Supporting Information

$(NH_4)_2S_2O_8$ Promoted Tandem Radical Cyclization of Quinazolin-4(3*H*)-ones with Oxamic Acids for Construction of Fused Quinazolinones under Metal-Free Conditions

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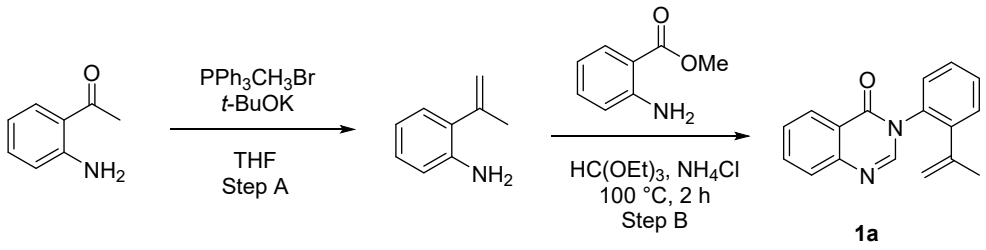
I. General Remarks

Unless otherwise specified, materials were purchased from commercial suppliers and used without further purification. All manipulations were performed in dried sealed tube equipped with a magnetic stir bar under nitrogen atmosphere. Except for the specially mentioned dry solvent, all the solvents were treated according to general methods. All the reactions were monitored by thin-

layer chromatography (TLC) and were visualized using UV light. The product purification was done using silica gel column chromatography. Thin-layer chromatography (TLC) characterization was performed with precoated silica gel GF254 (0.2 mm), while column chromatography characterization was performed with silica gel (200-300 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded with tetramethylsilane (TMS, δ = 0.00 ppm) as the internal standard. ^{1}H NMR spectra were recorded at 400 (Bruker), ^{13}C NMR spectra were recorded at 126 MHz (Bruker). Chemical shifts are reported in ppm downfield from Chloroform-d (δ = 7.26 ppm) or DMSO-d_6 (δ = 2.50 ppm; H_2O signal was found at δ = 3.34 ppm) for ^{1}H NMR and chemical shifts for ^{13}C NMR spectra are reported in ppm relative to the central Chloroform-d (δ = 77.0 ppm). Coupling constants were given in Hz. The following notations were used: br-broad, s-singlet, d-doublet, t-triplet, q-quartet, m-multiplet, dd-doublet of doublet, dt-doublet of triplet, td-triplet of doublet, ddd-doublet of doublet of doublet. Melting points were measured with WRS-1B melting point apparatus (Shanghai Shen Guang Instrument Co., Ltd., Shanghai, China).

II. Experimental Information

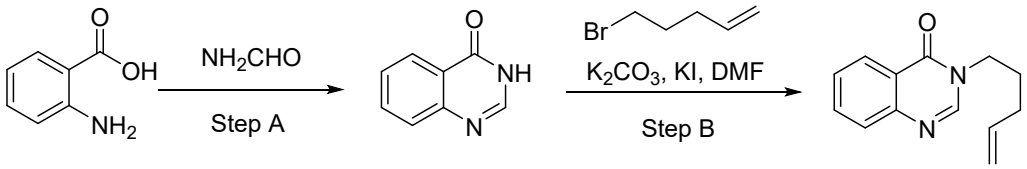
(a) Synthesis of conjugated quinazoline-4(3*H*)-one derivatives 1 (1a as an example) [1]



Step A: Synthesis of 2-(prop-1-en-2-yl) aniline: To a 250 mL oven-dried round-bottom flask was charged with methyltriphenylphosphonium bromide (10.72 g, 30 mmol) and THF (30 mL) under nitrogen atmosphere, followed by the addition of potassium tert-butoxide (3.36 g, 30 mmol) at 0 °C. The reaction mixture was allowed to warm to ambient temperature and stir for 30 minutes. Next, 2- aminoacetophenone (2.42 g, 10 mmol) was added. The reaction mixture was stirred at room temperature overnight. After completion, the reaction was quenched with water, and extracted with ethyl acetate (100 mL). The organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The reaction mixture was purified via flash column chromatography on silica gel to give 2-(prop-1-en-2-yl)aniline as a colorless oil.

Step B: Synthesis of quinazoline-4(3*H*)-one derivative 1a: A mixture of 2-amino-benzoic acid esters (2.5 mmol), 2-(prop-1-en-2-yl) aniline (3.0 mmol), ortho esters (3.8 mmol) and NH_4Cl (1.0 mmol) was heated with stirring at 100 °C for 2 h. After cooling to room temperature, water was added, and the product was extracted with ethyl acetate (2×30 mL). The organic layer was dried with anhydrous Na_2SO_4 and filtered. The filtrate was concentrated in vacuo. The crude product was purified by flash column chromatography on silica gel (PE:EA = 8:1) to afford quinazoline-4(3*H*)-one derivative **1a** as a white solid.

(b) Synthesis of quinazoline-4(3*H*)-one derivatives 1 (1n as an example) [2]

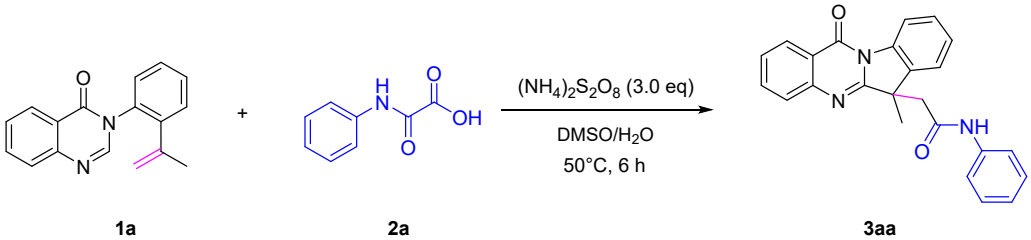


1n

Step A: Synthesis of quinazoline-4(3*H*)-one: To a 10 mL round-bottomed flask equipped with a stir bar were added anthranilic acid (1.37g, 10 mmol) and formamide (4.0 mL, 100 mmol). The reaction mixture was stirred at 130 °C for 4 h. After full consumption of anthranilic acid, the reaction mixture was cooled to room temperature and then poured into icy water. The resultant light precipitates were filtered and washed three times with water (100 mL) and dried over vacuum to give quinazoline-4(3*H*)-one, which was used for the next step without further purification.

Step B: Synthesis of quinazoline-4(3*H*)-one derivative 1n: A 150 mL round-bottom flask equipped with a magnetic stirrer bar was charged with quinazolin-4(3*H*)-one (731mg, 5 mmol), potassium carbonate (1.38g, 10 mmol), and DMF (50 ml). The resulting mixture was heated to 80 °C with stirring for 30 min. After that, KI (83, 5 mmol) was added and after stirring for further 15 min, brominated olefins (711μL, 6 mmol) diluted with DMF (7 mL) was dropwise added into the mixture. The reaction mixture was heated to 60 °C in an oil bath and stirred for 3 h. After the reaction completed, the resulting mixture was cooled to room temperature. The reaction mixture was washed with water and extracted with ethyl acetate three times. The combined organic layer was washed with brine, dried with anhydrous Na_2SO_4 and evaporated, and the residue was purified through flash column chromatography on silica gel to afford desired product **1a** as a white solid.

(c) General procedure for the synthesis of desired products 3 (3a as an example)

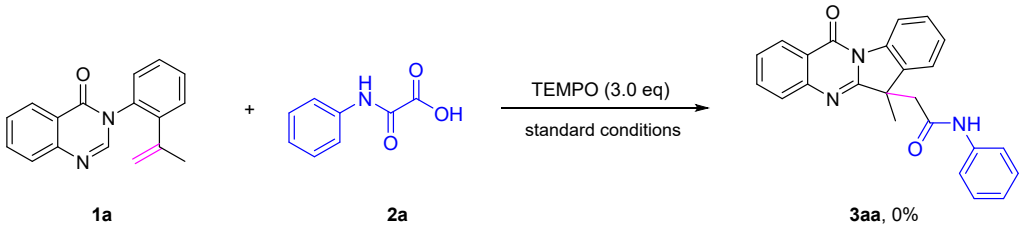


1a **2a** **3aa**

3-(2-(prop-1-en-2-yl)phenyl)quinazolin-4(3*H*)-one **1a** (0.2 mmol) and 2-oxo-2-(phenylamino)acetic acid **2a** (0.6 mmol) were added to a solution of $(NH_4)_2S_2O_8$ (0.6 mmol) in DMSO/H_2O (v/v=2 mL). The reaction mixture was stirred at 50℃. The progress of the reaction was monitored by TLC. Typically, the reaction was completed within 6 hours. After completion, 10 mL of saturated potassium carbonate solution was added, and the mixture was extracted with ethyl acetate (10 mL × 3). The solvent was then removed under vacuum. The residue was purified by flash column chromatography using a mixture of dichloromethane and ethyl acetate as the eluent, resulting in the desired product **3aa**, with a yield of 81%.

III. Mechanistic Studies

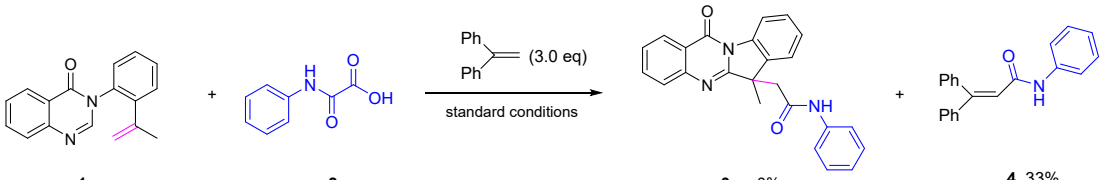
(a) Radical-trapping experiment using TEMPO as the radical scavenger



1a **2a** **3aa**, 0%

3-(2-(prop-1-en-2-yl)phenyl)quinazolin-4(3*H*)-one **1a** (0.2 mmol), 2-oxo-2-(phenylamino)acetic acid **2a** (0.6 mmol) and TEMPO (93.8 mg, 0.6 mmol) were added to a solution of $(NH_4)_2S_2O_8$ (0.6 mmol) in DMSO/H_2O (v/v=2 mL). The reaction mixture was stirred at 50℃. The progress of the reaction was monitored by TLC. Typically, the reaction was completed within 6 hours. After the specified time, no corresponding product **3aa** was formed by TLC analysis, suggesting that the in-situ formed phosphine radical might act as a key intermediate during this transformation.

(b) Control reaction using 1,1-diphenylethylene as the radical-trapping reagent

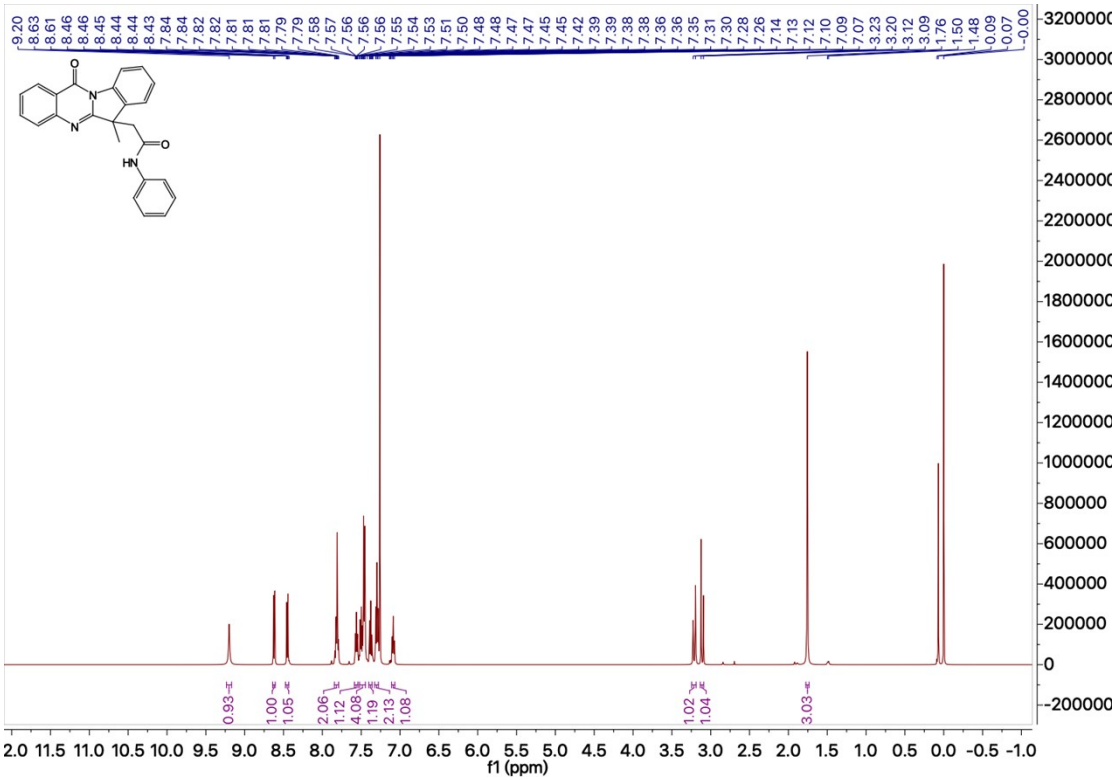


1a **2a** **3aa**, 0% **4**, 33% detected by LC-MS

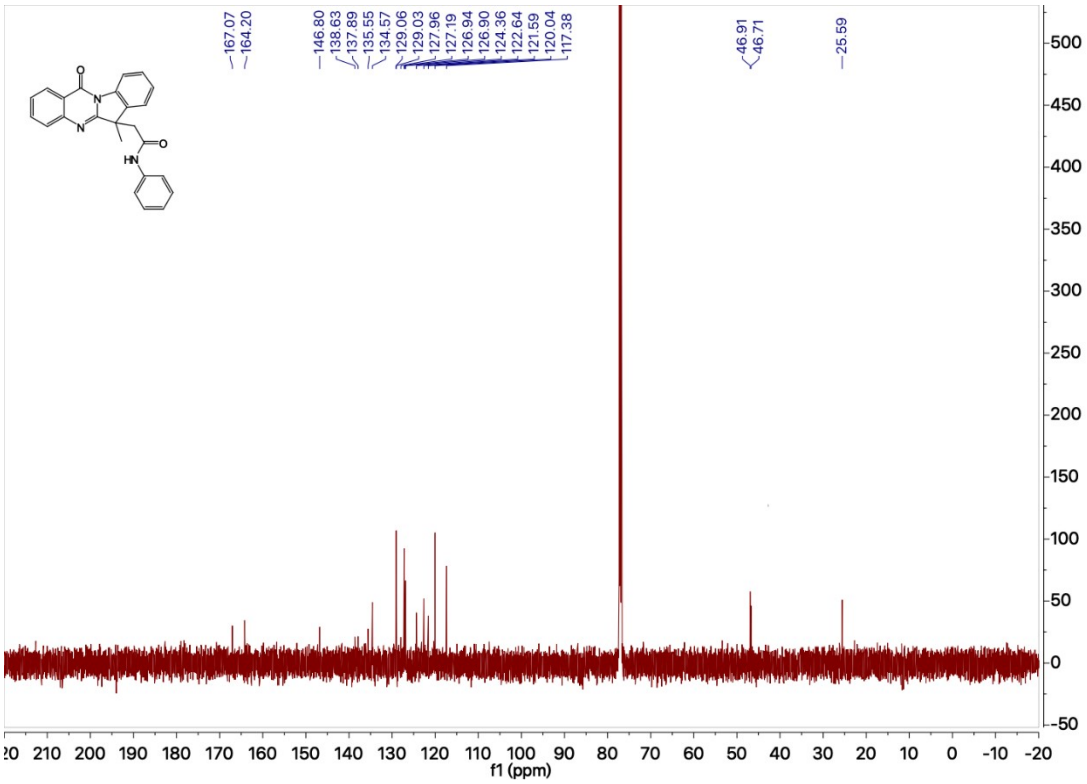
3-(2-(prop-1-en-2-yl)phenyl)quinazolin-4(3*H*)-one **1a** (0.2 mmol), 2-oxo-2-(phenylamino)acetic acid **2a** (0.6 mmol) and 1,1- diphenylethylene (106.4 μL, 0.6 mmol) were added to a solution of $(NH_4)_2S_2O_8$ (0.6 mmol) in DMSO/H_2O (v/v=2 mL). The reaction mixture was stirred at 50℃. The progress of the reaction was monitored by TLC. Typically, the reaction was completed within 6 hours. No corresponding product **3aa** was detected and the heck-type product **4** was isolated in 33.0% yield, indicating that this addition/cyclization scheme induced by the oxidant may proceed through a radical-based mechanism.

IV. NMR spectra of Products

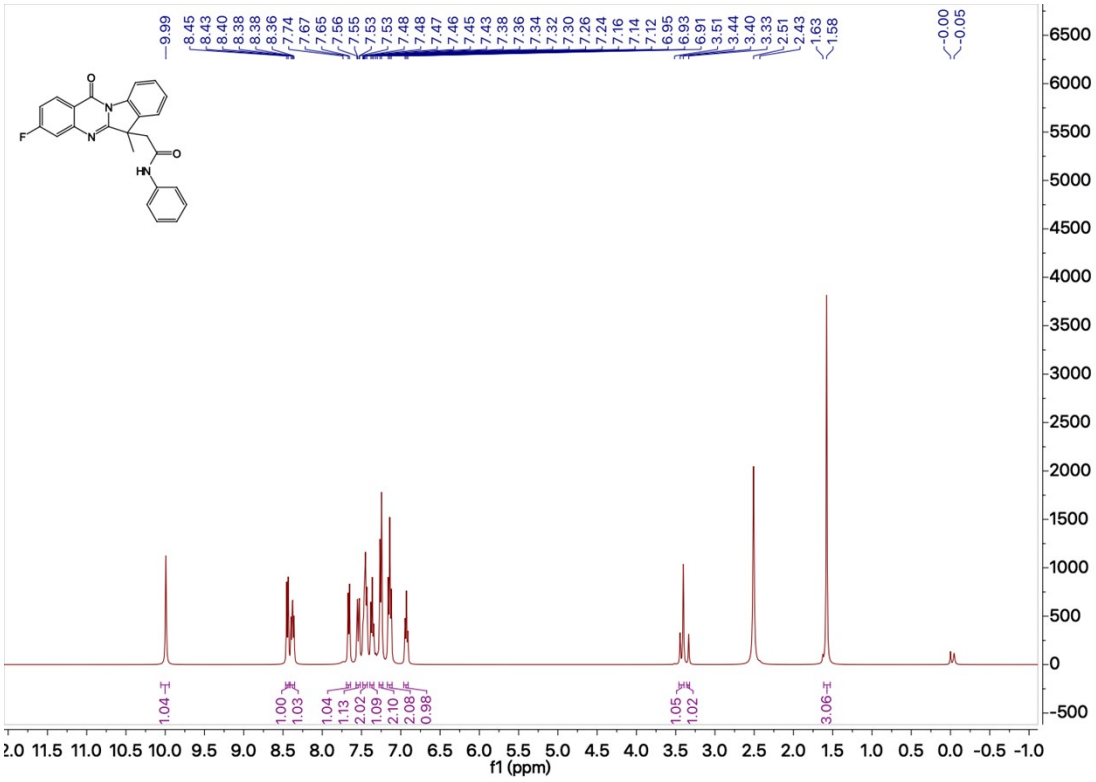
3aa ^{1}H Chloroform-*d*, 500 MHz



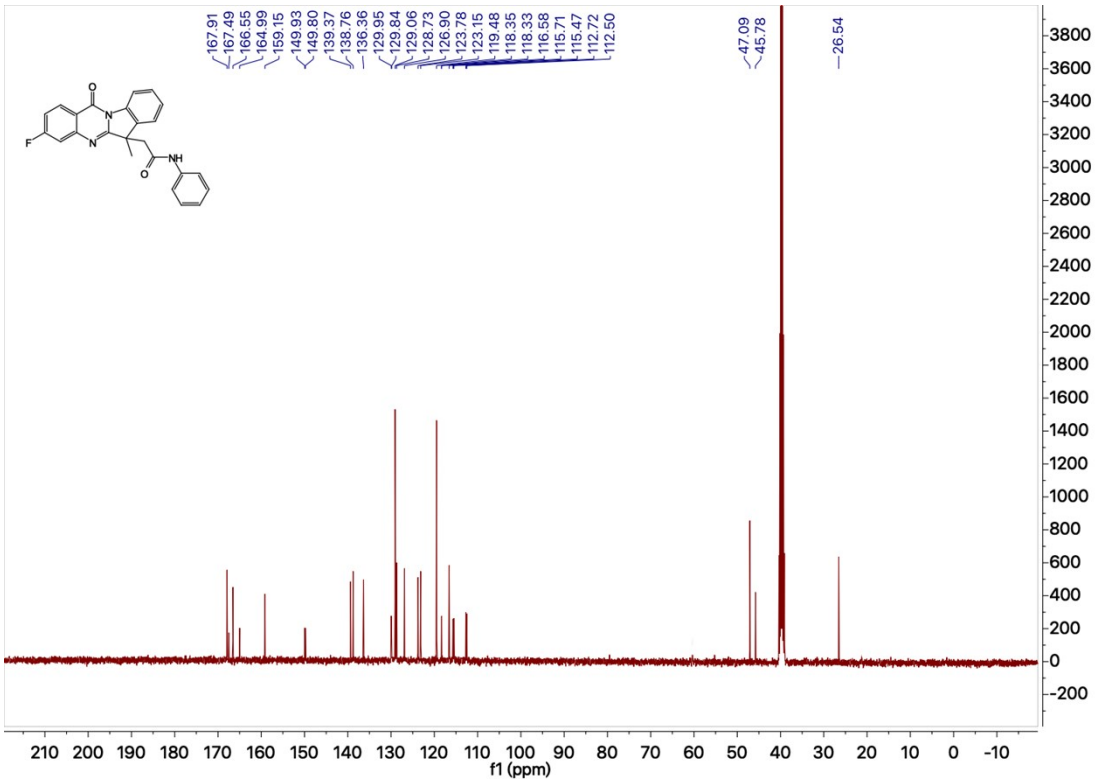
3aa $^{13}C\{1H\}$ Chloroform-*d*, 151 MHz



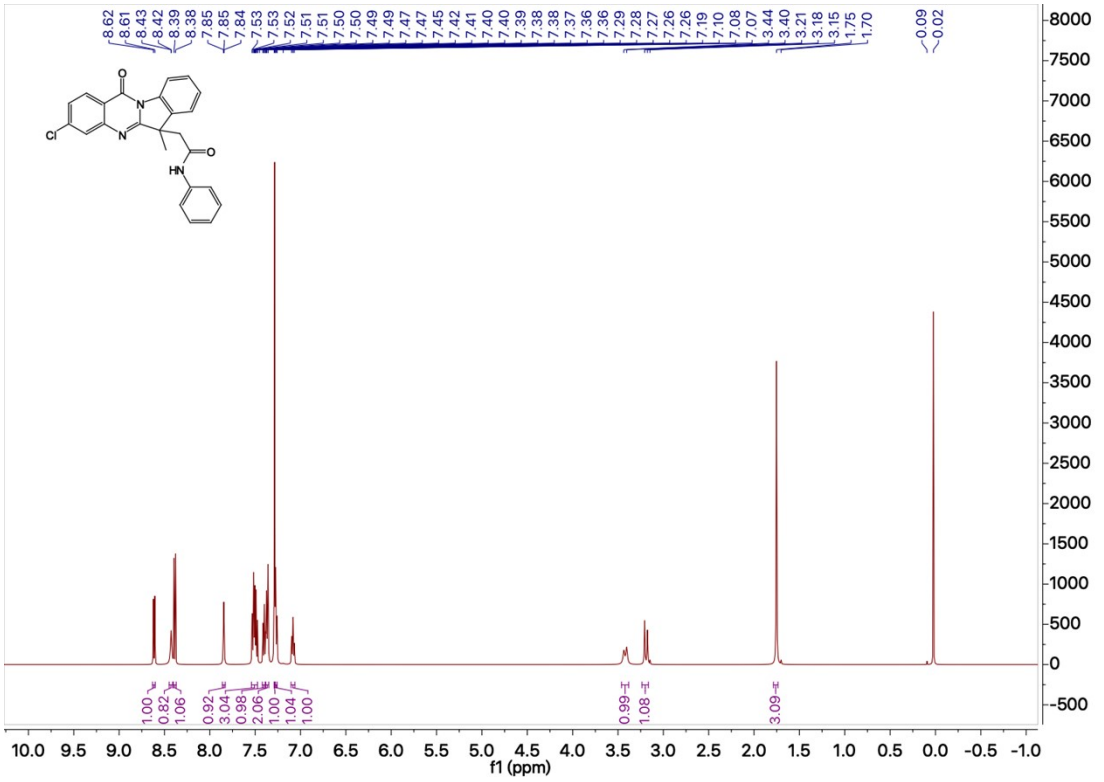
3ab ^{1}H DMSO-d_6, 400 MHz



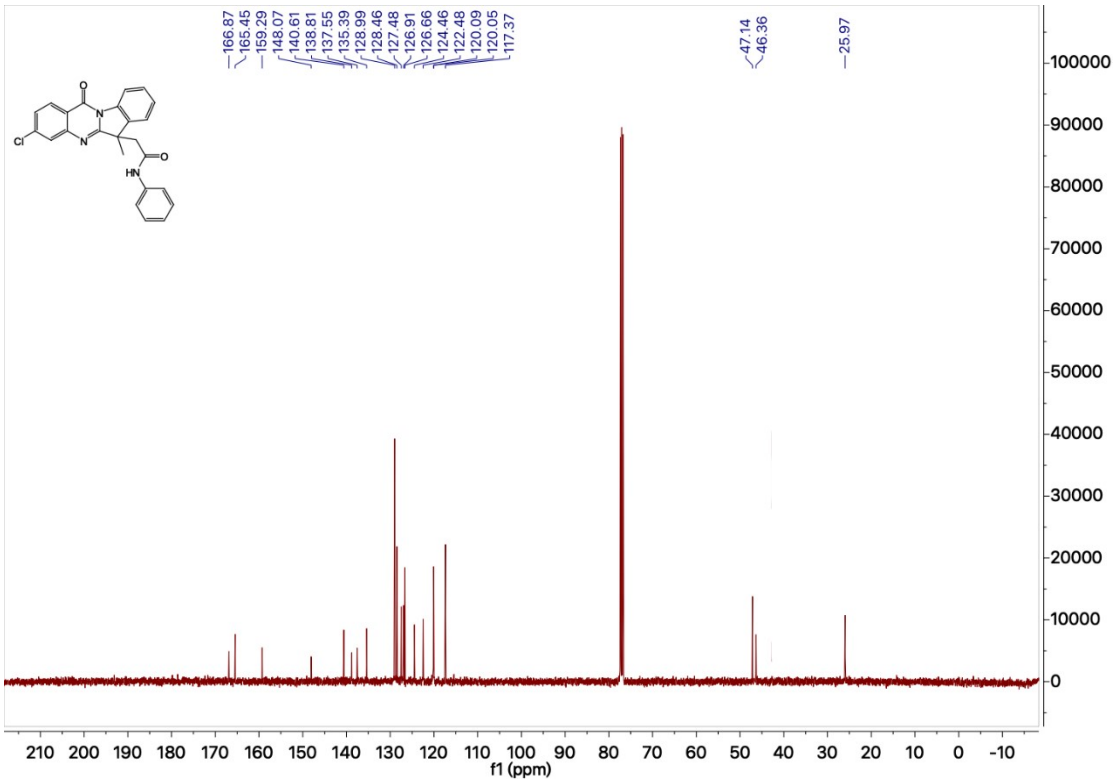
3ab $^{13}C\{1H\}$ DMSO-d_6, 101 MHz



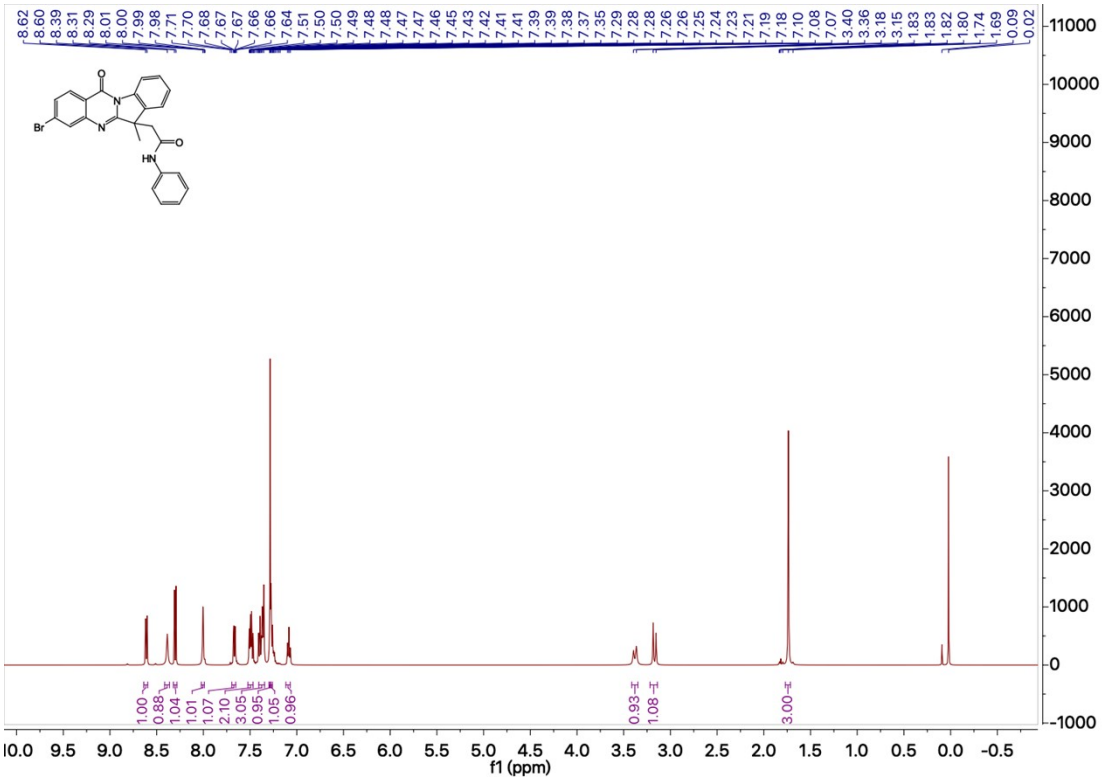
3ac ^{1}H Chloroform-*d*, 500 MHz



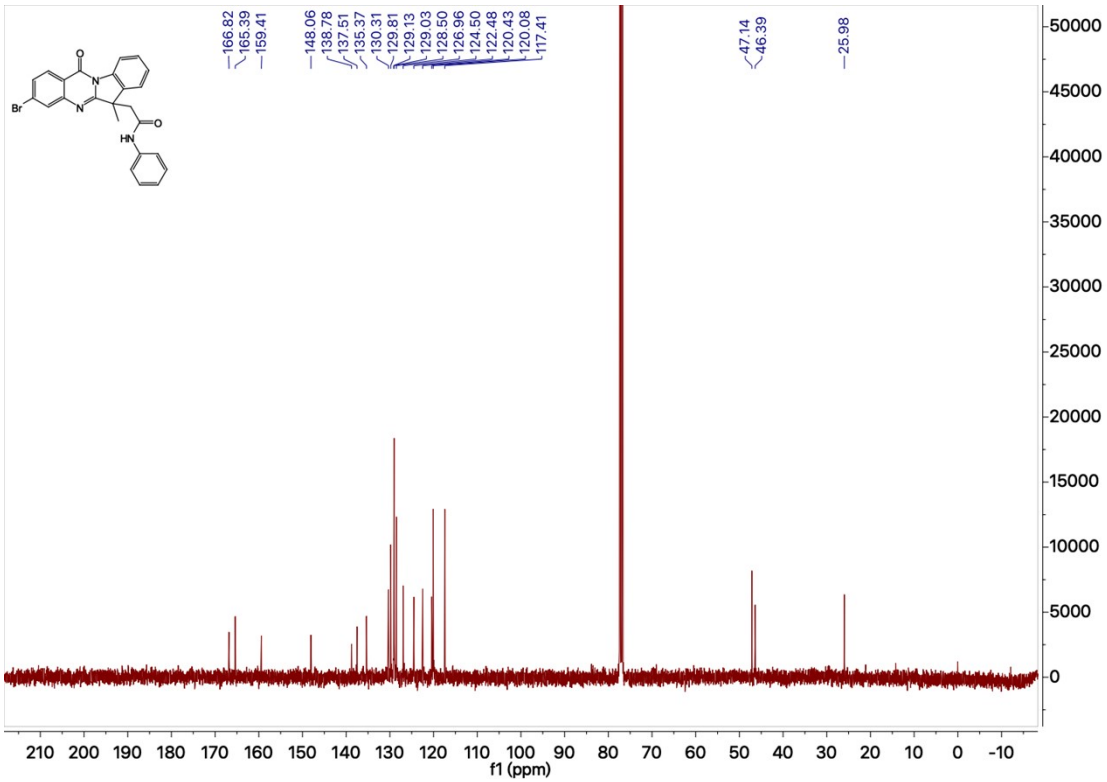
3ac $^{13}C\{1H\}$ Chloroform-*d*, 101 MHz



