Supporting Information

Cu(II)-catalyzed Friedel-Crafts reaction of 2-thiopyrimidine derivatives with aldehydes utilizing water as cocatalyst in the presence of surfactant: elucidation the role of water on reaction mechanism and tautomerism

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1. Experimental procedure

1.1. Materials and methods:

All the reagents were purchased from Sigma-Aldrich, TCI and Avra chemicals were used without further purification. All the reaction was performed in a round-bottom flask and monitored by Thin-layer chromatography (TLC, Merck silica gel 60 F_{254}). The FT-IR spectra were taken from Shimadzu Iraffinity-1s FT-IR spectrophotometer. The product was characterized by ^{1}H and ^{13}C-NMR spectra and it was recorded on Bruker 400/500MHz spectrometers at room temperature using DMSO-d_6 as a solvent having tetramethylsilane (TMS) as an internal standard. Data reported as s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, dt = doublet of triplets; coupling constant in Hz: integration. High-resolution mass spectroscopy (HRMS) of compounds was examined on an XEVO G2-XS QTOF mass spectrometer. The UV-visible spectra were obtained using a Shimadzu UV-1780 Spectrophotometer.

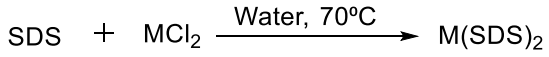
1.2. General procedure for the compound 3a-t:

4-Amino-6-hydroxy-2-mercatopyrimidine hydrate (**1**, 0.25 mmol, 35.7 mg) and 4-chlorobenzaldehyde (**2a**, 0.125 mmol, 17.6 mg) were added to the solution of $CuCl_2.2H_2O$(10 mol%) and SDS (20 mol%) in 2mL water and the resulted solution was stirred at room temperature. After 5h, product formation occurs (confirmed by TLC) and is allowed to stir for 24h.

Separation procedure A: The crude precipitate was separated by centrifugation at 10,000 rpm for 10 min with five consecutive cycle. In each cycle, residue was washed with mixture of hot water and ethanol. The final residue was dried in vacuum oven at 60ºC for overnight and isolated yield was determined.

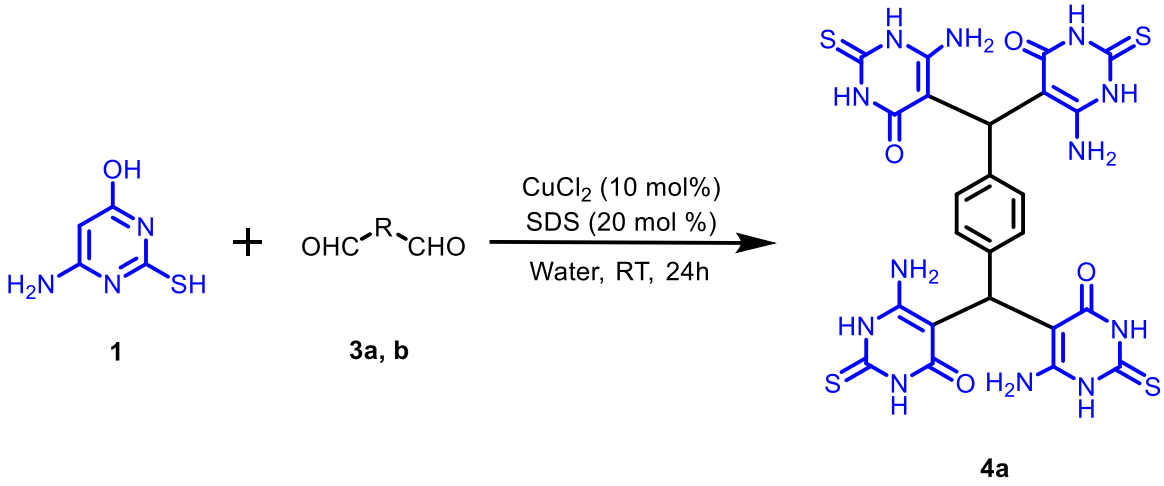
Separation procedure B: The obtained precipitate was filtered off, and the residue was washed with warm water (5 × 5 mL) and ethanol (1 × 5 mL). The final product was further purified through recrystallization in warm ethanol, and the crude residue was dried in vacuum oven at 60ºC for overnight.

1.3. General procedure for the preparation of Lewis acid surfactant combined catalyst (LASC):



The combined catalyst was prepared using the reported method.[1] Sodium dodecyl sulfate (SDS) (2 mmol) was dissolved in 10 mL distilled water and respective metal salt MCl_2 (1 mmol) (M = Cu, Sn) was added dropwise in it. Then, the reaction mixture was set up in an oil bath at 70ºC and stirred for 24 hours. The reaction mixture was cooled at room temperature, and the obtained precipitate was filtered out and dried in a vacuum oven.

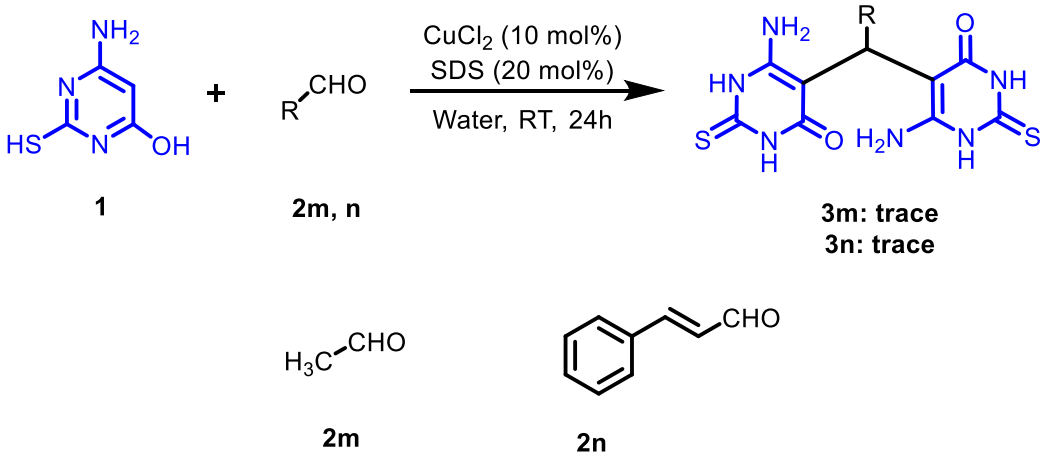
1.4. Reaction of 4-amino-6-hydroxy-2-mercatopyrimidine with di-aldehydes[a]:



Sl. No.	R	Yield (%)
1	1,4-dialdehyde (**3a**)	64
2	1,3-dialdehyde (**3b**)	n.r

[a]Reaction condition: **1** (0.25 mmol), **3** (0.125 mmol), and water (2 mL); n.r.; No reaction.

1.5. Unsuccessful aldehydes for the synthesis of bis-(2-thiopyrimidine) derivatives[a]:



[a]Reaction condition: **1** (0.25 mmol), **2** (0.125 mmol) and water (2 mL).

1.6. General procedure for gram-scale synthesis:

To the mixture of 4-Amino-6-hydroxy-2-mercatopyrimidine hydrate (**1**, 10 mmol, 1.43 g) and 4-chlorobenzaldehyde (**2a**, 5 mmol, 0.70 g), 50mL of water was added. Then the mixture of $CuCl_2.2H_2O$(10 mol%) and SDS (20 mol%) were added in it. The resulting solution was stirred for 24 hours at room temperature. After completion of the reaction, the obtained product **3a** (73%) was isolated by centrifugation at 10,000 rpm for 10 min. The obtained filtrate was further used in a reusability test.

1.7. General procedure for reusability:

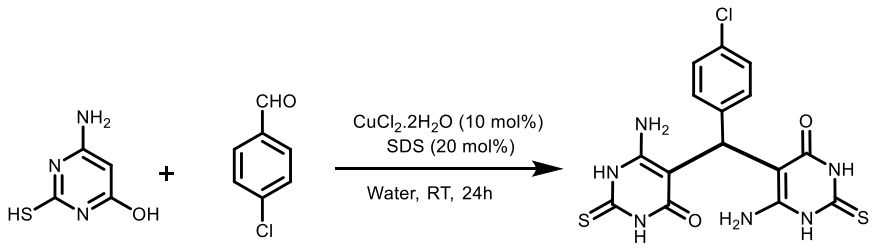
A reusability test was conducted using the filtrate that was collected in a gram-scale synthesis. At first cycle, 10 mL of filtrate was used to the mixture of 4-Amino-6-hydroxy-2-mercatopyrimidine hydrate (1, 1 mmol,) and 4-chlorobenzaldehyde (2a, 0.5 mmol). After 24 hours, and the obtained product **3a** (74%) was isolated by centrifugation and 98% of the filtrate was recovered. At the second cycle, 9 mL of filtrate was used for 1 mmol scale of the substrate and after completion of the reaction 71% of product **3a** was collected by centrifugation.

2. Analysis of green chemistry metrics:

The following equation have been used for the calculation of environmental factor (E-factor).

$$E\ factor = \frac{\text{Total mass of waste}}{\text{Mass of product}} = \frac{[\text{Mass of raw materials} - \text{mass of product}]}{\text{Mass of product}}$$

The following reaction was used for the calculation of E-factor



	1	2a	3a
M.W	143.02	140.00	408.02
	0.25 mmol	0.125 mmol	0.092 mmol
	35.75	17.57	37.56

Table S1. E-factor for the bis-(2-thiopyrimidne) derivatives.

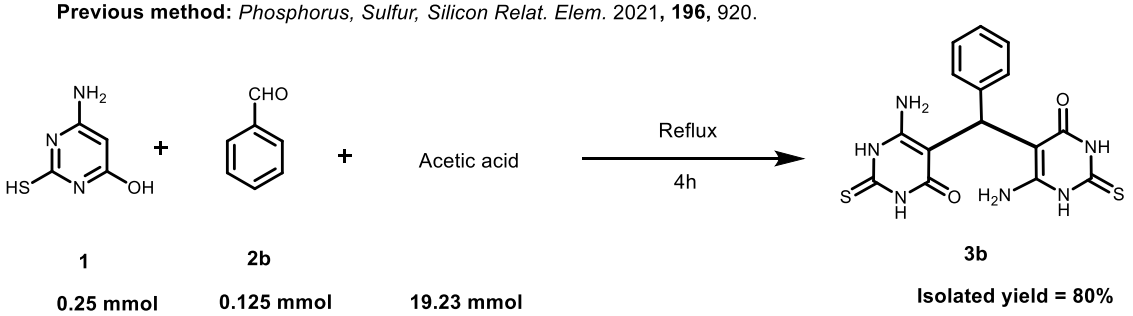
Product	Yield (%)	E-factor[a]	E-factor[b]
3a	74	0.41	0.85
3b	75	0.52	0.98
3c	74	0.47	0.92
3d	68	0.61	1.1
3e	71	0.55	1.03
3f	71	0.48	0.94
3g	73	0.43	0.88
3h	71	0.34	0.78
3i	73	0.54	1.01
3j	72	0.59	1.04
3k	73	0.61	1.1
3l	67	0.63	1.13

3o	58	1.07	1.72
3p	67	0.58	0.93
3q	72	0.31	0.71
3r	76	0.49	0.89
3s	78	0.31	0.71
3t	72	0.52	0.99

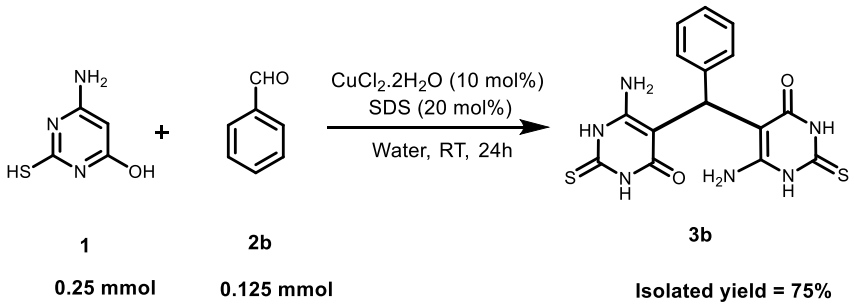
[a]Excluding the components of optimized reaction condition [b]Including the components of optimized reaction condition.

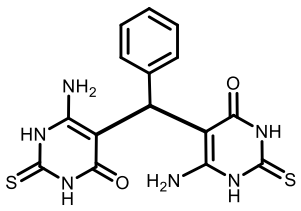
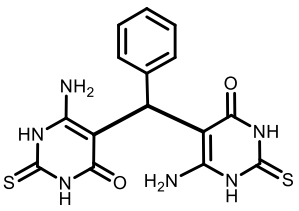
3. Comparison of green metrics (E-factor) and reaction condition with previously reported method:

Previous method: *Phosphorus, Sulfur, Silicon Relat. Elem.* 2021**, 196,** 920.



Our method

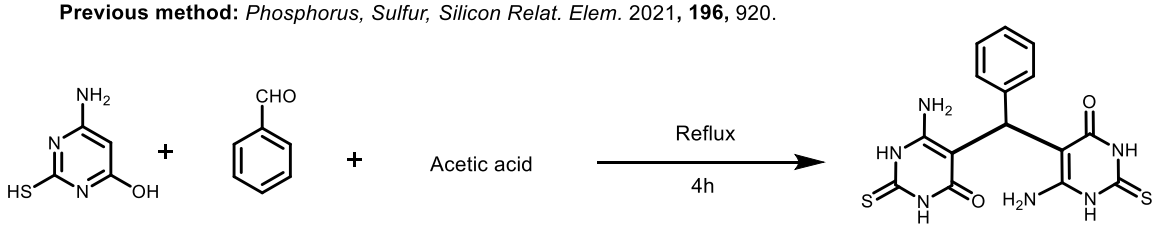


Parameters	Our method	Previous method
		

Optimized condition	$CuCl_2.2H_2O$ (10 mol%), SDS (20 mol%)	Acetic acid
Solvent	H_2O	Harmful acetic acid
Temperature	Room temperature	Reflux Acetic acid in reflux condition
Reaction time	24h	4h
Yield	75	80
E-factor	0.98	31.36

4. Ecoscale determination:

Previous method: *Phosphorus, Sulfur, Silicon Relat. Elem.* 2021**, 196,** 920.



1 **2b** **3b**

Reagents

Link

	identifier*	name	MF*	MW	density	purity*	ml	g	mmoles	equiv.
1		2-Mercapto-6-aminouracil	C4H5N3OS	143.1632		100%	0	0.486755	3.4	1
2		Benzaldehyde	C7H6O	106.12404	1.05	100%	0.17182	0.180411	1.7	0.5
3		Acetic acid	C2H4O2	60.05256	1.048	100%	15.58616	16.334296	272	80

Products

identifier*:	name:	MF*:	MW:	g:	mmoles:	g theor:	yield:
	Bis-product	C15H14N6O2S2	374.0620	0		1.271811	0

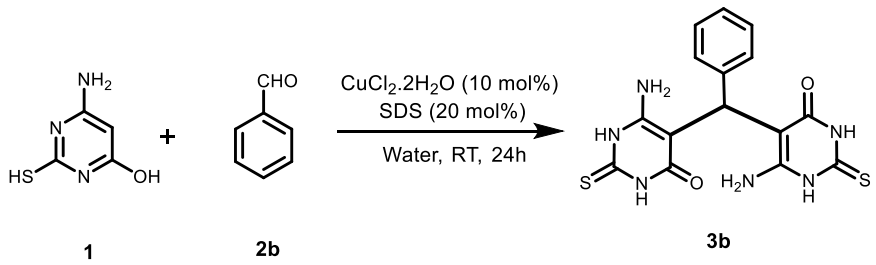
Conditions

Reagents

Name	mmoles	eq.	Bp	Hazard	Price
2-Mercapto-6-aminouracil	Infinity	1			
Benzaldehyde	Infinity	0.5	179		
Acetic acid	Infinity	80	117		

Yield	80		-10
Price / availability			-5
Safety			0
Technical setup	Possible items: Common set-up; Instruments for controlled addition of chemicals; Unconventional activation technique	Selected items: Common set-up	0
Temperature / time	Possible items: Heating, > 1h; Cooling to 0°C; Cooling, < 0°C	Selected items: Heating, > 1h	-3
Workup and purification	Possible items: Crystallization and filtration; Removal of solvent with bp > 150°C; Solid phase extration	Selected items: Crystallization and filtration	-1
EcoScale			81

Our method



1 2b 3b

Reagents

Link

	identifier*	name	MF*	MW	density	purity*	ml	g	mmoles	equiv.
1		4-Amino-6-hydroxy-2-mercaptopyrimidine mor	C4H5N3OS . H2	161.17848		100%	0	1.611785	10	2.9411764705
2		Benzaldehyde	C7H6O	106.12404	1.05	100%	0.505352	0.53062	5	1.4705882352
3		Copper(II) chloride dihydrate	Cl2Cu . 2H2O	170.48256	2.54	100%	0.033559	0.085241	0.5	0.1470588235
4		SDS	C12H25NaO4S	288.38		100%	0	0.57676	2	0.5882352941
5		Water	H2O	18.01528	1	100%	50	50	2775.4217530	816.30051561

Products

identifier*:	name:	MF*:	MW:	g:	mmoles:	g theor:	yield:
	Bis-product	C15H14N6O2S2	374.0620	0		1.271811	0

Conditions

Reagents

Name	mmoles	eq.	Bp	Hazard	Price
4-Amino-6-hydroxy-2-mercaptopyrimidine monohydrate	Infinity	2.94			
Benzaldehyde	Infinity	1.47	179		
Copper(II) chloride dihydrate	Infinity	0.14			
SDS	Infinity	0.58			
Water	Infinity	816.3			

Yield	75		-12.5
Price / availability			-5
Safety			-5
Technical setup	Possible items: Common set-up; Instruments for controlled addition of chemicals; Unconventional activation technique	Selected items: Common set-up	0
Temperature / time	Possible items: Room temperature, < 1h; Room temperature, < 24h; Heating, < 1h	Selected items: Room temperature, < 24h	-1
Workup and purification	Possible items: Crystallization and filtration; Removal of solvent with bp > 150°C; Solid phase extration	Selected items: Crystallization and filtration	-1
EcoScale			75.5

Based on green metrics such as E-factor, ecoscale and reaction condition, our method provide a more green technology, which is align with the previously published editorial report [green chem. 2020, 22, 13-15].

