Electronic Supplementary Material (ESI) for Chemical Science.

Electronic Supplementary Information

Directing group switch in copper-catalyzed electrophilic C–H amination/migratory annulation cascade: divergent access to benzimidazolone/benzimidazole

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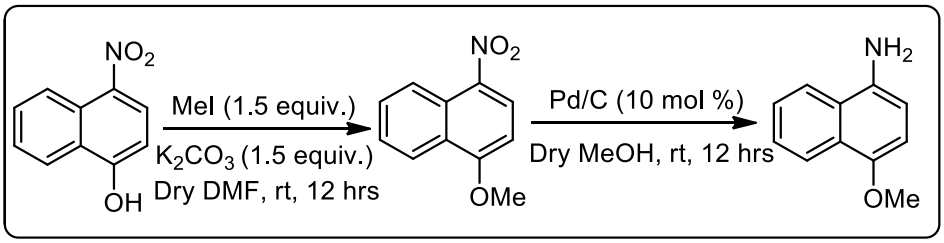
General Information: Air-sensitive reagents were handled under a dry nitrogen atmosphere. Unless otherwise stated, all commercial reagents were used without additional purification. Solvents were dried using standard methods and distilled before use. TLC was performed on silica gel plates (Merck silica gel 60, f_{254}), and the spots were visualized with UV light (254 and 365 nm) or by charring the plate dipped in $KMnO_4$ or vanillin charring solution. ^{1}H NMR spectra were recorded at 400 MHz (JEOL-JNM-ECZ400S/L1), ^{13}C NMR spectra were recorded at 100 MHz (JEOL-JNM-ECZ400S/L1) and ^{19}F NMR spectra were recorded at 376 MHz (JEOL-JNM-ECZ400S/L1) frequency in $CDCl_3$ solvent using TMS as the internal standard. Chemical shifts were measured in parts per million (ppm) referenced to 0.0 ppm for tetramethylsilane. The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br. = broad, dt = doublet of triplet, td = triplet of doublet, dd = doublet of doublet. Coupling constants, *J* were reported in Hertz unit (Hz). HRMS (m/z) were measured using ESI technique (Q-Tof Micro mass spectrometer). Crystals were grown in dichloromethane and crystal data was recorded in (Bruker Kappa Apex-2, CCD Area Detector) instrument.

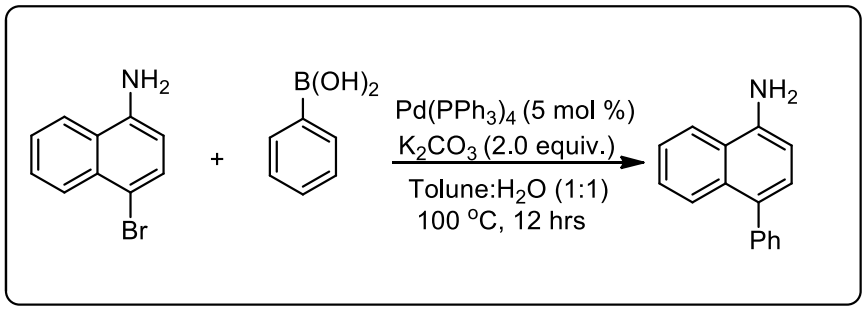
Preparation of starting materials:

Preparation of some 1-naphthylamines:



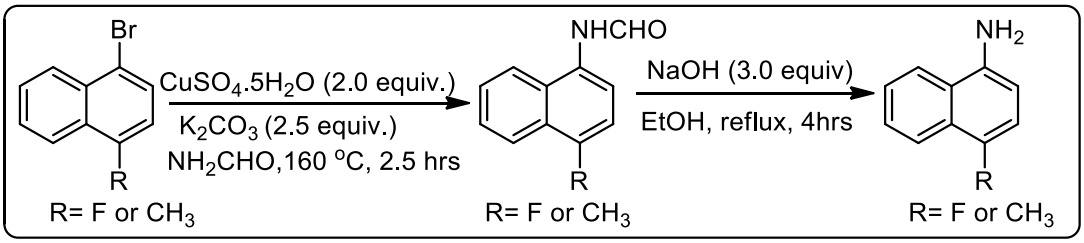
To a solution of 4-nitro-1-naphthol (106.0 mg, 0.4 mmol) in dry DMF (5.0 mL) were added K_2CO_3 (83.0 mg, 0.6 mmol) and MeI (58 µL, 0.6 mmol). The resulting reaction mixture was stirred at r.t. for 12 hrs. After completion of the reaction, the mixture was diluted with ethyl acetate and washed with chilled water, brine solution and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and finally the crude product was purified by column chromatography to afford the desired product.

To a solution of nitro compound (50 mg) in 5.0 mL MeOH was added 10% Pd/C (15 mg) and stirred for 12 hrs under H_2 atmosphere. Then the mixture was diluted with EtOAc (5 mL), filtered through celite, the filtrate was concentrated under reduced pressure to afford the crude compound which was purified by column chromatography to give the corresponding as purple colored viscous liquid which was used for amidation following **procedure1**.



Phenylboronic acid or 3-Furanylboronic acid (1.5 mmol, 1.5 equiv.), 4-bromo-1-naphthylamine (1.0 equiv.), K_2CO_3 (1.0 equiv.) and $Pd(PPh_3)_4$ (5 mol %) were added to an oven-dried sealed tube (15 mL) and toluene (2 mL) and H_2O (2 mL) were added into the tube which was then purged with nitrogen three times. The resulted solution was stirred at 100 °C for 8 hrs. The reaction mixture was cooled to r.t. and then extracted with ethyl acetate (3 × 15 mL). The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. This crude product was passed through short column.

These substituted 1-naphthylamine compounds were then used for amidation following **procedure1**.

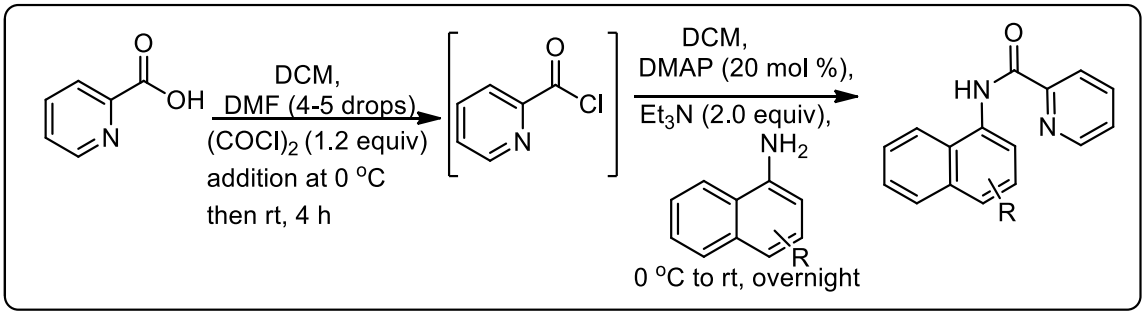


In an oven dried RB substituted 1-bromonaphthalene (2.5 mmol), K_2CO_3 (865 mg, 6.25 mmol), and copper(II) sulfate pentahydrate (750 mg, 5.0 mmol) was taken and to it formamide (10 mL)was added. The RB was fitted with reflux condenser and heated at 160 °C for 4 hrs. (**caution:** don't use pressure tube for this reaction). After cooling to room temperature the reaction mixture was mixed with ice cold water (50 mL) and extracted with ethyl acetate (3×20 mL). Combined organic layers were dried over Na_2SO_4 and evaporated. The crude product was used for the next step without further purification.

Aqueous (2 mL) sodium hydroxide (5.0 equiv.) was added to the ethanol (10 mL) solution of *N*-(naphthalen-1-yl)formamide. Resulting solution was heated to reflux for 6 hrs. Ethanol was evaporated and extracted with ethyl acetate (3×10 mL). The combined organic layer was dried over Na_2SO_4 and solvent was evaporated under reduced pressure. The crude mixture was purified by column chromatography to obtain naphthylamines. These substituted 1-naphthylamine compounds were then used for amidation following **procedure 1**.

General procedure for the preparation of picolinamides:

Procedure 1 for the preparation of picolinamides:



To an oven dried RB was charged with 2-picolinic acid or the corresponding acid (2.5 mmol) in dry DCM (5mL) was added 4-5 drops of DMF and the solution was stirred at 0 °C for 5 minutes. Then oxalyl chloride (0.26ml, 3 mmol) was added dropwise into the cooled solution of the acid which immediately formed rust-red color in case of 2-picolinic acid (other colors for other acids) with the gas bubbling and then stirred at 0 °C for 10 minutes. The reaction mixture was stirred at

room temperature for 4 hours. After completion, the excess oxalyl chloride was removed under *vacuum* to obtain crude acid chloride. Then, the crude pyridine-2-acid chloride was dissolved in 5mL dry DCM, and cooled to 0 ^{o}C and DMAP (61 mg, 0.5 mmol), Et_3N (0.7 mL, 5 mmol) and the naphthylamine (2.5 mmol) were successively added. Then the reaction mixture was stirred under room temperature for overnight. After completion as indicated by TLC, the mixture was diluted with 60 mL DCM and washed with 2N HCl (20 mL), brine solution (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and finally the crude product was purified by column chromatography to afford the 2-picolinamide (50-85% yield). This method was used for the synthesis of most of the substrates.

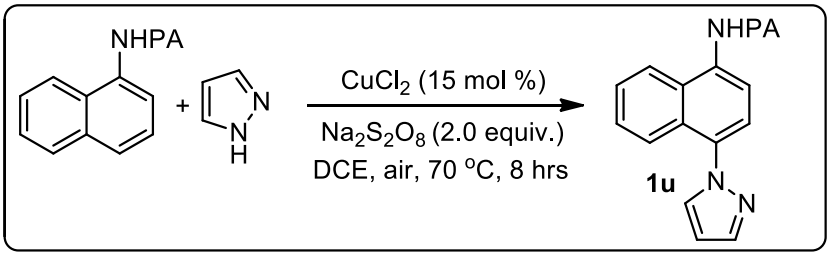
Procedure 2 for the preparation of picolinamides:

A RB containing pyridine-2-carboxylic acid (203 mg, 1.65 mmol), HATU (627 mg, 1.65 mmol) in dry DMF was cooled to 0 ^{o}C. Then DIPEA (0.43 ml, 2.5 mmol) and 5-amino isoquinoline (216 mg, 1.5 mmol) were successively added. The reaction mixture was stirred at r.t for overnight. Then the mixture was diluted with ethyl acetate and washed with chilled water, brine solution and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and finally the crude product was purified by column chromatography to afford **1aa**.

Procedure 3 for the preparation of picolinamides:

An oven dried RB charged with 5-methyl pyrazine-2- carboxylic acid (319 mg, 2.31 mmol), 1-naphthylamine (300 mg, 2.1 mmol), EDCI (443 mg, 2.31 mmol), HOBT (312 mg, 2.31 mmol)) in dry DCM was cooled to 0 ^{o}C and then DIPEA (1.1 ml, 6.3 mmol) was added. The reaction mixture was stirred at r.t for 12 hrs. Then the mixture was diluted with DCM and washed with water, brine solution and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and finally the crude product was purified by column chromatography to afford **1ad**. This method is also used for the synthesis of **1s**.

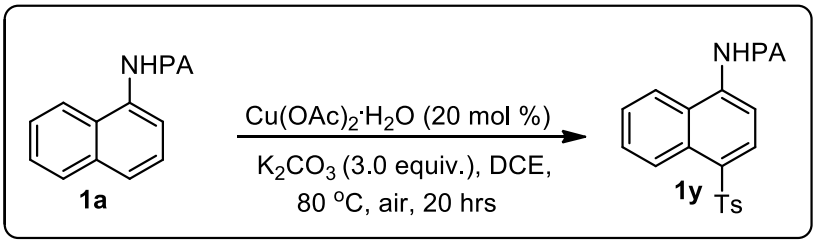
Procedure for the synthesis of 1u:



In an oven dried sealed tube charged with **1a** (496 mg, 2.0 mmol), pyrazole (544 mg, 4.0 equiv.), $CuCl_2$ (41 mg, 0.3 mmol), $Na_2S_2O_8$ (952 mg, 4.0 mmol) was added dry DCE (5ml) and heated at 70 ^{o}C for 8 hrs. Then the reaction mixture was cooled to r.t and diluted with DCM and washed with water, brine solution

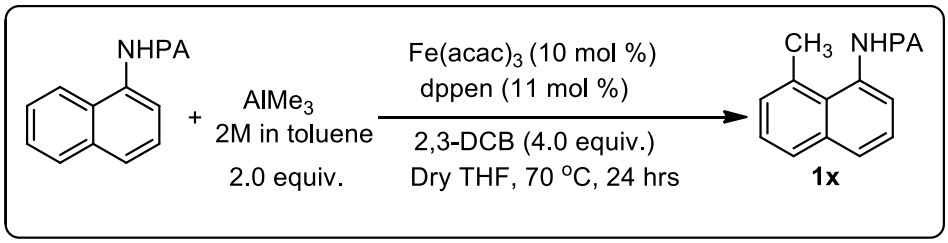
and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and finally the crude product was purified by column chromatography to afford **1u**. This method is also used for the synthesis of amide version of **4r**.

Procedure for the synthesis of 1y:



1a (248 mg, 1 mmol, 1.0 equiv.), K_2CO_3 (276.5 mg, 2.0 mmol), $Cu(OAc)_2 \cdot H_2O$ (40.0 mg, 0.2 mmol), TsCl (570 mg, 3.0 mmol) and DCE (5 mL) were successively added into a sealed tube. The mixture was stirred at 80 °C under air for 20 h. After cooling to ambient temperature, the resulting mixture was filtered through celite pad and washed with DCM. The filtrate was concentrated under vacuum and purified column chromatography using solvent mixtures of petroleum ether and ethyl acetate to give the product **1y.**

Procedure for the synthesis of 1x:



Under a nitrogen atmosphere, in an oven-dried two-necked RB a solution of $Fe(acac)_3$ (71 mg, 0.2 mmol) and (Z)-1,2-bis (diphenylphosphino)ethene (dppen) (88 mg, 0.22 mmol) in THF (1.0 ml) was injected into an anhydrous tetrahydrofuran (THF, 7 mL) solution of **1a** (496 mg, 2.0 mmol). Trimethylaluminum (2 ml, 4.0 mmol, 2.0 M in toluene) was slowly added. After stirring for 10 min to finish generating methane at r.t, 2,3-dichlorobutane (2,3-DCB) (0.9 ml, 8.0 mmol) was added via a syringe, and the RB was joined to reflux condenser and heated at 70 °C for 24 h. After cooling to r.t., the mixture was diluted with diethyl ether, and methanol (2.0 ml) was slowly added via a syringe at 0 °C to quench the aluminium reagent. Then the mixture was further diluted with diethyl ether and washed with water, brine solution and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and finally the crude product was purified by column chromatography to afford **1x.**

General Procedure for the preparation of *O*-benzoylhydroxylamines:

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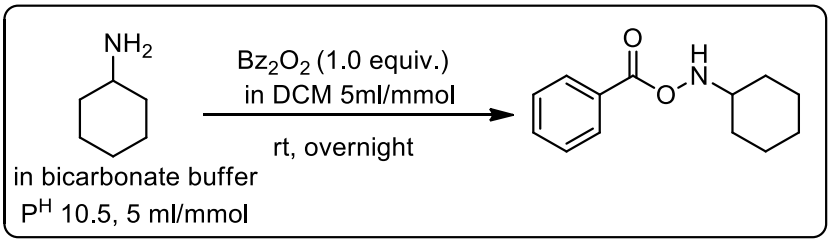
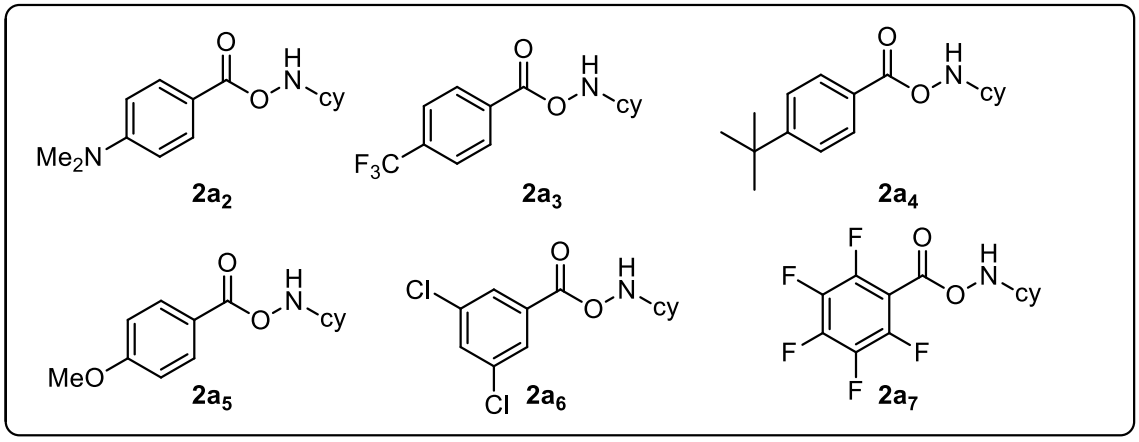


As reported in the literature [1-3] a solution of benzoyl peroxide (BPO, 1 equiv.) in CH_2Cl_2 (5 mL/mmol BPO) was added to a mixture of the amine (1 equiv.) and aqueous Na_2CO_3/$NaHCO_3$ buffer (pH 10.5) solution (5 mL/mmol amine) at room temperature overnight. (Note: The desired product in most cases had R_f values close to that of BPO). The aqueous layer was extracted three times with CH_2Cl_2. The organic layers were combined, dried over anhydrous Na_2SO_4, and concentrated. The crude residue was subjected to column chromatography for purification of the products. Using this protocol, *O*-benzoylhydroxylamine of other aliphatic primary amines were prepared. Most of the compounds are known in literature though ^{1}HNMR and ^{13}NMR spectral data of some compounds are given.

Preparation of P^H 10.5 bicarbonate buffer solution:

100 mL 0.1M $NaHCO_3$ solution = 840 mg $NaHCO_3$ in 100 mL water (solution A), 100 mL 0.1M Na_2CO_3 solution = 1.06 gm Na_2CO_3 in 100 mL water (solution B). For preparation 50 ml of P^H 10.5 = 5 mL solution A + 45 mL solution B.

2a$_4$, 2a$_5$, 2a$_6$, 2a$_7$ were synthesized using corresponding substituted benzoyl peroxides.

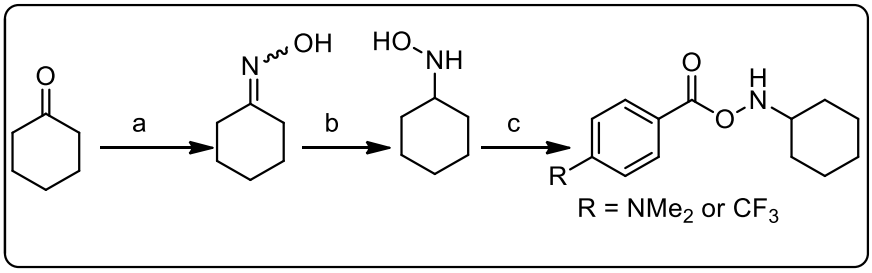


Synthesis of aryl acylperoxide

In a round-bottomed flask, the solution of acid chloride (5 mmol) in diethyl ether (2.5 mL) was cooled to 0 °C in an ice-bath. Then, hydrogen peroxide (0.294 g, 30 wt.% in H_2O, 2.86 mmol) was added dropwise over 10 minutes to the cold solution. This was followed by the dropwise addition of an aqueous solution of NaOH (0.252g, 6.32 mmol, 2 mL) over 20 minutes. The resulting white

precipitate was collected by filtration. After washing with water (3×5 mL) and diethyl ether (3×5 mL), the solid was air dried and used for the next step without any further purification. In some case if the compound was found to dissolve in ether, after evaporating ether the compound was extracted with DCM and dried over anhydrous Na_2SO_4 and after rotary evaporation of the solvent (<40 ^oC) the solid compound was obtained.

Synthesis of 2a$_2$ and 2a$_3$

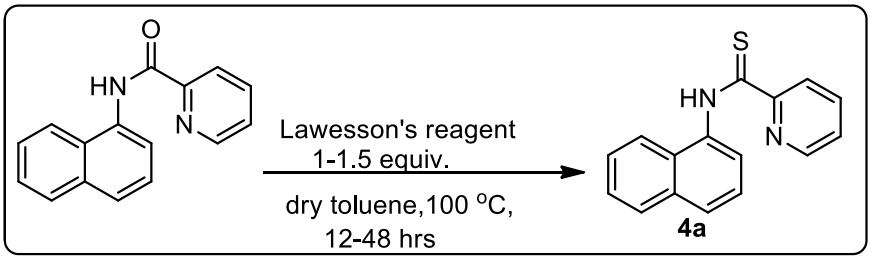


(a) A 100 ml round bottomed flask, equipped with a magnetic stirring bar, was charged with cyclohexanone (2.58 g, 25 mmol), hydroxylamine hydrochloride (2.57 g, 37.5 mmol), sodium acetate (5.13 g, 62.5 mmol), ethanol (10 mL) and water (30 mL). The reaction mixture was refluxed for 6 hrs and brought to room temperature. Thin layer chromatography in vanilline stain showed the complete conversion of cyclohexanone to cyclohexanone oxime. At this point, ethanol was evaporated using rotary evaporator. The residue was dissolved in 100 ml of EtOAc and washed sequentially with 20 mL of 1M HCl, 20 mL sat. $NaHCO_3$, 20 mL sat. NaCl, and organic layer was dried over Na_2SO_4.

(b) To a stirring solution of cyclohexanone oxime (2.86 g, 25 mmol, 1.0 equiv) in MeOH (30 mL) containing an altered pH strip were added solid $NaBH_3CN$ (2.32 g, 37.5 mmol, 1.5 equiv) and aqueous HCl (2.0 M, about 35 mL) over 15 min in such a way that the pH of the solution stayed within 2–3 during the duration of the addition. The reaction mixture was allowed to stir for an additional 3.5 h, and then was quenched with the addition of aqueous 15% NaOH (until pH = 10). MeOH was removed in vacuo. The remaining aqueous solution was extracted with CH_2Cl_2 (3 × 100 mL). The organic layers were combined, washed with brine (100 mL), dried over Na_2SO_4, and filtered. The filtrate was concentrated in vacuo. The crude residue was used for the next step.

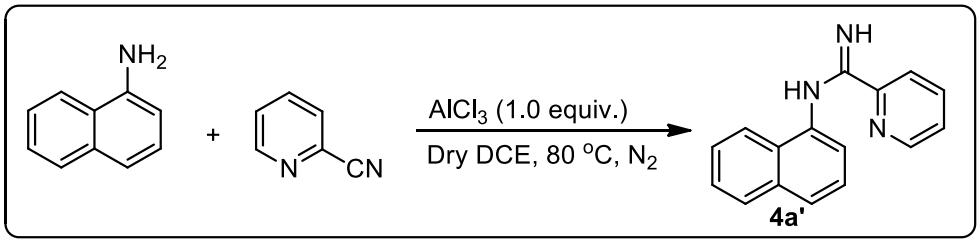
(c) An oven-dried round bottom flask was charged with the corresponding benzoic acid (1.1 equiv) and CH_2Cl_2 (0.3 M). The flask was placed in an ice-bath, and 1,1'-carbonyldiimidazole (1.1 equiv) was added. The mixture was stirred at this temperature for 30 min, at which time N-alkyl hydroxylamine (1.0 equiv) solution in dry CH_2Cl_2 was added dropwise. The ice-bath was removed, and the reaction mixture was allowed to stir at room temperature for 1-2 h. The resulting mixture was passed through a pad of Celite, and rinsed with CH_2Cl_2. The filtrate was concentrated and purified by column chromatography to give the corresponding amine electrophile.

General procedure for the preparation of thioamides from corresponding picolinamides:



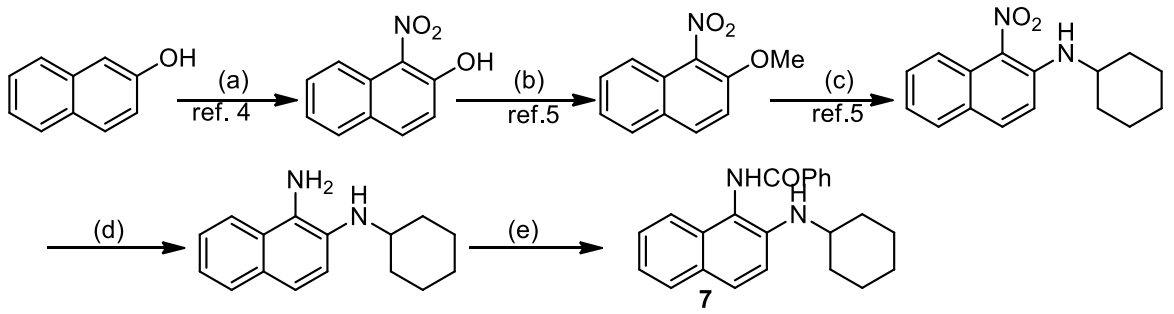
To a mixture of picolinamide (2.50 mmol) and Lawesson's reagent (0.52 g, 1.28 mmol) was added toluene (10 mL) and the solution refluxed for 12-48 hrs. The mixture was then filtered and solvent was removed under reduced pressure to afford a yellow solid material which was purified by column chromatography using solvent mixtures of petroleum ether and ethyl acetate to give the desired product (yellow solid). Using this method, thioamide of other amides were also prepared.

General procedure for the preparation of picolinimidamide:

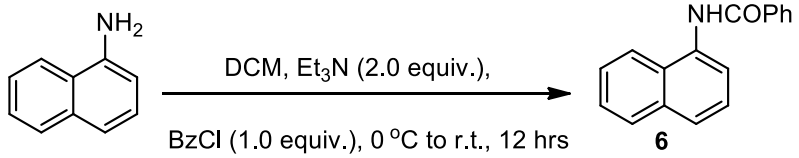


In an oven dried two-necked RB charged with 2-cyano pyridine (520 mg, 5.0 mmol) and 1-naphthylamine (715 mg, 5.0 mmol) under nitrogen atmosphere 10 ml dry DCE was added and cooled to 0 °C. Then $AlCl_3$ (665 mg, 5.0 mmol from glove box), was added portion wise to avoid overheating. The reaction mixture was stirred at this temperature for 10 minutes then at rt for 5 minutes. Then this mixture was heated to 80 °C for several hours under N_2 atmosphere. After consumtion of the starting materials. The reaction mixture was diluted with 20 mL dichloromethane and washed with 15 mL of 6N NaOH. The resulting organic layer was separated and dried over Na_2SO_4 and solvent was removed under reduced pressure. Then this crude product was washed with distilled hexane three times and dried under high vacuum to give the desired product which can be used without further purification.

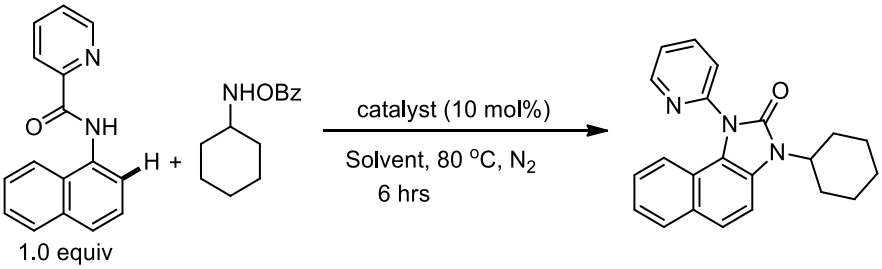
Procedure for the preparation of 6 and 7:



(a) $ZrO(NO_3)_2$ .xH_2O (1.0 equiv.), acetone, r.t., 3hrs, filter,solvent evaporation, column chromatography;
(b) KOH (3.0 equiv.), MeI (2.0 equiv.), acetone, reflux, 12 hrs, cooled to r.t., work-up, column chromatography;
(c) K_2CO_3 (4.0 equiv.), $CyNH_2$ (3.0 equiv.), DMF, 80 ^oC, 16 hrs, cooled to r.t., work-up, column chromatography;
(d) Pd/C, EtOAc, H_2, r.t, 3 hrs, filter on celite bed, solvent evaporation, used for next step immidiately;
(e) Et_3N (2.0 equiv.), BzCl (1.0 equiv.), DCM, r.t., 30 min, work-up, solvent evaporation, column chromatography.



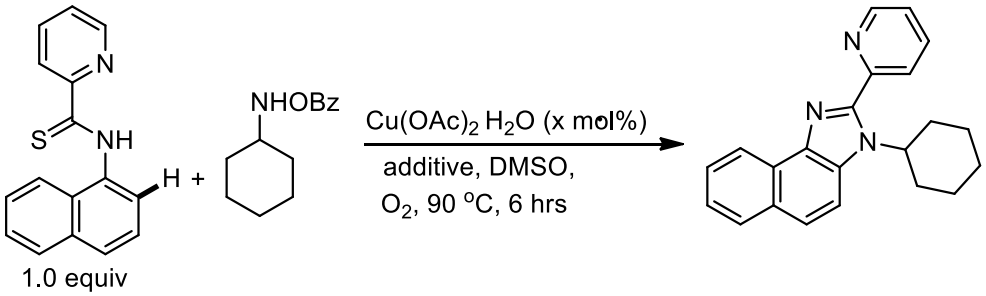
Optimization table for imidazolone product[a,b]:



Entry	Catalyst	Amine source	additive	solvent	Yield (%)
1	$Cu(OAc)_2.H_2O$	1.0	-	DMSO	44
2	$Cu(OAc)_2.H_2O$	1.5		DMSO	50
3	$Cu(OAc)_2.H_2O$	2.5	-	H_2O	0
4	$Cu(OAc)_2.H_2O$	2.5	-	Toluene	20
5	$Cu(OAc)_2.H_2O$	2.5	-	MeCN	39
6	$Cu(OAc)_2.H_2O$	2.5	-	1,4-Dioxane	62
7	$Cu(OAc)_2.H_2O$	2.5	-	THF	52
8	**$Cu(OAc)_2.H_2O$**	**2.5**	**-**	**DMSO**	**90**
10[c]	**$Cu(OAc)_2.H_2O$**	**2.5**	**-**	**DMSO**	**93**
11[d]	$Cu(OAc)_2.H_2O$	2.5	-	DMSO	87
12[e]	$Cu(OAc)_2.H_2O$	2.5	-	DMSO	56
13[c]	Cu	2.5	-	DMSO	83
14[f]	$Cu(OAc)_2.H_2O$	2.5	PIDA	DMSO	5<
15[f]	$Cu(OAc)_2.H_2O$	2.5	$K_2S_2O_8$	DMSO	12
16[f]	$Cu(OAc)_2.H_2O$	2.5	Bz_2O_2	DMSO	32
17[g]	$Cu(OAc)_2.H_2O$	1.2	Bz_2O_2	DMSO	58
18[h]	$Cu(OAc)_2.H_2O$	2.5	-	DMSO	0
19	$Pd(OAc)_2$	2.5	-	DMSO	5<
20	$Co(OAc)_2$	2.5	-	DMSO	20<
21	$Ni(OAc)_2$	2.5	-	DMSO	n.r.
22	$Mn(OAc)_2$	2.5	-	DMSO	n.r.
23	$FeBr_2$	2.5	-	DMSO	n.r.
24	$FeCl_2$	2.5	-	DMSO	n.r.

[a]All reactions were carried out in 0.2 mmol scale. [b]Yields refer to here are overall isolated yields. [c]5.0 mol% catalyst was used. [d]1.0 mol % catalyst was used. [e]Reaction was performed at room temperature. [f]Free amine was used as amine source and oxidant 2.5 equiv. [g]1.0 equiv Bz_2O_2 was used. [h]25% *ortho* aminated product was obtained without any copper catalyst.

Optimization table for imidazole product[a,b]:

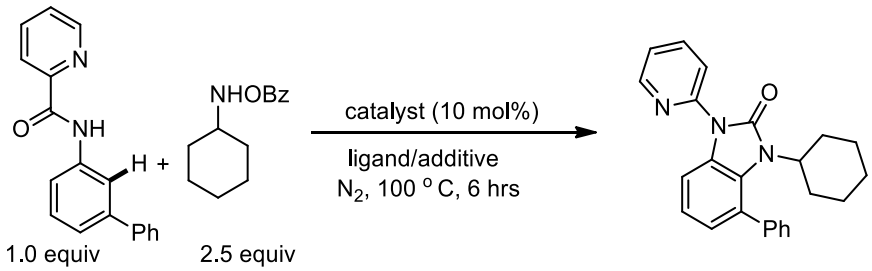


Entry	Amine source (equiv.)	$Cu(OAc)_2.H_2O$ (mol%)	Additive	Yield (%)
1[c]	2.5	10	-	38
2[d]	2.5	10	-	40
3	2.5	10	-	46

4	2.5	20	-	48
5	3.0	10	-	50
6	3.0	20	-	53
7[e]	3.0	20	-	34
8[f]	3.0	20	-	40
9[g]	3.0	20	-	40
10	3.0	20	1.2 equiv. K_2CO_3	58
11[h]	3.0	20	1.2 equiv. K_2CO_3	64
12[i]	**3.0**	**20**	**1.2 equiv. K_2CO_3**	**88**
13[i]	3.0	20	-	64
14[i]	3.0	10	1.2 equiv. K_2CO_3	70
15[i,j]	3.0	10	1.2 equiv. K_2CO_3	0

[a]All reactions were carried out in 0.2 mmol scale. [b]Yields refer to here are overall isolated yields. [c]Reaction was continued for 3 hrs. [d]Reaction was carried out at 100 °C. [e]Reaction was carried out in dry toluene. [f]Reaction was carried out in dry 1,4-dioxane. [g]Reaction was carried out in dry THF. [h]Reaction was carried out in air. [i]Reaction was carried under O_2 atm. [j]Reaction was performed with substrate **1a** instead of **4a**.

Optimization table for imidazolone product in 2-substituted aniline system[a,b]:

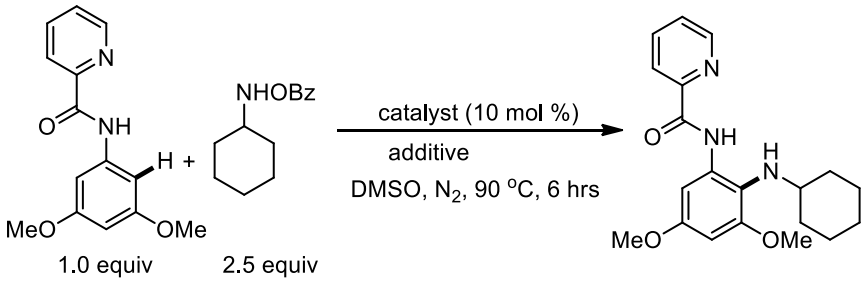


Entry	Catalyst	Additive (1.5 equiv.)	Ligand (20 mol %)	Solvent	Yield (%)
1[c]	$Cu(OAc)_2.H_2O$	-	-	DMSO	20
2[c]	$Pd(OAc)_2$	-	-	DMSO	nr
3[c]	$Co(OAc)_2.4H_2O$	-	-	DMSO	5 <
4	**$Cu(OAc)_2.H_2O$**	**-**	**-**	**DMSO**	**40**
5[d]	$Cu(OAc)_2.H_2O$	-	-	DMSO	27
6[e]	$Cu(OAc)_2.H_2O$	-	-	DMSO	27
7	$Cu(OAc)_2.H_2O$	-	-	Toluene	20
8	$Cu(OAc)_2.H_2O$	-	-	1,4-dioxane	32
9	$Cu(OAc)_2.H_2O$	-	-	MeCN	28
10	$Cu(OAc)_2.H_2O$	-	-	DCE	28
11	$Cu(OAc)_2.H_2O$	K_2CO_3	-	DMSO	15
12	$Cu(OAc)_2.H_2O$	$NaHCO_3$	-	DMSO	37

13	$Cu(OAc)_2.H_2O$	Li_2CO_3	-	DMSO	35
14	$Cu(OAc)_2.H_2O$	K_2CO_3	-	DMSO	32
15	$Cu(OAc)_2.H_2O$	Cs_2CO_3	-	DMSO	nr
16	$Cu(OAc)_2.H_2O$	$KHCO_3$	-	DMSO	30
17	$Cu(OAc)_2.H_2O$	LiO^tBu	-	DMSO	nr
18	$Cu(OAc)_2.H_2O$	$NaHCO_3$	dppb	DMSO	39
19	$Cu(OAc)_2.H_2O$	$NaHCO_3$	dppm	DMSO	27
20	$Cu(OAc)_2.H_2O$	$NaHCO_3$	dppe	DMSO	35
21	$Cu(OAc)_2.H_2O$	$NaHCO_3$	dppp	DMSO	27
22	$Cu(OAc)_2.H_2O$	$NaHCO_3$	dppf	DMSO	20
23	$Cu(OAc)_2.H_2O$	$NaHCO_3$	dppen	DMSO	27
24	$Cu(OAc)_2.H_2O$	-	1,10-phen	DMSO	18
25	$Cu(OAc)_2.H_2O$	-	PPh_3	DMSO	35
26	$Cu(OAc)_2.H_2O$	-	x-phos	DMSO	35
27	$Cu(OAc)_2.H_2O$	-	dtbbpy	DMSO	35
28	$Cu(OAc)_2.H_2O$	-	terpyridine	DMSO	35
29	$Cu(OTf)_2$	-	-	DMSO	35
30	Cu_2O	-	-	DMSO	33
31	$CuSO_4.5H_2O$	-	-	DMSO	35
32	CuCl	-	-	DMSO	28
33	$Cu(OAc)_2$	-	-	DMSO	35
34	$Cu(OAc)_2.H_2O$	Zn dust	-	DMSO	30
35	$Cu(OAc)_2.H_2O$	$Mn(OAc)_2$	-	DMSO	28
36	$Cu(OAc)_2.H_2O$	$Mn(OAc)_3$	-	DMSO	28

[a]All reactions were carried out in 0.2 mmol scale. [b]Yields refer to here are overall isolated yields. [c]Temperature was 80 °C. [d]20 mol % catalyst was used. [e]50 mol % catalyst was used.

Optimization table for amination product in aniline system[a,b]:

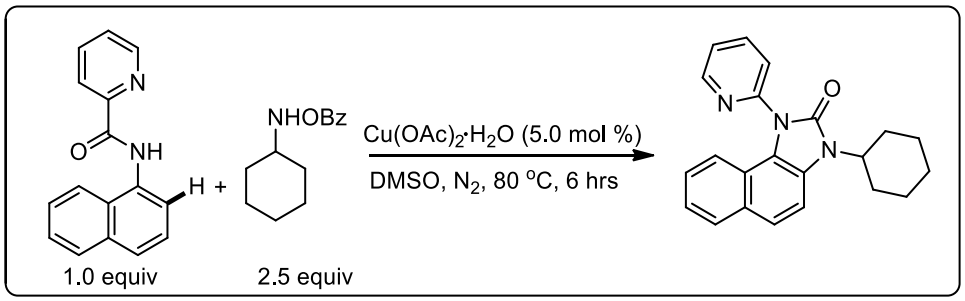


Entry	catalyst	additive	Yield (%)
1	$Cu(OAc)_2.H_2O$	-	35
2[c]	$Cu(OAc)_2.H_2O$	-	25
3	$Cu(OTf)_2$	-	10<
4	$Pd(OAc)_2$	-	nr
5	$Cu(OAc)_2.H_2O$	1,10-phen	15
6	$Cu(OAc)_2.H_2O$	K_2CO_3	58
7[d]	$Cu(OAc)_2.H_2O$	K_2CO_3	50

8[e]	$Cu(OAc)_2.H_2O$	K_2CO_3	54
9	$Cu(OAc)_2.H_2O$	Na_2CO_3	45
10	$Cu(OAc)_2.H_2O$	Cs_2CO_3	43
11	$Cu(OAc)_2.H_2O$	KOAc	30
12	**$Cu(OAc)_2.H_2O$**	**LiO^tBu**	**72**

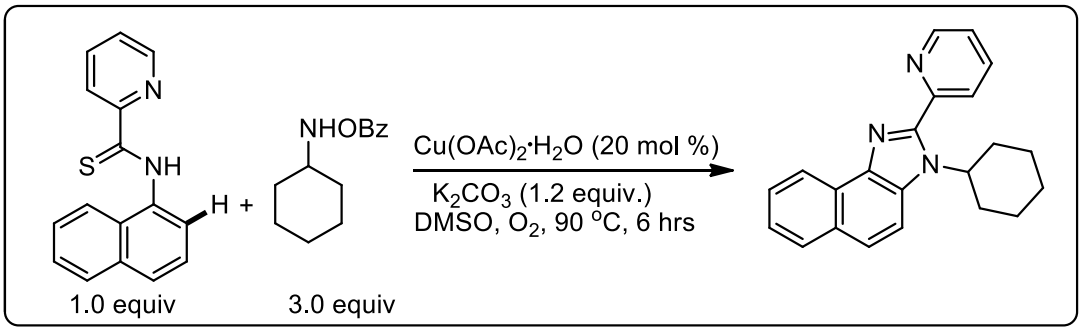
[a]All reactions were carried out in 0.2 mmol scale. [b]Yields refer to here are overall isolated yields. [c]Temperature 100 °C and time 12 hrs. [d]Air. [e]O_2 atm.

Representative Procedure 1 for imidazolone:



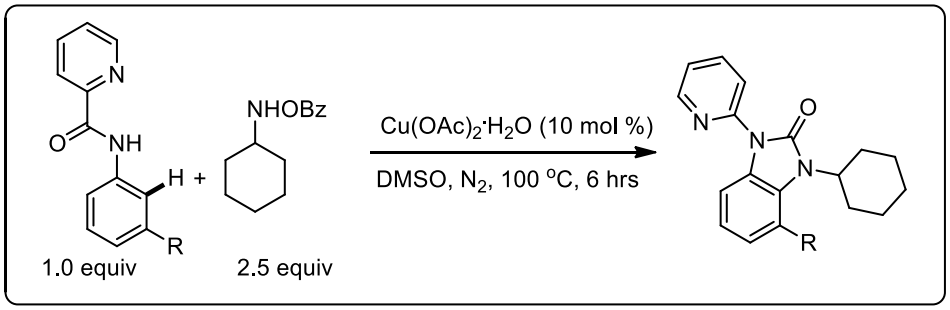
In an oven dried 15 mL sealed tube containing a stir bar was added corresponding picolinamide (0.2 mmol, 1.0 equiv), *O*-benzoylhydroxylamine (0.5 mmol, 2.5 equiv.) and $Cu(OAc)_2{\cdot}H_2O$ (0.01 mmol). Dry DMSO (2mL) was then added and N_2 gas was purged for 2 minutes. The mixture was stirred at 80 °C for 6 hrs. After allotted time the reaction mixture was cooled to room temperature. The mixture was diluted with EtOAc (15 mL) and washed with saturated aq. $NaHCO_3$ solution (25mL), followed by brine solution (25 mL) and dried over Na_2SO_4, and evaporated in *vacuo*. The crude mixture was loaded on a silica gel column chromatography and purified using (Hexane/EtOAc) to give the desired imidazolone product.

Representative Procedure for imidazole:



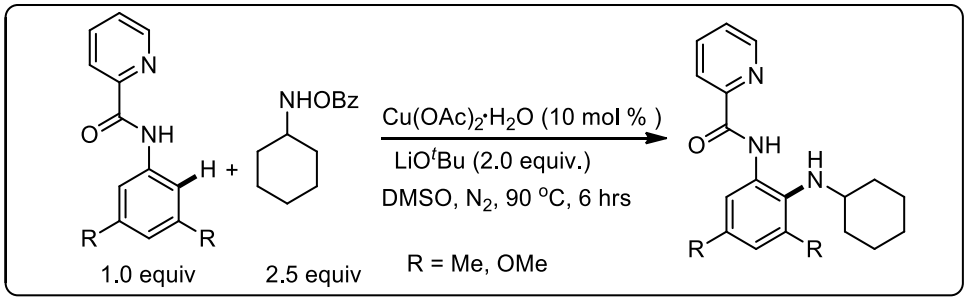
In an oven dried 15 mL sealed tube containing a stir bar was added corresponding thiopicolinamide (0.2 mmol, 1.0 equiv), *O*-benzoylhydroxylamine (0.5 mmol, 3.0 equiv.), $Cu(OAc)_2 \cdot H_2O$ (0.04 mmol) and K_2CO_3 (0.24 mmol). Dry DMSO (2mL) was then added and O_2 gas was purged for 2 minutes. **[Note**: amount of O_2 should be sufficient for better reaction and so large amount of empty space is required. For scale up reaction (2.0 mmol) 100 mL pressure tube was used**]**. The mixture was stirred at 90 ^oC for 6 hrs. After allotted time the reaction mixture was cooled to room temperature. The mixture was diluted with EtOAc (15 mL) and washed with saturated aq. $NaHCO_3$ solution (25mL), followed by brine solution (25 mL) and dried over Na_2SO_4, and evaporated in *vacuo*. The crude mixture was loaded on a silica gel column chromatography and purified using (Hexane/EtOAc) to give the desired imidazole product.

Representative Procedure 2 for imidazolone in 2-substituted aniline system:



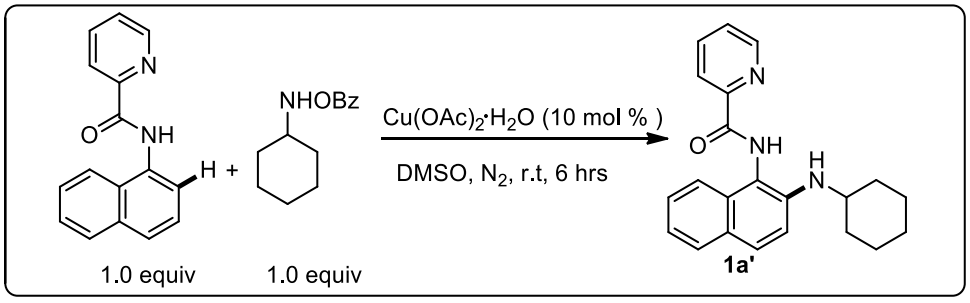
In an oven dried 15 mL sealed tube containing a stir bar was added corresponding picolinamide (0.2 mmol, 1.0 equiv), *O*-benzoylhydroxylamine (0.5 mmol, 2.5 equiv.) and $Cu(OAc)_2 \cdot H_2O$ (0.02 mmol). Dry DMSO (2mL) was then added and N_2 gas was purged for 2 minutes. The mixture was stirred at 100 ^oC for 6 hrs. After allotted time the reaction mixture was cooled to room temperature. The mixture was diluted with EtOAc (15 mL) and washed with saturated aq. $NaHCO_3$ solution (25mL), followed by brine solution (25 mL) and dried over Na_2SO_4, and evaporated in *vacuo*. The crude mixture was loaded on a silica gel column chromatography and purified using (Hexane/EtOAc) to give the desired imidazolone product.

Representative Procedure for amination in aniline system:



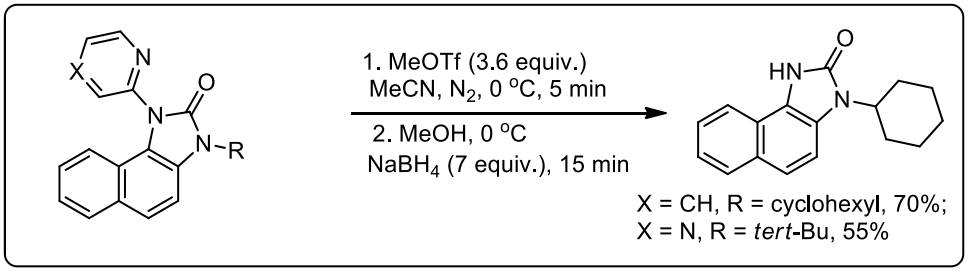
In an oven dried 15 mL sealed tube containing a stir bar was added corresponding picolinamide (0.2 mmol, 1.0 equiv), *O*-benzoylhydroxylamine (0.5 mmol, 2.5 equiv.), LiO^tBu (0.4 mmol, 2.0 equiv.) and $Cu(OAc)_2{\cdot}H_2O$ (0.02 mmol). Dry DMSO (2mL) was then added and N_2 gas was purged for 2 minutes. The mixture was stirred at 90 ^oC for 6 hrs. After allotted time the reaction mixture was cooled to room temperature. The mixture was diluted with EtOAc (15 mL) and washed with saturated aq. $NaHCO_3$ solution (25mL), followed by brine solution (25 mL) and dried over Na_2SO_4, and evaporated in *vacuo*. The crude mixture was loaded on a silica gel column chromatography and purified using (Hexane/EtOAc) to give the desired amination product.

Procedure for synthesis of compound 1a':



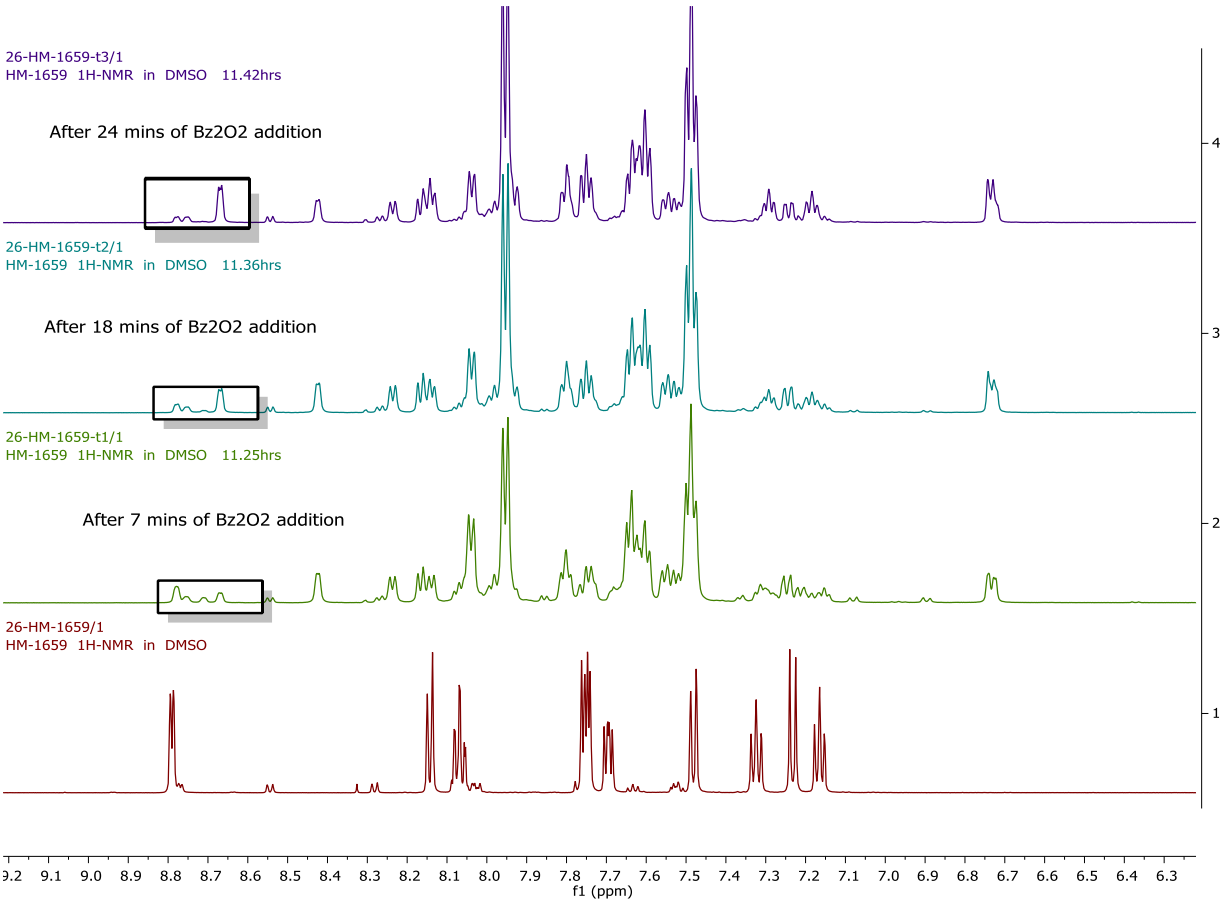
In an oven dried RB containing a stir bar was added picolinamide **1a** (2 mmol, 1.0 equiv), *O*-benzoylhydroxylamine (2 mmol, 1.0 equiv.) and $Cu(OAc)_2{\cdot}H_2O$ (0.2 mmol). Dry DMSO (15 mL) was then added and N_2 gas was purged for 2 minutes. The mixture was stirred at room temperature for 6 hrs. The mixture was diluted with EtOAc (100 mL) and washed with saturated aq. $NaHCO_3$ solution (50 mL), followed by brine solution (50 mL) and dried over Na_2SO_4, and evaporated in *vacuo*. The crude mixture was loaded on a silica gel column chromatography and purified using (Hexane/EtOAc) to give the amination product.

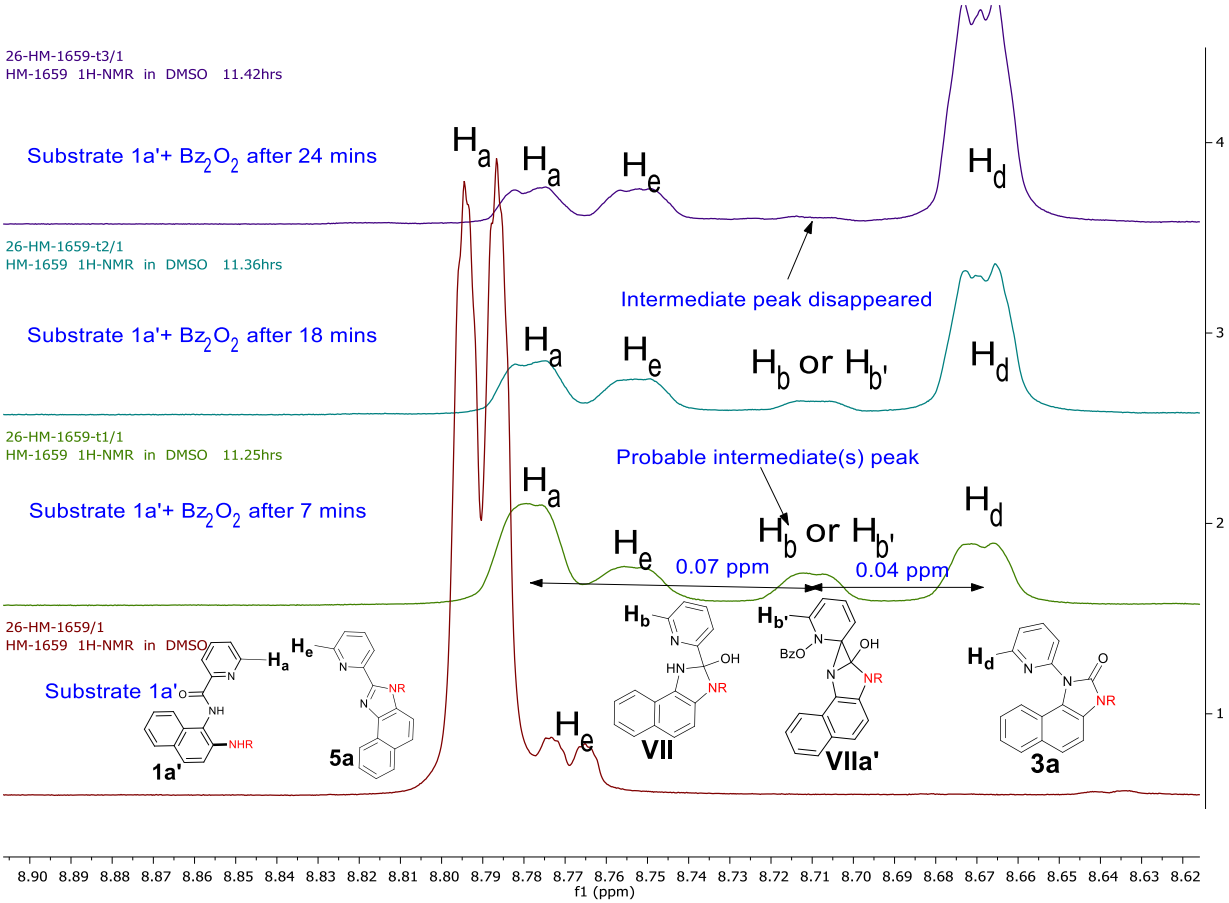
Deprotection of pyridyl group of Benzimidazolone product:



This deprotection was done according a condition for the deprotection of N-pyridyl group.[6] In an oven dried RB containing a stir bar was added the benzimidazolone and dry MeCN and it was cooled to 0 °C in an ice-bath under N_2 atmosphere. Ice-cooled MeOTf (3.6 equiv.) was added dropwise to this solution. After addition the mixture was stirred at r.t. for 10 minutes. Then to this mixture MeOH (4 mL) was added and further cooled to 0 °C in an ice-bath. $NaBH_4$ (7.0 equiv.) was added portion-wise and stirred at this temperature for 15 minutes. After that the solvent was evaporated and diluted with EtOAc, washed with water and dried over Na_2SO_4. This was concentrated under vacuum followed by column chromatography gave the desired product.

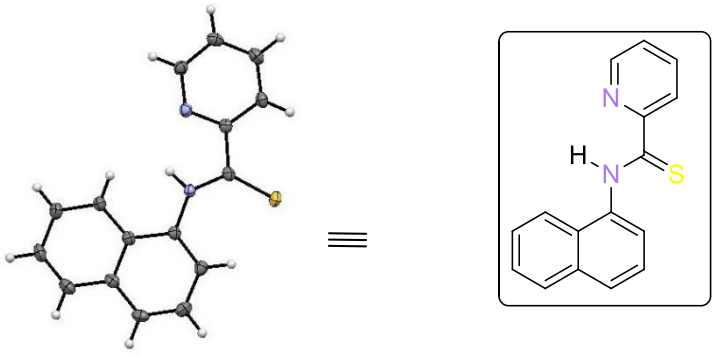
<u>Time dependent ^{1}H NMR experiment for mechanistic determination of intermediate</u>:





Crystal structure:

The crystals were grown in dichloromethane solvent. The pure compound was dissolved in dichloromethane slow evaporation led to the crystal **4a**. The crystal data was collected in X-ray spectroscopy (Bruker Kappa Apex-2, CCD Area Detector), and the data was analyzed using OLEX2 software. The structure is given below. The corresponding cif file has been uploaded separately as supporting information.



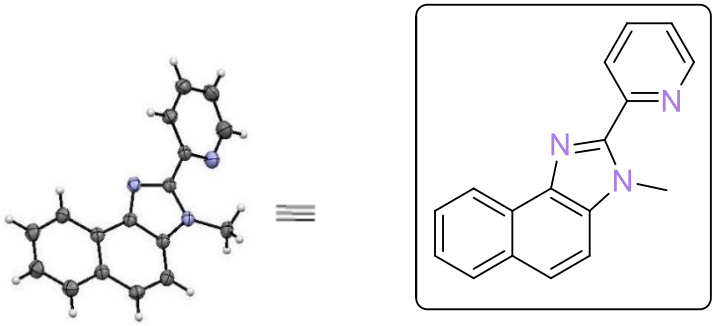
Thermal ellipsoid plot of **4a**. Ellipsoids are represented with 50% probability.

X-ray determined molecular structure of **4a,** CCDC: 2025280

Identification code	HM_643S_0m_a
Empirical formula	$C_{16}H_{12}N_2S$
Formula weight	264.34
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	6.1282(2)
b/Å	14.1422(4)
c/Å	14.4603(4)
α/°	90
β/°	95.2550(10)
γ/°	90
Volume/Å^3	1247.95(6)
Z	4
ρ_{calc}g/cm^3	1.407
μ/mm^{-1}	2.167
F(000)	552.0
Crystal size/mm^3	0.2 × 0.2 × 0.2
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	8.764 to 133.626
Index ranges	$-7 \leq h \leq 7$, $-16 \leq k \leq 16$, $-17 \leq l \leq 17$
Reflections collected	19122
Independent reflections	2213 [R_{int} = 0.0469, R_{sigma} = 0.0251]
Data/restraints/parameters	2213/0/172
Goodness-of-fit on F^2	1.078

Final R indexes [I>=2σ (I)]	R_1 = 0.0361, wR_2 = 0.0921
Final R indexes [all data]	R_1 = 0.0373, wR_2 = 0.0929
Largest diff. peak/hole / e Å^{-3}	0.26/-0.32

The crystals were grown in dichloromethane solvent. The pure compound was dissolved in dichloromethane slow evaporation led to the crystal **3aj**. The crystal data was collected in X-ray spectroscopy (Bruker Kappa Apex-2, CCD Area Detector), and the data was analyzed using OLEX2 software. The structure is given below. The corresponding cif file has been uploaded separately as supporting information.



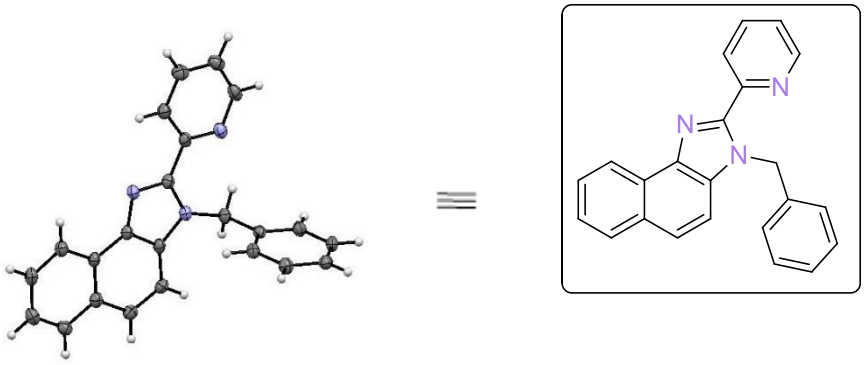
Thermal ellipsoid plot of **3aj**. Ellipsoids are represented with 50% probability.

