Supporting Information

A General Electron Donor–Acceptor Complex for Photoactivation of Arenes *via* Thianthrenation

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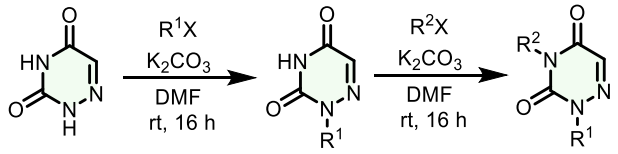
1. General Information

1.1 Materials and instruments

All reagents were purchased from commercial suppliers, which were used directly without further purification unless otherwise stated. TLC was performed on silica gel plates (F254, 200-300 mesh) using UV light (254/366 nm) for detection. Products were purified by column chromatography, which was carried out on 200-300 mesh of silica gel purchased from Qing Dao Hai Yang Chemical Industry Co. All the ^{1}H, ^{13}C, and ^{19}F NMR spectra were recorded on Bruker Avance 400 MHz operating at 400 MHz, 101 MHz, and 376 MHz, respectively. Proton chemical shifts δ were given in ppm using tetramethylsilane as internal standard. All NMR spectra were recorded in $CDCl_3$ or DMSO-d_6 at room temperature (20 ± 3 °C). High-resolution mass spectra (HRMS) were taken with a 3000-mass spectrometer, using Waters Q-Tof MS/MS system with the ESI technique. Absorption spectra were recorded on an Agilent 8453.

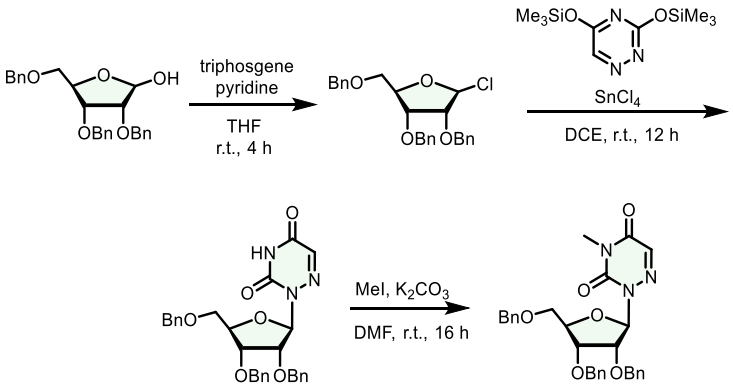
1.2 General procedure for the synthesis of azauracil substrates[1]



Alkyl halides (3.6 mmol, 0.9 equiv.) was added dropwise to a stirring solution of 6-azuracil (4.0 mmol, 1.0 equiv.), K_2CO_3 (2.0 mmol, 0.5 equiv.) in DMF (40 mL). The reaction mixture was allowed to stir at room temperature for 16 h. Then, the mixture was quenched with saturated Na_2CO_3 solution and extracted with DCM for three times. The organic layers were combined, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude products were purified through silica gel column chromatography using petroleum ether/ethyl acetate as eluent to give to afford the corresponding *N*-1-alkyl-6-azauracils.

Alkyl halides (2.0 mmol, 1.0 equiv.) was added dropwise to a stirring solution of *N*-1-alkyl-6-azauracils (2.0 mmol, 1.0 equiv.), K_2CO_3 (1.0 mmol, 0.5 equiv.) in DMF (20 mL). The reaction mixture was allowed to stir at room temperature for 16 h. Then, the mixture was quenched with saturated Na_2CO_3 solution and extracted with DCM for three times. The organic layers were combined, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude products were purified through silica gel column chromatography using petroleum ether/ethyl acetate as eluent to give to afford the corresponding *N*-1,*N*-3-dialkyl-6- azauracils.

1.3 General procedure and characterization data for the synthesis of azauracil ribonucleoside[1]

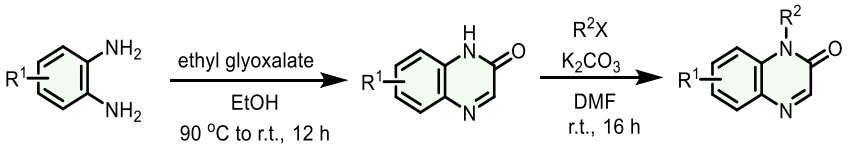


Triphosgene (653.4 mg, 2.2 mmol, 0.4 equiv.) was added dropwise to a stirring solution of (2R,3R,4R,5R)-3,4-bis(benzyloxy)-5-((benzyloxy)methyl)tetrahydrofuran-2-ol (2.31 g, 5.5 mmol, 1.0 equiv.) in THF (24 mL) under N_2 atmosphere. The mixture was allowed to stir at 10~15 ℃ for 2 minutes. Pyridine (0.55 mL) was added dropwise over 20 minutes at 10~15 ℃. The reaction mixture was allowed to stir at room temperature for 4 h. The reaction mixture was filtered and the solid residue was discarded. The crude chloride obtained as a solution in THF was used immediately for the coupling reaction.

To an oven-dried round bottom flask charged with crude chloride obtained (1.78 g, 5.0 mmol, 1.0 equiv., 24 mL solution in anhydrous THF) and 3,5-bis((trimethylsilyl)oxy)-1,2,4-triazine (1.67 g, 6.5 mmol, 1.3 equiv.) was added $SnCl_4$ (3.8 mL, 3.75 mmol, 0.75 equiv., 1 mol/L solution in CH_2Cl_2) dropwise at 0 ℃ under N_2 atmosphere. The reaction mixture was allowed to stir at room temperature for 12 h. The reaction was quenched with an aqueous $NaHCO_3$ solution and the mixture was extracted with EtOAc. The organic extracts were combined, dried over Na_2SO_4, and concentrated under reduced pressure. The residue was purified by flash chromatography (*n*-hexane/EtOAc = 4:1) to afford azauracil ribonucleoside in 25% yield as a pale yellow viscous liquid.

MeI (2.0 mmol, 1.0 equiv.) was added dropwise to a stirring solution of azauracil ribonucleoside (2.0 mmol, 1.0 equiv.), K_2CO_3 (1.0 mmol, 0.5 equiv.) in DMF (20 mL). The reaction mixture was allowed to stir at room temperature for 16 h. Then, the mixture was quenched with saturated Na_2CO_3 solution and extracted with DCM for three times. The organic layers were combined, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude products were purified through silica gel column chromatography using petroleum ether/ethyl acetate as eluent to give to afford the corresponding *N*-Methyl azauracil ribonucleoside.

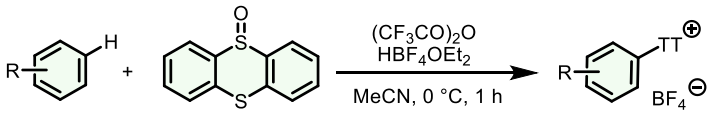
1.4 General procedure for the synthesis of quinoxalinone substrates[2]



Ethyl glyoxalate (1.1 equiv.) was added dropwise to a stirring solution of *o*-arylenediamine (1 equiv.) in ethanol. The reaction mixture was allowed to stir at room temperature for 1 h. The precipitated solid was filtered and washed with ethanol, then dried to give quinoxalinone.

To a suspension of quinoxalinone (1 equiv.) in DMF was added potassium carbonate (1.2 equiv.) and the corresponding halogenoalcane (1.6 equiv.). The mixture was stirred at room temperature overnight. Ethyl acetate and water were added. The aqueous layer was extracted twice with EtOAc. The combined organic layers were washed with a saturated solution of NaCl, dried over $MgSO_4$, filtered and evaporated under reduced pressure. The residue is purified by flash chromatography over silica gel to afford the desired product *N*-alkyl quinoxalinone.

1.5 General procedure for the synthesis of aryl sulfonium salt substrates[3]



Under an ambient atmosphere, a 20 mL glass vial was charged with arene (0.50 mmol, 1.0 equiv.) and dry MeCN (4.0 mL). After cooling to 0 °C, $HBF_4{\cdot}OEt_2$ (1.5 equiv.) was added to the vial while stirring the reaction mixture. After all solids were dissolved, thianthrenium-S-oxide (TTO) (0.50 mmol, 1.0 equiv.) was added in one portion to the solution at 0 ℃, leading to a suspension. Subsequently, trifluoroacetic anhydride (1.5 mmol, 3.0 equiv.) was added in one portion at 0 ℃, resulting in a color change to deep purple. The vial was sealed with a screw cap. The mixture was stirred at 0 ℃ for 1 h, subsequently the reaction mixture was warmed to 25 ℃ and stirred until all solids dissolved, and the intensity of the purple color decreased. The solution was poured onto a mixture of 20 mL dichloromethane, 20 mL saturated aqueous Na_2CO_3 solution, and 10 mL water. After stirring for 5 min at 25 °C, the mixture was poured into a separatory funnel, and the layers were separated. The dichloromethane layer was washed with aqueous $NaBF_4$ solution (2 × ca. 20 mL, 5 % w/w) and with water (2 × ca. 20 mL). The collected organic layers were then dried over $MgSO_4$, then filtered and concentrated under reduced pressure and purified by precipitation with Et_2O/DCM, and then repeated the precipitation procedure 3 times, the solid was dried in vacuo to afford the aryl sulfonium salts.

1.6 The spectrum of the lamp and the visible-light irradiation instrument

Photochemical reaction was carried out under visible light irradiation by a blue LED at 25 ºC. RLH-18 8-position Photo Reaction System manufactured by Beijing Roger Tech Ltd. was used in this system. Eight 10 W blue LEDs were equipped in this Photo reactor. The blue LED's energy peak wavelength is 430 nm, peak width at half-height is 18.4 nm, lirradiance@10 W is 237.57 mW/cm^2. The reaction vessel is borosilicate glass test tube and the distance between it

and the lamp is 15 mm, no filter applied.

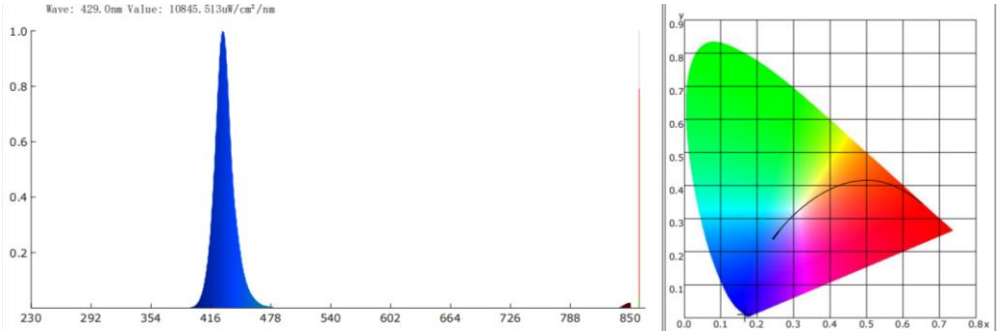


Figure S1. The spectrum of our lamp (white LED)

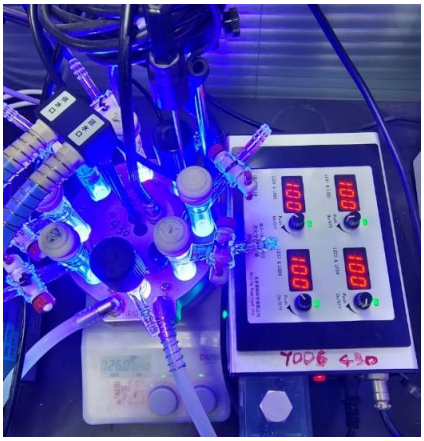
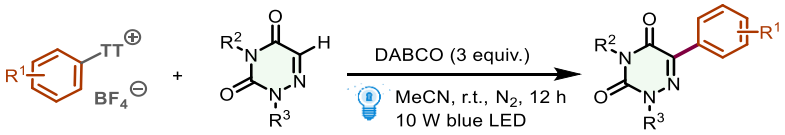


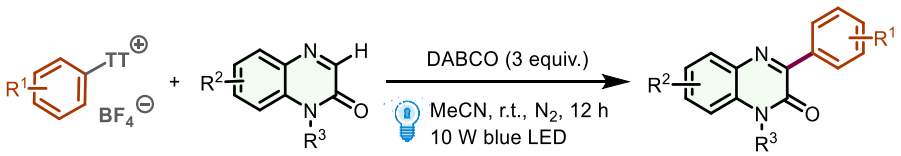
Figure S2. The visible-light irradiation instrument

2. Experimental procedures

2.1 General experimental procedures for the desired product



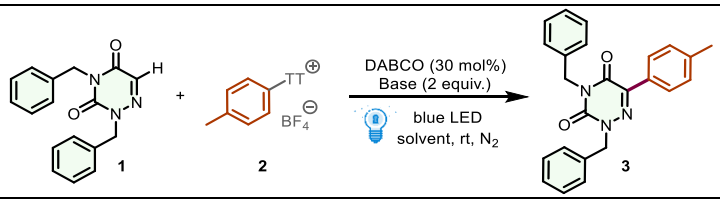
The mixture of azauracil (0.1 mmol), aryl sulfonium salt (0.2 mmol, 2 equiv.), DABCO (0.3 mmol, 3 equiv.) and CH_3CN (1.5 mL) were sequentially added in a 25 mL reaction vessel. Then the reaction vessel was irradiated with 10 W blue LED (430 nm) at room temperature under N_2 atmosphere for 12 h. After the reaction, the solvent was evaporated under vacuum. The reaction was quenched with aqueous $NaHCO_3$ solution and the mixture was extracted with EtOAc. The organic extracts were combined, dried over Na_2SO_4, and concentrated under reduced pressure. The crude products were purified by silica gel chromatography using petroleum ether/ethyl acetate as eluting solvent to give the desired products.



The mixture of quinoxalinone (0.1 mmol), aryl sulfonium salt (0.2 mmol, 2 equiv.), DABCO (0.3 mmol, 3 equiv.) and CH_3CN (1.5 mL) were sequentially added in a 25 mL reaction vessel. Then the reaction vessel was irradiated with 10 W blue LED (430 nm) at room temperature under N_2 atmosphere for 12 h. After the reaction, the solvent was evaporated under vacuum. The reaction was quenched with aqueous $NaHCO_3$ solution and the mixture was extracted with EtOAc. The organic extracts were combined, dried over Na_2SO_4, and concentrated under reduced pressure. The crude products were purified by silica gel chromatography using petroleum ether/ethyl acetate as eluting solvent to give the desired products.

2.2 Additional attempts to decrease the donor loading

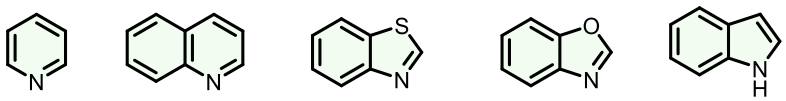
Table S1. Reactions with a catalytic amount of DABCO[a]



Entry	Base (2 equiv.)	Yield (%)
1	K_2CO_3	41
2	Cs_2CO_3	32
3	K_3PO_4	52
4	CH_3COONa	23
5	K_2HPO_4	61
6	$NaHCO_3$	20
7	KOH	66
8[b]	KOH	51
9[c]	KOH	27
10[d]	KOH	0

[a]Reaction conditions: **1** (0.1 mmol), **2** (0.2 mmol), DABCO (30 mol%), base (2 equiv.), and CH_3CN (1.5 mL) were irradiated with 10 W blue LED (430 nm) at room temperature under N_2 atmosphere for 12 h. Yields were given by ^1H NMR using 1,1,2,2-tetrachloroethane as an internal standard based on **1**. [b] 20 mol% DABCO was used. [c] 10 mol% DABCO was used. [d] In the absence of DABCO.

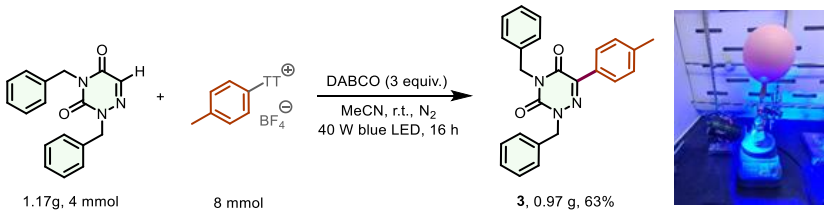
2.3 Unsuitable (hetero)aromatic cycles



Scheme S1. Unsuitable (hetero)aromatic cycles

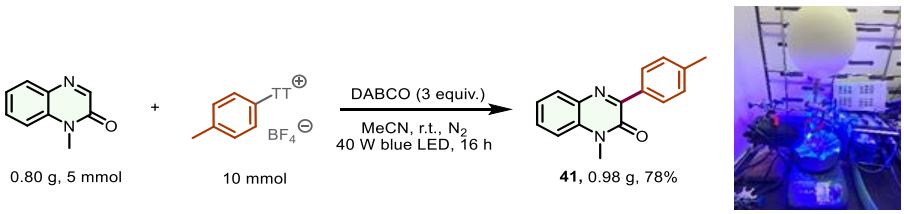
2.4 Gram-scale synthesis

The mixture of 2,4-dibenzyl-1,2,4-triazine-3,5(2H,4H)-dione (4 mmol), methylbenzene-derived sulfonium salt (8 mmol), DABCO (12 mmol) and CH_3CN (30 mL) were sequentially added in a 100 mL round bottom flask. And then the reaction system was carried out under 40 W blue LED (430 nm) at room temperature under N_2 atmosphere for 16 h. After reaction, the residue was quenched with saturated $NaHCO_3$ solution (10 mL), and ethyl acetate (15 mL) was added three times for extraction. The combined organic layers were dried over anhydrous Na_2SO_4. The residue was purified by silica gel chromatography (petroleum ether/ethyl acetate = 30/1) to afford the desired product (0.97 g, 63%).



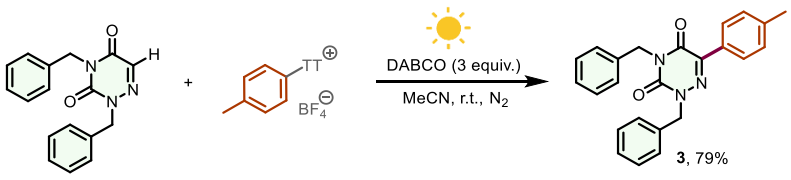
Scheme S2. Gram-scale synthesis of **3**

The mixture of 1-methylquinoxalin-2(1H)-one (5 mmol), methylbenzene-derived sulfonium salt (10 mmol), DABCO (15 mmol) and CH_3CN (30 mL) were sequentially added in a 100 mL round bottom flask. And then the reaction system was carried out under 40 W blue LED (430 nm) at room temperature under N_2 atmosphere for 16 h. After reaction, the residue was quenched with saturated $NaHCO_3$ solution (10 mL), and ethyl acetate (15 mL) was added three times for extraction. The combined organic layers were dried over anhydrous Na_2SO_4. The residue was purified by silica gel chromatography (petroleum ether/ethyl acetate = 20/1) to afford the desired product (0.98 g, 78%).



Scheme S3. Gram-scale synthesis of **41**

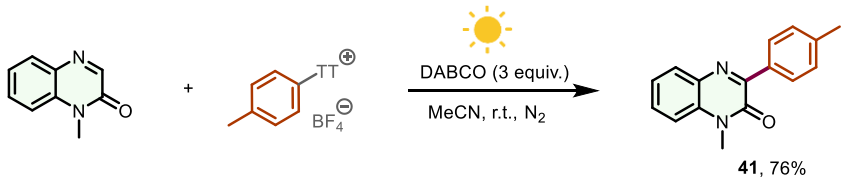
2.5 Irradiation with natural sunlight



Scheme S4. Synthesis of **3** under natural sunlight

The mixture of azauracil (0.1 mmol), aryl sulfonium salt (0.2 mmol, 2 equiv.), DABCO (0.3 mmol, 3 equiv.) and CH_3CN (1.5 mL) were sequentially added in a 25 mL reaction vessel. Then the reaction system was carried out under sunlight for 12 h (from 11:00 to 16:00;

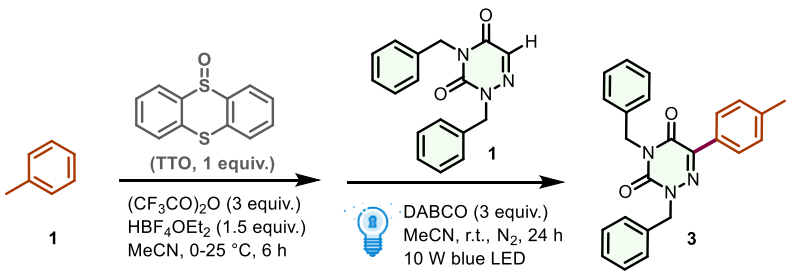
2021/06/04 and from 10:00 to 17:00; 2021/06/05. Zhengzhou, Henan province, China. Temperature: 25 ℃ – 29 ℃). After the reaction, the solvent was evaporated under vacuum. The reaction was quenched with aqueous $NaHCO_3$ solution and the mixture was extracted with EtOAc. The organic extracts were combined, dried over Na_2SO_4, and concentrated under reduced pressure. The crude products were purified by silica gel chromatography using petroleum ether/ethyl acetate as eluting solvent to give the desired products.



Scheme S5. Synthesis of **41** under natural sunlight

The mixture of quinoxalinone (0.1 mmol), aryl sulfonium salt (0.2 mmol, 2 equiv.), DABCO (0.3 mmol, 3 equiv.) and CH_3CN (1.5 mL) were sequentially added in a 25 mL reaction vessel. Then the reaction system was carried out under sunlight for 12 h (from 11:00 to 16:00; 2021/06/04 and from 10:00 to 17:00; 2021/06/05. Zhengzhou, Henan province, China. Temperature: 25 ℃ – 29 ℃). After similar operation, the crude products were purified by silica gel chromatography using petroleum ether/ethyl acetate as eluting solvent to give the desired products.

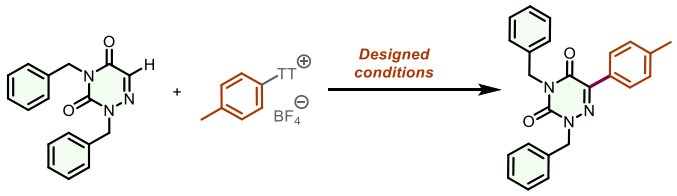
2.6 One-pot sequence



Under an ambient atmosphere, a 20 mL glass vial was charged with toluene (18.5 mg, 0.2 mmol) and MeCN (0.5 mL, c = 0.4 M). After cooling to 0 °C, $HBF_4{\cdot}OEt_2$ (1.5 equiv.) was added to the vial while stirring the reaction mixture. After all solids were dissolved, thianthrenium-S-oxide (TTO) (0.2 mmol, 1.0 equiv.) was added in one portion to the solution at 0 ℃, leading to a suspension. Subsequently, trifluoroacetic anhydride (0.6 mmol, 3.0 equiv.) was added in one portion at 0 ℃, resulting in a color change to deep purple. The vial was sealed with a screw cap. The mixture was stirred at 0 ℃ for 1 h. Subsequently, the reaction mixture was warmed to 25 ℃ and stirred until all solids dissolved, and the intensity of the purple color decreased. Then K_2CO_3 (82.9 mg, 0.6 mmol) was added and stirred for five minutes. Afterward, 2,4-dibenzyl-1,2,4-triazine-3,5(2*H*,4*H*)-dione **1** (0.1 mmol, 29.3 mg), DABCO (33.7 mg, 0.3 mmol) and

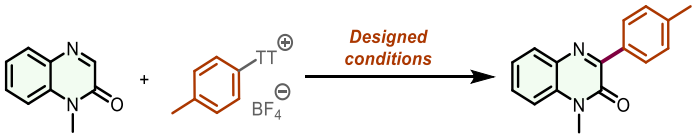
CH_3CN (1.5 mL) were added in the 25 mL reaction vial. Then the reaction vessel was irradiated with 10 W blue LED (430 nm) at room temperature under N_2 atmosphere for 24 h. After the reaction, the solvent was evaporated under vacuum. The crude product was purified by silica gel chromatography to give the desired product **3** in 37% yield.

2.7 Sensitivity assessment of reaction



Parameter	Variation		Description	Yield[b]
Concentration (*c*)	High *c*	*c* + 10% *c*	1.35 mL CH_3CN	79%
	Low *c*	*c* - 10% *c*	1.65 mL CH_3CN	75%
H_2O level	High H_2O	+ H_2O; V_{H2O} = 1%V_{rxn}	15 μL H_2O in 1.5 mL CH_3CN	73%
O_2 level	High O_2	O_2 balloon	O_2 balloon instead of air	40%
Temperature (*T*)	High *T*	*T* + 10 °C	35 °C	78%
	Low *T*	*T* – 10 °C	15 °C	73%
Light intensity (*W*)	Low *W*	*W*/16	0.6 W	0%
Scale	Big scale	n·30	3 mmol of **1a**	70%

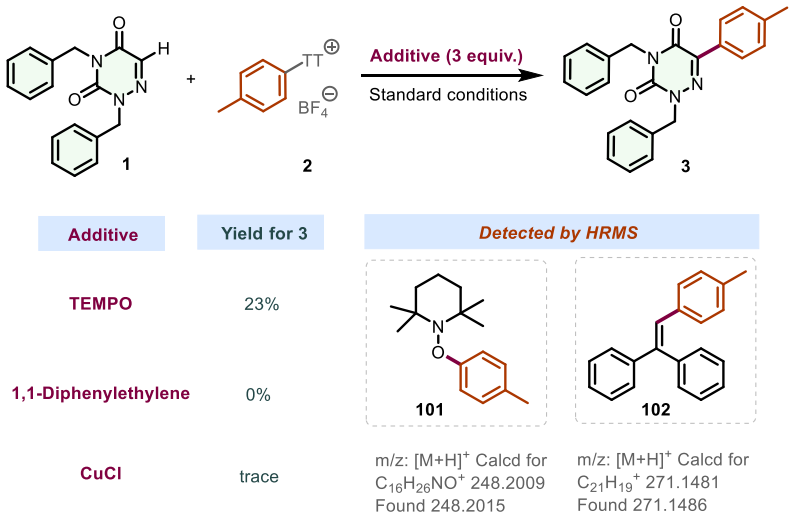
[a]Standard conditions: 2,4-dibenzyl-1,2,4-triazine-3,5(2H,4H)-dione (0.1 mmol), methylbenzene-derived sulfonium salt (0.2 mmol), DABCO (3 equiv), CH_3CN (1.5 mL), 430 nm blue LED (10 W), under N_2 for 12 h, room temperature. [b]The average yield of three parallel reactions. [c]Deviation from the yield of standard reaction.



Parameter	Variation		Description	Yield[b]
Concentration (*c*)	High *c*	*c* + 10% *c*	1.35 mL CH_3CN	80%
	Low *c*	*c* - 10% *c*	1.65 mL CH_3CN	78%
base dosage	High base	+ 1 equiv	4 equiv	76%
	Low base	- 1 equiv	2 equiv	56%
H_2O level	High H_2O	+ H_2O; V_{H2O} = 1%V_{rxn}	15 μL H_2O in 1.5 mL CH_3CN	78%
O_2 level	High O_2	O_2 balloon	O_2 balloon instead of air	32%
Temperature (*T*)	High *T*	*T* + 10 °C	35 °C	83%
	Low *T*	*T* – 10 °C	15 °C	74%
Light intensity (*W*)	Low *W*	*W*/16	0.6 W	0%
Scale	Big scale	n·30	3 mmol of **1a**	68%

[a]Standard conditions: 1-methylquinoxalin-2(1H)-one (0.1 mmol), methylbenzene-derived sulfonium salt (0.2 mmol), DABCO (3 equiv), CH_3CN (1.5 mL), 430 nm blue LED (10 W), under N_2 for 12 h, room temperature. [b]The average yield of three parallel reactions. [c]Deviation from the yield of standard reaction.

2.8 Control experiment



Scheme S6. Control experiments

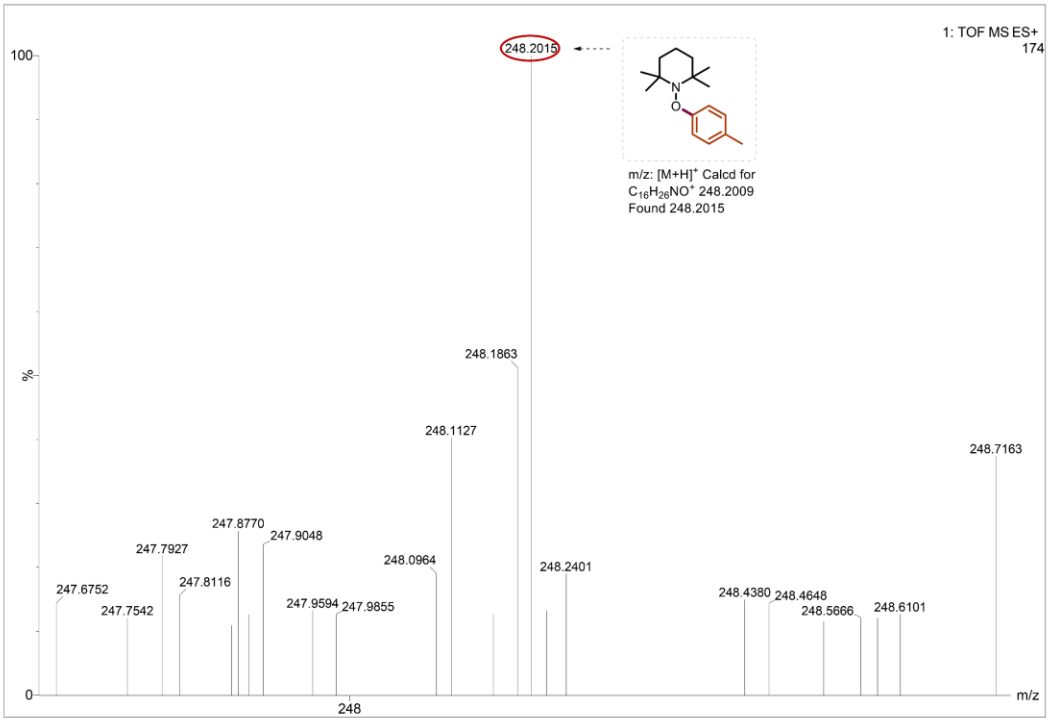


Figure S3. The HRMS analysis of compound **101**

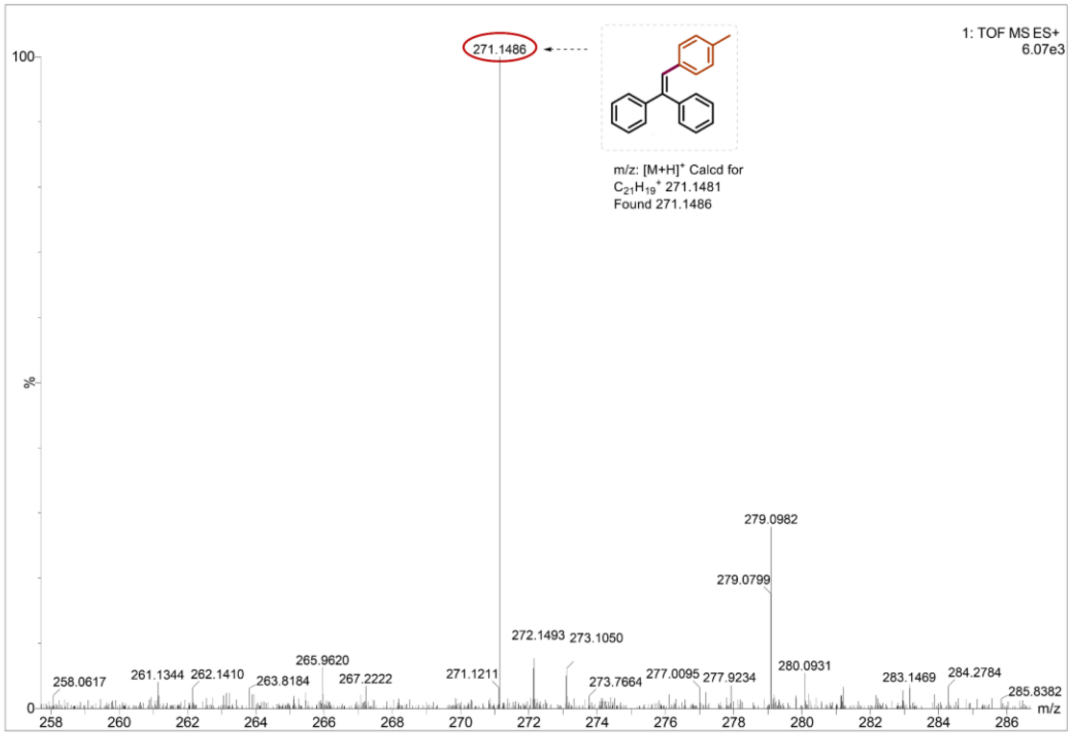
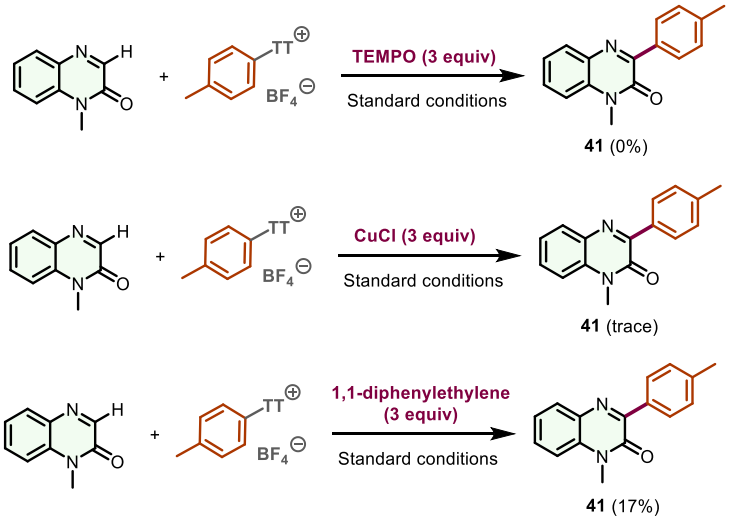


Figure S4. The HRMS analysis of compound **102**



Scheme S7. Control experiments

2.9 Titration experiments

^{1}H NMR spectra of mixtures of methylbenzene-derived sulfonium salt **2** and DABCO in $CDCl_3$ were recorded at 298 K. In an NMR tube, the total volume of the mixture was 0.6 mL, the concentration of methylbenzene-derived sulfonium salt (0.03 mmol) was kept constant at 0.05 M, and that of TMEDA was varied from 0 to 1.5 M. The molar ratios of methylbenzene-derived sulfonium salt : DABCO were 1:0, 1:1, 1:2, 1:3, 1:4, 1:5, 1:6, 1:10, 1:20, 1:30. $CDCl_3$ (δ = 7.2600) was used as an internal standard. The ^{1}H NMR signal of ArH in methylbenzene-

derived sulfonium salt **2** shifted upfield along with increasing the amount of DABCO, indicating the formation of EDA complex of methylbenzene-derived sulfonium salt with DABCO.

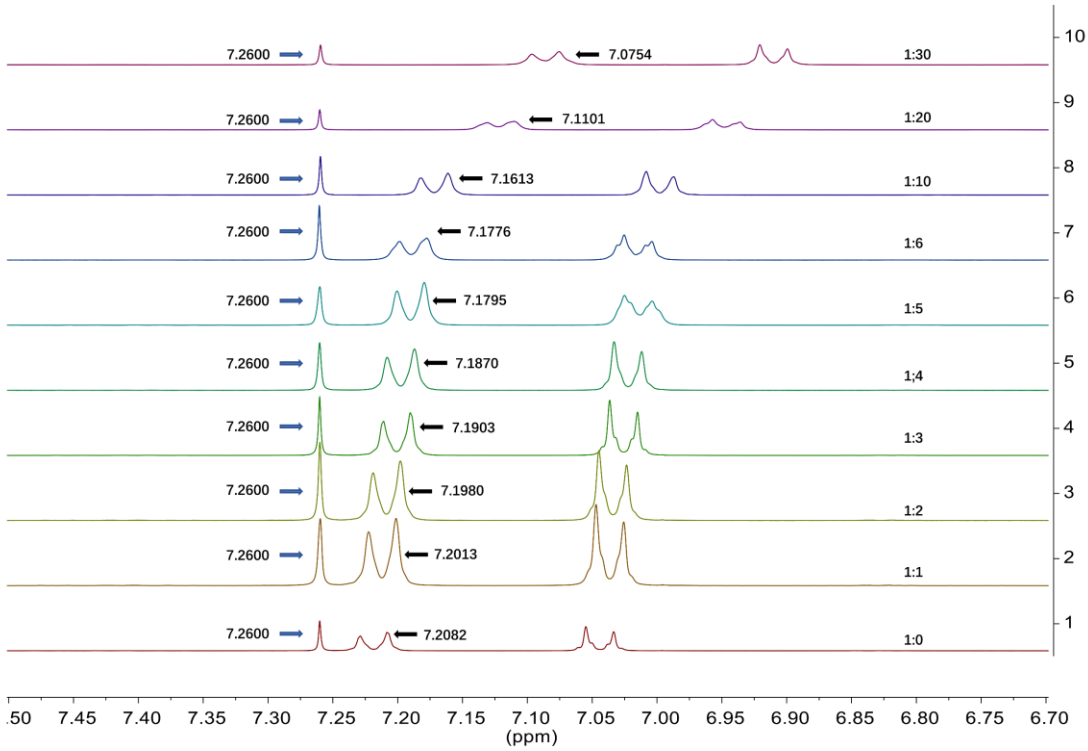


Figure S5. ^{1}H NMR shift of methylbenzene-derived sulfonium salt with DABCO.

2.10 In vitro antitumor activity

IC_{50} values of compounds against selected cell lines (μM)

Tumor types	Cell lines	IC_{50} (μM) Compound 37	Compound 92	Fluorouracil (5-Fu)
Lymphoma	Ramos	8.5	10.2	13.7

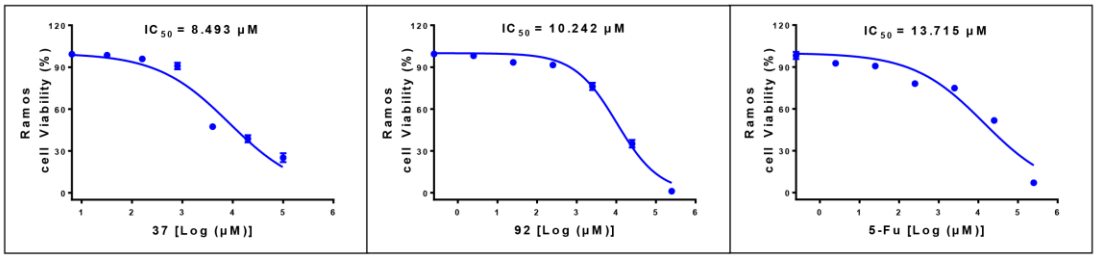


Figure S6. The in vitro antitumor activity of 37 and 92 against Ramos cells

2.11 Determination of the association constant (K_{DABCO})

^{1}H NMR for each sample was recorded and the changes of chemical shift (Δδ) for ArH in methylbenzene-derived sulfonium salt were used to draw the plot. The association constant of methylbenzene-derived sulfonium salt with DABCO (K_{DABCO}) was calculated: K_{DABCO} = c/a = 7.5589/7.3010 = 1.04 M^{-1}

Entry	[sulfonium salt]	1/[DABCO]	δ (ppm)	Δδ (ppm)	1/Δδ (ppm)
1	0.05	--	7.2082	--	--
2	0.05	20	7.2013	0.0069	144.9275362
3	0.05	10	7.198	0.0102	98.03921569
4	0.05	6.67	7.1903	0.0179	55.86592179
5	0.05	5	7.187	0.0212	47.16981132
6	0.05	4	7.1795	0.0287	34.84320557
7	0.05	3.33	7.1776	0.0306	32.67973856
8	0.05	2	7.1613	0.0469	21.32196162
9	0.05	1	7.1101	0.0981	10.19367992
10	0.05	0.67	7.0754	0.1328	7.530120482

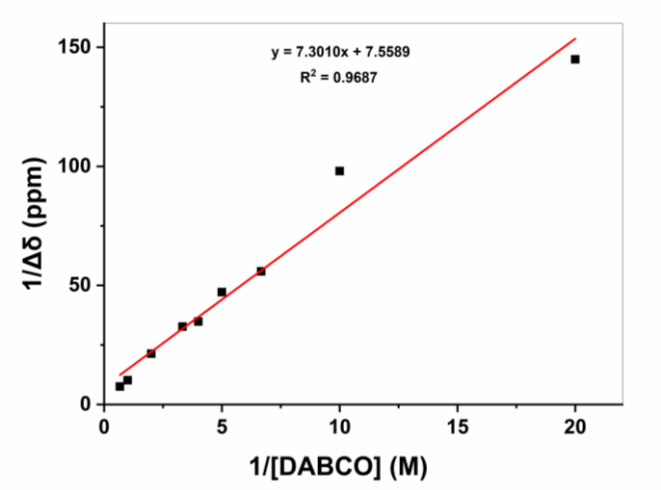


Figure S7. Plot for determination of the association constant (K_{DABCO})

2.12 Determination of binding stoichiometry of EDA complex

The binding stoichiometry between methylbenzene-derived sulfonium salt and DABCO was evaluated using Job's plot analysis: ^{1}H NMR spectra of mixtures of methylbenzene-derived sulfonium salt and DABCO in $CDCl_3$ were recorded at 298 K. $CDCl_3$ (δ = 7.2600) was used as an internal standard. The total volume of the mixture was 0.5 mL, and the total amount of methylbenzene-derived sulfonium salt and DABCO was kept constant at 0.1 mmol (0.2 M), while the amount of methylbenzene-derived sulfonium salt was varied from 0 to 0.1 mmol (0-0.2 M). The molar ratios of [methylbenzene-derived sulfonium salt]/[methylbenzene-derived sulfonium salt + DABCO] were 0.0, 0.2, 0.4, 0.5, 0.6, 0.8, 1.0. ^{1}H NMR for each sample was recorded and the changes of chemical shift (Δδ) for ArH in methylbenzene-derived sulfonium salt were used to draw the plot. The stoichiometry was determined by plotting ratios of [methylbenzene-derived sulfonium salt] × Δδ against ratios of [methylbenzene-derived sulfonium salt]/[methylbenzene-derived sulfonium salt + DABCO] to afford a maximum value.

X_{max} = b/(-2a) = 0.00149/(-2)×(-0.00153) ≈ 0.5. These data indicate that the formation of EDA complex of methylbenzene-derived sulfonium salt with DABCO in a binding stoichiometry of 1:1.

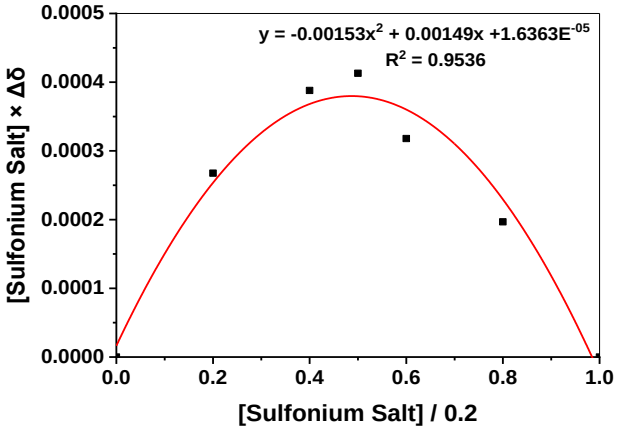


Figure S8. Job's plot

2.13 UV-vis absorbance experiment

A UV-vis absorbance experiment has been carried out for confirming the formation of EDA complex as illustrated below in Figure S9. In Figure S9, the red UV absorbance line came from compound **2** solution, the blue one came from DABCO solution, and the black one came from the mixed solution of compound **2** and DABCO. UV-vis spectra revealed that upon mixing compound **2** with DABCO, an obvious bathochromic shift of the UV-vis absorbance was observed, strongly suggesting that compound **2**-DABCO EDA complex might indeed be formed in the mixed solution.

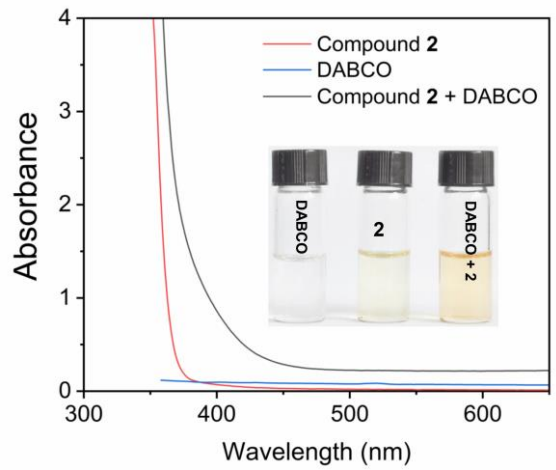


Figure S9. UV-vis absorption spectra. Red line: compound **2** (0.1 mmol) in 2 mL MeCN; Blue line: DABCO (0.1 mmol) in 2 mL MeCN; Black line: compound **2** (0.1 mmol) and DABCO (0.1 mmol) in 2 mL MeCN.

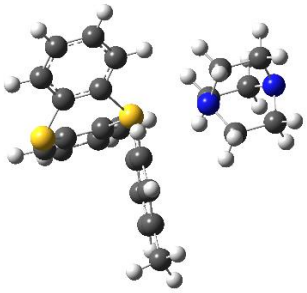
3. Computational method

3.1 Computational Details

In this work, we used Gaussian 16 software[1] for all calculations within the framework of DFT. All the molecular structures were computed with the B3LYP (Becke, three-parameter, Lee–Yang–Parr) hybrid functional[2] to describe the exchange–correlation energies. DFT-D3(BJ) method was considered in this work to calculate the weak interaction between methylbenzene-derived sulfonium salt **2** and DABCO.[3] Basis sets were employed for high-level B3LYP calculations at 6-31+G(d,p)[4] was adopted for atoms including C, N, S, and H. Vibrational frequency calculations were performed on all minima states, and each minima was identified to have no imaginary frequencies. The population analysis has also been performed by the natural bond orbital method.[5,6]

[1] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
[2] Devlin, F. J.; Finley, J. W.; Stephens, P. J.; Frisch, M. J. Ab Initio Calculation of Vibrational Absorption and Circular Dichroism Spectra Using Density Functional Force Fields: A Comparison of Local, Nonlocal, and Hybrid Density Functionals. J. Phys. Chem. 1995, 99, 16883– 16902, DOI: 10.1021/j100046a014
[3] JCP,132,154104(2010)
[4] McLean, A. D.; Chandler, G. S. Contracted Gaussian basis sets for molecular calculations. I. Second row atoms, Z=11-18. J. Chem. Phys. 1980, 72, 5639– 5648, DOI: 10.1063/1.438980
[5] A.E. Reed, L.A. Curtiss, F. Weinhold, Chem. Rev. 88, 899 (1988).
[6] E.D. Glendening, A.E. Reed, J.E. Carpenter, F. Weinhold, J. Am. Chem. Soc. 120, 12051 (1998).

3.2 Coordinates of Stationary Points

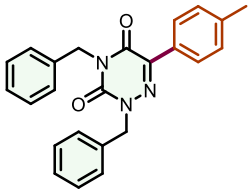


C	-3.89655600	-2.59927600	-2.58700800
C	-4.03645800	-2.31617500	-1.22781300
C	-3.03840900	-1.60551300	-0.54599000
C	-1.91138000	-1.18722000	-1.27225300
C	-1.74600200	-1.50251600	-2.62662700
C	-2.75070100	-2.20741100	-3.28715700
C	-0.47430600	-0.97098700	1.11682300
C	-1.61519900	-1.39607500	1.81863100
C	-1.43581200	-1.93743500	3.09812800
H	-2.29731900	-2.29039300	3.65600200
C	-0.15352500	-2.04700500	3.64011700
C	0.96988900	-1.64734600	2.91035400
C	0.82022900	-1.10848000	1.63120400
H	-4.67913800	-3.15250800	-3.09638700
H	-4.90975400	-2.66388400	-0.68512300
H	-0.85002200	-1.19057500	-3.15459200
H	-2.63850700	-2.44993700	-4.33836300
H	-0.03341600	-2.47068700	4.63228300
H	1.96315800	-1.75471900	3.33308200
H	1.68934500	-0.78660700	1.04826700
S	-3.27327800	-1.26331900	1.18344600
S	-0.63109700	-0.21117300	-0.49440200
C	-1.42487700	1.40229900	-0.17095000
C	-1.06291800	2.11937100	0.96915000
C	-2.26078700	1.95053700	-1.14469800
C	-1.57676200	3.40565900	1.14075500
H	-0.40511000	1.69398700	1.71951700
C	-2.76036300	3.23812900	-0.94897200
H	-2.53415400	1.39395500	-2.03496800
C	-2.43229100	3.98683000	0.19251100

H	-1.30330700	3.96419400	2.03123300
H	-3.41725700	3.66539500	-1.70118000
C	-3.00282900	5.36700100	0.40270000
H	-3.98711800	5.30778500	0.88300200
H	-2.35921900	5.97283100	1.04575300
H	-3.13376700	5.89387200	-0.54652800
C	6.04027500	-0.52791300	0.14451000
H	6.54899800	-1.43834700	-0.18934600
H	6.68766400	-0.04210700	0.88207500
C	5.06575000	-0.27993500	-2.03291800
H	4.99286900	0.39024900	-2.89622700
H	5.57820100	-1.18888400	-2.36539700
C	5.24701900	1.61844600	-0.57686700
H	5.89139200	2.10305900	0.16418700
H	5.17793000	2.28926100	-1.43991400
C	4.63120600	-0.84905600	0.74522700
H	4.55567200	-0.51861400	1.78794400
H	4.41927900	-1.92441700	0.72146400
C	3.83297100	1.30262700	0.01584600
H	3.75237400	1.62736600	1.05979000
H	3.03947900	1.80618500	-0.54931900
N	5.89971700	0.37284900	-1.01135700
N	3.57587300	-0.15580500	-0.03214900
C	3.65342700	-0.60558100	-1.44123600
H	3.44515400	-1.68176500	-1.46588700
H	2.85791100	-0.09997100	-2.00232100

4. Characterization Data for Products

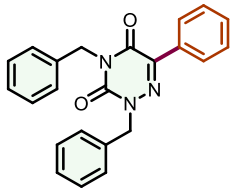
1,3-dibenzyl-6-(p-tolyl)-1,3,5-triazine-2,4(1H,3H)-dione (3)



White solid (31.4 mg, 82%); m.p. 130.5 – 132.1 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 (d, *J* = 8.2 Hz, 2H), 7.59 – 7.54 (m, 2H), 7.53 – 7.48 (m, 2H), 7.41 – 7.25 (m, 8H), 5.23 (s, 2H), 5.20 (s, 2H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.5, 148.8, 141.3, 140.3,

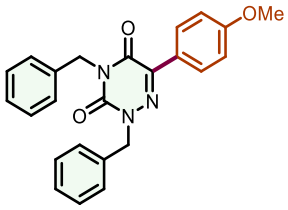
135.70, 135.68, 129.6, 129.3, 129.0, 128.82, 128.76, 128.6, 128.33, 128.28, 128.1, 55.7, 44.5, 21.4. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{24}H_{22}N_3O_2$, 384.1707; Found: 384.1718.

2,4-dibenzyl-6-phenyl-1,2,4-triazine-3,5(2H,4H)-dione (4)



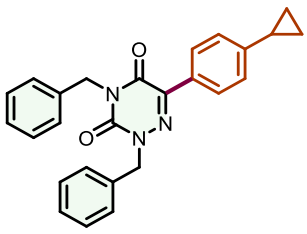
White solid (26.6 mg, 72%); m.p. 151.1 – 152.4 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.04 – 7.94 (m, 2H), 7.60 – 7.55 (m, 2H), 7.53 – 7.44 (m, 5H), 7.43 – 7.32 (m, 6H), 5.23 (d, *J* = 15.5 Hz, 4H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.5, 148.8, 141.2, 135.6, 135.6, 132.0, 130.0, 129.6, 128.84, 128.79, 128.6, 128.4, 128.33, 128.28, 128.1, 55.8, 44.5. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{23}H_{20}N_3O_2$, 370.1550; Found: 370.1559.

2,4-dibenzyl-6-(4-methoxyphenyl)-1,2,4-triazine-3,5(2H,4H)-dione (5)



White solid (30.3 mg, 76%); m.p. 114.3 – 115.1 °C; 1H NMR (400 MHz, Chloroform-d) δ 8.00 (d, J = 9.0 Hz, 2H), 7.59 – 7.54 (m, 2H), 7.49 (d, *J* = 6.5 Hz, 2H), 7.41 – 7.33 (m, 6H), 6.97 (d, *J* = 9.0 Hz, 2H), 5.21 (d, *J* = 11.7 Hz, 4H), 3.87 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.1, 155.6, 148.8, 140.9, 135.7, 134.5, 129.9, 129.5, 128.80, 128.76, 128.6, 128.3, 128.1, 124.6, 113.7, 55.6, 55.4, 44.4. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{24}H_{22}N_3O_3$, 400.1656; Found: 400.1661.

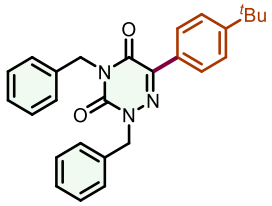
1,3-dibenzyl-6-(4-cyclopropylphenyl)-1,3,5-triazine-2,4(1H,3H)-dione (6)



White solid (22.9 mg, 56%); m.p. 107.4 – 108.9 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 (d, *J* = 8.4 Hz, 2H), 7.59 – 7.54 (m, 2H), 7.52 – 7.45 (m, 2H), 7.42 – 7.30 (m, 6H), 7.14 (d, *J* = 8.4 Hz, 2H), 5.21 (d, *J* = 12.4 Hz, 4H), 1.99 – 1.92 (m, 1H), 1.09 – 1.00 (m, 2H), 0.81 – 0.73

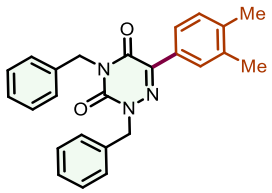
(m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.5, 148.8, 146.6, 141.2, 135.70, 135.67, 129.6, 129.1, 128.83, 128.76, 128.6, 128.34, 128.28, 128.1, 125.4, 55.7, 44.4, 15.5, 9.8. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{26}H_{24}N_3O_2$, 410.1863; Found: 410.1864.

2,4-dibenzyl-6-(4-(tert-butyl)phenyl)-1,2,4-triazine-3,5(2H,4H)-dione (7)



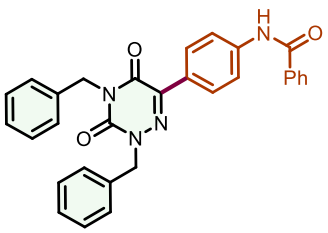
White solid (31.9 mg, 75%); m.p. 159.0 –159.4 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.94 – 7.89 (m, 2H), 7.57 – 7.55 (m, 2H), 7.50 – 7.46 (m, 4H), 7.41 – 7.30 (m, 6H), 5.21 (d, *J* = 11.2 Hz, 4H), 1.36 (s, 9H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.6, 153.3, 148.8, 141.3, 135.68, 135.66, 129.6, 129.2, 128.8, 128.7, 128.6, 128.3, 128.2, 128.1, 125.3, 55.7, 44.5, 34.8, 31.2. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{27}H_{28}N_3O_2$, 426.2176; Found: 426.2180.

1,3-dibenzyl-6-(3,4-dimethylphenyl)-1,3,5-triazine-2,4(1H,3H)-dione (8)



White solid (30.9 mg, 78%); m.p. 115.9 – 117.1 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.76 (s, 1H), 7.72 (d, *J* = 7.9 Hz, 1H), 7.59 – 7.54 (m, 2H), 7.52 – 7.47 (m, 2H), 7.41 – 7.30 (m, 6H), 7.22 (d, *J* = 7.9 Hz, 1H), 5.21 (d, *J* = 14.3 Hz, 4H), 2.34 (d, *J* = 5.3 Hz, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.6, 148.8, 141.5, 139.0, 136.5, 135.72, 135.70, 129.62, 129.58, 129.5, 129.4, 128.8, 128.7, 128.6, 128.3, 128.1, 126.0, 55.7, 44.4, 19.9, 19.8. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{25}H_{24}N_3O_2$, 398.1863; Found: 398.1874.

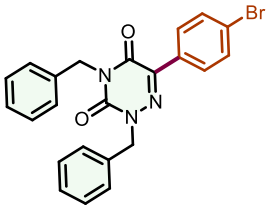
N-(4-(2,4-dibenzyl-3,5-dioxo-2,3,4,5-tetrahydro-1,2,4-triazin-6-yl)phenyl)benzamide (9)



White solid (23.7 mg, 48%); m.p. 142.1 – 143.4 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.12

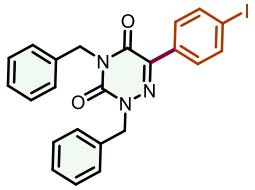
(s, 1H), 8.06 (d, J = 8.7 Hz, 2H), 7.88 (d, J = 7.3 Hz, 2H), 7.75 (d, J = 8.7 Hz, 2H), 7.58 – 7.54 (m, 3H), 7.50 – 7.46 (m, 4H), 7.41 – 7.31 (m, 6H), 5.20 (d, J = 19.7 Hz, 4H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 165.8, 155.5, 148.8, 140.4, 139.7, 135.62, 135.59, 134.7, 132.0, 129.5, 129.3, 128.9, 128.8, 128.6, 128.3, 128.1, 128.0, 127.1, 119.5, 55.7, 44.5. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{30}H_{25}N_4O_3$, 489.1921; Found: 489.1924.

1,3-dibenzyl-6-(4-bromophenyl)-1,3,5-triazine-2,4(1H,3H)-dione (10)



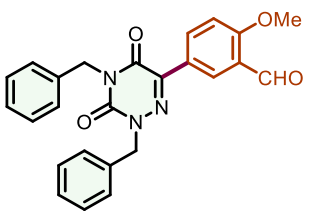
White solid (19.6 mg, 44%); m.p. 149.8 – 151.0 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.94 – 7.88 (m, 2H), 7.59 – 7.54 (m, 4H), 7.50 – 7.46 (m, 2H), 7.42 – 7.32 (m, 6H), 5.21 (d, J = 17.4 Hz, 4H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.3, 148.7, 140.1, 135.5, 135.4, 131.5, 130.9, 129.9, 129.6, 128.84, 128.83, 128.6, 128.4, 128.2, 124.6, 55.8, 44.6. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{23}H_{19}BrN_3O_2$, 448.0655; Found: 448.0670.

2,4-dibenzyl-6-(4-iodophenyl)-1,2,4-triazine-3,5(2H,4H)-dione (11)



White solid (28.2 mg, 57%); m.p. 112.7 – 113.9 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 – 7.72 (m, 4H), 7.54 (dd, J = 7.7, 1.6 Hz, 2H), 7.47 (dd, J = 7.8, 1.5 Hz, 2H), 7.42 – 7.32 (m, 6H), 5.20 (d, J = 17.1 Hz, 4H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.2, 148.7, 140.2, 137.5, 135.5, 135.4, 131.5, 129.9, 129.6, 128.84, 128.82, 128.6, 128.4, 128.2, 96.8, 55.8, 44.5. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{23}H_{19}IN_3O_2$, 496.0516; Found: 496.0518.

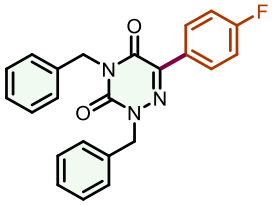
5-(2,4-dibenzyl-3,5-dioxo-2,3,4,5-tetrahydro-1,2,4-triazin-6-yl)-2-methoxybenzaldehyde (12)



White solid (23.1 mg, 54%); m.p. 89.2 – 89.9 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.50

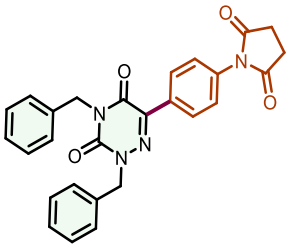
(s, 1H), 8.49 (d, *J* = 2.4 Hz, 1H), 8.30 (dd, *J* = 8.9, 2.4 Hz, 1H), 7.55 (dd, *J* = 7.8, 1.5 Hz, 2H), 7.48 (dd, *J* = 7.9, 1.4 Hz, 2H), 7.40 – 7.31 (m, 6H), 7.06 (d, *J* = 8.9 Hz, 1H), 5.21 (d, *J* = 18.9 Hz, 4H), 4.01 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.2, 162.7, 155.4, 148.7, 139.8, 135.8, 135.53, 135.50, 129.5, 129.1, 128.82, 128.79, 128.6, 128.3, 128.1, 124.9, 124.6, 111.4, 55.9, 55.8, 44.5. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{25}H_{22}N_3O_4$, 428.1605; Found: 428.1613.

2,4-dibenzyl-6-(4-fluorophenyl)-1,2,4-triazine-3,5(2H,4H)-dione (13)



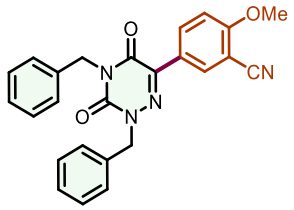
White solid (21.3 mg, 55%); m.p. 124.1 – 125.2 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.07 – 7.99 (m, 2H), 7.59 – 7.54 (m, 2H), 7.49 (d, *J* = 6.5 Hz, 2H), 7.42 – 7.31 (m, 6H), 7.13 (t, *J* = 8.7 Hz, 2H), 5.22 (d, *J* = 15.4 Hz, 4H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.8 (d, *J* = 250.8 Hz), 155.4, 148.7, 140.2, 135.5 (d, *J* = 2.3 Hz), 130.5, 130.4, 129.6, 128.8, 128.6, 128.4, 128.1, 115.5, 115.2, 55.7, 44.5. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -110.27. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{23}H_{19}FN_3O_2$, 388.1456; Found: 388.1460.

2,4-dibenzyl-6-(4-(2,5-dioxopyrrolidin-1-yl)phenyl)-1,2,4-triazine-3,5(2H,4H)-dione (14)



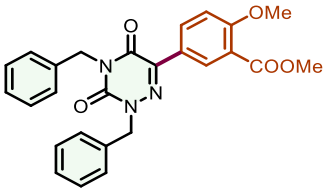
White solid (31.8 mg, 68%); m.p. 92.7 – 93.1 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.16 (d, *J* = 8.6 Hz, 2H), 7.57 – 7.54 (m, 2H), 7.50 – 7.47 (m, 2H), 7.42 – 7.32 (m, 8H), 5.23 (s, 2H), 5.19 (s, 2H), 2.93 (d, *J* = 6.0 Hz, 4H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.9, 155.3, 148.7, 140.0, 135.5, 135.4, 133.2, 132.1, 129.6, 129.2, 128.9, 128.8, 128.6, 128.4, 128.1, 126.1, 55.8, 44.5, 28.4. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{27}H_{23}N_4O_4$, 467.1714; Found: 467.1712.

5-(1,5-dibenzyl-4,6-dioxo-1,4,5,6-tetrahydro-1,3,5-triazin-2-yl)-2-methoxybenzonitrile (15)



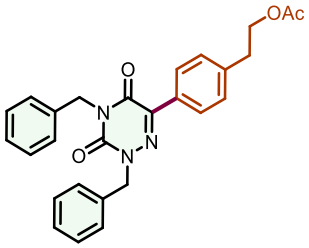
White solid (22.6 mg, 53%); m.p. 169.6 – 170.4 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 – 8.24 (m, 2H), 7.58 – 7.52 (m, 2H), 7.50 – 7.45 (m, 2H), 7.43 – 7.32 (m, 6H), 7.03 (d, *J* = 8.8 Hz, 1H), 5.21 (d, *J* = 18.7 Hz, 4H), 4.00 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.1, 155.3, 148.6, 138.6, 135.4, 135.3, 134.4, 133.8, 129.5, 128.9, 128.8, 128.6, 128.5, 128.2, 125.1, 116.0, 111.0, 102.1, 56.3, 55.8, 44.6. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{25}H_{21}N_4O_3$, 425.1608; Found: 425.1605.

Methyl-5-(2,4-dibenzyl-3,5-dioxo-2,3,4,5-tetrahydro-1,2,4-triazin-6-yl)-2-methoxybenzoate (16)



White solid (33.8 mg, 74%); m.p. 119.5 – 120.7 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.50 (d, *J* = 2.3 Hz, 1H), 8.19 (dd, *J* = 8.9, 2.4 Hz, 1H), 7.57 – 7.53 (m, 2H), 7.50 – 7.46 (m, 2H), 7.40 – 7.30 (m, 6H), 7.04 (d, *J* = 8.9 Hz, 1H), 5.21 (d, *J* = 17.6 Hz, 4H), 3.97 (s, 3H), 3.94 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.2, 160.3, 155.5, 148.7, 139.8, 135.6, 133.5, 131.9, 129.5, 128.8, 128.6, 128.3, 128.1, 124.2, 120.0, 111.7, 56.2, 55.7, 52.2, 44.5.. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{26}H_{24}N_3O_5$, 458.1710; Found: 458.1718.

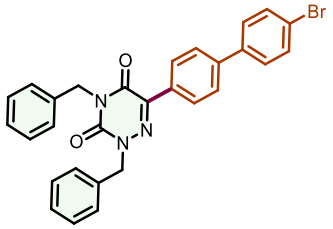
4-(2,4-dibenzyl-3,5-dioxo-2,3,4,5-tetrahydro-1,2,4-triazin-6-yl)phenethyl acetate (17)



White solid (32.7 mg, 72%); m.p. 104.2 – 105.5 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.94 (d, *J* = 8.3 Hz, 2H), 7.59 – 7.53 (m, 2H), 7.51 – 7.45 (m, 2H), 7.41 – 7.29 (m, 8H), 5.23 (s, 2H), 5.19 (s, 2H), 4.32 (t, *J* = 6.9 Hz, 2H), 3.00 (t, *J* = 6.9 Hz, 2H), 2.06 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 171.0, 155.5, 148.8, 141.0, 140.1, 135.62, 135.59, 130.4, 129.6, 128.82, 128.80, 128.77, 128.58, 128.56, 128.3, 128.1, 64.6, 55.7, 44.5, 34.9, 21.0. HRMS (ESI-TOF)

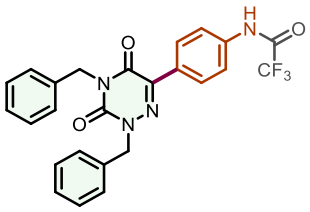
m/z: $[M + H]^+$ Calcd for $C_{27}H_{26}N_3O_4$, 456.1918; Found: 456.1923.

1,3-dibenzyl-6-(4'-bromo-[1,1'-biphenyl]-4-yl)-1,3,5-triazine-2,4(1H,3H)-dione (18)



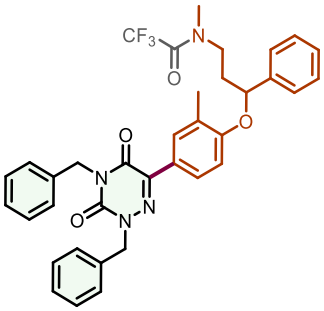
White solid (30.2 mg, 58%); m.p. 144.5 – 145.8 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.09 (d, *J* = 8.4 Hz, 2H), 7.66 – 7.56 (m, 6H), 7.51 (d, *J* = 8.5 Hz, 4H), 7.43 – 7.31 (m, 6H), 5.24 (d, *J* = 17.0 Hz, 4H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.5, 148.7, 141.4, 140.7, 139.2, 135.6, 135.5, 132.0, 131.3, 129.6, 128.94, 128.86, 128.8, 128.7, 128.6, 128.4, 128.1, 126.7, 122.1, 55.8, 44.5. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{29}H_{23}BrN_3O_2$, 524.0968; Found: 524.0970.

N-(4-(2,4-dibenzyl-3,5-dioxo-2,3,4,5-tetrahydro-1,2,4-triazin-6-yl)phenyl)-2,2,2-trifluoroacetamide (19)



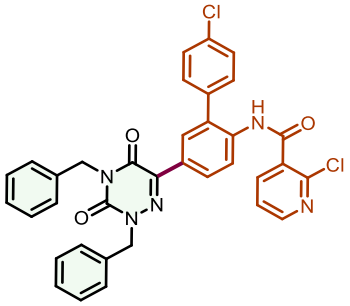
White solid (32.6 mg, 68%); m.p. 166.9 – 167.6 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.13 – 8.07 (m, 2H), 8.02 (s, 1H), 7.66 (d, *J* = 8.8 Hz, 2H), 7.57 – 7.53 (m, 2H), 7.50 – 7.46 (m, 2H), 7.43 – 7.30 (m, 6H), 5.22 (d, *J* = 19.1 Hz, 4H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.4, 154.7 (q, *J* = 37.7 Hz), 148.7, 139.9, 136.5, 135.5 (d, *J* = 4.7 Hz), 134.3, 130.2, 130.0, 129.5, 128.8, 128.6, 128.4, 128.2, 127.7, 119.9, 65.4, 55.8, 44.6. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -75.6. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{25}H_{20}F_3N_4O_3$, 481.1482; Found: 481.1490.

N-(3-(4-(2,4-dibenzyl-3,5-dioxo-2,3,4,5-tetrahydro-1,2,4-triazin-6-yl)-2-methylphenoxy)-3-phenylpropyl)-2,2,2-trifluoro-N-methylacetamide (20)



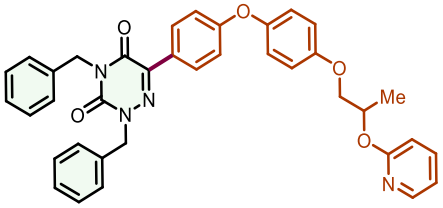
White solid (33.8 mg, 53%); m.p. 85.4 – 86.1 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.79 (s, 1H), 7.64 (dd, *J* = 8.6, 2.2 Hz, 1H), 7.52 (dd, *J* = 7.7, 1.6 Hz, 2H), 7.45 (dd, *J* = 7.8, 1.5 Hz, 2H), 7.38 – 7.27 (m, 11H), 6.62 (dd, *J* = 15.0, 8.7 Hz, 1H), 5.27 (dd, *J* = 8.4, 4.1 Hz, 1H), 5.19 (s, 2H), 5.16 (s, 2H), 3.80 – 3.55 (m, 2H), 3.18 – 3.03 (m, 3H), 2.41 (d, *J* = 4.1 Hz, 3H), 2.36 – 2.21 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.1, 156.9, 155.6, 148.8, 141.0, 141.0, 140.5, 140.1, 135.7, 130.8, 129.5, 129.0, 128.9, 128.7, 128.7, 128.5, 128.2, 128.2, 128.0, 127.4, 127.4, 126.8, 126.8, 125.6, 125.4, 124.5, 124.4, 112.2, 112.1, 55.6, 47.1, 46.6, 44.4, 37.5, 35.6, 35.4, 35.4, 34.8, 16.6, 16.5. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -68.93, -69.84. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{36}H_{34}F_3N_4O_4$, 643.2527; Found: 643.2535.

2-chloro-N-(4'-chloro-5-(2,4-dibenzyl-3,5-dioxo-2,3,4,5-tetrahydro-1,2,4-triazin-6-yl)-[1,1'-biphenyl]-2-yl)nicotinamide (21)



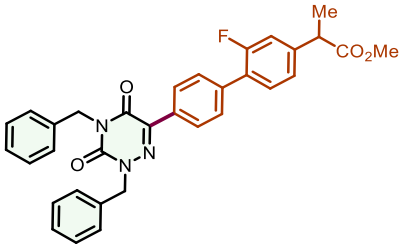
White solid (45.1 mg, 71%); m.p. 142.1 – 142.8 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.62 (d, *J* = 8.7 Hz, 1H), 8.49 (dd, *J* = 4.7, 1.9 Hz, 1H), 8.34 (s, 1H), 8.24 – 8.18 (m, 1H), 8.10 (dd, *J* = 8.7, 2.0 Hz, 1H), 8.00 (d, *J* = 2.1 Hz, 1H), 7.56 – 7.52 (m, 2H), 7.50 – 7.47 (m, 4H), 7.42 – 7.31 (m, 9H), 5.24 (s, 2H), 5.19 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.4, 155.4, 151.5, 148.7, 146.6, 140.5, 140.0, 136.0, 135.6, 135.52, 135.47, 134.8, 131.4, 130.9, 130.8, 130.2, 129.50, 129.46, 128.9, 128.83, 128.79, 128.63, 128.61, 128.4, 128.1, 123.0, 121.1, 55.8, 44.5. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{35}H_{26}Cl_2N_5O_3$, 634.1407; Found: 634.1424.

1,3-dibenzyl-6-(4-(4-(2-(pyridin-2-yloxy)propoxy)phenoxy)phenyl)-1,3,5-triazine-2,4(1H,3H)-dione (22)



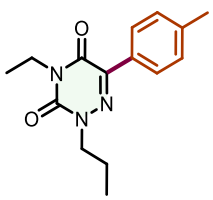
Yellow solid (39.2 mg, 64%); m.p. 62.7 – 64.5 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.19 (dd, *J* = 5.0, 1.5 Hz, 1H), 8.02 – 7.91 (m, 2H), 7.62 – 7.54 (m, 3H), 7.50 – 7.46 (m, 2H), 7.41 – 7.31 (m, 6H), 7.03 – 6.96 (m, 6H), 6.91 – 6.88 (m, 1H), 6.78 (d, *J* = 8.3 Hz, 1H), 5.67 – 5.60 (m, 1H), 5.21 (d, *J* = 11.6 Hz, 4H), 4.23 (dd, *J* = 9.9, 5.3 Hz, 1H), 4.12 (dd, *J* = 9.9, 4.8 Hz, 1H), 1.52 (d, *J* = 6.4 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.1, 160.3, 155.7, 155.6, 149.4, 148.8, 146.8, 140.7, 138.7, 135.7, 130.0, 129.5, 128.82, 128.77, 128.6, 128.3, 128.1, 126.1, 121.3, 116.83, 116.80, 115.9, 111.7, 71.1, 69.2, 55.7, 44.5, 17.0. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{37}H_{33}N_4O_5$, 613.2445; Found: 613.2454.

Methyl-2-(4'-(2,4-dibenzyl-3,5-dioxo-2,3,4,5-tetrahydro-1,2,4-triazin-6-yl)-2-fluoro-[1,1'-biphenyl]-4-yl)propanoate (23)



White solid (39.8 mg, 72%); m.p. 61.7 – 62.2 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.09 (d, *J* = 8.5 Hz, 2H), 7.66 – 7.62 (m, 2H), 7.60 – 7.56 (m, 2H), 7.53 – 7.49 (m, 2H), 7.47 – 7.33 (m, 7H), 7.22 – 7.15 (m, 2H), 5.26 (s, 2H), 5.22 (s, 2H), 3.81 (q, *J* = 7.2 Hz, 1H), 3.74 (s, 3H), 1.58 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.4, 159.8 (d, *J* = 249.1 Hz), 155.5, 148.8, 142.3 (d, *J* = 7.7 Hz), 140.8, 137.1, 135.62, 135.56, 131.3, 130.7 (d, *J* = 3.7 Hz), 129.6, 128.9, 128.8, 128.6, 128.5, 128.4, 128.1, 127.1, 127.0, 123.7 (d, *J* = 3.3 Hz), 115.4 (d, *J* = 23.5 Hz), 55.8, 52.3, 45.0, 44.5, 18.4. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -117.03. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{33}H_{29}FN_3O_4$, 550.2137; Found: 550.2149.

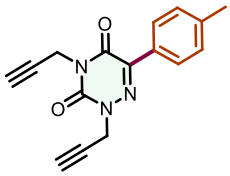
3-ethyl-1-propyl-6-(p-tolyl)-1,3,5-triazine-2,4(1H,3H)-dione (24)



White solid (20.0 mg, 73%); m.p. 96.5 – 97.5 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 –

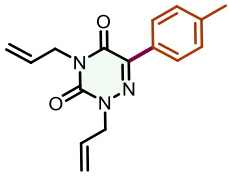
7.84 (m, 2H), 7.26 (d, J = 8.0 Hz, 2H), 4.14 (q, J = 7.2 Hz, 2H), 4.04 – 3.97 (m, 2H), 2.42 (s, 3H), 1.70 – 1.79 (m, 2H), 1.42 (t, J = 7.2 Hz, 3H), 1.01 (t, J = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.7, 148.5, 140.9, 140.0, 129.5, 129.0, 128.2, 47.1, 42.7, 21.4, 20.6, 13.5, 11.4. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{15}H_{20}N_3O_2$, 274.1550; Found: 274.1559.

2,4-di(prop-2-yn-1-yl)-6-(p-tolyl)-1,2,4-triazine-3,5(2H,4H)-dione (25)



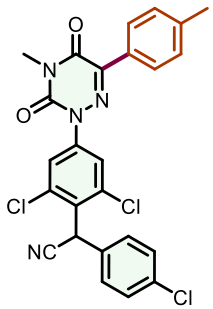
White solid (19.8 mg, 71%); m.p. 149.0 – 149.7 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.95 (d, J = 8.0 Hz, 2H), 7.27 (d, J = 8.4 Hz, 2H), 4.84 (dd, J = 30.2, 1.8 Hz, 4H), 2.42 (s, 4H), 2.27 (s, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.6, 147.5, 141.7, 140.8, 129.1, 128.6, 128.4, 76.8, 76.7, 73.7, 71.7, 41.7, 30.3, 21.5. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{16}H_{14}N_3O_2$, 280.1081; Found: 280.1079.

2,4-diallyl-6-(p-tolyl)-1,2,4-triazine-3,5(2H,4H)-dione (26)



White solid (16.1 mg, 57%); m.p. 92.0 – 92.7 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 (d, J = 8.2 Hz, 2H), 7.26 (d, J = 8.1 Hz, 2H), 6.08 – 5.89 (m, 2H), 5.41 – 5.26 (m, 4H), 4.67 (dd, J = 16.3, 6.1 Hz, 4H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.3, 148.3, 141.2, 140.3, 131.5, 130.5, 129.2, 129.0, 128.3, 119.3, 119.2, 54.4, 43.2, 21.4. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{16}H_{18}N_3O_2$, 284.1394; Found: 284.1400.

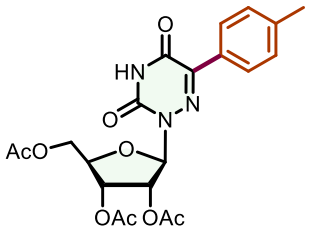
2-(4-chlorophenyl)-2-(2,6-dichloro-4-(4-methyl-3,5-dioxo-6-(p-tolyl)-4,5-dihydro-1,2,4-triazin-2(3H)-yl)phenyl)acetonitrile (27)



White solid (27.0 mg, 53%); m.p. 123.0 – 123.6 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.94

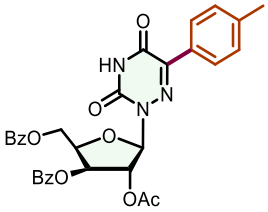
(d, *J* = 8.3 Hz, 2H), 7.87 (s, 2H), 7.40 – 7.29 (m, 6H), 6.22 (s, 1H), 3.53 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.0, 148.0, 142.7, 141.7, 141.3, 135.7, 134.3, 130.8, 129.9, 129.3, 129.2, 128.6, 128.4, 128.2, 125.0, 116.3, 37.0, 27.9, 21.5. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{25}H_{18}C_{l3}N_4O_2$, 511.0490; Found: 511.0501.

(2R,3R,4R,5R)-2-(acetoxymethyl)-5-(3,5-dioxo-6-(p-tolyl)-4,5-dihydro-1,2,4-triazin-2(3H)-yl)tetrahydrofuran-3,4-diyl diacetate (28)



White solid (23.5 mg, 51%); m.p. 107.0 – 107.5 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.62 (s, 1H), 7.95 (d, *J* = 8.2 Hz, 2H), 7.28 (d, *J* = 8.1 Hz, 2H), 6.42 (d, *J* = 2.8 Hz, 1H), 5.78 (dd, *J* = 5.3, 2.9 Hz, 1H), 5.67 – 5.59 (m, 1H), 4.39 (ddt, *J* = 10.6, 7.2, 3.2 Hz, 2H), 4.23 – 4.14 (m, 1H), 2.41 (s, 3H), 2.15 (d, *J* = 7.3 Hz, 6H), 1.84 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 170.6, 169.7, 169.6, 155.3, 148.0, 143.4, 141.3, 129.3, 128.4, 128.1, 88.1, 79.1, 73.1, 70.3, 62.8, 21.4, 20.54, 20.50, 20.4. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{21}H_{23}N_3NaO_9$, 484.1327; Found: 484.1333.

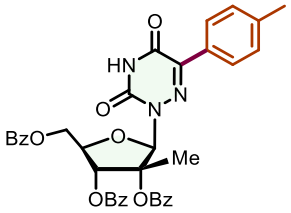
(2R,3R,4R,5R)-4-acetoxy-2-((benzoyloxy)methyl)-5-(3,5-dioxo-6-(p-tolyl)-4,5-dihydro-1,2,4-triazin-2(3H)-yl)tetrahydrofuran-3-yl benzoate (29)



White solid (30.4 mg, 52%); m.p. 129.5 – 130.2 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.41 (s, 1H), 8.01 – 7.93 (m, 4H), 7.74 (d, *J* = 8.2 Hz, 2H), 7.58 – 7.52 (m, 2H), 7.39 (t, *J* = 7.8 Hz, 2H), 7.31 (d, *J* = 7.8 Hz, 2H), 6.91 (d, *J* = 8.1 Hz, 2H), 6.35 (d, *J* = 3.6 Hz, 1H), 5.90 (dd, *J* = 3.6, 2.1 Hz, 1H), 5.76 (dd, *J* = 4.6, 2.0 Hz, 1H), 4.81 (dt, *J* = 6.6, 4.8 Hz, 1H), 4.70 (h, *J* = 6.8 Hz, 2H), 2.30 (s, 3H), 2.20 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 169.9, 166.1, 165.6, 155.3, 148.2, 143.4, 140.7, 133.5, 133.2, 130.0, 129.7, 129.4, 128.9, 128.7, 128.5, 128.4, 128.0, 89.7, 78.8, 76.3, 62.3, 21.4, 20.7. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{31}H_{27}N_3NaO_9$, 608.1640; Found: 608.1647.

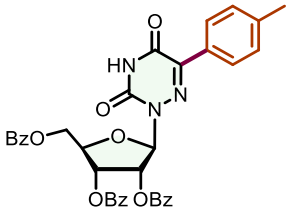
(2R,3R,4R,5R)-5-((benzoyloxy)methyl)-2-(3,5-dioxo-6-(p-tolyl)-4,5-dihydro-1,2,4-

triazin-2(3H)-yl)-3-methyltetrahydrofuran-3,4-diyl dibenzoate (30)



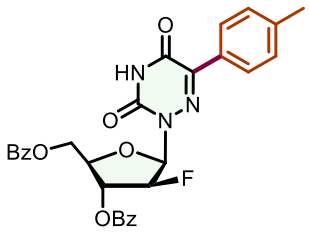
White solid (31.1 mg, 47%); m.p. 131.3 – 132.9 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.19 (s, 1H), 8.21 – 8.11 (m, 4H), 8.05 (d, *J* = 8.3 Hz, 2H), 7.97 – 7.89 (m, 2H), 7.64 (t, *J* = 7.4 Hz, 2H), 7.55 – 7.45 (m, 5H), 7.34 (d, *J* = 8.1 Hz, 2H), 7.28 – 7.22 (m, 3H), 6.25 (d, *J* = 8.8 Hz, 1H), 4.83 (ddd, *J* = 8.7, 7.1, 4.1 Hz, 1H), 4.72 (dd, *J* = 11.8, 4.1 Hz, 1H), 4.60 (dd, *J* = 11.8, 7.1 Hz, 1H), 2.45 (s, 3H), 1.89 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.1, 165.6, 164.9, 155.1, 147.9, 143.4, 141.4, 133.7, 133.5, 133.0, 130.2, 130.0, 129.9, 129.7, 129.6, 129.4, 129.0, 128.60, 128.56, 128.4, 128.2, 128.0, 88.4, 87.3, 65.0, 21.5, 17.6. HRMS (ESI-TOF) *m/z*: [M + Na]$^{+}$ Calcd for $C_{37}H_{31}N_3NaO_9$, 684.1953; Found: 684.1962.

(2R,3R,4R,5R)-2-((benzoyloxy)methyl)-5-(3,5-dioxo-6-(p-tolyl)-4,5-dihydro-1,2,4-triazin-2(3H)-yl)tetrahydrofuran-3,4-diyl dibenzoate (31)



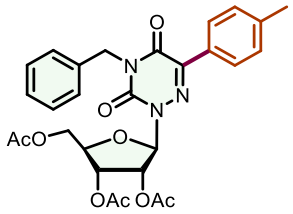
White solid (45.9 mg, 71%); m.p. 127.6 – 128.7 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.35 (s, 1H), 7.98 (dd, *J* = 12.0, 8.2 Hz, 8H), 7.58 (td, *J* = 7.4, 3.4 Hz, 2H), 7.44 (dq, *J* = 22.0, 7.4 Hz, 5H), 7.24 (dd, *J* = 8.2, 2.1 Hz, 3H), 6.68 (d, *J* = 2.9 Hz, 1H), 6.24 (dd, *J* = 5.4, 3.0 Hz, 1H), 6.06 (t, *J* = 6.1 Hz, 1H), 4.91 – 4.72 (m, 2H), 4.60 (dd, *J* = 12.1, 4.9 Hz, 1H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.2, 165.3, 165.2, 155.3, 147.9, 143.4, 141.2, 133.7, 133.6, 133.1, 129.9, 129.8, 129.7, 129.4, 129.3, 128.8, 128.7, 128.53, 128.50, 128.48, 128.3, 128.0, 88.6, 73.7, 71.3, 63.6, 21.5. HRMS (ESI-TOF) *m/z*: [M + Na]$^{+}$ Calcd for $C_{36}H_{29}N_3NaO_9$, 670.1796; Found: 670.1791.

((2R,3R,4R,5R)-3-(benzoyloxy)-5-(3,5-dioxo-6-(p-tolyl)-4,5-dihydro-1,2,4-triazin-2(3H)-yl)-4-fluorotetrahydrofuran-2-yl)methyl benzoate (32)



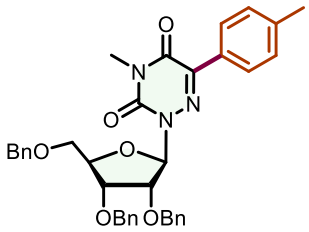
White solid (33.8 mg, 62%); m.p. 101.3 – 102.7 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.46 (s, 1H), 8.10 (d, *J* = 8.0 Hz, 2H), 7.96 (t, *J* = 7.4 Hz, 4H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.50 (t, *J* = 6.8 Hz, 3H), 7.43 – 7.12 (m, 5H), 6.82 (d, *J* = 6.4 Hz, 1H), 6.31 (dt, *J* = 16.2, 6.4 Hz, 1H), 5.66 (dt, *J* = 51.5, 6.1 Hz, 1H), 4.76 (dd, *J* = 11.6, 4.1 Hz, 1H), 4.70 – 4.62 (m, 1H), 4.53 (q, *J* = 6.5 Hz, 1H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.0, 165.5, 155.2, 148.3, 143.5, 141.2, 133.8, 133.1, 129.9, 129.7, 129.4, 128.7, 128.6, 128.5, 128.3, 128.0, 92.5 (d, *J* = 203.1 Hz), 82.9 (d, *J* = 16.9 Hz), 78.5 (d, *J* = 8.7 Hz), 75.7 (d, *J* = 22.8 Hz), 65.1, 21.5. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -202.82. HRMS (ESI-TOF) *m/z*: [M + Na]$^{+}$ Calcd for $C_{29}H_{24}FN_3NaO_7$, 568.1490; Found: 568.1495.

(2R,3R,4R,5R)-2-(acetoxymethyl)-5-(4-benzyl-3,5-dioxo-6-(p-tolyl)-4,5-dihydro-1,2,4-triazin-2(3H)-yl)tetrahydrofuran-3,4-diyl diacetate (33)



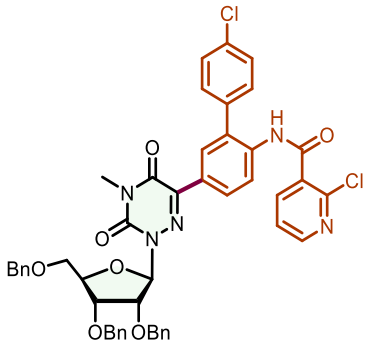
White solid (32.5 mg, 59%); m.p. 142.5 – 143.2 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 8.3 Hz, 2H), 7.59 – 7.53 (m, 2H), 7.36 – 7.26 (m, 5H), 6.46 (d, *J* = 2.9 Hz, 1H), 5.78 (dd, *J* = 5.3, 2.9 Hz, 1H), 5.69 – 5.58 (m, 1H), 5.25 – 5.13 (m, 2H), 4.41 – 4.32 (m, 2H), 4.22 – 4.15 (m, 1H), 2.41 (s, 3H), 2.15 (s, 3H), 2.13 (s, 3H), 1.82 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 170.6, 169.6, 169.5, 155.0, 148.6, 142.7, 141.0, 135.2, 129.8, 129.2, 128.7, 128.6, 128.5, 128.2, 88.9, 79.0, 73.1, 70.2, 62.8, 44.6, 21.4, 20.6, 20.5, 20.4. HRMS (ESI-TOF) *m/z*: [M + Na]$^{+}$ Calcd for $C_{28}H_{29}N_3NaO_9$, 574.1796; Found: 574.1805.