5. NMR yield determination:

$$\frac{np}{nis} = \frac{Ip}{Np} \times \frac{Nis}{Iis}$$

n_p = No. of mmole of product.

n_{is} = No. of mmole of internal standard (is).

I_p = Peak integration value of corresponds to the product.

N_p = No. of hydrogen atom corresponds to I_p.

I_{is} = Peak integration value of corresponds to the internal standard = 1.

N_{is} = No. of H-atom corresponds to I_{is} = 3.

Table S2.Time studies with different concentration of water.

Entries	Volume of water (H_2O)	Weight of internal standard taken (mg)[a]	n_{is}	I_{is}	N_{is}	I_p	N_p	Yield (%)[b]
1.	neat	-	-	-	-	-	-	0
2.	100 μL	5	0.029	1	3	0.02	1	7
3.	200 μL	5	0.029	1	3	0.03	1	20
4.	300 μL	5	0.029	1	3	0.05	1	52
5.	400 μL	5	0.029	1	3	0.05	1	69
6.	500 μL	5	0.029	1	3	0.044	1	77

Reaction condition: **1** (0.1 mmol), **2a** (0.05 mmol), $CuCl_2.2H_2O$ (10 mol%), SDS (20 mol%); a = taken internal standard 1,3,5-trimethoxybenzene, b = NMR yield (Samples were taken at each time point. A precise 50 μL of the reaction mixture was removed for each sampling, and the mixture was thoroughly dissolved in DMSO-d_6).

Table S3.Time studies in H_2O.

Entries	Time(h)	Weight of internal standard taken (mg)[a]	n_{is}	I_{is}	N_{is}	I_p	N_p	Yield (%)[b]
1	0	-	-	-	-	-	-	0
2	6	5	0.029	1	3	0.01	1	8
3	12	5	0.029	1	3	0.04	1	34
4	18	5	0.029	1	3	0.06	1	52
5	24	5	0.029	1	3	0.09	1	78

Reaction condition: 1 (0.2 mmol), 2a (0.1 mmol), $CuCl_2.2H_2O$ (10 mol%), SDS (20 mol%), H_2O = 1 ml.; a = taken internal standard 1,3,5-trimethoxybenzene, b = NMR yield (Samples were taken at each time point. A precise 100 μL of the reaction mixture was removed for each sampling, and the mixture was thoroughly dissolved in DMSO-d_6).

Table S4. Time studies in D_2O.

Entries	Time(h)	Weight of internal standard taken (mg)[a]	n_{is}	I_{is}	N_{is}	I_p	N_p	Yield (%)[b]
1.	0	-	-	-	-	-	-	0
2.	6	5	0.029	1	3	0.00	1	0
3.	12	5	0.029	1	3	0.02	1	17
4.	18	5	0.029	1	3	0.07	1	60
5.	24	5	0.029	1	3	0.08	1	69

Reaction condition: 1 (0.2 mmol), 2a (0.1 mmol), $CuCl_2.2H_2O$ (10 mol%), SDS (20 mol%), D_2O = 1 ml.; a = taken internal standard 1,3,5-trimethoxybenzene, b = NMR yield (Samples were taken at each time point. A precise 100 μL of the reaction mixture was removed for each sampling, and the mixture was thoroughly dissolved in DMSO-d_6).

6. Theoretical calculation

6.1. Experimental details:

The ORCA 5.0.3, 5.0.4 and 6.0.1 software packages were used for all calculations.[2] Geometry optimizations were performed using the r^{2}SCAN-3c composite DFT method[3] or hybrid PBE0 functional[4,5] with the minimally augmented ma-def2-TZVP basis set[6] for all other atoms along with D4 dispersion correction.[7] The RIJCOSX approximation[8] was used in all DFT calculations. In certain cases, the RI-MP2 and RI-SCS-MP2 wavefunction methods[9-11] with cc-pVTZ or aug-cc-pVTZ basis sets[12-14] were employed for geometry optimization. In the latter option the (aug-)cc-pVQZ/C auxiliary basis sets[15] was used for resolution of identity (RI) approximation.[16] The final geometries were generated involving *VeryTightSCF*, *TightOPT* and "*EnforceSctrictConvergence true*" keywords. The final single point energies were obtained using ωB97M-V functional[17] and def2-QZVP basis set.[18] The auxiliary basis sets in all DFT calculations (except of r^{2}SCAN-3c) were generated through the *AutoAux* keyword.[19] The time-dependent DFT calculations (TDDFT) were performed using the PBE0 functional and aug-cc-pVDZ basis set[13,14] for all atoms. The Tamm–Dancoff approximation (TDA)[20] were applied for all TDDFT calculations. The very dense integration grids were invoked by the *Defgrid3* keyword in all r^{2}SCAN-3c and ωB97M-V calculations. C-PCM[21] and SMD[22] implicit solvation models were used to account for solvation effects. Natural transition orbitals[23] were used for the visualization of electronic transitions. The ^{1}H-NMR shifts were calculated using TPSS functional[24] along with pcSseg-3 basis set.[25] The visualisation of molecular orbitals was made using the Avogadro 1.2 programme.[26] Free energy profile diagrams in the main text were drawn using mechaSVG 0.1.1 program.[27] In some cases the CYLview20 programme[28] was used for structural visualization. Sample ORCA input files are shown in Listings S1–S4. Cartesian coordinates of the DFT optimised structures are given as the xyz supplementary files. All the theoretical information for optimization of the final reaction products in neutral, protonated and deprotonated forms available in https://iochem-bd.bsc.es/browse/review-collection/100/328533/9d60a5f5805b8619b5d4e57b.

6.2. Keto-enol conformation of 3a:

The initial search for conformations of the **3a** ligand disclosed the presence of several configurations where the 4-amino-6-hydroxy-2-mercatopyrimidine groups are oriented in different manners and stabilized by the hydrogen bonds between –OH and –NH_2 groups. Hence, a full-angle scan of the 3a molecule at the r2SCAN-3c level, as implemented in the ORCA 5.0.4 software package, was performed to find all stable conformations. The r2SCAN-3c composite DFT method was used as the preliminary method due to its ability to generate accurate structures at a relatively low computational cost. The 1° step relaxed scan of the torsion <C–C–C–C angle formed by the two mercatopyrimidine rings revealed that the energy of the molecule differs much depending on the angle. Five tentative energy minima were detected, separated by rotational energy barriers up to 7 kcal mol^{-1} (Figure S1). Structure optimization of these five minima disclosed stable conformers where the –OH groups are directed towards the internal N atoms of the mercatopyrimidine ring (Figure S2, top). Another two stable conformers were detected when considering one of the –OH group rotated at 180° (Figure S2, bottom). As can be seen, the former group of conformers is more stable with the difference in the free Gibbs energies of ca. 6 kcal mol^{-1}.

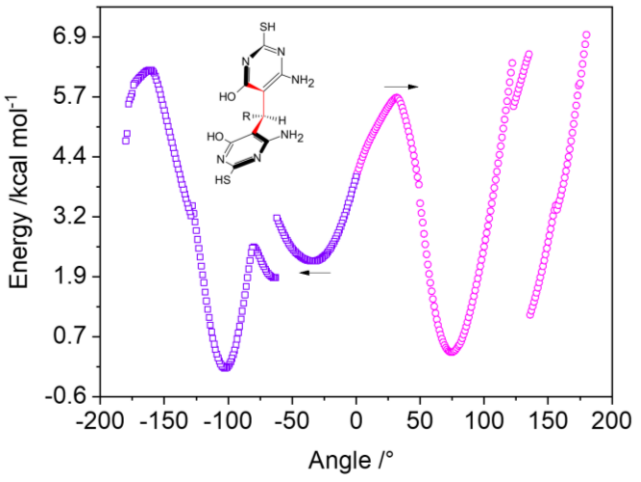


Figure S1. Relaxed scan of the rotation of the torsion angle (1 degree step) of the enol tautomer of **3a**. The scanned angle is highlighted by red colour. Energy designates single point energy. Arrows show the direction of the scan (0 → –180° and 0 → 180°).

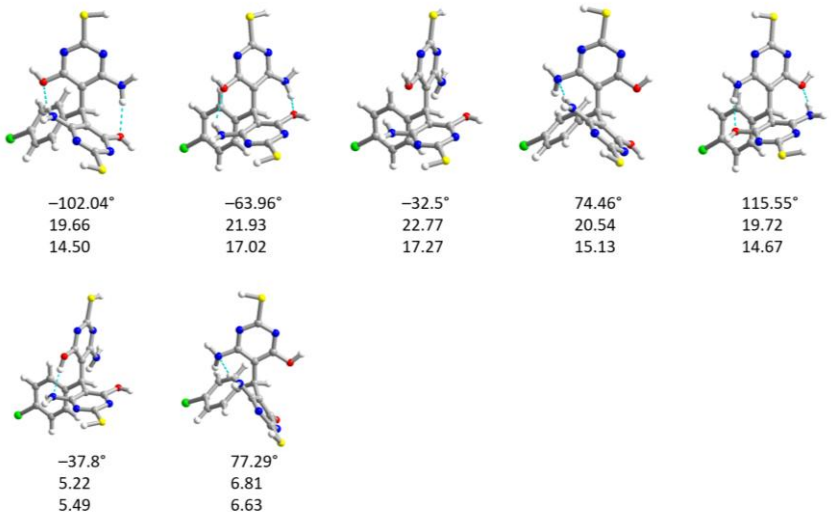


Figure S2. Stable conformers with the "regular" (top) and "rotated" (bottom) orientation of the –OH groups of the enol tautomer of **3a**. The numbers designate the torsion angle, electronic and Gibbs energies (top down), where the energies are given relative to the lowest energy keto tautomer having 96.97° torsion angle.

The relaxed scan of the similar torsion angle in the keto tautomer of 3a resulted in a much smaller number of conformations, which can be associated with the absence of flexible –OH and –SH groups in the keto form that could make strong H-bonds stabilizing intermediate structures (Figure S3). Full geometry relaxation of the configurations with the lowest energies found from the scan afforded two conformers having equal energies and another one having 10 kcal mol^{-1} Gibbs energy higher (Figure S4). The first two conformers are symmetrically related by reflection and are stabilized by strong N–H···O bonds. The latter conformer (angle 72.12°) exhibits two non-covalent N–H···π bondings.

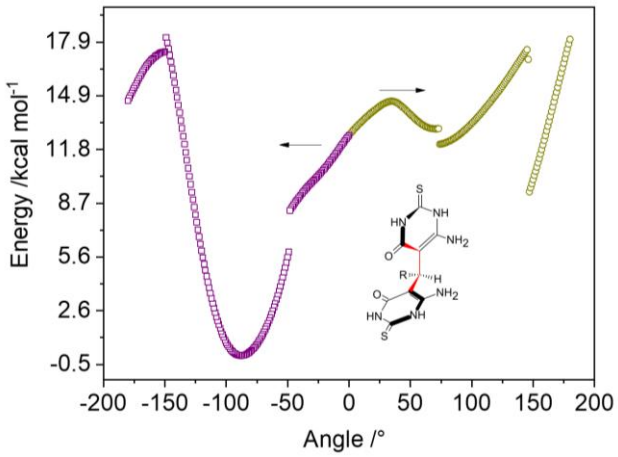


Figure S3. Relaxed scan of the rotation of the torsion angle (1 degree step) in keto tautomer of **3a**. The scanned angle is highlighted by red colour. Energy designates single point energy. Arrows show the direction of the scan (0 → –180° and 0 → 180°).

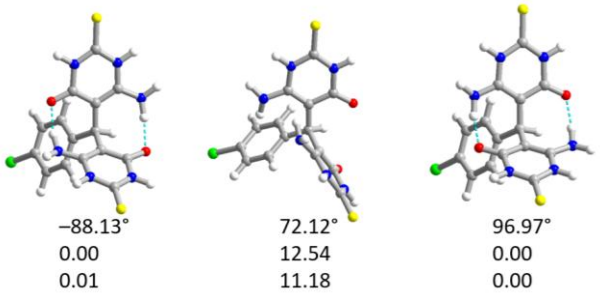


Figure S4. Stable conformers of the keto tautomer of 3a. The numbers designate the torsion angle, electronic and Gibbs energies (top down), where the energies are given relative to those of 96.97° conformer.

6.3. Keto-enol tautomer of 3a and solvation shell models of 3a:

At the r^{2}SCAN-3c level, the lowest energy keto tautomer was found to be more favorable (ΔG = –5.49 kcal mol^{-1}) than the most stable enol form. The respective tautomerization mechanism is expected to be mediated by a water molecule, H-bonded to the N and hydroxyl or sulphoxyl groups. Calculations at the r^{2}SCAN-3c // ωB97M-V/def2-QZVP level considering water reaction medium afforded relatively low barriers in the range 10.56 – 12.15 kcal mol^{-1} for the water-assisted tautomerization of a single –OH/N ⇌ =O/NH or –SH/N ⇌ =S/NH group. The two-step mechanism of complete tautomerization of one mercatopyrimidine is depicted in Figure S5. Although, this

mechanism is speculative since the tautomerization can proceed through the different simultaneously occurring pathways, the barriers and overall profile clearly demonstrate that the keto tautomer is favorable and the tautomerization can efficiently proceed in the presence of water.

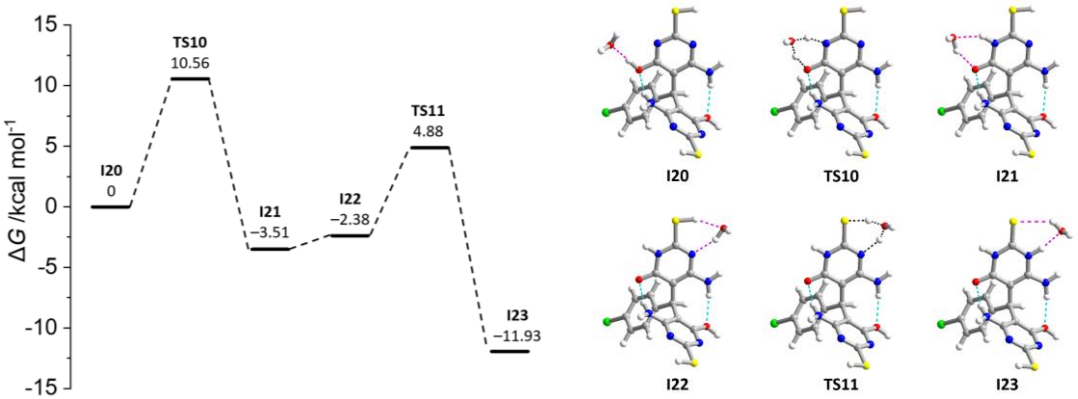


Figure S5. Left: The energy profile diagram for the water-mediated tautomerization of enol form to keto one of a single mercaptopyrimidine group in **3a** calculated at the r^{2}SCAN-3c // ωB97M-V/def2-QZVP level in water (C-PCM solvation model). Right: The structures of intermediates (**I**) and transition states (**TS**) for the energy profile.

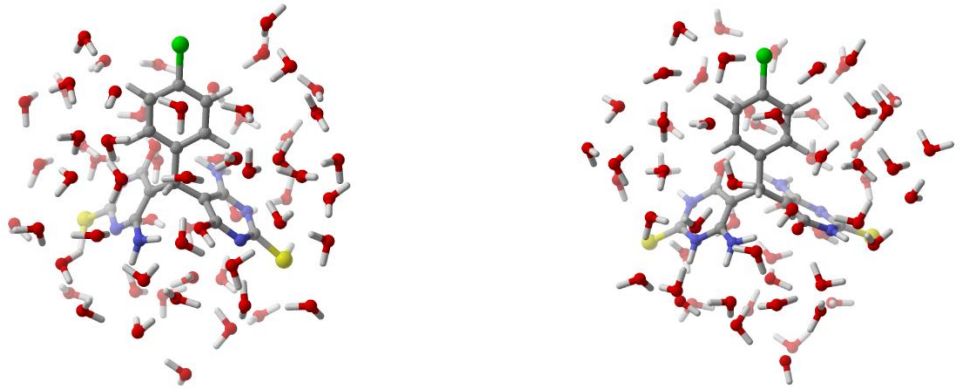


Figure S6: Geometries of the ^{enol}**3a·60H$_2$O** (left) and ^{keto}**3a·60H$_2$O** (right) assemblies optimized at the r^{2}SCAN-3c/CPCM(water) level. The starting models were obtained through the ORCA.SOLVATOR feature operating at the semiempirical GFN2-xTB level.