X-ray determined molecular structure of **3aj,** CCDC: 2025266

Identification code	HM_430A_0m_a
Empirical formula	$C_{18}H_{15}N_2$
Formula weight	259.32
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	10.9333(3)

b/Å	7.3400(2)
c/Å	16.2518(5)
α/°	90
β/°	98.6550(10)
γ/°	90
Volume/$Å^3$	1289.36(6)
Z	4
$\rho_{calc}g/cm^3$	1.336
μ/mm^{-1}	0.612
F(000)	548.0
Crystal size/mm^3	0.2 × 0.2 × 0.2
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	13.262 to 132.918
Index ranges	$-12 \leq h \leq 12$, $-8 \leq k \leq 8$, $-19 \leq l \leq 17$
Reflections collected	18364
Independent reflections	2259 [R_{int} = 0.0807, R_{sigma} = 0.0459]
Data/restraints/parameters	2259/0/183
Goodness-of-fit on F^2	1.056
Final R indexes [I>=2σ (I)]	R_1 = 0.0733, wR_2 = 0.2003
Final R indexes [all data]	R_1 = 0.0760, wR_2 = 0.2033
Largest diff. peak/hole / e $Å^{-3}$	0.55/-0.66

The crystals were grown in dichloromethane solvent. The pure compound was dissolved in dichloromethane slow evaporation led to the crystal **5h**. The crystal data was collected in X-ray spectroscopy (Bruker Kappa Apex-2, CCD Area Detector), and the data was analyzed using OLEX2 software. The structure is given below. The corresponding cif file has been uploaded separately as supporting information.



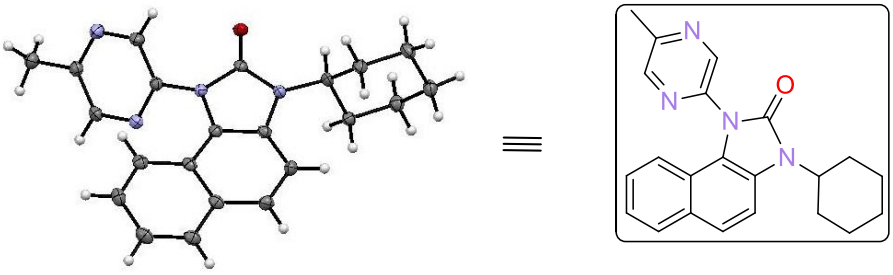
Thermal ellipsoid plot of **5h**. Ellipsoids are represented with 50% probability.

X-ray determined molecular structure of **5h,** CCDC: 2025275

Identification code	K_101_0m_a
Empirical formula	$C_{23}H_{18}N_3$
Formula weight	336.40
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	11.8246(5)
b/Å	8.7668(4)
c/Å	16.2183(7)
α/°	90
β/°	90.457(2)
γ/°	90
Volume/Å^3	1681.20(13)
Z	4
ρ_{calc}g/cm^3	1.329
μ/mm^{-1}	0.618
F(000)	708.0
Crystal size/mm^3	0.35 × 0.29 × 0.28
Radiation	CuKα (λ = 1.54178)

2Θ range for data collection/°	10.91 to 133.22
Index ranges	$-14 \leq h \leq 13, -10 \leq k \leq 10, -18 \leq l \leq 19$
Reflections collected	16494
Independent reflections	2930 [R_{int} = 0.0772, R_{sigma} = 0.0536]
Data/restraints/parameters	2930/0/235
Goodness-of-fit on F^2	1.105
Final R indexes [I>=2σ (I)]	R_1 = 0.0624, wR_2 = 0.1540
Final R indexes [all data]	R_1 = 0.0667, wR_2 = 0.1575
Largest diff. peak/hole / e $Å^{-3}$	0.25/-0.66

The crystals were grown in dichloromethane solvent. The pure compound was dissolved in dichloromethane slow evaporation led to the crystal **3ad**. The crystal data was collected in X-ray spectroscopy (Bruker Kappa Apex-2, CCD Area Detector), and the data was analyzed using OLEX2 software. The structure is given below. The corresponding cif file has been uploaded separately as supporting information.



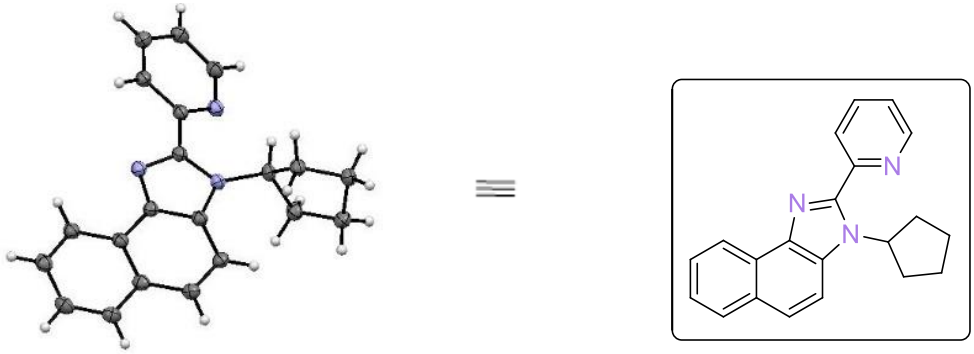
Thermal ellipsoid plot of **3ad**. Ellipsoids are represented with 50% probability.

X-ray determined molecular structure of **3ad,** CCDC: 2025269

Identification code	HM_583_0m_a
Empirical formula	$C_{2.44}H_{2.44}N_{0.44}O_{0.11}$
Formula weight	39.83
Temperature/K	100.0
Crystal system	triclinic
Space group	P-1
a/Å	7.9957(2)
b/Å	10.4307(2)
c/Å	12.5078(3)
α/°	67.7270(10)
β/°	89.0730(10)
γ/°	71.4000(10)
Volume/Å^3	908.36(4)
Z	18
ρ_{calc}g/cm^3	1.310
μ/mm^{-1}	0.658
F(000)	380.0
Crystal size/mm^3	0.80 × 0.28 × 0.27
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	7.692 to 133.402
Index ranges	$-9 \leq h \leq 8$, $-12 \leq k \leq 12$, $-14 \leq l \leq 14$
Reflections collected	28821
Independent reflections	3182 [R_{int} = 0.0634, R_{sigma} = 0.0334]
Data/restraints/parameters	3182/0/245

Goodness-of-fit on F^2	1.088
Final R indexes [I>=2σ (I)]	R_1 = 0.0424, wR_2 = 0.0985
Final R indexes [all data]	R_1 = 0.0438, wR_2 = 0.0994
Largest diff. peak/hole / e $Å^{-3}$	0.21/-0.25

The crystals were grown in dichloromethane solvent. The pure compound was dissolved in dichloromethane slow evaporation led to the crystal **5b**. The crystal data was collected in X-ray spectroscopy (Bruker Kappa Apex-2, CCD Area Detector), and the data was analyzed using OLEX2 software. The structure is given below. The corresponding cif file has been uploaded separately as supporting information.



Thermal ellipsoid plot of **5b**. Ellipsoids are represented with 50% probability.

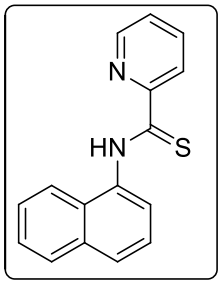
X-ray determined molecular structure of **5b,** CCDC: 2025279

Identification code	HM_788_1_0m_a
Empirical formula	$C_{21}H_{19}N_3$
Formula weight	313.41
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	15.2933(10)
b/Å	5.6759(9)
c/Å	18.003(3)
α/°	90
β/°	99.217(8)
γ/°	90
Volume/Å^3	1542.5(4)
Z	4
ρ_{calc}g/cm^3	1.3495
μ/mm^{-1}	0.627
F(000)	665.9
Crystal size/mm^3	0.2 × 0.2 × 0.2
Radiation	Cu Kα (λ = 1.54178)
2Θ range for data collection/°	5.86 to 143.7
Index ranges	$-18 \leq h \leq 18$, $-6 \leq k \leq 6$, $-21 \leq l \leq 22$
Reflections collected	22846
Independent reflections	2934 [R_{int} = 0.0804, R_{sigma} = 0.0465]
Data/restraints/parameters	2934/0/218
Goodness-of-fit on F^2	1.048

Final R indexes [I>=2σ (I)]	R_1 = 0.0531, wR_2 = 0.1361
Final R indexes [all data]	R_1 = 0.0570, wR_2 = 0.1400
Largest diff. peak/hole / e Å^{-3}	0.22/-0.34

Spectral data:

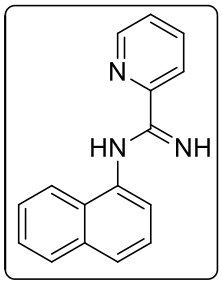
_N_-(naphthalen-1-yl)pyridine-2-carbothioamide (4a)



Column chromatography (SiO_2, eluting with 95:5 hexane/ethyl acetate) afforded the desired product as a yellow solid, mp 124-126 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 12.36 (s, 1H), 8.84 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 8.63-8.61 (m, 1H), 8.33 (d, J = 7.2 Hz, 1H), 8.03-7.99 (m, 1H), 7.95-7.89 (m, 2H), 7.85 (d, J = 8.4 Hz, 1H), 7.60-7.49 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.2, 151.5, 146.8, 137.7, 134.4, 134.3, 128.9, 128.4, 127.7, 126.8, 126.5, 126.3, 125.5, 125.3, 122.9, 121.6; HRMS (ESI, m/z) calcd. For $C_{16}H_{13}N_2S$ $[M+H]^+$: 265.0799; found: 265.0802.

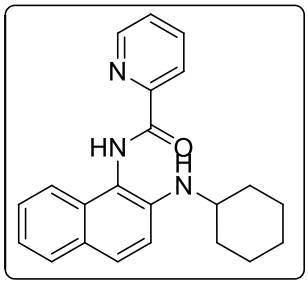
_N_-(naphthalen-1-yl)picolinimidamide (4a')



Washing with distilled hexane afforded the desired product as a violet solid, mp 118-120 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.63 (d, *J* = 8.0 Hz, 1H), 8.61-8.59 (m, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 7.89-7.83 (m, 2H), 7.59 (d, *J* = 8.4 Hz, 1H), 7.49-7.38 (m, 4H), 7.09 (d, *J* = 7.6 Hz, 1H), 6.29-5.17 (br. S); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.9, 151.3, 148.1, 137.0, 134.8, 128.1, 127.4, 126.4, 126.2, 125.4, 123.9, 123.4, 122.0, 116.3; HRMS (ESI, m/z) calcd. For $C_{16}H_{14}N_3$ $[M+H]^+$: 248.1188; found: 248.1185.

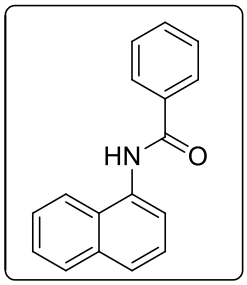
***N*-(2-(cyclohexylamino)naphthalen-1-yl)picolinamide (1a')**



Column chromatography (SiO_2, eluting with 85:15 hexane/ethyl acetate) afforded the desired product as a brown gummy liquid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.76 (s, 1H), 8.68-8.67 (m, 1H), 8.34 (dt, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 7.91 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.73-7.68 (m, 3H), 7.51-7.48 (m, 1H), 7.41-7.37 (m, 1H), 7.23-7.19 (m, 2H), 3.51-3.44 (m, 1H), 2.12-2.08 (m, 2H), 1.79-1.74 (m, 2H), 1.65-1.61 (m, 1H), 1.43-1.21 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.4, 149.8, 148.4, 141.5, 137.7, 131.5, 128.7, 128.3, 127.3, 127.0, 126.6, 122.8, 122.1, 120.5, 115.4, 113.0, 51.9, 33.8, 25.9, 25.1; HRMS (ESI, m/z) calcd. For $C_{22}H_{24}N_3O$ $[M+H]^+$: 346.1919; found: 346.1922.

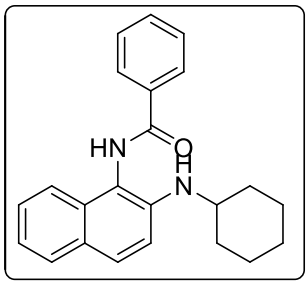
***N*-(naphthalen-1-yl)benzamide (6)**



Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as white fluffy solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.27 (s, 1H), 7.98-7.95 (m, 3H), 7.90-7.87 (m, 2H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.58-7.55 (m, 1H), 7.51-7.46 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.4, 134.9, 134.3, 132.5, 132.0, 128.94, 128.90, 127.6, 127.3, 126.5, 126.2, 126.1, 125.9, 121.5, 120.9.

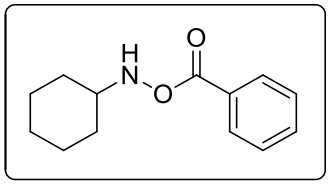
***N*-(2-(cyclohexylamino)naphthalen-1-yl)benzamide (7)**



Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as white fluffy solid.

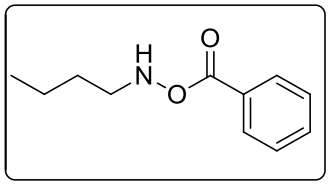
^{1}H NMR (400 MHz, $CDCl_3$ + CD_3OD): δ 8.01-7.98 (m, 2H), 7.68-7.64 (m, 2H), 7.58-7.51 (m, 2H), 7.49-7.45 (m, 2H), 7.33-7.28 (m, 1H), 7.17-7.01 (m, 2H), 3.39-3.30 (m, 1H), 1.98 (d, *J* = 12.8 Hz, 2H), 1.69-1.61 (m, 2H), 1.58-1.54 (m, 1H), 1.35-1.12 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$+ CD_3OD): δ 171.8, 137.7, 136.1, 135.6, 133.0, 132.8, 132.1, 132.0, 131.6, 131.0, 126.5, 124.8, 119.8, 56.8, 37.3, 33.6, 29.6, 28.9; HRMS (ESI, m/z) calcd. For $C_{23}H_{25}N_2O$ $[M+H]^+$: 345.1967; found: 345.1964.

_O_-benzoyl-_N_-cyclohexylhydroxylamine (2a)



Column chromatography (SiO_2, eluting with 98:2 hexane/ethyl acetate) afforded the desired product as colourless liquid.
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02-7.99 (m, 2H), 7.58-7.53 (m, 1H), 7.45-7.41 (m, 2H), 3.07-2.99 (m, 1H), 1.98-1.94 (m, 2H), 1.81-1.74 (m, 2H), 1.64-1.59 (m, 1H), 1.31-1.17 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.0, 133.3, 129.4, 128.6, 59.9, 30.4, 25.9, 24.1.

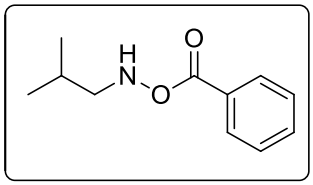
_O_-benzoyl-_N_-butylhydroxylamine (2g)



Column chromatography (SiO_2, eluting with 98:2 hexane/ethyl acetate) afforded the desired product as colourless liquid.

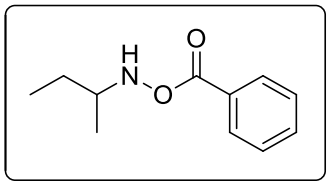
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03-7.99 (m, 2H), 7.86 (br. S, 1H), 7.58-7.54 (m, 1H), 7.46-7.42 (m, 2H), 3.13 (t, *J* = 7.2 Hz, 2H), 1.63-1.56 (m, 2H), 1.47-1.38 (m, 2H), 0.94 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.0, 133.4, 129.4, 128.6, 52.4, 29.3, 20.3, 13.9.

_O_-benzoyl-_N_-_iso_butylhydroxylamine (2h)



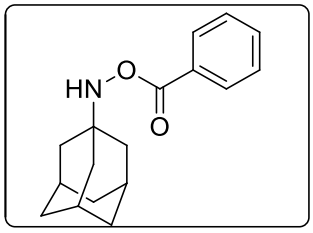
Column chromatography (SiO_2, eluting with 98:2 hexane/ethyl acetate) afforded the desired product as colourless liquid.
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02-7.99 (m, 2H), 7.96 (br. S, 1H), 7.58-7.54 (m, 1H), 7.46-7.41 (m, 2H), 2.95 (d, *J* = 6.8 Hz, 2H), 1.99-1.89 (m, 1H), 1.00 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.9, 133.4, 129.4, 128.6, 60.2, 26.5, 20.6.

_O_-benzoyl-_N_-(_sec_-butyl)hydroxylamine (2i)



Column chromatography (SiO_2, eluting with 98:2 hexane/ethyl acetate) afforded the desired product as colourless liquid.
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03-7.99 (m, 2H), 7.58-7.54 (m, 1H), 7.46-7.42 (m, 2H), 3.11 (sextet, *J* = 6.4 Hz, 1H), 1.71-1.61 (m, 1H), 1.50-1.39 (m, 1H), 1.17 (d, *J* = 6.4 Hz, 3H), 0.98 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.0, 133.3, 129.4, 128.6, 58.2, 26.8, 17.6, 10.3.

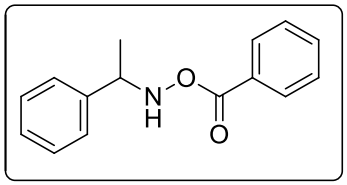
_N_-((3s,5s,7s)-adamantan-1-yl)-_O_-benzoylhydroxylamine (2m)



Column chromatography (SiO_2, eluting with 98:2 hexane/ethyl acetate) afforded the desired product as crystalline solid.

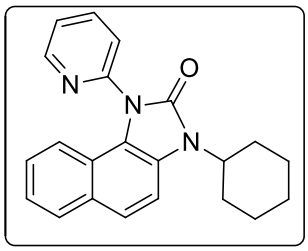
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03-8.01 (m, 2H), 7.59-7.55 (m, 1H), 7.47-7.43 (m, 2H), 2.11 (s, 3H), 1.76 (d, *J* = 2.8 Hz, 6H), 1.71-1.62 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.0, 133.3, 129.4, 128.6, 56.4, 40.1, 36.5, 29.2.

_O_-benzoyl-_N_-(1-phenylethyl)hydroxylamine (2n)



Column chromatography (SiO_2, eluting with 98:2 hexane/ethyl acetate) afforded the desired product as colourless liquid.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97-7.94 (m, 2H), 7.56-7.51 (m, 1H), 7.45-7.35 (m, 6H), 7.32-7.28 (m, 1H), 4.34 (q, *J* = 6.8 Hz, 2H), 1.55 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.9, 141.3, 133.4, 129.4, 128.7, 128.6, 128.5, 127.9, 127.2, 61.0, 19.8.

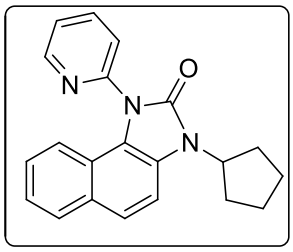
3-cyclohexyl-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3a)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a light brown solid (63.8 mg, 93% yield), mp 142-144 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.67-8.65 (m, 1H), 7.97 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.70 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.64 (d, *J* = 8.8 Hz, 1H), 7.51 (d, *J* = 8.8 Hz, 1H), 7.45-7.41 (m, 1H), 7.29-7.25 (m, 1H), 7.19-7.15 (m, 1H), 6.96 (d, *J* = 8.0 Hz, 1H), 4.42-4.34 (m, 1H), 2.33-2.22 (m, 2H), 1.99-1.92 (m, 4H), 1.77 (d, *J* = 12.8 Hz, 1H),1.53-1.42 (m, 2H), 1.36-1.29 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.7, 150.2, 149.6, 138.8, 129.9, 129.2, 126.0, 125.8, 123.7, 123.5, 123.2, 121.8, 121.3, 120.4, 110.4, 53.7, 30.4, 26.2, 25.5; HRMS (ESI, m/z) calcd. For $C_{22}H_{22}N_3O$ $[M+H]^+$: 344.1763; found: 344.1760.

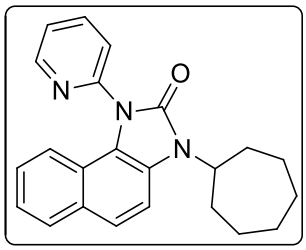
3-cyclopentyl-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3b)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a light brown solid (51 mg, 78% yield), mp 138-140 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.67-8.65 (m, 1H), 7.97 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.82 (dd, J_1 = 8.4 Hz, J_2 = 0.4 Hz, 1H), 7.69 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.65 (d, J = 8.8 Hz, 1H), 7.45-7.40 (m, 2H), 7.29-7.24 (m, 1H), 7.19-7.15 (m, 1H), 6.97 (d, J = 8.8 Hz, 1H), 4.97 (quintet, J = 8.8 Hz, 1H), 2.29-2.20 (m, 2H), 2.14-1.97 (m, 4H), 1.80-1.73 (m, 2H); ^{13}C NMR(100 MHz, $CDCl_3$):δ 153.9, 150.2, 149.6, 138.8, 130.0, 129.2, 125.8, 125.6, 123.8, 123.6, 123.5, 123.3, 121.9, 121.2, 120.5, 110.1, 54.0, 29.3, 25.3; HRMS (ESI, m/z) calcd. For $C_{21}H_{20}N_3O$ $[M+H]^+$: 330.1606; found: 330.1644.

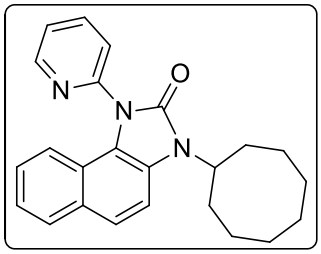
3-cycloheptyl-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3c)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a light brown solid (46.4 mg, 65% yield), mp 154-156 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.67-8.65 (m, 1H), 7.98 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.82 (d, J = 8.4 Hz, 1H), 7.70 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.64 (d, J = 8.8 Hz, 1H), 7.47-7.42 (m, 2H), 7.29-7.25 (m, 1H), 7.19-7.15 (m, 1H), 6.97 (d, J = 8.8 Hz, 1H), 4.62-4.55 (m, 1H), 2.37-2.29 (m, 2H), 2.07-2.03 (m, 2H), 1.88-1.85 (m, 2H), 1.73-1.64 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.5, 150. 2, 149.5, 138.8, 130.0, 129.2, 125.8, 125.7, 123.7, 123.49, 123.47, 123.3, 121.8, 121.3, 120.5, 110.5, 55.6, 32.9, 27.7, 25.9; HRMS (ESI, m/z) calcd. For $C_{23}H_{24}N_3O$ $[M+H]^+$: 358.1919; found: 358.1921.

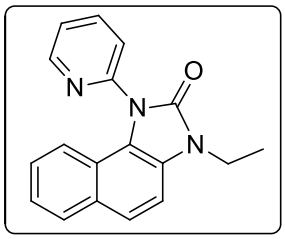
3-cyclooctyl-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3d)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a light brown solid (34 mg, 46% yield), mp 156-158 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.66-8.64 (m, 1H), 7.97 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.82 (d, J = 8.0 Hz, 1H), 7.71 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.64 (d, J = 8.8 Hz, 1H), 7.45-7.41 (m, 2H), 7.29-7.25 (m, 1H), 7.19-7.15 (m, 1H), 6.99 (d, J = 8.8 Hz, 1H), 4.75-4.69 (m, 1H), 2.39-2.31 (m, 2H), 2.02-1.97 (m, 2H), 1.89-1.84 (m, 2H), 1.79-1.60 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.5, 150.2, 149.5, 138.7, 130.0, 129.2, 125.8, 125.5, 123.6, 123.5, 123.4, 123.3, 121.9, 121.3, 120.5, 110.6, 54.1, 32.6, 26.4, 26.2, 25.5; HRMS (ESI, m/z) calcd. For $C_{24}H_{26}N_3O$ $[M+H]^+$: 372.2076; found: 372.2076.

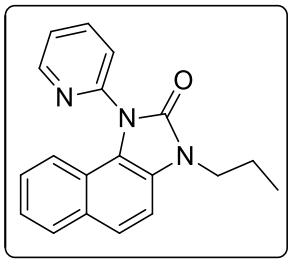
3-ethyl-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3e)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a light brown solid (29 mg, 50% yield), mp 96-98 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.68-8.66 (m, 1H), 7.98 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.84 (d, J = 8.0 Hz, 1H), 7.72-7.68 (m, 2H), 7.46-7.42 (m, 1H), 7.34 (d, J = 8.4 Hz, 1H), 7.31-7.27 (m, 1H), 7.22-7.18 (m, 1H), 7.02 (d, J = 9.2 Hz, 1H), 4.09 (q, J = 7.2 Hz, 2H), 1.43 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.9, 150.1, 149.6, 138.9, 130.4, 129.3, 126.2, 125.9, 123.8, 123.7, 123.5, 123.4, 121.8, 121.2, 120.5, 108.9, 36.3, 13.9; HRMS (ESI, m/z) calcd. For $C_{18}H_{16}N_3O$ $[M+H]^+$: 290.1293; found: 290.1296.

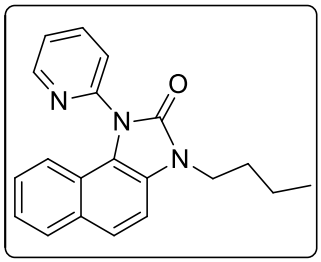
3-propyl-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3f)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a light brown solid (39.4 mg, 65% yield), mp 134-136 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.66 (d, *J* = 3.6 Hz, 1H), 7.97 (t, *J* = 7.6 Hz, 1H), 7.82 (d, *J* = 8.4 Hz, 1H), 7.71-7.66 (m, 2H), 7.45-7.41 (m, 1H), 7.33 (d, *J* = 8.4 Hz, 1H), 7.27 (t, *J* = 7.2 Hz, 1H), 7.19 (t, *J* = 8.0 Hz, 1H), 7.01 (d, *J* = 8.8 Hz, 1H), 3.98 (t, *J* = 7.2 Hz, 2H), 1.87 (sextet, *J* = 7.2 Hz, 2H), 1.02 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$):δ 154.2, 150.1, 149.6, 138.8, 130.4, 129.3, 126.6, 125.9, 123.8, 123.7, 123.5, 123.4, 121.7, 121.3, 120.5, 109.1, 43.1, 22.1, 11.5; HRMS (ESI, m/z) calcd. For $C_{19}H_{18}N_3O$ $[M+H]^+$: 304.1450; found: 304.1451.

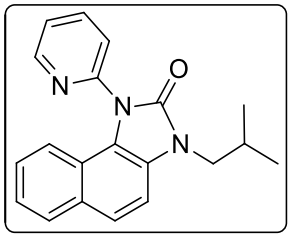
3-butyl-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3g)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a creamy white solid (52 mg, 82% yield), mp 104-106 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.68-8.67 (m, 1H), 7.99 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.85-7.83 (m, 1H), 7.72 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.47-7.43 (m, 1H), 7.34 (d, *J* = 8.8 Hz, 1H), 7.31-7.27 (m, 1H), 7.22-7.18 (m, 1H), 7.04-7.02 (m, 1H), 4.03 (t, *J* = 7.2 Hz, 2H), 1.86-1.79 (m, 2H), 1.51-1.41 (m, 2H), 0.97 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.2, 150.1, 149.5, 138.9, 130.4, 129.3, 126.6, 125.9, 123.8, 123.7, 123.5, 123.4, 121.7, 121.3, 120.5, 109.1, 41.3, 30.8, 20.2, 13.8; HRMS (ESI, m/z) calcd. For $C_{20}H_{20}N_3O$ $[M+H]^+$: 318.1606; found: 318.1657.

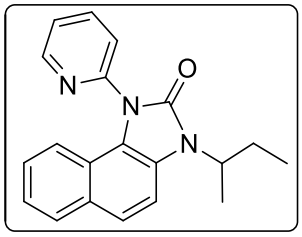
3-isobutyl-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3h)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a light brown solid (40 mg, 63% yield). mp 112-114 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.67 (s, 1H), 7.98 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.83 (d, J = 7.6 Hz, 1H), 7.72 (d, J = 8.0 Hz, 1H), 7.67 (d, J = 8.8 Hz, 1H), 7.46-7.43 (m, 1H), 7.34-7.26 (m, 2H), 7.22-7.18 (m, 1H), 7.03 (d, J = 8.4 Hz, 1H), 3.82 (d, J = 7.6 Hz, 2H), 2.34-2.24 (m, 1H), 1.02 (d, J = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.5, 150.1, 149.4, 138.8, 130.4, 129.3, 126.9, 125.9, 123.7, 123.5, 123.4, 121.6, 121.3, 120.5, 109.4, 48.9, 28.3, 20.3; HRMS (ESI, m/z) calcd. For $C_{20}H_{20}N_3O$ $[M+H]^+$: 318.1606; found: 318.1608.

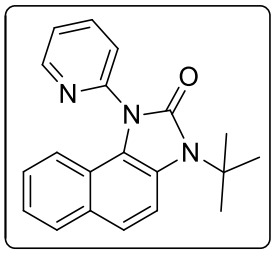
3-(sec-butyl)-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3i)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as light brown solid (60 mg, 95% yield), mp 112-114 °C.

^{1}H NMR (400 MHz, $CDCl_3$):δ 8.68-8.66 (m, 1H), 7.98 (td, J_1 = 7.6 Hz, J_2 = 2.0 Hz, 1H), 7.82 (d, J = 8.0 Hz, 1H), 7.71 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.65 (d, J = 8.4 Hz, 1H), 7.46-7.42 (m, 2H), 7.30-7.26 (m, 1H), 7.20-7.16 (m, 1H), 6.99 (dd, J_1 = 8.8 Hz, J_2 = 0.8 Hz, 1H), 4.61-4.51 (m, 1H), 2.24-2.13 (m, 1H), 1.98-1.87 (m, 1H), 1.61 (d, J = 6.8 Hz, 3H), 0.93 (t, J = 7.6 Hz, 3H),^{13}C NMR (100 MHz, $CDCl_3$): δ 153.9, 150.1, 149.5, 138.8, 130.0, 129.2, 126.0, 125.8, 123.7, 123.6, 123.5, 123.4, 121.8, 121.3, 120.5, 110.2, 51.8, 27.6, 18.8, 11.5; HRMS (ESI, m/z) calcd. For $C_{20}H_{20}N_3O$ $[M+H]^+$: 318.1606; found: 318.1610.

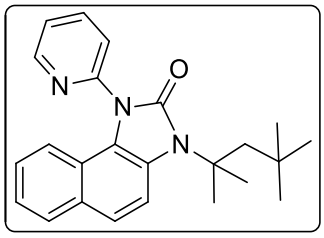
3-(tert-butyl)-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3j)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a creamy white powder (59.6 mg, 94% yield), mp 154−156 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.67 (dd, J_1 = 4.8 Hz, J_2 = 1.2 Hz, 1H), 7.96 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.79 (d, J = 8.0 Hz, 1H), 7.75 (d, J = 9.2 Hz, 1H), 7.66 (d, J = 8.0 Hz, 1H), 7.58 (d, J = 9.2 Hz, 1H), 7.45- 7.42 (m, 1H), 7.28-7.24 (m, 1H), 7.15-7.11 (m, 1H), 6.85 (d, J = 8.8 Hz, 1H), 1.88 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.1, 150.4, 149.7, 138.8, 129.7, 128.9, 126.6, 125.7, 124.0, 123.8, 123.7, 122.6, 122.4, 121.3, 120.0, 113.1, 58.8, 29.8; HRMS (ESI, m/z) calcd. For $C_{20}H_{20}N_3O$ $[M+H]^+$: 318.1606; found: 318.1606.

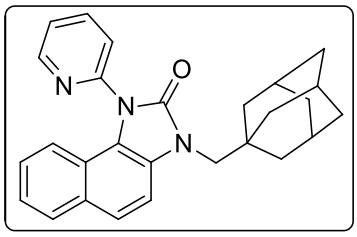
1-(pyridin-2-yl)-3-(2,4,4-trimethylpentan-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3k)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a creamy white solid (49 mg, 66% yield), mp 120−122 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.68-8.66 (m, 1H), 7.95 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.81-7.78 (m, 2H), 7.62 (dt, J_1 = 8.0 Hz, J_2 = 0.4 Hz, 1H), 7.59 (d, J = 8.8 Hz, 1H), 7.45-7.41 (m, 1H), 7.29-7.25 (m, 1H), 7.16-7.12 (m, 1H), 6.86 (d, J = 8.8 Hz, 1H), 2.18 (s, 2H), 1.98 (s, 6H), 0.92 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.4, 150.5, 149.8, 138.8, 129.6, 128.8, 127.1, 125.6, 124.0, 123.8, 123.7, 122.51, 122.49, 121.4, 120.0, 113.5, 62.4, 51.1, 31.9, 31.2, 31.0; HRMS (ESI, m/z) calcd. For $C_{24}H_{28}N_3O$ $[M+H]^+$: 374.2232; found: 374.2235.

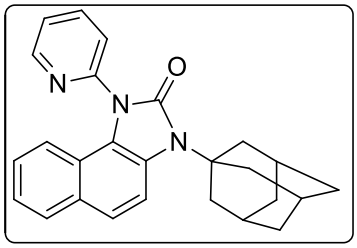
3-((3s)-adamantan-1-ylmethyl)-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3l)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 80:20 hexane/ethyl acetate) afforded the desired product as a light brown solid (59 mg, 72% yield), mp 198−200 °C.

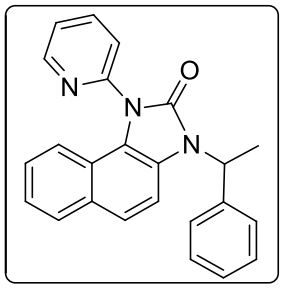
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.68 (d, J = 3.6 Hz, 1H), 7.98 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.84-7.82 (m, 1H), 7.73 (d, J = 8.0 Hz, 1H), 7.66 (d, J = 8.4 Hz, 1H), 7.46-7.43 (m, 1H), 7.38 (d, J = 8.8 Hz, 1H), 7.31-7.26 (m, 1H), 7.22-7.18 (m, 1H), 7.05-7.02 (m, 1H), 3.69 (s, 2H), 1.98 (s, 3H), 1.71-1.60 (m, 12H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.2, 150.1, 149.4, 138.9, 130.3, 129.3, 128.2, 125.9, 123.67, 123.66, 123.4, 121.6, 121.3, 120.3, 110.3, 53.9, 41.2, 36.8, 36.4, 28.3; HRMS (ESI, m/z) calcd. For $C_{27}H_{28}N_3O$ $[M+H]^+$: 410.2232; found: 410.2231.

3-((3s,5s,7s)-adamantan-1-yl)-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3m)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 80:20 hexane/ethyl acetate) afforded the desired product as a light brown solid (77 mg, 98% yield), mp 164-166 °C.
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.67-8.65 (m, 1H), 7.98-7.93 (m, 1H), 7.85 (dd, J_1 = 8.8 Hz, J_2 = 1.2 Hz, 1H), 7.78 (d, J = 8.0 Hz, 1H), 7.66-7.63 (m, 1H), 7.54 (d, J = 9.2 Hz, 1H), 7.44-7.41 (m, 1H), 7.28-7.23 (m, 1H), 7.14-7.10 (m, 1H), 6.85 (d, J = 9.2 Hz, 1H), 2.68 (s, 6H), 2.25 (s, 3H), 1.80 (dd, J_1 = 32.4 Hz, J_2 = 12.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.0, 150.5, 149.7, 138.7, 129.5, 128.8, 126.4, 125.6, 124.0, 123.72, 123.67, 122.6, 122.2, 121.3, 120.0, 113.6, 61.1, 40.9, 36.3, 30.1; HRMS (ESI, m/z) calcd. For $C_{26}H_{26}N_3O$ $[M+H]^+$: 396.2076; found: 396.2076

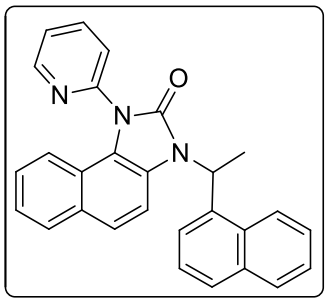
3-(1-phenylethyl)-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3n)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a pale yellow solid (48.2 mg, 66% yield), mp 136-138 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.70-8.69 (m, 1H), 8.01 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.78-7.75 (m, 2H), 7.49-7.44 (m, 4H), 7.36-7.32 (m, 2H), 7.29-7.24 (m, 2H), 7.19-7.16 (m, 1H), 7.02-6.98 (m, 2H), 6.01 (q, *J* = 7.2 Hz, 1H), 1.99 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.2, 150.1, 149.6, 139.8, 138.9, 130.1, 129.2, 128.8, 127.7, 126.9, 125.8, 125.4, 123.8, 123.7, 123.5, 123.4, 121.9, 121.2, 120.4, 110.8, 51.2, 17.7; HRMS (ESI, m/z) calcd. For $C_{24}H_{20}N_3O$ $[M+H]^+$: 366.1606; found: 366.1606.

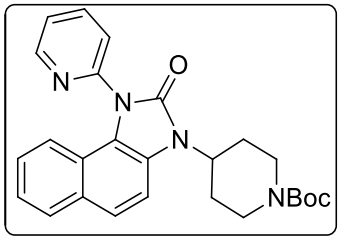
3-(1-(naphthalen-1-yl)ethyl)-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3o)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a light brown solid (73 mg, 88% yield), mp 222-224 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.69 (d, *J* = 4.8 Hz, 1H), 8.25 (d, *J* = 8.4 Hz, 1H), 8.01 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.96 (d, *J* = 7.2 Hz, 1H), 7.86 (d, *J* = 8.4 Hz, 1H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.68 (d, *J* = 8.4 Hz, 1H), 7.58 (t, *J* = 8.0 Hz, 1H), 7.51- 7.40 (m, 3H), 7.36 (d, *J* = 8.8 Hz, 1H), 7.22-7.18 (m, 1H), 7.14-7.10 (m, 2H), 6.93 (d, *J* = 8.8 Hz, 1H), 6.63 (q, *J* = 6.8 Hz, 1H), 2.11 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.9, 150.1, 149.7, 138.9, 134.9, 134.0, 131.8, 129.9, 129.4, 129.1, 128.9, 127.1, 126.1, 125.7, 125.6, 125.0, 124.8, 123.8, 123.59, 123.57, 123.51, 123.3, 122.0, 121.2, 120.3, 110.6, 48.9, 18.1; HRMS (ESI, m/z) calcd. For $C_{28}H_{22}N_3O$ $[M+H]^+$: 416.1763; found: 416.1766.

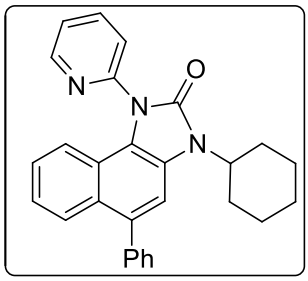
***tert*-butyl 4-(2-oxo-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-3(2H)-yl)piperidine-1-carboxylate (3p)**



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 70:30 hexane/ethyl acetate) afforded the desired product as a creamy white solid (80 mg, 90% yield), mp 174-176 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.68-8.66 (m, 1H), 7.99 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.83 (d, J = 8.0 Hz, 1H), 7.69 (dt, J_1 = 8.0 Hz, J_2 = 0.8Hz, 1H), 7.65 (d, J = 8.8 Hz, 1H), 7.48-7.45 (m, 2H), 7.31-7.27 (m, 1H), 7.20-7.16 (m, 1H), 6.94 (d, J = 8.8 Hz, 1H), 4.62-4,54 (m, 1H), 4.35-4.33 (br. S, 2H), 2.90 (t, J = 12.4 Hz, 2H), 2.50-2.40 (m, 2H), 1.92 (d, J = 12.4 Hz, 2H), 1.50 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.8, 153.6, 150.0, 149.7, 138.9, 130.1, 129.2, 125.9, 125.4, 123.9, 123.8, 123.52, 123.50, 121.9, 121.2, 120.4, 110.2, 80.0, 51.8, 29.5, 28.6; HRMS (ESI, m/z) calcd. For $C_{26}H_{29}N_4O_3$ $[M+H]^+$: 445.2240; found: 445.2237.

3-cyclohexyl-5-phenyl-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3q)

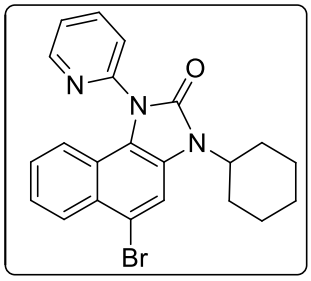


The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a creamy white solid (67.8 mg, 81% yield), mp 186-188 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.68-8.66 (m, 1H), 7.99 (td, J_1 = 7.6 Hz, J_2 = 2.0 Hz, 1H), 7.83-7.80 (m, 1H), 7.74 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.53-7.48 (m, 4H), 7.47-7.42 (m, 3H), 7.23-7.16 (m, 2H), 7.05-7.03 (m, 1H), 4.41-4.33 (m, 1H), 2.33-2.23 (m, 2H), 1.99-1.90 (m, 4H), 1.73 (d, J = 13.2 Hz, 1H), 1.50-1.40 (m, 2H), 1.32-1.26 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.9, 150.3, 149.6, 141.1, 138.8, 136.0, 130.5, 128.4, 128.2, 127.46, 127.44, 125.71, 125.67, 123.63,

123.61, 123.4, 121.51, 121.46, 120.6, 111.4, 53.8, 30.4, 26.1, 25.4; HRMS (ESI, m/z) calcd. For $C_{28}H_{26}N_3O$ $[M+H]^+$: 420.2076; found: 420.2075.

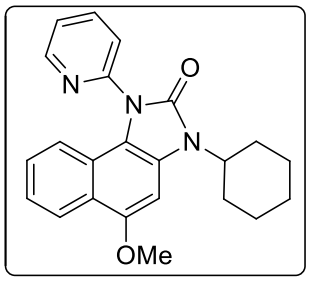
5-bromo-3-cyclohexyl-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3r)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a creamy white solid (68 mg, 81% yield), mp 168-170 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.65-8.63 (m, 1H), 8.25-8.22 (m, 1H), 7.98 (td, J_1 = 7.6 Hz, J_2 = 2.0 Hz, 1H), 7.83 (s, 1H), 7.69 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.46-7.43 (m, 1H), 7.40-7.35 (m, 1H), 7.40-7.35(m, 1H), 7.22-7.18 (m, 1H), 6.99-6.96 (m, 1H), 4.36-4.28 (m, 1H), 2.29-2.19 (m, 2H), 1.95 (d, J = 11.2 Hz, 4H), 1.77 (d, J = 12.8 Hz, 1H),1.52-1.42 (m, 2H), 1.38-1.30 (m, 1H);^{13}C NMR (100 MHz, $CDCl_3$): δ 153.6, 150.0, 149.7, 138.9, 128.5, 127.8, 126.5, 126.2, 124.9, 123.9, 123.5, 121.9, 121.7, 121.2, 116.7, 114.4, 53.9, 30.4, 26.1, 25.4; HRMS (ESI, m/z) calcd. For $C_{22}H_{21}BrN_3O$ $[M+H]^+$: 422.0868; found: 422.0886.

3-cyclohexyl-5-methoxy-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3s)

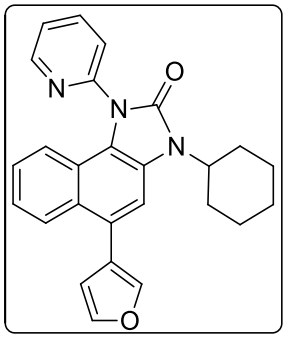


The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 70:30 hexane/ethyl acetate) afforded the desired product as a brown solid (44.7 mg, 60% yield), mp 166-168 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.64-8.62 (m, 1H), 8.27-8.25 (m, 1H), 7.95 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.70 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.41-7.37 (m, 1H), 7.29-7.25 (m, 1H), 7.22-7.18 (m, 1H), 6.98-6.96 (m, 1H), 6.87 (s, 1H), 4.35-4.27 (m, 1H), 4.05 (s, 3H), 2.34-2.24 (m, 2H), 1.99-1.93 (m, 4H), 1.78 (d, J = 12.8 Hz, 1H), 1.54-1.43 (m, 2H), 1.37-1.28 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$):δ 153.9, 152.6, 150.3, 149.4, 138.6, 126.5, 126.1, 123.3, 123.21, 123.18, 122.8,

121.8, 121.3, 121.0, 115.4, 90.8, 56.3, 53.8, 30.4, 26.2, 25.6; HRMS (ESI, m/z) calcd. For $C_{23}H_{24}N_3O_2$ $[M+H]^+$: 374.1869; found: 374.1874.

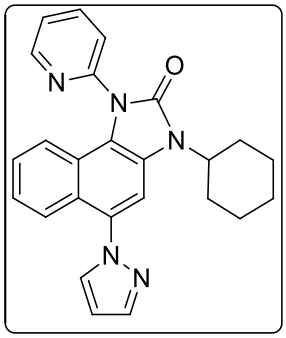
3-cyclohexyl-5-(furan-3-yl)-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3t)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a light brown solid (65.4 mg, 80% yield), mp 190-192 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.67-8.66 (m, 1H), 8.07-8.05 (m, 1H), 7.99 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.72 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.65 (dd, J_1 = 1.6 Hz, J_2 = 0.8 Hz, 1H), 7.59 (t, J = 1.6 Hz, 1H), 7.47-7.43 (m, 2H), 7.29-7.25 (m, 1H), 7.21-7.17 (m, 1H), 7.04-7.01 (m, 1H), 6.68 (dd, J_1 = 2.0 Hz, J_2 = 0.8 Hz, 1H), 4.40-4.32 (m, 1H), 2.33-2.22 (m, 2H), 1.99-1.91 (m, 4H), 1.76 (d, J = 12.8 Hz, 1H), 1.53-1.42 (m, 2H), 1.36-1.28 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.8, 150.2, 149.5, 143.0, 140.6, 138.9, 128.5, 127.0, 126.3, 125.8, 125.7, 123.8, 123.7, 123.4, 121.7, 121.6, 120.7, 113.0, 111.4, 53.8, 30.4, 26.1, 25.4; HRMS (ESI, m/z) calcd. For $C_{26}H_{24}N_3O$ $[M+H]^+$: 410.1869; found: 410.1870.

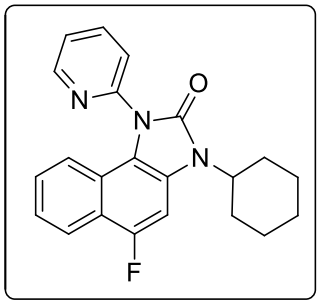
3-cyclohexyl-5-(1H-pyrazol-1-yl)-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3u)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 70:30 hexane/ethyl acetate) afforded the desired product as a creamy white solid (79.3 mg, 97% yield), mp 192-194 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.68-8.66 (m, 1H), 8.01 (td, J_1 = 7.6 Hz, J_2 = 2.0 Hz, 1H), 7.85-7.84 (m, 1H), 7.76 (dd, J_1 = 2.4 Hz, J_2 = 0.8 Hz, 1H), 7.73 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.62 (s, 1H), 7.54-7.51 (m, 1H), 7.48-7.45 (m, 1H), 7.30-7.25 (m, 1H), 7.23-7.19 (m, 1H), 7.05-7.02 (m, 1H), 6.56 (t, J = 2.0 Hz, 1H), 4.37-4.29 (m, 1H), 2.31-2.21 (m, 2H), 1.97-1.89 (m, 4H), 1.73 (d, J = 12.8 Hz, 1H), 1.49-1.39 (m, 2H), 1.33-1.25 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.8, 149.9, 149.7, 140.9, 139.0, 133.0, 132.6, 126.4, 126.1, 125.2, 124.9, 124.0, 123.96, 123.5, 122.5, 121.6, 120.5, 108.95, 106.7, 54.1, 30.3, 26.1, 25.3; HRMS (EI, m/z) calcd. For $C_{25}H_{24}N_5O$ $[M+H]^+$: 410.1981; found: 410.1985.

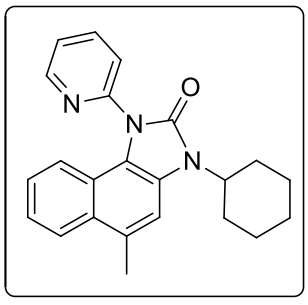
3-cyclohexyl-5-fluoro-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3v)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a light brown crystalline solid (47 mg, 65% yield), mp 142-144 °C.

^{1}H NMR (400 MHz, $CDCl_3$): 8.65-8.64 (m, 1H), 8.08 (d, J = 8.0 Hz, 1H), 7.98 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.71 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.45-7.42 (m, 1H), 7.35- 7.21 (m, 3H), 7.00-6.98 (m, 1H), 4.38-4.29 (m, 1H), 2.27-2.17 (m, 2H), 1.97-1.93 (m, 4H), 1.78 (d, J = 12.8 Hz, 1H), 1.53-1.41 (m, 2H), 1.36-1.29 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.5 (d, J = 244.7 Hz), 153.9, 150.0, 149.5, 138.9, 126.8, 125.2 (d, J = 12.5 Hz), 123.7, 123.69, 123.3, 121.7 (d, J = 6.3 Hz), 121.2 (d, J = 2.7 Hz), 120.8 (d, J = 4.8 Hz), 119.5 (d, J = 16.8 Hz), 117.9, 96.1 (d, J = 27.7 Hz), 53.9, 30.3, 26.1, 25.4; ^{19}F NMR (376 MHz, $CDCl_3$): δ -127.04 (s, 1F); HRMS (ESI, m/z) calcd. For $C_{22}H_{21}FN_3O_3$ $[M+H]^+$: 362.1669; found: 362.1667.

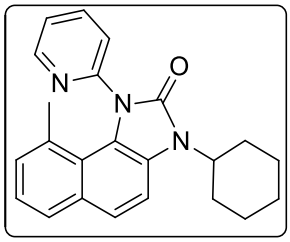
3-cyclohexyl-5-methyl-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3w)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a light brown solid (53.5 mg, 75% yield), mp 134-136 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.66-8.64 (m, 1H), 7.99-7.94 (m, 2H), 7.69 (dt, J_1 = 8.0 Hz, J_2 = 0.4 Hz, 1H), 7.43-7.40 (m, 1H), 7.37 (s, 1H), 7.34-7.30 (m, 1H), 7.21-7.16 (m, 1H), 7.02 (d, J = 8.4 Hz, 1H), 4.40-4.32 (m, 1H), 2.76 (s, 3H), 2.34-2.24 (m, 2H), 1.98-1.92 (m, 4H), 1.78 (d, J = 12.4 Hz, 1H), 1.53-1.43 (m, 2H), 1.39-1.31 (m, 1H), 1.25 (grease); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.8, 150.4, 149.5, 138.8, 129.6, 128.8, 125.7, 125.5, 125.3, 123.5, 123.39, 123.36, 121.8, 120.7, 120.5, 111.3, 53.7, 30.4, 26.2, 25.5, 20.3; HRMS (ESI, m/z) calcd. For $C_{23}H_{24}N_3O$ $[M+H]^+$: 358.1919; found: 358.1920.

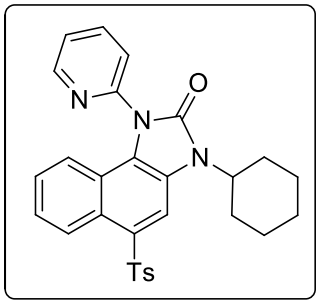
3-cyclohexyl-9-methyl-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3x)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a light brown solid (67.8 mg, 95 % yield), mp 164-166 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.33-8.31 (m, 1H), 7.87 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.78 (d, J = 8.0 Hz, 1H), 7.69-7.66 (m, 2H), 7.45 (d, J = 8.8 Hz, 1H), 7.25-7.20 (m, 2H), 7.08 (d, J = 7.2 Hz, 1H), 4.38-4.30 (m, 1H), 2.34-2.23 (m, 2H), 1.94 (d, J = 11.2 Hz, 4H), 1.77-1.74 (m, 4H), 1.51-1.41 (m, 2H), 1.36-1.28 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.1, 153.3, 148.3, 138.2, 131.1, 131.0, 129.0, 128.5, 127.1, 125.3, 123.5, 123.2, 122.2, 122.1, 121.6, 109.7, 53.9, 30.2, 26.2, 25.5, 21.7; HRMS (ESI, m/z) calcd. For $C_{23}H_{24}N_3O$ $[M+H]^+$: 358.1919; found: 358.1925.

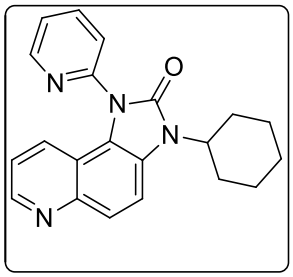
3-cyclohexyl-1-(pyridin-2-yl)-5-tosyl-1H-naphtho[1,2-d]imidazol-2(3H)-one (3y)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 70:30 hexane/ethyl acetate) afforded the desired product as a light brown powder (63.6 mg, 64% yield), mp 172-174 °C.

^{1}H NMR (400 MHz, $CDCl_3$): 8.63-8.62 (m, 1H), 8.60 (s, 1H), 8.58 (dt, J_1 = 8.8 Hz, J_2 = 0.8 Hz, 1H), 8.01 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.81-7.78 (m, 2H), 7.69 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.49-7.46 (m, 1H), 7.35- 7.31 (m, 1H), 7.25-7.23 (m, 2H), 7.19-7.14 (m, 1H), 7.00-6.97 (m, 1H), 4.45-4.37 (m, 1H), 2.39-2.28 (m, 5H), 2.00-1.96 (m, 4H), 1.79 (d, J = 12.4 Hz, 1H), 1.57-1.46 (m, 2H), 1.42-1.34 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.6, 149.8, 149.4, 144.0, 139.2, 130.1, 129.8, 127.3, 127.1, 126.3, 125.8, 125.7, 125.4, 124.4, 123.7, 122.2, 120.6, 114.2, 54.4, 30.4, 25.2, 21.6; HRMS (ESI, m/z) calcd. For $C_{29}H_{28}N_3O_3S$ $[M+H]^+$: 498.1851; found: 498.1853.

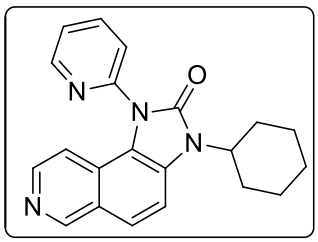
3-cyclohexyl-1-(pyridin-2-yl)-1H-imidazo[4,5-f]quinolin-2(3H)-one (3z)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 65:35 hexane/ethyl acetate) afforded the desired product as a creamy white powder (62 mg, 90% yield), mp 144-146 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.73 (d, J = 3.6 Hz, 1H), 8.64-8.62 (m, 1H), 8.01-7.93 (m, 2H), 7.74-7.72 (m, 2H), 7.45-7.41 (m, 2H), 7.11-7.08 (m, 1H), 4.42-4.34 (m, 1H), 2.32-2.21 (m, 2H), 1.97-1.92 (m, 4H), 1.77 (d, J = 12.8 Hz, 1H), 1.52-1.41 (m, 2H), 1.36-1.28 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.7, 149.7, 149.5, 148.8, 144.6, 139.0, 129.7, 126.2, 124.6, 123.9, 123.2, 121.1, 120.2, 115.9, 113.5, 53.9, 36.4, 26.1, 25.4; HRMS (ESI, m/z) calcd. For $C_{21}H_{20}N_4ONa$ $[M+Na]^+$: 367.1535; found: 367.1551.

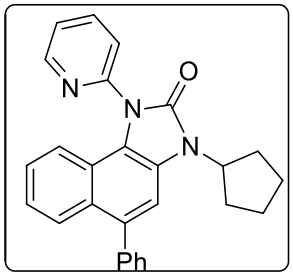
3-cyclohexyl-1-(pyridin-2-yl)-1H-imidazo[4,5-f]isoquinolin-2(3H)-one (3aa)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 65:35 hexane/ethyl acetate) afforded the desired product as a creamy white powder (56.4 mg, 82% yield), mp 160-162 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.20 (s, 1H), 8.68-8.66 (m, 1H), 8.20 (d, J = 5.6 Hz, 1H), 8.01 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.82 (d, J = 8.8 Hz, 1H), 7.74 (d, J = 7.6 Hz, 1H), 7.65 (d, J = 8.8 Hz, 1H), 7.49-7.46 (m, 1H), 6.84 (d, J = 6.0 Hz, 1H), 4.44-4.36 (m, 1H), 2.32-2.23 (m, 2H), 1.96 (d, J = 11.6 Hz, 4H), 1.79 (d, J = 12.8 Hz, 1H), 1.53-1.43 (m, 2H), 1.37-1.29 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.5, 152.8, 149.5, 149.3, 141.6, 139.0, 129.8, 124.0, 123.8, 123.2, 122.8, 120.5, 114.8, 111.8, 54.1, 30.4, 26.1, 25.4; HRMS (ESI, m/z) calcd. For $C_{21}H_{21}N_4O$ $[M+H]^+$: 345.1715; found: 345.1721.

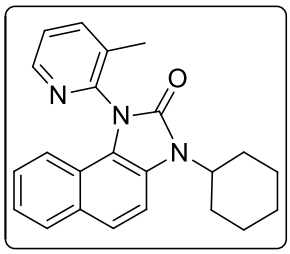
3-cyclopentyl-5-phenyl-1-(pyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3ab)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a creamy white powder (45.4 mg, 56% yield), mp 142-144 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.68-8.67 (m, 1H), 8.01 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.85-7.83 (m, 1H), 7,75 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.53-7.42 (m, 6H), 7.36 (s, 1H), 7.24-7.16 (m, 2H), 7.07-7.03 (m, 1H), 4.94 (quintet, J = 8.8 Hz, 1H), 2.31-2.22 (m, 2H), 2.13-2.06 (m, 2H), 2.01-1.92 (m, 2H), 1.76-1.70 (m, 2H); ^{13}C NMR: (100 MHz, $CDCl_3$):δ 154.0, 150.2, 149.6, 141.1, 138.9, 136.1, 130.4, 128.4, 128.3, 127.5, 127.4, 125.7, 125.5, 123.7, 123.6, 123.4, 121.5, 120.7, 111.1, 54.1, 29.3, 25.1; HRMS (ESI, m/z) calcd. For $C_{27}H_{24}N_3O$ $[M+H]^+$: 406.1919; found: 406.1917.

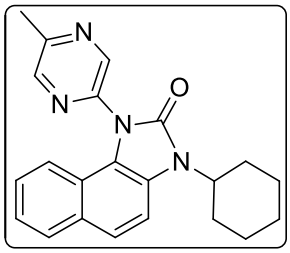
3-cyclohexyl-1-(3-methylpyridin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3ac)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a light brown crystalline solid (54.3 mg, 76% yield), mp 192-194 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.52 (s, 1H), 7.83-7.80 (m, 2H), 7.62 (d, *J* = 8.8 Hz, 1H), 7.54 (d, *J* = 8.4 Hz, 1H), 7.42 (dd, J_1 = 7.6 Hz, J_2 = 4.8 Hz, 1H), 7.26-7.22 (m, 1H), 7.13-7.09 (m, 1H), 6.63 (d, *J* = 8.8 Hz, 1H), 4.45-4.37 (m, 1H), 2.30-2.23 (m, 5H), 1.99-1.92 (m, 4H), 1.77 (d, *J* = 12.8 Hz, 1H), 1.53-1.44 (m, 2H), 1.37-1.29 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.0, 149.3, 147.6, 140.4, 133.4, 129.7, 129.1, 126.1, 125.8, 124.8, 123.5, 122.6, 122.1, 120.3, 119.9, 110.6, 53.6, 30.6, 30.5, 26.1, 25.5, 17.5; HRMS (ESI, m/z) calcd. For $C_{23}H_{24}N_3O$ $[M+H]^+$: 358.1919; found: 358.1921.

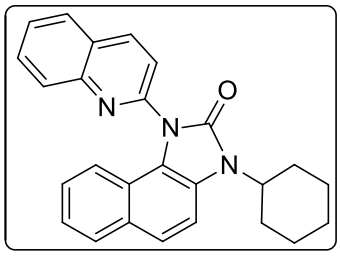
3-cyclohexyl-1-(5-methylpyrazin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3ad)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 70:30 hexane/ethyl acetate) afforded the desired product as a light brown solid (40.8 mg, 57% yield), mp 134-136 °C.

^{1}H NMR (400 MHz, $CDCl_3$): 8.89 (d, *J* = 0.8 Hz, 1H), 8.50 (s, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 8.8 Hz, 1H), 7.52 (d, *J* = 8.8 Hz, 1H), 7.32-7.28 (m, 1H), 7.24-7.19 (m, 1H), 6.98 (dd, J_1 = 8.8 Hz, J_2 = 0.8 Hz, 1H), 4.43-4.34 (m, 1H), 2.72 (s, 3H), 2.32-2.21(m, 2H), 1.98-1.93 (m, 4H), 1.78 (d, *J* = 12.4 Hz, 1H), 1.54-1.42 (m, 2H), 1.36-1.29 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$):δ 153.6, 153.5, 144.4, 143.4, 143.3, 129.9, 129.4, 126.4, 126.1, 123.72, 123.69, 121.5, 121.1, 120.3, 110.5, 53.9, 30.4, 26.1, 25.5, 21.4; HRMS (ESI, m/z) calcd. For $C_{22}H_{23}N_3O$ $[M+H]^+$: 359.1872; found: 359.1887.

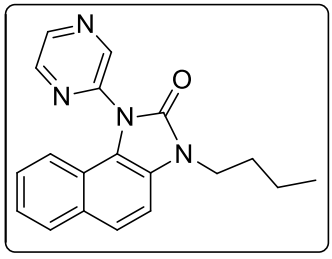
3-cyclohexyl-1-(quinolin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3ae)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a creamy white powder (57.4 mg, 73% yield), mp 188-190 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.42 (d, J = 8.4 Hz, 1H), 8.05-8.02 (m, 1H), 7.97 (dd, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.84-7.82 (m, 2H), 7.77-7.73 (m, 1H), 7.64-7.62 (m, 2H), 7.54 (d, J = 8.8 Hz, 1H), 7.28-7.24 (m, 1H), 7.08-7.07 (m, 2H), 4.46-4.38 (m, 1H), 2.35-2.25 (m, 2H), 2.01-1.93 (m, 4H), 1.78 (d, J = 13.2 Hz, 1H), 1.54-1.44 (m, 2H), 1.38-1.30 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.8, 149.6, 147.3, 138.9, 130.3, 130.0, 129.3, 129.1, 127.8, 127.6, 127.4, 126.3, 125.7, 123.5, 121.73, 121.68, 121.2, 120.7, 110.4, 53.7, 30.4, 26.2, 25.5; HRMS (ESI, m/z) calcd. For $C_{26}H_{24}N_3O$ $[M+H]^+$: 394.1919; found: 394.1920.