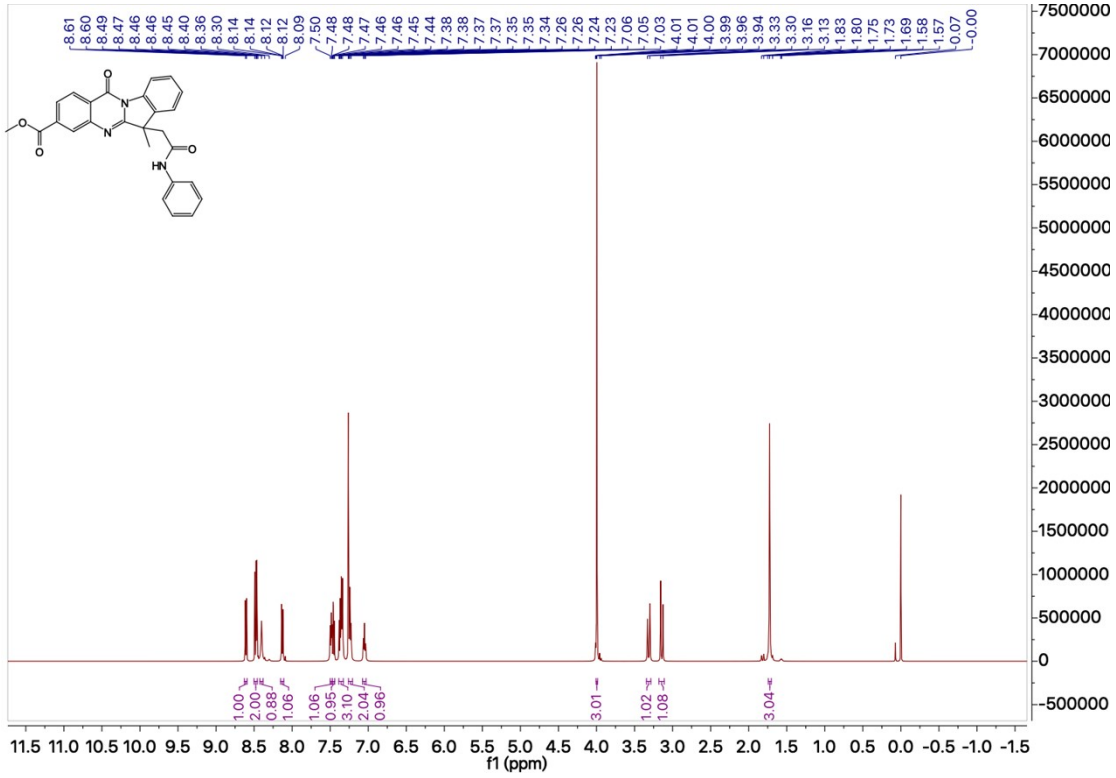
3ad ^{1}H Chloroform-*d*, 500 MHz



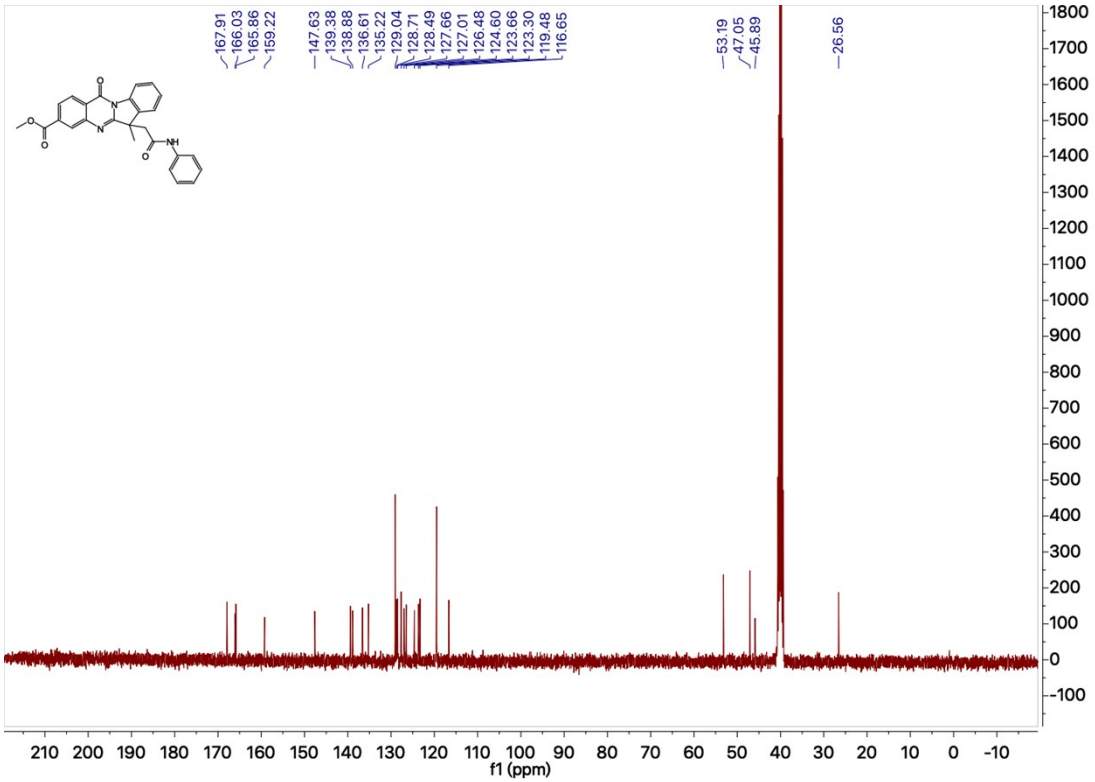
3ad $^{13}C\{1H\}$ Chloroform-*d*, 101 MHz



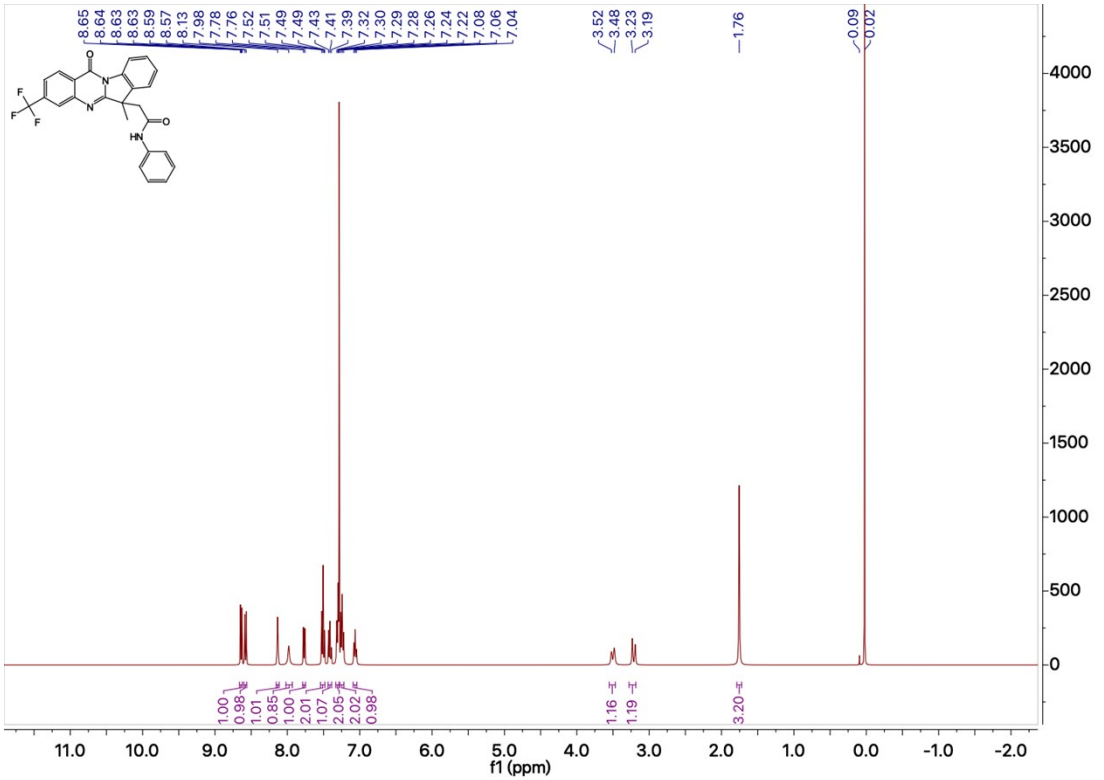
3ae ^{1}H Chloroform-*d*, 500 MHz



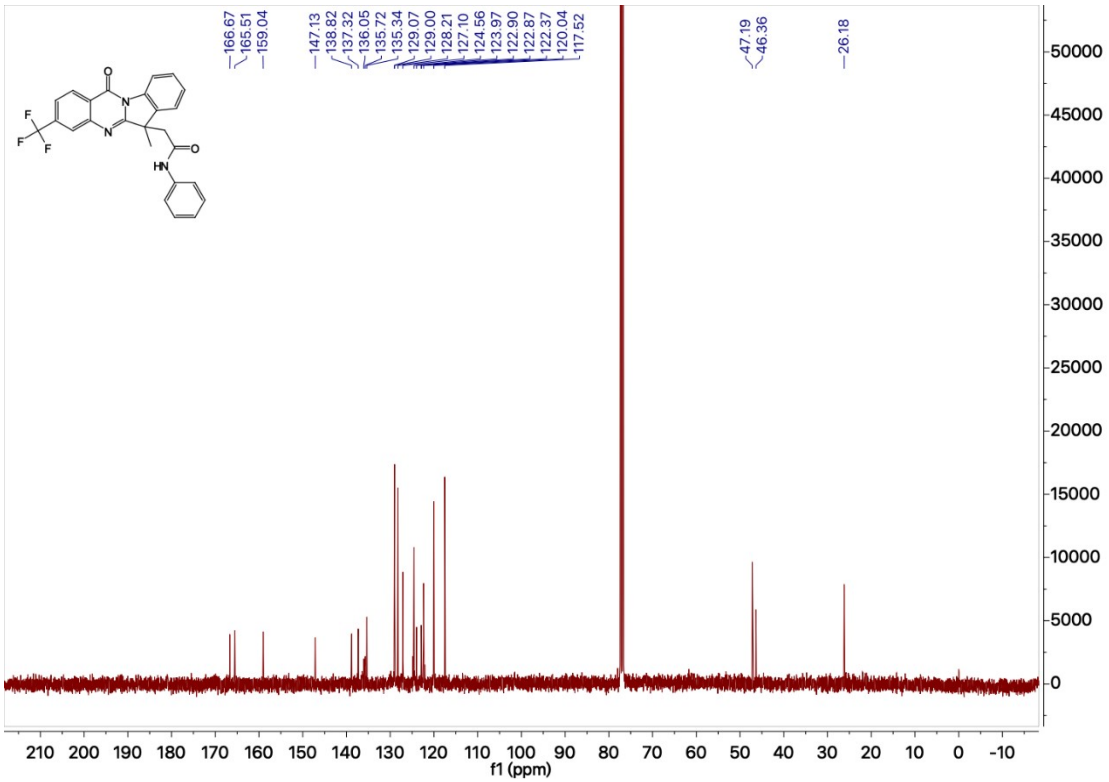
3ae $^{13}C\{1H\}$ DMSO-d_6, 101 MHz



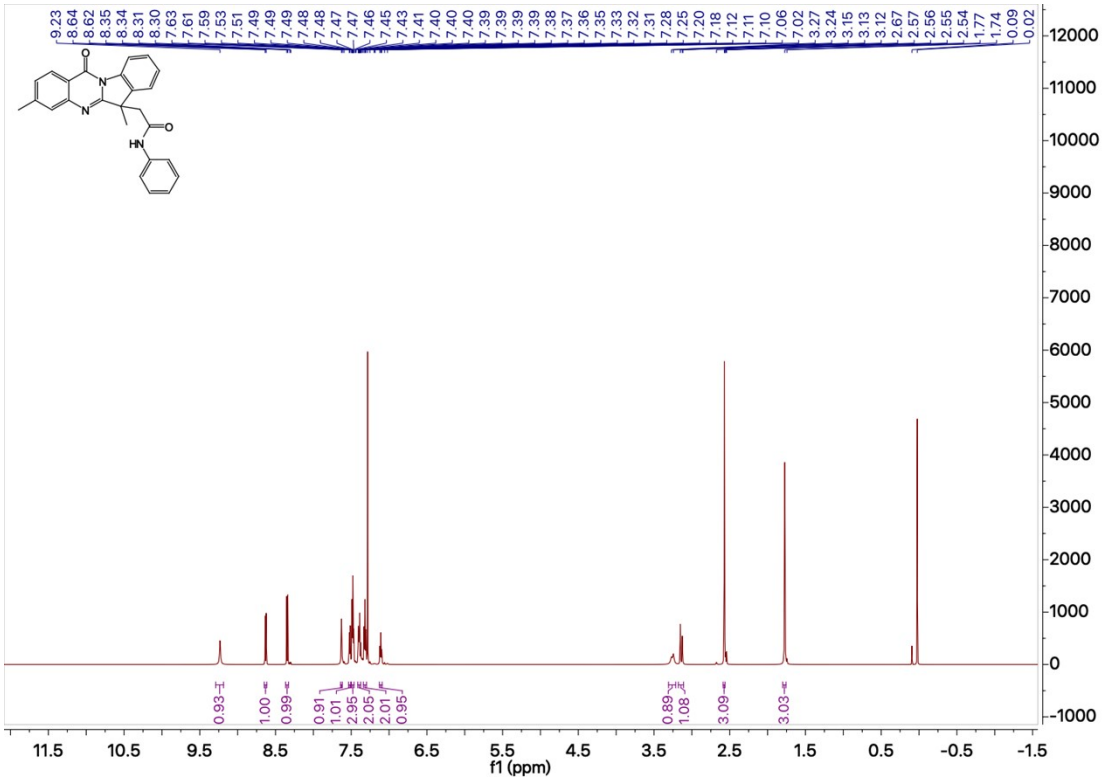
3af ^{1}H Chloroform-*d*, 400 MHz



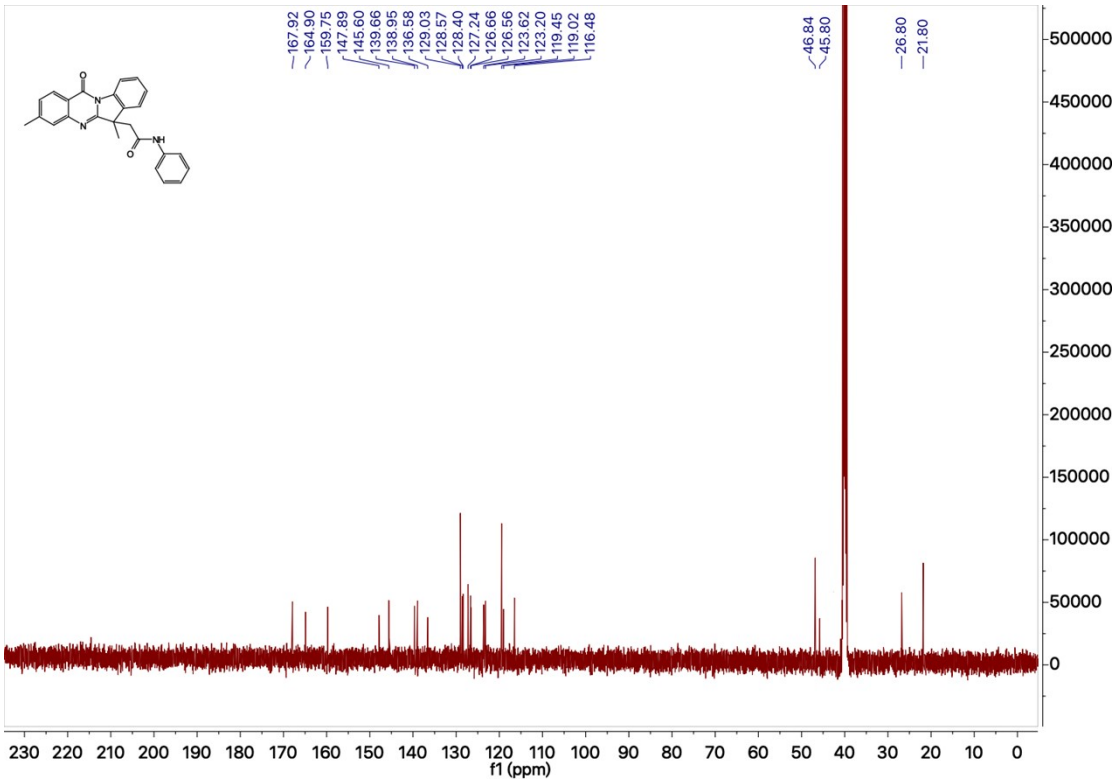
3af $^{13}C\{1H\}$ Chloroform-*d*, 101 MHz



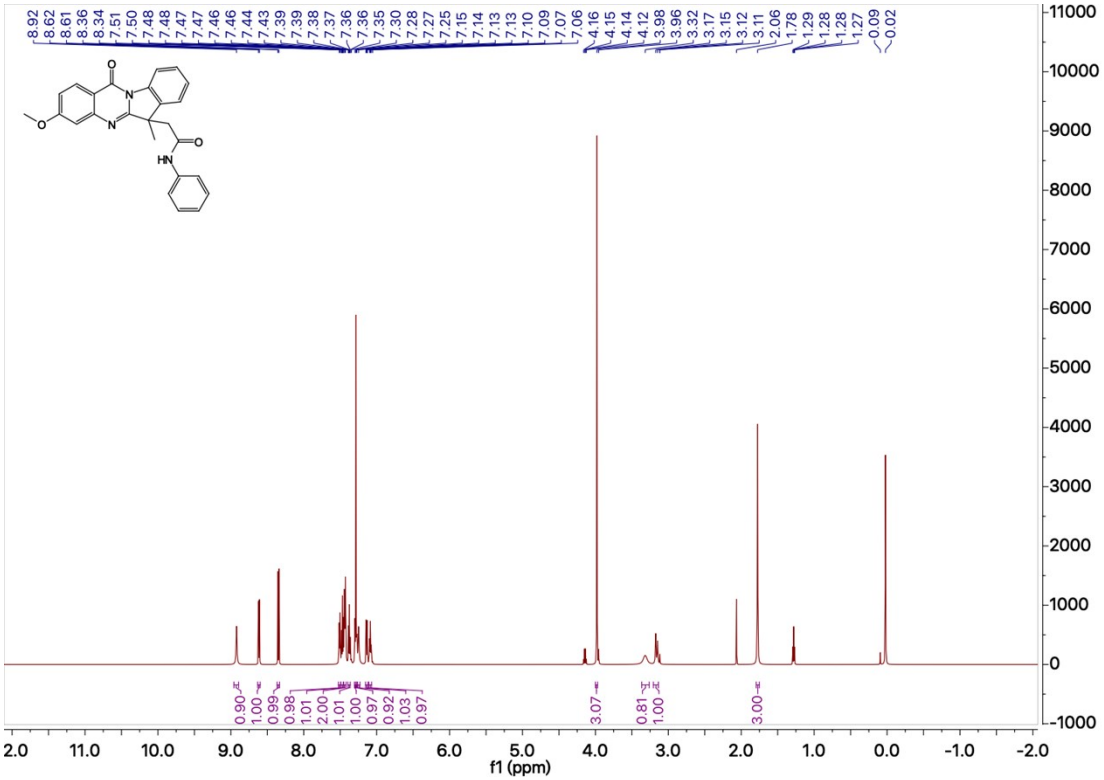
3ag ^{1}H Chloroform-*d*, 600 MHz



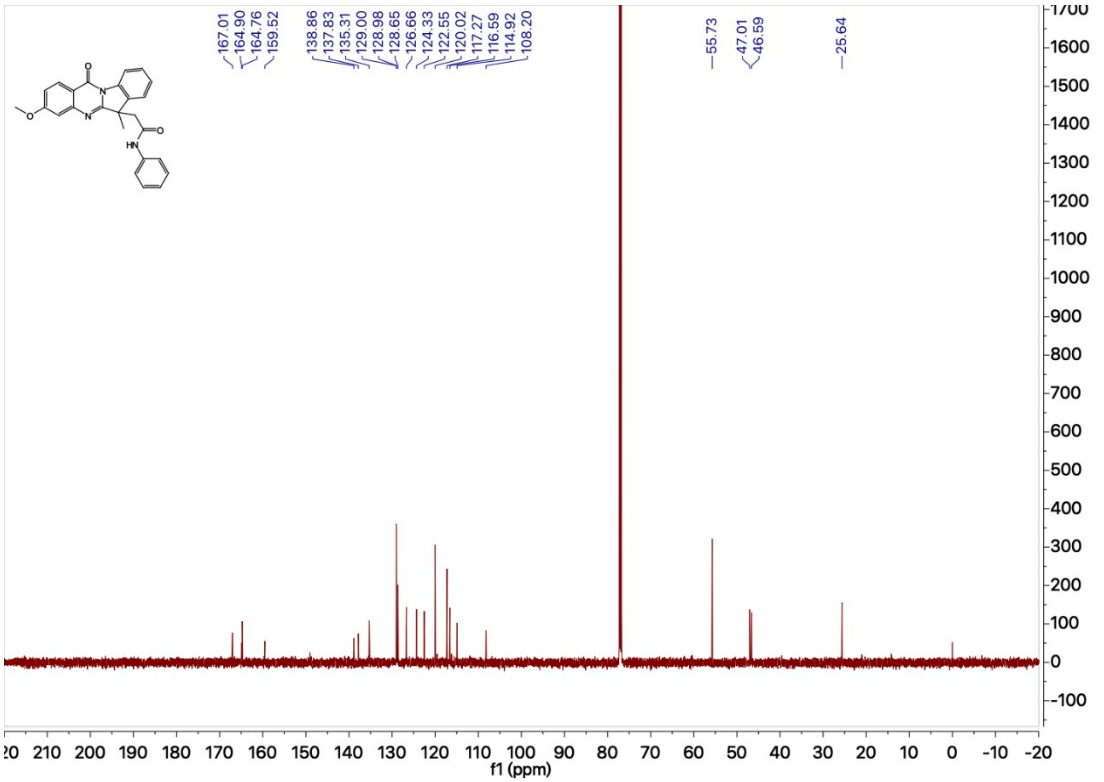
3ag $^{13}C\{1H\}$ DMSO-d_6, 126 MHz



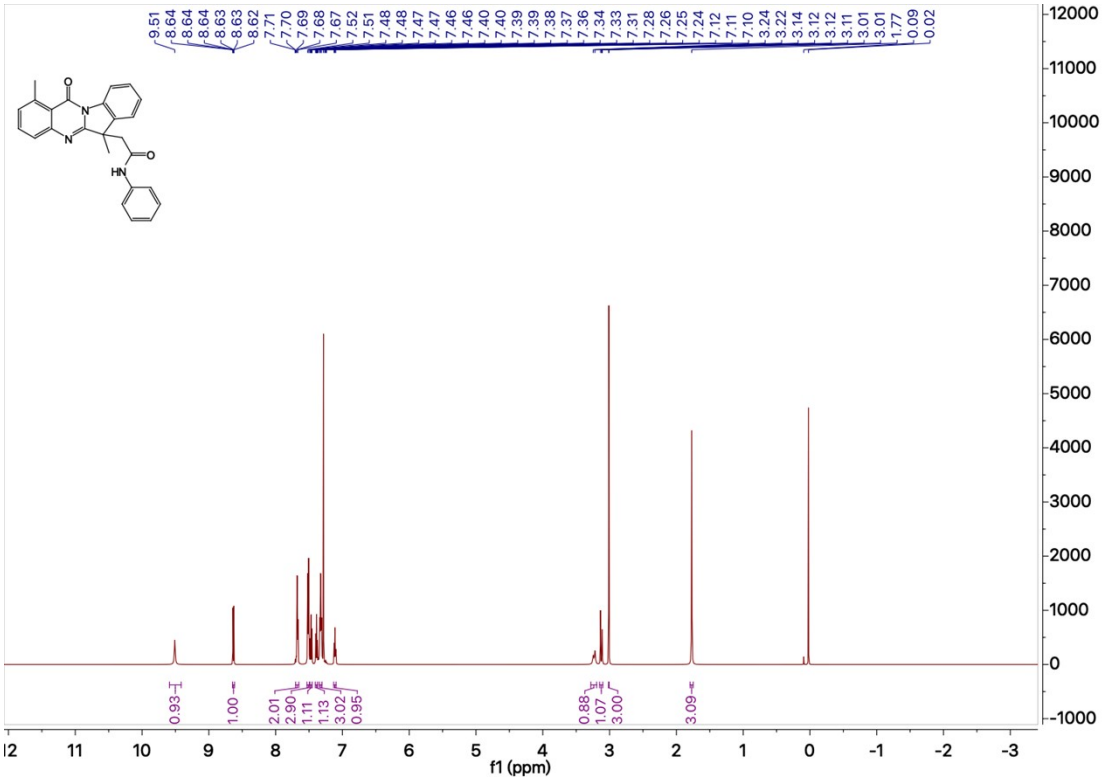
3ah ^{1}H Chloroform-*d*, 600 MHz



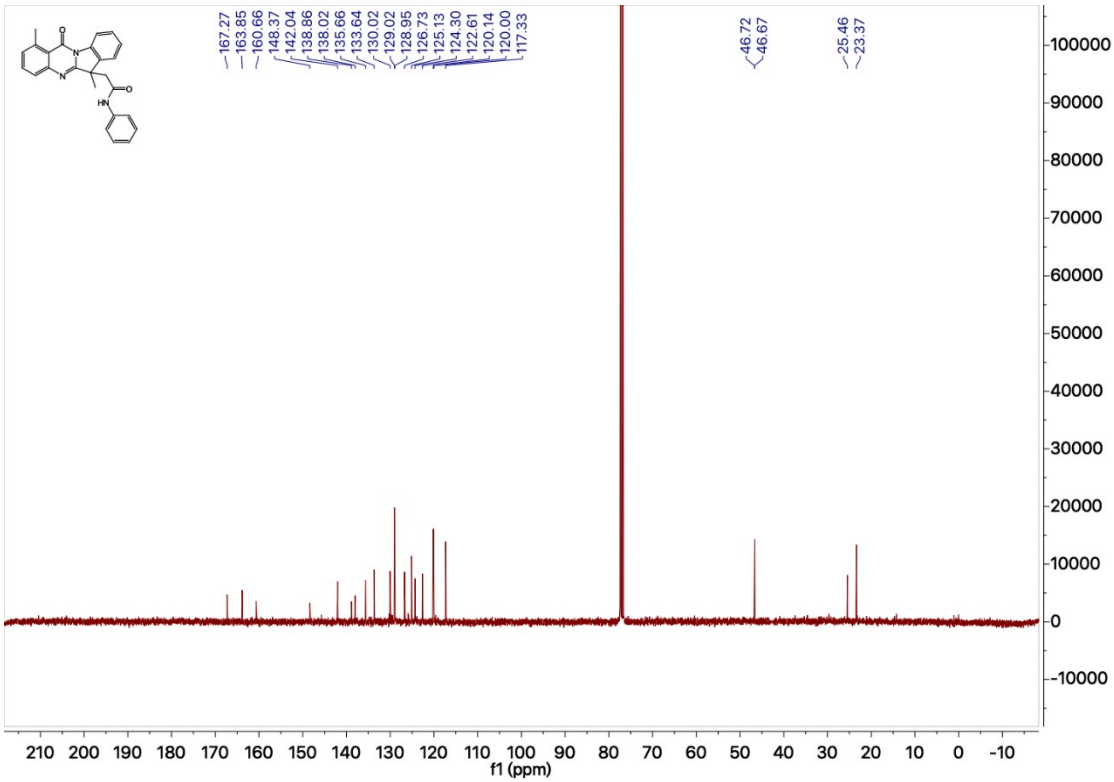
3ah $^{13}C\{1H\}$ Chloroform-*d*, 151 MHz