6.4. DFT calculated structures and TDDFT predicted UV/Spectra of 3a-3o.

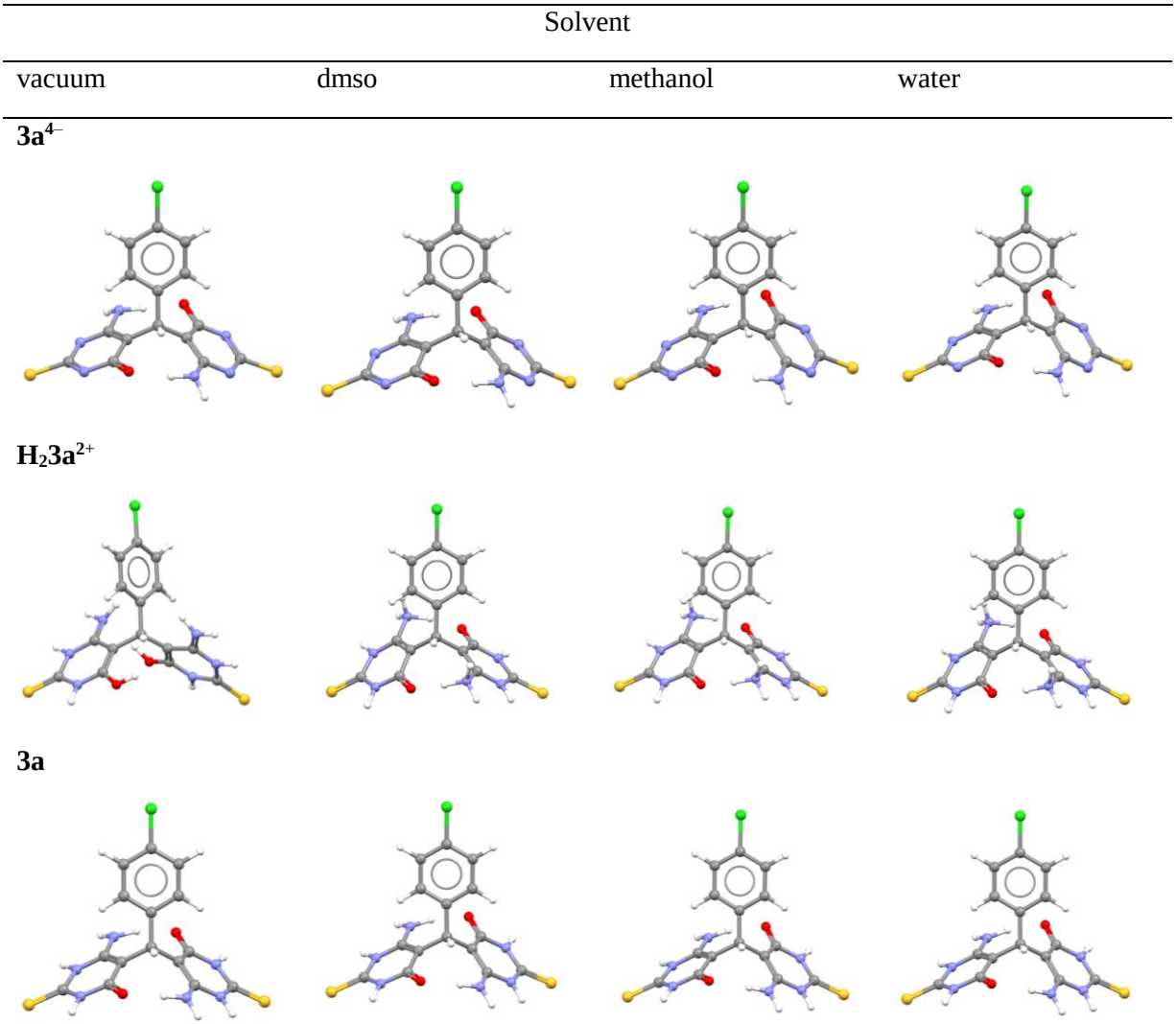
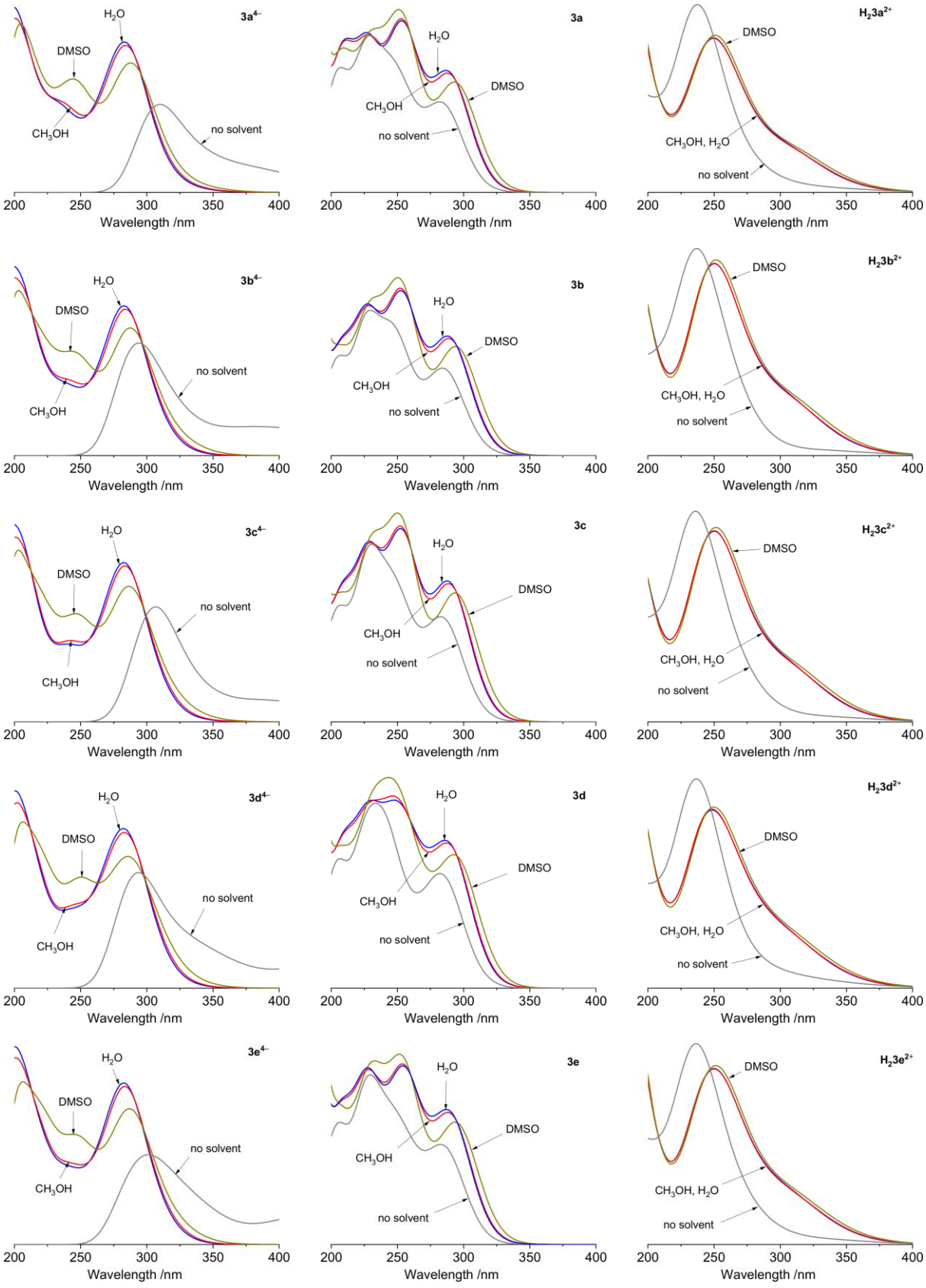
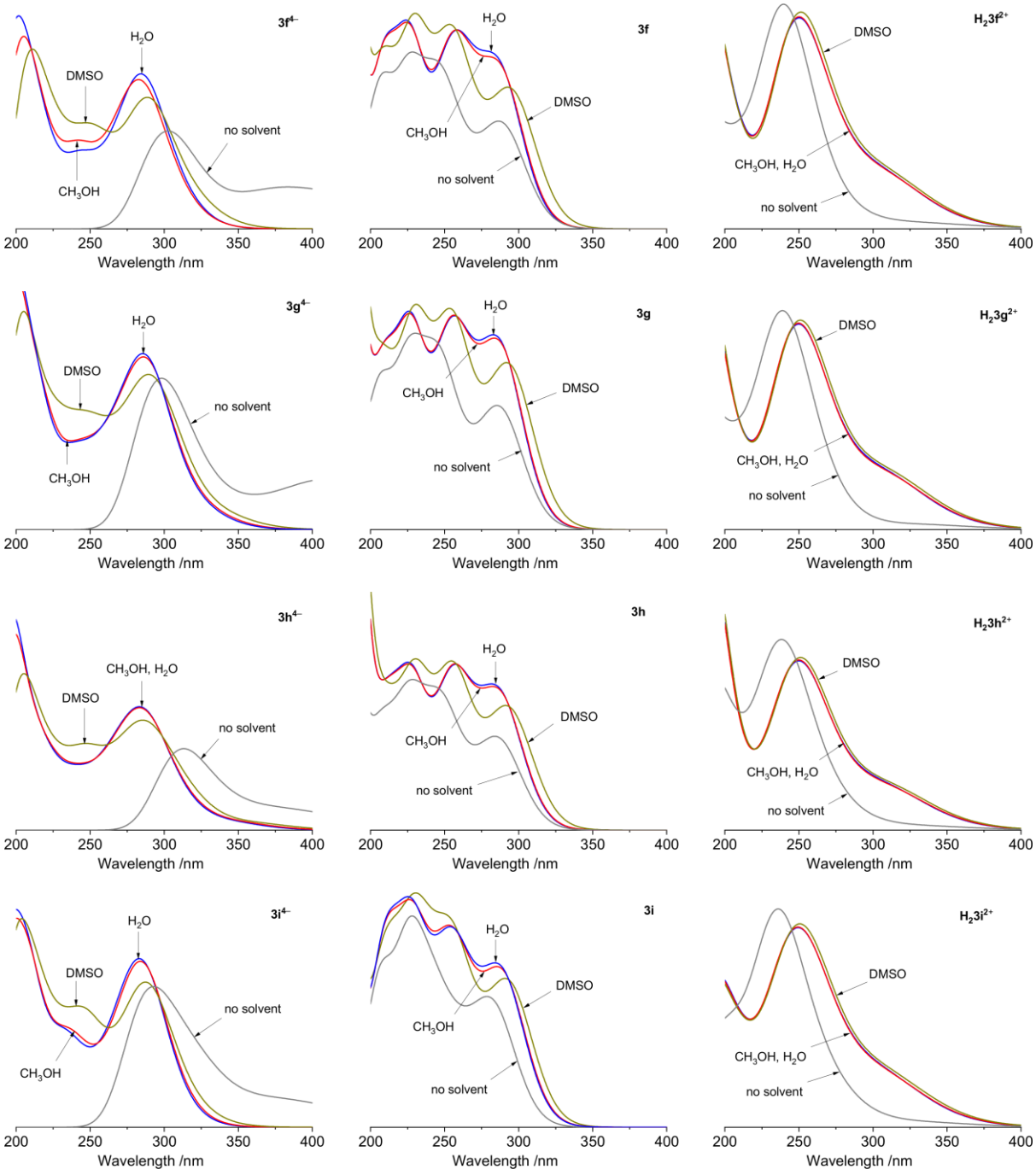
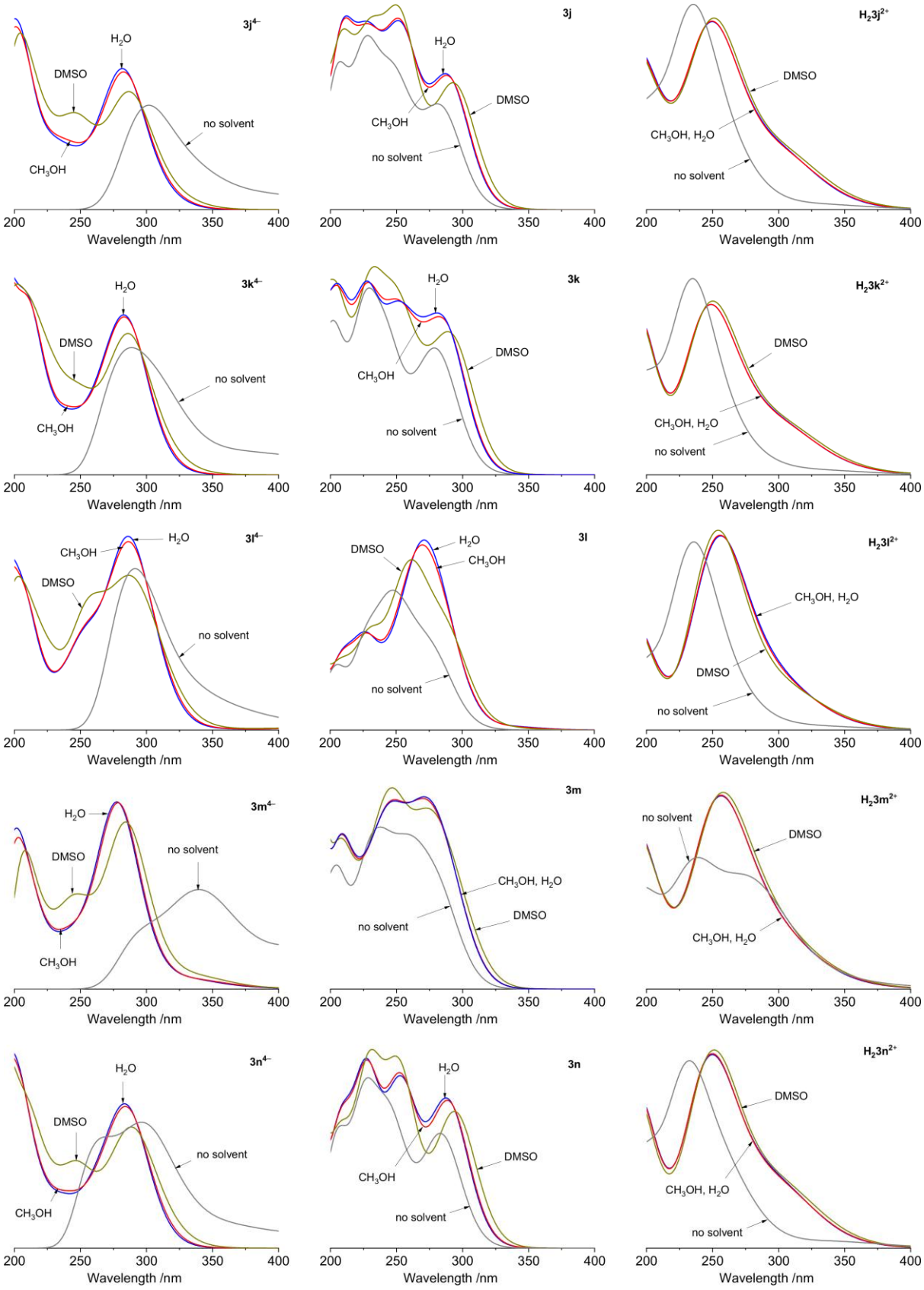


Figure S7. Molecular structures of the tautomer **3a** and its deprotonated (left) and protonated (right) derivatives optimized at the PBE0/ma-def2-TZVP level in water (SMD solvation model).


