

Electronic Supplementary Information

A one-pot synthesis of [1,2,3]triazolo[1,5-*a*]quinoxalines from 1-azido-2-isocyanoarenes with high bond-forming efficiency

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Table of Contents

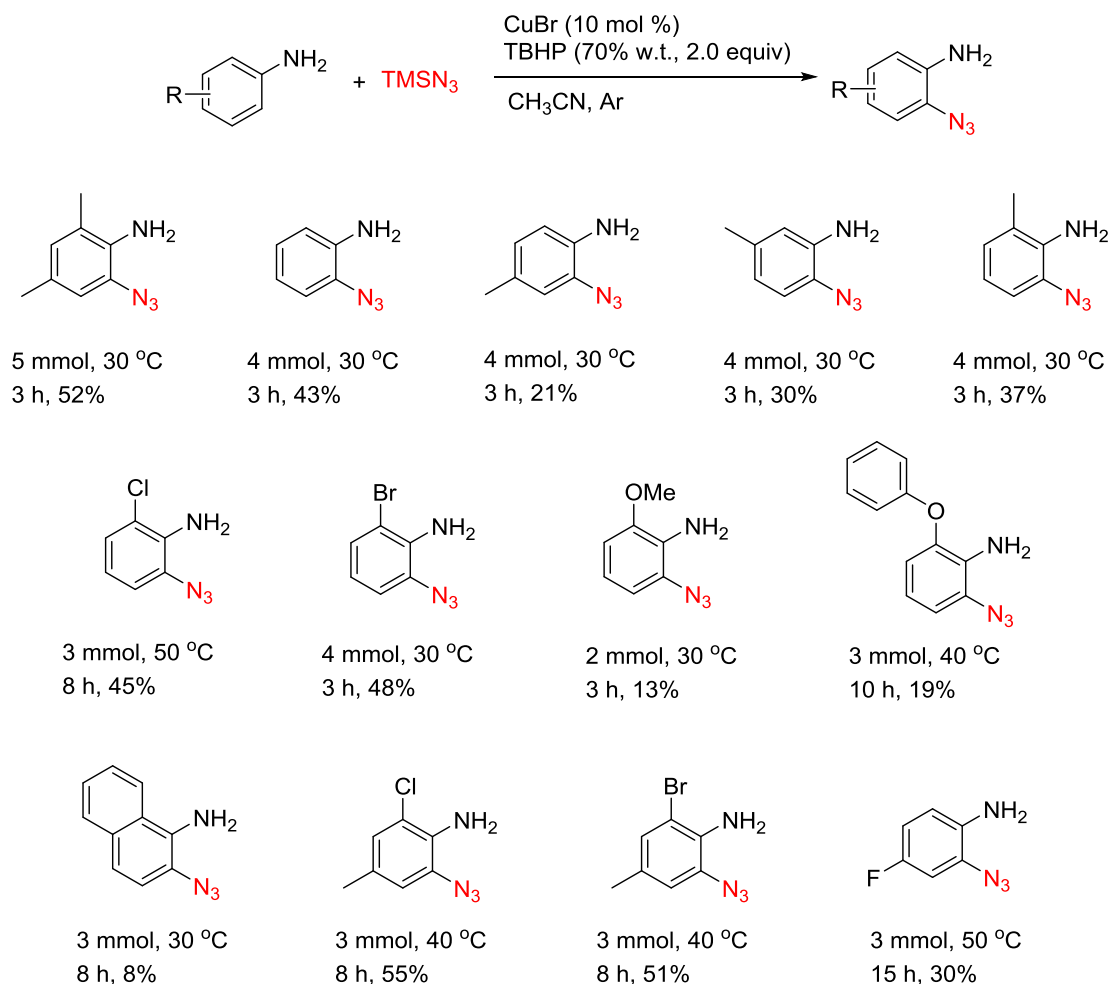
1. General Information	S2
2. Preparation of the Starting Materials.....	S3
2.1 Azidation of Anilines	S3
2.2 Preparation of 1-Azido-2-isocyanoarenes.....	S4
2.3 Preparation of Alkynes.....	S5
2.4 Preparation of Aldehydes	S5
3. Reaction Optimization and General Procedures.....	S6
3.1 Reaction Optimization for the Synthesis of 3a and 5a	S6
3.2 General Procedures for the Synthesis of 3 , and 5a	S8
3.3 General Procedures for the Synthesis of 6	S9
3.4 General Procedure for the Synthesis of 7	S11
4. Characterization Data	S13
5. References	S39
6. Copies of ¹ H, ¹³ C or ¹⁹ F NMR Spectra	S39

1. General Information

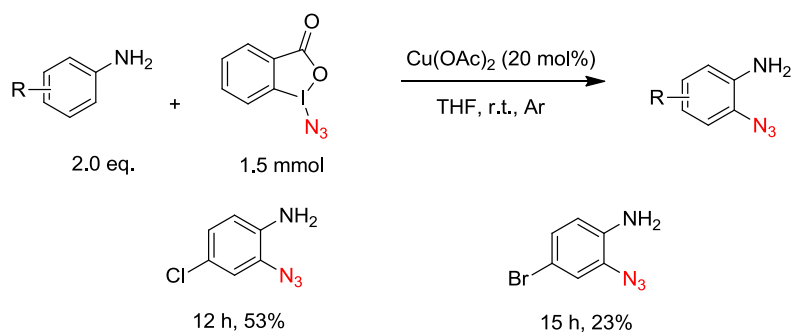
All the solvents and reagents were purchased from commercial suppliers. ^1H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on a 400 MHz or/and 500 MHz Bruker FT-NMR spectrometers. All chemical shifts were given as δ value (ppm) with reference to tetramethylsilane (TMS) as an internal standard. The peak patterns are indicated as follows: s, singlet; d, doublet; t, triplet; m, multiplet; q, quartet. The coupling constants, J , are reported in Hertz (Hz). High Resolution Mass (MS) analysis was obtained using on a LC/MSD TOF spectrometer system with Electrospray Ionization (ESI). Melting points were measured on a Mel-Temp apparatus and are uncorrected. IR was recorded on a Bruker Tensor 27 FT-IR spectrometer. Reactions were monitored by thin-layer chromatography (TLC) carried out on commercial silica gel plates (GF254) under UV light. Flash chromatography was performed on silica gel 60 (200–300 mesh).

2. Preparation of the Starting Materials

2.1 Azidation of Anilines

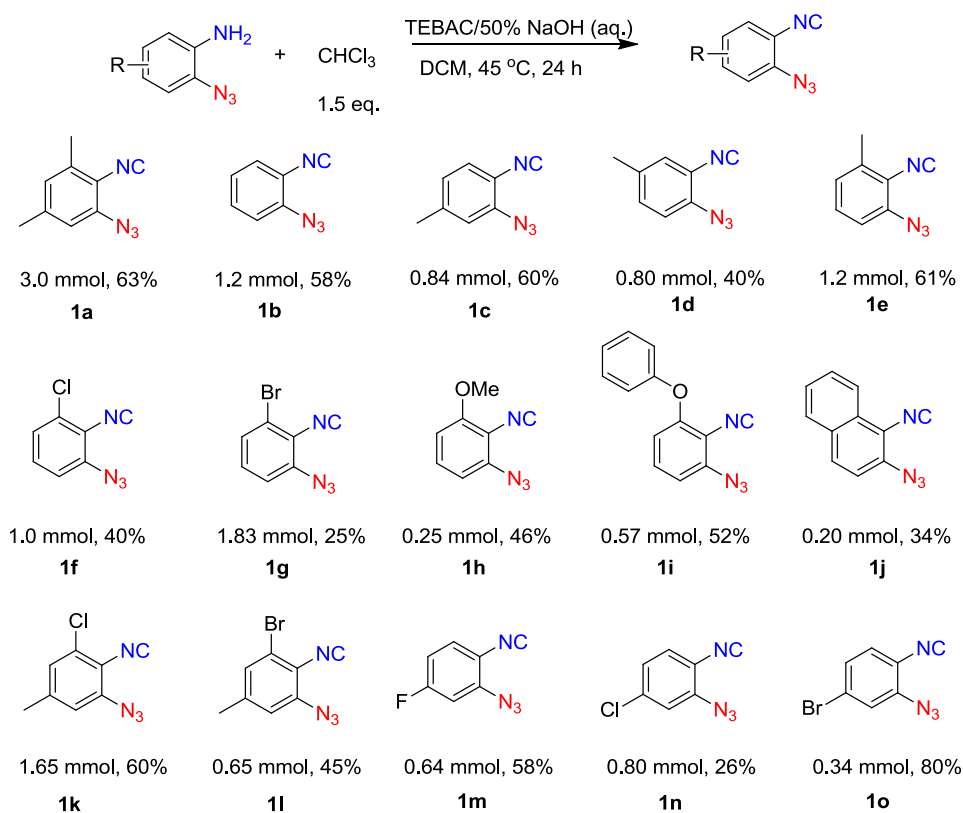


The above 2-azidoanilines were prepared by following a reported procedure with minor changes.¹ Anilines (1.0 equiv, 2.0-5.0 mmol scales) and CuBr (10 mol%) were added to a 25 mL Schlenk tube in Ar, followed by addition of TMSN₃ (1.5 equiv), TBHP (70 % w.t. in water, 2.0 equiv) and CH₃CN (4-8 mL). The mixture was stirred in Ar at the optimal temperature. After completion of the reaction, the solution was diluted with ethyl acetate, and concentrated under vacuum. The crude product was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 100/1 to 50/1) to afford the desired 2-azidoanilines.



The above 2-azidoanilines were prepared by following a reported procedure.² Togni azide (1.5 mmol) and Cu(OAc)₂ (20 mol%) were added to THF (6.0 mL) in a 25 mL Schlenk tube, followed by addition of aniline (2.0 equiv). The mixture was stirred at room temperature in Ar for 12-15 h. The solution was then diluted with ethyl acetate, and concentrated in vacuum to afford the crude product, which was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 100/1 to 50/1) to afford the desired 2-azidoanilines.

2.2 Preparation of 1-Azido-2-isocyanoarenes

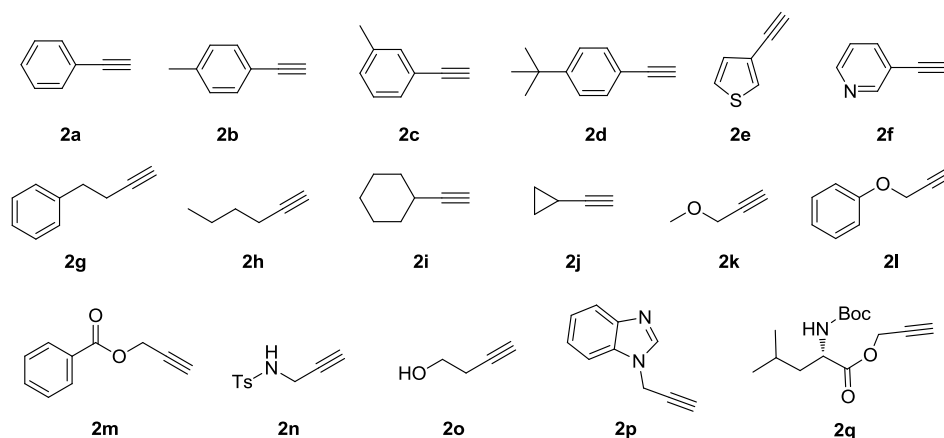


In a dry 25 mL round-bottom flask, 2-azidoaniline (1.0 equiv, 0.2-3.0 mmol), chloroform (1.5 equiv), dichloromethane (2-6 mL), aqueous sodium hydroxide (50%

solution, 3.6 equiv), and benzyltriethylammonium chloride (TEBAC, 0.14 mol %) were added. Then the mixture was heated under reflux for 24 h. After cooling down to room temperature, the solution was concentrated under vacuum and the crude reaction mixture was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate =100/1 to 50/1) to afford the desired product **1**.³

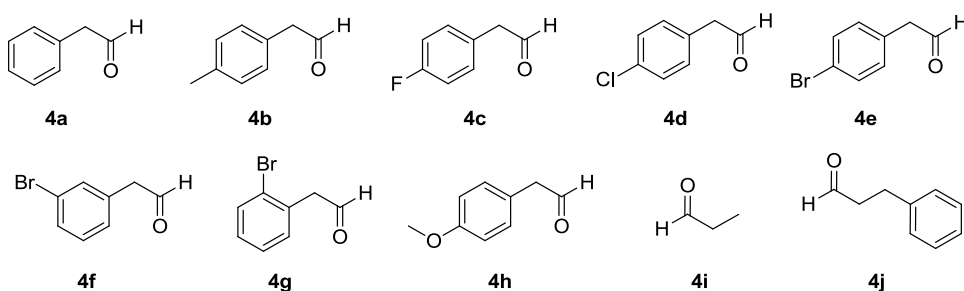
2.3 Preparation of Alkynes

Alkynes **2a–2k** and **2o** were purchased. Others (**2l–2n**, **2p** and **2q**) were prepared according to a reported literature.⁴



2.4 Preparation of Aldehydes

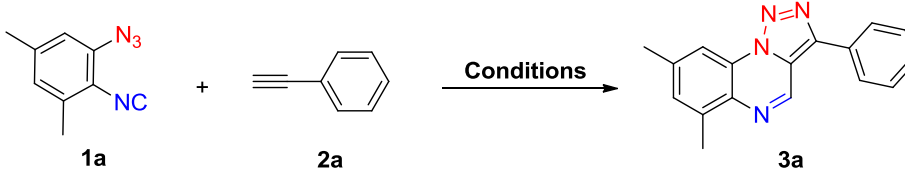
Aldehydes **4a**, **4i** and **4j** were purchased. Others (**4b–4h**) were prepared by oxidation of the corresponding aryl ethanols according to a reported literature.⁵



3. Reaction Optimization and General Procedures

3.1 Reaction Optimization for the Synthesis of 3a and 5a

Table S1. Reaction Optimization for the Synthesis of 3a^a

					
Entry	Catalyst (mol%)	Additive (equiv)	Solvent	Temp. (°C) /Time (h)	Isolated Yield (%)
1	CuSO ₄ (10)	Na ascorbate (0.2)	DMSO	50/18	N.R.
2	CuI (10)	Na ₂ CO ₃ (1.2)	DMSO	25/15	N.R.
3	CuI (10)	Na ₂ CO ₃ (1.2)	DMSO	45/15	trace
4	CuI (10)	Na ₂ CO ₃ (1.2)	DMSO	65/10	44
5	CuI (10)	--	DMSO	65/12	N.R.
6	CuI (10)	Na ₂ CO ₃ (1.2)	DMF	65/12	trace
7	CuI (10)	Na ₂ CO ₃ (1.2)	CH ₃ CN	65/15	N.R.
8	CuI (10)	Na ₂ CO ₃ (1.2)	EtOH	65/15	N.R.
9	CuCl (10)	Na ₂ CO ₃ (1.2)	DMSO	65/12	40
10	CuBr (10)	Na ₂ CO ₃ (1.2)	DMSO	65/12	40
11	CuTc (10)	Na ₂ CO ₃ (1.2)	DMSO	65/12	25
12	Cu(OAc) ₂ (10)	Na ₂ CO ₃ (1.2)	DMSO	65/12	55
13	Cu(OTf) ₂ (10)	Na ₂ CO ₃ (1.2)	DMSO	65/12	trace
14	CuOAc (10)	Na ₂ CO ₃ (1.2)	DMSO	65/12	N.R.
15	CuCl ₂ (10)	Na ₂ CO ₃ (1.2)	DMSO	65/12	22

16	Cu(OAc) ₂ (10)	Na ₂ CO ₃ (1.2)	DMSO	80/12	47
17	Cu(OAc) ₂ (10)	K ₂ CO ₃ (1.2)	DMSO	65/12	49
18	Cu(OAc) ₂ (10)	NaHCO ₃ (1.2)	DMSO	65/12	45
19	Cu(OAc) ₂ (10)	Cs ₂ CO ₃ (1.2)	DMSO	65/12	10
20	Cu(OAc) ₂ (10)	KF (1.2)	DMSO	65/12	20
21	Cu(OAc) ₂ (10)	NEt ₃ (1.2)	DMSO	65/12	23
22	Cu(OAc) ₂ (10)	PivOH (1.2)	DMSO	65/12	N.R.
23	Cu(OAc) ₂ (10)	Na ₂ CO ₃ (1.5)	DMSO	65/12	53
24	Cu(OAc) ₂ (10)	Na ₂ CO ₃ (1.2)	NMP	65/12	< 5
25	Cu(OAc) ₂ (10)	Na ₂ CO ₃ (1.2)	dioxane	65/12	10
26	Cu(OAc) ₂ (10)	Na ₂ CO ₃ (1.2)	toluene	65/12	62
27	Cu(OAc) ₂ (10)	Na ₂ CO ₃ (1.2)	THF	65/12	70
28	Cu(OAc) ₂ (10)	Na ₂ CO ₃ (1.2)	DCE	65/12	trace
29	Cu(OAc) ₂ (10)	Na ₂ CO ₃ (1.2)	<i>p</i> -xylene	65/12	58
30	Cu(OAc) ₂ (10)	Na ₂ CO ₃ (1.2)	toluene/DMSO O= 4/1 (v/v)	65/12	66
31	Cu(OAc)₂ (10)	Na₂CO₃ (1.2)	THF/DMSO = 4/1 (v/v)	65/12	73
32	Cu(OAc) ₂ (10)	Na ₂ CO ₃ (1.2)	THF/DMSO = 3/1 (v/v)	65/12	73
33	Cu(OAc) ₂ (10)	Na ₂ CO ₃ (1.2)	THF/DMSO = 2/1 (v/v)	65/12	68
34	Cu(OAc) ₂ (5)	Na ₂ CO ₃ (1.2)	THF/DMSO = 4/1 (v/v)	65/12	40

^a Reaction conditions: **1a** (0.1 mmol, 1.0 equiv), **2a** (0.15 mmol, 1.5 equiv), [Cu] (10 mol%), Na₂CO₃ (1.2 equiv) in solvent (1.5 mL).

Table S2. Reaction Optimization for the Synthesis of **5a**^a

Entry	Catalyst (10 mol%)	Solvent	Temp. (°C)	Yield (%) ^b
1	DBU	DMSO	50	93
2	^t BuOK	DMSO	50	85
3	K ₂ CO ₃	DMSO	50	38
4	DABCO	DMSO	50	< 10
5	DMAP	DMSO	50	20
6	NEt ₃	DMSO	50	< 5
7	L-proline	DMSO	50	89
8	pyrrolidine	DMSO	50	< 10
9	diethylamine	DMSO	50	< 5
10	DBU	DMSO	50	91 ^c
11	DBU	DMSO	r.t.	92^c

^a Reaction conditions: 1-azido-2-isocyano-3,5-dimethylbenzene (**1a**, 0.1 mmol, 1.0 equiv), 2-phenylacetaldehyde (**4a**, 0.15 mmol, 1.5 equiv), catalyst (10 mol%), DMSO (2.0 mL), 50 °C, in Ar, 3 h. ^b Isolated yield of **5a**. ^c **4a** (1.2 equiv).

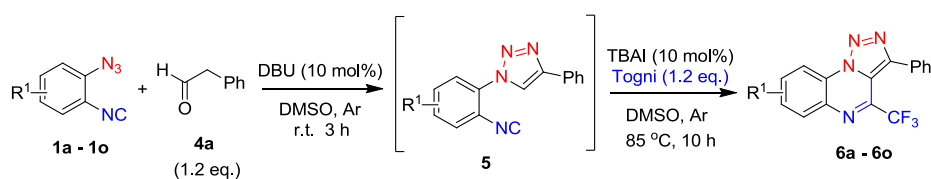
3.2 General Procedures for the Synthesis of **3**, and **5a**

In a dry 10 mL Schlenk tube, 1-azido-2-isocyanoarene **1** (0.1 mmol, 1.0 equiv) and acetylene **2** (0.15 mmol, 1.5 equiv), Cu(OAc)₂ (10 mol%), Na₂CO₃ (1.2 equiv) were mixed in THF/DMSO (v/v = 4/1, 1.5 mL) in Ar. Then the mixture was heated at 65 °C for 12 h (monitored by TLC). After completion of the reaction, it was cooled to

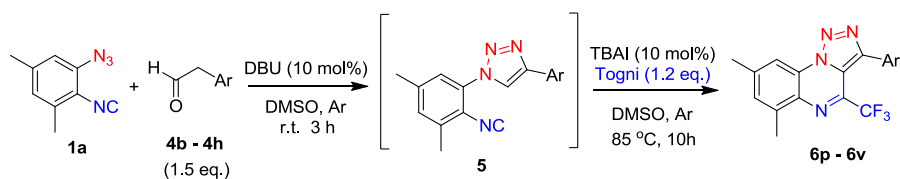
room temperature and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 10/1) to give the desired product **3**.

In a dry 10 mL Schlenk tube, 1-azido-2-isocyano-3,5-dimethylbenzene **1a** (0.1 mmol, 1.0 equiv) and 2-phenylacetaldehyde (**4a**, 0.15 mmol, 1.5 equiv), and DBU (10 mol%) were mixed in DMSO (2.0 mL) in Ar. Then, the mixture was stirred at 50 °C for 3 h. After cooling down to room temperature, it was quenched with water. The mixture was extracted with ethyl acetate and the organic layer was dried over Na₂SO₄. The resulting solution was directly filtered through a pad of silica gel using a sintered glass funnel, and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 7/1) to give 25.2 mg (92% yield) of **5a**.

3.3 General Procedures for the Synthesis of **6**

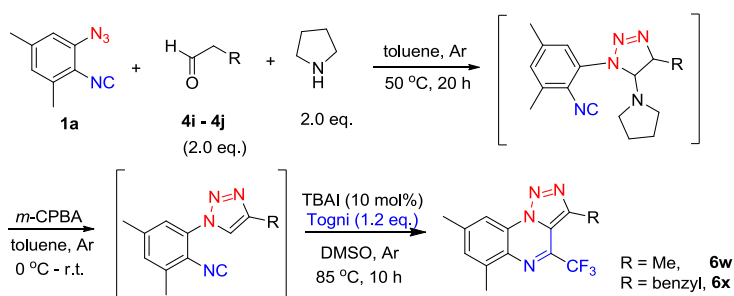


In a dry 10 mL Schlenk tube, 1-azido-2-isocyanobenzenes **1a-1o** (1.0 equiv, 0.1-0.2 mmol), phenylacetaldehyde (**4a**, 1.2 equiv), and DBU (10 mol%) were mixed in DMSO (2.0 mL) in Ar. Then the mixture was stirred at room temperature for 3 h. Then Togni reagent (II) (1.2 equiv), and TBAI (10 mol%) were added. The resulting mixture was heated at 85 °C in Ar for 10 h. The reaction was then quenched with water, extracted with ethyl acetate and dried over Na₂SO₄. The resulting solution was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate) to give the desired product.

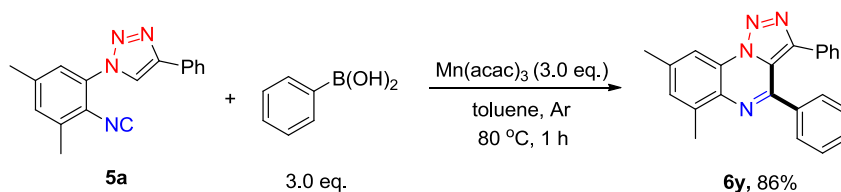


In a dry 10 mL Schlenk tube, 1-azido-2-isocyano-3,5-dimethylbenzene **1a** (1.0

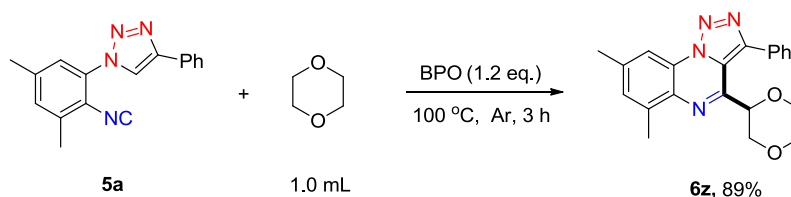
equiv, 0.1-0.2 mmol) and phenylacetaldehyde derivatives (**4b–4h**, 1.5 equiv), and DBU (10 mol%) were mixed in DMSO (2.0 mL) in Ar. Then the mixture was stirred at room temperature for 3 h. Then Togni reagent (II) (1.2 equiv), and TBAI (10 mol%) were added, and the mixture was heated at 85 °C in Ar for 10 h. The reaction was quenched with water, then extracted with ethyl acetate and dried over Na₂SO₄. The resulting solution was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate) to give the desired product.



In a dry 10 mL Schlenk tube, 1-azido-2-isocyano-3,5-dimethylbenzene **1a** (1.0 equiv, 0.15 mmol) and aldehydes (**4i–4j**, 2.0 equiv), pyrrolidine (2.0 equiv) and toluene (2.0 mL) were mixed in Ar. The mixture was heated at 50 °C for 20 h (monitored by TLC). After completion of the reaction, it was cooled to room temperature. Then, *m*-CPBA (1.5 equiv for **6w**, 3.0 equiv for **6x**) was added at 0 °C, and the resulting mixture was warmed up to room temperature for 5 h. The reaction was quenched with K₂CO₃ (aq.), extracted with ethyl acetate, and dried over Na₂SO₄. The concentrated residue was completely dried under reduced pressure. To this residue, DMSO (2.0 mL), Togni reagent (II) (1.2 equiv) and TBAI (10 mol%) were added successively. The mixture was heated at 85 °C in Ar for 10 h. Then, it was quenched with water, extracted with ethyl acetate and dried over Na₂SO₄. The resulting solution was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 15/1) to give the desired product.



In a dry 10 mL Schlenk tube, $\text{Mn}(\text{acac})_3$ (3.0 equiv) was added to a solution of 1-(2-isocyano-3,5-dimethylphenyl)-4-phenyl-1*H*-1,2,3-triazole **5a** (1.0 equiv, 0.05 mmol) and phenylboronic acid (3.0 equiv, 0.15 mmol) in toluene (1.0 mL). Then the mixture was heated at 80 °C for 1 h in Ar. After completion of the reaction, it was cooled to room temperature. The resulting solution was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 10/1) to give the desired product **6y** (15.0 mg, 86% yield).

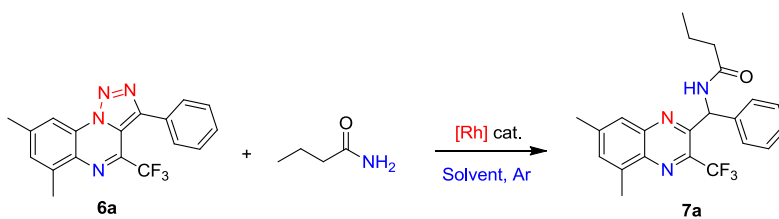


In a dry 10 mL Schlenk tube, benzoic peroxyanhydride (1.2 equiv) was added to a solution of 1-(2-isocyano-3,5-dimethylphenyl)-4-phenyl-1*H*-1,2,3-triazole **5a** (1.0 equiv, 0.05 mmol) in 1,4-dioxane (1.0 mL). Then the mixture was heated at 100 °C for 3 h in Ar. After completion of the reaction, it was cooled to room temperature. The resulting solution was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 10/1) to give the desired product **6z** (16.0 mg, 89% yield).

3.4 General Procedure for the Synthesis of 7

In a dry 10 mL Schlenk tube, [Rh] catalyst (2.5–5.0 mol%) was added to a solution of 6,8-dimethyl-3-phenyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline **6a** (1.0 equiv, 0.1 mmol) and N-H or O-H nucleophile (2.0 equiv, 0.2 mmol) in toluene (2.0 mL). Then the mixture was heated at optimal temperature for 24 h in Ar. After completion of the reaction, it was cooled to room temperature. The resulting solution was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 7/1) to give the desired product.

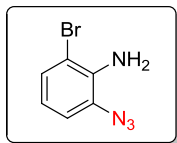
Table S3. Rh-catalyzed diversification of **6a**^a



Entry	Catalyst	Solvent	Temp. (°C)	Yield (%) ^b
			/Time (h)	
1	Rh ₂ (esp) ₂ (2.5 mol%)	toluene	120/24	50
2	Rh ₂ (esp) ₂ (2.5 mol%)	DCE	120/24	10
3	Rh ₂ (esp) ₂ (2.5 mol%)	<i>p</i> -xylene	120/24	48
4	Rh ₂ (esp) ₂ (2.5 mol%)	toluene	135/24	45
5	Rh ₂ (esp) ₂ (2.5 mol%)	toluene	100/24	< 5
6	Rh ₂ (esp) ₂ (2.5 mol%)	toluene	120/36	46
7	Rh ₂ (esp) ₂ (2.5 mol%)	toluene	120/24	12 ^c
8	Rh ₂ (esp) ₂ (4.0 mol%)	toluene	120/24	57
9	Rh₂(esp)₂ (5.0 mol%)	toluene	120/24	67
10	Rh ₂ (OAc) ₄ (5.0 mol%)	toluene	120/24	trace
11	Rh ₂ (OAc) ₄ (5.0 mol%)	DCE	120/24	N.R.
12	Rh ₂ (Oct) ₄ (2.5 mol%)	toluene	120/24	5
13	Rh ₂ (Oct) ₄ (2.5 mol%)	DCE	120/24	trace

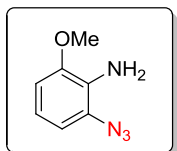
^a Reaction conditions: **6a** (1.0 equiv, 0.1 mmol), *N*-butyl amide (2.0 equiv, 0.2 mmol), [Rh] catalyst, solvent (2.0 mL), in Ar. ^b Isolated yields. ^c *N*-butyl amide (4.0 equiv) was used.

4. Characterization Data



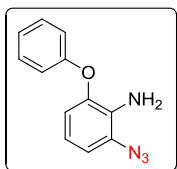
2-azido-6-bromoaniline

Brown solid. ^1H NMR (400 MHz, CDCl_3): δ 7.22-7.20 (m, 1H), 6.99-6.97 (m, 1H), 6.67-6.63 (m, 1H), 4.24 (br s, 2H); ^{13}C NMR (125 MHz, CDCl_3): 136.40, 128.59, 125.86, 118.74, 117.16, 109.41; HRMS (ESI) calcd for $\text{C}_6\text{H}_6\text{BrN}_2^+$ $[\text{M}+\text{H}-\text{N}_2]^+$ 184.9709, found 184.9708.



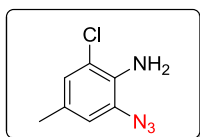
2-azido-6-methoxyaniline

Brown solid. ^1H NMR (400 MHz, CDCl_3): δ 6.77-6.70 (m, 2H), 6.62-6.60 (m, 1H), 3.89 (br s, 2H), 3.85 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): 147.72, 128.09, 125.08, 117.76, 110.70, 106.83, 55.76; HRMS (ESI) calcd for $\text{C}_7\text{H}_9\text{N}_2\text{O}^+$ $[\text{M}+\text{H}-\text{N}_2]^+$ 137.0709, found 137.0708.



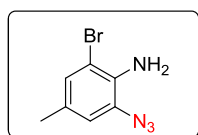
2-azido-6-phenoxyaniline

Brown solid. ^1H NMR (400 MHz, CDCl_3): δ 7.35-7.31 (m, 2H), 7.11-7.07 (m, 1H), 7.00-6.98 (m, 2H), 6.89-6.87 (m, 1H), 6.75-6.71 (m, 1H), 6.69-6.66 (m, 1H), 3.96 (br s, 2H); ^{13}C NMR (125 MHz, CDCl_3): 157.04, 143.85, 130.91, 129.82, 126.49, 123.13, 117.88, 117.54, 115.99, 113.84; HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{11}\text{N}_2\text{O}^+$ $[\text{M}+\text{H}-\text{N}_2]^+$ 199.0866, found 199.0863.



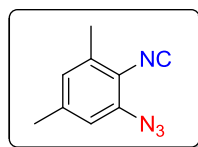
2-azido-6-chloro-4-methylaniline

Brown solid. ^1H NMR (500 MHz, CDCl_3): δ 6.87 (s, 1H), 6.74 (s, 1H), 4.03 (br s, 2H), 2.25 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): 132.80, 128.21, 125.95, 125.91, 119.66, 117.21, 20.40; HRMS (ESI) calcd for $\text{C}_7\text{H}_8\text{ClN}_2^+$ $[\text{M}+\text{H}-\text{N}_2]^+$ 155.0371, found 155.0369.



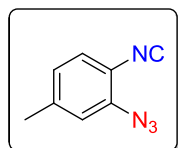
2-azido-6-bromo-4-methylaniline

Brown solid. ^1H NMR (400 MHz, CDCl_3): δ 7.04 (s, 1H), 6.78 (s, 1H), 4.08 (br s, 2H), 2.25 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): 133.92, 128.93, 128.72, 125.62, 117.84, 109.42, 20.22; HRMS (ESI) calcd for $\text{C}_7\text{H}_8\text{BrN}_2^+$ $[\text{M}+\text{H}-\text{N}_2]^+$ 198.9865, found 198.9858.



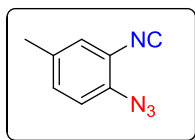
1-azido-2-isocyano-3,5-dimethylbenzene **1a**

Brown solid. ^1H NMR (400 MHz, CDCl_3): δ 6.84 (s, 1H), 6.82 (s, 1H), 2.36 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): 170.32, 140.24, 136.64, 136.45, 127.18, 116.90, 115.61, 21.34, 18.60; HRMS (ESI) calcd for $\text{C}_9\text{H}_9\text{N}_2^+$ $[\text{M}+\text{H}-\text{N}_2]^+$ 145.0760, found 145.0760.



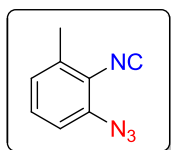
2-azido-1-isocyano-4-methylbenzene **1c**

Brown solid. ^1H NMR (400 MHz, CDCl_3): δ 7.19-7.16 (m, 1H), 6.92 (s, 1H), 6.87-6.85 (m, 1H), 2.32 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): 168.63, 141.23, 136.34, 127.72, 125.94, 119.58, 115.50, 21.39; HRMS (ESI) calcd for $\text{C}_8\text{H}_7\text{N}_2^+$ $[\text{M}+\text{H}-\text{N}_2]^+$ 131.0604, found 131.0604.



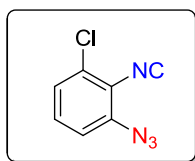
1-azido-2-isocyano-4-methylbenzene 1d

Brown solid. ^1H NMR (400 MHz, CDCl_3): δ 7.23–7.20 (m, 1H), 7.18 (s, 1H), 7.10–7.08 (m, 1H), 2.33 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): 169.05, 135.49, 133.95, 131.12, 128.37, 119.06, 117.75, 20.51; HRMS (ESI) calcd for $\text{C}_8\text{H}_7\text{N}_2^+$ $[\text{M}+\text{H}-\text{N}_2]^+$ 131.0604, found 131.0603.



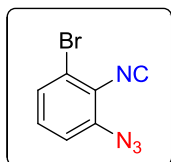
1-azido-2-isocyano-3-methylbenzene 1e

Brown solid. ^1H NMR (400 MHz, CDCl_3): δ 7.32–7.28 (m, 1H), 7.06–7.04 (m, 2H), 2.42 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): 171.22, 137.07, 136.84, 129.51, 126.25, 118.00, 116.42, 18.70; HRMS (ESI) calcd for $\text{C}_8\text{H}_7\text{N}_2^+$ $[\text{M}+\text{H}-\text{N}_2]^+$ 131.0604, found 131.0605.



1-azido-3-chloro-2-isocyanobenzene 1f

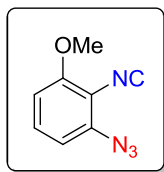
Brown solid. ^1H NMR (500 MHz, CDCl_3): δ 7.30–7.27 (m, 1H), 7.19–7.17 (m, 1H), 7.07–7.05 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3): 174.54, 138.83, 132.73, 130.20, 125.73, 117.44; HRMS (ESI) calcd for $\text{C}_7\text{H}_4\text{ClN}_2^+$ $[\text{M}+\text{H}-\text{N}_2]^+$ 151.0058, found 151.0058.



1-azido-3-bromo-2-isocyanobenzene 1g

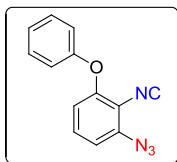
Brown solid. ^1H NMR (500 MHz, CDCl_3): δ 7.39–7.37 (m, 1H), 7.24–7.23 (m, 1H), 7.14–7.13 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3): 173.78, 138.69, 130.39, 128.71,

121.56, 118.90, 117.91; HRMS (ESI) calcd for $C_7H_4BrN_2^+$ $[M+H-N_2]^+$ 194.9552, found 194.9551.



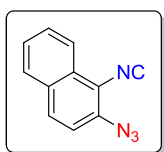
1-azido-2-isocyano-3-methoxybenzene 1h

Brown solid. 1H NMR (400 MHz, $CDCl_3$): δ 7.35-7.31 (m, 1H), 6.78 (d, J = 8.0 Hz, 1H), 6.72 (d, J = 8.0 Hz, 1H), 3.92 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 172.85, 156.39, 138.14, 130.14, 110.62, 107.98, 107.46, 56.38; HRMS (ESI) calcd for $C_8H_7N_2O^+$ $[M+H-N_2]^+$ 147.0553, found 147.0550.



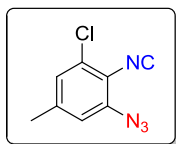
1-azido-2-isocyano-3-phenoxybenzene 1i

Brown solid. 1H NMR (400 MHz, $CDCl_3$): δ 7.33-7.30 (m, 2H), 7.21-7.18 (m, 1H), 7.17-7.11 (m, 1H), 6.99-6.97 (m, 2H), 6.83-6.81 (m, 1H), 6.55-6.53 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 173.62, 155.12, 154.81, 138.58, 130.15, 130.12, 125.06, 119.76, 113.41, 112.76, 109.83; HRMS (ESI) calcd for $C_{13}H_9N_2O^+$ $[M+H-N_2]^+$ 209.0709, found 209.0707.



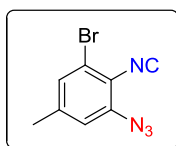
2-azido-1-isocyanonaphthalene 1j

Brown solid. 1H NMR (500 MHz, $CDCl_3$): δ 8.09-8.08 (m, 1H), 7.92-7.90 (m, 1H), 7.86-7.84 (m, 1H), 7.69-7.66 (m, 1H), 7.56-7.53 (m, 1H), 7.32-7.31 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 172.81, 134.58, 130.81, 130.44, 129.06, 128.79, 128.33, 126.69, 122.70, 116.75, 112.66; HRMS (ESI) calcd for $C_{11}H_7N_2^+$ $[M+H-N_2]^+$ 167.0604, found 167.0602.



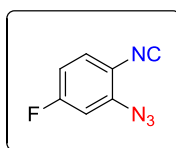
1-azido-3-chloro-2-isocyano-5-methylbenzene **1k**

Brown solid. ^1H NMR (500 MHz, CDCl_3): δ 7.04 (s, 1H), 6.89 (s, 1H), 2.37 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): 173.55, 141.48, 138.17, 132.04, 126.35, 117.96, 114.70, 21.47; HRMS (ESI) calcd for $\text{C}_8\text{H}_6\text{ClN}_2^+$ $[\text{M}+\text{H}-\text{N}_2]^+$ 165.0214, found 165.0212.



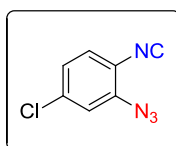
1-azido-3-bromo-2-isocyano-5-methylbenzene **1l**

Brown solid. ^1H NMR (400 MHz, CDCl_3): δ 7.22 (s, 1H), 6.94 (s, 1H), 2.38 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): 172.89, 141.62, 138.11, 129.39, 121.05, 118.48, 116.51, 21.25; HRMS (ESI) calcd for $\text{C}_8\text{H}_6\text{BrN}_2^+$ $[\text{M}+\text{H}-\text{N}_2]^+$ 208.9709, found 208.9705.



2-azido-4-fluoro-1-isocyanobenzene **1m**

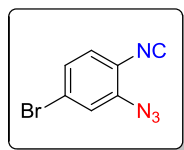
Brown solid. ^1H NMR (500 MHz, CDCl_3): δ 7.38-7.35 (m, 1H), 6.94-6.92 (m, 1H), 6.88-6.84 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3): 169.63, 162.58 (d, $J = 252.75$ Hz), 138.75 (d, $J = 9.63$ Hz), 129.57 (d, $J = 9.9$ Hz), 114.30, 112.51 (d, $J = 23.5$ Hz), 106.85 (d, $J = 26.5$ Hz); HRMS (ESI) calcd for $\text{C}_7\text{H}_4\text{FN}_2^+$ $[\text{M}+\text{H}-\text{N}_2]^+$ 135.0353, found 135.0354.



2-azido-4-chloro-1-isocyanobenzene **1n**

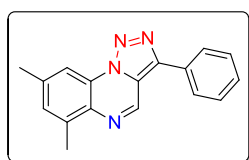
Brown solid. ^1H NMR (400 MHz, CDCl_3): δ 7.32-7.30 (m, 1H), 7.20-7.19 (m, 1H), 7.14-7.11 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3): 170.88, 138.04, 136.21, 128.89, 125.45, 119.51, 116.48; HRMS (ESI) calcd for $\text{C}_7\text{H}_4\text{ClN}_2^+$ $[\text{M}+\text{H}-\text{N}_2]^+$ 151.0058,

found 151.0058.



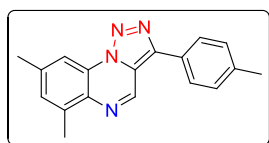
2-azido-4-bromo-1-isocyanobenzene 1o

Brown solid. ^1H NMR (500 MHz, CDCl_3): δ 7.36-7.35 (m, 1H), 7.29-7.27 (m, 1H), 7.24-7.23 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3): 170.98, 138.06, 129.00, 128.36, 123.88, 122.39, 116.87; HRMS (ESI) calcd for $\text{C}_7\text{H}_4\text{BrN}_2^+$ $[\text{M}+\text{H}-\text{N}_2]^+$ 194.9552, found 194.9551.



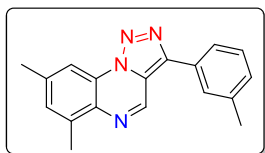
6,8-dimethyl-3-phenyl-[1,2,3]triazolo[1,5-a]quinoxaline 3a

Yellow solid, 0.1 mmol scale, 20.0 mg, 73% yield, mp 189-194 °C. ^1H NMR (400 MHz, CDCl_3): δ 9.32 (s, 1H), 8.34 (s, 1H), 8.05-8.03 (m, 2H), 7.58-7.54 (m, 2H), 7.49-7.45 (m, 1H), 7.38 (s, 1H), 2.77 (s, 3H), 2.58 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): 141.97, 141.04, 140.76, 138.48, 133.50, 131.17, 130.24, 129.23, 129.00, 127.22, 126.00, 123.38, 113.09, 21.88, 17.99; IR (cm^{-1}) 2953, 2923, 1617, 1503, 1448, 1374, 1133, 885, 860, 765, 689; HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{15}\text{N}_4^+$ $[\text{M}+\text{H}]^+$ 275.1291, found 275.1293.



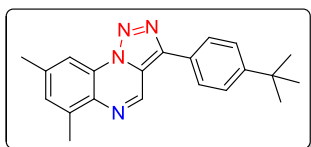
6,8-dimethyl-3-(p-tolyl)-[1,2,3]triazolo[1,5-a]quinoxaline 3b

Yellow solid, 0.1 mmol scale, 20.0 mg, 69% yield, mp 205-208 °C. ^1H NMR (400 MHz, CDCl_3): δ 9.29 (s, 1H), 8.33 (s, 1H), 7.93-7.91 (m, 2H), 7.37-7.35 (m, 2H), 7.35 (s, 1H), 2.76 (s, 3H), 2.57 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): 142.11, 140.92, 140.89, 139.07, 138.41, 133.47, 131.08, 129.91, 127.36, 127.08, 126.03, 123.21, 113.07, 21.86, 21.34, 17.98; IR (cm^{-1}) 2920, 2851, 1617, 1511, 1448, 1377, 856, 828, 773; HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{17}\text{N}_4^+$ $[\text{M}+\text{H}]^+$ 289.1448, found 289.1451.



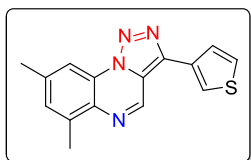
6,8-dimethyl-3-(*m*-tolyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline **3c**

Yellow solid, 0.1 mmol scale, 19.0 mg, 66% yield, mp 199-203 °C. ¹H NMR (400 MHz, CDCl₃): δ 9.32 (s, 1H), 8.33 (s, 1H), 7.88 (s, 1H), 7.82-7.80 (m, 1H), 7.46-7.42 (m, 1H), 7.38 (s, 1H), 7.28-7.26 (m, 1H), 2.76 (s, 3H), 2.57 (s, 3H), 2.47 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): 142.12, 140.98, 140.88, 139.00, 138.45, 133.49, 131.12, 130.09, 129.79, 129.10, 127.93, 126.01, 124.26, 123.36, 113.09, 21.87, 21.49, 17.97; IR (cm⁻¹) 2920, 2852, 1616, 1497, 1467, 1133, 876, 822, 793, 772, 696; HRMS (ESI) calcd for C₁₈H₁₇N₄⁺ [M+H]⁺ 289.1448, found 289.1453.



3-(4-(*tert*-butyl)phenyl)-6,8-dimethyl-[1,2,3]triazolo[1,5-*a*]quinoxaline **3d**

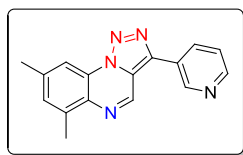
Yellow solid, 0.1 mmol scale, 23.0 mg, 70% yield, mp 182-184 °C. ¹H NMR (400 MHz, CDCl₃): δ 9.32 (s, 1H), 8.32 (s, 1H), 7.98 (d, *J* = 8.0 Hz, 2H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.36 (s, 1H), 2.76 (s, 3H), 2.57 (s, 3H), 1.40 (s, 9H); ¹³C NMR (125 MHz, CDCl₃): 152.28, 142.03, 140.91, 138.39, 133.46, 131.08, 127.37, 126.93, 126.19, 126.03, 123.23, 113.07, 34.80, 31.25, 21.86, 17.99; IR (cm⁻¹) 2959, 2866, 1619, 1510, 1476, 1362, 1268, 1114, 841, 774; HRMS (ESI) calcd for C₂₁H₂₃N₄⁺ [M+H]⁺ 331.1917, found 331.1916.



6,8-dimethyl-3-(thiophen-3-yl)-[1,2,3]triazolo[1,5-*a*]quinoxaline **3e**

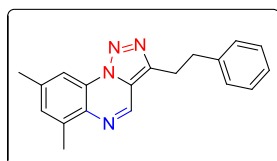
Yellow solid, 0.1 mmol scale, 16.0 mg, 57% yield, mp 233-235 °C. ¹H NMR (400 MHz, CDCl₃ with 1 drop of TFA): δ 9.46 (s, 1H), 8.38 (s, 1H), 8.00-7.99 (m, 1H), 7.76-7.75 (m, 1H), 7.58-7.56 (m, 1H), 7.45 (s, 1H), 2.79 (s, 3H), 2.61 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): 141.47, 140.60, 138.32, 133.21, 131.56, 130.53, 127.24, 126.21, 125.99, 123.45, 123.01, 113.23, 21.89, 18.13; IR (cm⁻¹) 2922, 2851, 1726,

1616, 1454, 1133, 859, 790, 773; HRMS (ESI) calcd for $C_{15}H_{13}N_4S^+$ $[M+H]^+$ 281.0855, found 281.0851.



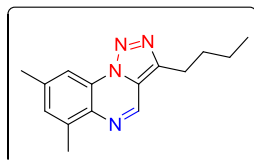
6,8-dimethyl-3-(pyridin-3-yl)-[1,2,3]triazolo[1,5-a]quinoxaline **3f**

Yellow solid, 0.1 mmol scale, 11.0 mg, 40% yield, mp 225-229 °C. 1H NMR (400 MHz, $CDCl_3$): δ 9.35 (s, 1H), 9.30 (br s, 1H), 8.73 (br s, 1H), 8.42-8.40 (m, 1H), 8.37 (s, 1H), 7.52 (br s, 1H), 7.43 (s, 1H), 2.79 (s, 3H), 2.60 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 150.00, 147.90, 141.52, 140.04, 138.76, 134.54, 133.60, 131.50, 126.68, 125.91, 124.14, 123.68, 113.13, 21.96, 18.01; IR (cm^{-1}) 2922, 2851, 1727, 1618, 1466, 1226, 1118, 860, 816, 704; HRMS (ESI) calcd for $C_{16}H_{14}N_5^+$ $[M+H]^+$ 276.1244, found 276.1244.



6,8-dimethyl-3-phenethyl-[1,2,3]triazolo[1,5-a]quinoxaline **3g**

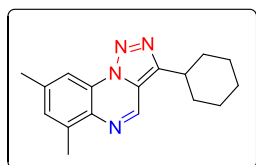
Yellow solid, 0.1 mmol scale, 17.0 mg, 56% yield, mp 98-100 °C. 1H NMR (400 MHz, $CDCl_3$): δ 8.50 (s, 1H), 8.23 (s, 1H), 7.28 (s, 1H), 7.20-7.16 (m, 2H), 7.14-7.09 (m, 3H), 3.56 (t, J = 7.6 Hz, 2H), 3.12 (t, J = 7.6 Hz, 2H), 2.65 (s, 3H), 2.49 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 142.10, 140.65, 140.57, 140.24, 138.38, 133.31, 130.93, 128.58, 128.52, 126.41, 126.04, 124.71, 113.03, 35.74, 27.59, 21.80, 18.05; IR (cm^{-1}) 3025, 2919, 2854, 1619, 1453, 1320, 1132, 889, 856, 740, 703; HRMS (ESI) calcd for $C_{19}H_{19}N_4^+$ $[M+H]^+$ 303.1604, found 303.1607.



3-butyl-6,8-dimethyl-[1,2,3]triazolo[1,5-a]quinoxaline **3h**

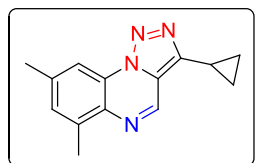
Yellow solid, 0.1 mmol scale, 15.0 mg, 59% yield, mp 95-97 °C. 1H NMR (400 MHz, $CDCl_3$): δ 9.02 (s, 1H), 8.30 (s, 1H), 7.36 (s, 1H), 3.12 (t, J = 7.6 Hz, 2H), 2.75 (s,

3H), 2.56 (s, 3H), 1.90-1.83 (m, 2H), 1.49-1.40 (m, 2H), 0.97 (t, $J = 7.6$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): 143.39, 140.58, 140.44, 138.37, 133.37, 130.90, 126.16, 124.50, 113.04, 31.75, 25.09, 22.35, 21.81, 18.05, 13.74; IR (cm^{-1}) 2955, 2929, 2861, 1619, 1439, 1375, 1104, 891, 850; HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{19}\text{N}_4^+$ $[\text{M}+\text{H}]^+$ 255.1604, found 255.1603.



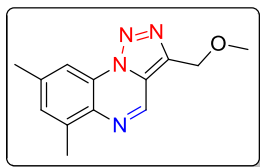
3-cyclohexyl-6,8-dimethyl-[1,2,3]triazolo[1,5-*a*]quinoxaline 3i

Yellow solid, 0.1 mmol scale, 20.0 mg, 71% yield, mp 175-177 °C. ^1H NMR (400 MHz, CDCl_3): δ 9.10 (s, 1H), 8.30 (s, 1H), 7.35 (s, 1H), 3.25-3.17 (m, 1H), 2.75 (s, 3H), 2.55 (s, 3H), 2.15-2.12 (m, 2H), 1.94-1.91 (m, 2H), 1.87-1.77 (m, 3H), 1.56-1.45 (m, 2H), 1.43-1.35 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3): 148.07, 140.82, 140.50, 138.31, 133.35, 130.85, 126.27, 123.73, 113.06, 36.20, 33.21, 26.42, 25.94, 21.80, 18.01; IR (cm^{-1}) 2924, 2851, 1619, 1486, 1448, 1361, 893, 846; HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{21}\text{N}_4^+$ $[\text{M}+\text{H}]^+$ 281.1761, found 281.1763.



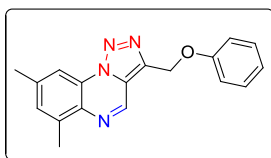
3-cyclopropyl-6,8-dimethyl-[1,2,3]triazolo[1,5-*a*]quinoxaline 3j

Yellow solid, 0.1 mmol scale, 16.0 mg, 67% yield, mp 157-159 °C. ^1H NMR (400 MHz, CDCl_3): δ 9.05 (d, $J = 5.2$ Hz, 1H), 8.25 (d, $J = 5.6$ Hz, 1H), 7.34 (d, $J = 4.0$ Hz, 1H), 2.74 (d, $J = 4.4$ Hz, 3H), 2.54 (d, $J = 3.2$ Hz, 3H), 2.33-2.27 (m, 1H), 1.25-1.22 (m, 2H), 1.20-1.15 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3): 144.93, 140.46, 140.37, 138.31, 133.43, 130.87, 126.19, 124.52, 112.97, 21.78, 18.04, 8.40, 6.54; IR (cm^{-1}) 2922, 1619, 1490, 1376, 1209, 1057, 850, 818; HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{15}\text{N}_4^+$ $[\text{M}+\text{H}]^+$ 239.1291, found 239.1287.



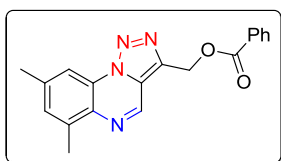
3-(methoxymethyl)-6,8-dimethyl-[1,2,3]triazolo[1,5-*a*]quinoxaline **3k**

Yellow solid, 0.1 mmol scale, 20.0 mg, 83% yield, mp 88-90 °C. ¹H NMR (400 MHz, CDCl₃): δ 9.19 (s, 1H), 8.29 (s, 1H), 7.37 (s, 1H), 5.01 (s, 2H), 3.50 (s, 3H), 2.75 (s, 3H), 2.56 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): 141.00, 140.78, 139.89, 138.55, 133.48, 131.13, 125.90, 125.21, 113.02, 66.54, 58.66, 21.81, 18.02; IR (cm⁻¹) 2923, 2852, 1619, 1487, 1197, 1108, 923, 847, 720; HRMS (ESI) calcd for C₁₃H₁₅N₄O⁺ [M+H]⁺ 243.1240, found 243.1244.



6,8-dimethyl-3-(phenoxymethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline **3l**

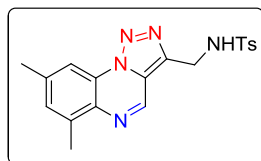
Yellow solid, 0.1 mmol scale, 16.0 mg, 53% yield, mp 155-157 °C. ¹H NMR (400 MHz, CDCl₃): δ 9.27 (s, 1H), 8.32 (s, 1H), 7.38 (s, 1H), 7.33-7.29 (m, 2H), 7.08-7.06 (m, 2H), 7.01-6.98 (m, 1H), 5.65 (s, 2H), 2.76 (s, 3H), 2.57 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): 157.93, 140.96, 140.94, 138.92, 138.59, 133.52, 131.25, 129.69, 125.89, 125.28, 121.65, 114.73, 113.03, 62.82, 21.84, 18.02; IR (cm⁻¹) 2922, 2852, 1598, 1488, 1227, 1204, 1035, 760, 675; HRMS (ESI) calcd for C₁₈H₁₇N₄O⁺ [M+H]⁺ 305.1397, found 305.1399.



(6,8-dimethyl-[1,2,3]triazolo[1,5-*a*]quinoxalin-3-yl)methyl benzoate **3m**

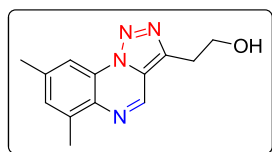
Yellow solid, 0.1 mmol scale, 28.0 mg, 84% yield, mp 138-141 °C. ¹H NMR (400 MHz, CDCl₃): δ 9.36 (s, 1H), 8.31 (s, 1H), 8.06-8.04 (m, 2H), 7.56-7.52 (m, 1H), 7.43-7.39 (m, 2H), 7.38 (s, 1H), 5.89 (s, 2H), 2.75 (s, 3H), 2.56 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): 166.32, 141.08, 140.66, 138.61, 137.30, 133.44, 133.32, 131.28, 129.75, 129.38, 128.42, 125.70, 125.47, 113.00, 57.58, 21.84, 17.97; IR (cm⁻¹) 2963, 2922, 2852, 1709, 1359, 1271, 1069, 858, 761, 706; HRMS (ESI) calcd for

$C_{19}H_{17}N_4O_2^+ [M+H]^+ 333.1346$, found 333.1349.



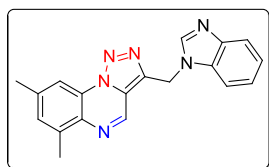
N-((6,8-dimethyl-[1,2,3]triazolo[1,5-*a*]quinoxalin-3-yl)methyl)-4-methylbenzenesulfonamide **3n**

Yellow solid, 0.1 mmol scale, 16.0 mg, 42% yield, mp 169-171 °C. 1H NMR (500 MHz, $CDCl_3$): δ 9.10 (s, 1H), 8.19 (s, 1H), 7.68 (d, $J = 8.0$ Hz, 2H), 7.39 (s, 1H), 7.14 (d, $J = 8.0$ Hz, 2H), 5.81 (br s, 1H), 4.67 (d, $J = 6.5$ Hz, 2H), 2.75 (s, 3H), 2.56 (s, 3H), 2.22 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 143.54, 141.07, 140.23, 138.74, 136.59, 133.39, 131.33, 129.61, 127.07, 126.39, 125.51, 124.62, 112.83, 38.43, 21.84, 21.21, 18.00; IR (cm^{-1}) 3191, 2922, 2851, 1619, 1435, 1330, 1157, 858, 658, 547; HRMS (ESI) calcd for $C_{19}H_{20}N_5O_2S^+ [M+H]^+ 382.1332$, found 382.1333.



2-((6,8-dimethyl-[1,2,3]triazolo[1,5-*a*]quinoxalin-3-yl)methyl)ethanol **3o**

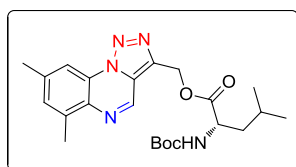
Yellow solid, 0.1 mmol scale, 14.0 mg, 58% yield, mp 132-134 °C. 1H NMR (400 MHz, $CDCl_3$): δ 9.04 (s, 1H), 8.12 (s, 1H), 7.32 (s, 1H), 4.14-4.13 (m, 2H), 3.34 (t, $J = 5.6$ Hz, 2H), 2.70 (s, 3H), 2.53 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 140.81, 140.74, 140.65, 138.32, 133.25, 131.04, 125.75, 125.16, 112.85, 61.45, 28.68, 21.80, 18.02; IR (cm^{-1}) 3351, 2921, 1728, 1621, 1483, 1061, 850, 665, 637; HRMS (ESI) calcd for $C_{13}H_{15}N_4O^+ [M+H]^+ 243.1240$, found 243.1243.



3-((1*H*-benzo[*d*]imidazol-1-yl)methyl)-6,8-dimethyl-[1,2,3]triazolo[1,5-*a*]quinoxaline **3p**

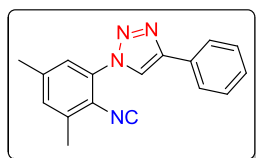
Yellow solid, 0.1 mmol scale, 24.0 mg, 73% yield, mp 212-216 °C. 1H NMR (500 MHz, $CDCl_3$): δ 8.41 (s, 1H), 8.19 (s, 1H), 8.19 (br s, 1H), 7.78 (br s, 1H), 7.44 (br s,

1H), 7.28 (s, 1H), 7.19 (m, 2H), 5.84 (s, 2H), 2.59 (s, 3H), 2.48 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): 141.45, 138.71, 136.84, 133.29, 131.48, 125.59, 124.55, 123.63, 122.63, 120.78, 112.90, 109.85, 40.75, 21.86, 17.85; IR (cm^{-1}) 3482, 2923, 2851, 1728, 1616, 1494, 1458, 1285, 1224, 1167, 743, 671; HRMS (ESI) calcd for $\text{C}_{19}\text{H}_{17}\text{N}_6^+$ $[\text{M}+\text{H}]^+$ 329.1509, found 329.1504.



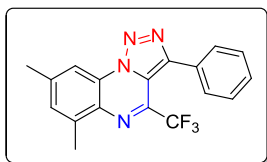
(S)-6,8-dimethyl-1-((tert-butoxycarbonyl)amino)-4-methylpentanoate-2-yl)-1H-1,2,3-triazolo[1,5-a]quinoxalin-3-yl)methyl-2-yl)amino)-4-methylpentanoate **3q**

Pale yellow liquid, 0.1 mmol scale, 32.0 mg, 72% yield. ^1H NMR (500 MHz, CDCl_3): δ 9.27 (s, 1H), 8.31 (s, 1H), 7.40 (s, 1H), 5.68 (s, 2H), 4.91-4.90 (m, 1H), 4.34 (d, J = 4.0 Hz, 1H), 2.76 (s, 3H), 2.57 (s, 3H), 1.67-1.57 (m, 2H), 1.49-1.43 (m, 1H), 1.39 (s, 9H), 0.88 (d, J = 7.5 Hz, 6H); ^{13}C NMR (125 MHz, CDCl_3): 173.36, 155.36, 141.08, 140.54, 138.71, 136.70, 133.46, 131.29, 125.63, 125.41, 112.96, 79.96, 57.64, 52.18, 41.38, 28.20, 24.73, 22.75, 21.84, 21.68, 17.95; IR (cm^{-1}) 3369, 2958, 2922, 1740, 1715, 1679, 1518, 1347, 1163, 854; HRMS (ESI) calcd for $\text{C}_{23}\text{H}_{32}\text{N}_5\text{O}_4^+$ $[\text{M}+\text{H}]^+$ 442.2449, found 442.2445.



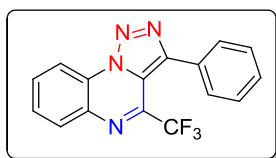
1-(2-isocyano-3,5-dimethylphenyl)-4-phenyl-1H-1,2,3-triazole **5a**

Yellow solid, 0.1 mmol scale, 25.2 mg, 92% yield, mp 94-96 $^{\circ}\text{C}$. ^1H NMR (400 MHz, CDCl_3): δ 8.29 (s, 1H), 7.92-7.90 (m, 2H), 7.47-7.43 (m, 2H), 7.41 (s, 1H), 7.39-7.35 (m, 1H), 7.24 (s, 1H), 2.49 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): 172.77, 148.03, 140.75, 136.94, 132.81, 131.91, 129.92, 128.85, 128.46, 125.95, 124.20, 120.51, 117.82, 21.18, 18.95; IR (cm^{-1}) 3135, 2921, 2115, 1697, 1611, 1585, 1475, 1452, 1351, 1231, 1207, 1072, 1024, 859, 766, 694; HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{15}\text{N}_4^+$ $[\text{M}+\text{H}]^+$ 275.1291, found 275.1291.



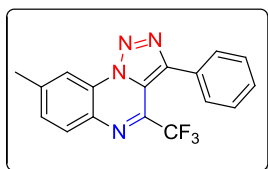
6,8-dimethyl-3-phenyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline **6a**

White solid, 0.1 mmol scale, 27.0 mg, 78% yield, mp 203-204 °C. ¹H NMR (400 MHz, CDCl₃): δ 8.45 (s, 1H), 7.60-7.59 (m, 2H), 7.52-7.50 (m, 3H), 7.48 (s, 1H), 2.81 (s, 3H), 2.64 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): 143.82, 142.87, 139.91, 138.42 (q, *J* = 38.5 Hz), 131.71, 131.16, 130.26, 130.20, 129.20, 128.06, 126.31, 120.59, 119.78 (q, *J* = 273.5 Hz), 113.17, 22.17, 17.51; ¹⁹F NMR (470 MHz, CDCl₃): -65.51 (s, 3F); IR (cm⁻¹) 2925, 1616, 1535, 1499, 1446, 1328, 1271, 1242, 1189, 1157, 969, 853, 782, 707; HRMS (ESI) calcd for C₁₈H₁₄F₃N₄⁺ [M+H]⁺ 343.1165, found 343.1168.



3-phenyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline **6b**⁶

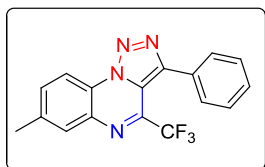
White solid, 0.1 mmol scale, 25.0 mg, 78% yield, mp 173-174 °C. ¹H NMR (400 MHz, CDCl₃): δ 8.83 (d, *J* = 8.0 Hz, 1H), 8.28 (d, *J* = 8.0 Hz, 1H), 7.97-7.93 (m, 1H), 7.86-7.82 (m, 1H), 7.60-7.58 (m, 2H), 7.53-7.52 (m, 3H); ¹³C NMR (125 MHz, CDCl₃): 143.49, 141.35 (q, *J* = 38.5 Hz), 134.15, 132.72, 130.87, 130.18, 129.94, 129.49, 129.39, 128.11, 126.38, 120.67, 119.52 (q, *J* = 274.0 Hz), 115.91; ¹⁹F NMR (470 MHz, CDCl₃): -65.75 (s, 3F); IR (cm⁻¹) 3094, 2922, 1606, 1584, 1494, 1468, 1337, 1191, 1139, 960, 776, 701; HRMS (ESI) calcd for C₁₆H₁₀F₃N₄⁺ [M+H]⁺ 315.0852, found 315.0851.



8-methyl-3-phenyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline **6c**⁶

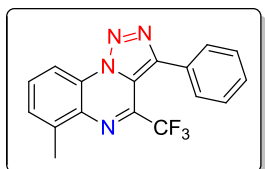
White solid, 0.2 mmol scale, 42.0 mg, 64% yield, mp 162-163 °C. ¹H NMR (400 MHz, CDCl₃): δ 8.62 (s, 1H), 8.14 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.60-7.58 (m, 2H), 7.52-7.50 (m, 3H), 2.71 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): 144.44, 143.23, 139.86 (q, *J* = 38.5 Hz), 132.28, 131.00, 130.48, 130.18, 130.07,

129.31, 128.09, 126.16, 120.73, 119.65 (q, $J = 273.5$ Hz), 115.56, 22.22; ^{19}F NMR (470 MHz, CDCl_3): -65.57 (s, 3F); IR (cm^{-1}) 3045, 2922, 1618, 1550, 1502, 1472, 1446, 1332, 1259, 1193, 1138, 1106, 961, 831, 704; HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{12}\text{F}_3\text{N}_4^+$ $[\text{M}+\text{H}]^+$ 329.1009, found 329.1012.



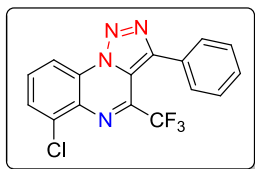
7-methyl-3-phenyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline 6d

White solid, 0.15 mmol scale, 20.0 mg, 41% yield, mp 188-189 °C. ^1H NMR (400 MHz, CDCl_3): δ 8.70 (d, $J = 8.0$ Hz, 1H), 8.07 (s, 1H), 7.76 (d, $J = 8.0$ Hz, 1H), 7.59-7.58 (m, 2H), 7.52-7.51 (m, 3H), 2.63 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): 143.35, 141.22 (q, $J = 38.5$ Hz), 140.17, 134.24, 134.12, 130.40, 130.20, 130.08, 129.35, 128.12, 124.29, 120.57, 119.59 (q, $J = 273.7$ Hz), 115.58, 21.43; ^{19}F NMR (470 MHz, CDCl_3): -65.71 (s, 3F); IR (cm^{-1}) 2922, 1587, 1556, 1449, 1309, 1256, 1227, 1143, 1112, 962, 833, 762, 701; HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{12}\text{F}_3\text{N}_4^+$ $[\text{M}+\text{H}]^+$ 329.1009, found 329.1017.



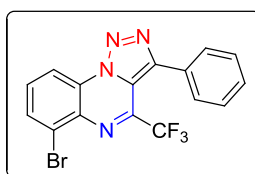
6-methyl-3-phenyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline 6e

White solid, 0.1 mmol scale, 23.0 mg, 70% yield, mp 174-175 °C. ^1H NMR (400 MHz, CDCl_3): δ 8.64 (d, $J = 8.0$ Hz, 1H), 7.82-7.78 (m, 1H), 7.67-7.65 (m, 1H), 7.60-7.59 (m, 2H), 7.53-7.51 (m, 3H), 2.85 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): 143.14, 140.42, 139.60 (q, $J = 38.3$ Hz), 132.92, 132.25, 130.18, 130.12, 129.29, 128.09, 126.45, 120.49, 119.64 (q, $J = 273.6$ Hz), 113.40, 17.64; ^{19}F NMR (470 MHz, CDCl_3): -65.70 (s, 3F); IR (cm^{-1}) 2925, 1604, 1487, 1412, 1382, 1324, 1243, 1189, 1136, 1095, 1015, 966, 771, 741, 696; HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{12}\text{F}_3\text{N}_4^+$ $[\text{M}+\text{H}]^+$ 329.1009, found 329.1011.



