Regioselectivity-Switchable Catalytic Annulations of Alkynyl α-Diketones and α-Cyanoketones

Sakkani Nagaraju,[†] Shuhua Liu,[†] Jinggong Liu,[§] Shuang Yang,[‡] Rui Liu,[‡] Zhizhou Chen,[‡] Banoth Paplal,[†] and Xinqiang Fang*[,‡]

[†]Shandong Analysis and Test Center, Qilu University of Technology (Shandong Academy of Sciences), Jinan 250014, China

[‡]State Key Laboratory of Structural Chemistry, Center for Excellence in Molecular Synthesis, Fujian Institute of Research on the Structure of Matter, University of Chinese Academy of Sciences, Fuzhou 350100, China

[§]Orthopedics Department, Guangdong Provincial Hospital of Traditional Chinese Medicine, The Second Affiliated Hospital of Guangzhou University of Chinese Medicine, No. 111 Dade Road, Guangzhou 510120, China.

E-mail: xqfang@fjirsm.ac.cn

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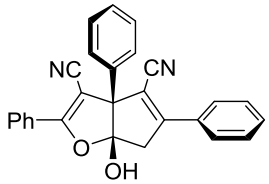
I. General Information

Commercially available chemicals were directly used without further purification, unless otherwise mentioned, all experiments and manipulations involving air- or moisture-sensitive compounds were performed using standard Schlenk technique. All solvents were purified and dried using typical procedures. Proton nuclear magnetic resonance (^{1}H NMR) spectra were

recorded on a Bruker AVANCE III HD400 (400 MHz) and ECZ600S (600 MHz) spectrometer. Chemical shifts were recorded in parts per million (ppm, δ) relative to tetramethylsilane (δ = 0.00 ppm) or acetone-D6 (δ = 2.09 ppm), chloroform (δ = 7.26 ppm) and dimethyl sulfoxide-D6 (δ = 2.50 ppm). ^{1}H NMR splitting patterns are designated as singlet (s), doublet (d), triplet (t), quartet (q), dd (doublet of doublets); m (multiplet), and etc. All first-order splitting patterns were assigned on the basis of the appearance of the multiplet. Splitting patterns that could not be easily interpreted are designated as multiplet (m) or broad (br). Carbon nuclear magnetic resonance (^{13}C NMR) spectra were recorded on a Bruker AVANCE III HD400 (400 MHz) (100 MHz) and ECZ600S (600 MHz) (150 MHz) spectrometers. High resolution mass spectral analysis (HRMS) was performed on Thermo Fisher Scientific LTQ FT Ultra mass spectrometer. The determination of *e.e.* was performed via chiral HPLC analysis using Shimadzu LC-20AD HPLC workstation. X-ray crystallography analysis was performed on Agilent Super Nova X-ray diffractionmeter. Optical rotations were measured using a 1 mL cell with a 5dm path length on an INESA SGW-1 polarimeter and are reported as follows: $[\alpha]^{rt}_{D}$ (c in g per 100 mL solvent). Analytical thin-layer chromatography (TLC) was carried out on WFH-203 F254 pre-coated silica gel plate (0.2 mm thickness). Visualization was performed using a UV lamp or 2,4-Dinitrophenylhydrazine or potassium permanganate stain or phosphomolybdic acid.

II. X-ray crystallographic analysis

Method for single crystals cultivation: a pure solid sample (10–20 mg) was dissolved in dichloromethane/acetone (2 mL) in a vial at room temperature, and petroleum ether/hexane (0.1 mL) was added into the above solution slowly while keeping the sample completely dissolved. The vial was properly sealed with parafilm and kept at room temperature to allow the slow evaporation of the solvents until a single crystal was obtained.



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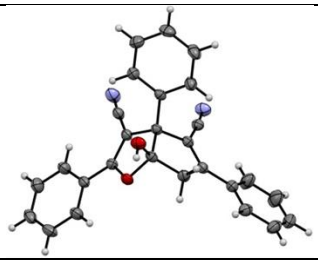
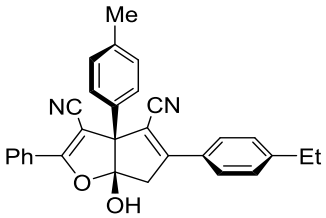
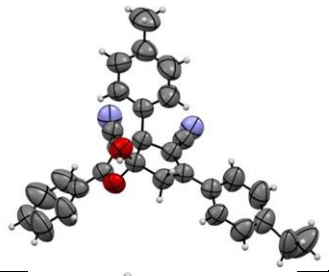
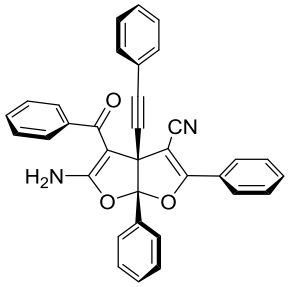
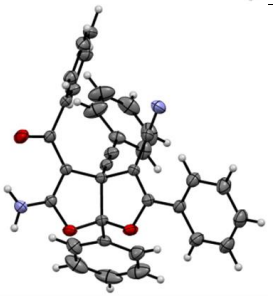
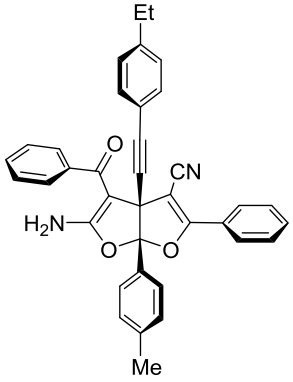
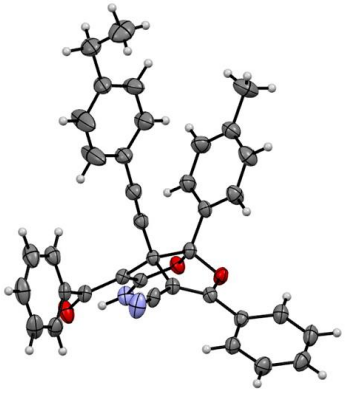
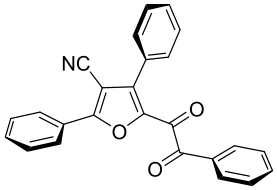
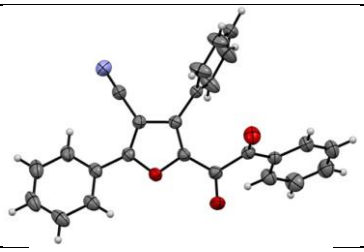
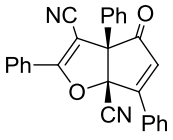
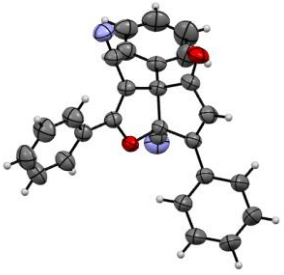


 **3i** (CCDC 1961047)	
 **4a** (CCDC 1961048)	
 **4i** (CCDC 1961052)	
 **5a** (CCDC 1961053)	
 **3aa** (CCDC 1962410)	

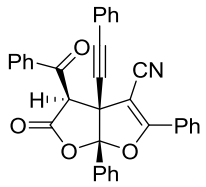
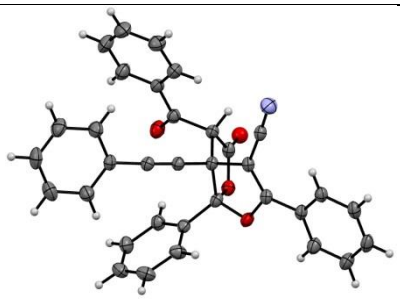
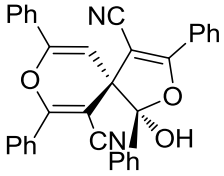
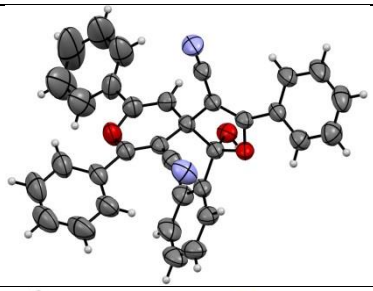
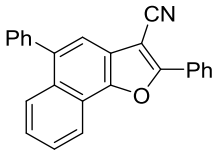
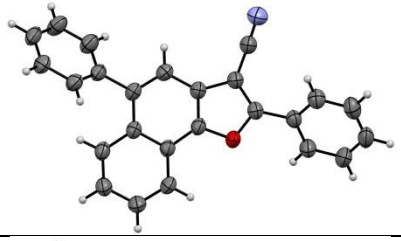
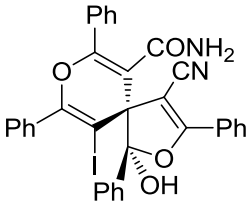
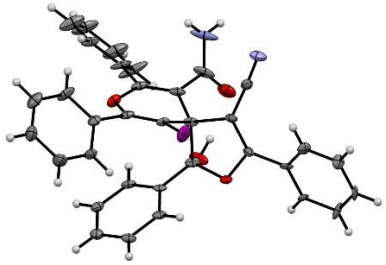
 **4aa** (CCDC 1961055)	
 **4ab** (CCDC 1961056)	
 **4ac** (CCDC 1961057)	
 **4ad** (CCDC 1961058)	

Table S1: Crystal data and structure refinement for **3a**

Identification code	3a
Empirical formula	$C_{28}H_{19}N_2O$
Formula weight	402.46
Temperature/K	150.00(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	9.72011(12)
b/Å	16.17976(18)
c/Å	12.95619(15)
α/°	90
β/°	90.8322(11)
γ/°	90
Volume/Å^3	2037.39(4)
Z	4
ρ_{calc}g/cm^3	1.3120

μ/mm^{-1}	0.666
F(000)	842.6
Crystal size/mm^3	0.1 × 0.05 × 0.05
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.74 to 148.6
Index ranges	$-11 \leq h \leq 12$, $-17 \leq k \leq 20$, $-15 \leq l \leq 16$
Reflections collected	24339
Independent reflections	4075 [R_{int} = 0.0451, R_{sigma} = 0.0238]
Data/restraints/parameters	4075/0/280
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0432, wR_2 = 0.1105
Final R indexes [all data]	R_1 = 0.0453, wR_2 = 0.1121
Largest diff. peak/hole / e $Å^{-3}$	0.49/-0.24

Table S2: Crystal data and structure refinement for **3i**

Identification code	3i
Empirical formula	$C_{30}H_{19}N_2O_2$
Formula weight	444.54
Temperature/K	291.86(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	10.6094(3)
b/Å	18.1146(6)
c/Å	12.8174(3)
α/°	90
β/°	95.312(2)
γ/°	90
Volume/$Å^3$	2452.74(12)
Z	4
$\rho_{calc}g/cm^3$	1.2037
μ/mm^{-1}	0.598
F(000)	938.8
Crystal size/mm^3	0.06 × 0.05 × 0.05
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.48 to 149.32
Index ranges	$-13 \leq h \leq 12$, $-22 \leq k \leq 21$, $-15 \leq l \leq 15$
Reflections collected	14194
Independent reflections	4820 [R_{int} = 0.0250, R_{sigma} = 0.0308]
Data/restraints/parameters	4820/1/328
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0619, wR_2 = 0.2013
Final R indexes [all data]	R_1 = 0.0848, wR_2 = 0.2250
Largest diff. peak/hole / e $Å^{-3}$	0.26/-0.16

Table S3: Crystal data and structure refinement for **4a**

Identification code	4a
Empirical formula	$C_{34}H_{22}N_2O_3$
Formula weight	506.57
Temperature/K	150.00(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.85928(10)
b/Å	24.8961(3)
c/Å	11.99933(13)
α/°	90
β/°	95.2548(10)
γ/°	90
Volume/Å^3	2635.47(5)
Z	4
ρ_{calc}g/cm^3	1.2766
μ/mm^{-1}	0.657
F(000)	1059.3
Crystal size/mm^3	0.03 × 0.02 × 0.02
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/ °	7.1 to 148.4
Index ranges	$-10 \leq h \leq 10$, $-29 \leq k \leq 30$, $-14 \leq l \leq 8$
Reflections collected	16547
Independent reflections	5207 [R_{int} = 0.0313, R_{sigma} = 0.0298]
Data/restraints/parameters	5207/1/352
Goodness-of-fit on F^2	1.025
Final R indexes [I>=2σ (I)]	R_1 = 0.0404, wR_2 = 0.1025
Final R indexes [all data]	R_1 = 0.0462, wR_2 = 0.1063
Largest diff. peak/hole / e Å^{-3}	0.31/-0.32

Table S4: Crystal data and structure refinement for **4i**

Identification code	F3
Empirical formula	$C_{37}H_{28}N_2O_3$
Formula weight	548.65
Temperature/K	180.00(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.96653(10)
b/Å	27.5380(3)
c/Å	12.02475(12)
α/°	90
β/°	93.3639(10)
γ/°	90
Volume/Å^3	2964.04(6)

Z	4
ρ_{calc}g/cm^3	1.2294
μ/mm^{-1}	0.621
F(000)	1155.6
Crystal size/mm^3	0.1 × 0.06 × 0.05
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.42 to 148.46
Index ranges	$-8 \leq h \leq 11$, $-32 \leq k \leq 33$, $-14 \leq l \leq 14$
Reflections collected	17378
Independent reflections	5857 [R_{int} = 0.0278, R_{sigma} = 0.0278]
Data/restraints/parameters	5857/0/381
Goodness-of-fit on F^2	1.029
Final R indexes [I>=2σ (I)]	R_1 = 0.0470, wR_2 = 0.1266
Final R indexes [all data]	R_1 = 0.0524, wR_2 = 0.1342
Largest diff. peak/hole / e Å^{-3}	0.45/-0.43

Table S5: Crystal data and structure refinement for **5a**

Identification code	5a
Empirical formula	$C_{25}NO_3H_{0.13}$
Formula weight	377.40
Temperature/K	149.99(10)
Crystal system	orthorhombic
Space group	Pbca
a/Å	9.75613(13)
b/Å	9.51207(13)
c/Å	40.8263(6)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3788.73(9)
Z	8
ρ_{calc}g/cm^3	1.3232
μ/mm^{-1}	0.706
F(000)	1573.1
Crystal size/mm^3	0.1 × 0.04 × 0.02
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.66 to 148.42
Index ranges	$-9 \leq h \leq 12$, $-7 \leq k \leq 11$, $-49 \leq l \leq 49$
Reflections collected	12081
Independent reflections	3744 [R_{int} = 0.0283, R_{sigma} = 0.0314]
Data/restraints/parameters	3744/0/261
Goodness-of-fit on F^2	1.023
Final R indexes [I>=2σ (I)]	R_1 = 0.0414, wR_2 = 0.1089
Final R indexes [all data]	R_1 = 0.0467, wR_2 = 0.1129
Largest diff. peak/hole / e Å^{-3}	0.17/-0.27

Table S6: Crystal data and structure refinement for **3aa**

Identification code	29-09-19
Empirical formula	$C_{27}H_{16}N_2O_2$
Formula weight	400.42
Temperature/K	294.12(10)
Crystal system	triclinic
Space group	P-1
a/Å	10.5132(3)
b/Å	12.0199(3)
c/Å	12.1585(3)
α/°	67.192(3)
β/°	66.023(3)
γ/°	88.369(2)
Volume/Å^3	1278.80(6)
Z	2
ρ_{calc}g/cm^3	1.040
μ/mm^{-1}	0.530
F(000)	416.0
Crystal size/mm^3	0.05 × 0.05 × 0.03
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/ °	8.074 to 148.16
Index ranges	$-13 \leq h \leq 12$, $-12 \leq k \leq 14$, $-15 \leq l \leq 14$
Reflections collected	13002
Independent reflections	5002 [R_{int} = 0.0281, R_{sigma} = 0.0303]
Data/restraints/parameters	5002/0/281
Goodness-of-fit on F^2	1.058
Final R indexes [I>=2σ (I)]	R_1 = 0.0447, wR_2 = 0.1378
Final R indexes [all data]	R_1 = 0.0502, wR_2 = 0.1434
Largest diff. peak/hole / e Å^{-3}	0.19/-0.19

Table S7: Crystal data and structure refinement for **4aa**

Identification code	17-08-19
Empirical formula	$C_{34}H_{21}NO_4$
Formula weight	507.55
Temperature/K	150.00(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.5919(2)
b/Å	8.32758(18)
c/Å	29.5069(6)
α/°	90
β/°	96.5718(18)

γ/°	90
Volume/Å^3	2585.56(9)
Z	4
ρ_{calc}g/cm^3	1.3038
μ/mm^{-1}	0.690
F(000)	1059.4
Crystal size/mm^3	0.05 × 0.05 × 0.05
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.04 to 147.98
Index ranges	-13 ≤ h ≤ 13, -5 ≤ k ≤ 10, -36 ≤ l ≤ 36
Reflections collected	13977
Independent reflections	5115 [R_{int} = 0.0288, R_{sigma} = 0.0309]
Data/restraints/parameters	5115/0/351
Goodness-of-fit on F^2	1.043
Final R indexes [I>=2σ (I)]	R_1 = 0.0418, wR_2 = 0.1070
Final R indexes [all data]	R_1 = 0.0464, wR_2 = 0.1104
Largest diff. peak/hole / e Å^{-3}	0.54/-0.46

Table S8: Crystal data and structure refinement for **4ab**

Identification code	28-08-19
Empirical formula	$C_{31}H_{19.41}N_2O_3$
Formula weight	506.57
Temperature/K	296(6)
Crystal system	triclinic
Space group	P-1
a/Å	8.05071(12)
b/Å	11.75708(19)
c/Å	16.5493(3)
α/°	95.7815(14)
β/°	96.8159(14)
γ/°	107.5854(14)
Volume/Å^3	1467.16(4)
Z	2
ρ_{calc}g/cm^3	1.1466
μ/mm^{-1}	0.590
F(000)	529.7
Crystal size/mm^3	0.05 × 0.02 × 0.02
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.44 to 148.5
Index ranges	-9 ≤ h ≤ 9, -11 ≤ k ≤ 14, -20 ≤ l ≤ 19
Reflections collected	14519
Independent reflections	5712 [R_{int} = 0.0295, R_{sigma} = 0.0388]
Data/restraints/parameters	5712/0/384
Goodness-of-fit on F^2	1.214

Final R indexes [I>=2σ (I)]	R_1 = 0.0905, wR_2 = 0.2782
Final R indexes [all data]	R_1 = 0.1053, wR_2 = 0.2986
Largest diff. peak/hole / e Å^{-3}	1.51/-0.32

Table S9: Crystal data and structure refinement for **4ac**

Identification code	exp_1148
Empirical formula	$C_{25}H_{15}NO$
Formula weight	345.40
Temperature/K	296.21(10)
Crystal system	triclinic
Space group	P-1
a/Å	9.7693(2)
b/Å	10.1301(2)
c/Å	10.3864(3)
α/°	92.8322(18)
β/°	117.303(2)
γ/°	100.9856(18)
Volume/Å^3	885.53(4)
Z	2
ρ_{calc}g/cm^3	1.2953
μ/mm^{-1}	0.618
F(000)	361.1
Crystal size/mm^3	0.1 × 0.03 × 0.02
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	9 to 148.32
Index ranges	-12 ≤ h ≤ 10, -12 ≤ k ≤ 11, -12 ≤ l ≤ 12
Reflections collected	8809
Independent reflections	3458 [R_{int} = 0.0314, R_{sigma} = 0.0376]
Data/restraints/parameters	3458/0/244
Goodness-of-fit on F^2	1.034
Final R indexes [I>=2σ (I)]	R_1 = 0.0416, wR_2 = 0.1064
Final R indexes [all data]	R_1 = 0.0501, wR_2 = 0.1128
Largest diff. peak/hole / e Å^{-3}	0.17/-0.24

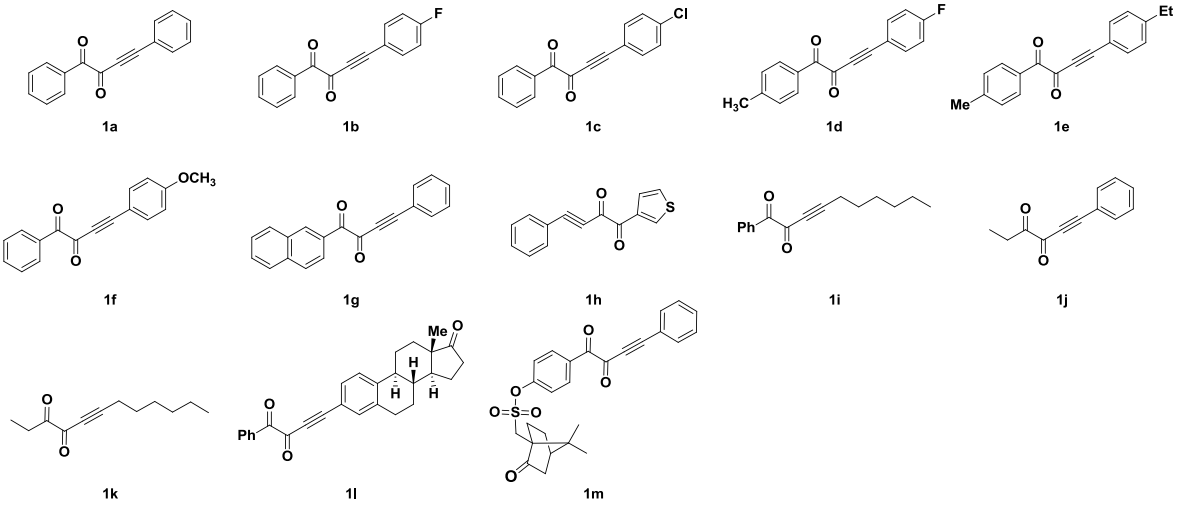
Table S10: Crystal data and structure refinement for **4ad**

Identification code	23-08-19-3
Empirical formula	$C_{68}H_{46}I_2N_4O_8$
Formula weight	1300.89
Temperature/K	150.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	9.4655(2)

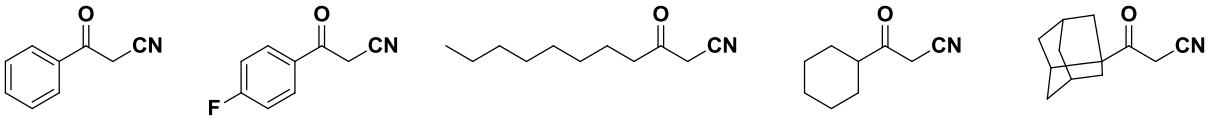
b/Å	11.3208(2)
c/Å	14.0572(3)
α/°	86.973(2)
β/°	89.871(2)
γ/°	76.103(2)
Volume/$Å^3$	1460.11(5)
Z	1
$\rho_{calc}g/cm^3$	1.479
μ/mm^{-1}	8.949
F(000)	652.0
Crystal size/mm^3	0.07 × 0.07 × 0.07
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.3 to 148.22
Index ranges	$-11 \leq h \leq 10$, $-14 \leq k \leq 12$, $-17 \leq l \leq 12$
Reflections collected	15168
Independent reflections	5668 [R_{int} = 0.0518, R_{sigma} = 0.0405]
Data/restraints/parameters	5668/35/395
Goodness-of-fit on F^2	1.204
Final R indexes [I>=2σ (I)]	R_1 = 0.0588, wR_2 = 0.1448
Final R indexes [all data]	R_1 = 0.0592, wR_2 = 0.1449
Largest diff. peak/hole / e $Å^{-3}$	1.19/-1.23

III. General procedures for the preparation of substrates

1. Substrates **1a-1k**[1a] and **1l**, **m**[1b] were known in the literature and prepared by following the literature procedure.



2. Substrates **2a-2e** were prepared according to the literature report.[2a-b]



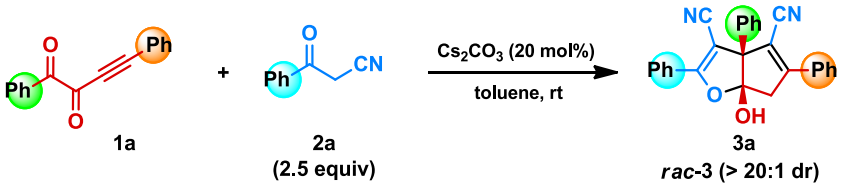
2a 2b 2c 2d 2e

References:

1. (a) X. Kong, G. Zhang, S. Yang, X. Liu, X. Fang, *Adv. Synth. Catal*. **2017**, *359*, 2729–2734; (b) Z. Zhang, X. Jiang, *Org. Lett.* 2014, 16, 4400–4403.

2. (a) S. Havel, P. Khirsariya, N. Akavaram, K. Paruch, B. J.-P. Carbain, *J. Org. Chem.* **2018**, *83*, 15380–15405; (b) C. Zheng, X. Zhang, M. Ijaz Hussain, M. Huang, Q. Liu, Y. Xiong, X. Zhu, *Tetrahedron lett.* **2017**, *58*, 574–577.

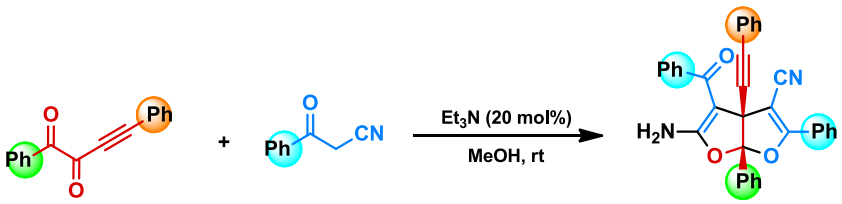
IV. Typical procedure for the synthesis of compounds 3



1a 2a (2.5 equiv) 3a *rac*-3 (> 20:1 dr)

To a dried schlenk tube equiped with stirring bar was added **1a** (0.234 g, 1.0 mmol), **2a** (0.362 g, 2.5 mmol), Cs_2CO_3 (0.65 g, 0.2 mmol, 20 mol%) under argon atmosphere. The tube was evacuated and back filled with argon for three times. Then 5 mL of dry toluene was added to the mixture, the resulted reaction mixture was allowed to stir at room temperature for 10 h. The progress of the reaction was monitored by the TLC. After completion of the reaction the solvent was removed under reduced pressure and the resulted residue was purified by column chromatography on silica gel using petroleum ether-ethyl acetate (10:1 v/v) as eluent to afford product **3a** (0.301 g, 75% yield).

V. Typical procedure for the synthesis of compounds 4

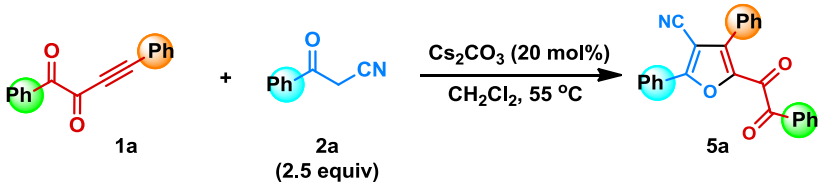


1a 2a (2.5 equiv) 4a *rac*-4 (> 20:1 dr)

To a dried schlenk tube equipped with stirring bar was added **1a** (0.234 g 1.0 mmol), **2a** (0.362 g, 2.5 mmol), Et_3N (0.027 g, 0.2 mmol, 20 mol %) under argon atmosphere. The tube was evacuated and back filled with argon for three times. Then 5 mL of methanol was added

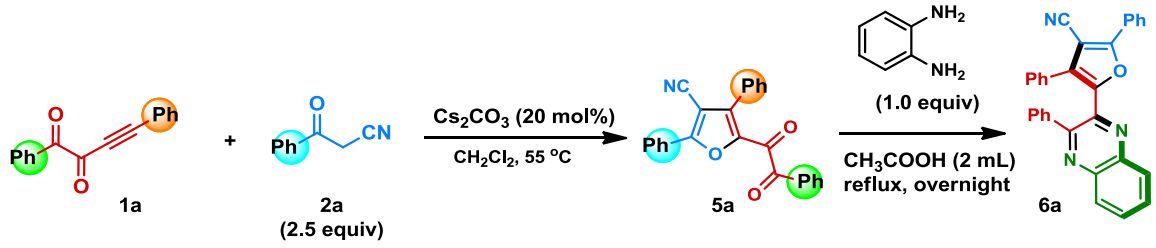
to the mixture, the resulted reaction mixture was allowed to stir at room temperature for 10 h. The progress of the reaction was monitored by the TLC. After completion of the reaction, the solvent was removed under reduced pressure and the resulted residue was purified by column chromatography on silica gel using petroleum ether-ethyl acetate (5:1 v/v) as eluent to afford product **4a** (0.400 g, 79% yield).

VI. Typical procedure of the synthesis of compounds 5



Substrate **1a** (0.234 g 1.0 mmol), **2a** (0.145 g, 1.0 mmol) and Cs_2CO_3 (0.065 g, 0.2 mmol, 20 mol%) were added to a dried schlenk tube containing stirring bar, then 5 mL of dry CH_2Cl_2 was added to it at room temperature under argon atmosphere. The resulted reaction mixture was allowed to stir at 55 ℃ using an oil bath for 5 h. The progress of the reaction was monitored by the TLC. After completion of the reaction, the solvent was removed under reduced pressure and the resulted residue was purified by column chromatography on silica gel using petroleum ether-ethyl acetate (5:1 v/v) as eluent to afford product **5a** (0.340 g, 79% yield).

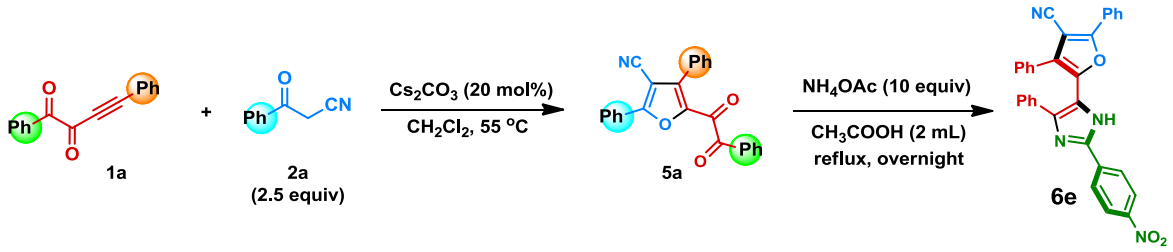
VII. Typical procedure of the synthesis of compounds 6a-6d



Substrate **1a** (0.234. g 1.0 mmol), **2a** (0.145 g, 1.0 mmol) and Cs_2CO_3 (0.065 g, 0.2 mmol, 20 mol%) were added to a dried schlenk tube containing stirring bar, then 5 mL of dry CH_2Cl_2 was added to it at room temperature under argon atmosphere. The resulted reaction mixture was allowed to stir at 55 ℃ using an oil bath for 5 h. The progress of the reaction was monitored by the TLC. After completion of the reaction, the solvent was removed by rota evaporator and the crude residue was used without purification. To this crude product 2 mL of acetic acid and benzene-1,2-diamine (0.108 g 1.00 mmol) were added. Then the reaction

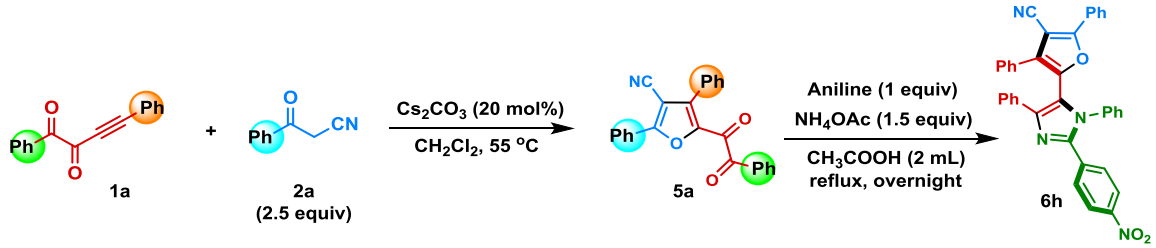
mixture was refluxed using an oil bath overnight. After completion of the reaction, solvent was removed under reduced pressure. Water was added to it and the mixture was extracted with ethyl acetate (5 mL) for three times. The resulted organic layer was dried over $MgSO_4$. The solvent was removed under reduced pressure and the resulted residue was purified by column chromatography on silica gel using petroleum ether-ethyl acetate (10:1 v/v) as eluent to afford product **6a** (0.348 g, 78% yield).

VIII. Typical procedure of the synthesis of compounds 6e-6g, 6j



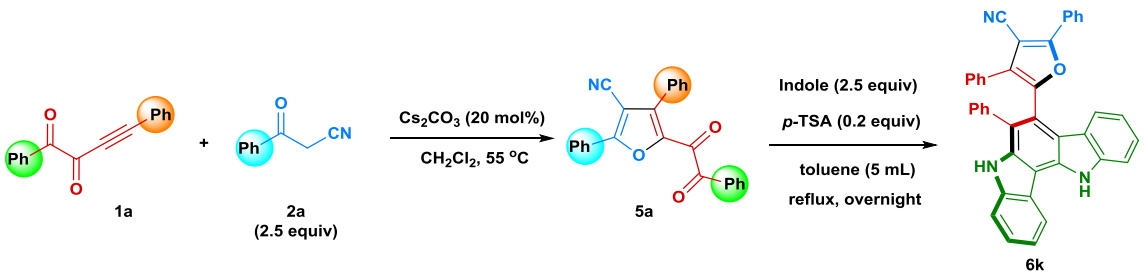
Substrate **1a** (0.234 g 1.0 mmol), **2a** (0.145 g, 1.0 mmol) and Cs_2CO_3 (0.065 g, 0.2 mmol, 20 mol%) were added to a dried schlenk tube containing stirring bar, then 5 mL of dry CH_2Cl_2 was added to it at room temperature under argon atmosphere. The resulted reaction mixture was allowed to stir at 55 ℃ using an oil bath for 5 h. The progress of the reaction was monitored by the TLC. After completion of the reaction the solvent was removed and the crude residue was used without purification. To this crude product 2 mL of acetic acid and aldehyde (0.151 g, 1.0 mmol) and NH_4OAc (0.771 g, 10.0 mmol) were added. Then the reaction mixture was refluxed using an oil bath overnight. After completion of the reaction, solvent was removed under reduced pressure. Water was added to it and the mixture was extracted with ethyl acetate (5 mL) for three times. The resulted organic layer was dried over $MgSO_4$. The solvent was removed under reduced pressure and the resulted residue was purified by column chromatography on silica gel using petroleum ether-ethyl acetate (10:1 v/v) as eluent to afford product **6e** (0.418 g, 83% yield).

IX. Typical procedure of the synthesis of compounds 6h-6j



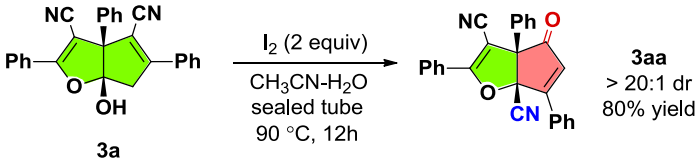
Substrate **1a** (0.234 g 1.0 mmol), **2a** (0.145 g, 1.0 mmol) and Cs_2CO_3 (0.065 g, 0.2 mmol, 20 mol%) were added to a dried schlenk tube containing stirring bar, then 5 mL of dry CH_2Cl_2 was added to it at room temperature under argon atmosphere. The resulted reaction mixture was allowed to stir at 55 ℃ using an oil bath for 5 h. The progress of the reaction was monitored by the TLC. After completion of the reaction, the solvent was removed and the crude residue was used without purification. To this crude product 2 mL of acetic acid, aldehyde (0.151 g, 1.0 mmol), NH_4OAc (0.115 g, 1.5 mmol), aniline (0.092 g 1.0 mmol) were added. Then the reaction mixture was refluxed using an oil bath overnight. After completion of the reaction, solvent was removed under reduced pressure. Water was added to it and the mixture was extracted with ethyl acetate (5 mL) for three times. The resulted organic layer was dried over $MgSO_4$. The solvent was removed under reduced pressure and the resulted residue was purified by column chromatography on silica gel using petroleum ether-ethyl acetate (10:1 v/v) as eluent to afford product **6h** (0.452 g, 77% yield).

X. Typical procedure of the synthesis of compound 6k

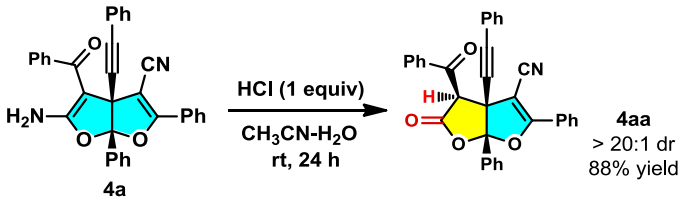


Substrate **1a** (0.234 g 1.00 mmol), **2a** (0.145 g, 1.00 mmol) and Cs_2CO_3 (0.065 g, 0.2 mmol, 20 mol%) were added to a dried schlenk tube containing stirring bar, then 5 mL of dry CH_2Cl_2 was added to it at room temperature under argon atmosphere. The resulted reaction mixture was allowed to stir at 55 ℃ using an oil bath for 5 h. The progress of the reaction was monitored by the TLC. After completion of the reaction the solvent was removed and the crude residue was used without purification. To this crude 5 mL of toluene, indole (0.292 g 2.5 mmol), *p*-TSA (0.034 g, 0.2 equiv) were added. Then the reaction mixture was refluxed using an oil bath for overnight. After completion of the reaction, the solvent was removed under reduced pressure and the resulted residue was purified by column chromatography on silica gel using petroleum ether-ethyl acetate (5:1 v/v) as eluent to afford product **6k (**0.414 g, 72% yield).

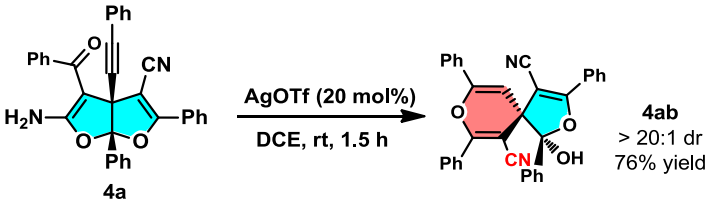
XI. Procedures for the derivatizations of products



To a dried sealed tube equipped with stirring bar was added **3a** (0.402 g, 1.0 mmol), iodine (0.507, 2.0 mmol) under argon atmosphere. Then 10 mL of acetonitrile and water (9:1) added to it, the mixture was allowed to stir at 90 ℃ using an oil bath for overnight. After completion of reaction, the reaction mixture was diluted with water and extracted with ethyl acetate. The organic layer was washed with satd. $Na_2S_2O_3$ solution and satd. brine, dried over anhydrous $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel using petroleum ether-ethyl acetate (10:1 v/v) as eluent to afford product **3aa** (0.325 g, 80% yield).

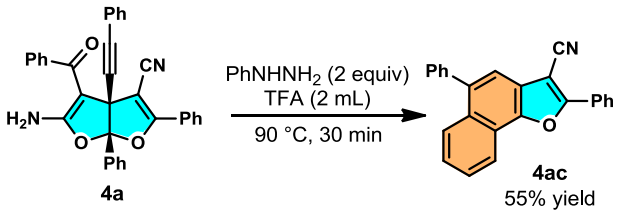


To a 50 mL round-bottom flask, **4a** (0.506 g, 1.0 mmol), acetonitrile (2 mL), H_2O (0.27 g, 1.5 mmol) and 4N HCl (75 μL, 0.30 mmol) was sequentially added. The round-bottom flask was sealed and the reaction mixture was stirred at room temperature for 24 h. The progress of the reaction was monitored by the TLC. After completion of the reaction, the resulting mixture was diluted with water (10 mL) and extracted with ethyl acetate (3 x 10 mL). The combined organic layers were washed with satd. brine dried over anhydrous $MgSO_4$ and concentrated in vacuo. The crude reaction mixture was purified by column chromatography on silica gel petroleum ether-ethyl acetate (5:1 v/v) to give **4aa** (0.450 g, 88% yield).

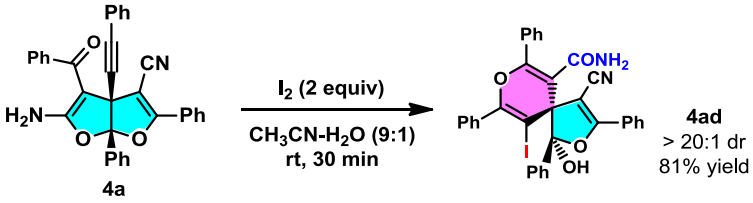


To a dried schlenk tube equipped with stirring bar, **4a** (0.506 g, 1.0 mmol), AgOTf (0.05 g, 0.2 mmol) were added under argon atmosphere. The tube was evacuated and back filled with argon for three times. Then 10 mL of dichloroethane was added to the mixture, the resulted reaction mixture was allowed to stir at room temperature for 1.5 h. The progress of the reaction was monitored by the TLC. After completion of the reaction, the solvent was removed under reduced pressure and the resulted residue was purified by column

chromatography on silica gel using petroleum ether-ethyl acetate (10:1 v/v) as eluent to afford product **4ab (**0.390 g, 76% yield).

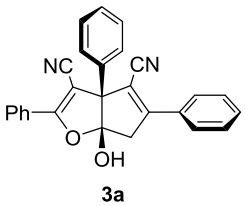


To a dried 50 mL round-bottom flask equipped with stirring bar, **4a** (0.506 g, 1 mmol), phenyl hydrazine (0.196 g, 2 mmol) and TFA (2 mL) were added under argon atmosphere.. Then the reaction mixture was stirred at 90 ℃ using an oil bath for 5 h. The progress of the reaction was monitored by the TLC. After completion of the reaction, the solvent was removed under reduced pressure and the resulted residue was purified by column chromatography on silica gel using petroleum ether-ethyl acetate (10:1 v/v) as eluent to afford product **4ac** (0.191 g, 55% yield).

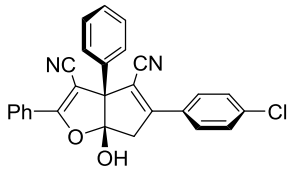


To a solution of **4a** (0.505 g, 1.0 mmol) in acetonitrile and water (9:1) was added iodine (0.507 g, 2.0 mmol). The mixture was allowed to stirred at room temperature for 30 min. The progress of the reaction was monitored by the TLC. After completion of reaction, the reaction mixture was diluted with water and extracted with ethyl acetate. The organic layer was washed with satd. $Na_2S_2O_3$ solution and satd. brine, dried over anhydrous $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel using petroleum ether-ethyl acetate (10:1 v/v) as eluent to afford product **4ad** (0.531 g, 81% yield).

XII. Characterization of new compounds

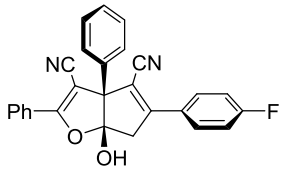


6a-hydroxy-2,3a,5-triphenyl-6,6a-dihydro-3a*H*-cyclopenta[*b*]furan-3,4-dicarbonitrile (3a): Purified using petroleum ether-ethyl acetate (10:1 v/v). White solid, mp 203–204 ^{o}C, 0.301 g, 75% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.11 (d, *J* = 7.2 Hz, 2H), 7.87 (s, 2H), 7.56–7.44 (m, 11H), 3.72 (d, *J* = 18.7 Hz, 1H), 3.54 (d, *J* = 18.7 Hz, 1H), 3.19 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 155.0, 132.5, 132.0, 131.6, 131.5, 130.0, 129.8, 129.1, 129.0, 127.7, 127.7, 127.6, 127.0, 115.8, 115.6, 114.8, 109.0, 85.2, 72.1, 47.4; HRMS (ESI, m/z): calcd. for $C_{27}H_{18}O_2N_2Na^+$ 425.1260, found 425.1256; IR (KBr thin film, cm^{-1}): ν 3564, 3328, 2922, 2209, 1616, 1495, 1448, 1356, 1262, 1182, 764.



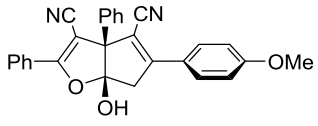
3b

5-(4-chlorophenyl)-6a-hydroxy-2,3a-diphenyl-6,6a-dihydro-3a*H*-cyclopenta[*b*]furan-3,4-dicarbonitrile (3b): Purified using petroleum ether-ethyl acetate (10:1 v/v). White solid, mp 203–204 ^{o}C, 0.353 g, 81% yield. ^{1}H NMR (400 MHz, DMSO–D6) δ 8.21 (s, 1H), 7.99–7.91 (m, 4H), 7.64–7.42(m, 9H), 3.75 (d, *J* = 18.7 Hz, 5H), 3.49 (d, *J* = 18.1 Hz, 2H), 2.08 (s, 1H); ^{13}C NMR (100 MHz, DMSO–D6) δ 168.6, 155.1, 136.3, 133.7, 133.0, 131.2, 130.1, 129.6, 129.5, 129.2, 129.0, 128.5, 127.8, 127.6, 117.5, 117.0, 116.3, 109.4, 84.7, 71.3, 46.0; HRMS (ESI, m/z): calcd. for $C_{27}H_{17}ClN_2O_2Na^+$ 459.0871, found 459.0869; IR (KBr thin film, cm^{-1}): ν 3561, 2920, 2213, 1648, 1280, 1268, 1100, 764, 694.



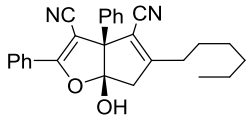
3c

5-(4-fluorophenyl)-6a-hydroxy-2,3a-diphenyl-6,6a-dihydro-3a*H*-cyclopenta[*b*]furan-3,4-dicarbonitrile (3c): Purified using petroleum ether-ethyl acetate (10:1 v/v). White solid, mp 168–169 ^{o}C, 0.327 g, 78% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.7 Hz, 2H), 7.89–7.86 (m, 2H), 7.55–7.43 (m, 10H), 3.71 (d, *J* = 18.7 Hz, 1H), 3.54 (d, *J* = 18.7 Hz, 1H), 3.24 (s, 1H); ^{13}C NMR (150 MHz $CDCl_3$) δ 165.9, 155.0, 138.8, 131.9, 131.6, 130.0, 129.9, 129.4, 129.2, 129.0, 127.8 (d, *J* = 3.5 Hz), 125.6, 115.6 (d, *J* = 6.1 Hz), 115.0, 108.9, 85.7, 72.2, 47.4; IR (KBr thin film, cm^{-1}): ν 3436, 2922, 2232, 1671, 1659, 1596, 1505, 1420, 1385, 1238, 1094, 860, 834, 753.



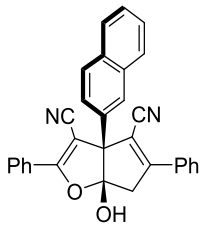
3d

6a-hydroxy-5-(4-methoxyphenyl)-2,3a-diphenyl-6,6a-dihydro-3a*H*-cyclopenta[*b*]furan-3,4-dicarbonitrile (3d): Purified using petroleum ether-ethyl acetate (10:1 v/v). White solid, mp 178–177 ^{o}C, 0.300 g, 69% yield. ^{1}H NMR (400 MHz, DMSO–D6) δ 8.15 (s, 1H), 8.01 (d, *J* = 6.9 Hz, 2H), 7.90 (d, *J* = 8.5 Hz, 2H), 7.65–7.62 (m, 2H), 7.53–7.49 (m, 2H), 7.46–7.39 (m, 3H), 7.12 (d, *J* = 8.5 Hz, 2H), 3.84 (s, 3H), 3.75 (d, *J* = 18.9 Hz, 1H), 3.43 (d, *J* = 18.9 Hz, 1H); ^{13}C NMR (100 MHz, DMSO–D6) δ 168.3, 162.0, 155.4, 134.1, 132.9, 130.1, 129.6, 129.2, 128.9, 128.5, 127.9, 127.6, 124.7, 117.1, 117.1 114.9, 106.0, 85.2, 71.1, 56.0, 45.9; HRMS (ESI, m/z): calcd. for $C_{28}H_{20}O_3N_2Na^+$ 455.1366, found 455.1369; IR (KBr thin film, cm^{-1}): ν 3311, 2928, 2210, 1650, 1507, 1458, 1274, 1018, 838, 764, 750, 694.



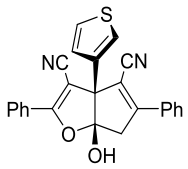
3e

5-hexyl-6a-hydroxy-2,3a-diphenyl-6,6a-dihydro-3a*H*-cyclopenta[*b*]furan-3,4-dicarbonitrile (3e): Purified using petroleum ether-ethyl acetate (10:1 v/v). Colourless liquid, 0.253 g, 62% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.07 (d, *J* = 7.6 Hz, 2H), 7.57–7.53 (m, 1H), 7.49 (t, *J* = 6.9 Hz, 4H), 7.49–7.42 (m, 1H), 7.35 (d, *J* = 7.4 Hz, 2H), 3.20 (d, *J* = 19.2 Hz, 1H), 3.04 (d, *J* = 19.2 Hz, 1H), 2.64–2.48 (m, 2H), 1.61–1.56 (m, 2H), 1.43–1.29 (m, 6H), 0.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8, 163.1, 132.4, 132.2, 129.8, 129.6, 128.9, 127.6, 127.5, 127.2, 115.9, 115.8, 114.2, 111.8, 85.2, 71.0, 47.3, 31.4, 31.2, 28.9, 27.3, 22.5, 14.0; HRMS (ESI, m/z): calcd. for $C_{27}H_{26}O_2N_2Na^+$ 433.1886, found 433.1888; IR (KBr thin film, cm^{-1}): ν 3337, 2925, 2207, 1648, 1450, 1341, 1256, 1091, 764, 750.



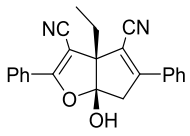
3f

6a-hydroxy-3a-(naphthalen-2-yl)-2,5-diphenyl-6,6a-dihydro-3a*H*-cyclopenta[*b*]furan-3,4-dicarbonitrile (3f): Purified using petroleum ether-ethyl acetate (10:1 v/v). White solid, mp 152–153 ^{o}C, 0.332 g, 73% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.19–8.11 (m, 2H), 8.02–7.87 (m, 6H), 7.58–7.47 (m, 9H), 3.75 (d, *J* = 18.8 Hz, 1H), 3.59 (d, *J* = 18.8 Hz, 1H), 3.32 (s, 1H); ^{13}CNMR (150 MHz, $CDCl_3$) δ 167.1, 155.0, 133.6, 133.4, 132.5, 131.7, 131.5, 129.9, 129.5, 129.1, 129.0, 128.4, 127.8, 127.7, 127.7 127.6, 127.3, 127.1, 127.0, 124.5, 115.8, 115.6, 109.1, 85.2, 72.2, 47.5; HRMS (ESI, m/z): calcd. for $C_{31}H_{20}O_2\ N_2Na^+$ 475.1417, found 475.1414; IR (KBr thin film, cm^{-1}): ν 3417, 2928, 2204, 1648, 1462, 1286, 1141, 763, 753, 697.



3g

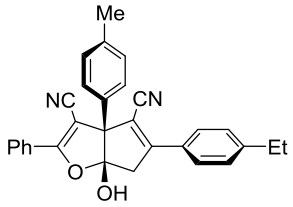
6a-hydroxy-2,5-diphenyl-3a-(thiophen-3-yl)-6,6a-dihydro-3a*H*-cyclopenta[*b*]furan-3,4-dicarbonitrile (3g): Purified using petroleum ether-ethyl acetate (10:1 v/v). White solid, mp 180–181 ^{o}C, 0.292 g, 72% yield. ^{1}H NMR (400 MHz, DMSO–D6) δ 8.40 (s, 1H), 8.00 (d, *J* = 7.0 Hz, 2H), 7.89 (d, *J* = 3.4 Hz, 2H), 7.71–7.57 (m, 6H), 7.21 (s, 2H), 3.81 (d, *J* = 19.1 Hz, 1H), 3.53 (d, *J* = 19.1 Hz, 1H); ^{13}C NMR (100 MHz, DMSO–D6) δ 168.4, 156.2, 137.6, 133.1, 132.1, 131.9, 129.7, 129.6, 128.2, 128.2, 128.1, 127.7, 127.6, 117.0, 116.7, 116.3, 109.2, 85.0, 68.4, 45.6; HRMS (ESI, m/z): calcd. for $C_{25}H_{16}O_2\ N_2NaS^+$ 431.0825, found 431.0826; IR (KBr thin film, cm^{-1}): ν 3405, 2928, 2204, 1656, 1389, 1280, 1262, 1024, 1262, 763, 747.



3h

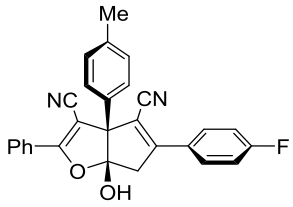
3a-ethyl-6a-hydroxy-2,5-diphenyl-6,6a-dihydro-3a*H*-cyclopenta[*b*]furan-3,4 dicarbonitrile (3h): Purified using petroleum ether-ethyl acetate (10:1 v/v). White solid, mp 152–153 ^{o}C, 0.240 g, 67% yield. ^{1}H NMR (400 MHz, DMSO–D6) δ 8.50 (s, 1H), 7.92 (d, *J* = 6.6 Hz, 2H), 7.81 (d, *J* = 2.9 Hz, 2H), 7.60 (d, *J* = 7.0 Hz, 3H), 7.53 (s, 2H), 3.71 (d, *J* = 19.0 Hz, 1H), 3.45 (d, *J* = 19.0 Hz, 1H), 2.04 (q, *J* = 7.3 Hz, 2H), 1.01 (t, *J* = 7.2 Hz, 3H); ^{13}CNMR (150 MHz, DMSO–D6) δ 166.5, 154.9, 132.8, 132.4, 131.5, 129.6, 129.5, 127.9,

127.5, 117.4, 116.9, 116.2, 108.6, 85.4, 65.8, 47.3, 23.5, 8.9; HRMS (ESI, m/z): calcd. for $C_{23}H_{18}O_2\ N_2Na^+$ 377.1260, found 377.1264; IR (KBr thin film, cm^{-1}): ν 3387, 3320, 2981, 2207, 1698, 1618, 1495, 1347, 1185, 997.



3i

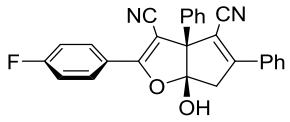
5-(4-ethylphenyl)-6a-hydroxy-2-phenyl-3a-(p-tolyl)-6,6a-dihydro-3a*H*-cyclopenta[*b*]furan-3,4-dicarbonitrile (3i): Purified using petroleum ether-ethyl acetate (10:1 v/v). White solid, mp 174–175 ^oC, 0.332 g, 74% yield. ^1H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 6.3 Hz, 2H), 7.79 (d, *J* = 6.8 Hz, 2H), 7.53–7.46 (m, 3H), 7.29 (s, 6H), 3.67 (d, *J* = 18.5 Hz, 2H), 3.48 (d, *J* = 18.5 Hz, 2H), 3.43 (s, 1H), 2.71 (d, *J* = 6.8 Hz, 2H), 2.37 (s, 3H), 1.26 (s, 3H); ^{13}CNMR (150 MHz, $CDCl_3$) δ 167.0, 154.7, 148.3, 139.7, 132.3, 130.4, 129.2, 129.1, 128.6, 128.5, 127.8, 127.8, 127.7, 127.6, 127.2, 115.9, 114.8, 107.9, 85.3, 71.8, 47.1, 34.7, 28.9, 15.3; HRMS (ESI, m/z): calcd. for $C_{30}H_{24}O_2\ N_2Na^+$ 467.1730, found 467.1729; IR (KBr thin film, cm^{-1}): ν 3399, 2920, 2207, 1647, 1600, 1509, 1462, 1260, 1182, 764, 744, 700.



3j

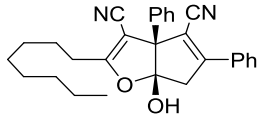
5-(4-fluorophenyl)-6a-hydroxy-2-phenyl-3a-(p-tolyl)-6,6a-dihydro-3a*H*-cyclopenta[*b*]furan-3,4-dicarbonitrile (3j): Purified using petroleum ether-ethyl acetate (10:1 v/v). White solid, mp 160–161 ^oC, 0.348 g, 80% yield. ^1H NMR (400 MHz, DMSO–D6) δ 8.18 (s, 1H), 8.04 (s, 4H), 7.68 (s, 3H), 7.49–7.44 (m, 2H), 7.35 (s, 3H), 3.79 (d, *J* = 18.7 Hz, 1H), 3.51 (d, *J* = 18.8 Hz, 1H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, DMSO–D6) δ 168.4, 165.1, 162.6, 154.9, 138.4, 132.9, 130.8 (d, *J* = 9.0 Hz), 129.8. 129.6, 128.9 (d, *J* = 3.0 Hz), 128.4, 127.9, 127.6, 117.4, 117.0, 116.7, 116.5, 108.8, 85.0, 71.0, 46.2, 21.2; HRMS (ESI, m/z): calcd. for $C_{28}H_{19}O_2\ N_2F\ Na^+$ 457.1323, found 457.1320; IR (KBr thin film, cm^{-1}):

ν 3355, 3078, 2916, 2206, 1745, 1615, 1602, 1512, 1447, 1341, 1274, 1188, 1024, 1002, 844, 764, 750.



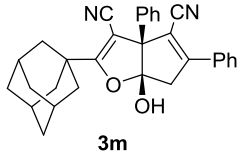
3k

2-(4-fluorophenyl)-6a-hydroxy-3a,5-diphenyl-6,6a-dihydro-3a*H*-cyclopenta[*b*]furan-3,4-dicarbonitrile (3k): Purified using petroleum ether-ethyl acetate (10:1 v/v). White solid, mp 165–167 ^{o}C, 0.327 g, 78% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 6.4 Hz, 2H), 7.85 (s, 2H), 7.50–7.42 (m, 10H), 3.69 (d, *J* = 18.5 Hz, 1H), 3.50 (d, *J* = 18.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.2, 155.0, 138.7, 131.9, 131.6, 129.8, 129.8, 129.3, 129.2, 128.9, 127.7 (d, *J* = 2.0 Hz), 125.5, 115.7, 115.6, 115.1, 108.7, 85.4, 72.0, 47.1; IR (KBr thin film, cm^{-1}): ν 3420, 3317, 2925, 2222, 1652, 1490, 1458, 1274, 1088, 1018, 841, 759.



3l

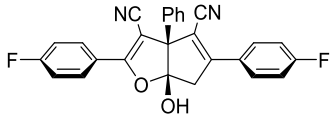
6a-hydroxy-2-octyl-3a,5-diphenyl-6,6a-dihydro-3a*H*-cyclopenta[*b*]furan-3,4-dicarbonitrile (3l): Purified using petroleum ether-ethyl acetate (10:1 v/v). White solid, mp 120–121 ^{o}C, 0.334 g, 77% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86–7.83 (m, 2H), 7.52–7.49 (m, 5H), 7.47–7.43 (m 1H), 7.40–7.33 (m, 2H), 3.57 (d, *J* = 18.7 Hz, 1H), 3.47 (d, *J* = 18.7 Hz, 1H), 2.61–2.51 (m, 2H), 1.71–1.64 (m, 2H), 1.41–1.23 (m, 10 H), 0.87 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.2, 153.5, 131.1, 130.6, 130.4, 128.8, 128.6, 128.1, 126.6, 126.5, 114.8, 114.5, 113.7, 108.3, 86.5, 70.1, 46.3, 30.7, 28.1, 28.0, 28.0, 27.4, 25.2, 21.6, 13.0; HRMS (ESI, m/z): calcd. for $C_{29}H_{30}O_2N_2Na^+$ 461.2199, found 461.2196; IR (KBr thin film, cm^{-1}): ν 3367, 2925, 2213, 1642, 1456, 1259, 1194, 991, 991, 753, 691.