3a4–
H2O
DMSO
CH3OH
no solvent
200 250 300 350 400
Wavelength /nm
3a
H2O
DMSO
CH3OH
no solvent
200 250 300 350 400
Wavelength /nm
H23a2+
DMSO
CH3OH, H2O
no solvent
200 250 300 350 400
Wavelength /nm
3b4–
H2O
DMSO
CH3OH
no solvent
200 250 300 350 400
Wavelength /nm
3b
H2O
DMSO
CH3OH
no solvent
200 250 300 350 400
Wavelength /nm
H23b2+
DMSO
CH3OH, H2O
no solvent
200 250 300 350 400
Wavelength /nm
3c4–
H2O
DMSO
CH3OH
no solvent
200 250 300 350 400
Wavelength /nm
3c
H2O
DMSO
CH3OH
no solvent
200 250 300 350 400
Wavelength /nm
H23c2+
DMSO
CH3OH, H2O
no solvent
200 250 300 350 400
Wavelength /nm
3d4–
H2O
DMSO
CH3OH
no solvent
200 250 300 350 400
Wavelength /nm
3d
H2O
DMSO
CH3OH
no solvent
200 250 300 350 400
Wavelength /nm
H23d2+
DMSO
CH3OH, H2O
no solvent
200 250 300 350 400
Wavelength /nm
3e4–
H2O
DMSO
CH3OH
no solvent
200 250 300 350 400
Wavelength /nm
3e
H2O
DMSO
CH3OH
no solvent
200 250 300 350 400
Wavelength /nm
H23e2+
DMSO
CH3OH, H2O
no solvent
200 250 300 350 400
Wavelength /nm


3f4−
H2O
DMSO
no solvent
CH3OH
Wavelength /nm
3f
H2O
CH3OH
DMSO
no solvent
Wavelength /nm
H23f2+
DMSO
CH3OH, H2O
no solvent
Wavelength /nm
3g4−
H2O
DMSO
no solvent
CH3OH
Wavelength /nm
3g
H2O
CH3OH
DMSO
no solvent
Wavelength /nm
H23g2+
DMSO
CH3OH, H2O
no solvent
Wavelength /nm
3h4−
CH3OH, H2O
DMSO
no solvent
Wavelength /nm
3h
H2O
CH3OH
DMSO
no solvent
Wavelength /nm
H23h2+
DMSO
CH3OH, H2O
no solvent
Wavelength /nm
3i4−
H2O
DMSO
no solvent
CH3OH
Wavelength /nm
3i
H2O
CH3OH
DMSO
no solvent
Wavelength /nm
H23i2+
DMSO
CH3OH, H2O
no solvent
Wavelength /nm


3j4−
H2O
DMSO
no solvent
CH3OH
3j
H2O
CH3OH
DMSO
no solvent
H23j2+
DMSO
CH3OH, H2O
no solvent
3k4−
H2O
DMSO
no solvent
CH3OH
3k
H2O
CH3OH
DMSO
no solvent
H23k2+
DMSO
CH3OH, H2O
no solvent
3l4−
CH3OH
H2O
DMSO
no solvent
3l
DMSO
H2O
CH3OH
no solvent
H23l2+
CH3OH, H2O
DMSO
no solvent
3m4−
H2O
DMSO
no solvent
CH3OH
3m
CH3OH, H2O
no solvent
DMSO
H23m2+
no solvent
DMSO
CH3OH, H2O
3n4−
H2O
DMSO
no solvent
CH3OH
3n
H2O
CH3OH
DMSO
no solvent
H23n2+
DMSO
CH3OH, H2O
no solvent
200
250
300
350
400
Wavelength /nm

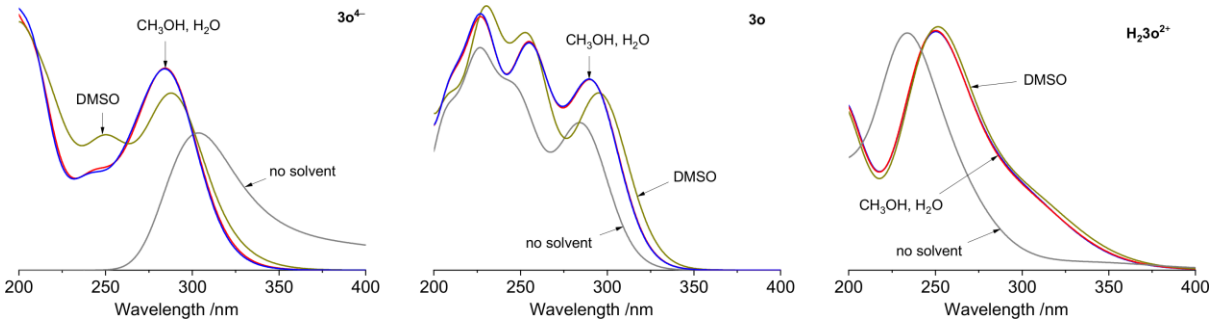


Figure S8. Theoretical UV-Vis spectra of neutral, protonated and deprotonated forms calculated by TDDFT at the PBE0/aug-cc-pVDZ level considering first 200 excited states for the different solvents (SMD model; structures optimized at the PBE0/ma-def2-TZVP level) or in vacuum. The following Gaussian broadening parameters were applied when building the spectra through the orca_mapspc routine: *-w6500* for cationic and *-w4000* for neutral and anionic structures. These parameters were selected based on the experimental findings (see the main text).

Table S5. Bonds (Å) and angles (°) of the N–H···O hydrogen contacts in the protonated (**$H_2$3a^{2+}**) and deprotonated (**3a^{4-}**) forms of the keto tautomer of **3a** optimized at various levels of theory.[a]

Method	*d*(N···O)	*d*(N–H)	*d*(H···O)	∠(N–H···O)
$H_2$3a^{2+}				
r^{2}SCAN-3c, C-PCM (water)	2.655	1.070	1.612	163.41
	2.738	1.061	1.700	164.69
r^{2}SCAN-3c, C-PCM (DMSO)	2.652	1.070	1.609	163.47
	2.732	1.061	1.694	164.72
r^{2}SCAN-3c, SMD (DMSO)	2.653	1.070	1.609	163.72
	2.736	1.061	1.698	165.01
RI-MP2/cc-pVTZ, SMD (DMSO) [b]	2.649	1.057	1.625	161.56
	2.721	1.052	1.697	163.27
RI-SCS-MP2/aug-cc-pVTZ, SMD (DMSO) [c]	2.702	1.047	1.703	158.01
	2.785	1.043	1.781	160.24
PBE0/ma-def2-TZVP, SMD (DMSO) [d]	2.625	1.071	1.572	166.05
	2.697	1.063	1.651	166.85
3a^{4-}				
r^{2}SCAN-3c, SMD (DMSO)	2.784	1.034	1.753	174.22
	2.887	1.028	1.862	175.52
RI-SCS-MP2/aug-cc-pVTZ, SMD (DMSO) [c]	2.778	1.029	1.752	174.20
	2.864	1.026	1.842	173.77
PBE0/ma-def2-TZVP, SMD (DMSO) [d]	2.743	1.034	1.712	174.51
	2.830	1.029	1.803	173.80
PBE0/ma-def2-TZVP, SMD (DMSO) [d,f]	2.742	1.034	1.712	174.16
	2.826	1.029	1.800	174.80

[a] SCF and geometry optimization convergence criteria: *VeryTightSCF*, *TightOPT*, "*EnforceStrictConvergence true*", default integration grids; [b] correlation auxiliary basis set cc-pVQZ/C; [b] correlation auxiliary basis set aug-cc-pVQZ/C; [d] automatic generation of auxiliary basis sets (*AutoAux*); [e] integration grids *Defgrid3*.

Table S6. TDDFT-predicted absorption maxima (nm) after Gaussian broadening.

solvent		water			methanol			DMSO	
me-dium	acidic	neutral	basic	acidic	neutral	basic	acidic	neutral	basic
3a	250	286	283	250	288	284	251	293	287
3b	250	287	283	250	289	284	251	294	287
3c	250	287	283	250	288	283	251	294	286
3d	248	286	282	248	287	283	250	292	286
3e	250	287	282	250	288	284	251	294	286
3f	250	282	285	250	282	283	251	283	288
3g	250	283	286	250	284	286	251	292	289
3h	250	283	283	250	283	283	252	292	286
3i	250	285	283	250	285	284	251	291	287
3j	250	287	281	250	288	282	251	293	287
3k	249	280	283	249	282	283	250	288	286
3l	256	271	286	256	270	286	254	262	286
3m	256	270	278	256	270	278	258	272	284
3n	250	288	283	250	289	284	251	294	288
3o	251	290	284	251	290	284	252	295	288

6.5. Sample ORCA input files

Listing S1. Sample ORCA input for the final geometry optimization.

```
! PBE0 ma-def2-TZVP AutoAux D4 VeryTightSCF TightOPT
%basis
  PCDTrimAuxJ Coulomb
  PCDTrimAuxC Coulomb
  PCDTrimAuxJK Coulomb
  PCDThresh -1
end
%pal nproc 10 end
%maxcore 10000
%cpcm
  SMD true
  SMDSolvent "DMSO"
end
%geom
  EnforceStrictConvergence true
end
* xyzfile 0 1 FileName.xyz
```

Listing S2. Sample ORCA input for geometry optimization at the RI-SCS-MP2 level.

```
! RI-SCS-MP2 aug-cc-pVTZ aug-cc-pVQZ/C VeryTightSCF TightOPT
%pal nproc 128 end
%maxcore 4000
%cpcm
  SMD true
  SMDSolvent "DMSO"
end
%geom
  EnforceStrictConvergence true
end
* xyzfile 2 1 FileName.xyz
```

Listing S3. Sample ORCA input for the TDDFT calculation of excited states and UV-Vis spectra.

```
! PBE0 aug-cc-pVDZ AutoAux D4 VeryTightSCF
%pal nproc 10 end
%basis
  PCDTrimAuxJ Coulomb
  PCDTrimAuxJK Coulomb
  PCDTrimAuxC Coulomb
  PCDThresh -1
end
%maxcore 10000
%cpcm
  SMD true
  SMDSolvent "dmso"
end
%tddft
  nroots 200
```

```
  maxdim 100
  DoNTO true
  NTOStates 1,2,3,4,5,6,7,8,9,10
end
* xyzfile 0 1 FileName.xyz
```

Listing S4. Sample ORCA input for the calculation of 1H NMR chemical shielding.

```
! TPSS pcSseg-3 AutoAux Defgrid3 VeryTightSCF NMR NoFrozenCore
%pal nproc 22 end
%maxcore 10000
%cpcm
  SMD true
  SMDSolvent "DMSO"
end
* xyzfile 2 1 FileName.xyz
%eprnmr
  nuclei = all H {shift}
  Tau Dobson
end
```

Listing S5. Sample ORCA input for the modelling of solvation shells.

```
! XTB ALPB(water)
%pal nproc 24 end
%solvator NSolv 60 end
* xyzfile 0 1 FileName.xyz
```

7. UV/Vis, FT-IR, ^{1}H & ^{13}C-NMR, HRMS data of compounds 3a-q.

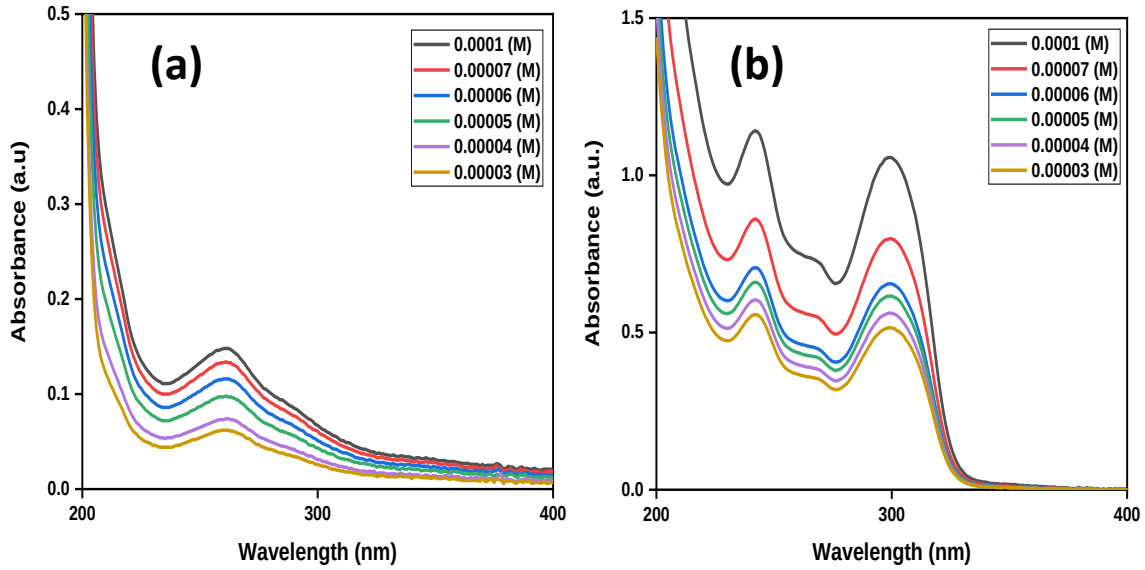


Figure S9. UV-Visible spectra of compound **3a** with different concentration at (a) acidic and (b) basic P^{H}.

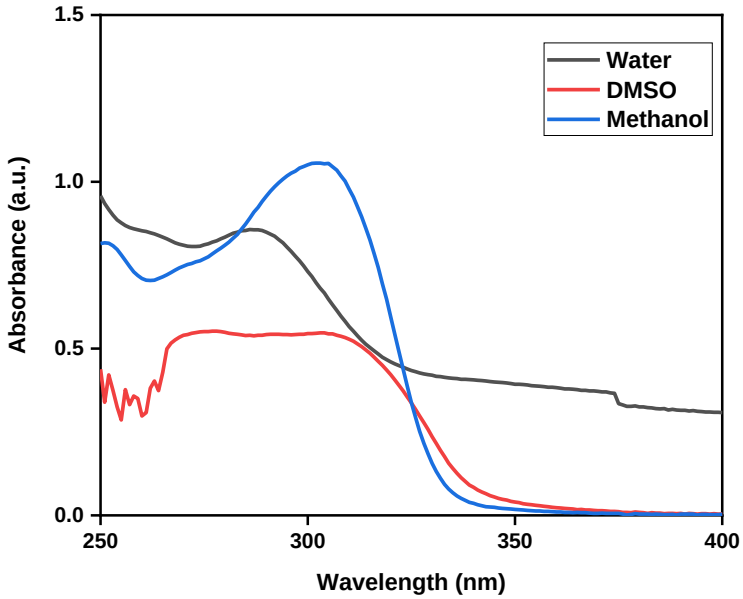


Figure S10. UV-Visible spectra of **3a** in neutral solvent.

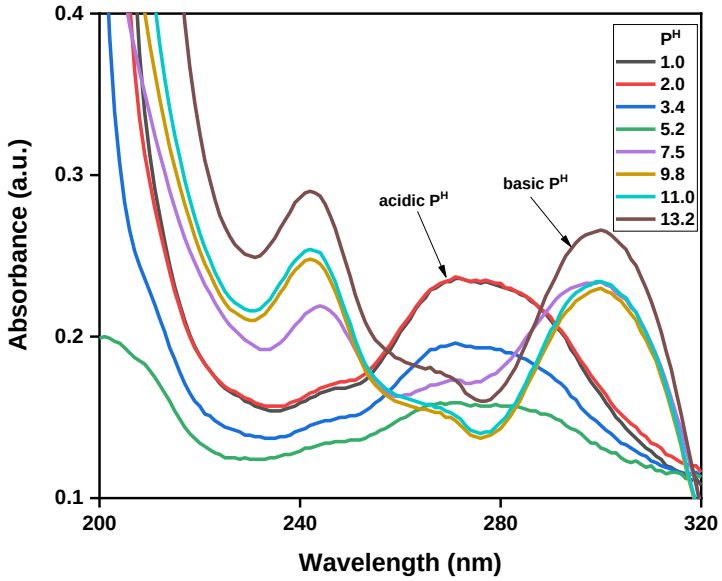


Figure S11. The UV-Visible spectra of **3a** at different P^H in aqueous solution.

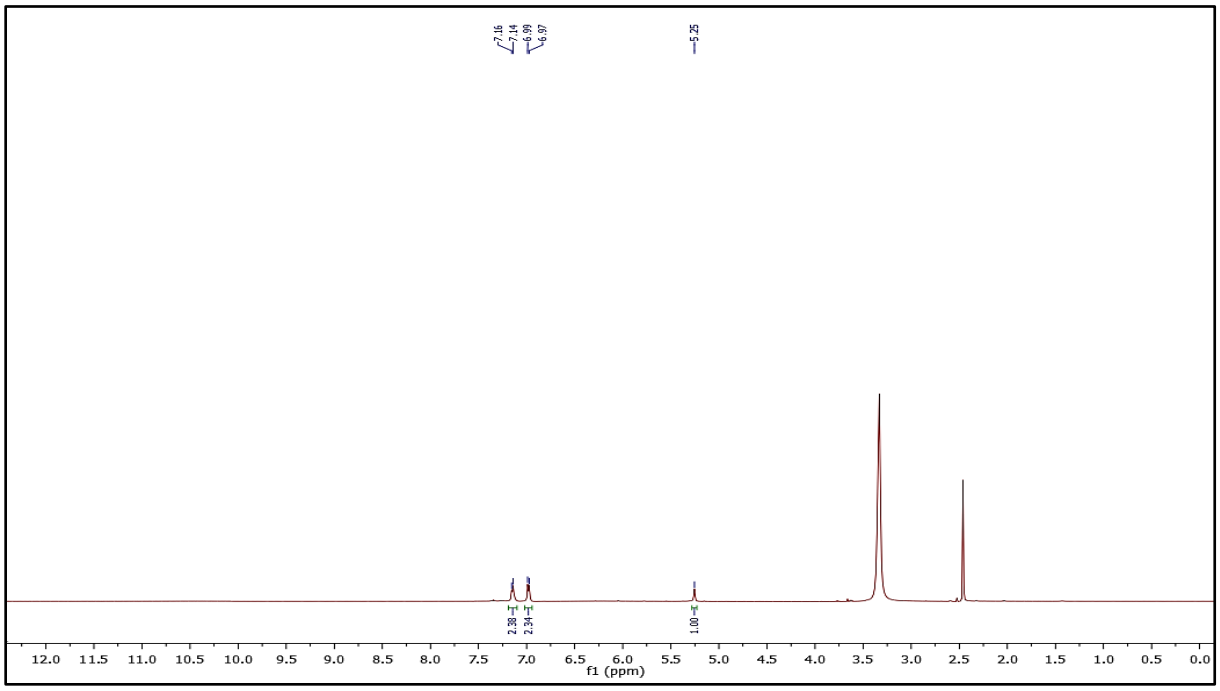


Figure S12. ^{1}H-NMR of compound **3a** in DMSO-d_6 in basic condition. Basified with 2 equivalents of NaOH solution (NaOH dissolve in D_2O).