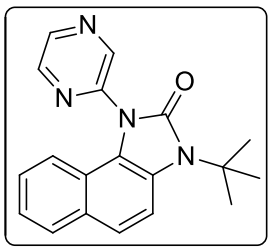
3-butyl-1-(pyrazin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3af)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 70:30 hexane/ethyl acetate) afforded the desired product as a light brown crystalline solid (41.3 mg, 65% yield), mp 140-142 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.07 (s, 1H), 8.69-8.63 (m, 2H), 7.86 (d, J = 8.0 Hz, 1H), 7.73 (d, J = 8.8 Hz, 1H), 7.36-7.30 (m, 2H), 7.27-7.23 (m, 1H), 7.04 (d, J = 8.4 Hz, 1H), 4.03 (t, J = 7.2 Hz, 2H), 1.86-1.79 (m, 2H), 1.50-1.41 (m, 2H), 0.97 (t, J = 7.6 Hz, 3H);^{13}C NMR (100 MHz, $CDCl_3$): δ 153.9, 146.9, 144.4, 143.7, 143.4, 130.4, 129.6, 127.2, 126.2, 124.6, 123.8, 121.3, 121.0, 120.4, 109.2, 41.5, 30.7, 20.2, 13.8; HRMS (ESI, m/z) calcd. For $C_{19}H_{18}N_4O$ $[M+H]^+$: 319.1559; found: 319.1558.

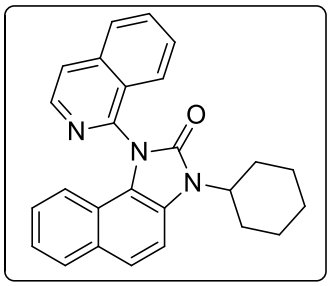
3-(tert-butyl)-1-(pyrazin-2-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3ag)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 70:30 hexane/ethyl acetate) afforded the desired product as a creamy white powder (62.3 mg, 98% yield), mp 148-150 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.00 (d, *J* = 1.6 Hz, 1H), 8.68 (d, *J* = 2.4 Hz, 1H), 8.63 (dd, J_1 = 2.4 Hz, J_2 = 1.2 Hz, 1H), 7.82 (d, *J* = 8.4 Hz, 1H), 7.76 (d, *J* = 9.2 Hz, 1H), 7.63 (d, *J* = 9.2 Hz, 1H), 7.32-7.28 (m, 1H), 7.21-7.16 (m, 1H), 6.85 (d, *J* = 8.4 Hz, 1H), 1.88 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.8, 147.2, 145.1, 143.8, 143.6, 129.7, 129.1, 127.2, 126.0, 123.9, 123.2, 121.9, 121.3, 119.9, 113.1, 59.1, 29.8; HRMS (ESI, m/z) calcd. For $C_{19}H_{19}N_4O$ $[M+H]^+$: 319.1559; found: 319.1563.

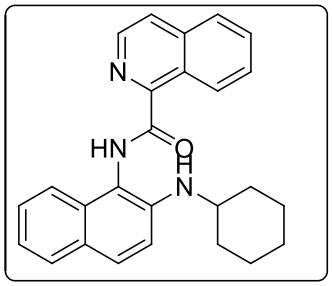
3-cyclohexyl-1-(isoquinolin-1-yl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (3ah)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 70:30 hexane/ethyl acetate) afforded the desired product as a white powder (23.6 mg, 30% yield), mp 184-186 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.60 (d, *J* = 5.6 Hz, 1H), 8.00 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 8.8 Hz, 1H), 7.91 (d, *J* = 6.0 Hz, 1H), 7.82-7.56 (m, 2H), 7.67 (d, *J* = 8.8 Hz, 1H), 7.61-7.57 (m, 2H), 7.22-7.18 (m, 1H), 6.99-6.95 (m, 1H), 6.44 (d, *J* = 8.4 Hz, 1H), 4.99-4.41 (m, 1H), 2.37-2.27 (m, 2H), 2.07-1.95 (m, 4H), 1.79 (d, *J* = 11.6 Hz, 1H), 1.56-1.44 (m, 2H), 1.39-1.31 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.8, 141.7, 138.5, 131.5, 129.8, 129.1, 128.9, 127.1, 126.7, 126.1, 125.6, 123.5, 123.1, 122.8, 120.4, 120.1, 110.6, 53.7, 30.7, 26.2, 25.5; HRMS (ESI, m/z) calcd. For $C_{26}H_{24}N_3O$ $[M+H]^+$: 394.1919; found: 394.1920.

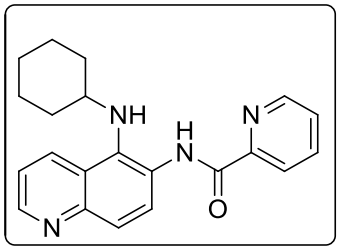
***N*-(2-(cyclohexylamino)naphthalen-1-yl)isoquinoline-1-carboxamide (3ah')**



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 85:15 hexane/ethyl acetate) afforded the desired product as a yellow fluffy solid (32.4 mg, 41% yield), mp 134-136 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.96 (S, 1H), 9.67-9.64 (m, 1H), 8.62 (d, J = 5.6 Hz, 1H), 7.92-7.90 (m, 2H), 7.81 (d, J = 8.4 Hz, 1H), 7.78- 7.69 (m, 4H), 7.43-7.39 (m, 1H), 7.28-7.21 (m, 2H), 3.52-3.46 (m, 1H), 2.12-2.09 (m, 2H), 1.79-1.74 (m, 2H), 1.64-1.60 (m, 1H), 1.42-1.19 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.2, 160.5, 154.8, 147.9, 140.5, 131.6, 130.8, 129.1, 128.3, 128.0, 127.4, 127.1, 127.0, 125.0, 122.3, 120.8, 110.9, 33.6, 25.9, 25.0; HRMS (ESI, m/z) calcd. For $C_{26}H_{26}N_3O$ $[M+H]^+$: 396.2076; found: 396.2078.

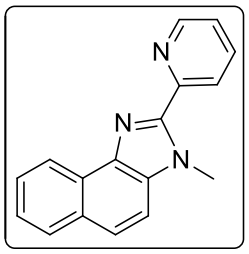
_N_-(5-(cyclohexylamino)quinolin-6-yl)picolinamide (3ai)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 80:20 hexane/ethyl acetate) afforded the desired product as a pale yellow solid (42.2 mg, 61% yield), mp 146-148 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 10.98 (s, 1H), 8.87 (d, J = 9.2 Hz, 1H), 8.81 (dd, J_1 = 4.0 Hz, J_2 = 1.6 Hz, 1H), 8.67-8.65 (m, 1H), 8.33 (dt, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 8.29-8.27 (m, 1H), 7.94-7.89 (m, 2H), 7.49-7.46 (m, 1H), 7.37 (dd, J_1 = 8.4 Hz, J_2 = 4.0 Hz, 1H), 3.35 (s, 1H), 3.02-2.95 (m, 1H), 2.06-2.02 (m, 2H), 1.73-1.68 (m, 2H), 1.59-1.55 (m, 1H), 1.39-1.30 (m, 2H), 1.67-1.08 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.3, 150.4, 148.9, 148.2, 146.2, 137.7, 131.6, 131.0, 130.6, 126.5, 125.9, 125.5, 123.6, 122.6, 120.8, 58.6, 34.8, 25.9, 25.4; HRMS (ESI, m/z) calcd. For $C_{21}H_{23}N_4O_3$ $[M+H]^+$: 347.1872; found: 347.1889.

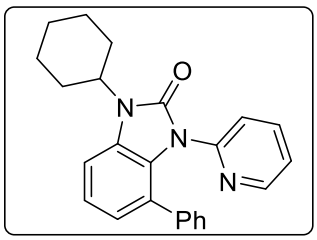
3-methyl-2-(pyridin-2-yl)-3H-naphtho[1,2-d]imidazole (3aj)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as a colorless crystalline solid (26 mg, 50% yield), mp 108-110 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.74 (d, J = 8.0 Hz, 1H), 8.70-8.68 (m, 1H), 8.51 (d, J = 8.0 Hz, 1H), 7.93 (d, J = 8.0 Hz, 1H), 7.85 (td, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 7.74 (d, J = 8.8 Hz, 1H), 7.66-7.62 (m, 1H), 7.56-7.48 (m, 2H), 7.33-7.30 (m, 1H), 4.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.9, 148.7, 148.3, 138.2, 136.9, 133.6, 130.6, 128.6, 127.2, 126.7, 124.8, 124.73, 124.67, 123.4, 122.1, 110.5, 33.1; HRMS (ESI, m/z) calcd. For $C_{17}H_{14}N_3$ $[M+H]^+$: 260.1188; found: 260.1196.

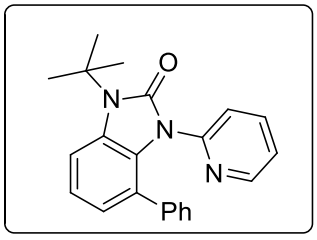
1-cyclohexyl-4-phenyl-3-(pyridin-2-yl)-1H-benzo[d]imidazol-2(3H)-one (3ak)



The general procedure 2 for imidazolone was followed. Column chromatography (SiO_2, eluting with 80:20 hexane/ethyl acetate) afforded the desired product as a white solid (29.5 mg, 40% yield), mp 196-198 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87-7.85 (m, 1H), 7.54 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.32 (d, J = 8.0 Hz, 1H), 7.25-7.17 (m, 2H), 7.06-6.89 (m, 7H), 4.38-4.29 (m, 1H), 2.32-2.22 (m, 2H), 1.94 (d, J = 10.8 Hz, 4H), 1.76 (d, J = 12.8 Hz, 1H), 1.51-1.42 (m, 2H), 1.35-1.25 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.5, 148.5, 148.1, 138.7, 137.3, 130.2, 128.3, 127.6, 126.4, 126.1, 125.7, 123.8, 122.2, 122.0, 121.9, 108.3, 53.6, 29.9, 26.1, 25.5; HRMS (ESI, m/z) calcd. For $C_{24}H_{24}N_3O$ $[M+H]^+$: 370.1919; found: 370.1913.

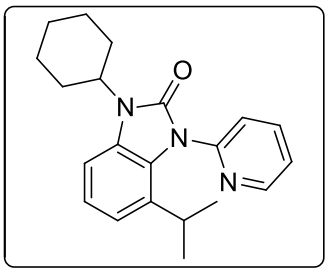
1-(tert-butyl)-4-phenyl-3-(pyridin-2-yl)-1H-benzo[d]imidazol-2(3H)-one (3al)



The general procedure 2 for imidazolone was followed was followed. Column chromatography (SiO_2, eluting with 80:20 hexane/ethyl acetate) afforded the desired product as a white solid (20.5 mg, 30% yield), mp 228-230 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 (d, *J* = 3.6 Hz, 1H), 7.51-7.46 (m, 2H), 7.23 (d, *J* = 7.6 Hz, 1H), 7.14 (t, *J* = 8.0 Hz, 1H), 7.03-6.89 (m, 7H), 1.86 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.8, 148.6, 148.1, 138.8, 137.2, 130.9, 128.4, 127.6, 126.3, 126.2, 125.6, 123.8, 122.8, 121.9, 121.5, 111.2, 58.7, 29.6; HRMS (ESI, m/z) calcd. For $C_{22}H_{22}N_3O$ $[M+H]^+$: 344.1763; found: 344.1752.

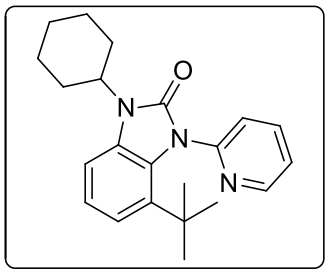
1-cyclohexyl-4-isopropyl-3-(pyridin-2-yl)-1H-benzo[d]imidazol-2(3H)-one (3am)



The general procedure 2 for imidazolone was followed was followed. Column chromatography (SiO_2, eluting with 80:20 hexane/ethyl acetate) afforded the desired product as a creamy white solid (43.5 mg, 65% yield), mp 164-166 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.58 (dd, J_1 = 4.8 Hz, J_2 = 2.0 Hz, 1H), 7.89 (td, J_1 = 7.6 Hz, J_2 = 2.0 Hz, 1H), 7.57 (d, *J* = 8.0 Hz, 1H), 7.37-7.34 (m, 1H), 7.12-7.04 (m, 2H), 7.00-6.98 (m, 1H), 4.29-4.21 (m, 1H), 2.46-2.36 (m, 1H), 2.27-2.16 (m, 2H), 1.89 (d, *J* = 11.2 Hz, 4H), 1.73 (d, *J* = 12.8 Hz, 1H), 1.48-1.38 (m, 2H), 1.32-1.24 (m, 1H), 1.02 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.9, 150.6, 149.0, 138.4, 132.4, 129.8, 126.1, 123.5, 123.4, 122.3, 119.0, 106.9, 53.5, 29.9, 27.7, 26.1, 25.5, 23.2; HRMS (ESI, m/z) calcd. For $C_{21}H_{26}N_3O$ $[M+H]^+$: 336.2076; found: 336.2067.

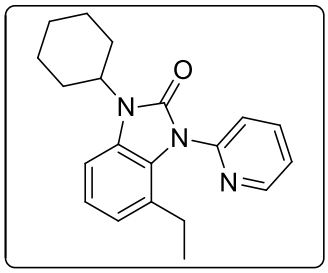
4-(tert-butyl)-1-cyclohexyl-3-(pyridin-2-yl)-1H-benzo[d]imidazol-2(3H)-one (3an)



The general procedure 2 for imidazolone was followed was followed. Column chromatography (SiO_2, eluting with 80:20 hexane/ethyl acetate) afforded the desired product as a creamy white solid (40 mg, 57% yield), mp 160-162 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.49 (dd, J_1 = 4.8 Hz, J_2 = 1.6 Hz, 1H), 7.86 (td, J_1 = 7.6 Hz, J_2 = 2.0 Hz, 1H), 7.60 (d, J = 8.0 Hz, 1H), 7.31-7.28 (m, 1H), 7.17 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.12-7.04 (m, 2H), 4.22-4.14 (m, 1H), 2.29-2.18 (m, 2H), 1.91-1.85 (m, 4H), 1.72 (d, J = 12.8 Hz, 1H), 1.46-1.35 (m, 2H), 1.30-1.22 (m, 1H), 1.07 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.6, 153.8, 148.7, 138.1, 136.5, 132.2, 127.3, 124.5, 123.2, 122.6, 121.7, 107.1, 53.8, 34.9, 31.4, 29.7, 26.2, 25.5; HRMS (ESI, m/z) calcd. For $C_{22}H_{28}N_3O$ $[M+H]^+$: 350.2232; found: 350.2225.

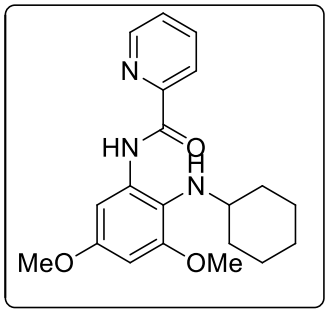
1-cyclohexyl-4-ethyl-3-(pyridin-2-yl)-1H-benzo[d]imidazol-2(3H)-one (3ao)



The general procedure 2 for imidazolone was followed was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as a creamy white solid (16 mg, 25% yield).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.60-8.58 (m, 1H), 7.89 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.58 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.37-7.34 (m, 1H), 7.09-7.04 (m, 2H), 6.89-6.88 (m, 1H), 4.30-4.22 (m, 1H), 2.26-2.19 (m, 4H), 1.89 (d, J = 9.6 Hz, 4H), 1.73 (d, J = 12.8 Hz, 1H), 1.48-1.38 (m, 2H), 1.32-1.24 (m, 1H), 0.89 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.8, 150.0, 148.9, 138.3, 129.7, 127.4, 126.6, 123.6, 123.4, 122.4, 122.1, 107.2, 53.5, 29.9, 26.1, 25.5, 25.1, 14.2; HRMS (ESI, m/z) calcd. For $C_{20}H_{24}N_3O$ $[M+H]^+$: 322.1919; found: 322.1913.

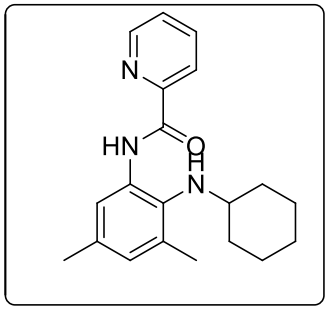
***N*-(2-(cyclohexylamino)-3,5-dimethoxyphenyl)picolinamide (3ap)**



The general procedure for amination in aniline system was followed was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as a gummy liquid (51 mg, 72% yield).

^{1}H NMR (400 MHz, $CDCl_3$): δ 11.04 (s, 1H), 8.62-8.60 (m, 1H), 8.25 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.89 (d, J = 2.8 Hz, 1H), 7.85 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.43-7.39 (m, 1H), 6.25 (d, J = 2.8 Hz, 1H), 3.82 (s, 3H), 3.77 (s, 3H), 2.74-2.68 (m, 1H), 1.93 (d, J = 12.8 Hz, 2H), 1.69-1.65 (m, 2H), 1.50 (s, 1H), 1.27-1.19 (m, 3H), 1.15-1.09 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.0, 156.8, 154.9, 150.6, 148.3, 137.5, 134.8, 126.2, 122.3, 119.5, 95.9, 94.9, 57.8, 55.7, 55.6, 34.2, 26.1, 25.3; HRMS (ESI, m/z) calcd. For $C_{20}H_{26}N_3O_3$ $[M+H]^+$: 356.1974; found: 356.1973.

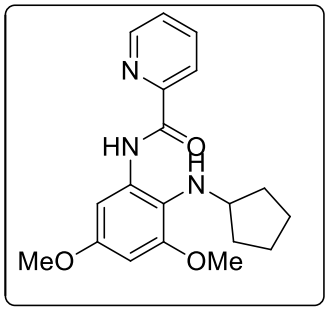
_N_-(2-(cyclohexylamino)-3,5-dimethylphenyl)picolinamide (3aq)



The general procedure for amination in aniline system was followed. Column chromatography (SiO_2, eluting with 95:5 hexane/ethyl acetate) afforded the desired product as a gummy liquid (33.5 mg, 52% yield).

^{1}H NMR (400 MHz, $CDCl_3$): δ 10.87 (s, 1H), 8.63-8.61 (m, 1H), 8.29 (dt, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 8.23 (s, 1H), 7.88 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.45-7.42 (m, 1H), 6.75 (m, 1H), 2.84-2.77 (m, 1H), 2.31 (s, 3H), 2.26 (s, 3H), 2.06-2.03 (m, 2H), 1.71-1.68 (m, 2H), 1.55-1.54 (m, 1H), 1.32-1.25 (m, 2H), 1.13-1.08 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.9, 150.8, 148.1, 137.5, 133.5, 133.2, 131.5, 126.6, 126.1, 122.4, 118.6, 58.0, 34.7, 25.9, 25.5, 21.3, 18.3; HRMS (ESI, m/z) calcd. For $C_{20}H_{26}N_3O$ $[M+H]^+$: 324.2076; found: 324.2066.

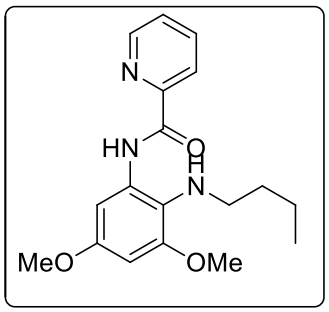
_N_-(2-(cyclopentylamino)-3,5-dimethoxyphenyl)picolinamide (3ar)



The general procedure for amination in aniline system was followed was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as a gummy liquid (34 mg, 50% yield).

^{1}H NMR (400 MHz, $CDCl_3$): δ 11.13 (s, 1H), 8.64-8.62 (m, 1H), 8.26 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.92 (d, J = 2.4 Hz, 1H), 7.86 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.45-7.41 (m, 1H), 6.26 (d, J = 2.8 Hz, 1H), 3.84 (s, 3H), 3.79 (s, 3H), 3.47 (quintet, J = 5.6 Hz, 1H), 1.80-1.70 (m, 4H), 1.56-1.46 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.1, 157.1, 155.2, 150.6, 148.3, 137.5, 135.3, 126.2, 122.3, 119.9, 95.8, 95.0, 60.8, 55.6, 33.2, 23.6; HRMS (ESI, m/z) calcd. For $C_{19}H_{24}N_3O_3$ $[M+H]^+$: 342.1818; found: 342.1819.

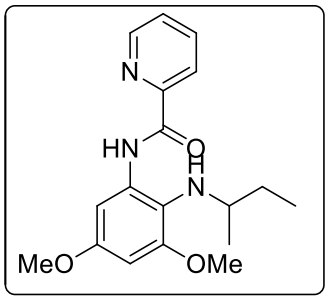
_N_-(2-(butylamino)-3,5-dimethoxyphenyl)picolinamide (3as)



The general procedure for amination in aniline system was followed was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as a gummy liquid (31 mg, 47% yield).

^{1}H NMR (400 MHz, $CDCl_3$): δ 11.03 (s, 1H), 8.65-8.63 (m, 1H), 8.28-8.25 (m, 1H), 7.90-7.86 (m, 2H), 7.46-7.43 (m, 1H), 6.28 (d, J = 2.4 Hz, 1H), 3.84 (s, 3H), 3.81 (s, 3H), 2.85 (t, J = 7.2 Hz, 2H), 1.61 (quintet, J = 7.2 Hz, 2H), 1.49-1.39 (m, 2H), 0.89 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.3, 157.1, 154.6, 150.5, 148.3, 137.5, 134.5, 126.3, 122.3, 96.2, 95.2, 55.8, 55.7, 49.8, 32.8, 20.3, 14.1; HRMS (ESI, m/z) calcd. For $C_{18}H_{24}N_3O_3$ $[M+H]^+$: 330.1818; found: 330.1822.

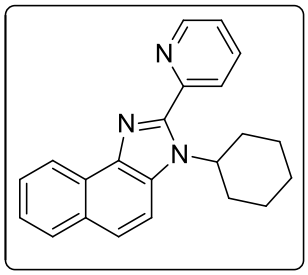
_N_-(2-(sec-butylamino)-3,5-dimethoxyphenyl)picolinamide (3at)



The general procedure for amination in aniline system was followed was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as a gummy liquid (27.6 mg, 42% yield).

^{1}H NMR (400 MHz, $CDCl_3$): δ 11.03 (s, 1H), 8.63-8.62 (m, 1H), 8.26 (dt, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 7.89-7.85 (m, 2H), 7.45-7.42 (m, 1H), 6.27 (d, J = 2.4 Hz, 1H), 3.84 (s, 3H), 3.79 (s, 3H), 2.98-2.90 (m, 1H), 1.68-1.57 (m, 1H), 1.47-1.39 (m, 1H), 1.04 (d, J = 6.4 Hz, 3H), 0.95 (t, J = 12.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.1, 156.9, 154.9, 150.6, 148.3, 137.5, 134.9, 126.2, 122.3, 96.1, 95.1, 55.7, 30.2, 19.9, 10.5; HRMS (ESI, m/z) calcd. For $C_{18}H_{24}N_3O_3$ $[M+H]^+$: 330.1818; found: 330.1826.

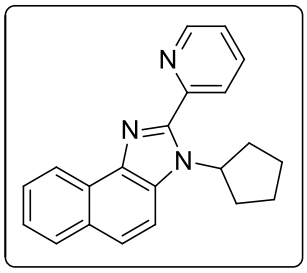
3-cyclohexyl-2-(pyridin-2-yl)-3H-naphtho[1,2-d]imidazole (5a)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as a white solid (58 mg, 88% yield), mp 88-90°C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.77 (d, J = 8.0 Hz, 1H), 8.72-8.70 (m, 1H), 8.36 (d, J = 8.0 Hz, 1H), 7.92 (d, J = 8.0 Hz, 1H), 7.89-7.83 (m, 2H), 7.68 (d, J = 8.8 Hz, 1H), 7.64-7.60 (m, 1H), 7.51-7.47 (m, 1H), 7.36-7.33 (m, 1H), 5.59-5.52 (m, 1H), 2.39-2.29 (m, 2H), 2.16-2.12 (m, 2H), 1.99-1.94 (m, 2H), 1.81 (d, J = 12.4 Hz, 1H), 1.52-1.34 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.9, 137.0, 131.3, 130.1, 128.6, 128.2, 126.6, 125.83, 125.8, 124.9, 123.81, 123.79, 123.55, 123.53, 122.2, 113.7, 57.2, 31.8, 26.3, 25.6; HRMS (ESI, m/z) calcd. For $C_{22}H_{22}N_3$ $[M+H]^+$: 328.1814; found: 328.1822.

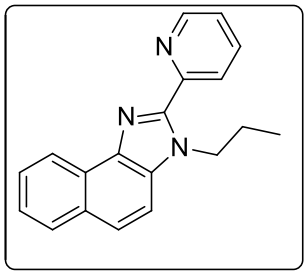
3-cyclopentyl-2-(pyridin-2-yl)-3H-naphtho[1,2-d]imidazole (5b)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as a light brown solid (50 mg, 80% yield), mp 146−148 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.73-8.72 (m, 1H), 8.51-8.48 (m, 1H), 8.25 (dt, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 8.02-7.98 (m, 2H), 7.81 (d, J = 9.2 Hz, 1H), 7.75 (d, J = 9.2 Hz, 1H), 7.62-7.58 (m, 1H), 7.50-7.46 (m, 2H), 6.09 (quintet, J = 9.2 Hz, 1H), 2.25-2.14 (m, 4H), 2.05-1.98 (m, 2H), 1.75-1.68 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.1, 149.4, 149.3, 138.9, 137.9, 130.9, 130.2, 128.9, 127.4, 126.9, 125.7, 125.3, 124.5, 124.1, 121.8, 113.7, 57.7, 31.0, 25.3; HRMS (ESI, m/z) calcd. For $C_{21}H_{20}N_3$ $[M+H]^+$: 314.1657; found: 314.1653.

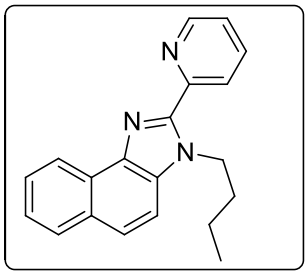
3-propyl-2-(pyridin-2-yl)-3H-naphtho[1,2-d]imidazole (5c)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as a light brown solid (40 mg, 70% yield), mp 58-60 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.75 (d, J = 8.0 Hz, 1H), 8.68-8.66 (m, 1H), 8.52 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.93 (d, J = 8.4 Hz, 1H), 7.84 (td, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.72 (d, J = 8.8 Hz, 1H), 7.66-7.62 (m, 1H), 7.55 (d, J = 8.8 Hz, 1H), 7.52-7.48 (m, 1H), 7.31-7.28 (m, 1H), 4.89 (t, J = 7.2 Hz, 2H), 1.98-1.89 (m, 2H), 0.93 (t, J = 7.2 Hz, 3H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.0, 148.7, 148.0, 138.2, 136.8, 133.1, 130.6, 128.5, 127.3, 126.6, 124.74, 124.66, 124.5, 123.3, 122.0, 110.9, 47.2, 24.0, 11.4; HRMS (ESI, m/z) calcd. For $C_{19}H_{18}N_3$ $[M+H]^+$: 288.1501; found: 288.1497.

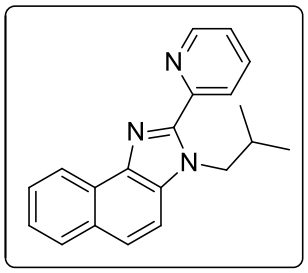
3-butyl-2-(pyridin-2-yl)-3H-naphtho[1,2-d]imidazole (5d)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as a light brown solid (50 mg, 83% yield), mp 158-160 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.69 (d, J = 8.4 Hz, 1H), 9.41 (d, J = 8.0 Hz, 1H), 8.78 (d, J = 4.4 Hz, 1H), 8.12 (td, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 7.97 (d, J = 2.0 Hz, 1H), 7.95 (d, J = 3.2 Hz, 1H), 7.86-7.82 (m, 1H), 7.68-7.61 (m, 2H), 7.54 (dd, J_1 = 7.6 Hz, J_2 = 4.8 Hz, 1H), 5.04 (t, J = 7.6 Hz, 2H), 1.98-1.94 (m, 2H), 1.44 (sextet, J = 7.6 Hz, 2H), 0.97 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.6, 143.7, 143.2, 138.4, 131.7, 130.1, 129.2, 129.0, 128.6, 128.2, 127.8, 126.5, 125.3, 109.6, 46.9, 32.0, 20.0, 13.6; HRMS (ESI, m/z) calcd. For $C_{20}H_{20}N$ $[M+H]^+$: 302.1657; found: 302.1663.

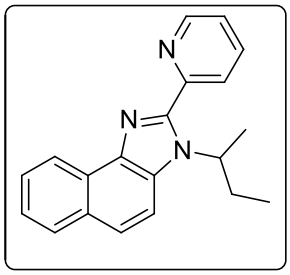
3-isobutyl-2-(pyridin-2-yl)-3H-naphtho[1,2-d]imidazole (5e)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as a brown solid (52 mg, 86% yield), mp 74-76 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.76-8.73 (m, 1H), 8.67-8.66 (m, 1H), 8.52 (dt, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.93 (d, J = 7.6 Hz, 1H), 7.84 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.72 (d, J = 8.8 Hz, 1H), 7.66-7.62 (m, 1H), 7.55 (d, J = 9.2 Hz, 1H), 7.52-7.47 (m, 1H), 7.32-7.28 (m, 1H), 4.79 (d, J = 7.2 Hz, 2H), 2.31-2.20 (m, 1H), 0.88 (d, J = 6.4 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.2, 148.5, 148.2, 138.2, 136.8, 133.5, 130.5, 128.5, 127.3, 126.6, 124.8, 124.7, 124.4, 123.3, 122.0, 111.3, 52.6, 30.1, 20.2; HRMS (ESI, m/z) calcd. For $C_{20}H_{20}N_3$ $[M+H]^+$: 302.1579; found: 302.1658.

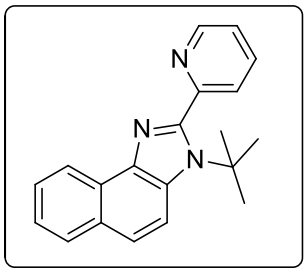
3-(sec-butyl)-2-(pyridin-2-yl)-3H-naphtho[1,2-d]imidazole (5f)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as a light brown solid (48 mg, 80% yield), mp 88-90 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.76 (d, J = 8.0 Hz, 1H), 8.70-8.68 (m, 1H), 8.37 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.92 (d, J = 8.0 Hz, 1H), 7.85 (td, J_1 = 7.6 Hz, J_2 = 2.0 Hz, 1H), 7.77 (d, J = 8.8 Hz, 1H), 7.67 (d, J = 8.8 Hz, 1H), 7.65-7.61 (m, 1H), 7.52-7.47 (m, 1H), 7.33-7.30 (m, 1H), 5.89-5.81 (m, 1H), 2.33-2.21 (m, 1H), 2.03-1.92 (m, 1H), 1.76 (d, J = 7.2 Hz, 3H), 0.74 (d, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.3, 149.2, 148.7, 139.1, 136.9, 131.1, 130.1, 128.3, 127.4, 126.5, 125.7, 124.8, 123.8, 123.4, 122.1, 113.3, 54.9, 28.8, 20.2, 11.2; HRMS (ESI, m/z) calcd. For $C_{20}H_{20}N_3$ $[M+H]^+$: 302.1579; found: 302.1660.

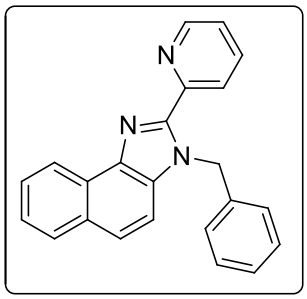
3-(tert-butyl)-2-(pyridin-2-yl)-3H-naphtho[1,2-d]imidazole (5g)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 80:20 hexane/ethyl acetate) afforded the desired product as light brown solid (43 mg, 72 % yield), mp 146-148 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.75 (d, J = 8.0 Hz, 1H), 8.71-8.69 (m, 1H), 7.92-7.88 (m, 2H), 7.84 (td, J_1 = 7.6 Hz, J_2 = 2.0 Hz, 1H), 7.77 (d, J = 7.6 Hz, 1H), 7.70 (d, J = 9.2 Hz, 1H), 7.61-7.57 (m, 1H), 7.51-7.47 (m, 1H), 7.40-7.37 (m, 1H), 1.70 (m, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.9, 136.6, 130.0, 128.0, 126.6, 125.9, 125.1, 124.0, 123.6, 122.5, 122.4, 114.9, 31.5; HRMS (ESI, m/z) calcd. For $C_{20}H_{20}N_3$ $[M+H]^+$:302.1579; found:302.1660.

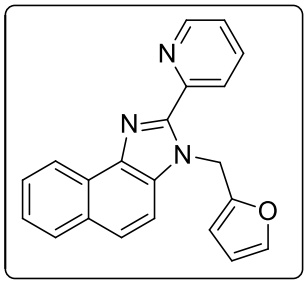
3-benzyl-2-(pyridin-2-yl)-3H-naphtho[1,2-d]imidazole (5h)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as a pale yellow solid (26.8 mg, 40% yield), mp 144-142 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.78 (d, J = 8.4 Hz, 1H), 8.62-8.60 (m, 1H), 8.57 (d, J = 8.0 Hz, 1H), 7.91 (d, J = 8.0 Hz, 1H), 7.84 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.67-7.63 (m, 2H), 7.52- 7.48 (m, 1H), 7.44 (d, J = 8.8 Hz, 1H), 7.30-7.27 (m, 1H), 7.22-7.13 (m, 5H), 6.30 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.6, 148.7, 147.9, 137.6, 136.9, 133.2, 130.7, 128.7, 128.5, 127.5, 127.1, 126.8, 124.9, 124.7, 123.6, 122.1, 111.1, 49.2; HRMS (ESI, m/z) calcd. For $C_{24}H_{18}N_3$ $[M+H]^+$: 336.1501; found: 336.1502.

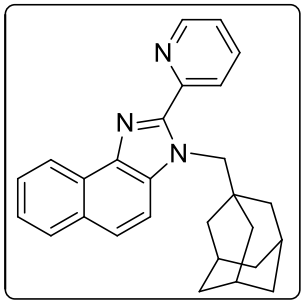
3-(furan-2-ylmethyl)-2-(pyridin-2-yl)-3H-naphtho[1,2-d]imidazole (5i)



The general procedure 1 for imidazolone was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as a yellow solid (24.7 mg, 38% yield), mp 122-124 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.75 (d, J = 8.4 Hz, 1H), 8.71-8.69 (m, 1H), 8.56 (d, J = 8.0 Hz, 1H), 7.93 (d, J = 8.4 Hz, 1H), 7.86 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.76-7.70 (m, 2H), 7.66-7.62 (m, 1H), 7.52-7.48 (m, 1H), 7.35-7.31 (m, 1H), 7.26 (dd, J_1 = 1.6 Hz, J_2 = 0.8 Hz, 1H), 6.29 (s, 2H), 6.22-6.19 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.8, 148.5, 147.4, 142.3, 137.0, 133.1, 130.7, 128.5, 127.0, 126.7, 124.9, 124,8, 123.6, 122.1, 111.1, 110.5, 108.3, 42.3; HRMS (ESI, m/z) calcd. For $C_{21}H_{16}N_3O$ $[M+H]^+$: 326.1293; found: 326.1294.

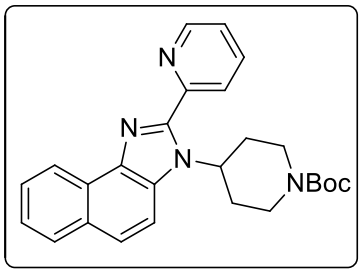
3-((3r,5r,7r)-adamantan-1-ylmethyl)-2-(pyridin-2-yl)-3H-naphtho[1,2-d]imidazole (5j)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as a creamy white solid (61 mg, 78% yield), mp 176−178 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.75 (d, J = 8.0 Hz, 1H), 8.67-8.65 (m, 1H), 8.41 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.93 (d, J = 8.0 Hz, 1H), 7.86 (td, J_1 = 7.6 Hz, J_2 = 2.0 Hz, 1H), 7.70 (d, J = 8.8 Hz, 1H), 7.66-7.62 (m, 1H), 7.59 (d, J = 8.8 Hz, 1H), 7.51-7.47 (m, 1H), 7.33-7.30 (m, 1H), 1.79 (s, 3H), 1.57-1.36 (m, 14H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.0, 149.1, 148.4, 137.1, 134.2, 130.4, 128.7, 128.4, 127.1, 126.7, 125.2, 124.8, 124.1, 123.5, 122.0, 112.4, 55.8, 41.0, 36.8, 36.6, 28.3; HRMS (ESI, m/z) calcd. For $C_{27}H_{28}N_3$ $[M+H]^+$: 394.2283; found: 394.2304.

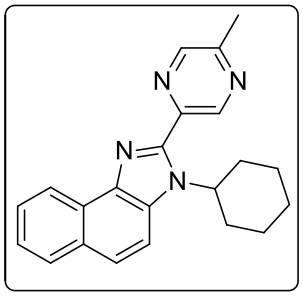
***tert*-butyl 4-(2-(pyridin-2-yl)-3H-naphtho[1,2-d]imidazol-3-yl)piperidine-1-carboxylate (5k)**



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 85:15 hexane/ethyl acetate) afforded the desired product as a creamy white solid (59 mg, 69 % yield), mp 112-114 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.76 (d, J = 8.0 Hz, 1H), 8.69-8.67 (m, 1H), 8.44 (d, J = 8.0 Hz, 1H), 7.93-7.87 (m, 2H), 7.74 (d, J = 9.2 Hz, 1H), 7.68 (d, J = 9.2 Hz, 1H), 7.65-7.61 (m, 1H), 7.52-7.48 (m, 1H), 7.37-7.34 (m, 1H), 5.94-5.85 (m, 1H), 4.35 (s, 2H), 2.88 (t, J = 9.6 Hz, 2H), 2.59-2.49 (m, 2H), 2.10 (dd, J_1 = 12.0 Hz, J_2 = 2.0 Hz, 2H), 1.53 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.9, 148.8, 148.3, 137.2, 131.1, 130.1, 128.3, 126.8, 125.8, 125.1, 124.3, 123.7, 122.1, 113.2, 80.0, 55.4, 30.8, 28.6; HRMS (ESI, m/z) calcd. For $C_{26}H_{29}N_4O_2$ $[M+H]^+$: 429.2291; found: 429.2285.

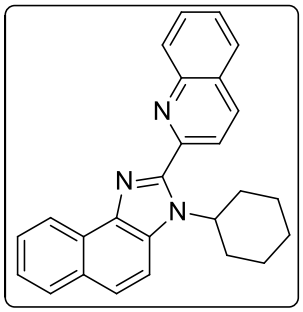
3-cyclohexyl-2-(5-methylpyrazin-2-yl)-3H-naphtho[1,2-d]imidazole (5l)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 85:15 hexane/ethyl acetate) afforded the desired product as a pale yellow powder (40.3 mg, 59% yield), mp 188-190 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.46 (s, 1H), 8.74 (d, *J* = 8.0 Hz, 1H), 8.51 (s, 1H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.82 (d, *J* = 9.2 Hz, 1H), 7.68 (d, *J* = 9.2 Hz, 1H), 7.65-7.61 (m, 1H), 7.52-7.48 (m, 1H), 5.45-5.37 (m, 1H), 2.65 (s, 3H), 2.38-2.29 (m, 2H), 2.11 (d, *J* = 11.2 Hz, 2H), 1.96 (d, *J* = 12.8 Hz, 2H), 1.81 (d, *J* = 11.6 Hz, 1H), 1.50-1.34 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.1, 146.17, 146.16, 145.7, 142.7, 131.5, 130.1, 128.3, 127.3, 126.7, 125.0, 124.1, 122.1, 113.5, 57.3, 31.9, 26.2, 25.6, 21.7; HRMS (ESI, m/z) calcd. For $C_{22}H_{23}N_4$ $[M+H]^+$: 343.1923; found: 343.1926.

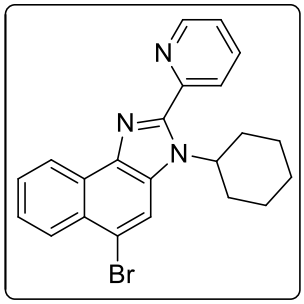
3-cyclohexyl-2-(quinolin-2-yl)-3H-naphtho[1,2-d]imidazole (5m)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as a creamy white solid (38 mg, 50% yield), mp 180-182 °C.

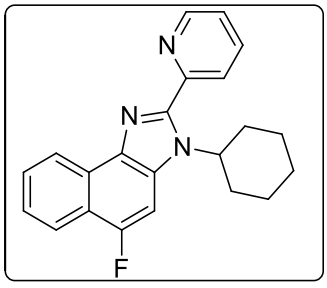
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.80 (d, *J* = 8.0 Hz, 1H), 8.61 (d, *J* = 8.8 Hz, 1H), 8.31 (d, *J* = 8.4 Hz, 1H), 8.11 (d, *J* = 8.8 Hz, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.89-7.86 (m, 2H), 7.78-7.73 (m, 1H), 7.70 (d, *J* = 9.2 Hz, 1H), 7.67-7.63 (m, 1H), 7.60-7.56 (m, 1H), 7.53-7.49 (m, 1H), 6.14-6.06 (m, 1H), 2.47-2.37 (m, 2H), 2.27-2.24 (m, 2H), 2.02 (d, *J* = 13.6 Hz, 2H), 1.85 (d, *J* = 12.8 Hz, 1H), 1.61-1.50 (m, 2H), 1.47-1.39 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.0, 148.3, 147.4, 136.6, 132.0, 130.1, 129.83, 129.79, 128.3, 127.8, 127.6, 127.5, 127.2, 126.6, 124.9, 124.1, 122.9, 122.2, 113.8, 57.5, 32.0, 26.5, 25.8; HRMS (ESI, m/z) calcd. For $C_{26}H_{24}N_3$ $[M+H]^+$: 378.1970; found: 378.1974.

5-bromo-3-cyclohexyl-2-(pyridin-2-yl)-3H-naphtho[1,2-d]imidazole (5n)



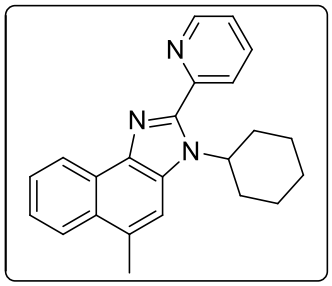
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as a creamy white powder (67 mg, 83% yield), mp 154-156 °C.
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.79 (d, J = 8.0 Hz, 1H), 8.72-8.70 (m, 1H), 8.35 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 8.31-8.29 (m, 1H), 8.19 (s, 1H), 7.88 (td, J_1 = 7.6 Hz, J_2 = 2.0 Hz, 1H), 7.69-7.65 (m, 1H), 7.62-7.57 (m, 1H), 7.38-7.34 (m, 1H), 5.59-5.52 (m, 1H), 2.33-2.23 (m, 2H), 2.16-2.12 (m, 2H), 2.00-1.96 (m, 2H), 1.82-1.79 (m, 1H), 1.52-1.37 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.9, 137.0, 131.2, 128.6, 128.2, 127.8, 127.3, 126.8, 126.1, 125.8, 123.7, 122.5, 117.6, 57.4, 31.9, 26.2, 25.5; HRMS (ESI, m/z) calcd. For $C_{22}H_{21}BrN_3$ $[M+H]^+$: 406.0919; found: 406.0926.

3-cyclohexyl-5-fluoro-2-(pyridin-2-yl)-3H-naphtho[1,2-d]imidazole (5o)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as a white solid (63.5 mg, 92% yield), mp 128-130 °C.
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.77 (d, J = 8.0 Hz, 1H), 8.71-8.69 (m, 1H), 8.34 (d, J = 8.0 Hz, 1H), 8.14 (d, J = 8.0 Hz, 1H), 7.87 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.69-7.66 (m, 1H), 7.57-7.53 (m, 2H), 7.36-7.33 (m, 1H), 5.61-5.23 (m, 1H), 2.31-2.21 (m, 2H), 2.15-2.11 (m, 2H), 1.99-1.95 (m, 2H), 1.82-1.78 (m, 1H), 1.52-1.33 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.7 (d, J = 245.4 Hz), 151.0, 148.9, 136.9, 129.9 (d, J = 13.4 Hz), 128.6, 127.6, 127.4 (d, J = 5.3 Hz), 125.5, 125.0, 123.5, 122.1, 121.3 (d, J = 5.7 Hz), 120.8 (d, J = 18.2 Hz), 98.2 (d, J = 27.3 Hz), 57.2, 31.7, 26.2, 25.6; ^{19}F NMR (376 MHz, $CDCl_3$): δ -126.54 (s, 1F); HRMS (ESI, m/z) calcd. For $C_{22}H_{21}FN_3$ $[M+H]^+$: 346.1720; found: 346.1719.

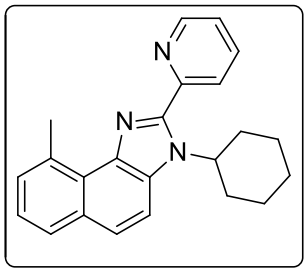
3-cyclohexyl-5-methyl-2-(pyridin-2-yl)-3H-naphtho[1,2-d]imidazole (5p)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as creamy white solid (58 mg, 85% yield), mp 132-134 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.95 (s, 1H), 8.73-8.71 (m, 1H), 8.48 (s, 1H), 8.04 (d, J = 8.4 Hz, 1H), 7.93-7.89 (m, 1H), 7.69-7.65 (m, 2H), 7.58-7.55 (m, 1H), 7.38-7.35 (m, 1H), 5.59-5.50 (m, 1H), 2.81 (s, 3H), 2.40-2.31 (m, 2H), 2.16-2.12 (m, 2H), 1.99-1.96 (m, 2H), 1.83-1.79 (m, 1H), 1.52-1.37 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.2, 148.8, 148.0, 137.9, 136.9, 131.1, 130.1, 129.4, 127.3, 126.3, 125.6, 124.7, 123.3, 122.6, 113.9, 57.1, 31.9, 26.3, 25.6, 20.7; HRMS (ESI, m/z) calcd. For $C_{23}H_{24}N_3$ $[M+H]^+$: 342.1970; found: 342.1971.

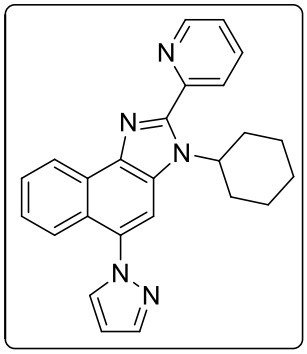
3-cyclohexyl-9-methyl-2-(pyridin-2-yl)-3H-naphtho[1,2-d]imidazole (5q)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/ethyl acetate) afforded the desired product as a creamy white solid (54.5 mg, 80% yield), mp 140-142 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.70-8.68 (m, 1H), 8.42 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.87-7.82 (m, 2H), 7.79-7.76 (m, 1H), 7.67 (d, J = 8.8 Hz, 1H), 7.43-7.36 (m, 2H), 7.32- 7.29 (m, 1H), 5.86-5.78 (m, 1H), 3.29 (s, 3H), 2.43-2.33 (m, 2H), 2.16-2.11 (m, 2H), 1.99- 1.95 (m, 2H), 1.81 (d, J = 11.2 Hz, 1H), 1.55-1.35 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.6, 147.3, 136.8, 135.0, 132.53, 132.48, 131.0, 128.5, 126.5, 126.4, 125.7, 124.6, 124.2, 123.2, 113.5, 56.9, 31.7, 26.3, 25.7, 23.8; HRMS (ESI, m/z) calcd. For $C_{23}H_{24}N_3$ $[M+H]^+$: 342.1970; found: 342.1973.

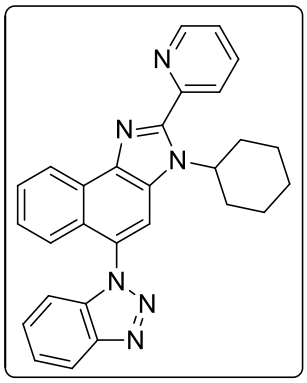
3-cyclohexyl-5-(1H-pyrazol-1-yl)-2-(pyridin-2-yl)-3H-naphtho[1,2-d]imidazole (5r)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 80:20 hexane/ethyl acetate) afforded the desired product as a creamy white solid (43 mg, 55% yield), mp 174-176 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.85 (d, *J* = 8.0 Hz, 1H), 8.73-8.71 (m, 1H), 8.38 (d, *J* = 8.0 Hz, 1H), 7.95 (s, 1H), 7.92-7.84 (m, 3H), 7.68-7.64 (m, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.50-7.46 (m, 1H), 7.39-7.35 (m, 1H), 6.58 (t, *J* = 2.0 Hz, 1H), 5.62-5.54 (m, 1H), 2.34-2.23 (m, 2H), 2.17-2.13 (m, 2H), 1.96-1.91 (m, 2H), 1.76 (d, *J* = 12.4 Hz, 1H), 1.50-1.40 (m, 2H), 1.37-1.29 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.9, 149.0, 140.8, 137.1, 133.5, 132.5, 129.9, 127.3, 127.2, 126.6, 126.0, 125.9, 123.8, 123.6, 122.5, 112.1, 106.5, 57.5, 32.0, 26.2, 25.4; HRMS (ESI, m/z) calcd. For $C_{25}H_{24}N_5$ $[M+H]^+$: 394.2032; found: 394.2036.

5-(1H-benzo[d][1,2,3]triazol-1-yl)-3-cyclohexyl-2-(pyridin-2-yl)-3H-naphtho[1,2-d]imidazole (5s)

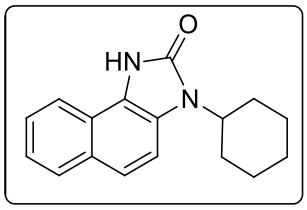


The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 80:20 hexane/ethyl acetate) afforded the desired product as a creamy white solid (43.5 mg, 49% yield), mp 214-216 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.90 (d, *J* = 8.0 Hz, 1H), 8.74-8.73 (m, 1H), 8.40 (d, *J* = 7.6 Hz, 1H), 8.26-8.21 (m, 1H), 8.07 (s, 1H), 7.91 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.71-7.67 (m, 1H), 7.51-7.46 (m, 2H), 7.45-7.37 (m, 2H), 7.30-7.27 (m, 2H), 5.67-5.59 (m, 1H), 2.29-2.16 (m, 4H),

1.91 (d, *J* = 13.2 Hz, 2H), 1.72 (d, *J* = 12.8 Hz, 1H), 1.49-1.38 (m, 2H), 1.31-1.20 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.6, 150.5, 149.0, 145.8, 140.3, 137.1, 135.4, 130.0, 128.3, 128.1, 127.6, 127.5, 126.2, 125.96, 125.92, 124.4, 123.9, 123.2, 122.8, 120.3, 113.6, 110.7, 57.6, 32.1, 26.1, 25.3; HRMS (ESI, m/z) calcd. For $C_{28}H_{25}N_6$ $[M+H]^+$: 445.2141; found: 445.2140.

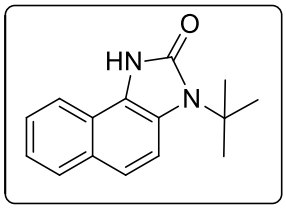
3-cyclohexyl-1H-naphtho[1,2-d]imidazol-2(3H)-one (8a)



Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a light pink solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 11.40 (s, 1H), 8.04 (d, *J* = 8.0 Hz, 1H) 7.85 (d, *J* = 8.4 Hz, 1H), 7.58-7.53 (m, 2H), 7.50 (d, *J* = 8.8 Hz, 1H), 7.41-7.37 (m, 1H), 4.51-4.24 (m, 1H), 2.28-2.18 (m, 2H), 1.99-1.94 (m, 4H), 1.81 (d, *J* = 12.8 Hz, 1H), 1.59-1.48 (m, 2H), 1.39-1.32 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.4, 129.1, 128.6, 126.5, 124.9, 124.2, 122.5, 121.4, 120.6, 119.9, 110.9, 53.1, 30.8, 26.1, 25.5; HRMS (ESI, m/z) calcd. For $C_{17}H_{19}N_2O$ $[M+H]^+$: 267.1497; found: 267.1506.

3-(*tert*-butyl)-1H-naphtho[1,2-d]imidazol-2(3H)-one (8b)



Column chromatography (SiO_2, eluting with 75:25 hexane/ethyl acetate) afforded the desired product as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 11.71 (s, 1H), 8.05 (d, *J* = 8.4 Hz, 1H) 7.83 (d, *J* = 8.4 Hz, 1H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.54-7-49 (m, 2H), 7.41-7.39 (m, 1H), 1.91 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.3, 128.8, 128.3, 126.2, 125.7, 124.3, 123.2, 120.7, 120.6, 119.7, 113.3, 58.6, 29.8; HRMS (ESI, m/z) calcd. For $C_{15}H_{17}N_2O$ $[M+H]^+$: 241.1341; found: 241.1344.

References.

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2) Phanstiel, O.; Wang, Q. X.; Powell, D. H.; Ospina, M. P.; Leeson, B. A., *J. Org. Chem.*, 1999, **64**, 803-806.
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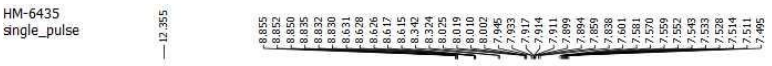
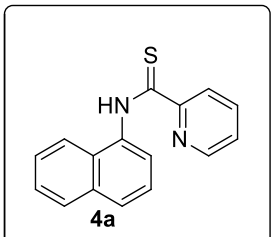
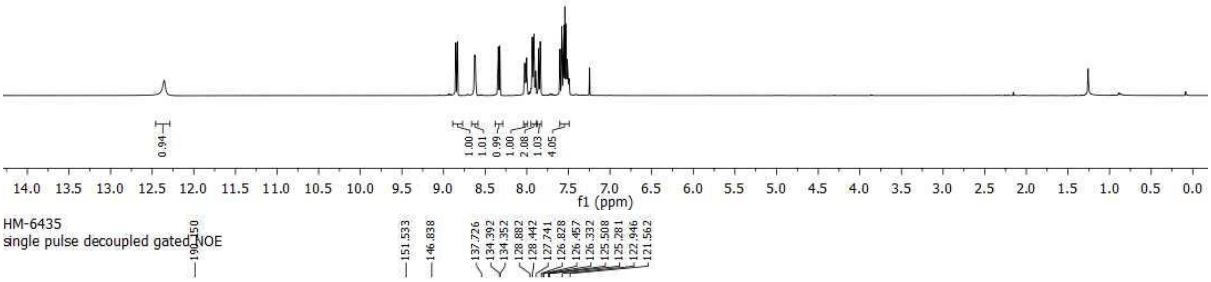
5) Beesu, M.; Malladi, S. S.; Fox, L. M.; Jones, C. D.; Dixit, A.; David, S. A., *J. Med. Chem.*, 2014, **57**, 7325-7341.
6) Smout, V.; Peschiulli, A.; Verbeeck, S.; Mitchell, E. A.; Herrebout, W.; Bultinck, P.; Vande Velde, C. M. L.; Berthelot, D.; Meerpoel, L.; Maes, B. U. W., *J. Org. Chem.*, 2013, **78**, 9803-9814.