2-((2R,3R,4R,5R)-3,4-bis(benzyloxy)-5-((benzyloxy)methyl)tetrahydrofuran-2-yl)-4-methyl-6-(p-tolyl)-1,2,4-triazine-3,5(2H,4H)-dione (34)



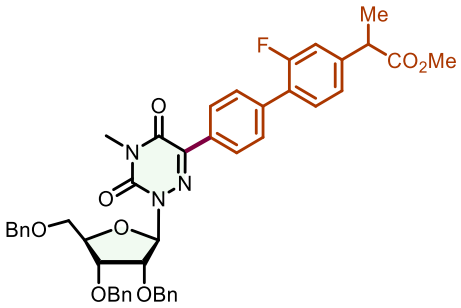
White solid (41.4 mg, 67%); m.p. 112.9 – 114.1 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 (d, *J* = 8.2 Hz, 2H), 7.35 – 7.30 (m, 7H), 7.29 – 7.25 (m, 6H), 7.23 (dt, *J* = 6.0, 3.3 Hz, 2H), 7.19 (d, *J* = 8.1 Hz, 2H), 6.49 (d, *J* = 3.6 Hz, 1H), 4.67 (dd, *J* = 12.1, 4.2 Hz, 2H), 4.60 (dd, *J* = 12.1, 4.1 Hz, 2H), 4.55 – 4.45 (m, 2H), 4.39 (dt, *J* = 7.5, 3.8 Hz, 2H), 4.31 (t, *J* = 5.5 Hz, 1H), 3.63 (qd, *J* = 10.8, 4.5 Hz, 2H), 3.40 (s, 3H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.3, 148.7, 141.4, 140.3, 137.9, 137.6, 137.4, 129.1, 129.0, 128.43, 128.40, 128.36, 128.3, 128.1, 128.0, 127.96, 127.93, 127.6, 89.5, 81.4, 78.6, 76.6, 73.4, 72.5, 72.4, 69.7, 27.5, 21.5. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{37}H_{38}N_3O_6$, 620.2755; Found: 620.2753.

N-(5-(2-((2R,3R,4R,5R)-3,4-bis(benzyloxy)-5-((benzyloxy)methyl)tetrahydrofuran-2-yl)-4-methyl-3,5-dioxo-2,3,4,5-tetrahydro-1,2,4-triazin-6-yl)-4'-chloro-[1,1'-biphenyl]-2-yl)-2-chloronicotinamide (35)



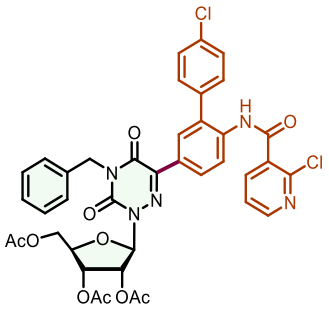
White solid (37.4 mg, 43%); m.p. 62.0 – 63.1 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.57 (d, *J* = 8.7 Hz, 1H), 8.49 (dd, *J* = 4.7, 1.9 Hz, 1H), 8.34 (s, 1H), 8.22 (d, *J* = 7.4 Hz, 1H), 7.93 (d, *J* = 2.0 Hz, 1H), 7.87 (dd, *J* = 8.8, 1.9 Hz, 1H), 7.46 – 7.40 (m, 3H), 7.36 – 7.27 (m, 14H), 7.19 (dd, *J* = 6.7, 2.4 Hz, 2H), 6.49 (d, *J* = 3.8 Hz, 1H), 4.72 – 4.53 (m, 5H), 4.44 – 4.37 (m, 4H), 4.30 (t, *J* = 5.3 Hz, 1H), 3.65 – 3.56 (m, 2H), 3.40 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.4, 155.2, 151.6, 148.6, 146.6, 140.4, 140.1, 137.8, 137.5, 137.4, 136.1, 135.6, 134.9, 131.3, 130.8, 130.4, 129.5, 128.8, 128.6, 128.5, 128.44, 128.4, 128.3, 128.02, 127.98, 127.96, 127.6, 127.5, 123.0, 121.2, 89.6, 81.5, 78.6, 73.3, 72.6, 72.5, 69.6, 27.5. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{48}H_{42}Cl_2N_5O_7$, 870.2456; Found: 870.2460.

Methyl-2-(4'-(2-((2R,3R,4R,5R)-3,4-bis(benzyloxy)-5-((benzyloxy)methyl)tetrahydrofuran-2-yl)-4-methyl-3,5-dioxo-2,3,4,5-tetrahydro-1,2,4-triazin-6-yl)-2-fluoro-[1,1'-biphenyl]-4-yl)propanoate (36)



White solid (49.5 mg, 63%); m.p. 108.7 – 109.4 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 (d, *J* = 8.6 Hz, 2H), 7.61 – 7.54 (m, 2H), 7.46 (s, 1H), 7.36 – 7.23 (m, 16H), 6.52 (d, *J* = 3.7 Hz, 1H), 4.76 – 4.58 (m, 5H), 4.53 (dd, *J* = 12.4, 8.1 Hz, 2H), 4.44 – 4.33 (m, 3H), 3.83 (q, *J* = 7.2, 6.2 Hz, 1H), 3.75 (s, 3H), 3.70 – 3.62 (m, 2H), 3.43 (s, 3H), 1.60 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.4, 159.8 (d, *J* = 249.2 Hz), 155.6, 155.3, 148.7, 142.5 (d, *J* = 7.7 Hz), 140.9, 138.1, 137.9, 137.7, 137.6, 137.4, 137.3, 137.2, 134.4, 131.1, 130.7 (d, *J* = 3.6 Hz), 128.8 (d, *J* = 3.2 Hz), 128.5, 128.5, 128.4, 128.3, 128.1, 128.0, 128.0, 127.6, 127.6, 127.5, 127.0 (d, *J* = 13.3 Hz), 125.6, 123.8 (d, *J* = 3.3 Hz), 115.5 (d, *J* = 23.5 Hz), 89.5, 81.5, 78.5, 76.4, 73.4, 72.5, 72.4, 69.6, 52.3, 45.0, 31.3, 27.6, 18.5. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -117.02. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{46}H_{45}FN_3O_8$, 786.3185; Found: 786.3187.

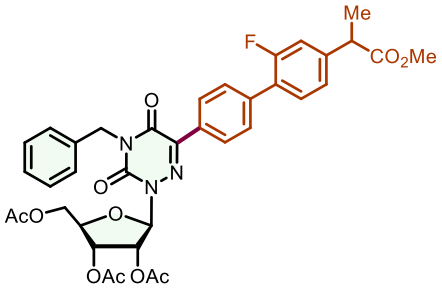
(2R,3R,4R,5R)-2-(acetoxymethyl)-5-(4-benzyl-6-(4'-chloro-6-(2-chloronicotinamido)-[1,1'-biphenyl]-3-yl)-3,5-dioxo-4,5-dihydro-1,2,4-triazin-2(3H)-yl)tetrahydrofuran-3,4-diyl diacetate compound with methane (37)



White solid (33.5 mg, 41%); m.p. 100.0 – 101.1 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.66 (d, *J* = 8.7 Hz, 1H), 8.48 (dd, *J* = 4.7, 2.0 Hz, 1H), 8.37 (s, 1H), 8.23 – 8.18 (m, 1H), 8.13 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.99 (d, *J* = 2.1 Hz, 1H), 7.57 – 7.53 (m, 2H), 7.50 – 7.46 (m, 2H), 7.42 – 7.31 (m, 6H), 6.44 (d, *J* = 2.9 Hz, 1H), 5.78 (dd, *J* = 5.4, 2.9 Hz, 1H), 5.60 – 5.54 (m, 1H), 5.18 (d, *J* = 2.7 Hz, 2H), 4.42 – 4.32 (m, 2H), 4.20 – 4.14 (m, 1H), 2.14 (s, 3H), 2.12 (s, 3H), 1.86 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 170.4, 169.4, 169.4, 154.9, 151.5, 148.5, 146.6, 141.6, 140.4, 136.6, 135.4, 135.1, 134.9, 131.6, 131.0, 130.8, 130.5, 129.7, 129.5, 129.2, 128.6, 128.3, 128.0, 123.0, 121.2, 89.2, 73.0, 70.3, 62.9, 44.7, 20.5, 20.4, 20.4. HRMS (ESI-TOF) *m/z*:

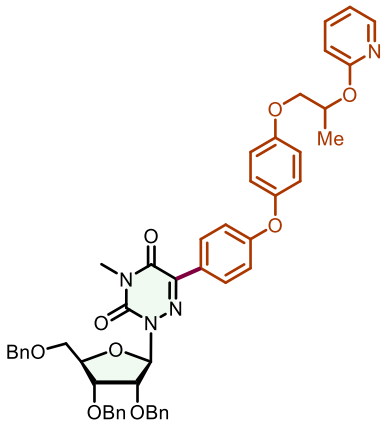
$[M + Na]^+$ Calcd for $C_{40}H_{37}C_{l2}N_5NaO_{10,}$ 840.1810; Found: 840.1815.

(2R,3R,4R,5R)-2-(acetoxymethyl)-5-(4-benzyl-6-(2'-fluoro-4'-(1-methoxy-1-oxopropan-2-yl)-[1,1'-biphenyl]-4-yl)-3,5-dioxo-4,5-dihydro-1,2,4-triazin-2(3H)-yl)tetrahydrofuran-3,4-diyl diacetate (38)



White solid (33.7 mg, 47%); m.p. 97.0 – 98.1 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.10 (d, *J* = 8.5 Hz, 2H), 7.70 – 7.62 (m, 2H), 7.62 – 7.55 (m, 2H), 7.44 (t, *J* = 8.0 Hz, 1H), 7.38 – 7.32 (m, 3H), 7.22 – 7.13 (m, 2H), 6.47 (d, *J* = 3.0 Hz, 1H), 5.81 (dd, *J* = 5.3, 3.0 Hz, 1H), 5.65 – 5.60 (m, 1H), 5.29 – 5.15 (m, 2H), 4.44 – 4.35 (m, 2H), 4.21 (dd, *J* = 12.0, 4.6 Hz, 1H), 3.79 (q, *J* = 7.2 Hz, 1H), 3.73 (s, 3H), 2.16 (s, 3H), 2.13 (s, 3H), 1.82 (s, 3H), 1.56 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.3, 170.6, 169.6, 169.5, 161.0, 155.0, 148.6, 142.3, 137.8, 135.1, 130.69, 130.67, 130.7, 129.8, 129.6, 129.0 (d, *J* = 3.1 Hz), 128.7 (d, *J* = 4.9 Hz), 128.3, 127.0, 126.8, 123.7 (d, *J* = 3.1 Hz), 115.4 (d, *J* = 23.5 Hz), 89.0, 79.1, 73.0, 70.3, 62.8, 52.3, 45.0, 44.7, 20.5 (d, *J* = 5.3 Hz), 20.3, 18.4. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -116.94. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{37}H_{37}FN_3O_{11}$, 718.2407; Found: 718.2412.

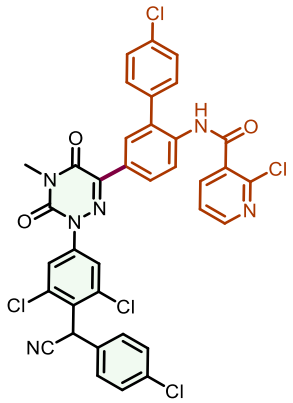
2-((2R,3R,4R,5R)-3,4-bis(benzyloxy)-5-((benzyloxy)methyl)tetrahydrofuran-2-yl)-4-methyl-6-(4-(4-(2-(pyridin-2-yloxy)propoxy)phenoxy)phenyl)-1,2,4-triazine-3,5(2H,4H)-dione (39)



Colorless oil (38.2 mg, 45%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.19 (dd, *J* = 4.9, 1.6 Hz,

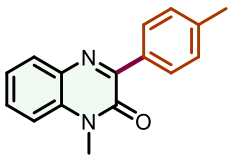
1H), 7.77 (d, *J* = 8.9 Hz, 2H), 7.60 (td, *J* = 8.1, 7.4, 1.9 Hz, 1H), 7.34 – 7.22 (m, 14H), 7.07 – 6.99 (m, 4H), 6.94 – 6.84 (m, 3H), 6.81 – 6.75 (m, 1H), 6.50 (d, *J* = 3.5 Hz, 1H), 5.65 (h, *J* = 6.1 Hz, 1H), 4.74 – 4.54 (m, 5H), 4.52 – 4.45 (m, 2H), 4.40 (d, *J* = 5.1 Hz, 2H), 4.34 – 4.30 (m, 1H), 4.26 (dd, *J* = 9.9, 5.3 Hz, 1H), 4.14 (dd, *J* = 9.9, 4.8 Hz, 1H), 3.69 – 3.58 (m, 2H), 3.40 (s, 3H), 1.53 (d, *J* = 6.4 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.2, 160.4, 155.8, 155.3, 149.2, 148.7, 146.8, 140.7, 138.7, 137.9, 137.6, 137.4, 130.0, 128.43, 128.40, 128.3, 128.03, 127.99, 128.0, 127.9, 127.6, 127.5, 125.8, 121.4, 116.8, 116.7, 116.0, 111.7, 89.5, 81.4, 76.5, 73.4, 72.5, 72.3, 71.1, 69.7, 69.2, 27.5, 17.0. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{50}H_{49}N_4O_9$, 849.3494; Found: 849.3494.

2-chloro-N-(4'-chloro-5-(2-(3,5-dichloro-4-((4-chlorophenyl)(cyano)methyl)phenyl)-4-methyl-3,5-dioxo-2,3,4,5-tetrahydro-1,2,4-triazin-6-yl)-[1,1'-biphenyl]-2-yl)nicotinamide (40)



White solid (26.6 mg, 35%); m.p. 147.3 – 148.6 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.69 (d, *J* = 8.7 Hz, 1H), 8.50 (dd, *J* = 4.7, 2.0 Hz, 1H), 8.41 (s, 1H), 8.23 (dd, *J* = 7.7, 1.7 Hz, 1H), 8.16 (dd, *J* = 8.8, 2.1 Hz, 1H), 8.00 (d, *J* = 2.1 Hz, 1H), 7.84 (s, 2H), 7.52 – 7.48 (m, 2H), 7.43 – 7.33 (m, 7H), 6.22 (s, 1H), 3.54 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.4, 155.0, 151.6, 147.8, 146.6, 141.6, 141.5, 140.6, 136.9, 135.8, 135.3, 135.1, 134.4, 131.6, 130.9, 130.7, 130.6, 130.5, 130.2, 129.6, 129.3, 129.2, 128.3, 127.6, 125.2, 123.0, 121.1, 116.2, 37.0, 28.0. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{36}H_{22}Cl_5N_6O_3$, 761.0191; Found: 761.0186.

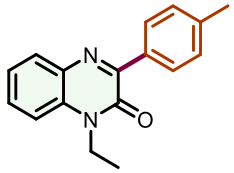
1-methyl-3-(p-tolyl)quinoxalin-2(1H)-one (41)[4]



Yellow solid (21.5 mg, 86%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.24 (d, *J* = 8.2 Hz, 2H), 7.96 – 7.90 (m, 1H), 7.59 – 7.51 (m, 1H), 7.38 – 7.26 (m, 4H), 3.76 (s, 3H), 2.42 (s, 3H); ^{13}C

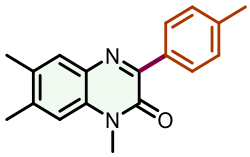
NMR (101 MHz, Chloroform-*d*) δ 154.8, 154.0, 140.6, 133.4, 133.3, 133.2, 130.3, 130.0, 129.5, 128.8, 123.7, 113.5, 29.3, 21.5.

1-ethyl-3-(p-tolyl)quinoxalin-2(1H)-one (42)



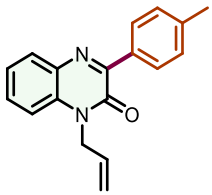
Light yellow solid (22.5 mg, 85%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.25 (d, *J* = 8.2 Hz, 2H), 7.95 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.55 (td, *J* = 7.8, 7.2, 1.4 Hz, 1H), 7.38 – 7.32 (m, 2H), 7.29 (d, *J* = 8.2 Hz, 2H), 4.39 (q, *J* = 7.2 Hz, 2H), 2.42 (s, 3H), 1.42 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.3, 154.0, 140.6, 133.5, 133.3, 132.2, 130.6, 130.0, 129.6, 128.8, 123.5, 113.4, 37.6, 21.5, 12.4.

1,6,7-trimethyl-3-(p-tolyl)quinoxalin-2(1H)-one (43)[5]



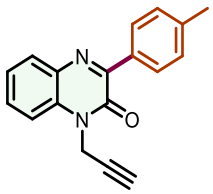
Yellow solid (21.7 mg, 78%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.22 (d, *J* = 8.1 Hz, 2H), 7.65 (s, 1H), 7.26 (d, *J* = 8.2 Hz, 2H), 7.05 (s, 1H), 3.70 (s, 3H), 2.40 (s, 6H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.8, 152.7, 140.2, 139.9, 133.6, 132.5, 131.6, 131.3, 130.4, 129.4, 128.7, 114.1, 29.1, 21.5, 20.6, 19.2.

1-allyl-3-(p-tolyl)quinoxalin-2(1H)-one (44)



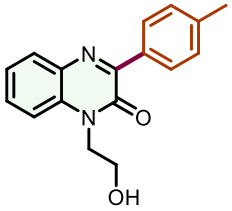
Yellow solid (20.5 mg, 74%); m.p. 107.3 – 108.05 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.27 (d, *J* = 8.2 Hz, 2H), 7.98 – 7.91 (m, 1H), 7.57 – 7.47 (m, 1H), 7.32 (dt, *J* = 20.5, 7.7 Hz, 4H), 5.98 (m, *J* = 15.6, 10.3, 5.1 Hz, 1H), 5.25 (dd, *J* = 27.0, 13.9 Hz, 2H), 4.97 (d, *J* = 5.1 Hz, 2H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.3, 154.0, 140.7, 133.3, 133.2, 132.5, 130.7, 130.4, 129.9, 129.6, 128.8, 123.6, 118.1, 114.0, 44.7, 21.5. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{18}H_{16}N_2NaO$, 299.1155; Found: 299.1157

1-(prop-2-yn-1-yl)-3-(p-tolyl)quinoxalin-2(1H)-one (45)



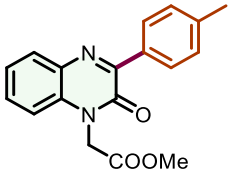
Light yellow solid (19.2 mg, 70%); m.p. 170.4 – 171.5 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.25 (d, *J* = 8.3 Hz, 2H), 7.94 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.58 (m, *J* = 8.6, 7.3, 1.5 Hz, 1 H), 7.49 – 7.45 (m, 1H), 7.41 – 7.36 (m, 1H), 7.28 (d, *J* = 8.1 Hz, 2H), 5.11 (d, *J* = 2.5 Hz, 2H), 2.42 (s, 3H), 2.30 (t, *J* = 2.5 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.83, 153.78, 140.9, 133.3, 133.0, 131.8, 130.5, 130.2, 129.6, 128.9, 124.1, 114.0, 73.1, 31.7, 21.6. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{18}H_{14}N_2NaO$, 297.0998; Found: 297.1003.

1-(2-hydroxyethyl)-3-(p-tolyl)quinoxalin-2(1H)-one (46)



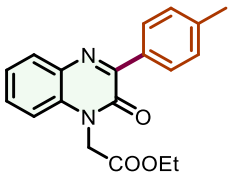
Yellow solid (18.3 mg, 65%); m.p. 163.4 – 164.4 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.23 (d, *J* = 8.2 Hz, 2H), 7.97 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.59 – 7.53 (m, 1H), 7.44 (d, *J* = 8.3 Hz, 1H), 7.39 (t, *J* = 7.9 Hz, 1H), 7.31 (d, *J* = 8.1 Hz, 2H), 4.57 (t, *J* = 5.5 Hz, 2H), 4.10 (t, *J* = 5.5 Hz, 2H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.8, 153.8, 140.8, 133.5, 133.0, 132.7, 130.6, 130.1, 129.5, 128.9, 123.9, 113.7, 60.8, 45.2, 21.5. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{17}H_{16}N_2NaO_2$, 303.1104; Found: 303.1106.

methyl 2-(2-oxo-3-(p-tolyl)quinoxalin-1(2H)-yl)acetate (47)



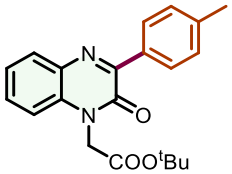
Yellow solid (16.5 mg, 54%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.29 (d, *J* = 8.3 Hz, 2H), 7.99 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.55 (ddd, *J* = 8.5, 7.4, 1.5 Hz, 1H), 7.42 – 7.37 (m, 1H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.14 – 7.10 (m, 1H), 5.13 (s, 2H), 3.82 (s, 3H), 2.45 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.8, 154.3, 153.7, 140.9, 133.2, 133.0, 132.4, 130.7, 130.2, 129.6, 128.8, 124.0, 112.9, 52.9, 43.6, 21.5.

ethyl 2-(2-oxo-3-(p-tolyl)quinoxalin-1(2H)-yl)acetate (48) [5]



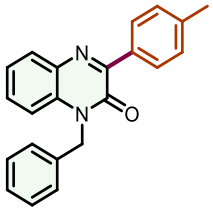
Yellow solid (22.3 mg, 69%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.29 (d, *J* = 8.2 Hz, 2H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.56 – 7.50 (m, 1H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.11 (d, *J* = 8.3 Hz 1H), 5.10 (s, 2H), 4.29 (q, *J* = 7.1 Hz 2H), 2.44 (s, 3H), 1.31 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.3, 154.4, 153.7, 140.8, 133.2, 133.0, 132.5, 130.7, 130.2, 129.6, 128.8, 124.0, 113.0, 62.1, 43.8, 21.5, 14.1.

tert-butyl 2-(2-oxo-3-(p-tolyl)quinoxalin-1(2H)-yl)acetate (49)



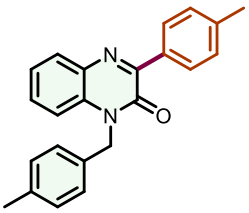
Yellow solid (24.5 mg, 70%); m.p. 123.9 – 125.0 °C; ^{1}H NMR (400 MHz, Chloroform-d) δ 8.25 (d, J = 8.2 Hz, 2H), 7.95 (dd, J = 8.0, 1.3 Hz, 1H), 7.55 – 7.49 (m, 1H), 7.38 – 7.33 (m, 1H), 7.28 (d, J = 8.1 Hz, 2H), 7.09 (d, J = 8.3 Hz, 1H), 5.00 (s, 2H), 2.42 (s, 3H), 1.47 (s, 9H). ^{13}C NMR (101 MHz, Chloroform-d) δ 166.3, 154.4, 153.8, 140.8, 133.2, 133.1, 132.5, 130.6, 130.1, 129.6, 128.8, 123.9, 113.0, 83.1, 44.4, 28.0, 21.5. HRMS (ESI-TOF) *m/z*: $[M + Na]^{+}$ Calcd for $C_{21}H_{22}N_2NaO_3$, 373.1523; Found: 373.1527.

1-benzyl-3-(p-tolyl)quinoxalin-2(1H)-one (50) [5]



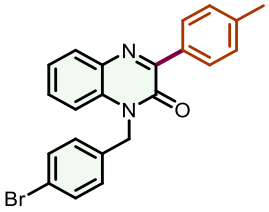
Light yellow solid (25.8 mg, 79%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.33 (d, *J* = 8.2 Hz, 2H), 7.97 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.46 (m, *J* = 8.5, 8.0, 1.5 Hz, 1H), 7.32 (m, *J* = 9.3, 4.5 Hz, 9H), 5.60 (s, 2H), 2.46 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.9, 154.1, 140.8, 135.4, 133.4, 133.3, 132.6, 130.5, 130.0, 129.6, 128.93, 128.86, 127.7, 127.0, 123.7, 114.3, 46.1, 21.6.

1-(4-methylbenzyl)-3-(p-tolyl)quinoxalin-2(1H)-one (51)



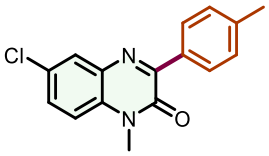
Light yellow solid (27.8 mg, 82%); m.p. 162.8 – 163.5 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.29 (d, *J* = 8.2 Hz, 2H), 7.92 (d, *J* = 8.1 Hz, 1H), 7.44 – 7.38 (m, 1H), 7.33 – 7.27 (m, 4H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H), 5.52 (s, 2H), 2.42 (s, 3H), 2.30 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.9, 154.1, 140.7, 137.4, 133.4, 133.3, 132.7, 132.4, 130.4, 130.0, 129.63, 129.58, 128.9, 127.0, 123.7, 114.3, 45.9, 21.6, 21.1. HRMS (ESI-TOF) *m/z*: [M + Na]$^{+}$ Calcd for $C_{23}H_{20}N_2NaO$, 363.1468; Found: 363.1473.

1-(4-bromobenzyl)-3-(p-tolyl)quinoxalin-2(1H)-one (52)



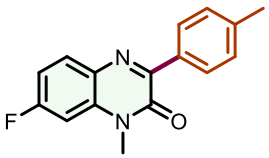
Yellow solid (25.5 mg, 63%); m.p. 149.7 – 150.2 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.29 (d, *J* = 8.1 Hz, 2H), 7.95 (d, *J* = 7.8 Hz, 1H), 7.47 – 7.41 (m, 3H), 7.32 (dd, *J* = 16.1, 8.0 Hz, 3H), 7.19 (m, *J* = 13.1, 8.4 Hz, 3H), 5.50 (s, 2H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.8, 154.0, 140.9, 134.5, 133.4, 133.1, 132.4, 132.1, 130.6, 130.1, 129.6, 128.9, 128.8, 123.9, 121.6, 114.0, 45.6, 21.6. HRMS (ESI-TOF) *m/z*: [M + Na]$^{+}$ Calcd for $C_{22}H_{17}BrN_2NaO$, 427.0416; Found: 427.0423.

6-chloro-1-methyl-3-(p-tolyl)quinoxalin-2(1H)-one (53) [5]



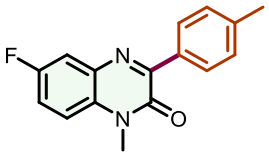
Yellow solid (19.4 mg, 68%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.25 (d, *J* = 8.3 Hz, 2H), 7.91 (d, *J* = 2.3 Hz, 1H), 7.49 (dd, *J* = 8.9, 2.4 Hz, 1H), 7.29 (d, *J* = 8.2 Hz, 2H), 7.24 (d, *J* = 8.9 Hz, 1H), 3.74 (s, 3H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.0, 154.4, 141.1, 133.6, 132.9, 132.0, 129.9, 129.6, 129.5, 128.93, 128.87, 114.6, 29.5, 21.6.

7-fluoro-1-methyl-3-(p-tolyl)quinoxalin-2(1H)-one (54) [5]



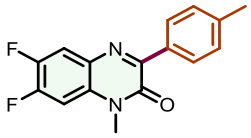
Light yellow solid (19.3 mg, 72%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.20 (d, *J* = 8.1 Hz, 2H), 7.88 (dd, *J* = 8.8, 6.0 Hz, 1H), 7.27 (d, *J* = 8.1 Hz, 2H), 7.05 (td, *J* = 8.5, 2.5 Hz, 1H), 6.98 (dd, *J* = 10.0, 2.4 Hz, 1H), 3.69 (s, 3H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 164.5, 162.0, 154.6, 152.8 (d, *J* = 3.7 Hz), 140.7, 134.7 (d, *J* = 11.4 Hz), 133.1, 132.2 (d, *J* = 10.3 Hz), 129.9 (d, *J* = 1.7 Hz), 129.4, 128.8, 111.5 (d, *J* = 23.5 Hz), 100.5 (d, *J* = 27.9 Hz), 29.5, 21.5. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -107.45.

6-fluoro-1-methyl-3-(p-tolyl)quinoxalin-2(1H)-one (55) [5]



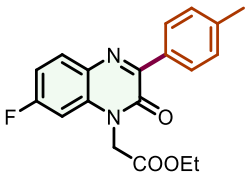
Light yellow solid (19.8 mg, 74%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.23 (d, *J* = 8.2 Hz, 2H), 7.91 (dd, *J* = 8.8, 6.0 Hz, 1H), 7.30 (d, *J* = 8.1 Hz, 2H), 7.09 (td, *J* = 8.5, 2.5 Hz, 1H), 7.02 (dd, *J* = 10.0, 2.5 Hz, 1H), 3.73 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 164.5, 162.0, 154.6, 152.8 (d, *J* = 3.6 Hz), 140.7, 134.7 (d, *J* = 11.3 Hz), 133.1, 132.2 (d, *J* = 10.5 Hz), 129.9 (d, *J* = 2.0 Hz), 129.4, 128.8, 111.5 (d, *J* = 23.6 Hz), 100.5 (d, *J* = 27.8 Hz), 29.5, 21.5. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -107.45.

6,7-difluoro-1-methyl-3-(p-tolyl)quinoxalin-2(1H)-one (56)



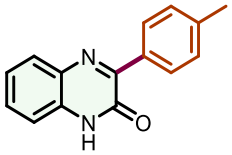
Yellow solid (20.6 mg, 72%); m.p. 161.3 – 162.6 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.24 (d, *J* = 8.3 Hz, 2H), 7.71 (dd, *J* = 10.3, 8.3 Hz, 1H), 7.29 (d, *J* = 8.1 Hz, 2H), 7.10 (dd, *J* = 11.4, 7.1 Hz, 1H), 3.69 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.3, 154.0 (d, *J* = 3.7 Hz), 152.6 (d, *J* = 14.6 Hz), 150.1 (d, *J* = 14.5 Hz), 148.0 (d, *J* = 14.0 Hz), 145.5 (d, *J* = 14.0 Hz), 141.1, 132.7, 130.4 (dd, *J* = 8.9, 1.8 Hz), 129.5, 129.3 (dd, *J* = 9.6, 2.8 Hz), 128.8, 117.6 (dd, *J* = 17.9, 2.2 Hz), 102.1 (d, *J* = 23.1 Hz), 29.7, 21.5. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -131.04 (d, *J* = 22.3 Hz), -142.19 (d, *J* = 22.4 Hz). HRMS (ESI-TOF) *m/z*: [M + Na]$^{+}$ Calcd for $C_{16}H_{12}F_2N_2NaO$, 309.0810; Found: 309.0811.

ethyl 2-(7-fluoro-2-oxo-3-(p-tolyl)quinoxalin-1(2H)-yl)acetate (57)



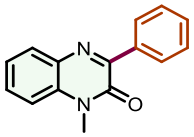
White solid (19.7 mg, 58%); m.p. 175.9 – 176.6 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.29 (d, *J* = 8.3 Hz, 2H), 7.67 (dd, *J* = 8.7, 2.9 Hz, 1H), 7.33 – 7.25 (m, 4H), 7.07 (dd, *J* = 9.2, 4.6 Hz, 1H), 5.09 (s, 2H), 4.29 (q, *J* = 7.1 Hz, 2H), 2.45 (s, 3H), 1.31 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.1, 158.9 (d, *J* = 243.9 Hz), 154.9, 154.0, 141.3, 133.8 (d, *J* = 11.4 Hz), 132.7, 129.7, 129.1 (d, *J* = 2.1 Hz), 128.9, 117.8 (d, *J* = 24.2 Hz), 115.9 (d, *J* = 22.4 Hz), 114.1 (d, *J* = 8.9 Hz), 62.2, 44.0, 21.5, 14.1. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -118.70. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{19}H_{18}FN_2O_3$, 341.1269; Found: 341.1269.

3-(p-tolyl)quinoxalin-2(1H)-one (58) [5]



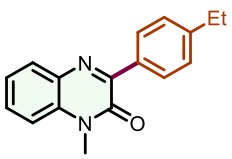
Light yellow solid (8.03 mg, 34%); ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.53 (s, 1H), 8.27 (d, *J* = 8.1 Hz, 2H), 7.82 (d, *J* = 7.8 Hz, 1H), 7.52 (t, *J* = 7.6 Hz, 1H), 7.36 – 7.26 (m, 4H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.1, 154.2, 140.5, 133.4, 132.5, 132.4, 130.5, 129.6, 129.1, 128.9, 123.8, 115.5, 21.5.

1-methyl-3-phenylquinoxalin-2(1H)-one (59)[4]



White solid (18.2 mg, 77%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.33 (dd, *J* = 6.4, 3.0 Hz, 2H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.62 – 7.56 (m, 1H), 7.53 – 7.49 (m, 3H), 7.42 – 7.34 (m, 2H), 3.79 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.7, 154.2, 136.1, 133.4, 133.1, 130.5, 130.3, 129.5, 128.1, 123.7, 113.6, 29.3.

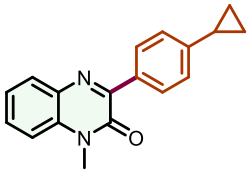
3-(4-ethylphenyl)-1-methylquinoxalin-2(1H)-one (60) [5]



Yellow solid (22.9 mg, 87%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.31 – 8.25 (m, 2H), 7.96

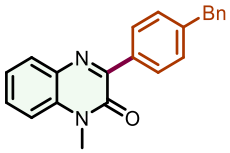
(dd, J = 8.0, 1.4 Hz, 1H), 7.58 (ddd, J = 8.5, 7.4, 1.5 Hz, 1H), 7.41 – 7.32 (m, 4H), 3.79 (s, 3H), 2.74 (q, J = 7.6 Hz, 2H), 1.30 (t, J = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.8, 154.1, 146.9, 133.6, 133.3, 133.2, 130.3, 130.0, 129.6, 127.7, 123.7, 113.5, 29.3, 28.9, 15.5.

3-(4-cyclopropylphenyl)-1-methylquinoxalin-2(1H)-one (61)



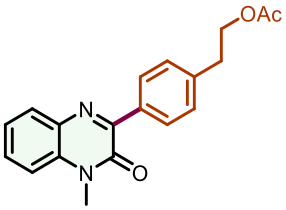
Yellow solid (22.9 mg, 83%); m.p. 112.9 – 113.6 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.27 (d, J = 8.4 Hz, 2H), 7.95 (dd, J = 8.0, 1.3 Hz, 1H), 7.60 – 7.55 (m, 1H), 7.41 – 7.33 (m, 2H), 7.19 (d, J = 8.4 Hz, 2H), 3.79 (s, 3H), 1.99 (m, J = 13.4, 8.5, 5.1 Hz, 1H), 1.08 – 1.02 (m, 2H), 0.83 – 0.78 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.8, 153.9, 146.9, 133.3, 133.2, 130.3, 130.0, 129.5, 125.2, 123.6, 113.5, 29.3, 15.6, 9.8. HRMS (ESI-TOF) *m/z*: [M + Na]$^{+}$ Calcd for $C_{18}H_{16}N_2NaO$, 299.1155; Found: 299.1159.

3-(4-benzylphenyl)-1-methylquinoxalin-2(1H)-one (62)[6]



Light yellow solid (23.3 mg, 71%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.25 (d, J = 8.2 Hz, 2H), 7.95 – 7.90 (m, 1H), 7.58 – 7.53 (m, 1H), 7.38 – 7.27 (m, 6H), 7.21 (m, J = 7.3 Hz, 3H), 4.05 (s, 2H), 3.76 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.8, 154.0, 143.6, 140.7, 134.0, 133.3, 133.2, 130.4, 130.1, 129.7, 129.0, 128.8, 128.5, 126.1, 123.7, 113.5, 41.9, 29.3.

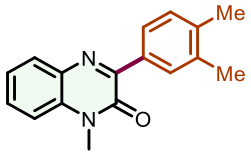
4-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenethyl acetate (63)



Yellow solid (22.1 mg, 69%); m.p. 102.7 – 103.5 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.30 (d, J = 8.2 Hz, 2H), 7.98 – 7.93 (m, 1H), 7.61 – 7.55 (m, 1H), 7.41 – 7.33 (m, 4H), 4.34 (t, J = 7.0 Hz, 2H), 3.78 (s, 3H), 3.03 (t, J = 6.9 Hz, 2H), 2.07 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 171.0, 154.7, 153.8, 140.3, 134.5, 133.3, 133.1, 130.4, 130.2, 129.7, 128.6, 123.7, 113.6, 64.7, 35.0, 29.3, 21.0. HRMS (ESI-TOF) *m/z*: [M + Na]$^{+}$ Calcd for $C_{19}H_{18}N_2NaO_3$,

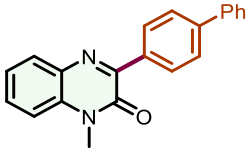
345.1210; Found: 345.1214.

3-(3,4-dimethylphenyl)-1-methylquinoxalin-2(1H)-one (64)[7]



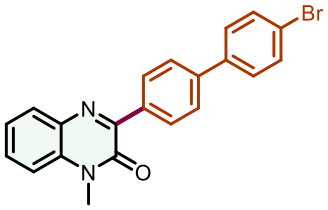
Light yellow solid (17.2 mg, 65%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.11 (d, *J* = 10.2 Hz, 2H), 7.96 (d, *J* = 7.7 Hz, 1H), 7.56 (t, *J* = 7.3 Hz, 1H), 7.40 – 7.31 (m, 2H), 7.28 (d, *J* = 3.5 Hz, 1H), 3.78 (s, 3H), 2.38 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.8, 154.2, 139.4, 136.2, 133.7, 133.3, 133.2, 130.5, 130.3, 129.9, 129.4, 127.2, 123.6, 113.5, 29.2, 19.9, 19.8.

3-([1,1'-biphenyl]-4-yl)-1-methylquinoxalin-2(1H)-one (65)[6]



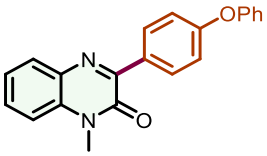
Yellow solid (24.5 mg, 78%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.49 – 8.45 (m, 2H), 7.99 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.77 – 7.73 (m, 2H), 7.72 – 7.68 (m, 2H), 7.62 – 7.57 (m, 1H), 7.50 (t, *J* = 7.5 Hz, 2H), 7.43 – 7.35 (m, 3H), 3.82 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.8, 153.6, 143.0, 140.6, 135.0, 133.4, 133.2, 130.5, 130.3, 130.0, 128.8, 127.7, 127.2, 126.8, 123.8, 113.6, 29.3.

3-(4'-bromo-[1,1'-biphenyl]-4-yl)-1-methylquinoxalin-2(1H)-one (66)



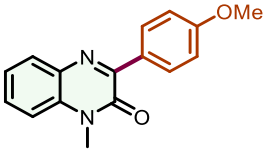
Yellow solid (30.3 mg, 78%); m.p. 159.8 – 160.6 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.45 (d, *J* = 8.3 Hz, 2H), 7.98 (d, *J* = 7.8 Hz, 1H), 7.69 (d, *J* = 8.3 Hz, 2H), 7.60 (m, *J* = 8.4 Hz, 3H), 7.54 (d, *J* = 8.4 Hz, 2H), 7.42 – 7.34 (m, 2H), 3.80 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.7, 153.4, 141.6, 139.5, 135.4, 133.4, 133.1, 131.9, 130.5, 130.4, 130.2, 128.8, 126.5, 123.8, 122.0, 113.6, 29.3. HRMS (ESI-TOF) *m/z*: [M + H]$^{+}$ Calcd for $C_{21}H_{16}BrN_2O$, 391.0441; Found: 391.0444.

1-methyl-3-(4-phenoxyphenyl)quinoxalin-2(1H)-one (67)[4]



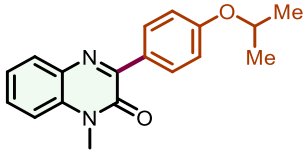
Yellow solid (28.5 mg, 87%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.40 (d, *J* = 8.7 Hz, 2H), 7.95 (d, *J* = 7.8 Hz, 1H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.42 – 7.34 (m, 4H), 7.18 (t, *J* = 7.4 Hz, 1H), 7.11 (d, *J* = 8.6 Hz, 4H), 3.79 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.4, 156.5, 154.8, 153.2, 133.2, 133.1, 131.5, 130.9, 130.3, 130.1, 129.8, 123.8, 123.7, 119.5, 117.9, 113.6, 29.3.

3-(4-methoxyphenyl)-1-methylquinoxalin-2(1H)-one (68)[4]



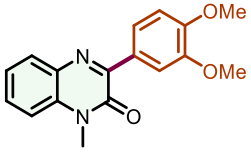
Light yellow solid (25.1 mg, 94%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.42 (d, *J* = 8.9 Hz, 2H), 7.96 – 7.90 (m, 1H), 7.58 – 7.52 (m, 1H), 7.40 – 7.31 (m, 2H), 7.02 (d, *J* = 8.9 Hz, 2H), 3.90 (s, 3H), 3.78 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.5, 154.8, 153.2, 133.2, 133.1, 131.4, 130.1, 129.7, 128.8, 123.6, 113.49, 113.47, 55.4, 29.3.

3-(4-isopropoxyphenyl)-1-methylquinoxalin-2(1H)-one (69)



Yellow solid (22.9 mg, 78%); m.p. 170.4 – 170.8 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.39 – 8.35 (m, 2H), 7.90 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.56 – 7.49 (m, 1H), 7.37 – 7.28 (m, 2H), 6.97 (d, *J* = 8.9 Hz, 2H), 4.65 (m, *J* = 6.1 Hz, 1H), 3.75 (s, 3H), 1.37 (d, *J* = 6.1 Hz, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.9, 154.8, 153.2, 133.2, 133.1, 131.4, 130.1, 129.7, 128.4, 123.6, 115.1, 113.5, 69.9, 29.2, 22.0. HRMS (ESI-TOF) *m/z*: $[M + H]^{+}$ Calcd for $C_{18}H_{19}N_2O_2$, 295.1441; Found: 295.1443.

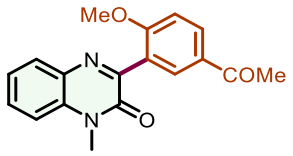
3-(3,4-dimethylphenyl)-1-methylquinoxalin-2(1H)-one (70)[8]



Yellow solid (26.2 mg, 88%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.17 (dd, *J* = 8.5, 1.9 Hz,

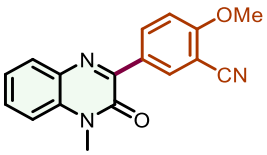
1H), 8.06 (d, *J* = 1.8 Hz, 1H), 7.96 – 7.91 (m, 1H), 7.58 – 7.52 (m, 1H), 7.40 – 7.31 (m, 2H), 6.97 (d, *J* = 8.6 Hz, 1H), 4.02 (s, 3H), 3.97 (s, 3H), 3.77 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.8, 152.7, 151.2, 148.4, 133.09, 133.08, 130.1, 129.8, 128.9, 123.7, 123.5, 113.5, 112.4, 110.4, 56.0, 29.3.

3-(5-acetyl-2-methoxyphenyl)-1-methylquinoxalin-2(1H)-one (71)



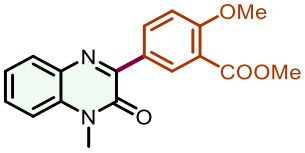
Light yellow solid (9.5 mg, 31%); m.p. 163.4 – 164.4 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.16 – 8.11 (m, 1H), 8.08 (s, 1H), 7.97 (d, *J* = 7.8 Hz, 1H), 7.64 (t, *J* = 7.8 Hz, 1H), 7.41 (t, *J* = 7.7 Hz, 2H), 7.08 (d, *J* = 8.7 Hz, 1H), 3.91 (s, 3H), 3.79 (s, 3H), 2.60 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 196.3, 161.8, 156.3, 154.2, 133.8, 132.9, 131.8, 131.0, 130.7, 130.5, 130.3, 126.6, 123.7, 113.7, 111.0, 56.2, 29.4, 26.4. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{18}H_{16}N_2NaO_3$, 331.1053; Found: 331.1059.

2-methoxy-5-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)benzonitrile (72)



Yellow solid (20.9 mg, 72%); m.p. 210.7 – 211.5 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.81 – 8.70 (m, 2H), 7.93 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.60 (ddd, *J* = 8.6, 7.4, 1.5 Hz, 1H), 7.42 – 7.34 (m, 2H), 7.06 (d, *J* = 8.9 Hz, 1H), 4.02 (s, 3H), 3.79 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.4, 154.5, 150.7, 135.9, 135.5, 133.3, 132.9, 130.6, 130.4, 129.0, 124.0, 116.2, 113.7, 110.7, 101.8, 56.3, 29.3. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{17}H_{14}N_3O_2$, 292.1081; Found: 292.1082.

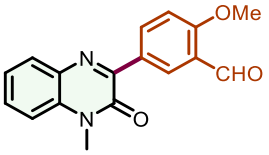
methyl 2-methoxy-5-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)benzoate (73)



Yellow solid (23.8 mg, 73%); m.p. 131.0 – 132.2 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.94 (s, 1H), 8.65 (d, *J* = 8.5 Hz, 1H), 7.95 (d, *J* = 7.8 Hz, 1H), 7.57 (t, *J* = 7.6 Hz, 1H), 7.37 (dd, *J* = 20.4, 7.9 Hz, 2H), 7.09 (d, *J* = 8.9 Hz, 1H), 4.00 (s, 3H), 3.95 (s, 3H), 3.78 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.3, 160.7, 154.7, 152.0, 135.0, 133.3, 133.2, 133.0, 130.3,

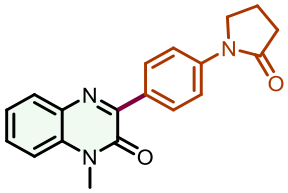
130.1, 128.2, 123.8, 119.7, 113.6, 111.4, 56.2, 52.1, 29.3. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{18}H_{16}N_2NaO_4$, 347.1002; Found: 347.1009.

2-methoxy-5-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)benzaldehyde (74)



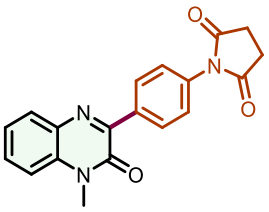
Yellow solid (15.2 mg, 52%); m.p. 195.8 – 196.2 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.50 (s, 1H), 8.88 (d, *J* = 2.3 Hz, 1H), 8.72 (dd, *J* = 8.8, 2.3 Hz, 1H), 7.99 – 7.89 (m, 1H), 7.62 – 7.53 (m, 1H), 7.40 – 7.32 (m, 2H), 7.08 (d, *J* = 8.9 Hz, 1H), 4.01 (s, 3H), 3.77 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.5, 163.0, 154.7, 152.0, 137.3, 133.2, 133.0, 130.9, 130.4, 130.3, 128.9, 124.5, 123.8, 113.6, 111.1, 56.0, 29.3. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{17}H_{15}N_2O_3$, 295.1077; Found: 295.1082.

1-methyl-3-(4-(2-oxopyrrolidin-1-yl)phenyl)quinoxalin-2(1H)-one (75)



Yellow solid (24.5 mg, 77%); m.p. 176.1 – 176.5 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.45 (d, *J* = 8.8 Hz, 2H), 7.96 – 7.91 (m, 1H), 7.78 (d, *J* = 8.9 Hz, 2H), 7.59 – 7.53 (m, 1H), 7.40 – 7.31 (m, 2H), 3.93 (t, *J* = 7.0 Hz, 2H), 3.77 (s, 3H), 2.66 (t, *J* = 8.1 Hz, 2H), 2.19 (q, *J* = 7.7 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.5, 154.8, 152.9, 141.2, 133.2, 133.1, 131.8, 130.34, 130.32, 130.1, 123.7, 118.7, 113.5, 48.6, 32.9, 29.3, 17.9. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{19}H_{17}N_3NaO_2$, 342.1213; Found: 342.1214.

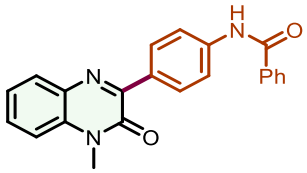
1-(4-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)pyrrolidine-2,5-dione (76)



Yellow solid (25.9 mg, 78%); m.p. 262.0 – 262.6 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.35 (d, *J* = 8.5 Hz, 2H), 7.93 – 7.89 (m, 1H), 7.71 – 7.66 (m, 1H), 7.62 (d, *J* = 8.0 Hz, 1H), 7.43 (dd, *J* = 11.7, 8.0 Hz, 3H), 3.72 (s, 3H), 2.83 (s, 4H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 177.3, 154.4, 152.9, 136.0, 134.7, 133.8, 132.7, 131.3, 130.2, 130.1, 126.8, 124.2, 115.3, 29.8, 29.0.

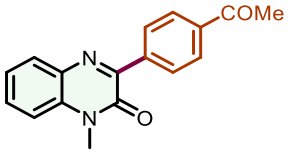
HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{19}H_{15}N_3NaO_3$, 356.1006; Found: 356.1008.

N-(4-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)benzamide (77)



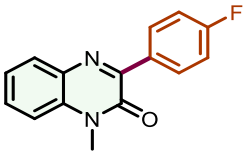
Yellow solid (26.2 mg, 74%); m.p. 208.2 – 208.8 °C;^{1}H NMR (400 MHz, DMSO-d_6) δ 10.48 (s, 1H), 8.37 (d, *J* = 8.8 Hz, 2H), 8.01 (d, *J* = 7.1 Hz, 2H), 7.95 (d, *J* = 8.8 Hz, 2H), 7.89 – 7.85 (m, 1H), 7.66 – 7.60 (m, 2H), 7.59 – 7.53 (m, 3H), 7.43 – 7.38 (m, 1H), 3.70 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 166.2, 154.5, 152.5, 141.6, 135.2, 133.6, 132.8, 132.2, 131.5, 130.7, 130.5, 129.9, 128.9, 128.2, 124.0, 119.7, 115.1, 29.7. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{22}H_{17}N_3NaO_2$, 378.1213; Found: 378.1217.

3-(4-acetylphenyl)-1-methylquinoxalin-2(1H)-one (78) [5]



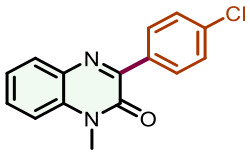
Yellow solid (19.2 mg, 69%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.46 (d, *J* = 8.5 Hz, 2H), 8.07 (d, *J* = 8.5 Hz, 2H), 8.00 – 7.95 (m, 1H), 7.66 – 7.60 (m, 1H), 7.44 – 7.36 (m, 2H), 3.80 (s, 3H), 2.67 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 197.9, 154.6, 152.8, 140.3, 137.9, 133.5, 133.0, 131.0, 130.7, 129.8, 127.9, 123.9, 113.7, 29.4, 26.8.

3-(4-fluorophenyl)-1-methylquinoxalin-2(1H)-one (79)[4]



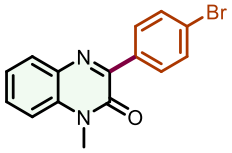
Yellow solid (16.0 mg, 63%); ^{1}H NMR (400 MHz, Chloroform-d) δ 8.47 – 8.38 (m, 2H), 7.95 (dd, J = 8.0, 1.3 Hz, 1H), 7.59 (ddd, J = 8.6, 7.4, 1.5 Hz, 1H), 7.43 – 7.33 (m, 2H), 7.21 – 7.14 (m, 2H), 3.79 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 164.2 (d, J = 251.0 Hz), 154.7, 152.7, 133.3, 133.0, 132.2 (d, J = 3.2 Hz), 131.8 (d, J = 8.5 Hz), 130.4 (d, J = 2.7 Hz), 123.8, 115.2, 114.9, 113.6, 29.3. ^{19}F NMR (376 MHz, Chloroform-d) δ -110.04.

3-(4-chlorophenyl)-1-methylquinoxalin-2(1H)-one (80)[4]



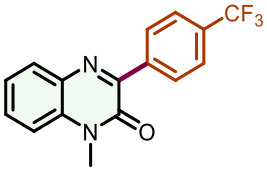
Yellow solid (17.0 mg, 63%); ^{1}H NMR (400 MHz, Chloroform-d) δ 8.37 (d, J = 8.5 Hz, 2H), 7.94 (d, J = 7.8 Hz, 1H), 7.59 (t, J = 7.5 Hz, 1H), 7.46 (d, J = 8.5 Hz, 2H), 7.42 – 7.33 (m, 2H), 3.78 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 154.6, 152.6, 136.5, 134.4, 133.4, 133.0, 131.0, 130.55, 130.48, 128.3, 123.8, 113.6, 29.3.

3-(4-bromophenyl)-1-methylquinoxalin-2(1H)-one (81)[4]



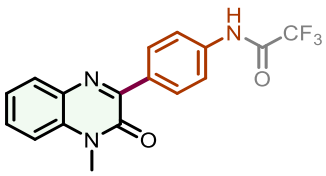
Yellow solid (17.9 mg, 57%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.32 – 8.25 (m, 2H), 7.94 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.64 – 7.57 (m, 3H), 7.41 – 7.33 (m, 2H), 3.78 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.5, 152.7, 134.9, 133.4, 133.0, 131.23, 131.20, 130.6, 130.5, 125.1, 123.9, 113.6, 29.3.

1-methyl-3-(4-(trifluoromethyl)phenyl)quinoxalin-2(1H)-one (82)[4]



Yellow solid (23.1 mg, 76%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.48 (d, *J* = 8.2 Hz, 2H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.74 (d, *J* = 8.3 Hz, 2H), 7.61 (t, *J* = 7.8 Hz, 1H), 7.44 – 7.32 (m, 2H), 3.77 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.5, 152.4, 139.3 (d, *J* = 1.5 Hz), 133.5, 132.9, 131.7 (q, *J* = 32.3 Hz), 131.0, 130.7, 129.9, 124.9 (q, *J* = 3.9 Hz), 124.1 (q, *J* = 272.3 Hz), 123.9, 113.7, 29.3. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.80.

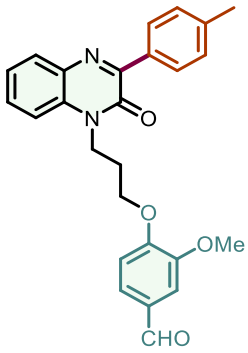
2,2,2-trifluoro-N-(4-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)acetamide (83)



Yellow solid (22.6 mg, 65%); m.p. 205.1 – 206.2 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.39 – 8.34 (m, 2H), 7.88 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.84 – 7.79 (m, 2H), 7.66 (ddd, *J* = 8.5, 7.1, 1.5

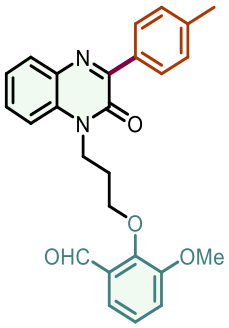
Hz, 1H), 7.59 (dd, *J* = 8.4, 1.0 Hz, 1H), 7.44 – 7.39 (m, 1H), 3.70 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.1 (q, *J* = 37.4 Hz), 154.4, 152.3, 138.5, 133.7, 133.4, 132.7, 131.0, 130.6, 130.0, 124.1, 120.6, 116.2 (q, *J* = 289.0 Hz), 115.2, 29.7. ^{19}F NMR (376 MHz, DMSO-d_6) δ -73.85. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{17}H_{12}F_3N_3NaO_2$, 370.0774; Found: 370.0777.

3-methoxy-4-(3-(2-oxo-3-(p-tolyl)quinoxalin-1(2H)-yl)propoxy)benzaldehyde (84)



Light yellow solid (23.3 mg, 54%); m.p. 172.7 – 173.1 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.86 (s, 1H), 8.08 (d, *J* = 8.1 Hz, 1H), 8.01 (d, *J* = 7.9 Hz, 2H), 7.83 (d, *J* = 8.2 Hz, 1H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.42 (d, *J* = 5.9 Hz, 2H), 7.29 (d, *J* = 7.8 Hz, 2H), 6.97 (d, *J* = 8.5 Hz, 1H), 4.81 (t, *J* = 6.0 Hz, 2H), 4.33 (d, *J* = 6.3 Hz, 2H), 3.91 (s, 3H), 2.47 (m, *J* = 11.7 Hz, 5H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 190.8, 155.3, 153.9, 149.9, 146.5, 139.8, 139.7, 139.0, 133.3, 130.2, 129.53, 129.49, 128.9, 126.8, 126.58, 126.55, 111.6, 109.5, 66.1, 63.2, 56.0, 28.6, 21.4. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{26}H_{24}N_2NaO_4$, 451.1628; Found: 451.1632.

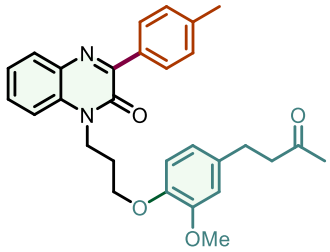
3-methoxy-2-(3-(2-oxo-3-(p-tolyl)quinoxalin-1(2H)-yl)propoxy)benzaldehyde (85)



White solid (20.5 mg, 48%); m.p. 116.7 – 118.1 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.49 (s, 1H), 8.08 (d, *J* = 8.1 Hz, 1H), 8.04 (d, *J* = 8.1 Hz, 2H), 7.88 (d, *J* = 8.1 Hz, 1H), 7.69 – 7.64 (m, 1H), 7.62 – 7.57 (m, 1H), 7.45 (dd, *J* = 5.6, 3.8 Hz, 1H), 7.30 (d, *J* = 8.8 Hz, 2H), 7.17 – 7.12 (m, 2H), 4.84 (t, *J* = 6.2 Hz, 2H), 4.37 (t, *J* = 6.3 Hz, 2H), 3.80 (s, 3H), 2.43 (m, *J* = 12.4 Hz, 5H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 190.0, 155.4, 153.0, 151.7, 146.5, 139.764,

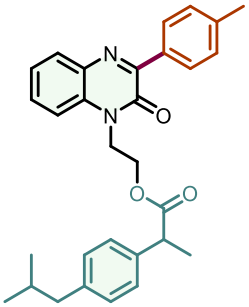
139.756, 139.0, 133.3, 130.0, 129.6, 129.5, 128.9, 126.69, 126.68, 124.1, 119.3, 118.1, 71.8, 63.4, 56.0, 29.6, 21.4. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{26}H_{24}N_2NaO_4$, 451.1628; Found: 451.1637.

1-(3-(2-methoxy-4-(3-oxobutyl)phenoxy)propyl)-3-(p-tolyl)quinoxalin-2(1H)-one (86)



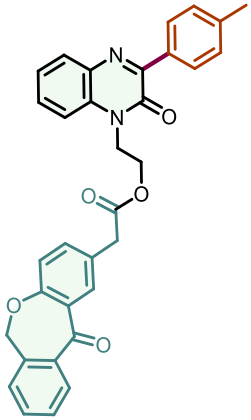
White solid (30.1 mg, 64%); m.p. 88.9 – 90.1 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.08 (d, *J* = 8.1 Hz, 1H), 8.02 (d, *J* = 8.0 Hz, 2H), 7.85 (d, *J* = 8.2 Hz, 1H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.58 (t, *J* = 7.3 Hz, 1H), 7.30 (d, *J* = 9.0 Hz, 2H), 6.82 (d, *J* = 8.1 Hz, 1H), 6.76 – 6.65 (m, 2H), 4.79 (t, *J* = 6.0 Hz, 2H), 4.23 (t, *J* = 6.3 Hz, 2H), 3.84 (s, 3H), 2.89 – 2.82 (m, 2H), 2.75 (t, *J* = 7.3 Hz, 2H), 2.46 (s, 3H), 2.44 – 2.39 (m, 2H), 2.16 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 208.1, 155.4, 149.5, 146.7, 146.6, 139.8, 139.7, 139.0, 134.2, 133.3, 129.6, 129.4, 128.93, 128.90, 126.65, 126.63, 120.2, 113.7, 112.3, 66.2, 63.6, 55.9, 45.4, 30.1, 29.4, 28.8, 21.5. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{29}H_{31}N_2O_4$, 471.2278; Found: 471.2277.

2-(2-oxo-3-(p-tolyl)quinoxalin-1(2H)-yl)ethyl 2-(4-isobutylphenyl)propanoate (87)



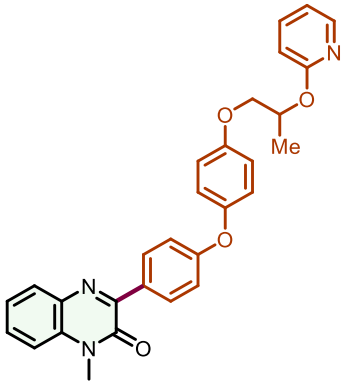
Colourless oil (37.8 mg, 81%); m.p. 96.5 – 98.2 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.27 (d, *J* = 8.2 Hz, 2H), 7.95 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.48 – 7.52 (m, 1H), 7.44 – 7.30 (m, 4H), 7.13 – 7.04 (m, 4H), 4.64 – 4.44 (m, 4H), 3.63 (q, *J* = 7.2 Hz, 1H), 2.41 – 2.48 (m, 5H), 1.80 – 1.90 (m, 1H), 1.45 (d, *J* = 7.2 Hz, 3H), 0.91 (d, *J* = 6.6 Hz, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.7, 154.6, 153.7, 140.74, 140.69, 137.2, 133.3, 133.1, 132.8, 130.5, 130.1, 129.5, 129.4, 128.8, 127.1, 123.7, 113.7, 61.2, 45.03, 45.01, 41.1, 30.1, 22.4, 21.5, 18.3. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{30}H_{33}N_2O_3$, 469.2486; Found: 469.2496.

2-(2-oxo-3-(p-tolyl)quinoxalin-1(2H)-yl)ethyl-2-(11-oxo-6,11-dihydrodibenzo[b,e]oxepin-2-yl)acetate (88)



Yellow solid (37.6 mg, 71%); m.p. 136.4-137.6 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.28 (d, *J* = 8.2 Hz, 2H), 8.07 (d, *J* = 2.3 Hz, 1H), 7.92 (ddd, *J* = 10.2, 7.9, 1.3 Hz, 2H), 7.61 – 7.29 (m, 10H), 6.98 (d, *J* = 8.4 Hz, 1H), 5.19 (s, 2H), 4.62 (t, *J* = 6.0 Hz, 2H), 4.55 (t, *J* = 5.5 Hz, 2H), 3.60 (s, 2H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 190.7, 171.4, 160.5, 154.6, 153.7, 140.7, 140.4, 136.3, 135.5, 133.3, 133.1, 132.80, 132.76, 132.5, 130.6, 130.2, 129.6, 129.5, 129.3, 128.8, 127.8, 127.2, 125.1, 123.8, 121.2, 113.5, 73.6, 61.3, 41.1, 40.0, 21.5. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{33}H_{27}N_2O_5$, 531.1914; Found: 531.1920.

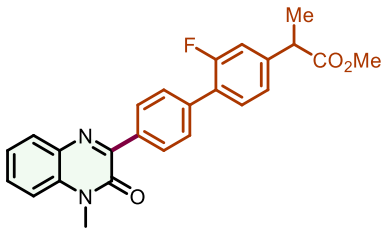
1-methyl-3-(4-(4-(2-(pyridin-2-yloxy)propoxy)phenoxy)phenyl)quinoxalin-2(1H)-one (89)



Yellow solid (28.6 mg, 60%); m.p. 87.4 – 89.1 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.37 (d, *J* = 8.7 Hz, 2H), 8.18 (d, *J* = 3.9 Hz, 1H), 7.94 (d, *J* = 7.9 Hz, 1H), 7.58 (q, *J* = 8.2 Hz, 2H), 7.40 – 7.32 (m, 2H), 7.04 (d, *J* = 6.9 Hz, 4H), 6.98 (d, *J* = 9.0 Hz, 2H), 6.91 – 6.86 (m, 1H), 6.77 (d, *J* = 8.3 Hz, 1H), 5.67 – 5.59 (m, 1H), 4.23 (dd, *J* = 9.8, 5.3 Hz, 1H), 4.12 (dd, *J* = 9.8, 4.8 Hz, 1H), 3.78 (s, 3H), 1.52 (d, *J* = 6.4 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.2, 160.5, 155.6, 154.8, 153.2, 149.6, 146.8, 138.7, 133.2, 133.1, 131.4, 130.3, 130.2, 130.0, 123.7, 121.2, 116.8, 116.7, 115.9, 113.5, 111.7, 71.1, 69.3, 29.3, 17.0. HRMS (ESI-TOF) *m/z*: [M +

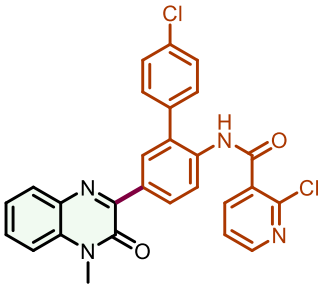
Na]$^+$ Calcd for $C_{29}H_{25}N_3NaO_4$, 502.1737; Found: 502.1744.

Methyl-2-(2-fluoro-4'-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)-[1,1'-biphenyl]-4-yl)propanoate (90)



Yellow solid (36.2 mg, 87%); m.p. 133.3 – 133.8 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.45 (d, *J* = 8.4 Hz, 2H), 7.97 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.69 (dd, *J* = 8.3, 1.3 Hz, 2H), 7.62 – 7.56 (m, 1H), 7.48 (t, *J* = 8.0 Hz, 1H), 7.43 – 7.33 (m, 2H), 7.23 – 7.13 (m, 2H), 3.80 (q, *J* = 7.4 Hz, 1H), 3.80 (s, 3H), 3.73 (s, 3H), 1.57 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.4, 159.8 (d, *J* = 249.2 Hz), 154.7, 153.5, 142.2 (d, *J* = 7.6 Hz), 137.4 (d, *J* = 1.5 Hz), 135.4, 133.4, 133.2, 130.8 (d, *J* = 3.7 Hz), 130.5, 130.4, 129.7, 128.6 (d, *J* = 3.1 Hz), 127.4 (d, *J* = 13.3 Hz), 123.7, 123.6 (d, *J* = 3.3 Hz), 115.4 (d, *J* = 23.6 Hz), 113.6, 52.2, 45.0 (d, *J* = 1.5 Hz), 29.3, 18.4. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -116.84. HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{25}H_{22}FN_2O_3$, 417.1609; Found: 417.1608.

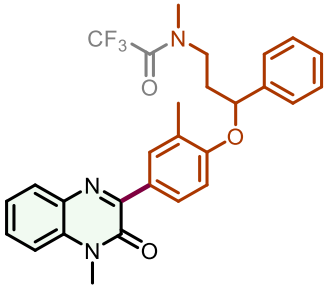
2-chloro-N-(4'-chloro-5-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)-[1,1'-biphenyl]-2-yl)nicotinamide (91)



Yellow solid (30.8 mg, 62%); m.p. 162.1 – 163.9 °C;^{1}H NMR (400 MHz, DMSO-d_6) δ 10.29 (s, 1H), 8.50 (dd, *J* = 4.7, 1.6 Hz, 1H), 8.42 – 8.25 (m, 2H), 7.98 – 7.87 (m, 2H), 7.82 (d, *J* = 8.4 Hz, 1H), 7.70 – 7.63 (m, 1H), 7.60 (d, *J* = 7.9 Hz, 1H), 7.55 (m, 5H), 7.45 – 7.39 (m, 1H), 3.71 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.6, 154.5, 152.4, 150.8, 146.9, 138.4, 138.0, 136.3, 135.5, 134.5, 133.7, 133.4, 132.8, 132.7, 131.9, 131.24, 131.16, 130.1, 129.6, 128.9, 126.6, 124.1, 123.5, 115.2, 29.7. HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{27}H_{19}Cl_2N_4O_2$, 501.0880; Found: 501.0882.

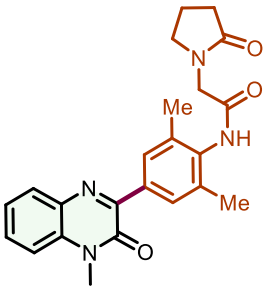
2,2,2-trifluoro-N-methyl-N-(3-(2-methyl-4-(4-methyl-3-oxo-3,4-dihydroquinoxalin-

2-yl)phenoxy)-3-phenylpropyl)acetamide (92)



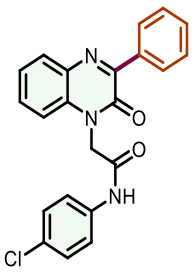
Colorless oil (37.6mg, 74%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.25 – 8.16 (m, 1H), 8.07 (dd, *J* = 8.6, 2.0 Hz, 1H), 7.88 (d, *J* = 7.9 Hz, 1H), 7.50 (t, *J* = 7.8 Hz, 1H), 7.38 – 7.26 (m, 7H), 6.69 (dd, *J* = 16.0, 8.7 Hz, 1H), 5.33 (dd, *J* = 8.0, 4.4 Hz, 1H), 3.81 – 3.64 (m, 5H), 3.16 – 3.03 (m, 3H), 2.46 (d, *J* = 3.7 Hz, 3H), 2.37 – 2.23 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.5, 157.3, 157.1, 157.0, 156.73, 156.68, 154.7, 153.34, 153.28, 140.6, 140.2, 133.12, 133.07, 132.11, 132.07, 130.0, 129.74, 129.70, 128.9, 128.83, 128.79, 128.7, 128.6, 128.1, 128.0, 126.53, 126.50, 125.6, 125.5, 123.6, 123.58, 118.0, 117.9, 115.1, 115.0, 113.5, 112.1, 112.0, 47.1, 46.59, 46.56, 37.5, 35.60, 35.56, 35.49, 35.41, 35.38, 34.8, 29.2, 16.7, 16.6. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -68.94, -69.85. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{28}H_{26}F_3N_3NaO_3$, 532.1818; Found: 532.1816.

N-(2,6-dimethyl-4-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)-2-(2-oxopyrrolidin-1-yl)acetamide (93)



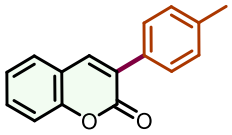
Yellow solid (29.1 mg, 72%); m.p. 116.0 – 116.5 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.11 (s, 1H), 8.04 (s, 2H), 7.91 (d, *J* = 7.8 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.34 (dd, *J* = 16.0, 8.5 Hz, 2H), 4.12 (s, 2H), 3.73 (s, 3H), 3.61 (t, *J* = 7.0 Hz, 2H), 2.46 (t, *J* = 8.1 Hz, 2H), 2.28 (s, 6H), 2.11 (d, *J* = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 176.3, 166.8, 154.6, 153.3, 135.6, 134.77, 134.75, 133.2, 133.0, 130.4, 130.2, 129.4, 123.7, 113.5, 48.6, 47.5, 30.4, 29.3, 18.6, 18.1. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{23}H_{24}N_4NaO_3$, 427.1741; Found: 427.1740.

N-(4-chlorophenyl)-2-(2-oxo-3-phenylquinoxalin-1(2H)-yl)acetamide (94)[9]



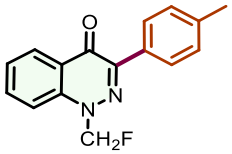
Yellow solid (27.9 mg, 72%);[1]H NMR (400 MHz, DMSO-d_6) δ 10.63 (s, 1H), 8.30 – 8.24 (m, 2H), 7.95 (dd, J = 8.0, 1.5 Hz, 1H), 7.67 – 7.58 (m, 4H), 7.55 – 7.49 (m, 3H), 7.46 – 7.42 (m, 1H), 7.41 – 7.37 (m, 2H), 5.22 (s, 2H). [13]C NMR (101 MHz, DMSO-d_6) δ 165.5, 154.4, 153.3, 138.0, 136.1, 133.6, 132.8, 131.2, 130.8, 130.2, 129.8, 129.2, 128.4, 127.6, 124.2, 121.2, 115.2, 46.1.

3-(p-tolyl)-2H-chromen-2-one (95)[10]



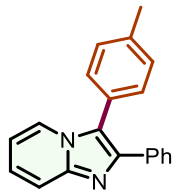
White solid (11.1 mg, 47%); [1]H NMR (400 MHz, Chloroform-*d*) δ 7.81 (s, 1H), 7.64 (d, J = 8.1 Hz, 2H), 7.57 – 7.52 (m, 2H), 7.38 (d, J = 8.1 Hz, 1H), 7.33 – 7.27 (m, 3H), 2.42 (s, 3H). [13]C NMR (101 MHz, Chloroform-*d*) δ 160.7, 153.4, 139.2, 138.9, 131.8, 131.2, 129.2, 128.4, 128.3, 127.8, 124.4, 119.8, 116.4, 21.3.

1-(fluoromethyl)-3-(p-tolyl)cinnolin-4(1H)-one (96)



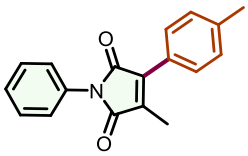
White solid (16.4 mg, 61%); m.p. 106.5 – 107.9 °C; [1]H NMR (400 MHz, Chloroform-*d*) δ 8.48 – 8.40 (m, 1H), 8.04 (d, J = 8.2 Hz, 2H), 7.79 (ddd, J = 8.6, 7.2, 1.4 Hz, 1H), 7.60 (d, J = 8.6 Hz, 1H), 7.50 (t, J = 7.6 Hz, 1H), 7.31 – 7.28 (m, 2H), 6.45 (s, 1H), 6.32 (s, 1H), 2.43 (s, 3H). [13]C NMR (101 MHz, Chloroform-*d*) δ 170.7, 147.3 (d, J = 2.7 Hz), 140.5 (d, J = 2.9 Hz), 139.4, 134.2, 130.7, 128.8 (d, J = 21.1 Hz), 126.8, 125.4, 124.3, 114.3, 93.0, 91.0, 21.4. [19]F NMR (376 MHz, Chloroform-*d*) δ -170.13. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{16}H_{14}FN_2O$, 269.1085; Found: 269.1090.

2-phenyl-3-(p-tolyl)imidazo[1,2-a]pyridine (97)[11]



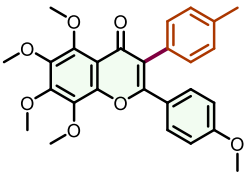
Brown Solid (11.0 mg, 39%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.97 – 7.95 (m, 1H), 7.74 – 7.68 (m, 3H), 7.36 – 7.18 (m, 8H), 6.75 – 6.71 (m, 1H), 2.48 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 144.7, 142.2, 138.8, 134.3, 130.6, 130.3, 128.2, 128.0, 127.4, 126.8, 124.5, 123.3, 121.1, 117.5, 112.1, 21.5.

3-methyl-1-phenyl-4-(p-tolyl)-1H-pyrrole-2,5-dione compound with methane (98)



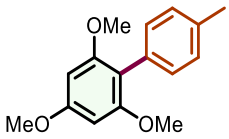
Yellow solid (10.1 mg, 34%); m.p. 138.3-139.4 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.58 (d, *J* = 8.2 Hz, 2H), 7.52 – 7.47 (m, 2H), 7.46 – 7.42 (m, 2H), 7.40 – 7.36 (m, 1H), 7.34 (d, *J* = 8.1 Hz, 2H), 2.45 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 170.9, 169.9, 140.1, 137.2, 135.9, 131.9, 129.6, 129.4, 129.0, 127.6, 126.0, 21.5, 10.2. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{19}H_{20}NO_2$, 294.1489; Found: 294.1499.

5,6,7,8-tetramethoxy-2-(4-methoxyphenyl)-3-(p-tolyl)-4H-chromen-4-one (99)



White solid (16.7 mg, 36%); m.p. 170.5 – 171.3 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.43 – 7.36 (m, 2H), 7.19 – 7.11 (m, 4H), 6.84 – 6.76 (m, 2H), 4.13 (s, 3H), 4.02 (s, 3H), 3.97 (s, 3H), 3.94 (s, 3H), 3.82 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 176.4, 160.8, 158.9, 151.2, 148.6, 147.5, 144.0, 137.8, 137.2, 131.1, 131.0, 130.1, 129.2, 125.4, 122.0, 114.5, 113.5, 62.2, 62.0, 61.8, 61.7, 55.3, 21.3. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{27}H_{27}O_7$, 463.1751; Found: 463.1754.

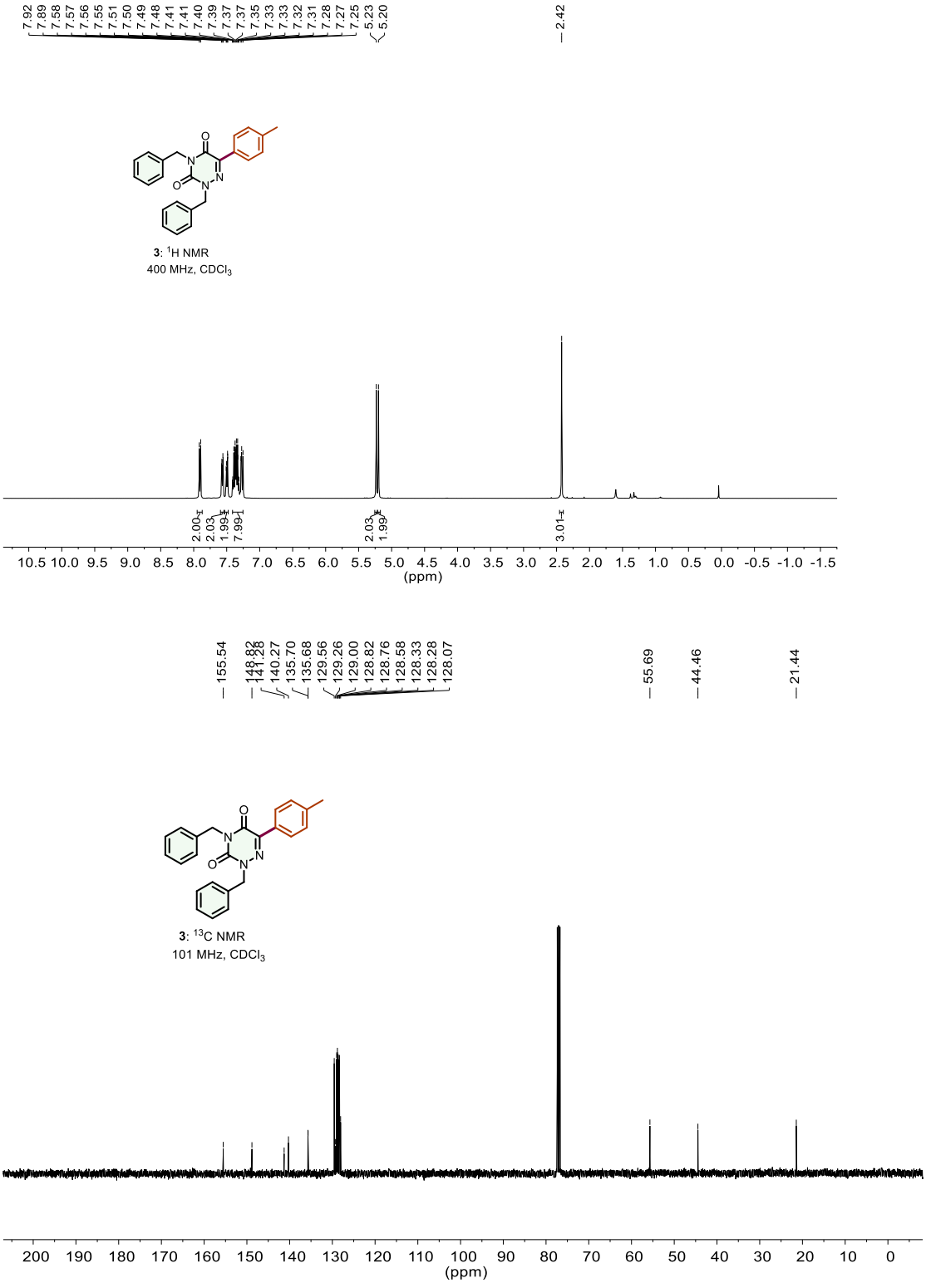
2,4,6-trimethoxy-4'-methyl-1,1'-biphenyl (100)[12]

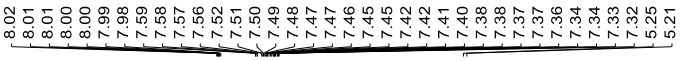


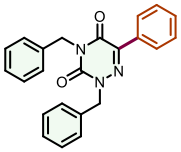
White solid (15.8 mg, 61%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.28 – 7.20 (m, 4H), 6.26

(s, 2H), 3.89 (s, 3H), 3.75 (s, 6H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 160.3, 158.4, 136.0, 131.0, 131.0, 128.5, 112.4, 90.9, 55.9, 55.4, 21.4.

