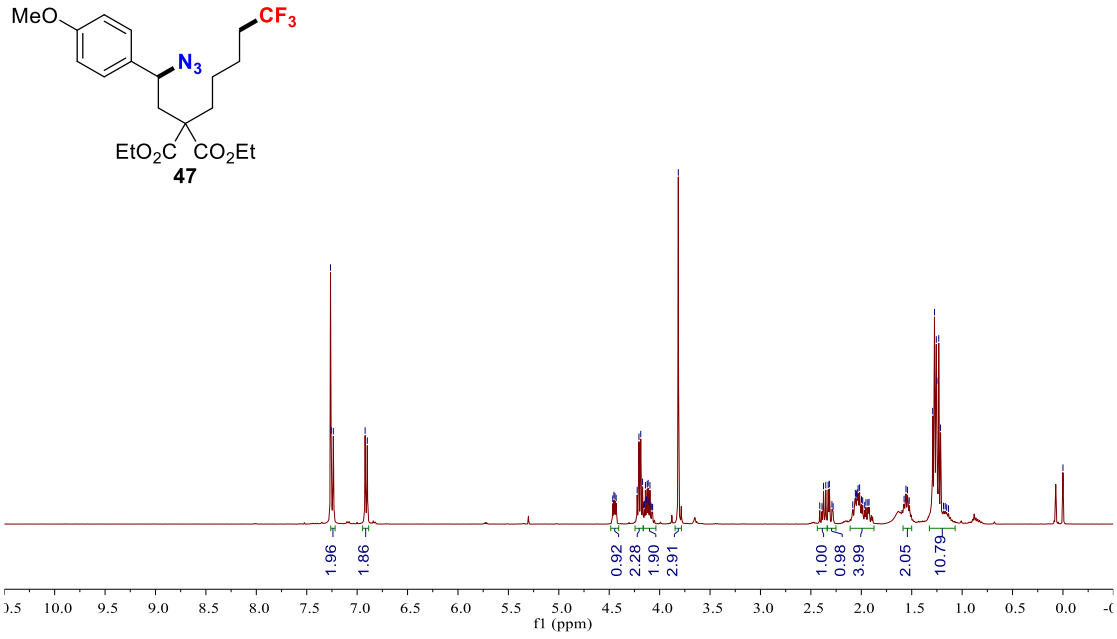

-66.25
-66.28
-66.30
N3
CF3
EtO2C CO2Et
45
1.00
141.02
f1 (ppm)

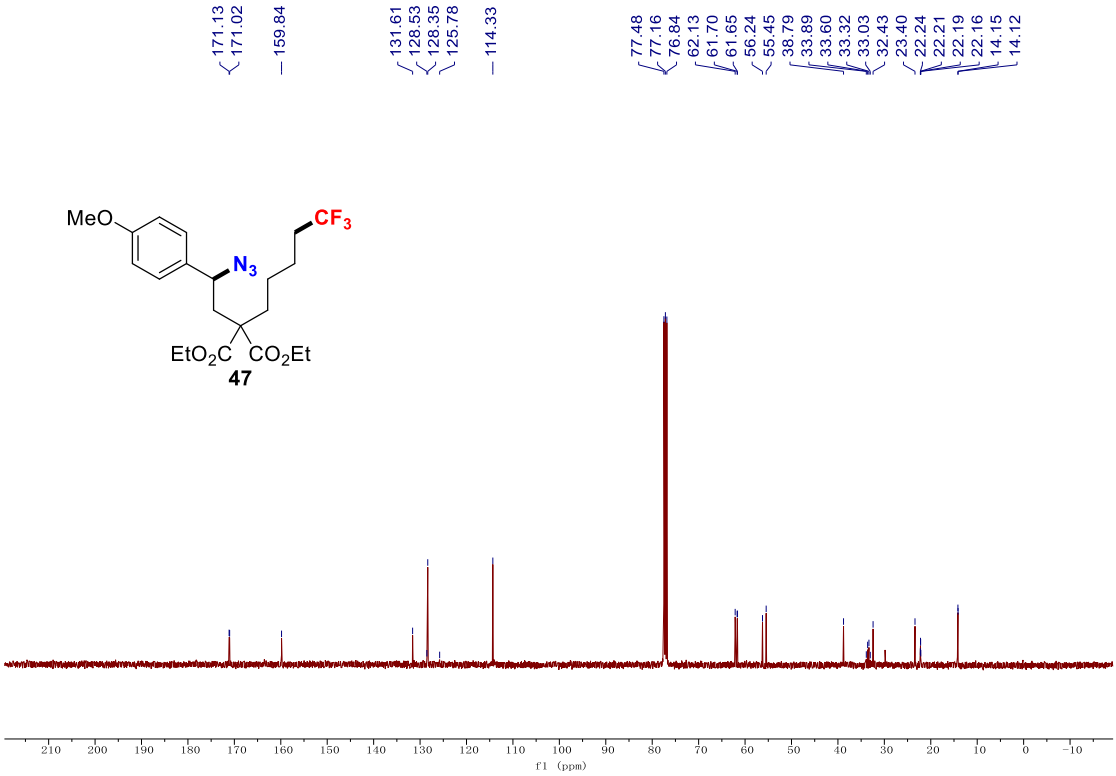

7.41 7.41 7.39 7.37 7.35 7.35 7.34 7.34 7.29 7.29 7.27 7.26 4.42 4.40 4.38 4.21 4.19 4.18 4.17 4.16 4.16 4.15 4.15 4.14 4.13 2.09 2.07 2.05 2.05 2.04 2.02 2.00 1.99 1.92 1.90 1.87 1.83 1.82 1.80 1.77 1.71 1.70 1.70 1.69 1.67 1.66 1.64 1.63 1.61 1.42 1.40 1.38 1.35 1.26 1.24 1.23 1.22 1.21 1.20

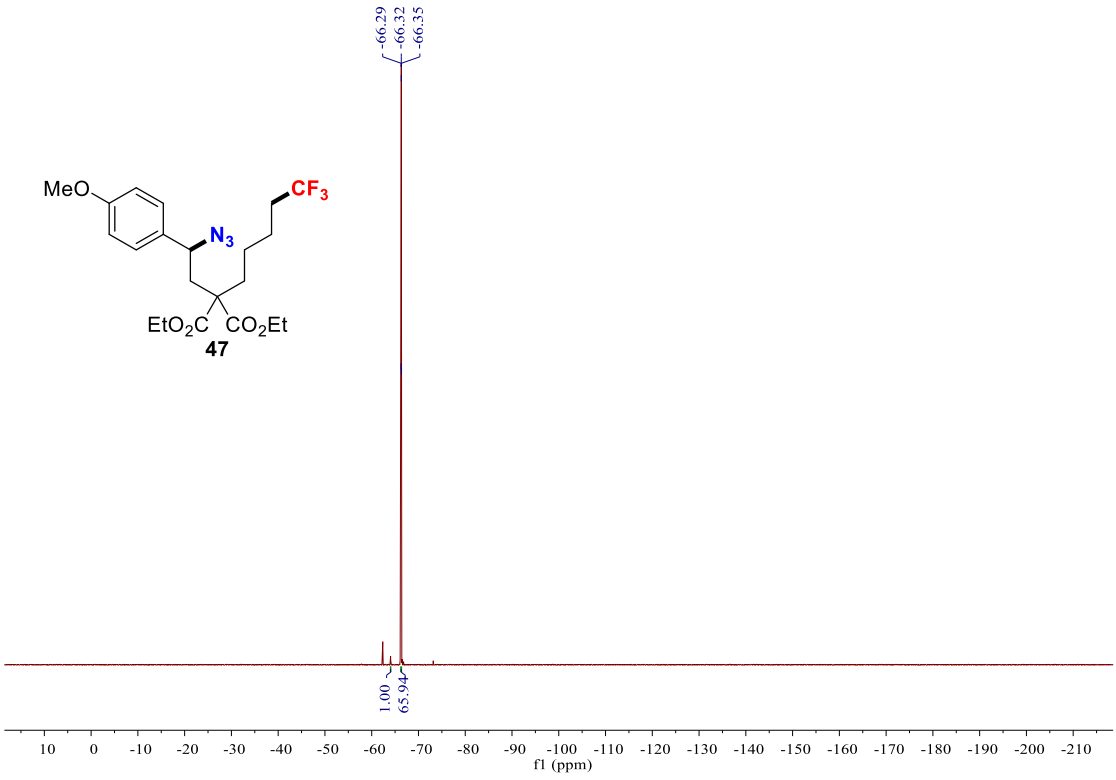

CF3
N3
EtO2C CO2Et
46
2.84
1.95
0.93
4.00
3.09
2.08
1.08
2.41
2.24
6.80
f1 (ppm)