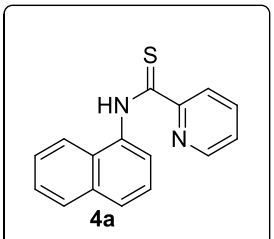
^{1}H NMR and ^{13}C NMR Spectra:



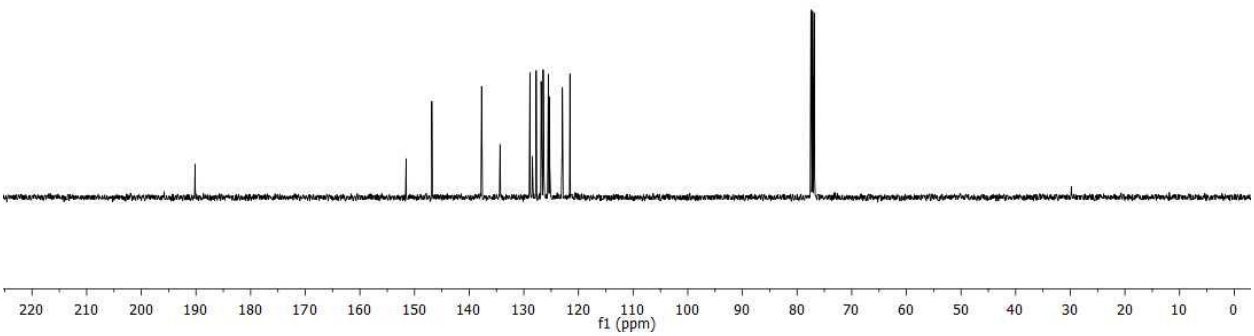


400 MHz, $CDCl_3$

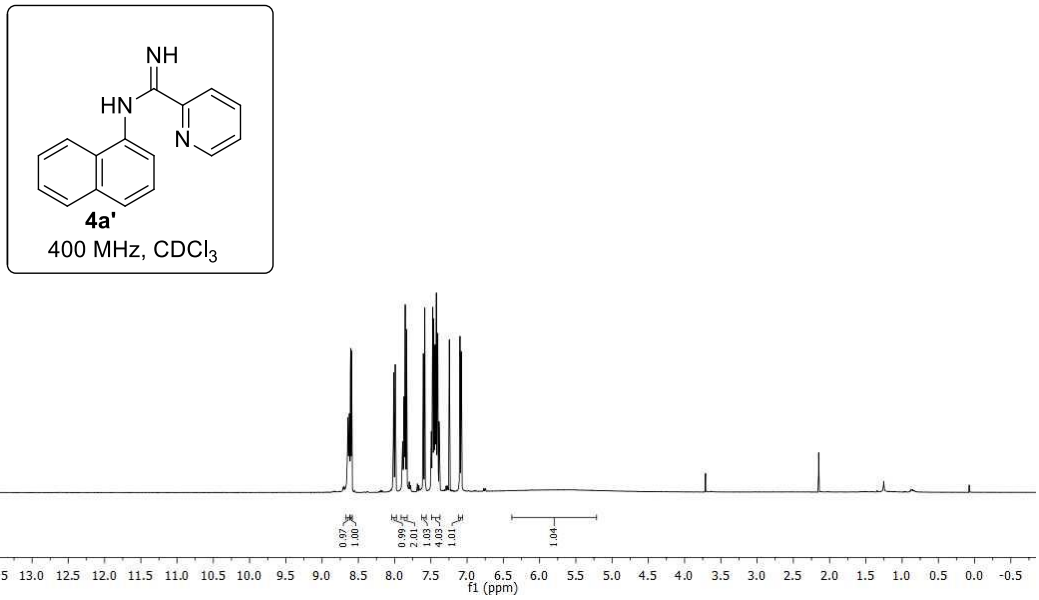




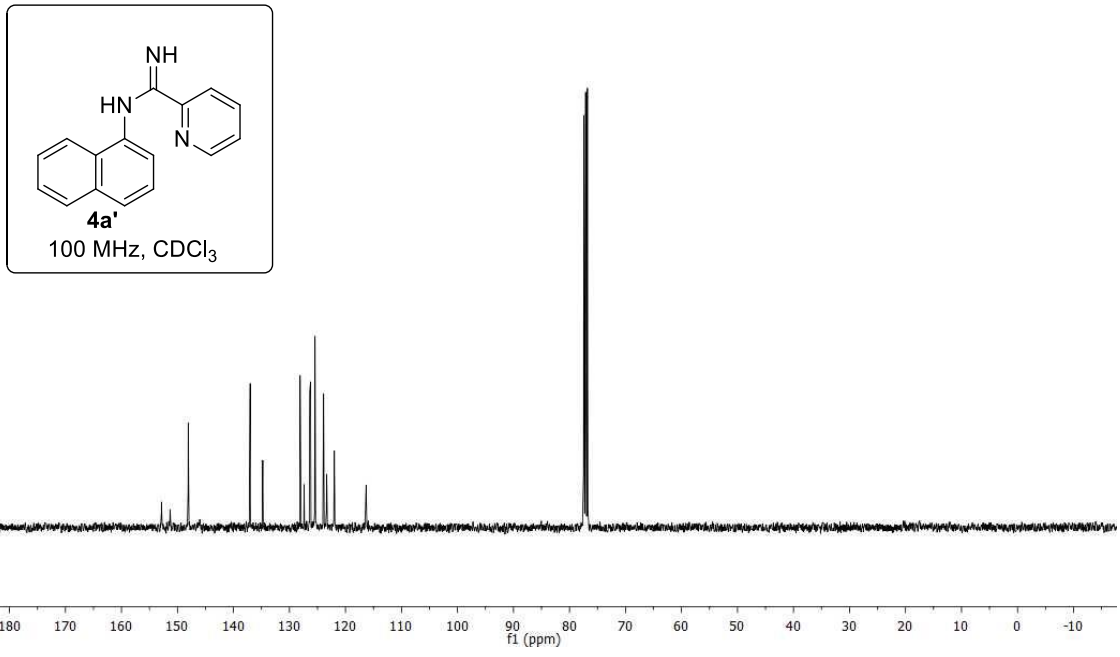
100 MHz, $CDCl_3$

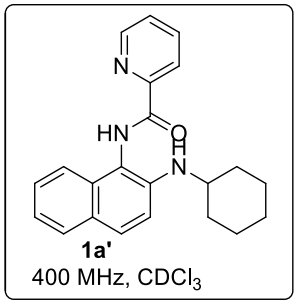



HM-682
single_pulse


NH
HN
N
4a'
400 MHz, CDCl3
f1 (ppm)

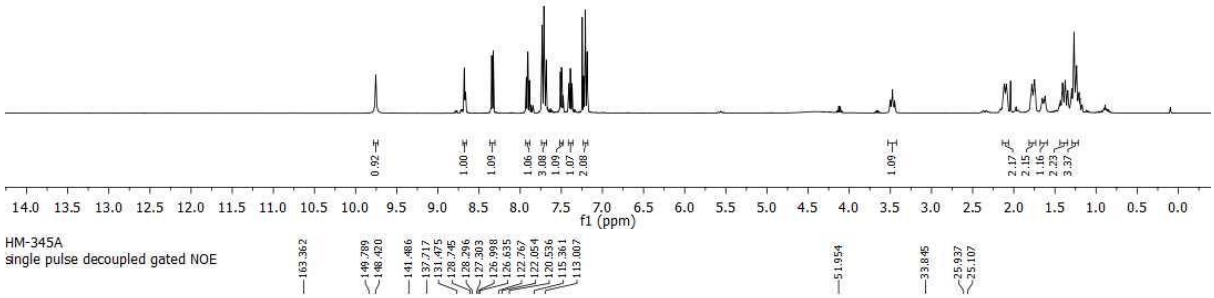

HM-682
single pulse decoupled gated NOE

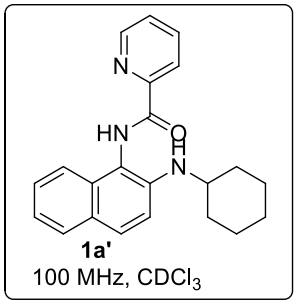

NH
HN
N
4a'
100 MHz, CDCl3
f1 (ppm)



1a'

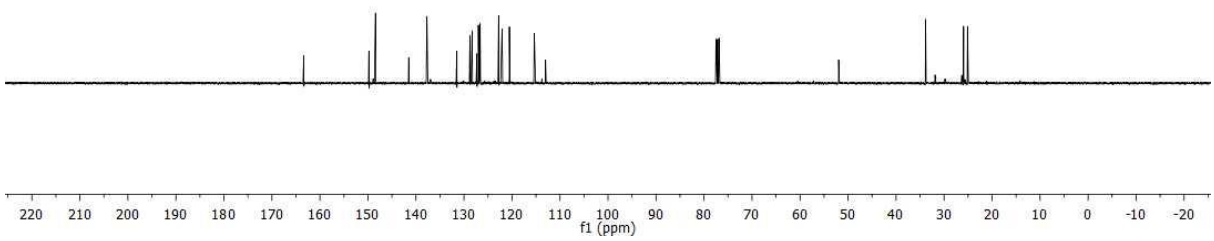
400 MHz, $CDCl_3$

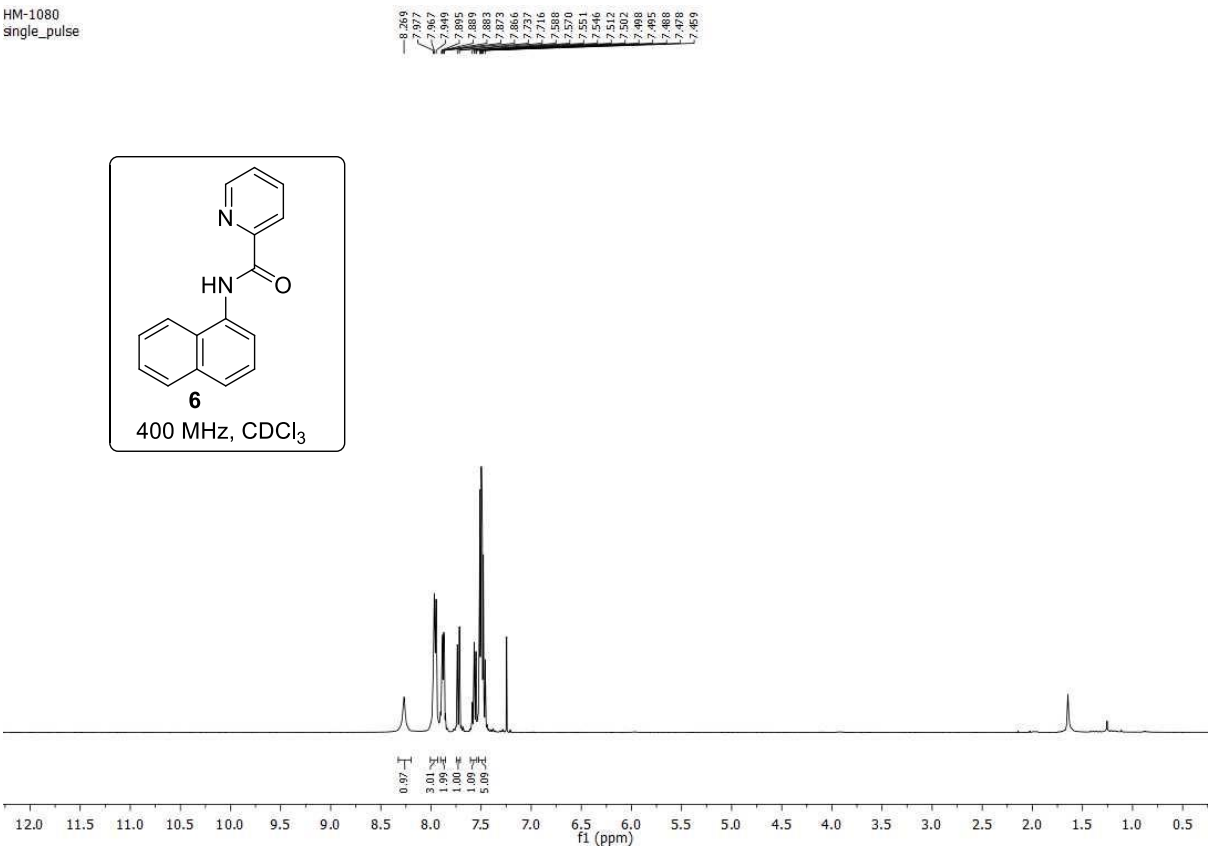




1a'

100 MHz, $CDCl_3$




HM-1080
single_pulse
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7.977
7.967
7.949
7.895
7.889
7.883
7.873
7.866
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7.570
7.551
7.546
7.512
7.502
7.498
7.495
7.488
7.478
7.459
N
HN
O
6
400 MHz, CDCl3
0.97
3.01
1.99
1.00
1.09
5.09
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


HM-1080
single pulse decoupled gated NOE
166.407
134.915
134.258
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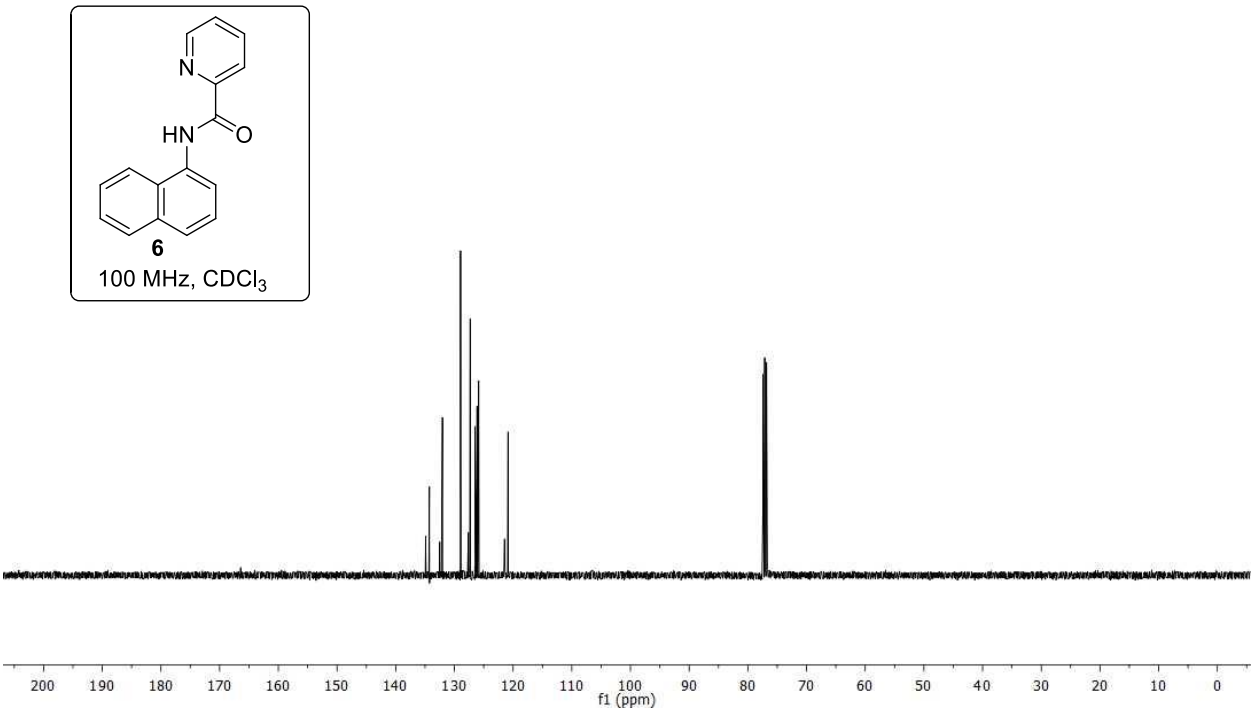
120.862


N
HN
O
6
100 MHz, CDCl3
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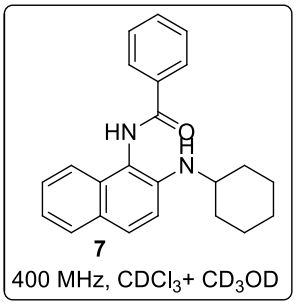
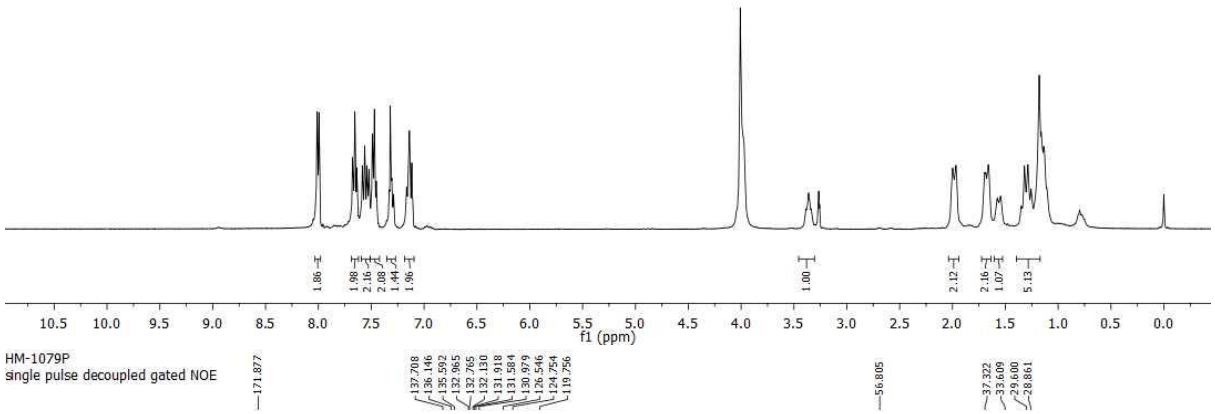
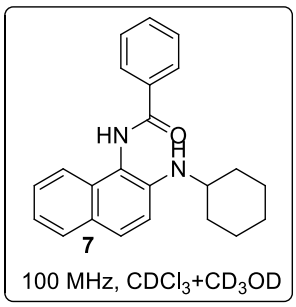
f1 (ppm)


HM-1079P
single_pulse


HN
O
N
7
400 MHz, CDCl3+ CD3OD

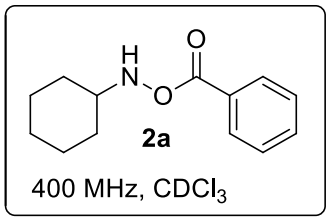

1.86
1.98
2.16
2.08
1.44
1.96
1.00
2.12
2.16
1.07
5.13
f1 (ppm)

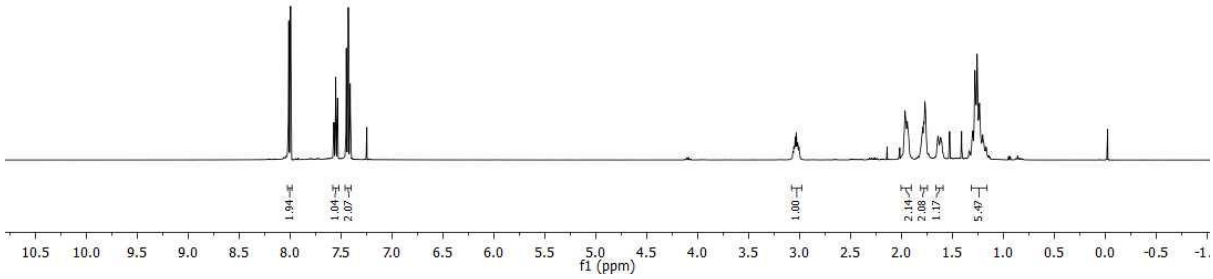
HM-1079P
single pulse decoupled gated NOE


HN
O
N
7
100 MHz, CDCl3+CD3OD

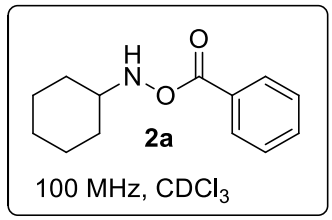
f1 (ppm)

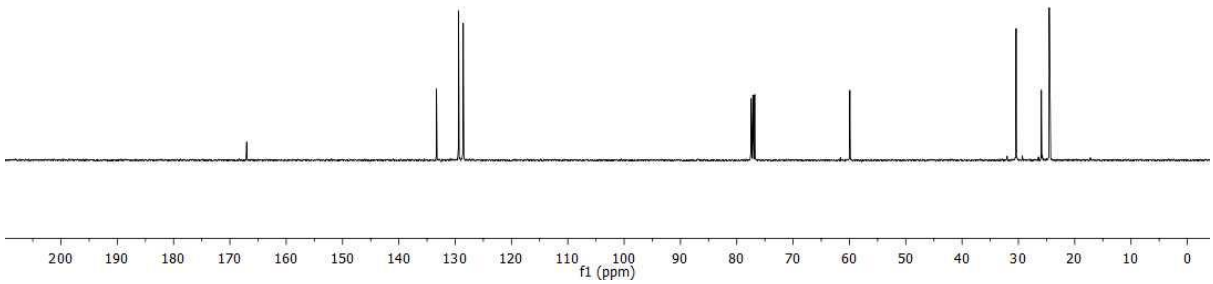
HM-1587
single_pulse

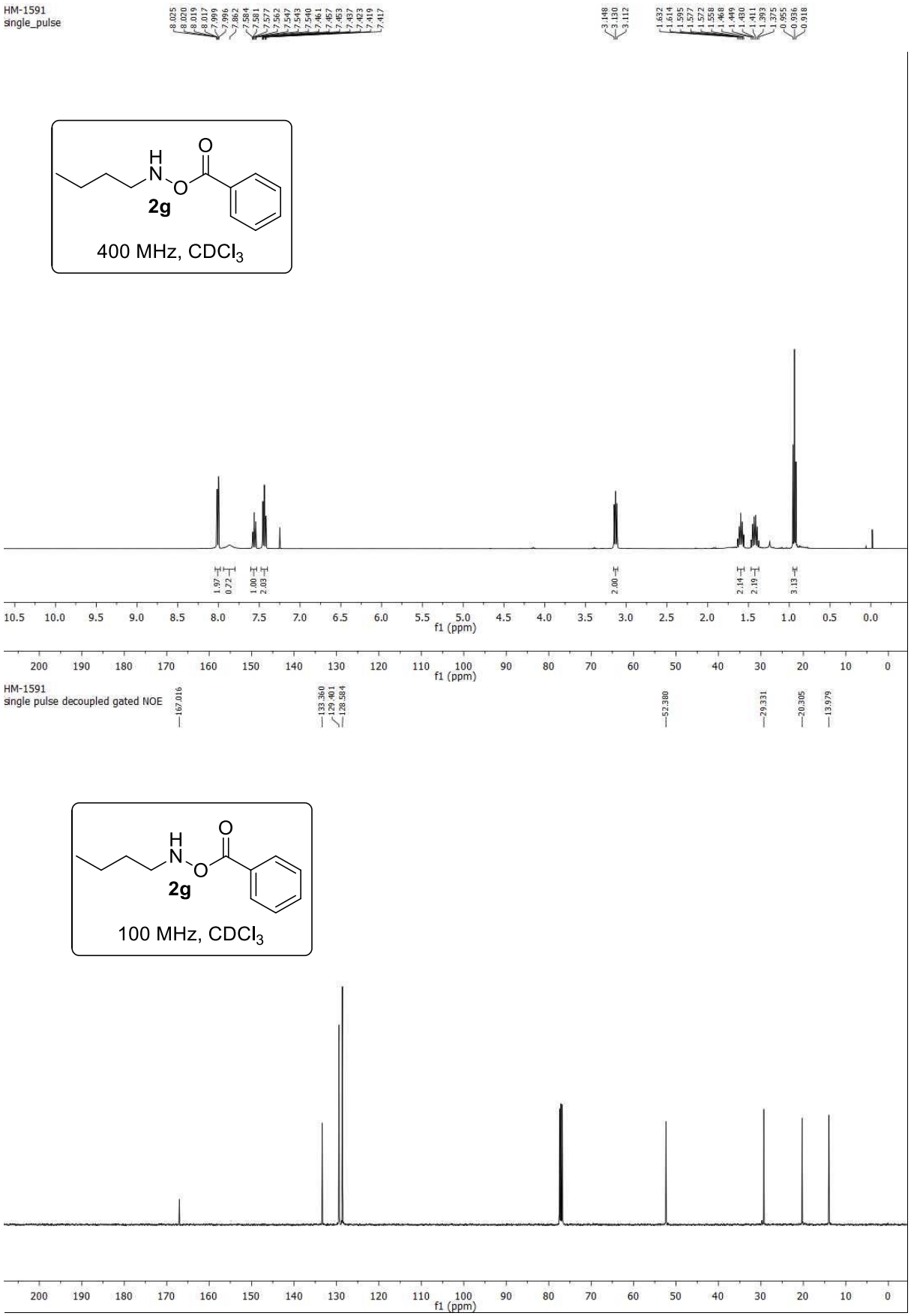


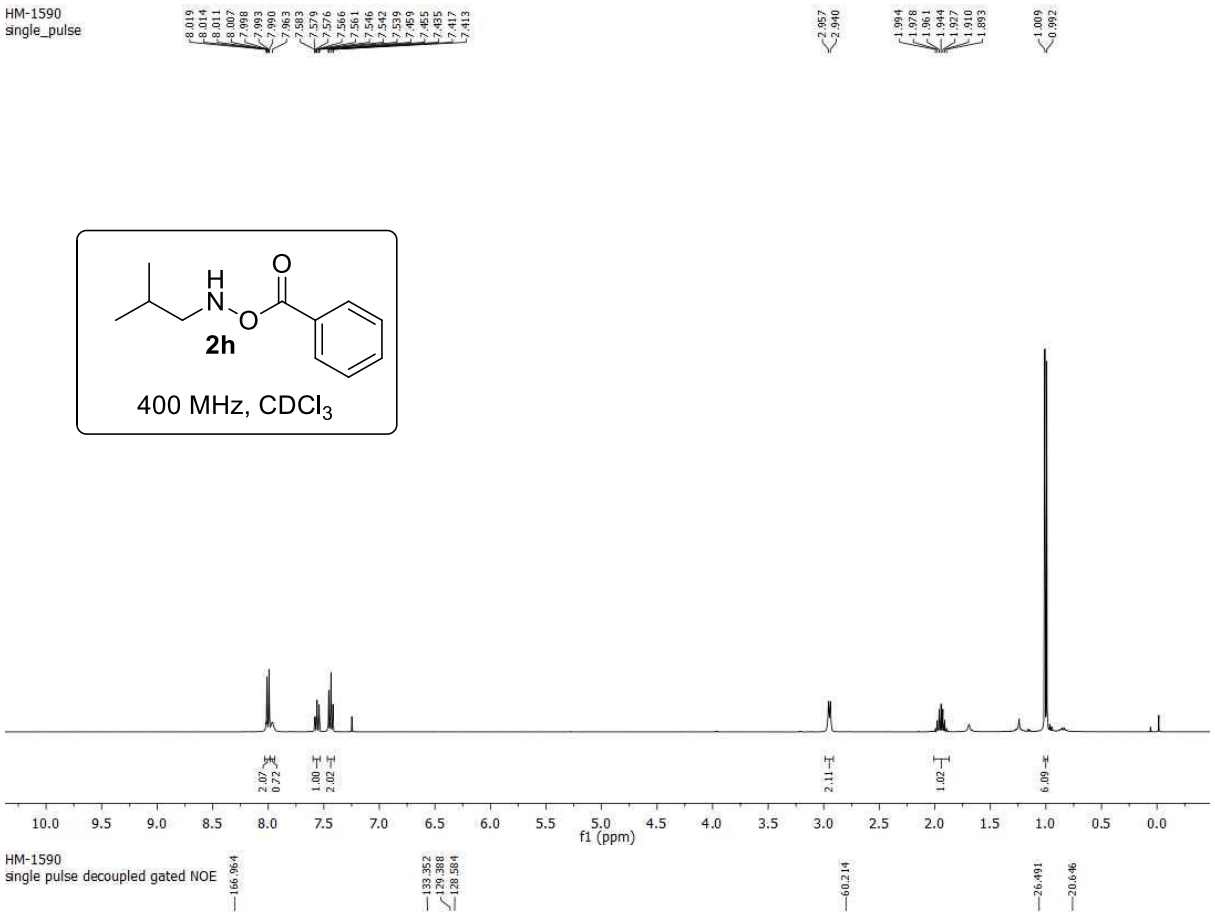


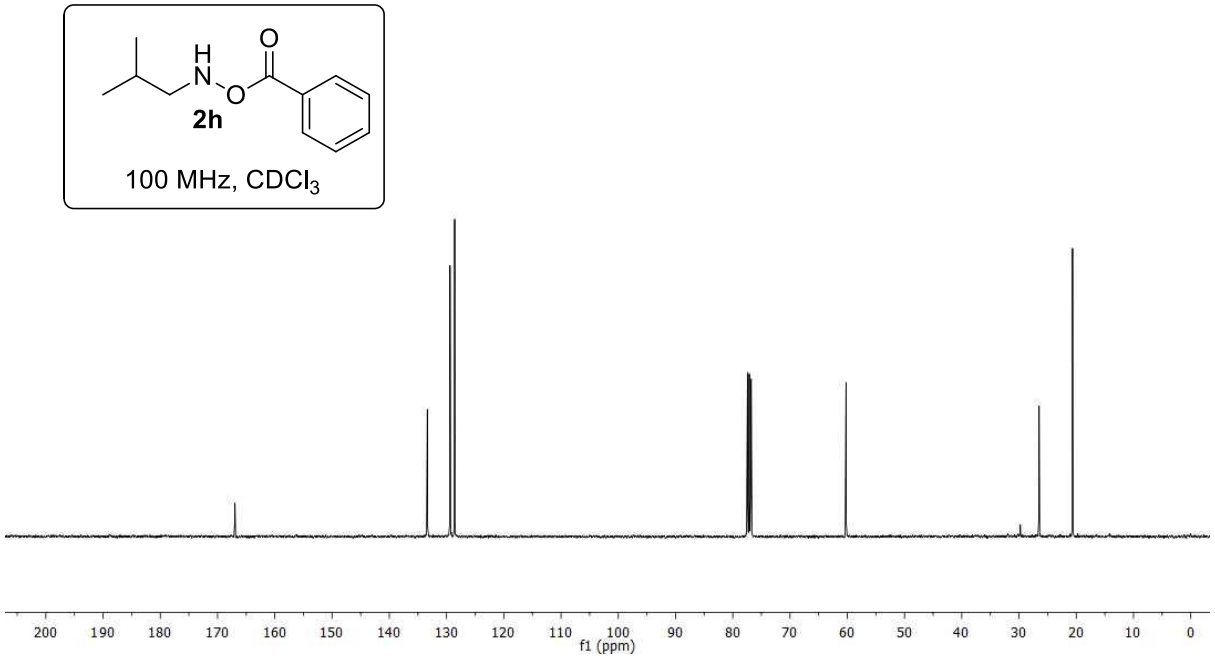
HM-1587
single pulse decoupled gated NOE



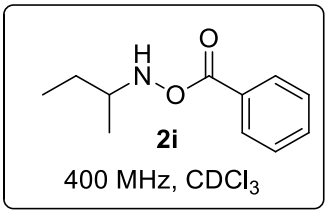


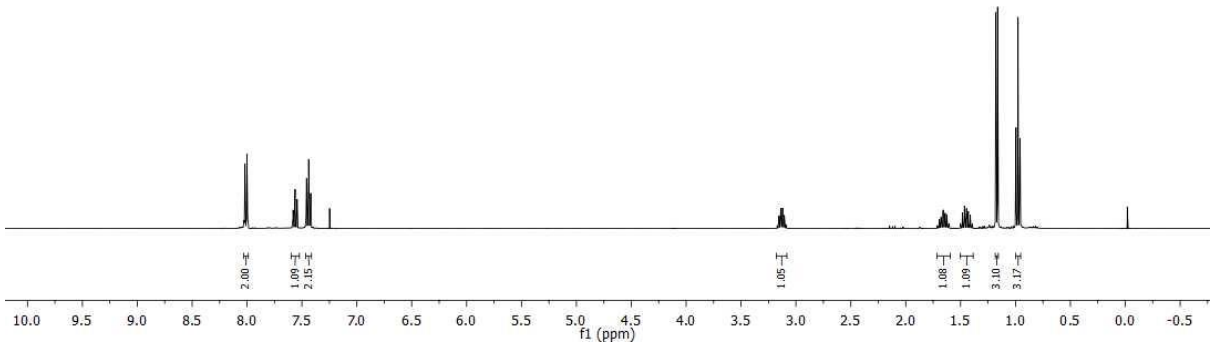

HM-1591
single_pulse
2g
400 MHz, CDCl3
f1 (ppm)
HM-1591
single pulse decoupled gated NOE
2g
100 MHz, CDCl3
f1 (ppm)


HM-1590
single_pulse
2h
400 MHz, CDCl3
f1 (ppm)
HM-1590
single pulse decoupled gated NOE

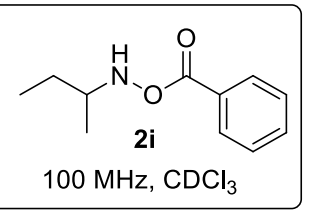

2h
100 MHz, CDCl3
f1 (ppm)

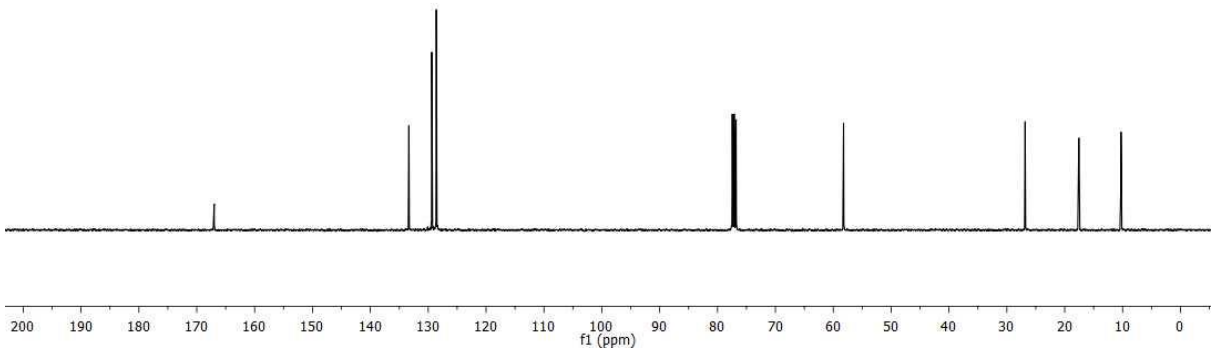

BHM-1588
single_pulse
8.026
8.022
8.019
8.001
7.997
7.584
7.581
7.577
7.567
7.562
7.557
7.547
7.543
7.540
7.461
7.458
7.454
7.441
7.438
7.420
7.419
7.416
3.170
3.154
3.138
3.122
3.106
3.090
1.712
1.693
1.674
1.644
1.625
1.606
1.502
1.483
1.465
1.448
1.430
1.412
1.394
1.179
1.163
0.995
0.977
0.958


H
N
O
O
2i
400 MHz, CDCl3

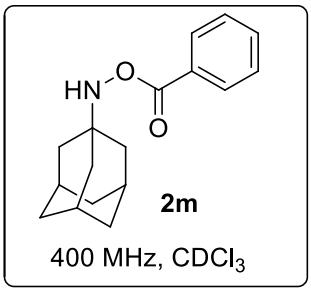

2.00
1.09
2.15
1.05
1.08
1.09
3.10
3.17
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

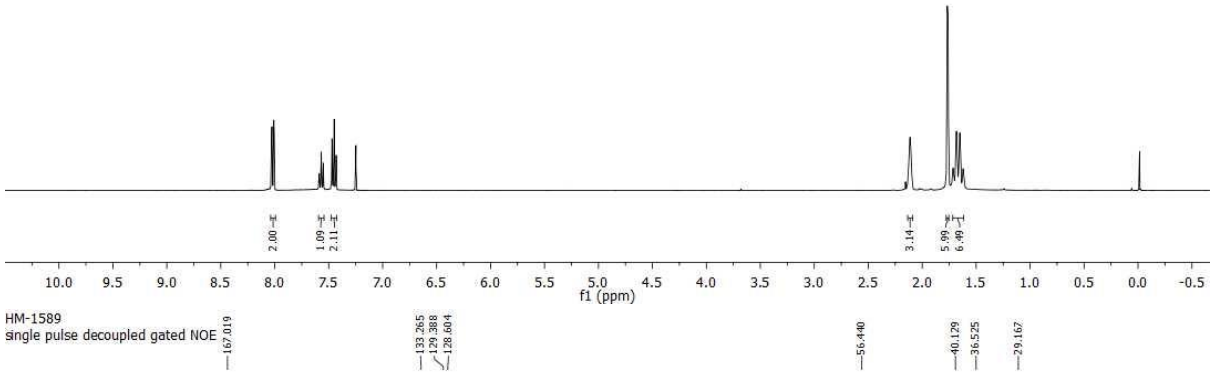

HM-1588
single pulse decoupled gated NOE
166.993
133.338
129.384
128.595
58.220
26.839
17.558
10.268


H
N
O
O
2i
100 MHz, CDCl3

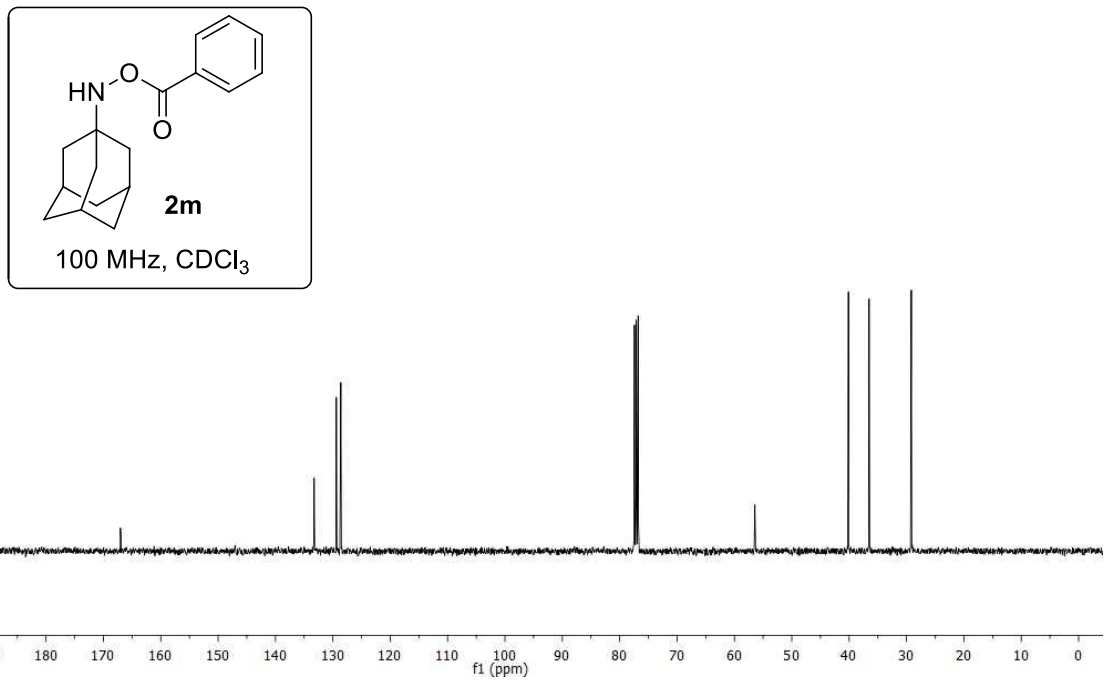

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

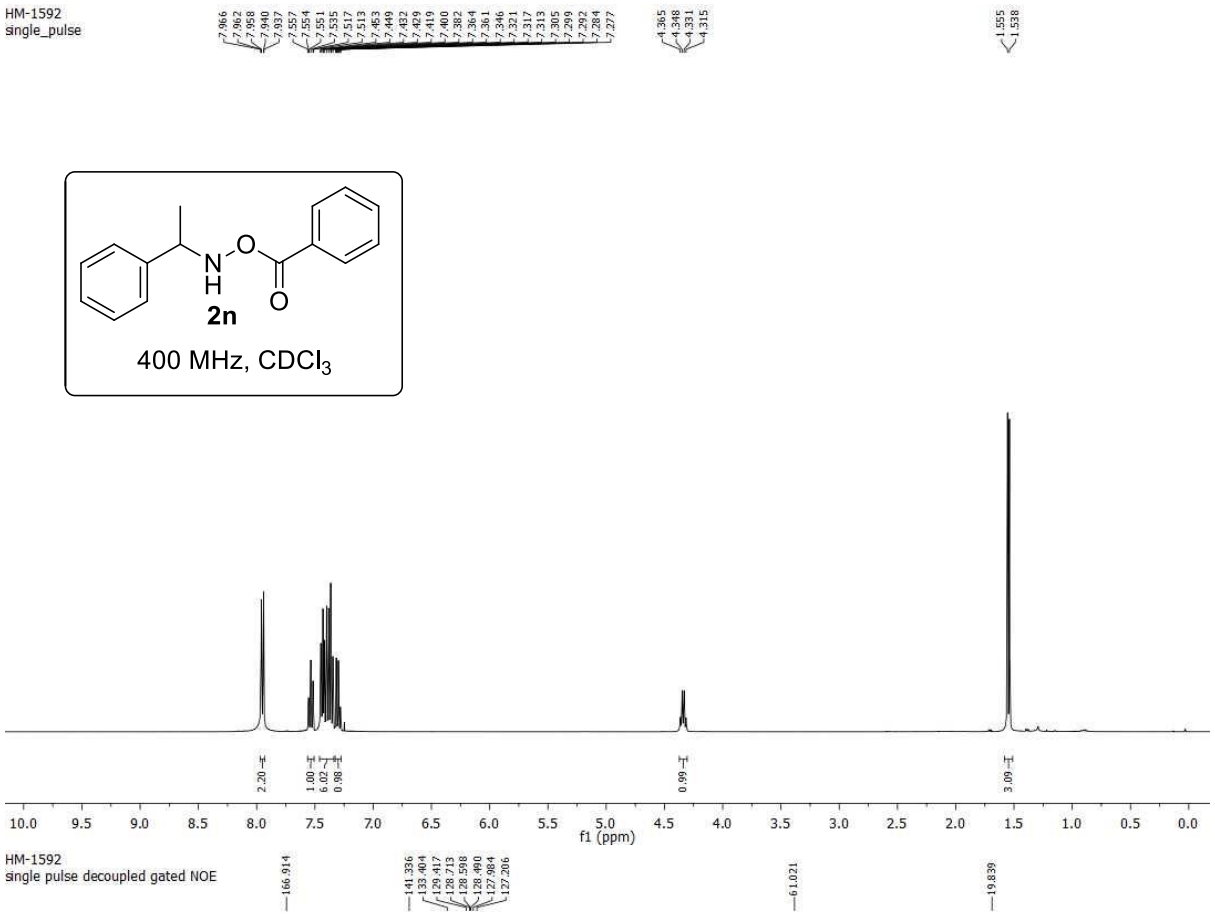
HM-1589
single_pulse



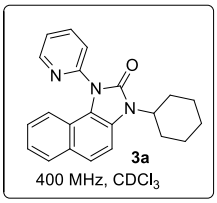


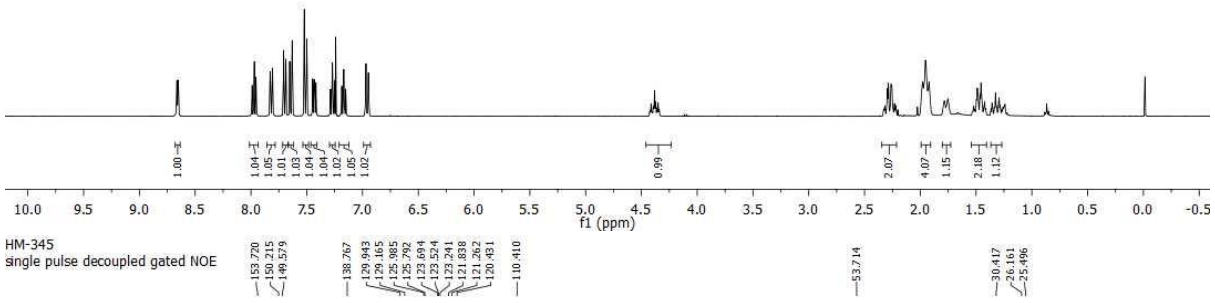
HM-1589
single pulse decoupled gated NOE



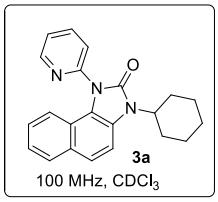

HM-1592
single_pulse
7.966
7.962
7.958
7.940
7.937
7.557
7.554
7.551
7.535
7.517
7.513
7.463
7.449
7.432
7.429
7.419
7.400
7.382
7.364
7.361
7.346
7.321
7.317
7.313
7.305
7.299
7.292
7.284
7.277
4.365
4.348
4.331
4.315
1.555
1.538
2n
400 MHz, CDCl3
2.20
1.00
6.02
0.98
0.99
3.09
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
HM-1592
single pulse decoupled gated NOE
166.914
141.336
133.404
129.417
128.773
128.598
128.490
127.984
127.206
61.021
19.839
2n
100 MHz, CDCl3
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

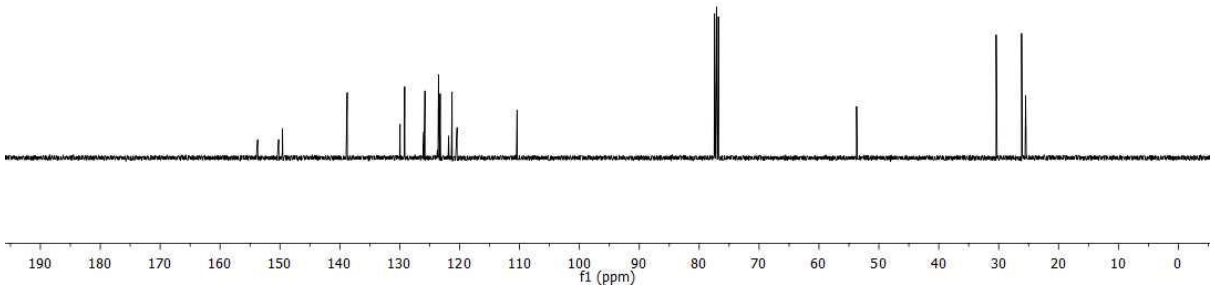

HM-345
single_pulse


3a
400 MHz, CDCl3

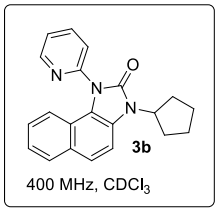

1.00
1.04
1.05
1.01
1.03
1.04
1.04
1.02
1.05
1.02
0.99
2.07
4.07
1.15
2.18
1.12
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

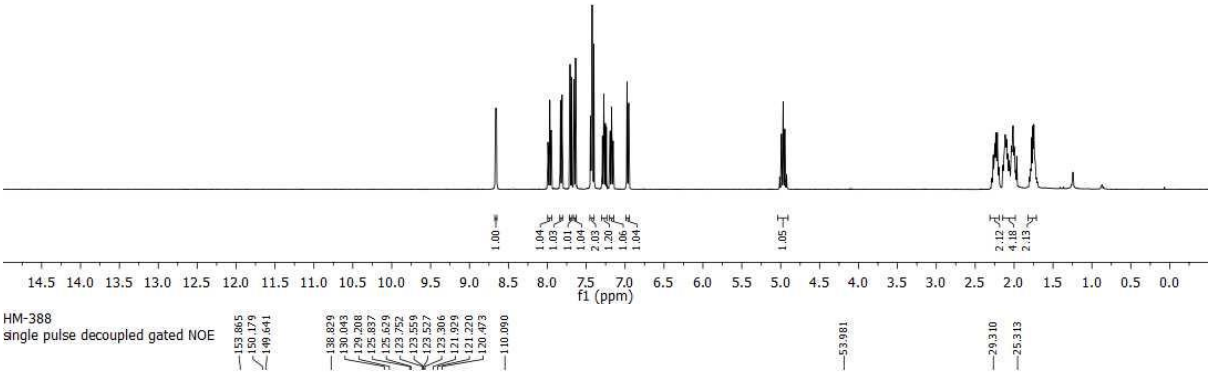
HM-345
single pulse decoupled gated NOE
153.720
150.215
149.579
138.767
129.943
129.165
125.985
125.792
123.694
123.524
123.241
121.838
121.262
120.431
110.410
53.714
30.417
26.161
25.496

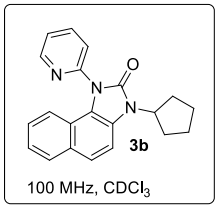

3a
100 MHz, CDCl3

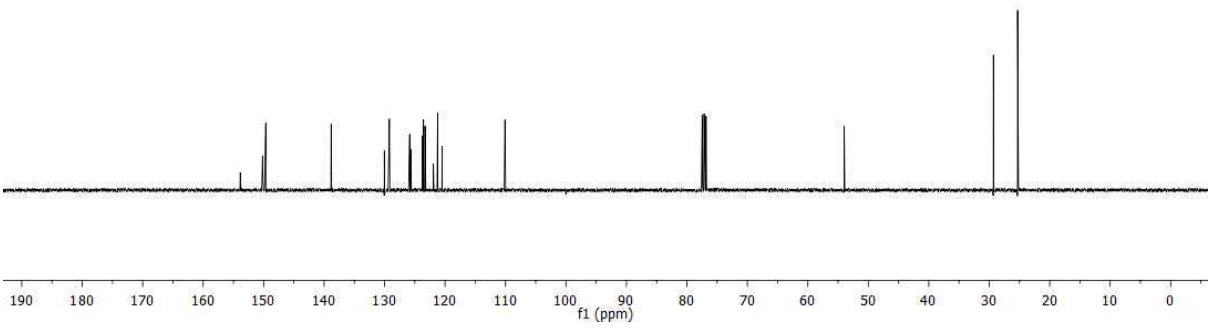

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


HM-388
single_pulse

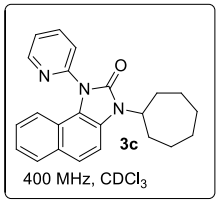

3b
400 MHz, CDCl3

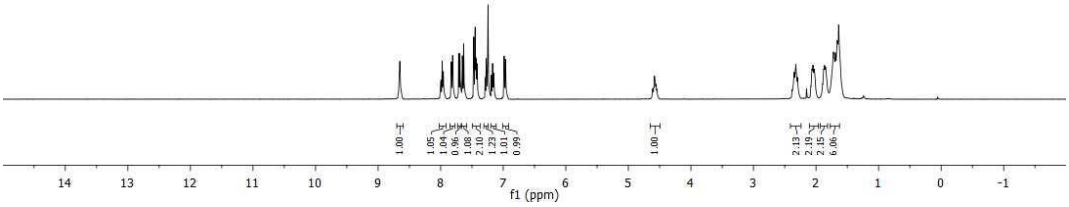

f1 (ppm)
HM-388
single pulse decoupled gated NOE

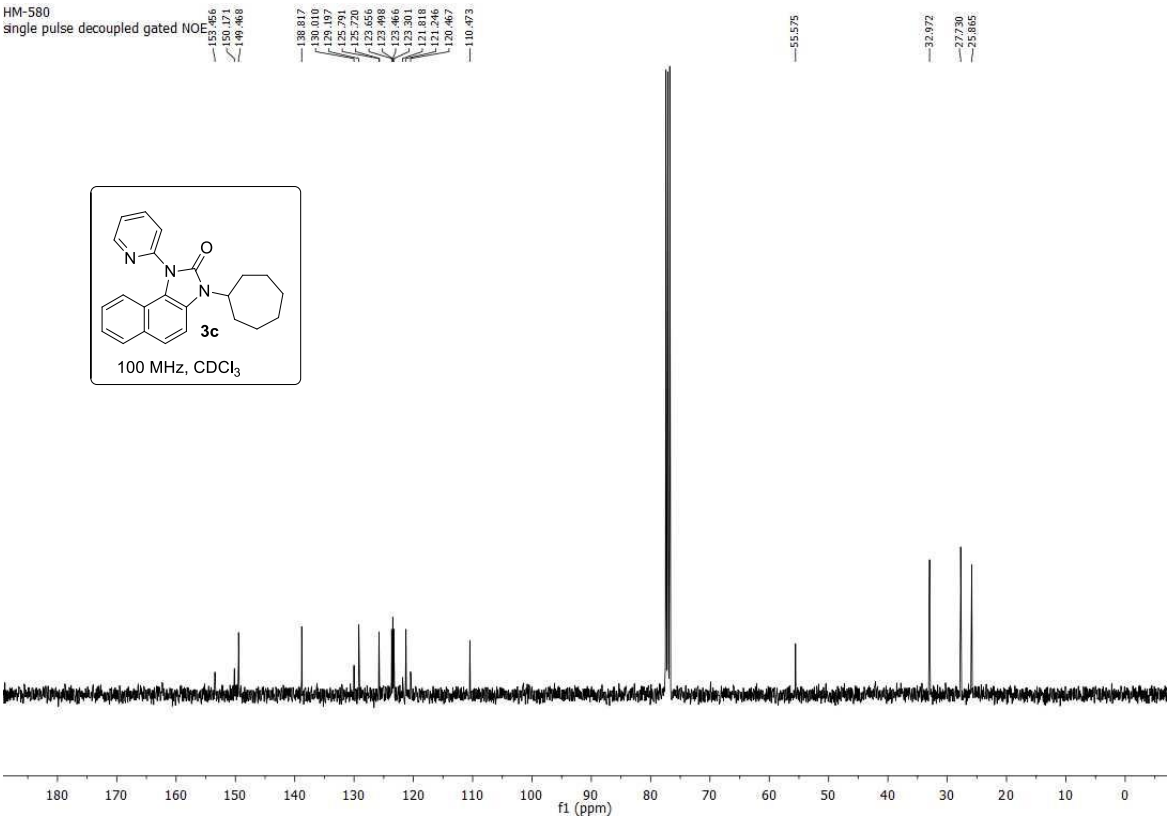

3b
100 MHz, CDCl3


f1 (ppm)


HM-580
single_pulse

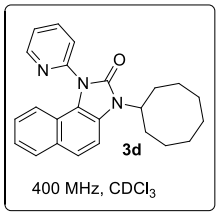

3c
400 MHz, CDCl3

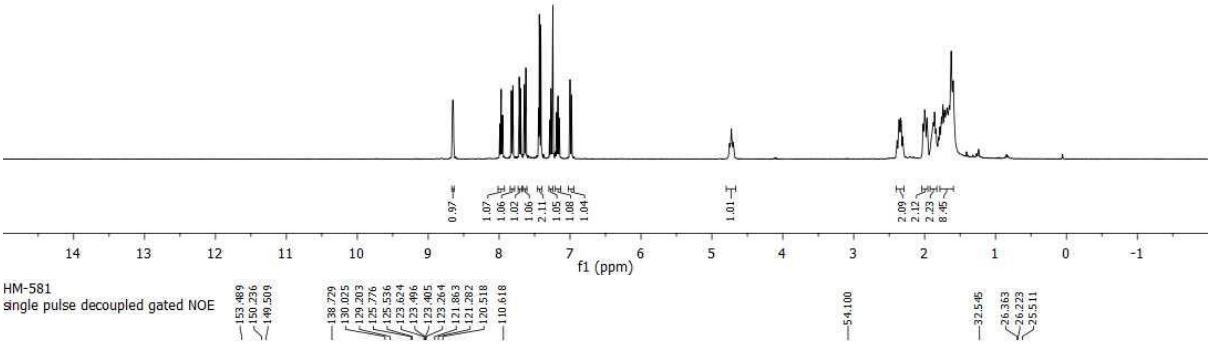

f1 (ppm)

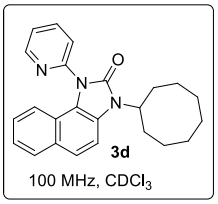

HM-580
single pulse decoupled gated NOE
f1 (ppm)

3c
100 MHz, CDCl3

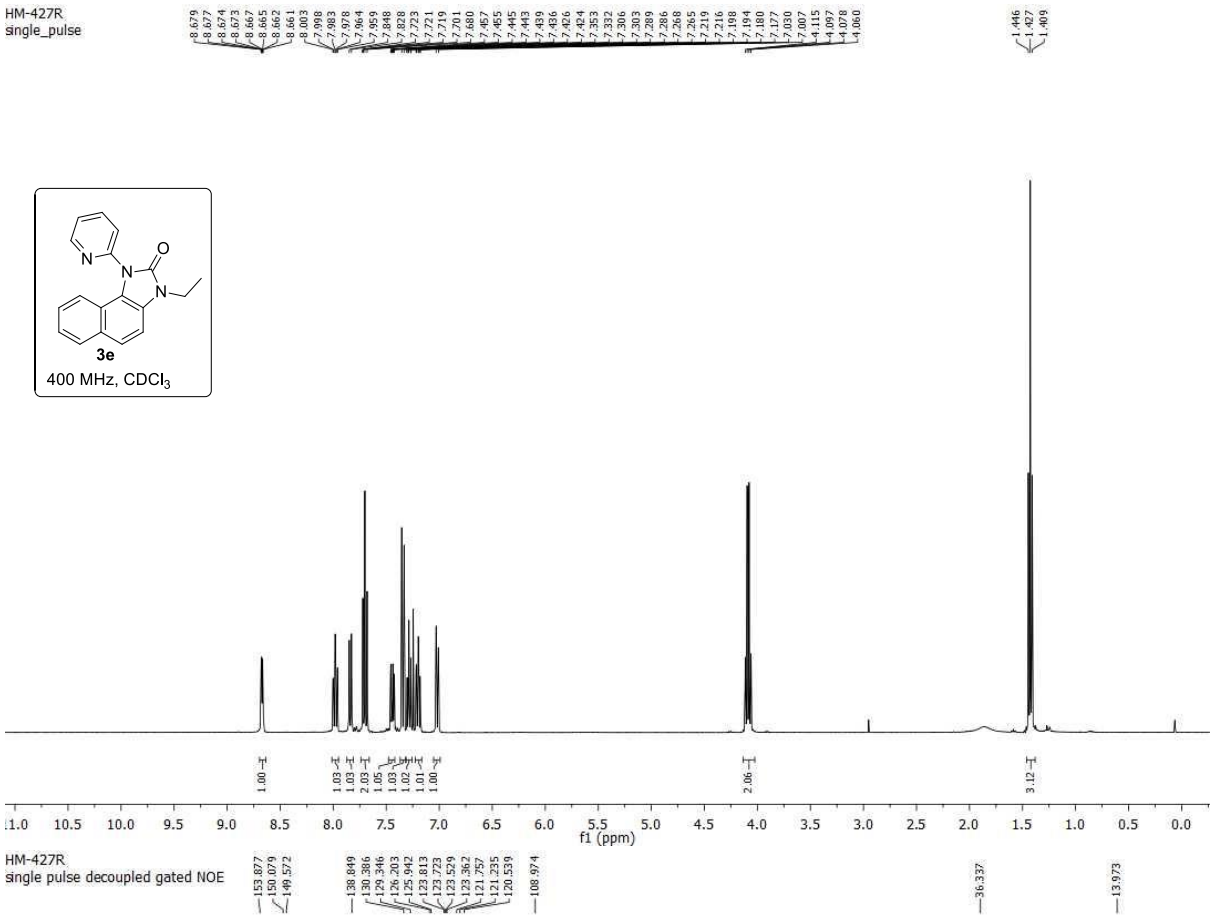

HM-581
single_pulse

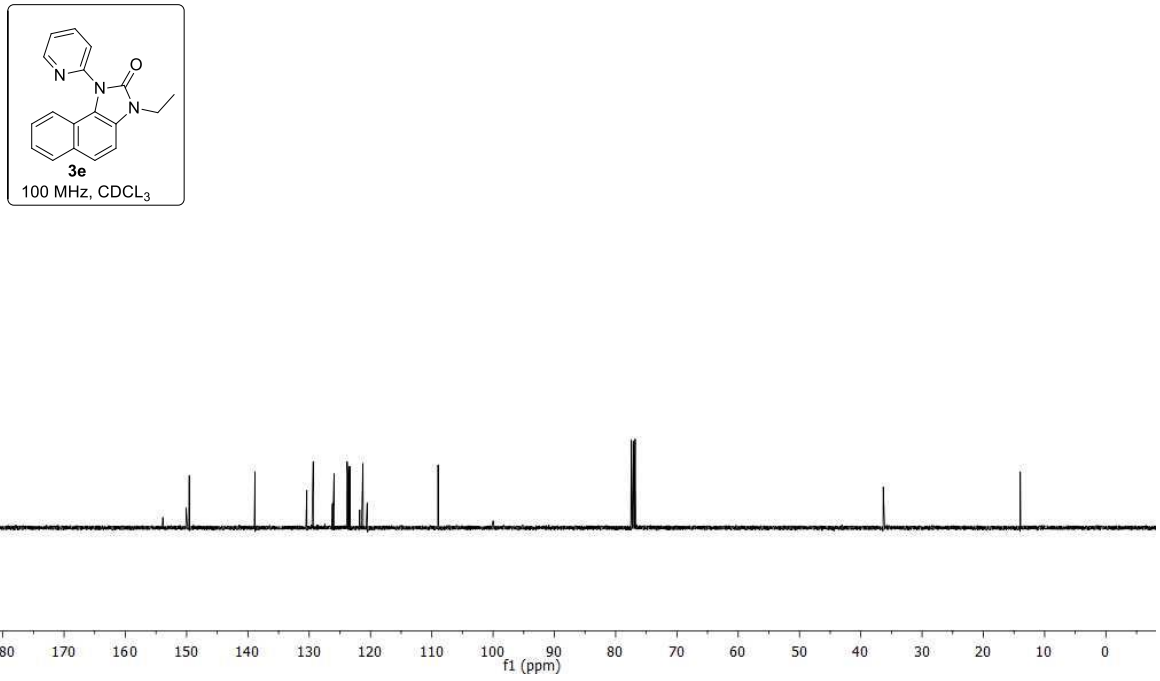

3d
400 MHz, CDCl3

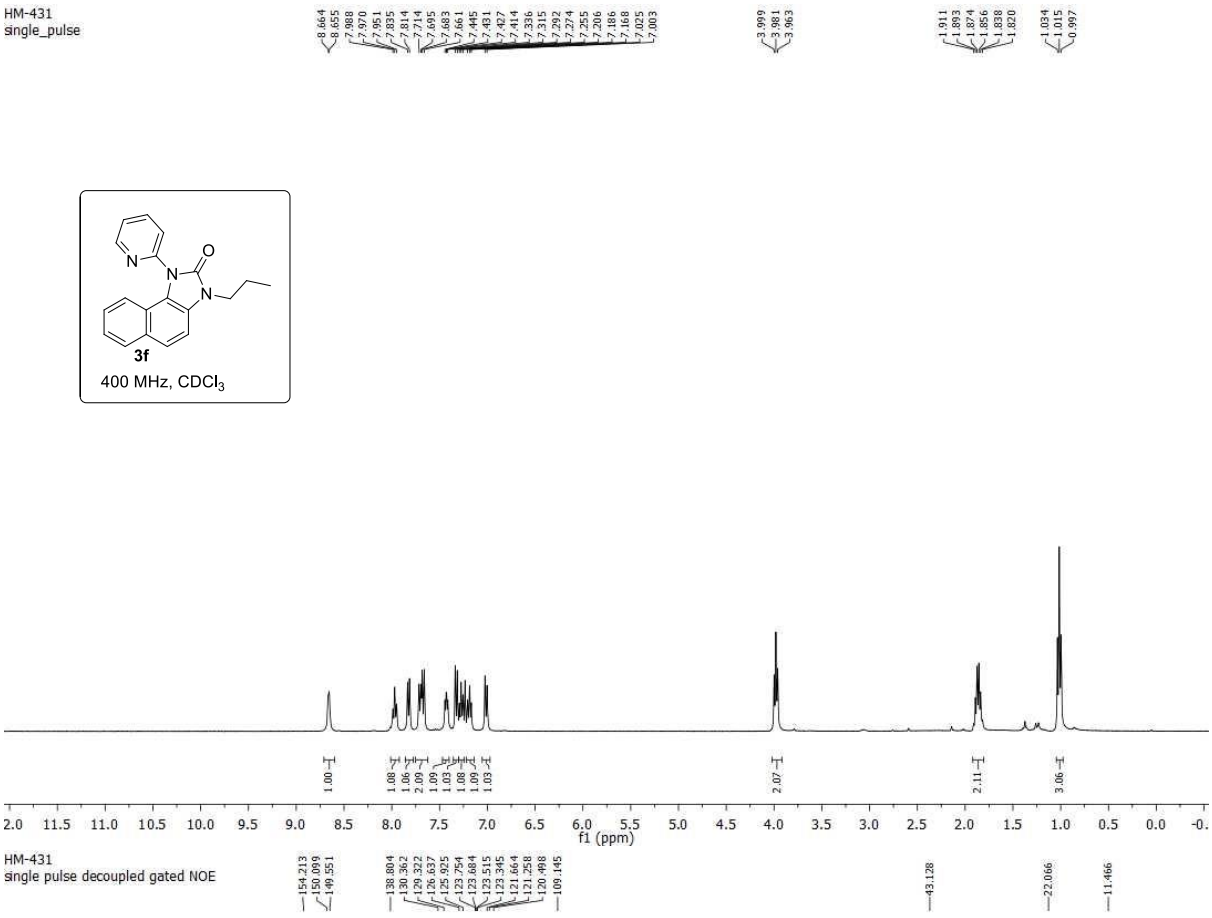

f1 (ppm)
HM-581
single pulse decoupled gated NOE

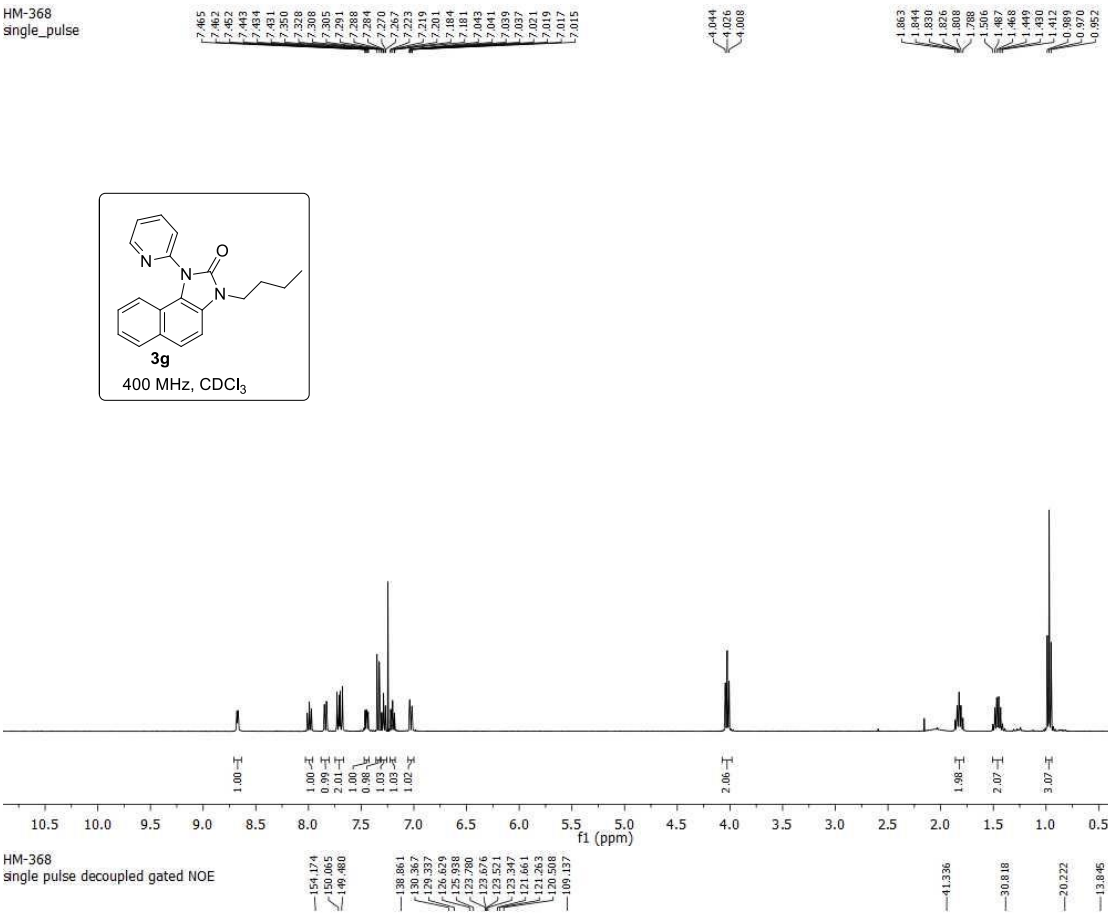

3d
100 MHz, CDCl3

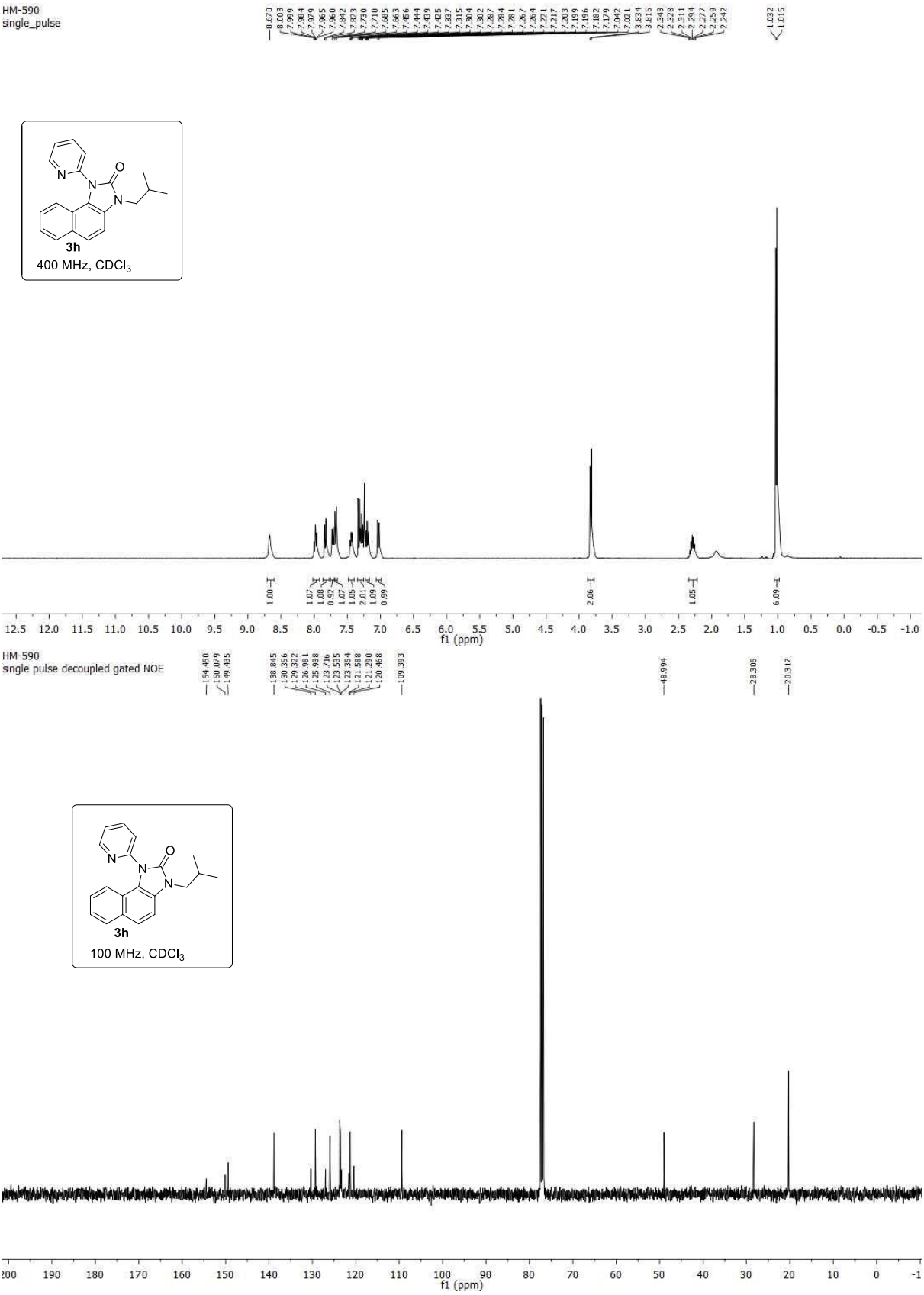
f1 (ppm)