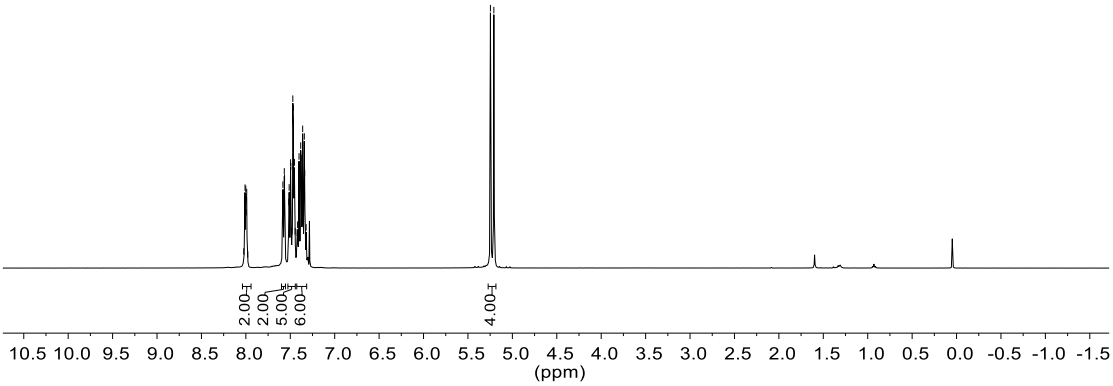
5. NMR Copies of Products

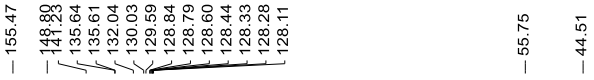


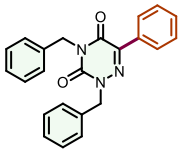




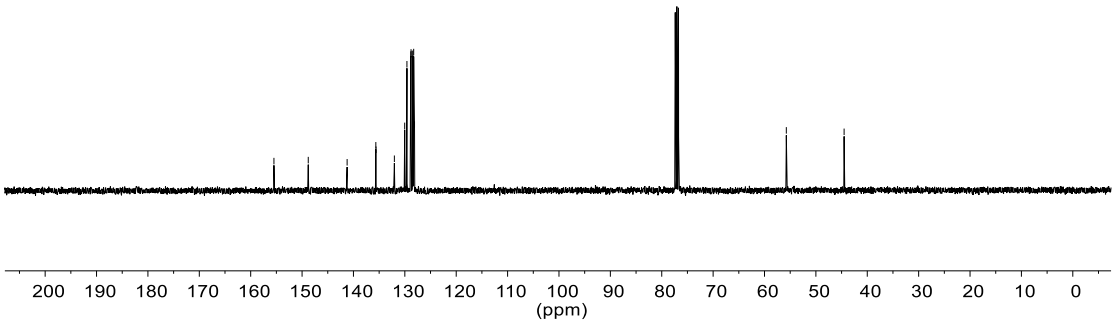
4: ^{1}H NMR
400 MHz, $CDCl_3$

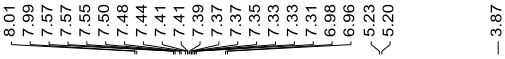


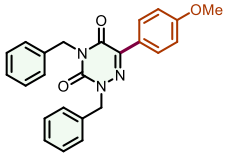




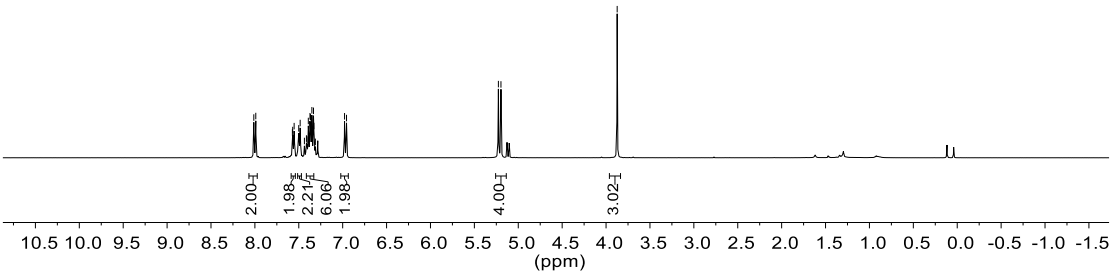
4: ^{13}C NMR
101 MHz, $CDCl_3$

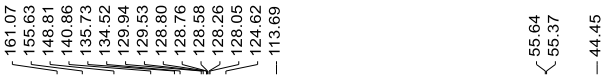


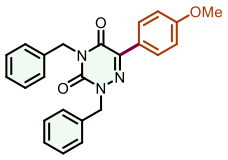




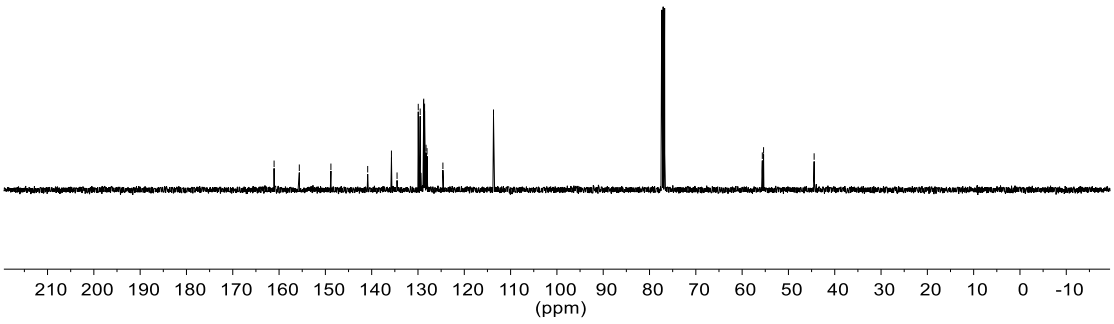
5: ^{1}H NMR
400 MHz, $CDCl_3$

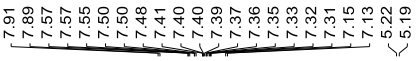


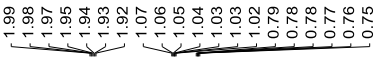


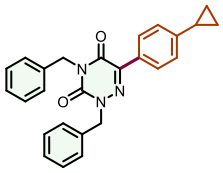


5: ^{13}C NMR
101 MHz, $CDCl_3$

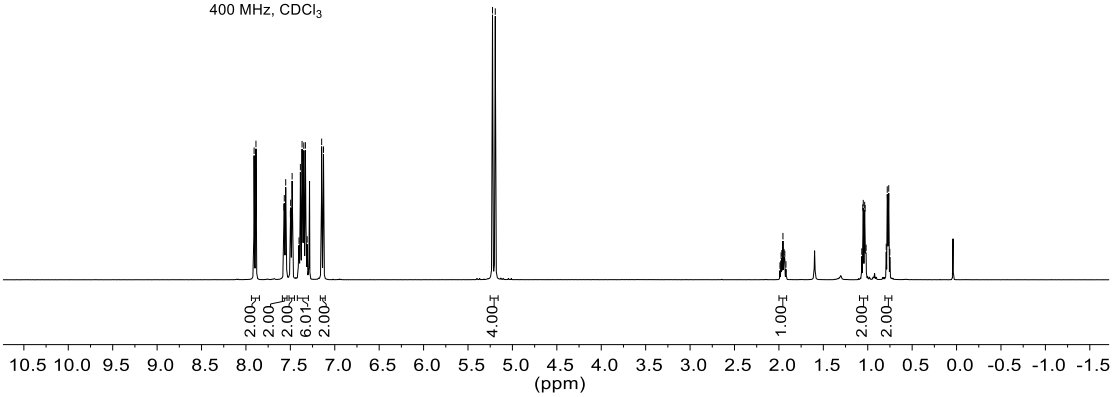


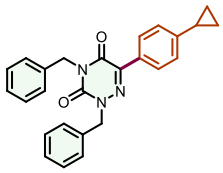




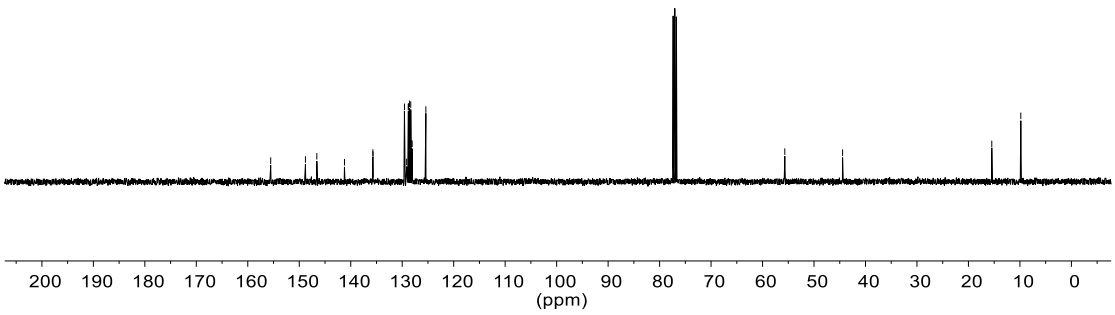


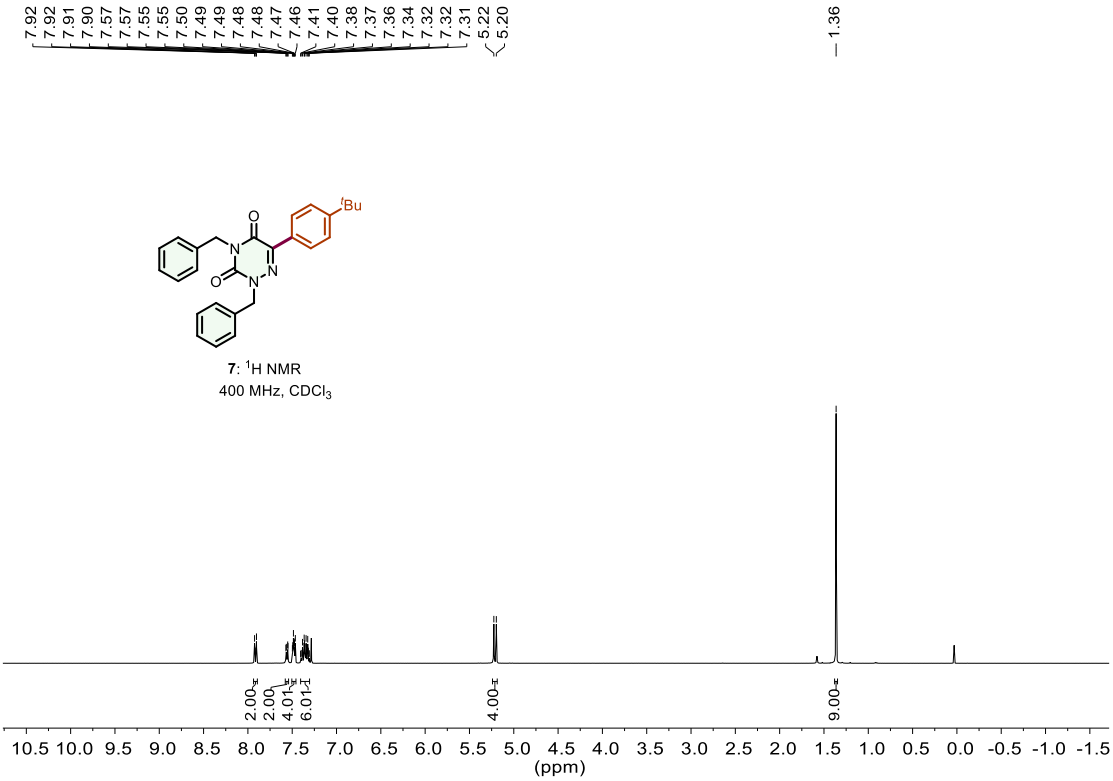
6: ^{1}H NMR
400 MHz, $CDCl_3$



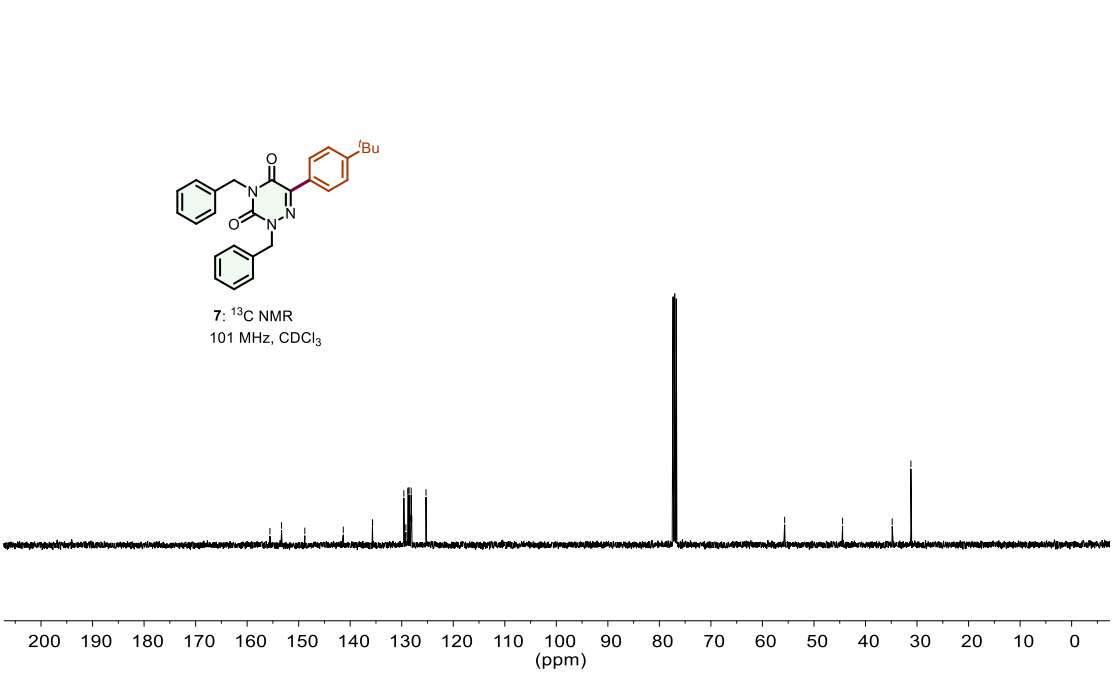


6: ^{13}C NMR
101 MHz, $CDCl_3$

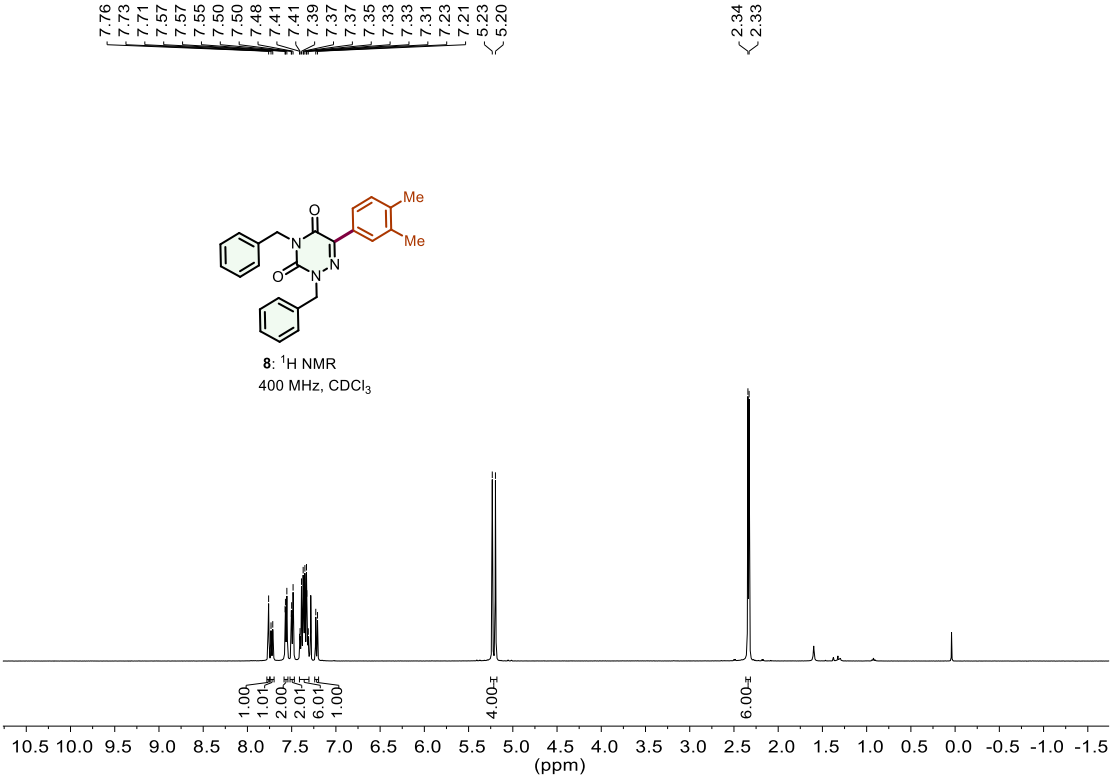


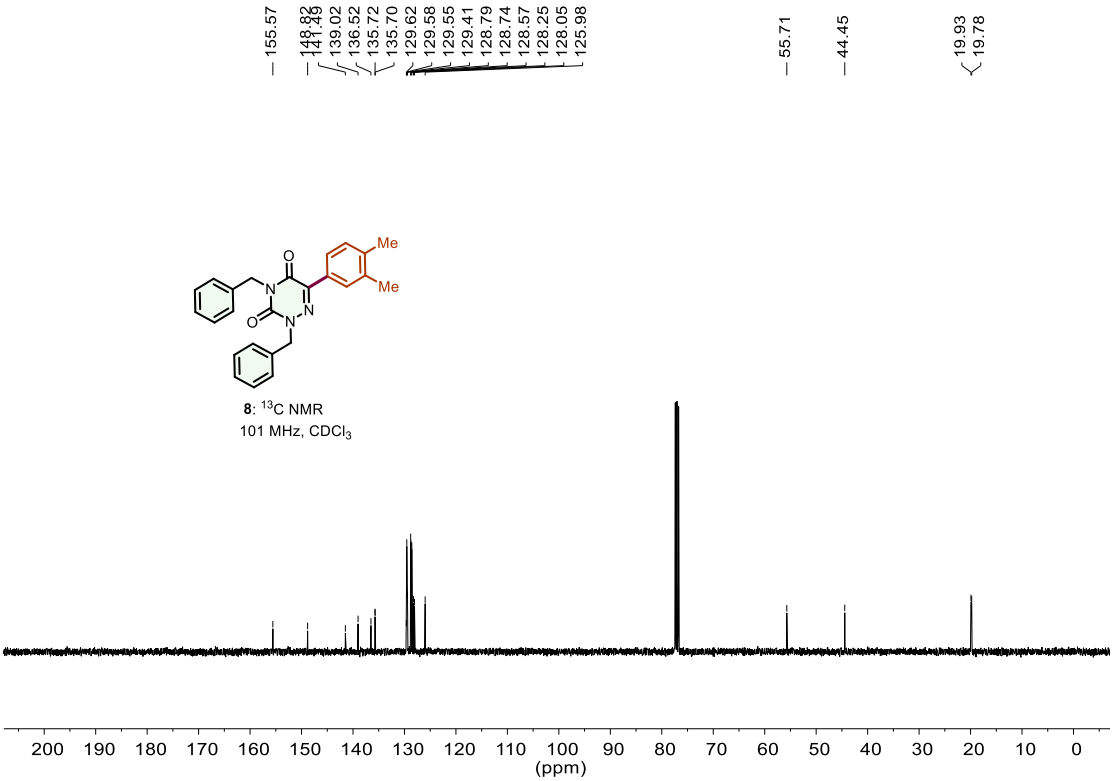


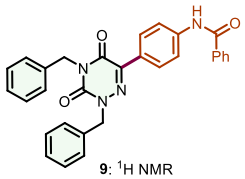
7: ^{1}H NMR
400 MHz, $CDCl_3$



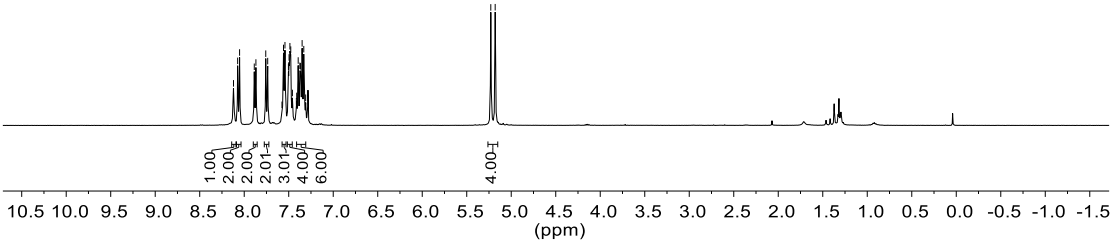
7: ^{13}C NMR
101 MHz, $CDCl_3$

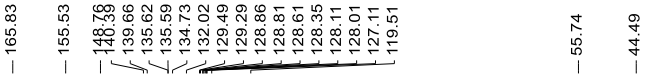

7.76
7.73
7.71
7.57
7.57
7.55
7.50
7.50
7.48
7.41
7.41
7.39
7.37
7.37
7.35
7.33
7.33
7.31
7.23
7.21
5.23
5.20
2.34
2.33
Me
Me
O
N
N
O
N
8: 1H NMR
400 MHz, CDCl3
1.00
1.01
2.00
2.01
6.01
1.00
4.00
6.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)

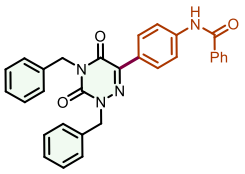

155.57
148.82
141.49
139.02
136.52
135.72
135.70
129.62
129.58
129.55
129.41
128.79
128.74
128.57
128.25
128.05
125.98
55.71
44.45
19.93
19.78
Me
Me
O
N
N
O
N
8: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)



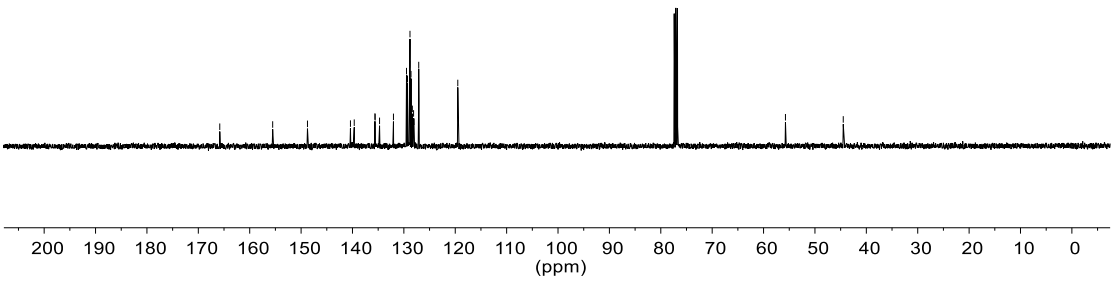
9: ^{1}H NMR
400 MHz, $CDCl_3$

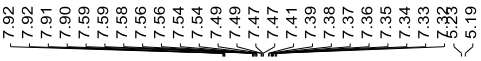


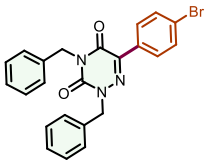




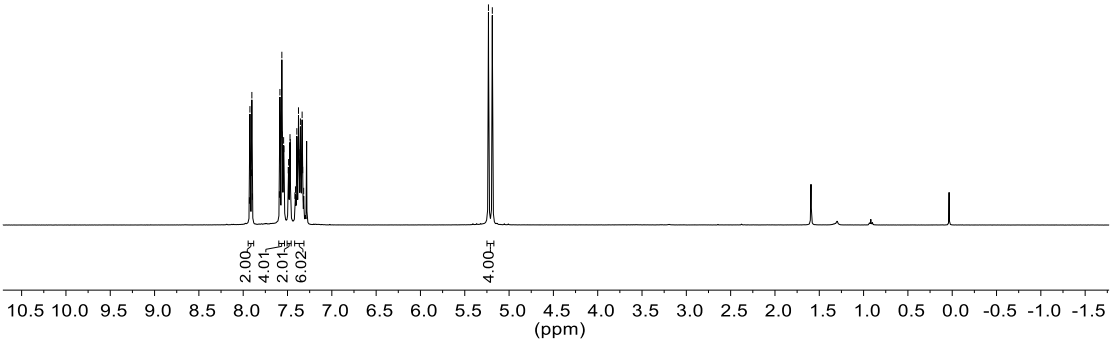
9: ^{13}C NMR
101 MHz, $CDCl_3$

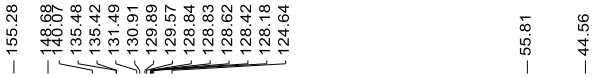


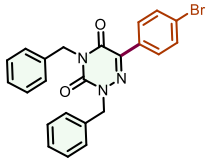




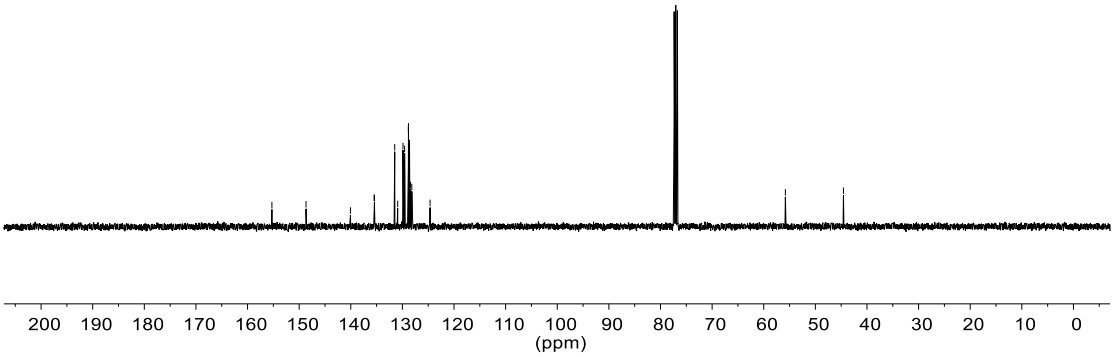
10: ^{1}H NMR
400 MHz, $CDCl_3$

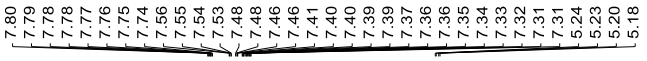


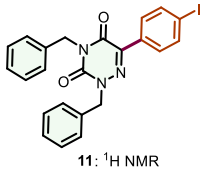




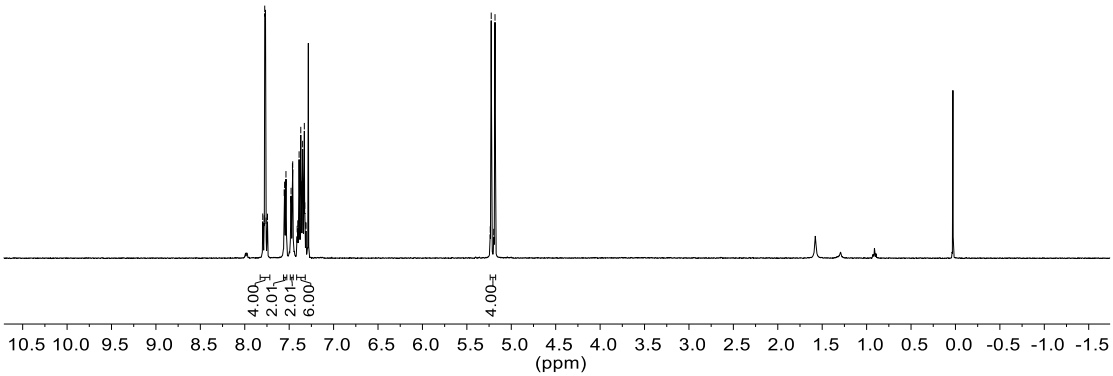
10: ^{13}C NMR
101 MHz, $CDCl_3$

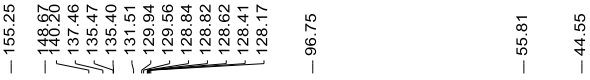


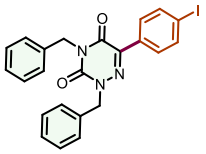




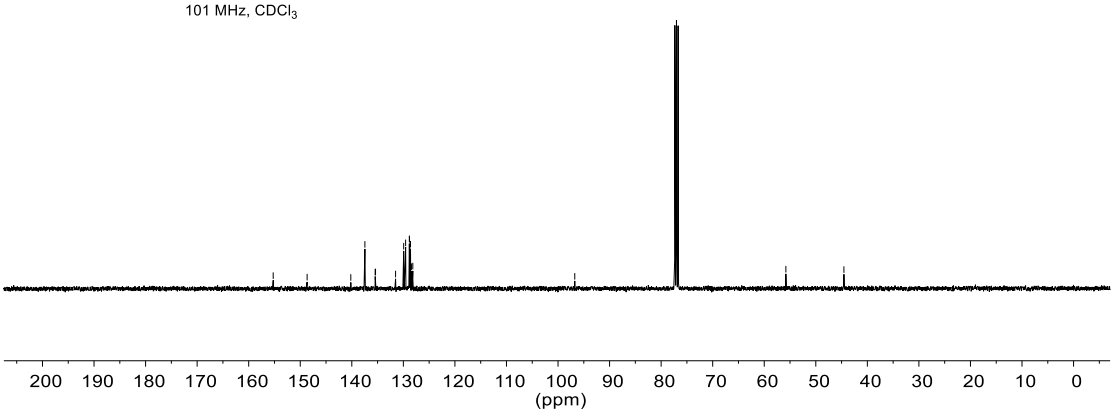
11: ^{1}H NMR
400 MHz, $CDCl_3$

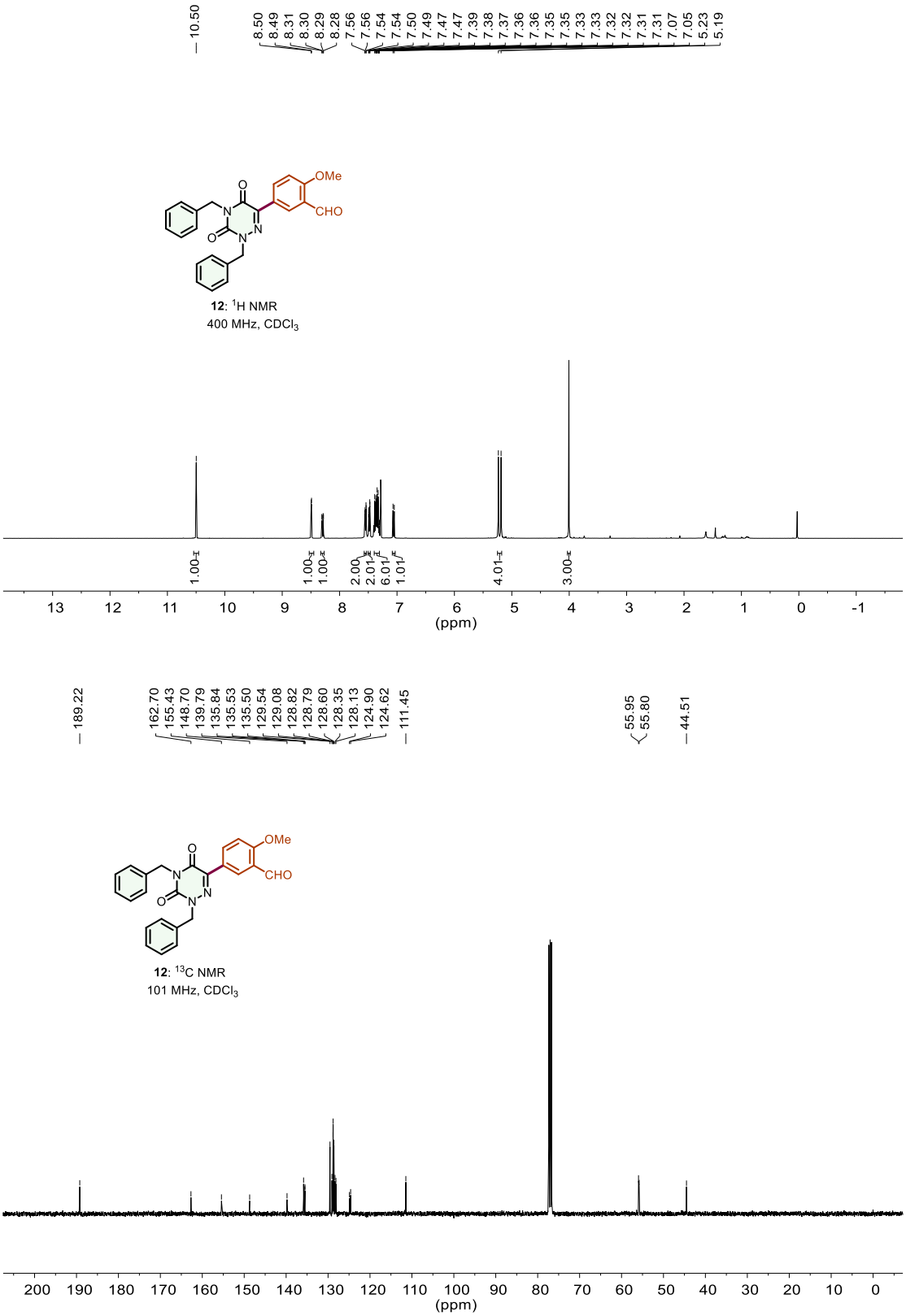


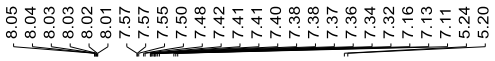


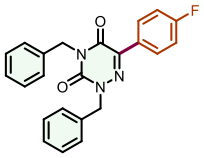


11: ^{13}C NMR
101 MHz, $CDCl_3$

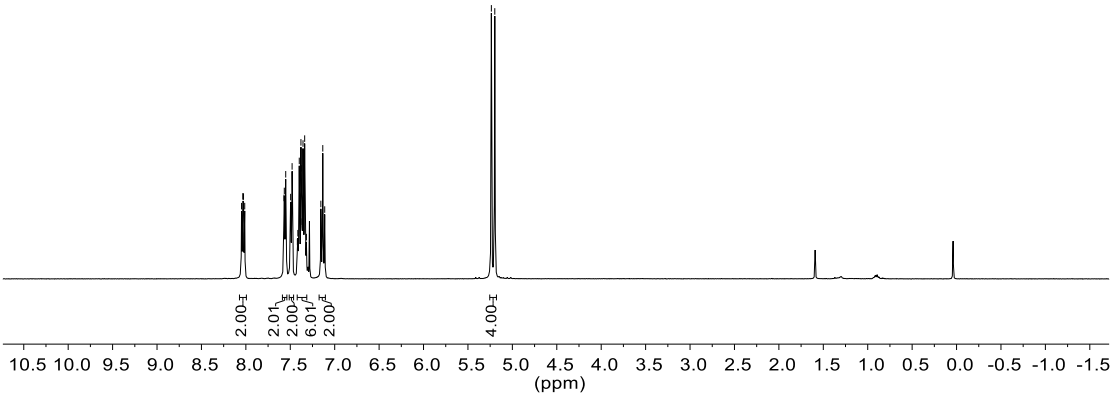


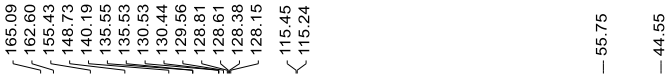

10.50
8.50
8.49
8.31
8.30
8.29
8.28
7.56
7.56
7.54
7.54
7.50
7.49
7.47
7.47
7.39
7.38
7.37
7.36
7.36
7.35
7.35
7.33
7.33
7.32
7.32
7.31
7.31
7.07
7.05
5.23
5.19
OMe
CHO
12: 1H NMR
400 MHz, CDCl3
1.00
1.00
1.00
2.00
2.01
6.01
1.01
4.01
3.00
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
(ppm)
189.22
162.70
155.43
148.70
139.79
135.84
135.53
135.50
129.54
129.08
128.82
128.79
128.60
128.35
128.13
124.90
124.62
111.45
55.95
55.80
44.51
OMe
CHO
12: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

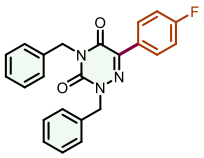




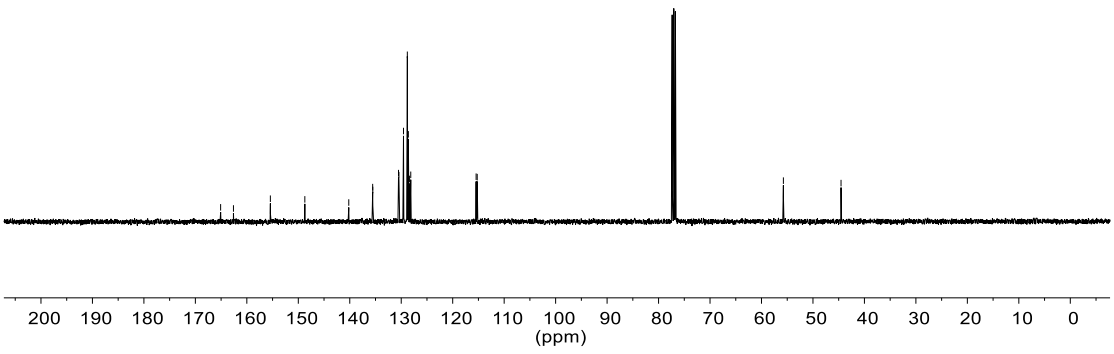
13: ^{1}H NMR
400 MHz, $CDCl_3$

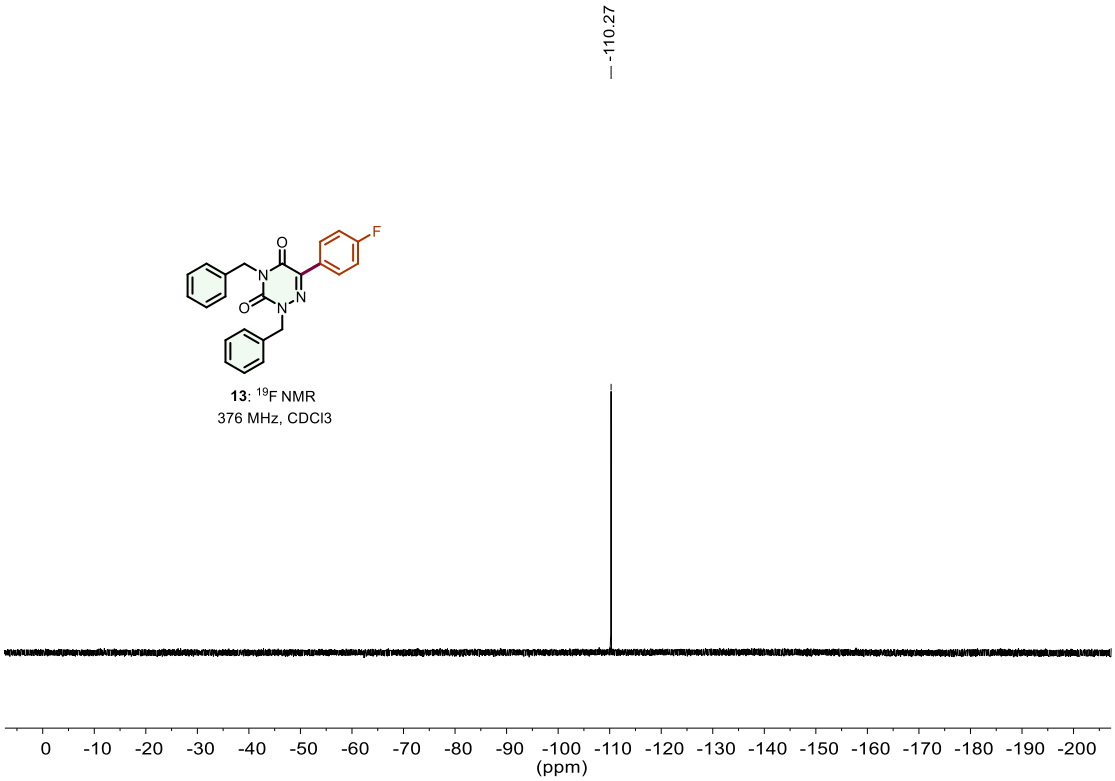


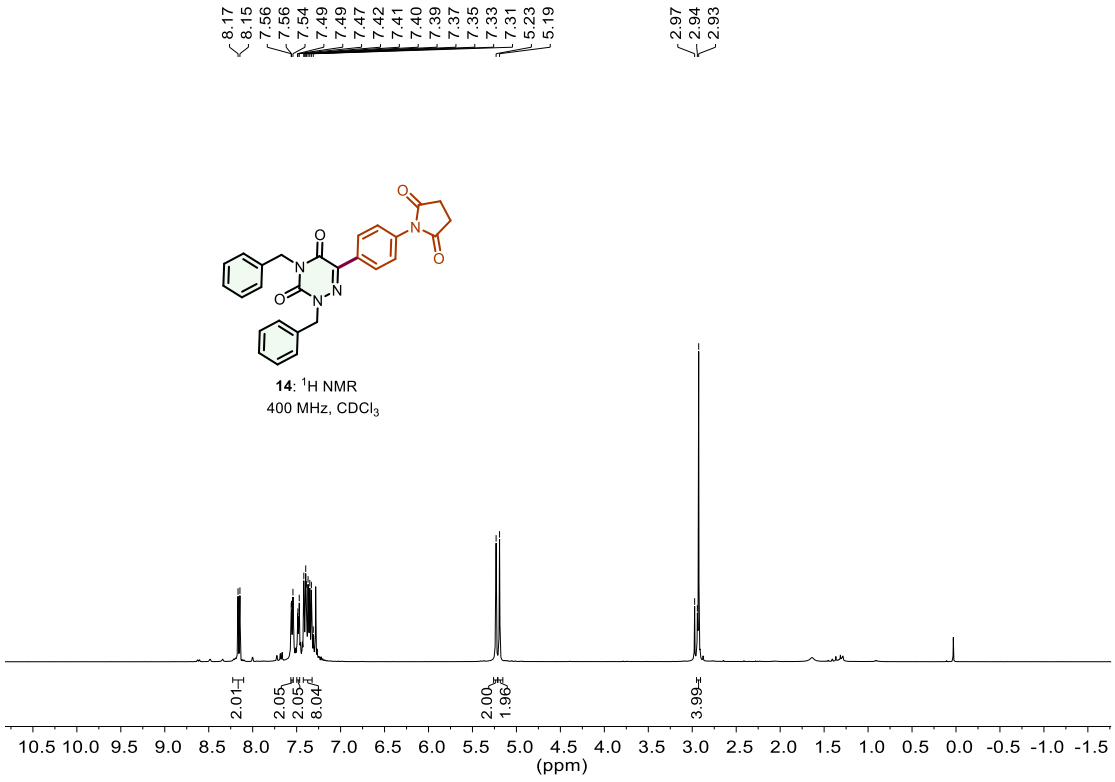


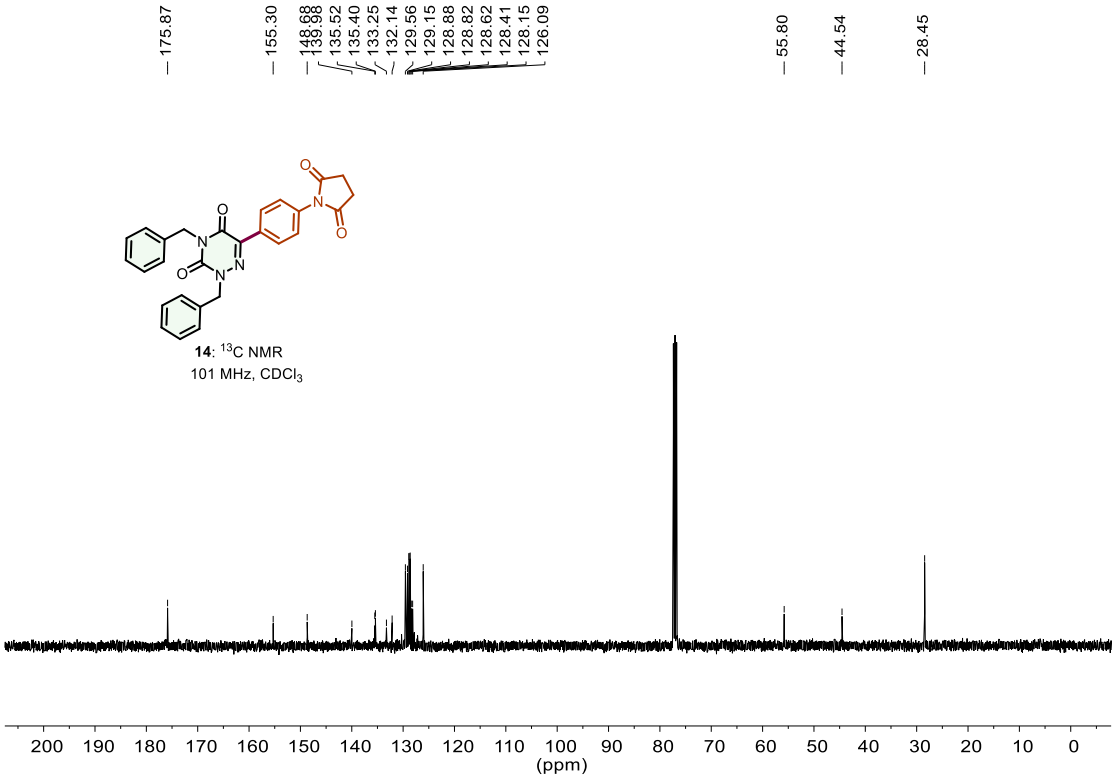


13: ^{13}C NMR
101 MHz, $CDCl_3$

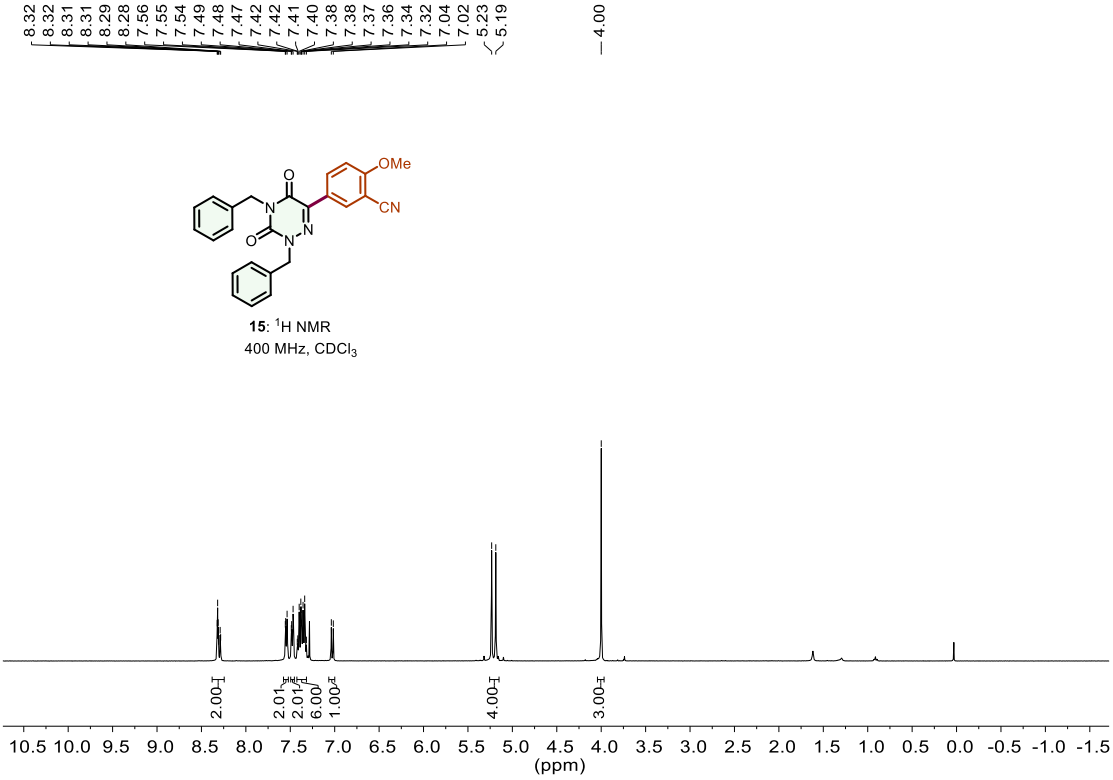



-110.27
F
O
N
N
O
N
13: 19F NMR
376 MHz, CDCl3
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
(ppm)

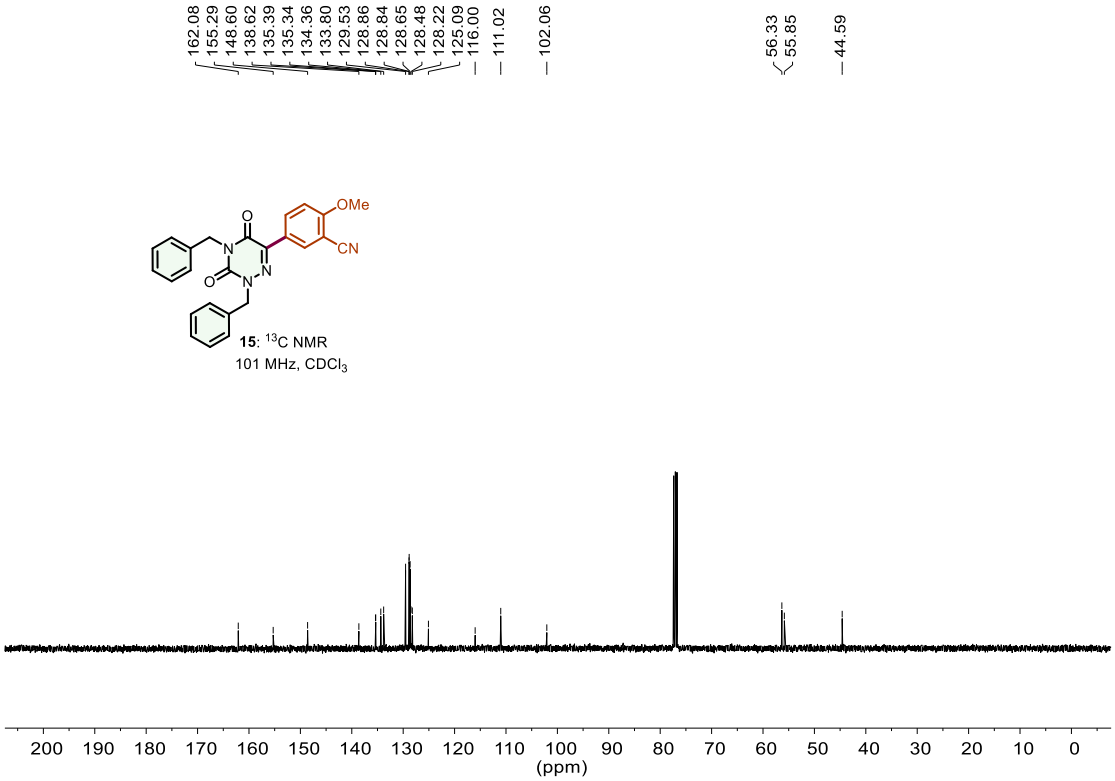

8.17
8.15
7.56
7.56
7.54
7.49
7.49
7.47
7.42
7.41
7.40
7.39
7.37
7.35
7.33
7.31
5.23
5.19
2.97
2.94
2.93
O
N
O
N
O
N
O
14: 1H NMR
400 MHz, CDCl3
2.01
2.05
2.05
8.04
2.00
1.96
3.99
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)



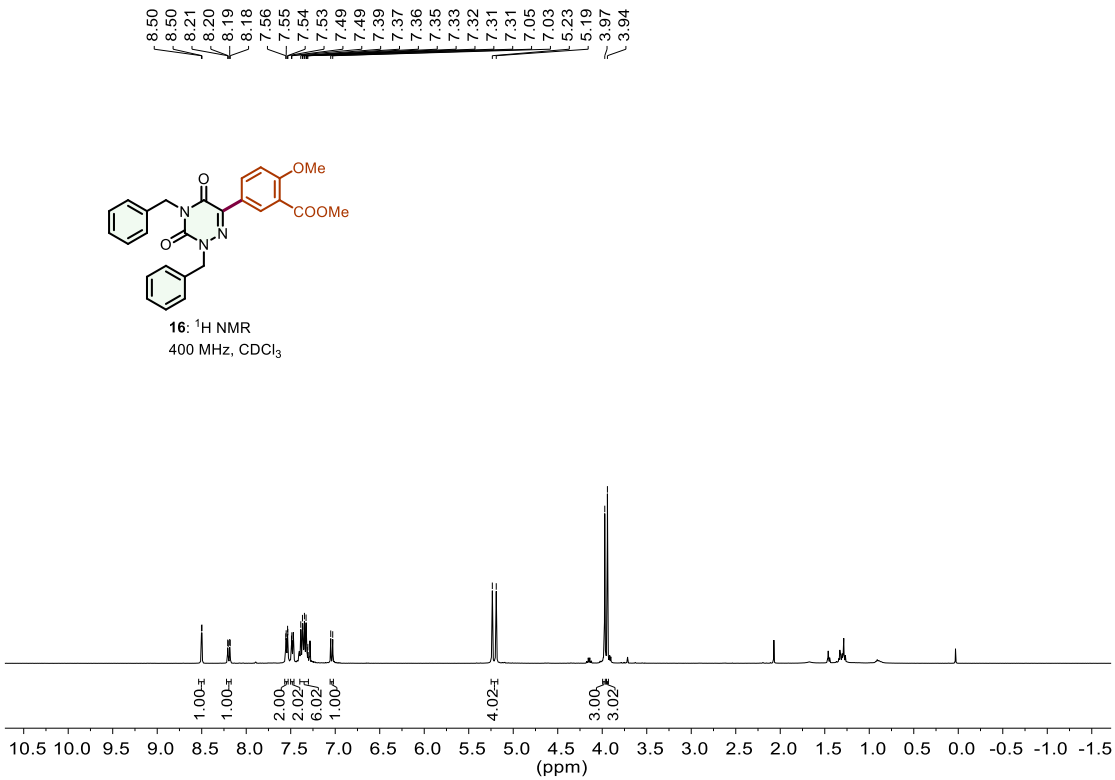
14: ^{13}C NMR
101 MHz, $CDCl_3$



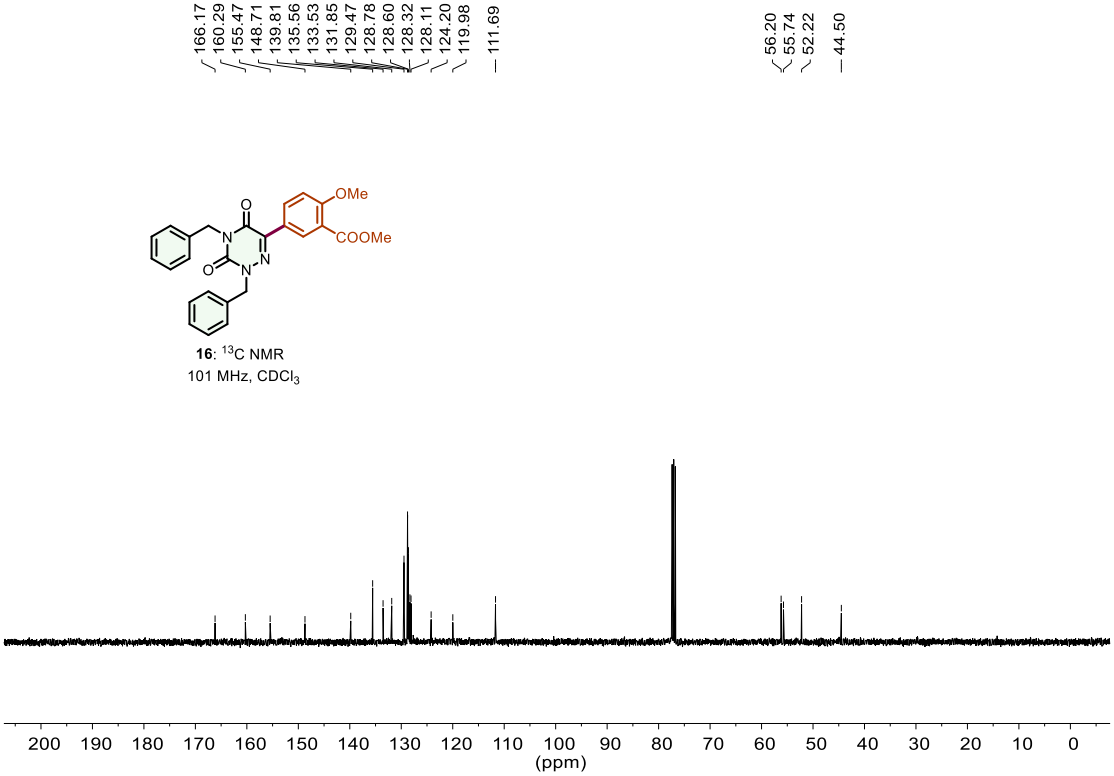
15: ^{1}H NMR
400 MHz, $CDCl_3$



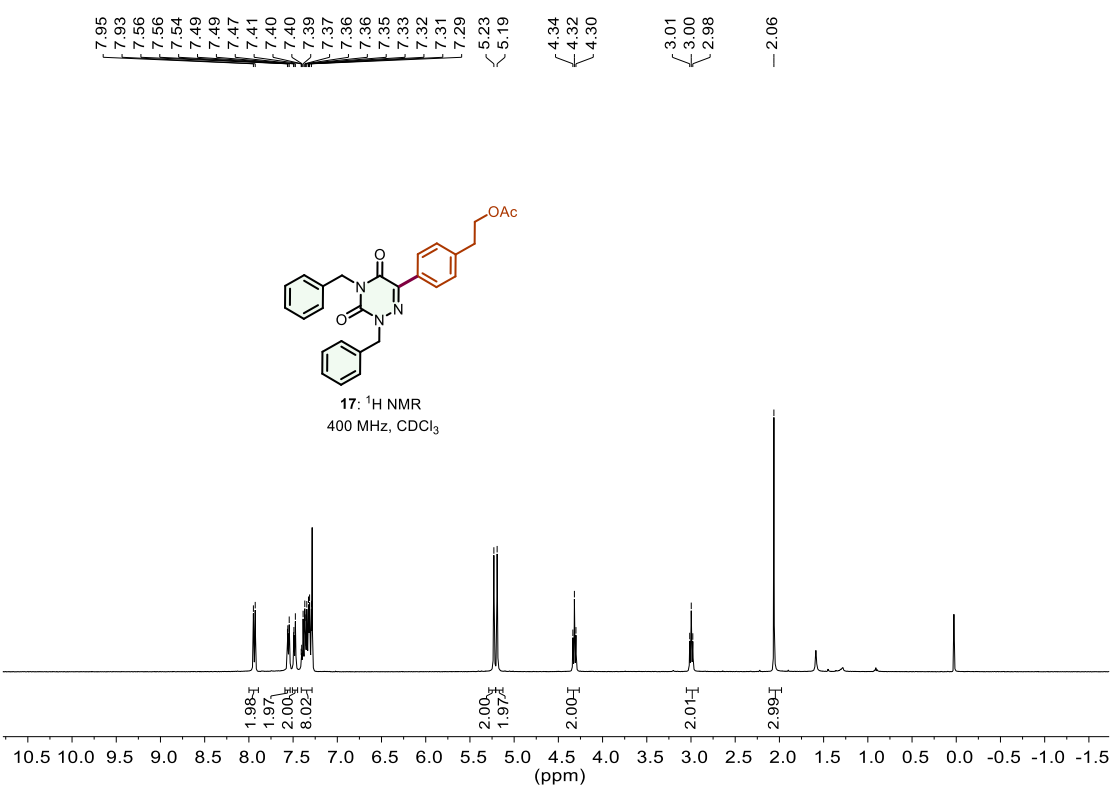
15: ^{13}C NMR
101 MHz, $CDCl_3$



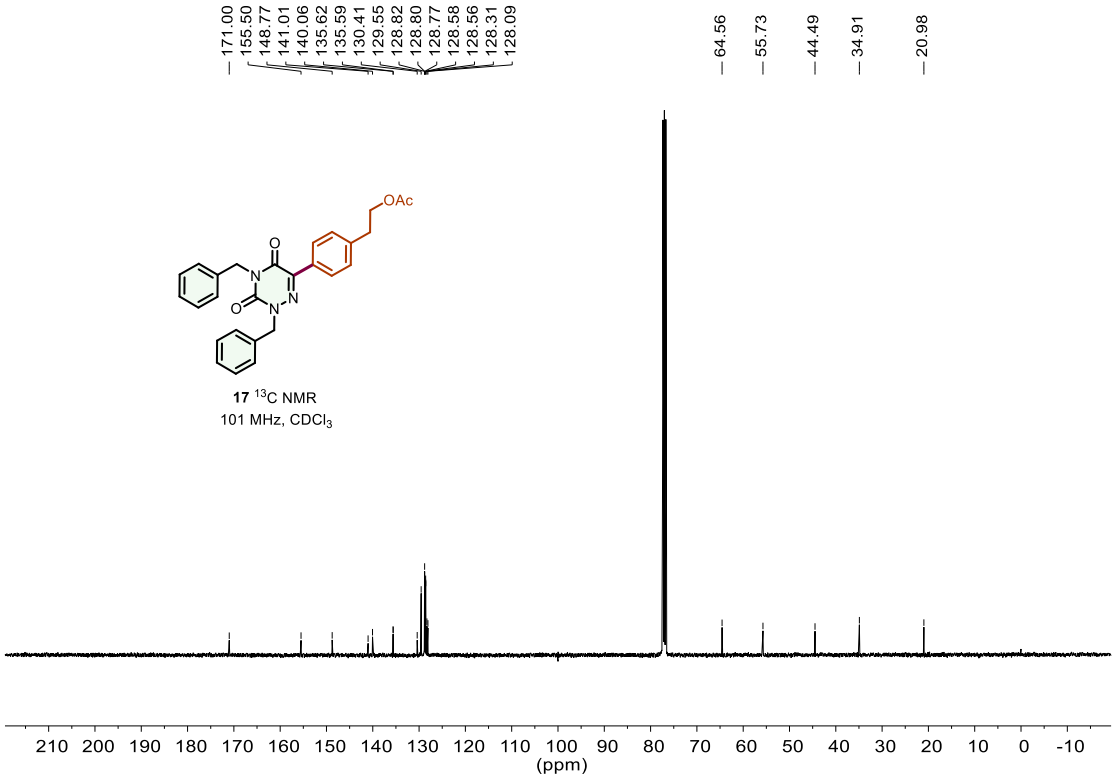
16: ^{1}H NMR
400 MHz, $CDCl_3$



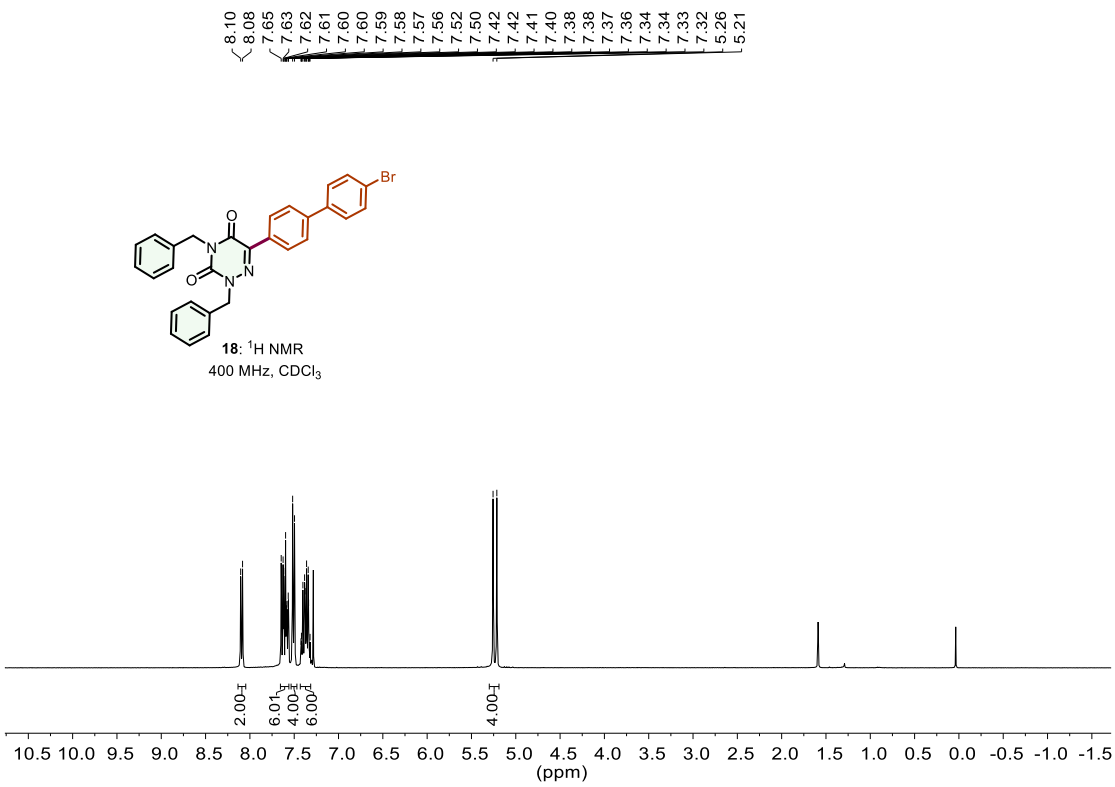
16: ^{13}C NMR
101 MHz, $CDCl_3$



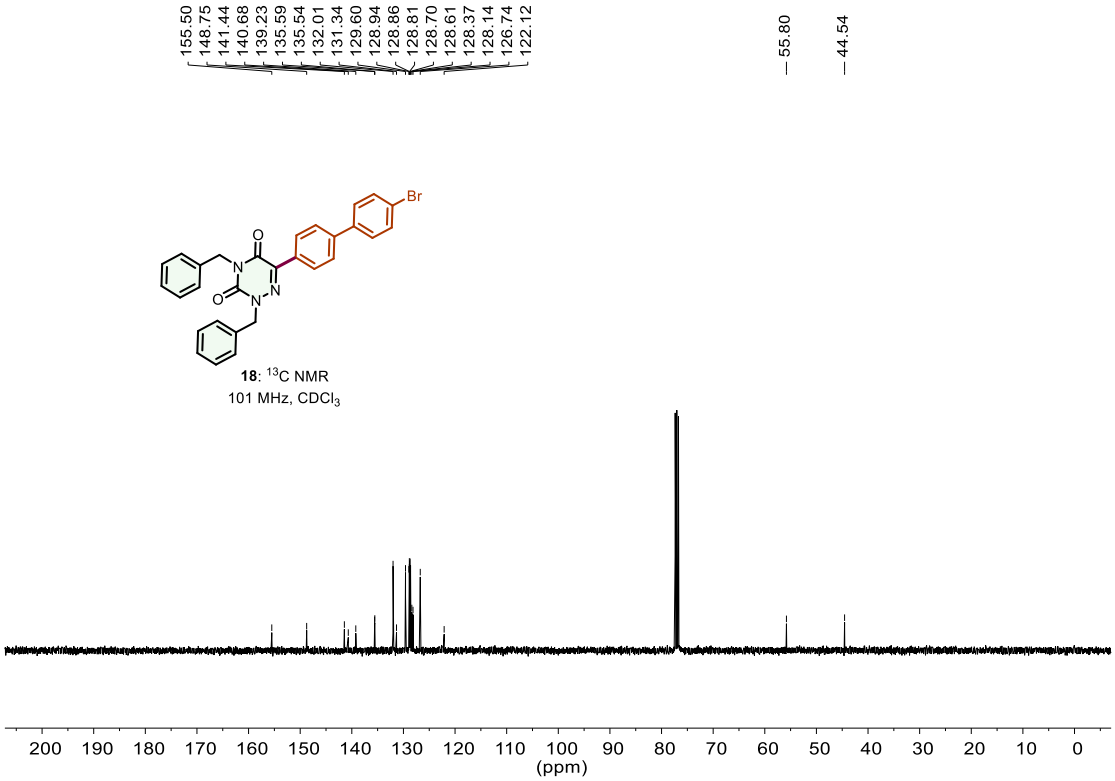
17: ^{1}H NMR
400 MHz, $CDCl_3$



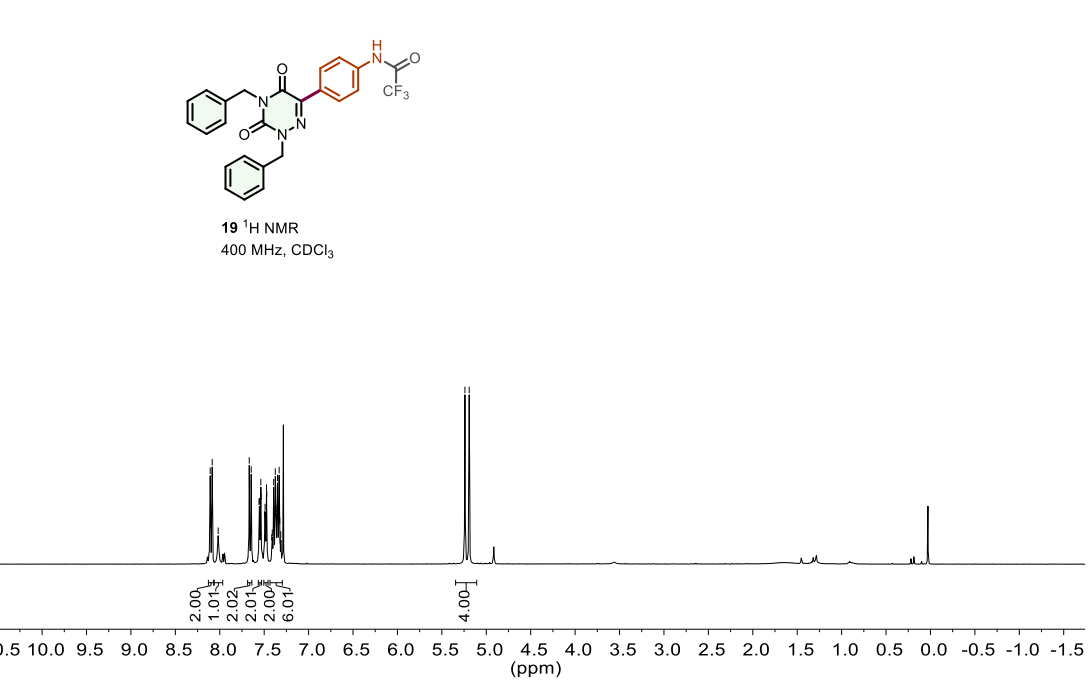
17 ^{13}C NMR
101 MHz, $CDCl_3$



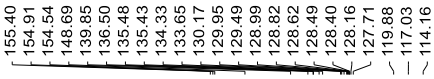
18: ^{1}H NMR
400 MHz, $CDCl_3$

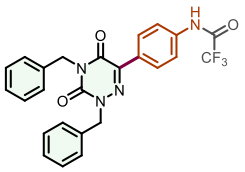


18: ^{13}C NMR
101 MHz, $CDCl_3$

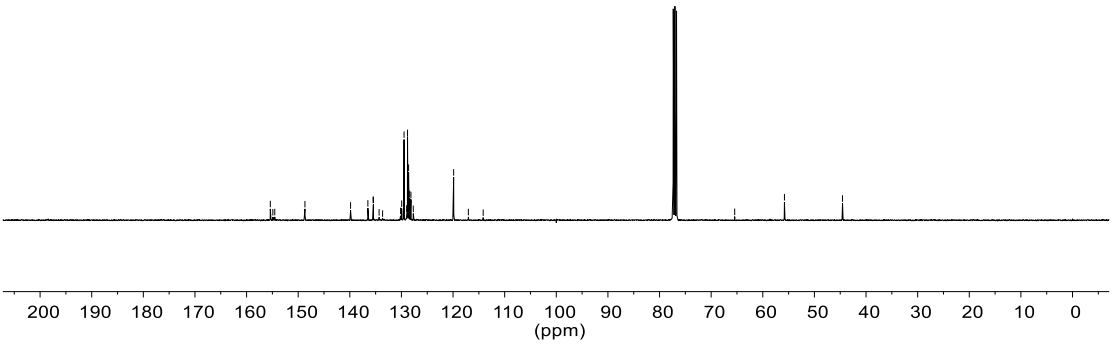


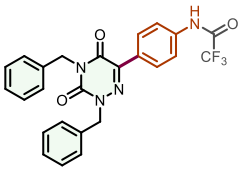
19 ^{1}H NMR
400 MHz, $CDCl_3$



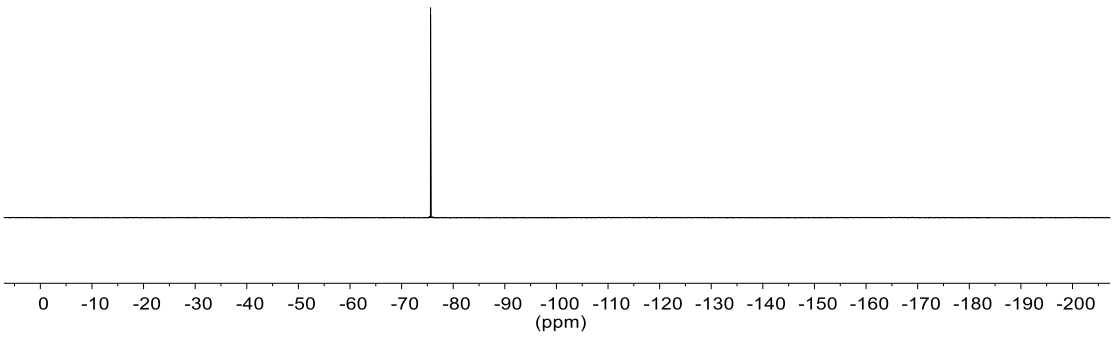


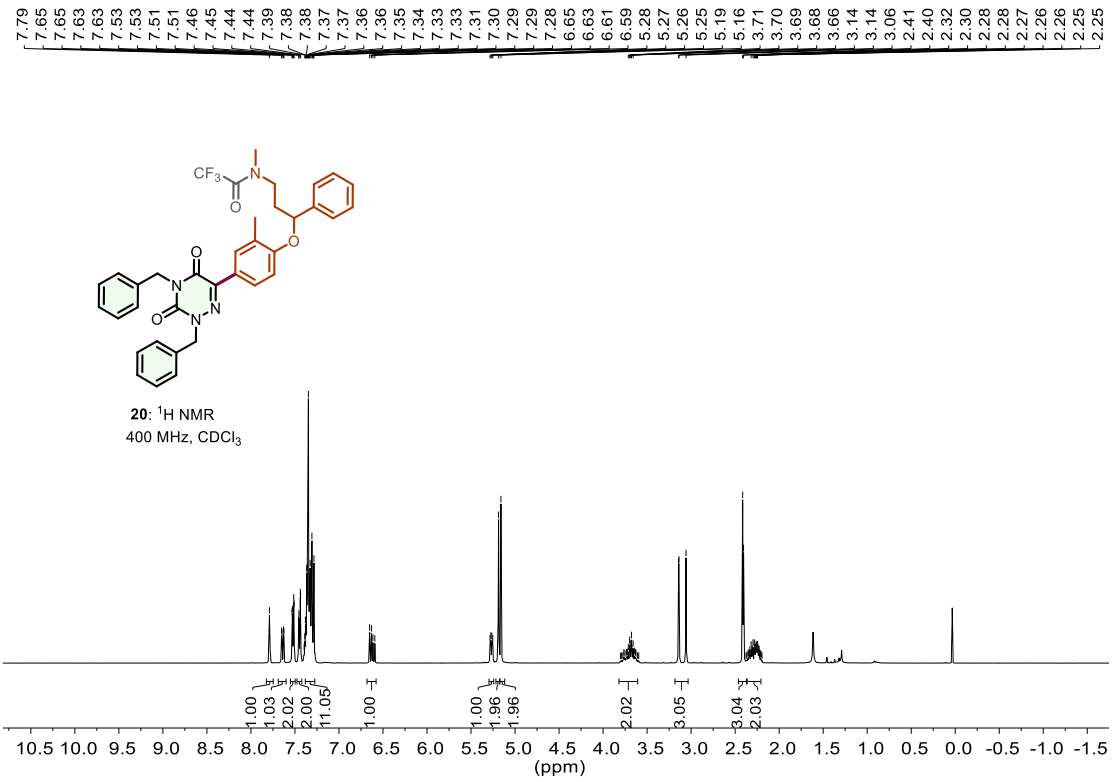
19: ^{13}C NMR
101 MHz, $CDCl_3$

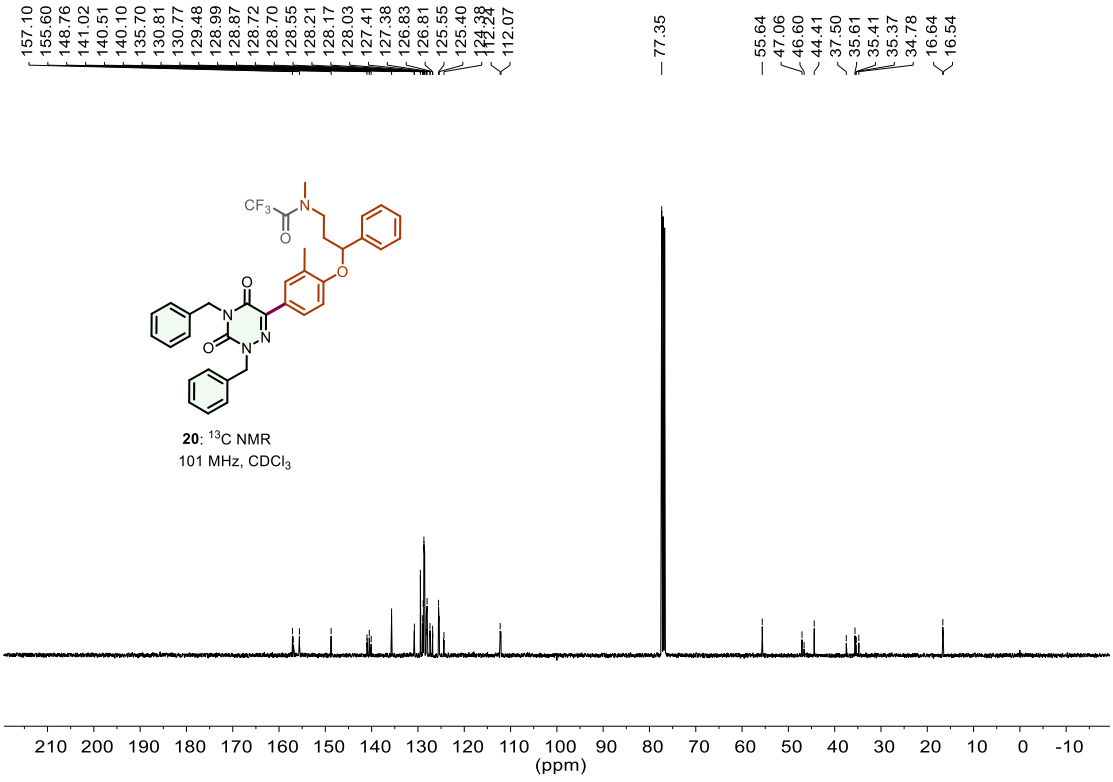


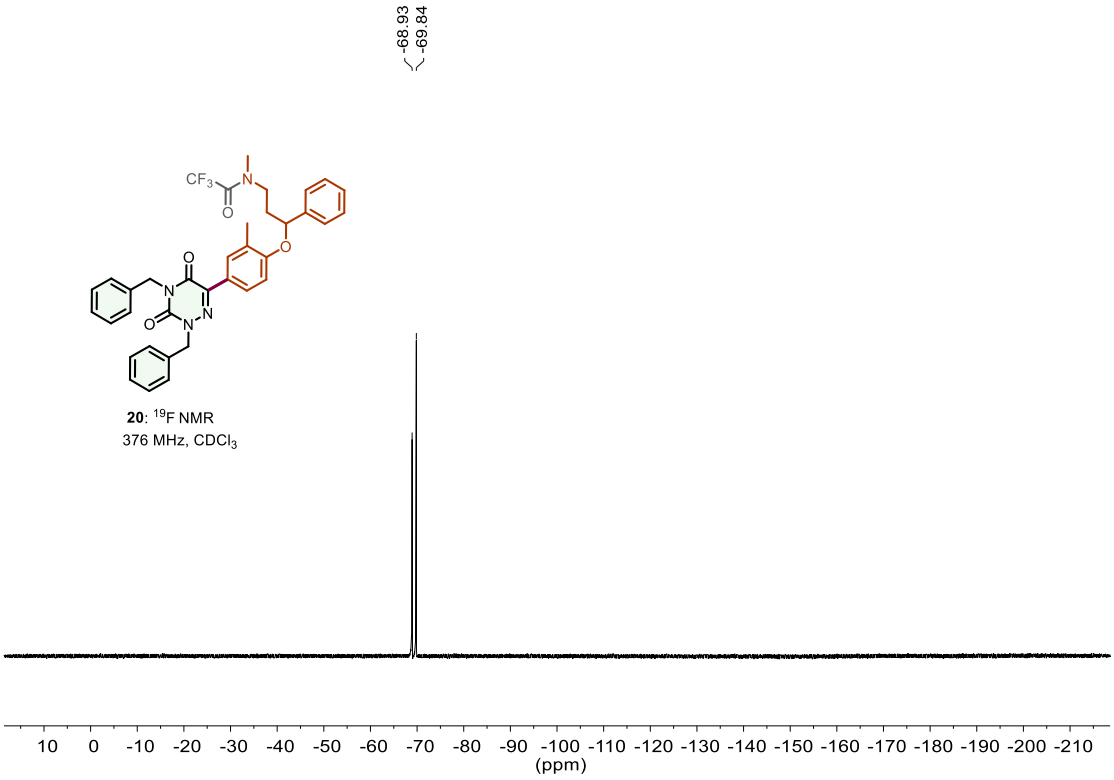


19: ^{19}F NMR
376 MHz, $CDCl_3$

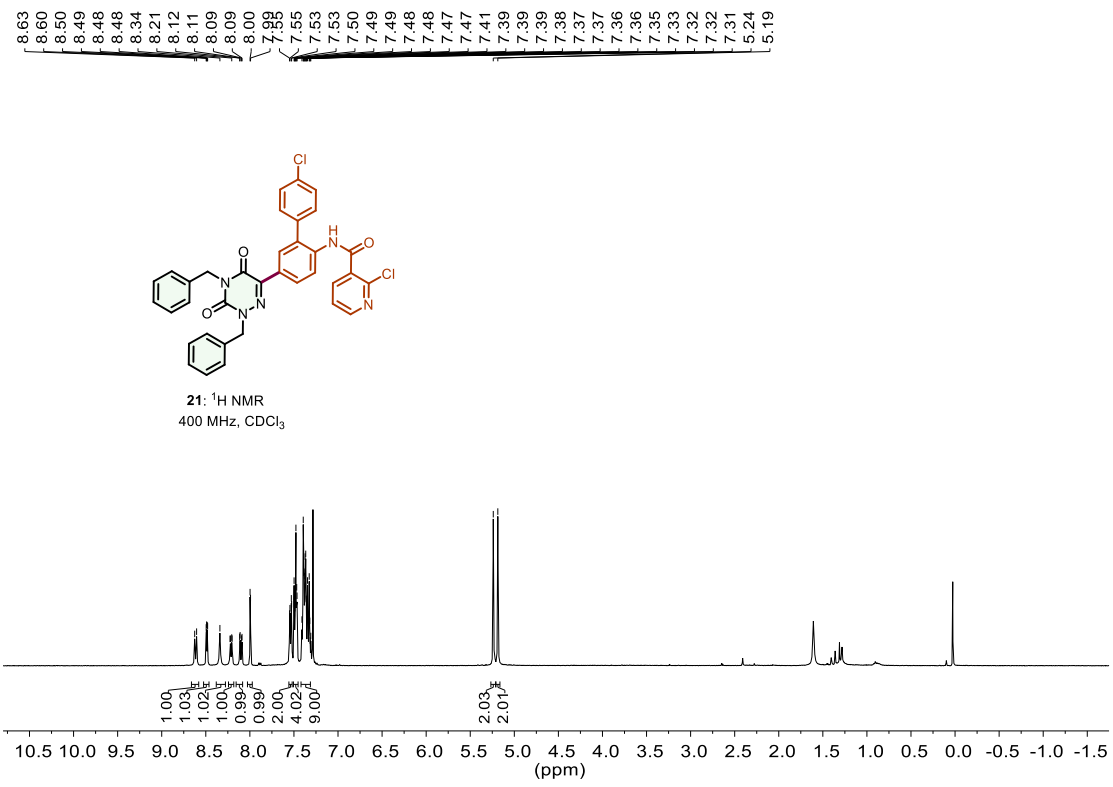



7.79 7.65 7.65 7.63 7.63 7.53 7.53 7.51 7.51 7.46 7.45 7.44 7.44 7.39 7.38 7.38 7.37 7.37 7.36 7.36 7.35 7.34 7.33 7.33 7.31 7.30 7.29 7.29 7.28 6.65 6.63 6.61 6.59 5.28 5.27 5.26 5.25 5.19 5.16 3.71 3.70 3.69 3.68 3.66 3.14 3.14 3.06 2.41 2.40 2.32 2.30 2.28 2.28 2.27 2.26 2.26 2.25 2.25
20: 1H NMR
400 MHz, CDCl3
1.00 1.03 2.02 2.00 11.05 1.00 1.00 1.96 1.96 2.02 3.05 3.04 2.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)

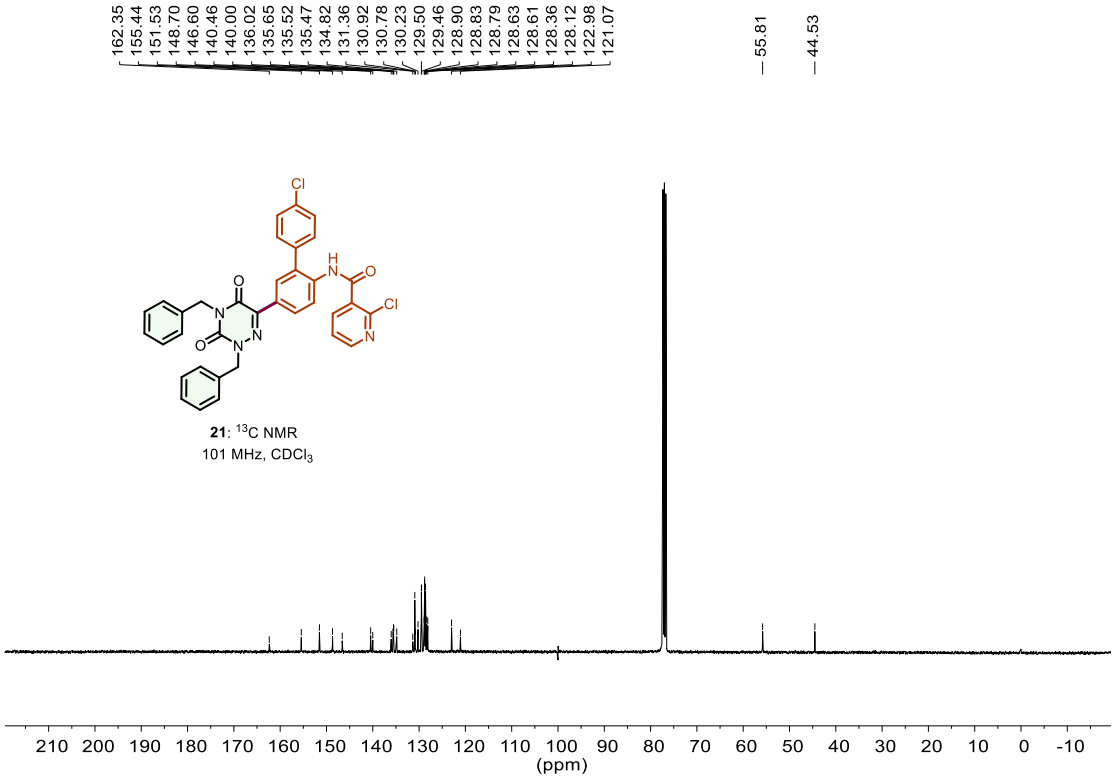

157.10 155.60 148.76 141.02 140.51 140.10 135.70 130.81 130.77 129.48 128.99 128.87 128.72 128.70 128.55 128.21 128.17 128.03 127.41 127.38 126.83 126.81 125.55 125.40 112.24 112.07
77.35
55.64 47.06 46.60 44.41 37.50 35.61 35.41 35.37 34.78 16.64 16.54
20: 13C NMR
101 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)