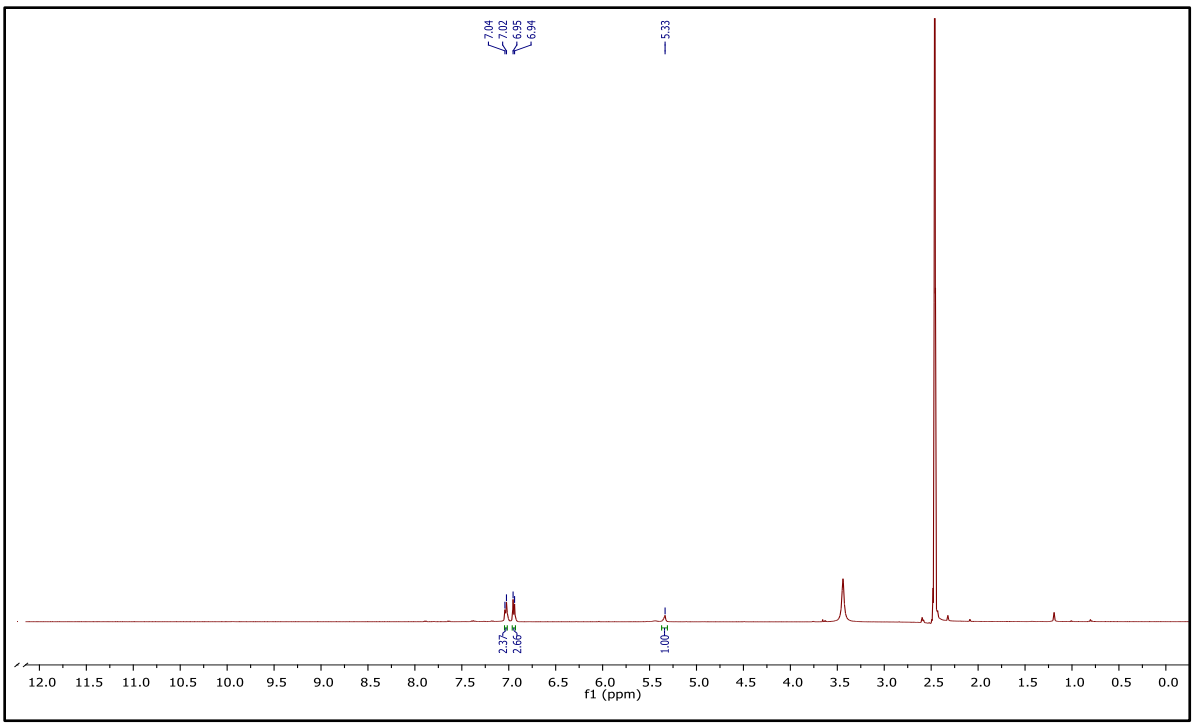


Figure S13. ^{1}H-NMR of compound **3a** in DMSO-d_6 in basic condition. Basified with 4 equivalents of NaOH solution (Solid NaOH dissolve in D_2O).

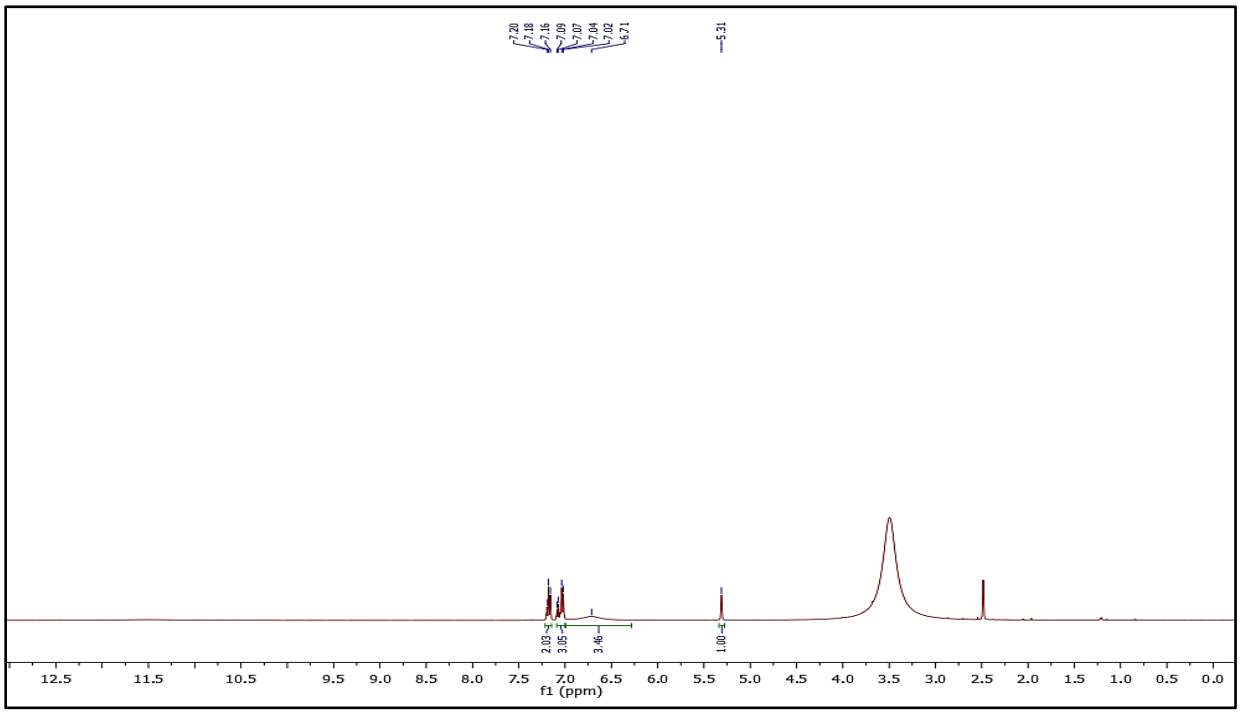


Figure S14. ^{1}H-NMR of compound **3b** in DMSO-d_6 in basic condition. Basified with 4 equivalents of NaOH solution (Solid NaOH dissolve in H_2O).

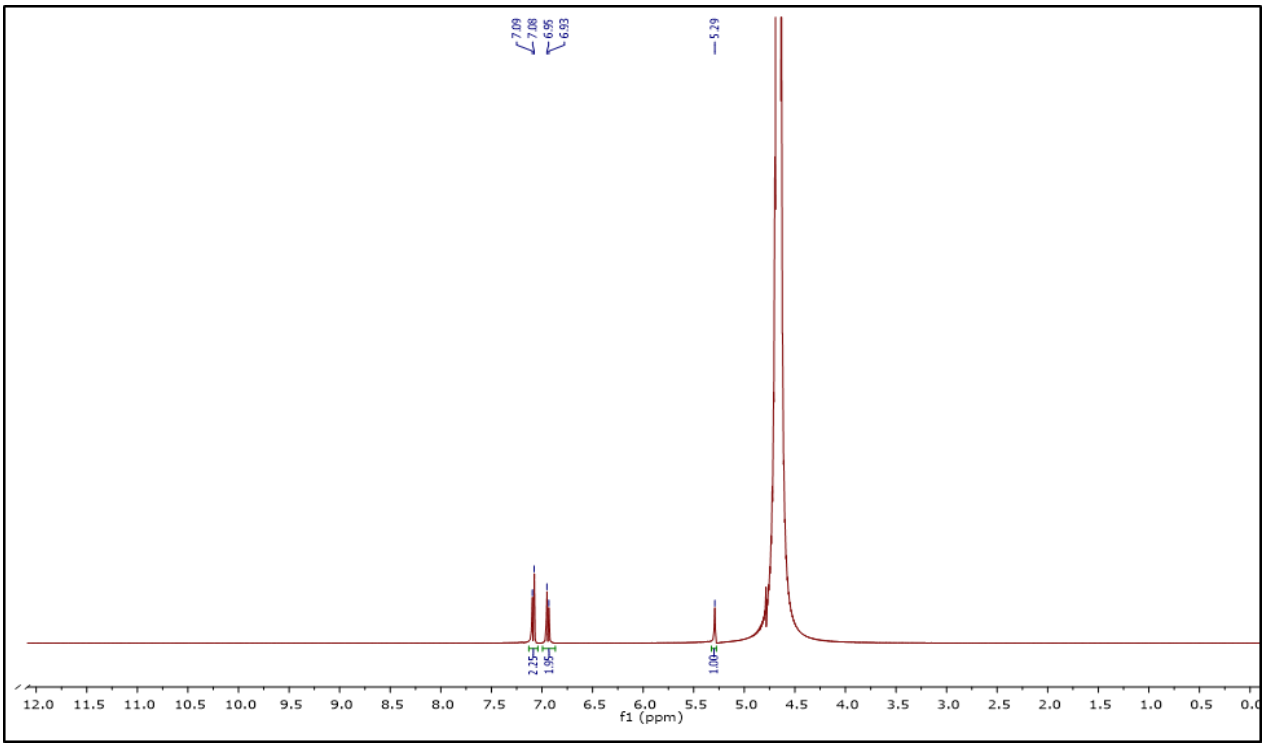


Figure S15. ^{1}H-NMR of compound **3a** in D_2O in basic condition. Basified with 4 equivalents of NaOH.

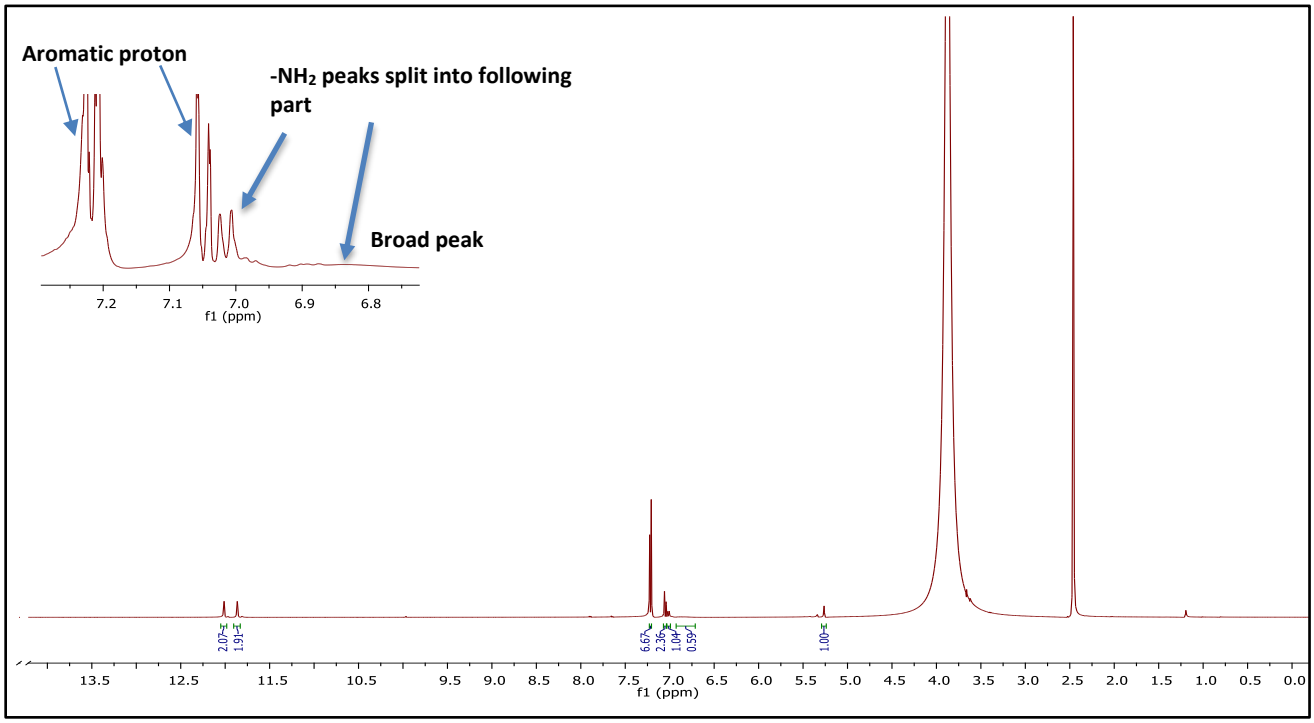


Figure S16. ^{1}H-NMR of compound **3a** in DMSO-d_6 in acidic condition. Acidified with 4 equivalents of 35 % HCl solution.

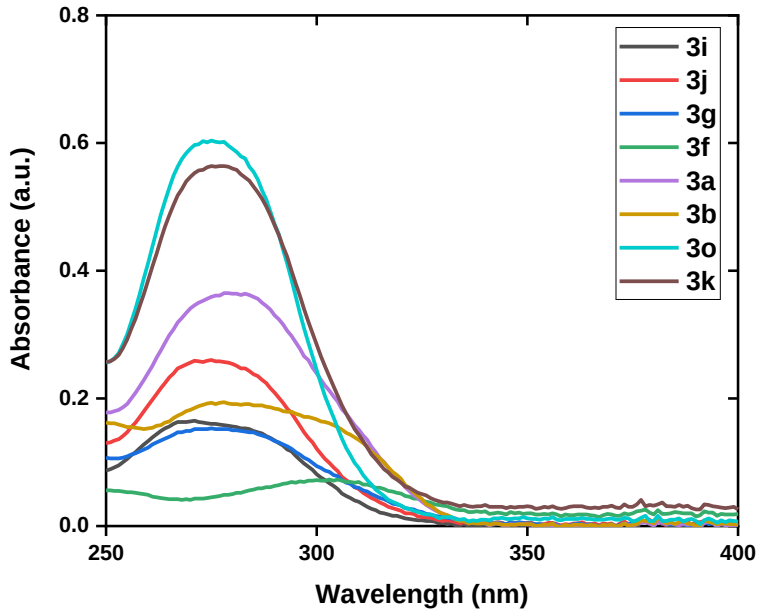


Figure S17. UV-visible spectra of some compounds in acidic water.

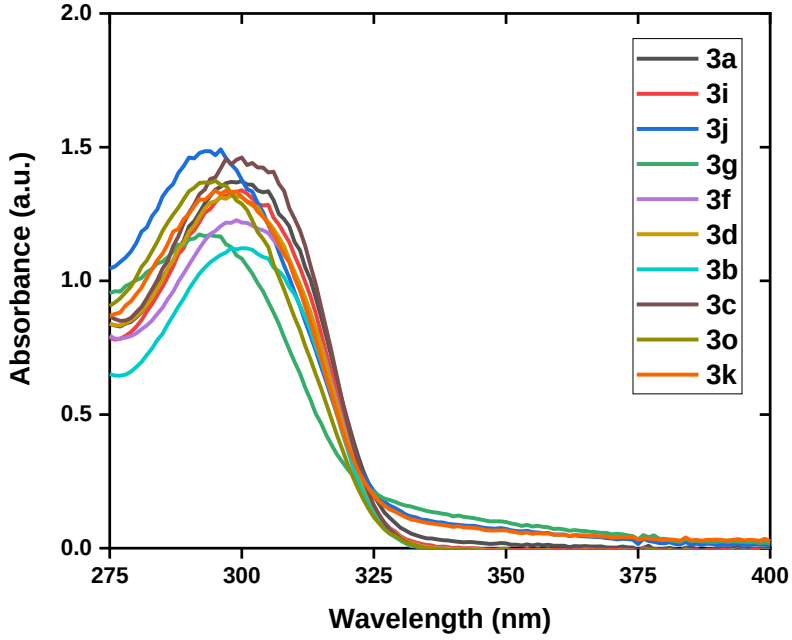


Figure S18. UV-visible spectra of some compounds in basic water.

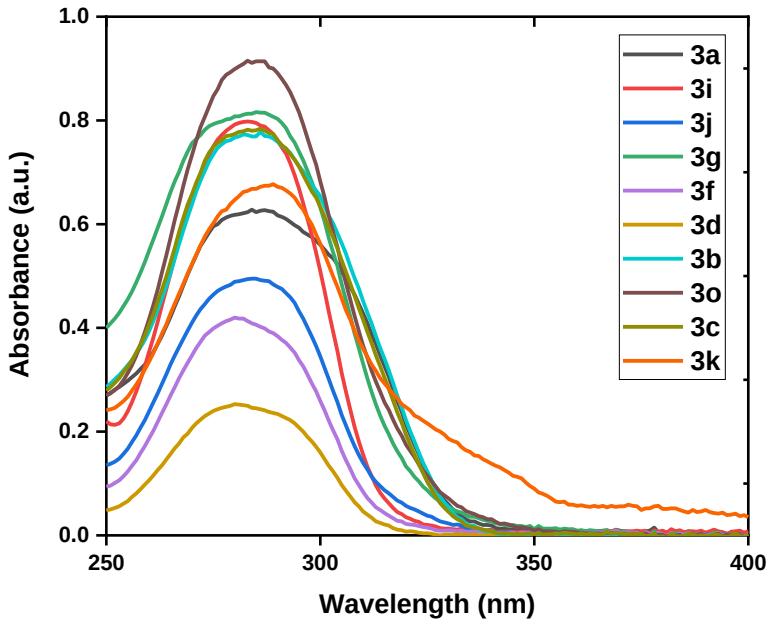


Figure S19. UV-visible spectra of some compounds in acidic methanol.