HM-427R
single_pulse
3e
400 MHz, CDCl3
f1 (ppm)
HM-427R
single pulse decoupled gated NOE

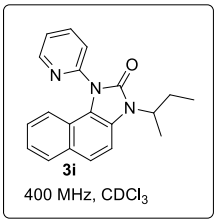

3e
100 MHz, CDCL3
f1 (ppm)

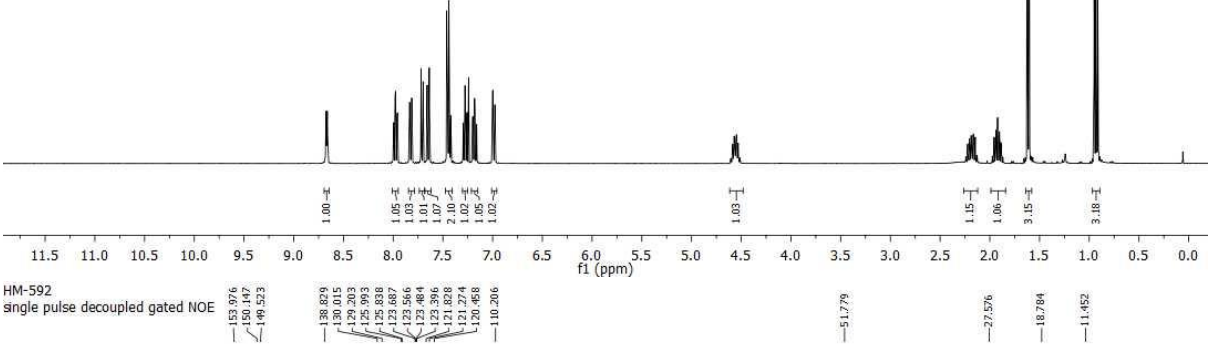

HM-431
single_pulse
3f
400 MHz, CDCl3
f1 (ppm)
HM-431
single pulse decoupled gated NOE
3f
100 MHz, CDCl3
f1 (ppm)

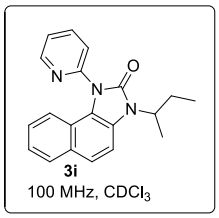

HM-368
single_pulse
3g
400 MHz, CDCl3
f1 (ppm)
HM-368
single pulse decoupled gated NOE
3f
100 MHz, CDCl3
f1 (ppm)

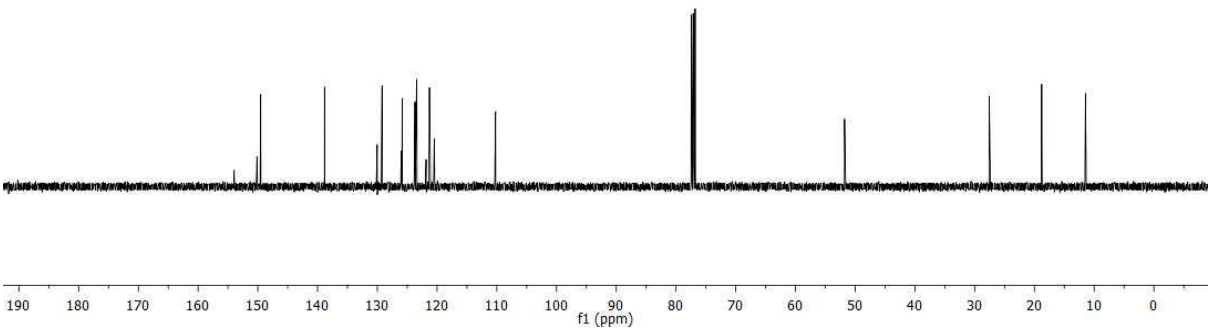

HM-590
single_pulse
3h
400 MHz, CDCl3
f1 (ppm)
HM-590
single pulse decoupled gated NOE
3h
100 MHz, CDCl3
f1 (ppm)


HM-592
single_pulse

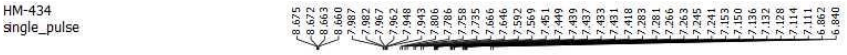

3i
400 MHz, CDCl3

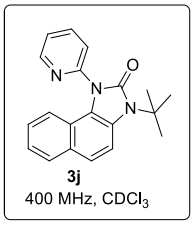

f1 (ppm)
HM-592
single pulse decoupled gated NOE


3i
100 MHz, CDCl3


f1 (ppm)

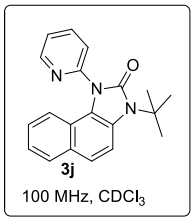
HM-434
single_pulse



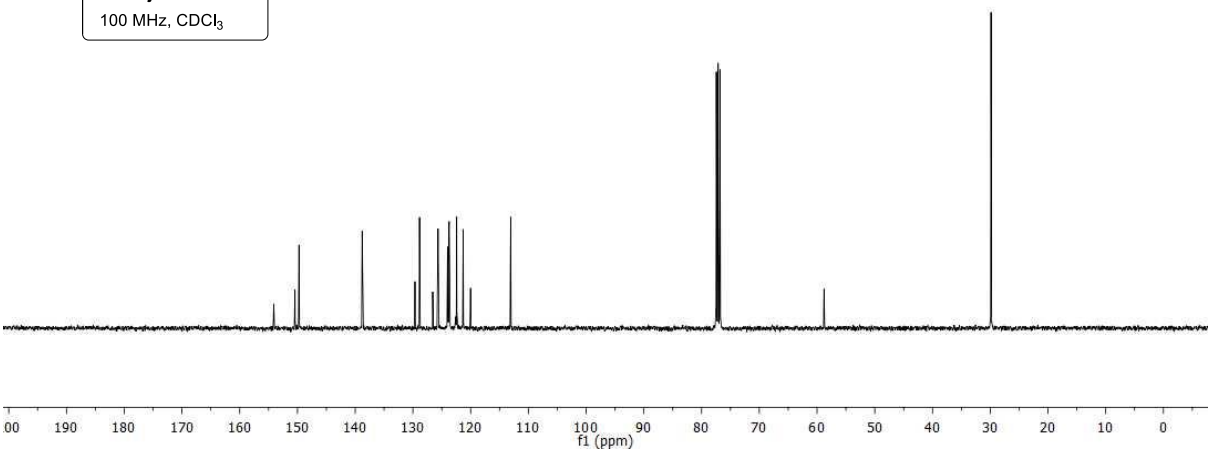


3j
400 MHz, $CDCl_3$

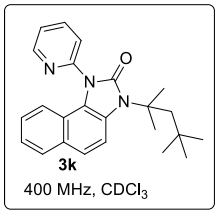
HM-434
single pulse decoupled gated NOE

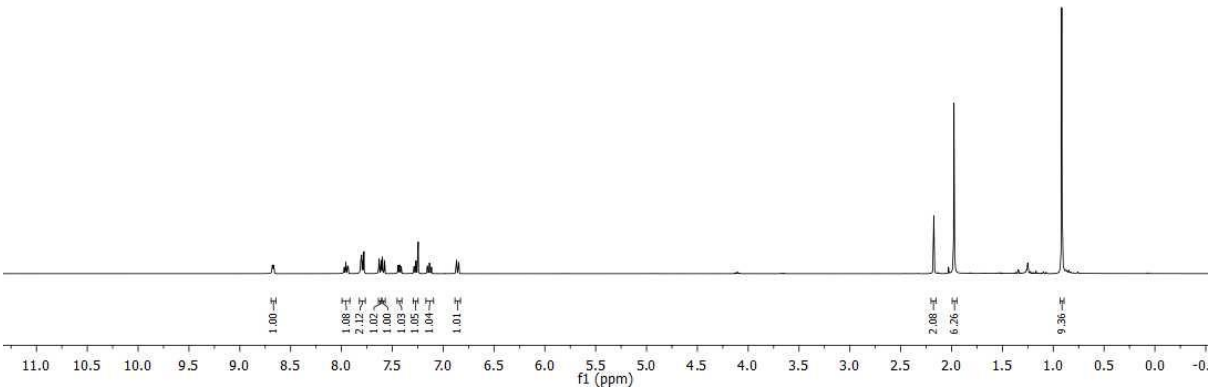


3j
100 MHz, $CDCl_3$

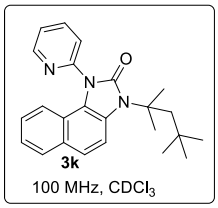


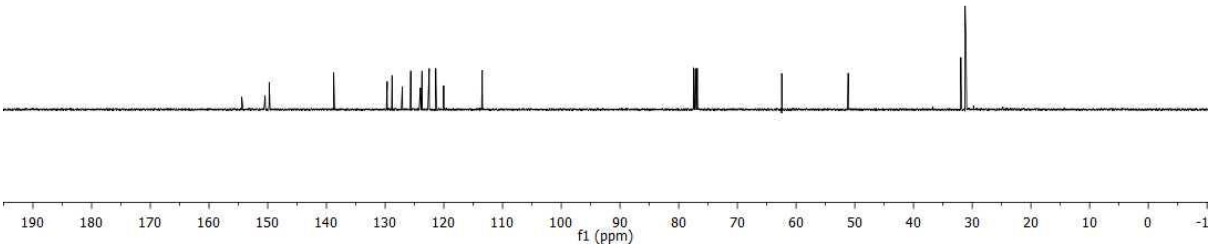
HM-393
single_pulse



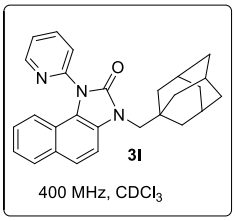


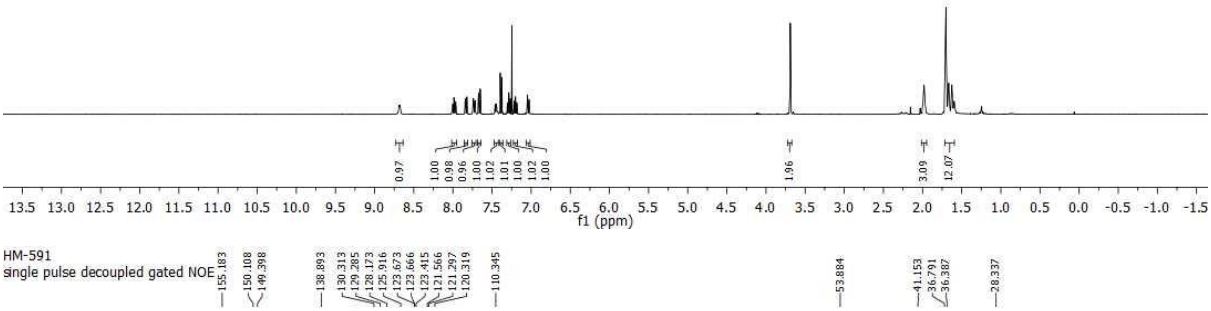
HM-393
single pulse decoupled gated NOE



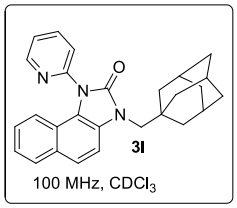


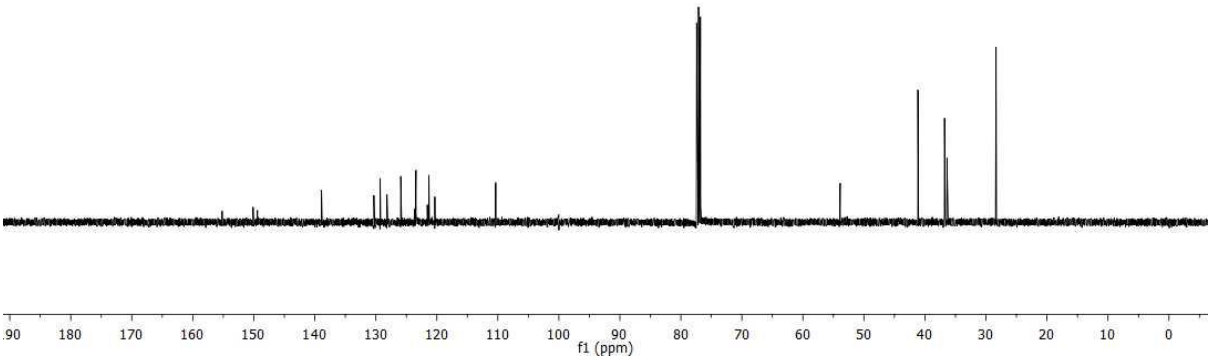

HM-591
single_pulse

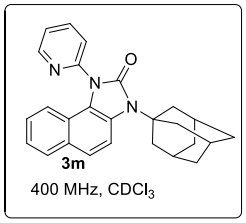

3l
400 MHz, CDCl3

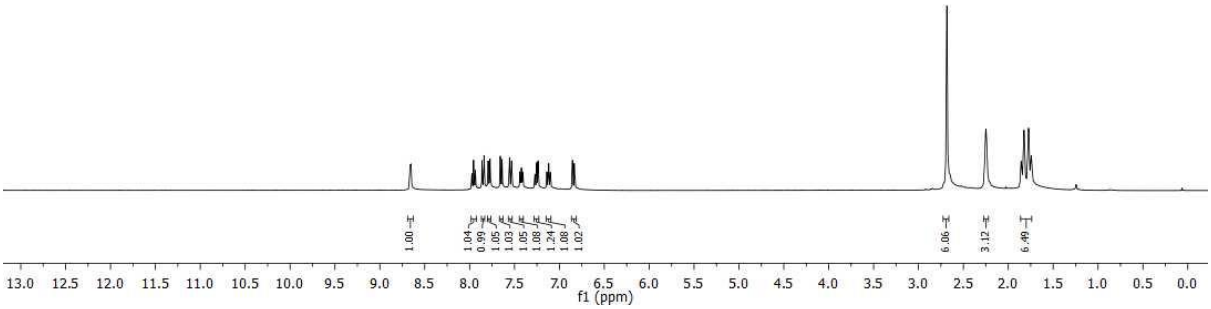

f1 (ppm)

HM-591
single pulse decoupled gated NOE

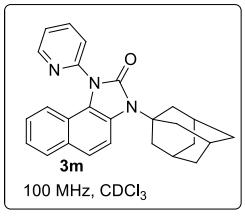

3l
100 MHz, CDCl3

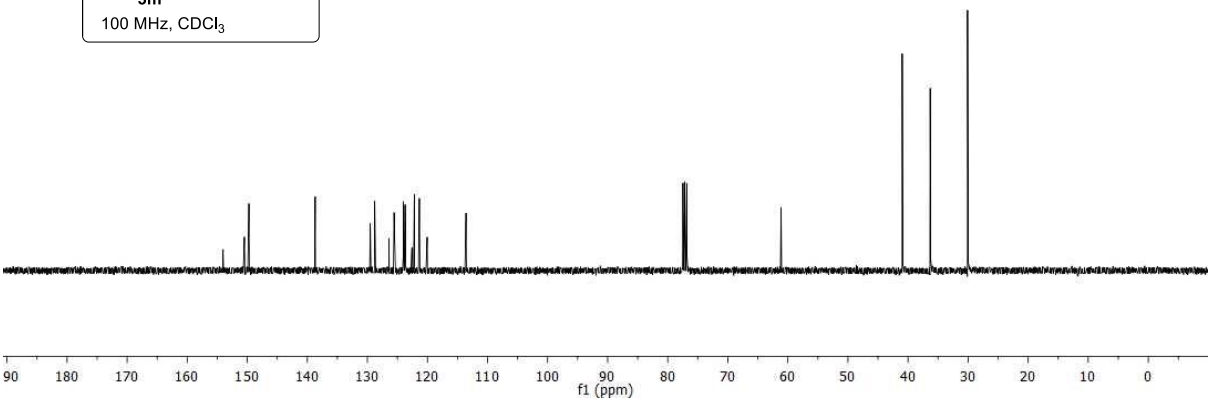

f1 (ppm)


3m
400 MHz, CDCl3

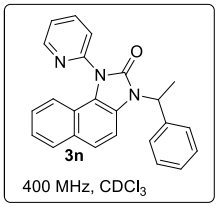

1.00
1.04
0.99
1.05
1.03
1.05
1.08
1.24
1.08
1.02
6.06
3.12
6.49
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

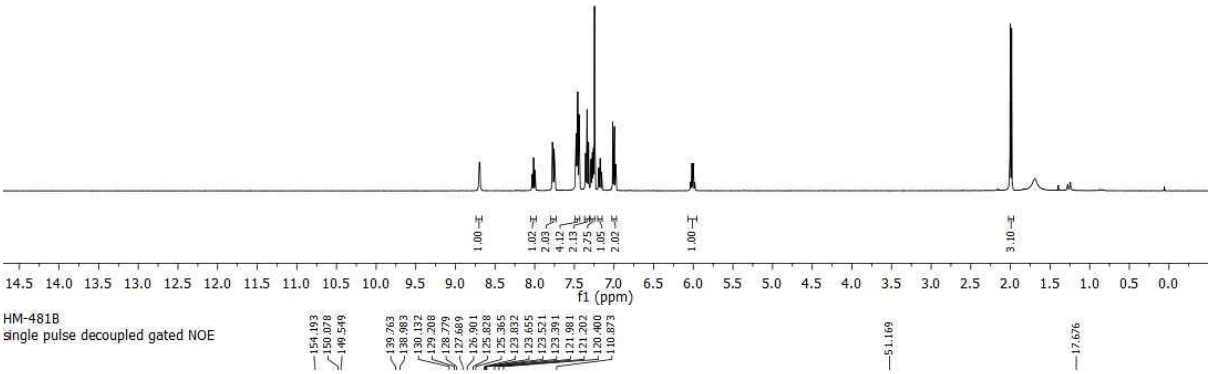

HM-594
single pulse decoupled gated NOE
154.031
150.476
149.719
138.684
129.519
128.781
126.396
125.559
124.003
123.727
123.670
122.580
122.183
121.345
120.045
113.576
61.123
40.962
36.305
30.086


3m
100 MHz, CDCl3

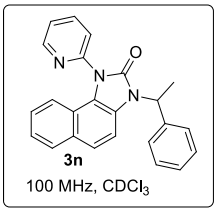

90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


HM-581B
single_pulse


3n
400 MHz, CDCl3

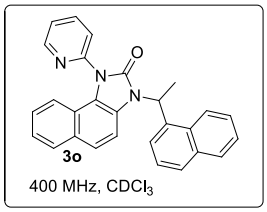

f1 (ppm)

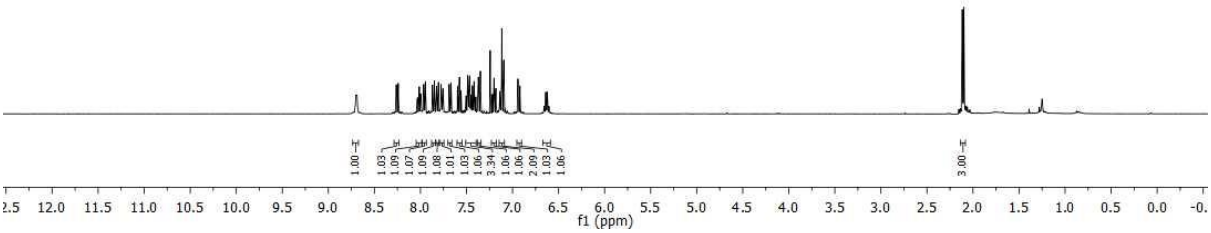
HM-481B
single pulse decoupled gated NOE


3n
100 MHz, CDCl3

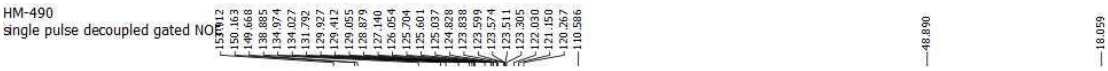
f1 (ppm)

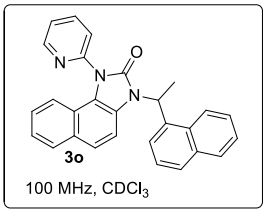
HM-490
single_pulse

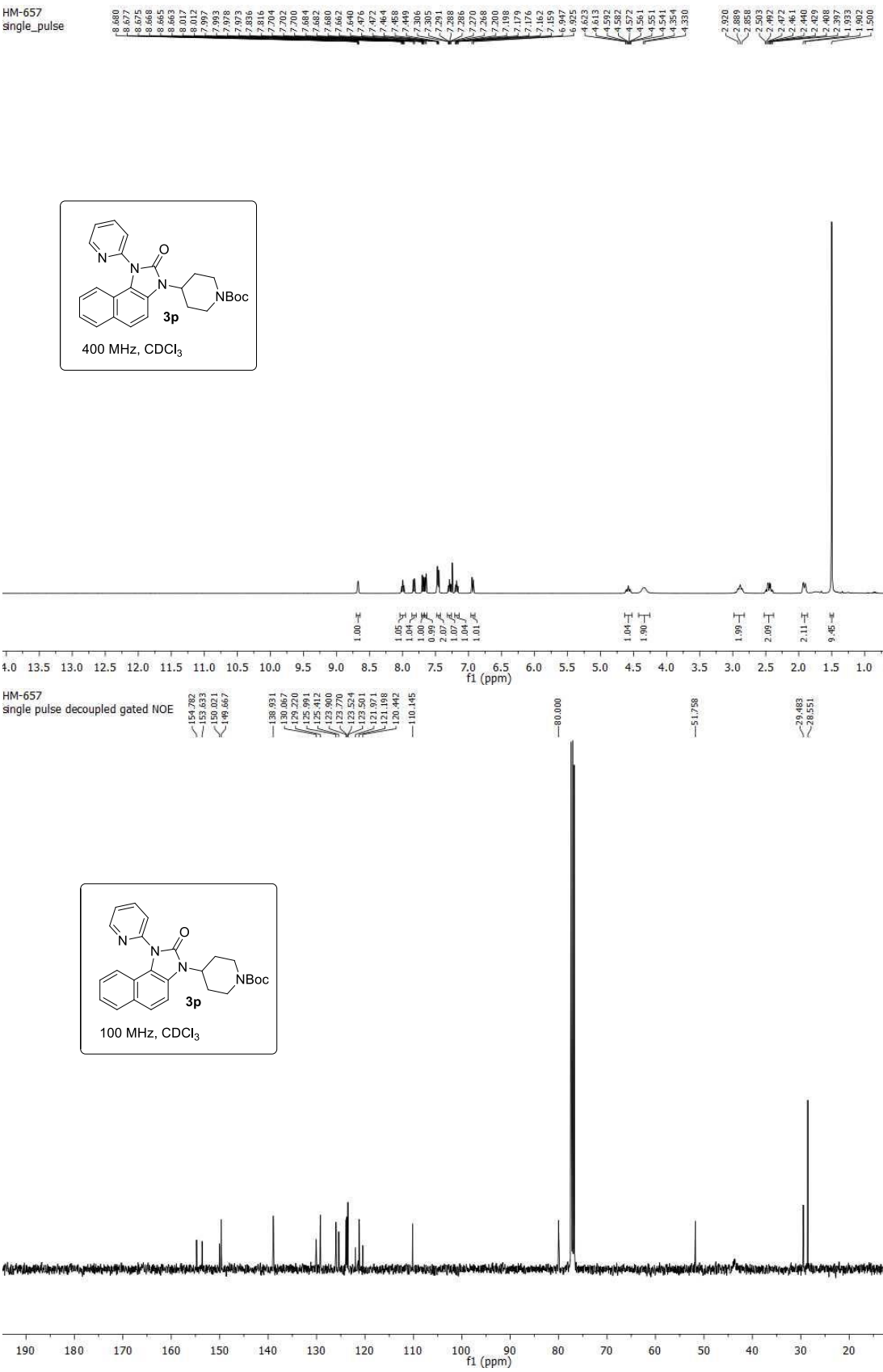


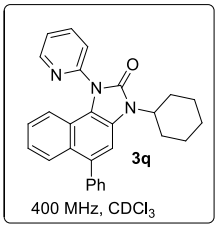


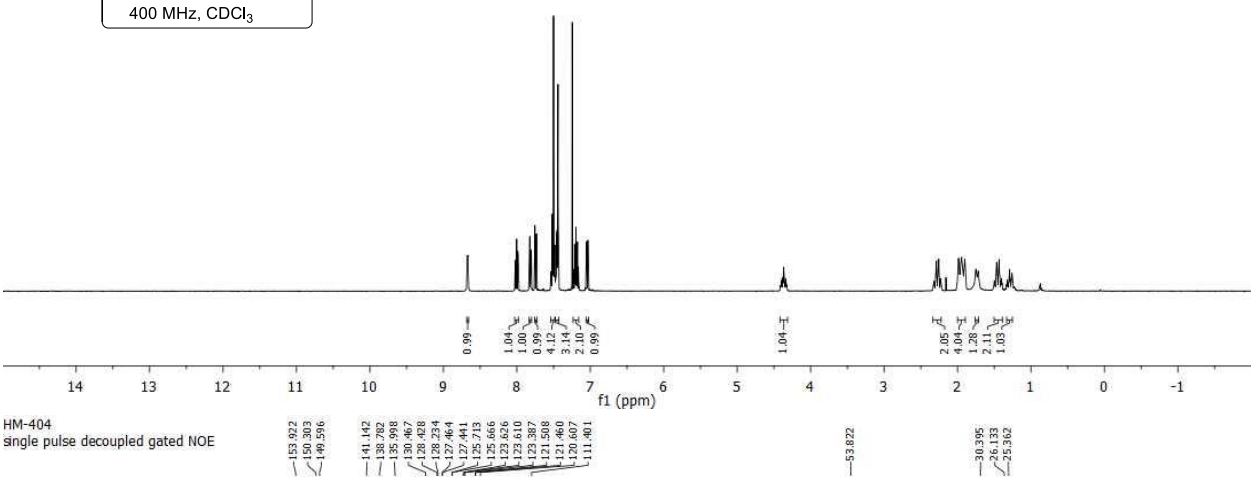
HM-490
single pulse decoupled gated NOE



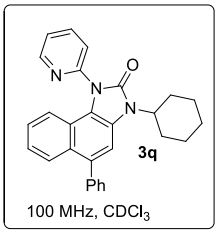


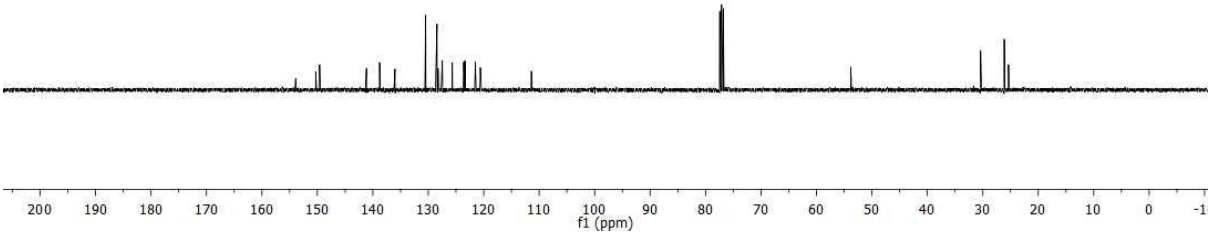

HM-657
single_pulse
3p
400 MHz, CDCl3
f1 (ppm)
HM-657
single pulse decoupled gated NOE
3p
100 MHz, CDCl3
f1 (ppm)



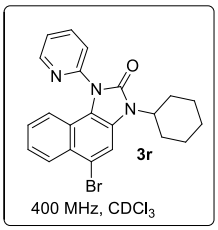


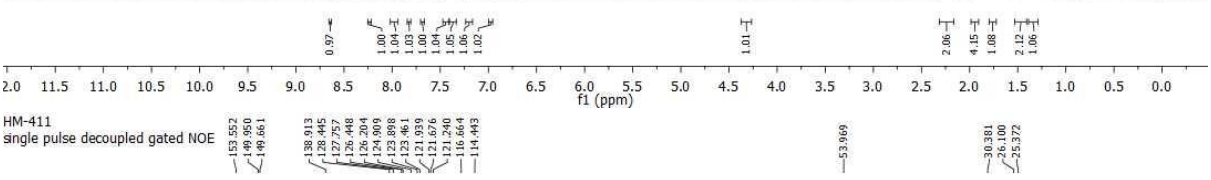
HM-404
single pulse decoupled gated NOE



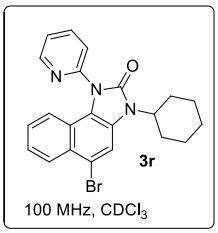


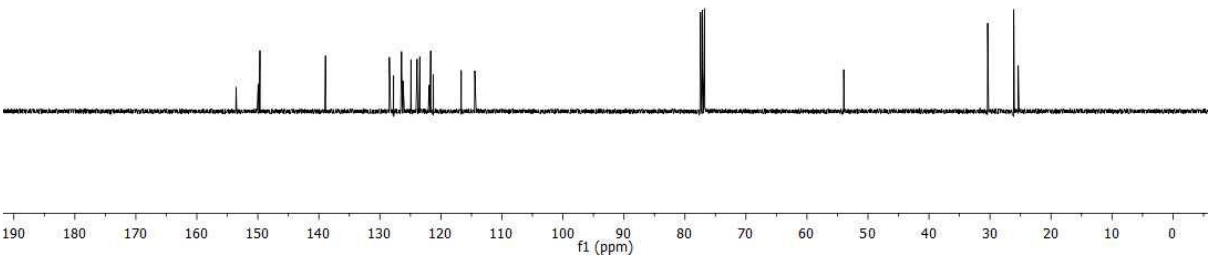

HM-411
single_pulse

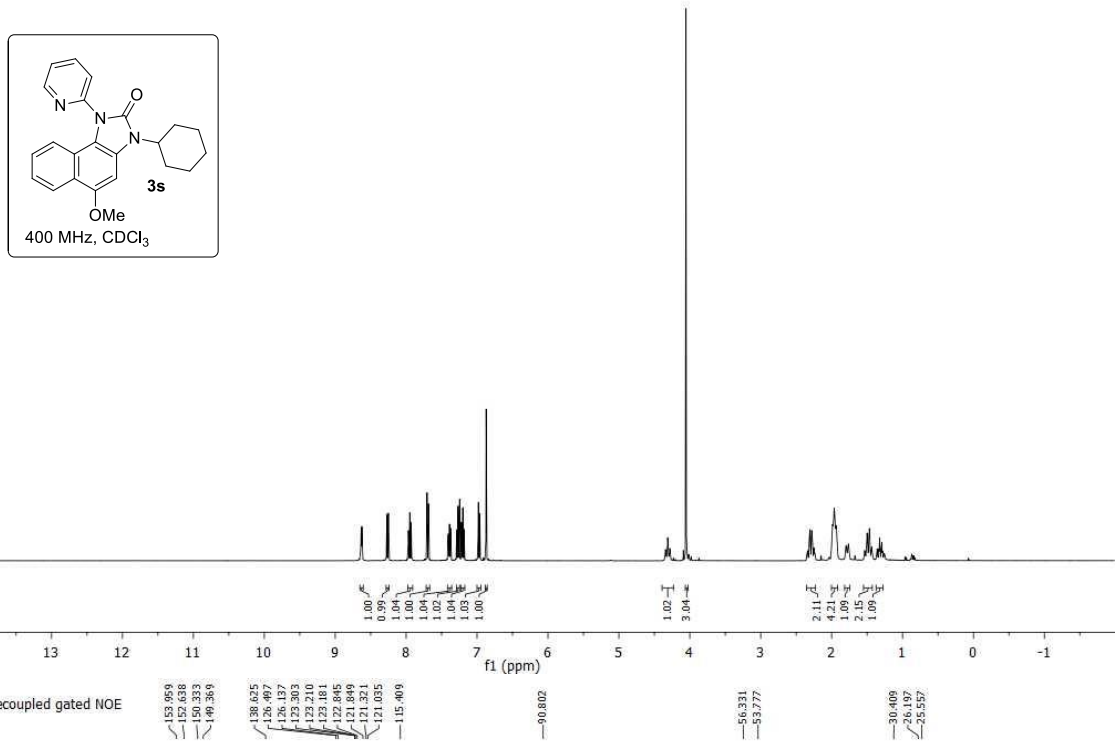

3r
Br
400 MHz, CDCl3


f1 (ppm)

HM-411
single pulse decoupled gated NOE

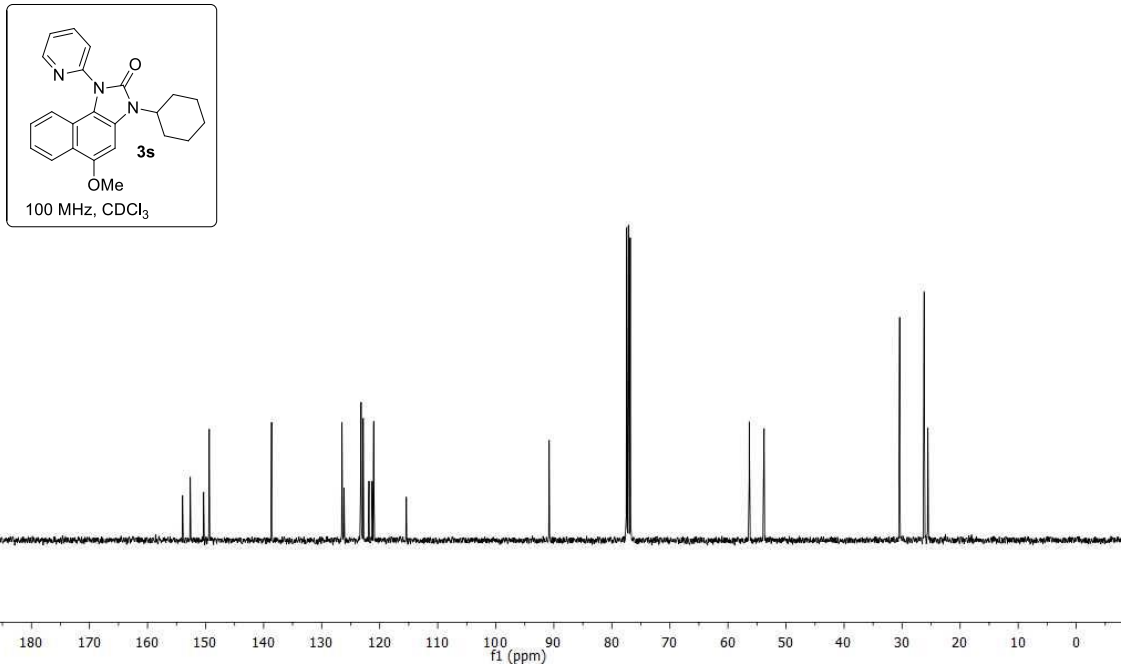

3r
Br
100 MHz, CDCl3

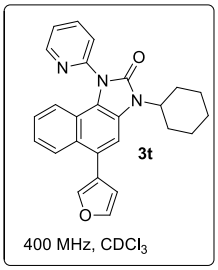

f1 (ppm)

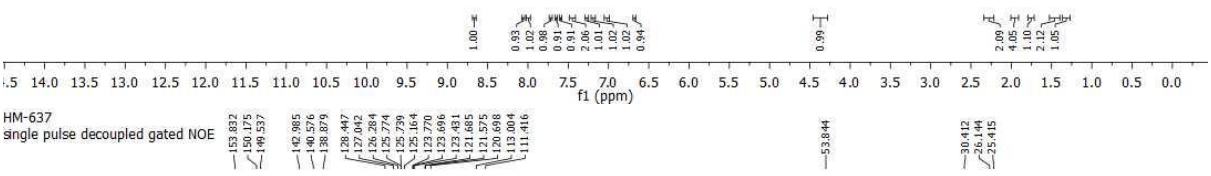


HM-613
single pulse decoupled gated NOE

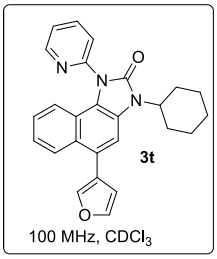
153.959
152.638
150.333
149.369
138.625
126.497
126.137
125.303
123.210
123.181
122.845
121.849
121.321
121.035
115.409
90.802
56.331
53.777
30.409
26.197
25.557

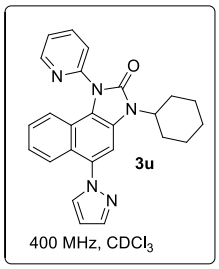


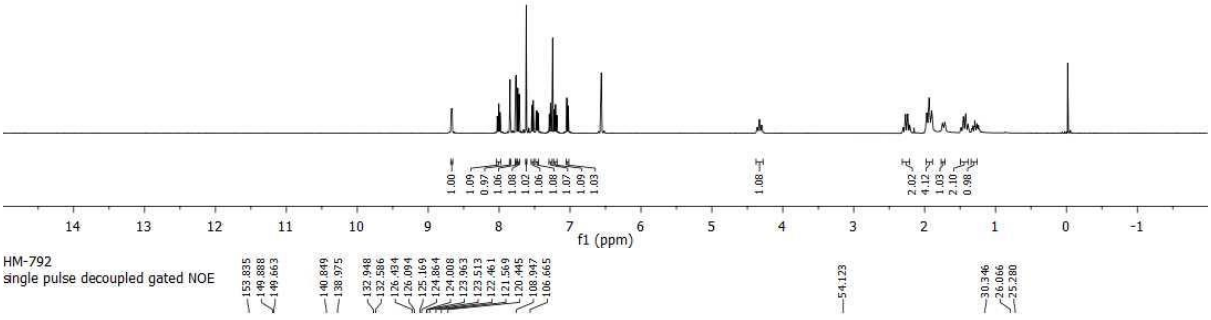




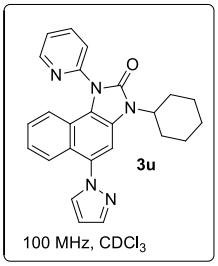
HM-637
single pulse decoupled gated NOE

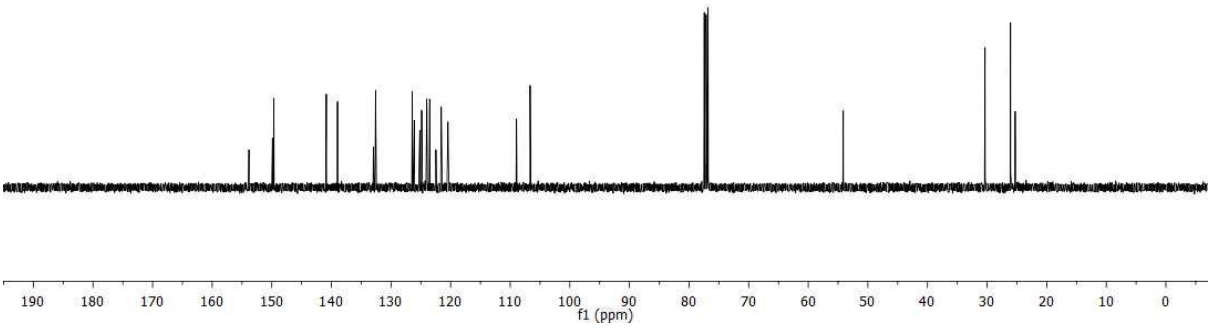




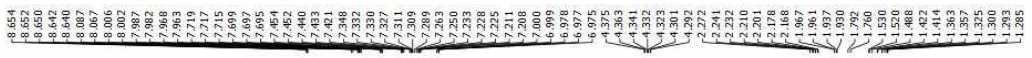


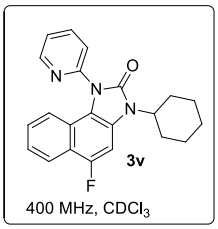
HM-792
single pulse decoupled gated NOE

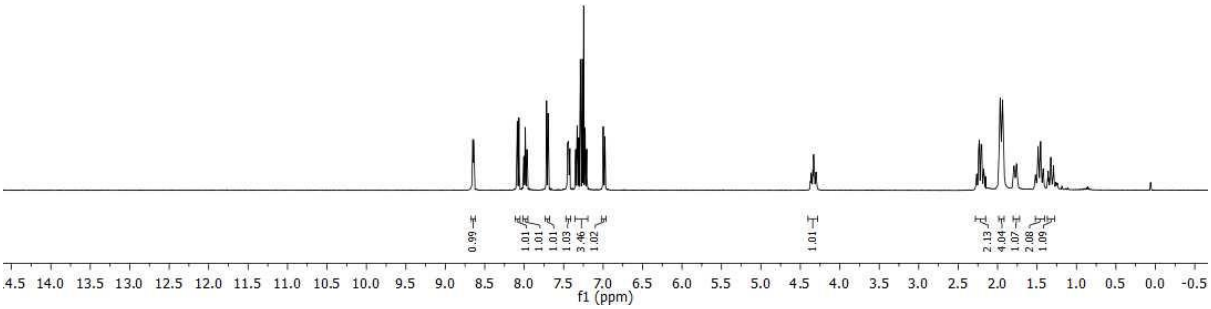




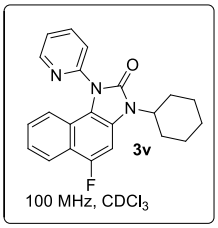
HM-826
single_pulse

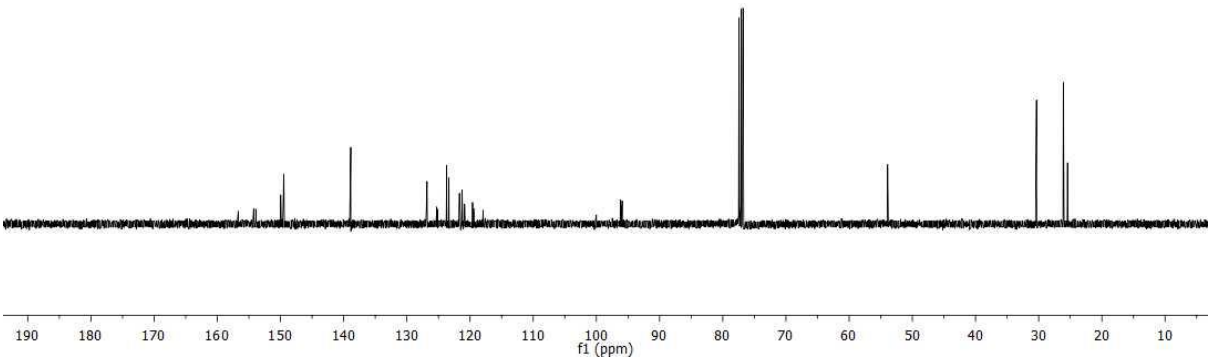




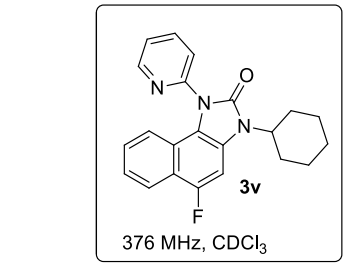


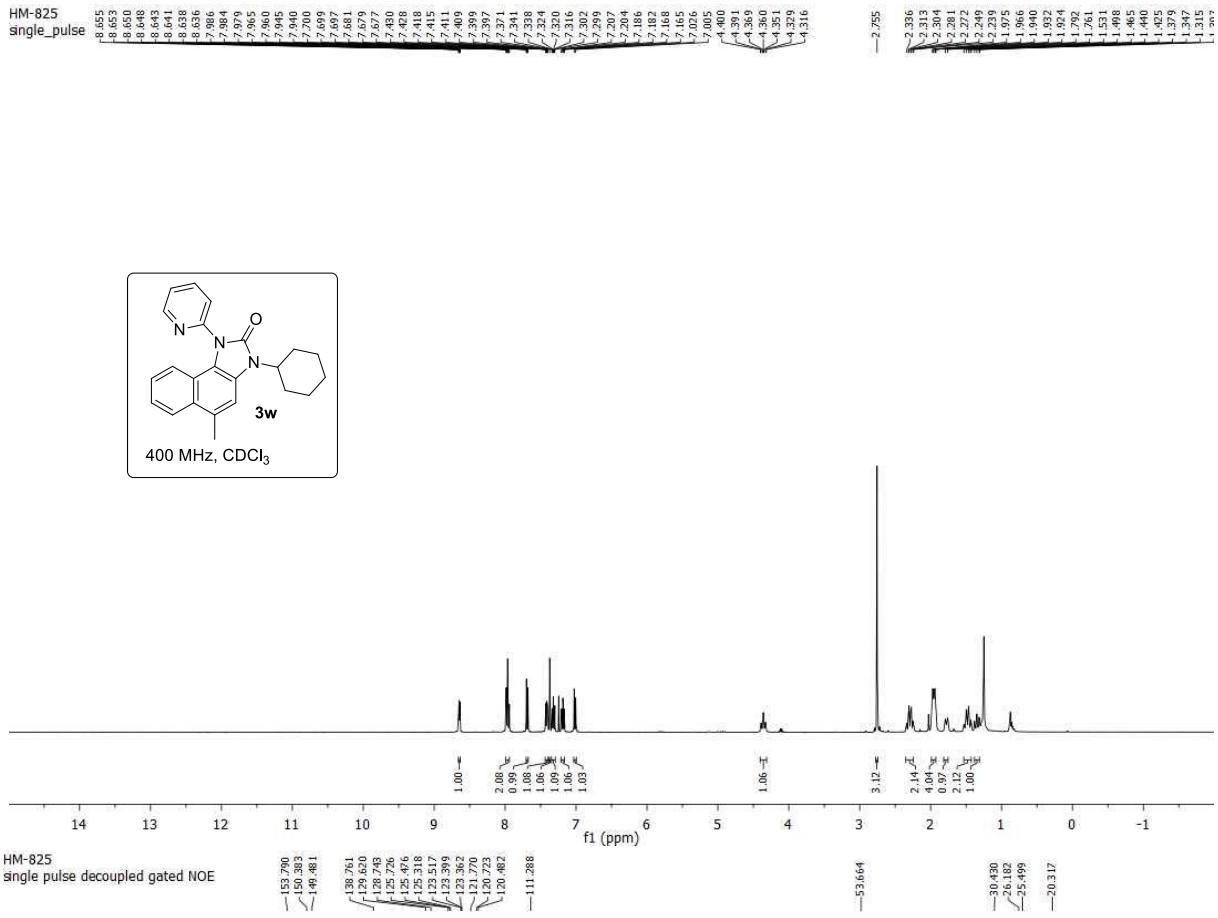
HM-826
single pulse decoupled gated NOE

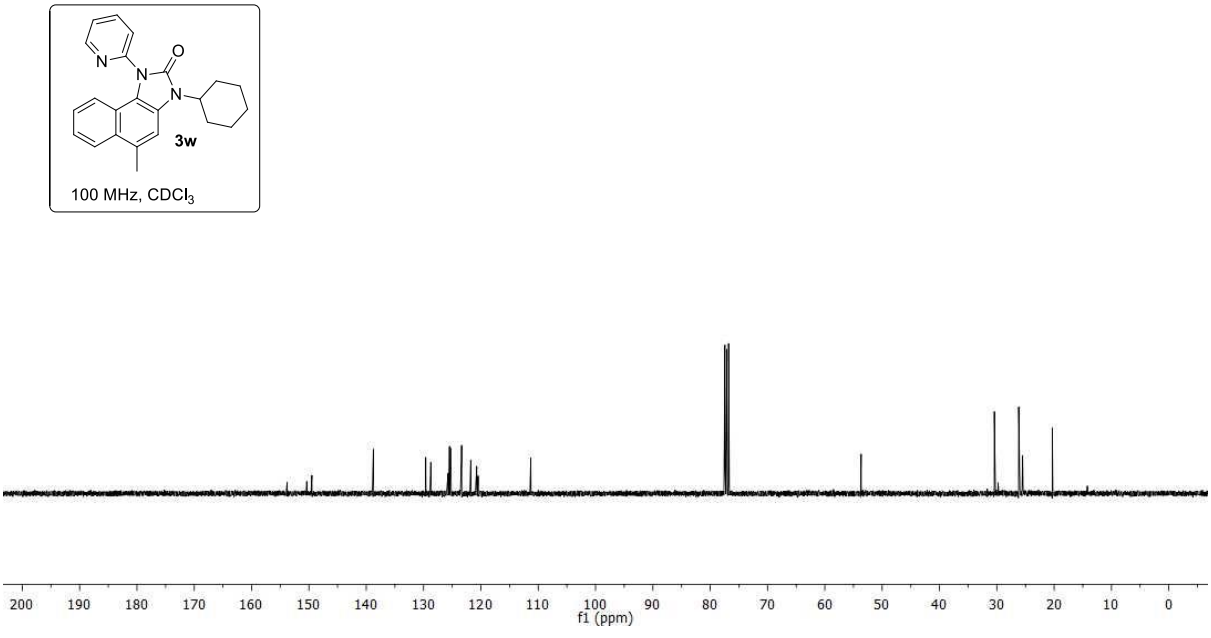




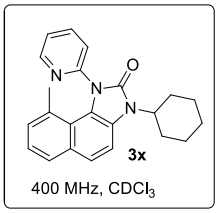
HM-826
single pulse decoupled gated NOE

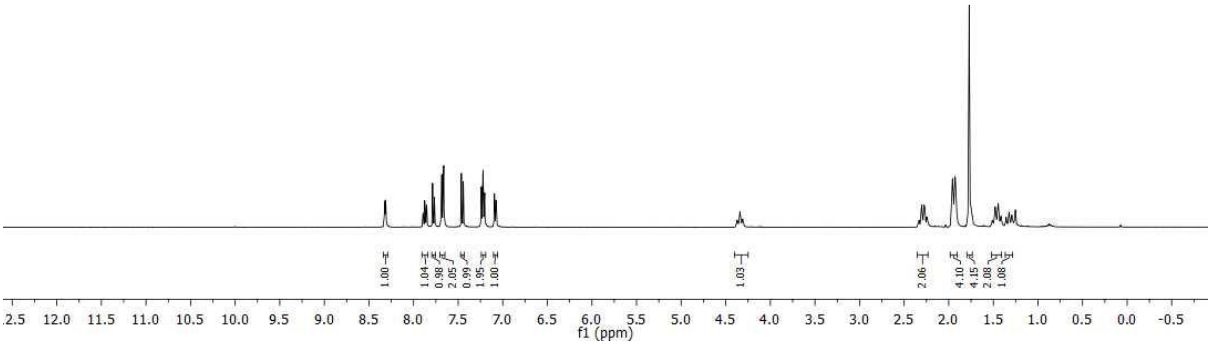



HM-825
single_pulse
3w
400 MHz, CDCl3
f1 (ppm)
HM-825
single pulse decoupled gated NOE

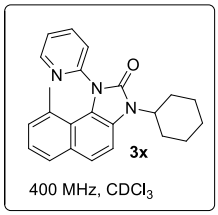

3w
100 MHz, CDCl3
f1 (ppm)

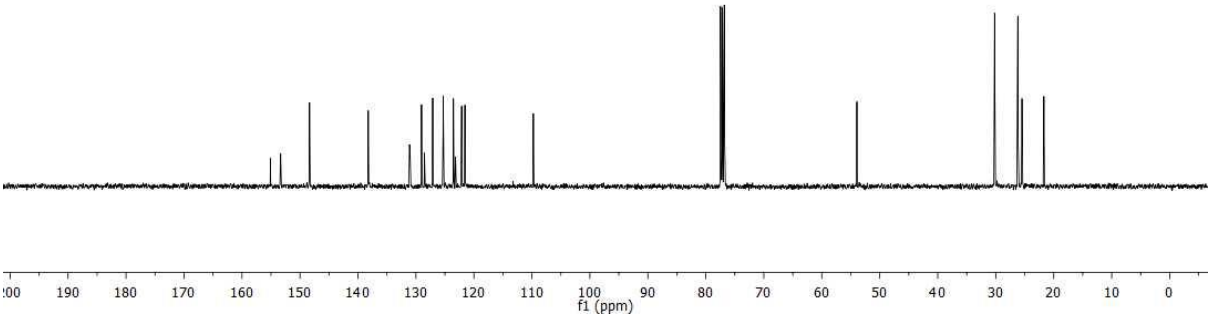
HM-810
single_pulse

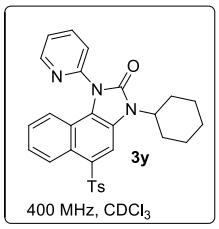


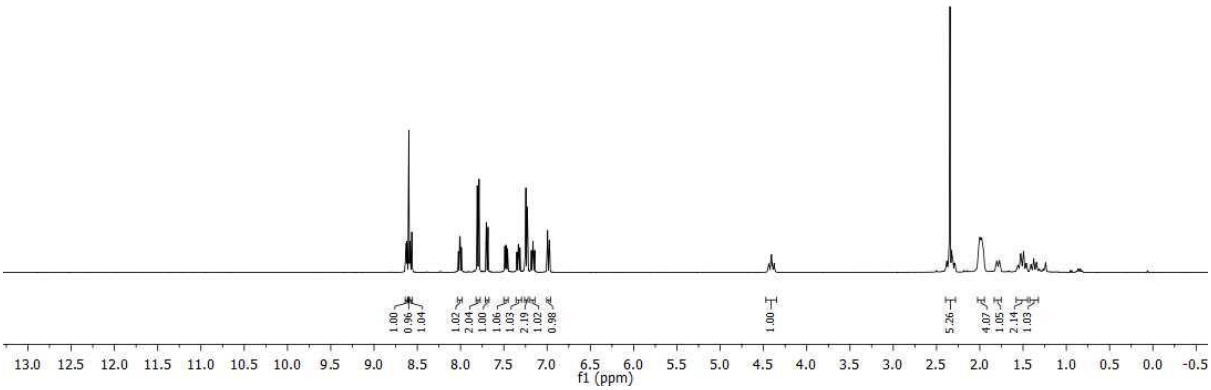


HM-810
single pulse decoupled gated NOE

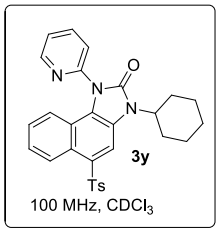


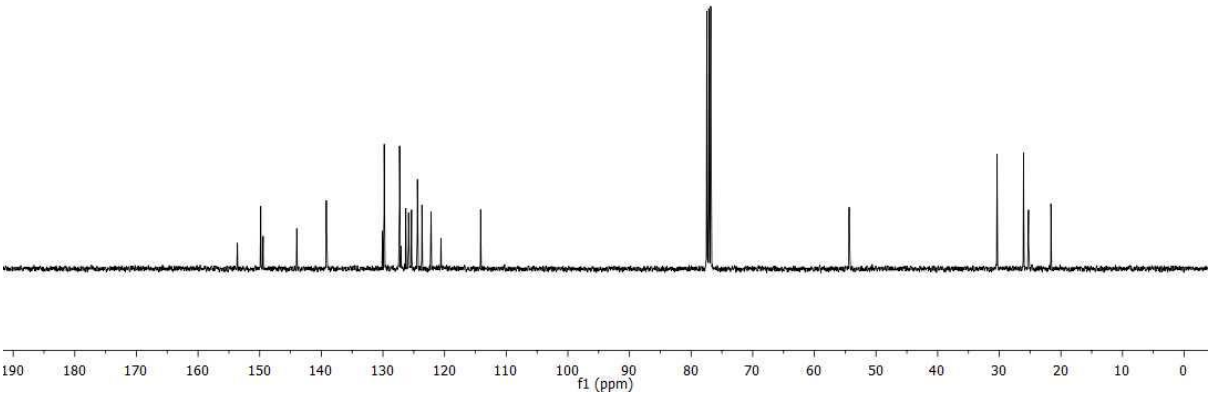



3y
Ts
400 MHz, CDCl3

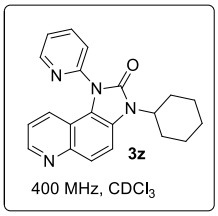

f1 (ppm)

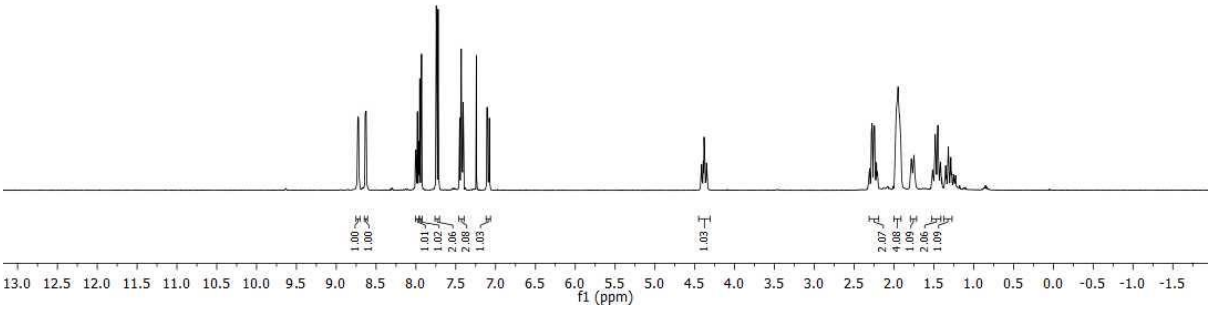

HM-927
single pulse decoupled gated NOE


3y
Ts
100 MHz, CDCl3

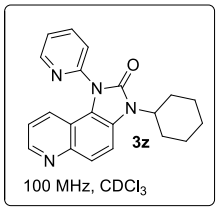

f1 (ppm)

