

- Electronic Supplementary Information-

**Copper-Mediated Etherification of Arenes with
Alkoxysilanes Directed by
(2-Aminophenyl)pyrazole Group**

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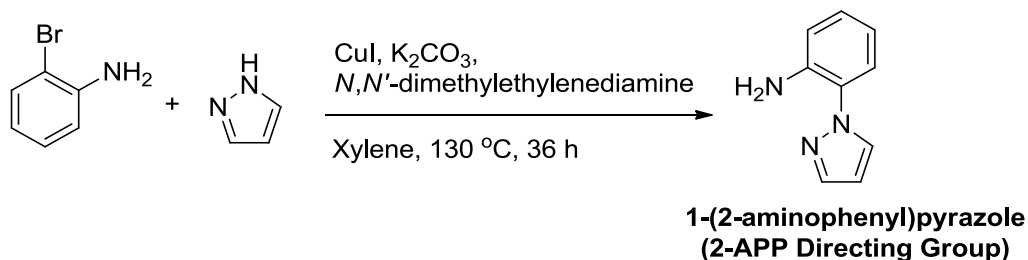
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1. General Information

All non-aqueous reactions were carried out under an atmosphere of nitrogen unless otherwise stated. All reactions were carried out using anhydrous solvent. Anhydrous Et₃N and CH₂Cl₂ were dried over calcium hydride. The anhydrous Cu(OAc)₂ and orthosilicates are purchased from Alfa-Aesar company. All the alcohols used were commercially purchased and used without further purification. Extra dry DMSO was purchased from Acros Organics Company. All reactions were monitored by thin layer chromatography (TLC) on Merck 60 F 254 precoated silica plates and visualized using a UV lamp (366 or 254 nm) or by use of potassium permanganate, 5 g K₂CO₃, / 100 mL water. Products were isolated by column chromatography (Merck silica gel 100-200μm). Yields refer to chromatographically and spectroscopically homogenous materials unless noted otherwise. ¹³C and ¹H NMR spectra were recorded on a Bruker 400 or Bruker 500 MHz spectrometers. Chemical shift values (δ) are reported in ppm and calibrated to the residual solvent peak CDCl₃ δ = 7.2600 ppm for ¹H, δ = 77.16 for ¹³C; or calibrated to tetramethylsilane (δ = 0.00). All NMR spectra were recorded at ambient temperature (290 K) unless otherwise noted. ¹H NMR spectra are reported as follows: chemical shift (multiplicity, coupling constant, integration). The following abbreviations are used to indicate multiplicities: s, singlet; d, doublet; t, triplet; q, quartet; quint, quintet; sext, sextet; sept, septet; m, multiplet; dd, doublet of doublet; dt, doublet of triplet; dq, doublet of quartet; td, triplet of doublet; tt, triplet of triplet; dq, doublet of quartet; br, broad. Mass spectra were recorded by electron spray ionization (ESI) method on a Q-TOF Micro with lock spray source. The crystal data were collected and integrated using a BrukerAxis kappa apex2 CCD diffractometer, with graphite monochromated Mo-Kα radiation.

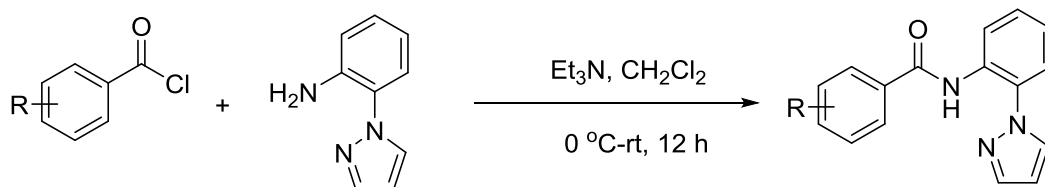
2. Synthesis of the 2-APP directing group and amides 1a-t.

2.1. Synthesis of the APP directing group¹



An oven dried two neck round bottom flask bearing septum in side arm was cooled to room temperature under a steady stream of nitrogen gas flow. The flask was charged with stirring bar, 2-bromoaniline (10 mmol), pyrazole (1.2 equiv), powdered K_2CO_3 (2.1 equiv), 20 mol% *N,N'*-dimethylethylenediamine, and 10 mL of *p*-xylene. The mixture was degassed for 15 min and CuI was added (5 mol %). The resulting mixture was kept stirring on the pre heated oil bath (130 °C) for 36 h (monitored by TLC). After cooling to room temperature, 100 mL of H_2O and a few crystals of EDTA were added to facilitate workup. The mixture was extracted with three 100 mL portions of CH_2Cl_2 . The combined organic layer was dried over $MgSO_4$ and filtered. The solvent was removed by rotary evaporation to leave oily residue. The residue was purified by column chromatography by using 4:1 hexanes : ethyl acetate as the eluent to provide pure product as pale yellow solid (1.08 g, 68% yield).

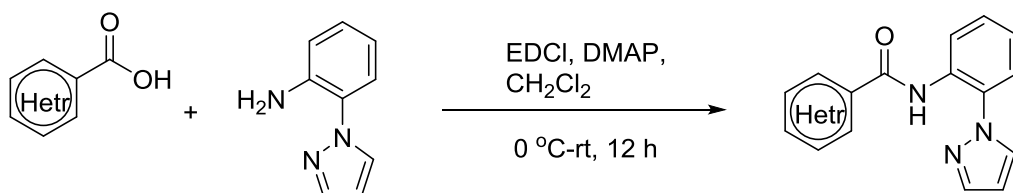
2.2. Synthesis of the amides 1a-1t²



An acid chloride (3 mmol, prepared from the corresponding carboxylic acid or commercially purchased) and 1-(2-aminophenyl)pyrazole (3 mmol) were added to a 50 mL round-bottom flask and then dissolved with CH_2Cl_2 (10 mL). Et_3N (5 mmol) was added to the vigorously stirred solution via a syringe. The reaction mixture was stirred at room

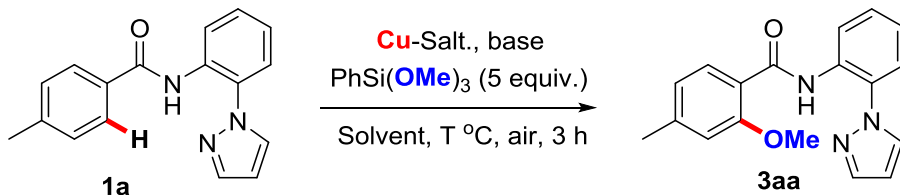
temperature for 12 h and quenched with saturated NaHCO₃ solution. After adding H₂O (75 mL), it was extracted with CH₂Cl₂ (75 mL x 3). Combined organic phase was washed with brine, dried over MgSO₄, and then filtered. The solvent was removed in a rotary evaporator and resulting crude product was purified by column chromatography on silica gel by using hexane : ethyl acetate as the eluent (90-95% yields).

2.3. Synthesis of the amides 1o-p²



A heterocyclic carboxylic acid (4 mmol) and 1-(2-aminophenyl)pyrazole (5 mmol) were taken to a 50 mL round-bottom flask and dissolved with CH₂Cl₂ (20 mL). DMAP (0.5 mmol) and EDCI (6 mmol) were added to the mixture under ice bath and then stirred for 12 h at room temperature. Saturated NaHCO₃ solution was added to the mixture to quench the reaction and then extracted with CH₂Cl₂ (100 mL x 3). Combined organic phase was washed with saturated brine solution, dried over Na₂SO₄, and then filtered. The solvent was removed in a rotary evaporator. The crude product was purified by column chromatography on silica gel by using hexane : ethyl acetate as the eluent (70-80% yields).

3. Optimization of the methoxylation reaction with amide **1a** and phenyltrimethoxysilane^a

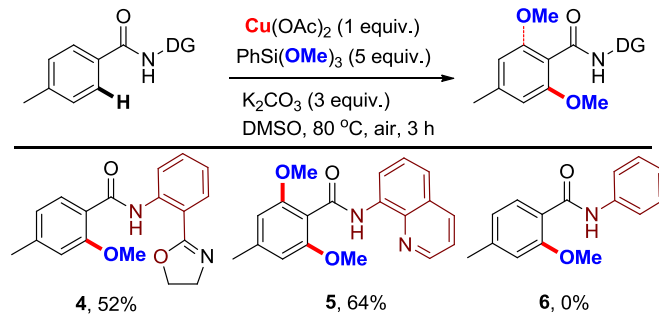


S.No	Cu-Salt	Base (equiv)	Oxidant (equiv)	Solvent (1 mL)	Temp. (°C)	Atm. (N ₂ /Air)	Yield (%) ^b
1	Cu(OAc) ₂	KHCO ₃ (3)	--	DMSO	80	Air	78
2	Cu(OAc) ₂	Na ₂ CO ₃ (3)	--	DMSO	80	Air	48
3	Cu(OAc)₂	K₂CO₃ (3)	--	DMSO	80	Air	87
4	Cu(OAc) ₂	Ag ₂ CO ₃ (1)	--	DMSO	80	Air	23
5	Cu(OAc) ₂	K ₂ CO ₃ (3)	--	DMSO	80	N ₂	26
6	Cu(OAc) ₂	K ₂ CO ₃ (3)	--	DMSO	100	Air	50
7	Cu(OAc) ₂	K ₂ CO ₃ (3)	--	DMSO	90	Air	82
8	Cu(OAc) ₂	K ₂ CO ₃ (2)	--	DMSO	80	Air	80
9	Cu(OAc) ₂	K ₂ CO ₃ (1)	--	DMSO	80	Air	58
10 ^c	Cu(OAc) ₂	K ₂ CO ₃ (3)	--	DMSO	80	Air	78
11 ^d	Cu(OAc) ₂	K ₂ CO ₃ (3)	--	DMSO	80	Air	62
12 ^e	Cu(OAc) ₂	K ₂ CO ₃ (3)	--	DMSO	80	Air	16
13 ^f	Cu(OAc) ₂	K ₂ CO ₃ (3)	--	DMSO	80	Air	41
14	Cu(OAc) ₂ ·H ₂ O	K ₂ CO ₃ (3)	--	DMSO	80	Air	83
15	CuCl ₂	K ₂ CO ₃ (3)	--	DMSO	80	Air	54
16	Cu(TFA) ₂ ·H ₂ O	K ₂ CO ₃ (3)	--	DMSO	80	Air	Trace
17	Cu(OTf) ₂	K ₂ CO ₃ (3)	--	DMSO	80	Air	Trace
18	(CuOH) ₂ CO ₃ ·H ₂ O	K ₂ CO ₃ (3)	--	DMSO	80	Air	28
19	Cu(OAc) ₂	K ₂ CO ₃ (3)	--	DMF	80	Air	46
20	Cu(OAc) ₂	K ₂ CO ₃ (3)	--	PhMe	80	Air	0
21	Cu(OAc) ₂	K ₂ CO ₃ (3)	--	MeCN	80	Air	0
22 ^e	Cu(OAc) ₂	Ag ₂ CO ₃ (1)	--	DMSO	80	N ₂	Trace
23 ^e	Cu(OAc) ₂	K ₂ CO ₃ (1)	Ag ₂ CO ₃ (2)	DMSO	80	N ₂	Trace
24 ^e	Cu(OAc) ₂	K ₂ CO ₃ (1)	Ag ₂ O (2)	DMSO	80	N ₂	Trace
25 ^e	Cu(OAc) ₂	K ₂ CO ₃ (1)	K ₂ S ₂ O ₈ (2)	DMSO	80	N ₂	Trace
26 ^e	Cu(OAc) ₂	K ₂ CO ₃ (1)	MnO ₂ (2)	DMSO	80	N ₂	Trace
27 ^e	Cu(OAc) ₂	K ₂ CO ₃ (1)	PhI(OAc) ₂	DMSO	80	N ₂	Trace

^aConditions: **1a** (0.1 mmol), Cu(OAc)₂ (0.1 mmol), PhSi(OMe)₃ (**2a**), Base (3 equiv.), air, DMSO (1 mL), 80 °C, 3h.

^bYields are isolated quantities. ^c4 equivalent of **2a** was used. ^d3 equivalent of **2a** was used. ^eCu(OAc)₂ (30 mol%) was used. ^fCu(OAc)₂ (50 mol%) was used.

3.1 Scope of the directing groups for methoxylation reaction



4 Typical copper mediated $\text{Csp}^2\text{-H}$ alkoxylation reaction using alkoxy silanes.

To an oven dried reaction tube (10 × 1.5 cm) was added amides **1a-1p** (0.1 mmol, 1 equiv.), $\text{Cu}(\text{OAc})_2$ (0.1 mmol), alkoxy silane (0.5 mmol, 5 equiv.), K_2CO_3 (0.3 mmol), and DMSO (1 mL). The reaction mixture was stirred at 80 °C (or given time in respective table) for stipulated time under air. After completion (TLC monitored), it was cooled and NH_4OH (2 ml) was added. The reaction mixture was transferred to a separating funnel and partitioned between CH_2Cl_2 and H_2O . Aqueous layer was extracted with CH_2Cl_2 (3 x 30 mL), then washed with brine, dried over MgSO_4 and evaporated under reduced pressure. In order to get pure alkoxyated product, the resulting residue was purified by column chromatography on silica gel with a gradient eluent of hexane and ethyl acetate. For the amides **1k**, **1l**, **1o** and **1p** TBAI (1 equiv.) was added as an additive along with the reagents.

5 Typical copper mediated $\text{Csp}^2\text{-H}$ alkoxylation reaction using alcohols.

To an oven dried reaction tube (10 × 1.5 cm) was added amide **1** (0.1 mmol, 1 equiv.), $\text{Cu}(\text{OAc})_2$ (0.1 mmol), alcohol (15 / 5 / 2 equiv.), Si_2Me_6 (1 equiv.), K_2CO_3 (0.3 mmol), and DMSO (1 mL). The reaction mixture was stirred at 80 °C for stipulated time under air. After completion (TLC monitored), NH_4Cl (2 ml) was added to the reaction tube and the reaction mixture was transferred to a separating funnel and partitioned between CH_2Cl_2 and H_2O . Aqueous layer was extracted with CH_2Cl_2 (3 x 30 mL), then washed with brine, dried over MgSO_4 and evaporated under reduced pressure. In order to get pure alkoxyated product, the resulting residue was purified by column chromatography on silica gel with a gradient eluent of hexane and ethyl acetate. For the amides **1k** and **1o**, TBAI (1 equiv.) was added as an additive along with the reagents.

Product Table

Table 2

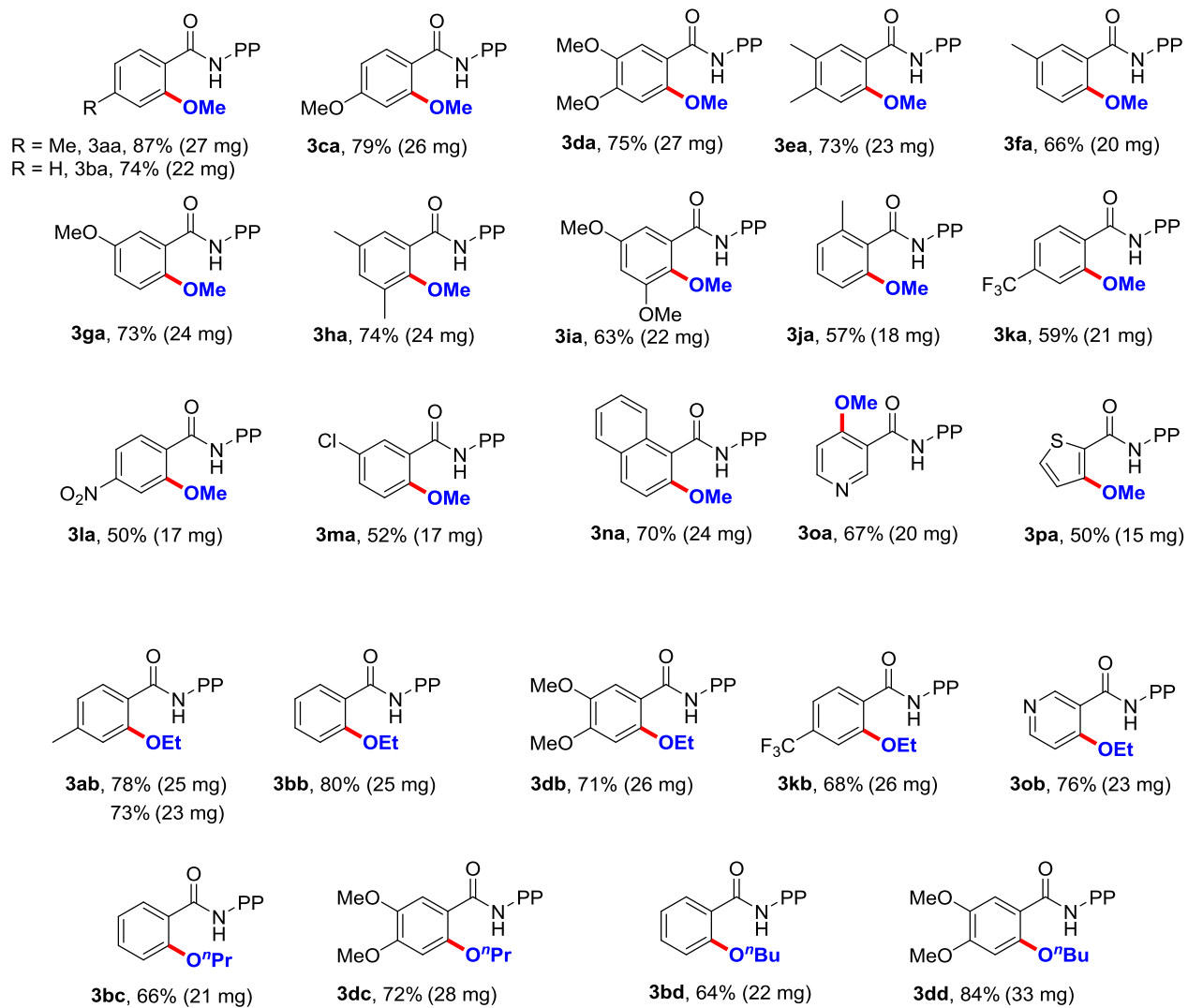
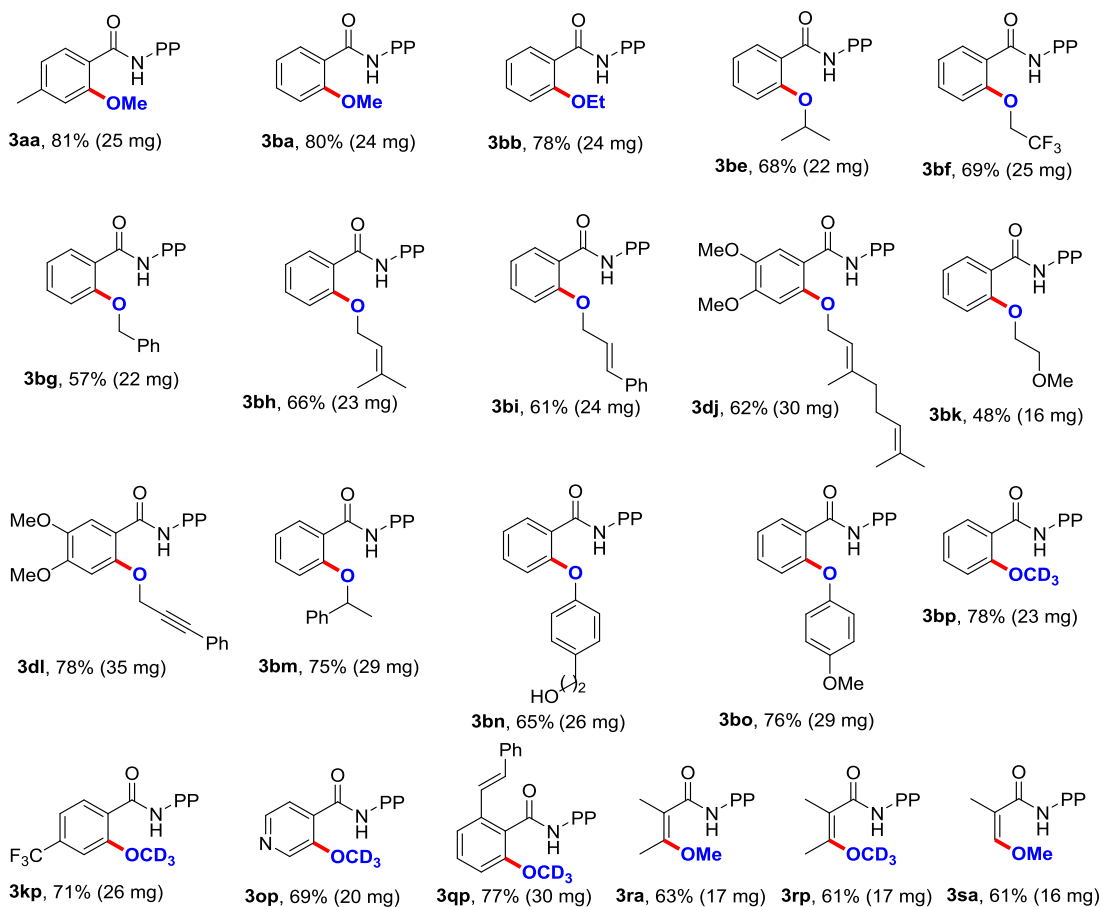
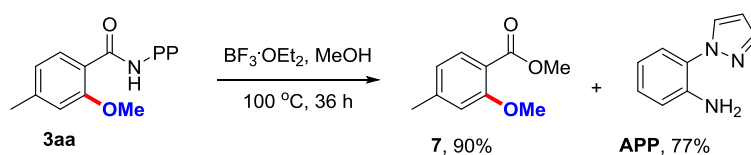


Table 3



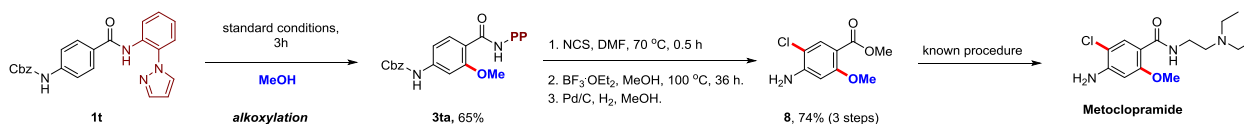
6. General procedure for the removal of the directing group³



To a 10 mL pressure tube equipped with a stir bar was added **3aa** (62 mg, 0.2 mmol, 1 equiv.). Then, $\text{BF}_3 \cdot \text{Et}_2\text{O}$ (0.18 mL, 6 equiv.) and dry methanol (3.5 mL) was added drop wise to the stirred solution in this sequence. The resulting mixture was stirred at 100°C for 36 h. After cooling to rt, Et_3N (0.32 mL, 10 equiv.) was added drop wise to the reaction mixture with stirring. After removal of the volatile components, the crude reaction mixture was directly loaded onto silica gel column and purification with gradient eluent of hexane and

ethyl acetate (9:1) mixture to give the pure product **7** as colorless oil (32 mg, 90% yield) and 2-APP directing group in 77% yield (25 mg).

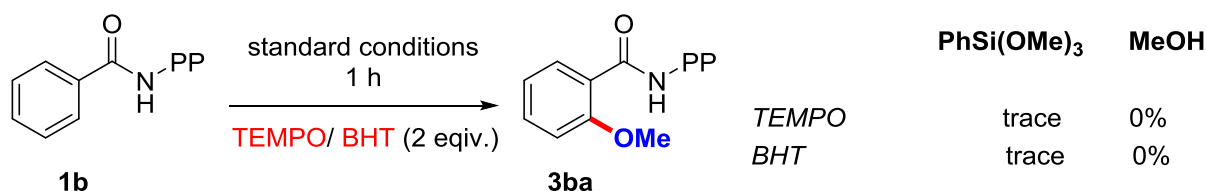
7. Formal Synthesis of Metoclopramide



The standardized methoxylation condition for the amide **1t** (4.0 mmol) delivered the methoxylated product **3ta** in 65% yield (1.17 g). Electrophilic chlorination of **3ta** (0.25 mmol) using *N*-chlorosuccinimide⁴ was carried out at 70 °C in DMF solvent for 30 minutes. The crude chlorinated product was sequentially subjected to the general procedure for the removal of the 2-APP directing group and the Pd/C hydrogenative removal of the Cbz protection⁵ to give the metoclopramide precursor **8** in 74% yield (40.0 mg). Synthesis of metoclopramide was previously reported with compound **8** [(a). S. Kato, T. Morie, T. Kon, N. Yoshida, T. Karasawa and J. Matsumoto, *J. Med. Chem.*, 1991, **34**, 616. (b). C. G. Jørgensen, B. Frølund, J. Kehler, A. A. Jensen, *ChemMedChem* 2011, **6**, 725].

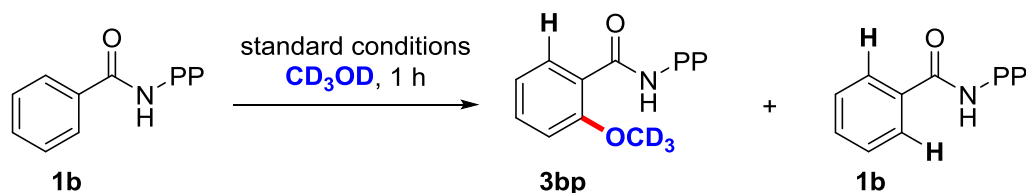
8. Control Experiments

8.1 Reactions with radical scavengers



In order to probe the reaction mechanism, we have performed methoxylation reaction in presence of radical scavenger under our stander reaction condition for 1 h. When stoichiometric amount of radical scavengers TEMPO or BHT used, trace amount of methoxylated product was observed when phenyltrimethoxy silane is used as methoxy source where as in the case of methanol reaction was completely arrested.

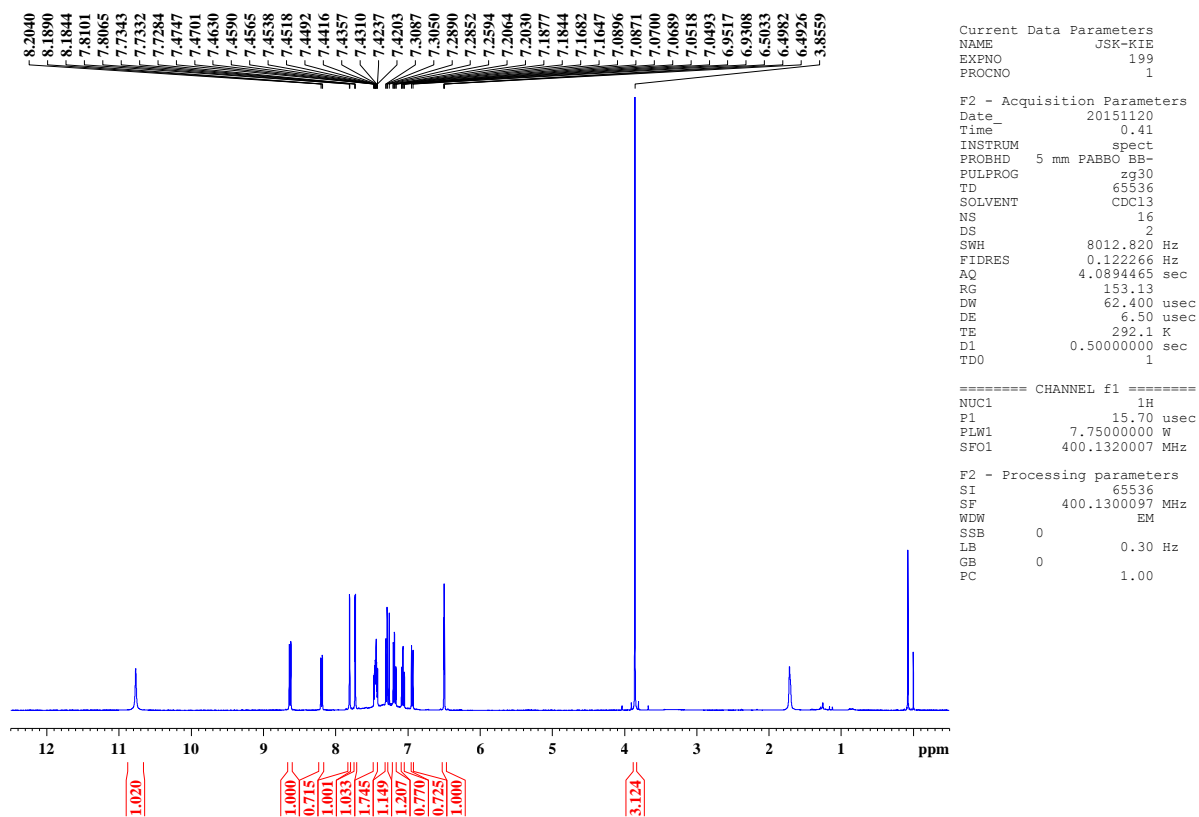
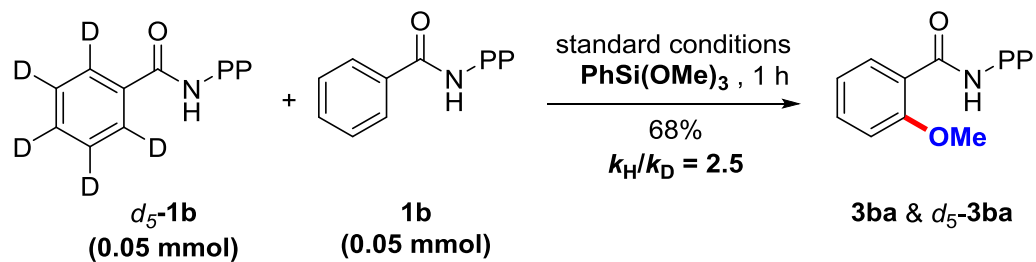
8.2 Reactions with methanol- d_4

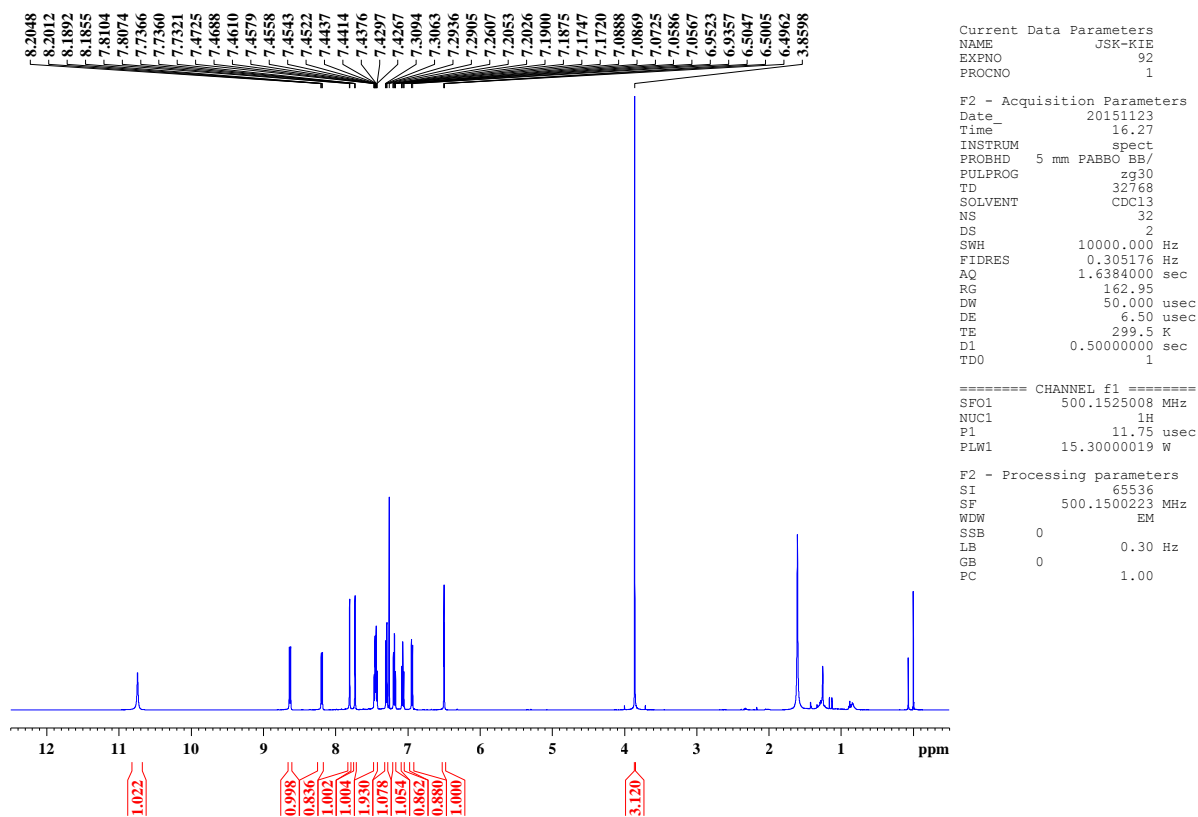
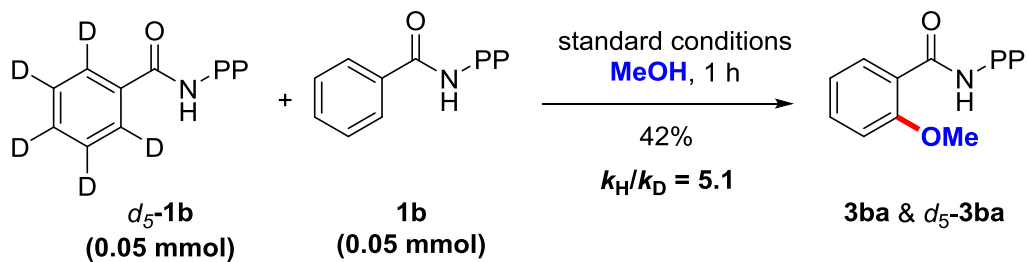


To investigate the reversibility of the copper mediated C-H bond cleavage, the methoxylation reaction was performed with methanol- d_4 under standard reaction condition for 1 h. From 1H -NMR spectrum, confirm no deuterium incorporation was detected in the product as well in recovered starting material.

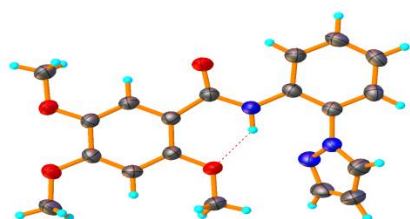
8.3 Intermolecular Kinetic Isotope Effect Experiments:

To demonstrate the intermolecular kinetic isotope effect (KIE), a 1 : 1 mixture of **1b** and the pentadeuterated substrate d_5 -**1b** was subjected to the standard reaction condition for 1 h and the products were isolated by column chromatography (silica gel, 15 % EtOAc : Hexane). From the 1H NMR, analysis of the H/D ratio on the phenyl ring reveals that, intermolecular KIE of k_H/k_D nearly 2.5 with phenyltrimethoxysilane as nucleophile (68% conversion) and k_H/k_D is nearly 5.1 when methanol is used as nucleophile (42% conversion).

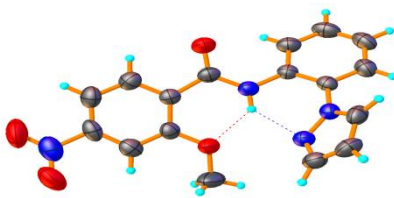




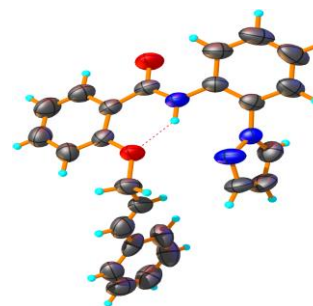
ORTEP diagram



3da (CCDC 1479824)



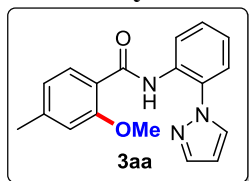
3la (CCDC 1479825)



3bi (CCDC 1479826)

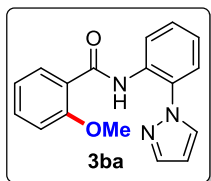
9. Spectroscopic data

2-Methoxy-4-methyl-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3aa): colorless solid, ^1H -



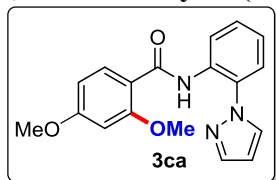
NMR (400 MHz, CDCl_3): δ 10.66 (s, 1H), 8.62 (dd, $J = 8.3, 1.2$ Hz, 1H), 8.08 (d, $J = 7.8$ Hz, 1H), 7.806-7.801 (m, 1H), 7.72-7.71 (m, 1H), 7.45-7.41 (m, 1H), 7.30-7.27 (m, 1H), 7.19-7.15 (m, 1H), 6.88-6.86 (m, 1H), 6.73 (s, 1H), 6.49-6.48 (m, 1H), 3.83 (s, 3H), 2.38 (s, 3H). ^{13}C -**NMR** (100 MHz, CDCl_3): δ 163.88, 144.18, 140.92, 133.43, 132.42, 130.84, 130.51, 128.78, 125.12, 123.89, 123.82, 122.01, 111.95, 106.93, 55.60, 21.74. **HRMS-ESI**: Calcd. for $\text{C}_{18}\text{H}_{17}\text{N}_3\text{O}_2\text{Na}$ $[\text{M}+\text{Na}]^+$ 330.1218, found 330.1243.

2-Methoxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3ba): colorless solid, ^1H -**NMR** (400



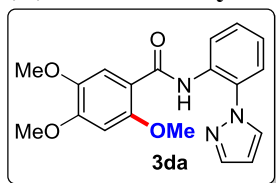
MHz, CDCl_3): δ 10.74 (s, 1H), 8.63 (dd, $J = 8.3, 1.2$ Hz, 1H), 8.19 (dd, $J = 7.79, 1.85$ Hz, 1H), 7.80-7.79 (m, 1H), 7.73-7.72 (m, 1H), 7.46-7.41 (m, 2H), 7.30-7.27 (m, 1H), 7.19-7.15 (m, 1H), 7.08-7.04 (m, 1H), 6.94-6.92 (m, 1H), 6.49-6.48 (m, 1H), 3.84 (s, 3H). ^{13}C -**NMR** (100 MHz, CDCl_3): δ 163.85, 157.39, 140.97, 133.23, 132.44, 130.83, 130.55, 128.79, 125.04, 124.07, 123.85, 121.97, 121.16, 111.21, 106.99, 55.68. **HRMS-ESI**: Calcd. For $\text{C}_{17}\text{H}_{16}\text{N}_3\text{O}_2$ $[\text{M}+\text{H}]^+$ 294.1237, found 294.1237.

2,4-Dimethoxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3ba): colorless solid, ^1H -**NMR**



(400 MHz, CDCl_3): δ 10.59 (s, 1H), 8.61 (dd, $J = 8.37, 1.24$ Hz, 1H), 8.17 (d, $J = 8.7$ Hz, 1H), 7.806-7.802 (m, 1H), 7.719-7.714 (m, 1H), 7.44-7.40 (m, 1H), 7.28 (dd, $J = 7.8, 1.6$ Hz, 1H), 7.18-7.14 (m, 1H), 6.58 (dd, $J = 8.8, 2.3$ Hz, 1H), 6.49-6.48 (m, 1H), 6.43 (d, $J = 2.3$ Hz, 1H), 3.84 (s, 3H), 3.82 (s, 3H). ^{13}C -**NMR** (100 MHz, CDCl_3): δ 163.85, 163.61, 158.82, 140.91, 134.19, 133.47, 130.88, 130.53, 128.80, 125.17, 123.84, 114.79, 106.95, 105.37, 98.33, 55.68, 55.55.

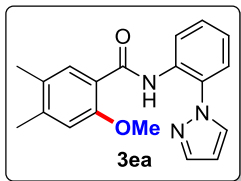
2,4,5-Trimethoxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3ba): colorless solid, ^1H -**NMR**



(400 MHz, CDCl_3): δ 10.66 (s, 1H), 8.61 (dd, $J = 8.3, 1.2$ Hz, 1H), 7.82-7.81 (m, 1H), 7.75 (s, 1H), 7.72 (dd, $J = 2.4, 0.49$ Hz, 1H), 7.46-7.41 (m, 1H), 7.29 (dd, $J = 7.9, 1.5$ Hz, 1H), 7.17 (td, $J = 7.7, 1.4$ Hz, 1H), 6.51-

6.49 (m, 1H), 6.48 (s, 1H), 3.93 (s, 3H), 3.90 (s, 3H), 3.84 (s, 3H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 163.56, 152.91, 152.77, 143.30, 140.93, 133.52, 130.89, 130.56, 128.83, 125.29, 123.89, 123.81, 114.19, 113.22, 106.96, 96.29, 56.35, 56.31, 56.15.

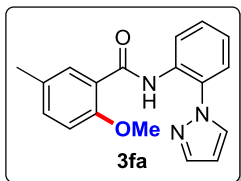
2-Methoxy-4,5-dimethyl-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3ea): colorless semi-



solid, $^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 10.62 (s, 1H), 8.63–8.60 (m, 1H), 7.94 (s, 1H), 7.80–7.79 (m, 1H), 7.717–7.710 (m, 1H), 7.45–7.41 (m, 1H), 7.29 (dd, $J = 7.9, 1.5$ Hz, 1H), 7.19–7.14 (m, 1H), 6.70 (s, 1H), 6.49–6.48

(m, 1H), 3.80 (s, 3H), 2.28 (s, 3H), 2.23 (s, 3H). $^{13}\text{C-NMR}$ (125 MHz, CDCl_3): δ 164.08, 155.46, 142.63, 140.96, 133.51, 133.14, 130.91, 130.59, 129.24, 128.88, 125.28, 123.91, 123.82, 118.94, 112.68, 106.98, 55.73, 20.32, 18.70.

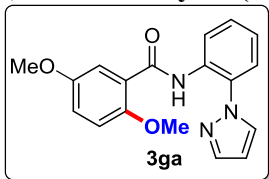
2-Methoxy-5-methyl-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3fa): colorless semi-solid,



$^1\text{H-NMR}$ (500 MHz, CDCl_3): δ 10.70 (s, 1H), 8.63–8.61 (m, 1H), 7.99 (s, 1H), 7.804–7.801 (m, 1H), 7.724–7.720 (m, 1H), 7.45–7.42 (m, 1H), 7.30–7.28 (m, 1H), 7.25–7.23 (m, 1H), 7.19–7.16 (m, 1H), 6.83–6.82 (m, 1H),

6.496–6.493 (m, 1H), 3.81 (s, 3H), 2.32 (s, 3H). $^{13}\text{C-NMR}$ (125 MHz, CDCl_3): δ 164.03, 155.40, 140.99, 134.15, 133.71, 133.36, 132.69, 130.87, 130.59, 130.52, 128.85, 127.76, 125.17, 124.03, 123.83, 121.50, 111.22, 106.98, 55.77, 20.36.