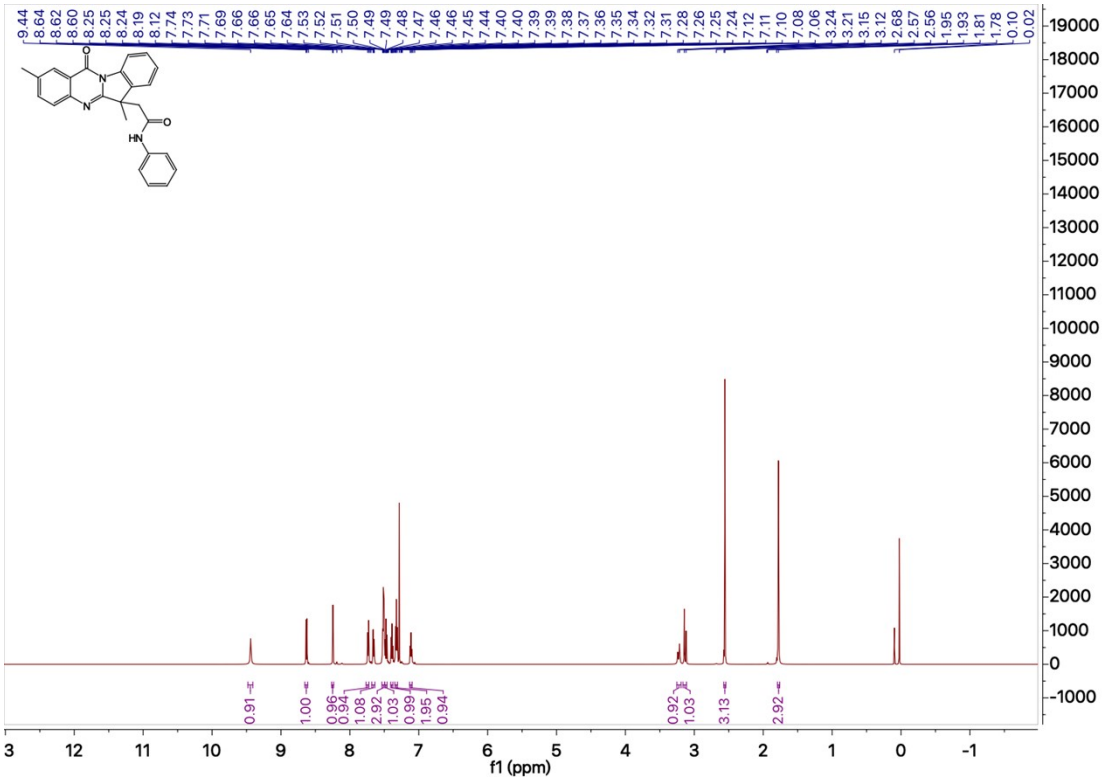
3ai ^{1}H Chloroform-*d*, 600 MHz



3ai $^{13}C\{1H\}$ Chloroform-*d*, 101 MHz



3aj ^{1}H Chloroform-*d*, 600 MHz



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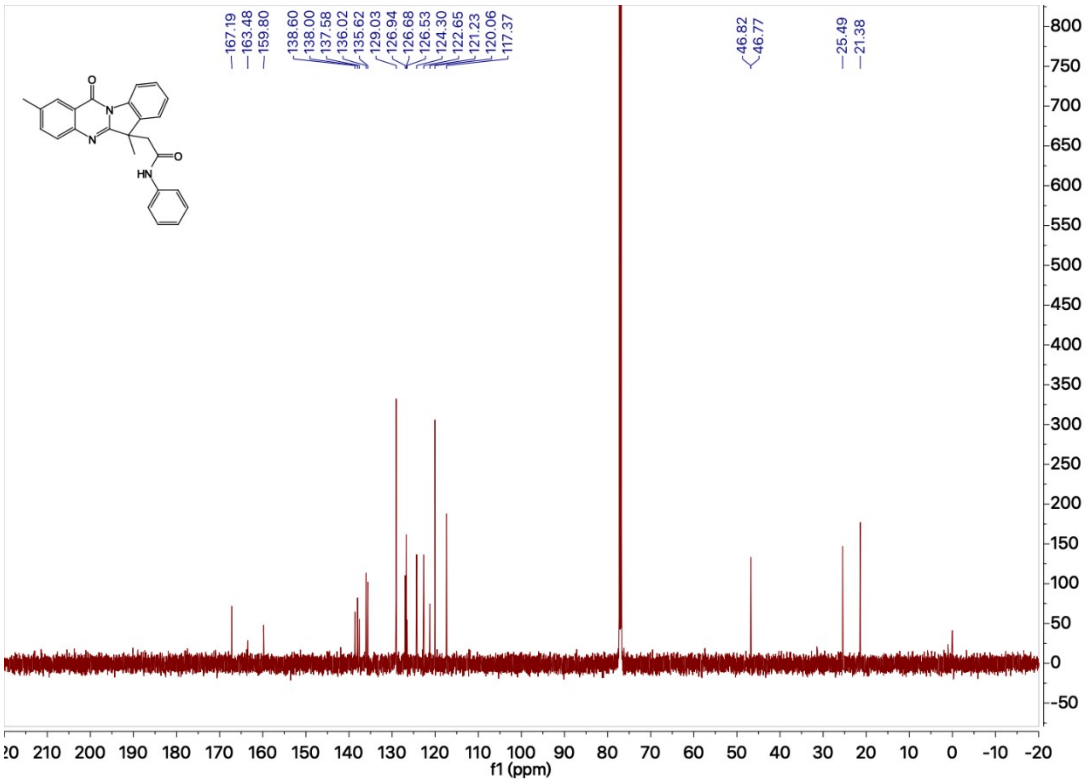
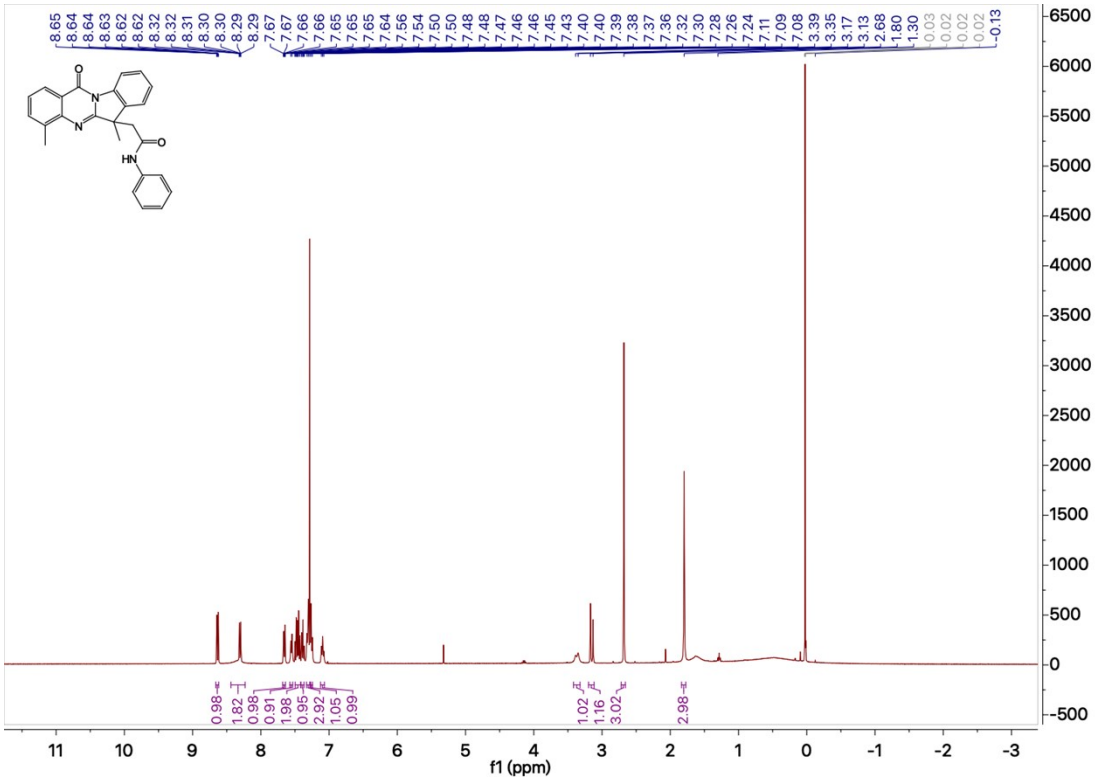
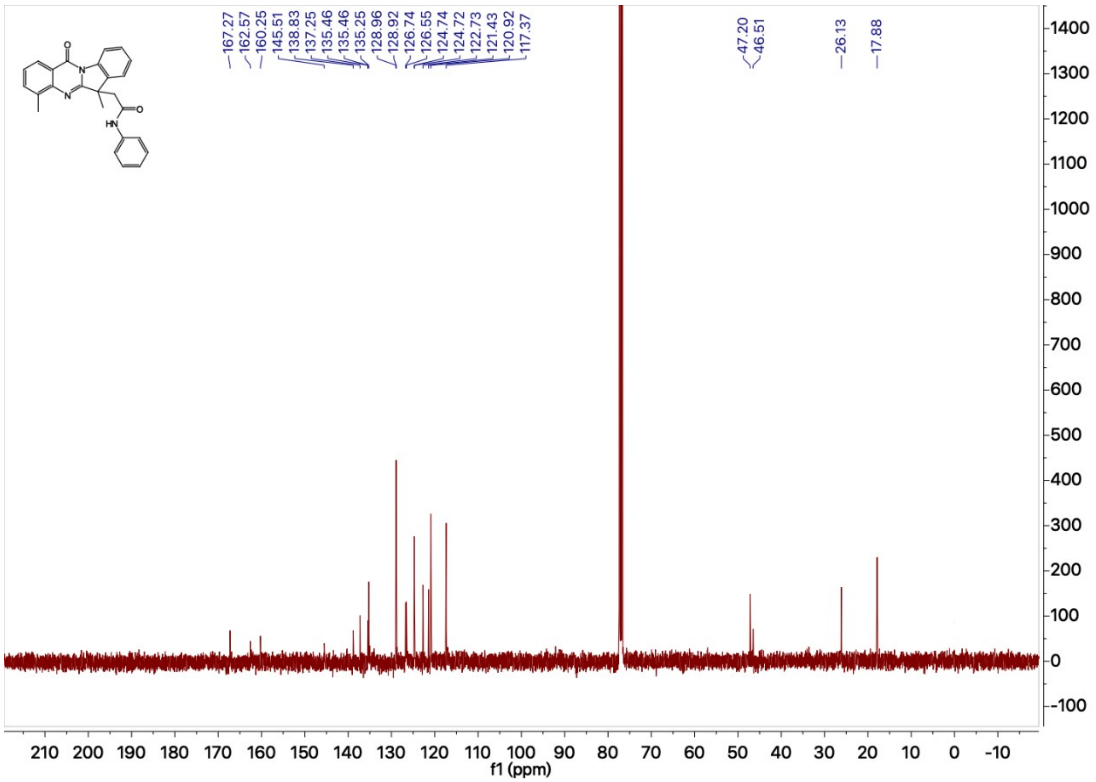


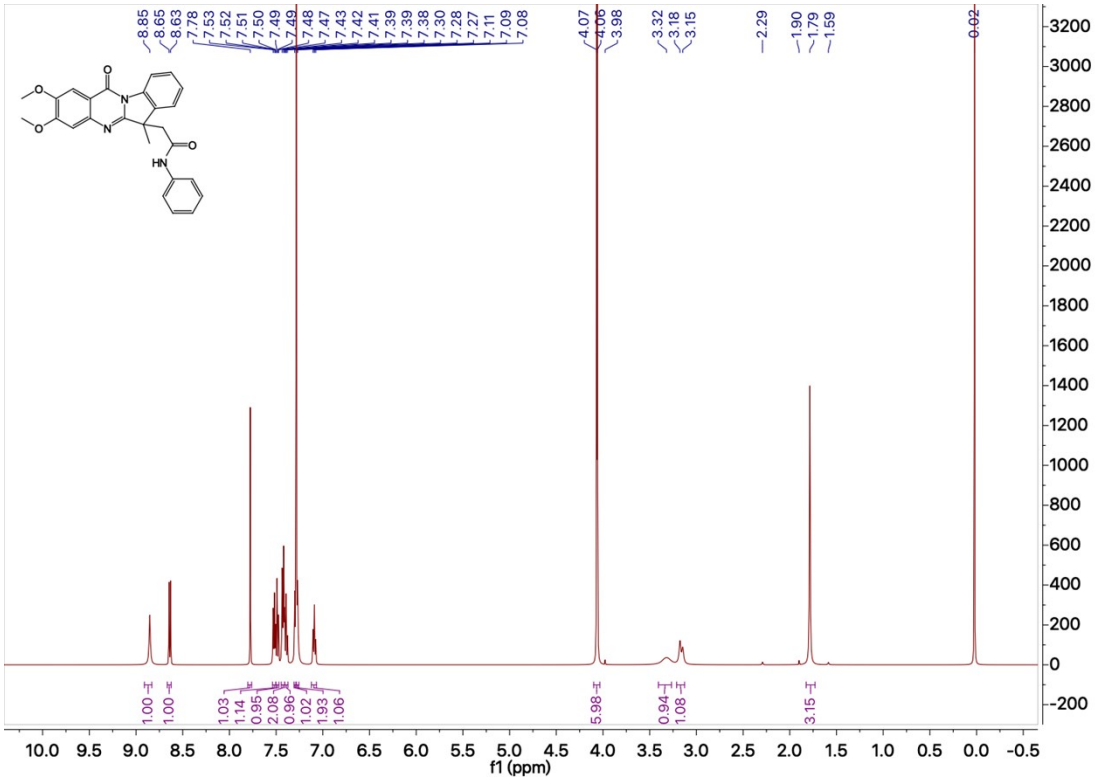
3ak ^{1}H Chloroform-*d*, 400 MHz



3ak $^{13}C\{1H\}$ Chloroform-*d*, 101 MHz



3al ^{1}H Chloroform-*d*, 500 MHz



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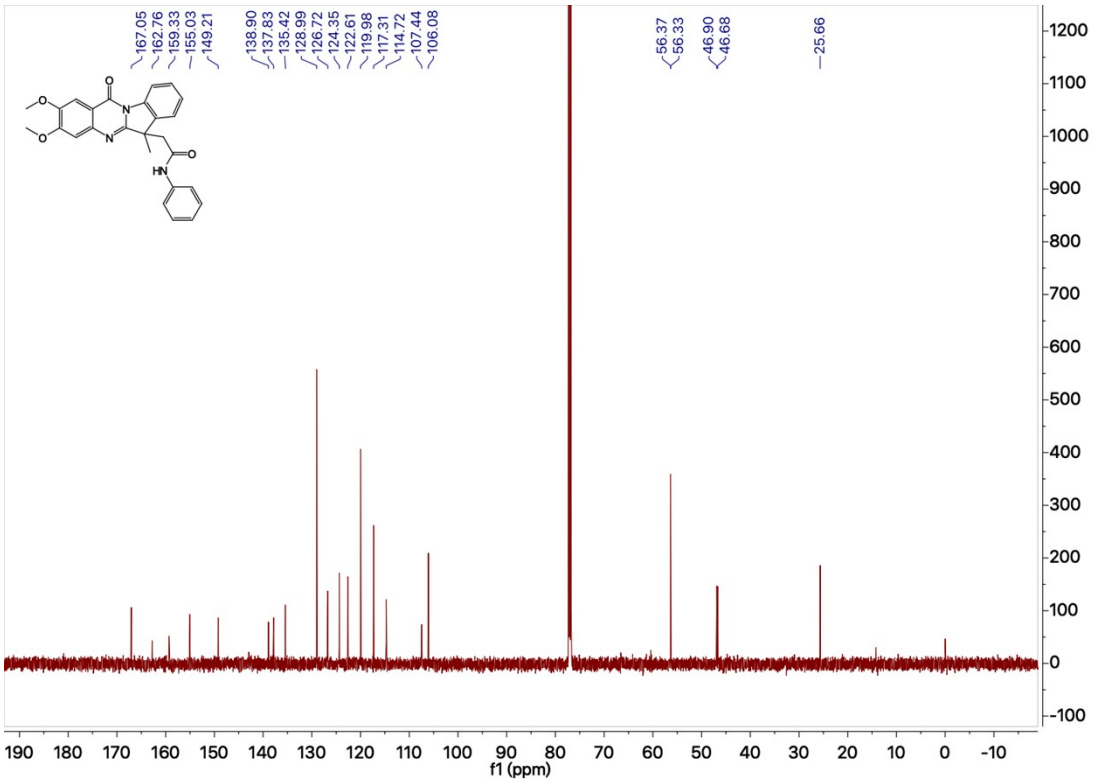

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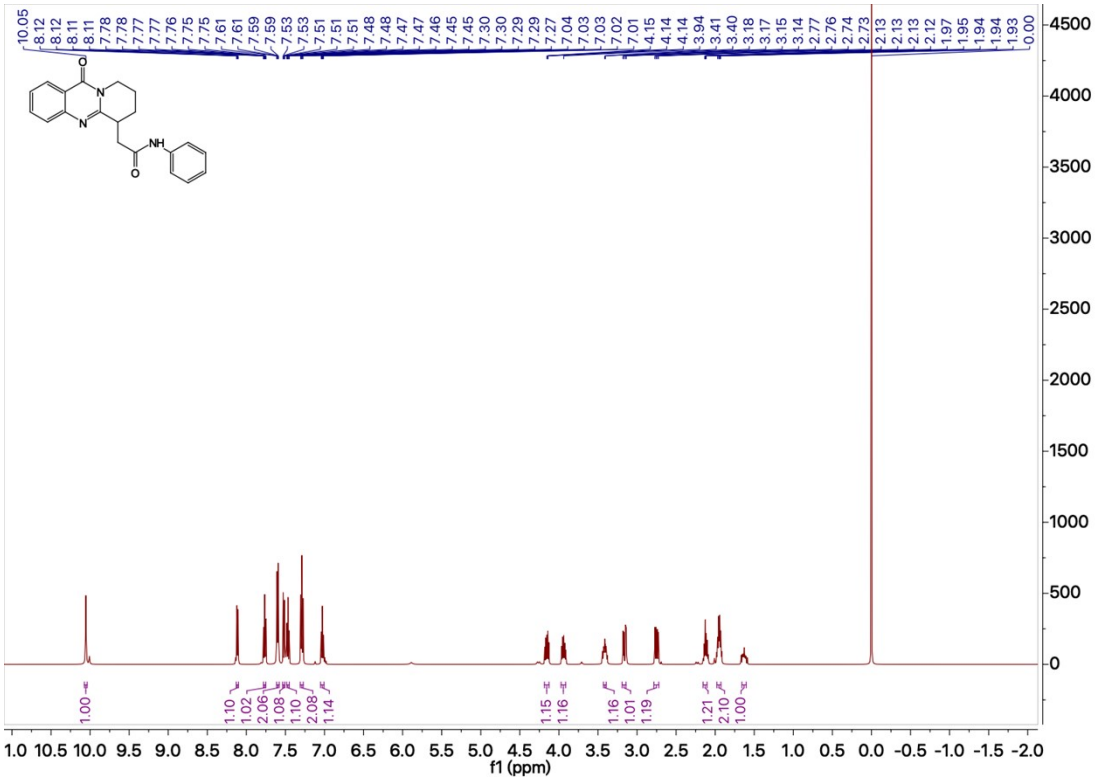

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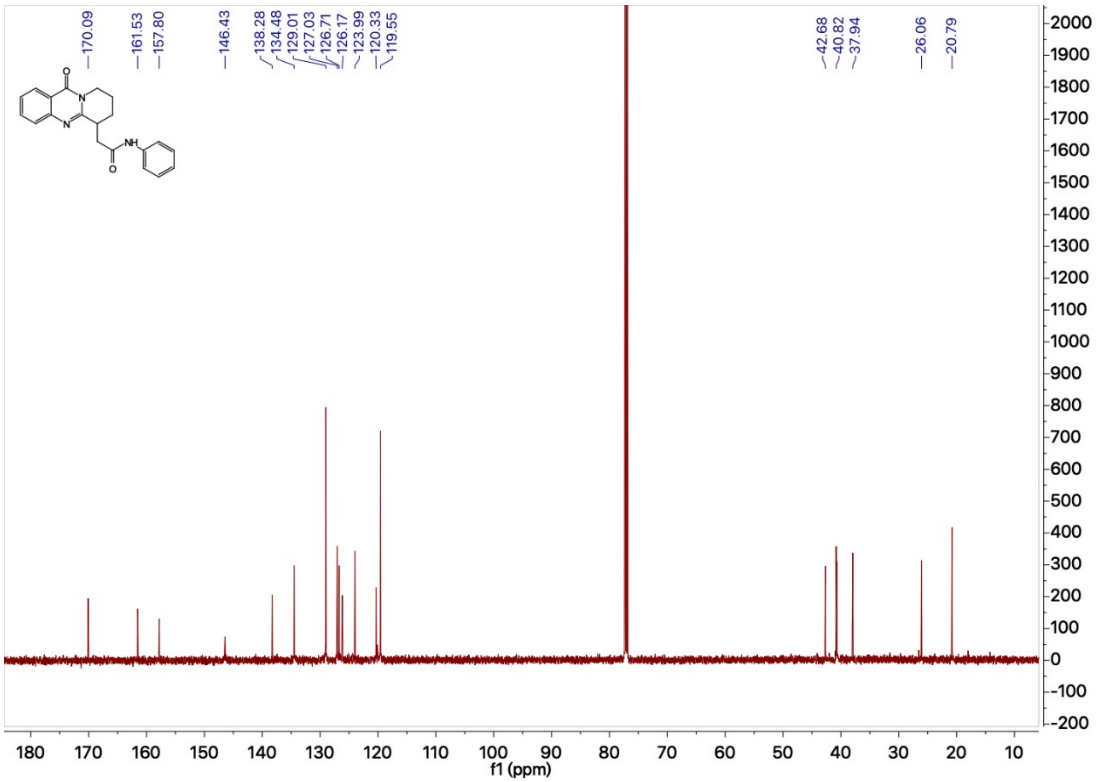
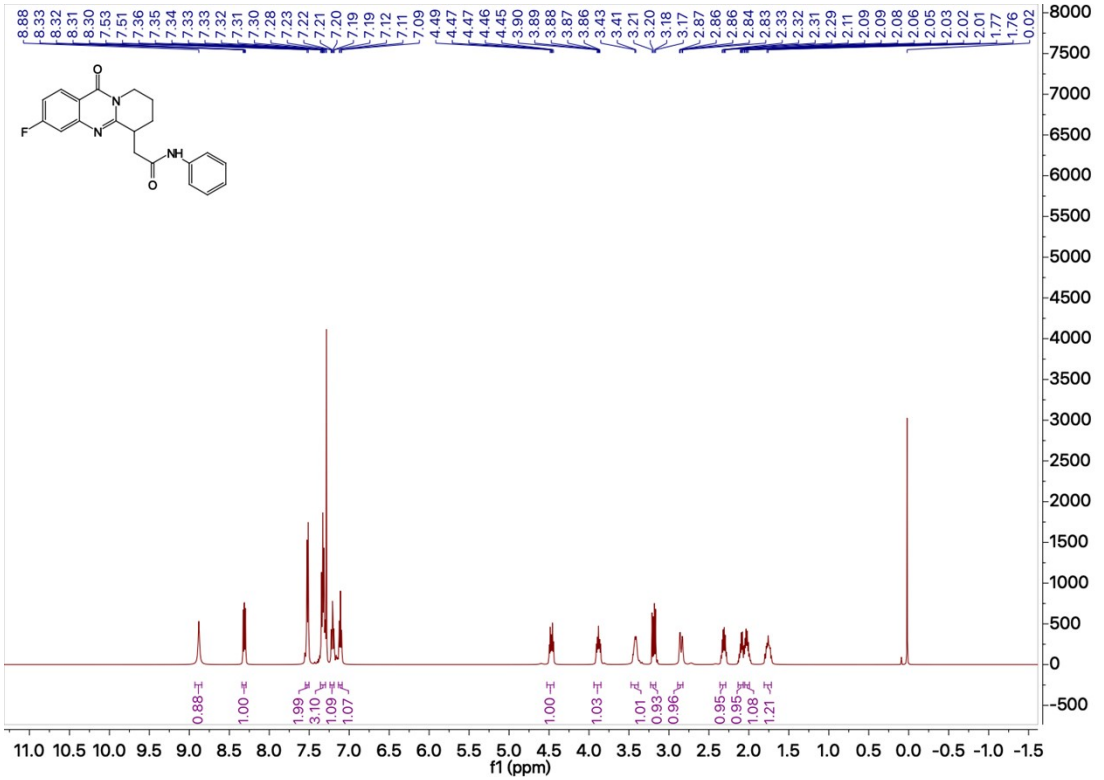
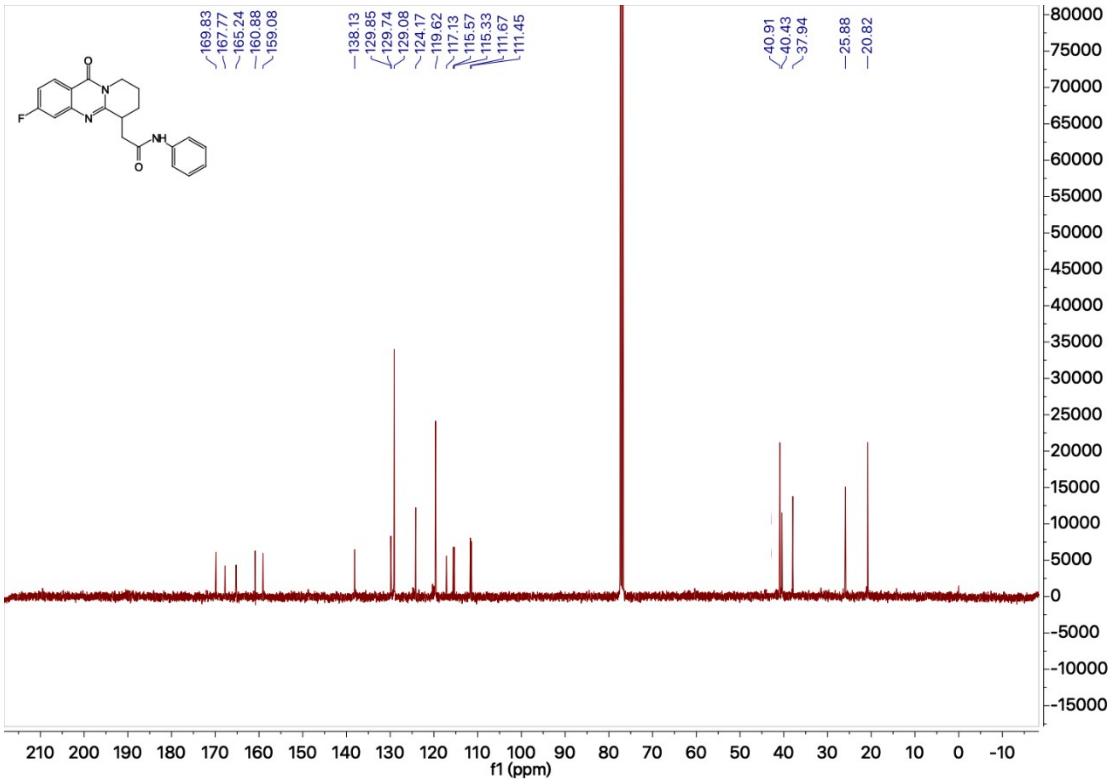


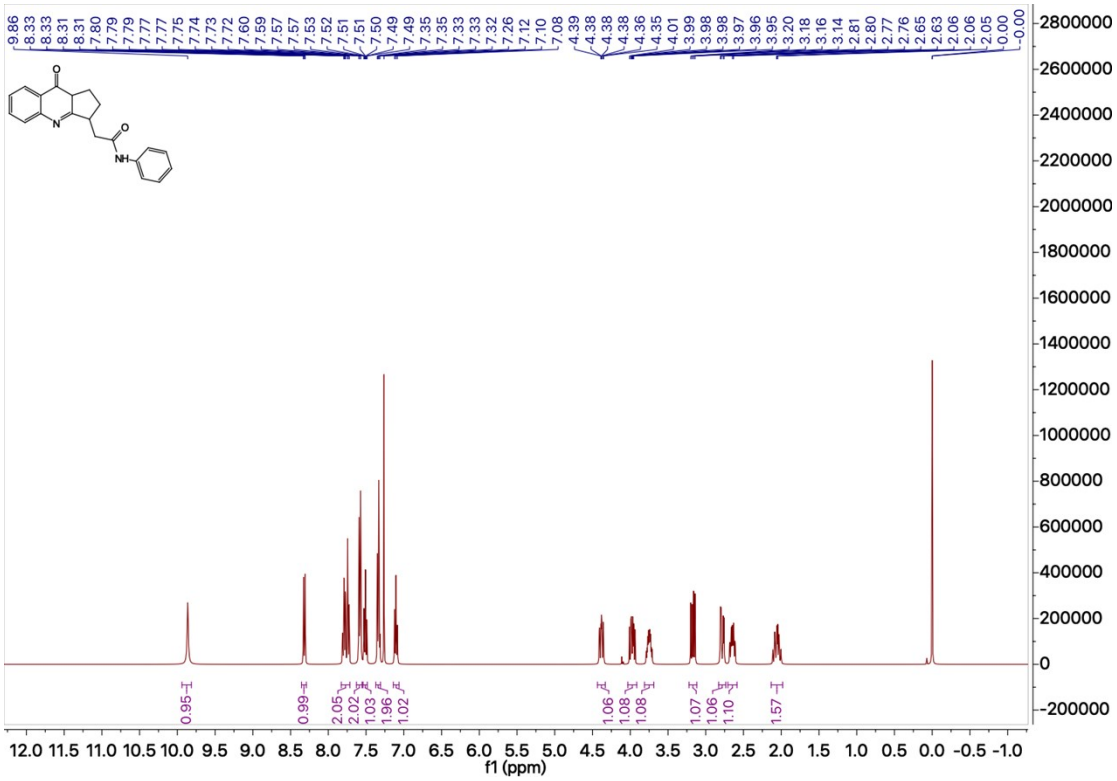
3ao ^{1}H Chloroform-*d*, 500 MHz



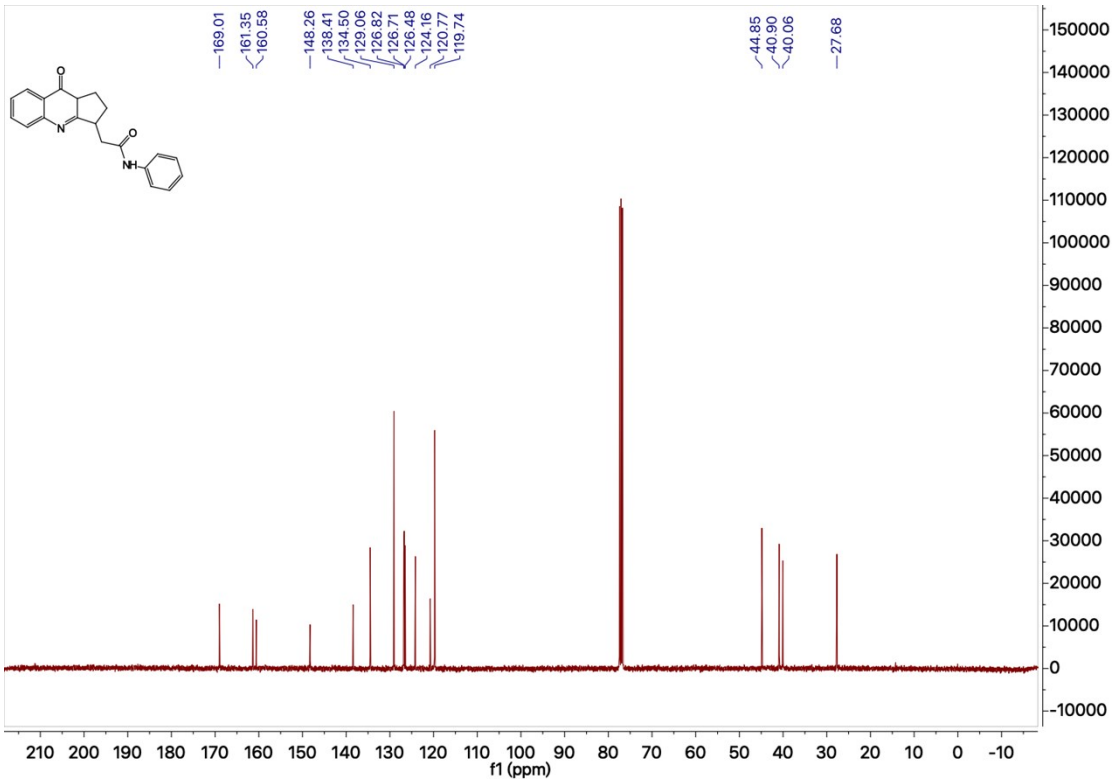
3ao $^{13}C\{1H\}$ Chloroform-*d*, 101 MHz