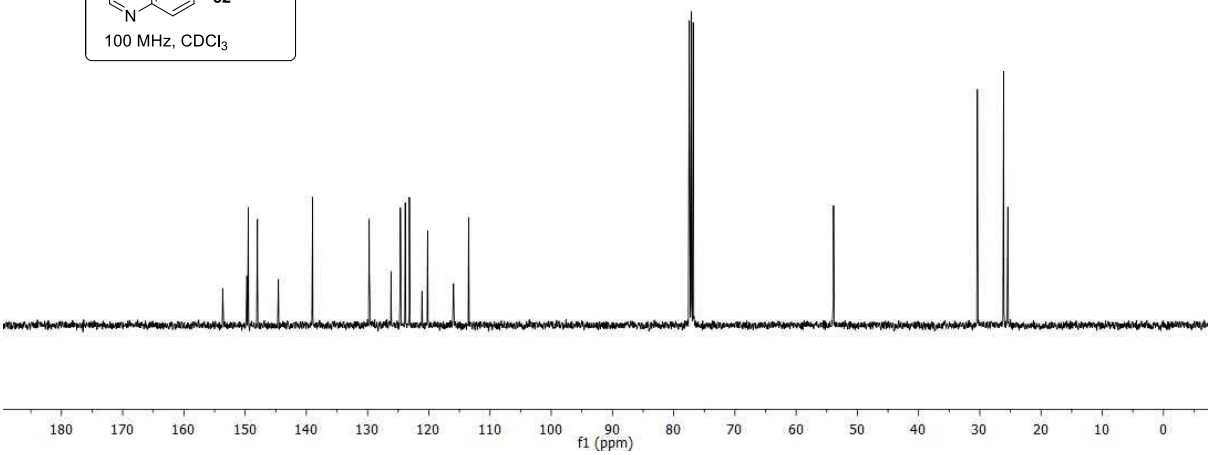
HM-412
single_pulse



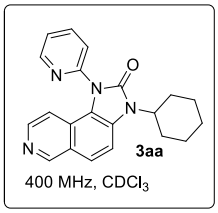


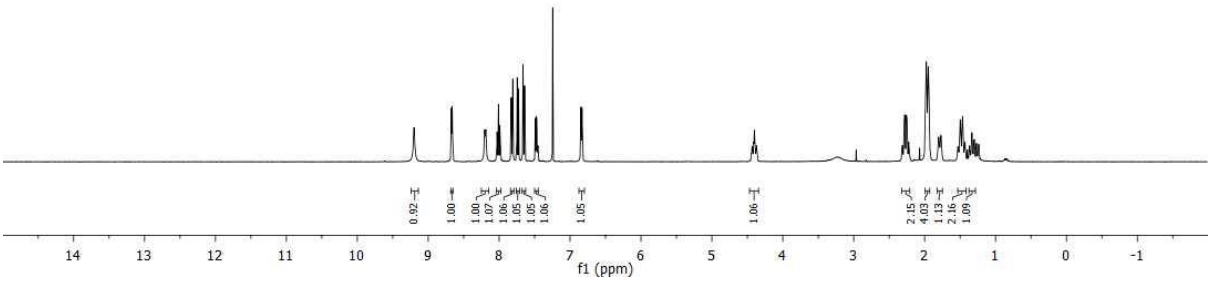
HM-412
single pulse decoupled gated NOE



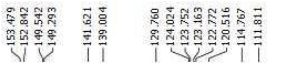


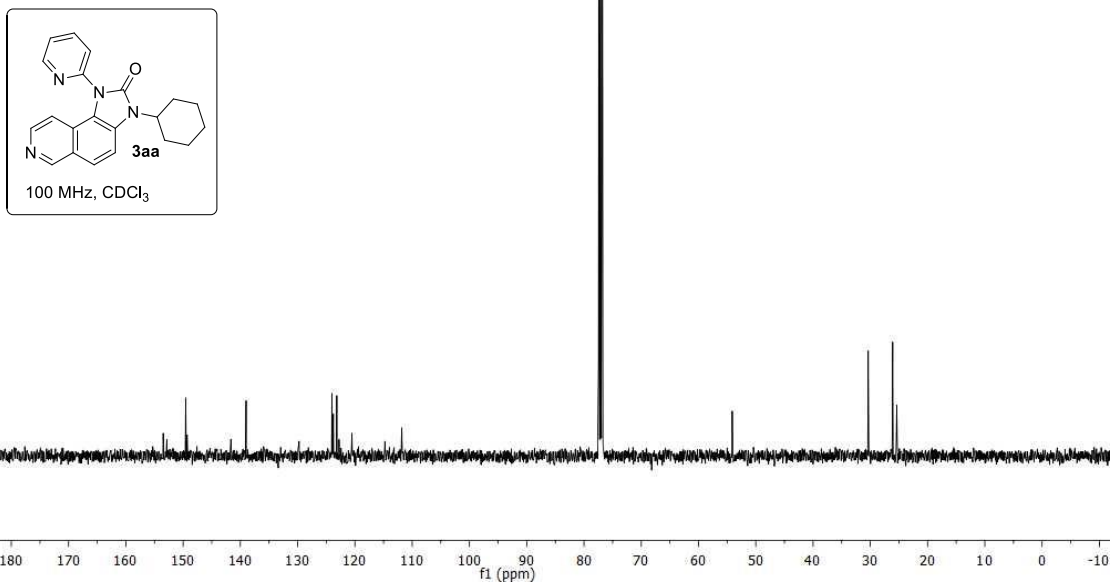
HM-644
single_pulse



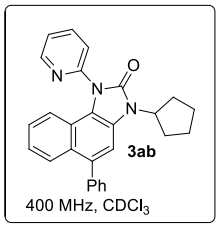


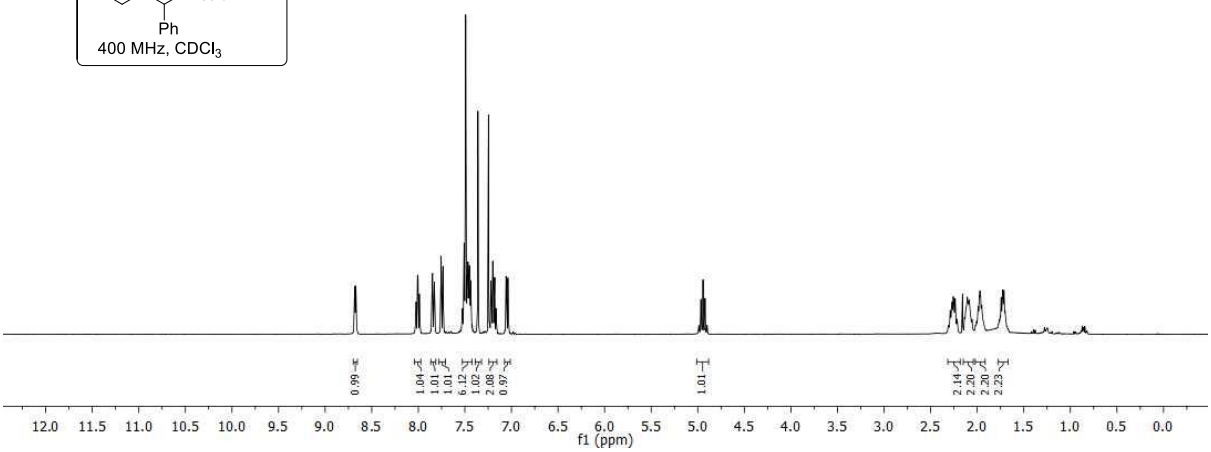
HM-644
single pulse decoupled gated NOE

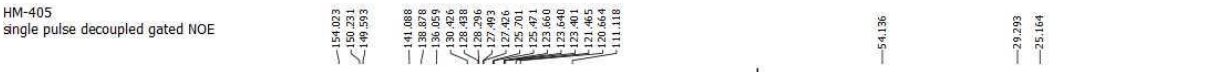


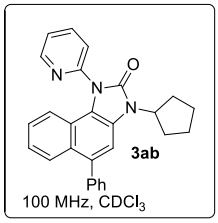



HM-405
single_pulse

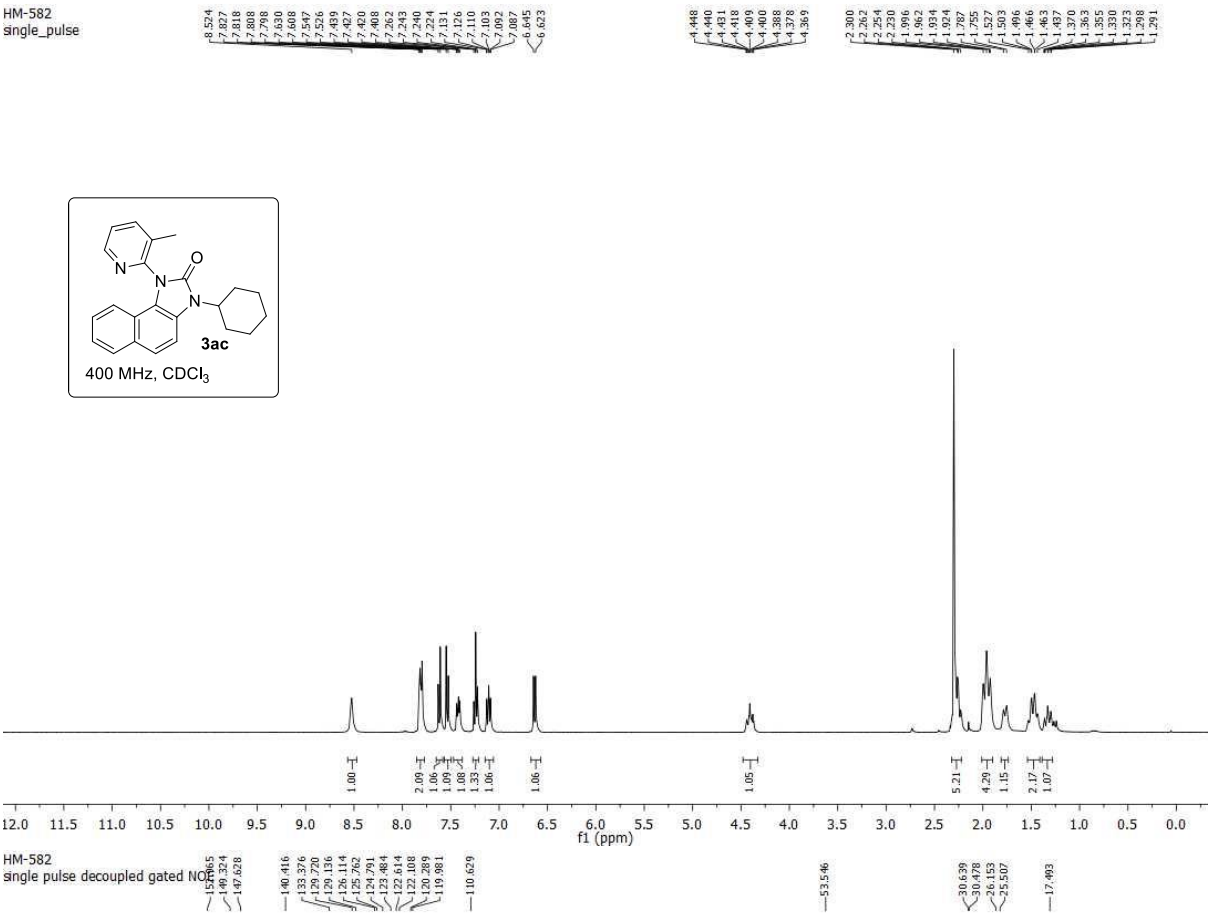

3ab
Ph
400 MHz, CDCl3


f1 (ppm)

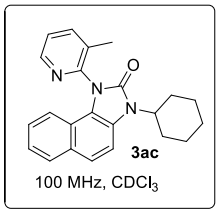

HM-405
single pulse decoupled gated NOE

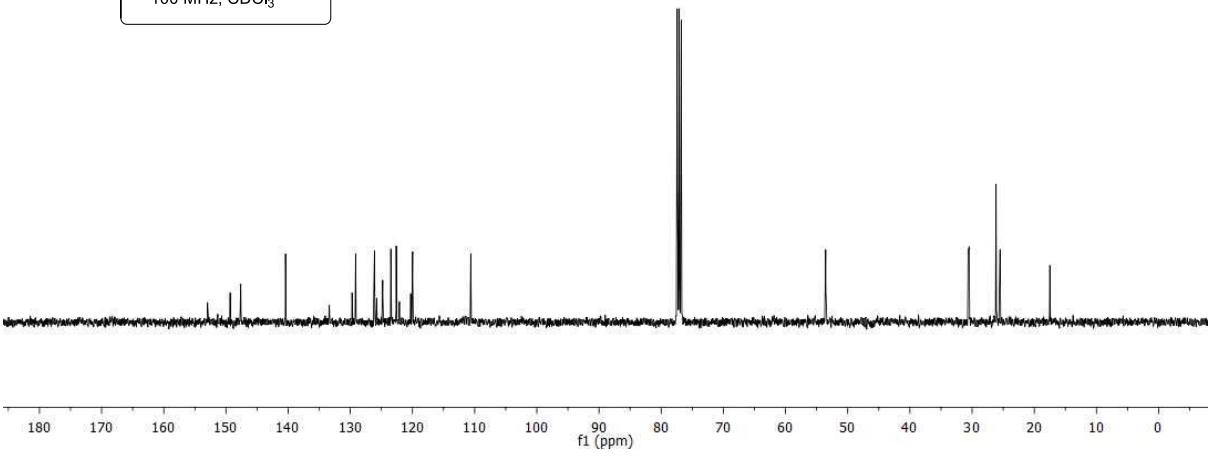

3ab
Ph
100 MHz, CDCl3

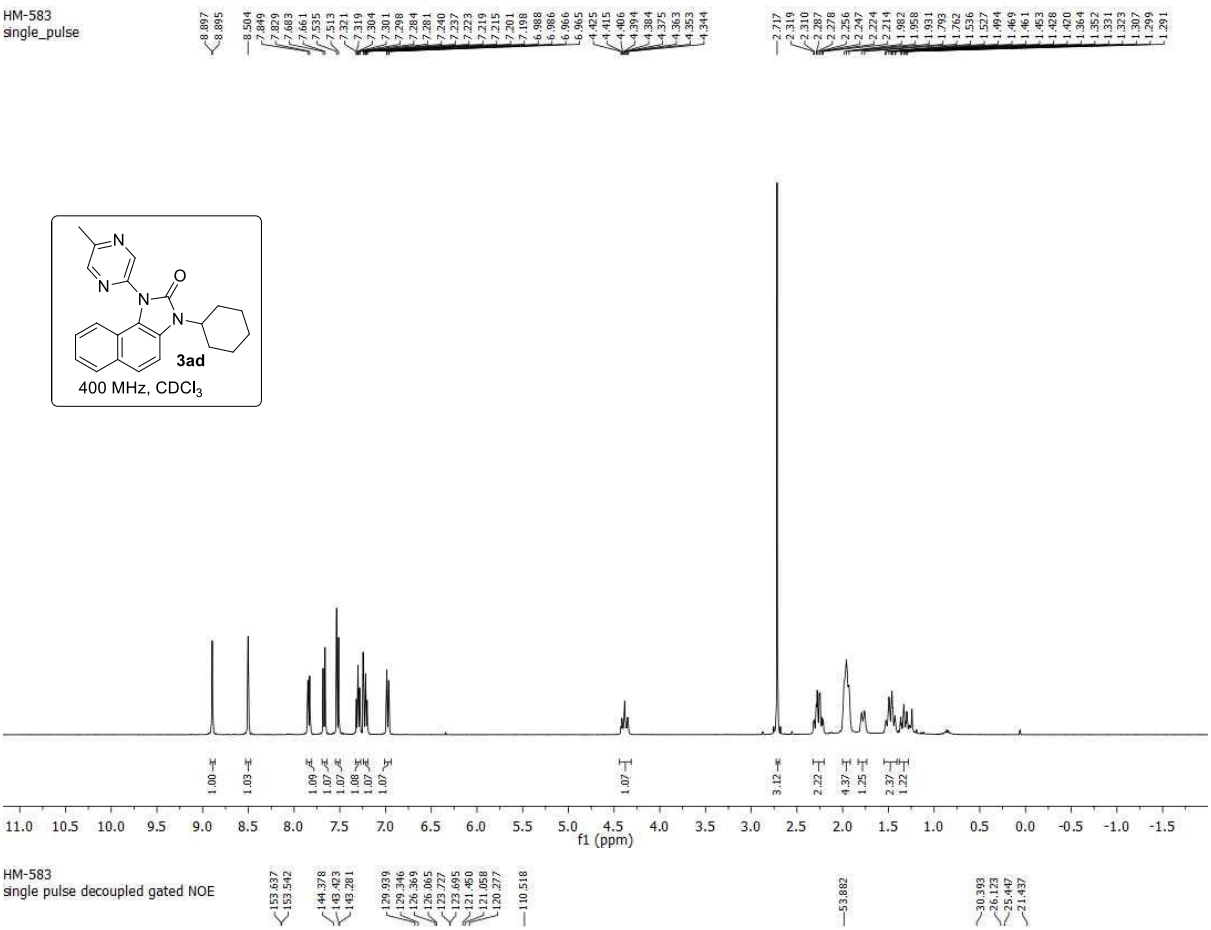
f1 (ppm)


HM-582
single_pulse
3ac
400 MHz, CDCl3
f1 (ppm)

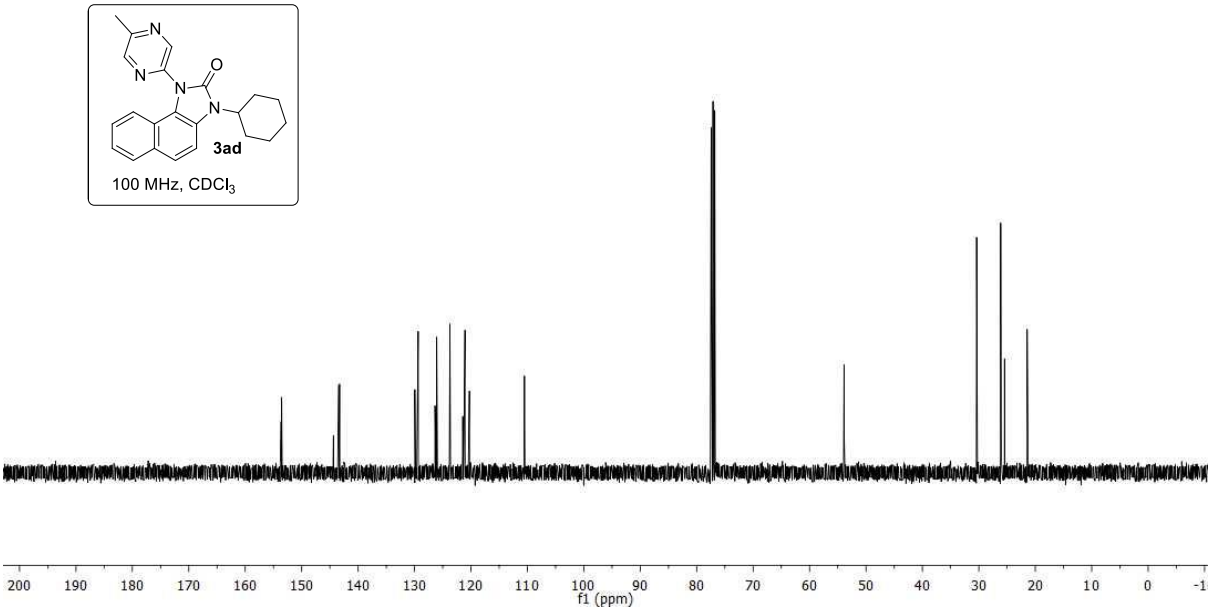
HM-582
single pulse decoupled gated NOE
f1 (ppm)


3ac
100 MHz, CDCl3

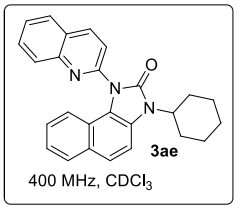

f1 (ppm)

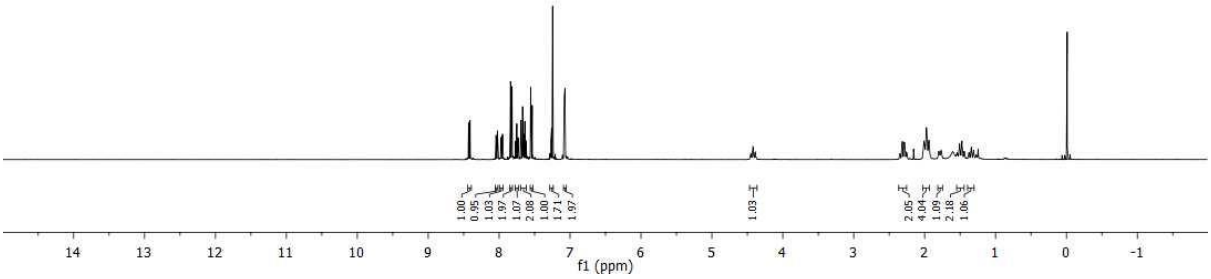

HM-583
single_pulse
3ad
400 MHz, CDCl3
f1 (ppm)

HM-583
single pulse decoupled gated NOE

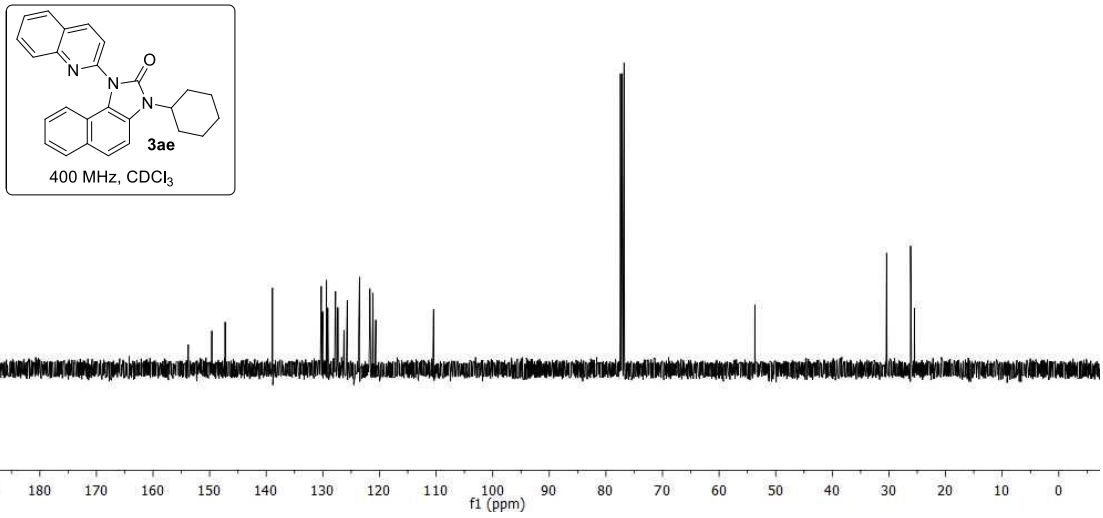

3ad
100 MHz, CDCl3
f1 (ppm)

HM-584
single_pulse

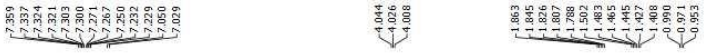


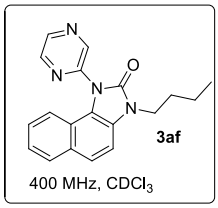


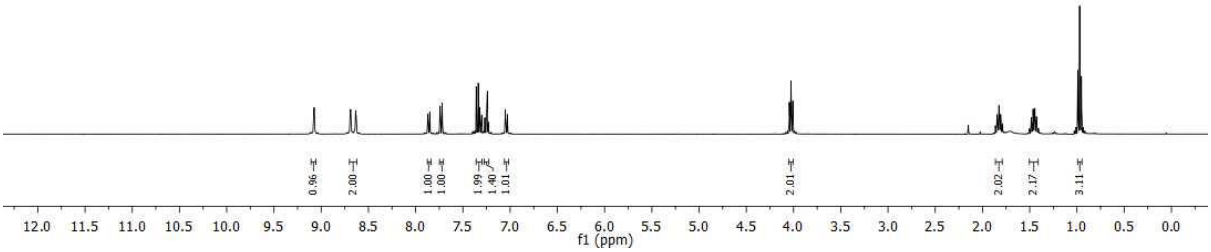
HM-584
single pulse decoupled gated NOE



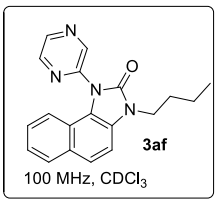
HM-426
single_pulse

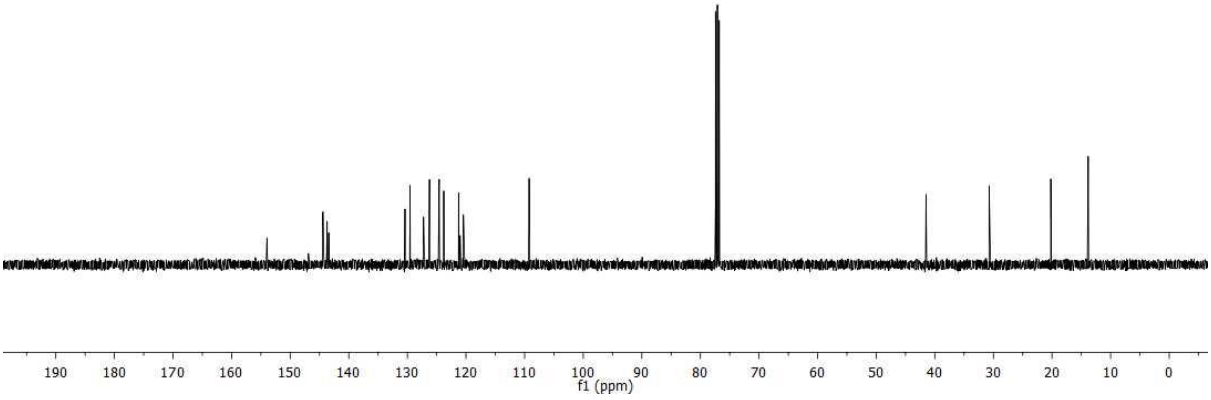


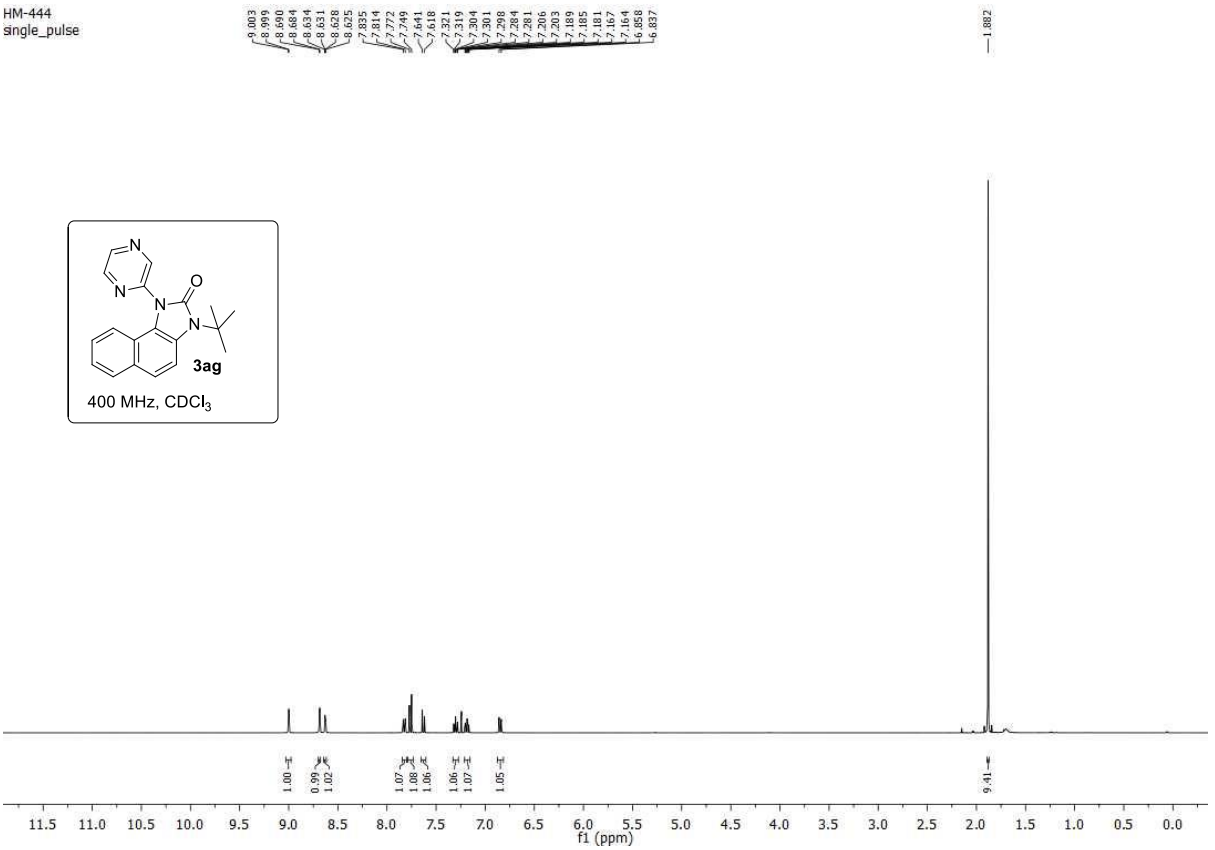


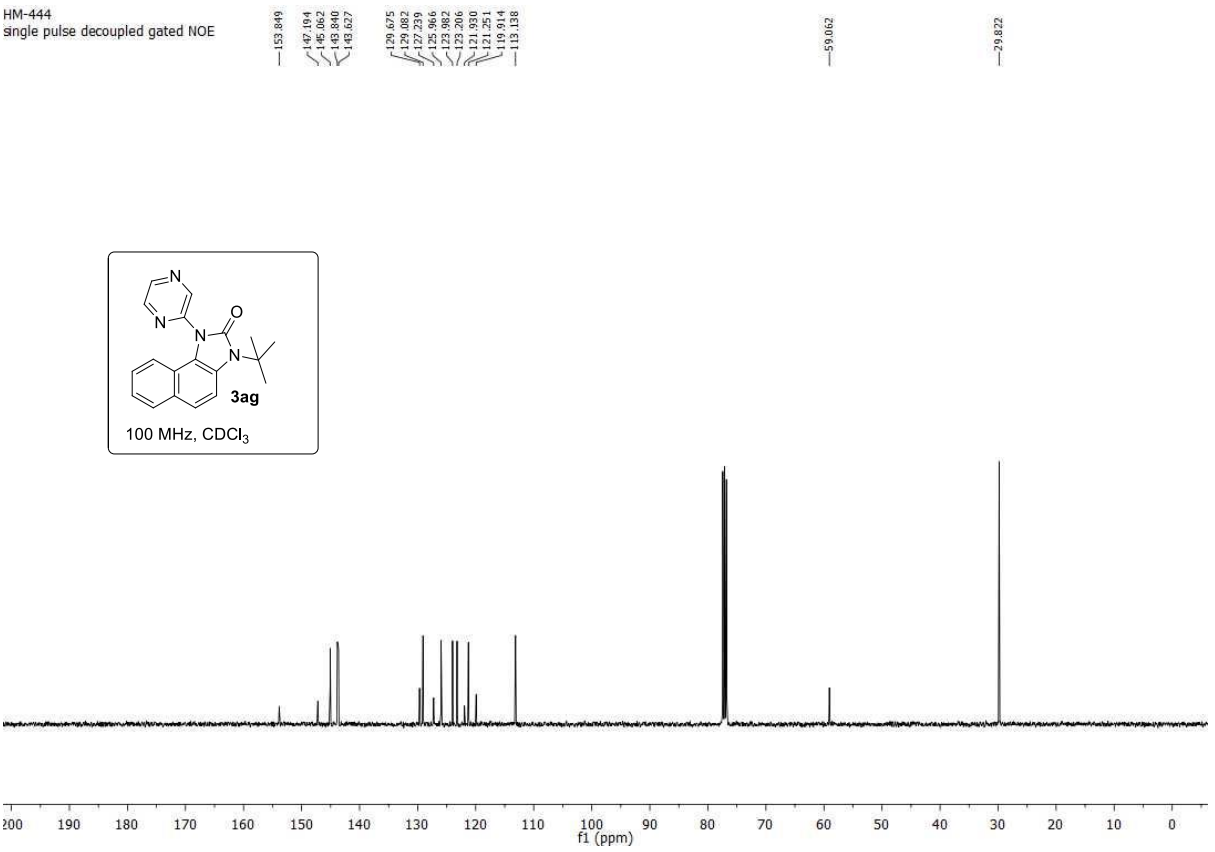


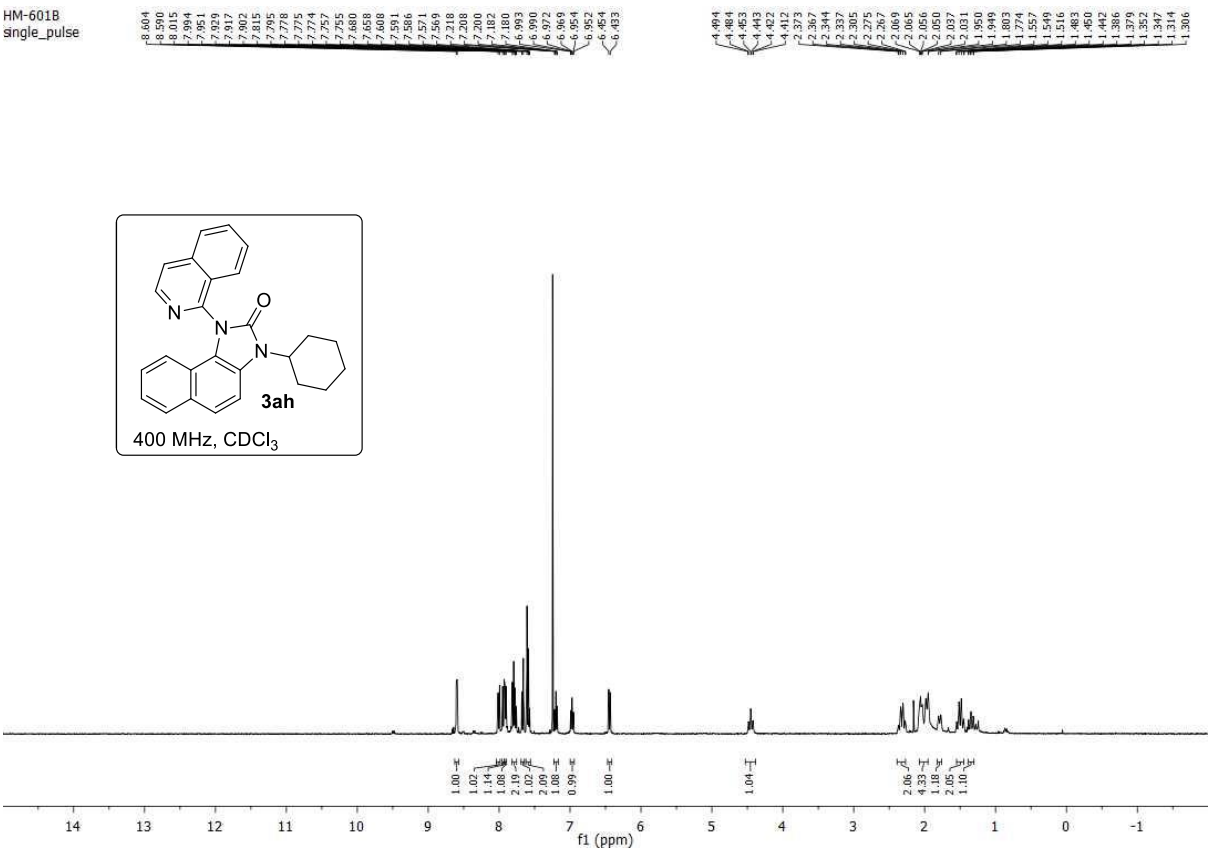
HM-426
single pulse decoupled gated NOE

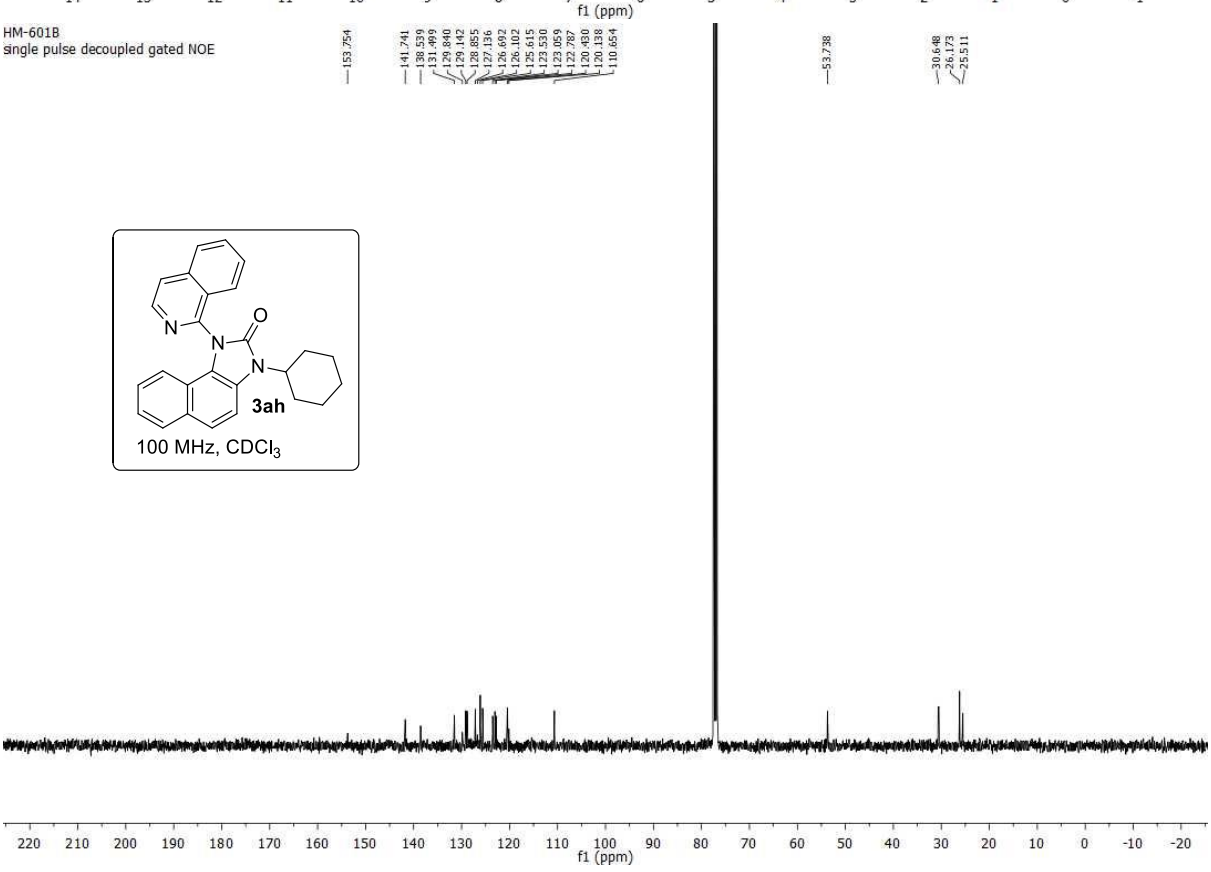


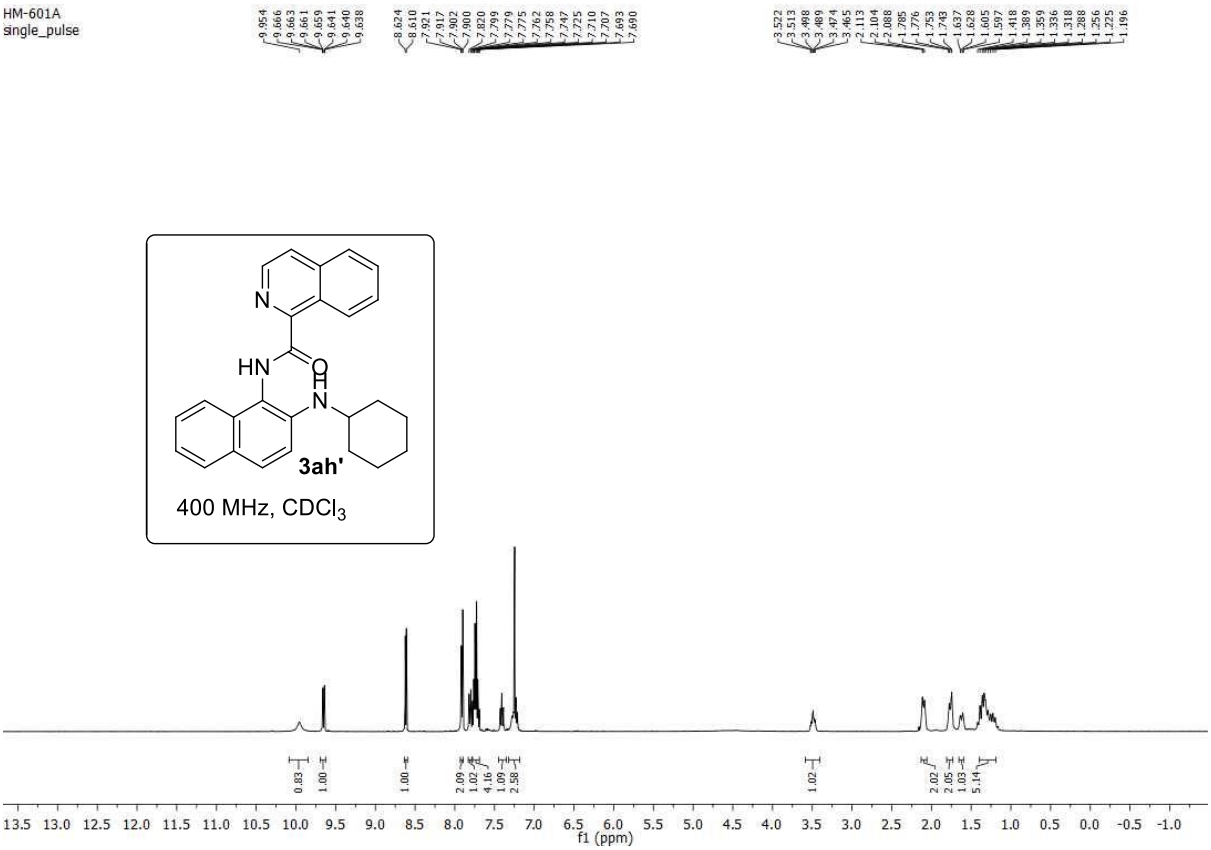


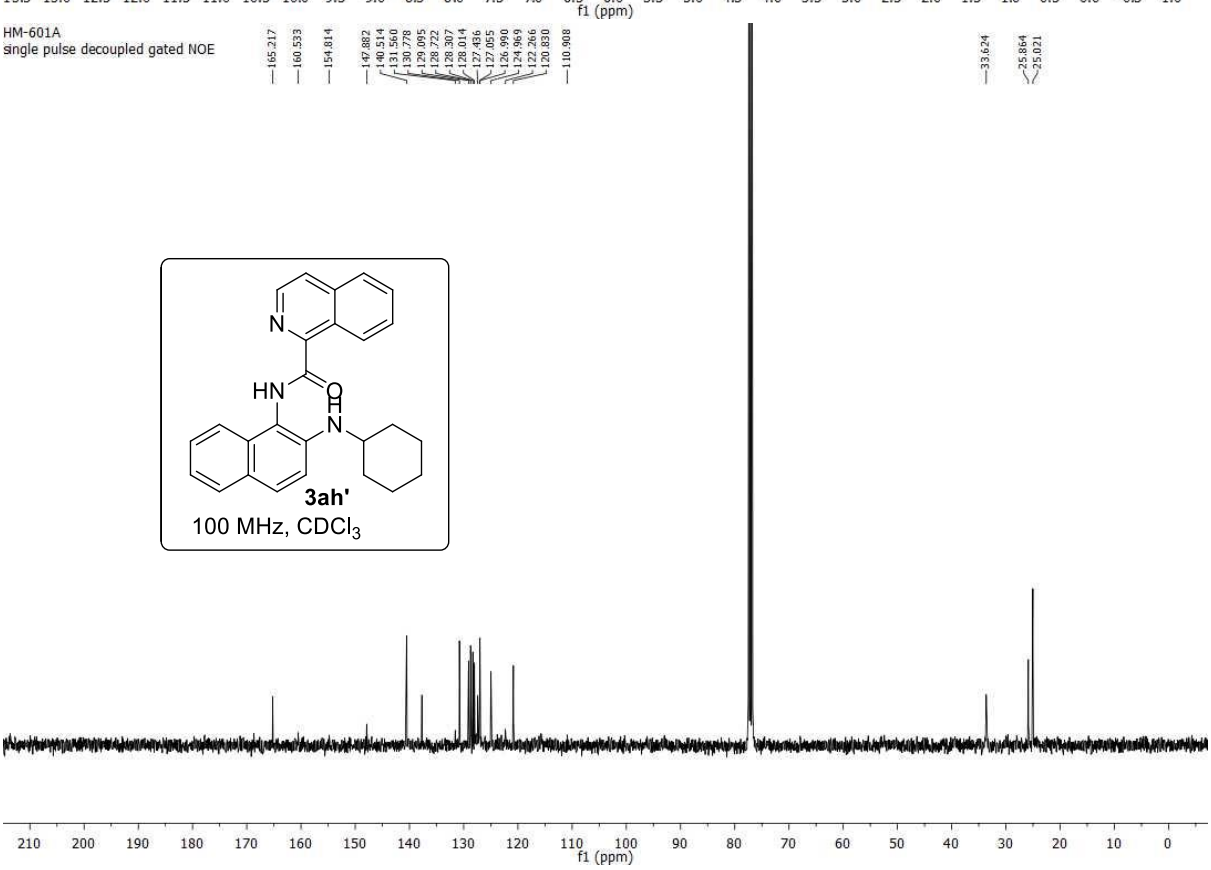

HM-444
single_pulse
3ag
400 MHz, CDCl3
f1 (ppm)

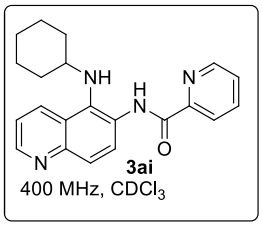

HM-444
single pulse decoupled gated NOE
3ag
100 MHz, CDCl3
f1 (ppm)

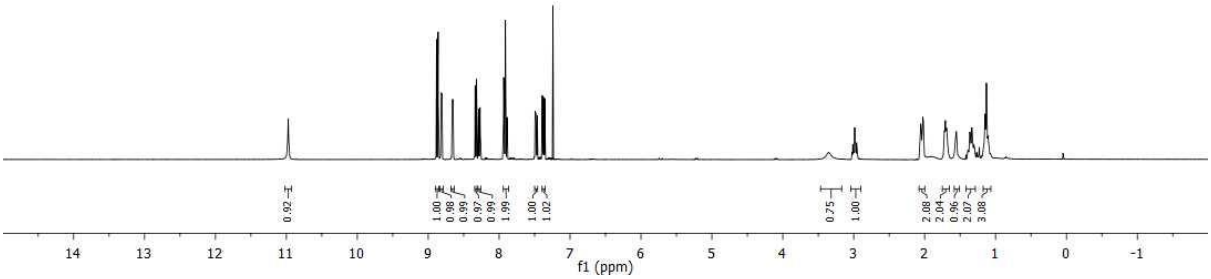

HM-601B
single_pulse
3ah
400 MHz, CDCl3
f1 (ppm)


HM-601B
single pulse decoupled gated NOE
3ah
100 MHz, CDCl3
f1 (ppm)

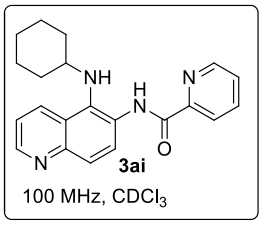

HM-601A
single_pulse
3ah'
400 MHz, CDCl3
f1 (ppm)

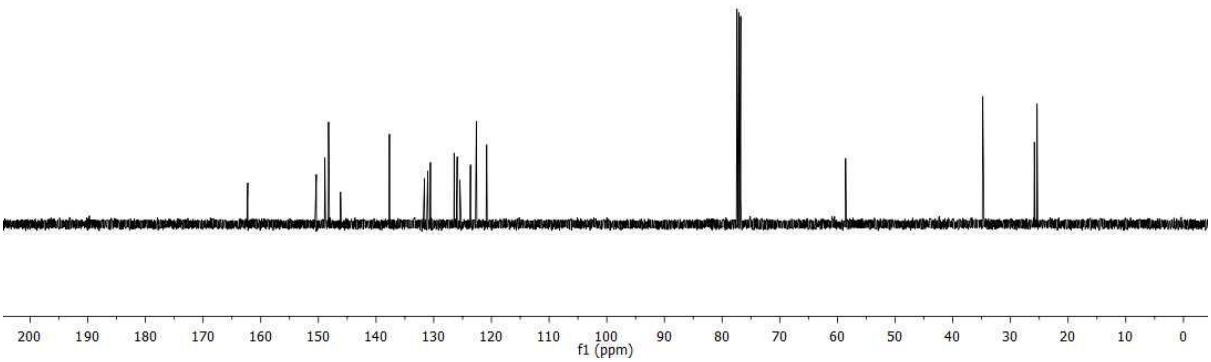

HM-601A
single pulse decoupled gated NOE
3ah'
100 MHz, CDCl3
f1 (ppm)

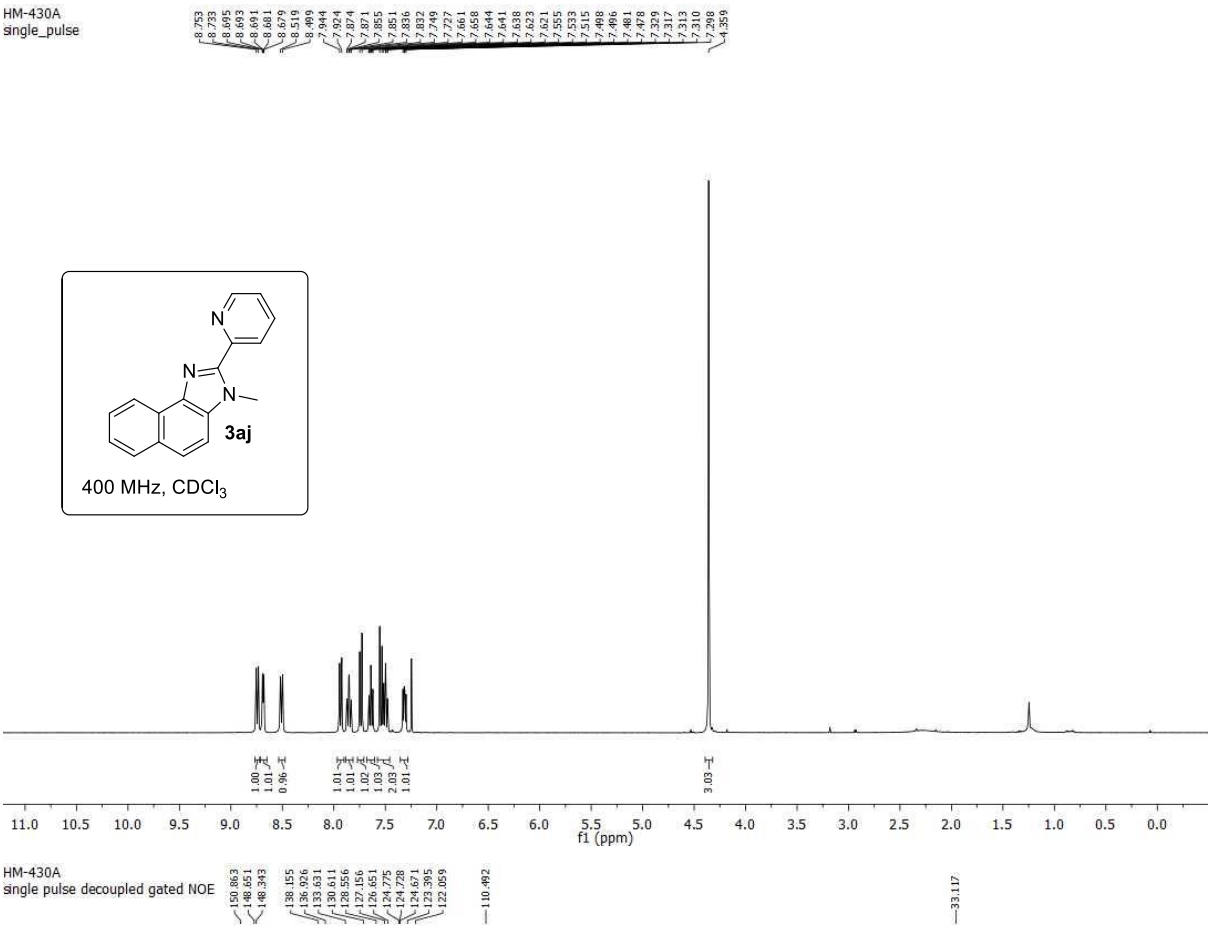

NH
H
N
N
O
N
3ai
400 MHz, CDCl3

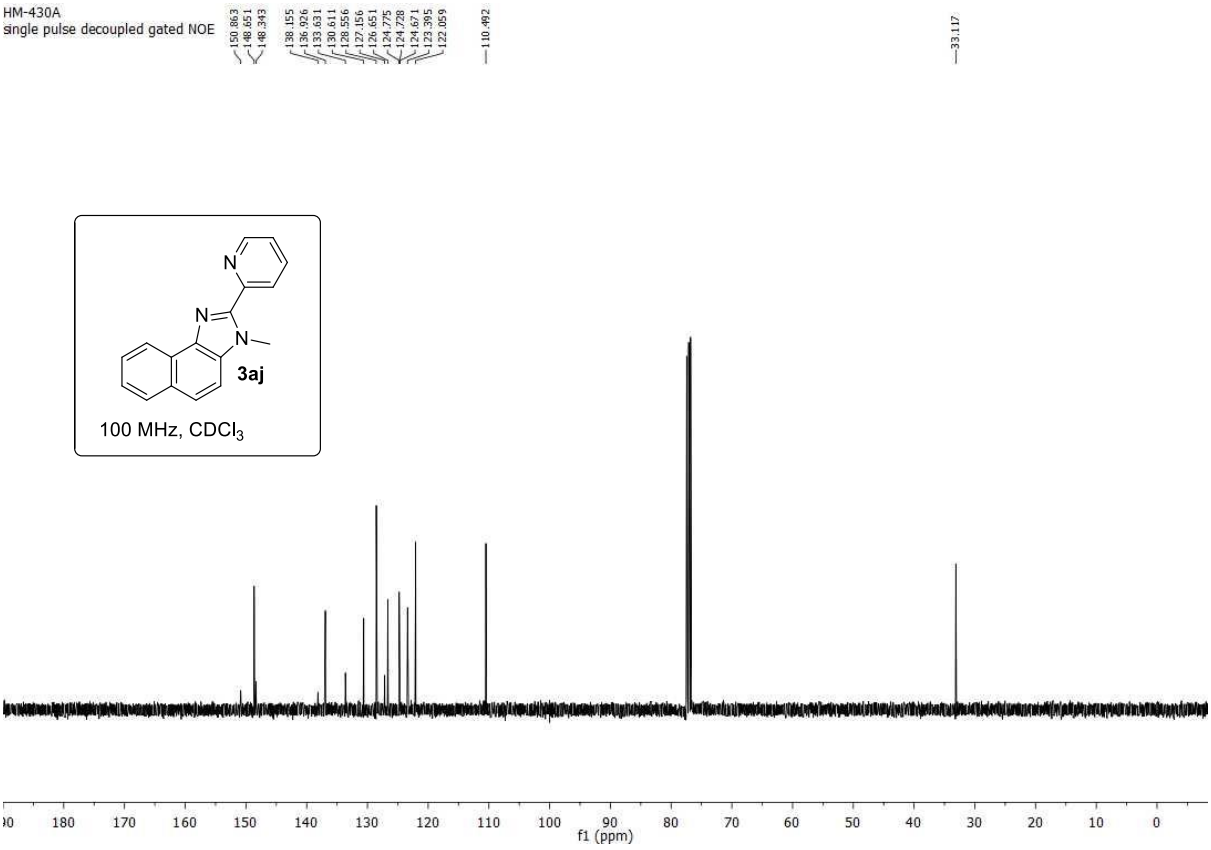

f1 (ppm)

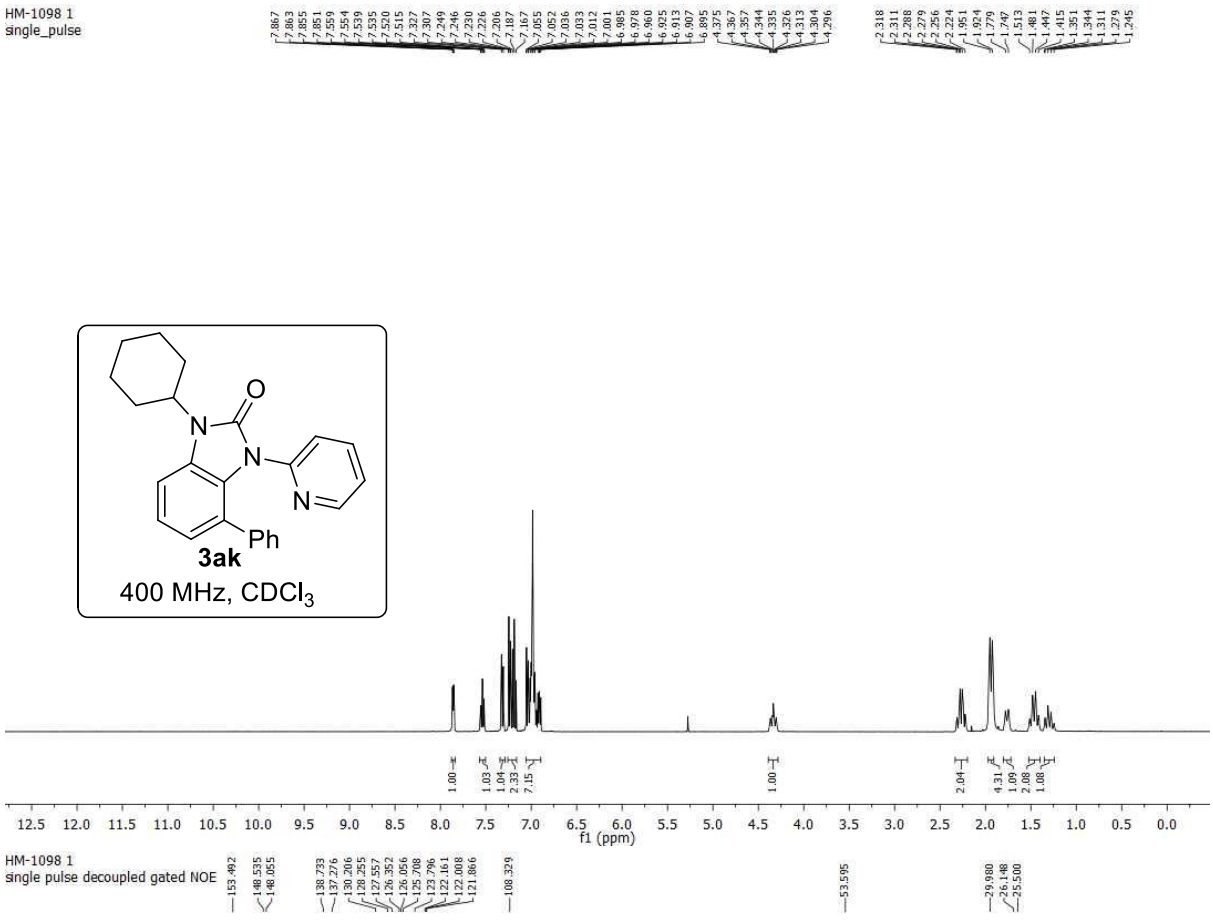

HM-421 1
single pulse decoupled gated NOE

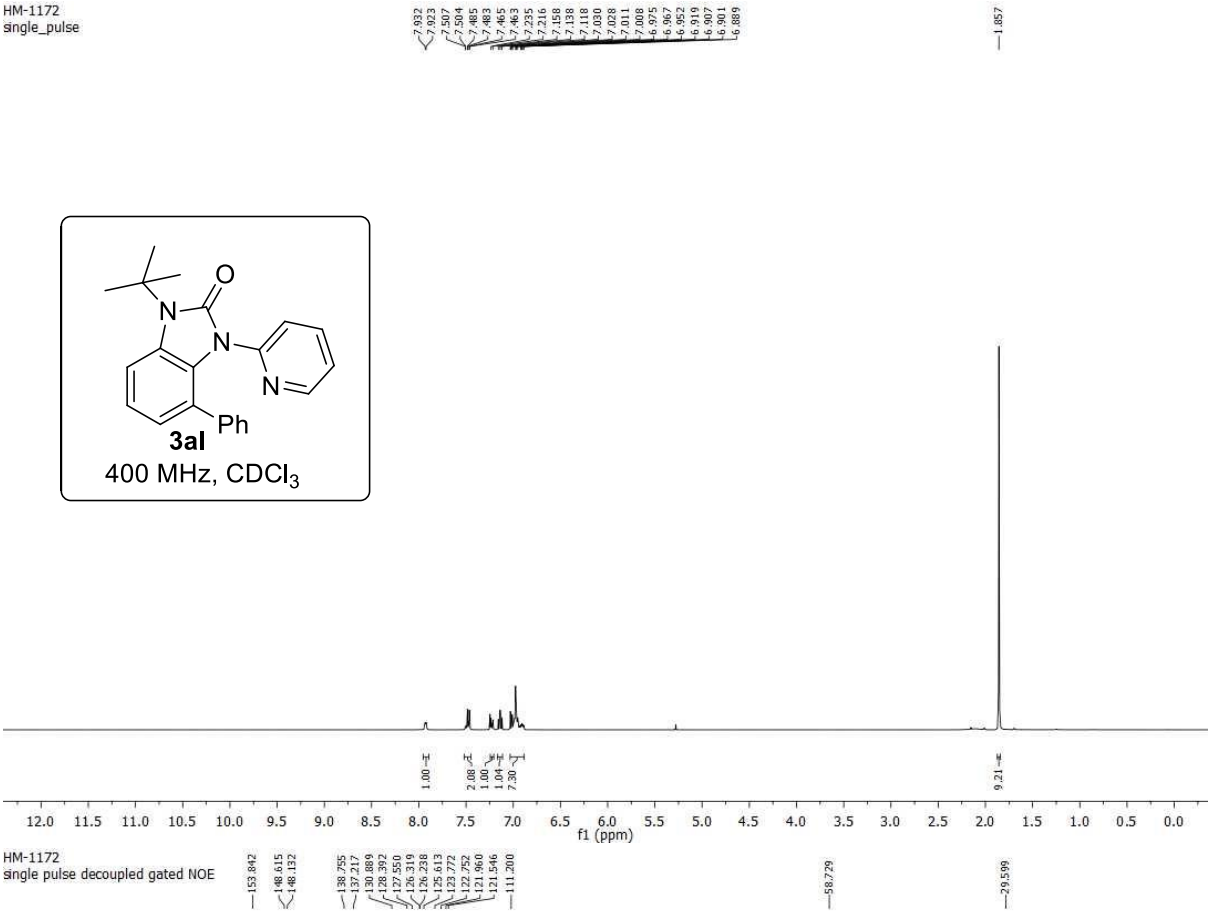

NH
H
N
N
O
N
3ai
100 MHz, CDCl3

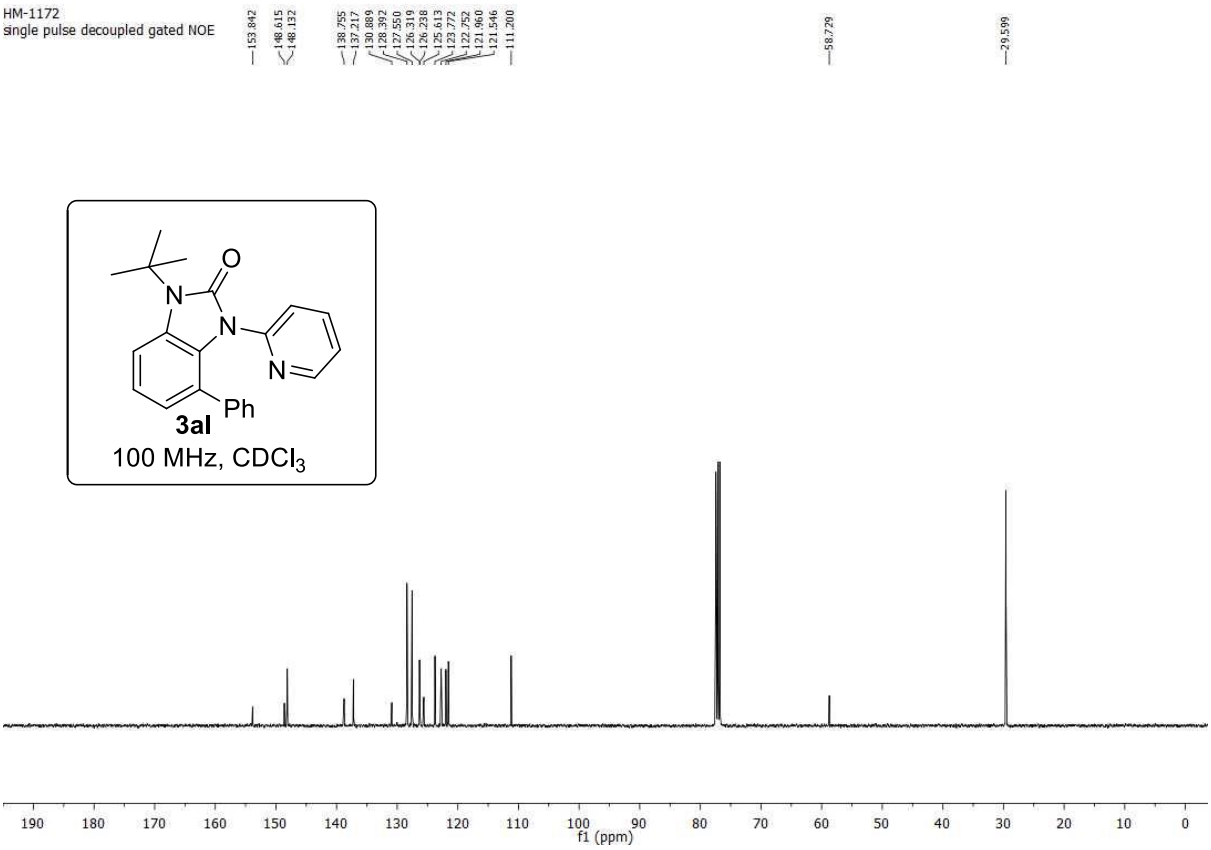

f1 (ppm)