3m

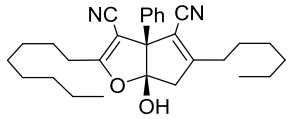
2-(adamantan-1-yl)-6a-hydroxy-3a,5-diphenyl-6,6a-dihydro-3a*H*-cyclopenta[*b*]furan-3,4-dicarbonitrile (3m): Purified using petroleum ether-ethyl acetate (10:1 v/v). White solid, mp 208–209 ^{o}C, 0.318 g, 69% yield. ^{1}H NMR (400 MHz, DMSO–D6) δ 7.88–7.86 (m, 2H),

7.56 (s, 3H), 7.48 (t, *J* = 7.2 Hz, 2H), 7.42–7.38 (m, 1H), 7.33 (d, *J* = 7.4 Hz, 2H), 3.56 (d, *J* = 18.8 Hz, 1H), 3.37 (d, *J* = 18.8 Hz, 1H), 3.35 (s, 1H), 2.01 (s, 9H), 1.71 (s, 6H); ^{13}C NMR (100 MHz, DMSO–D6) δ 180.6, 156.0, 134.1, 132.5, 131.6, 129.5, 129.0, 128.7, 128.5, 128.1, 116.7, 116.5, 116.3, 109.1, 83.6, 79.7, 70.7, 46.5, 39.2, 37.3, 36.3, 27.7; HRMS (ESI, m/z): calcd. for $C_{31}H_{28}O_2N_2Na^+$ 483.2043, found 483.2042; IR (KBr thin film, cm^{-1}): ν 3334, 2910, 2212, 1692, 1612, 1453, 1268, 1180, 1100, 844, 751, 697.



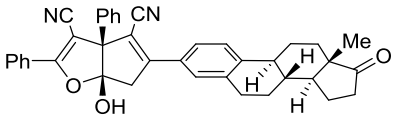
3n

2,5-bis(4-fluorophenyl)-6a-hydroxy-3a-phenyl-6,6a-dihydro-3a*H*-cyclopenta[*b*]furan-3,4-dicarbonitrile (3n): Purified using petroleum ether-ethyl acetate (10:1 v/v). White solid, mp 184–185 ^{o}C, 0.333 g, 77% yield. ^{1}H NMR (600 MHz, CD_3OD) δ 8.05 (d, *J* = 8.4 Hz, 2H), 7.94 (dd, *J* = 8.2, 5.3 Hz, 2H), 7.55 (d, *J* = 8.4 Hz, 2H), 7.50–7.46 (m, 2H), 7.41 (d, *J* = 7.4 Hz, 3H), 7.26 (t, *J* = 8.6 Hz, 2H), 3.43 (s, 1H), 3.30 (s, H), 3.29 (s, 1H); ^{13}C NMR (150 MHz, CD_3OD) δ 167.7, 165.0, 163.4, 154.1 , 138.0, 133.2, 129.9 (d, *J* = 8.8 Hz), 129.0, 128.8, 128.6, 128.5, 127.9, 126.6, 116.2, 115.8, 115.7, 115.5, 85.0, 71.2; IR (KBr thin film, cm^{-1}): ν 3293, 2924, 2211, 1598, 1508, 1495, 1339, 1259, 1100, 1006, 844, 744.



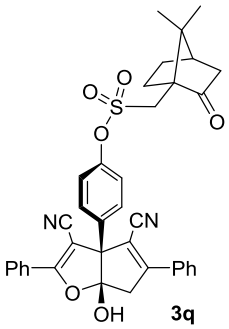
3o

5-hexyl-6a-hydroxy-2-octyl-3a-phenyl-6,6a-dihydro-3a*H*-cyclopenta[*b*]furan-3,4-dicarbonitrile (3o): Purified using petroleum ether-ethyl acetate (10:1 v/v). Colourless liquid, 0.298 g, 67% yield. ^{1}HNMR (600 MHz, $CDCl_3$) δ 7.48 (t, *J* = 7.5 Hz, 2H), 7.42 (t, *J* = 7.3 Hz, 1H), 7.28–7.24 (m, 2H), 3.07 (d, *J* = 19.3 Hz, 1H), 2.97 (d, *J* = 19.3 Hz, 1H), 2.86 (s, 1H), 2.58–2.49 (m, 3H), 1.66–1.61 (m, 2H), 1.58–1.53 (m, 3H), 1.37–1.23 (m, 16H), 0.91–0.86 (m, 6H); ^{13}CNMR (150 MHz, $CDCl_3$) δ 174.8, 162.6, 132.2, 129.9, 129.6, 127.5, 116.8, 114.7, 114.1, 112.2, 87.8, 70.2, 47.5, 31.9, 31.5, 31.2, 29.2, 29.2, 29.1, 28.9, 28.4, 27.4, 26.4, 22.7, 22.6, 14.2, 14.1; HRMS (ESI, m/z): calcd. for $C_{29}H_{38}O_2N_2Na^+$ 469.2825, found 469.2830; IR (KBr thin film, cm^{-1}): ν 3361, 2955, 2216, 1642, 1465, 1262, 1188, 1085, 971, 749.



3p

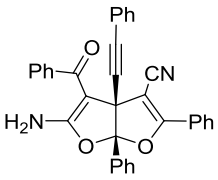
6a-hydroxy-5-((8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-3-yl)-2,3a-diphenyl-6,6a-dihydro-3a*H*-cyclopenta[*b*]furan-3,4-dicarbonitrile (3p): Purified using petroleum ether-ethyl acetate (10:1 v/v). Colourless gummy liquid, 0.455 g, 78% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.08 (d, *J* = 7.6 Hz, 2H), 7.86–7.84 (m, 2H), 7.56–7.53 (m, 1H), 7.50–7.47 (m, 6H), 7.40 (dd, *J* = 8.7, 1.6 Hz, 2H), 3.80 (dd, *J* = 15.0, 2.5 Hz, 1H), 3.67 (d, *J* = 18.8 Hz, 1H), 3.50 (dd, *J* = 18.7, 1.2 Hz, 1H), 3.23 (dd, *J* = 15.0, 2.7 Hz, 1H), 2.51–2.45 (m, 1H), 2.42–2.37 (m, 1H), 2.14 (t, *J* = 4.4 Hz, 1H), 2.11–2.04 (m, 1H), 1.95 (d, *J* = 18.6 Hz, 1H), 1.75–1.69 (m, 1H), 1.47–1.41 (m, 1H), 1.30–1.24 (m, 1H), 1.13 (s, 3H), 1.04 (t, *J* = 7.2 Hz, 1H), 0.90 (d, *J* = 2.7 Hz, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 214.3, 167.8, 155.2, 149.8, 132.6, 131.8, 131.7, 131.6, 129.9, 129.2, 129.0, 127.8, 127.7, 127.3, 123.1, 116.3, 115.6, 108.7, 84.8, 71.4, 58.3, 48.2, 48.2, 48.1, 47.0, 42.9, 42.5, 26.9, 25.3, 19.9, 19.8; HRMS (ESI, m/z): calcd. for $C_{39}H_{34}O_3N_2Na^+$ 601.2462, found 601.2456; IR (KBr thin film, cm^{-1}): ν 3352, 2934, 2204, 1739, 1453, 1386, 1268, 1200, 1088, 749, 694.



3q

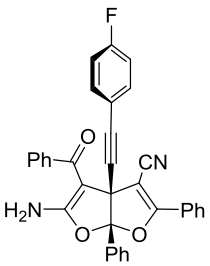
4-(3,4-dicyano-6a-hydroxy-2,5-diphenyl-6,6a-dihydro-3a*H*-cyclopenta[*b*]furan-3a-yl)phenyl ((1*R*,4*R*)-7,7-dimethyl-2-oxobicyclo[2.2.1]heptan-1-yl)methanesulfonate (3q): Purified using petroleum ether-ethyl acetate (10:1 v/v). Colourless gummy liquid, 0.491 g, 77% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 7.6 Hz, 2H), 7.83–7.74 (m, 2H), 7.49–7.37 (m, 7H), 7.30 (d, *J* = 8.2 Hz, 2H), 7.19 (s, 1H), 4.23 (s, 1H), 3.70 (d, *J* = 15.0 Hz, 1H), 3.59 (d, *J* = 18.7 Hz, 1H), 3.42 (d, *J* = 18.7 Hz, 1H), 3.13 (d, *J* = 15.0 Hz, 1H), 2.41–2.27 (m, 2H), 2.05–1.97 (m, 1H), 1.85 (d, *J* = 18.6 Hz, 1H), 1.69–1.58 (m, 1H), 1.37–1.33 (m, 1H), 1.22–1.15 (m, 1H), 1.04 (s, 3H), 0.80 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 213.4, 166.7, 154.1, 148.6, 131.5, 130.7, 130.5, 130.5, 128.8, 128.1, 127.9, 126.7, 126.6, 126.0, 121.9,

114.8, 114.5, 114.3, 107.6, 83.7, 70.2, 57.1, 47.1, 47.0, 45.8, 41.8, 41.4, 25.8, 24.1, 18.8, 18.7; HRMS (ESI, m/z): calcd. for $C_{37}H_{32}O_6N_2NaS^+$ 655.1873, found 655.1869; IR (KBr thin film, cm^{-1}): ν 3305, 3193, 2920, 2204, 1748, 1645, 1506, 1271, 1015, 865, 764, 753, 691.



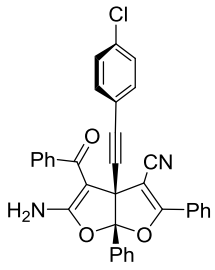
4a

5-amino-4-benzoyl-2,6a-diphenyl-3a-(phenylethynyl)-3a,6a-dihydrofuro[2,3-*b*]furan-3-carbonitrile (4a): Purified using petroleum ether-ethyl acetate (5:1 v/v). White solid, mp 210–211 °C, 0.400 g, 79% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 6.1 Hz, 2H), 7.74 (d, *J* = 5.9 Hz, 2H), 7.64–7.28 (m, 10H), 7.25–7.15 (m, 3H), 6.81 (d, *J* = 5.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.0, 167.6, 164.1, 139.8, 133.1, 131.3, 130.2, 129.3, 128.9, 127.9, 127.5, 127.3, 127.0, 126.8, 126.5, 126.5, 125.5, 125.2, 120.8, 120.1, 113.6, 91.4, 90.7, 90.1, 84.3, 60.0; HRMS (ESI, m/z): calcd. for $C_{34}H_{22}N_2O_3H^+$ 507.1703, found 507.1701; IR (KBr thin film, cm^{-1}): ν 3311, 2920, 2854, 2216, 1648, 1565, 1474, 1286, 1262, 1018, 1018, 763, 750, 697.



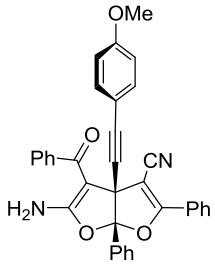
4b

5-amino-4-benzoyl-3a-((4-fluorophenyl)ethynyl)-2,6a-diphenyl-3a,6a-dihydrofuro[2,3-*b*]furan-3-carbonitrile (4b): Purified using petroleum ether-ethyl acetate (5:1 v/v). White solid, mp 130–131 °C, 0.423 g, 80% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.0 Hz, 2H), 7.60 (d, *J* = 6.7 Hz, 2H), 7.39–7.23 (m, 11H), 6.75–6.64 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.0, 168.7, 165.2, 163.8, 161.3, 140.8, 134.2, 133.1 (d, *J* = 8.4 Hz), 132.4, 130.4, 129.9, 129.0, 128.4, 127.9, 127.5 (d, *J* = 9.0 Hz), 126.5, 126.2, 121.1, 117.9 (d, *J* = 3.4 Hz), 115.4 (d, *J* = 219.6 Hz), 114.7, 92.3, 91.1, 90.7, 85.0, 61.1; HRMS (ESI, m/z): calcd. for $C_{34}H_{21}FO_3N_2H^+$ 525.1609, found 525.1606; IR (KBr thin film, cm^{-1}): ν 3358, 2957, 2920, 2263, 2210, 1683, 1650, 1589, 1462, 1399, 1328, 1271, 1220, 1095, 1015, 932, 821, 764, 750, 688.



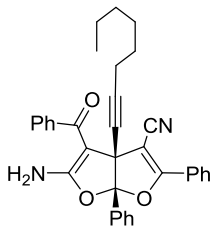
4c

5-amino-4-benzoyl-3a-((4-chlorophenyl)ethynyl)-6a-hydroxy-2-phenyl-3a,6a-dihydrofuro[2,3-*b*]furan-3-carbonitrile (4c): Purified using petroleum ether-ethyl acetate (5:1 v/v). White solid, mp 218–219 ^{o}C, 0.440 g, 82% yield. ^{1}H NMR (400 MHz, DMSO–D6) δ 8.77 (s, 2H), 7.99 (d, *J* = 7.2 Hz, 2H), 7.69–7.56 (m, 10H), 7.44–7.33 (m, 5H), 6.80 (d, *J* = 8.3 Hz, 2H); ^{13}C NMR (100 MHz, DMSO–D6) δ 189.3, 168.2, 165.3, 141.5, 134.2, 134.1, 133.3, 133.0, 131.0, 130.0, 129.9, 129.2, 129.0, 128.2, 127.6, 127.5, 126.5, 126.4, 120.5, 120.2, 115.3, 91.4, 90.2, 89.6, 87.1, 61.2; HRMS (ESI, m/z): calcd. for $C_{34}H_{21}ClO_3N_2H^+$ 541.1313, found 541.1315; IR (KBr thin film, cm^{-1}): ν 3299, 3063, 2924, 2289, 2216, 1650, 1497, 1465, 1277, 1100, 1024, 912, 835, 764, 753, 700.



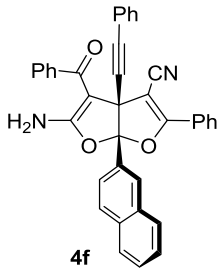
4d

5-amino-4-benzoyl-6a-hydroxy-3a-((4-methoxyphenyl)ethynyl)-2-phenyl-3a,6a-dihydrofuro[2,3-*b*]furan-3-carbonitrile (4d): Purified using petroleum ether-ethyl acetate (5:1 v/v). White solid, mp 218–219 ^{o}C, 0.405 g, 74% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.01 (d, *J* = 7.4 Hz, 2H), 7.75 (d, *J* = 7.2 Hz, 2H), 7.55–7.41 (m, 9H), 7.36 (t, *J* = 7.3 Hz, 2H), 6.76–6.68 (m, 4H), 3.75 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.1, 168.7, 165.1, 159.7, 140.9, 134.3, 132.7, 132.3, 130.3, 129.9, 129.0, 128.3, 127.9, 127.6, 127.6, 126.6, 126.3, 121.2, 114.7, 114.0, 113.7, 92.7, 91.8, 91.3, 84.0, 61.1, 55.3; HRMS (ESI, m/z): calcd. for $C_{35}H_{24}O_4N_2H^+$ 537.1809, found 537.181; IR (KBr thin film, cm^{-1}): ν 3308, 3069, 2928, 2307, 2219, 1718, 1659, 1605, 1464, 1249, 1180, 1032, 1180, 1032, 906, 835, 765, 698.



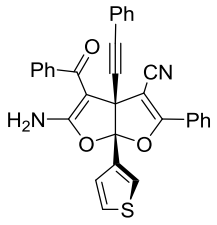
4e

5-amino-4-benzoyl-6a-hydroxy-3a-(oct-1-yn-1-yl)-2-phenyl-3a,6a-dihydrofuro[2,3-*b*]furan-3-carbonitrile (4e): Purified using petroleum ether-ethyl acetate (5:1 v/v). Colourless liquid, 0.333 g, 64% yield**.** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83–7.80 (m, 2H), 7.53–7.50 (m, 2H), 7.34–7.16 (m, 11H), 1.59 (t, *J* = 6.5 Hz, 2H), 1.09–0.99 (m, 2H), 0.95–0.74 (m, 6H), 0.68 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 192.0, 168.7, 164.8, 140.9, 134.3, 132.2, 130.2, 129.8, 129.0, 128.2, 127.7, 127.6, 126.8, 126.3, 121.2, 115.0, 93.5, 92.9, 91.9, 76.3, 60.7, 31.3, 28.3, 27.8, 22.5, 18.6, 14.2; HRMS (ESI, m/z): calcd. for $C_{34}H_{30}O_3N_2H^+$ 515.2329, found 515.2326; IR (KBr thin film, cm^{-1}): ν 3317, 3181, 2923, 2298, 2219, 1650, 1471, 1283, 1077, 1012, 764.



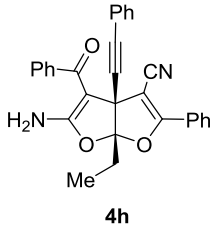
4f

5-amino-4-benzoyl-6a-(naphthalen-2-yl)-2-phenyl-3a-(phenylethynyl)-3a,6a-dihydrofuro[2,3-*b*]furan-3-carbonitrile (4f): Purified using petroleum ether-ethyl acetate (5:1 v/v). White solid, mp 190–191 ^{o}C, 0.446 g, 80% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.07–8.02 (m, 3H), 7.92–7.88 (m, 3H), 7.76 (d, *J* = 7.3 Hz, 2H), 7.59–7.34 (m, 9H), 7.11 (t, *J* = 7.4 Hz, 1H), 6.99 (t, *J* = 7.6 Hz, 2H), 6.55 (d, *J* = 7.5 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 192.2, 168.8, 165.3, 140.9, 134.1, 132.5, 132.5, 131.5, 131.2, 130.0, 129.1, 128.9, 128.5, 128.2, 128.0, 127.8, 127.7, 127.6, 127.5, 126.9, 126.7, 126.1, 123.4, 121.7, 121.3, 114.7, 92.6, 92.0, 91.4, 85.5, 61.3; HRMS (ESI, m/z): calcd. for $C_{38}H_{24}O_3N_2Na^+$ 579.1679, found 579.1675; IR (KBr thin film, cm^{-1}): ν 3311, 2921, 2304, 2225, 1650, 1463, 1274, 1194, 994, 765, 691.



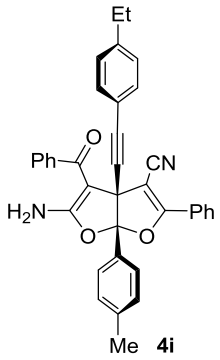
4g

5-amino-4-benzoyl-2-phenyl-3a-(phenylethynyl)-6a-(thiophen-3-yl)-3a,6a-dihydrofuro[2,3-*b*]furan-3-carbonitrile (4g): Purified using petroleum ether-ethyl acetate (5:1 v/v). White solid, mp 179–180 ^{o}C, 0.4032 g, 78% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.7 Hz, 2H), 7.75 (d, *J* = 7.4 Hz, 2H), 7.53–7.42 (m, 6H), 7.38 (t, *J* = 7.4 Hz, 2H), 7.29 (d, *J* = 3.0 Hz, 1H), 7.20 (t, *J* = 7.4 Hz, 2H), 7.15–7.10 (m, 1H), 6.98 (d, *J* = 7.4 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 192.2, 168.0, 164.9, 140.8, 136.2, 131.5, 130.1, 129.0, 128.7, 128.2, 128.1, 127.8, 127.7, 127.5, 127.4, 126.5, 122.0, 120.0, 114.5, 92.2, 91.5, 91.1, 84.7; HRMS (ESI, m/z): calcd. for $C_{32}H_{20}O_3N_2SH^+$ 513.1267, found 513.1266; IR (KBr thin film, cm^{-1}): ν 3317, 3066, 2925, 2301, 2216, 1653, 1492, 1458, 1257, 1411, 1257, 1079, 752, 690.



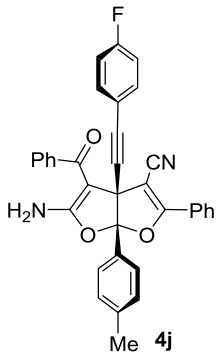
4h

5-amino-4-benzoyl-6a-ethyl-2-phenyl-3a-(phenylethynyl)-3a,6a-dihydrofuro[2,3-b]furan-3-carbonitrile (4h): Purified using petroleum ether-ethyl acetate (5:1 v/v). White solid, mp 90–92 ^{o}C, 0.30 g, 66% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.3 Hz, 2H), 7.67–7.64 (m, 2H), 7.47–7.22 (m, 11H), 2.24 (q, *J* = 7.5 Hz, 2H), 1.18 (t, *J* = 7.4 Hz, 3H); ^{13}CNMR (150 MHz, $CDCl_3$) δ 191.4, 168.6, 164.9, 141.1, 132.3, 131.7, 129.9, 129.0, 128.9, 128.5, 128.1, 127.5, 127.5, 126.9, 122.4, 122.1, 115.2, 93.0, 91.2, 90.2, 84.8, 57.7, 28.6, 7.1; HRMS (ESI, m/z): calcd. for $C_{30}H_{22}O_3N_2H^+$ 459.1703, found 459.1702; IR (KBr thin film, cm^{-1}): ν 3202, 3125, 2921, 2292, 2219, 1653, 1507, 1456, 1259, 1094, 763, 750, 703.



4i

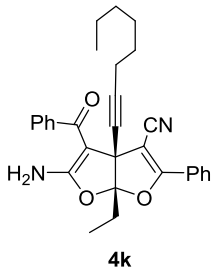
5-amino-4-benzoyl-3a-((4-ethylphenyl)ethynyl)-2-phenyl-6a-(*p*-tolyl)-3a,6a-dihydrofuro[2,3-*b*]furan-3-carbonitrile (4I): Purified using petroleum ether-ethyl acetate (5:1 v/v). White solid, mp 215–216 ^{o}C, 0.372 g, 76% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 5.1 Hz, 2H), 7.75 (d, *J* = 4.7 Hz, 2H), 7.51–7.38 (m, 8H), 7.27 (d, *J* = 7.7 Hz, 2H), 7.01 (d, *J* = 5.7 Hz, 2H), 6.75 (d, *J* = 5.7 Hz, 2H), 2.58 (d, *J* = 6.1 Hz, 2H), 2.42 (s, 3H), 1.18 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 192.2, 168.8, 165.2, 145.0, 140.9, 140.5, 131.4, 131.3, 131.3, 129.1, 129.0, 128.0, 127.7, 127.6, 127.6, 126.7, 126.2, 121.5, 119.2, 114.7, 92.8, 92.0, 91.3, 84.9, 61.1, 28.9, 15.4; HRMS (ESI, m/z): calcd. for $C_{37}H_{28}O_3N_2H^+$ 549.2173, found 549.2171; IR (KBr thin film, cm^{-1}): ν 3122, 2921, 2298, 2216, 1651, 1562, 1507, 1456, 1274, 1097, 763, 756, 703.



4j

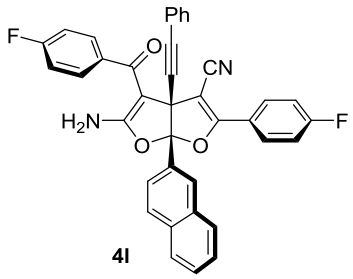
5-amino-4-benzoyl-3a-((4-fluorophenyl)ethynyl)-2-phenyl-6a-(*p*-tolyl)-3a,6a-dihydrofuro[2,3-*b*]furan-3-carbonitrile (4J): Purified using petroleum ether-ethyl acetate (5:1 v/v). White solid, mp 126–127 ^{o}C, 0.422 g, 78% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.2 Hz, 2H), 7.73–7.70 (m, 2H), 7.52–7.32 (m, 8H), 7.26 (d, *J* = 9.7 Hz, 2H), 6.89–6.75 (m, 4H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.9, 168.8, 165.2, 163.8, 161.3, 140.9, 140.5, 133.2 (d, *J* = 8.4 Hz), 132.4, 131.3, 129.9, 129.0, 127.9, 127.5 (d, *J* = 7.3 Hz), 126.6, 126.2, 121.3, 118.1 (d, *J* = 3.3 Hz), 115.5, 115.2, 114.8, 92.3, 91.1, 90.6, 85.2, 61.0, 21.3; HRMS (ESI, m/z): calcd. for $C_{35}H_{23}FO_3N_2H^+$ 539.1765, found 539.1764; IR (KBr

thin film, cm^{-1}): ν 3320, 2928, 2928, 2207, 1651, 1509, 1458, 1271, 1227, 1015, 1015, 844, 764, 750, 694.



4k

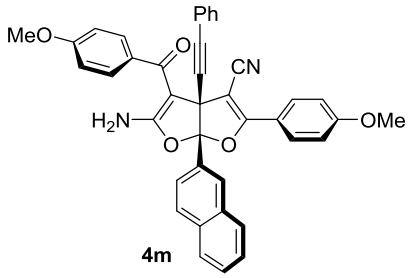
5-amino-4-benzoyl-6a-ethyl-3a-(oct-1-yn-1-yl)-2-phenyl-3a,6a-dihydrofuro[2,3-b]furan-3-carbonitrile (4k): Purified using petroleum ether-ethyl acetate (5:1 v/v). White solid, mp 126–127 ^{o}C, 0.368 g, 78% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 7.2 Hz, 2H), 7.61–7.58 (m, 2H), 7.38–7.29 (m, 6H), 2.14–2.07 (m, 2H), 2.03 (t, *J* = 7.0 Hz, 2H), 1.36–1.28 (m, 2H), 1.28–1.14 (m, 6H), 1.10 (t, *J* = 7.4 Hz, 3H), 0.79 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.4, 168.3, 164.3, 141.1, 132.0, 129.5, 128.7, 127.7, 127.4, 127.4, 126.9, 122.3, 115.2, 93.2, 91.4, 77.4, 75.5, 57.2, 31.3, 28.6, 28.3, 28.2, 22.5, 18.9, 14.1, 6.9; HRMS (ESI, m/z): calcd. for $C_{30}H_{30}O_3N_2H^+$ 467.2329, found 467.2328; IR (KBr thin film, cm^{-1}): ν 3311, 3190, 2923, 2263, 2207, 1653, 1471, 1380, 1274, 1094, 912, 912, 750, 694.



4l

5-amino-4-(4-fluorobenzoyl)-2-(4-fluorophenyl)-6a-(naphthalen-2-yl)-3a-(phenylethynyl)-3a,6a-dihydrofuro[2,3-*b*]furan-3-carbonitrile (4l): Purified using petroleum ether-ethyl acetate (5:1 v/v). White solid, mp 145–146 ^{o}C, 0.490 g, 83% yield. ^{1}HNMR (600 MHz, $CDCl_3$) δ 8.01–8.00 (m, 3H), 7.94–7.90 (m, 3H), 7.68 (d, *J* = 8.4 Hz, 2H), 7.61–7.52 (m, 3H), 7.48 (d, *J* = 8.6 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 7.14 (t, *J* = 7.5 Hz, 1H), 7.03 (t, *J* = 7.7 Hz, 2H), 6.51 (d, *J* = 7.4 Hz, 2H); ^{13}CNMR (150 MHz, $CDCl_3$) δ 190.8, 169.0, 164.0, 139.1, 138.8, 136.0, 134.1, 132.5, 131.1, 129.5, 129.1, 129.0, 128.8, 128.7, 128.3, 128.1 (d, *J* = 6.4 Hz), 128.0, 127.7 (d, *J* = 17.9 Hz), 127.0, 126.0, 125.0, 123.2, 121.4 (d, *J* = 4.1 Hz), 114.7, 92.7, 92.2, 91.9, 84.9; HRMS (ESI, m/z): calcd. for $C_{38}H_{22}F_2O_3N_2H^+$ 593.1671, found 593.1670; IR (KBr thin film, cm^{-1}): ν 3309, 2950, 2330,

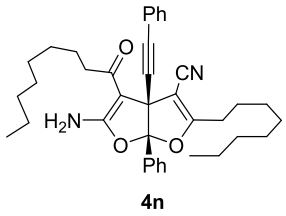
2235, 224, 11693, 1654, 1579, 1469, 1389, 1332, 1264, 1243, 1085, 1017, 935, 831, 754, 770, 678.



4m

5-amino-4-(4-methoxybenzoyl)-2-(4-methoxyphenyl)-6a-(naphthalen-2-yl)-3a-(phenylethynyl)-3a,6a-dihydrofuro[2,3-*b*]furan-3-carbonitrile (4m):

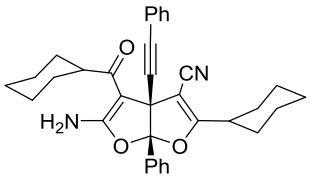
Purified using petroleum ether-ethyl acetate (5:1 v/v). White solid, mp 215–216 ^{o}C, 0.44 g, 71% yield.^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.7 Hz, 3H), 7.91 (d, *J* = 7.7 Hz, 3H), 7.82 (d, *J* = 6.9 Hz, 2H), 7.58–7.54 (m, 3H), 7.12 (s, 1H), 7.00–6.96 (m, 4H), 6.86 (d, *J* = 6.8 Hz, 2H), 6.57 (d, *J* = 5.9 Hz, 2H), 3.85 (s, 3H), 3.77 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 191.4, 168.7, 165.2, 162.8, 161.3, 134.1, 133.7, 132.5, 131.8, 131.1, 129.7, 129.7, 128.9, 128.4, 128.1, 128.0, 127.7, 127.5, 126.8, 126.1, 123.6, 121.9, 120.9, 119.2, 115.5, 114.4, 113.2, 92.6, 91.9, 89.2, 86.1, 61.3, 55.6, 55.3; HRMS (ESI, m/z): calcd. for $C_{40}H_{28}O_5N_2H^+$ 617.2071, found 617.2069; IR (KBr thin film, cm^{-1}): ν 3315, 2931, 2319, 2215, 1653, 1442, 1264, 1020, 828, 774, 760, 684.



4n

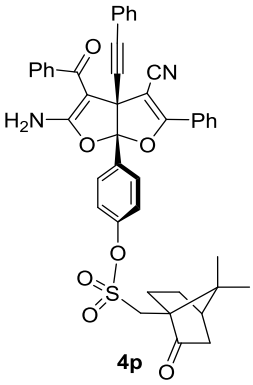
(3a*S*,6a*R*)-5-amino-4-nonanoyl-2-octyl-6a-phenyl-3a-(phenylethynyl)-3a,6a-dihydrofuro[2,3-*b*]furan-3-carbonitrile (4n): Purified using petroleum ether-ethyl acetate (5:1 v/v). Colourless liquid, 0.477 g, 89% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47–7.39 (m, 5H), 7.23–7.15 (m, 3H), 6.90 (d, *J* = 7.1 Hz, 2H), 3.03–2.94 (m, 1H), 2.76–2.68 (m, 1H), 2.63–2.51 (m, 2H), 1.78–1.62 (m, 4H), 1.44–1.18 (m, 20H), 0.89–0.81 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.2, 172.3, 166.9, 134.5, 131.2, 130.2, 128.6, 128.3, 128.1, 125.9, 121.9, 121.4, 114.9, 93.8, 91.6, 91.1, 84.3, 60.3, 39.6, 31.9, 31.8, 29.7, 29.6, 29.3, 29.1, 29.0, 28.1, 26.2, 25.1, 22.7, 22.7, 14.1, 14.1; HRMS (ESI, m/z): calcd. for $C_{38}H_{46}O_3N_2H^+$

579.3581, found 579.3579; IR (KBr thin film, cm^{-1}): ν 3340, 2922, 2295, 2219, 1659, 1490, 1464, 1271, 1015, 1100, 918, 838, 759, 697.



4o

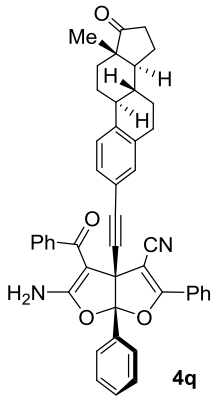
5-amino-4-(cyclohexanecarbonyl)-2-cyclohexyl-6a-phenyl-3a-(phenylethynyl)-3a,6a-dihydrofuro[2,3-*b*]furan-3-carbonitrile (4o): Purified using petroleum ether-ethyl acetate (5:1 v/v). Colour less liquid, 0.402 g, 77% yield**.** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47–7.37 (m, 5H), 7.25–7.14 (m, 3H), 6.88–6.85 (m, 2H), 3.18–3.12 (m, 1H), 2.73–2.62 (m, 1H), 2.03 (d, *J* = 12.3 Hz, 1H), 1.91–1.22 (m, 19H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.8, 175.7, 167.5, 134.7, 131.2, 130.2, 128.5, 128.3, 128.1, 125.9, 121.9, 121.2, 114.5, 91.7, 91.4, 90.3, 84.5, 60.1, 46.9, 38.1, 30.0, 29.6, 29.4, 29.0, 26.1, 25.8, 25.5, 25.5, 25.4, 25.1; HRMS (ESI, m/z): calcd. for $C_{34}H_{34}O_3N_2H^+$ 519.2642, found 519.2638; IR (KBr thin film, cm^{-1}): ν 3358, 2930, 2298, 2222, 1665, 1479, 1268, 1191, 1032, 962, 757, 697.



4p

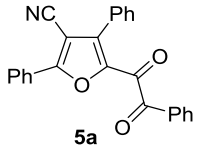
4-(2-amino-3-benzoyl-4-cyano-5-phenyl-3a-(phenylethynyl)-3a,6a-dihydrofuro[2,3-b]furan-6a-yl)phenyl((1*R*)-7,7-dimethyl-2-oxobicyclo[2.2.1]heptan-1-yl)methanesulfonate (4p): Purified using petroleum ether-ethyl acetate (5:1 v/v). Colour less liquid, 0.589 g, 80% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.99 (d, *J* = 7.5 Hz, 2H), 7.73 (d, *J* = 7.2 Hz, 2H), 7.57 (d, *J* = 8.7 Hz, 2H), 7.54–7.50 (m, 1H), 7.48–7.41 (m, 5H), 7.38–7.34 (m, 2H), 7.25–7.16 (m 3H), 6.86 (d, *J* = 7.7 Hz, 2H), 3.82 (d, *J* = 15.0 Hz, 1H), 3.20 (dd, *J* = 15.0, 3.2 Hz, 1H), 2.55–2.49 (m, 1H), 2.44–2.38 (m, 1H), 2.17–2.13 (m, 1H), 2.09–2.06 (m, 1H), 1.97 (d, *J* = 18.5 Hz, 1H), 1.74–1.69 (m, 1H), 1.48–1.40 (m, 1H), 1.13 (d, *J* = 2.5 Hz, 3H), 0.87 (d, *J* = 1.8 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 214.1, 192.1, 168.5, 165.0,

150.5, 140.8, 133.3, 132.5, 131.4, 130.1, 129.1, 128.8, 128.3, 128.0, 127.6, 127.6, 126.4, 122.2, 121.6, 121.5, 120.6, 114.5, 92.4, 91.3, 85.0, 61.2, 58.2, 48.2, 48.1, 42.9, 42.5, 31.0, 27.0, 25.2, 20.0, 19.8; HRMS (ESI, m/z): calcd. for $C_{44}H_{36}O_7N_2SH^+$ 737.2316, found 737.2318; IR (KBr thin film, cm^{-1}): ν 3328, 3140, 2963, 2287, 2213, 1747, 1651, 1507, 1457, 1384, 1259, 1156, 1015, 870, 759, 703.



4q

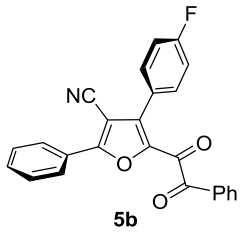
5-amino-4-benzoyl-3a-(((8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-3-yl)ethynyl)-2,6a-diphenyl-3a,6a-dihydrofuro[2,3-*b*]furan-3-carbonitrile (4q): Purified using petroleum ether-ethyl acetate (5:1 v/v). Colour less liquid, 0.553 g, 81% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 7.5 Hz, 2H), 7.76 (d, *J* = 7.3 Hz, 2H), 7.54–7.36 (m, 9H), 7.38 (t, *J* = 7.3 Hz, 2H), 7.09 (d, *J* = 8.0 Hz, 1H), 6.59 (d, *J* = 9.3 Hz, 2H), 2.78 (d, *J* = 4.7 Hz, 2H), 2.54–2.46 (m, 1H), 2.34 (d, *J* = 5.5 Hz, 1H), 2.26–1.93 (m, 5H), 1.58–1.37 (m, 5H), 1.26 (s, 1H), 0.89 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 220.9, 192.1, 168.8, 165.2, 140.9, 140.6, 136.4, 134.3, 132.4, 131.9, 130.3, 130.0, 129.0, 128.5, 128.4, 128.0, 127.6, 127.6, 126.7, 126.3, 125.1, 121.2, 119.3, 114.7, 92.7, 92.0, 91.3, 84.8, 61.2, 50.5, 48.0, 44.4, 37.9, 35.9, 31.6, 29.1, 26.3, 25.6, 21.6, 13.9; HRMS (ESI, m/z): calcd. for $C_{46}H_{37}O_4N_2NaH^+$ 705.2738, found 705.2733; IR (KBr thin film, cm^{-1}): ν 3352, 3193, 2922, 2289, 2213, 1733, 1651, 1453, 1277, 1256, 1088, 764, 750, 694.



5a

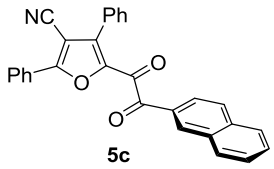
5-(2-oxo-2-phenylacetyl)-2,4-diphenylfuran-3-carbonitrile (5a): Purified using petroleum ether-ethyl acetate (5:1 v/v). Yellow solid, mp 126–127 ^{o}C, 0.340 g, 79% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12–8.09 (m, 2H), 7.86 (d, *J* = 7.4 Hz, 4H), 7.65 (t, *J* = 7.4 Hz, 2H),

7.57–7.42 (m, 8H), 7.38 (t, *J* = 7.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.1, 181.9, 162.9, 143.9, 139.6, 135.0, 132.3, 130.4, 129.8, 129.6, 129.4, 129.0, 128.7, 127.0, 126.7, 126.4, 113.1, 96.4; HRMS (ESI, m/z): calcd. for $C_{25}H_{15}O_3NNa^+$ 400.0944, found 400.0941; IR (KBr thin film, cm^{-1}): ν 3061, 2922, 2227, 1671, 1652, 1479, 1230, 862.



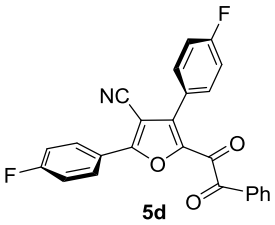
5b

4-(4-fluorophenyl)-5-(2-oxo-2-phenylacetyl)-2-phenylfuran-3-carbonitrile (5b): Purified using petroleum ether-ethyl acetate (5:1 v/v). Yellow solid, mp 140–141 ^{o}C, 0.312 g, 79% yield. ^{1}HNMR (600 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.7 Hz, 2H), 7.88–7.84 (m, 2H), 7.67–7.63 (m, 1H), 7.52–7.43 (m, 7H), 7.38–7.36 (m, 2H); ^{13}CNMR (150 MHz, $CDCl_3$) δ 191.1, 181.9, 161.7, 144.1, 139.6, 138.7, 135.1, 132.4, 130.6, 130.0 129.8, 129.7, 129.1, 128.8, 128.0, 126.9, 125.0, 113.0, 96.8; HRMS (ESI, m/z): calcd. for $C_{25}H_{14}O_3NFNa^+$ 418.0850, found 418.0851; IR (KBr thin film, cm^{-1}): ν 2981, 2212, 1681, 1625, 1525, 1421, 1375, 1238, 1084, 870, 621.



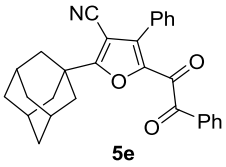
5c

5-(2-(naphthalen-2-yl)-2-oxoacetyl)-2,4-diphenylfuran-3-carbonitrile (5c): Purified using petroleum ether-ethyl acetate (5:1 v/v). Yellow solid, mp 181–182 ^{o}C, 0.337 g, 79% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.40 (s, 1H), 8.12 (d, *J* = 7.1 Hz, 2H), 7.95–7.89 (m, 4H), 7.66 (t, *J* = 7.7 Hz,1H), 7.58 (d, *J* = 7.5 Hz,1H), 7.57–7.51 (m, 5H), 7.44 (t, *J* = 7.3 Hz, 1H), 7.37 (t, *J* = 7.5 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 191.3, 182.1, 163.0, 144.1, 139.8, 136.5, 133.4, 132.4, 132.3, 130.5, 130.1, 129.8, 129.7, 129.5, 129.3, 128.8, 128.1, 127.4, 127.2, 126.9, 126.6, 123.7, 113.3, 96.5; HRMS (ESI, m/z): calcd. for $C_{29}H_{17}O_3NNa^+$ 450.1100, found 450.1101; IR (KBr thin film, cm^{-1}): ν 3061, 2921, 2233, 1698, 1671, 1558, 1448, 1400, 1268, 719, 770.



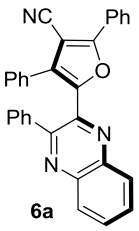
5d

2,4-bis(4-fluorophenyl)-5-(2-oxo-2-phenylacetyl)furan-3-carbonitrile (5d): Purified using petroleum ether-ethyl acetate (5:1 v/v). Yellow solid, mp 174–175 ^{o}C, 0.3102 g, 77% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.6 Hz, 2H), 7.88 (d, *J* = 7.6 Hz, 2H), 7.68 (t, *J* = 7.4 Hz, 1H), 7.54–7.49 (m, 6H), 7.10 (t, *J* = 8.5 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 191.1, 181.8, 164.8, 163.1, 161.7, 144.1, 138.8, 138.5, 135.3, 132.2, 131.8 (d, *J* = 8.8 Hz), 129.9 (d, *J* = 6.2 Hz), 129.2, 128.0, 124.9, 122.9, 116.1 (d, *J* = 21.8 Hz), 112.9, 96.7; HRMS (ESI, m/z): calcd. for $C_{25}H_{13}F_2O_3NNa^+$ 436.0756, found 436.0759; IR (KBr thin film, cm^{-1}): ν 2916, 2232, 1671, 1645, 1505, 1420, 1385, 1238, 1094, 860, 611.



5e

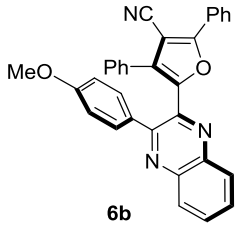
2-((1*S*, 3*S*)-adamantan-1-yl)-5-(2-oxo-2-phenylacetyl)-4-phenylfuran-3-carbonitrile (5e): Purified using petroleum ether-ethyl acetate (5:1 v/v). Pale yellow solid, mp 117–118 ^{o}C, 0.347 g, 78% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.81–7.78 (m, 2H), 7.62 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 2H), 7.41–7.35 (m, 3H), 7.30 (t, *J* = 7.6 Hz, 2H), 2.14–2.10 (m, 9H), 1.77 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 191.4, 182.0, 175.6, 143.3, 139.2, 134.9, 132.5, 130.2, 129.8, 129.7, 129.0, 128.6, 127.4, 112.9, 96.1, 39.8, 37.7, 36.1, 27.8; HRMS (ESI, m/z): calcd. for $C_{29}H_{25}O_3NNa^+$ 458.1727, found 458.1728; IR (KBr thin film, cm^{-1}): ν 2922, 2851, 2233, 1682, 1670, 1518, 1450, 1391, 1262, 882.



6a

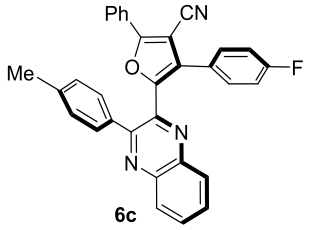
2,4-diphenyl-5-(3-phenylquinoxalin-2-yl)furan-3-carbonitrile (6a): Purified using petroleum ether-ethyl acetate (10:1 v/v). Yellow solid, mp 198–199 ^{o}C, 0.348 g, 78% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (t, *J* = 7.1 Hz, 2H), 7.92 (d, *J* = 3.8 Hz, 2H), 7.82 (s, 2H),

7.46 (s, 3H), 7.30–7.19 (m, 8H), 7.11 (d, *J* = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 153.9, 146.3, 142.7, 141.7, 140.9, 138.1, 131.3, 130.7, 130.5, 129.4, 129.4, 129.2, 129.1, 128.9, 128.9, 128.7, 127.6, 125.9, 114.5, 94.2; HRMS (ESI, m/z): calcd. for $C_{31}H_{19}ON_3H^+$ 450.1601, found 450.1604; IR (KBr thin film, cm^{-1}): ν 2919, 2227, 1647, 1542, 1380, 1380, 1097, 767.



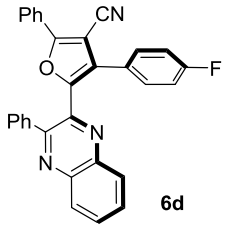
6b

5-(3-(4-methoxyphenyl)quinoxalin-2-yl)-2,4-diphenylfuran-3-carbonitrile (6b): Purified using petroleum ether-ethyl acetate (10:1 v/v). Yellow solid, mp 166–167 ^{o}C, 0.359 g, 75% yield**.** ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18–8.13 (m, 2H), 7.91–7.88 (m, 2H), 7.84–7.79 (m, 2H), 7.46 (d, *J* = 3.6 Hz, 3H), 7.33–7.26 (m, 5H), 7.07 (d, *J* = 8.6 Hz, 2H), 6.76 (d, *J* = 8.6 Hz, 2H), 3.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.2, 159.9, 153.9, 145.9, 142.9, 141.6, 140.9, 138.2, 131.2, 130.6, 130.5, 130.0, 129.4, 129.3, 129.1, 128.9, 128.3, 127.7, 125.8, 121.2, 114.6, 114.1, 94.3, 55.4; HRMS (ESI, m/z): calcd. for $C_{32}H_{21}O_2N_3H^+$ 480.1707, found 480.1710; IR (KBr thin film, cm^{-1}): ν 3058, 2940, 2227, 1612, 1511, 1253, 1100, 1177, 1029, 770, 697.



6c

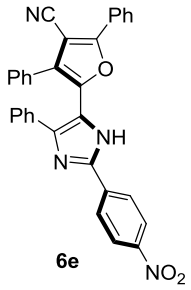
4-(4-fluorophenyl)-2-phenyl-5-(3-(p-tolyl)quinoxalin-2-yl)furan-3-carbonitrile (6c): Purified using petroleum ether-ethyl acetate (10:1 v/v). Yellow solid, mp 178–179 ^{o}C, 0.356 g, 74% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16–8.10 (m, 2H), 7.91–7.89 (m, 2H), 7.84–7.77 (m, 2H), 7.47 (d, *J* = 4.6 Hz, 3H), 7.18–7.06 (m, 6H), 6.92 (t, *J* = 8.4 Hz, 2H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.1, 161.6, 160.3, 153.8, 146.5, 142.5, 141.7, 140.7, 139.1, 135.2, 131.2, 130.8, 130.6 (d, *J* = 8.4 Hz), 130.4, 129.3 (d, *J* = 10.7 Hz), 129.1 (d, *J* = 3.7 Hz), 128.4, 128.0, 127.6, 125.9, 125.0 (d, *J* = 3.3 Hz), 115.7, 115.5, 114.4, 94.1, 21.3; HRMS (ESI, m/z): calcd. for $C_{32}H_{20}OFN_3Na^+$ 504.1483, found 504.1481; IR (KBr thin film, cm^{-1}): ν 3061, 2916, 2227, 1609, 1509, 1231, 1103, 947, 840, 765, 685.



6d

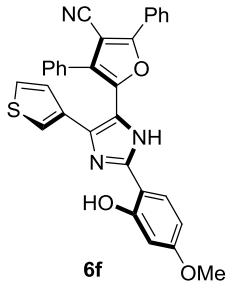
4-(4-fluorophenyl)-2-phenyl-5-(3-phenylquinoxalin-2-yl)furan-3-carbonitrile (6d):

Purified using petroleum ether-ethyl acetate (10:1 v/v). Yellow solid, mp 166–167 ^{o}C, 0.372 g, 80% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.17– 8.11 (m, 2H), 7.91–7.88 (m, 2H), 7.84–7.78 (m, 2H), 7.49–7.42 (m, 3H), 7.34–7.24 (m, 5H), 7.12–7.08 (m, 2H), 6.96–6.88 (m, 2H); ^{13}H NMR (150 MHz, $CDCl_3$) δ 163.8, 162.1, 160.4, 153.8, 146.4, 142.5, 141.8, 140.9, 138.2, 131.4, 130.9, 130.6 (d, *J* = 30 Hz), 129.5, 129.4, 129.2, 129.1, 128.5 (d, *J* = 2.4 Hz), 128.3, 127.6, 125.9, 125.1, 115.9, 115.7, 114.4, 94.2; HRMS (ESI, m/z): calcd. for $C_{31}H_{18}OFN_3Na^+$ 490.1326, found 490.1324; IR (KBr thin film, cm^{-1}): ν 3069, 2925, 2225, 1553, 1509, 1341, 1221, 1091, 844, 773, 697, 573.



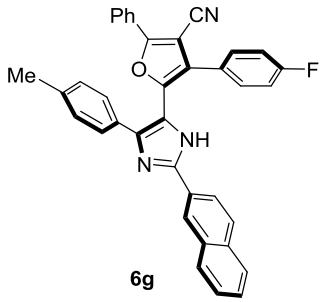
6e

5-(2-(4-nitrophenyl)-4-phenyl-1*H*-imidazol-5-yl)-2,4-diphenylfuran-3-carbonitrile (6e): Purified using petroleum ether-ethyl acetate (10:1 v/v). Yellow solid, mp 181–182 ^{o}C, 0.418 g, 83% yield. ^{1}H NMR (400 MHz, DMSO–D6) δ 13.46 (s, 1H), 8.38–8.26 (m, 4H), 7.86 (s, 2H), 7.57–7.34 (m, 13H); ^{13}C NMR (150 MHz, DMSO-D6) δ 158.6, 147.5, 145.4, 144.9, 136.0, 134.6, 131.1, 130.0, 129.8, 129.4, 129.1, 129.0, 128.8, 128.3, 127.8, 126.6, 125.5, 125.4, 124.9, 115.1, 94.1; HRMS (ESI, m/z): calcd. for $C_{32}H_{20}O_3N_4Na^+$ 531.1428, found 531.1429; IR (KBr thin film, cm^{-1}): ν 3647, 2922, 2849, 2225, 1639, 1508, 1339, 1256, 853, 767, 695.



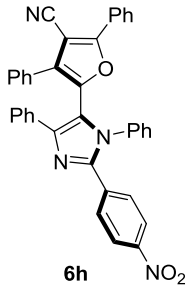
6f

5-(2-(2-hydroxy-4-methoxyphenyl)-4-(thiophen-3-yl)-1*H*-imidazol-5-yl)-2,4-diphenylfuran-3-carbonitrile (6f): Purified using petroleum ether-ethyl acetate (10:1 v/v). Yellow solid, mp 290–291 ^{o}C, 0.417 g, 81% yield. ^{1}H NMR (600 MHz, DMSO–D6) δ 12.28 (s, 0.33H), 11.76 (s, 0.47H), 8.05–6.88 (m, 14H), 6.54–6.43 (m, 2H), 3.75–3.71 (m, 3H); ^{13}CNMR (150 MHz, DMSO-D6) δ 162.1, 161.9, 160.6, 158.8, 158.8, 158.7, 148.1, 147.5, 143.9, 139.9, 135.3, 135.1, 131.7, 131.2, 130.2, 130.1, 130.0, 129.8, 129.5, 129.4, 129.3, 129.2, 129.1, 128.8, 128.4, 128.3, 128.2, 128.1, 127.7, 127.6, 127.1, 127.0, 126.2, 126.0, 125.6, 125.3, 124.6, 124.4, 115.0, 112.7, 107.0, 106.7, 106.5, 106.2, 106.0, 102.0, 101.9, 94.6, 93.8, 55.8; HRMS (ESI, m/z): calcd. for $C_{31}H_{21}O_3N_3SH^+$ 516.1376, found 516.1378; IR (KBr thin film, cm^{-1}): ν 3350, 2215, 1525, 1505, 1450, 1356, 1327, 1215, 879, 721, 721, 657.



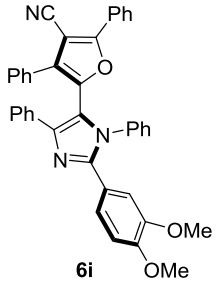
6g

4-(4-fluorophenyl)-5-(2-(naphthalen-2-yl)-4-(*p*-tolyl)-1*H*-imidazol-5-yl)-2-phenylfuran-3-carbonitrile (6g): Purified using petroleum ether-ethyl acetate (10:1 v/v). Yellow solid, mp 287–288 ^{o}C, 0.425 g, 78% yield. ^{1}H NMR (400 MHz, DMSO–D_6) δ 13.10 (s, 1H), 8.77 (d, *J* = 8.5 Hz, 1H), 8.02–7.97 (m, 3H), 7.77–7.68 (m, 3H), 7.65–7.44 (m, 9H), 7.34 (t, *J* = 8.6 Hz, 2H), 7.28 (d, *J* = 7.6 Hz, 2H), 2.38 (s, 3H); ^{13}CNMR (150 MHz, DMSO–D_6) δ 163.3, 161.7, 157.8, 146.6, 146.4, 138.2, 134.1, 132.7, 132.1 (d, *J* = 9.7 Hz), 131.0, 130.6, 129.9 (d, *J* = 7.1 Hz), 129.6, 128.8, 128.5 (d, *J* = 2.7 Hz), 128.4, 127.9, 127.4, 127.2, 127.1, 127.0, 126.9, 126.9, 126.7, 125.7, 125.4, 123.4, 115.9 (d, *J* = 90 Hz), 115.1, 94.5, 21.3; HRMS (ESI, m/z): calcd. for $C_{37}H_{24}FON_3Na^+$ 568.1796, found 568.1793; IR (KBr thin film, cm^{-1}): ν 3317, 2916, 2224, 1642, 1548, 1506, 1383, 1230, 1159, 935, 853, 770, 691, 588.



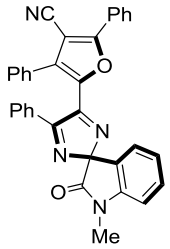
6h

5-(2-(4-nitrophenyl)-1,4-diphenyl-1*H*-imidazol-5-yl)-2,4-diphenylfuran-3-carbonitrile (6h): Purified using petroleum ether-ethyl acetate (10:1 v/v). Yellow solid, mp 117–118 ^{o}C, 0.452 g, 77% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.9 Hz, 2H), 7.98–7.94 (m, 2H), 7.75 (d, *J* = 7.1 Hz, 2H), 7.61 (d, *J* = 8.9 Hz, 2H), 7.52–7.47 (m, 3H), 7.39–7.29 (m, 4H), 7.26–7.19 (m, 5H), 7.07 (d, *J* = 6.6 Hz, 2H), 6.78 (s, 2H); ^{13}CNMR (150 MHz, $CDCl_3$) δ 161.0, 147.5, 145.9, 144.9, 138.9, 135.8, 135.6, 132.8, 130.9, 130.3, 129.7, 129.5, 129.3, 128.9, 128.8, 128.3, 128.0, 127.7, 127.2, 126.6, 125.7, 123.6, 120.1, 114.5, 93.5; HRMS (ESI, m/z): calcd. for $C_{38}H_{24}O_3N_4H^+$ 585.1921, found 585.1920; IR (KBr thin film, cm^{-1}): ν 2922, 2227, 1595, 1527, 1508, 1496, 1386, 1347, 1265, 859, 765, 753, 692.



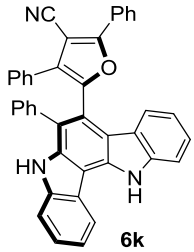
6i

5-(2-(3,4-dimethoxyphenyl)-1,4-diphenyl-1H-imidazol-5-yl)-2,4-diphenylfuran-3-carbonitrile (6i): Purified using petroleum ether-ethyl acetate (10:1 v/v). Yellow solid, mp 244–245 ^{o}C, 0.482, 81% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 6.6 Hz, 2H), 7.44–7.37 (m, 5H), 7.30–7.23 (m, 6H), 7.17–7.13 (m, 1H), 7.08–7.05 (m, 4H), 6.94 (s, 1H), 6.86 (d, *J* = 7.6 Hz, 3H), 6.69 (d, *J* = 8.4 Hz, 1H), 3.83 (s, 3H), 3.63 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.8, 149.4, 148.4, 147.4, 144.8, 137.0, 134.5, 130.4, 130.1, 129.9, 129.4, 129.3, 129.1, 128.9, 128.7, 128.5, 128.2, 128.1, 128.0, 127.9, 127.8, 125.6, 125.5, 122.6, 121.4, 115.1, 111.8, 110.6, 94.1, 55.8, 55.6; HRMS (ESI, m/z): calcd. for $C_{40}H_{29}O_3N_3H^+$ 600.2282, found 600.2285; IR (KBr thin film, cm^{-1}): ν 3069, 2925, 2225, 1524, 1492, 1442, 1256, 1229, 1147, 1021, 1021, 935, 935, 850, 765, 765, 691.



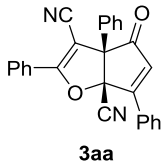
6j

5-(1'-methyl-2'-oxo-4-phenylspiro[imidazole-2,3'-indolin]-5-yl)-2,4-diphenylfuran-3-carbonitrile (6j): Purified using petroleum ether-ethyl acetate (10:1 v/v). White solid, mp 258–259 ^{o}C, 0.429 g, 83% yield. ^{1}H NMR (600 MHz, DMSO–D_6) δ 8.32 (d, *J* = 7.7 Hz, 1H), 8.00 (d, *J* = 8.0 Hz, 2H), 7.69 (t, *J* = 7.7 Hz, 1H), 7.61–7.49 (m, 6H), 7.42 (t, *J* = 7.4 Hz, 1H), 7.33–7.20 (m, 8H), 3.60 (s, 3H); ^{13}C NMR (100 MHz, DMSO–D_6) δ 160.3, 145.8, 145.2, 140.3, 137.6, 132.4, 132.2, 131.5, 130.1, 129.3, 129.3, 129.2, 129.1, 129.1, 129.1, 128.2, 127.7, 127.2, 125.9, 124.3, 124.2, 116.1, 115.0, 113.1, 111.6, 93.2, 31.4; HRMS (ESI, m/z): calcd. for $C_{34}H_{22}O_2N_4H^+$ 519.1816, found 519.1819; IR (KBr thin film, cm^{-1}): ν 2922, 2852, 2227, 1712, 1656, 1598, 1559, 1484, 1484, 1344, 1321, 750.



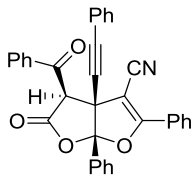
6k

2,4-diphenyl-5-(6-phenyl-5,12-dihydroindolo[3,2-*a*]carbazol-7-yl)furan-3-carbonitrile (6k): Purified using petroleum ether-ethyl acetate (5:1 v/v). White solid, mp 116–117 ^{o}C, 0.414 g, 72% yield. ^{1}H NMR (600 MHz, DMSO–D_6) δ 12.08 (s, 1H), 11.51 (s, 1H), 8.75–8.69 (m, 1H), 7.94–7.87 (m, 2H), 7.65–7.08 (m, 17H), 6.83–6.59 (m, 3H); ^{13}C NMR (100 MHz, DMSO–D_6) δ 159.6, 147.6, 140.4, 139.6, 139.5, 139.1, 136.8, 135.3, 130.9, 130.2, 129.9, 129.0, 128.5, 128.2, 128.2, 127.9, 126.7, 125.6, 125.1, 124.4, 123.7, 121.8, 121.6, 120.6, 119.7, 119.5, 115.5, 113.9, 111.7, 111.6, 106.1, 104.0, 92.7; HRMS (ESI, m/z): calcd. for $C_{41}H_{25}ON_3Na^+$ 598.1890, found 598.1891; IR (KBr thin film, cm^{-1}): ν 3317, 3055, 2931, 2853, 2224, 1495, 1462, 1374, 1256, 1026, 744, 697.



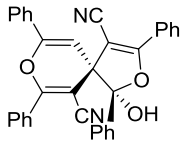
3aa

4-oxo-2,3a,6-triphenyl-4,6a-dihydro-3a*H*-cyclopenta[*b*]furan-3,6a-dicarbonitrile(3aa): Purified using petroleum ether-ethyl acetate (10:1 v/v). White solid, mp 110–111 ^{o}C, 0.325 g, 80% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (d, *J* = 7.5 Hz, 2H), 8.01 (d, *J* = 6.9 Hz, 2H), 7.61–7.57 (m, 4H), 7.53–7.46 (m, 5H), 7.38 (d, *J* = 7.2 Hz, 2H), 7.13 (s, 1H); ^{13}CNMR (150 MHz, $CDCl_3$) δ 198.2, 165.9, 163.1, 133.2, 133.0, 130.2, 130.1, 129.8, 129.7, 129.3, 129.0, 128.7, 128.4, 127.7, 125.8, 114.0, 113.3, 90.5, 85.7, 71.5; HRMS (ESI, m/z): calcd. for $C_{27}H_{16}O_2N_2H^+$ 401.1285, found 401.1281; IR (KBr thin film, cm-1): 3358, 3187, 2920, 2215, 1727, 1656, 1344, 1286, 1135, 766, 751, 688.