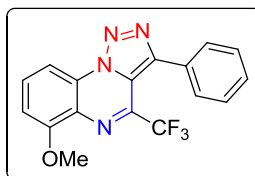
6-chloro-3-phenyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline **6f**

White solid, 0.2 mmol scale, 45.0 mg, 64% yield, mp 126-127 °C. ¹H NMR (500 MHz, CDCl₃): δ 8.72 (dd, *J* = 7.0, 1.2 Hz, 1H), 7.91-7.89 (m, 1H), 7.86-7.83 (m, 1H), 7.59-7.58 (m, 2H), 7.55-7.51 (m, 3H); ¹³C NMR (125 MHz, CDCl₃): 143.80, 141.64 (q, *J* = 39.1 Hz), 136.10, 132.68, 131.49, 130.15, 130.05, 129.57, 128.19, 127.68, 120.76, 119.36 (q, *J* = 274.1 Hz), 114.52; ¹⁹F NMR (470 MHz, CDCl₃): -65.68 (s, 3F); IR (cm⁻¹) 3081, 2923, 1598, 1472, 1445, 1410, 1320, 1237, 1190, 1137, 1074, 963, 797, 772, 740, 696; HRMS (ESI) calcd for C₁₆H₉ClF₃N₄⁺ [M+H]⁺ 349.0462, found 349.0466.



6-bromo-3-phenyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline **6g**

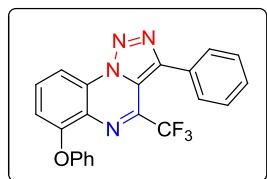
Yellow solid, 0.2 mmol scale, 48.0 mg, 61% yield, mp 156-158 °C. ¹H NMR (400 MHz, CDCl₃): δ 8.78 (d, *J* = 8.0 Hz, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 7.79-7.75 (m, 1H), 7.60-7.52 (m, 5H); ¹³C NMR (125 MHz, CDCl₃): 143.66, 141.76 (q, *J* = 39.1 Hz), 133.41, 132.99, 132.48, 130.16, 129.59, 129.55, 128.18, 127.56, 126.61, 120.76, 119.29 (q, *J* = 274.3 Hz), 115.22; ¹⁹F NMR (470 MHz, CDCl₃): -65.67 (s, 3F); IR (cm⁻¹) 3066, 1600, 1566, 1471, 1445, 1414, 1320, 1306, 1235, 1193, 1142, 962, 792, 772, 739, 693; HRMS (ESI) calcd for C₁₆H₉BrF₃N₄⁺ [M+H]⁺ 392.9957, found 392.9960.



6-methoxy-3-phenyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline **6h**

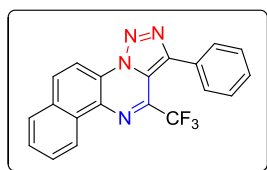
White solid, 0.1 mmol scale, 26.0 mg, 76% yield, mp 206-207 °C. ¹H NMR (500 MHz, CDCl₃): δ 8.40 (d, *J* = 7.5 Hz, 1H), 7.91-7.89 (m, 1H), 7.61-7.55 (m, 5H),

7.28-7.26 (m, 1H), 4.17 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): 156.95, 143.35, 139.31 (q, $J = 38.5$ Hz), 133.67, 130.20, 129.97, 129.35, 128.10, 127.42, 125.07, 120.73 (q, $J = 273.6$ Hz), 118.54, 109.99, 107.43, 56.86; ^{19}F NMR (470 MHz, CDCl_3): -65.28 (s, 3F); IR (cm^{-1}) 3104, 2922, 1605, 1536, 1499, 1440, 1322, 1282, 1184, 1138, 1102, 965, 799, 765, 740, 695; HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{12}\text{F}_3\text{N}_4\text{O}^+$ $[\text{M}+\text{H}]^+$ 345.0958, found 345.0959.



6-phenoxy-3-phenyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline 6i

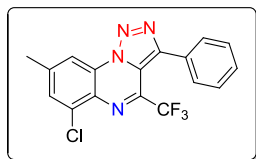
White solid, 0.15 mmol scale, 30.0 mg, 49% yield, mp 214-215 °C. ^1H NMR (400 MHz, CDCl_3): δ 8.49 (d, $J = 8.0$ Hz, 1H), 7.82-7.77 (m, 1H), 7.61-7.59 (m, 2H), 7.53-7.52 (m, 3H), 7.45-7.41 (m, 2H), 7.26-7.22 (m, 1H), 7.19-7.16 (m, 3H); ^{13}C NMR (125 MHz, CDCl_3): 156.02, 155.87, 143.57, 140.11 (q, $J = 38.6$ Hz), 133.25, 130.21, 130.10, 129.90, 129.43, 128.14, 127.60, 126.27, 124.96, 120.79, 120.30, 119.53 (q, $J = 273.9$ Hz), 116.35, 109.56; ^{19}F NMR (470 MHz, CDCl_3): -65.41 (s, 3F); IR (cm^{-1}) 3099, 2921, 1605, 1586, 1566, 1540, 1484, 1320, 1266, 1189, 1136, 1094, 970, 798, 764, 741, 695; HRMS (ESI) calcd for $\text{C}_{22}\text{H}_{14}\text{F}_3\text{N}_4\text{O}^+$ $[\text{M}+\text{H}]^+$ 407.1114, found 407.1118.



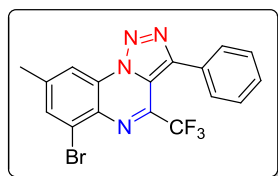
1-phenyl-12-(trifluoromethyl)benzo[f][1,2,3]triazolo[1,5-*a*]quinoxaline 6j

White solid, 0.1 mmol scale, 15.8 mg, 43% yield, mp 232-234 °C. ^1H NMR (500 MHz, CDCl_3): δ 9.18 (d, $J = 8.2$ Hz, 1H), 8.85 (d, $J = 9.0$ Hz, 1H), 8.35 (d, $J = 9.0$ Hz, 1H), 8.07 (d, $J = 8.0$ Hz, 1H), 7.88-7.85 (m, 1H), 7.80-7.77 (m, 1H), 7.65-7.64 (m, 2H), 7.55-7.53 (m, 3H); ^{13}C NMR (125 MHz, CDCl_3): 142.83, 139.74 (q, $J = 38.8$ Hz), 134.28, 132.66, 130.41, 130.24, 130.20, 129.35, 129.07, 128.43, 128.34, 128.17, 124.53, 124.20, 119.9 (q, $J = 273.6$ Hz), 121.42, 113.42; ^{19}F NMR (470 MHz, CDCl_3): -65.12 (s, 3F); IR (cm^{-1}) 2921, 1734, 1702, 1589, 1391, 1286, 1142, 1087, 965, 818,

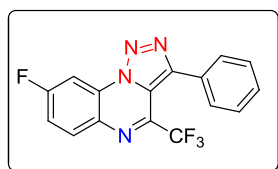
764, 698; HRMS (ESI) calcd for $C_{20}H_{12}F_3N_4^+$ $[M+H]^+$ 365.1009, found 365.1011.



6-chloro-8-methyl-3-phenyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline **6k**
White solid, 0.2 mmol scale, 45.2 mg, 62% yield, mp 192-194 °C. 1H NMR (500 MHz, $CDCl_3$): δ 8.51 (s, 1H), 7.72 (s, 1H), 7.59-7.58 (m, 2H), 7.53-7.51 (m, 3H), 2.67 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 144.73, 143.54, 140.44 (q, J = 38.8 Hz), 135.50, 131.31, 130.16, 129.71, 129.55, 129.49, 128.16, 127.35, 120.81, 119.5 (q, J = 274.1 Hz), 114.31, 22.14; ^{19}F NMR (470 MHz, $CDCl_3$): -65.52 (s, 3F); IR (cm^{-1}) 3045, 2921, 1604, 1474, 1446, 1385, 1326, 1246, 1193, 1144, 1113, 1005, 964, 918, 857, 820, 770, 729, 708; HRMS (ESI) calcd for $C_{17}H_{11}ClF_3N_4^+$ $[M+H]^+$ 363.0619, found 363.0622.

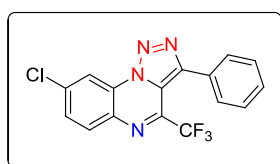


6-bromo-8-methyl-3-phenyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline **6l**
Yellow solid, 0.15 mmol scale, 40.0 mg, 65% yield, mp 175-176 °C. 1H NMR (400 MHz, $CDCl_3$): δ 8.56 (s, 1H), 7.93 (s, 1H), 7.60-7.58 (m, 2H), 7.53-7.51 (m, 3H), 2.67 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 145.04, 143.41, 139.31 (q, J = 38.5 Hz), 134.70, 130.56, 130.17, 129.70, 129.49, 128.16, 127.17, 126.07, 120.80, 120.73 (q, J = 273.6 Hz), 115.01, 22.01; ^{19}F NMR (470 MHz, $CDCl_3$): -65.52 (s, 3F); IR (cm^{-1}) 3041, 2921, 1605, 1473, 1446, 1406, 1312, 1230, 1194, 1143, 1110, 963, 857, 787, 769, 728, 708; HRMS (ESI) calcd for $C_{17}H_{11}BrF_3N_4^+$ $[M+H]^+$ 407.0114, found 407.0118.



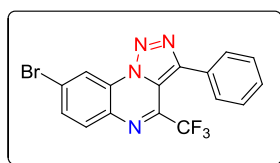
8-fluoro-3-phenyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline **6m**⁶
White solid, 0.2 mmol scale, 44.1 mg, 66% yield, mp 177-178 °C. 1H NMR (500 MHz, $CDCl_3$): δ 8.48 (dd, J = 8.0, 2.7 Hz, 1H), 8.30 (dd, J = 9.0, 5.0 Hz, 1H),

7.59-7.55 (m, 3H), 7.54-7.50 (m, 3H); ^{13}C NMR (125 MHz, CDCl_3): 164.37 (d, $J = 256.3$ Hz), 143.65, 140.66 (d, $J = 39.2$ Hz), 140.65 (q, $J = 38.6$ Hz), 133.41 (d, $J = 10.0$ Hz), 130.32 (d, $J = 148.3$ Hz), 130.21, 129.57, 128.22, 127.51 (d, $J = 12.5$ Hz), 120.59, 119.54 (q, $J = 276.5$ Hz), 118.37 (d, $J = 23.7$ Hz), 102.90 (d, $J = 27.9$ Hz); ^{19}F NMR (470 MHz, CDCl_3): -65.68 (s, 3F), -100.62- -100.66 (m, 1F); IR (cm^{-1}) 3074, 2922, 1618, 1568, 1503, 1479, 1416, 1254, 1221, 1192, 1137, 964, 856, 769, 699; HRMS (ESI) calcd for $\text{C}_{16}\text{H}_9\text{F}_4\text{N}_4^+$ $[\text{M}+\text{H}]^+$ 333.0758, found 333.0757.



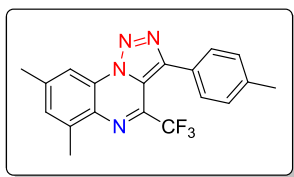
8-chloro-3-phenyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline **6n**

White solid, 0.1 mmol scale, 18.0 mg, 51% yield, mp 164-166 °C. ^1H NMR (500 MHz, CDCl_3): δ 8.82 (d, $J = 2.2$ Hz, 1H), 8.22 (d, $J = 8.8$ Hz, 1H), 7.79 (dd, $J = 8.5$, 2.0 Hz, 1H), 7.59-7.57 (m, 2H), 7.55-7.50 (m, 3H); ^{13}C NMR (125 MHz, CDCl_3): 143.81, 141.50 (q, $J = 38.8$ Hz), 139.17, 132.65, 132.11, 130.37, 130.20, 129.66, 129.62, 128.24, 126.89, 120.74, 119.47 (q, $J = 274.1$ Hz), 116.02; ^{19}F NMR (470 MHz, CDCl_3): -65.74 (s, 3F); IR (cm^{-1}) 3075, 2920, 1603, 1566, 1467, 1447, 1322, 1233, 1184, 1135, 1087, 959, 863, 843, 761, 700; HRMS (ESI) calcd for $\text{C}_{16}\text{H}_9\text{ClF}_3\text{N}_4^+$ $[\text{M}+\text{H}]^+$ 349.0462, found 349.0458.



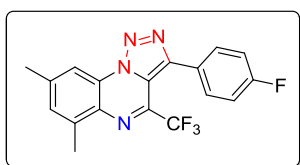
8-bromo-3-phenyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline **6o**

Yellow solid, 0.15 mmol scale, 40.0 mg, 68% yield, mp 146-147 °C. ^1H NMR (500 MHz, CDCl_3): δ 8.99 (d, $J = 4.5$ Hz, 1H), 8.14-8.12 (m, 1H), 7.95-7.93 (m, 1H), 7.58-7.56 (m, 2H), 7.54-7.50 (m, 3H); ^{13}C NMR (125 MHz, CDCl_3): 143.84, 141.65 (q, $J = 38.5$ Hz), 133.20, 132.99, 132.11, 130.20, 129.65, 129.61, 128.24, 127.24, 126.98, 120.76, 119.49 (q, $J = 273.8$ Hz), 119.07; ^{19}F NMR (470 MHz, CDCl_3): -65.77 (s, 3F); IR (cm^{-1}) 3084, 2922, 1602, 1566, 1466, 1446, 1414, 1185, 1139, 1069, 957, 862, 839, 757, 699; HRMS (ESI) calcd for $\text{C}_{16}\text{H}_9\text{BrF}_3\text{N}_4^+$ $[\text{M}+\text{H}]^+$ 392.9957, found 392.9953.



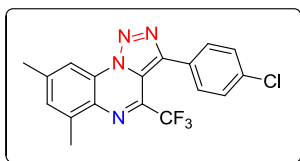
6,8-dimethyl-3-(*p*-tolyl)-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline **6p**

Yellow solid, 0.15 mmol scale, 35.2 mg, 66% yield, mp 199-200 °C. ^1H NMR (400 MHz, CDCl_3): δ 8.42 (s, 1H), 7.49-7.47 (m, 2H), 7.45 (s, 1H), 7.32-7.30 (m, 2H), 2.79 (s, 3H), 2.62 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): 143.73, 143.01, 139.86, 139.15, 138.52 (q, $J = 38.1$ Hz), 131.64, 131.13, 130.05, 128.80, 127.33, 126.34, 120.54, 119.81 (q, $J = 273.5$ Hz), 113.15, 22.16, 21.40, 17.51; ^{19}F NMR (470 MHz, CDCl_3): -65.45 (s, 3F); IR (cm^{-1}) 3032, 2925, 1617, 1506, 1483, 1323, 1189, 1139, 1099, 969, 961, 858, 823, 720; HRMS (ESI) calcd for $\text{C}_{19}\text{H}_{16}\text{F}_3\text{N}_4$ ⁺ $[\text{M}+\text{H}]^+$ 357.1322, found 357.1325.



3-(4-fluorophenyl)-6,8-dimethyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline **6q**

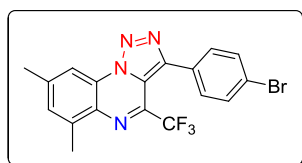
White solid, 0.2 mmol scale, 39.0 mg, 54% yield, mp 174-175 °C. ^1H NMR (400 MHz, CDCl_3): δ 8.42 (s, 1H), 7.59-7.55 (m, 2H), 7.48 (s, 1H), 7.22-7.18 (m, 2H), 2.79 (s, 3H), 2.64 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): 163.49 (d, $J = 247.4$ Hz), 143.99, 141.80, 139.99, 138.21 (q, $J = 38.5$ Hz), 132.13 (d, $J = 8.1$ Hz), 131.83, 131.16, 126.32 (d, $J = 3.1$ Hz), 126.28, 120.68, 119.79 (q, $J = 273.3$ Hz), 115.24 (d, $J = 21.8$ Hz), 113.17, 22.20, 17.52; ^{19}F NMR (470 MHz, CDCl_3): -65.52 (s, 3F); -110.90 (m, 1F); IR (cm^{-1}) 2924, 1619, 1561, 1506, 1484, 1324, 1241, 1189, 1143, 1099, 862, 842, 721; HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{13}\text{F}_4\text{N}_4$ ⁺ $[\text{M}+\text{H}]^+$ 361.1071, found 361.1073.



3-(4-chlorophenyl)-6,8-dimethyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline

6r

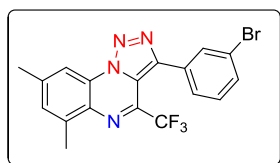
White solid, 0.15 mmol scale, 25.0 mg, 45% yield, mp 165-167 °C. ¹H NMR (400 MHz, CDCl₃): δ 8.45 (s, 1H), 7.55-7.48 (m, 5H), 2.81 (s, 3H), 2.65 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): 144.07, 141.63, 140.04, 138.16 (q, *J* = 37.5 Hz), 135.56, 131.90, 131.55, 131.21, 128.80, 128.44, 126.28, 120.64, 119.80 (q, *J* = 272.5 Hz), 113.21, 22.23, 17.55; ¹⁹F NMR (470 MHz, CDCl₃): -65.42 (s, 3F); IR (cm⁻¹) 2923, 1618, 1538, 1498, 1478, 1323, 1273, 1240, 1190, 1141, 1100, 969, 961, 857, 831, 717; HRMS (ESI) calcd for C₁₈H₁₃ClF₃N₄⁺ [M+H]⁺ 377.0775, found 377.0774.



3-(4-bromophenyl)-6,8-dimethyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-a]quinoxaline

6s

Yellow solid, 0.1 mmol scale, 25.0 mg, 60% yield, mp 124-125 °C. ¹H NMR (500 MHz, CDCl₃): δ 8.44 (s, 1H), 7.66-7.64 (m, 2H), 7.50-7.46 (m, 3H), 2.81 (s, 3H), 2.65 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): 144.08, 141.64, 140.03, 138.13 (q, *J* = 38.1 Hz), 131.91, 131.78, 131.40, 131.19, 129.28, 126.25, 123.82, 120.58, 119.79 (q, *J* = 273.5 Hz), 113.19, 22.24, 17.55; ¹⁹F NMR (470 MHz, CDCl₃): -65.39 (s, 3F); IR (cm⁻¹) 2922, 1744, 1618, 1559, 1323, 1146, 1096, 1067, 1007, 969, 961, 810, 779; HRMS (ESI) calcd for C₁₈H₁₃BrF₃N₄⁺ [M+H]⁺ 421.0270, found 421.0274.

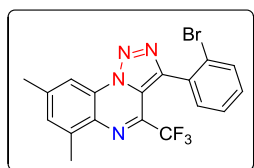


3-(3-bromophenyl)-6,8-dimethyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-a]quinoxaline

6t

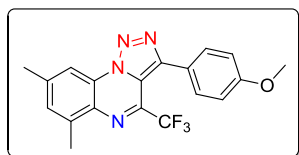
Yellow solid, 0.15 mmol scale, 39.0 mg, 62% yield, mp 170-172 °C. ¹H NMR (400 MHz, CDCl₃): δ 8.43 (s, 1H), 7.77 (s, 1H), 7.66-7.64 (m, 1H), 7.54-7.52 (m, 1H), 7.49 (s, 1H), 7.40-7.36 (m, 1H), 2.80 (s, 3H), 2.64 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): 144.12, 141.19, 140.04, 138.08 (q, *J* = 38.1 Hz), 133.19, 132.33, 132.24, 131.92, 131.20, 129.59, 128.90, 126.21, 122.08, 120.62, 119.78 (q, *J* = 273.4 Hz), 113.20, 22.22, 17.53; ¹⁹F NMR (470 MHz, CDCl₃): -65.46 (s, 3F); IR (cm⁻¹) 2920, 1615,

1491, 1319, 1269, 1238, 1190, 1130, 972, 863, 777; HRMS (ESI) calcd for $C_{18}H_{13}BrF_3N_4^+$ $[M+H]^+$ 421.0270, found 421.0273.



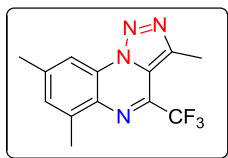
3-(2-bromophenyl)-6,8-dimethyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline
6u

Yellow solid, 0.15 mmol scale, 38.0 mg, 60% yield, mp 184-185 °C. 1H NMR (400 MHz, $CDCl_3$): δ 8.47 (s, 1H), 7.75-7.73 (m, 1H), 7.49 (s, 1H), 7.46-7.45 (m, 2H), 7.42-7.37 (m, 1H), 2.80 (s, 3H), 2.65 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 144.02, 141.08, 140.07, 138.17 (q, J = 38.4 Hz), 132.52, 131.83, 131.36, 131.30, 131.03, 126.86, 126.32, 125.29, 121.30, 119.78 (q, J = 273.6 Hz), 113.25, 22.20, 17.56; ^{19}F NMR (470 MHz, $CDCl_3$): -66.43 (s, 3F); IR (cm^{-1}) 2924, 1619, 1562, 1470, 1382, 1324, 1242, 1189, 1141, 1103, 968, 859; HRMS (ESI) calcd for $C_{18}H_{13}BrF_3N_4^+$ $[M+H]^+$ 421.0270, found 421.0274.



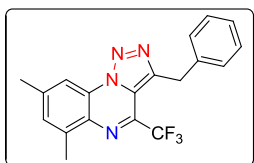
3-(4-methoxyphenyl)-6,8-dimethyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline
6v

Yellow solid, 0.1 mmol scale, 20.0 mg, 54% yield, mp 145-146 °C. 1H NMR (400 MHz, $CDCl_3$): δ 8.44 (s, 1H), 7.52 (d, J = 8.0 Hz, 2H), 7.47 (s, 1H), 7.03 (d, J = 8.0 Hz, 2H), 3.90 (s, 3H), 2.80 (s, 3H), 2.64 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 160.43, 143.75, 142.78, 139.90, 138.55 (q, J = 38.1 Hz), 131.68, 131.50, 131.18, 126.41, 122.55, 120.58, 119.84 (q, J = 273.4 Hz), 113.61, 113.18, 55.32, 22.20, 17.55; ^{19}F NMR (470 MHz, $CDCl_3$): -65.47 (s, 3F); IR (cm^{-1}) 2923, 1655, 1575, 1558, 1379, 1322, 1209, 1175, 1134, 1098, 969, 850, 720; HRMS (ESI) calcd for $C_{19}H_{16}F_3N_4O^+$ $[M+H]^+$ 373.1271, found 373.1273.



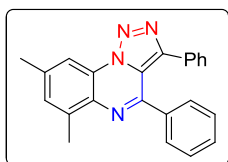
3,6,8-trimethyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline **6w**

Yellow solid, 0.15 mmol scale, 18.0 mg, 43% yield, mp 108-110 °C. ¹H NMR (400 MHz, CDCl₃): δ 8.32 (s, 1H), 7.42 (s, 1H), 2.79 (s, 3H), 2.77 (s, 3H), 2.59 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): 143.40, 139.89, 138.64, 138.16 (q, *J* = 38.0 Hz), 131.49, 131.04, 126.50, 121.10, 120.13 (q, *J* = 272.6 Hz), 113.05, 22.09, 17.53, 12.08 (q, *J* = 3.6 Hz); ¹⁹F NMR (470 MHz, CDCl₃): -66.72 (s, 3F); IR (cm⁻¹) 2923, 2851, 1743, 1618, 1488, 1464, 1381, 1332, 1243, 1180, 1119, 853, 741; HRMS (ESI) calcd for C₁₃H₁₂F₃N₄⁺ [M+H]⁺ 281.1009, found 281.1006.



3-benzyl-6,8-dimethyl-4-(trifluoromethyl)-[1,2,3]triazolo[1,5-*a*]quinoxaline **6x**

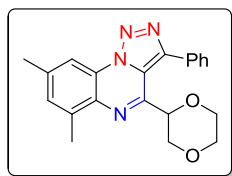
White solid, 0.15 mmol scale, 14.0 mg, 26% yield, mp 147-148 °C. ¹H NMR (400 MHz, CDCl₃): δ 8.37 (s, 1H), 7.44 (s, 1H), 7.33-7.30 (m, 3H), 7.28-7.26 (m, 1H), 7.22-7.18 (m, 1H), 4.56 (s, 2H), 2.78 (s, 3H), 2.61 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): 143.68, 141.04, 139.93, 138.05, 138.08 (q, *J* = 37.9 Hz), 131.59, 130.99, 128.68, 128.40, 126.52, 120.89, 120.15 (q, *J* = 272.9 Hz), 113.10, 31.82 (d, *J* = 2.9 Hz), 22.15, 17.52; ¹⁹F NMR (470 MHz, CDCl₃): -66.21 (s, 3F); IR (cm⁻¹) 3030, 2923, 1617, 1493, 1342, 1240, 1185, 1137, 872, 726, 716; HRMS (ESI) calcd for C₁₉H₁₆F₃N₄⁺ [M+H]⁺ 357.1322, found 357.1325.



6,8-dimethyl-3,4-diphenyl-[1,2,3]triazolo[1,5-*a*]quinoxaline **6y**

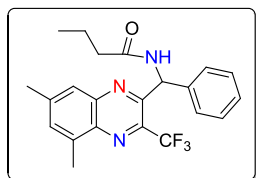
White solid, 0.05 mmol scale, 15.0 mg, 86% yield, mp 133-135 °C. ¹H NMR (400 MHz, CDCl₃): δ 8.45 (s, 1H), 7.49-7.47 (m, 2H), 7.43 (s, 1H), 7.36-7.32 (m, 1H), 7.28-7.25 (m, 2H), 7.23-7.21 (m, 2H), 7.19-7.15 (m, 3H), 2.83 (s, 3H), 2.62 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): 150.97, 143.29, 140.34, 138.51, 136.63, 133.57, 131.12,

130.74, 129.98, 129.74, 129.29, 128.16, 127.93, 127.78, 125.03, 122.44, 112.99, 21.95, 17.87; IR (cm⁻¹) 2954, 2921, 1730, 1614, 1446, 1385, 1181, 849, 762, 732, 698; HRMS (ESI) calcd for C₂₃H₁₉N₄⁺ [M+H]⁺ 351.1604, found 351.1615.



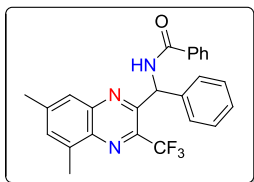
4-(1,4-dioxan-2-yl)-6,8-dimethyl-3-phenyl-[1,2,3]triazolo[1,5-*a*]quinoxaline **6z**

White solid, 0.05 mmol scale, 16.0 mg, 89% yield, mp 164-165 °C. ¹H NMR (500 MHz, CDCl₃): δ 8.38 (s, 1H), 7.73-7.72 (m, 2H), 7.57-7.52 (m, 3H), 7.39 (s, 1H), 4.84-4.82 (m, 1H), 4.31-4.27 (m, 1H), 4.13-4.11 (m, 1H), 3.66-3.65 (m, 2H), 3.55-3.52 (m, 1H), 3.29-3.24 (m, 1H), 2.75 (s, 3H), 2.59 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): 148.32, 142.94, 141.20, 138.74, 132.45, 131.62, 131.11, 129.78, 128.96, 128.35, 125.68, 123.32, 113.03, 73.50, 68.21, 66.71, 66.14, 21.96, 17.68; IR (cm⁻¹) 2922, 2852, 1691, 1453, 1423, 1325, 1290, 1179, 915, 706, 666; HRMS (ESI) calcd for C₂₁H₂₁N₄O₂⁺ [M+H]⁺ 361.1659, found 361.1660.



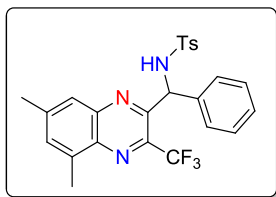
N-((5,7-dimethyl-3-(trifluoromethyl)quinoxalin-2-yl)(phenyl)methyl)butyramide **7a**

White solid, 0.1 mmol of **6a**, Rh₂(esp)₂ (5.0 mol%), *N*-butyl amide (2.0 equiv), 27.0 mg, 67% yield, mp 179-180 °C. ¹H NMR (500 MHz, CDCl₃): δ 7.84 (s, 1H), 7.55 (s, 1H), 7.39-7.36 (m, 3H), 7.29-7.22 (m, 3H), 6.87 (d, *J* = 8.0 Hz, 1H), 2.77 (s, 3H), 2.63 (s, 3H), 2.27 (t, *J* = 7.5 Hz, 2H), 1.73-1.66 (m, 2H), 0.93 (t, *J* = 7.5 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃): 171.78, 151.06, 143.62, 142.59, 140.09, 138.46 (q, *J* = 37.6 Hz), 138.31, 137.47, 133.51, 128.62, 128.21, 127.88, 125.31, 121.49 (q, *J* = 274.4 Hz), 53.52 (d, *J* = 3.0 Hz), 38.59, 22.16, 18.98, 16.76, 13.74; ¹⁹F NMR (470 MHz, CDCl₃): -63.22 (s, 3F); IR (cm⁻¹) 3296, 2959, 2931, 1637, 1542, 1348, 1314, 1229, 1184, 1138, 1043, 861, 763, 729, 703; HRMS (ESI) calcd for C₂₂H₂₃F₃N₃O⁺ [M+H]⁺ 402.1788, found 402.1790.



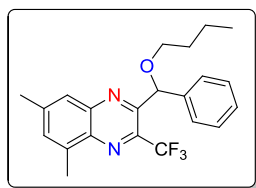
N-((5,7-dimethyl-3-(trifluoromethyl)quinoxalin-2-yl)(phenyl)methyl)benzamide **7b**

White solid, 0.1 mmol of **6a**, Rh₂(esp)₂ (5.0 mol%), benzamide (1.5 equiv), 32.0 mg, 73% yield, mp 184-185 °C. ¹H NMR (500 MHz, CDCl₃): δ 8.22 (d, *J* = 10.0 Hz, 1H), 7.88-7.86 (m, 3H), 7.56 (s, 1H), 7.52-7.49 (m, 1H), 7.46-7.43 (m, 4H), 7.31-7.28 (m, 2H), 7.26-7.23 (m, 1H), 7.05 (d, *J* = 7.5 Hz, 1H), 2.78 (s, 3H), 2.62 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): 165.96, 150.82, 143.68, 142.46, 139.89, 138.45 (q, *J* = 35.9 Hz), 138.31, 137.52, 134.24, 133.57, 131.60, 128.64, 128.54, 128.29, 127.96, 127.12, 125.33, 121.45 (q, *J* = 274.3 Hz), 53.93 (d, *J* = 2.7 Hz), 22.12, 16.72; ¹⁹F NMR (470 MHz, CDCl₃): -63.17 (s, 3F); IR (cm⁻¹) 3314, 2921, 1640, 1537, 1492, 1347, 1314, 1231, 1185, 1136, 1083, 1040, 729, 718; HRMS (ESI) calcd for C₂₅H₂₁F₃N₃O⁺ [M+H]⁺ 436.1631, found 436.1635.



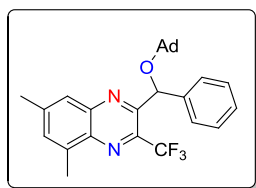
N-((5,7-dimethyl-3-(trifluoromethyl)quinoxalin-2-yl)(phenyl)methyl)-4-methylbenzenesulfonamide **7c**

White solid, 0.1 mmol of **6a**, Rh₂(esp)₂ (5.0 mol%), *p*-toluenesulfonamide (1.5 equiv), 26.7 mg, 55% yield, mp 141-142 °C. ¹H NMR (500 MHz, CDCl₃): δ 7.65 (s, 1H), 7.52 (s, 1H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.20 (s, 5H), 6.81 (d, *J* = 8.0 Hz, 2H), 6.64 (d, *J* = 10.0 Hz, 1H), 6.14 (d, *J* = 10.0 Hz, 1H), 2.72 (s, 3H), 2.61 (s, 3H), 2.06 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): 149.38, 143.71, 142.79, 142.19, 138.37, 138.01, 137.92 (q, *J* = 35.1 Hz), 137.19, 136.98, 133.61, 128.99, 128.60, 128.10, 128.06, 126.92, 125.18, 121.23 (q, *J* = 274.0 Hz), 57.64 (d, *J* = 2.8 Hz), 22.11, 21.04, 16.60; ¹⁹F NMR (470 MHz, CDCl₃): -63.11 (s, 3F); IR (cm⁻¹) 3247, 2922, 1597, 1339, 1229, 1189, 1169, 1136, 1043, 929, 731, 702, 675, 554; HRMS (ESI) calcd for C₂₅H₂₃F₃N₃O₂S⁺ [M+H]⁺ 486.1458, found 486.1460.



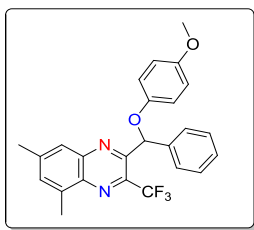
2-(butoxy(phenyl)methyl)-5,7-dimethyl-3-(trifluoromethyl)quinoxaline **7d**

Colorless oil, 0.05 mmol of **6a**, Rh₂(esp)₂ (2.5 mol%), 1-butanol (2.0 equiv), 13.1 mg, 67% yield. ¹H NMR (500 MHz, CDCl₃): δ 7.81 (s, 1H), 7.58-7.56 (m, 2H), 7.48 (s, 1H), 7.36-7.33 (m, 2H), 7.29-7.27 (m, 1H), 6.02 (s, 1H), 3.62-3.57 (m, 1H), 3.53-3.49 (m, 1H), 2.76 (s, 3H), 2.55 (s, 3H), 1.69-1.62 (m, 2H), 1.43-1.36 (m, 2H), 0.89 (t, *J* = 7.5 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃): 152.44, 143.50, 142.92, 139.41, 138.60 (q, *J* = 34.6 Hz), 137.80, 137.16, 133.37, 128.16, 127.98, 127.87, 126.11, 121.96 (q, *J* = 274.1 Hz), 79.65, 69.83, 31.72, 22.00, 19.24, 16.68, 13.81; ¹⁹F NMR (470 MHz, CDCl₃): -62.27 (s, 3F); IR (cm⁻¹) 2932, 1618, 1456, 1384, 1351, 1229, 1191, 1117, 1044, 865, 816, 758, 743, 727; HRMS (ESI) calcd for C₂₂H₂₄F₃N₂O⁺ [M+H]⁺ 389.1835, found 389.1838.



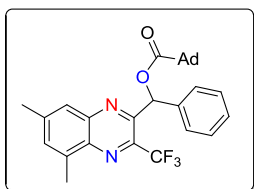
2-((adamantan-1-yloxy)(phenyl)methyl)-5,7-dimethyl-3-(trifluoromethyl)quinoxaline **7e**

White solid, 0.1 mmol of **6a**, Rh₂(esp)₂ (4.0 mol%), 1-adamantanol (1.5 equiv), 22.0 mg, 47% yield, mp 166-167 °C. ¹H NMR (400 MHz, CDCl₃): δ 7.89 (s, 1H), 7.50 (s, 1H), 7.44-7.43 (m, 2H), 7.28-7.24 (m, 2H), 7.22-7.18 (m, 1H), 6.40 (s, 1H), 2.77 (s, 3H), 2.58 (s, 3H), 2.08 (s, 3H), 1.77 (s, 6H), 1.57 (s, 6H); ¹³C NMR (125 MHz, CDCl₃): 154.86, 143.21, 142.92, 141.78, 138.19 (q, *J* = 34.7 Hz), 137.88, 137.10, 133.13, 128.00, 127.57, 127.24, 125.93, 121.80 (q, *J* = 273.8 Hz), 75.27, 71.69, 42.49, 36.27, 30.71, 22.07, 16.69; ¹⁹F NMR (470 MHz, CDCl₃): -62.13 (s, 3F); IR (cm⁻¹) 2913, 2852, 1619, 1547, 1454, 1348, 1227, 1189, 1126, 1083, 1035, 862, 814, 762, 743, 728, 719, 696; HRMS (ESI) calcd for C₂₈H₃₀F₃N₂O⁺ [M+H]⁺ 467.2305, found 467.2309.



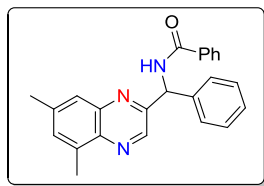
2-((4-methoxyphenoxy)(phenyl)methyl)-5,7-dimethyl-3-(trifluoromethyl)quinoxaline
7f

White solid, 0.1 mmol of **6a**, Rh₂(esp)₂ (4.0 mol%), 4-methoxyphenol (1.5 equiv), 20.0 mg, 45% yield, mp 108-110 °C. ¹H NMR (400 MHz, CDCl₃): δ 7.83 (s, 1H), 7.60-7.58 (m, 2H), 7.51 (s, 1H), 7.37-7.31 (m, 2H), 7.29-7.27 (m, 1H), 6.93-6.91 (m, 2H), 6.75-6.73 (m, 3H), 3.71 (s, 3H), 2.76 (s, 3H), 2.56 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): 154.51, 152.06, 151.14, 143.35, 143.22, 138.51, 138.33 (q, *J* = 34.9 Hz), 137.91, 137.28, 133.65, 128.38, 128.22, 127.94, 126.13, 121.83 (q, *J* = 273.8 Hz), 117.89, 114.52, 79.56 (d, *J* = 2.5 Hz), 55.55, 22.02, 16.67; ¹⁹F NMR (470 MHz, CDCl₃): -62.40 (s, 3F); IR (cm⁻¹) 2920, 1616, 1556, 1507, 1354, 1228, 1186, 1041, 878, 818, 767, 669; HRMS (ESI) calcd for C₂₅H₂₂F₃N₂O₂⁺ [M+H]⁺ 439.1628, found 439.1625.



(5,7-dimethyl-3-(trifluoromethyl)quinoxalin-2-yl)(phenyl)methyl
adamantane-1-carboxylate **7g**

White solid, 0.05 mmol of **6a**, Rh₂(esp)₂ (4.0 mol%), adamantane-1-carboxylic acid (1.5 equiv), 13.0 mg, 51% yield, mp 169-170 °C. ¹H NMR (400 MHz, CDCl₃): δ 7.75 (s, 1H), 7.53-7.50 (m, 3H), 7.36-7.30 (m, 3H), 7.12 (s, 1H), 2.75 (s, 3H), 2.58 (s, 3H), 2.02 (s, 3H), 1.96 (s, 6H), 1.71 (s, 6H); ¹³C NMR (125 MHz, CDCl₃): 176.72, 150.75, 143.11, 138.23 (q, *J* = 35.4 Hz), 138.04, 137.24, 137.13, 133.37, 128.47, 128.42, 128.36, 125.72, 121.66 (q, *J* = 274.4 Hz), 73.49 (d, *J* = 2.6 Hz), 40.72, 38.67, 36.49, 27.95, 22.06, 16.69; ¹⁹F NMR (470 MHz, CDCl₃): -62.95 (s, 3F); IR (cm⁻¹) 2917, 2902, 2852, 1733, 1619, 1550, 1455, 1348, 1227, 1196, 1138, 1070, 1048, 993, 858, 812, 761, 746, 727; HRMS (ESI) calcd for C₂₉H₃₀F₃N₂O₂⁺ [M+H]⁺ 495.2254, found 495.2255.



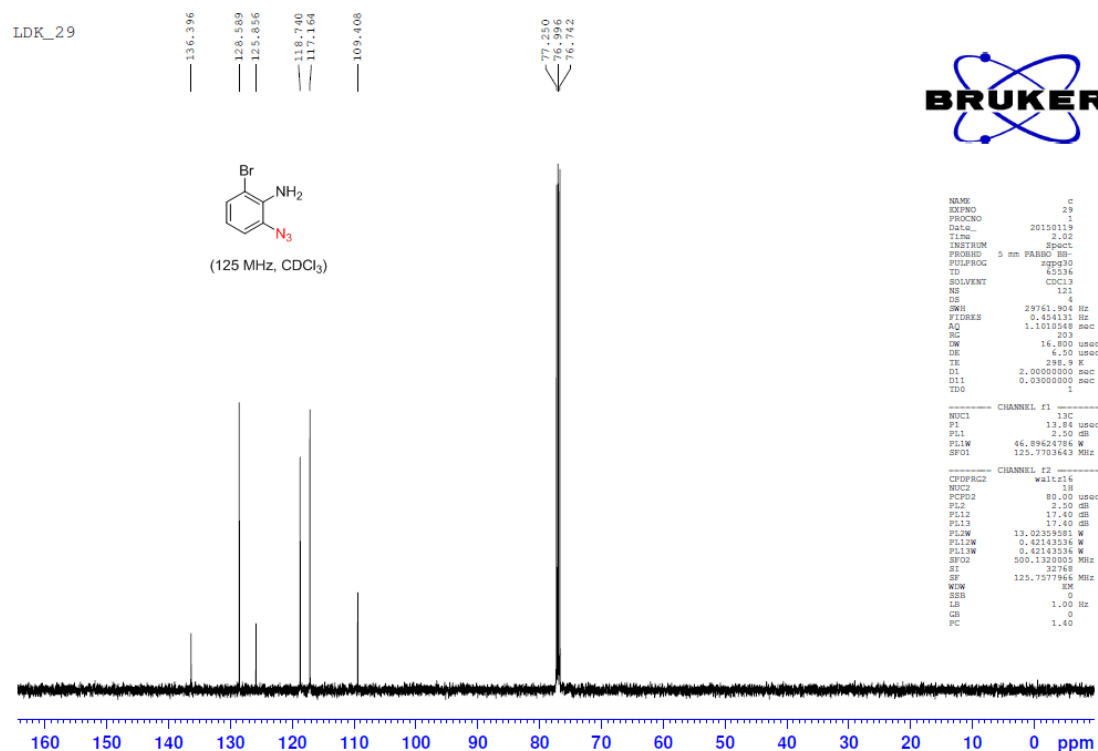
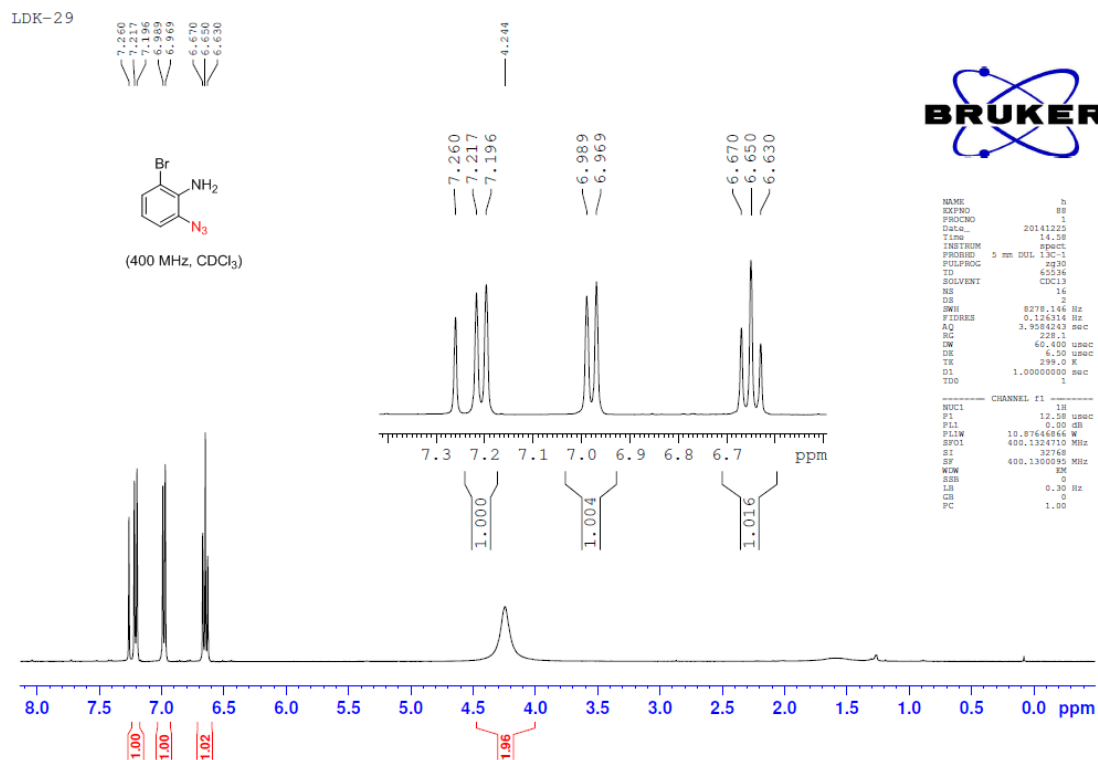
N*-((5,7-dimethylquinoxalin-2-yl)(phenyl)methyl)benzamide **7h*

White solid, 0.05 mmol of **3a**, Rh₂(esp)₂ (4.0 mol%), benzamide (1.5 equiv), 12.0 mg, 65% yield, mp 182-185 °C. ¹H NMR (400 MHz, CDCl₃): δ 8.74 (s, 1H), 8.58 (d, *J* = 6.0 Hz, 1H), 7.96-7.94 (m, 2H), 7.78 (s, 1H), 7.56-7.53 (m, 1H), 7.52-7.45 (m, 5H), 7.33-7.30 (m, 2H), 7.26-7.23 (m, 1H), 6.58 (d, *J* = 6.4 Hz, 1H), 2.74 (s, 3H), 2.58 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): 166.48, 152.95, 142.92, 141.34, 140.75, 140.61, 139.58, 137.13, 134.35, 132.25, 131.62, 128.93, 127.99, 127.80, 127.19, 125.76, 56.35, 21.81, 17.10; IR (cm⁻¹) 3340, 2919, 2850, 1644, 1531, 1486, 1353, 1029, 860, 734, 716, 619; HRMS (ESI) calcd for C₂₄H₂₂N₃O⁺ [M+H]⁺ 368.1757, found 368.1754.

5. References

1. C. Tang, N. Jiao, *J. Am. Chem. Soc.* 2012, **134**, 18924.
2. Y. Fan, W. Wan, G. Ma, W. Gao, H. Jiang, S. Zhu, J. Hao, *Chem. Commun.* 2014, **50**, 5733.
3. O. Kaufhold, A. Flores-Figueroa, T. Pape, F. E. Hahn, *Organometallics* 2009, **28**, 896.
4. S. P. Bew, G. D. Hiatt-Gipson, *J. Org. Chem.* 2010, **75**, 3897.
5. E. J. Corey, J. W. Suggs, *Tetrahedron Lett.* 1975, **31**, 2647.
6. Z. Chen, J. Zhu, H. Xie, S. Li, Y. Wu, Y. Gong, *Adv. Synth. Catal.* 2010, **352**, 1296.

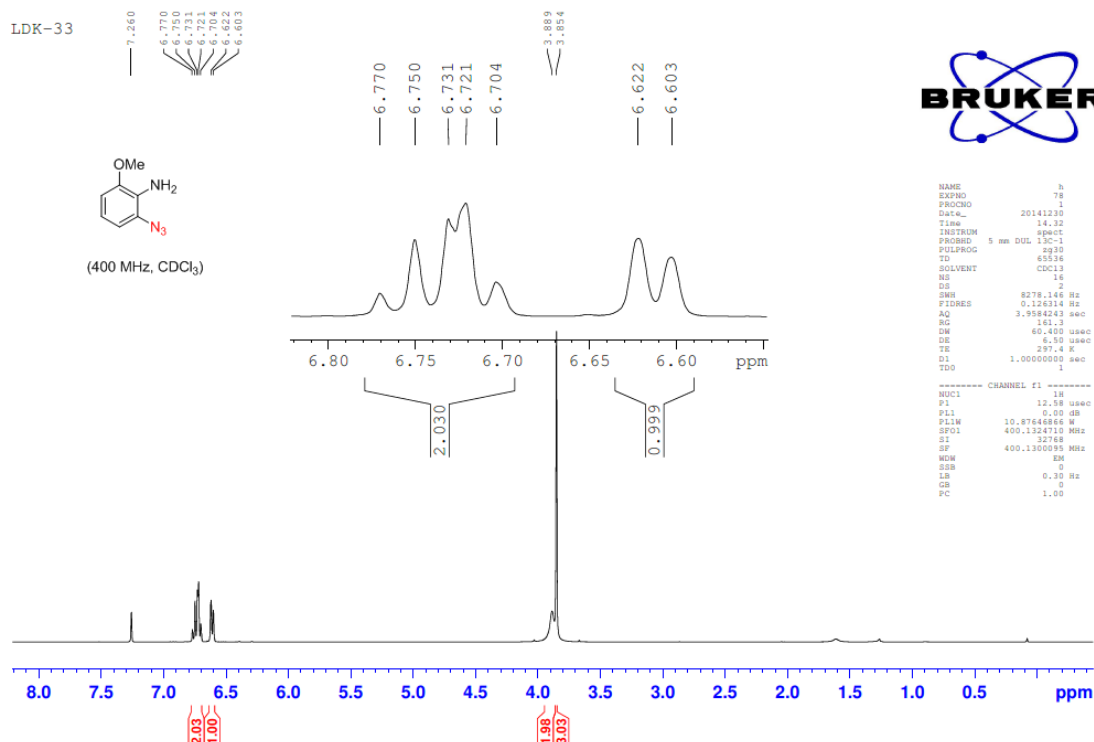
6. Copies of ^1H , ^{13}C or ^{19}F NMR Spectra



LDK-33



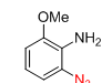
(400 MHz, CDCl₃)



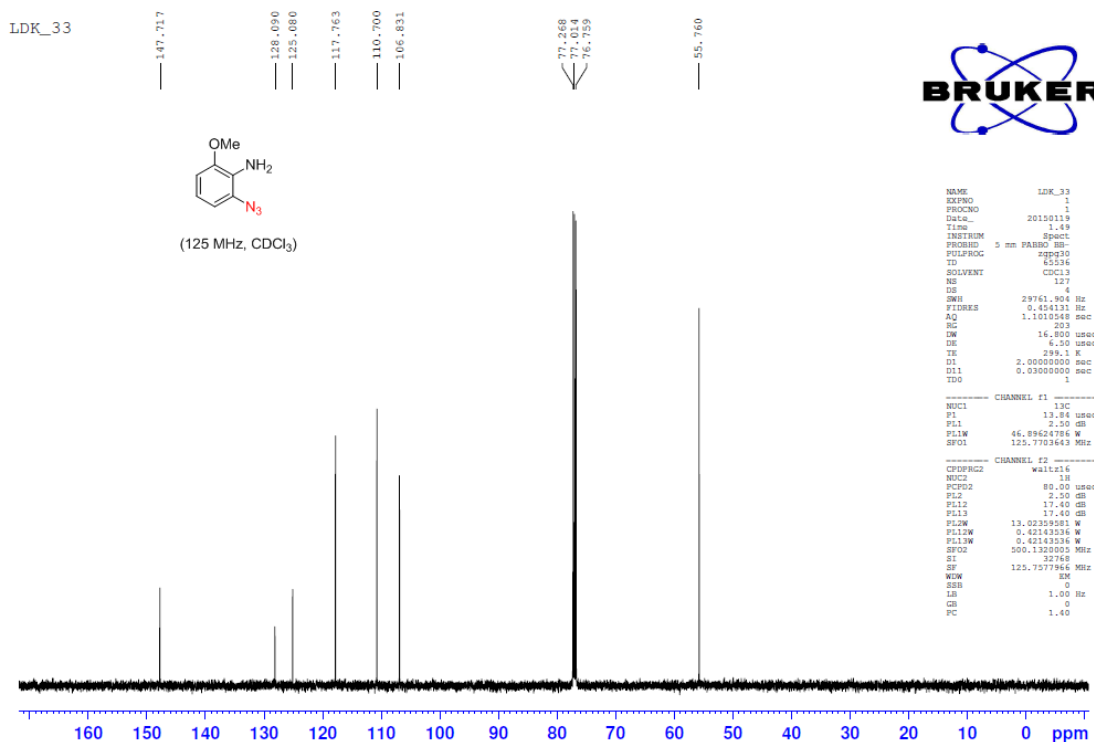
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PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           8278.146 Hz
FIDRES       0.124314 Hz
AQ           3.9584243 sec
RG            160.1
DM           60.400 usec
DE           6.50 usec
TE           297.4 K
D1           1.00000000 sec
TD0
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NUC1          1H
P1            12.38 usec
PL1           0.00 dB
PL1W          10.8764686 W
SFO1          400.1324710 MHz
SI            32768
SF            400.1300000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
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LDK_33

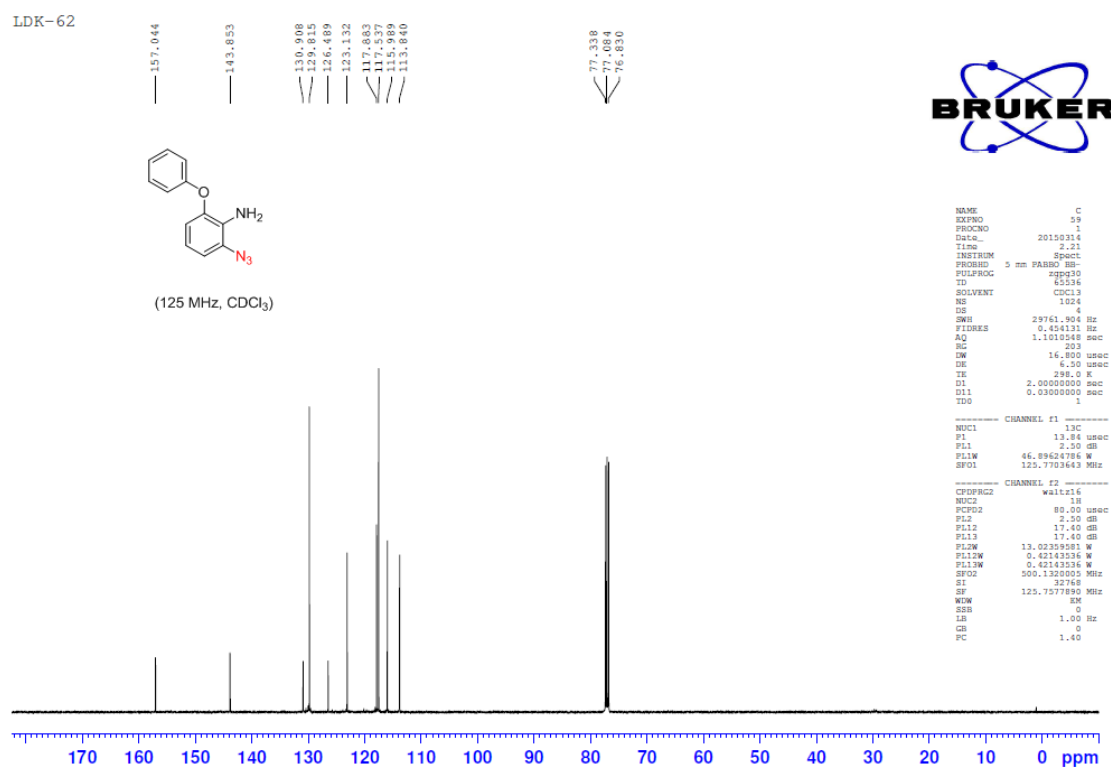
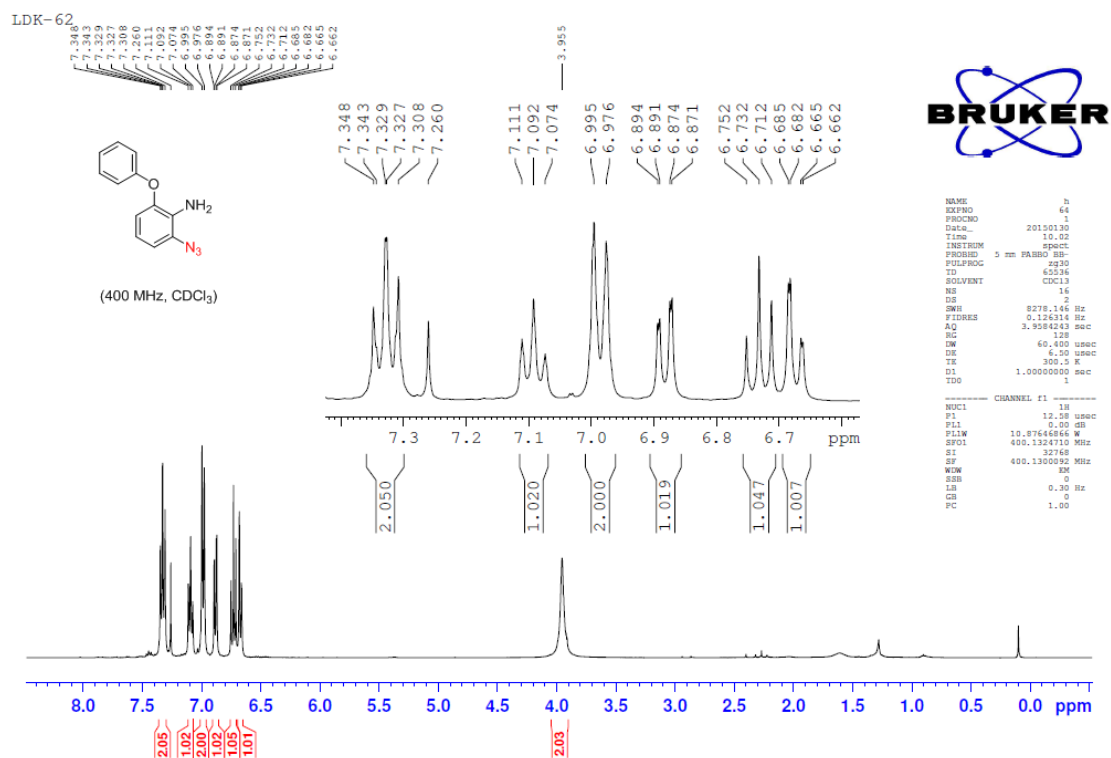


(125 MHz, CDCl₃)

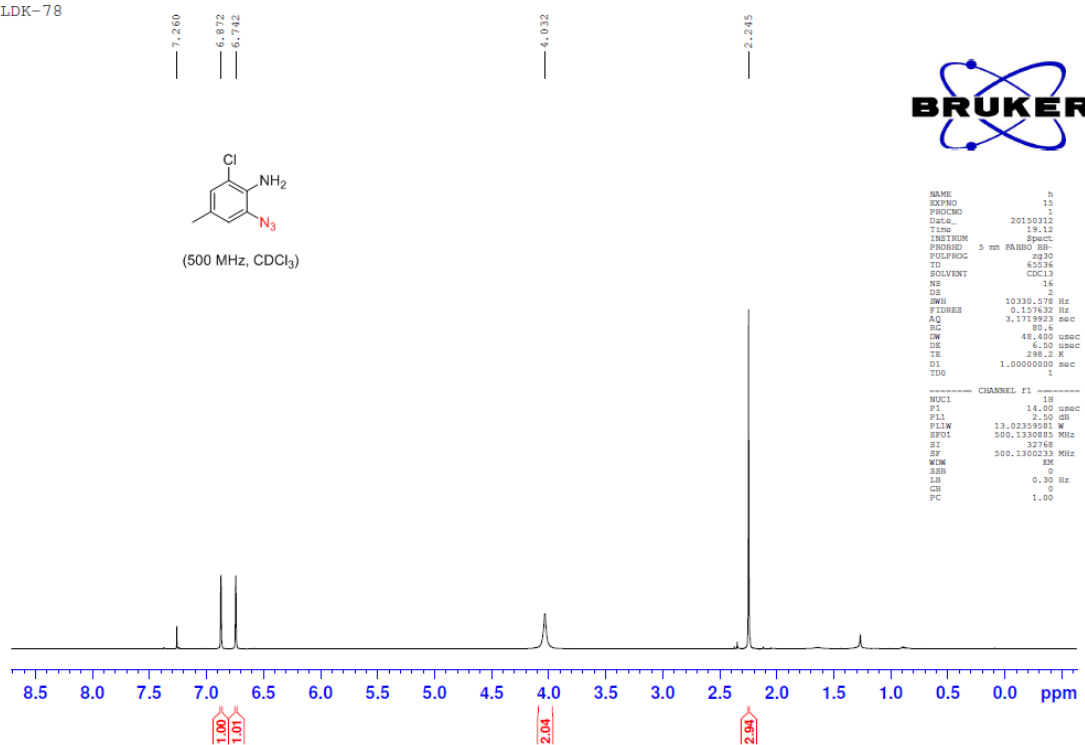


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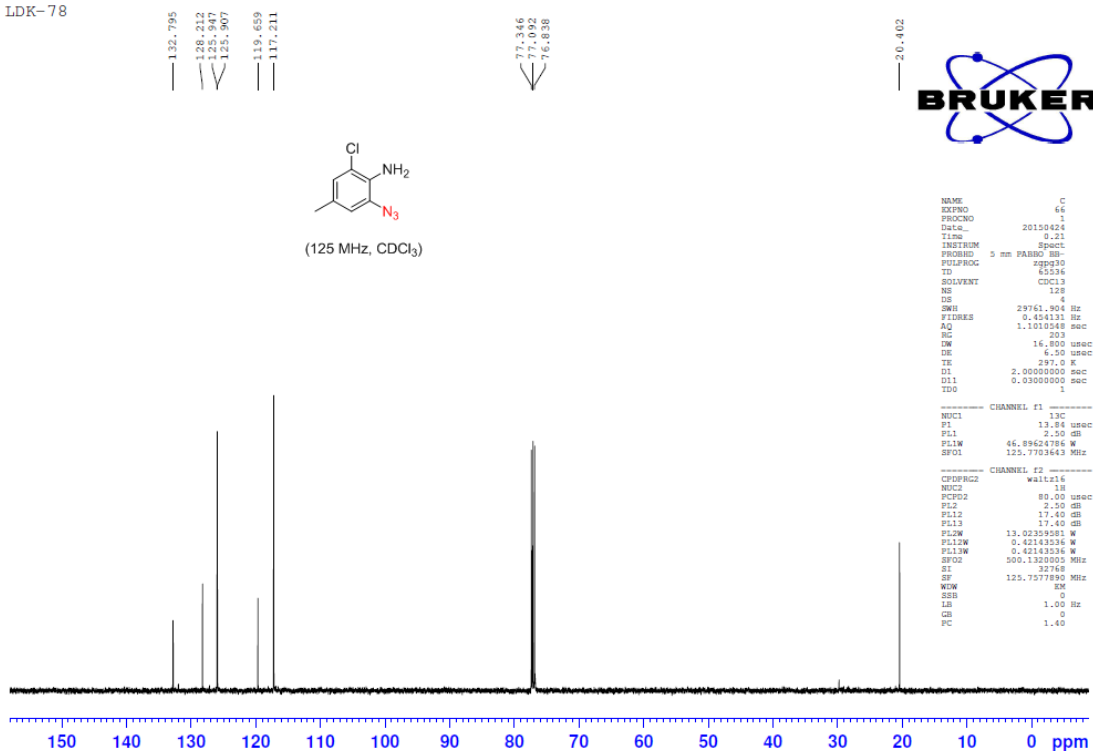
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INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            127
DS            4
SWH           29761.904 Hz
FIDRES       0.456131 Hz
AQ           1.1019548 sec
RG            203
DM           16.800 usec
DE           6.30 usec
TE           299.1 K
D1           2.00000000 sec
D11           0.03000000 sec
TD0           1
----- CHANNEL f1 -----
NUC1          13C
P1            13.84 usec
PL1           2.30 dB
PL1W          46.8963478 W
SFO1          125.7703643 MHz
----- CHANNEL f2 -----
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           2.30 dB
PL12          17.40 dB
PL13          17.40 dB
PL2W          13.02359581 W
PL12W         0.42143536 W
PL13W         0.42143536 W
SFO2          500.1320000 MHz
SI            32768
SF            125.7577964 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
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LDK-78



LDK-78

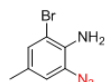
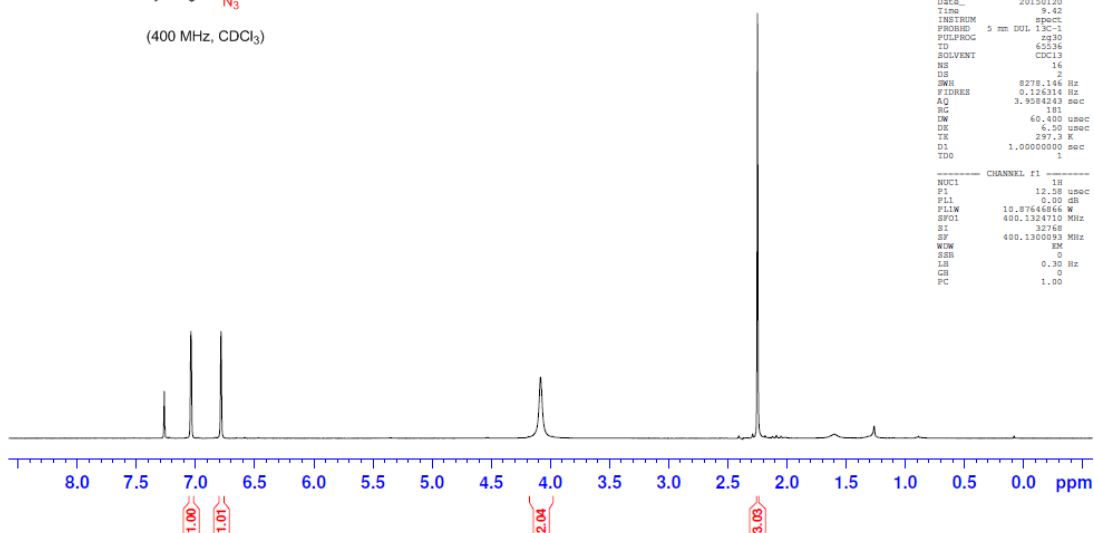


ldk-53

7.261
7.035
6.781

4.082

2.248

(400 MHz, CDCl₃)

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PROCNO    1
Date_     20150120
Time      8.42
INSTRUM    spect
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PULPROG    zg30
TD         65536
SOLVENT    CDCl3
NS         16
DS         2
SWH         8278.144 Hz
FIDRES     0.125314 Hz
AQ         3.9584243 sec
RG         181
DW         60.400 usec
DE         6.200 usec
TE         297.3 K
D1         1.00000000 sec
D11        1
===== CHANNEL f1 =====
NUC1       1H
P1         12.50 usec
PL1        0.00 dB
PL1W       18.8764868 W
SFO1       400.1324710 MHz
SI         32768
SF         400.1300000 MHz
WDW        EM
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GB         0
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LDK_53

133.915

128.630

128.721

125.621

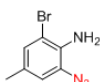
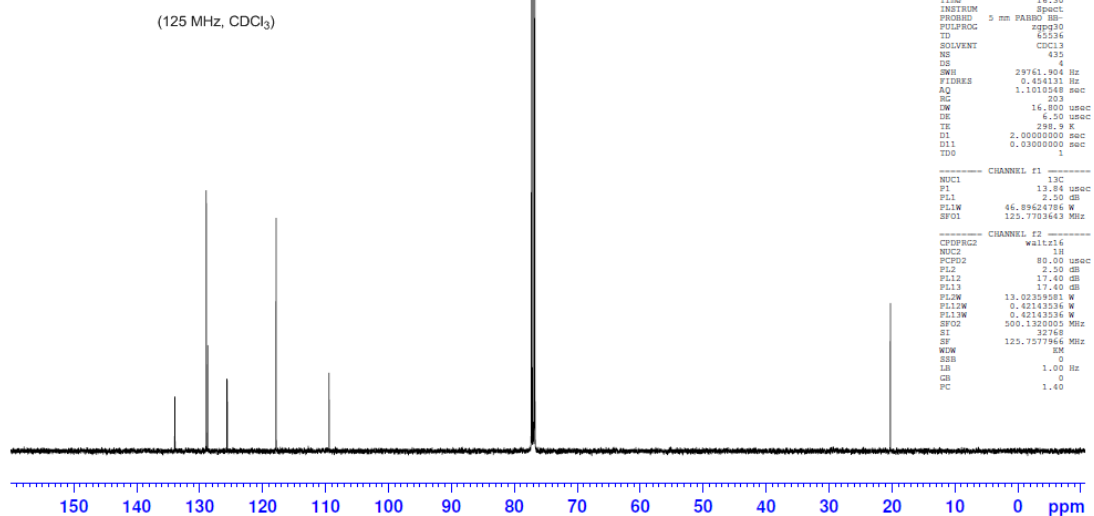
117.843

109.421

77.242

76.734

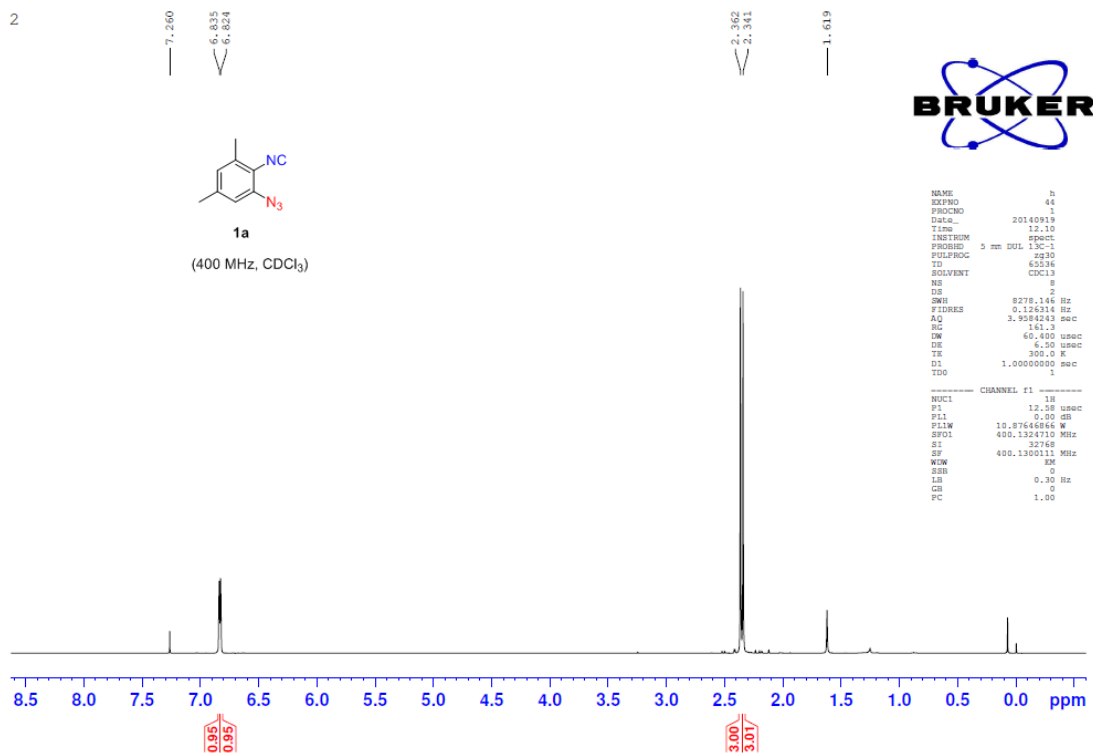
20.221

(125 MHz, CDCl₃)

