Electronic Supplementary Material (ESI) for RSC Advances.
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Supplementary data

1. Reagents & Instruments

For antioxidant activity: The antioxidant activity was run at the Unit of genetic engineering and biotechnology, Faculty of Science, Mansoura University. The analyses were run at unit of genetic engineering and biotechnology, Mansoura University using Spectrophotometric apparatus (Spekol 11 spectrophotometer, analytic Jena AG, Jena, Germany). UV lamp (Vilber Lourmat-6.LC, VILBER Smart Imaging, Marne-la-Vallée, France). 1,1-Diphenyl-2-picrylhydrazyl (DPPH•), ascorbic acid, sulfuric acid, sodium phosphate, ammonium heptamolybdate, and DMSO were purchased from Sigma Aldrich (St. Louis, USA).

Characterization of the nanocatalyst: The FTIR analyses were run on Thermo-Fisher Nicolet IS10, USA Spectrophotometer in the range of 400-4000 cm^{-1} in transmission attitude.

Zeta potential analyses were run on HORIBA SZ-100 with a holder (24.8 °C), dispersion medium viscosity (0.898 mPa.s), conductivity (0.289 mS/cm), and electrode voltage (3.3 V).

The SEM analysis was run on SEM-type FEI Czech (accelerating voltage at 25 kV).

The TEM analyses were run on a (Thermoscientific, Talos F200i) using the carbon-coated grid (Type G 200, 3.05 µ diameter, TAAP, USA).

Characterization of the synthesized compounds: Elemental microanalyses were carried out at Microanalytical Unit, Faculty of Science, Cairo University. Perkin-Elmer 1000 FT-IR infrared spectrometer (horizontal attenuated total reflection (HATR)) was used to record the Infrared spectra. The commercial reagents and solvents were acquired and utilized in their form. The distilled solvents were used as freshly prepared ones to accomplish the reactions. The mass spectra had been recorded on Kratos MS apparatus and the ionizing voltage was 70 ev. DEPT spectra are displayed in the upside direction because they are caused by the positive signal of the carbon-13 nuclei. DEPT spectra are a type of 13C NMR experiment that can be used to distinguish between different types of carbon atoms, such as primary, secondary, tertiary, and quaternary carbons. The angle of the DEPT experiment is typically set to 90° or 135°. A 90° DEPT experiment will produce a spectrum with positive peaks for primary and tertiary carbons and negative peaks for secondary and quaternary carbons. A 135° DEPT experiment will produce a spectrum with positive peaks for primary and quaternary carbons and negative peaks for secondary and tertiary carbons.

Here is a diagram that shows the different types of carbon atoms and the signals they produce in DEPT spectra:

Carbon type	90° DEPT	135° DEPT
Primary	Positive	Positive
Secondary	Negative	Negative
Tertiary	Positive	Negative
Quaternary	Negative	Positive

2. Procedures of Antioxidant Activity

2.1. DPPH• assay

The antioxidant activity of the newly synthesized benzopyrimido[4,5-*d*]azoninone derivatives was evaluated by DPPH• assay [1]. A solution of DPPH• (0.135 mM) was used as a positive control, methanol (80%) as a negative control, and ascorbic acid as a reference standard. The samples were prepared in a serial dilution using methanol (80%). DPPH• solution (1 mL) was added to each tube and then incubated at room temperature for 30 min. The absorbance of each tube was recorded at 517 nm of wavelength (λ). The exponential curves were plotted for the % DPPH• remaining versus the sample concentration to estimate the values of IC_{50} in mg/mL. The values of IC_{50} were calculated to rationalize the comparison between the results of the investigated samples, in which an inverse relationship between the antioxidant capacity of the sample with the IC_{50} values [2]. The percentages of remaining DPPH• were calculated from Equation (1):

$$Remaining\ \ DPPH^{\bullet}\ (\%) = (DPPH^{\bullet})_{T} / (DPPH^{\bullet})_{T=0} \times 100 \qquad \text{Equation (1)}$$

2.2. Phosphomolybdate assay

The total antioxidant capacity was assessed by the phosphomolybdate method to investigate the antioxidant activity of the synthesized benzopyrimido[4,5-*d*]azoninone derivatives. A modified procedure was applied, in which the results were expressed as mg ascorbic acid equivalent per 100 grams of dry sample [3]. A freshly prepared reagent (0.6 M sulfuric acid, 28 mM sodium phosphate, 4 mM ammonium molybdate) was used. 3 mL of the standard reagent was mixed with 300 μL of the tested sample and incubated for 90 min at 95 °C. The intensity in the blue color of the samples was measured at λ= 695 nm. A negative control was prepared by mixing the standard reagent with 300 μL of distilled water instead of the tested sample [4].

References

[1] Kitts, D.D.; Wijewickreme, A.N.; Hu, C. Antioxidant properties of a North American ginseng extract. Molecular and cellular biochemistry 2000, 203, 1-10.

[2] Parejo, I.; Codina, C.; Petrakis, C.; Kefalas, P. Evaluation of scavenging activity assessed by Co (II)/EDTA-induced luminol chemiluminescence and DPPH·(2,2-diphenyl-1-picrylhydrazyl) free radical assay. Journal of Pharmacological and toxicological Methods 2000, 44, 507-512.

[3] Prieto, P.; Pineda, M.; Aguilar, M. Spectrophotometric quantitation of antioxidant capacity through the formation of a phosphomolybdenum complex: specific application to the determination of vitamin E. Analytical biochemistry 1999, 269, 337-341.

[4] Belyagoubi-Benhammou, N.; Belyagoubi, L.; Gismondi, A.; Di Marco, G.; Canini, A.; Atik Bekkara, F. GC/MS analysis, and antioxidant and antimicrobial activities of alkaloids extracted by polar and a polar solvents from the stems of *Anabasis articulata*. Medicinal Chemistry Research 2019, 28, 754-767.

Antioxidant results

Table S1. The results antioxidant activity expressed as % Remaining DPPH and % Scavenging activity at different concentrations of the tested samples.

Sample	Ar	Concentrations (mg/mL)	% Remaining DPPH	% Scavenging activity
3a	C_6H_5	0.212	26.28	73.72
		0.106	43.86	56.14
		0.053	62.67	37.33
		0.026	87.56	12.44
3b	2,4-$(Cl)_2$-C_6H_3	0.424	39.04	60.96
		0.212	58.63	41.37
		0.106	76.98	23.02
		0.053	91.14	8.865
3c	4-Cl-C_6H_4	0.524	27.22	72.78
		0.262	36.55	63.45
		0.131	56.61	43.39
		0.066	77.29	22.71
3d	2,6-$(Cl)_2$-C_6H_3	1.104	30.95	69.05
		0.552	32.66	67.34
		0.276	54.12	45.88
		0.138	69.36	30.64
3e	4-NMe_2-C_6H_4	0.313	18.35	81.65
		0.157	27.22	72.78
		0.078	46.19	53.81
		0.039	65.79	34.21
3f	2-OH-C_6H_4	0.096	11.51	88.49
		0.048	34.84	65.16
		0.024	57.85	42.15
		0.012	74.18	25.82
3g	3,5-$(Br)_2$-C_6H_3	0.49	30.64	69.36
		0.245	58.32	41.68
		0.123	72.63	27.37
		0.061	78.07	21.93
3h	4-OMe-C_6H_4	0.214	18.97	81.03
		0.107	34.37	65.63
		0.054	49.92	50.08
		0.027	75.89	24.11

3i	5-Br-benzo[*d*][1,3]dioxol-6-yl	0.204	23.33	76.67
		0.102	36.08	63.92
		0.051	58.01	41.99
		0.025	83.2	16.8
3j	2-pyridyl	0.12	42.3	57.7
		0.06	55.21	44.79
		0.03	72.63	27.37
		0.015	84.29	15.71
3k	1-naphthyl	0.22	23.17	76.83
		0.11	44.95	55.05
		0.055	64.39	35.61
		0.028	75.43	24.57
Ascorbic acid	--	0.062	15.27	84.73
		0.031	39.08	60.92
		0.016	61.07	38.93
		0.008	74.81	25.19

Table S2. The results antioxidant activity of the tested samples applying DPPH and phosphomolybdate assays.

Samples	**IC_{50} (mg/mL) DPPH Assay [a]**	**Total antioxidant capacity (mg AAE/ 100 gm DS) [b]**
3a	0.099 ±1.34	5276.654±2.59
3b	0.304±3.02	1966.205±3.74
3c	0.204±1.52	2392.291±1.98
3d	0.362±0.97	1412.344±3.76
3e	0.068±3.36	7017.389±3.38
3f	0.03±0.45	7894.563±2.92
3g	0.284±1.57	2104.67±3.49
3h	0.067±2.01	7575.59±2.86
3i	0.08±1.56	6379.444±4.18
3j	0.088±1.08	5422.528±3.36
3k	0.095±2.16	5342.785±2.70

[a] The values of IC_{50} in mg/mL using DPPH assay. Values are average ($n = 3$) ± SD.

[b] mg ascorbic acid equivalent/100 gm dry sample (DS). Values are average ($n = 3$) ± SD.

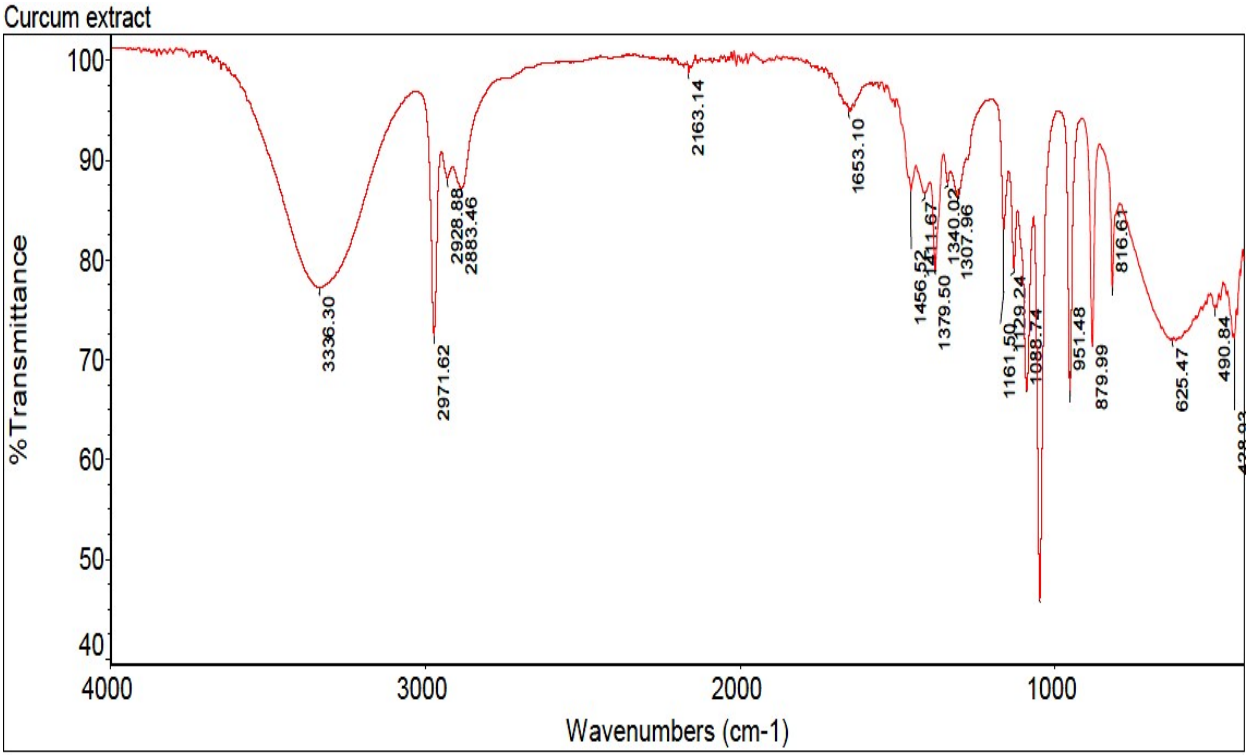


Fig. S1. FTIR analysis of turmeric ethanol extract.

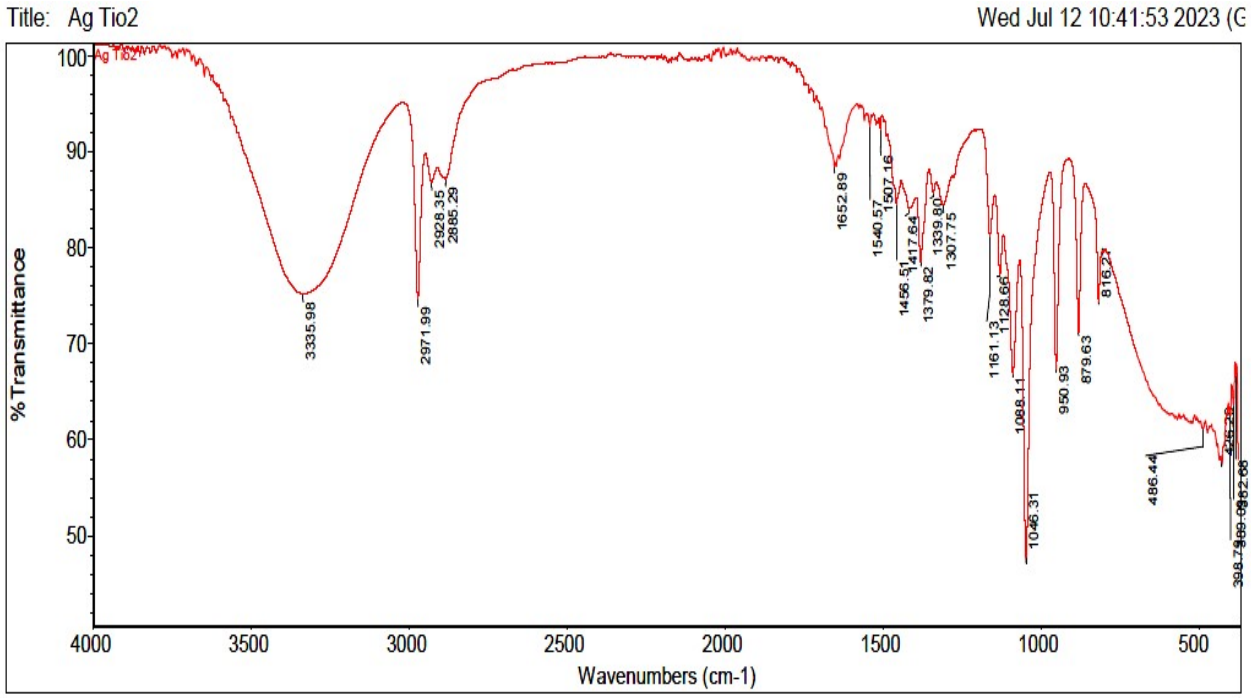


Fig. S2. FTIR analysis of Ag-TiO_2 bmNPs.

Turmeric extract				Ag-TiO_2 bmNPs			
Position:	398.36	Intensity:	78.865	Position:	382.68	Intensity:	66.557
Position:	428.93	Intensity:	72.114	Position:	389.09	Intensity:	63.569
Position:	490.84	Intensity:	75.160	Position:	398.79	Intensity:	62.526
Position:	625.47	Intensity:	71.833	Position:	426.29	Intensity:	57.599
Position:	816.61	Intensity:	77.289	Position:	816.27	Intensity:	74.376
Position:	879.99	Intensity:	71.339	Position:	879.63	Intensity:	71.202
Position:	951.48	Intensity:	66.896	Position:	950.93	Intensity:	67.319
Position:	1046.94	Intensity:	45.910	Position:	1046.31	Intensity:	47.693
Position:	1088.74	Intensity:	66.944	Position:	1088.11	Intensity:	66.860
Position:	1129.24	Intensity:	79.205	Position:	1128.66	Intensity:	77.230
Position:	1161.50	Intensity:	83.092	Position:	1161.13	Intensity:	81.111
Position:	1307.96	Intensity:	86.353	Position:	1307.75	Intensity:	84.418
Position:	1340.02	Intensity:	87.670	Position:	1339.80	Intensity:	85.634
Position:	1379.50	Intensity:	78.989	Position:	1379.82	Intensity:	78.452
Position:	1411.67	Intensity:	86.696	Position:	1417.64	Intensity:	84.025
Position:	1456.52	Intensity:	86.916	Position:	1456.51	Intensity:	84.432
Position:	1653.10	Intensity:	94.880	Position:	1507.16	Intensity:	92.228
Position:	2163.14	Intensity:	98.731	Position:	1540.57	Intensity:	92.608
Position:	2883.46	Intensity:	87.149	Position:	1652.89	Intensity:	88.386
Position:	2928.88	Intensity:	88.146	Position:	2885.29	Intensity:	87.211
Position:	2971.62	Intensity:	72.431	Position:	2928.35	Intensity:	86.845
Position:	3336.30	Intensity:	77.255	Position:	2971.99	Intensity:	74.609
				Position:	3335.98	Intensity:	75.185

Fig. S3. The results of the FTIR analysis of turmeric extract and Ag-TiO_2 bmNPs.

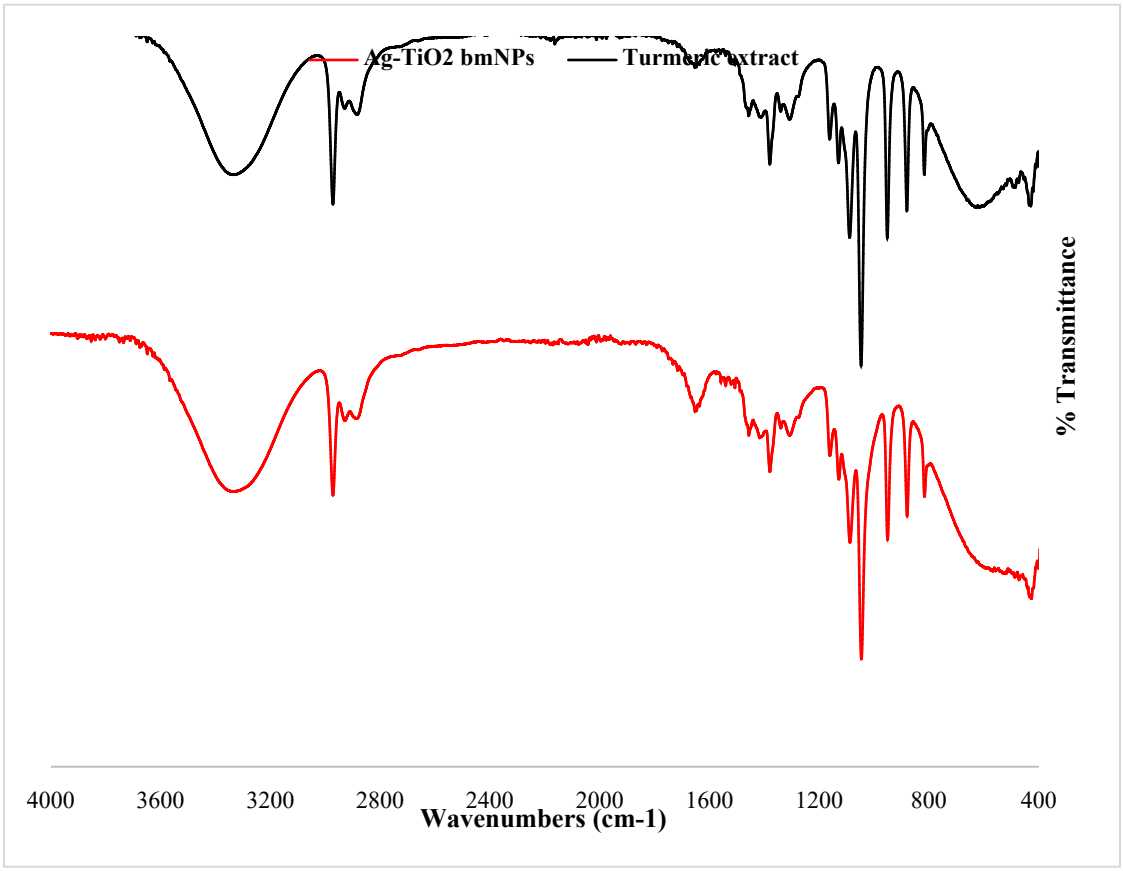
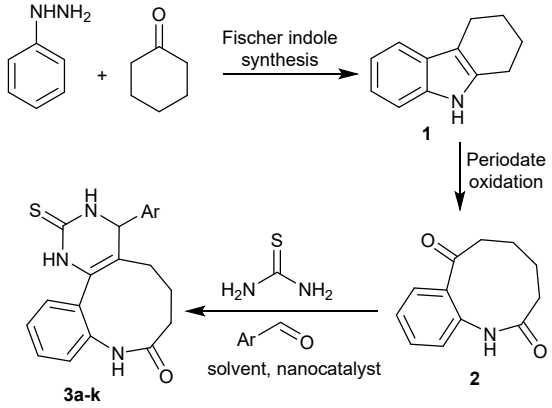
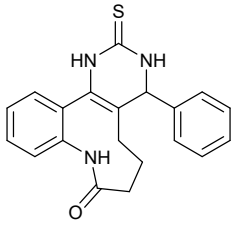
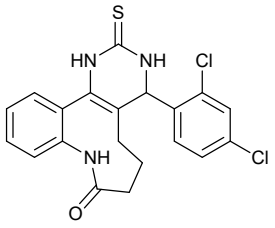
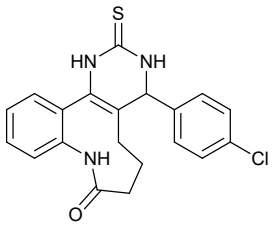
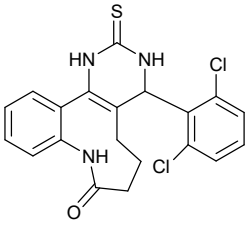
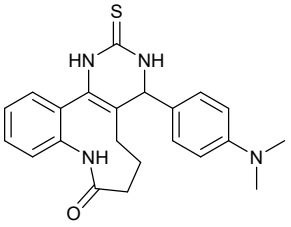
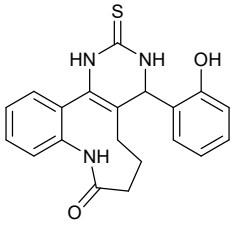


Fig. S4. FT-IR analysis of turmeric extract, and Ag-TiO_2 bmNPs.

Table S3. XRD analysis of the nanocatalyst.

Pos. [°2Th.]	Height [cts]	FWHM [°2Th.]	d-spacing [Å]	Rel. Int. [%]	Tip width [°2Th.]	Matched by
25.4282	294.02	0.1771	3.50289	100.00	0.2125	01-073-1764
27.9393	51.89	0.2362	3.19350	17.65	0.2834	00-006-0480
32.3090	81.99	0.3542	2.77088	27.89	0.4251	00-006-0480
37.8764	72.28	0.1771	2.37542	24.58	0.2125	01-073-1764
46.2968	45.27	0.4133	1.96110	15.40	0.4959	00-006-0480
48.1503	75.29	0.1771	1.88985	25.61	0.2125	01-073-1764
54.0300	46.50	0.2362	1.69726	15.82	0.2834	01-073-1764
55.1796	50.89	0.2362	1.66459	17.31	0.2834	01-073-1764
57.5827	12.51	0.4723	1.60071	4.25	0.5668	00-006-0480
62.7931	28.94	0.3542	1.47984	9.84	0.4251	01-073-1764
68.8952	10.12	0.3542	1.36292	3.44	0.4251	01-073-1764
70.3194	10.57	0.3542	1.33876	3.59	0.4251	01-073-1764
75.1116	25.78	0.1771	1.26480	8.77	0.2125	01-073-1764
82.9333	6.21	0.8640	1.16327	2.11	1.0368	01-073-1764



		
3a	**3b**	**3c**
		

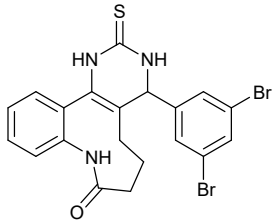
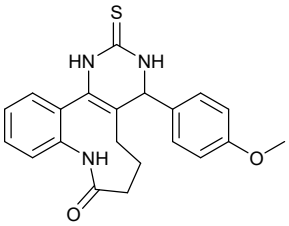
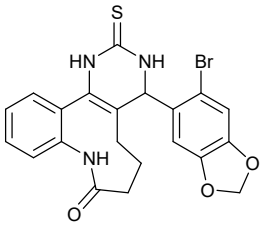
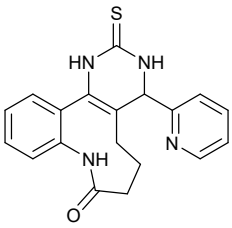
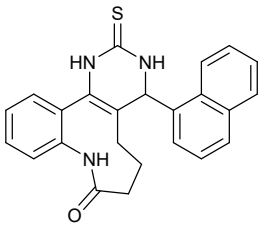
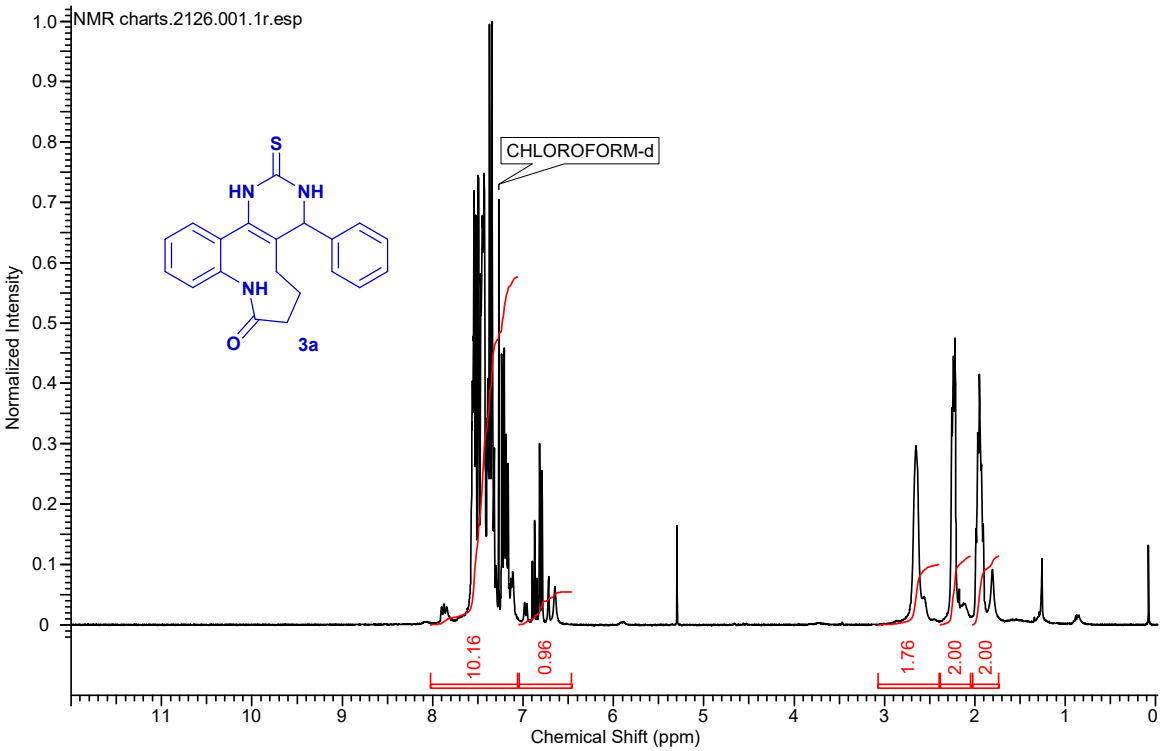
3d	3e	3f
		
3g	**3h**	**3i**
		
3j	**3k**	

Fig. S5. Synthesis of 4-(aryl)-2-thioxo-1,2,3,4,5,6,7,9-octahydro-8*H*-benzo[*b*]pyrimido[4,5-*d*]azonin-8-one derivatives.

Spectral Charts



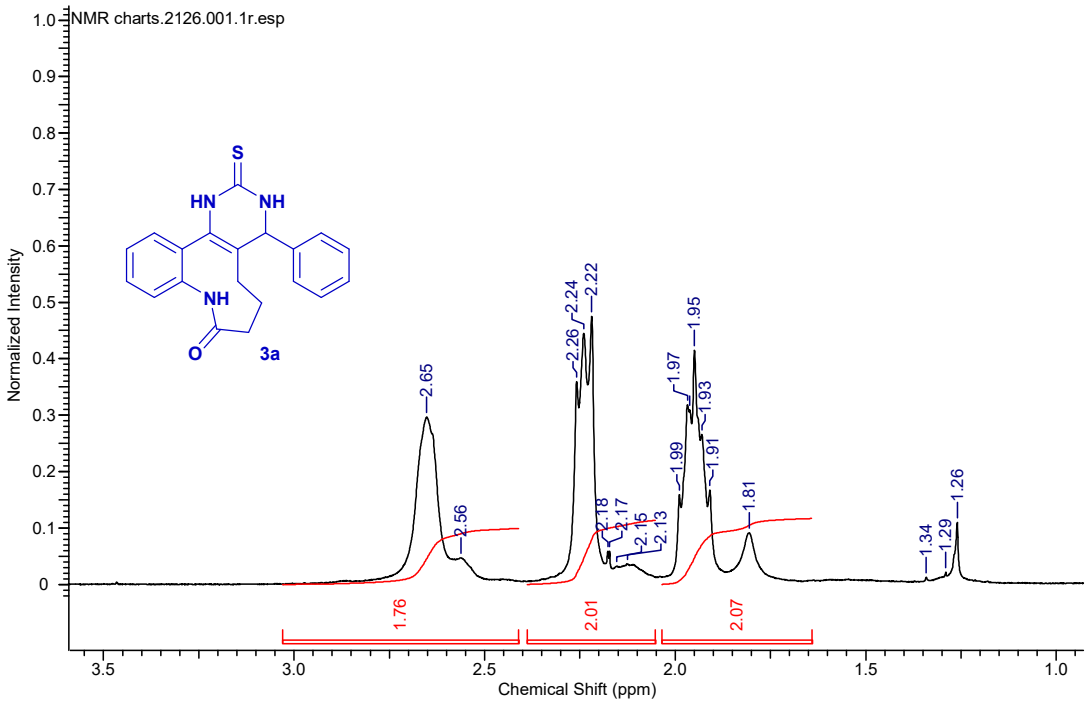


Fig. S6. [1]H-NMR spectrum of compound **3a**.

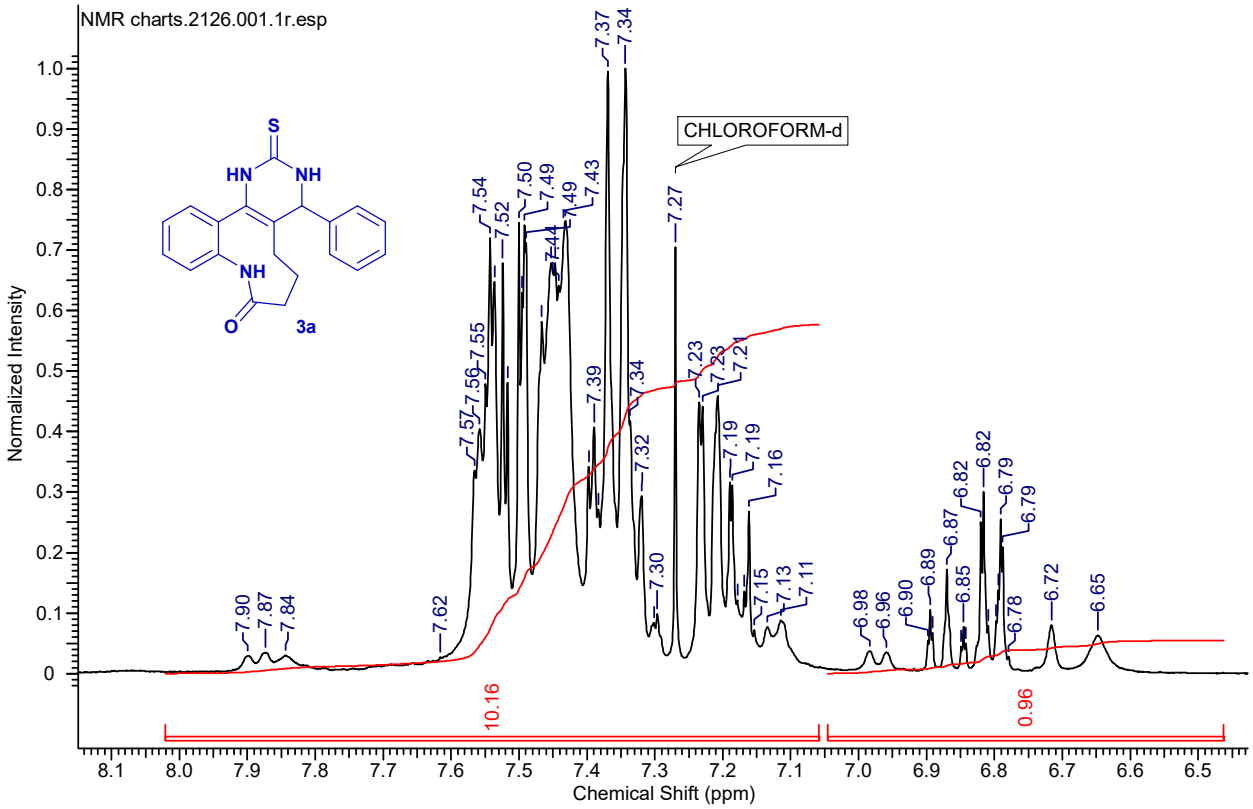
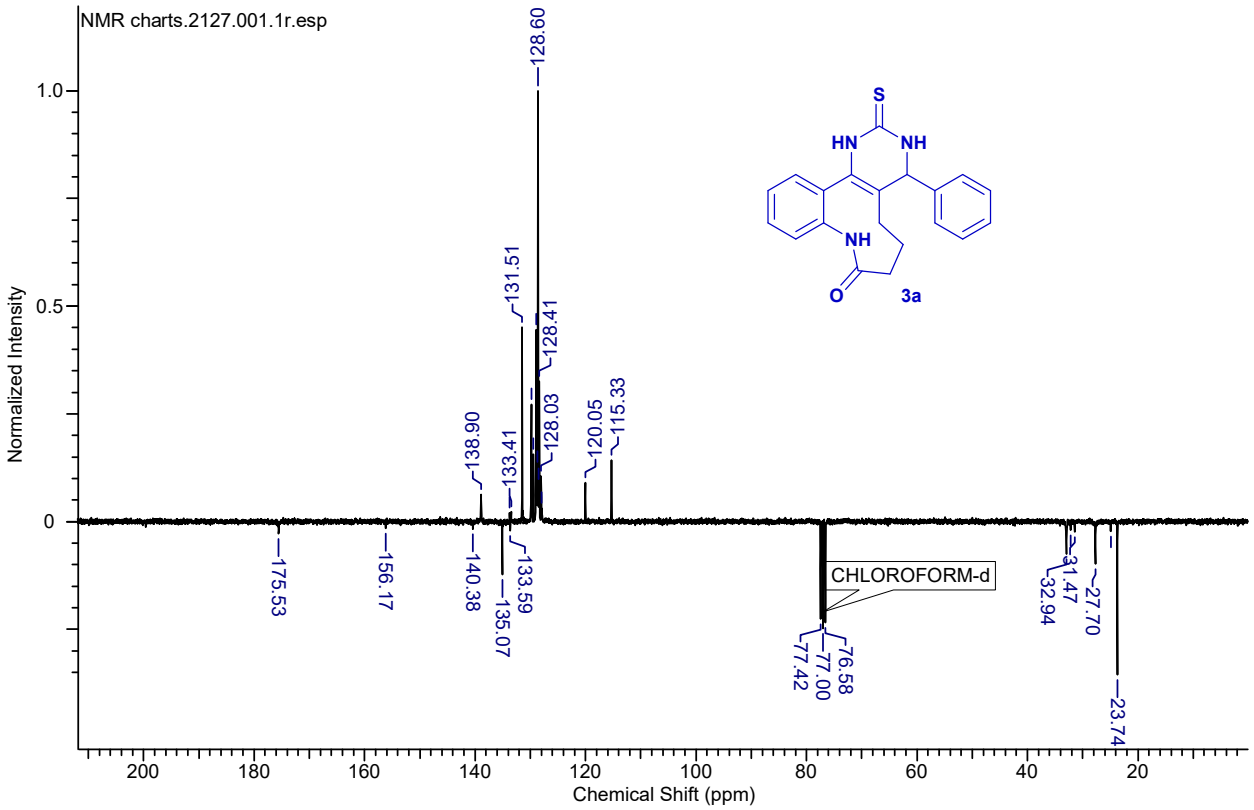