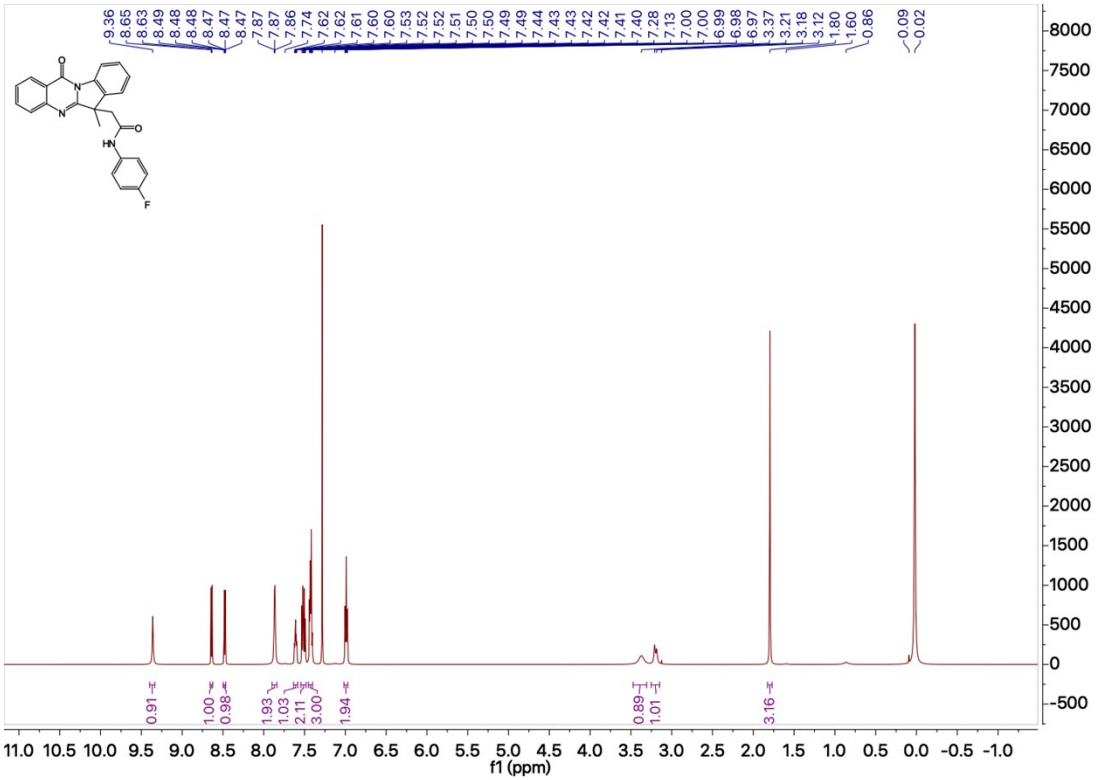
3as ^{1}H Chloroform-*d*, 400 MHz



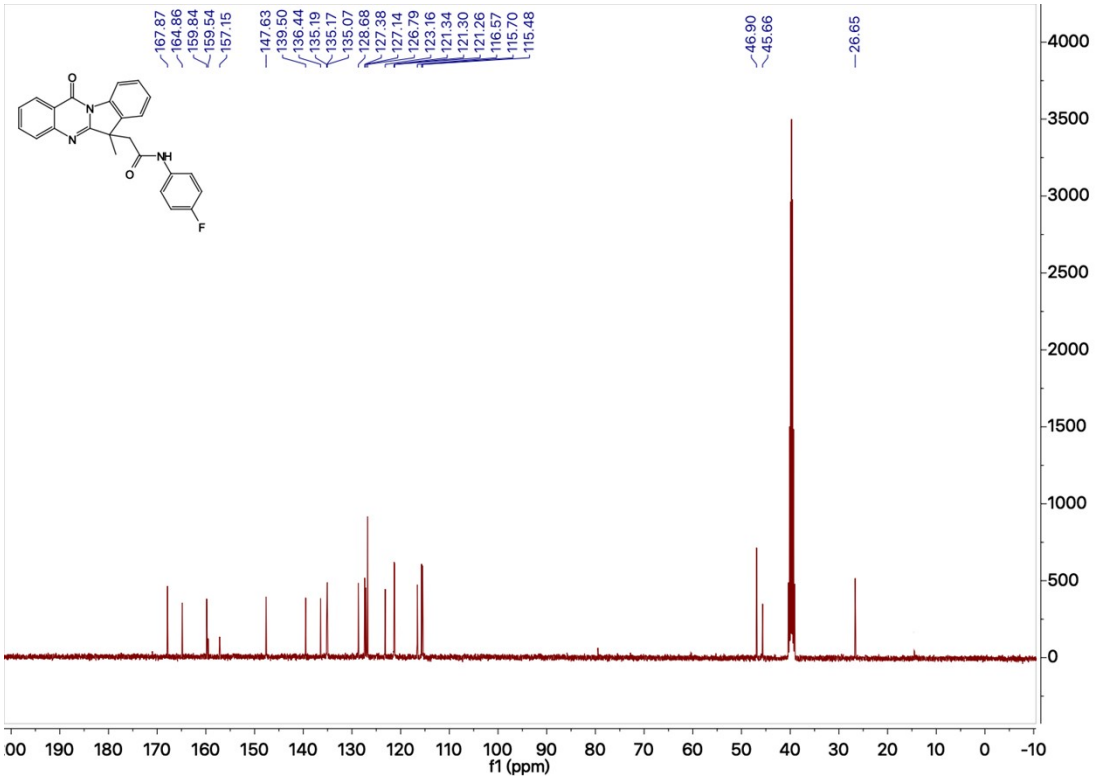
3as $^{13}C\{1H\}$ Chloroform-*d*, 101 MHz



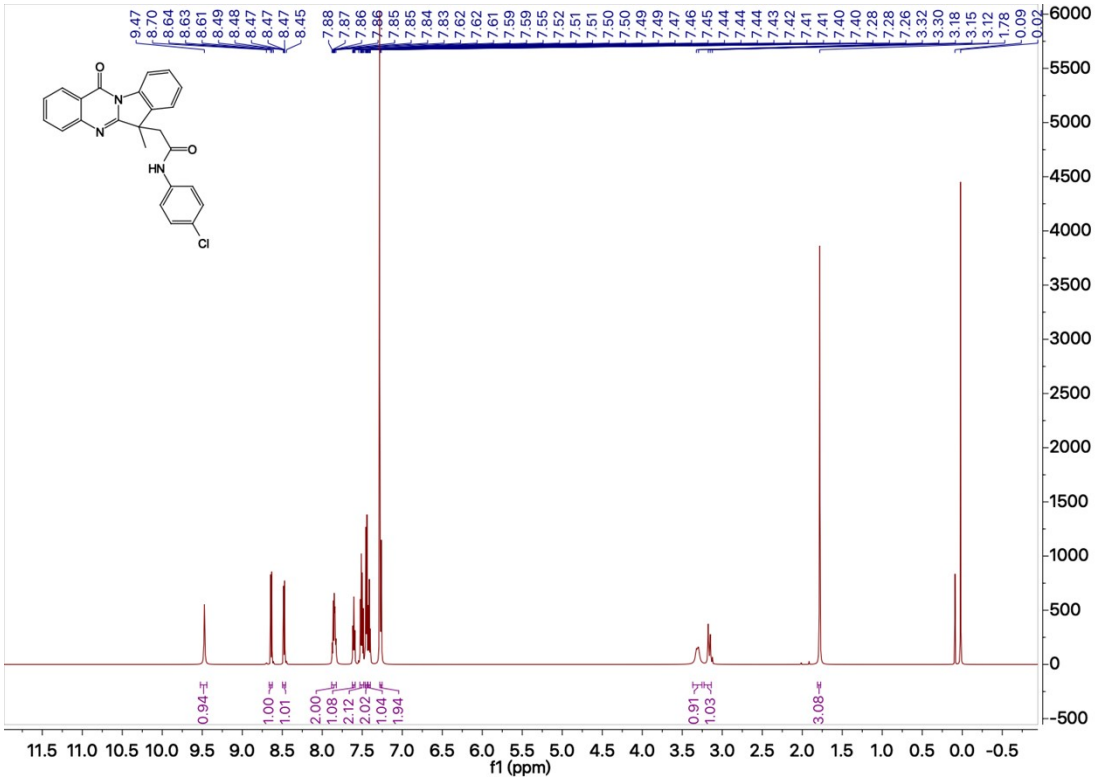
3ba ^{1}H Chloroform-*d*, 600 MHz



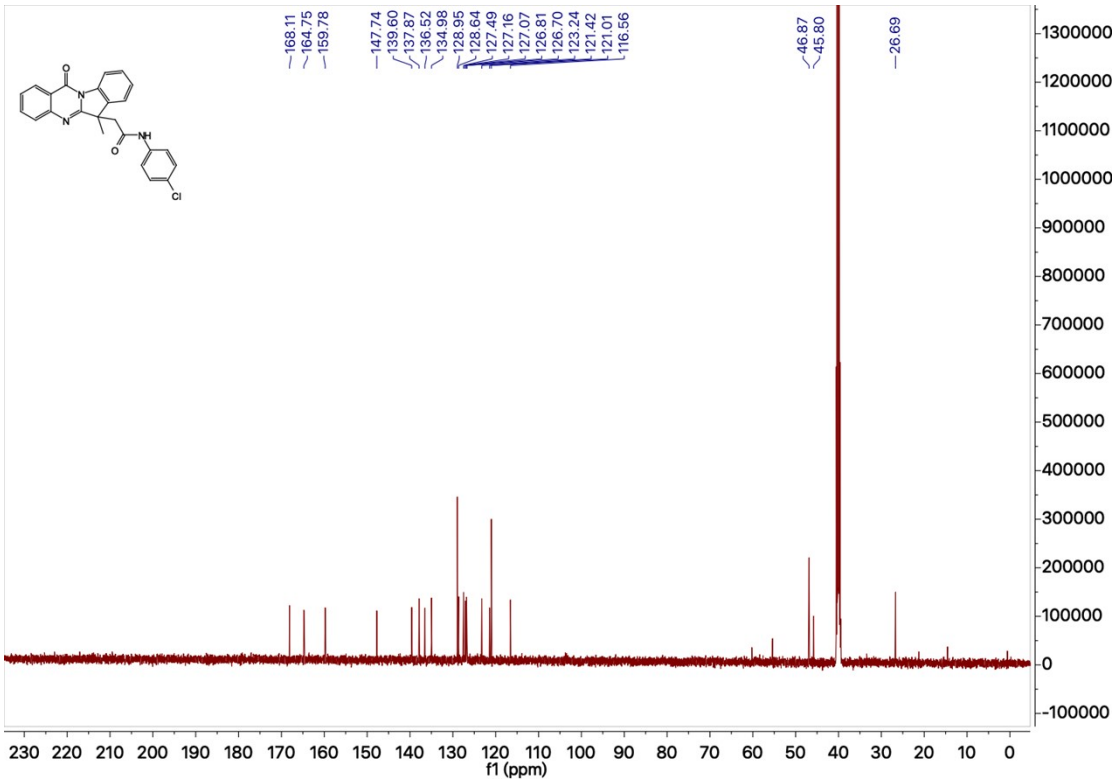
3ba $^{13}C\{1H\}$ DMSO-d_6, 101 MHz



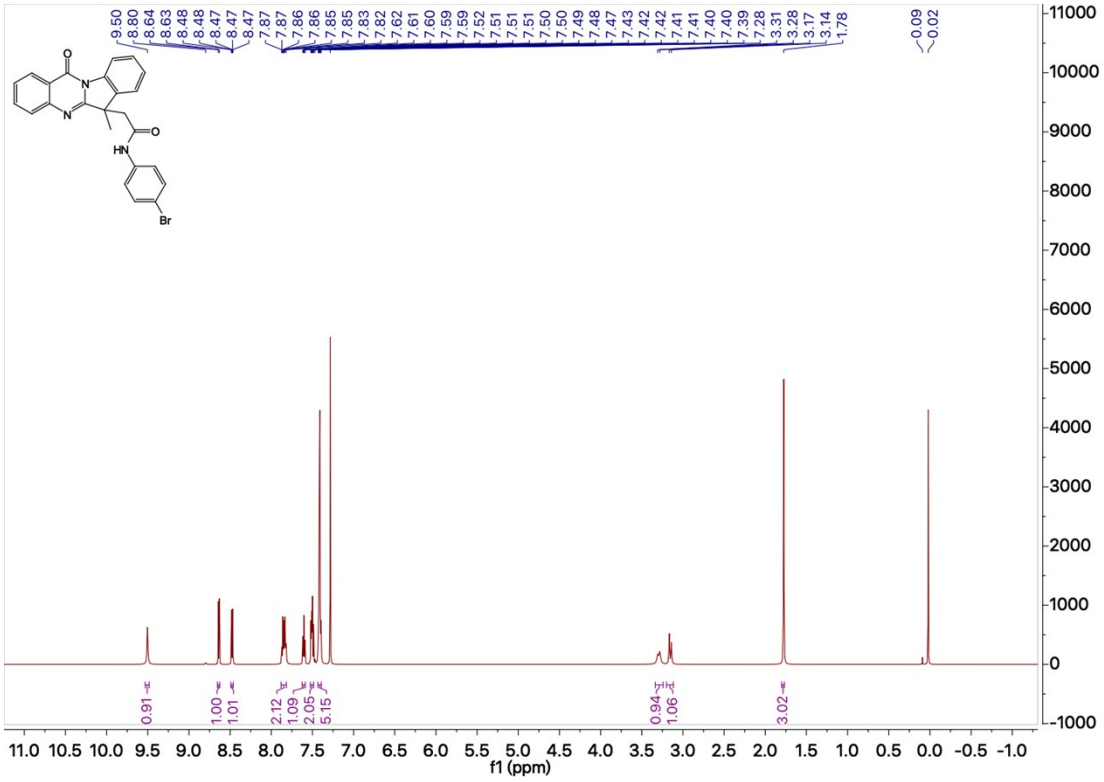
3ca ^{1}H Chloroform-d, 600 MHz



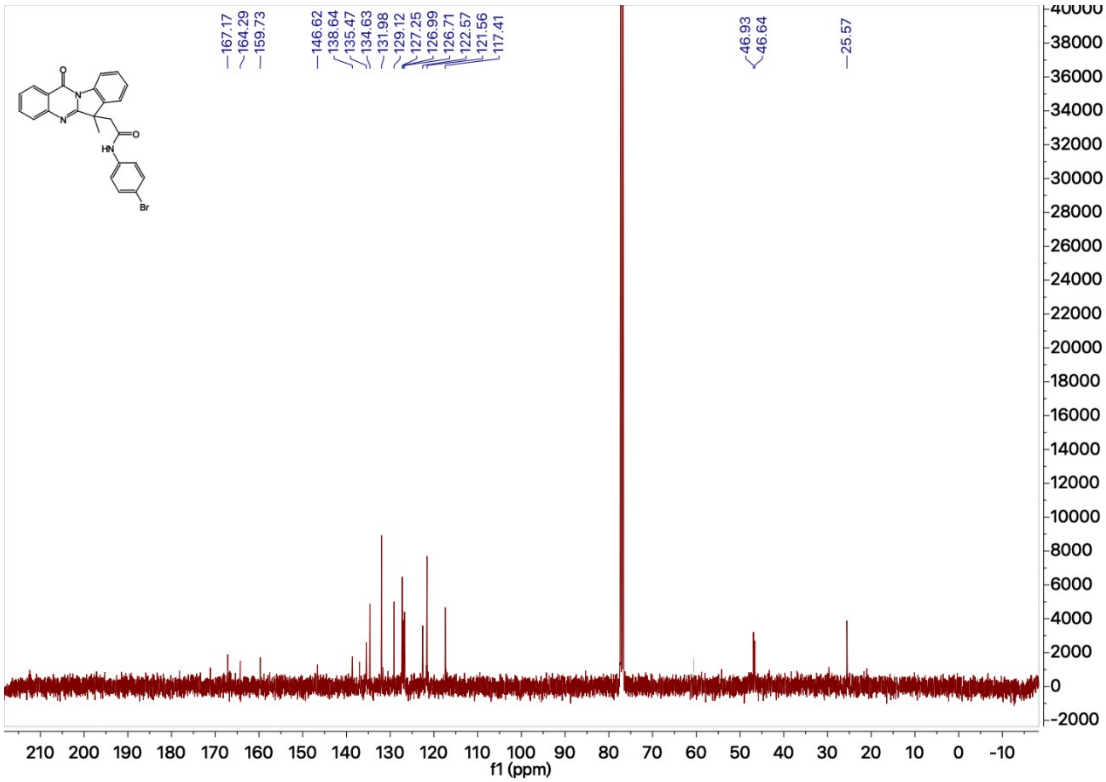
3ca $^{13}C\{1H\}$ DMSO-d_6, 126 MHz



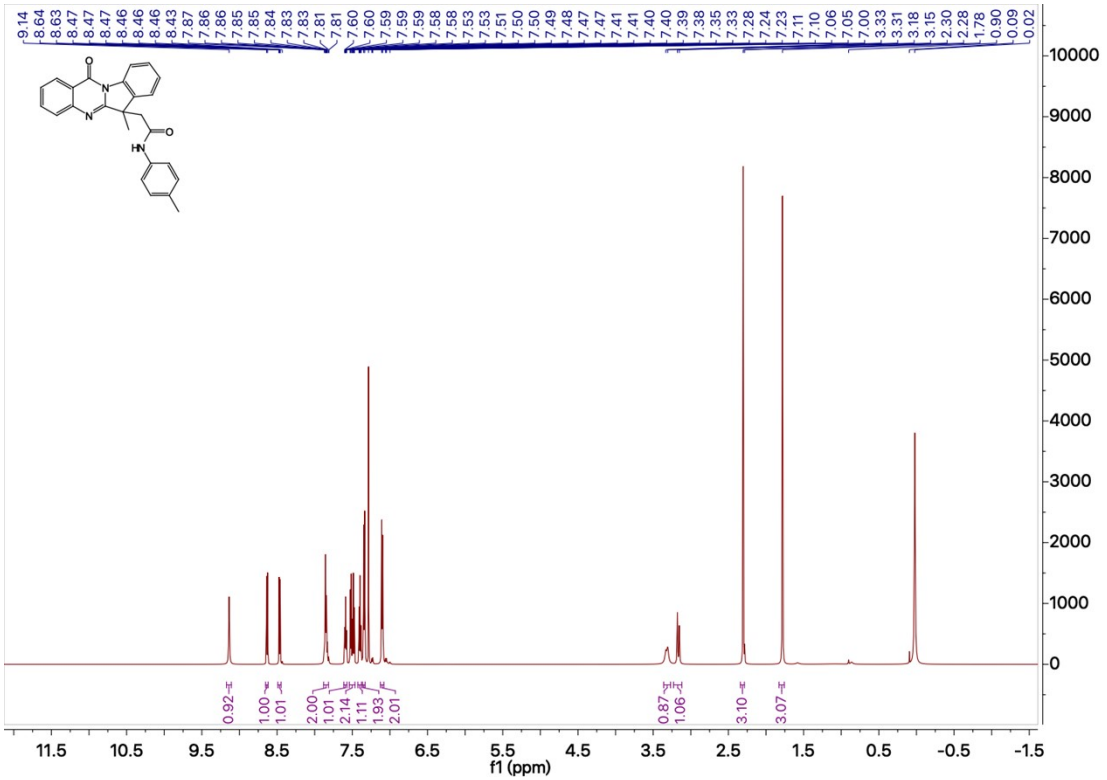
3da ^{1}H Chloroform-d, 600 MHz



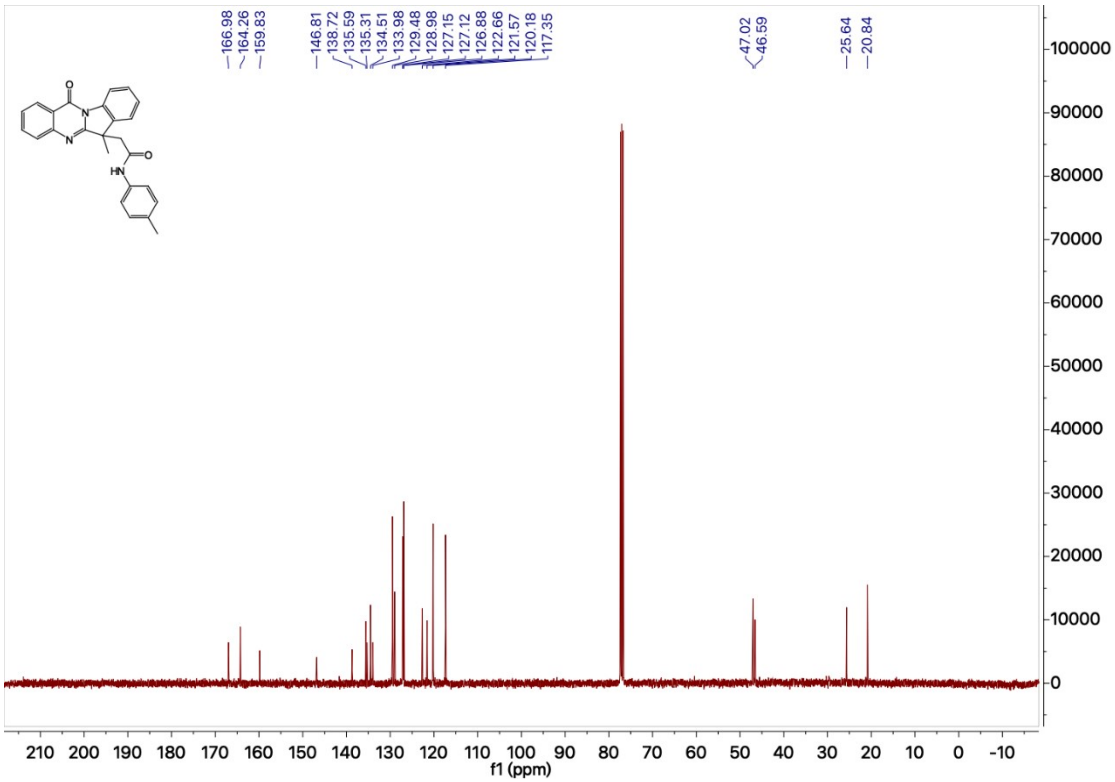
3da $^{13}C\{1H\}$ Chloroform-*d*, 101 MHz



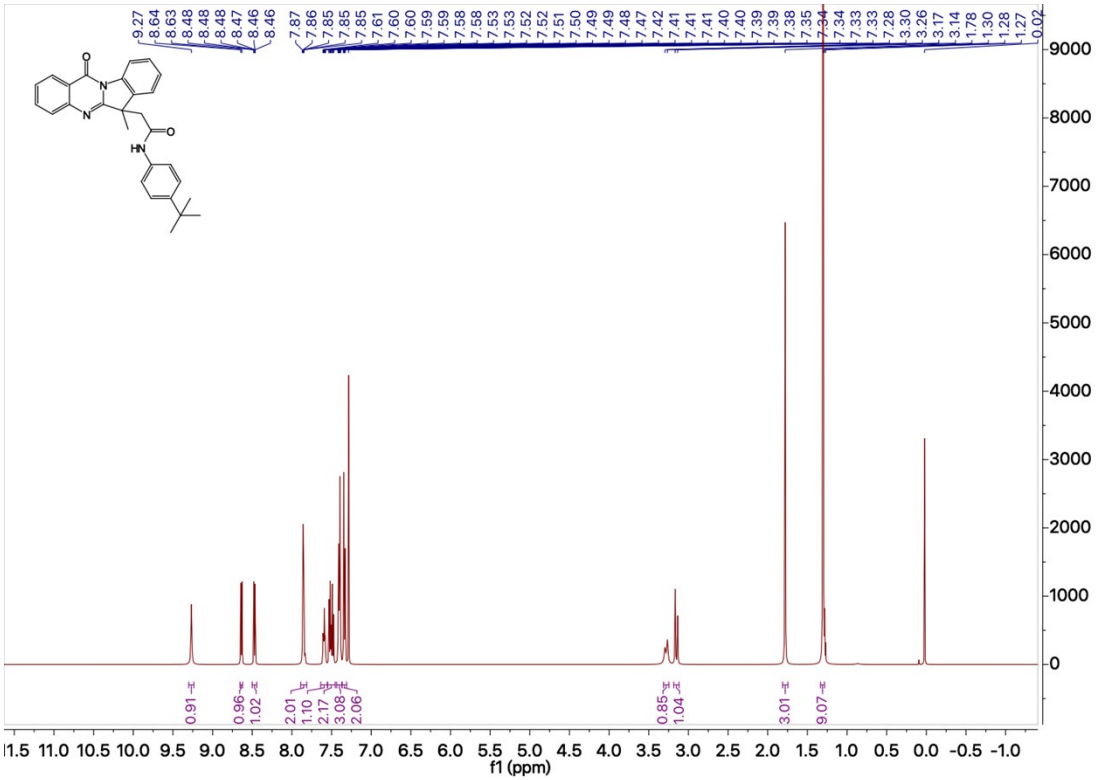
3ea ^{1}H Chloroform-*d*, 600 MHz



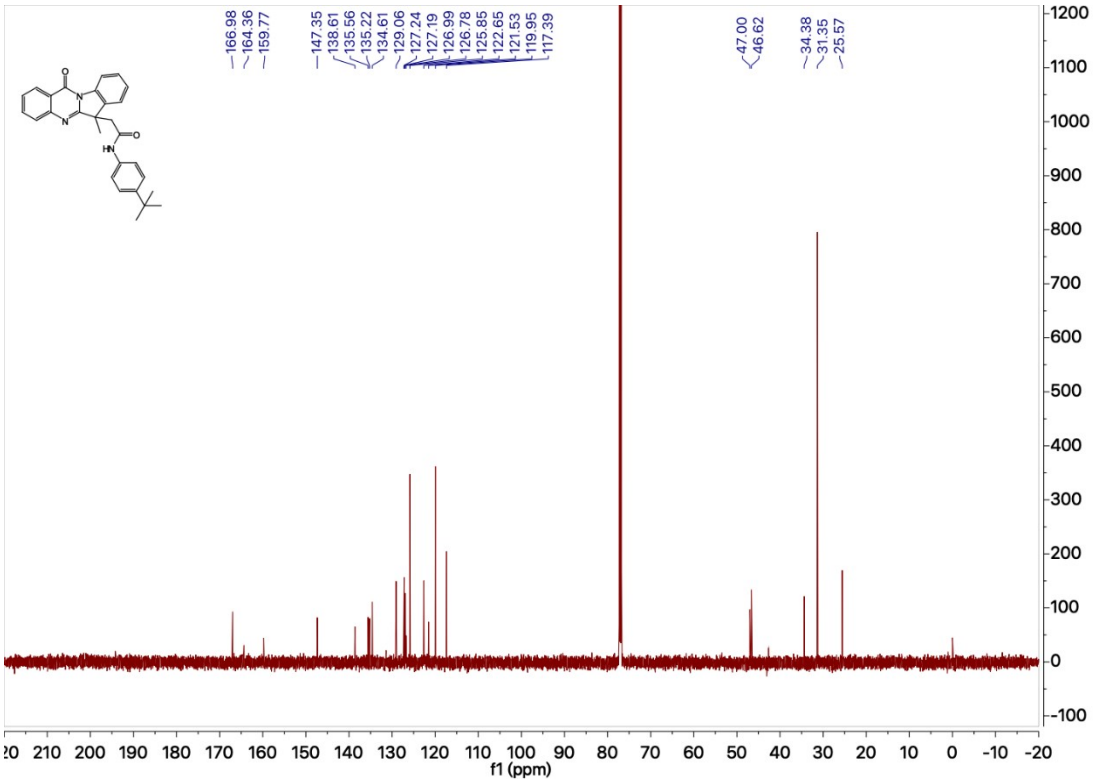
3ea $^{13}C\{1H\}$ Chloroform-*d*, 101 MHz



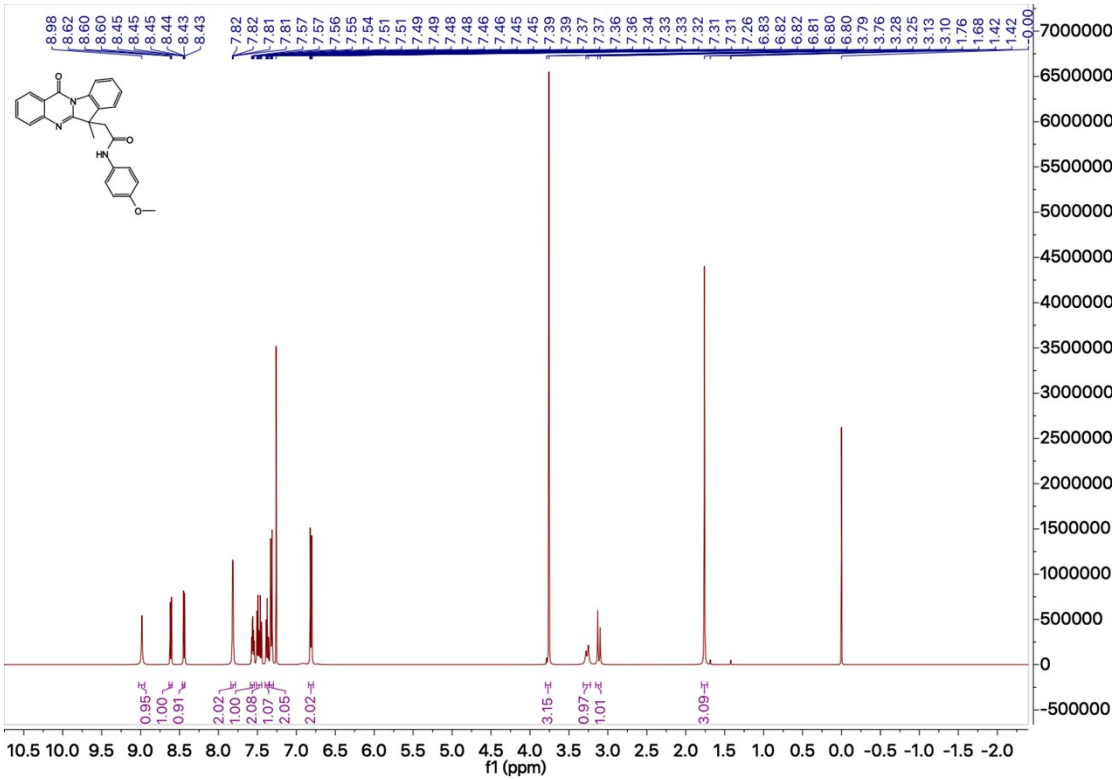
3fa ^{1}H Chloroform-*d*, 500 MHz



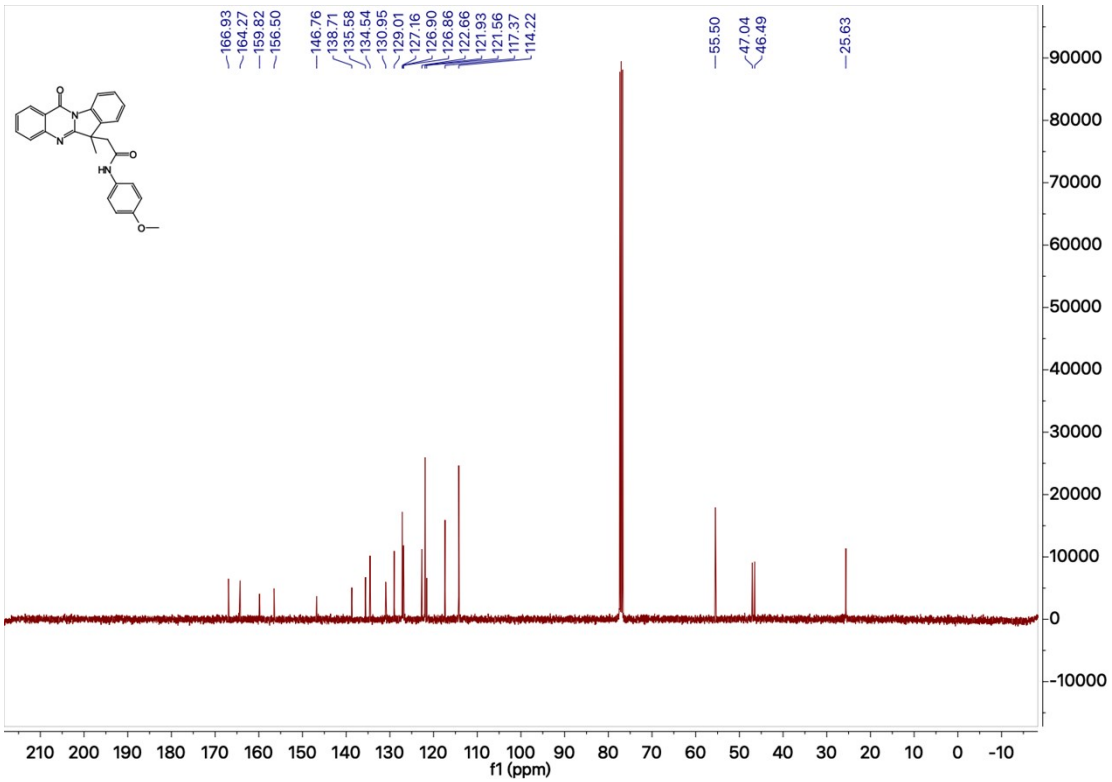
3fa $^{13}C\{1H\}$ Chloroform-*d*, 151 MHz