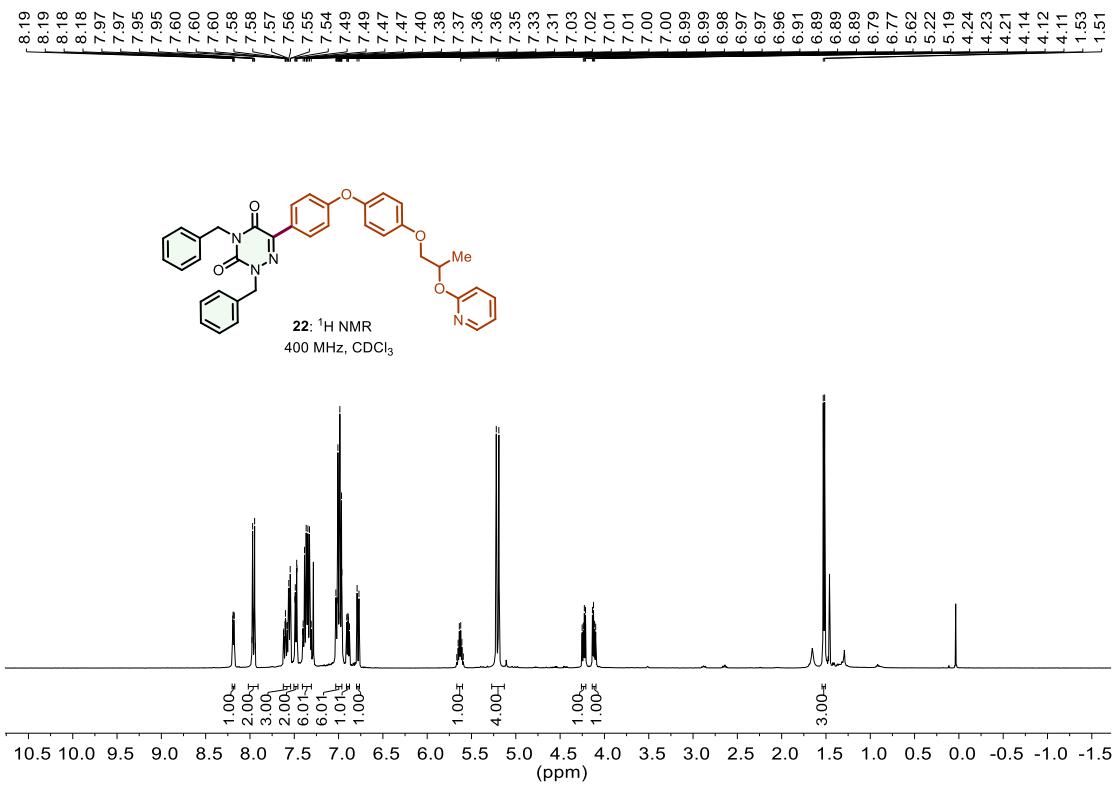
20: ^{19}F NMR
376 MHz, $CDCl_3$



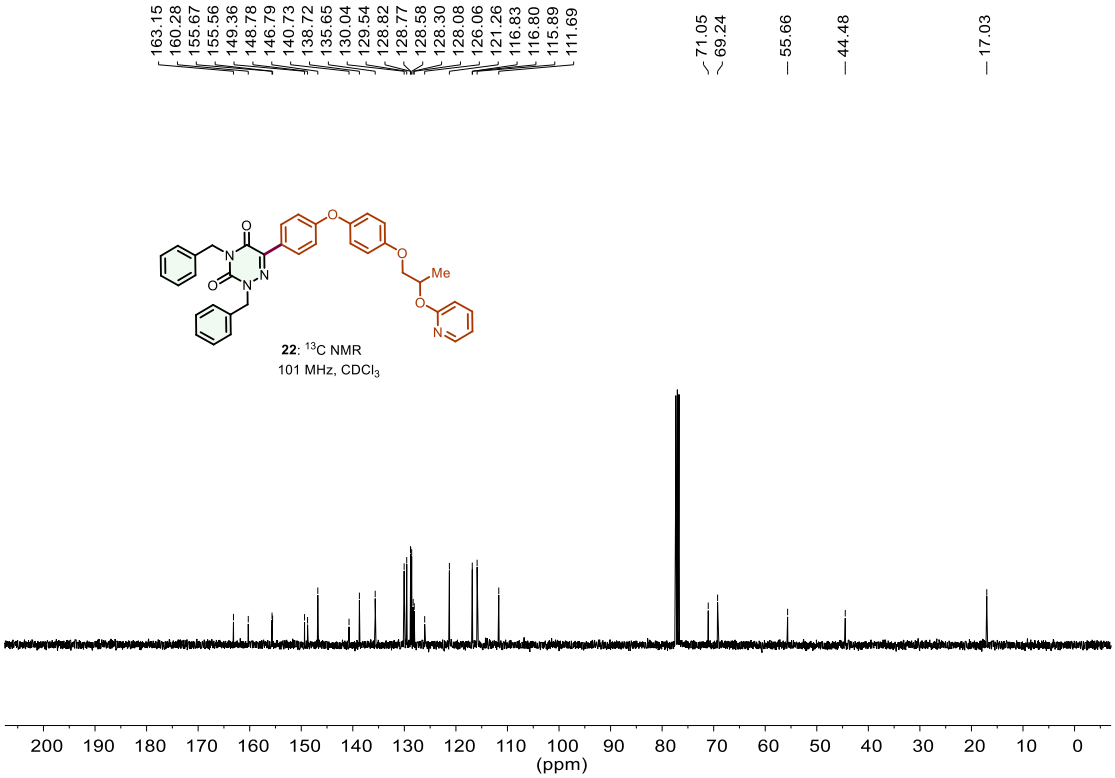
21: ^{1}H NMR
400 MHz, $CDCl_3$

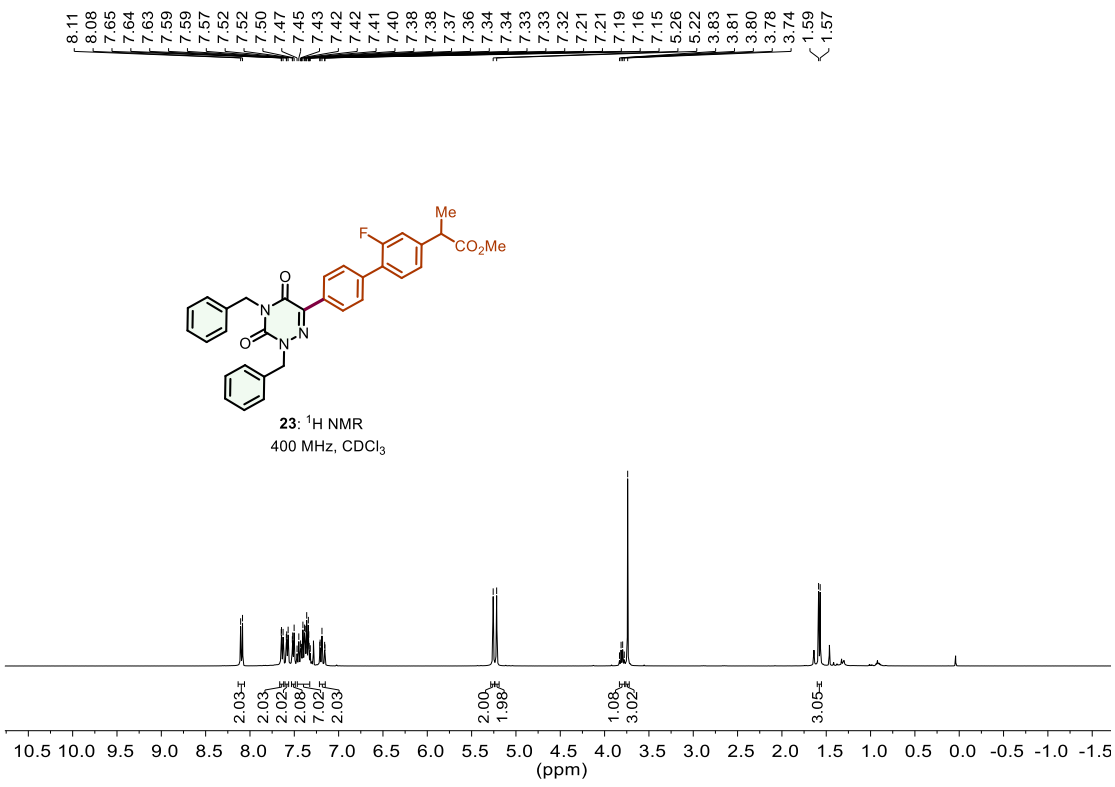


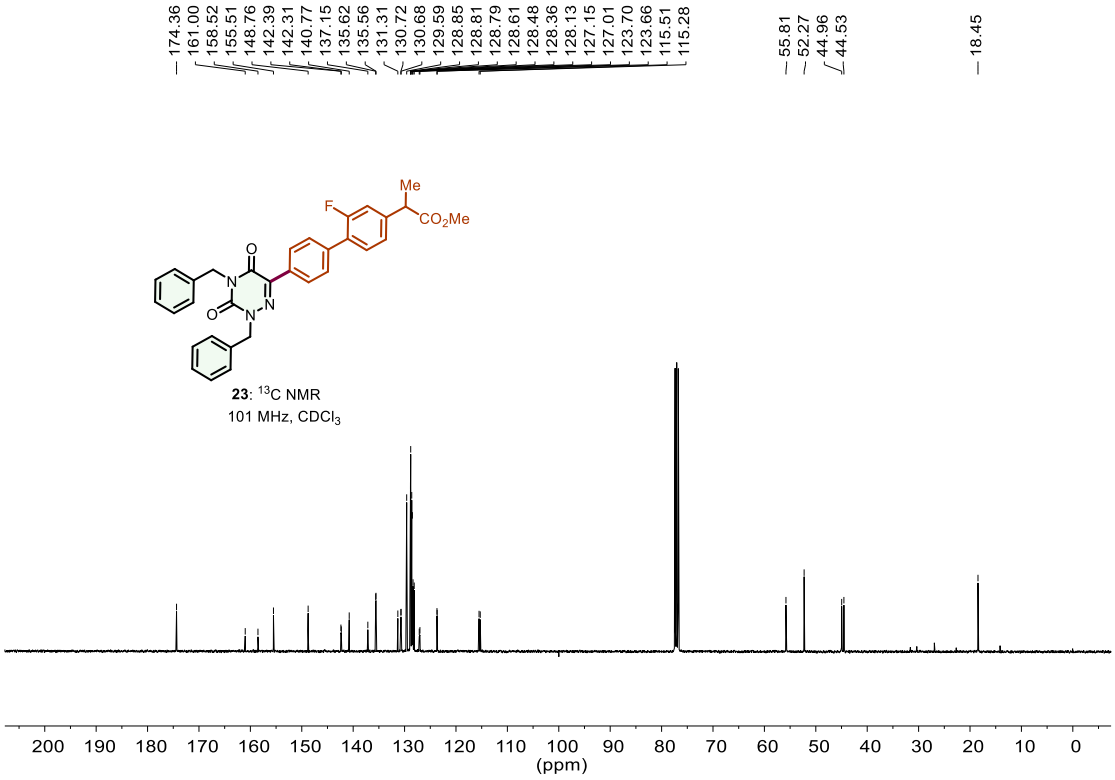
21: ^{13}C NMR
101 MHz, $CDCl_3$

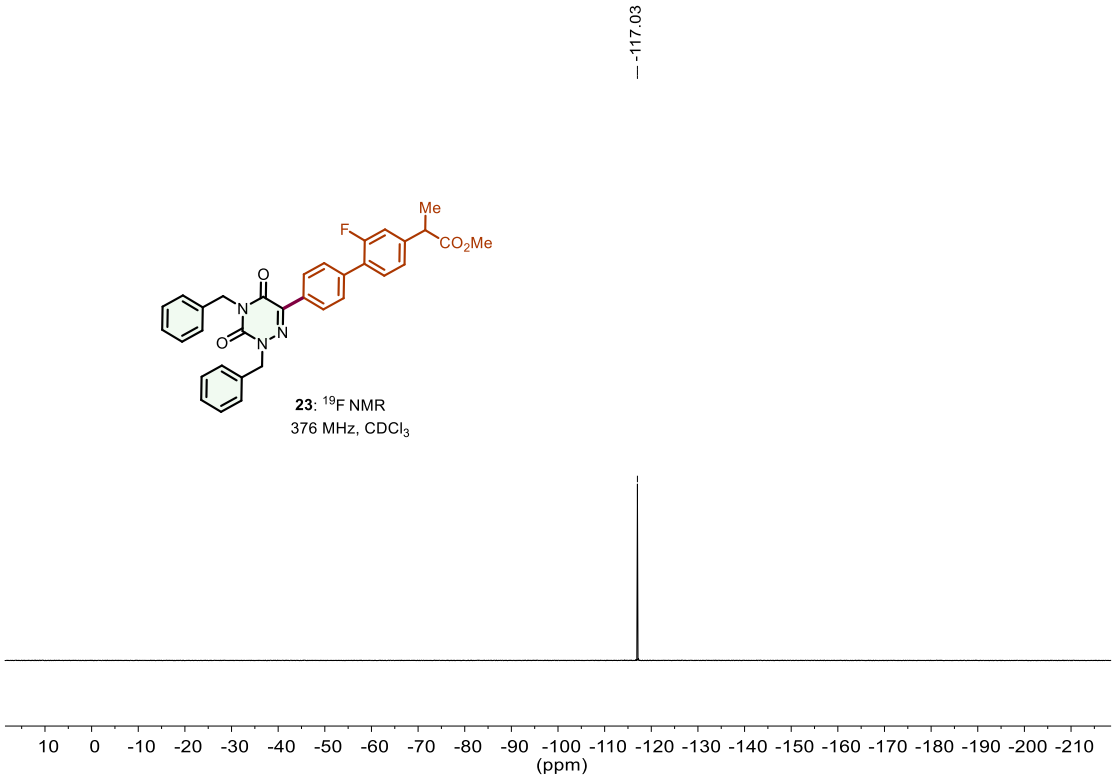


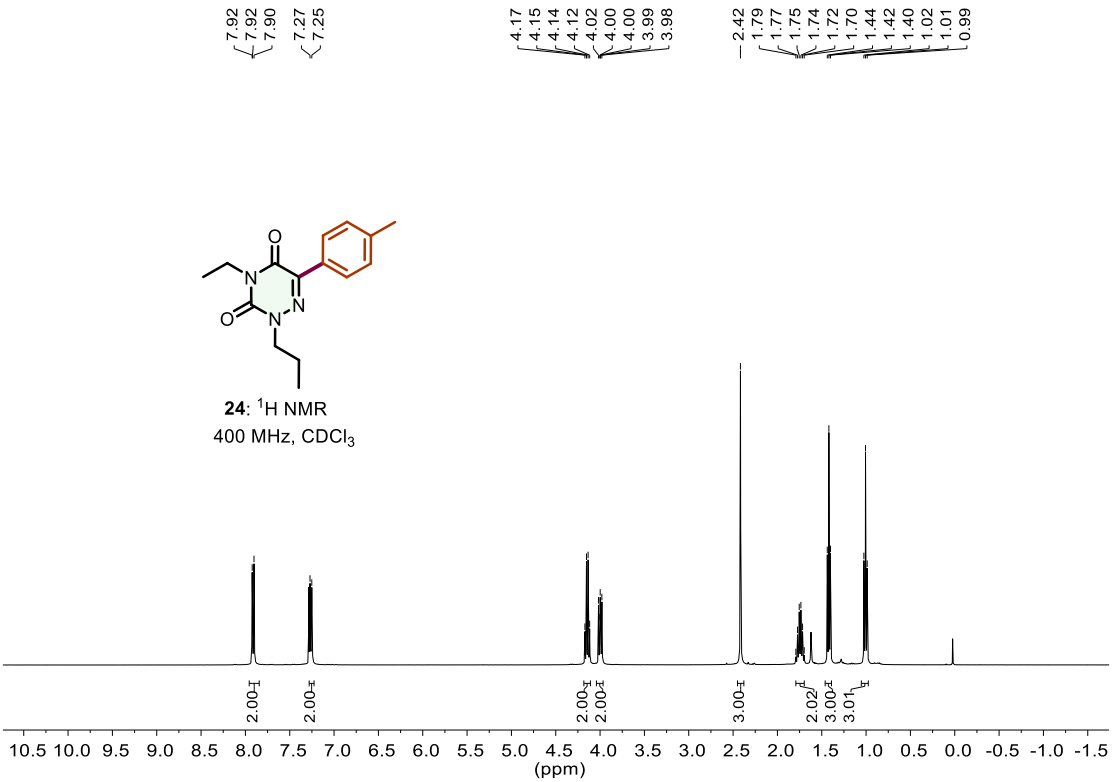
22: ^{1}H NMR
400 MHz, $CDCl_3$

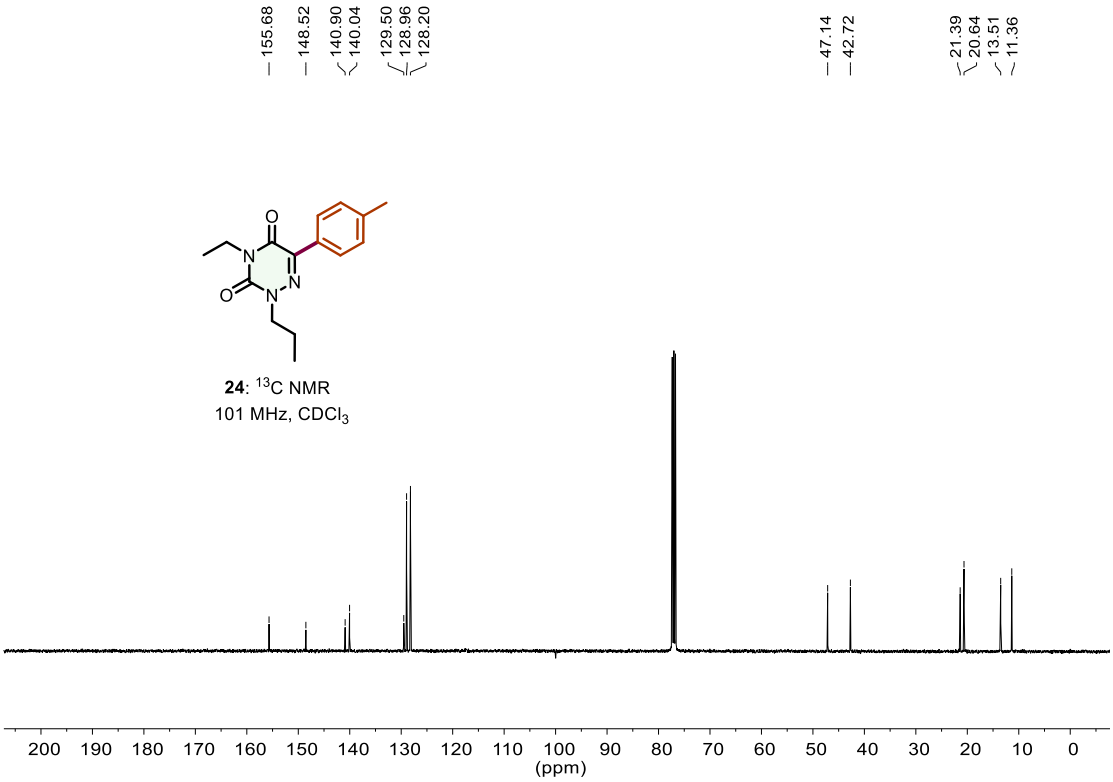

163.15
160.28
155.67
155.56
149.36
148.78
146.79
140.73
138.72
135.65
130.04
129.54
128.82
128.77
128.58
128.30
128.08
126.06
121.26
116.83
116.80
115.89
111.69
71.05
69.24
55.66
44.48
17.03
Me
22: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

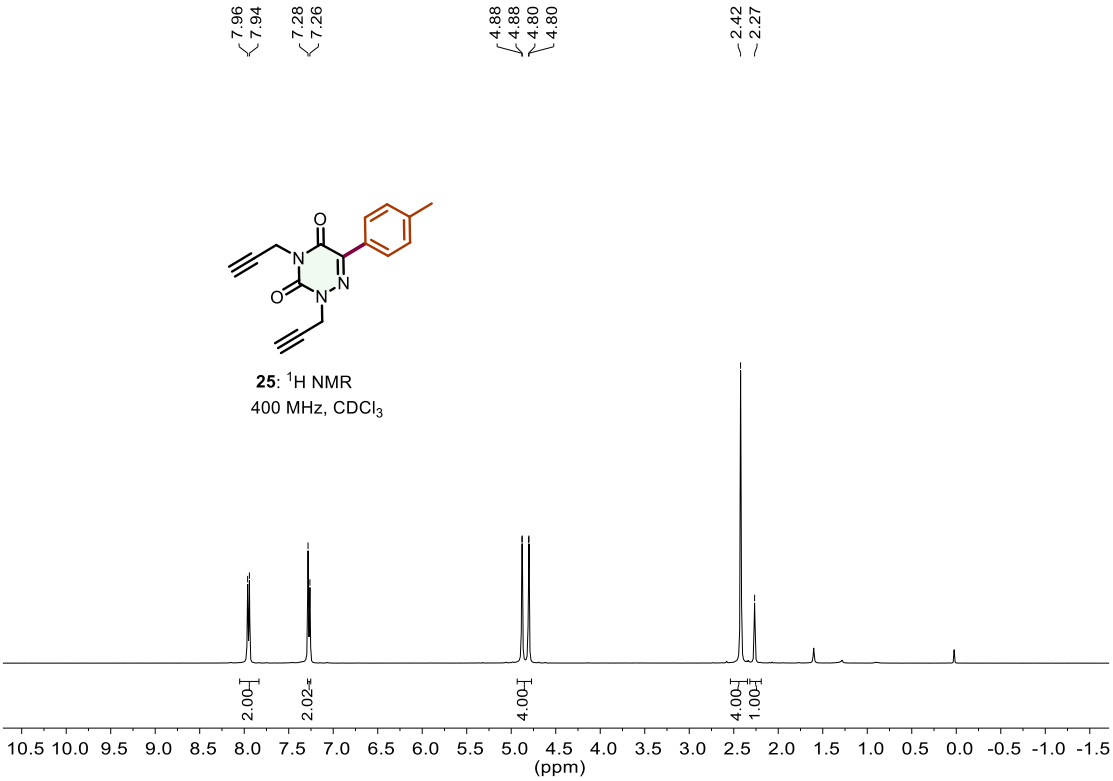

8.11
8.08
7.65
7.64
7.63
7.59
7.59
7.57
7.52
7.52
7.50
7.47
7.45
7.43
7.42
7.42
7.41
7.40
7.38
7.38
7.37
7.36
7.34
7.34
7.33
7.33
7.32
7.21
7.21
7.19
7.16
7.15
5.26
5.22
3.83
3.81
3.80
3.78
3.74
1.59
1.57
Me
F
CO2Me
23: 1H NMR
400 MHz, CDCl3
2.03
2.03
2.02
2.08
7.02
2.03
2.00
1.98
1.08
3.02
3.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)


174.36
161.00
158.52
155.51
148.76
142.39
142.31
140.77
137.15
135.62
135.56
131.31
130.72
130.68
129.59
128.85
128.81
128.79
128.61
128.48
128.36
128.13
127.15
127.01
123.70
123.66
115.51
115.28
55.81
52.27
44.96
44.53
18.45
Me
F
CO2Me
O
N
N
O
N
23: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

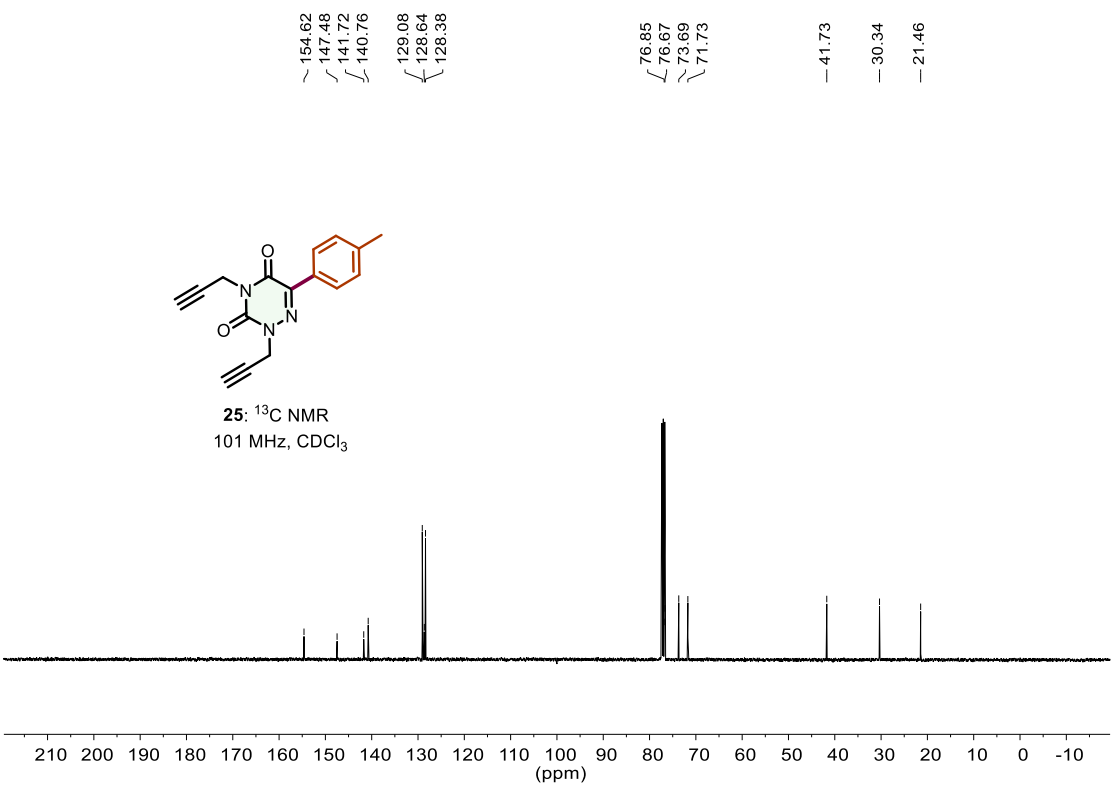

-117.03
Me
F
CO2Me
O
N
N
O
N
23: 19F NMR
376 MHz, CDCl3
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
(ppm)


7.92
7.92
7.90
7.27
7.25
4.17
4.15
4.14
4.12
4.02
4.00
4.00
3.99
3.98
2.42
1.79
1.77
1.75
1.74
1.72
1.70
1.44
1.42
1.40
1.02
1.01
0.99
24: 1H NMR
400 MHz, CDCl3
2.00
2.00
2.00
2.00
3.00
2.02
3.00
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)

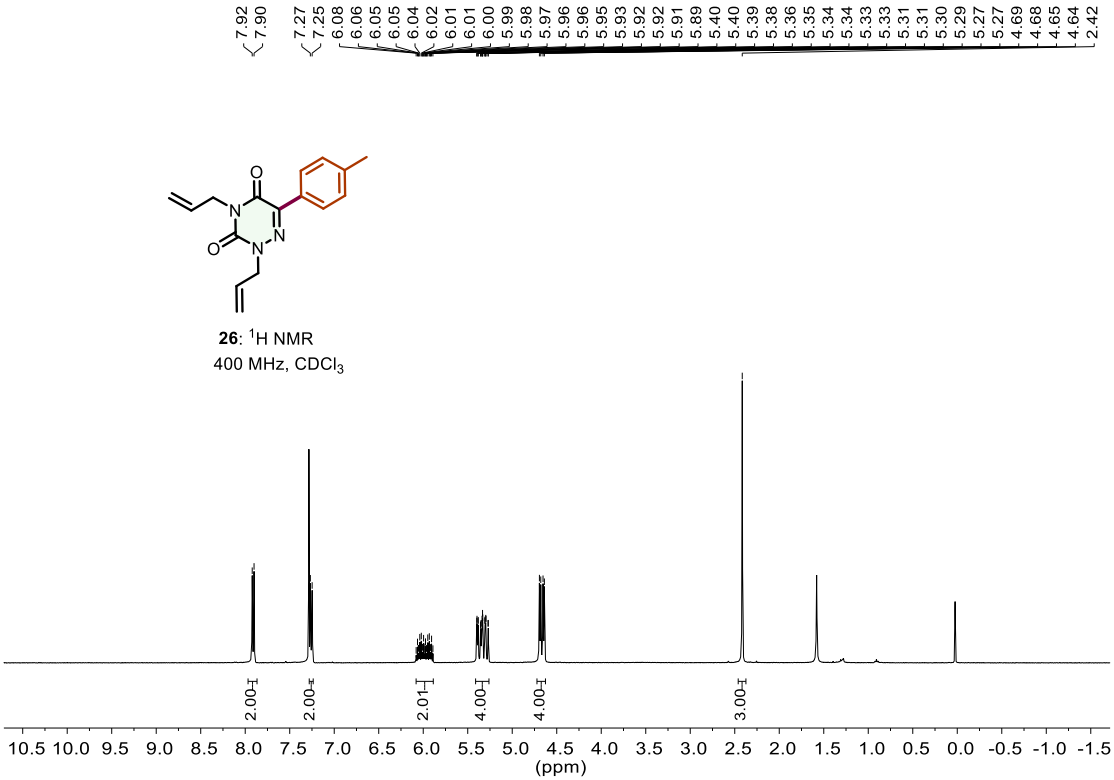

155.68
148.52
140.90
140.04
129.50
128.96
128.20
47.14
42.72
21.39
20.64
13.51
11.36
24: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

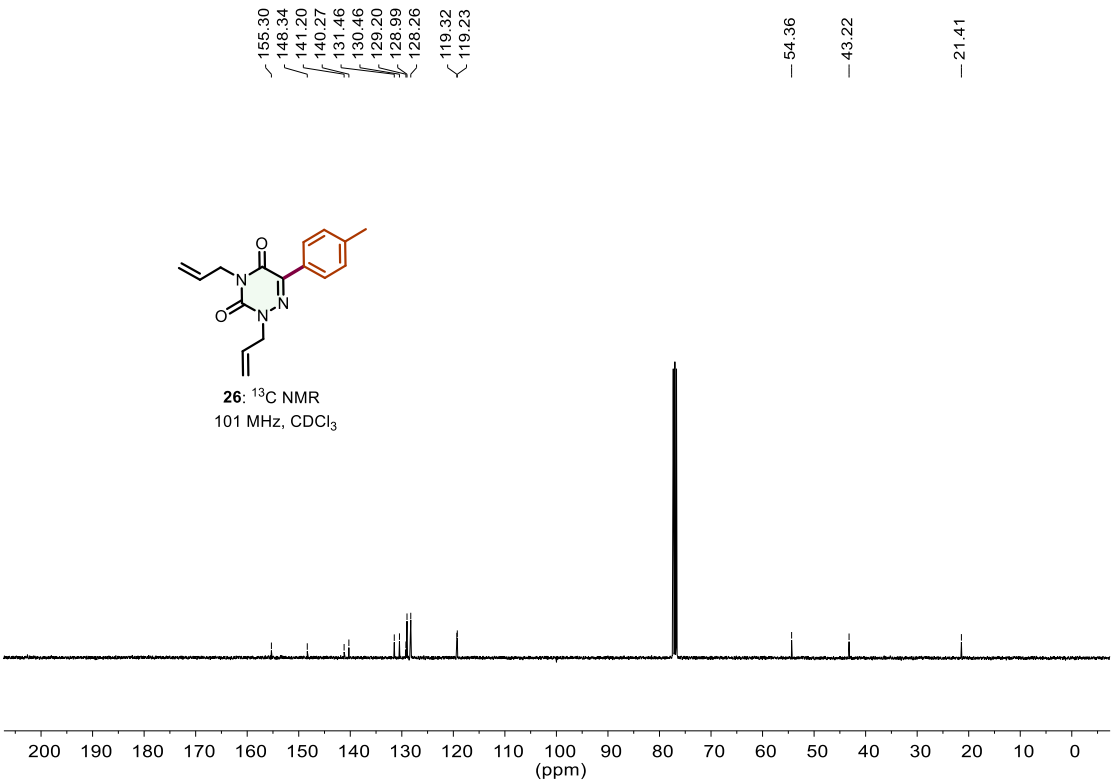


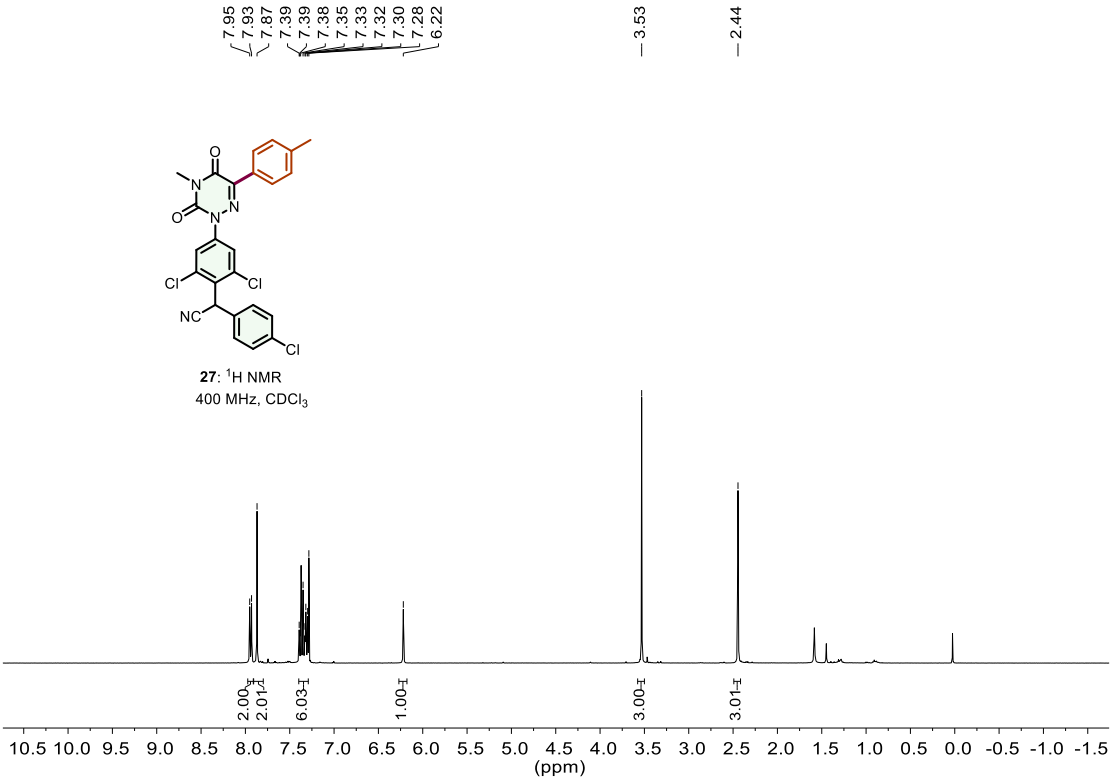
25: ^{1}H NMR
400 MHz, $CDCl_3$

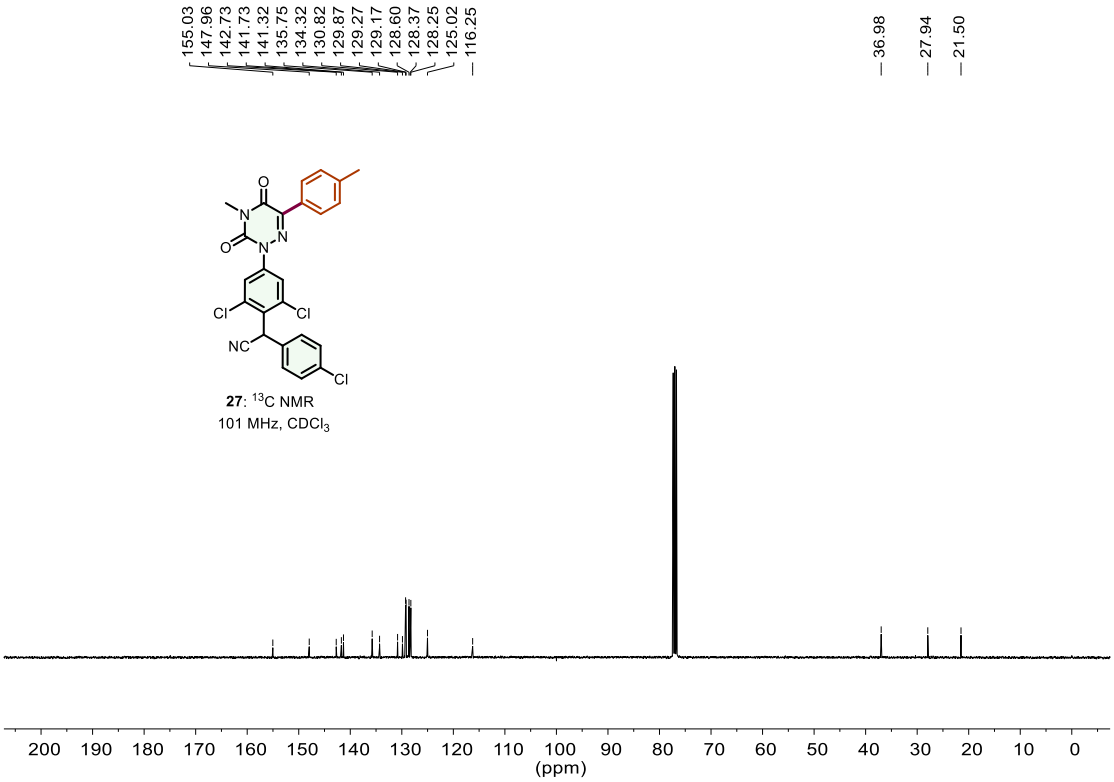


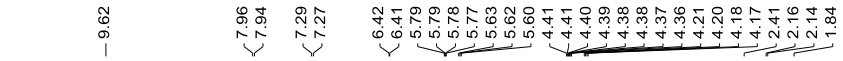
25: ^{13}C NMR
101 MHz, $CDCl_3$

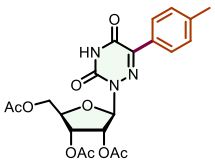

7.92
7.90
7.27
7.25
6.08
6.06
6.05
6.05
6.04
6.02
6.01
6.01
6.00
5.99
5.98
5.97
5.96
5.96
5.95
5.93
5.92
5.92
5.91
5.89
5.40
5.40
5.39
5.38
5.36
5.35
5.34
5.34
5.33
5.33
5.31
5.31
5.30
5.29
5.27
5.27
4.69
4.68
4.65
4.64
2.42
O
N
O
N
N
26: 1H NMR
400 MHz, CDCl3
2.00
2.00
2.01
4.00
4.00
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)


155.30
148.34
141.20
140.27
131.46
130.46
129.20
128.99
128.26
119.32
119.23
54.36
43.22
21.41
O
N
O
N
N
26: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

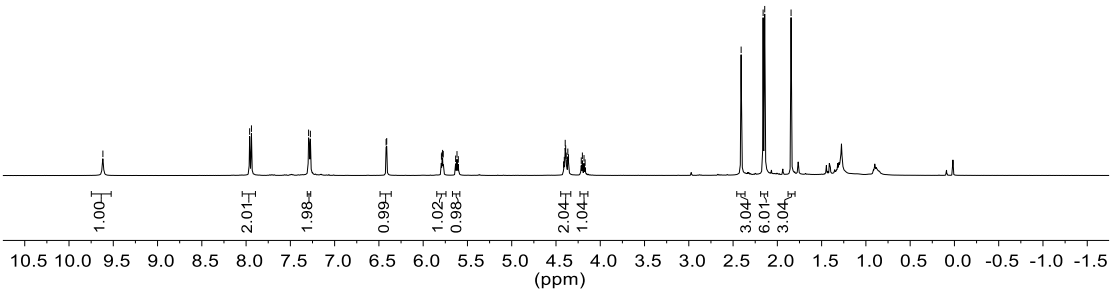

7.95
7.93
7.87
7.39
7.39
7.38
7.35
7.33
7.32
7.30
7.28
6.22
3.53
2.44
O
N
N
O
N
Cl
Cl
NC
Cl
27: 1H NMR
400 MHz, CDCl3
2.00
2.01
6.03
1.00
3.00
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)

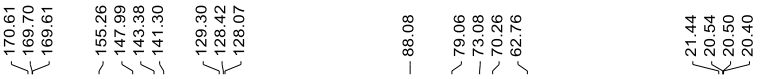

155.03
147.96
142.73
141.73
141.32
135.75
134.32
130.82
129.87
129.27
129.17
128.60
128.37
128.25
125.02
116.25
36.98
27.94
21.50
O
N
N
O
N
Cl
Cl
NC
Cl
27: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

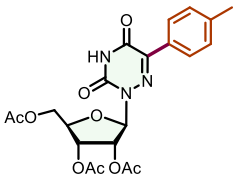




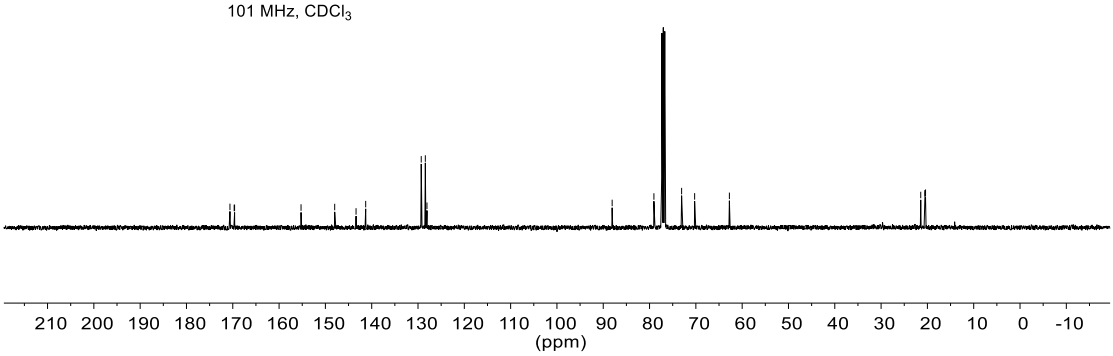
28: ^{1}H NMR
400 MHz, $CDCl_3$

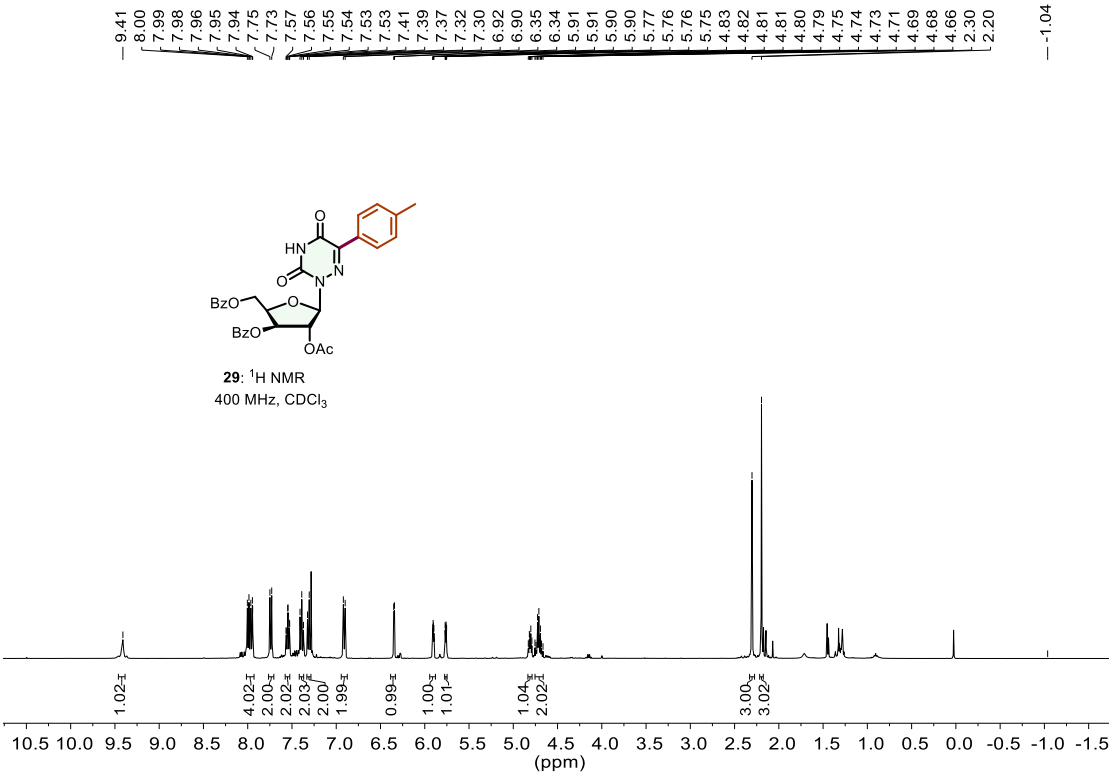


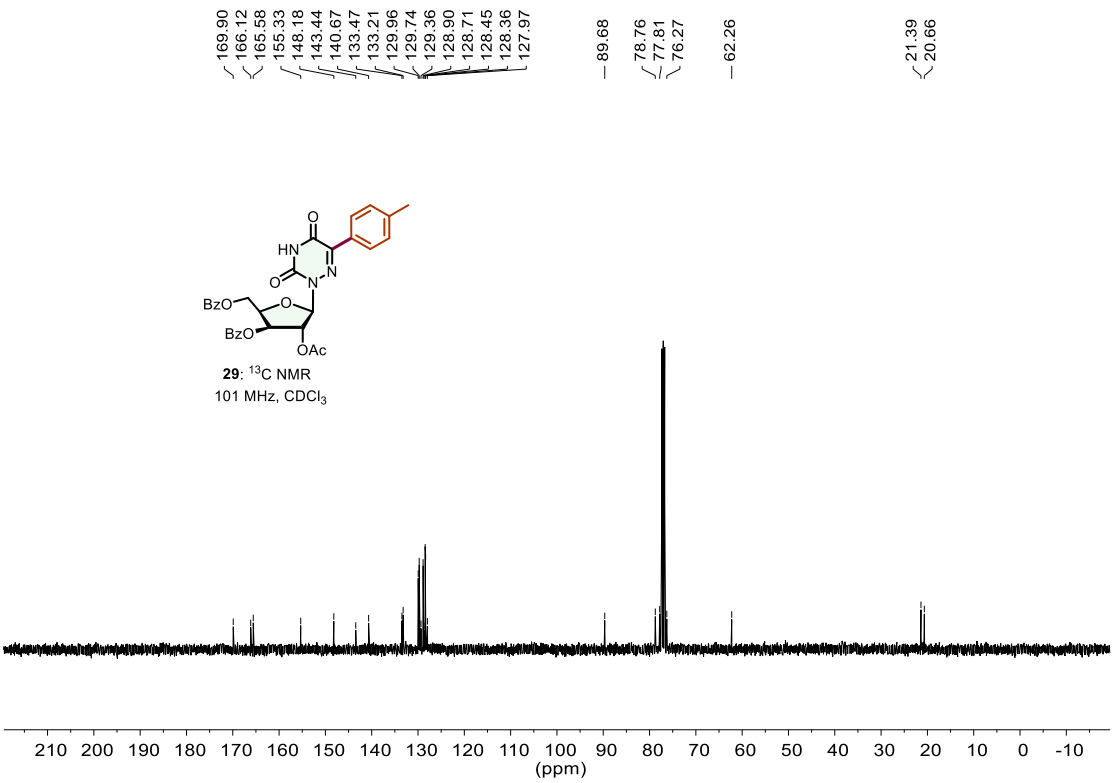


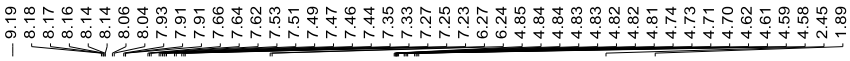


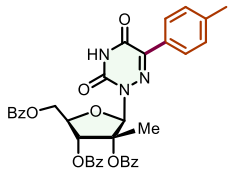
28: ^{13}C NMR
101 MHz, $CDCl_3$



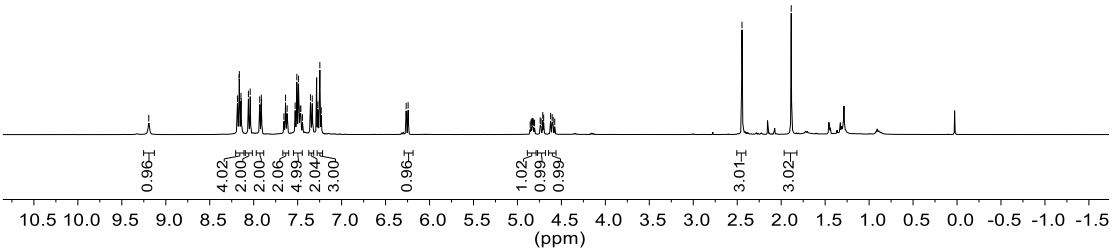

9.41
8.00
7.99
7.98
7.96
7.95
7.94
7.75
7.73
7.57
7.56
7.55
7.54
7.53
7.53
7.41
7.39
7.37
7.32
7.30
6.92
6.90
6.35
6.34
5.91
5.91
5.90
5.90
5.77
5.76
5.76
5.75
4.83
4.82
4.81
4.81
4.80
4.79
4.75
4.74
4.73
4.71
4.69
4.68
4.66
2.30
2.20
-1.04
HN
O
N
BzO
BzO
OAc
29: 1H NMR
400 MHz, CDCl3
1.02
4.02
2.00
2.02
2.03
2.00
1.99
0.99
1.00
1.01
1.04
2.02
3.00
3.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)

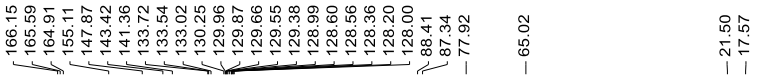

169.90
166.12
165.58
155.33
148.18
143.44
140.67
133.47
133.21
129.96
129.74
129.36
128.90
128.71
128.45
128.36
127.97
89.68
78.76
77.81
76.27
62.26
21.39
20.66
HN
O
N
BzO
BzO
OAc
29: 13C NMR
101 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)