Fig. S6. [1]H-NMR spectrum of compound **3a**.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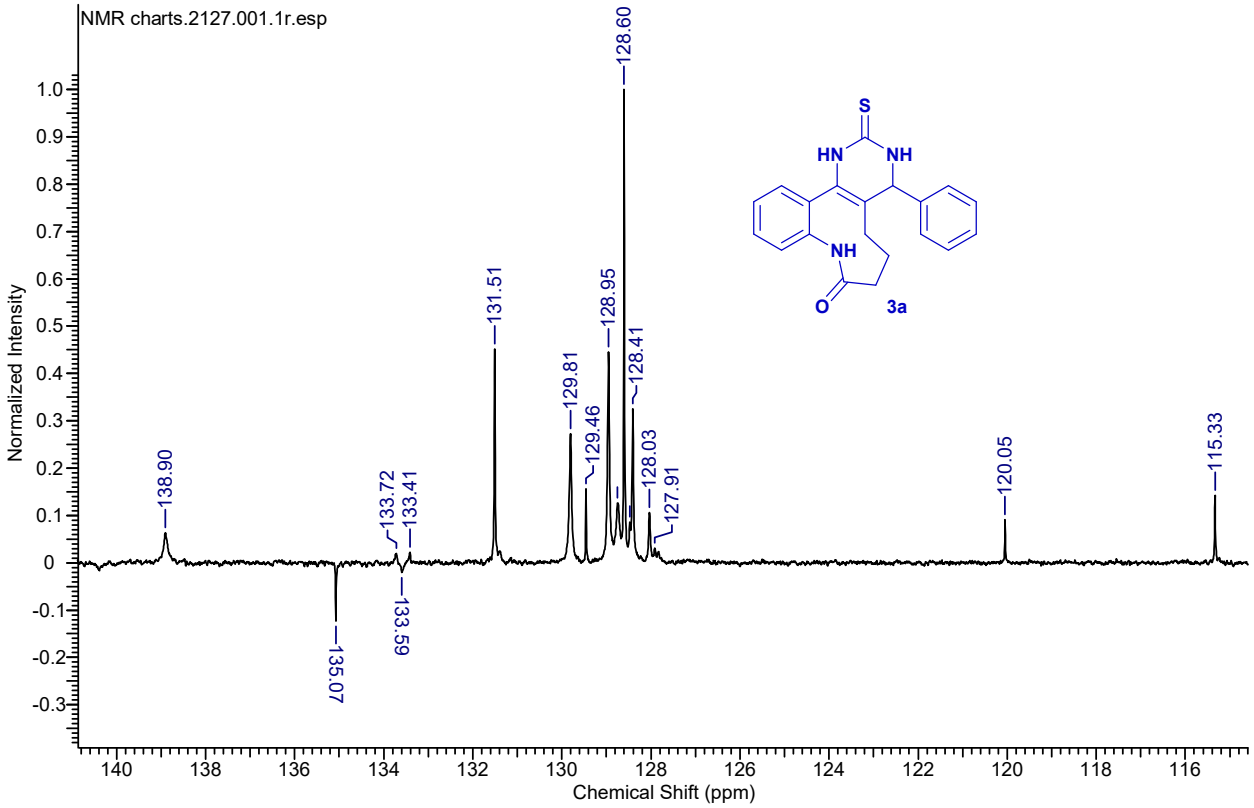
131.51
128.41
128.03
120.05
115.33
138.90
133.41
175.53
156.17
140.38
135.07
133.59
CHLOROFORM-d
77.42
77.00
76.58
32.94
31.47
27.70
23.74
3a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Normalized Intensity
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135.07
133.59
120.05
115.33
3a

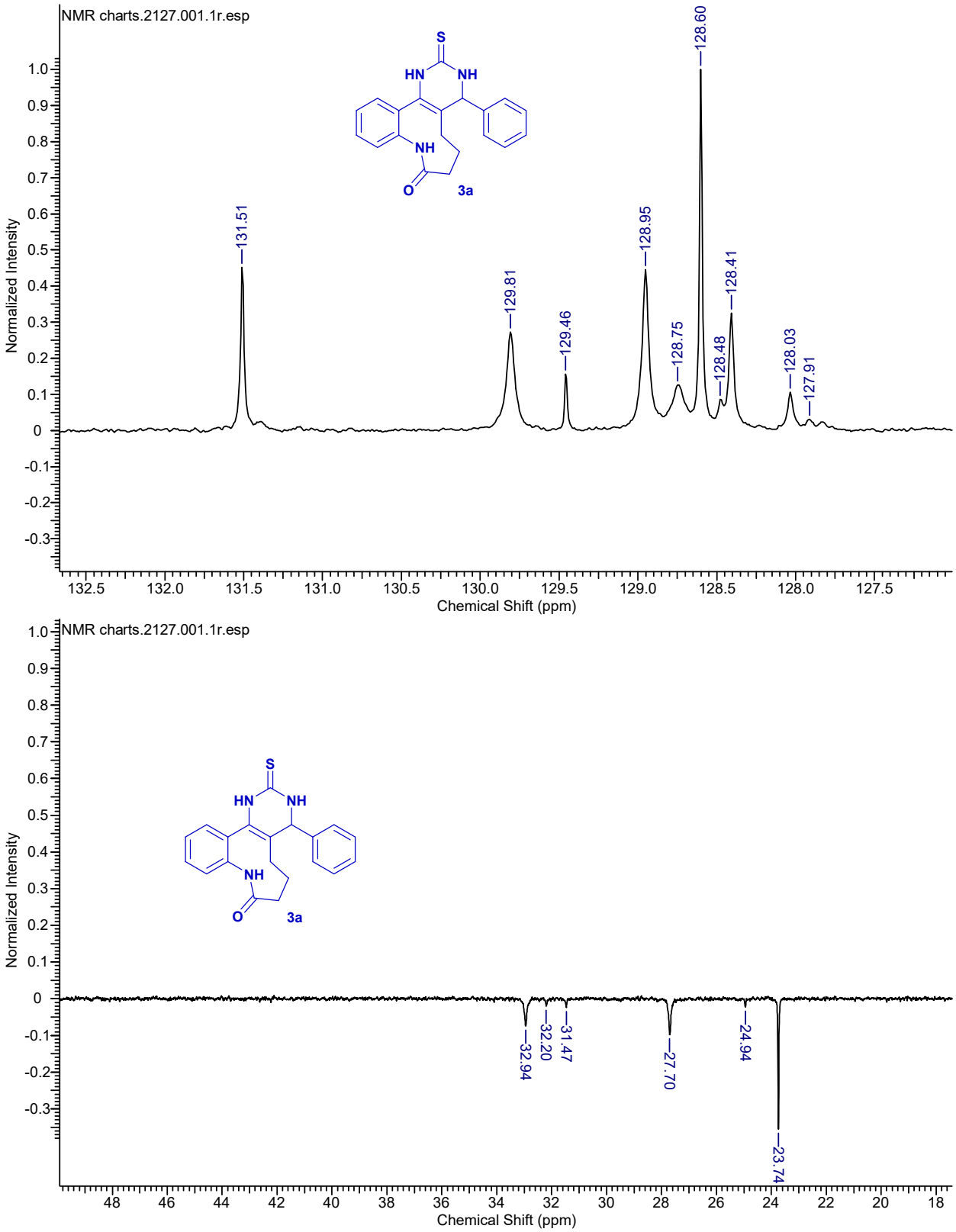


Fig. S7. ^{13}C-NMR spectrum of compound **3a**.

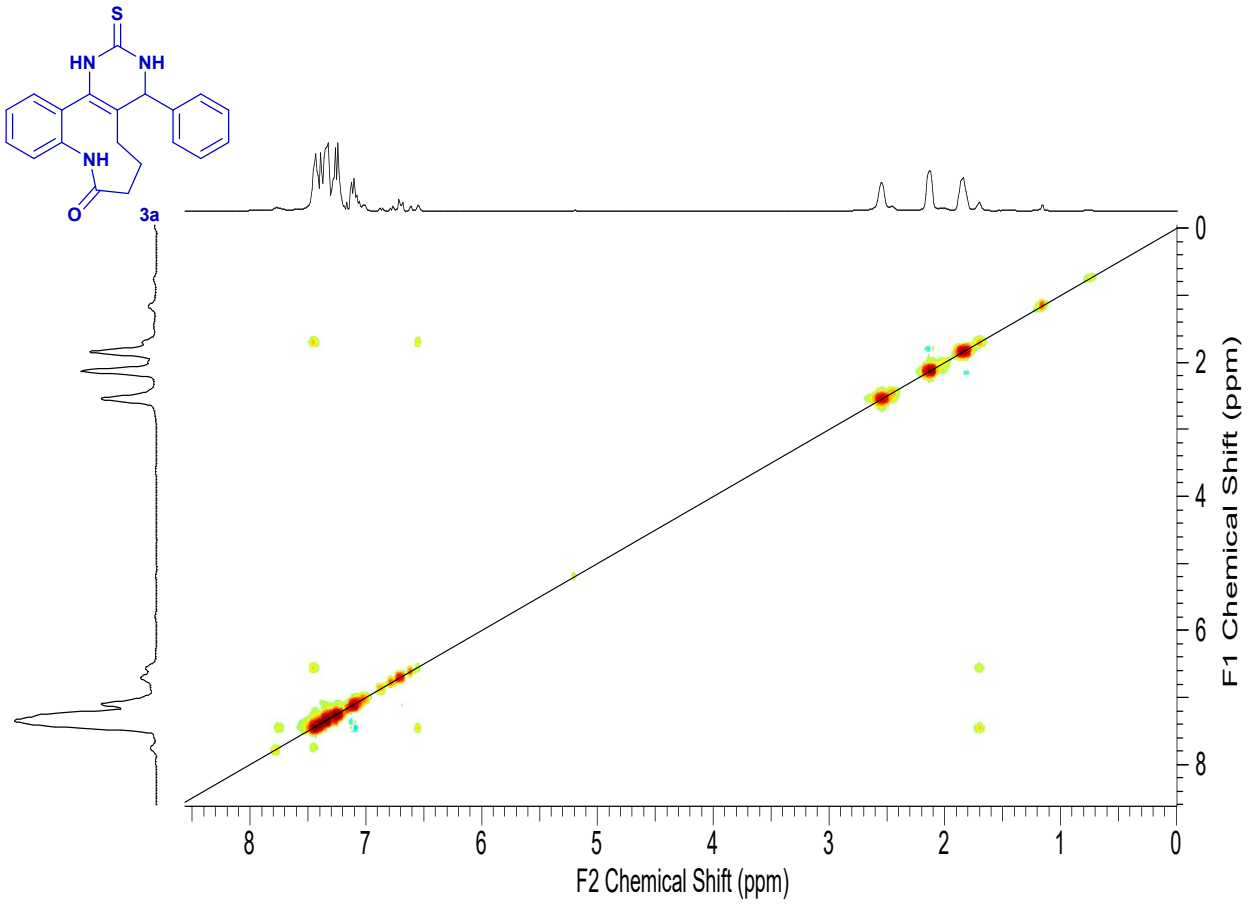


Fig. S8. 2D-NMR spectrum (COSY) of compound **3a**.

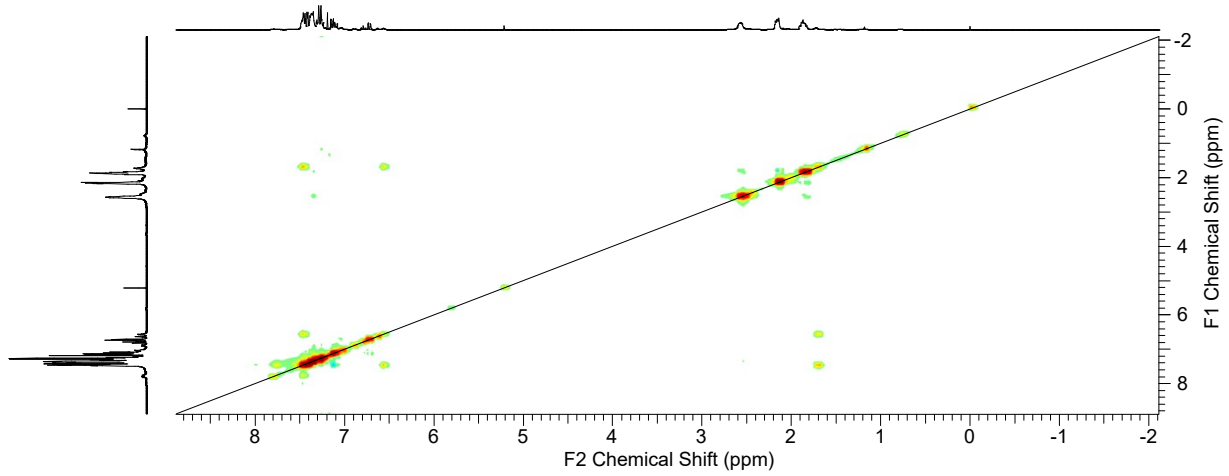


Fig. S9. 2D-NMR spectrum (NOESY) of compound **3a**.

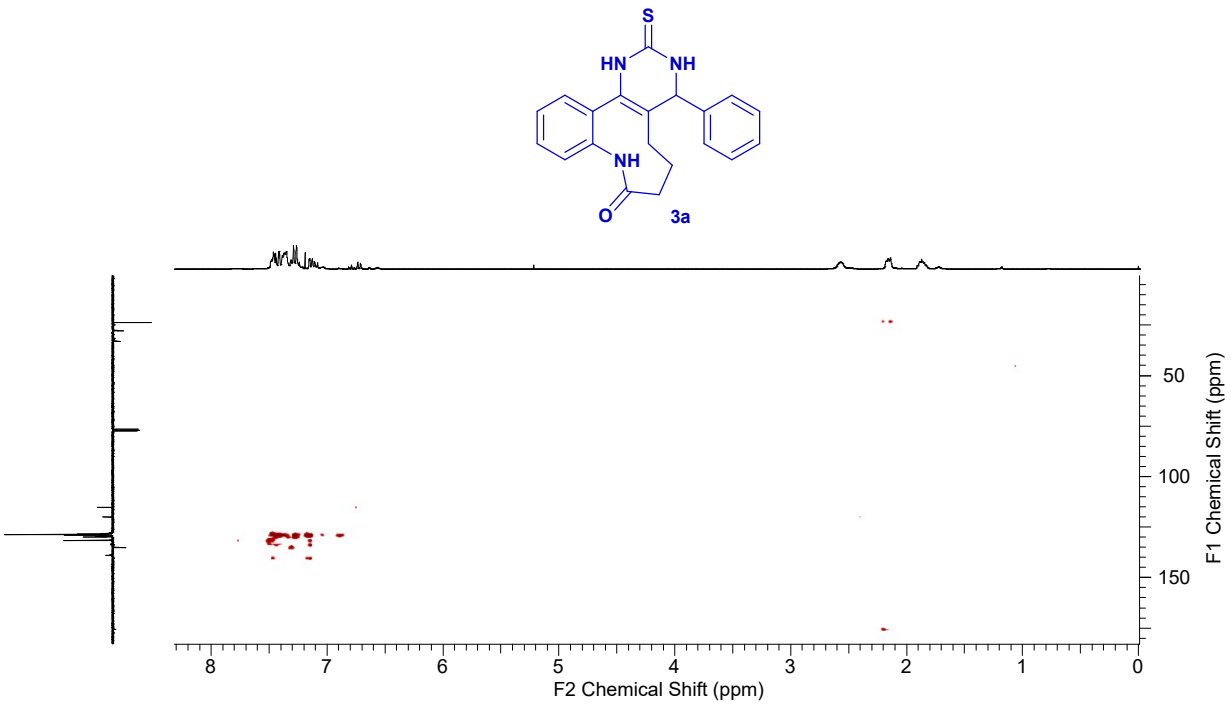
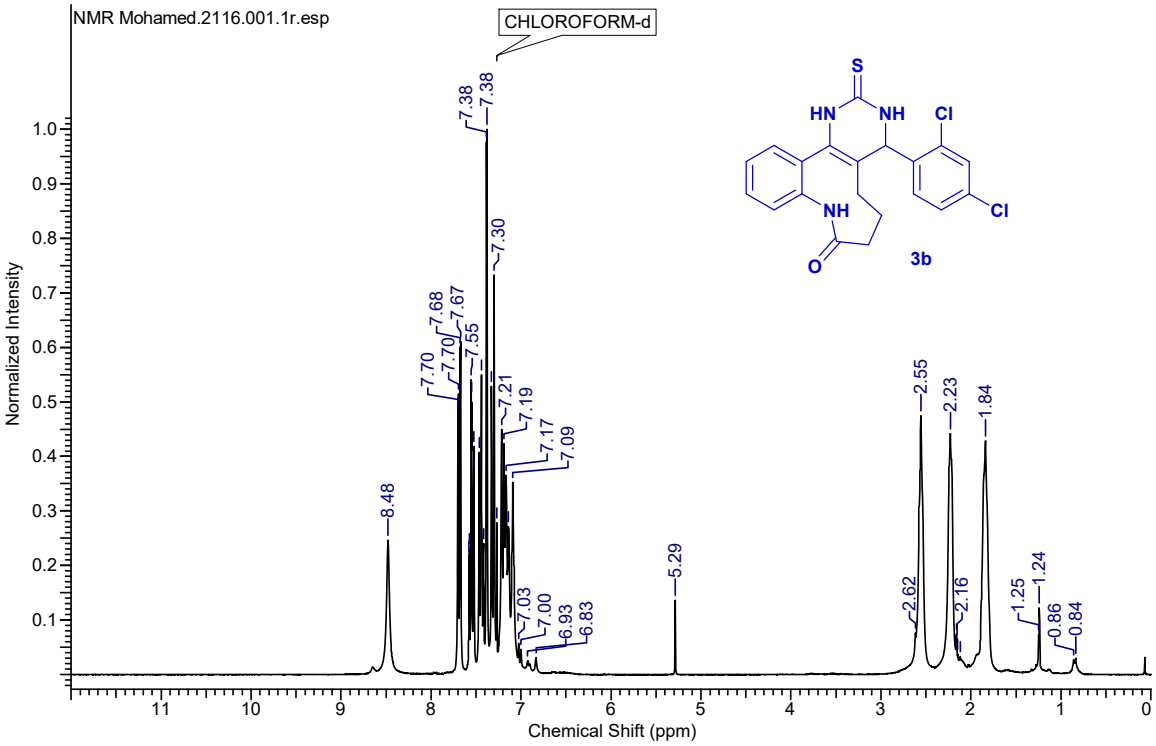


Fig. S10. 2D-NMR spectrum (HMBC) of compound **3a**.



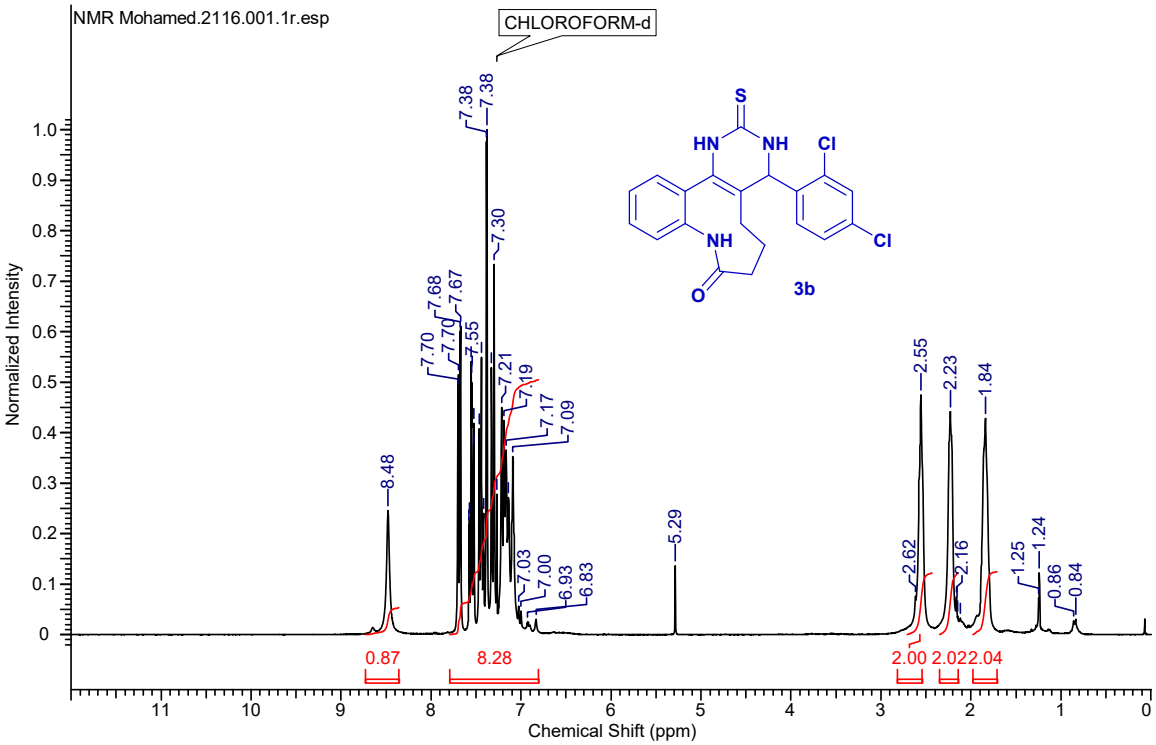
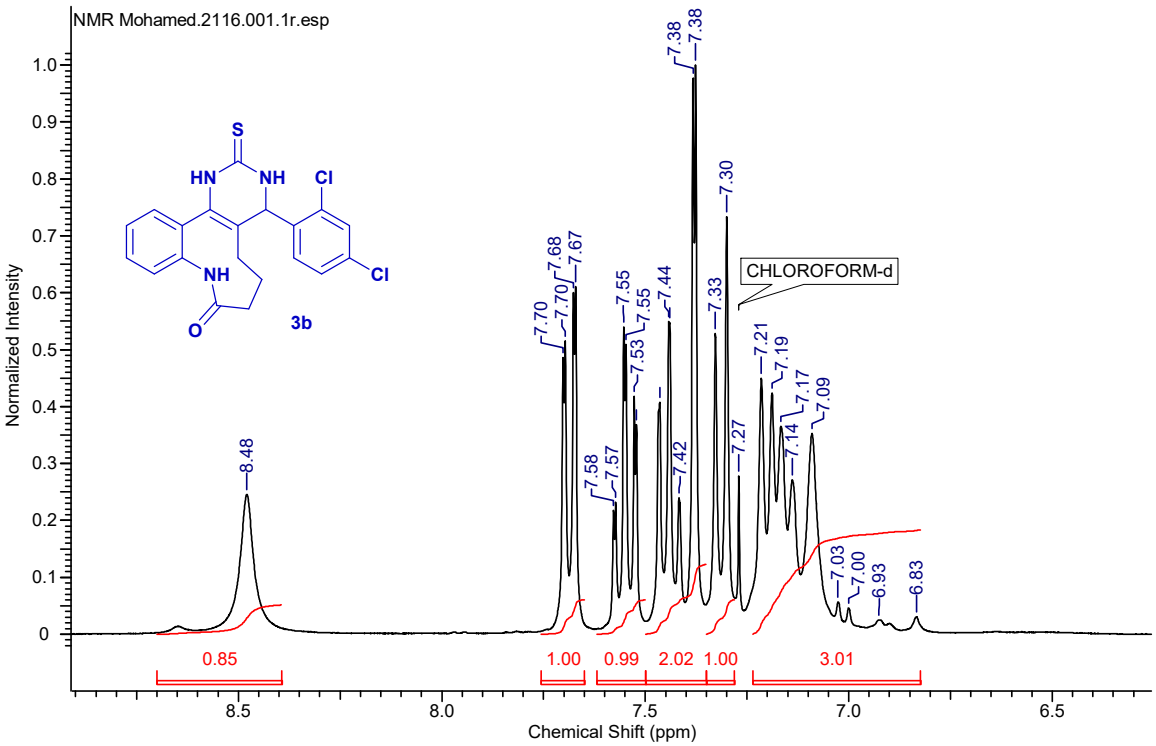


Fig. S11. [1]H-NMR spectrum of compound **3b**.



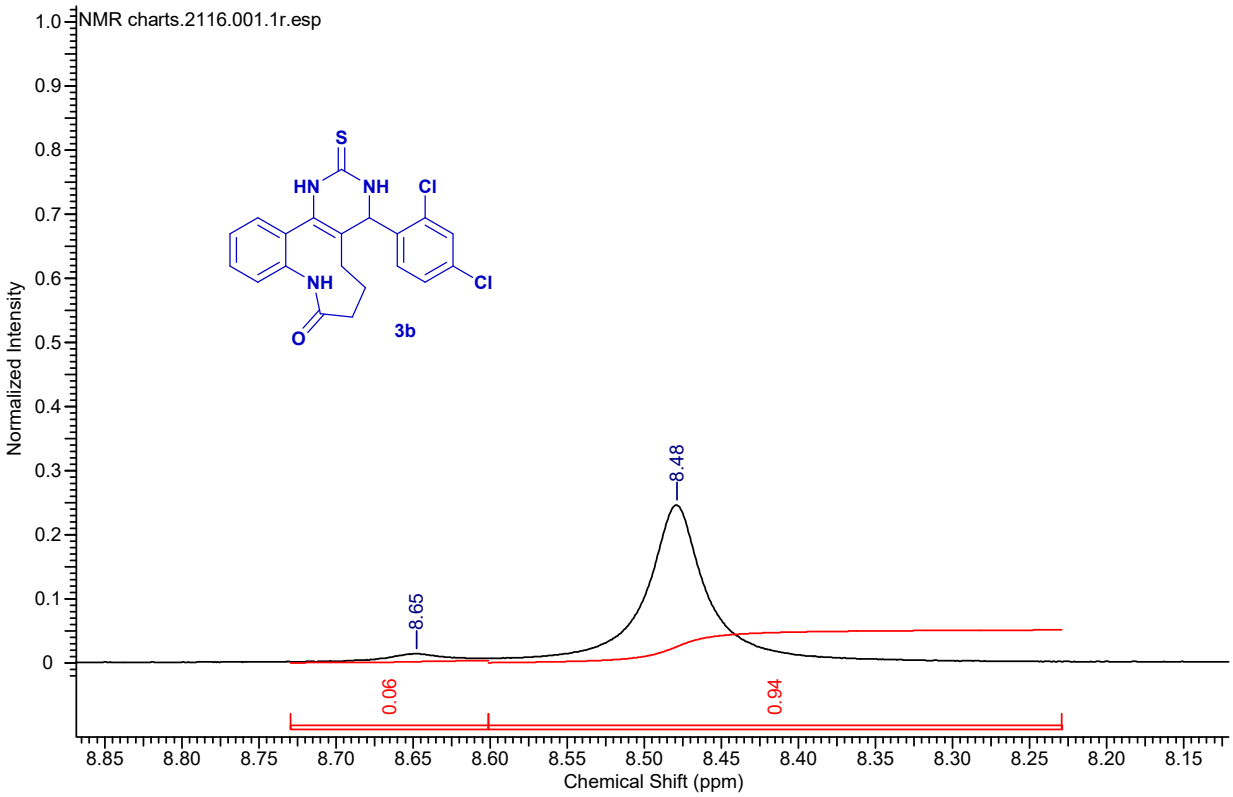
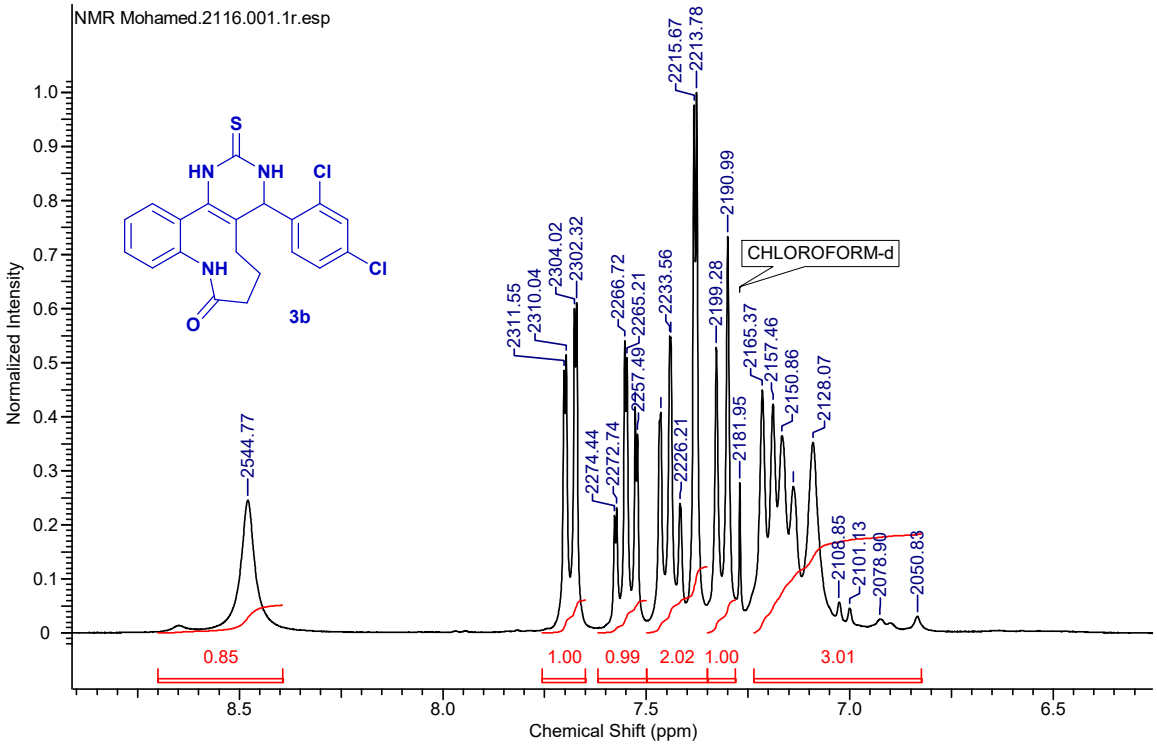


Fig. S11. ^{1}H-NMR spectrum of compound **3b**.



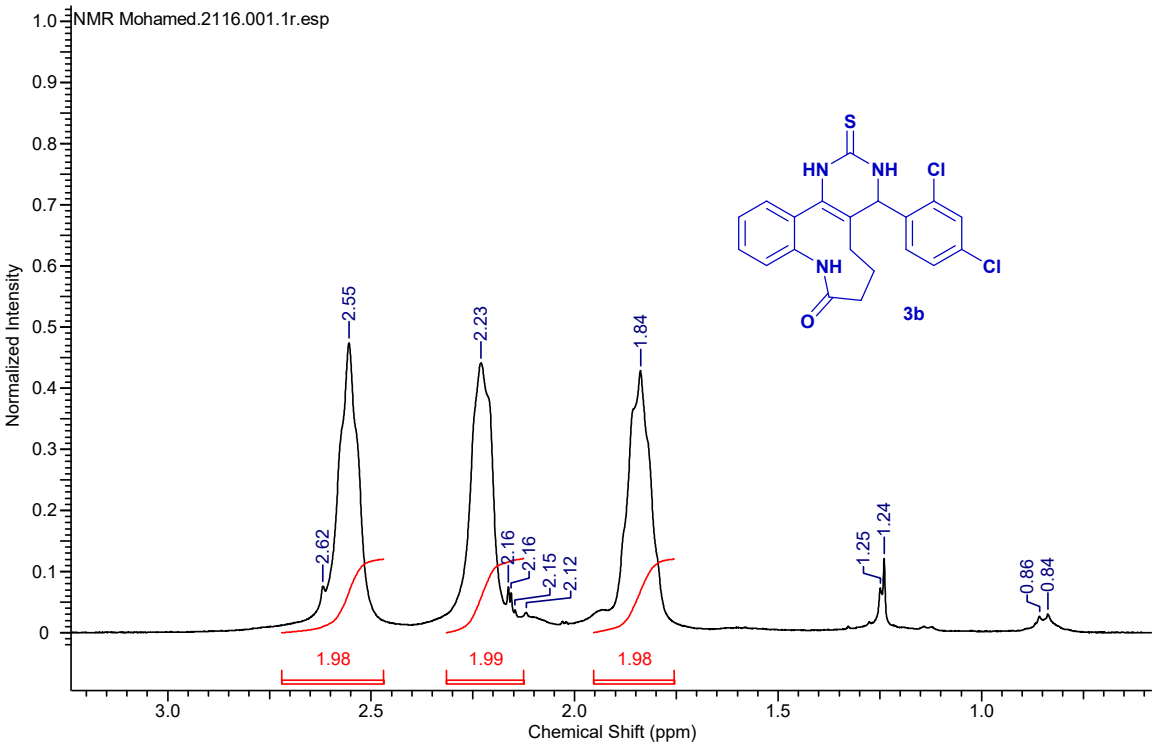
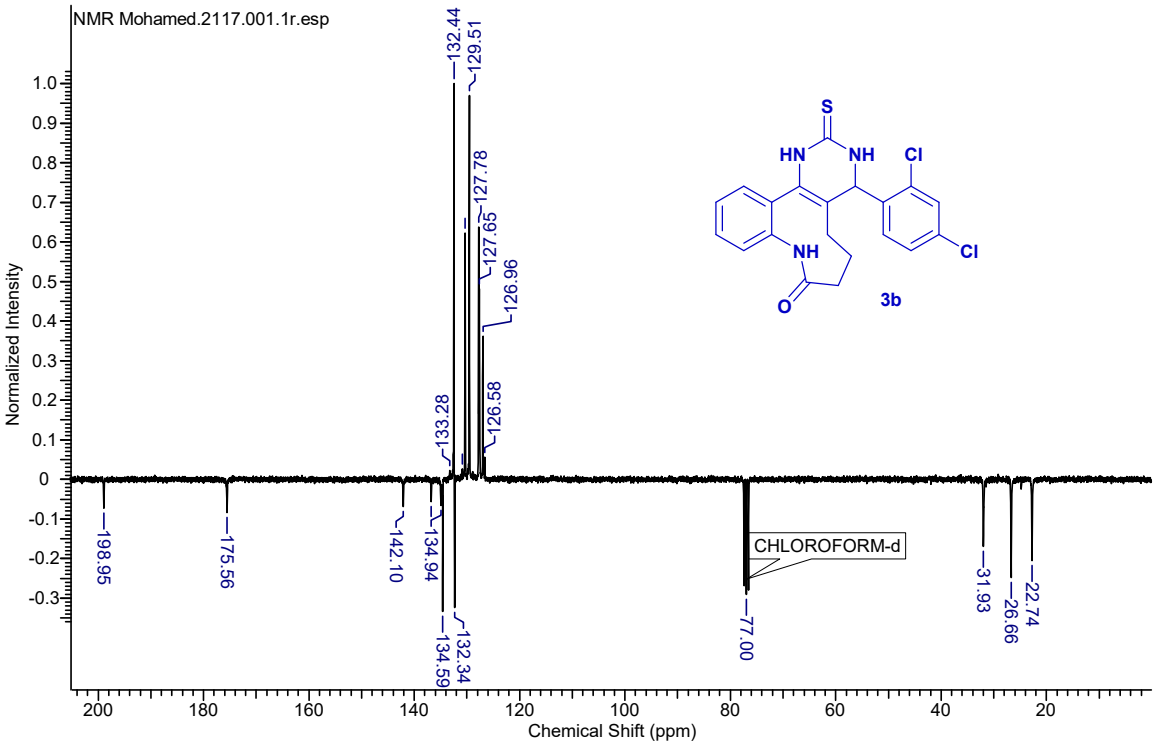


Fig. S11. ^{1}H-NMR spectrum of compound **3b**.