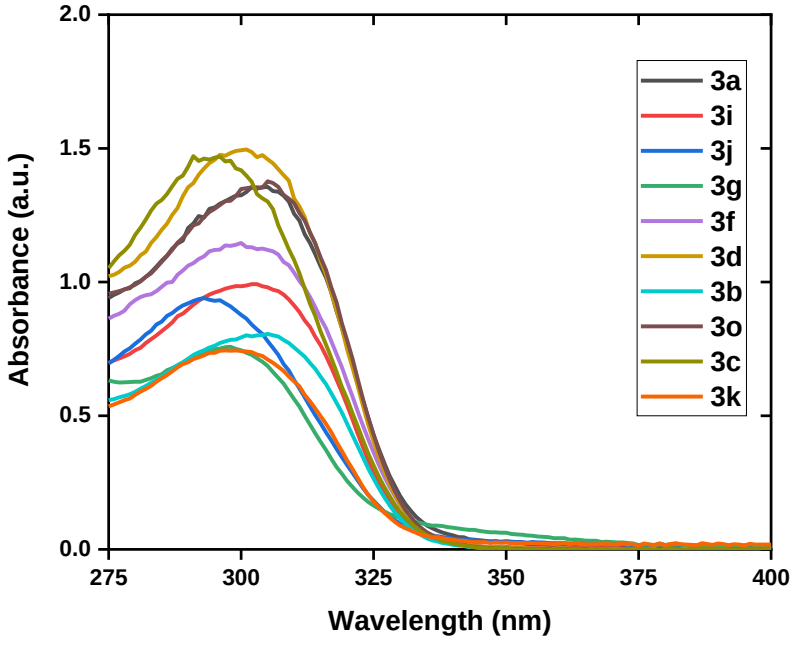


Figure S20. UV-visible spectra of some compounds in basic methanol.

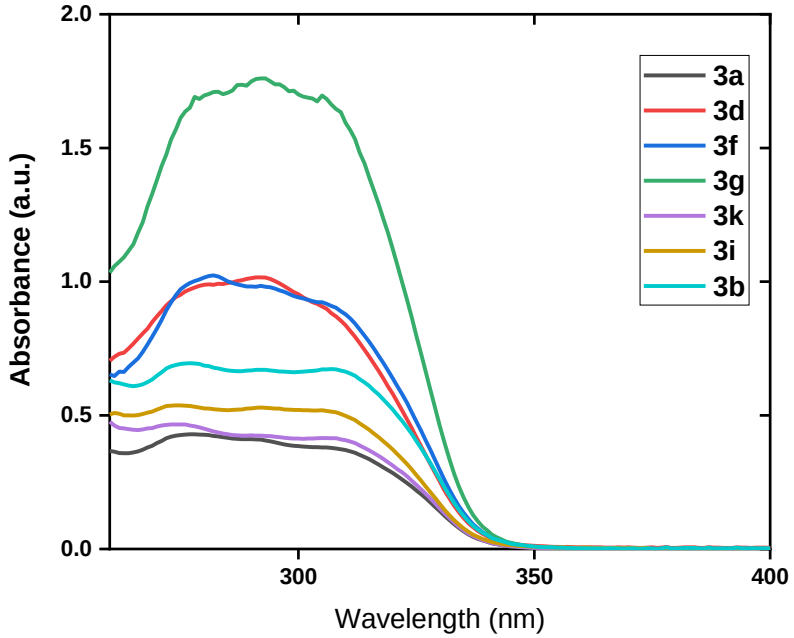


Figure S21. UV-visible spectra of some compounds in acidic DMSO.

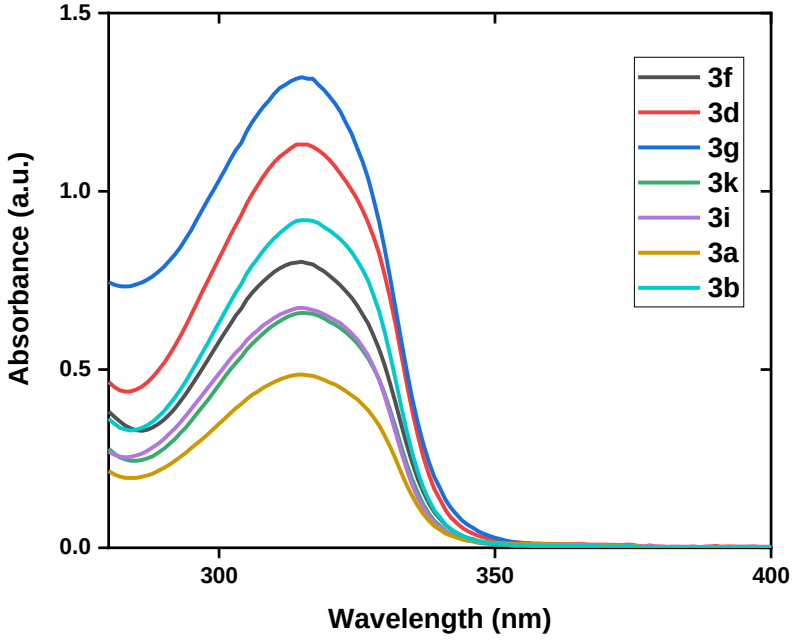
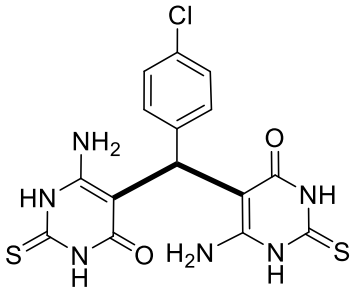


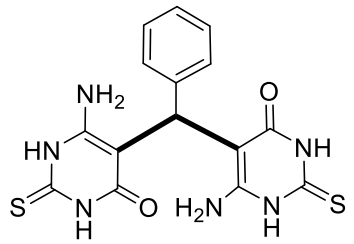
Figure S22. UV-visible spectra of some compounds in basic DMSO.

(5,5'-((4-chlorophenyl)methylene)bis(6-amino-2-mercaptopyrimidin-4-ol)) (3a):



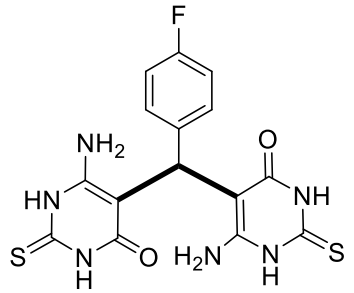
White solid (37.3 mg, 74%), **FT-IR (cm^{-1}):** 3339, 3143, 1597, 1539, 1173; **^{1}H-NMR (400 MHz, DMSO-d$_6$)** δ: 12.0 (s, 2H), 11.86 (s, 2H), 7.25 (d, J = 8.5 Hz, 2H), 7.09 (d, J = 8.3 Hz, 2H), 6.78 (s, 4H), 5.32 (s, 1H); **^{13}C-NMR (101 MHz, DMSO-d$_6$)** δ: 173.3, 163.5, 153.9, 137.5, 130.4, 129.0, 128.2, 90.4, 32.6; **HRMS (ESI):** calculated for $C_{15}H_{13}ClN_6O_2S_2Na$ [M + Na] $^{+}$: 431.0128; found: 431.0143.

(5,5'-(phenylmethylene)bis(6-amino-2-mercaptopyrimidin-4-ol)) (3b):



White solid (35.1 mg, 75%), **FT-IR (cm^{-1}):** 3392, 3050, 2895, 1633, 1600, 1546,1172; **^{1}H-NMR (500 MHz, DMSO-d$_6$)** δ: 12.05 (s, 2H), 11.83 (s, 2H), 7.22 (dd, *J* = 10.4, 4.6 Hz, 2H), 7.14 – 7.06 (m, 3H), 6.78 (s, 4H), 5.35 (s, 1H); **^{13}C-NMR (101 MHz, DMSO-d$_6$)** δ: 173.2, 163.5, 153.8, 138.4, 135.1, 129.9, 129.6, 128.3, 126.9, 125.8, 90.7, 32.9; **HRMS (ESI):** calculated for $C_{15}H_{15}N_6O_2S_2$ [M + H] $^{+}$: 375.0698; found: 375.0691.

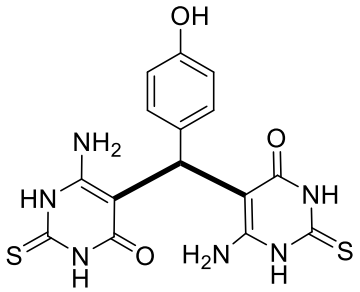
(5,5'-((4-fluorophenyl)methylene)bis(6-amino-2-mercaptopyrimidin-4-ol)) (3c):



White solid (36.3 mg, 74%), **FT-IR (cm^{-1}):** 3353, 3156, 1698, 1672, 1538, 1170; **^{1}H-NMR (500 MHz, DMSO-d$_6$)** δ: 12.05 (s, 2H), 11.83 (s, 2H), 7.10 – 7.07 (m, 2H), 7.02 (t, J = 8.8 Hz, 2H), 6.76 (s, 4H), 5.31

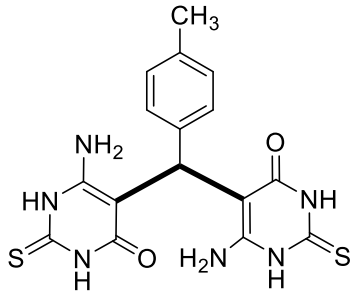
(s, 1H); **^{13}C-NMR (126 MHz, DMSO-d$_6$)** δ: 173.3, 163.5, 161.8, 159.9, 134.4, 128.9, 114.9, 90.7, 32.4; **HRMS (ESI):** calculated for $C_{15}H_{14}FN_6O_2S_2$ [M + H] $^+$: 393.0604; found: 393.0600.

(5,5'-((4-hydroxyphenyl)methylene)bis(6-amino-2-mercaptopyrimidin-4-ol)) (3d):



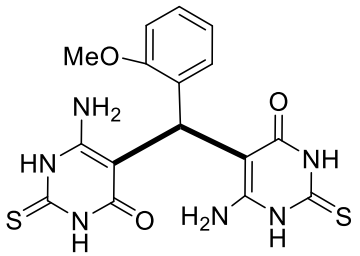
White solid (33.2 mg, 68%), **FT-IR (cm^{-1}):** 3334, 3142, 1629, 1535, 1169; **^{1}H-NMR (400 MHz, DMSO-d$_6$)** δ: 12.03 (s, 2H), 11.79 (s, 2H), 9.07 (s, 1H), 6.84 (d, *J* = 8.1 Hz, 2H), 6.75 (s, 4H), 6.61 (d, *J* = 8.6 Hz, 2H), 5.24 (s, 1H); **^{13}C-NMR (101 MHz, DMSO-d$_6$)** δ: 173.1, 163.4, 155.5, 153.8, 128.1, 127.9, 115.2, 91.1, 32.1; **HRMS (ESI):** calculated for $C_{15}H_{15}N_6O_3S_2$ [M + H] $^+$: 391.0647; found: 391.0642.

(5,5'-(p-tolylmethylene)bis(6-amino-2-mercaptopyrimidin-4-ol)) (3e):



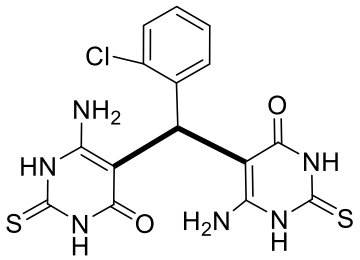
White solid (37.4 mg, 71%), **FT-IR (cm^{-1}):** 3395, 2882, 1624, 1598, 1545, 1170; **^{1}H-NMR (500 MHz, DMSO-d$_6$)** δ: 12.03 (s, 2H), 11.81 (s, 2H), 7.02 (d, *J* = 8.1 Hz, 2H), 6.94 (d, *J* = 7.9 Hz, 2H), 6.76 (s, 4H), 5.30 (s, 1H), 2.22 (s, 3H); **^{13}C-NMR (126 MHz, DMSO-d$_6$)** δ: 173.3, 163.5, 153.9, 135.3, 134.6, 128.9, 126.9, 90.9, 32.6, 21.0; **HRMS (ESI):** calculated for $C_{16}H_{17}N_6O_2S_2$ [M + H] $^+$: 389.0854; found: 389.0855.

(5,5'-((2-methoxyphenyl)methylene)bis(6-amino-2-mercaptopyrimidin-4-ol)) (3f):



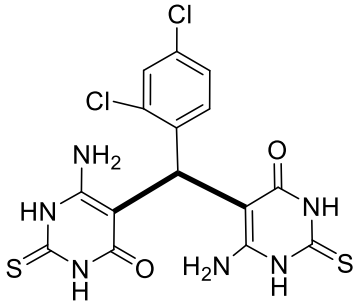
White solid (35.9 mg, 71%), **FT-IR (cm^{-1}):** 3386, 3317, 1637, 1612, 1550, 1172; **^{1}H-NMR (400 MHz, DMSO-d$_6$)** δ: 11.93 (s, 2H), 11.79 (s, 2H), 7.12 (t, *J* = 8.4 Hz, 1H), 7.03 (d, *J* = 7.5 Hz, 1H), 6.84-6.78 (m, 2H), 6.51 (s, 4H), 5.25 (s, 1H), 3.62 (s, 3H); **^{13}C-NMR (101 MHz, DMSO-d$_6$)** δ: 172.9, 163.1, 157.7, 153.2, 127.9, 127.5, 120.3, 111.0, 91.3, 56.0, 29.6. **HRMS (ESI):** calculated for $C_{16}H_{17}N_6O_3S_2$ [M + H] $^{+}$: 405.0804; found: 405.0807.

(5,5'-((2-chlorophenyl)methylene)bis(6-amino-2-mercaptopyrimidin-4-ol)) (3g):



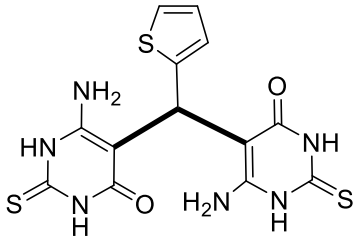
White solid (37.2 mg, 73%), **FT-IR (cm^{-1}):** 3380, 3133, 1634, 1543, 1166; **^{1}H-NMR (400 MHz, DMSO-d$_6$)** δ: 12.04 (s, 2H), 11.90 (s, 2H), 7.35-7.15 (m, 4H), 6.58 (s, 4H), 5.30 (s, 1H); **^{13}C-NMR (101 MHz, DMSO-d$_6$)** δ: 173.2, 163.0, 153.6, 137.5, 132.8, 129.9, 129.4, 128.0, 127.1, 90.2, 32.4. Spectroscopic data matched with ref [29].

(5,5'-((2,4-dichlorophenyl)methylene)bis(6-amino-2-mercaptopyrimidin-4-ol)) (3h):



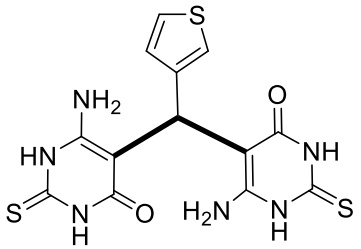
White solid (39.2 mg, 71%), **FT-IR (cm^{-1}):** 3379, 3124, 1630, 1596, 1170; **^{1}H-NMR (500 MHz, DMSO-d$_6$)** δ: 12.05 (s, 2H), 11.91 (s, 2H), 7.45 (d, J = 2.2 Hz, 1H), 7.32 (dd, J = 8.5 Hz, 1H), 7.27 (d, J = 8.4 Hz, 1H), 6.56 (s, 4H), 5.26 (s, 1H); **^{13}C-NMR (126 MHz, DMSO-d$_6$)** δ: 173.3, 163.1, 153.6, 136.8, 133.6, 131.6, 130.9, 129.3, 127.2, 89.9, 32.2; **HRMS (ESI):** calculated for $C_{15}H_{13}Cl_2N_6O_2S_2$ [M + H] $^{+}$: 442.9918; found: 442.9913.

(5,5'-(thiophen-2-ylmethylene)bis(6-amino-2-mercaptopyrimidin-4-ol)) (3i):



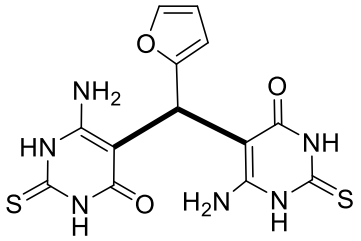
White solid (34.7 mg, 73%), **FT-IR (cm^{-1}):** 3379, 2898, 1632, 1601, 1547, 1170; **^{1}H-NMR (500 MHz, DMSO- d$_6$)** δ: 12.08 (s, 2H), 11.83 (s, 2H), 7.26 (d, *J* = 5.1 Hz, 1H), 6.90 – 6.84 (m, 5H, four –NH_2 proton and one H^a protons are merged), 6.66-6.64 (m, 1H), 5.48 (s, 1H); **^{13}C-NMR (101 MHz, DMSO-d$_6$)** δ: 173.4, 163.7, 153.6, 144.0, 126.8, 124.3, 124.2, 91.4, 30.4; **HRMS (ESI):** calculated for $C_{13}H_{13}N_6O_2S_3$ [M + H] $^+$: 381.0262; found: 381.0263.

(5,5'-(thiophen-3-ylmethylene)bis(6-amino-2-mercaptopyrimidin-4-ol)) (3j):



White solid (34.2 mg, 72%), **FT-IR (cm^{-1}):** 3382, 3157, 1631, 1600, 1547, 1173; **^{1}H-NMR (400 MHz, DMSO-d$_6$)** δ: 12.03 (s, 2H), 11.79 (s, 2H), 7.31 (dd, J = 5.0 Hz, 1H), 6.95 – 6.93 (m, 1H), 6.81-6.76 (m, 5H, four –NH_2 proton and one H^a protons are merged), 5.20 (s, 1H); **^{13}C-NMR (101 MHz, DMSO-d$_6$)** δ: 186.5, 175.0, 173.1, 163.3, 162.1, 154.8, 153.5, 139.5, 129.1, 128.4, 125.3, 120.1, 91.5, 78.7, 30.3; **HRMS (ESI):** calculated for $C_{13}H_{13}N_6O_2S_3$ [M + H] $^+$: 381.0262; found: 381.0255.