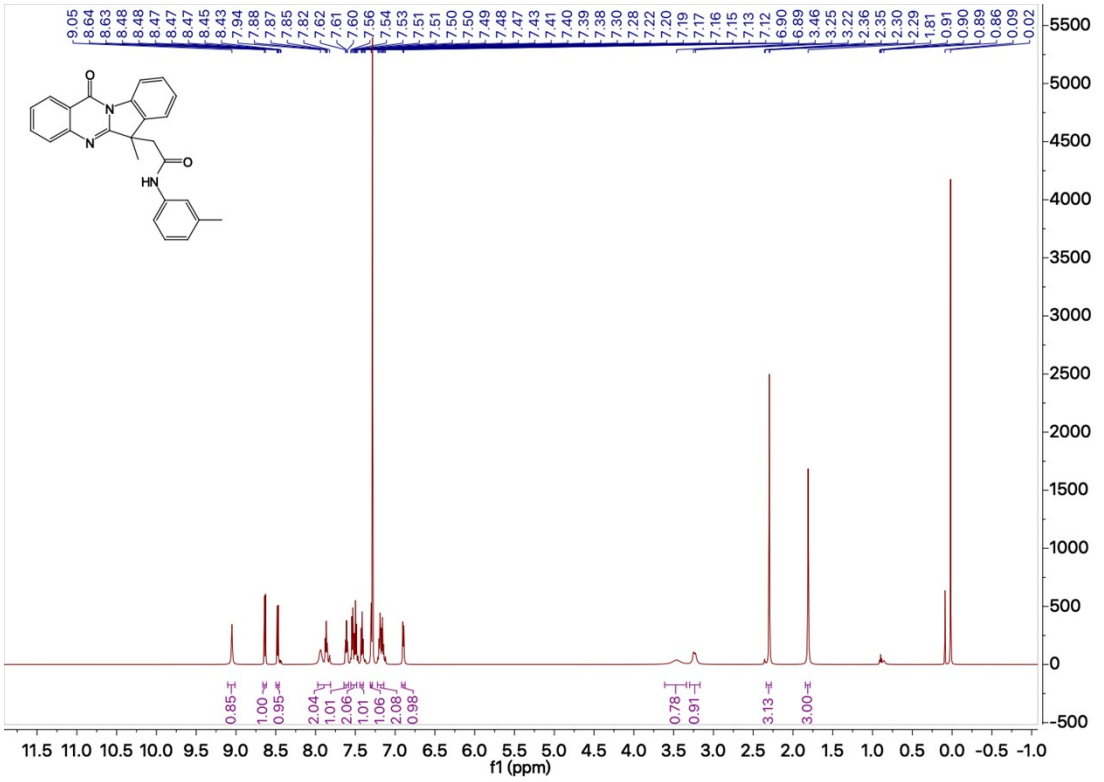
3ga ^{1}H Chloroform-*d*, 500 MHz



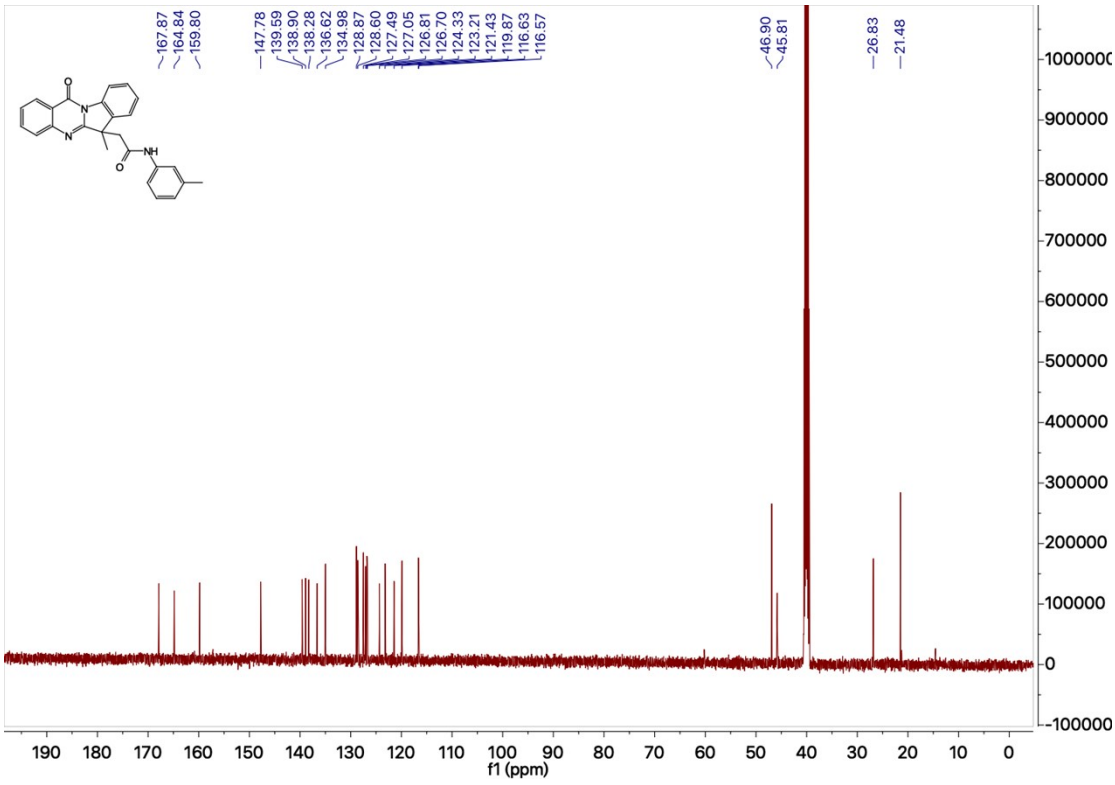
3ga $^{13}C\{1H\}$ Chloroform-*d*, 101 MHz



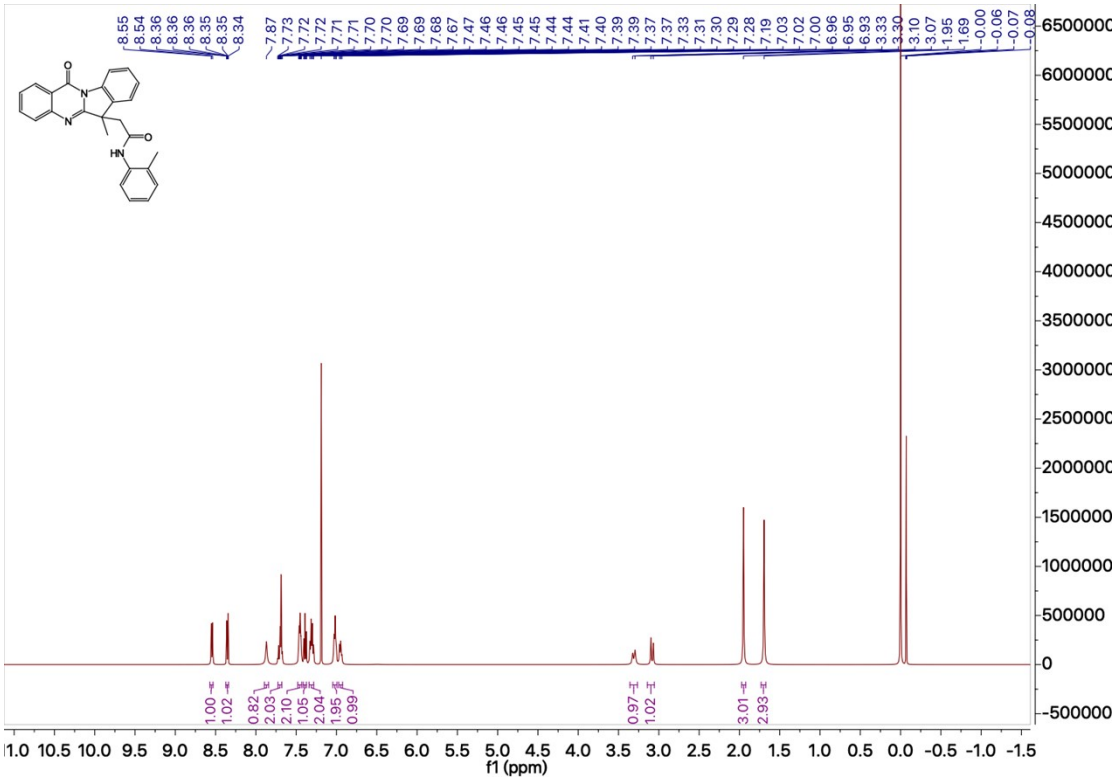
3ha ^{1}H Chloroform-*d*, 600 MHz



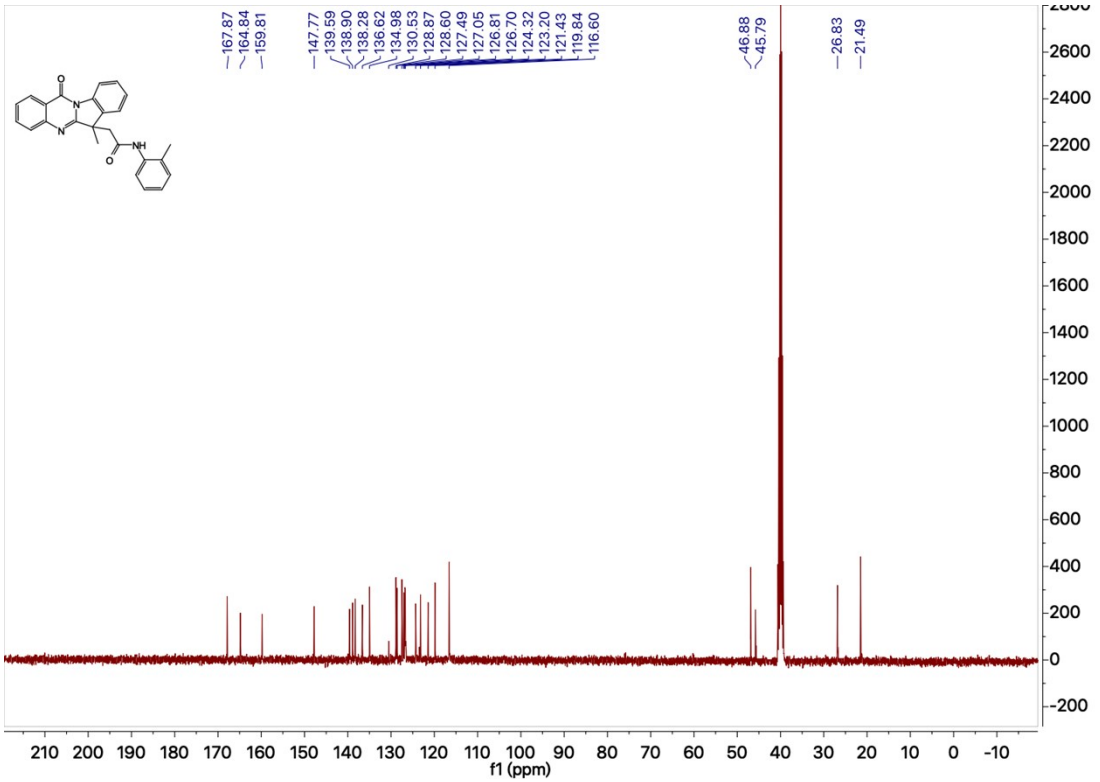
3ha $^{13}C\{1H\}$ DMSO-d_6, 101 MHz



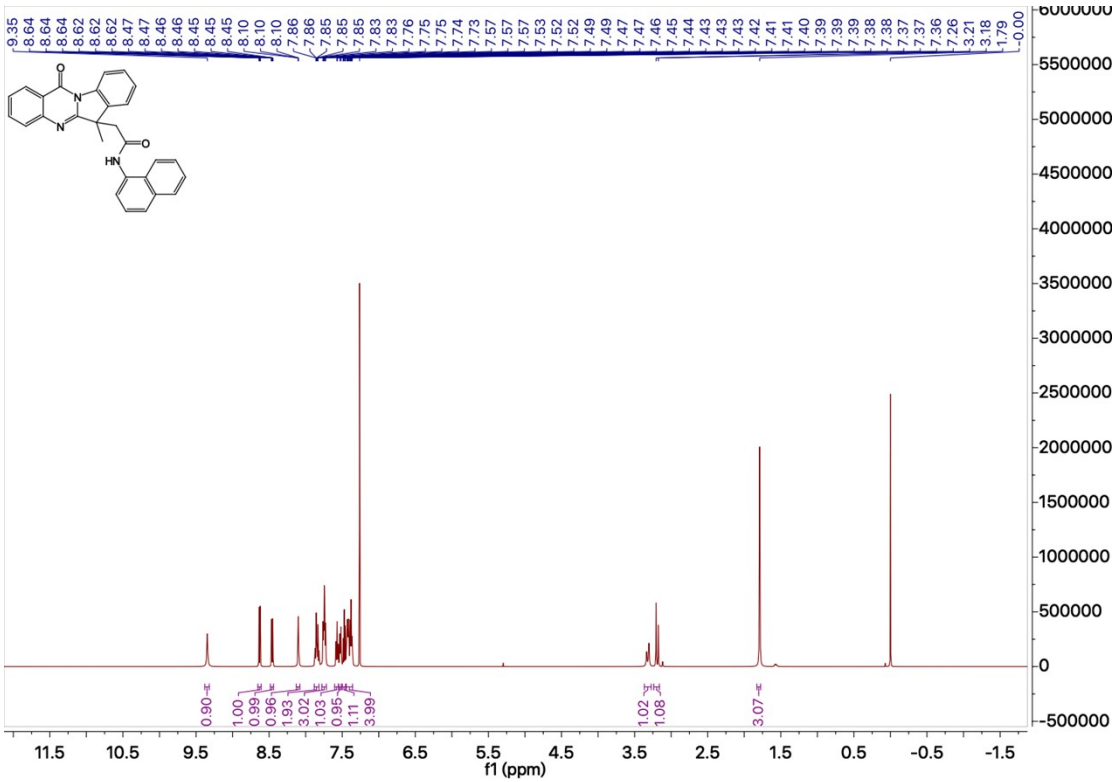
3ia ^{1}H Chloroform-d, 500 MHz



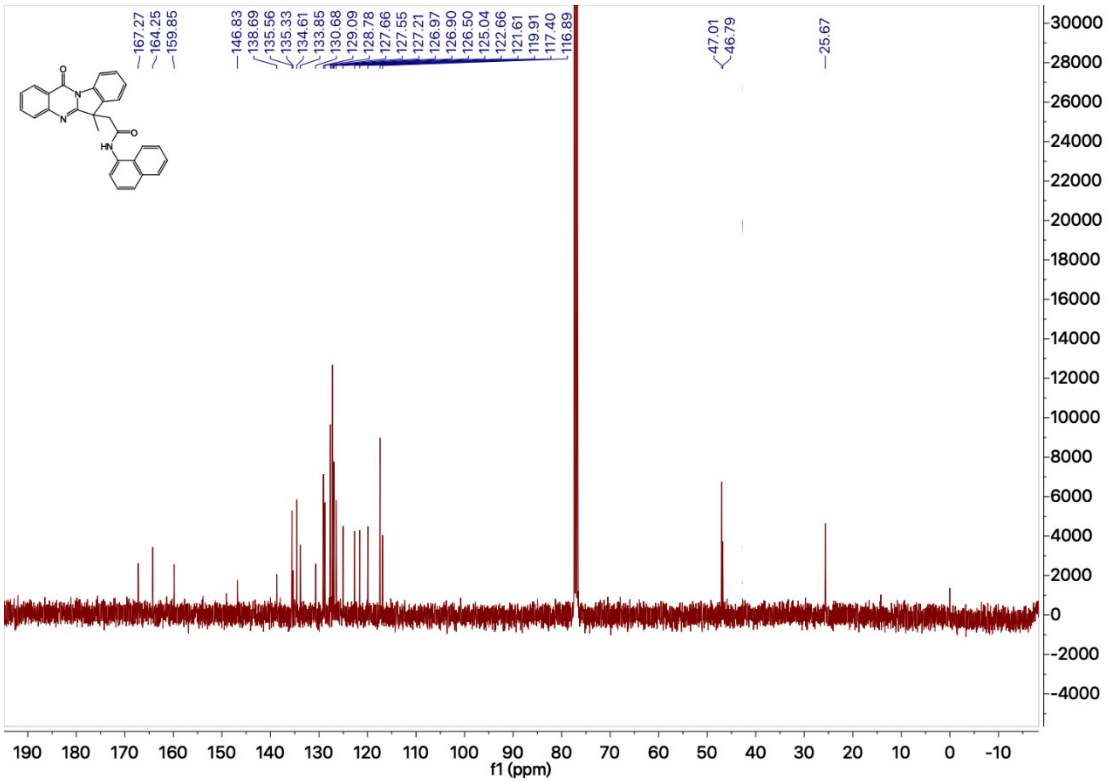
3ia $^{13}C\{1H\}$ DMSO-d_6, 101 MHz



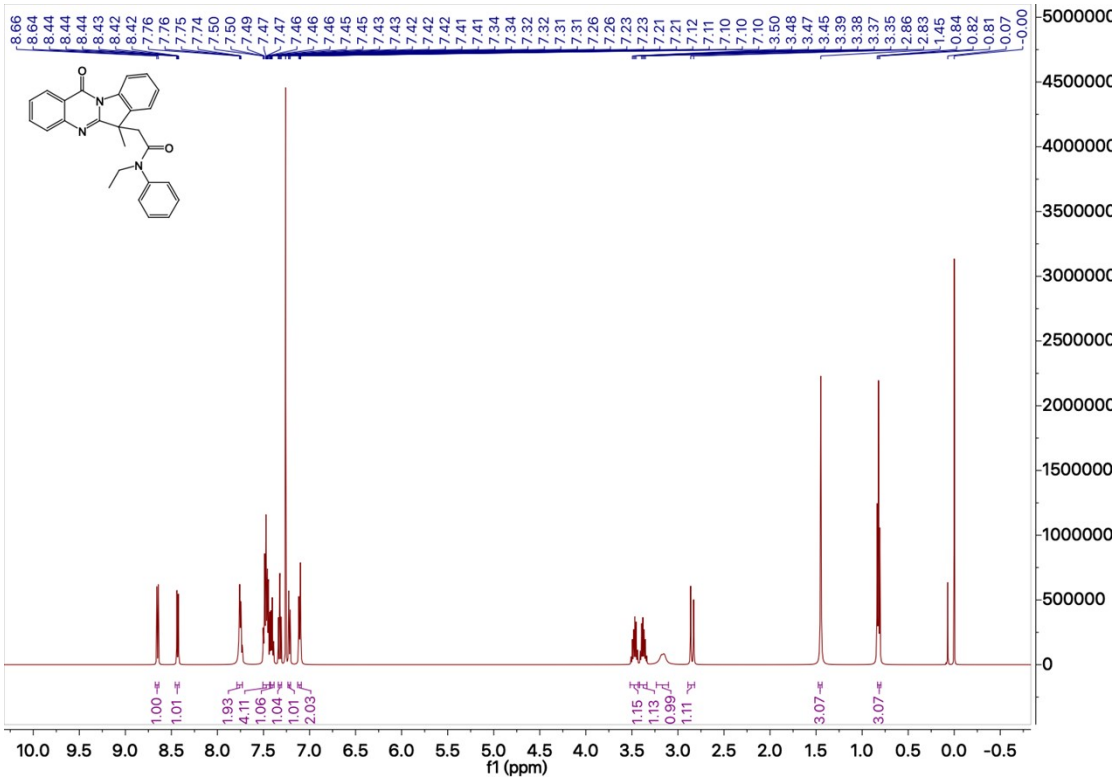
3ja ^{1}H Chloroform-d, 500 MHz



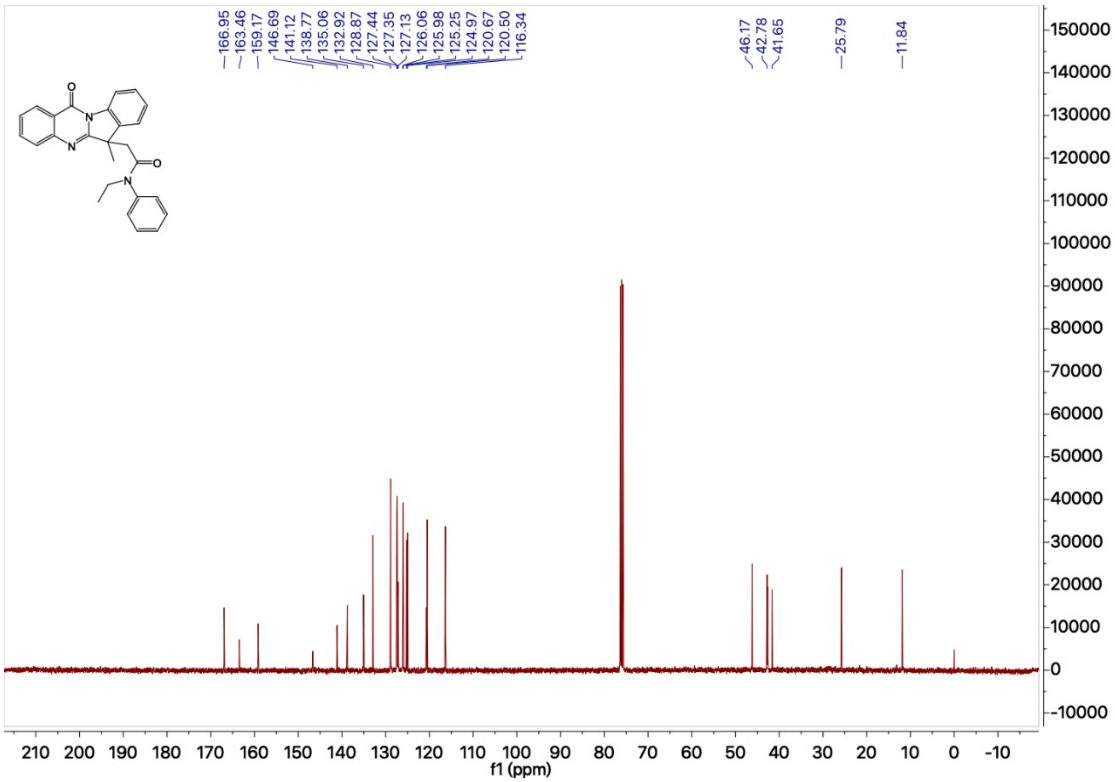
3ja $^{13}C\{1H\}$ Chloroform-*d*, 101 MHz



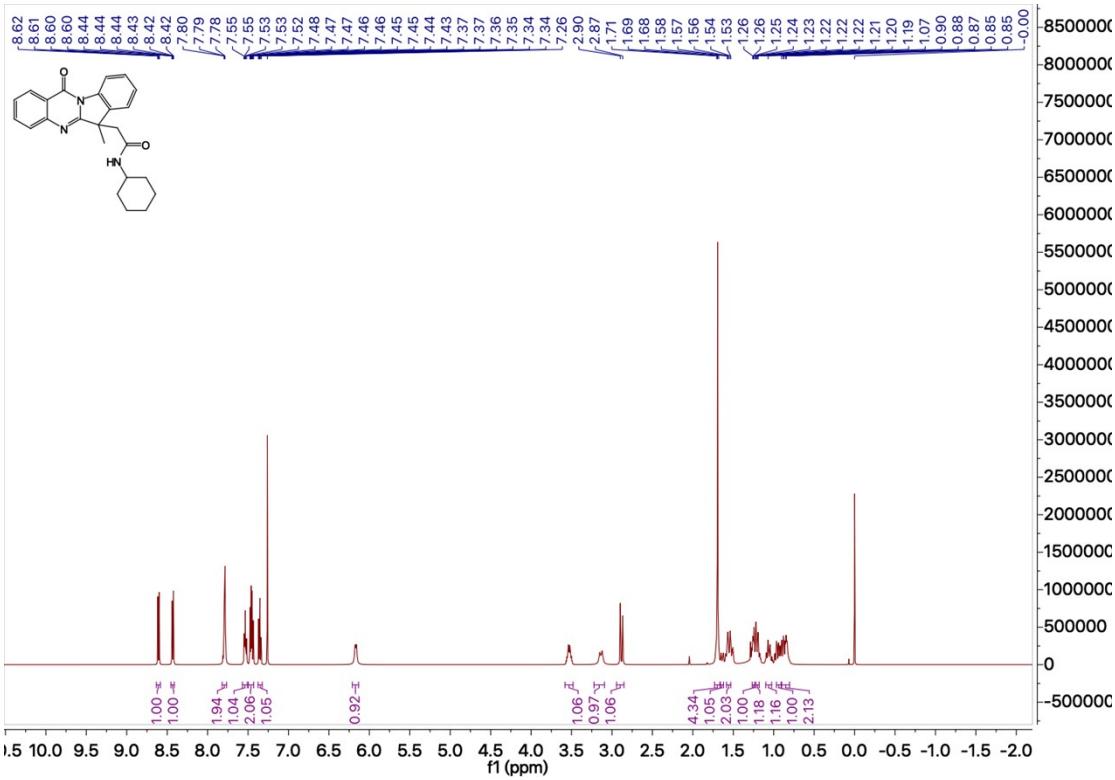
3ka ^{1}H Chloroform-*d*, 500 MHz



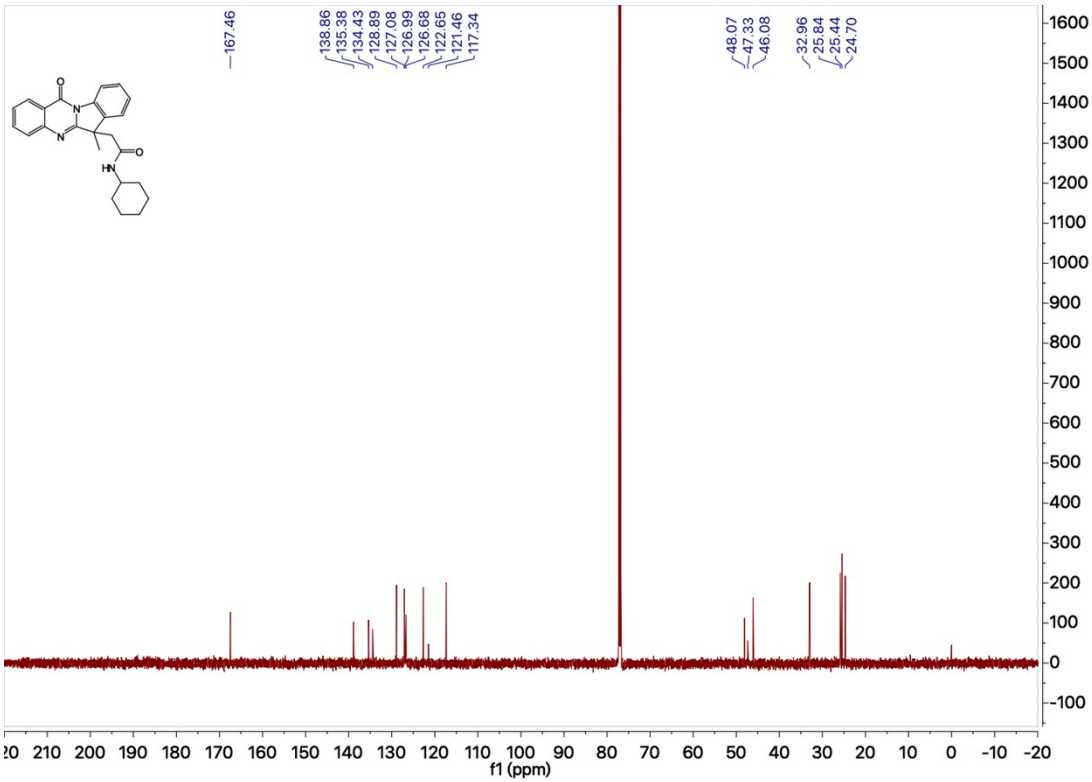
3ka $^{13}C\{1H\}$ Chloroform-*d*, 101 MHz