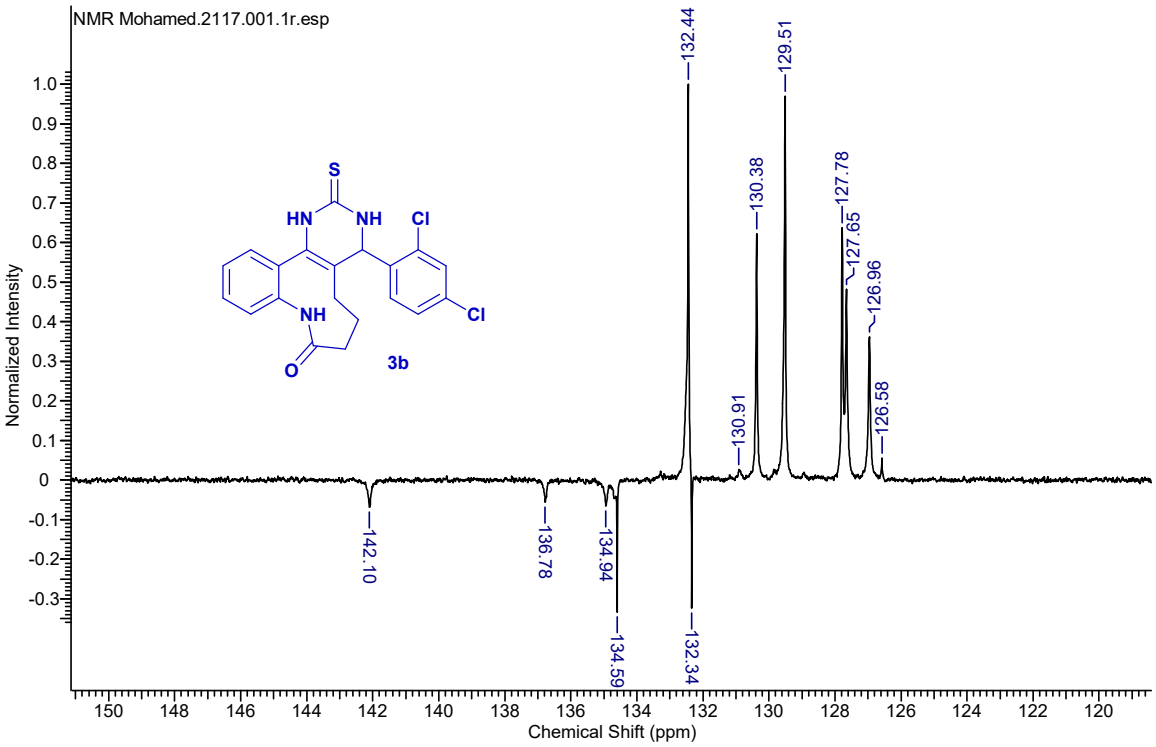


Fig. S12. ^{13}C-NMR spectrum of compound **3b**.

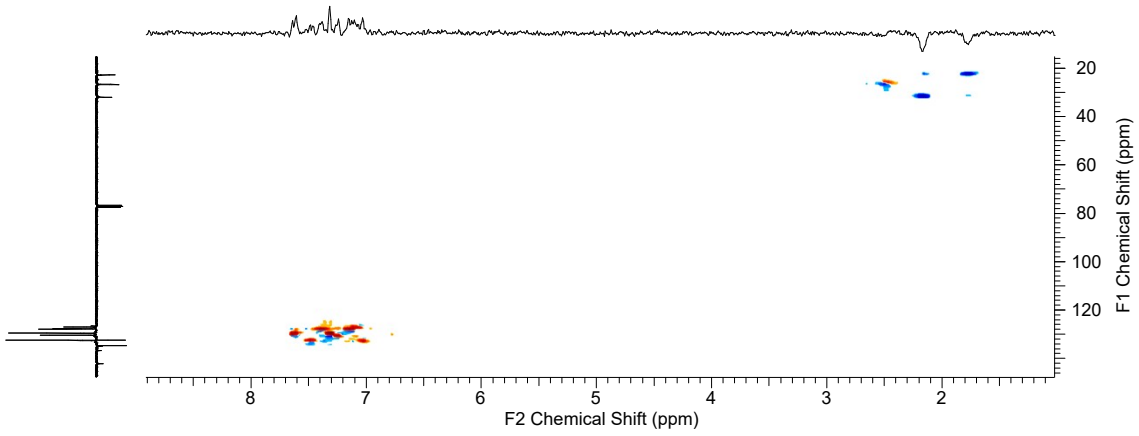


Fig. S13. 2D-NMR spectrum (**HSQC**) of compound **3b**.

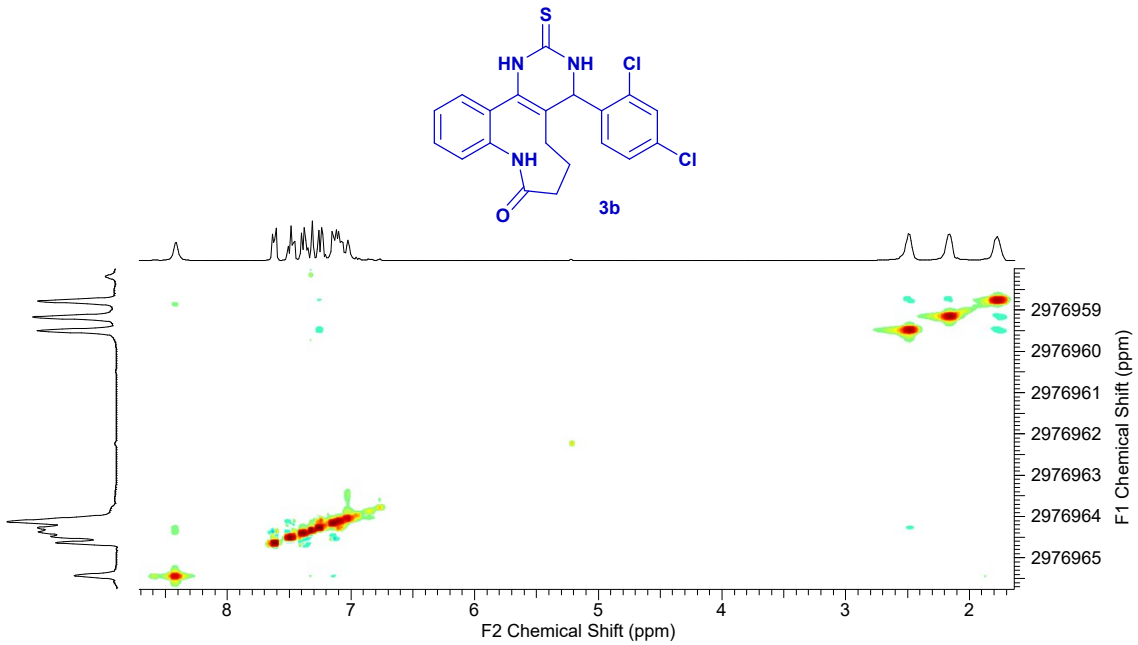


Fig. S14. 2D-NMR spectrum (**COSY**) of compound **3b**.

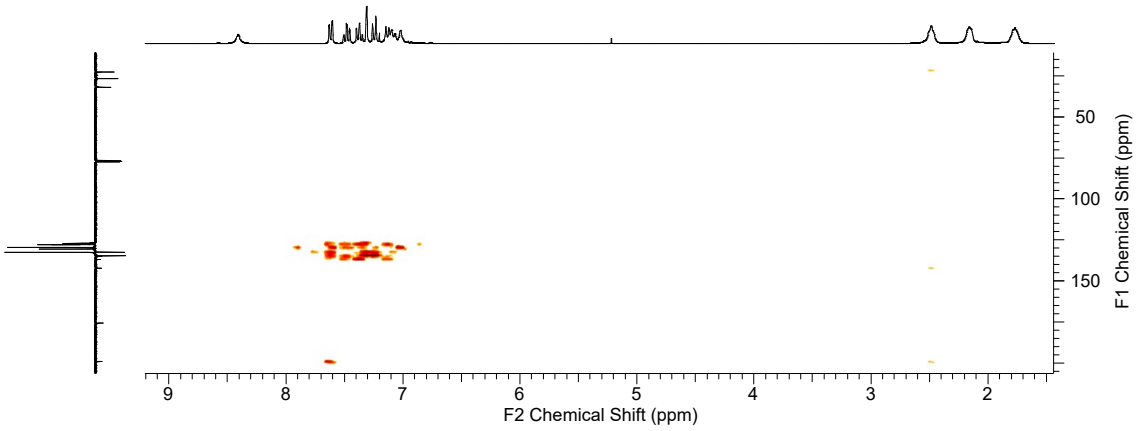


Fig. S15. 2D-NMR spectrum (**HMBC**) of compound **3b**.

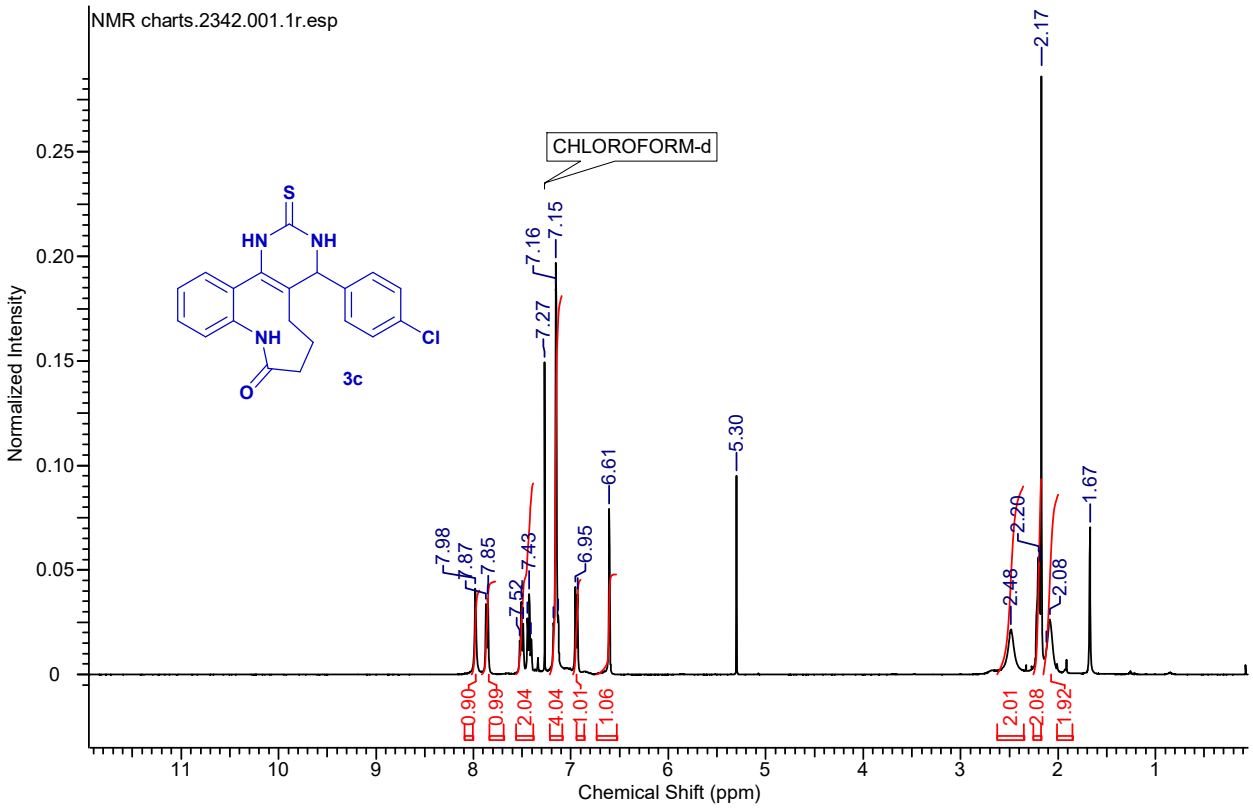
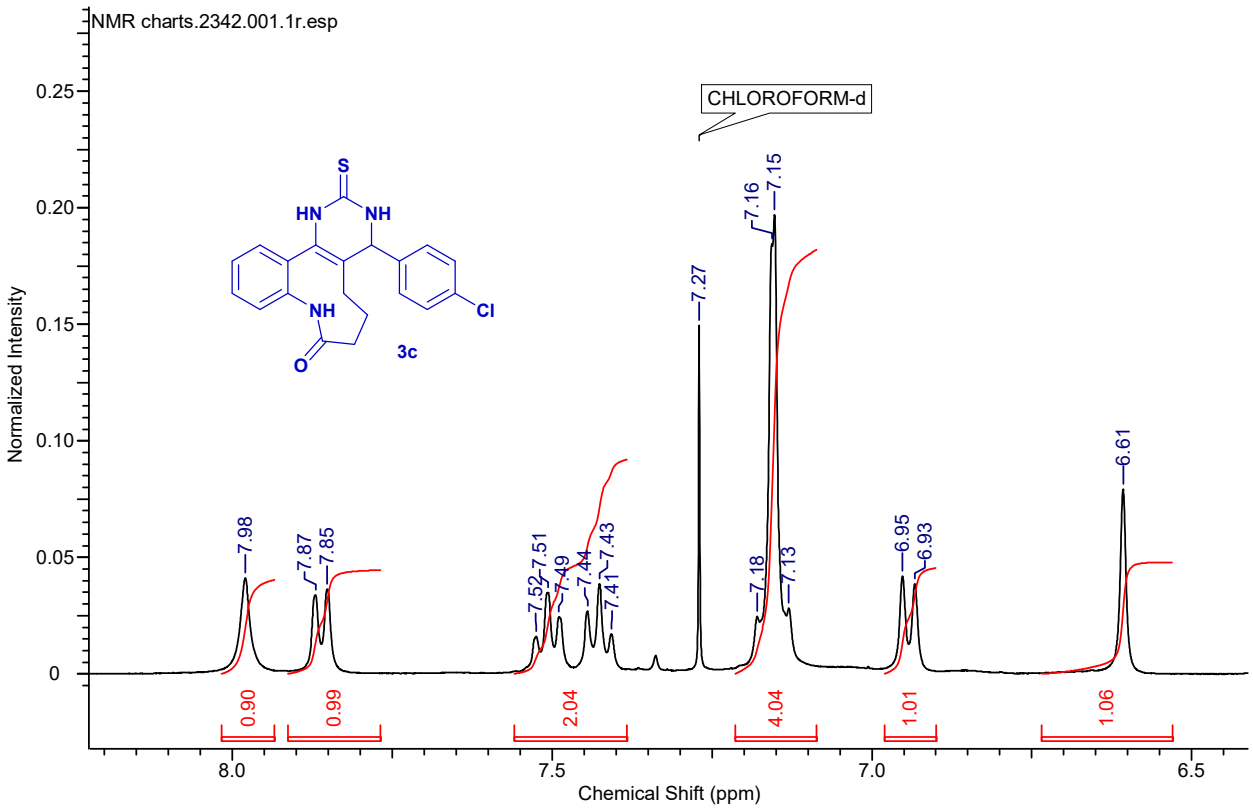


Fig. S16. ^{1}H-NMR spectrum of compound **3c**.



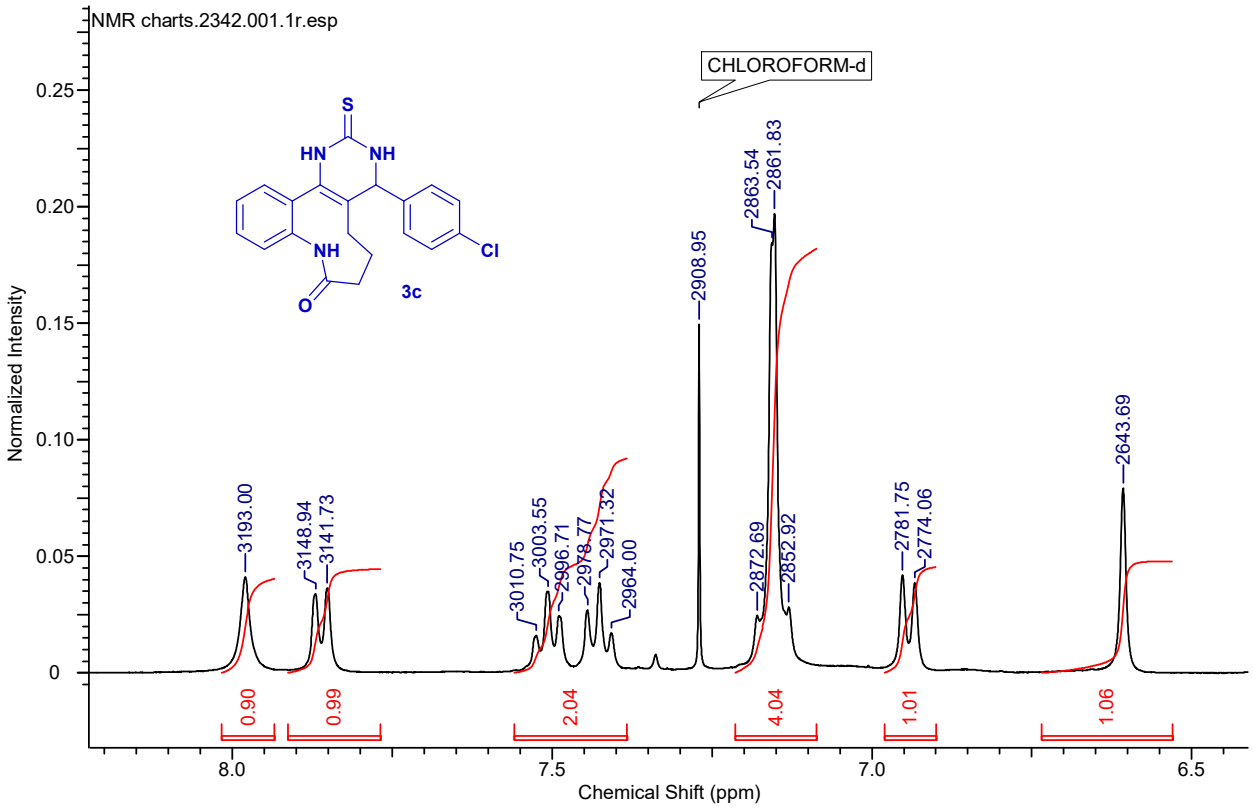


Fig. S16-A. ^{1}H-NMR spectrum of compound **3c**.

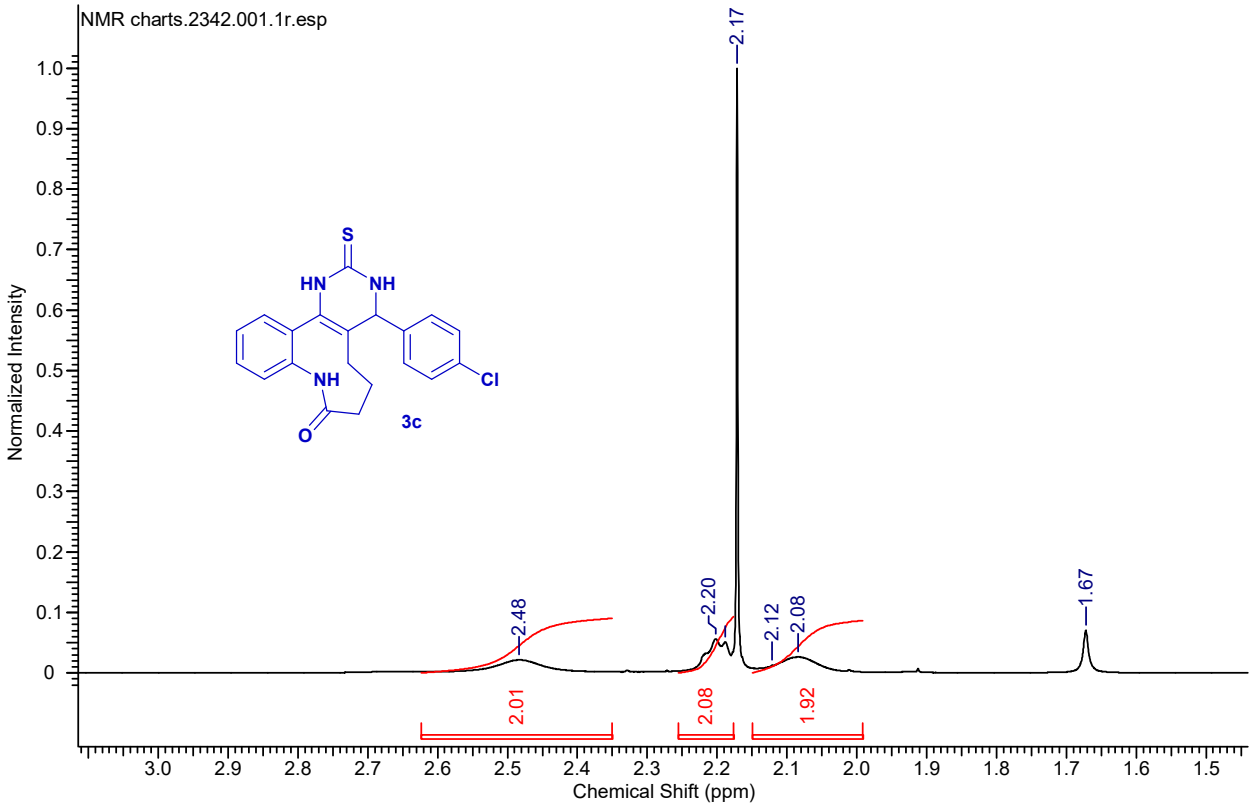


Fig. S16-B. ^{1}H-NMR spectrum of compound **3c**.

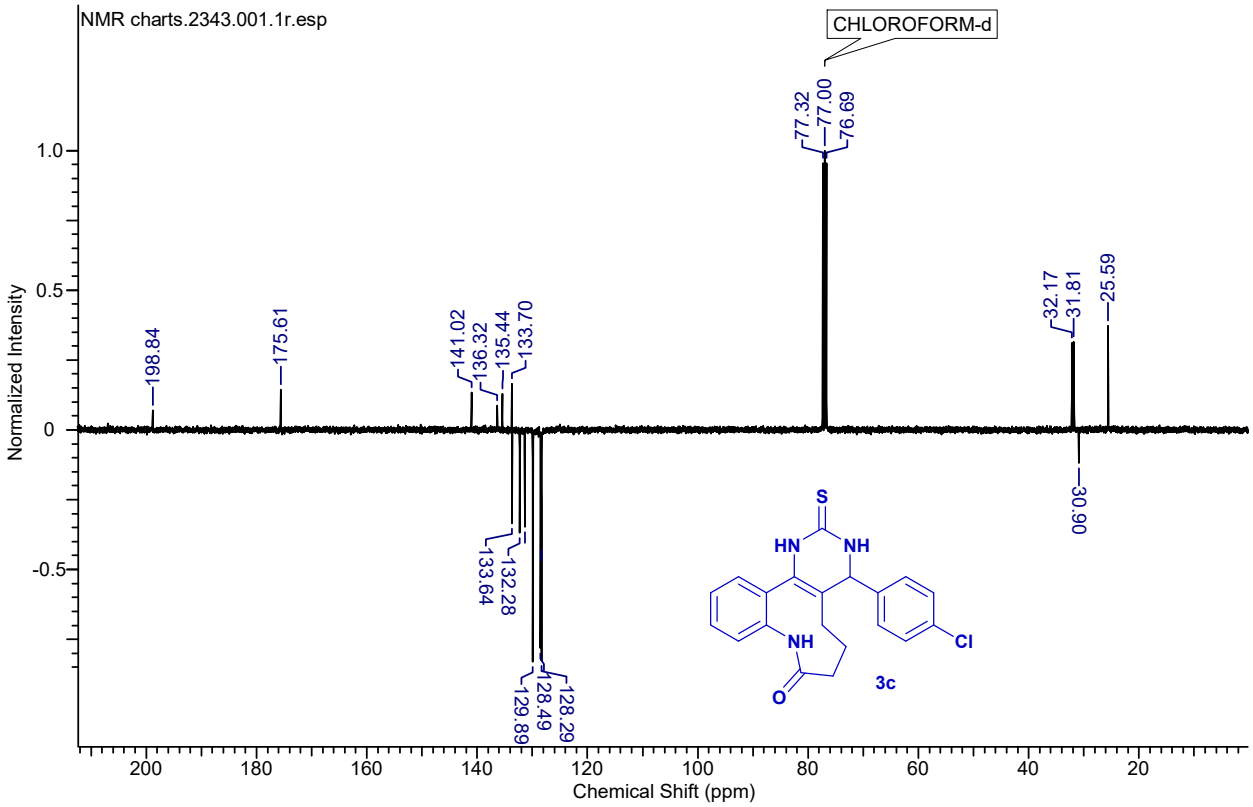
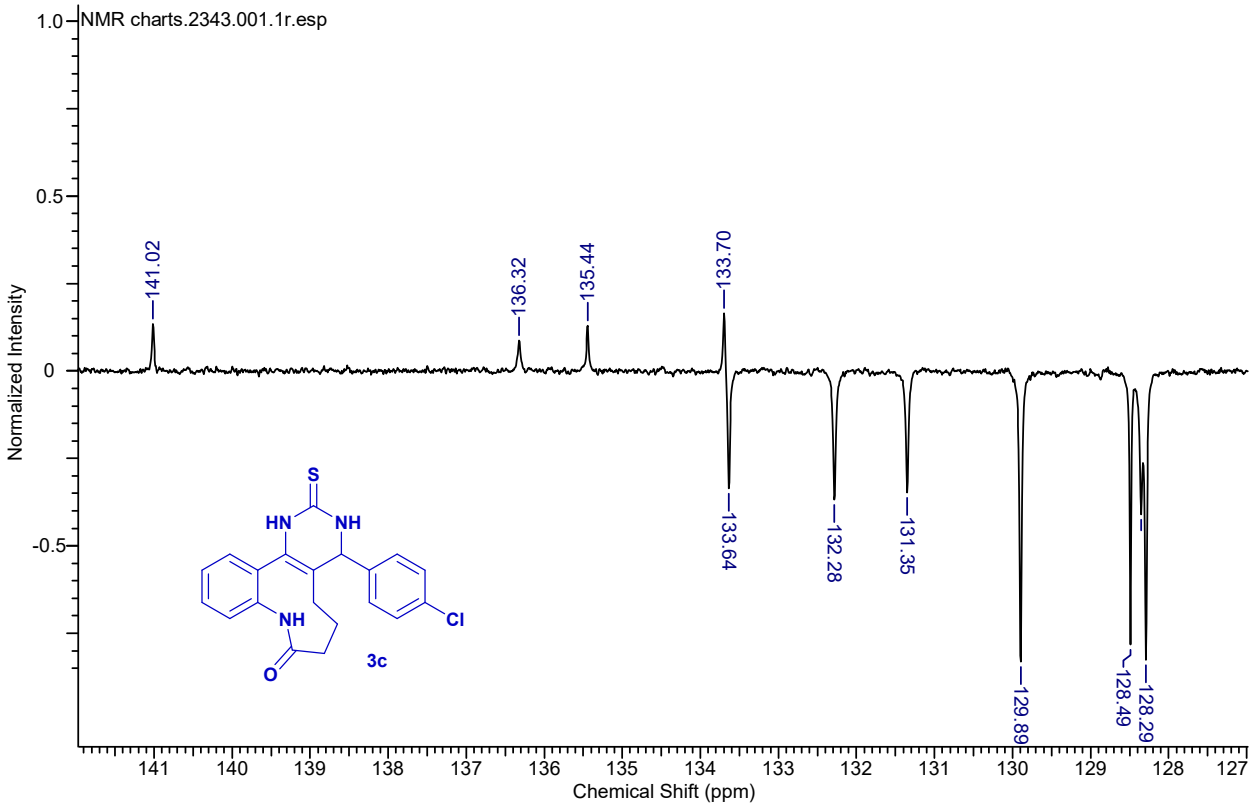


Fig. S17. ^{13}C-NMR spectrum of compound **3c**.



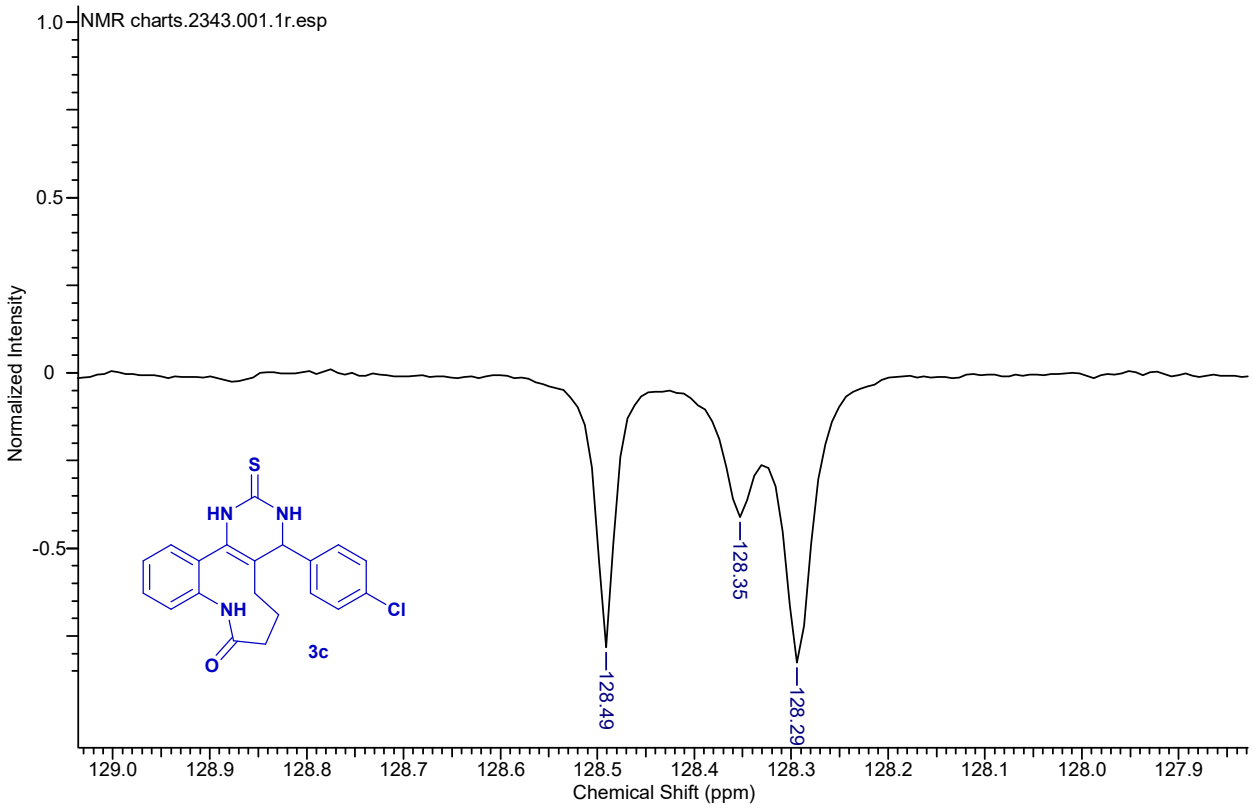


Fig. S17-A. ^{13}C-NMR spectrum of compound **3c**.

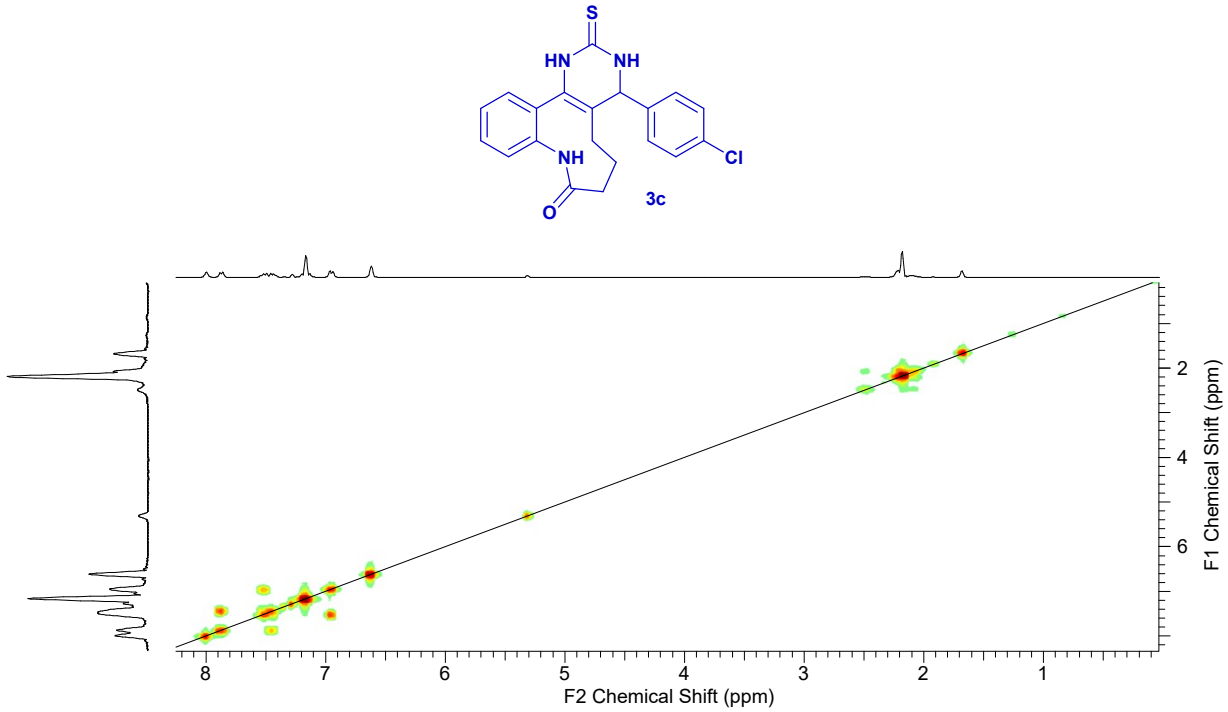


Fig. S18. 2D-NMR spectrum (**COSY**) of compound **3c**.

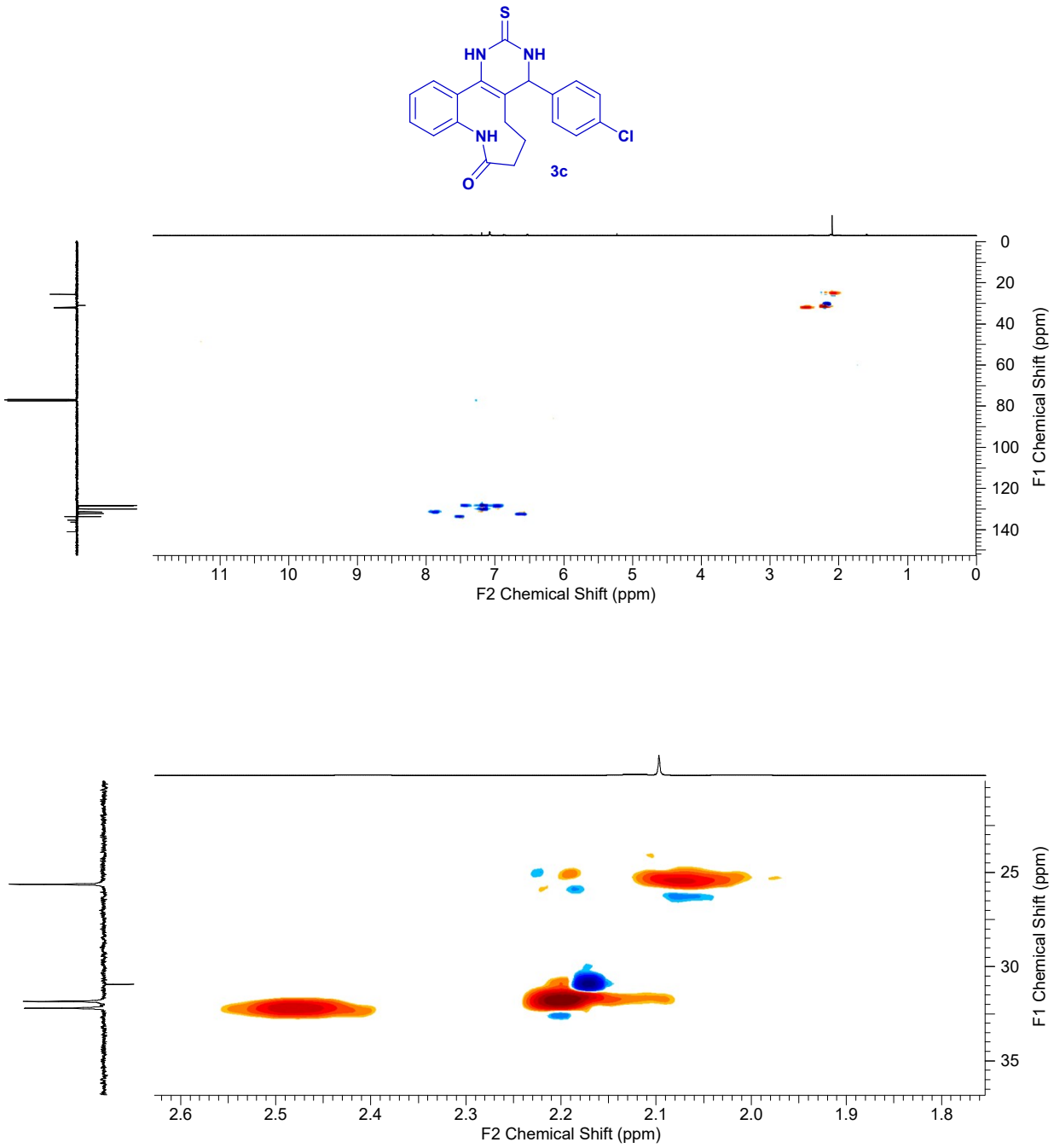


Fig. S19. 2D-NMR spectrum (**HSQC**) of compound **3c**.