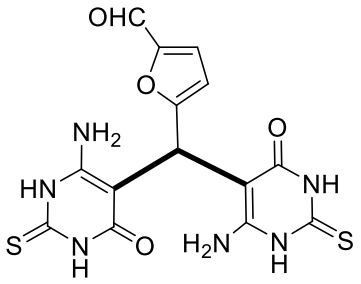
(**5,5'-(furan-2-ylmethylene)bis(6-amino-2-mercaptopyrimidin-4-ol)) (3k):**



White solid (33.2 mg, 73%), **FT-IR (cm^{-1}):** 3401, 3168, 2900, 1630, 1606, 1544, 1166; **^{1}H-NMR (500 MHz, DMSO-d$_6$)** δ: 12.05 (s, 2H), 11.82 (s, 2H), 7.43 (s, 1H), 6.79 (s, 4H), 6.22 (dd, J = 3.1 Hz, 1H), 6.00

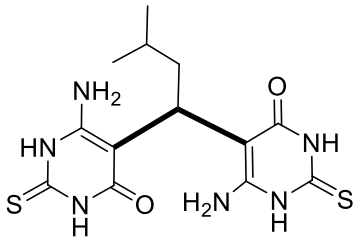
(s, 1H), 5.22 (s, 1H); **^{13}C-NMR (126 MHz, DMSO-d$_6$)** δ: 173.4, 163.2, 153.4, 152.1, 141.7, 110.6, 106.1, 89.9, 29.0; **HRMS (ESI):** calculated for $C_{13}H_{13}N_6O_3S_2$ $[M + H]^+$: 365.0491; found: 365.0487.

(5-(bis(4-amino-6-hydroxy-2-mercaptopyrimidin-5-yl)methyl)furan-2-carbaldehyde) (3l):



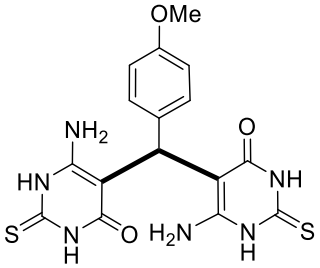
White solid (32.8 mg, 67%), **FT-IR (cm^{-1}):** 3379, 3170, 1627, 1535, 1157; **^{1}H-NMR (500 MHz, DMSO-d$_6$)** δ: 12.14 (s, 1H), 11.92 (s, 1H), 9.42 (s, 1H), 7.43 (d, J = 3.6 Hz, 1H), 6.78 (br, 4H), 6.40 (dd, J = 3.6, 1.3 Hz, 1H), 5.33 (s, 1H). **^{13}C-NMR (126 MHz, DMSO-d$_6$)** δ: 177.7, 173.5, 163.2, 160.4, 153.5, 152.0, 121.8, 110.1, 89.1, 29.5; **HRMS (ESI):** calculated for $C_{14}H_{13}N_6O_4S_2$ $[M + H]^+$: 393.0440; found: 393.0445.

(5,5'-(3-methylbutane-1,1-diyl)bis(6-amino-2-mercaptopyrimidin-4-ol)) (3o) :



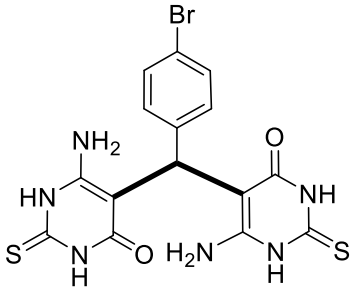
White solid (25.7 mg, 58%), **FT-IR (cm^{-1}):** 3389, 3058, 2891, 1635, 1597, 1548, 1173; **^{1}H-NMR (400 MHz, DMSO-d$_6$)** δ: 11.98 (s, 2H), 11.73 (s, 2H), 6.37 (s, 4H), 4.70 (s, 1H), 3.94 (t, J = 8.0 Hz, 1H), 1.89 (br, 2H), 1.36 – 1.26 (m, 1H), 0.79 (d, J = 6.6 Hz, 6H); **^{13}C-NMR (101 MHz, DMSO-d$_6$)** δ: 175.0, 172.9, 162.1, 154.8, 78.6, 37.4, 26.9, 26.6, 22.9; **HRMS (ESI):** calculated for $C_{13}H_{19}N_6O_2S_2$ $[M + H]^+$: 355.1011; found: 355.0990.

5,5'-((4-methoxyphenyl)methylene)bis(6-amino-2-thioxo-2,3-dihydropyrimidin-4(1H)-one) (3p):



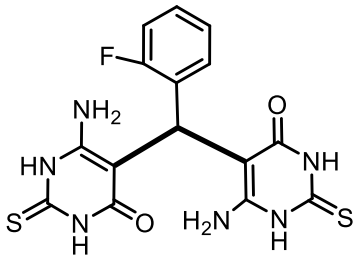
White solid (33.8 mg, 67 %), **FT-IR (cm^{-1}):** 3387, 3066, 1631, 1543, 1172; **^{1}H-NMR (500 MHz, DMSO-d$_6$)** δ: 12.02 (s, 2H), 11.80 (s, 2H), 6.96 (d, J = 7.9 Hz, 2H), 6.78 (m, 6H, merge four -NH_2 proton and two benzene ring proton), 5.29 (s, 1H), 3.70 (s, 3H); **^{13}C-NMR (126 MHz, DMSO-d$_6$)** δ: 173.3, 163.5, 157.6, 153.9, 130.0, 129.9, 128.0, 113.8, 91.1, 55.5, 32.2; **HRMS (ESI):** calculated for $C_{16}H_{17}N_6O_3S_2$ [M + H] $^+$: 405.0804; found: 405.0807.

5,5'-((4-bromophenyl)methylene)bis(6-amino-2-thioxo-2,3-dihydropyrimidin-4(1H)-one) (3q):



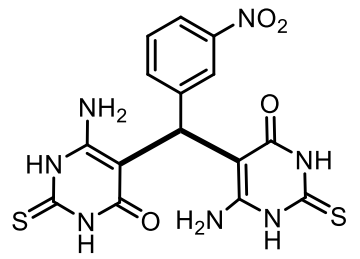
White solid (40.7 mg, 72 %), **FT-IR (cm^{-1}):** 3325, 3128, 1593, 1535, 1168; **^{1}H-NMR (500 MHz, DMSO-d$_6$)** δ: 12.05 (s, 2H), 11.83 (s, 2H), 7.34 (d, J = 8.5 Hz, 2H), 7.00 (d, J = 8.0 Hz, 2H), 6.73 (br, 4H), 5.25 (s, 1H); **^{13}C-NMR (126 MHz, DMSO-d$_6$)** δ: 173.3, 163.5, 153.9, 138.1, 131.1, 129.5, 118.9, 90.4, 32.8; **HRMS (ESI):** calculated for $C_{15}H_{14}BrN_6O_2S_2$ [M + H] $^+$: 452.9803; found: 452.9807.

5,5'-((2-fluorophenyl)methylene)bis(6-amino-2-thioxo-2,3-dihydropyrimidin-4(1H)-one) (3r):



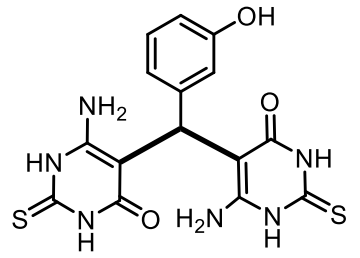
White solid (36.8 mg, 76%), **FT-IR (cm^{-1}):** 3394, 2901, 1605, 1543, 1206; **^{1}H-NMR (500 MHz, DMSO-d$_6$)** δ: 12.05 (s, 2H), 11.87 (s, 2H), 7.20 (dd, J = 6.4 Hz, 1H), 7.13 (t, J = 7.9 Hz, 1H), 7.07 (td, J = 7.6 Hz, 1H), 7.01 (dd, J = 8.6 Hz, 1H), 6.62 (s, 4H), 5.37 (s, 1H); **^{13}C-NMR (126 MHz, DMSO-d$_6$)** δ: 173.2, 172.6, 163.3, 162.2, 160.2, 153.3, 129.1, 128.3, 126.3, 124.3, 115.4, 115.3, 90.3, 29.1; Spectroscopic data matched with ref [29].

5,5'-((3-nitrophenyl)methylene)bis(6-amino-2-thioxo-2,3-dihydropyrimidin-4(1H)-one) (3s):



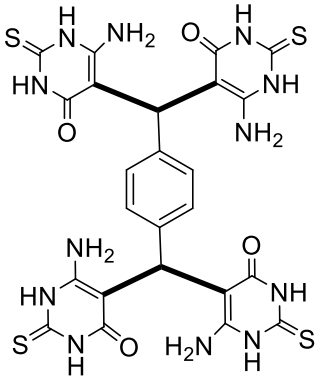
White solid (40.8 mg, 78%), **FT-IR (cm^{-1}):** 3399, 2894, 1702, 1603, 1554, 1274; **^{1}H-NMR (500 MHz, DMSO-d$_6$)** δ: 12.13 (s, 2H), 11.92 (s, 2H), 8.02 (dd, J = 7.4 Hz, 1H), 7.84 (s, 1H), 7.58 (d, J = 7.1 Hz, 1H), 7.53 (t, J = 7.9 Hz, 1H), 6.79 (s, 4H), 5.44 (s, 1H). ; **^{13}C-NMR (126 MHz, DMSO-d$_6$)** δ: 173.5, 172.6, 163.5, 154.0, 148.3, 141.4, 134.3, 129.9, 121.8, 121.2, 89.8, 33.0; **HRMS (ESI):** calculated for $C_{15}H_{14}N_7O_4S_2$ $[M + H]^+$: 420.0549; found: 420.0546.

5,5'-((3-hydroxyphenyl)methylene)bis(6-amino-2-thioxo-2,3-dihydropyrimidin-4(1H)-one) (3t):



White solid (35.1 mg, 72%), **FT-IR (cm^{-1}):** 3399, 2902, 1699, 1605, 1553, 1201; **^{1}H-NMR (500 MHz, DMSO-d$_6$)** δ: 12.05 (s, 2H), 11.83 (s, 2H), 9.07 (s, 1H), 7.00 (t, J = 7.5 Hz, 1H), 6.77 (s, 4H), 6.50 (d, J = 7.9 Hz, 3H), 5.27 (s, 1H); **^{13}C-NMR (126 MHz, DMSO-d$_6$)** δ: 173.3, 172.6, 163.5, 157.7, 153.9, 140.0, 129.3, 117.7, 113.8, 112.8, 90.9, 32.9; **HRMS (ESI):** calculated for $C_{15}H_{15}N_6O_3S_2$ [M + H] $^{+}$: 391.0647; found: 391.0644.

5,5',5'',5'''-(1,4-phenylenebis(methanetriyl))tetrakis(6-amino-2-thioxo-2,3-dihydropyrimidin-4(1H)-one) (4a):



White solid (214.6 mg, 64%), **FT-IR (cm^{-1}):** 3378, 3197, 2899, 1632, 1599, 1543, 1173; **^{1}H-NMR (400 MHz, DMSO-d$_6$)** δ: 12.05 (s, 4H), 11.91 (s, 4H), 7.44 (d, J = 9.4 Hz, 2H), 7.25 (d, J = 5.9 Hz, 2H), 6.53 (s, 8H), 5.29 (s, 2H); **^{13}C-NMR (101 MHz, DMSO-d$_6$)** δ: 173.2, 162.9, 162.1, 154.8, 153.5, 140.4, 130.5, 128.6, 128.2, 127.9, 89.9, 78.6, 33.3, 29.5; **HRMS (ESI):** calculated for $C_{24}H_{23}N_{12}O_4S_2$ [M + H]$^{+}$: 671.0848; found: 671.0841.

8. References

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9. FT-IR, ^{1}H and ^{13}C-NMR spectra

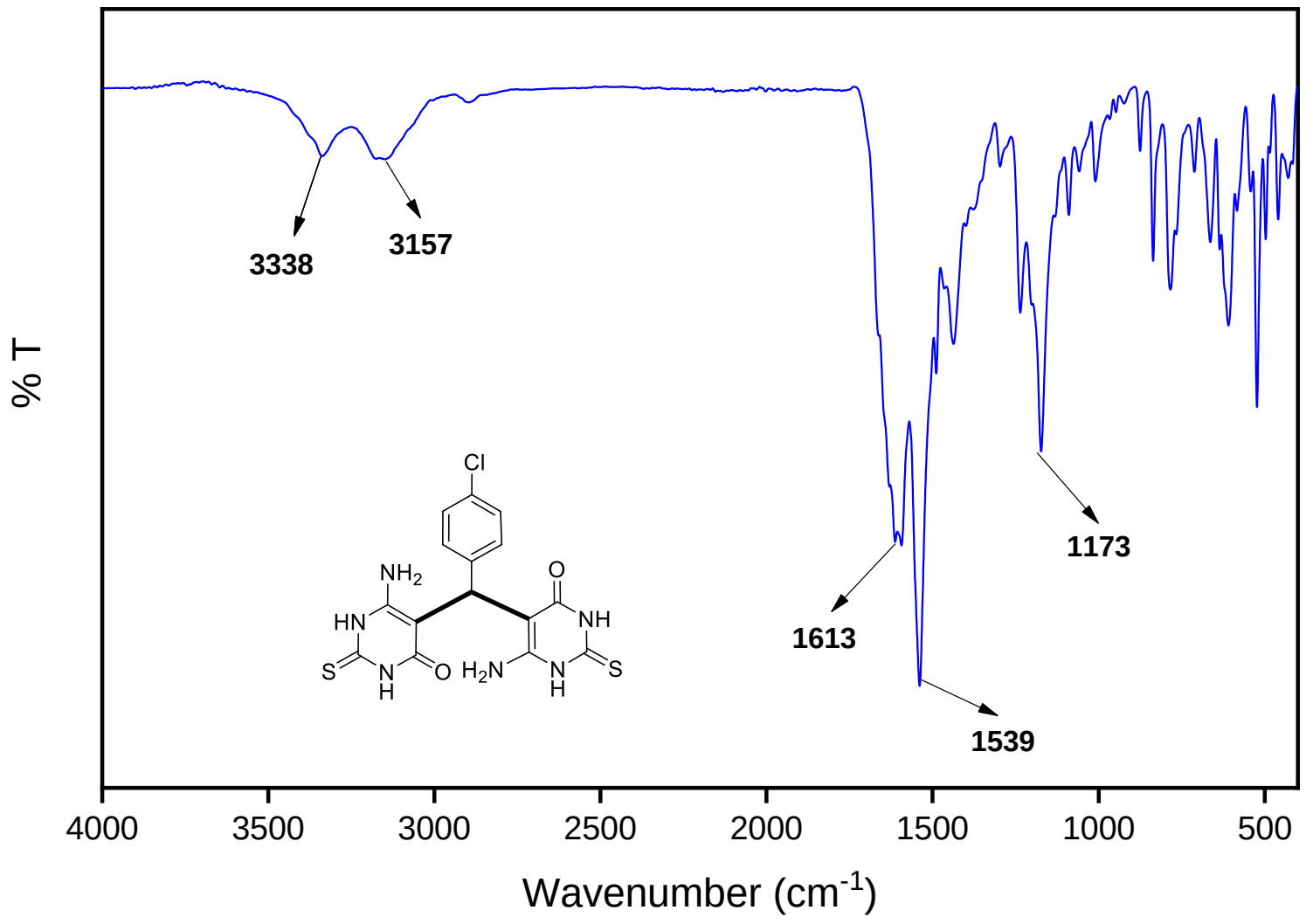

Figure S23. FT-IR spectra of compound **3a**.

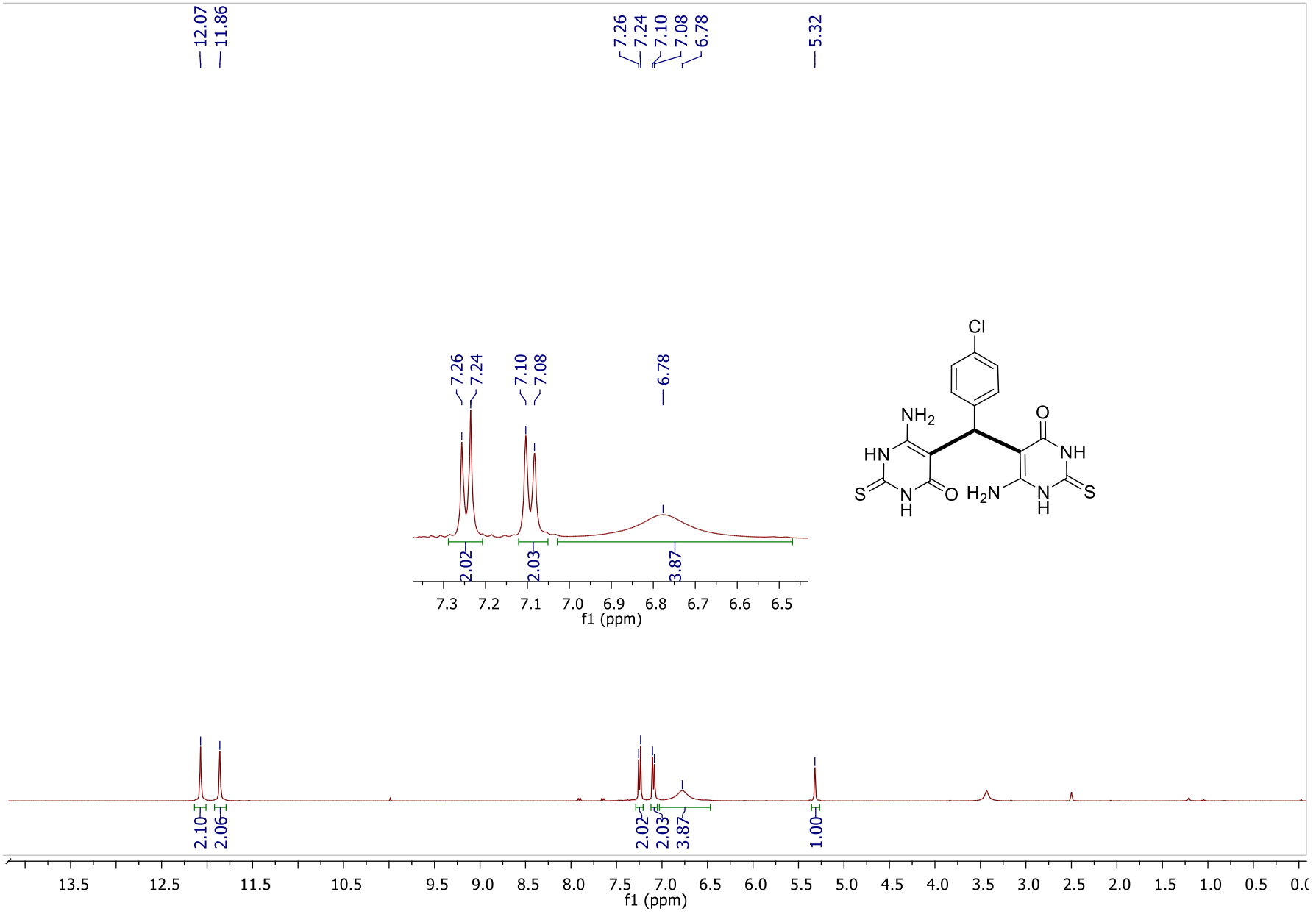

Figure S24. ^{1}H-NMR (400 MHz, DMSO-d_6) spectra of compound **3a**.