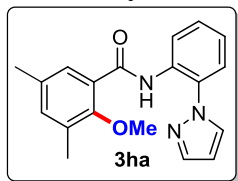
2,5-Dimethoxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3ga): colorless solid, $^1\text{H-NMR}$



(400 MHz, CDCl_3): δ 10.71 (s, 1H), 8.54 (dd, $J = 8.3, 1.1$ Hz, 1H), 7.74 (d, $J = 1.6$ Hz, 1H), 7.68 (d, $J = 3.2$ Hz, 1H), 7.66 (d, $J = 2.0$ Hz, 1H), 7.39–7.35 (m, 1H), 7.23 (dd, $J = 7.7, 1.5$ Hz, 1H), 7.12 (td, $J = 7.7, 1.3$

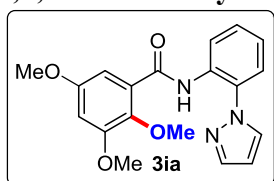
Hz, 1H), 6.94 (dd, $J = 9.0, 3.2$ Hz, 1H), 6.80 (d, $J = 9.0$ Hz, 1H), 6.43 (t, $J = 2.0$ Hz, 1H), 3.74 (s, 3H), 3.73 (s, 3H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 163.61, 153.77, 151.74, 140.94, 133.25, 130.91, 130.63, 128.87, 125.21, 124.19, 123.89, 119.97, 115.71, 112.73, 107.03, 56.20, 55.86.

2-Methoxy-3,5-dimethyl-N-(2-(1H-pyrazol-1-yl)phenyl)benzamide (3ha): colorless semi



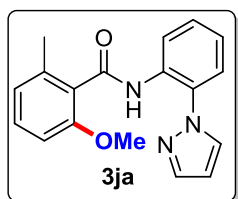
solid, $^1\text{H-NMR}$ (500 MHz, CDCl_3): δ 10.85 (s, 1H), 8.69 (d, $J = 8.3$ Hz, 1H), 7.81 (s, 1H), 7.724-7.720 (m, 1H), 7.67 (s, 1H), 7.46-7.43 (m, 1H), 7.31-7.30 (m, 1H), 7.20-7.17 (m, 1H), 7.11 (s, 1H), 6.50-6.49 (m, 1H), 3.51 (s, 3H), 2.30 (s, 3H), 2.26 (s, 3H). $^{13}\text{C-NMR}$ (125 MHz, CDCl_3): δ 164.63, 154.51, 141.42, 135.56, 133.82, 133.29, 131.40, 130.44, 129.59, 128.75, 124.78, 124.05, 123.47, 107.15, 61.25, 20.66, 15.88.

2,3,5-Trimethoxy-N-(2-(1H-pyrazol-1-yl)phenyl)benzamide (3ia): colorless solid, $^1\text{H-NMR}$



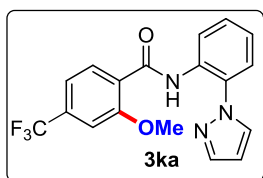
(400 MHz, CDCl_3): δ 10.94 (s, 1H), 8.67-8.65 (m, 1H), 7.85-7.84 (m, 1H), 7.72-7.71 (m, 1H), 7.47-7.42 (m, 1H), 7.32-7.29 (m, 1H), 7.22-7.18 (m, 2H), 6.62-6.61 (m, 1H), 6.51-6.50 (m, 1H), 3.85 (s, 3H), 3.82 (s, 3H), 3.65 (s, 3H). $^{13}\text{C-NMR}$ (125 MHz, CDCl_3): δ 163.80, 155.94, 153.48, 142.08, 141.54, 133.24, 130.65, 130.53, 128.77, 126.89, 125.16, 124.25, 123.67, 107.26, 104.55, 104.13, 61.47, 56.08, 55.73.

2-Methoxy-6-methyl-N-(2-(1H-pyrazol-1-yl)phenyl)benzamide (3ja): colorless semi-solid,



$^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 10.11 (s, 1H), 8.63-8.61 (m, 1H), 7.80-7.79 (m, 1H), 7.67-7.66 (m, 1H), 7.45-7.40 (m, 1H), 7.34-7.32 (m, 1H), 7.23-7.18 (m, 2H), 6.82-6.80 (m, 1H), 6.75-6.72 (m, 1H), 6.47-6.45 (m, 1H), 3.66 (s, 3H), 2.32 (s, 3H). $^{13}\text{C-NMR}$ (125 MHz, CDCl_3): δ 166.24, 156.24, 141.09, 137.49, 131.97, 130.33, 130.11, 129.74, 128.29, 126.57, 124.28, 123.64, 123.10, 122.89, 108.37, 106.98, 55.66, 19.33.

2-Methoxy-4-trifluoromethyl-N-(2-(1H-pyrazol-1-yl)phenyl)-benzamide (3ka): colorless

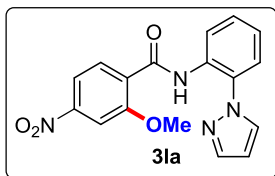


semi-solid, $^1\text{H-NMR}$ (500 MHz, CDCl_3): δ 10.87 (s, 1H), 8.63 (dd, $J = 8.3, 1.2$ Hz, 1H), 8.28-8.26 (m, 1H), 7.81-7.80 (m, 1H), 7.76-7.75 (m, 1H), 7.46-7.43 (m, 1H), 7.34-7.30 (m, 2H), 7.22-7.19 (m, 1H), 7.16 (s, 1H), 6.51-6.50 (m, 1H), 3.93 (s, 3H). $^{13}\text{C-NMR}$ (125 MHz, CDCl_3): δ 162.60, 157.30, 141.07,

134.67 (q, J_{C-F} 32.5 Hz), 133.17, 132.62, 130.77, 130.48, 128.75, 125.41, 124.69, 124.57, 123.88, 123.48 (q, J_{C-F} 272.9 Hz), 117.84 (q, J_{C-F} 3.6 Hz), 108.34 (q, J_{C-F} 3.7 Hz), 107.18, 56.12.

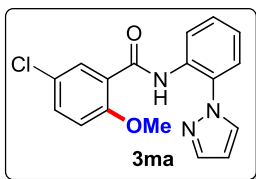
HRMS-ESI: Calcd. for $C_{18}H_{14}F_3N_3O_2Na$ $[M+Na]^+$ 384.0936, found 384.0953.

2-Methoxy-4-nitro-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)-benzamide (3la): yellow solid, 1H -NMR



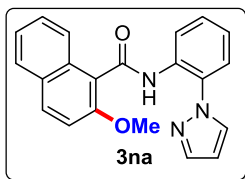
(400 MHz, $CDCl_3$): δ 10.97 (s, 1H), 8.62 (dd, $J = 8.3, 1.2$ Hz, 1H), 8.32 (d, $J = 8.65$ Hz, 1H), 7.91 (dd, $J = 8.6, 2.1$ Hz, 1H), 7.82-7.80 (m, 2H), 7.78-7.77 (m, 1H), 7.47-7.43 (m, 1H), 7.33-7.31 (m, 1H), 7.25-7.21 (m, 1H), 6.53-6.52 (m, 1H), 3.99 (s, 3H). ^{13}C -NMR (125 MHz, $CDCl_3$): δ 161.88, 157.47, 150.53, 141.12, 133.50, 132.23, 130.74, 130.40, 128.72, 127.91, 124.80, 124.48, 123.87, 115.89, 107.28, 106.64, 56.55. **HRMS-ESI:** Calcd. for $C_{17}H_{14}N_4O_4Na$ $[M+Na]^+$ 384.0936, found 384.0911.

2-Methoxy-5-chloro-*N*-(2-(1*H*-pyrazol-1-yl)phenyl) benzamide (3ma): colorless solid, 1H -NMR



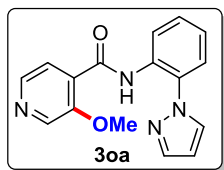
(400 MHz, $CDCl_3$): δ 10.78 (s, 1H), 8.60 (dd, $J = 8.3, 1.0$ Hz, 1H), 8.15 (d, $J = 2.7$ Hz, 1H), 7.80 (d, $J = 1.6$ Hz, 1H), 7.74 (d, $J = 2.3$ Hz, 1H), 7.46-7.42 (m, 1H), 7.38 (dd, $J = 8.8, 2.7$ Hz, 1H), 7.30 (dd, $J = 7.9, 1.5$ Hz, 1H), 7.20 (td, $J = 7.6, 1.3$ Hz, 1H), 6.88 (d, $J = 8.8$ Hz, 1H), 6.51-6.49 (m, 1H), 3.85 (s, 3H). ^{13}C -NMR (100 MHz, $CDCl_3$): δ 162.50, 155.89, 141.00, 132.82, 132.75, 132.09, 130.79, 130.53, 128.77, 126.54, 124.88, 124.36, 123.87, 123.44, 112.74, 107.08, 56.10. **HRMS-ESI:** Calcd. for $C_{17}H_{14}ClN_3O_2Na$ $[M+Na]^+$ 350.0672, found 350.0655.

2-Methoxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)-1-naphthamide (3na): colorless solid, 1H -NMR



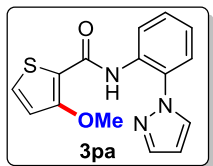
(500 MHz, $CDCl_3$): δ 10.39 (s, 1H), 8.80 (d, $J = 8.3$ Hz, 1H), 8.02-8.00 (m, 1H), 7.89-7.87 (m, 1H), 7.80-7.77 (m, 2H), 7.56 (s, 1H), 7.48-7.43 (m, 2H), 7.36-7.33 (m, 2H), 7.26-7.20 (m, 2H), 6.43-6.42 (m, 1H), 3.79 (s, 3H). ^{13}C -NMR (125 MHz, $CDCl_3$): δ 165.68, 153.83, 132.19, 131.66, 130.26, 129.67, 128.86, 128.33, 127.97, 127.58, 124.39, 124.27, 124.13, 123.13, 123.51, 123.12, 120.42, 112.88, 106.96, 56.51. **HRMS-ESI:** Calcd. for $C_{21}H_{18}N_3O_2$ $[M+H]^+$ 344.1394, found 344.1397.

3-Methoxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)pyridine-4-carboxamide (3oa): colorless semi-



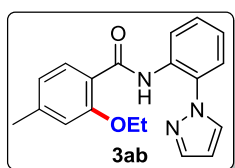
solid, $^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 10.73 (s, 1H), 8.60 (dd, $J = 8.3, 1.2$ Hz, 1H), 8.13 (d, $J = 8.5$ Hz, 1H), 7.80 (d, $J = 1.5$ Hz, 1H), 7.74-7.73 (m, 1H), 7.46-7.42 (m, 1H), 7.31-7.28 (m, 1H), 7.21-7.17 (m, 1H), 7.05 (dd, $J = 8.5, 1.9$ Hz, 1H), 6.94 (d, $J = 1.9$ Hz, 1H), 6.51-6.50 (m, 1H), 3.87 (s, 3H). $^{13}\text{C-NMR}$ (125 MHz, CDCl_3): δ 162.92, 157.74, 141.00, 138.96, 133.61, 130.82, 130.51, 128.79, 124.88, 124.29, 123.90, 121.50, 120.66, 111.97, 107.00, 56.09. **HRMS-ESI:** Calcd. for $\text{C}_{16}\text{H}_{14}\text{N}_4\text{O}_2$ $[\text{M}+\text{H}]^+$ 317.1006, found 317.1014.

3-Methoxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)thiophene-2-carboxamide (3pa): colorless semi-



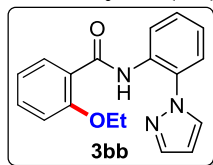
solid, $^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 10.11 (s, 1H), 8.58 (dd, $J = 8.3, 1.2$ Hz, 1H), 7.82 (d, $J = 1.7$ Hz, 1H), 7.72 (d, $J = 2.3$ Hz, 1H), 7.43-7.38 (m, 2H), 7.29-7.26 (m, 1H), 7.15 (td, $J = 7.6, 1.3$ Hz, 1H), 6.81 (d, $J = 5.5$ Hz, 1H), 6.51-6.50 (m, 1H), 3.90 (s, 3H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 160.15, 156.79, 140.90, 133.14, 130.80, 130.13, 128.86, 125.10, 123.82, 123.31, 117.07, 115.44, 107.00, 58.77. **HRMS-ESI:** Calcd. for $\text{C}_{15}\text{H}_{14}\text{N}_3\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$ 300.0807, found 300.0795.

2-Ethoxy-4-methyl-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3ab): colorless semi-solid, $^1\text{H-}$



NMR (400 MHz, CDCl_3): δ 10.56 (s, 1H), 8.50 (dd, $J = 8.3, 1.2$ Hz, 1H), 8.04 (d, $J = 8.0$ Hz, 1H), 7.74-7.71 (m, 2H), 7.44-7.40 (m, 1H), 7.31 (dd, $J = 8.0, 1.5$ Hz, 1H), 7.20-7.16 (m, 1H), 6.88-6.84 (m, 1H), 6.74 (s, 1H), 6.45-6.44 (m, 1H), 4.15 (q, $J = 7.0$ Hz, 2H), 2.36 (s, 3H), 1.33 (t, $J = 7.0$ Hz, 3H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 164.25, 156.60, 143.98, 140.88, 132.68, 132.35, 131.06, 130.61, 128.45, 124.84, 124.66, 124.29, 121.89, 119.71, 113.11, 107.02, 64.48, 21.78, 14.30. **HRMS-ESI:** Calcd. for $\text{C}_{19}\text{H}_{20}\text{N}_3\text{O}_2$ $[\text{M}+\text{H}]^+$ 322.1550, found 322.1549.

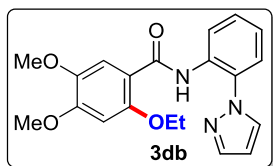
2-Ethoxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3bb): colorless semi-solid, $^1\text{H-NMR}$



(400 MHz, CDCl_3): δ 10.67 (s, 1H), 8.51 (dd, $J = 8.3, 0.9$ Hz, 1H), 8.14 (dd, $J = 7.8, 1.8$ Hz, 1H), 7.75-7.73 (m, 2H), 7.45-7.40 (m, 2H), 7.33 (dd, $J = 8.0, 1.5$ Hz, 1H), 7.22-7.18 (m, 1H), 7.06-7.02 (m, 1H), 6.95-6.93 (m,

1H), 6.47-6.46 (m, 1H), 4.17 (q, $J = 7.0$ Hz, 2H), 1.35 (t, $J = 7.0$ Hz, 3H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 164.25, 156.63, 140.84, 133.10, 132.54, 132.36, 130.96, 130.67, 128.53, 124.76, 124.66, 124.48, 122.46, 120.98, 112.37, 107.11, 64.56, 14.30.

2-Ethoxy-3,4-dimethoxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3bb): colorless semi-

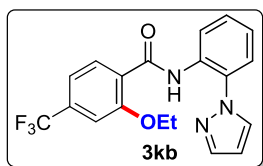


solid, $^1\text{H-NMR}$ (500 MHz, CDCl_3): δ 10.57 (s, 1H), 8.46–8.44 (m, 1H), 7.766-7.762 (m, 1H), 7.72-7.71 (m, 2H), 7.44-7.41 (m, 1H), 7.33-7.31 (m, 1H), 7.25-7.18 (m, 1H), 6.49, (s, 1H), 6.47-6.46 (m, 1H), 4.14 (q, $J = 7.0$ Hz, 2H), 3.91 (s, 3H), 3.88 (s, 3H), 1.32 (t, $J = 7.0$ Hz, 3H). $^{13}\text{C-NMR}$

(125 MHz, CDCl_3): δ 163.92, 152.81, 151.92, 143.42, 140.86, 132.81, 131.12, 130.74, 128.57, 125.09, 124.75, 124.38, 114.04, 113.95, 107.08, 97.94, 65.78, 56.29, 56.14, 14.45.

HRMS-ESI: Calcd. for $\text{C}_{20}\text{H}_{22}\text{N}_3\text{O}_4[\text{M}+\text{H}]^+$ 388.1605, found 368.1641.

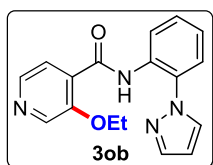
2-Ethoxy-4trifluoromethyl-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3kb): colorless semi-



solid, $^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 10.81 (s, 1H), 8.54 (dd, $J = 8.3, 1.2$ Hz, 1H), 8.20 (d, $J = 8.0$ Hz, 1H), 7.76-7.74 (m, 2H), 7.46-7.42 (m, 1H), 7.33 (dd, $J = 8.0, 1.5$ Hz, 1H), 7.31-7.29 (m, 1H), 7.25-7.20 (m, 1H), 7.17 (s, 1H), 6.48-6.47 (m, 1H), 4.23 (q, $J = 7.0$ Hz, 2H), 1.40 (t, $J = 7.0$ Hz, 3H). $^{13}\text{C-NMR}$ (125

MHz, CDCl_3): δ 163.06, 156.55, 141.02, 134.46 (q, $J_{\text{C-F}}$ 31.4 Hz), 132.99, 132.00, 130.72, 130.49, 128.44, 126.07, 124.78, 124.49, 124.28, 123.51 (q, $J_{\text{C-F}}$ 274 Hz), 117.65 (q, $J_{\text{C-F}}$ 4.1 Hz), 109.35 (q, $J_{\text{C-F}}$ 4.0 Hz), 107.26, 65.17, 14.18.

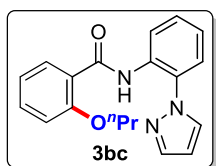
3-Ethoxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)pyridine-4-carboxamide (3ob): colorless semi-solid,



$^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 10.66 (s, 1H), 8.50 (dd, $J = 8.2, 1.1$ Hz, 1H), 8.06 (d, $J = 8.4$ Hz, 1H), 7.74-7.73 (m, 2H), 7.45-7.40 (m, 1H), 7.32 (dd, $J = 8.0, 1.5$ Hz, 1H), 7.22-7.18 (m, 1H), 7.03 (d, $J = 8.4, 1.9$ Hz, 1H), 6.94 (d, $J = 1.9$ Hz, 1H), 6.47-6.46 (m, 1H), 4.17 (q, $J = 7.0$ Hz, 2H), 1.38 (t, $J = 7.0$ Hz, 3H). $^{13}\text{C-NMR}$

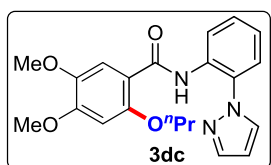
(100 MHz, CDCl_3): δ 163.30, 157.00, 140.93, 138.70, 133.46, 132.25, 130.87, 130.53, 128.42, 124.59, 124.56, 124.49, 121.28, 112.93, 107.14, 65.07, 14.15.

2-Propoxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3bc): colorless semi-solid, $^1\text{H-NMR}$



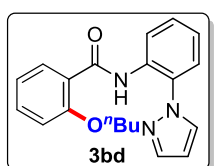
(400 MHz, CDCl_3): δ 10.63 (s, 1H), 8.52–8.50 (m, 1H), 8.13–8.11 (m, 1H), 7.73–7.72 (m, 2H), 7.45–7.40 (m, 2H), 7.33–7.31 (m, 1H), 7.22–7.18 (m, 1H), 7.06–7.02 (m, 1H), 6.96–6.94 (m, 1H), 6.46–6.45 (m, 1H), 4.05–4.01 (m, 2H), 1.78–1.69 (m, 2H), 0.94–0.91 (m, 3H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 164.30, 156.81, 140.91, 132.99, 132.45, 132.28, 131.01, 130.52, 128.41, 124.64, 124.43, 122.68, 120.99, 112.54, 107.03, 70.60, 21.84, 10.22. **HRMS-ESI:** Calcd. for $\text{C}_{19}\text{H}_{20}\text{N}_3\text{O}_2$ $[\text{M}+\text{H}]^+$ 322.1556, found 322.1573.

2-Propoxy-4,5-dimethoxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3dc): colorless semi-



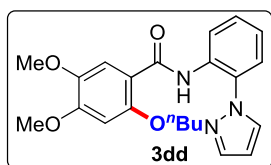
solid, $^1\text{H-NMR}$ (500 MHz, CDCl_3): δ 10.56 (s, 1H), 8.45 (dd, $J = 8.3, 1.1$ Hz, 1H), 7.74 (d, $J = 1.6$ Hz, 1H), 7.72 (d, $J = 2.2$ Hz, 1H), 7.70 (s, 1H), 7.44–7.41 (m, 1H), 7.33–7.32 (m, 1H), 7.21–7.18 (m, 1H), 6.5 (s, 1H), 6.46–6.45 (m, 1H), 4.01–3.99 (m, 2H), 3.92 (s, 3H), 3.89 (s, 3H), 1.75–1.67 (m, 2H), 0.93–0.90 (m, 3H). $^{13}\text{C-NMR}$ (125 MHz, CDCl_3): δ 163.96, 152.79, 152.16, 143.42, 140.93, 132.67, 131.20, 130.61, 128.44, 124.98, 124.78, 124.38, 114.08, 113.94, 107.04, 98.04, 71.84, 56.29, 56.13, 22.02, 10.27.

2-Butoxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3bd): colorless semi-solid, $^1\text{H-NMR}$



(400 MHz, CDCl_3): δ 10.63 (s, 1H), 8.52–8.50 (m, 1H), 8.13–8.11 (m, 1H), 7.74–7.72 (m, 2H), 7.45–7.40 (m, 2H), 7.34–7.32 (m, 1H), 7.22–7.18 (m, 1H), 7.06–7.02 (m, 1H), 6.96–6.94 (m, 1H), 6.46–6.45 (m, 1H), 4.09–4.05 (m, 2H), 1.72–1.65 (m, 2H), 1.41–1.31 (m, 2H), 0.92–0.89 (m, 3H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 164.31, 156.80, 140.92, 132.99, 132.42, 132.29, 131.00, 130.49, 128.38, 124.63, 124.42, 122.68, 120.96, 112.50, 107.04, 68.85, 30.43, 19.00, 13.76.

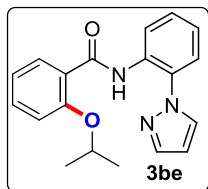
2-Butoxy-4,5-dimethoxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3dd): colorless semi-



solid, $^1\text{H-NMR}$ (500 MHz, CDCl_3): δ 10.55 (s, 1H), 8.46–8.45 (m, 1H), 7.75–7.72 (m, 2H), 7.70 (s, 1H), 7.44–7.41 (m, 1H), 7.34–7.32 (m, 1H), 7.21–7.18 (m, 1H), 6.50 (s, 1H), 6.46–6.45 (m, 1H), 4.05–4.02 (m, 2H), 3.92 (s, 3H), 3.89 (s, 3H), 1.68–1.62 (m, 2H), 1.39–1.31 (m, 2H), 0.92–0.89 (m, 3H). $^{13}\text{C-NMR}$ (125 MHz, CDCl_3): δ 163.98, 152.78, 152.15, 143.39, 140.94, 132.62,

131.19, 130.59, 128.41, 124.97, 124.78, 124.39, 114.05, 113.96, 107.06, 97.97, 70.03, 56.29, 56.13, 30.60, 19.01, 13.80. **HRMS-ESI:** Calcd. for $C_{22}H_{26}N_3O_4$ $[M+H]^+$ 396.1923, found 396.1943.

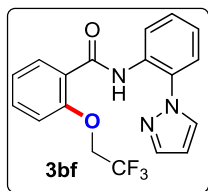
2-Isopropoxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3be): colorless solid, **1H -NMR** (400



MHz, $CDCl_3$): δ 10.48 (s, 1H), 8.43 (dd, $J = 8.2, 1.0$ Hz, 1H), 8.13 (dd, $J = 7.8, 1.8$ Hz, 1H), 7.74-7.72 (m, 2H), 7.45-7.39 (m, 2H), 7.35 (dd, $J = 7.9, 1.5$ Hz, 1H), 7.24-7.19 (m, 1H), 7.06-7.02 (m, 1H), 6.96-6.94 (m, 1H), 6.45-6.44 (m, 1H), 4.62 (q, $J = 6.1$ Hz, 1H), 1.31 (d, $J = 6.1$ Hz, 6H) **^{13}C -NMR** (100

MHz, $CDCl_3$): δ 164.49, 156.03, 141.13, 132.95, 132.38, 132.10, 131.40, 130.52, 128.27, 125.08, 124.76, 124.67, 123.34, 120.97, 114.12, 107.14, 72.35, 21.79. **HRMS-ESI:** Calcd. for $C_{19}H_{20}N_3O_2$ $[M+H]^+$ 322.1550, found 322.1551.

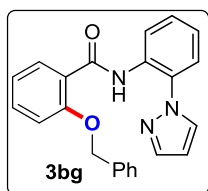
2-(2,2,2-Trifluoroethoxy)-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3bf): colorless solid,



1H -NMR (400 MHz, $CDCl_3$): δ 10.64 (s, 1H), 8.57 (d, $J = 8.1$ Hz, 1H), 7.98 (dd, $J = 7.7, 1.7$ Hz, 1H), 7.78-7.72 (m, 1H), 7.48-7.41 (m, 2H), 7.33 (dd, $J = 7.9, 1.5$ Hz, 1H), 7.23-7.15 (m, 2H), 7.02 (d, $J = 8.3$ Hz, 1H), 6.47-6.46 (m, 1H), 4.46 (q, $J_{H-F} = 8.2$ Hz, 2H). **^{13}C -NMR** (100 MHz, $CDCl_3$): δ 163.74,

155.23, 140.97, 132.82, 132.05, 131.89, 130.42, 130.31, 128.34, 125.37, 124.57, 124.08, 123.78, 123.49, 123.07 (q, $J_{C-F} = 279.9$ Hz), 114.69, 107.12, 67.37 (q, $J_{C-F} = 36$ Hz). **HRMS-ESI:** Calcd. for $C_{18}H_{15}F_3N_3O_2$ $[M+H]^+$ 361.0913, found 361.0923.

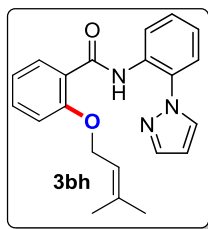
2-benzyloxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3bg): colorless solid, **1H -NMR** (400



MHz, $CDCl_3$): δ 10.84 (s, 1H), 8.62 (dd, $J = 8.3, 1.0$ Hz, 1H), 8.16 (dd, $J = 7.8, 1.8$ Hz, 1H), 7.67 (d, $J = 2.3$ Hz, 1H), 7.57 (d, $J = 1.8$ Hz, 1H), 7.46-7.42 (m, 1H), 7.34-7.27 (m, 7H), 7.21-7.17 (m, 1H), 7.05-7.01 (m, 1H), 6.86-6.83 (m, 1H), 6.36-6.34 (m, 1H), 5.25 (s, 2H). **^{13}C -NMR** (100 MHz, $CDCl_3$): δ

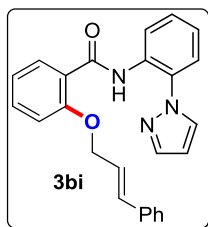
164.10, 156.33, 141.12, 136.31, 132.97, 132.39, 130.69, 130.57, 128.69, 128.62, 127.92, 126.46, 124.87, 124.23, 124.14, 122.86, 121.42, 113.55, 107.00, 70.63. **HRMS-ESI:** Calcd. for $C_{23}H_{20}N_3O_2$ $[M+H]^+$ 370.1556, found 370.1583.

2-(3-methylbut-2-en-1-yl)oxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3bh): colorless



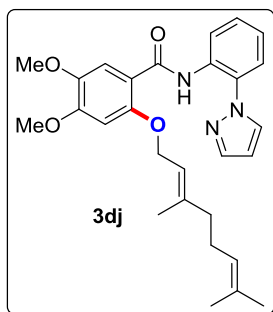
semi-solid, $^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 10.71 (s, 1H), 8.56 (dd, $J = 8.3$, 1.0 Hz, 1H), 8.17 (dd, $J = 7.8$, 1.8 Hz, 1H), 7.74-7.72 (m, 2H), 7.45-7.38 (m, 2H), 7.32 (dd, $J = 7.8$, 1.5 Hz, 1H), 7.22-7.17 (m, 1H), 7.06-7.02 (m, 1H), 6.92-6.90 (m, 1H), 6.47-6.46 (m, 1H), 5.31-5.29 (m, 1H), 4.67-4.66 (m, 2H), 1.73 (s, 3H), 1.71 (s, 3H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 164.14, 156.61, 141.00, 137.20, 132.96, 132.81, 132.42, 130.92, 130.56, 128.50, 124.84, 124.38, 124.25, 122.52, 121.00, 119.64, 112.97, 106.99, 66.09, 25.68, 18.33. **HRMS-ESI:** Calcd. for $\text{C}_{21}\text{H}_{22}\text{N}_3\text{O}_2$ $[\text{M}+\text{H}]^+$ 348.1712, found 348.1726.

2-cinnamyloxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3bi): colorless solid, $^1\text{H-NMR}$



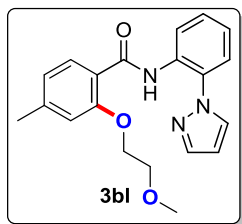
(400 MHz, CDCl_3): δ 10.82 (s, 1H), 8.62-8.60 (m, 1H), 8.18-8.16 (m, 1H), 7.72-7.70 (m, 2H), 7.45-7.38 (m, 2H), 7.35-7.17 (m, 7H), 7.07-7.04 (m, 1H), 7.01-6.99 (m, 1H), 6.63 (d, $J = 15.9$ Hz, 1H), 6.43-6.42 (m, 1H), 6.34 (td, $J = 15.9$, 5.4 Hz, 1H), 4.85 (d, $J = 5.4$ Hz, 2H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 164.06, 156.46, 141.12, 136.09, 133.16, 133.04, 132.87, 132.44, 130.71, 130.60, 128.65, 124.57, 128.08, 126.60, 124.73, 124.24, 123.86, 122.77, 121.36, 113.17, 107.04, 69.66. **HRMS-ESI:** Calcd. for $\text{C}_{25}\text{H}_{21}\text{N}_3\text{O}_2\text{Na}$ $[\text{M}+\text{Na}]^+$ 418.1512, found 418.1531.

2-((3,7-dimethylocta-2,6-dien-1-yl)oxy)-4,5-dimethoxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)-



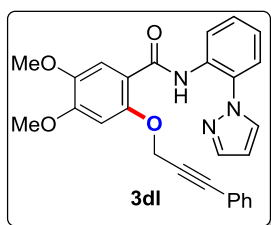
benzamide (3dj): colorless semi-solid, $^1\text{H-NMR}$ (500 MHz, CDCl_3): δ 10.62 (s, 1H), 8.48-8.47 (m, 1H), 7.70-7.69 (m, 1H), 7.66-7.64 (m, 2H), 7.37-7.34 (m, 1H), 7.24-7.22 (m, 1H), 7.12-7.09 (m, 1H), 6.40-6.39 (m, 2H), 5.25-5.22 (m, 1H), 4.95-4.93 (m, 1H), 4.60-4.59 (m, 2H), 3.81 (s, 1H), 3.80 (s, 3H), 1.99-1.94 (m, 4H), 1.64 (s, 3H), 1.55 (s, 3H), 1.48 (s, 3H). $^{13}\text{C-NMR}$ (125 MHz, CDCl_3): δ 163.83, 152.60, 151.92, 143.32, 141.00, 140.53, 133.24, 132.02, 130.88, 130.70, 128.63, 125.18, 124.24, 124.06, 123.52, 119.94, 113.94, 106.98, 98.42, 67.02, 56.27, 56.00, 39.44, 26.24, 25.62, 17.71, 16.76. **HRMS-ESI:** Calcd. for $\text{C}_{28}\text{H}_{33}\text{N}_3\text{O}_4\text{Na}$ $[\text{M}+\text{Na}]^+$ 498.2369, found 498.2371.

2-(2-methoxyethoxy)-4-methoxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3ak): colorless



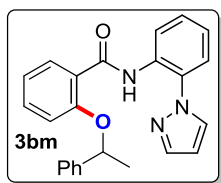
semi-solid, $^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 10.52 (s, 1H), 8.36-8.34 (m, 1H), 8.02-8.00 (m, 1H), 7.77-7.74 (m, 2H), 7.45-7.36 (m, 2H), 7.24-7.20 (m, 1H), 6.89-6.87 (m, 1H), 6.80 (s, 1H), 6.46-6.45 (m, 1H), 4.23-4.21 (m, 2H), 3.69-3.66 (m, 2H), 3.31 (s, 3H), 2.37 (s, 3H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 164.21, 156.72, 144.08, 140.51, 132.31, 132.24, 131.45, 130.91, 128.51, 125.33, 124.79, 122.47, 119.95, 113.91, 107.08, 70.23, 68.48, 59.16, 21.76. **HRMS-ESI:** Calcd. for $\text{C}_{20}\text{H}_{22}\text{N}_3\text{O}_3[\text{M}+\text{H}]^+$ 352.1656, found 352.1655.

2-((3-phenylprop-2-yn-1-yl)oxy)-4,5-dimethoxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3dl): colorless solid,



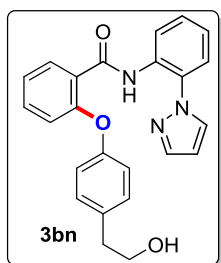
$^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 10.72 (s, 1H), 8.63 (dd, $J = 8.3, 1.3$ Hz, 1H), 7.91-7.90 (m, 1H), 7.75-7.73 (m, 2H), 7.45-7.41 (m, 1H), 7.39-7.36 (m, 2H), 7.34-7.29 (m, 4H), 7.17 (td, $J = 7.6, 1.3$ Hz, 1H), 6.84 (s, 1H), 6.53-6.51 (m, 1H), 4.95 (s, 2H), 3.93 (s, 3H), 3.91 (s, 3H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 163.44, 152.56, 150.75, 143.92, 141.18, 133.42, 131.65, 130.80, 130.45, 129.00, 128.76, 128.45, 125.04, 123.89, 123.68, 121.81, 114.41, 113.90, 107.05, 98.74, 88.67, 83.21, 58.24, 56.27, 56.17. **HRMS-ESI:** Calcd. for $\text{C}_{27}\text{H}_{23}\text{N}_3\text{O}_4 \text{Na}[\text{M}+\text{Na}]^+$ 476.1565, found 476.1586.

2-(1-phenylethoxy)-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3bm): colorless semi-solid,



$^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 10.68 (s, 1H), 8.46 (d, $J = 8.2$ Hz, 1H), 8.07 (dd, $J = 7.8, 1.7$ Hz, 1H), 7.76-7.75 (m, 1H), 7.66-7.65 (m, 1H), 7.46-7.42 (m, 1H), 7.36-7.28 (m, 6H), 7.27-7.21 (m, 2H), 7.00-6.96 (m, 1H), 6.74-6.72 (m, 1H), 6.43-6.42 (m, 1H), 5.37 (q, $J = 6.5$ Hz, 1H), 1.62 (d, $J = 6.5$ Hz, 3H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 164.54, 156.02, 142.13, 141.29, 132.75, 132.05, 132.02, 131.34, 130.41, 128.70, 128.21, 127.71, 125.45, 125.23, 124.74, 124.46, 123.34, 121.18, 114.87, 107.13, 78.37, 24.24.

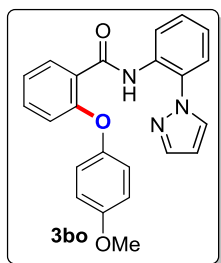
2-(4-(2-hydroxyethyl)phenoxy)-N-(2-(1H-pyrazol-1-yl)phenyl)benzamide (3bn): colorless solid,



$^1\text{H-NMR}$ (400 MHz, CDCl_3): 10.94 (s, 1H), 8.59-8.57 (m, 1H), 8.21 (dd, $J = 1.7, 7.8$ Hz, 1H), 7.67-7.66 (m, 1H), 7.42-7.38 (m, 1H), 7.36-7.32 (m, 1H), 7.26-7.23 (m, 3H), 7.21-7.13 (m, 3H), 6.98-6.96 (m, 2H), 6.79-6.77 (m, 1H), 6.28-6.27 (m, 1H), 3.87 (t, $J = 6.6$ Hz, 2H), 2.88 (t, $J = 6.6$ Hz, 2H), 1.7 (brs, 1H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 163.56, 156.06, 153.81,

141.13, 135.10, 132.97, 132.54, 132.37, 130.56, 130.44, 130.21, 128.37, 124.36, 124.26, 123.85, 123.01, 120.79, 117.24, 106.89, 63.70, 38.50. **HRMS-ESI:** Calcd. for $\text{C}_{24}\text{H}_{22}\text{N}_3\text{O}_3[\text{M}+\text{H}]^+$ 400.1656, found 400.1650.

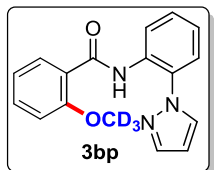
2-(4-methoxyphenoxy)-N-(2-(1H-pyrazol-1-yl)phenyl)benzamide (3bo): colorless solid, $^1\text{H-NMR}$



(400 MHz, CDCl_3): δ 10.96 (s, 1H), 8.62 (δ d, $J = 8.4, 0.9$ Hz, 1H), 8.24 (dd, $J = 7.9, 1.9$ Hz, 1H), 7.66-7.65 (m, 1H), 7.44-7.40 (m, 1H), 7.34-7.29 (m, 1H), 7.26-7.24 (m, 1H), 7.19-7.09 (m, 3H), 7.00-6.93 (m, 4H), 6.71-6.69 (m, 1H), 6.25-6.24 (m, 1H), 3.85 (s, 3H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 163.57, 157.04, 156.90, 148.10, 141.18, 132.95, 132.84, 132.48,

130.64, 130.18, 128.43, 124.50, 124.25, 122.97, 122.42, 122.37, 116.02, 114.94, 106.81, 55.71. **HRMS-ESI:** Calcd. for $\text{C}_{23}\text{H}_{20}\text{N}_3\text{O}_3[\text{M}+\text{H}]^+$ 386.1505, found 386.1519.

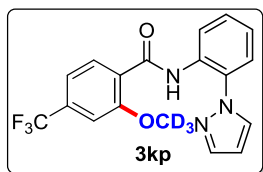
2-Trideuteromethoxy-N-(2-(1H-pyrazol-1-yl)phenyl)benzamide (3bp): colorless solid, $^1\text{H-NMR}$



(400 MHz, CDCl_3): δ 10.75 (s, 1H), 8.64 (dd, $J = 8.3, 1.1$ Hz, 1H), 8.20 (dd, $J = 7.8, 1.8$ Hz, 1H), 7.81-7.80 (m, 1H), 7.74-7.73 (m, 1H), 7.47-7.42 (m, 2H), 7.31-7.28 (m, 1H), 7.19 (td, $J = 7.8, 1.5$ Hz, 1H), 7.09-7.05 (m, 1H), 6.93 (dd, $J = 8.3, 0.8$ Hz, 1H), 6.50-6.49 (m, 1H). $^2\text{D-NMR}$ (76 MHz, CDCl_3): δ 3.83 (s).

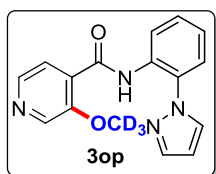
$^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 163.84, 157.38, 140.96, 133.24, 132.46, 130.83, 130.55, 128.80, 125.05, 124.06, 123.84, 121.94, 121.14, 111.18, 106.99. **LRMS:** Calcd. for $\text{C}_{17}\text{H}_{12}\text{D}_3\text{N}_3\text{O}_2\text{Na}[\text{M}+\text{Na}]^+$ 319.1, found 319.3.

2-Trideuteromethoxy-4-trifluoromethyl-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3bp):



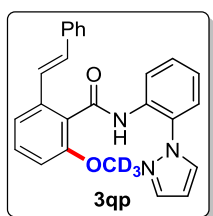
colorless semi-solid, $^1\text{H-NMR}$ (500 MHz, CDCl_3): δ 10.89 (s, 1H), 8.63-8.62 (m, 1H), 8.28 (d, $J = 8.1$ Hz, 1H), 7.814-7.810 (m, 1H), 7.76-7.75 (m, 1H), 7.47-7.43 (m, 1H), 7.34-7.31 (m, 1H), 7.21 (td, $J = 7.5, 1.3$ Hz, 1H), 7.16 (s, 1H), 6.52-6.51 (m, 1H). $^2\text{D-NMR}$ (76 MHz, CDCl_3): δ 3.91 (s). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 162.57, 157.26, 141.03, 134.48 (q, $J_{\text{C-F}} = 33.0$ Hz), 133.15, 132.61, 130.74, 130.46, 128.73, 125.37, 124.82, 124.67, 124.49, 123.85, 123.46 (q, $J_{\text{C-F}} = 273$ Hz), 117.80 (q, $J_{\text{C-F}} = 3.6$ Hz), 108.30 (q, $J_{\text{C-F}} = 3.6$ Hz), 107.13.

3-Trideuteromethoxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)pyridine-4-carboxamide (3op):



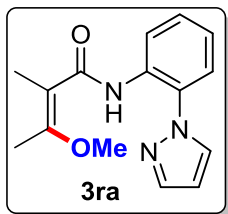
colorless semi-solid, $^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 10.73 (s, 1H), 8.60 (dd, $J = 8.4, 1.0$ Hz, 1H), 8.13 (d, $J = 8.4$ Hz, 1H), 7.80 (d, $J = 1.7$ Hz, 1H), 7.73 (d, $J = 2.4$ Hz, 1H), 7.46-7.41 (m, 1H), 7.29 (dd, $J = 7.9, 1.5$ Hz, 1H), 7.21-7.17 (m, 1H), 7.05 (dd, $J = 8.5, 1.9$ Hz, 1H), 6.93 (d, $J = 1.9$ Hz, 1H), 6.56-6.50 (m, 1H). $^2\text{D-NMR}$ (76 MHz, CDCl_3): δ 3.85 (s). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 162.89, 157.72, 140.97, 138.93, 133.59, 132.91, 130.79, 130.49, 128.76, 124.87, 124.26, 123.86, 121.46, 120.64, 111.94, 107.07.