4aa

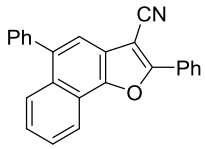
4-benzoyl-5-oxo-2,6a-diphenyl-3a-(phenylethynyl)-3a,4,5,6a-tetrahydrofuro[2,3-*b*]furan-3-carbonitrile (4aa): Purified using petroleum ether-ethyl acetate (5:1 v/v). White solid, mp 148–149 ^{o}C, 0.450 g, 88% yield**.** ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.09 (dd, *J* = 20.9, 6.9 Hz, 4H), 7.78 (d, *J* = 4.7 Hz, 2H), 7.62 (s, 2H), 7.56–7.47 (m, 7H), 7.14–7.13 (m, 1H), 7.01 (t, *J* = 6.7 Hz, 2H), 6.44 (d, *J* = 6.7 Hz, 2H), 5.32 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 191.4, 168.9, 165.0, 135.8, 134.6, 133.4, 133.0, 131.2, 130.5, 129.5, 129.3, 129.2, 129.1, 128.1, 128.0, 128.0, 127.4, 125.9, 120.5, 117.5, 115.1, 94.6, 87.5, 80.8, 58.8, 57.4; HRMS (ESI, m/z): calcd. for $C_{34}H_{21}O_4NH^+$ 508.1453, found 508.1456; IR (KBr thin film, cm^{-1}): ν 3072, 2922, 2216, 1809, 1682, 1634, 1449, 1268, 1207, 978, 758, 687.



4ab

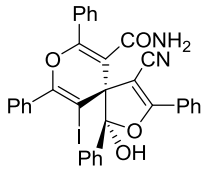
1-hydroxy-1,3,7,9-tetraphenyl-2,8-dioxaspiro[4.5]deca-3,6,9-triene-4,6-dicarbonitrile (4ab): Purified using petroleum ether-ethyl acetate (10:1 v/v). White solid, mp 136–137 ^{o}C, 0.390 g, 76% yield. ^{1}H NMR (600 MHz, CD_3OD) δ 8.14 (d, *J* = 7.3 Hz, 2H), 7.79 (d, *J* = 6.9 Hz, 2H), 7.70 (d, *J* = 5.4 Hz, 2H), 7.65–7.57 (m, 4H), 7.50–7.43 (m, 6H), 7.36 (t, *J* = 7.3 Hz, 2H), 7.22 (d, *J* = 7.2 Hz, 2H), 6.18 (s, 1H); ^{13}C NMR (150 MHz, CD_3OD) δ 166.5, 162.4, 150.5, 138.4, 132.2, 131.9, 131.4, 131.3, 129.7, 129.2, 129.1, 128.8, 128.6, 128.2, 128.0, 127.3, 126.4, 124.8, 116.9, 116.1, 113.2, 96.3, 89.1, 88.0, 56.7; HRMS (ESI, m/z): calcd. for

$C_{34}H_{22}O_3N_2H^+$ 507.1703, found 507.1700; IR (KBr thin film, cm^{-1}): ν 3199, 2922, 2208, 1647, 1507, 1263, 1122, 1092, 764, 700.



4ac

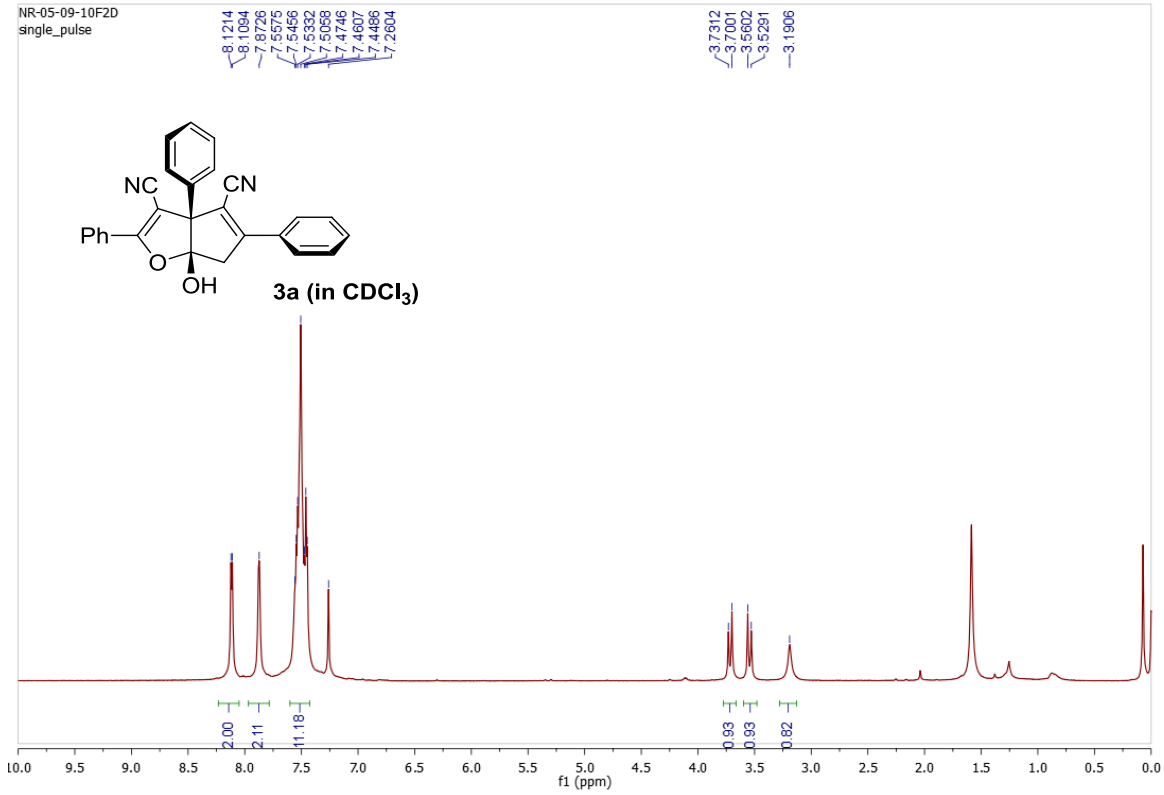
2,5-diphenylnaphtho[1,2-*b*]furan-3-carbonitrile (4ac): Purified using petroleum ether-ethyl acetate (10:1 v/v). Light yellow solid, mp 189–190 ^oC, 0.191 g, 55% yield. ^1H NMR (600 MHz, $CDCl_3$) δ 8.42 (d, *J* = 7.8 Hz, 1H), 8.27 (d, *J* = 7.4 Hz, 2H), 7.95 (d, *J* = 8.5 Hz, 1H), 7.68–7.65 (m, 2H), 7.58 (t, *J* = 7.4 Hz, 2H), 7.54–7.45 (m, 7H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.0, 149.0, 140.1, 138.6, 131.0, 130.9, 130.3, 129.4, 128.5, 128.2, 127.8, 127.5, 127.2, 126.5, 126.3, 122.9, 121.0, 120.2, 118.1, 114.5, 89.3; HRMS (ESI, m/z): calcd. for $C_{25}H_{15}ONH^+$ 346.1226, found 346.1224; IR (KBr thin film, cm^{-1}): ν 3061, 2922, 2226, 1652, 1634, 1565, 1497, 1268, 1141, 759.

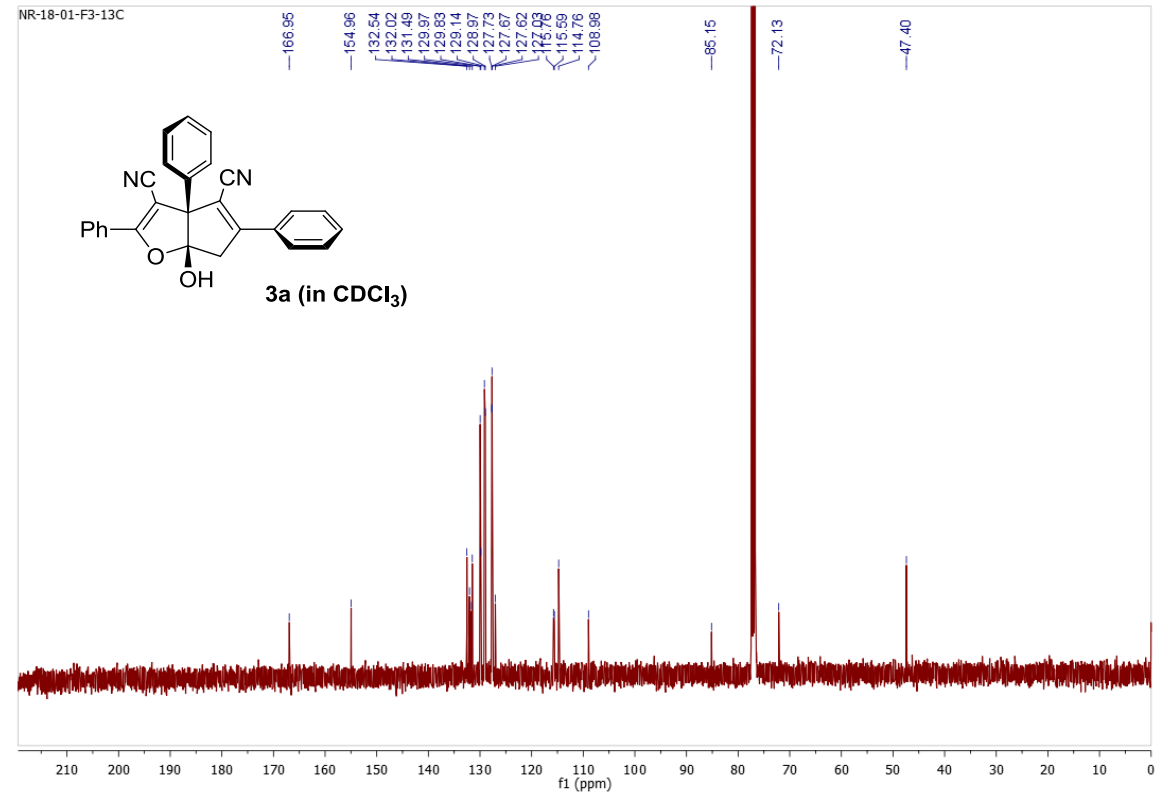


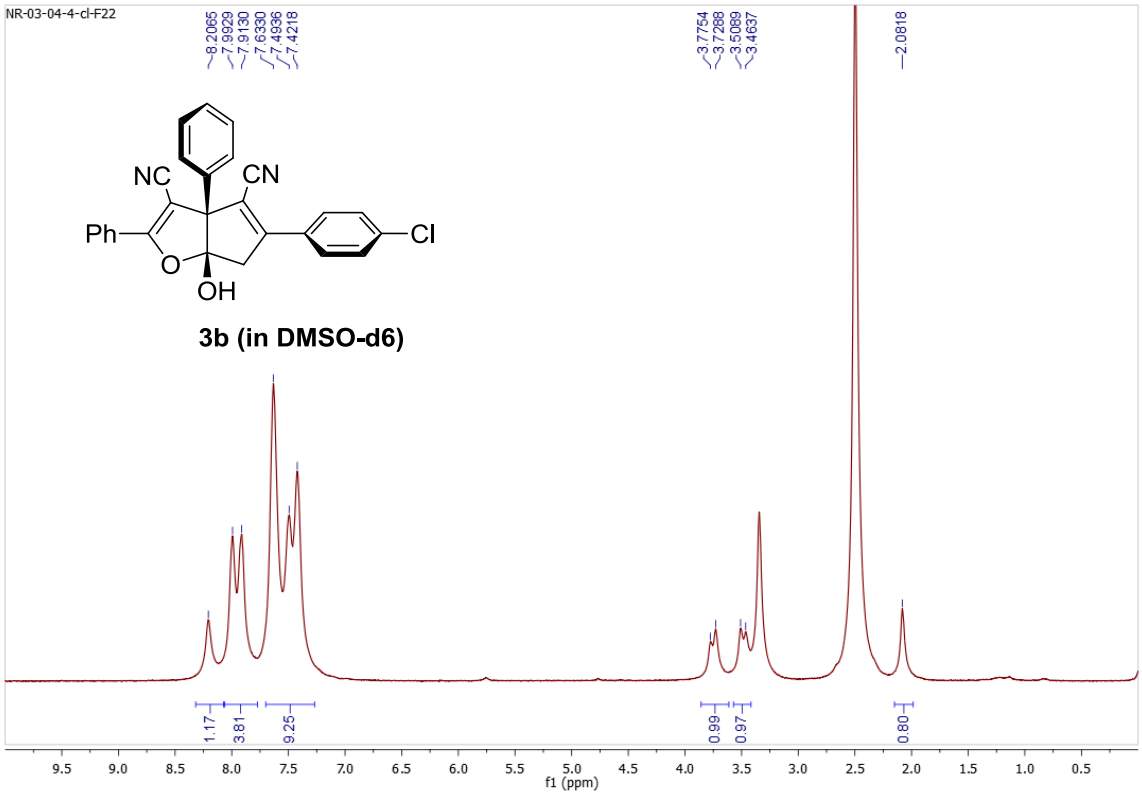
4ad

4-cyano-1-hydroxy-10-iodo-1,3,7,9-tetraphenyl-2,8-dioxaspiro[4.5]deca-3,6,9-triene-6-carboxamide (4ad): Purified using petroleum ether-ethyl acetate (10:1 v/v). Light yellow solid, mp 165–166 ^oC, 0.531g, 81% yield. ^1H NMR (400 MHz, $CDCl_3$) δ 9.84 (s, 1H), 8.19 (d, *J* = 6.7 Hz, 2H), 7.77 (d, *J* = 6.5 Hz, 2H), 7.69 (d, *J* = 6.5 Hz, 2H), 7.56–7.40 (m, 7H), 7.36–7.26 (m, 4H), 6.84 (d, *J* = 6.9 Hz, 2H), 5.86 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.0, 166.9, 156.5, 152.1, 138.5, 132.3, 131.6, 131.5, 129.7, 129.4, 129.2, 129.0, 128.9, 128.0, 128.0, 127.8, 127.3, 117.1, 115.2, 102.3, 91.0, 82.6, 62.8; HRMS (ESI, m/z): calcd. for $C_{34}H_{24}O_4N_2IH^+$ 651.0775, found 651.0777; IR (KBr thin film, cm^{-1}): ν 3069, 2922, 2206, 1653, 1447, 1261, 1132, 1026, 765, 694.

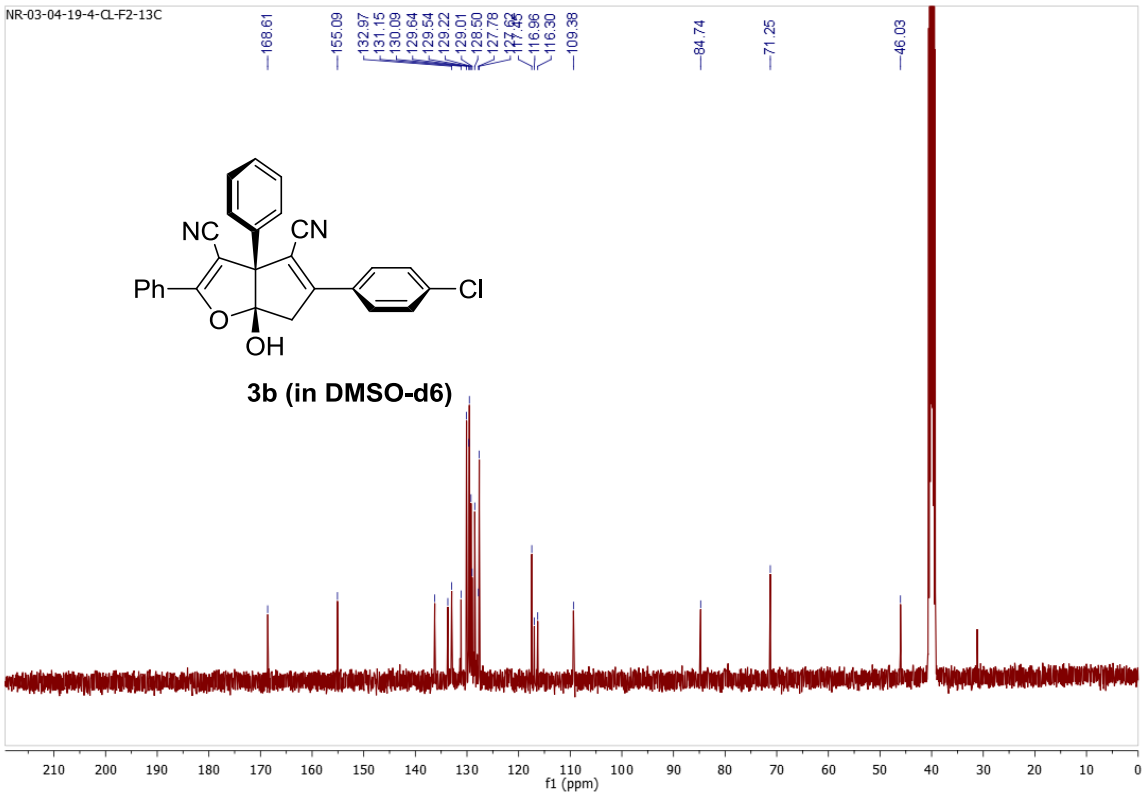
XIII. ^{1}H NMR and ^{13}C NMR spectra of new compounds



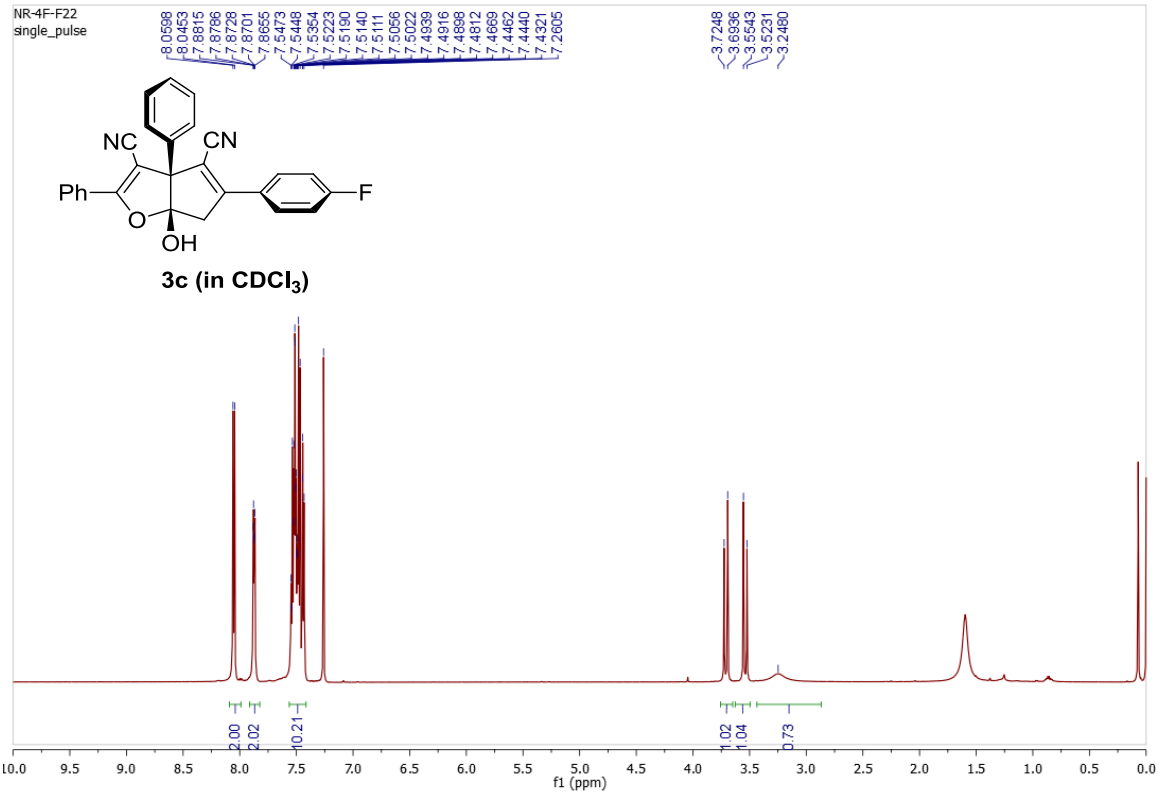




3b (in DMSO-d6)



3b (in DMSO-d6)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NC
CN
Ph
O
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F
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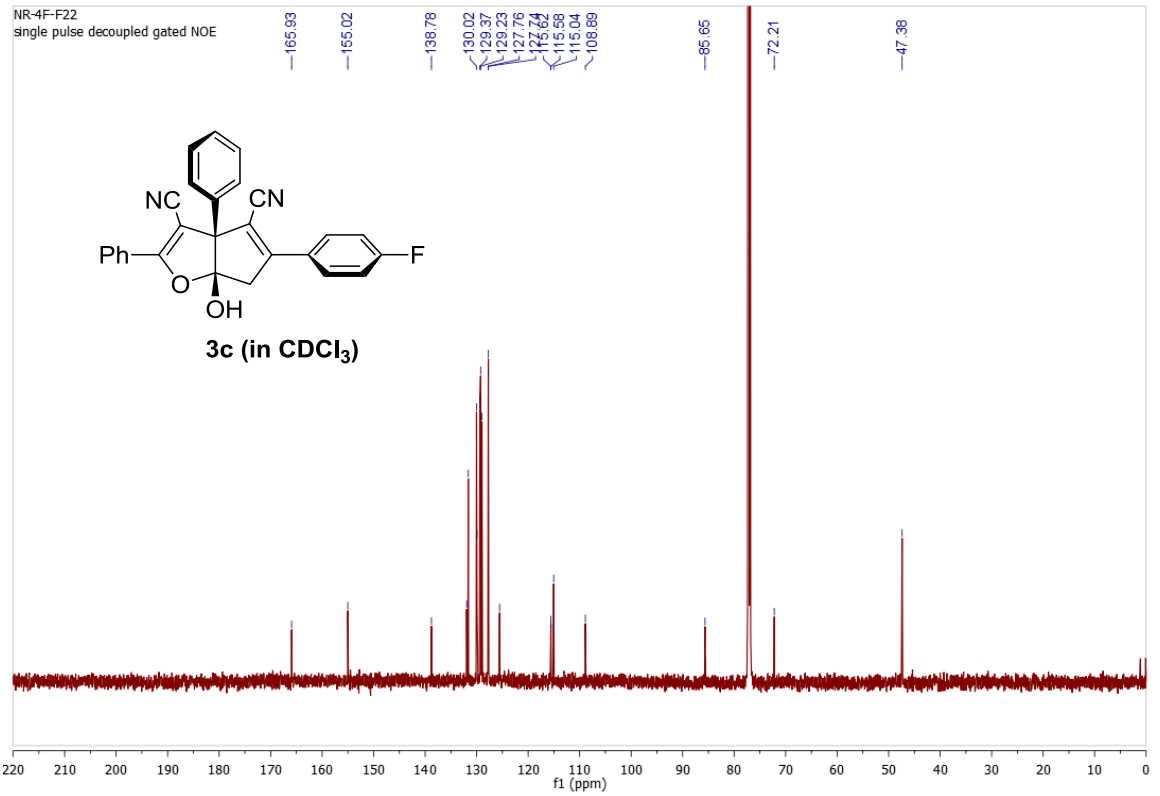
1.02
1.04
0.73
f1 (ppm)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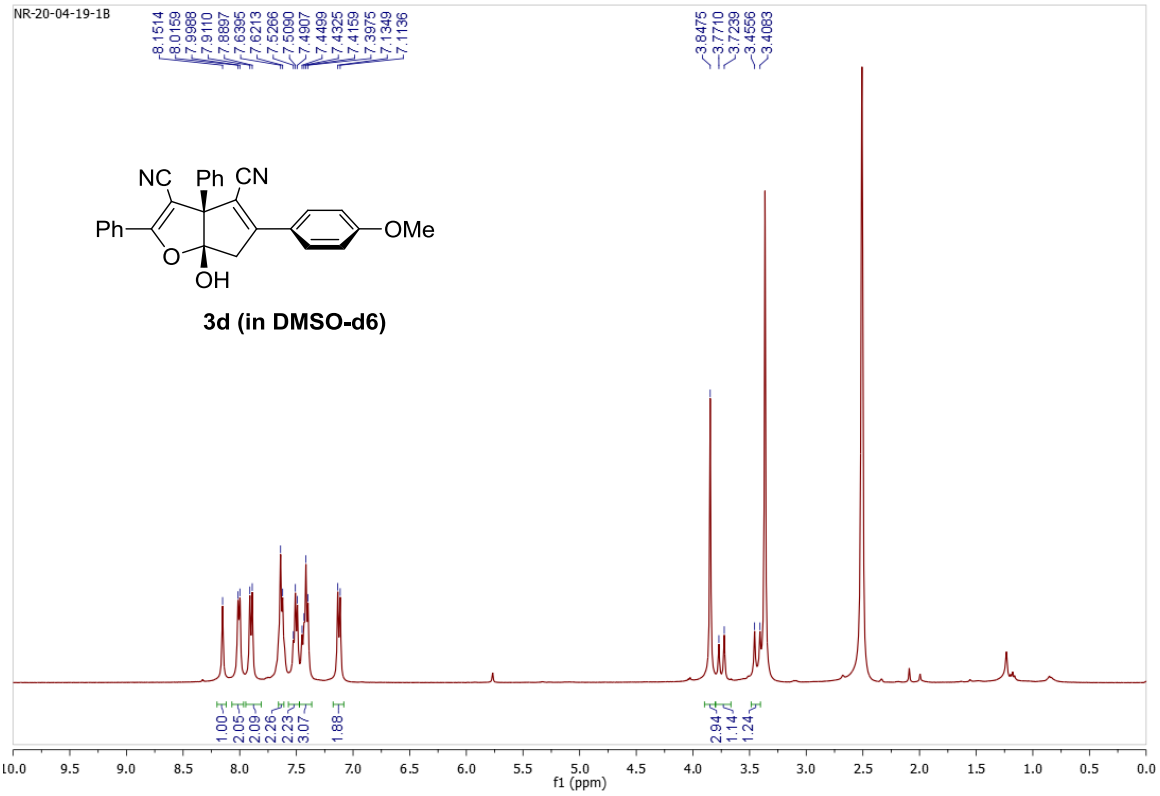
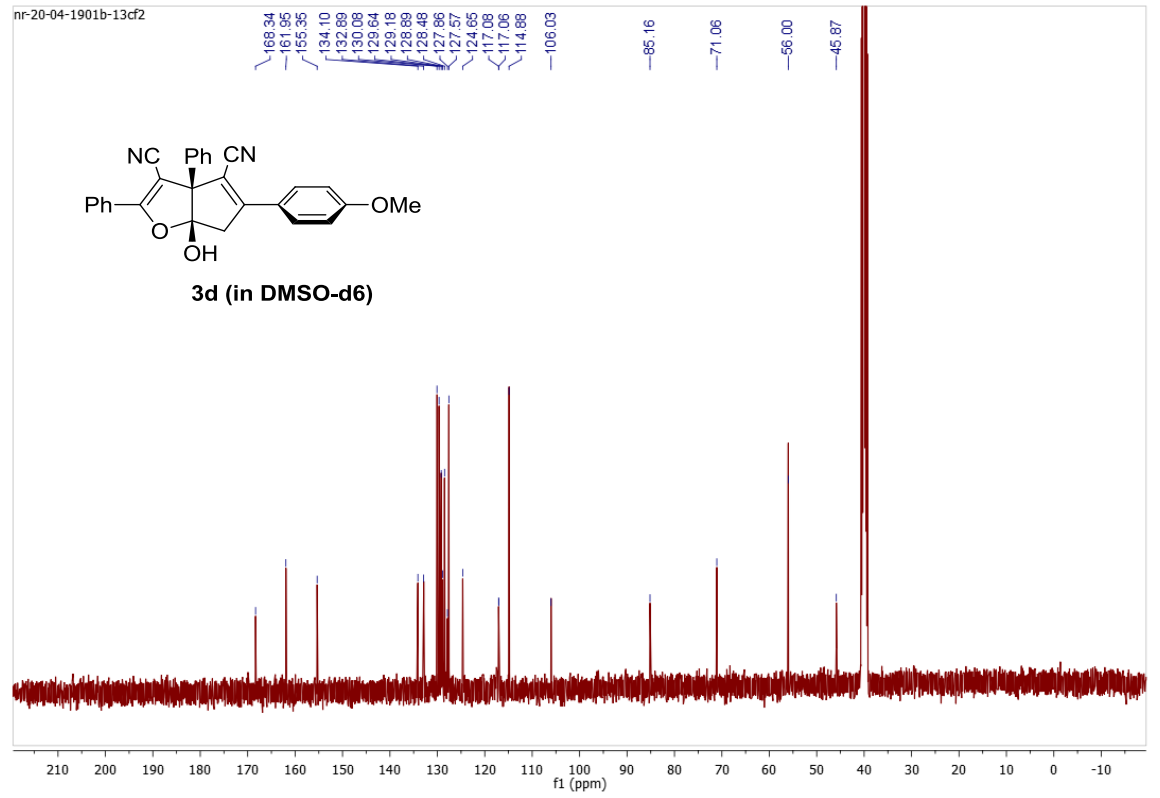
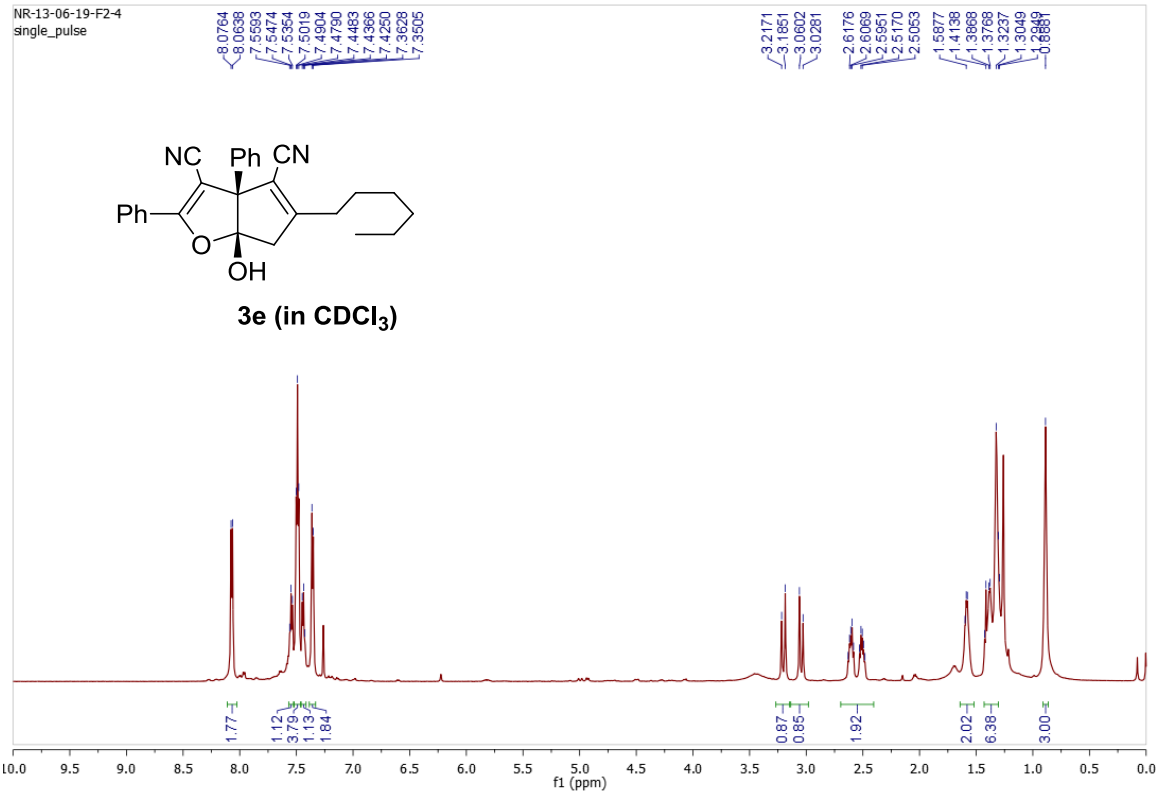
NC
CN
Ph
O
OH
F
3c (in CDCl3)
f1 (ppm)



3d (in DMSO-d6)



3d (in DMSO-d6)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Ph
O
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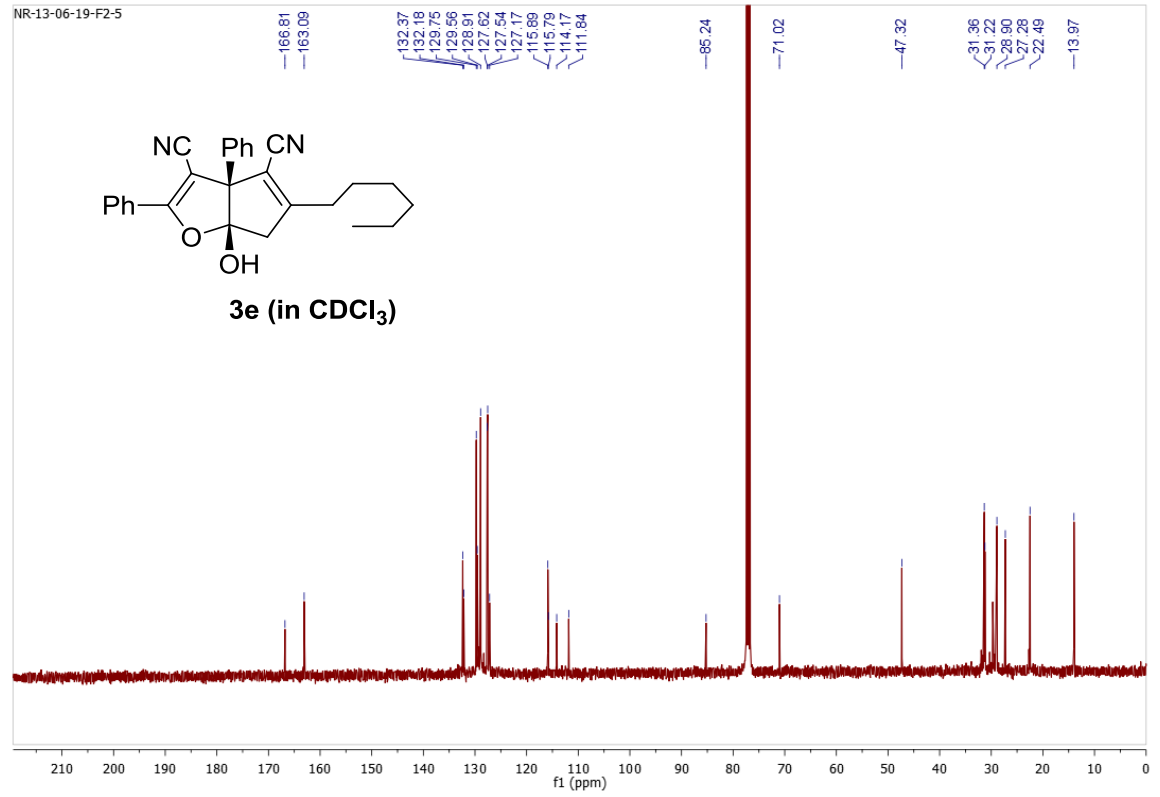
f1 (ppm)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Ph
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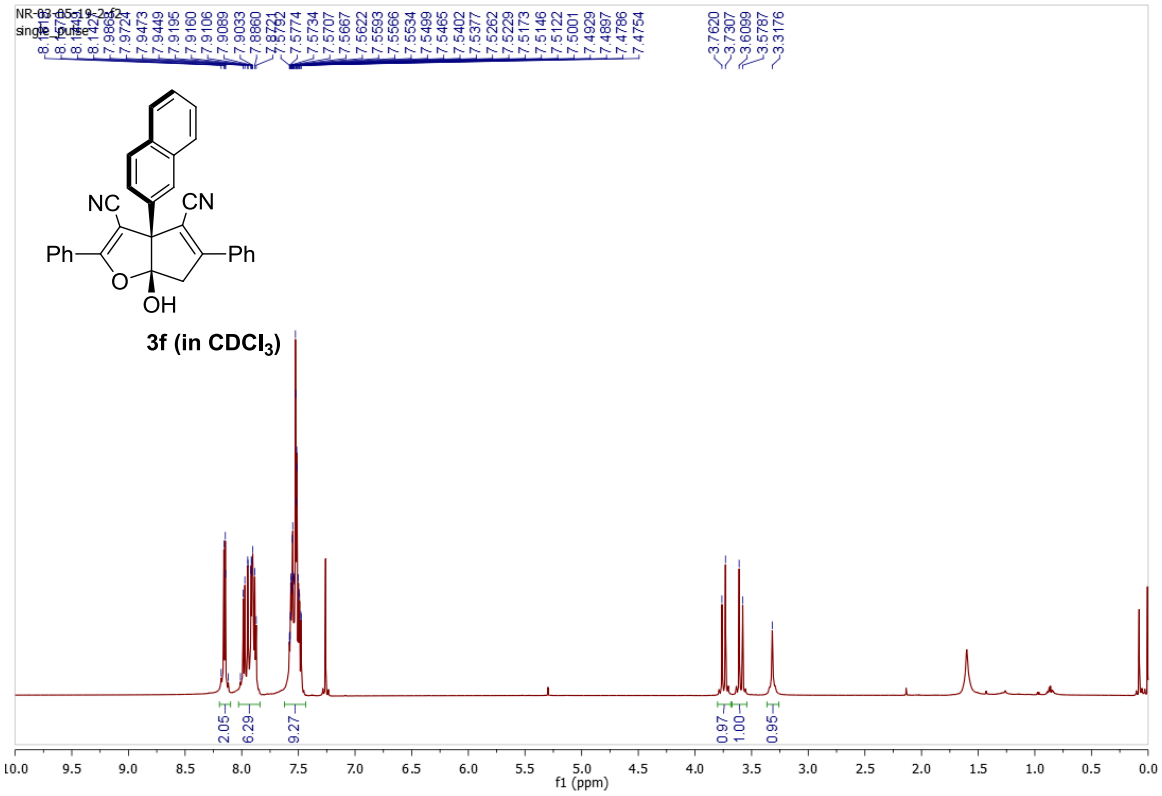
3e (in CDCl3)
f1 (ppm)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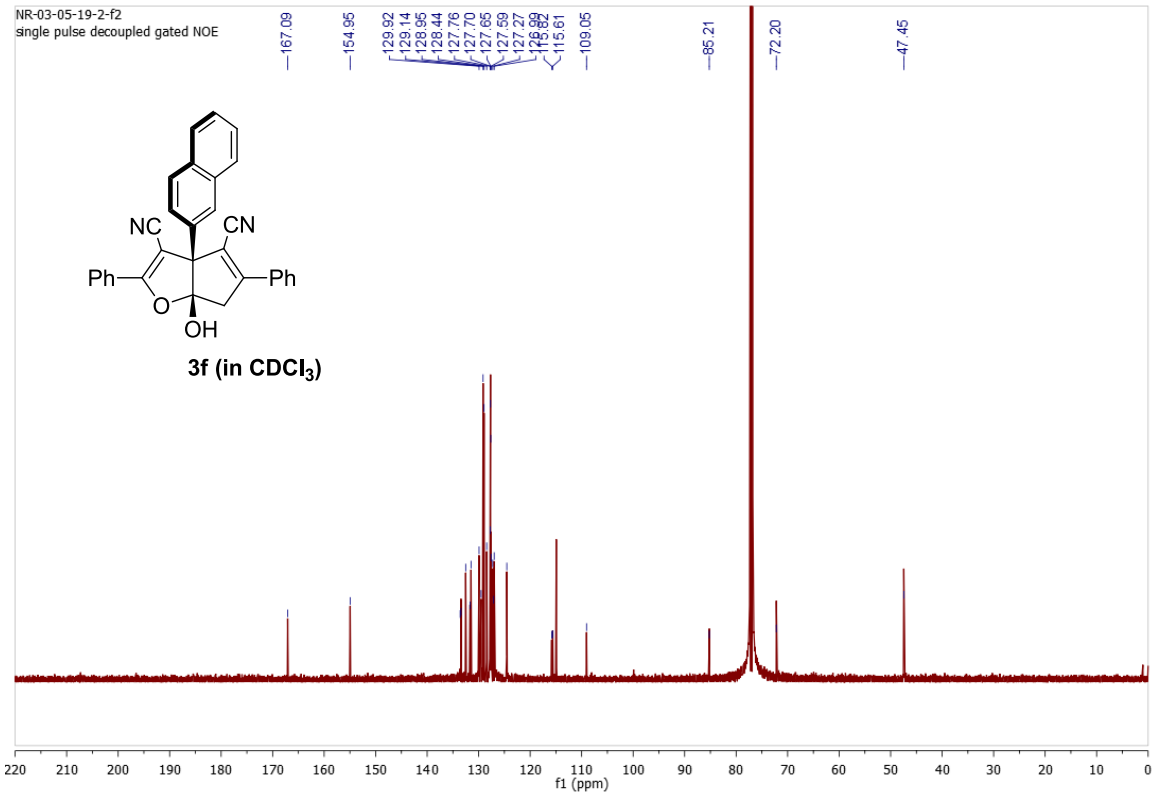
CN
Ph
Ph
O
OH
3f (in CDCl3)
f1 (ppm)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Ph
Ph
O
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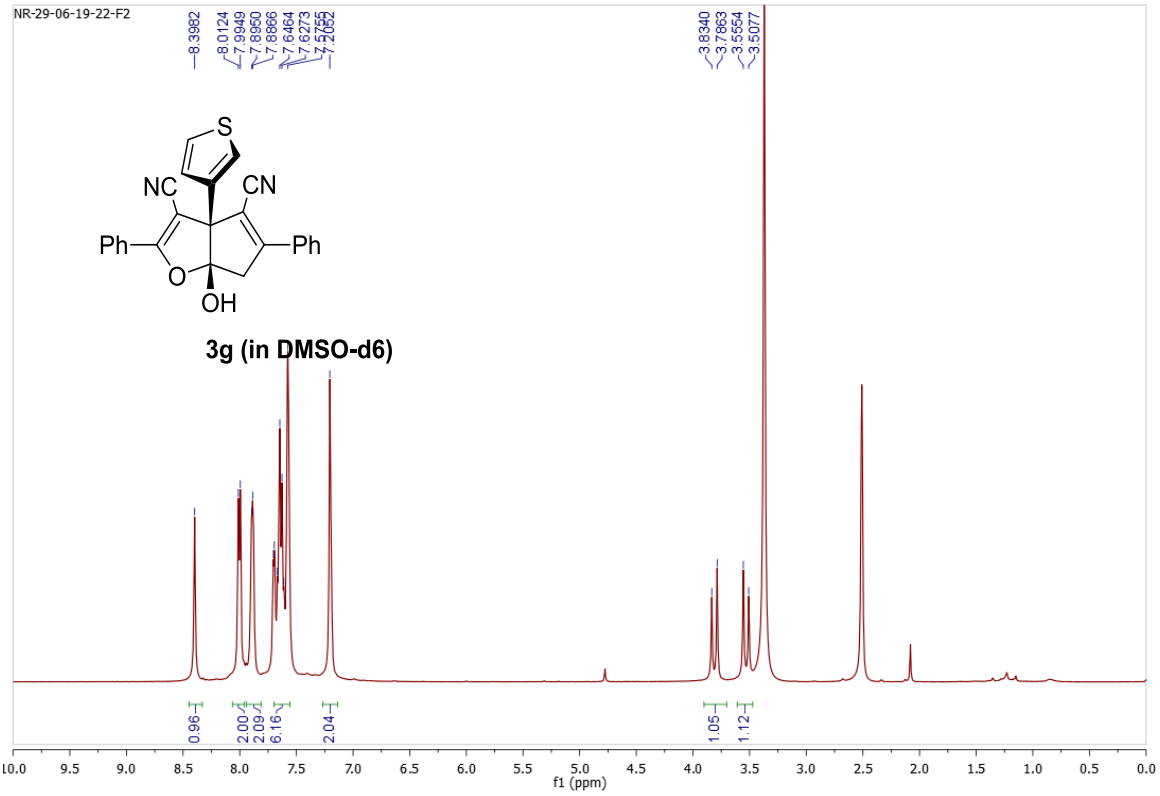
3f (in CDCl3)
f1 (ppm)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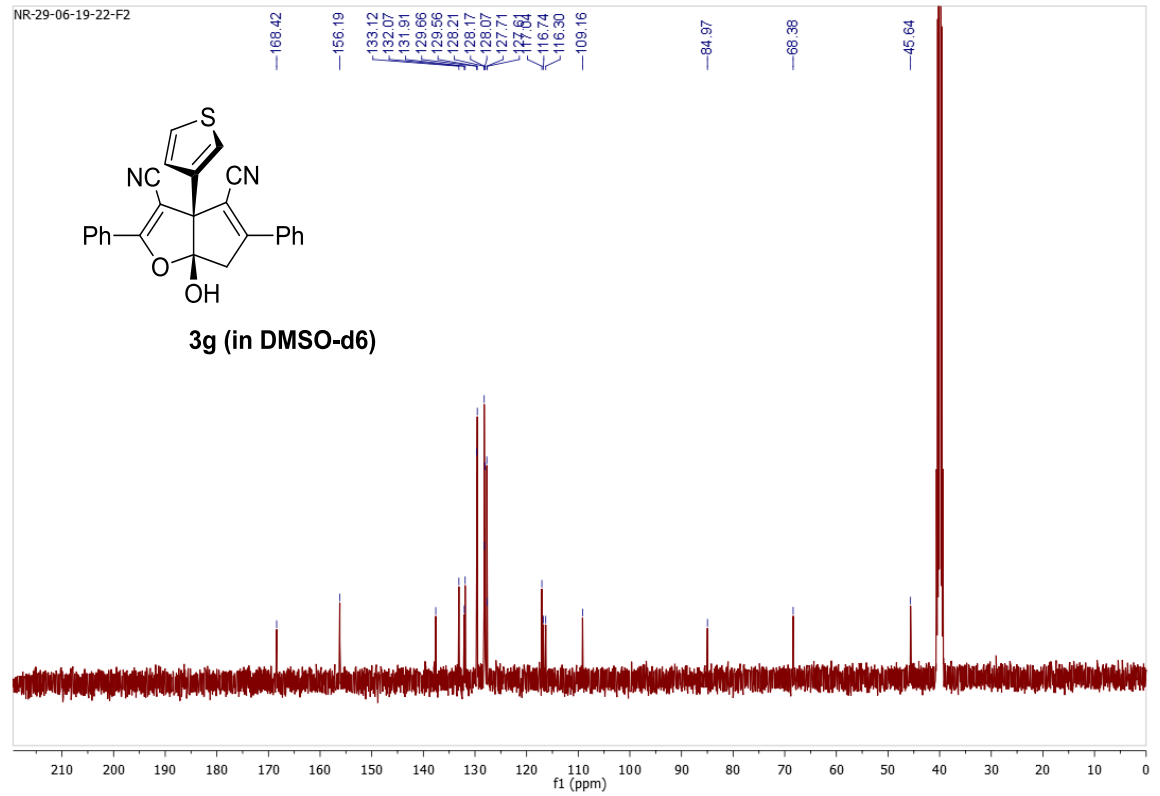
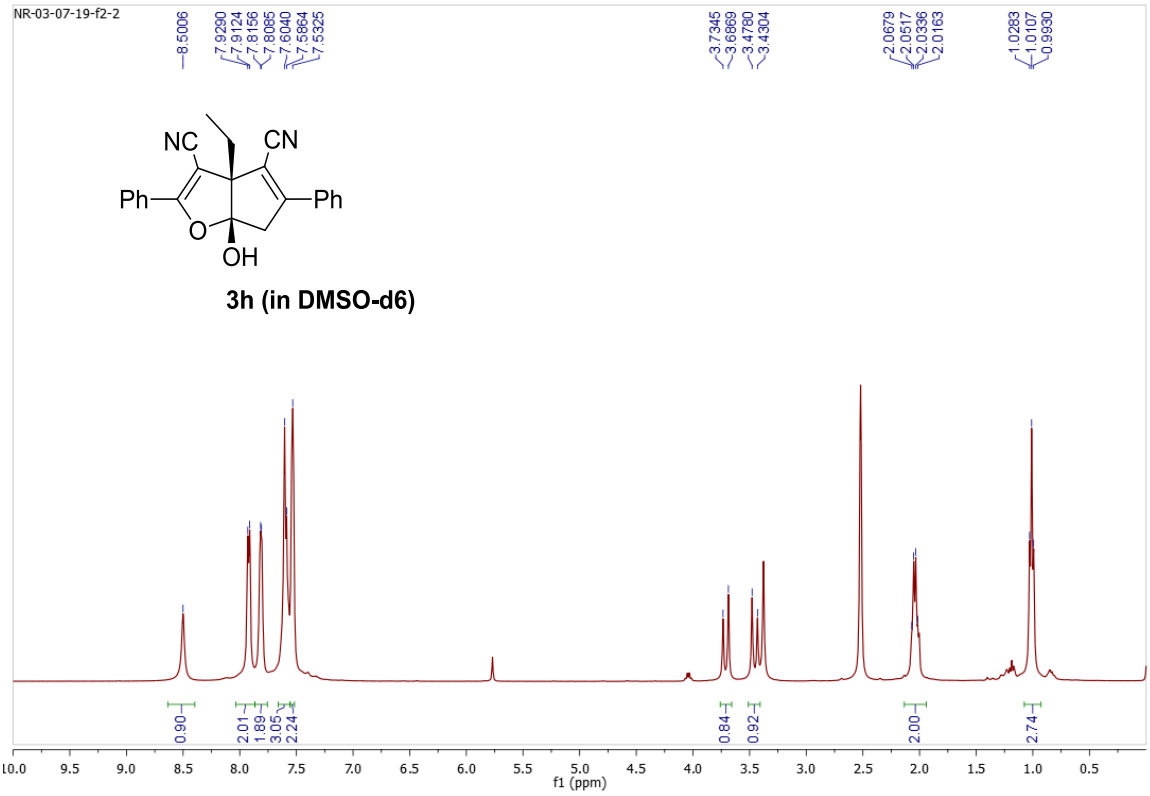
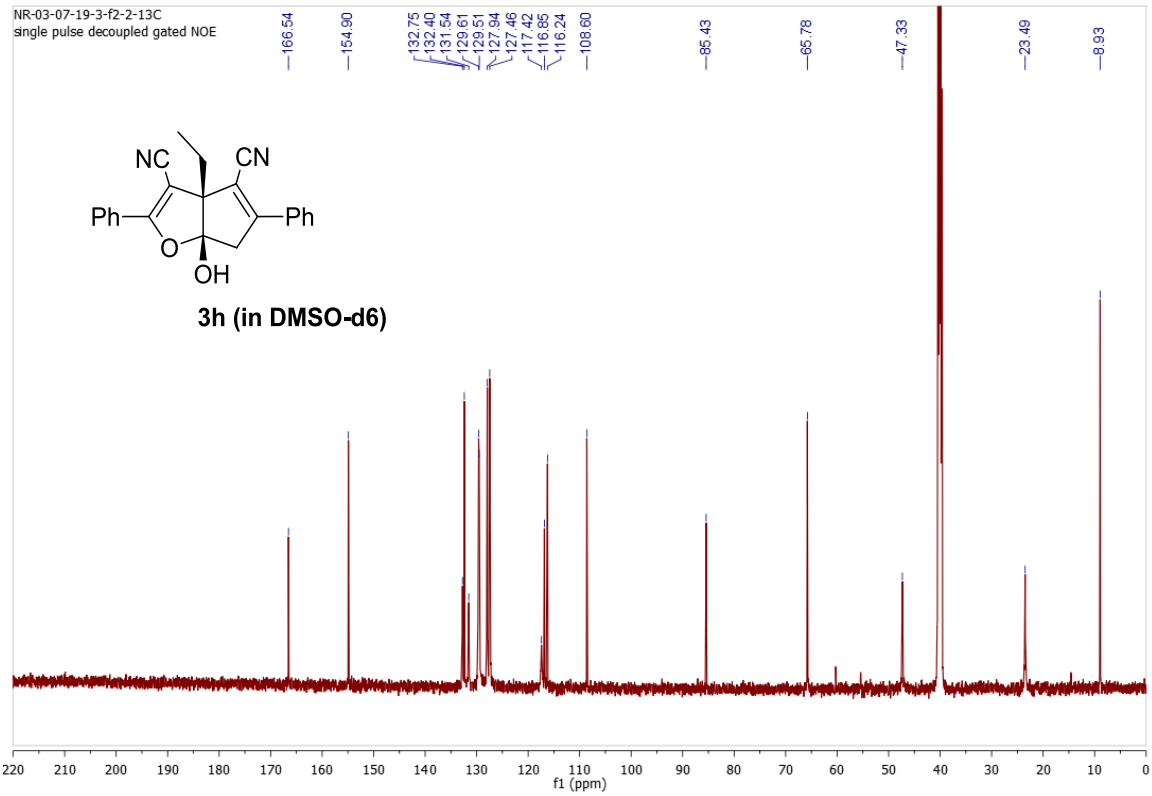
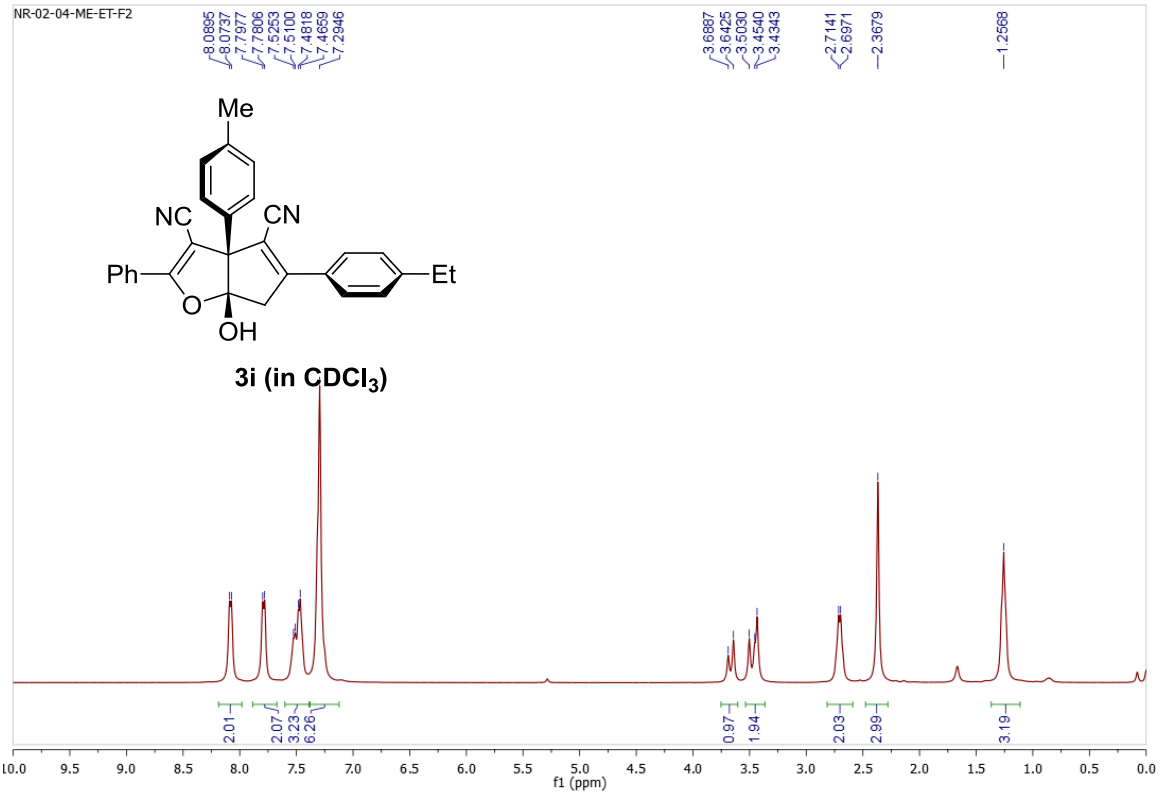
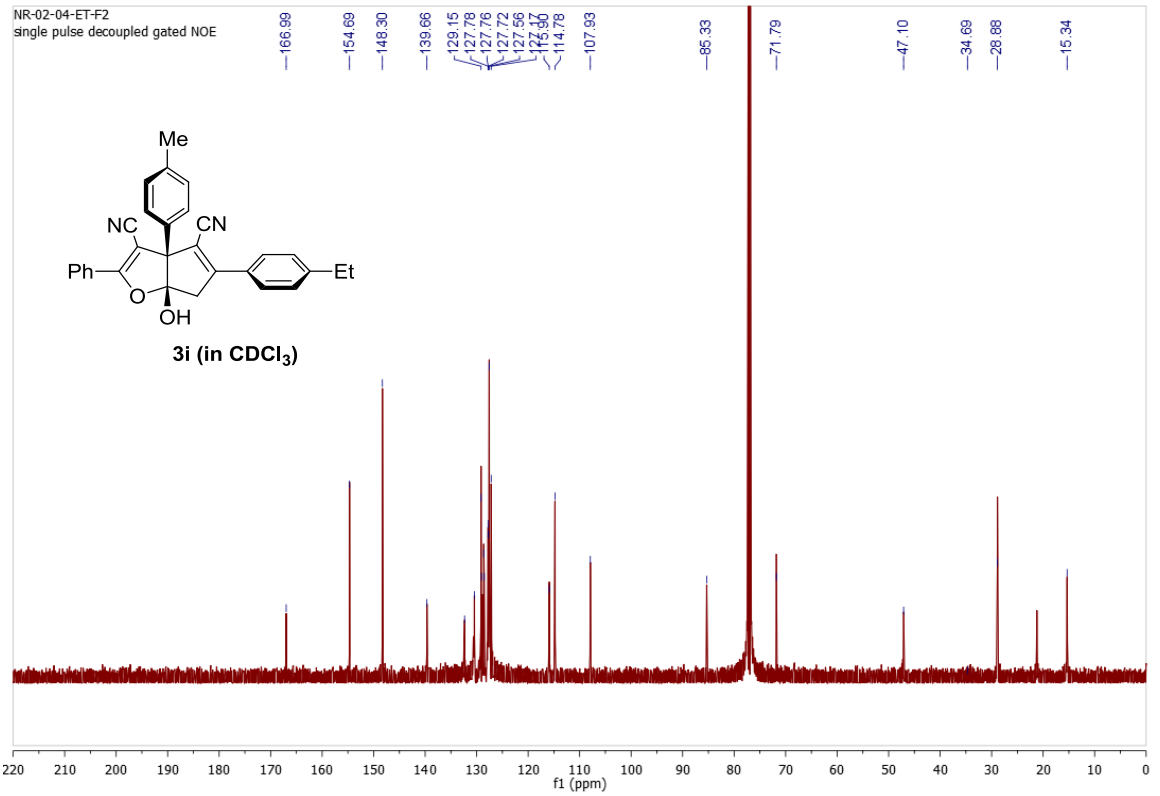
S
NC
CN
Ph
Ph
O
OH
3g (in DMSO-d6)
0.96
2.00
2.09
6.16
2.04
1.05
1.12
f1 (ppm)