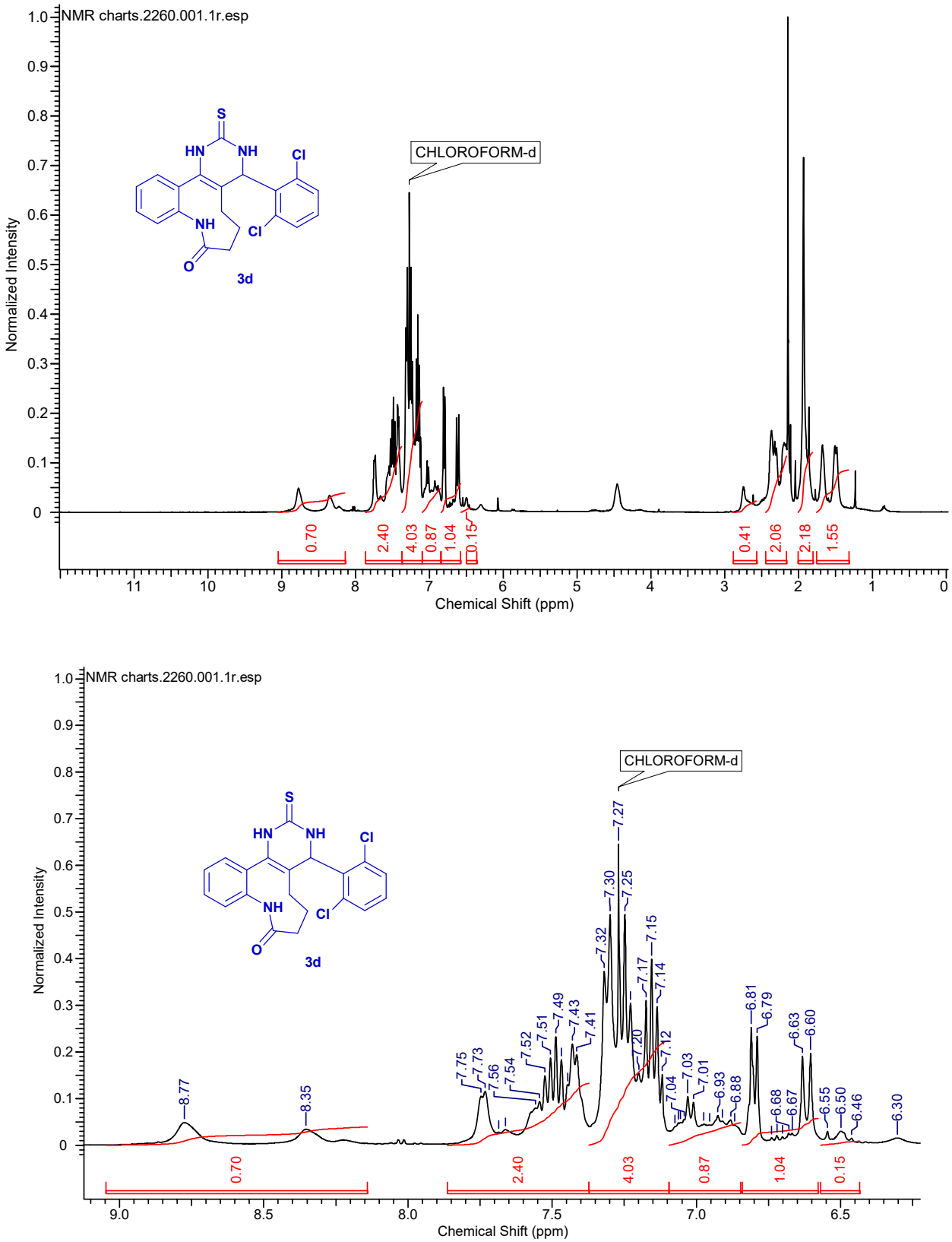
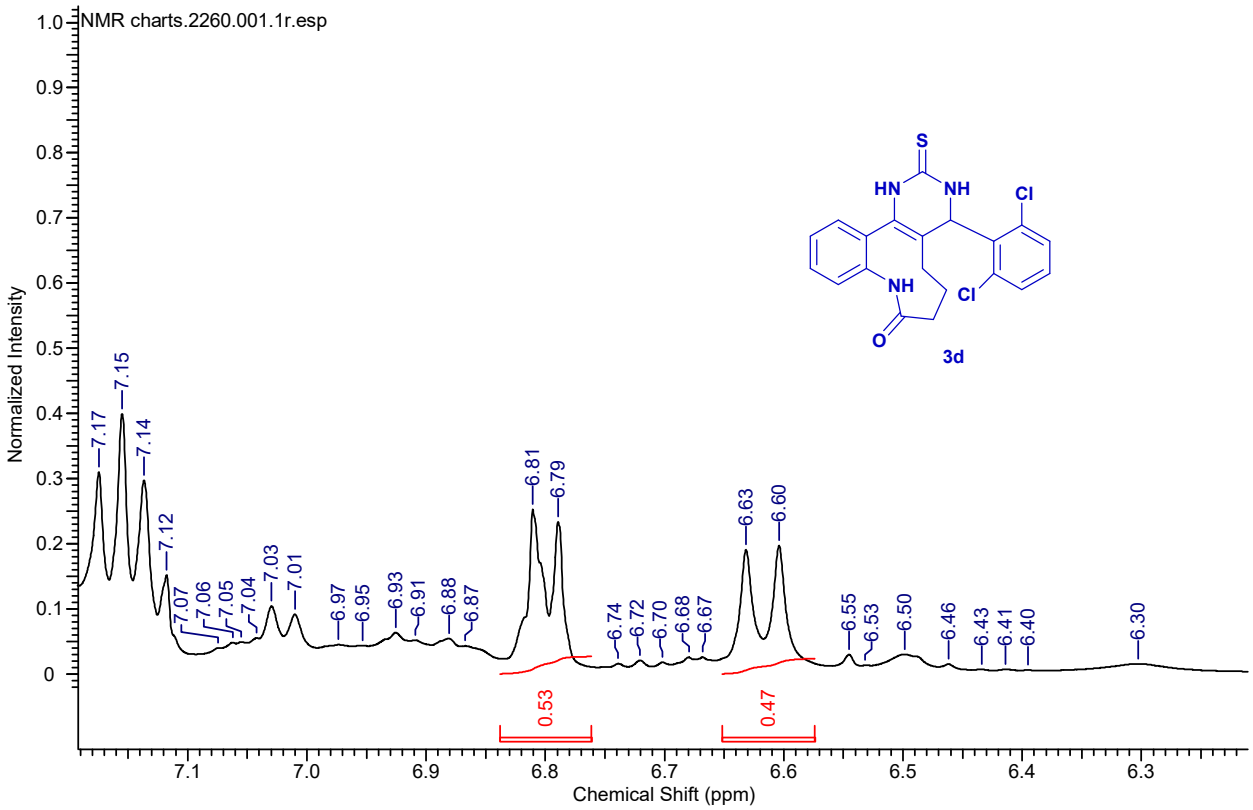


Fig. S20. ^{1}H-NMR spectrum of compound **3d**.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Normalized Intensity
Chemical Shift (ppm)
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7.15
7.14
7.12
7.07
7.06
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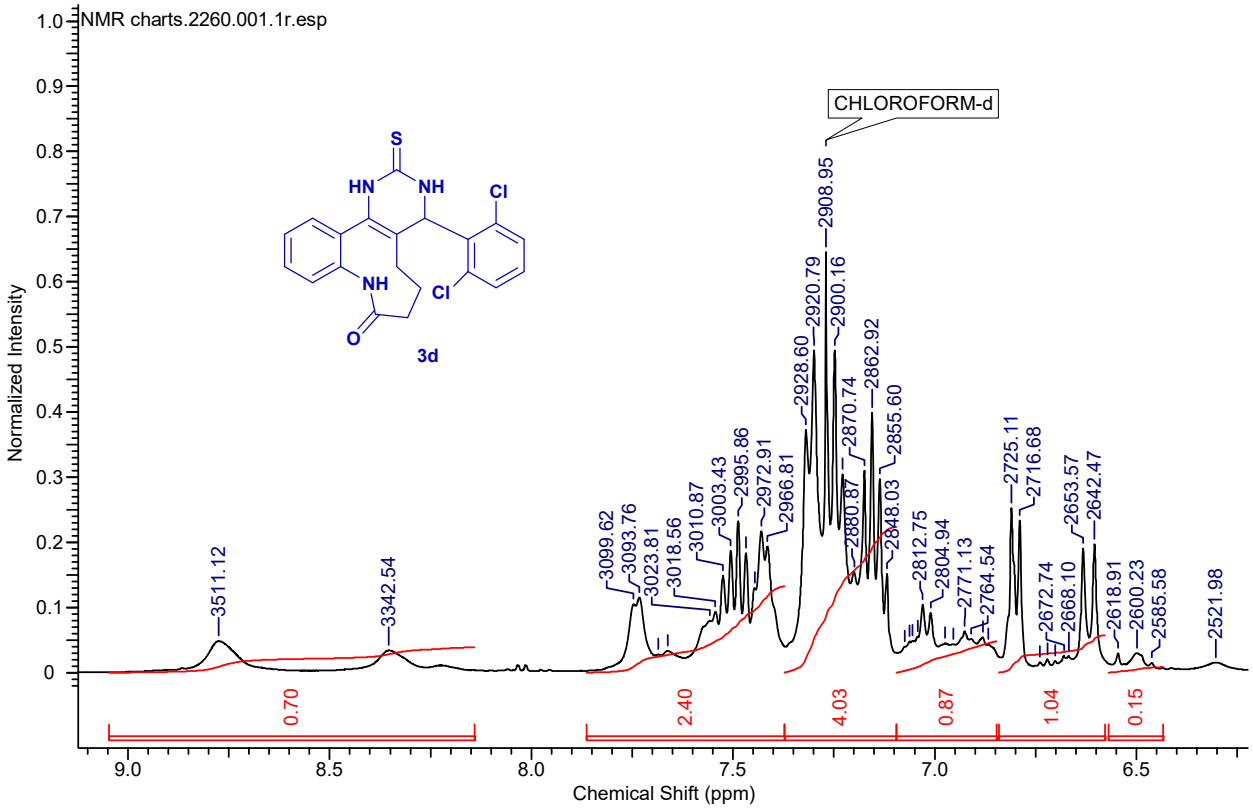
7.04
7.03
7.01
6.97
6.95
6.93
6.91
6.88
6.87
6.81
6.79
6.74
6.72
6.70
6.68
6.67
6.63
6.60
6.55
6.53
6.50
6.46
6.43
6.41
6.40
6.30
0.53
0.47
S
HN
NH
Cl
NH
Cl
O
3d


NMR charts.2260.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
CHLOROFORM-d
3511.12
3342.54
3099.62
3093.76
3023.81
3018.56
3010.87
3003.43
2995.86
2972.91
2966.81
2928.60
2920.79
2908.95
2900.16
2880.87
2870.74
2862.92
2855.60
2848.03
2812.75
2804.94
2771.13
2764.54
2725.11
2716.68
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2668.10
2653.57
2642.47
2618.91
2600.23
2585.58
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4.03
0.87
1.04
0.15
S
HN
NH
Cl
NH
Cl
O
3d

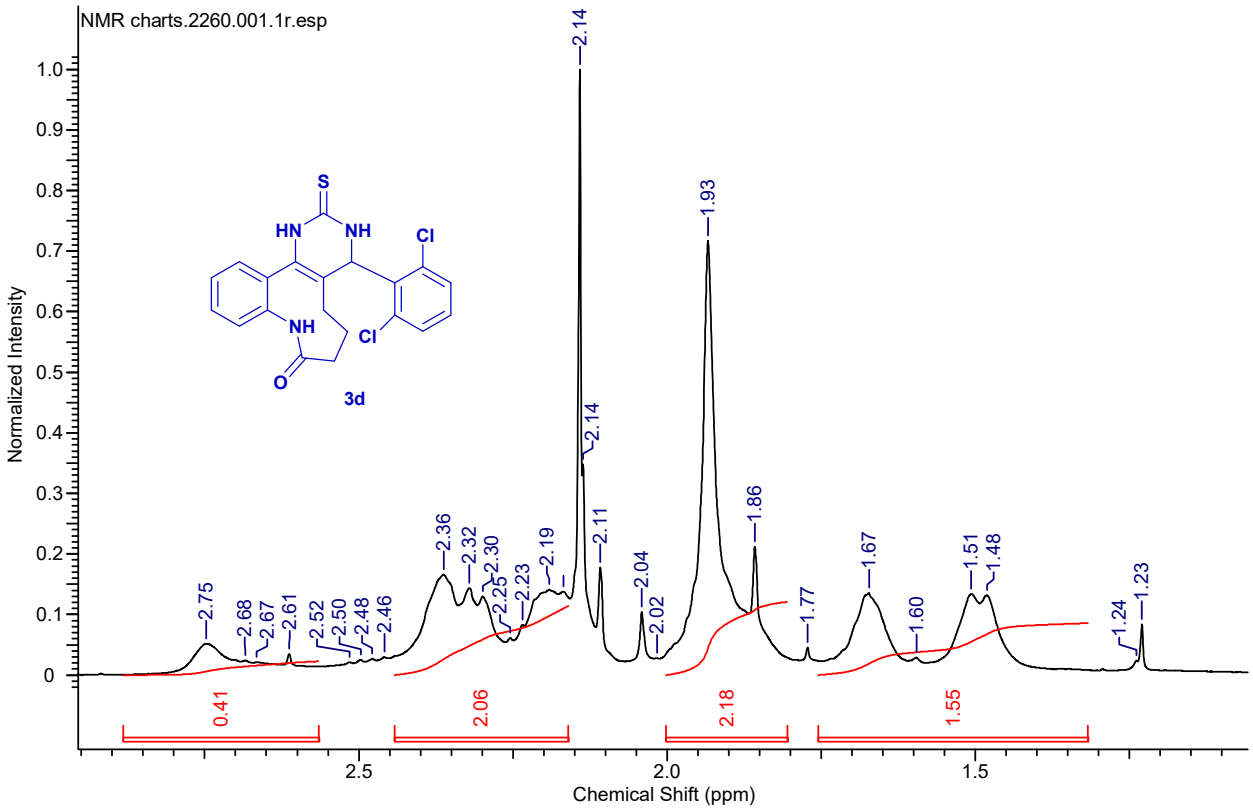
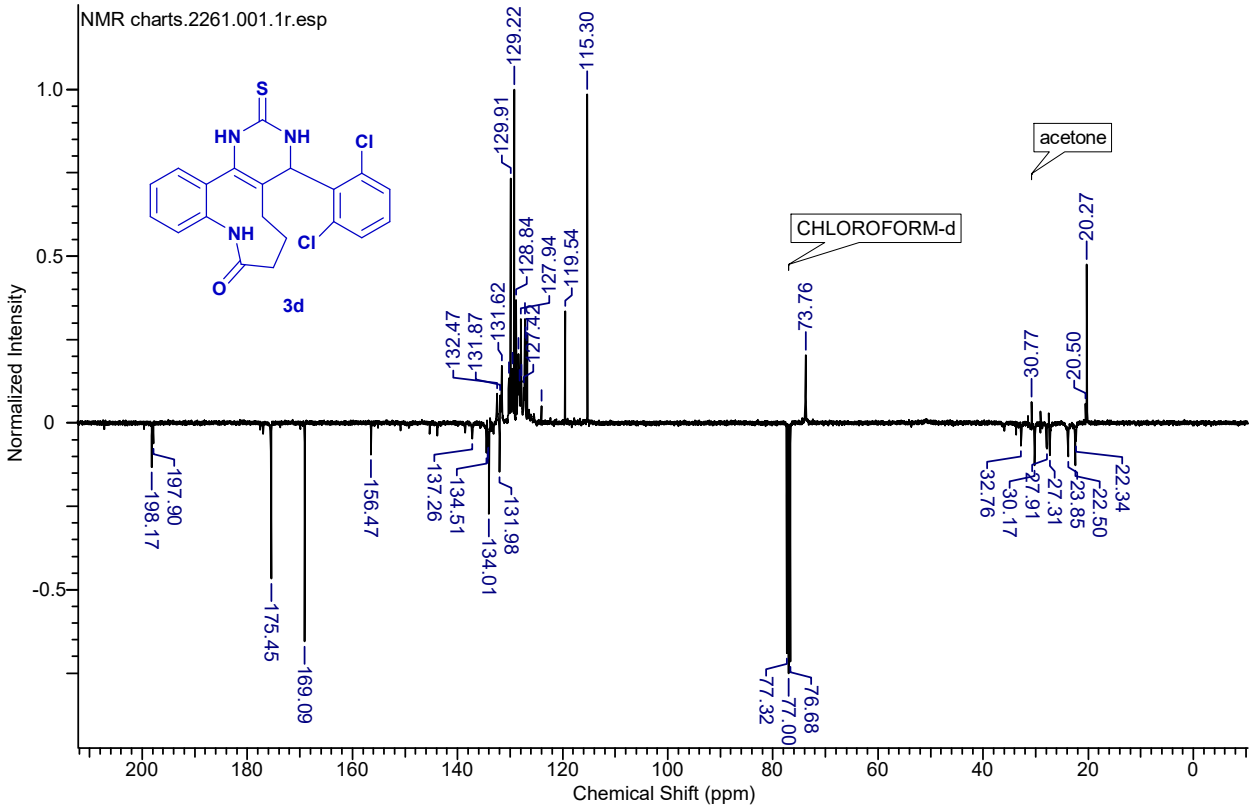


Fig. S20-A. ^{1}H-NMR spectrum of compound **3d**.



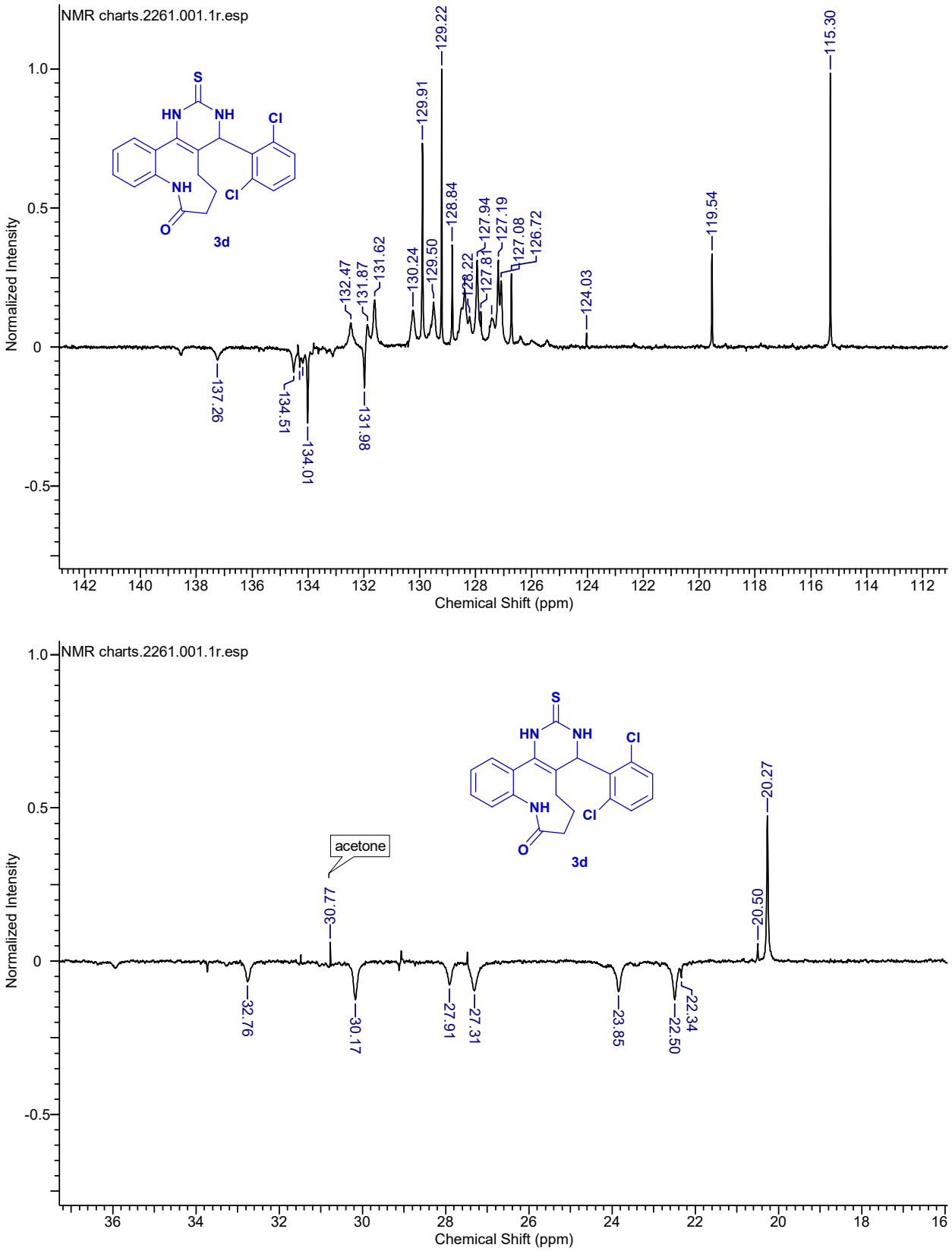


Fig. S21. ^{13}C-NMR spectrum of compound **3d**.

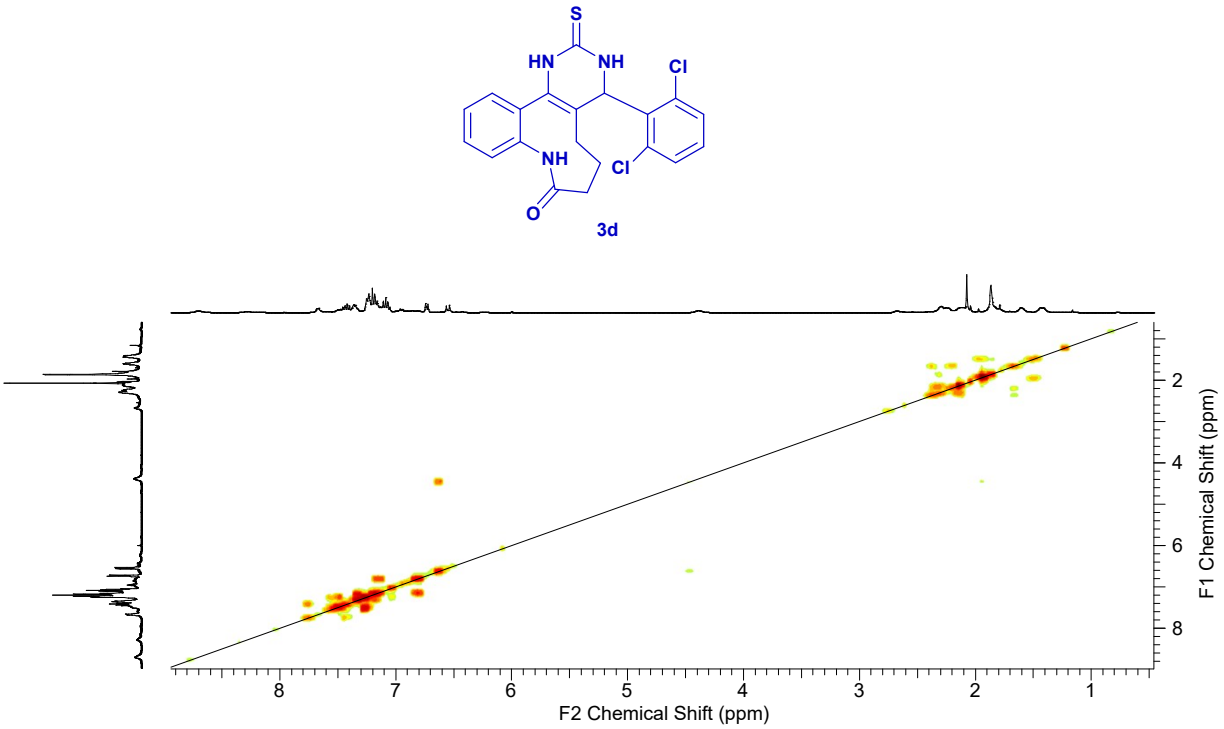


Fig. S22. 2D-NMR spectrum (**COSY**) of compound **3d**.

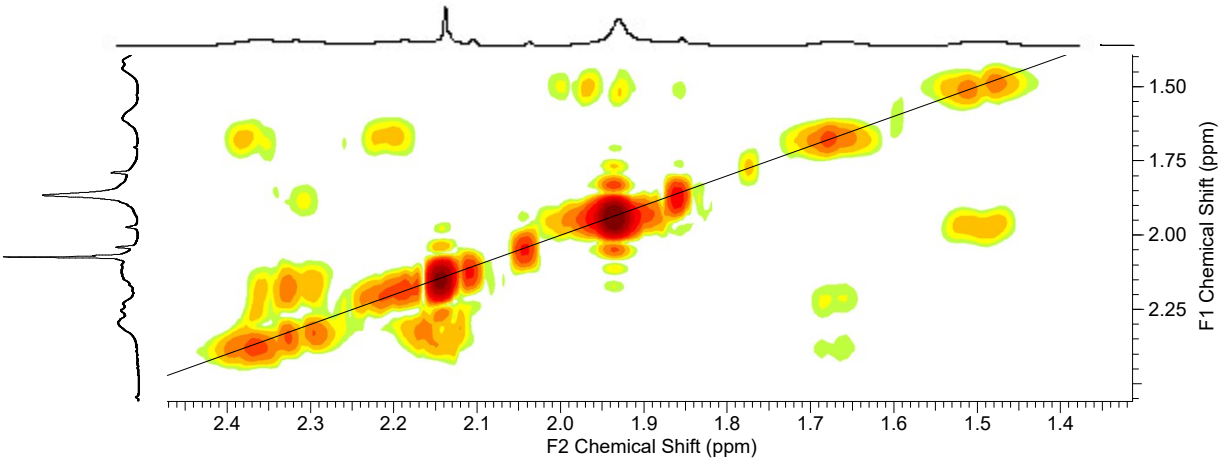
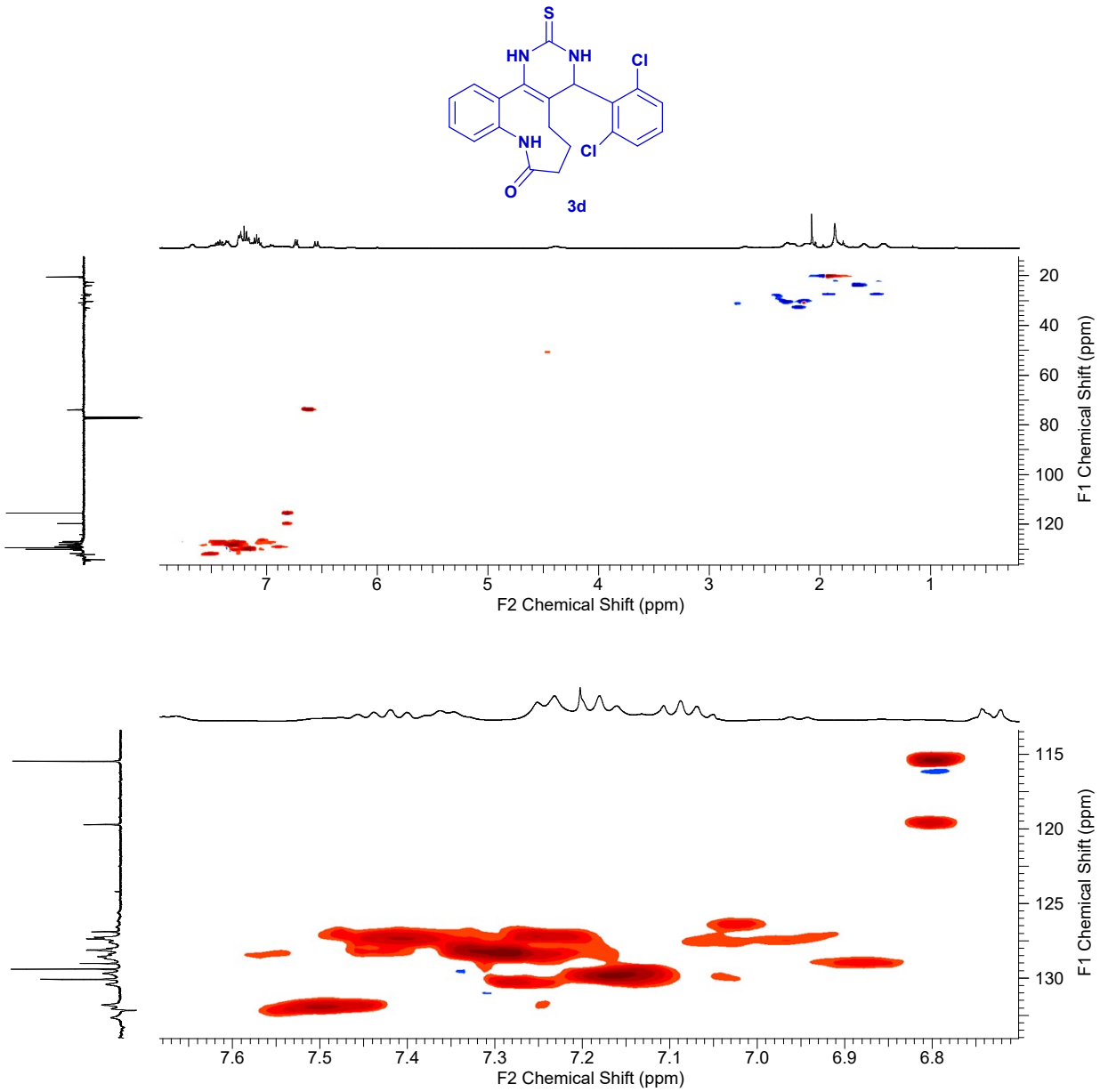


Fig. S23. 2D-NMR spectrum (**COSY**) of compound **3d**.


S
HN
NH
Cl
NH
Cl
O
3d
20
40
60
80
100
120
F1 Chemical Shift (ppm)
7
6
5
4
3
2
1
F2 Chemical Shift (ppm)
115
120
125
130
F1 Chemical Shift (ppm)
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
F2 Chemical Shift (ppm)

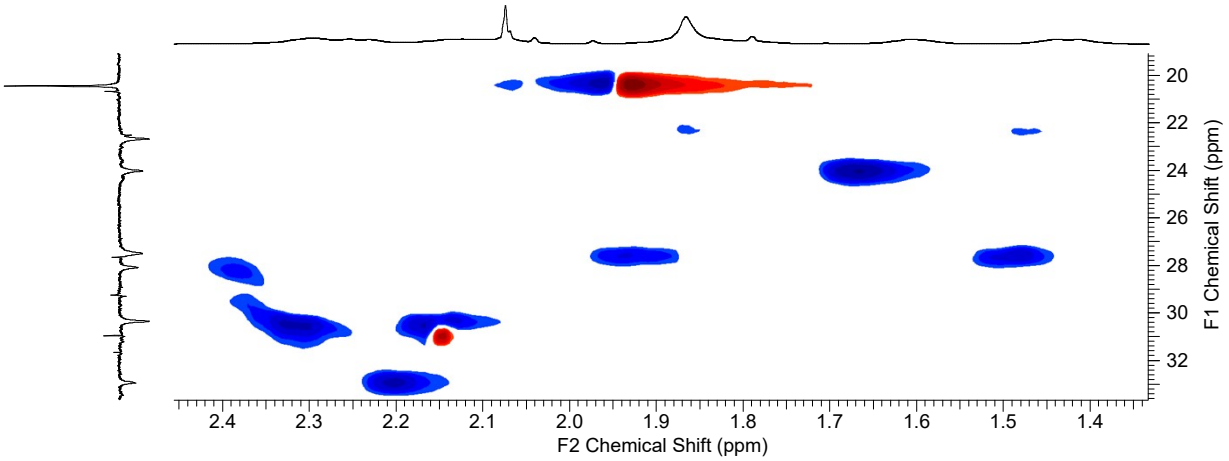
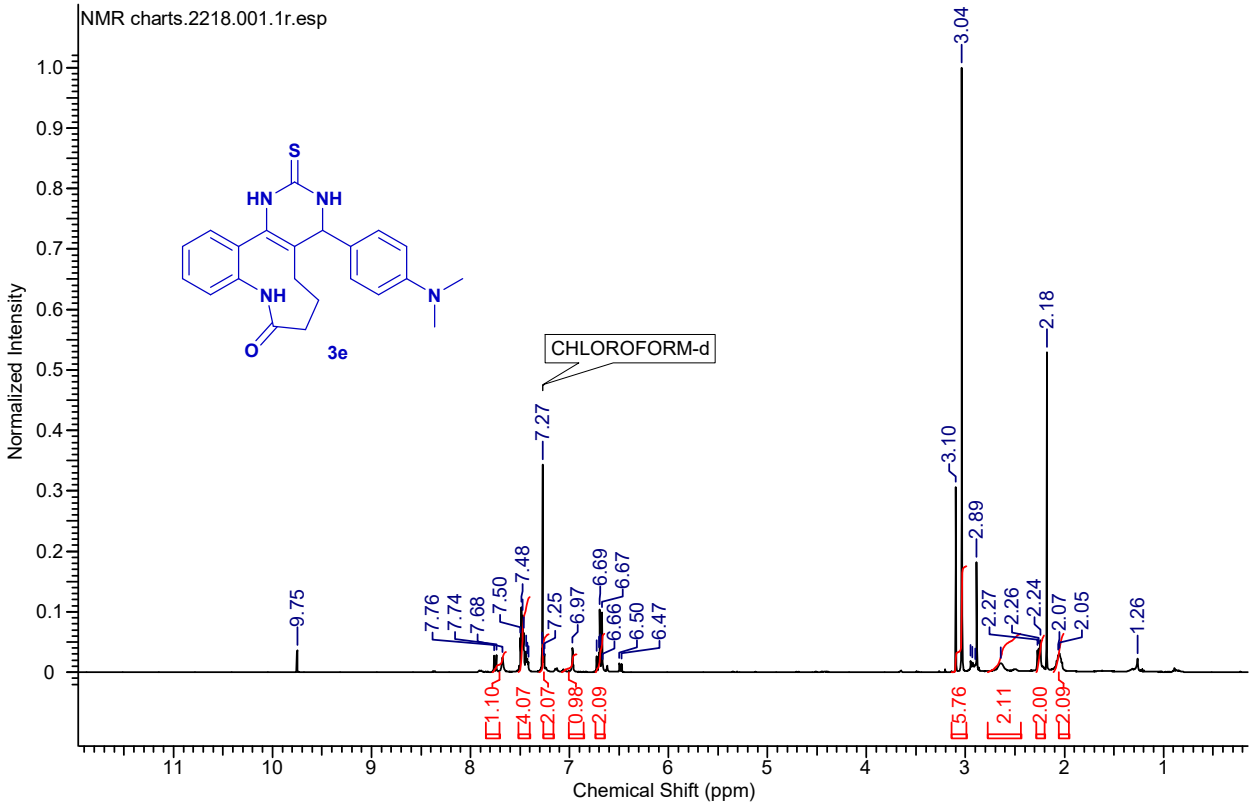


Fig. S24. 2D-NMR spectrum (**HSQC**) of compound **3d**.