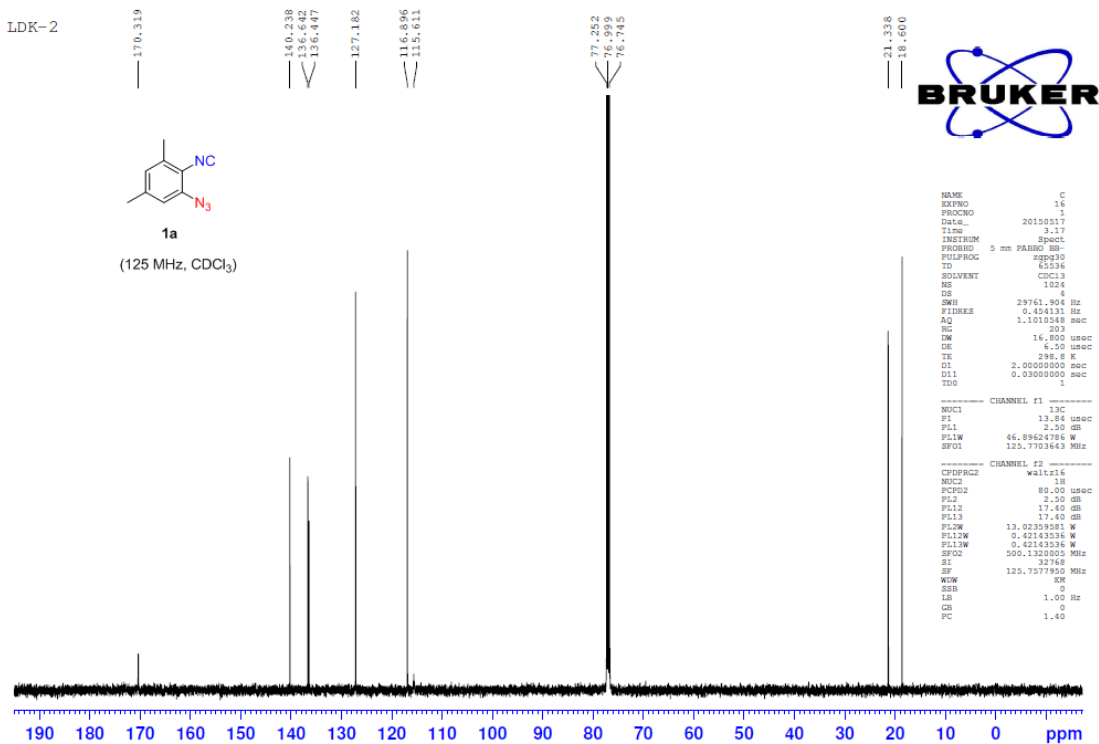
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PROCNO    1
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DS         4
SWH         29761.904 Hz
FIDRES     0.424131 Hz
AQ         1.1010248 sec
RG         203
DW         16.800 usec
DE         6.200 usec
TE         298.9 K
D1         2.00000000 sec
D11        0.03000000 sec
D10        1
===== CHANNEL f1 =====
NUC1       13C
P1         13.84 usec
PL1        2.20 dB
PL1W       46.8962478 W
SFO1       125.7703643 MHz
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        2.20 dB
PL12       17.40 dB
PL13       17.40 dB
PL2W       13.0235981 W
PL12W      0.4214303 W
PL13W      0.4214303 W
SFO2       500.1320000 MHz
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SF         125.7577964 MHz
WDW        EM
SSB        0
LB         1.00 Hz
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PC         1.40
  
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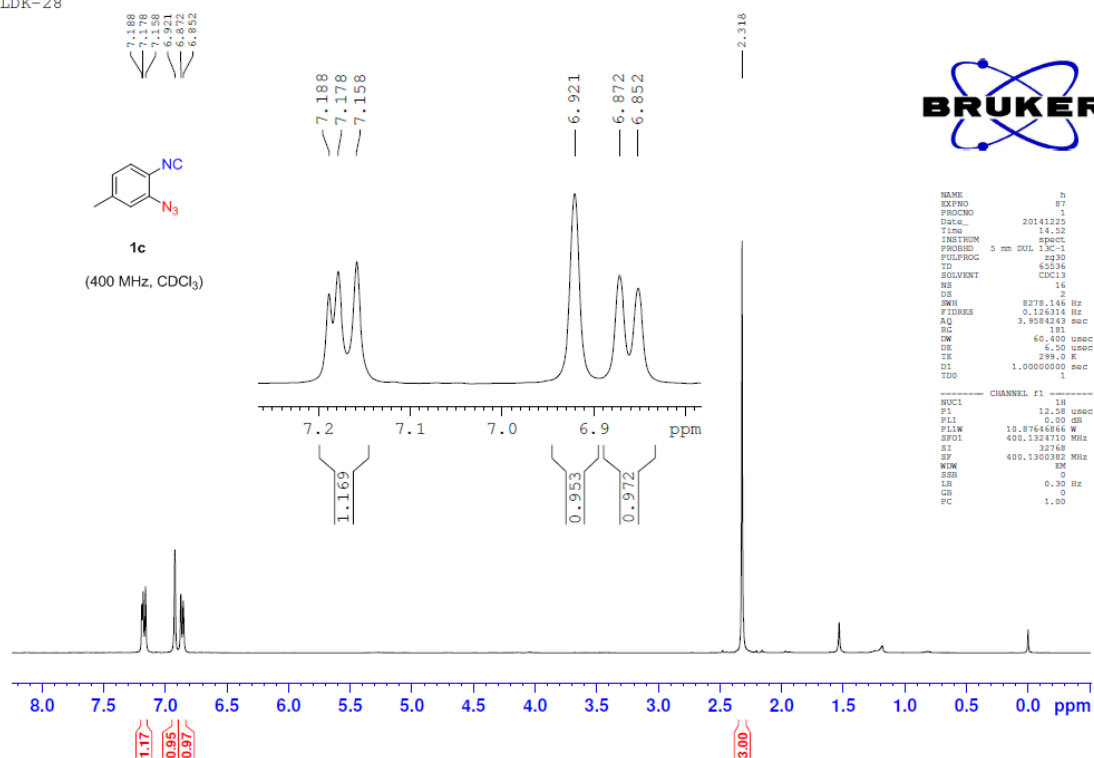
2



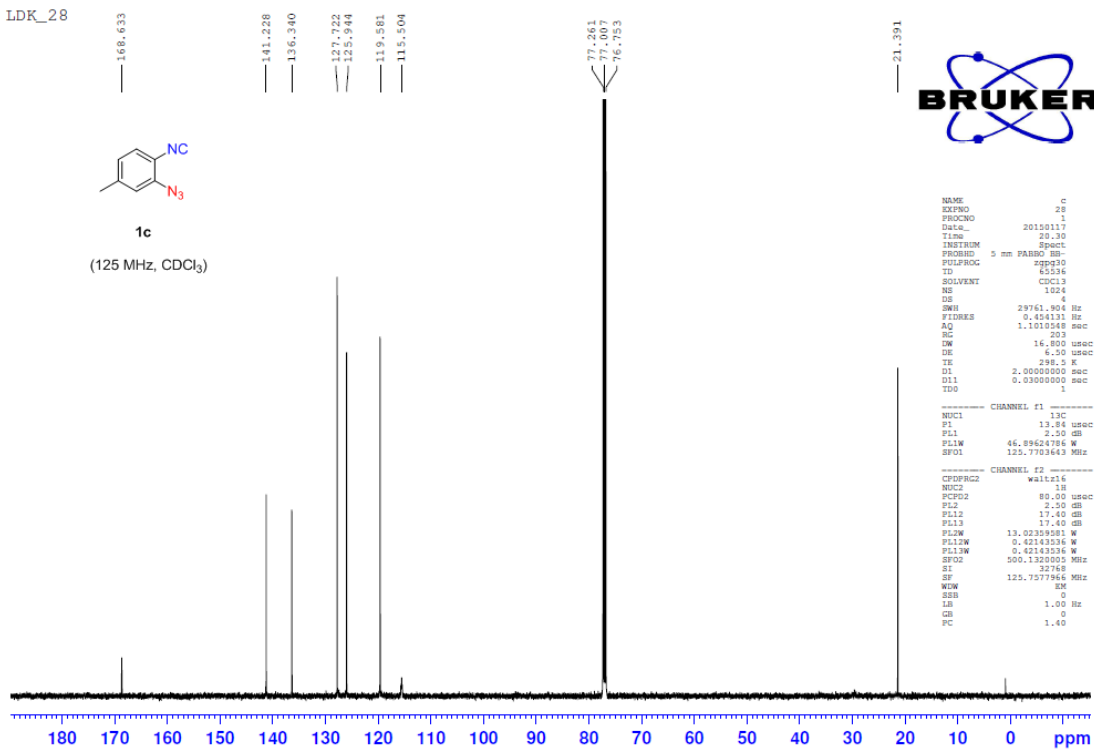
LDK-2



LDK-28



LDK_28

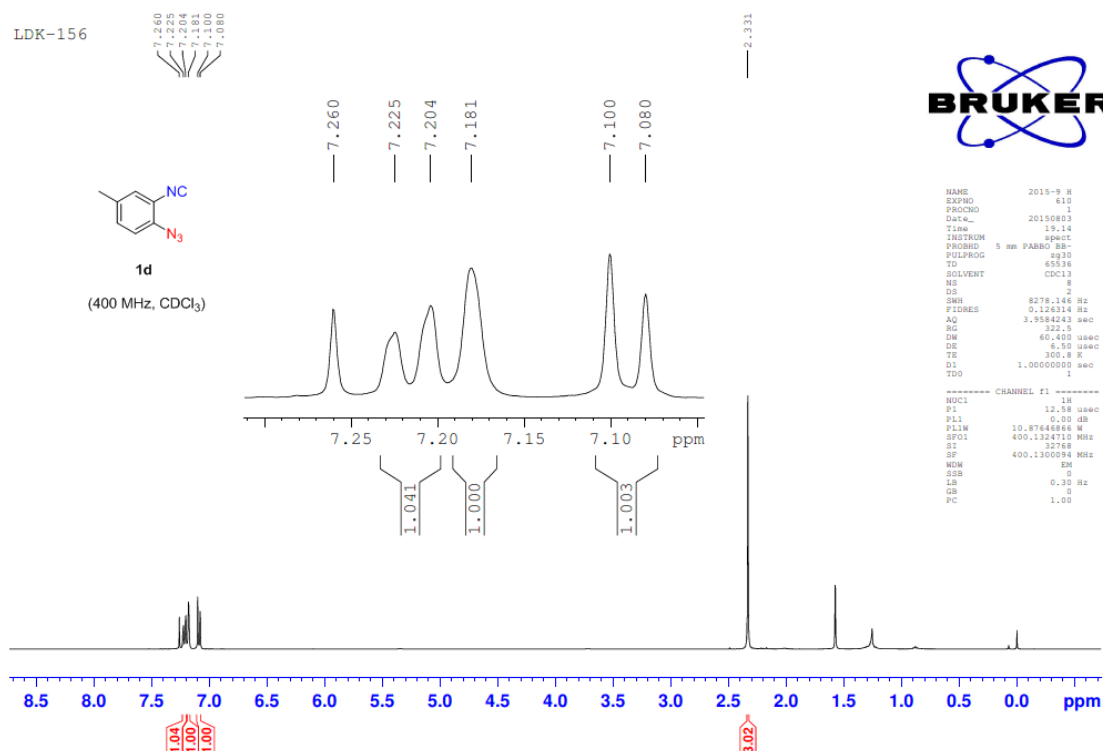


LDK-156



1d

(400 MHz, CDCl₃)

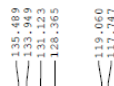


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Time 19:14
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
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FIDRES 0.12314 Hz
AQ 3.9584243 sec
RG 322.5
OW 65.405 usec
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TE 300.2 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 1H
P1 12.50 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324715 MHz
SI 32768
SF 400.1320094 MHz
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SSB 0
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GB 0
PC 1.00

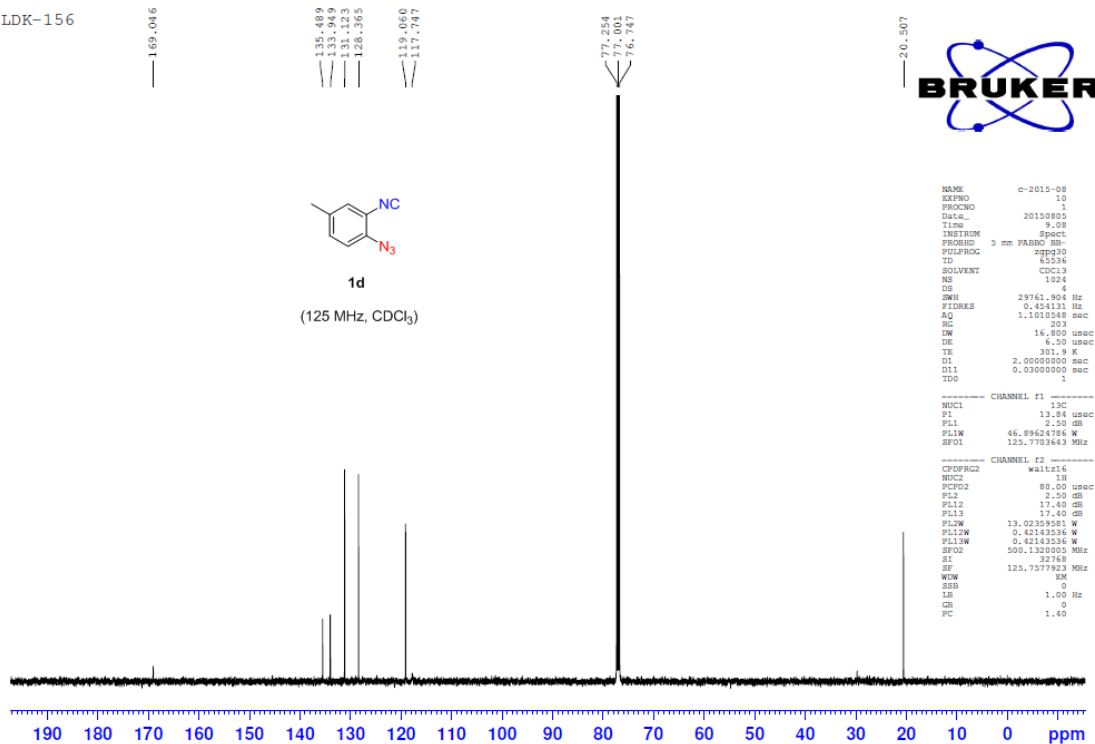
LDK-156

169.046



1d

(125 MHz, CDCl₃)

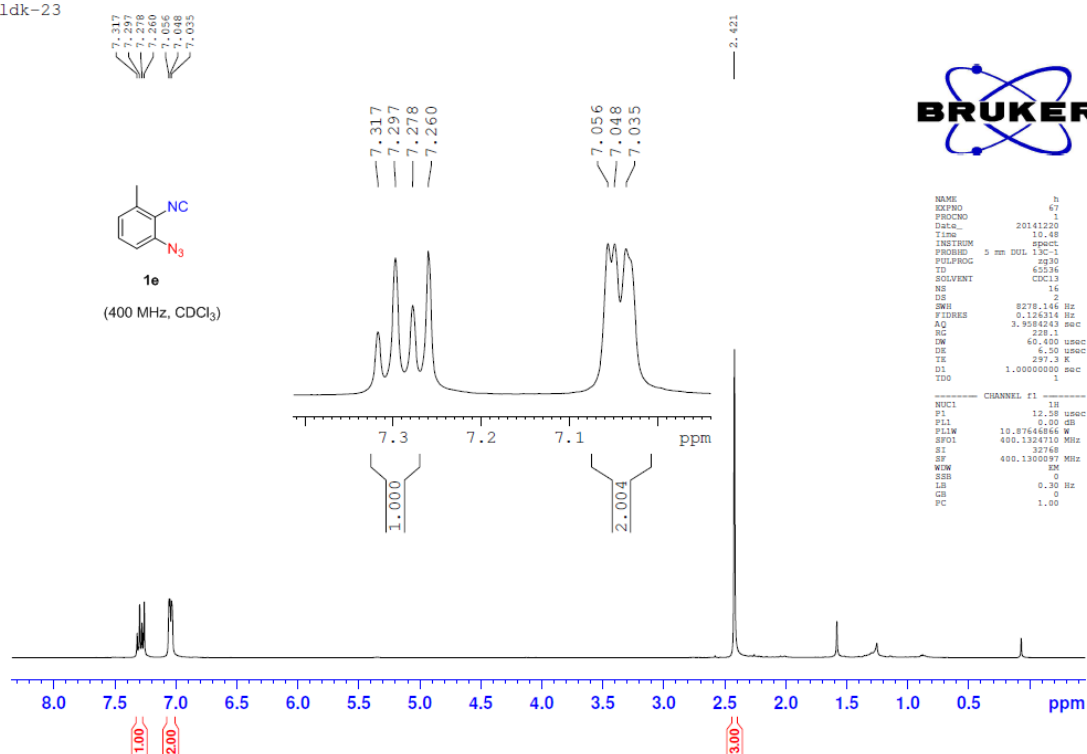


NAME c-2015-08
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PROCNO 1
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.424231 Hz
AQ 1.1010548 sec
RG 253
OW 16.800 usec
DE 6.50 usec
TE 301.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

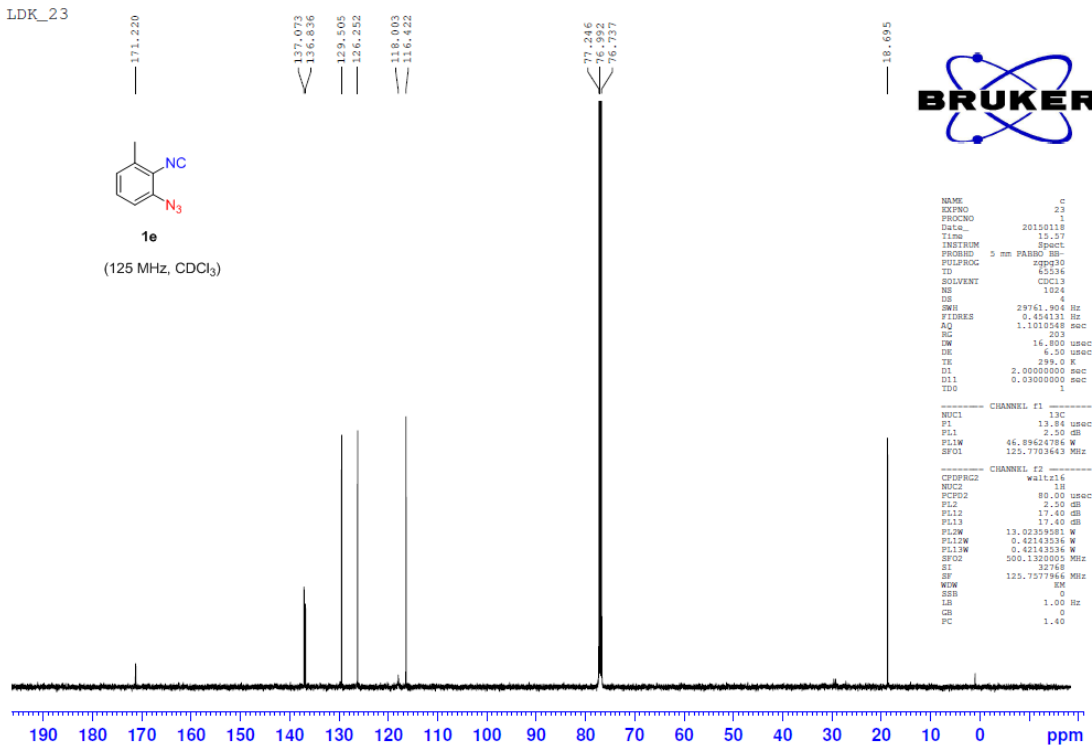
----- CHANNEL f1 -----
NUC1 13C
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PL1 2.20 dB
PL1W 46.89624756 W
SFO1 125.7703643 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.20 dB
PL12 17.40 dB
PL13 17.40 dB
PL1W 13.02359581 W
PL12W 0.42143535 W
PL13W 0.42143535 W
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SI 32768
SF 125.7577923 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

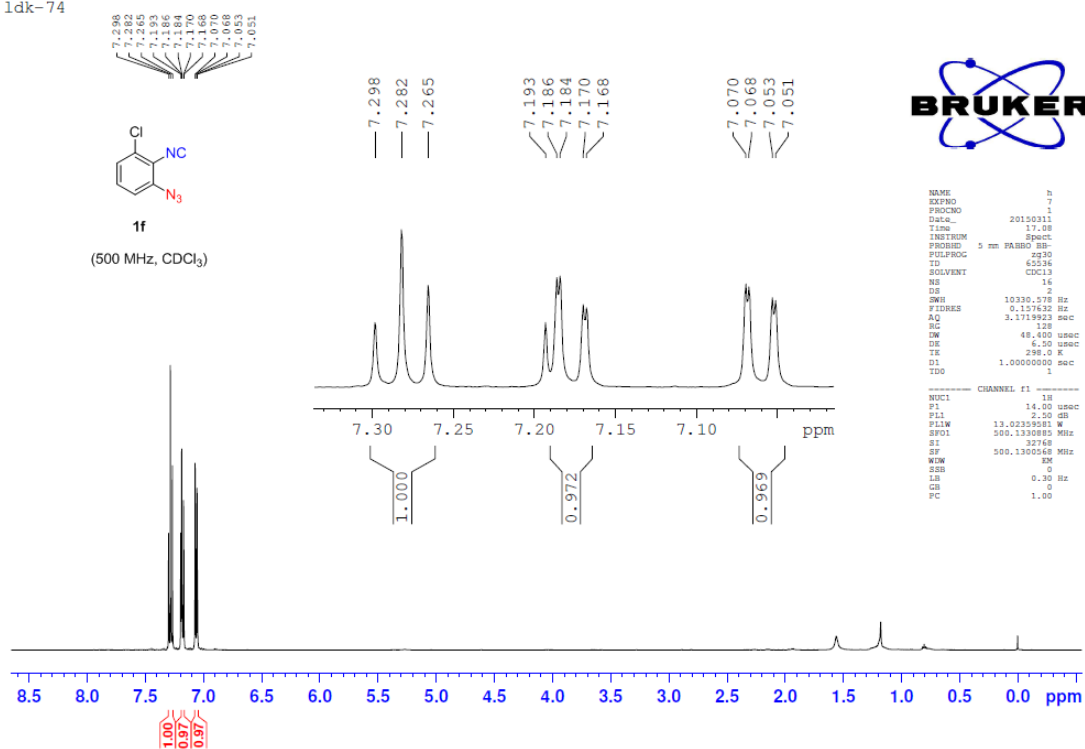
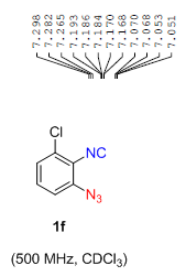
ldk-23



LDK_23



ldk-74



```

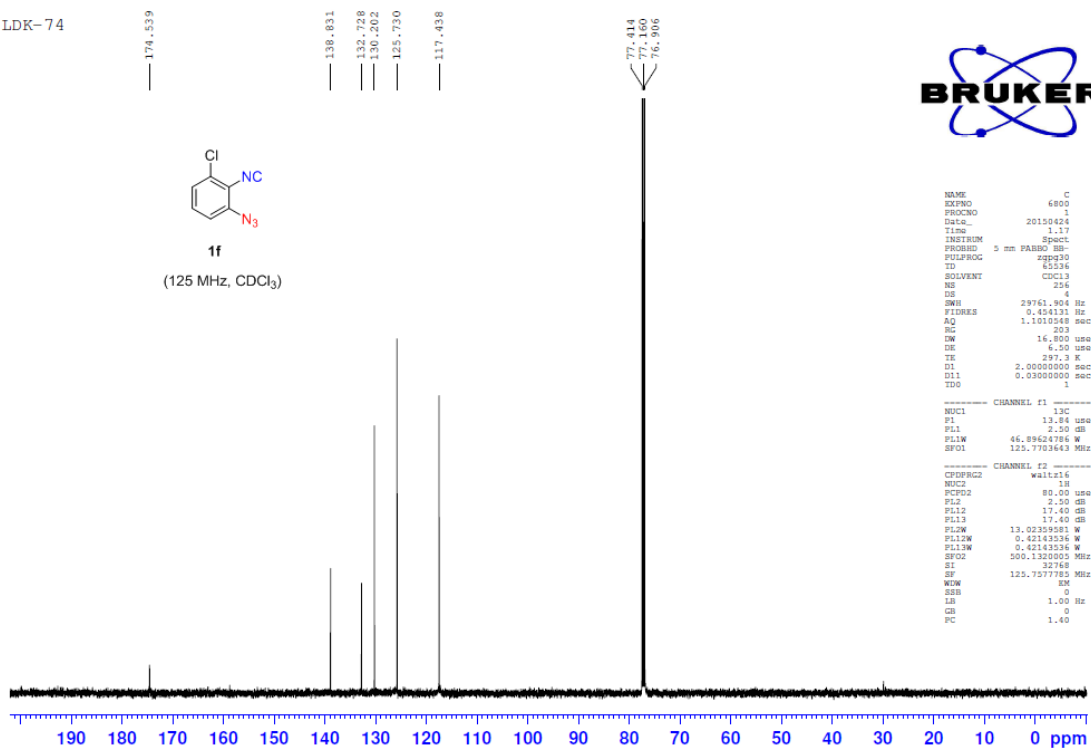
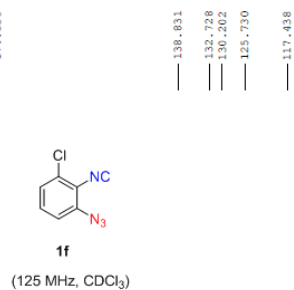
NAME      h
EXPNO     7
PROCNO    1
Date_     20150311
Time      17.08
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zg30
TD         65536
SOLVENT    CDCl3
NS         14
DS         2
SWH         10330.778 Hz
FIDRES     0.107632 Hz
AQ         3.1719923 sec
RG         138
WDW         48.400 usec
SSB         0
DE         6.50 usec
TE         298.0 K
D1         1.00000000 sec
TD0        1
  
```

CHANNEL F1

```

NUC1      1H
P1        14.00 usec
PL1       2.50 dB
PL1W      13.02359581 W
SF01      500.1330882 MHz
SI        32768
SF         500.1330882 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

LDK-74



```

NAME      C
EXPNO     6800
PROCNO    1
Date_     20150624
Time      1.17
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         256
DS         4
SWH         29761.904 Hz
FIDRES     0.454131 Hz
AQ         1.1010348 sec
RG         203
WDW         16.800 usec
SSB         0
DE         6.50 usec
TE         297.3 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
  
```

CHANNEL F1

```

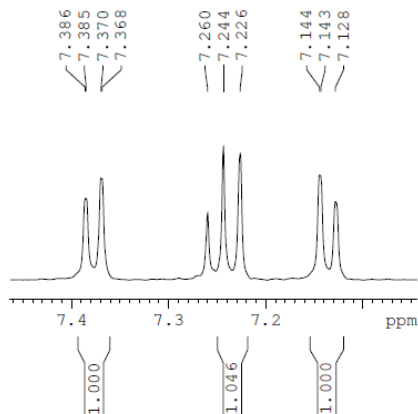
NUC1      13C
P1        13.84 usec
PL1       2.50 dB
PL1W      46.89624786 W
SF01      125.7703643 MHz
  
```

CHANNEL F2

```

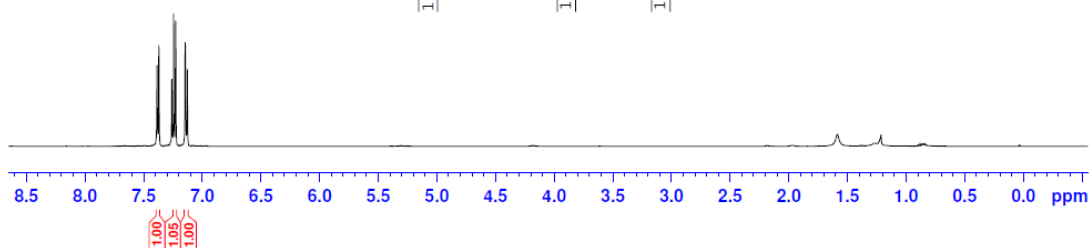
CPDPRG2   waitz16
NUC2      1H
PCPD2     80.00 usec
PL2       2.50 dB
PL2W      17.40 dB
PL13      17.40 dB
PL1W      13.02359581 W
PL12W     0.42143536 W
PL13W     0.42143536 W
SF02      500.1320005 MHz
SI        32768
SF         125.7577782 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

LDK-108

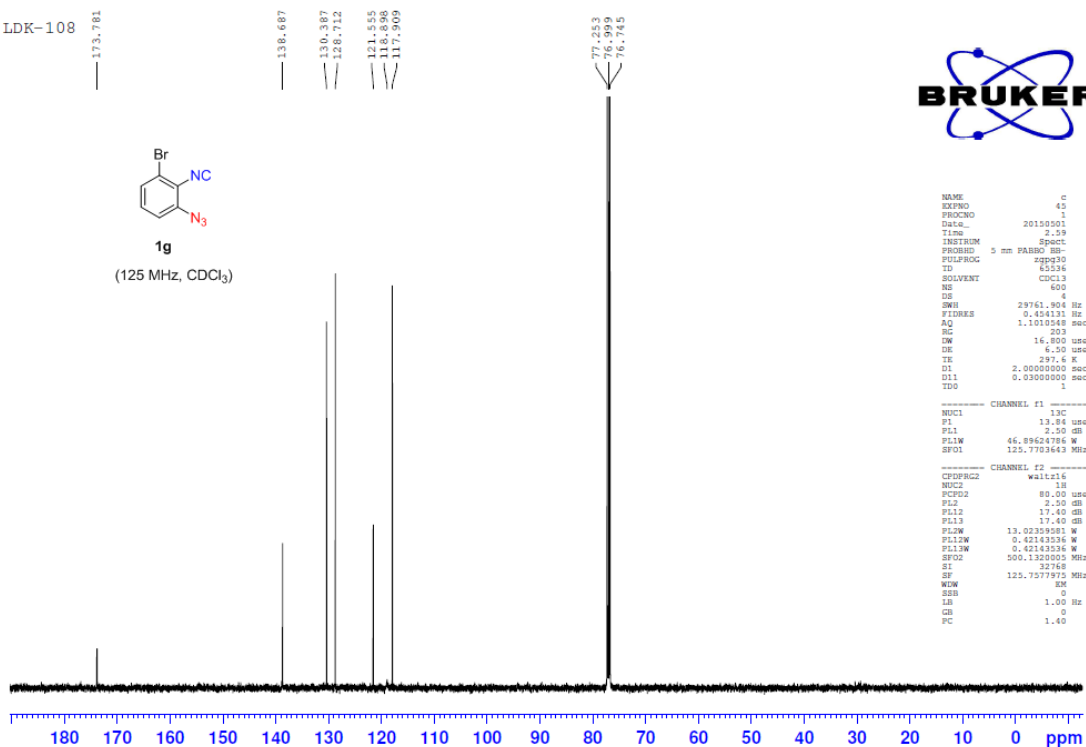
**1g**(500 MHz, CDCl₃)

NAME h
EXPNO 20
PROCNO 1
Date_ 20150430
Time 20.34
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 14
DS 2
SWH 10330.578 Hz
FIDRES 0.157625 Hz
AQ 3.1719923 sec
RG 203
LW 48.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0

CHANNEL F1
NUC1 1H
P1 14.00 usec
PL1 2.50 dB
PL1W 13.02339881 W
SFO1 500.1300000 MHz
SI 32768
SF 500.1300000 MHz
WIM EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



LDK-108

**1g**(125 MHz, CDCl₃)

NAME j c
EXPNO 45
PROCNO 1
Date_ 20150501
Time 2.59
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 600
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010248 sec
RG 203
LW 16.000 usec
DE 6.50 usec
TE 297.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0

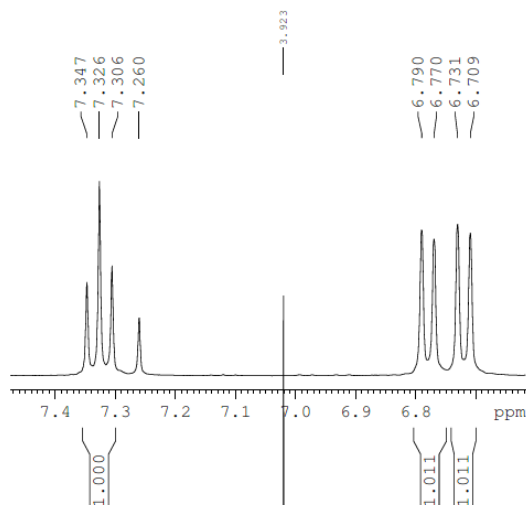
CHANNEL F1
NUC1 13C
P1 13.84 usec
PL1 2.50 dB
PL1W 46.89624786 W
SFO1 125.7703643 MHz

CHANNEL F2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
P12 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL1W 13.02339881 W
PL1W 0.42143936 W
PL1W 0.42143936 W
SFO2 500.1300000 MHz
SI 32768
SF 125.7577975 MHz
WIM EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

LDK-152

7.347
7.326
7.306
7.260

6.790
6.770
6.731
6.709

**1h**(400 MHz, CDCl₃)

NAME 2015-9 H
EXPNO 1
PROCNO 1
Date_ 20150722
Time 22.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4
DS 2
SWH 8278.144 Hz
FIDRES 0.12314 Hz
AQ 3.9584243 sec
RG 256
DW 60.400 usec
DE 16.50 usec
TE 300.2 K
D1 1.0000000 sec
TDO

===== CHANNEL f1 =====
NUC1 1H
P1 12.58 usec
PL1 0.00 dB
PL1W 10.874888 W
SFO1 400.1324710 MHz
SI 32768
SF 400.130092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

LDK-152

172.847

156.385

138.138

130.144

119.451

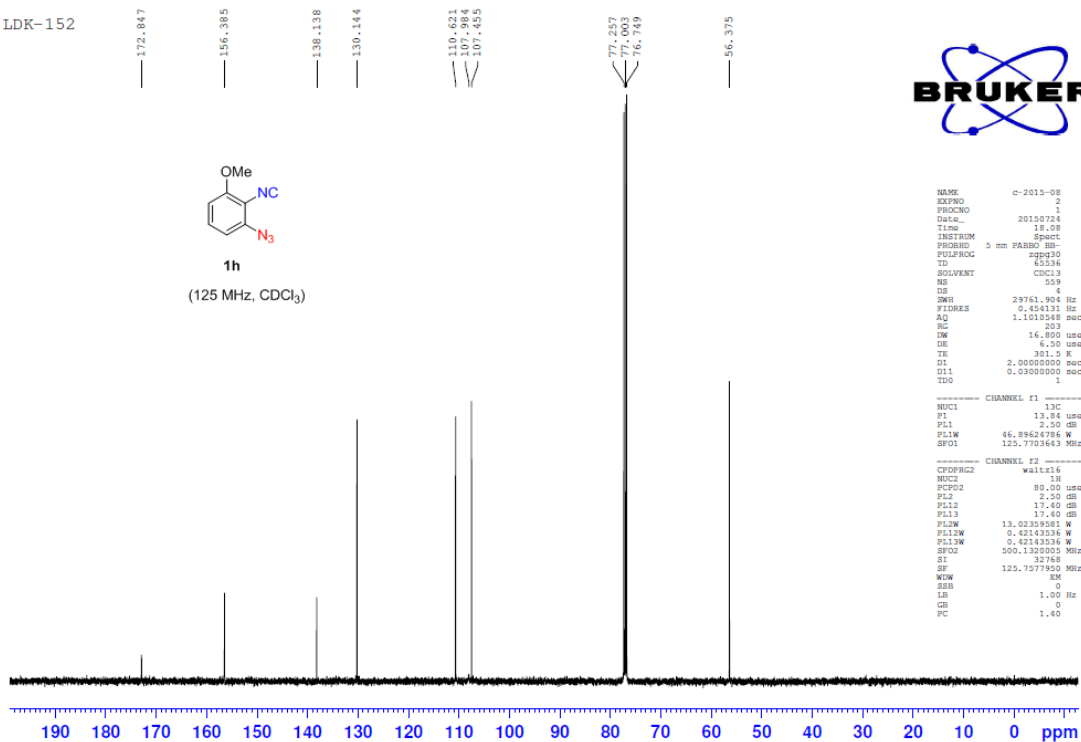
107.984

107.455

77.257

76.749

96.375

**1h**(125 MHz, CDCl₃)

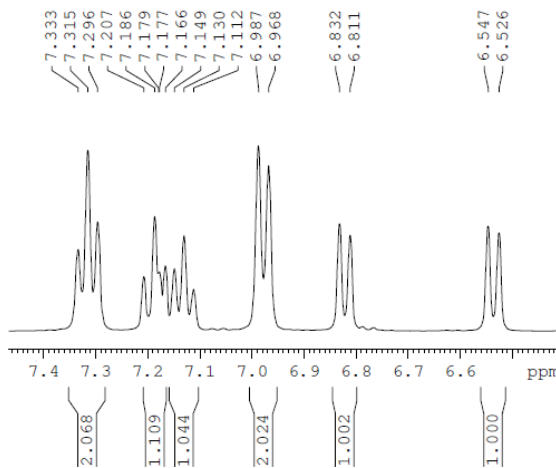
NAME C-2015-08
EXPNO 2
PROCNO 1
Date_ 20150724
Time 16.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 509
DS 4
SWH 29761.904 Hz
FIDRES 0.424121 Hz
AQ 1.1010548 sec
RG 259
DW 16.800 usec
DE 4.20 usec
TE 301.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 13.84 usec
PL1 2.50 dB
PL1W 46.8962478 W
SFO1 125.7703643 MHz
===== CHANNEL f2 =====
CPOPC2 waltz16
NUC2 1H
PCPO2 80.00 usec
PL2 2.50 dB
PL2 17.40 dB
PL3 17.40 dB
PL2W 13.0235958 W
PL3W 0.4214333 W
SFO2 500.132092 MHz
SI 32768
SF 125.7577950 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ldk-59



1i
(400 MHz, CDCl₃)



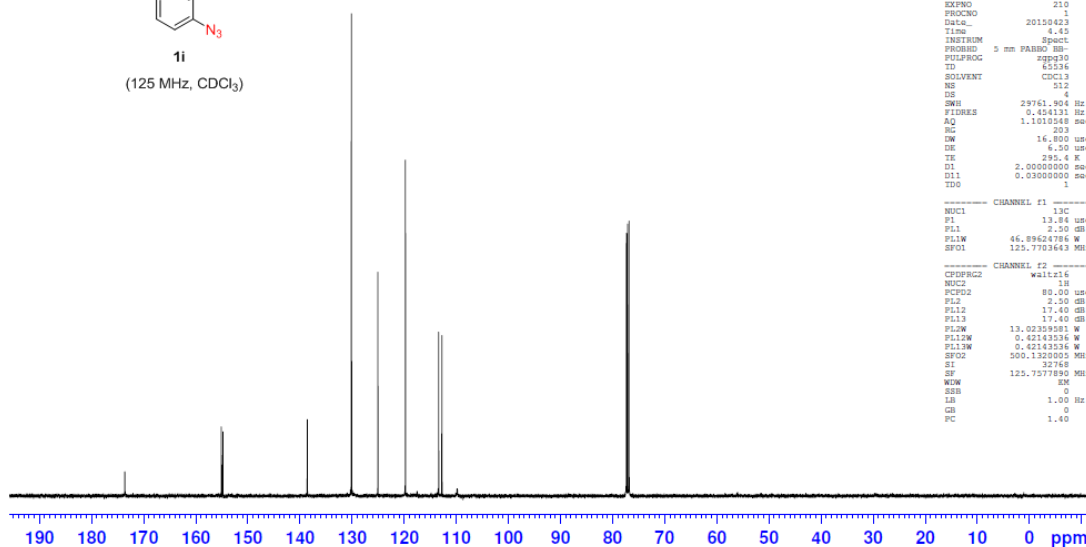
NAME 1i
EXPNO 33
PROCNO 20150129
Date_ 7.19
Time 8:05
INSTRUM spect
PROBHD 5 mm DOL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.144 Hz
FIDRES 0.126314 Hz
AQ 3.8580243 sec
RG 80.5
DW 60.400 usec
DE 6.50 usec
TE 299.2 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 13C
P1 12.50 usec
PL1 0.00 dB
PL1W 10.87645064 W
SFO1 400.1324710 MHz
SI 32769
SF 400.1300427 MHz
WUW 0
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

LDK-59



1i
(125 MHz, CDCl₃)



NAME 1i
EXPNO 23
PROCNO 20150423
Date_ 4.15
Time 8:05
INSTRUM spect
PROBHD 5 mm PABBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.458131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 295.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

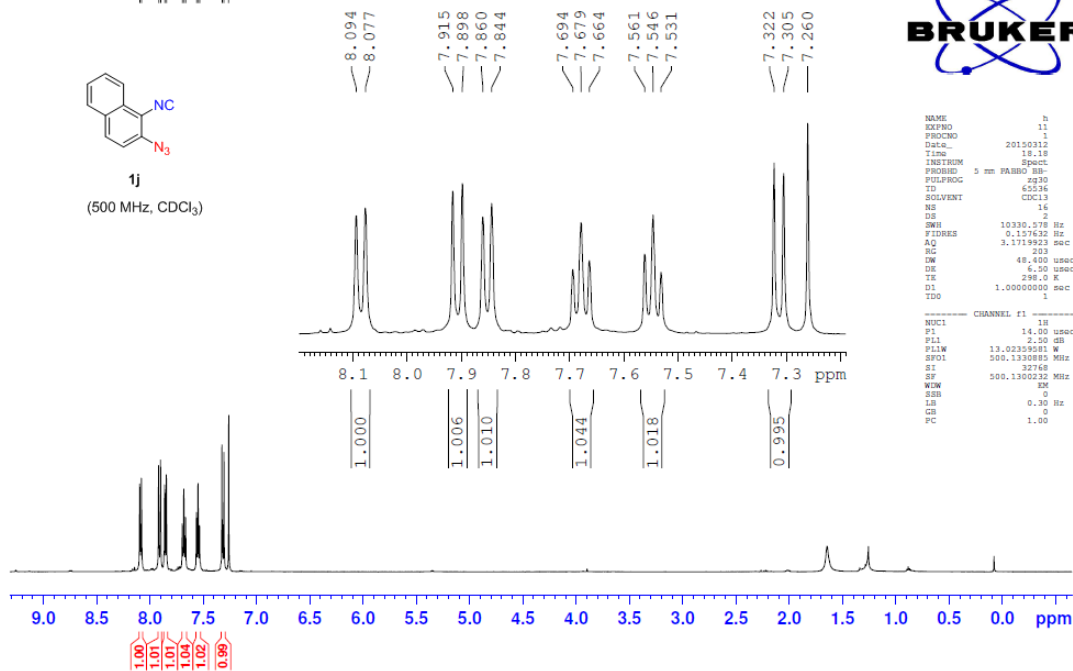
----- CHANNEL f1 -----
NUC1 13C
P1 13.84 usec
PL1 2.50 dB
PL1W 46.89624706 W
SFO1 125.7703643 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 89.50 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL1W 13.02309081 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320050 MHz
SI 32769
SF 125.7577890 MHz
WUW 0
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

LDK-77



1j
(500 MHz, CDCl₃)



```

NAME      h
EXPNO     1
PROCNO    1
Data_     20150311
Time      18.18
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zg30
TD         65536
SOLVENT    CDCl3
NS         14
DS         2
SWH        10330.378 Hz
AQ         0.157632 sec
RG         203
WDW         48.400 usec
DE         6.50 usec
TE         298.0 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         14.00 usec
PL1        2.50 dB
PL1W       13.02339081 W
SFO1       500.1330885 MHz
SI         32768
SF         500.1330232 MHz
WUM        0
SBB        0
LB         0.30 Hz
GB         0
PC         1.00

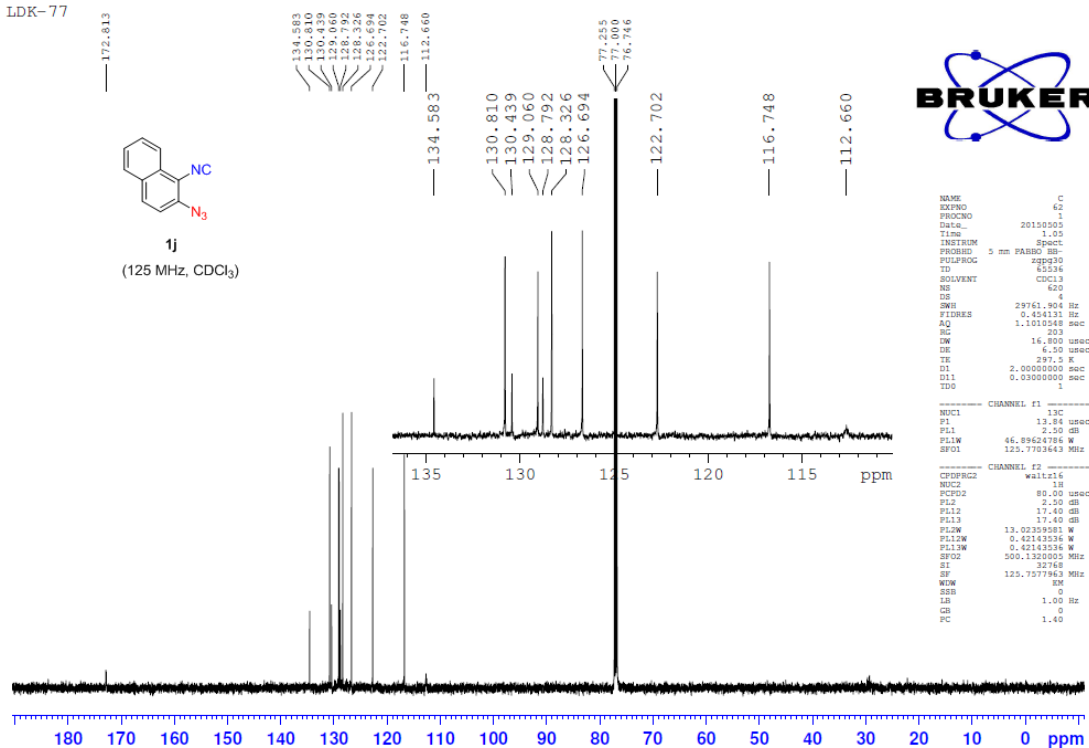
```

LDK-77

— 172.813



1j
(125 MHz, CDCl₃)



```

NAME      c
EXPNO     62
PROCNO    1
Data_     20150505
Time      1.00
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         620
DS         4
SWH        29761.904 Hz
AQ         0.424131 sec
RG         1.1010548 sec
WDW         16.800 usec
DE         6.50 usec
TE         297.5 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

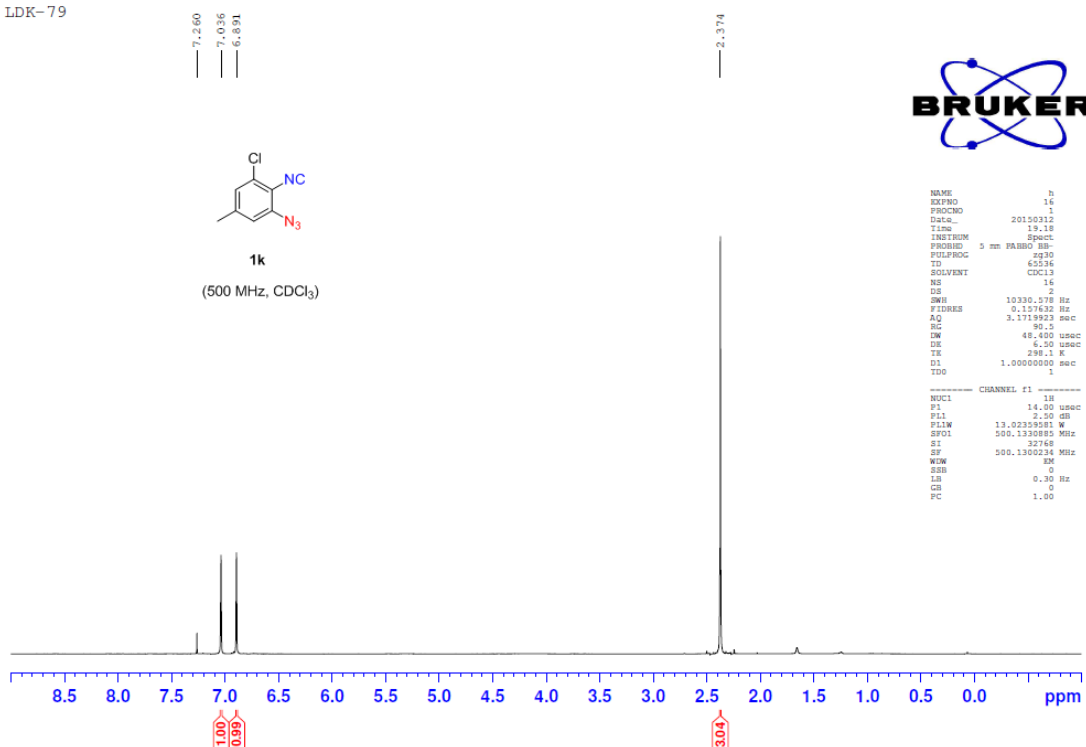
===== CHANNEL f1 =====
NUC1       13C
P1         13.84 usec
PL1        2.50 dB
PL1W       46.89624786 W
SFO1       125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        2.50 dB
PL12       17.40 dB
PL13       17.40 dB
PL2W       13.02339081 W
PL1W       0.42143536 W
SFO2       500.1330885 MHz
SI         32768
SF         125.7577963 MHz
WUM        0
SBB        0
LB         1.00 Hz
GB         0
PC         1.40

```

LDK-79

7.260
7.036
6.891

**1k**(500 MHz, CDCl₃)

LDK-79

173.549

141.483

138.167

132.035

126.351

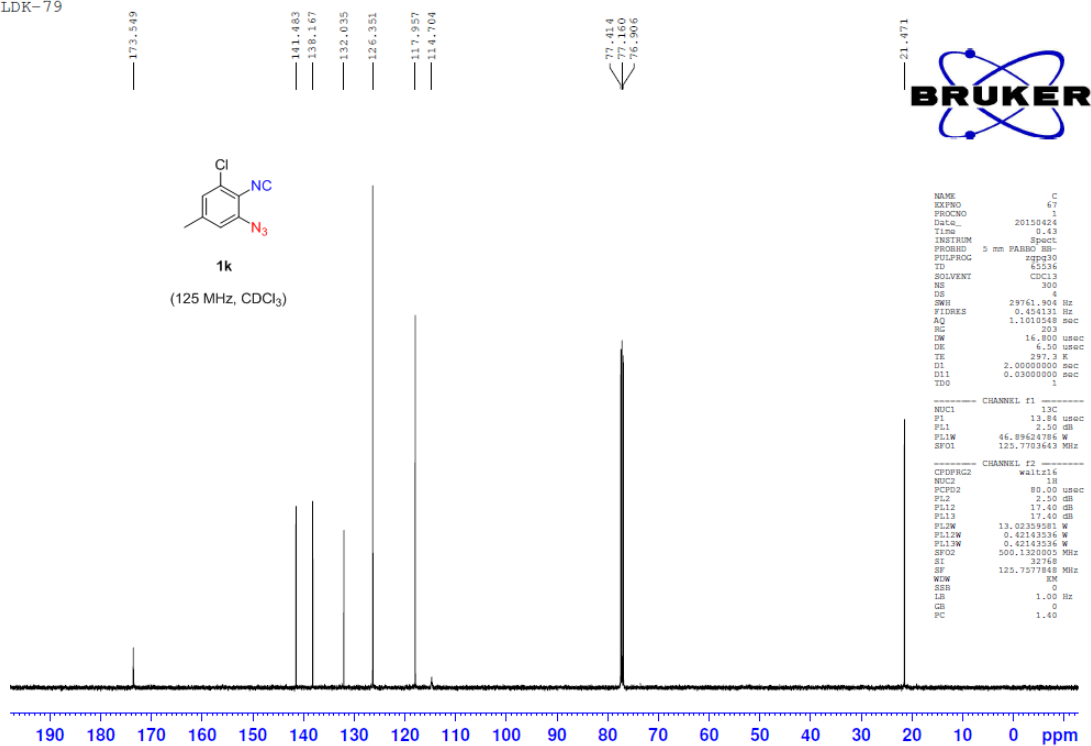
117.957

114.704

77.414

77.000

76.596

**1k**(125 MHz, CDCl₃)

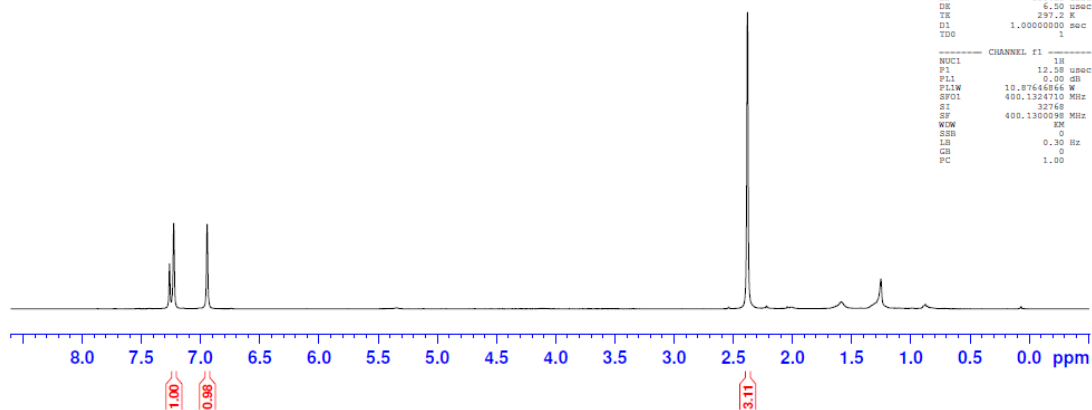
LDK-55

7.260
7.224
6.941

2.377



11

(400 MHz, CDCl₃)

```

NAME      h
EXPNO     12
PROCNO    1
Date_     20150123
Time      2:23
INSTRUM    spect
PROBHD     5 mm DOL 13C-1
PULPROG    zg30
TD         65536
SOLVENT    CDCl3
NS         16
DS         2
SWH        8278.144 Hz
FIDRES     0.126314 Hz
AQ         3.9584243 sec
RG         256
WDW        60.400 usec
DE         6.50 usec
TE         297.2 K
D1         1.00000000 sec
TD0        1
----- CHANNEL f1 -----
NUC1       1H
P1         12.50 usec
PL1        0.00 dB
PL1W       10.8764686 W
SFO1       400.1324711 MHz
SI         32768
SF         400.130099 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

```

LDK-55

172.587

141.618
138.105

129.394

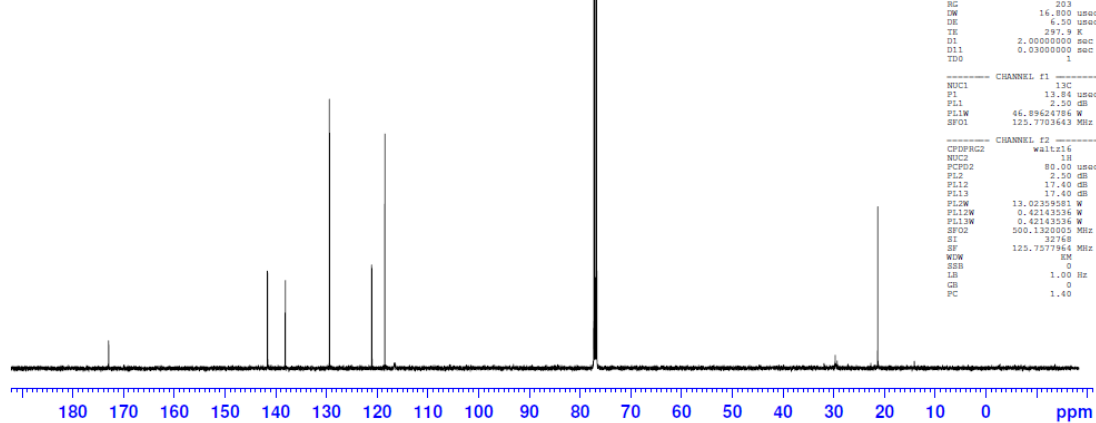
121.052
118.480
116.511

77.255
77.001
76.747

21.252



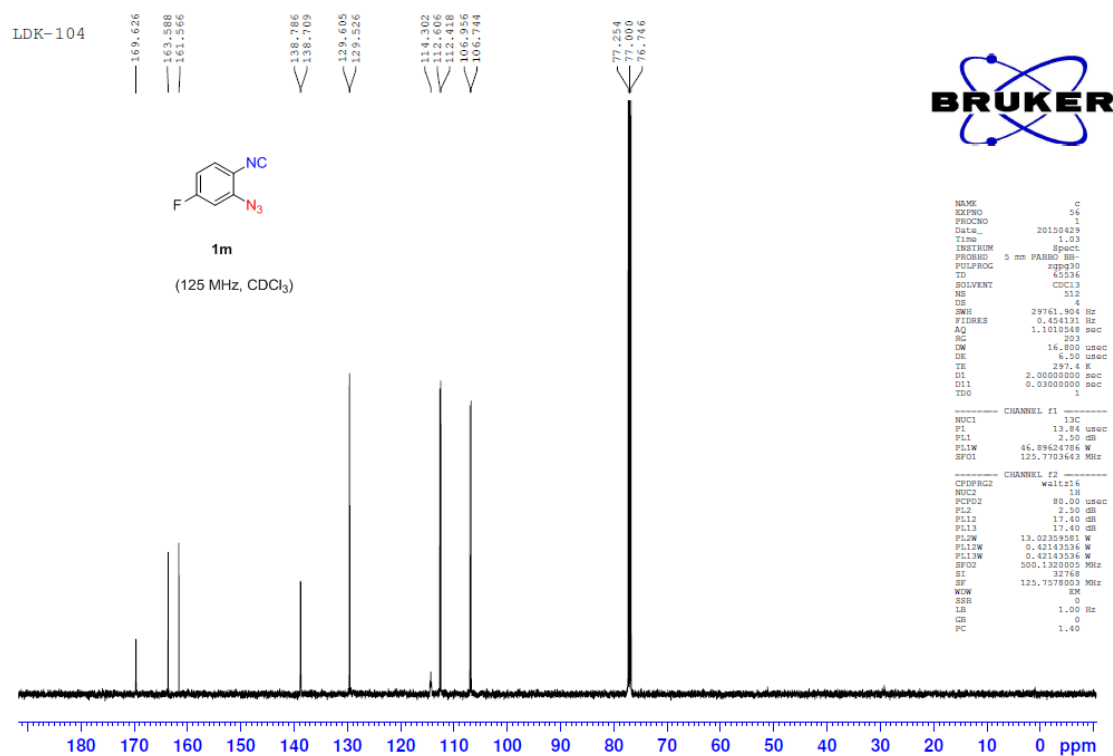
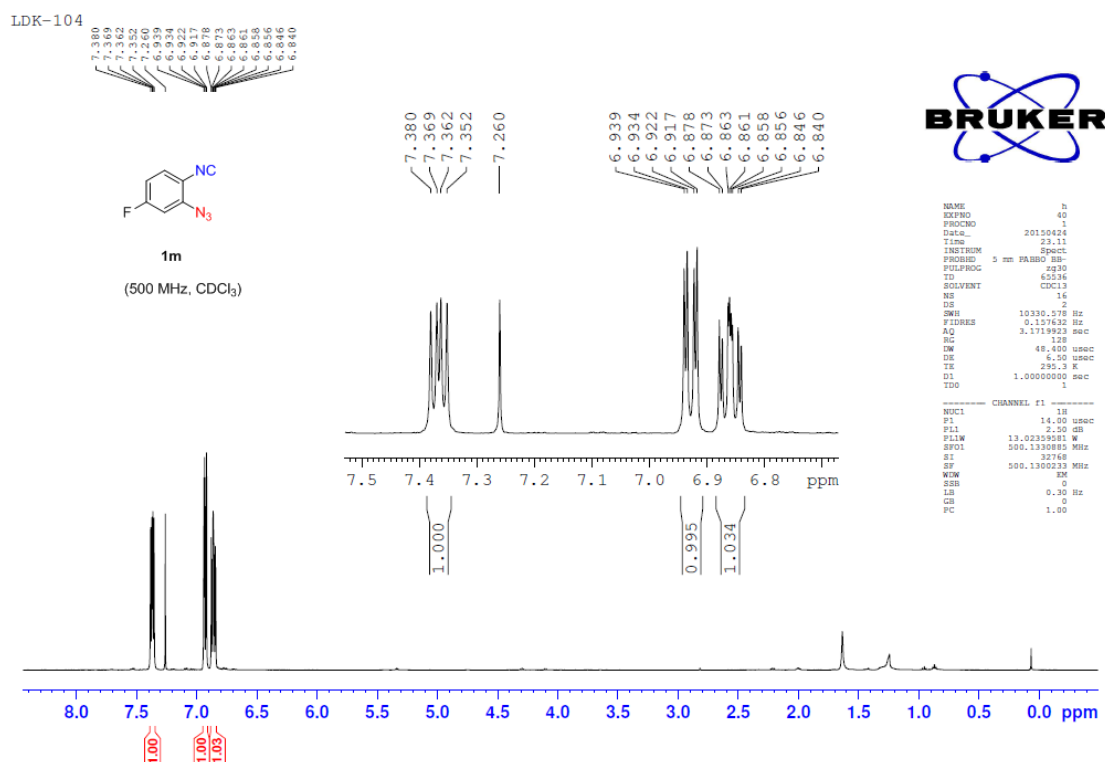
11

(125 MHz, CDCl₃)

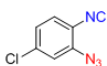
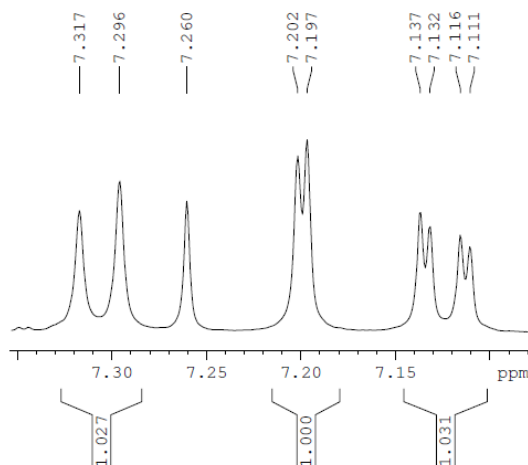
```

NAME      C
EXPNO     51
PROCNO    1
Date_     20150313
Time      6:24
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         1204
DS         4
SWH        29761.904 Hz
FIDRES     0.424131 Hz
AQ         1.1010268 sec
RG         203
WDW        14.800 usec
DE         6.50 usec
TE         297.2 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
----- CHANNEL f1 -----
NUC1       13C
P1         13.84 usec
PL1        2.50 dB
PL1W       46.8962478 W
SFO1       125.7703643 MHz
----- CHANNEL f2 -----
wait1216
NUC2       1H
PCPD2      80.00 usec
PL2        2.50 dB
PL12       17.40 dB
PL13       17.40 dB
PL2W       13.02359581 W
PL12W      0.42143538 W
PL13W      0.42143538 W
SFO2       500.1320000 MHz
SI         32768
SF         125.7577964 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```

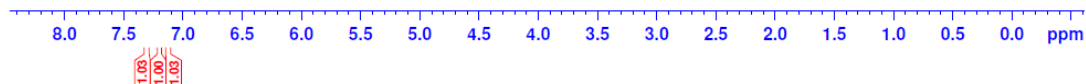


LDK-118

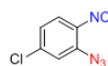
(400 MHz, CDCl₃)

NAME h
EXPRO 2700
PROCNO 1
Date_ 20150509
Time 19.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.144 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 362
DW 60.400 usec
DE 6.50 usec
TK 300.9 K
D1 1.00000000 sec
TDO 1

CHANNEL f1
NUC1 1H
P1 12.28 usec
PL1 0.00 dB
PL1W 10.87646844 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300091 MHz
WOW RM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



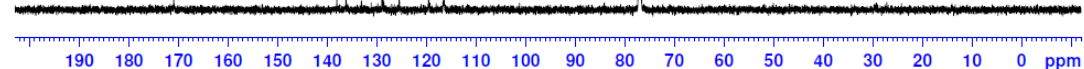
LDK-118

(125 MHz, CDCl₃)

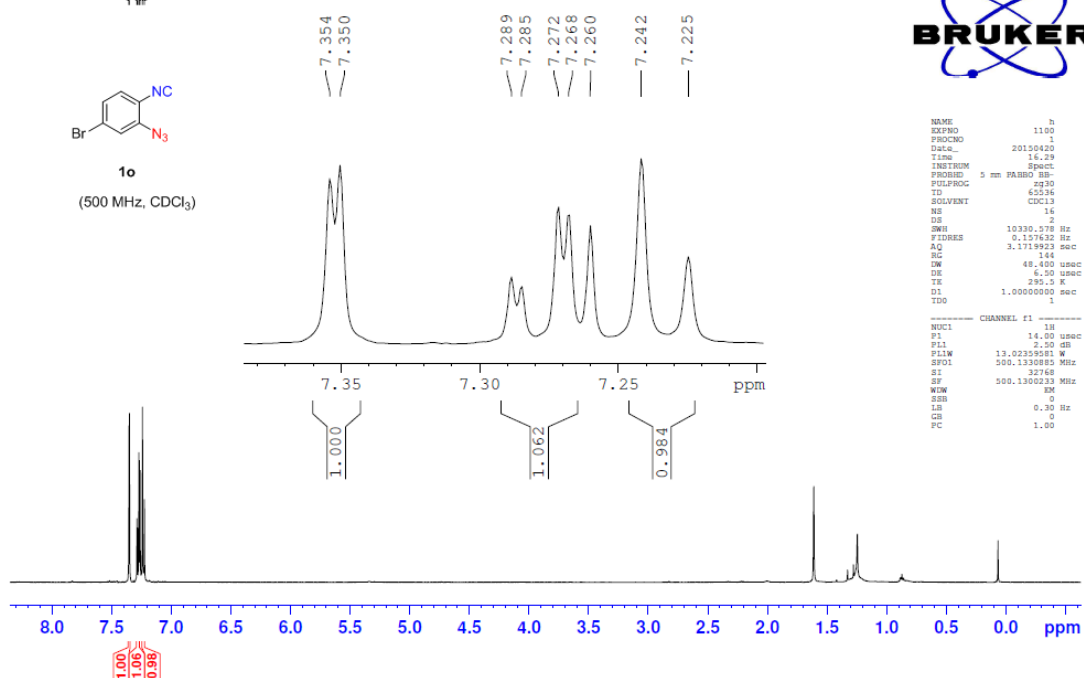
NAME LDK-118
EXPRO 1
PROCNO 1
Date_ 20150511
Time 0.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 975
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TK 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

CHANNEL f1
NUC1 13C
P1 13.84 usec
PL1 2.50 dB
PL1W 46.89624794 W
SFO1 125.7703643 MHz

CHANNEL f2
CPDPRG2 wait1216
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02309581 W
PL12W 0.42143336 W
PL13W 0.42143336 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577949 MHz
WOW RM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.354
7.350
7.289
7.285
7.272
7.268
7.260
7.242

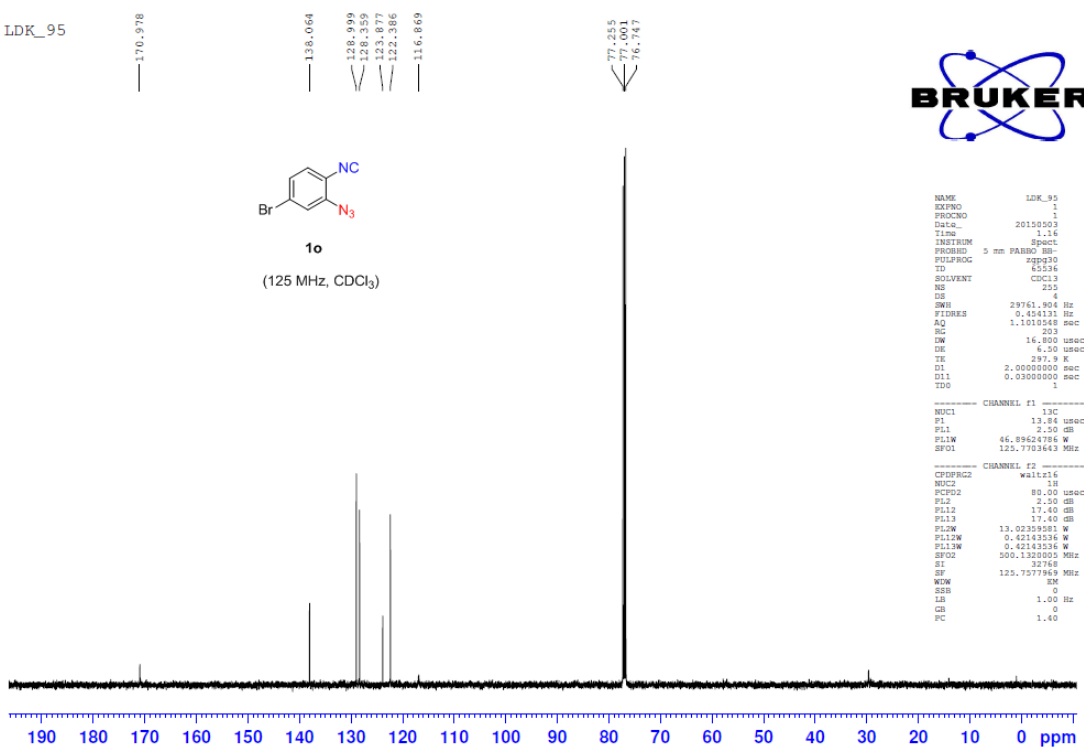