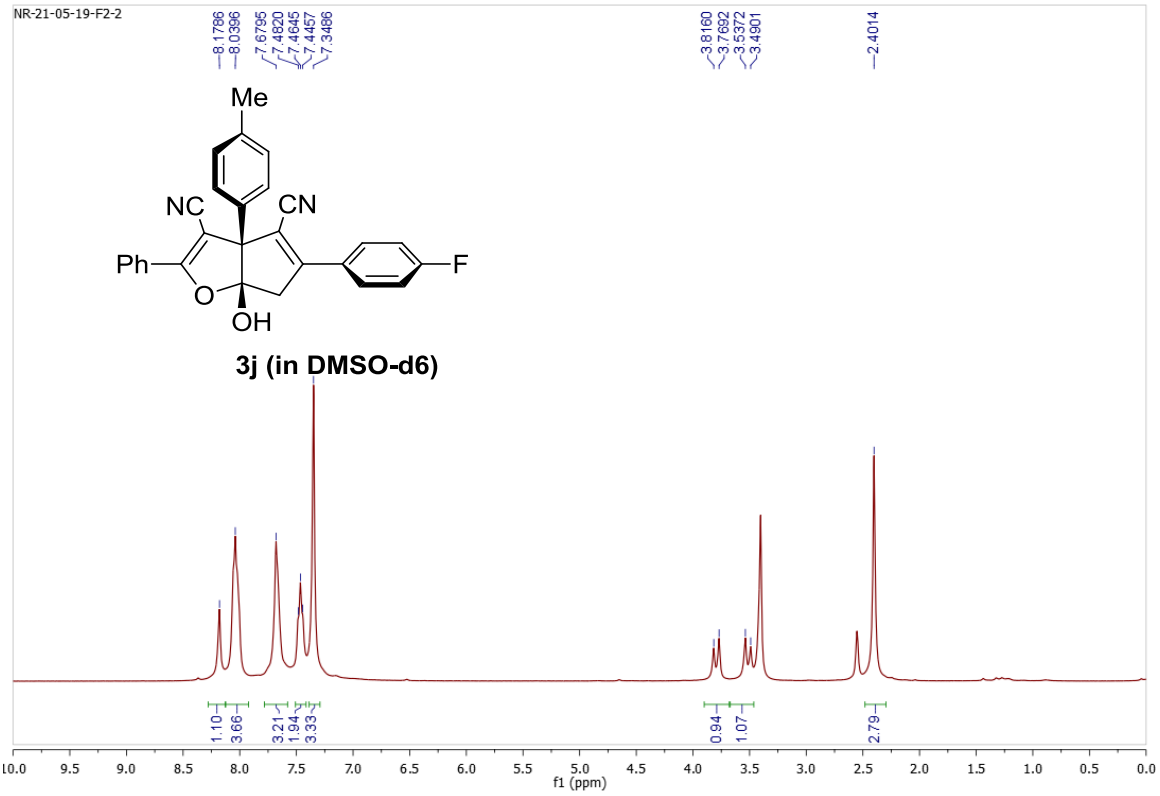

NR-29-06-19-22-F2
168.42
156.19
133.12
132.07
131.91
129.66
129.56
128.21
128.17
128.07
127.71
116.74
116.30
109.16
84.97
68.38
45.64
S
NC
CN
Ph
Ph
O
OH
3g (in DMSO-d6)
f1 (ppm)

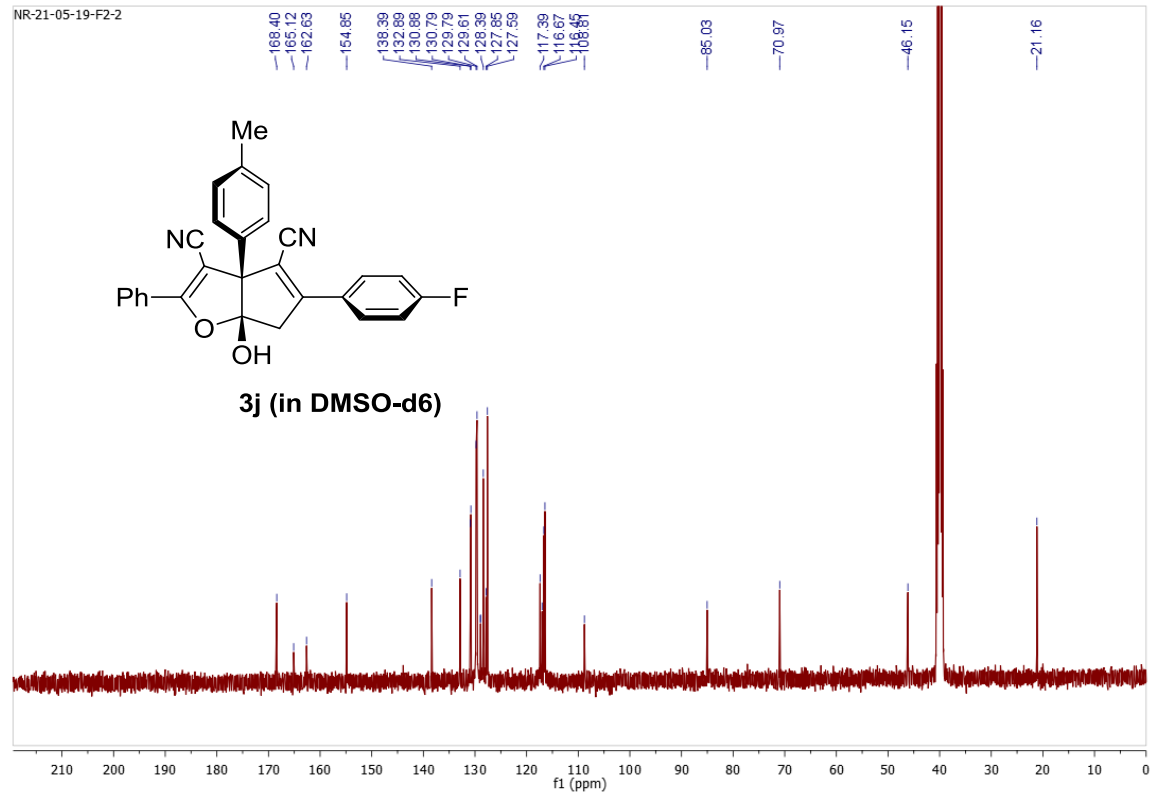

NR-03-07-19-f2-2
8.5006
7.9290
7.9124
7.8156
7.8085
7.6040
7.5864
7.5325
3.7345
3.6869
3.4780
3.4304
2.0679
2.0517
2.0336
2.0163
1.0283
1.0107
0.9930
NC
CN
Ph
Ph
O
OH
3h (in DMSO-d6)
0.90
2.01
1.89
3.05
2.24
0.84
0.92
2.00
2.74
f1 (ppm)

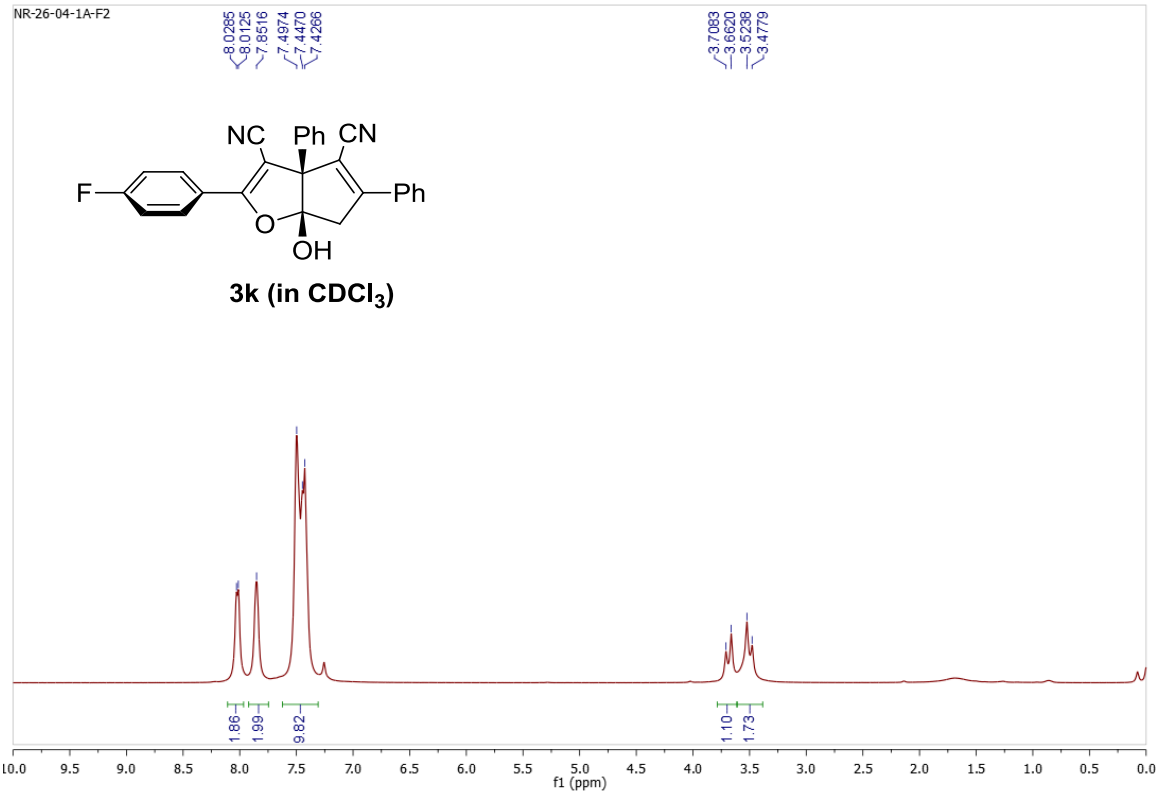

NR-03-07-19-3-f2-2-13C
single pulse decoupled gated NOE
166.54
154.90
132.75
132.40
131.54
129.61
129.51
127.94
127.46
117.42
116.85
116.24
108.60
85.43
65.78
47.33
23.49
8.93
NC
CN
Ph
Ph
O
OH
3h (in DMSO-d6)
f1 (ppm)


NR-02-04-ME-ET-F2
8.0895
8.0737
7.7977
7.7806
7.5253
7.5100
7.4818
7.4659
7.2946
3.6887
3.6425
3.5030
3.4540
3.4343
2.7141
2.6971
2.3679
1.2568
Me
NC
CN
Ph
O
OH
Et
3i (in CDCl3)
2.01
2.07
3.23
6.26
0.97
1.94
2.03
2.99
3.19
f1 (ppm)

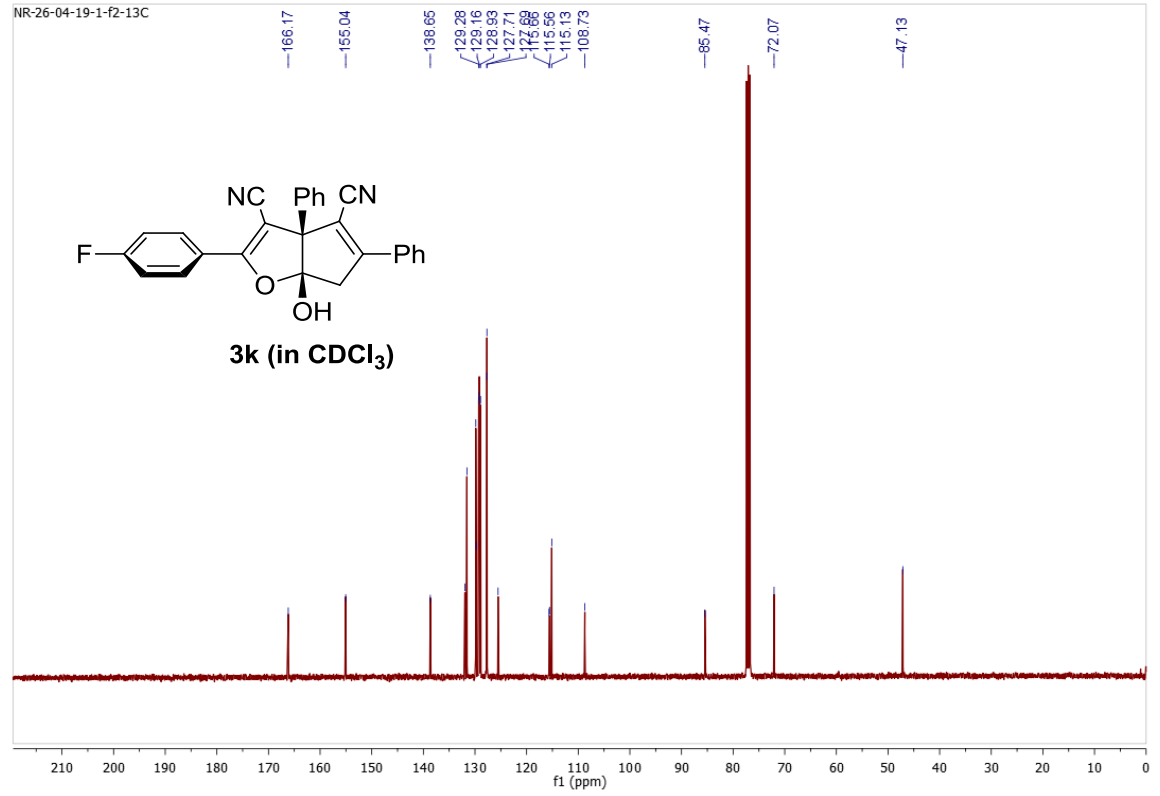

NR-02-04-ET-F2
single pulse decoupled gated NOE
166.99
154.69
148.30
139.66
129.15
127.78
127.76
127.72
127.56
115.90
114.78
107.93
85.33
71.79
47.10
34.69
28.88
15.34
Me
NC
CN
Ph
O
OH
Et
3i (in CDCl3)
f1 (ppm)


NR-21-05-19-F2-2
8.1786
8.0396
7.6795
7.4820
7.4645
7.4457
7.3486
3.8160
3.7692
3.5372
3.4901
2.4014
Me
NC
CN
Ph
O
F
OH
3j (in DMSO-d6)
1.10
3.66
3.21
1.94
3.33
0.94
1.07
2.79
f1 (ppm)

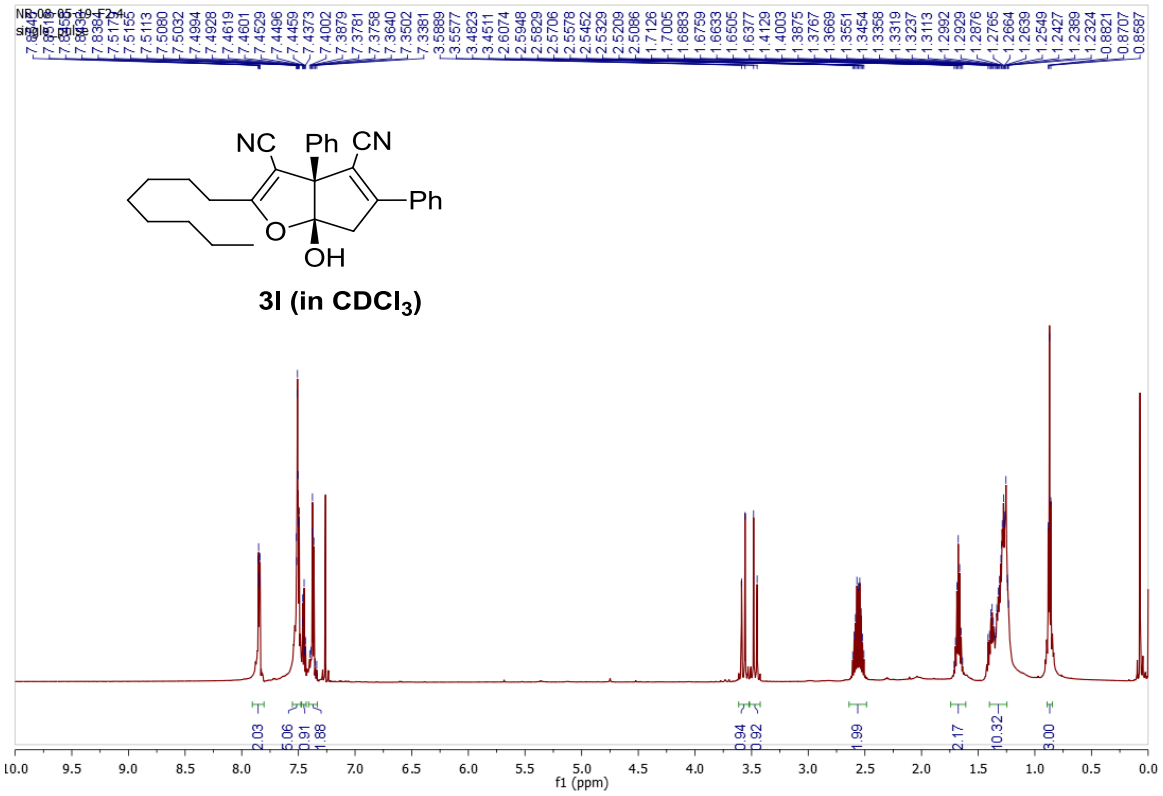

NR-21-05-19-F2-2
168.40
165.12
162.63
154.85
138.39
132.89
130.88
130.79
129.79
129.61
128.39
127.85
127.59
117.39
116.67
85.03
70.97
46.15
21.16
Me
NC
CN
Ph
O
F
OH
3j (in DMSO-d6)
f1 (ppm)

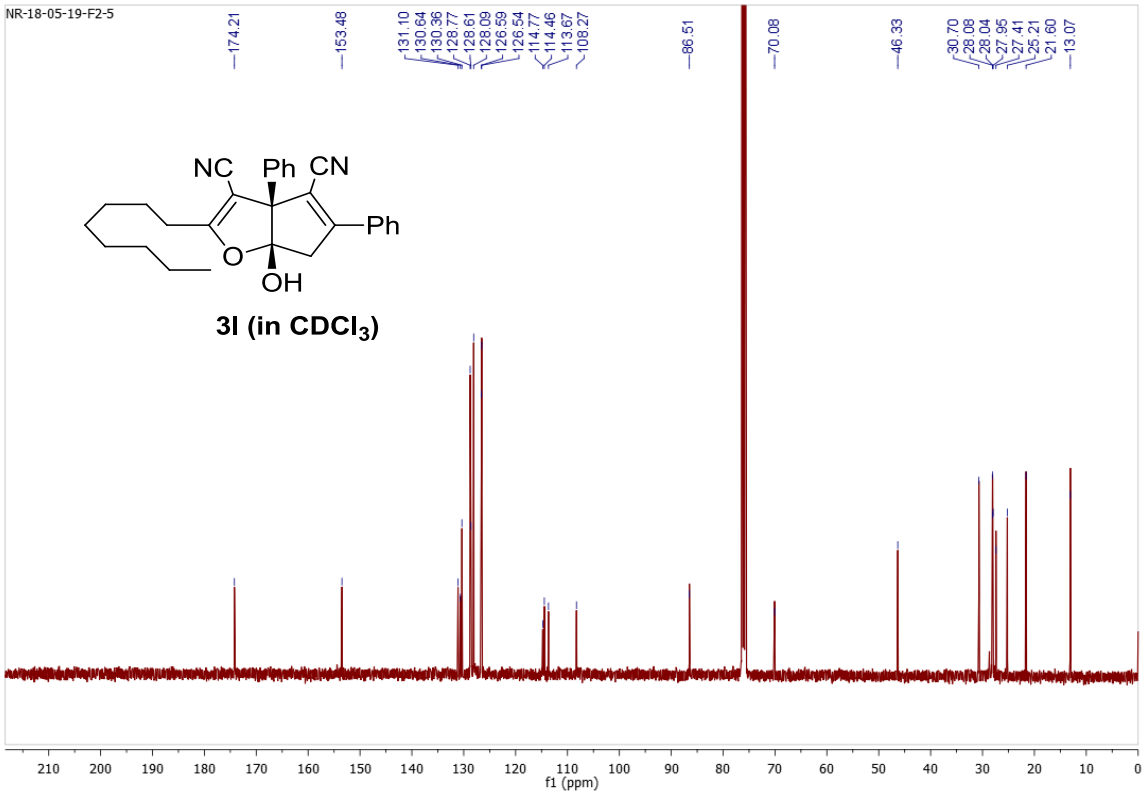


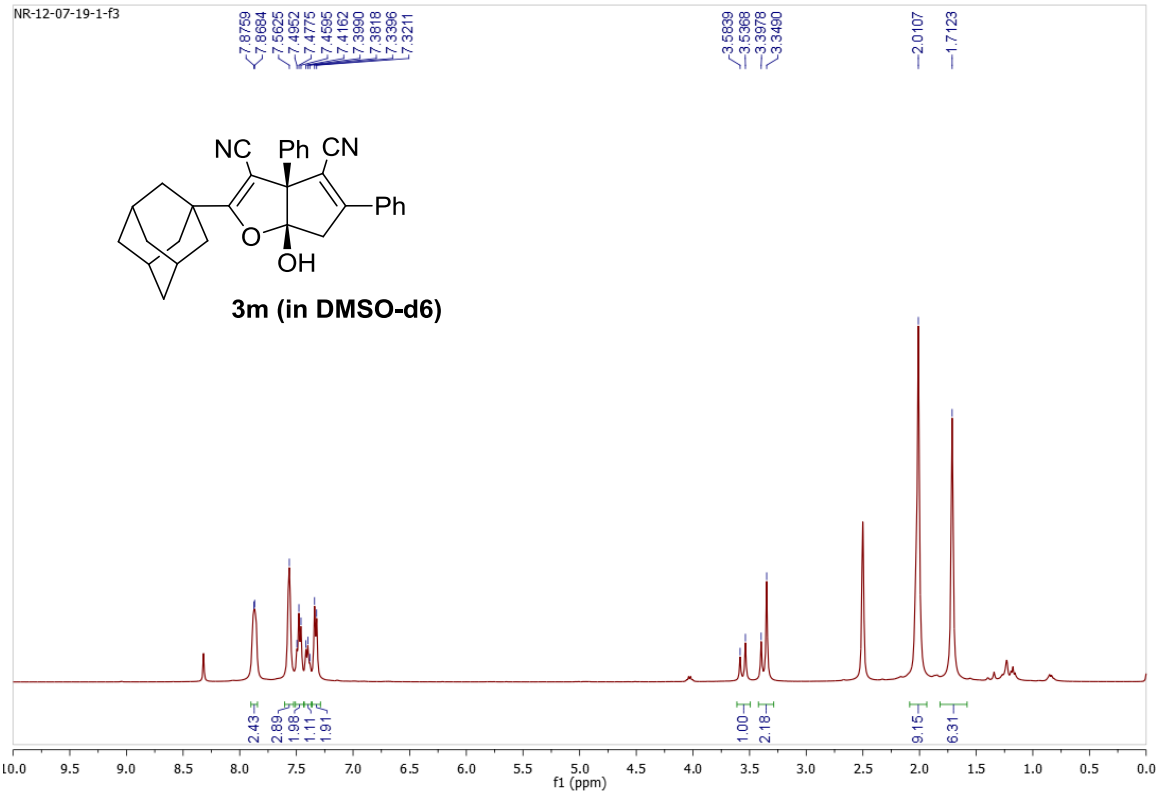
3k (in $CDCl_3$)

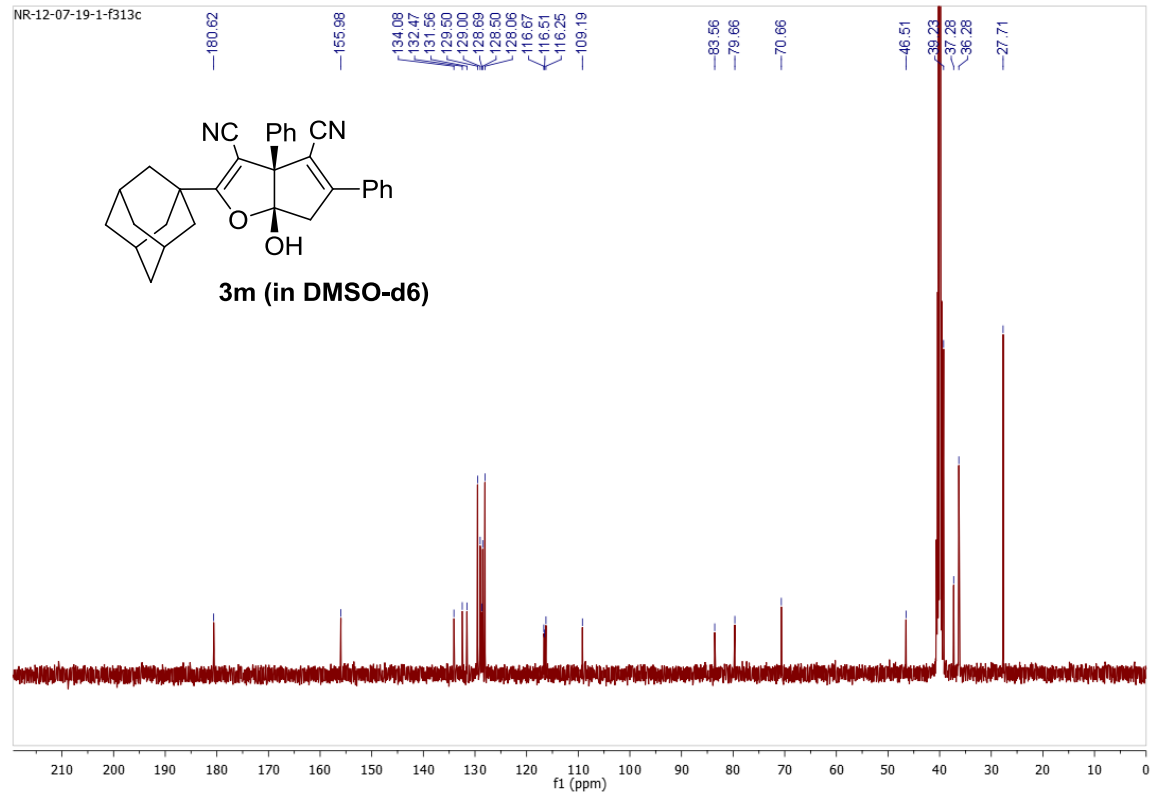


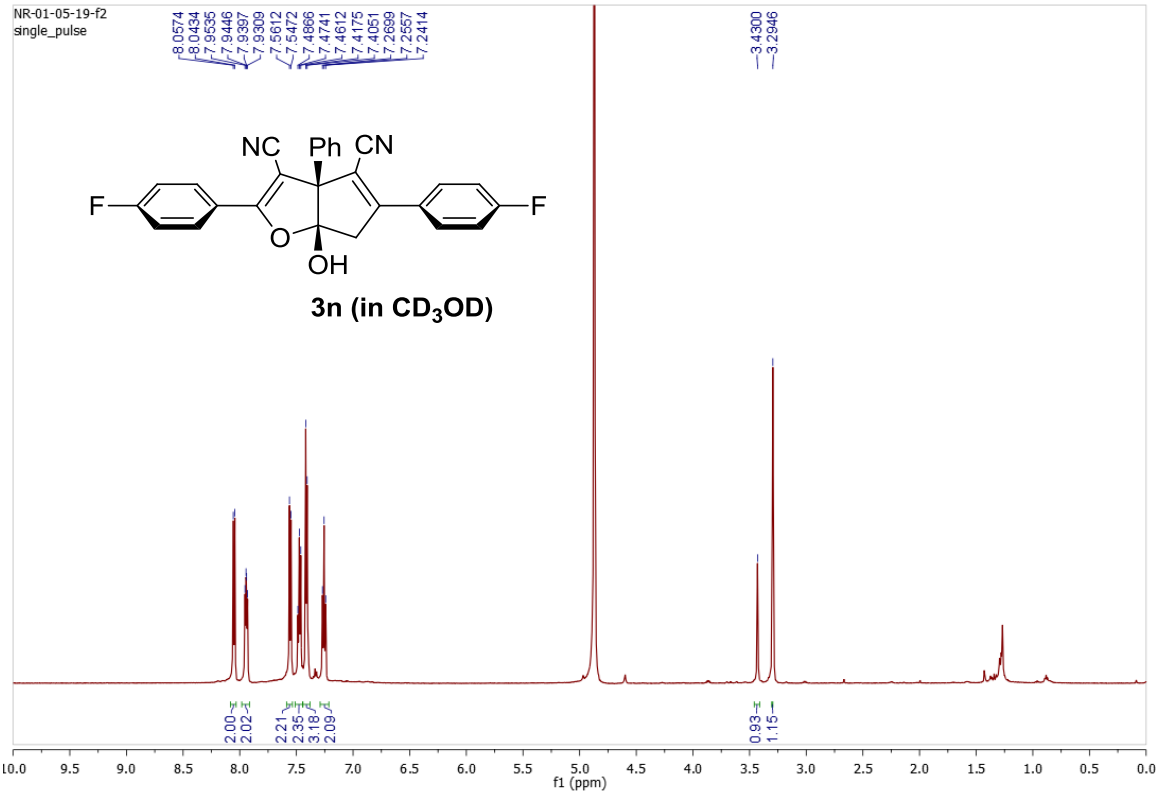
3k (in $CDCl_3$)

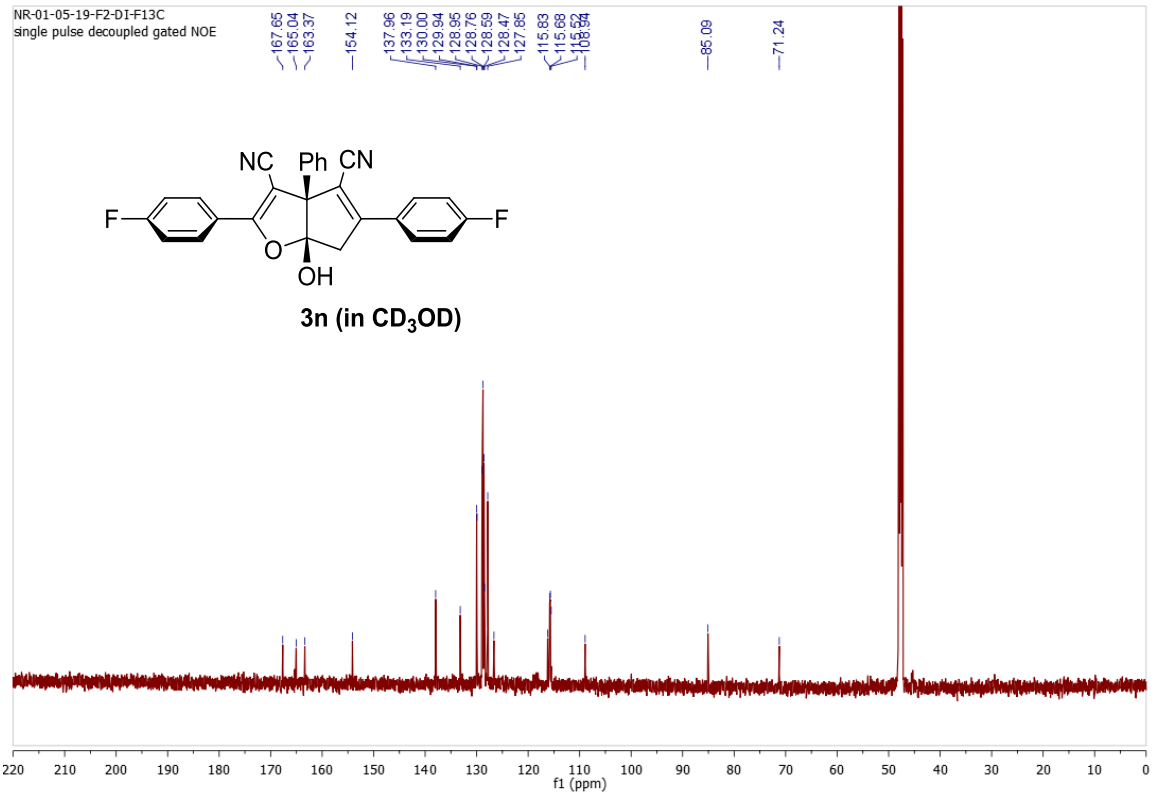

NC
Ph
CN
Ph
O
OH
3l (in CDCl3)
f1 (ppm)

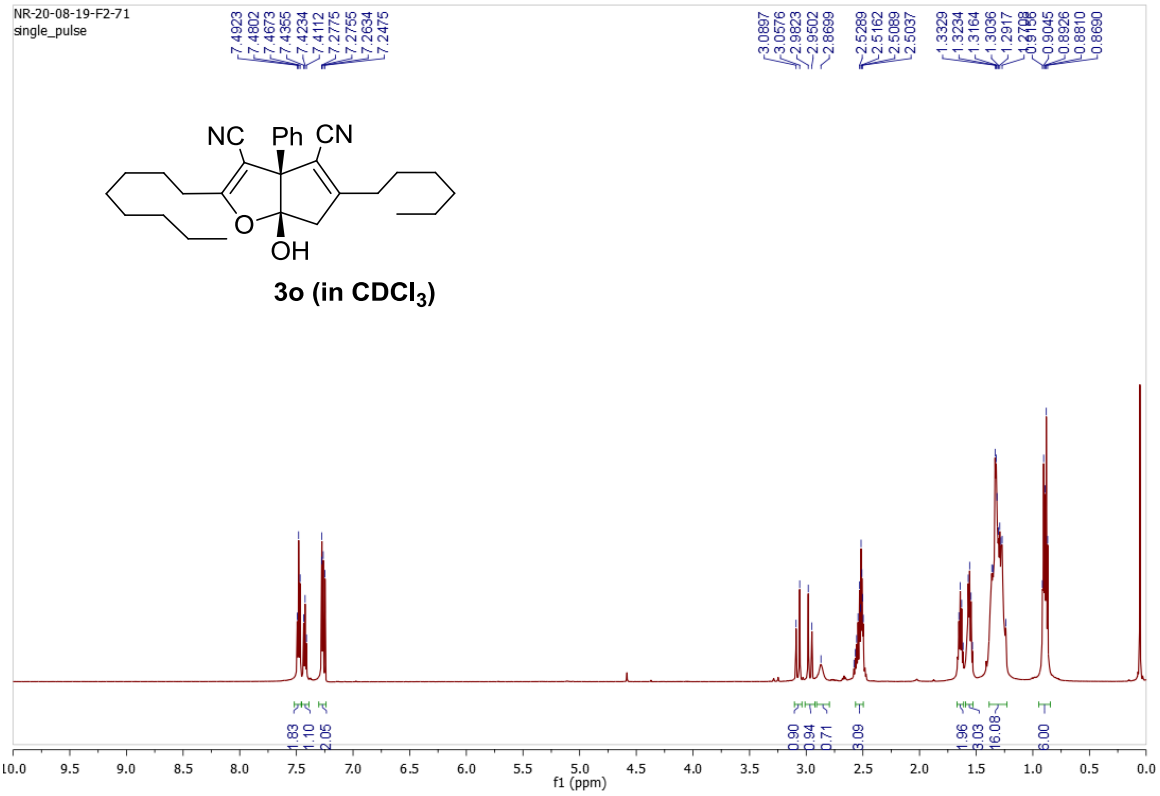

NR-18-05-19-F2-5
NC
Ph
CN
Ph
O
OH
3l (in CDCl3)
f1 (ppm)

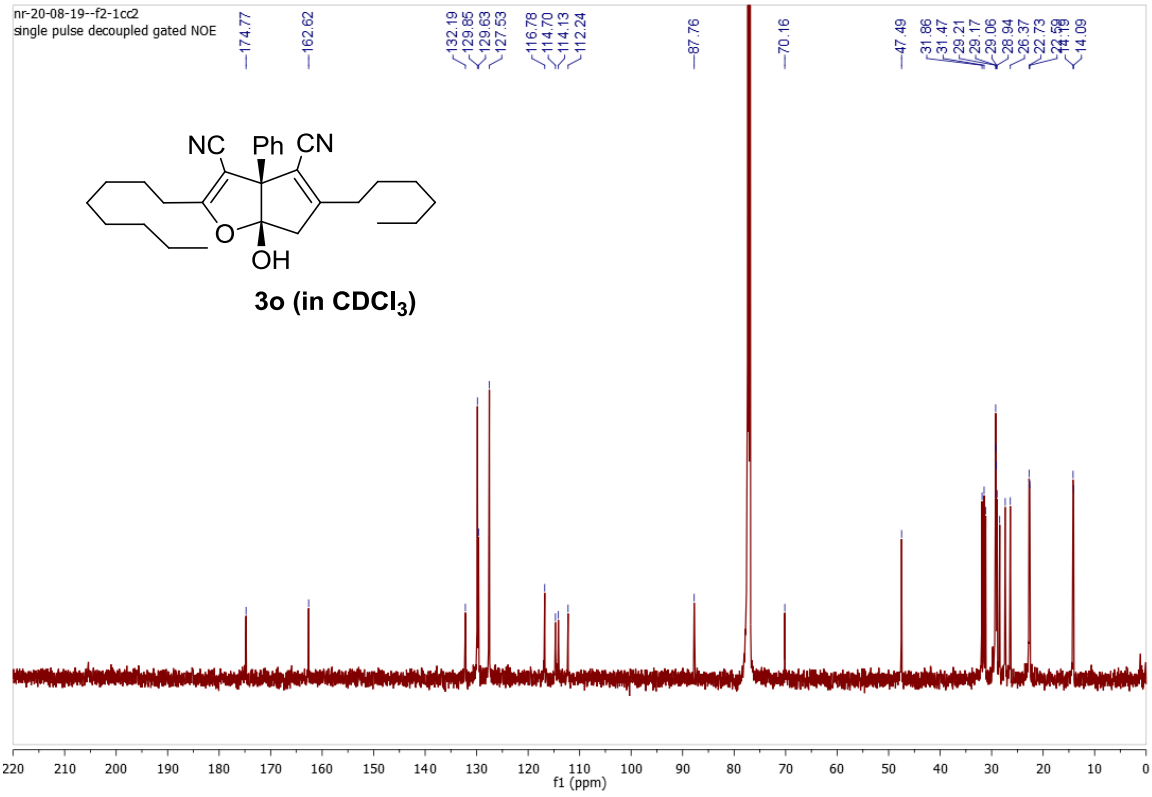

NR-12-07-19-1-f3
7.8759
7.8684
7.5625
7.4952
7.4775
7.4595
7.4162
7.3990
7.3818
7.3396
7.3211
3.5839
3.5368
3.3978
3.3490
2.0107
1.7123
NC
Ph
CN
Ph
O
OH
3m (in DMSO-d6)
2.43
2.89
1.98
1.11
1.91
1.00
2.18
9.15
6.31
f1 (ppm)

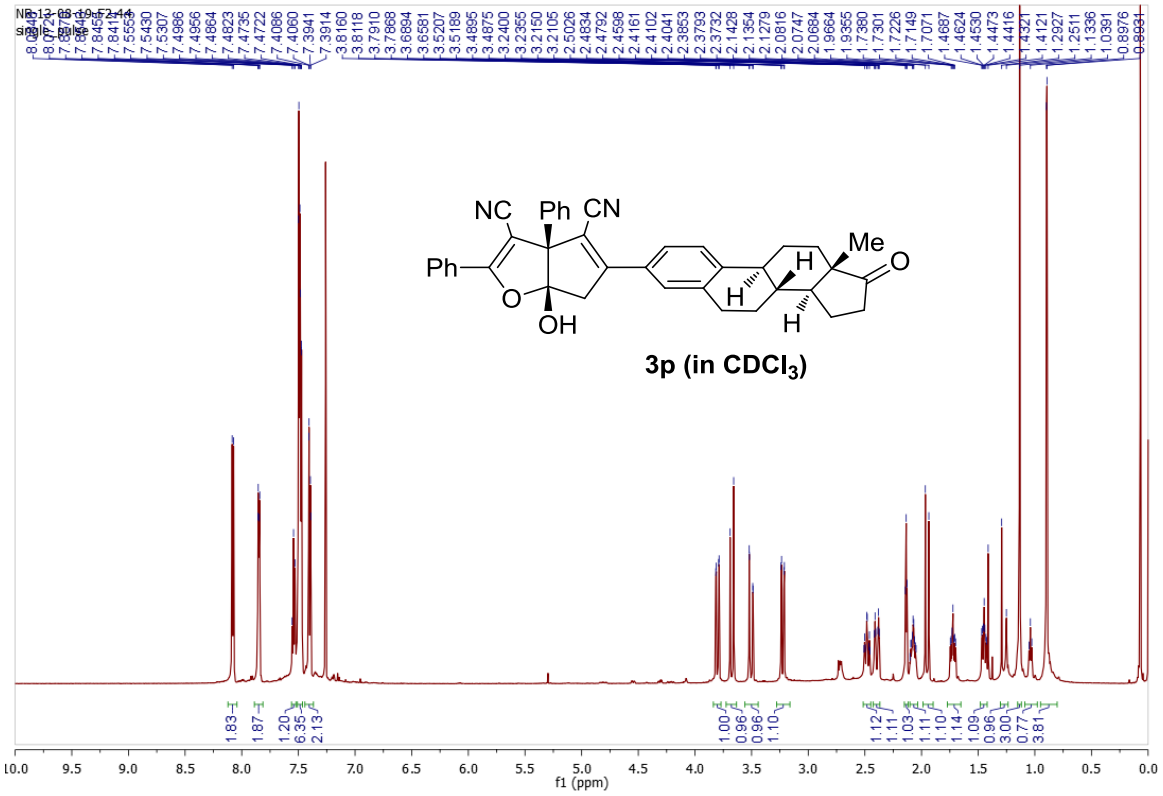

NR-12-07-19-1-f313c
180.62
155.98
134.08
132.47
131.56
129.50
129.00
128.69
128.50
128.06
116.67
116.51
116.25
109.19
83.56
79.66
70.66
46.51
39.23
37.28
36.28
27.71
NC
Ph
CN
Ph
O
OH
3m (in DMSO-d6)
f1 (ppm)

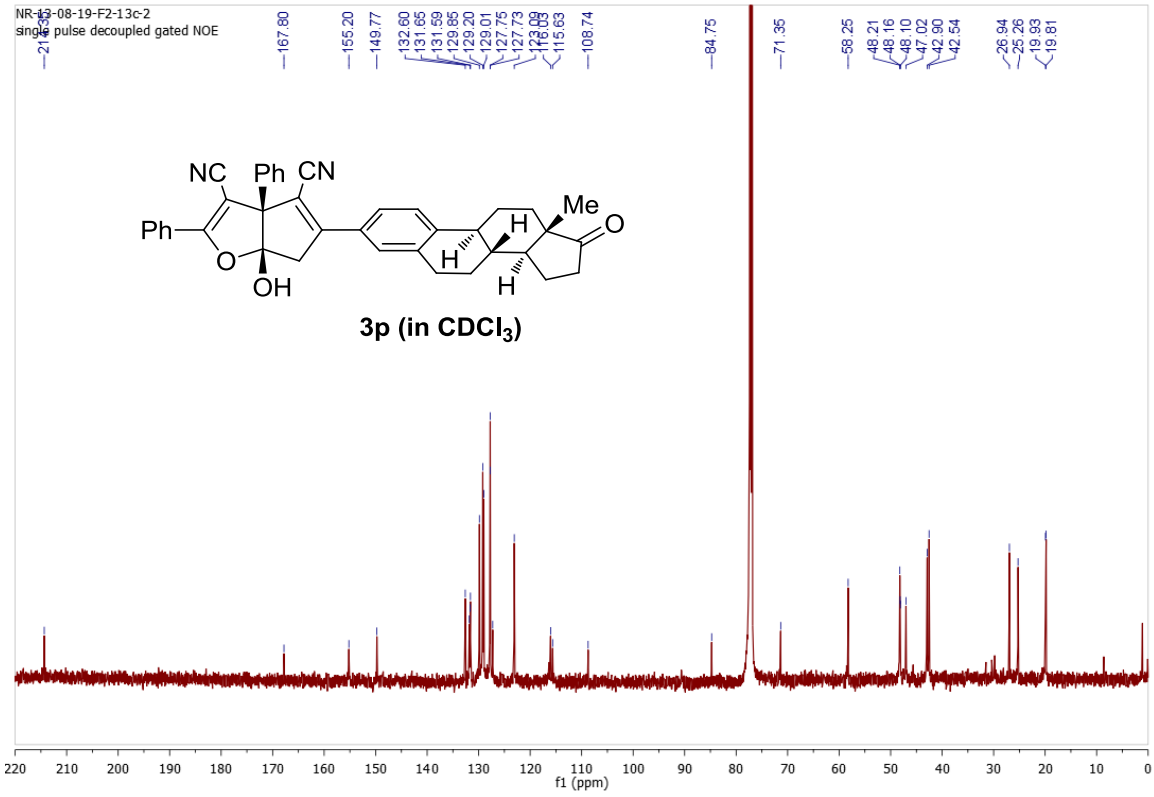

NR-01-05-19-f2
single_pulse
8.0574
8.0434
7.9535
7.9446
7.9397
7.9309
7.5612
7.5472
7.4866
7.4741
7.4612
7.4175
7.4051
7.2699
7.2557
7.2414
3.4300
3.2946
NC
Ph
CN
F
F
O
OH
3n (in CD3OD)
2.00
2.02
2.21
2.35
3.18
2.09
0.93
1.15
f1 (ppm)

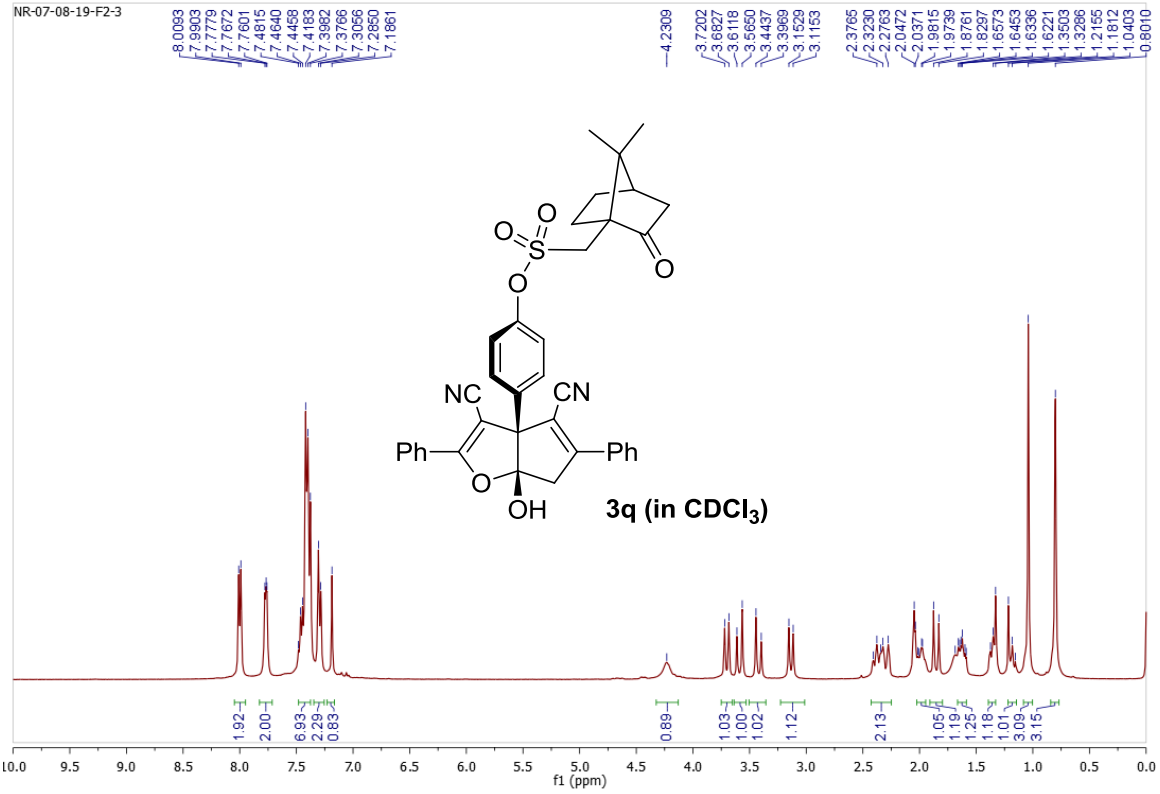

NR-01-05-19-F2-DI-F13C
single pulse decoupled gated NOE
167.65
165.04
163.37
154.12
137.96
133.19
130.00
129.94
128.95
128.76
128.59
128.47
127.85
115.83
115.68
85.09
71.24
NC
Ph
CN
F
F
O
OH
3n (in CD3OD)
f1 (ppm)

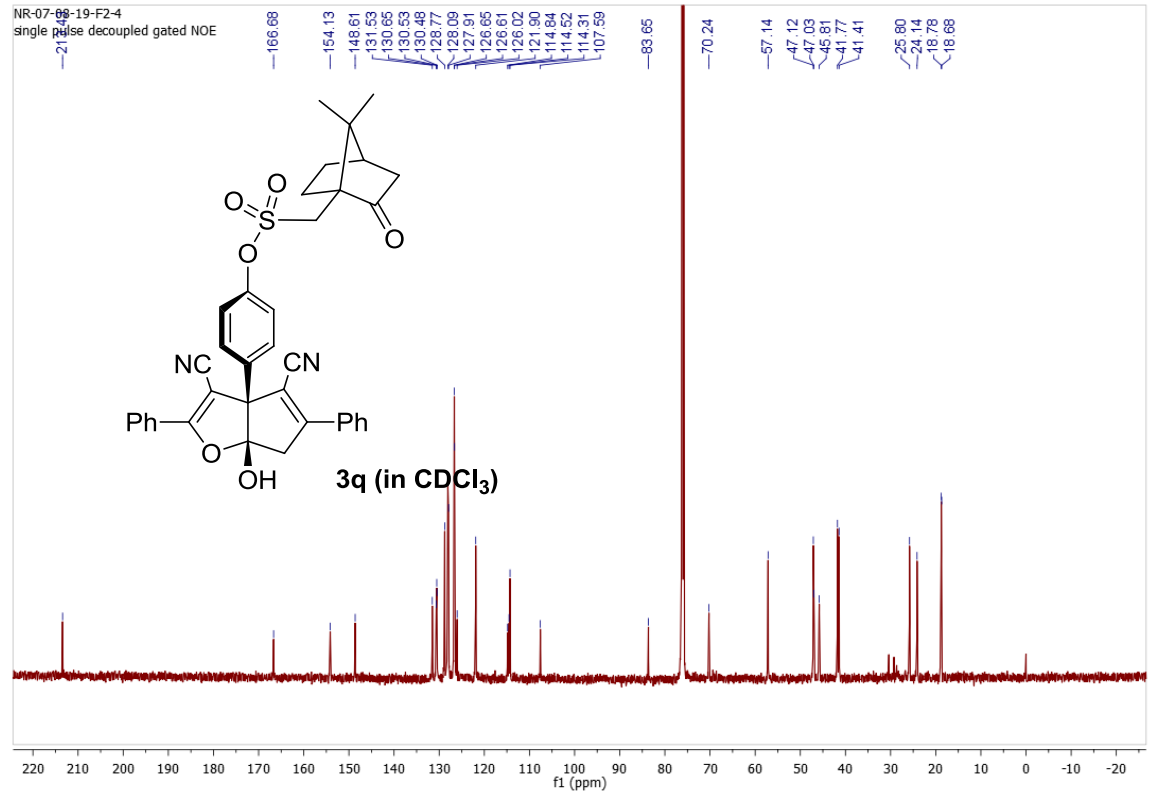

NR-20-08-19-F2-71
single_pulse
NC
Ph
CN
O
OH
3o (in CDCl3)
f1 (ppm)

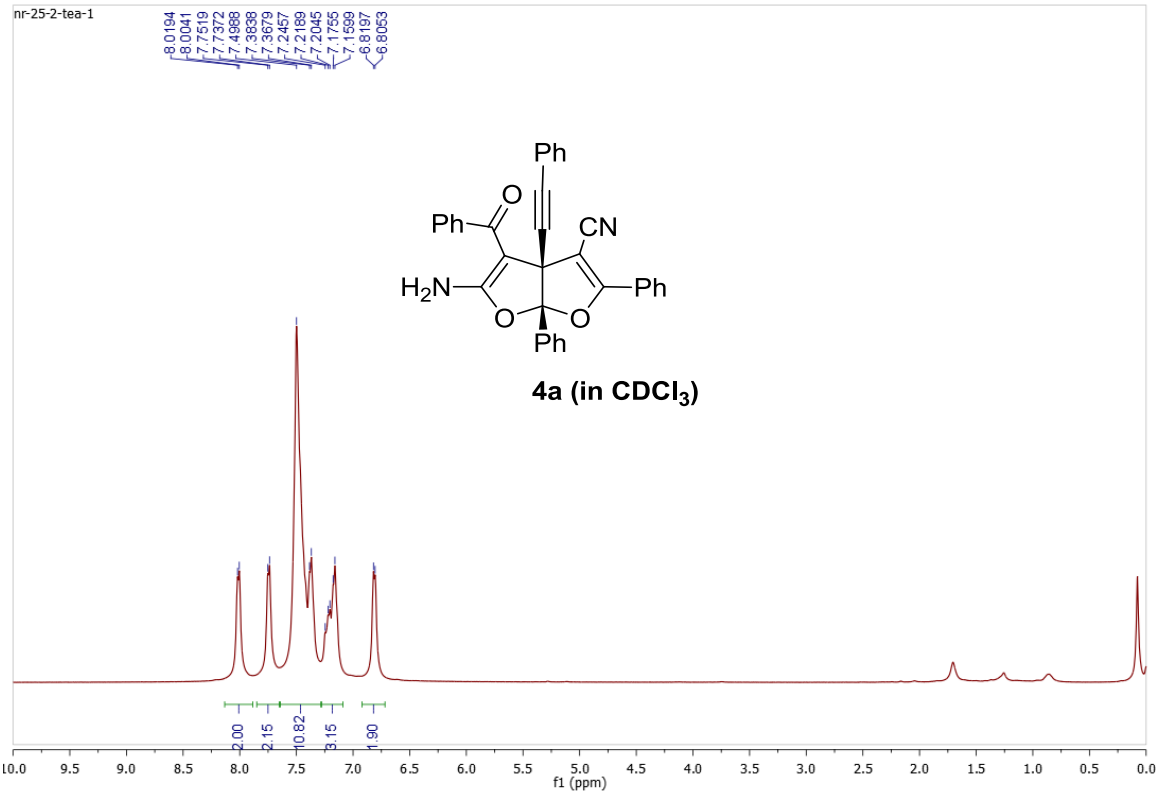

nr-20-08-19--f2-1cc2
single pulse decoupled gated NOE
NC
Ph
CN
O
OH
3o (in CDCl3)
f1 (ppm)


NC
Ph
CN
Ph
O
OH
Me
O
H
H
H
3p (in CDCl3)
f1 (ppm)

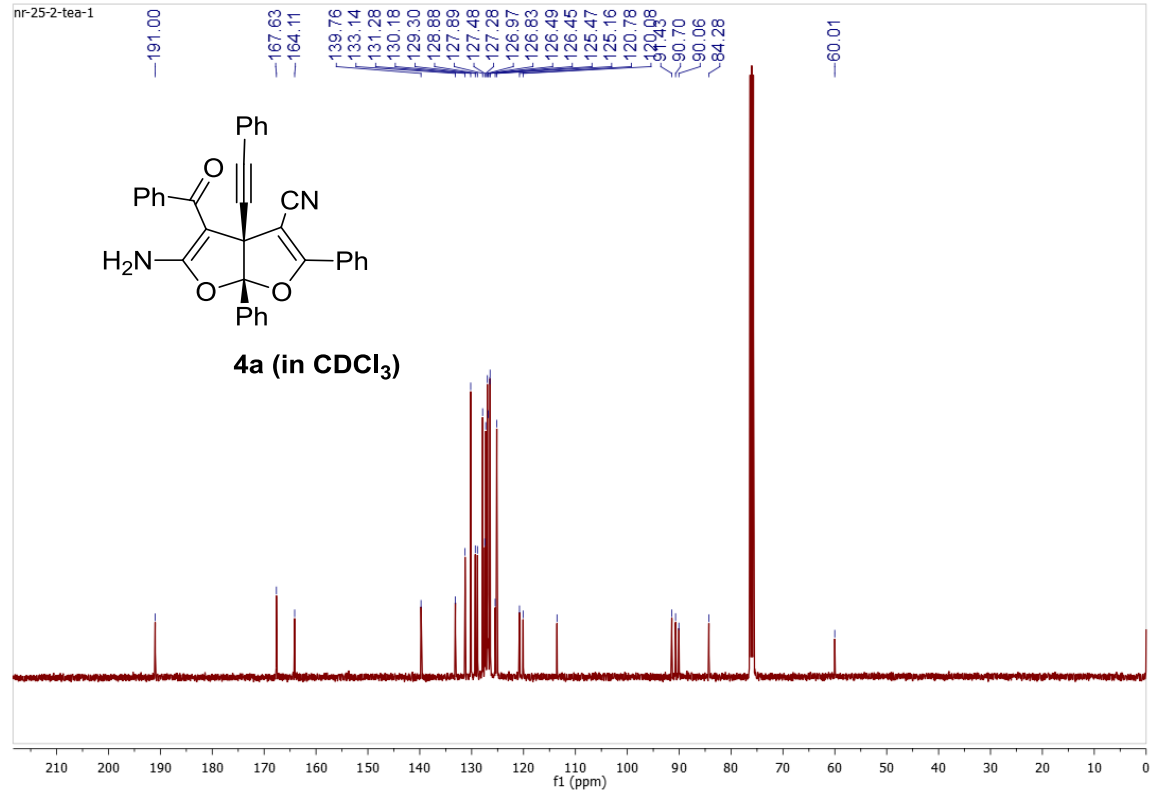

NR-13-08-19-F2-13c-2
single pulse decoupled gated NOE
NC
Ph
CN
Ph
O
OH
Me
O
H
H
H
3p (in CDCl3)
f1 (ppm)


NR-07-08-19-F2-3
3q (in CDCl3)
f1 (ppm)

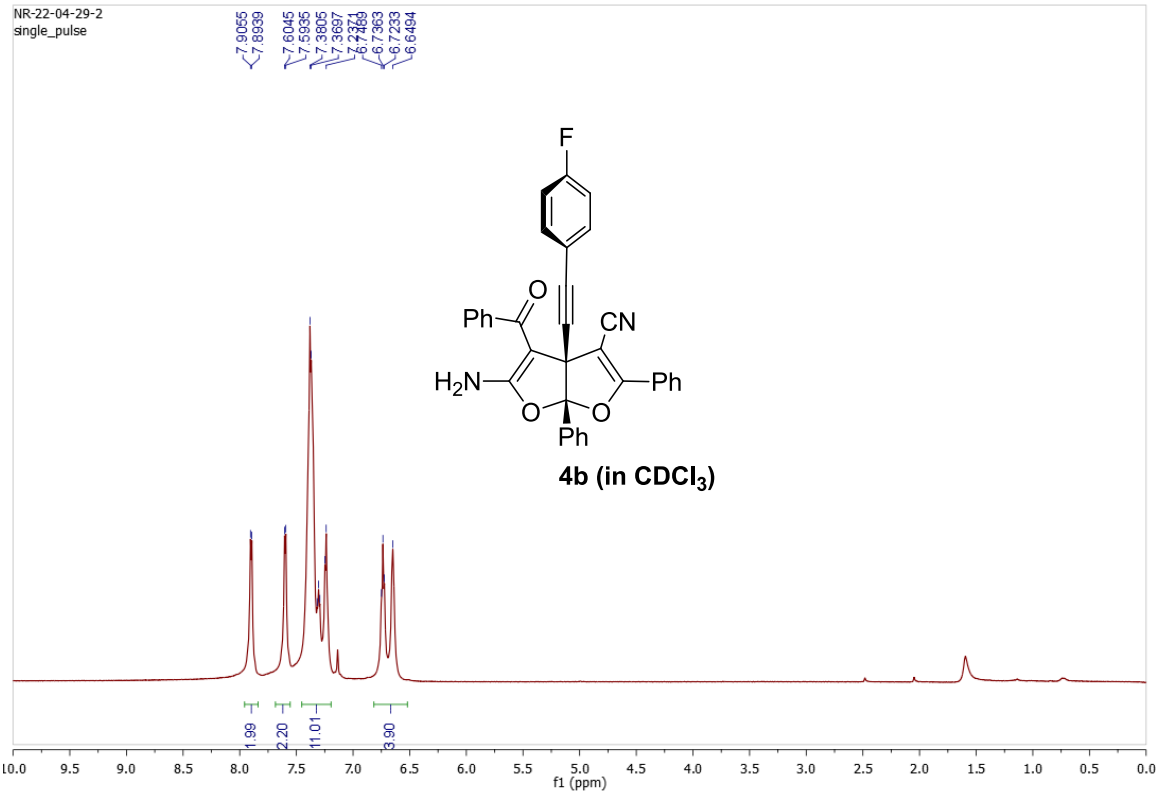

NR-07-08-19-F2-4
single pulse decoupled gated NOE
3q (in CDCl3)
f1 (ppm)