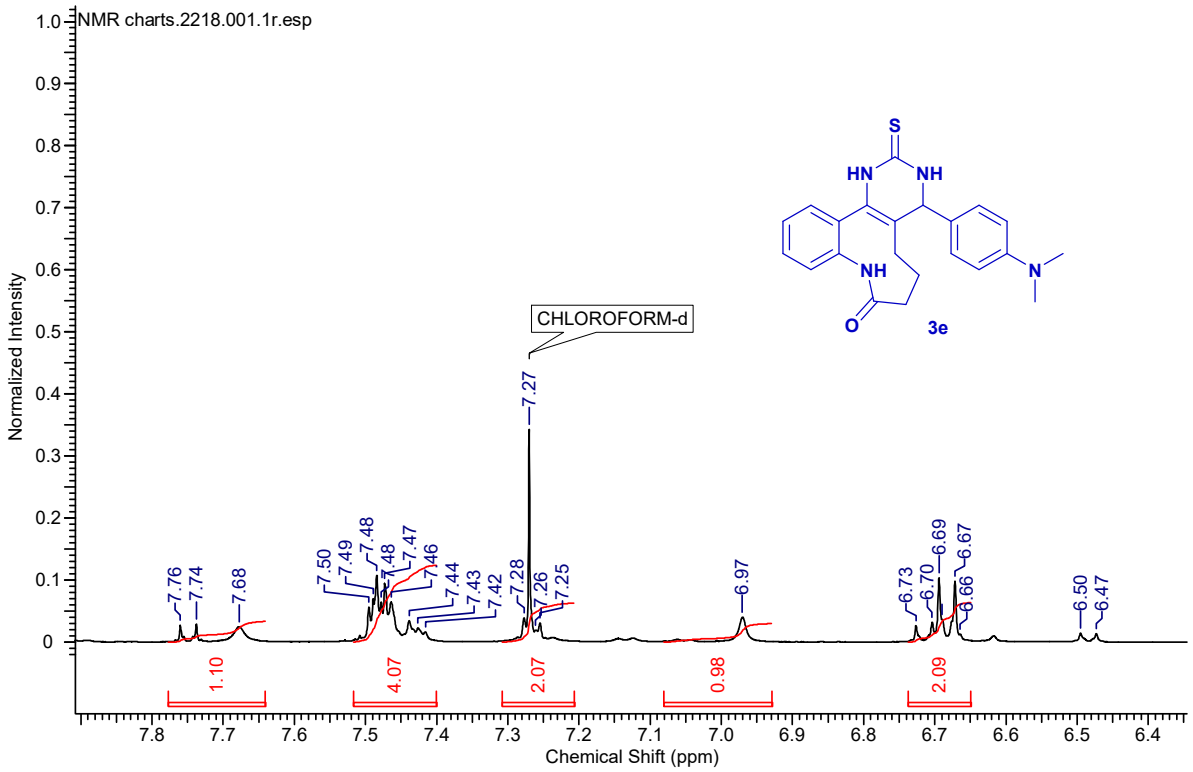
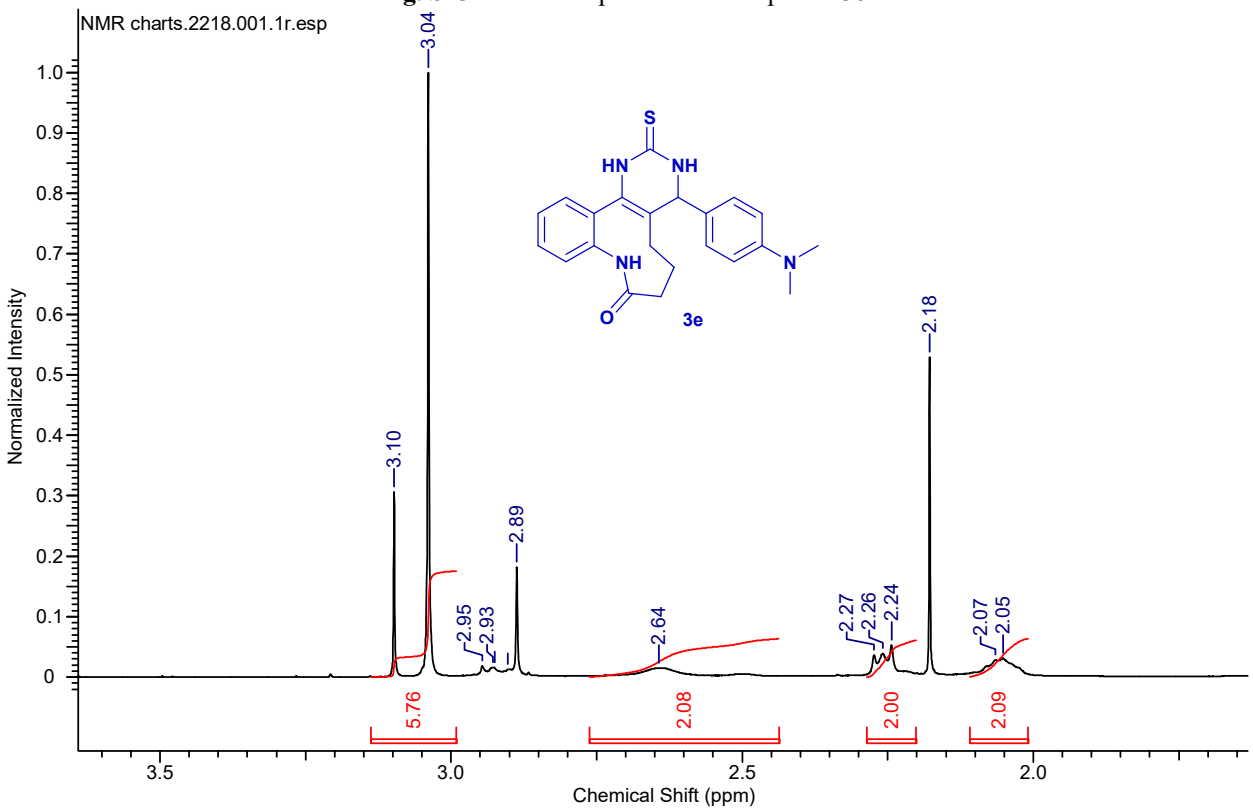


Fig. S25. [1]H-NMR spectrum of compound **3e**.



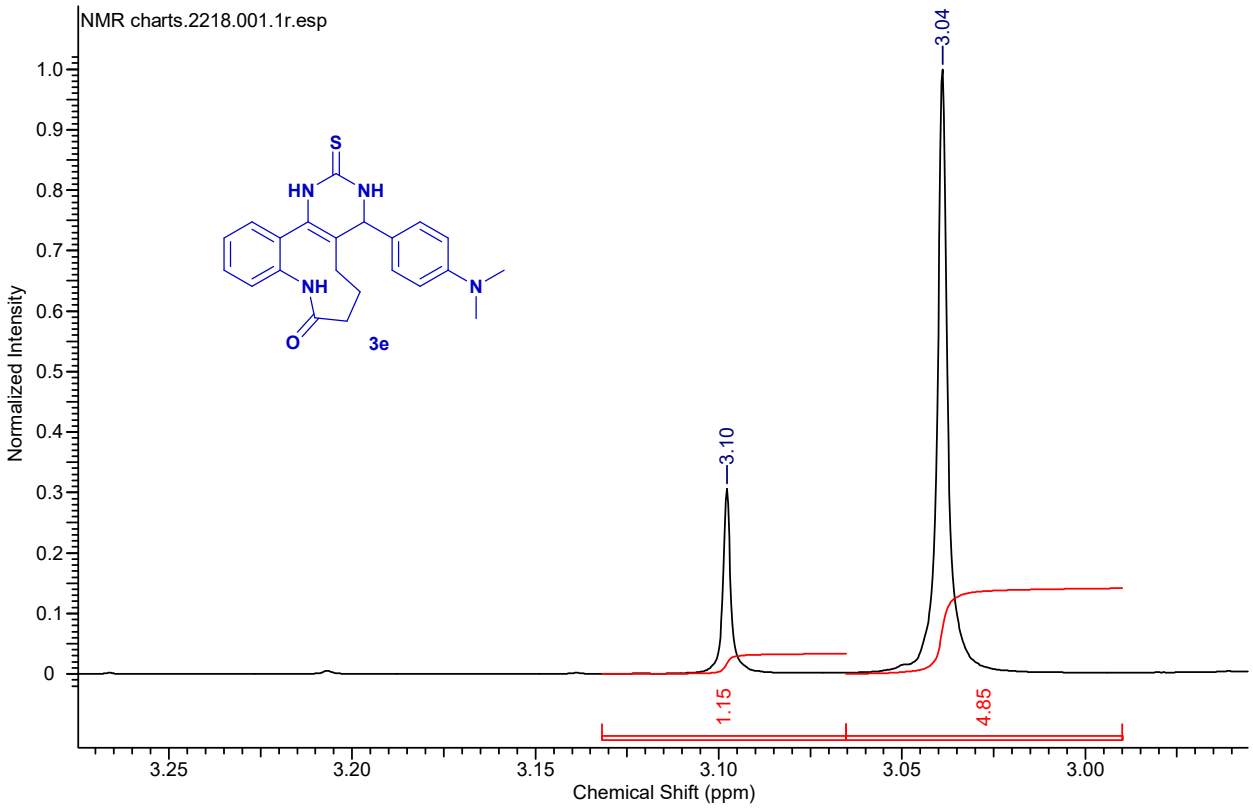


Fig. S25-A. ^{1}H-NMR spectrum of compound **3e**.

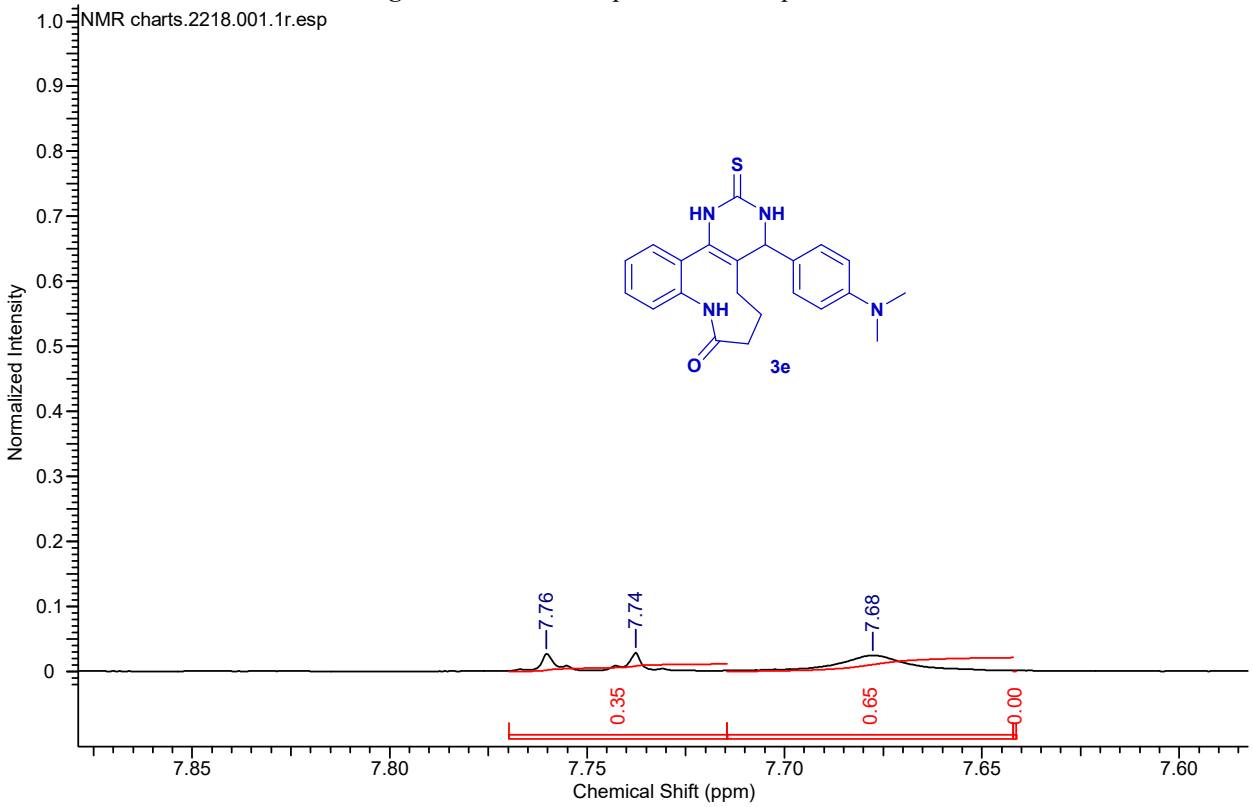


Fig. S25-B. ^{1}H-NMR spectrum of compound **3e**.

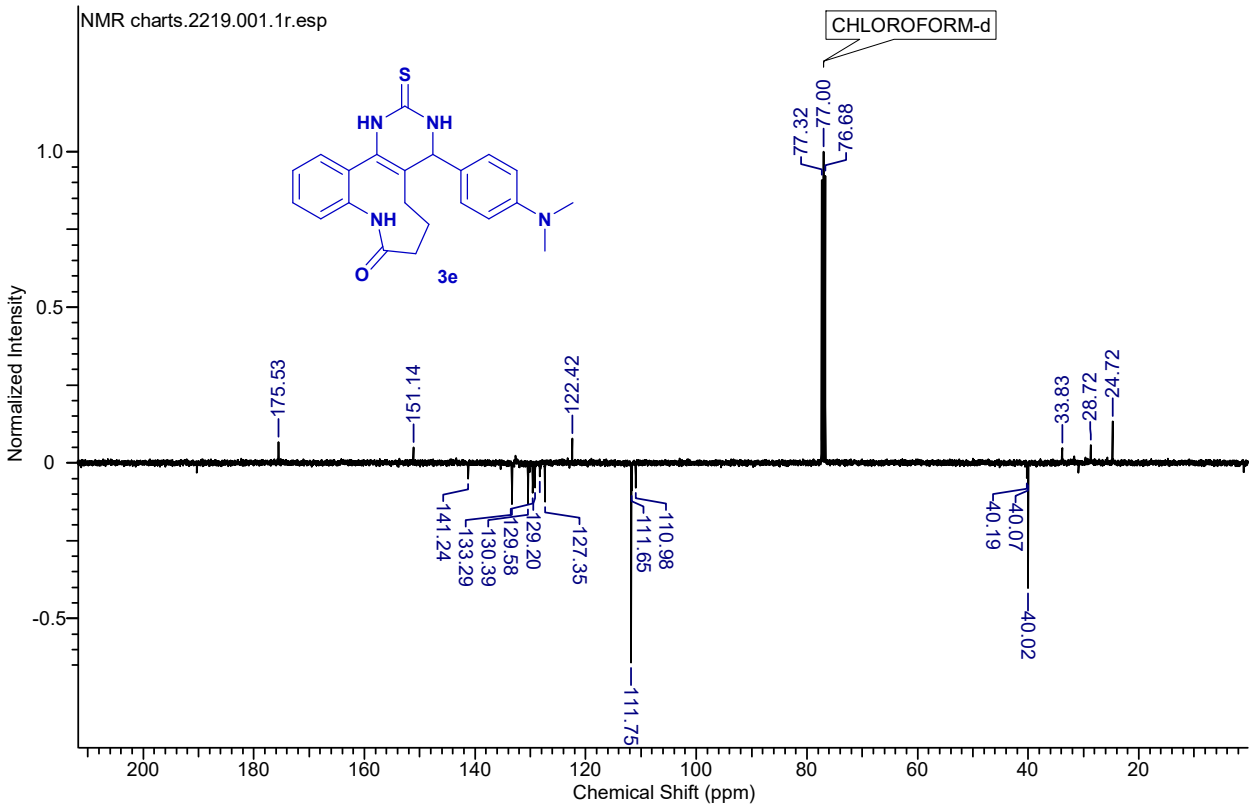
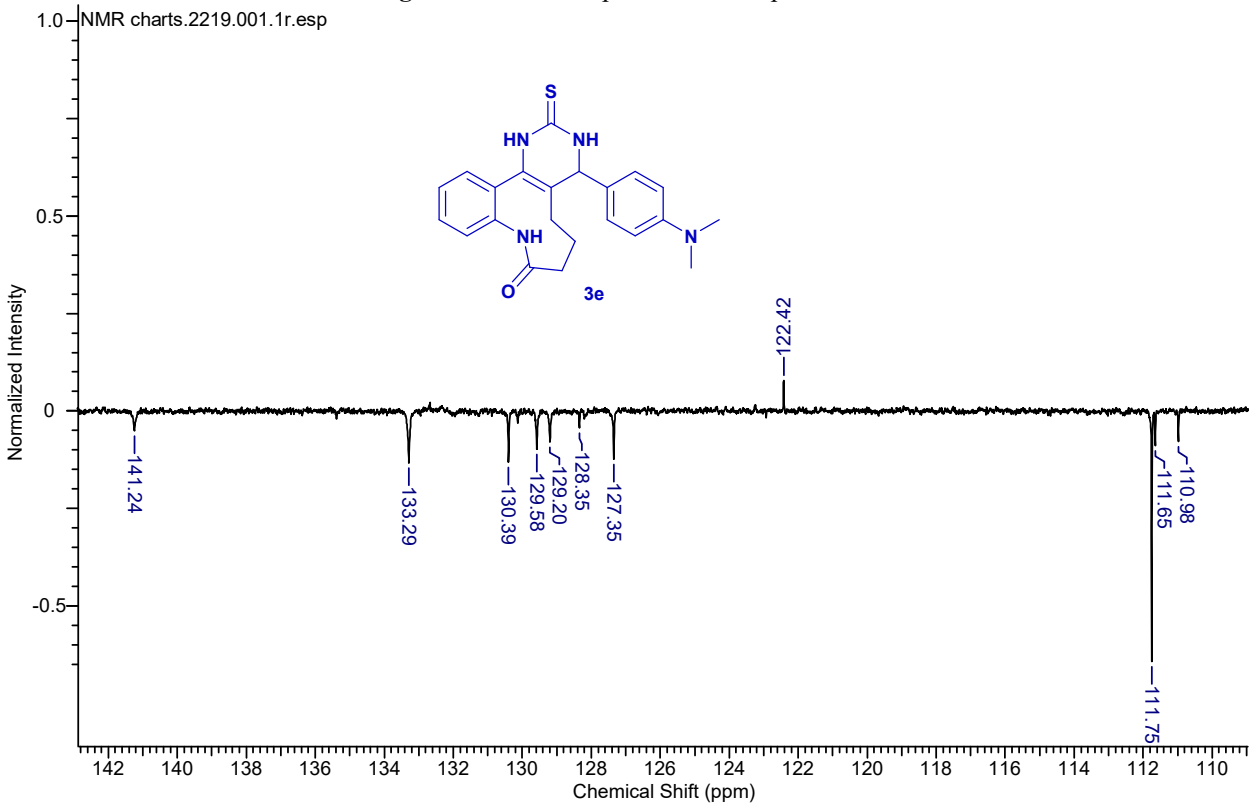


Fig. S26. ^{13}C-NMR spectrum of compound **3e**.



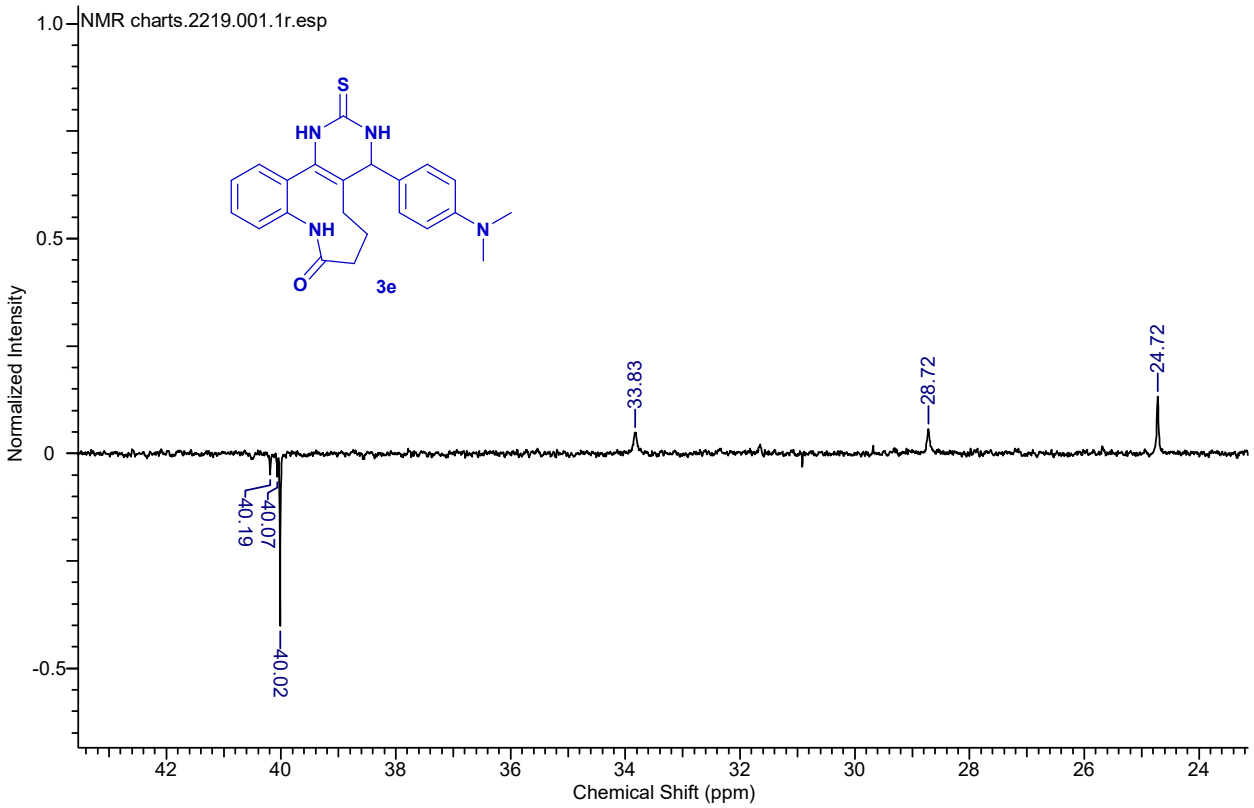
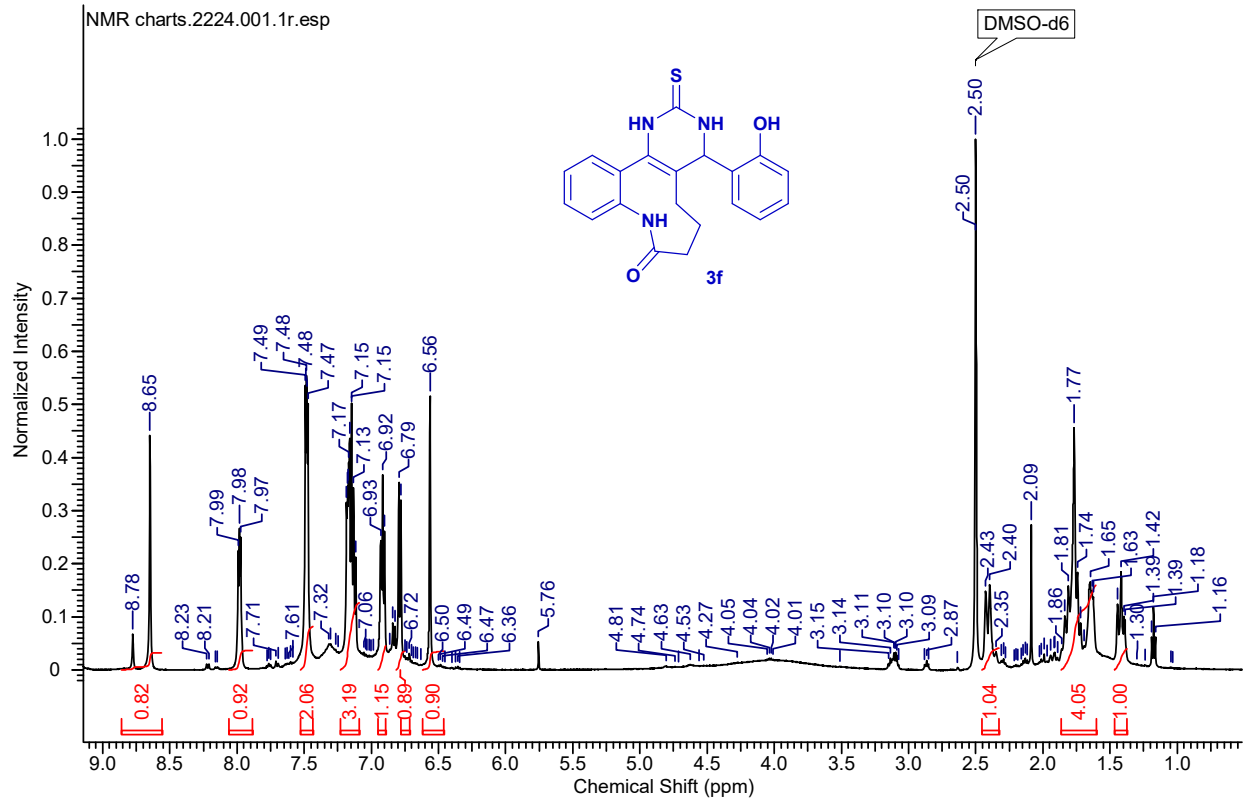


Fig. S26-A. ^{13}C-NMR spectrum of compound **3e**.



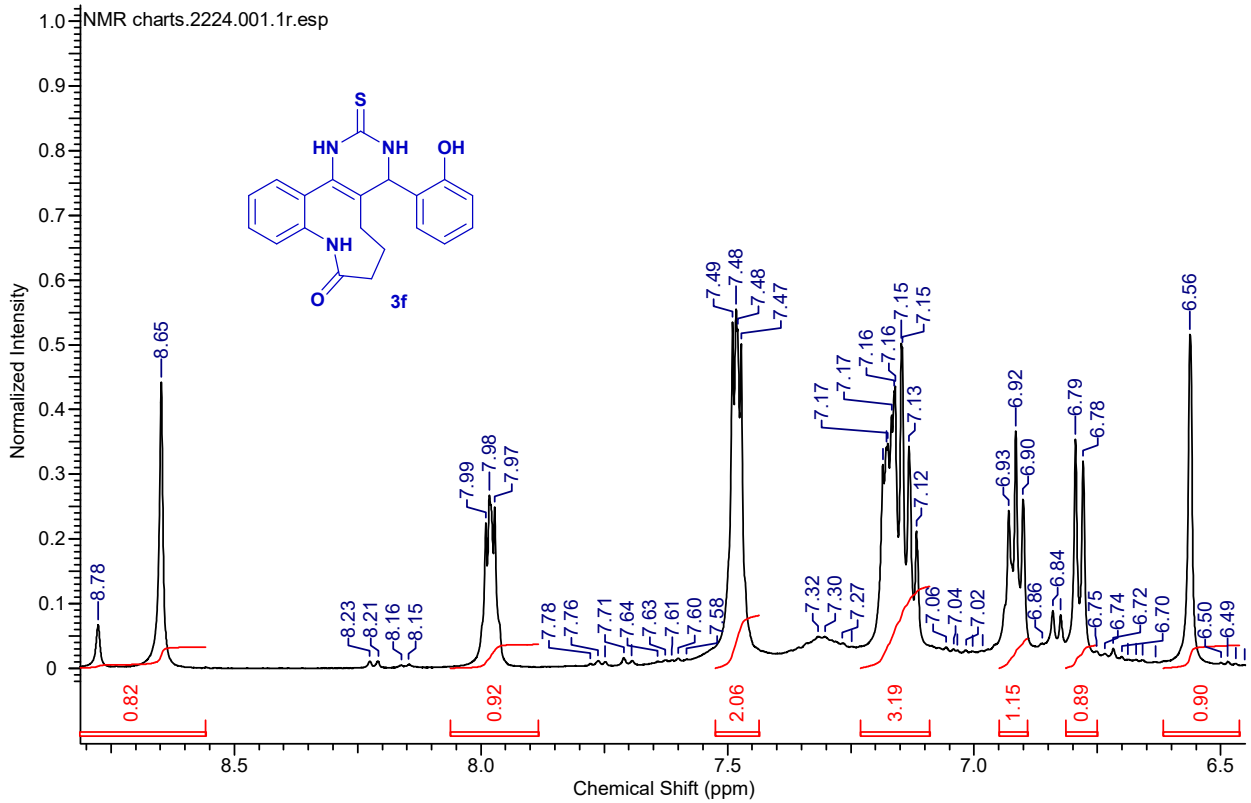
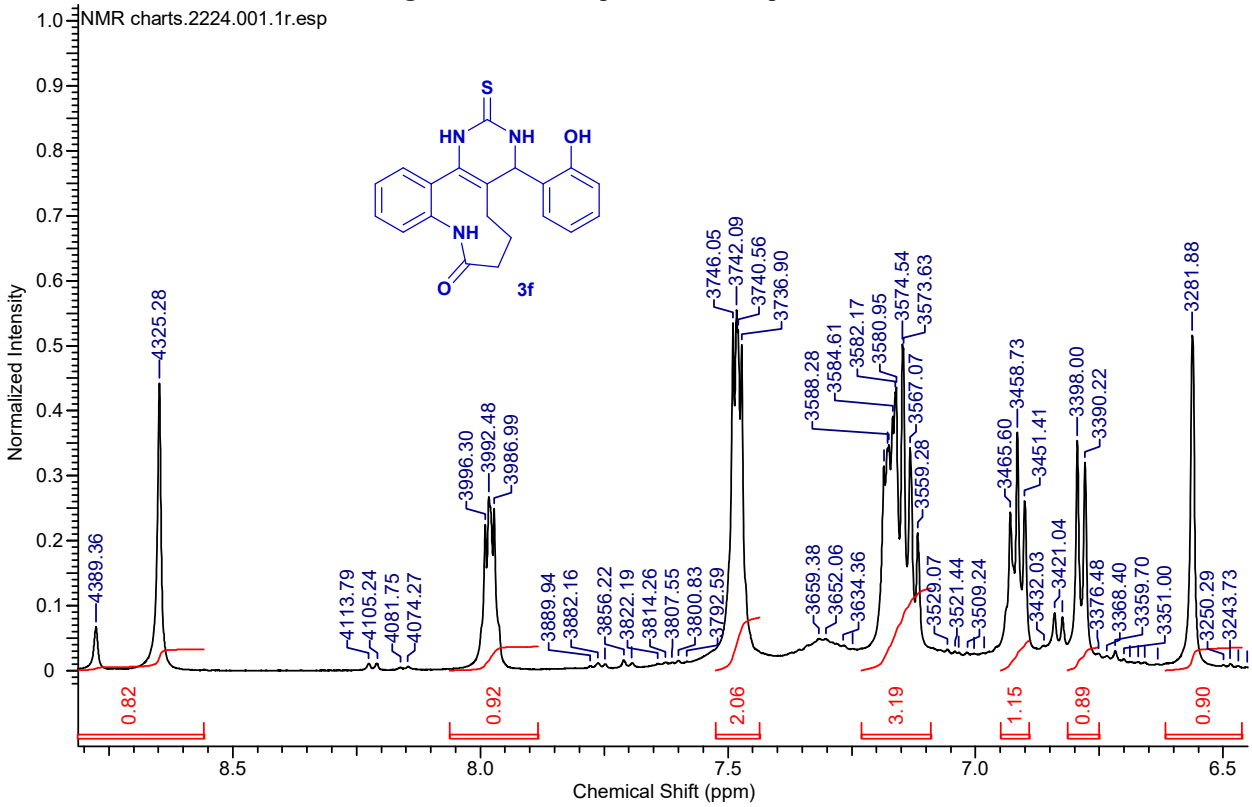


Fig. S27. [1]H-NMR spectrum of compound **3f**.



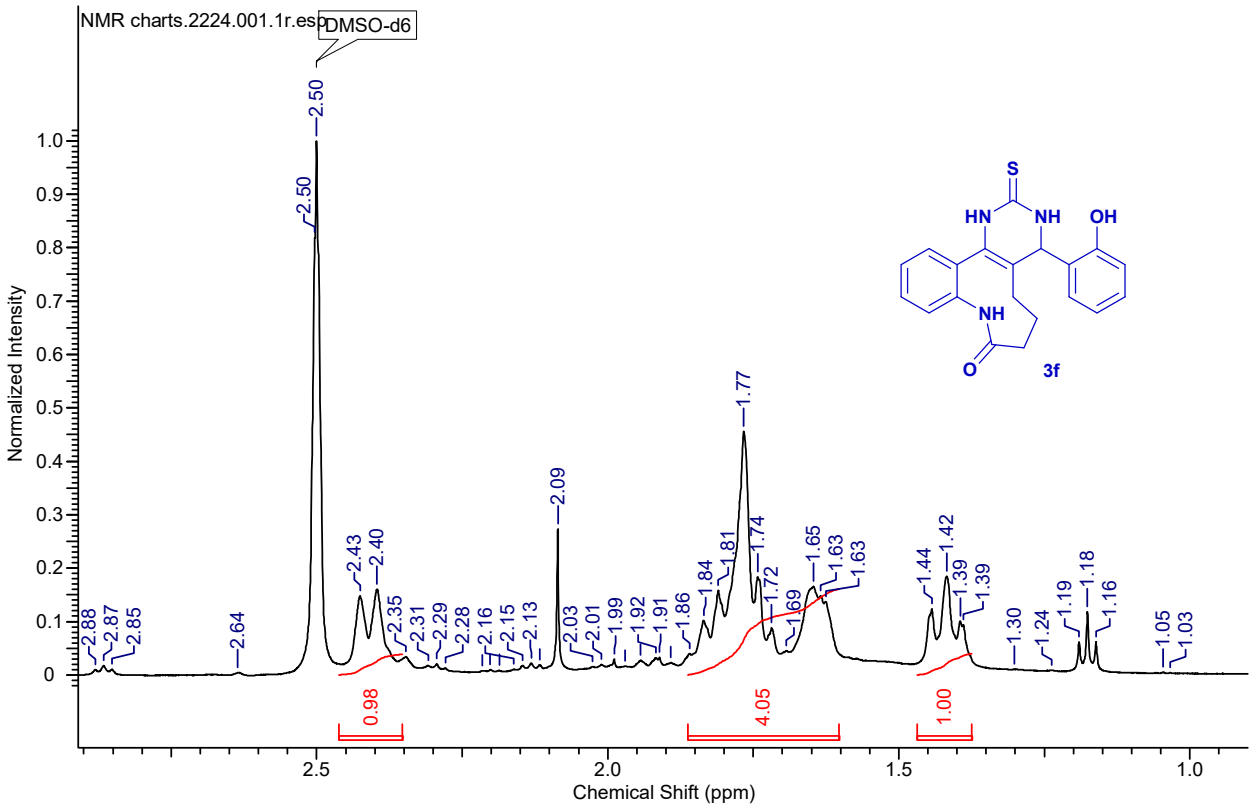


Fig. S27. ^{1}H-NMR spectrum of compound **3f**.

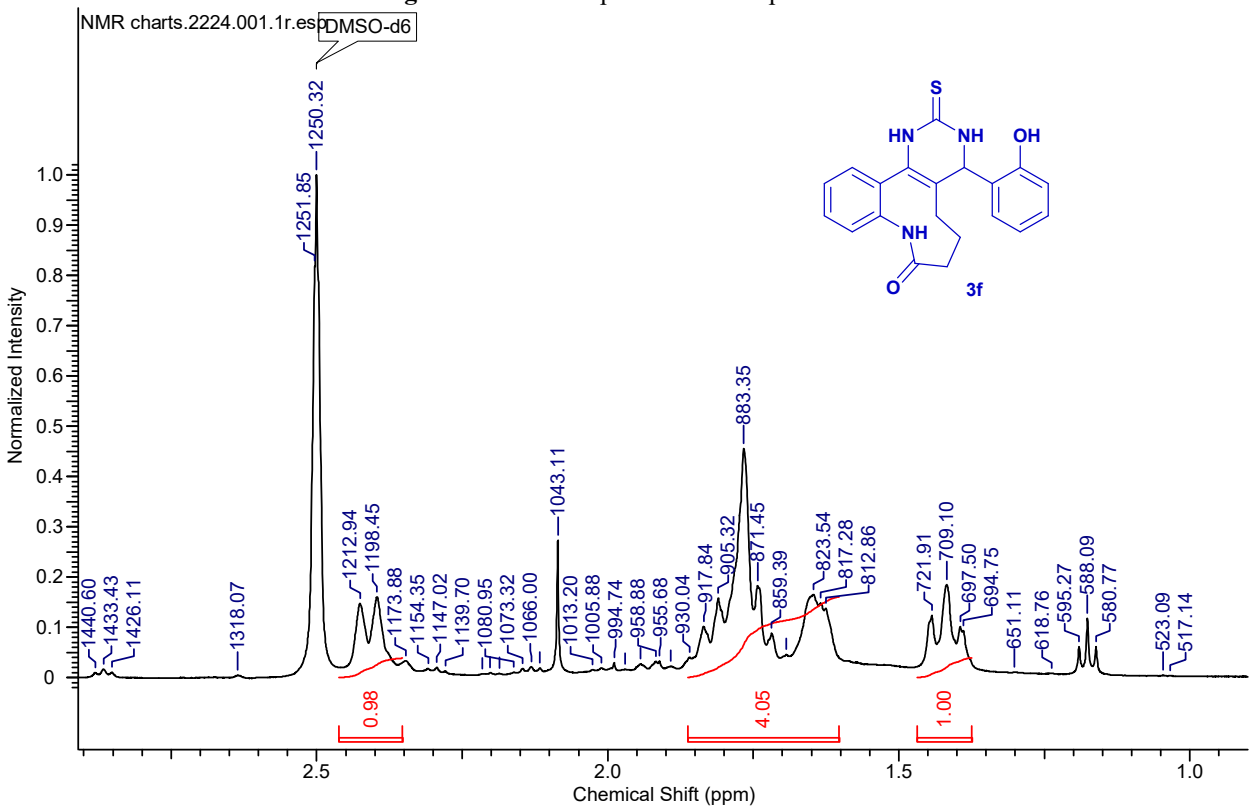


Fig. S27. ^{1}H-NMR spectrum of compound **3f**.