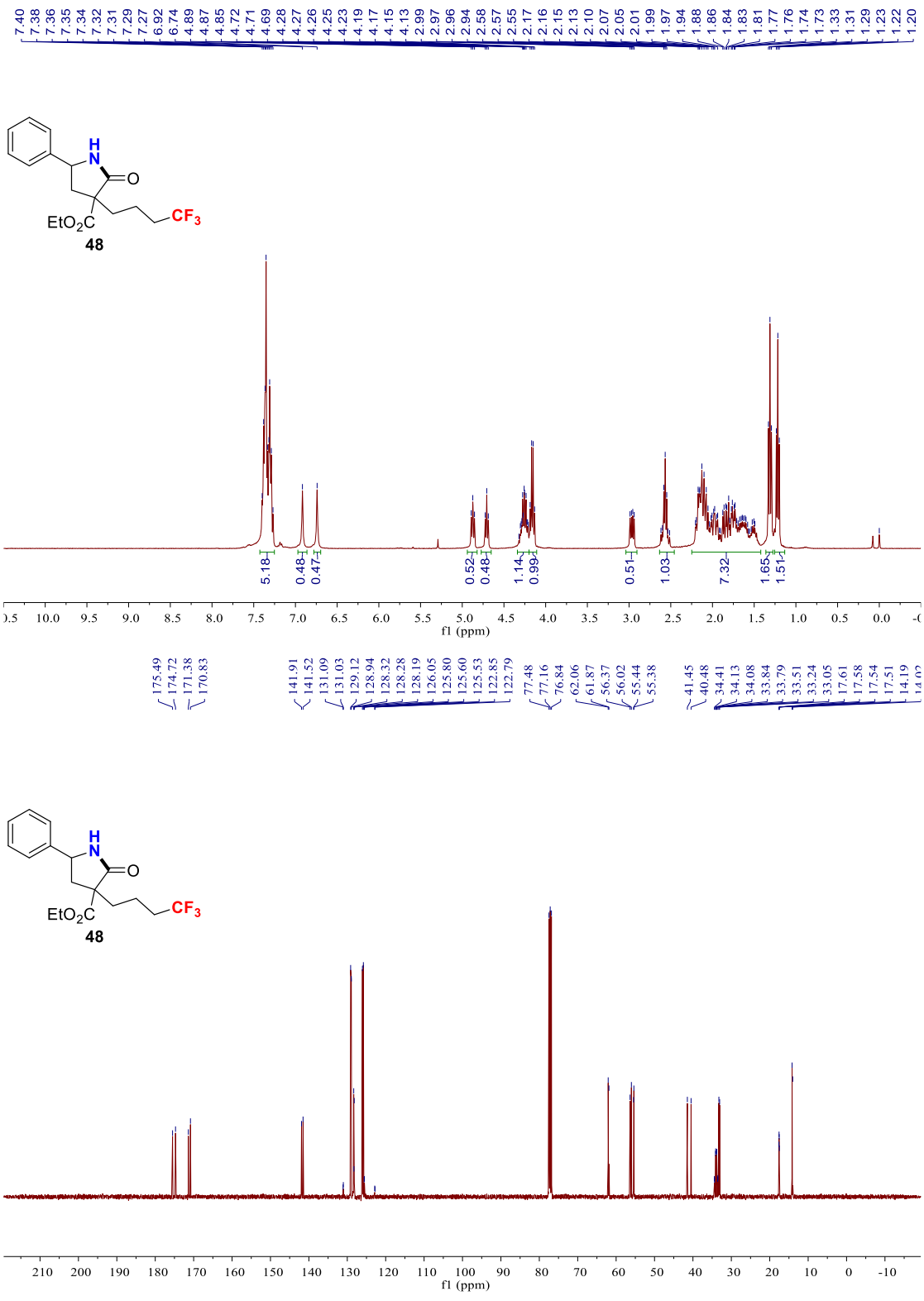

171.07
139.10
129.04
128.64
126.97
66.20
61.62
61.59
56.97
31.74
30.92
29.21
14.19
14.16
CF3
N3
EtO2C CO2Et
46
f1 (ppm)

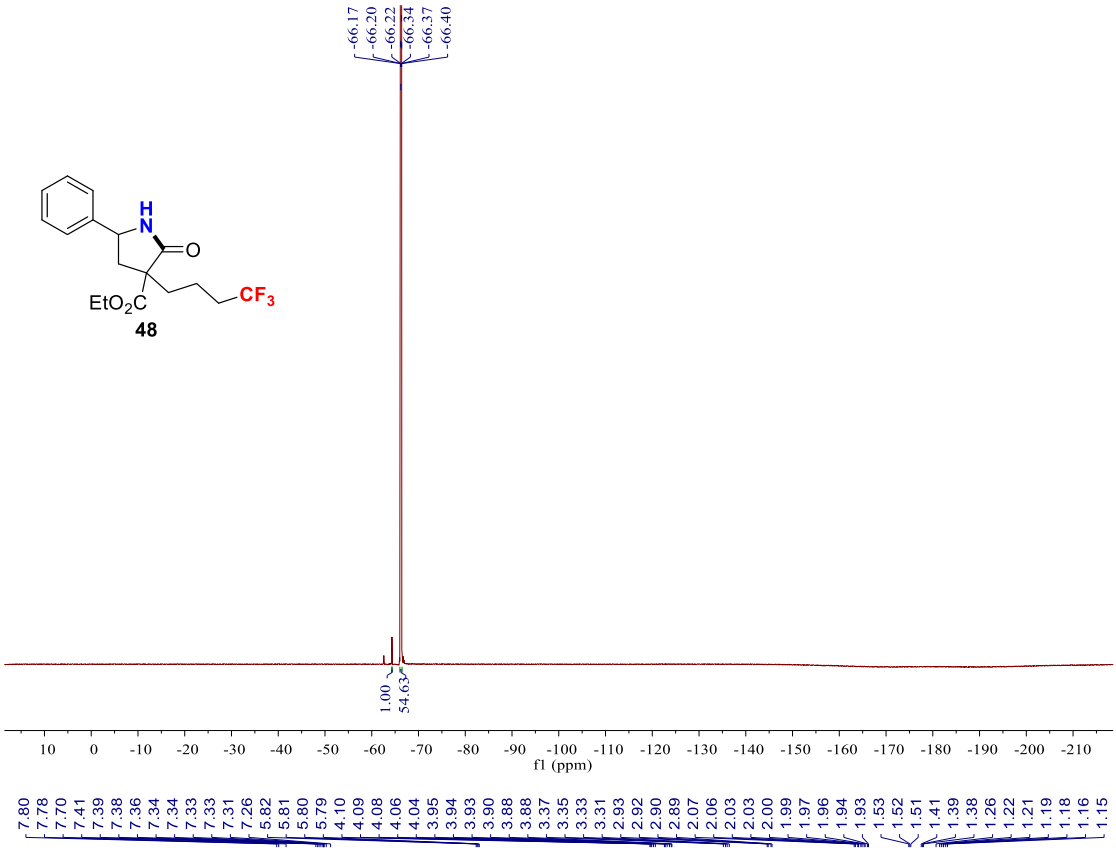

-66.25
-66.28
-66.31
CF3
N3
EtO2C CO2Et
46
1.00
112.02
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)
7.26 7.26 7.24 6.92 6.90 4.46 4.45 4.44 4.43 4.22 4.21 4.19 4.17 4.16 4.15 4.14 4.13 4.12 4.11 4.11 4.10 4.09 4.08 4.07 3.81 2.41 2.39 2.37 2.35 2.33 2.32 2.29 2.28 2.08 2.06 2.05 2.05 2.04 2.03 2.02 2.00 1.99 1.97 1.95 1.93 1.92 1.58 1.56 1.54 1.52 1.29 1.27 1.26 1.25 1.23 1.21 1.19 1.17 -0.00

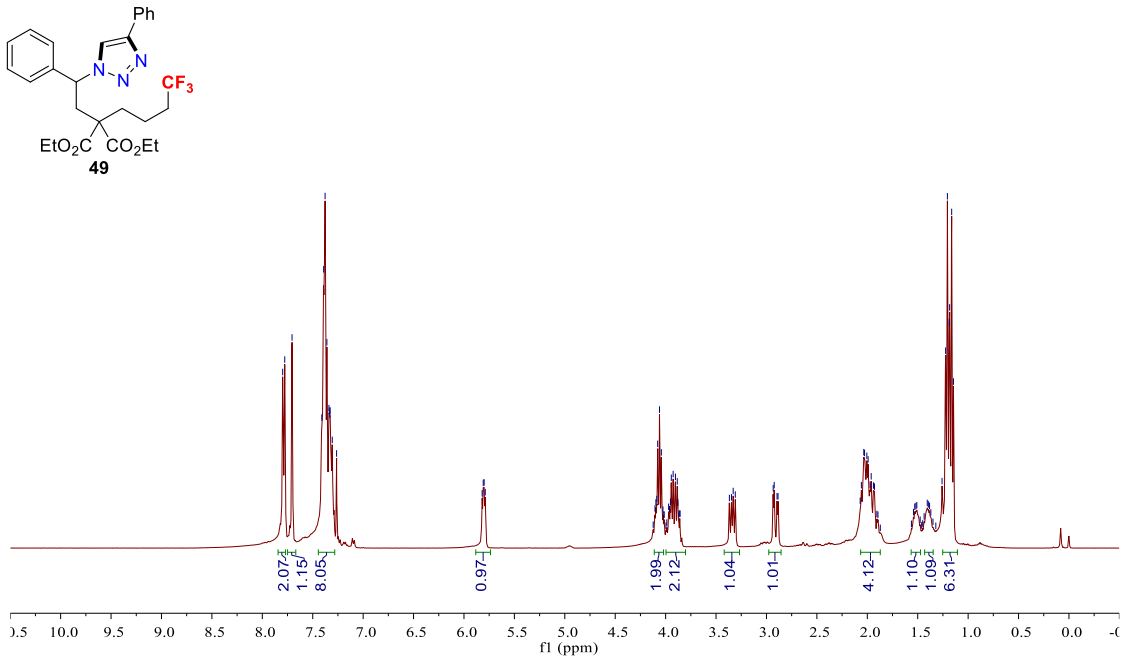

MeO
CF3
N3
EtO2C CO2Et
47
1.96
1.86
0.92
2.28
1.90
2.91
1.00
0.98
3.99
2.05
10.79
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

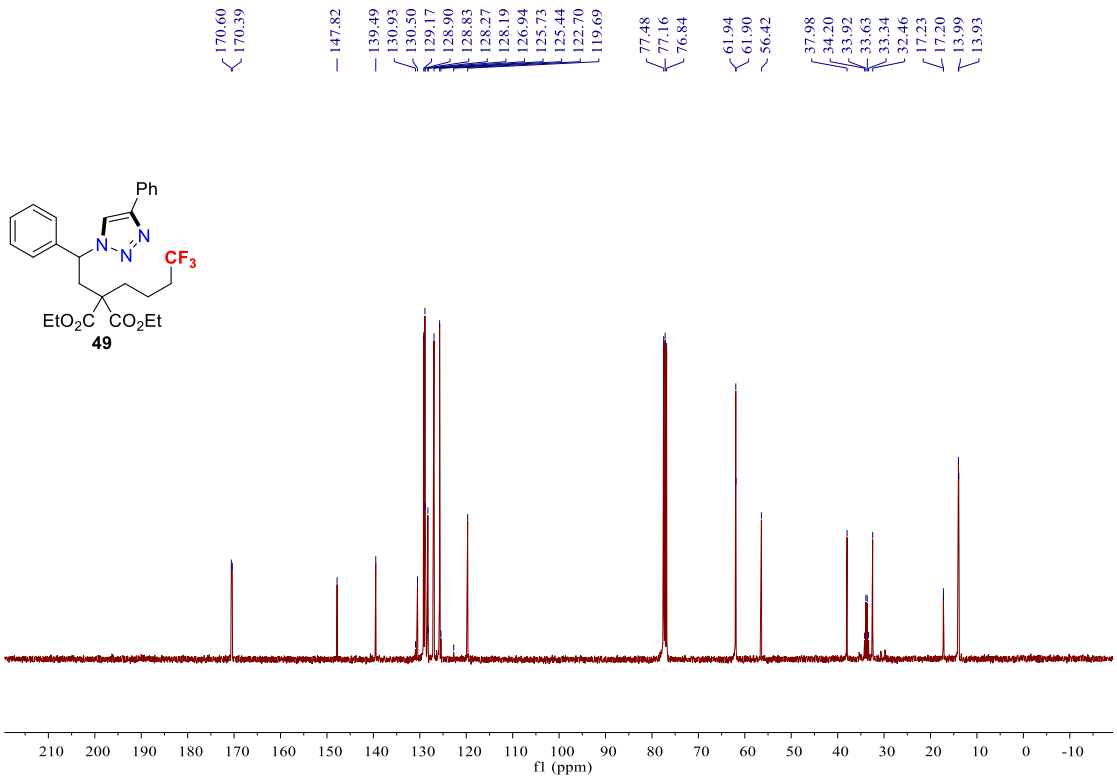

171.13
171.02
159.84
131.61
128.53
128.35
125.78
114.33
77.48
77.16
76.84
62.13
61.70
61.65
56.24
55.45
38.79
33.89
33.60
33.32
33.03
32.43
23.40
22.24
22.21
22.19
22.16
14.15
14.12
MeO
CF3
N3
EtO2C
CO2Et
47
f1 (ppm)