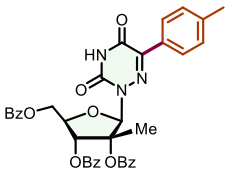




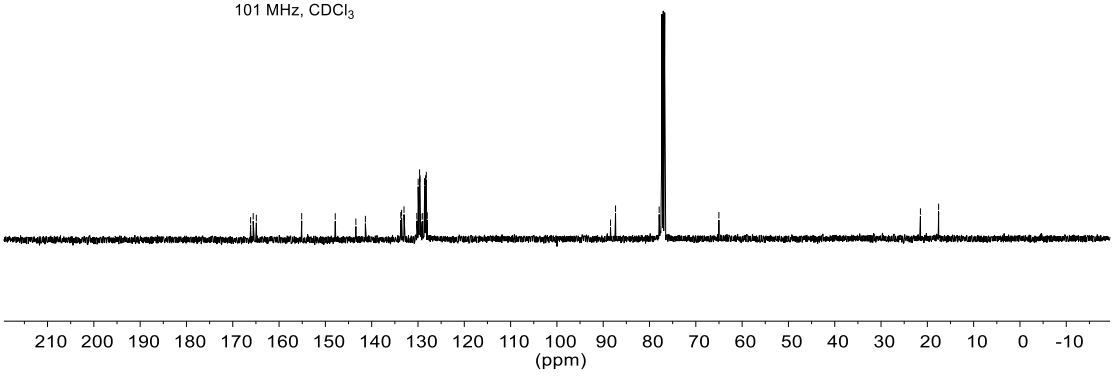
30: ^{1}H NMR
400 MHz, $CDCl_3$

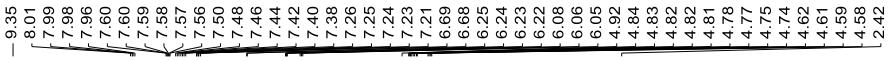


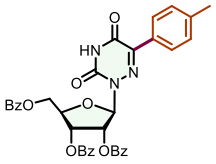




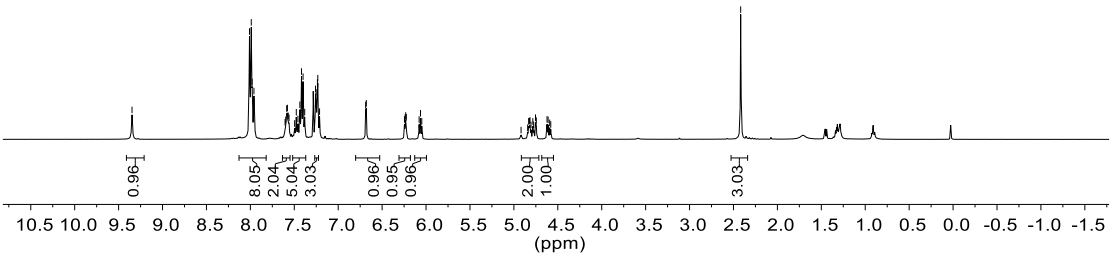
30: ^{13}C NMR
101 MHz, $CDCl_3$

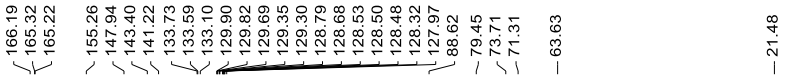


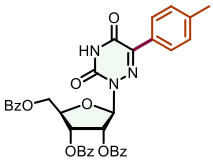




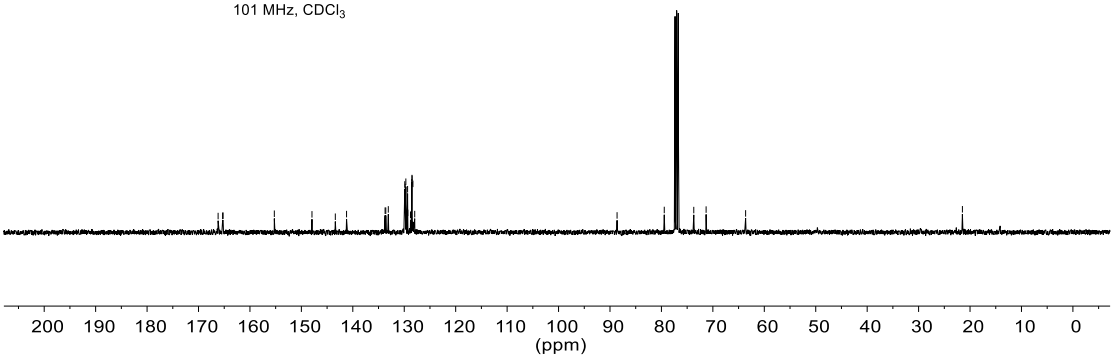
31 ^{1}H NMR
400 MHz, $CDCl_3$

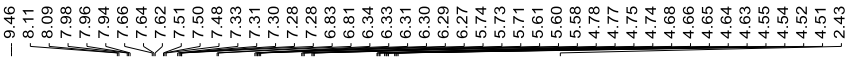


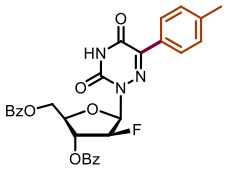




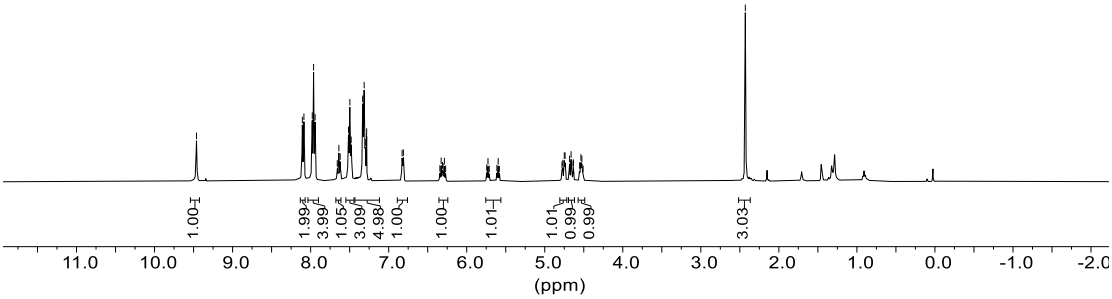
31: ^{13}C NMR
101 MHz, $CDCl_3$

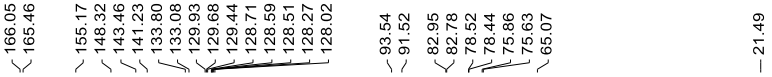


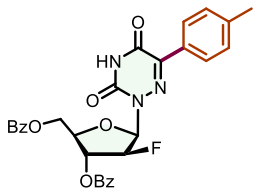




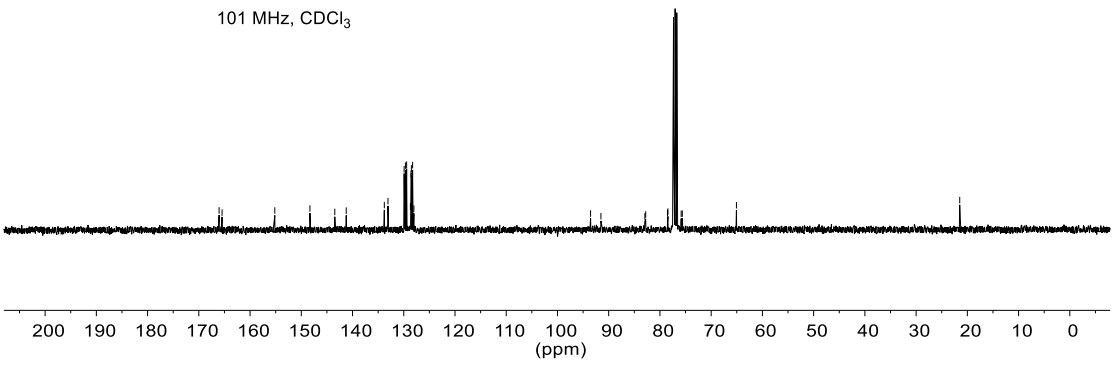
32: ^{1}H NMR
400 MHz, $CDCl_3$

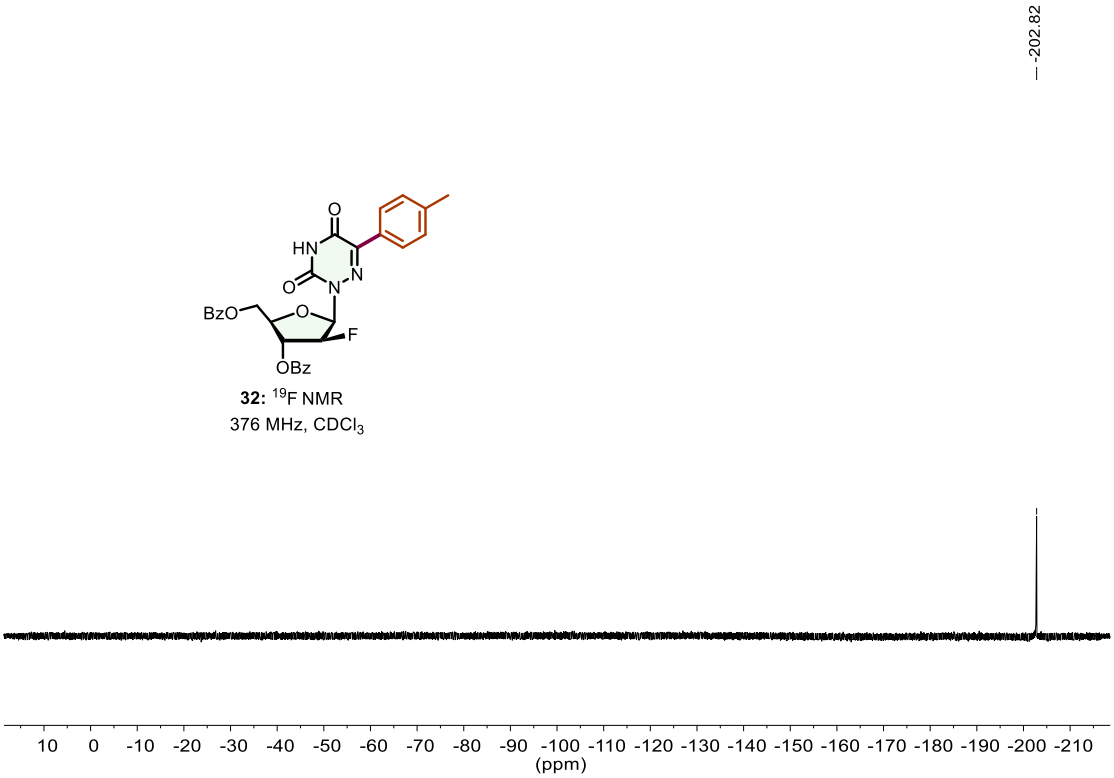




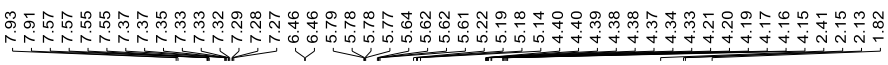


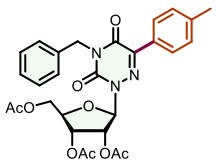
32: ^{13}C NMR
101 MHz, $CDCl_3$



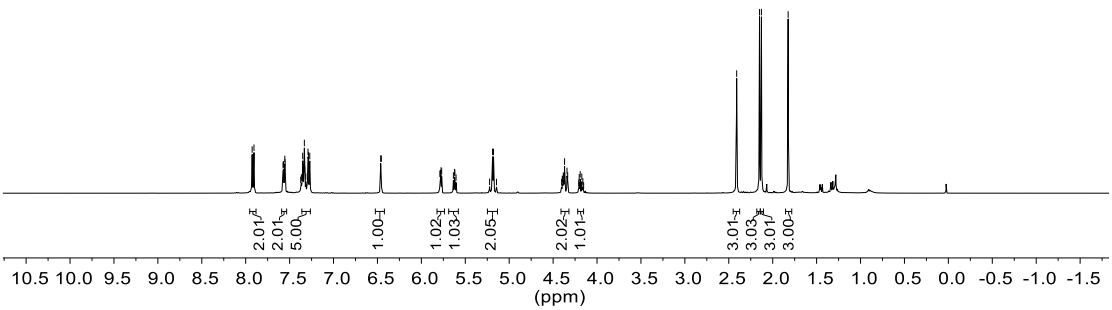


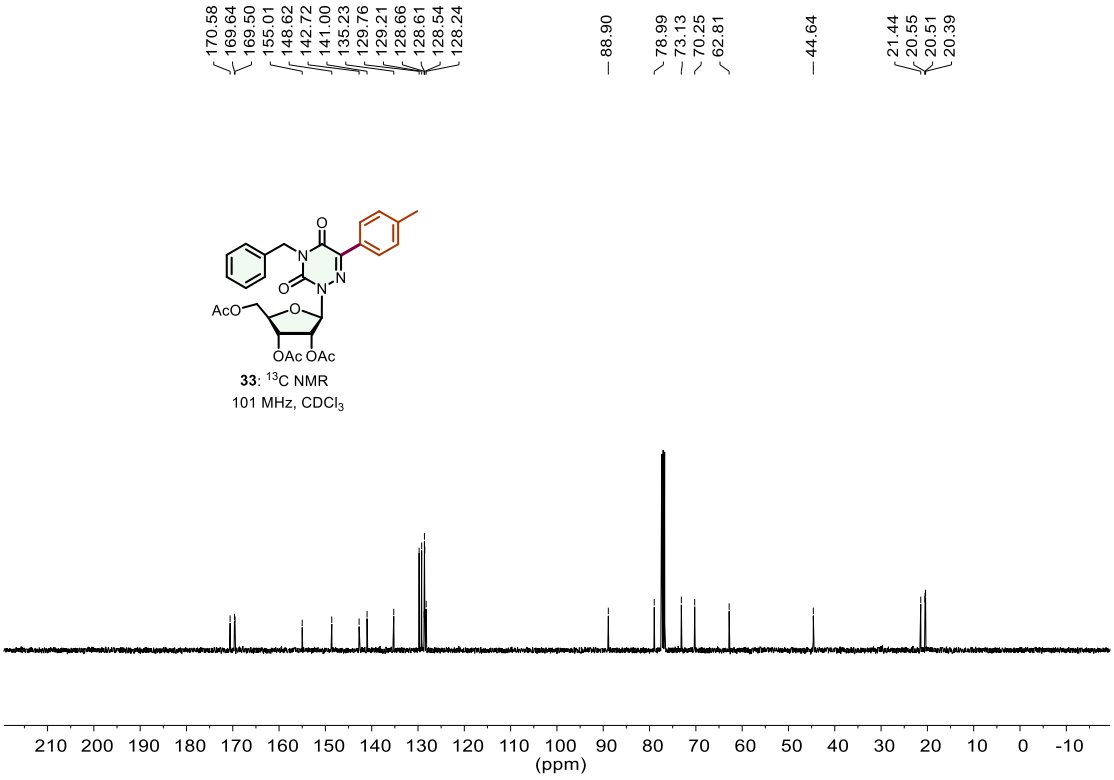
32: ^{19}F NMR
376 MHz, $CDCl_3$



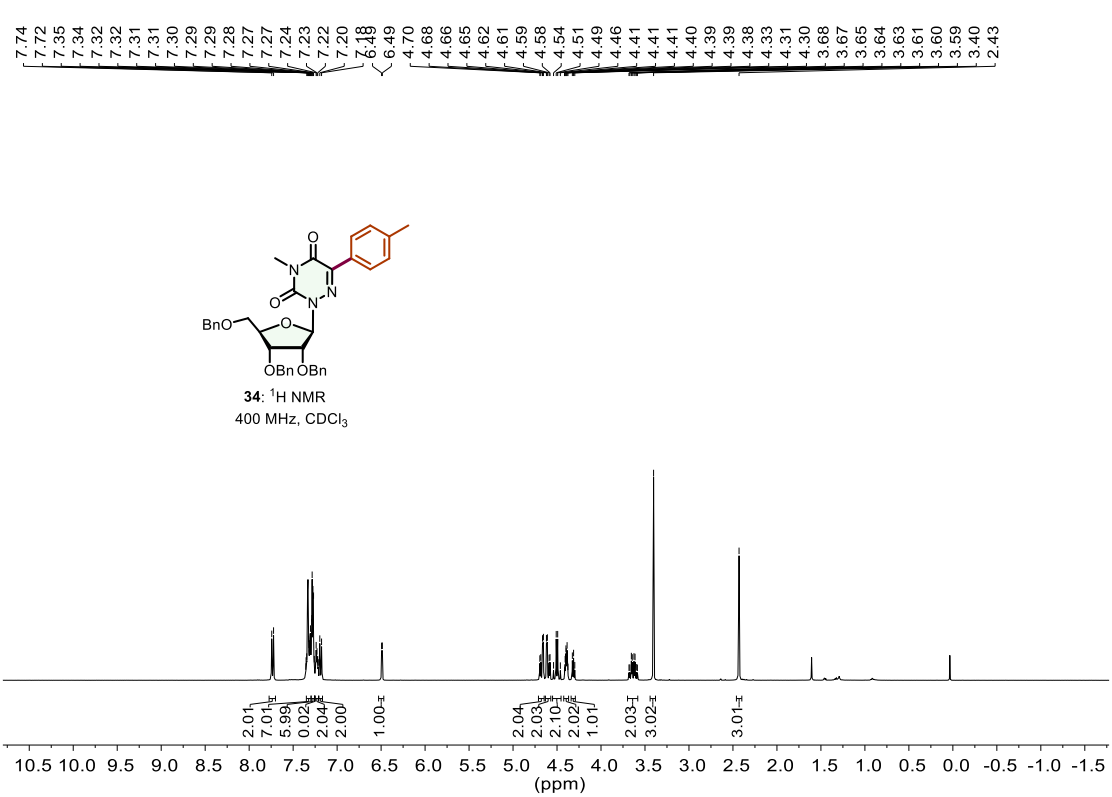


33: ^{1}H NMR
400 MHz, $CDCl_3$

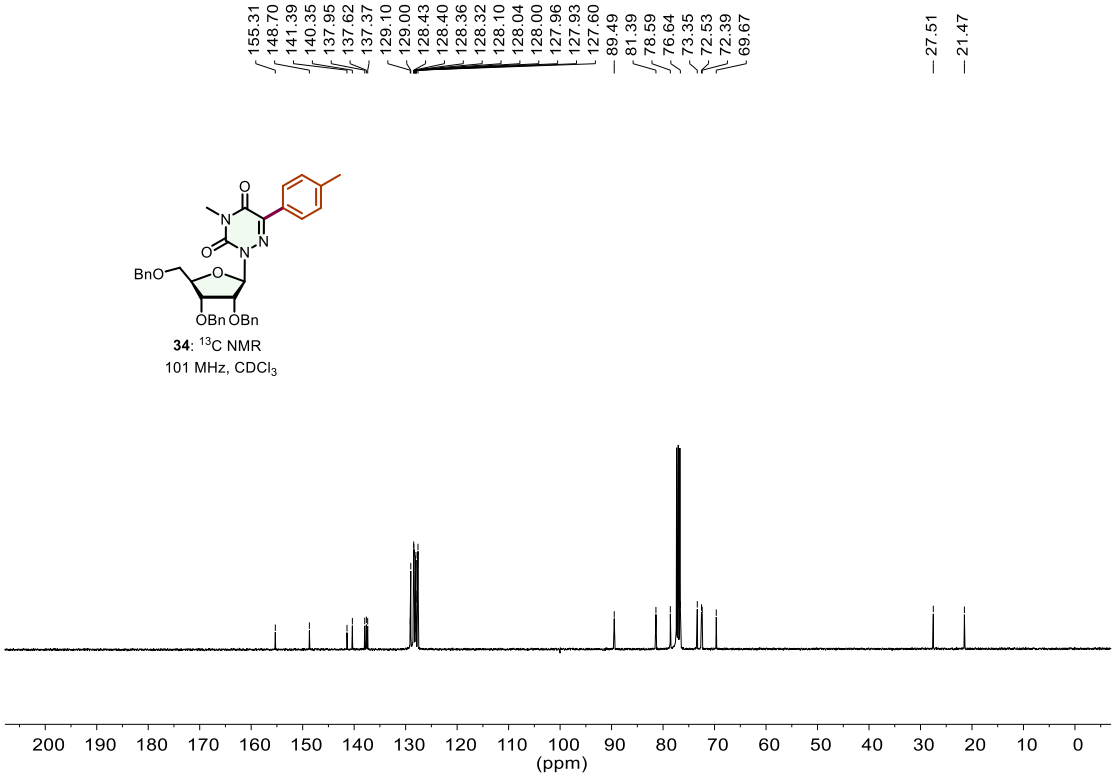




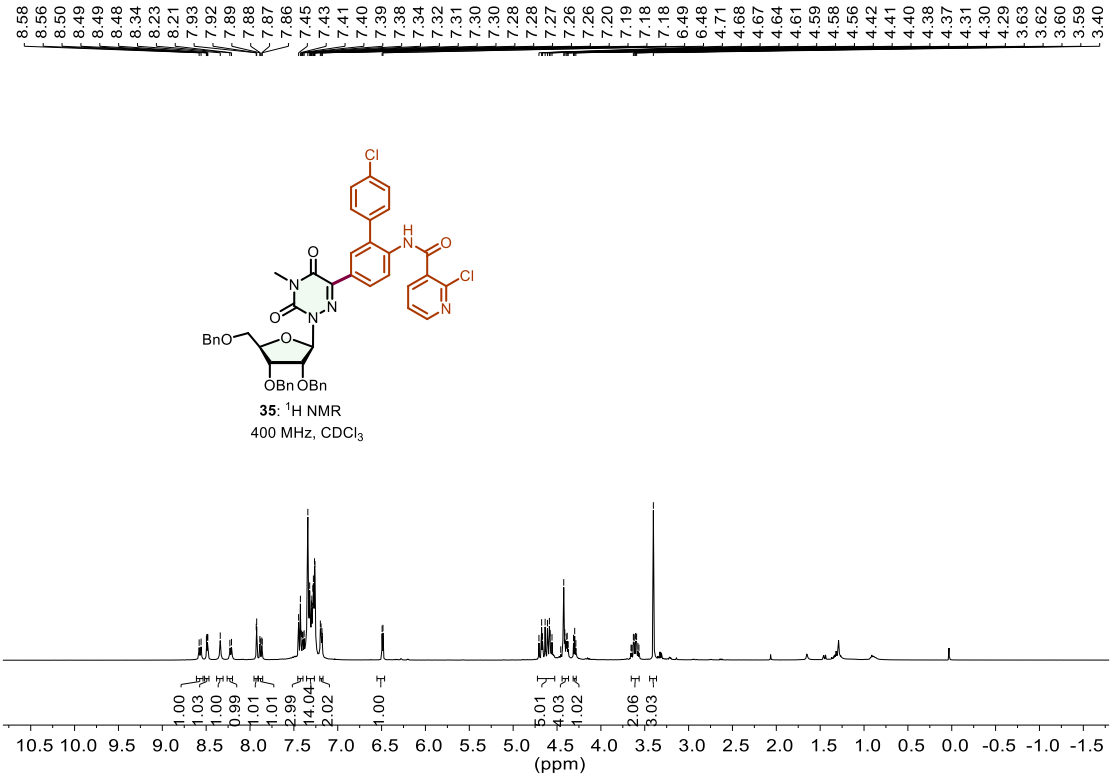
33: ^{13}C NMR
101 MHz, $CDCl_3$



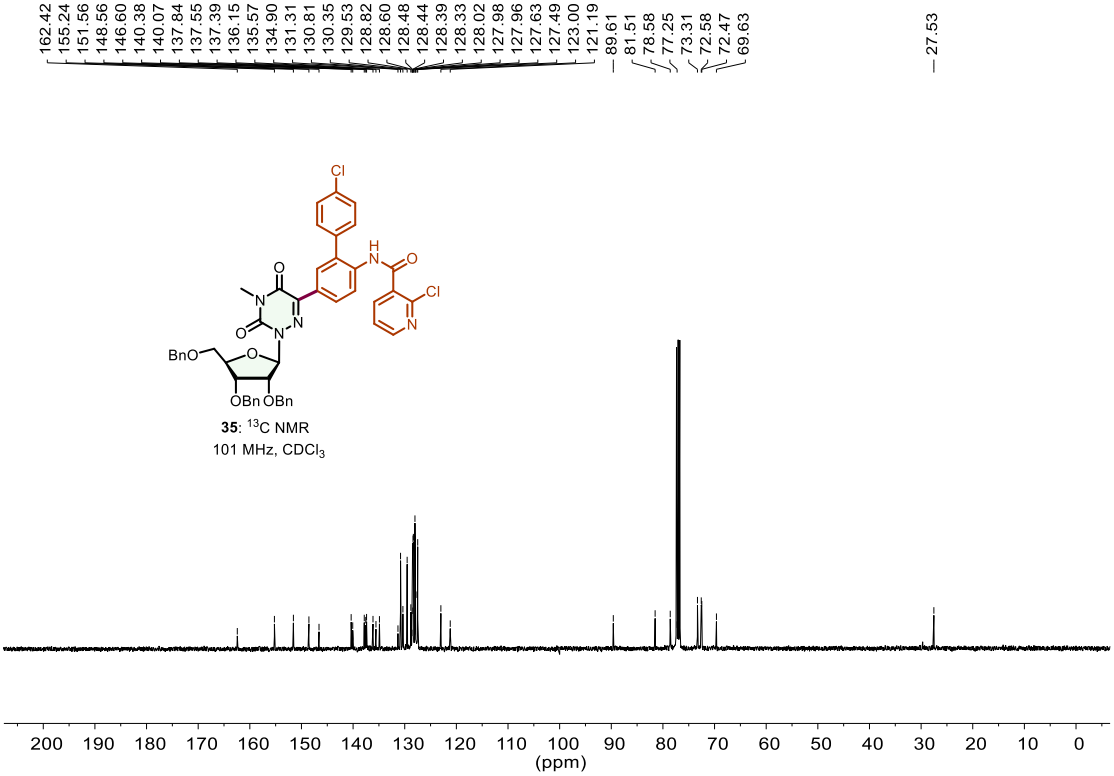
34: ^{1}H NMR
400 MHz, $CDCl_3$



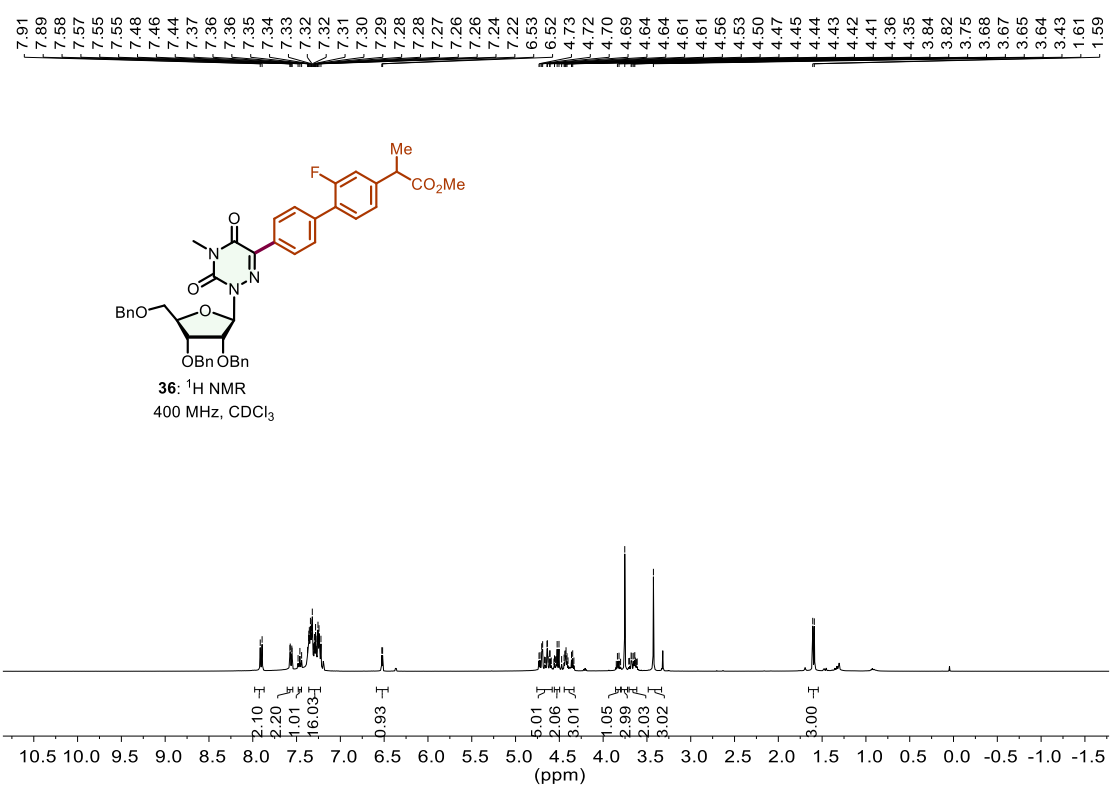
34: ^{13}C NMR
101 MHz, $CDCl_3$



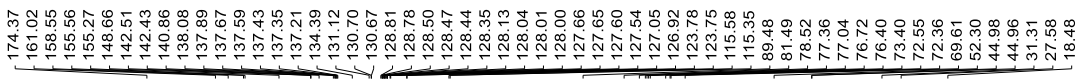
35: ^{1}H NMR
400 MHz, $CDCl_3$

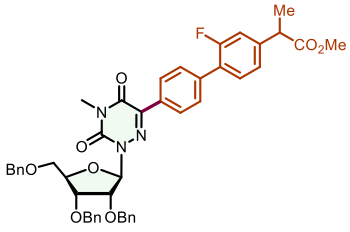


35: ^{13}C NMR
101 MHz, $CDCl_3$

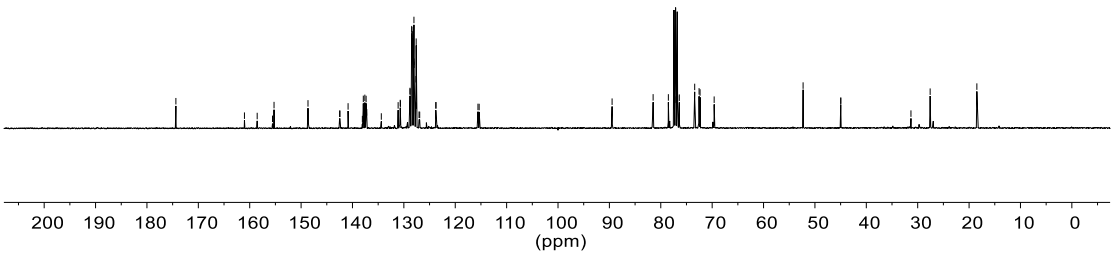


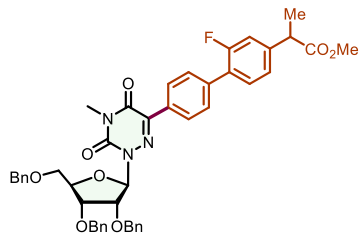
36: ^{1}H NMR
400 MHz, $CDCl_3$



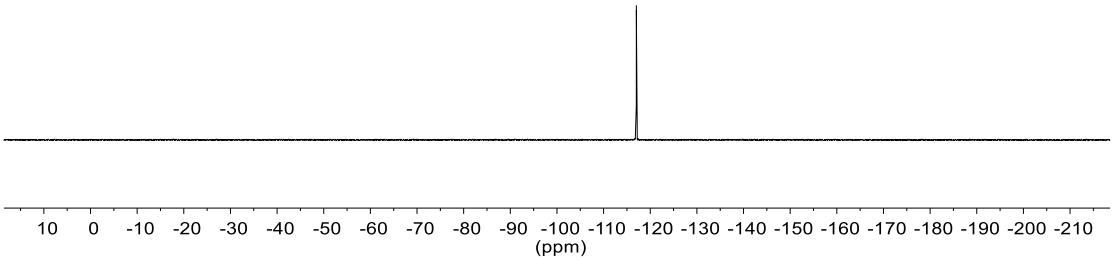


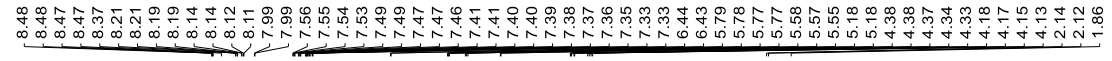
36: ^{13}C NMR
101 MHz, $CDCl_3$

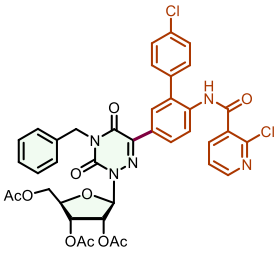




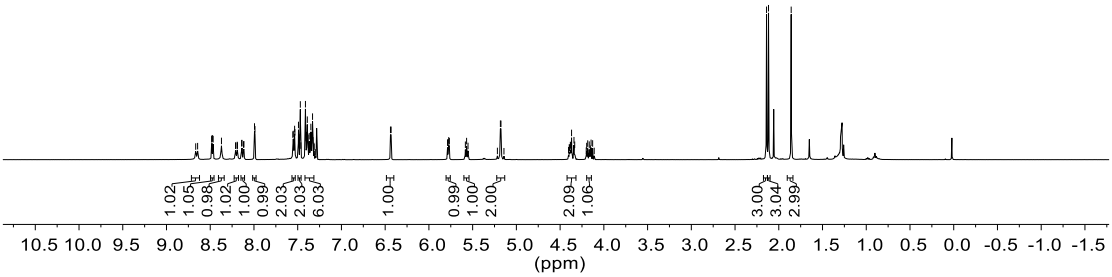
36: ^{19}F NMR
376 MHz, $CDCl_3$

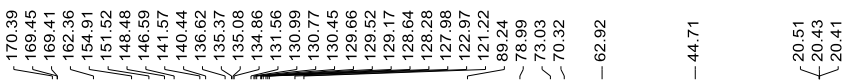


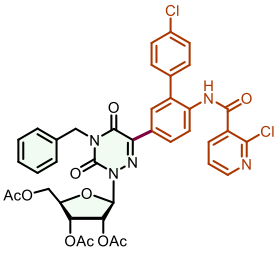




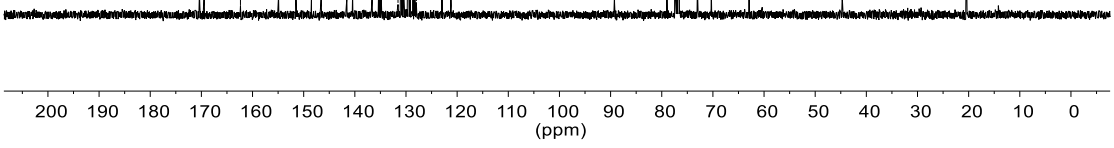
37: ^{1}H NMR
400 MHz, $CDCl_3$

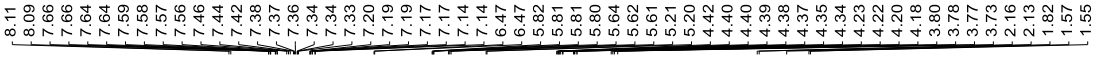


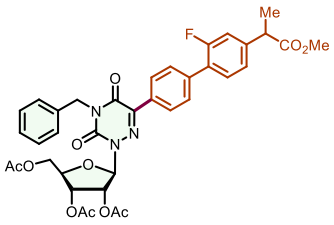




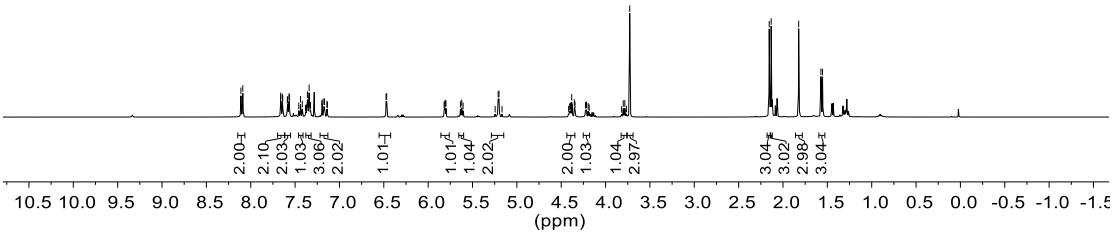
37: ^{13}C NMR
101 MHz, $CDCl_3$

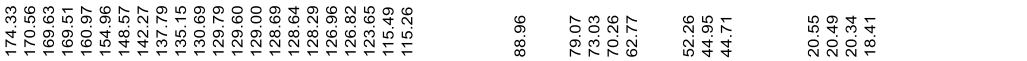


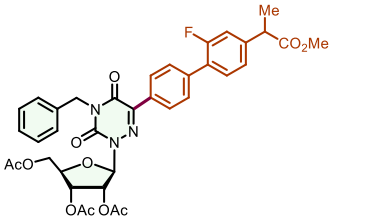




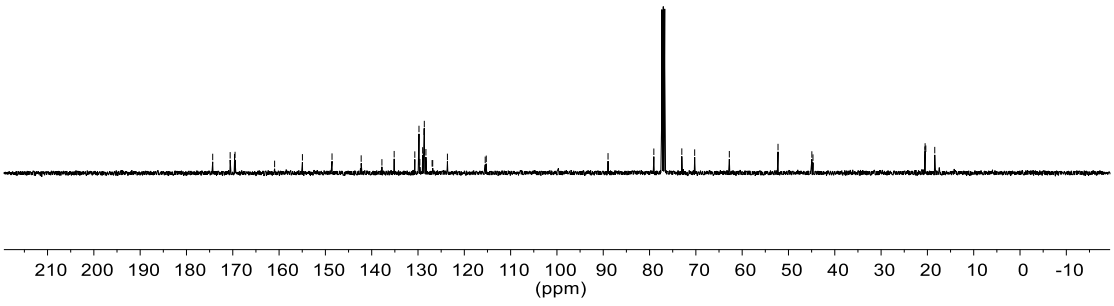
38: ^{1}H NMR
400 MHz, $CDCl_3$

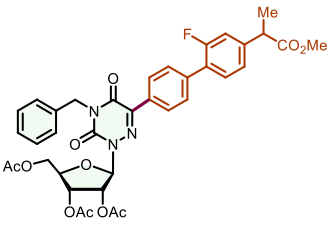




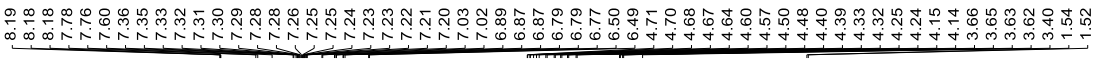


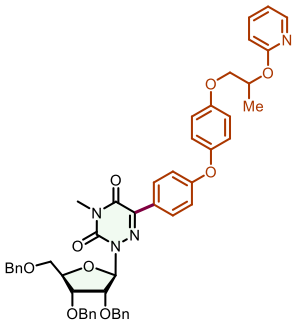
38: ^{13}C NMR
101 MHz, $CDCl_3$



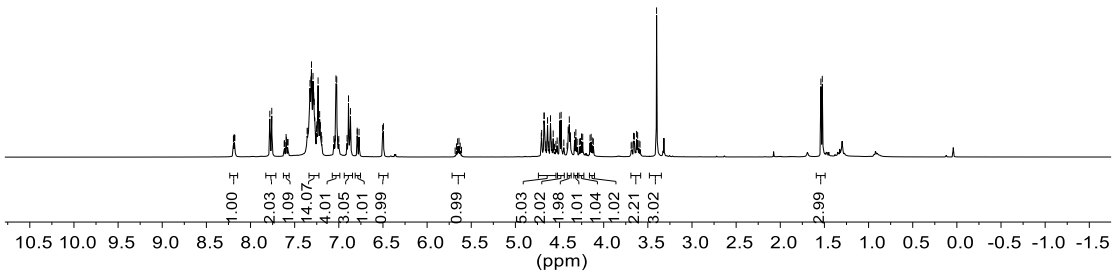


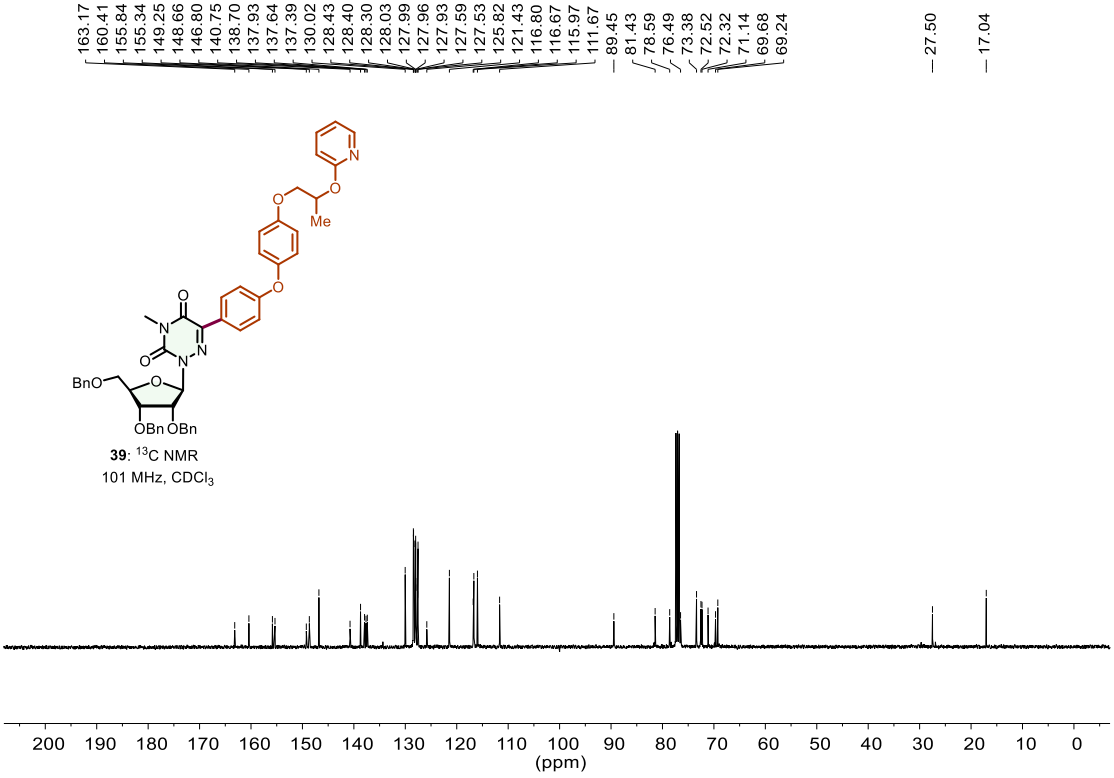
38: ^{19}F NMR
376 MHz, $CDCl_3$



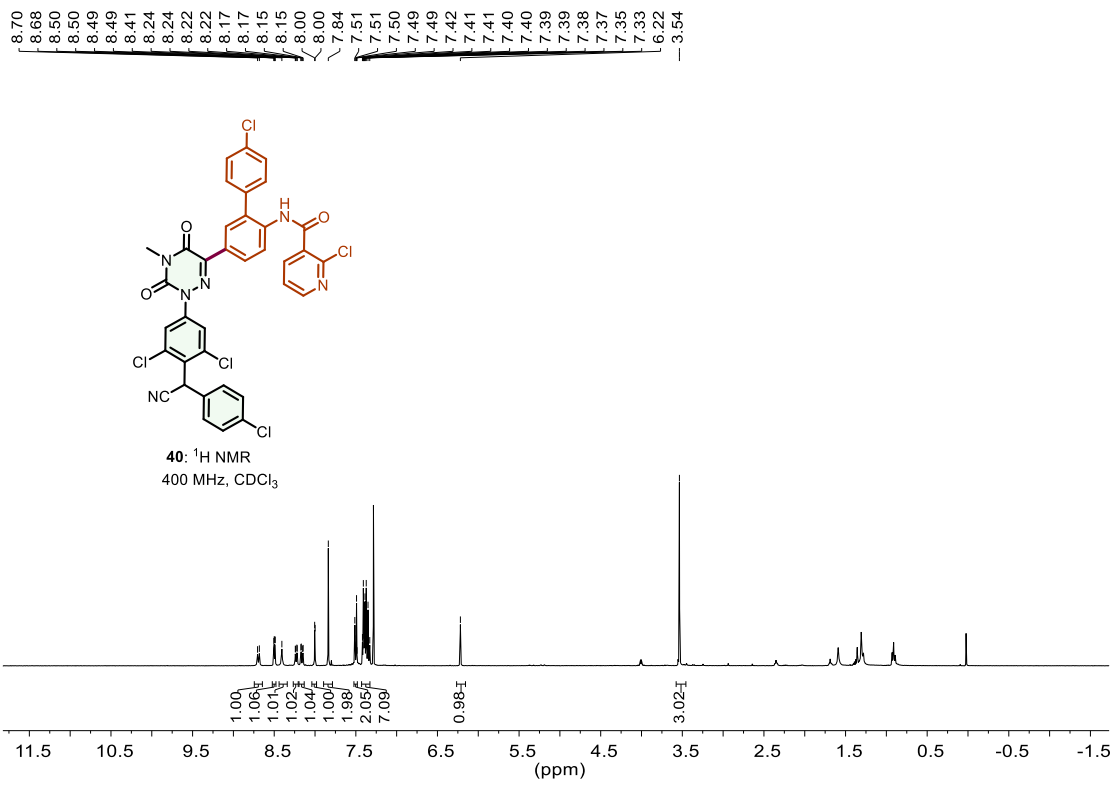


39: ^{1}H NMR
400 MHz, $CDCl_3$

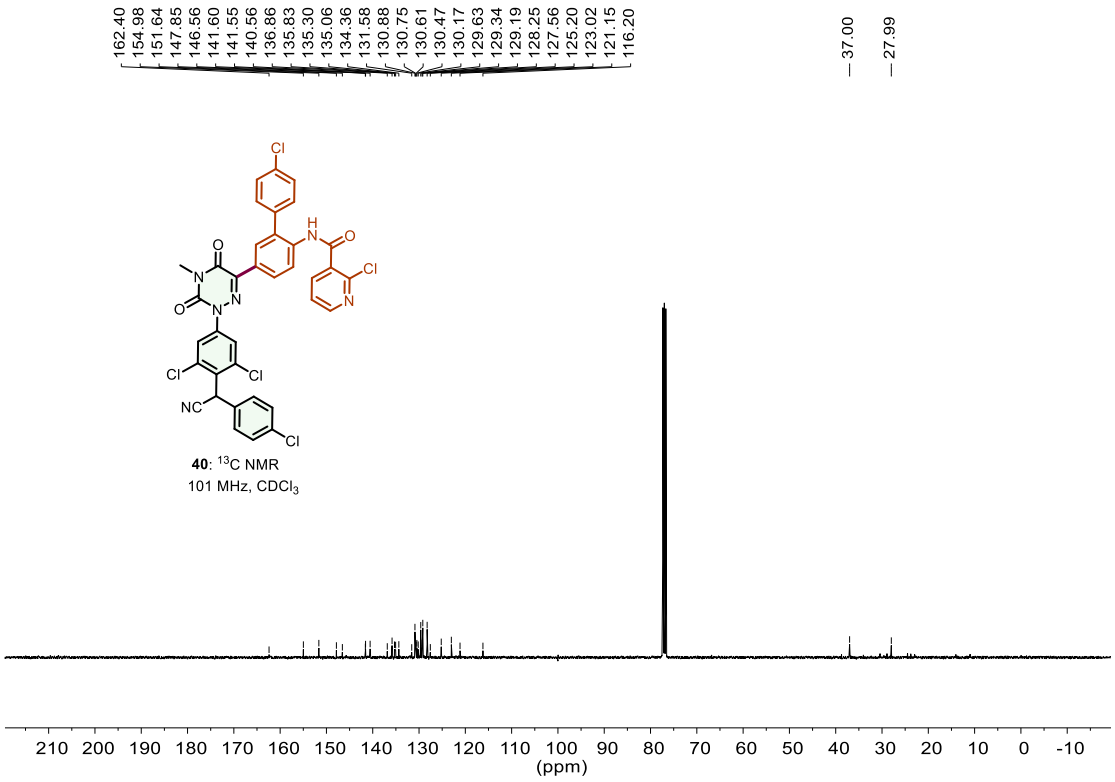


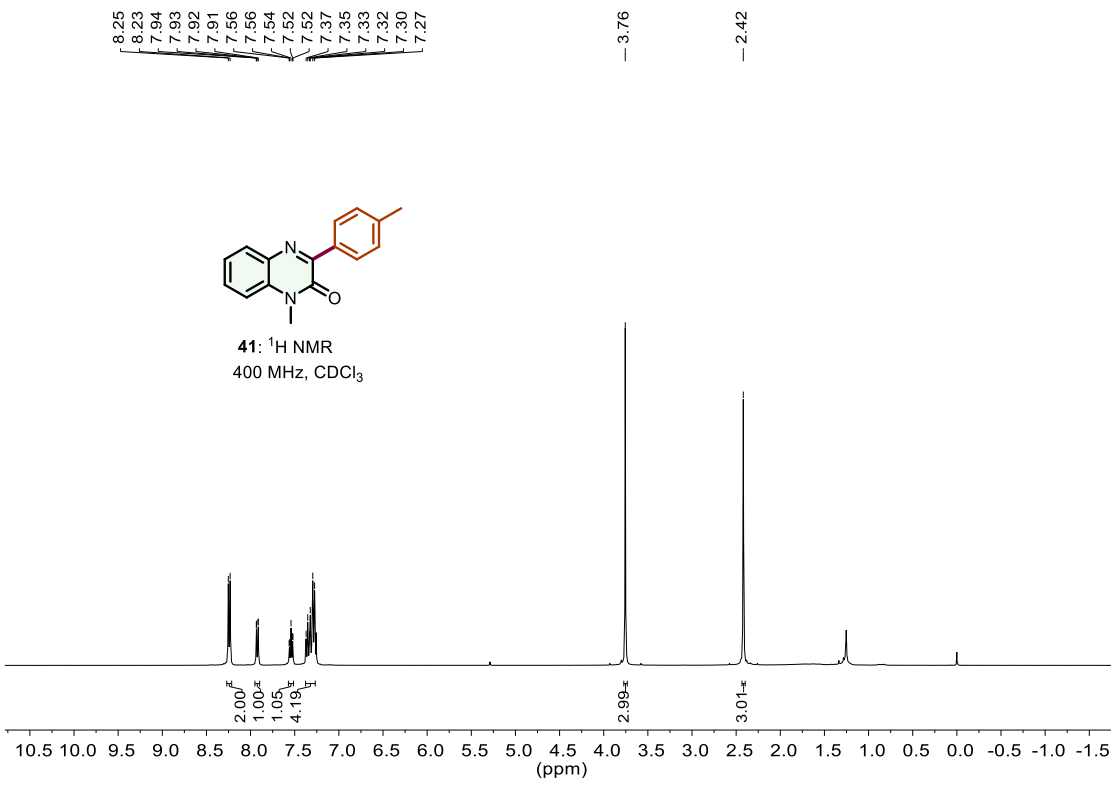


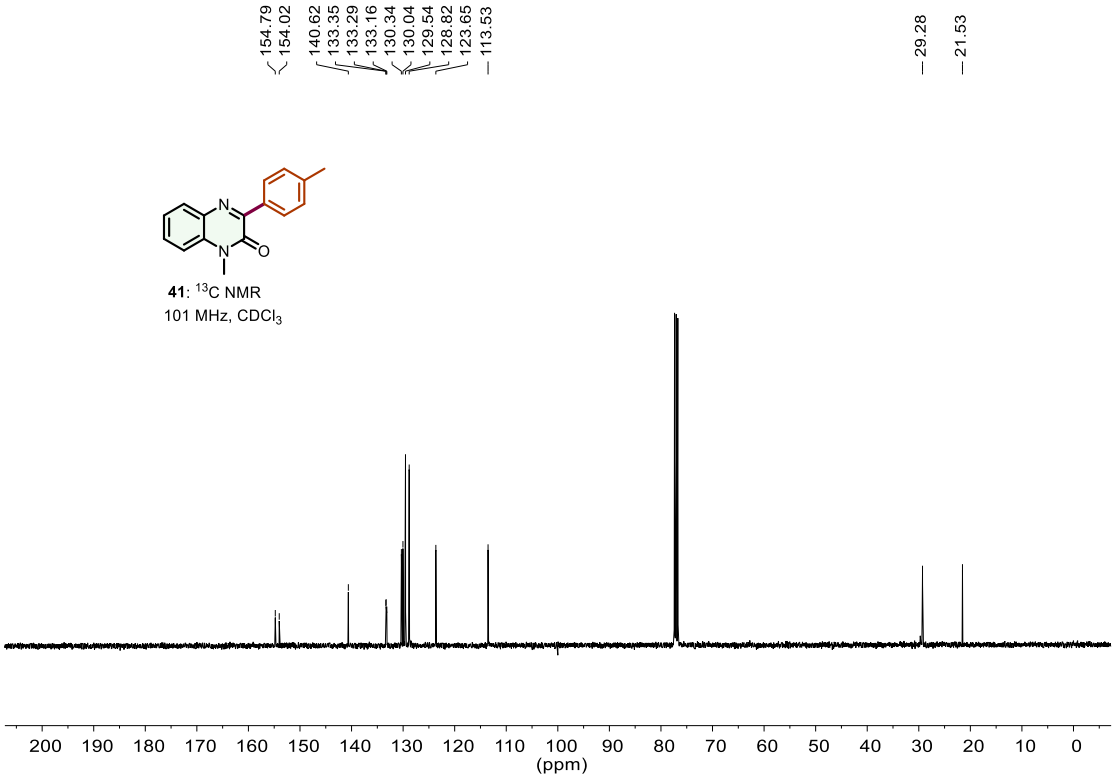
39: ^{13}C NMR
101 MHz, $CDCl_3$

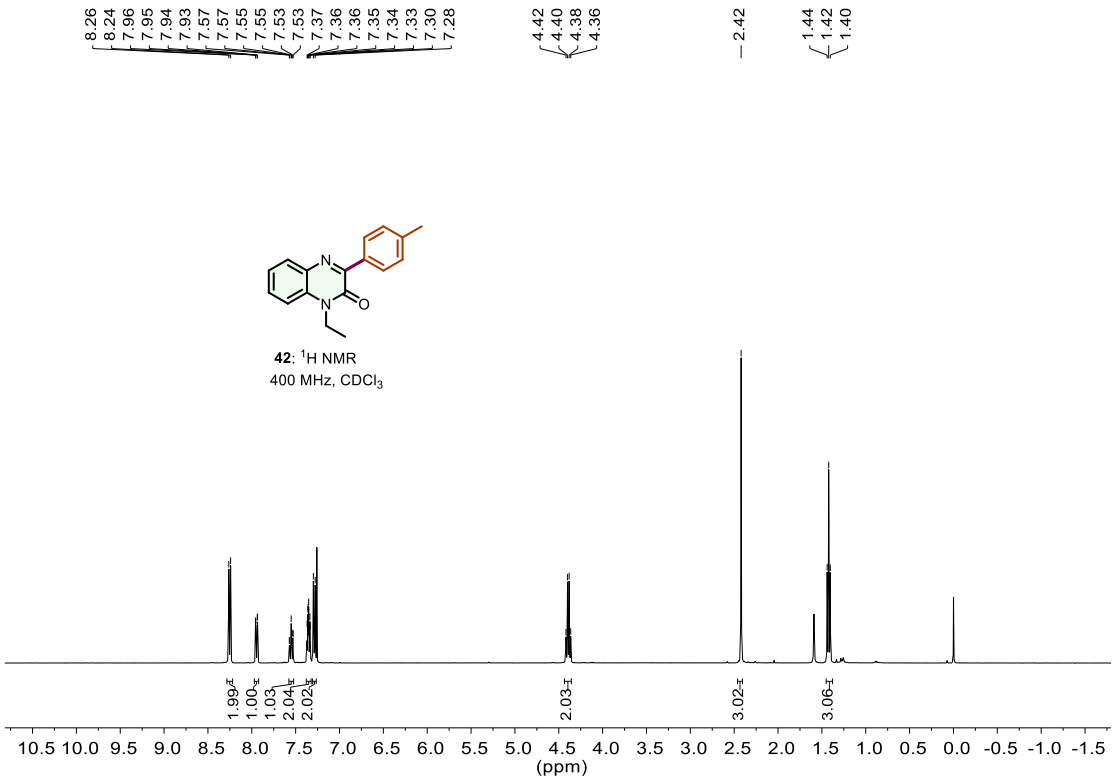


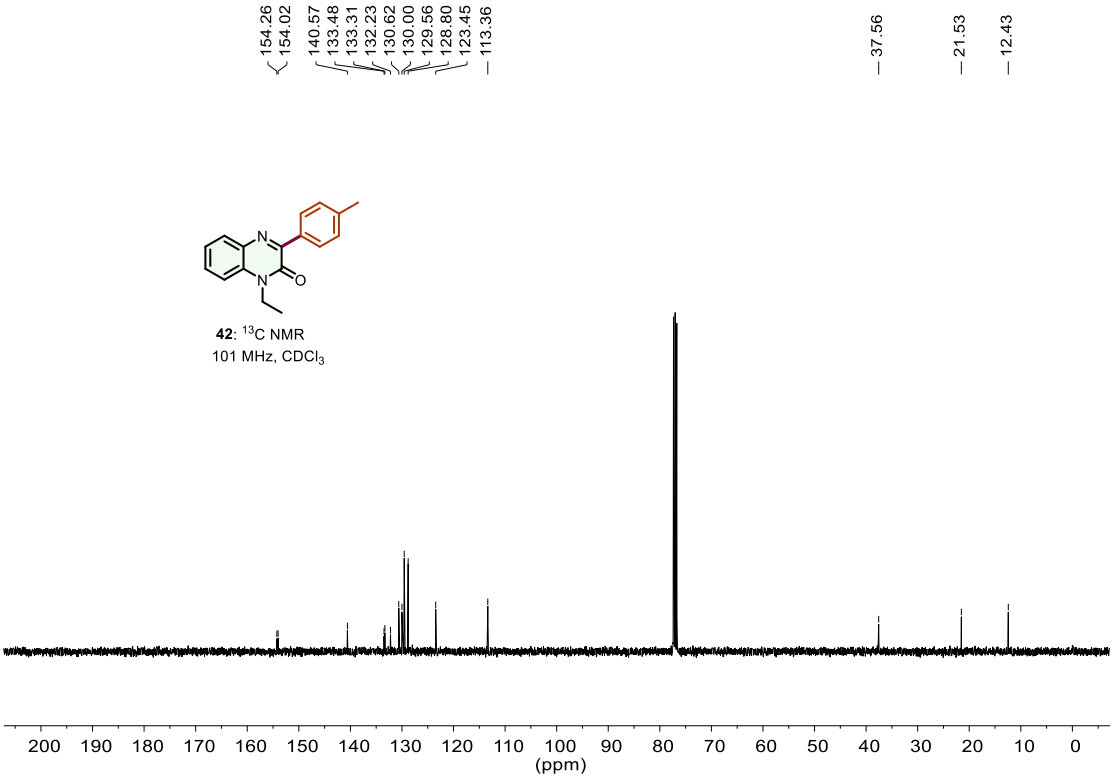
40: ^{1}H NMR
400 MHz, $CDCl_3$

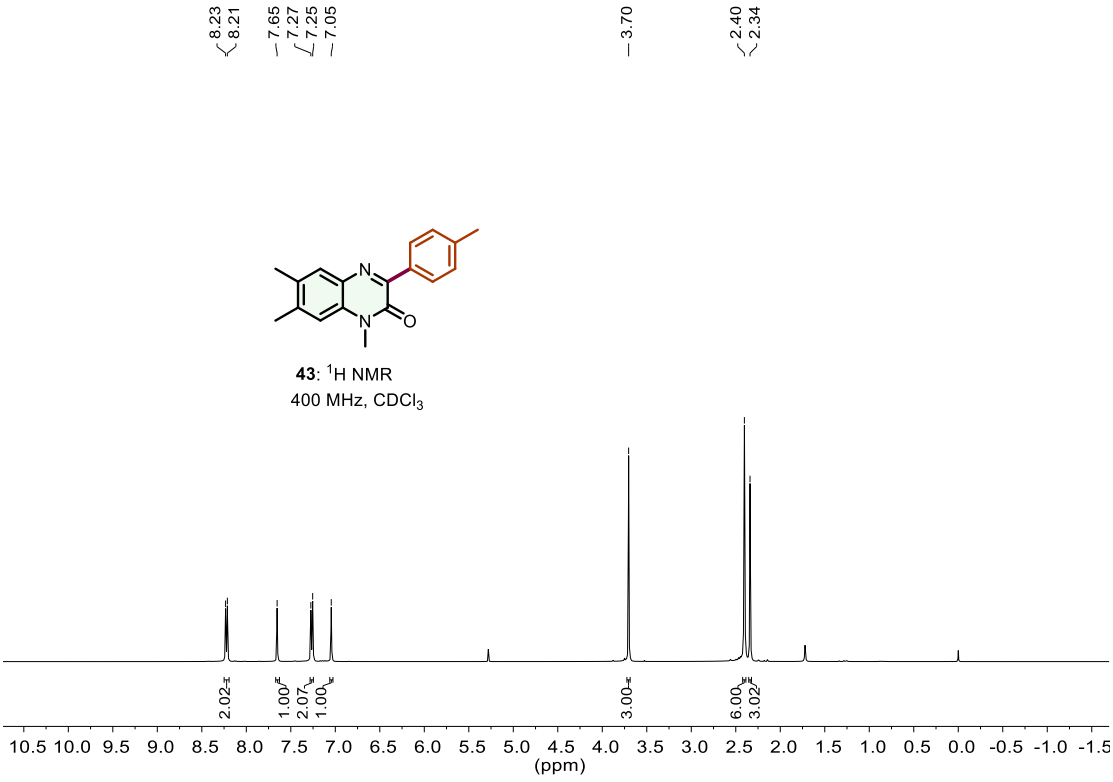

162.40
154.98
151.64
147.85
146.56
141.60
141.55
140.56
136.86
135.83
135.30
135.06
134.36
131.58
130.88
130.75
130.61
130.47
130.17
129.63
129.34
129.19
128.25
127.56
125.20
123.02
121.15
116.20
37.00
27.99
40: 13C NMR
101 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)

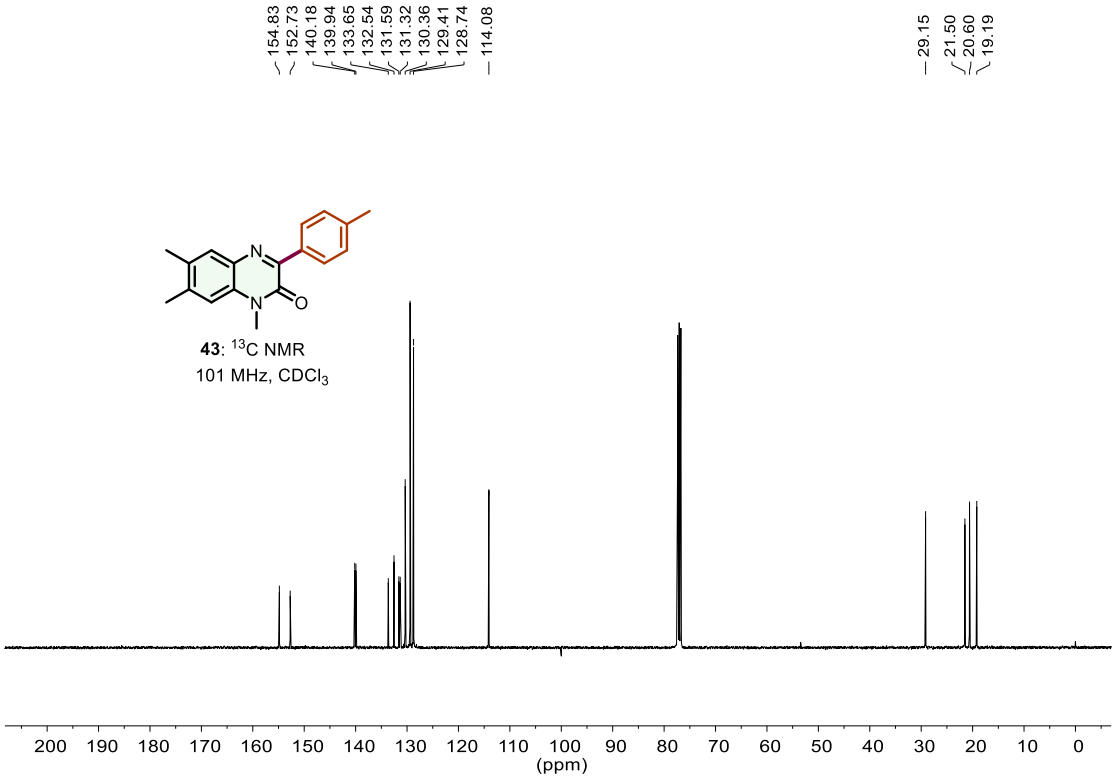

8.25
8.23
7.94
7.93
7.92
7.91
7.56
7.56
7.54
7.52
7.52
7.37
7.35
7.33
7.32
7.30
7.27
3.76
2.42
41: 1H NMR
400 MHz, CDCl3
2.00
1.00
1.05
4.19
2.99
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)


154.79
154.02
140.62
133.35
133.29
133.16
130.34
130.04
129.54
128.82
123.65
113.53
29.28
21.53
41: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

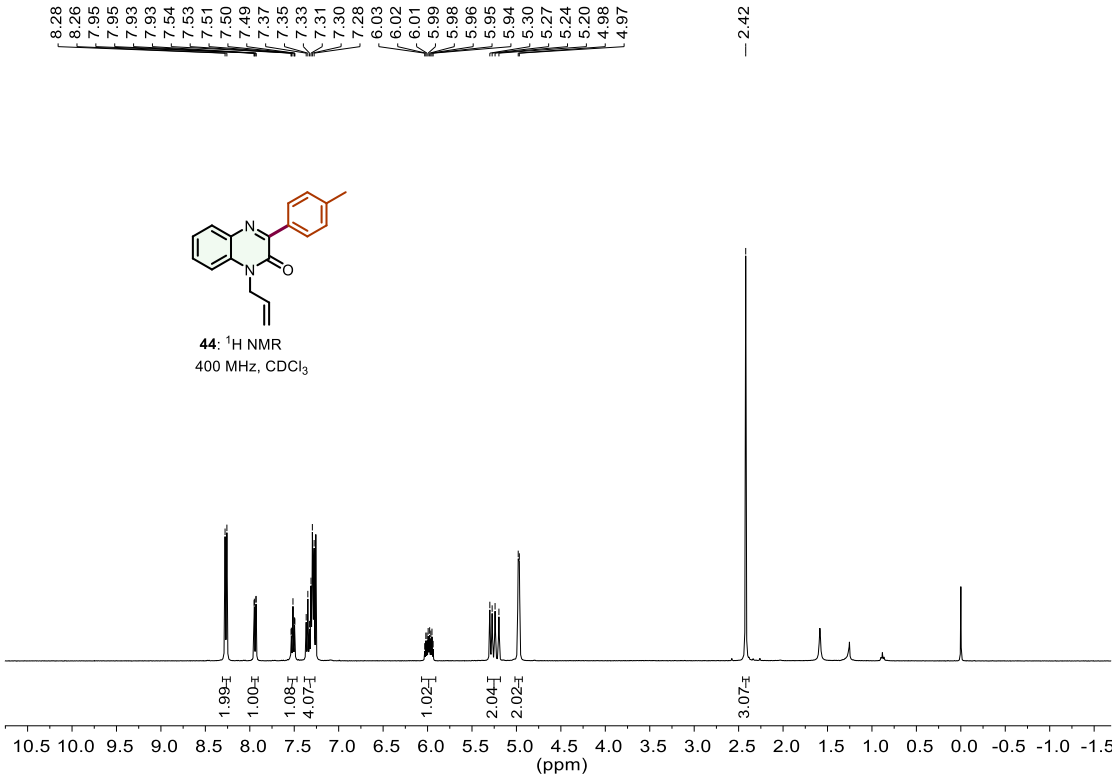

8.26
8.24
7.96
7.95
7.94
7.93
7.57
7.57
7.55
7.55
7.53
7.53
7.37
7.36
7.36
7.35
7.34
7.33
7.30
7.28
4.42
4.40
4.38
4.36
2.42
1.44
1.42
1.40
42: 1H NMR
400 MHz, CDCl3
1.99
1.00
1.03
2.04
2.02
2.03
3.02
3.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)


154.26
154.02
140.57
133.48
133.31
132.23
130.62
130.00
129.56
128.80
123.45
113.36
37.56
21.53
12.43
42: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

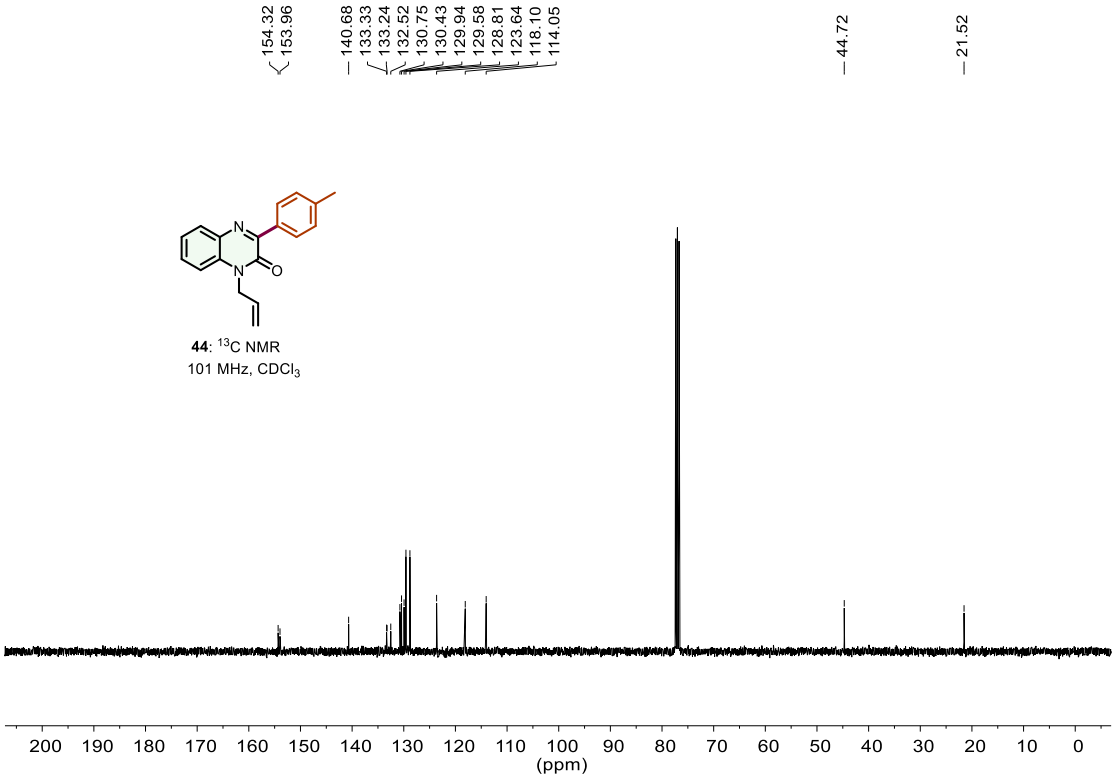

8.23
8.21
7.65
7.27
7.25
7.05
3.70
2.40
2.34
43: 1H NMR
400 MHz, CDCl3
2.02
1.00
2.07
1.00
3.00
6.00
3.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)



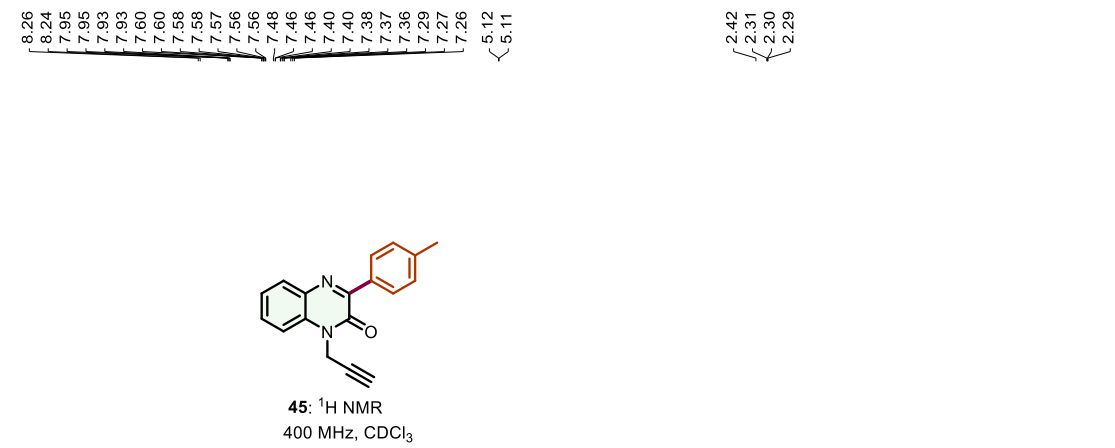
43: ^{13}C NMR
101 MHz, $CDCl_3$



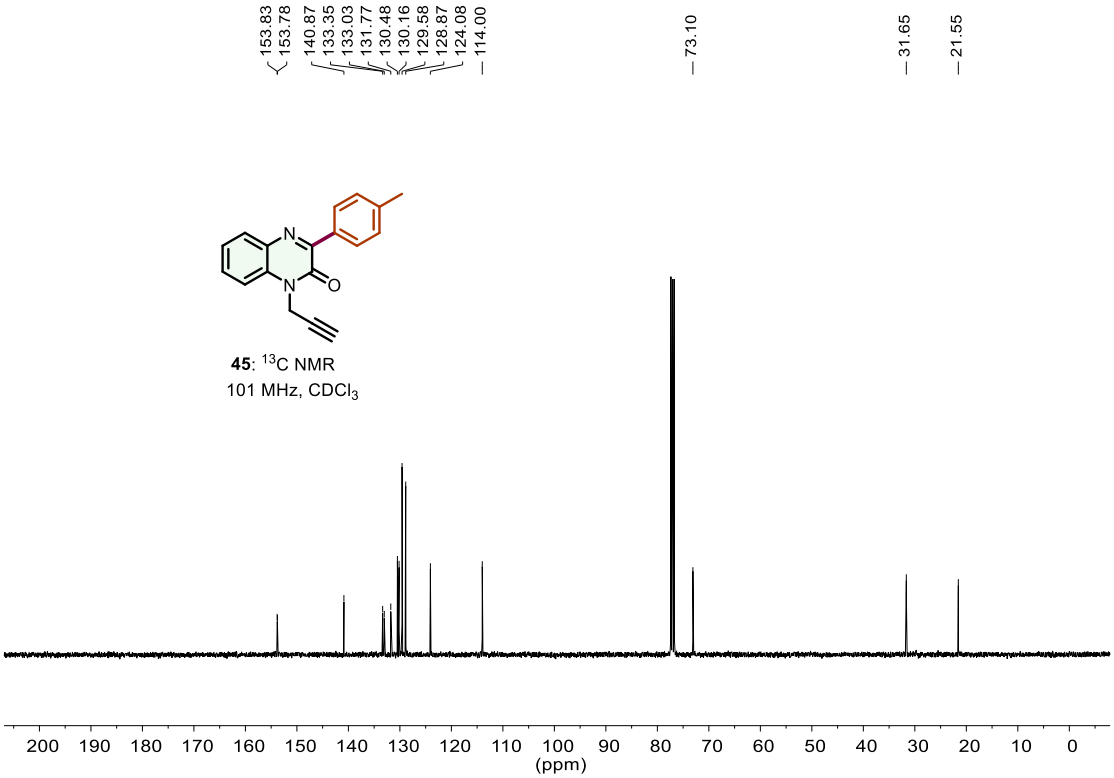
44: ^{1}H NMR
400 MHz, $CDCl_3$



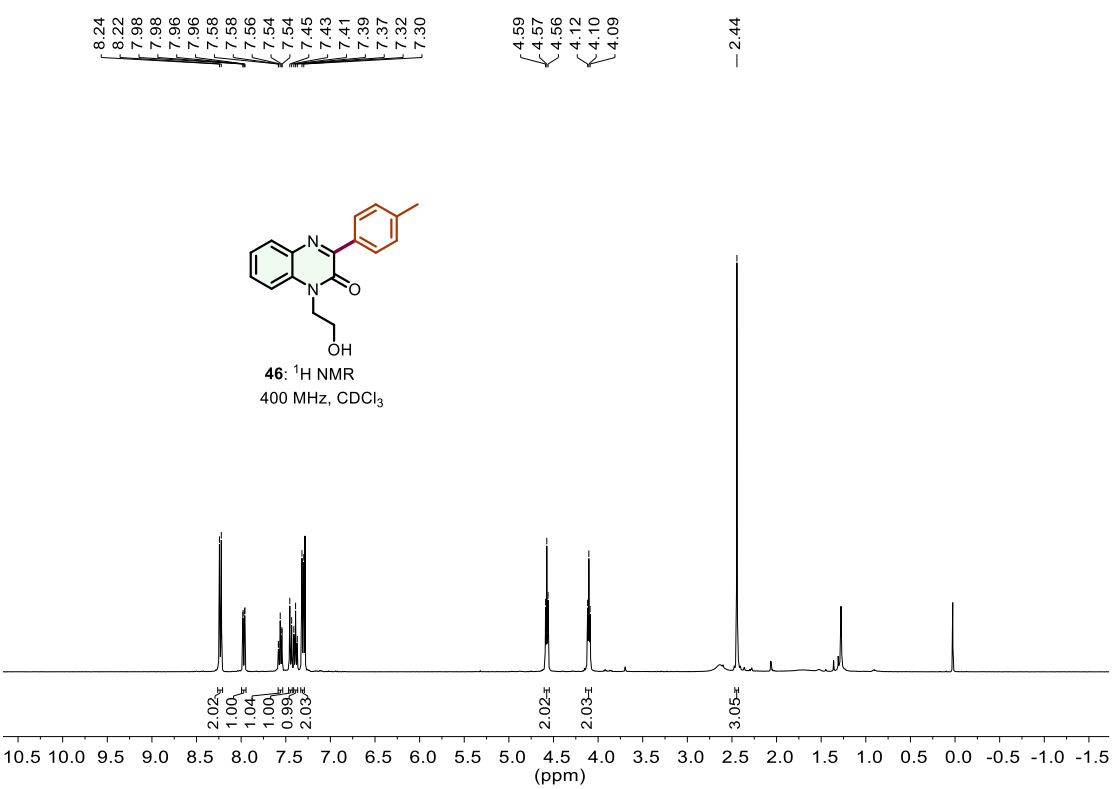
44: ^{13}C NMR
101 MHz, $CDCl_3$



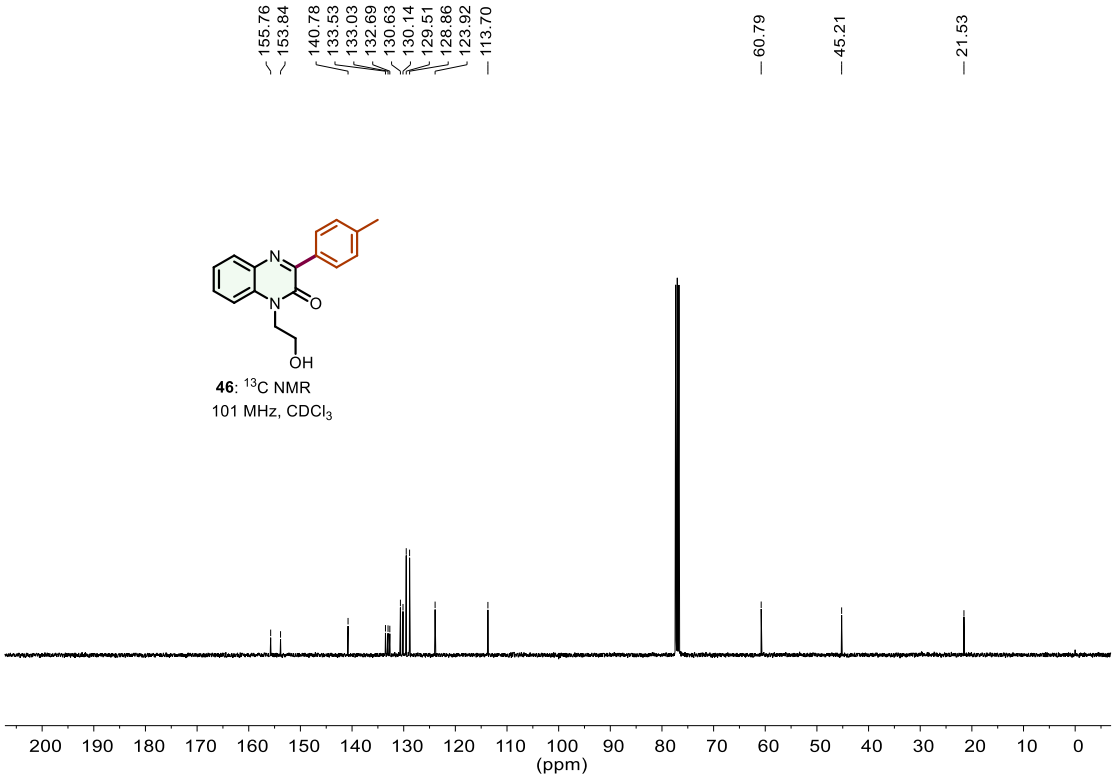
45: ^{1}H NMR
400 MHz, $CDCl_3$



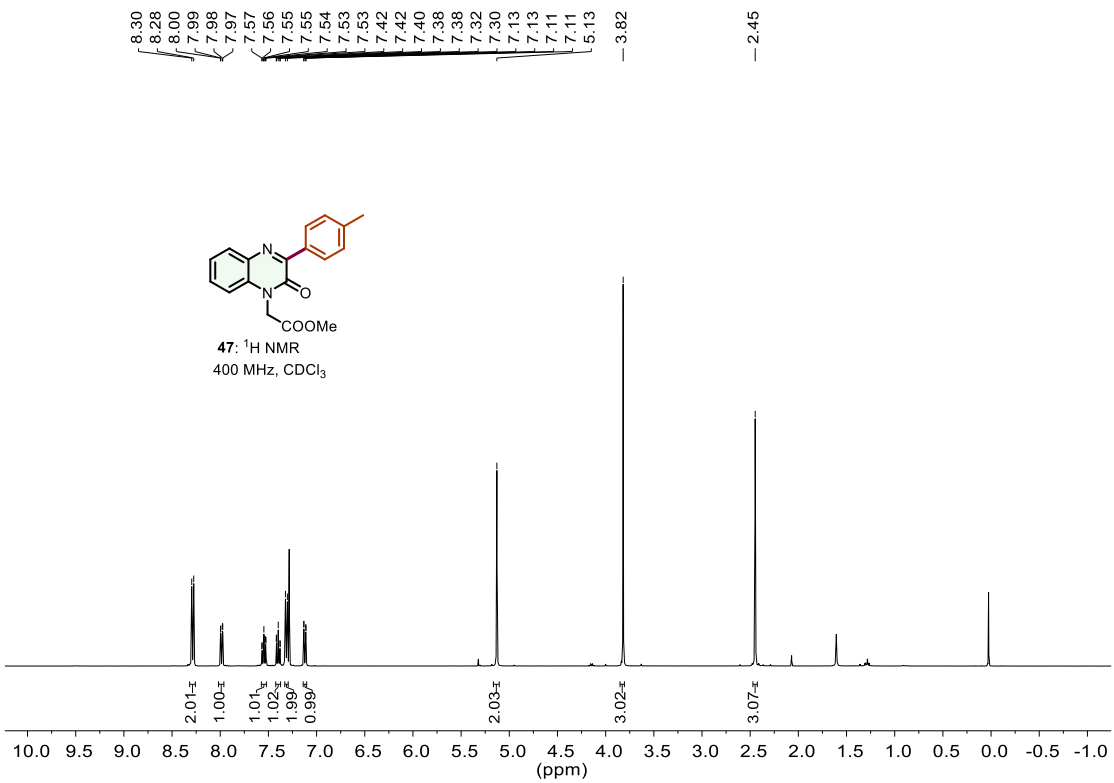
45: ^{13}C NMR
101 MHz, $CDCl_3$



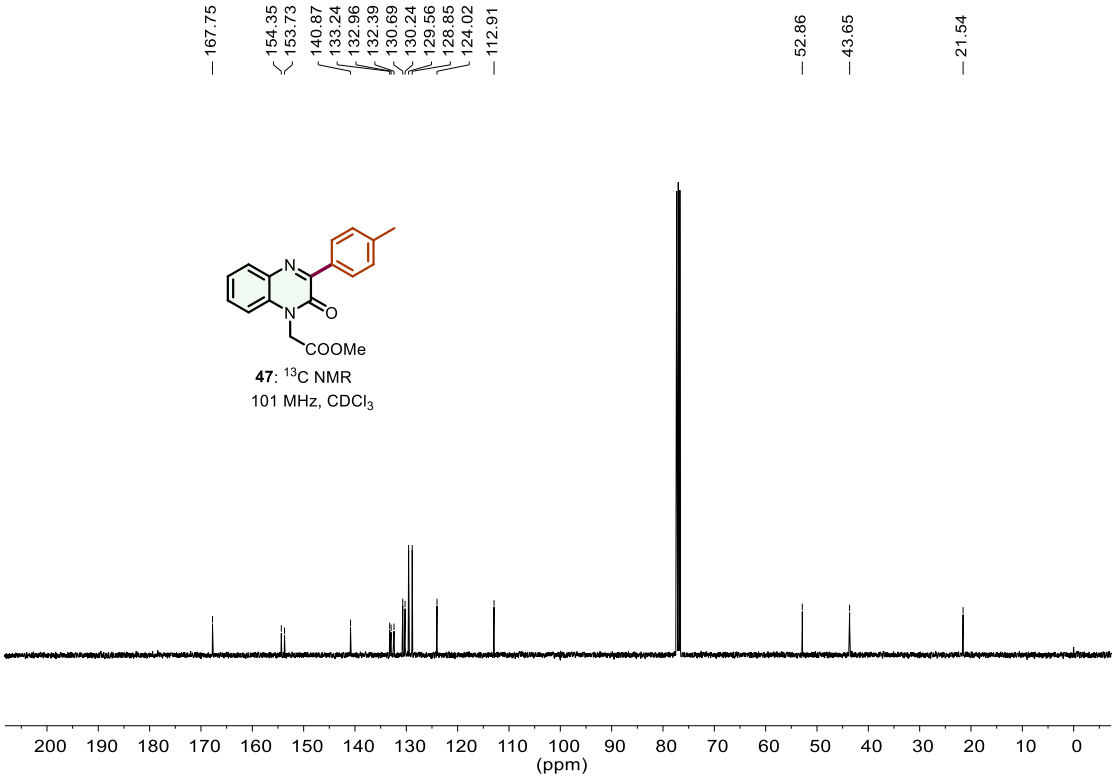
46: ^{1}H NMR
400 MHz, $CDCl_3$



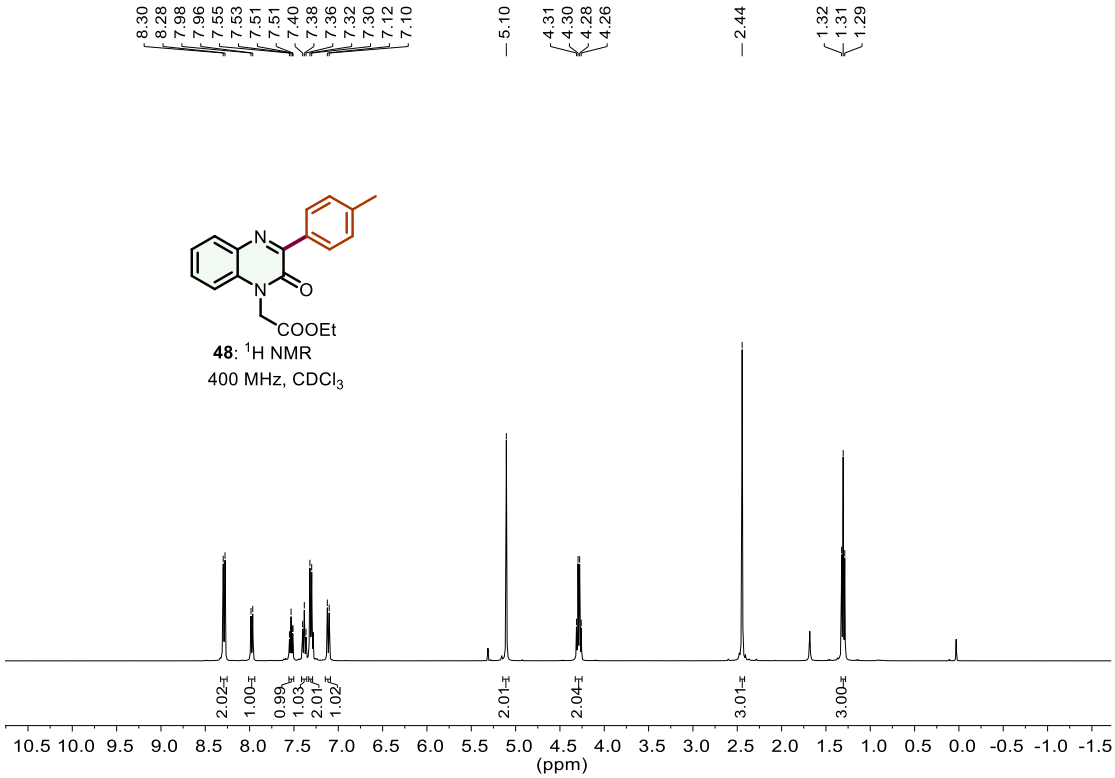
46: ^{13}C NMR
101 MHz, $CDCl_3$



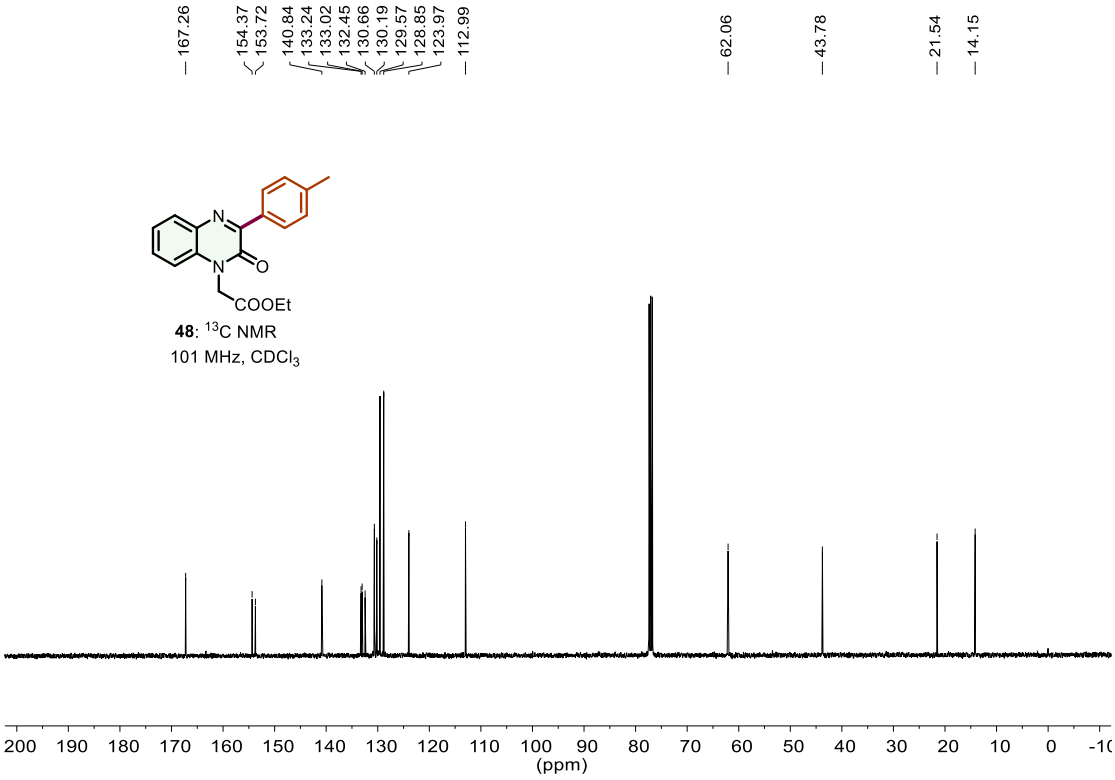
47: ^{1}H NMR
400 MHz, $CDCl_3$



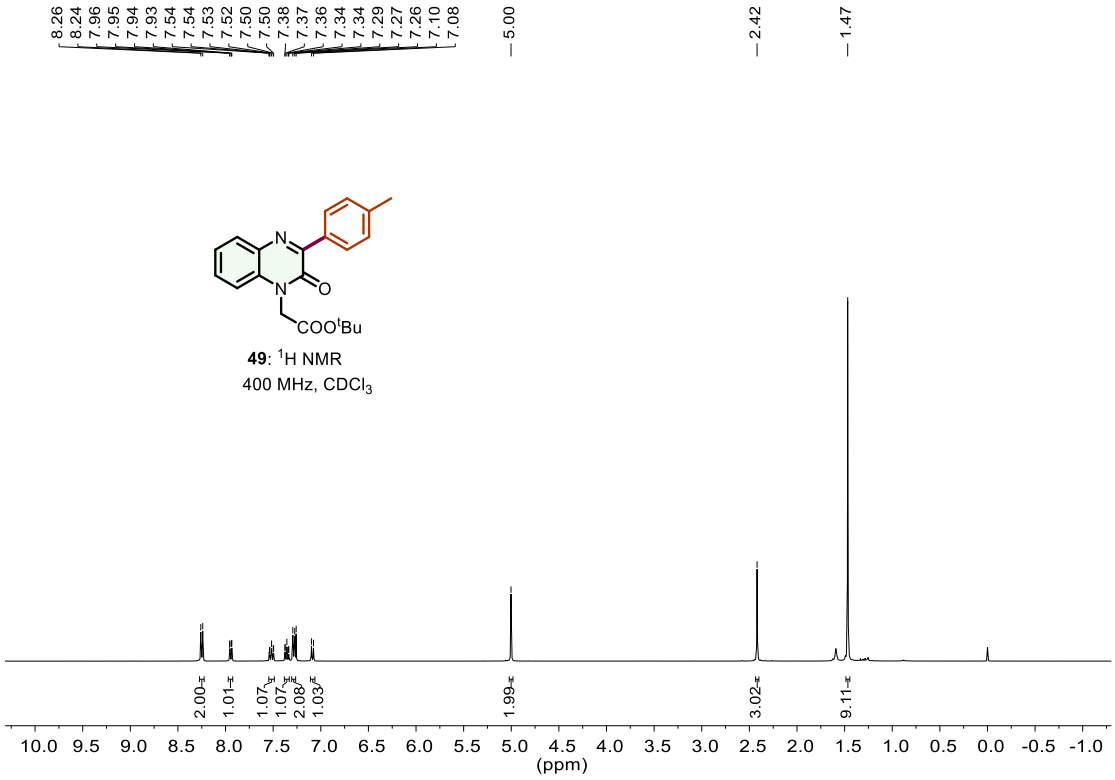
47: ^{13}C NMR
101 MHz, $CDCl_3$



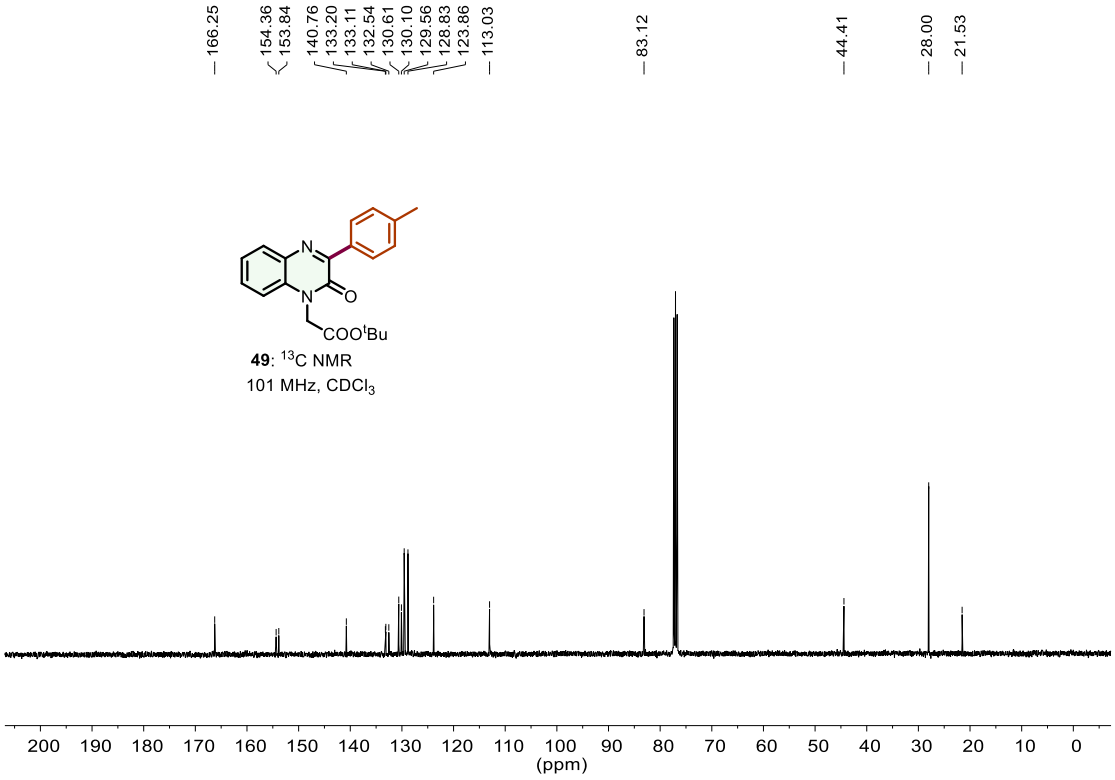
48: ^{1}H NMR
400 MHz, $CDCl_3$



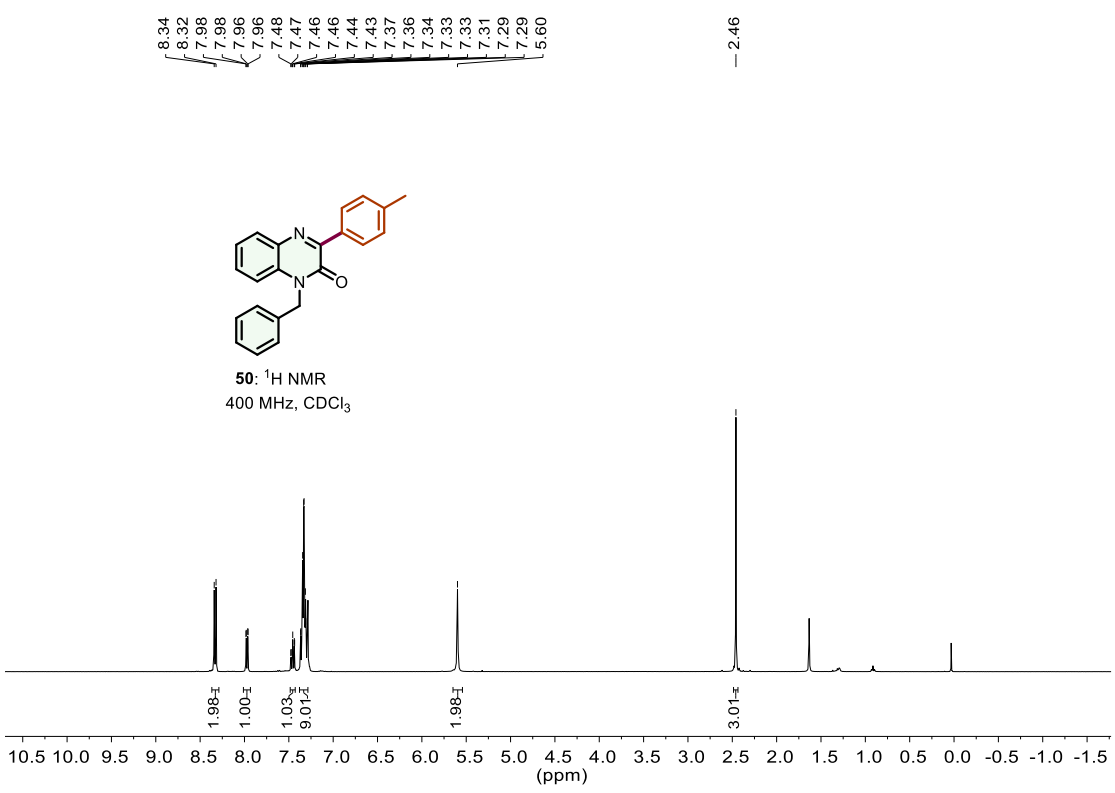
48: ^{13}C NMR
101 MHz, $CDCl_3$



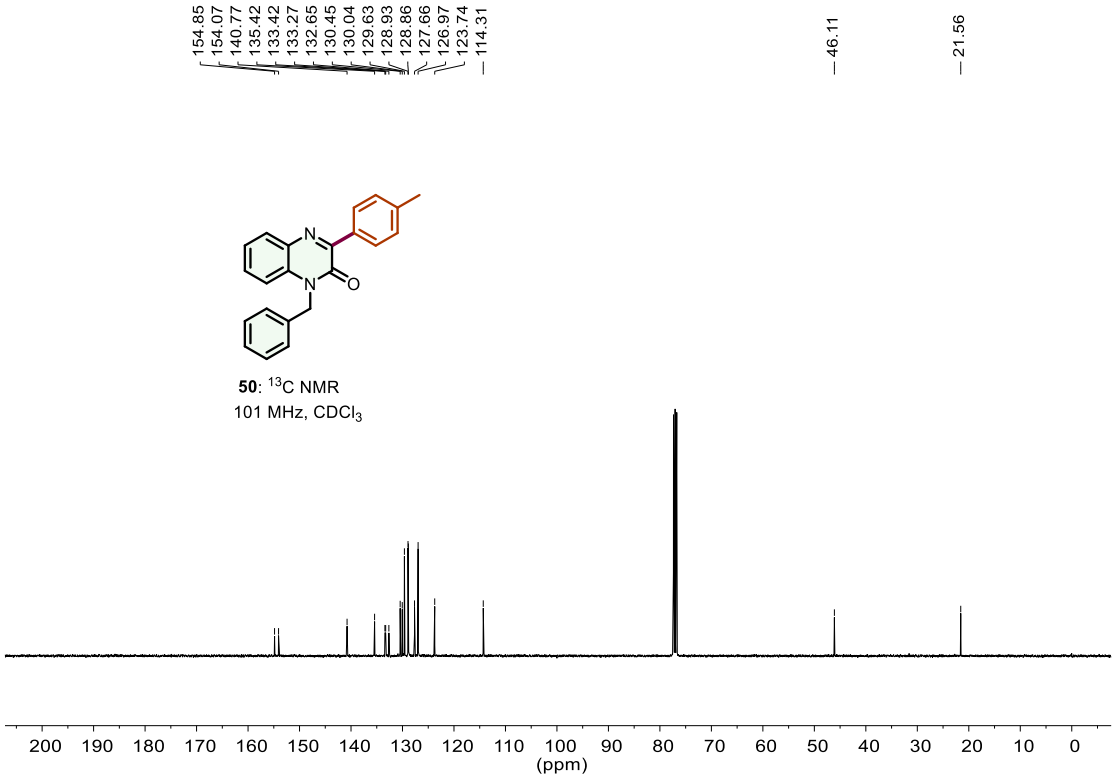
49: ^{1}H NMR
400 MHz, $CDCl_3$

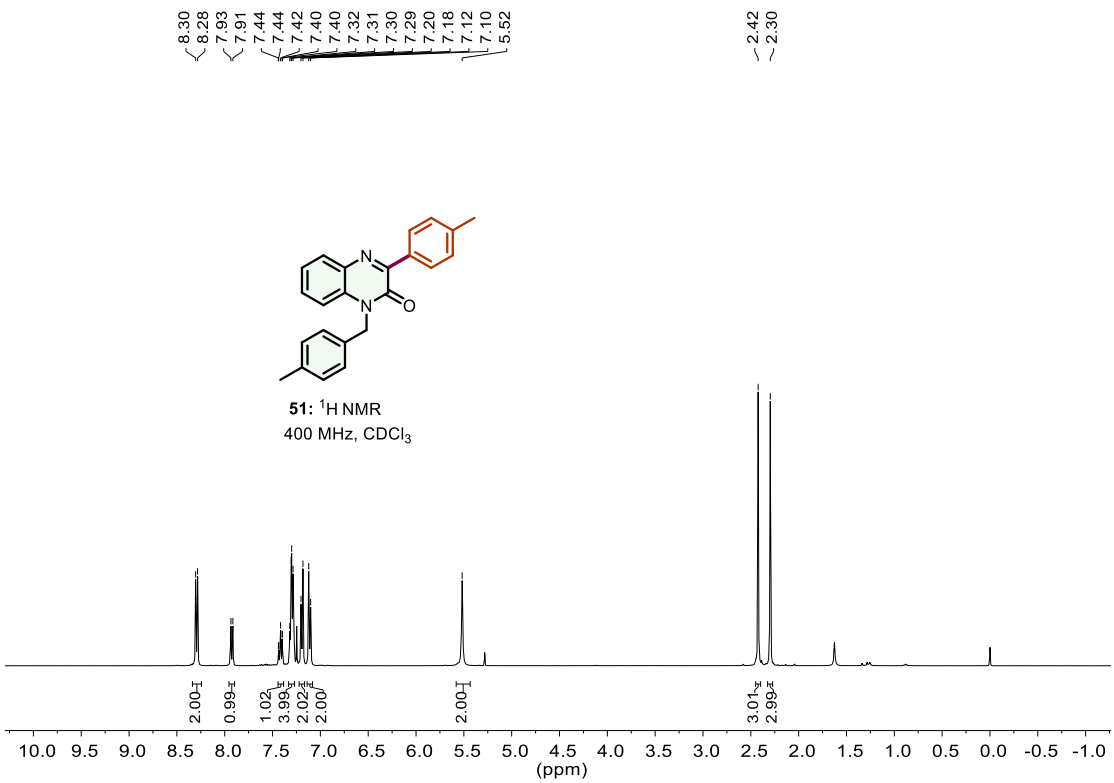


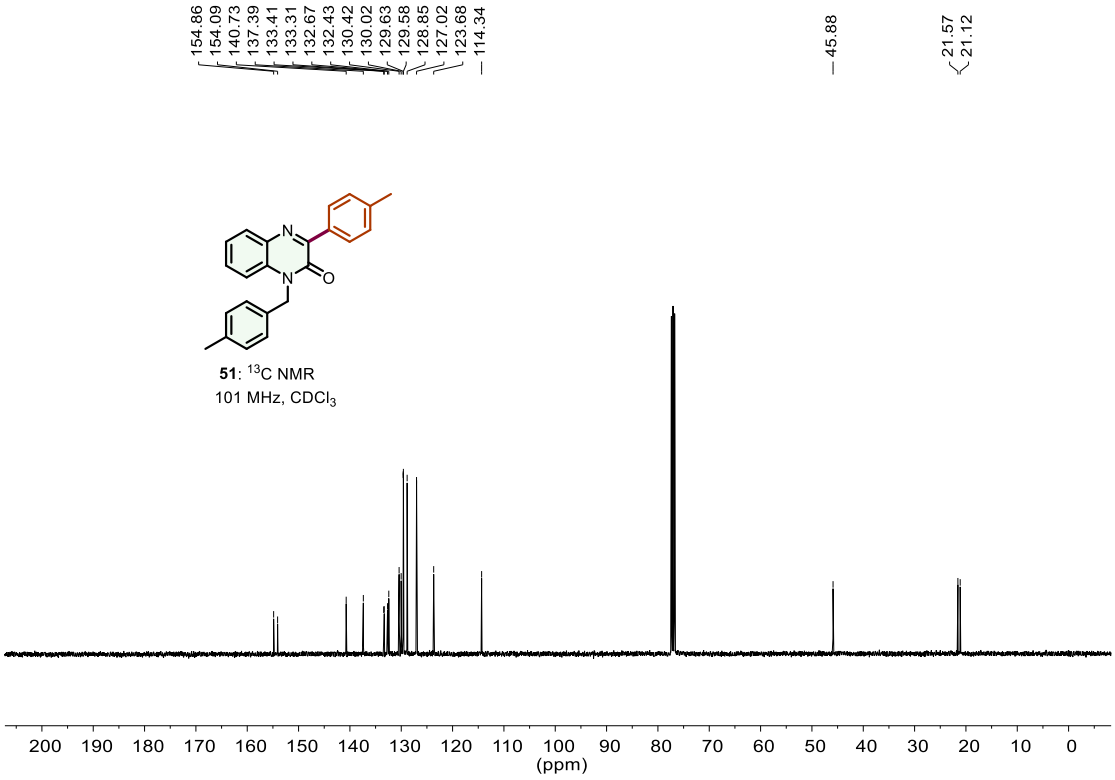
49: ^{13}C NMR
101 MHz, $CDCl_3$

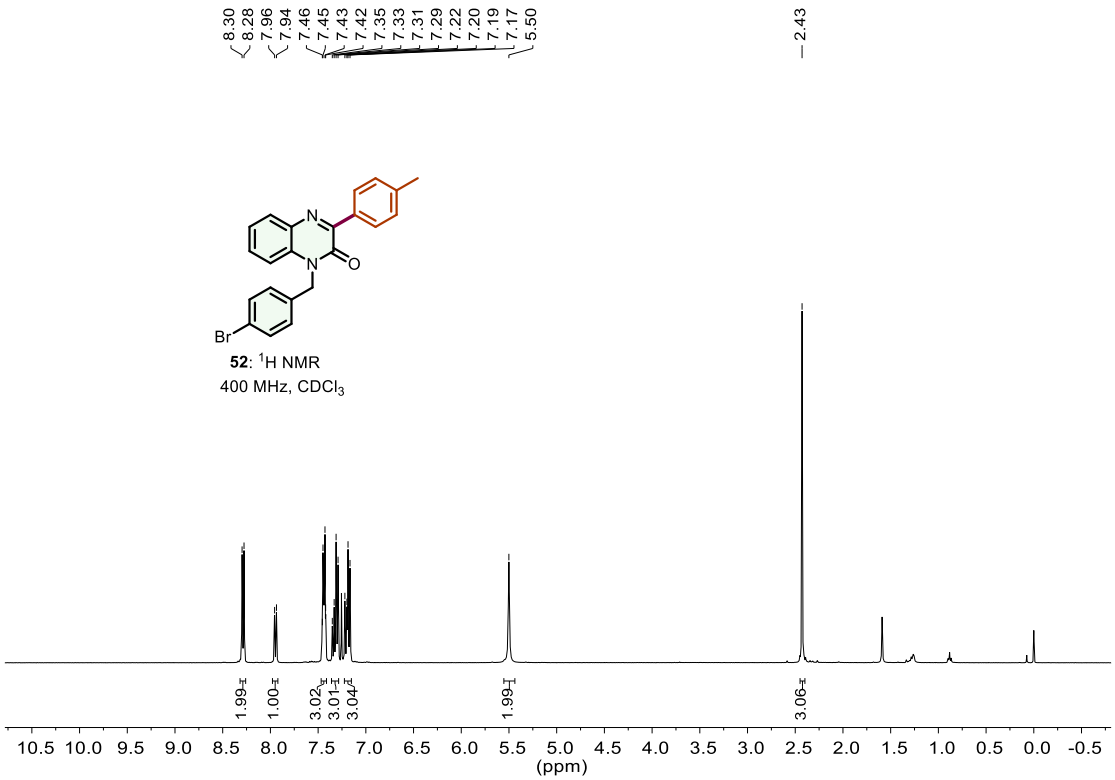


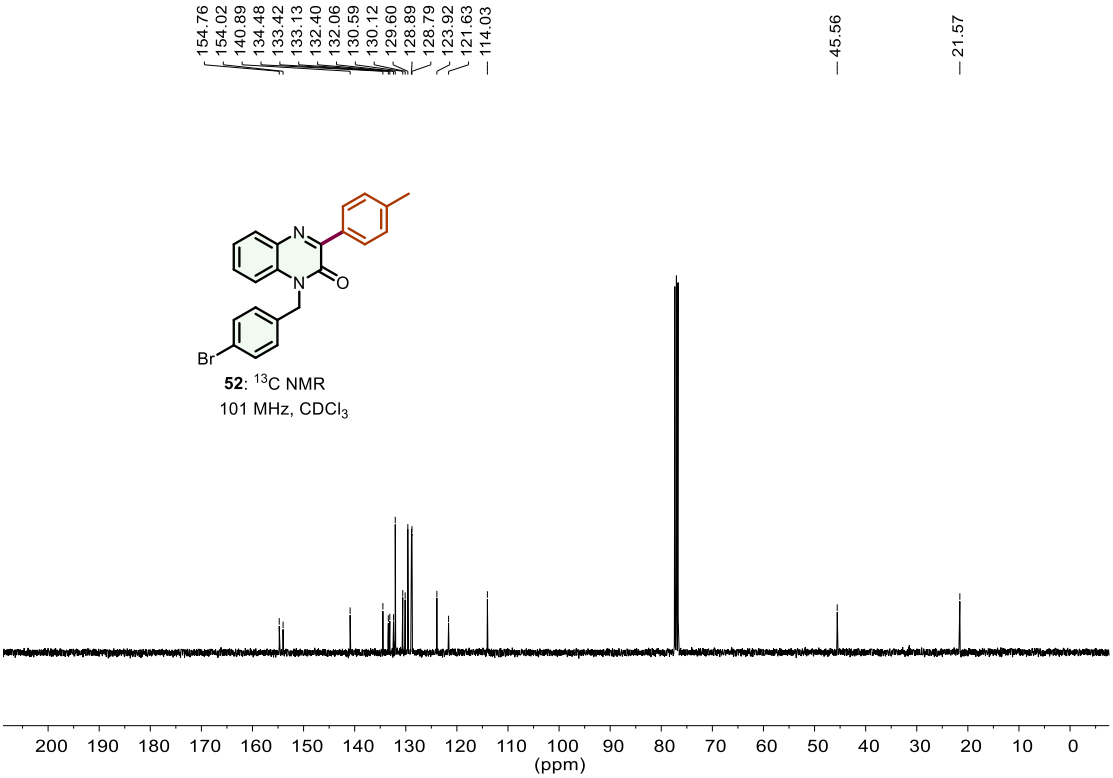
50: ^{1}H NMR
400 MHz, $CDCl_3$


154.85
154.07
140.77
135.42
133.42
133.27
132.65
130.45
130.04
129.63
128.93
128.86
127.66
126.97
123.74
114.31
46.11
21.56
N
N
O
50: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

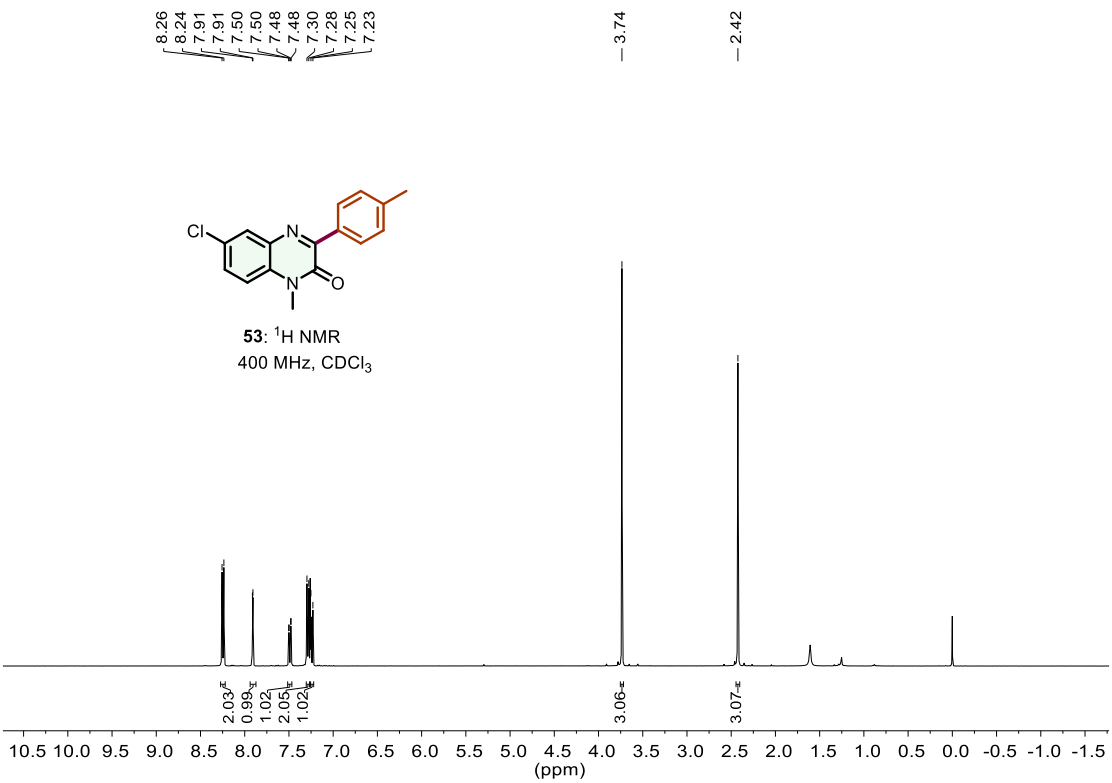

8.30
8.28
7.93
7.91
7.44
7.44
7.42
7.40
7.40
7.32
7.31
7.30
7.29
7.20
7.18
7.12
7.10
5.52
2.42
2.30
N
N
O
51: 1H NMR
400 MHz, CDCl3
2.00
0.99
1.02
3.99
2.02
2.00
2.00
3.01
2.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
(ppm)


154.86
154.09
140.73
137.39
133.41
133.31
132.67
132.43
130.42
130.02
129.63
129.58
128.85
127.02
123.68
114.34
45.88
21.57
21.12
N
N
O
51: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

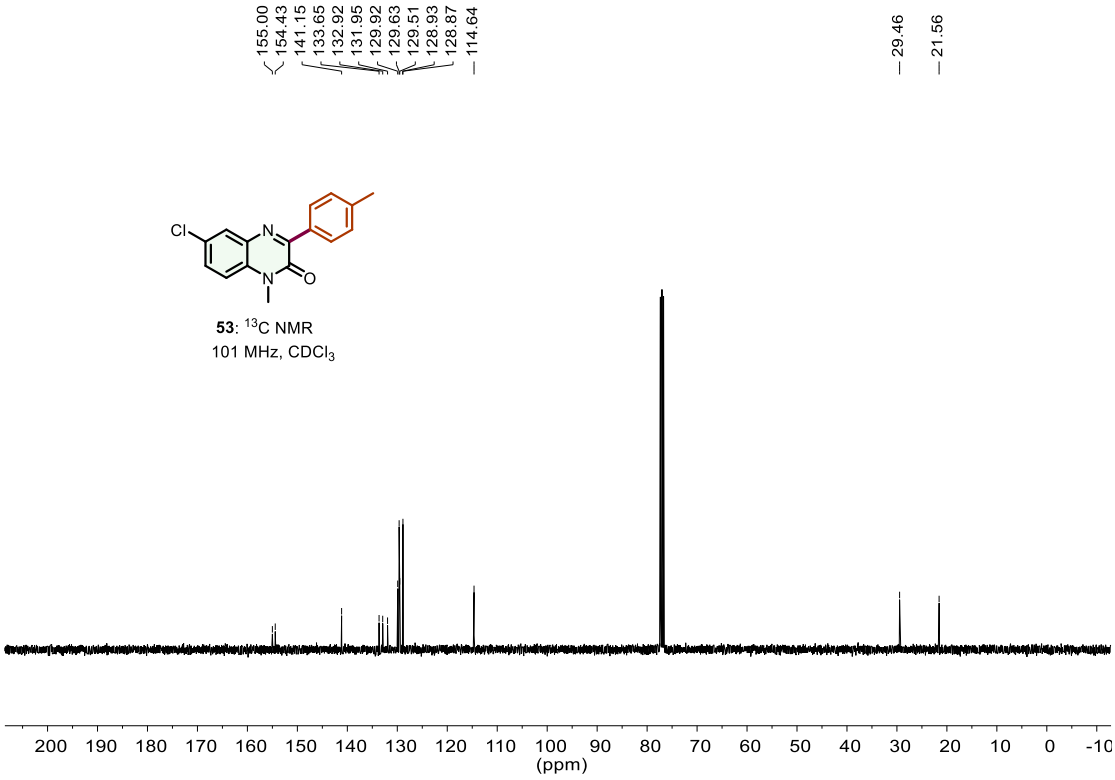

8.30
8.28
7.96
7.94
7.46
7.45
7.43
7.42
7.35
7.33
7.31
7.29
7.22
7.20
7.19
7.17
5.50
2.43
N
N
O
Br
52: 1H NMR
400 MHz, CDCl3
1.99
1.00
3.02
3.01
3.04
1.99
3.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)



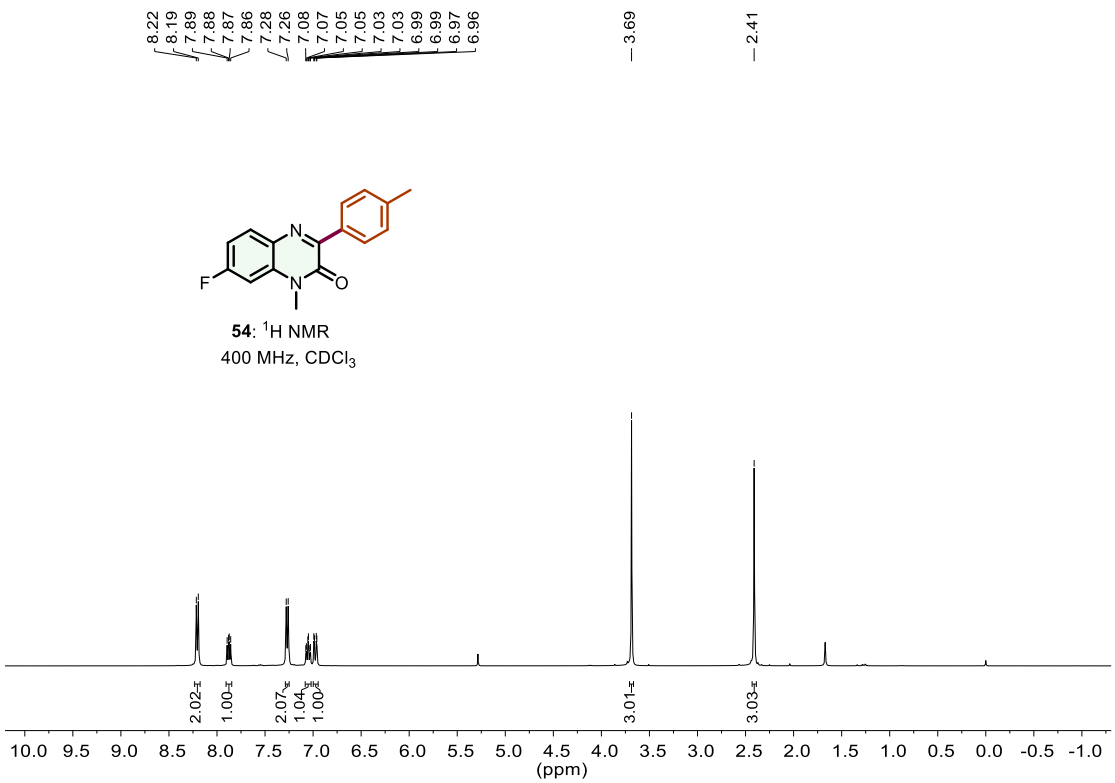
52: ^{13}C NMR
101 MHz, $CDCl_3$



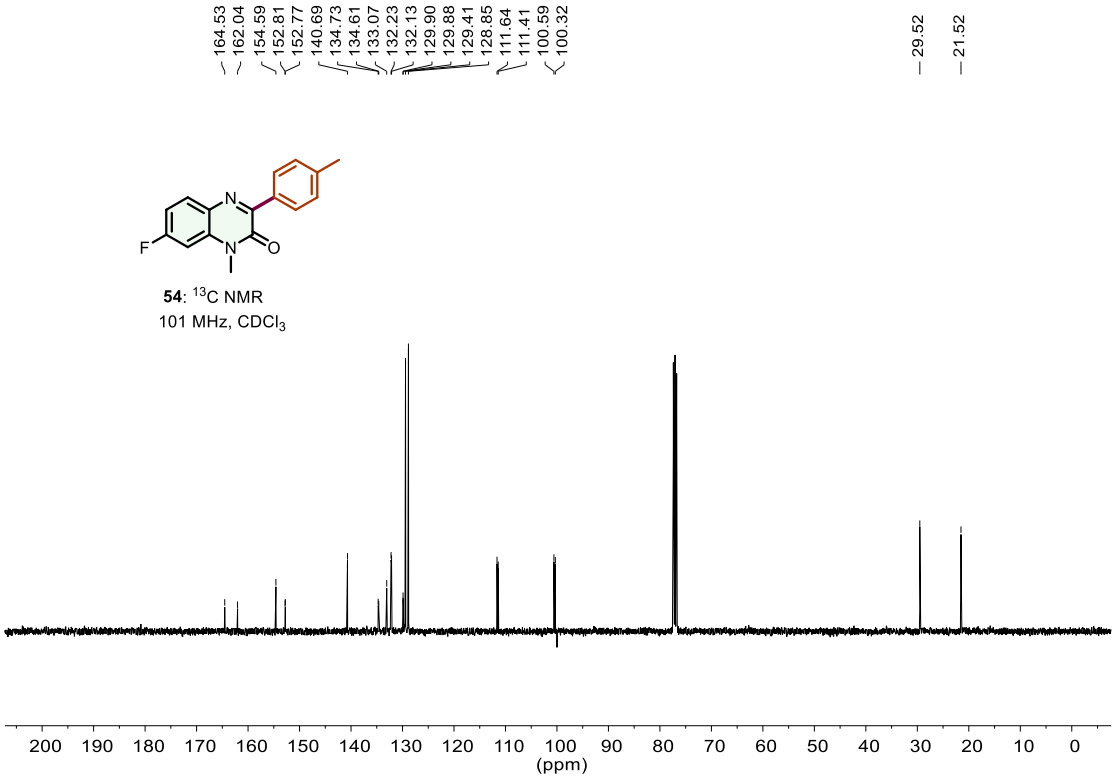
53: ^{1}H NMR
400 MHz, $CDCl_3$



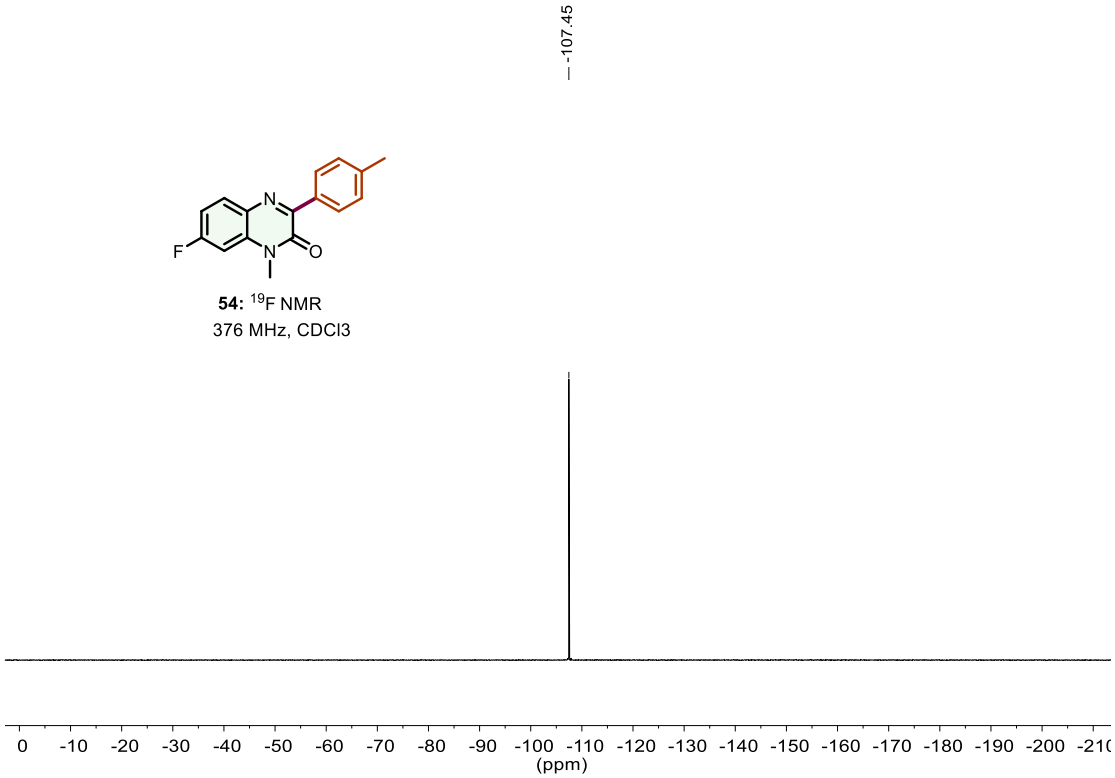
53: ^{13}C NMR
101 MHz, $CDCl_3$



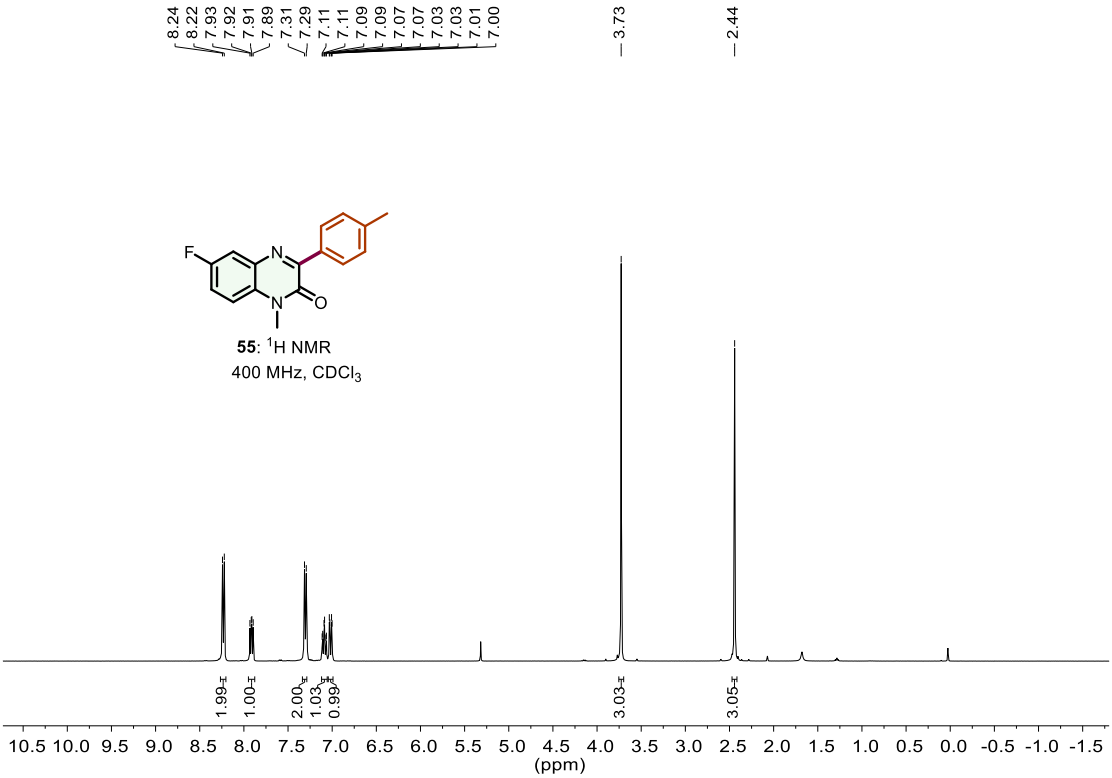
54: ^{1}H NMR
400 MHz, $CDCl_3$

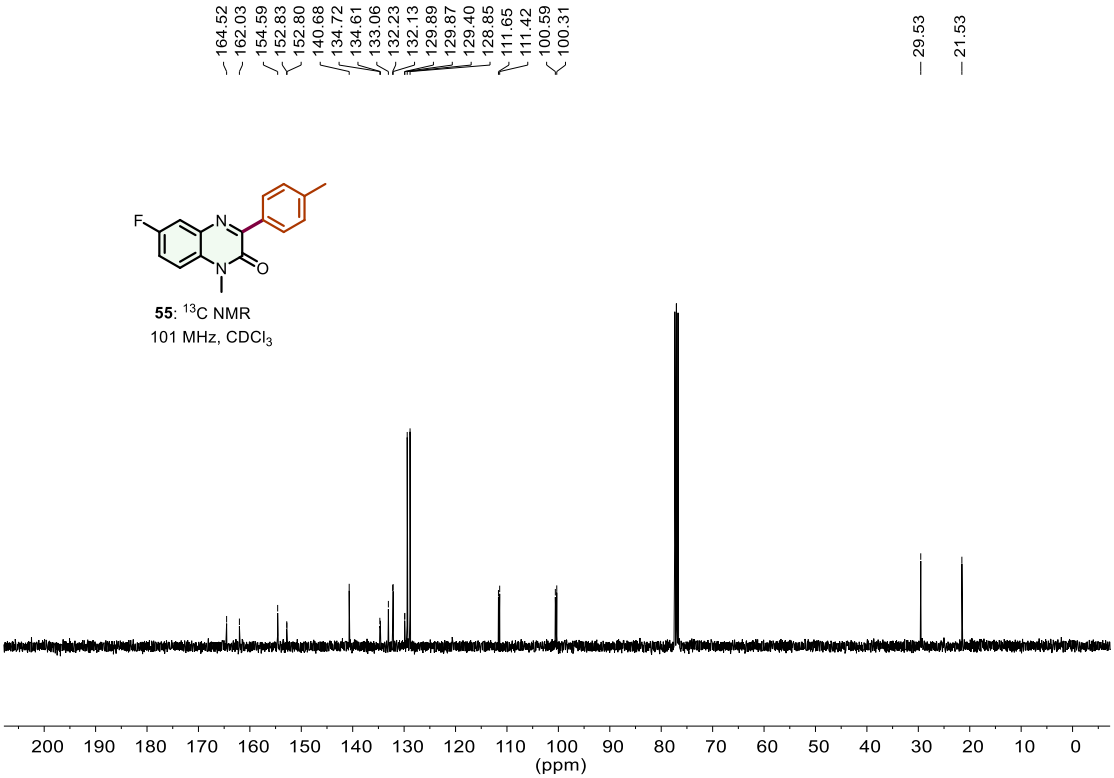


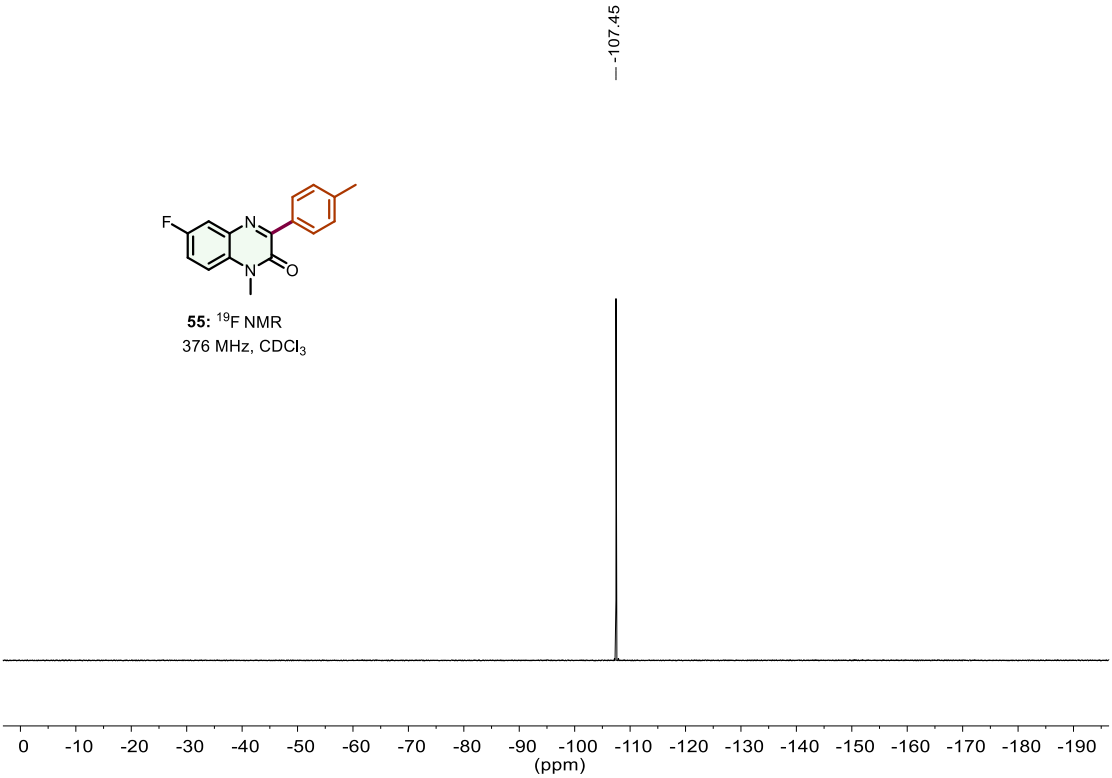
54: ^{13}C NMR
101 MHz, $CDCl_3$



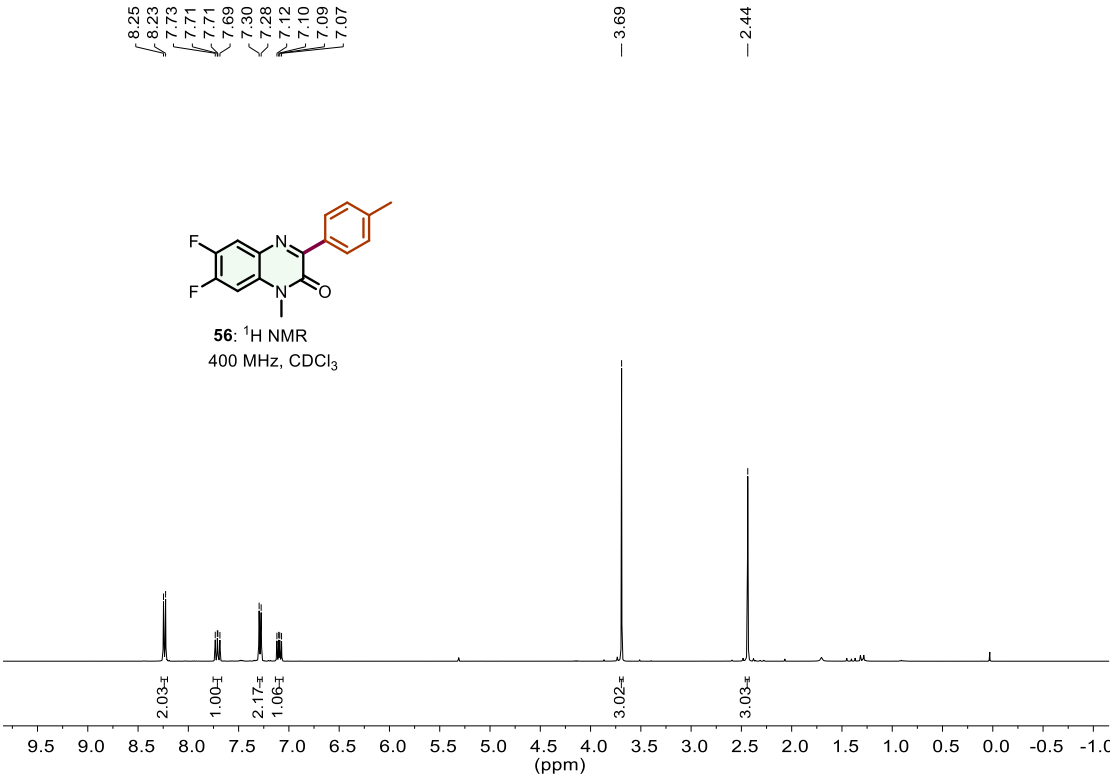
54: ^{19}F NMR
376 MHz, CDCl3


8.24
8.22
7.93
7.92
7.91
7.89
7.31
7.29
7.11
7.11
7.09
7.09
7.07
7.07
7.03
7.03
7.01
7.00
3.73
2.44
F
N
O
N
55: 1H NMR
400 MHz, CDCl3
1.99
1.00
2.00
1.03
0.99
3.03
3.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)