```

NAME
KXPROB 1100
PHOBROD
DATE 20150420
TIME 16.29
INSTRUM NMR
PROBHD 5 mm PABBO-BB
PULPROG zgpg
PC 6.50
TD 32768
SOLVENT CDCl3
NS 16
DS 2
AQH 10390.576 Hz
FIDRES 0.1571923 Hz
RG 13.7119923 sec
RG 164
WC 48.400
DE 48.400 usec
TE 295.2 K
D1 1.00000000 sec
D0 1
===== CHANNEL f1 =====
NUC1 F1 16
P1 14.400 usec
P12 2.500 gHz
P13 15.000 W
SFO1 103.625893 MHz
SF 32768
SS 500.1302333 MHz
WINDW EM
SBS 0
GB 0.30 Hz
GB 0
PC 1.000

```

LDK_95

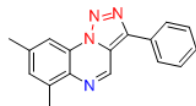


NAME	LDN-35
EXPNO	1
PROCNO	1
DATE_	20110505
TIME	1:16
INSTRUM	1
PROBHD	5 mm PABBO HD
PULPROG	zgpg30
TD	85536
NS	CC123
DS	2
SC	20
RG	29761.904 Hz
FIDRES	0.456131 Hz
WDW	1.1010000000000000
SSB	0
LB	203
GB	0
DE	6.3000000000000000
TE	297.879 K
D1	2.0000000000000000
D11	0.0300000000000000
TDO	1

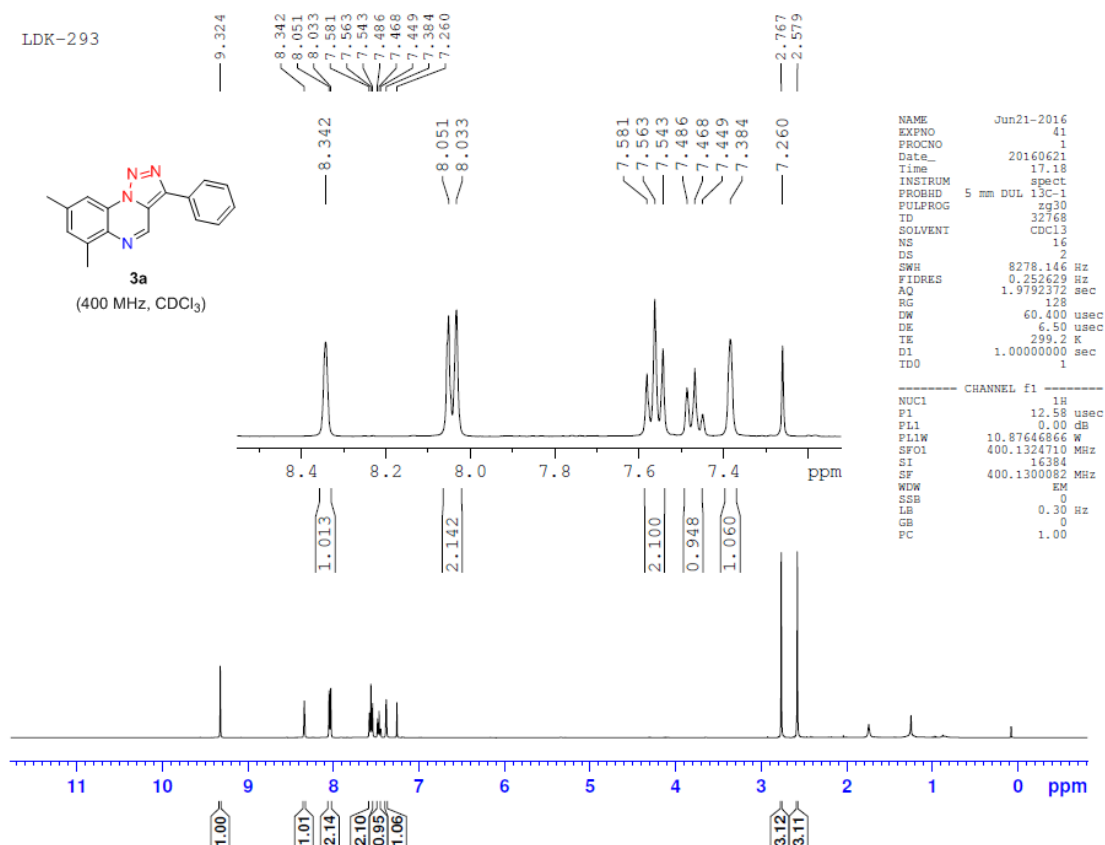
NAME	CHANNEL F1
NUC1	13C
P1	13.8400000000000000
PL1	0
AF1	46.9842769400000000
FLN1	125.7702645 Hz

NAME	CHANNEL F2
CPDPRG2	waltz16
NUC2	89Yb
P2	80.0000000000000000
PL2	2.2500000000000000
PL3	1.0000000000000000
PL13	17.4000000000000000
PL14	13.0200000000000000
PL12W	0.4212159356 Hz
PL12C	0.4212159356 Hz
PL12F	500.1250000000000000
SR	32768
DE	125.7702645 Hz
TE	297.879 K
DS	2
SSB	0
LB	1.0000000000000000
GB	0
DE	1.0000000000000000

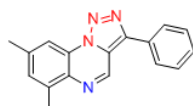
LDK-293



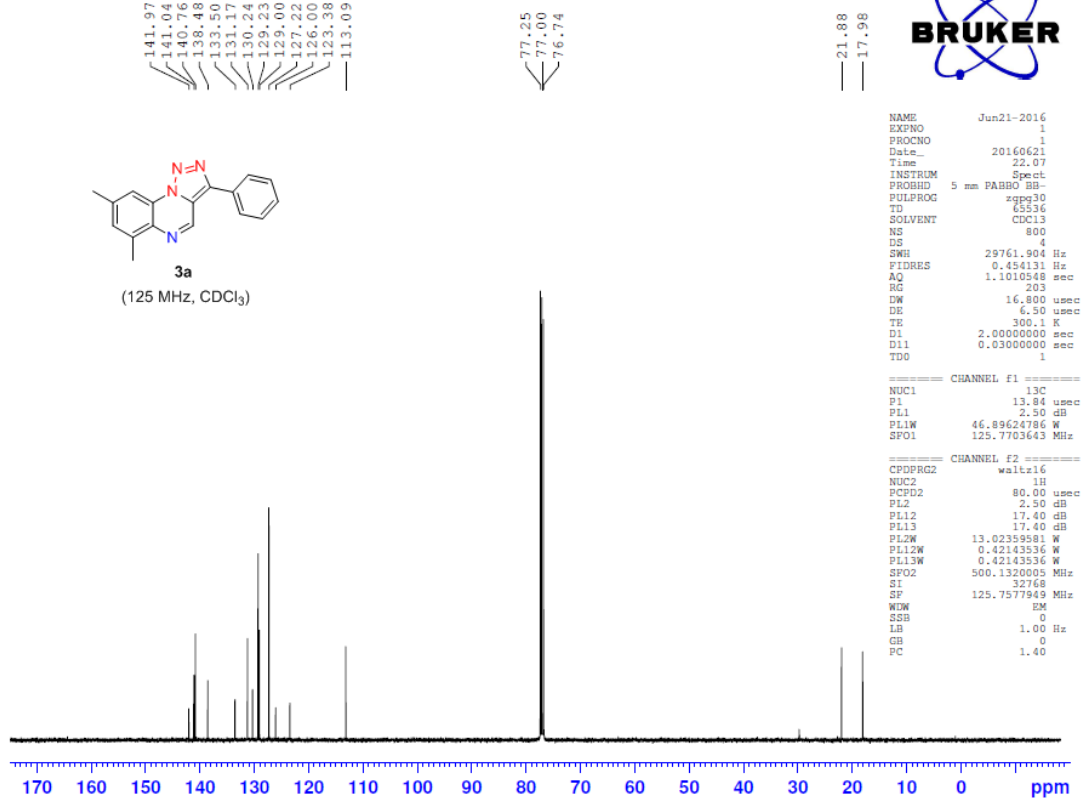
3a
(400 MHz, CDCl₃)



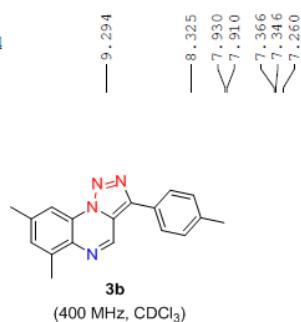
LDK-293 click



3a
(125 MHz, CDCl₃)



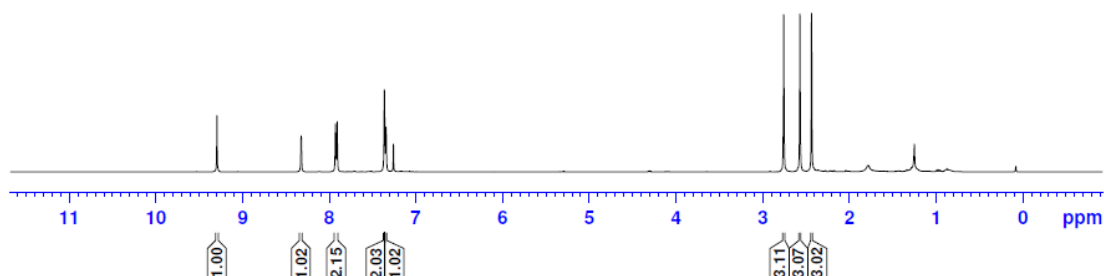
LDK-294



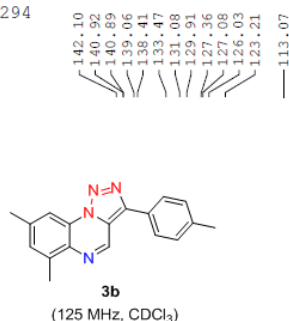
```

NAME      Jun29-2016
EXPNO     23
PROCNO    1
Date_     20160629
Time      14.37
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         16
DS         2
SWH        8278.146 Hz
FIDRES     0.252629 Hz
AQ         1.9792372 sec
RG         90.5
DW         60.400 usec
DE         6.50 usec
TE         299.3 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         12.58 usec
PL1        0.00 dB
PL1W       10.87646866 W
SFO1       400.1324710 MHz
SI         16384
SF         400.1300079 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



ldk-294

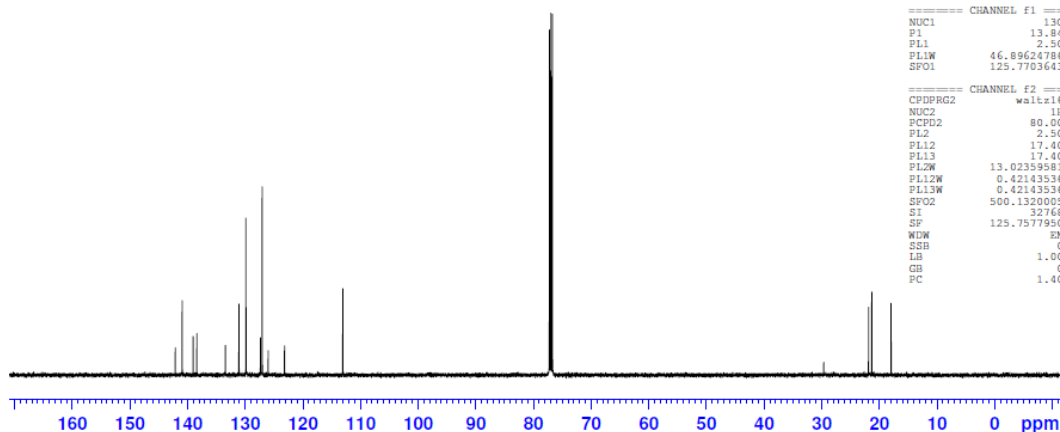


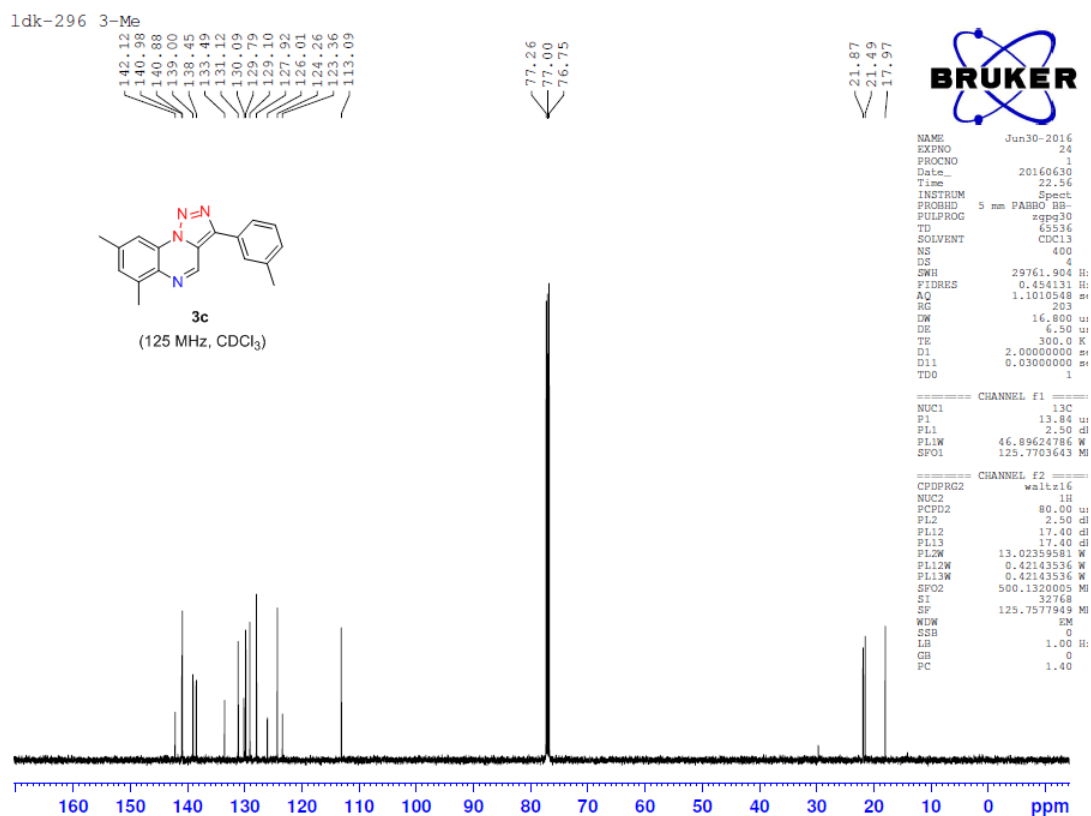
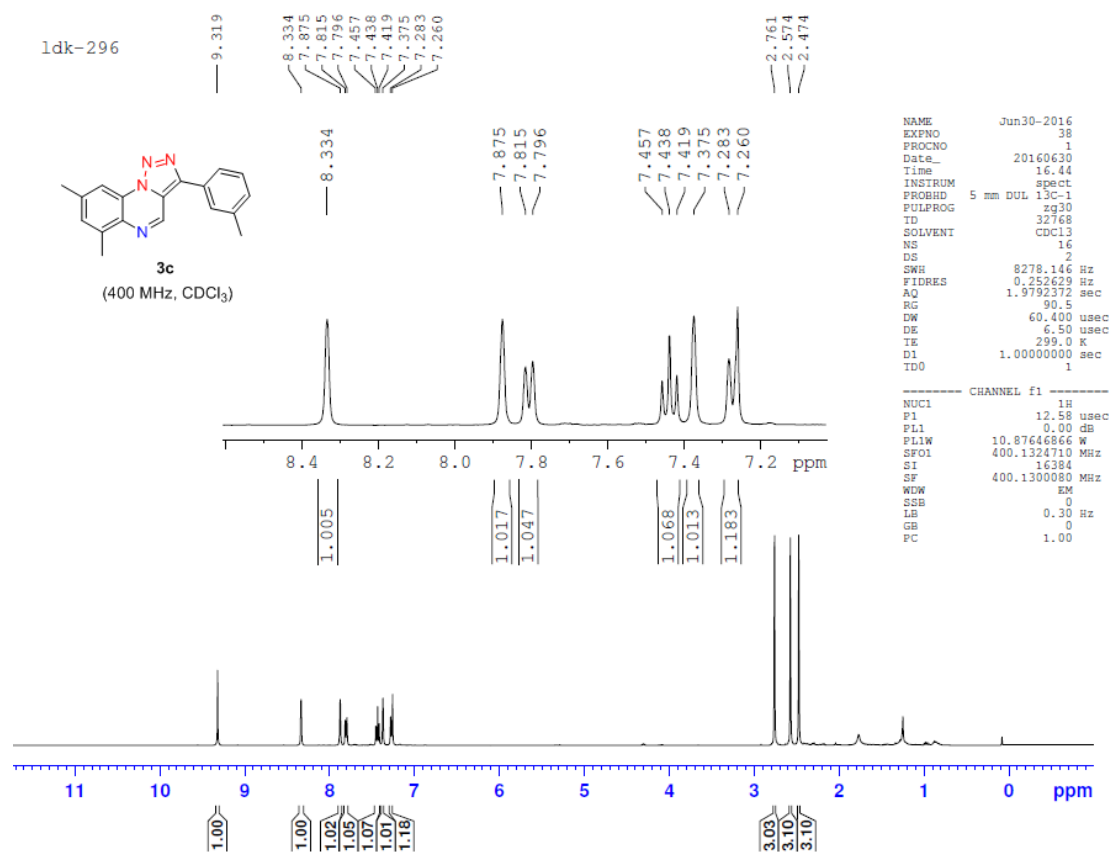
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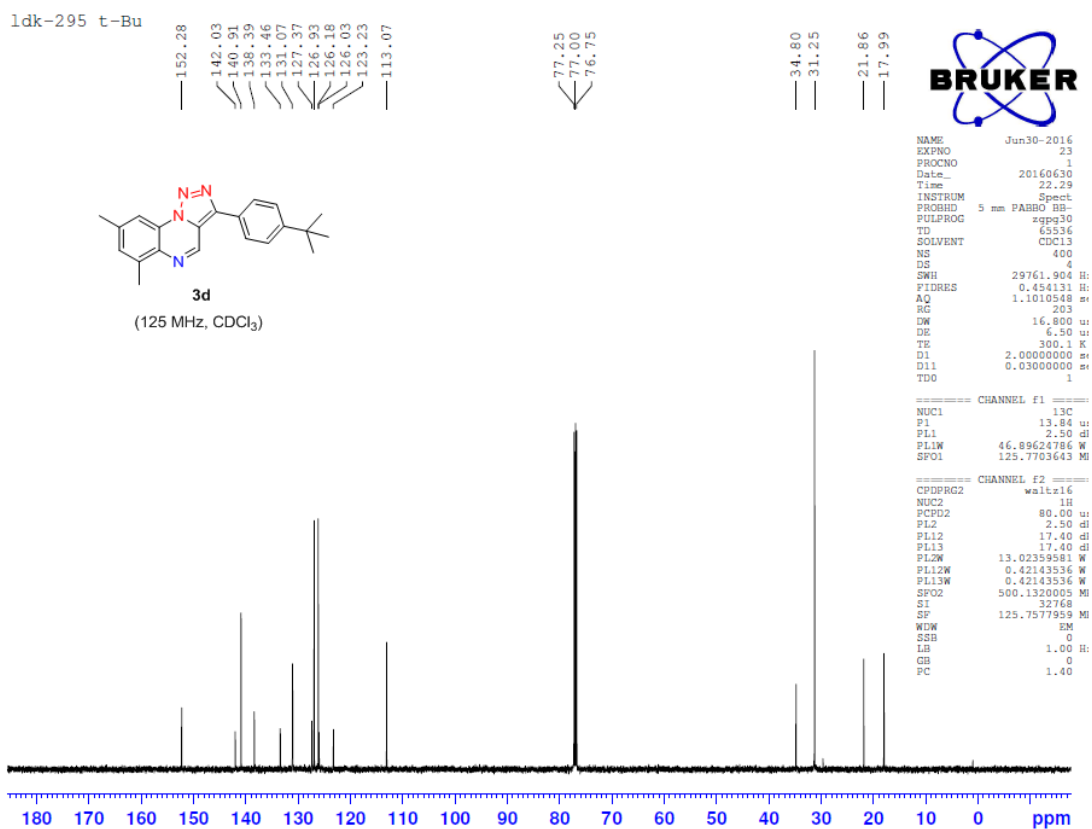
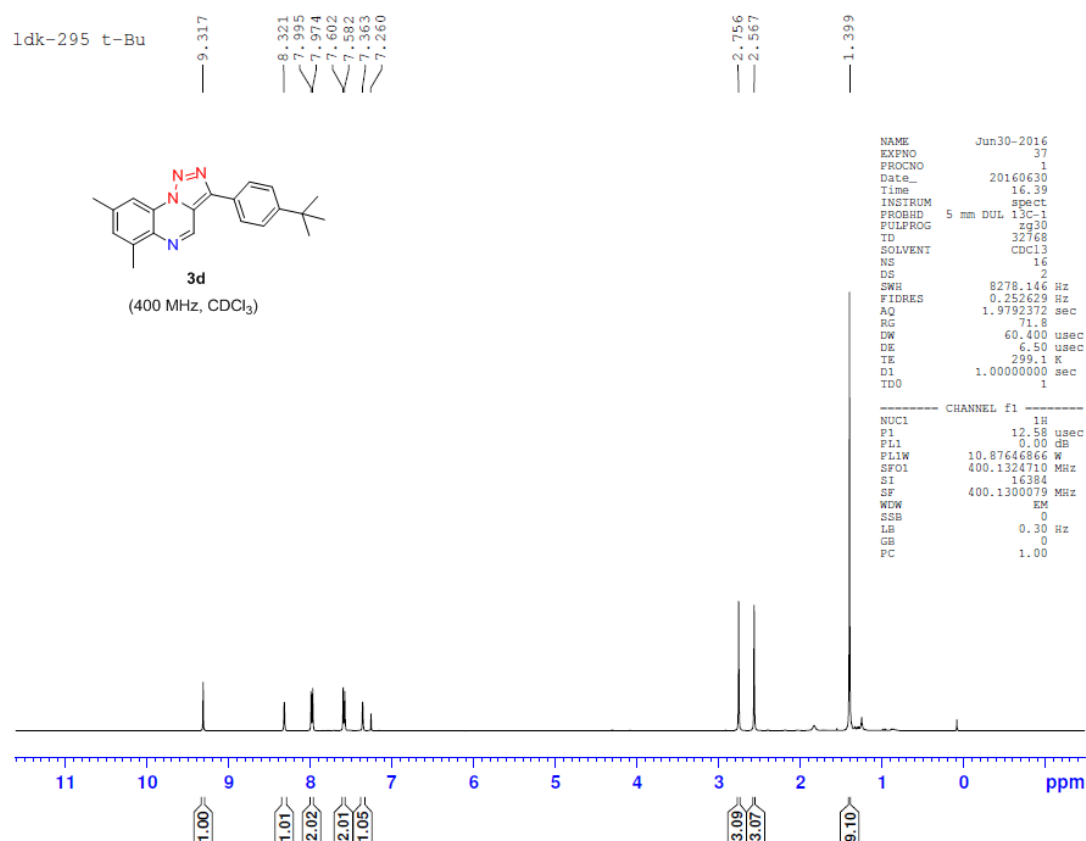
NAME      Jun29-2016
EXPNO     7
PROCNO    1
Date_     20160629
Time      19.32
INSTRUM   Spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         500
DS         4
SWH        29761.904 H:
FIDRES     0.454131 H:
AQ         1.1010548 s:
RG         203
DW         16.800 u:
DE         6.50 u:
TE         300.1 K
D1         2.00000000 s:
D11        0.03000000 s:
TD0        1

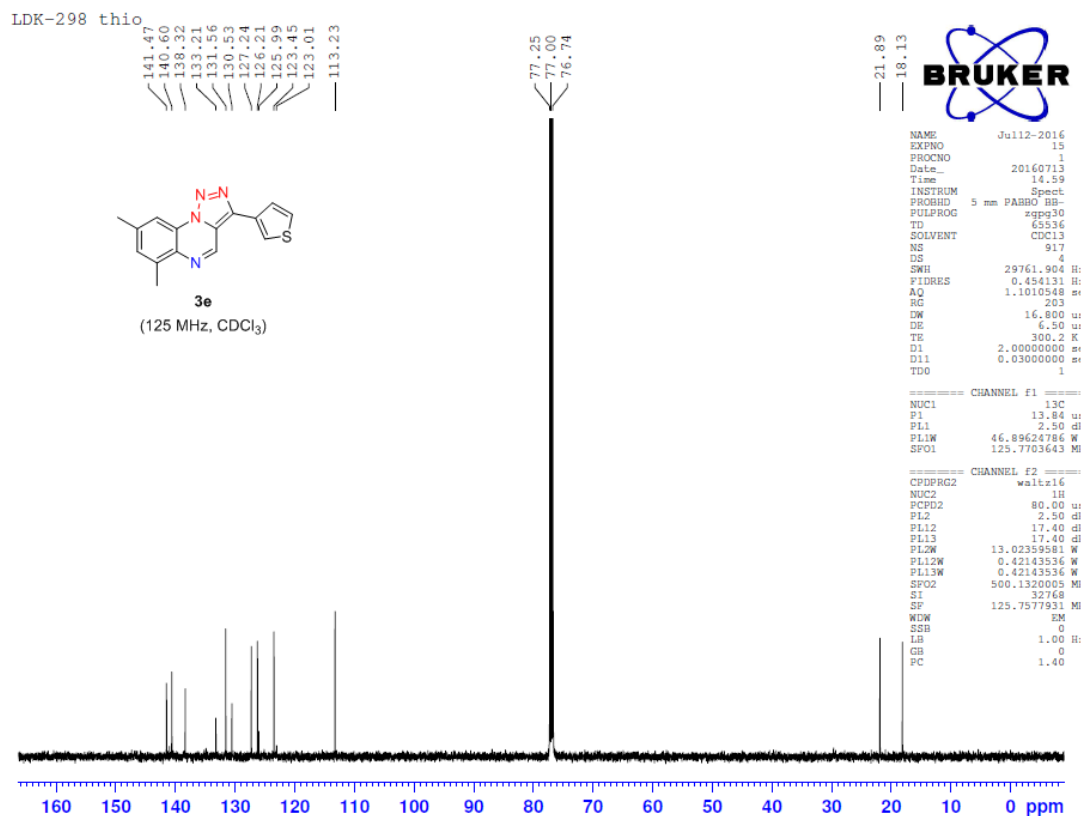
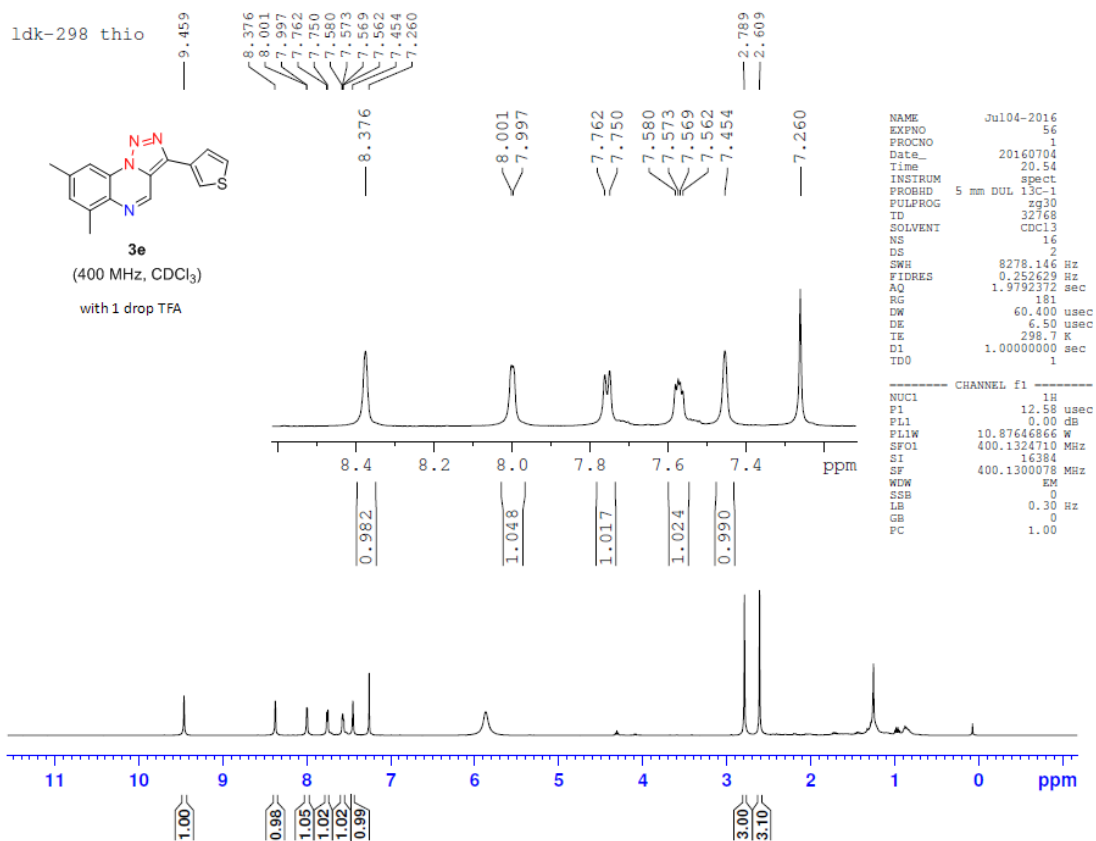
===== CHANNEL f1 =====
NUC1       13C
P1         13.84 u:
PL1        2.50 dB
PL1W       46.89624786 W
SFO1       125.7703643 M:

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 u:
PL2        2.50 dB
PL12       17.40 dB
PL13       17.40 dB
PL1W       13.02359581 W
PL12W      0.42143536 W
PL13W      0.42143536 W
SFO2       500.1320005 M:
SI         32768
SF         125.7577950 M:
WDW        EM
SSB        0
LB         1.00 H:
GB         0
PC         1.40
  
```

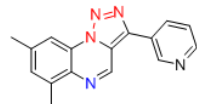




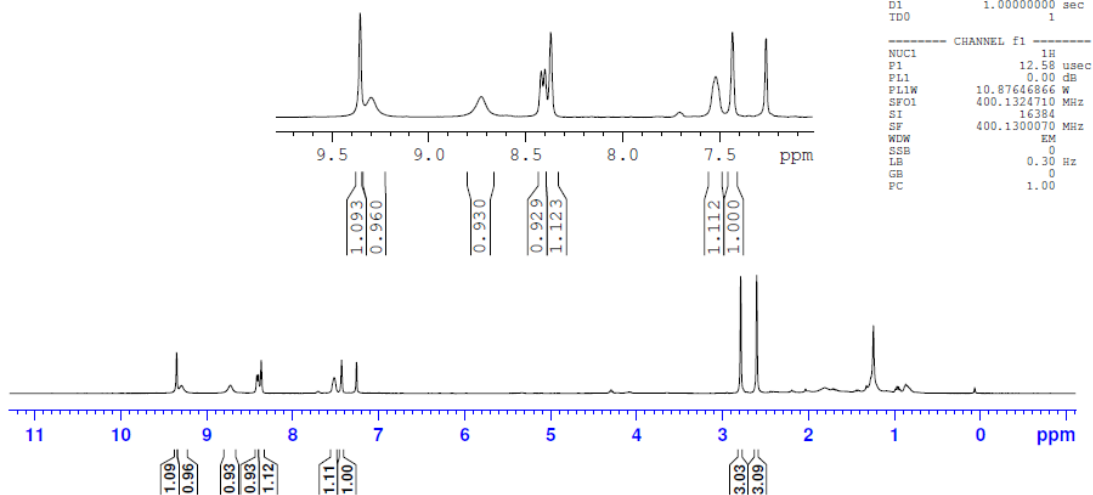




LDK-309 3-Py



3f
(400 MHz, CDCl₃)

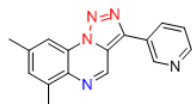


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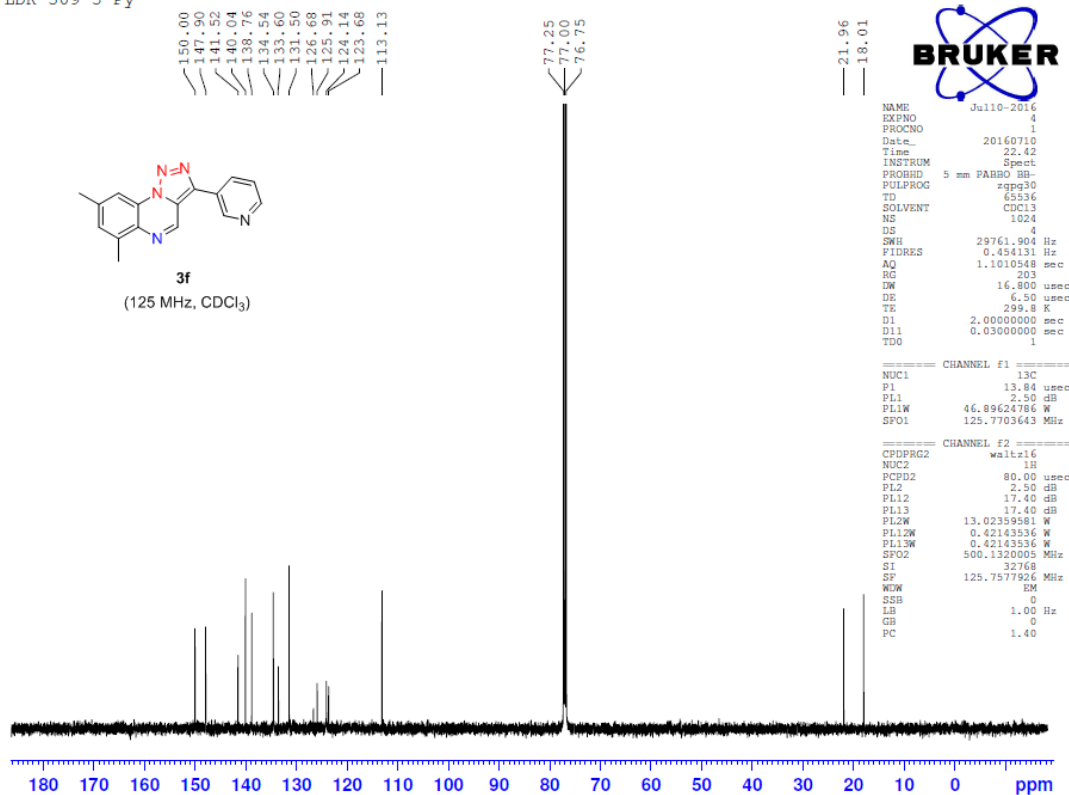
NAME      Jul10-2016
EXPNO     14
PROCNO    1
Date_     20160710
Time      17.33
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         16
DS         2
SWH        8278.146 Hz
FIDRES     0.252629 Hz
AQ         1.9792372 sec
RG         181
DW         60.400 usec
DE         6.50 usec
TE         298.6 K
D1         1.00000000 sec
D11        1
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         12.58 usec
PL1        0.00 dB
PL1W       10.87646866 W
SFO1       400.1324710 MHz
SI         16384
SF         400.1300070 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

LDK-309 3-Py



3f
(125 MHz, CDCl₃)

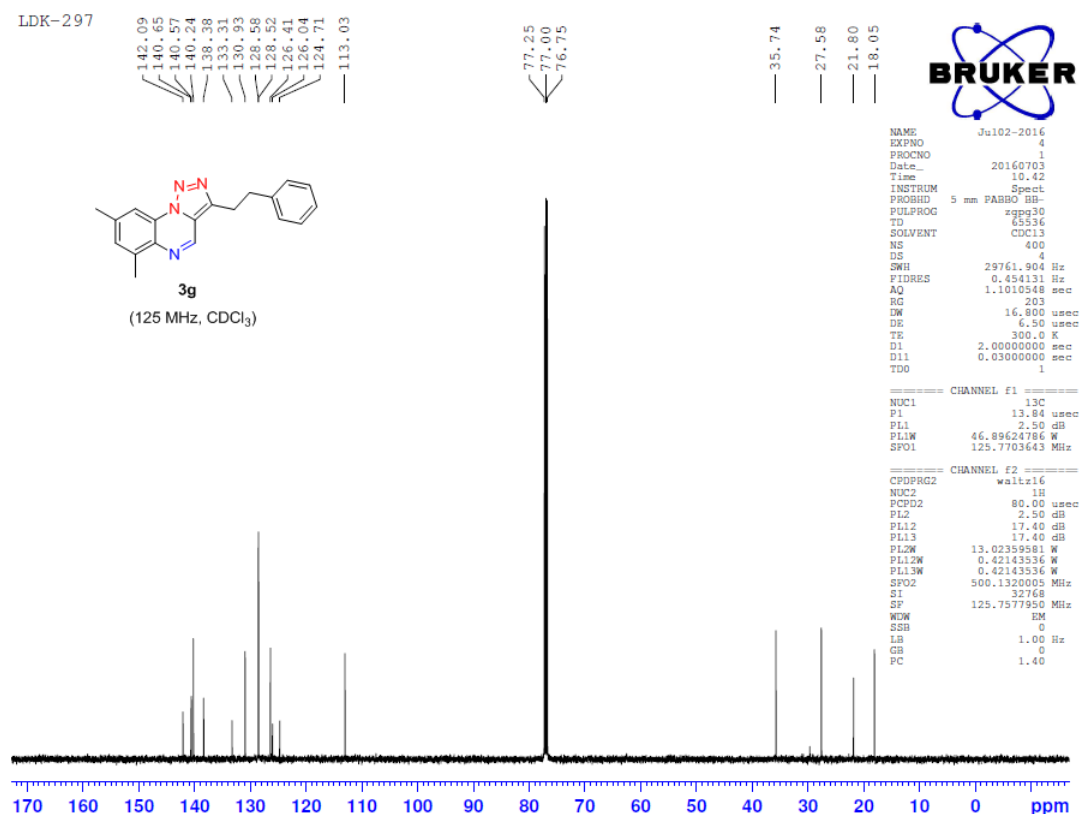
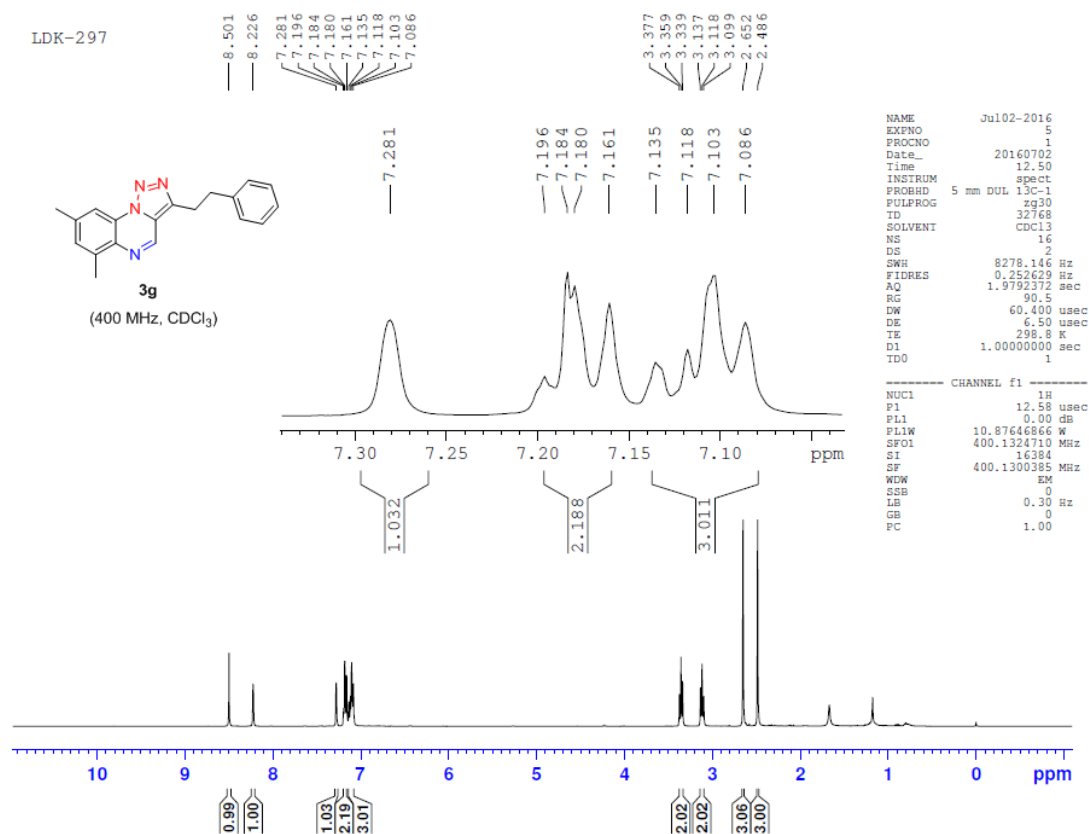


```

NAME      Jul10-2016
EXPNO     4
PROCNO    1
Date_     20160710
Time      22.42
INSTRUM   Spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         1024
DS         4
SWH        29761.904 Hz
FIDRES     0.454131 Hz
AQ         1.1010548 sec
RG         203
DW         16.800 usec
DE         6.50 usec
TE         299.8 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         13.84 usec
PL1        2.50 dB
PL1W       46.89624786 W
SFO1       125.7703643 MHz

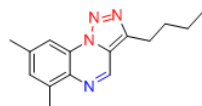
===== CHANNEL f2 =====
CPDPRG2   waitz16
NUC2       1H
PCPD2     80.00 usec
PL2        2.50 dB
PL12       17.40 dB
PL13       17.40 dB
PL1W       13.02359581 W
PL12W      0.42143536 W
PL13W      0.42143536 W
SFO2       500.1320005 MHz
SI         32768
SF         125.7577926 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



LDK-299 C4H9

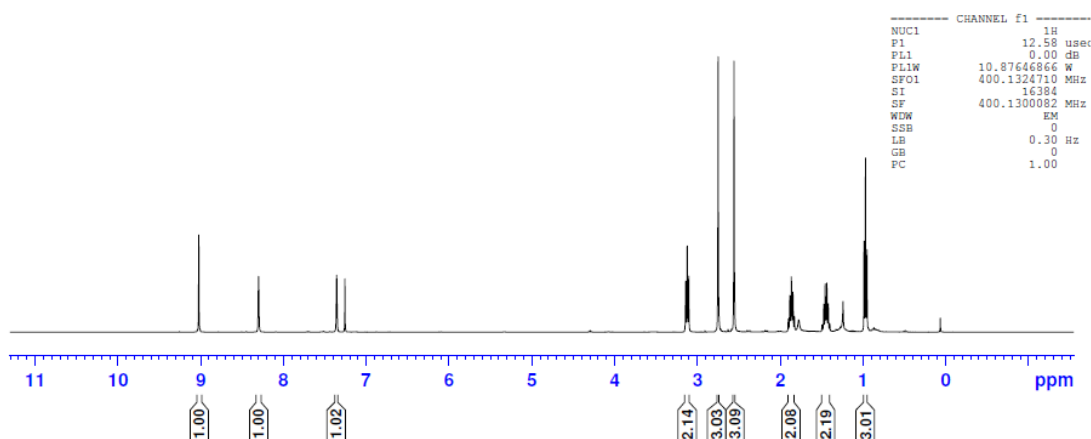
9.021
8.298
7.360
7.260

3.143
3.124
3.105
2.751
2.559
1.904
1.885
1.866
1.847
1.828
1.494
1.476
1.457
1.438
1.420
1.401
0.989
0.970
0.952



3h

(400 MHz, CDCl₃)



NAME Jul03-2016
EXPNO 4
PROCNO 1
Date_ 20160703
Time 15.28
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 4
SWH 8278.16 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 90.5
DW 60.400 usec
DE 6.50 usec
TE 298.8 K
D1 1.00000000 sec
TD0 1

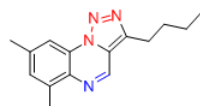
CHANNEL f1
NUC1 1H
P1 12.58 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 16384
SF 400.1300082 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

LDK-299 C4H9

143.39
140.58
140.44
138.37
133.37
130.90
126.16
124.50
113.04

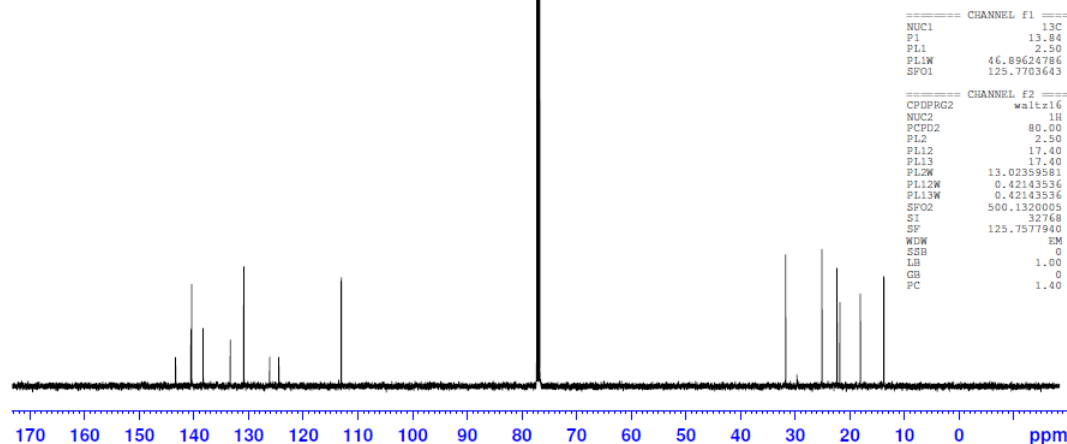
77.25
77.00
76.74

31.75
25.09
22.35
21.81
18.05
13.74



3h

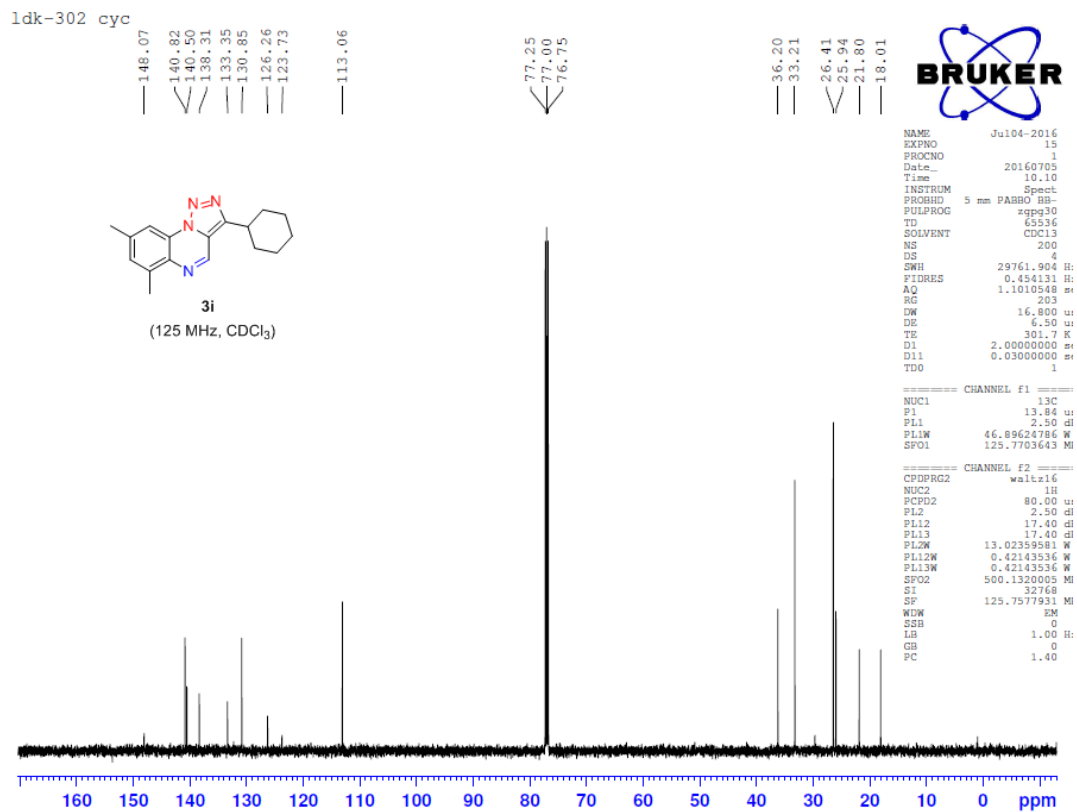
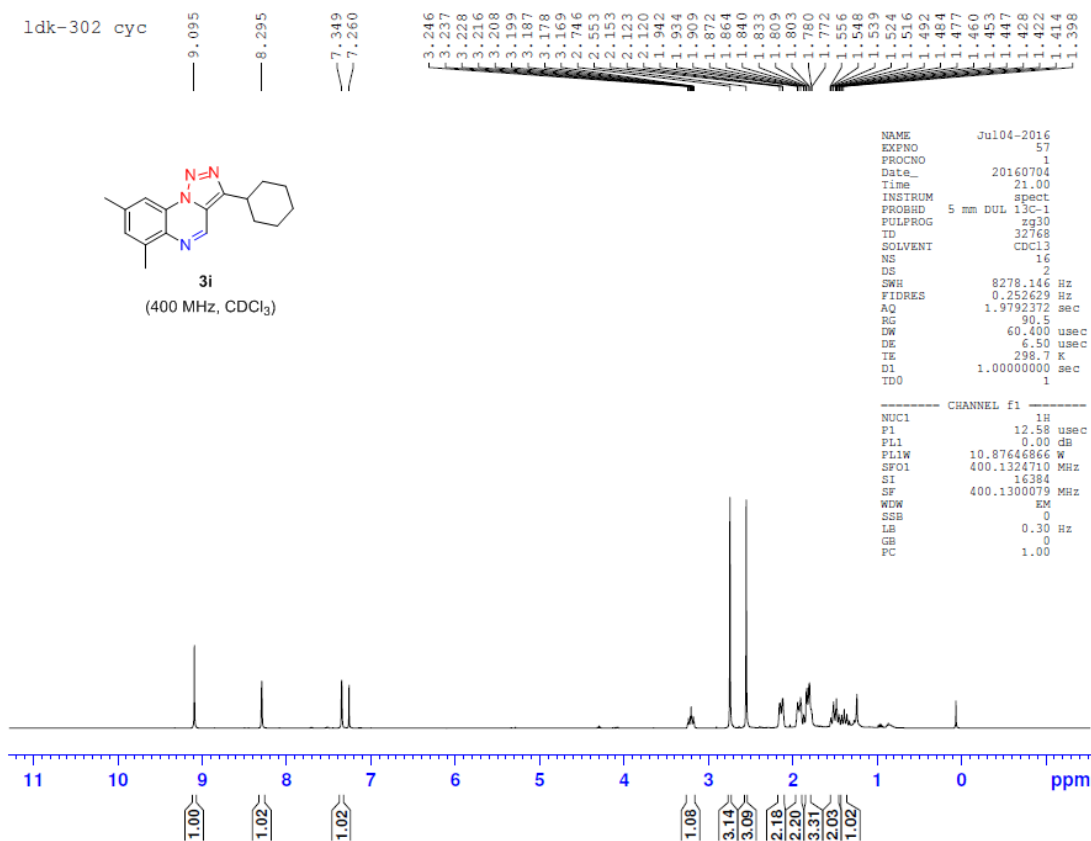
(125 MHz, CDCl₃)

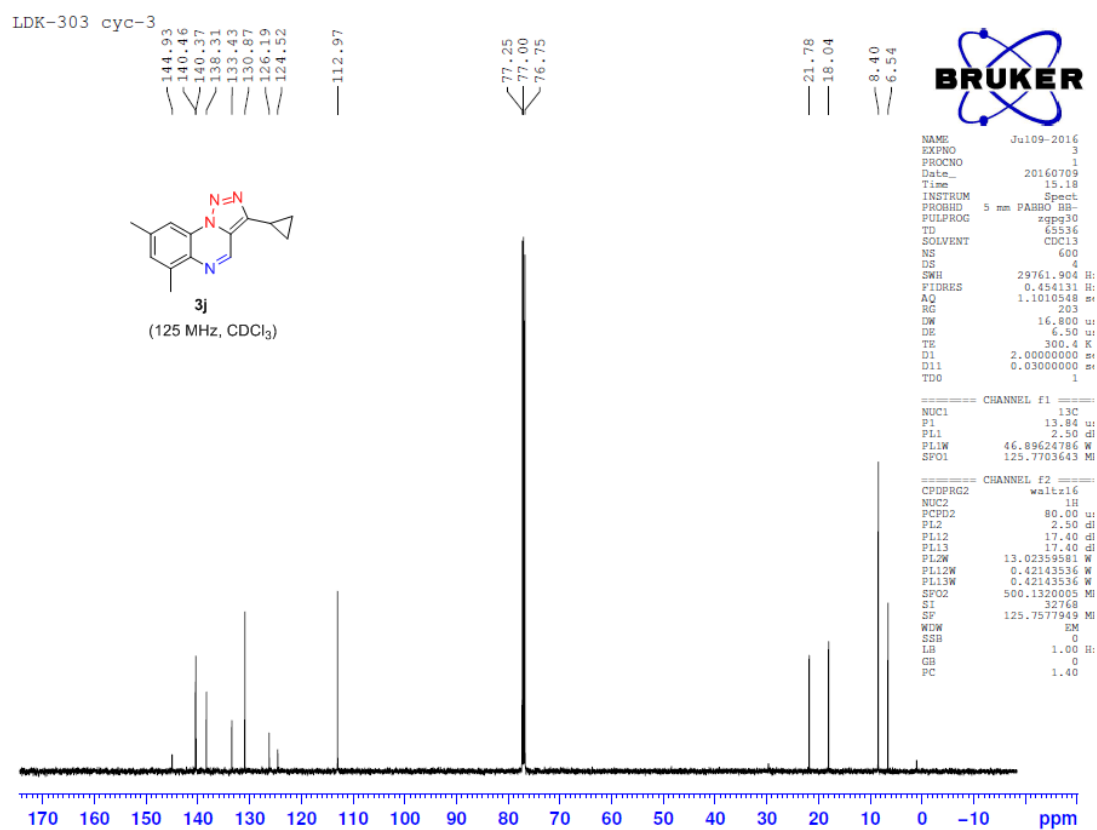
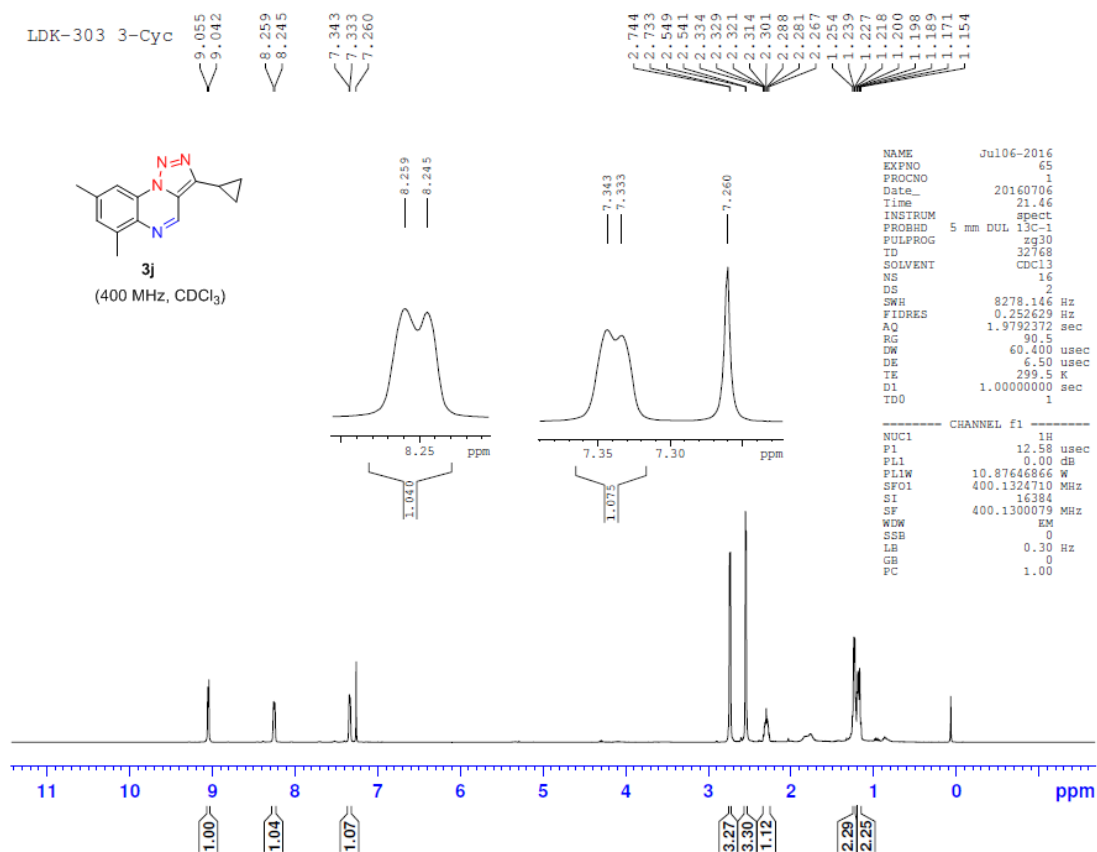


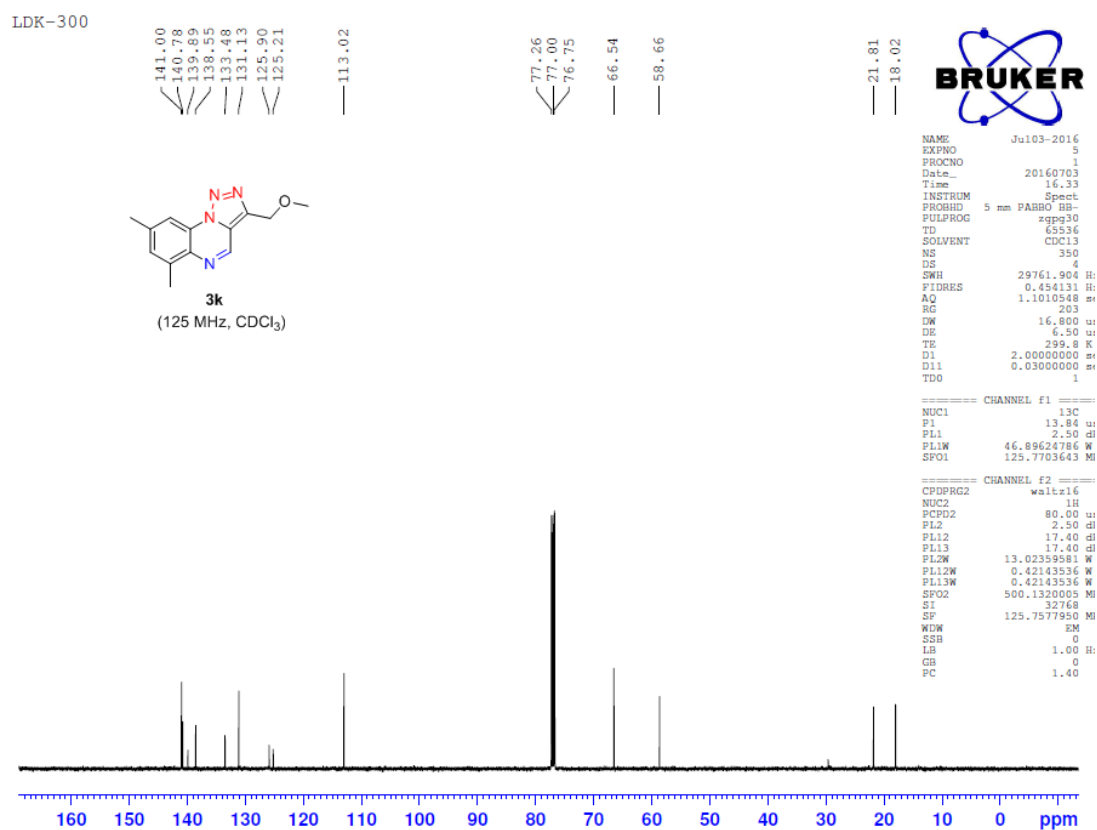
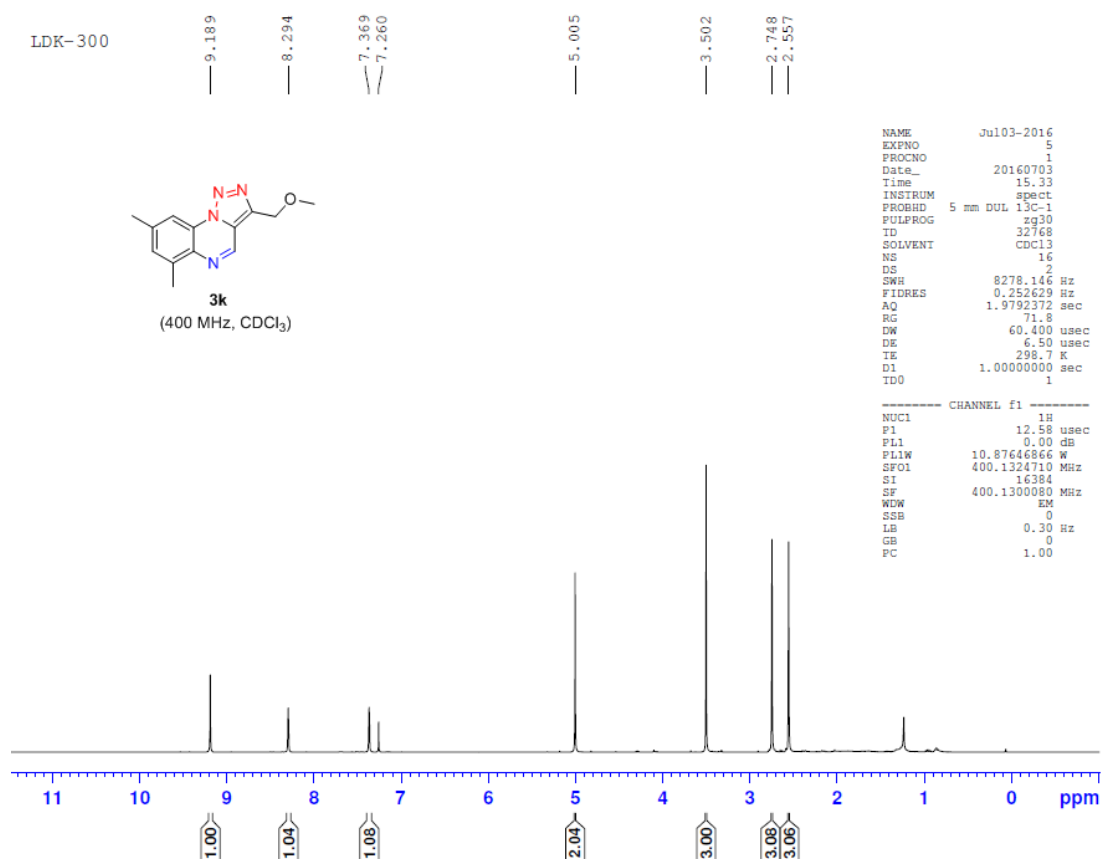
NAME Jul03-2016
EXPNO 4
PROCNO 1
Date_ 20160703
Time 16.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65936
SOLVENT CDCl3
NS 350
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

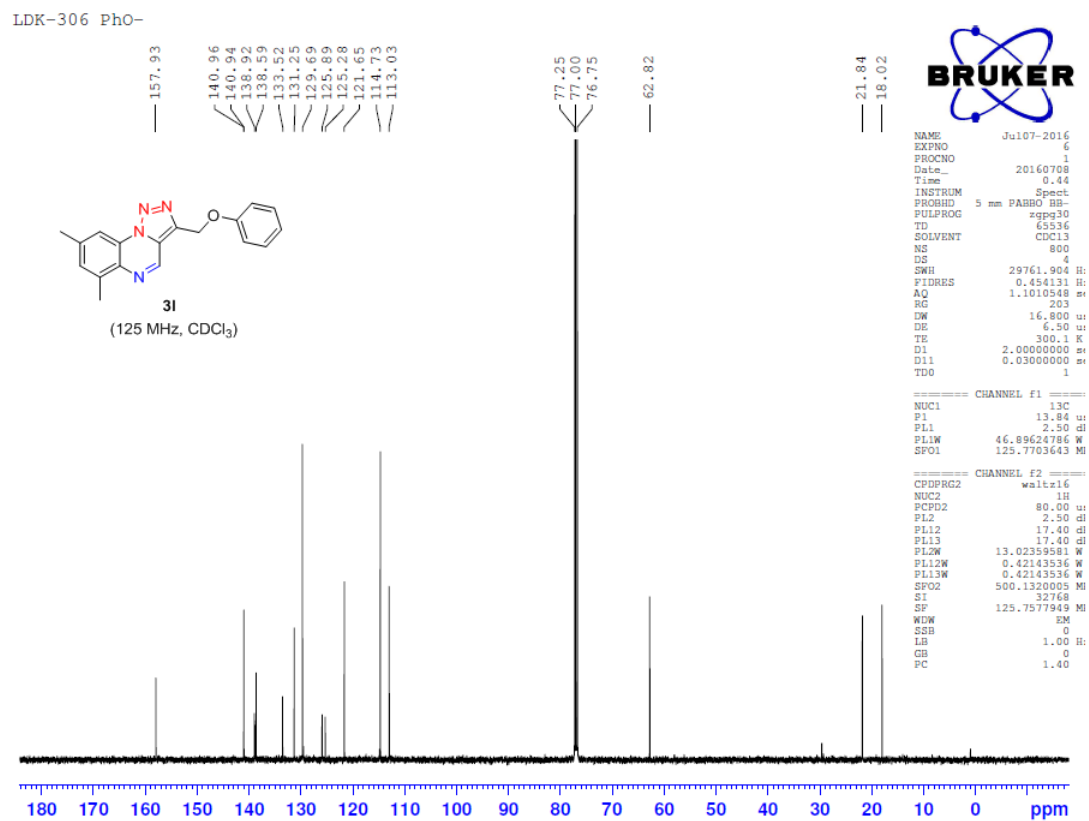
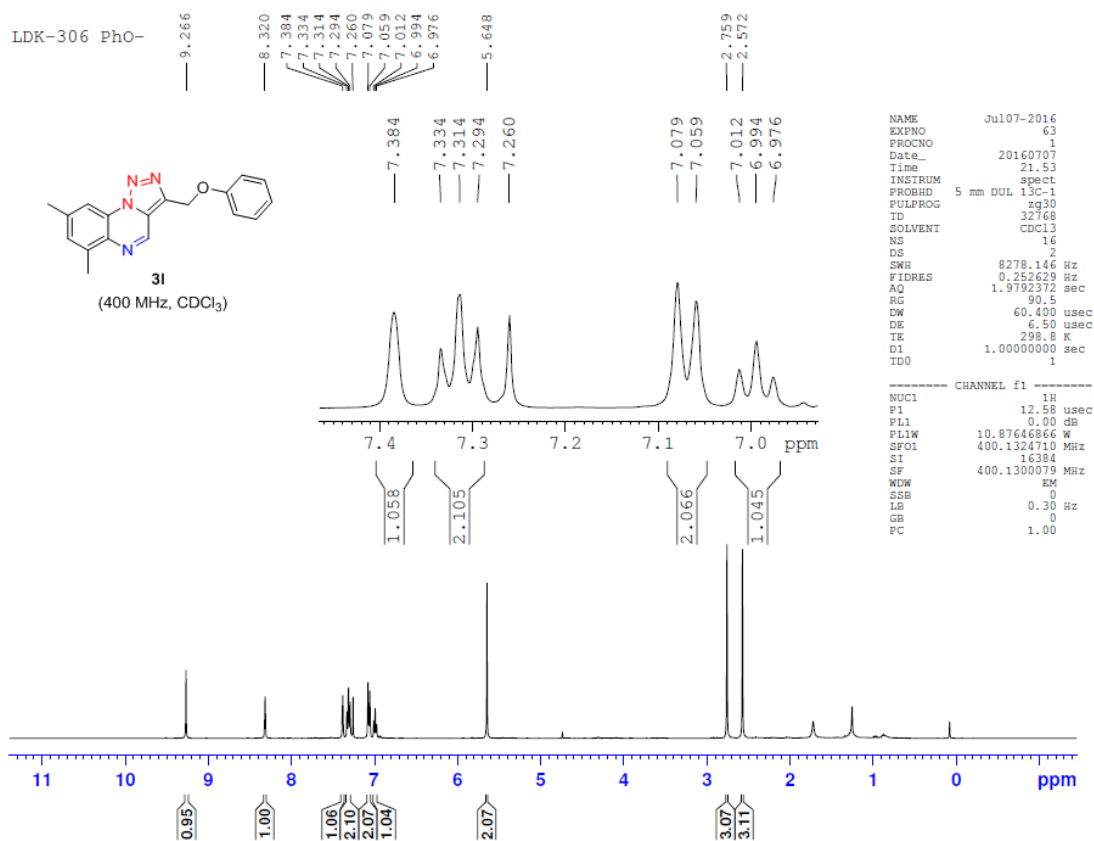
CHANNEL f1
NUC1 13C
P1 13.84 usec
PL1 2.50 dB
PL1W 46.89624786 W
SFO1 125.7763643 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577940 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