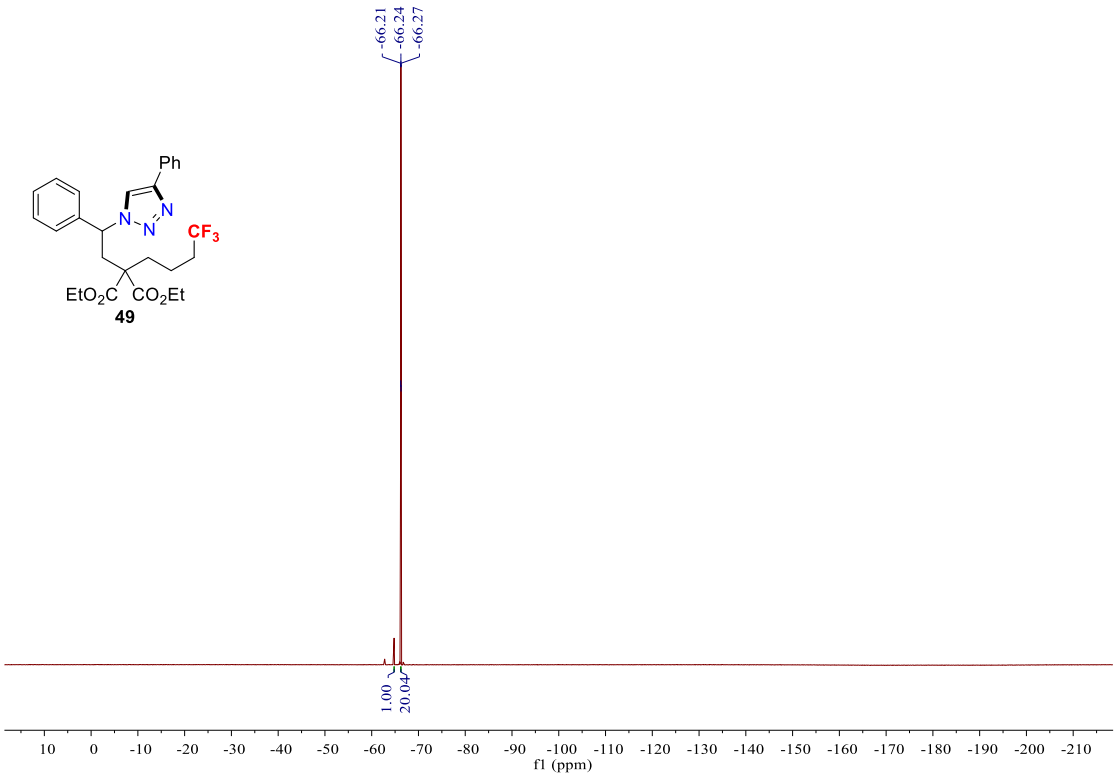

-66.29
-66.32
-66.35
MeO
CF3
N3
EtO2C
CO2Et
47
1.00
65.94
f1 (ppm)

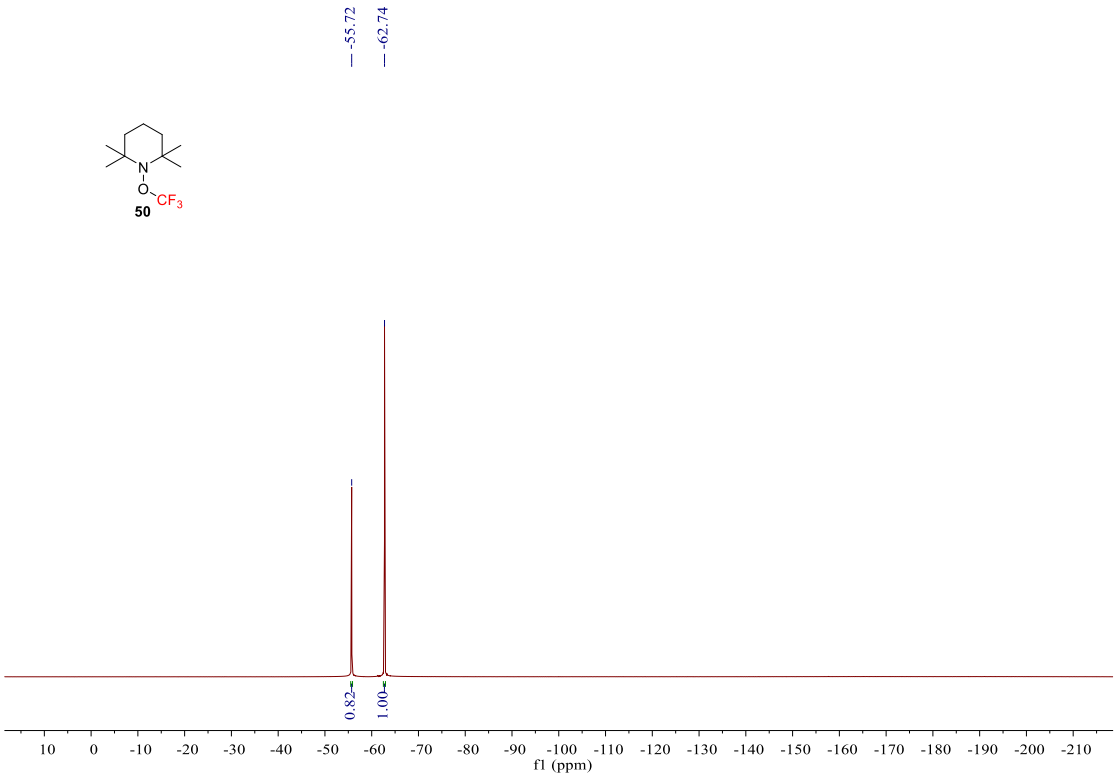

7.40 7.38 7.36 7.35 7.34 7.32 7.31 7.29 7.27 6.92 6.74 4.89 4.87 4.85 4.72 4.71 4.69 4.28 4.27 4.26 4.25 4.23 4.19 4.17 4.15 4.13 2.99 2.97 2.96 2.94 2.58 2.57 2.55 2.17 2.16 2.15 2.13 2.10 2.07 2.05 2.01 1.99 1.97 1.94 1.88 1.86 1.84 1.83 1.81 1.77 1.76 1.74 1.73 1.33 1.31 1.29 1.23 1.22 1.20
H
N
O
EtO2C
CF3
48
5.18 0.48 0.47 0.52 0.48 1.14 0.99 0.51 1.03 7.32 1.65 1.51
f1 (ppm)
175.49 174.72 171.38 170.83 141.91 141.52 131.09 131.03 129.12 128.94 128.32 128.28 128.19 126.05 125.80 125.60 125.53 122.85 122.79 77.48 77.16 76.84 62.06 61.87 56.37 56.02 55.44 55.38 41.45 40.48 34.41 34.13 34.08 33.84 33.79 33.51 33.24 33.05 17.61 17.58 17.54 17.51 14.19
H
N
O
EtO2C
CF3
48
f1 (ppm)

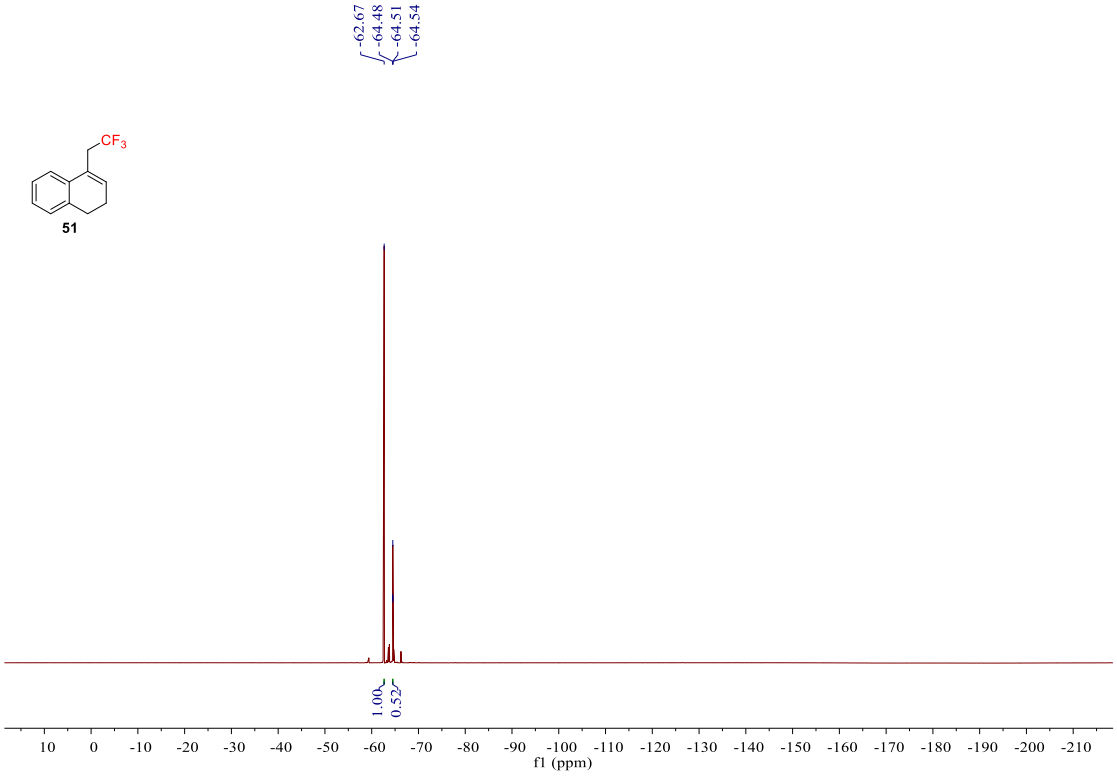

-66.17
-66.20
-66.22
-66.34
-66.37
-66.40
H
N
O
EtO2C
CF3
48
1.00
54.63
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)
7.80 7.78 7.70 7.41 7.39 7.38 7.36 7.34 7.34 7.33 7.33 7.31 7.26 5.82 5.81 5.80 5.79 4.10 4.09 4.08 4.06 4.04 3.95 3.94 3.93 3.90 3.88 3.88 3.37 3.35 3.33 3.31 2.93 2.92 2.90 2.89 2.07 2.06 2.03 2.03 2.00 1.99 1.97 1.96 1.94 1.93 1.53 1.52 1.51 1.41 1.39 1.38 1.26 1.22 1.21 1.19 1.18 1.16 1.15