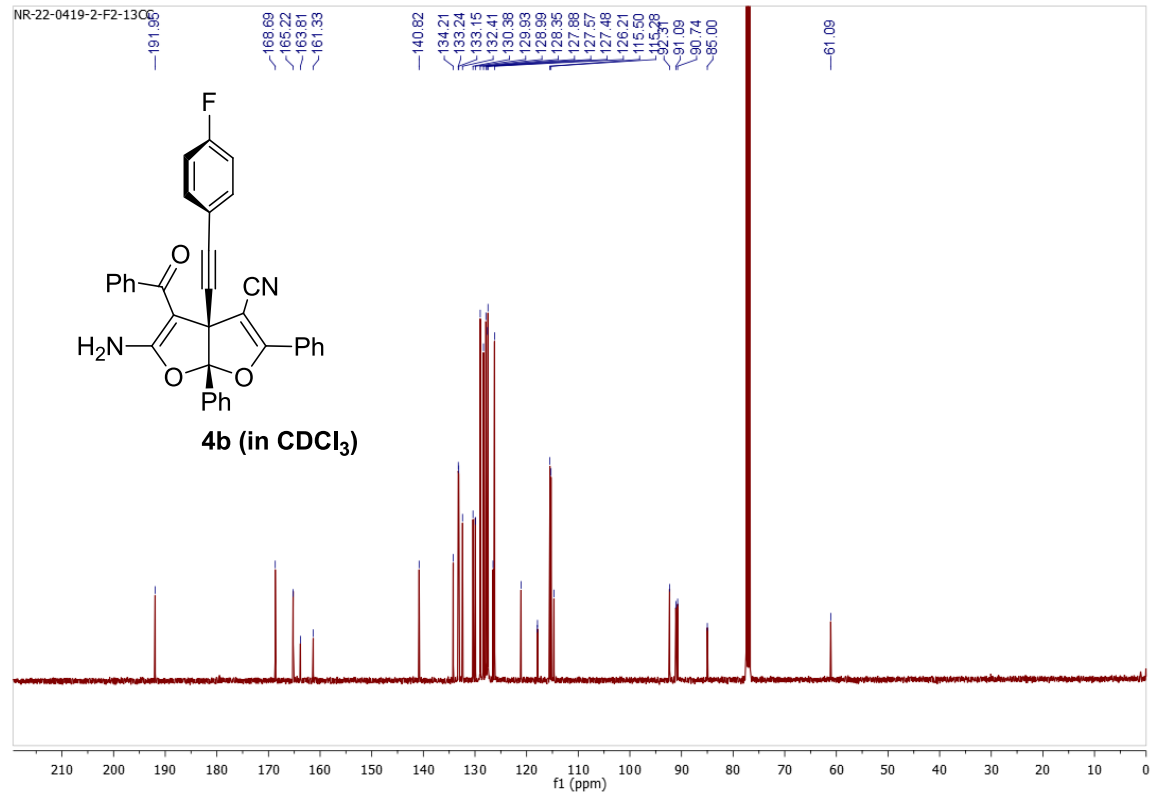


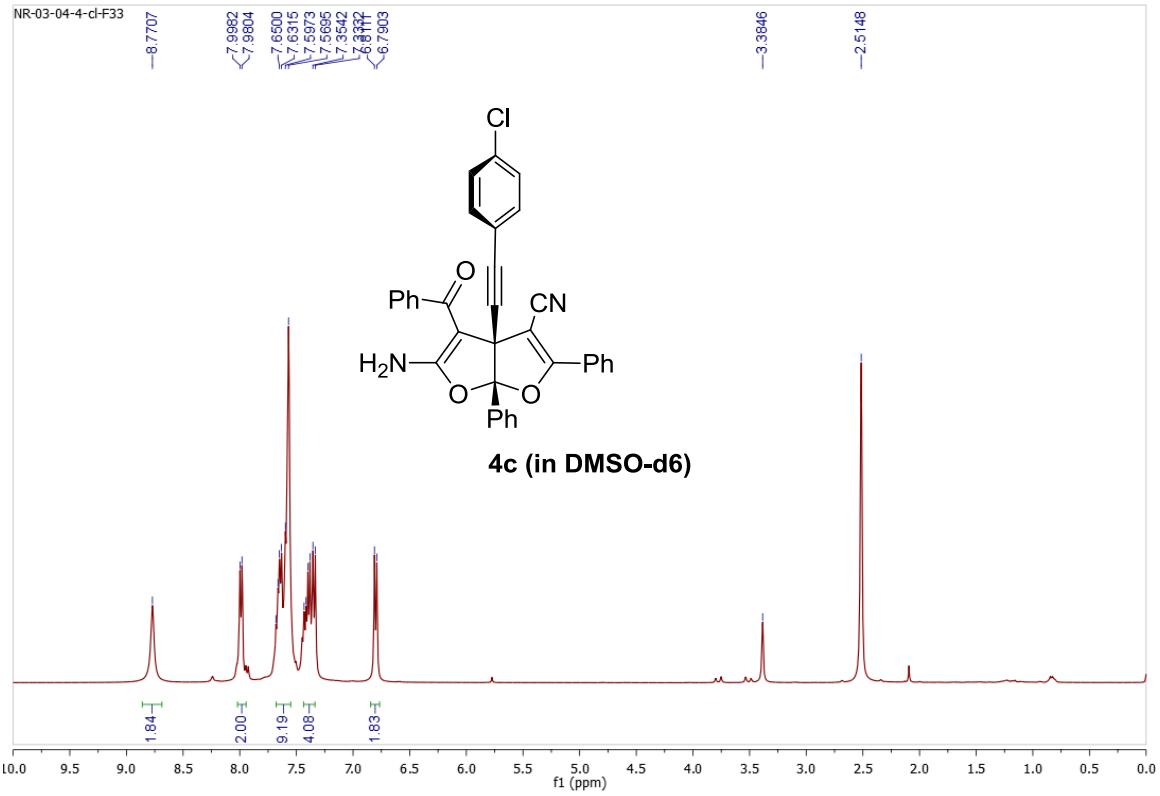
4a (in $CDCl_3$)

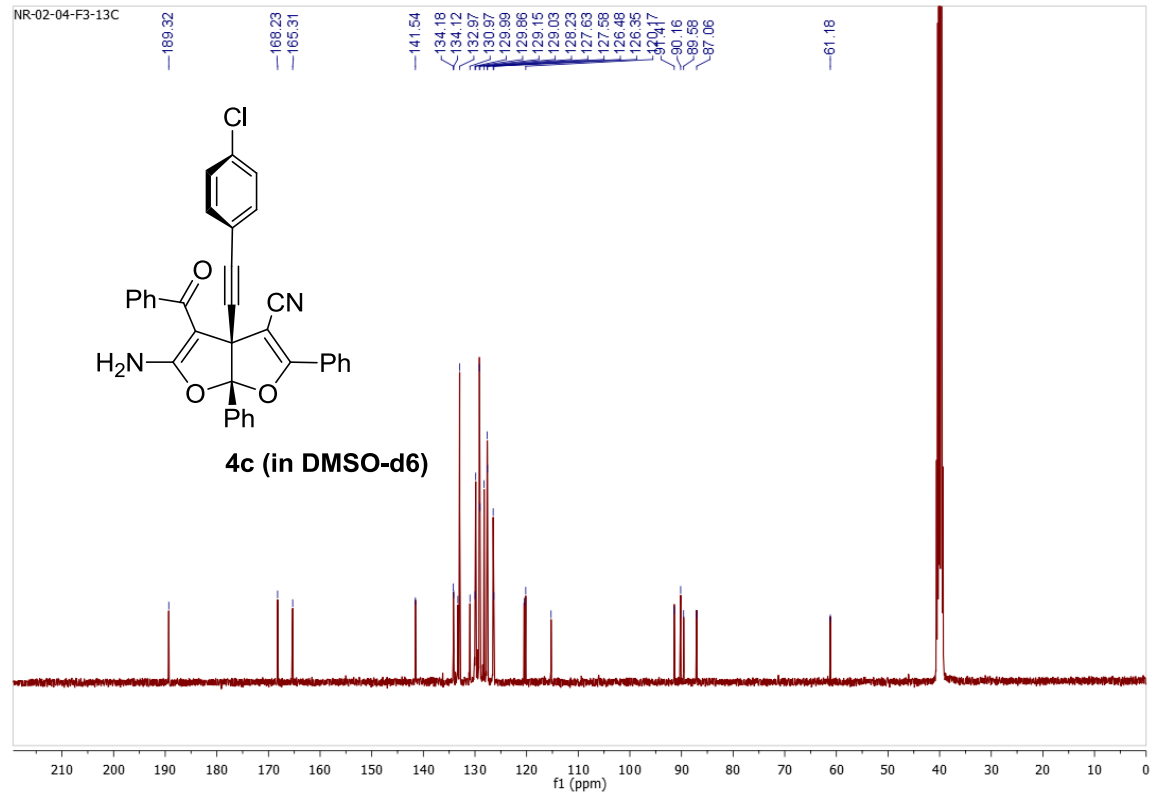


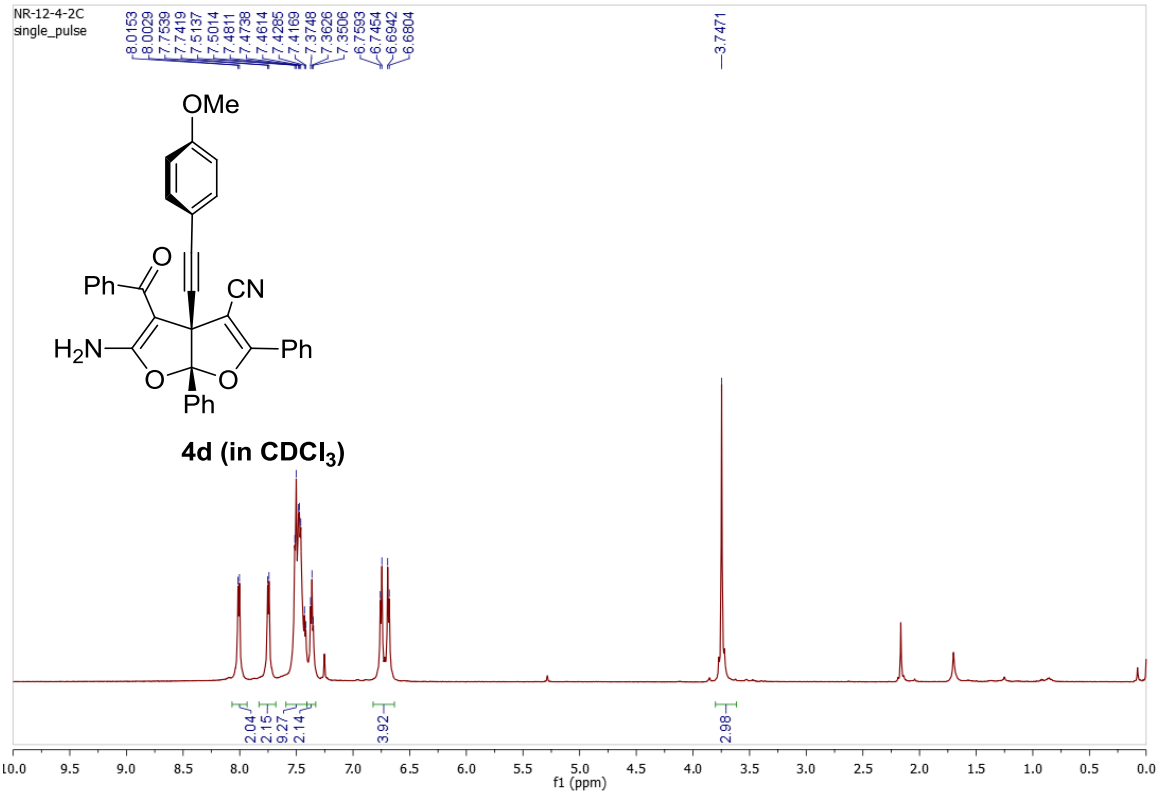
4a (in $CDCl_3$)

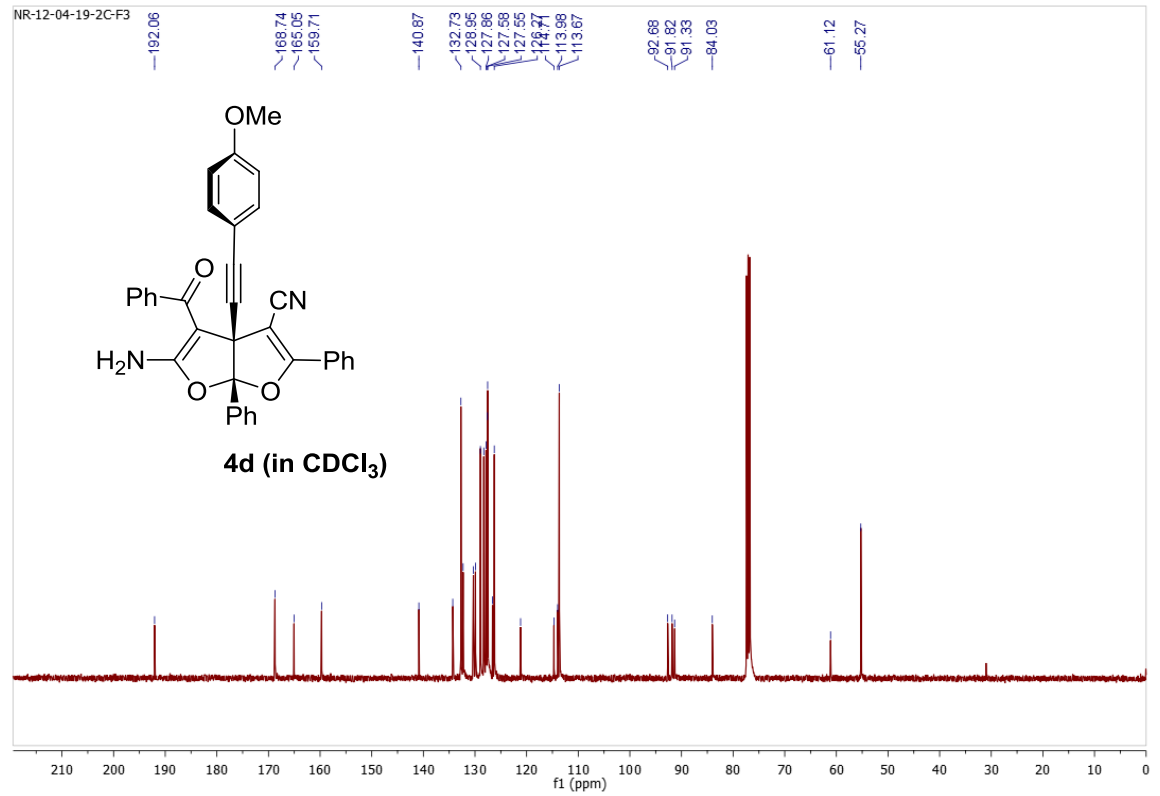

NR-22-04-29-2
single_pulse
7.9055
7.8939
7.6045
7.5935
7.3805
7.3697
7.2371
7.2289
6.7363
6.7233
6.6494
F
O
Ph
CN
H2N
Ph
O
O
Ph
4b (in CDCl3)
1.99
2.20
11.01
3.90
f1 (ppm)

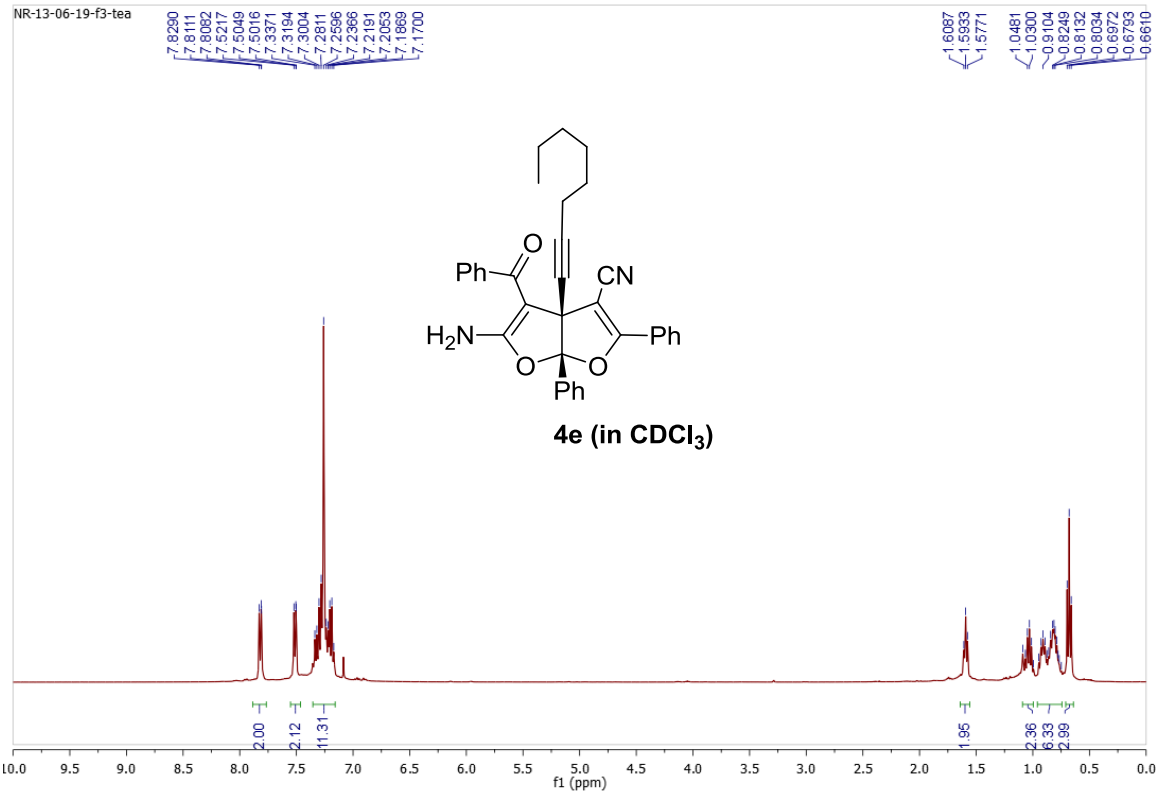

NR-22-0419-2-F2-13CC
191.95
168.69
165.22
163.81
161.33
140.82
134.21
133.24
133.15
132.41
130.38
129.93
128.99
128.35
127.88
127.57
127.48
126.21
115.50
115.28
92.31
91.09
90.74
85.00
61.09
F
O
Ph
CN
H2N
Ph
O
O
Ph
4b (in CDCl3)
f1 (ppm)


NR-03-04-4-cl-F33
8.7707
7.9982
7.9804
7.6500
7.6315
7.5973
7.5695
7.3542
7.3332
6.7903
3.3846
2.5148
Cl
O
Ph
CN
H2N
Ph
O
O
Ph
4c (in DMSO-d6)
1.84
2.00
9.19
4.08
1.83
f1 (ppm)

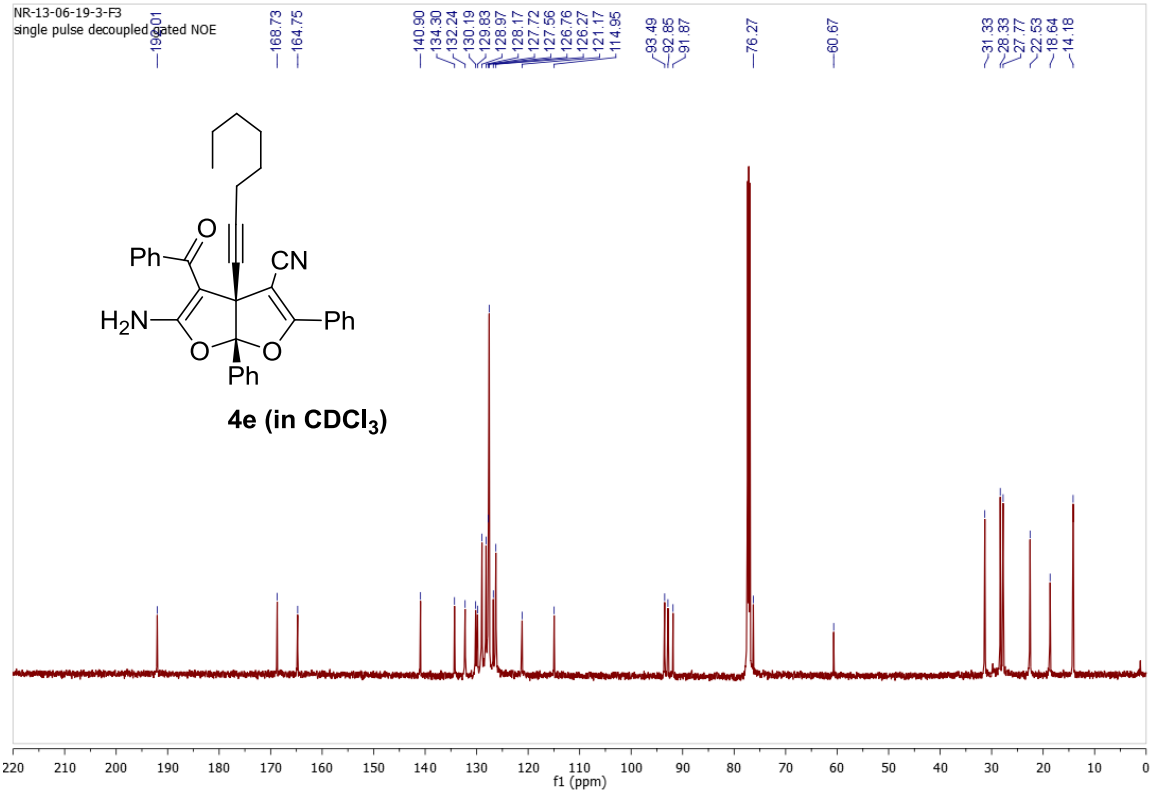

NR-02-04-F3-13C
189.32
168.23
165.31
141.54
134.18
134.12
132.97
130.97
129.99
129.86
129.15
129.03
128.23
127.63
127.58
126.48
126.35
120.17
91.41
90.16
89.58
87.06
61.18
Cl
O
Ph
CN
H2N
Ph
O
O
Ph
4c (in DMSO-d6)
f1 (ppm)


NR-12-4-2C
single_pulse
8.0153
8.0029
7.7539
7.7419
7.5137
7.5014
7.4811
7.4738
7.4614
7.4285
7.4169
7.3748
7.3626
7.3506
6.7593
6.7454
6.6942
6.6804
3.7471
OMe
O
Ph
CN
H2N
Ph
O
O
Ph
4d (in CDCl3)
2.04
2.15
9.27
2.14
3.92
2.98
f1 (ppm)

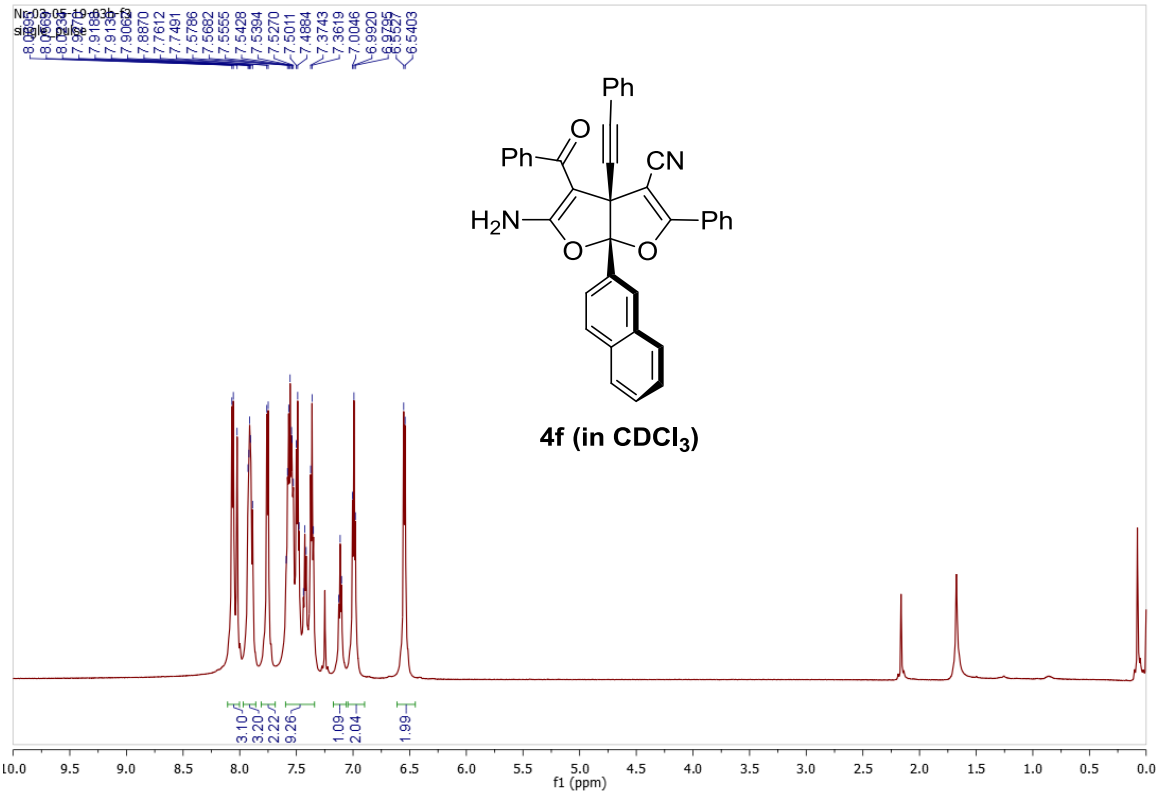

NR-12-04-19-2C-F3
192.06
168.74
165.05
159.71
140.87
132.73
128.95
127.86
127.58
127.55
113.98
113.67
92.68
91.82
91.33
84.03
61.12
55.27
OMe
O
Ph
CN
H2N
Ph
O
O
Ph
4d (in CDCl3)
f1 (ppm)

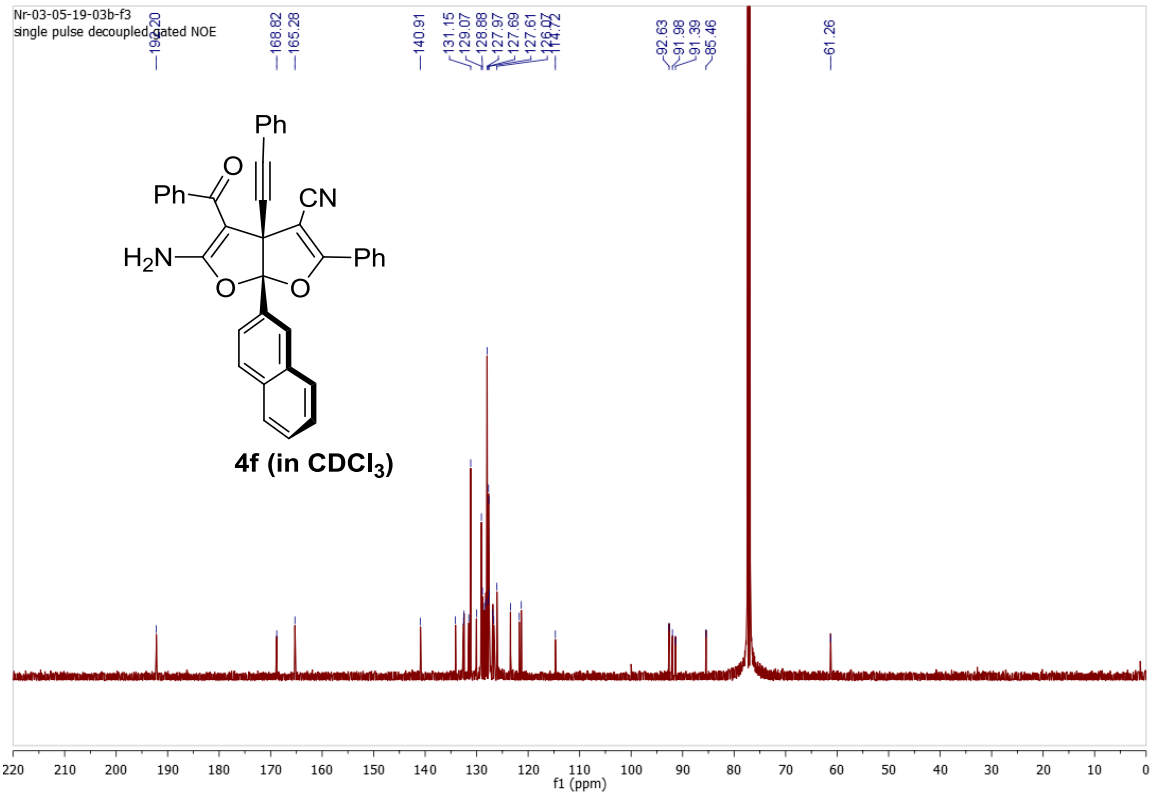


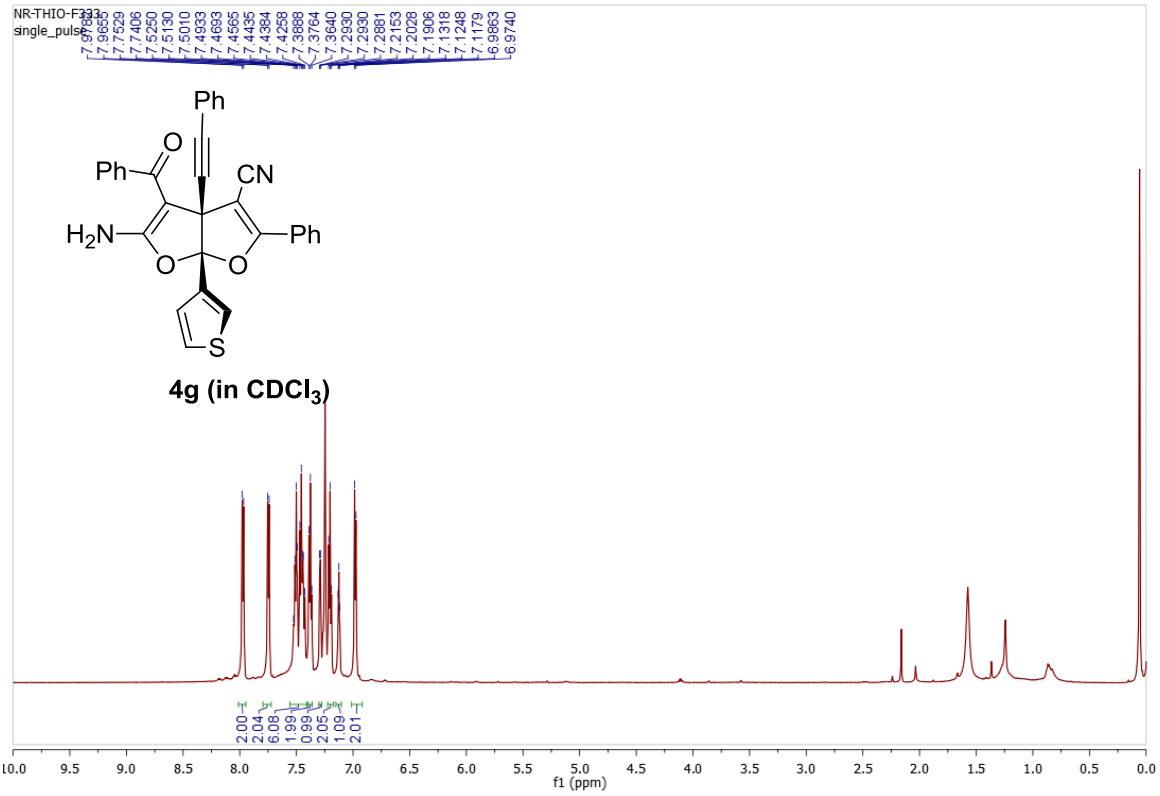
4e (in $CDCl_3$)

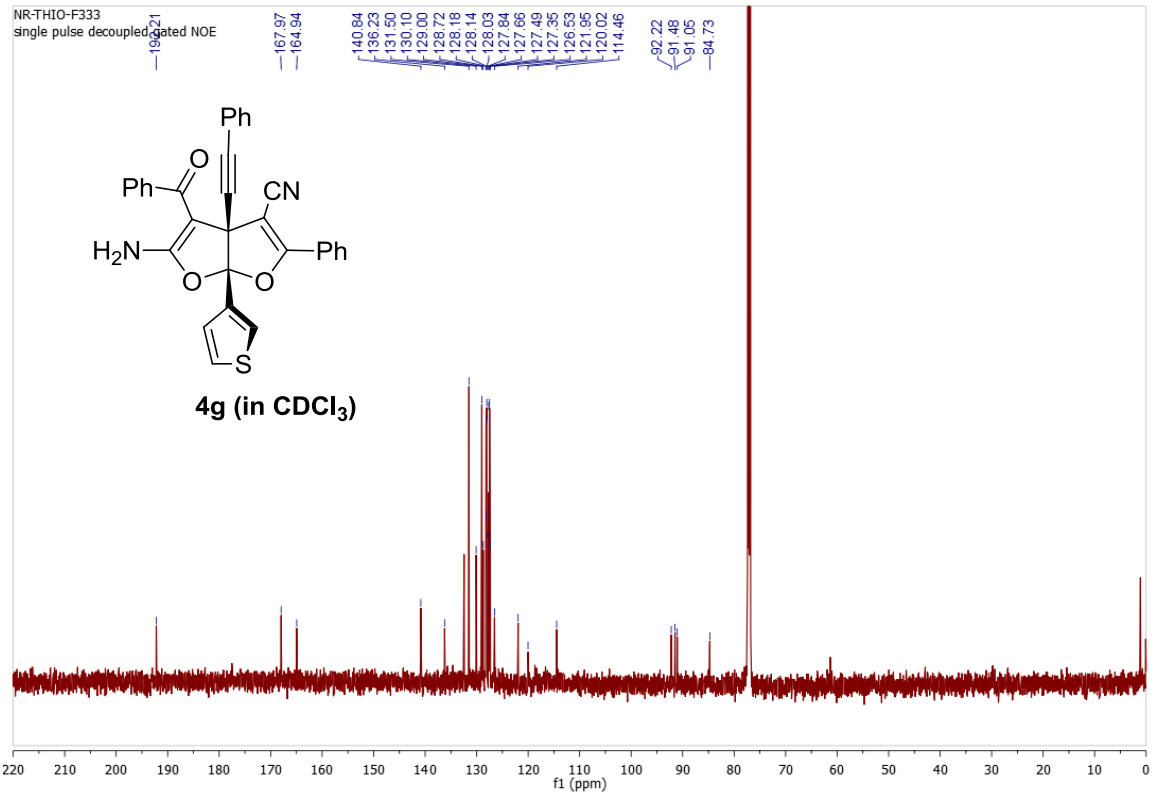


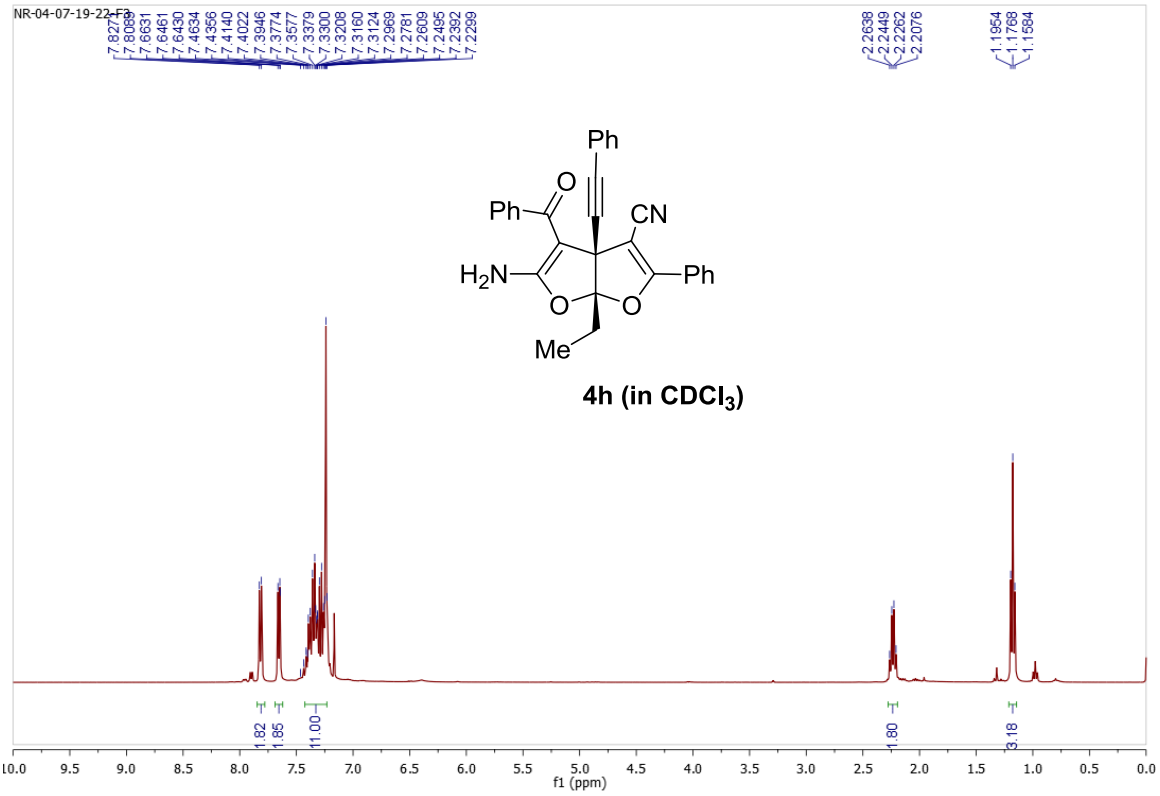
4e (in $CDCl_3$)

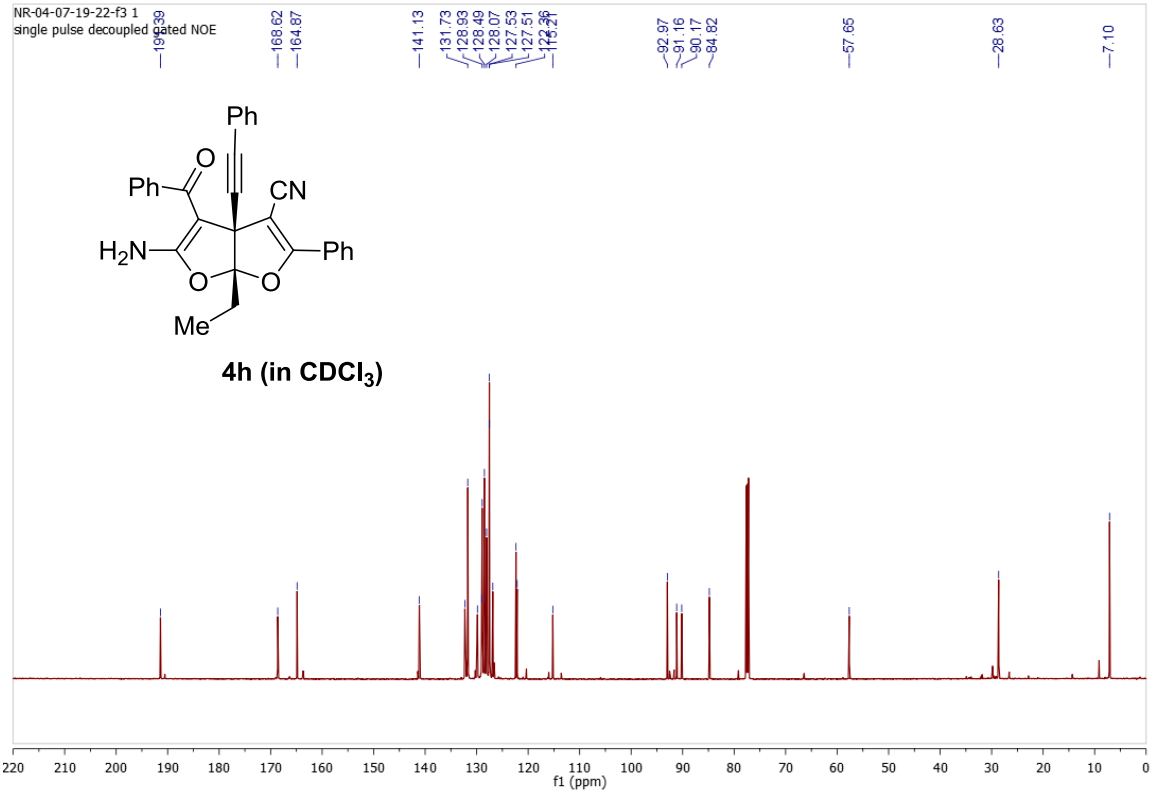

Nr-03-05-19-03b-f3
single pulse
Ph
O
Ph
CN
H2N
O
O
Ph
4f (in CDCl3)
3.10
3.20
2.22
9.26
1.09
2.04
1.99
f1 (ppm)

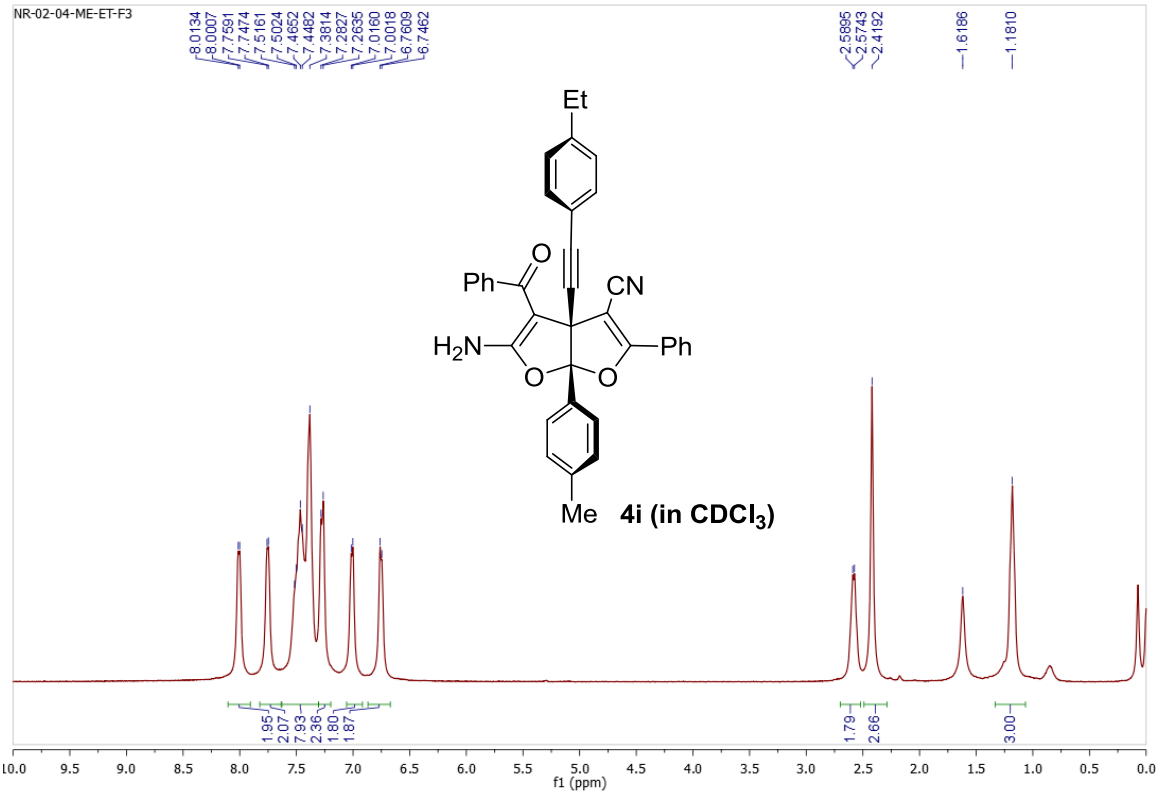

Nr-03-05-19-03b-f3
single pulse decoupled, gated NOE
168.82
165.28
140.91
131.15
129.07
128.88
127.97
127.69
127.61
92.63
91.98
91.39
85.46
61.26
Ph
O
Ph
CN
H2N
O
O
Ph
4f (in CDCl3)
f1 (ppm)

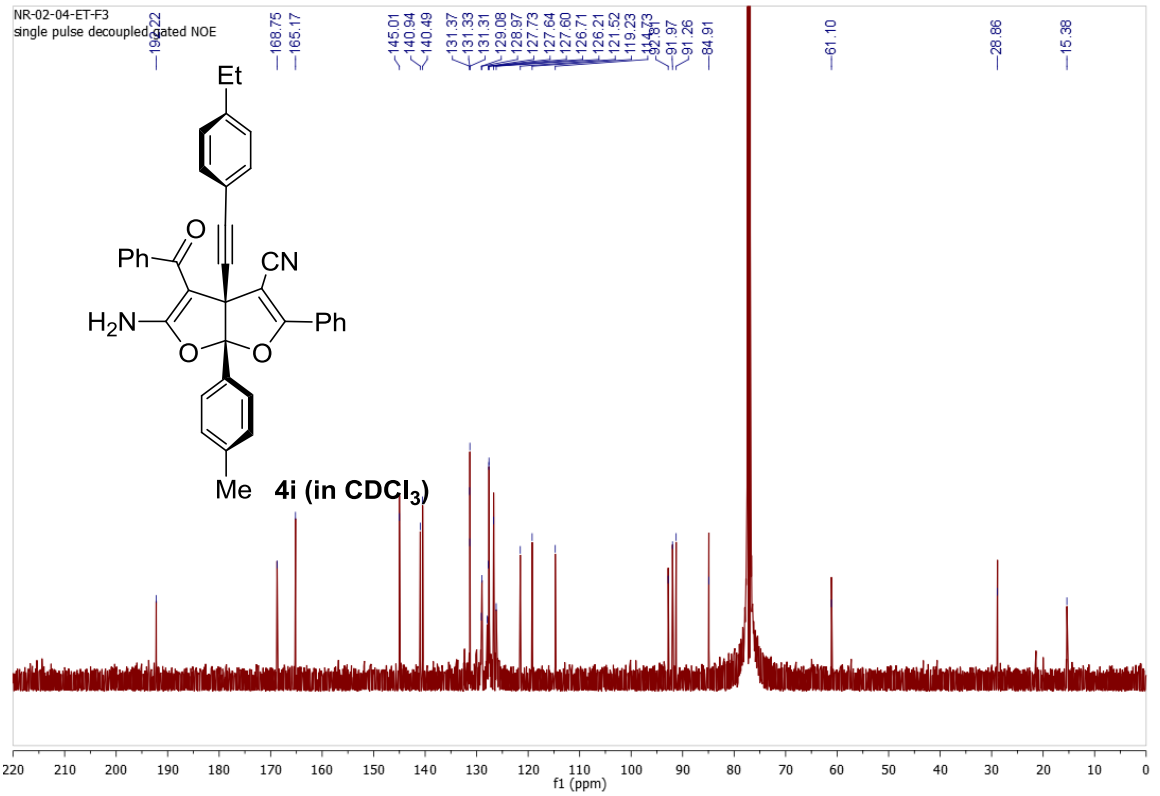

NR-THIO-F333
single_pulse
Ph
O
Ph
CN
H2N
Ph
O
O
S
4g (in CDCl3)
f1 (ppm)

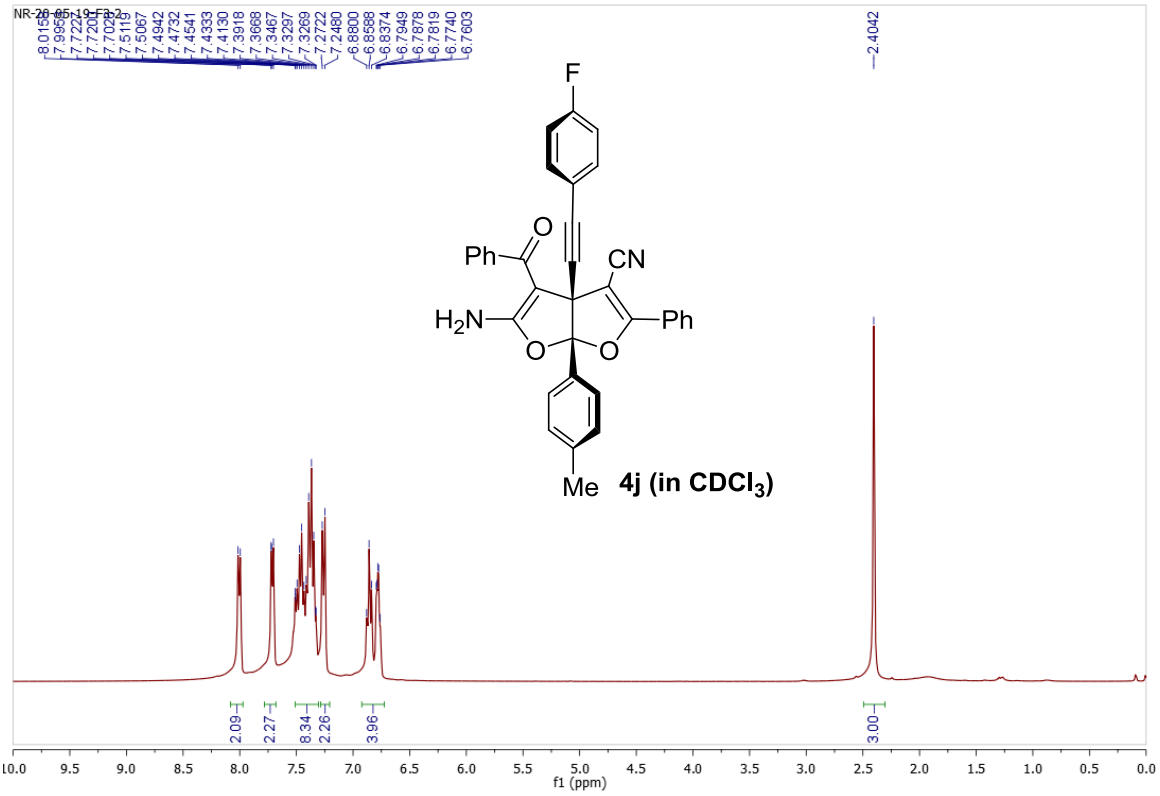

NR-THIO-F333
single pulse decoupled gated NOE
Ph
O
Ph
CN
H2N
Ph
O
O
S
4g (in CDCl3)
f1 (ppm)

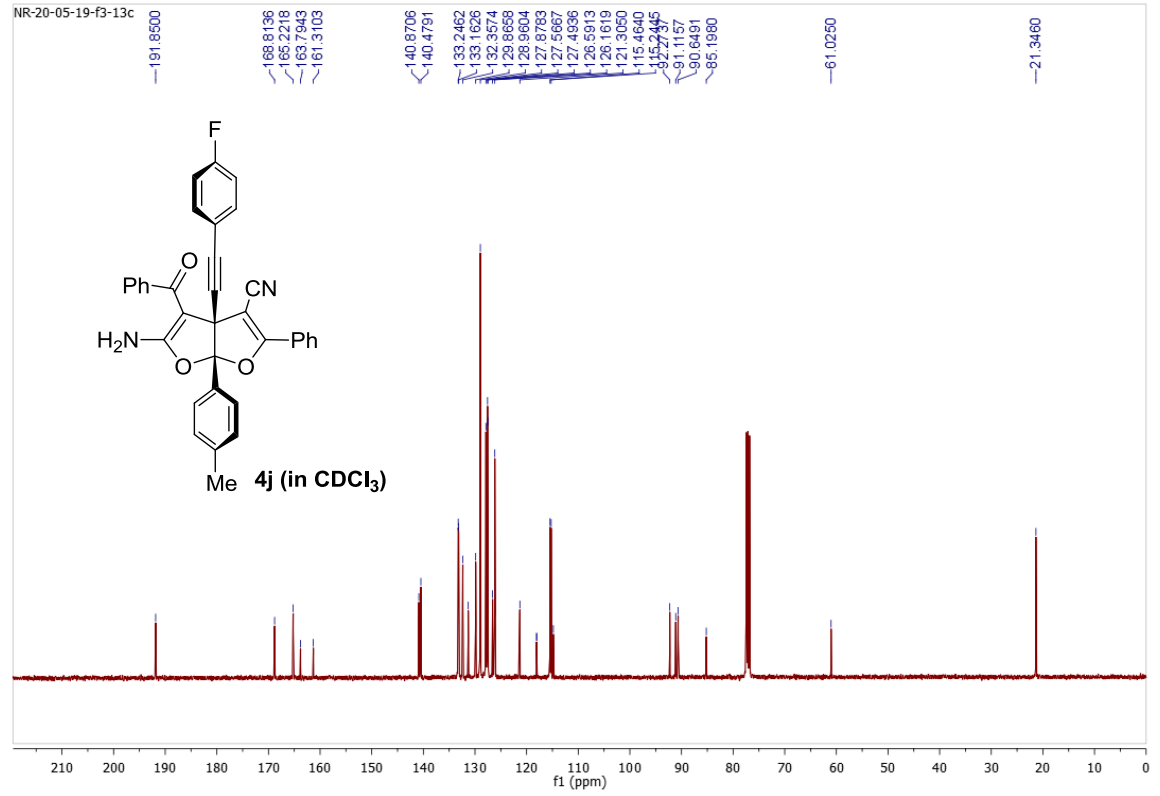

NR-04-07-19-22-F3
7.8272
7.8089
7.6631
7.6461
7.6430
7.4634
7.4356
7.4140
7.4022
7.3946
7.3774
7.3577
7.3379
7.3300
7.3208
7.3160
7.3124
7.2969
7.2781
7.2609
7.2495
7.2392
7.2299
2.2638
2.2449
2.2262
2.2076
1.1954
1.1768
1.1584
Ph
O
Ph
CN
H2N
Ph
O
O
Me
4h (in CDCl3)
1.82
1.85
11.00
1.80
3.18
f1 (ppm)

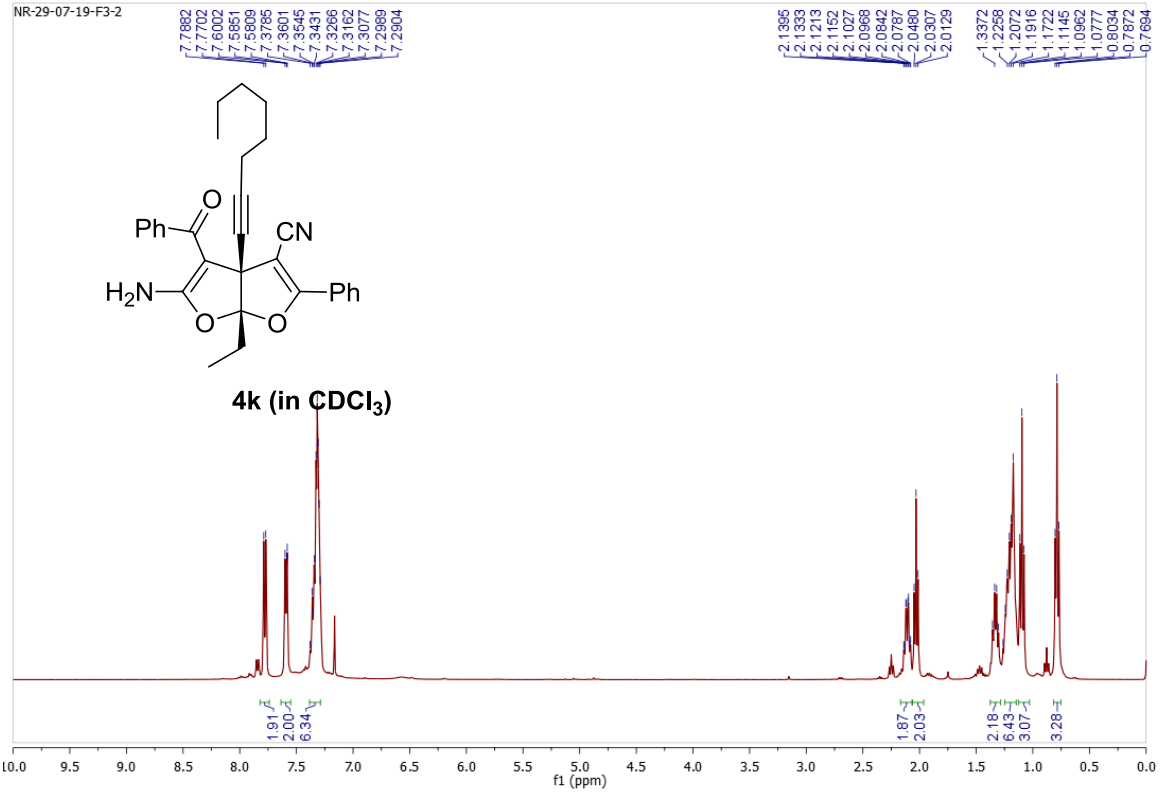

NR-04-07-19-22-f3 1
single pulse decoupled gated NOE
168.62
164.87
141.13
131.73
128.93
128.49
128.07
127.53
127.51
92.97
91.16
90.17
84.82
57.65
28.63
7.10
Ph
O
Ph
CN
H2N
Ph
O
O
Me
4h (in CDCl3)
f1 (ppm)

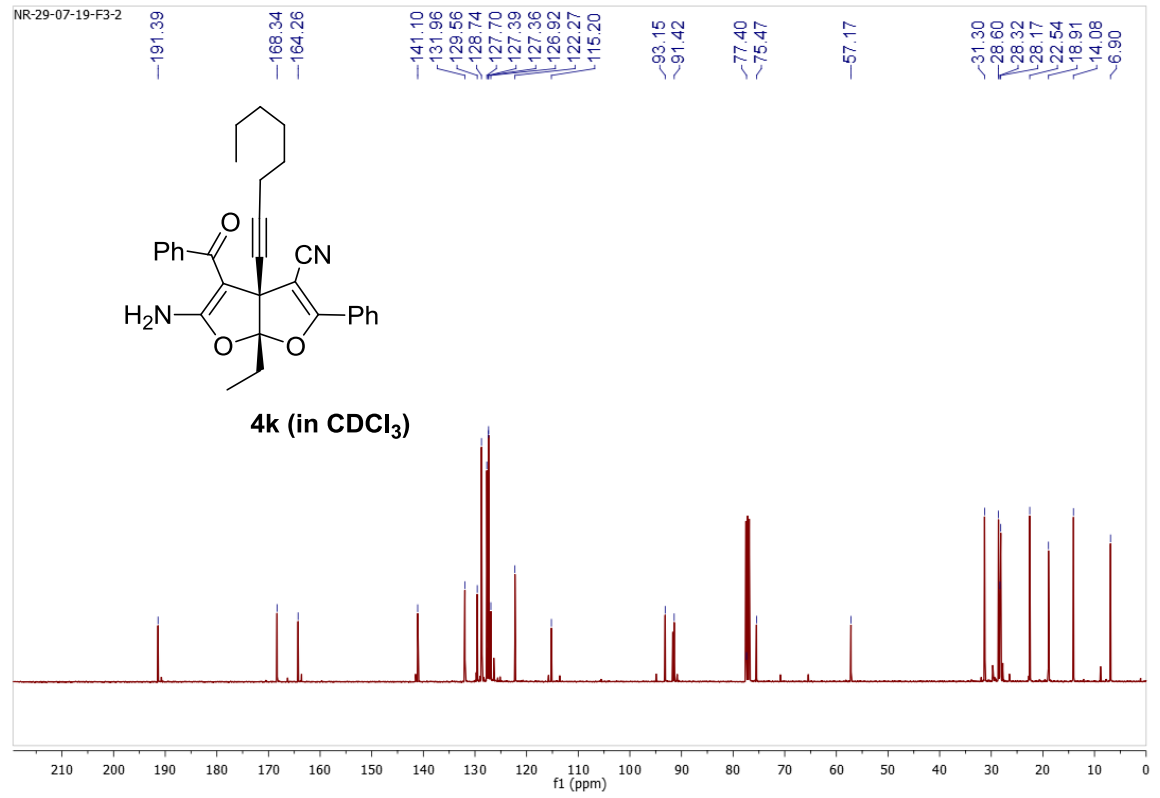

NR-02-04-ME-ET-F3
8.0134
8.0007
7.7591
7.7474
7.5161
7.5024
7.4652
7.4482
7.3814
7.2827
7.2635
7.0160
7.0018
6.7609
6.7462
2.5895
2.5743
2.4192
1.6186
1.1810
Et
O
Ph
CN
H2N
O
O
Ph
Me
4i (in CDCl3)
1.95
2.07
7.93
2.36
1.80
1.87
1.79
2.66
3.00
f1 (ppm)