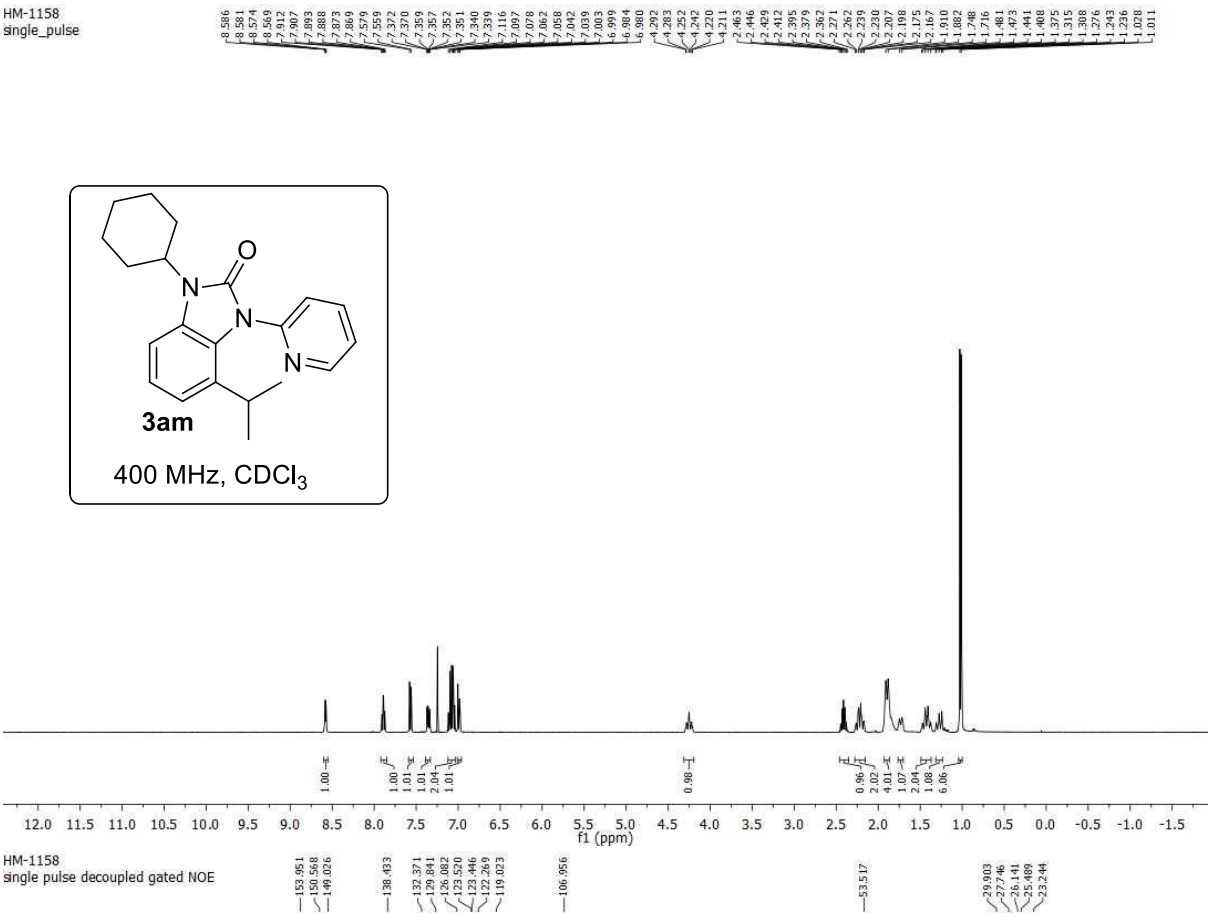

HM-430A
single_pulse
3aj
400 MHz, CDCl3
f1 (ppm)


HM-430A
single pulse decoupled gated NOE
3aj
100 MHz, CDCl3
f1 (ppm)

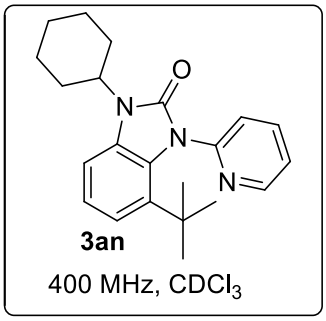

HM-1098 1
single_pulse
3ak
400 MHz, CDCl3
f1 (ppm)
HM-1098 1
single pulse decoupled gated NOE
3ak
100 MHz, CDCl3
f1 (ppm)


HM-1172
single_pulse
3al
400 MHz, CDCl3
f1 (ppm)

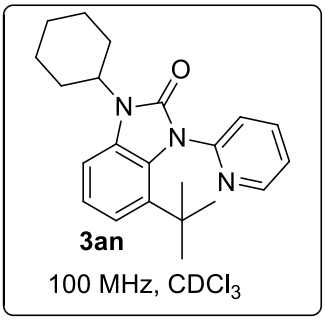

HM-1172
single pulse decoupled gated NOE
3al
100 MHz, CDCl3
f1 (ppm)

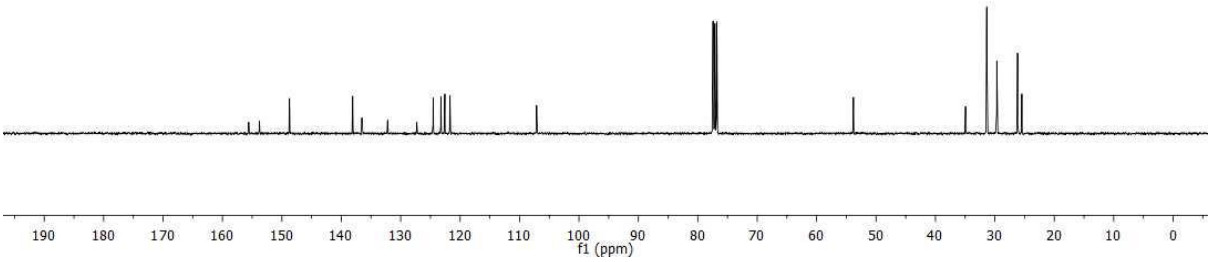

HM-1158
single_pulse
3am
400 MHz, CDCl3
f1 (ppm)
HM-1158
single pulse decoupled gated NOE
3am
100 MHz, CDCl3
f1 (ppm)

HM-1168
single_pulse

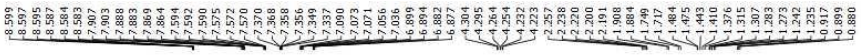


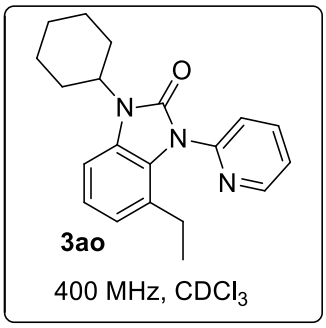
HM-1168
single pulse decoupled gated NOE

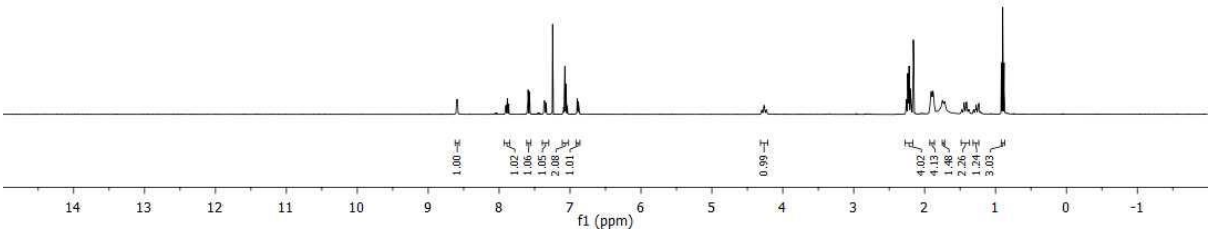




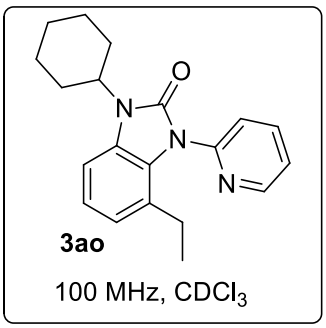
HM-1147
single_pulse



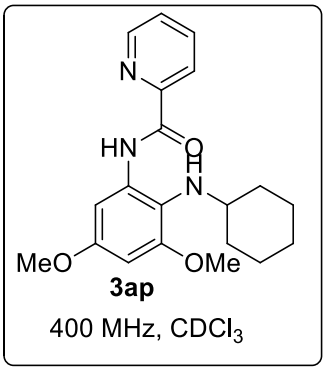




HM-1147
single pulse decoupled gated NOE

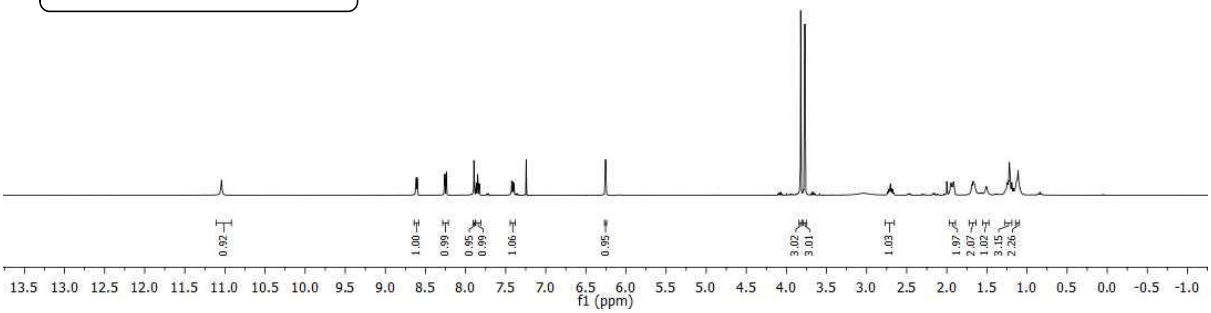


HM-1130
single_pulse

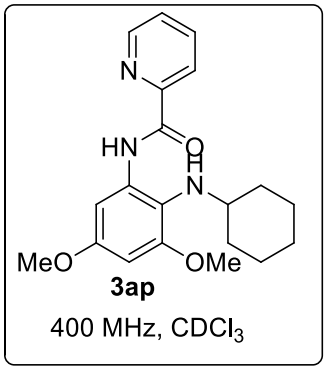


3ap

400 MHz, $CDCl_3$

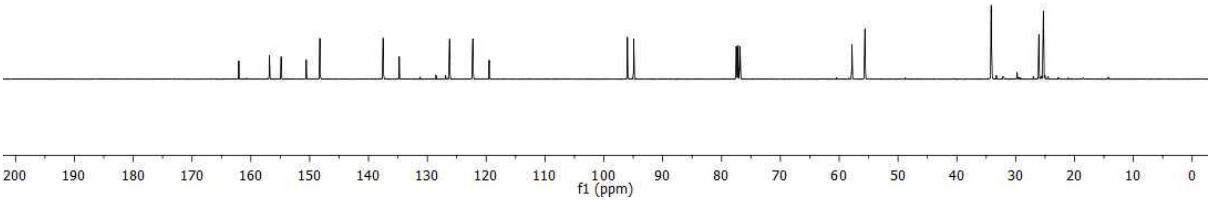


HM-1130
single pulse decoupled gated NOE

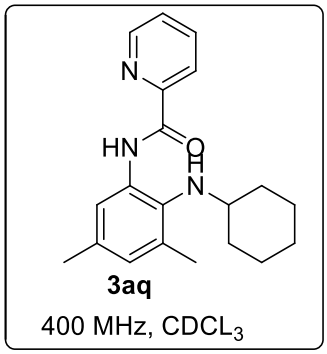


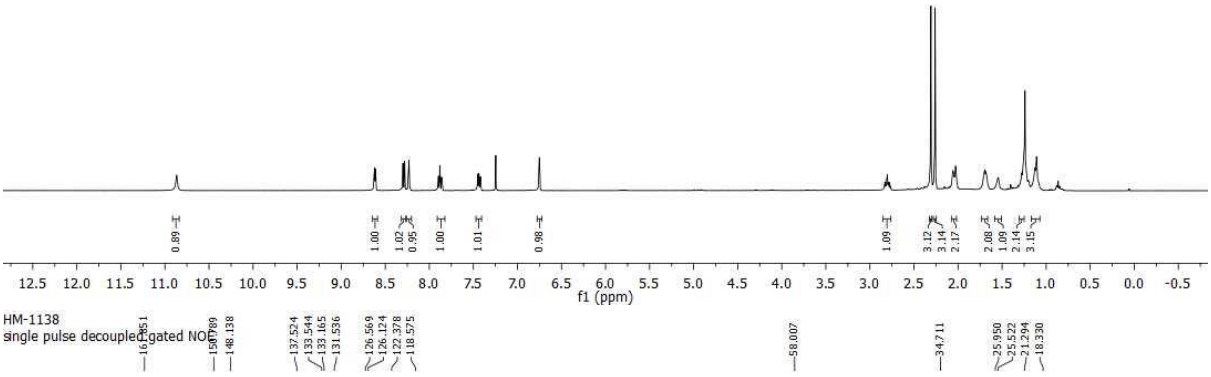
3ap

400 MHz, $CDCl_3$

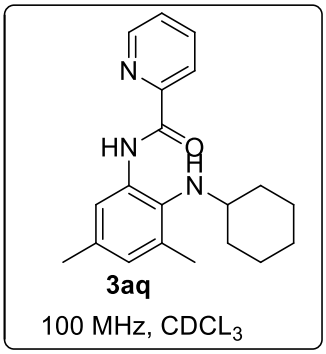


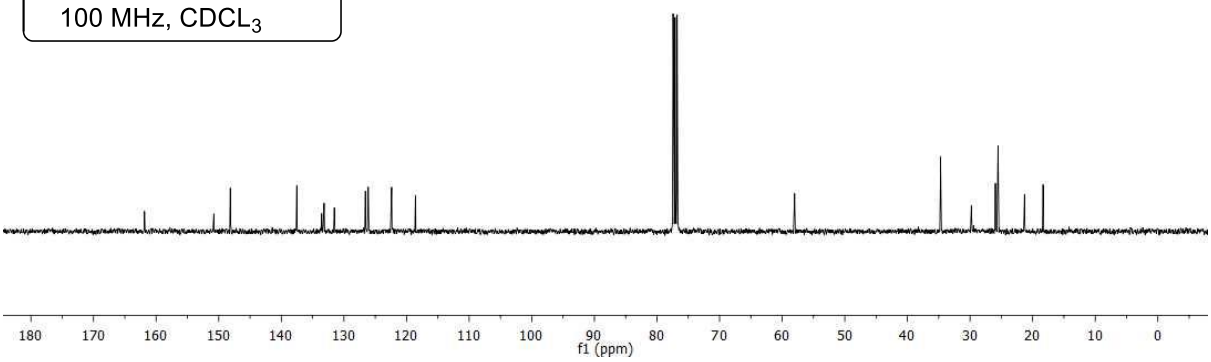

HM-1138
single_pulse


3aq
400 MHz, CDCL3

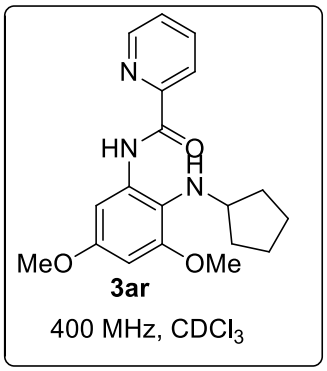

f1 (ppm)

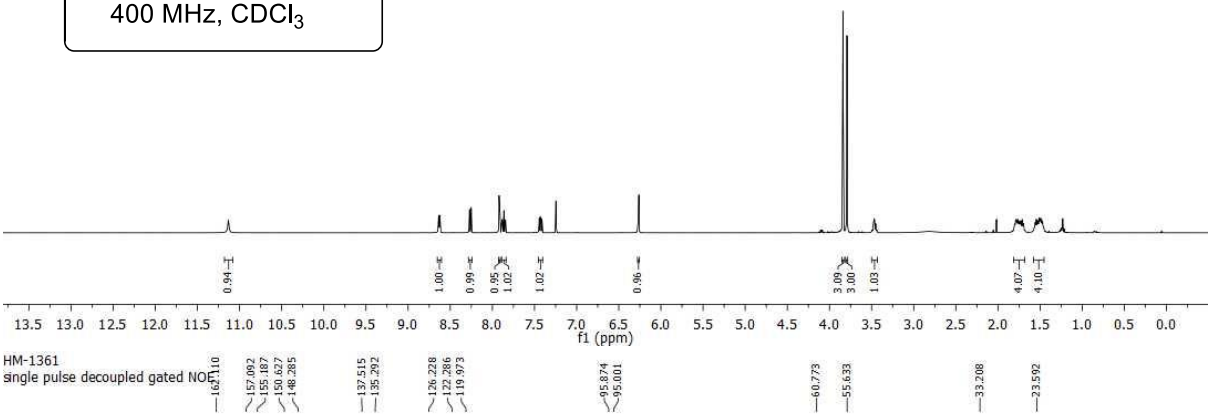
HM-1138
single pulse decoupled gated NOE

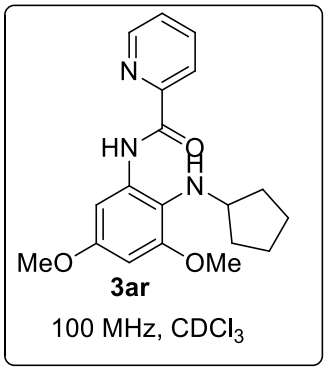

3aq
100 MHz, CDCL3

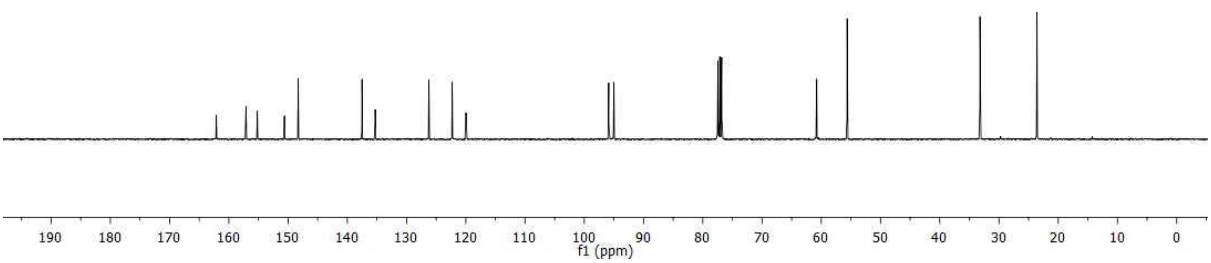

f1 (ppm)


HM-1361
single_pulse

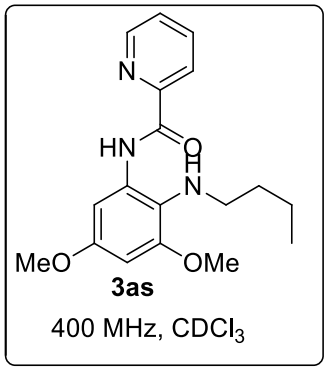

HN
O
H
N
MeO
OMe
3ar
400 MHz, CDCl3

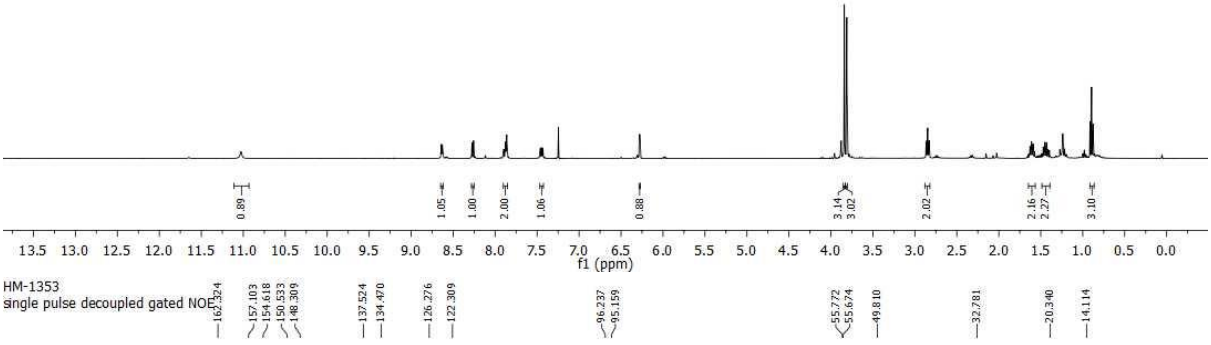

f1 (ppm)
HM-1361
single pulse decoupled gated NOE


HN
O
H
N
MeO
OMe
3ar
100 MHz, CDCl3

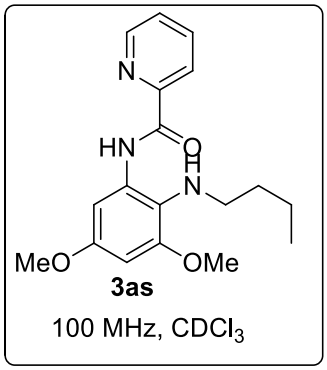

f1 (ppm)

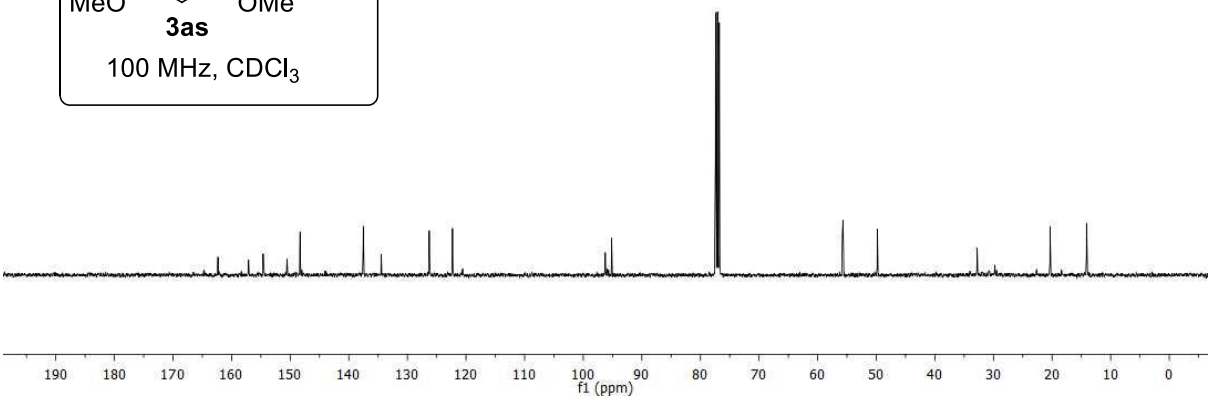

HM-1353
single_pulse


N
HN
O
N
MeO
OMe
3as
400 MHz, CDCl3

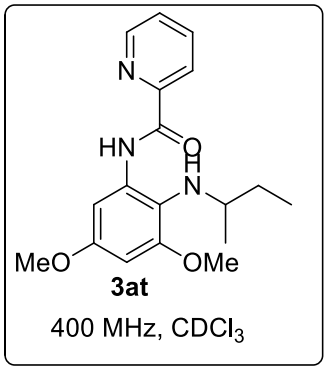

f1 (ppm)

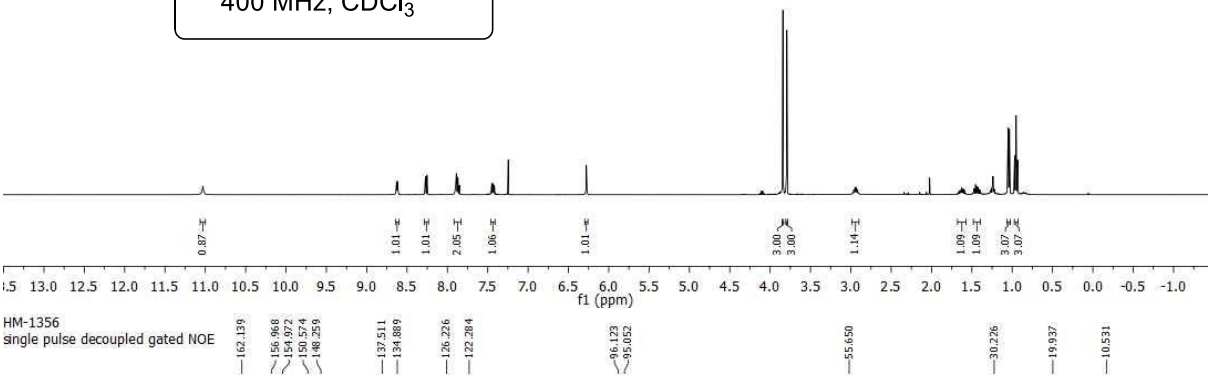
HM-1353
single pulse decoupled gated NOE


N
HN
O
N
MeO
OMe
3as
100 MHz, CDCl3

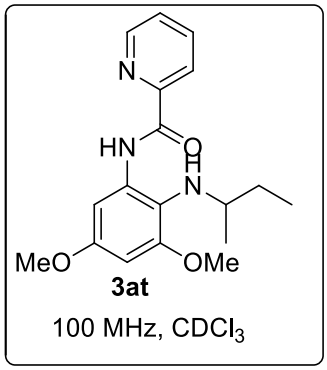

f1 (ppm)

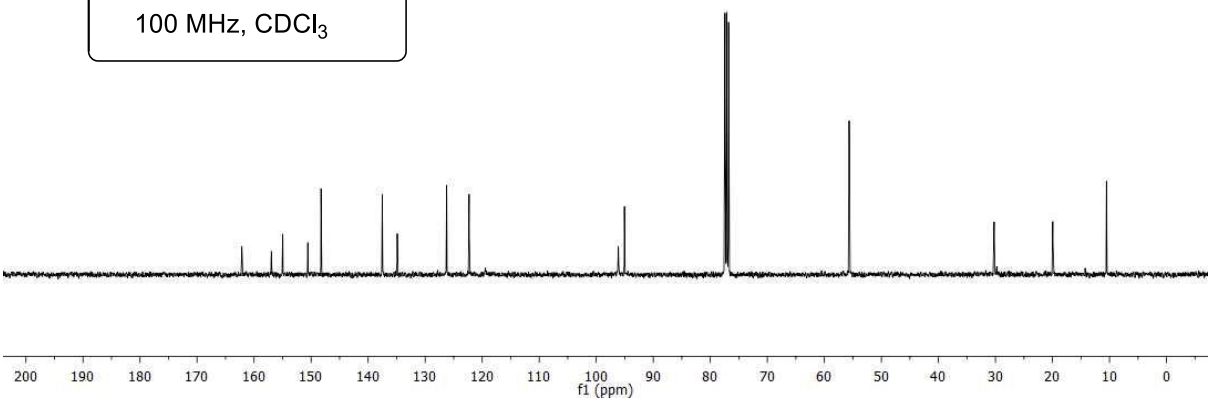

HM-1356
single_pulse


N
HN
O
H
N
MeO
OMe
3at
400 MHz, CDCl3

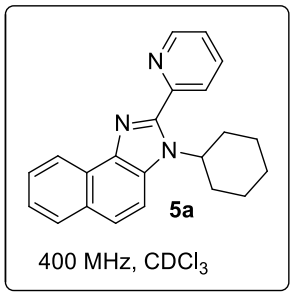

f1 (ppm)

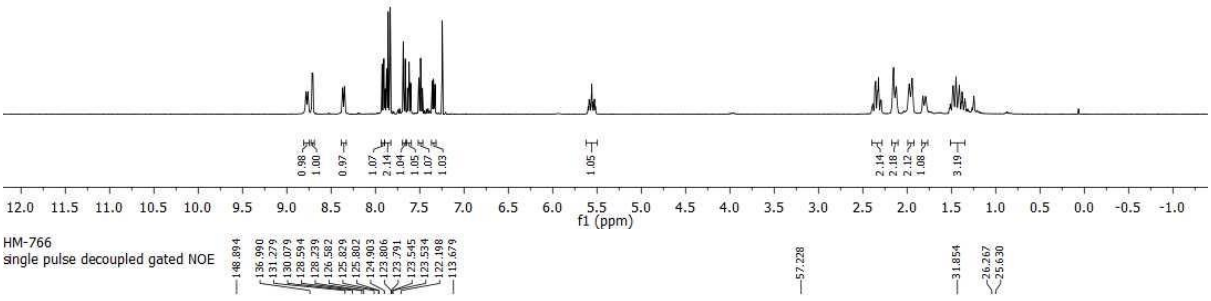
HM-1356
single pulse decoupled gated NOE


N
HN
O
H
N
MeO
OMe
3at
100 MHz, CDCl3

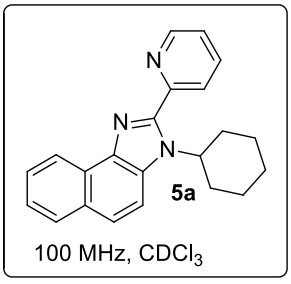

f1 (ppm)

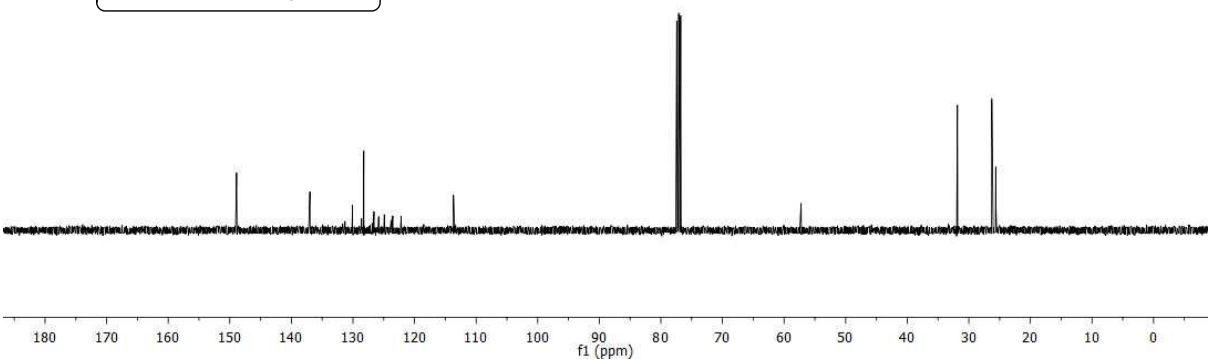

HM-766
single_pulse

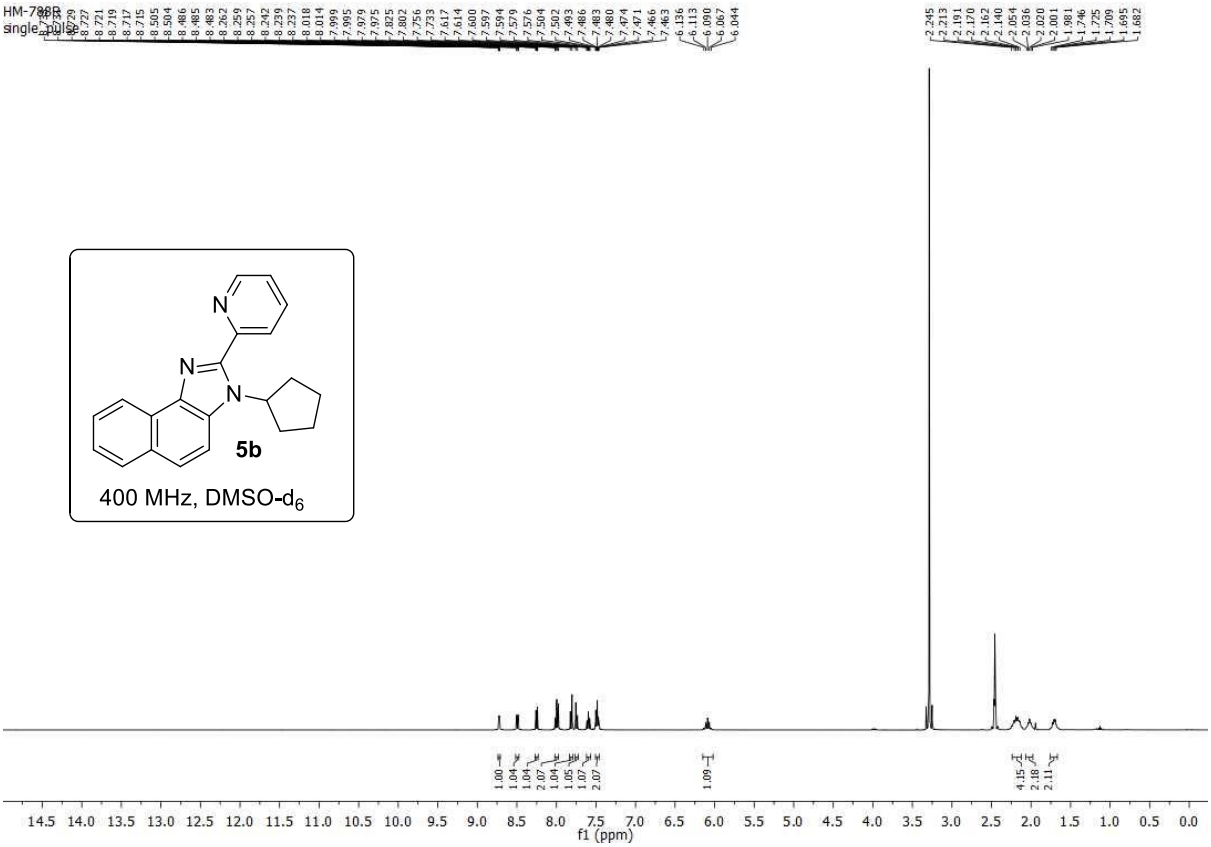

5a
400 MHz, CDCl3

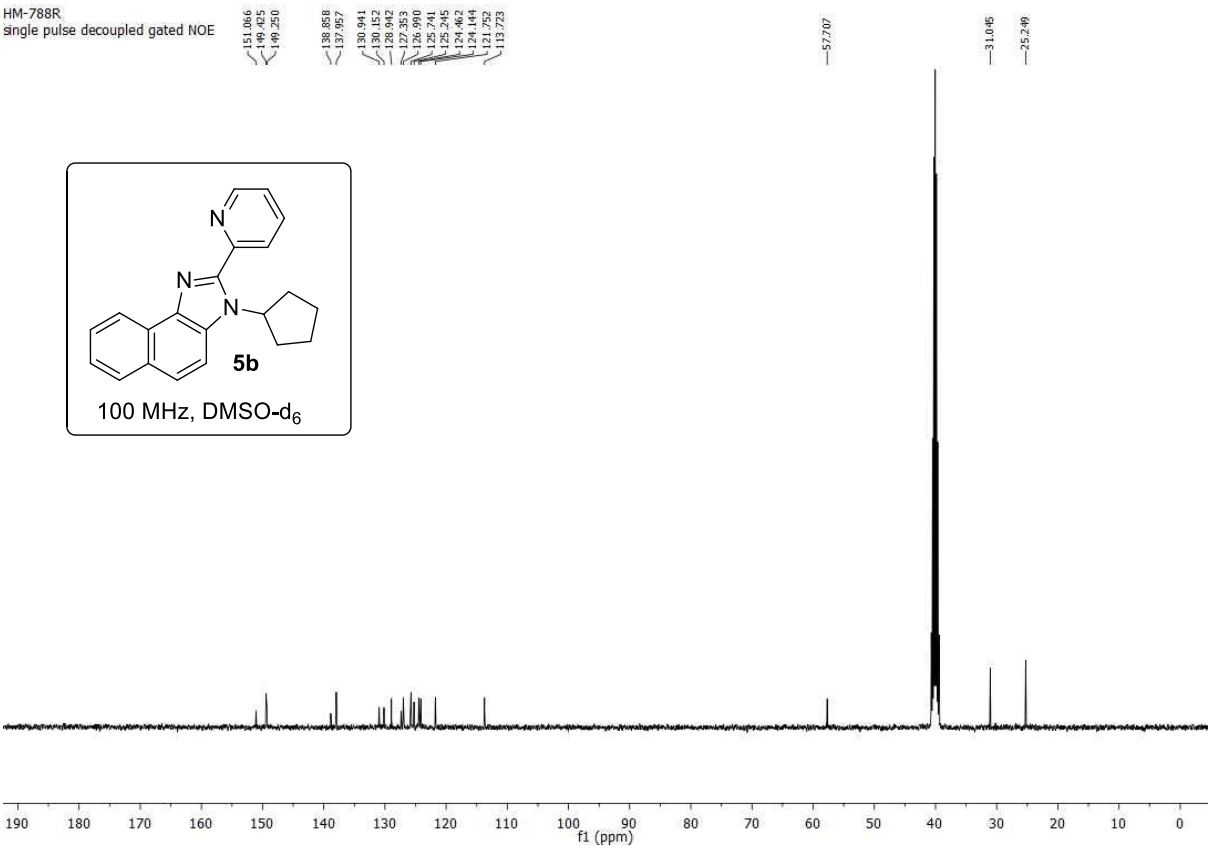

0.98
1.00
0.97
1.07
2.14
1.04
1.05
1.07
1.03
1.05
2.14
2.18
2.12
1.08
3.19
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

HM-766
single pulse decoupled gated NOE
148.894
136.990
131.279
130.979
128.994
128.239
126.592
125.822
125.802
124.903
123.806
123.791
123.545
123.534
122.198
113.679
57.228
31.854
26.267
25.630

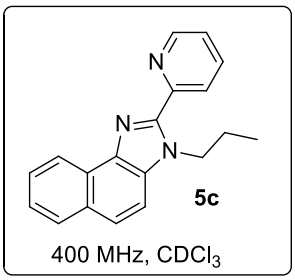

5a
100 MHz, CDCl3

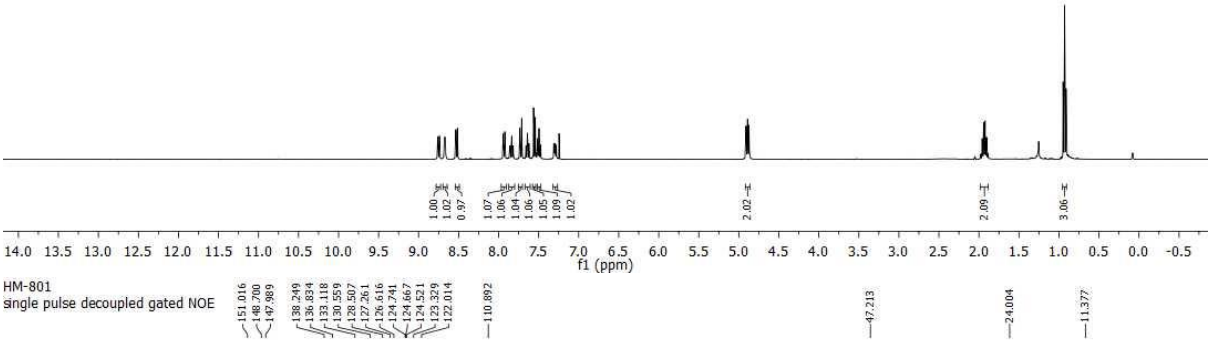

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

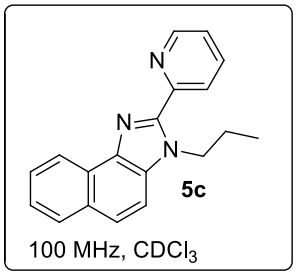

HM-788R
single pulse
5b
400 MHz, DMSO-d6
f1 (ppm)

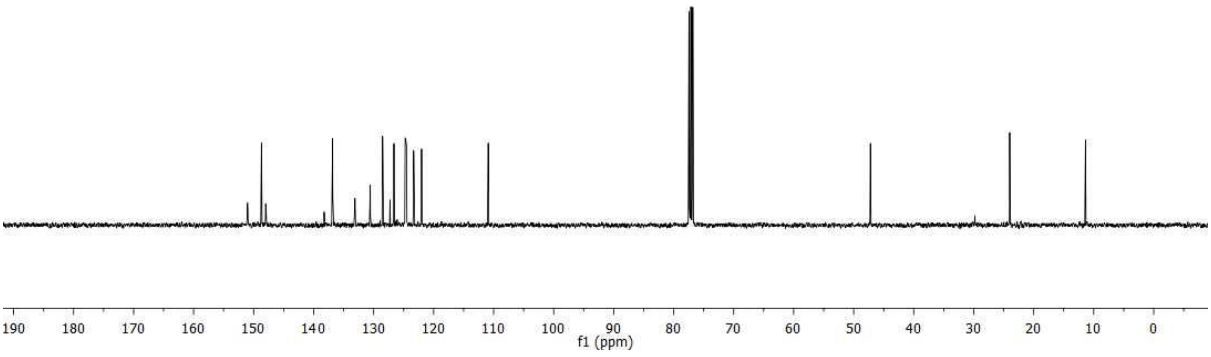

HM-788R
single pulse decoupled gated NOE
5b
100 MHz, DMSO-d6
f1 (ppm)

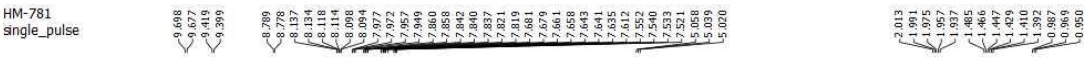

HM-801
single_pulse

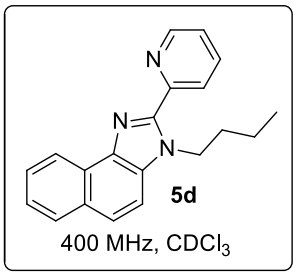

5c
400 MHz, CDCl3

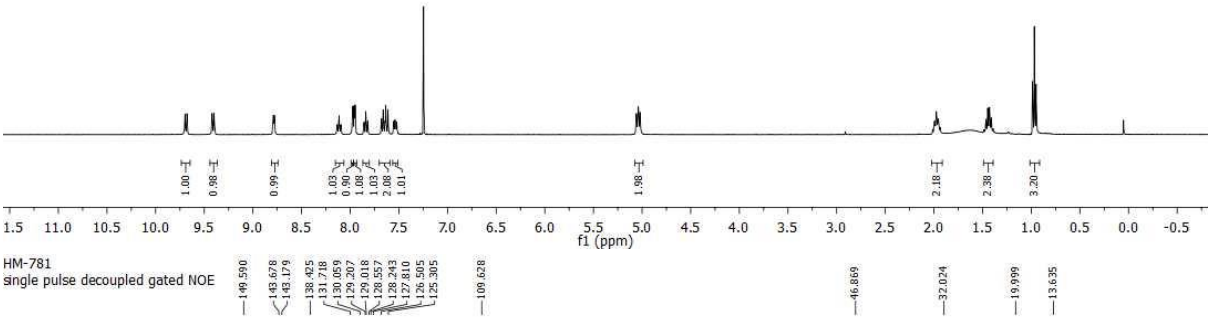

f1 (ppm)
HM-801
single pulse decoupled gated NOE


5c
100 MHz, CDCl3

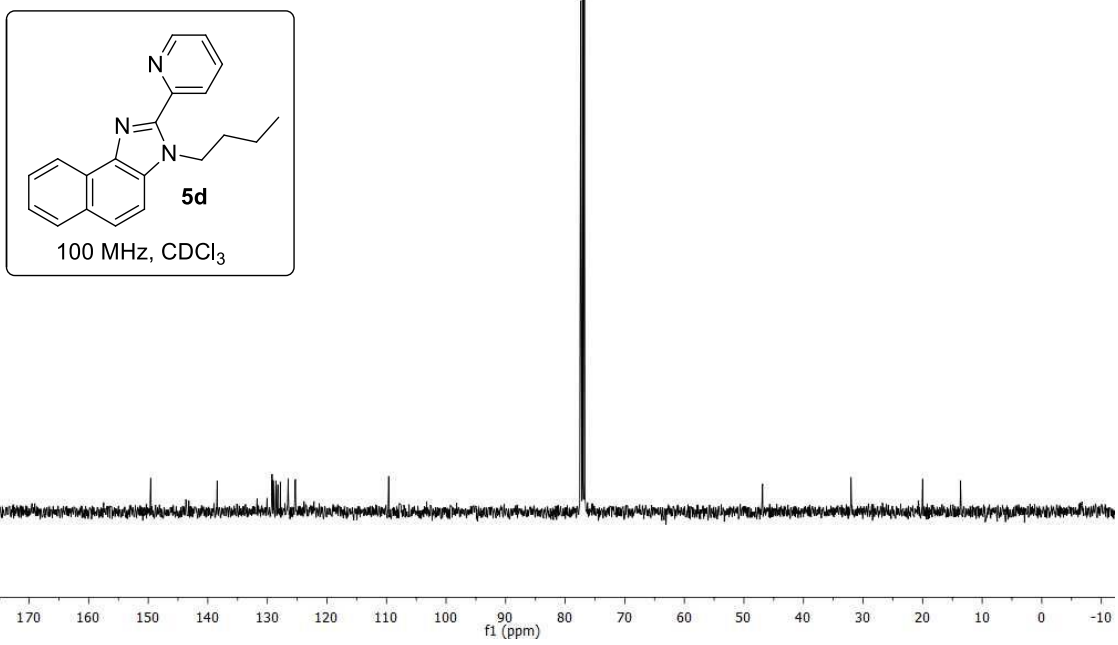

f1 (ppm)


HM-781
single_pulse


5d
400 MHz, CDCl3

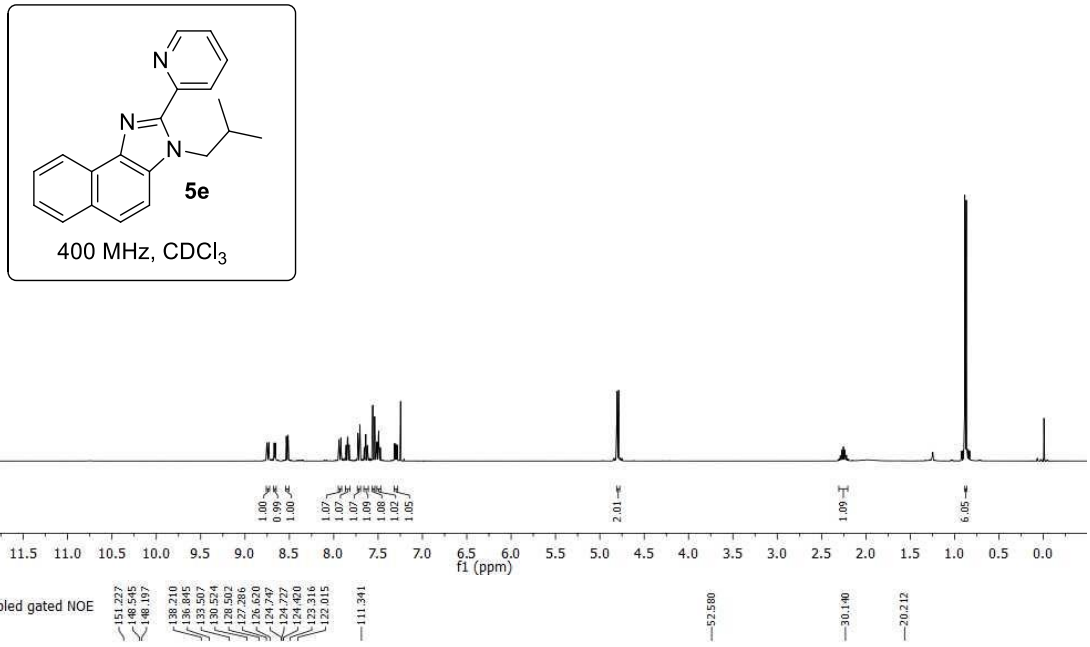

f1 (ppm)

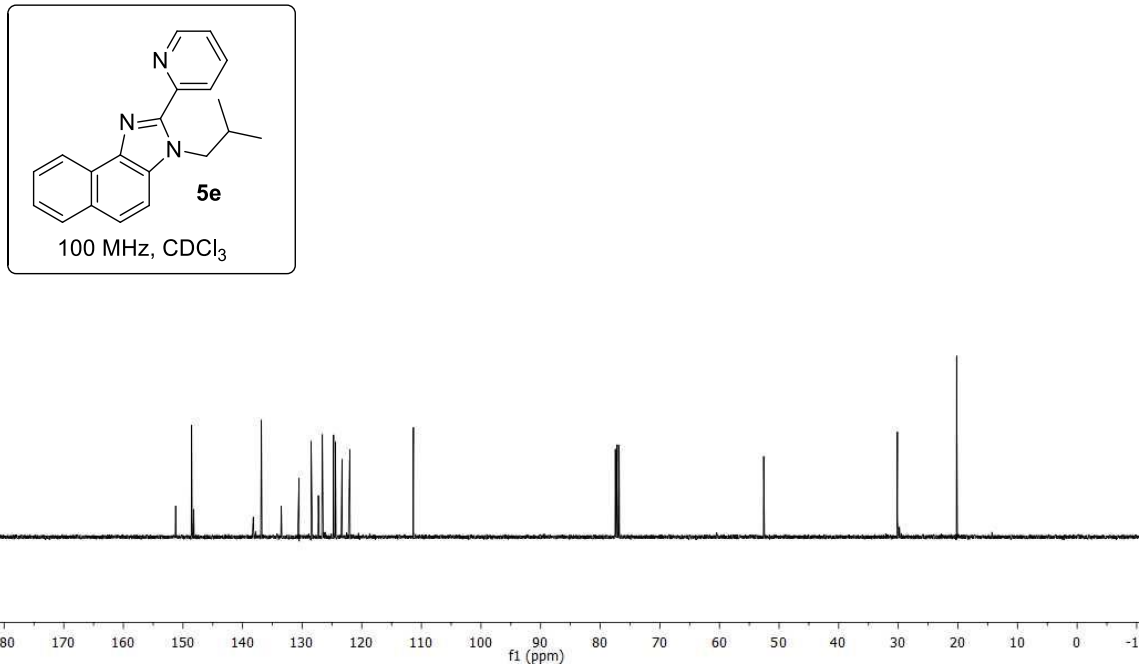
HM-781
single pulse decoupled gated NOE


f1 (ppm)

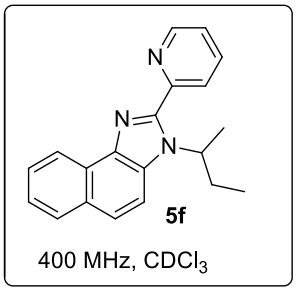
5d
100 MHz, CDCl3

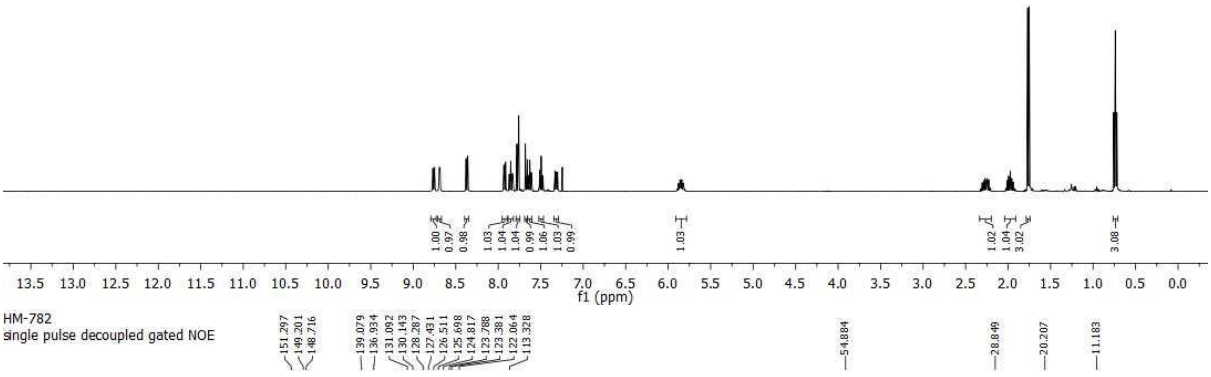

HM-815
single_pulse

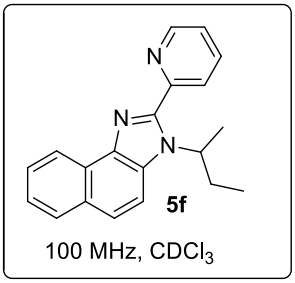

5e
400 MHz, CDCl3
1.00
0.99
1.00
1.07
1.07
1.07
1.09
1.08
1.02
1.05
2.01
1.09
6.05
3.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
HM-815
single pulse decoupled gated NOE
151.227
148.545
148.197
138.210
136.845
133.507
130.524
128.502
127.286
126.620
124.747
124.727
124.420
123.316
122.015
111.341
52.580
30.140
20.212

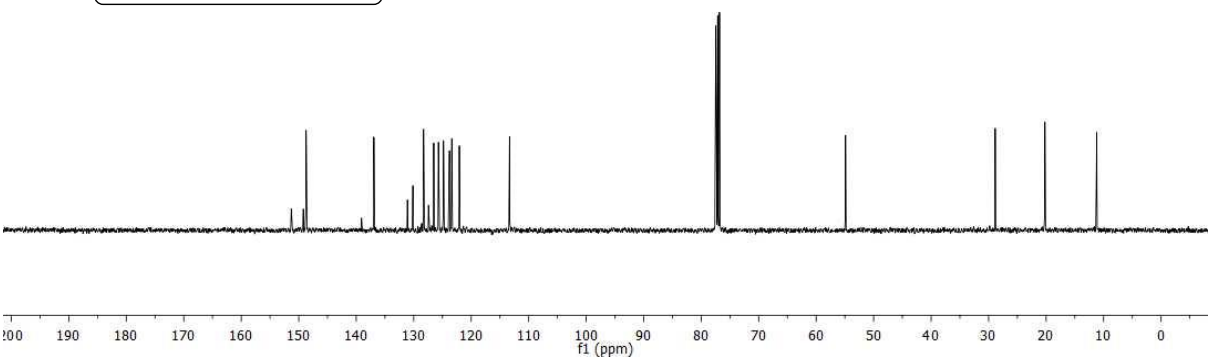

5e
100 MHz, CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

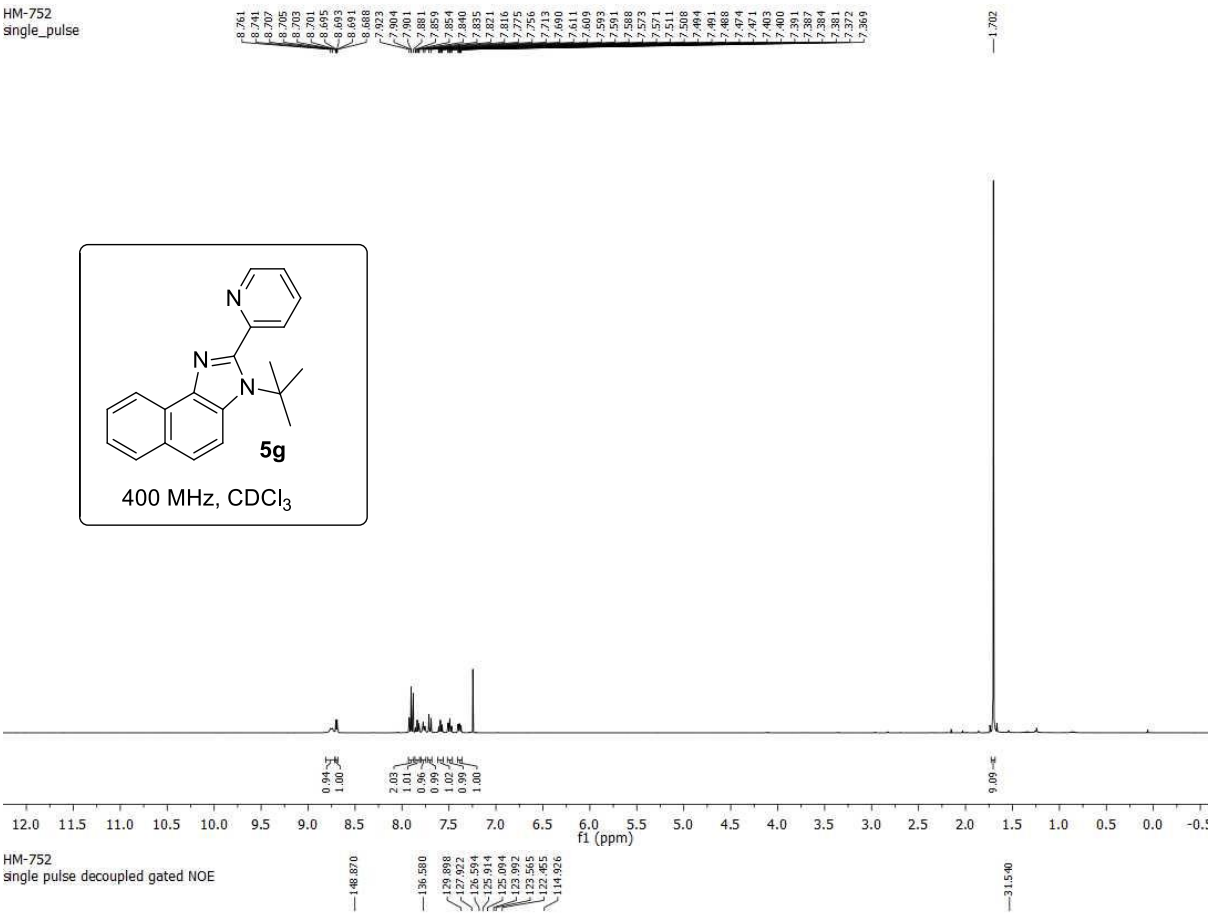

HM-782
single_pulse

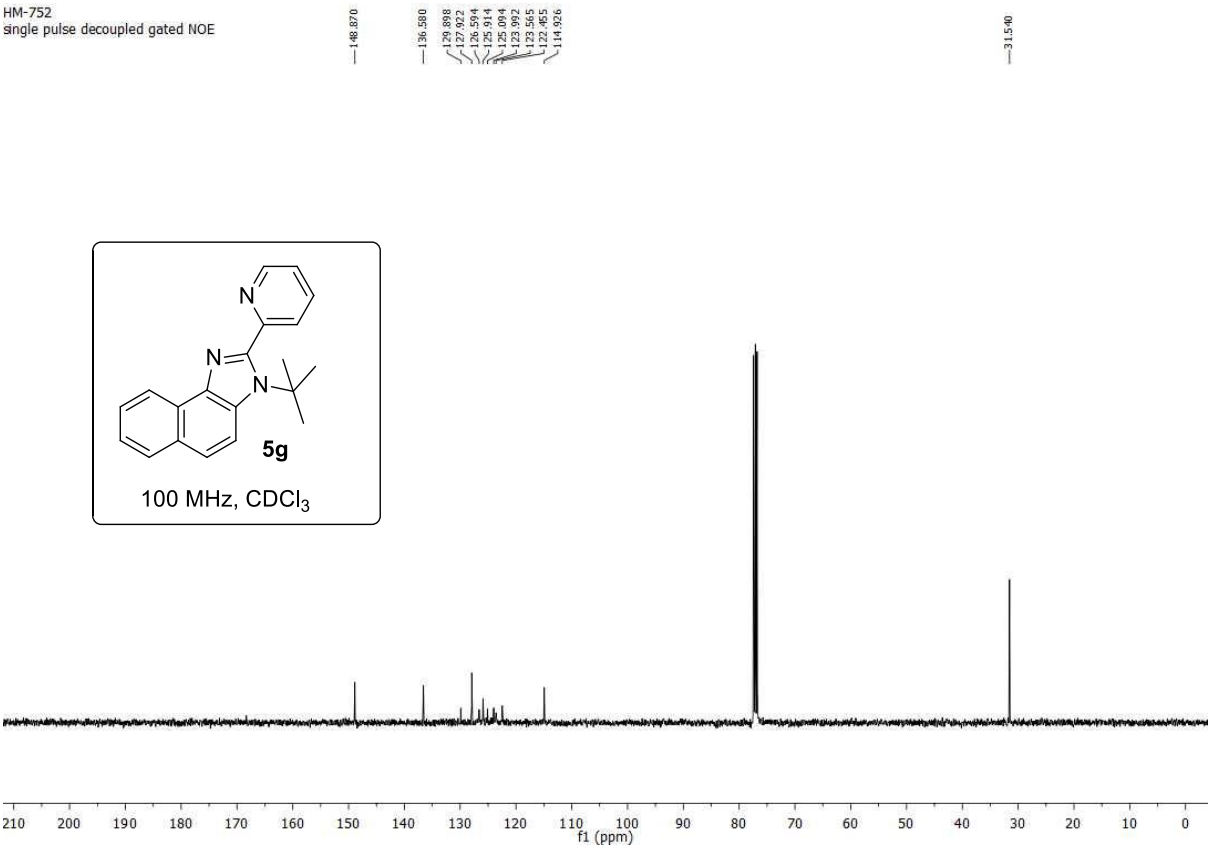

5f
400 MHz, CDCl3


f1 (ppm)
HM-782
single pulse decoupled gated NOE

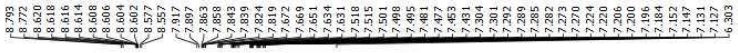

5f
100 MHz, CDCl3

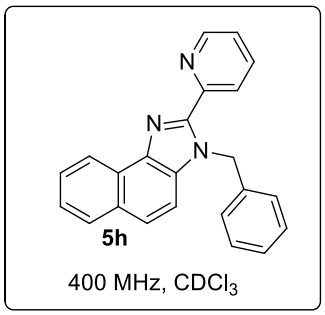

f1 (ppm)