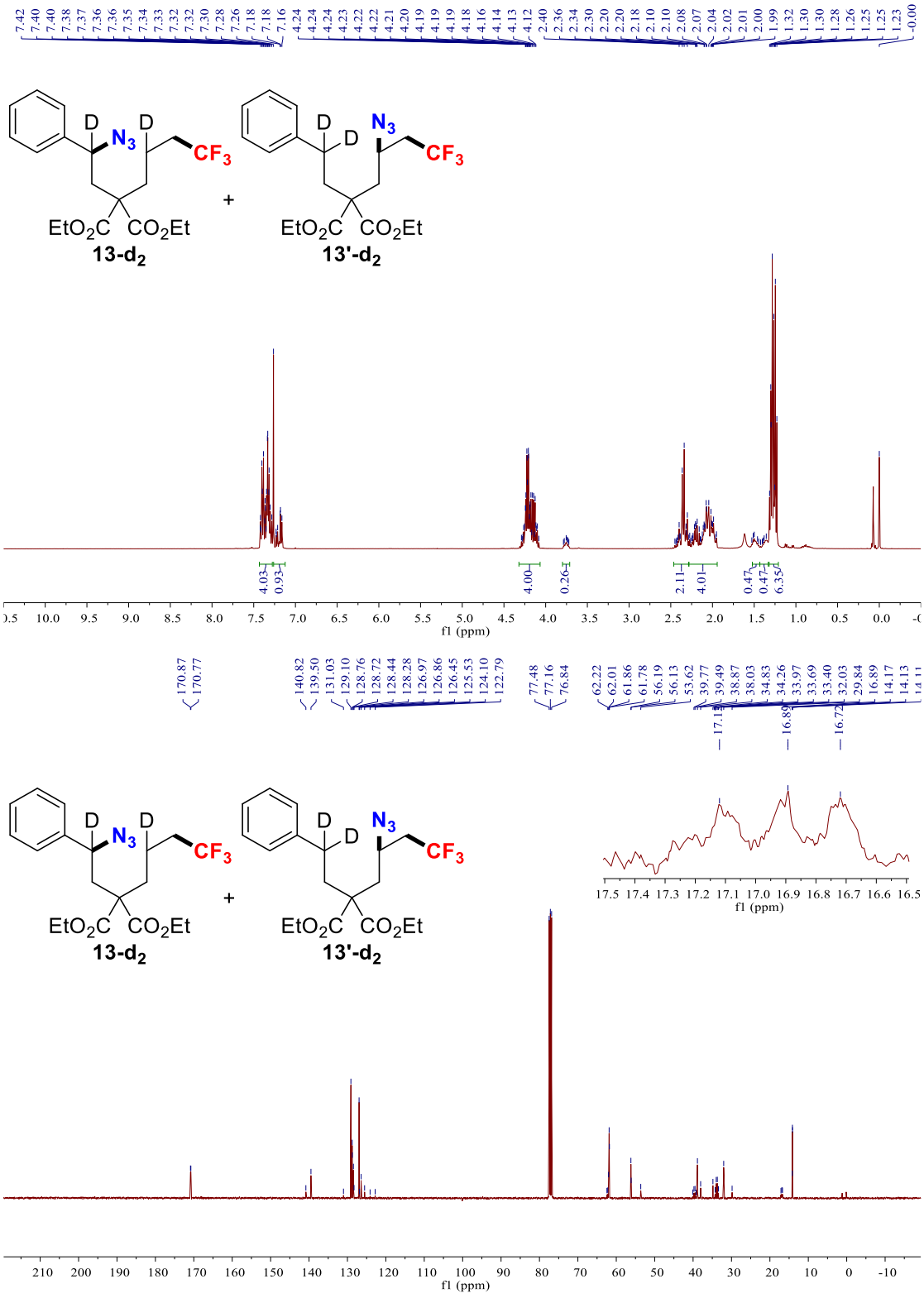

Ph
N
N
N
CF3
EtO2C
CO2Et
49
2.07
1.15
8.05
0.97
1.99
2.12
1.04
1.01
4.12
1.10
1.09
6.31
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

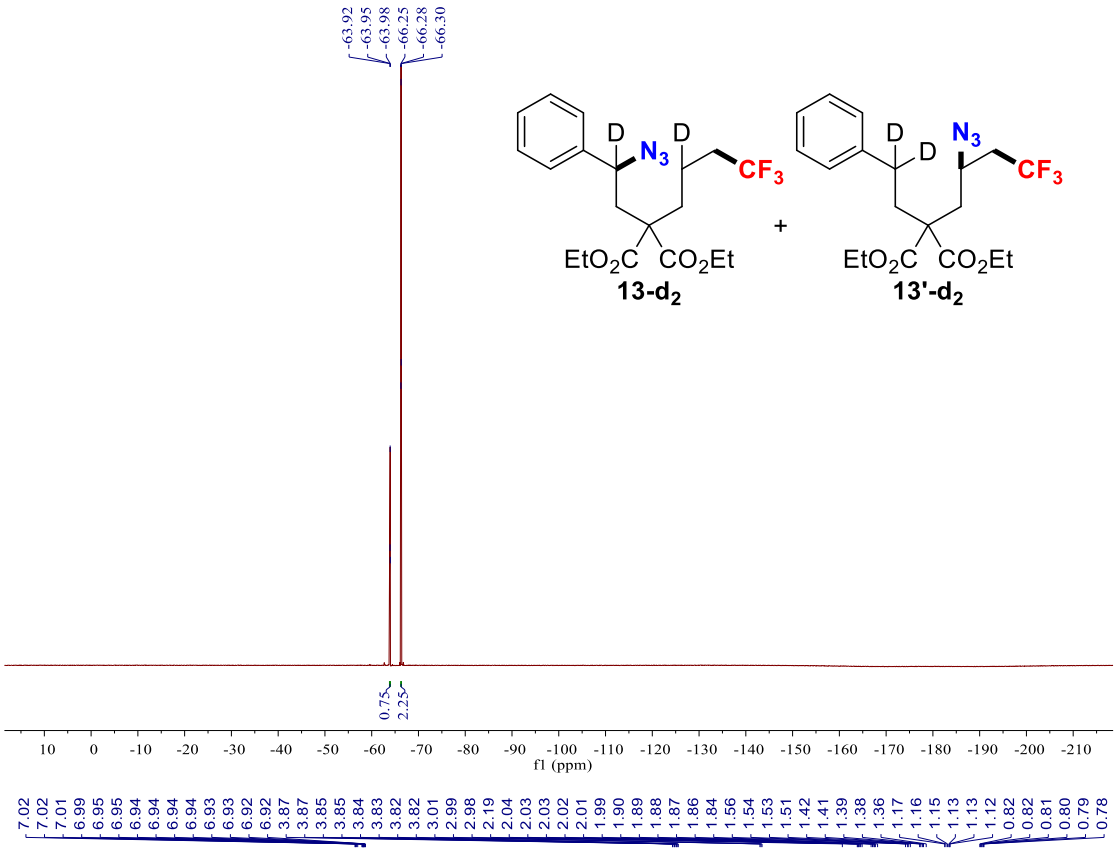

170.60
170.39
147.82
139.49
130.93
130.50
129.17
128.90
128.83
128.27
128.19
126.94
125.73
125.44
122.70
119.69
77.48
77.16
76.84
61.94
61.90
56.42
37.98
34.20
33.92
33.63
33.34
32.46
17.23
17.20
13.99
13.93
Ph
CF3
EtO2C CO2Et
49
f1 (ppm)

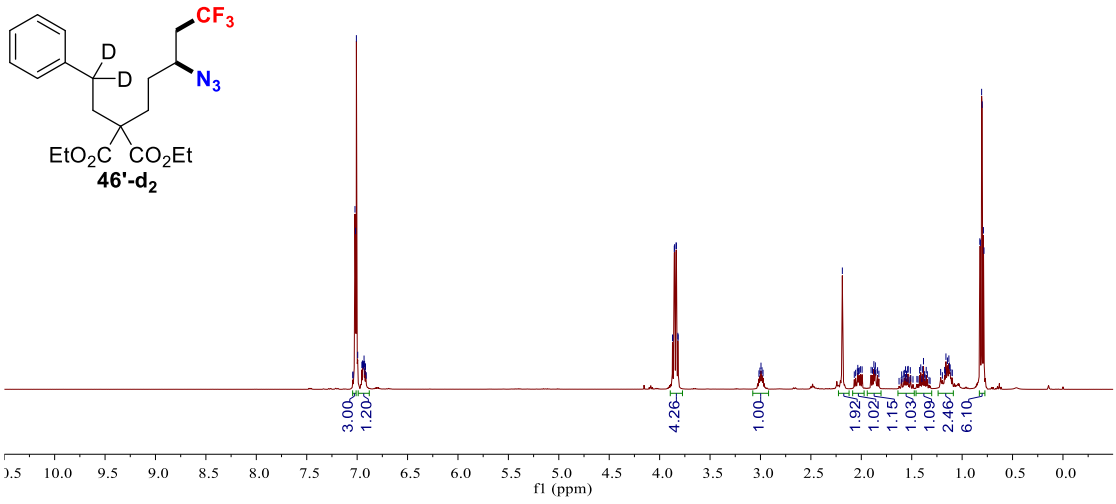

-66.21
-66.24
-66.27
Ph
CF3
EtO2C CO2Et
49
1.00
20.04
f1 (ppm)

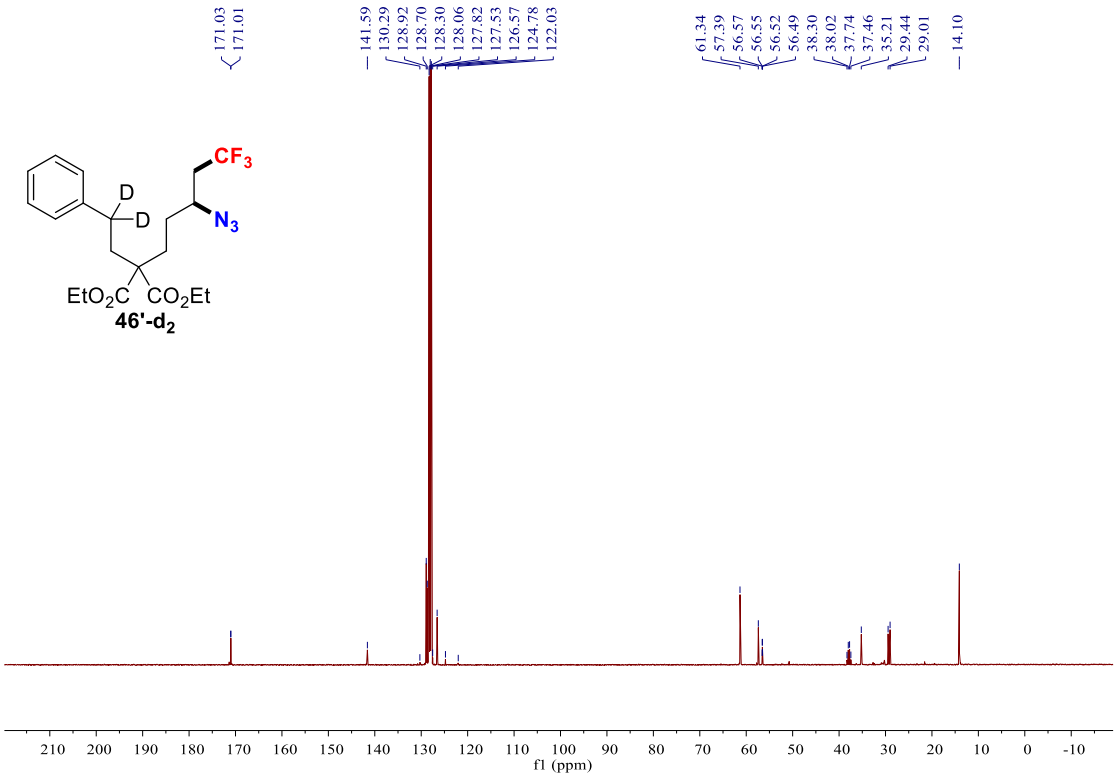

-55.72
-62.74
N
O
CF3
50
0.82
1.00
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