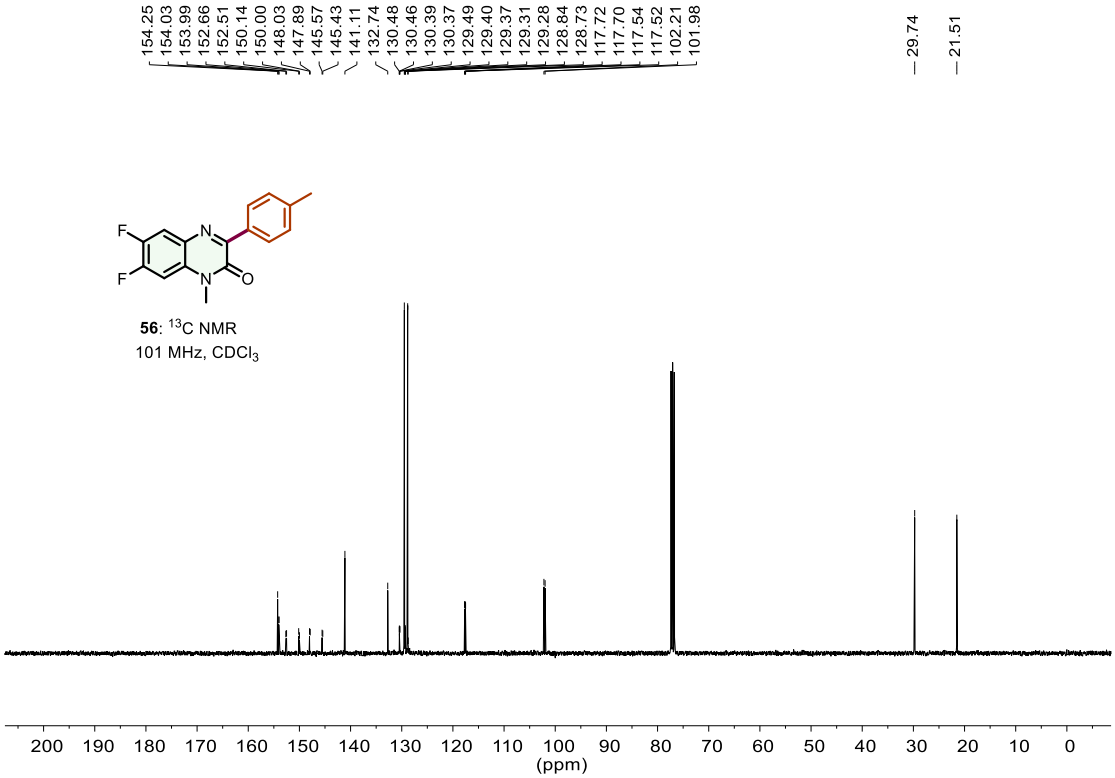

164.52
162.03
154.59
152.83
152.80
140.68
134.72
134.61
133.06
132.23
132.13
129.89
129.87
129.40
128.85
111.65
111.42
100.59
100.31
29.53
21.53
F
N
O
N
55: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)



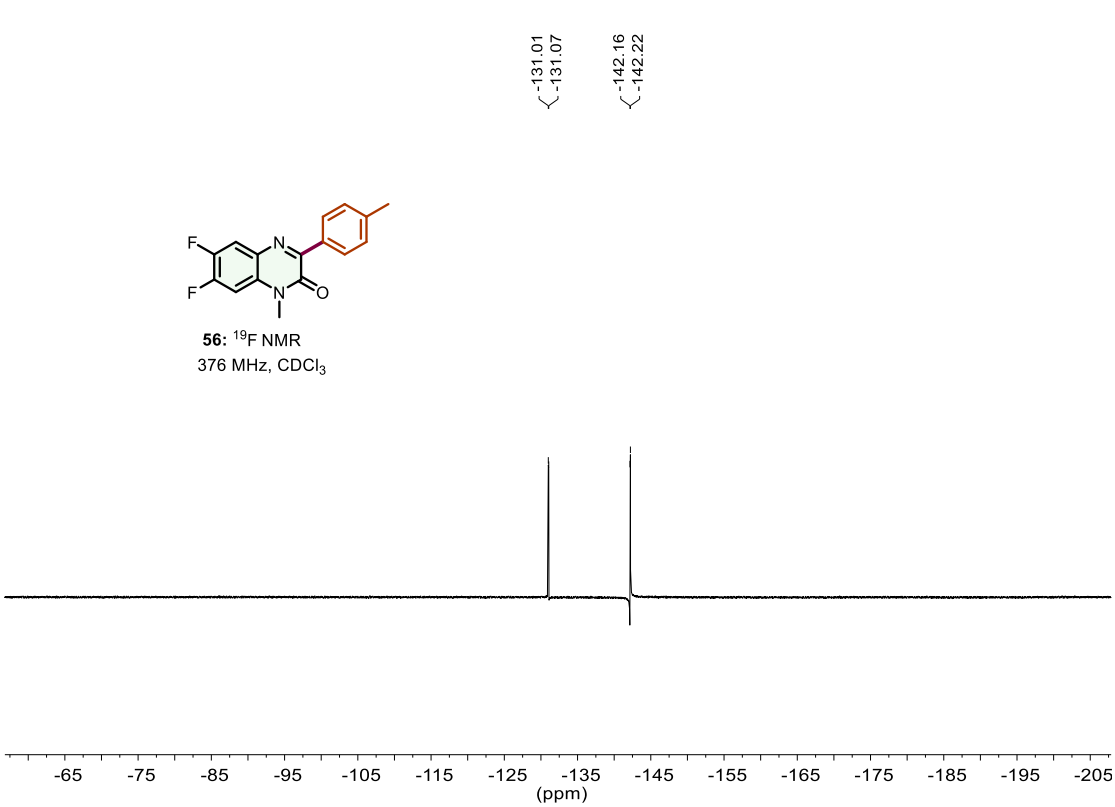
55: ^{19}F NMR
376 MHz, $CDCl_3$



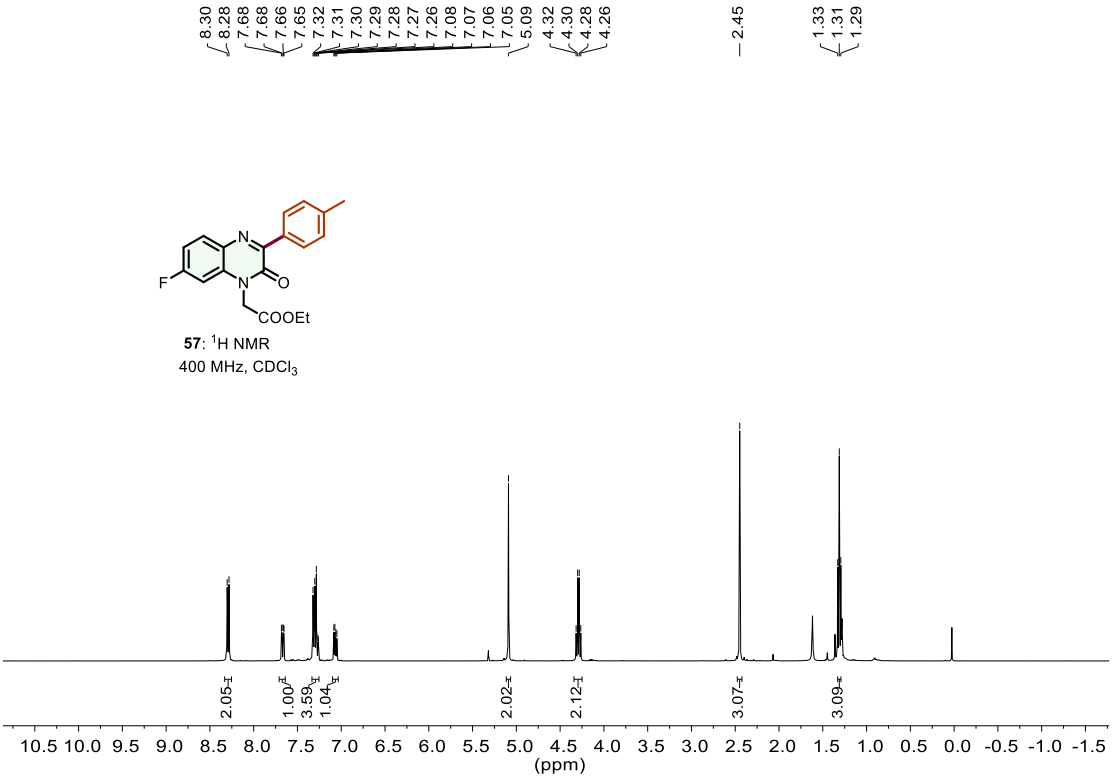
56: ^{1}H NMR
400 MHz, $CDCl_3$

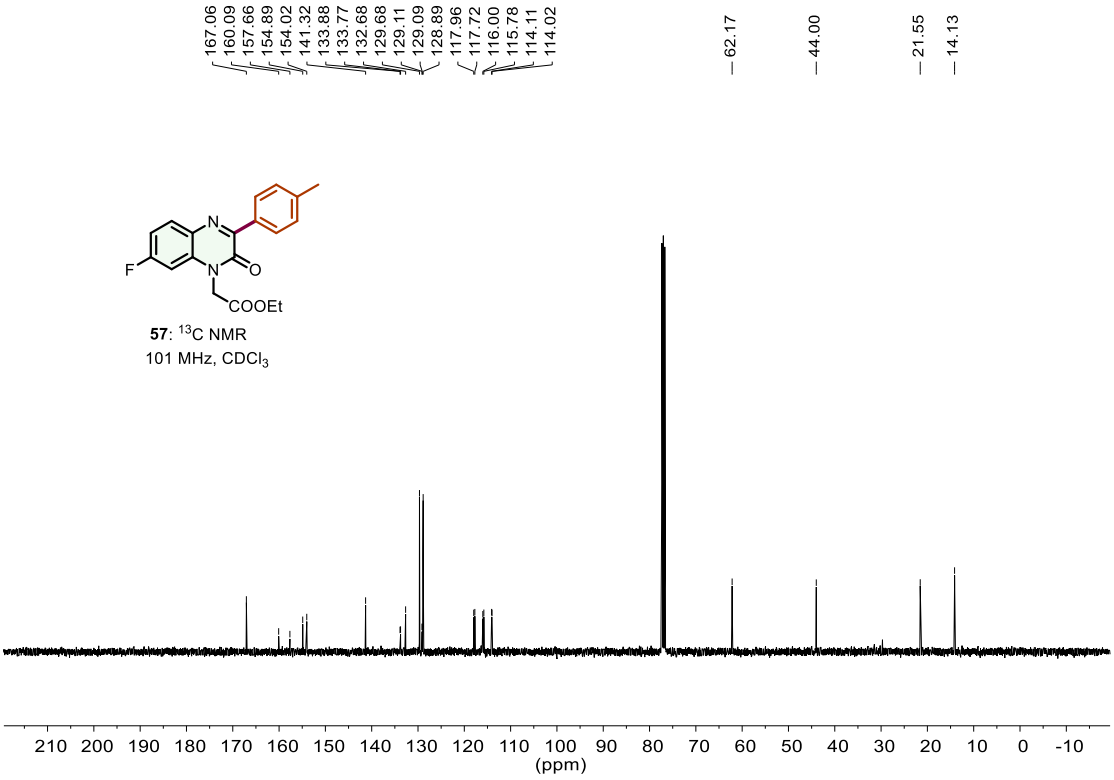


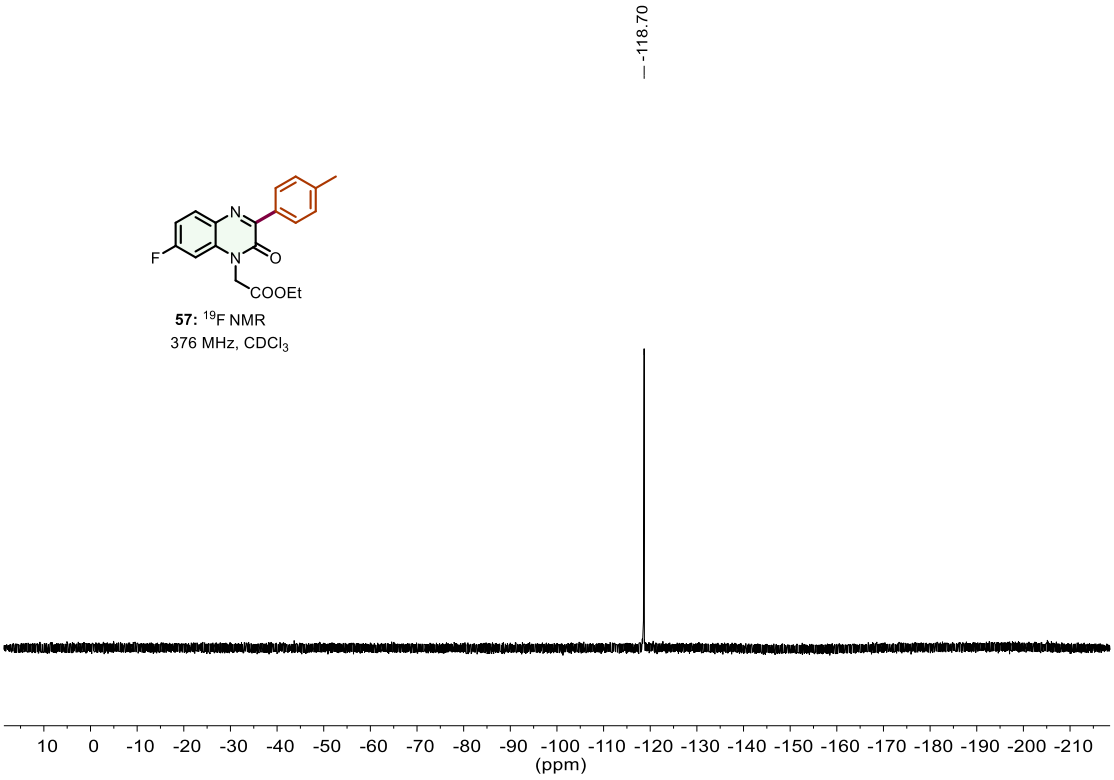
56: ^{13}C NMR
101 MHz, $CDCl_3$



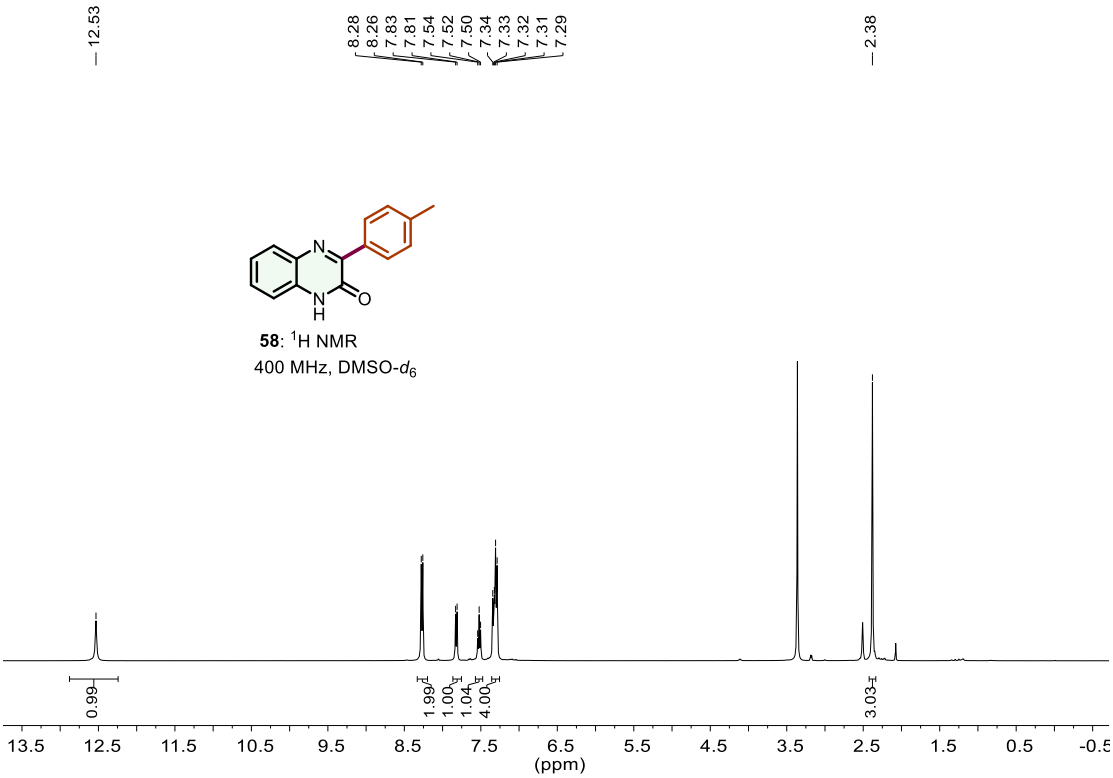
56: ^{19}F NMR
376 MHz, $CDCl_3$


8.30
8.28
7.68
7.68
7.66
7.65
7.32
7.31
7.30
7.29
7.28
7.27
7.26
7.08
7.07
7.06
7.05
5.09
4.32
4.30
4.28
4.26
2.45
1.33
1.31
1.29
F
N
N
O
COOEt
57: 1H NMR
400 MHz, CDCl3
2.05
1.00
3.59
1.04
2.02
2.12
3.07
3.09
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)

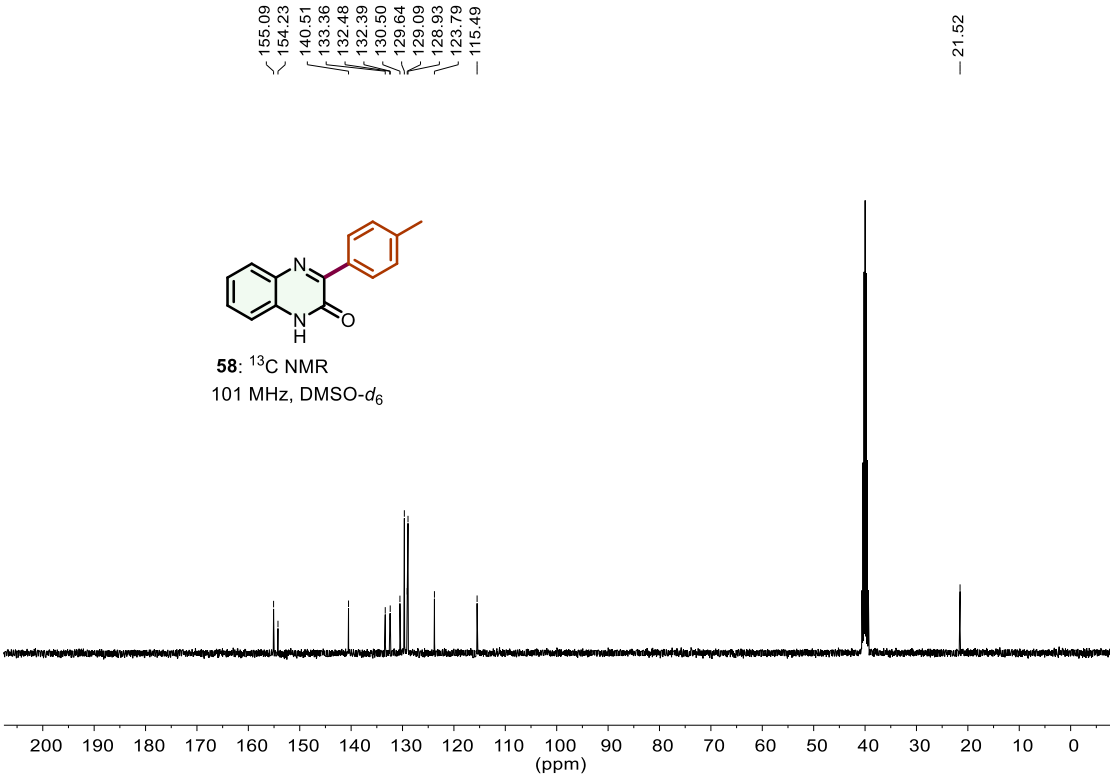

167.06
160.09
157.66
154.89
154.02
141.32
133.88
133.77
132.68
129.68
129.11
129.09
128.89
117.96
117.72
116.00
115.78
114.11
114.02
62.17
44.00
21.55
14.13
F
N
N
O
COOEt
57: 13C NMR
101 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)



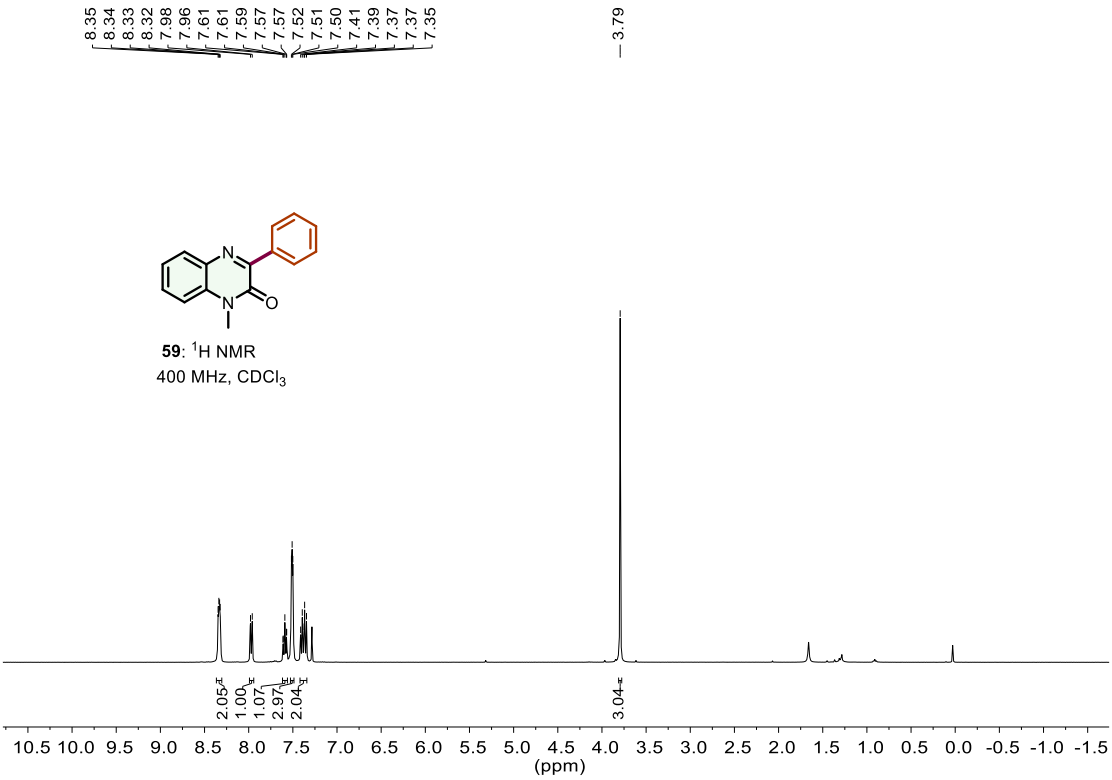
57: ^{19}F NMR
376 MHz, $CDCl_3$



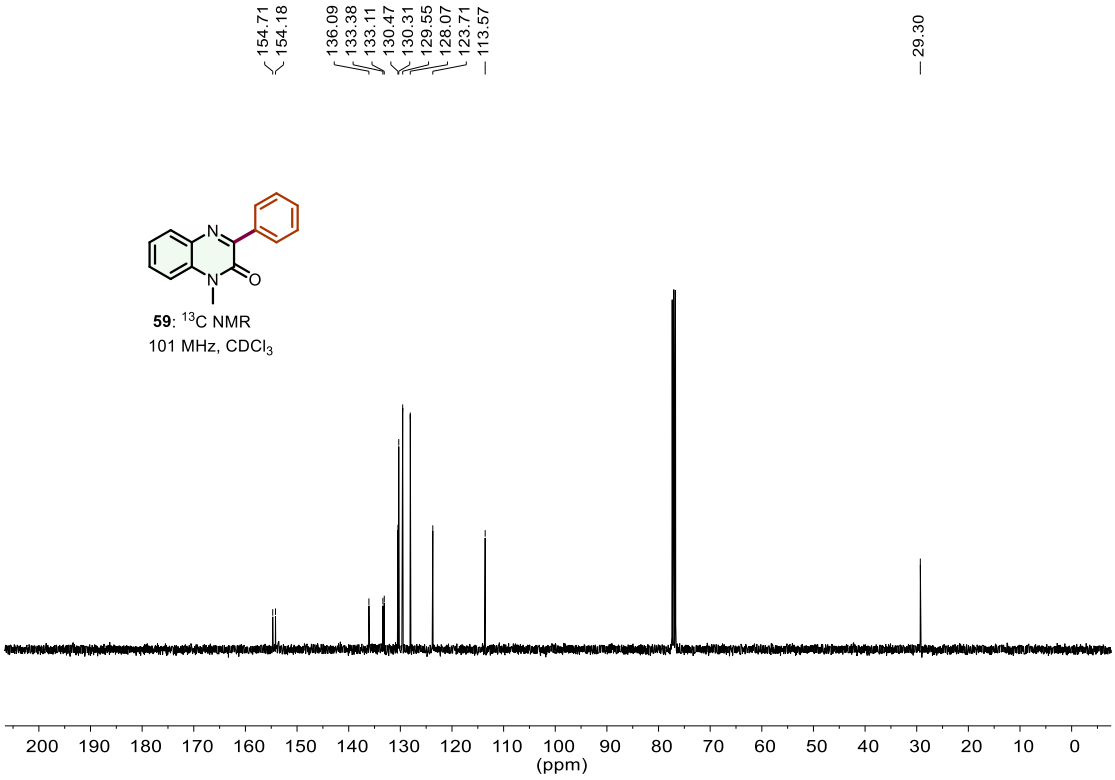
58: ^{1}H NMR
400 MHz, DMSO-d_6

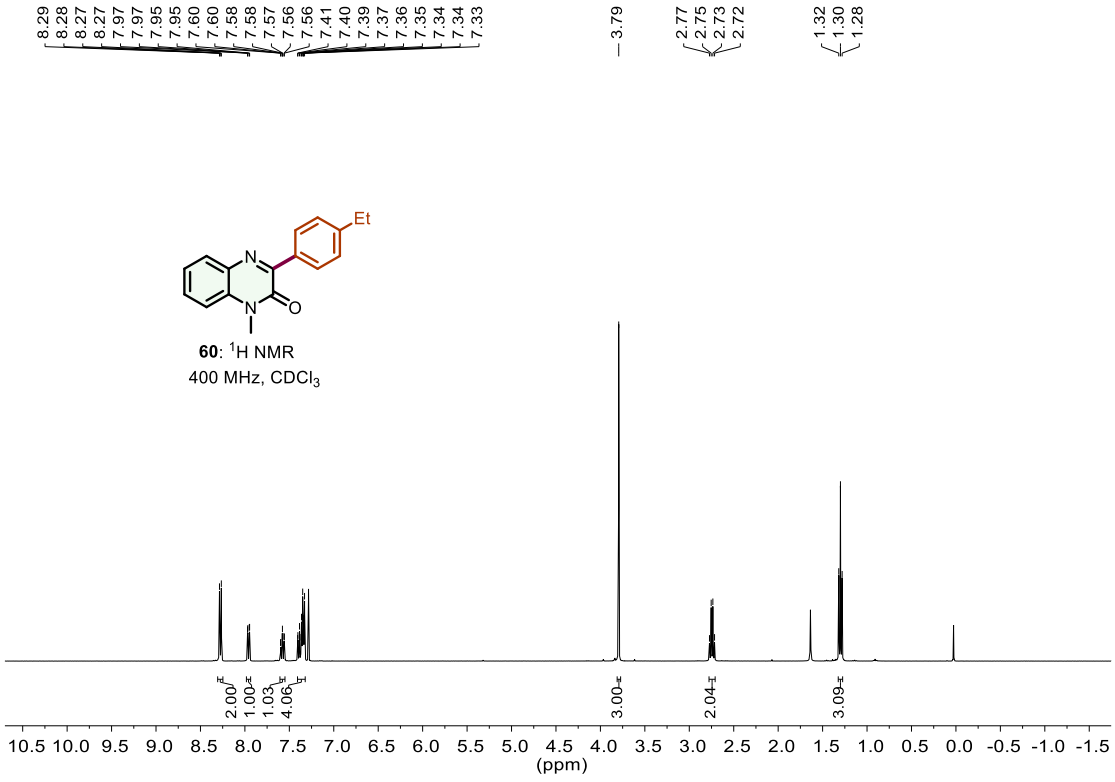


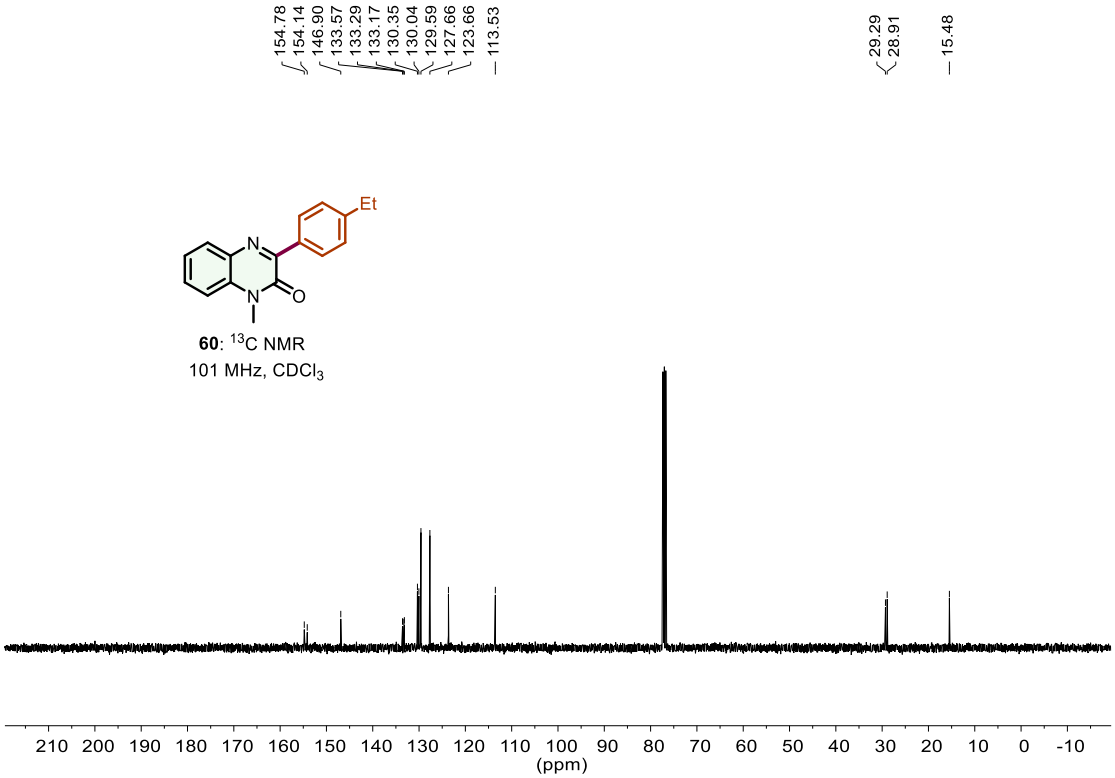
58: ^{13}C NMR
101 MHz, DMSO-d_6



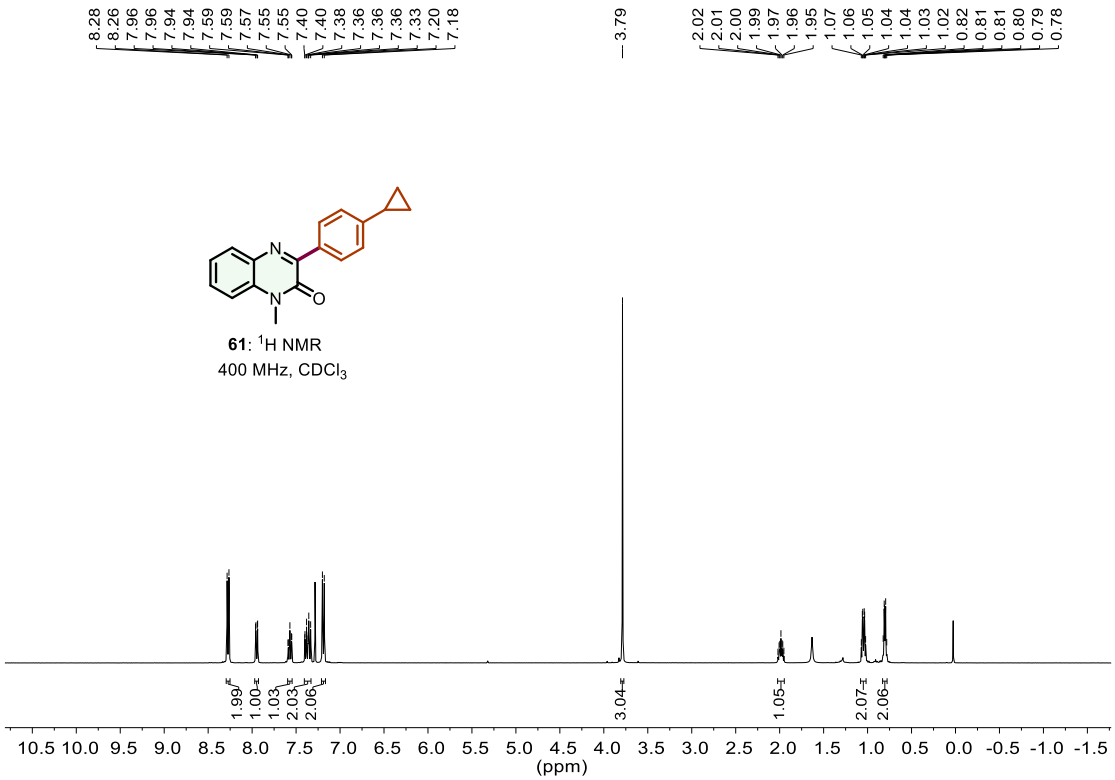
59: ^{1}H NMR
400 MHz, $CDCl_3$


154.71
154.18
136.09
133.38
133.11
130.47
130.31
129.55
128.07
123.71
113.57
29.30
59: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

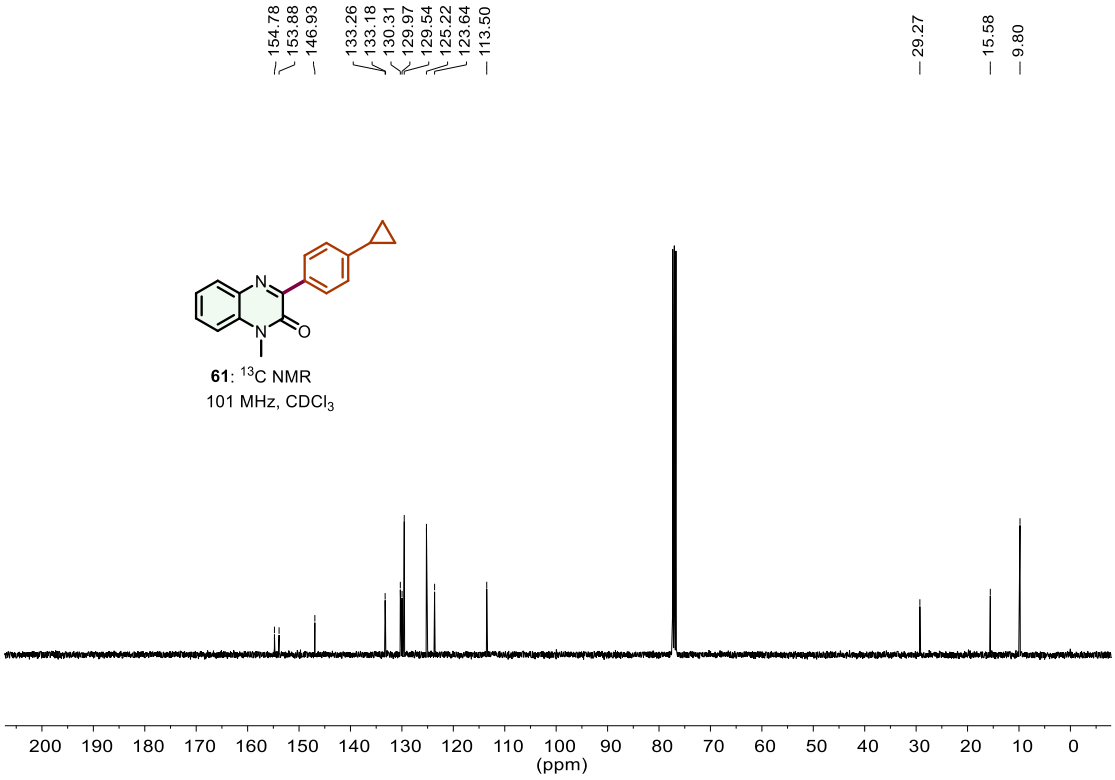

8.29
8.28
8.27
8.27
7.97
7.97
7.95
7.95
7.60
7.58
7.58
7.57
7.56
7.56
7.41
7.40
7.39
7.37
7.36
7.35
7.34
7.34
7.33
3.79
2.77
2.75
2.73
2.72
1.32
1.30
1.28
Et
60: 1H NMR
400 MHz, CDCl3
2.00
1.00
1.03
4.06
3.00
2.04
3.09
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)

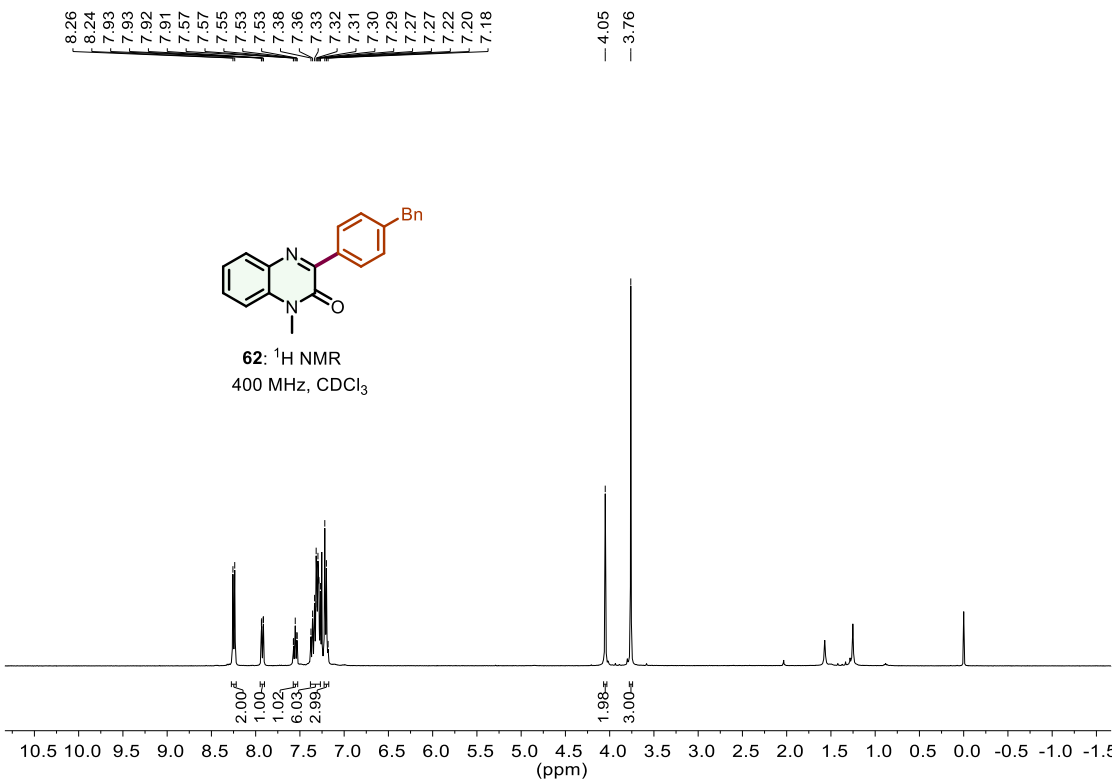


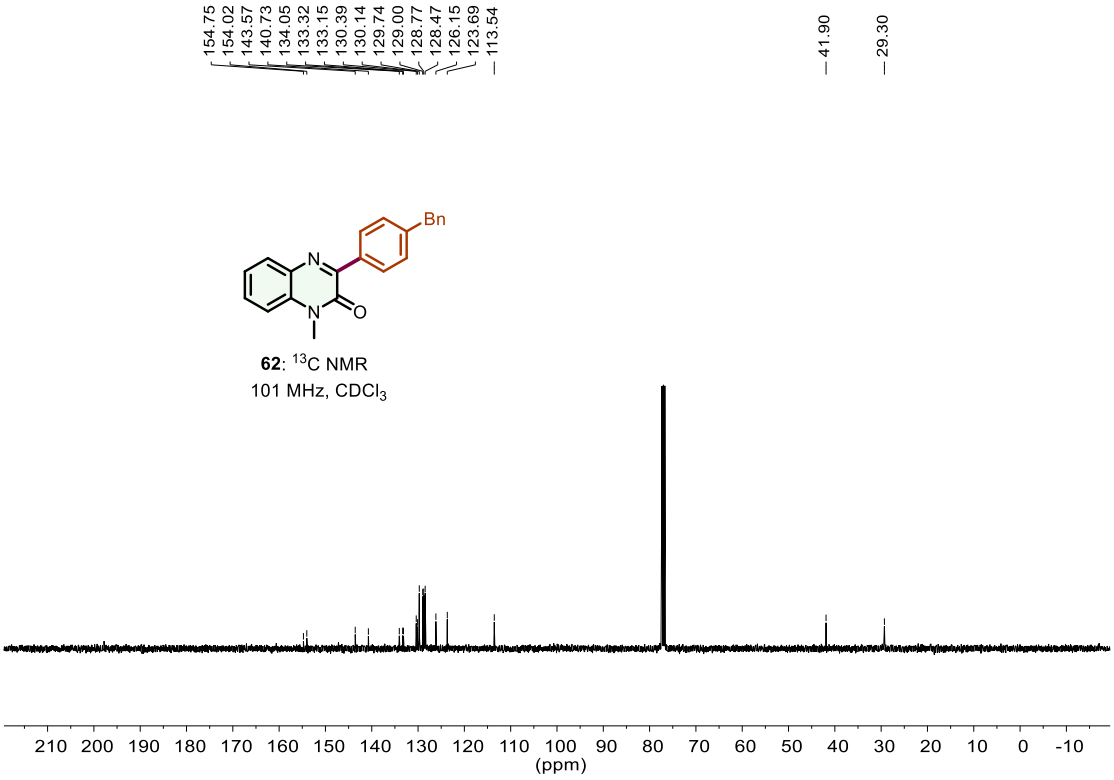
60: ^{13}C NMR
101 MHz, $CDCl_3$



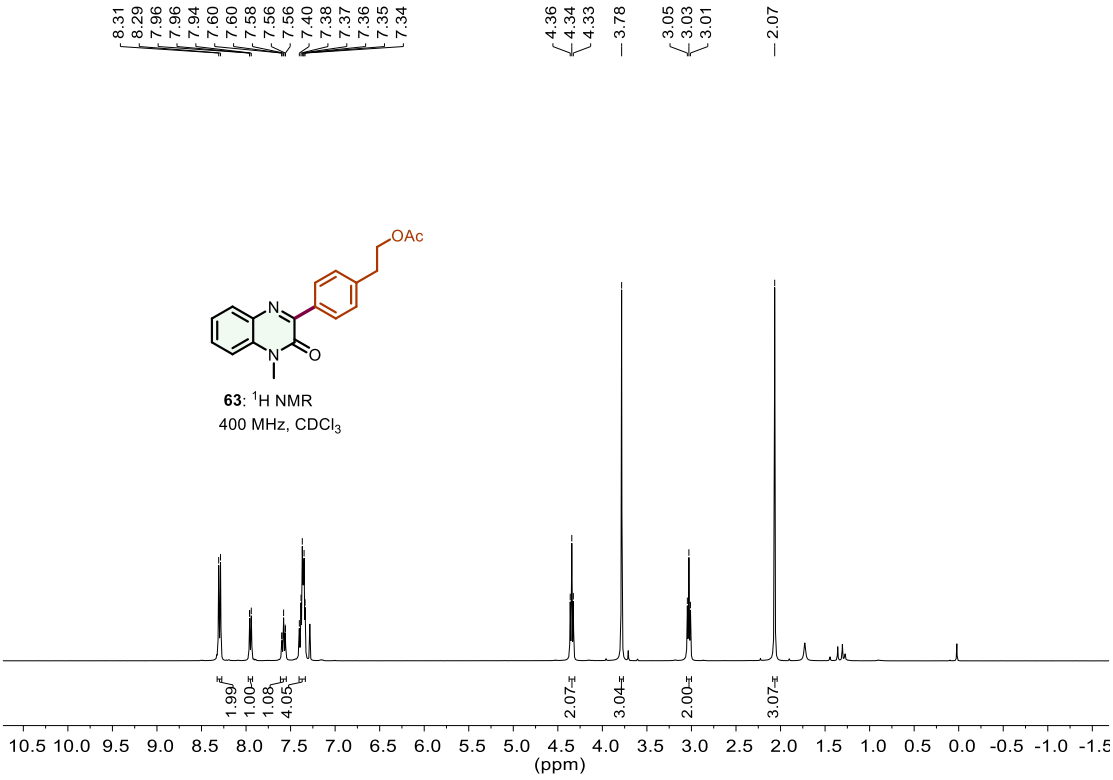
61: ^{1}H NMR
400 MHz, $CDCl_3$


154.78
153.88
146.93
133.26
133.18
130.31
129.97
129.54
125.22
123.64
113.50
29.27
15.58
9.80
61: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

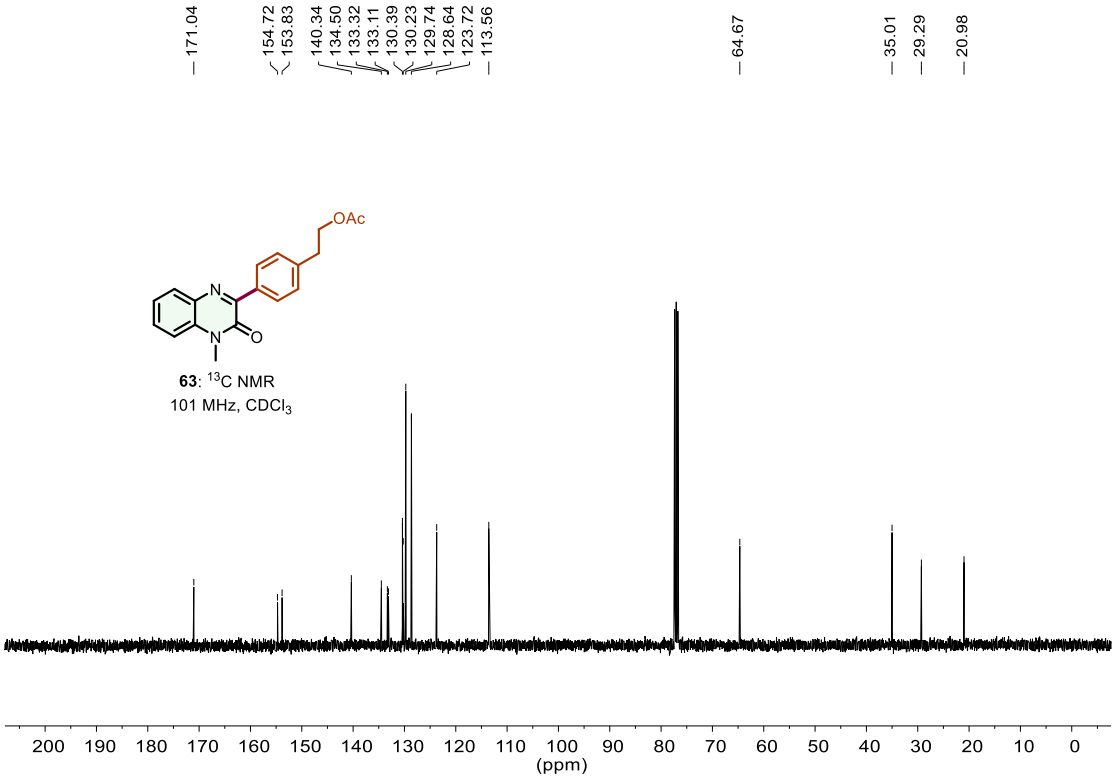

8.26
8.24
7.93
7.93
7.92
7.91
7.57
7.57
7.55
7.53
7.53
7.38
7.36
7.33
7.32
7.31
7.30
7.29
7.27
7.27
7.22
7.20
7.18
4.05
3.76
Bn
62: 1H NMR
400 MHz, CDCl3
2.00
1.00
1.02
6.03
2.99
1.98
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
(ppm)

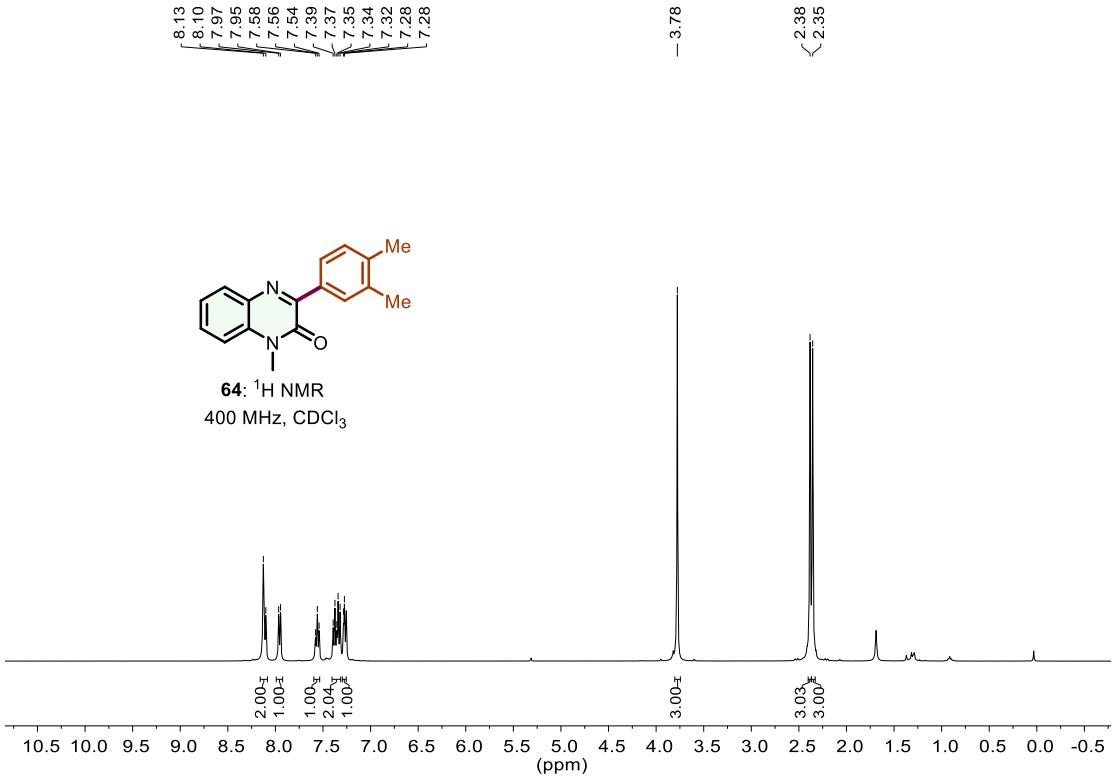


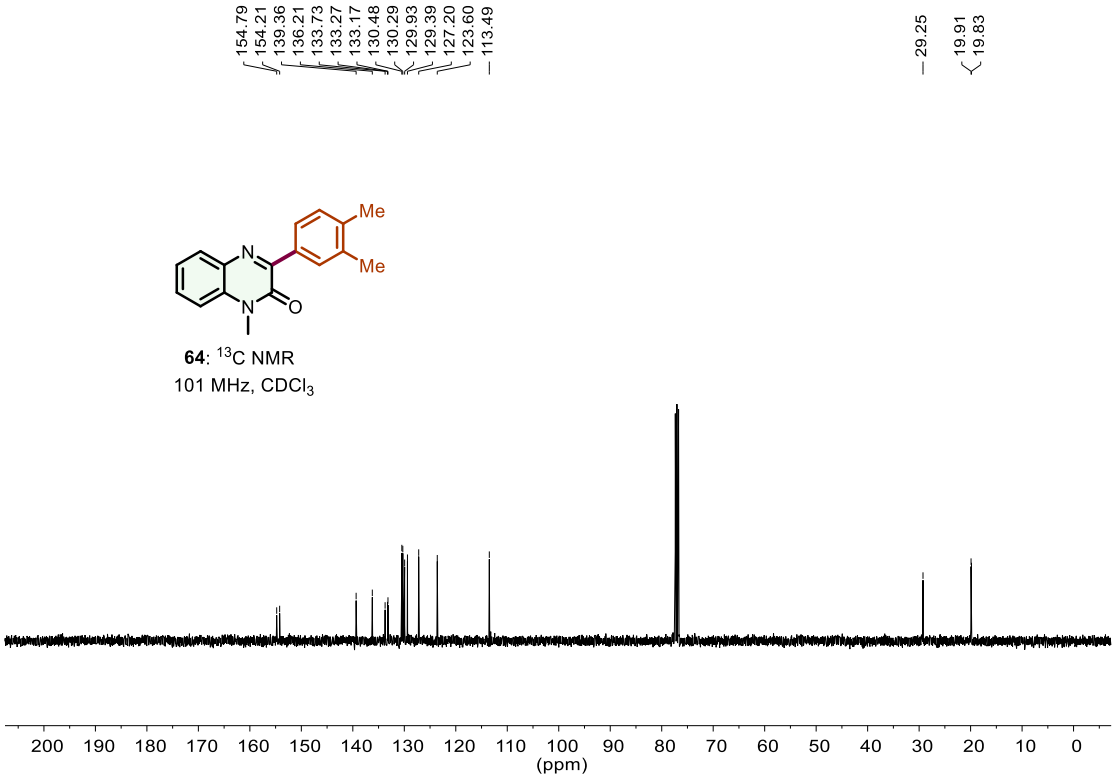
62: ^{13}C NMR
101 MHz, $CDCl_3$



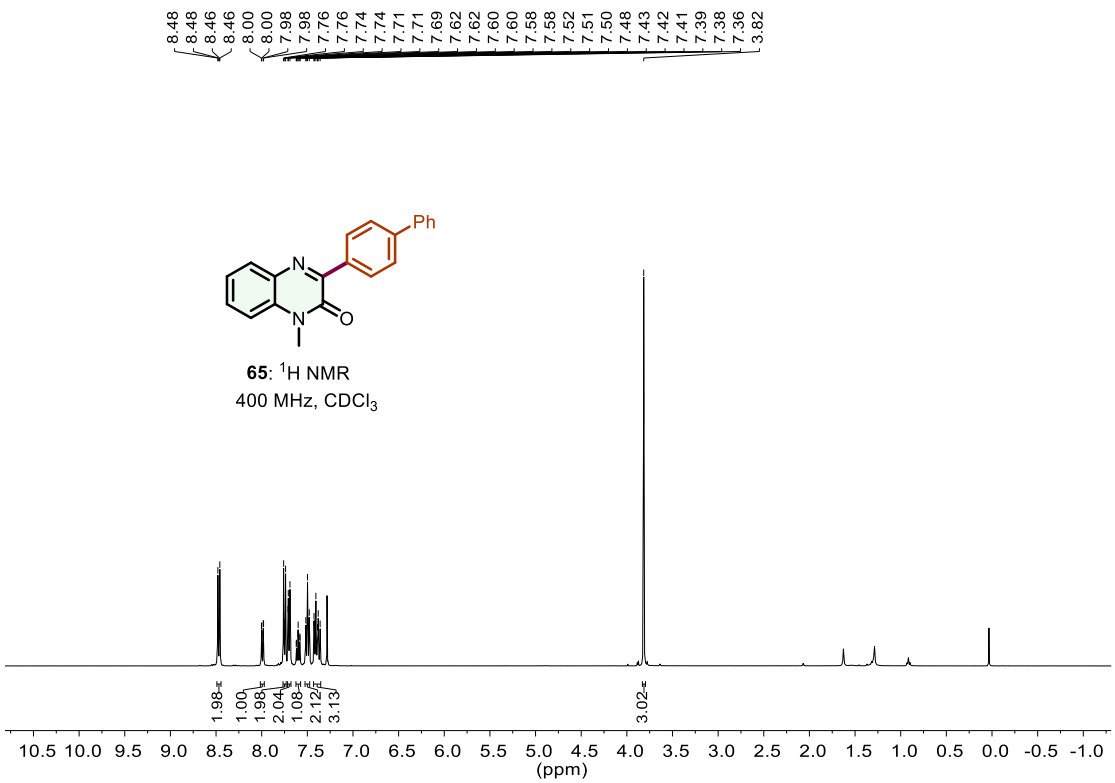
63: ^{1}H NMR
400 MHz, $CDCl_3$


171.04
154.72
153.83
140.34
134.50
133.32
133.11
130.39
130.23
129.74
128.64
123.72
113.56
64.67
35.01
29.29
20.98
OAc
N
N
O
63: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

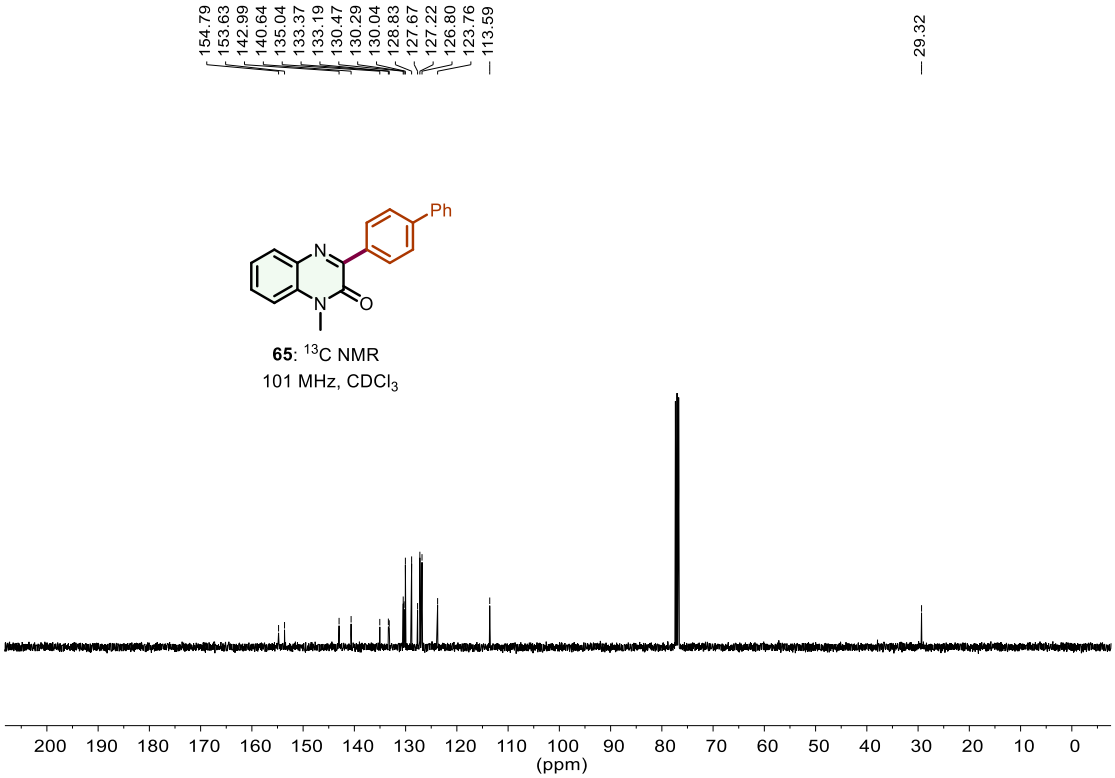

8.13
8.10
7.97
7.95
7.58
7.56
7.54
7.39
7.37
7.35
7.34
7.32
7.28
7.28
3.78
2.38
2.35
Me
Me
N
N
O
64: 1H NMR
400 MHz, CDCl3
2.00
1.00
1.00
2.04
1.00
3.00
3.03
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)