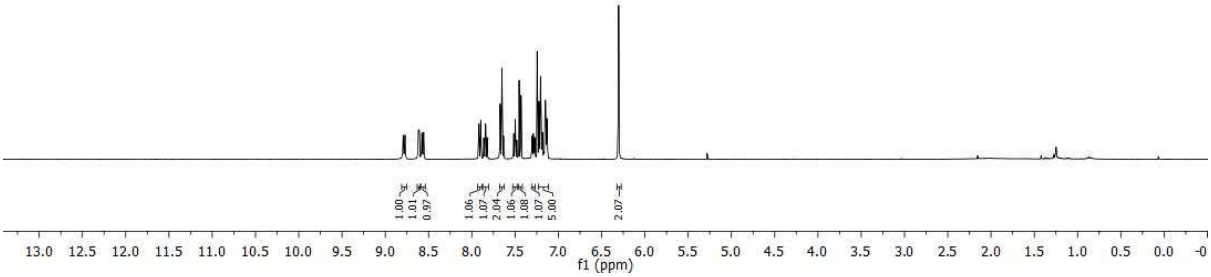

HM-752
single_pulse
8.761
8.741
8.707
8.705
8.703
8.701
8.695
8.693
8.691
8.688
7.923
7.904
7.901
7.881
7.859
7.854
7.840
7.835
7.821
7.816
7.775
7.756
7.713
7.690
7.611
7.609
7.593
7.591
7.588
7.573
7.571
7.511
7.508
7.494
7.491
7.488
7.474
7.471
7.403
7.400
7.391
7.387
7.384
7.381
7.372
7.369
1.702
N
N
N
5g
400 MHz, CDCl3
0.94
1.00
2.03
1.01
0.96
0.99
1.02
0.99
1.00
9.09
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


HM-752
single pulse decoupled gated NOE
148.870
136.580
129.898
127.922
126.594
125.914
125.094
123.992
123.565
122.455
114.926
31.540
N
N
N
5g
100 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

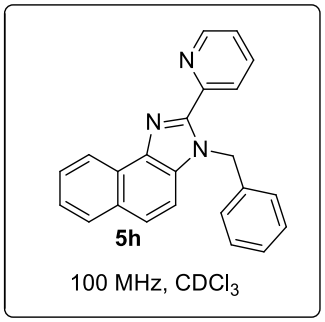
HM-482G
single_pulse



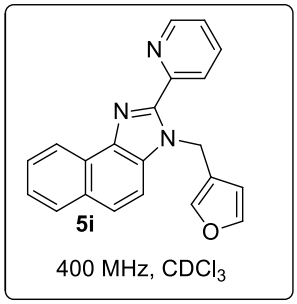


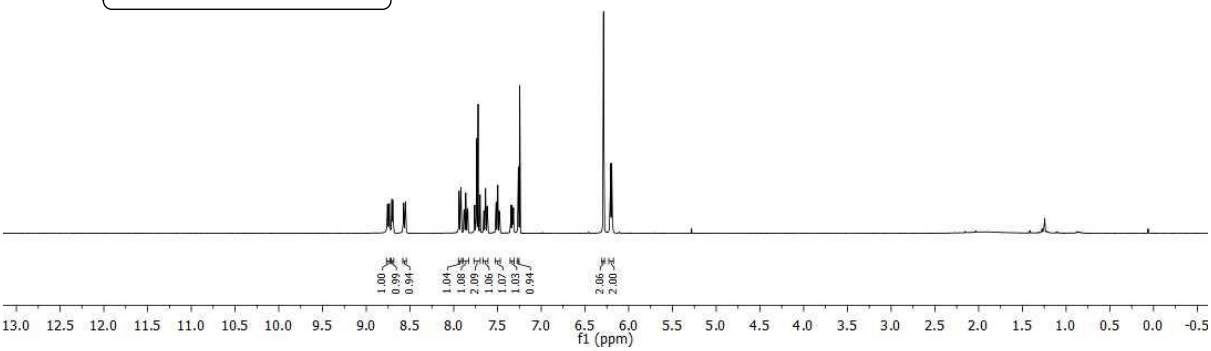


HM-482G
single pulse decoupled gated NOE

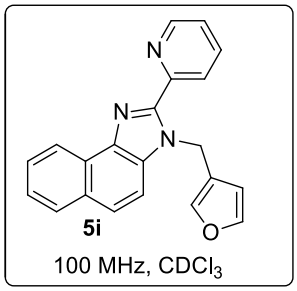


HM-417G
single_pulse

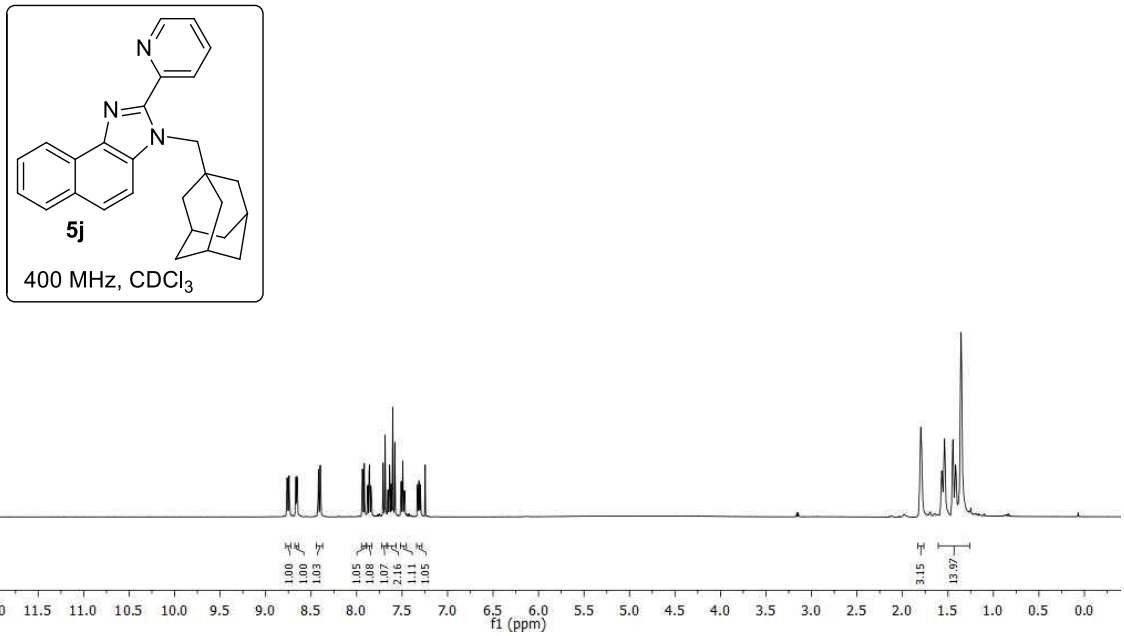




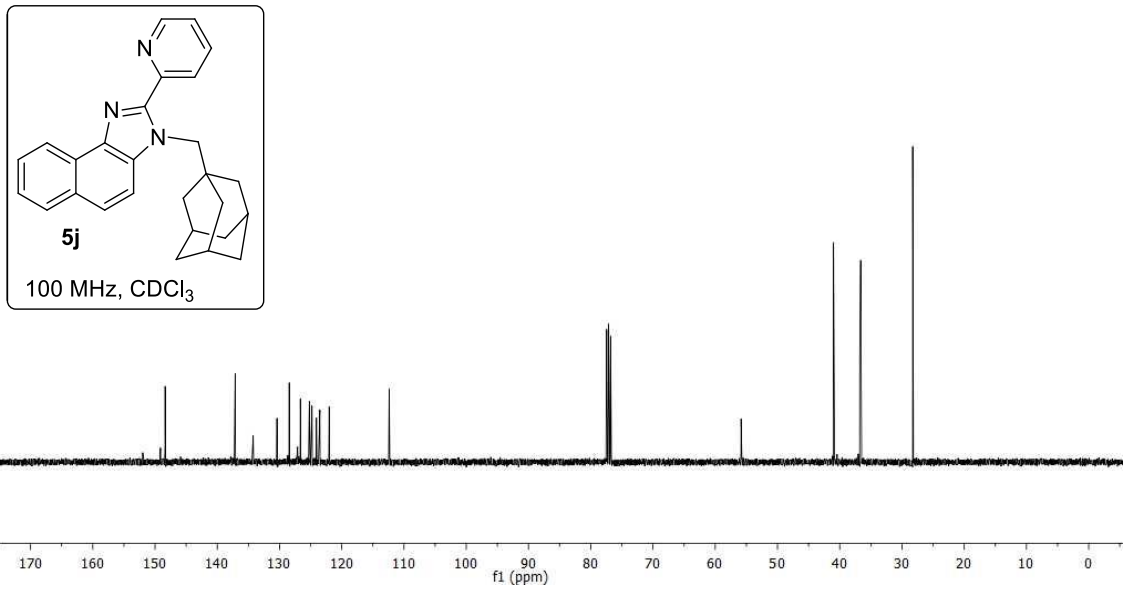
HM-417G
single pulse decoupled gated NOE



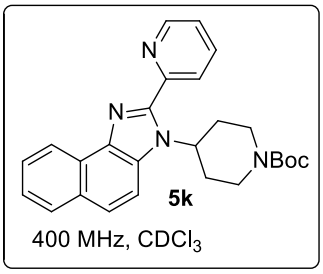

HM-783
single_pulse


5j
400 MHz, CDCl3
f1 (ppm)


HM-783
single pulse decoupled gated NOE

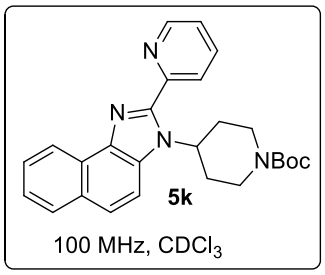

5j
100 MHz, CDCl3
f1 (ppm)

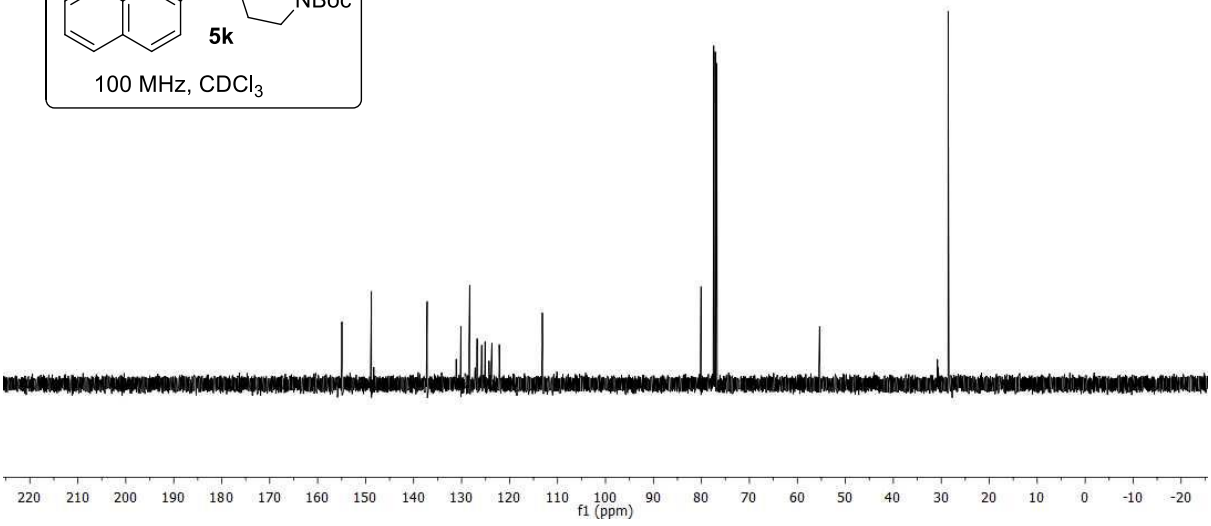

HM-787
single_pulse

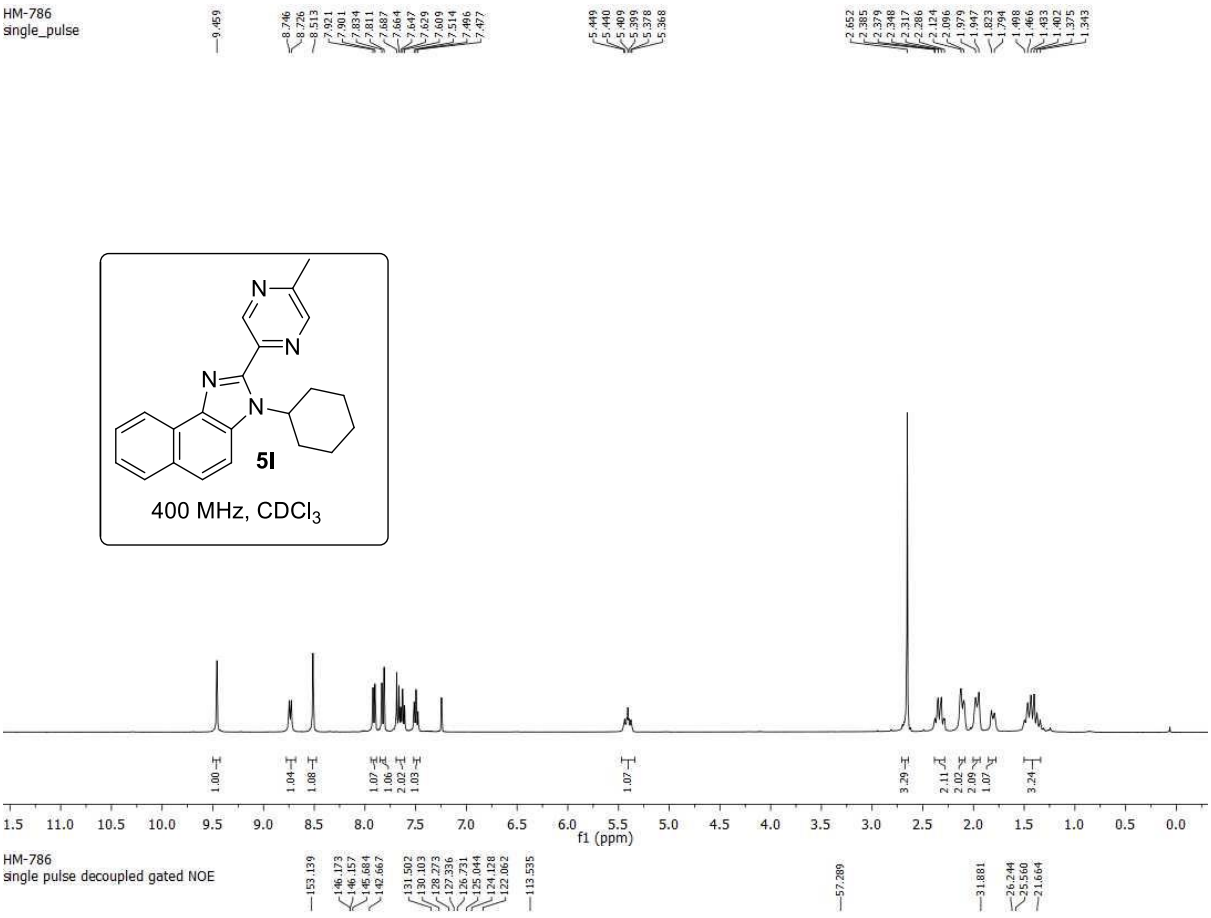

N
N
N
NBoc
5k
400 MHz, CDCl3

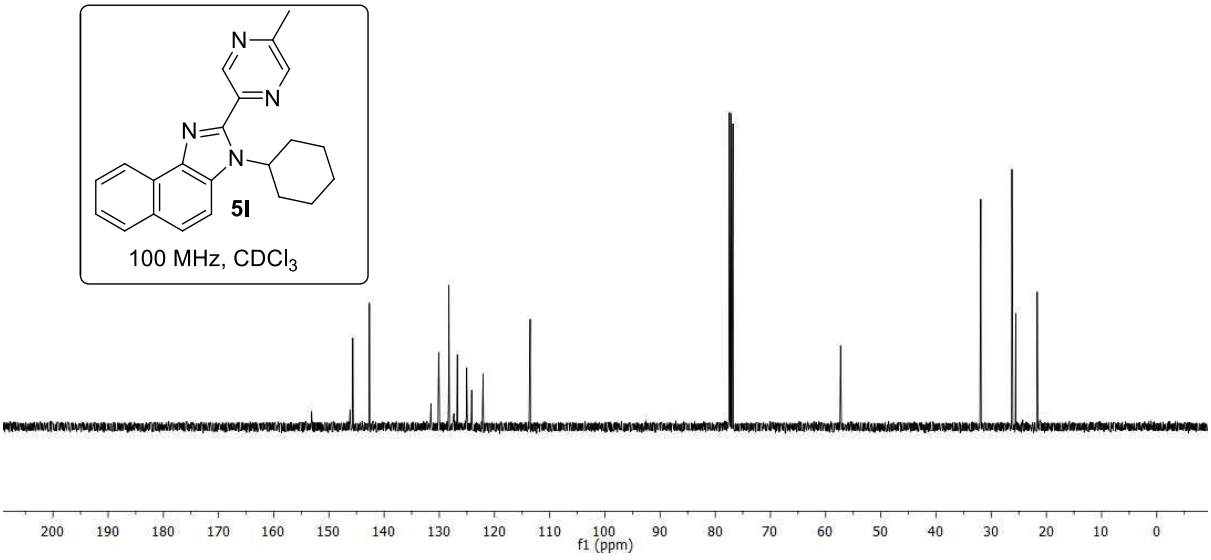
1.00
1.02
1.03
2.11
1.03
1.03
1.08
1.06
1.03
1.04
1.94
2.04
2.09
2.12
9.26
14.5 14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

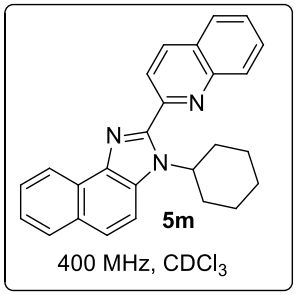
HM-787
single pulse decoupled gated NOE
154.951
148.794
148.292
137.175
131.123
130.146
128.312
126.769
125.613
125.108
124.266
123.698
122.150
113.161
80.089
55.363
30.779
28.572

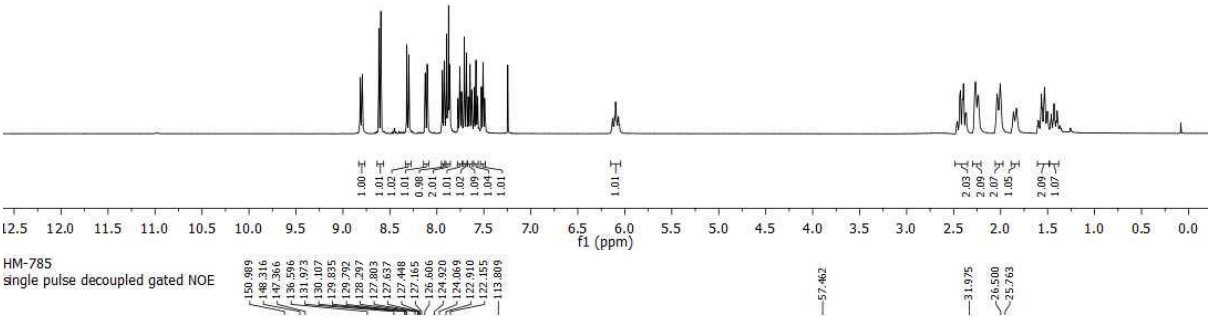

N
N
N
NBoc
5k
100 MHz, CDCl3


220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

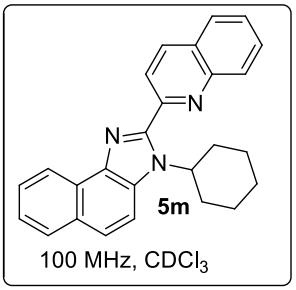

HM-786
single_pulse
5l
400 MHz, CDCl3
f1 (ppm)
HM-786
single pulse decoupled gated NOE

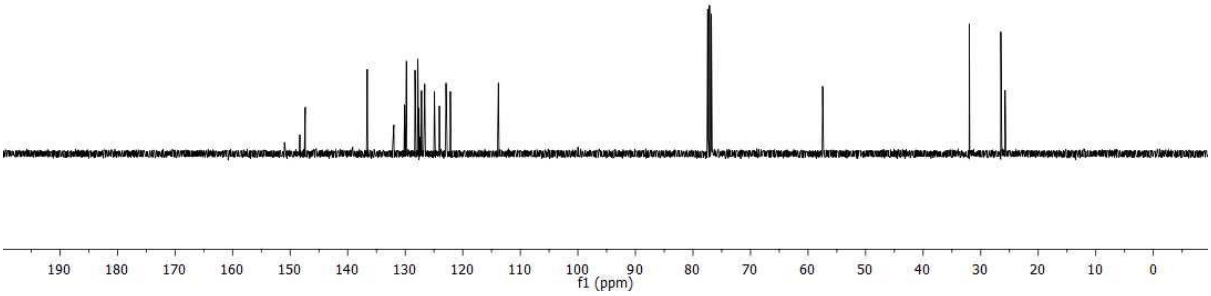

5l
100 MHz, CDCl3
f1 (ppm)

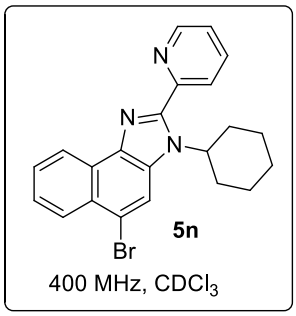

5m
400 MHz, CDCl3

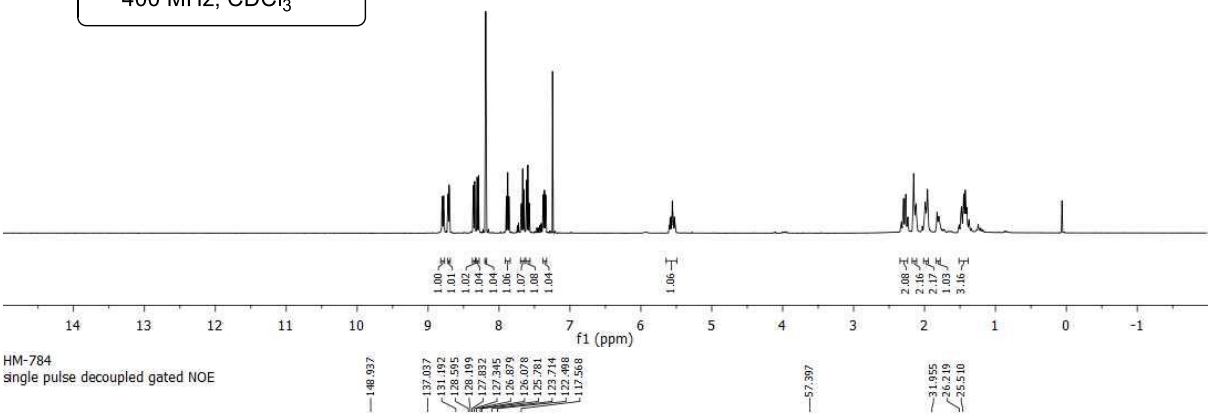

f1 (ppm)

HM-785
single pulse decoupled gated NOE

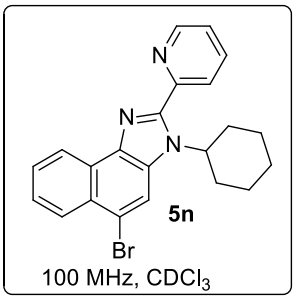

5m
100 MHz, CDCl3

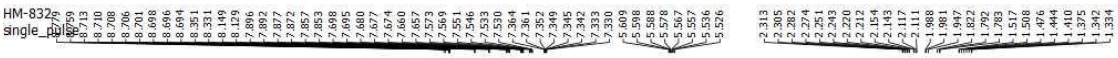

f1 (ppm)

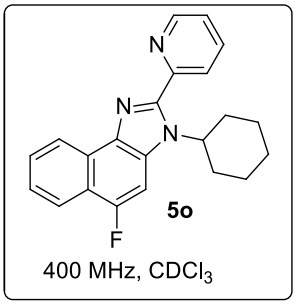


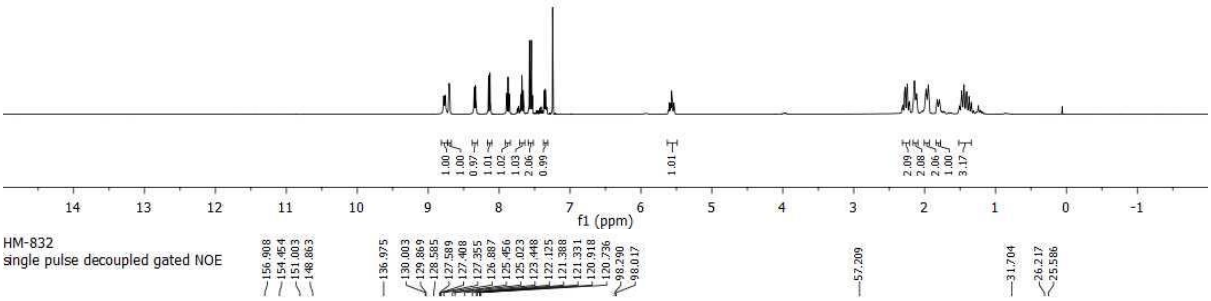


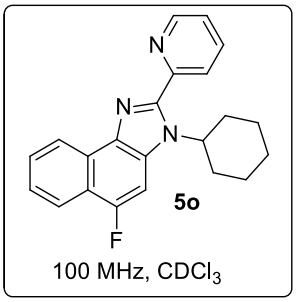
HM-784
single pulse decoupled gated NOE

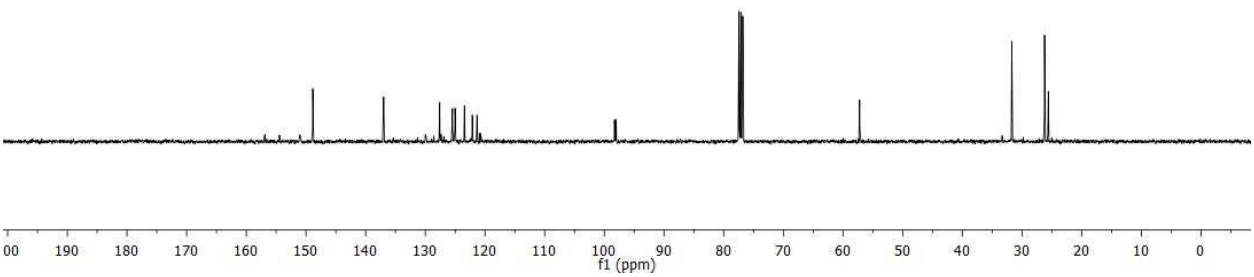



HM-832
single_pulse

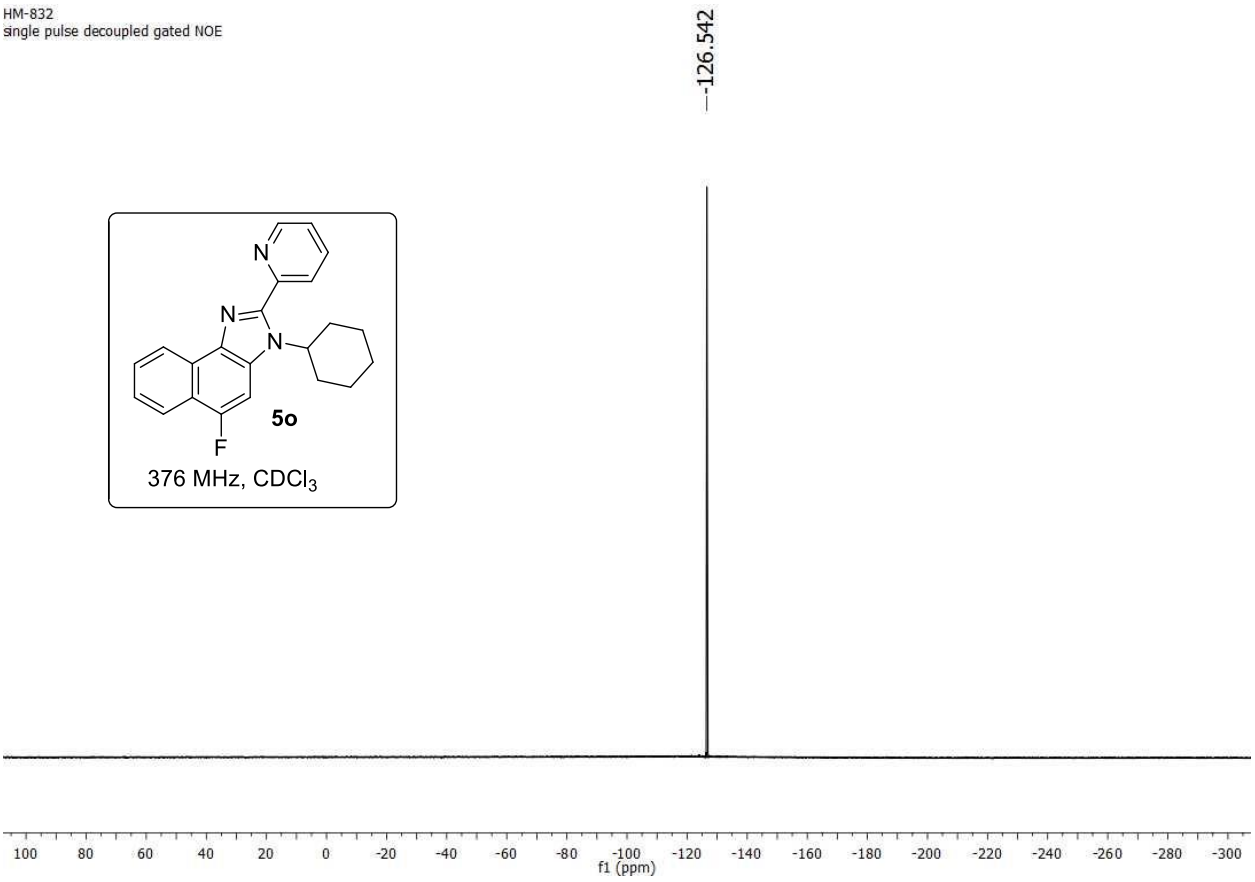

5o
400 MHz, CDCl3

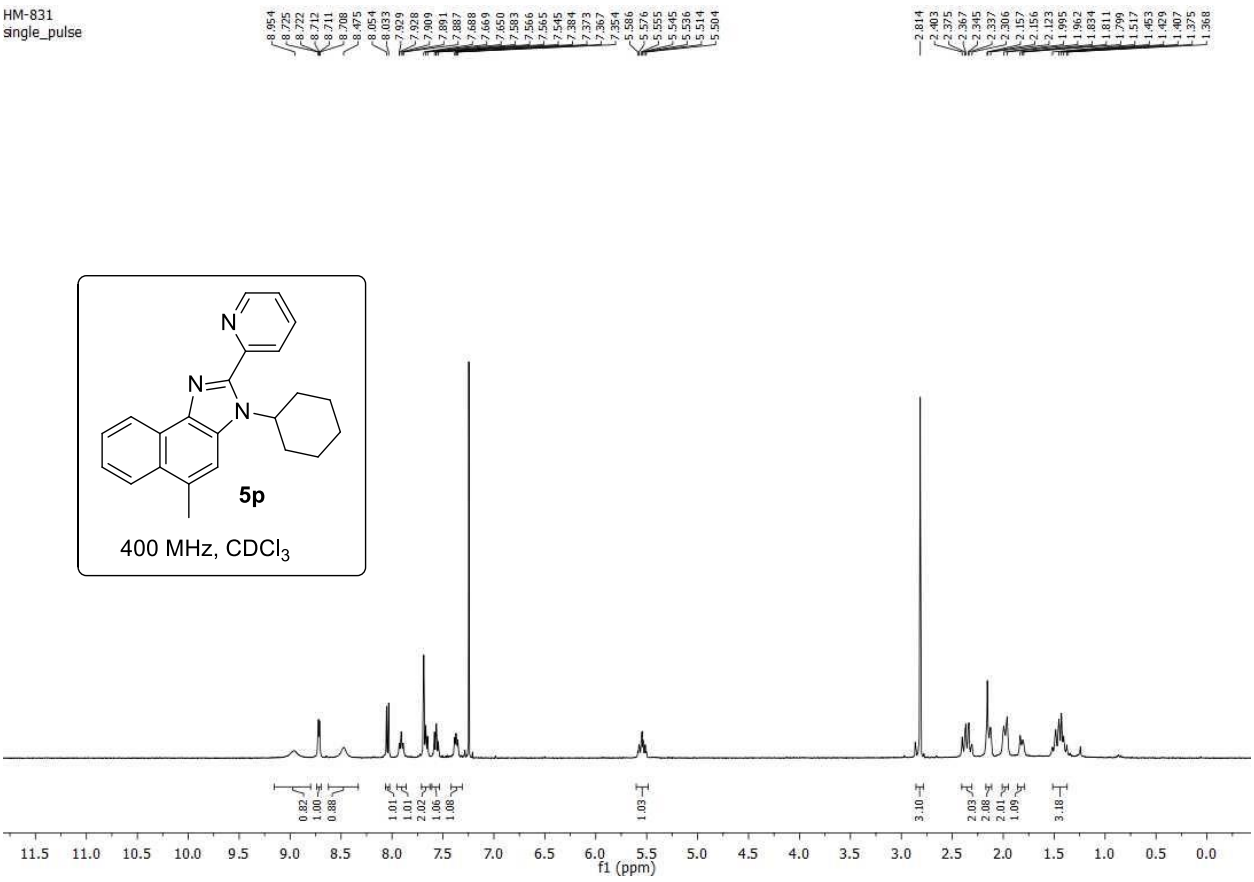

f1 (ppm)
HM-832
single pulse decoupled gated NOE

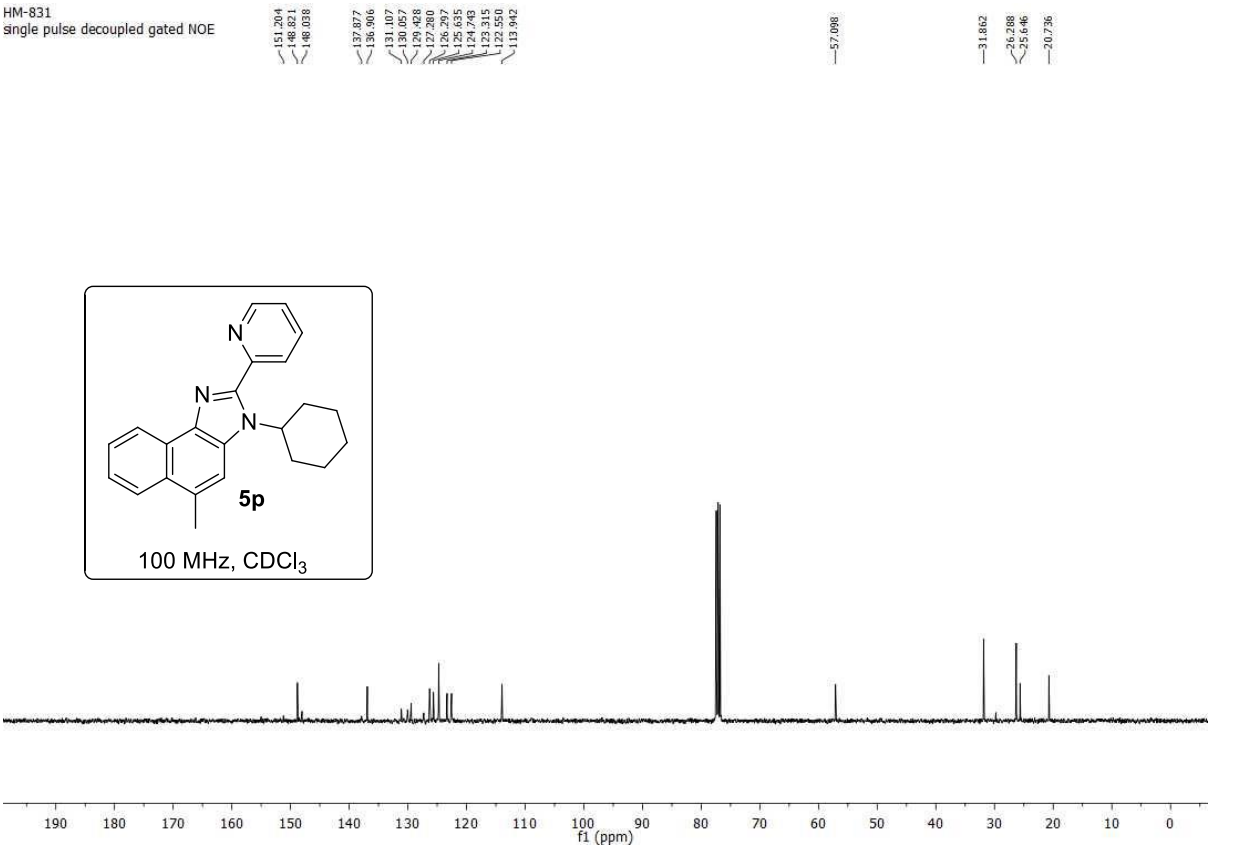

5o
100 MHz, CDCl3


f1 (ppm)

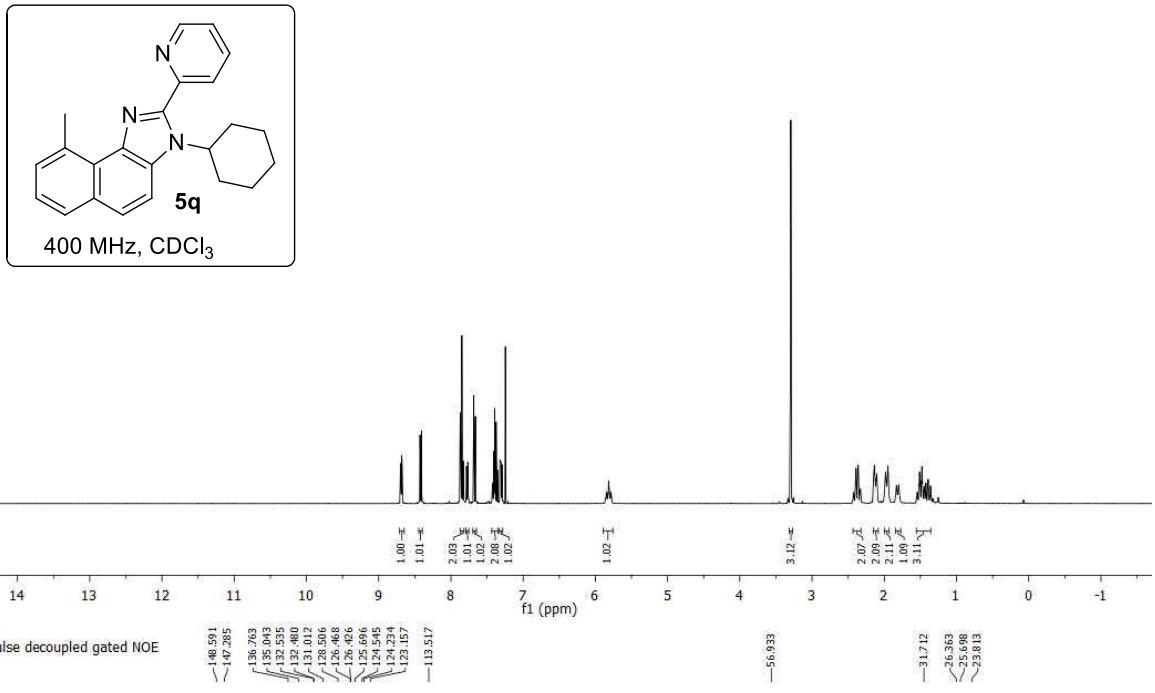
HM-832
single pulse decoupled gated NOE



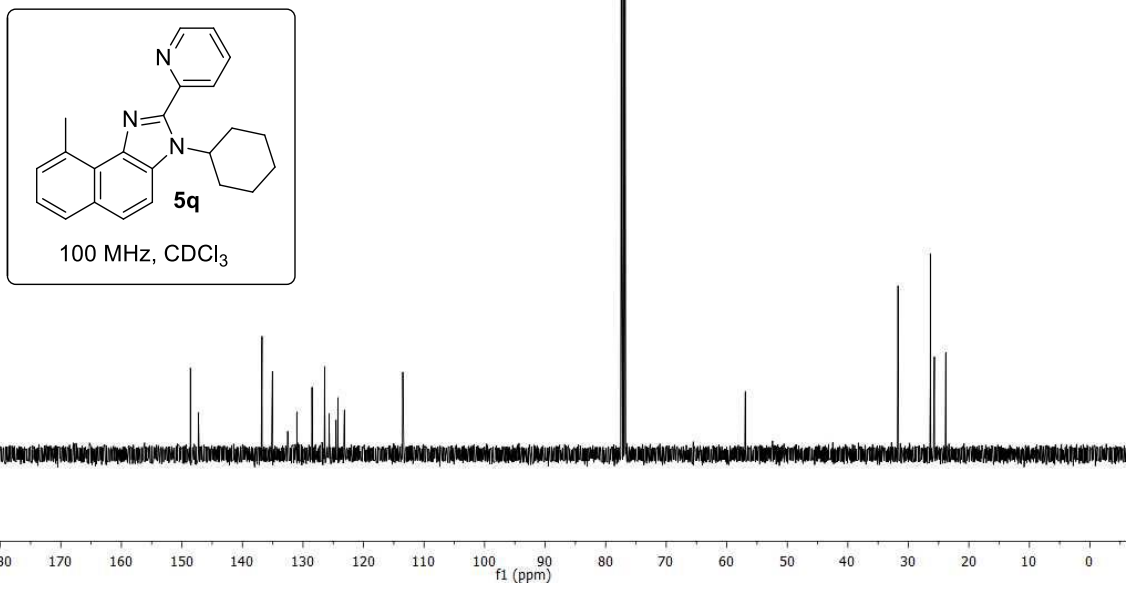

HM-831
single_pulse
5p
400 MHz, CDCl3
f1 (ppm)

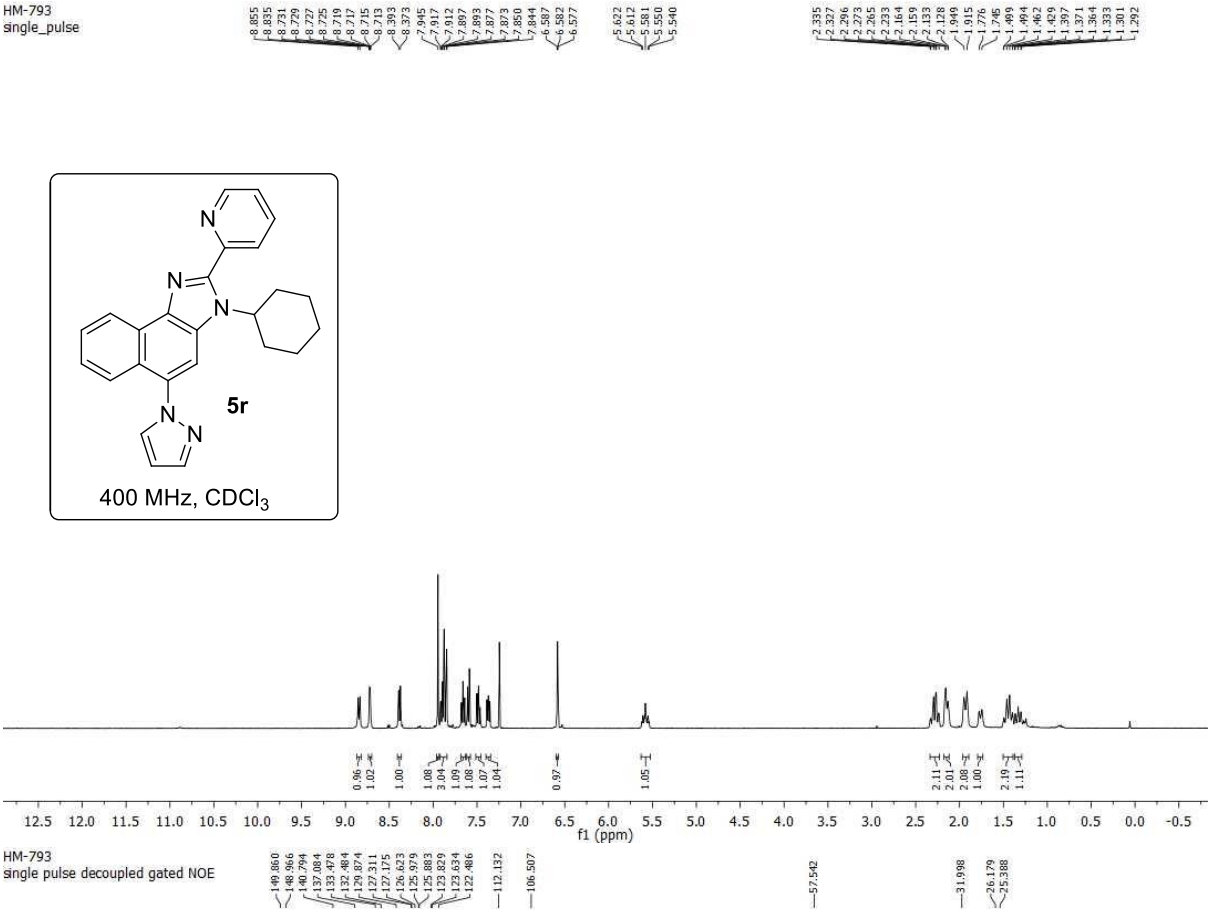

HM-831
single pulse decoupled gated NOE
5p
100 MHz, CDCl3
f1 (ppm)

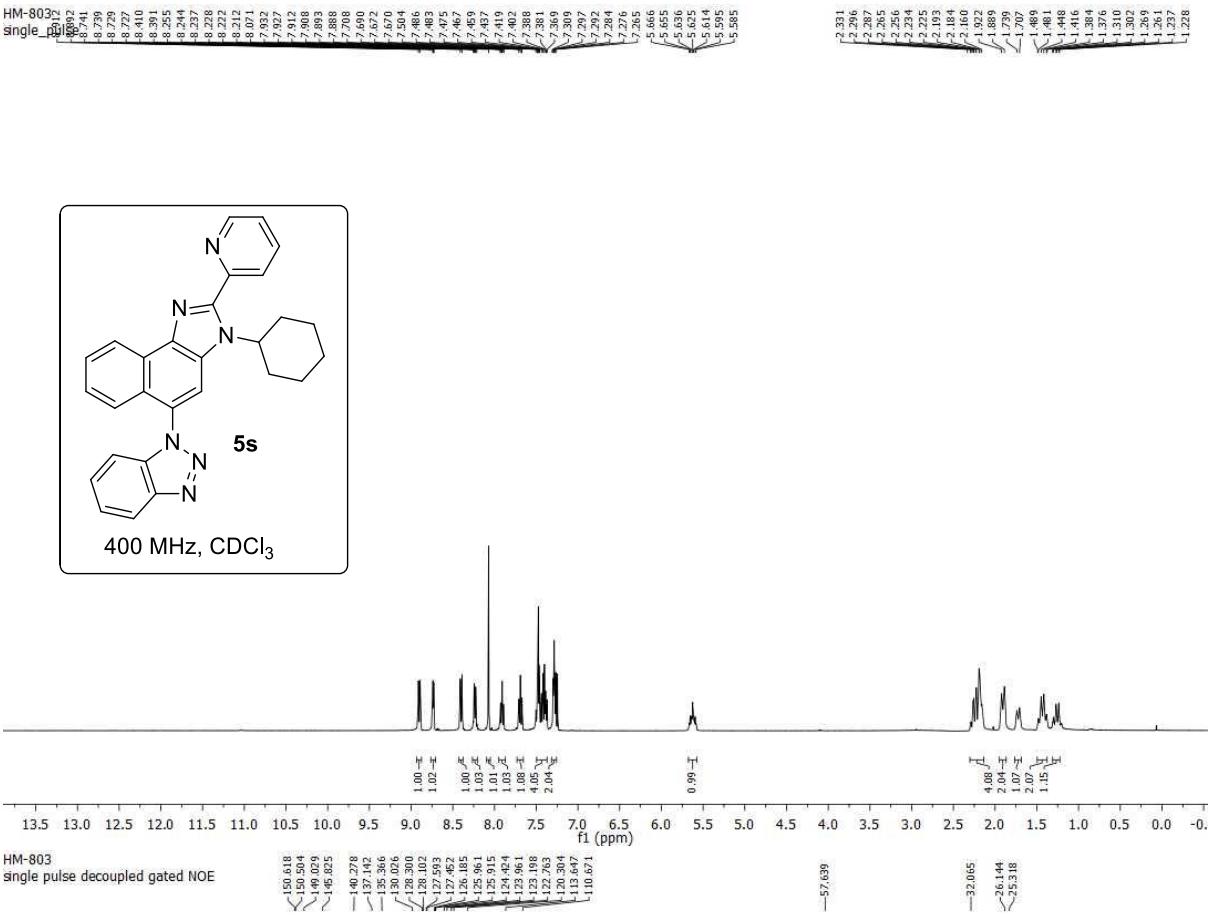

HM-817
single pulse

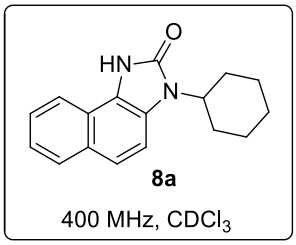

5q
400 MHz, CDCl3
f1 (ppm)

HM-817
single pulse decoupled gated NOE


5q
100 MHz, CDCl3
f1 (ppm)

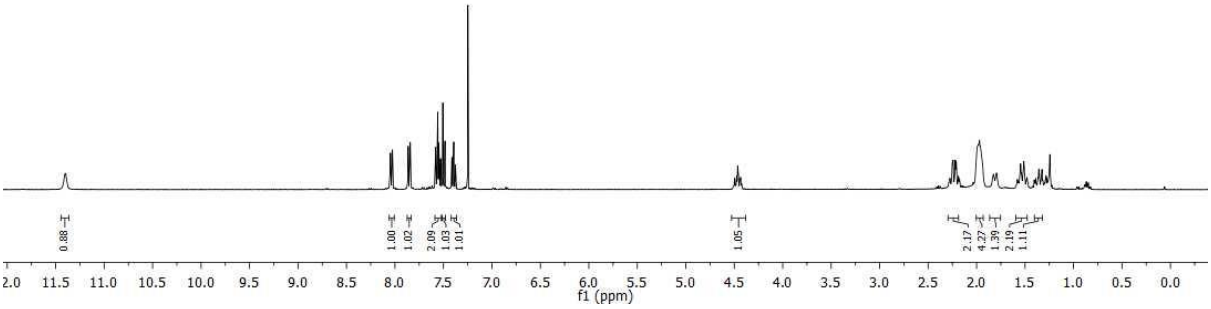

HM-793
single_pulse
5r
400 MHz, CDCl3
f1 (ppm)
HM-793
single pulse decoupled gated NOE
5r
100 MHz, CDCl3
f1 (ppm)

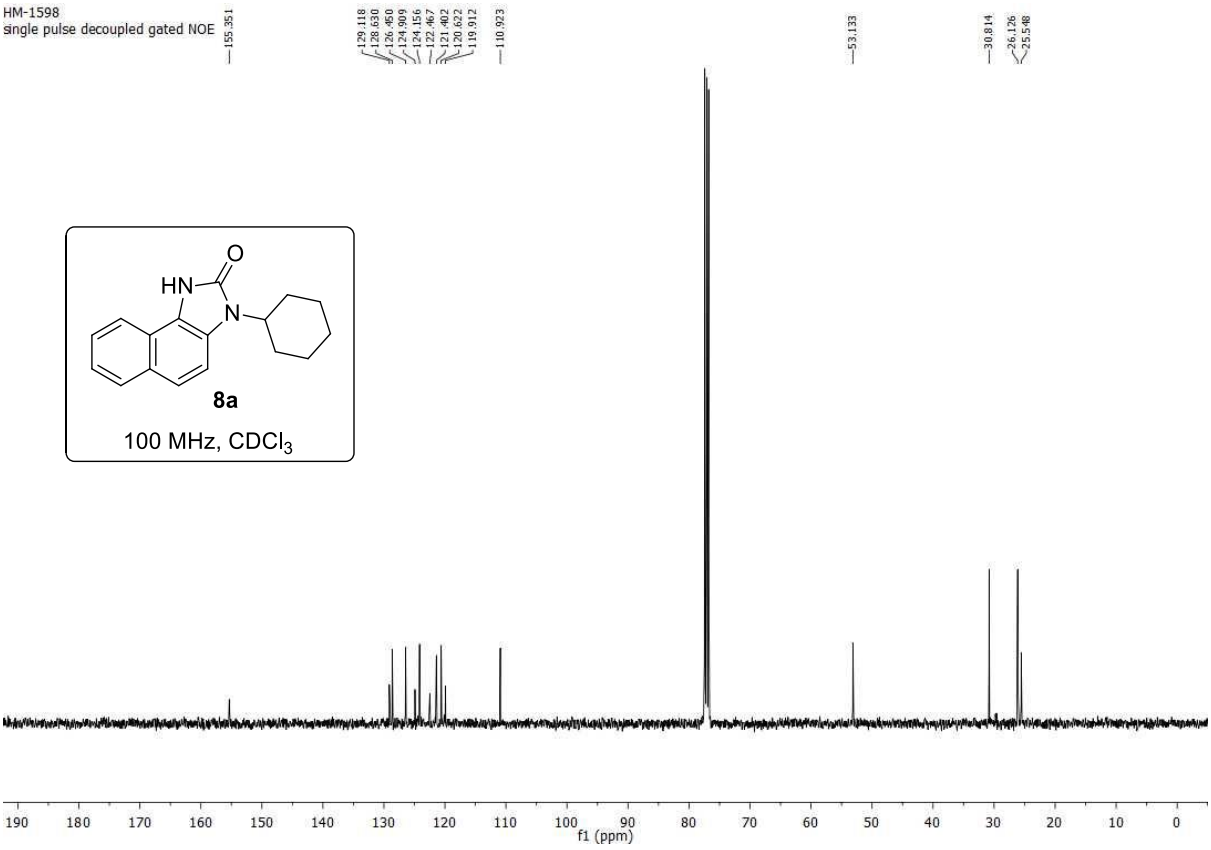

HM-803
single_pulse
5s
400 MHz, CDCl3
f1 (ppm)
HM-803
single pulse decoupled gated NOE
5s
100 MHz, CDCl3
f1 (ppm)



8a

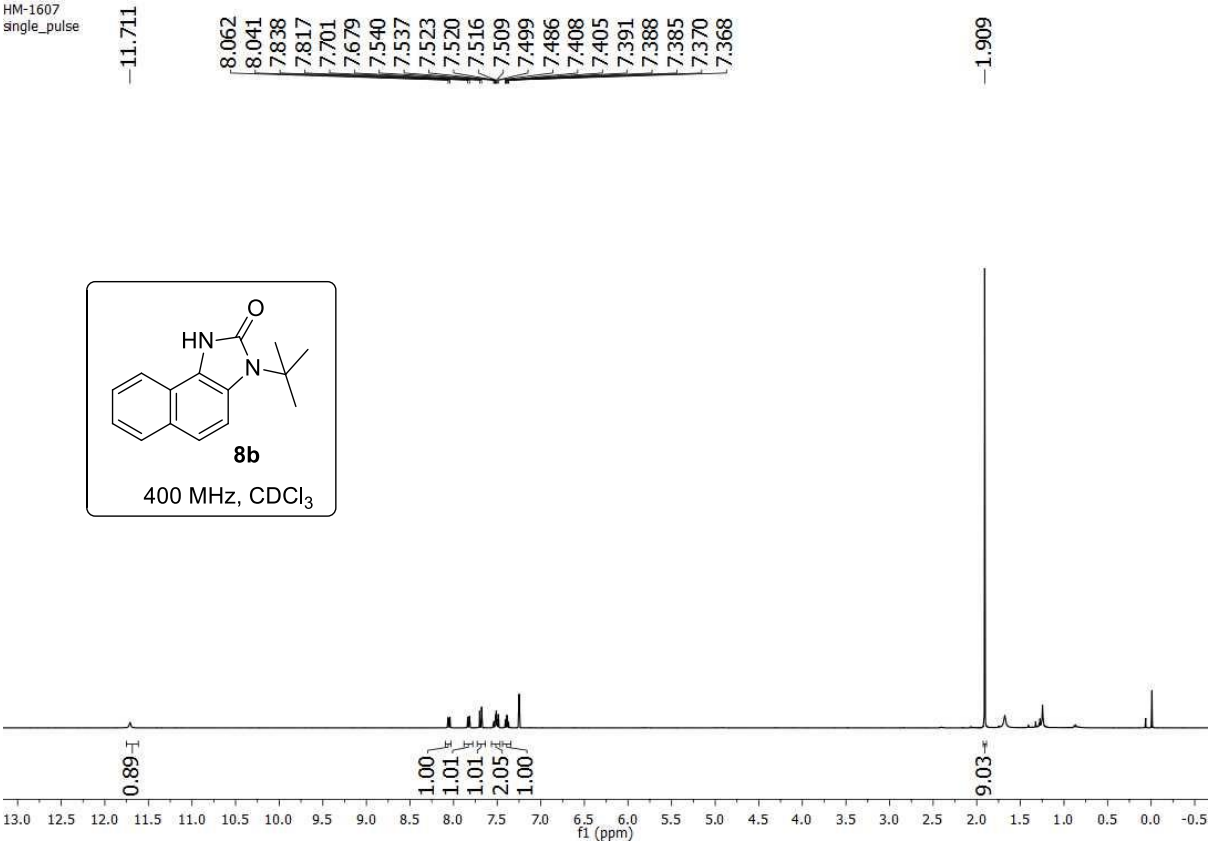
400 MHz, $CDCl_3$

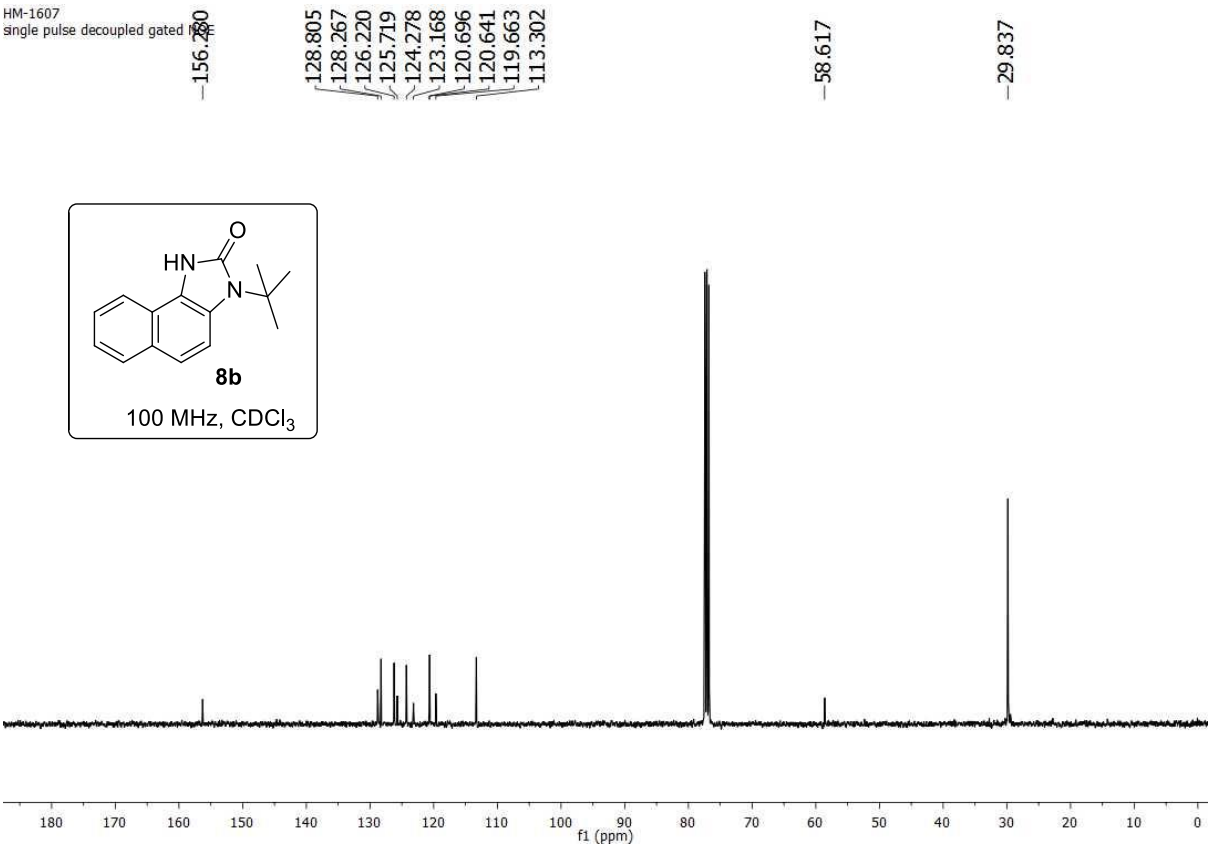




8a

100 MHz, $CDCl_3$


HM-1607
single_pulse
11.711
8.062
8.041
7.838
7.817
7.701
7.679
7.540
7.537
7.523
7.520
7.516
7.509
7.499
7.486
7.408
7.405
7.391
7.388
7.385
7.370
7.368
1.909
HN
O
N
8b
400 MHz, CDCl3
0.89
1.00
1.01
1.01
2.05
1.00
9.03
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


HM-1607
single pulse decoupled gated
156.280
128.805
128.267
126.220
125.719
124.278
123.168
120.696
120.641
119.663
113.302
58.617
29.837
HN
O
N
8b
100 MHz, CDCl3
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)