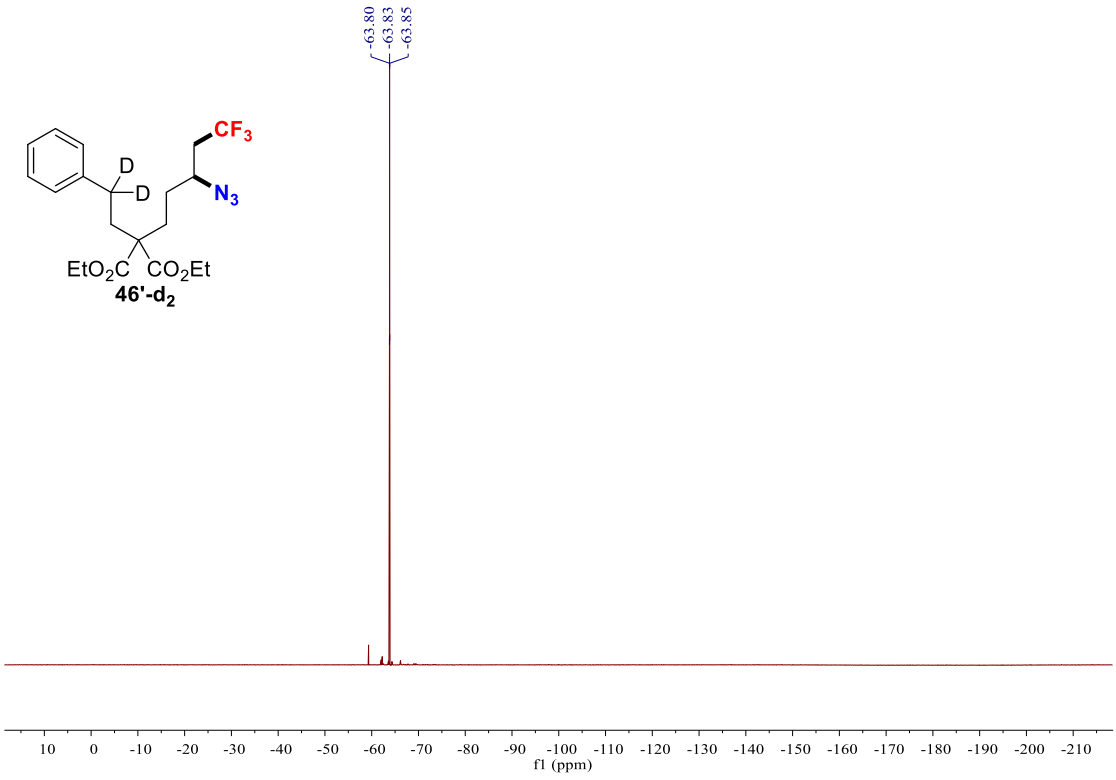

-62.67
-64.48
-64.51
-64.54
CF3
51
1.00
0.52
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

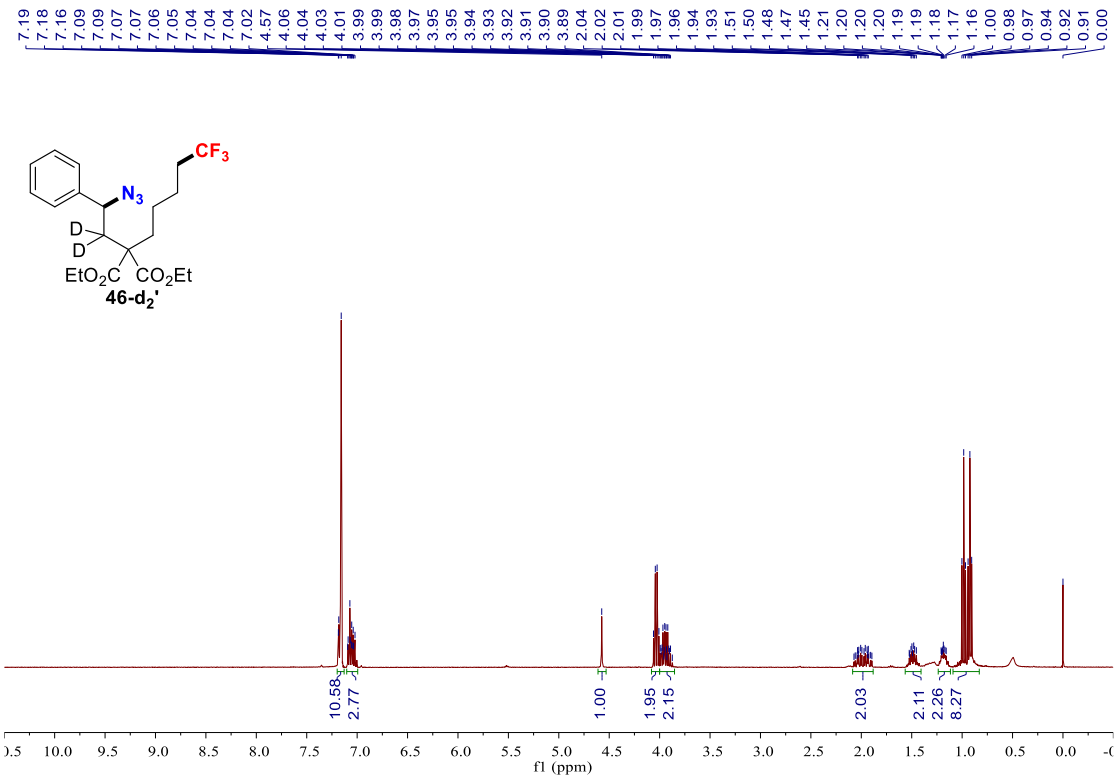

13-d2
13'-d2
fl (ppm)

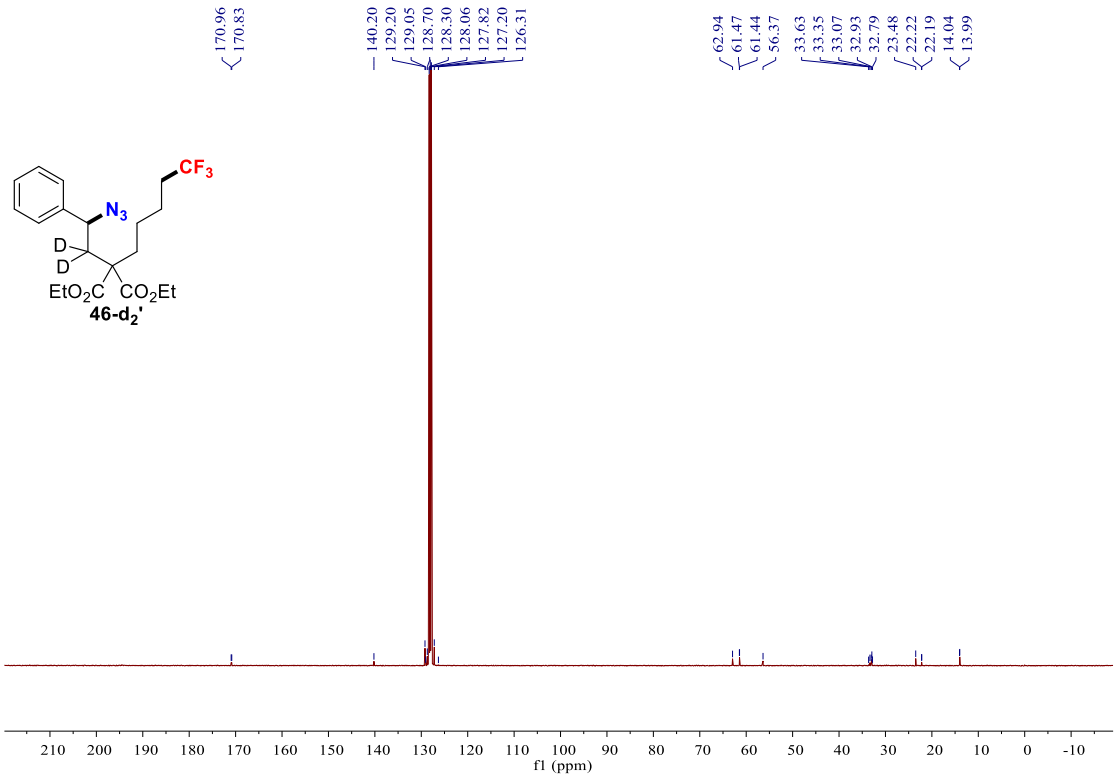

-63.92
-63.95
-63.98
-66.25
-66.28
-66.30
D
N3
D
CF3
EtO2C
CO2Et
13-d2
+
D
D
N3
CF3
EtO2C
CO2Et
13'-d2
0.75
2.25
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

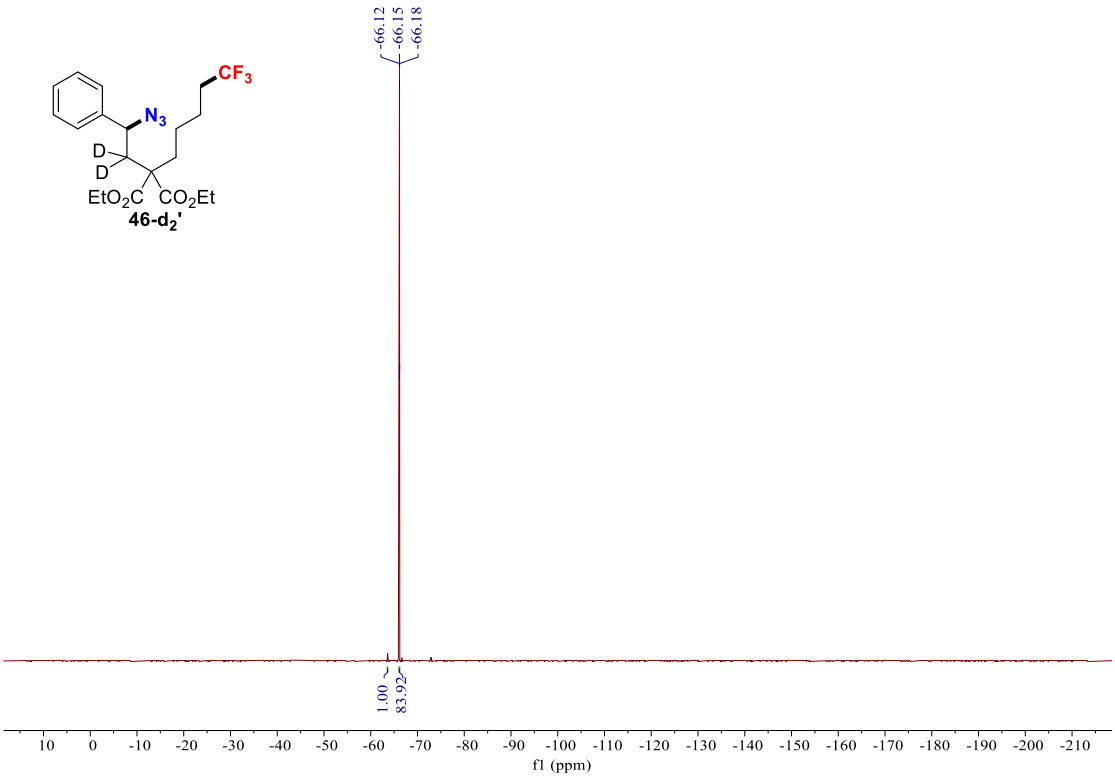

CF3
D
D
N3
EtO2C
CO2Et
46'-d2
3.00
1.20
4.26
1.00
1.92
1.02
1.15
1.03
1.09
2.46
6.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