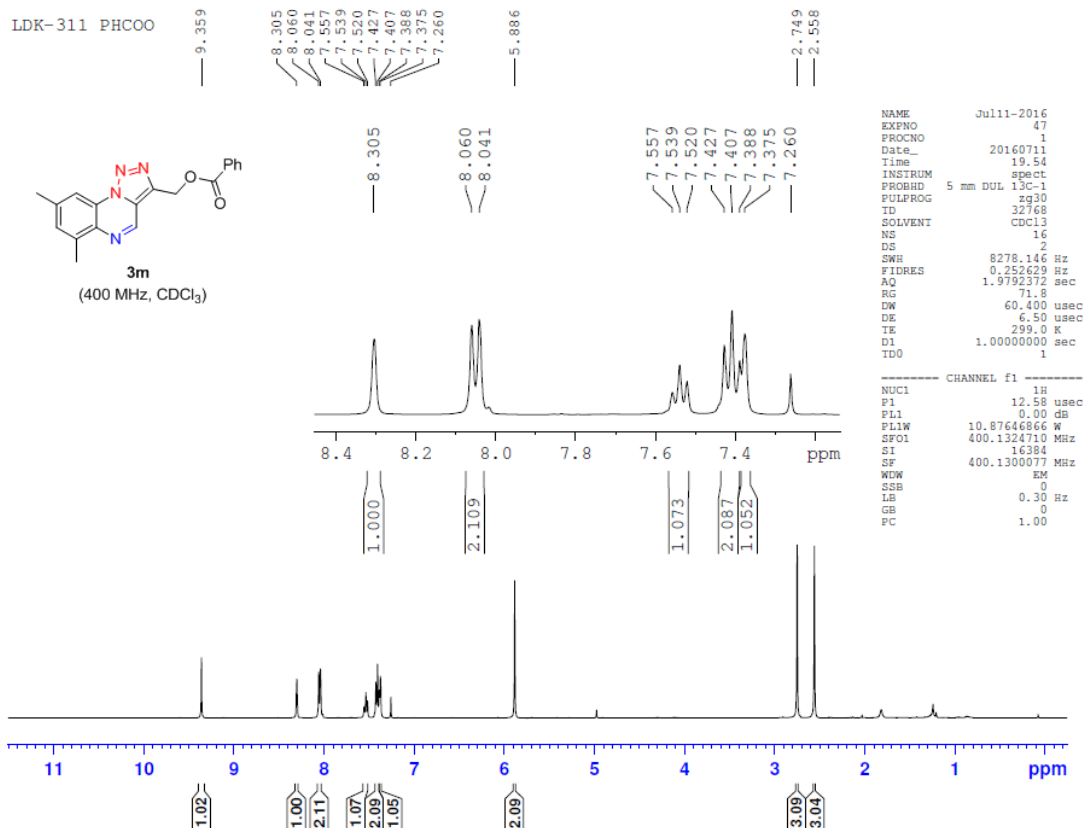
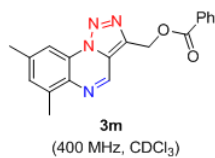








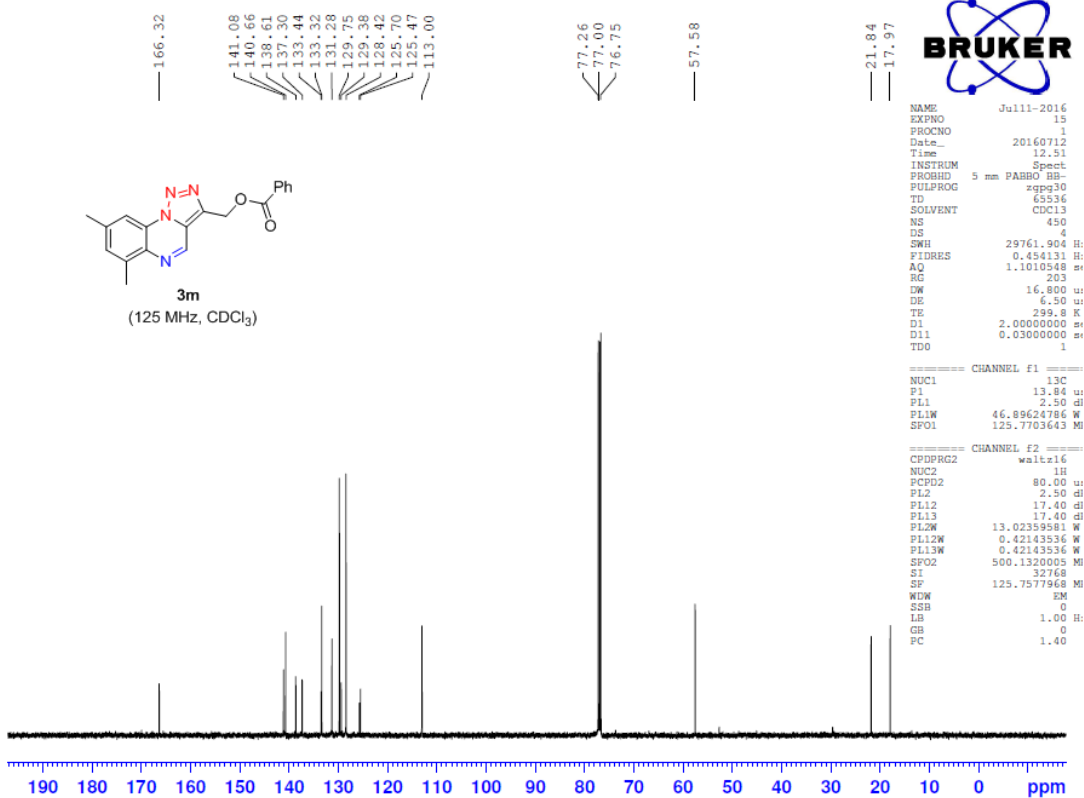
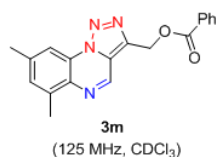
LDK-311 PhCOO



NAME Jul11-2016
EXPNO 47
PROCNO 1
Date_ 20160711
Time 19.54
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 71.8
DW 60.400 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 12.58 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 16384
SF 400.1300077 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ldk-311 PhCOO

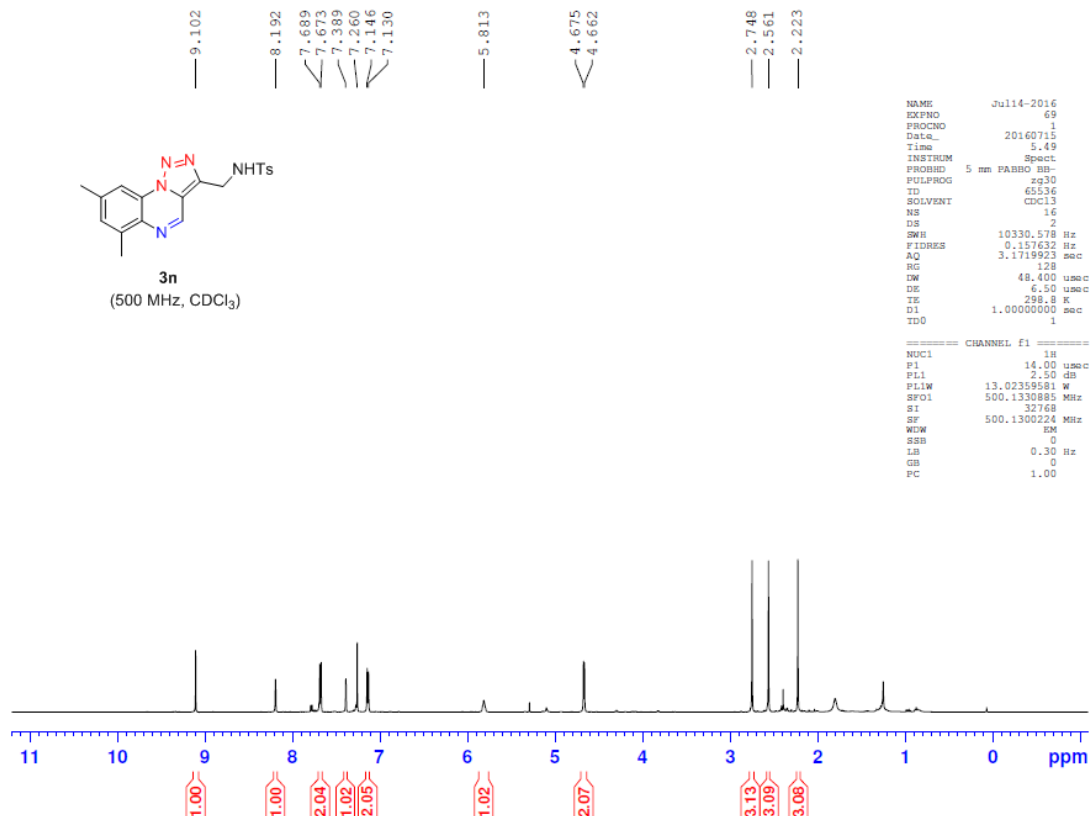
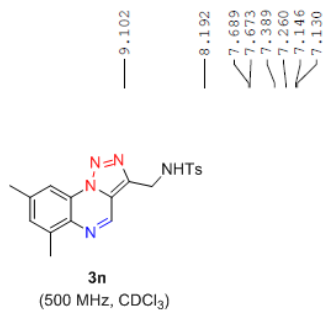


NAME Jul11-2016
EXPNO 15
PROCNO 1
Date_ 20160712
Time 12.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 450
DS 4
SWH 29761.904 H:
FIDRES 0.454131 H:
AQ 1.1010548 sr
RG 203
DW 16.800 u:
DE 6.50 u:
TE 299.8 K
D1 2.00000000 sr
D11 0.03000000 sr
TD0 1

CHANNEL f1
NUC1 13C
P1 13.84 u:
PL1 2.50 dB
PL1W 46.89624786 W
SFO1 125.7703643 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 u:
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359881 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577968 MHz
WDW EM
SSB 0
LB 1.00 H:
GB 0
PC 1.40

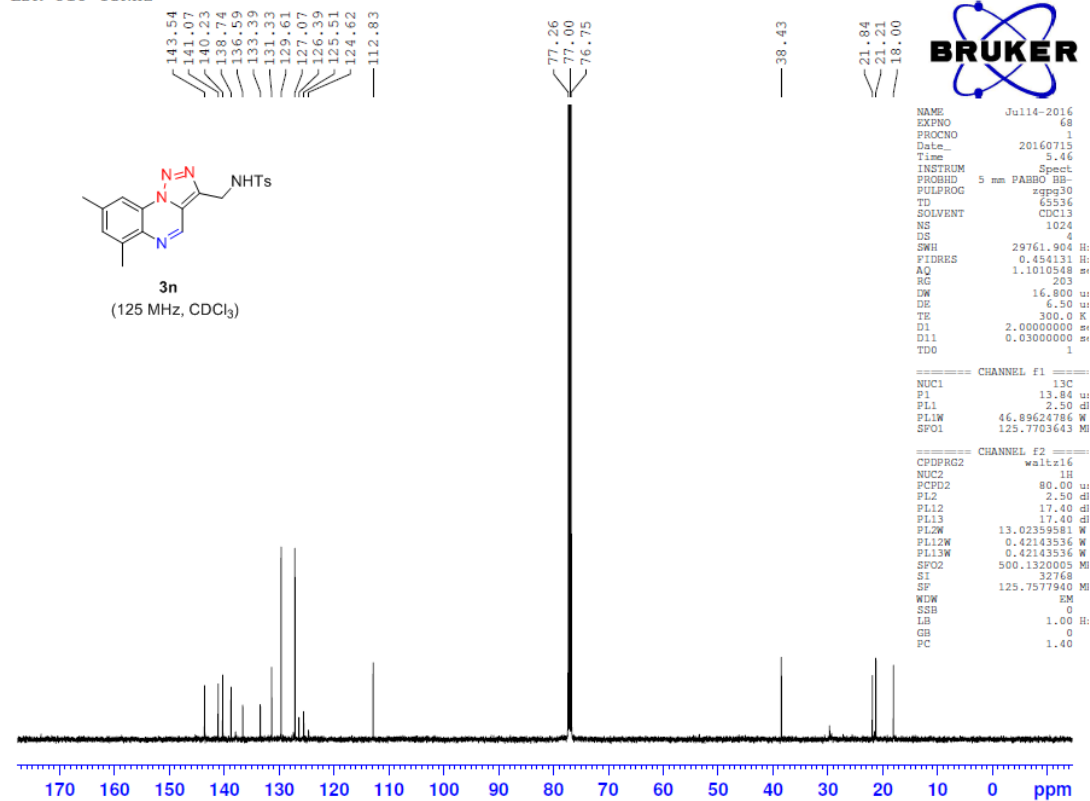
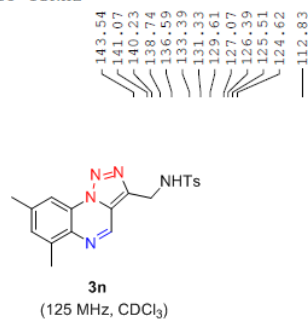
LDK-315 TsNH2



```

NAME      Jul14-2016
EXPNO     69
PROCNO    1
Date_     20160715
Time      5.49
INSTRUM   Spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1719923 sec
RG         128
DW         48.400 usec
DE         6.50 usec
TE         298.8 K
D1         1.00000000 sec
TDO        1
===== CHANNEL f1 =====
NUC1       1H
P1         14.00 usec
PL1        2.50 dB
PL1W       13.02359581 W
SFO1       500.1330885 MHz
SI         32768
SF         500.1300224 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

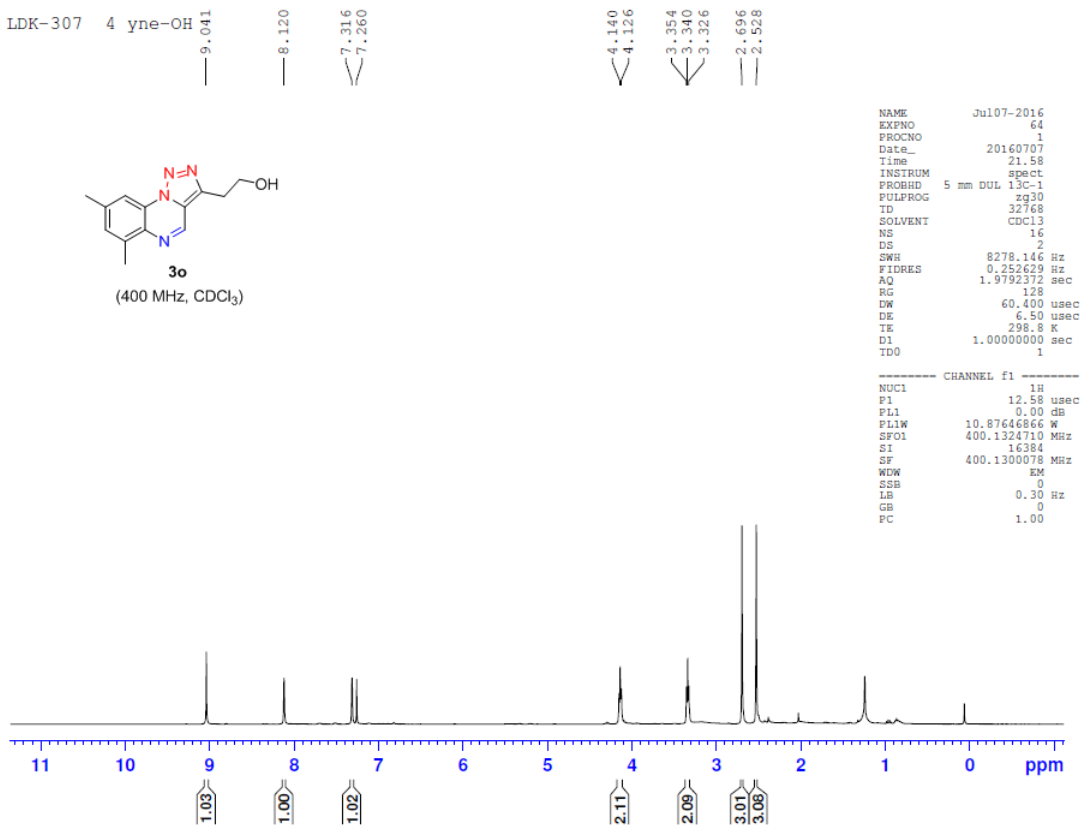
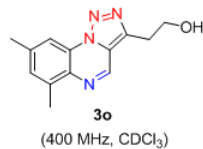
LDK-315 TsNH2



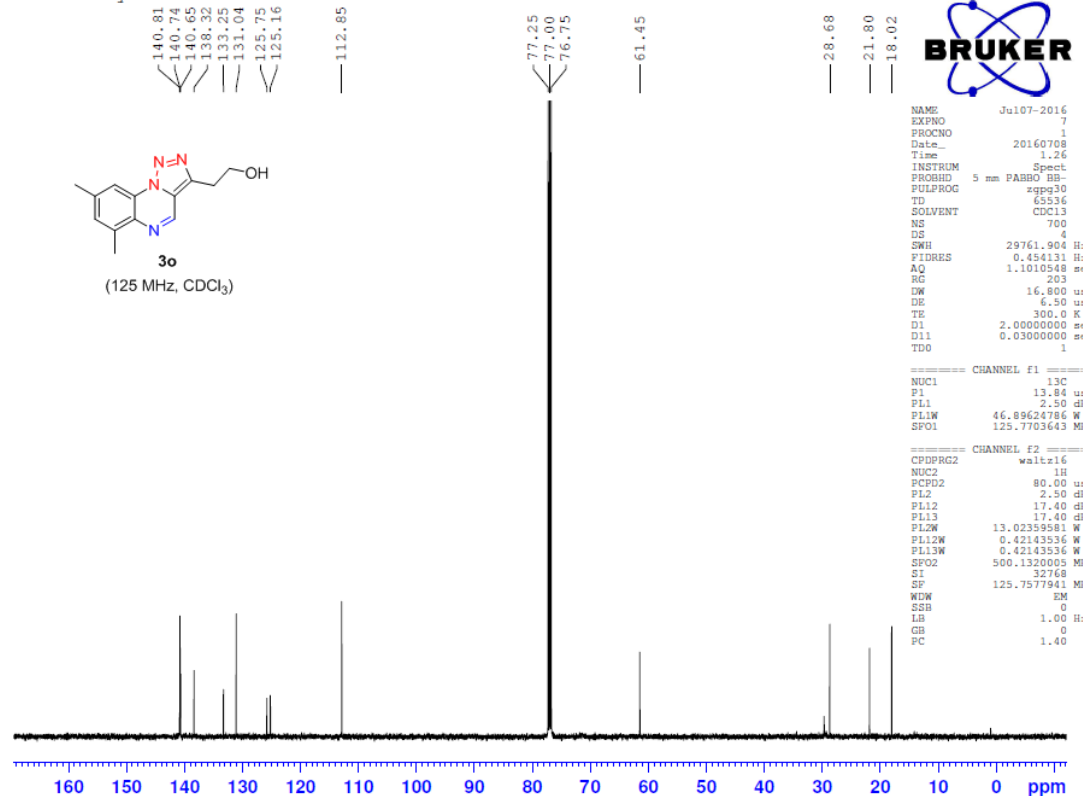
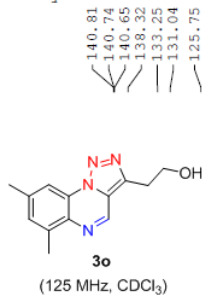
```

NAME      Jul14-2016
EXPNO     68
PROCNO    1
Date_     20160715
Time      5.46
INSTRUM   Spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         1024
DS         4
SWH        29761.904 Hz
FIDRES     0.4548131 Hz
AQ         1.1010548 sec
RG         203
DW         16.800 usec
DE         6.50 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        1
===== CHANNEL f1 =====
NUC1       13C
P1         13.84 usec
PL1        2.50 dB
PL1W       46.89624786 W
SFO1       125.7703643 MHz
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        2.50 dB
PL12       17.40 dB
PL13       17.40 dB
PL1W       13.02359581 W
PL12W      0.42143536 W
PL13W      0.42143536 W
SF02       500.1320005 MHz
SI         32768
SF         125.7577940 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

LDK-307 4-yne-OH



LDK-307 4-yne-OH

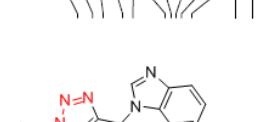


Chemical structure of **3p** is shown above the spectrum. The structure is a benzimidazole derivative with a 2-phenyl-1H-benzimidazole-5-yl group attached to a 2-methyl-1H-benzimidazole-5-yl group.

3p
(500 MHz, CDCl₃)

¹H NMR spectrum (500 MHz, CDCl₃) showing peaks at 8.406, 8.190, 7.781, 7.441, 7.284, 7.193, 5.835, 2.592, and 2.476 ppm. Integration values are provided below the peaks: 0.98, 1.94, 0.96, 0.91, 1.01, 2.36, 2.03, 3.06, and 3.07.

¹³C NMR spectrum (100 MHz, CDCl₃) showing peaks at 155.2, 154.8, 154.7, 154.6, 154.5, 154.4, 154.3, 154.2, 154.1, 154.0, 153.9, 153.8, 153.7, 153.6, 153.5, 153.4, 153.3, 153.2, 153.1, 153.0, 152.9, 152.8, 152.7, 152.6, 152.5, 152.4, 152.3, 152.2, 152.1, 152.0, 151.9, 151.8, 151.7, 151.6, 151.5, 151.4, 151.3, 151.2, 151.1, 151.0, 150.9, 150.8, 150.7, 150.6, 150.5, 150.4, 150.3, 150.2, 150.1, 150.0, 149.9, 149.8, 149.7, 149.6, 149.5, 149.4, 149.3, 149.2, 149.1, 149.0, 148.9, 148.8, 148.7, 148.6, 148.5, 148.4, 148.3, 148.2, 148.1, 148.0, 147.9, 147.8, 147.7, 147.6, 147.5, 147.4, 147.3, 147.2, 147.1, 147.0, 146.9, 146.8, 146.7, 146.6, 146.5, 146.4, 146.3, 146.2, 146.1, 146.0, 145.9, 145.8, 145.7, 145.6, 145.5, 145.4, 145.3, 145.2, 145.1, 145.0, 144.9, 144.8, 144.7, 144.6, 144.5, 144.4, 144.3, 144.2, 144.1, 144.0, 143.9, 143.8, 143.7, 143.6, 143.5, 143.4, 143.3, 143.2, 143.1, 143.0, 142.9, 142.8, 142.7, 142.6, 142.5, 142.4, 142.3, 142.2, 142.1, 142.0, 141.9, 141.8, 141.7, 141.6, 141.5, 141.4, 141.3, 141.2, 141.1, 141.0, 140.9, 140.8, 140.7, 140.6, 140.5, 140.4, 140.3, 140.2, 140.1, 140.0, 139.9, 139.8, 139.7, 139.6, 139.5, 139.4, 139.3, 139.2, 139.1, 139.0, 138.9, 138.8, 138.7, 138.6, 138.5, 138.4, 138.3, 138.2, 138.1, 138.0, 137.9, 137.8, 137.7, 137.6, 137.5, 137.4, 137.3, 137.2, 137.1, 137.0, 136.9, 136.8, 136.7, 136.6, 136.5, 136.4, 136.3, 136.2, 136.1, 136.0, 135.9, 135.8, 135.7, 135.6, 135.5, 135.4, 135.3, 135.2, 135.1, 135.0, 134.9, 134.8, 134.7, 134.6, 134.5, 134.4, 134.3, 134.2, 134.1, 134.0, 133.9, 133.8, 133.7, 133.6, 133.5, 133.4, 133.3, 133.2, 133.1, 133.0, 132.9, 132.8, 132.7, 132.6, 132.5, 132.4, 132.3, 132.2, 132.1, 132.0, 131.9, 131.8, 131.7, 131.6, 131.5, 131.4, 131.3, 131.2, 131.1, 131.0, 130.9, 130.8, 130.7, 130.6, 130.5, 130.4, 130.3, 130.2, 130.1, 130.0, 129.9, 129.8, 129.7, 129.6, 129.5, 129.4, 129.3, 129.2, 129.1, 129.0, 128.9, 128.8, 128.7, 128.6, 128.5, 128.4, 128.3, 128.2, 128.1, 128.0, 127.9, 127.8, 127.7, 127.6, 127.5, 127.4, 127.3, 127.2, 127.1, 127.0, 126.9, 126.8, 126.7, 126.6, 126.5, 126.4, 126.3, 126.2, 126.1, 126.0, 125.9, 125.8, 125.7, 125.6, 125.5, 125.4, 125.3, 125.2, 125.1, 125.0, 124.9, 124.8, 124.7, 124.6, 124.5, 124.4, 124.3, 124.2, 124.1, 124.0, 123.9, 123.8, 123.7, 123.6, 123.5, 123.4, 123.3, 123.2, 123.1, 123.0, 122.9, 122.8, 122.7, 122.6, 122.5, 122.4, 122.3, 122.2, 122.1, 122.0, 121.9, 121.8, 121.7, 121.6, 121.5, 121.4, 121.3, 121.2, 121.1, 121.0, 120.9, 120.8, 120.7, 120.6, 120.5, 120.4, 120.3, 120.2, 120.1, 120.0, 119.9, 119.8, 119.7, 119.6, 119.5, 119.4, 119.3, 119.2, 119.1, 119.0, 118.9, 118.8, 118.7, 118.6, 118.5, 118.4, 118.3, 118.2, 118.1, 118.0, 117.9, 117.8, 117.7, 117.6, 117.5, 117.4, 117.3, 117.2, 117.1, 117.0, 116.9, 116.8, 116.7, 116.6, 116.5, 116.4, 116.3, 116.2, 116.1, 116.0, 115.9, 115.8, 115.7, 115.6, 115.5, 115.4, 115.3, 115.2, 115.1, 115.0, 114.9, 114.8, 114.7, 114.6, 114.5, 114.4, 114.3, 114.2, 114.1, 114.0, 113.9, 113.8, 113.7, 113.6, 113.5, 113.4, 113.3, 113.2, 113.1, 113.0, 112.9, 112.8, 112.7, 112.6, 112.5, 112.4, 112.3, 112.2, 112.1, 112.0, 111.9, 111.8, 111.7, 111.6, 111.5, 111.4, 111.3, 111.2, 111.1, 111.0, 110.9, 110.8, 110.7, 110.6, 110.5, 110.4, 110.3, 110.2, 110.1, 110.0, 109.9, 109.8, 109.7, 109.6, 109.5, 109.4, 109.3, 109.2, 109.1, 109.0, 108.9, 108.8, 108.7, 108.6, 108.5, 108.4, 108.3, 108.2, 108.1, 108.0, 107.9, 107.8, 107.7, 107.6, 107.5, 107.4, 107.3, 107.2, 107.1, 107.0, 106.9, 106.8, 106.7, 106.6, 106.5, 106.4, 106.3, 106.2, 106.1, 106.0, 105.9, 105.8, 105.7, 105.6, 105.5, 105.4, 105.3, 105.2, 105.1, 105.0, 104.9, 104.8, 104.7, 104.6, 104.5, 104.4, 104.3, 104.2, 104.1, 104.0, 103.9, 103.8, 103.7, 103.6, 103.5, 103.4, 103.3, 103.2, 103.1, 103.0, 102.9, 102.8, 102.7, 102.6, 102.5, 102.4, 102.3, 102.2, 102.1, 102.0, 101.9, 101.8, 101.7, 101.6, 101.5, 101.4, 101.3, 101.2, 101.1, 101.0



3p
 (125 MHz, CDCl₃)

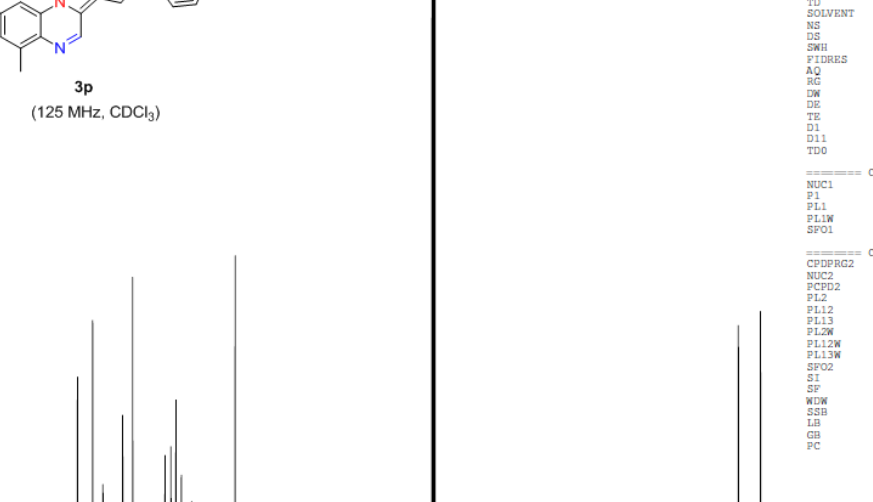
141.45
 138.71
 136.64
 133.29
 131.48
 125.59
 124.53
 123.63
 122.63
 120.78
 112.90
 109.85

77.25
 77.00
 76.75

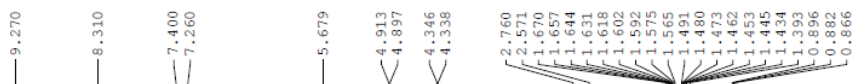
— 40.75

— 21.86
 — 17.85


 NAME Jul14-2016
 EXPNO 70
 PROCNO 1
 Date_ 20160715
 Time 6.37
 INSTRUM Spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 800
 DS 4
 SWH 29761.904 H:
 FIDRES 0.454131 H:
 AQ 1.1010548 s:
 RG 203
 DW 16.800 u:
 DE 6.50 u:
 TE 299.9 K
 D1 2.00000000 s:
 D11 0.03000000 s:
 TD0 1
 ===== CHANNEL f1 =====
 NUC1 13C
 P1 13.84 u:
 PL1 2.50 dB
 PL1W 46.89624786 W
 SFO1 125.7703643 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 u:
 PL2 2.50 dB
 PL12 17.40 dB
 PL13 17.40 dB
 PLW 13.02359581 W
 PL12W 0.42143536 W
 PL13W 0.42143536 W
 SFO2 500.1320005 MHz
 SI 32768
 SF 125.7577974 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



LDK-310

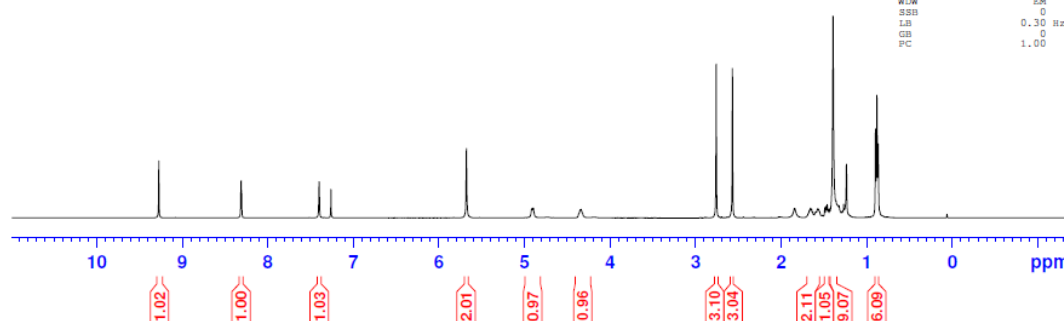


3q

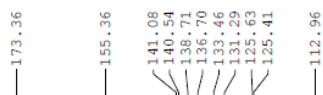
(500 MHz, CDCl₃)

NAME Jul14-2016
EXPNO 51
PROCNO 1
Date_ 20160714
Time 19.41
INSTRUM Spect
PROBHD 5 mm PARBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 80.6
DW 48.400 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 2.50 dB
PL1W 13.02359581 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300223 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



LDK-310 Aminoacid



3q

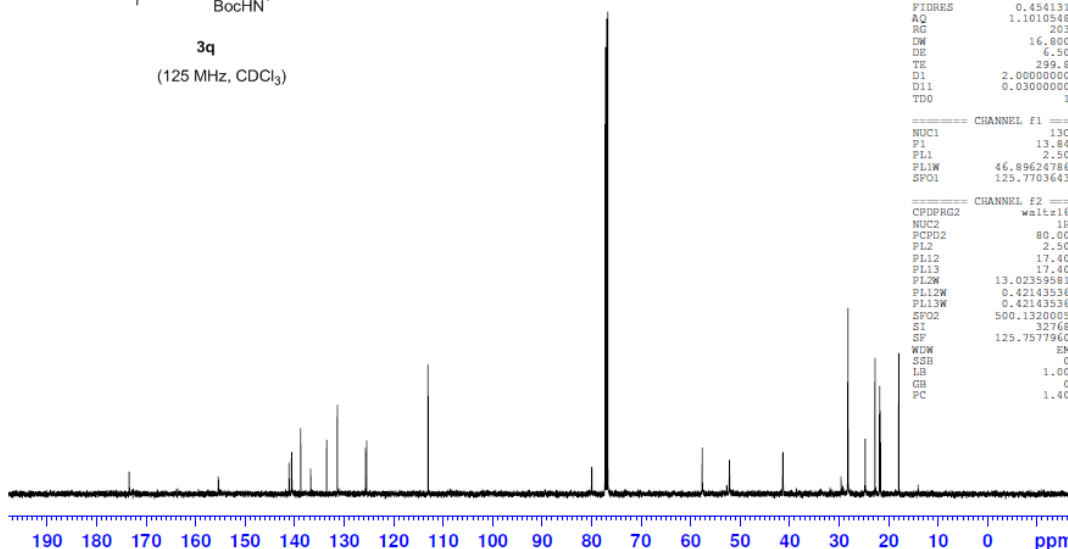
(125 MHz, CDCl₃)



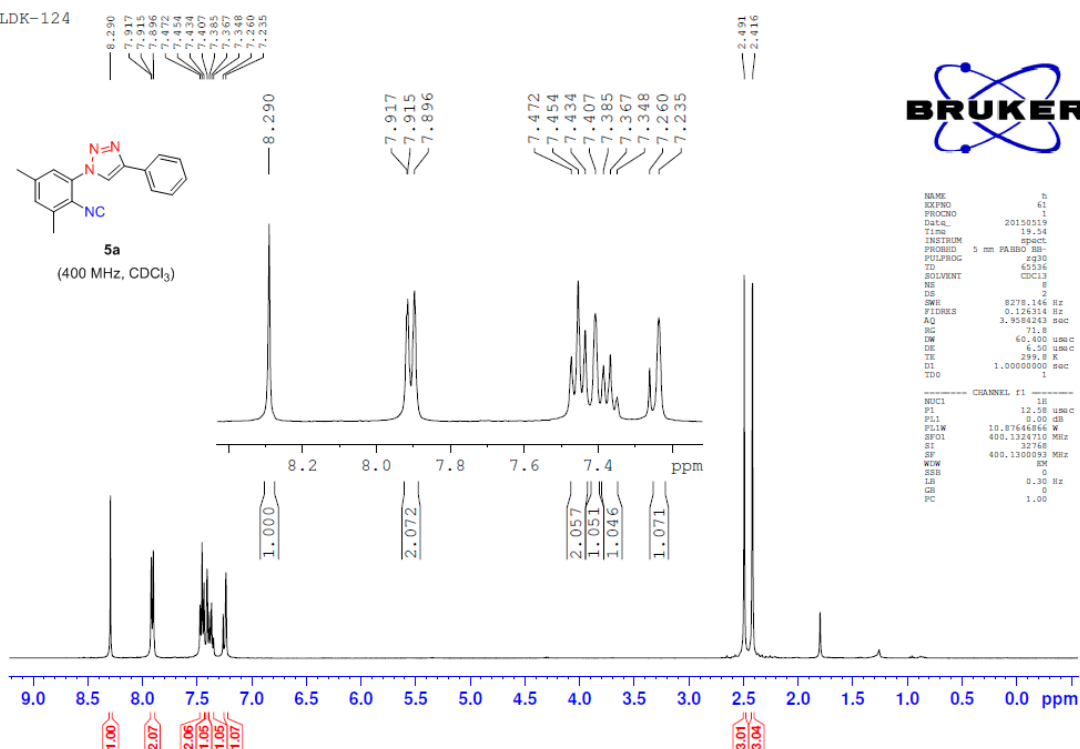
NAME Jul10-2016
EXPNO 2
PROCNO 1
Date_ 20160710
Time 18.34
INSTRUM Spect
PROBHD 5 mm PARBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 500
DS 29761.904 H:
SWH 0.454131 H:
FIDRES 1.1010548 M:
AQ 203
RG 16.800 M:
DW 6.50 M:
DE 298.8 K
TE 2.00000000 M:
D1 0.03000000 M:
D11 1
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 13.84 M:
PL1 2.50 dB
PL1W 46.89624786 W
SFO1 125.7703643 M:

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 M:
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1330005 M:
SI 32768
SF 125.7577960 M:
WDW EM
SSB 0
LB 1.00 H:
GB 0
PC 1.40



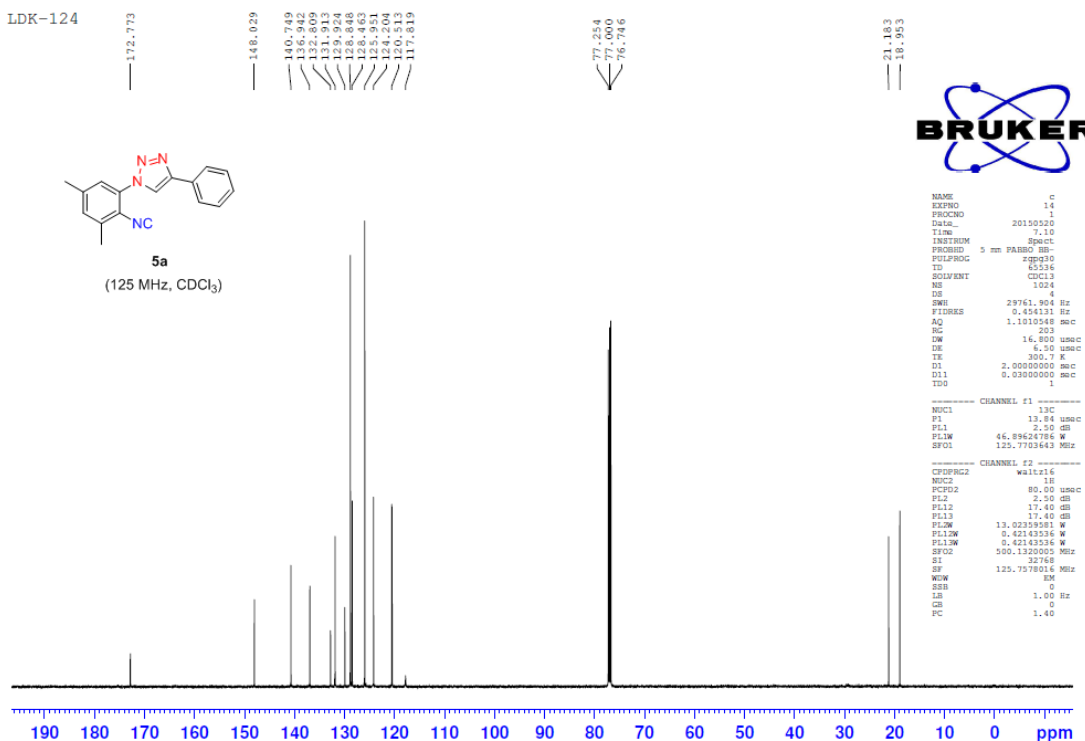
LDK-124



```

NAME      5
EXPNO     1
PROCNO    1
F2 - 20150319
Time      19.54
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         2
DS         2
SWH         8278.146 Hz
FIDRES     0.126314 Hz
AQ         3.9584243 sec
RG         512
DE         60.400 umsec
DS         4.50 umsec
TE         299.8 K
D1         1.00000000 sec
D11
D10
===== CHANNEL f1 =====
NUC1       13C
P1         12.50 umsec
PL1        2.00 dB
PL1W       10.8764848 W
SFO1       400.1324710 MHz
SI         32768
SF         400.1300993 MHz
WDW         EM
SSB         0
LB         0.30 Hz
GB         0
PC         1.00
  
```

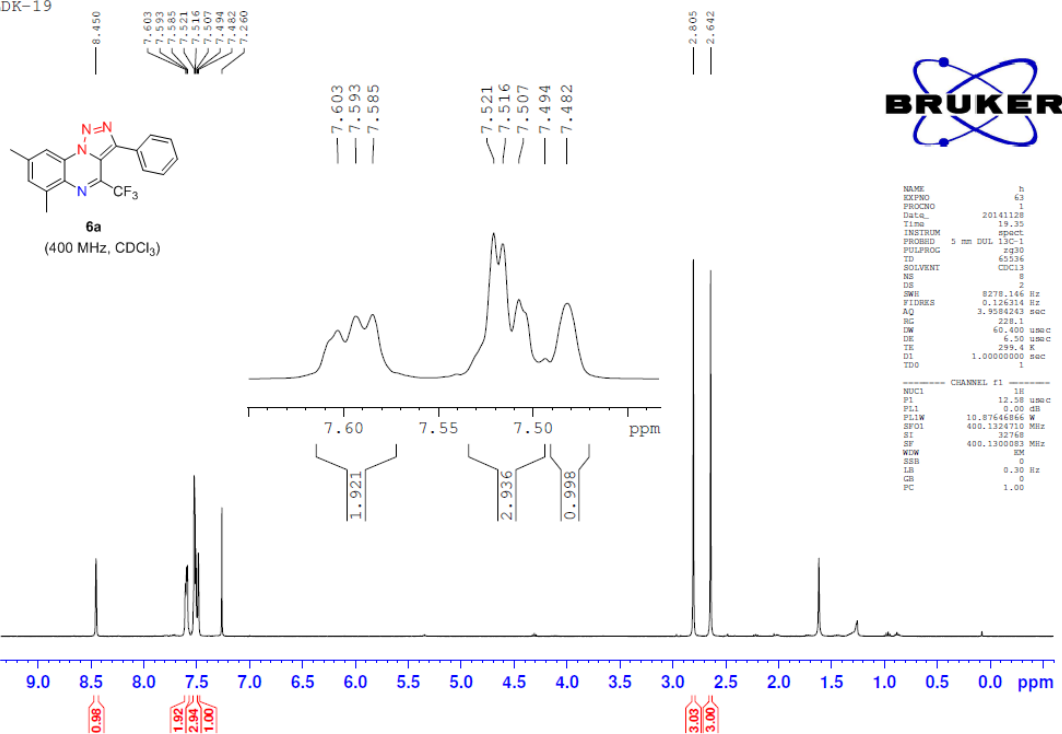
LDK-124



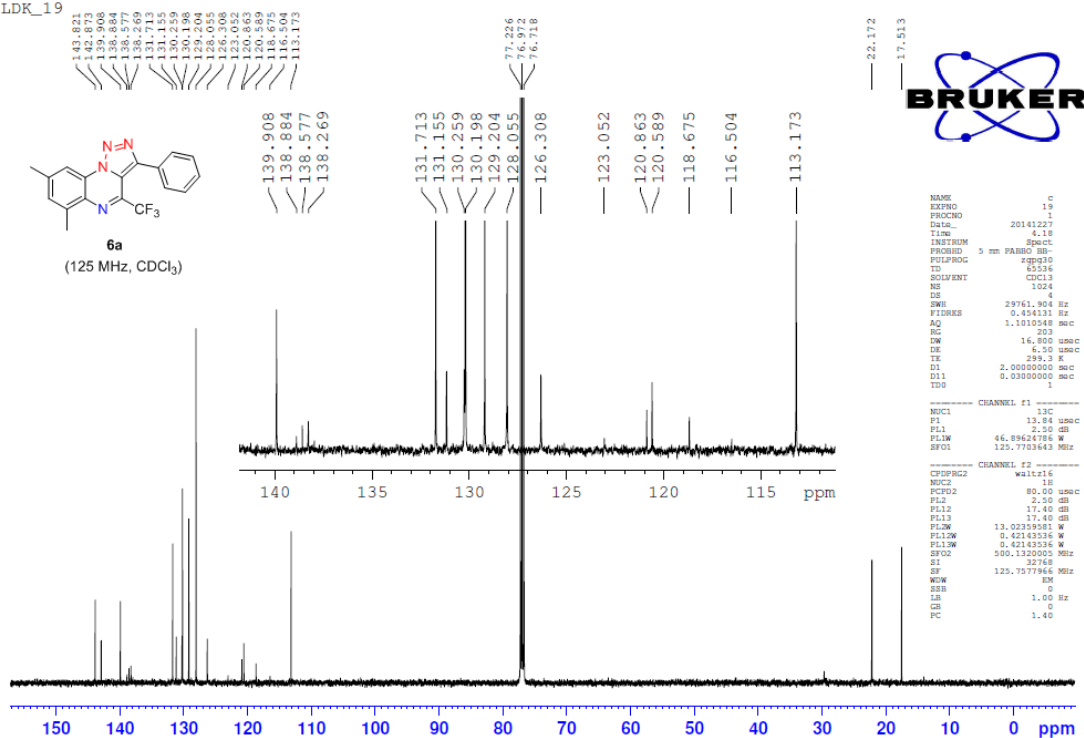
```

NAME      c
EXPNO     14
PROCNO    1
F2 - 20150319
Time      7.10
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         4
DS         4
SWH         29761.904 Hz
FIDRES     0.454131 Hz
AQ         1.1010548 sec
RG         203
DE         16.800 umsec
DS         4.50 umsec
TE         300.7 K
D1         2.00000000 sec
D11
D10
===== CHANNEL f1 =====
NUC1       13C
P1         12.50 umsec
PL1        2.00 dB
PL1W       46.89624796 W
SFO1       125.7703643 MHz
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 umsec
PL2        2.50 dB
PL2W       17.40 dB
PL12       17.40 dB
PL13       17.40 dB
PL1W       13.02359381 W
PL12W      0.42143536 W
PL13W      0.42143536 W
SFO2       500.1320005 MHz
SI         32768
SF         125.7578016 MHz
WDW         EM
SSB         0
LB         1.00 Hz
GB         0
PC         1.40
  
```

LDK-19

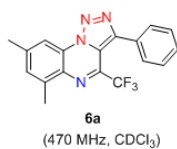


LDK_19



LDK-19

- 65.51

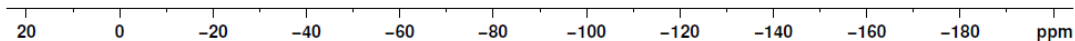


```

NAME      f
EXPNO     5
PROCNO    1
Date_     20150516
Time      21.14
INSTRUM    Spect
PROBHD     5 mm PABBO HS-
PULPROG    zgpg30
TD         131072
SOLVENT    CDCl3
NS         16
DS         4
SWH        113636.367 Hz
FIDRES     0.866977 Hz
AQ         0.5767668 sec
RG         203
DW         4.400 usec
DE         6.50 usec
TE         297.9 K
D1         1.00000000 sec
TDO        1

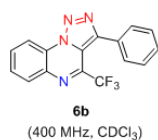
----- CHANNEL f1 -----
NUC1      19F
P1        14.00 usec
PL1       -2.00 dB
PL1W      29.89784813 W
SFO1      470.5453180 MHz
SI        65536
SF        470.5923770 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

```



ldk-26

8.836
8.815
8.290
8.269
7.969
7.950
7.930
7.857
7.838
7.819
7.597
7.579
7.530
7.515
7.240



8.836
8.815
8.290
8.269
7.969
7.950
7.930
7.857
7.838
7.819
7.597
7.579
7.530
7.515

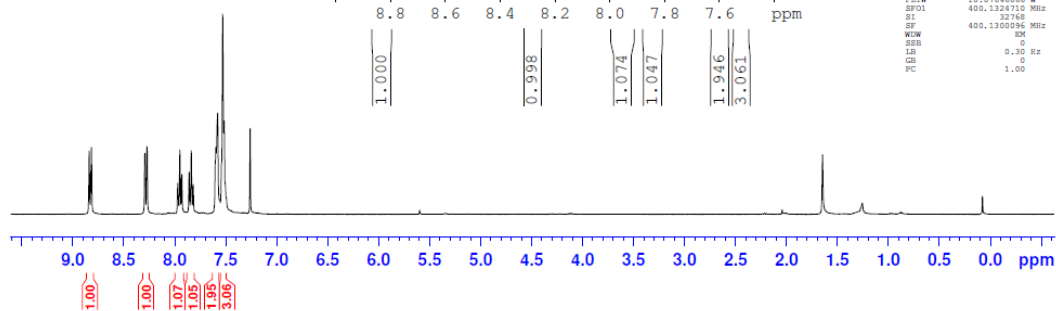


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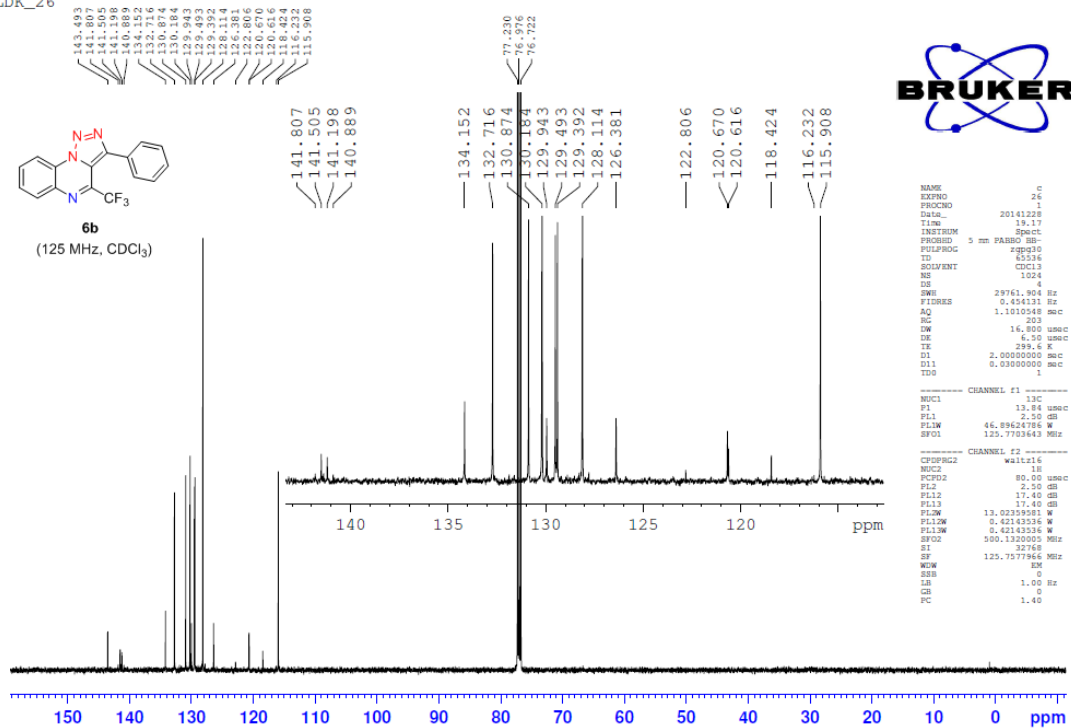
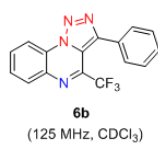
NAME      h
EXPNO     79
PROCNO    1
Date_     20141220
Time      11.05
INSTRUM    spect
PROBHD     5 mm DUL 13C-1
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         16
DS         2
SWH        8278.146 Hz
FIDRES     0.126214 Hz
AQ         3.3584243 sec
RG         238.1
DW         6.400 usec
DE         6.50 usec
TE         297.2 K
D1         1.00000000 sec
TDO        1

----- CHANNEL f1 -----
NUC1      1H
P1        12.08 usec
PL1       0.00 dB
PL1W      10.87646866 W
SFO1      400.1324710 MHz
SI        32768
SF        400.1300000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

```



LDK_26

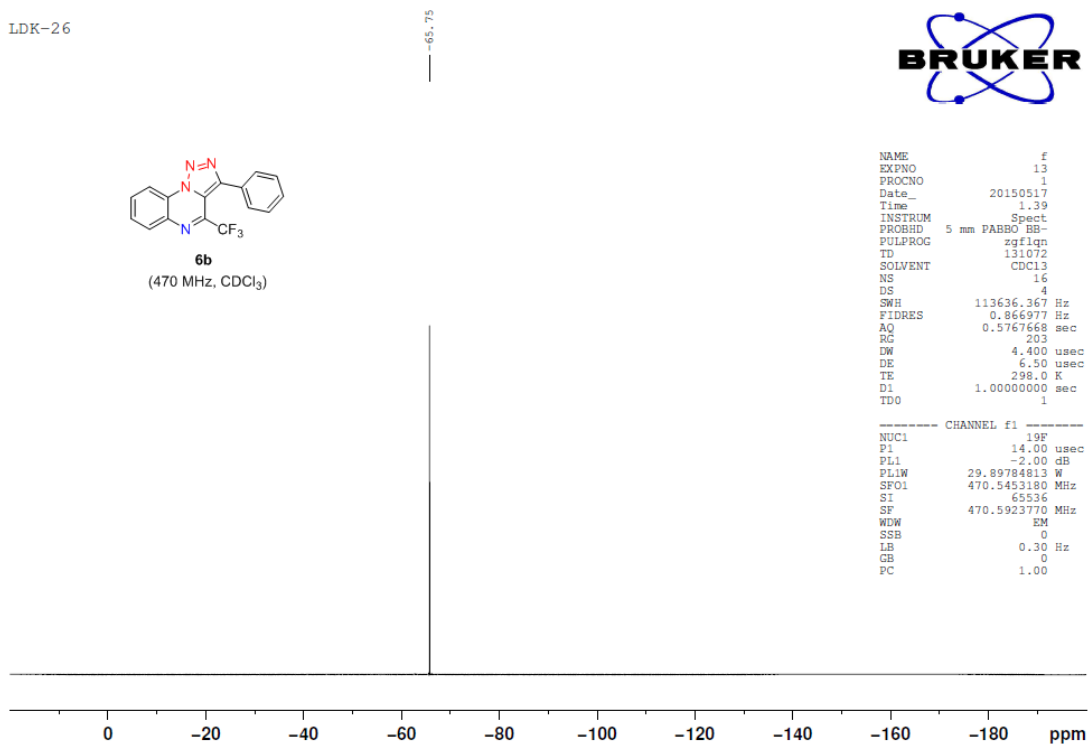
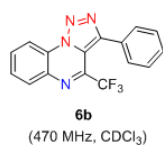


NAME EXPNO 26
PROCNO 1
Date_ 20141228
Time 19.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 1024
DS 4
SWH 28761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 13C
P1 13.84 usec
PL1 2.20 dB
PL1W 46.8962175 W
SFO1 125.7703643 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL2 17.40 dB
PL3 17.40 dB
PL3 17.40 dB
PL2W 13.02359581 W
PL3W 0.42143336 W
PL1W 0.42143336 W
SFO2 500.1320000 MHz
SI 32768
SF 125.7577964 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

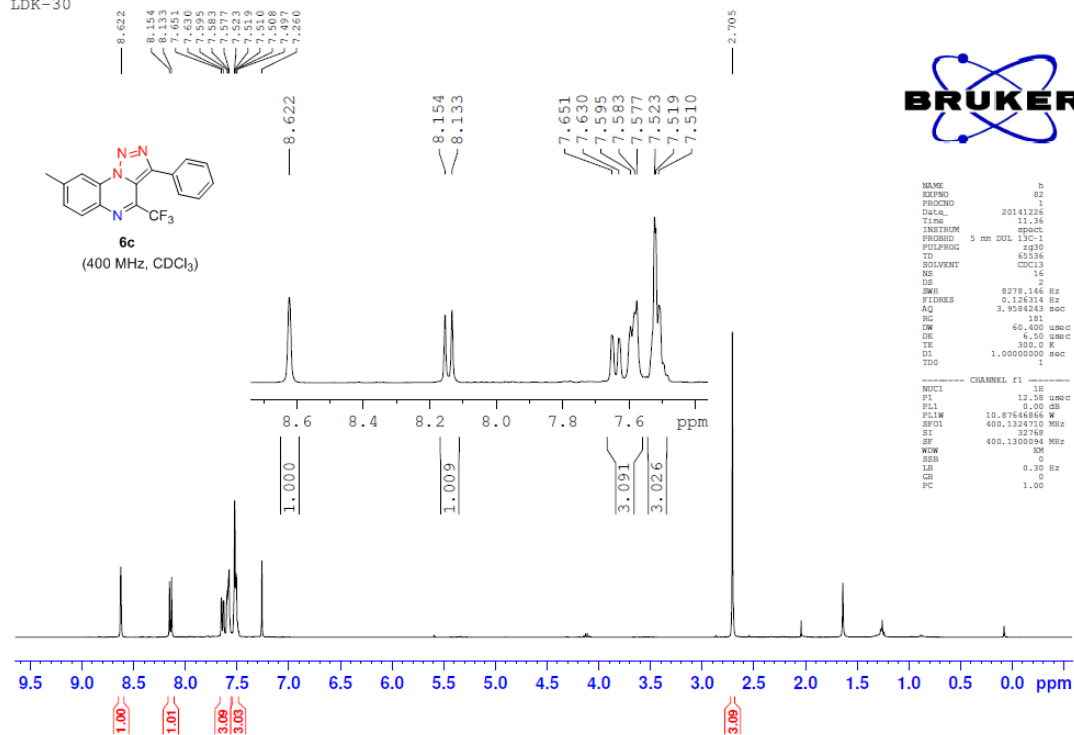
LDK-26



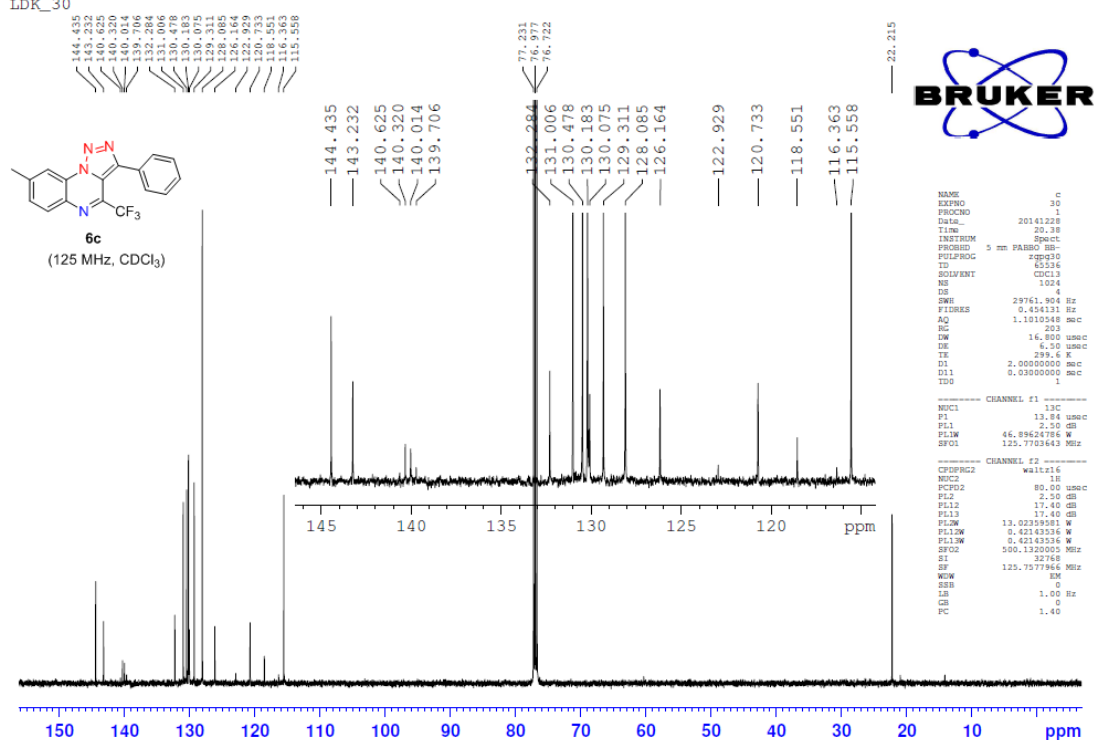
NAME f
EXPNO 13
PROCNO 1
Date_ 20150517
Time 1.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfg1qn
TD 131072
SOLVENT CDCl₃
NS 16
DS 4
SWH 113636.367 Hz
FIDRES 0.866977 Hz
AQ 0.5767668 sec
RG 203
DW 4.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 19F
P1 14.00 usec
PL1 -2.00 dB
PL1W 29.89784813 W
SFO1 470.5453180 MHz
SI 65536
SF 470.5923770 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

LDK-30

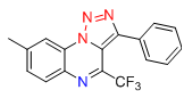


LDK_30



LDK-30

— 65.57



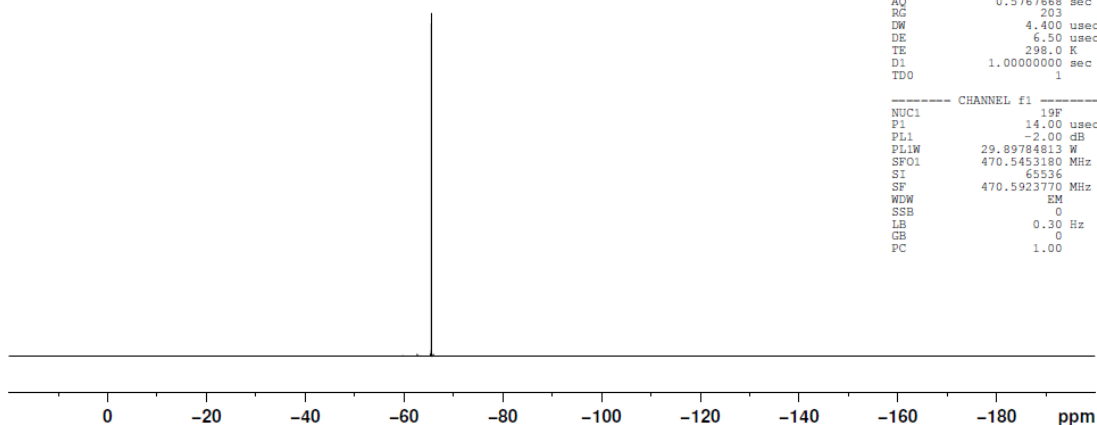
6c
(470 MHz, CDCl₃)

```

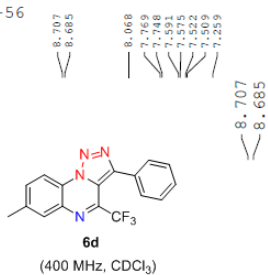
NAME          f
EXPNO         14
PROCNO        1
Date_         20150517
Time          1.43
INSTRUM       Spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            131072
SOLVENT       CDCl3
NS            16
DS            4
SWH           113636.367 Hz
FIDRES        0.866977 Hz
AQ            0.5767668 sec
RG            203
DW            4.400 usec
DE            6.50 usec
TE            298.0 K
D1            1.00000000 sec
TD0           1

----- CHANNEL f1 -----
NUC1          19F
P1            14.00 usec
PL1           -2.00 dB
PL1W          29.89784813 W
SFO1          470.5453180 MHz
SI            55536
SF            470.5923770 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```



LDK-56



6d
(400 MHz, CDCl₃)