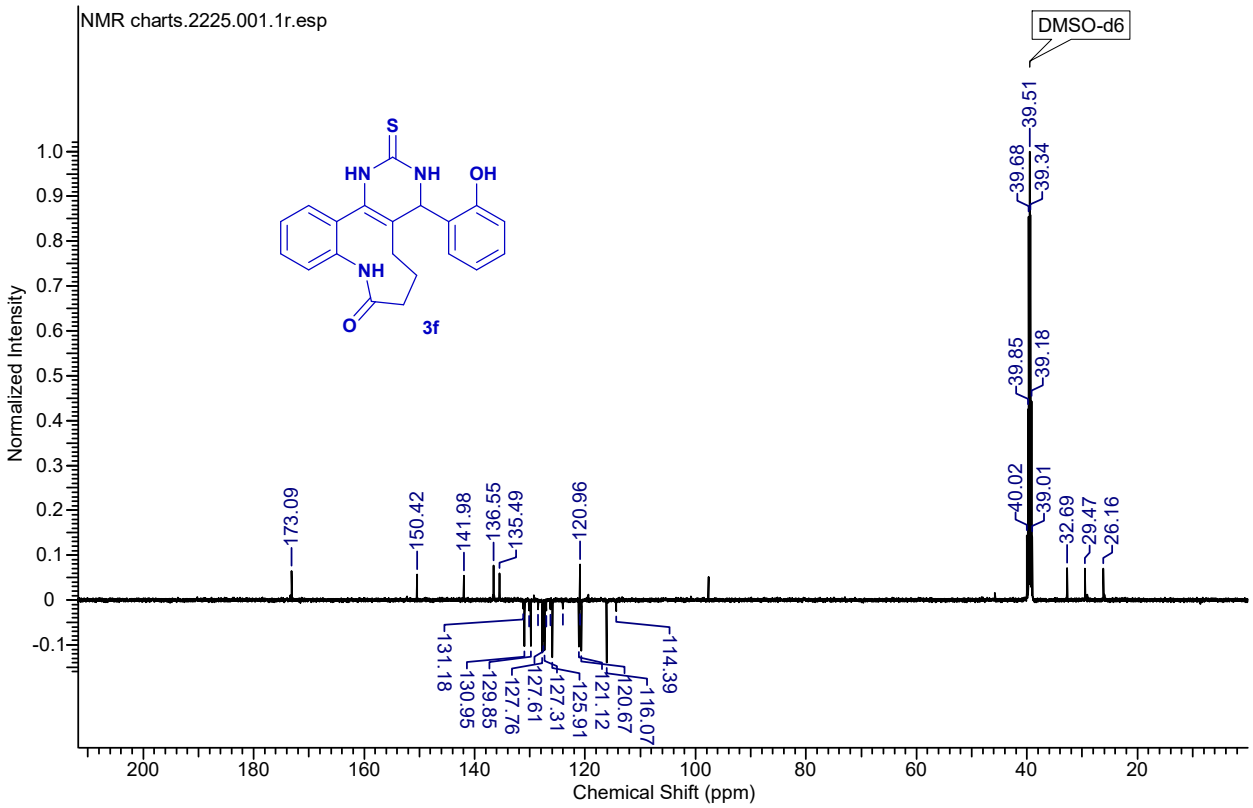


Fig. S28. ^{13}C-NMR spectrum of compound **3f**.

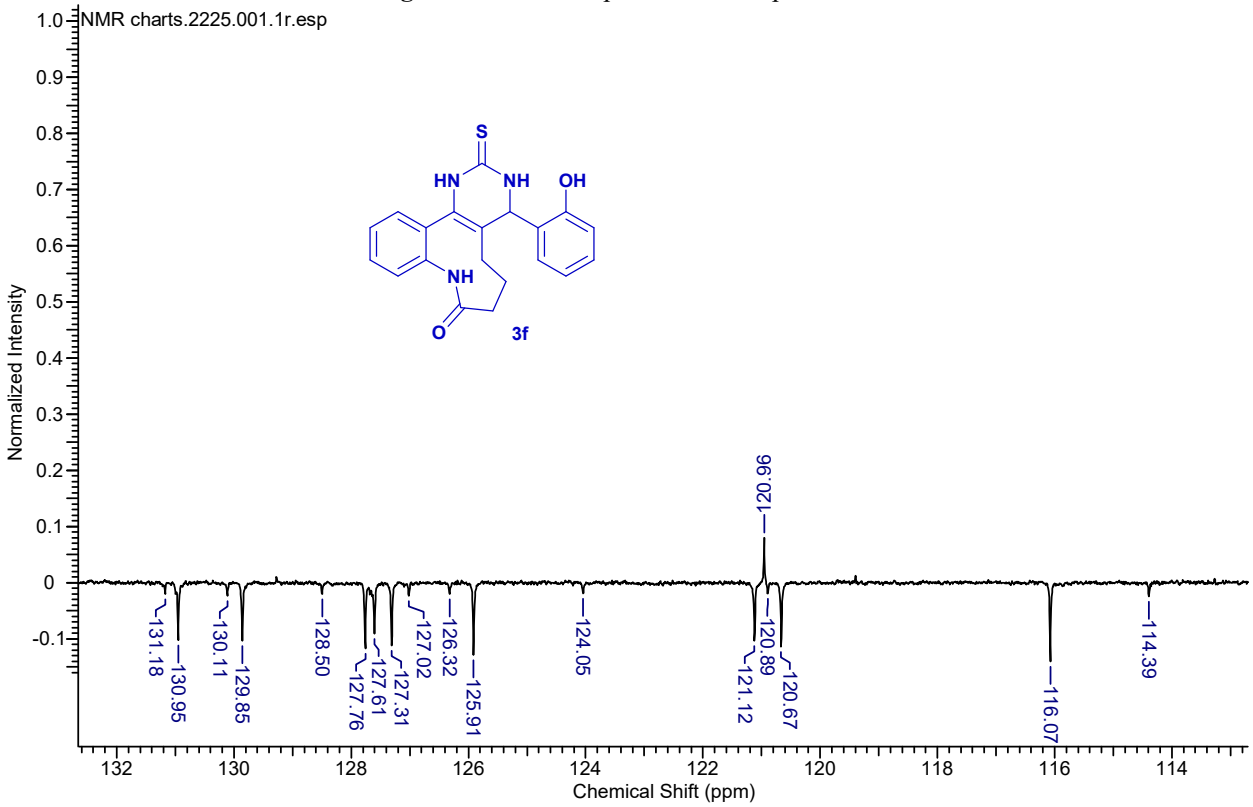


Fig. S28-a. ^{13}C-NMR spectrum of compound **3f**.

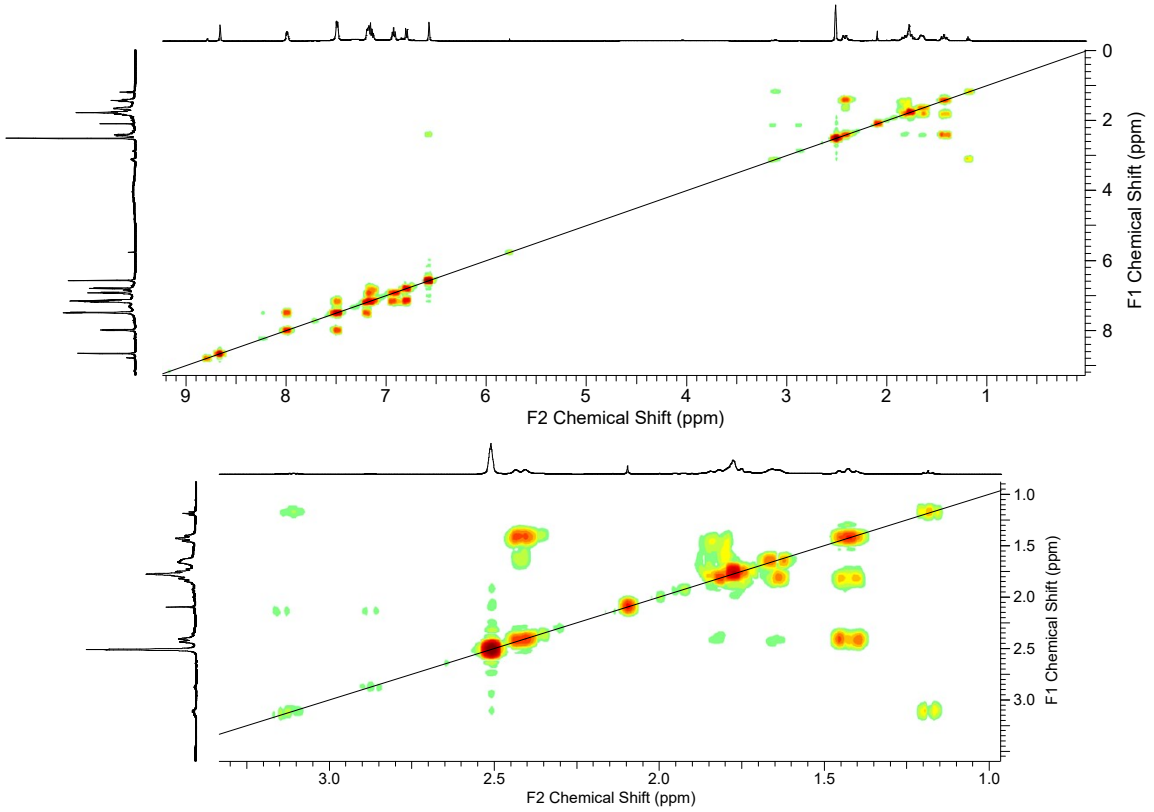
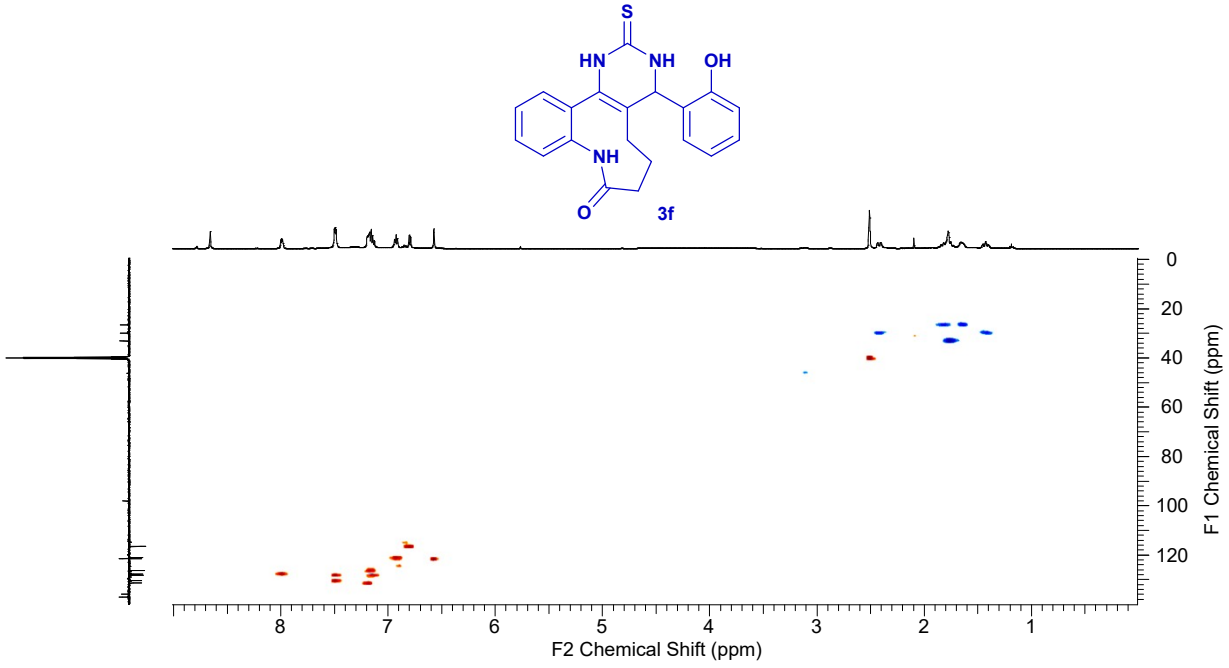


Fig. S29. 2D-NMR spectrum (**COSY**) of compound **3f**.



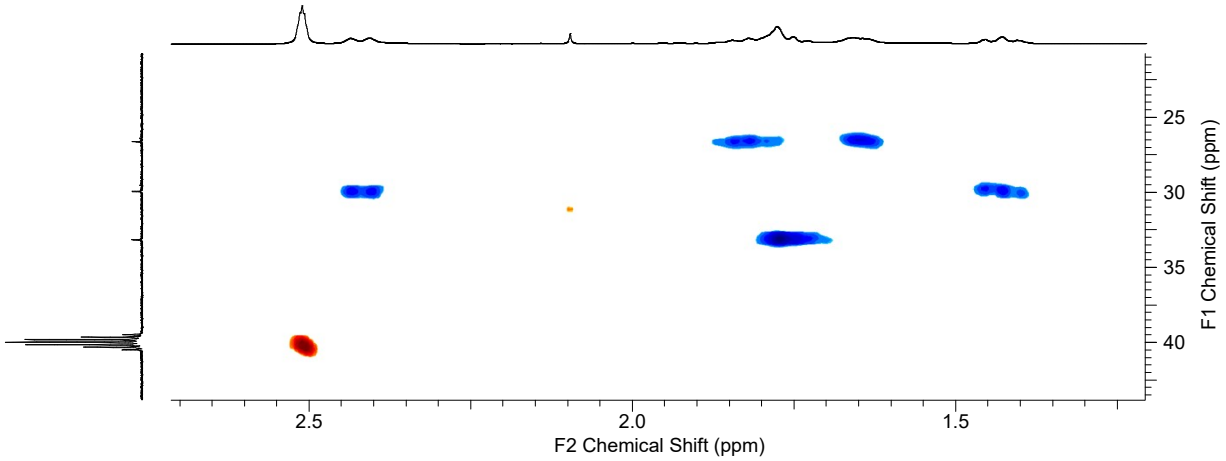


Fig. S30. 2D-NMR spectrum (**HSQC**) of compound **3f**.

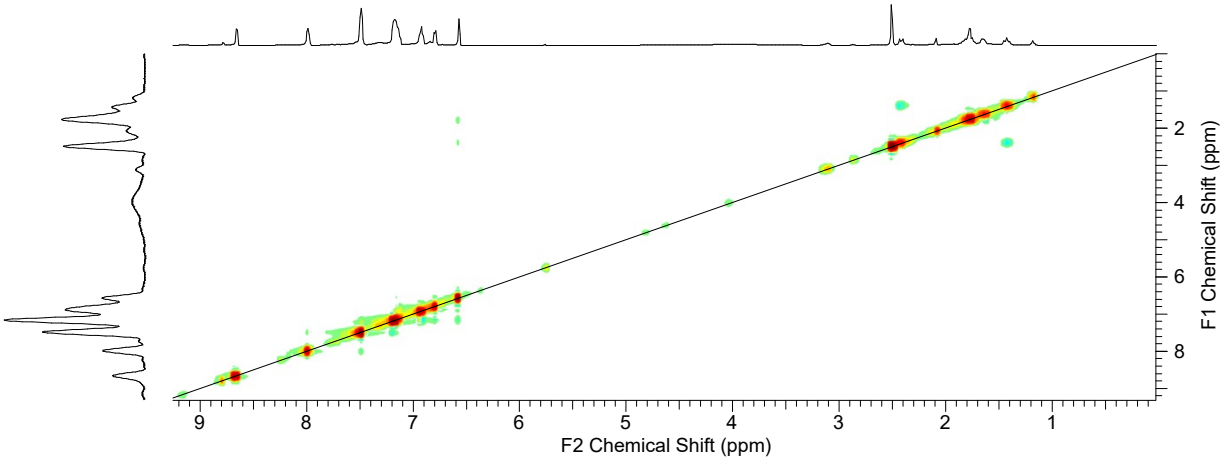


Fig. S31. 2D-NMR spectrum (**NOESY**) of compound **3f**.

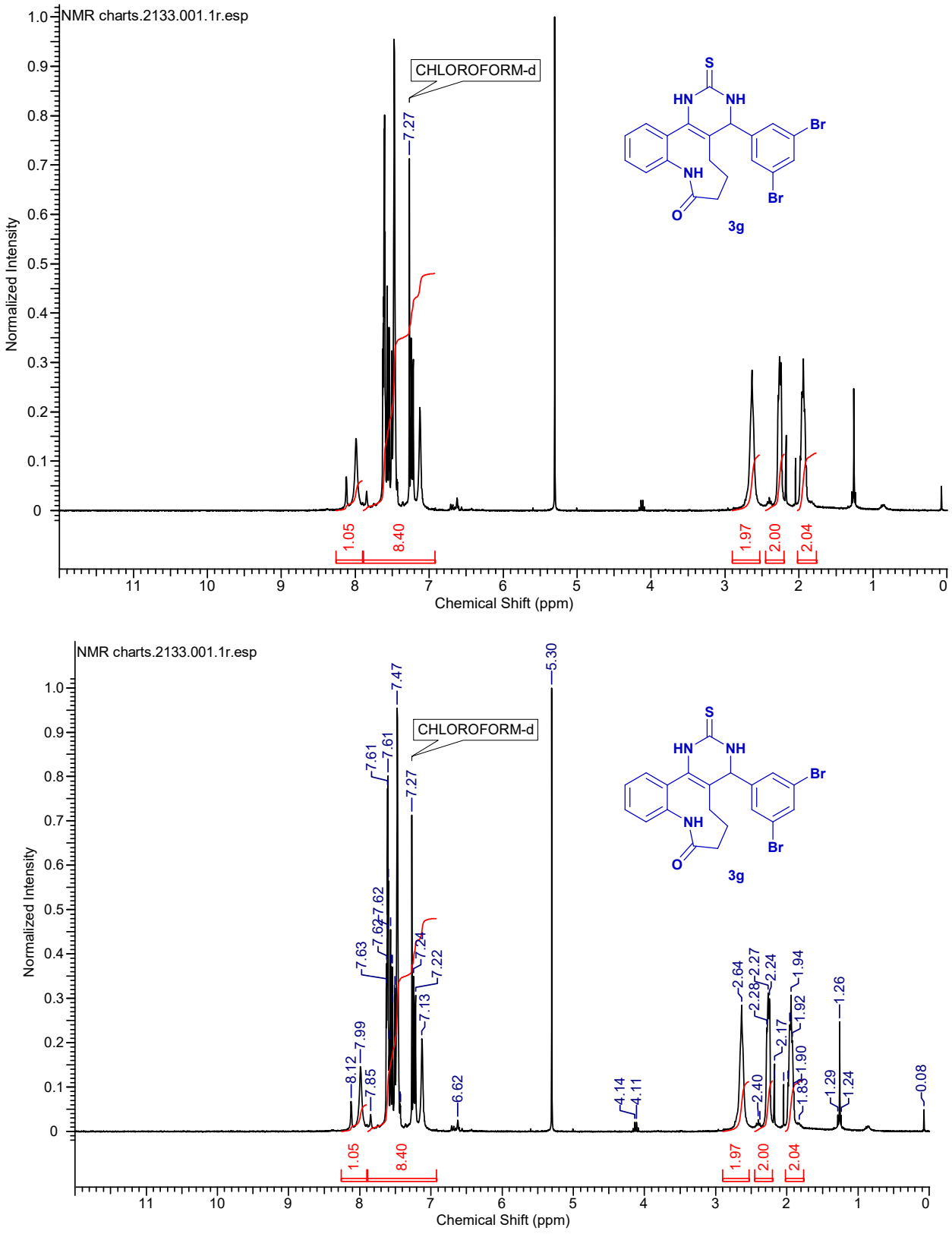


Fig. S32. ^{1}H-NMR spectrum of compound **3g**.

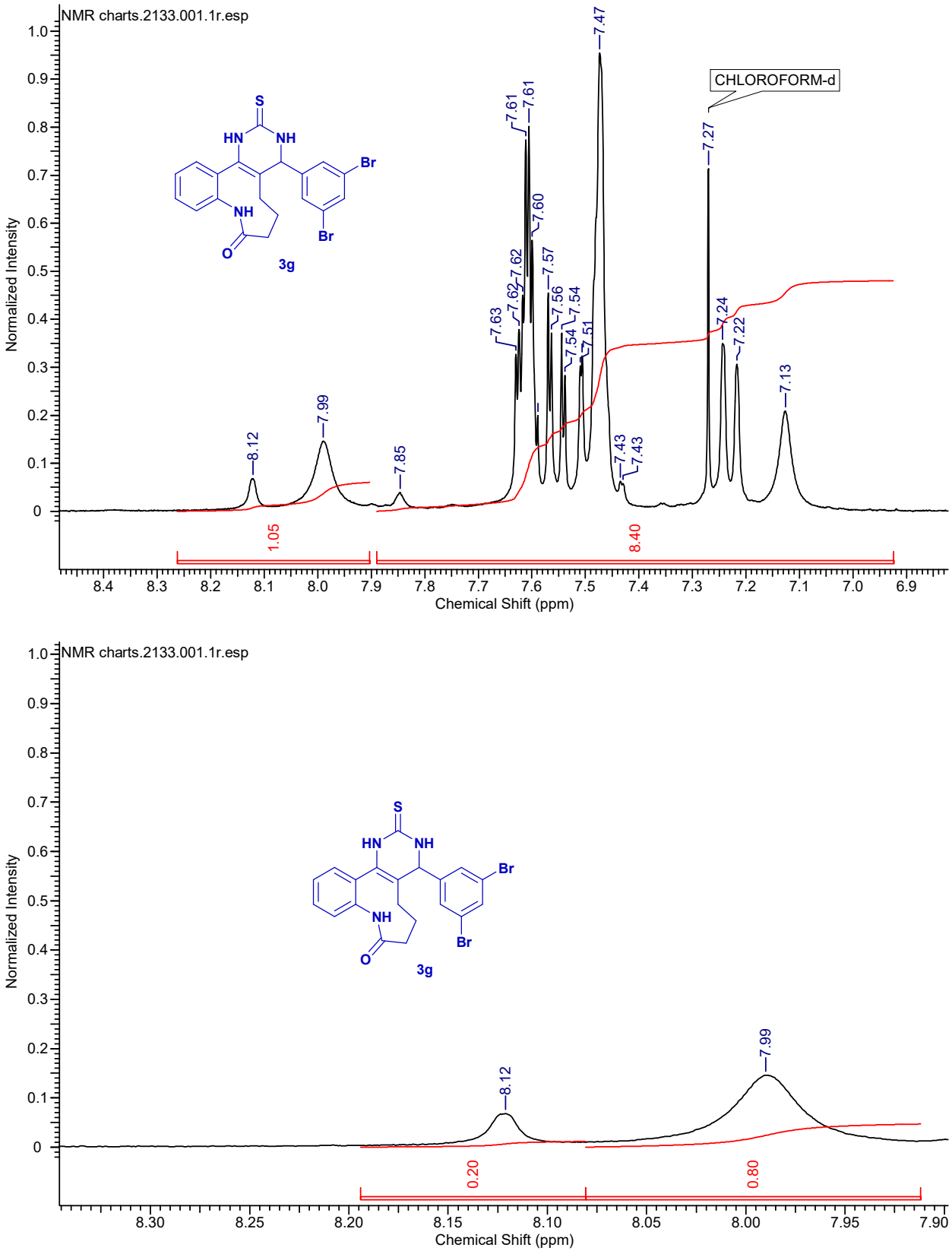


Fig. S32. ^{1}H-NMR spectrum of compound **3g**.

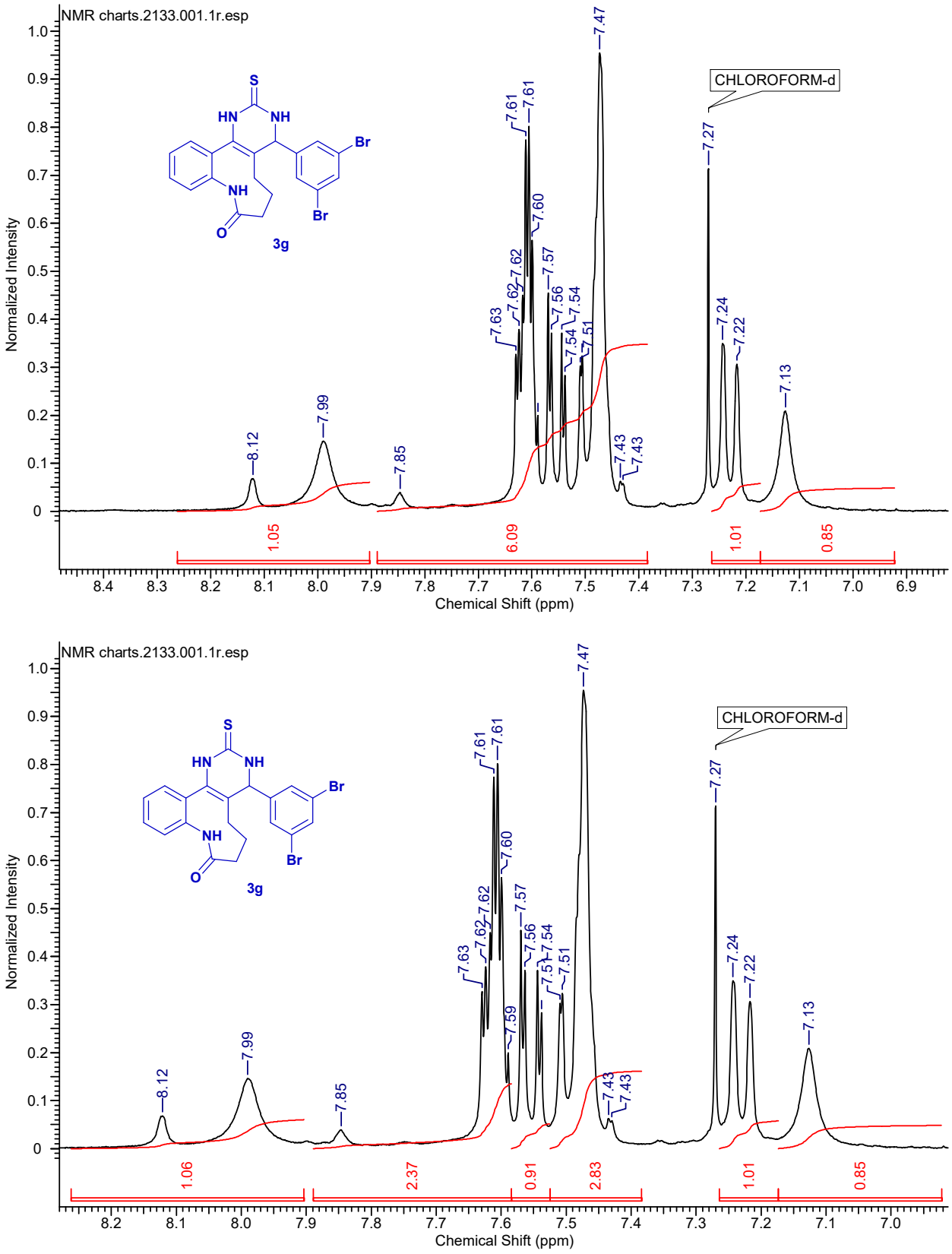


Fig. S32. ^{1}H-NMR spectrum of compound **3g**.

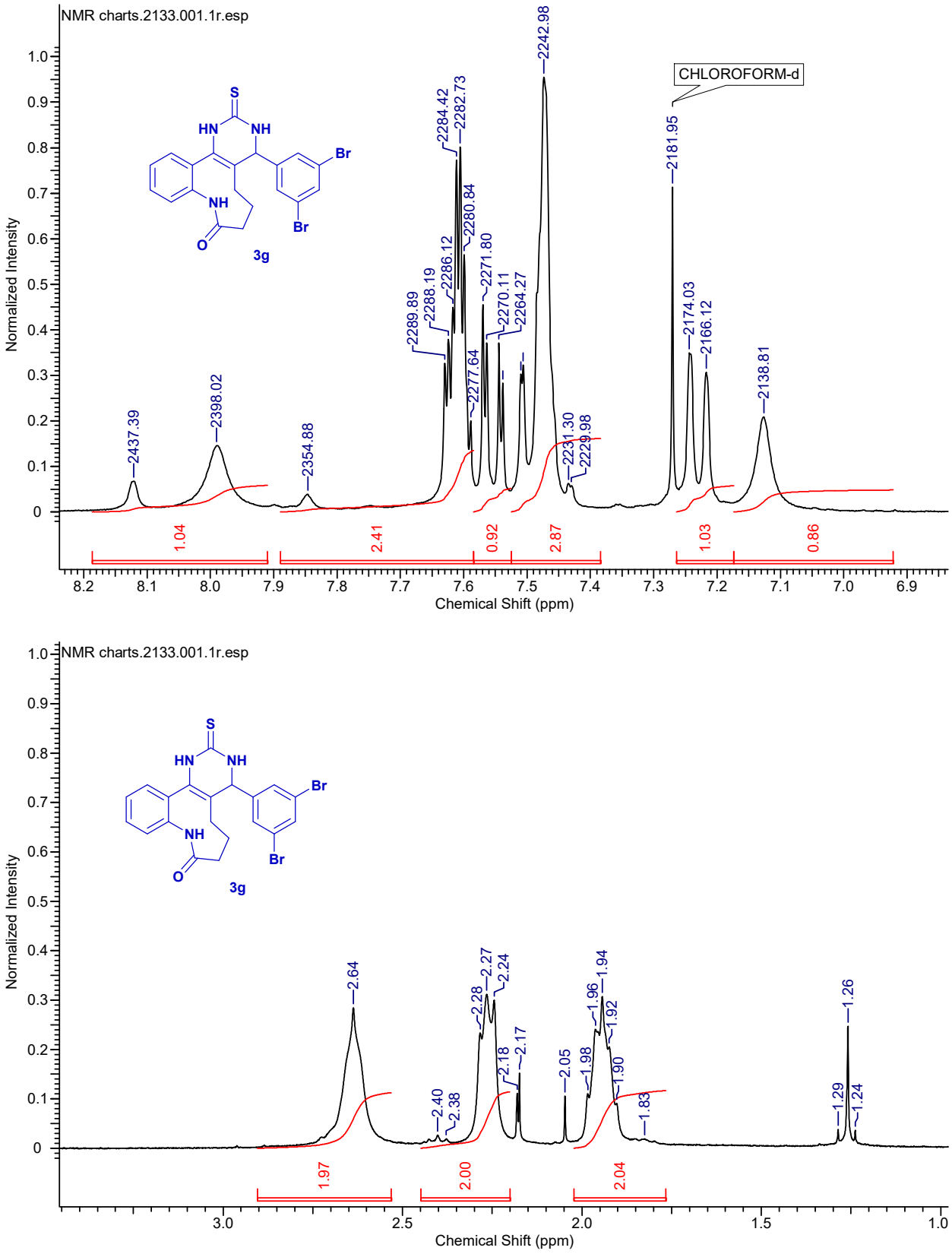


Fig. S32. ^{1}H-NMR spectrum of compound **3g**.

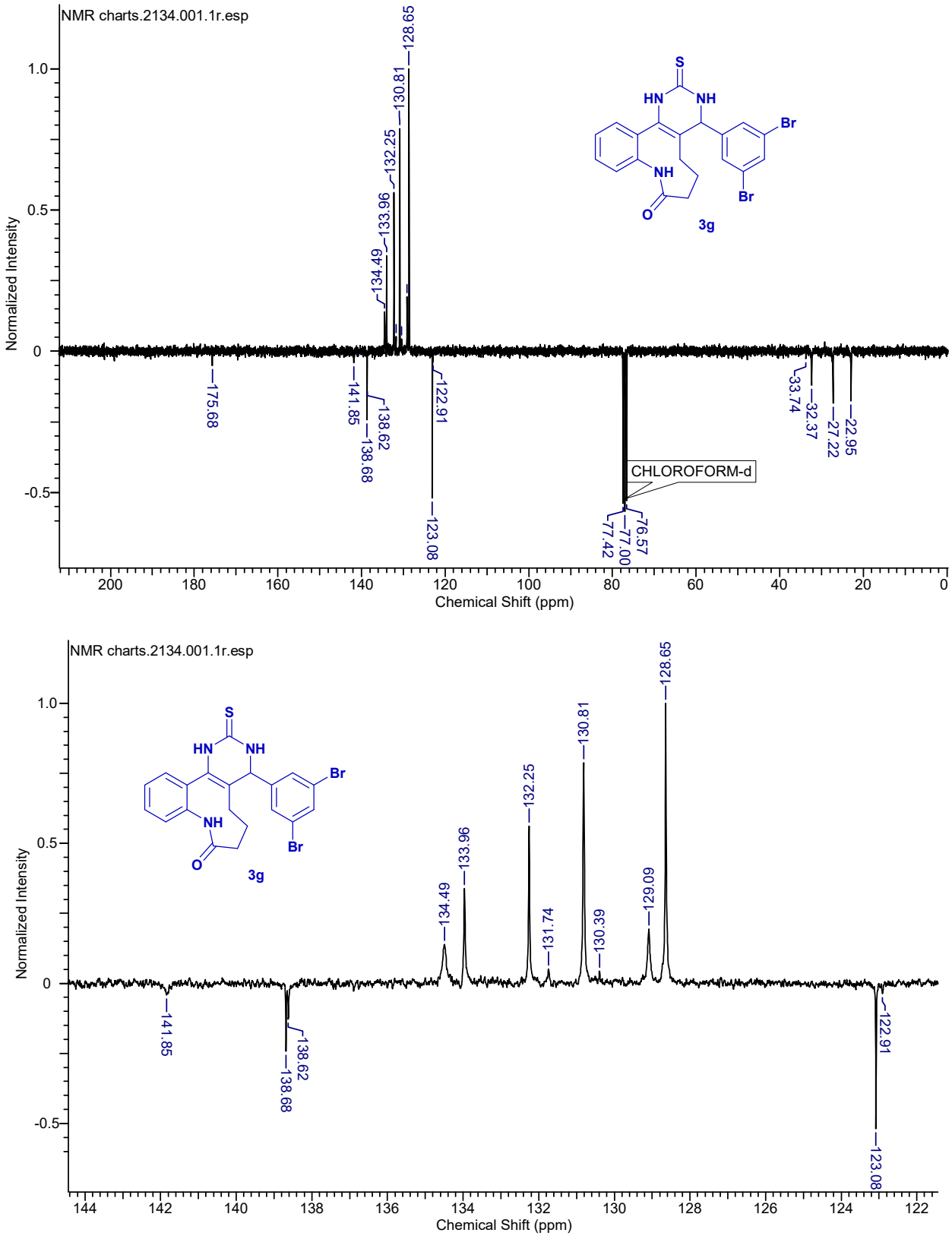


Fig. S33. ^{13}C-NMR spectrum of compound **3g**.