171.03
171.01
141.59
130.29
128.92
128.70
128.30
128.06
127.82
127.53
126.57
124.78
122.03
61.34
57.39
56.57
56.55
56.52
56.49
38.30
38.02
37.74
37.46
35.21
29.44
29.01
14.10
CF3
D
D
N3
EtO2C CO2Et
46'-d2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

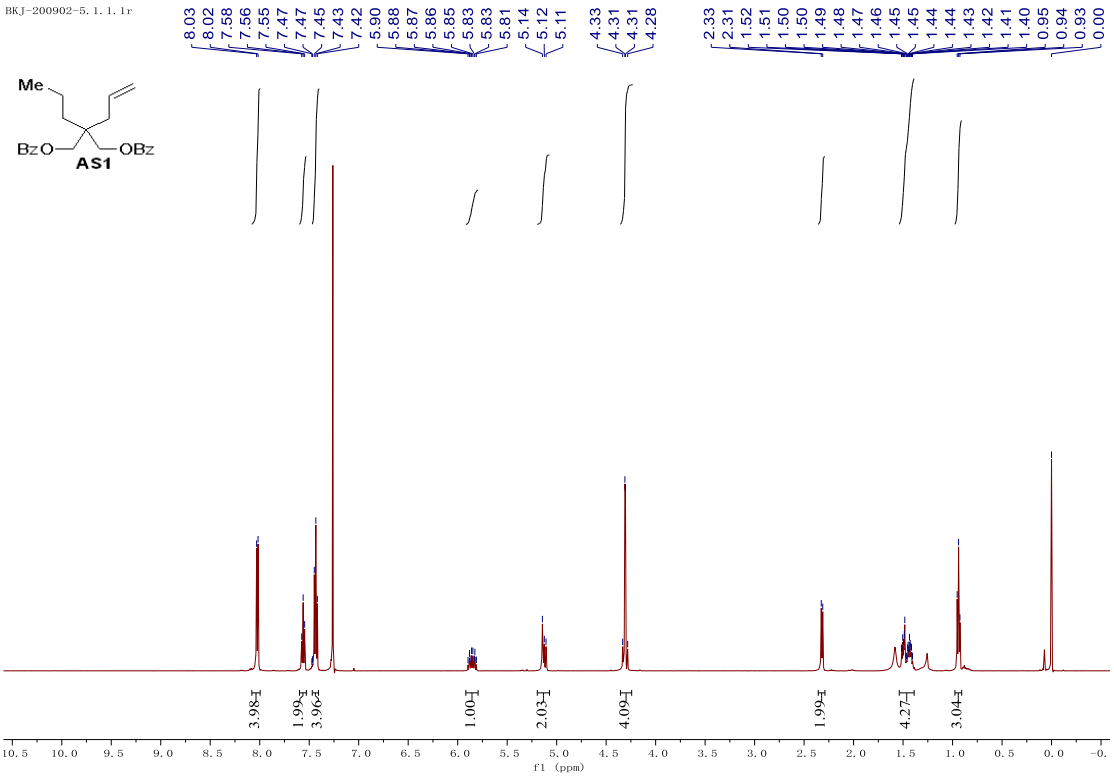

-63.80
-63.83
-63.85
CF3
D
D
N3
EtO2C CO2Et
46'-d2
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

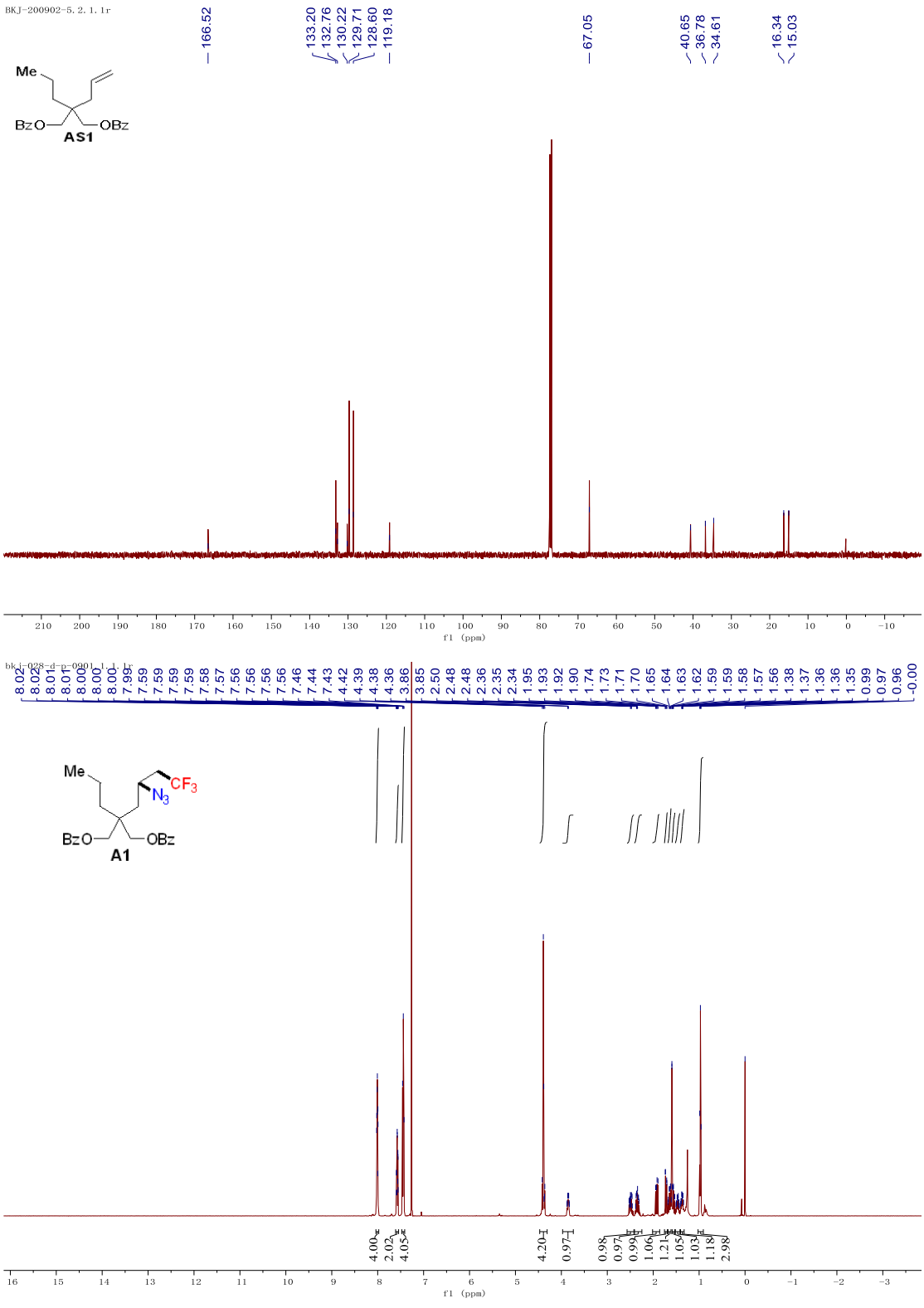

7.19 7.18 7.16 7.09 7.09 7.07 7.07 7.06 7.05 7.04 7.04 7.04 7.02 4.57 4.06 4.04 4.03 4.01 3.99 3.99 3.98 3.97 3.95 3.95 3.94 3.93 3.92 3.91 3.90 3.89 2.04 2.02 2.01 1.99 1.97 1.96 1.94 1.93 1.51 1.50 1.48 1.47 1.45 1.21 1.20 1.20 1.19 1.19 1.18 1.17 1.16 1.00 0.98 0.97 0.94 0.92 0.91 0.00
CF3
N3
D
D
EtO2C CO2Et
46-d2'
10.58
2.77
1.00
1.95
2.15
2.03
2.11
2.26
8.27
f1 (ppm)

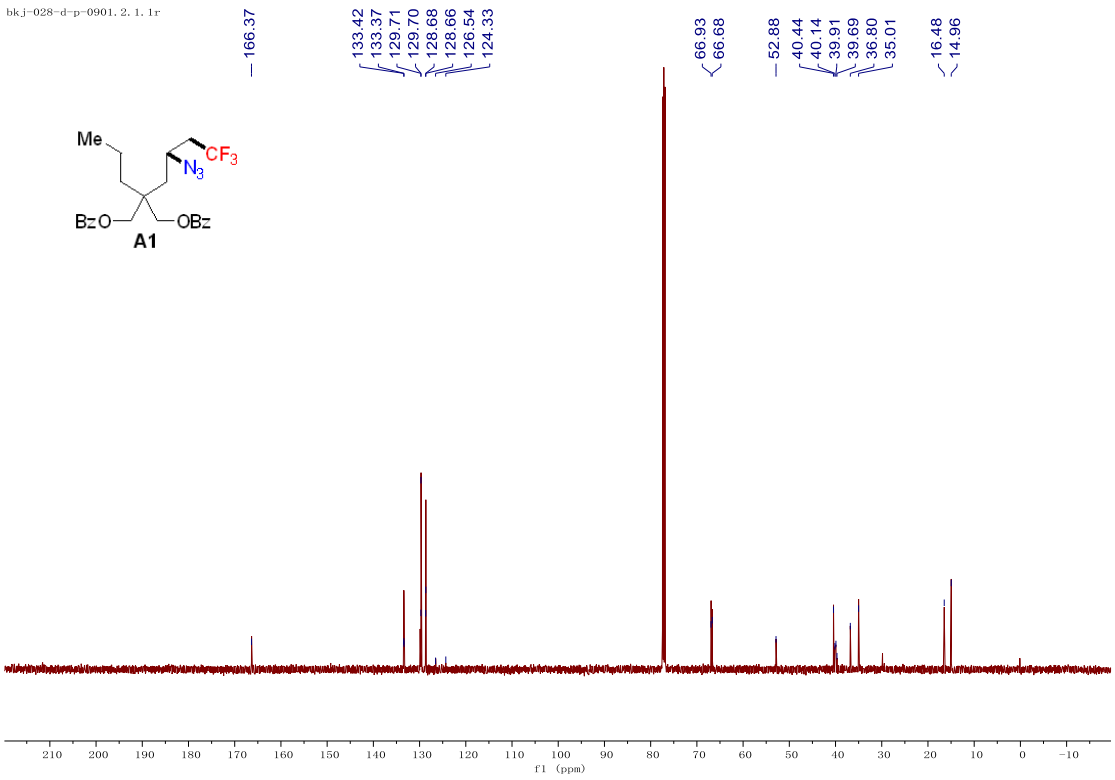

170.96 170.83 140.20 129.20 129.05 128.70 128.30 128.06 127.82 127.20 126.31 62.94 61.47 61.44 56.37 33.63 33.35 33.07 32.93 32.79 23.48 22.22 22.19 14.04 13.99
CF3
N3
D
D
EtO2C CO2Et
46-d2'
f1 (ppm)