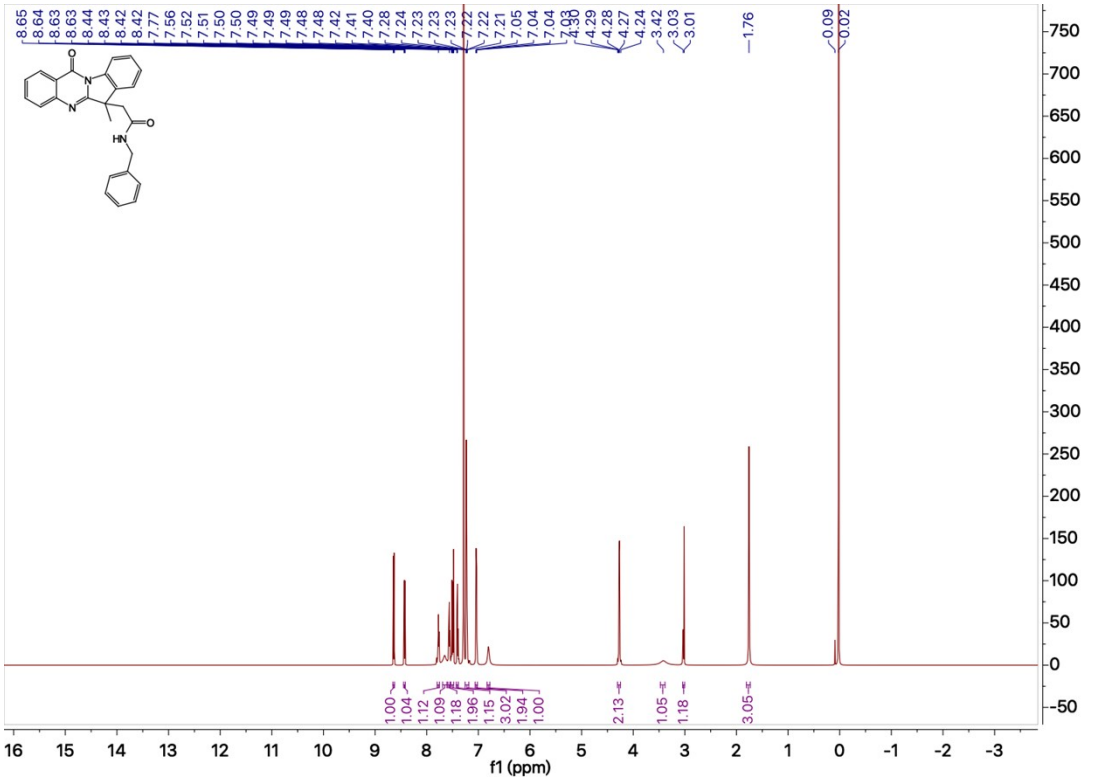
3la ^{1}H Chloroform-*d*, 500 MHz



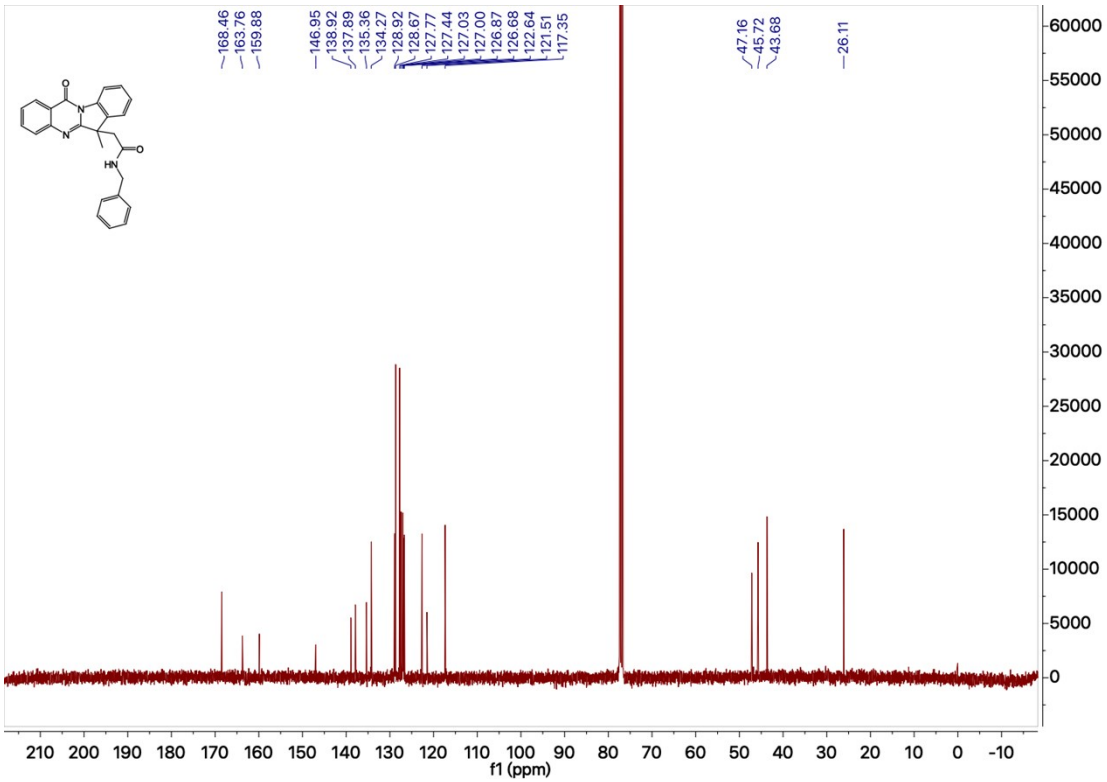
3la $^{13}C\{1H\}$ Chloroform-*d*, 151 MHz



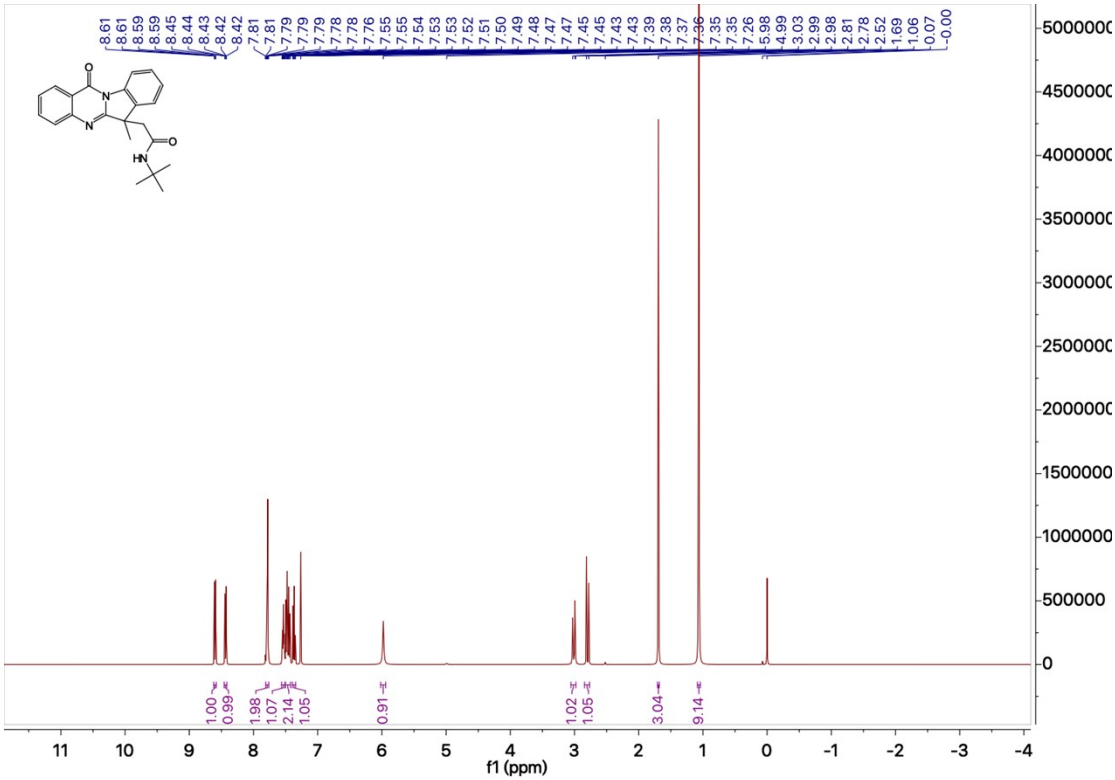
3ma ^{1}H Chloroform-*d*, 600 MHz



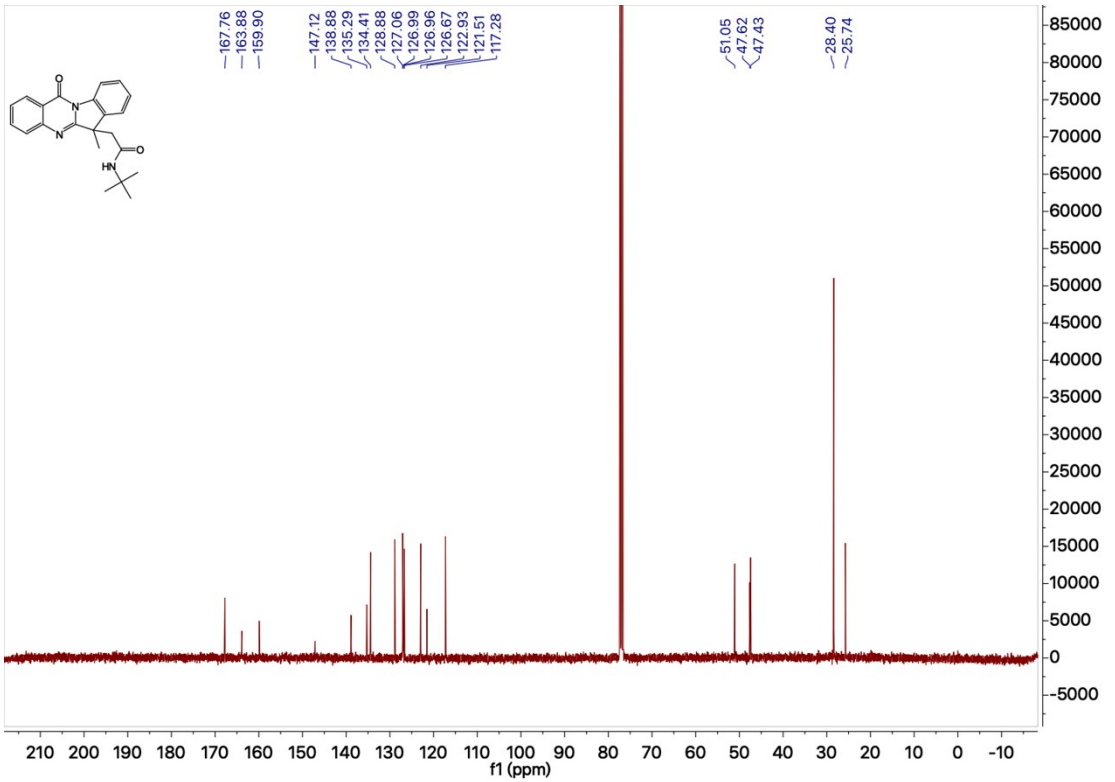
3ma $^{13}C\{1H\}$ Chloroform-*d*, 101 MHz



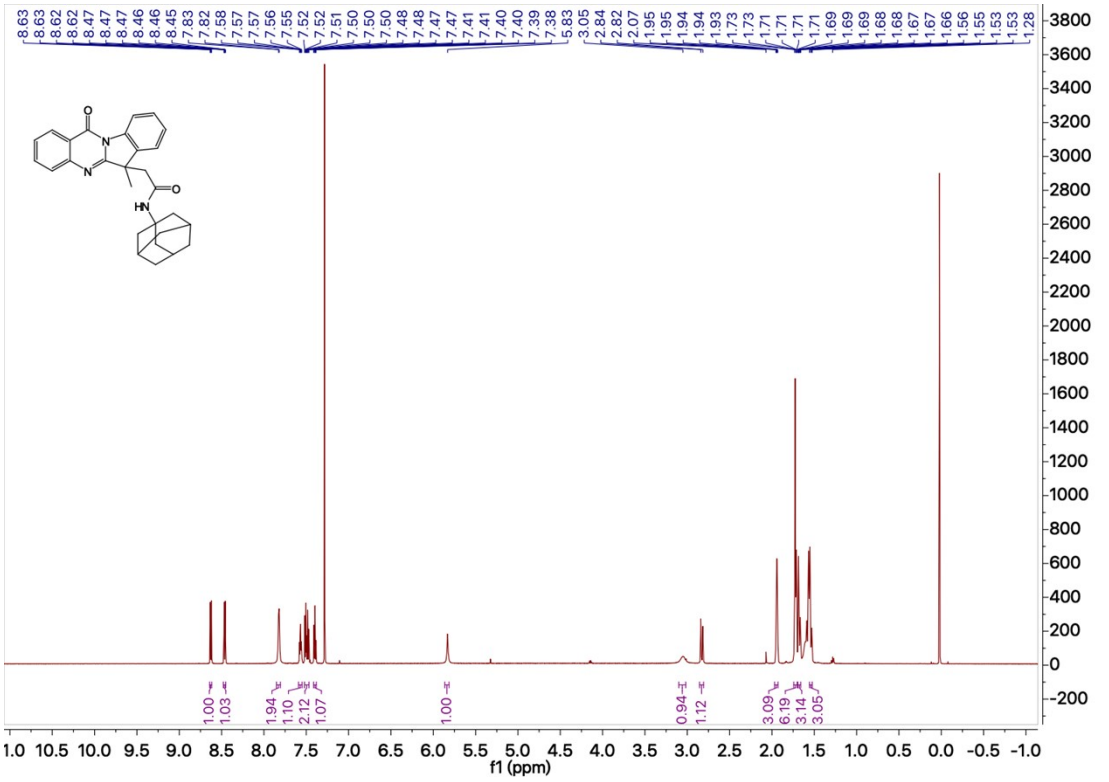
3na ^{1}H Chloroform-*d*, 400 MHz



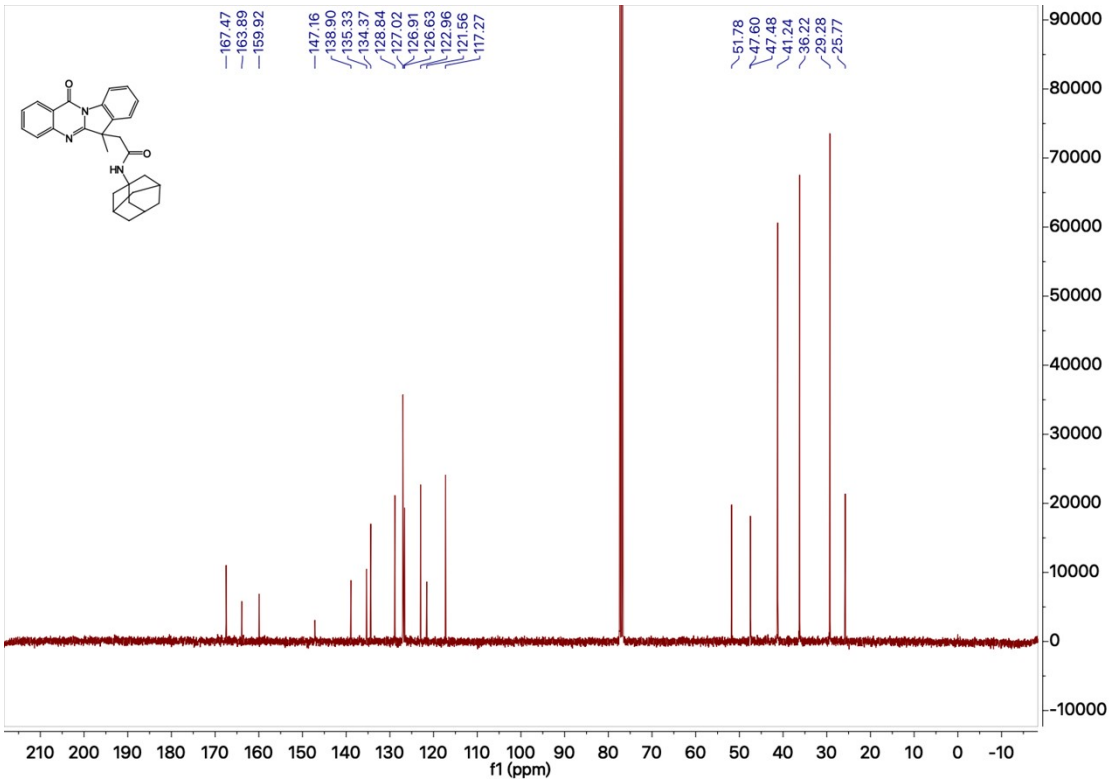
3na $^{13}C\{1H\}$ Chloroform-*d*, 101 MHz



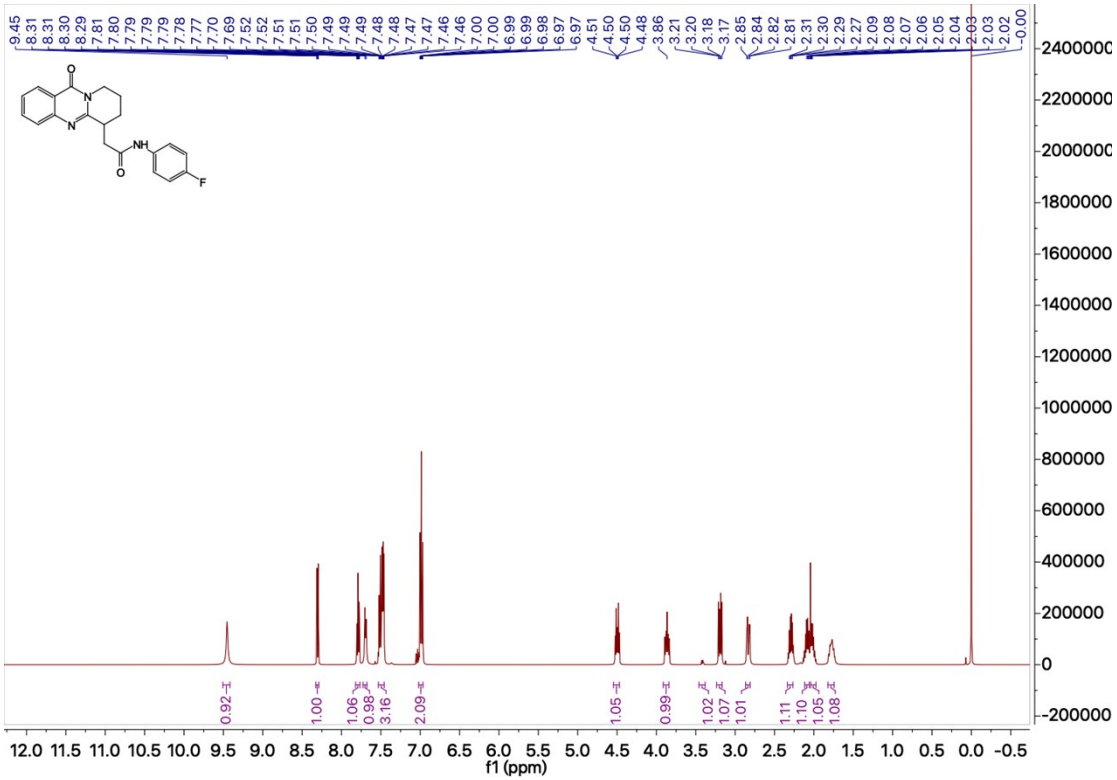
3oa ^{1}H Chloroform-*d*, 600 MHz



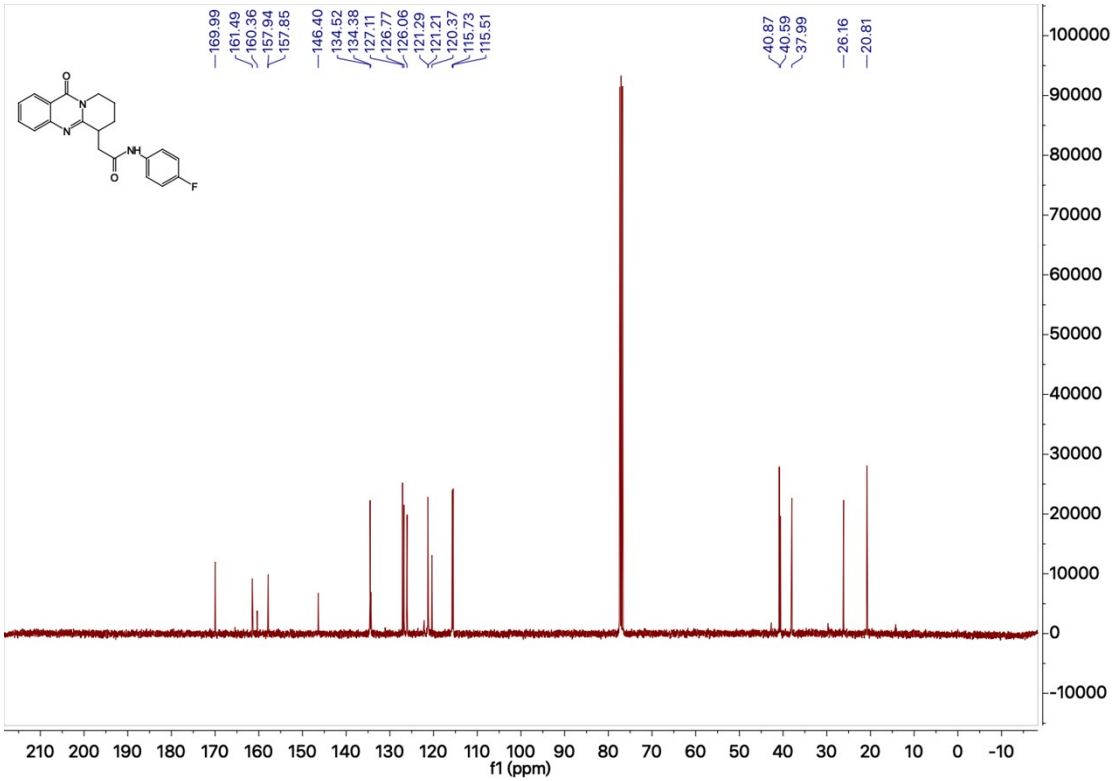
3oa $^{13}C\{1H\}$ Chloroform-*d*, 101 MHz



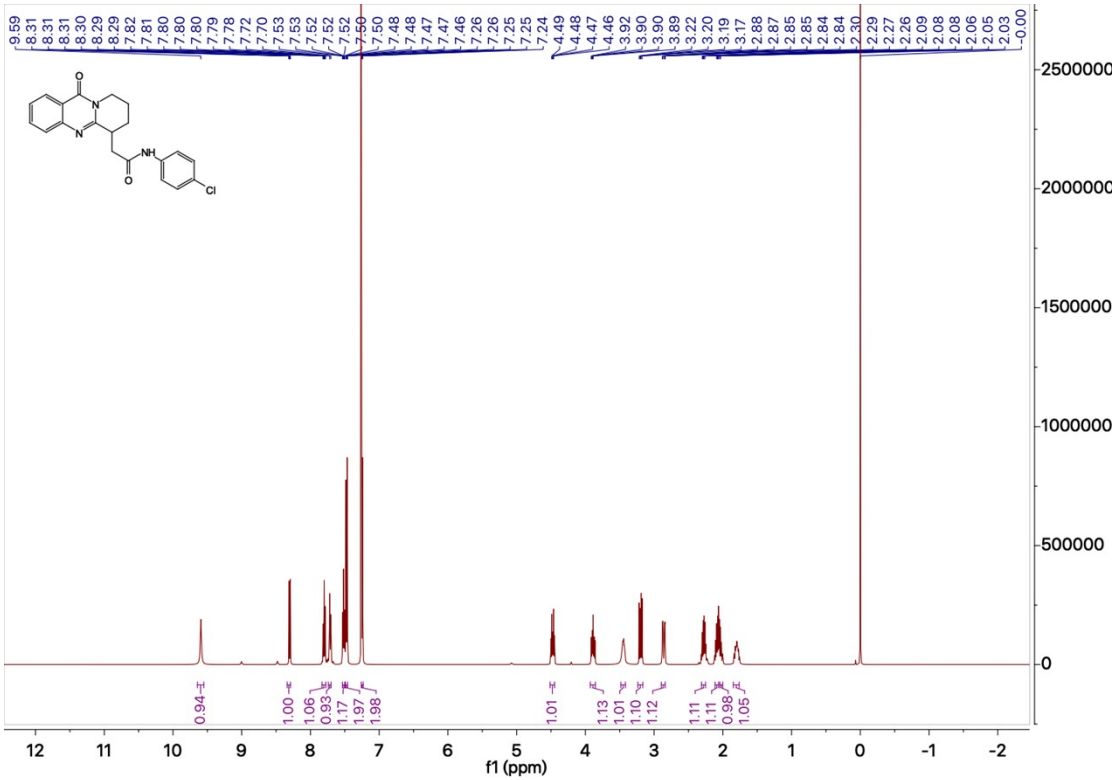
3qa ^{1}H Chloroform-*d*, 500 MHz



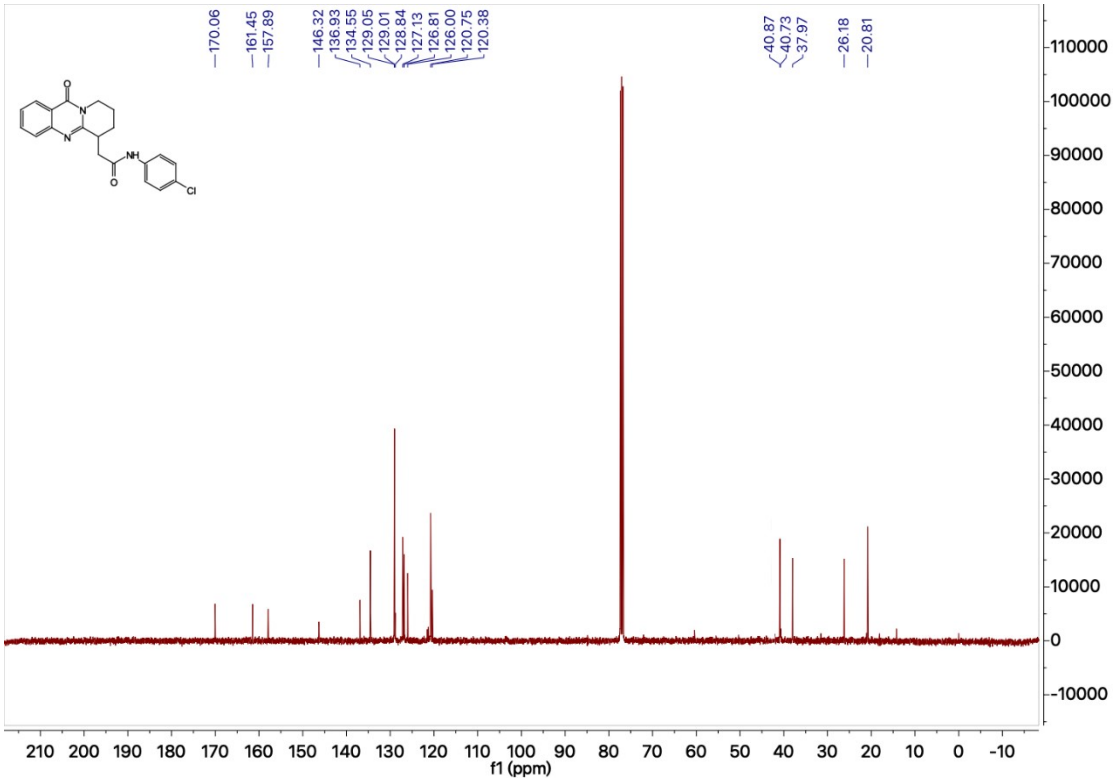
3qa $^{13}C\{1H\}$ Chloroform-*d*, 101 MHz



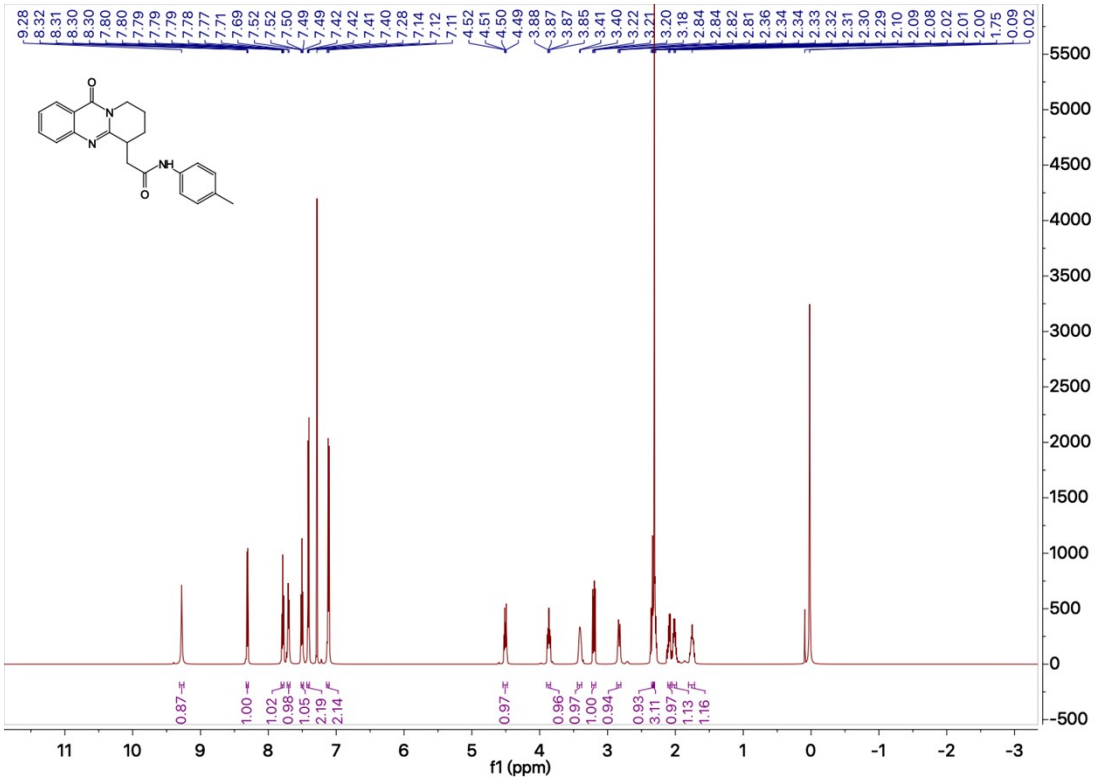
3ra ^{1}H Chloroform-*d*, 500 MHz



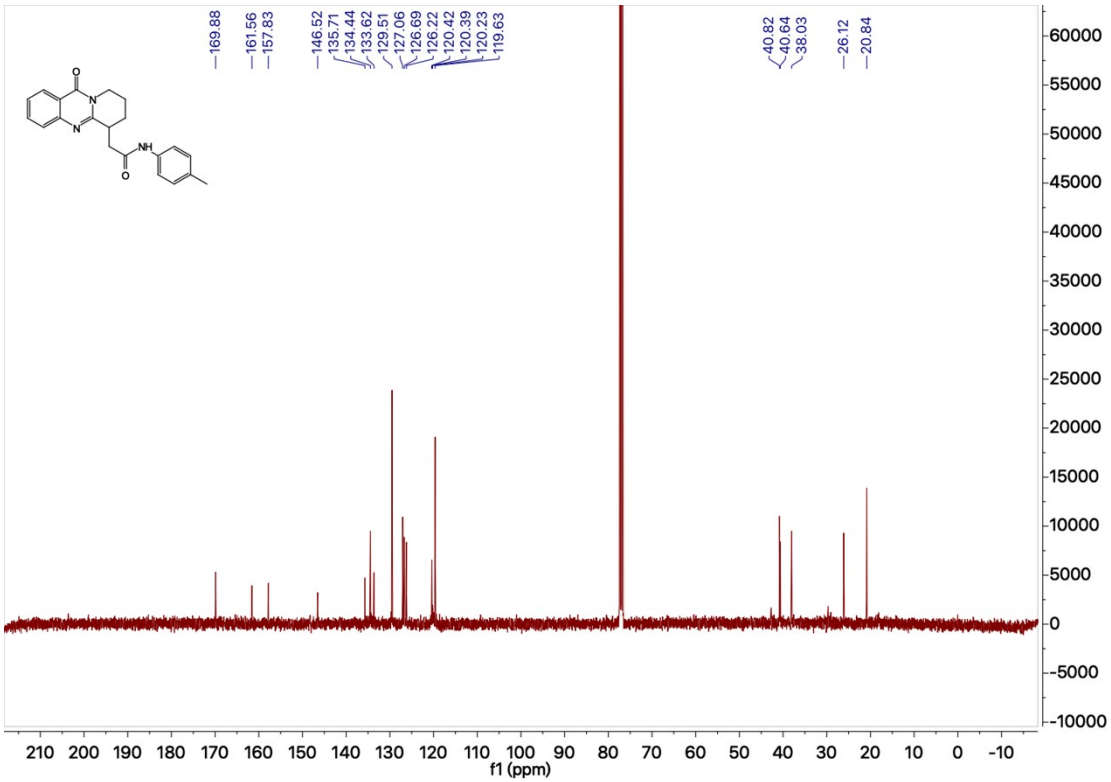
3ra $^{13}C\{1H\}$ Chloroform-*d*, 101 MHz