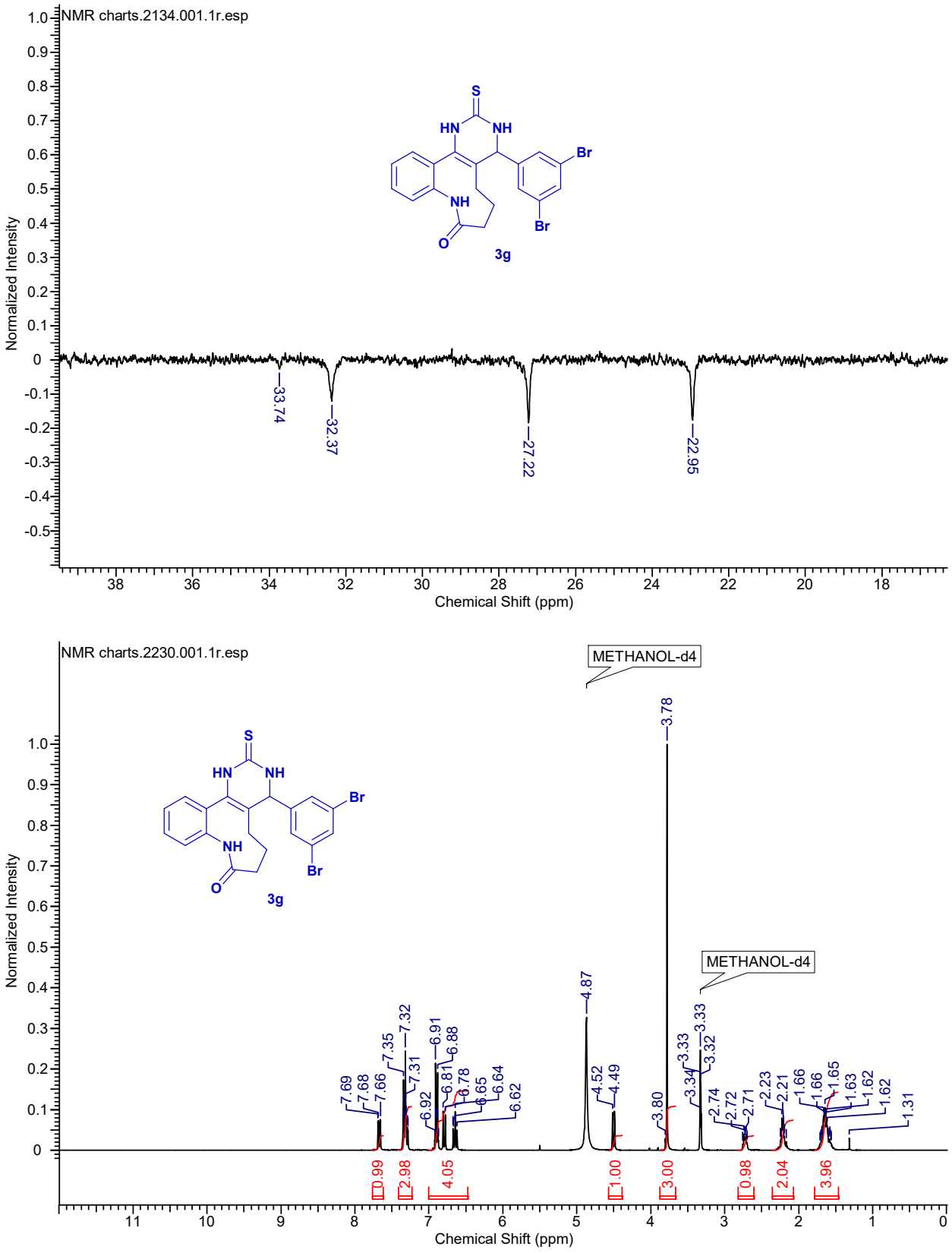


Fig. S33. ^{13}C-NMR spectrum of compound **3g**.

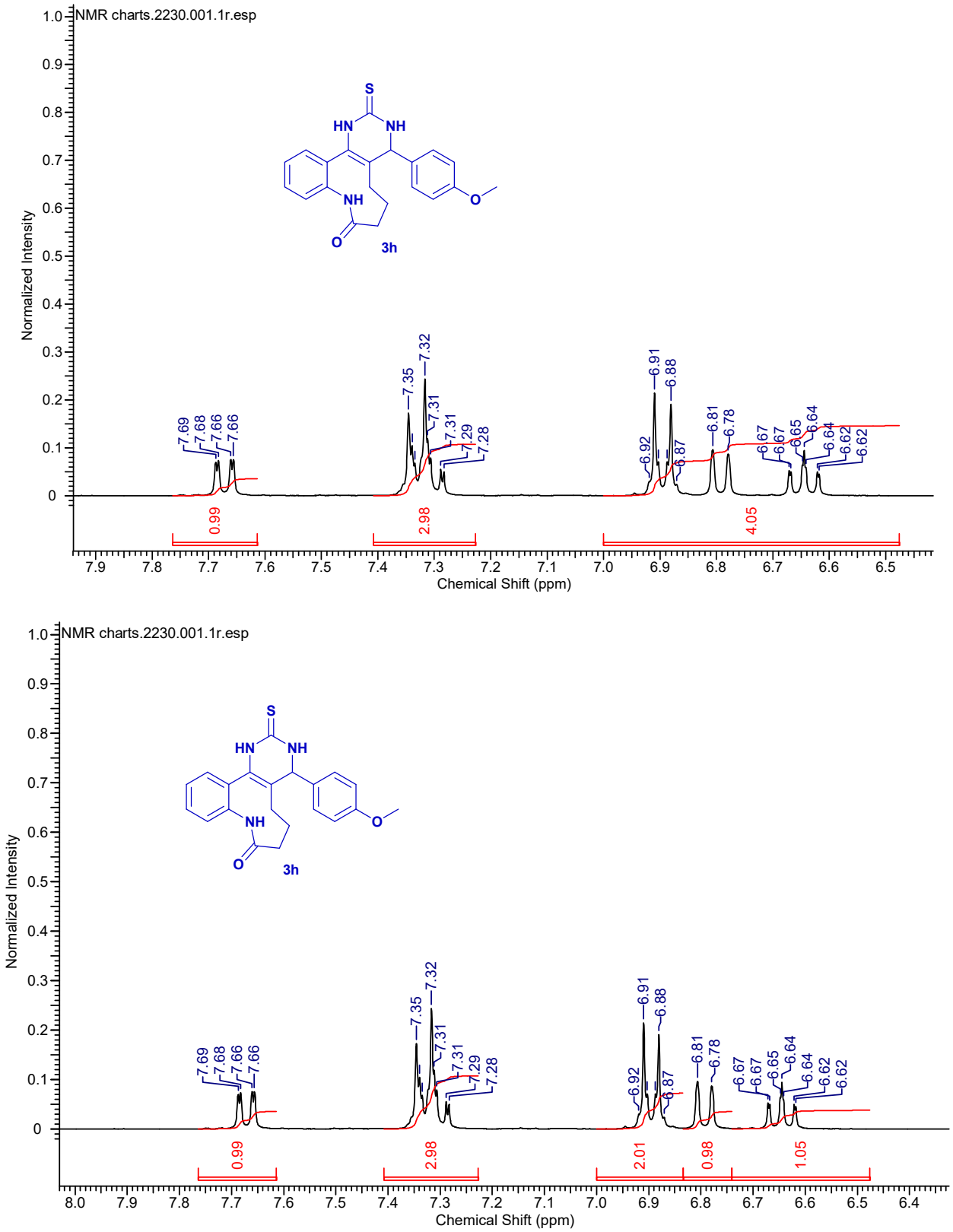


Fig. S34. ^{1}H-NMR spectrum of compound **3h**.

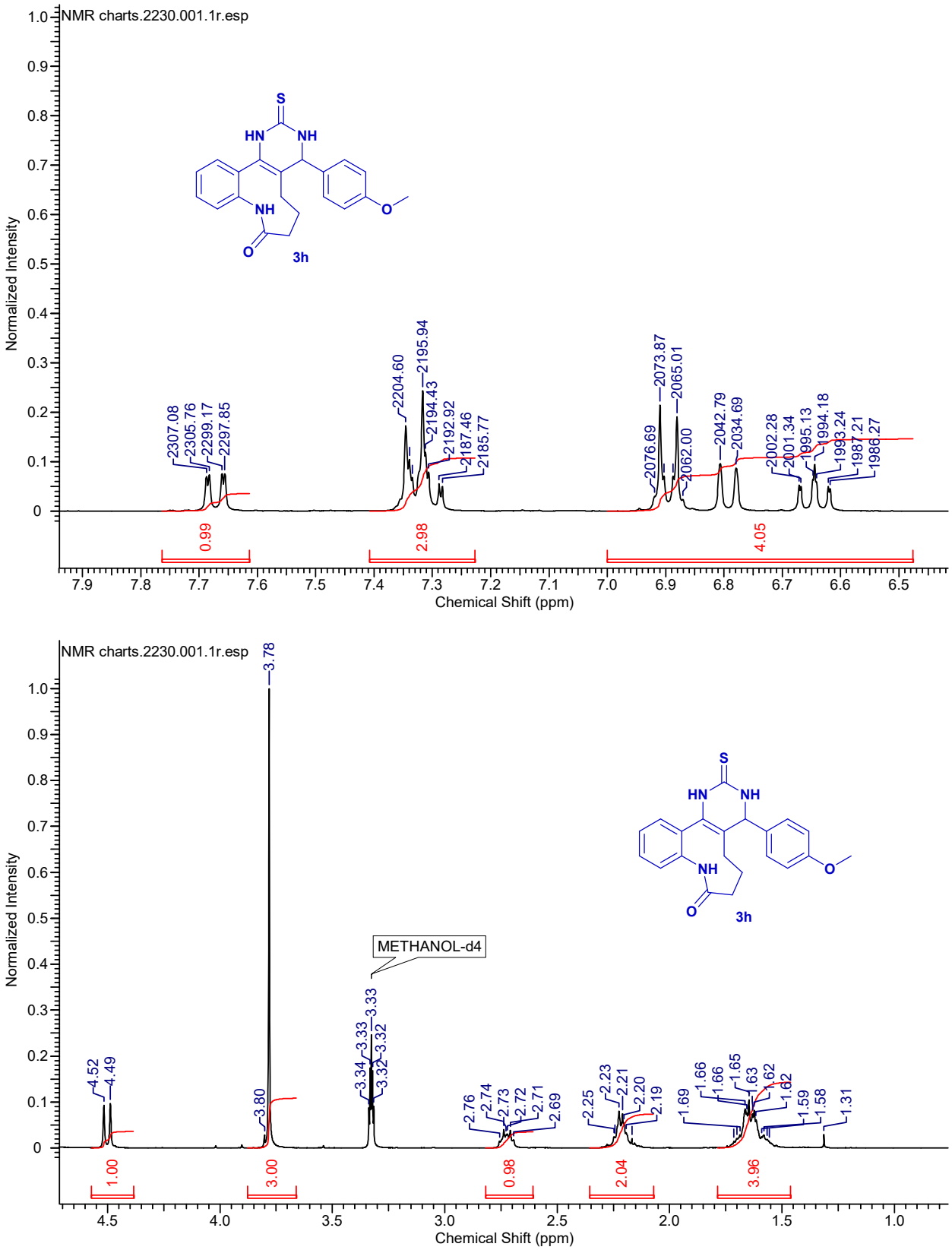


Fig. S34. ^{1}H-NMR spectrum of compound **3h**.

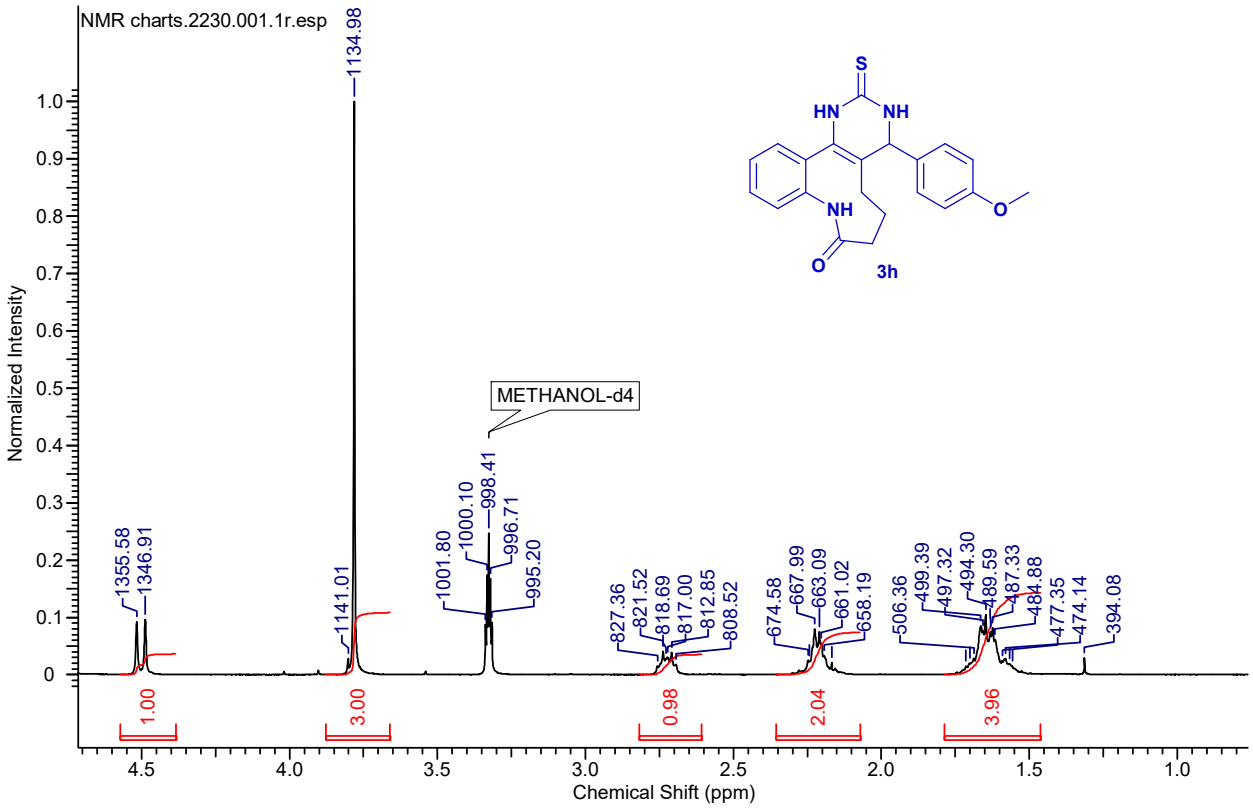


Fig. S34. [1]H-NMR spectrum of compound **3h**.

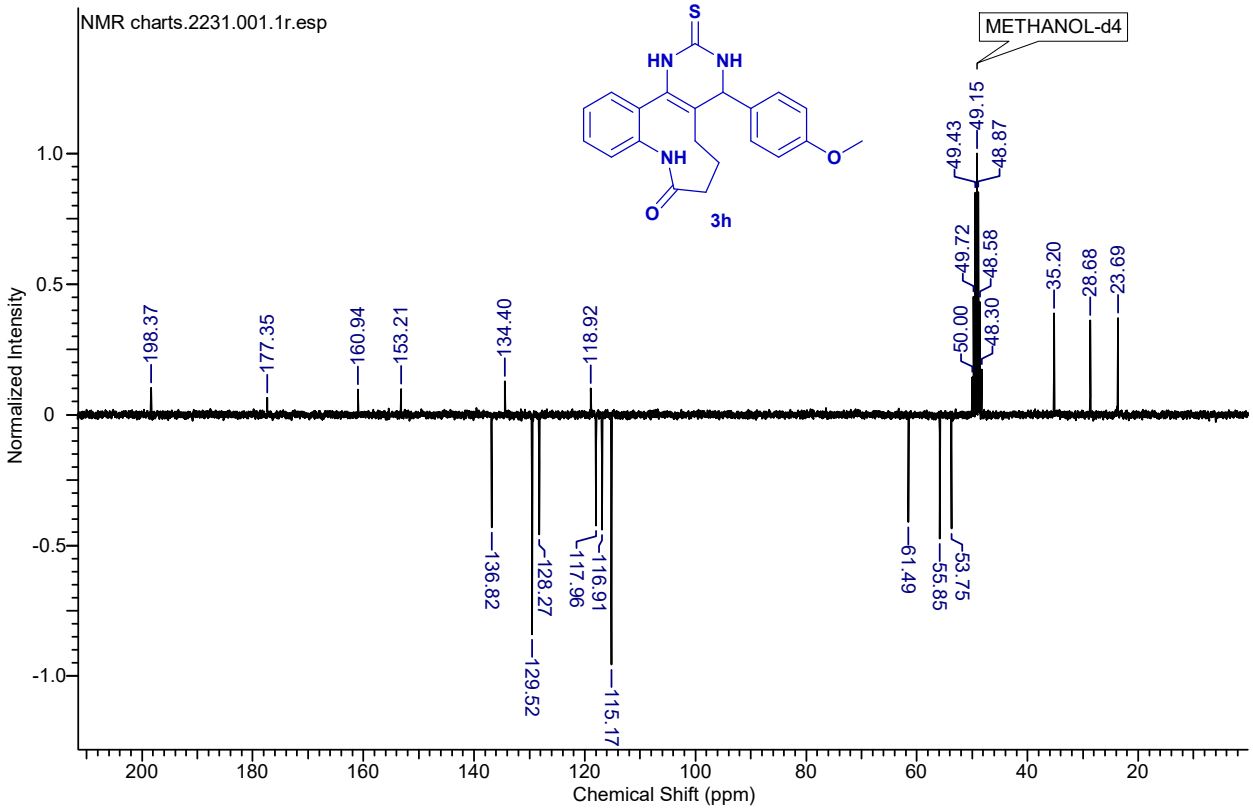


Fig. S35. [13]C-NMR spectrum of compound **3h**.

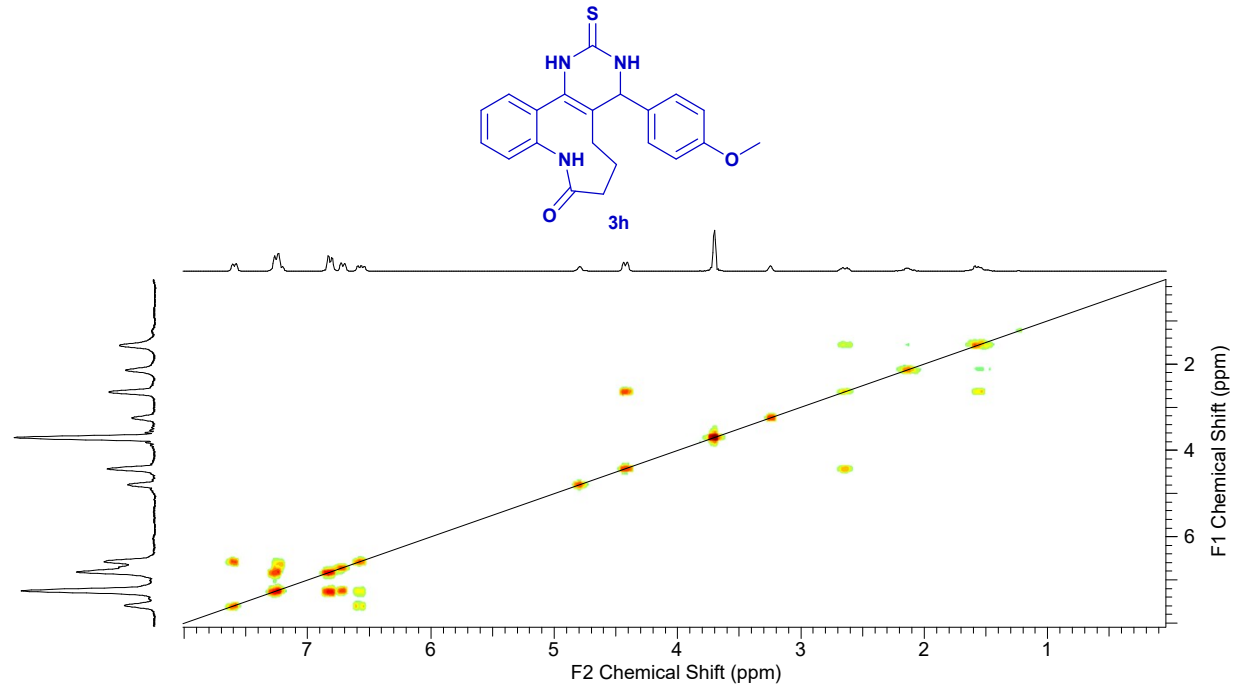


Fig. S36. 2D NMR spectrum (**COSY**) of compound **3h**.

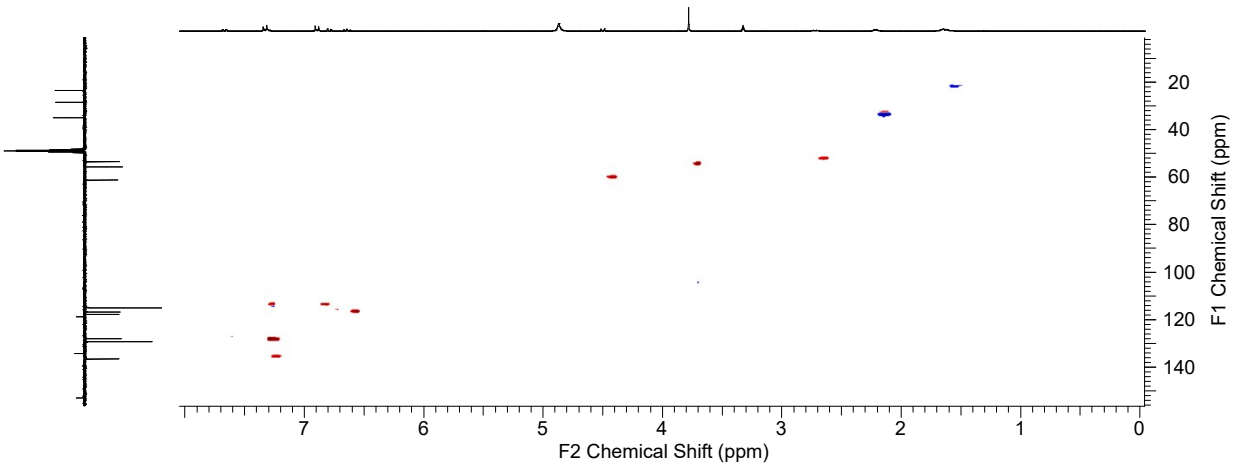


Fig. S37. 2D NMR spectrum (**HSQC**) of compound **3h**.

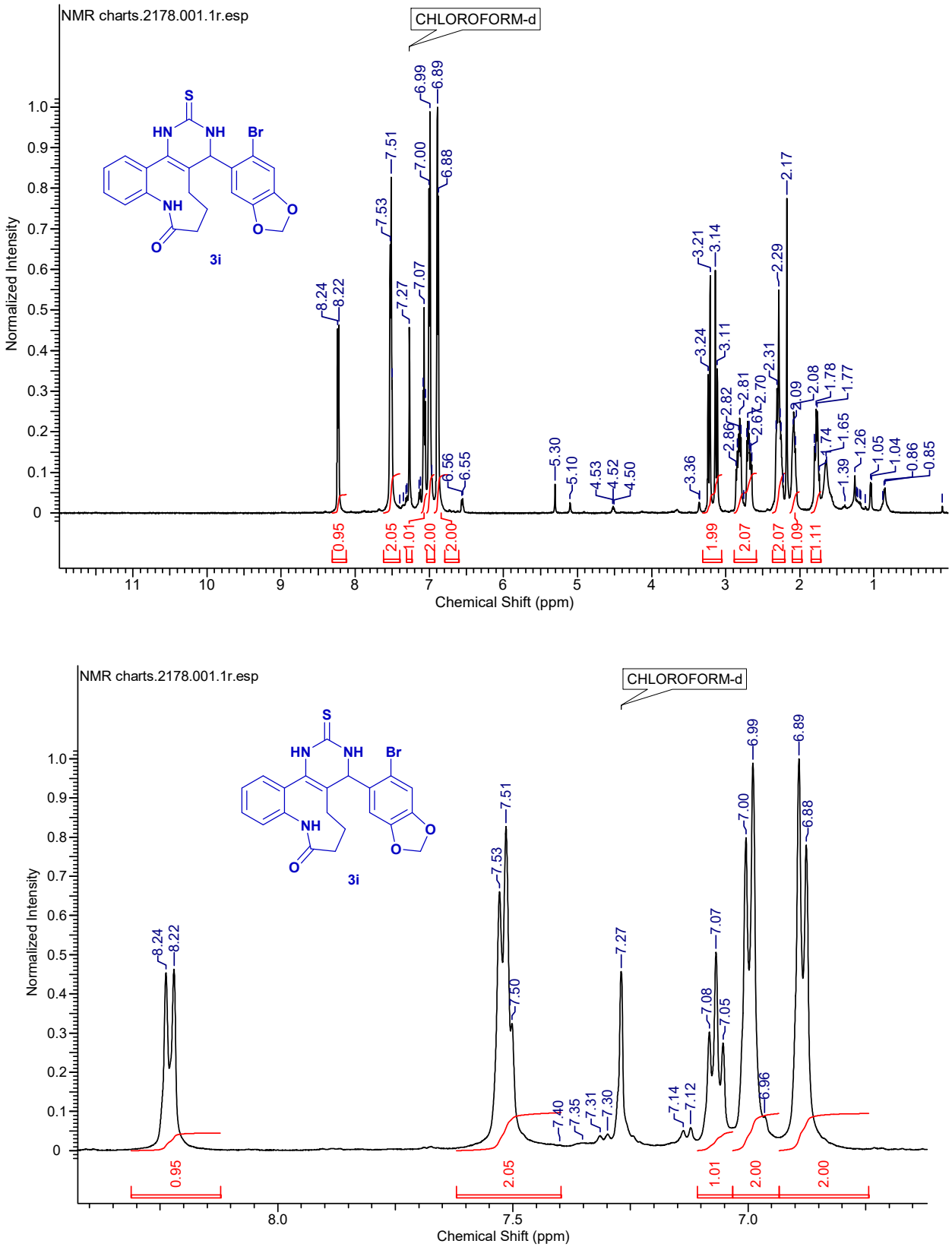


Fig. S38. ^{1}H-NMR spectrum of compound **3i**.

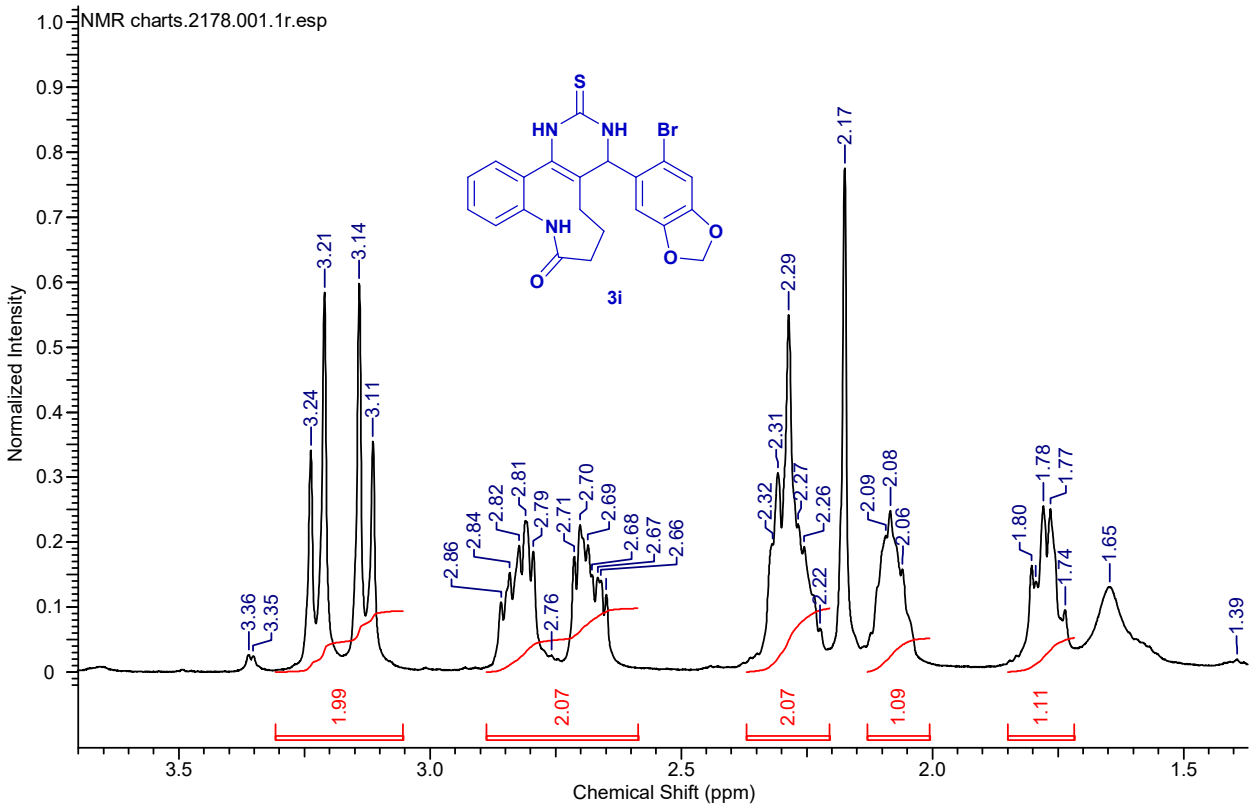


Fig. S38. [1]H-NMR spectrum of compound **3i**.

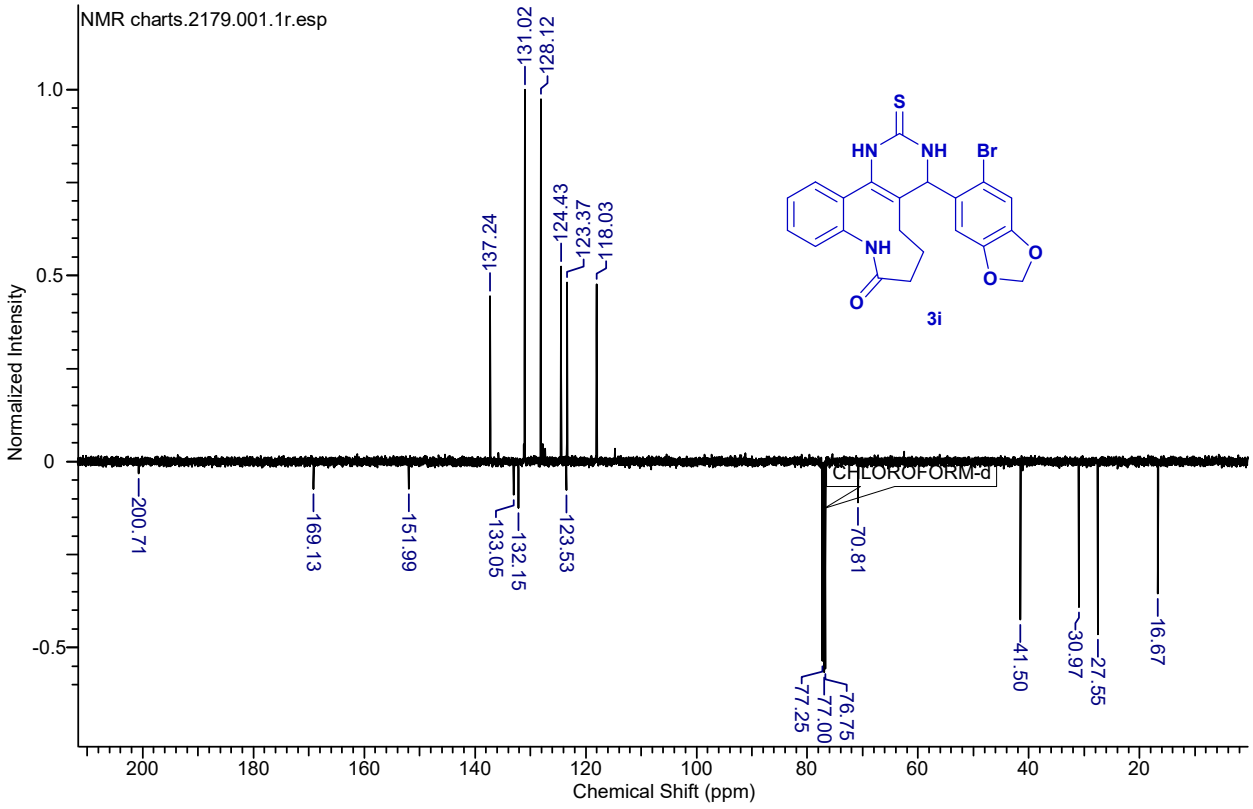


Fig. S39. [13]C-NMR spectrum of compound **3i**.

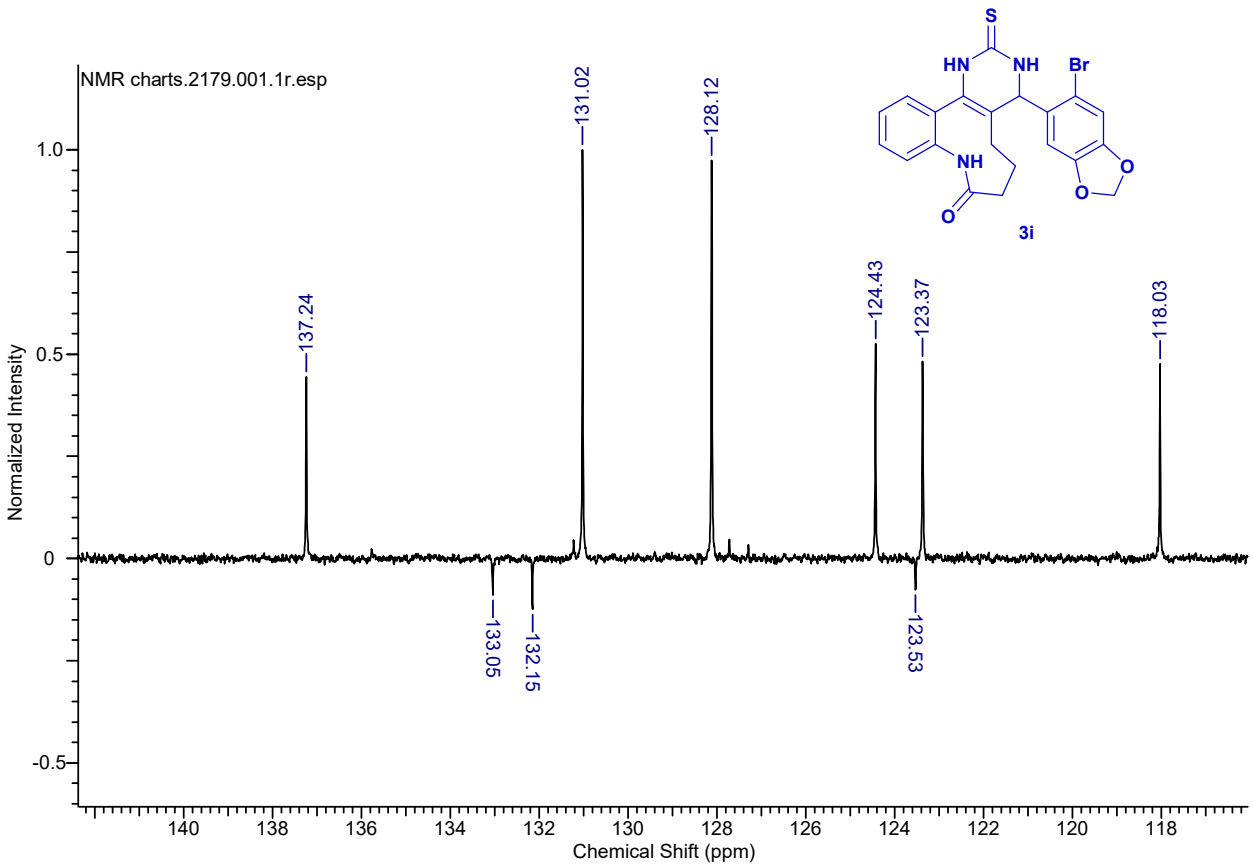


Fig. S39. ^{13}C-NMR spectrum of compound **3i**.