2-Trideuteromethoxy-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)-6-styrylbenzamide (3qp): colorless



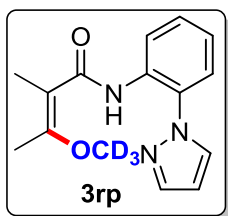
solid, $^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 10.18 (s, 1H), 8.56 (dd, $J = 8.2, 1.2$ Hz, 1H), 7.60 (d, $J = 2.3$ Hz, 1H), 7.51 (d, $J = 1.6$ Hz, 1H), 7.39-7.35 (m, 1H), 7.31-7.29 (m, 2H), 7.25 (m, 4H), 7.19-7.11 (m, 4H), 6.95 (d, $J = 16$ Hz, 1H), 6.74 (dd, $J = 7.8, 1.0$ Hz, 1H), 6.22-6.21 (m, 1H). $^2\text{D-NMR}$ (76 MHz, CDCl_3): δ 3.69 (s). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 165.78, 156.44, 141.00, 137.10, 136.88, 131.74, 131.57, 130.39, 130.12, 129.82, 128.53, 128.22, 127.84, 126.87, 125.73, 125.37, 124.47, 123.82, 122.99, 118.05, 109.83, 106.97.

(Z)-3-Methoxy-N-(2-(1H-pyrazol-1-yl)phenyl)2-methylbut-2-enamide (3ra): colorless solid,



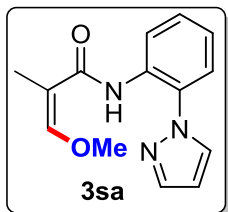
$^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 10.35 (s, 1H), 8.47 (dd, $J = 8.4, 1.2$ Hz, 1H), 7.71-7.70 (m, 1H), 7.62-7.61 (m, 1H), 7.33-7.28 (m, 1H), 7.16 (dd, $J = 7.8, 1.5$ Hz, 1H), 7.06-7.01 (m, 1H), 6.42-6.40 (m, 1H), 3.50 (s, 3H), 1.94 (s, 3H), 1.77 (s, 3H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 160.05, 157.26, 140.89, 133.92, 130.86, 130.04, 128.81, 125.24, 123.25, 109.14, 106.85, 55.80, 15.07, 14.22. **HRMS:** Calcd. for $\text{C}_{15}\text{H}_{17}\text{N}_3\text{O}_2\text{Na}$ $[\text{M}+\text{Na}]^+$ 294.1218, found 294.1238.

(Z)-3-Trideuteromethoxy-N-(2-(1H-pyrazol-1-yl)phenyl)2-methylbut-2-enamide (3rp):



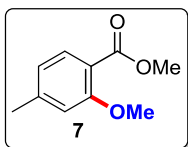
colorless solid, $^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 10.42 (s, 1H), 8.55 (dd, $J = 8.3, 1.2$ Hz, 1H), 7.78-7.77 (m, 1H), 7.69-7.68 (m, 1H), 7.40-7.36 (m, 1H), 7.24 (dd, $J = 7.8, 1.5$ Hz, 1H), 7.11 (td, $J = 7.5, 1.3$ Hz, 1H), 6.49-6.48 (m, 1H), 2.01 (s, 3H), 1.85 (s, 3H). $^2\text{D-NMR}$ (76 MHz, CDCl_3): δ 3.55 (s). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 166.07, 157.26, 140.88, 133.93, 130.87, 130.05, 128.82, 125.26, 123.25, 109.06, 106.84, 15.08, 14.21.

3-Methoxy-N-(2-(1H-pyrazol-1-yl)phenyl)2-methylacrylamide (3sa): colorless semi-solid,



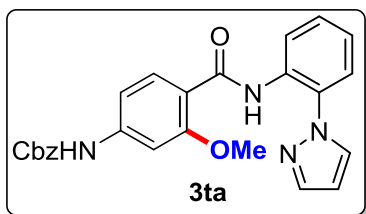
$^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 9.98 (s, 1H), 8.58 (dd, $J = 8.4, 4.8$ Hz, 1H), 7.78 (d, $J = 1.4$ Hz, 1H), 7.68-7.67 (m, 1H), 7.41-7.37 (m, 1H), 7.25 (dd, $J = 7.8, 1.5$ Hz, 1H), 7.14-7.10 (m, 1H), 6.49-6.48 (m, 1H), 6.40 (q, $J = 1.3$ Hz, 1H), 3.67 (s, 3H), 1.74 (d, $J = 1.3$ Hz, 3H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 164.93, 151.17, 140.80, 133.79, 130.87, 129.95, 128.97, 125.40, 123.39, 122.92, 108.82, 106.97, 61.29, 14.74.

Methyl-2-methoxy-4-methyl benzoate (7): colorless oil, $^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 7.73-



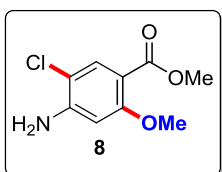
7.71(m, 1H), 6.80-6.78 (m, 2H), 3.89 (s, 3H), 3.87 (s, 3H), 2.38 (s, 3H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 166.61, 159.36, 144.63, 131.86, 120.96, 112.78, 55.94, 51.85, 21.95.

2-methoxy-4-benzylcarbamate-*N*-(2-(1*H*-pyrazol-1-yl)phenyl)benzamide (3qa): colorless



solid, $^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 10.63 (s, 1H), 8.57 (dd, $J = 8.4, 1.2$ Hz, 1H), 8.10 (d, $J = 8.5$ Hz, 1H), 7.82-7.81 (m, 1H), 7.73-7.72 (m, 1H), 7.49 (s, 1H), 7.44-7.34 (m, 7H), 7.29 (dd, $J = 7.8, 1.3$ Hz, 1H), 7.21-7.17 (td, $J = 7.3, 1.3$ Hz, 1H), 7.02 (s, 1H), 6.71 (dd, $J = 8.5, 2.0$ Hz, 1H), 6.51-6.50 (m, 1H), 5.20 (s, 2H), 3.85 (s, 3H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 163.46, 158.48, 152.95, 142.62, 140.78, 135.66, 133.32, 133.26, 131.01, 130.56, 128.91, 128.69, 128.53, 128.30, 125.18, 124.09, 124.04, 116.50, 110.45, 107.04, 101.01, 67.30, 55.79. **HRMS-ESI:** Calcd. for $\text{C}_{25}\text{H}_{22}\text{N}_4\text{O}_4\text{Na}$ $[\text{M}+\text{Na}]^+$ 465.1539, found 465.1539.

Methyl-4-amino-5-chloro-2-methoxy benzoate (8): colorless solid, $^1\text{H-NMR}$ (400 MHz,

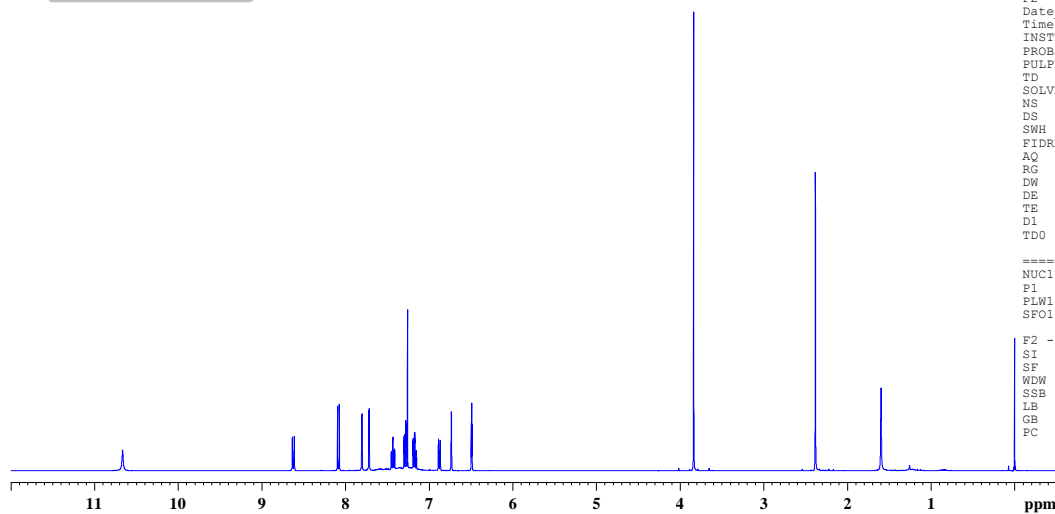
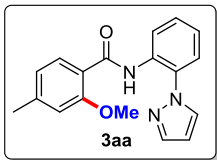


CDCl_3): δ 7.82 (s, 1H), 6.29 (s, 1H), 4.44 (s, 2H), 3.85 (s, 3H), 3.83 (s, 3H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 165.16, 160.19, 147.71, 133.40, 110.03, 109.84, 98.28, 56.16, 51.65.

References:

1. B. J. Liddle, R. M. Silva, T. J. Morin, F. P. Macedo, R. Shukla, S. V. Lindeman, and J. R. Gardinier. *J. Org. Chem.*, 2007, **72**, 5637.
2. M. Shang, S. Z. Sun, H. X. Dai and J.-Q. Yu, *J. Am. Chem. Soc.*, 2014, **136**, 3354.
3. L. D. Tran and O. Daugulis, *Angew. Chem. Int. Ed.* 2012, **51**, 5188.
4. S. Kato, T. Morie, T. Kon, N. Yoshida, T. Karasawa and J. Matsumoto, *J. Med. Chem.*, 1991, **34**, 616.
5. T. Terai, H. Ito, K. Kikuchi and T. Nagano, *Chem. Eur. J.*, 2012, **18**, 7377.

10.6654
8.6359
8.6328
8.6151
8.6119
8.0947
8.0748
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7.8052
7.8015
7.7222
7.7210
7.7162
7.7152
7.4550
7.4511
7.4330
7.4156
7.4117
7.3905
7.2965
7.2807
7.2768
7.2586
7.1929
7.1895
7.1741
7.1707
7.1547
7.1512
6.8888
6.8870
6.8688
6.8670
6.7350
6.4965
6.4914
6.4858
3.8367
2.3821



```
lab mmb-jsk-234
itm-Proton(-5to15) CDCl3 /opt/topspin nmr 10
Current Data Parameters
NAME JSK-234-4-me-OMe
EXPNO 36
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150806
Time 15.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 298.5 K
D1 0.5000000 sec
TDO 1
```

```
===== CHANNEL f1 =====
NUC1 1H
P1 15.70 usec
PLW1 7.7500000 W
SFO1 400.1320007 MHz
```

```
F2 - Processing parameters
SI 65536
SF 400.1300100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
```

1.0
1.0
1.0
1.0
1.1
1.1
1.1
1.0
1.0
1.0
1.0
3.1
3.1
21.74

163.88
144.18
140.92
133.43
132.42
130.84
130.51
128.78
125.12
123.89
123.82
122.01
111.95
106.93
77.35
77.04
76.72
55.60
21.74

```
lab mmbjsk-1-40-1
iitm_carbonsort CDCl3 /opt/topspin nmr 6
```

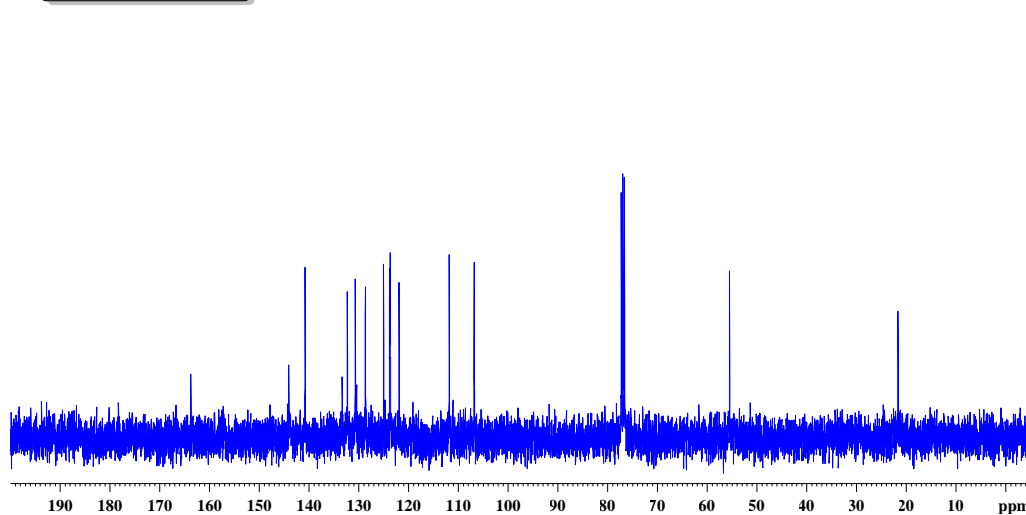
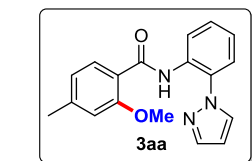
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Current Data Parameters
NAME 4-methyl-OMe
EXPNO 61
PROCNO 1
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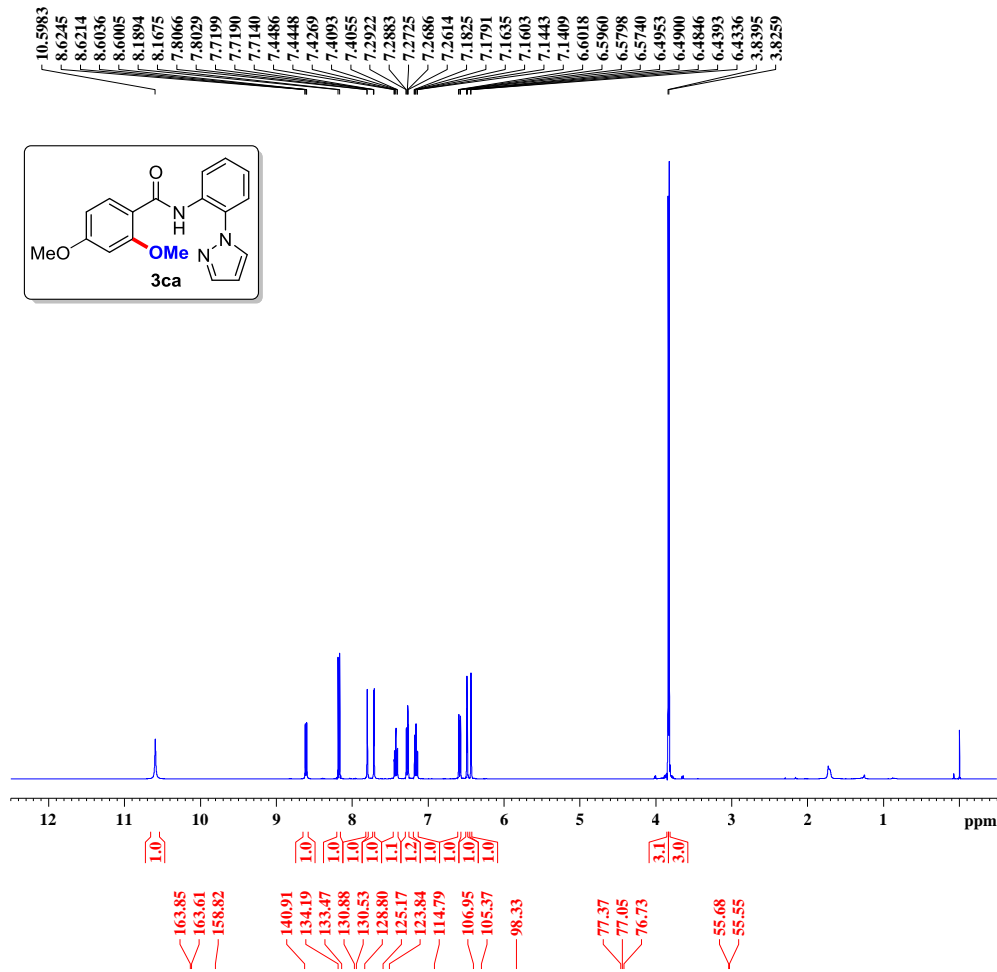
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F2 - Acquisition Parameters
Date_ 20150412
Time 16.09
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 306.1 K
D1 1.0000000 sec
D11 0.0300000 sec
TDO 1
```

```
===== CHANNEL f1 =====
NUC1 13C
P1 15.00 usec
PLW1 76.0000000 W
SFO1 100.6226269 MHz
```

```
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 8.5000000 W
PLW12 0.0850000 W
PLW13 0.0688500 W
SFO2 400.1316005 MHz
```

```
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```





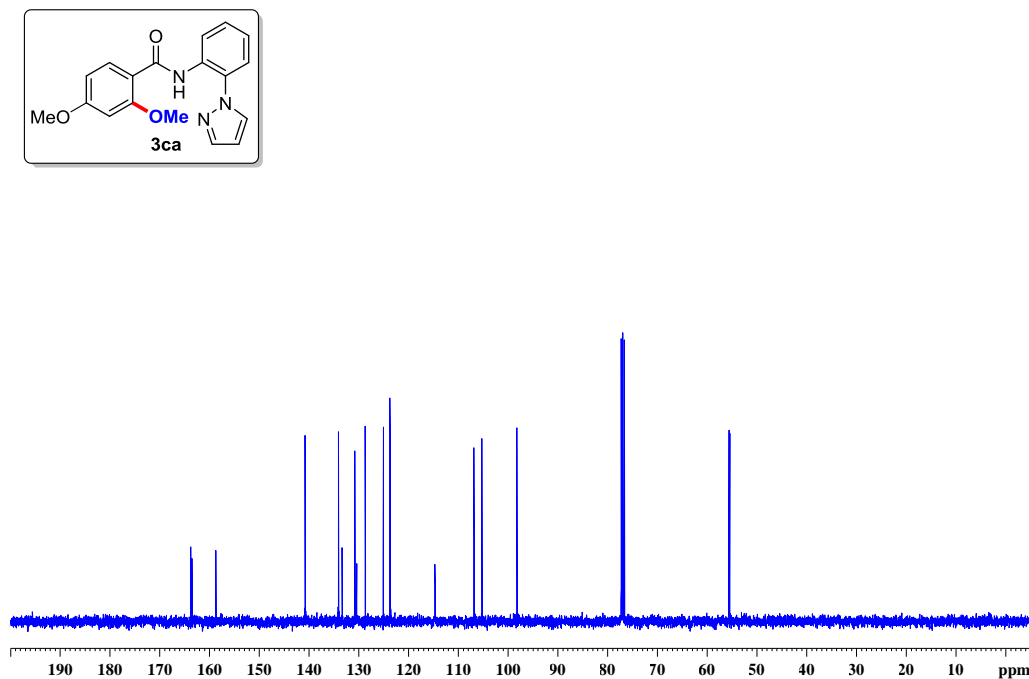
Current Data Parameters
NAME jsk-4-ome-Ome
EXPNO 46
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160210
Time 17.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 138.85
DW 62.400 usec
DE 6.50 usec
TE 297.2 K
D1 0.50000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

lab mmb-jsk-4-ome
iitm_carbonshort CDCl3 /opt/topspin nmr 9



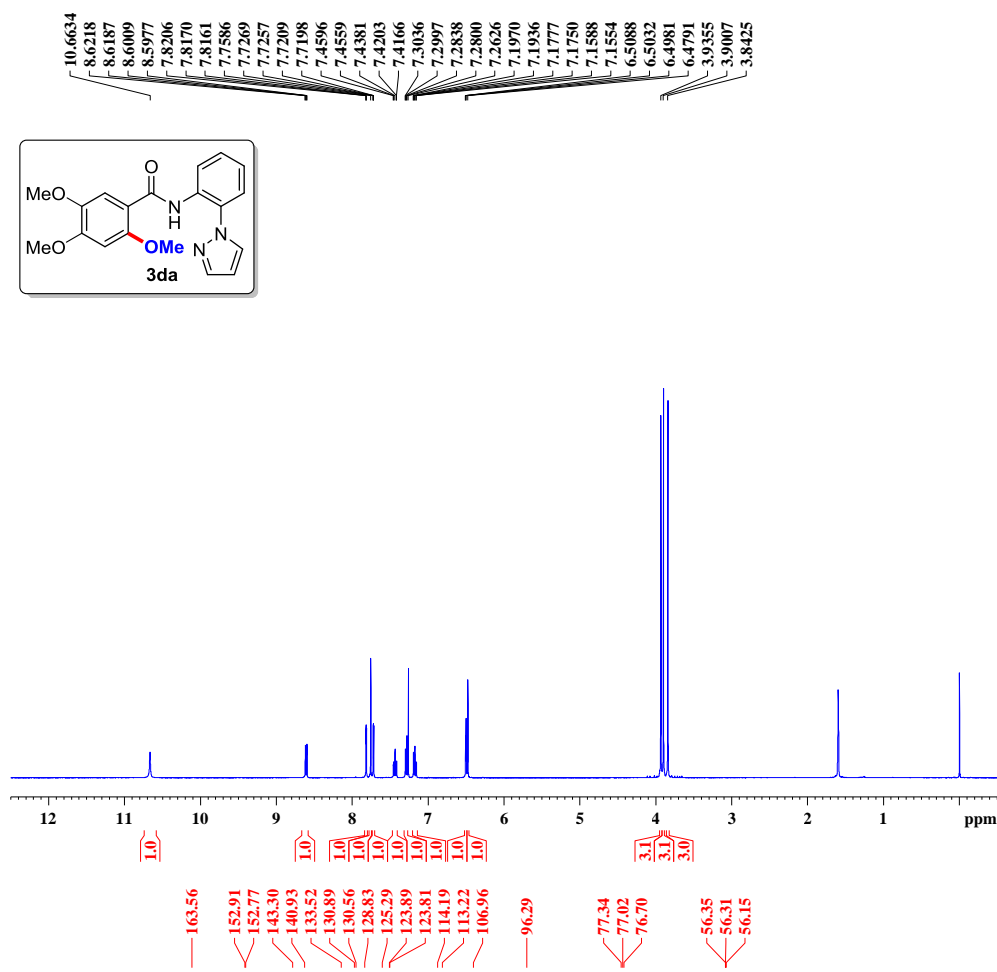
Current Data Parameters
NAME jsk-4-ome-Ome
EXPNO 49
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160210
Time 18.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



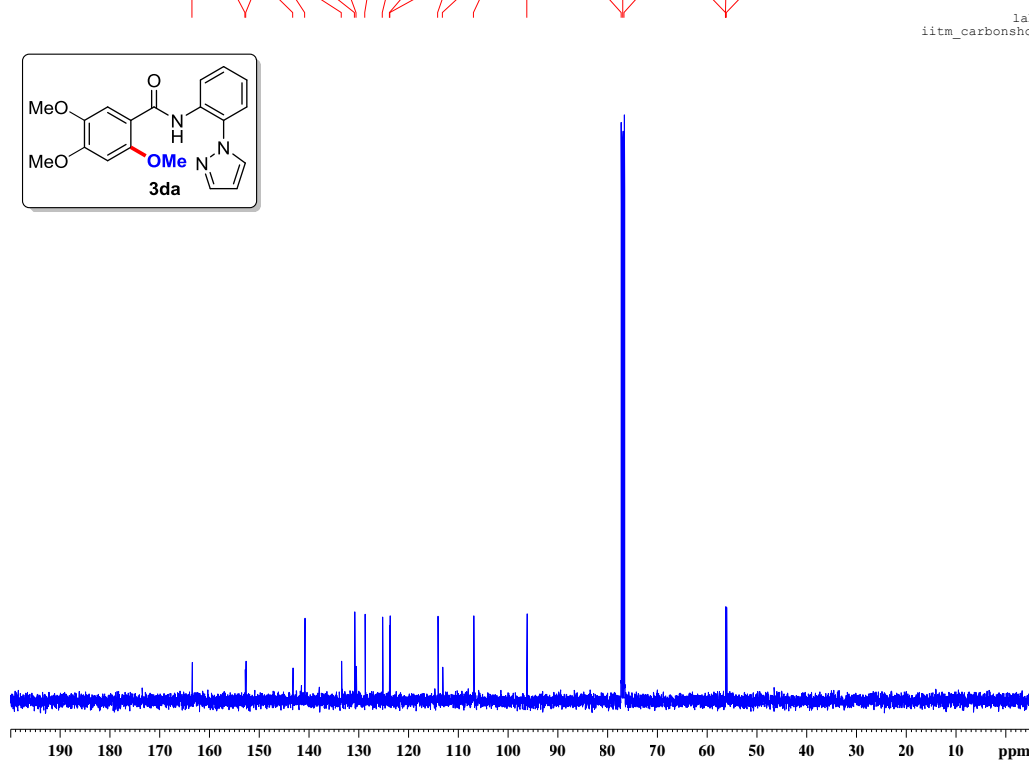
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Current Data Parameters
NAME          3,4-diome
EXPNO         28
PROCNO        1

F2 - Acquisition Parameters
Date_         20160410
Time          3.31
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG            200.34
DW            62.400 usec
DE            6.50 usec
TE            299.1 K
D1            0.50000000 sec
TDO           1

===== CHANNEL f1 =====
SFO1          400.1320007 MHz
NUC1           1H
P1            15.70 usec
PLW1          7.75000000 W

F2 - Processing parameters
SI            65536
SF            400.1300085 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```



```

lab mmb-jsk-34-ome
iitm_carbonshort CDCl3 /opt/topspin nmr 8

Current Data Parameters
NAME          3,4-diome
EXPNO         29
PROCNO        1

F2 - Acquisition Parameters
Date_         20160410
Time          3.44
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            16540
SOLVENT       CDCl3
NS            512
DS            4
SWH           24038.461 Hz
FIDRES        1.453353 Hz
AQ            0.3440320 sec
RG            200.34
DW            20.800 usec
DE            6.50 usec
TE            299.5 K
D1            1.00000000 sec
D11           0.03000000 sec
TDO           1

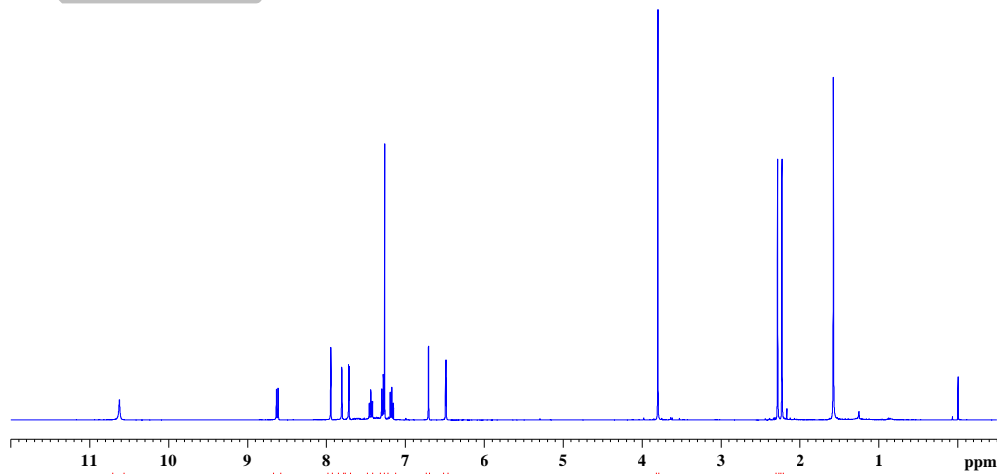
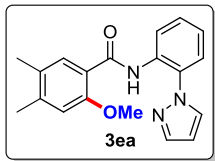
===== CHANNEL f1 =====
SFO1          100.6228289 MHz
NUC1           13C
P1            9.25 usec
PLW1          47.00000000 W

===== CHANNEL f2 =====
SFO2          400.1316005 MHz
NUC2           1H
CPDPRG[2]     waltz16
PCPD2         90.00 usec
PLW2          7.75000000 W
PLW12         0.23583399 W
PLW13         0.11863000 W

F2 - Processing parameters
SI            32768
SF            100.6127690 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

10.6221
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8.6089
7.9426
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7.8007
7.7998
7.7177
7.7166
7.7118
7.7107
7.4573
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7.4180
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7.2998
7.2959
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7.2762
7.1911
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2.2308



Current Data Parameters
NAME JSK-264
EXPNO 186
PROCNO 1

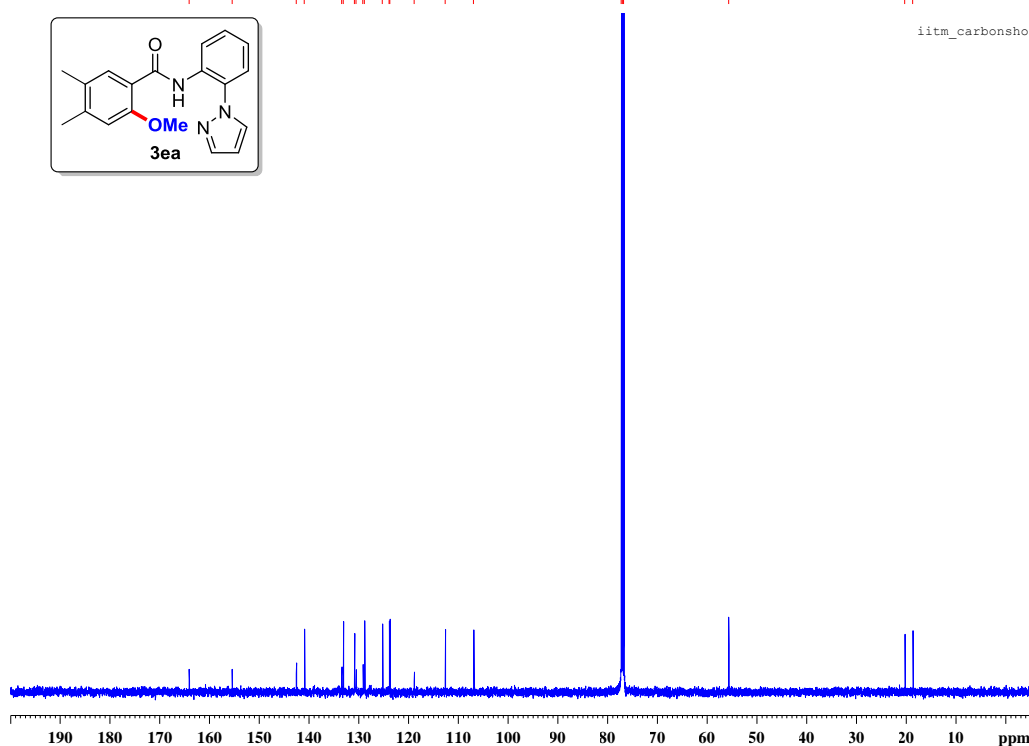
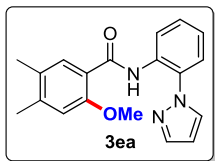
F2 - Acquisition Parameters
Date_ 20150826
Time 11.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 298.9 K
D1 0.50000000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 1H
P1 15.70 usec
PLW1 7.7500000 W
SF01 400.1320007 MHz

F2 - Processing parameters
SI 65536
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

164.08
155.46
142.63
140.96
133.51
133.14
130.91
130.59
129.24
128.88
125.28
123.91
123.82
118.94
112.68
106.96

77.30
77.05
76.80
55.73
20.32
18.70



Lab mmb
jsk-267
iitm_carbonshort CDC13 /opt/topspin iitm 4

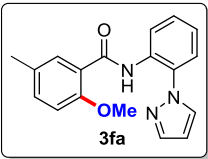
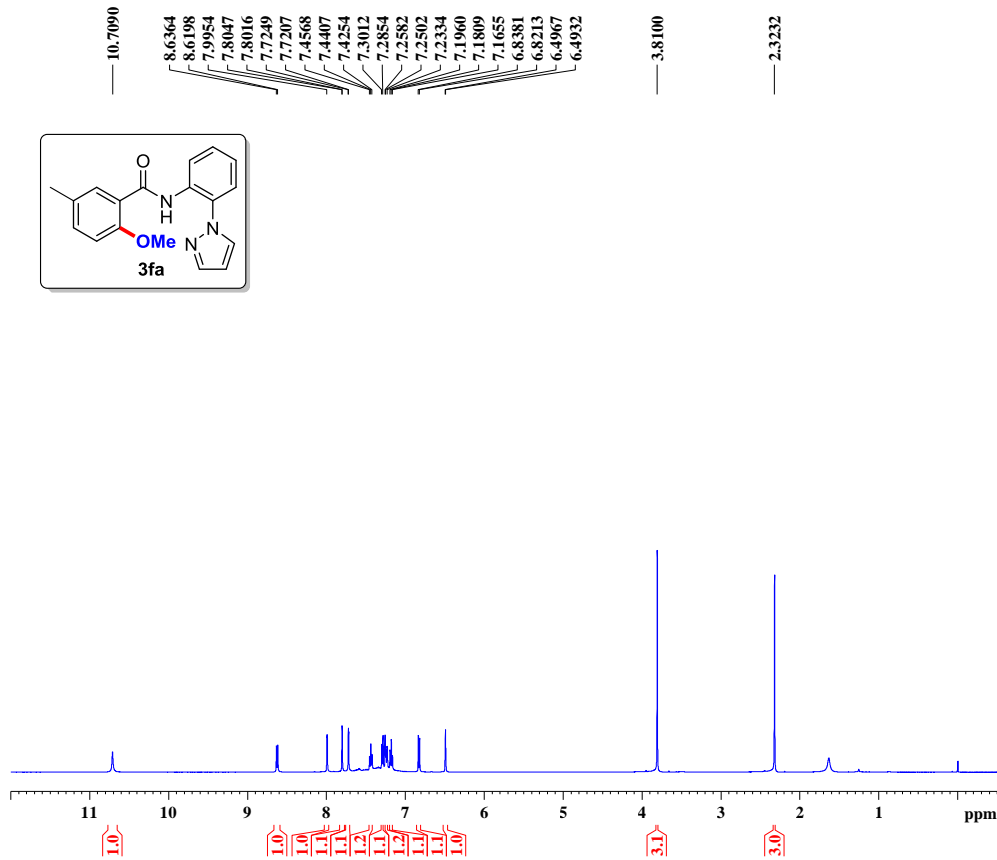
Current Data Parameters
NAME JSK-267
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150826
Time_ 18.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 20480
SOLVENT CDC13
NS 2000
DS 4
SWH 29761.904 Hz
FIDRES 1.453218 Hz
AQ 0.3440640 sec
RG 202.34
DW 16.800 usec
DE 6.50 usec
TE 294.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TDO 1

==== CHANNEL f1 =====
SF01 125.7753932 MHz
NUC1 13C
P1 9.63 usec
PLW1 103.0000000 W

==== CHANNEL f2 =====
SF02 500.1520006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 15.30000019 W
PLW12 0.33006001 W
PLW13 0.21123999 W

F2 - Processing parameters
SI 32768
SF 125.7628180 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



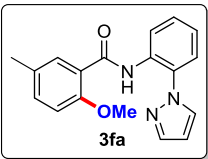
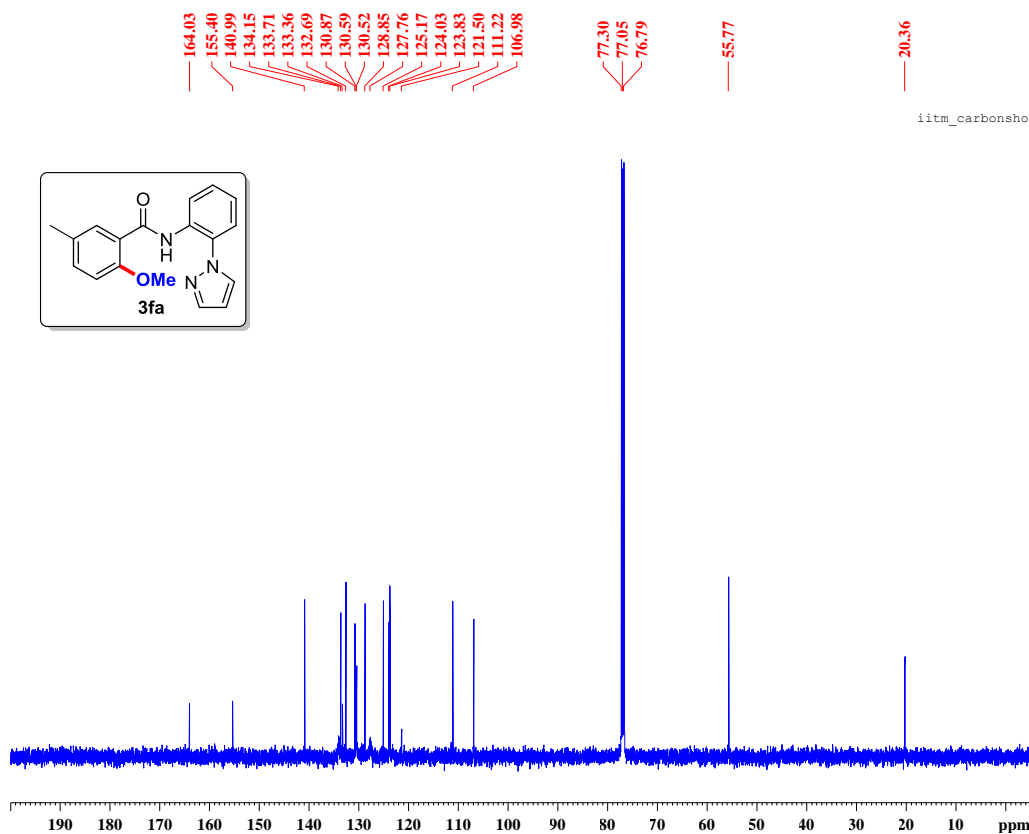
```

Current Data Parameters
NAME      JSK-300 3-me-OMe
EXPNO     21
PROCNO    1

F2 - Acquisition Parameters
Date_     20150927
Time      12.43
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         32
DS         2
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         1.6384000 sec
RG         138.53
DW         50.000 usec
DE         6.50 usec
TE         296.9 K
D1         0.50000000 sec
TDO        1

===== CHANNEL f1 =====
SF01      500.1525008 MHz
NUC1       1H
P1         11.75 usec
PLW1      15.30000019 W

F2 - Processing parameters
SI         65536
SF         500.1500232 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



```

Lab mmb
jsk-300
iitm_carbonshort CDCl3 /opt/topspin iitm 9

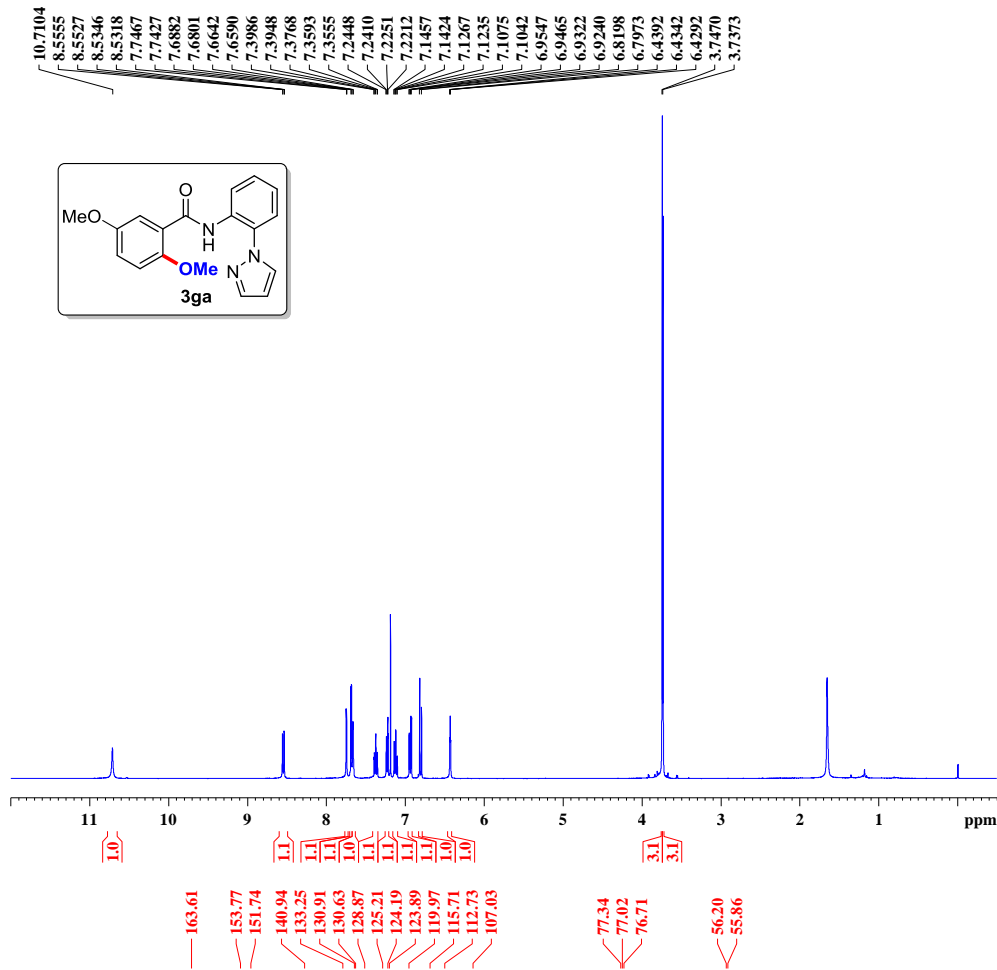
Current Data Parameters
NAME      JSK-300 3-me-OMe
EXPNO     22
PROCNO    1

F2 - Acquisition Parameters
Date_     20150927
Time      12.57
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD         20480
SOLVENT   CDCl3
NS         512
DS         4
SWH        29761.904 Hz
FIDRES     1.453218 Hz
AQ         0.3440640 sec
RG         202.34
DW         16.800 usec
DE         6.50 usec
TE         297.7 K
D1         1.00000000 sec
D11        0.03000000 sec
TDO        1

===== CHANNEL f1 =====
SF01      125.7753932 MHz
NUC1       13C
P1         9.63 usec
PLW1      103.00000000 W

===== CHANNEL f2 =====
SF02      500.1520006 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2     80.00 usec
PLW2      15.30000019 W
PLW12     0.33006001 W
PLW13     0.21123999 W

F2 - Processing parameters
SI         32768
SF         125.7628180 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



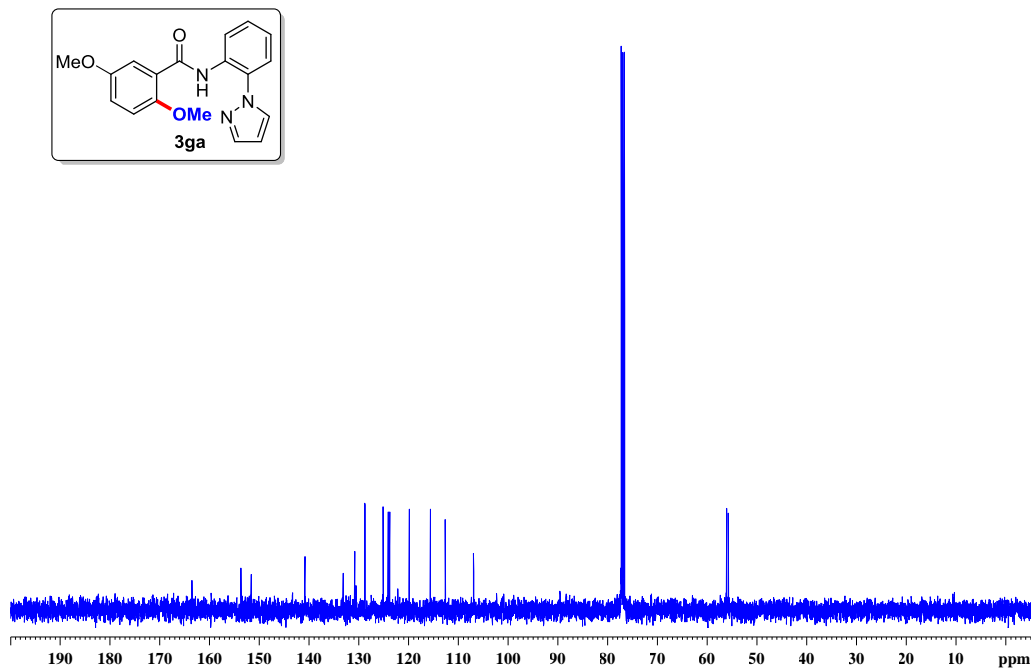
```
Current Data Parameters
NAME      JSK-3-Ome Ome
EXPNO    222
PROCNO   1