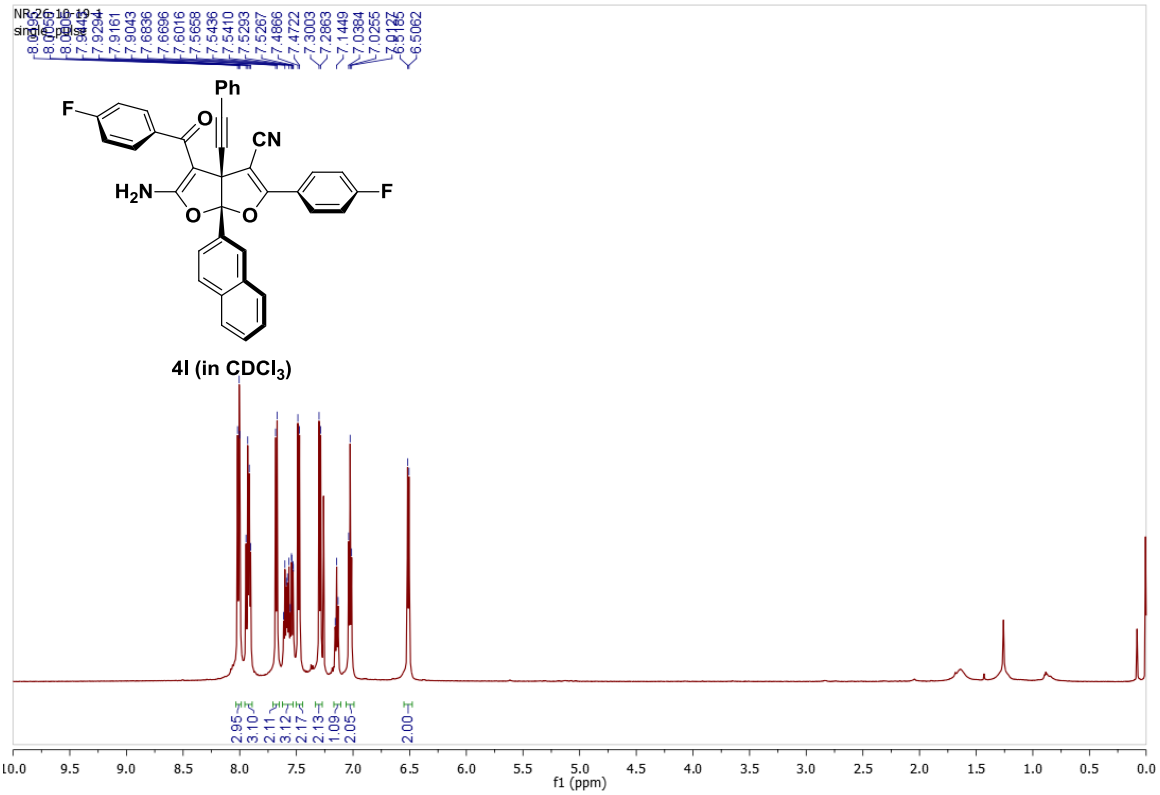

NR-02-04-ET-F3
single pulse decoupled, gated NOE
168.75
165.17
145.01
140.94
140.49
131.37
131.33
131.31
129.08
128.97
127.73
127.64
127.60
126.71
126.21
121.52
119.23
92.81
91.97
91.26
84.91
61.10
28.86
15.38
Et
O
Ph
CN
H2N
O
O
Ph
Me
4i (in CDCl3)
f1 (ppm)

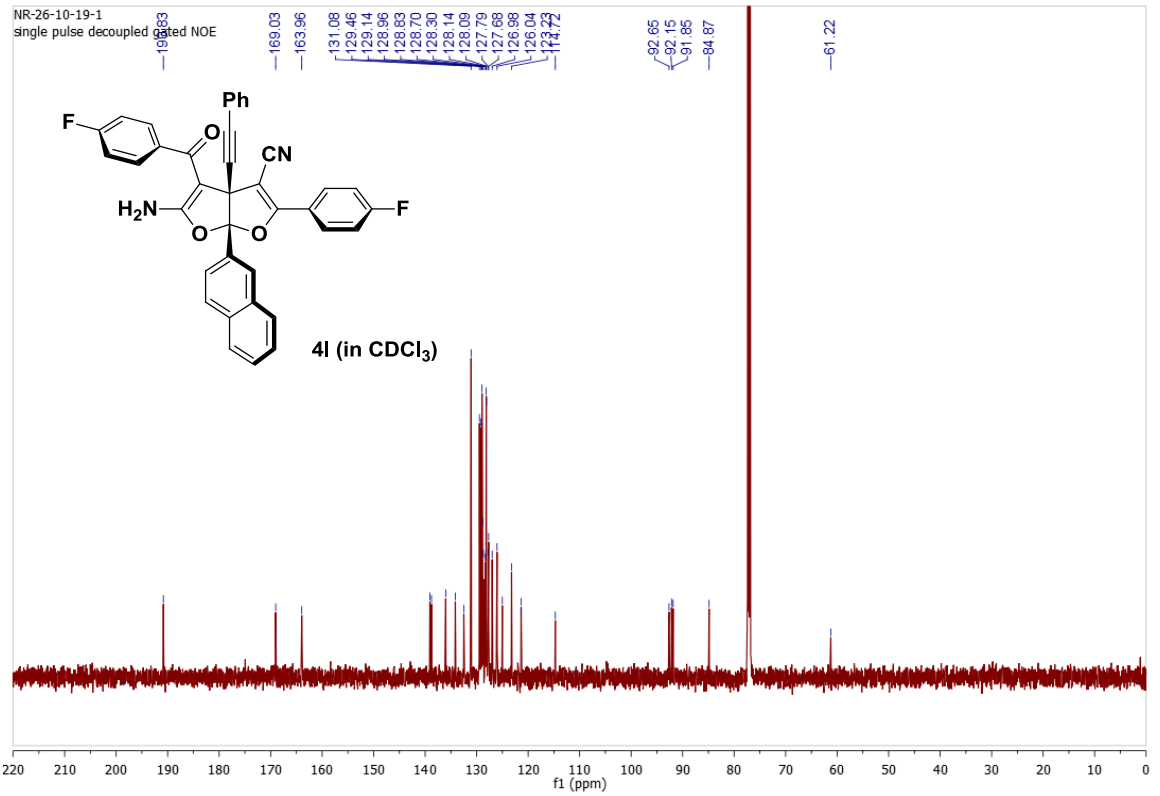

NR-20-05-19-F3c2
8.0156
7.9956
7.7224
7.7200
7.7024
7.5119
7.5067
7.4942
7.4732
7.4541
7.4333
7.4130
7.3918
7.3668
7.3467
7.3297
7.3269
7.2722
7.2480
6.8800
6.8588
6.8374
6.7949
6.7878
6.7819
6.7740
6.7603
2.4042
F
O
Ph
CN
H2N
O
O
Ph
Me
4j (in CDCl3)
2.09
2.27
8.34
2.26
3.96
3.00
f1 (ppm)

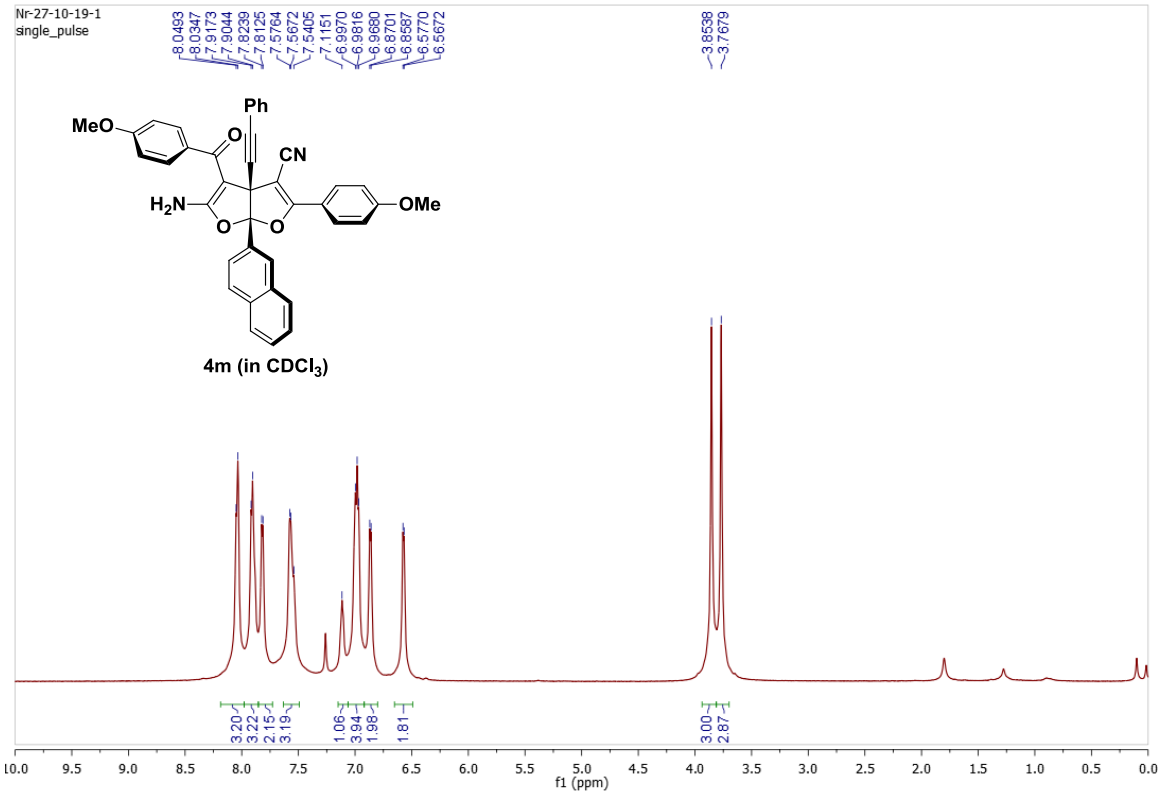

NR-20-05-19-f3-13c
191.8500
168.8136
165.2218
163.7943
161.3103
140.8706
140.4791
133.2462
133.1626
132.3574
129.8658
128.9604
127.8783
127.5667
127.4936
126.5913
126.1619
121.3050
115.4640
115.2345
91.1157
90.6491
85.1980
61.0250
21.3460
F
O
Ph
CN
H2N
O
O
Ph
Me
4j (in CDCl3)
f1 (ppm)

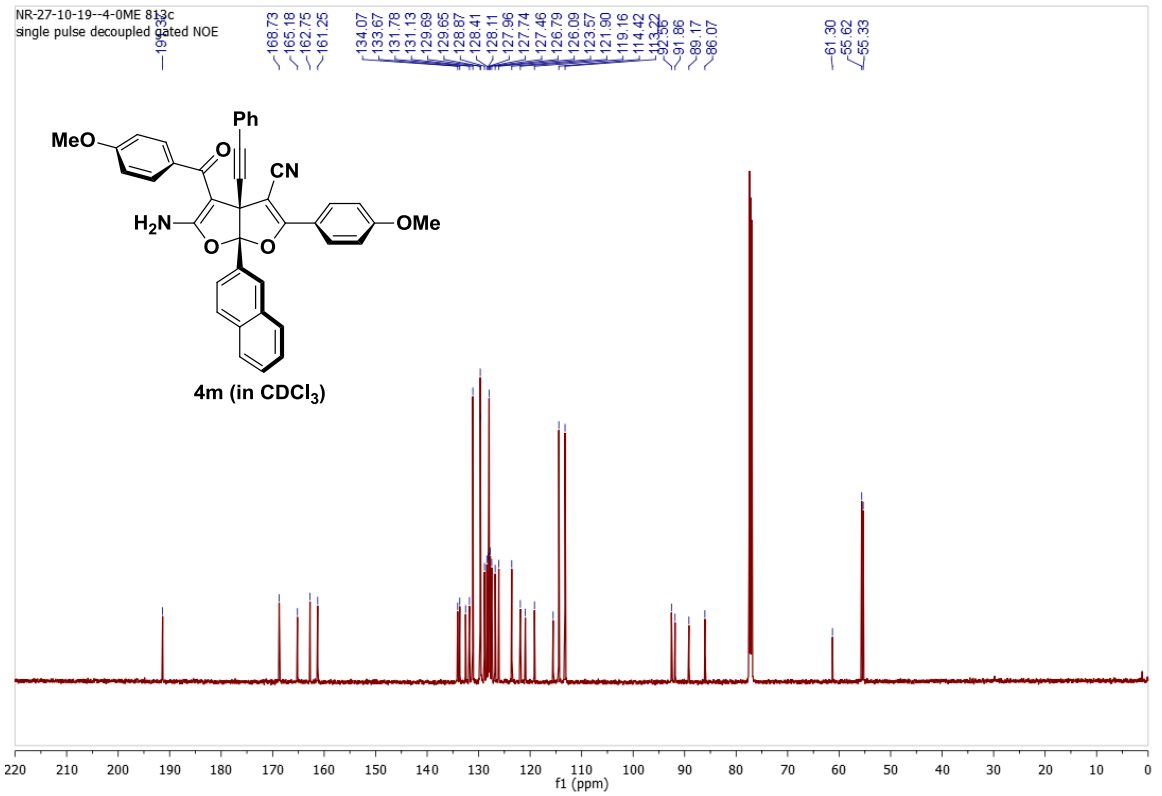

NR-29-07-19-F3-2
7.7882
7.7702
7.6002
7.5851
7.5809
7.3785
7.3601
7.3545
7.3431
7.3266
7.3162
7.3077
7.2989
7.2904
2.1395
2.1333
2.1213
2.1152
2.1027
2.0968
2.0842
2.0787
2.0480
2.0307
2.0129
1.3372
1.2258
1.2072
1.1916
1.1722
1.1145
1.0962
1.0777
0.8034
0.7872
0.7684
Ph
O
CN
H2N
Ph
O
O
4k (in CDCl3)
1.91
2.00
6.34
1.87
2.03
2.18
6.43
3.07
3.28
f1 (ppm)

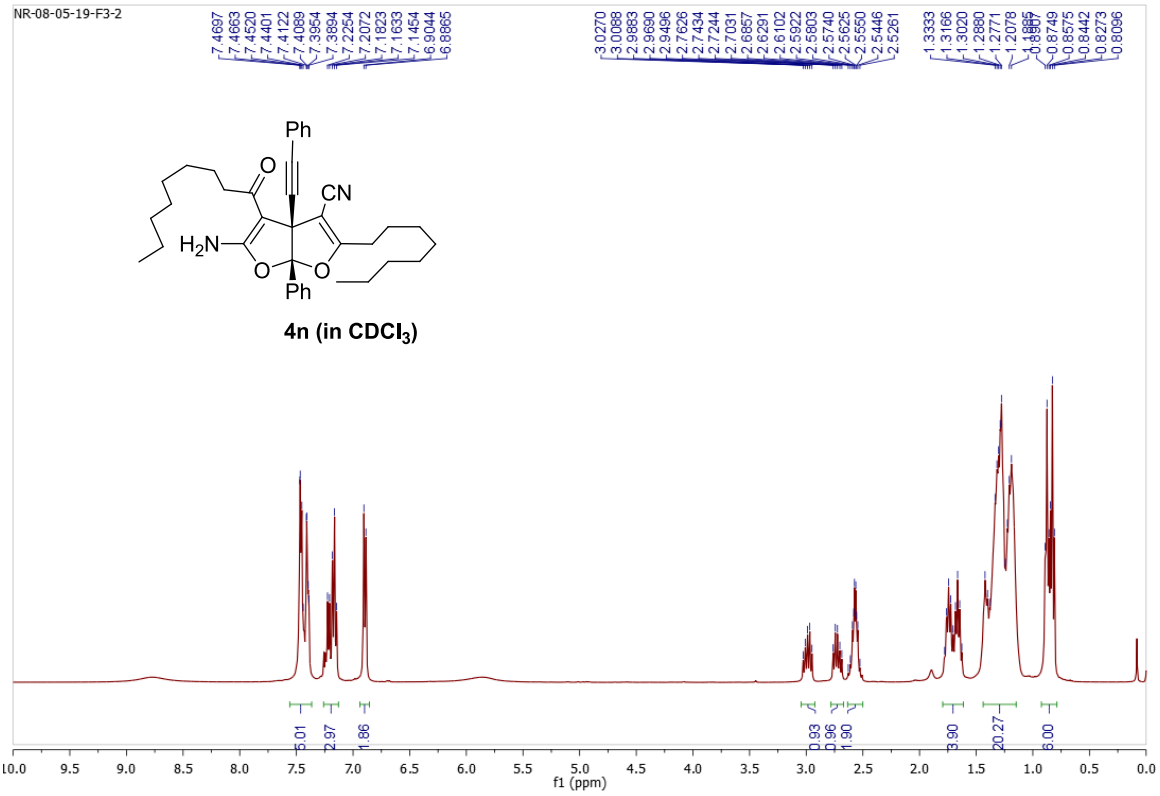

NR-29-07-19-F3-2
191.39
168.34
164.26
141.10
131.96
129.56
128.74
127.70
127.39
127.36
126.92
122.27
115.20
93.15
91.42
77.40
75.47
57.17
31.30
28.60
28.32
28.17
22.54
18.91
14.08
6.90
Ph
O
CN
H2N
Ph
O
O
4k (in CDCl3)
f1 (ppm)

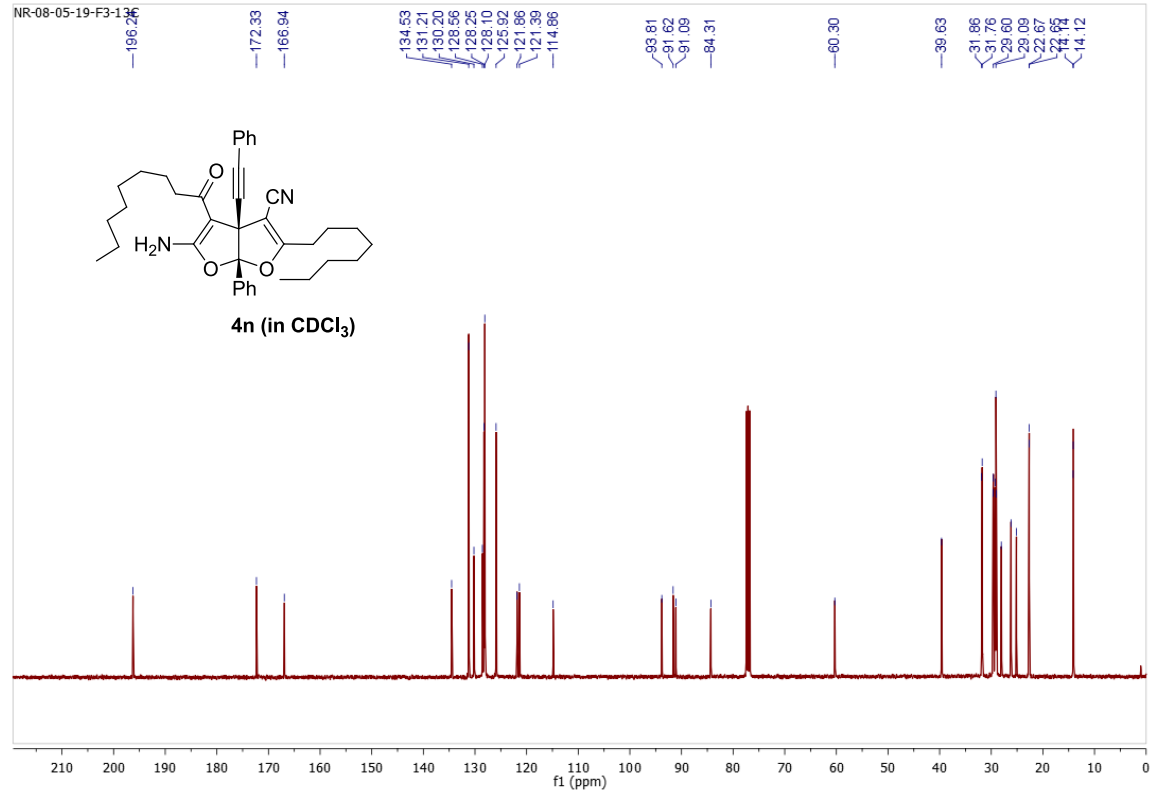

NR-26-10-19-1
single pulse
Ph
F
O
CN
H_2N
O
O
F
4l (in $CDCl_3$)
2.95
3.10
2.11
3.12
2.17
2.13
1.09
2.05
2.00
f1 (ppm)

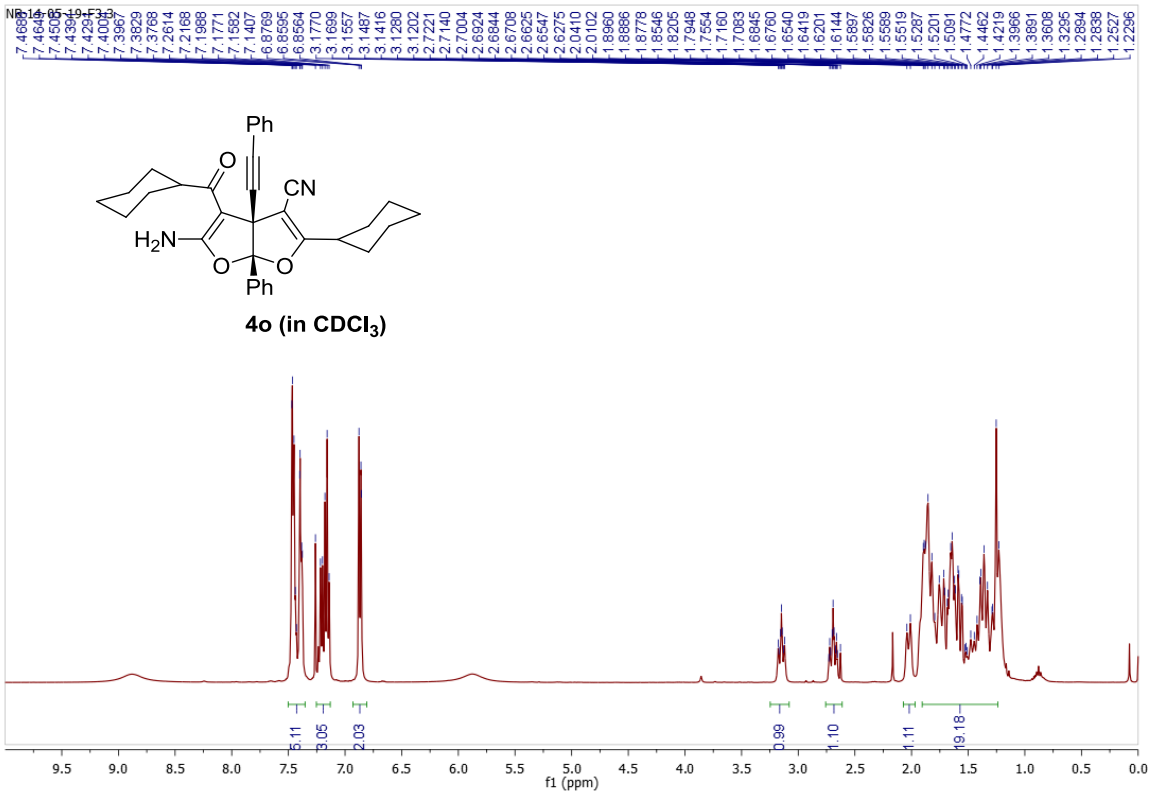

NR-26-10-19-1
single pulse decoupled gated NOE
169.03
163.96
131.08
129.46
129.14
128.96
128.83
128.70
128.30
128.14
128.09
127.79
127.68
126.98
126.04
92.65
92.15
91.85
84.87
61.22
Ph
F
O
CN
H_2N
O
O
F
4l (in $CDCl_3$)
f1 (ppm)


Nr-27-10-19-1
single_pulse
8.0493
8.0347
7.9173
7.9044
7.8239
7.8125
7.5764
7.5672
7.5405
7.1151
6.9970
6.9816
6.9680
6.8701
6.8587
6.5770
6.5672
3.8538
3.7679
Ph
MeO
O
CN
H2N
O
O
OMe
4m (in CDCl3)
3.20
3.22
2.15
3.19
1.06
3.94
1.98
1.81
3.00
2.87
f1 (ppm)

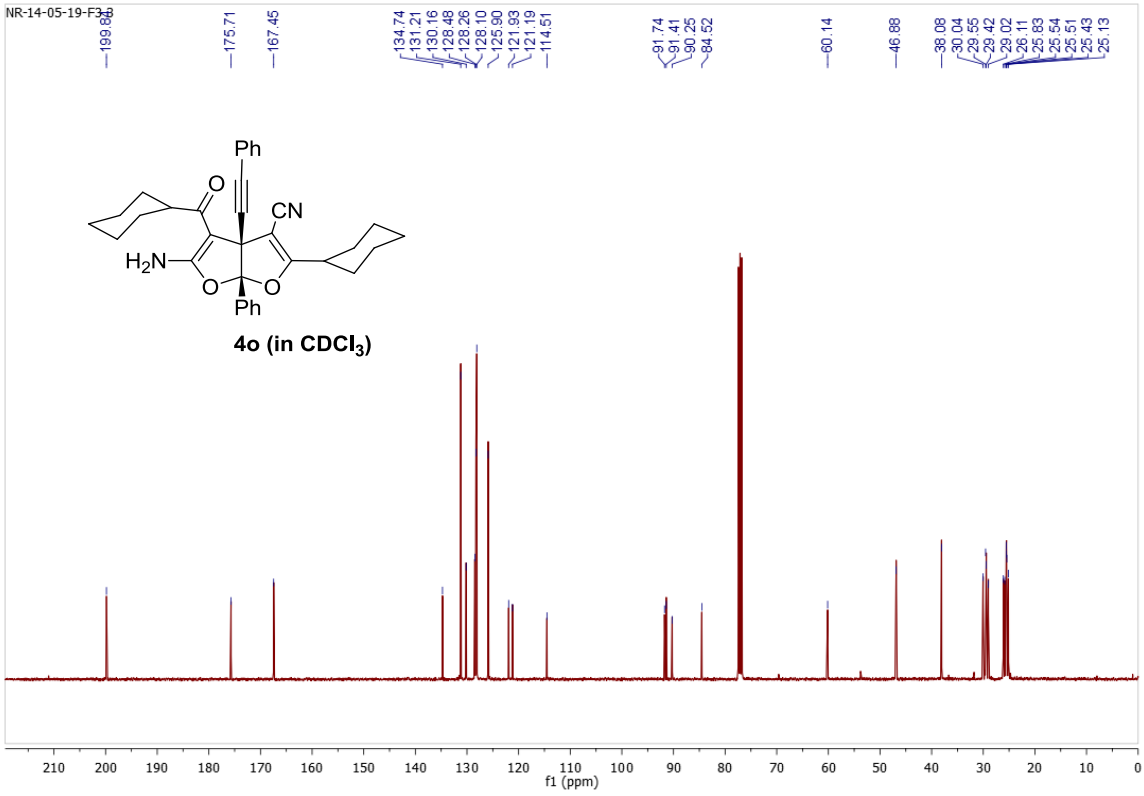

NR-27-10-19--4-0ME 813c
single pulse decoupled gated NOE
168.73
165.18
162.75
161.25
134.07
133.67
131.78
131.13
129.69
129.65
128.87
128.41
128.11
127.96
127.74
127.46
126.79
126.09
123.57
121.90
119.16
114.42
113.22
92.56
91.86
89.17
86.07
61.30
55.62
55.33
Ph
MeO
O
CN
H2N
O
O
OMe
4m (in CDCl3)
f1 (ppm)


NR-08-05-19-F3-2
Ph
O
CN
H2N
O
O
Ph
4n (in CDCl3)
f1 (ppm)

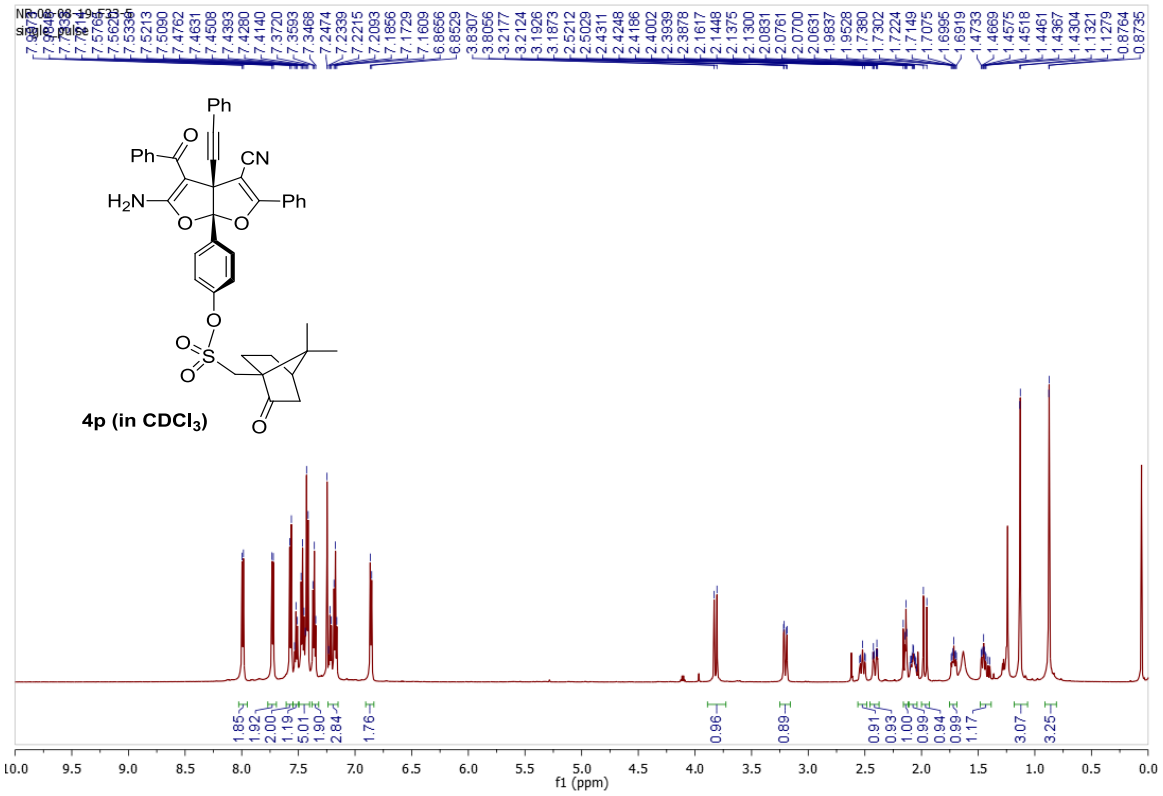

NR-08-05-19-F3-13C
Ph
O
CN
H2N
O
O
Ph
4n (in CDCl3)
f1 (ppm)

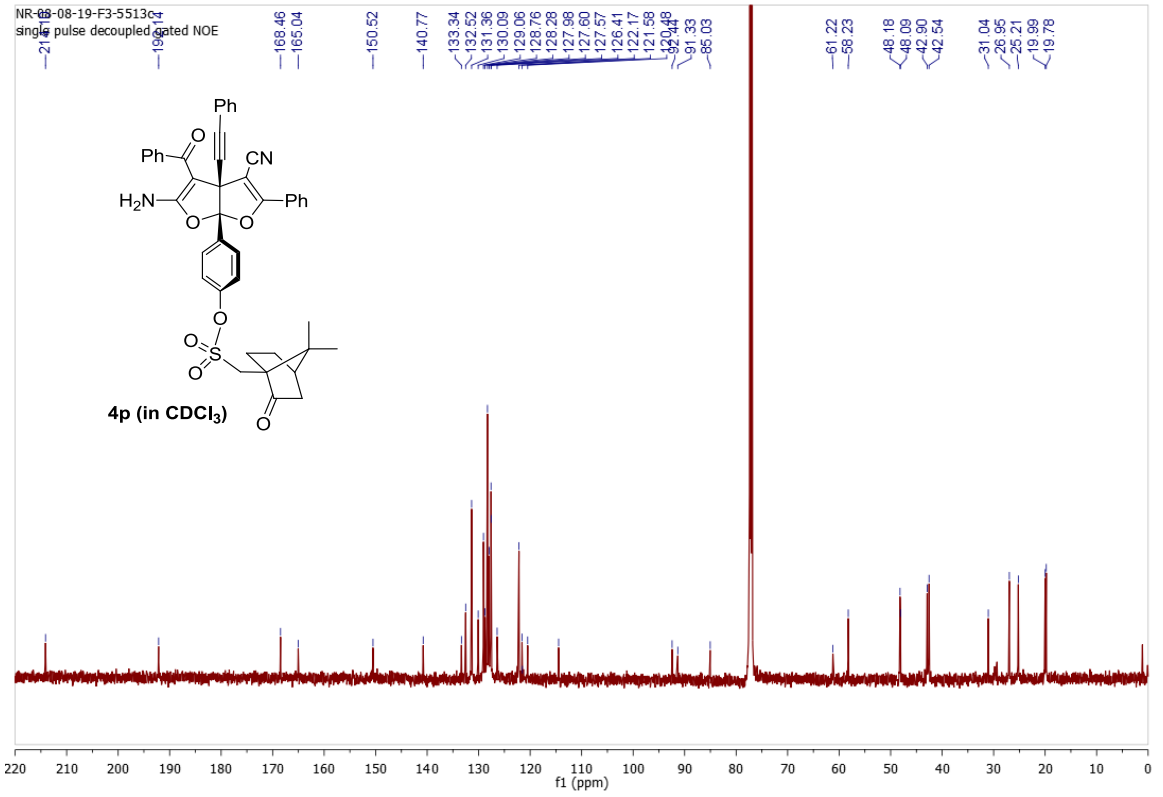


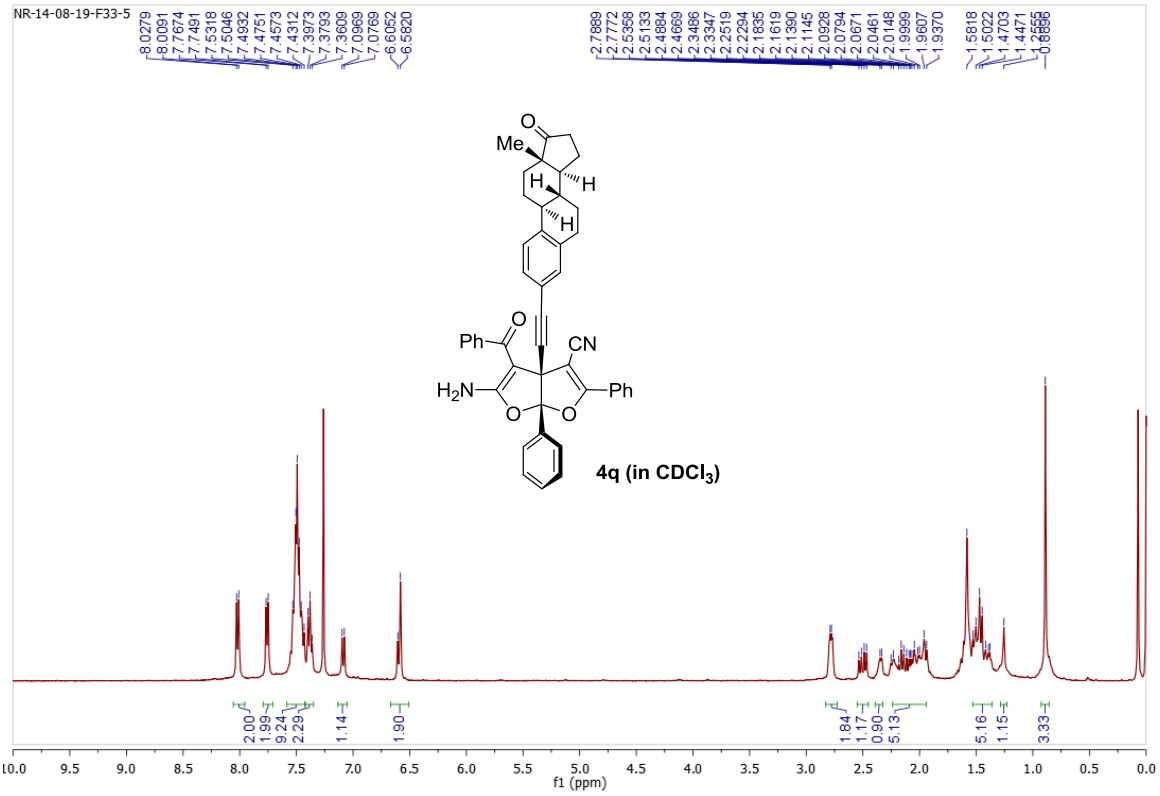
4o (in $CDCl_3$)

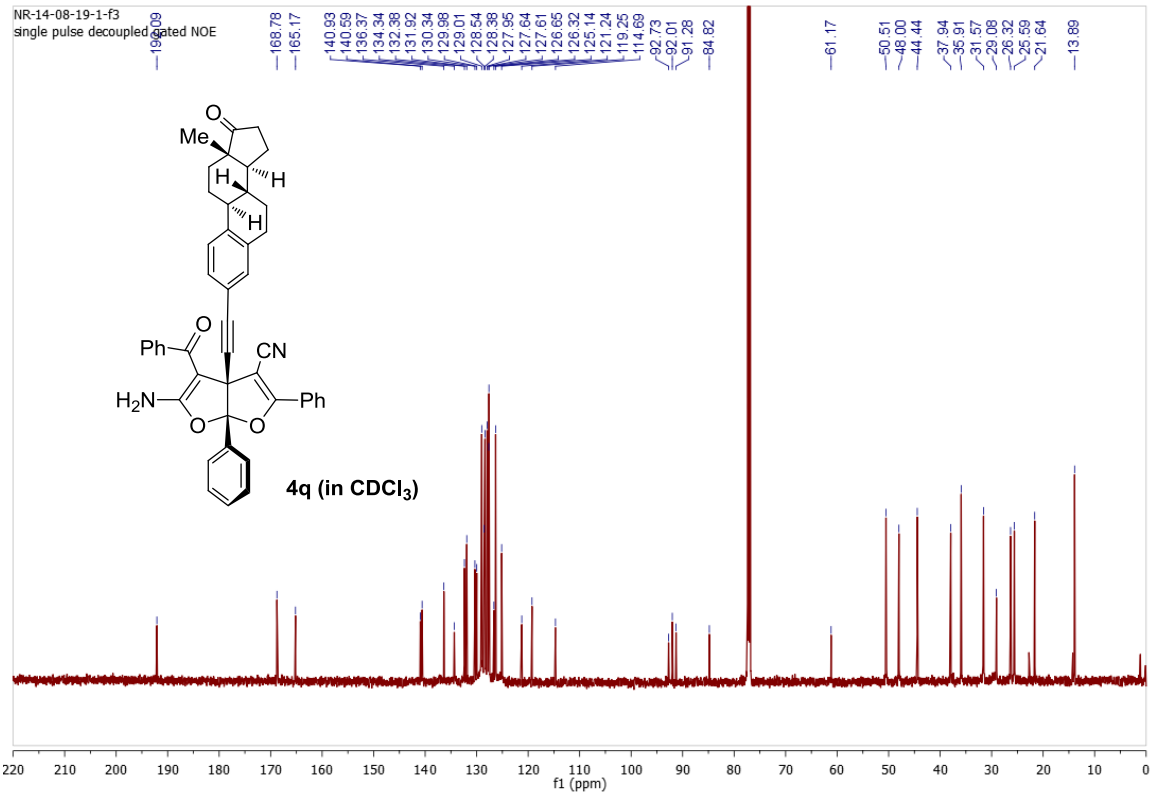


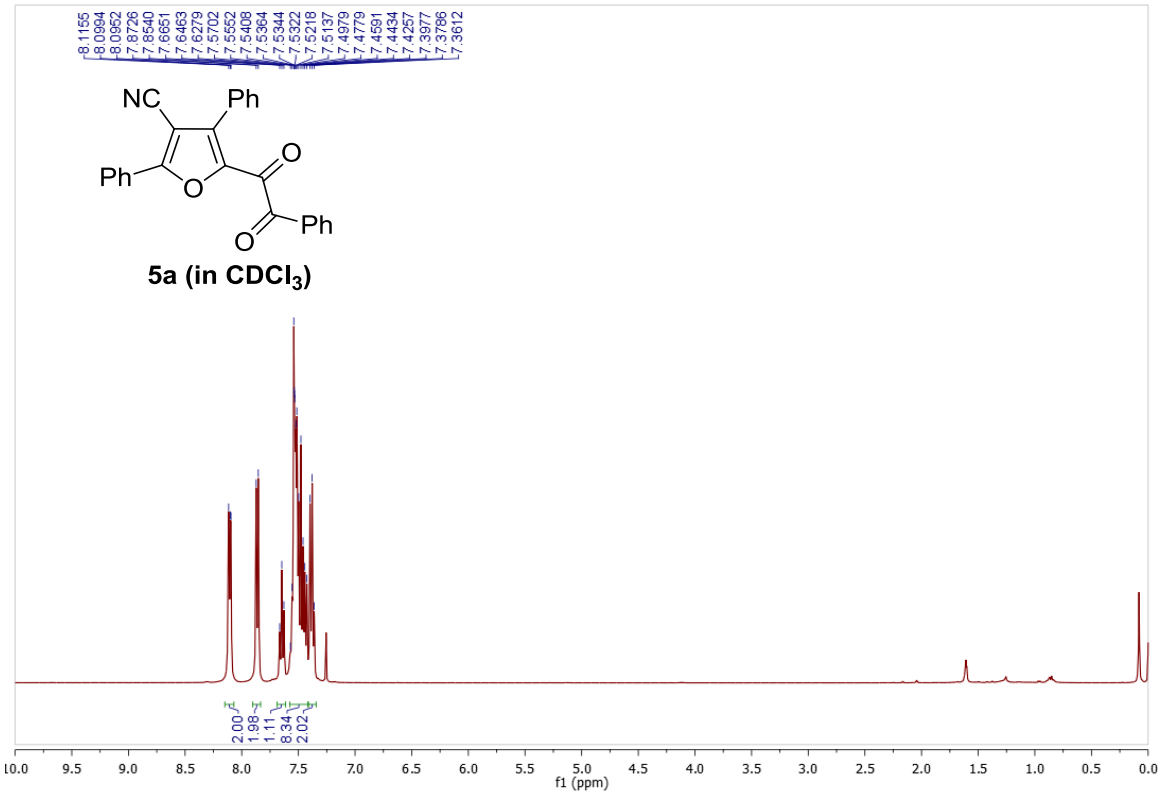
4o (in $CDCl_3$)

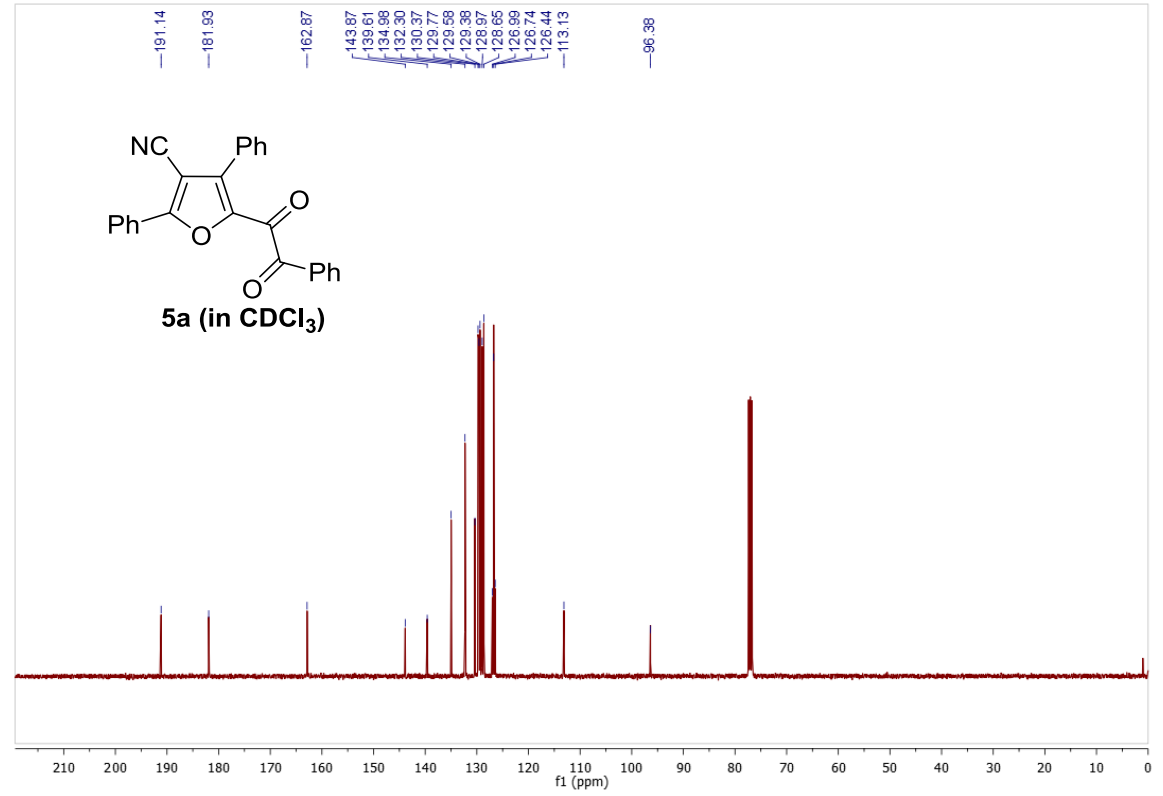

NR-08-08-19-F23-5
single pulse
Ph
O
Ph
CN
H2N
O
O
Ph
O
O
S
O
O
4p (in CDCl3)
1.85
1.92
2.00
1.19
5.01
1.90
2.84
1.76
0.96
0.89
0.91
0.93
1.00
0.99
0.94
0.99
1.17
3.07
3.25
f1 (ppm)

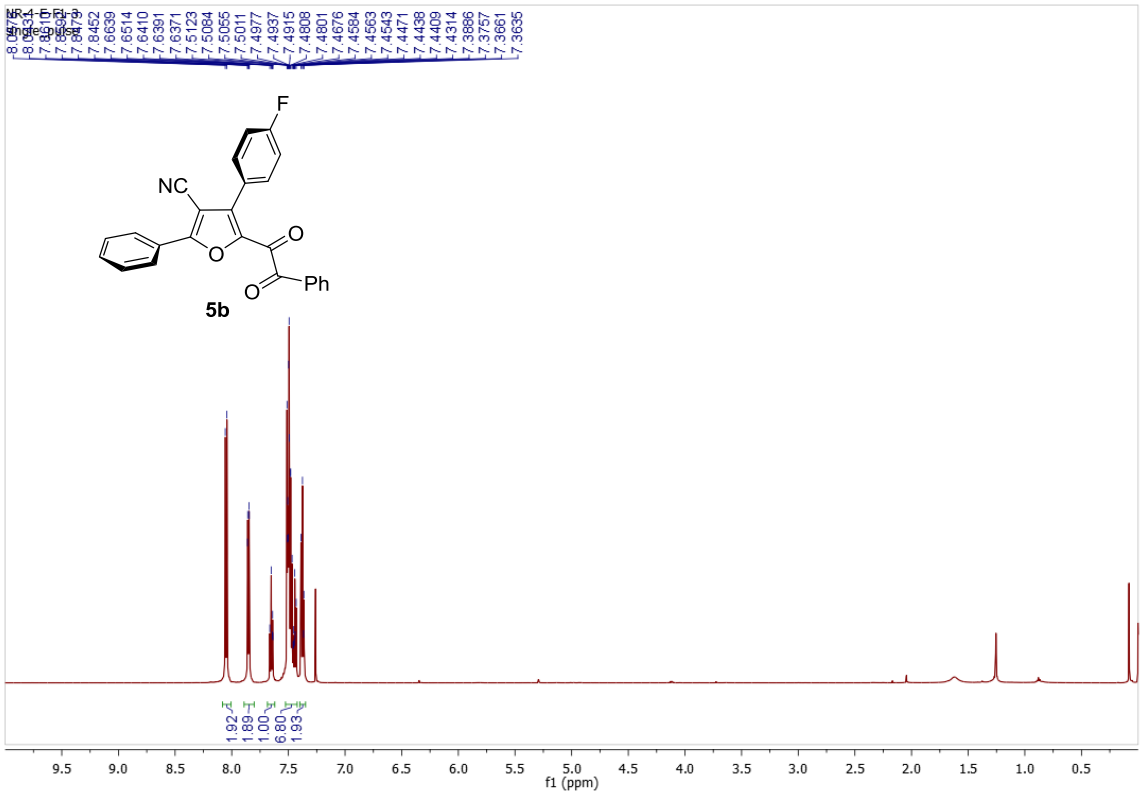

NR-08-08-19-F3-5513c
single pulse decoupled gated NOE
168.46
165.04
150.52
140.77
133.34
132.52
131.36
130.09
129.06
128.76
128.28
127.98
127.60
127.57
126.41
122.17
121.58
120.48
92.44
91.33
85.03
61.22
58.23
48.18
48.09
42.90
42.54
31.04
26.95
25.21
19.99
19.78
Ph
O
Ph
CN
H2N
O
O
Ph
O
O
S
O
O
4p (in CDCl3)
f1 (ppm)

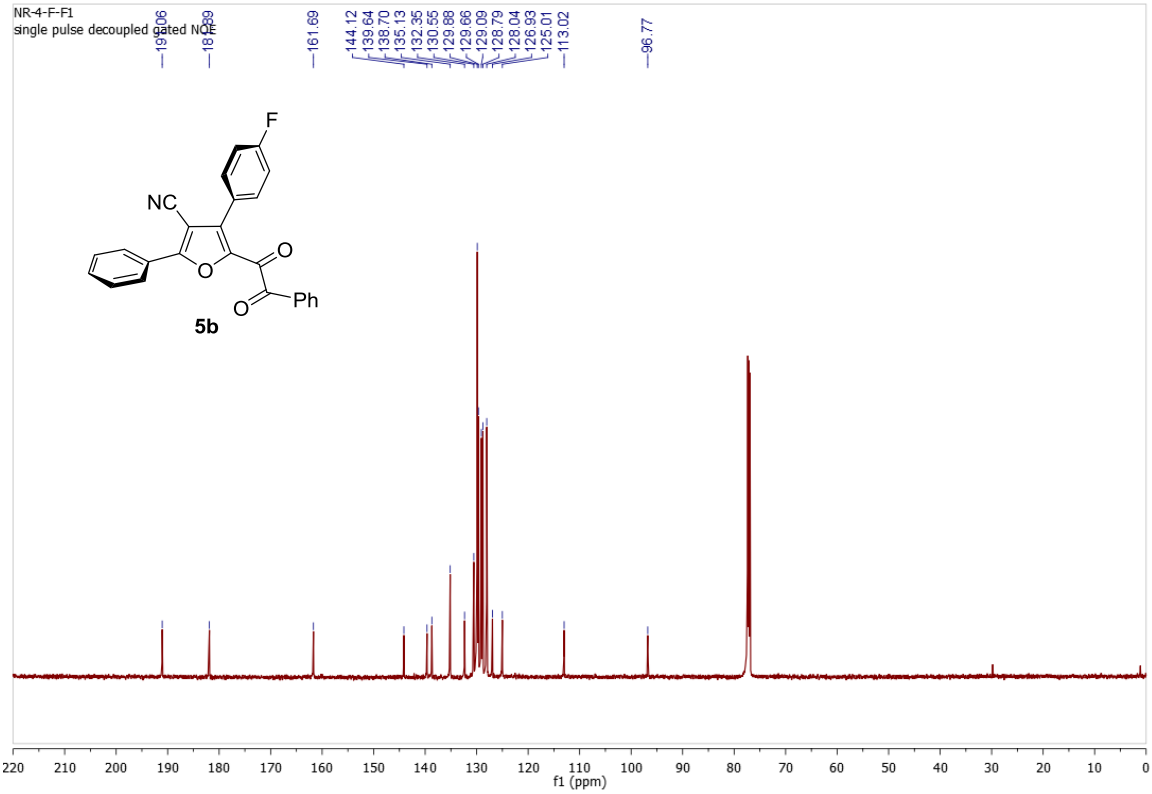

NR-14-08-19-F33-5
8.0279
8.0091
7.7674
7.7491
7.5318
7.5046
7.4932
7.4751
7.4573
7.4312
7.3973
7.3793
7.3608
7.0969
7.0769
6.6052
6.5820
2.7889
2.7772
2.5368
2.5133
2.4884
2.4669
2.3486
2.3347
2.2519
2.2294
2.1835
2.1619
2.1390
2.1145
2.0928
2.0794
2.0671
2.0461
2.0148
1.9999
1.9607
1.9370
1.5818
1.5022
1.4703
1.4471
Me
H
H
H
O
Ph
O
CN
H_2N
O
O
Ph
4q (in $CDCl_3$)
2.00
1.99
9.24
2.29
1.14
1.90
1.84
1.17
0.90
5.13
5.16
1.15
3.33
f1 (ppm)

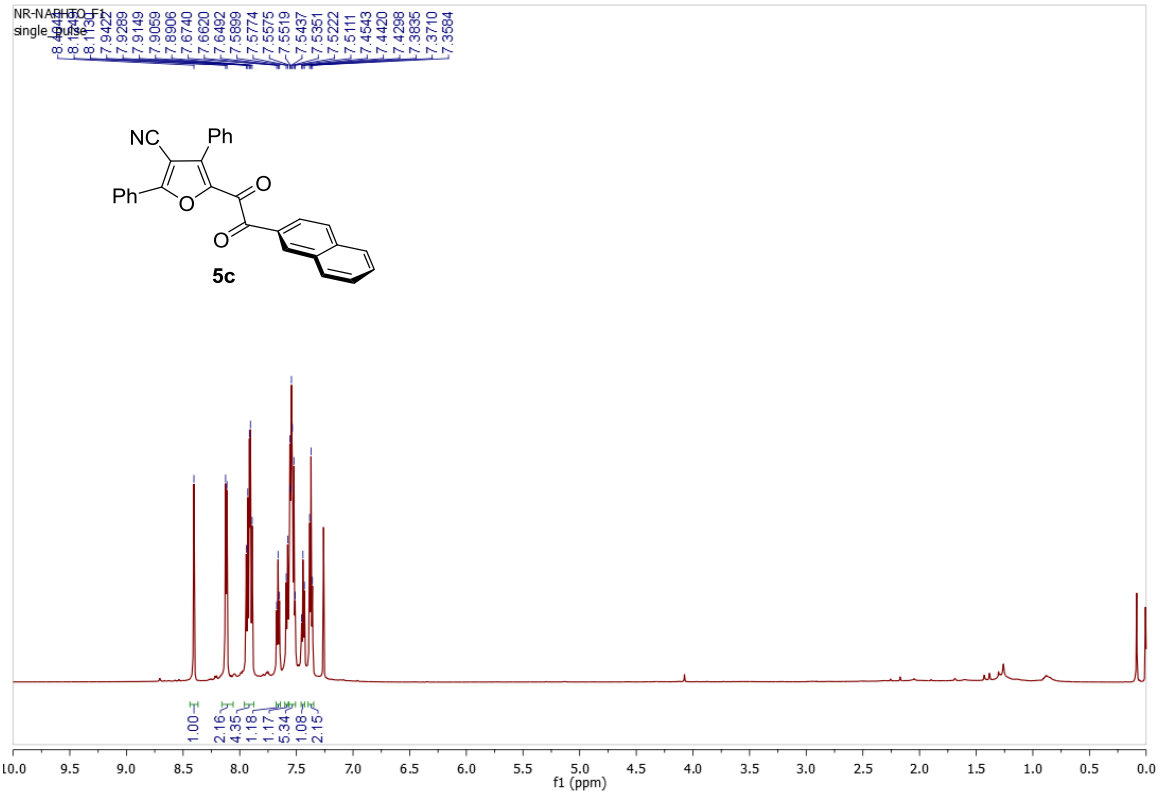

NR-14-08-19-1-f3
single pulse decoupled gated NOE
168.78
165.17
140.93
140.59
136.37
134.34
132.38
131.92
130.34
129.98
129.01
128.54
128.38
127.95
127.64
127.61
126.65
126.32
125.14
121.24
119.25
114.69
92.73
92.01
91.28
84.82
61.17
50.51
48.00
44.44
37.94
35.91
31.57
29.08
26.32
25.59
21.64
13.89
Me
H
H
H
O
Ph
O
CN
H_2N
O
O
Ph
4q (in $CDCl_3$)
f1 (ppm)

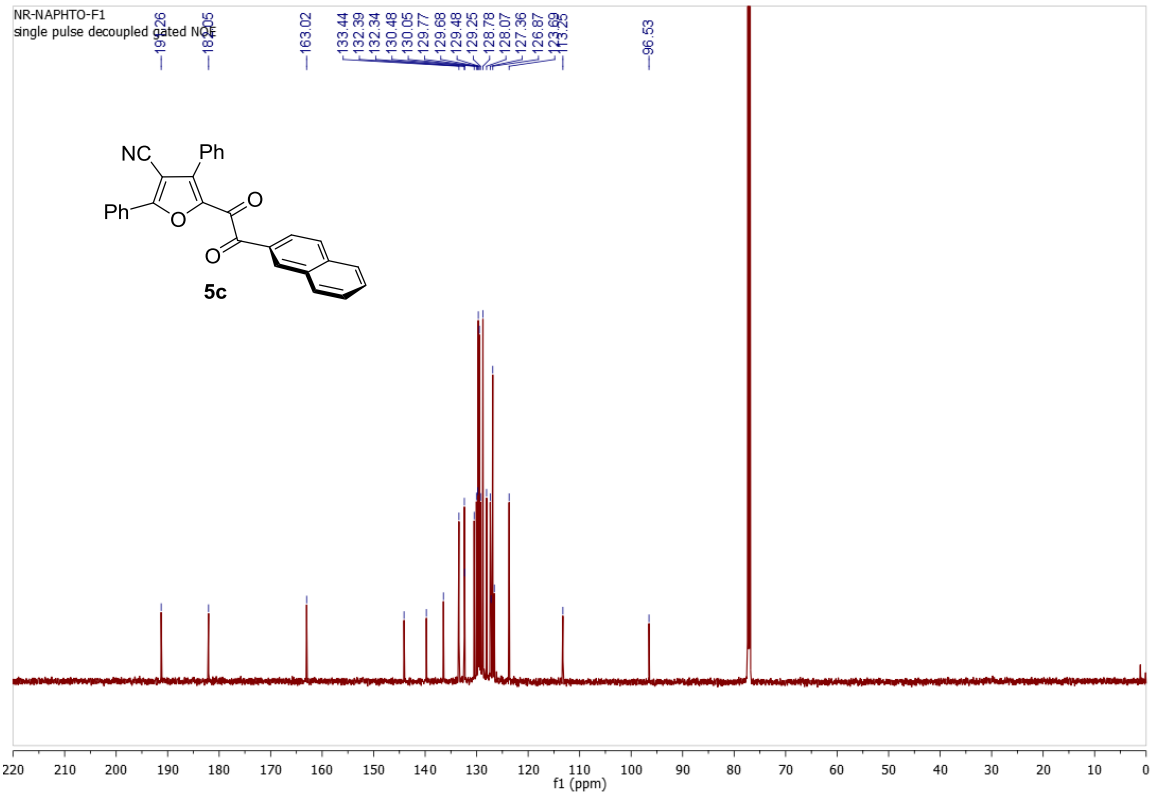

8.1155
8.0994
8.0952
7.8726
7.8540
7.6651
7.6463
7.6279
7.5702
7.5552
7.5408
7.5364
7.5344
7.5322
7.5218
7.5137
7.4979
7.4779
7.4591
7.4434
7.4257
7.3977
7.3786
7.3612
NC
Ph
Ph
O
O
Ph
5a (in CDCl3)
2.00
1.98
1.11
8.34
2.02
f1 (ppm)