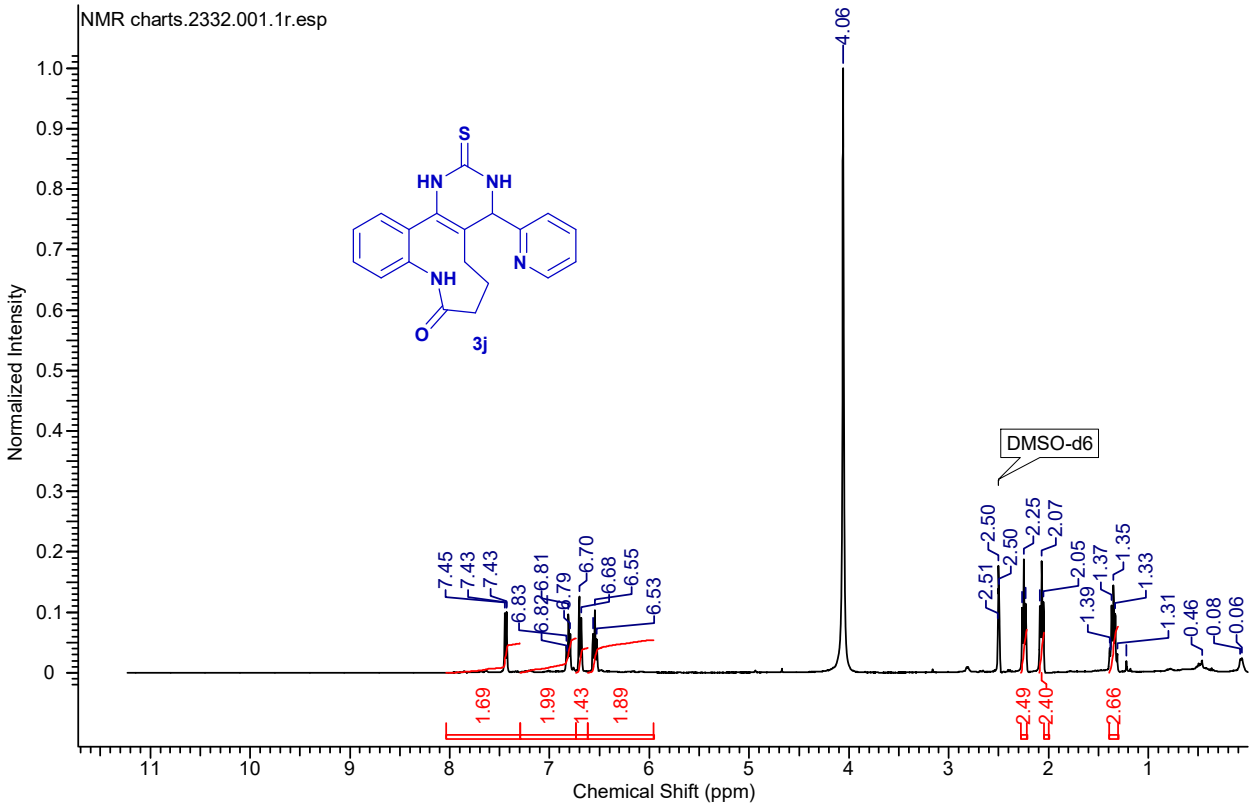
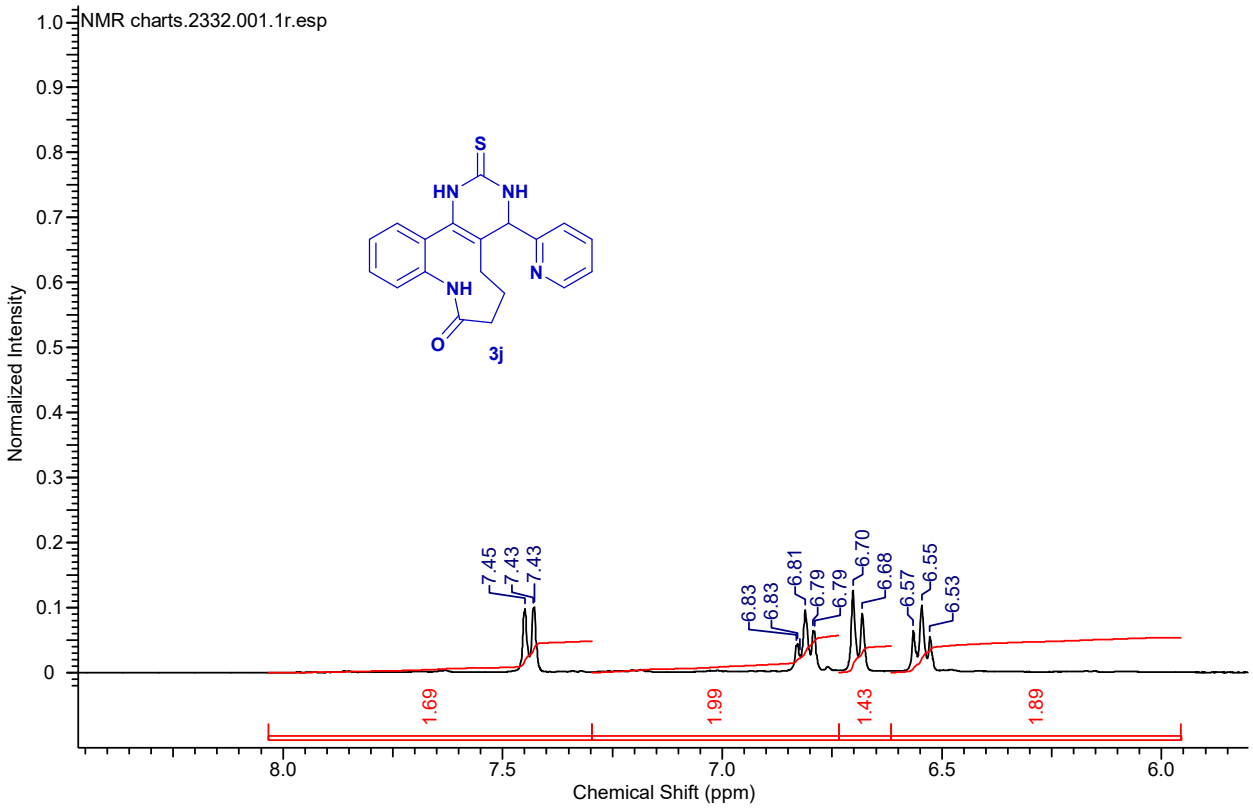


Fig. S40. ^{1}H-NMR spectrum of compound **3j**.



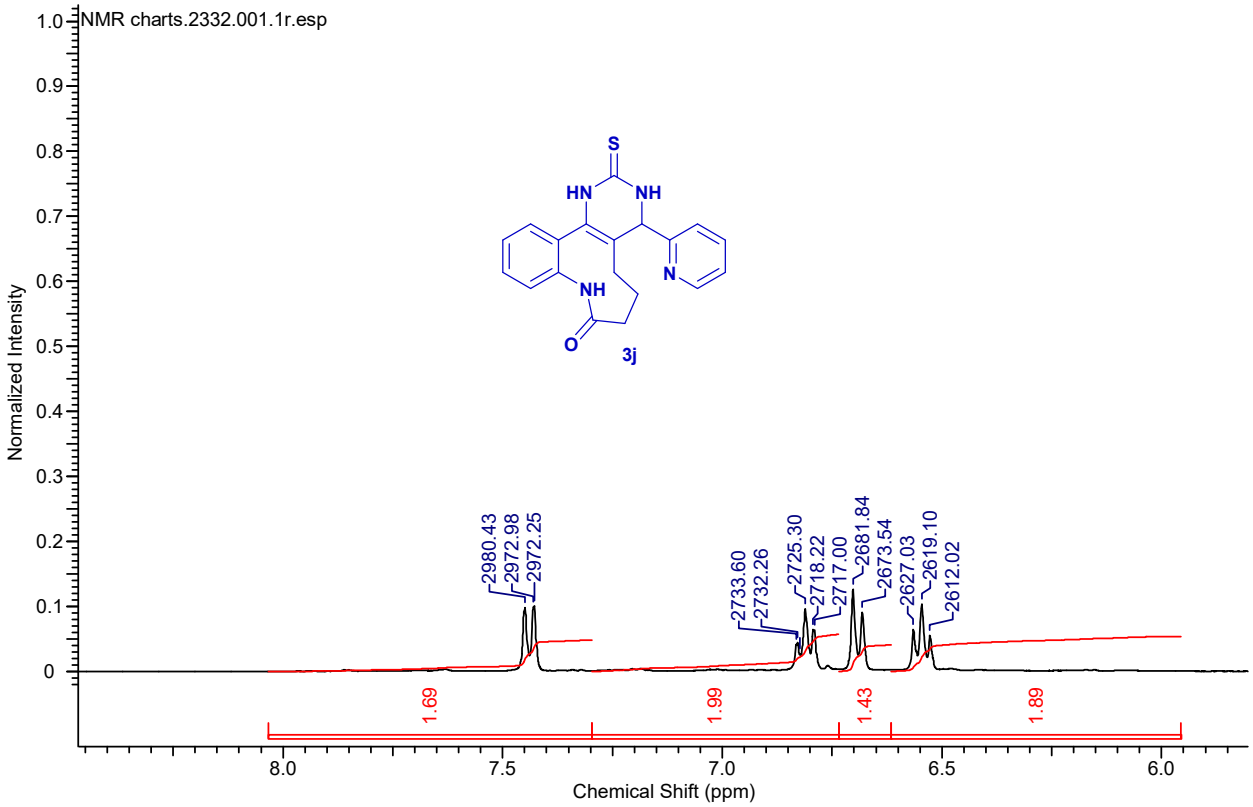


Fig. S40. [1]H-NMR spectrum of compound **3j**.

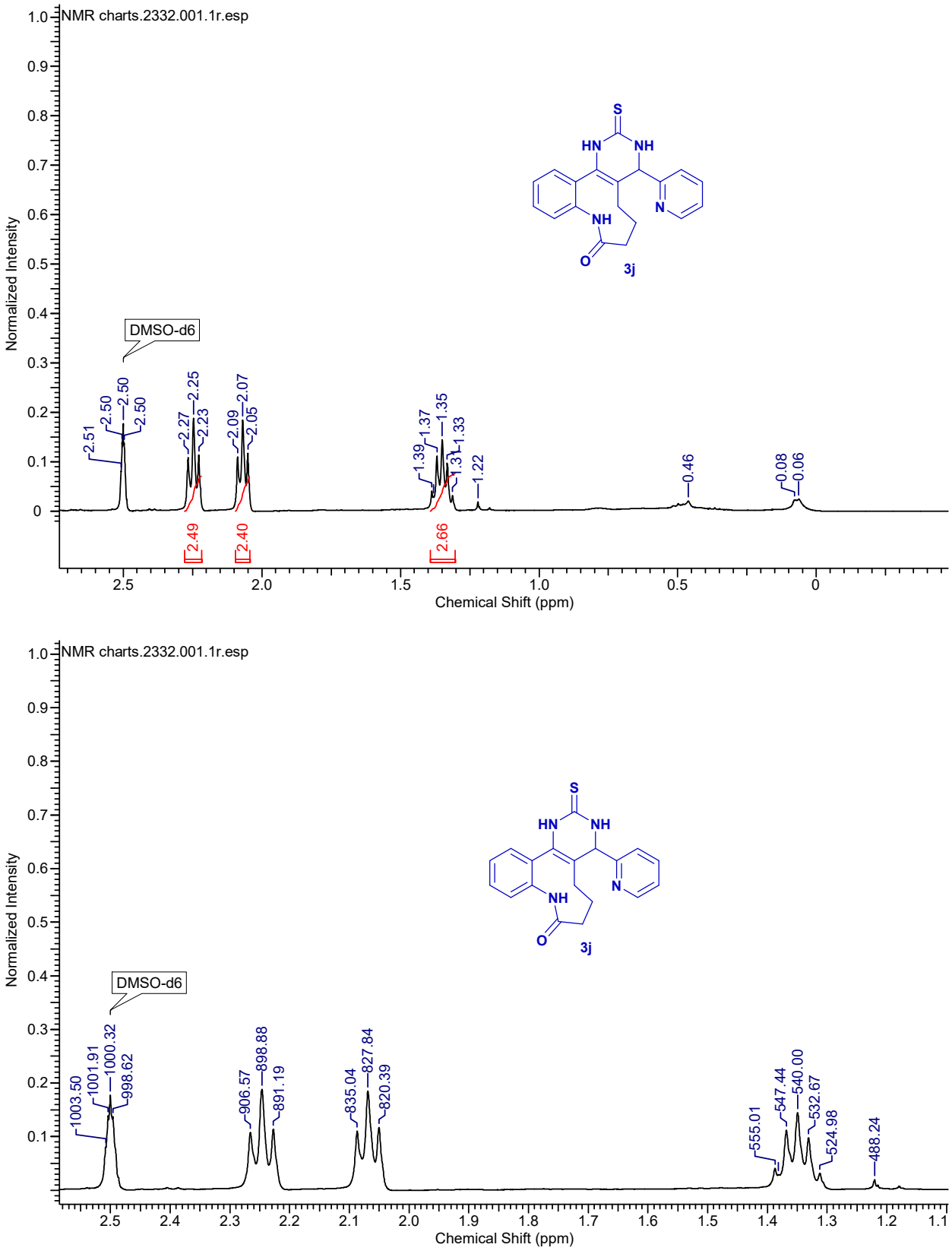


Fig. S40. ^{1}H-NMR spectrum of compound **3j**.

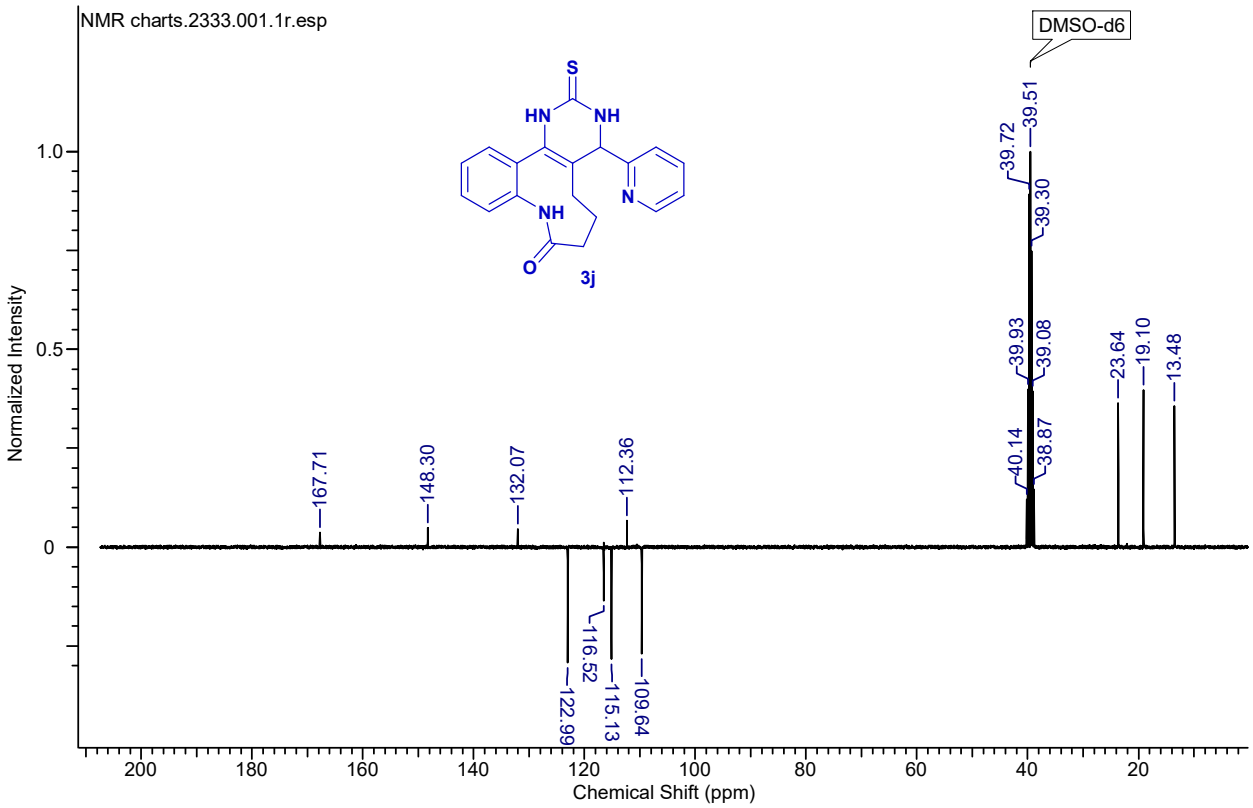


Fig. S41. ^{13}C-NMR spectrum of compound **3j**.

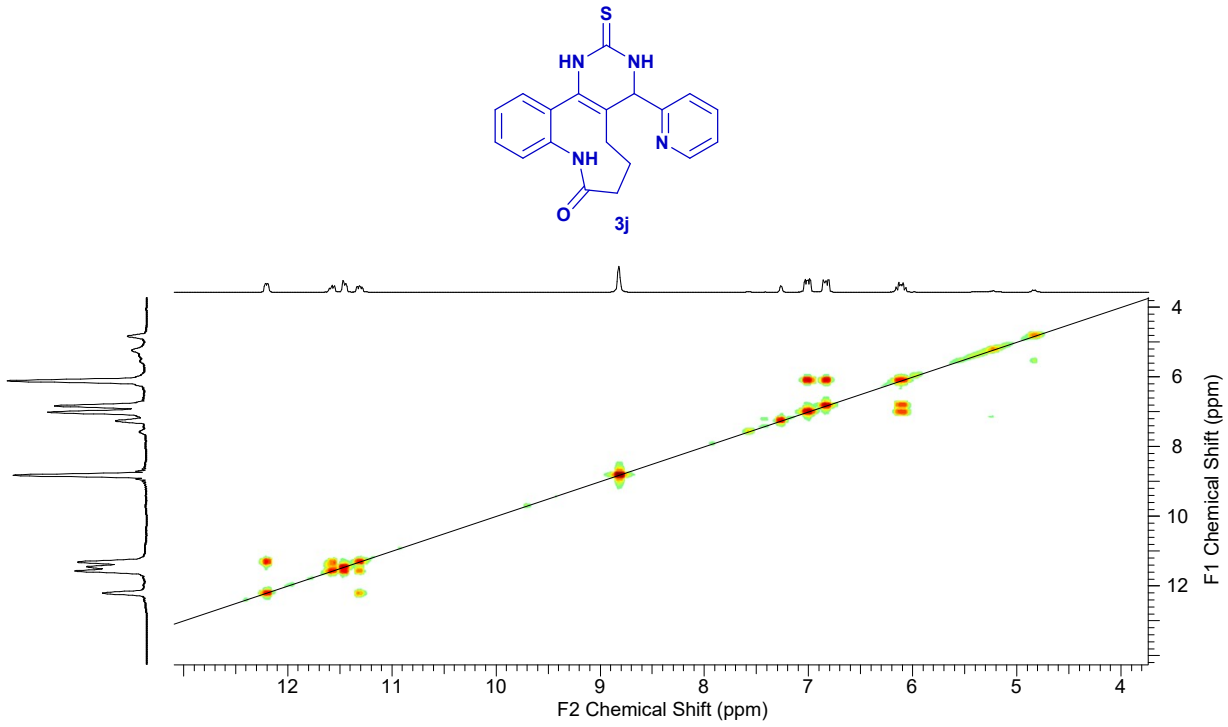


Fig. S42. 2D-NMR spectrum (**COSY**) of compound **3j**.

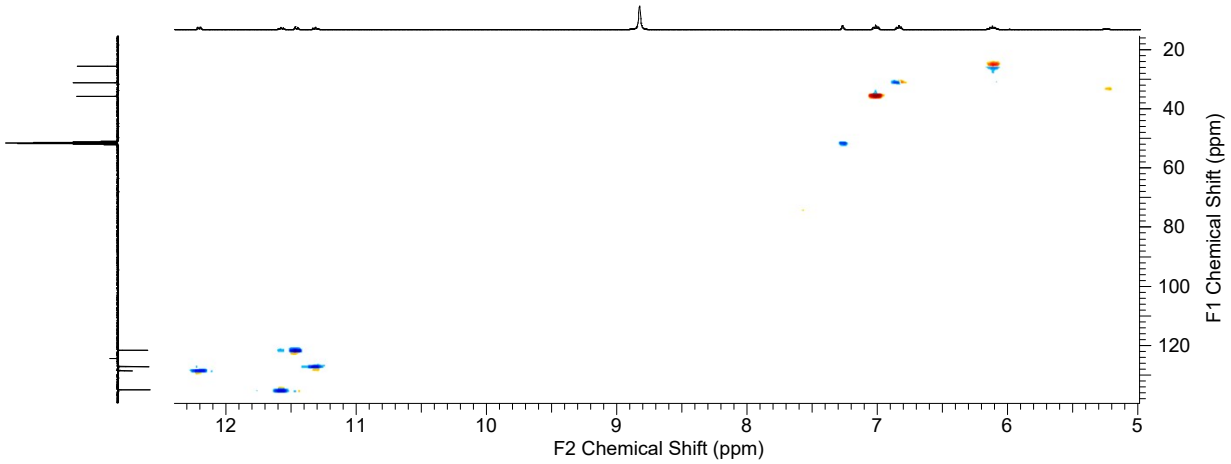


Fig. S43. 2D-NMR spectrum (**HSQC**) of compound **3j**.

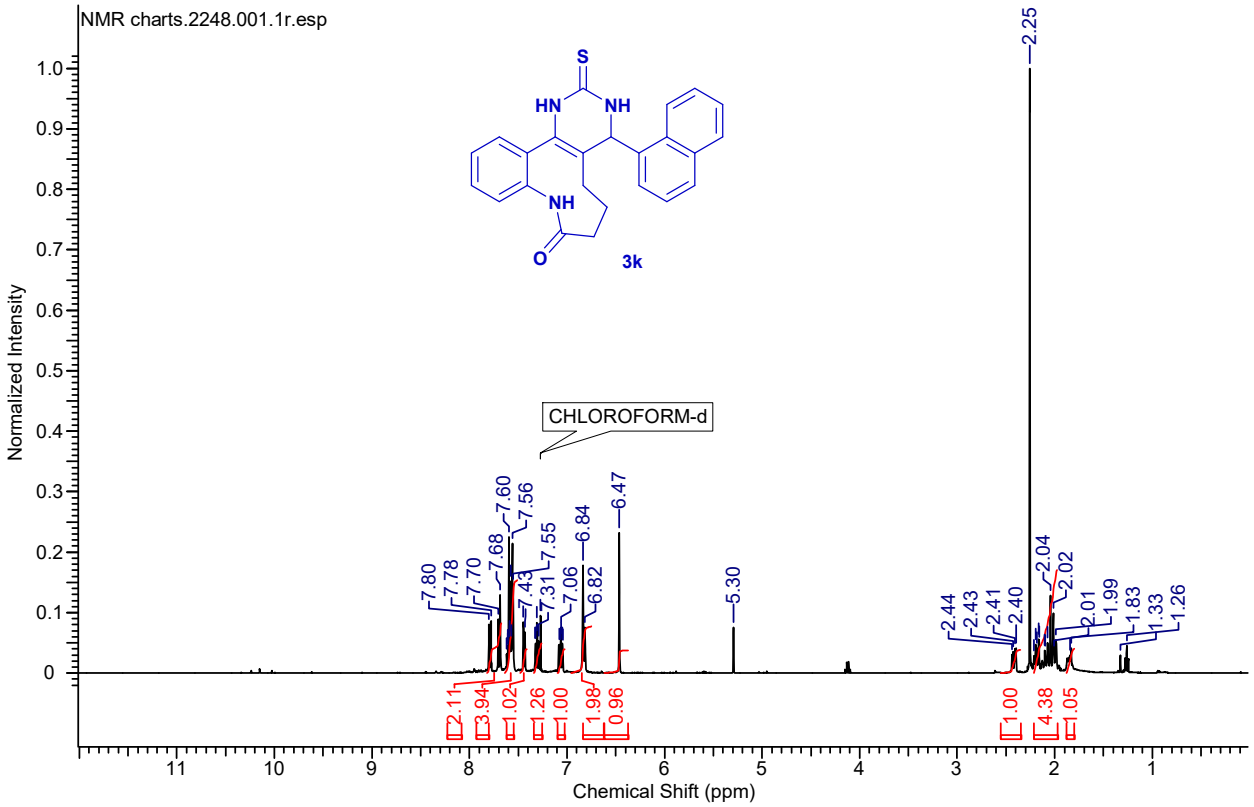


Fig. S44. ^{1}H-NMR spectrum of compound **3k**.

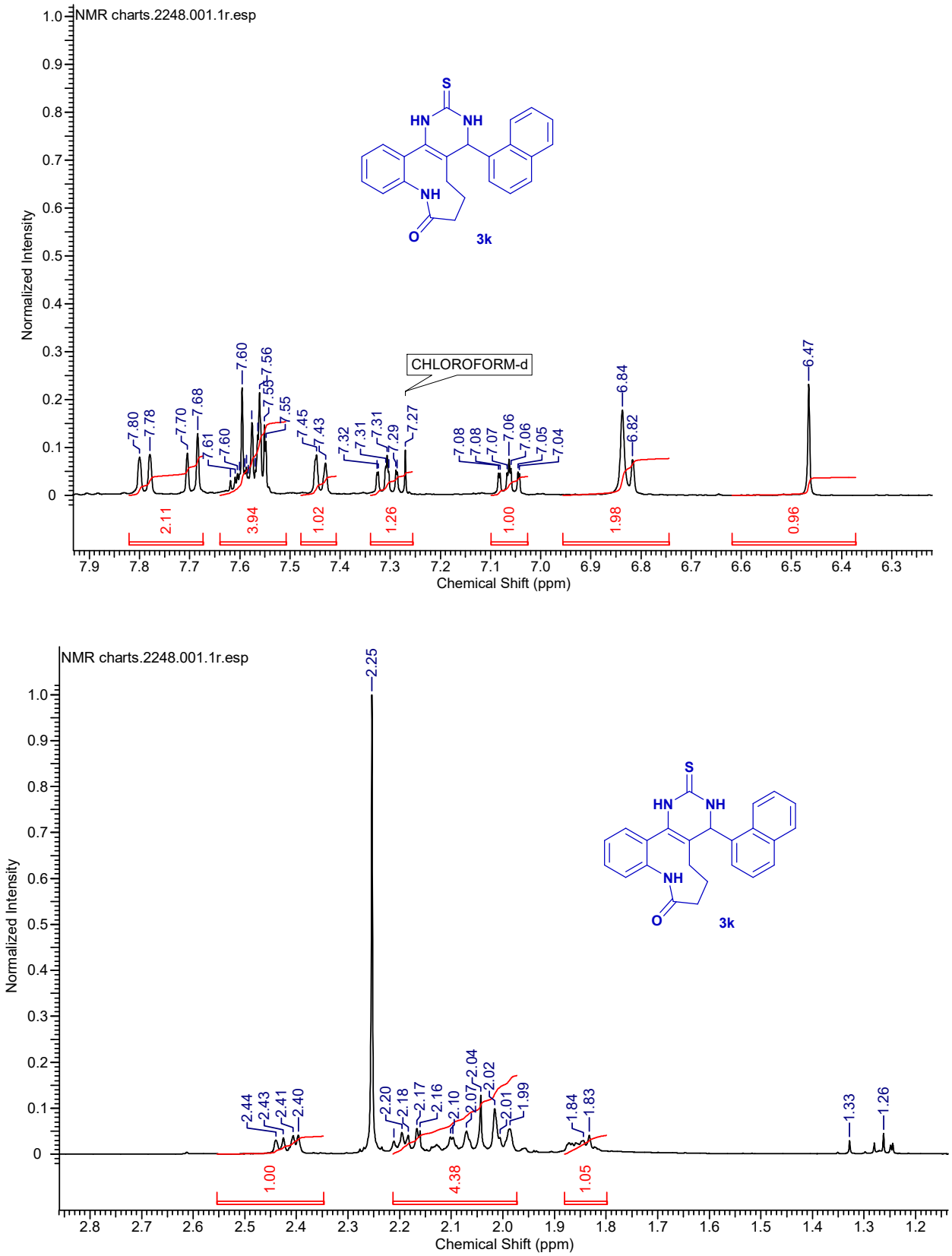


Fig. S44. ^{1}H-NMR spectrum of compound **3k**.

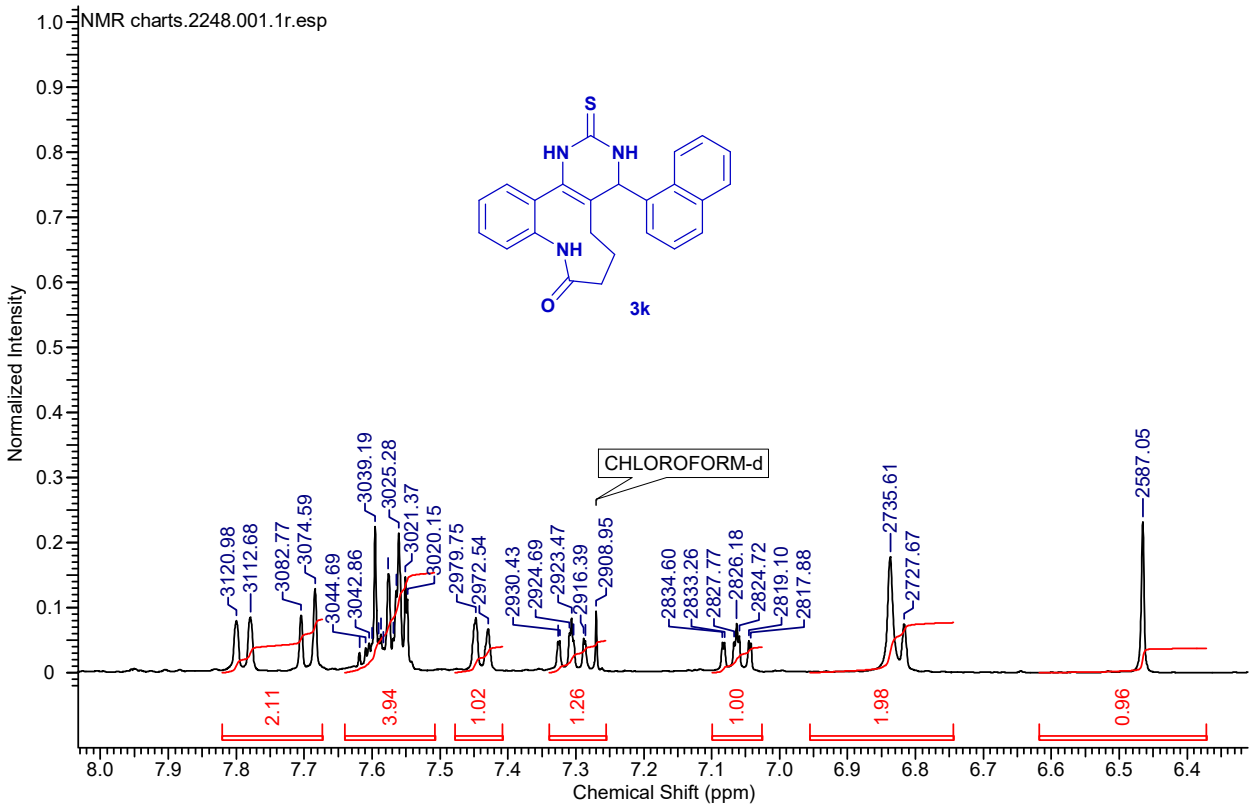


Fig. S44. [1]H-NMR spectrum of compound **3k**.

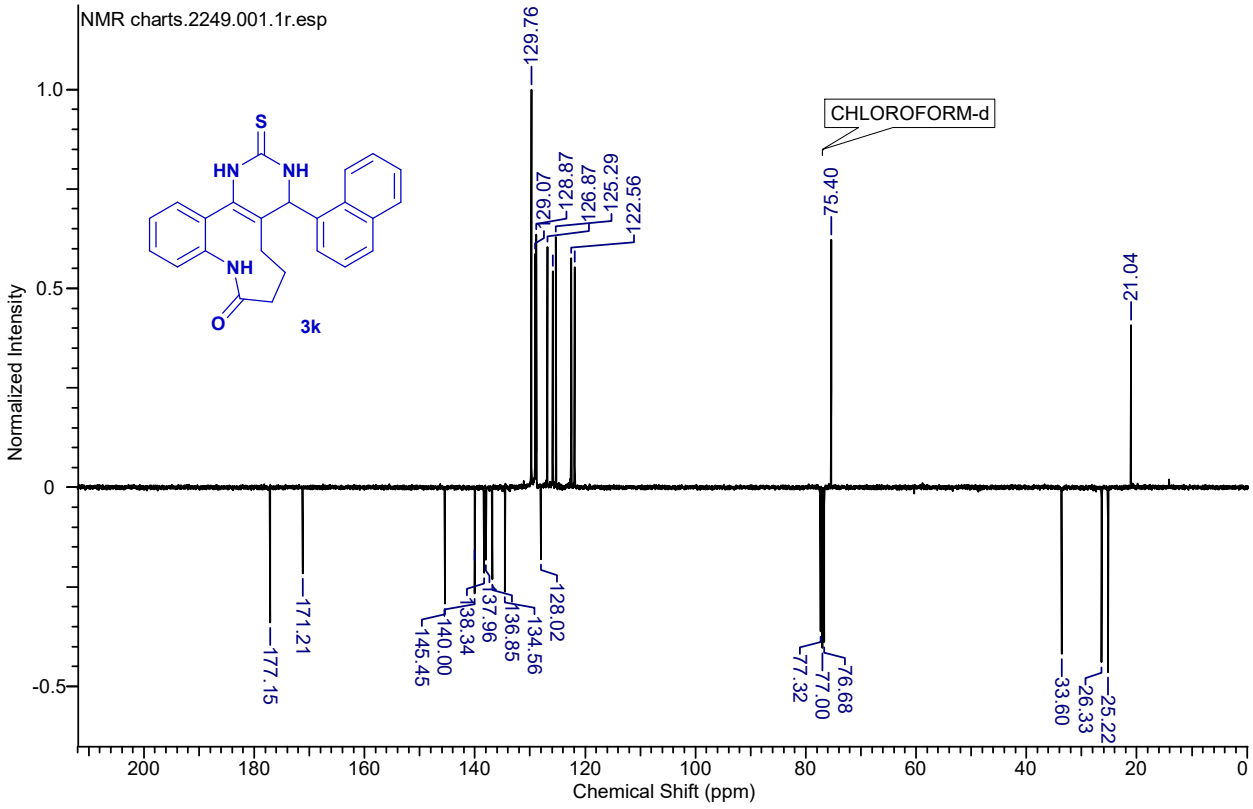


Fig. S45. [13]C-NMR spectrum of compound **3k**.

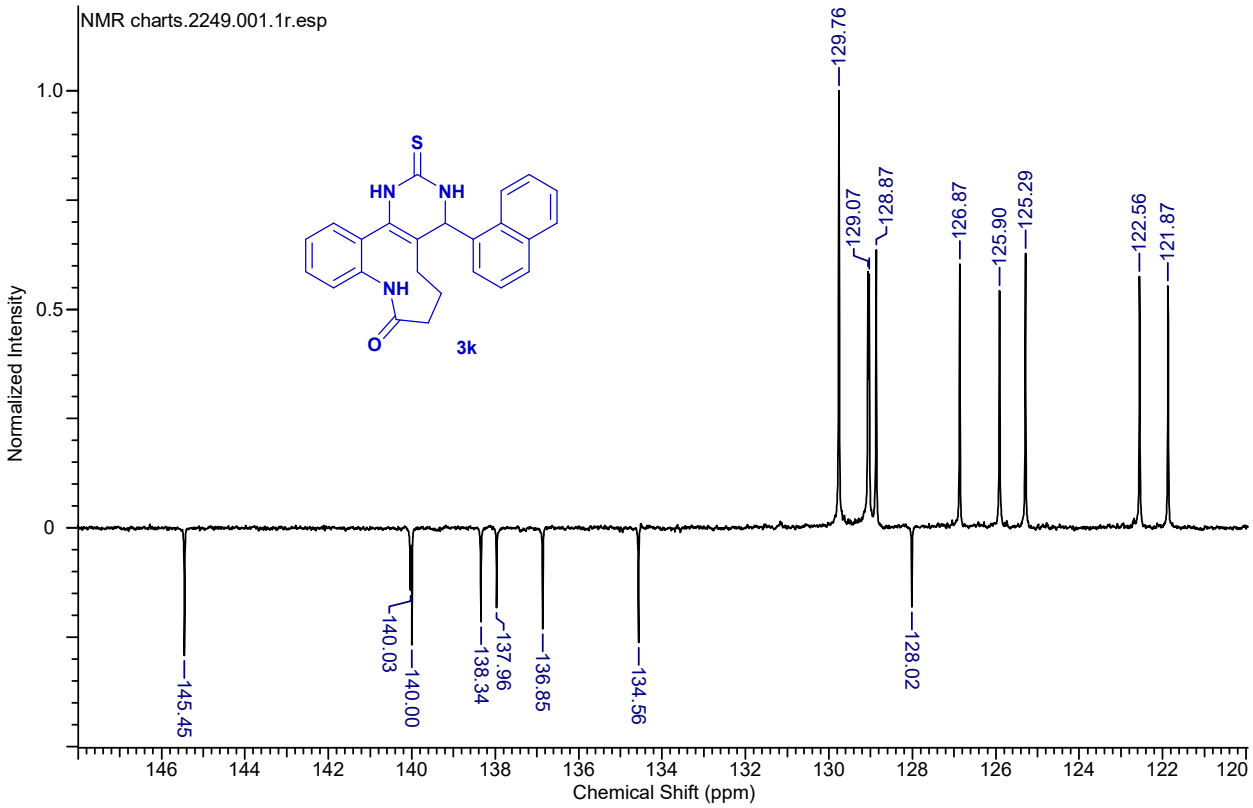


Fig. S45. ^{13}C-NMR spectrum of compound **3k**.