F2 - Acquisition Parameters
Date_    20160131
Time     11.45
INSTRUM spect
PROBHD   5 mm PABBO BB-
PULPROG zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ       4.0894465 sec
RG       200.34
DW       62.400 usec
DE       6.50 usec
TE       297.3 K
D1       0.50000000 sec
TDO      1

===== CHANNEL f1 =====
SF01    400.1320007 MHz
NUC1    1H
P1      15.70 usec
PLW1    7.75000000 W

F2 - Processing parameters
SI      65536
SF      400.1300378 MHz
WDW     EM
SSB     0
LB      0.30 Hz
GB      0
PC      1.00
```

lab mmb-jsk-3ome
iitm_carbonshort CDCl3 /opt/topspin nmr 2



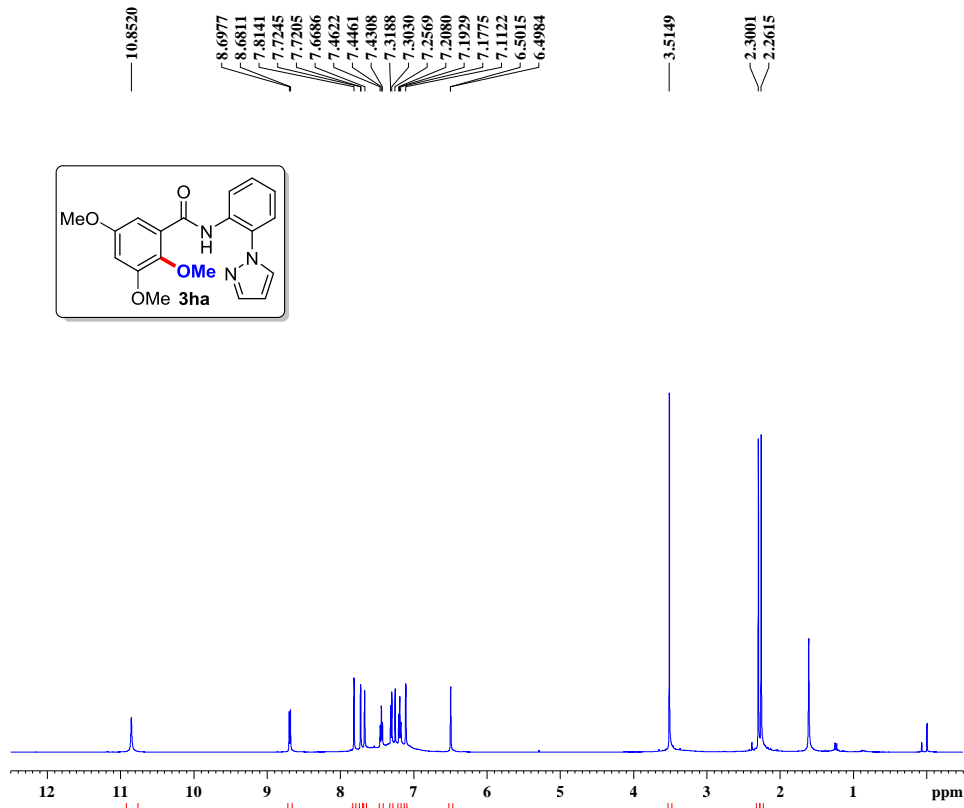
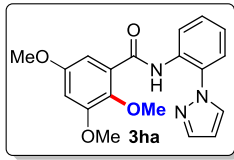
```
Current Data Parameters
NAME      JSK-3-Ome Ome
EXPNO    223
PROCNO   1

F2 - Acquisition Parameters
Date_    20160131
Time     11.51
INSTRUM spect
PROBHD   5 mm PABBO BB-
PULPROG zgpg30
TD       16540
SOLVENT  CDCl3
NS       256
DS       4
SWH      24038.461 Hz
FIDRES   1.453353 Hz
AQ       0.3440320 sec
RG       200.34
DW       20.800 usec
DE       6.50 usec
TE       297.8 K
D1       1.00000000 sec
D11      0.03000000 sec
TDO      1

===== CHANNEL f1 =====
SF01    100.6228289 MHz
NUC1    13C
P1      9.25 usec
PLW1    47.00000000 W

===== CHANNEL f2 =====
SF02    400.1316005 MHz
NUC2    1H
CPDPRG2 waltz16
PCPD2   90.00 usec
PLW2    7.75000000 W
PLW12   0.23583999 W
PLW13   0.11863000 W

F2 - Processing parameters
SI      32768
SF      100.6127690 MHz
WDW     EM
SSB     0
LB      1.00 Hz
GB      0
PC      1.40
```



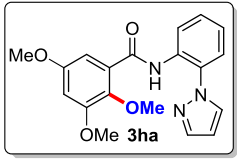
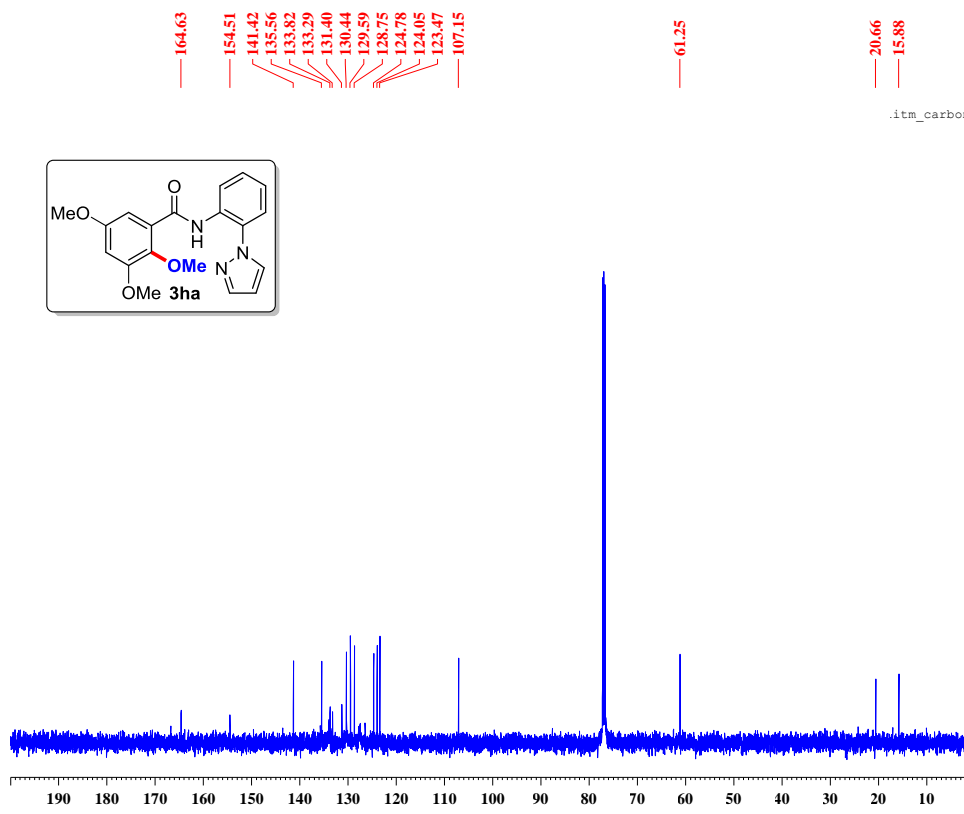
```

Current Data Parameters
NAME      JSK-299 3,5-dime-ome 500
EXPNO    9
PROCNO   1

F2 - Acquisition Parameters
Date_    20150923
Time     10.09
INSTRUM spect
PROBHD   5 mm PABBO BB/
PULPROG zg30
TD       32768
SOLVENT  CDCl3
NS       32
DS       2
SWH      10000.000 Hz
FIDRES   0.305176 Hz
AQ       1.6384000 sec
RG       162.95
DW       50.000 usec
DE       6.50 usec
TE       297.7 K
D1       0.50000000 sec
TD0      1

===== CHANNEL f1 =====
SFO1    500.1525008 MHz
NUC1    1H
P1      11.75 usec
PLW1    15.30000019 W

F2 - Processing parameters
SI      6536
SF      500.1500242 MHz
WDW     EM
SSB     0
LB      0.30 Hz
GB      0
PC      1.00
  
```



```

Lab mmb
JSK-299
.itm_carbonshort CDCl3 /opt/topspin iitm 14

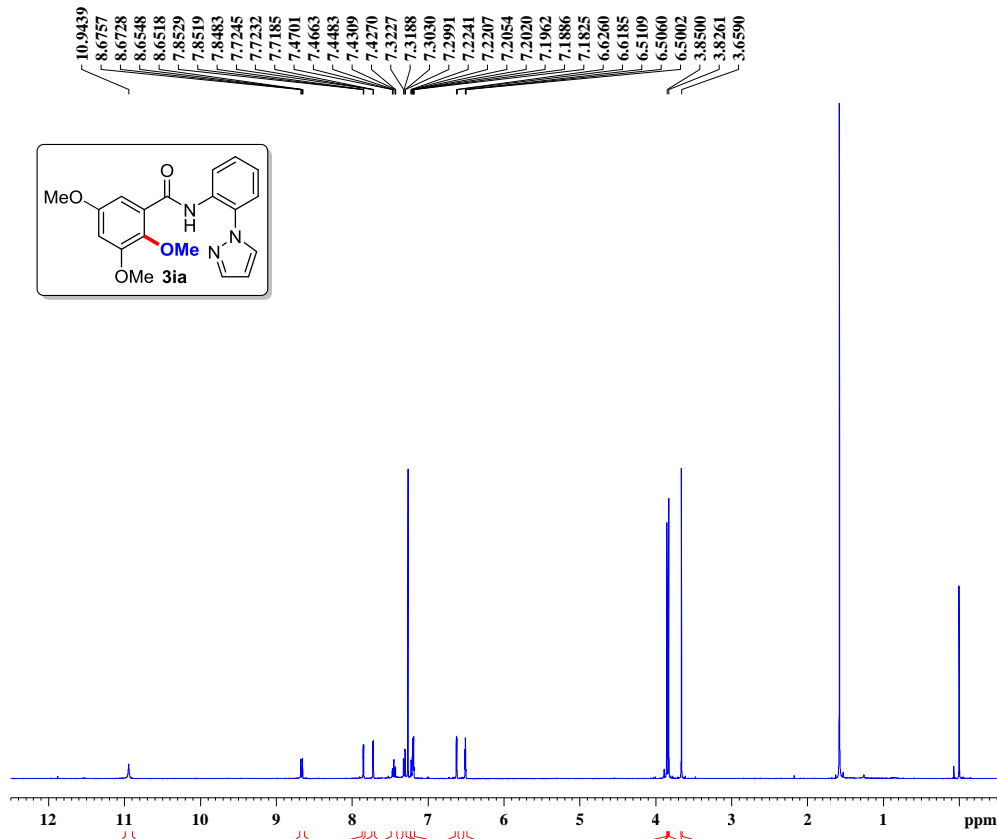
Current Data Parameters
NAME      JSK-299 3,5-dime-ome 500
EXPNO    10
PROCNO   1

F2 - Acquisition Parameters
Date_    20150923
Time     10.21
INSTRUM spect
PROBHD   5 mm PABBO BB/
PULPROG zgpg30
TD       20480
SOLVENT  CDCl3
NS       256
DS       4
SWH      29761.904 Hz
FIDRES   1.453218 Hz
AQ       0.3440640 sec
RG       202.34
DW       16.800 usec
DE       6.50 usec
TE       298.1 K
D1       1.00000000 sec
D11     0.03000000 sec
TD0      1

===== CHANNEL f1 =====
SFO1    125.7753932 MHz
NUC1    13C
P1      9.63 usec
PLW1    103.00000000 W

===== CHANNEL f2 =====
SFO2    500.1520006 MHz
NUC2    1H
CPDPRG[2] waltz16
PCPD2   80.00 usec
PLW2    15.30000019 W
PLW12   0.33006001 W
PLW13   0.21123999 W

F2 - Processing parameters
SI      32768
SF      125.7628180 MHz
WDW     EM
SSB     0
LB      1.00 Hz
GB      0
PC      1.40
  
```



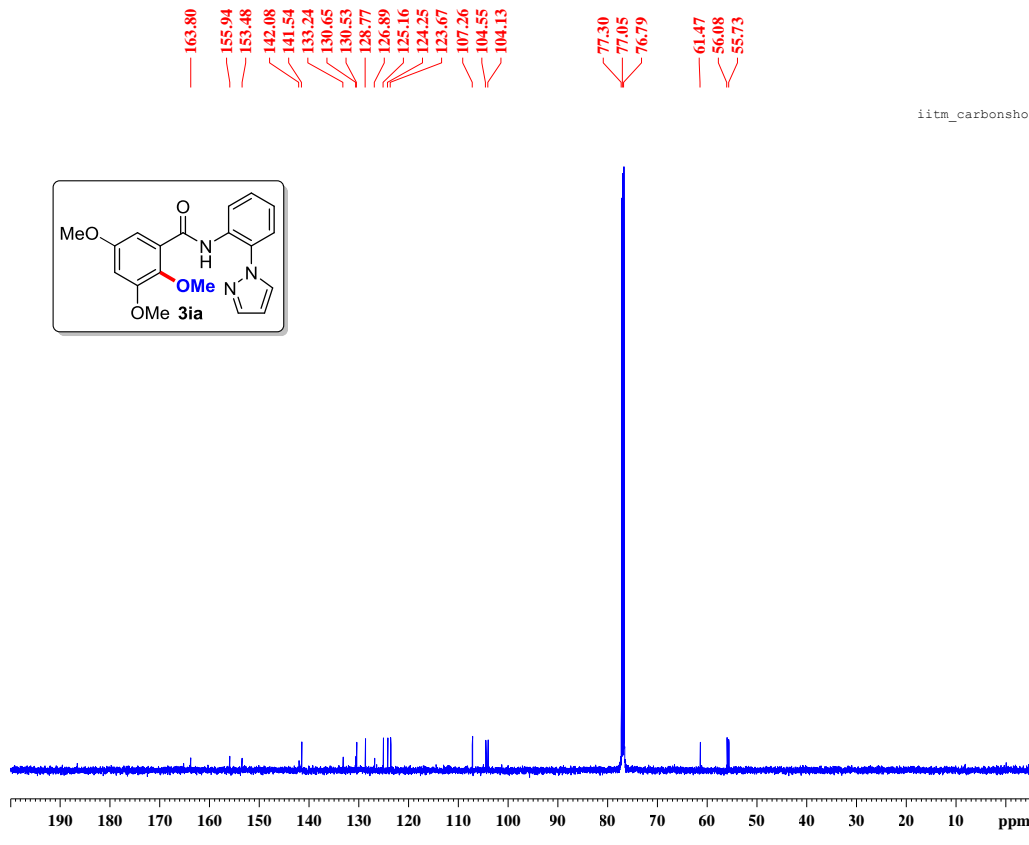
```

Current Data Parameters
NAME          JSK-283
EXPNO        27
PROCNO       1

F2 - Acquisition Parameters
Date_        20150903
Time         21.08
INSTRUM     spect
PROBHD      5 mm PABBO BB-
PULPROG     zg30
TD          65536
SOLVENT     CDCl3
NS          16
DS          2
SWH         8012.820 Hz
FIDRES     0.122266 Hz
AQ         4.0894465 sec
RG         200.34
DW         62.400 usec
DE         6.50 usec
TE         296.1 K
D1         0.50000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1        1H
P1          15.70 usec
PLW1       7.75000000 W
SF01       400.1320007 MHz

F2 - Processing parameters
SI          65536
SF         400.1300085 MHz
WDW         EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.00
  
```



```

Lab mmb
-jsk-35-ome
iitm_carbonshort CDCl3 /opt/topspin iitm 5

Current Data Parameters
NAME          3,5-ome
EXPNO        83
PROCNO       1

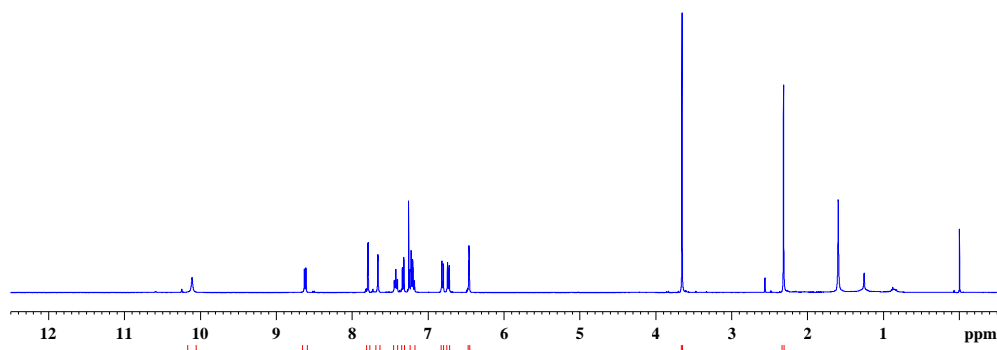
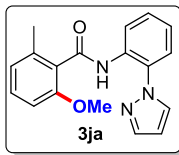
F2 - Acquisition Parameters
Date_        20160413
Time         1.27
INSTRUM     spect
PROBHD      5 mm PABBO BB/
PULPROG     zgpg30
TD          20480
SOLVENT     CDCl3
NS          2000
DS          4
SWH         29761.904 Hz
FIDRES     1.453218 Hz
AQ         0.3440640 sec
RG         202.34
DW         16.800 usec
DE         6.50 usec
TE         296.0 K
D1         1.00000000 sec
D11        0.03000000 sec
TDO        1

===== CHANNEL f1 =====
SF01       125.7753932 MHz
NUC1        13C
P1          9.63 usec
PLW1       103.0000000 W

===== CHANNEL f2 =====
SF02       500.1520006 MHz
NUC2        1H
CPDPRG2     waltz16
PCPD2       80.00 usec
PLW2       15.30000019 W
PLW12      0.33006001 W
PLW13      0.21123999 W

F2 - Processing parameters
SI          32768
SF         125.7628180 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
  
```

10.1089
8.6347
8.6319
8.6140
8.6112
7.7988
7.7975
7.7927
7.7914
7.6668
7.6629
7.4498
7.4466
7.4284
7.4180
7.4107
7.4074
7.3435
7.3398
7.3235
7.3199
7.2593
7.2471
7.2269
7.2232
7.2195
7.2069
7.2042
7.2008
7.1843
7.1810
6.8220
6.8029
6.7465
6.7257
6.4693
6.4641
6.4585
3.6570
2.3190



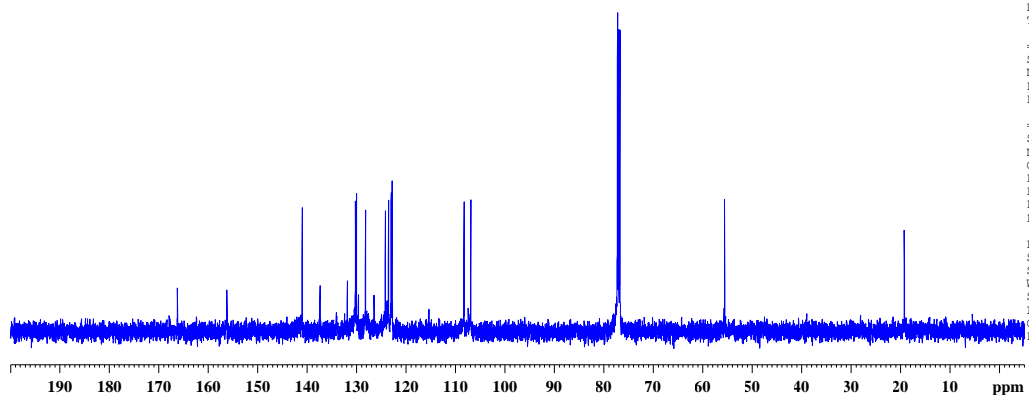
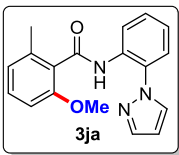
1.0
1.1
1.1
1.1
1.1
2.0
1.1
1.1
1.0
3.0
3.1
19.33

```
Current Data Parameters
NAME      2,3-dione
EXPNO    25
PROCNO    1

F2 - Acquisition Parameters
Date_     20160410
Time      3.12
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8012.820 Hz
FIDRES     0.122266 Hz
AQ         4.0894465 sec
RG         200.34
DW         62.400 usec
DE         6.50 usec
TE         299.1 K
D1         0.50000000 sec
TDO        1

===== CHANNEL f1 =====
SF01      400.1320007 MHz
NUC1       1H
P1         15.70 usec
PLW1       7.75000000 W

F2 - Processing parameters
SI         65536
SF         400.1300098 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```



```
Lab mmb
JSK-292
itm_carbonshort CDCl3 /opt/topspin iitm 14

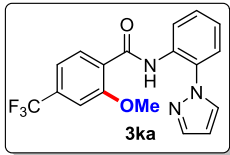
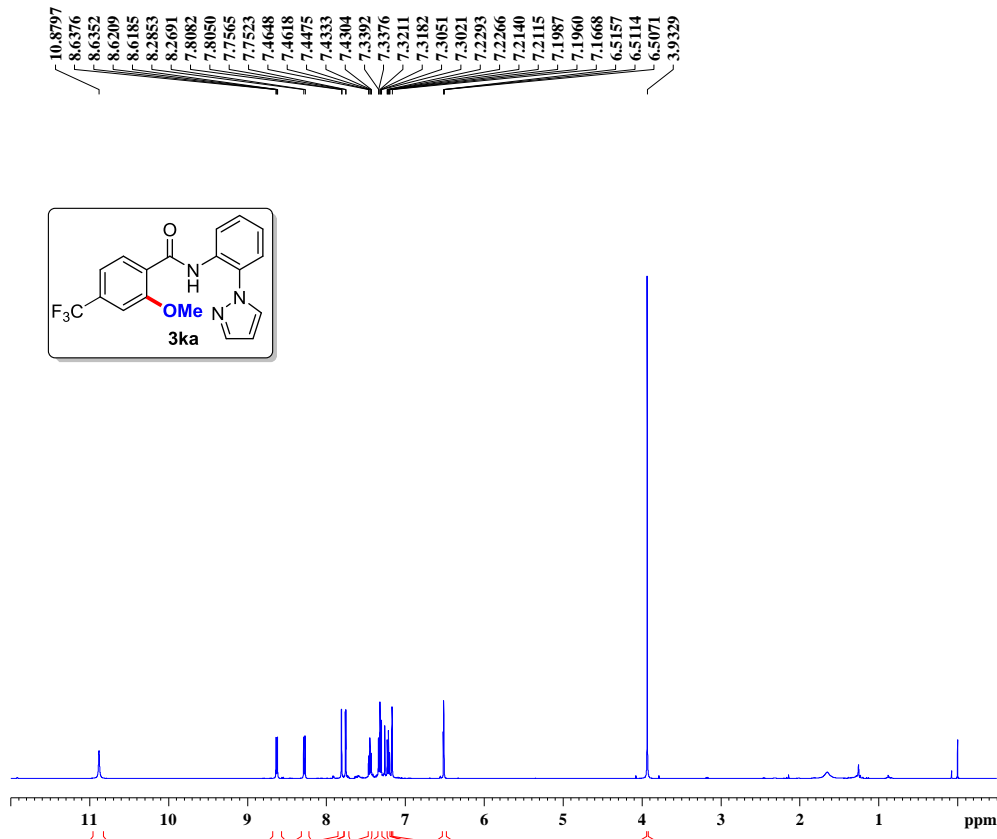
Current Data Parameters
NAME      JSK-292-2-m3 OMe 500
EXPNO    6
PROCNO    1

F2 - Acquisition Parameters
Date_     20150916
Time      8.50
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         20480
SOLVENT   CDCl3
NS         512
DS         4
SWH        29761.904 Hz
FIDRES     1.453218 Hz
AQ         0.3440640 sec
RG         202.34
DW         16.800 usec
DE         6.50 usec
TE         298.8 K
D1         1.00000000 sec
D11        0.03000000 sec
TDO        1

===== CHANNEL f1 =====
SF01      125.7753932 MHz
NUC1       13C
P1         9.63 usec
PLW1       103.00000000 W

===== CHANNEL f2 =====
SF02      500.1520006 MHz
NUC2       1H
CPDPRG[2] waltz16
PCPD2     80.00 usec
PLW2      15.30000019 W
PLW12     0.33006001 W
PLW13     0.21123999 W

F2 - Processing parameters
SI         32768
SF         125.7628180 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

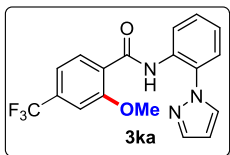
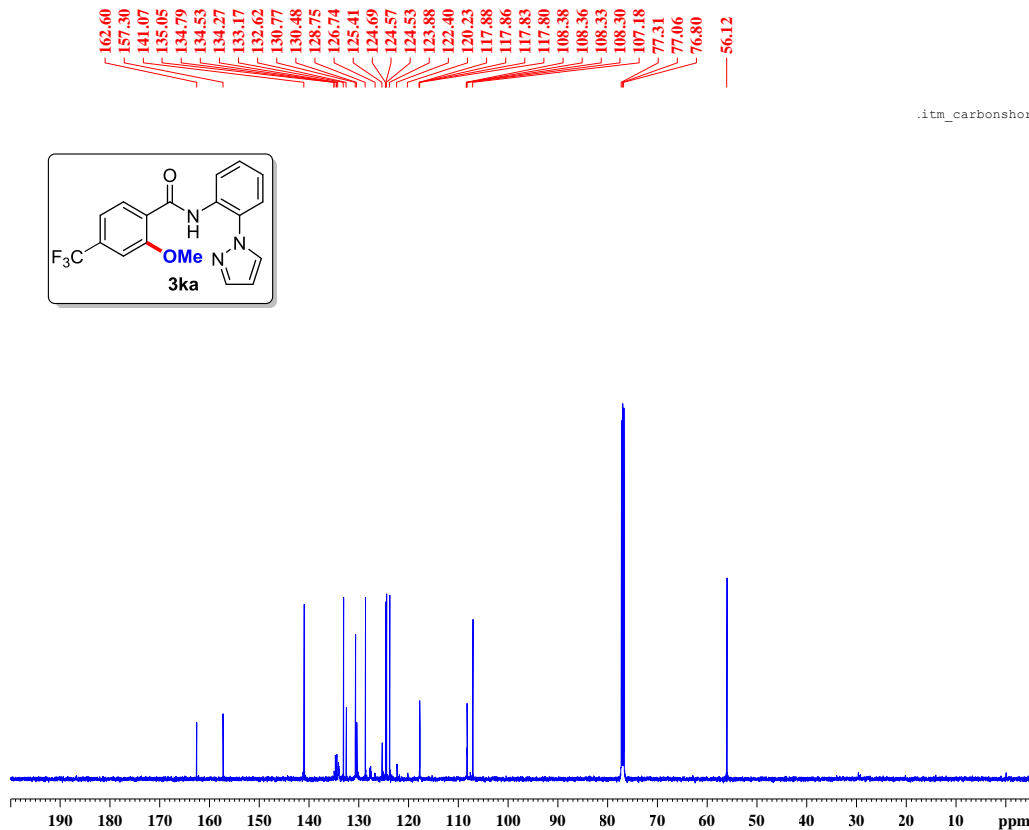


```
Current Data Parameters
NAME      4-CF3-methoxy
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20151103
Time      12.38
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD        32768
SOLVENT   CDCl3
NS        16
DS        2
SWH       10000.000 Hz
FIDRES    0.305176 Hz
AQ        1.6384000 sec
RG        114.76
DW        50.000 usec
DE        6.50 usec
TE        299.3 K
D1        0.50000000 sec
TDO       1

===== CHANNEL f1 =====
SF01     500.1525008 MHz
NUC1     1H
P1       11.75 usec
PLW1     15.30000019 W

F2 - Processing parameters
SI       65536
SF       500.1500229 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
```



```
Lab mmb
j3k-342-4
.itm_carbonshort CDCl3 /opt/topspin iitm 11

Current Data Parameters
NAME      4-CF3-methoxy
EXPNO     18
PROCNO    1

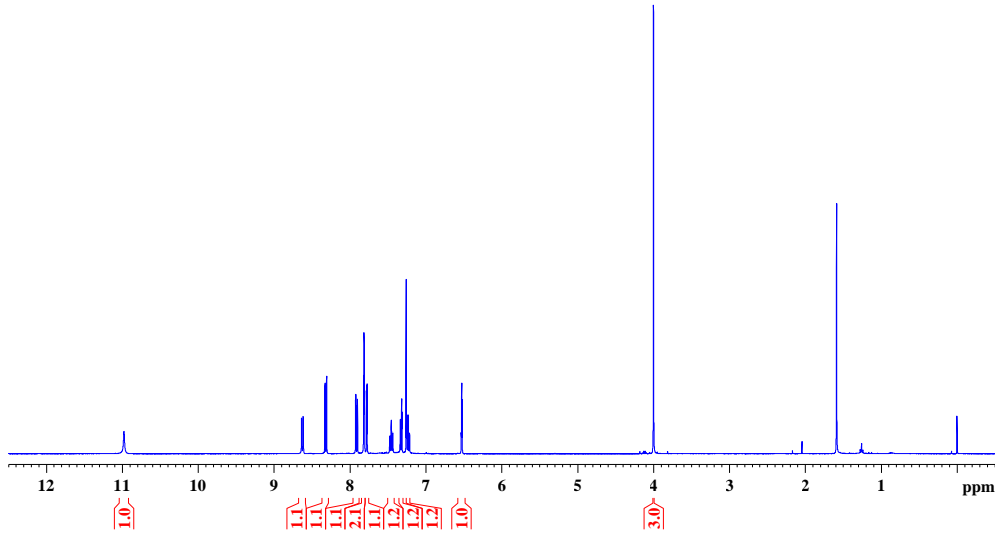
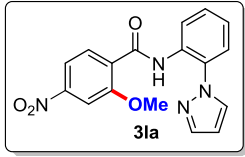
F2 - Acquisition Parameters
Date_     20151104
Time      2.43
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD        20480
SOLVENT   CDCl3
NS        2000
DS        4
SWH       29761.904 Hz
FIDRES    1.453218 Hz
AQ        0.3440640 sec
RG        202.34
DW        16.800 usec
DE        6.50 usec
TE        296.5 K
D1        1.00000000 sec
D11       0.03000000 sec
TDO       1

===== CHANNEL f1 =====
SF01     125.7753932 MHz
NUC1     13C
P1       9.63 usec
PLW1     103.00000000 W

===== CHANNEL f2 =====
SF02     500.1520006 MHz
NUC2     1H
CPDPRG2   waltz16
PCPD2    80.00 usec
PLW2     15.30000019 W
PLW12    0.33006001 W
PLW13    0.21123999 W

F2 - Processing parameters
SI       32768
SF       125.7628180 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
```

10.9789
8.6390
8.6359
8.6182
8.6150
8.5297
8.3082
7.9268
7.9215
7.9053
7.9001
7.8202
7.8148
7.8099
7.8086
7.7819
7.7804
7.7758
7.7743
7.4777
7.4741
7.4562
7.4384
7.4349
7.3393
7.3355
7.3194
7.3157
7.2613
7.2559
7.2524
7.2373
7.2362
7.2339
7.2176
7.2141
6.5331
6.5281
6.5272
6.5222
3.9997



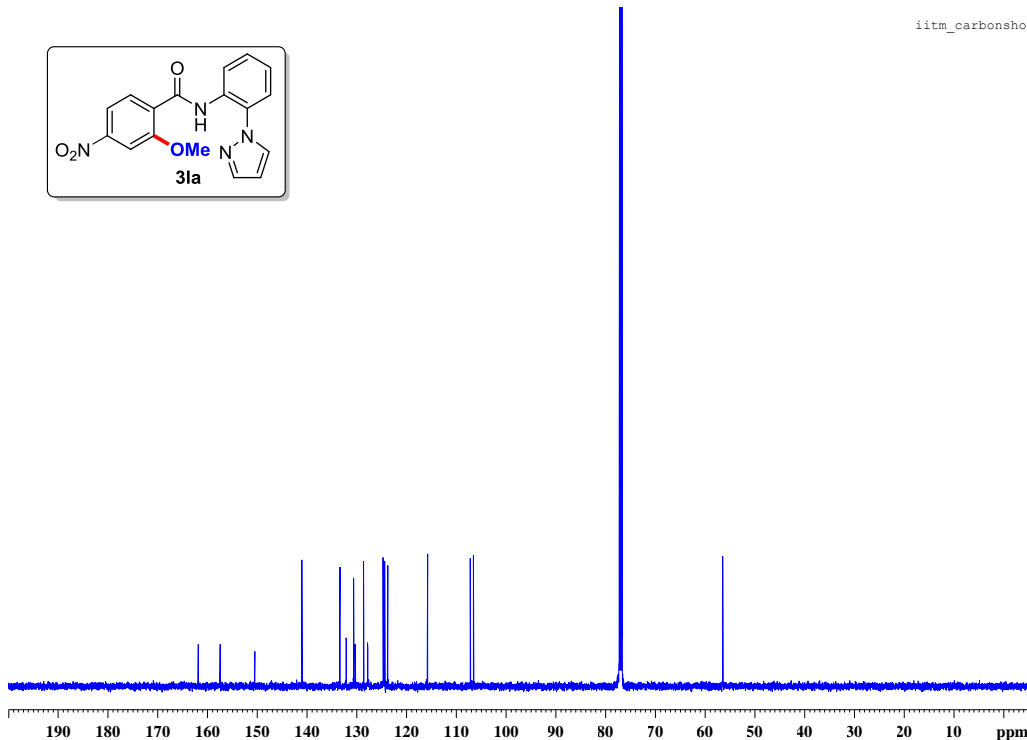
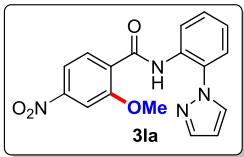
Current Data Parameters
NAME JSK-265
EXPNO 192
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150826
Time 12.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 299.0 K
D1 0.5000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.70 usec
PLW1 7.7500000 W
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 65536
SF 400.1300089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

161.88
157.47
150.53
141.12
133.50
132.23
130.74
130.40
128.72
127.91
124.80
124.48
123.87
115.89
107.28
106.64
77.31
77.06
76.80
56.55



Lab mmb
jks-266
iitm_carbonshort CDCl3 /opt/topspin iitm 5

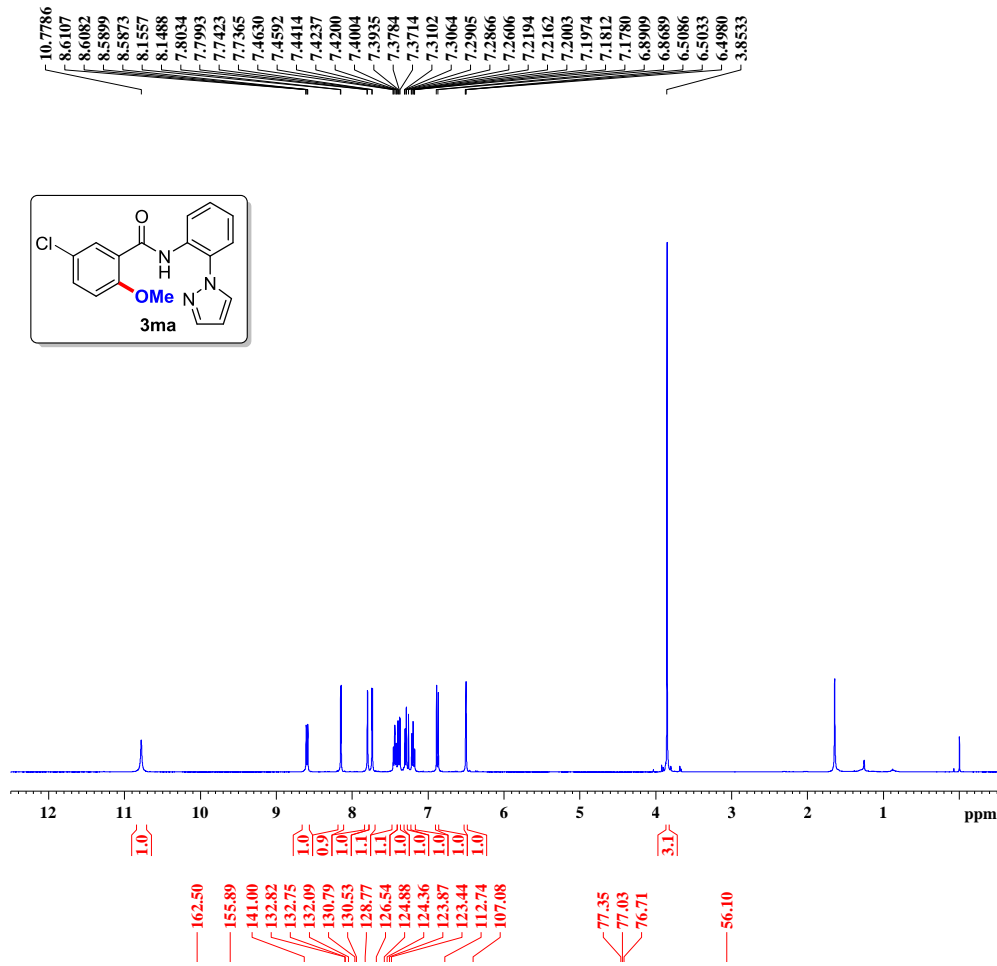
Current Data Parameters
NAME JSK-266
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150826
Time 19.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 20480
SOLVENT CDCl3
NS 2000
DS 4
SWH 29761.904 Hz
FIDRES 1.453218 Hz
AQ 0.3440640 sec
RG 202.34
DW 16.800 usec
DE 6.50 usec
TE 293.7 K
D1 1.0000000 sec
D11 0.0300000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 125.7753932 MHz
NUC1 13C
P1 9.63 usec
PLW1 103.0000000 W

===== CHANNEL f2 =====
SFO2 500.1520006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 15.30000019 W
PLW12 0.33006001 W
PLW13 0.21123999 W

F2 - Processing parameters
SI 32768
SF 125.7628180 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



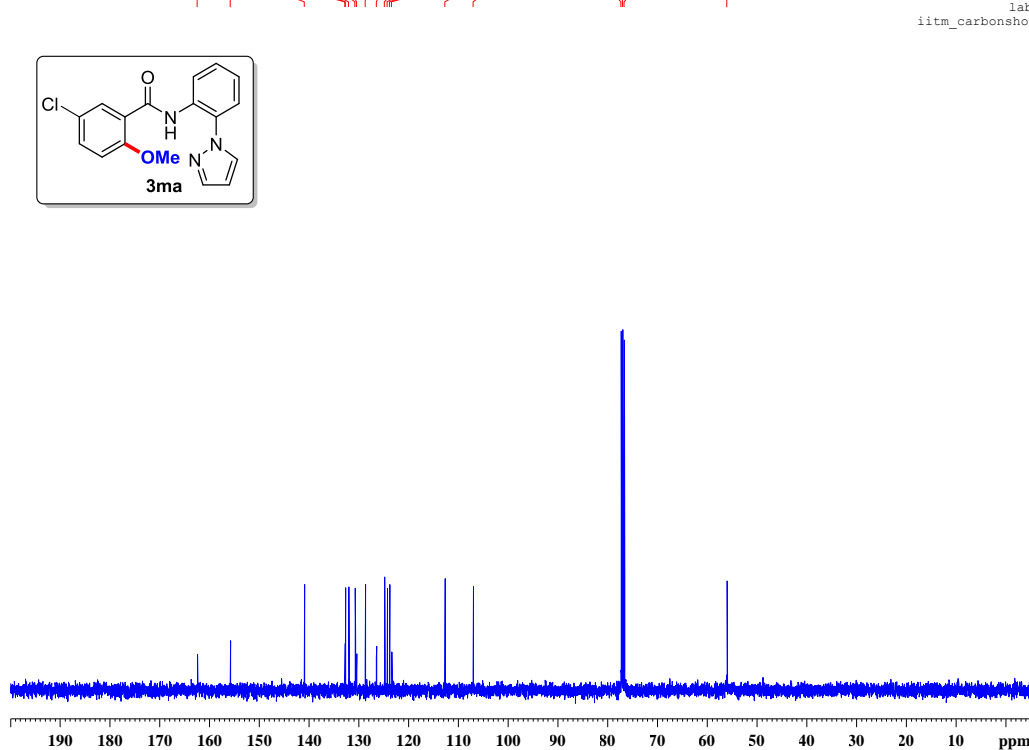
```