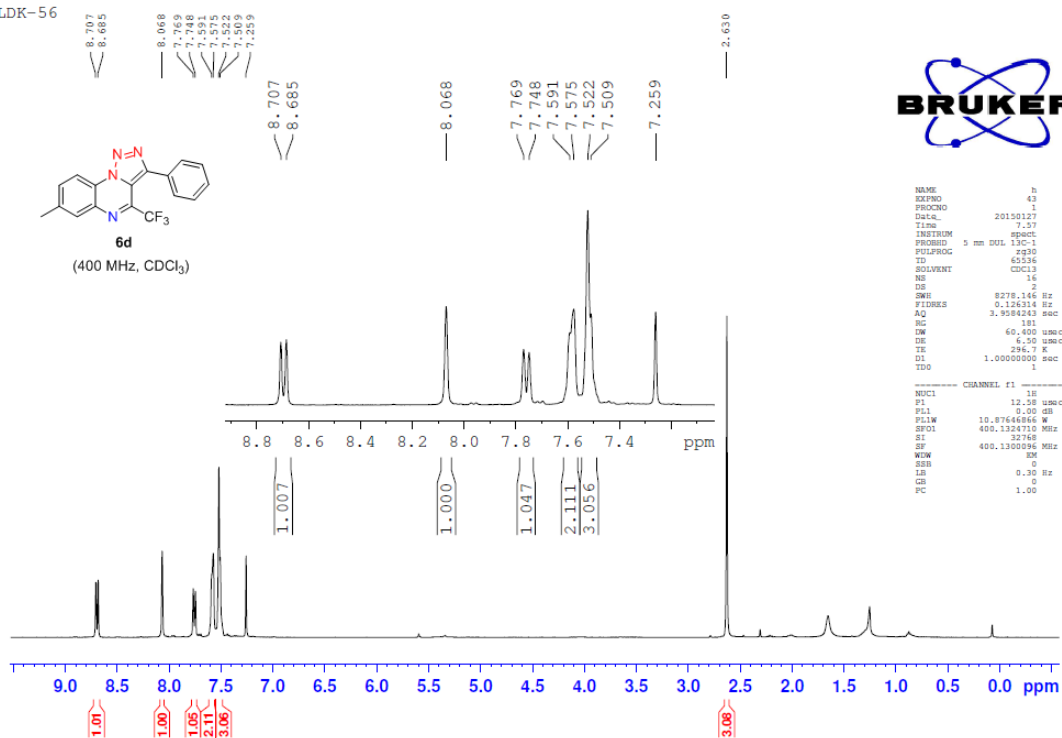


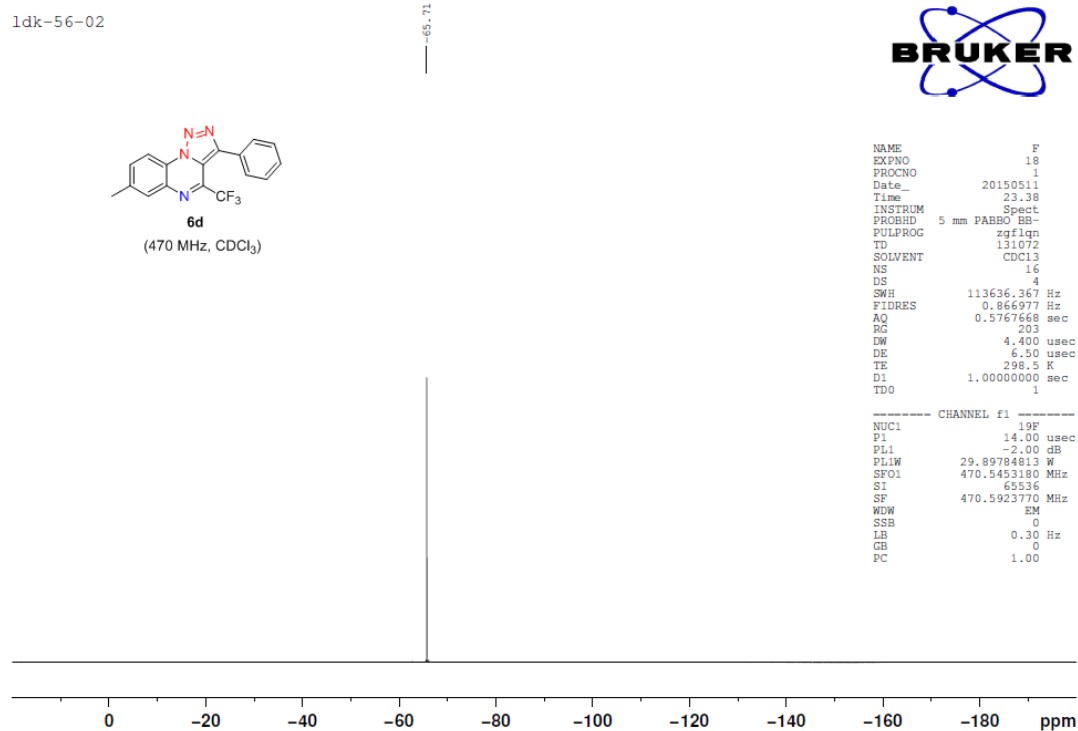
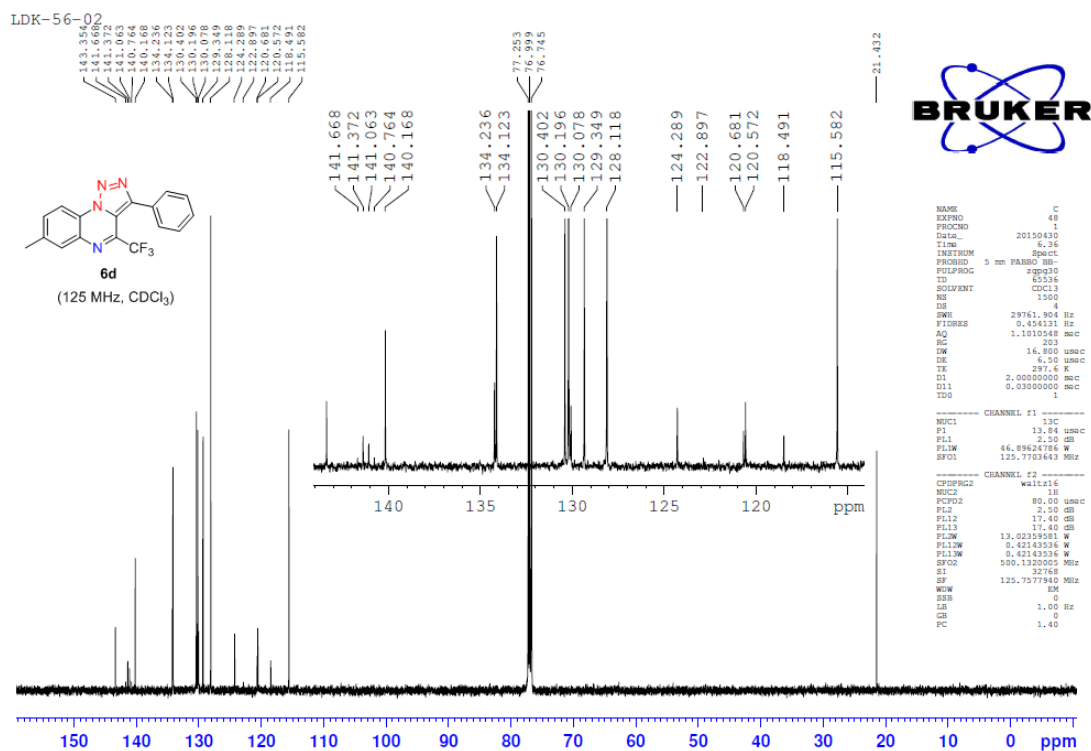
```

NAME          h
EXPNO         43
PROCNO        1
Date_         20150127
Time          7.57
INSTRUM       spect
PROBHD        5 mm DUL 130-1
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           8278.146 Hz
FIDRES        0.126314 Hz
AQ            3.9584243 sec
RG            181
DW            60.400 usec
DE            6.50 usec
TE            296.7 K
D1            1.00000000 sec
TD0           1

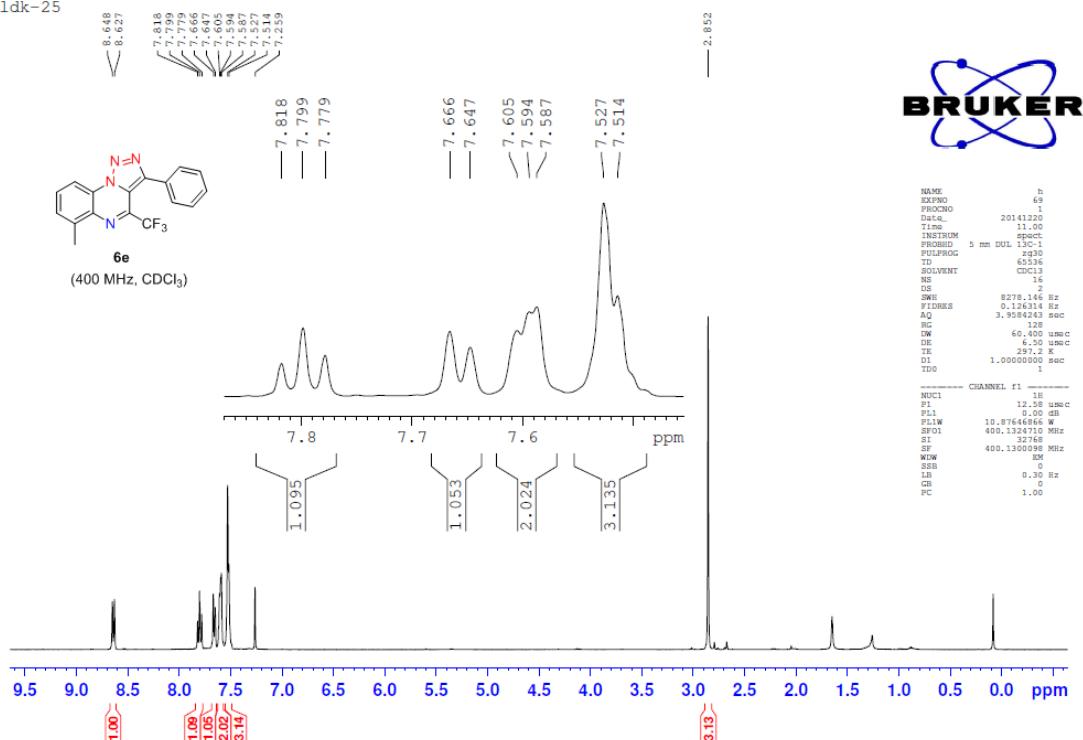
----- CHANNEL f1 -----
NUC1          1H
P1            12.58 usec
PL1           0.00 dB
PL1W          10.87646866 W
SFO1          400.1324710 MHz
SI            32768
SF            400.1300096 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```

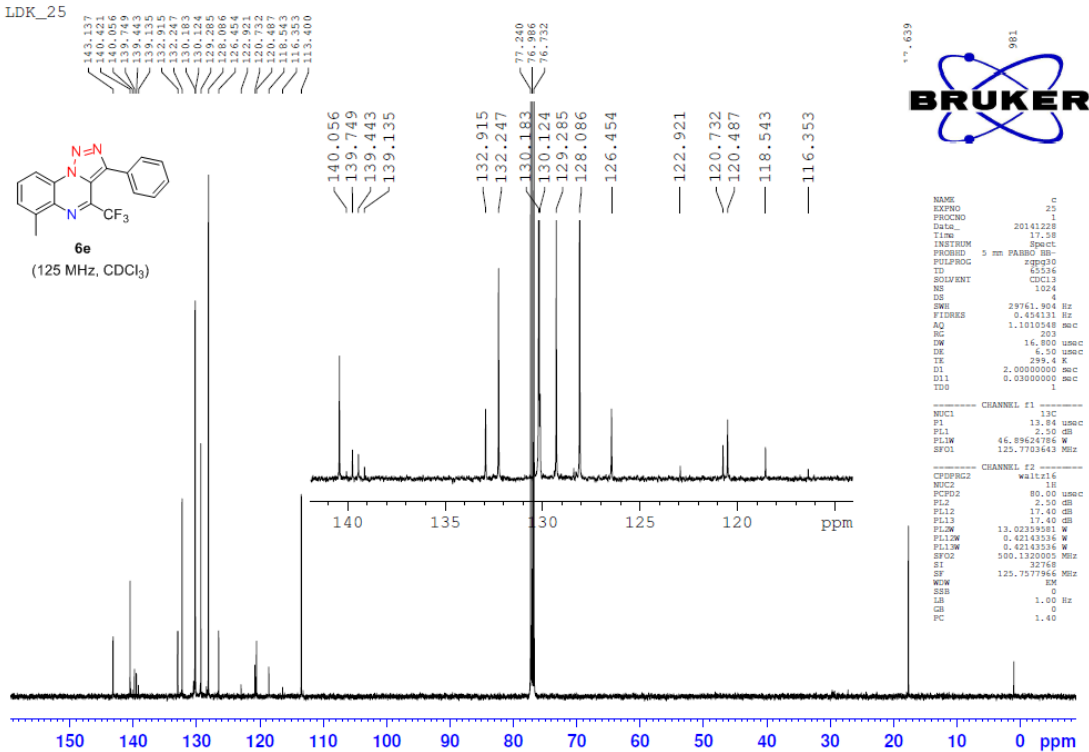




ldk-25



LDK_25



LDK-25

-65, 70

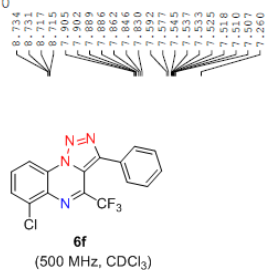


NAME f
EXPNO 6
PROCNO 1
Date_ 20150516
Time_ 21.19
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 131072
SOLVENT CDCl₃
NS 16
DS 4
SWH 113636.367 Hz
FIDRES 0.866977 Hz
AQ 0.5767668 sec
RG 203
DW 4.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.0000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 19F
P1 14.00 usec
PL1 -2.00 dB
PL1W 29.89784813 W
SFO1 470.5453180 MHz
SI 65536
SF 470.5923770 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

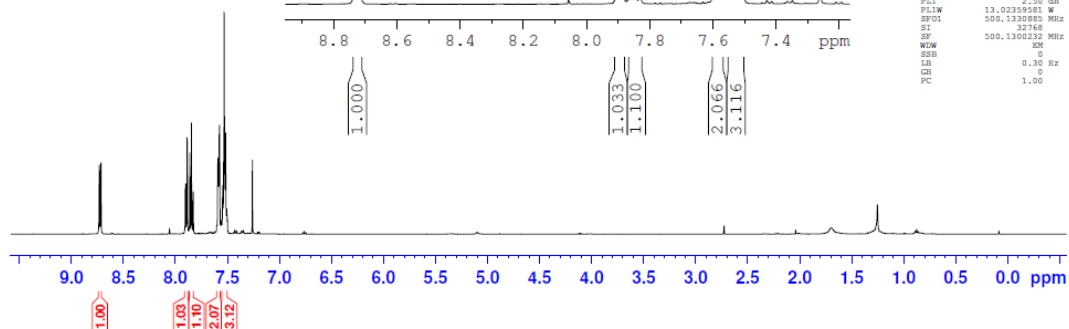
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

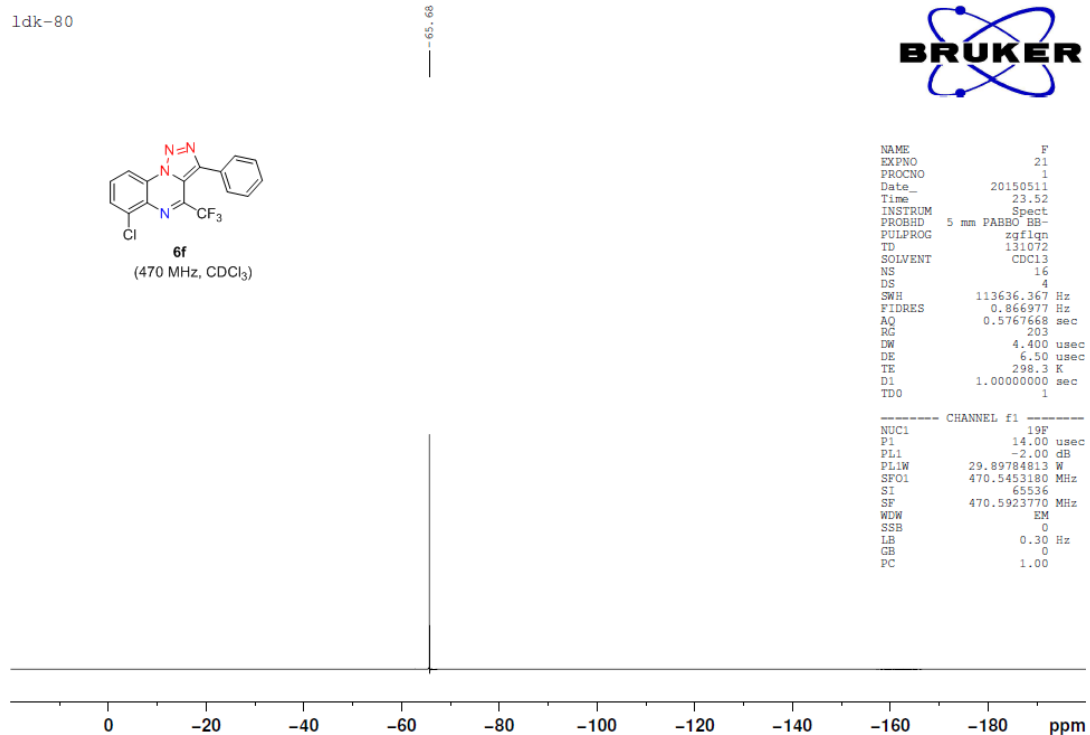
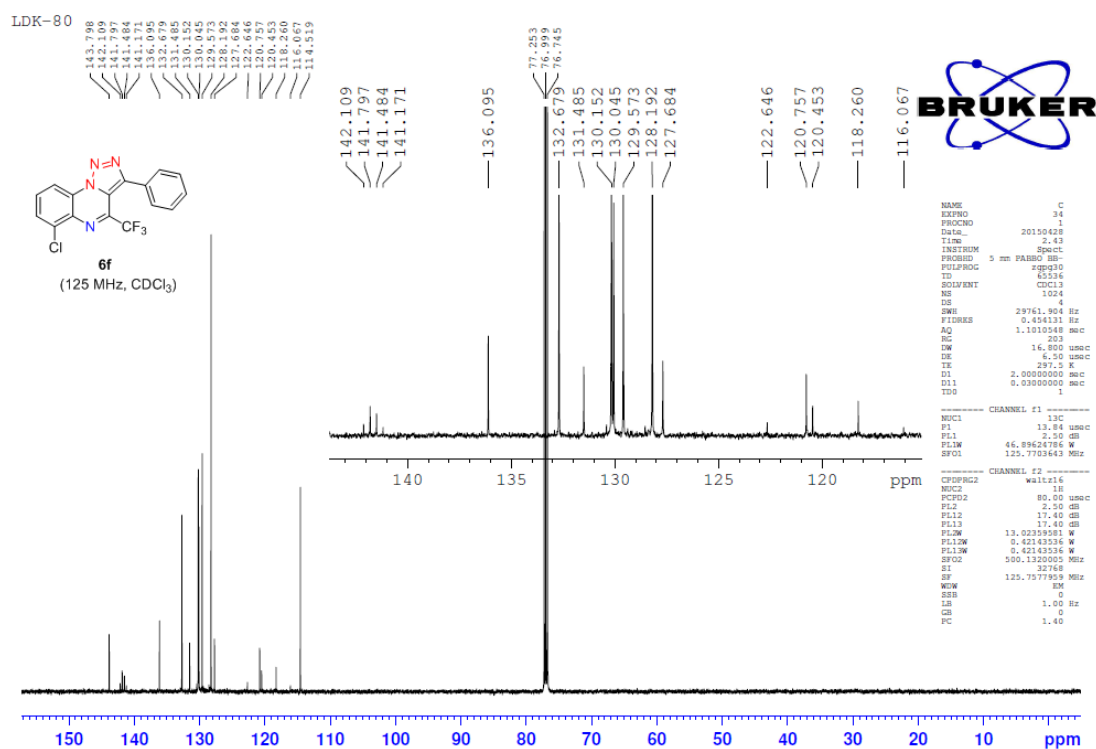
LDK-80



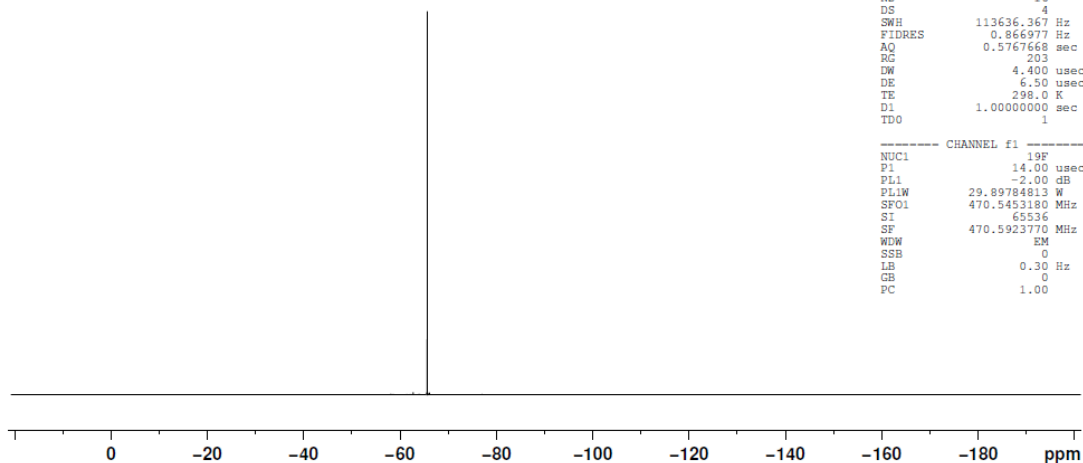
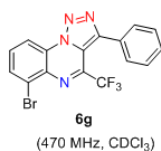
NAME h
EXPNO 1200
PROCNO 1
Date_ 20150312
Time_ 18.24
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157522 Hz
AQ 3.1719923 sec
RG 101
DW 48.600 usec
DE 6.50 usec
TE 298.0 K
D1 1.0000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 1H
P1 14.00 usec
PL1 2.50 dB
PL1W 13.02339581 W
SFO1 500.1360885 MHz
SI 32768
SF 500.1360885 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





— -65.67



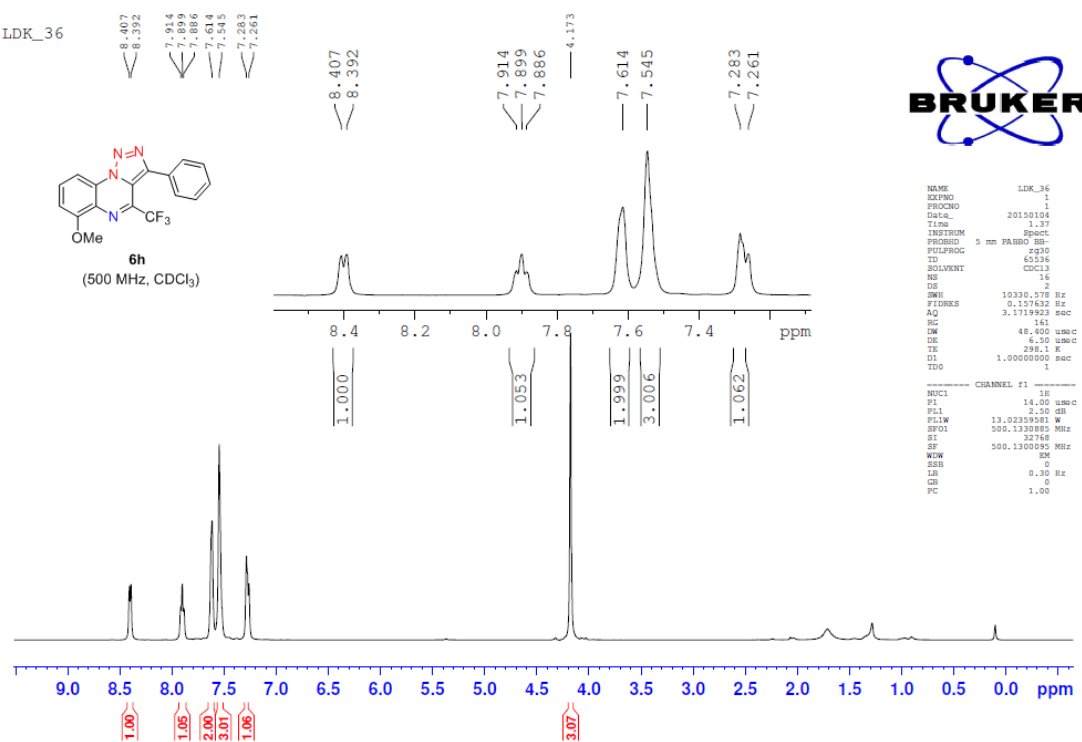
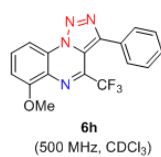
NAME		f
EXPNO	7	
PROCNO	1	
Date_	20150516	
Time	21.24	
INSTRUM	Spect	
PROBHD	5 mm PABBO BB	
PULPROG	zgpg	
TD	131072	
SOLVENT	CDCl3	
NS	16	
DS	5	
SWH	113636.367	Hz
FIDRES	0.869777	Hz
AQ	0.5767668	sec
RG	203	
DW	4.400	usec
DE	6.50	usec
TE	298.0	K
D1	1.00000000	sec
TD0	1	

```

----- CHANNEL f1 -----
NUC1              19F
P1                14.00 usec
PL1              -2.00 dB
PL1W             29.89784813 W
SFO1             470.5453180 MHz
SI               65536
SF              470.5923770 MHz
WDW              EM
SSB              0
LB              0.30 Hz
GB              0
PC              1.00

```

LDK_36



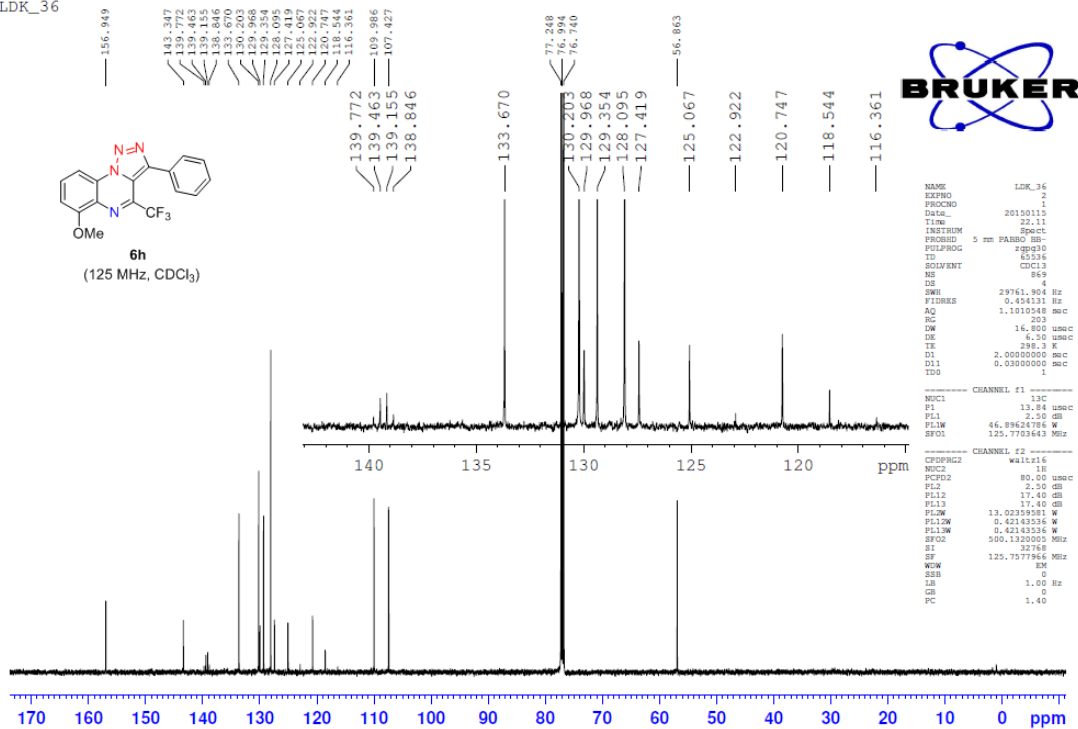
NAME	LDK_36
EXPNO	1
PROCNO	1
Date_	20150104
Time	1.37
INSTRUM	Spect
FREQID	5 mm F400 NMR
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	161
DE	48.400 usec
DW	6.50 usec
TE	298.1 K
D1	1.00000000 sec
TD0	1

```

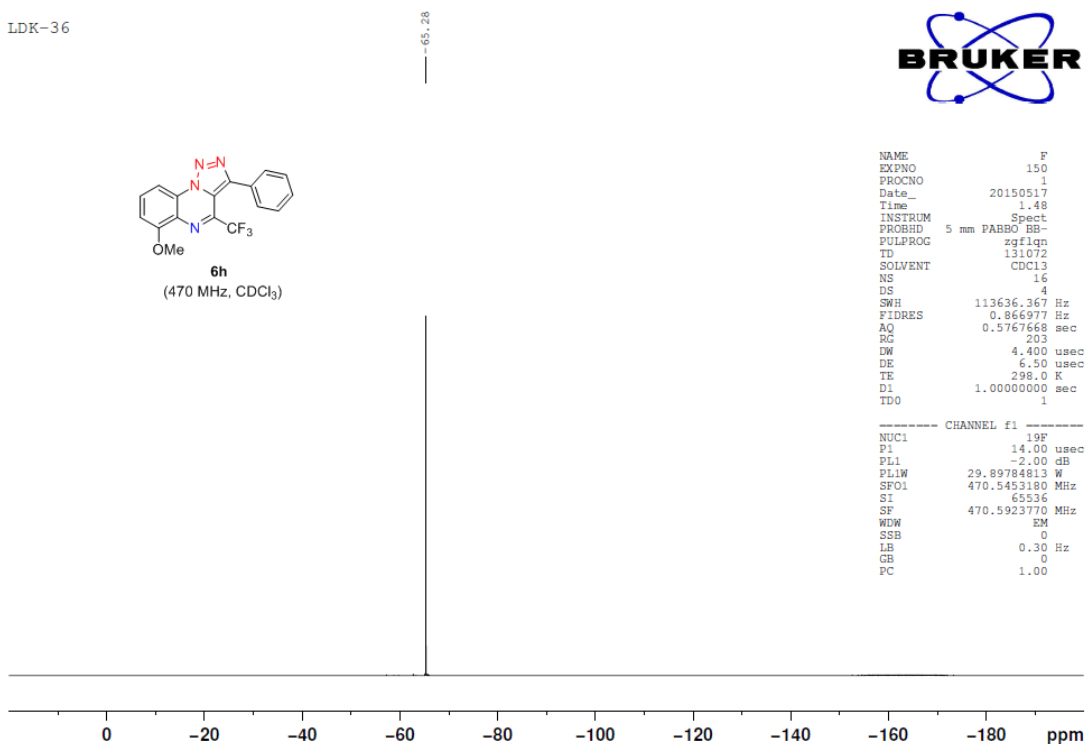
----- CHANNEL F1 -----
NUC1              1H
P1                14.00 usec
PL1              2.50 dB
PLW1             13.02359581 W
SF01             500.1330885 MHz
SI               32768
SF              500.1300895 MHz
WDW              EM
SSB              0
LB              0.30 Hz
GB              0
PC              1.00

```

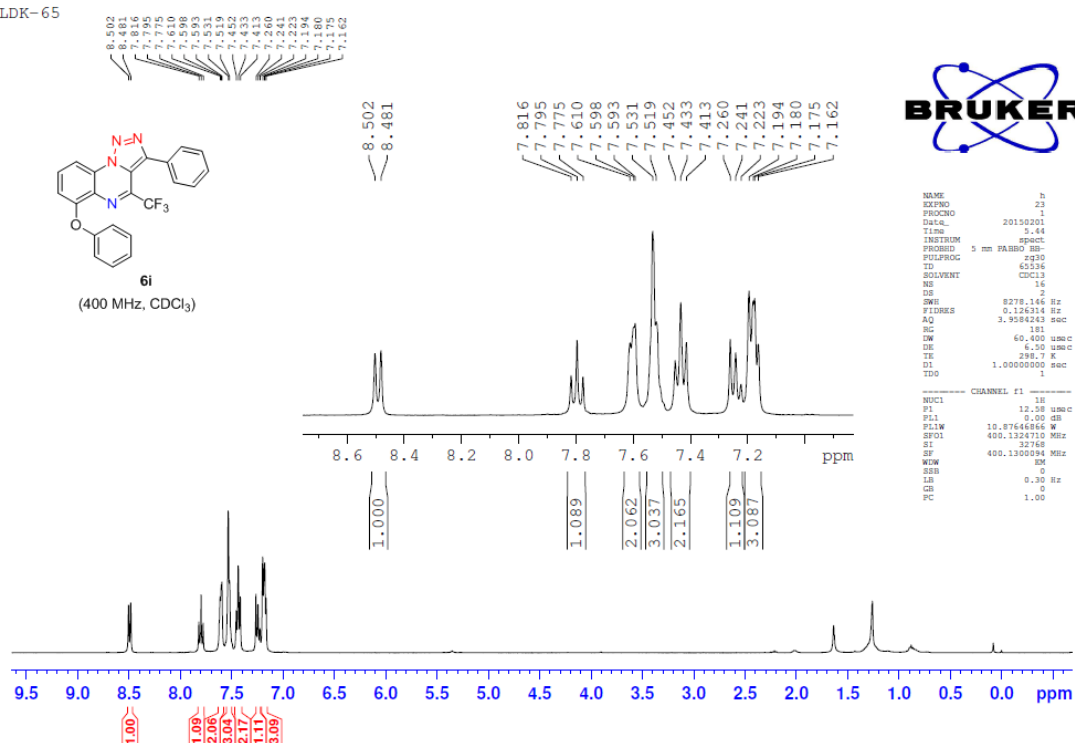
LDK_36



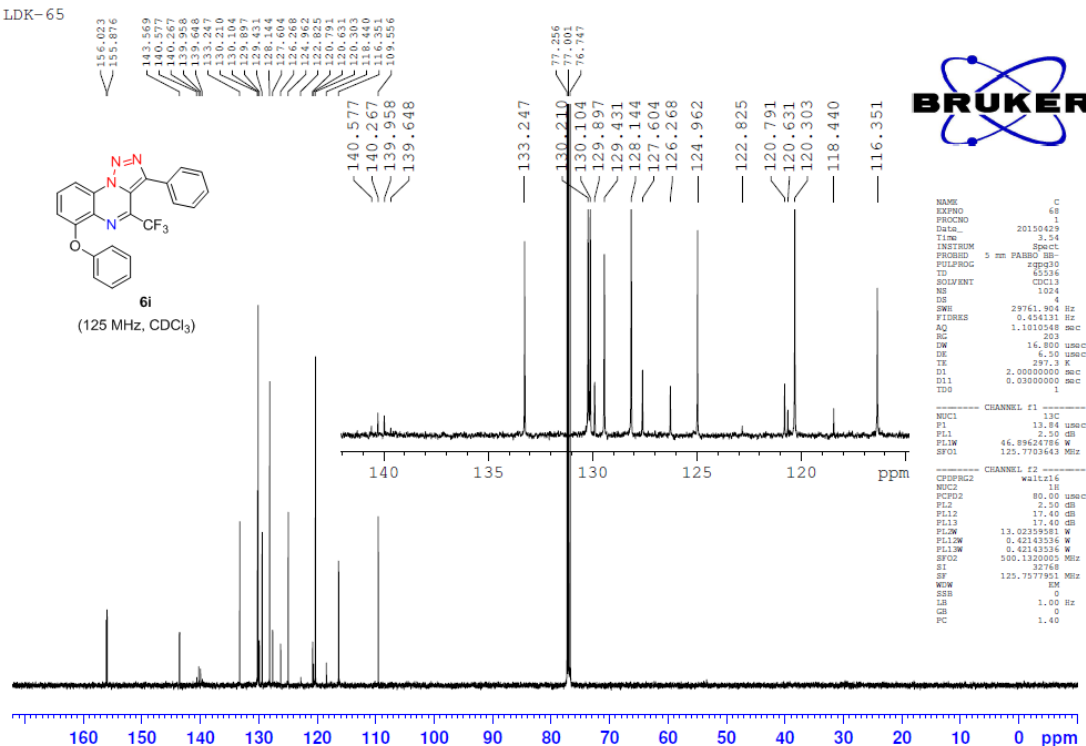
LDK-36



LDK-65

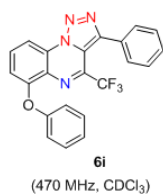


LDK-65



1dk-65

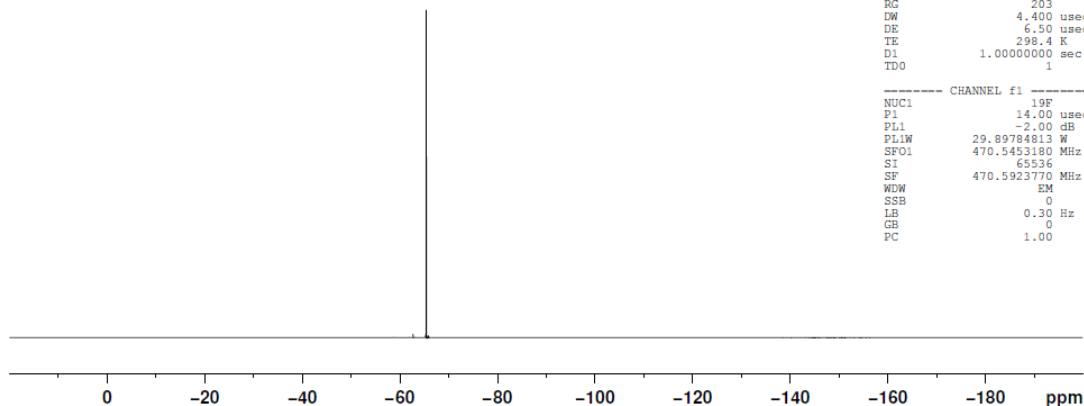
— -65.41



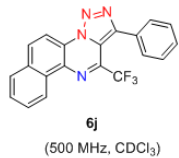
```

NAME          F
EXPNO         20
PROCNO        1
Date_         20150511
Time          23.47
INSTRUM       Spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            131072
SOLVENT       CDCl3
NS            16
DS            4
SWH           113636.367 Hz
FIDRES        0.866977 Hz
AQ            0.5767668 sec
RG            203
DE            4.400 usec
TE            298.4 K
D1            1.00000000 sec
TD0           1

----- CHANNEL f1 -----
NUC1          19F
P1            14.00 usec
PL1           2.00 dB
PL1W          29.89784813 W
SFO1          470.5453180 MHz
SI            65536
SF            470.5923770 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```



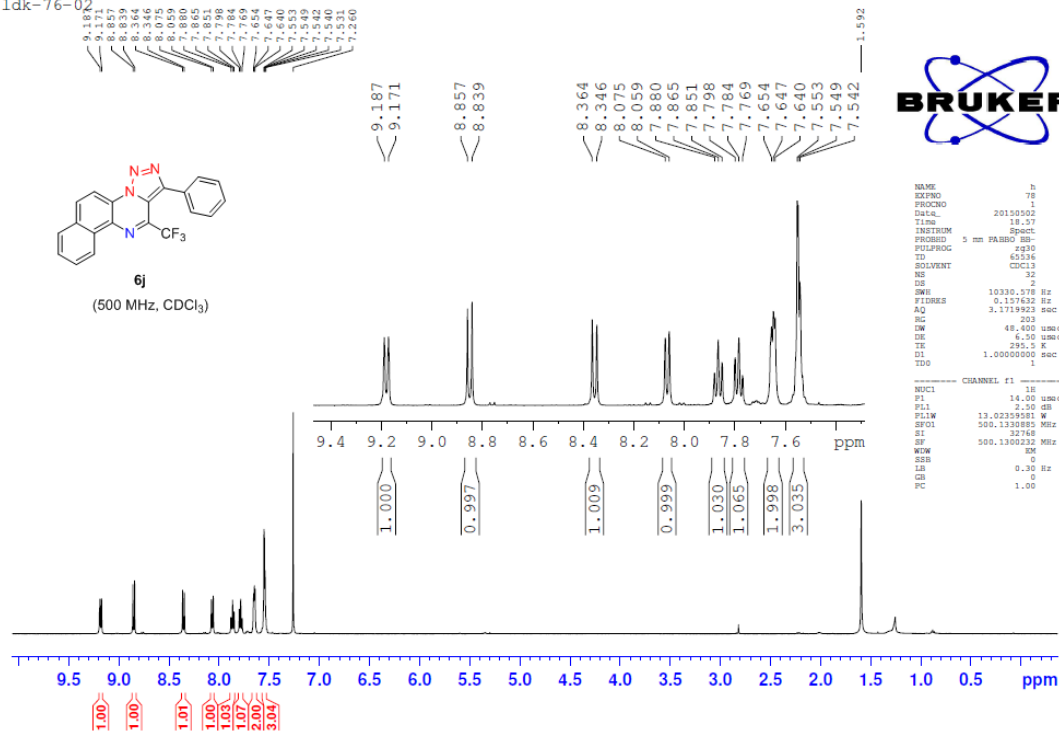
1dk-76-02

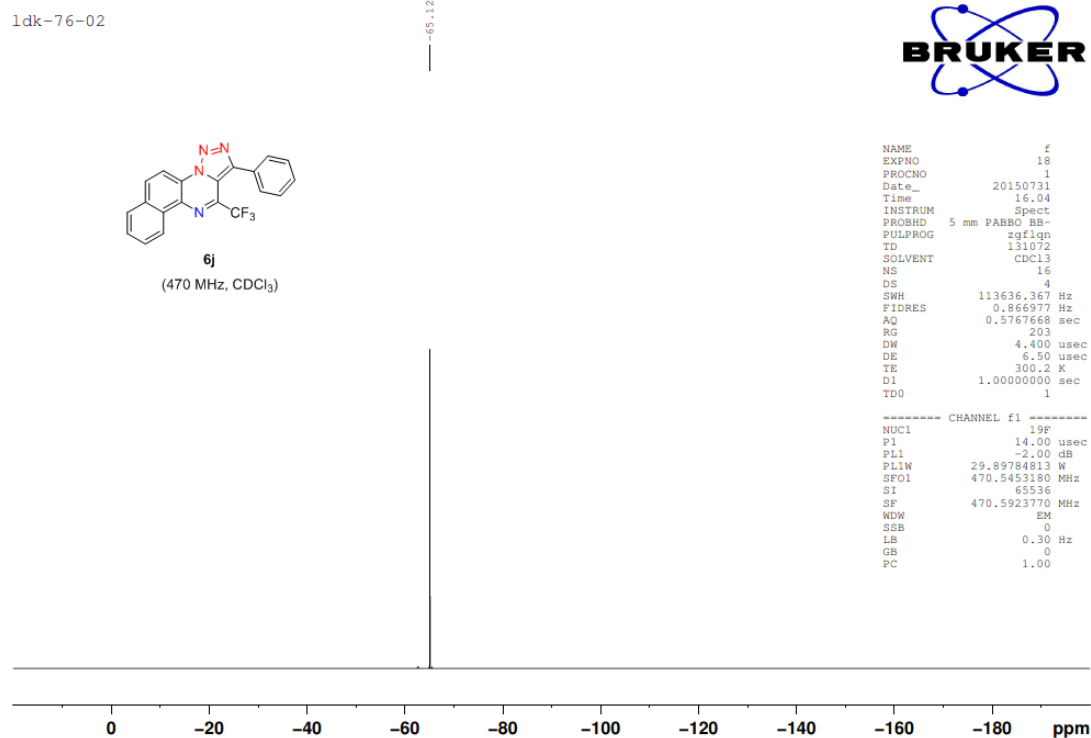
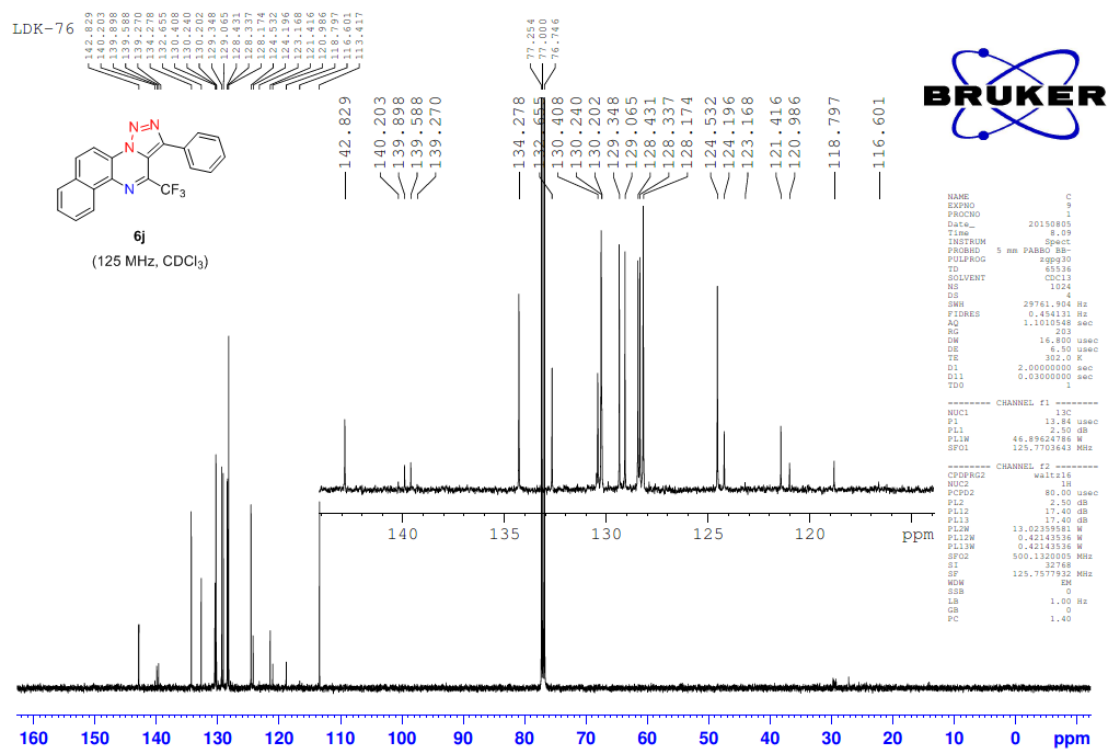


```

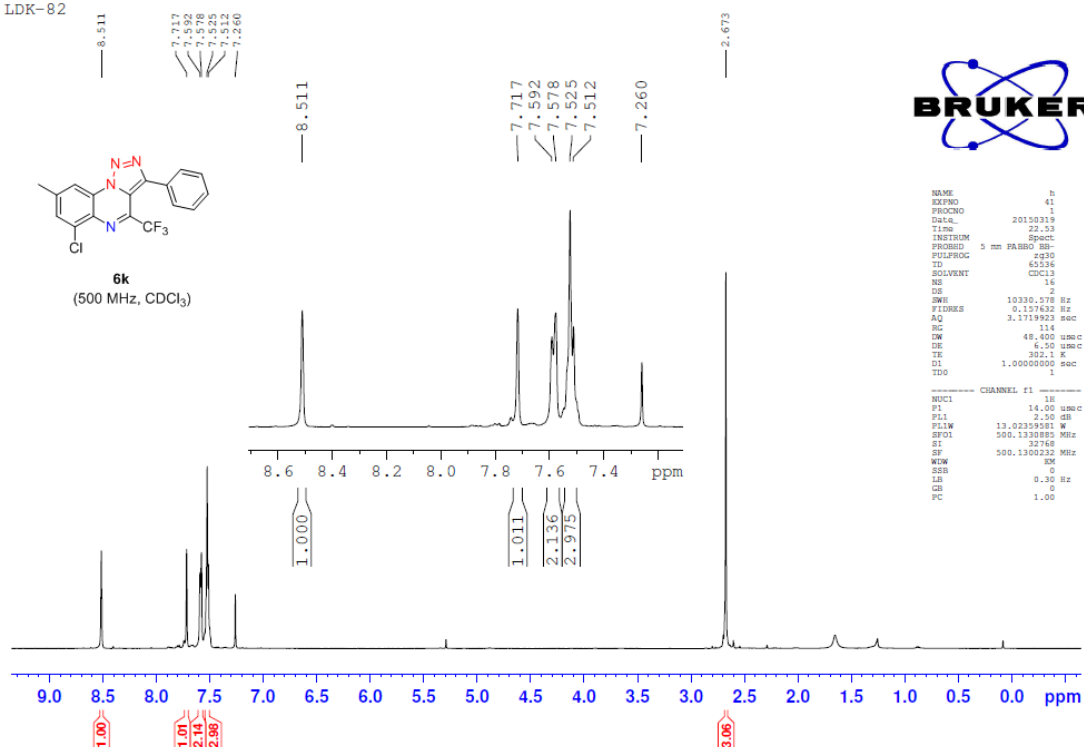
NAME          h
EXPNO         78
PROCNO        1
Date_         20150502
Time          18.57
INSTRUM       Spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            32
DS            2
SWH           10330.578 Hz
FIDRES        0.127632 Hz
AQ            3.1719923 sec
RG            203
DE            4.400 usec
TE            295.5 K
D1            1.00000000 sec
TD0           1

----- CHANNEL f1 -----
NUC1          1H
P1            14.00 usec
PL1           2.00 dB
PL1W          13.02359581 W
SFO1          500.1360882 MHz
SI            32768
SF            500.1360882 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

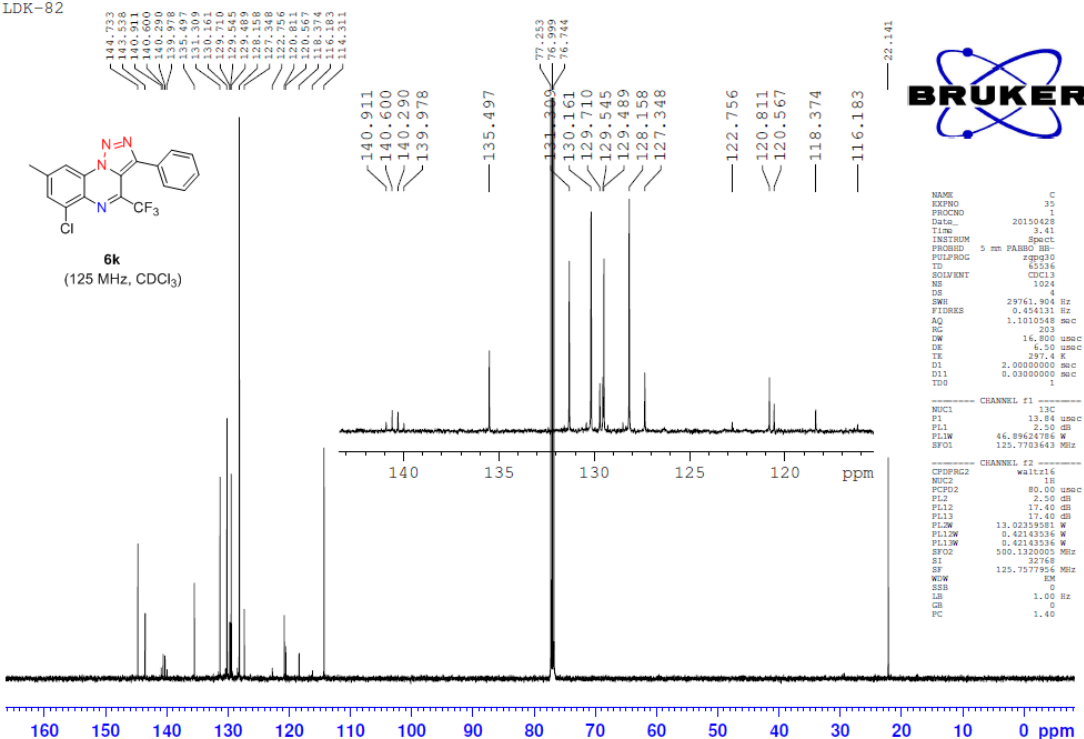




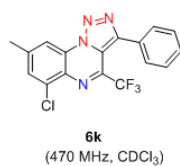
LDK-82



LDK-82



ldk-82

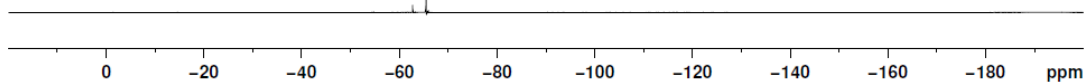


— 65.52

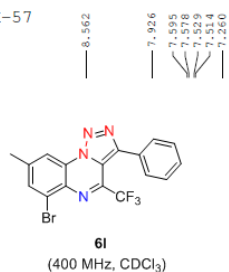


```
NAME      F
EXPNO     22
PROCNO    1
Date_     20150511
Time      23.57
INSTRUM   Spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         131072
SOLVENT   CDCl3
NS         16
DS         4
SWH        113636.367 Hz
FIDRES     0.866977 Hz
AQ         0.5767668 sec
RG         203
DW         4.400 usec
DE         6.50 usec
TE         298.2 K
D1         1.00000000 sec
TD0        1
```

```
----- CHANNEL f1 -----
NUC1      19F
P1         14.00 usec
PL1        -2.00 dB
PL1W       29.89784813 W
SFO1       470.5453180 MHz
SI         65536
SF         470.5923770 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```



LDK-57



— 8.562

— 7.926

— 7.595

— 7.578

— 7.529

— 7.514

— 7.260

— 8.562

— 7.926

— 7.595

— 7.578

— 7.529

— 7.514

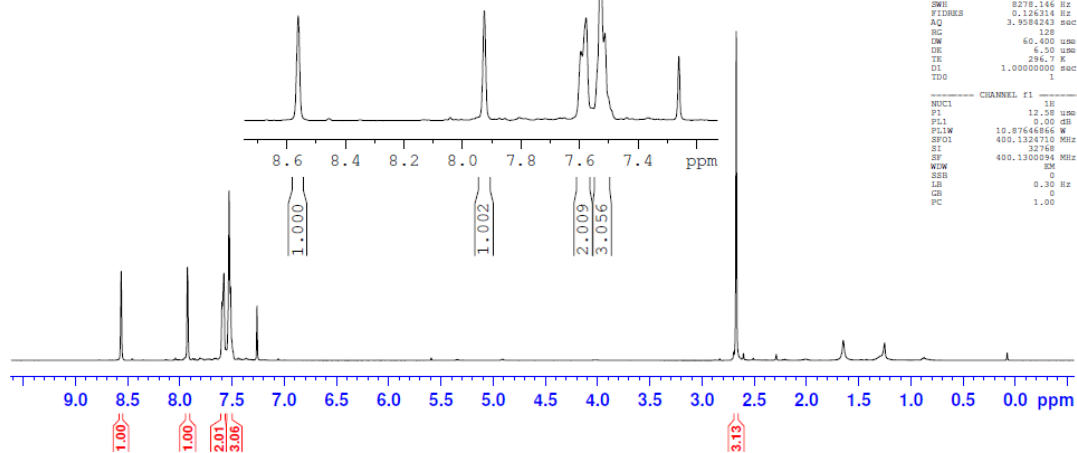
— 7.260

— 2.674



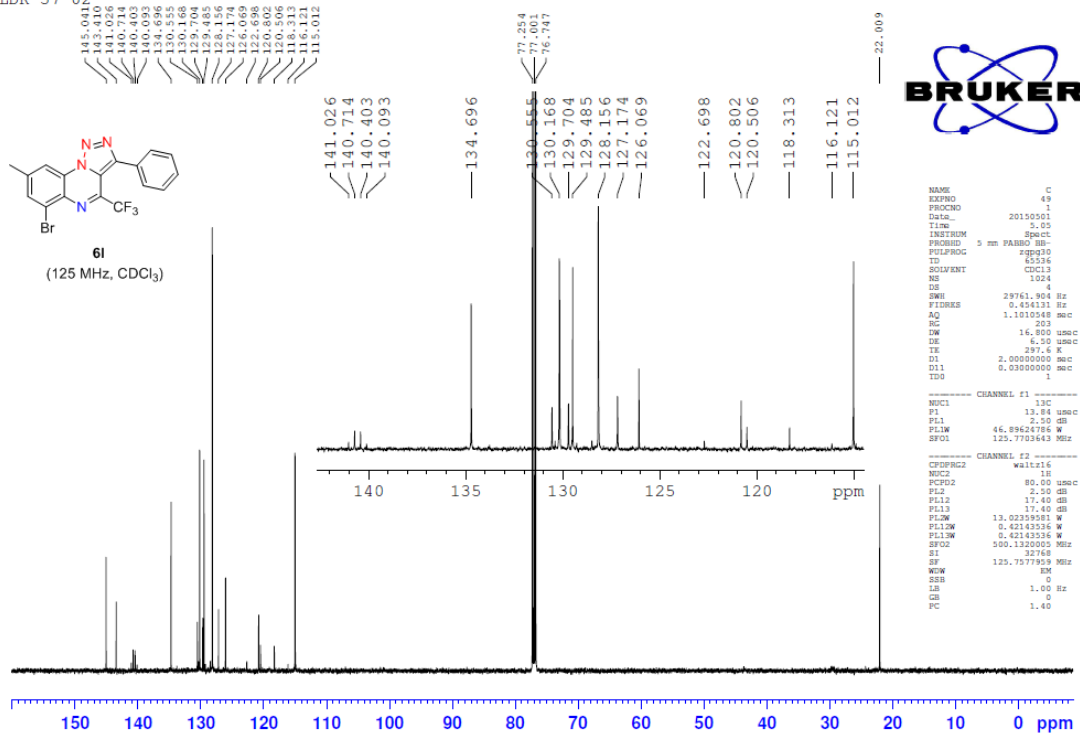
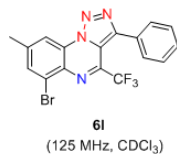
```
NAME      h
EXPNO     4400
PROCNO    1
Date_     20150127
Time      12.03
INSTRUM   spect
PROBHD    5 mm DOL 13C-1
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8278.144 Hz
FIDRES     0.125314 Hz
AQ         3.9084243 sec
RG         128
DW         60.400 usec
DE         6.50 usec
TE         296.7 K
D1         1.00000000 sec
TD0        1
```

```
----- CHANNEL f1 -----
NUC1      1H
P1         12.50 usec
PL1         0.00 dB
PL1W       10.87544895 W
SFO1       400.1324710 MHz
SI         32768
SF         400.1300934 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

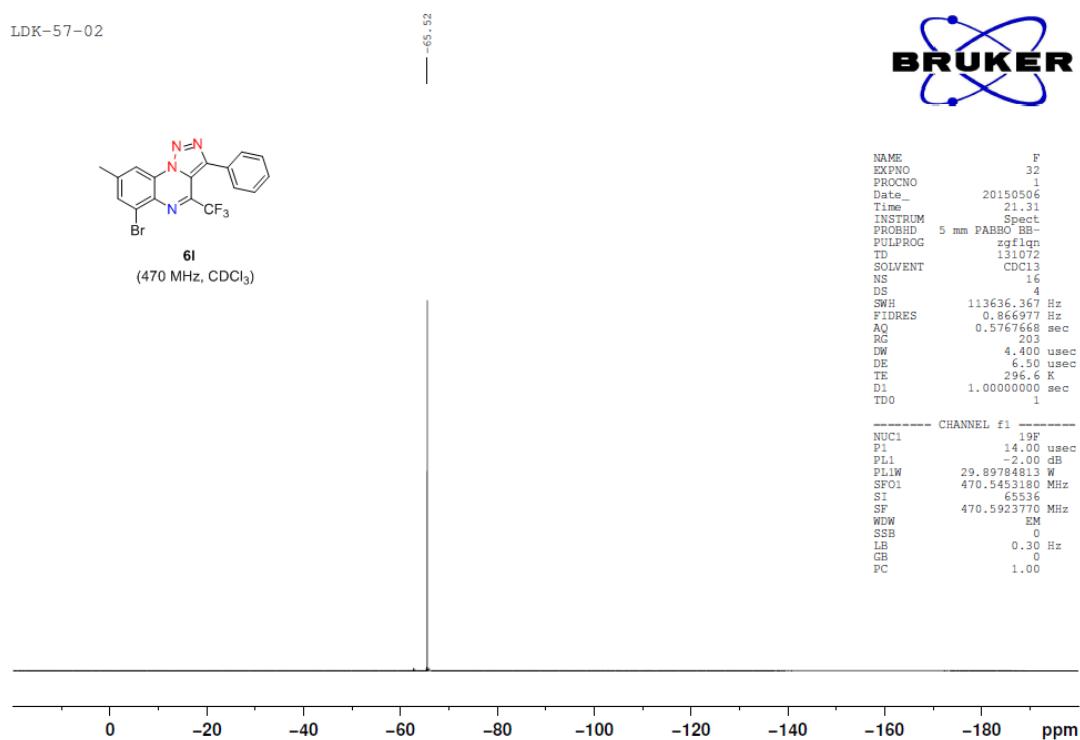
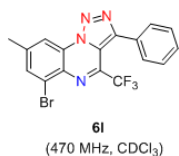


LDK-57-02

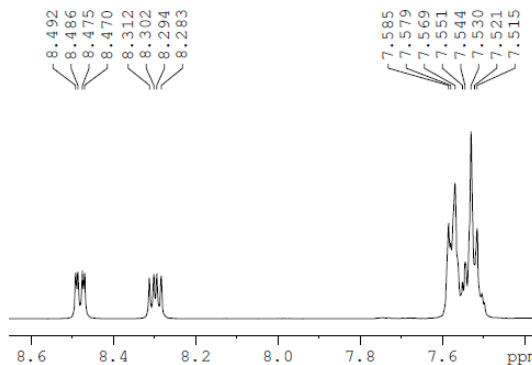
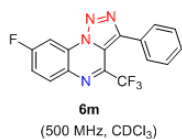
145.041N
144.516
141.026
140.714
140.403
139.592
134.696
130.555
130.168
129.704
129.485
128.156
127.174
126.089
125.506
120.802
120.506
118.313
116.121
115.012



LDK-57-02

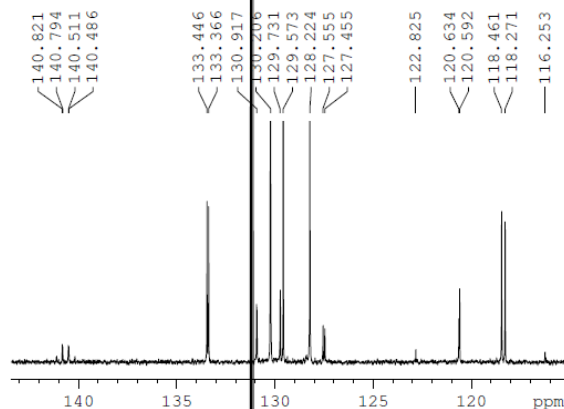
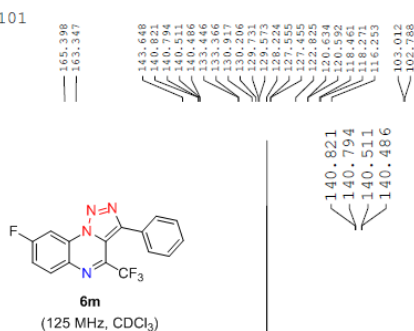


ldk-101



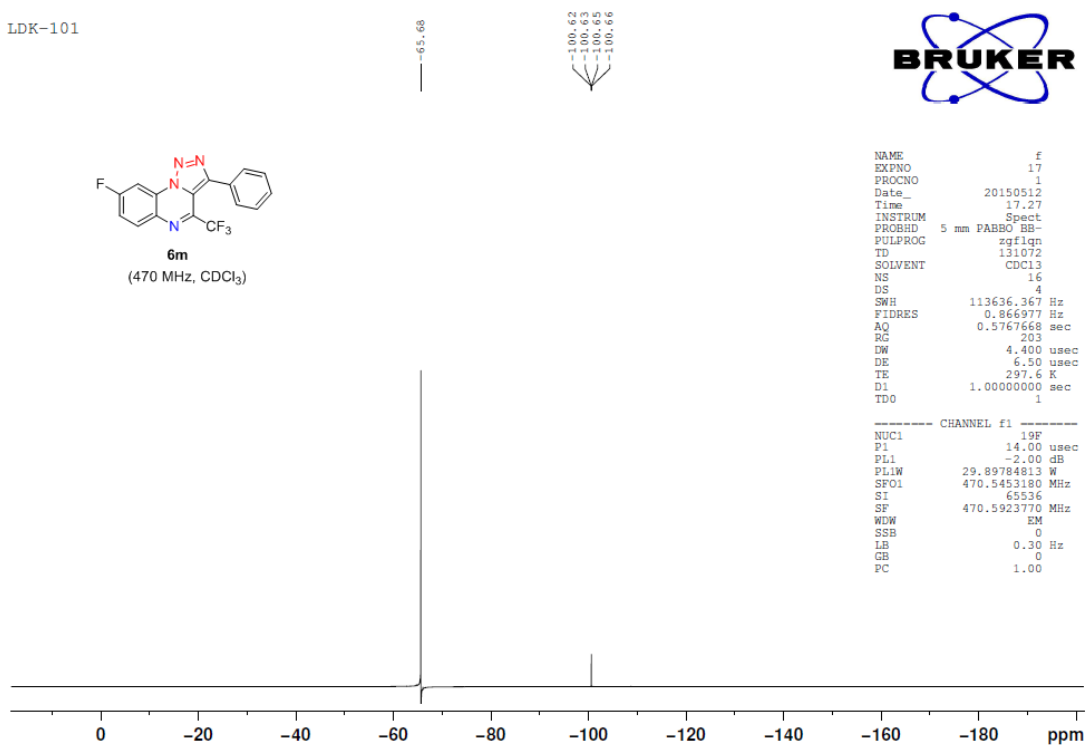
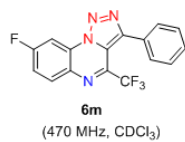
NAME h
EXPNO 24
PROCNO 1
Date_ 20150421
Time 21:01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.137632 Hz
AQ 3.1719923 sec
RG 128
DW 48.400 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TDO
----- CHANNEL f1 -----
NUC1 1H
P1 14.00 usec
PL1 2.50 dB
PL1W 13.02359581 W
SFO1 500.1330880 MHz
ST 32768
SF 500.1330233 MHz
WDW RM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

LDK-101



NAME c
EXPNO 602
PROCNO 1
Date_ 20150421
Time 11:26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1600
DS 4
SWH 29761.904 Hz
FIDRES 0.404131 Hz
AQ 1.1010248 sec
RG 203
DW 14.900 usec
DE 6.50 usec
TE 297.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO
----- CHANNEL f1 -----
NUC1 13C
P1 13.84 usec
PL1 2.50 dB
PL1W 46.89624786 W
SFO1 125.7703643 MHz
----- CHANNEL f2 -----
CFDPGR2 waitx16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL1W 0.42143336 W
PL1W 0.42143336 W
SFO2 500.1330205 MHz
ST 32768
SF 125.7577890 MHz
WDW RM
SSB 0
LB 1.40 Hz
GB 0
PC 1.40

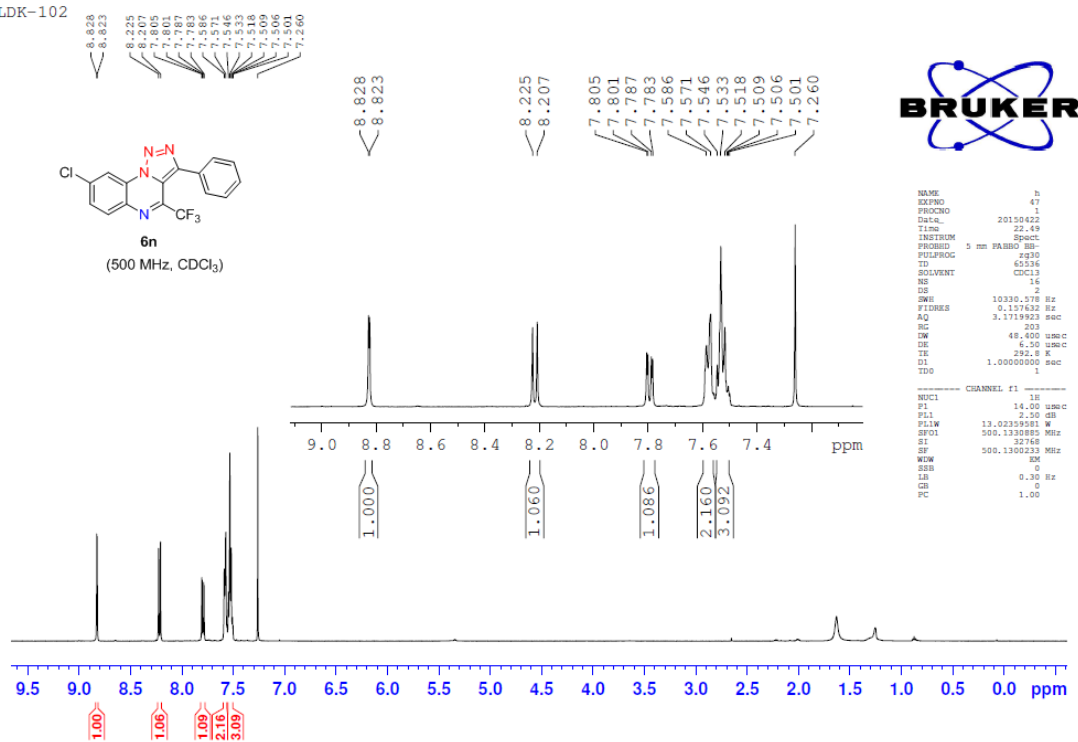
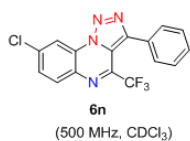
LDK-101



NAME f
EXPNO 17
PROCNO 1
Date_ 20150512
Time 17.27
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 131072
SOLVENT CDCl₃
NS 16
DS 4
SWH 113636.367 Hz
FIDRES 0.866977 Hz
AQ 0.5767668 sec
RG 203
DW 4.400 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 13C
P1 14.00 usec
PL1 -2.00 dB
PL1W 29.89784813 W
SFO1 470.5453180 MHz
SI 65536
SF 470.5923770 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

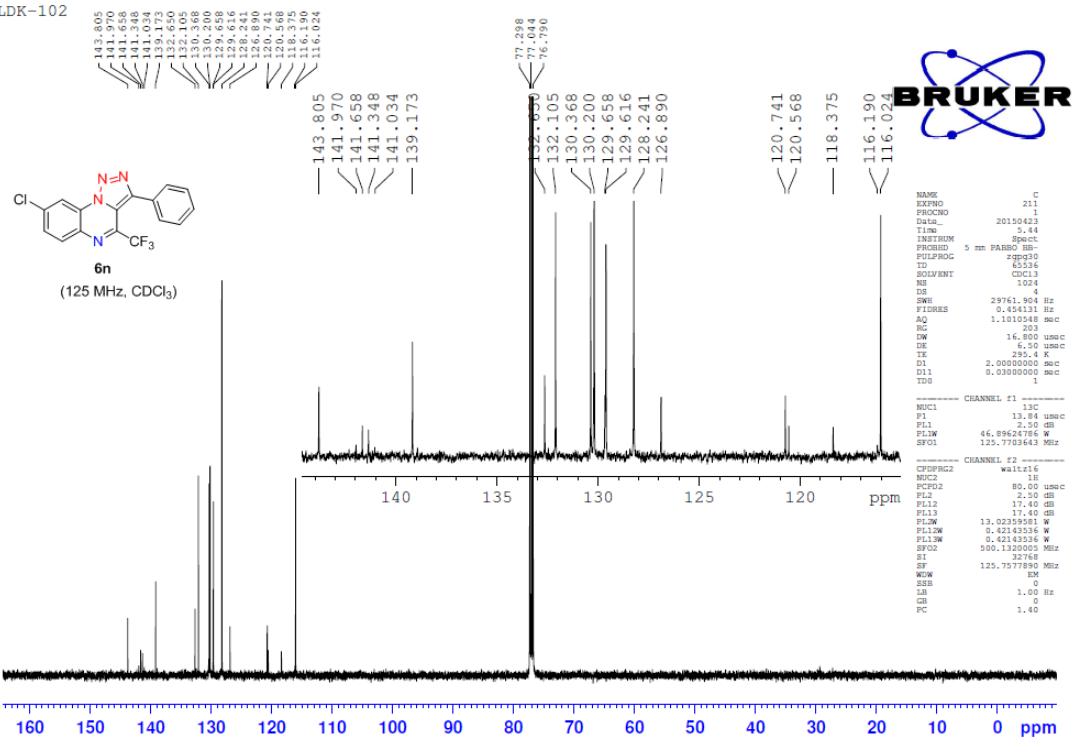
LDK-102



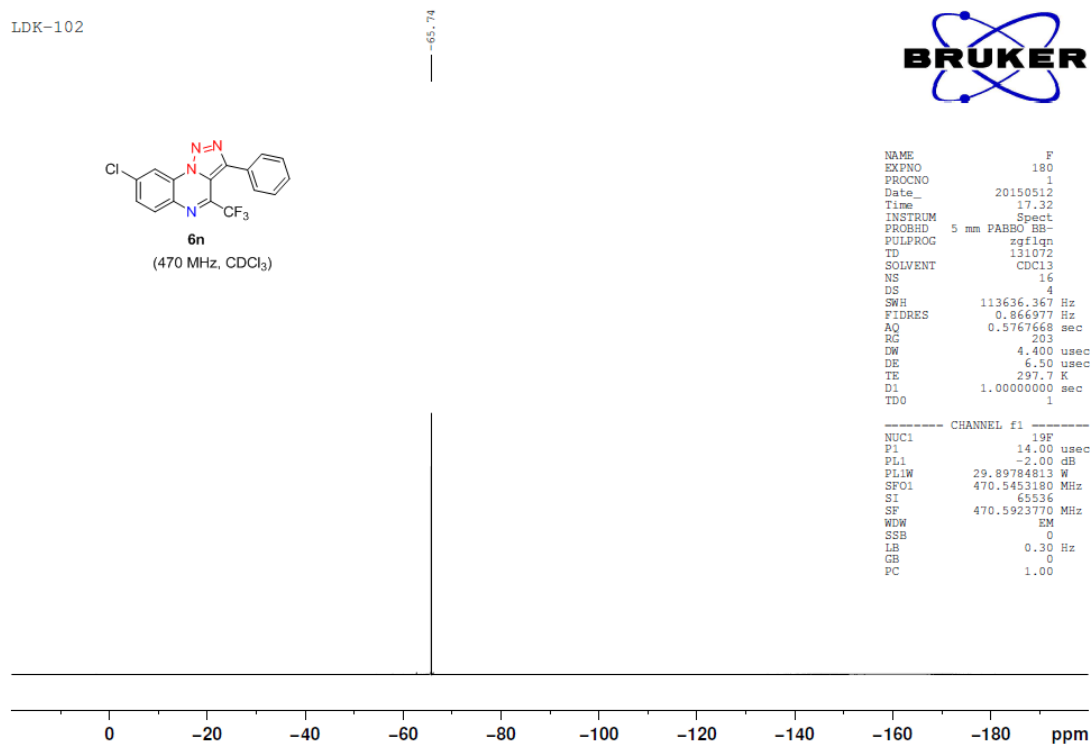
NAME h
EXPNO 47
PROCNO 1
Date_ 20150422
Time 22.49
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.151932 Hz
AQ 3.1719923 sec
RG 203
DW 48.400 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec
TD0 1

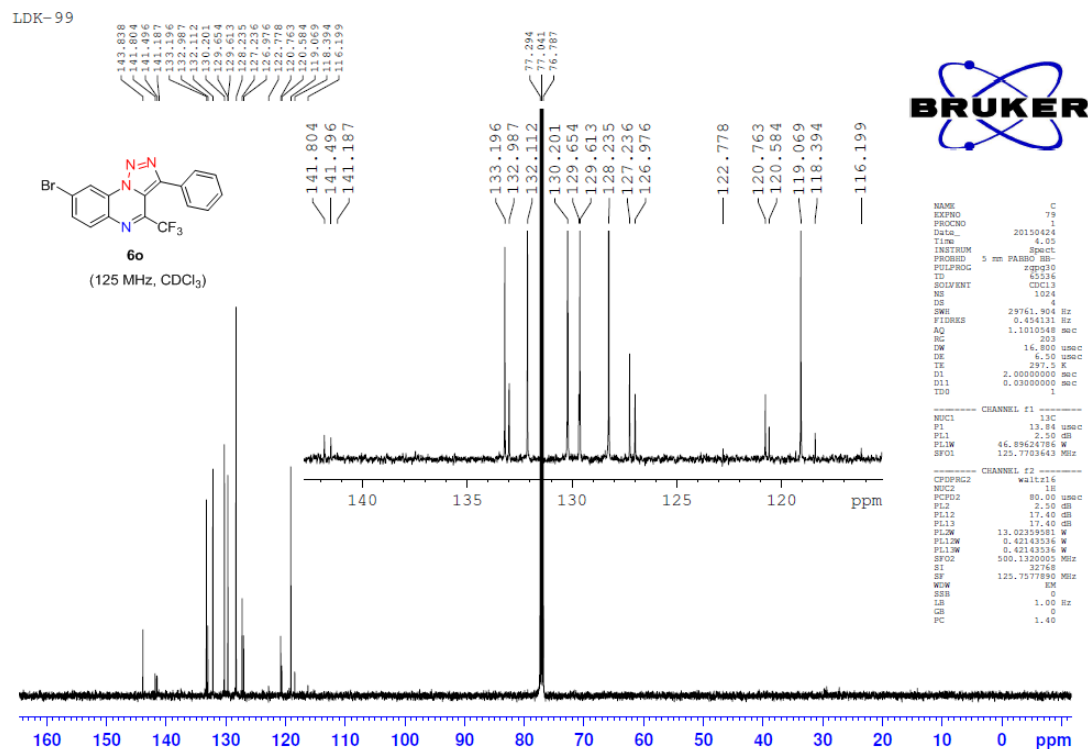
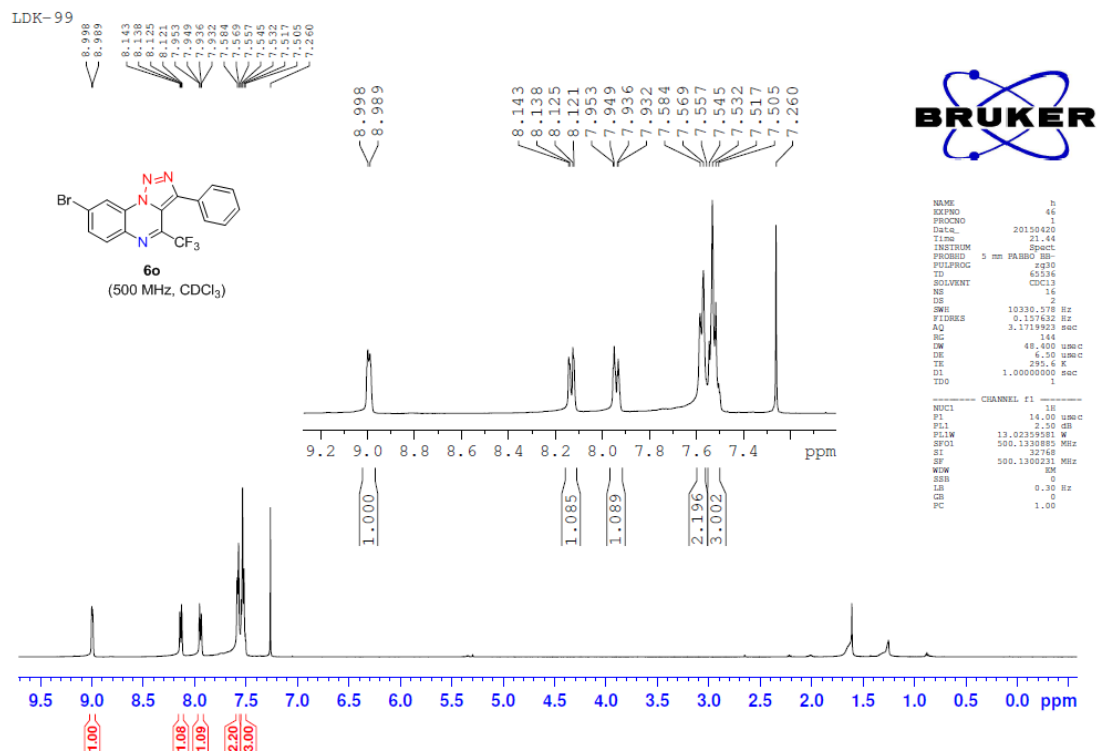
----- CHANNEL f1 -----
NUC1 1H
P1 14.00 usec
PL1 2.50 dB
PL1W 13.02359881 W
SFO1 500.130882 MHz
SI 32768
SF 500.1308823 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

LDK-102



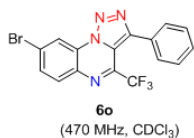
LDK-102





LDK-99

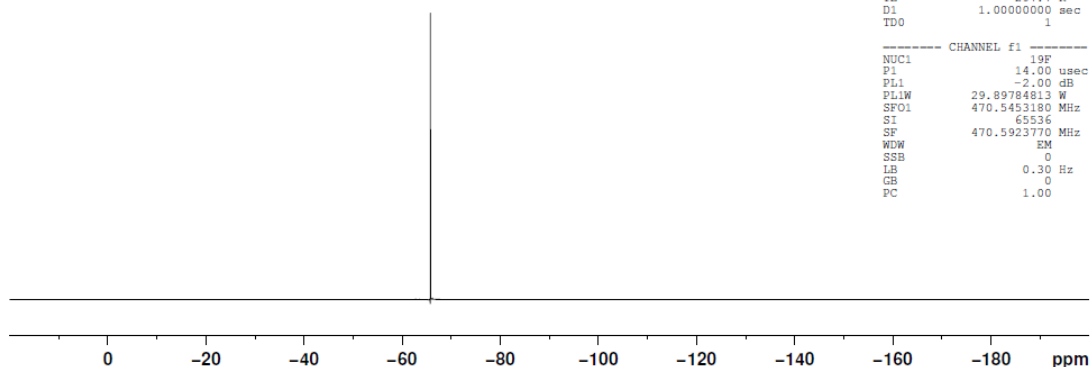
— 65.77



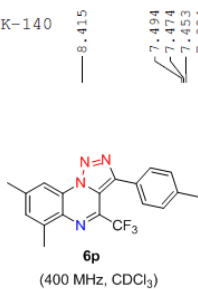
```