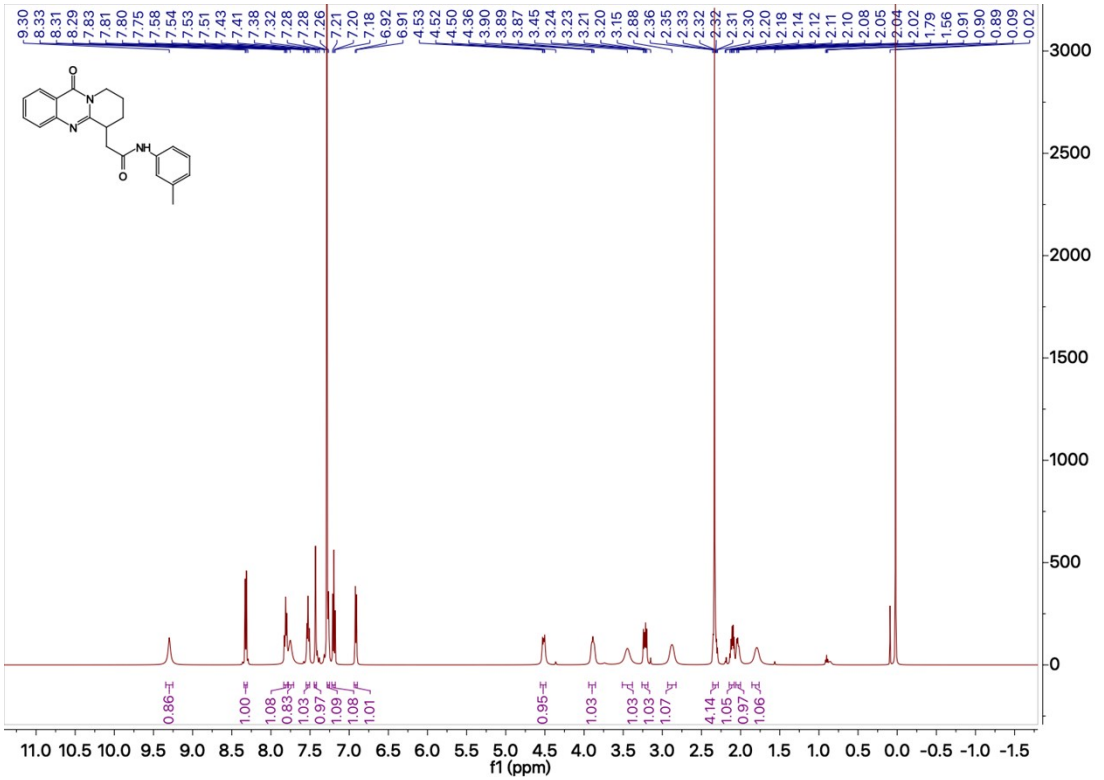
3sa ^{1}H Chloroform-*d*, 600 MHz



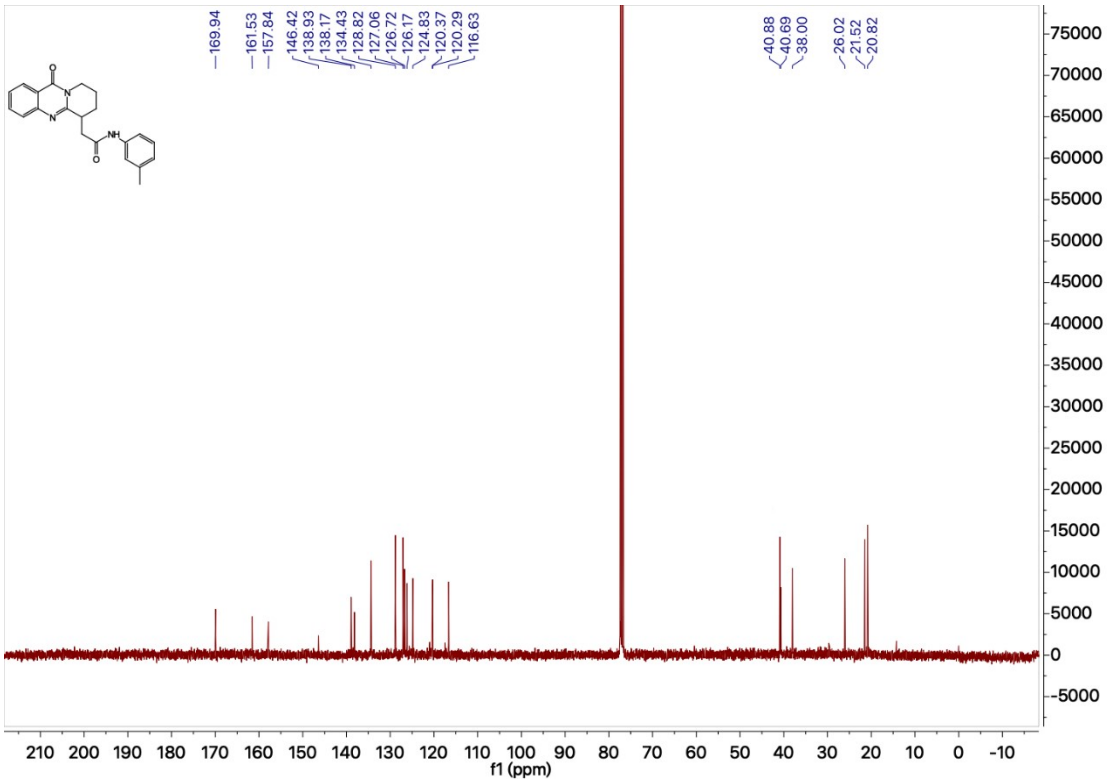
3sa $^{13}C\{1H\}$ Chloroform-*d*, 101 MHz



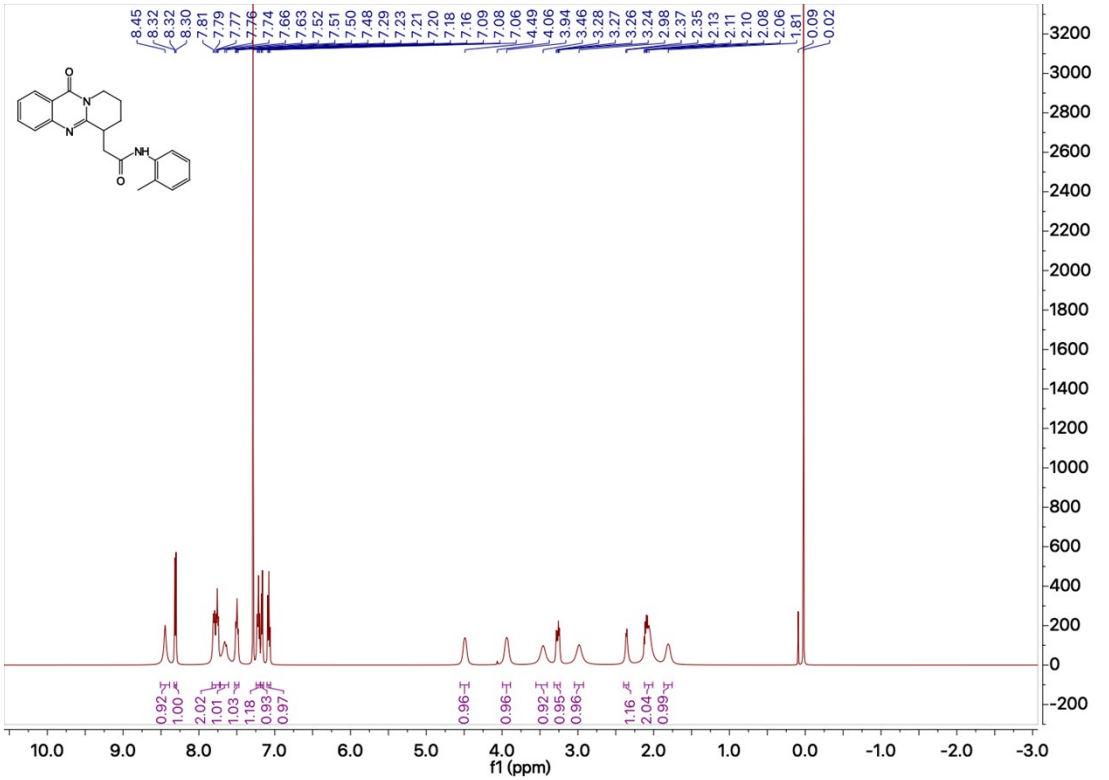
3ta ^{1}H Chloroform-*d*, 500 MHz



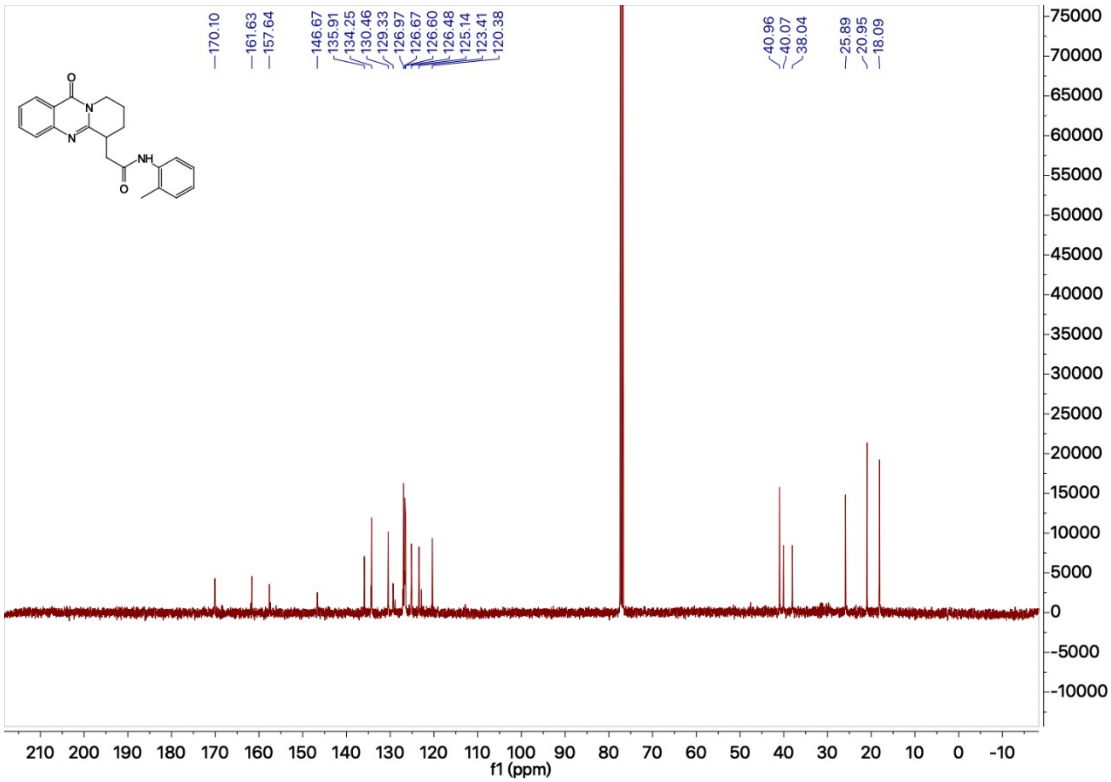
3ta ^{13}C{1H} Chloroform-*d*, 101 MHz



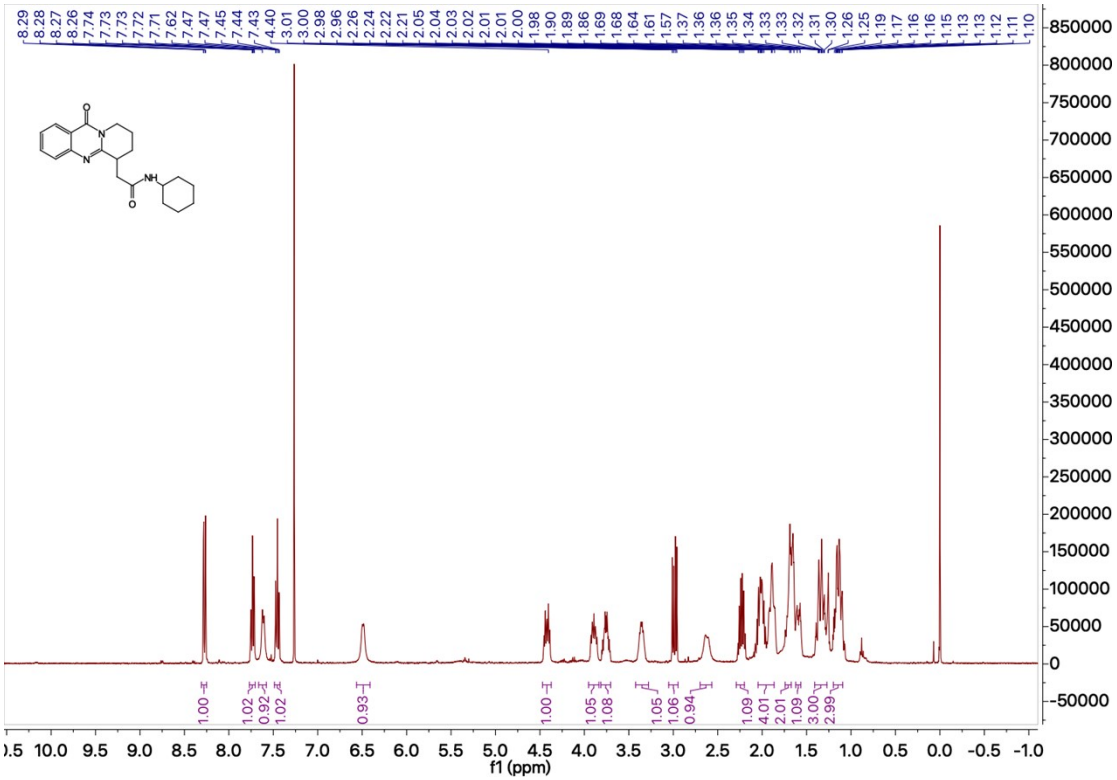
3ua ^{1}H Chloroform-*d*, 500 MHz



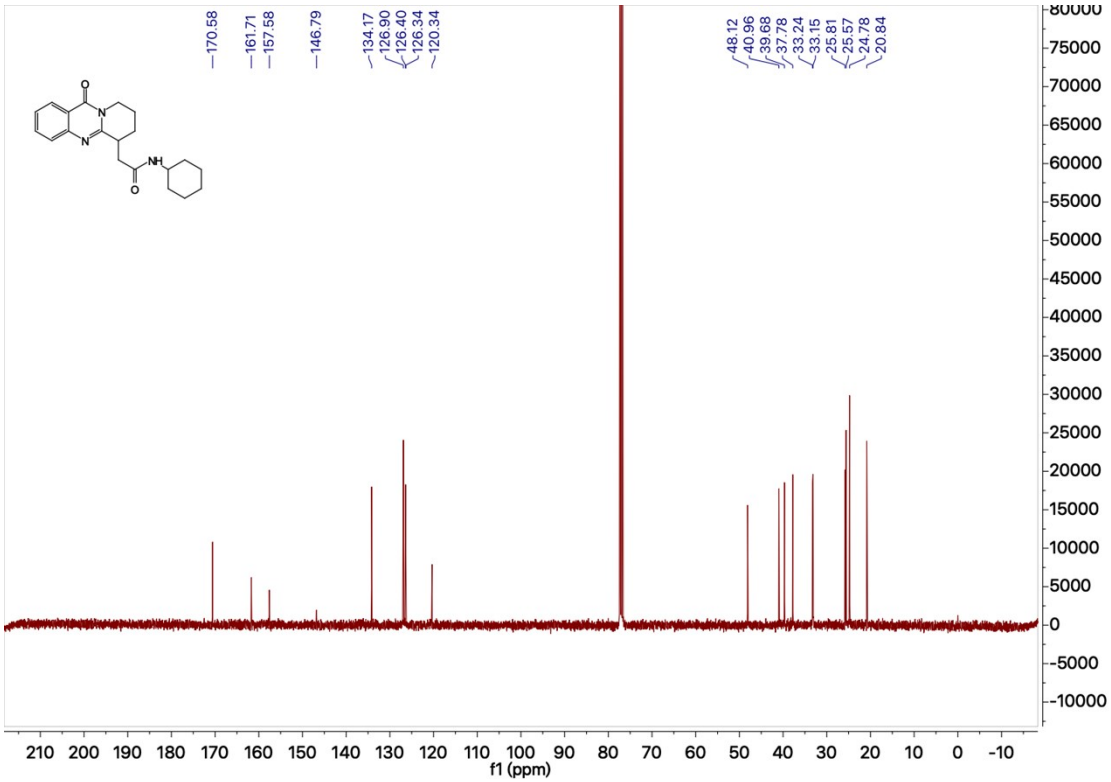
3ua $^{13}C\{1H\}$ Chloroform-*d*, 101 MHz



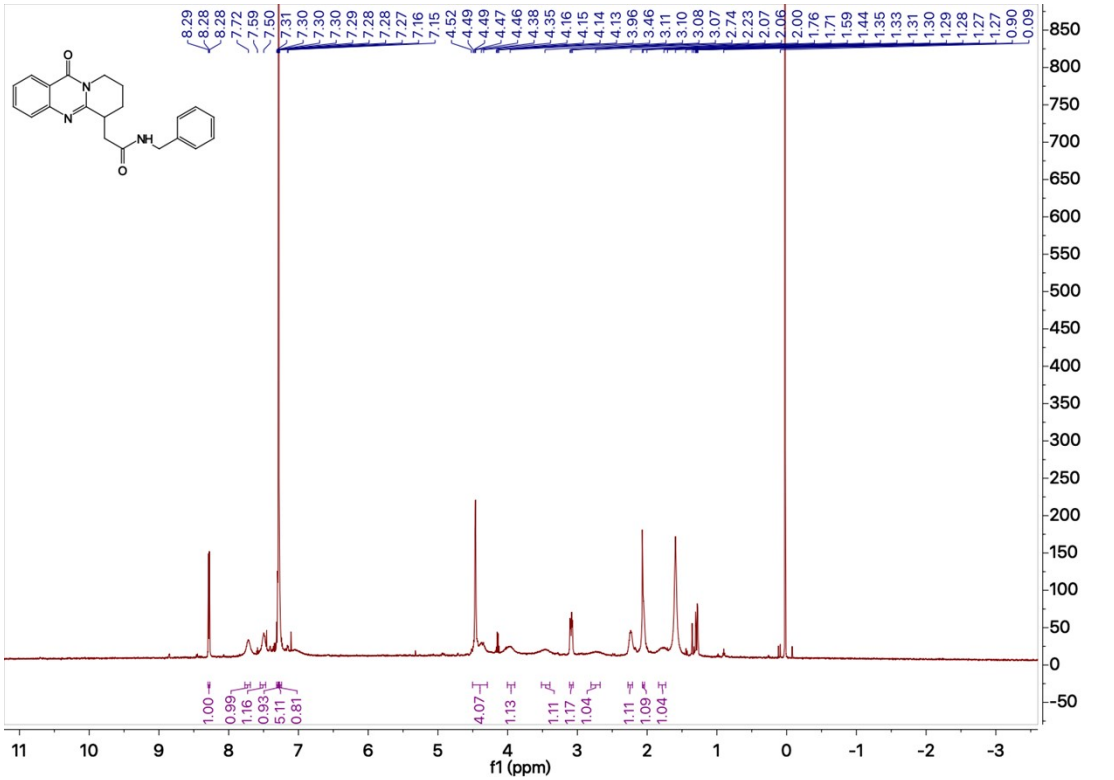
3va ^{1}H Chloroform-*d*, 400 MHz



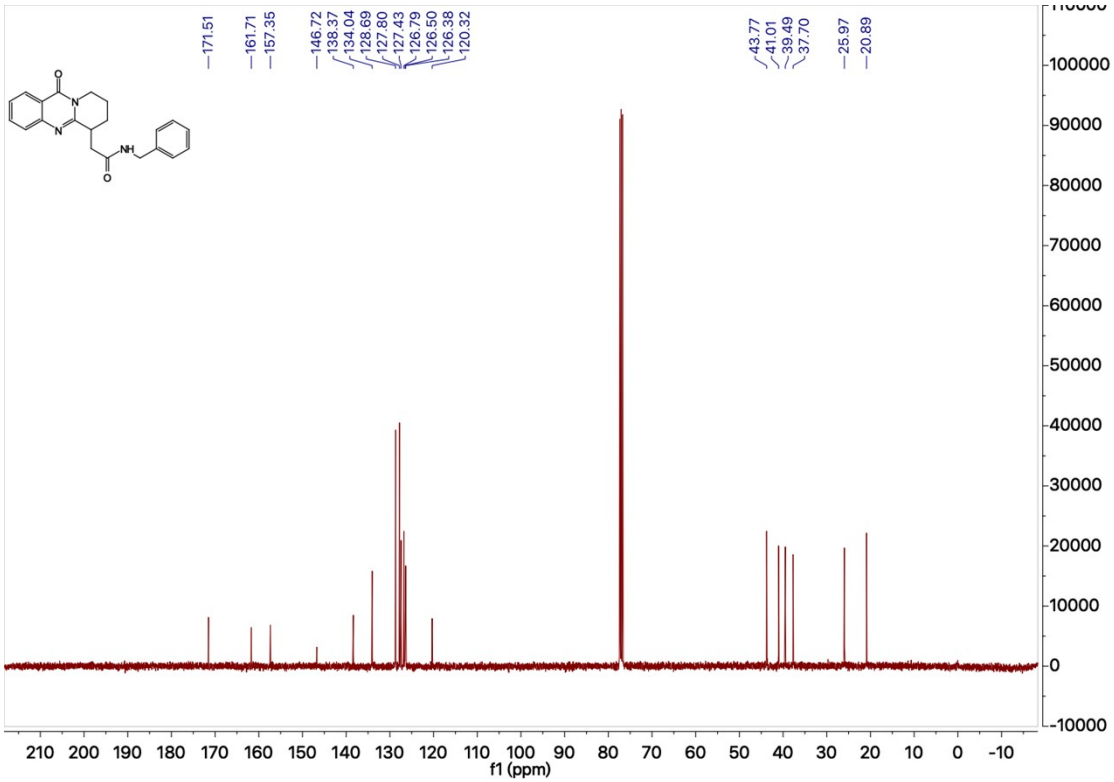
3va ^{13}C{1H} Chloroform-*d*, 101 MHz



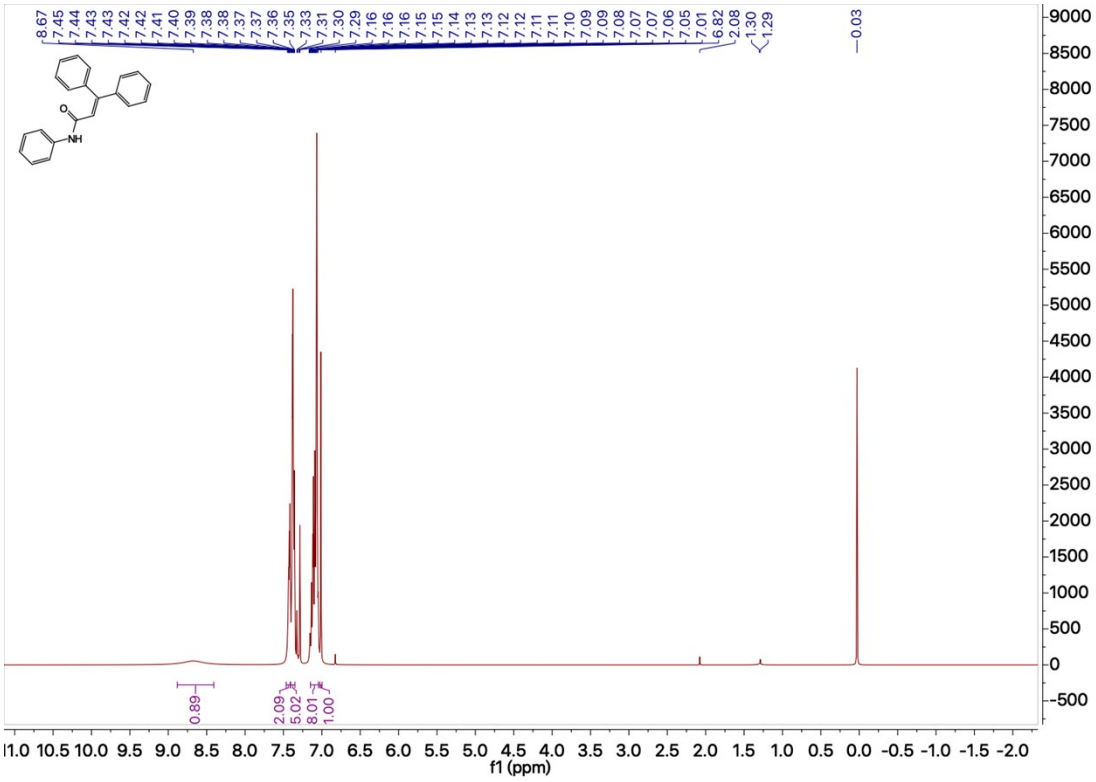
3wa ^{1}H Chloroform-*d*, 600 MHz



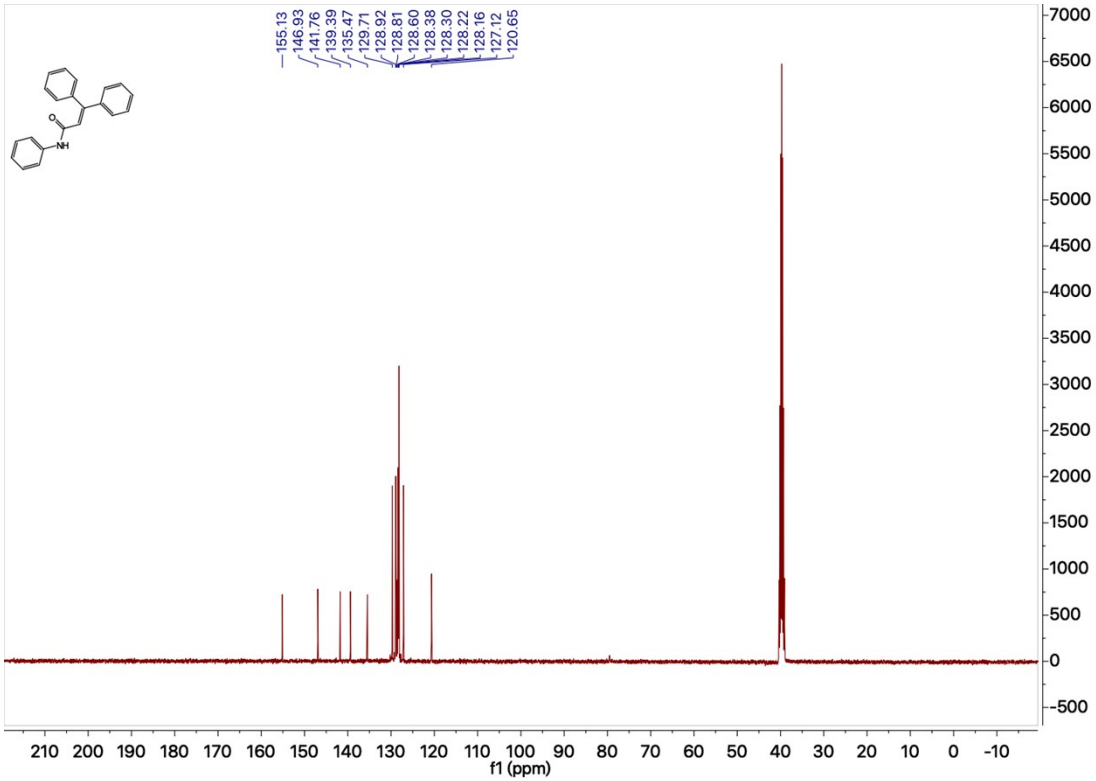
3wa $^{13}C\{1H\}$ Chloroform-*d*, 101 MHz



4 ^{1}H Chloroform-*d*, 400 MHz



4 $^{13}C\{1H\}$ DMSO-d_6, 101 MHz



V. Computational Details

The density functional theory (DFT) calculations were carried out with the VASP code[3]. The Perdew–Burke–Ernzerhof (PBE) functional within generalized gradient approximation (GGA)[4] was used to process the exchange–correlation, while the projectoraugmented-wave pseudopotential (PAW)[5] was applied with a kinetic energy cut-off of 500 eV, which was utilized to describe the expansion of the electronic eigenfunctions. The vacuum thickness was set to be 20 Å to minimize interlayer interactions. The Brillouin-zone integration was sampled by a Γ-centered 1 × 1 × 1 Monkhorst–Pack k-point. All atomic positions were fully relaxed until energy and force reached a tolerance of 1×10^{-5} eV and 0.03 eV/Å, respectively. The dispersion corrected DFT-D method was employed to consider the long-range interactions[6]. Employing the climbing image nudged elastic band method (CI-NEB), we computed the minimum energy pathway of the cyclization reaction along with its corresponding activation barrier.

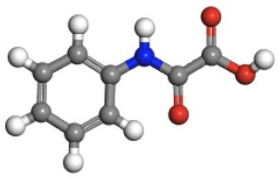
The Gibbs free energy change (ΔG) was calculated by computational hydrogen electrode (CHE) model as follows:

$$\Delta G = \Delta E + \Delta ZPE - T\Delta S \qquad (1)$$

where ΔE is the reaction energy obtained by the total energy difference between the reactant and product molecules absorbed on the catalyst surface and ΔS is the change in entropy for each reaction, ΔZPE is the zero-point energy correction to the Gibbs free energy. T represents temperature (323.15 K).