Current Data Parameters
NAME          mmb40416
EXPNO        124
PROCNO       1

F2 - Acquisition Parameters
Date_        20160416
Time         10.04
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zg30
TD           65536
SOLVENT      CDCl3
NS           16
DS           2
SWH          8012.820 Hz
FIDRES       0.122266 Hz
AQ           4.0894465 sec
RG           200.34
DW           62.400 usec
DE           6.50 usec
TE           299.9 K
D1           0.50000000 sec
TDO         1

===== CHANNEL f1 =====
SF01         400.1320007 MHz
NUC1         1H
P1           15.70 usec
PLW1         7.75000000 W

F2 - Processing parameters
SI           65536
SF           400.1300093 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
  
```



```

lab mmb-jsk-3cl-ome
iitm_carbonshort CDCl3 /opt/topspin nmr 15

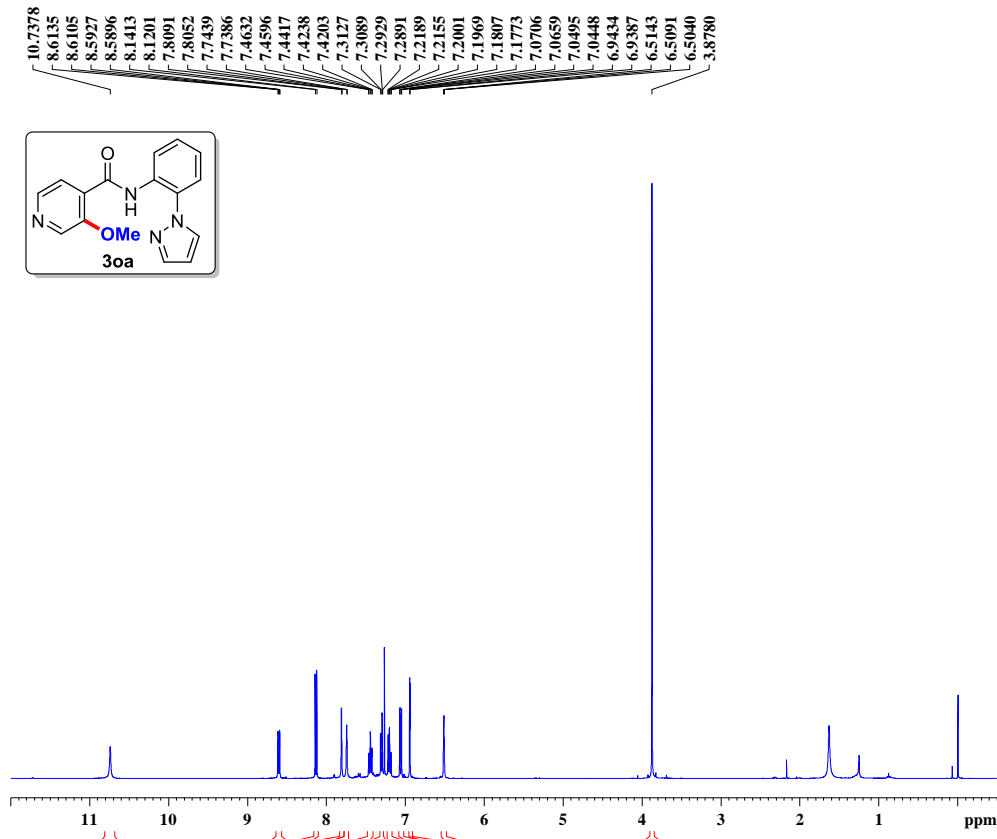
Current Data Parameters
NAME          mmb40416
EXPNO        125
PROCNO       1

F2 - Acquisition Parameters
Date_        20160416
Time         10.11
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zgpg30
TD           16540
SOLVENT      CDCl3
NS           256
DS           4
SWH          24038.461 Hz
FIDRES       1.453353 Hz
AQ           0.3440320 sec
RG           200.34
DW           20.800 usec
DE           6.50 usec
TE           300.3 K
D1           1.00000000 sec
D11          0.03000000 sec
TDO         1

===== CHANNEL f1 =====
SF01         100.6228289 MHz
NUC1         13C
P1           9.25 usec
PLW1         47.00000000 W

===== CHANNEL f2 =====
SF02         400.1316005 MHz
NUC2         1H
CPDPRG[2]    waltz16
PCPD2        90.00 usec
PLW2         7.75000000 W
PLW12        0.23583999 W
PLW13        0.11863000 W

F2 - Processing parameters
SI           32768
SF           100.6127690 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```

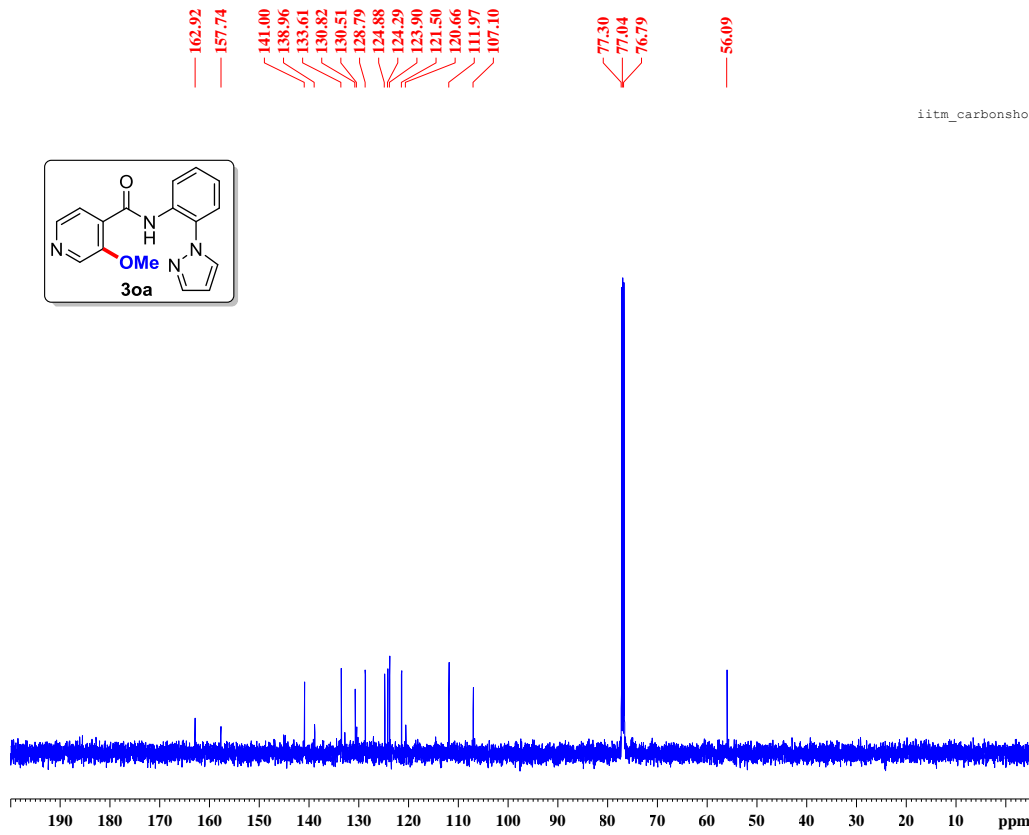
```

Current Data Parameters
NAME          JSK-343
EXPNO         73
PROCNO        1

F2 - Acquisition Parameters
Date_         20151108
Time          12.58
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG            200.34
DW            62.400 usec
DE            6.50 usec
TE            293.9 K
D1            0.50000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            15.70 usec
PLW1          7.75000000 W
SF01          400.1320007 MHz

F2 - Processing parameters
SI            65536
SF            400.1300084 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```



```

Lab mmb
iitm_carbonshort CDCl3 /opt/topspin iitm 7

Current Data Parameters
NAME          JSK-343
EXPNO         48
PROCNO        1

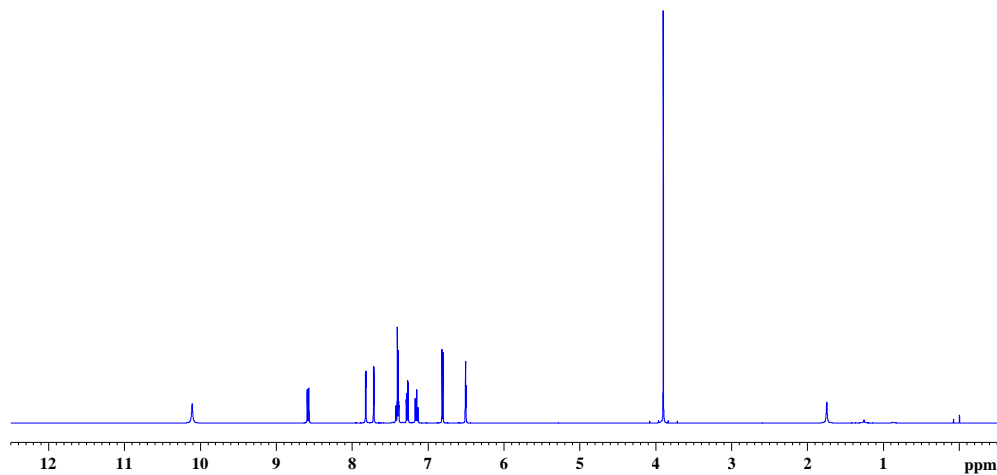
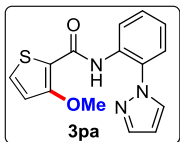
F2 - Acquisition Parameters
Date_         20151106
Time          15.30
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       zgpg30
TD            20480
SOLVENT       CDCl3
NS            256
DS            4
SWH           29761.904 Hz
FIDRES        1.453218 Hz
AQ            0.3440640 sec
RG            202.34
DW            16.800 usec
DE            6.50 usec
TE            298.6 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
SF01          125.7753932 MHz
NUC1          13C
P1            9.63 usec
PLW1          103.00000000 W

===== CHANNEL f2 =====
SF02          500.1520006 MHz
NUC2          1H
CPDPRG[2]    waltz16
PCPD2         80.00 usec
PLW2          15.30000019 W
PLW12         0.33006001 W
PLW13         0.21123999 W

F2 - Processing parameters
SI            32768
SF            125.7628180 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

10.1128
8.5965
8.5934
8.5755
8.5725
8.8263
7.8219
7.7225
7.7166
7.4300
7.4261
7.4087
7.3949
7.3908
7.3868
7.2898
7.2859
7.2701
7.2661
7.2635
7.1749
7.1717
7.1559
7.1526
7.1367
7.1334
6.8195
6.8057
6.5133
6.5080
6.5027
3.9036



1.0
1.1
1.0
1.1
1.2
1.1
1.1
1.0
1.0
160.15
156.79
140.90
133.14
130.78
130.13
128.86
125.10
123.82
123.31
117.07
115.44
107.00
77.38
77.06
76.74
3.0
58.77

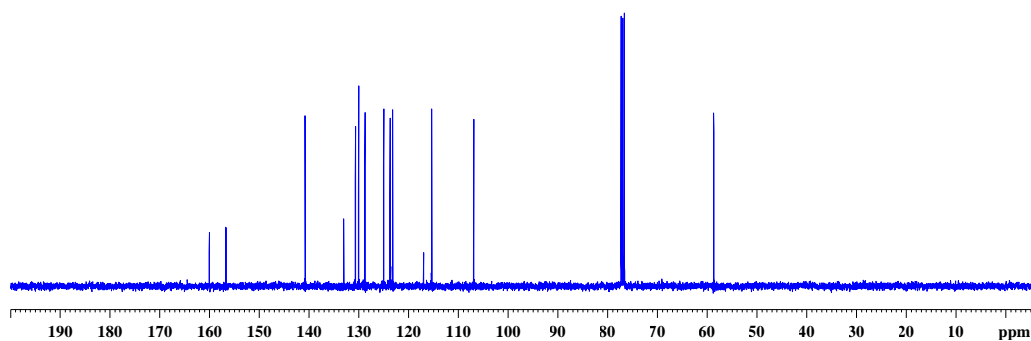
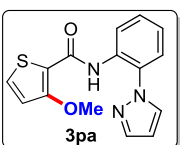
```
Current Data Parameters
NAME          JSK
EXPNO         71
PROCNO        1

F2 - Acquisition Parameters
Date_         20160415
Time          7.59
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDC13
NS            16
DS            2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG            138.85
DW            62.400 usec
DE            6.50 usec
TE            299.8 K
D1            0.50000000 sec
TDO           1

===== CHANNEL f1 =====
SF01          400.1320007 MHz
NUC1           1H
P1            15.70 usec
PLW1          7.75000000 W

F2 - Processing parameters
SI            65536
SF            400.1300083 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```

lab mmbjck-2-thio-ome
iitm_carbonsshort CDC13 /opt/topspin nmr 3



```
Current Data Parameters
NAME          JSK
EXPNO         72
PROCNO        1

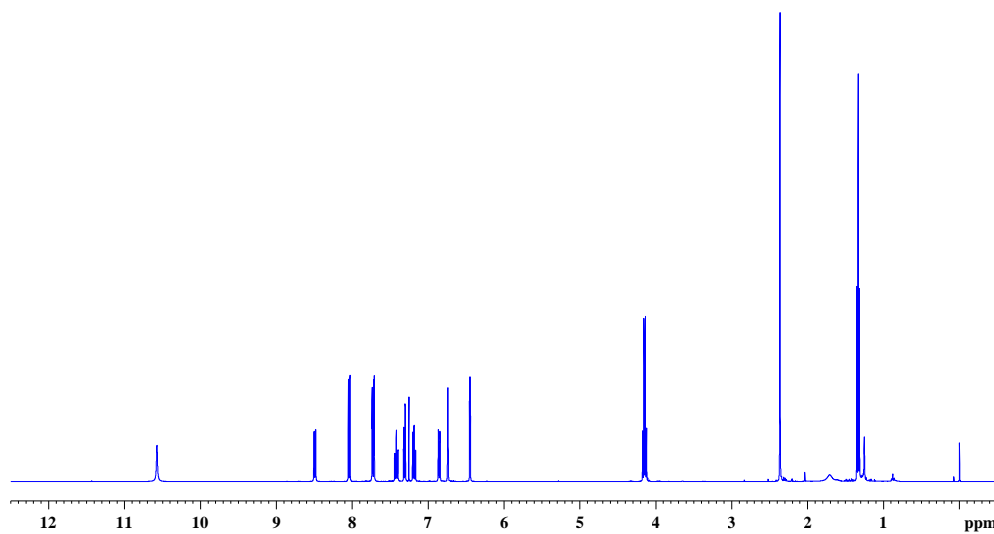
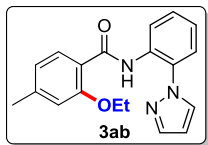
F2 - Acquisition Parameters
Date_         20160415
Time          8.12
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            16540
SOLVENT       CDC13
NS            512
DS            4
SWH           24038.461 Hz
FIDRES        1.453353 Hz
AQ            0.3440320 sec
RG            200.34
DW            20.800 usec
DE            6.50 usec
TE            300.2 K
D1            1.00000000 sec
D11           0.03000000 sec
TDO           1

===== CHANNEL f1 =====
SF01          100.6228289 MHz
NUC1           13C
P1            9.25 usec
PLW1          47.00000000 W

===== CHANNEL f2 =====
SF02          400.1316005 MHz
NUC2           1H
CPDPRG[2]     waltz16
PCPD2         90.00 usec
PLW2          7.75000000 W
PLW12         0.23583399 W
PLW13         0.11863000 W

F2 - Processing parameters
SI            32768
SF            100.6127690 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```

10.5760
8.5089
8.5059
8.4881
8.4851
8.0536
8.0337
7.7404
7.7369
7.7359
7.7192
7.7178
7.7131
7.7117
7.4401
7.4222
7.4045
7.4009
7.3264
7.3226
7.3065
7.3027
7.2092
7.2057
7.1905
7.1899
7.1871
7.1709
7.1675
6.8694
6.8678
6.8659
6.8644
6.8493
6.8479
6.8460
6.8445
6.7432
6.4569
6.4519
6.4512
6.4462
4.1755
4.1580
4.1404
4.1229
2.3665
1.3541
1.3367
1.3191



Current Data Parameters
NAME JSK-263
EXPNO 155
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150823
Time 10.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
FULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 138.85
DW 62.400 usec
DE 6.50 usec
TE 299.0 K
D1 0.50000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W
SFO1 400.1320007 MHz

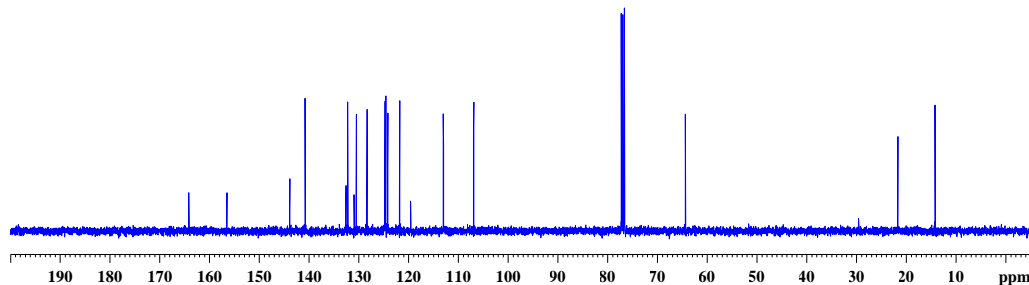
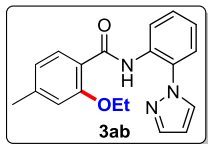
F2 - Processing parameters
SI 65536
SF 400.1300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

164.25
156.60
143.98
140.88
132.68
132.35
131.06
130.61
128.45
124.84
124.66
124.29
121.89
119.71
113.11
107.02

64.48

21.78
14.30

lab mmb-jsk-263
iitm_carbonshort CDC13 /opt/topspin nmr 9



Current Data Parameters
NAME JSK-263
EXPNO 156
PROCNO 1

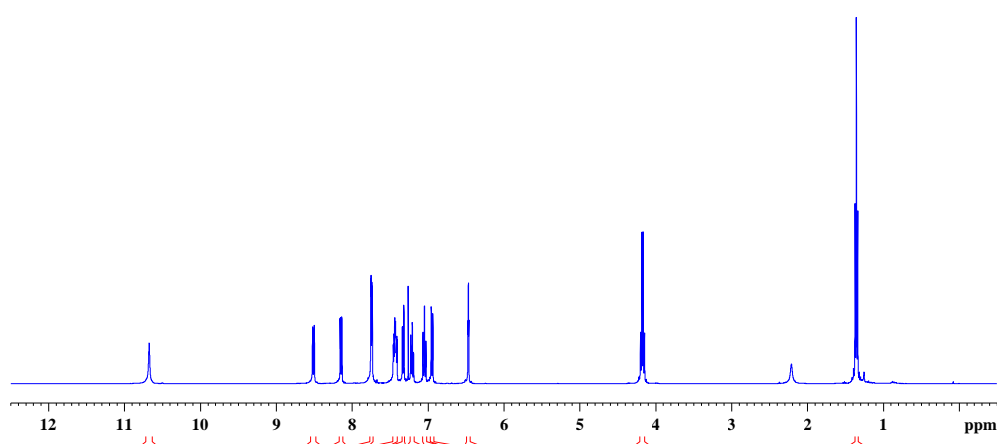
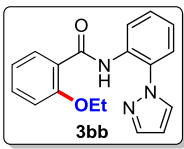
F2 - Acquisition Parameters
Date_ 20150823
Time_ 11.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
FULPROG zgpg30
TD 16540
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 299.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO1 100.6228289 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

10.6739
8.5208
8.5185
8.5001
8.4977
8.1563
8.1517
8.1367
8.1322
7.7523
7.7482
7.7392
7.7334
7.4494
7.4447
7.4371
7.4312
7.4285
7.4266
7.4239
7.4196
7.4159
7.4103
7.4057
7.3385
7.3348
7.3186
7.3149
7.2599
7.2283
7.2249
7.2063
7.2063
7.0664
7.0640
7.0460
7.0286
7.0262
6.9577
6.9370
6.4723
6.4671
6.4618
4.1980
4.1805
4.1630
4.1455
1.3713
1.3539
1.3363

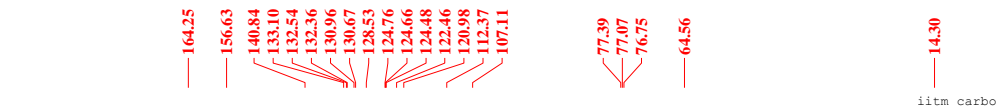


```
Current Data Parameters
NAME      ph-ethyl
EXPNO    34
PROCNO    1

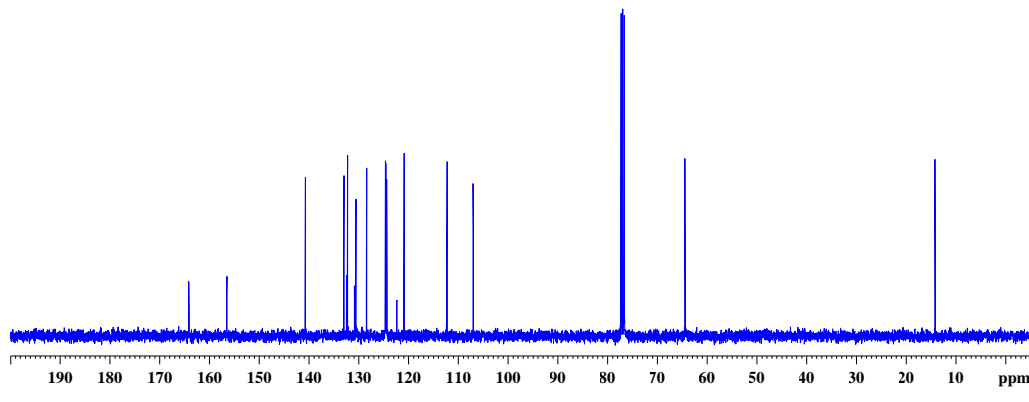
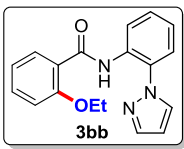
F2 - Acquisition Parameters
Date_     20151009
Time      5.23
INSTRUM   spect
PROBHD    5 mm PABBO BB-
FULPROG   zg30
TD         65536
SOLVENT   CDC13
NS         16
DS         2
SWH        8012.820 Hz
FIDRES    0.122266 Hz
AQ         4.0894465 sec
RG         124.58
DW         62.400 usec
DE         6.50 usec
TE         293.2 K
D1         0.50000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         15.70 usec
PLW1       7.75000000 W
SFO1       400.1320007 MHz

F2 - Processing parameters
SI         65536
SF         400.1300094 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```



lab mmbjsk-311
iitm_carbonshort CDC13 /opt/topspin nmr 12



```
Current Data Parameters
NAME      ph-ethyl
EXPNO    35
PROCNO    1

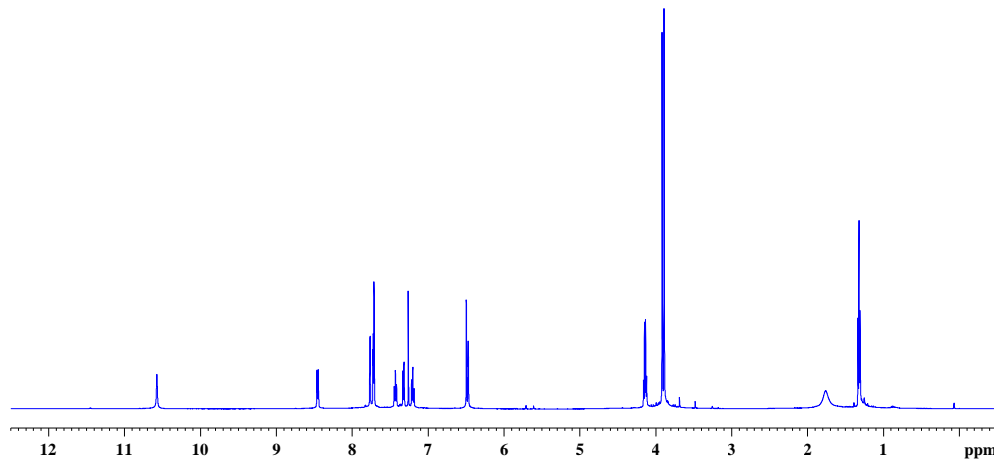
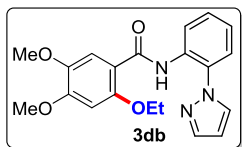
F2 - Acquisition Parameters
Date_     20151009
Time      5.30
INSTRUM   spect
PROBHD    5 mm PABBO BB-
FULPROG   zgpg30
TD         16540
SOLVENT   CDC13
NS         256
DS         4
SWH        24038.461 Hz
FIDRES    1.453353 Hz
AQ         0.3440320 sec
RG         200.34
DW         20.800 usec
DE         6.50 usec
TE         294.0 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         9.25 usec
PLW1       47.00000000 W
SFO1       100.6228289 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PLW2       7.75000000 W
PLW12      0.23583999 W
PLW13      0.19103000 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI         32768
SF         100.6127690 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

10.5726
8.4645
8.4622
8.4479
8.4456
7.7663
7.7629
7.7255
7.7208
7.7105
7.4477
7.4449
7.4302
7.4163
7.4135
7.3334
7.3306
7.3176
7.3148
7.2601
7.2540
7.2170
7.2145
7.1992
7.1864
7.1839
6.4942
6.4752
6.4709
6.4669
4.1599
4.1460
4.1320
4.1180
3.9155
3.8896
1.3346
1.3207
1.3067



Current Data Parameters
NAME 3,4-dimethyl ethyl
EXPNO 27
PROCNO 1

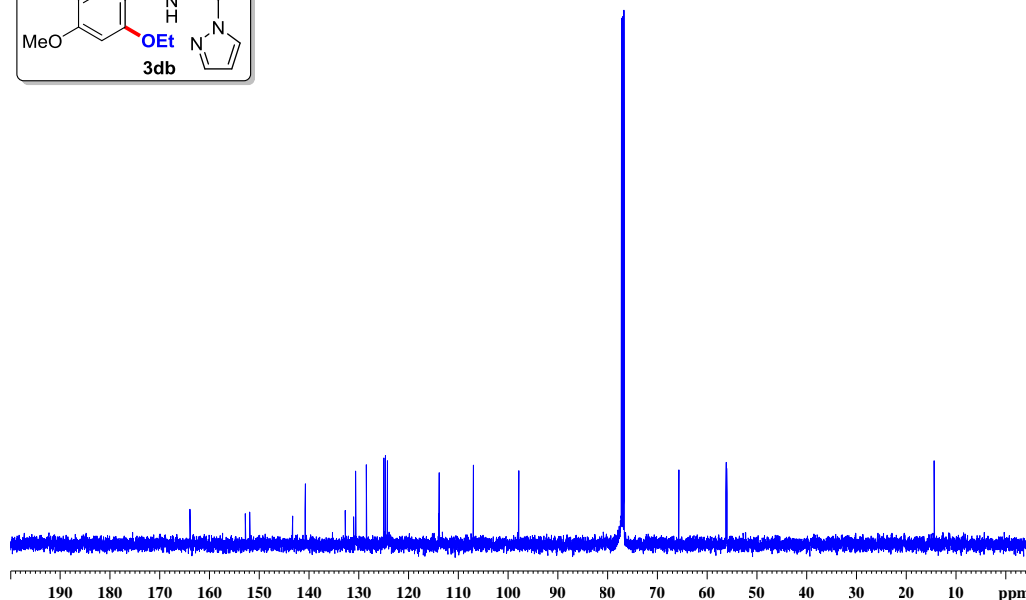
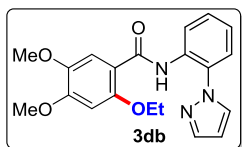
F2 - Acquisition Parameters
Date_ 20151021
Time 13.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 32
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384000 sec
RG 138.53
DW 50.000 usec
DE 6.50 usec
TE 298.5 K
D1 0.50000000 sec
TDO 1

===== CHANNEL f1 =====
SF01 500.1525008 MHz
NUC1 1H
P1 11.75 usec
PLW1 15.30000019 W

F2 - Processing parameters
SI 65536
SF 500.1500223 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

163.92
152.81
151.92
143.42
140.86
132.81
131.12
130.74
128.57
125.09
124.75
124.38
114.04
113.95
107.08
97.94
77.30
77.05
76.79
65.78
56.29
56.14
14.45

Lab mmb
jshk-333-1
iitm_carbonshort CDC13 /opt/topspin iitm 6



Current Data Parameters
NAME 3,4-dimethyl ethyl
EXPNO 28
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151021
Time_ 14.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 20480
SOLVENT CDC13
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 1.453218 Hz
AQ 0.3440640 sec
RG 202.34
DW 16.800 usec
DE 6.50 usec
TE 299.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TDO 1

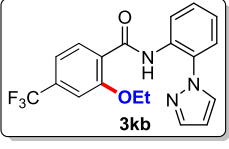
===== CHANNEL f1 =====
SF01 125.7753932 MHz
NUC1 13C
P1 9.63 usec
PLW1 103.0000000 W

===== CHANNEL f2 =====
SF02 500.1520006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 15.30000019 W
PLW12 0.33006001 W
PLW13 0.21123999 W

F2 - Processing parameters
SI 32768
SF 125.7628180 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

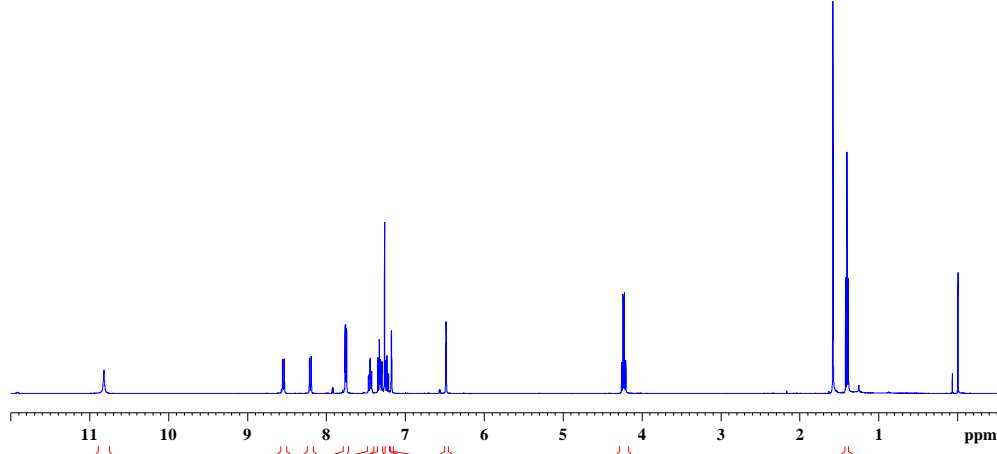
10.8175
8.5541
8.5512
8.5334
8.5305
8.2111
8.1911
7.7606
7.7545
7.7463
7.7417
7.4664
7.4627
7.4448
7.4272
7.4235
7.3479
7.3440
7.3280
7.3242
7.3147
7.3127
7.2944
7.2924
7.2514
7.2480
7.2326
7.2293
7.2131
7.2096
7.1741
6.4878
6.4827
6.4771
4.2616
4.2441
4.2265
4.2090

1.4235
1.4060
1.3885



Current Data Parameters
NAME JSK-378-1- 4cf3-oet
EXPNO 202
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160226
Time 23.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 298.4 K
D1 0.50000000 sec
TD0 1

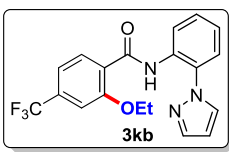


===== CHANNEL f1 =====
SF01 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

163.06
156.55
141.02
134.59
132.99
132.00
130.72
130.49
128.44
126.07
124.78
124.61
124.49
124.28
122.43
117.69
117.65
117.62
117.59
109.39
109.37
109.33
109.31
107.26
77.31
77.06
76.81
65.17

14.19



Lab mmb
jsk-378-1
iitm_carbonshort CDCl3 /opt/topspin iitm 6

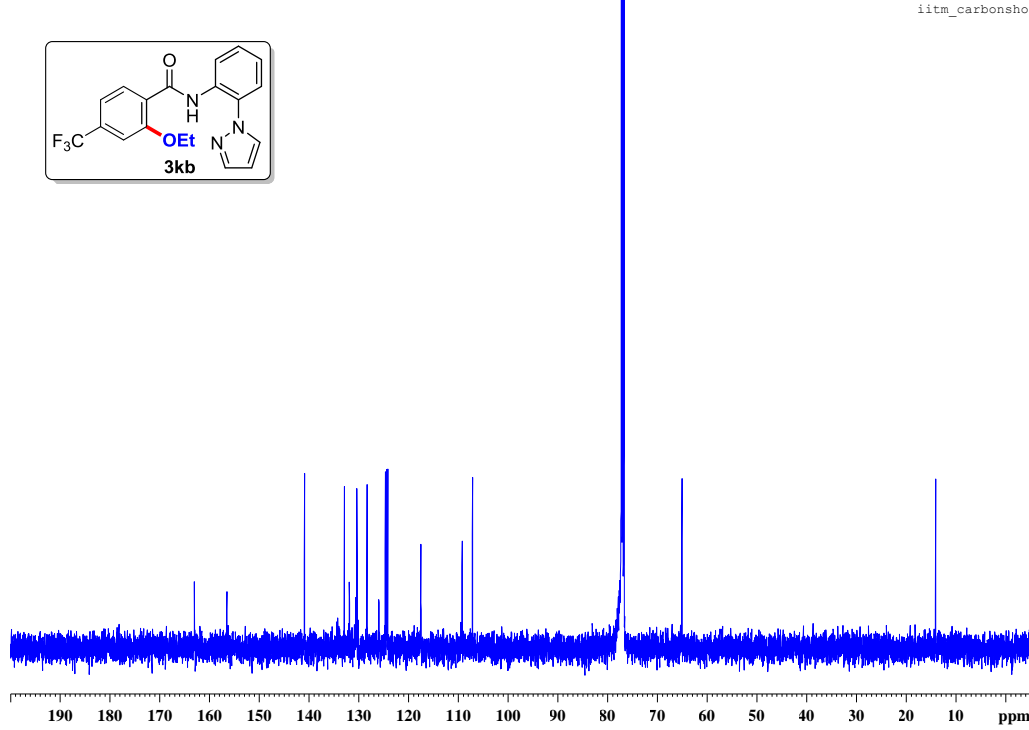
Current Data Parameters
NAME JSK-378-1- 4cf3-oet
EXPNO 70
PROCNO 1

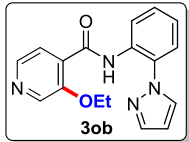
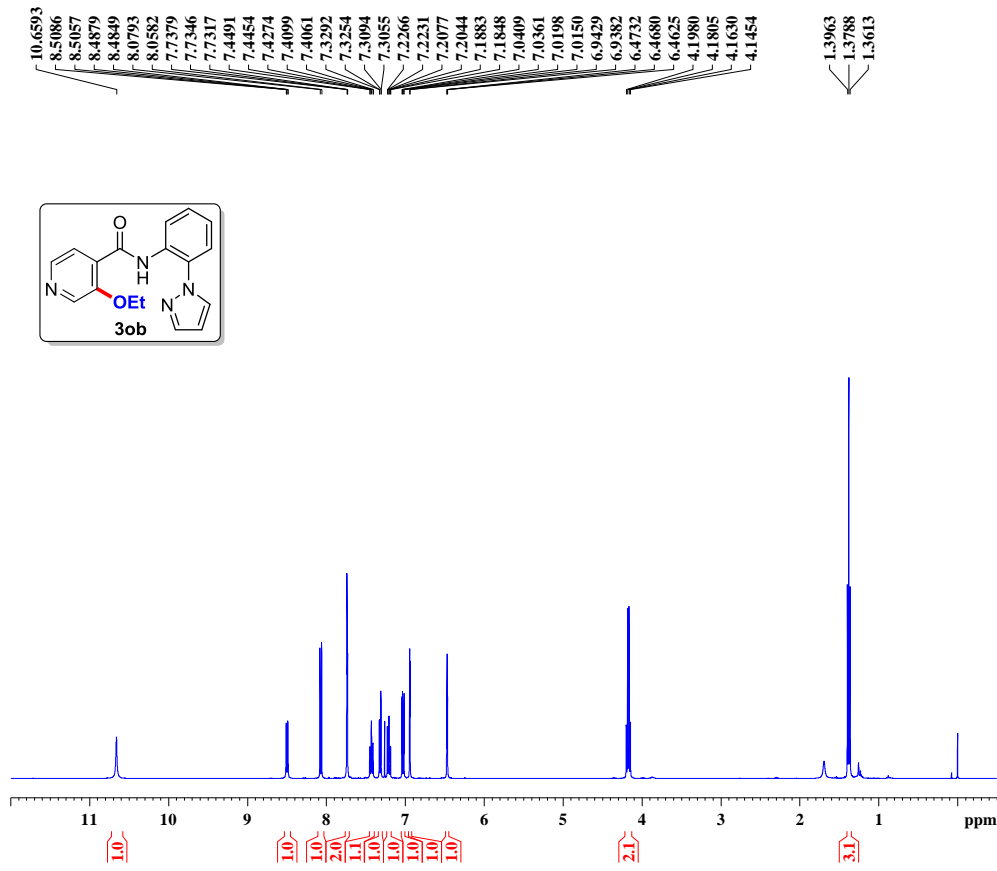
F2 - Acquisition Parameters
Date_ 20160225
Time 2.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 20480
SOLVENT CDCl3
NS 2000
DS 4
SWH 29761.904 Hz
FIDRES 1.453218 Hz
AQ 0.3440640 sec
RG 202.34
DW 16.800 usec
DE 6.50 usec
TE 294.4 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 125.7753932 MHz
NUC1 13C
P1 9.63 usec
PLW1 103.00000000 W

===== CHANNEL f2 =====
SF02 500.1520006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 15.30000019 W
PLW12 0.33006001 W
PLW13 0.21123999 W

F2 - Processing parameters
SI 32768
SF 125.7628180 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



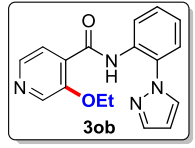


Current Data Parameters
 NAME JSK-363 4-py-oet
 EXPNO 80
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160120
 Time 6.21
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 138.85
 DW 62.400 usec
 DE 6.50 usec
 TE 297.8 K
 D1 0.50000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 400.1320007 MHz
 NUC1 1H
 P1 15.70 usec
 PLW1 7.75000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300097 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



lab mmbjsk-363
 iitm_carbonshort CDCl3 /opt/topspin nmr 4

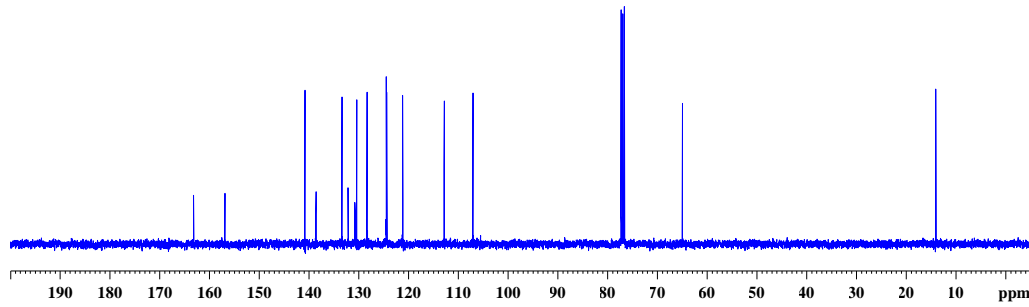
Current Data Parameters
 NAME JSK-363 4-py-oet
 EXPNO 120
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160121
 Time_ 9.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 16540
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 24038.461 Hz
 FIDRES 1.453353 Hz
 AQ 0.3440320 sec
 RG 200.34
 DW 20.800 usec
 DE 6.50 usec
 TE 297.5 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

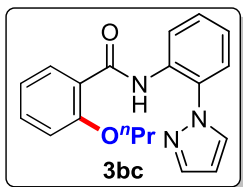
===== CHANNEL f1 =====
 SF01 100.6228289 MHz
 NUC1 13C
 P1 9.25 usec
 PLW1 47.00000000 W

===== CHANNEL f2 =====
 SF02 400.1316005 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 7.75000000 W
 PLW12 0.23583999 W
 PLW13 0.11863000 W

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

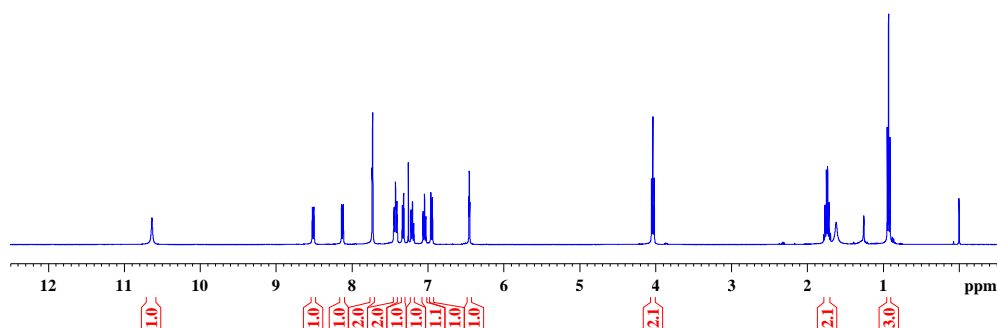


10.6370
8.9219
8.9012
8.1389
8.1344
8.1194
8.1149
7.7341
7.7282
7.7262
7.4513
7.4465
7.4417
7.4281
7.4258
7.4237
7.4209
7.4122
7.4074
7.4026
7.3995
7.3358
7.3196
7.3160
7.2256
7.2222
7.2059
7.2036
7.1873
7.1839
7.0659
7.0636
7.0452
7.0282
7.0258
6.9609
6.9400
6.4600
6.4543
6.4494
6.0528
4.0353
4.0179
1.7861
1.7676
1.7495
1.7314
1.7134
1.6954
0.9472
0.9287
0.9100



Current Data Parameters
NAME ph-propyl
EXPNO 73
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150915
Time 7.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 298.9 K
D1 0.5000000 sec
TDO 1

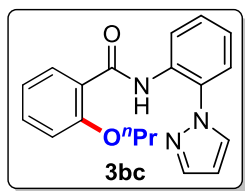


164.30
156.81
140.91
132.99
132.45
132.28
131.01
130.52
128.41
124.64
124.43
122.68
120.99
112.54
107.03