NAME          F
EXPNO         16
PROCNO        1
Date_         20150512
Time          17.22
INSTRUM       Spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            131072
SOLVENT       CDCl3
NS            16
DS            4
SWH           113636.367 Hz
FIDRES        0.866977 Hz
AQ            0.5767668 sec
RG            203
DW            4.400 usec
DE            6.50 usec
TE            297.7 K
D1            1.00000000 sec
TD0           1

----- CHANNEL f1 -----
NUC1          19F
P1            14.00 usec
PL1           -2.00 dB
PL1W          29.89784813 W
SFO1          470.5453180 MHz
SI            65536
SF            470.5923770 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```



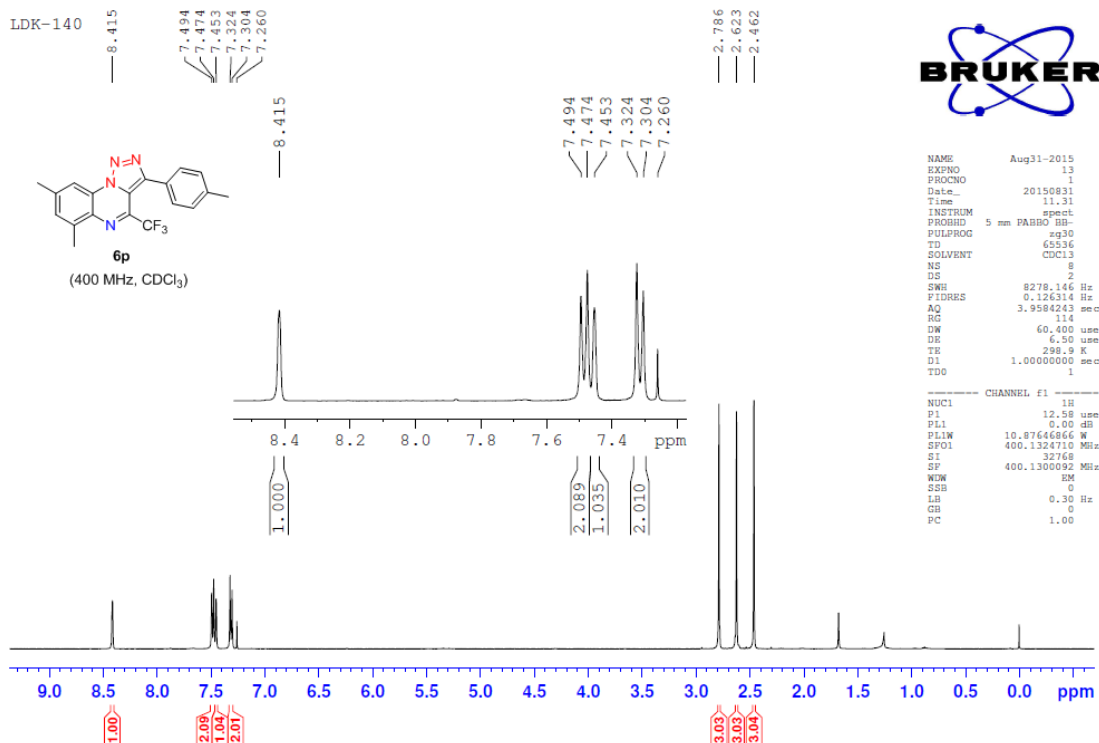
LDK-140

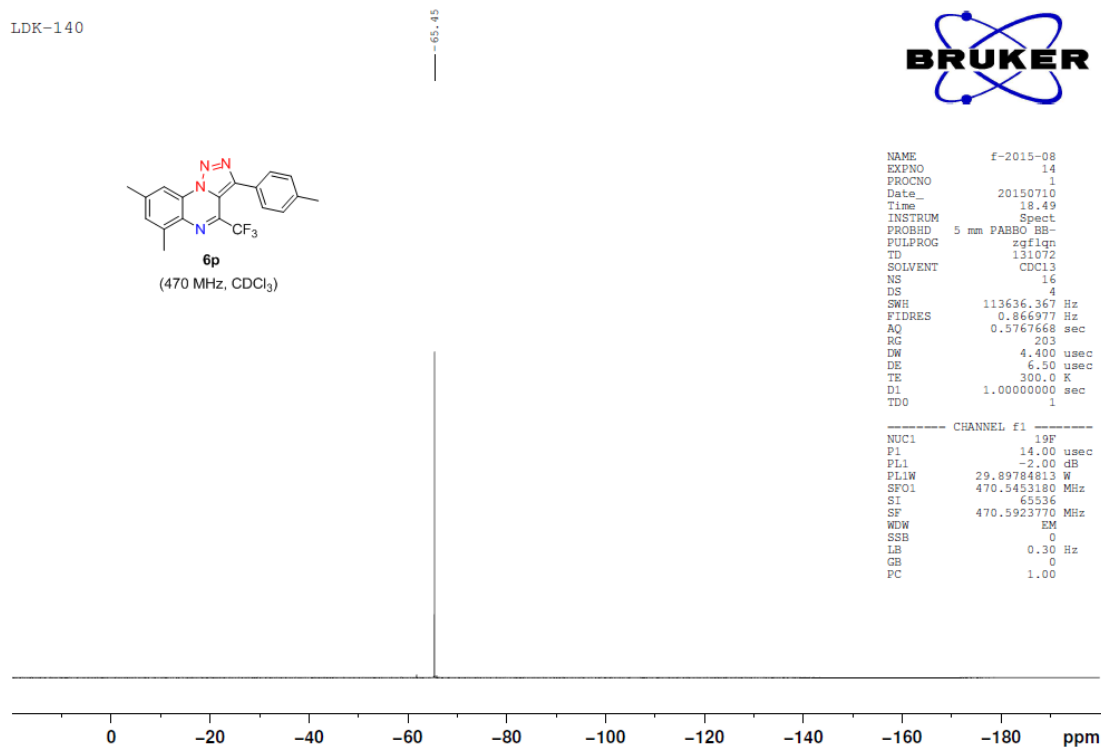
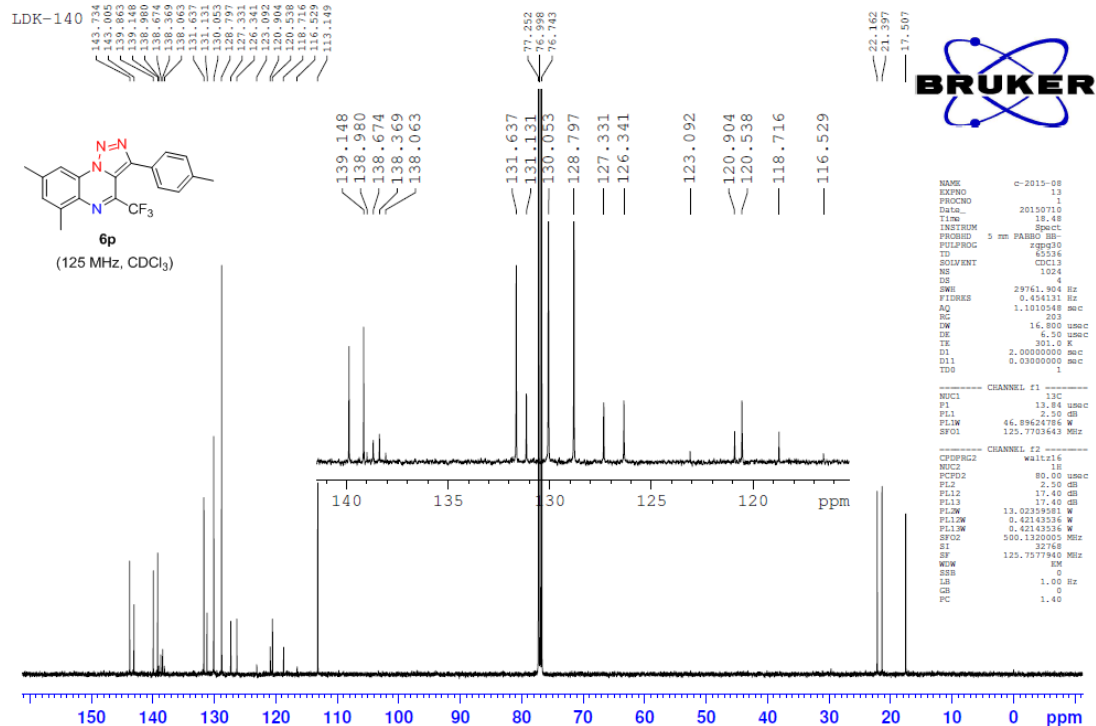


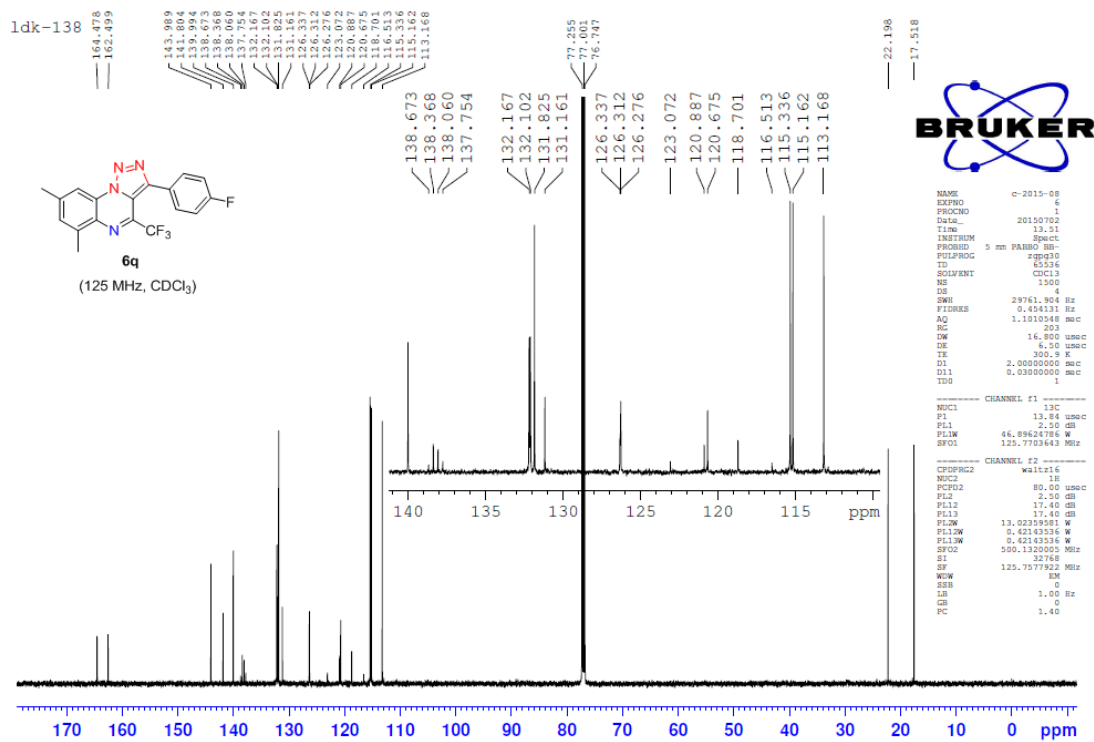
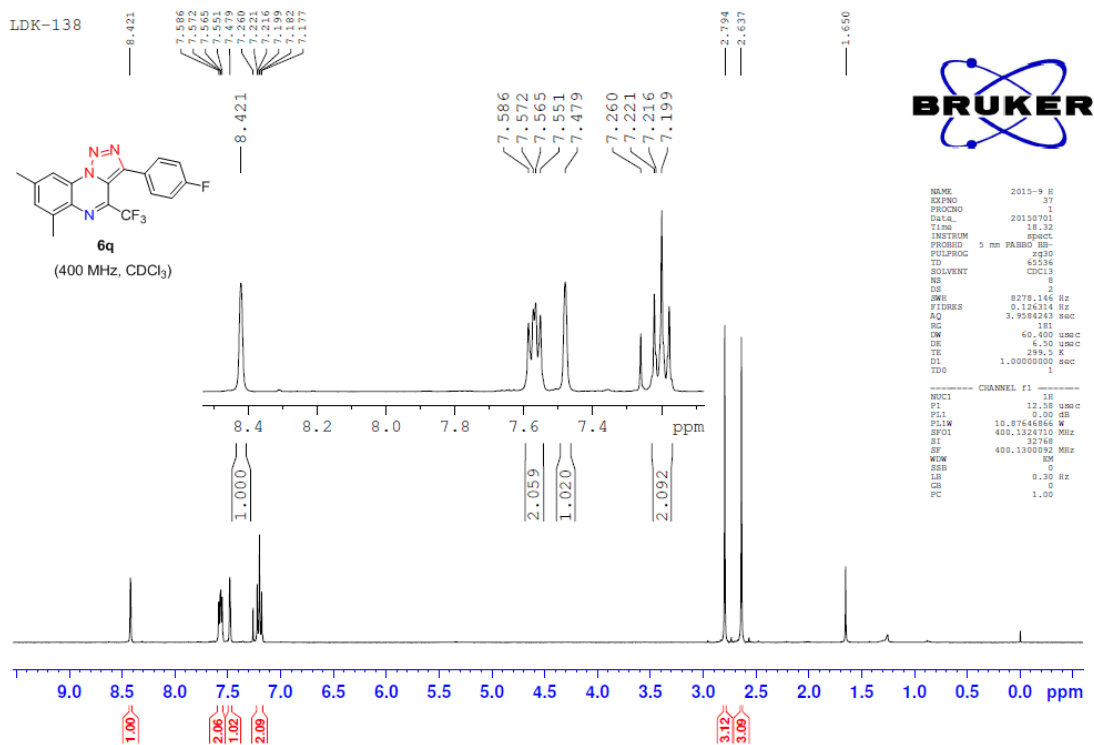
```

NAME          Aug31-2015
EXPNO         13
PROCNO        1
Date_         20150831
Time          11.31
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            8
DS            2
SWH           8278.146 Hz
FIDRES        0.126314 Hz
AQ            3.9584243 sec
RG            114
DW            60.400 usec
DE            6.50 usec
TE            298.9 K
D1            1.00000000 sec
TD0           1

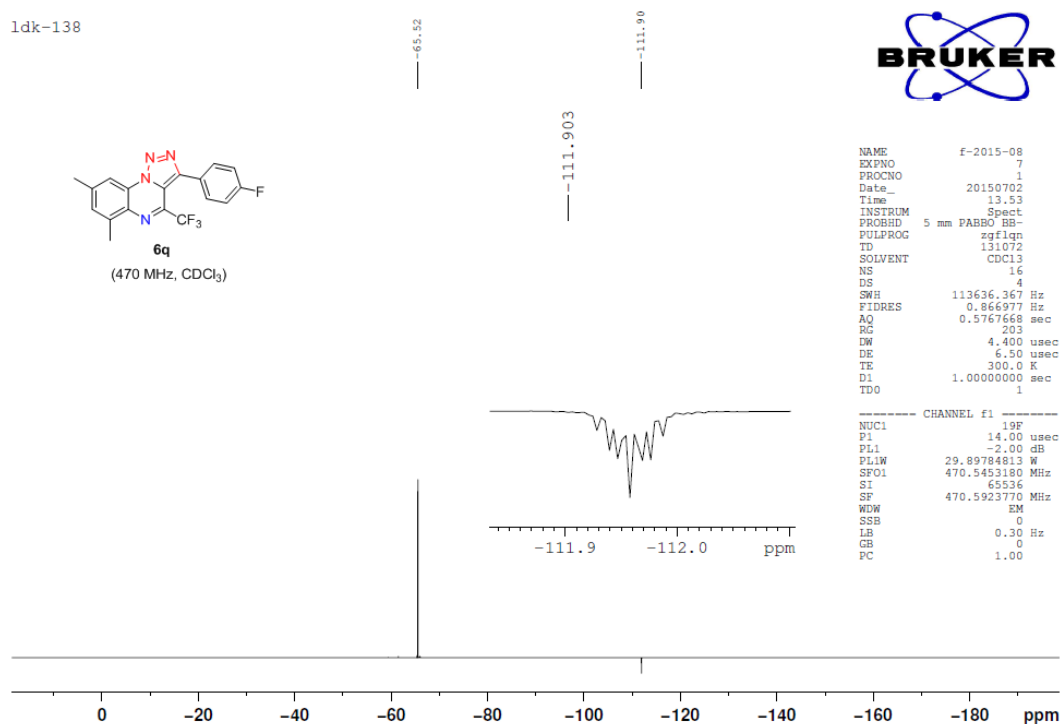
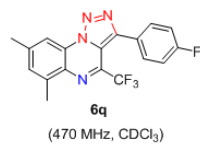
----- CHANNEL f1 -----
NUC1          1H
P1            12.58 usec
PL1           0.00 dB
PL1W          10.87646866 W
SFO1          400.1324710 MHz
SI            32768
SF            400.1300092 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```



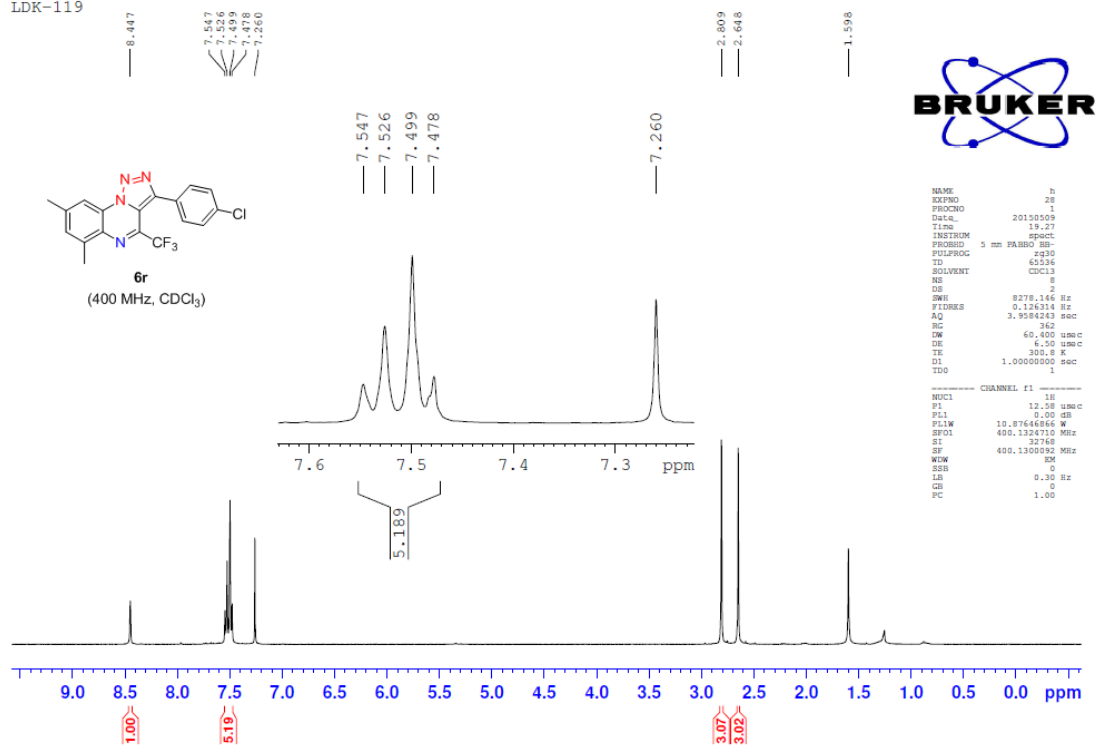
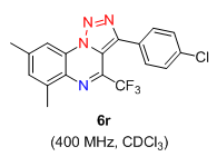


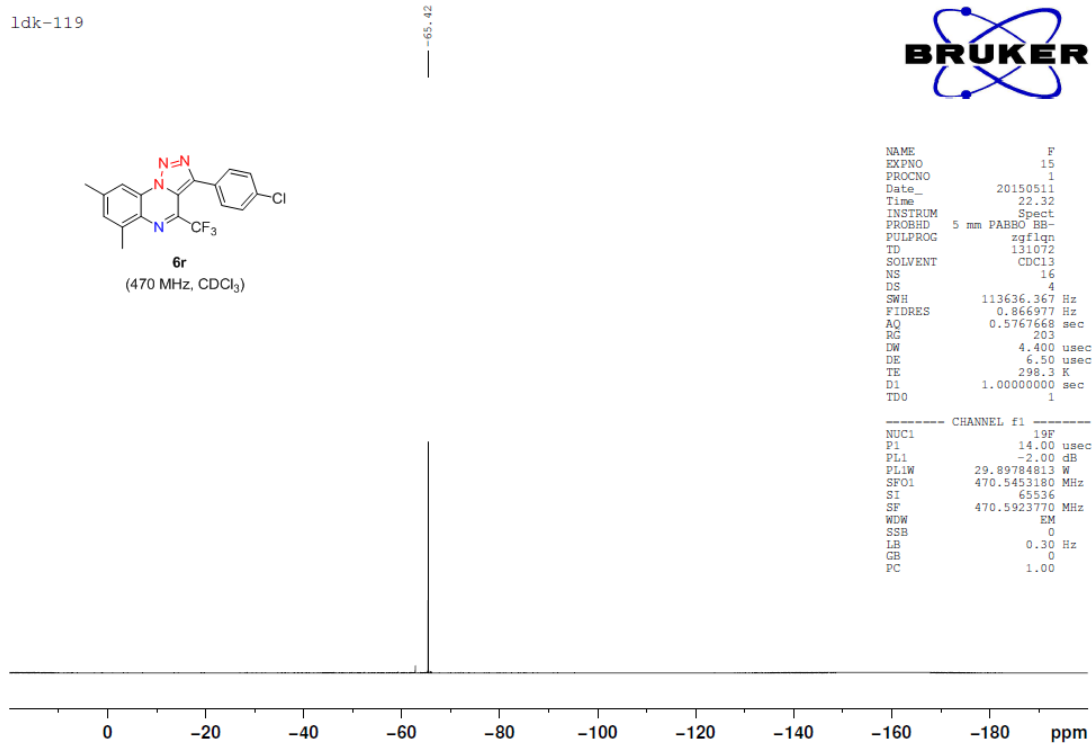
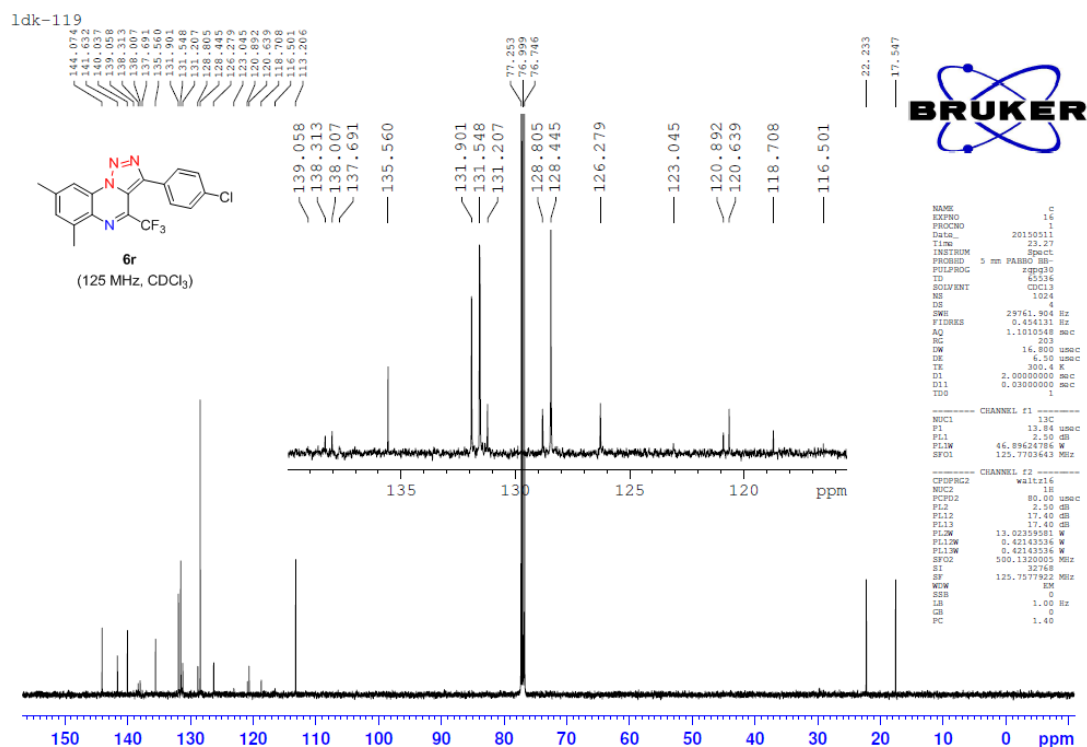


ldk-138

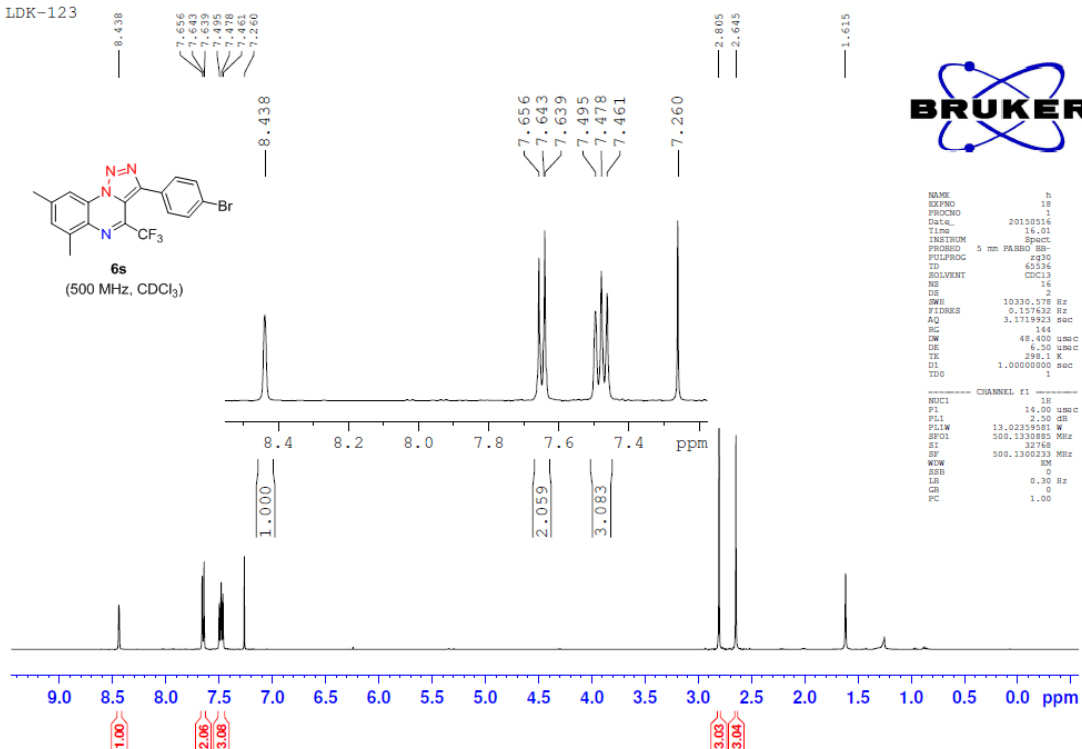


LDK-119





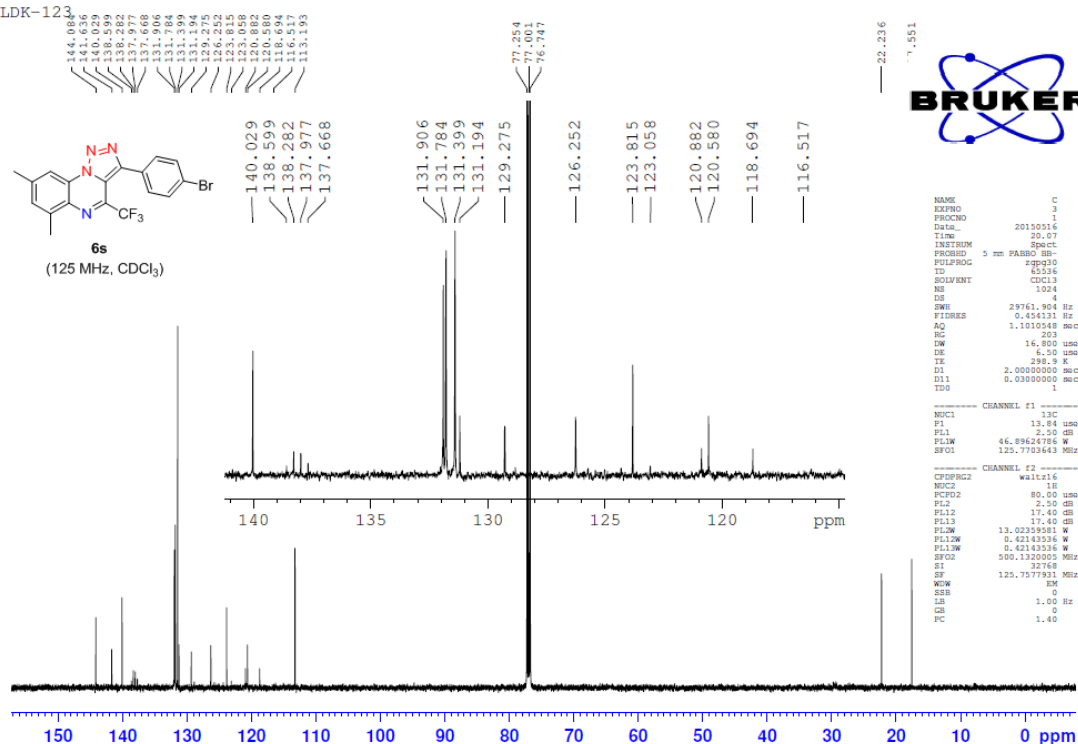
LDK-123



```

NAME      h
EXPNO     1
PROCNO    1
DATE_     20150516
TIME      16.01
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zgpg30
TD          65536
SOLVENT    CDCl3
NS          16
DS          2
SWH         10330.578 Hz
FIDRES     0.137432 Hz
AQ          3.1719923 sec
RG          144
IN          48.400 usec
DE          6.50 usec
TE          298.1 K
D1          1.00000000 sec
TDO         1
----- CHANNEL f1 -----
NUC1       13C
P1          14.00 usec
PL1         2.50 dB
PL1W       13.02359581 W
SFO1       500.1330885 MHz
SI          32768
SF          500.1330233 MHz
WDW         EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.00
  
```

LDK-123

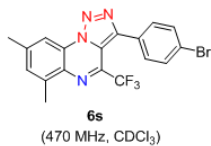


```

NAME      c
EXPNO     3
PROCNO    1
DATE_     20150516
TIME      20.07
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zgpg30
TD          65536
SOLVENT    CDCl3
NS          1024
DS          2
SWH         29761.904 Hz
FIDRES     0.454131 Hz
AQ          1.1010548 sec
RG          16
IN          16.800 usec
DE          6.50 usec
TE          298.9 K
D1          2.00000000 sec
D11         0.03000000 sec
TDO         1
----- CHANNEL f1 -----
NUC1       13C
P1          13.84 usec
PL1         2.50 dB
PL1W       46.89624786 W
SFO1       125.7703643 MHz
----- CHANNEL f2 -----
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2         2.50 dB
PL2W       17.40 dB
PL3         13.02359581 W
PL1W       0.42143336 W
PL3W       0.42143336 W
SFO2       500.1330233 MHz
SI          32768
SF          125.7577931 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
  
```

LDK-123

-65.39

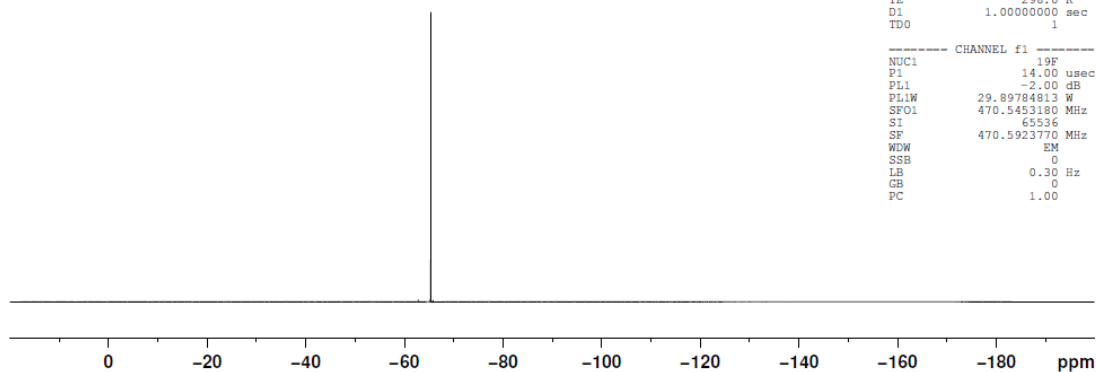


```

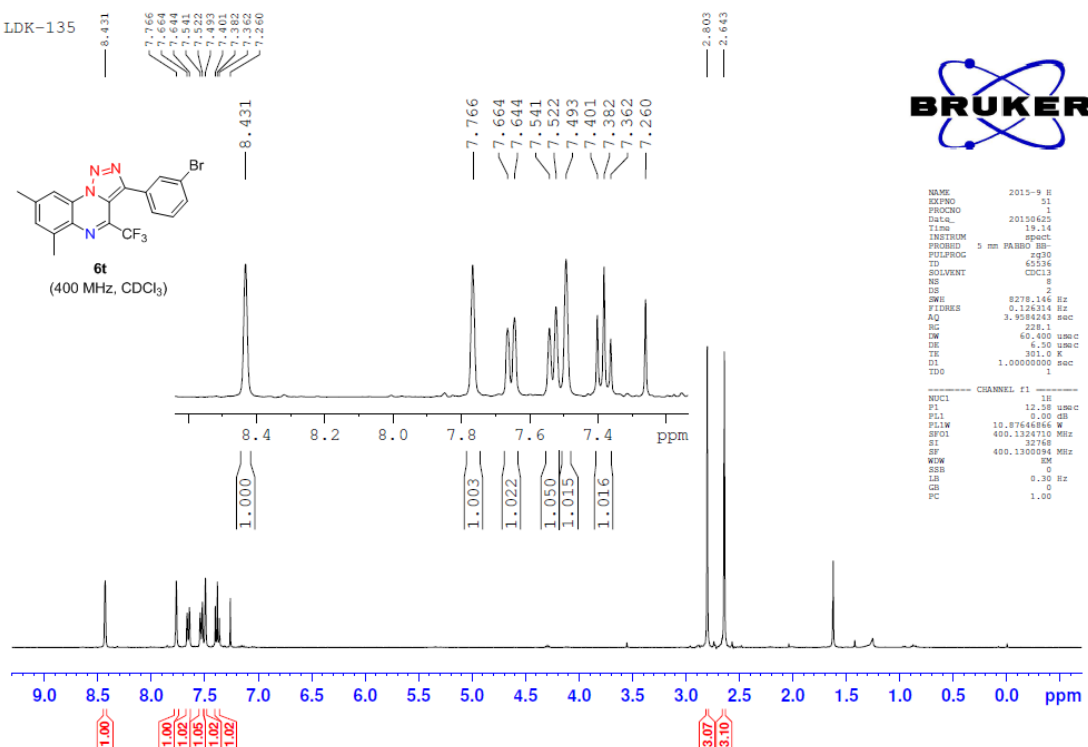
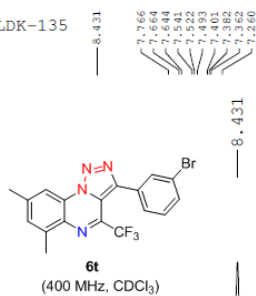
NAME          f
EXPNO         2
PROCNO        1
Date_         20150516
Time          19.11
INSTRUM       Spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            131072
SOLVENT       CDCl3
NS            16
DS            4
SWH           113636.367 Hz
FIDRES        0.866977 Hz
AQ            0.5767668 sec
RG            203
DW            4.400 usec
DE            6.50 usec
TE            298.0 K
D1            1.00000000 sec
TD0           1

----- CHANNEL f1 -----
NUC1          19F
P1            14.00 usec
PL1           -2.00 dB
PL1W          29.89784813 W
SFO1          470.5453180 MHz
SI            65536
SF            470.5923770 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```



LDK-135

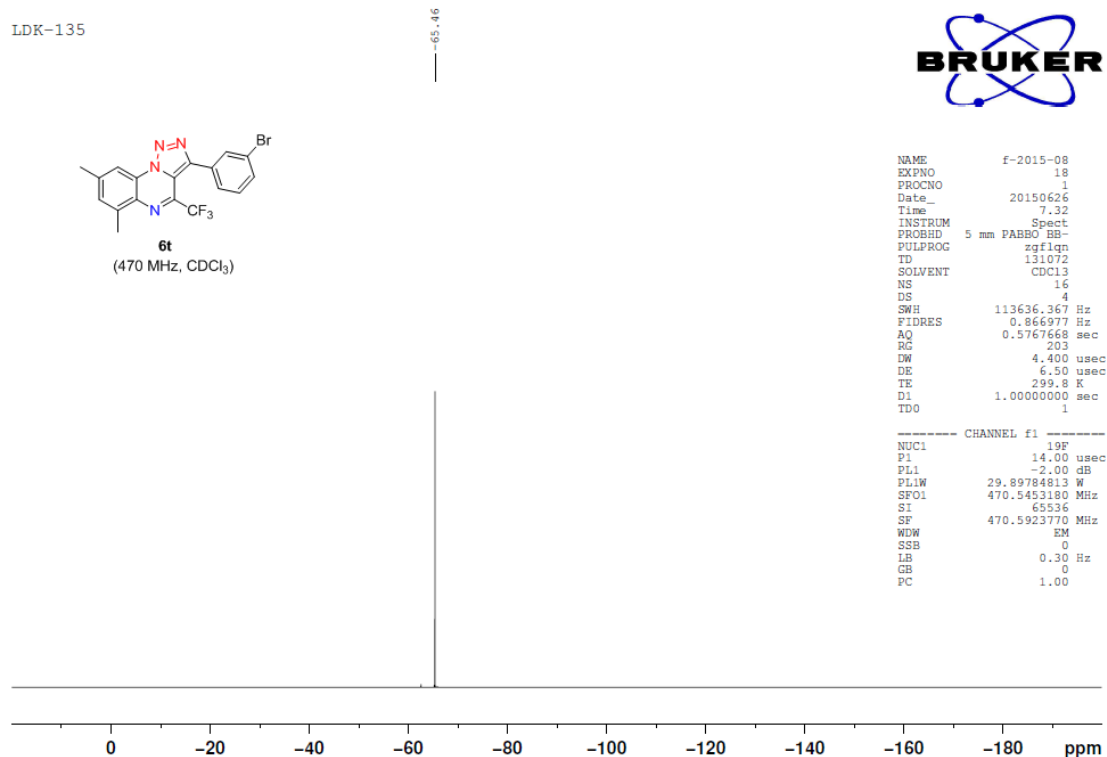
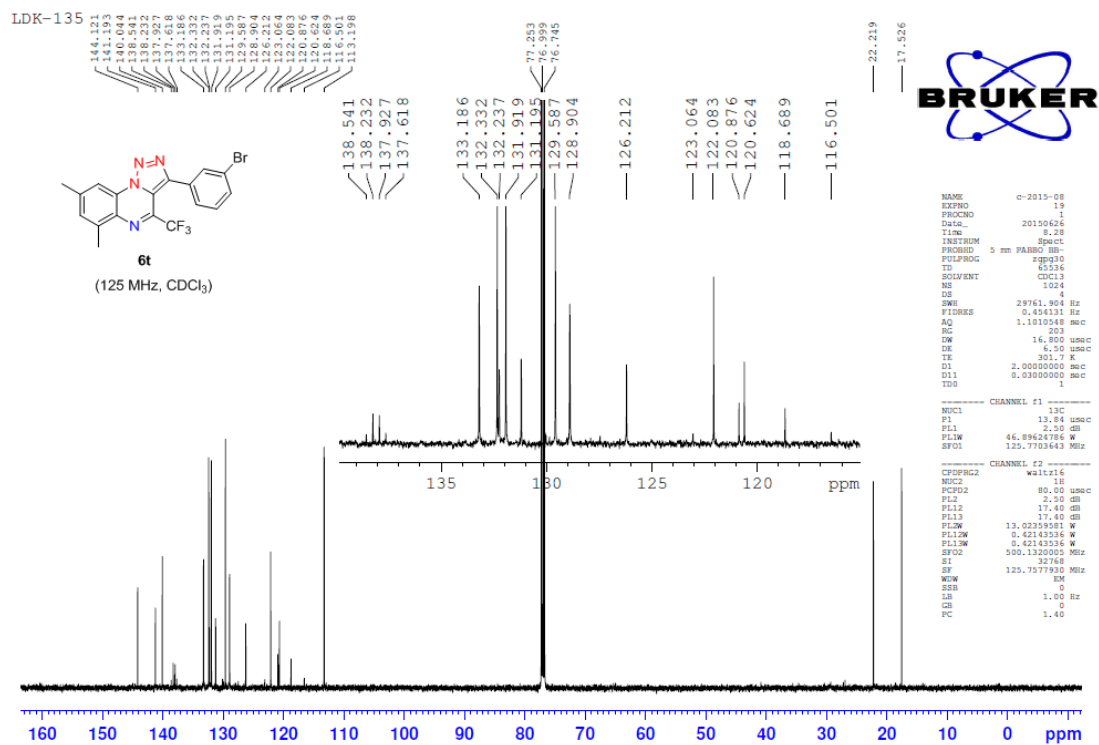


```

NAME          2015-9-8
EXPNO         51
PROCNO        1
Date_         20150625
Time          19.14
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            8
DS            2
SWH           8278.146 Hz
FIDRES        0.126314 Hz
AQ            3.8082823 sec
RG            228.1
DW            60.400 usec
DE            6.50 usec
TE            301.0 K
D1            1.00000000 sec
TD0           1

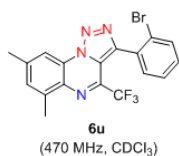
----- CHANNEL f1 -----
NUC1          1H
P1            12.50 usec
PL1           0.00 dB
PL1W          10.87646866 W
SFO1          400.1324710 MHz
SI            32768
SF            400.1300894 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```



ldk-137

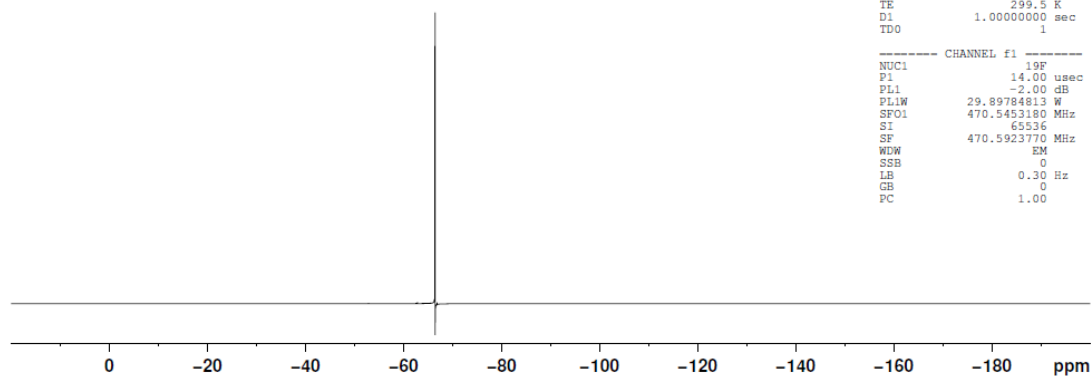
— 66.43



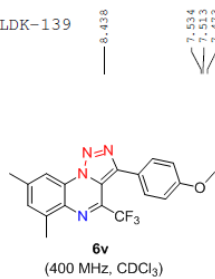
```

NAME      f-2015-08
EXPNO     29
PROCNO    1
Date_     20150702
Time      6.37
INSTRUM    Spect
PROBHD     5 mm PABBO BB-
PULPROG    zgpg30
TD         131072
SOLVENT    CDCl3
NS         16
DS         4
SWH        113636.367 Hz
FIDRES     0.866977 Hz
AQ         0.5767668 sec
RG         203
DE         4.400 usec
TE         299.5 K
D1         1.00000000 sec
TD0        1
----- CHANNEL f1 -----
NUC1       19F
P1         14.00 usec
PL1        -2.00 dB
PL1W       29.89784813 W
SFO1       470.5453180 MHz
SI         65536
SF         470.5923770 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

```



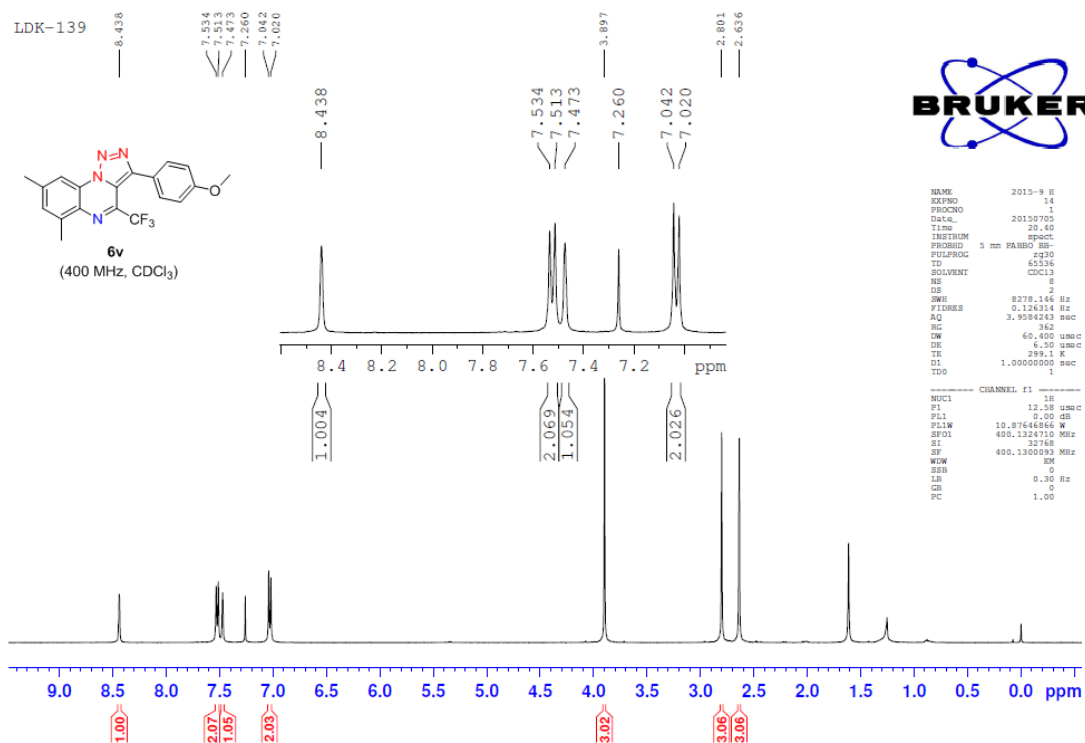
LDK-139

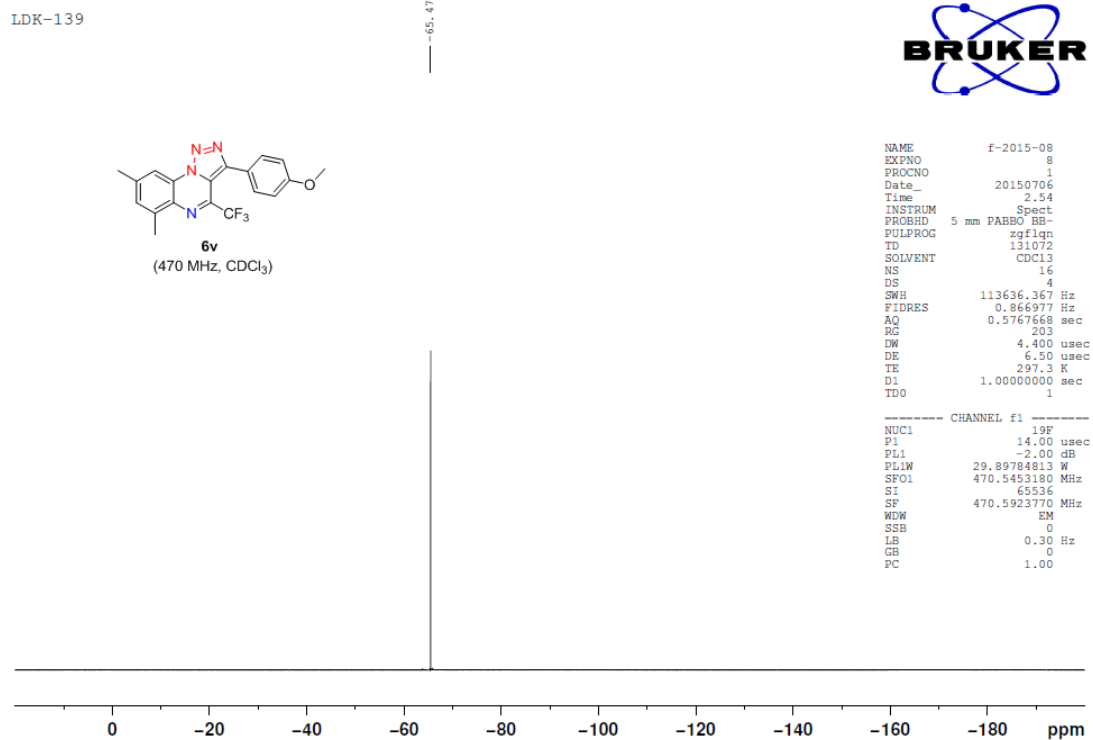
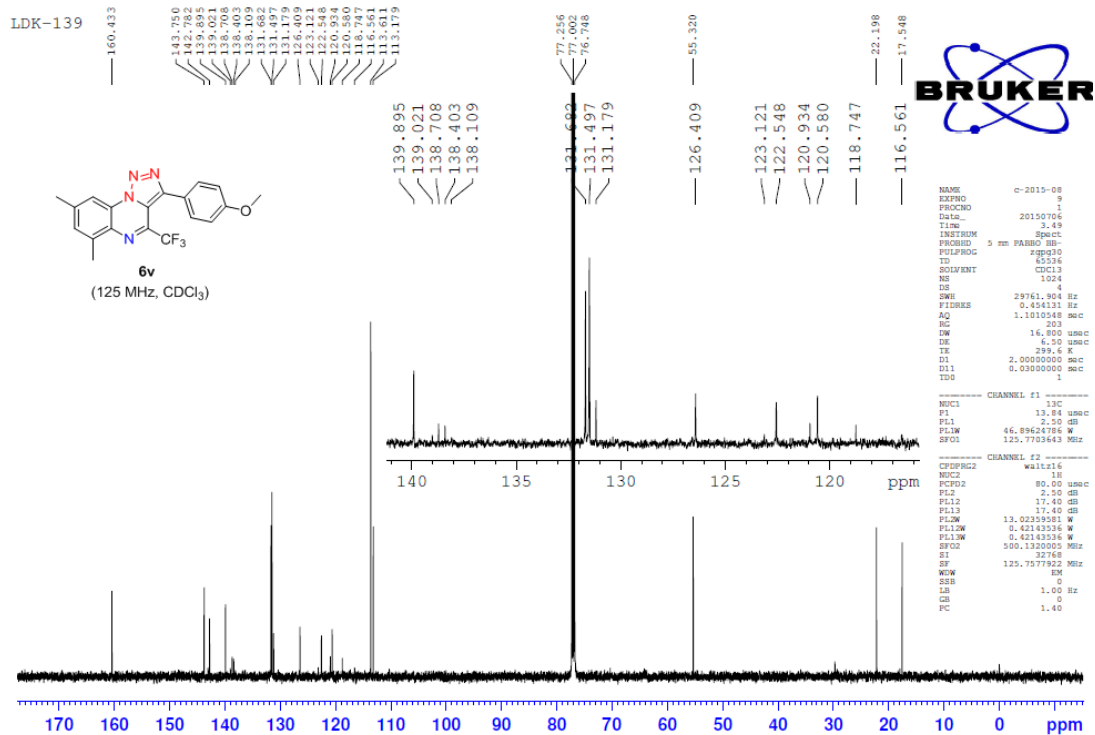


```

NAME      2015-9-8
EXPNO     14
PROCNO    1
Date_     20150705
Time      20.40
INSTRUM    5 mm PABBO BB-
PROBHD     5 mm PABBO BB-
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         8
DS         2
SWH        8278.146 Hz
FIDRES     0.126314 Hz
AQ         3.9284243 sec
RG         362
DE         60.000 usec
TE         299.1 K
D1         1.00000000 sec
TD0        1
----- CHANNEL f1 -----
NUC1       1H
P1         12.58 usec
PL1        0.00 dB
PL1W       10.87646486 W
SFO1       400.1324710 MHz
SI         32768
SF         400.1300933 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

```

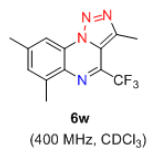




LDK-131-02

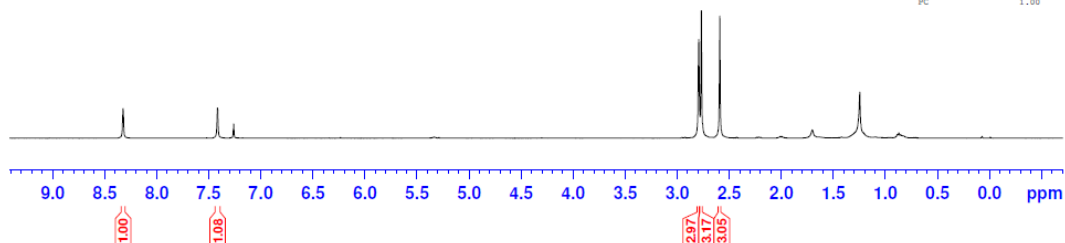
8.322
7.415
7.260

2.794
2.768
2.591

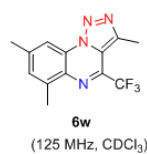


NAME 2015-9 H
EXPNO 43
PROCNO 1
Date_ 20150616
Time 16:12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126316 Hz
AQ 3.9584243 sec
RG 181
DW 60.400 usec
DE 6.50 usec
TE 300.2 K
D1 1.00000000 sec
TD0

CHANNEL f1
NUC1 13
P1 12.00 usec
PL1 0.00 dB
PL1W 10.8764846 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



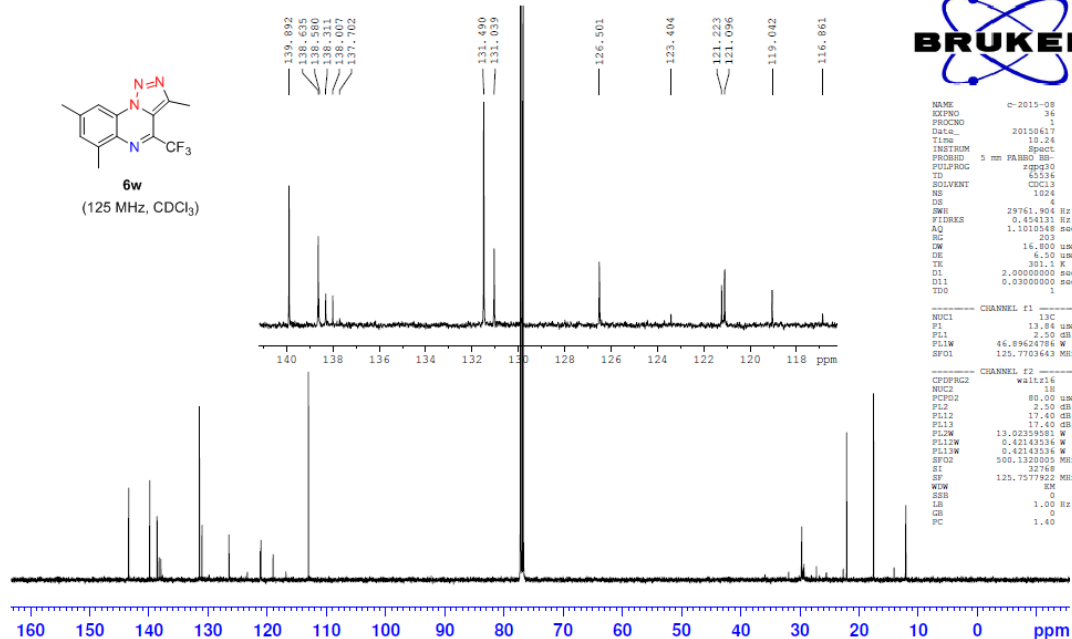
LDK-131-02



NAME c-2015-08
EXPNO 16
PROCNO 1
Date_ 20150617
Time 17:14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.900 usec
DE 6.50 usec
TE 301.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

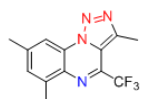
CHANNEL f1
NUC1 13C
P1 13.84 usec
PL1 2.50 dB
PL1W 46.89624786 W
SFO1 125.7703643 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 13
PCPD2 80.00 usec
PL2 2.50 dB
PL2W 17.40 dB
PL13 17.40 dB
PL12W 13.02339351 W
PL12W 0.42143336 W
PL12W 0.42143336 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577852 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



LDK-131

— 66.72

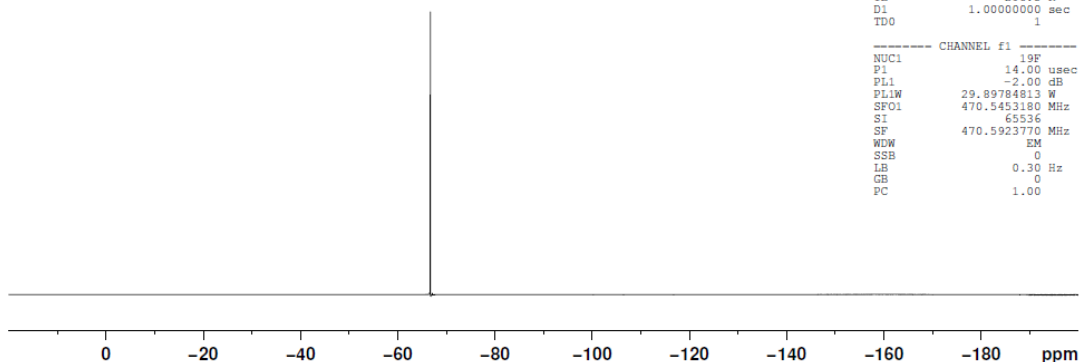


6w
(470 MHz, CDCl₃)

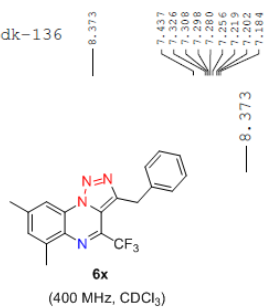
```

NAME      f-2015-08
EXPNO     11
PROCNO    1
Date_     20150608
Time      2.36
INSTRUM   Spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         131072
SOLVENT   CDCl3
NS         16
DS         4
SWH        113636.367 Hz
FIDRES     0.866977 Hz
AQ         0.5767668 sec
RG         203
DW         4.400 usec
DE         6.50 usec
TE         298.3 K
D1         1.00000000 sec
TD0        1

----- CHANNEL f1 -----
NUC1       13C
P1         14.00 usec
PL1        -2.00 dB
PL1W       29.89784813 W
SFO1       470.5453180 MHz
SI         65536
SF         470.5923770 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



ldk-136



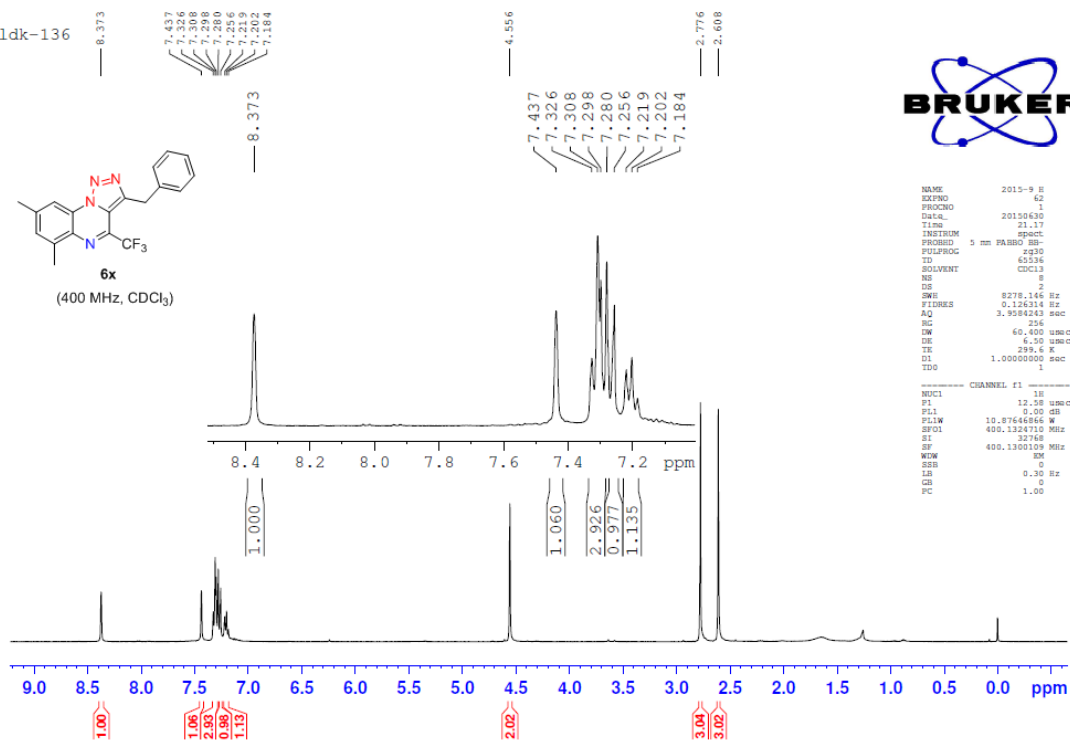
6x
(400 MHz, CDCl₃)