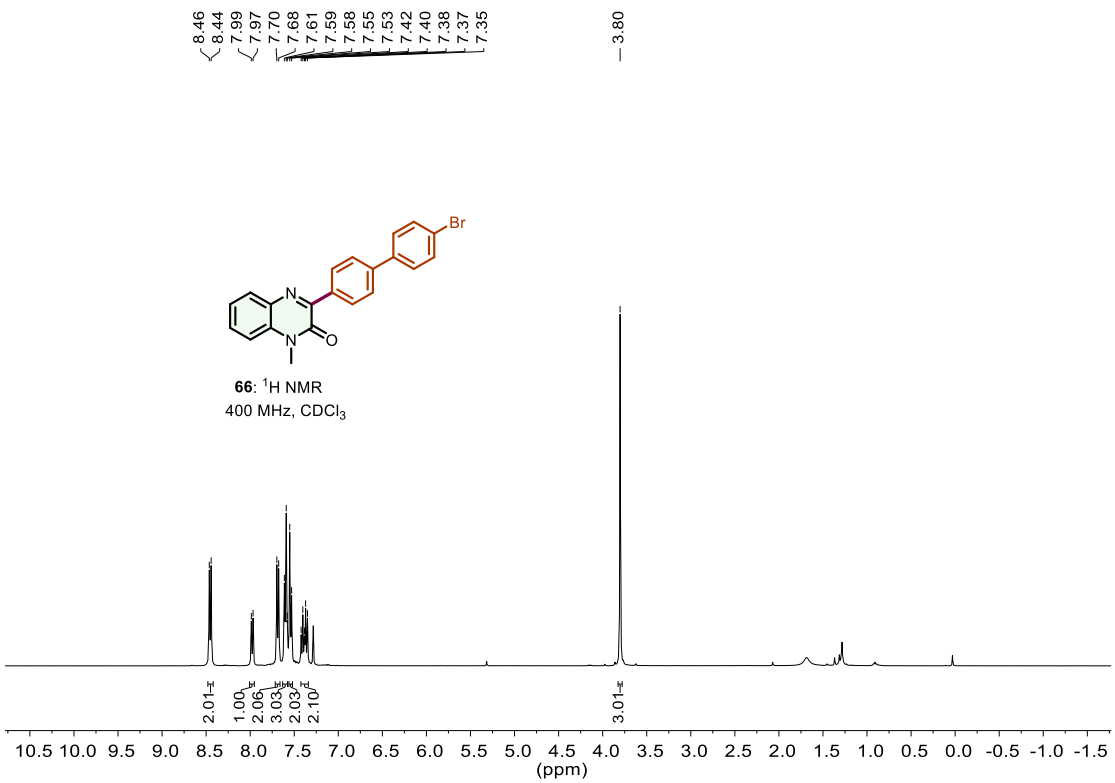
64: ^{13}C NMR
101 MHz, $CDCl_3$



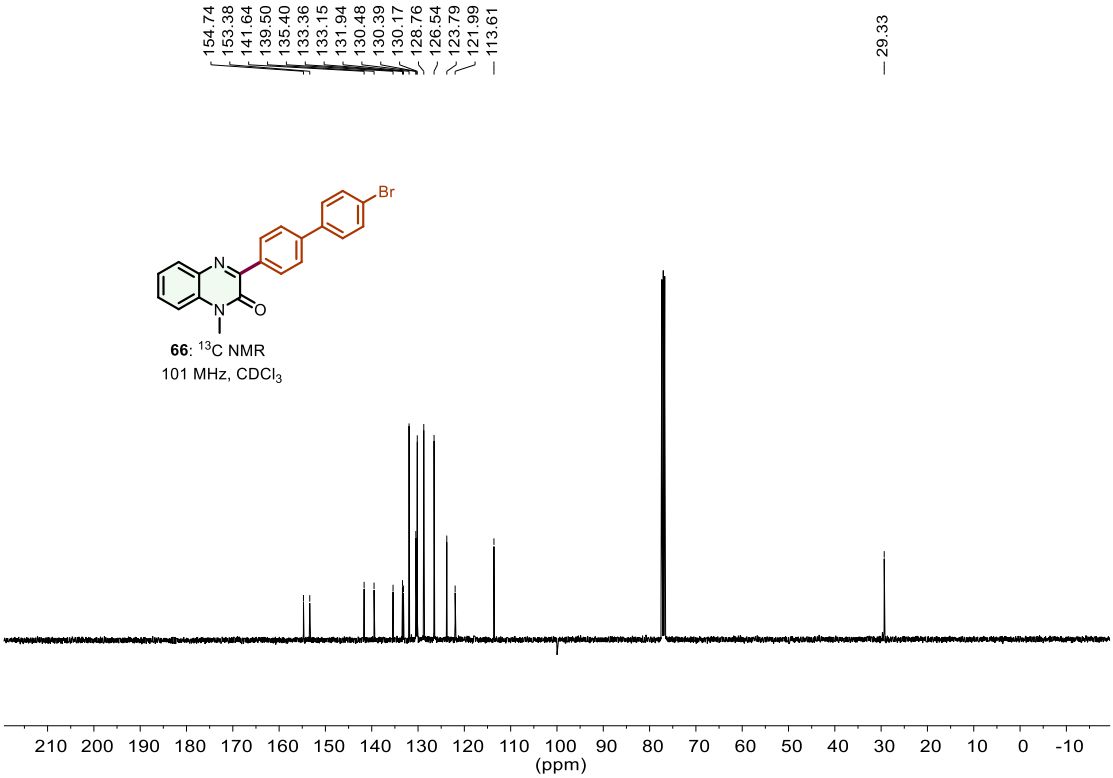
65: ^{1}H NMR
400 MHz, $CDCl_3$



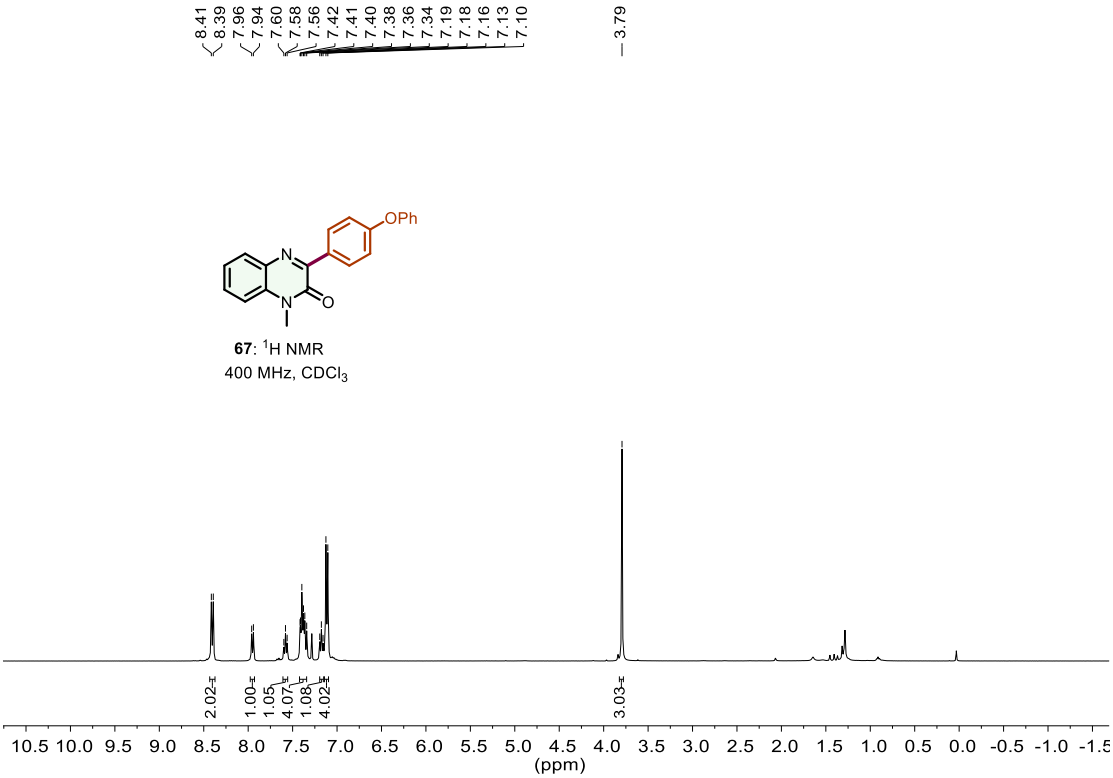
65: ^{13}C NMR
101 MHz, $CDCl_3$



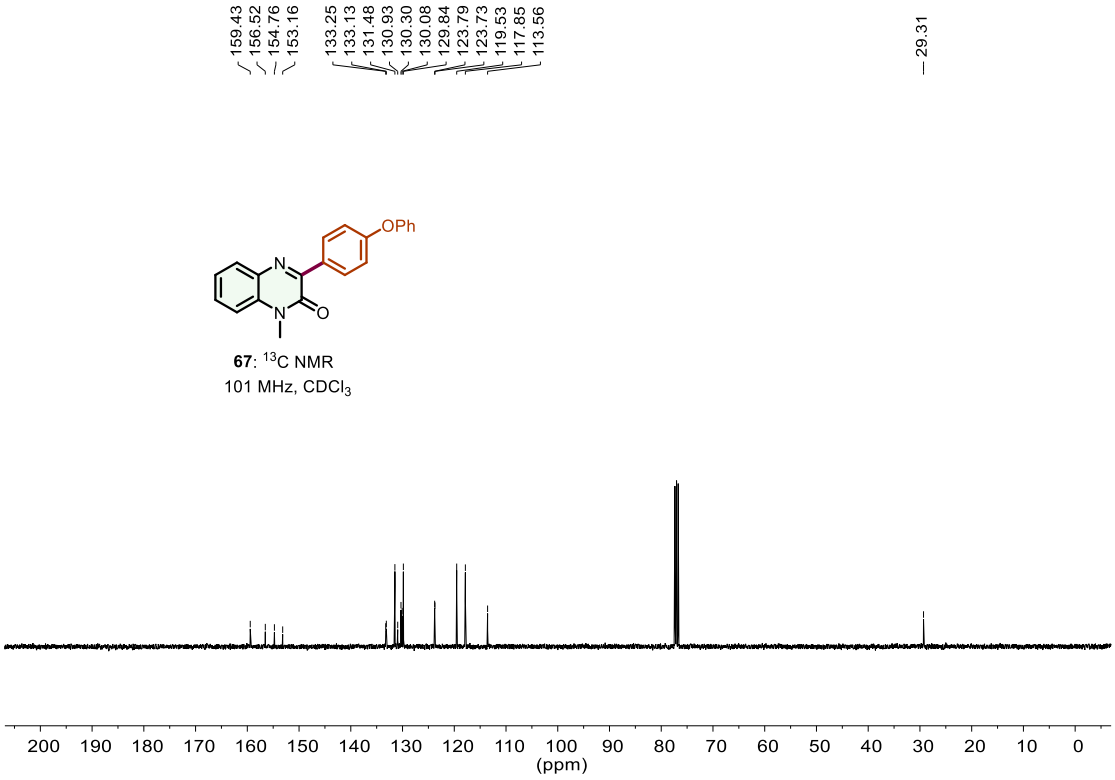
66: ^{1}H NMR
400 MHz, $CDCl_3$



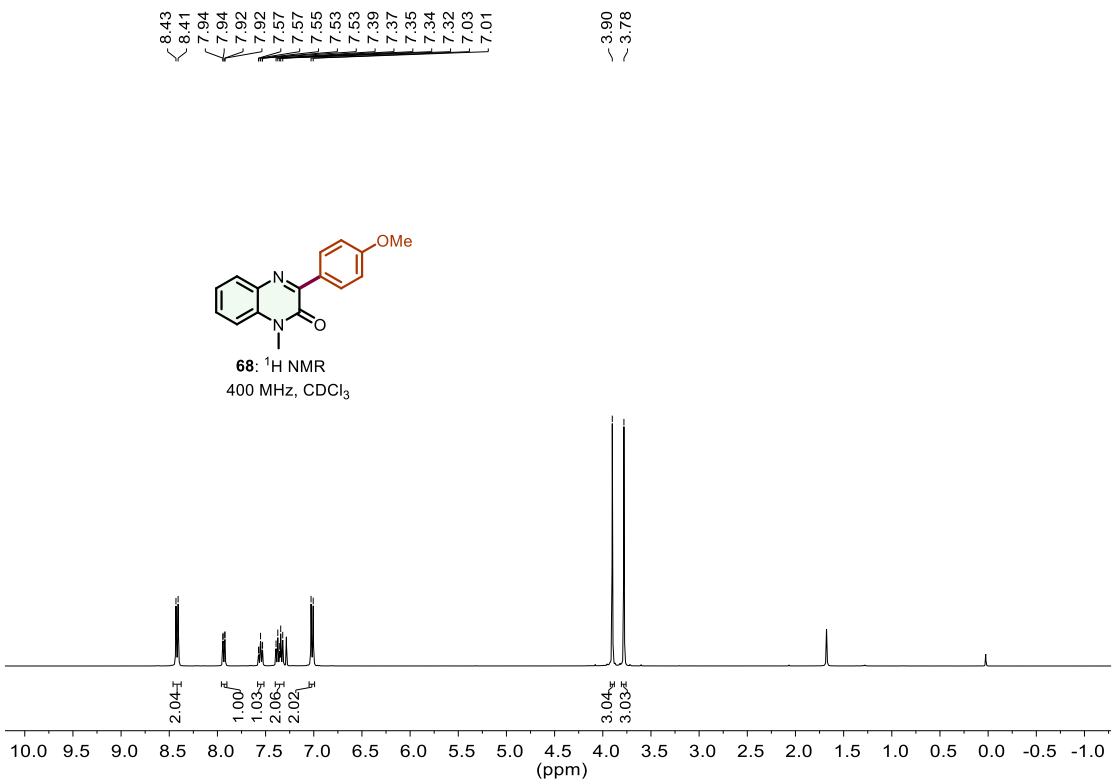
66: ^{13}C NMR
101 MHz, $CDCl_3$



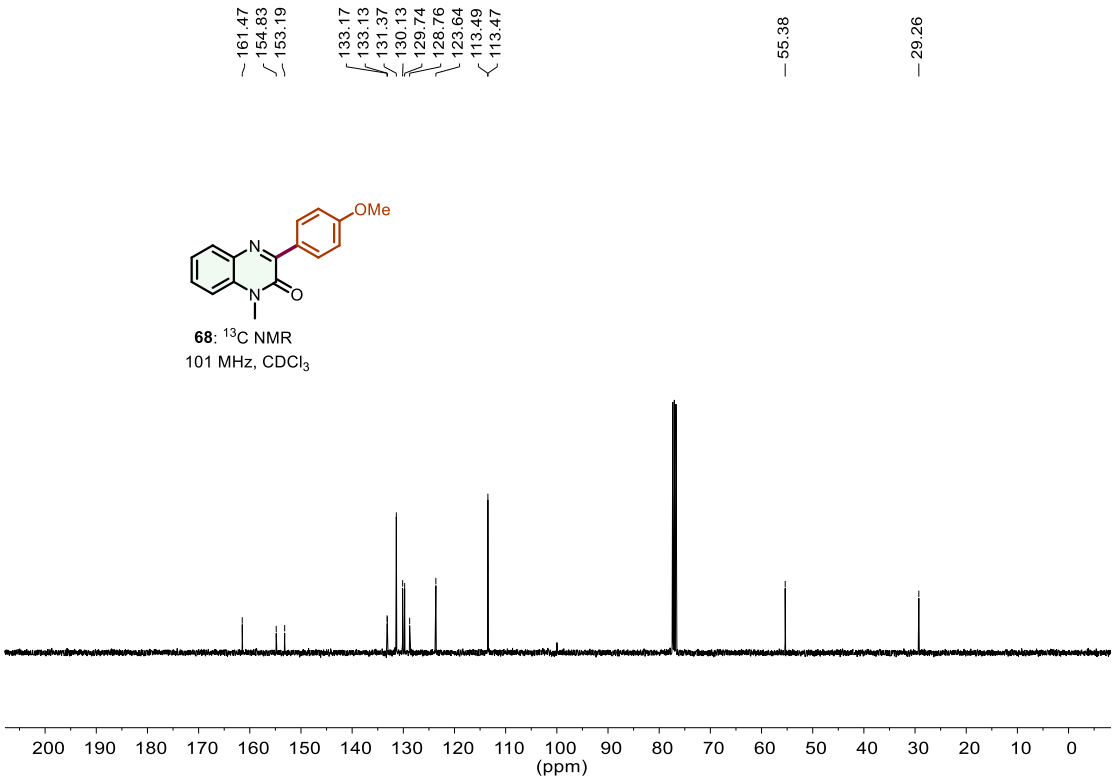
67: ^{1}H NMR
400 MHz, $CDCl_3$



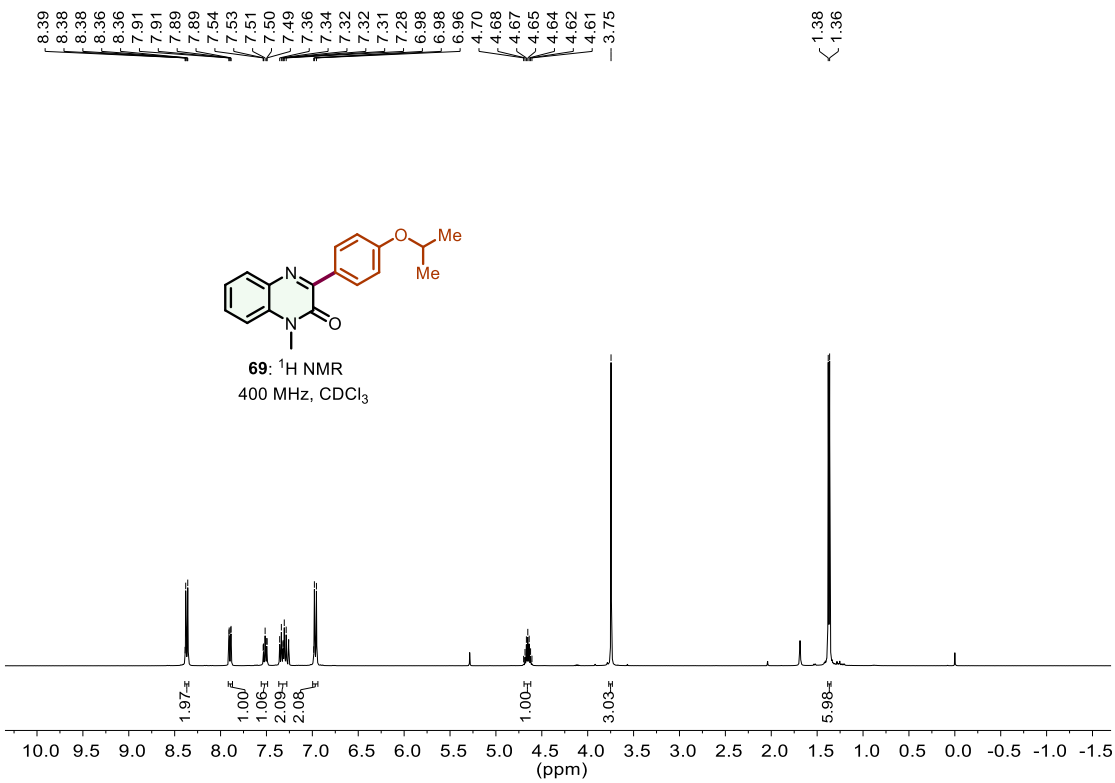
67: ^{13}C NMR
101 MHz, $CDCl_3$



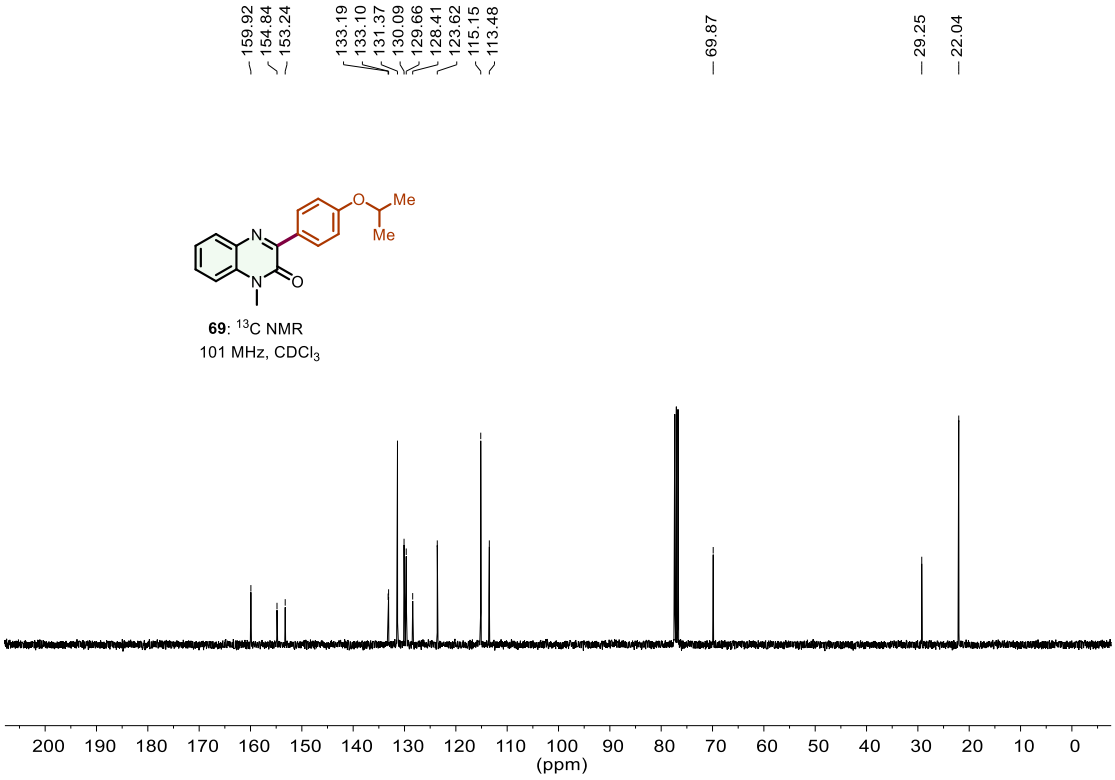
68: ^{1}H NMR
400 MHz, $CDCl_3$



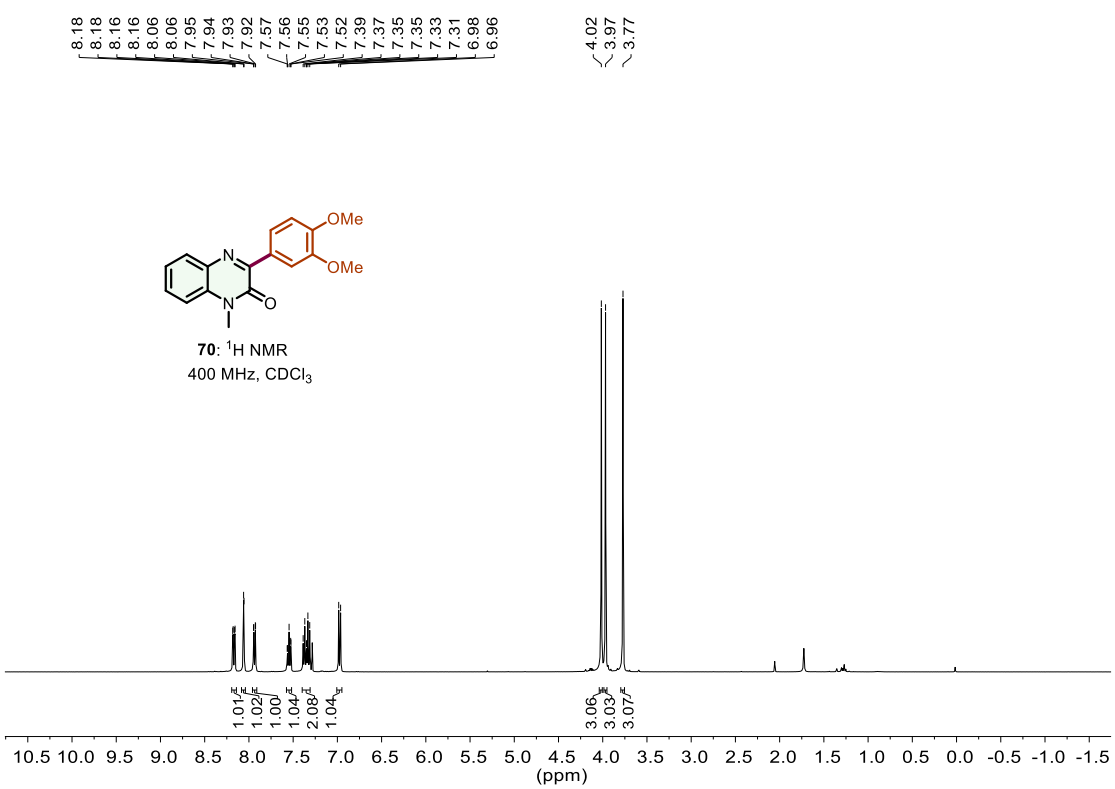
68: ^{13}C NMR
101 MHz, $CDCl_3$



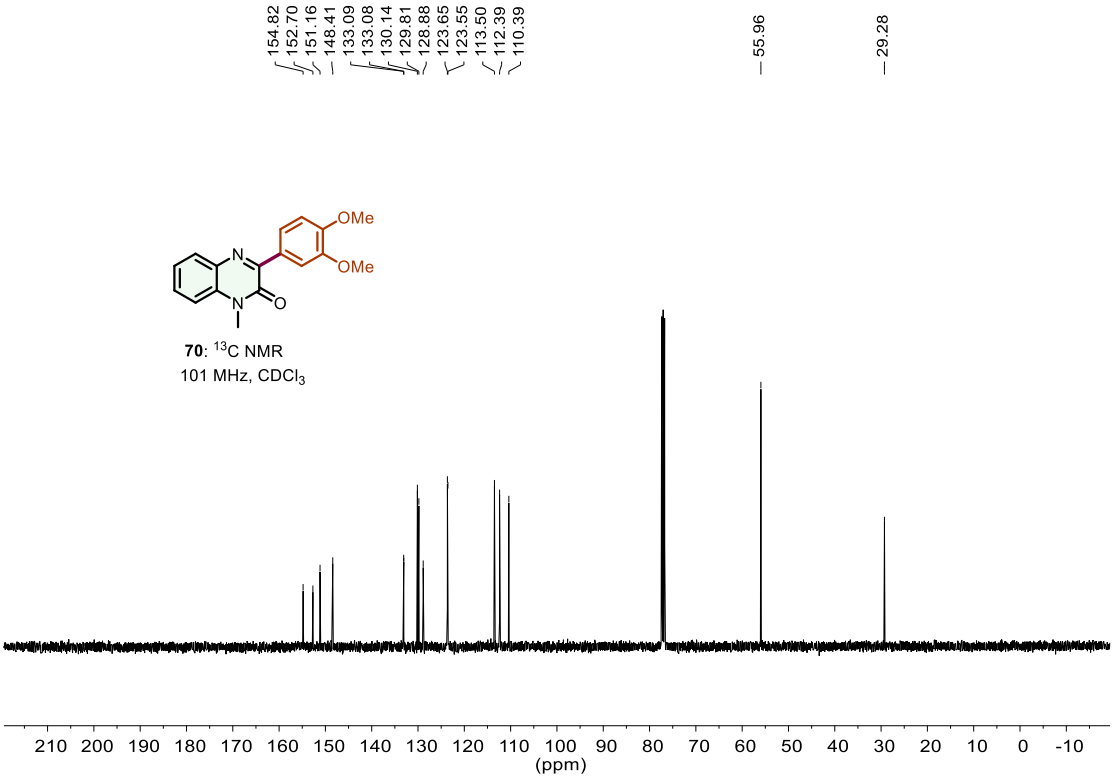
69: ^{1}H NMR
400 MHz, $CDCl_3$



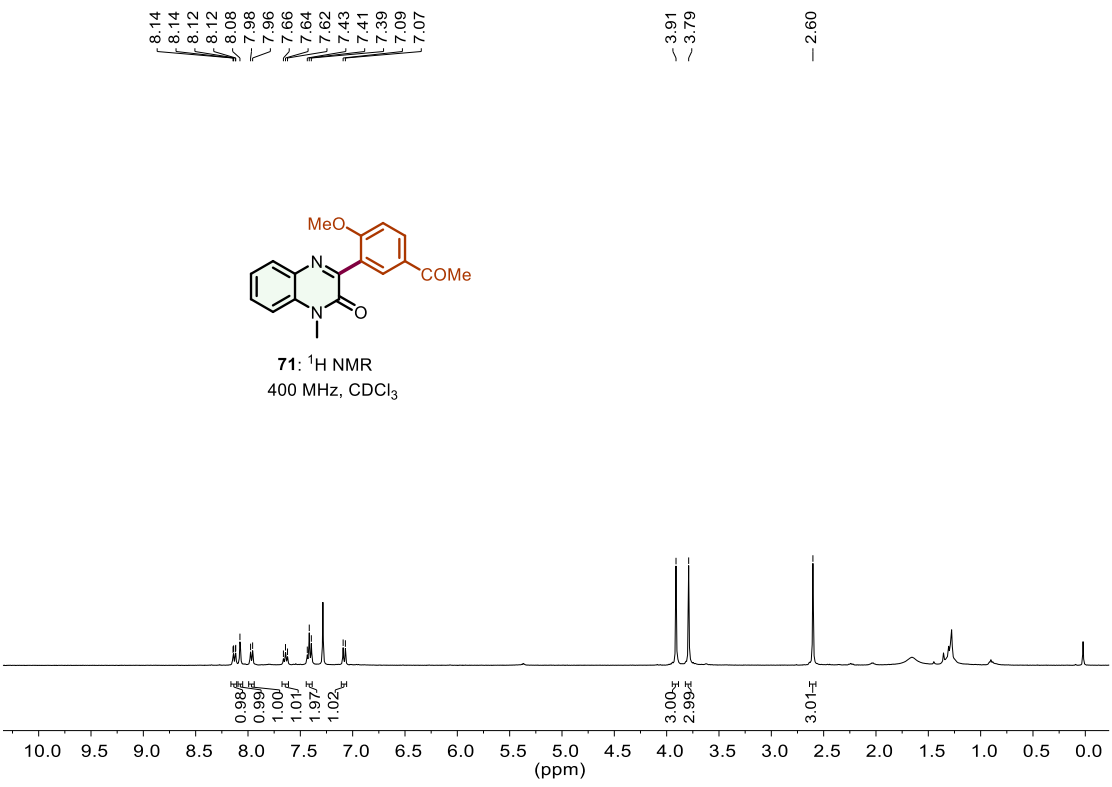
69: ^{13}C NMR
101 MHz, $CDCl_3$



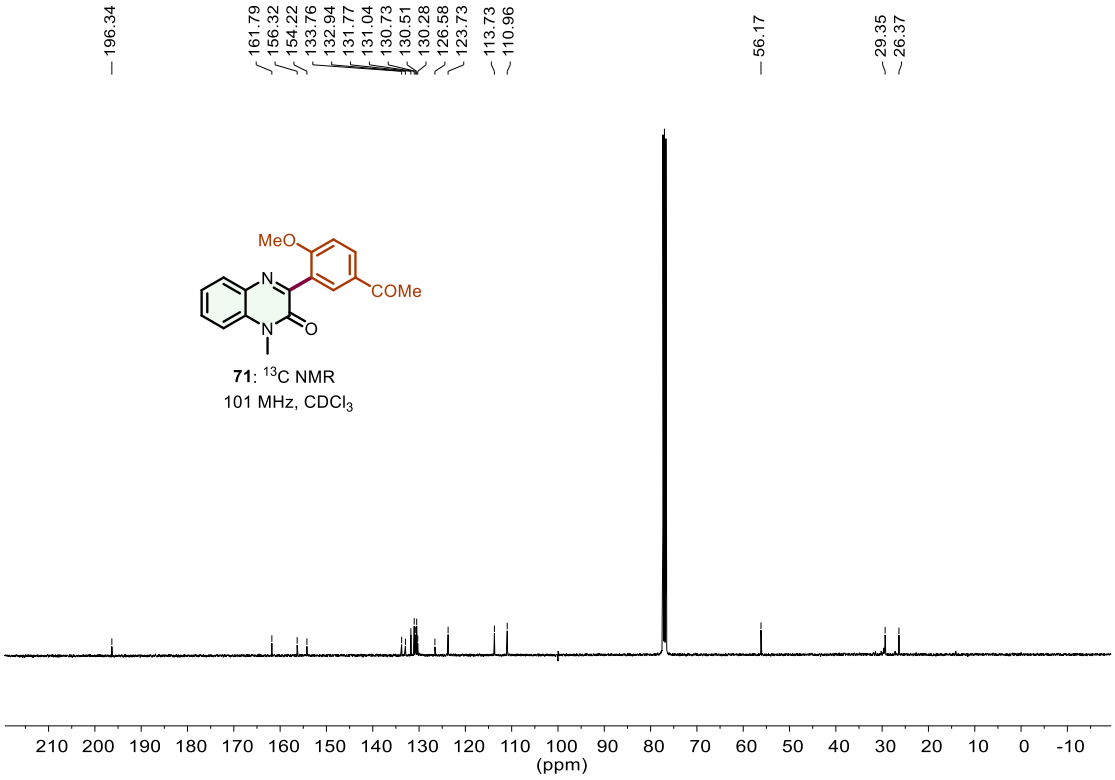
70: ^{1}H NMR
400 MHz, $CDCl_3$



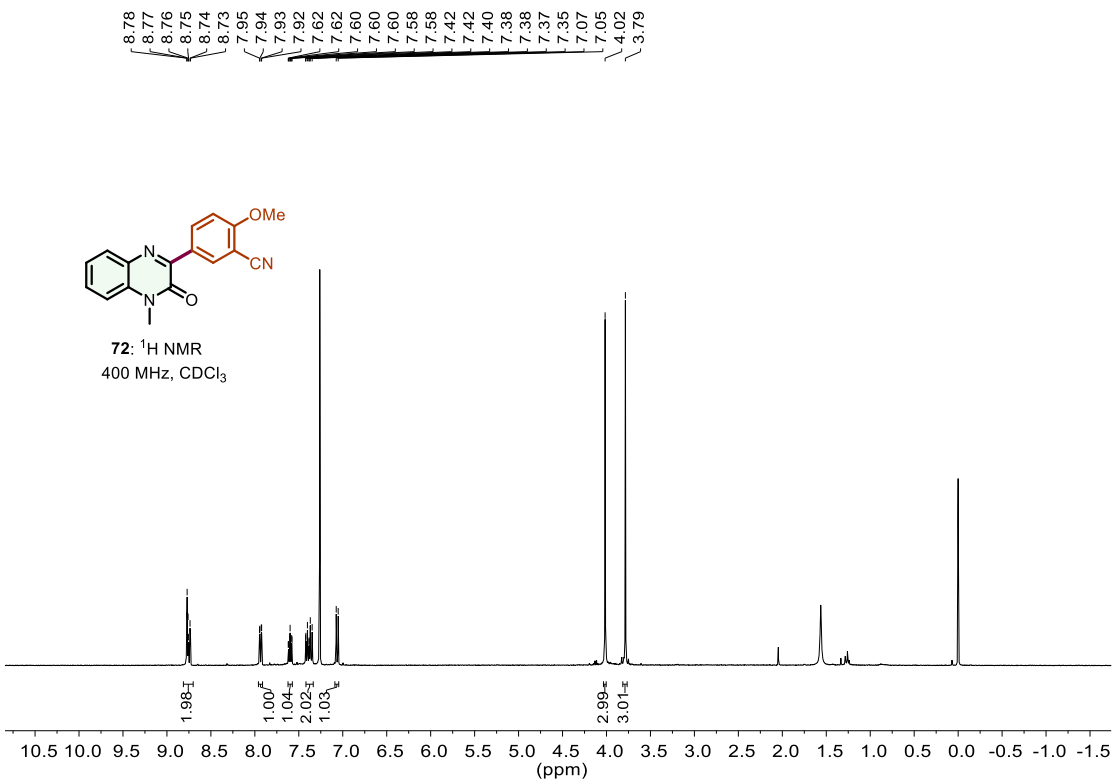
70: ^{13}C NMR
101 MHz, $CDCl_3$



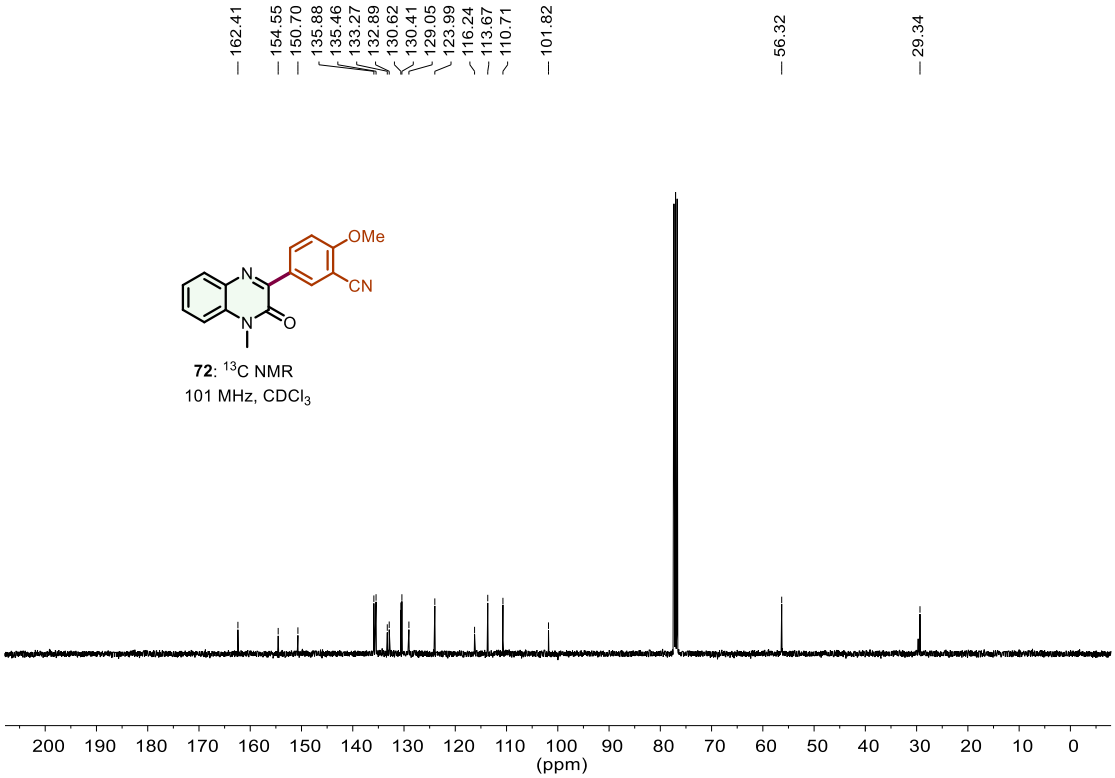
71: ^{1}H NMR
400 MHz, $CDCl_3$



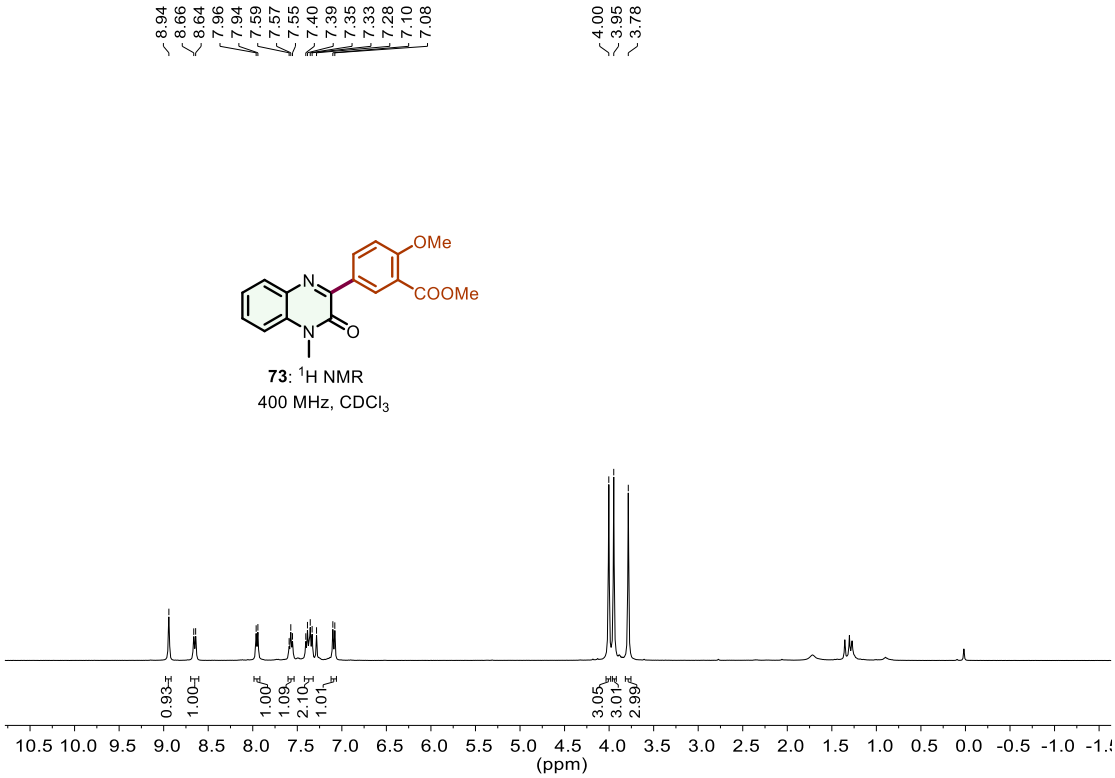
71: ^{13}C NMR
101 MHz, $CDCl_3$



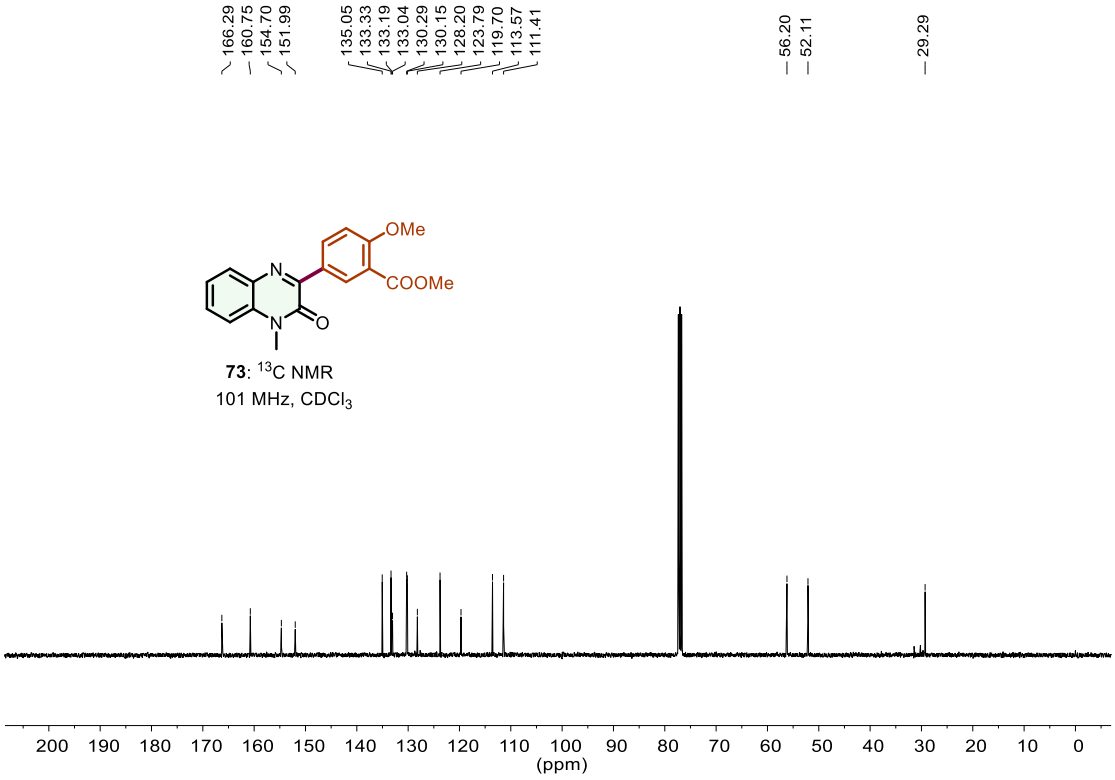
72: ^{1}H NMR
400 MHz, $CDCl_3$



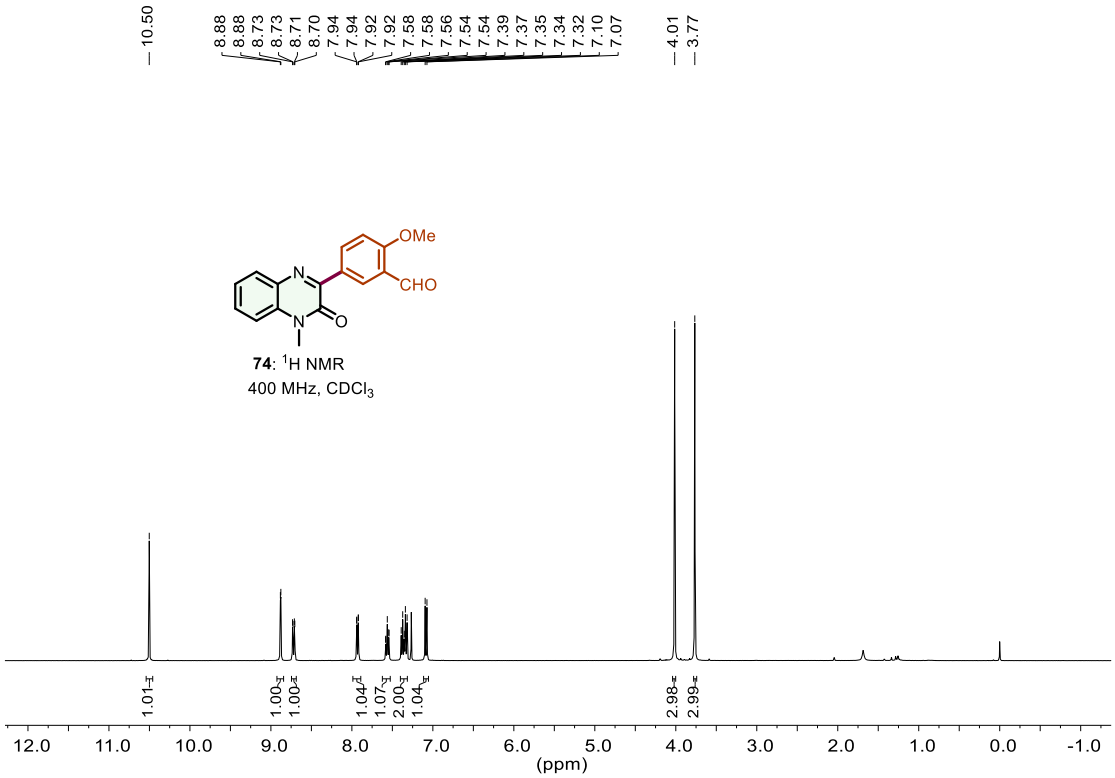
72: ^{13}C NMR
101 MHz, $CDCl_3$



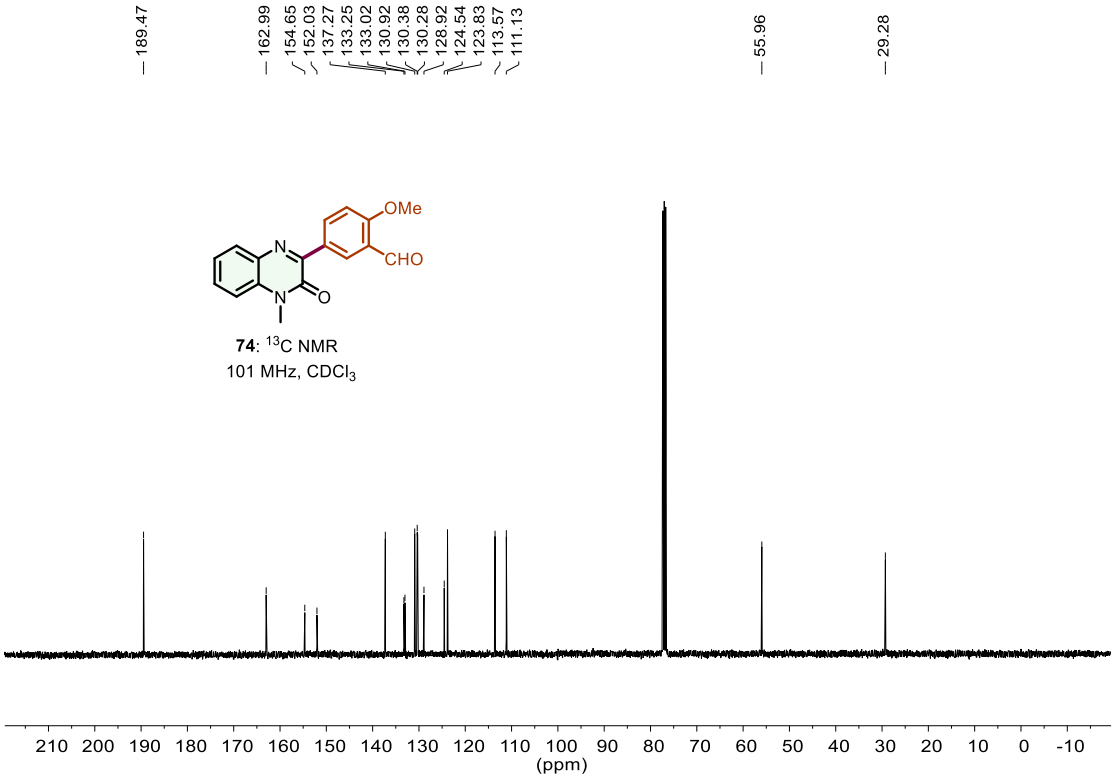
73: ^{1}H NMR
400 MHz, $CDCl_3$



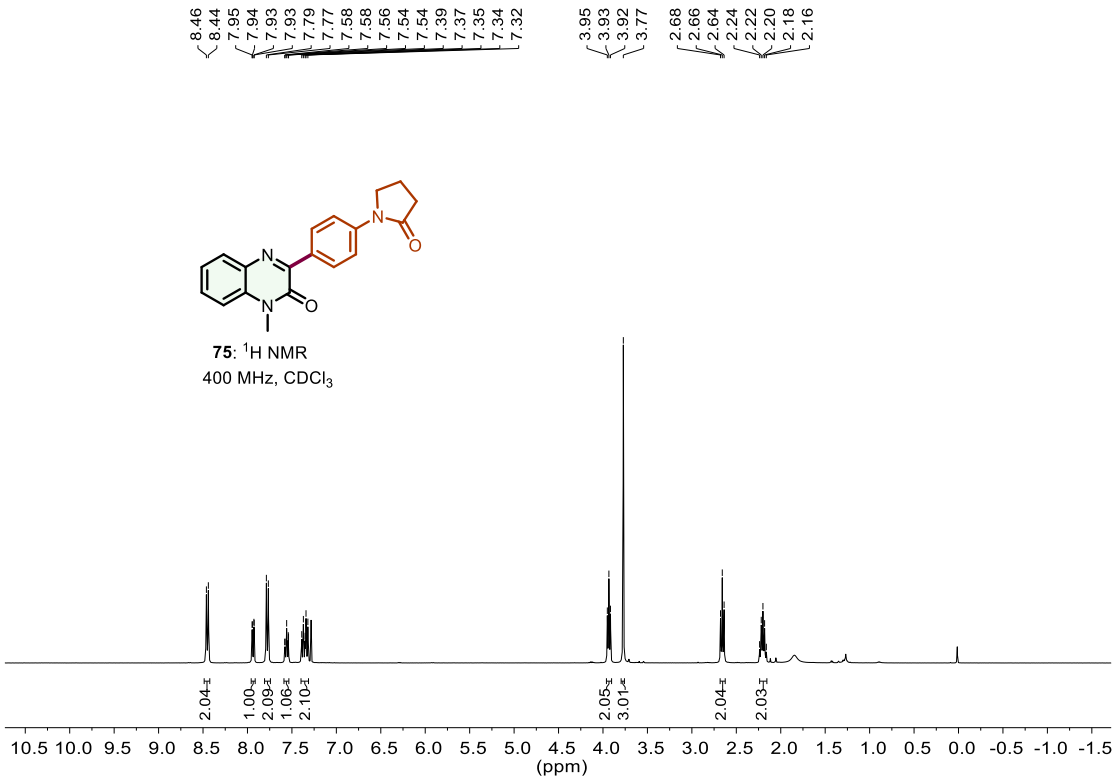
73: ^{13}C NMR
101 MHz, $CDCl_3$



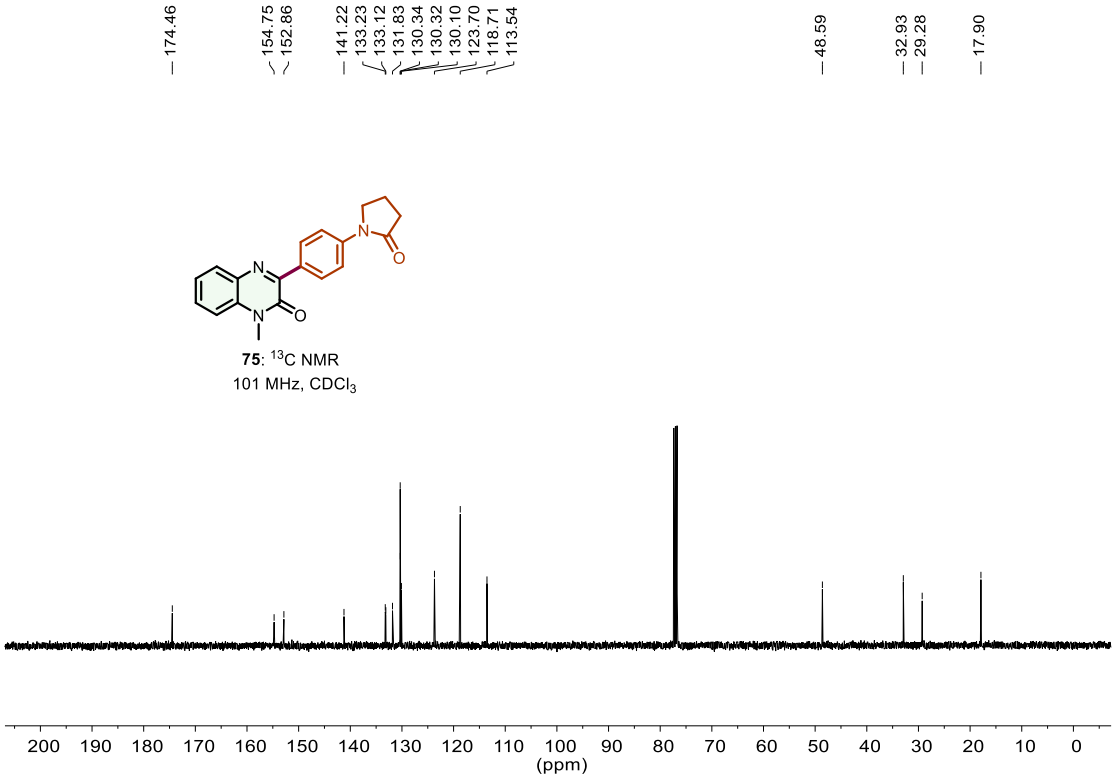
74: ^{1}H NMR
400 MHz, $CDCl_3$

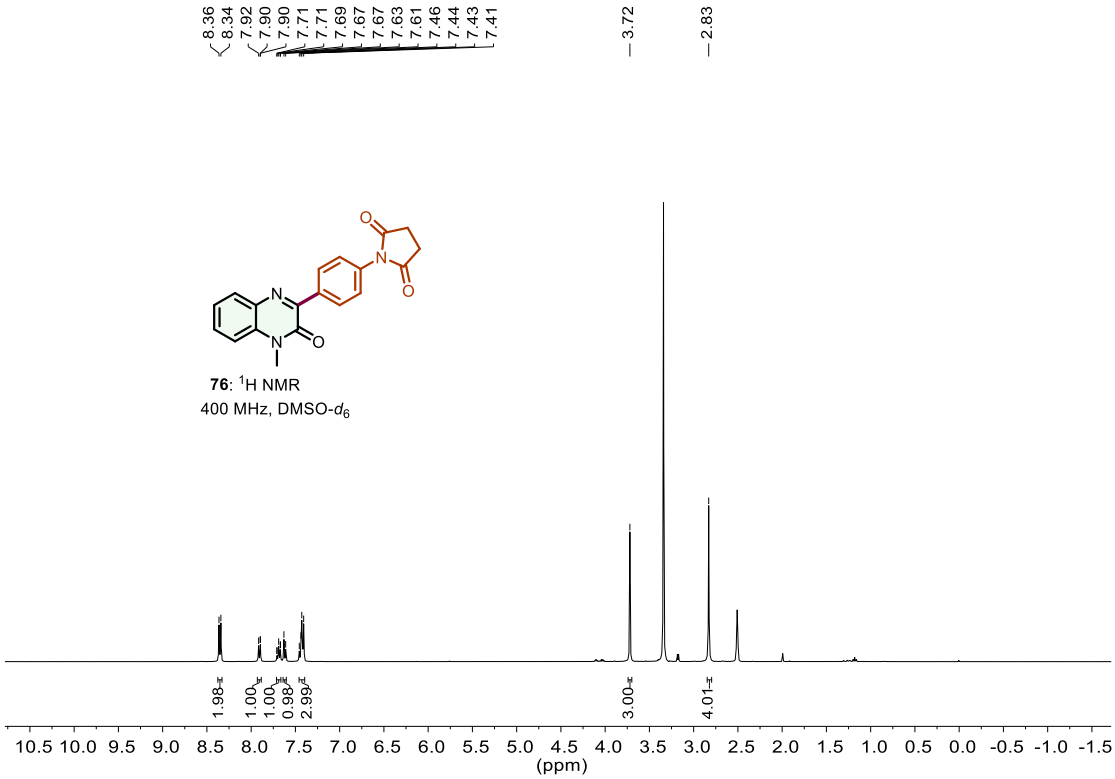


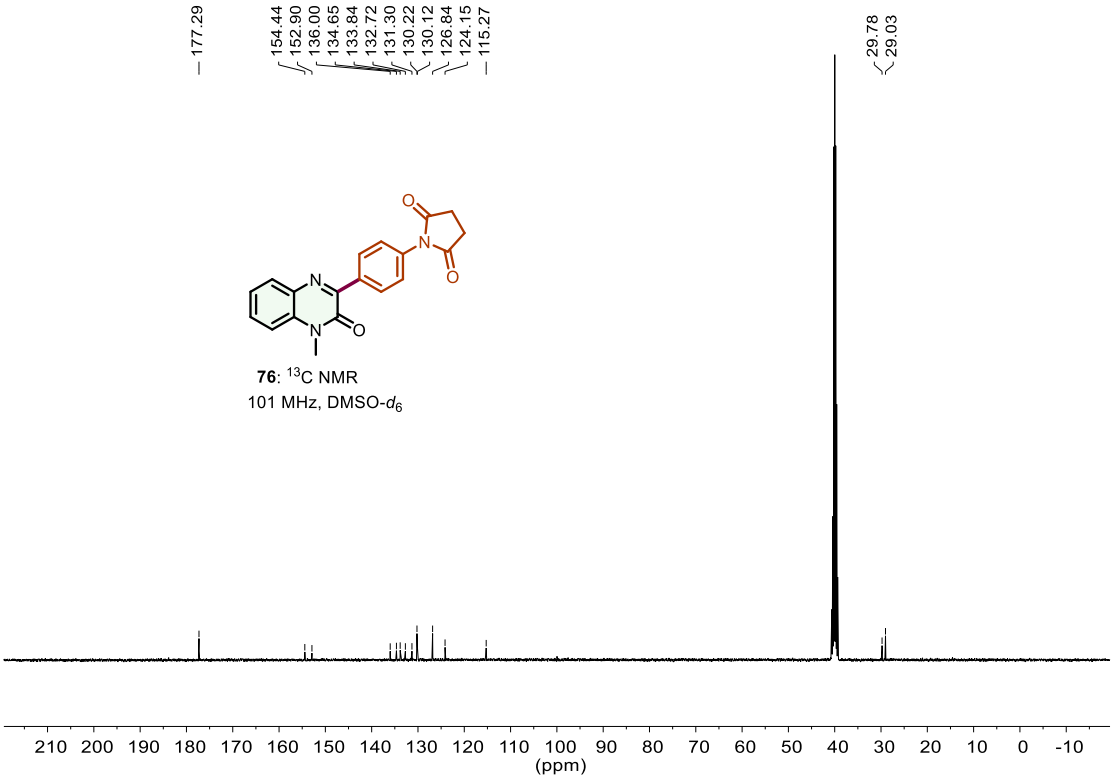
74: ^{13}C NMR
101 MHz, $CDCl_3$



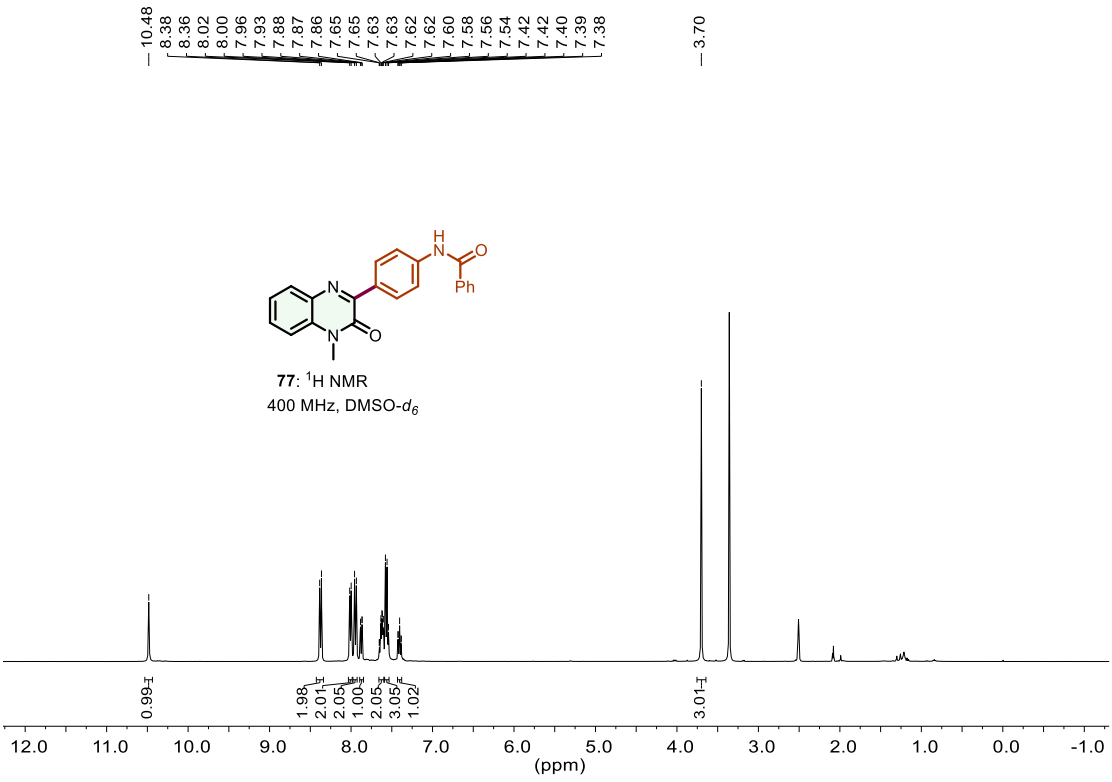
75: ^{1}H NMR
400 MHz, $CDCl_3$


174.46
154.75
152.86
141.22
133.23
133.12
131.83
130.34
130.32
130.10
123.70
118.71
113.54
48.59
32.93
29.28
17.90
75: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

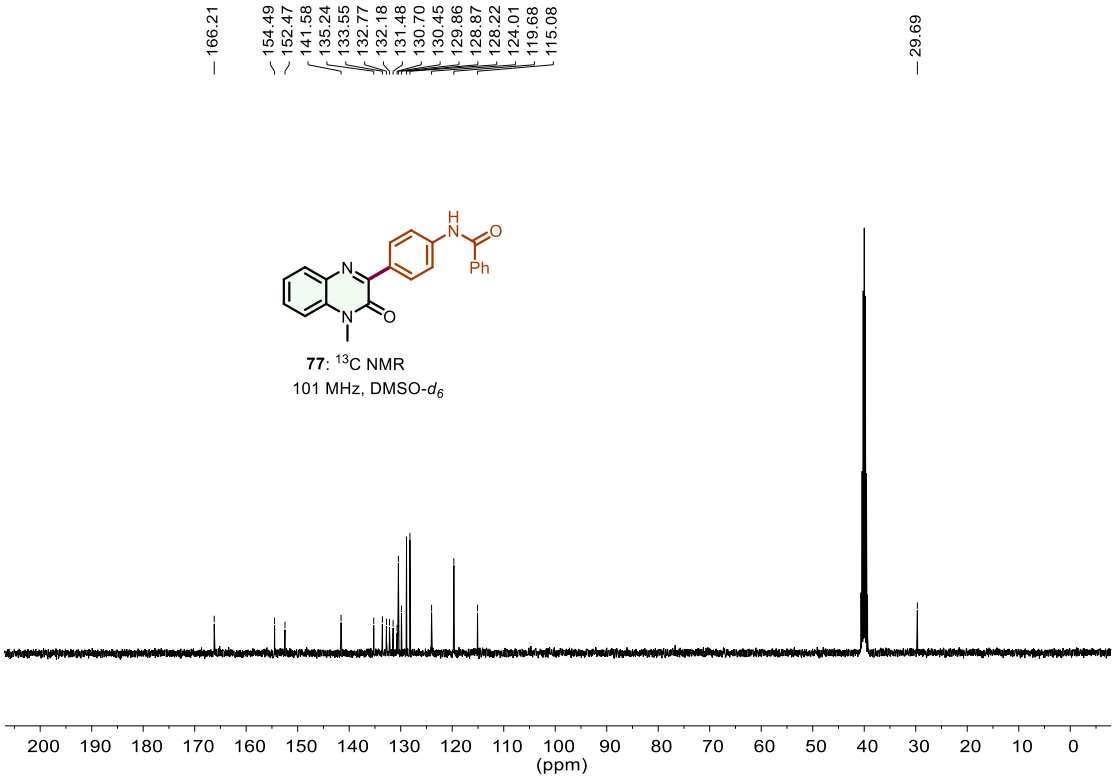

8.36
8.34
7.92
7.90
7.90
7.71
7.71
7.69
7.67
7.67
7.63
7.61
7.46
7.44
7.43
7.41
3.72
2.83
76: 1H NMR
400 MHz, DMSO-d6
1.98
1.00
1.00
0.98
2.99
3.00
4.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)



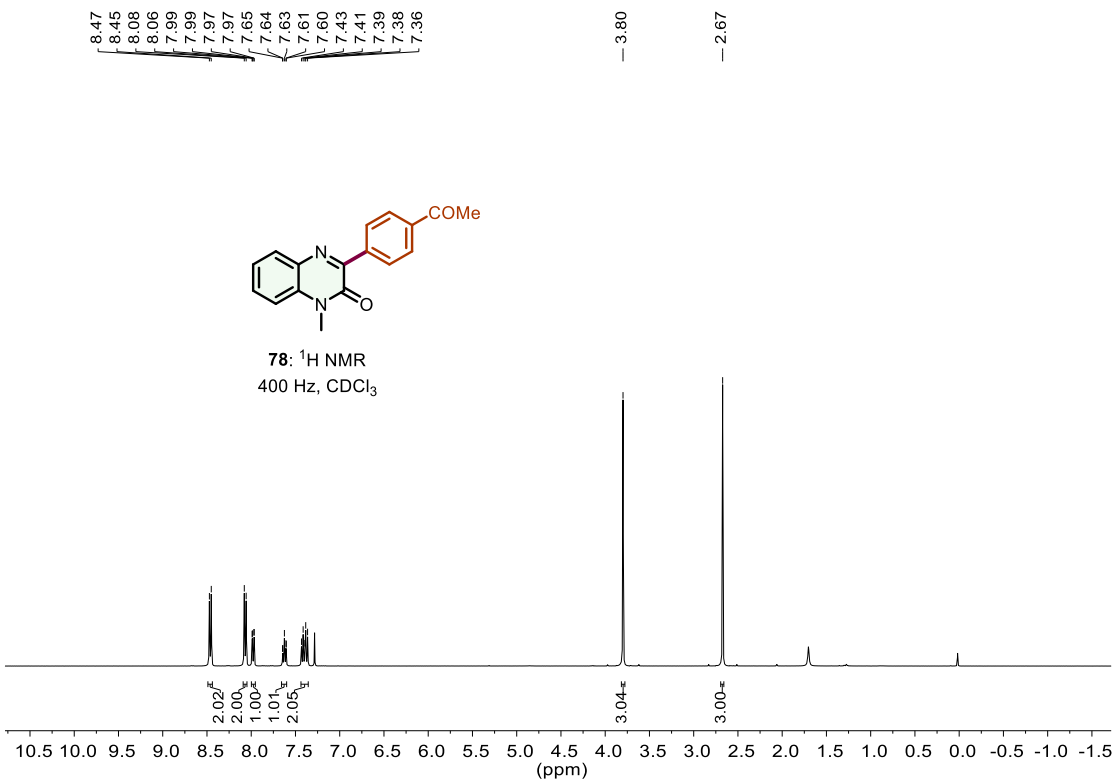
76: ^{13}C NMR
101 MHz, DMSO-d_6



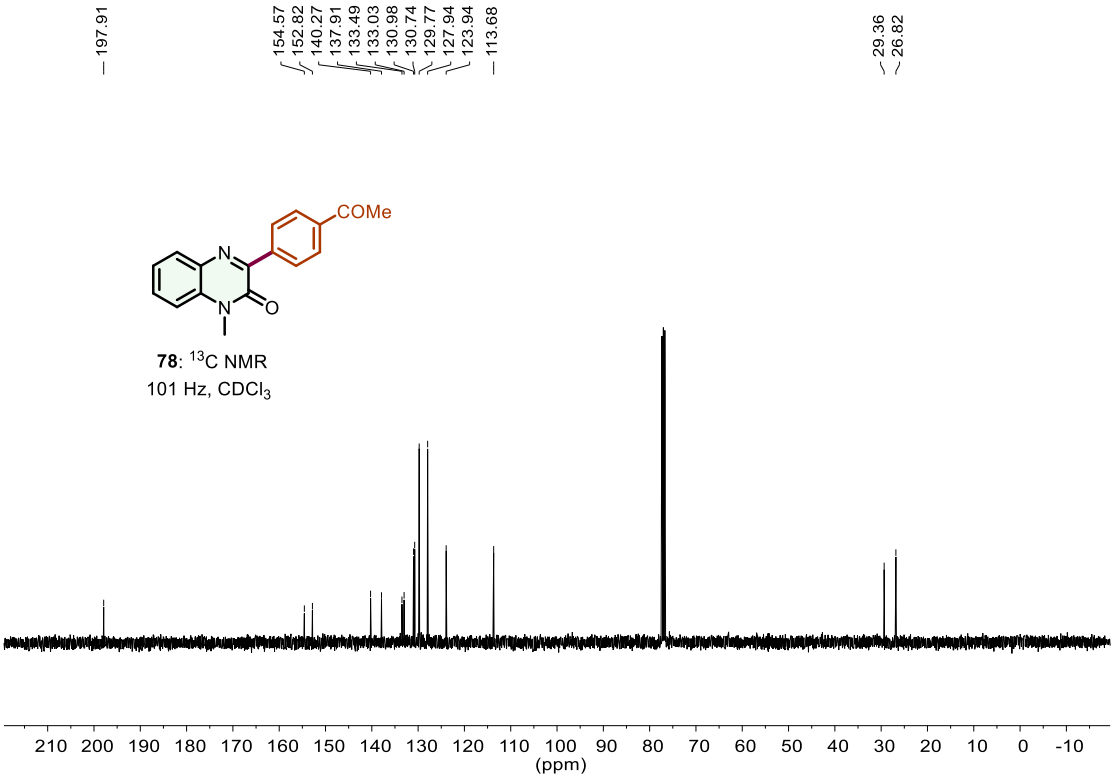
77: ^{1}H NMR
400 MHz, DMSO-d_6

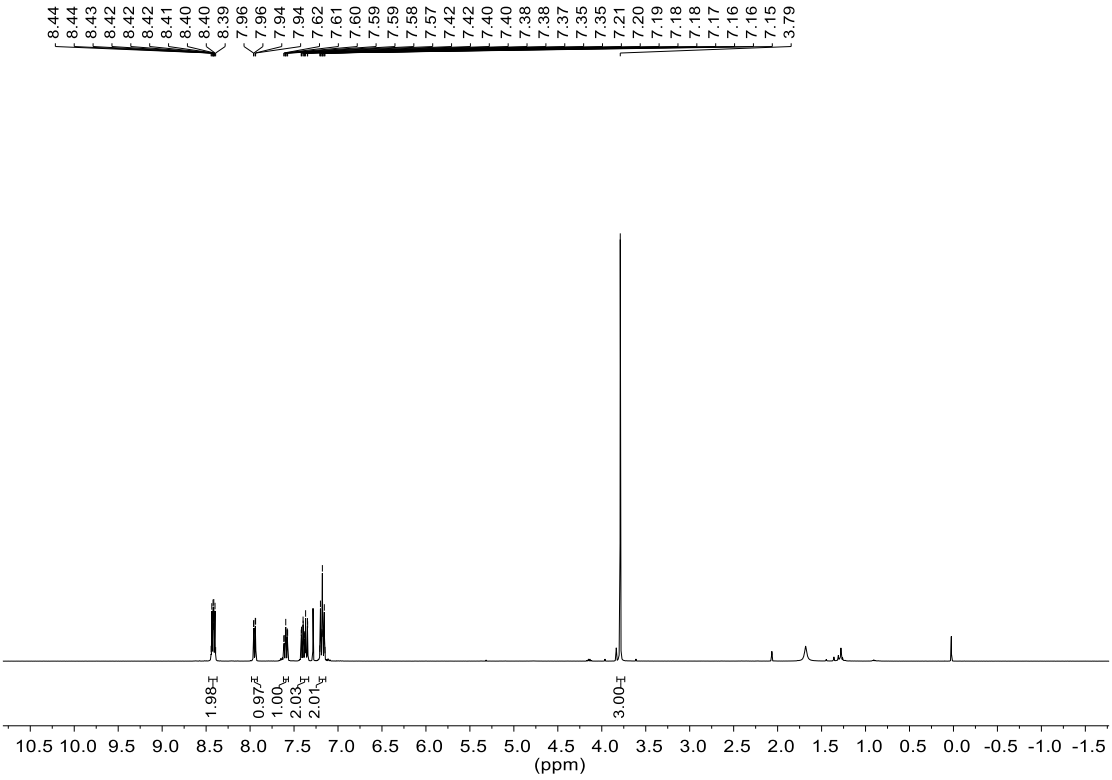


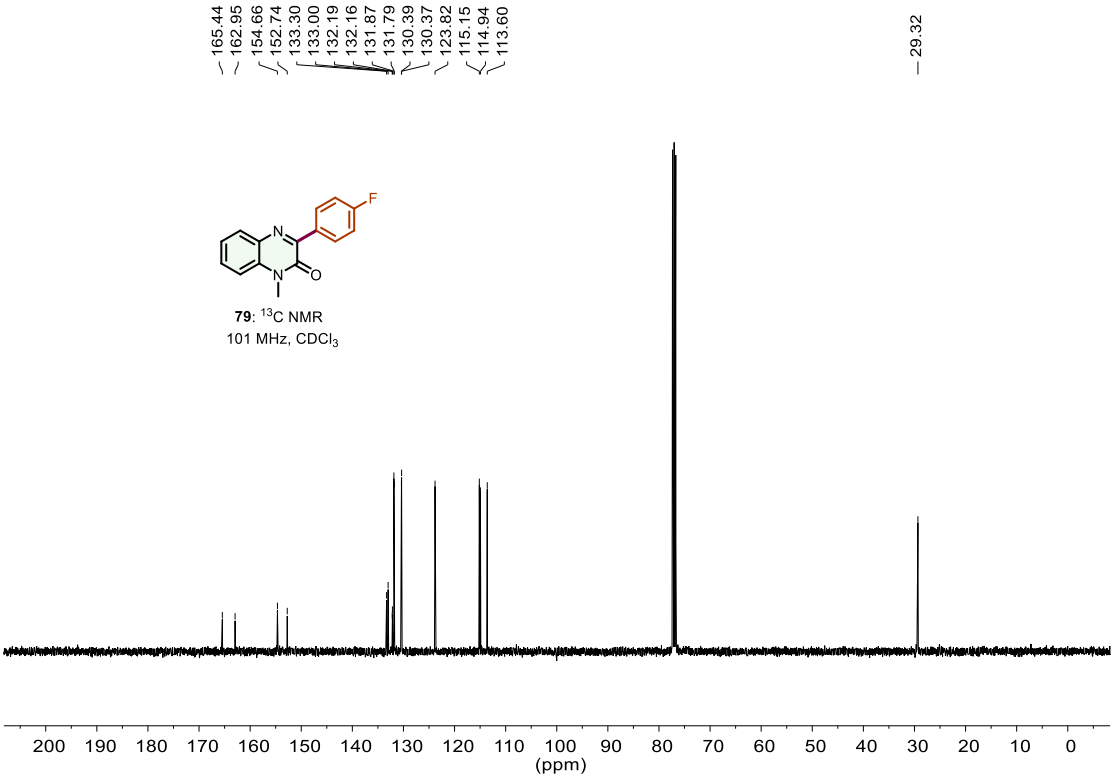
77: ^{13}C NMR
101 MHz, DMSO-d_6



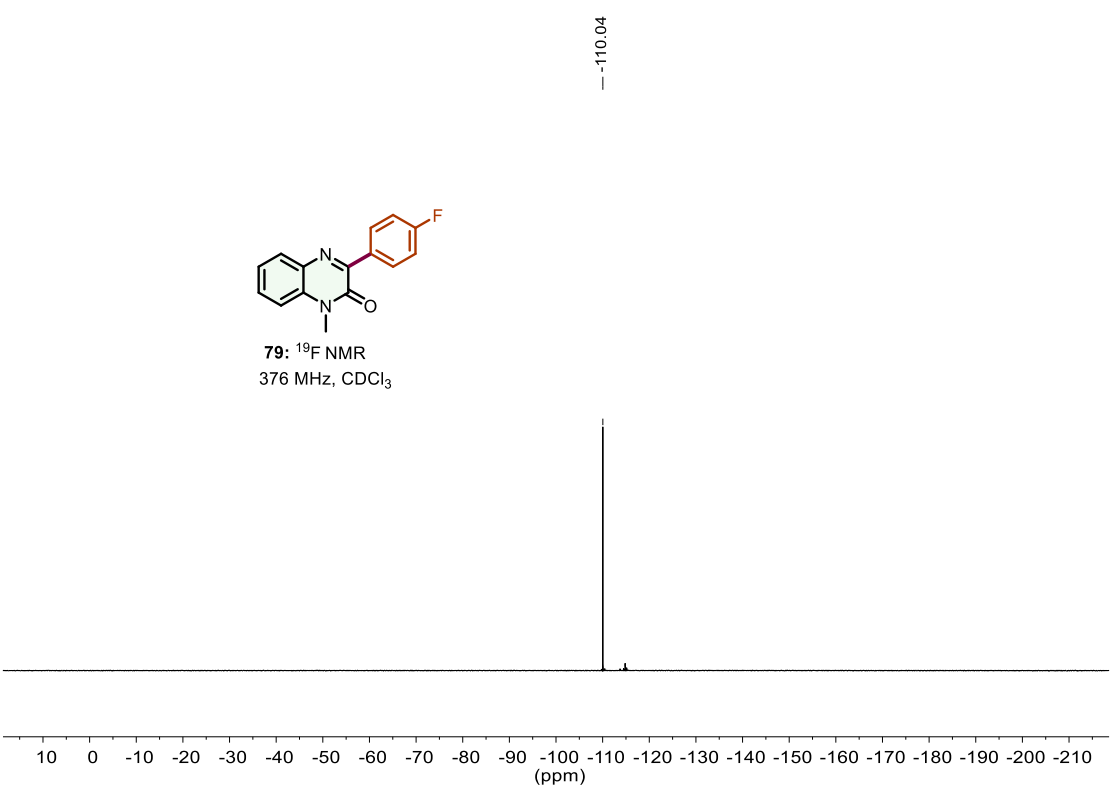
78: ^{1}H NMR
400 Hz, $CDCl_3$


197.91
154.57
152.82
140.27
137.91
133.49
133.03
130.98
130.74
129.77
127.94
123.94
113.68
29.36
26.82
COMe
N
N
O
78: 13C NMR
101 Hz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)

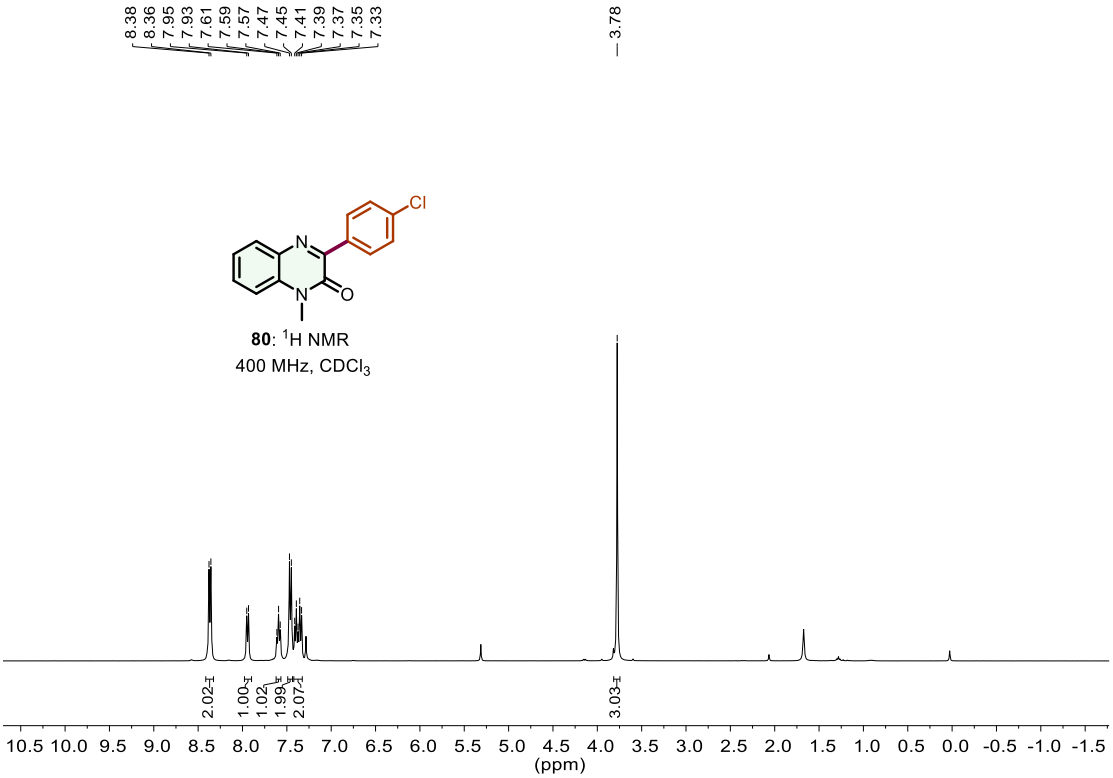

8.44
8.44
8.43
8.42
8.42
8.42
8.41
8.40
8.40
8.39
7.96
7.96
7.94
7.94
7.62
7.61
7.60
7.59
7.59
7.58
7.57
7.42
7.40
7.40
7.38
7.37
7.35
7.35
7.21
7.20
7.19
7.18
7.18
7.17
7.16
7.16
7.15
3.79
1.98
0.97
1.00
2.03
2.01
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)

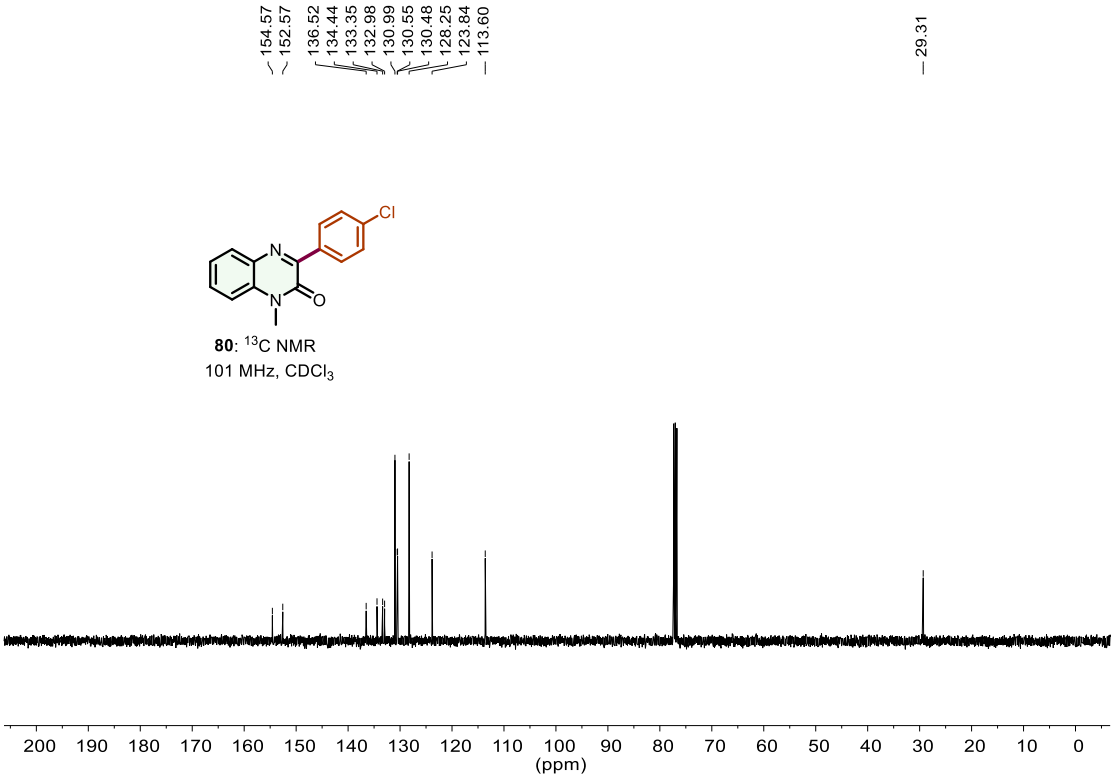


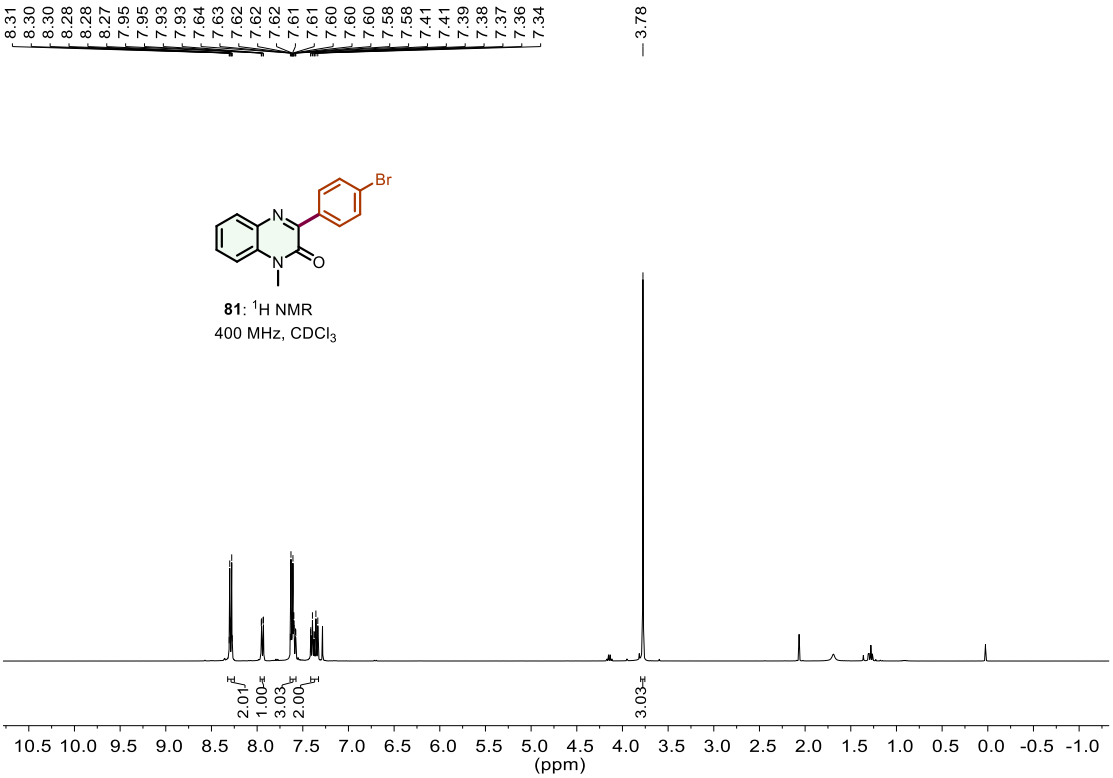
79: ^{13}C NMR
101 MHz, $CDCl_3$

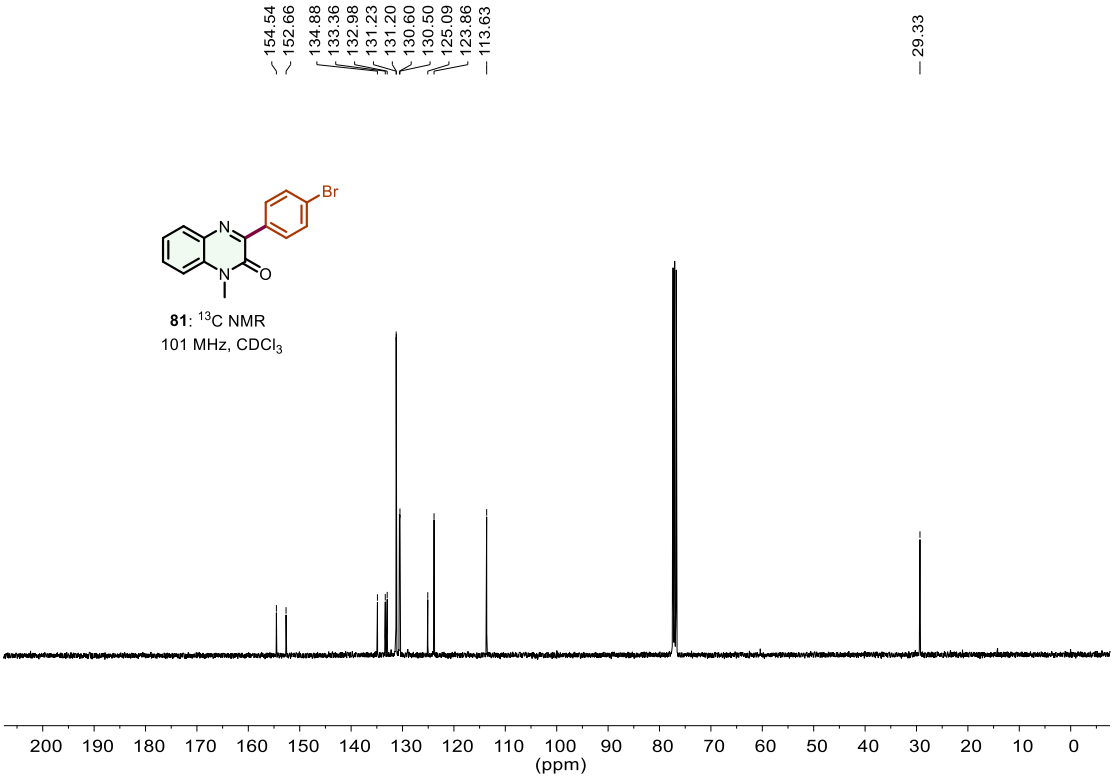


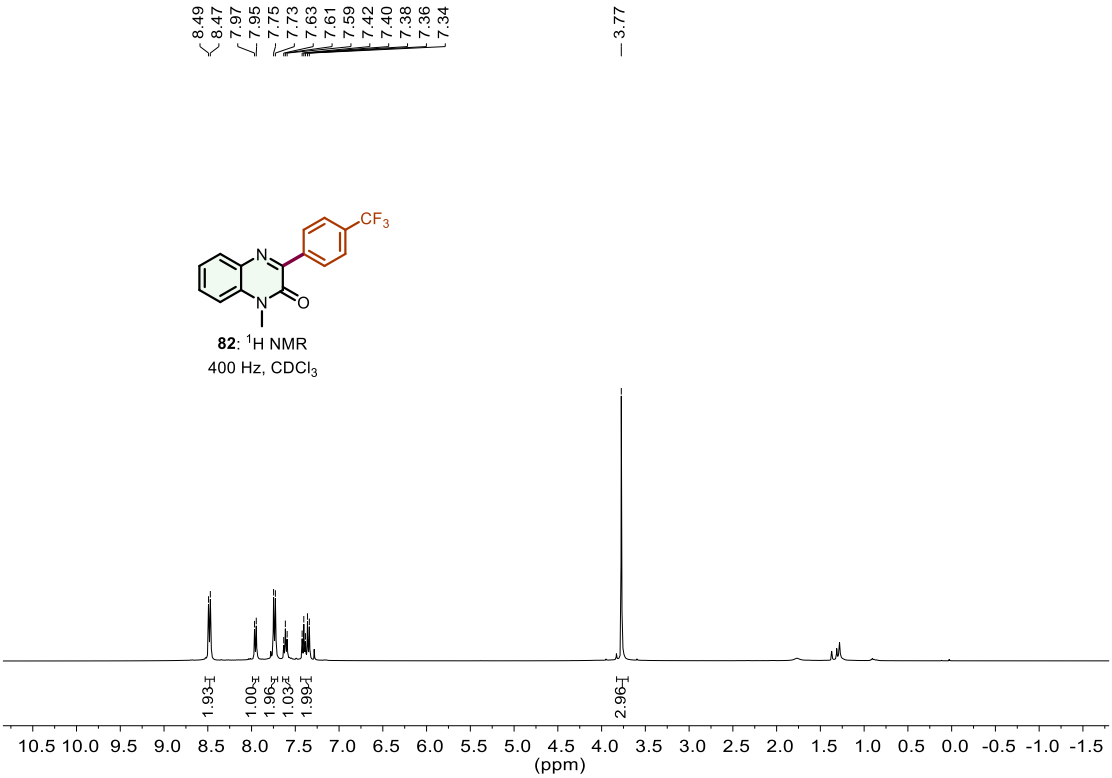
79: ^{19}F NMR
376 MHz, $CDCl_3$

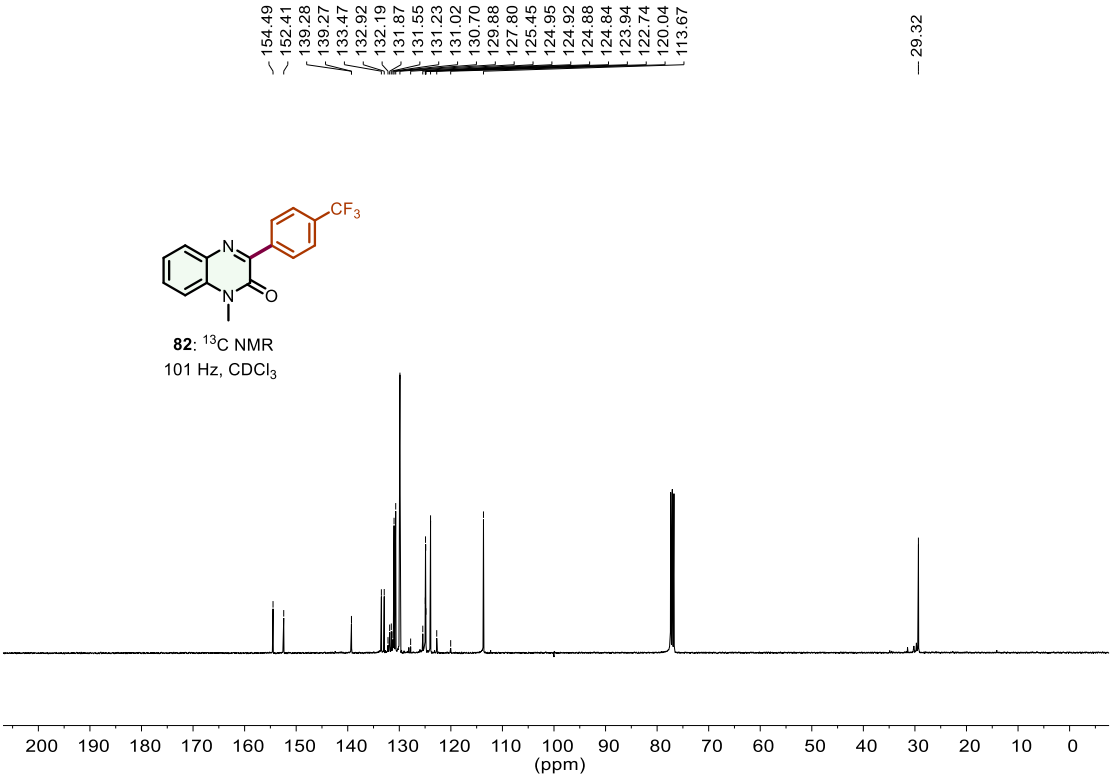

8.38
8.36
7.95
7.93
7.61
7.59
7.57
7.47
7.45
7.41
7.39
7.37
7.35
7.33
3.78
Cl
N
O
N
80: 1H NMR
400 MHz, CDCl3
2.02
1.00
1.02
1.99
2.07
3.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)

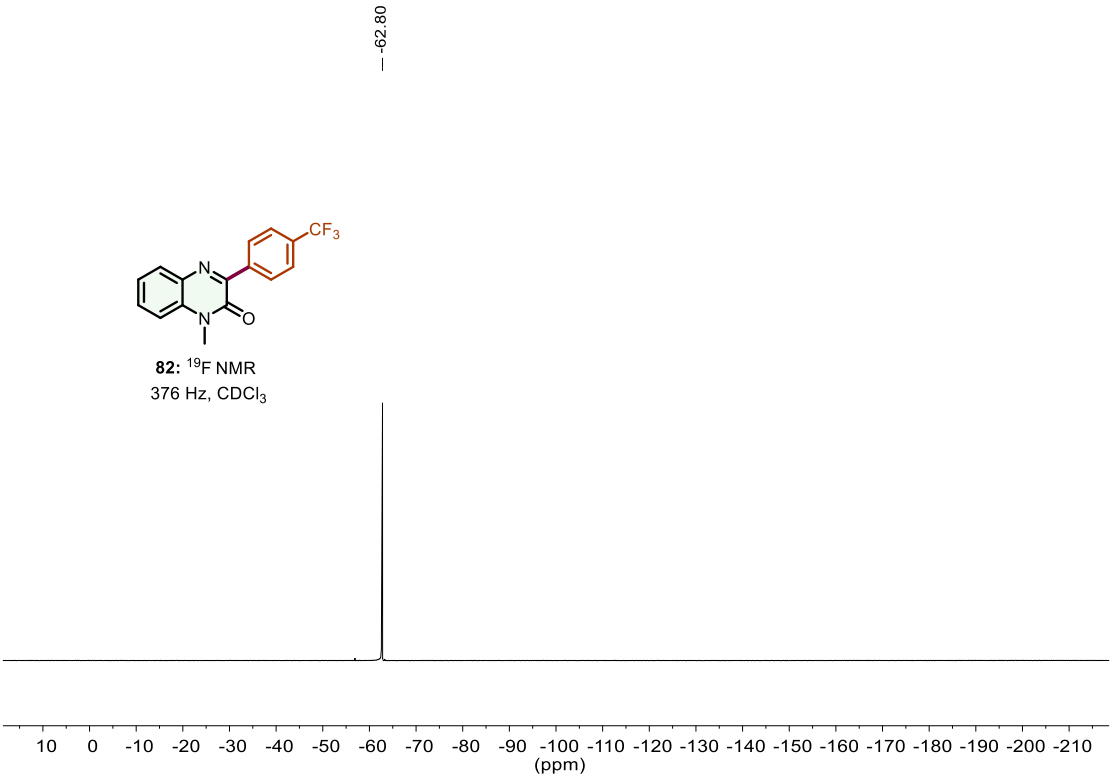

154.57
152.57
136.52
134.44
133.35
132.98
130.99
130.55
130.48
128.25
123.84
113.60
29.31
Cl
N
O
N
80: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


8.31
8.30
8.30
8.28
8.28
8.27
7.95
7.95
7.93
7.93
7.64
7.63
7.62
7.62
7.62
7.61
7.61
7.60
7.60
7.60
7.58
7.58
7.41
7.41
7.39
7.38
7.37
7.36
7.34
3.78
Br
N
O
N
81: 1H NMR
400 MHz, CDCl3
2.01
1.00
3.03
2.00
3.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
(ppm)

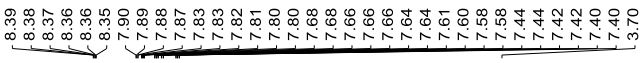

154.54
152.66
134.88
133.36
132.98
131.23
131.20
130.60
130.50
125.09
123.86
113.63
29.33
Br
N
O
N
81: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

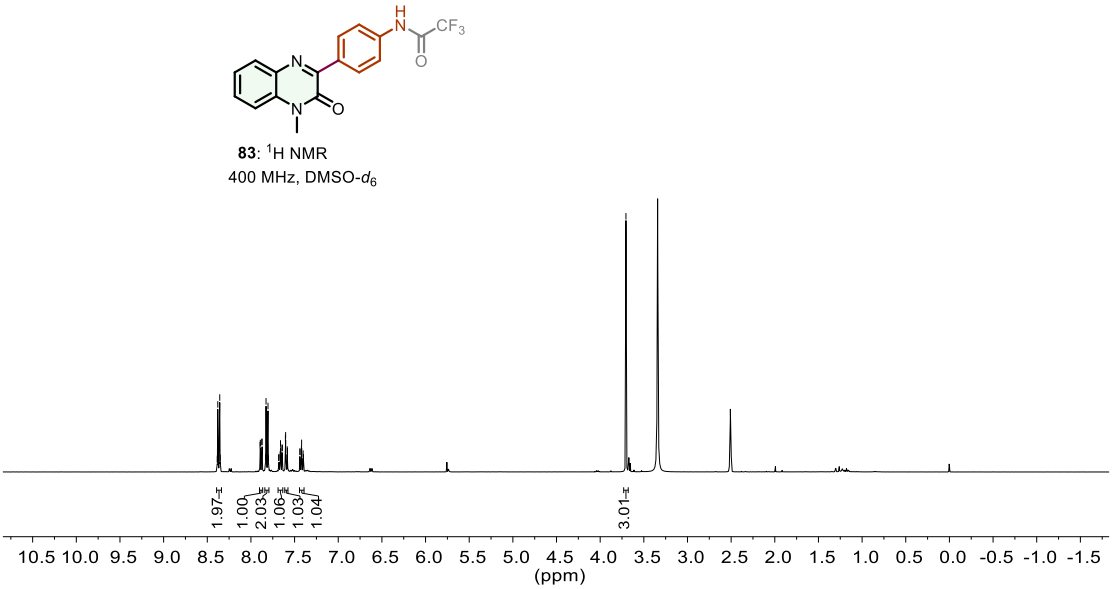

8.49
8.47
7.97
7.95
7.75
7.73
7.63
7.61
7.59
7.42
7.40
7.38
7.36
7.34
3.77
CF3
N
O
N
82: 1H NMR
400 Hz, CDCl3
1.93
1.00
1.96
1.03
1.99
2.96
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)


154.49
152.41
139.28
139.27
133.47
132.92
132.19
131.87
131.55
131.23
131.02
130.70
129.88
127.80
125.45
124.95
124.92
124.88
124.84
123.94
122.74
120.04
113.67
29.32
CF3
N
O
N
82: 13C NMR
101 Hz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

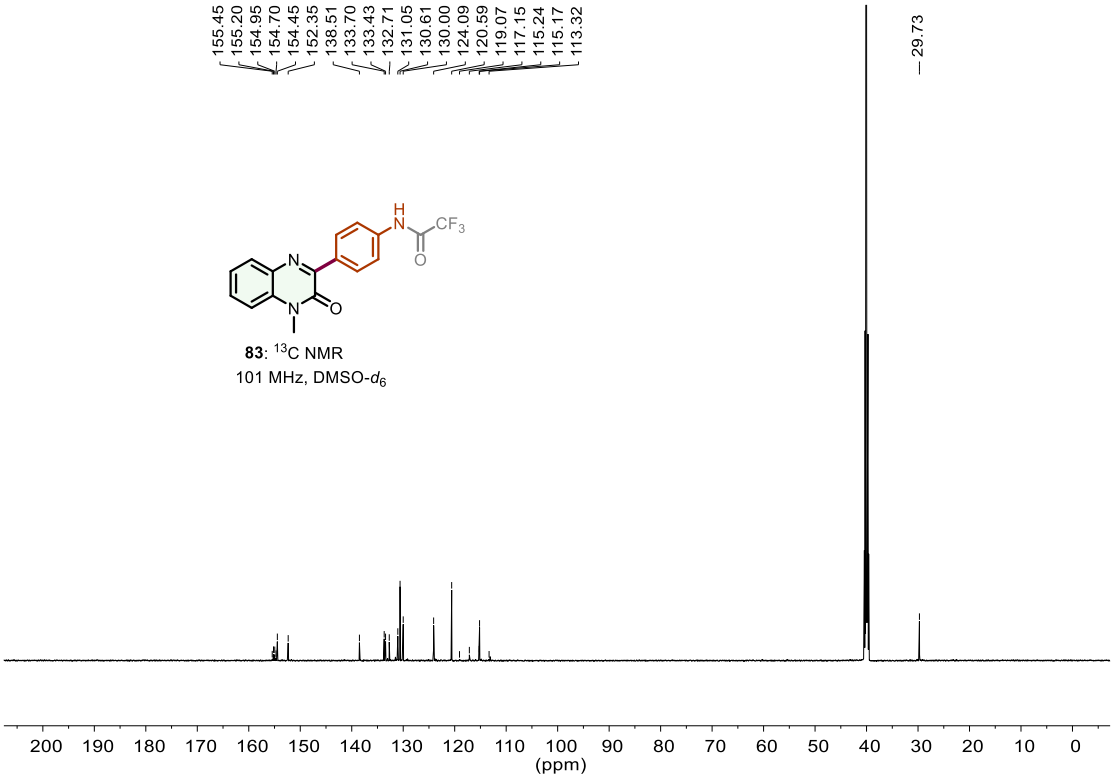


82: ^{19}F NMR
376 Hz, $CDCl_3$

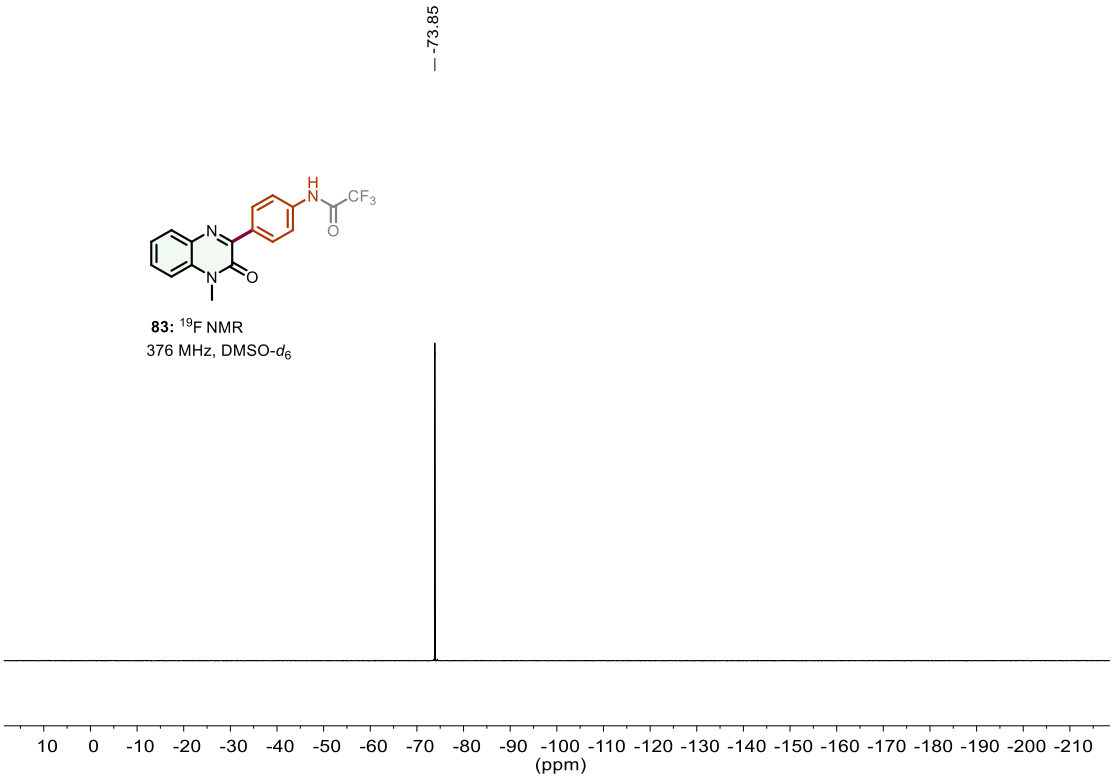




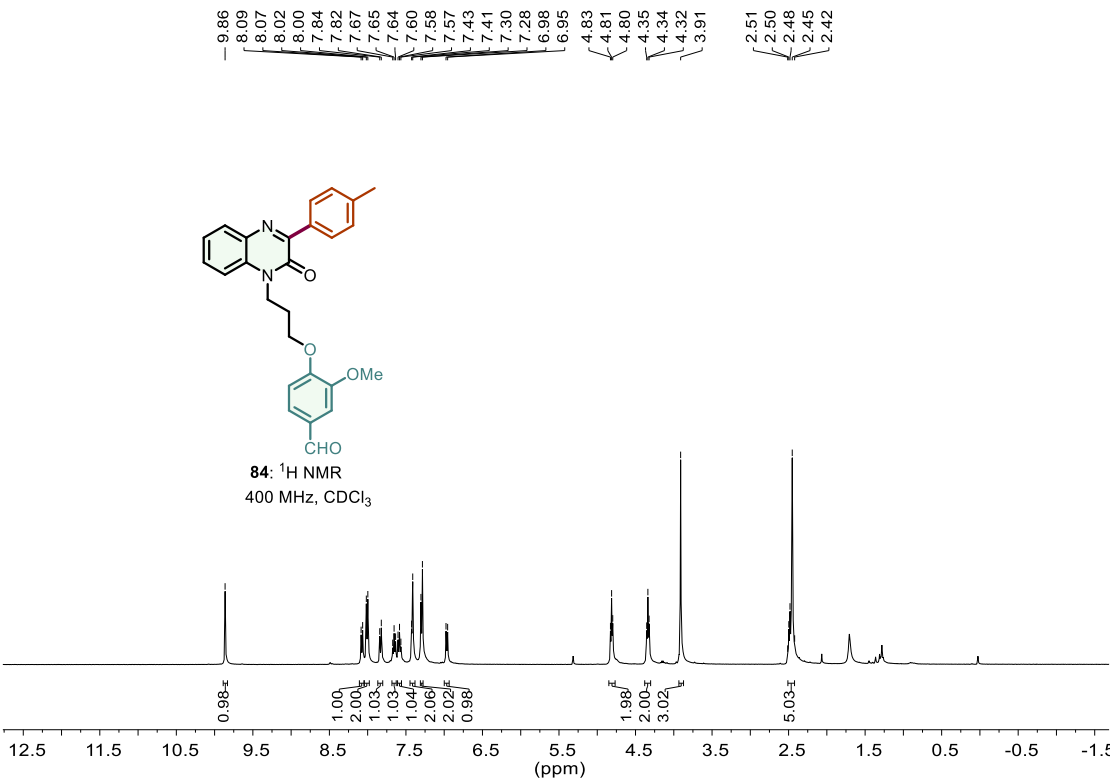
83: ^{1}H NMR
400 MHz, DMSO-d_6

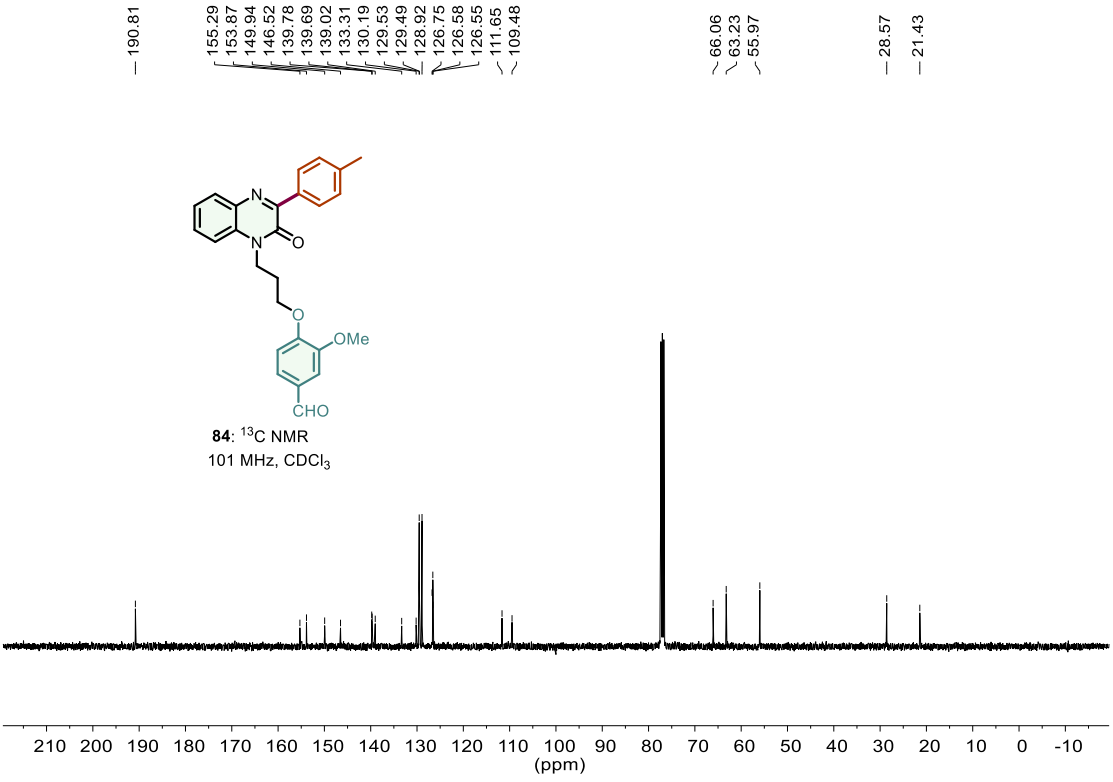


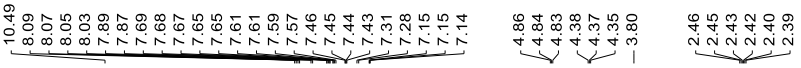
83: ^{13}C NMR
101 MHz, DMSO-d_6

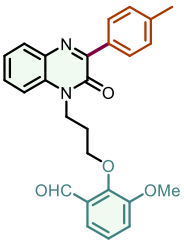


83: ^{19}F NMR
376 MHz, DMSO-d_6

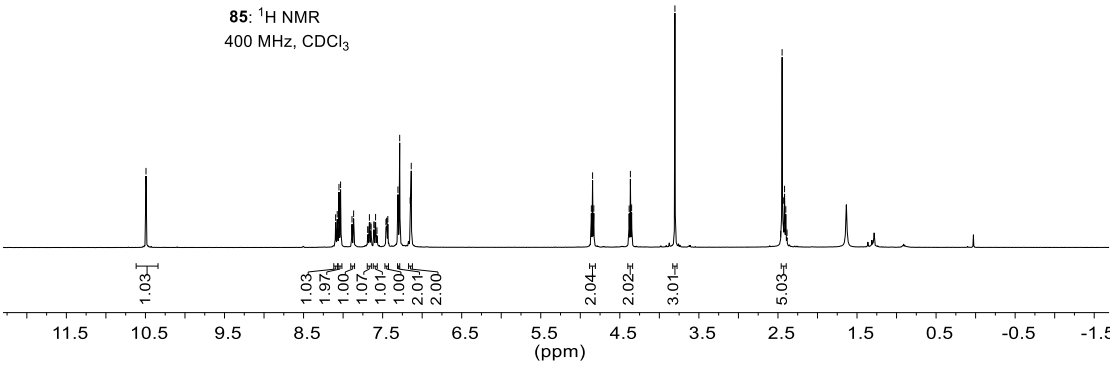

9.86
8.09
8.07
8.02
8.00
7.84
7.82
7.67
7.65
7.64
7.60
7.58
7.57
7.43
7.41
7.30
7.28
6.98
6.95
4.83
4.81
4.80
4.35
4.34
4.32
3.91
2.51
2.50
2.48
2.45
2.42
OMe
CHO
84: 1H NMR
400 MHz, CDCl3
0.98
1.00
2.00
1.03
1.03
1.04
2.06
2.02
0.98
1.98
2.00
3.02
5.03
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
(ppm)