(1) 3D Structure and Coordinates of all Stationary Point

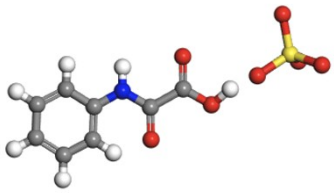
2a



C1	C	0.37217	0.58980	0.49278	0.00000	Uiso	1.00
C2	C	0.30415	0.55378	0.49280	0.00000	Uiso	1.00
C3	C	0.30133	0.47687	0.49282	0.00000	Uiso	1.00
C4	C	0.36651	0.43602	0.49278	0.00000	Uiso	1.00
C5	C	0.43454	0.47197	0.49279	0.00000	Uiso	1.00
C6	C	0.43749	0.54898	0.49274	0.00000	Uiso	1.00
N7	N	0.50378	0.58541	0.49270	0.00000	Uiso	1.00
C8	C	0.56940	0.54774	0.49274	0.00000	Uiso	1.00
C9	C	0.63553	0.58705	0.49244	0.00000	Uiso	1.00
O10	O	0.70136	0.55017	0.49351	0.00000	Uiso	1.00
O11	O	0.57084	0.47229	0.49301	0.00000	Uiso	1.00
O12	O	0.63436	0.66253	0.49302	0.00000	Uiso	1.00
H13	H	0.37420	0.64676	0.49266	0.00000	Uiso	1.00
H14	H	0.25586	0.58408	0.49278	0.00000	Uiso	1.00

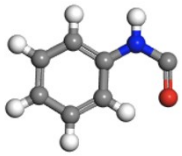
H15	H	0.25095	0.45014	0.49276	0.00000	Uiso	1.00
H16	H	0.36442	0.37904	0.49285	0.00000	Uiso	1.00
H17	H	0.48249	0.44138	0.49274	0.00000	Uiso	1.00
H18	H	0.50429	0.64085	0.49249	0.00000	Uiso	1.00
H19	H	0.73852	0.57949	0.52240	0.00000	Uiso	1.00

Ts-1



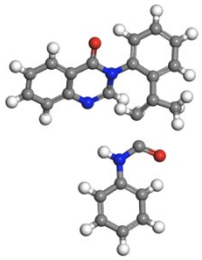
C1	C	0.22156	0.58767	0.49278	0.00000	Uiso	1.00
C2	C	0.15354	0.55164	0.49280	0.00000	Uiso	1.00
C3	C	0.15073	0.47473	0.49282	0.00000	Uiso	1.00
C4	C	0.21591	0.43388	0.49278	0.00000	Uiso	1.00
C5	C	0.28394	0.46983	0.49279	0.00000	Uiso	1.00
C6	C	0.28689	0.54685	0.49274	0.00000	Uiso	1.00
N7	N	0.35318	0.58327	0.49270	0.00000	Uiso	1.00
C8	C	0.41879	0.54560	0.49274	0.00000	Uiso	1.00
C9	C	0.49561	0.58812	0.49244	0.00000	Uiso	1.00
O10	O	0.56144	0.55124	0.49351	0.00000	Uiso	1.00
O11	O	0.42024	0.47015	0.49301	0.00000	Uiso	1.00
O12	O	0.49443	0.66360	0.49302	0.00000	Uiso	1.00
H13	H	0.22360	0.64463	0.49266	0.00000	Uiso	1.00
H14	H	0.10526	0.58194	0.49278	0.00000	Uiso	1.00
H15	H	0.10035	0.44800	0.49276	0.00000	Uiso	1.00
H16	H	0.21382	0.37691	0.49285	0.00000	Uiso	1.00
H17	H	0.33189	0.43924	0.49274	0.00000	Uiso	1.00
H18	H	0.35368	0.63871	0.49249	0.00000	Uiso	1.00
H19	H	0.60552	0.58778	0.52181	0.00000	Uiso	1.00
O20	O	0.81968	0.64365	0.54661	0.00000	Uiso	1.00
S21	S	0.74527	0.66935	0.49338	0.00000	Uiso	1.00
O22	O	0.66900	0.61884	0.51916	0.00000	Uiso	1.00
O23	O	0.72772	0.76190	0.50592	0.00000	Uiso	1.00
O24	O	0.76462	0.65294	0.40180	0.00000	Uiso	1.00

A



C1	C	0.37217	0.58980	0.49278	0.00000	Uiso	1.00
C2	C	0.30415	0.55378	0.49280	0.00000	Uiso	1.00
C3	C	0.30133	0.47687	0.49282	0.00000	Uiso	1.00
C4	C	0.36651	0.43602	0.49278	0.00000	Uiso	1.00
C5	C	0.43454	0.47197	0.49279	0.00000	Uiso	1.00
C6	C	0.43749	0.54898	0.49274	0.00000	Uiso	1.00
N7	N	0.50378	0.58541	0.49270	0.00000	Uiso	1.00
C8	C	0.56940	0.54774	0.49274	0.00000	Uiso	1.00
O9	O	0.57084	0.47229	0.49301	0.00000	Uiso	1.00
H10	H	0.37420	0.64676	0.49266	0.00000	Uiso	1.00
H11	H	0.25586	0.58408	0.49278	0.00000	Uiso	1.00
H12	H	0.25095	0.45014	0.49276	0.00000	Uiso	1.00
H13	H	0.36442	0.37904	0.49285	0.00000	Uiso	1.00
H14	H	0.48249	0.44138	0.49274	0.00000	Uiso	1.00
H15	H	0.50429	0.64085	0.49249	0.00000	Uiso	1.00

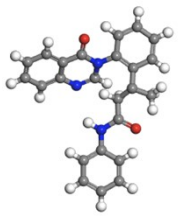
TS-2



C1	C	0.28377	0.72031	0.53128	0.00000	Uiso	1.00
C2	C	0.21481	0.68679	0.52389	0.00000	Uiso	1.00
C3	C	0.20776	0.62181	0.48311	0.00000	Uiso	1.00
C4	C	0.26961	0.59055	0.44947	0.00000	Uiso	1.00
C5	C	0.33852	0.62402	0.45715	0.00000	Uiso	1.00
C6	C	0.34563	0.68845	0.49835	0.00000	Uiso	1.00
C7	C	0.41503	0.72043	0.50690	0.00000	Uiso	1.00
N8	N	0.47579	0.68696	0.47704	0.00000	Uiso	1.00
C9	C	0.46723	0.62621	0.43279	0.00000	Uiso	1.00
N10	N	0.39933	0.59413	0.42392	0.00000	Uiso	1.00
O11	O	0.42265	0.78439	0.54626	0.00000	Uiso	1.00
C12	C	0.54381	0.71894	0.48635	0.00000	Uiso	1.00
C13	C	0.54830	0.79580	0.48237	0.00000	Uiso	1.00
C14	C	0.61682	0.83076	0.48134	0.00000	Uiso	1.00

C15	C	0.68118	0.78896	0.48510	0.00000	Uiso	1.00
C16	C	0.67692	0.71275	0.49443	0.00000	Uiso	1.00
C17	C	0.60847	0.67766	0.49875	0.00000	Uiso	1.00
C18	C	0.60799	0.60323	0.52011	0.00000	Uiso	1.00
C19	C	0.67987	0.57890	0.50662	0.00000	Uiso	1.00
C20	C	0.55604	0.55752	0.48640	0.00000	Uiso	1.00
C21	C	0.56349	0.45536	0.50354	0.00000	Uiso	1.00
N22	N	0.50096	0.41278	0.50322	0.00000	Uiso	1.00
C23	C	0.50485	0.33740	0.50928	0.00000	Uiso	1.00
C24	C	0.57296	0.30128	0.51035	0.00000	Uiso	1.00
C25	C	0.57586	0.22438	0.51369	0.00000	Uiso	1.00
C26	C	0.51074	0.18341	0.51620	0.00000	Uiso	1.00
C27	C	0.44270	0.21937	0.51555	0.00000	Uiso	1.00
C28	C	0.43978	0.29625	0.51212	0.00000	Uiso	1.00
O29	O	0.62979	0.42533	0.52320	0.00000	Uiso	1.00
H30	H	0.28901	0.76837	0.56127	0.00000	Uiso	1.00
H31	H	0.16909	0.71001	0.54855	0.00000	Uiso	1.00
H32	H	0.15682	0.59700	0.47768	0.00000	Uiso	1.00
H33	H	0.26435	0.54276	0.41902	0.00000	Uiso	1.00
H34	H	0.51236	0.60457	0.40561	0.00000	Uiso	1.00
H35	H	0.50067	0.82675	0.47799	0.00000	Uiso	1.00
H36	H	0.61985	0.88750	0.47689	0.00000	Uiso	1.00
H37	H	0.73202	0.81454	0.48210	0.00000	Uiso	1.00
H38	H	0.72473	0.68219	0.49979	0.00000	Uiso	1.00
H39	H	0.69003	0.57970	0.45056	0.00000	Uiso	1.00
H40	H	0.68739	0.52622	0.52669	0.00000	Uiso	1.00
H41	H	0.71647	0.61385	0.53280	0.00000	Uiso	1.00
H42	H	0.56108	0.56294	0.42993	0.00000	Uiso	1.00
H43	H	0.50449	0.57485	0.50319	0.00000	Uiso	1.00
H44	H	0.45147	0.43711	0.49708	0.00000	Uiso	1.00
H45	H	0.62128	0.33121	0.50787	0.00000	Uiso	1.00
H46	H	0.62625	0.19779	0.51411	0.00000	Uiso	1.00
H47	H	0.51290	0.12652	0.51856	0.00000	Uiso	1.00
H48	H	0.39447	0.18908	0.51752	0.00000	Uiso	1.00
H49	H	0.38933	0.32275	0.51142	0.00000	Uiso	1.00

B

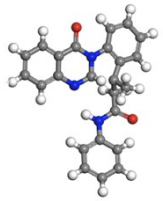


C1	C	0.28594	0.69317	0.53128	0.00000	Uiso	1.00

C2	C	0.21698	0.65965	0.52389	0.00000	Uiso	1.00
C3	C	0.20993	0.59468	0.48311	0.00000	Uiso	1.00
C4	C	0.27178	0.56341	0.44947	0.00000	Uiso	1.00
C5	C	0.34070	0.59689	0.45715	0.00000	Uiso	1.00
C6	C	0.34780	0.66132	0.49835	0.00000	Uiso	1.00
C7	C	0.41720	0.69329	0.50690	0.00000	Uiso	1.00
N8	N	0.47796	0.65982	0.47704	0.00000	Uiso	1.00
C9	C	0.46940	0.59907	0.43279	0.00000	Uiso	1.00
N10	N	0.40150	0.56699	0.42392	0.00000	Uiso	1.00
O11	O	0.42482	0.75725	0.54626	0.00000	Uiso	1.00
C12	C	0.54598	0.69180	0.48635	0.00000	Uiso	1.00
C13	C	0.55047	0.76866	0.48237	0.00000	Uiso	1.00
C14	C	0.61899	0.80362	0.48134	0.00000	Uiso	1.00
C15	C	0.68335	0.76182	0.48510	0.00000	Uiso	1.00
C16	C	0.67909	0.68561	0.49443	0.00000	Uiso	1.00
C17	C	0.61064	0.65052	0.49875	0.00000	Uiso	1.00
C18	C	0.61016	0.57609	0.52011	0.00000	Uiso	1.00
C19	C	0.68204	0.55176	0.50662	0.00000	Uiso	1.00
C20	C	0.55821	0.53038	0.48640	0.00000	Uiso	1.00
C21	C	0.56349	0.45536	0.50354	0.00000	Uiso	1.00
N22	N	0.50096	0.41278	0.50322	0.00000	Uiso	1.00
C23	C	0.50485	0.33740	0.50928	0.00000	Uiso	1.00
C24	C	0.57296	0.30128	0.51035	0.00000	Uiso	1.00
C25	C	0.57586	0.22438	0.51369	0.00000	Uiso	1.00
C26	C	0.51074	0.18341	0.51620	0.00000	Uiso	1.00
C27	C	0.44270	0.21937	0.51555	0.00000	Uiso	1.00
C28	C	0.43978	0.29625	0.51212	0.00000	Uiso	1.00
O29	O	0.62979	0.42533	0.52320	0.00000	Uiso	1.00
H30	H	0.29118	0.74123	0.56127	0.00000	Uiso	1.00
H31	H	0.17126	0.68287	0.54855	0.00000	Uiso	1.00
H32	H	0.15899	0.56986	0.47768	0.00000	Uiso	1.00
H33	H	0.26653	0.51562	0.41902	0.00000	Uiso	1.00
H34	H	0.51453	0.57743	0.40561	0.00000	Uiso	1.00
H35	H	0.50284	0.79961	0.47799	0.00000	Uiso	1.00
H36	H	0.62202	0.86036	0.47689	0.00000	Uiso	1.00
H37	H	0.73420	0.78740	0.48210	0.00000	Uiso	1.00
H38	H	0.72691	0.65505	0.49979	0.00000	Uiso	1.00
H39	H	0.69220	0.55256	0.45056	0.00000	Uiso	1.00
H40	H	0.68956	0.49908	0.52669	0.00000	Uiso	1.00
H41	H	0.71865	0.58671	0.53280	0.00000	Uiso	1.00
H42	H	0.56325	0.53580	0.42993	0.00000	Uiso	1.00
H43	H	0.50666	0.54771	0.50319	0.00000	Uiso	1.00
H44	H	0.45147	0.43711	0.49708	0.00000	Uiso	1.00
H45	H	0.62128	0.33121	0.50787	0.00000	Uiso	1.00

H46	H	0.62625	0.19779	0.51411	0.00000	Uiso	1.00
H47	H	0.51290	0.12652	0.51856	0.00000	Uiso	1.00
H48	H	0.39447	0.18908	0.51752	0.00000	Uiso	1.00
H49	H	0.38933	0.32275	0.51142	0.00000	Uiso	1.00

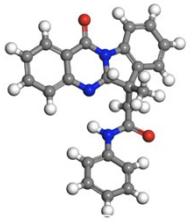
TS-3



C1	C	0.28329	0.72357	0.50504	0.00000	Uiso	1.00
C2	C	0.21476	0.68869	0.50120	0.00000	Uiso	1.00
C3	C	0.21080	0.61193	0.49617	0.00000	Uiso	1.00
C4	C	0.27531	0.57003	0.49568	0.00000	Uiso	1.00
C5	C	0.34361	0.60492	0.50028	0.00000	Uiso	1.00
C6	C	0.34764	0.68144	0.50392	0.00000	Uiso	1.00
C7	C	0.41651	0.71511	0.50468	0.00000	Uiso	1.00
N8	N	0.47885	0.67255	0.50325	0.00000	Uiso	1.00
C9	C	0.47471	0.59695	0.50775	0.00000	Uiso	1.00
N10	N	0.40691	0.56405	0.50070	0.00000	Uiso	1.00
O11	O	0.42186	0.79047	0.50537	0.00000	Uiso	1.00
C12	C	0.54622	0.70556	0.49547	0.00000	Uiso	1.00
C13	C	0.56387	0.77960	0.48745	0.00000	Uiso	1.00
C14	C	0.63722	0.79716	0.47082	0.00000	Uiso	1.00
C15	C	0.68982	0.74074	0.46189	0.00000	Uiso	1.00
C16	C	0.66968	0.66646	0.47012	0.00000	Uiso	1.00
C17	C	0.59688	0.65016	0.48788	0.00000	Uiso	1.00
C18	C	0.56681	0.57886	0.49815	0.00000	Uiso	1.00
C19	C	0.59544	0.55016	0.56347	0.00000	Uiso	1.00
C20	C	0.58254	0.52985	0.44109	0.00000	Uiso	1.00
C21	C	0.57618	0.45794	0.46802	0.00000	Uiso	1.00
N22	N	0.51042	0.42062	0.46528	0.00000	Uiso	1.00
C23	C	0.50661	0.34775	0.48601	0.00000	Uiso	1.00
C24	C	0.57079	0.30741	0.50058	0.00000	Uiso	1.00
C25	C	0.56618	0.23376	0.52253	0.00000	Uiso	1.00
C26	C	0.49748	0.19997	0.52975	0.00000	Uiso	1.00
C27	C	0.43336	0.23971	0.51446	0.00000	Uiso	1.00
C28	C	0.43793	0.31342	0.49243	0.00000	Uiso	1.00
O29	O	0.63823	0.42359	0.49366	0.00000	Uiso	1.00
H30	H	0.28640	0.78040	0.50821	0.00000	Uiso	1.00
H31	H	0.16698	0.71970	0.50189	0.00000	Uiso	1.00
H32	H	0.16012	0.58616	0.49276	0.00000	Uiso	1.00
H33	H	0.27245	0.51322	0.49204	0.00000	Uiso	1.00

H34	H	0.52427	0.82023	0.49316	0.00000	Uiso	1.00
H35	H	0.65271	0.85171	0.46466	0.00000	Uiso	1.00
H36	H	0.74374	0.75415	0.44914	0.00000	Uiso	1.00
H37	H	0.70803	0.62486	0.46326	0.00000	Uiso	1.00
H38	H	0.65154	0.54224	0.55747	0.00000	Uiso	1.00
H39	H	0.57036	0.50018	0.57462	0.00000	Uiso	1.00
H40	H	0.58561	0.58656	0.60622	0.00000	Uiso	1.00
H41	H	0.63754	0.53617	0.42768	0.00000	Uiso	1.00
H42	H	0.55051	0.54010	0.39504	0.00000	Uiso	1.00
H43	H	0.46447	0.44699	0.44866	0.00000	Uiso	1.00
H44	H	0.62188	0.33166	0.49451	0.00000	Uiso	1.00
H45	H	0.61370	0.20426	0.53346	0.00000	Uiso	1.00
H46	H	0.49409	0.14546	0.54616	0.00000	Uiso	1.00
H47	H	0.38242	0.21460	0.51960	0.00000	Uiso	1.00
H48	H	0.39035	0.34277	0.48129	0.00000	Uiso	1.00
H49	H	0.49941	0.57910	0.55566	0.00000	Uiso	1.00

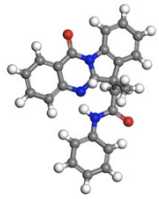
C



C1	C	0.28100	0.68847	0.50733	0.00000	Uiso	1.00
C2	C	0.21998	0.64212	0.50026	0.00000	Uiso	1.00
C3	C	0.23000	0.56611	0.49262	0.00000	Uiso	1.00
C4	C	0.30101	0.53616	0.49311	0.00000	Uiso	1.00
C5	C	0.36227	0.58224	0.50060	0.00000	Uiso	1.00
C6	C	0.35198	0.65884	0.50649	0.00000	Uiso	1.00
C7	C	0.41318	0.70538	0.50951	0.00000	Uiso	1.00
N8	N	0.48076	0.67344	0.50600	0.00000	Uiso	1.00
C9	C	0.49135	0.59946	0.50510	0.00000	Uiso	1.00
N10	N	0.43232	0.55255	0.50117	0.00000	Uiso	1.00
O11	O	0.40560	0.78036	0.51374	0.00000	Uiso	1.00
C12	C	0.54622	0.70556	0.49547	0.00000	Uiso	1.00
C13	C	0.56387	0.77960	0.48745	0.00000	Uiso	1.00
C14	C	0.63722	0.79716	0.47082	0.00000	Uiso	1.00
C15	C	0.68982	0.74074	0.46189	0.00000	Uiso	1.00
C16	C	0.66968	0.66646	0.47012	0.00000	Uiso	1.00
C17	C	0.59688	0.65016	0.48788	0.00000	Uiso	1.00
C18	C	0.56681	0.57886	0.49815	0.00000	Uiso	1.00
C19	C	0.59544	0.55016	0.56347	0.00000	Uiso	1.00
C20	C	0.58254	0.52985	0.44109	0.00000	Uiso	1.00

C21	C	0.57618	0.45794	0.46802	0.00000	Uiso	1.00
N22	N	0.51042	0.42062	0.46528	0.00000	Uiso	1.00
C23	C	0.50661	0.34775	0.48601	0.00000	Uiso	1.00
C24	C	0.57079	0.30741	0.50058	0.00000	Uiso	1.00
C25	C	0.56618	0.23376	0.52253	0.00000	Uiso	1.00
C26	C	0.49748	0.19997	0.52975	0.00000	Uiso	1.00
C27	C	0.43336	0.23971	0.51446	0.00000	Uiso	1.00
C28	C	0.43793	0.31342	0.49243	0.00000	Uiso	1.00
O29	O	0.63823	0.42359	0.49366	0.00000	Uiso	1.00
H30	H	0.27365	0.74476	0.51250	0.00000	Uiso	1.00
H31	H	0.16739	0.66405	0.50046	0.00000	Uiso	1.00
H32	H	0.18480	0.53195	0.48675	0.00000	Uiso	1.00
H33	H	0.30818	0.47986	0.48783	0.00000	Uiso	1.00
H34	H	0.52427	0.82023	0.49316	0.00000	Uiso	1.00
H35	H	0.65271	0.85171	0.46466	0.00000	Uiso	1.00
H36	H	0.74374	0.75415	0.44914	0.00000	Uiso	1.00
H37	H	0.70803	0.62486	0.46326	0.00000	Uiso	1.00
H38	H	0.65154	0.54224	0.55747	0.00000	Uiso	1.00
H39	H	0.57036	0.50018	0.57462	0.00000	Uiso	1.00
H40	H	0.58561	0.58656	0.60622	0.00000	Uiso	1.00
H41	H	0.63754	0.53617	0.42768	0.00000	Uiso	1.00
H42	H	0.55051	0.54010	0.39504	0.00000	Uiso	1.00
H43	H	0.46447	0.44699	0.44866	0.00000	Uiso	1.00
H44	H	0.62188	0.33166	0.49451	0.00000	Uiso	1.00
H45	H	0.61370	0.20426	0.53346	0.00000	Uiso	1.00
H46	H	0.49409	0.14546	0.54616	0.00000	Uiso	1.00
H47	H	0.38242	0.21460	0.51960	0.00000	Uiso	1.00
H48	H	0.39035	0.34277	0.48129	0.00000	Uiso	1.00
H49	H	0.49315	0.59649	0.56199	0.00000	Uiso	1.00

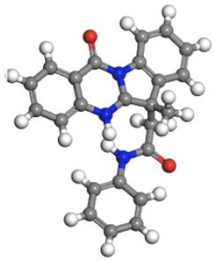
TS-4



C1	C	0.28332	0.66897	0.49807	0.00000	Uiso	1.00
C2	C	0.22506	0.61907	0.50445	0.00000	Uiso	1.00
C3	C	0.23953	0.54415	0.51493	0.00000	Uiso	1.00
C4	C	0.31225	0.51908	0.51958	0.00000	Uiso	1.00
C5	C	0.37069	0.56889	0.51354	0.00000	Uiso	1.00
C6	C	0.35594	0.64386	0.50233	0.00000	Uiso	1.00
C7	C	0.41442	0.69308	0.49472	0.00000	Uiso	1.00
N8	N	0.48421	0.66573	0.49887	0.00000	Uiso	1.00

C9	C	0.49974	0.59299	0.51333	0.00000	Uiso	1.00
N10	N	0.44226	0.54413	0.51874	0.00000	Uiso	1.00
O11	O	0.40214	0.76653	0.48225	0.00000	Uiso	1.00
C12	C	0.54658	0.70336	0.48766	0.00000	Uiso	1.00
C13	C	0.55721	0.77765	0.47243	0.00000	Uiso	1.00
C14	C	0.62991	0.80204	0.46296	0.00000	Uiso	1.00
C15	C	0.68887	0.75184	0.46896	0.00000	Uiso	1.00
C16	C	0.67545	0.67718	0.48433	0.00000	Uiso	1.00
C17	C	0.60279	0.65448	0.49328	0.00000	Uiso	1.00
C18	C	0.57796	0.58245	0.50802	0.00000	Uiso	1.00
C19	C	0.60802	0.55597	0.57384	0.00000	Uiso	1.00
C20	C	0.59796	0.53633	0.44966	0.00000	Uiso	1.00
C21	C	0.58403	0.46277	0.46775	0.00000	Uiso	1.00
N22	N	0.51361	0.43539	0.46516	0.00000	Uiso	1.00
C23	C	0.49902	0.36313	0.48270	0.00000	Uiso	1.00
C24	C	0.55562	0.31503	0.50359	0.00000	Uiso	1.00
C25	C	0.53969	0.24170	0.52081	0.00000	Uiso	1.00
C26	C	0.46721	0.21616	0.51729	0.00000	Uiso	1.00
C27	C	0.41059	0.26407	0.49675	0.00000	Uiso	1.00
C28	C	0.42648	0.33742	0.47946	0.00000	Uiso	1.00
O29	O	0.64187	0.41804	0.48617	0.00000	Uiso	1.00
H30	H	0.27272	0.72439	0.49006	0.00000	Uiso	1.00
H31	H	0.17123	0.63756	0.50134	0.00000	Uiso	1.00
H32	H	0.19635	0.50720	0.51937	0.00000	Uiso	1.00
H33	H	0.32281	0.46364	0.52761	0.00000	Uiso	1.00
H34	H	0.51315	0.81360	0.46837	0.00000	Uiso	1.00
H35	H	0.64029	0.85692	0.45157	0.00000	Uiso	1.00
H36	H	0.74243	0.77010	0.46203	0.00000	Uiso	1.00
H37	H	0.71842	0.64002	0.48879	0.00000	Uiso	1.00
H38	H	0.66473	0.55316	0.56913	0.00000	Uiso	1.00
H39	H	0.58719	0.50404	0.58467	0.00000	Uiso	1.00
H40	H	0.59443	0.59111	0.61661	0.00000	Uiso	1.00
H41	H	0.65413	0.54136	0.44140	0.00000	Uiso	1.00
H42	H	0.57050	0.55179	0.40217	0.00000	Uiso	1.00
H43	H	0.47183	0.46889	0.45063	0.00000	Uiso	1.00
H44	H	0.60934	0.33338	0.50641	0.00000	Uiso	1.00
H45	H	0.58167	0.20628	0.53611	0.00000	Uiso	1.00
H46	H	0.45547	0.16183	0.52988	0.00000	Uiso	1.00
H47	H	0.35683	0.24524	0.49430	0.00000	Uiso	1.00
H48	H	0.38447	0.37275	0.46415	0.00000	Uiso	1.00
H49	H	0.47218	0.58030	0.58573	0.00000	Uiso	1.00

D



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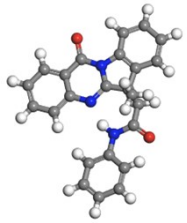
C3	C	0.23953	0.54415	0.51493	0.00000	Uiso	1.00
C4	C	0.31225	0.51908	0.51958	0.00000	Uiso	1.00
C5	C	0.37069	0.56889	0.51354	0.00000	Uiso	1.00
C6	C	0.35594	0.64386	0.50233	0.00000	Uiso	1.00
C7	C	0.41442	0.69308	0.49472	0.00000	Uiso	1.00
N8	N	0.48421	0.66573	0.49887	0.00000	Uiso	1.00
C9	C	0.49974	0.59299	0.51333	0.00000	Uiso	1.00
N10	N	0.44226	0.54413	0.51874	0.00000	Uiso	1.00
O11	O	0.40214	0.76653	0.48225	0.00000	Uiso	1.00
C12	C	0.54658	0.70336	0.48766	0.00000	Uiso	1.00
C13	C	0.55721	0.77765	0.47243	0.00000	Uiso	1.00
C14	C	0.62991	0.80204	0.46296	0.00000	Uiso	1.00
C15	C	0.68887	0.75184	0.46896	0.00000	Uiso	1.00
C16	C	0.67545	0.67718	0.48433	0.00000	Uiso	1.00
C17	C	0.60279	0.65448	0.49328	0.00000	Uiso	1.00
C18	C	0.57796	0.58245	0.50802	0.00000	Uiso	1.00
C19	C	0.60802	0.55597	0.57384	0.00000	Uiso	1.00
C20	C	0.59796	0.53633	0.44966	0.00000	Uiso	1.00
C21	C	0.58403	0.46277	0.46775	0.00000	Uiso	1.00
N22	N	0.51361	0.43539	0.46516	0.00000	Uiso	1.00
C23	C	0.49902	0.36313	0.48270	0.00000	Uiso	1.00
C24	C	0.55562	0.31503	0.50359	0.00000	Uiso	1.00
C25	C	0.53969	0.24170	0.52081	0.00000	Uiso	1.00
C26	C	0.46721	0.21616	0.51729	0.00000	Uiso	1.00
C27	C	0.41059	0.26407	0.49675	0.00000	Uiso	1.00
C28	C	0.42648	0.33742	0.47946	0.00000	Uiso	1.00
O29	O	0.64187	0.41804	0.48617	0.00000	Uiso	1.00
H30	H	0.27272	0.72439	0.49006	0.00000	Uiso	1.00
H31	H	0.17123	0.63756	0.50134	0.00000	Uiso	1.00
H32	H	0.19635	0.50720	0.51937	0.00000	Uiso	1.00
H33	H	0.32281	0.46364	0.52761	0.00000	Uiso	1.00
H34	H	0.51315	0.81360	0.46837	0.00000	Uiso	1.00
H35	H	0.64029	0.85692	0.45157	0.00000	Uiso	1.00
H36	H	0.74243	0.77010	0.46203	0.00000	Uiso	1.00
H37	H	0.71842	0.64002	0.48879	0.00000	Uiso	1.00

H38	H	0.66473	0.55316	0.56913	0.00000	Uiso	1.00
H39	H	0.58719	0.50404	0.58467	0.00000	Uiso	1.00
H40	H	0.59443	0.59111	0.61661	0.00000	Uiso	1.00
H41	H	0.65413	0.54136	0.44140	0.00000	Uiso	1.00
H42	H	0.57050	0.55179	0.40217	0.00000	Uiso	1.00
H43	H	0.47183	0.46889	0.45063	0.00000	Uiso	1.00
H44	H	0.60934	0.33338	0.50641	0.00000	Uiso	1.00
H45	H	0.58167	0.20628	0.53611	0.00000	Uiso	1.00
H46	H	0.45547	0.16183	0.52988	0.00000	Uiso	1.00
H47	H	0.35683	0.24524	0.49430	0.00000	Uiso	1.00
H48	H	0.38447	0.37275	0.46415	0.00000	Uiso	1.00
H49	H	0.45241	0.49011	0.52632	0.00000	Uiso	1.00

3aa



C1	C	0.28271	0.66586	0.49862	0.00000	Uiso	1.00
C2	C	0.22642	0.61385	0.50602	0.00000	Uiso	1.00
C3	C	0.24368	0.53964	0.51735	0.00000	Uiso	1.00
C4	C	0.31724	0.51721	0.52124	0.00000	Uiso	1.00
C5	C	0.37372	0.56889	0.51356	0.00000	Uiso	1.00
C6	C	0.35627	0.64352	0.50213	0.00000	Uiso	1.00
C7	C	0.41292	0.69506	0.49375	0.00000	Uiso	1.00
N8	N	0.48337	0.66939	0.49652	0.00000	Uiso	1.00
C9	C	0.50041	0.59754	0.50768	0.00000	Uiso	1.00
N10	N	0.44607	0.54615	0.51667	0.00000	Uiso	1.00
O11	O	0.39809	0.76830	0.48295	0.00000	Uiso	1.00
C12	C	0.54672	0.70601	0.48741	0.00000	Uiso	1.00
C13	C	0.55908	0.78016	0.47312	0.00000	Uiso	1.00
C14	C	0.63233	0.80303	0.46400	0.00000	Uiso	1.00
C15	C	0.69027	0.75155	0.46910	0.00000	Uiso	1.00
C16	C	0.67551	0.67699	0.48368	0.00000	Uiso	1.00
C17	C	0.60250	0.65535	0.49296	0.00000	Uiso	1.00
C18	C	0.57743	0.58271	0.50692	0.00000	Uiso	1.00
C19	C	0.60258	0.55747	0.57507	0.00000	Uiso	1.00
C20	C	0.59957	0.53504	0.45068	0.00000	Uiso	1.00
C21	C	0.58443	0.46170	0.46878	0.00000	Uiso	1.00
N22	N	0.51372	0.43500	0.46533	0.00000	Uiso	1.00
C23	C	0.49821	0.36276	0.48243	0.00000	Uiso	1.00
C24	C	0.55407	0.31390	0.50361	0.00000	Uiso	1.00

C25	C	0.53709	0.24080	0.52086	0.00000	Uiso	1.00
C26	C	0.46429	0.21623	0.51716	0.00000	Uiso	1.00
C27	C	0.40844	0.26478	0.49605	0.00000	Uiso	1.00
C28	C	0.42537	0.33791	0.47874	0.00000	Uiso	1.00
O29	O	0.64170	0.41617	0.48698	0.00000	Uiso	1.00
H30	H	0.26991	0.72079	0.49032	0.00000	Uiso	1.00
H31	H	0.17192	0.63027	0.50309	0.00000	Uiso	1.00
H32	H	0.20193	0.50123	0.52281	0.00000	Uiso	1.00
H33	H	0.32988	0.46225	0.52956	0.00000	Uiso	1.00
H34	H	0.51586	0.81710	0.46918	0.00000	Uiso	1.00
H35	H	0.64387	0.85782	0.45334	0.00000	Uiso	1.00
H36	H	0.74412	0.76884	0.46202	0.00000	Uiso	1.00
H37	H	0.71787	0.63903	0.48733	0.00000	Uiso	1.00
H38	H	0.65940	0.55321	0.57382	0.00000	Uiso	1.00
H39	H	0.57983	0.50627	0.58561	0.00000	Uiso	1.00
H40	H	0.58699	0.59411	0.61587	0.00000	Uiso	1.00
H41	H	0.65615	0.53939	0.44541	0.00000	Uiso	1.00
H42	H	0.57501	0.54992	0.40144	0.00000	Uiso	1.00
H43	H	0.47248	0.46890	0.45016	0.00000	Uiso	1.00
H44	H	0.60802	0.33155	0.50664	0.00000	Uiso	1.00
H45	H	0.57851	0.20487	0.53645	0.00000	Uiso	1.00
H46	H	0.45175	0.16212	0.53000	0.00000	Uiso	1.00
H47	H	0.35449	0.24661	0.49328	0.00000	Uiso	1.00
H48	H	0.38387	0.37378	0.46325	0.00000	Uiso	1.00

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