77.34
77.02
76.70
70.60

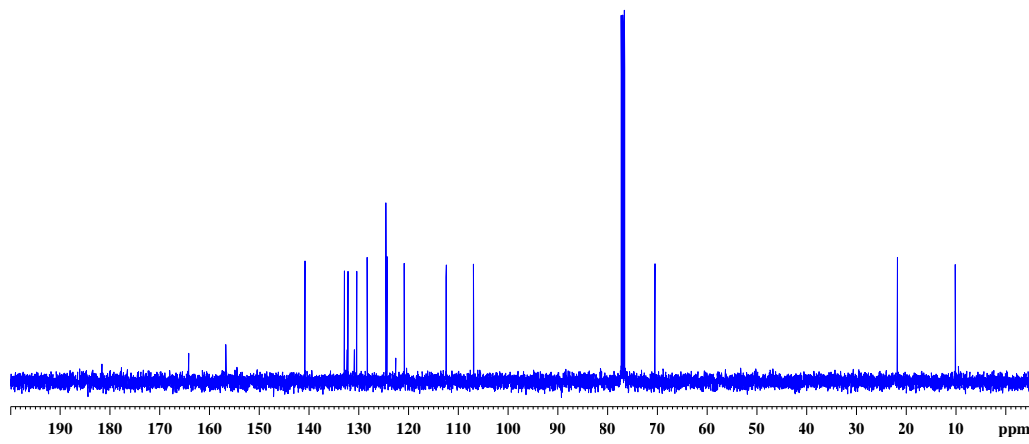
21.84
10.22

lab mmb-jsk-293B
iitm_carbonshort CDCl3 /opt/topspin nmr 13



Current Data Parameters
NAME ph-propyl
EXPNO 74
PROCNO 1

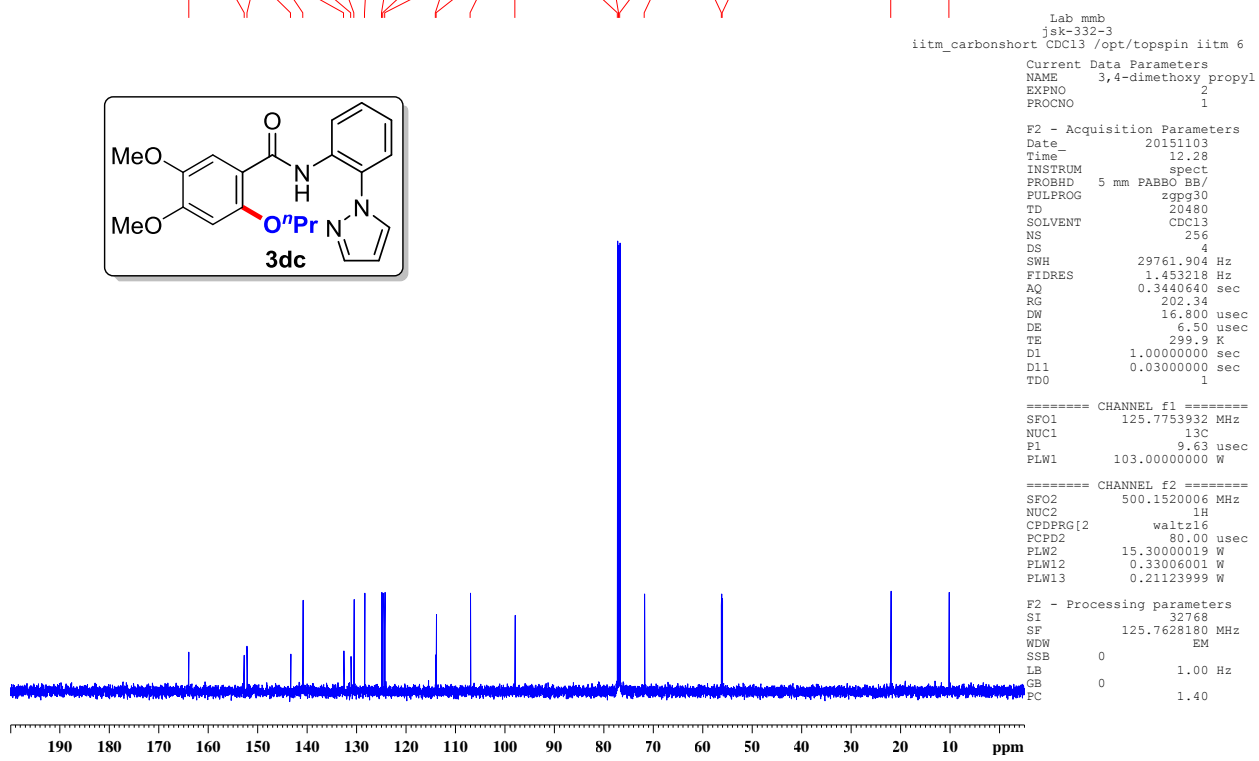
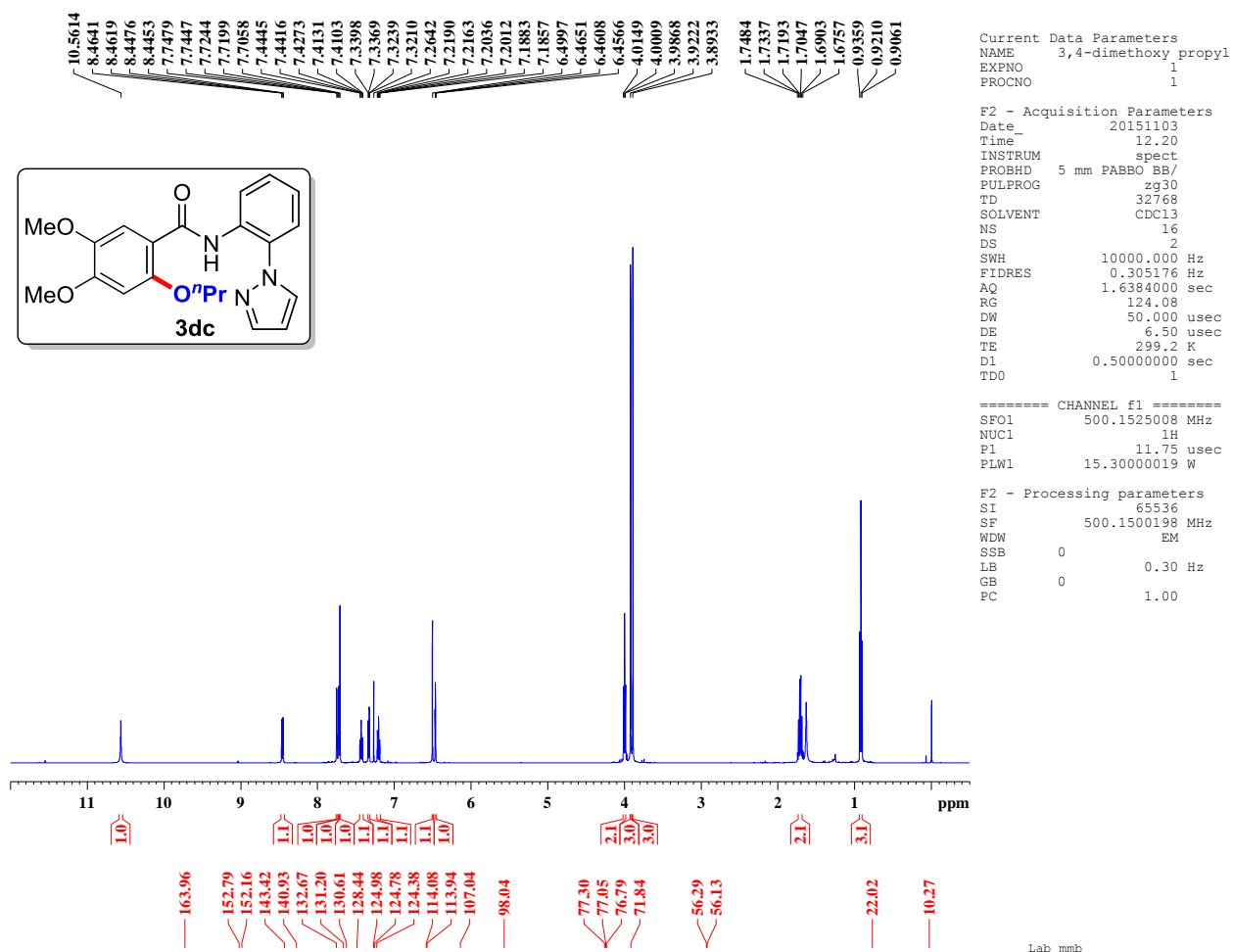
F2 - Acquisition Parameters
Date_ 20150915
Time 7.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 299.7 K
D1 1.0000000 sec
D11 0.0300000 sec
TDO 1



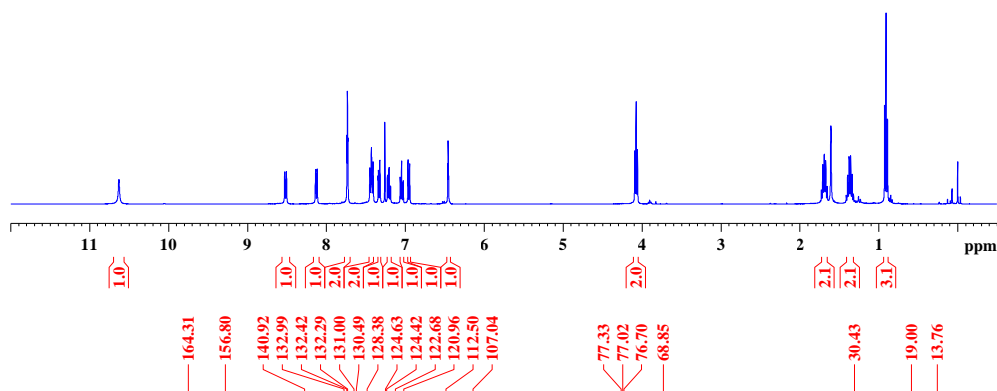
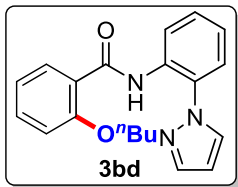
==== CHANNEL f1 =====
NUC1 13C
P1 9.25 usec
PLW1 47.0000000 W
SFO1 100.6228289 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.7500000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



10.6278
8.5246
8.5041
8.1384
8.1339
8.1189
8.1144
7.7382
7.7320
7.7272
7.4513
7.4475
7.4428
7.4291
7.4268
7.4222
7.4121
7.4083
7.4037
7.3427
7.3389
7.3228
7.3191
7.2267
7.2233
7.2070
7.2046
7.0655
7.0632
7.0449
7.0278
7.0255
6.9638
6.9430
6.4615
6.4558
6.4509
4.0916
4.0740
4.0564
1.7083
1.6900
1.6712
1.3938
1.3748
1.3560
1.3375
0.9257
0.9073
0.8887



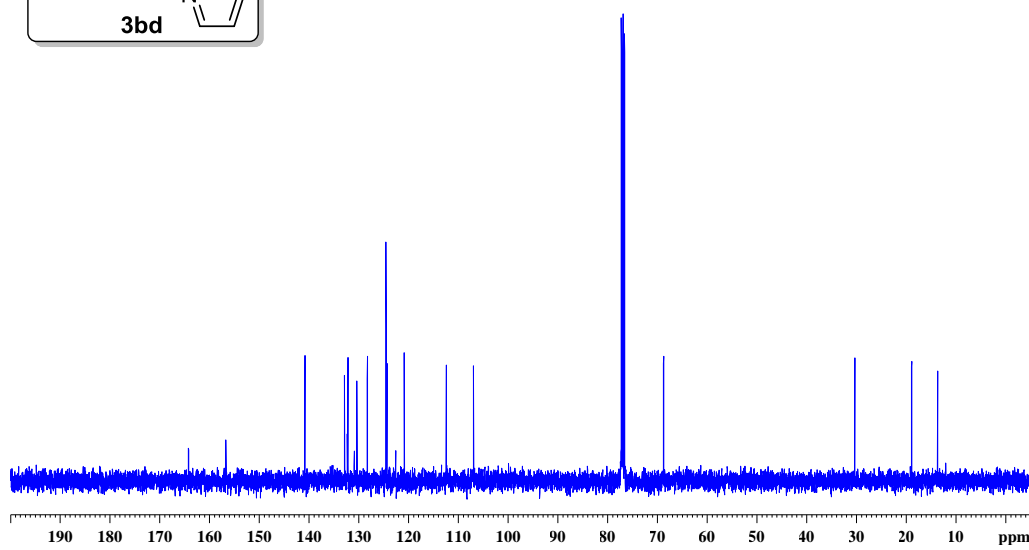
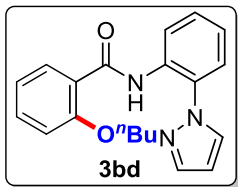
```
Current Data Parameters
NAME      ph-butyl
EXPNO    76
PROCNO    1

F2 - Acquisition Parameters
Date_     20150915
Time      8.02
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD        65536
SOLVENT   CDC13
NS        16
DS        2
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ        4.0894465 sec
RG        200.34
DW        62.400 usec
DE        6.50 usec
TE        298.9 K
D1        0.50000000 sec
TD0       1

===== CHANNEL f1 =====
NUC1      1H
P1        15.70 usec
PLW1     7.75000000 W
SFO1     400.1320007 MHz

F2 - Processing parameters
SI        65536
SF        400.1300101 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
```

lab mmb-jsk-293C
iitm_carbonshort CDC13 /opt/topspin nmr 14



```
Current Data Parameters
NAME      ph-butyl
EXPNO    77
PROCNO    1

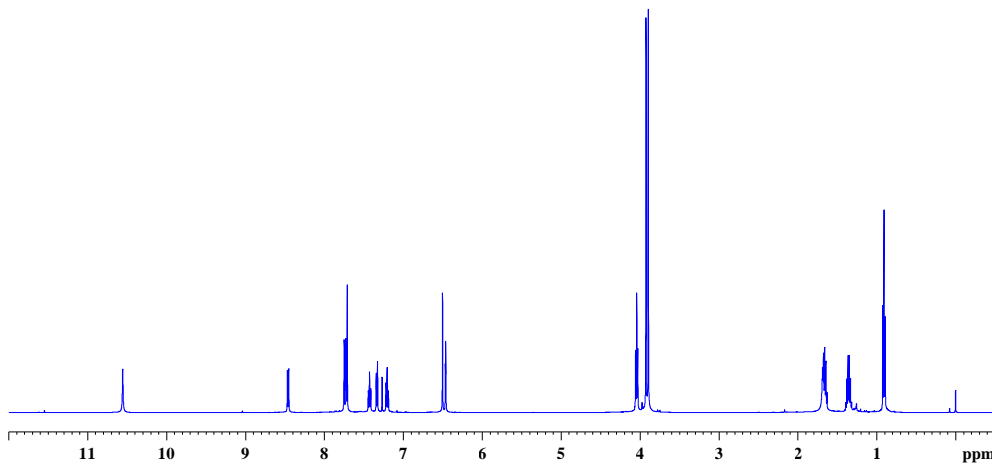
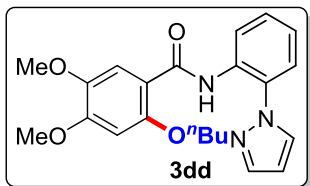
F2 - Acquisition Parameters
Date_     20150915
Time      8.09
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        16540
SOLVENT   CDC13
NS        256
DS        4
SWH       24038.461 Hz
FIDRES    1.453353 Hz
AQ        0.3440320 sec
RG        200.34
DW        20.800 usec
DE        6.50 usec
TE        299.6 K
D1        1.00000000 sec
D11       0.03000000 sec
TD0       1

===== CHANNEL f1 =====
NUC1      13C
P1        9.25 usec
PLW1     47.00000000 W
SFO1     100.6228289 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2      1H
PCPD2    90.00 usec
PLW2     7.75000000 W
PLW12    0.23583999 W
PLW13    0.19103000 W
SFO2     400.1316005 MHz

F2 - Processing parameters
SI        32768
SF        100.6127690 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
```

10.5539
8.4672
8.4506
7.7491
7.7458
7.7280
7.7233
7.7082
7.4435
7.4409
7.4268
7.4122
7.4096
7.3422
7.3396
7.3264
7.3237
7.2666
7.2188
7.2167
7.2037
7.1881
7.1862
6.5012
6.4652
6.4614
6.4571
4.0543
4.0403
4.0262
3.9226
3.8937
1.6876
1.6739
1.6592
1.6439
1.6295
1.3913
1.3764
1.3614
1.3463
1.3315
1.3168
0.9221
0.9073
0.8925



Current Data Parameters
NAME 3,4-dimethoxy butyl
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151103
Time 12.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
FULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384000 sec
RG 101.5
DW 50.000 usec
DE 6.50 usec
TE 299.0 K
D1 0.50000000 sec
TDO 1

===== CHANNEL f1 =====
SF01 500.1525008 MHz
NUC1 1H
P1 11.75 usec
PLW1 15.30000019 W

F2 - Processing parameters
SI 65536
SF 500.1500186 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

163.98
152.78
152.15
143.39
140.94
132.62
131.19
130.59
128.41
124.97
124.78
124.39
114.05
113.96
107.06
97.97
77.32
77.06
76.81
70.03
56.29
56.13
30.60
19.01
13.80

Lab mmb
j3k-333-2
iitm_carbonshort CDC13 /opt/topspin iitm 7

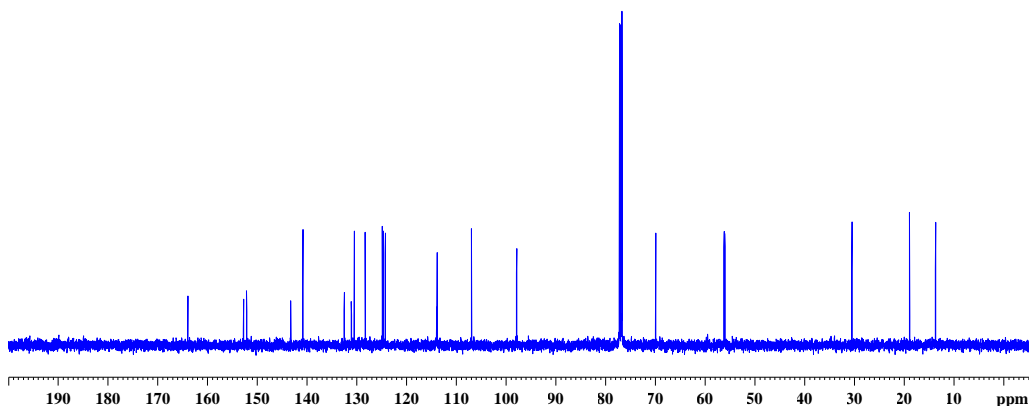
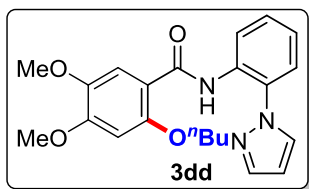
Current Data Parameters
NAME 3,4-dimethoxy butyl
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151103
Time 13.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
FULPROG zgpg30
TD 20480
SOLVENT CDC13
NS 256
DS 4
SWH 29761.904 Hz
FIDRES 1.453218 Hz
AQ 0.3440640 sec
RG 202.34
DW 16.800 usec
DE 6.50 usec
TE 299.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TDO 1

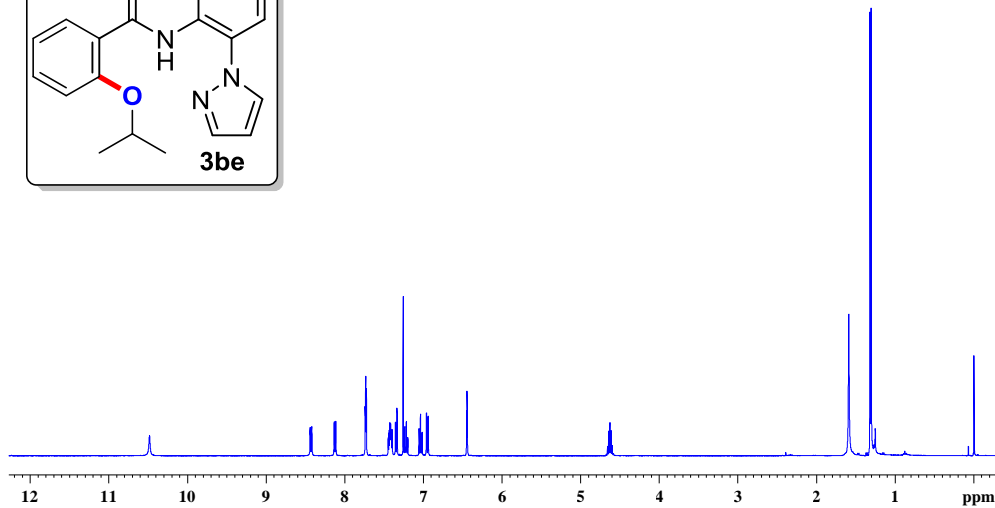
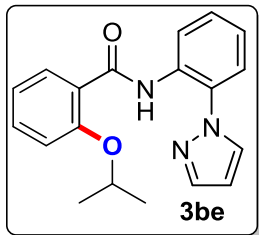
===== CHANNEL f1 =====
SF01 125.7753932 MHz
NUC1 13C
P1 9.63 usec
PLW1 103.00000000 W

===== CHANNEL f2 =====
SF02 500.1520006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 15.30000019 W
PLW12 0.33006001 W
PLW13 0.21123999 W

F2 - Processing parameters
SI 32768
SF 125.7628180 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



10.4819
8.4438
8.4412
8.4232
8.4205
8.1392
8.1346
8.1196
8.1150
7.7413
7.7365
7.7346
7.7284
7.4476
7.4410
7.4362
7.4297
7.4228
7.4200
7.4182
7.4154
7.4125
7.4085
7.4019
7.3972
7.3895
7.3857
7.3396
7.3358
7.2602
7.2414
7.2379
7.2222
7.2192
7.2030
7.0595
7.0570
7.0392
7.0217
7.0193
6.9636
6.9429
6.4536
6.4482
6.4430
4.6452
4.6299
4.6147
1.3223
1.3070



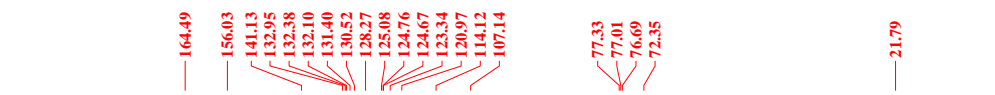
Current Data Parameters
NAME JSK
EXPNO 97
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160415
Time 10.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 299.8 K
D1 0.50000000 sec
TD0 1

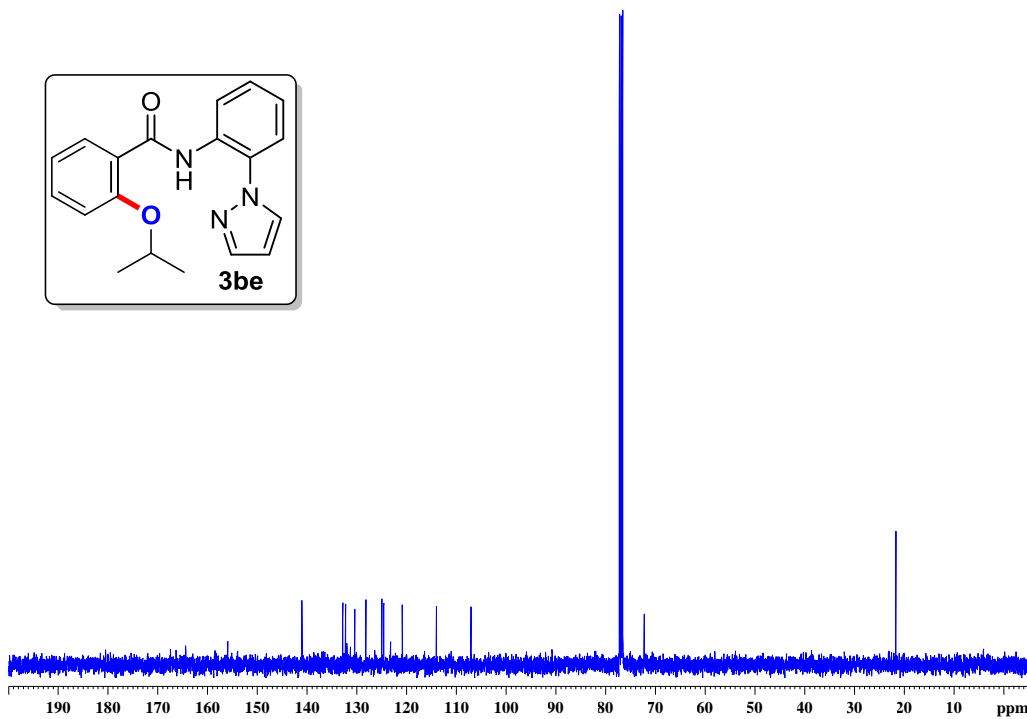
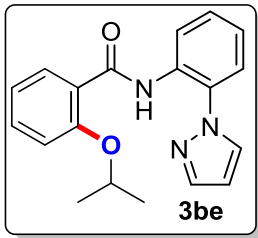
===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1.0
1.1
2.1
2.1
1.1
1.1
1.1
1.1
1.1
1.0
1.1
3.0
3.1
21.79



lab mmb-jsk-ph-ivr
iitm_carbonshort CDCl3 /opt/topspin nmr 8



Current Data Parameters
NAME ph-ivr
EXPNO 117
PROCNO 1

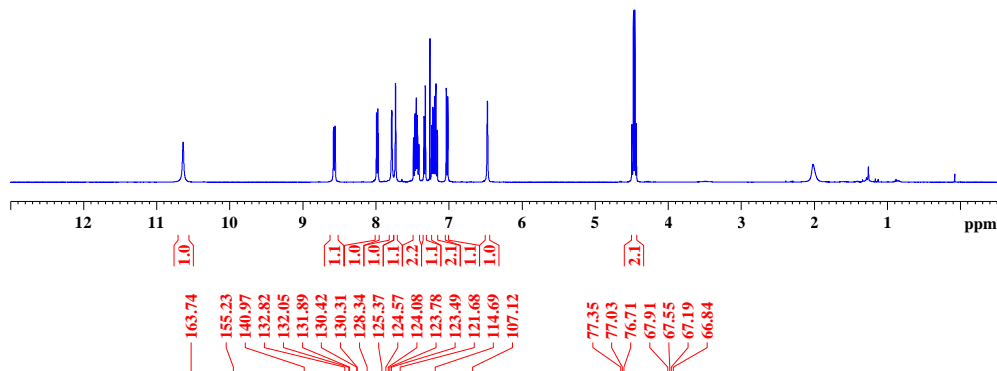
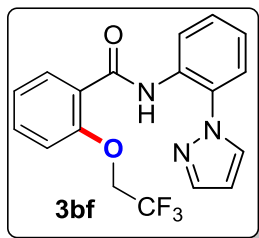
F2 - Acquisition Parameters
Date_ 20160415
Time 14.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 300.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

10.6388
8.5796
8.5591
7.9335
7.9891
7.9741
7.9697
7.7847
7.7805
7.7323
7.7291
7.4870
7.4825
7.4685
7.4661
7.4641
7.4618
7.4518
7.4479
7.4433
7.4308
7.4129
7.4096
7.3431
7.3394
7.3232
7.3196
7.2381
7.2348
7.2189
7.2162
7.1980
7.1959
7.1778
7.1771
7.1602
7.1579
7.0368
7.0160
6.4794
6.4740
6.4688
4.4963
4.4758
4.4553
4.4349



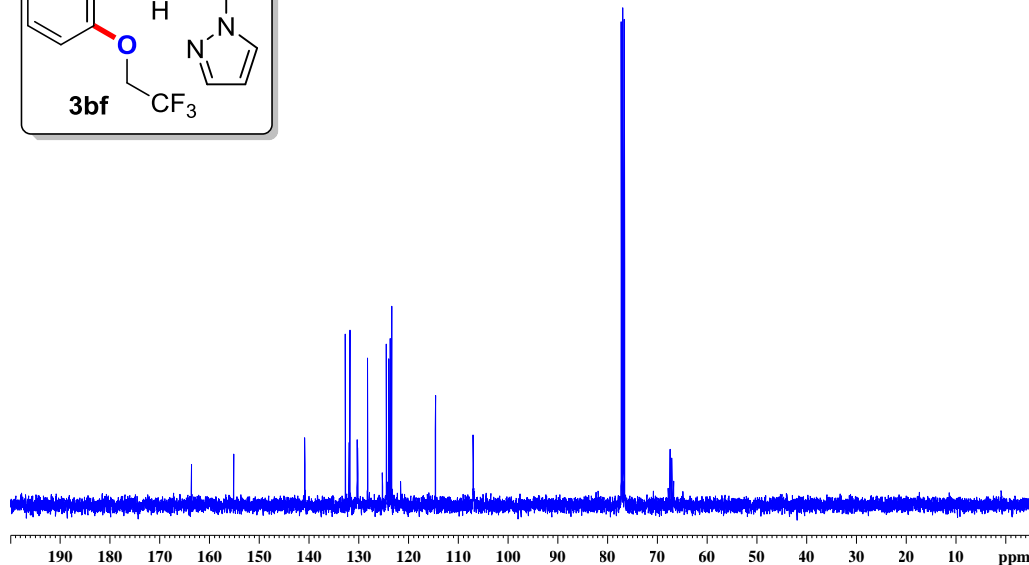
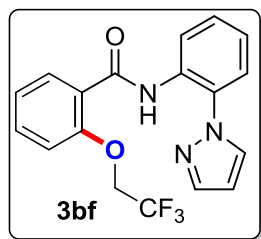
Current Data Parameters
NAME ph-TF ethanol
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151002
Time 18.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.77
DW 62.400 usec
DE 6.50 usec
TE 298.7 K
D1 0.5000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.70 usec
PLW1 7.7500000 W
SF01 400.1320007 MHz

F2 - Processing parameters
SI 65536
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

lab mmbjsk-306
iitm_carbonshort CDCl3 /opt/topspin nmr 16



Current Data Parameters
NAME ph-TF ethanol
EXPNO 10
PROCNO 1

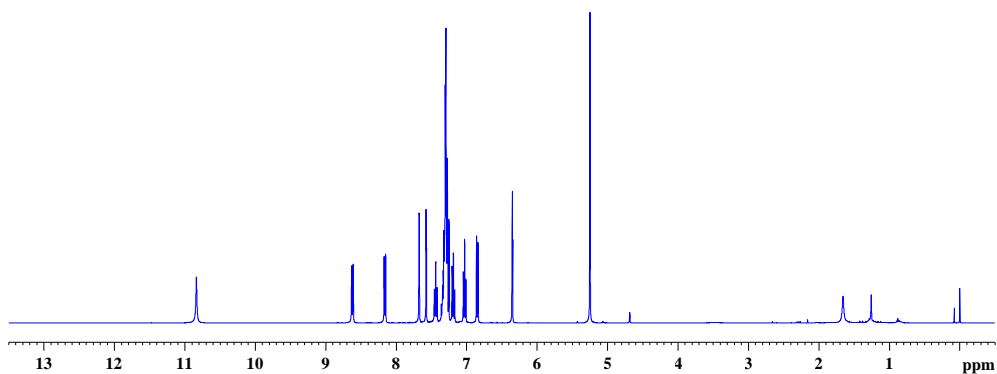
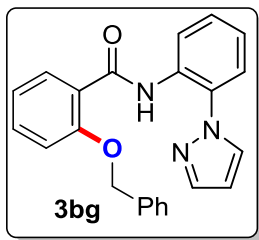
F2 - Acquisition Parameters
Date_ 20151002
Time 18.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 299.6 K
D1 1.0000000 sec
D11 0.0300000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.25 usec
PLW1 47.0000000 W
SF01 100.6228289 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.7500000 W
PLW12 0.2358399 W
PLW13 0.1910300 W
SF02 400.1316005 MHz

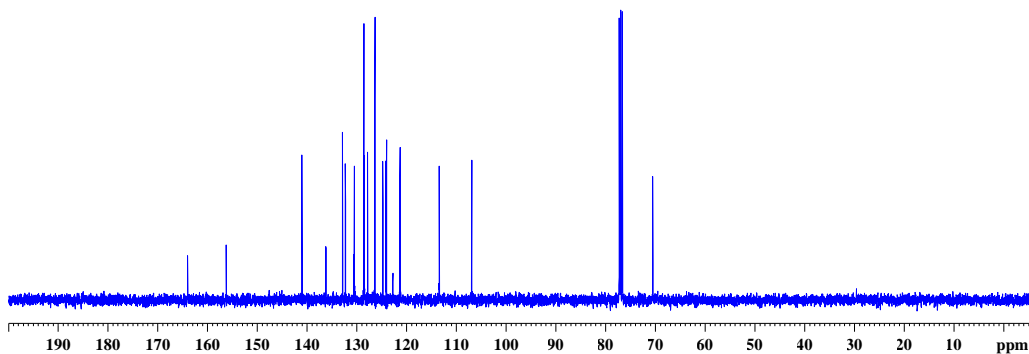
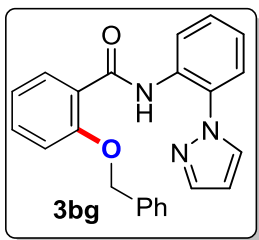
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

10.8389
8.6347
8.6323
8.6139
8.6115
8.1735
8.1689
8.1539
8.1493
7.6788
7.6729
7.5789
7.5745
7.4622
7.4584
7.4405
7.4230
7.4191
7.3410
7.3328
7.3278
7.3237
7.3193
7.3144
7.3116
7.3065
7.2963
7.2893
7.2775
7.2734
7.2103
7.2070
7.1915
7.1883
7.1721
7.1688
7.0499
7.0476
7.0301
7.0121
7.0098
6.8616
6.8601
6.8407
6.8389
6.3578
6.3526
6.3471
5.2498



164.10
156.33
141.12
136.31
132.97
132.39
130.69
130.57
128.69
128.62
127.92
126.46
124.87
124.23
124.14
122.86
121.42
113.55
107.00
77.36
77.04
76.72
70.63

lab mmbjsk-307
iitm_carbonsshort CDC13 /opt/topspin nmr 1



Current Data Parameters
NAME JSK-307 benzyl
EXPNO 186
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150929
Time_ 17.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 153.13
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 0.50000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W
SF01 400.1320007 MHz

F2 - Processing parameters
SI 65536
SF 400.1300124 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
NAME JSK-307 benzyl
EXPNO 187
PROCNO 1

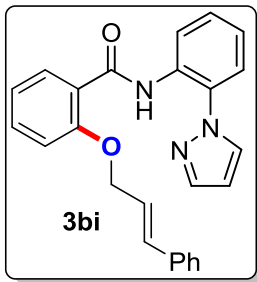
F2 - Acquisition Parameters
Date_ 20150929
Time_ 17.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16540
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SF01 100.6228289 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

10.8194
8.6174
8.5969
8.1834
8.1796
8.1640
8.1602
7.7251
7.7222
7.7055
7.7004
7.4540
7.4352
7.4249
7.4082
7.3900
7.3857
7.3563
7.3385
7.3227
7.3047
7.2867
7.2615
7.2574
7.2507
7.2449
7.2099
7.2072
7.1886
7.1719
7.1690
7.0794
7.0612
7.0433
7.0418
7.0106
6.9899
6.6495
6.6093
6.4301
6.4252
6.4202
6.3729
6.3593
6.3457
6.3329
6.3191
6.3055
4.8585
4.8476

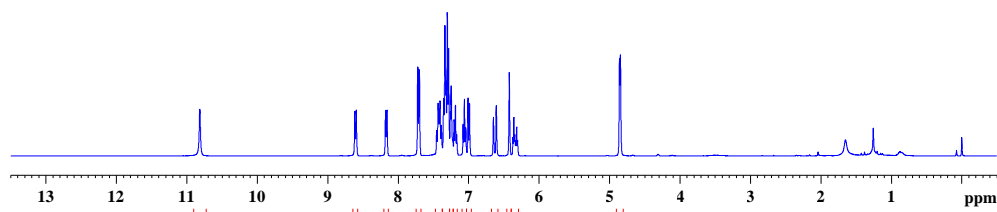


Current Data Parameters
NAME JSK-308 cinnamyl
EXPNO 189
PROCNO 1

F2 - Acquisition Parameters
Date 20150929
Time 17.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 153.13
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 0.50000000 sec
TDO 1

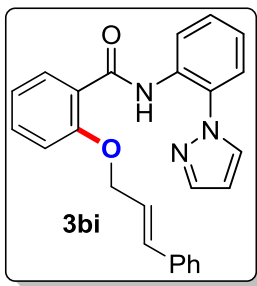
===== CHANNEL f1 =====
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W
SF01 400.1320007 MHz

F2 - Processing parameters
SI 65536
SF 400.1300131 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



164.06
156.46
141.12
136.09
133.16
133.04
132.87
132.44
130.71
130.60
128.65
128.57
128.08
126.60
124.73
124.24
123.86
122.77
121.36
113.17
107.04
77.36
77.04
76.72
69.66

lab mmbjsk-308
iitm_carbonsshort CDCl3 /opt/topspin nmr 2



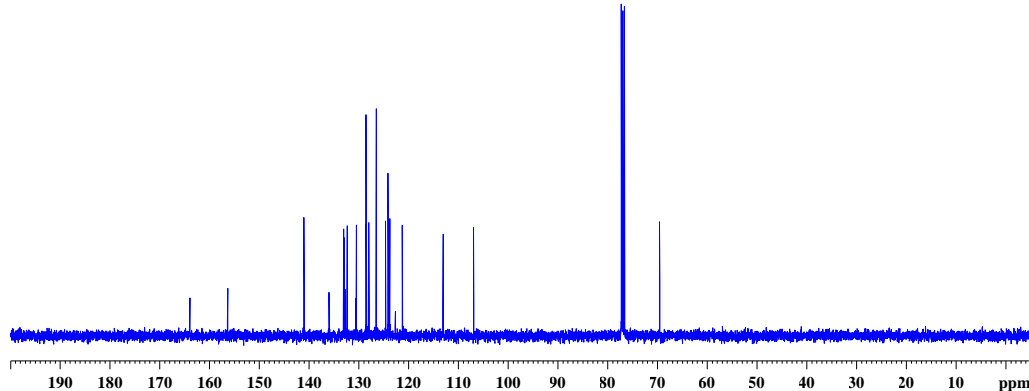
Current Data Parameters
NAME JSK-308 cinnamyl
EXPNO 190
PROCNO 1

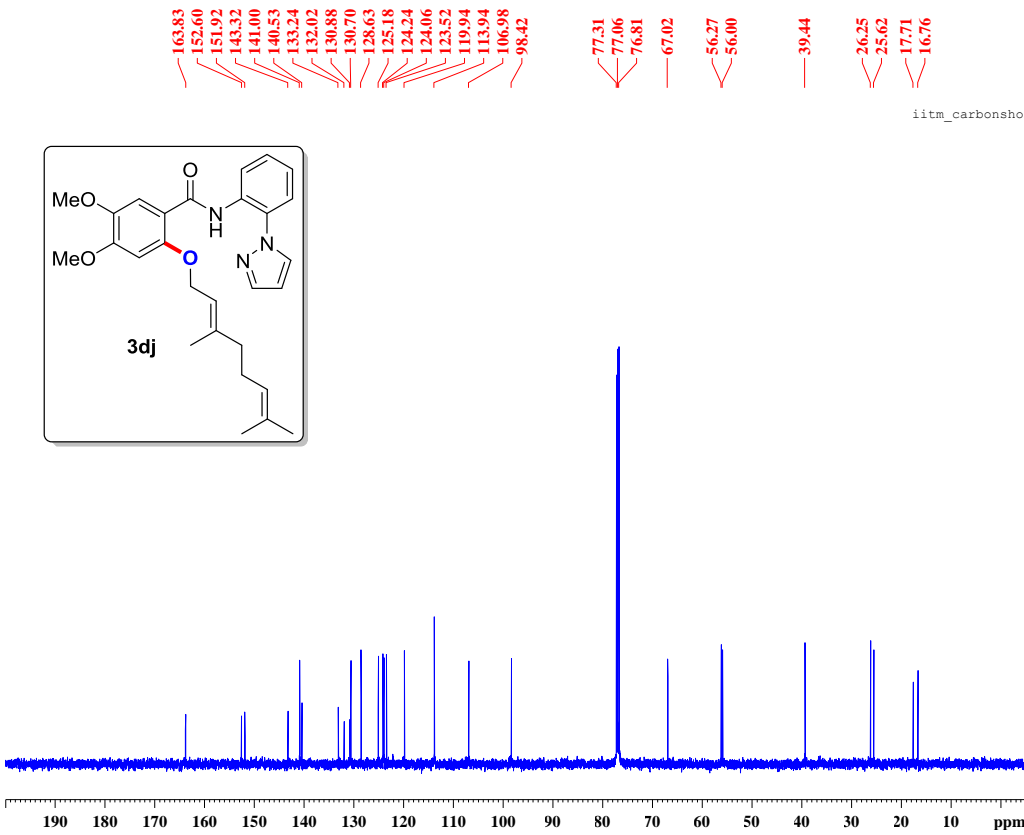
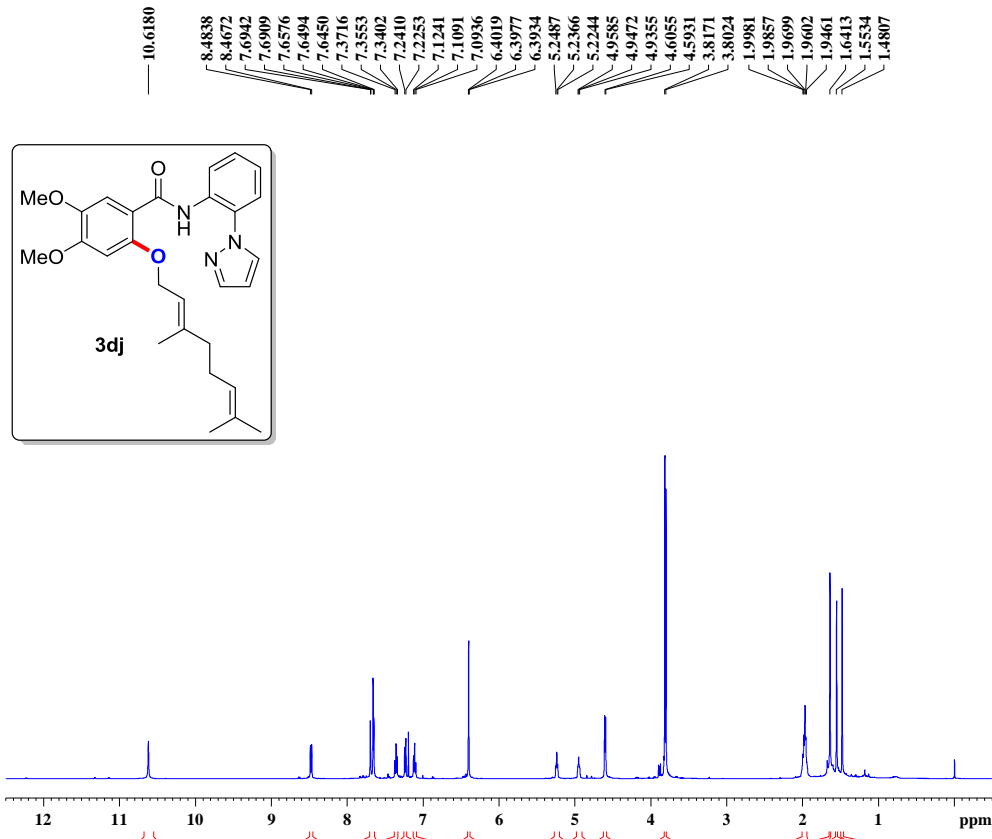
F2 - Acquisition Parameters
Date 20150929
Time 17.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 298.9 K
D1 1.00000000 sec
D11 0.03000000 sec
TDO 1