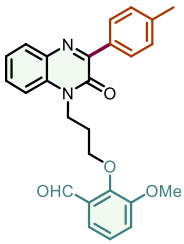

190.81
155.29
153.87
149.94
146.52
139.78
139.69
139.02
133.31
130.19
129.53
129.49
128.92
126.75
126.58
126.55
111.65
109.48
66.06
63.23
55.97
28.57
21.43
OMe
CHO
84: 13C NMR
101 MHz, CDCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
(ppm)



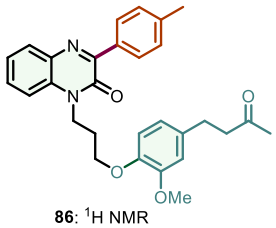


85: ^{1}H NMR
400 MHz, $CDCl_3$

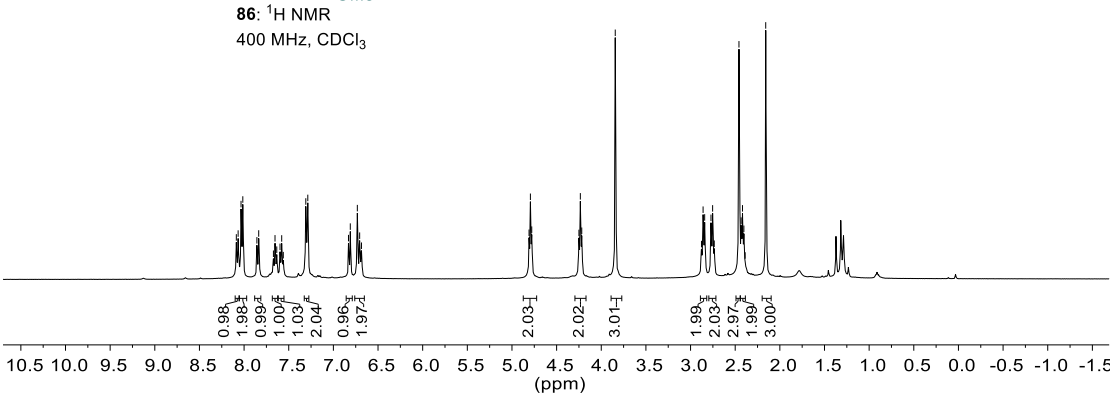


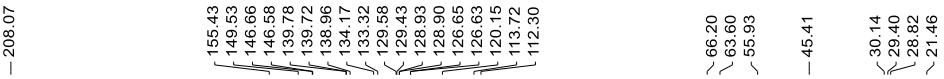


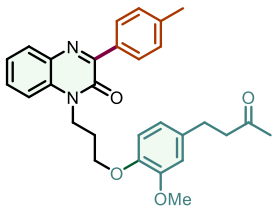
85: ^{13}C NMR
101 MHz, $CDCl_3$



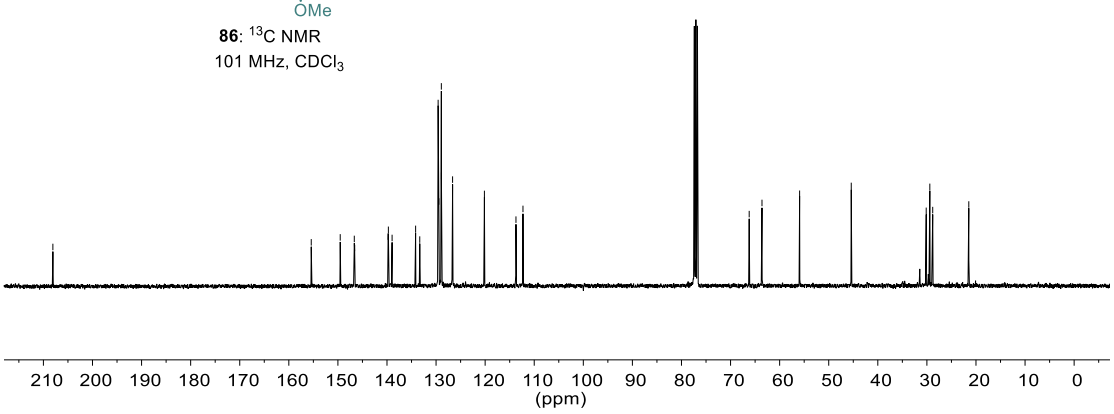
86: ^{1}H NMR
400 MHz, $CDCl_3$



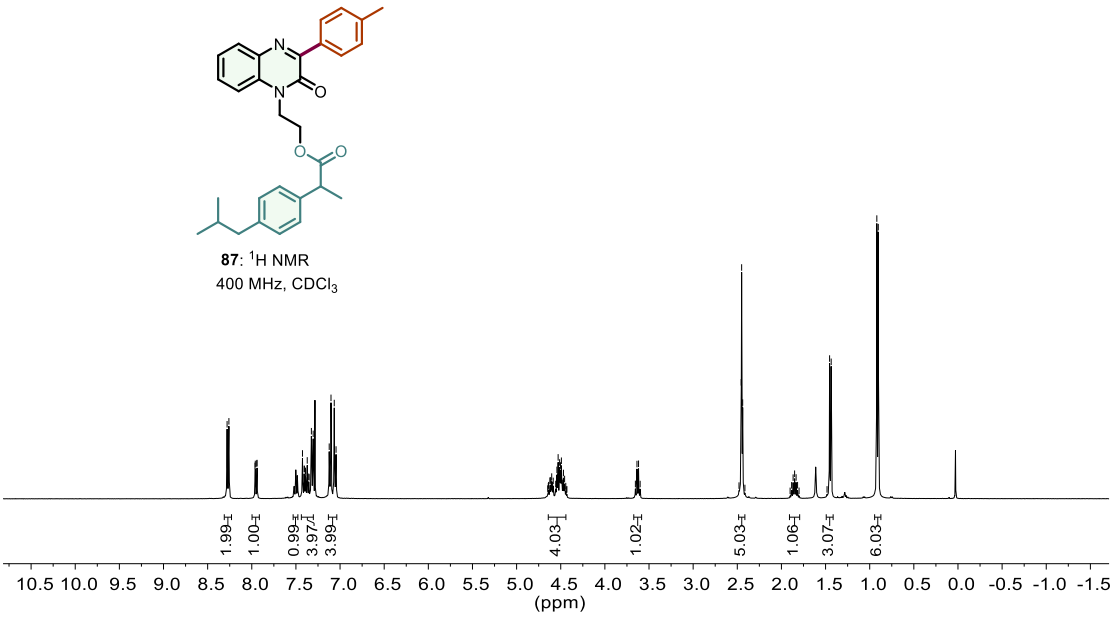




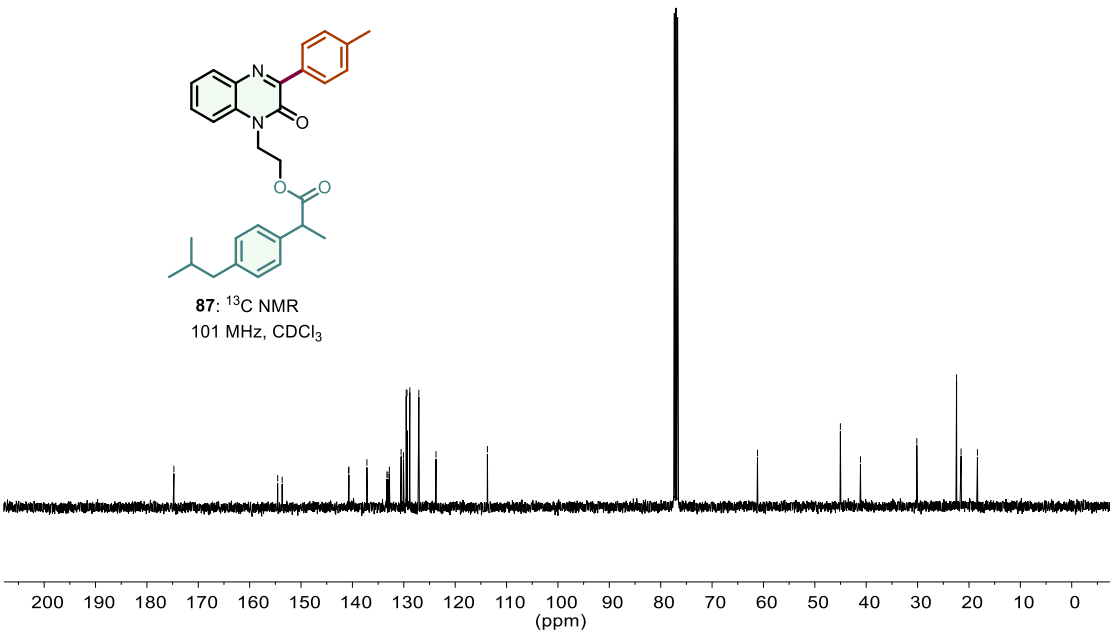
86: ^{13}C NMR
101 MHz, $CDCl_3$

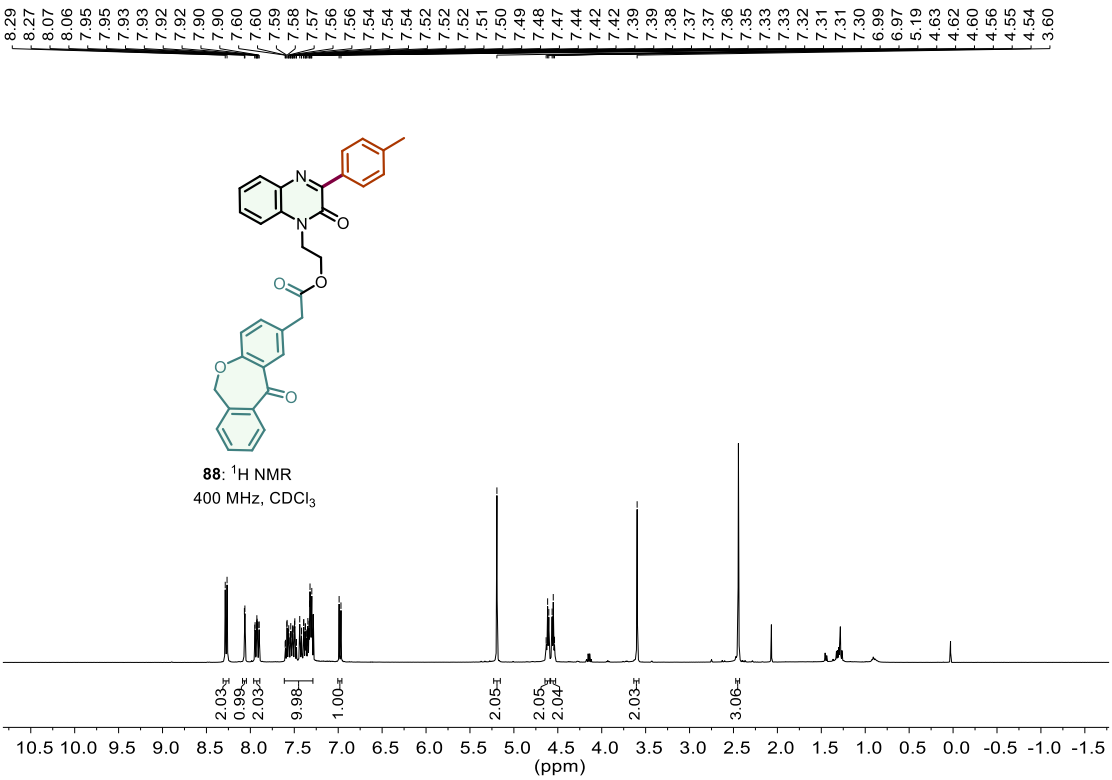


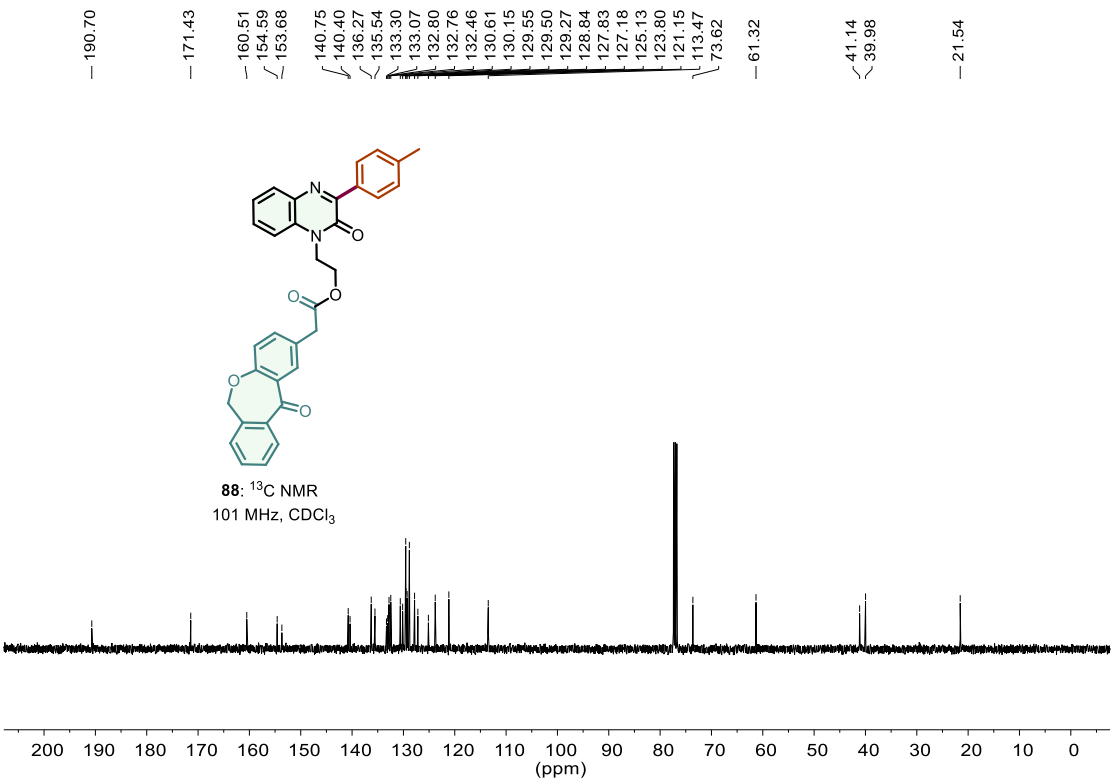

8.28
8.26
7.96
7.96
7.94
7.94
7.43
7.41
7.40
7.39
7.39
7.37
7.35
7.35
7.32
7.30
7.12
7.10
7.07
7.05
4.65
4.64
4.64
4.62
4.62
4.61
4.60
4.59
4.59
4.56
4.54
4.53
4.51
4.50
4.49
4.48
4.47
4.46
4.44
4.43
3.65
3.64
3.62
3.60
2.48
2.46
2.45
2.44
2.41
1.88
1.87
1.85
1.83
1.82
1.45
1.44
0.92
0.90

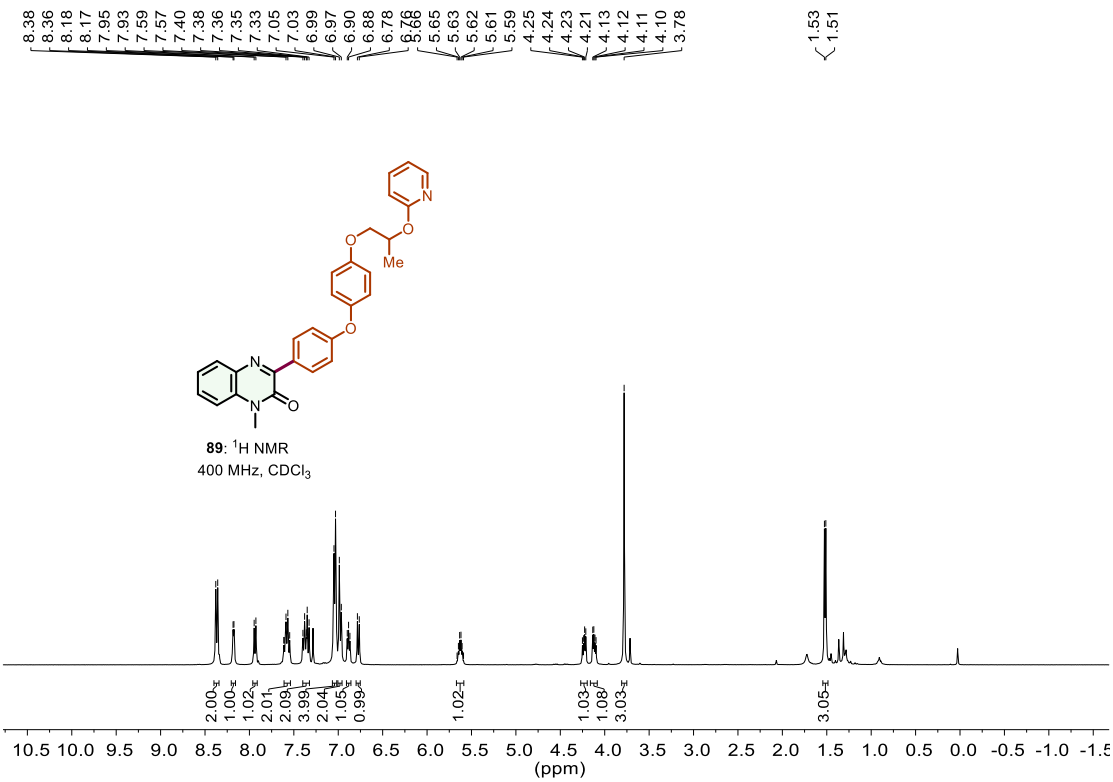

87: 1H NMR
400 MHz, CDCl3
1.99
1.00
0.99
3.97
3.99
4.03
1.02
5.03
1.06
3.07
6.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)

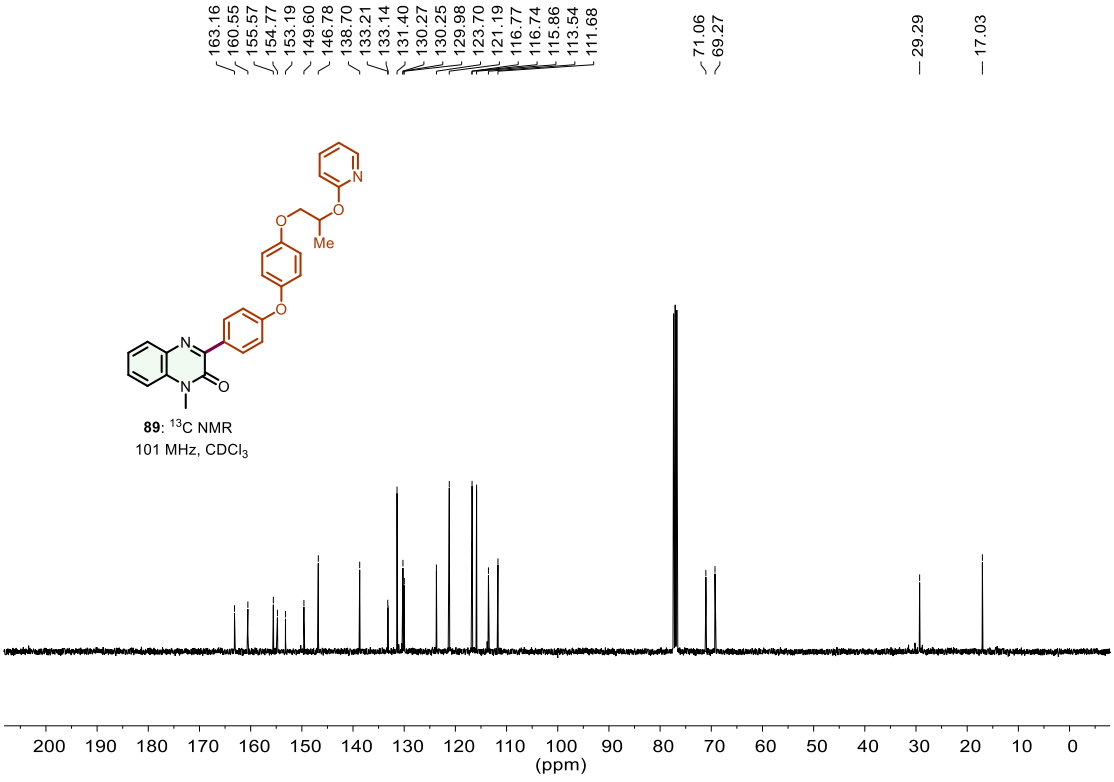

174.75
154.56
153.68
140.74
140.69
137.18
133.29
133.08
132.81
130.52
130.07
129.53
129.37
128.83
127.07
123.73
113.73
61.16
45.03
45.01
41.12
30.15
22.42
21.54
18.35

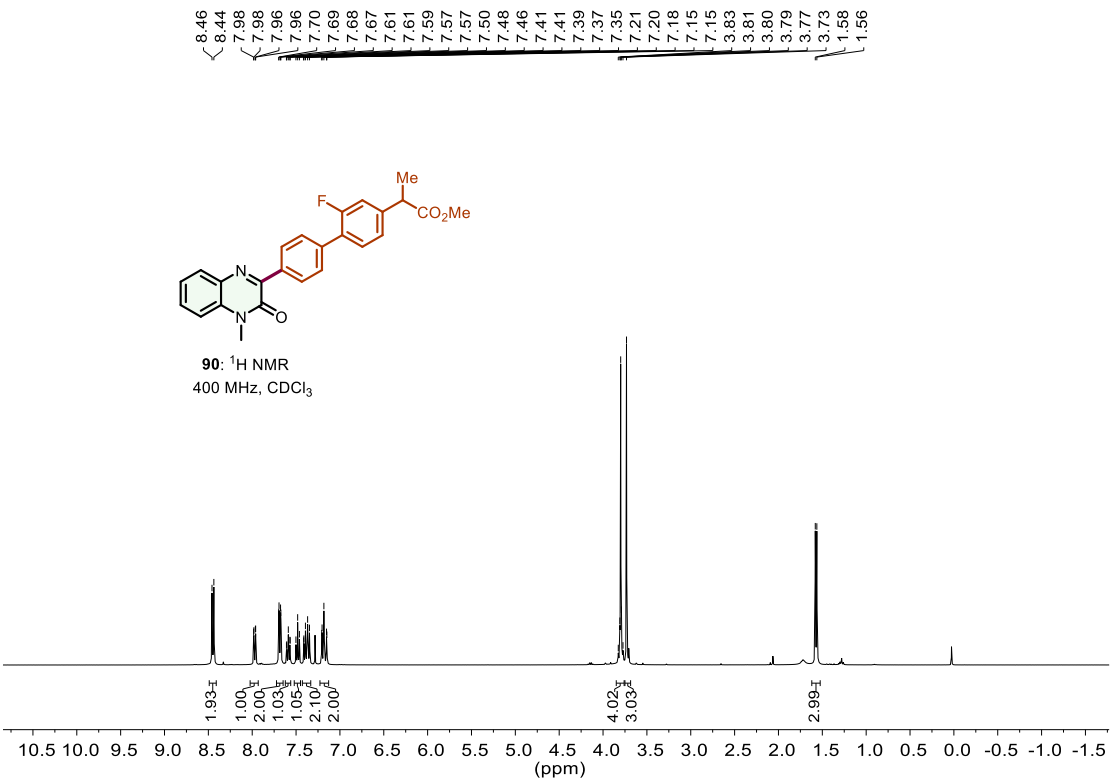

87: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

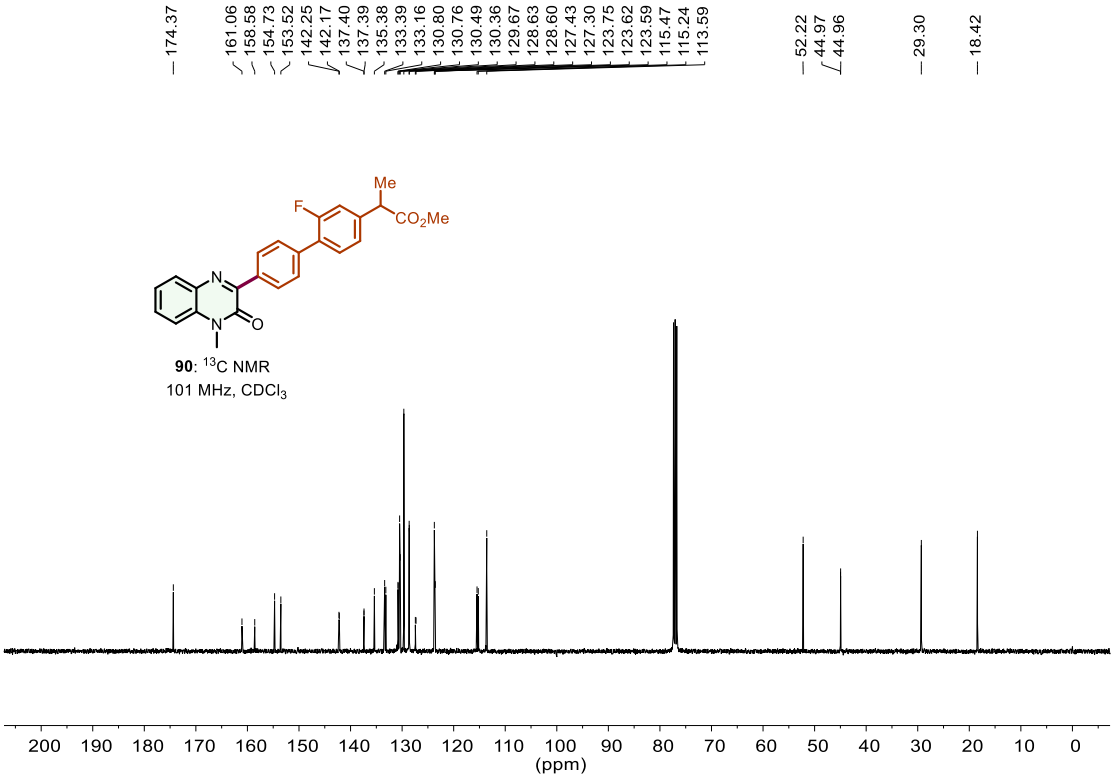

8.29 8.27 8.07 8.06 7.95 7.95 7.93 7.93 7.92 7.92 7.90 7.90 7.60 7.60 7.59 7.58 7.57 7.56 7.56 7.54 7.54 7.54 7.52 7.52 7.52 7.51 7.50 7.49 7.48 7.47 7.44 7.42 7.42 7.39 7.39 7.38 7.37 7.37 7.36 7.35 7.33 7.33 7.32 7.31 7.31 7.30 6.99 6.97 5.19 4.63 4.62 4.60 4.56 4.55 4.54 3.60
88: 1H NMR
400 MHz, CDCl3
2.03 0.99 2.03 9.98 1.00 2.05 2.05 2.04 2.03 3.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)

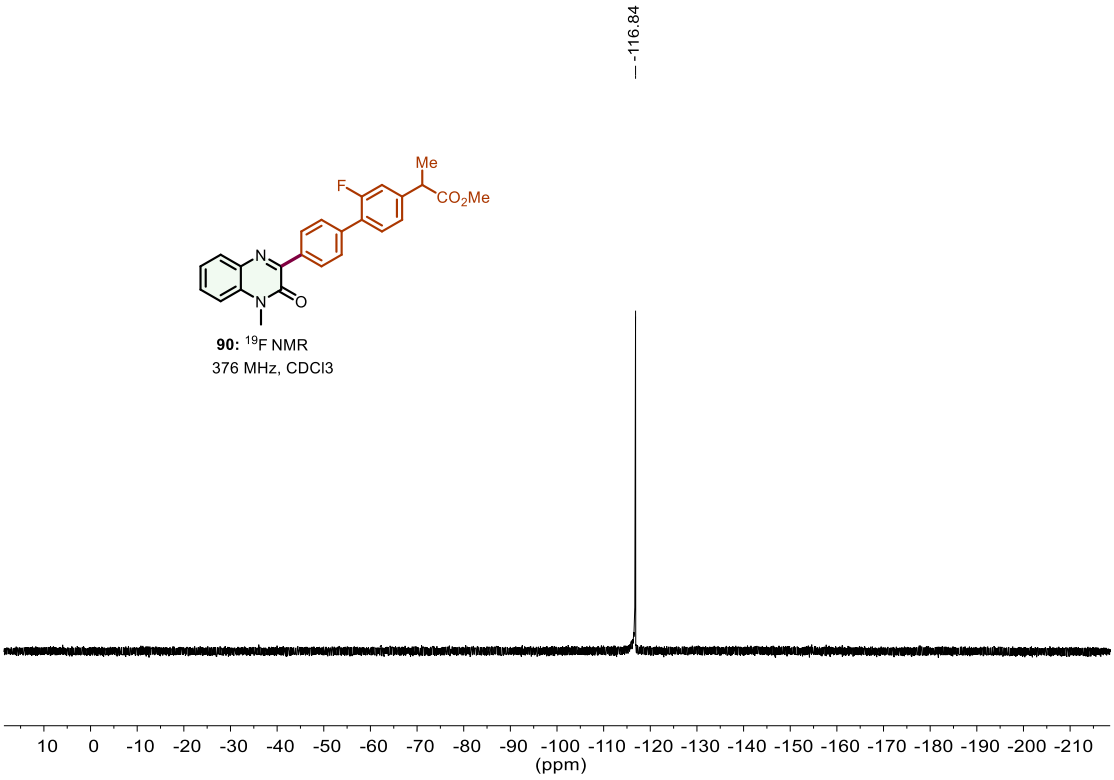

190.70 171.43 160.51 154.59 153.68 140.75 140.40 136.27 135.54 133.30 133.07 132.80 132.76 132.46 130.61 130.15 129.55 129.50 129.27 128.84 127.83 127.18 125.13 123.80 121.15 113.47 73.62 61.32 41.14 39.98 21.54
88: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


8.38
8.36
8.18
8.17
7.95
7.93
7.59
7.57
7.40
7.38
7.36
7.35
7.33
7.05
7.03
6.99
6.97
6.90
6.88
6.78
6.76
6.66
5.65
5.63
5.62
5.61
5.59
4.25
4.24
4.23
4.21
4.13
4.12
4.11
4.10
3.78
1.53
1.51
89: 1H NMR
400 MHz, CDCl3
2.00
1.00
1.02
2.01
3.99
2.04
1.05
0.99
1.02
1.03
1.08
3.03
3.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)

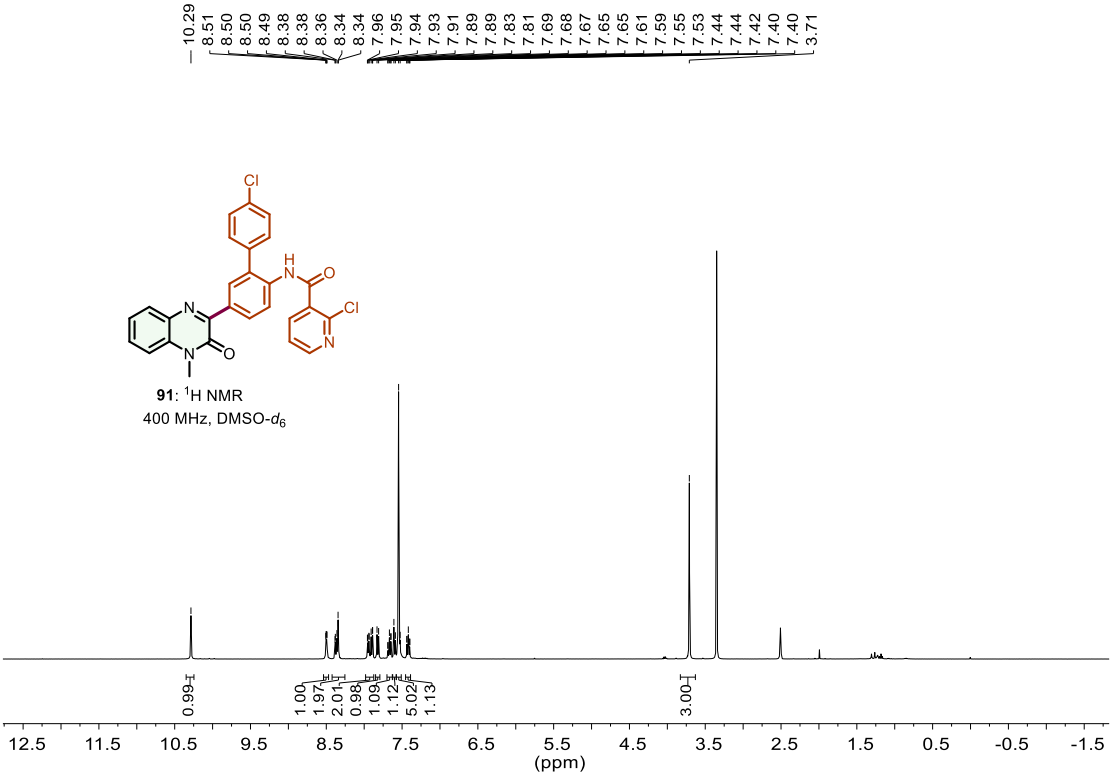

163.16
160.55
155.57
154.77
153.19
149.60
146.78
138.70
133.21
133.14
131.40
130.27
130.25
129.98
123.70
121.19
116.77
116.74
115.86
113.54
111.68
71.06
69.27
29.29
17.03
89: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


8.46
8.44
7.98
7.98
7.96
7.96
7.70
7.69
7.68
7.67
7.61
7.61
7.59
7.57
7.57
7.50
7.48
7.46
7.41
7.41
7.39
7.37
7.35
7.21
7.20
7.18
7.15
7.15
3.83
3.81
3.80
3.79
3.77
3.73
1.58
1.56
Me
F
CO2Me
N
O
N
O
90: 1H NMR
400 MHz, CDCl3
1.93
1.00
2.00
1.03
1.05
2.10
2.00
4.02
3.03
2.99
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
(ppm)

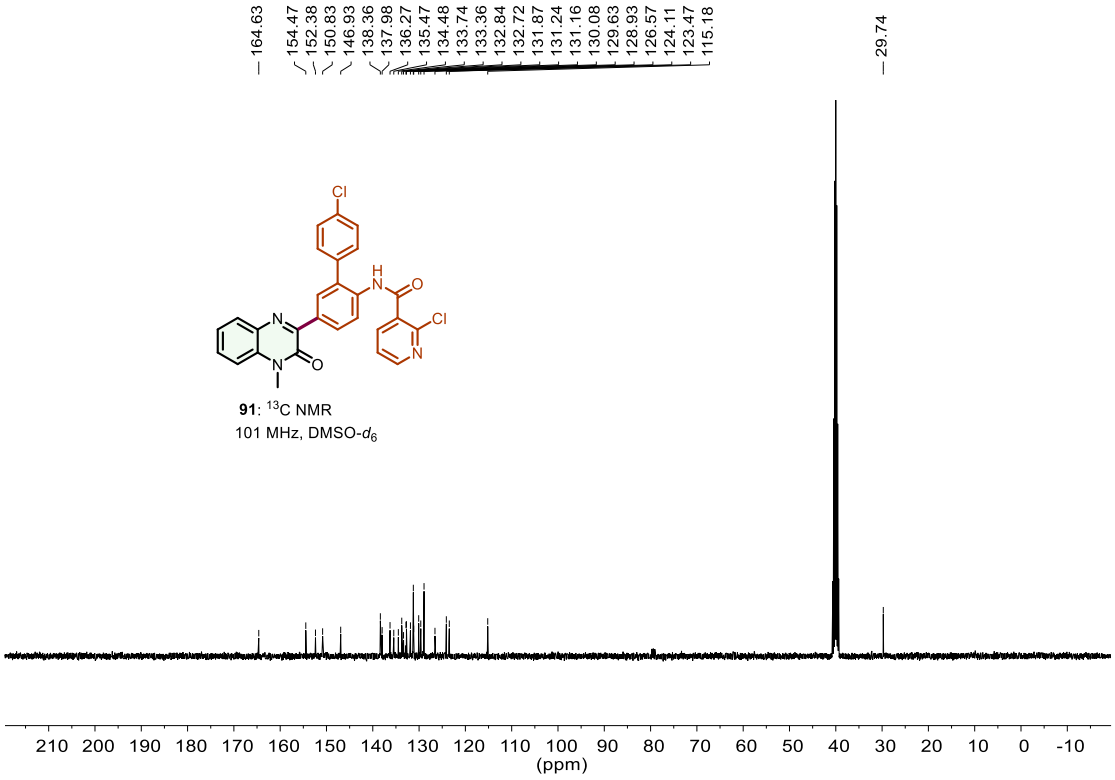

174.37
161.06
158.58
154.73
153.52
142.25
142.17
137.40
137.39
135.38
133.39
133.16
130.80
130.76
130.49
130.36
129.67
128.63
128.60
127.43
127.30
123.75
123.62
123.59
115.47
115.24
113.59
52.22
44.97
44.96
29.30
18.42
Me
F
CO2Me
N
O
N
O
90: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)



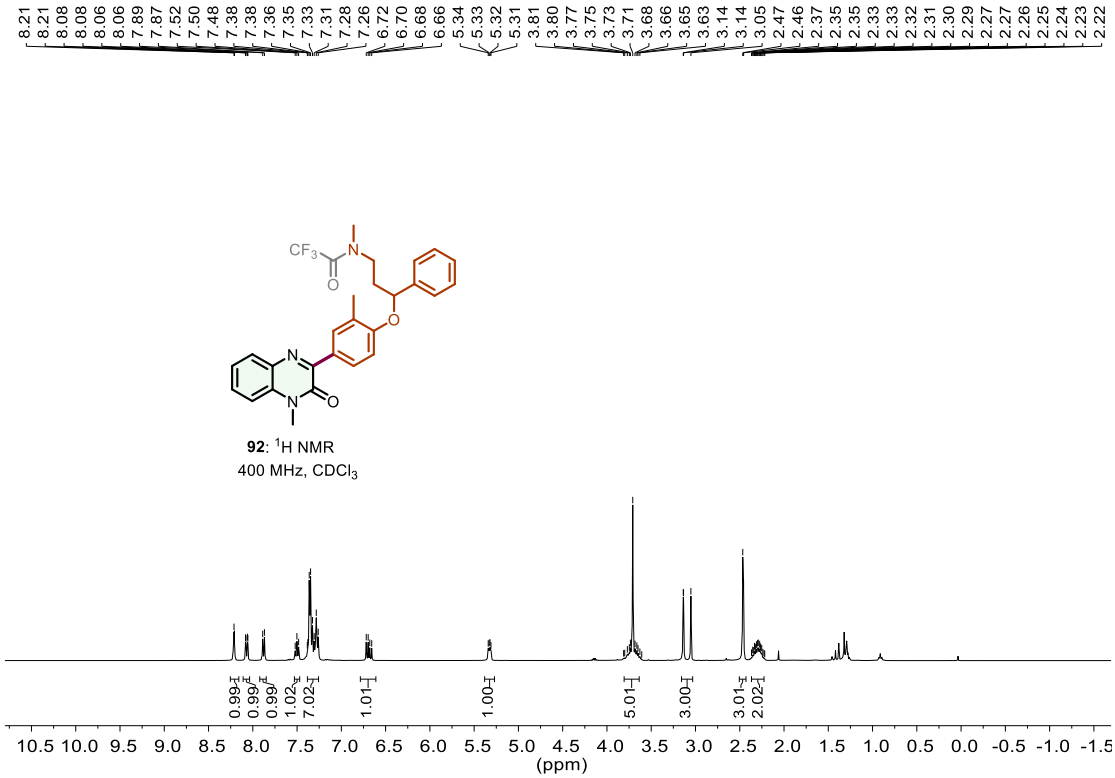
90: ^{19}F NMR
376 MHz, CDCl3



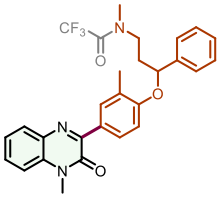
91: ^{1}H NMR
400 MHz, DMSO-d_6



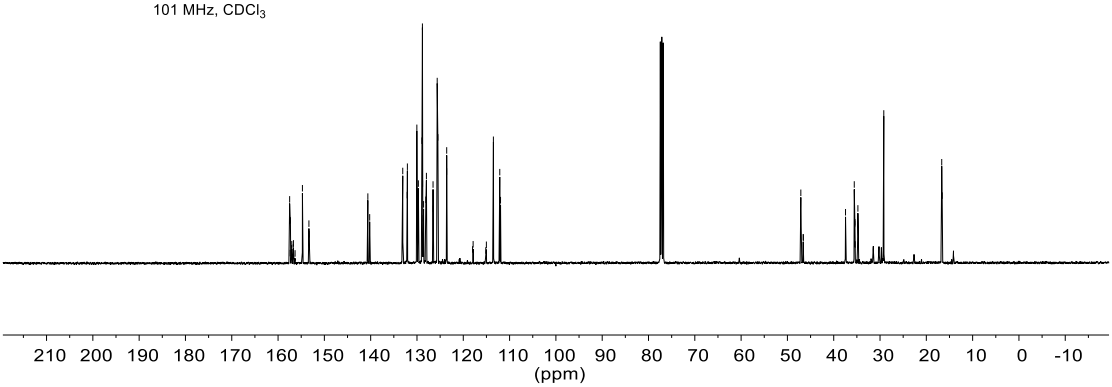
91: ^{13}C NMR
101 MHz, DMSO-d_6

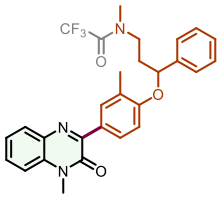


92: ^{1}H NMR
400 MHz, $CDCl_3$

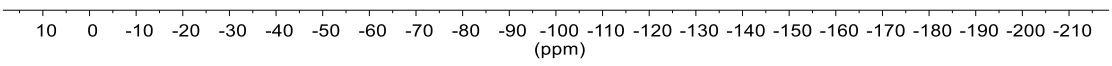


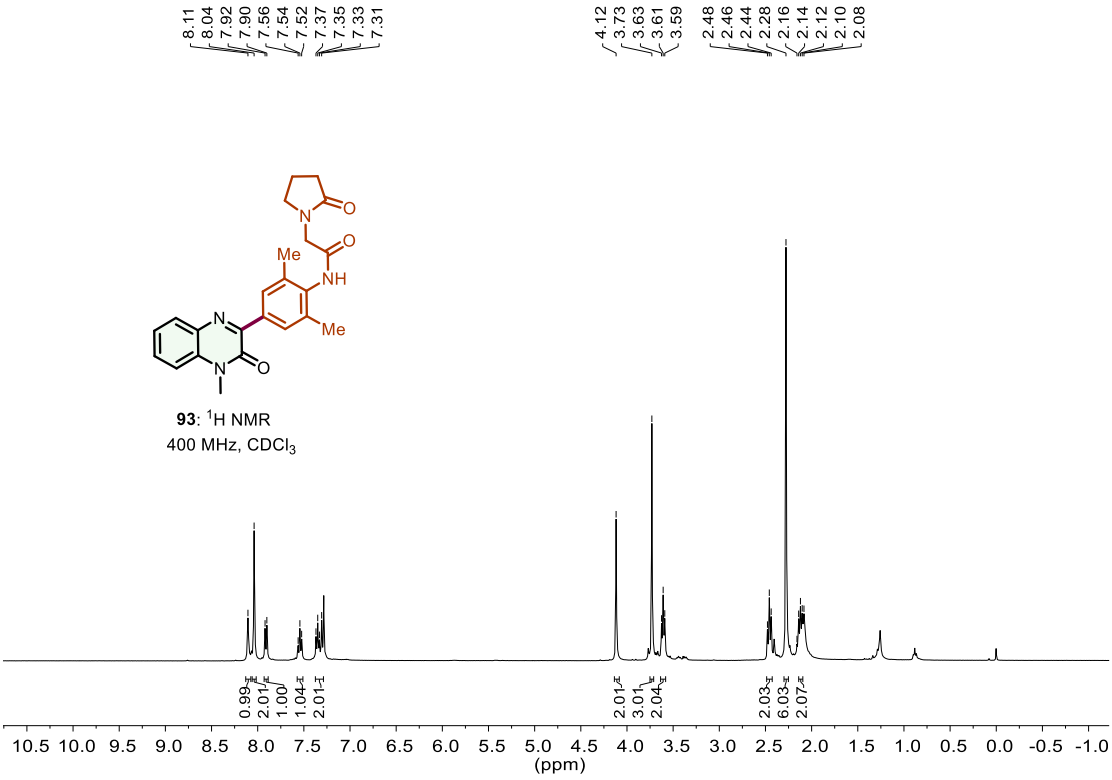
92: ^{13}C NMR
101 MHz, $CDCl_3$



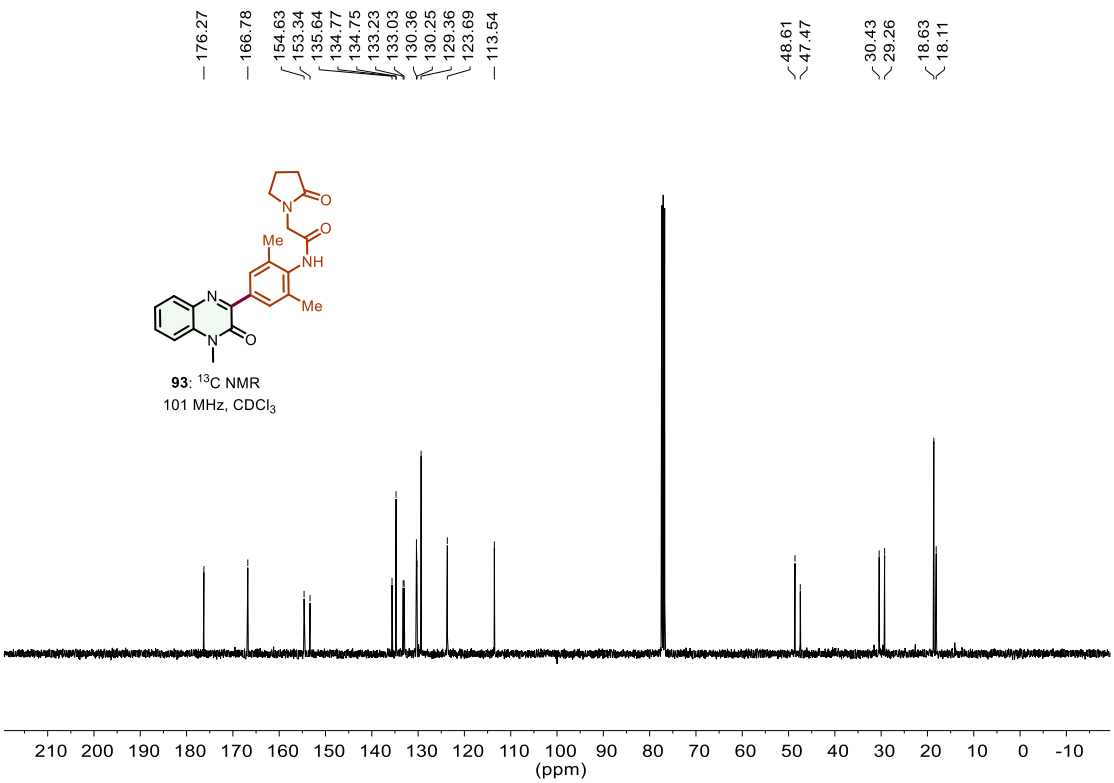


92: ^{19}F NMR
376 MHz, $CDCl_3$

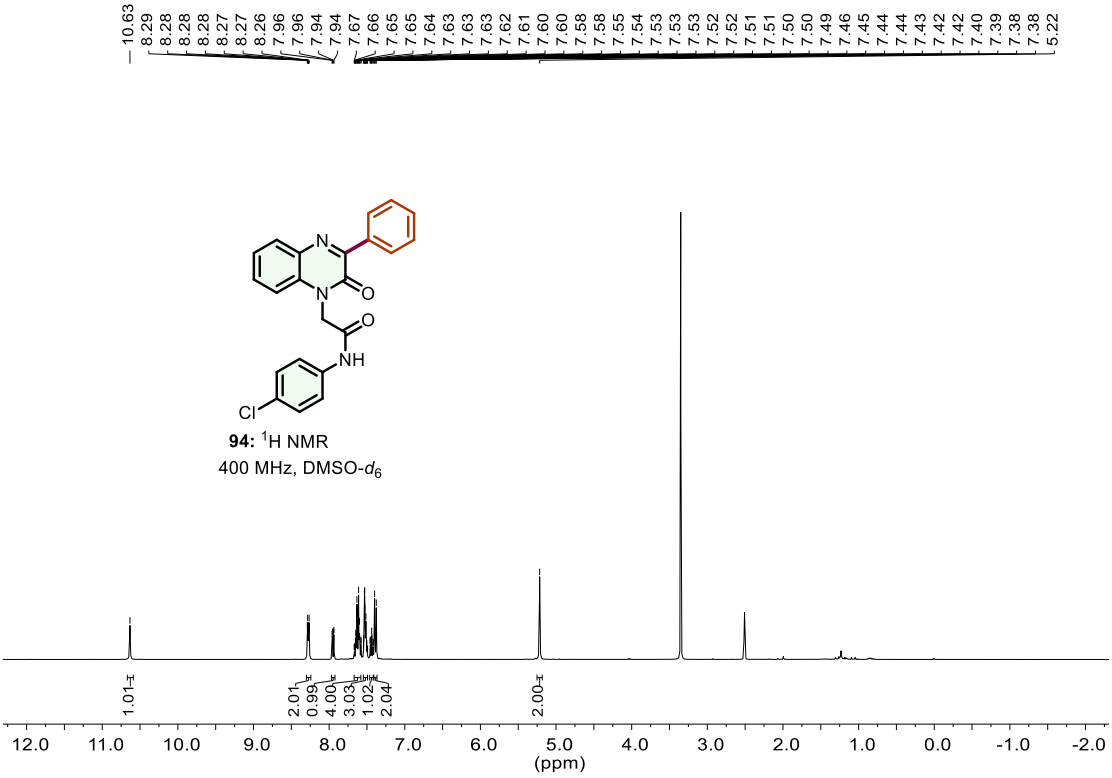


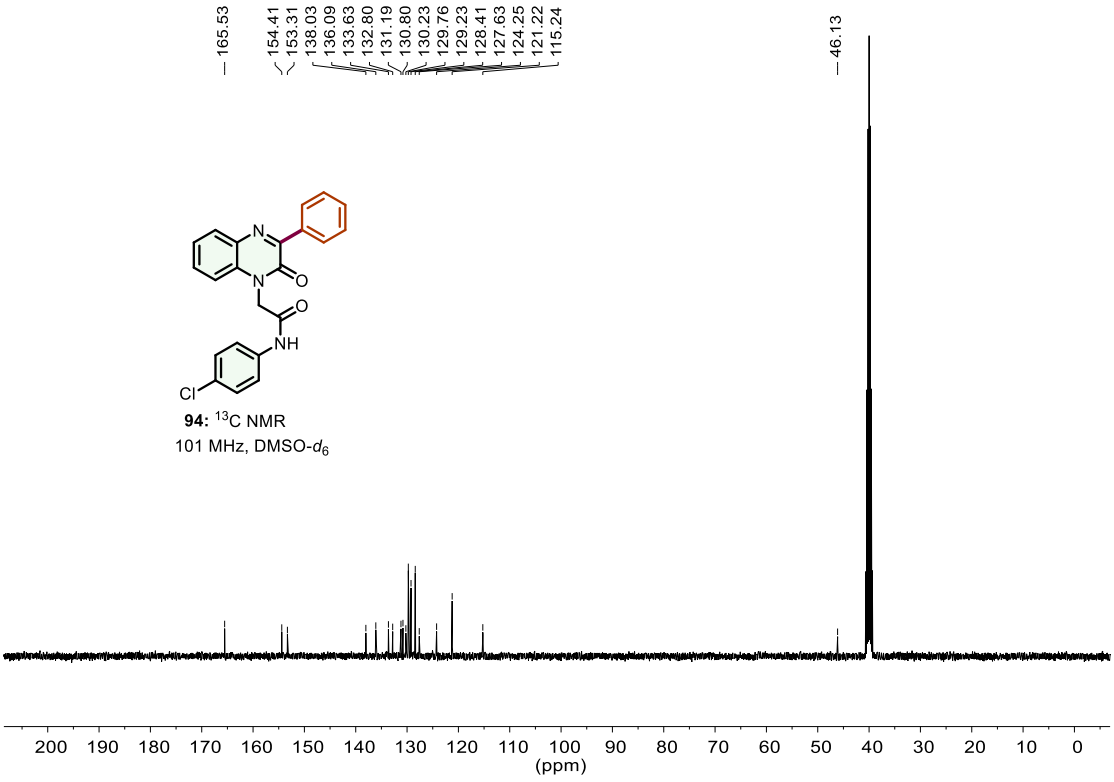


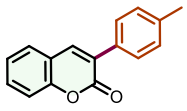
93: ^{1}H NMR
400 MHz, $CDCl_3$



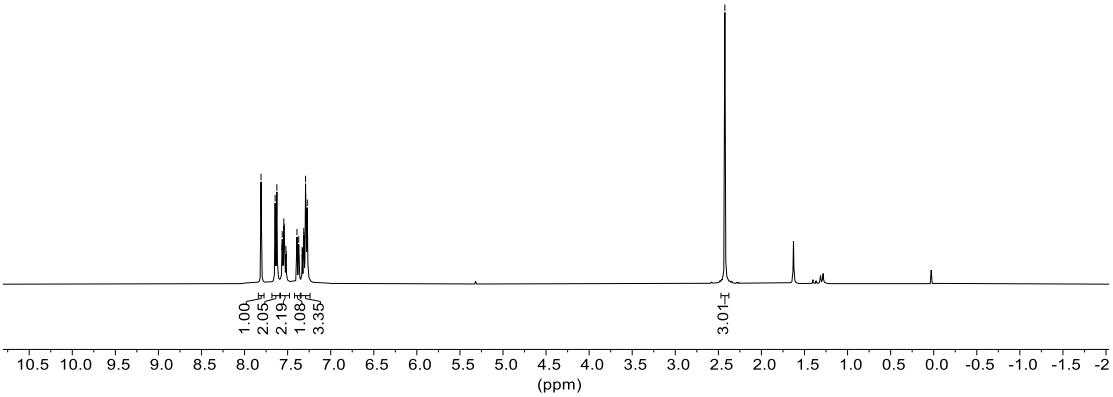
93: ^{13}C NMR
101 MHz, $CDCl_3$

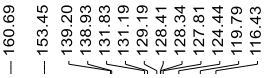

10.63
8.29
8.28
8.28
8.28
8.27
8.27
8.26
7.96
7.96
7.94
7.94
7.67
7.66
7.65
7.65
7.64
7.63
7.63
7.63
7.62
7.61
7.60
7.60
7.58
7.58
7.55
7.54
7.53
7.53
7.53
7.52
7.52
7.51
7.51
7.50
7.50
7.49
7.46
7.45
7.44
7.44
7.43
7.42
7.42
7.40
7.39
7.38
7.38
5.22
N
N
O
O
NH
Cl
94: 1H NMR
400 MHz, DMSO-d6
1.01
2.01
0.99
4.00
3.03
1.02
2.04
2.00
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
(ppm)

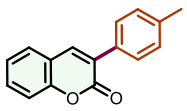

165.53
154.41
153.31
138.03
136.09
133.63
132.80
131.19
130.80
130.23
129.76
129.23
128.41
127.63
124.25
121.22
115.24
46.13
N
N
O
O
NH
Cl
94: 13C NMR
101 MHz, DMSO-d6
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)



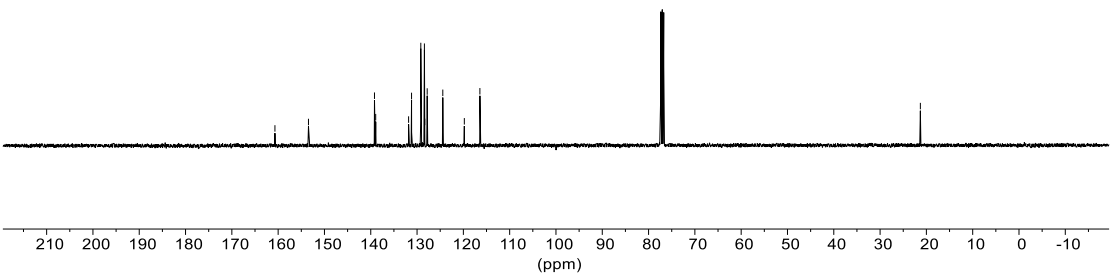
95: ^{1}H NMR
400 MHz, $CDCl_3$

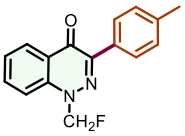




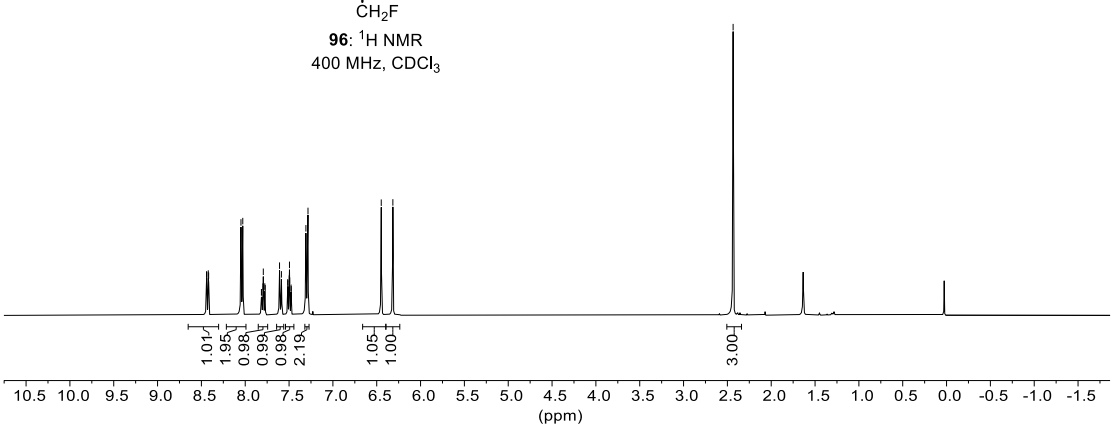


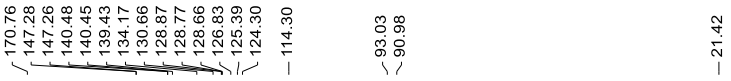
95: ^{13}C NMR
400 MHz, $CDCl_3$

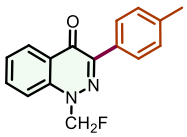




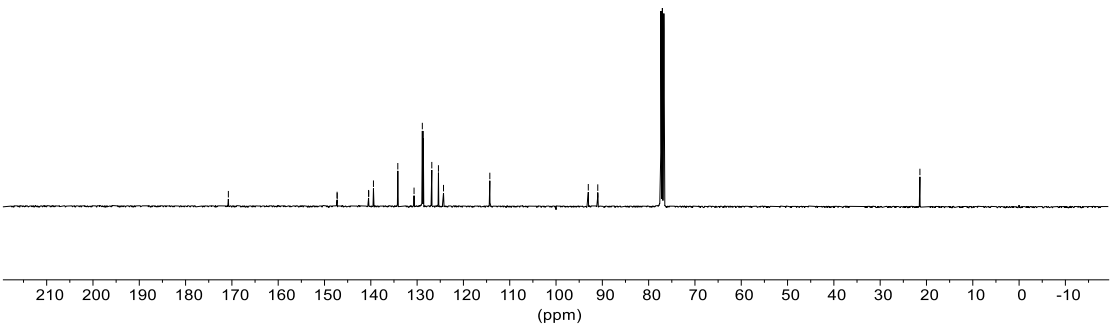
96: ^{1}H NMR
400 MHz, $CDCl_3$

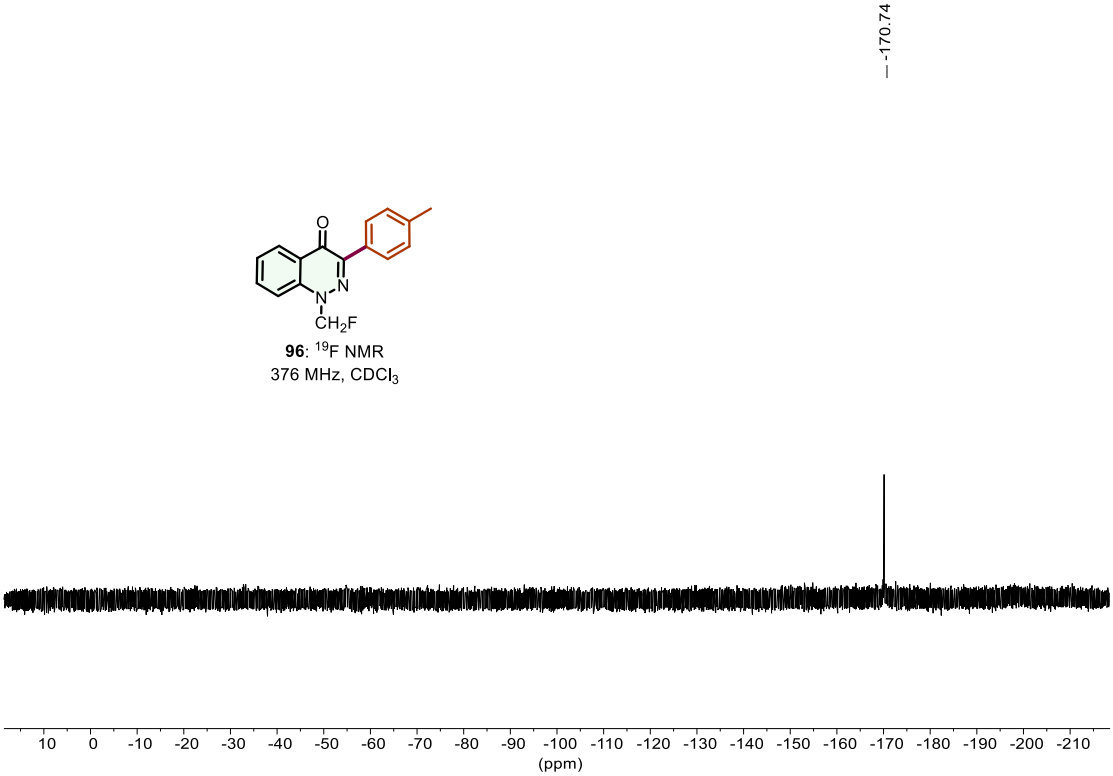




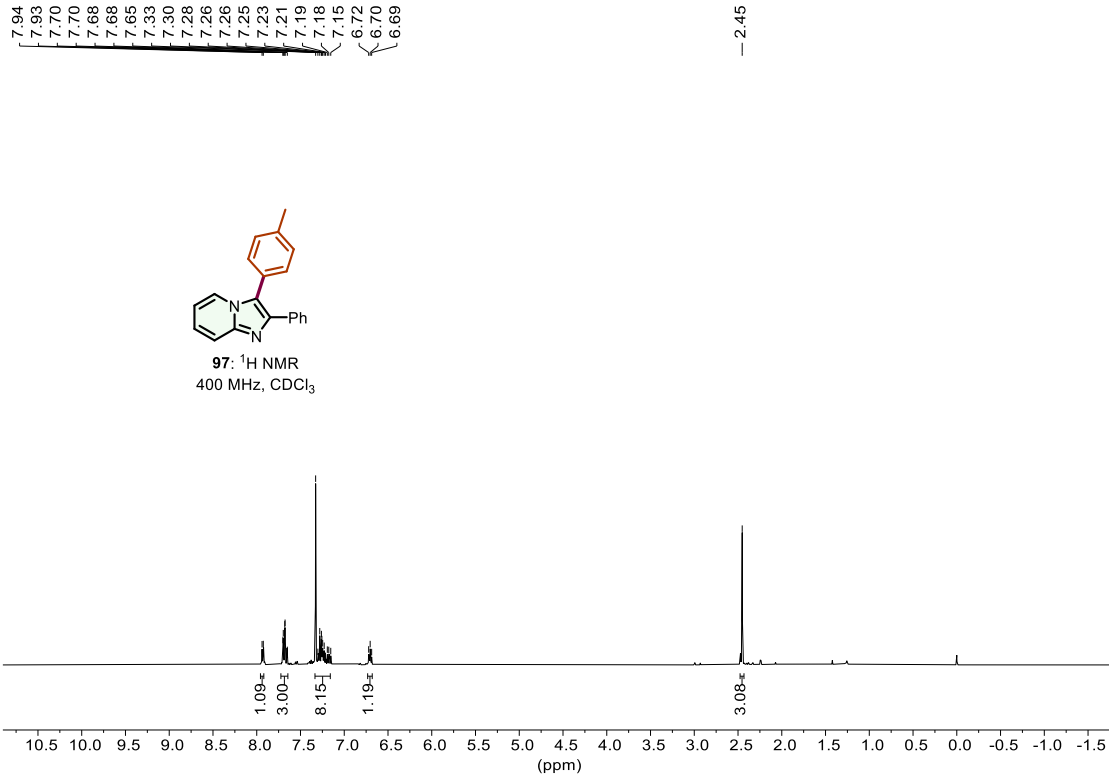


96: ^{13}C NMR
101 MHz, $CDCl_3$

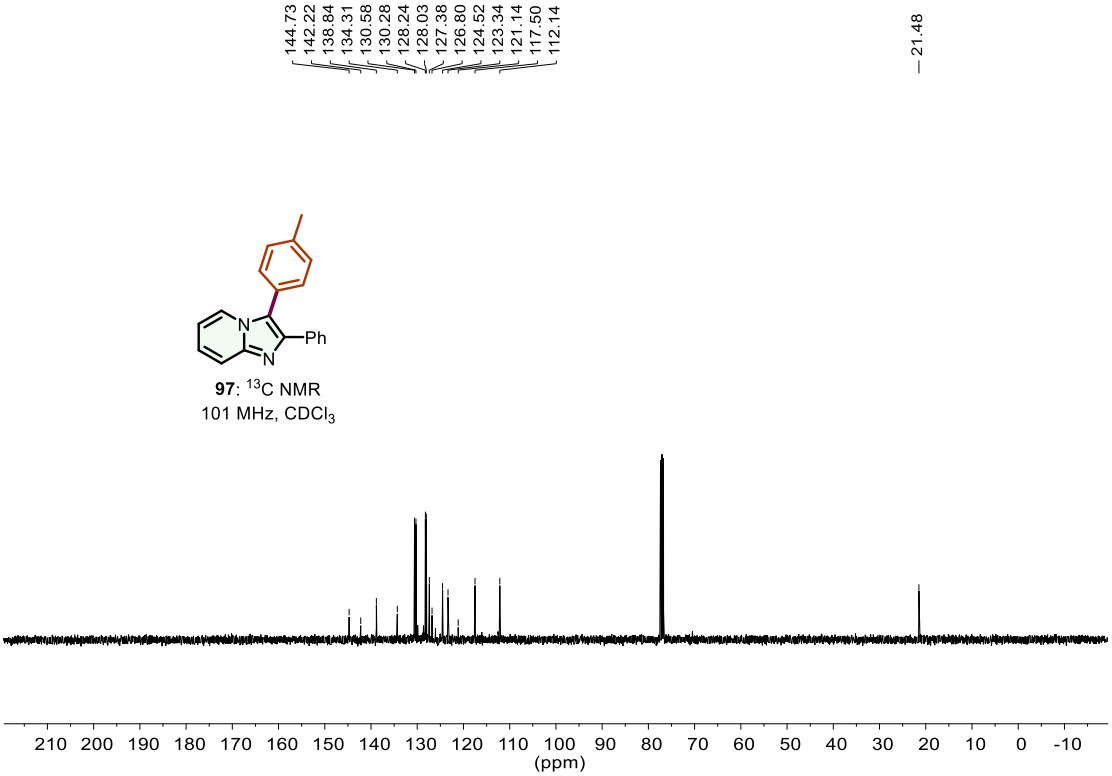




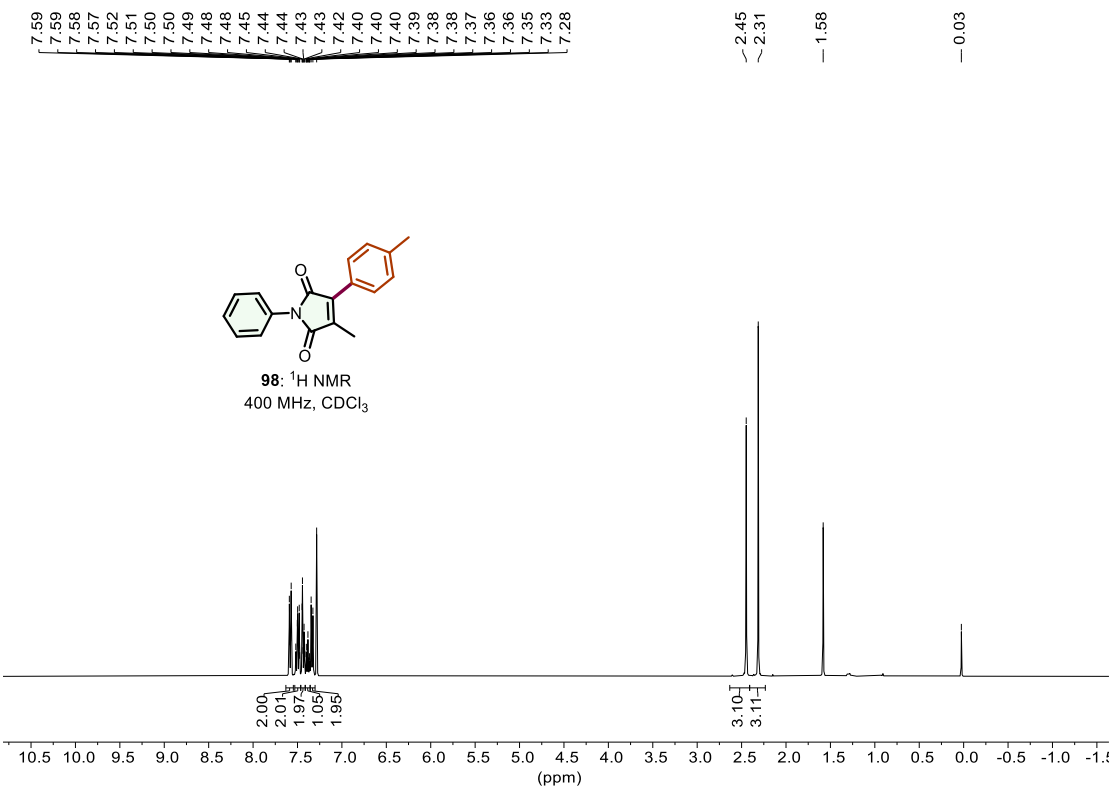
96: ^{19}F NMR
376 MHz, $CDCl_3$



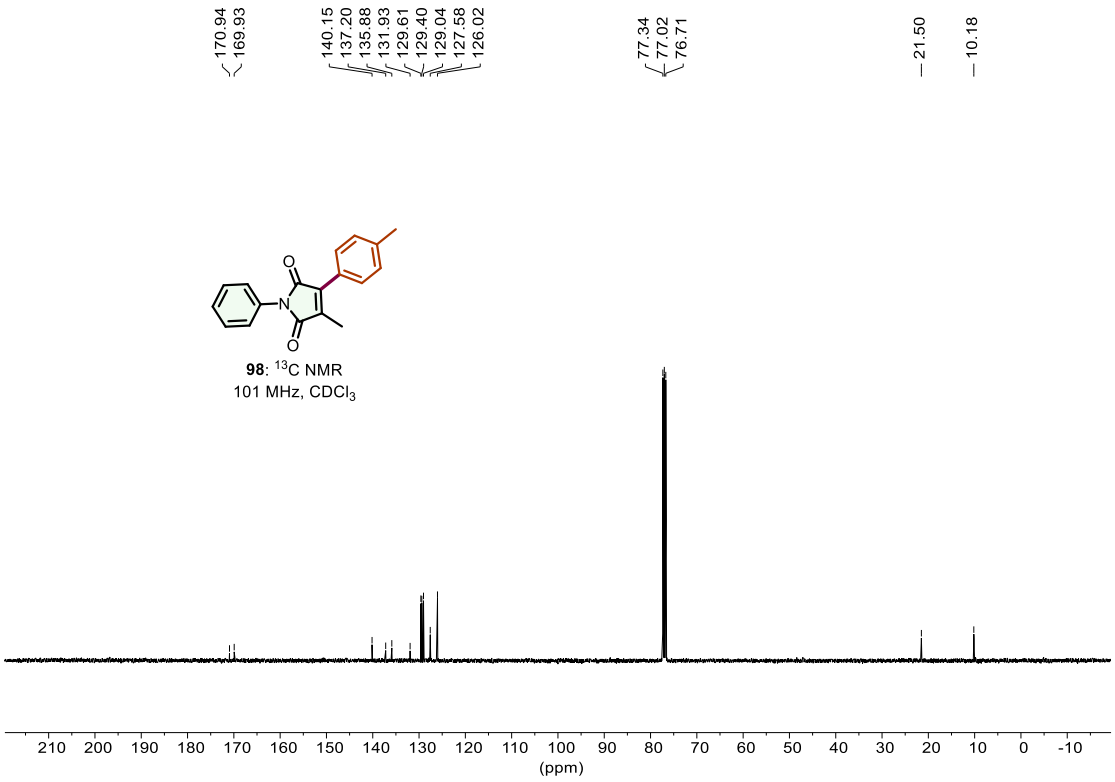
97: ^{1}H NMR
400 MHz, $CDCl_3$

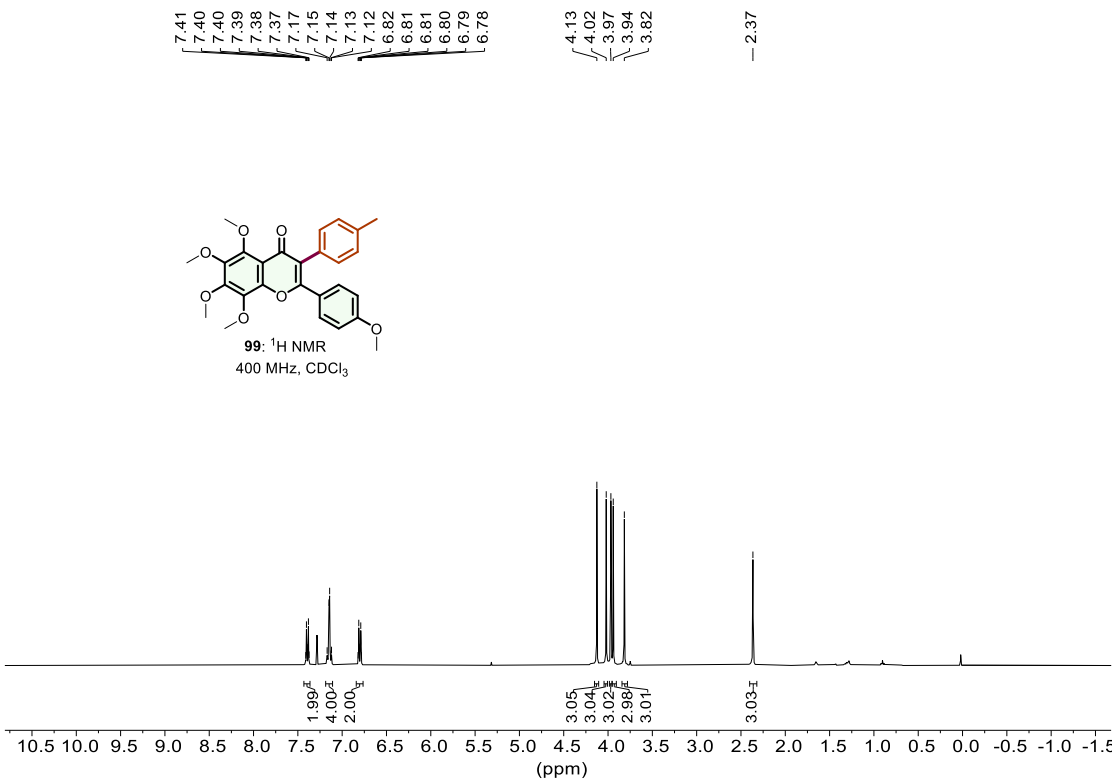


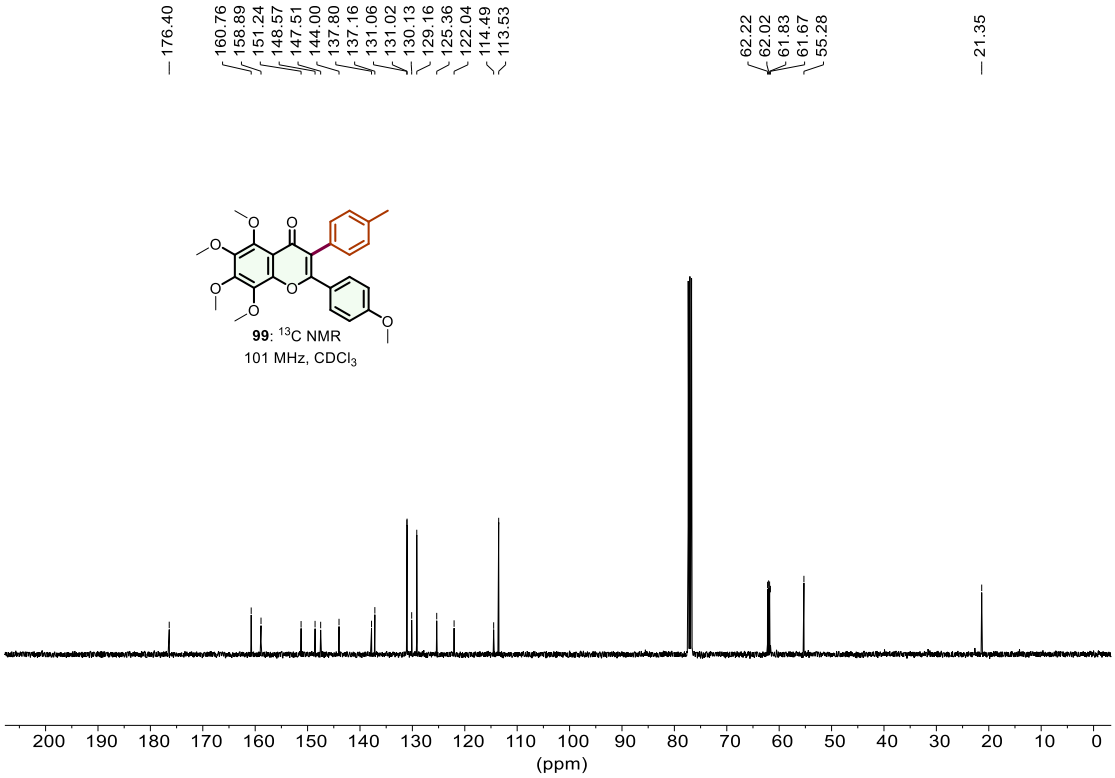
97: ^{13}C NMR
101 MHz, $CDCl_3$

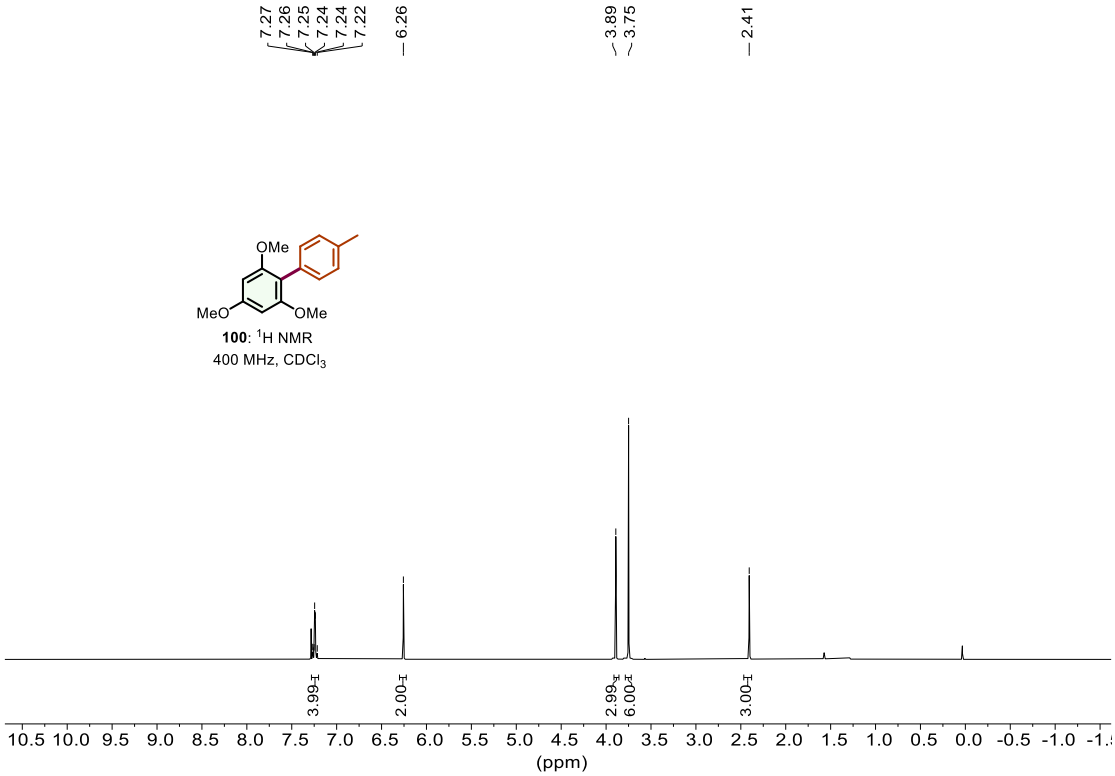


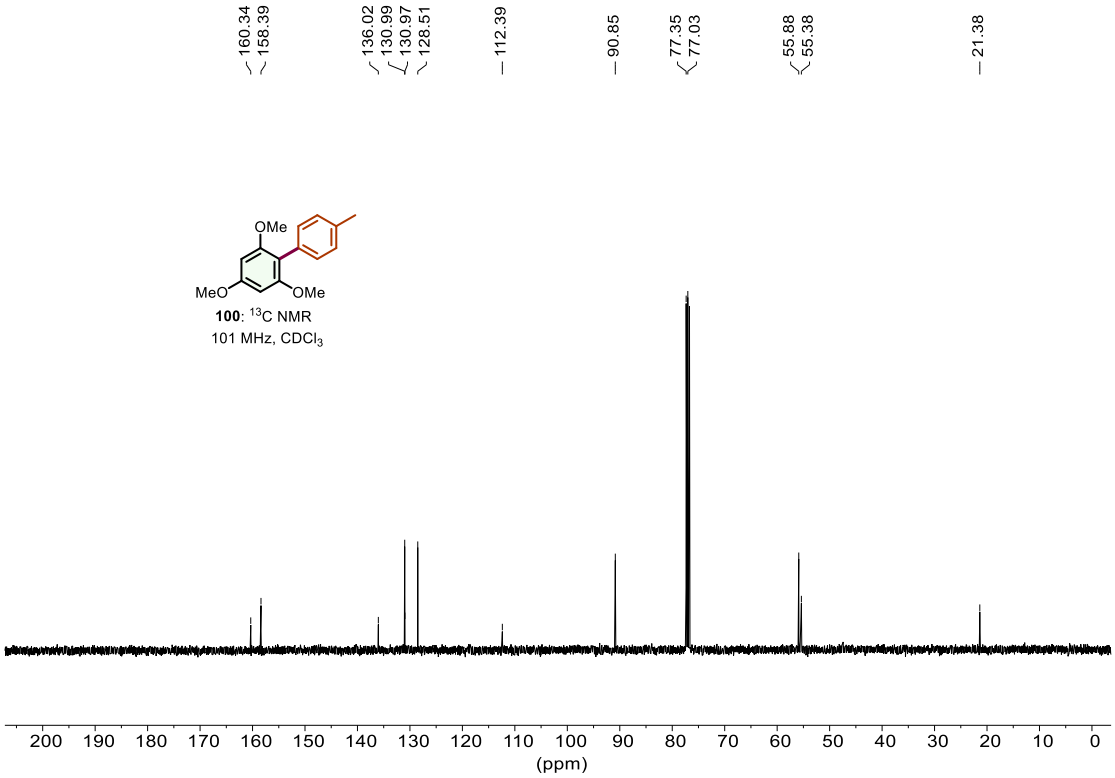
98: ^{1}H NMR
400 MHz, $CDCl_3$


170.94
169.93
140.15
137.20
135.88
131.93
129.61
129.40
129.04
127.58
126.02
77.34
77.02
76.71
21.50
10.18
98: 13C NMR
101 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)


7.41
7.40
7.40
7.39
7.38
7.37
7.17
7.15
7.14
7.13
7.12
6.82
6.81
6.81
6.80
6.79
6.78
4.13
4.02
3.97
3.94
3.82
2.37
99: 1H NMR
400 MHz, CDCl3
1.99
4.00
2.00
3.05
3.04
3.02
2.98
3.01
3.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
(ppm)


176.40
160.76
158.89
151.24
148.57
147.51
144.00
137.80
137.16
131.06
131.02
130.13
129.16
125.36
122.04
114.49
113.53
62.22
62.02
61.83
61.67
55.28
21.35
99: 13C NMR
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


7.27
7.26
7.25
7.24
7.24
7.22
6.26
3.89
3.75
2.41
OMe
MeO
OMe
100: 1H NMR
400 MHz, CDCl3
3.99
2.00
2.99
6.00
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
(ppm)



6. Reference

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