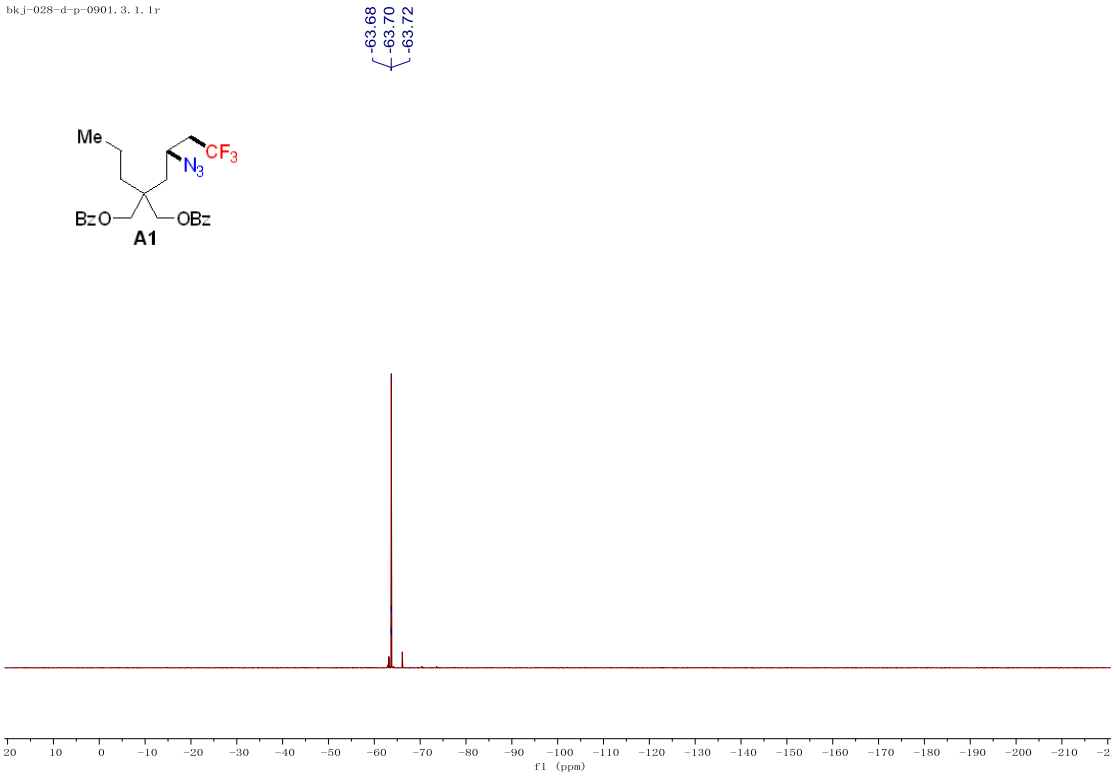


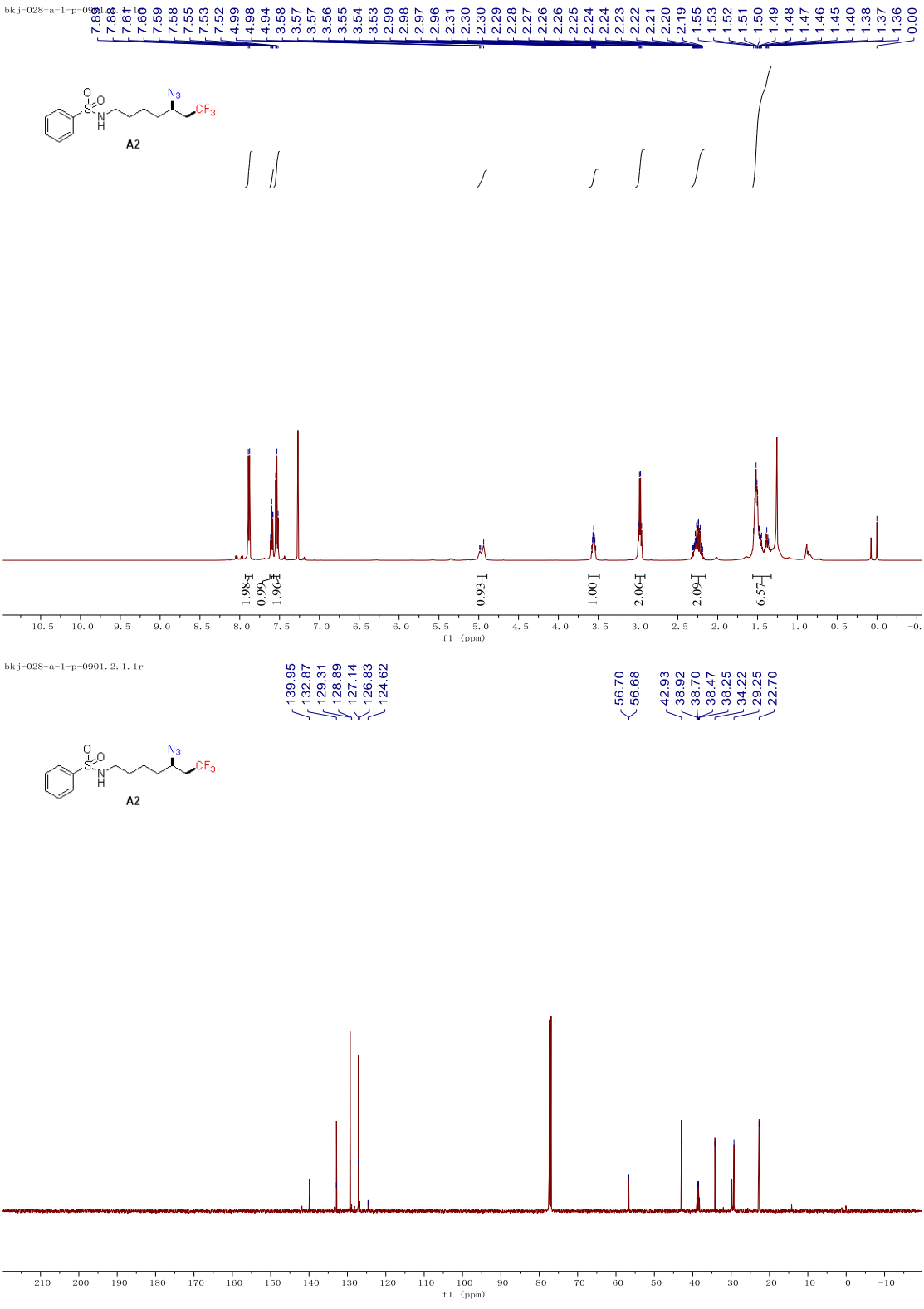
Alternative testing:

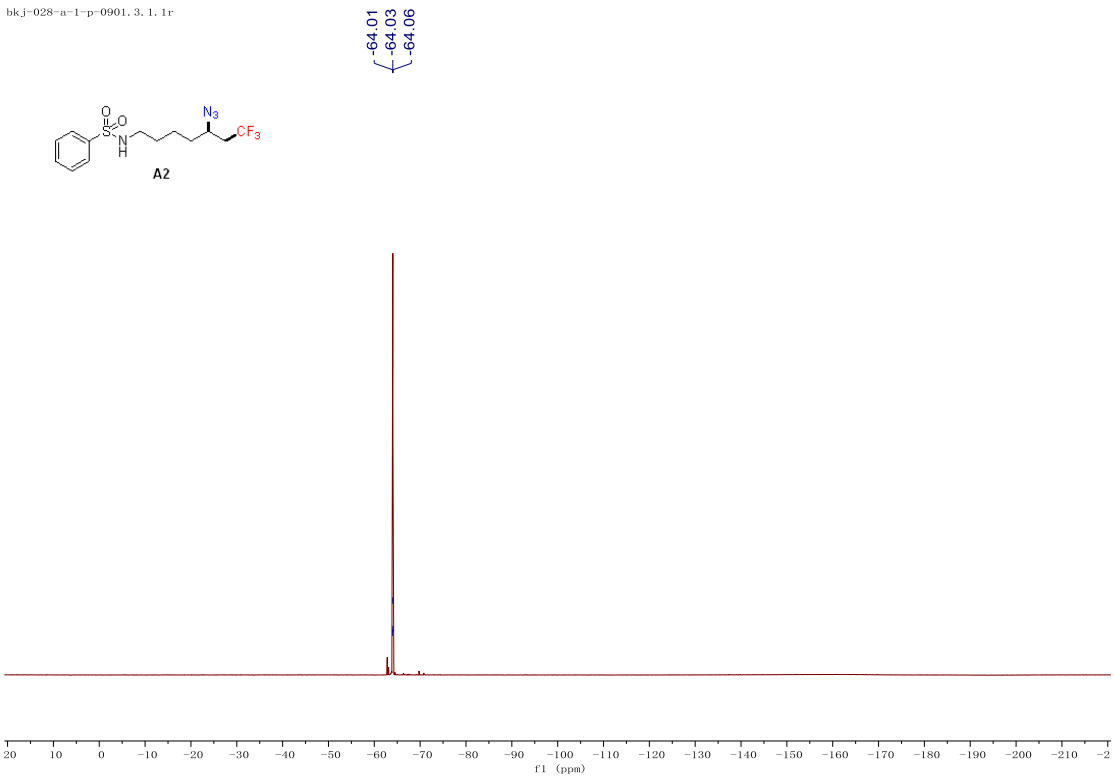


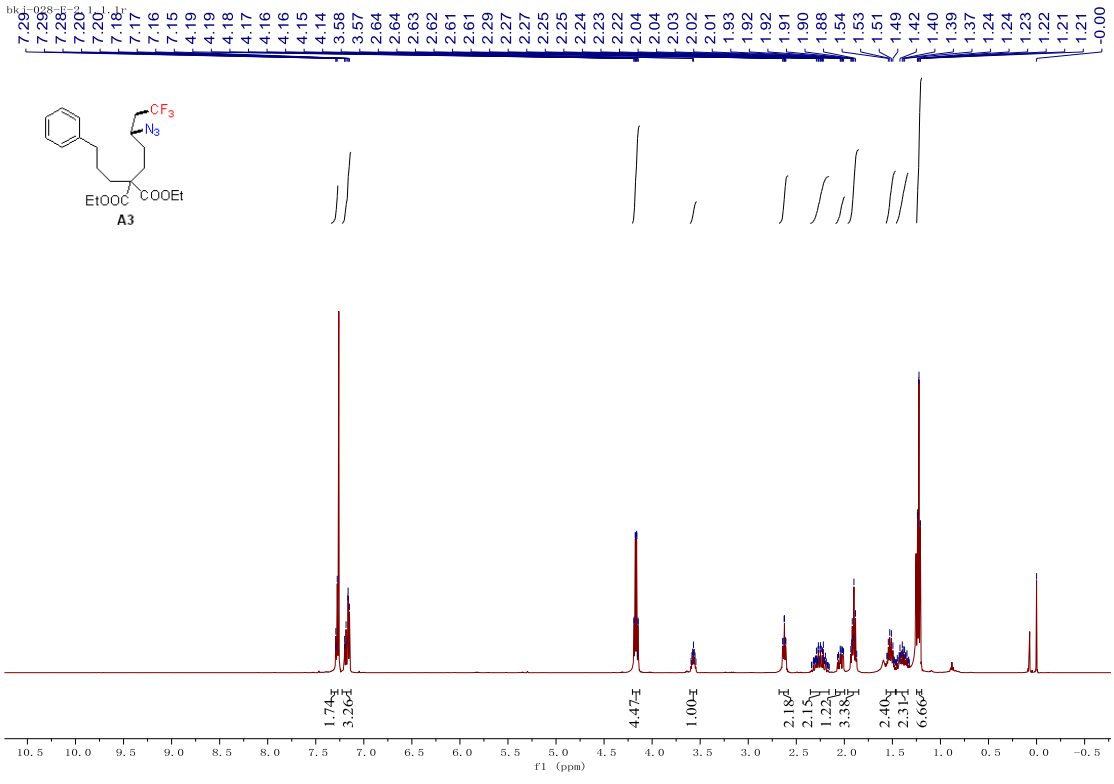

BKJ-200902-5.2.1.1r
166.52
133.20
132.76
130.22
129.71
128.60
119.18
67.05
40.65
36.78
34.61
16.34
15.03
Me
BzO
OBz
AS1
f1 (ppm)
Me
CF3
N3
BzO
OBz
A1
4.00
2.02
4.05
4.20
0.97
0.98
0.97
0.99
1.06
1.21
1.05
1.03
1.18
2.98
f1 (ppm)

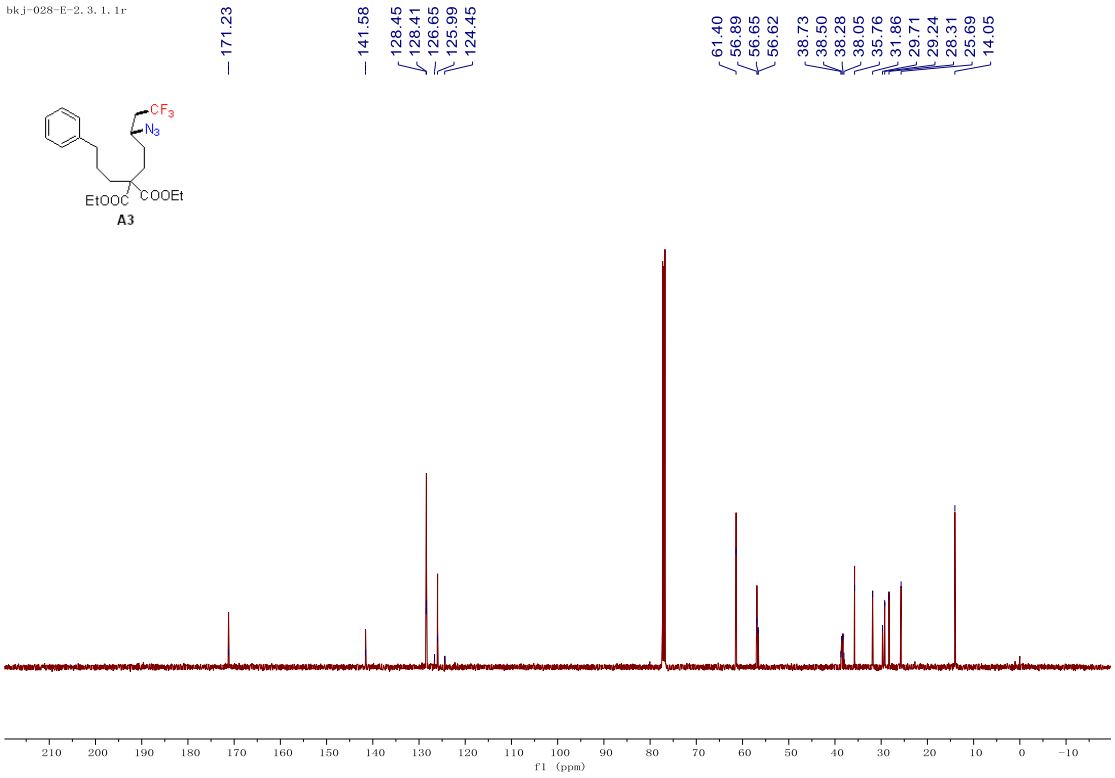

bkj-028-d-p-0901.2.1.1r
166.37
133.42
133.37
129.71
129.70
128.68
128.66
126.54
124.33
66.93
66.68
52.88
40.44
40.14
39.91
39.69
36.80
35.01
16.48
14.96
Me
CF3
N3
BzO
OBz
A1
f1 (ppm)

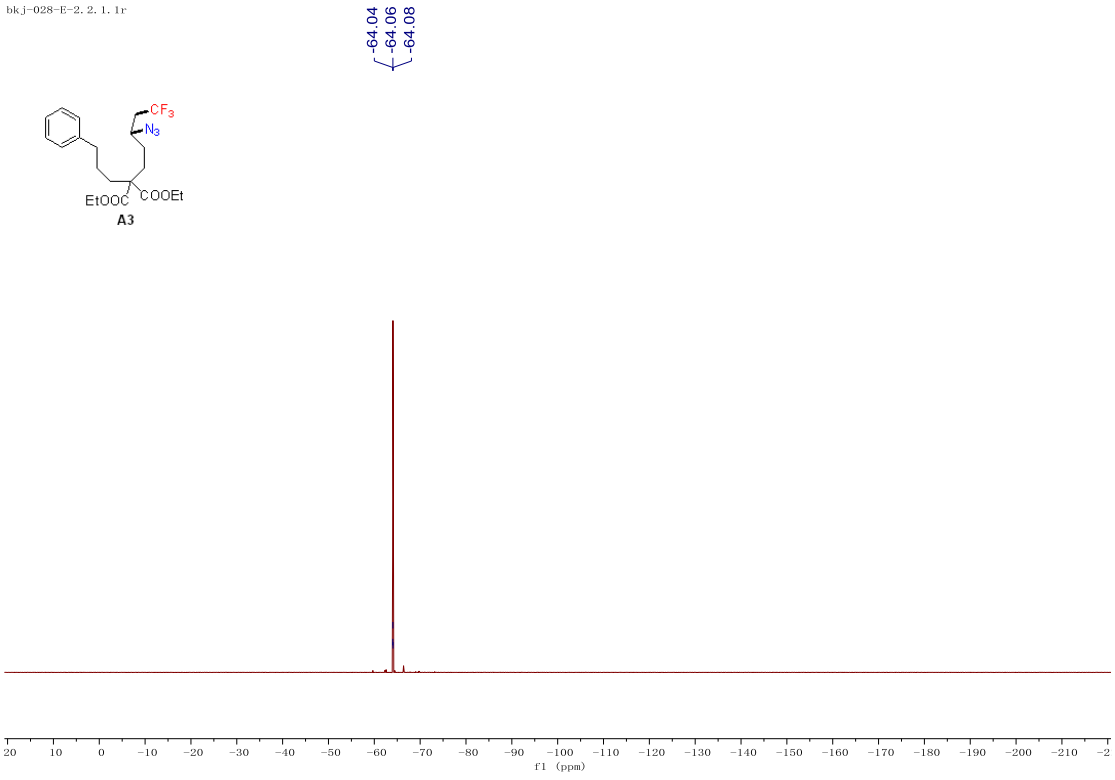

bkj-028-d-p-0901.3.1.1r
-63.68
-63.70
-63.72
Me
CF3
N3
BzO
OBz
A1
f1 (ppm)


bkj-028-a-1-p-0901.2.1.1r
7.89 7.88 7.61 7.60 7.59 7.58 7.55 7.53 7.52 4.99 4.98 4.94 3.58 3.57 3.56 3.55 3.54 3.53 2.99 2.98 2.97 2.96 2.31 2.30 2.29 2.28 2.27 2.26 2.26 2.25 2.24 2.24 2.23 2.22 2.21 2.20 2.19 1.55 1.53 1.52 1.51 1.50 1.49 1.48 1.47 1.46 1.45 1.40 1.38 1.37 1.36 0.00
A2
1.98 0.96 1.96 0.93 1.00 2.06 2.09 6.57
f1 (ppm)
bkj-028-a-1-p-0901.2.1.1r
139.95 132.87 129.31 128.89 127.14 126.83 124.62
56.70 56.68 42.93 38.92 38.70 38.47 38.25 34.22 29.25 22.70
A2
f1 (ppm)


bkj-028-a-1-p-0901.3.1.1r
-64.01
-64.03
-64.06
A2
f1 (ppm)


7.29
7.28
7.20
7.18
7.17
7.16
7.15
4.19
4.18
4.17
4.16
4.15
4.14
3.58
3.57
2.64
2.63
2.62
2.61
2.29
2.27
2.25
2.24
2.23
2.22
2.04
2.03
2.02
2.01
1.93
1.92
1.91
1.90
1.88
1.54
1.53
1.51
1.49
1.42
1.40
1.39
1.37
1.24
1.23
1.22
1.21
-0.00
A3
1.74
3.26
4.47
1.00
2.18
2.15
1.23
3.38
2.40
2.31
6.66
f1 (ppm)


bkj-028-E-2.3.1.1r
171.23
141.58
128.45
128.41
126.65
125.99
124.45
61.40
56.89
56.65
56.62
38.73
38.50
38.28
38.05
35.76
31.86
29.71
29.24
28.31
25.69
14.05
CF3
N3
EtOOC
COOEt
A3
f1 (ppm)


bkj-028-E-2.2.1.1r
-64.04
-64.06
-64.08
CF3
N3
EtOOC
COOEt
A3
f1 (ppm)