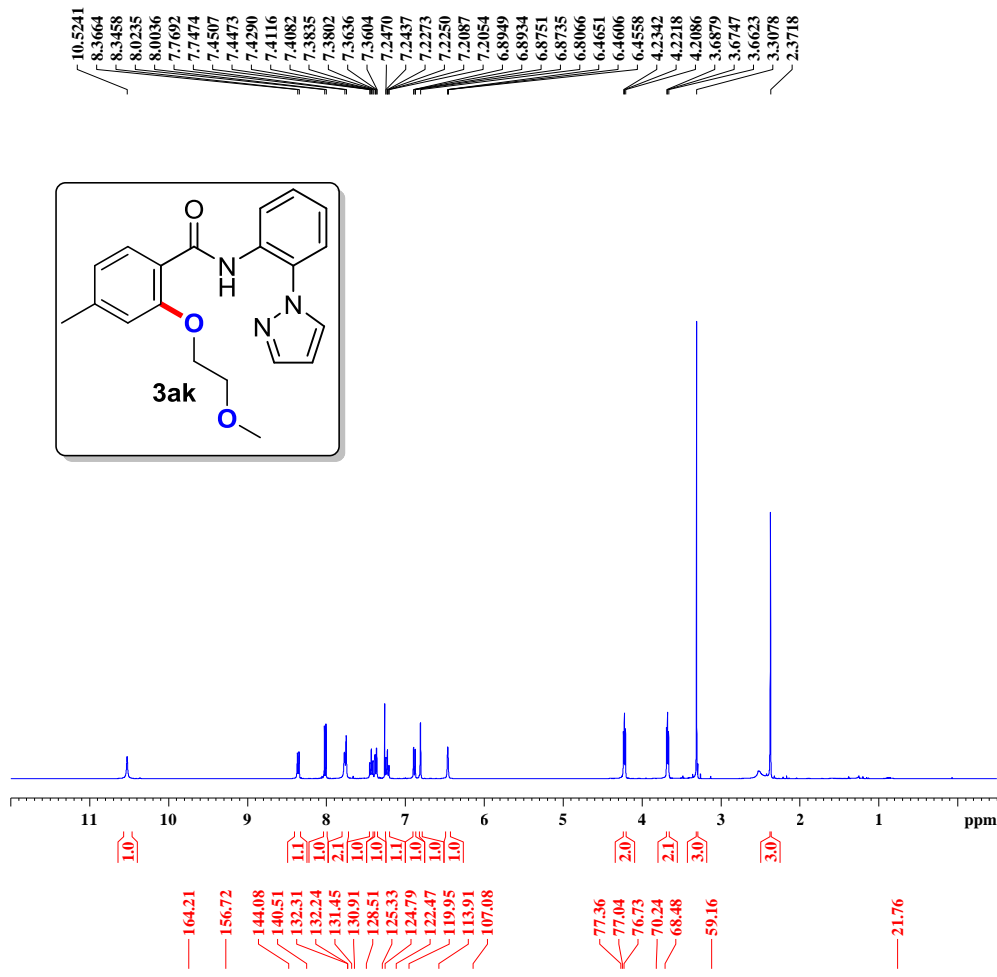
===== CHANNEL f1 =====
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SF01 100.6228289 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





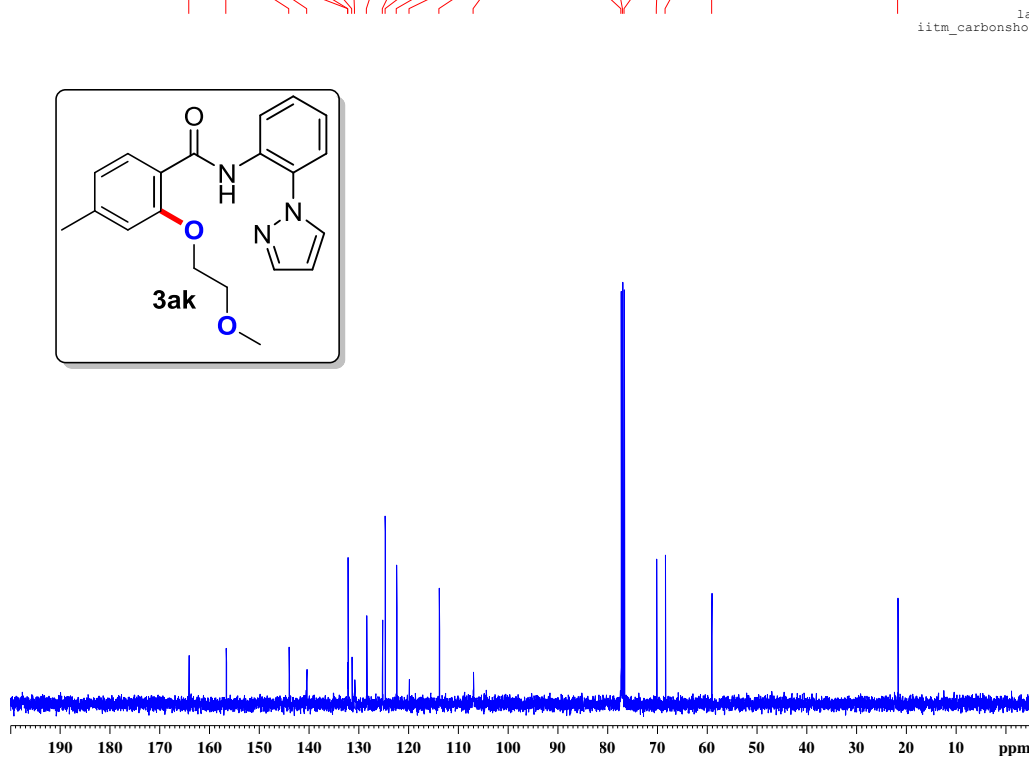


```
Current Data Parameters
NAME      JSK-320-3
EXPNO    87
PROCNO   1

F2 - Acquisition Parameters
Date_    20151016
Time     10.47
INSTRUM spect
PROBHD   5 mm PABBO BB-
PULPROG zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ       4.0894465 sec
RG       153.13
DW       62.400 usec
DE       6.50 usec
TE       295.2 K
D1       0.50000000 sec
TD0      1

===== CHANNEL f1 =====
NUC1     1H
P1       15.70 usec
PLW1    7.75000000 W
SF01    400.1320007 MHz

F2 - Processing parameters
SI       65536
SF       400.1300094 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
```



```
lab mmb-jsk-320-3
iitm_carbonshort CDCl3 /opt/topspin nmr 11

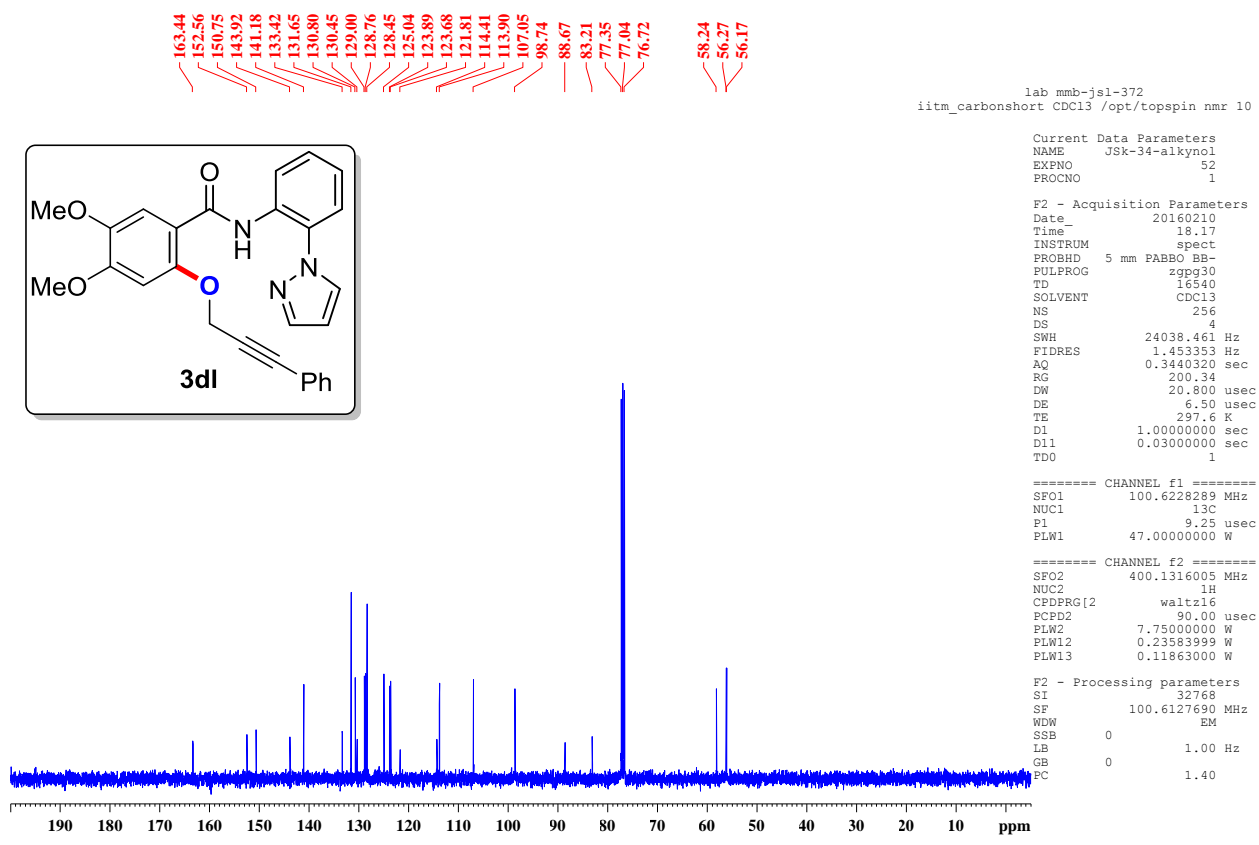
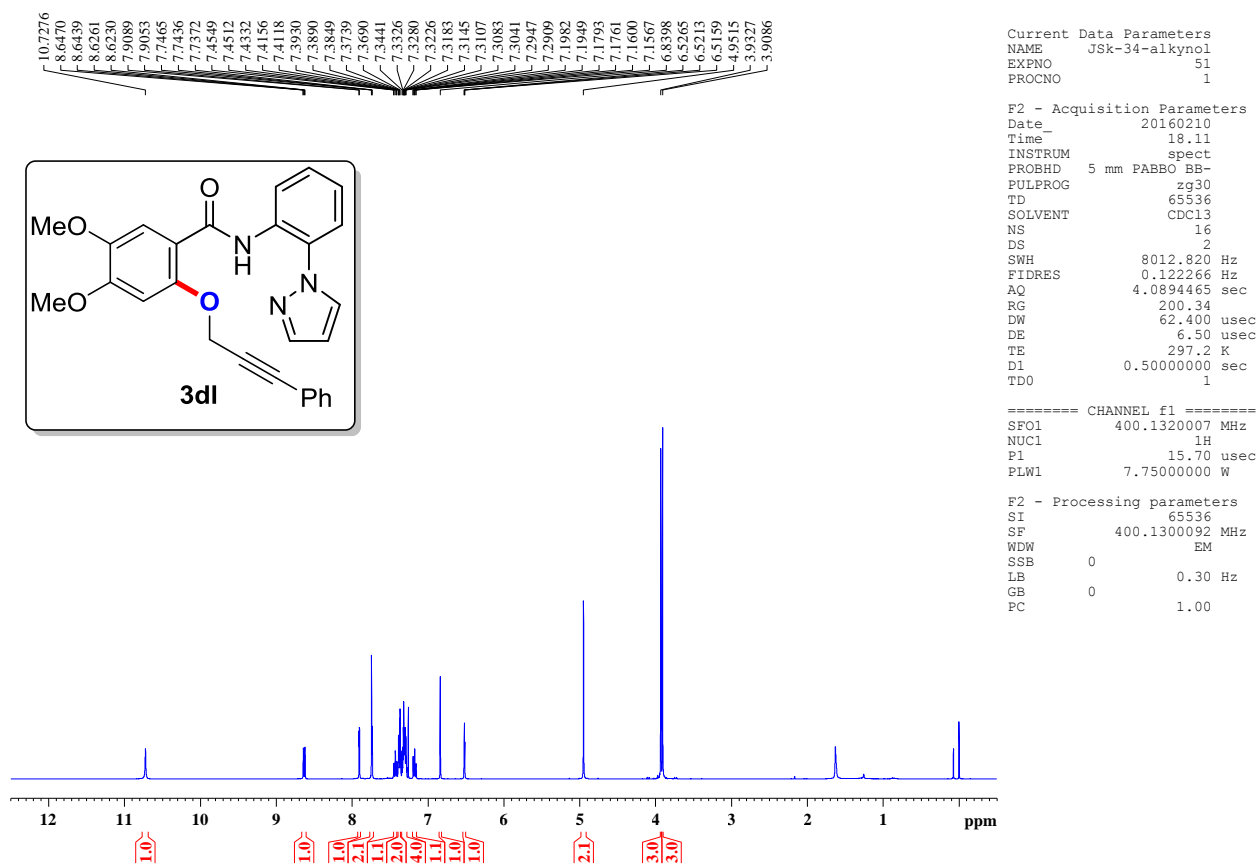
Current Data Parameters
NAME      JSK-320-3
EXPNO    88
PROCNO   1

F2 - Acquisition Parameters
Date_    20151016
Time     10.55
INSTRUM spect
PROBHD   5 mm PABBO BB-
PULPROG zgpg30
TD       16540
SOLVENT  CDCl3
NS       256
DS       4
SWH      24038.461 Hz
FIDRES   1.453353 Hz
AQ       0.3440320 sec
RG       200.34
DW       20.800 usec
DE       6.50 usec
TE       296.0 K
D1       1.00000000 sec
D11      0.03000000 sec
TD0      1

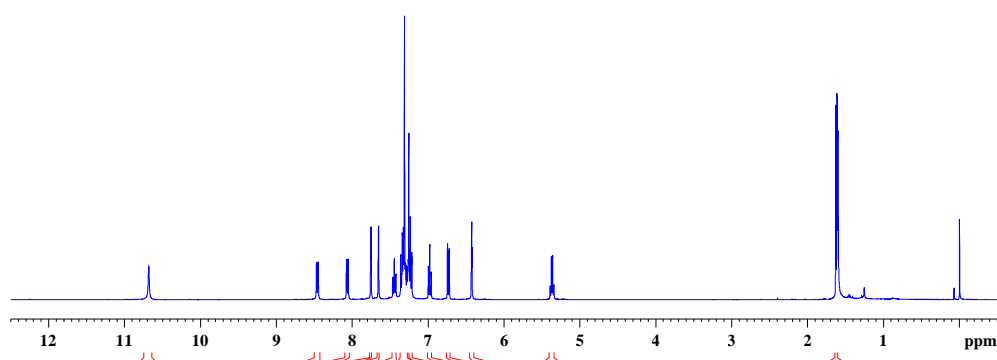
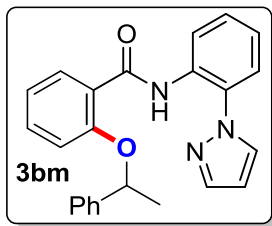
===== CHANNEL f1 =====
NUC1     13C
P1       9.25 usec
PLW1    47.00000000 W
SF01    100.6228289 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2   90.00 usec
PLW2    7.75000000 W
PLW12   0.23583999 W
PLW13   0.19103000 W
SF02    400.1316005 MHz

F2 - Processing parameters
SI       32768
SF       100.6127690 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
```



10.6849
8.4728
8.4523
8.0803
8.0759
8.0608
8.0564
7.7600
7.7546
7.6596
7.6558
7.4483
7.4308
7.4273
7.3652
7.3616
7.3454
7.3417
7.3360
7.3310
7.3288
7.3200
7.3146
7.3032
7.2993
7.2873
7.2825
7.2722
7.2658
7.2577
7.2421
7.2379
7.2354
7.2211
7.2219
7.2195
7.2166
7.0017
6.9995
6.9810
6.9640
6.9618
6.7467
6.7259
6.4341
6.4289
6.4234
5.3781
5.3619
1.6299
1.6136



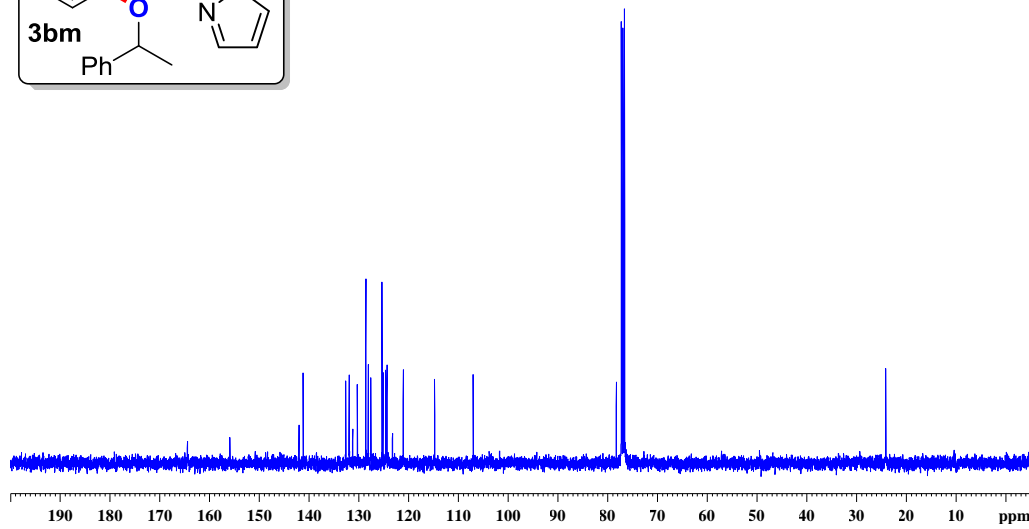
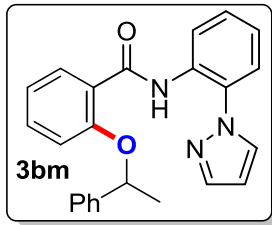
164.54
156.02
142.13
141.29
132.75
132.05
131.34
130.41
128.70
128.21
127.71
125.45
125.23
124.74
124.46
123.34
121.18
114.87
107.13
78.37
77.34
77.03
76.71
24.24

Current Data Parameters
NAME JSK-377-3
EXPNO 90
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160213
Time 22.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 297.1 K
D1 0.50000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300110 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Lab mmbjsk-377-d
iitm_carbonshort CDCl3 /opt/topspin nmr 5

Current Data Parameters
NAME JSK-377-3
EXPNO 91
PROCNO 1

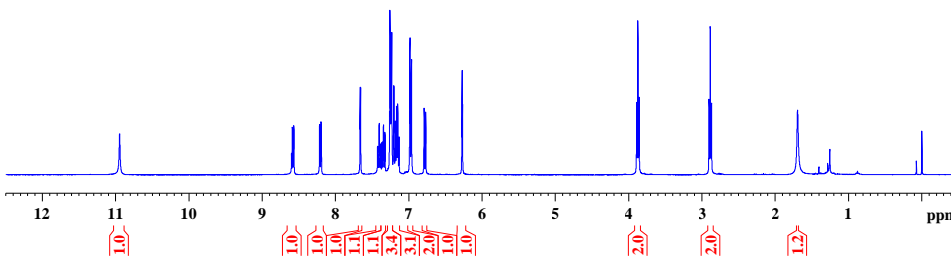
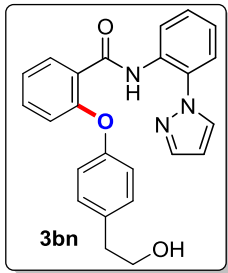
F2 - Acquisition Parameters
Date_ 20160213
Time_ 23.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

10.9436
8.5937
8.5730
8.2196
8.2153
8.2000
8.1956
7.6666
7.6667
7.6607
7.4069
7.3510
7.3483
7.3466
7.3440
7.3303
7.2618
7.2659
7.2591
7.2565
7.2514
7.2464
7.2422
7.2351
7.2078
7.2040
7.1880
7.1846
7.1743
7.1714
7.1696
7.1661
7.1545
7.1501
6.9873
6.9826
6.9704
6.9660
6.7942
6.7920
6.7734
6.7712
6.2788
6.2738
6.2681
3.8931
3.8766
3.8601
2.9048
2.8883
2.8719
1.6964



```
Current Data Parameters
NAME JSK-335-ph-phenylethanol
EXPNO 70
PROCNO 1

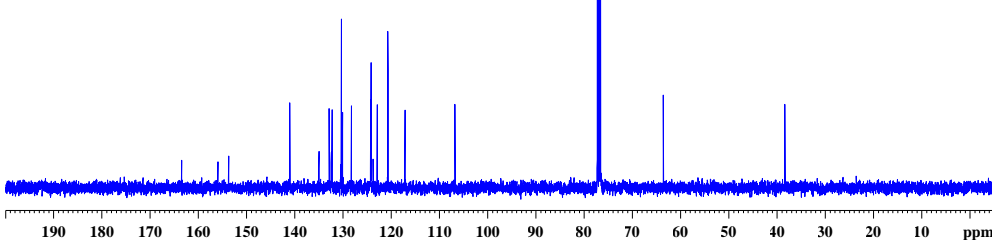
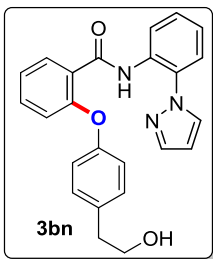
F2 - Acquisition Parameters
Date_ 20160120
Time 4.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.089465 sec
RG 153.13
DW 62.400 usec
DE 6.50 usec
TE 299.1 K
D1 0.5000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
```

163.56
156.06
153.81
141.13
135.10
132.97
132.54
132.37
130.56
130.44
130.21
128.37
124.36
124.26
123.85
123.01
120.79
117.24
106.89
77.36
77.04
76.73
63.70
38.50

lab mmb-jsk-353
iitm_carbonshort CDCl3 /opt/topspin nmr 12



```
Current Data Parameters
NAME JSK-335-ph-phenylethanol
EXPNO 190
PROCNO 1

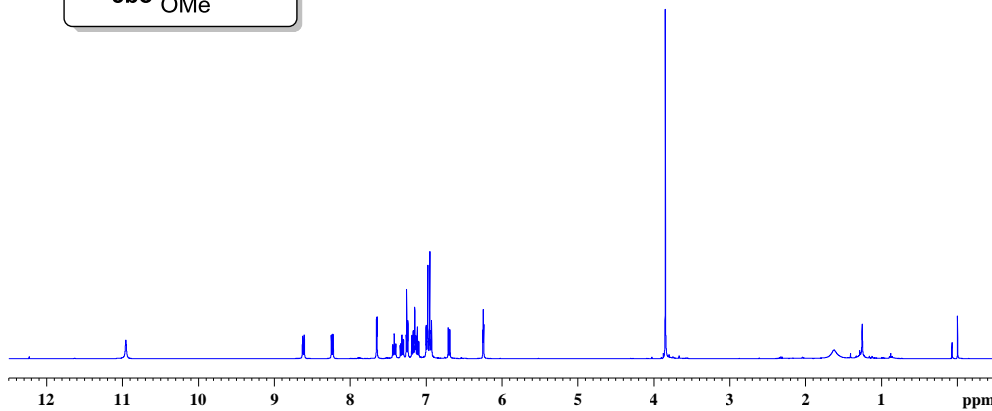
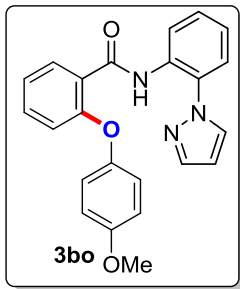
F2 - Acquisition Parameters
Date_ 20151117
Time 22.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 291.9 K
D1 1.0000000 sec
D11 0.0300000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO1 100.6228289 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz

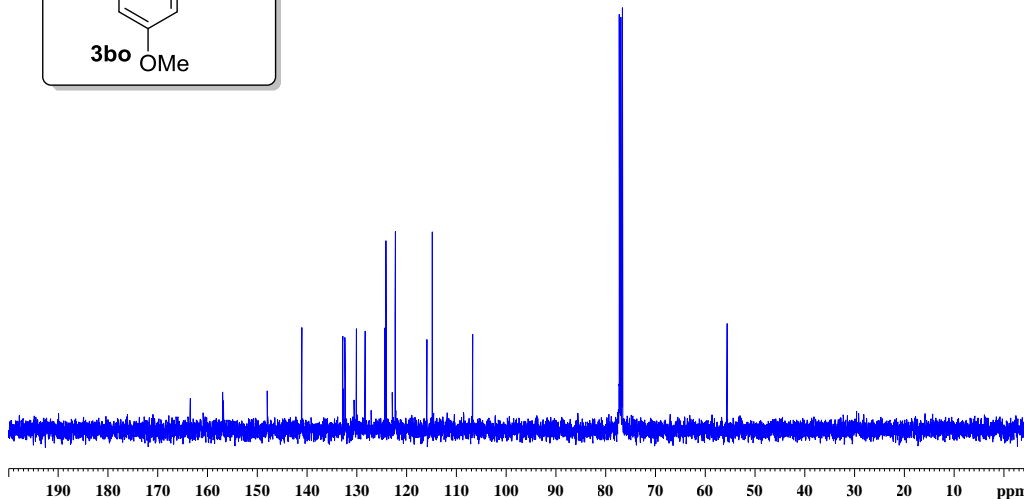
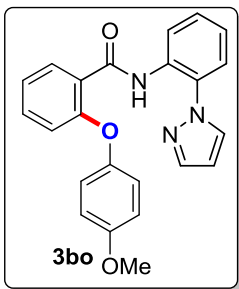
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

10.9596
8.6318
8.6294
8.6110
8.6086
8.2516
8.2472
8.2319
8.2275
7.6558
7.6507
7.4237
7.3252
7.3223
7.3208
7.3180
7.3044
7.2998
7.2656
7.2590
7.2459
7.2421
7.1926
7.1892
7.1740
7.1707
7.1542
7.1504
7.1382
7.1355
7.1182
7.1004
7.0031
6.9967
6.9864
6.9800
6.9729
6.9612
6.9540
6.9475
6.9373
6.9309
6.7118
6.7097
6.6909
6.6889
6.2545
6.2493
6.2437
3.8506



163.58
157.04
156.90
148.10
141.18
132.95
132.85
132.48
130.65
130.18
128.44
124.50
124.25
122.97
122.42
122.37
116.03
114.94
106.81
77.35
77.03
76.72
55.71

lab mmbjsk-363
iitm_carbonshort CDCl3 /opt/topspin nmr 6



Current Data Parameters
NAME JSK-ph-4OmePhenol
EXPNO 73
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160120
Time 5.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.9
DW 62.400 usec
DE 6.50 usec
TE 299.3 K
D1 0.50000000 sec
TDO 1

===== CHANNEL f1 =====
SF01 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

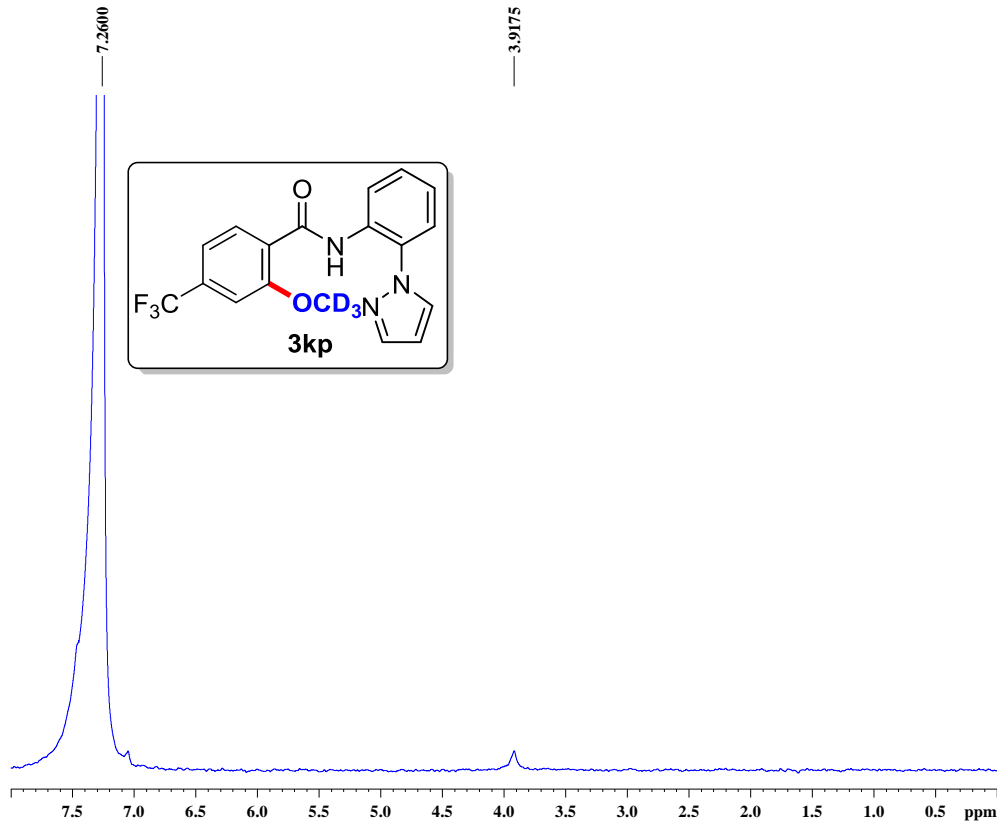
Current Data Parameters
NAME JSK-ph-4OmePhenol
EXPNO 126
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160121
Time_ 10.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 297.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
SF01 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SF02 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



```

Current Data Parameters
NAME      Cd3 2D NMR
EXPNO    92
PROCNO   1

F2 - Acquisition Parameters
Date_    20160226
Time     9.42
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg2h
TD       65536
SOLVENT  None
NS       1
DS       1
SWH      921.376 Hz
FIDRES   0.014059 Hz
AQ       35.5642014 sec
RG       3.88
DW       542.667 usec
DE       6.50 usec
TE       300.0 K
D1       1.00000000 sec
D11      0.03000000 sec
TD0      1

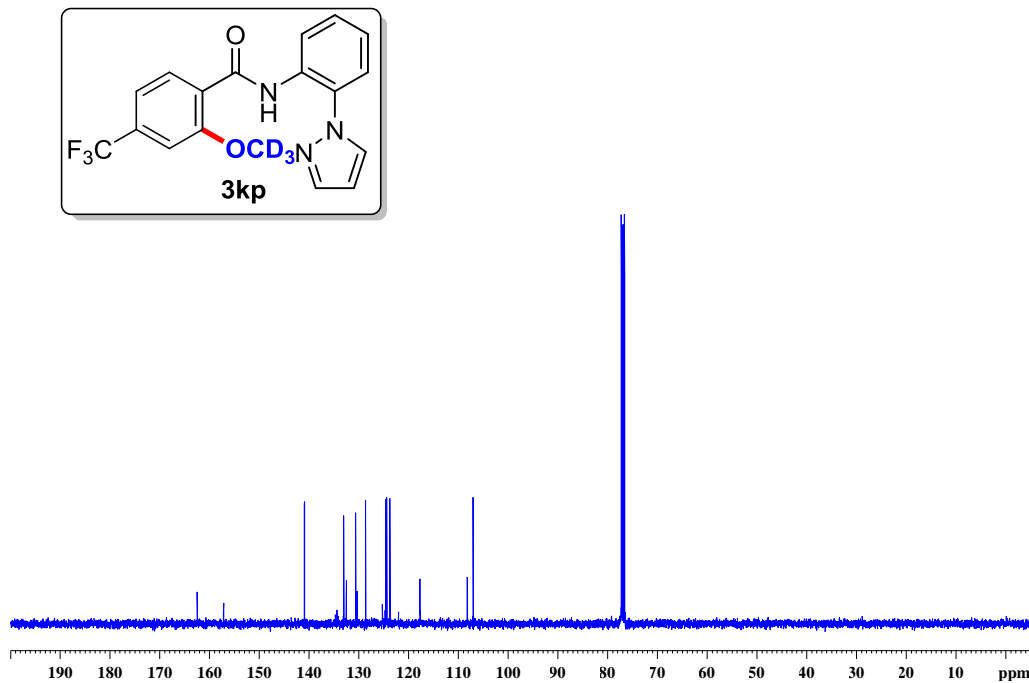
===== CHANNEL f1 =====
SFO1     76.7764539 MHz
NUC1     2H
P1       530.00 usec
PLW1     1.79999995 W

F2 - Processing parameters
SI       65536
SF       76.7760296 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.00
  
```

162.57
157.27
141.03
134.48
132.61
130.74
128.73
125.37
124.82
124.67
124.49
123.85
122.10
117.86
117.82
117.75
117.78
108.36
108.32
108.28
108.25
107.14
77.34
77.02
76.70

```

lab mmbjsk-378-2-f
iitm_carbonshort CDCl3 /opt/topspin nmr 4
  
```



```

Current Data Parameters
NAME      JSK-378-2 4CF3 CD3
EXPNO    145
PROCNO   1

F2 - Acquisition Parameters
Date_    20160222
Time     1.28
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD       16540
SOLVENT  CDCl3
NS       1000
DS       4
SWH      24038.461 Hz
FIDRES   1.453353 Hz
AQ       0.3440320 sec
RG       200.34
DW       20.800 usec
DE       6.50 usec
TE       298.3 K
D1       1.00000000 sec
D11      0.03000000 sec
TD0      1

===== CHANNEL f1 =====
SFO1     100.6228289 MHz
NUC1     13C
P1       9.25 usec
PLW1     47.00000000 W

===== CHANNEL f2 =====
SFO2     400.1316005 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    90.00 usec
FLW2     7.75000000 W
FLW12    0.23583999 W
FLW13    0.11863000 W

F2 - Processing parameters
SI       32768
SF       100.6127690 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```

10.7288
8.6179
8.6152
8.5970
8.5943
8.1393
8.1182
7.8037
7.7993
7.7391
7.7332
7.4588
7.4550
7.4368
7.4195
7.4157
7.3079
7.3040
7.2881
7.2843
7.2608
7.2126
7.2094
7.1938
7.1906
7.1744
7.1711
7.0655
7.0608
7.0444
7.0397
6.9329
6.9283
6.5082
6.5031
6.4975

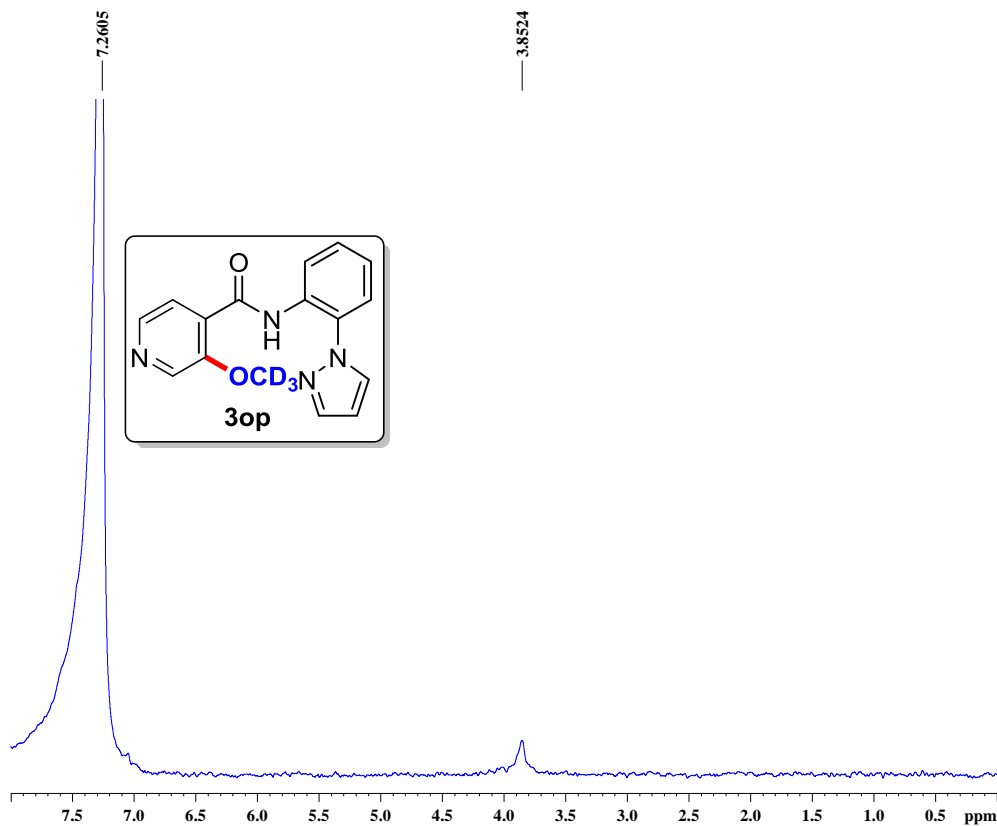
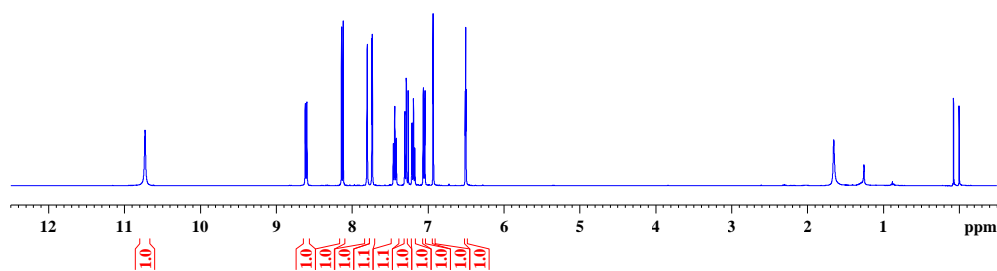
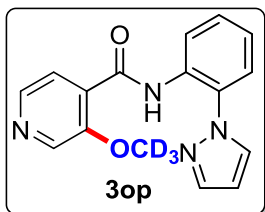
```

Current Data Parameters
NAME      JSK-378-3-py-cd3
EXPNO     139
PROCNO    1

F2 - Acquisition Parameters
Date_     20160221
Time      23.39
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8012.820 Hz
FIDRES     0.122266 Hz
AQ         4.0894465 sec
RG         200.34
DW         62.400 usec
DE         6.50 usec
TE         297.8 K
D1         0.50000000 sec
TDO        1

===== CHANNEL f1 =====
SF01      400.1320007 MHz
NUC1       1H
P1         15.70 usec
PLW1       7.75000000 W

F2 - Processing parameters
SI         65536
SF         400.1300094 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



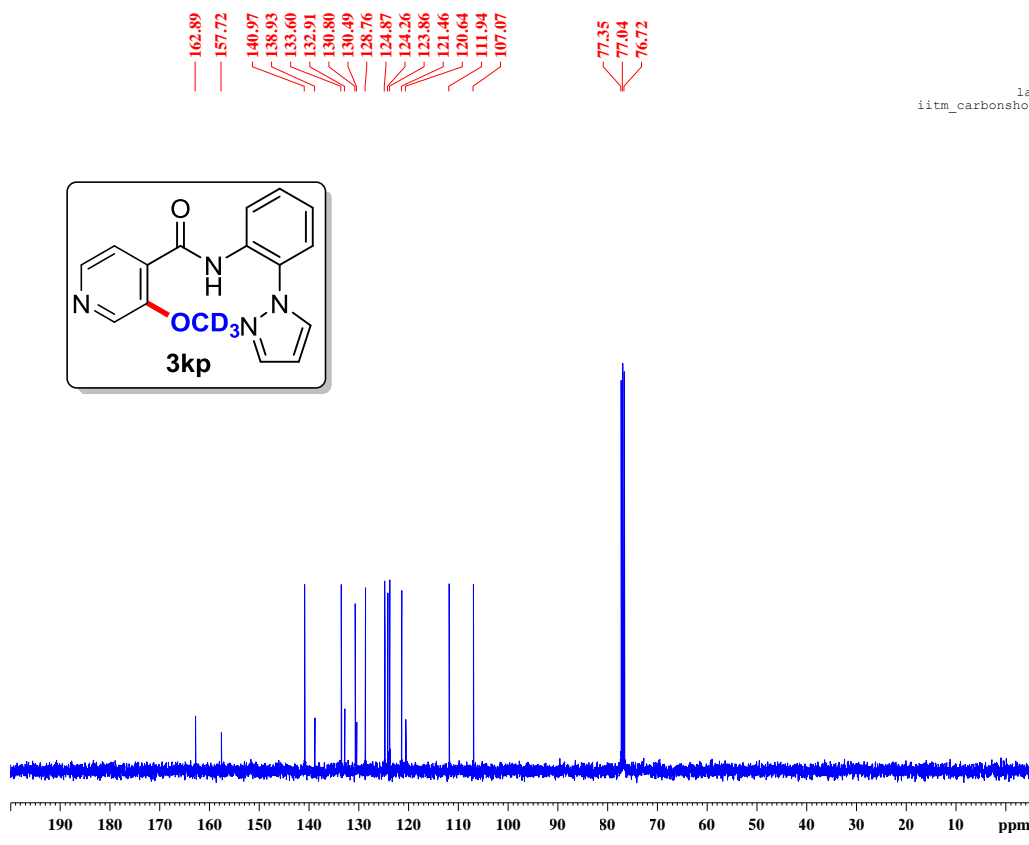
```