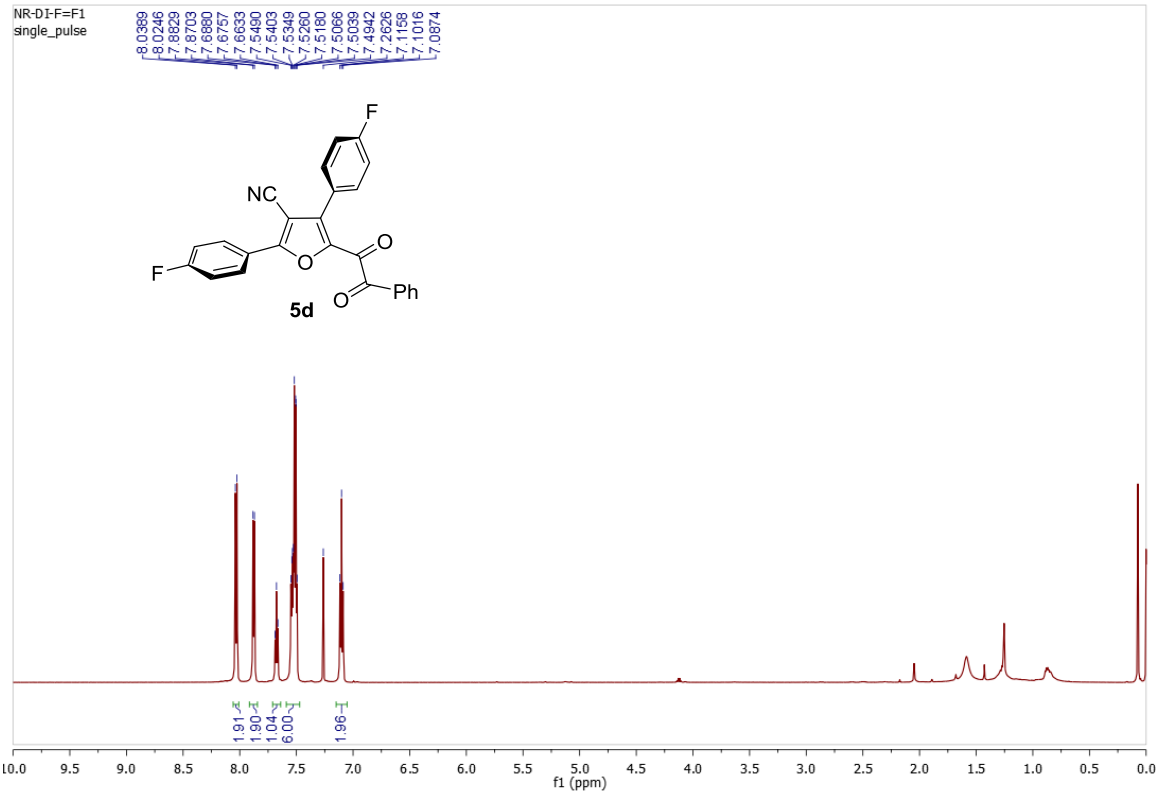

191.14
181.93
162.87
143.87
139.61
134.98
132.30
130.37
129.77
129.58
129.38
128.97
128.65
126.99
126.74
126.44
113.13
96.38
NC
Ph
Ph
O
O
Ph
5a (in CDCl3)
f1 (ppm)

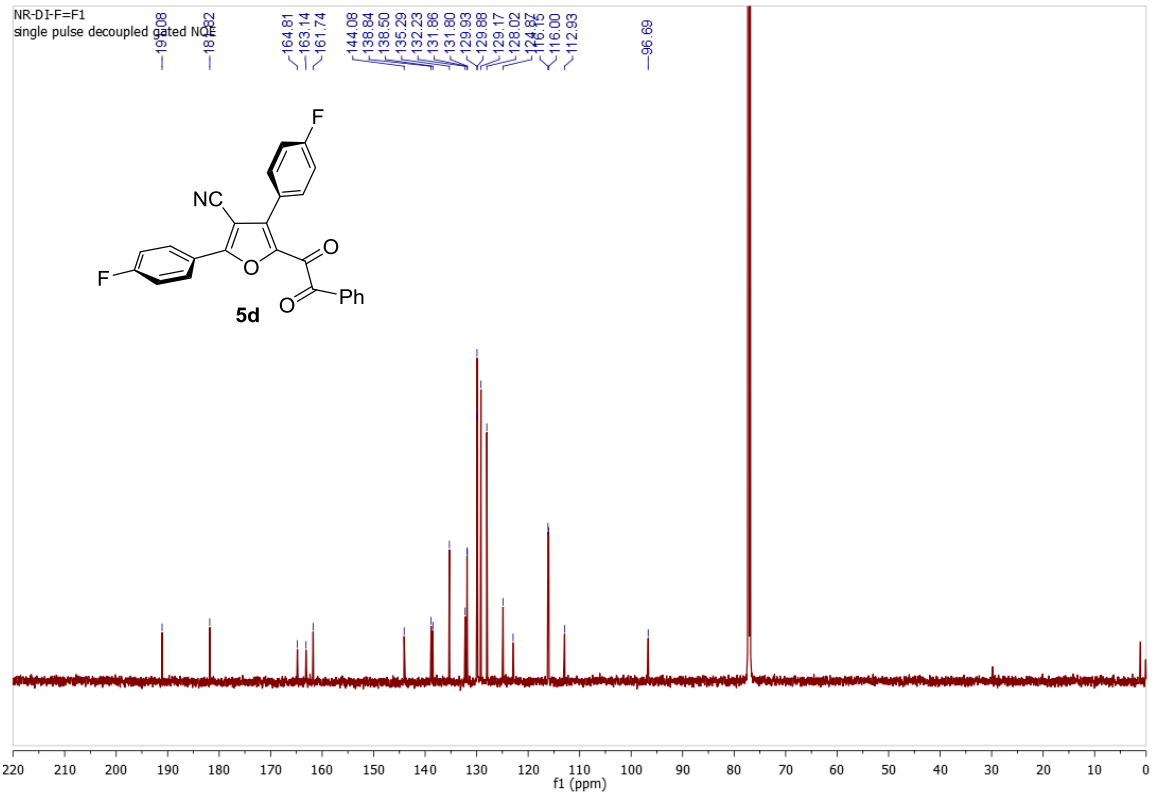

NR-4-F-F1
single pulse
8.1476
8.1331
7.8452
7.6639
7.6514
7.6410
7.6391
7.6371
7.5123
7.5084
7.5055
7.5011
7.4977
7.4937
7.4915
7.4808
7.4801
7.4676
7.4584
7.4563
7.4543
7.4471
7.4438
7.4409
7.4314
7.3886
7.3757
7.3661
7.3635
F
NC
O
O
O
Ph
5b
1.92
1.89
1.00
6.80
1.93
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

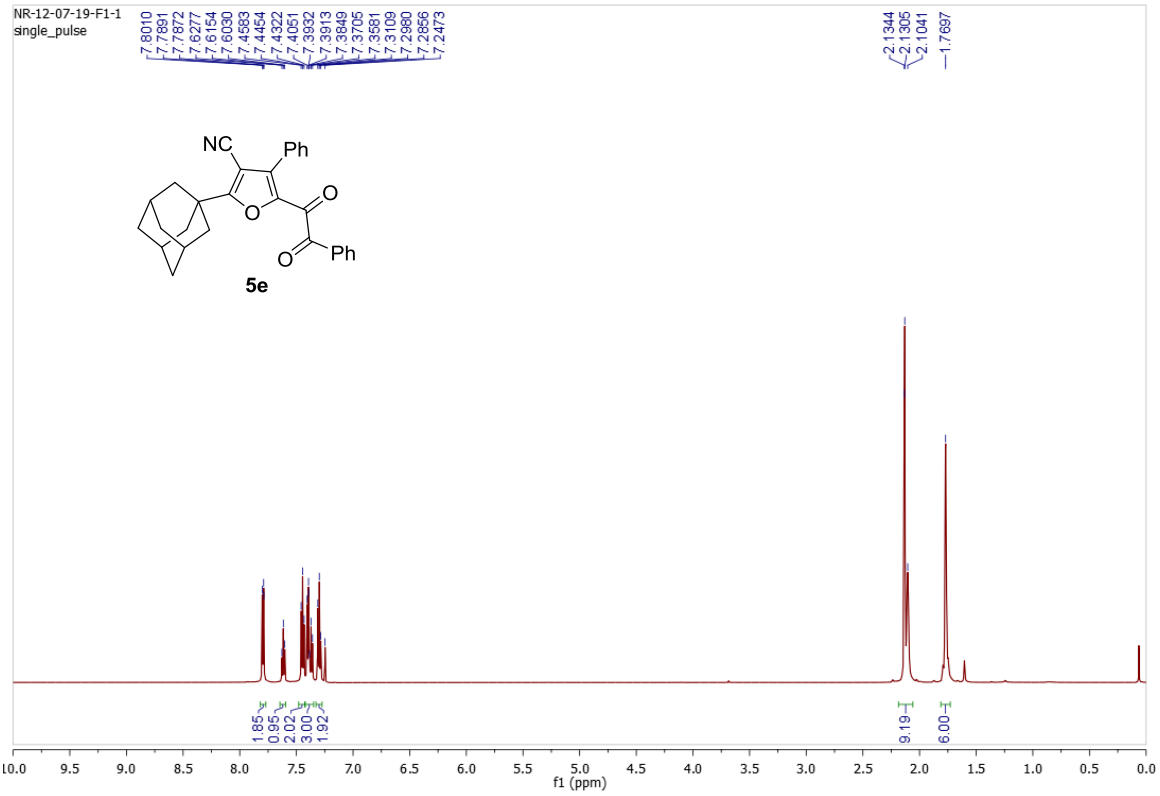

NR-4-F-F1
single pulse decoupled gated NOE
190.06
178.39
161.69
144.12
139.64
138.70
135.13
132.35
130.55
129.88
129.66
129.09
128.79
128.04
126.93
125.01
113.02
96.77
F
NC
O
O
O
Ph
5b
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

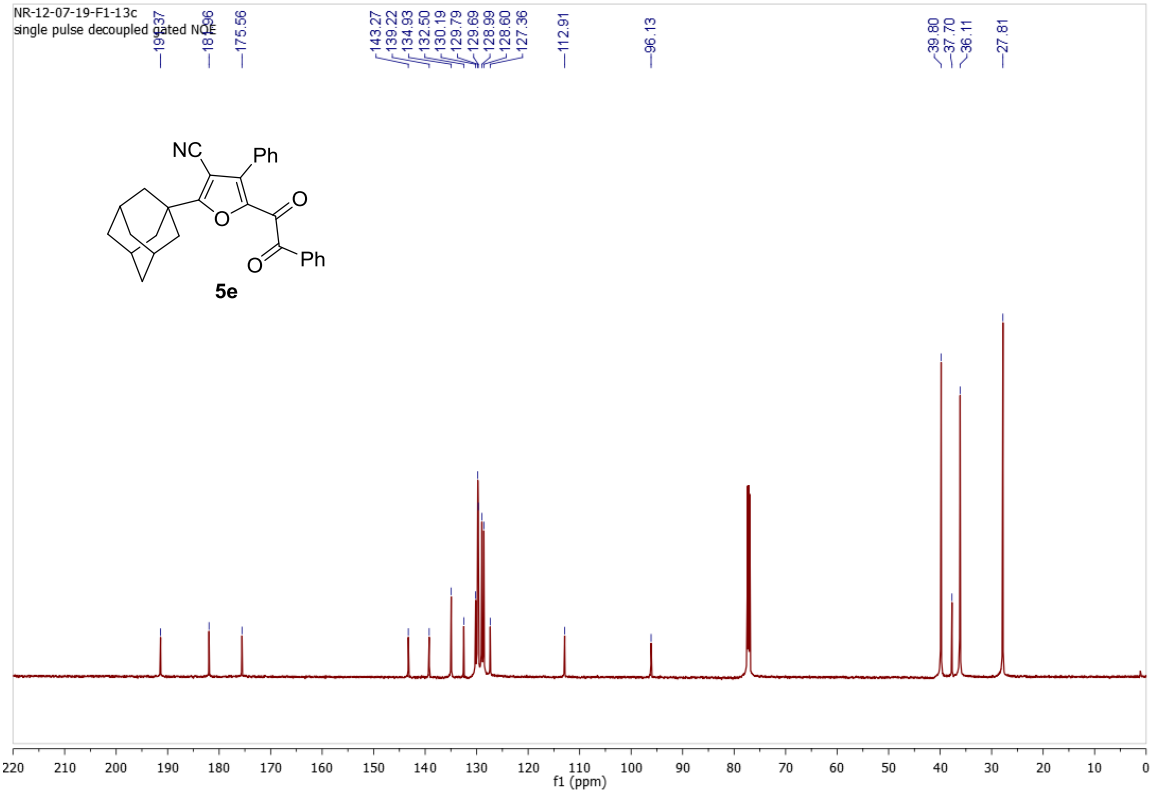

NR-NAPHTO-F1
single_pulse
NC
Ph
Ph
O
O
O
5c
1.00
2.16
4.35
1.17
1.18
5.34
1.08
2.15
f1 (ppm)

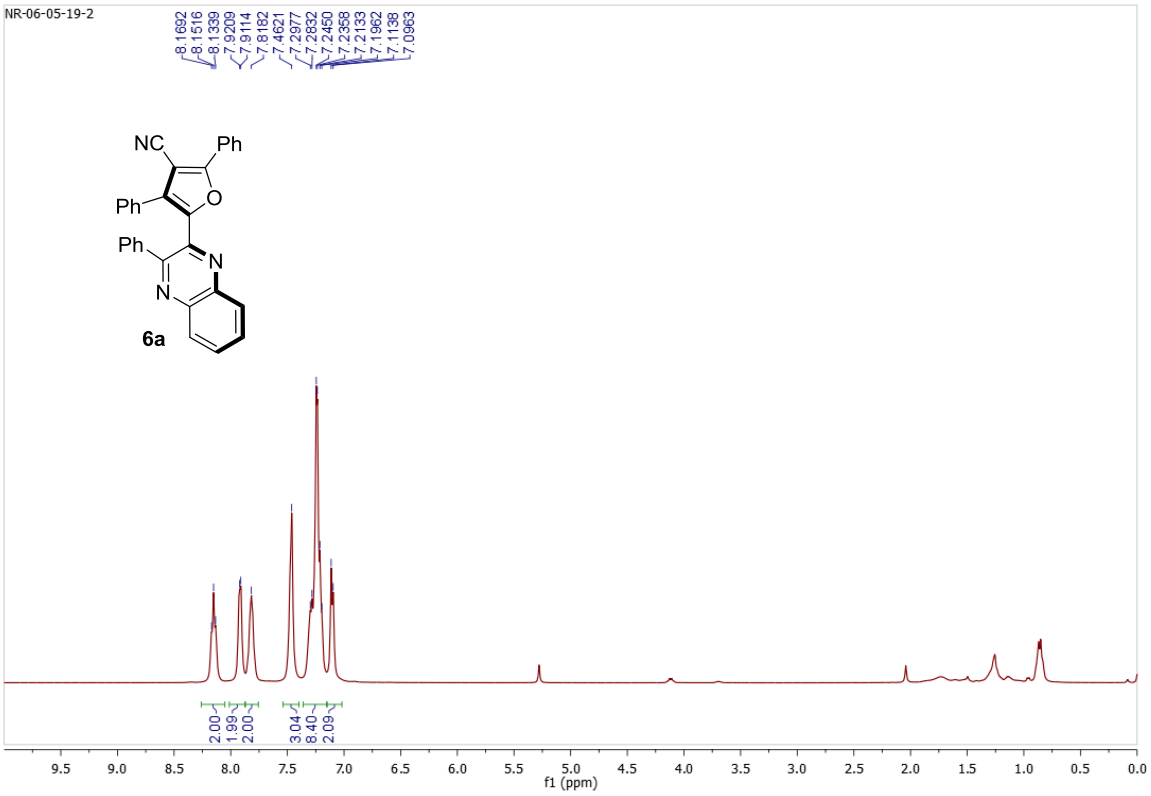

NR-NAPHTO-F1
single pulse decoupled gated NOE
163.02
133.44
132.39
132.34
130.48
130.05
129.77
129.68
129.48
129.25
128.78
128.07
127.36
126.87
96.53
NC
Ph
Ph
O
O
O
5c
f1 (ppm)

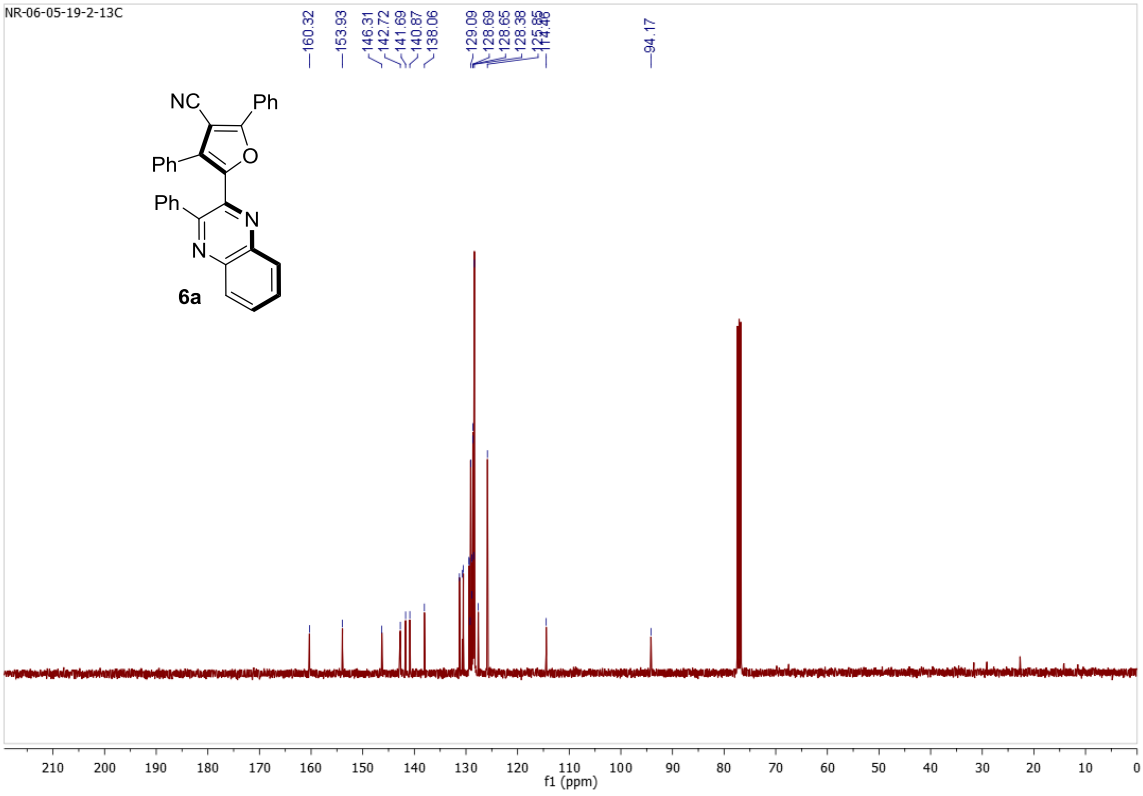

NR-DI-F=F1
single_pulse
8.0389
8.0246
7.8829
7.8703
7.6880
7.6757
7.6633
7.5490
7.5403
7.5349
7.5260
7.5160
7.5066
7.5039
7.4942
7.2626
7.1158
7.1016
7.0874
F
NC
O
F
O
O
Ph
5d
1.91
1.90
1.04
6.00
1.96
f1 (ppm)

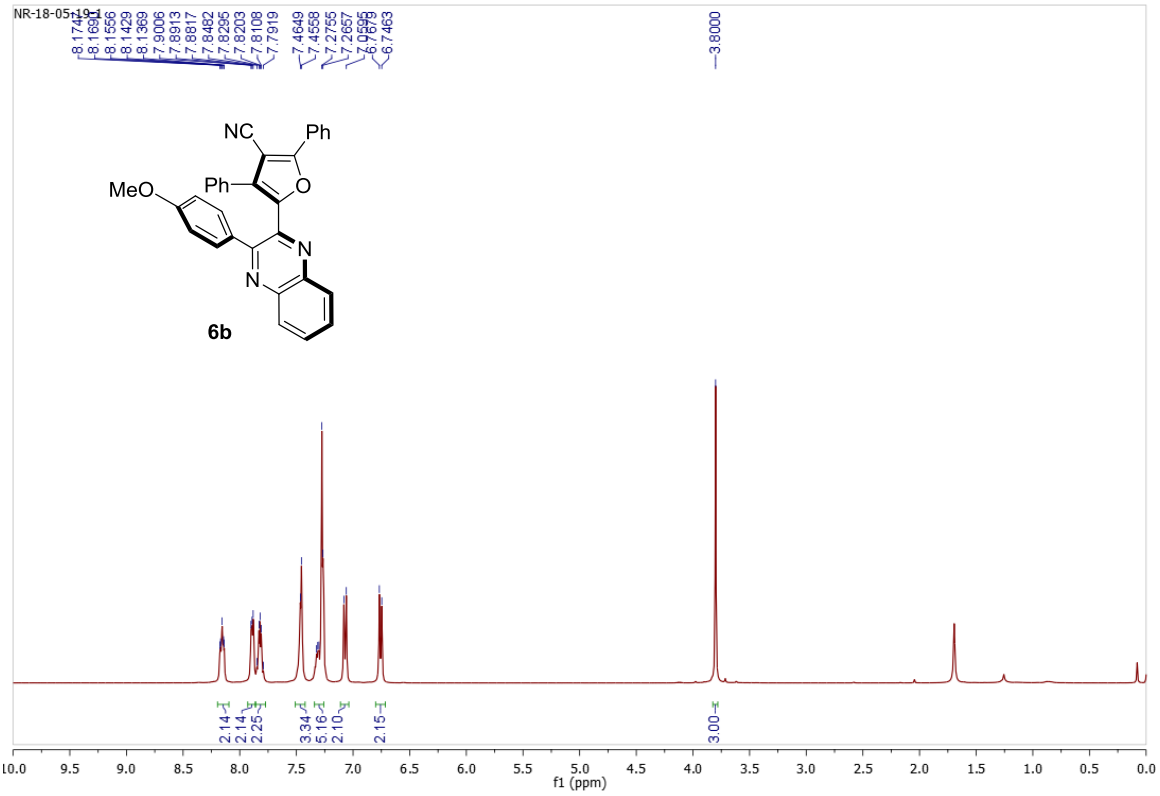

NR-DI-F=F1
single pulse decoupled gated NOE
164.81
163.14
161.74
144.08
138.84
138.50
135.29
132.23
131.86
131.80
129.93
129.88
129.17
128.02
116.00
112.93
96.69
F
NC
O
F
O
O
Ph
5d
f1 (ppm)

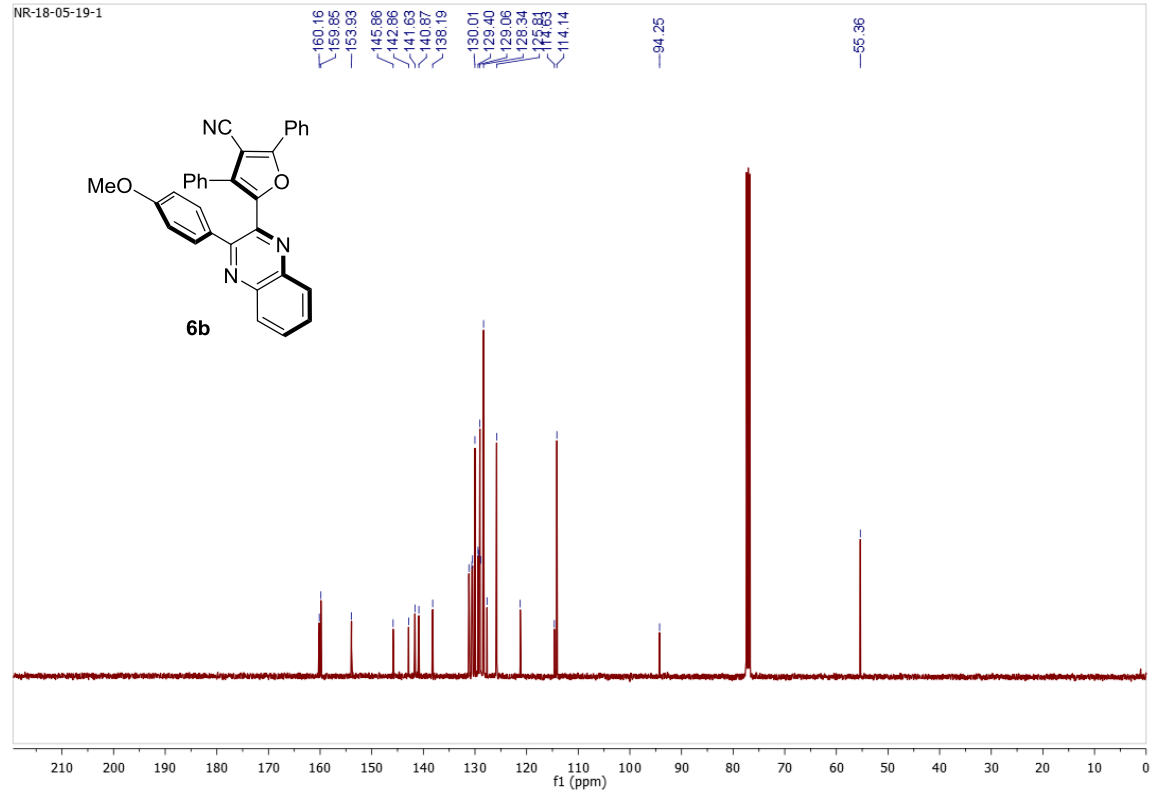

NR-12-07-19-F1-1
single_pulse
7.8010
7.7891
7.7872
7.6277
7.6154
7.6030
7.4583
7.4454
7.4322
7.4051
7.3932
7.3913
7.3848
7.3705
7.3581
7.3109
7.2980
7.2856
7.2473
2.1344
2.1305
2.1041
1.7697
NC
Ph
O
O
O
Ph
5e
1.85
0.95
2.02
3.00
1.92
9.19
6.00
f1 (ppm)

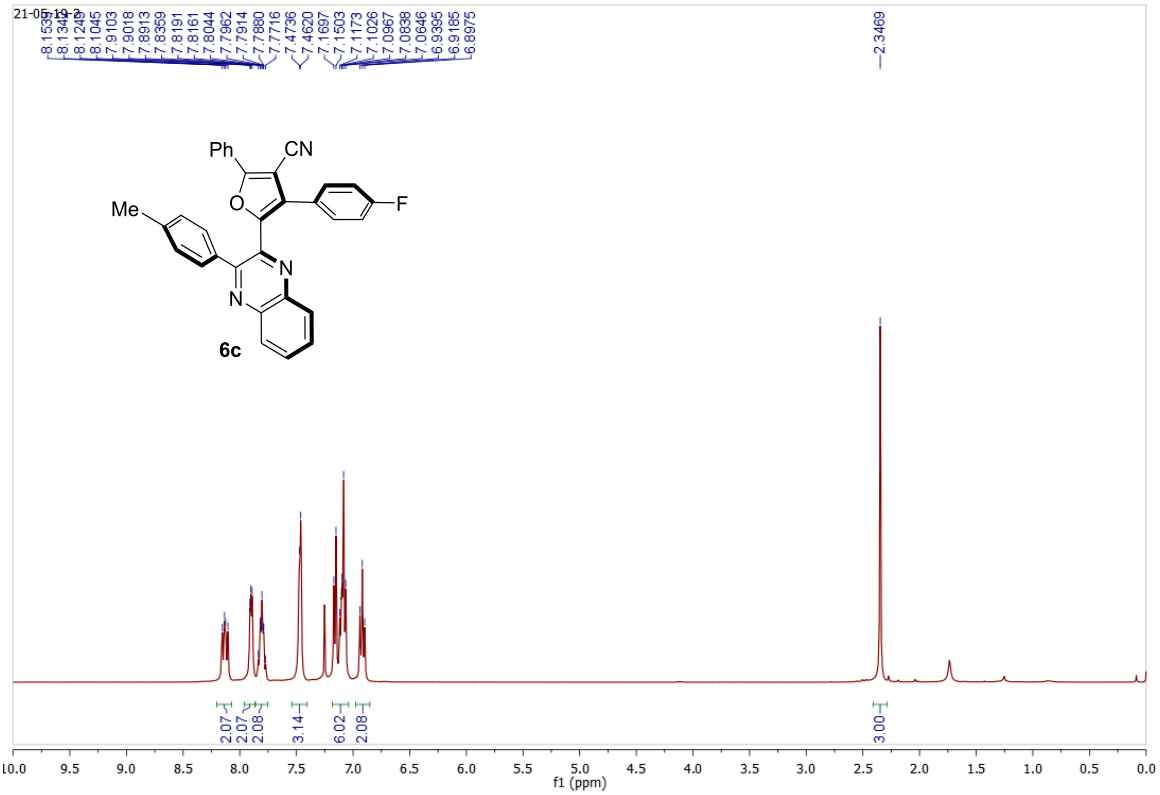

NR-12-07-19-F1-13c
single pulse decoupled gated NOE
175.56
143.27
139.22
134.93
132.50
130.19
129.79
129.69
128.99
128.60
127.36
112.91
96.13
39.80
37.70
36.11
27.81
NC
Ph
O
O
O
Ph
5e
f1 (ppm)

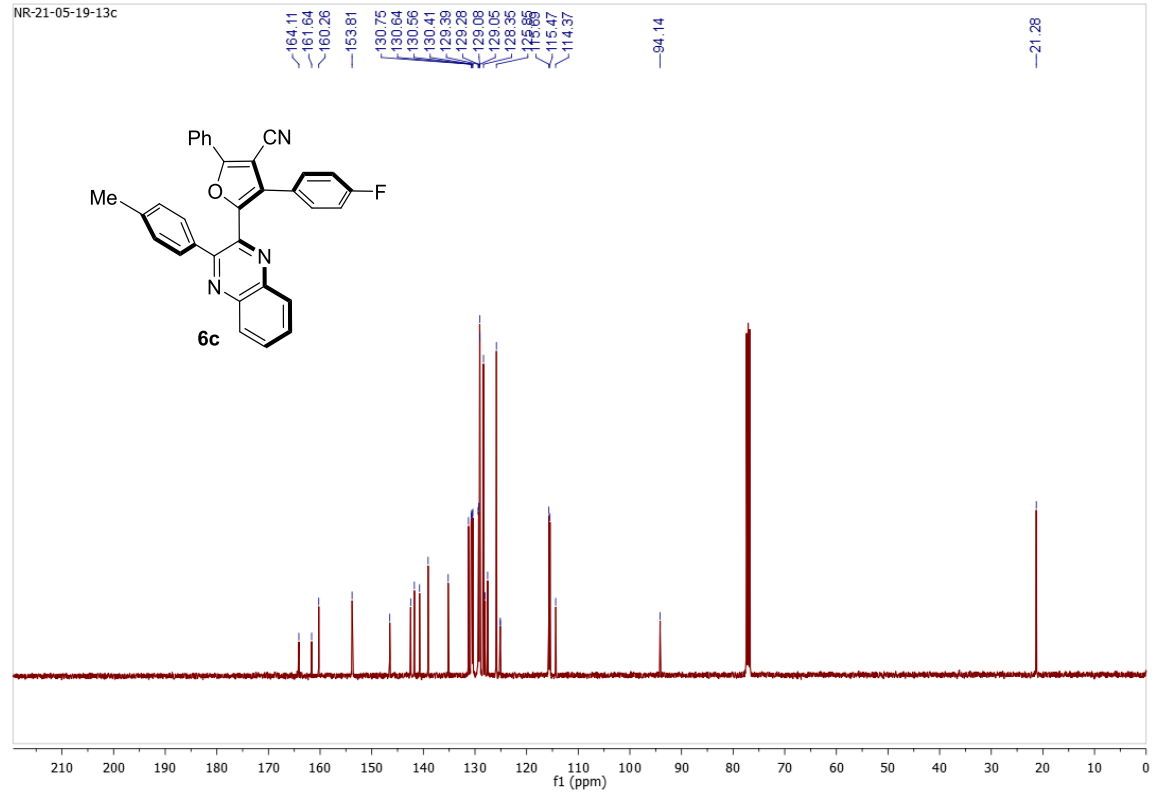

NR-06-05-19-2
8.1692
8.1516
8.1339
7.9209
7.9114
7.8182
7.4621
7.2977
7.2832
7.2450
7.2358
7.2133
7.1962
7.1138
7.0963
NC
Ph
Ph
O
Ph
N
N
6a
2.00
1.99
2.00
3.04
8.40
2.09
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

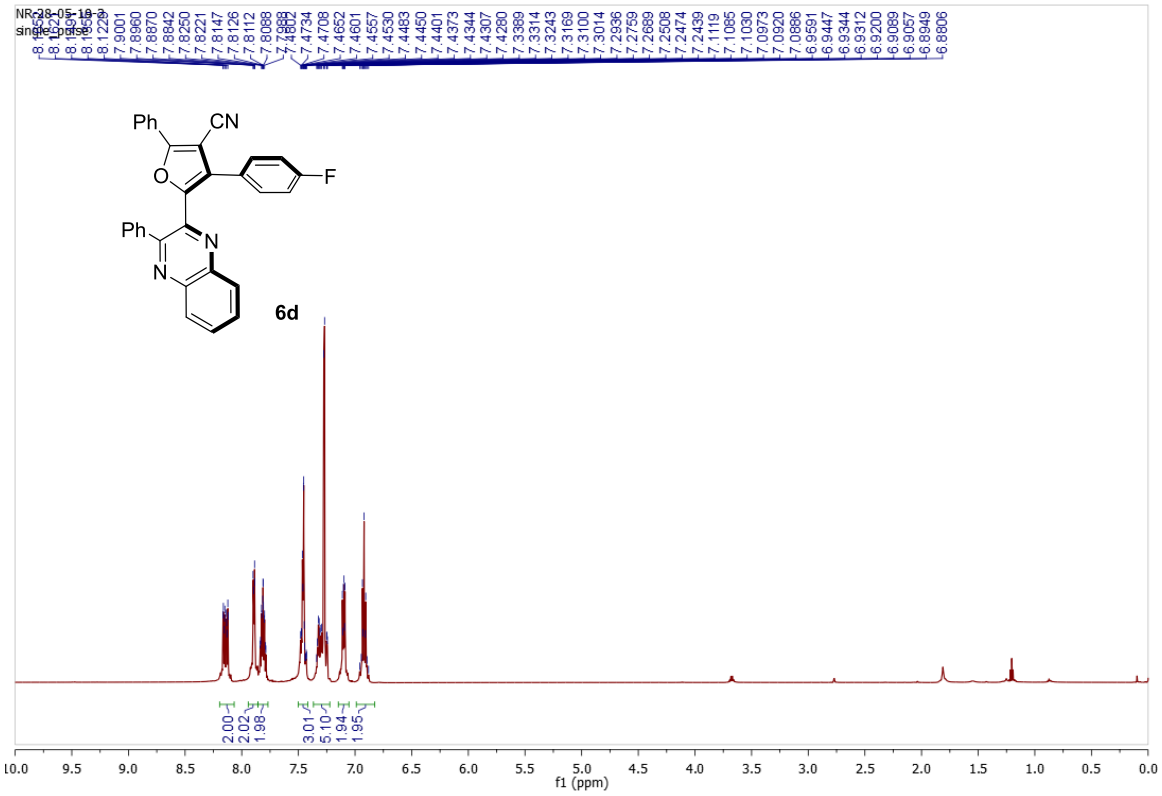

NR-06-05-19-2-13C
160.32
153.93
146.31
142.72
141.69
140.87
138.06
129.09
128.69
128.65
128.38
94.17
NC
Ph
Ph
O
Ph
N
N
6a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

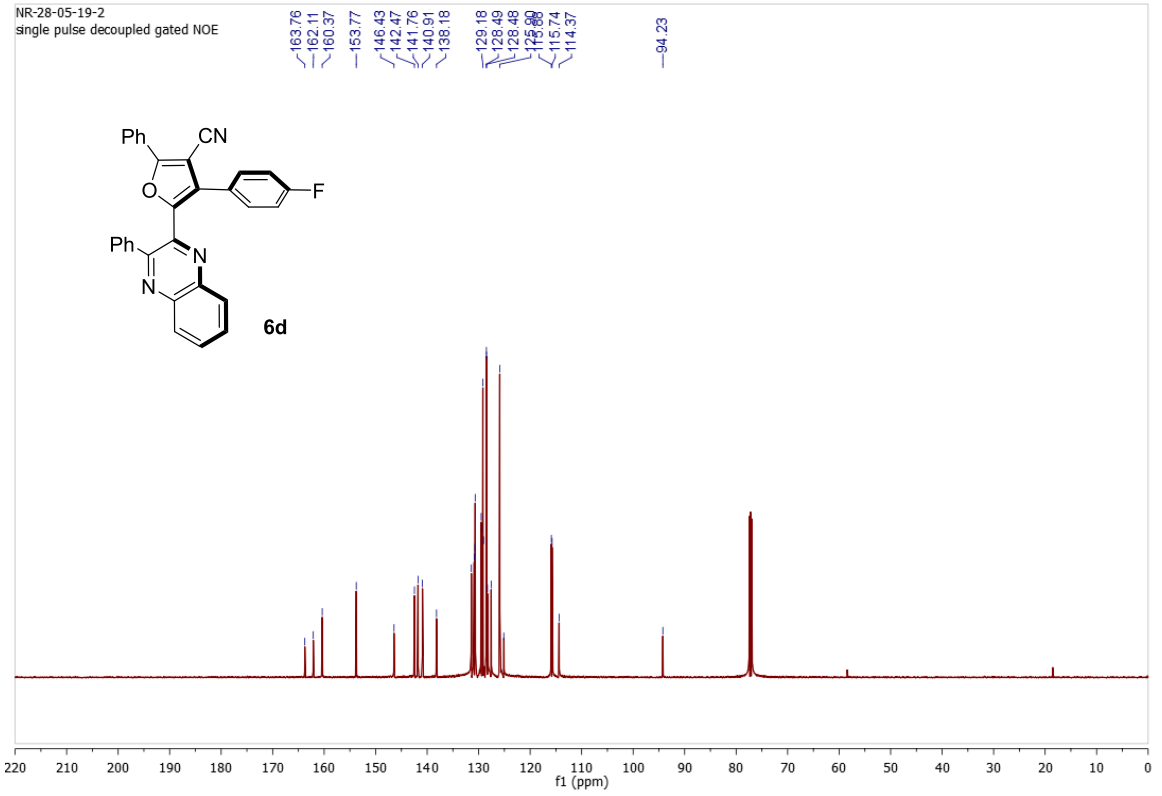

NR-18-05-19-1
8.1744
8.1691
8.1556
8.1429
8.1369
7.9006
7.8913
7.8817
7.8482
7.8295
7.8203
7.8108
7.7919
7.4649
7.4558
7.2755
7.2657
6.7463
3.8000
NC
Ph
Ph
O
MeO
N
N
6b
2.14
2.14
2.25
3.34
5.16
2.10
2.15
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

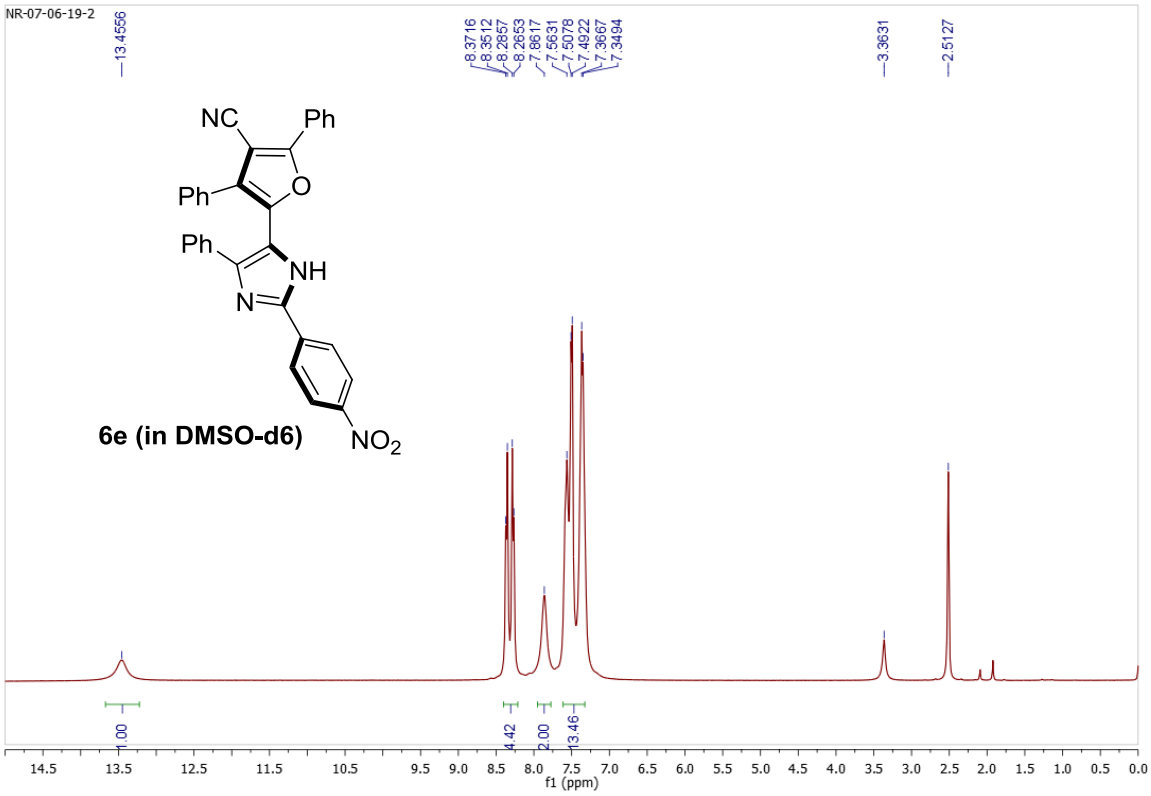

NR-18-05-19-1
160.16
159.85
153.93
145.86
142.86
141.63
140.87
138.19
130.01
129.40
129.06
128.34
114.14
94.25
55.36
NC
Ph
Ph
O
MeO
N
N
6b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

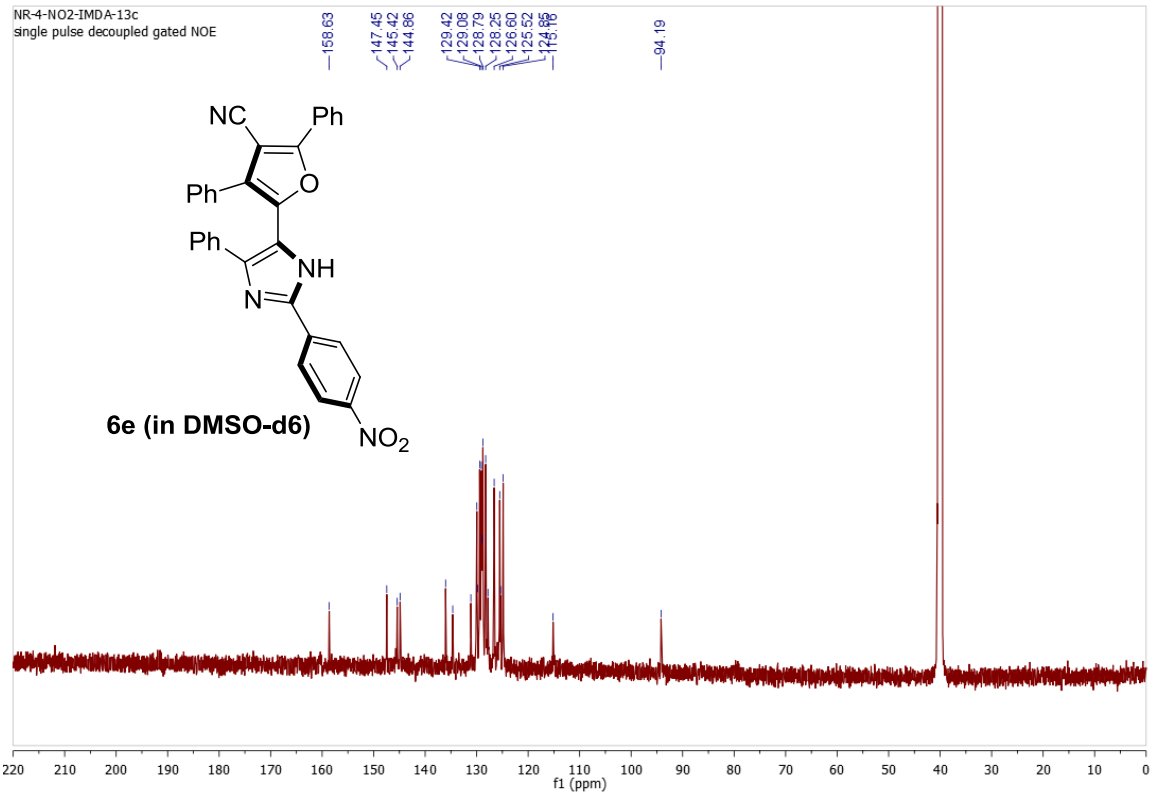

21-05-19-2
8.1539
8.1342
8.1249
8.1045
7.9103
7.9018
7.8913
7.8359
7.8191
7.8161
7.8044
7.7962
7.7914
7.7880
7.7716
7.4736
7.4620
7.1697
7.1503
7.1173
7.1026
7.0967
7.0838
7.0646
6.9395
6.9185
6.8975
2.3469
Ph
CN
O
F
Me
N
N
6c
2.07
2.07
2.08
3.14
6.02
2.08
3.00
f1 (ppm)

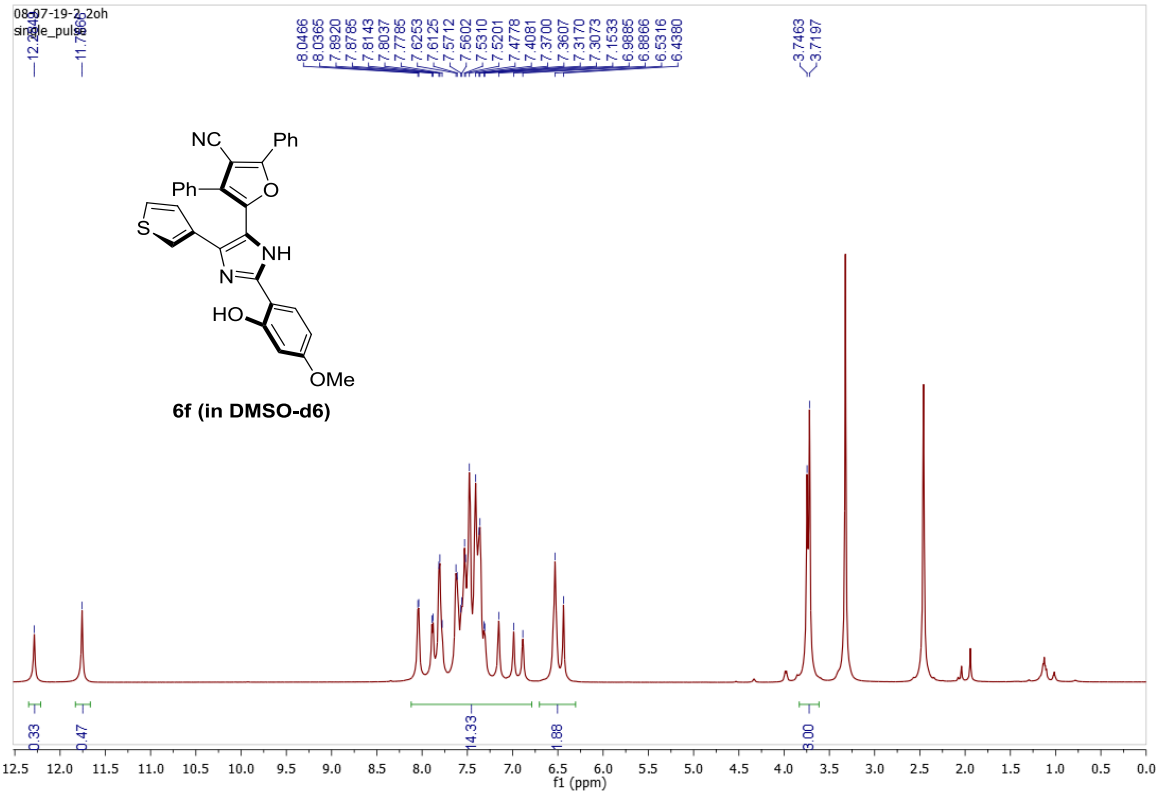

NR-21-05-19-13c
164.11
161.64
160.26
153.81
130.75
130.64
130.56
130.41
129.39
129.28
129.08
129.05
128.35
115.47
114.37
94.14
21.28
Ph
CN
O
F
Me
N
N
6c
f1 (ppm)

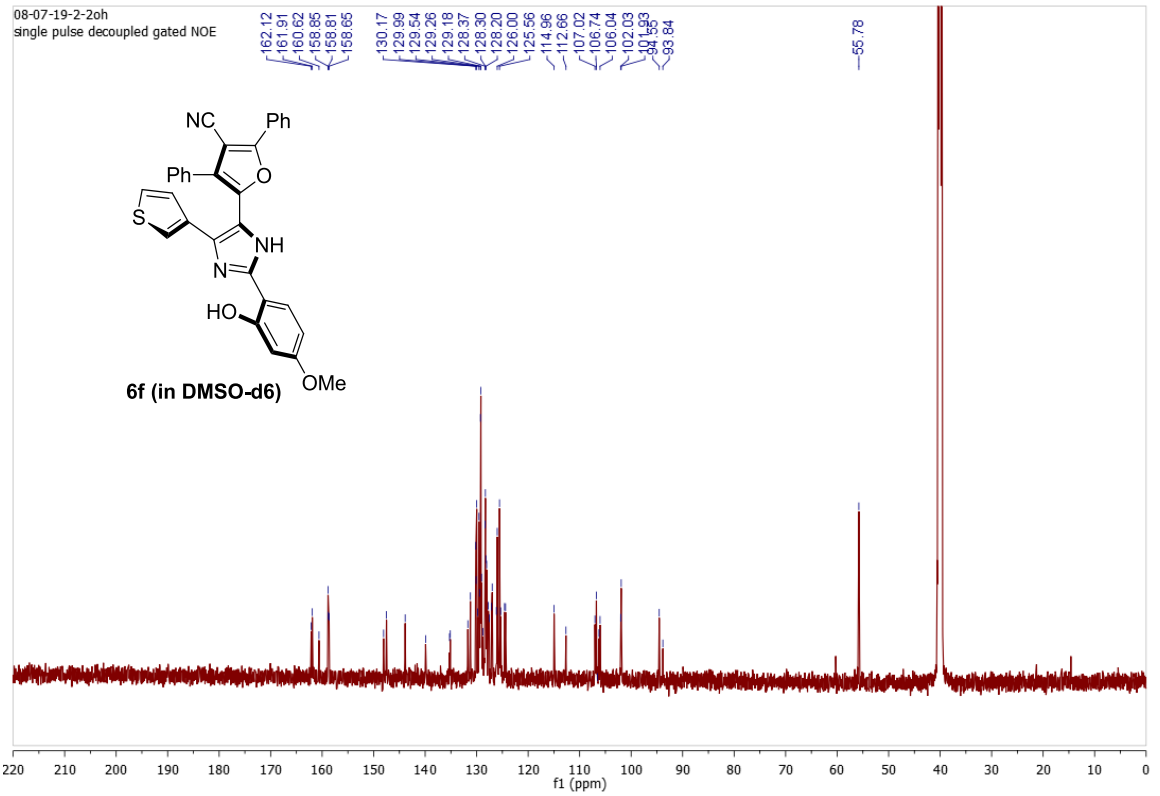

NR-28-05-19-3
single pulse
Ph
CN
O
F
Ph
N
N
6d
2.00
2.02
1.98
3.01
5.10
1.94
1.95
f1 (ppm)

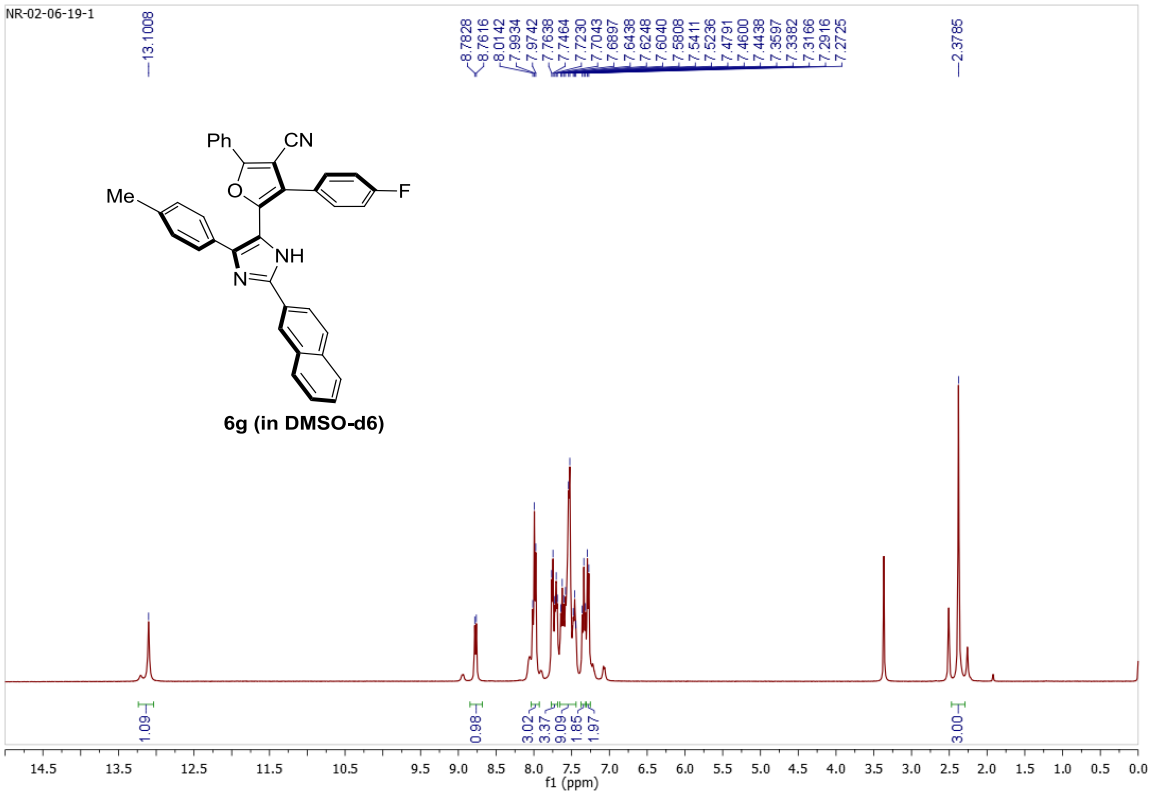

NR-28-05-19-2
single pulse decoupled gated NOE
163.76
162.11
160.37
153.77
146.43
142.47
141.76
140.91
138.18
129.18
128.49
128.48
115.74
114.37
94.23
Ph
CN
O
F
Ph
N
N
6d
f1 (ppm)


NR-07-06-19-2
13.4556
8.3716
8.3512
8.2857
8.2653
7.8617
7.5631
7.5078
7.4922
7.3667
7.3494
3.3631
2.5127
NC
Ph
Ph
O
Ph
NH
N
NO2
6e (in DMSO-d6)
1.00
4.42
2.00
13.46
f1 (ppm)

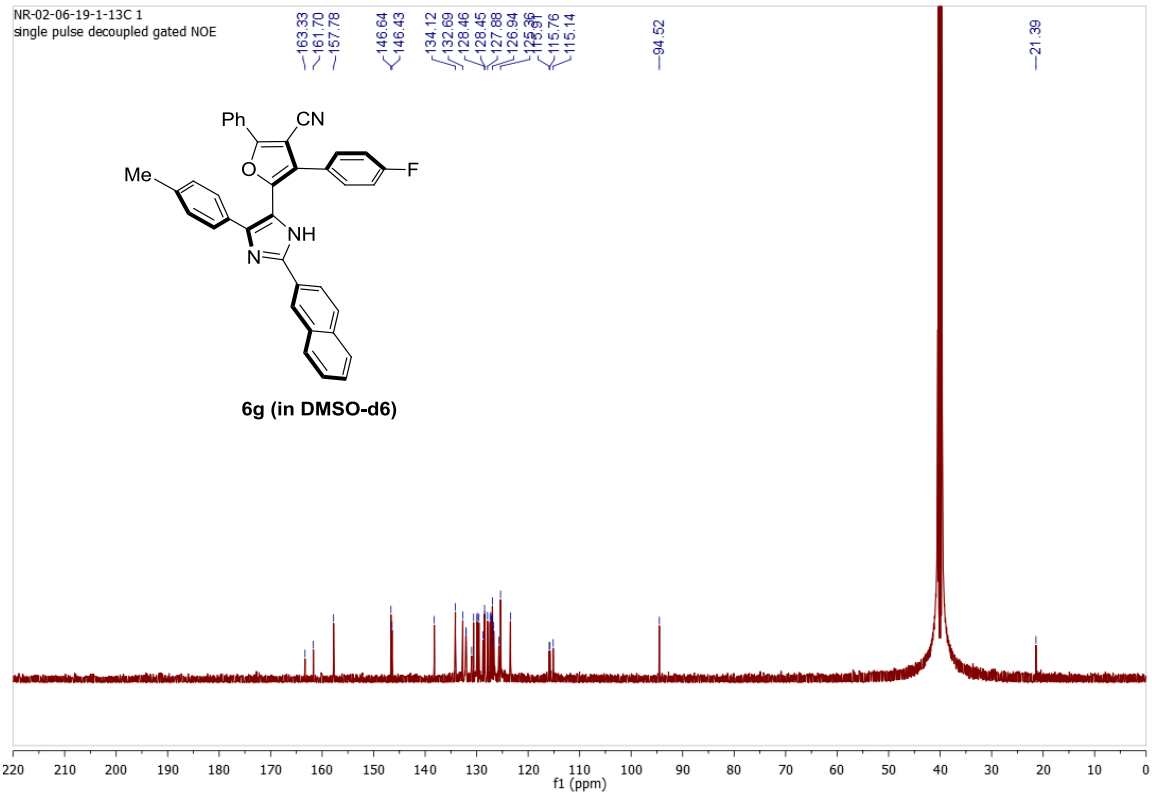

NR-4-NO2-IMDA-13c
single pulse decoupled gated NOE
158.63
147.45
145.42
144.86
129.42
129.08
128.79
128.25
126.60
125.52
94.19
NC
Ph
Ph
O
Ph
NH
N
NO2
6e (in DMSO-d6)
f1 (ppm)


08-07-19-2-2oh
single_pulse
12.44
11.76
8.0466
8.0365
7.8920
7.8785
7.8143
7.8037
7.7785
7.6253
7.6125
7.5712
7.5602
7.5310
7.5201
7.4778
7.4081
7.3700
7.3607
7.3170
7.3073
7.1533
6.9885
6.8866
6.5316
6.4380
3.7463
3.7197
NC
Ph
Ph
O
S
NH
N
HO
OMe
6f (in DMSO-d6)
0.33
0.47
14.33
1.88
3.00
f1 (ppm)