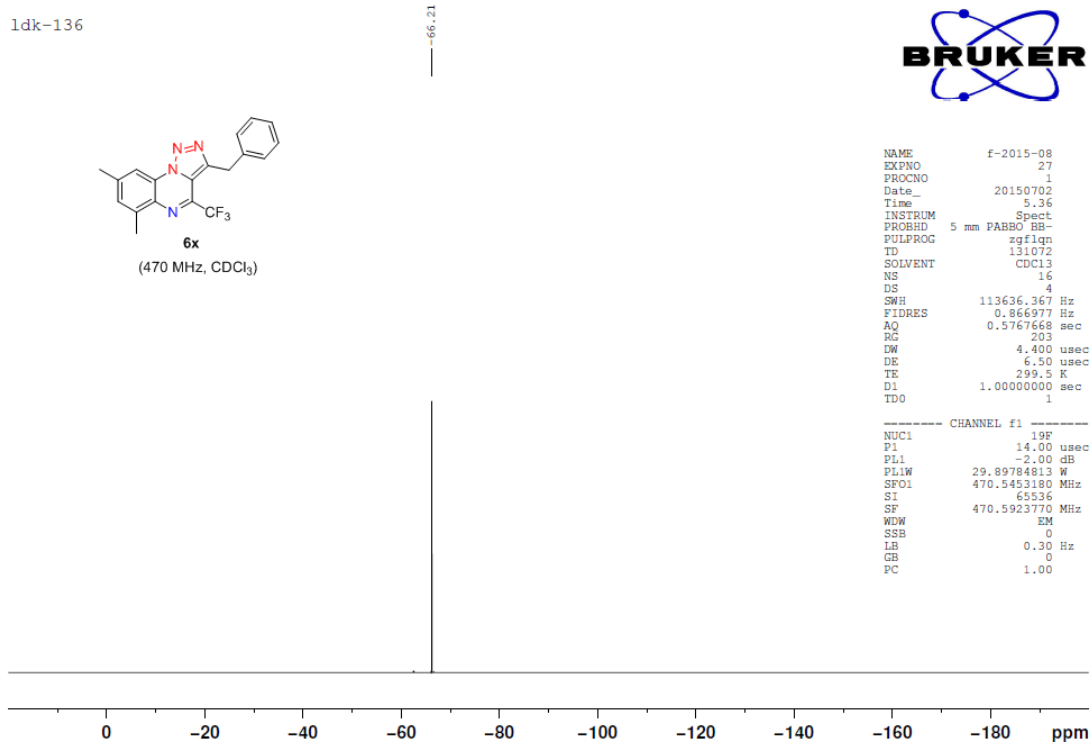
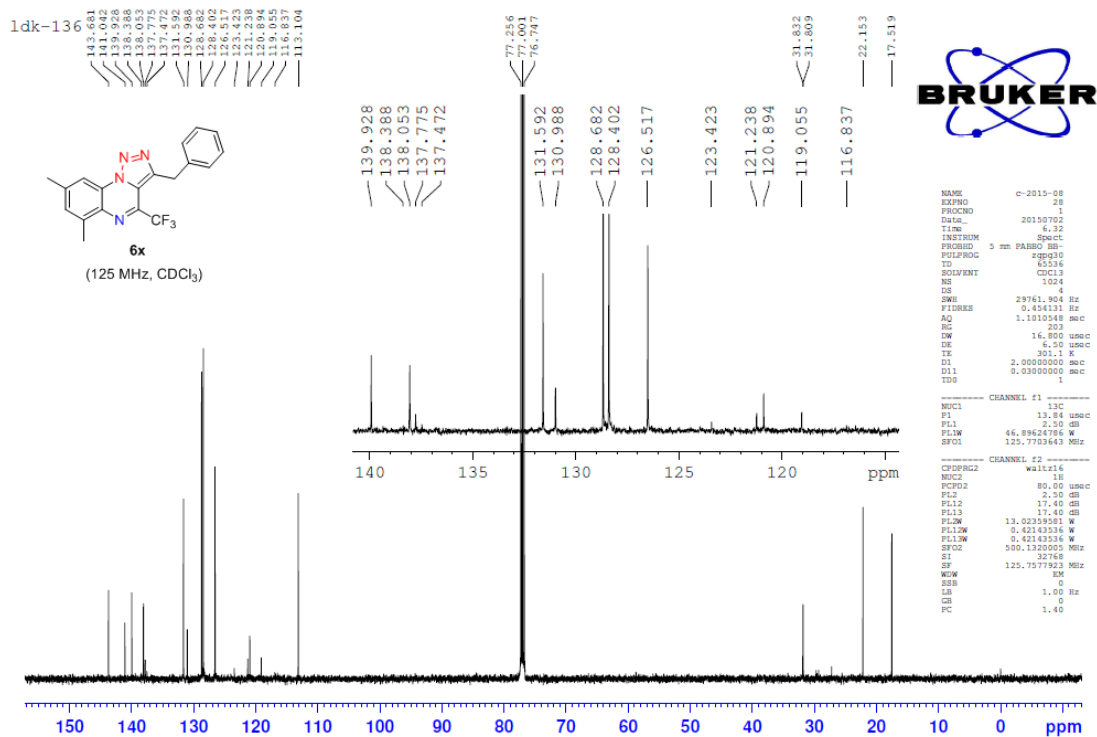


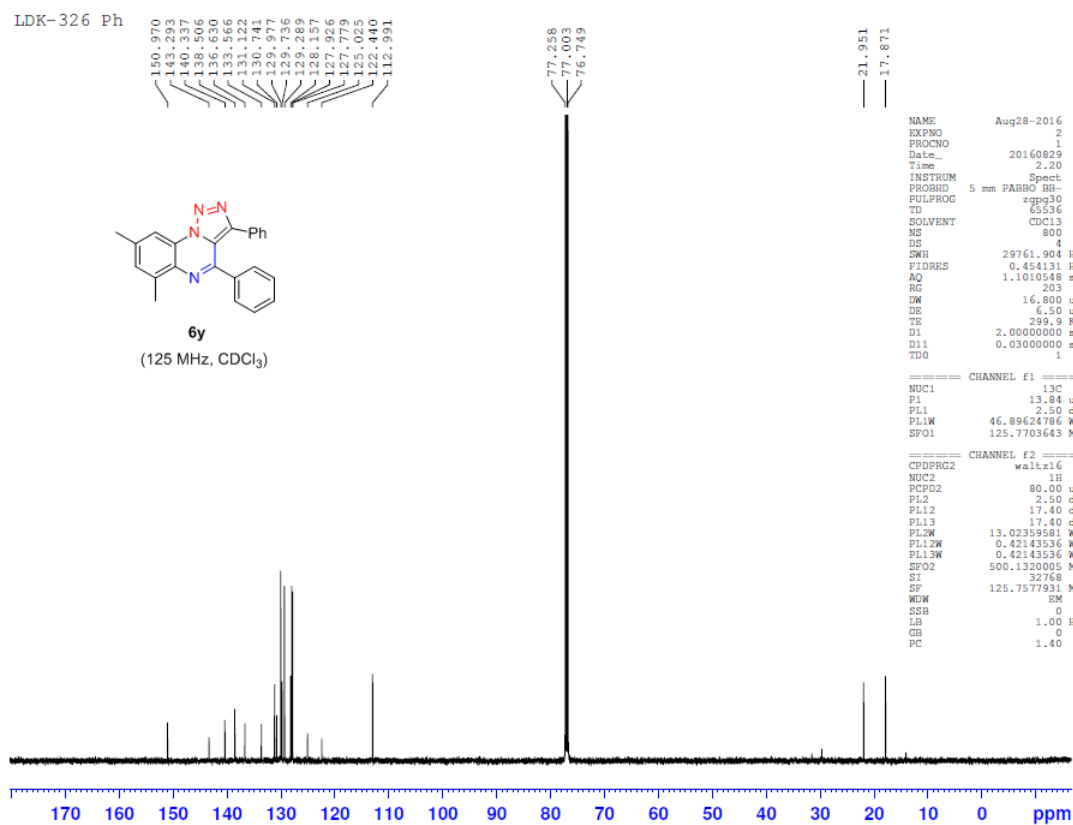
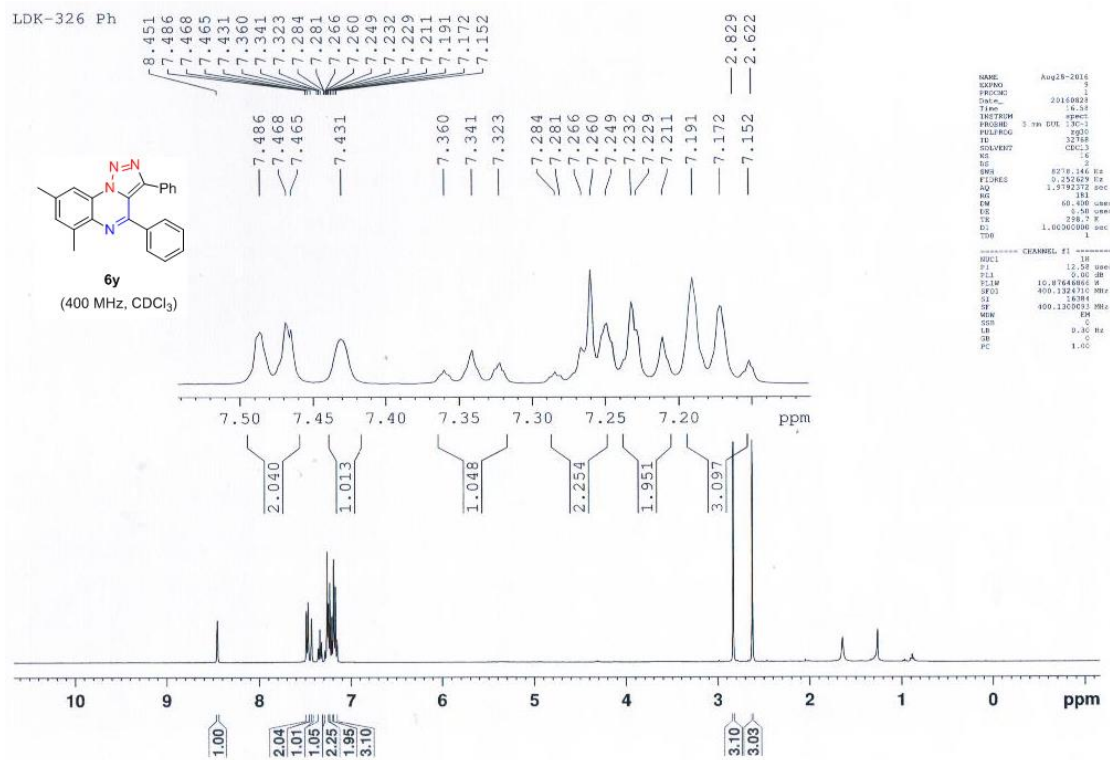
```

NAME      2015-9-8
EXPNO     62
PROCNO    1
Date_     20150630
Time      21.17
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         2
SWH        8278.146 Hz
FIDRES     0.125214 Hz
AQ         3.9584243 sec
RG         256
DW         60.600 usec
DE         6.50 usec
TE         298.4 K
D1         1.00000000 sec
TD0        1

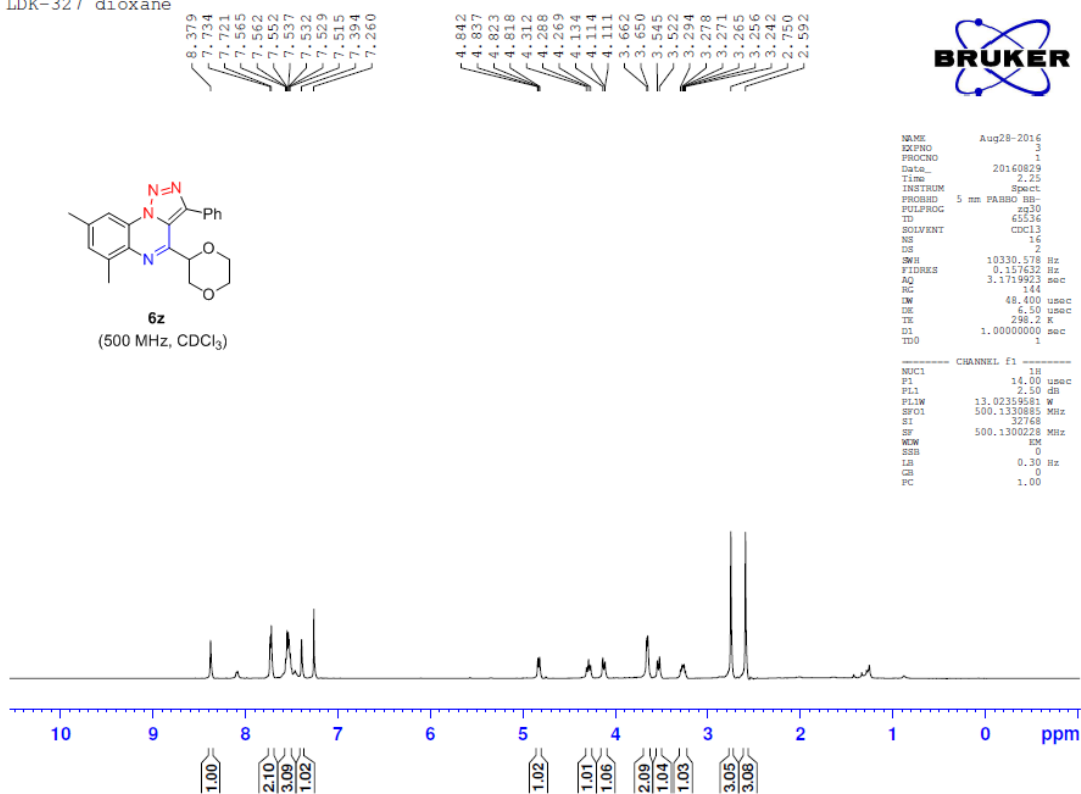
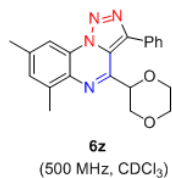
----- CHANNEL f1 -----
NUC1       1H
P1         12.50 usec
PL1        0.00 dB
PL1W       10.87644886 W
SFO1       400.1304710 MHz
SI         32768
SF         400.1300109 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```







LDK-327 dioxane

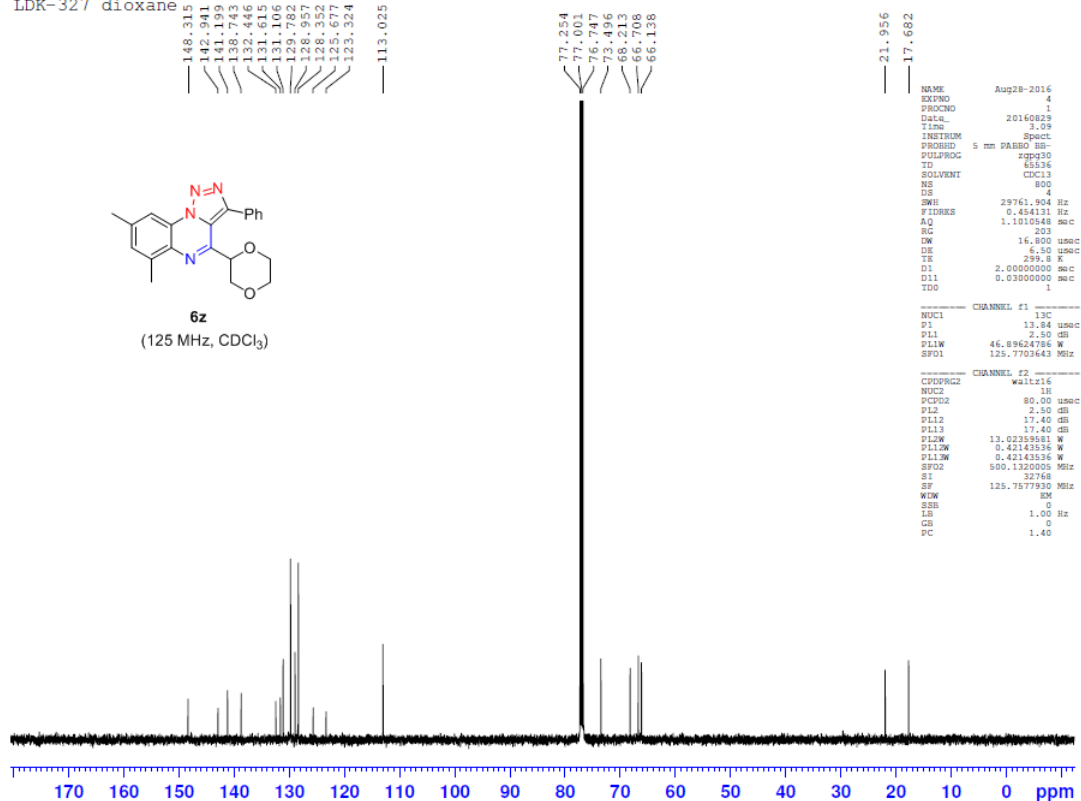
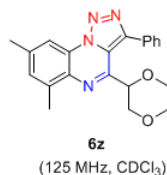


```

NAME      Aug28-2016
EXPNO     3
PROCNO    1
Date_     20160829
Time      2.25
INSTRUM   Spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.151632 Hz
AQ         3.1719923 sec
RG         144
IN         48.400 usec
DE         6.50 usec
TE         298.2 K
D1         1.00000000 sec
D11        1
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         14.00 usec
PL1        2.50 dB
PL1W       13.02339581 W
SFO1       500.1330881 MHz
SI         32768
SF         500.1300223 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

LDK-327 dioxane



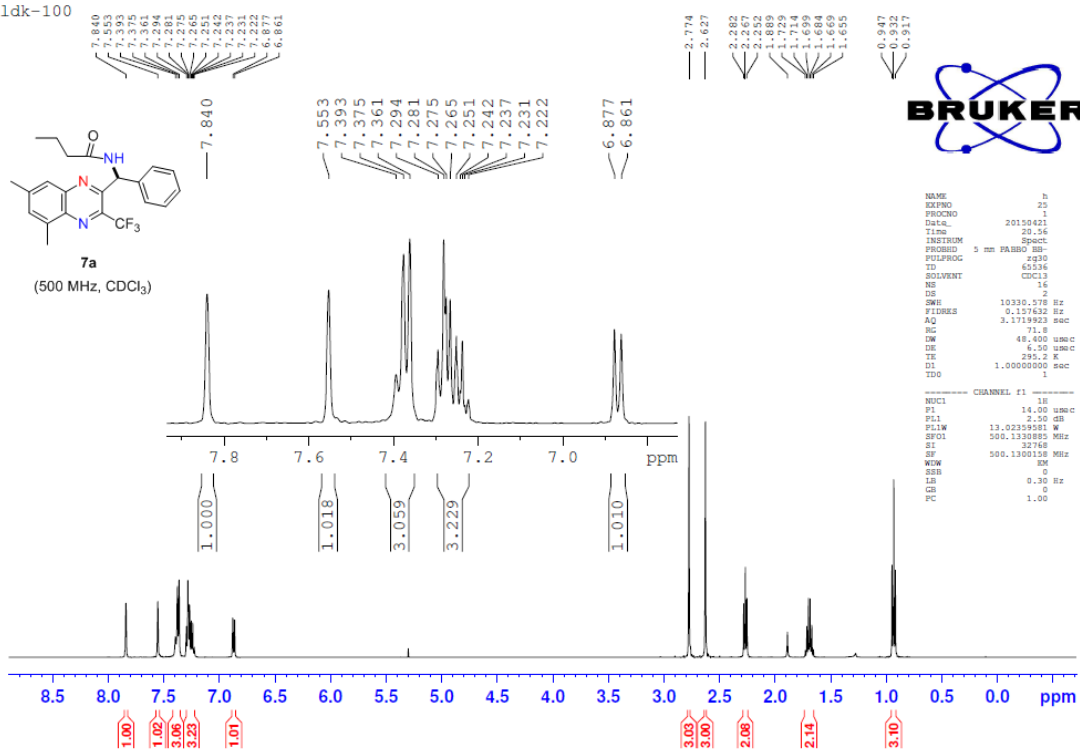
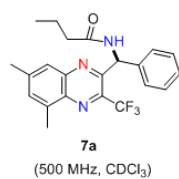
```

NAME      Aug28-2016
EXPNO     4
PROCNO    1
Date_     20160829
Time      3.09
INSTRUM   Spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         4
SWH        29761.904 Hz
FIDRES     0.404131 Hz
AQ         1.1010548 sec
RG         103
IN         16.800 usec
DE         6.50 usec
TE         298.2 K
D1         2.00000000 sec
D11        1
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         13.84 usec
PL1        2.50 dB
PL1W       46.89624786 W
SFO1       125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
PL2       2.50 dB
PL12      17.40 dB
PL13      17.40 dB
PL1W      13.02339581 W
PL12W     0.42143536 W
PL13W     0.42143536 W
SFO2      500.1320005 MHz
SI         32768
SF         125.7577930 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

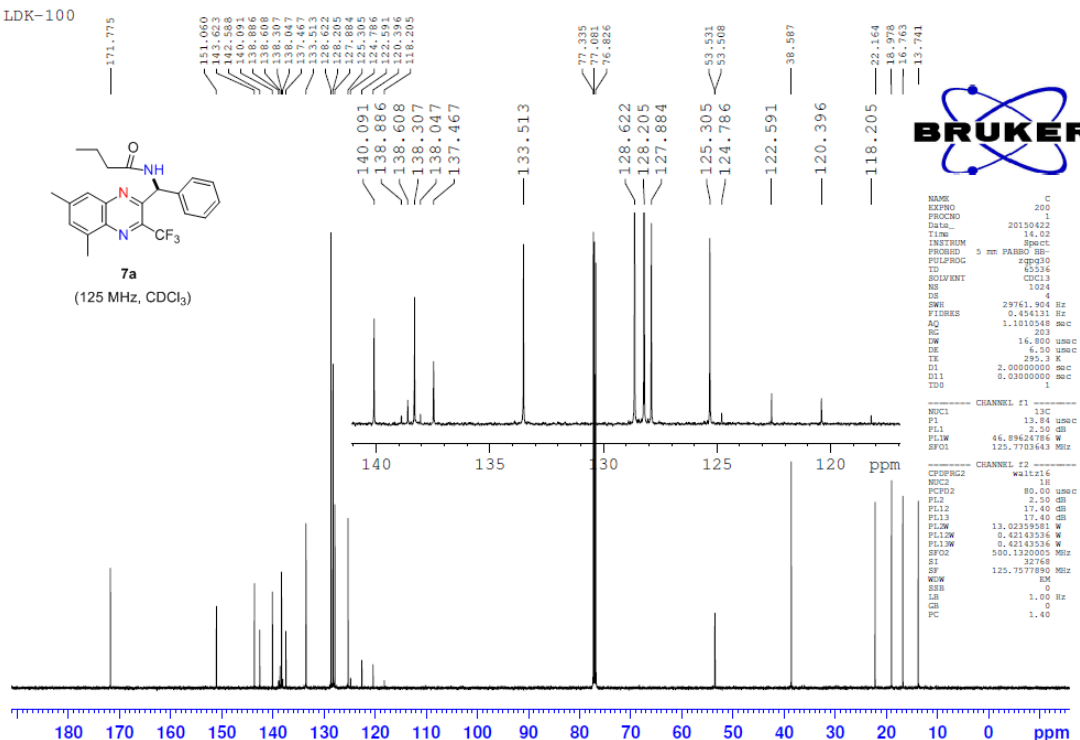
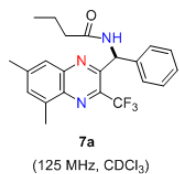
ldk-100



NAME h
EXPNO 25
PROCNO 1
Date_ 20150421
Time 22.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157432 Hz
AQ 3.1719923 sec
RG 71.8
RW 48.400 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TD0

CHANNEL f1
NUC1 1H
P1 14.00 usec
PL1 2.50 dB
PL1W 13.02359581 W
SFO1 500.1330892 MHz
SI 32768
SF 500.1330892 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

LDK-100



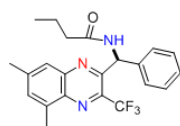
NAME C
EXPNO 200
PROCNO 1
Date_ 20150421
Time 14.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 1024
DS 2
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010342 sec
RG 203
RW 16.800 usec
DE 6.50 usec
TE 295.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0

CHANNEL f1
NUC1 13C
P1 13.00 usec
PL1 2.50 dB
PL1W 46.89424784 W
SFO1 125.7703441 MHz

CHANNEL f2
waitz16
NUC2 1H
PCPD2 80.00 usec
P2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL1W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1330892 MHz
SI 32768
SF 125.7577892 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

LDK-100

-63.22



7a
(470 MHz, CDCl₃)

```

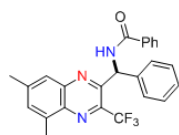
NAME          F
EXPNO         30
PROCNO        1
Date_         20150506
Time_         21.19
INSTRUM       Spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            131072
SOLVENT       CDCl3
NS            16
DS            4
SWH           113636.367 Hz
FIDRES        0.866977 Hz
AQ            0.5767668 sec
RG            203
DW            4.400 usec
DE            6.50 usec
TE            296.4 K
D1            1.0000000 sec
TD0           1
  
```

```

----- CHANNEL f1 -----
NUC1          19F
P1            14.00 usec
PL1           -2.00 dB
PL1W          29.89784813 W
SFO1          470.5453180 MHz
SI            65536
SF            470.5923770 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

LDK-105



7b
(500 MHz, CDCl₃)



```

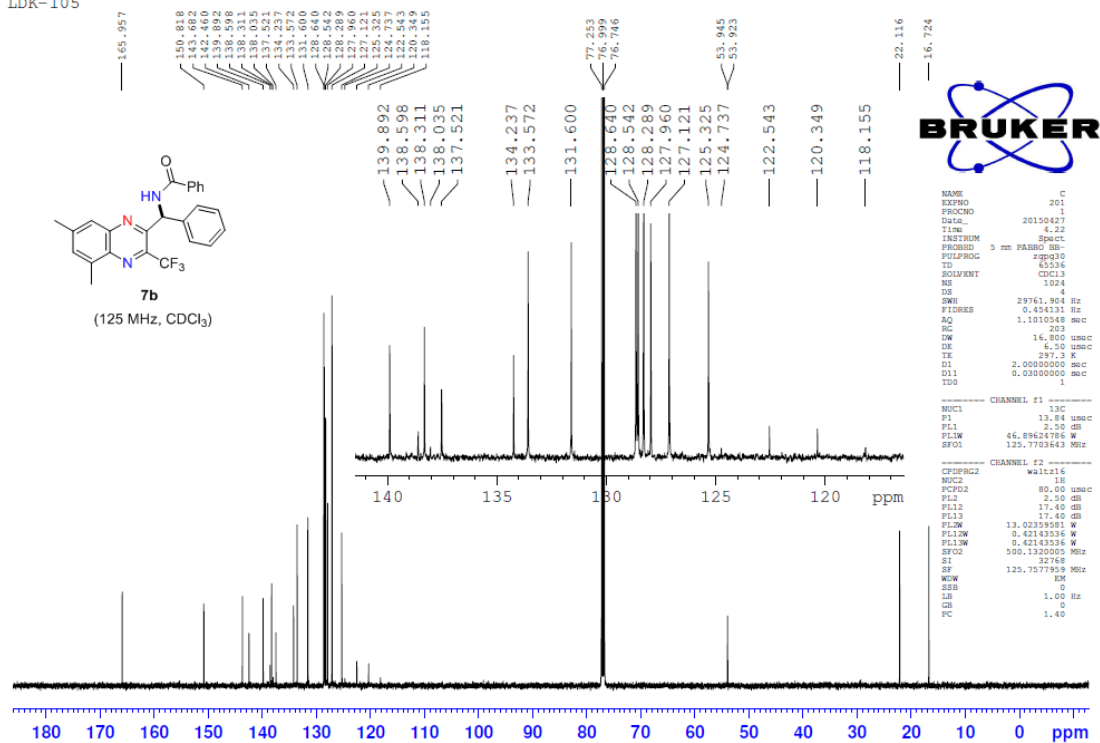
NAME          b
EXPNO         42
PROCNO        1
Date_         20150425
Time_         2.36
INSTRUM       Spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           10330.578 Hz
FIDRES        0.137532 Hz
AQ            3.1719923 sec
RG            114
DW            48.400 usec
DE            6.50 usec
TE            296.0 K
D1            1.0000000 sec
TD0           1
  
```

```

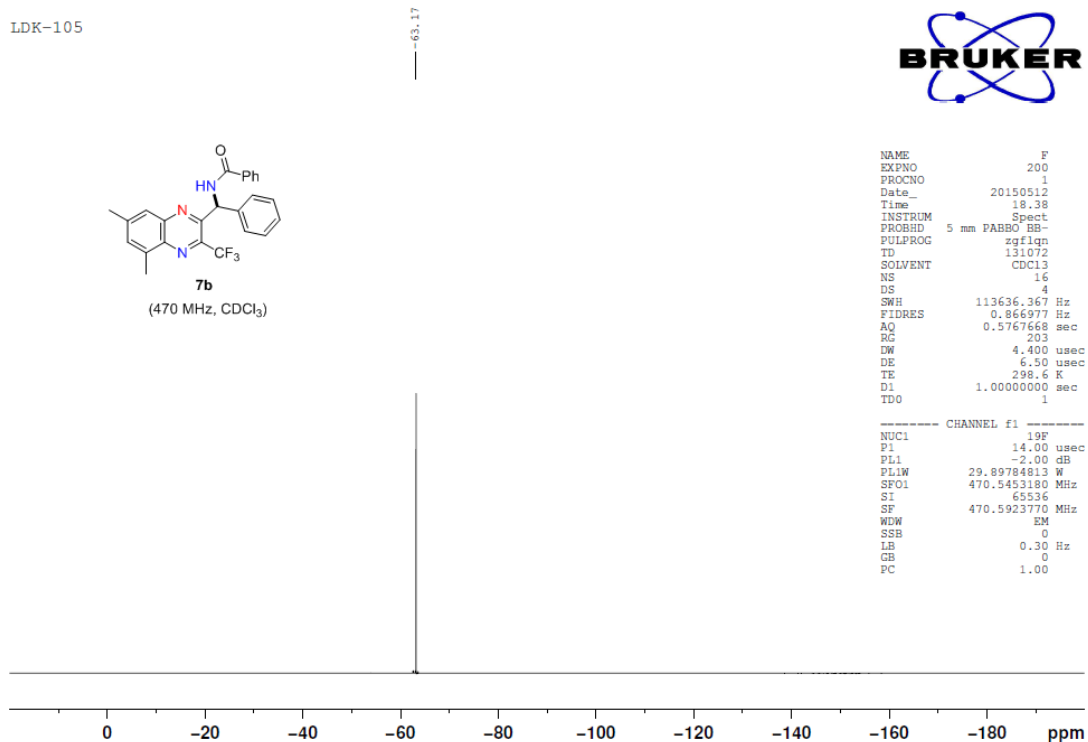
----- CHANNEL f1 -----
NUC1          1H
P1            14.00 usec
PL1           -2.00 dB
PL1W          13.02359881 W
SFO1          500.1330885 MHz
SI            32768
SF            500.1300231 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

LDK-105

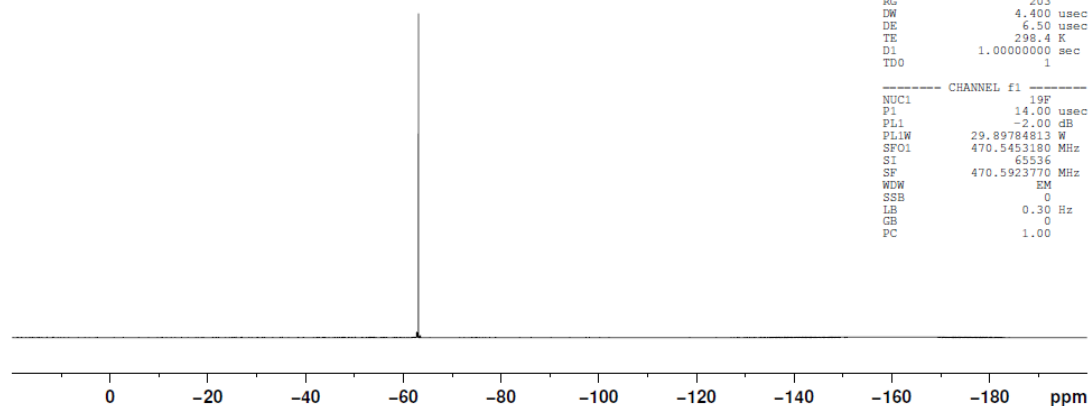
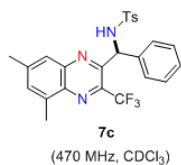


LDK-105



LDK-106

-63.11



```

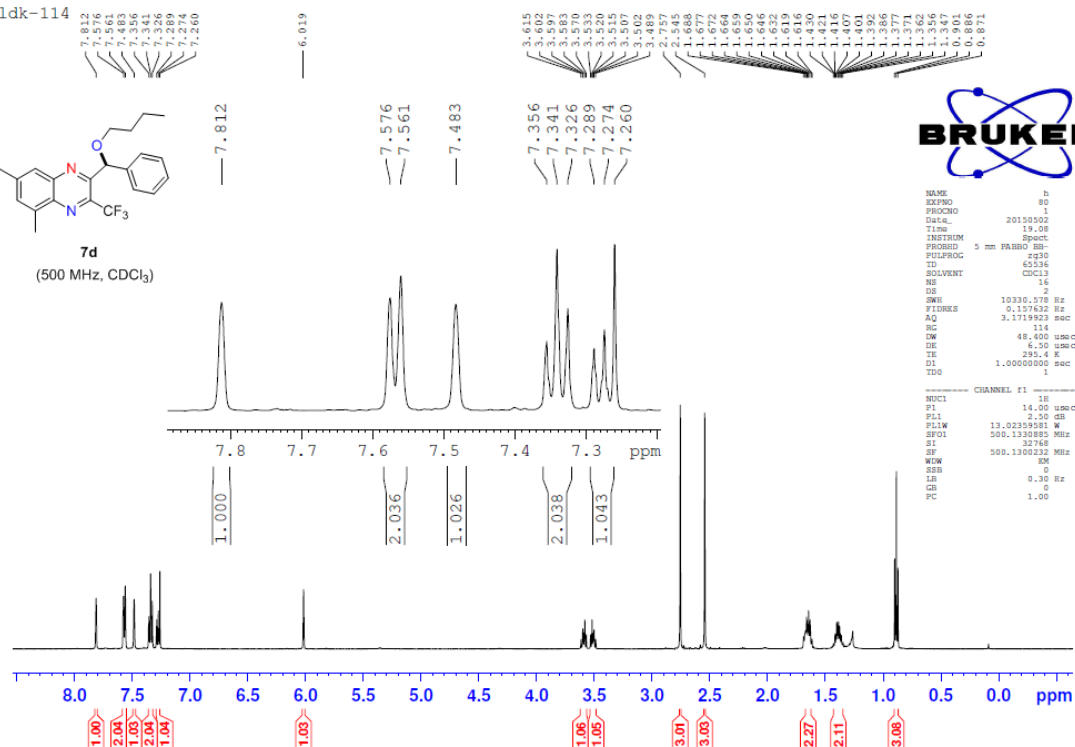
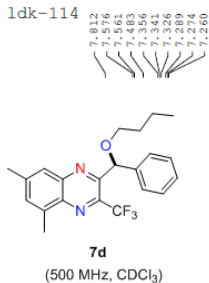
NAME      F
EXPNO     210
PROCNO    1
Date_     20150512
Time      18.43
INSTRUM   Spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         131072
SOLVENT   CDCl3
NS         16
DS         4
SWH        113636.367 Hz
FIDRES     0.866977 Hz
AQ         0.5767668 sec
RG         203
DW         4.400 usec
DE         6.50 usec
TE         298.4 K
D1         1.00000000 sec
TDO        1
  
```

----- CHANNEL f1 -----

```

NUC1      13C
P1        14.00 usec
PL1       -2.00 dB
PL1W      29.89784813 W
SFO1      470.5453180 MHz
SI        65536
SF         470.5923770 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

ldk-114



```

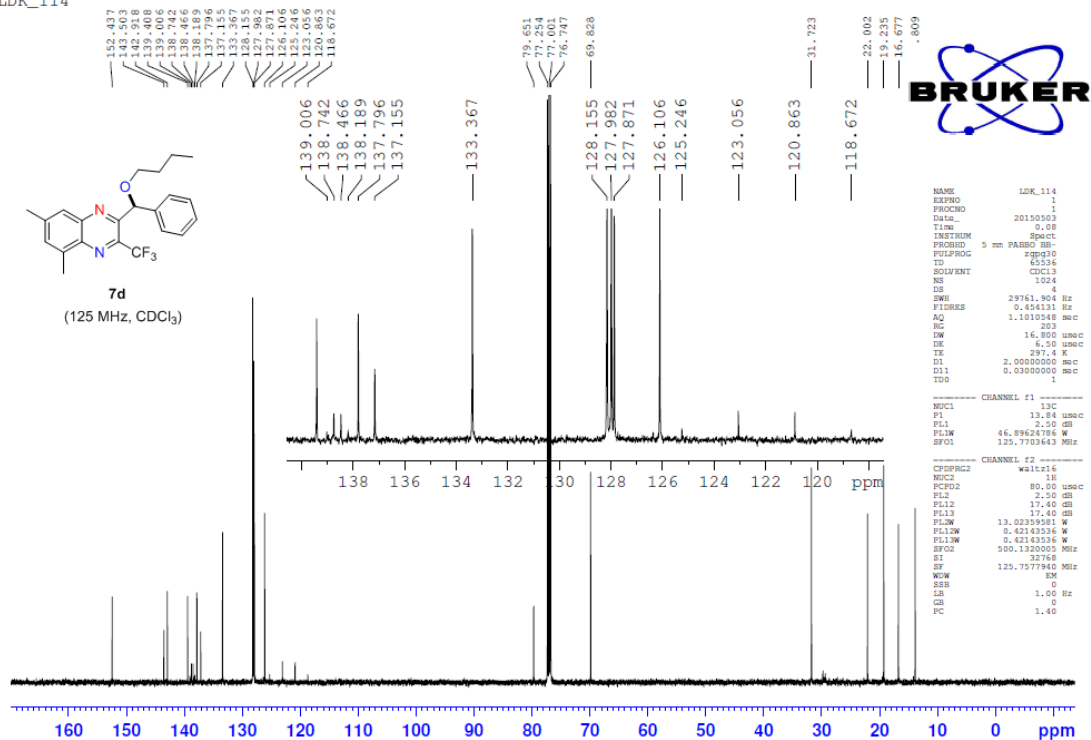
NAME      b
EXPNO     80
PROCNO    1
Date_     20150502
Time      19.08
INSTRUM   Spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.127632 Hz
AQ         3.1718923 sec
RG         114
DW         48.400 usec
DE         6.50 usec
TE         298.4 K
D1         1.00000000 sec
TDO        1
  
```

----- CHANNEL f1 -----

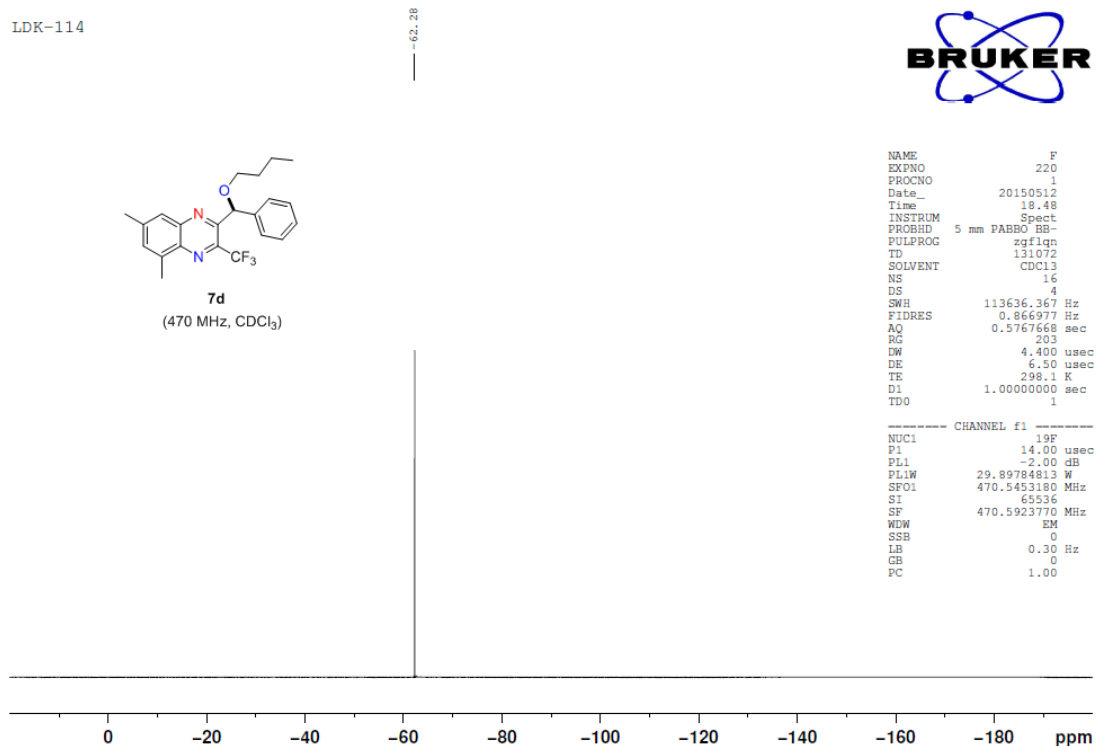
```

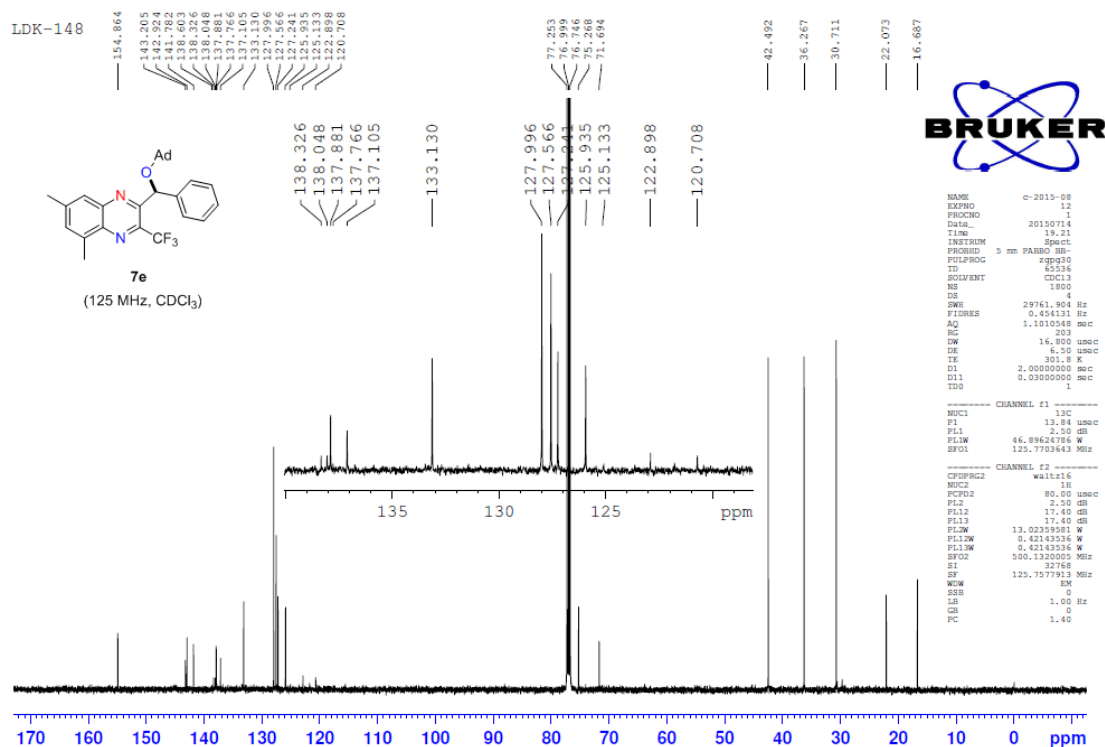
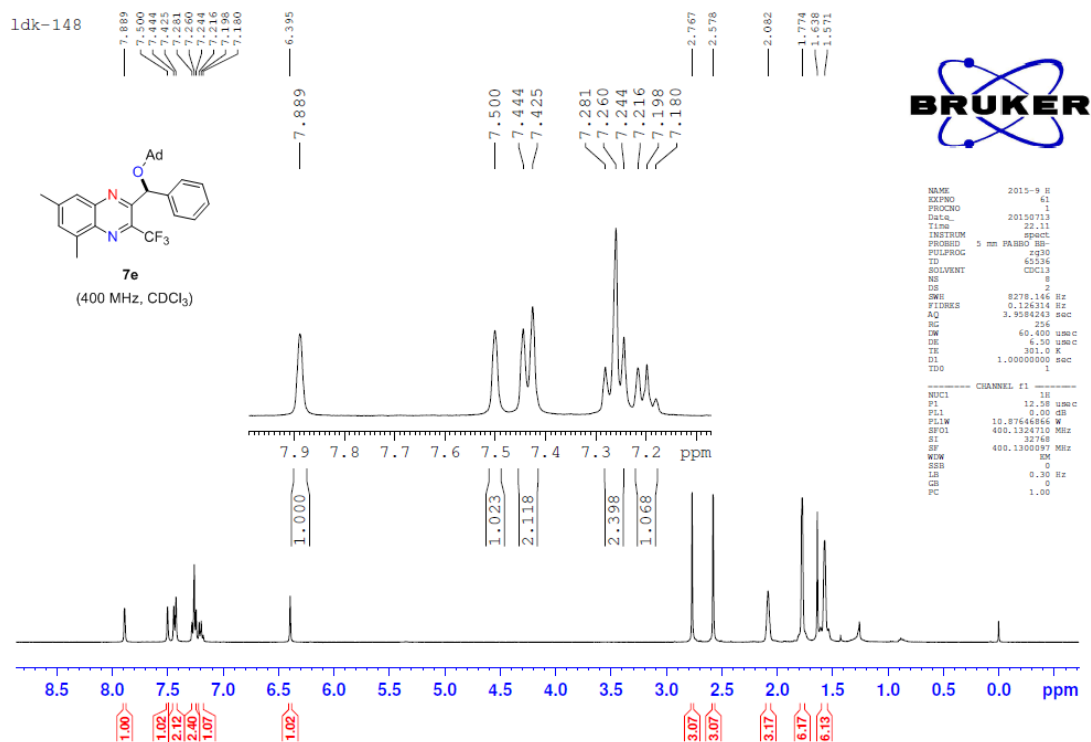
NUC1      1H
P1        14.00 usec
PL1       -2.50 dB
PL1W      13.02359081 W
SFO1      500.1320895 MHz
SI        32768
SF         500.1300232 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

LDK_114



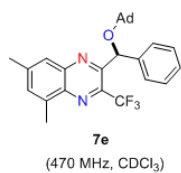
LDK-114





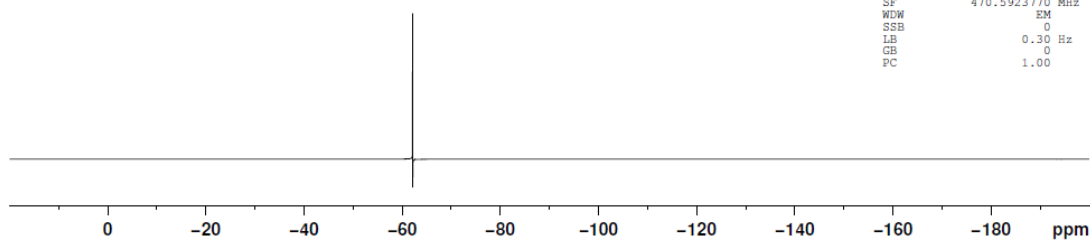
LDK-148

-62.13

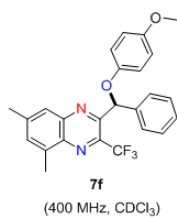


NAME f-2015-08
 EXPNO 13
 PROCNO 1
 Date_ 20150714
 Time 19.23
 INSTRUM Spect
 PROBD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 131072
 SOLVENT CDCl₃
 NS 16
 DS 4
 SWH 113636.367 Hz
 FIDRES 0.866977 Hz
 AQ 0.5767668 sec
 RG 203
 DW 4.400 usec
 DE 6.50 usec
 TE 300.6 K
 D1 1.00000000 sec
 TDO 1

CHANNEL f1
 NUC1 19F
 P1 14.00 usec
 PL1 -2.00 dB
 PL1W 29.89784813 W
 SFO1 470.5453180 MHz
 SI 65536
 SF 470.5923770 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

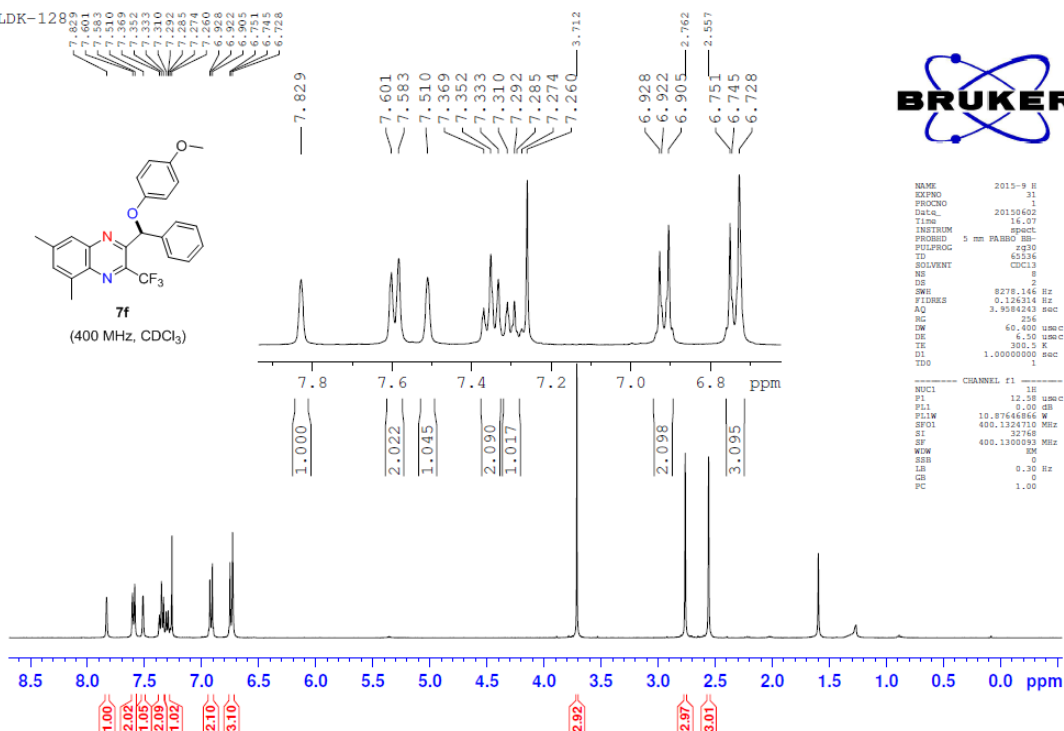


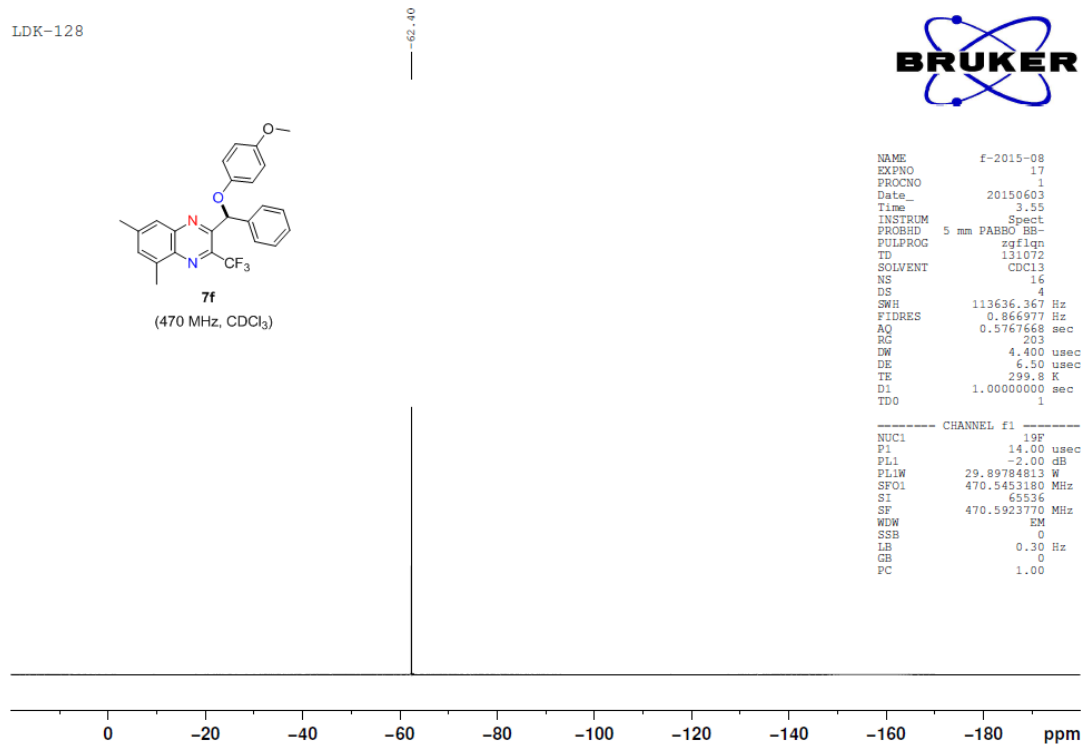
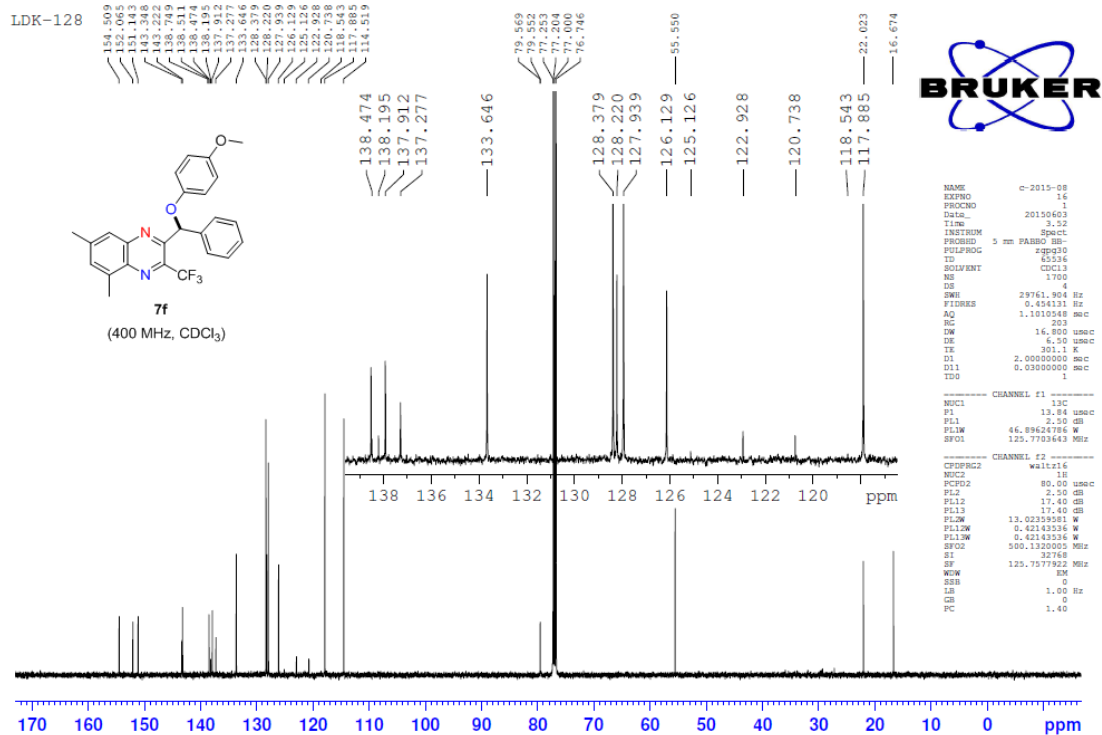
LDK-129

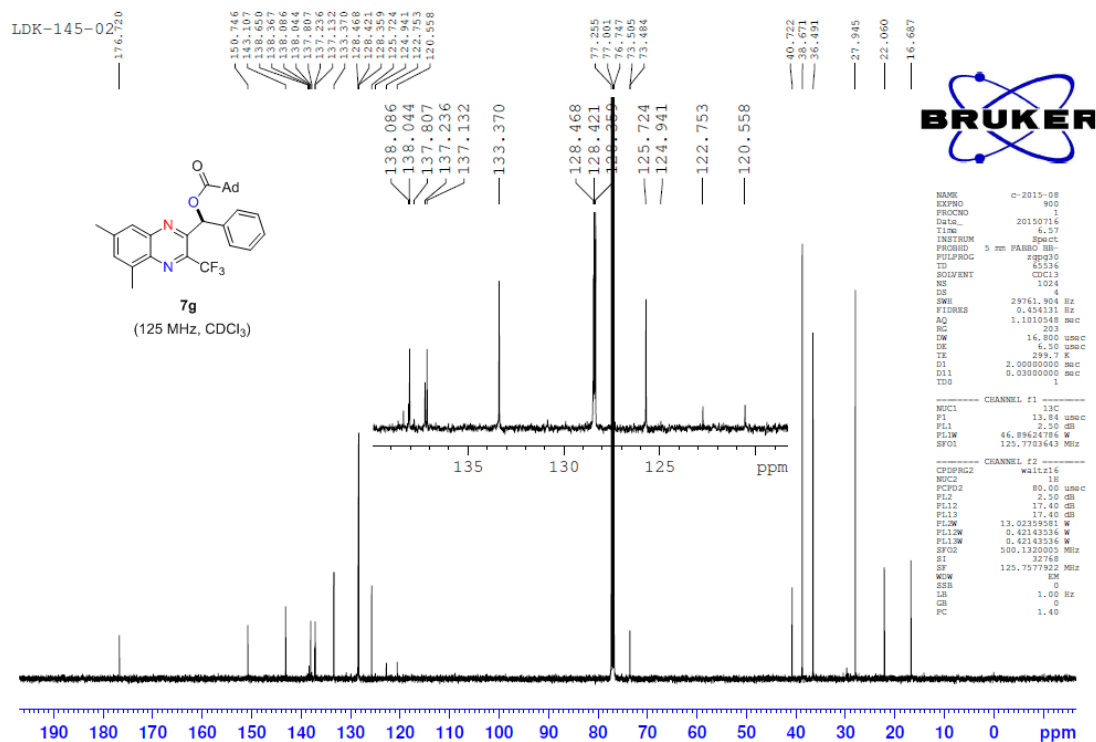
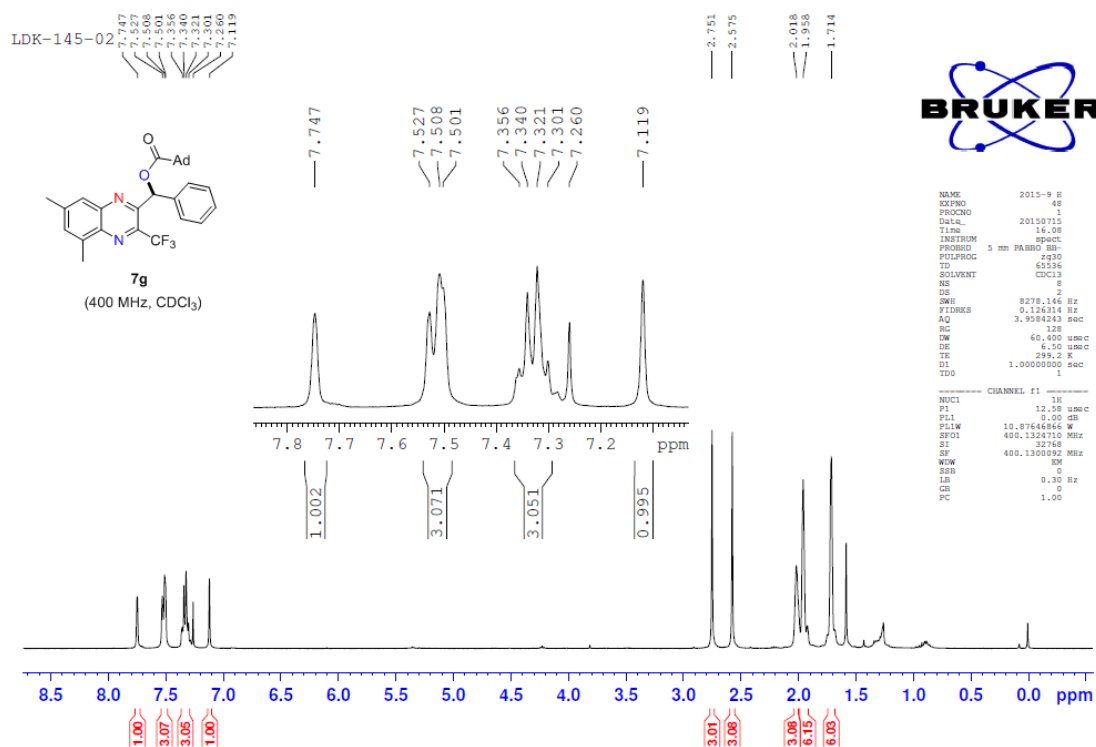


NAME 2015-9 E
 EXPNO 31
 PROCNO 1
 Date_ 2010602
 Time 16.57
 INSTRUM spect
 PROBD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 8
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 256
 DW 60.400 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.00000000 sec
 TDO 1

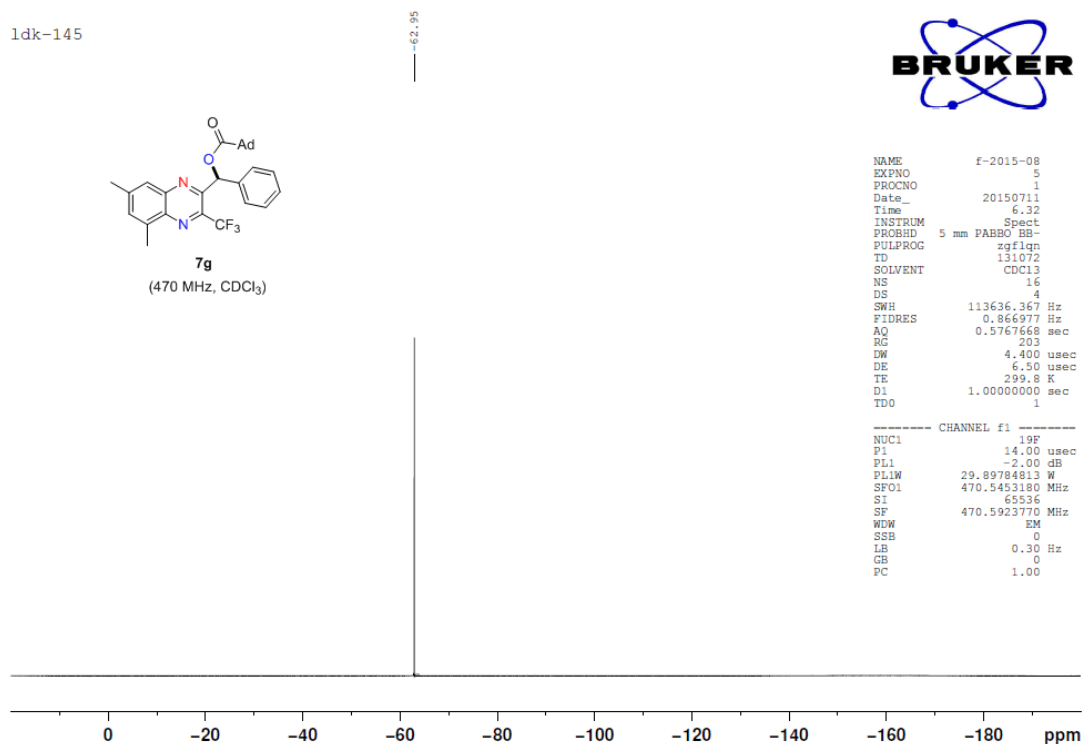
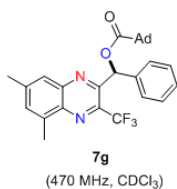
CHANNEL f1
 NUC1 1H
 P1 12.50 usec
 PL1 0.00 dB
 PL1W 10.8764686 W
 SFO1 400.1324710 MHz
 SI 32768
 SF 400.1300933 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00







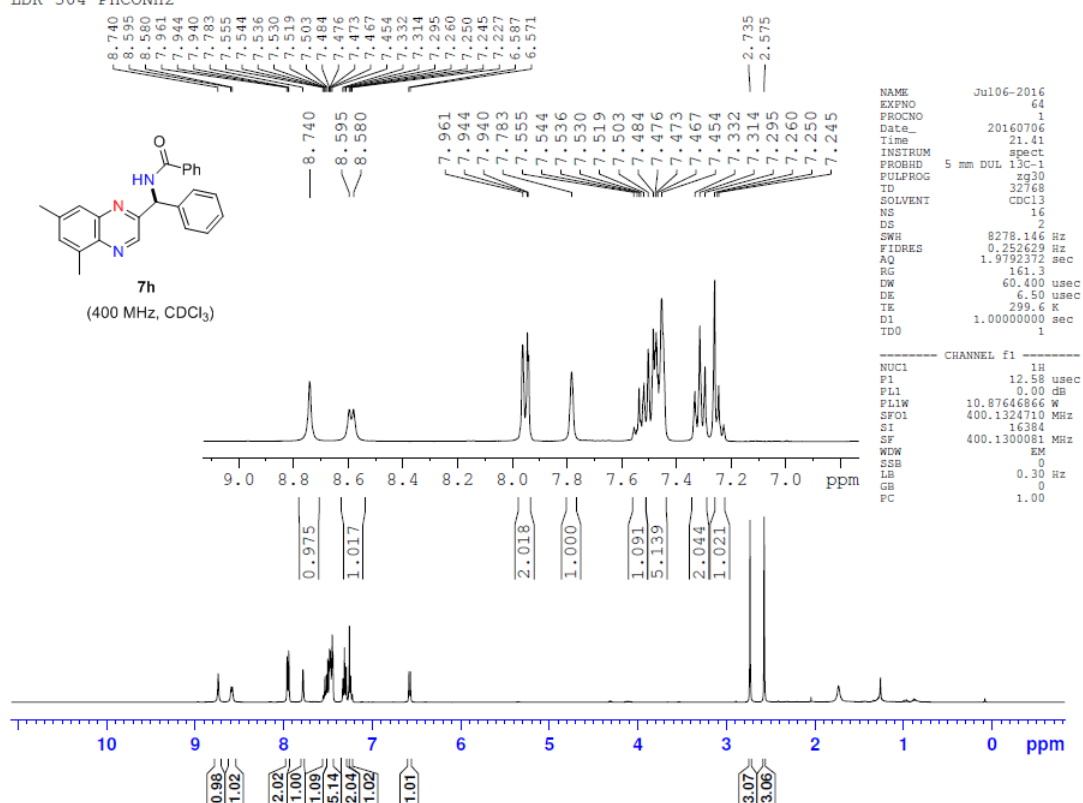
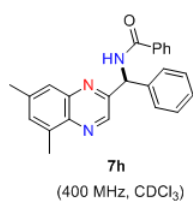
ldk-145



NAME f-2015-08
EXPNO 5
PROCNO 1
Date_ 20150711
Time 6.32
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 113636.367 Hz
FIDRES 0.866977 Hz
AQ 0.5767668 sec
RG 203
DW 4.400 usec
DE 6.50 usec
TE 299.8 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 13C
P1 14.00 usec
PL1 -2.00 dB
PL1W 29.89784813 W
SFO1 470.5453180 MHz
SI 65536
SF 470.5923770 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

LDK-304 PhCONH2



NAME Ju106-2016
EXPNO 64
PROCNO 1
Date_ 20160706
Time 21.41
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 161.3
DW 60.400 usec
DE 6.50 usec
TE 299.6 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 12.58 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 16384
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

LDK-304 PhCONH2