Current Data Parameters
NAME      Cd3 2D NMR
EXPNO     87
PROCNO    1

F2 - Acquisition Parameters
Date_     20160229
Time      11.33
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg2h
TD         65536
SOLVENT   None
NS         1
DS         1
SWH        921.376 Hz
FIDRES     0.014059 Hz
AQ         35.5642014 sec
RG         3.88
DW         542.667 usec
DE         6.50 usec
TE         300.0 K
D1         1.00000000 sec
D11        0.03000000 sec
TDO        1

===== CHANNEL f1 =====
SF01      76.7764539 MHz
NUC1       2H
P1         530.00 usec
PLW1       1.79999995 W

F2 - Processing parameters
SI         65536
SF         76.7760748 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.00
  
```



lab mmb-jsk-378-3
iitm_carbonshort CDCl3 /opt/topspin nmr 15

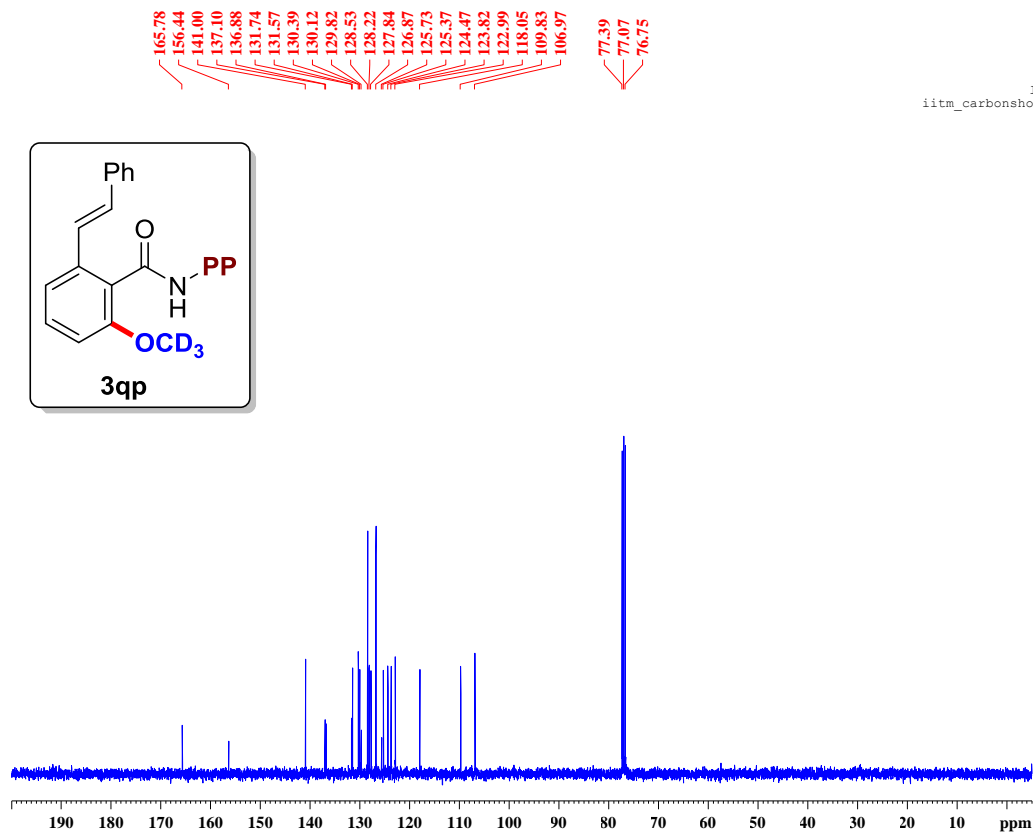
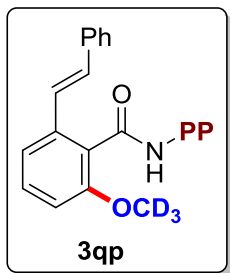
Current Data Parameters
NAME JSK-378-3-py-cd3
EXPNO 140
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160221
Time_ 23.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 298.3 K
D1 1.0000000 sec
D11 0.0300000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



lab mmbjsk-414
iitm_carbonshort CDCl3 /opt/topspin nmr 4

```

Current Data Parameters
NAME          mmb40616
EXPNO         260
PROCNO        1

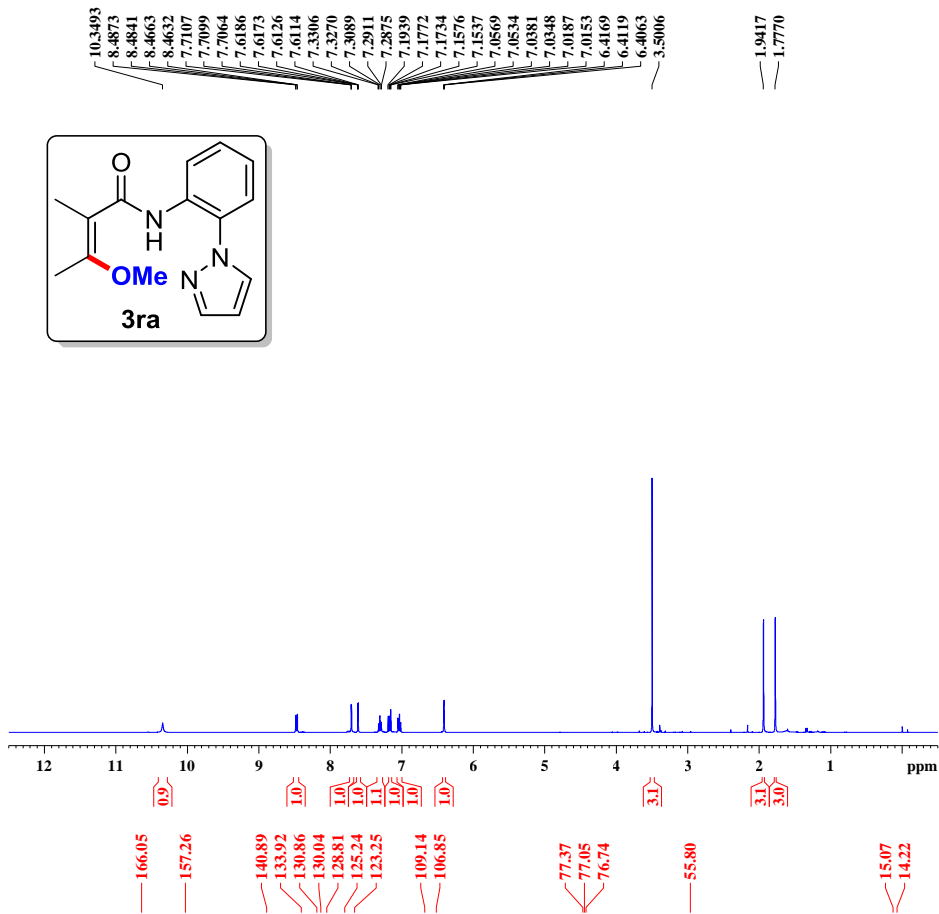
F2 - Acquisition Parameters
Date_         20160623
Time_         9.38
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            16340
SOLVENT       CDCl3
NS            256
DS            4
SWH           24038.461 Hz
FIDRES        1.453353 Hz
AQ            0.3440320 sec
RG            200.34
DW            20.800 usec
DE            6.50 usec
TE            294.5 K
D1            1.0000000 sec
D11           0.0300000 sec
TD0           1

===== CHANNEL f1 =====
SFO1          100.6228289 MHz
NUC1           13C
P1            9.25 usec
PLW1          47.0000000 W

===== CHANNEL f2 =====
SFO2          400.1316005 MHz
NUC2           1H
PCPD2         waltz16
PLW2          7.7500000 W
PLW12         0.23583999 W
PLW13         0.11863000 W

F2 - Processing parameters
SI            32768
SF            100.6127690 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```



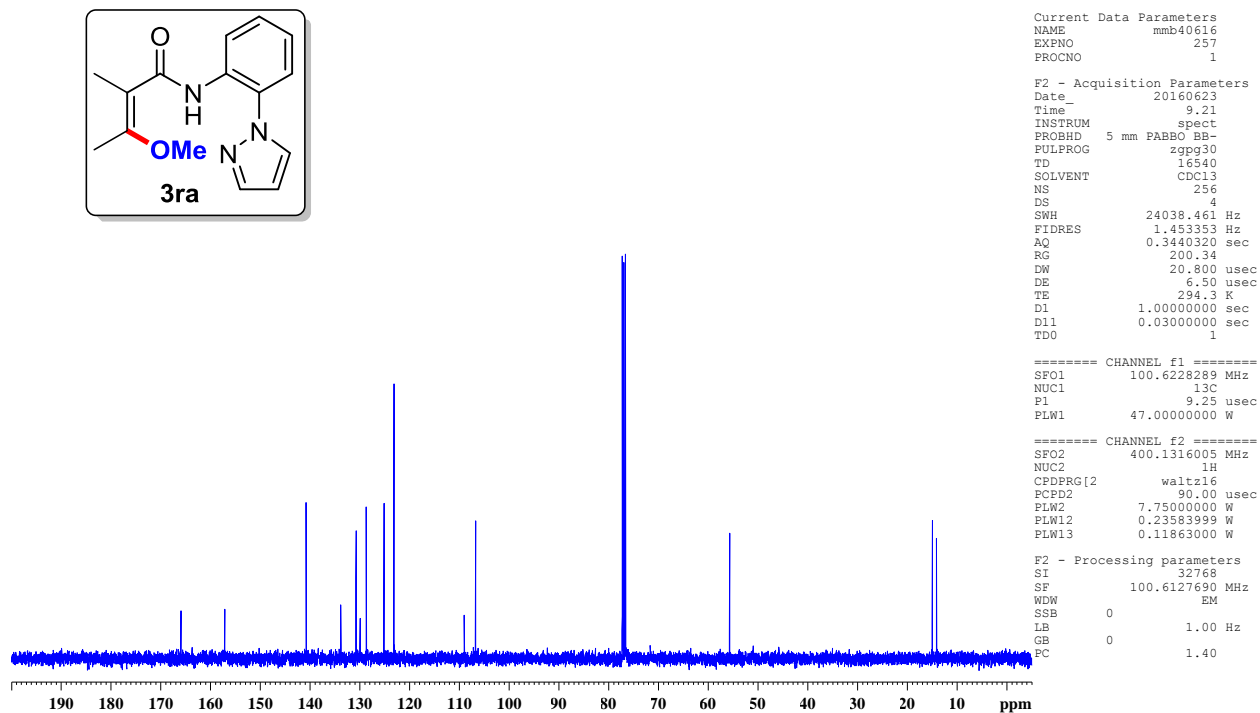
Current Data Parameters
 NAME mmb40616
 EXPNO 256
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160623
 Time_ 9.19
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 153.13
 DW 62.400 usec
 DE 6.50 usec
 TE 293.9 K
 D1 0.50000000 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 400.1320007 MHz
 NUC1 1H
 P1 15.70 usec
 PLW1 7.75000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300362 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

lab mmbjsk-415
 iitm_carbonshort CDCl3 /opt/topspin nmr 3



Current Data Parameters
 NAME mmb40616
 EXPNO 257
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160623
 Time_ 9.21
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 16540
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 24038.461 Hz
 FIDRES 1.453353 Hz
 AQ 0.3440320 sec
 RG 200.34
 DW 20.800 usec
 DE 6.50 usec
 TE 294.3 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TDO 1

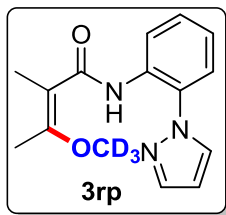
==== CHANNEL f1 =====
 SFO1 100.6228289 MHz
 NUC1 13C
 P1 9.25 usec
 PLW1 47.00000000 W

==== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 7.75000000 W
 PLW12 0.23583999 W
 PLW13 0.11863000 W

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

10.4210
8.5575
8.5543
8.5366
8.5333
7.7841
7.7831
7.7796
7.6922
7.6908
7.6862
7.6849
7.4056
7.4019
7.3838
7.3663
7.3625
7.2649
7.2513
7.2474
7.2316
7.2277
7.1316
7.1282
7.1128
7.1095
7.0935
7.0900
6.4913
6.4862
6.4807

2.0152
1.8504

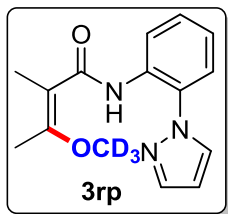
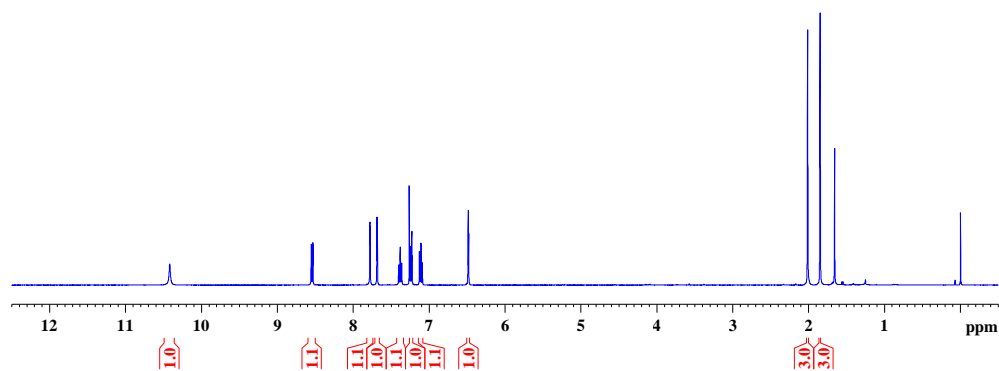


Current Data Parameters
NAME mmb40616
EXPNO 277
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160624
Time 4.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 293.9 K
D1 0.5000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300077 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



7.2602

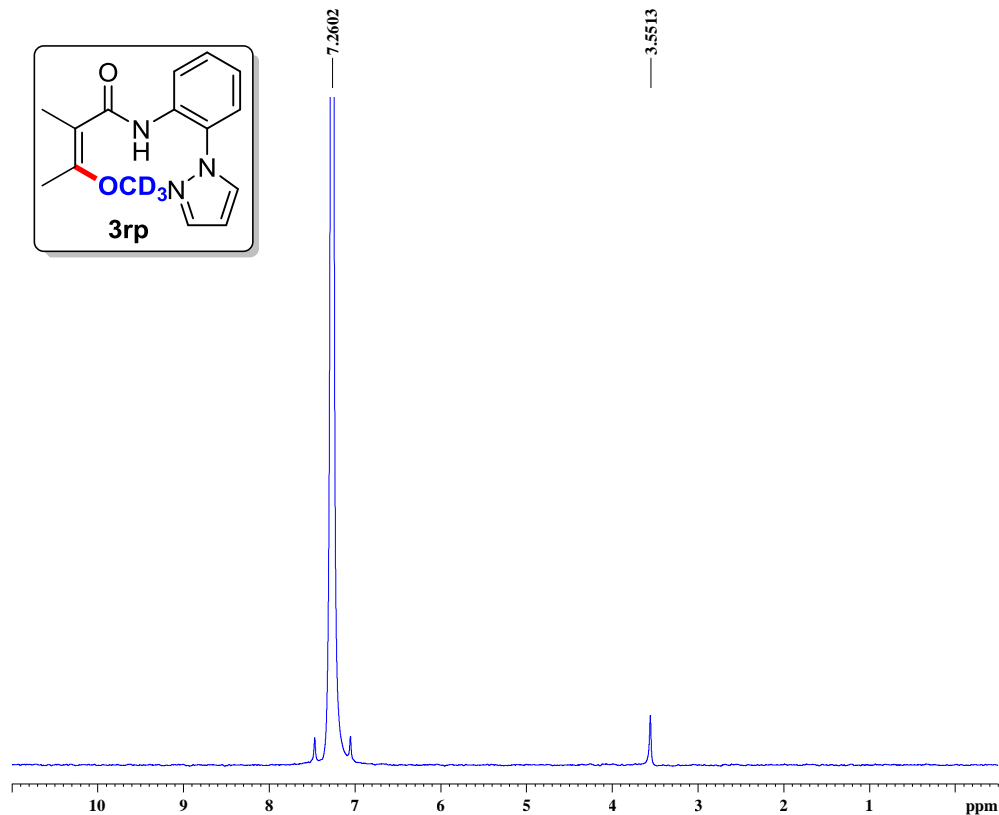
3.5513

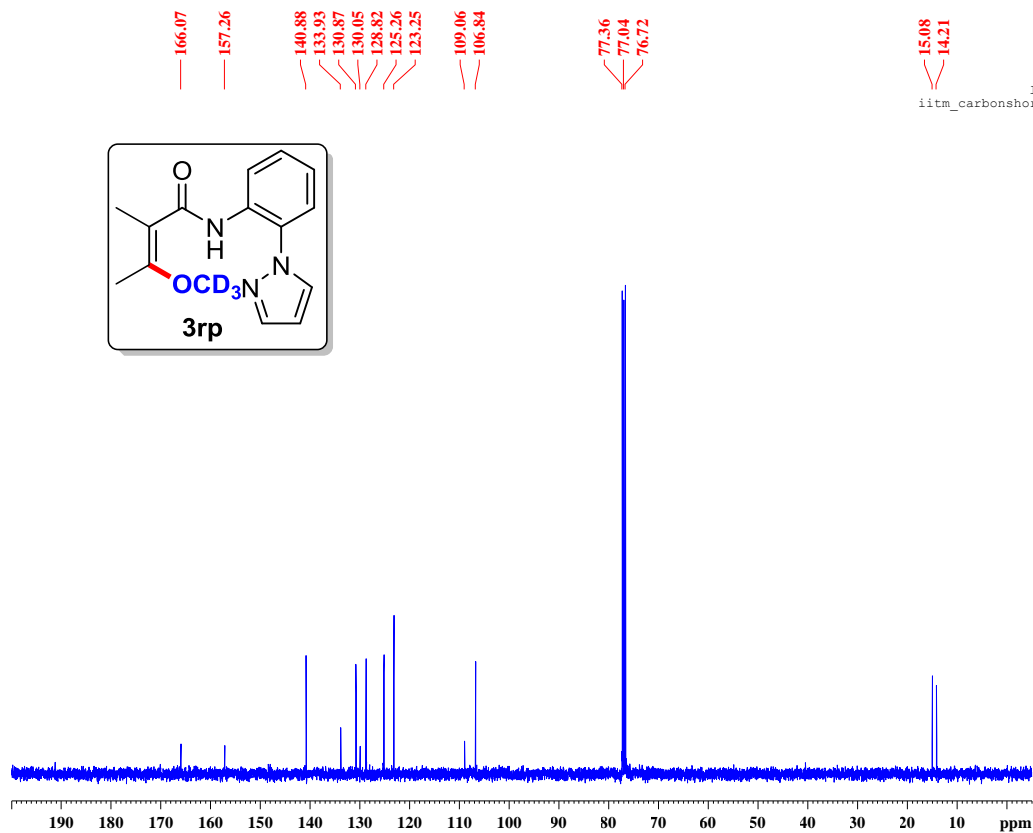
Current Data Parameters
NAME mmb50616
EXPNO 69
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160624
Time 11.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg2h
TD 65536
SOLVENT None
NS 1
DS 1
SWH 921.376 Hz
FIDRES 0.014059 Hz
AQ 35.5642014 sec
RG 2.18
DW 542.667 usec
DE 6.50 usec
TE 300.0 K
D1 1.0000000 sec
D11 0.0300000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 76.7764539 MHz
NUC1 2H
P1 530.00 usec
PLW1 1.79999995 W

F2 - Processing parameters
SI 65536
SF 76.7760710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00





lab mmbjsk-416
iitm_carbonshort CDCl3 /opt/topspin nmr 10

```

Current Data Parameters
NAME          mmb40616
EXPNO         278
PROCNO        1

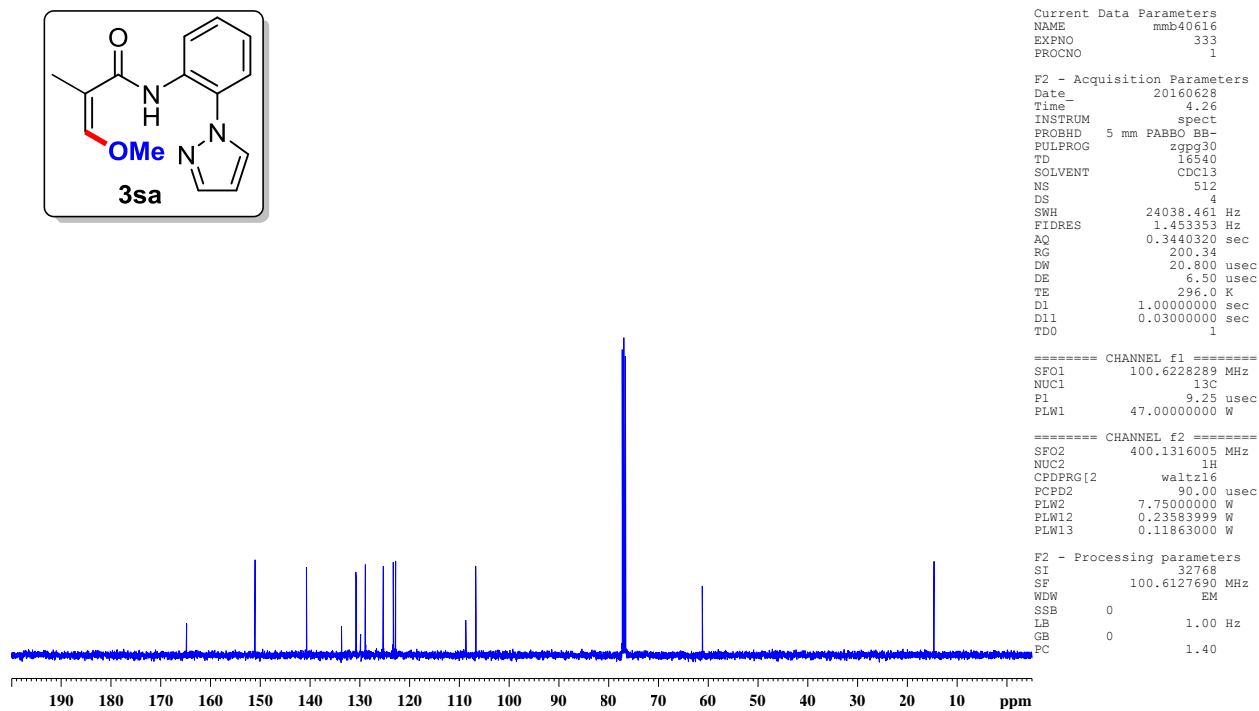
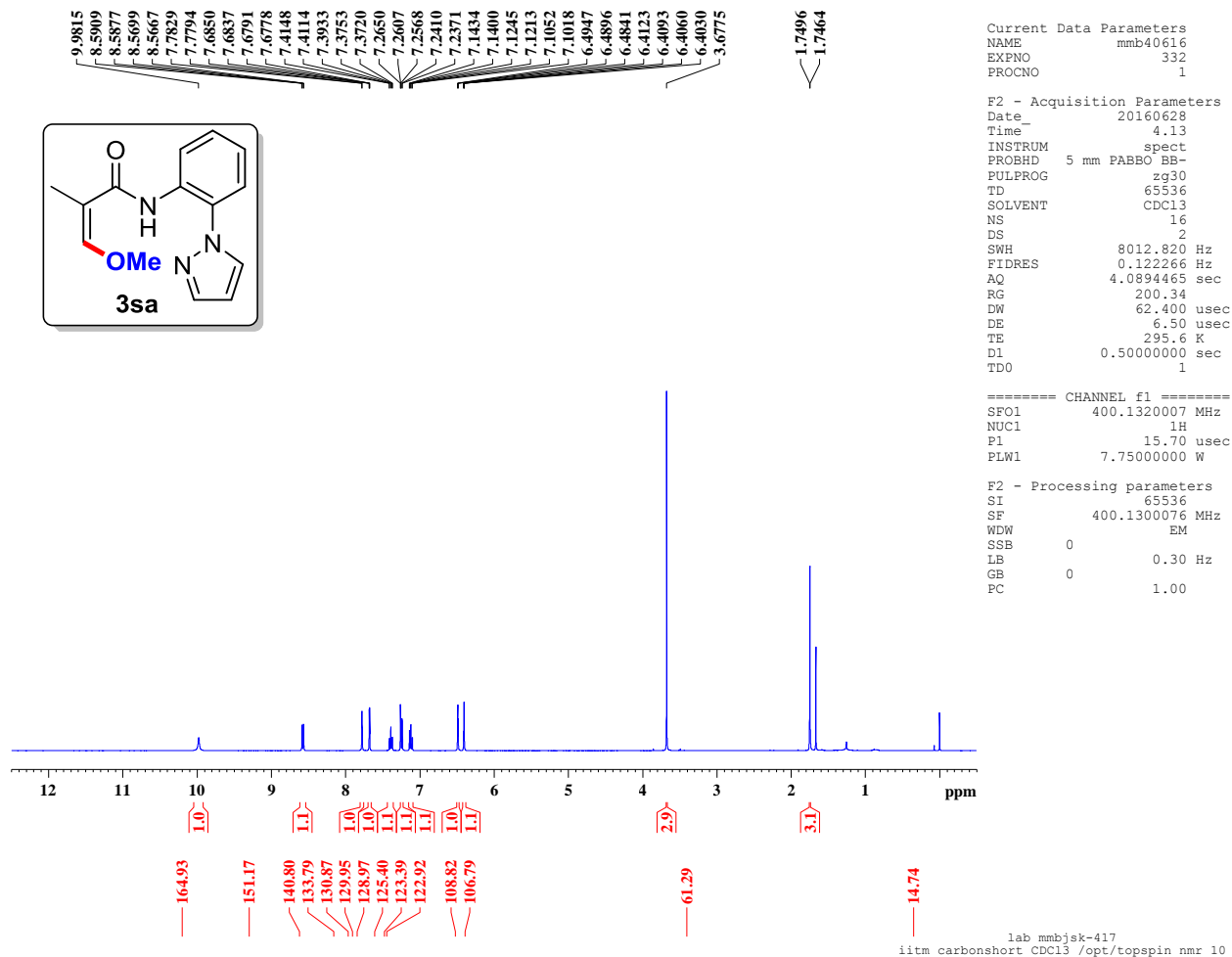
F2 - Acquisition Parameters
Date_         20160624
Time          4.58
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            16340
SOLVENT       CDCl3
NS            512
DS            4
SWH           24038.461 Hz
FIDRES        1.453353 Hz
AQ            0.3440320 sec
RG            200.34
DW            20.800 usec
DE            6.50 usec
TE            294.2 K
D1            1.0000000 sec
D11           0.0300000 sec
TD0           1

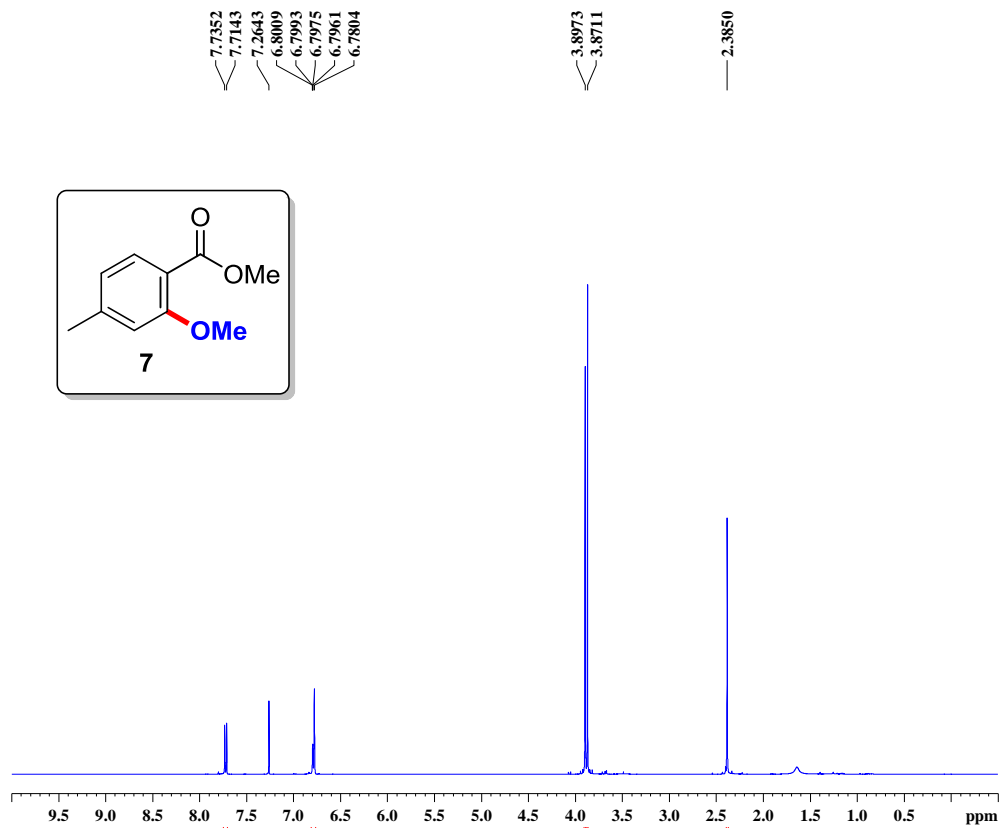
===== CHANNEL f1 =====
SFO1          100.6228289 MHz
NUC1           13C
P1             9.25 usec
PLW1          47.0000000 W

===== CHANNEL f2 =====
SFO2          400.1316005 MHz
NUC2           1H
PCPDPRG[2]    waltz16
PCPD2         90.00 usec
PLW2          7.7500000 W
PLW12         0.23583999 W
PLW13         0.11863000 W

F2 - Processing parameters
SI            32768
SF            100.6127690 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```





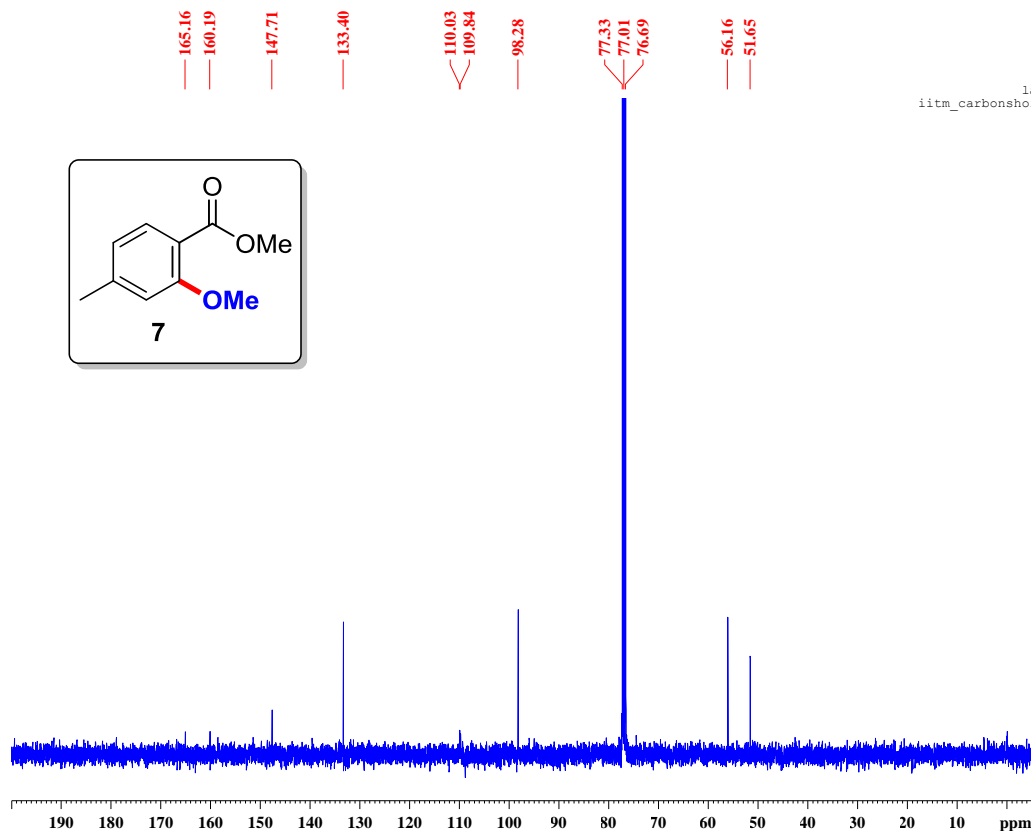
```

Current Data Parameters
NAME          mmb41015
EXPNO         48
PROCNO        1

F2 - Acquisition Parameters
Date_         20151010
Time_         13.10
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            200.34
DW            62.400 usec
DE            6.50 usec
TE            295.0 K
D1            0.5000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            15.70 usec
PLW1          7.7500000 W
SFO1          400.1320007 MHz

F2 - Processing parameters
SI            65536
SF            400.1300076 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```



```

lab mmb-jsk-mcpa
iitm_carbonshort CDCl3 /opt/topspin nmr 11

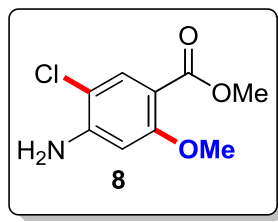
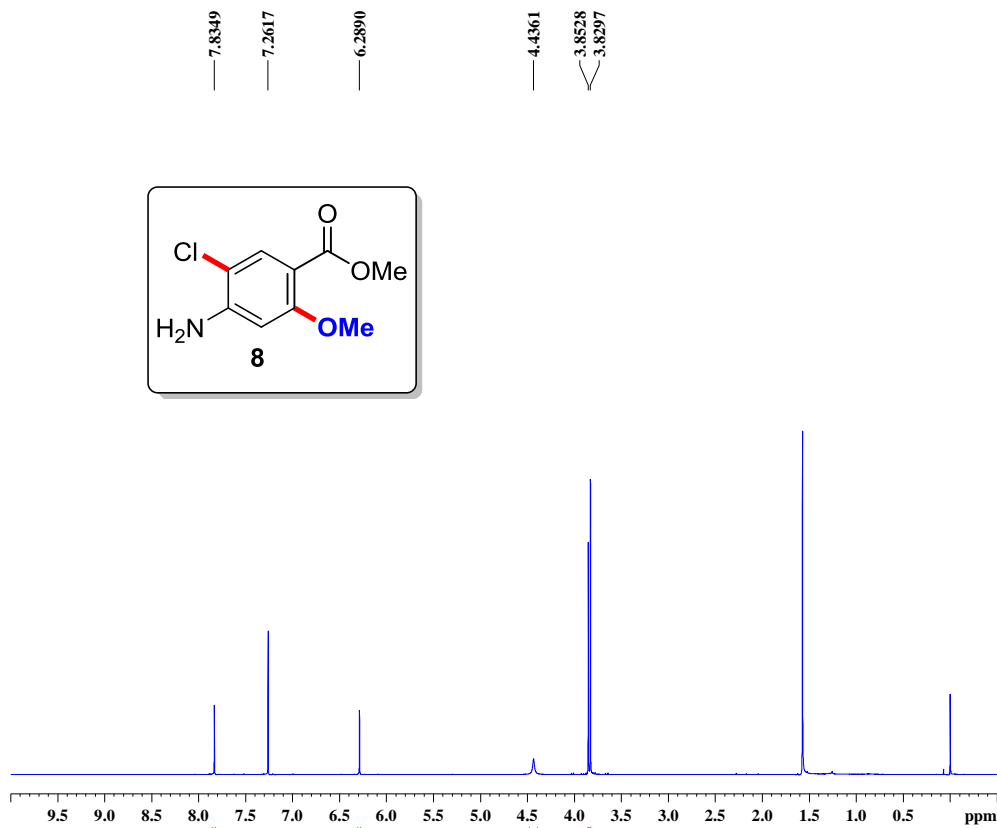
Current Data Parameters
NAME          MCpramide
EXPNO         239
PROCNO        1

F2 - Acquisition Parameters
Date_         20160229
Time_         2.00
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            16540
SOLVENT       CDCl3
NS            2000
DS            4
SWH           24038.461 Hz
FIDRES        1.453353 Hz
AQ            0.3440320 sec
RG            200.34
DW            20.800 usec
DE            6.50 usec
TE            298.9 K
D1            1.0000000 sec
D11           0.0300000 sec
TD0           1

===== CHANNEL f1 =====
SFO1          100.6228289 MHz
NUC1          13C
P1            9.25 usec
PLW1          47.0000000 W

===== CHANNEL f2 =====
SFO2          400.1316005 MHz
NUC2          1H
CPDPRG[2]     waltz16
PCPD2         90.00 usec
PLW2          7.7500000 W
PLW12         0.2358399 W
PLW13         0.1186300 W

F2 - Processing parameters
SI            32768
SF            100.6127690 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

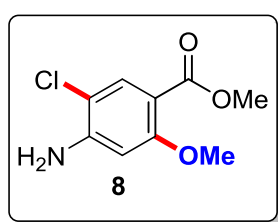
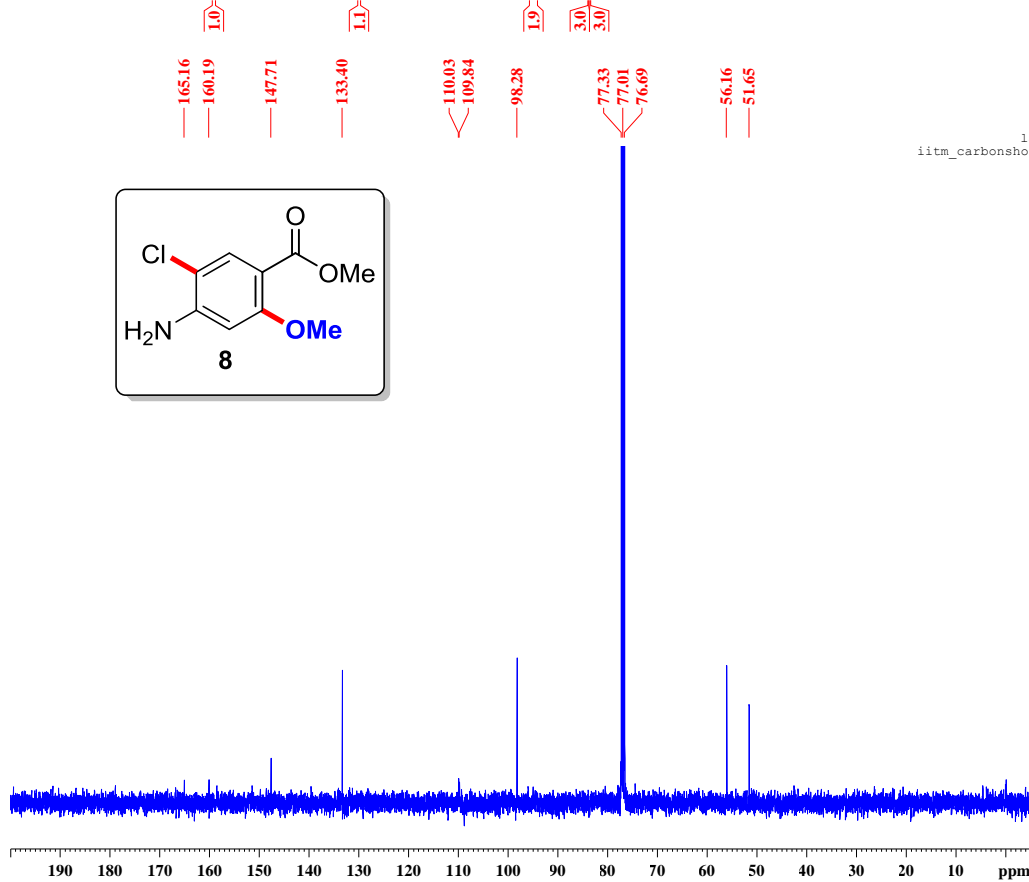



```
Current Data Parameters
NAME      MCpramide
EXPNO    208
PROCNO   1

F2 - Acquisition Parameters
Date_    20160227
Time     23.15
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ       4.0894465 sec
RG       200.34
DW       62.490 usec
DE       6.50 usec
TE       299.5 K
D1       0.5000000 sec
D11      1
TD0      1
```

```
===== CHANNEL f1 =====
SFO1    400.1320007 MHz
NUC1    1H
P1      15.70 usec
PLW1    7.75000000 W

F2 - Processing parameters
SI      65536
SF      400.1300089 MHz
WDW     EM
SSB     0
LB      0.30 Hz
GB      0
PC      1.00
```



```
lab mmb-jsk-mcpa
iitm_carbonshort CDCl3 /opt/topspin nmr 11
```

```
Current Data Parameters
NAME      MCpramide
EXPNO    239
PROCNO   1

F2 - Acquisition Parameters
Date_    20160229
Time     2.00
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD       16540
SOLVENT  CDCl3
NS       2000
DS       4
SWH      24038.461 Hz
FIDRES   1.453353 Hz
AQ       0.3440320 sec
RG       200.34
DW       20.800 usec
DE       6.50 usec
TE       298.9 K
D1       1.0000000 sec
D11      0.03000000 sec
TD0      1
```

```
===== CHANNEL f1 =====
SFO1    100.6228289 MHz
NUC1    13C
P1      9.25 usec
PLW1    47.00000000 W
```

```
===== CHANNEL f2 =====
SFO2    400.1316005 MHz
NUC2    1H
CPDPRG2 waltz16
PCPD2   90.00 usec
PLW2    7.75000000 W
PLW12   0.23583999 W
PLW13   0.11863000 W
```

```
F2 - Processing parameters
SI      32768
SF      100.6127690 MHz
WDW     EM
SSB     0
LB      1.00 Hz
GB      0
PC      1.40
```