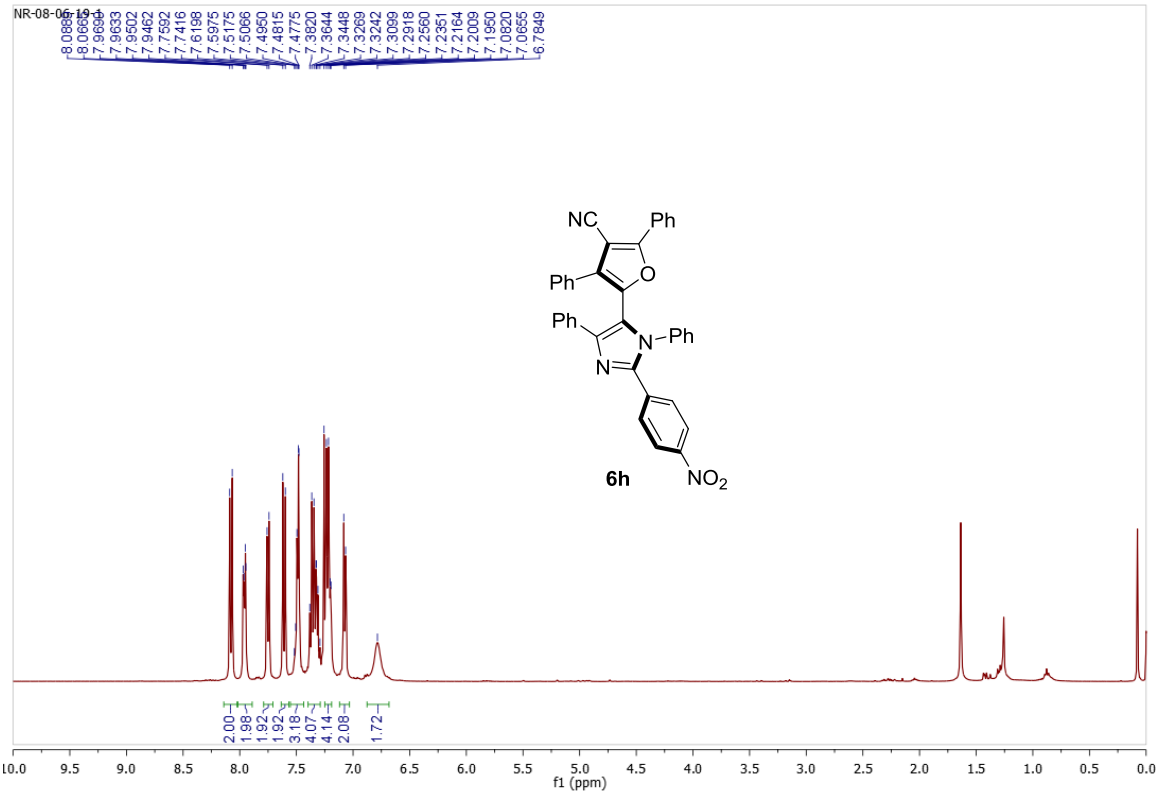

08-07-19-2-2oh
single pulse decoupled gated NOE
162.12
161.91
160.62
158.85
158.81
158.65
130.17
129.99
129.54
129.26
129.18
128.37
128.30
128.20
126.00
125.56
114.96
112.66
107.02
106.74
106.04
102.03
93.84
55.78
NC
Ph
Ph
O
S
NH
N
HO
OMe
6f (in DMSO-d6)
f1 (ppm)

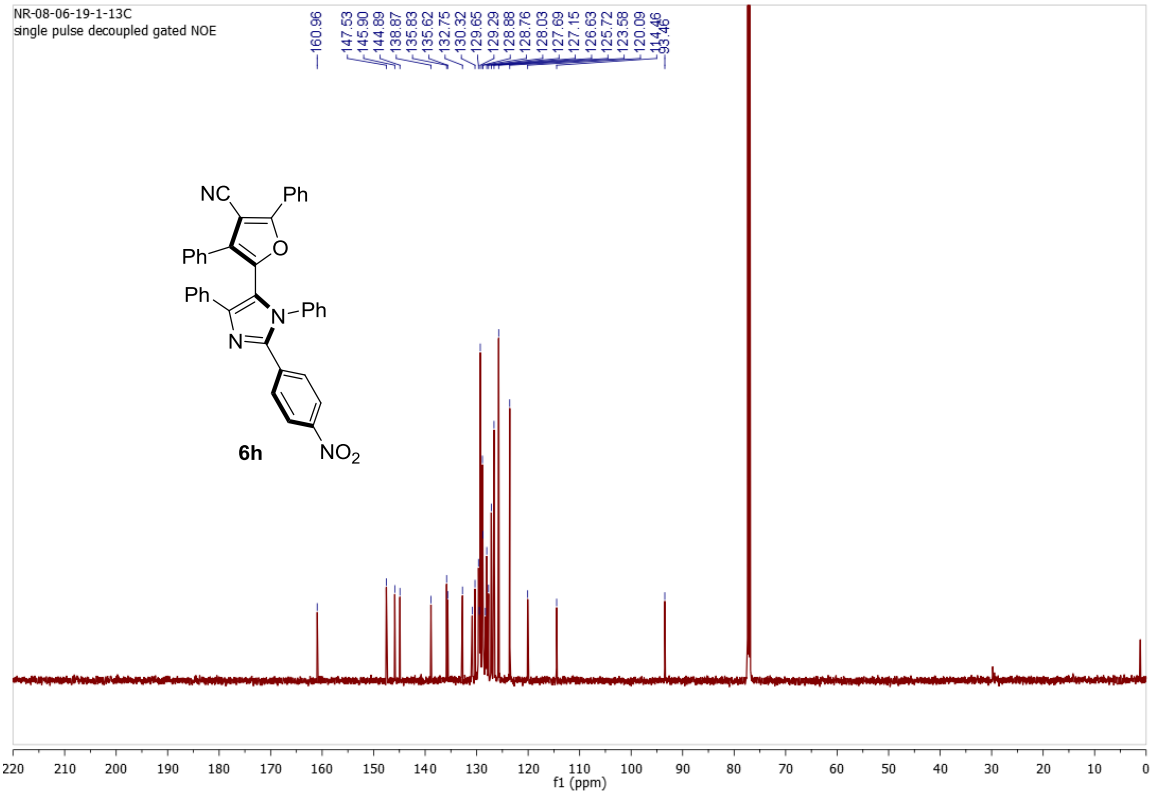


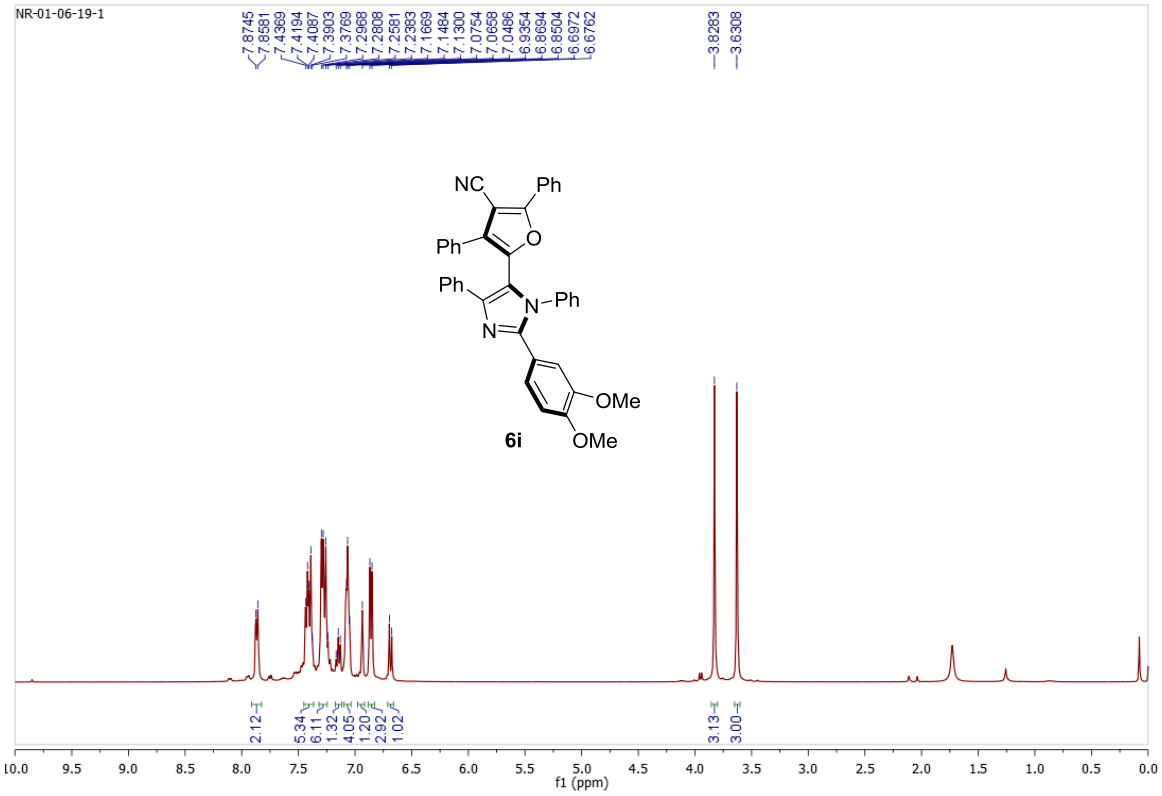
6g (in DMSO-d6)

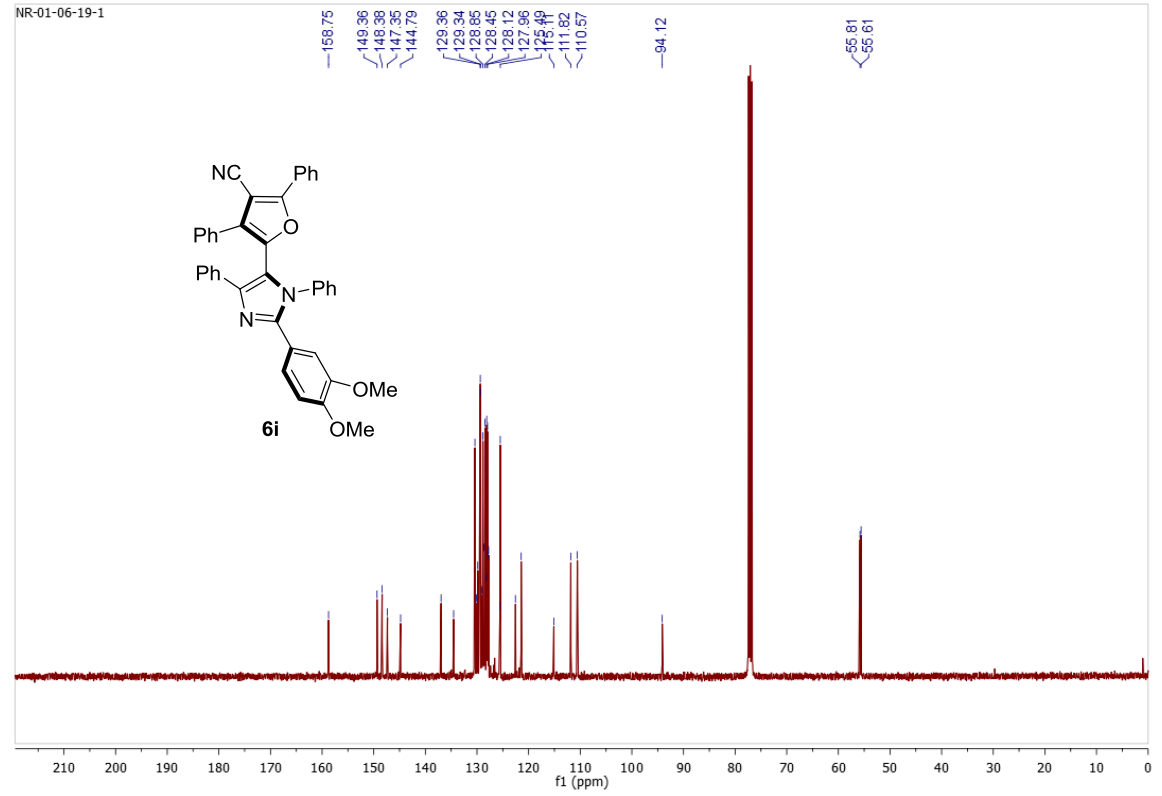


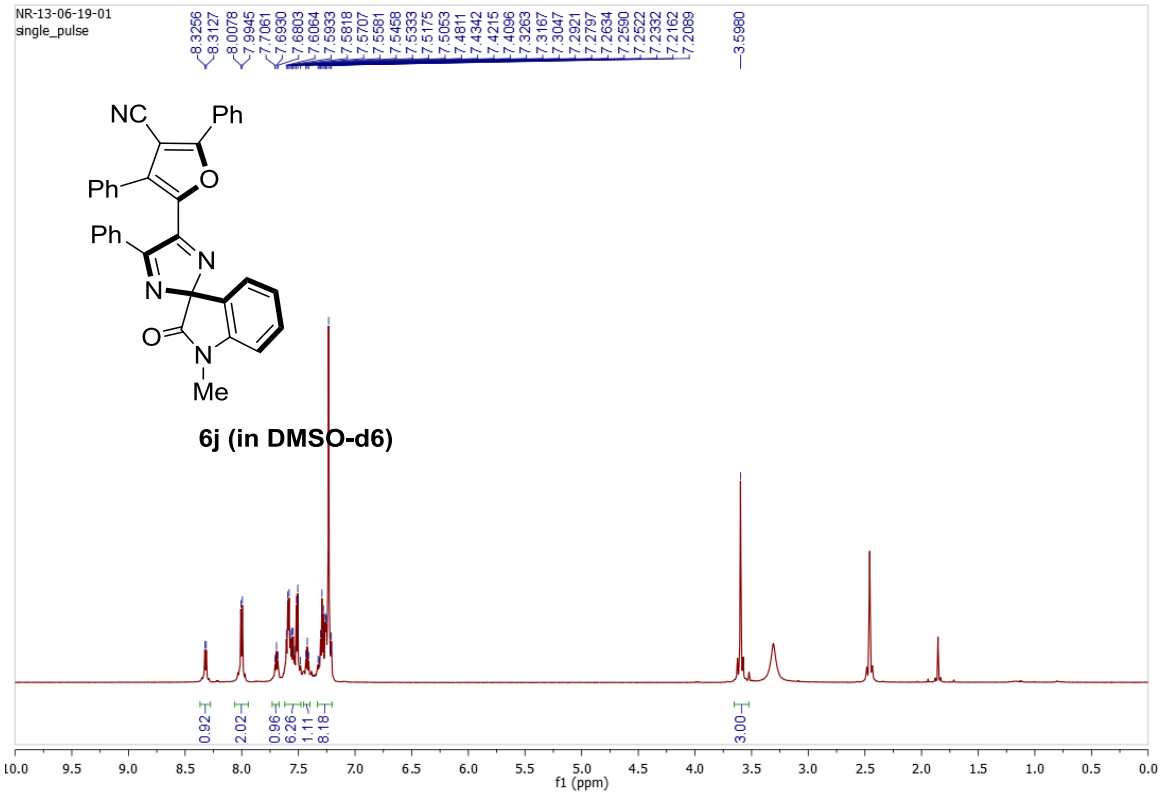
6g (in DMSO-d6)

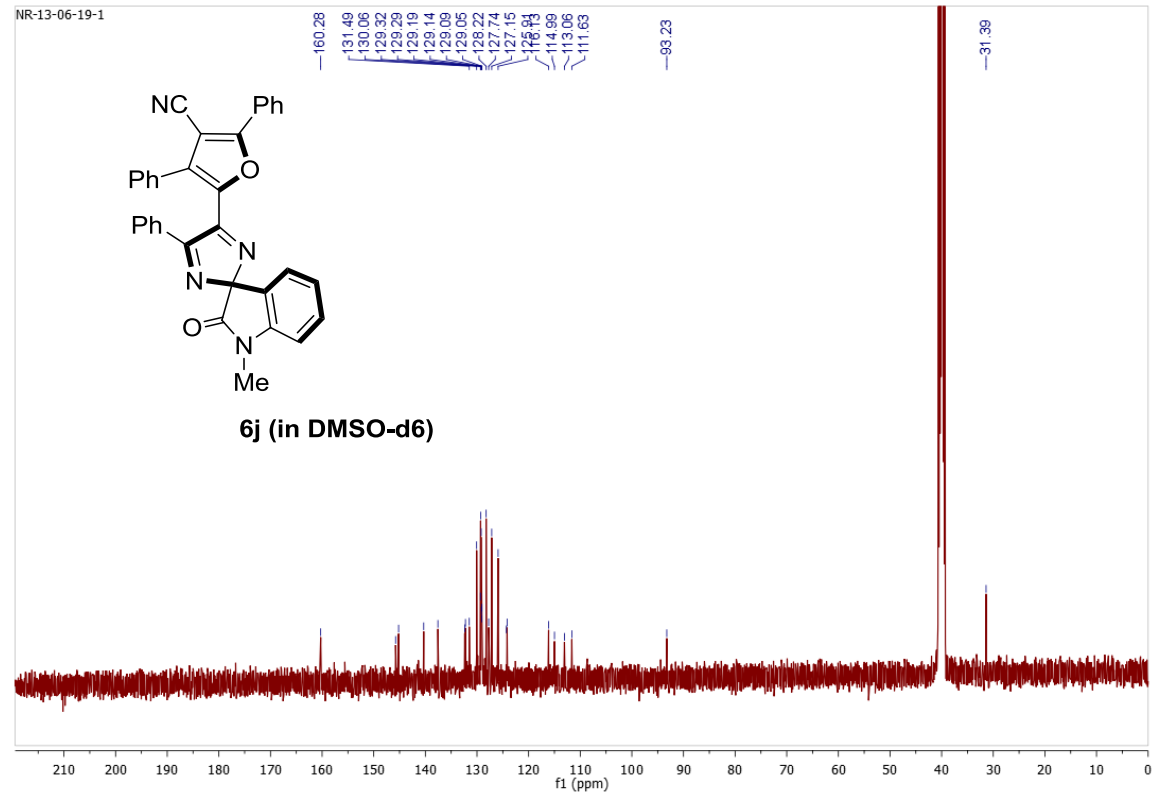

NR-08-06-19-1
8.0885
8.0665
7.9699
7.9633
7.9502
7.9462
7.7592
7.7416
7.6198
7.5975
7.5175
7.5066
7.4950
7.4815
7.4775
7.3820
7.3644
7.3448
7.3269
7.3242
7.3099
7.2918
7.2560
7.2351
7.2164
7.2009
7.1950
7.0820
7.0655
6.7849
NC
Ph
Ph
O
Ph
N
Ph
N
6h
NO2
2.00
1.98
1.92
1.92
3.18
4.07
4.14
2.08
1.72
f1 (ppm)

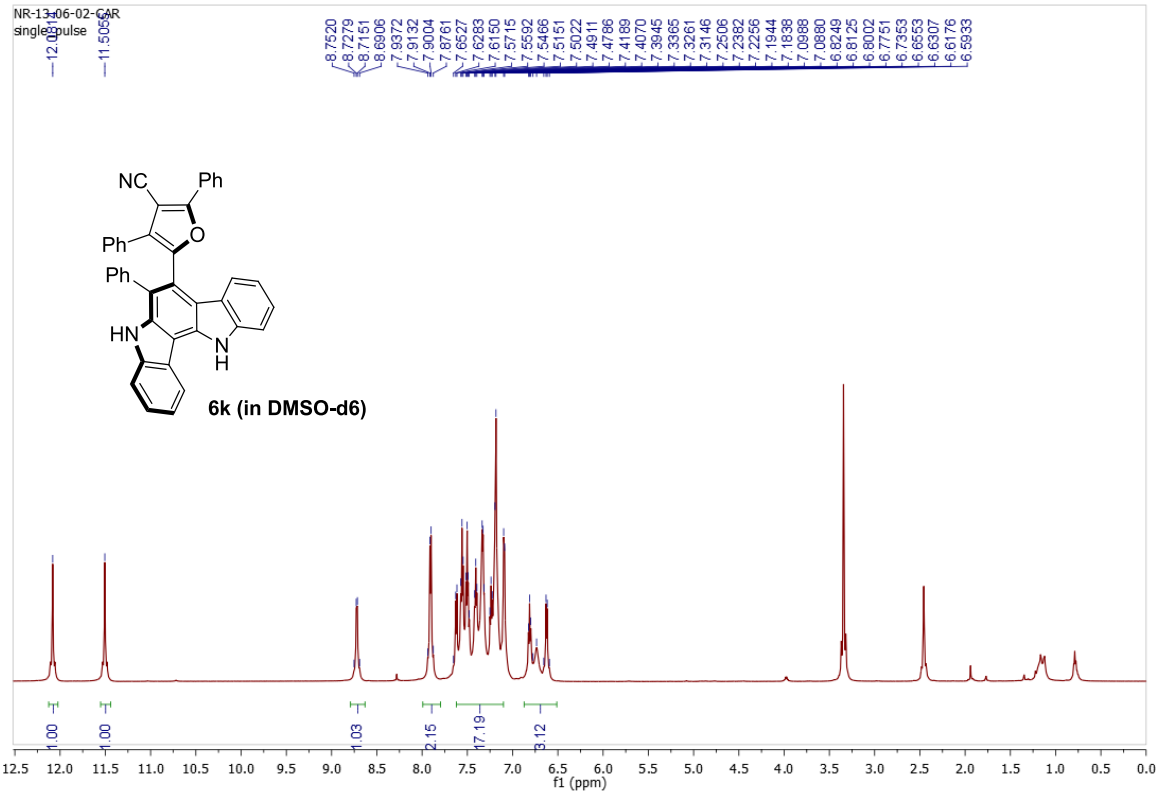

NR-08-06-19-1-13C
single pulse decoupled gated NOE
160.96
147.53
145.90
144.89
138.87
135.83
135.62
132.75
130.32
129.65
129.29
128.88
128.76
128.03
127.69
127.15
126.63
125.72
123.58
120.09
114.46
93.46
NC
Ph
Ph
O
Ph
N
Ph
N
6h
NO2
f1 (ppm)

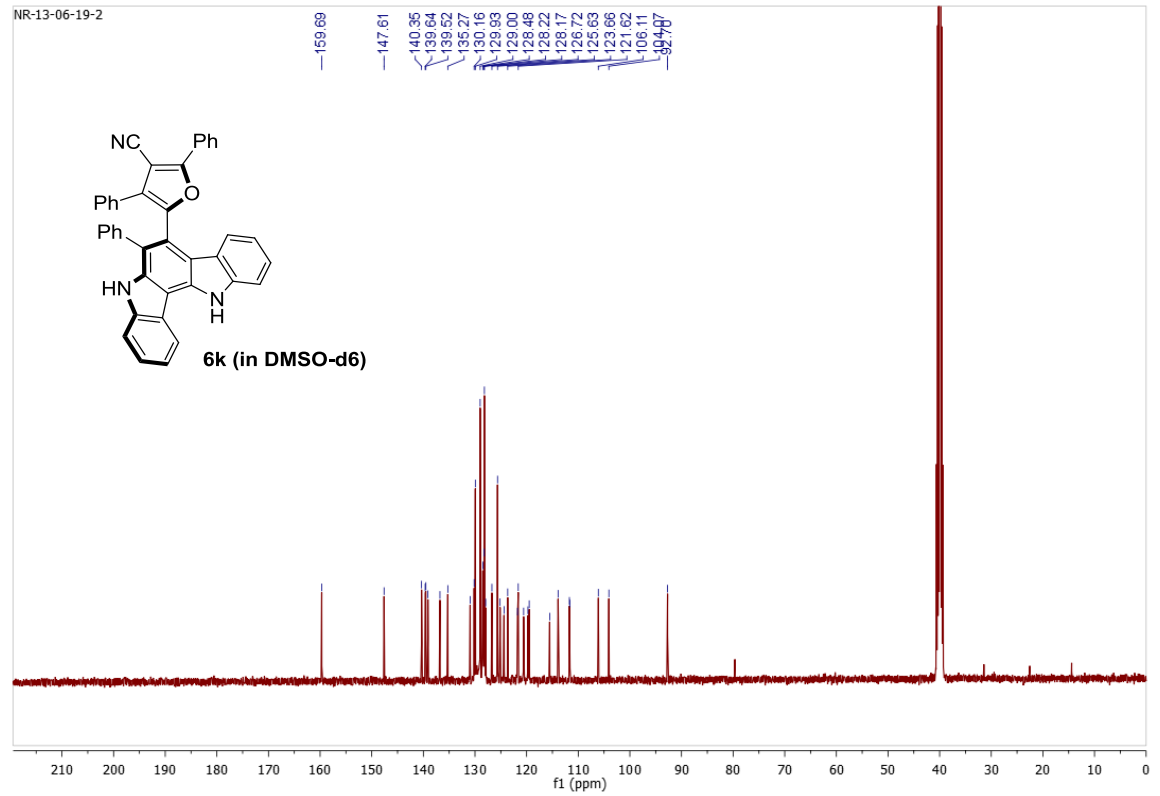

NR-01-06-19-1
7.8745
7.8581
7.4369
7.4194
7.4087
7.3903
7.3769
7.2968
7.2808
7.2581
7.2383
7.1669
7.1484
7.1300
7.0754
7.0658
7.0486
6.9354
6.8694
6.8504
6.6972
6.6762
3.8283
3.6308
NC
Ph
Ph
O
Ph
N
Ph
N
OMe
OMe
6i
2.12
5.34
6.11
1.32
4.05
1.20
2.92
1.02
3.13
3.00
f1 (ppm)

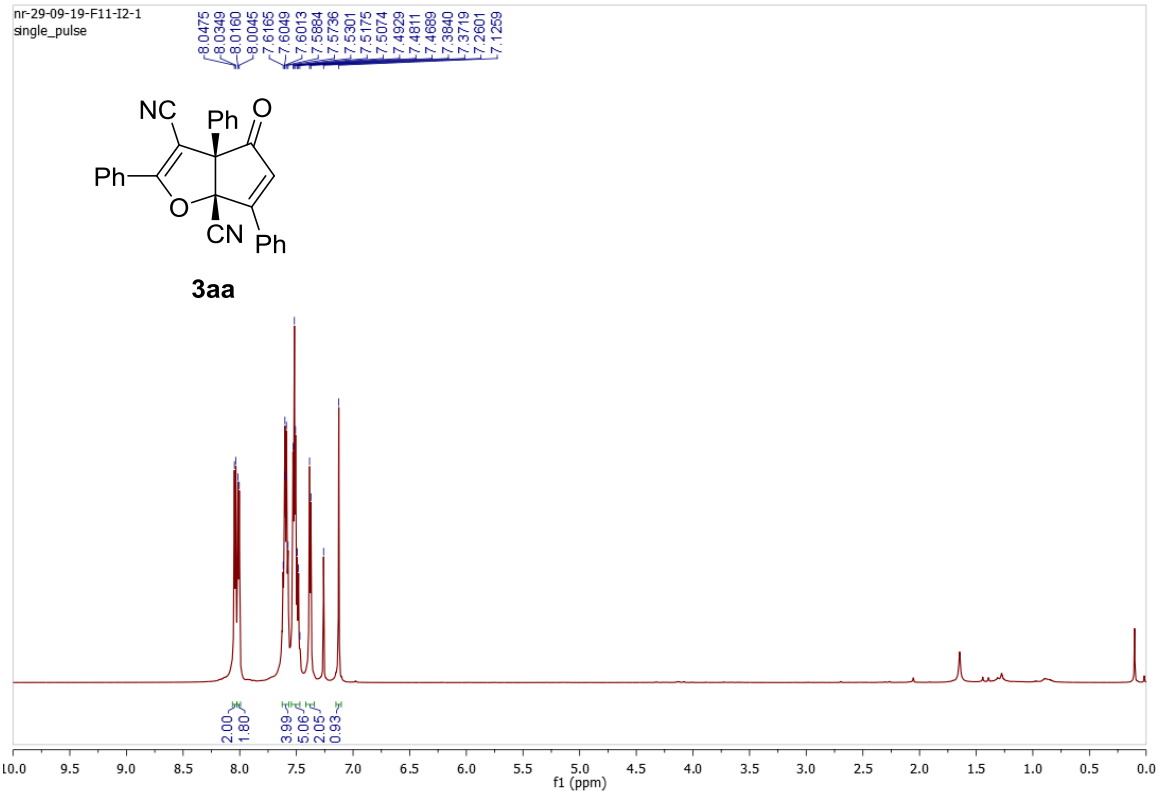

NR-01-06-19-1
158.75
149.36
148.38
147.35
144.79
129.36
129.34
128.85
128.45
128.12
127.96
125.49
115.11
111.82
110.57
94.12
55.81
55.61
NC
Ph
Ph
O
Ph
N
Ph
N
OMe
OMe
6i
f1 (ppm)

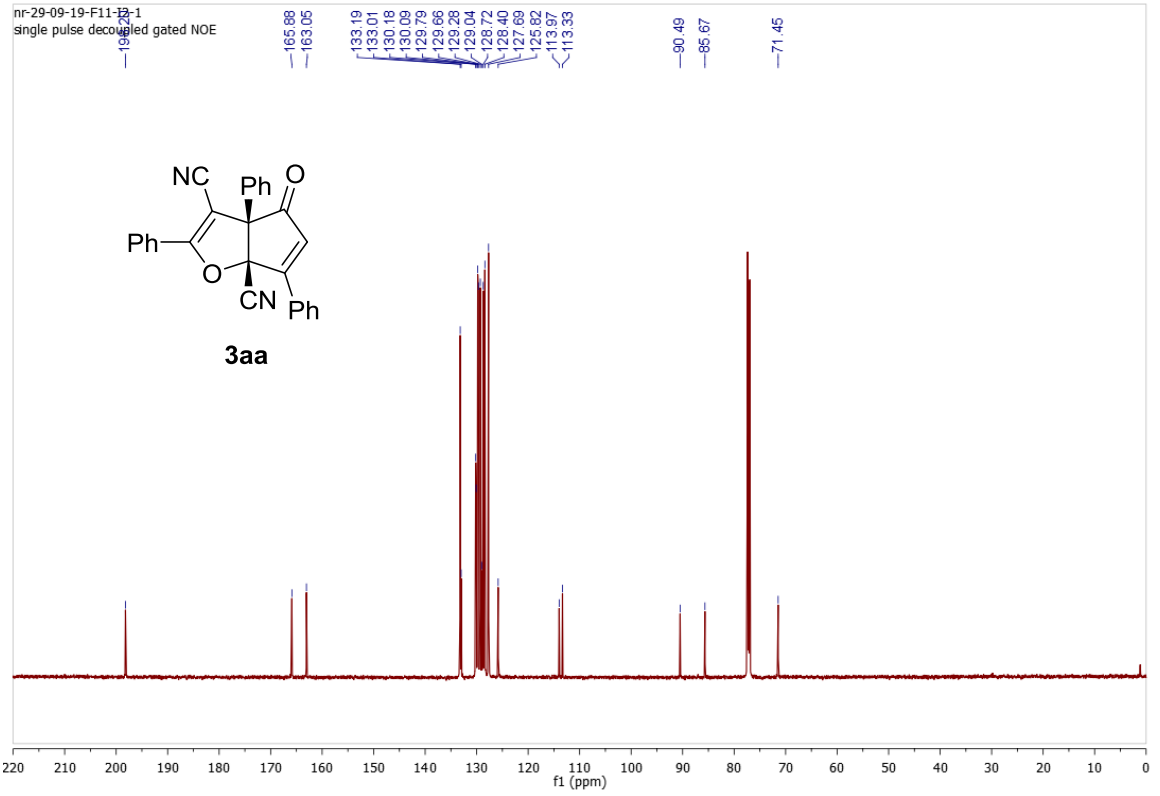

NR-13-06-19-01
single_pulse
8.3256
8.3127
8.0078
7.9945
7.7061
7.6930
7.6803
7.6064
7.5933
7.5818
7.5707
7.5581
7.5458
7.5333
7.5175
7.5053
7.4811
7.4342
7.4215
7.4096
7.3263
7.3167
7.3047
7.2921
7.2797
7.2634
7.2590
7.2522
7.2332
7.2162
7.2089
3.5980
NC
Ph
Ph
O
Ph
N
N
O
N
Me
6j (in DMSO-d6)
0.92
2.02
0.96
6.26
1.11
8.18
3.00
f1 (ppm)

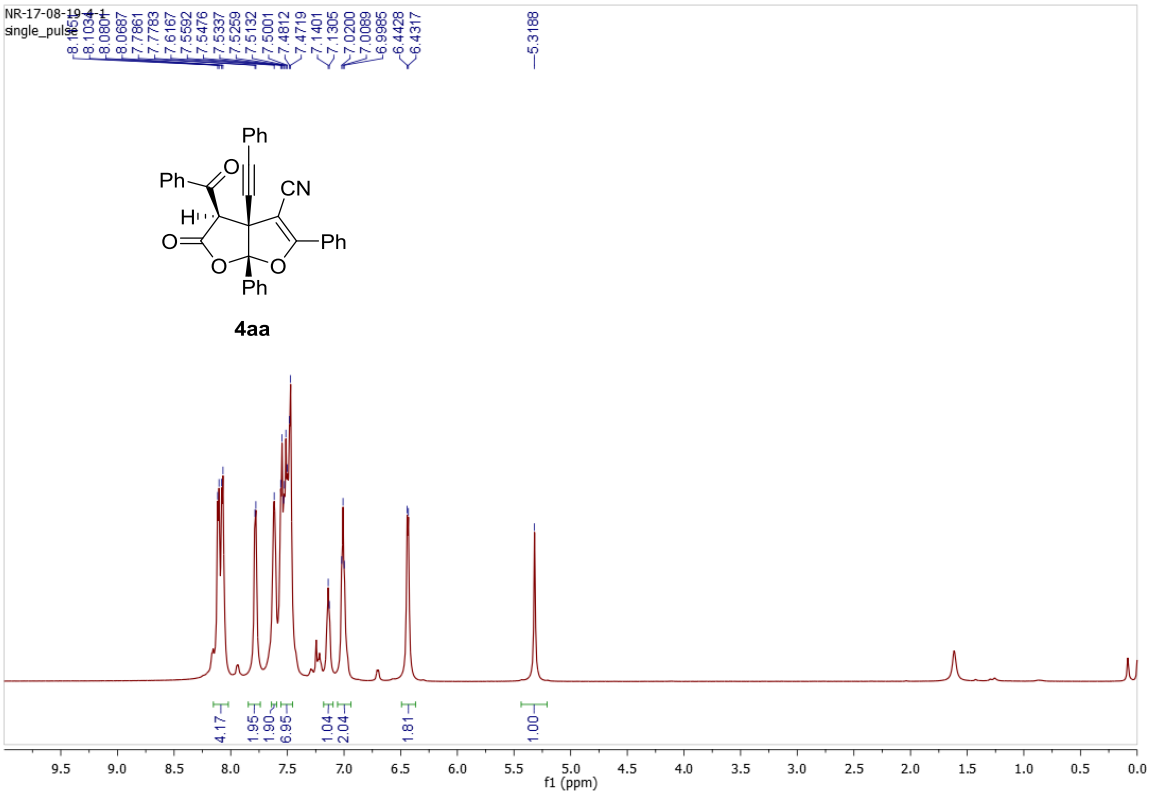

NR-13-06-19-1
160.28
131.49
130.06
129.32
129.29
129.19
129.14
129.09
129.05
128.22
127.74
127.15
125.91
116.13
114.99
113.06
111.63
93.23
31.39
NC
Ph
Ph
O
Ph
N
N
O
N
Me
6j (in DMSO-d6)
f1 (ppm)


NR-13-06-02-CAR
single pulse
12.011
11.505
8.7520
8.7279
8.7151
8.6906
7.9372
7.9132
7.9004
7.8761
7.6527
7.6283
7.6150
7.5715
7.5592
7.5466
7.5151
7.5022
7.4911
7.4786
7.4189
7.4070
7.3945
7.3365
7.3261
7.3146
7.2506
7.2382
7.2256
7.1944
7.1838
7.0988
7.0880
6.8249
6.8125
6.8002
6.7751
6.7353
6.6553
6.6307
6.6176
6.5933
NC
Ph
Ph
Ph
O
HN
N
H
6k (in DMSO-d6)
1.00
1.00
1.03
2.15
17.19
3.12
f1 (ppm)

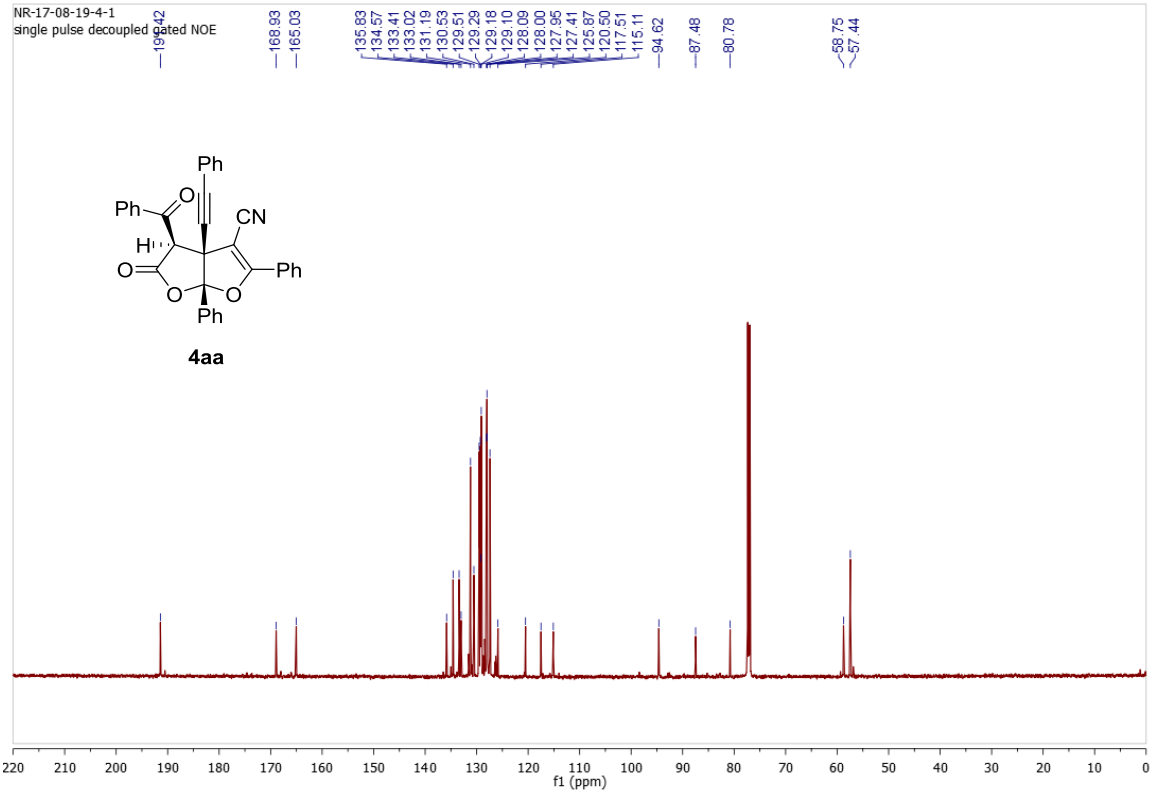

NR-13-06-19-2
159.69
147.61
140.35
139.64
139.52
135.27
130.16
129.93
129.00
128.48
128.22
128.17
126.72
125.63
123.66
121.62
106.11
94.47
92.70
NC
Ph
Ph
Ph
O
HN
N
H
6k (in DMSO-d6)
f1 (ppm)


nr-29-09-19-F11-I2-1
single_pulse
8.0475
8.0349
8.0160
8.0045
7.6165
7.6049
7.6013
7.5884
7.5736
7.5301
7.5175
7.5074
7.4929
7.4811
7.4689
7.3840
7.3719
7.2601
7.1259
NC
Ph
O
Ph
O
CN
Ph
3aa
2.00
1.80
3.99
5.06
2.05
0.93
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)

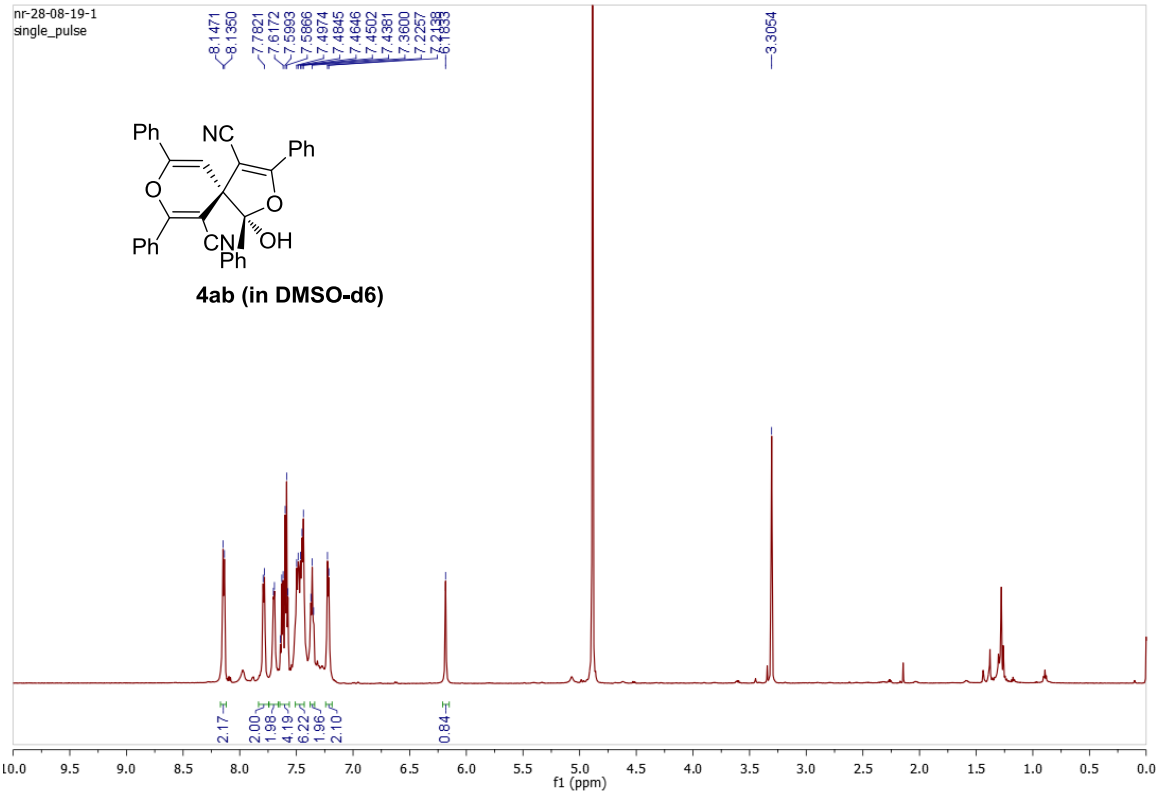

nr-29-09-19-F11-I2-1
single pulse decoupled gated NOE
165.88
163.05
133.19
133.01
130.18
130.09
129.79
129.66
129.28
129.04
128.72
128.40
127.69
125.82
113.97
113.33
90.49
85.67
71.45
NC
Ph
O
Ph
O
CN
Ph
3aa
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


NR-17-08-19-4-1
single_pulse
8.1655
8.1034
8.0801
8.0687
7.7861
7.7783
7.6167
7.5592
7.5476
7.5337
7.5259
7.5132
7.5001
7.4812
7.4719
7.1401
7.1305
7.0200
7.0089
6.9985
6.4428
6.4317
5.3188
Ph
O
Ph
CN
H
O
Ph
O
O
Ph
4.17
1.95
1.90
6.95
1.04
2.04
1.81
1.00
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)

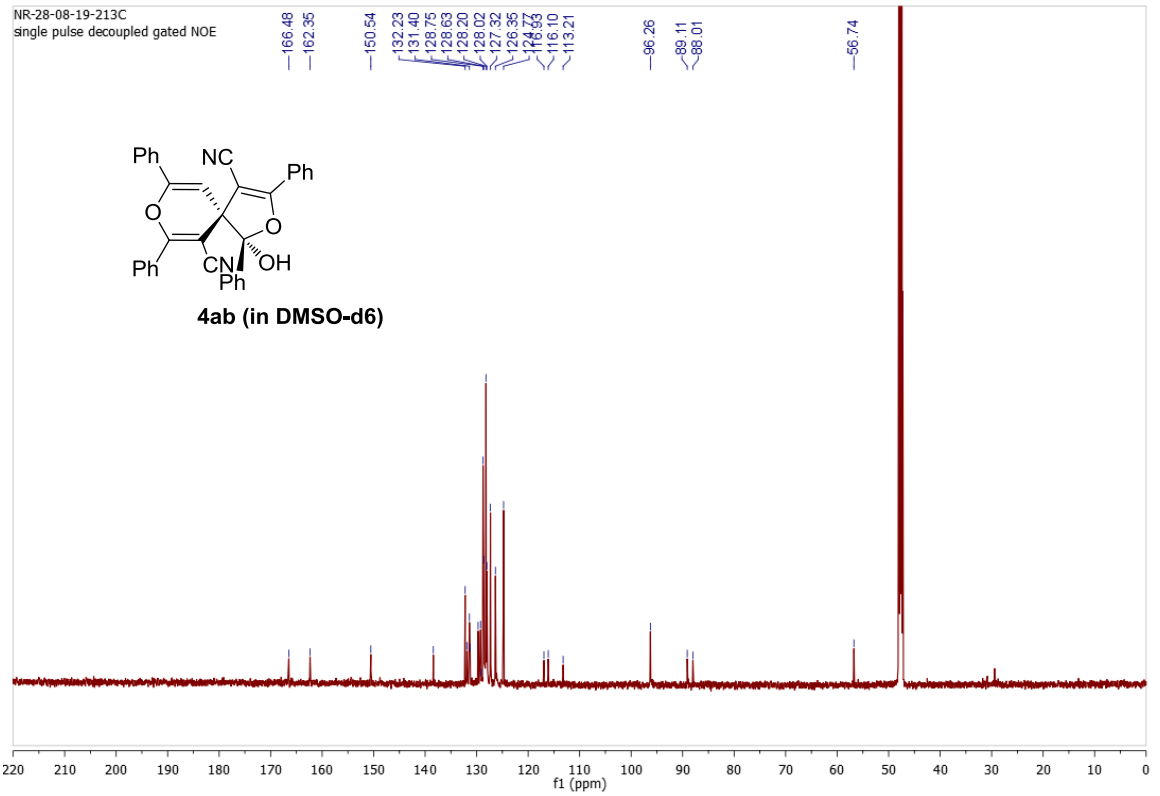
4aa


NR-17-08-19-4-1
single pulse decoupled gated NOE
168.93
165.03
135.83
134.57
133.41
133.02
131.19
130.53
129.51
129.29
129.18
129.10
128.09
128.00
127.95
127.41
125.87
120.50
117.51
115.11
94.62
87.48
80.78
58.75
57.44
Ph
O
Ph
CN
H
O
Ph
O
O
Ph
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

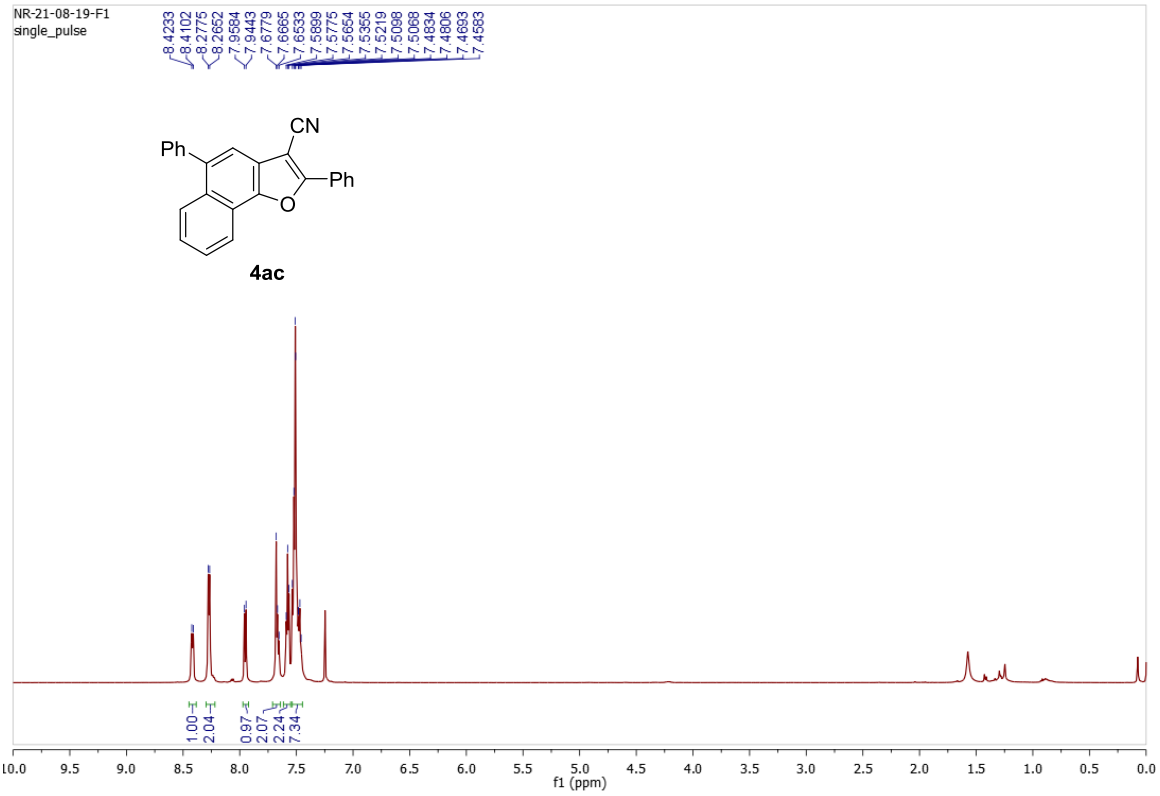
4aa

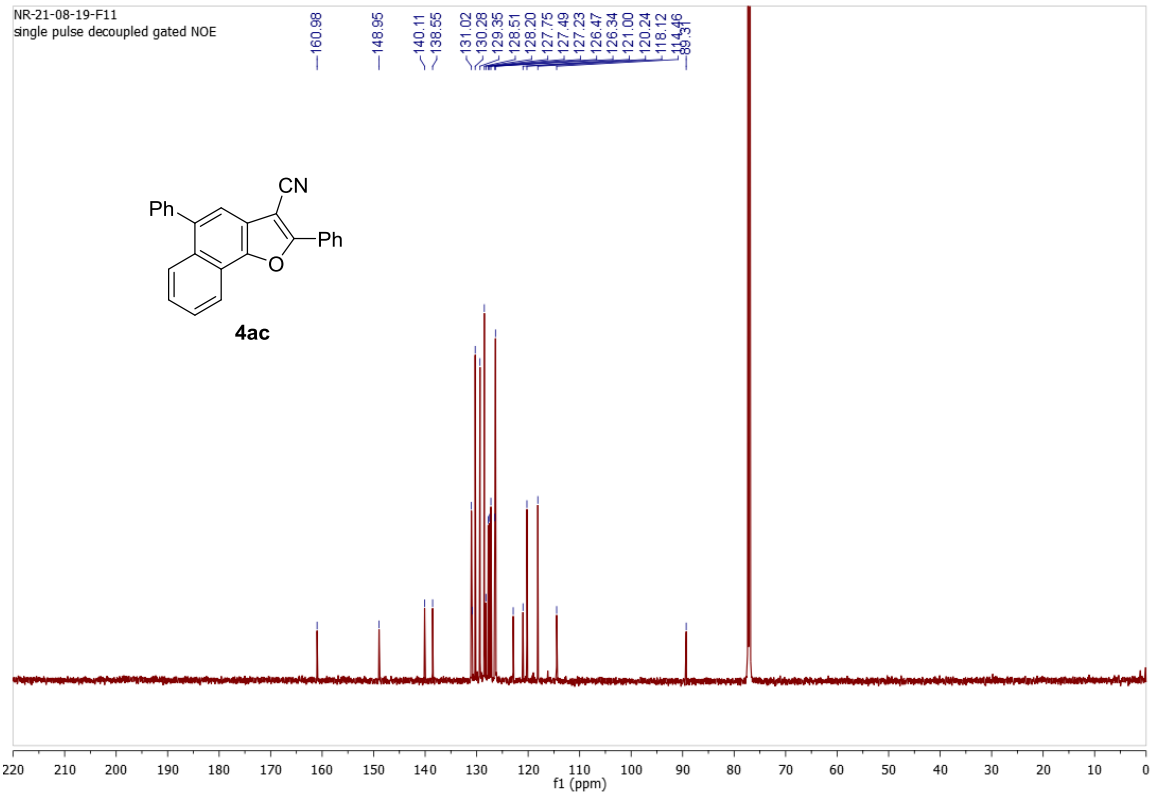


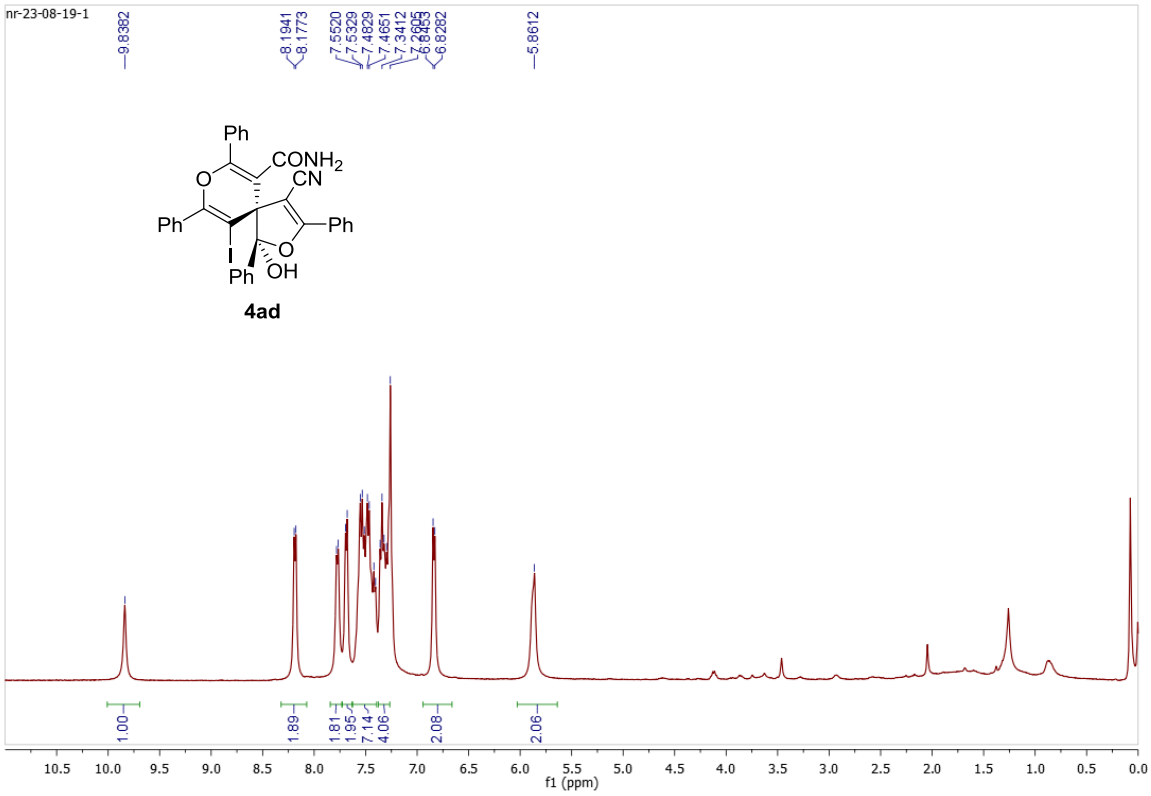
4ab (in DMSO-d6)



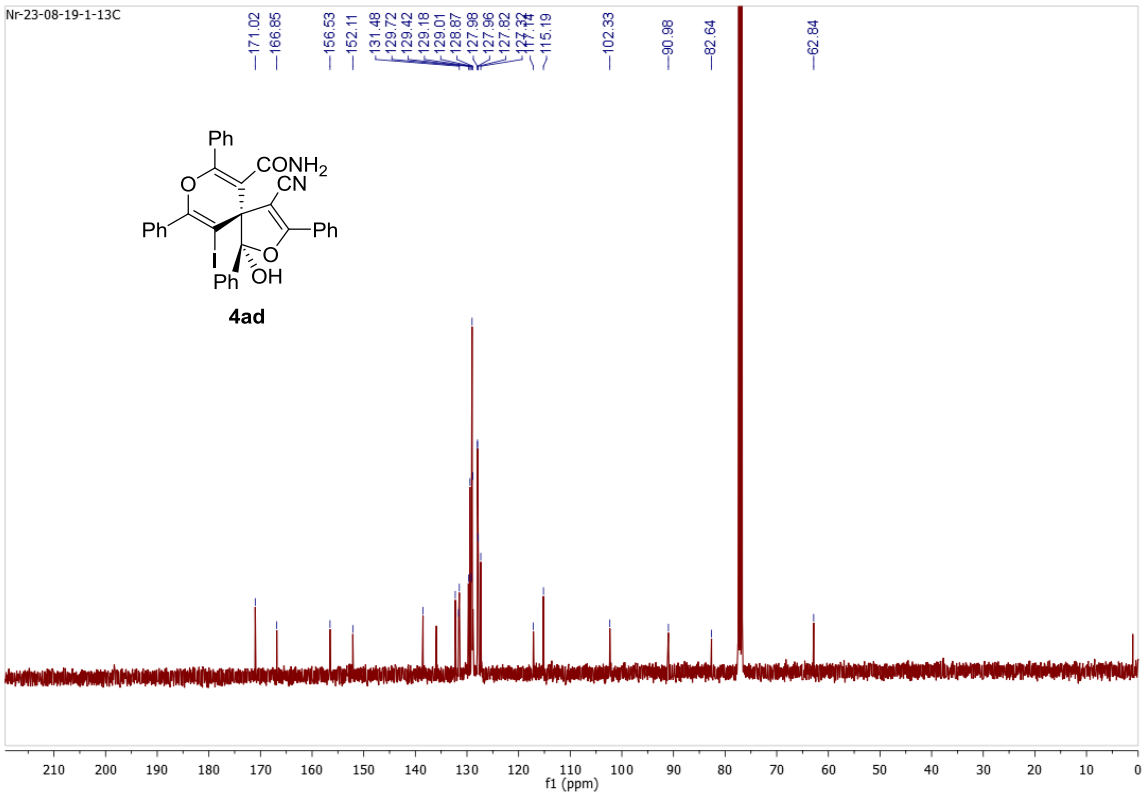
4ab (in DMSO-d6)


NR-21-08-19-F1
single_pulse
8.4233
8.4102
8.2775
8.2652
7.9584
7.9443
7.6779
7.6665
7.6533
7.5899
7.5775
7.5654
7.5355
7.5219
7.5098
7.5068
7.4834
7.4806
7.4693
7.4583
CN
Ph
Ph
O
4ac
1.00
2.04
0.97
2.07
2.24
7.34
f1 (ppm)


NR-21-08-19-F11
single pulse decoupled gated NOE
160.98
148.95
140.11
138.55
131.02
130.28
129.35
128.51
128.20
127.75
127.49
127.23
126.47
126.34
121.00
120.24
118.12
114.46
89.31
CN
Ph
Ph
O
4ac
f1 (ppm)


nr-23-08-19-1
9.8382
8.1941
8.1773
7.5520
7.5329
7.4829
7.4651
7.3412
6.8282
5.8612
Ph
CONH2
CN
O
Ph
Ph
I
O
Ph
OH
1.00
1.89
1.81
1.95
7.14
4.06
2.08
2.06
f1 (ppm)

4ad


Nr-23-08-19-1-13C
171.02
166.85
156.53
152.11
131.48
129.72
129.42
129.18
129.01
128.87
127.98
127.96
127.82
115.19
102.33
90.98
82.64
62.84
Ph
CONH2
CN
O
Ph
Ph
I
O
Ph
OH
f1 (ppm)

4ad