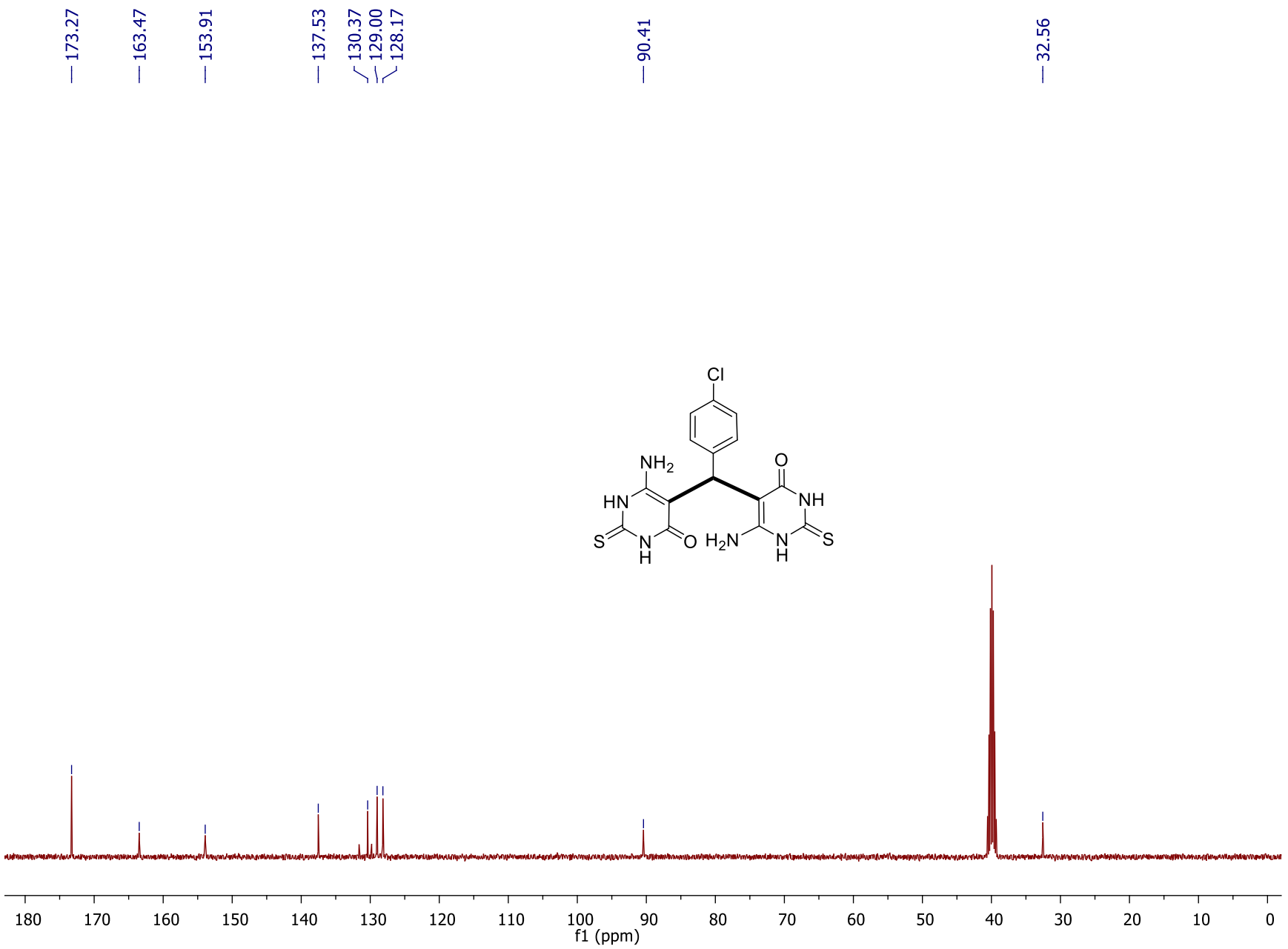

Figure S25. ^{13}C-NMR (101 MHz, DMSO-d_6) spectra of compound **3a**.

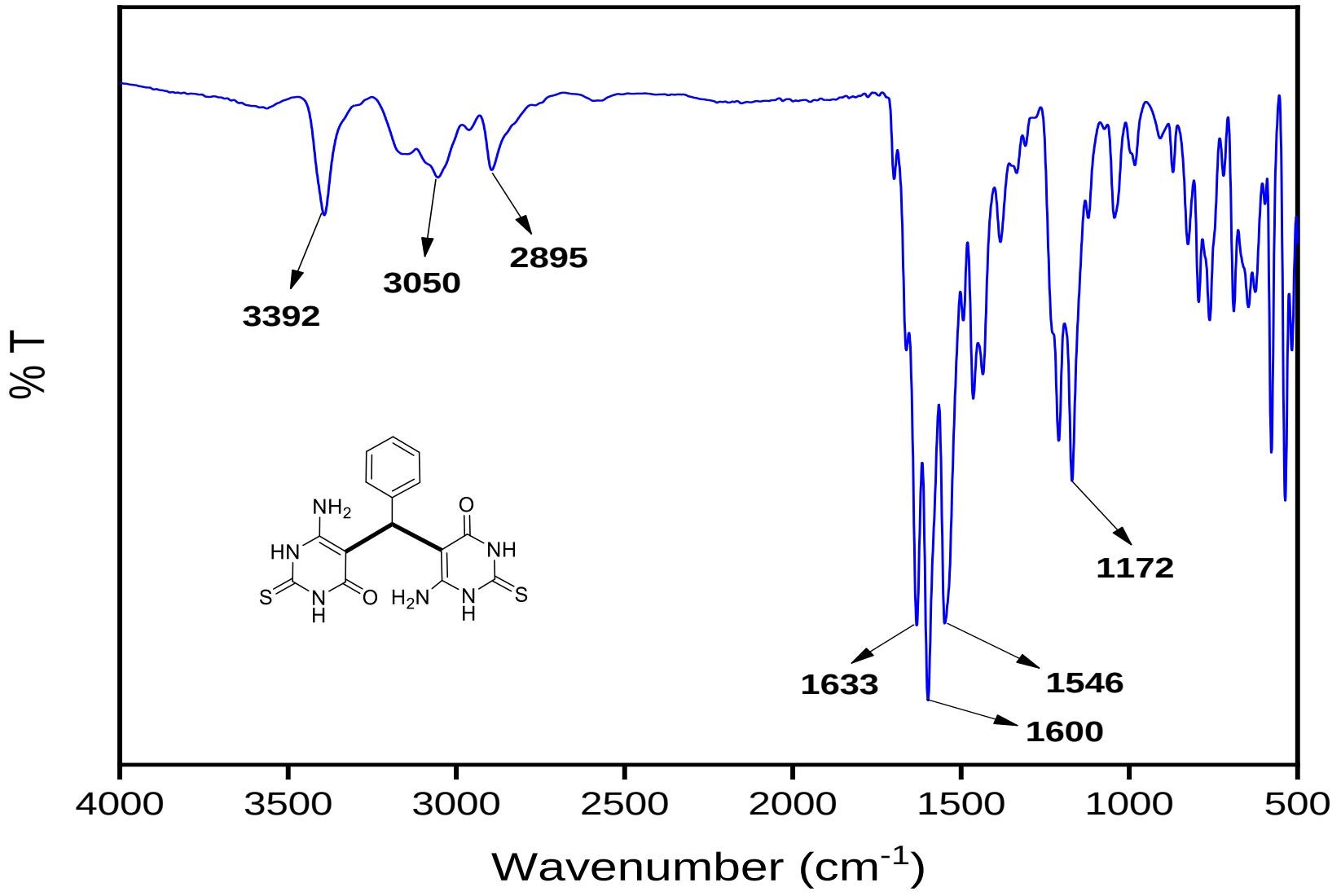

Figure S26. FT-IR spectra of compound **3b**.

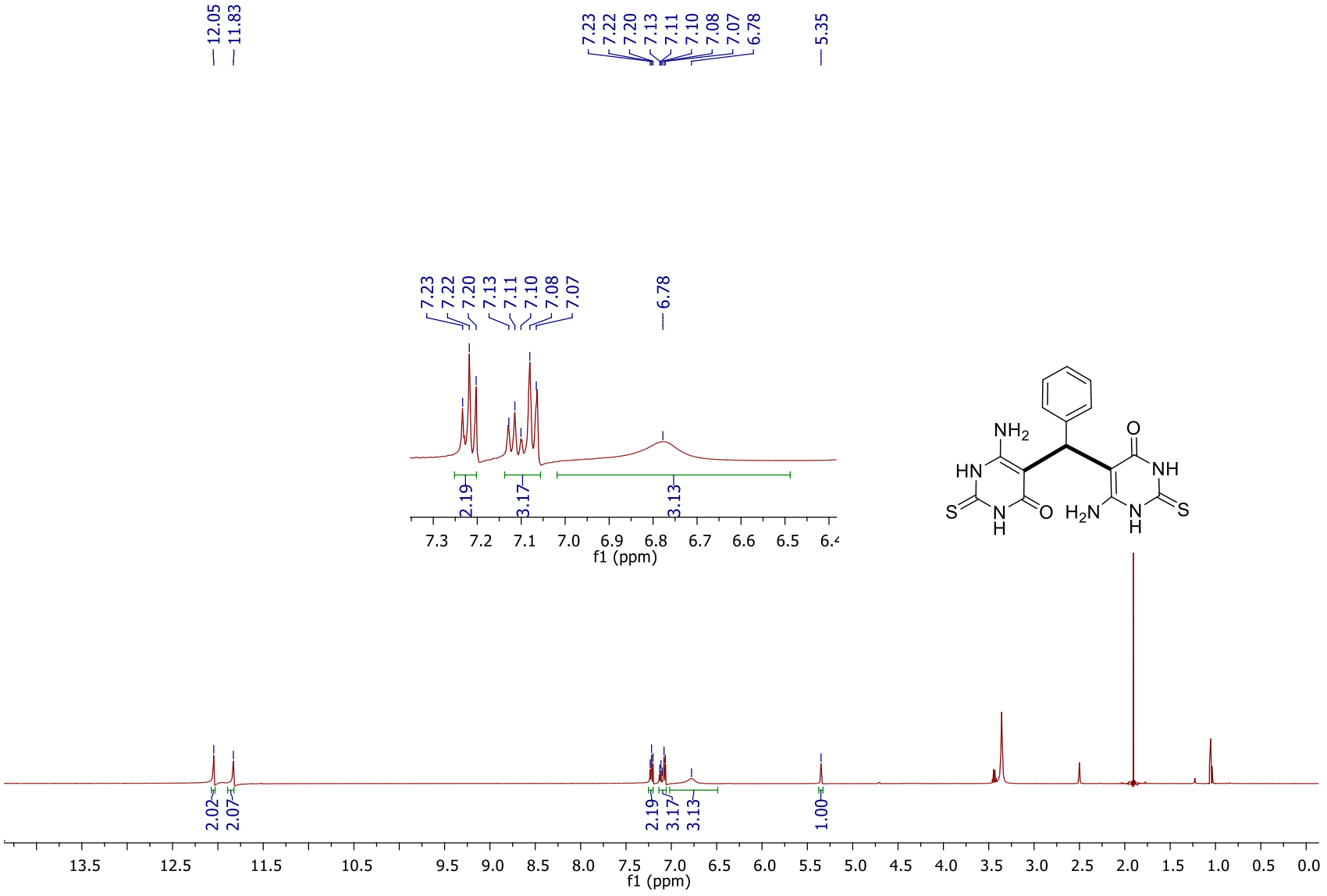

Figure S27. ^{1}H-NMR (500 MHz, DMSO-d_6) spectra of compound **3b**.

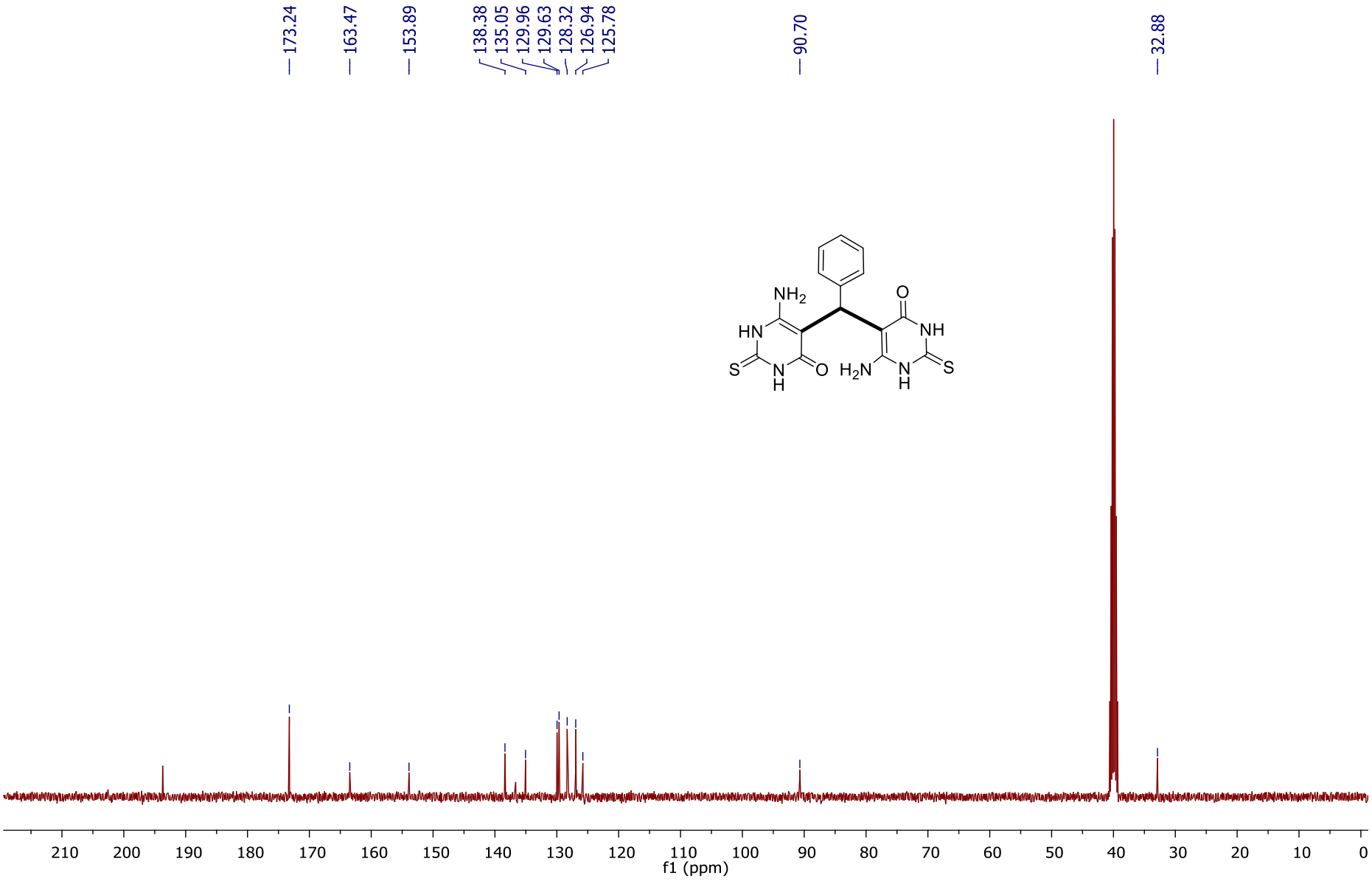

Figure S28. ^{13}C-NMR (101 MHz, DMSO-d_6) spectra of compound **3b**.

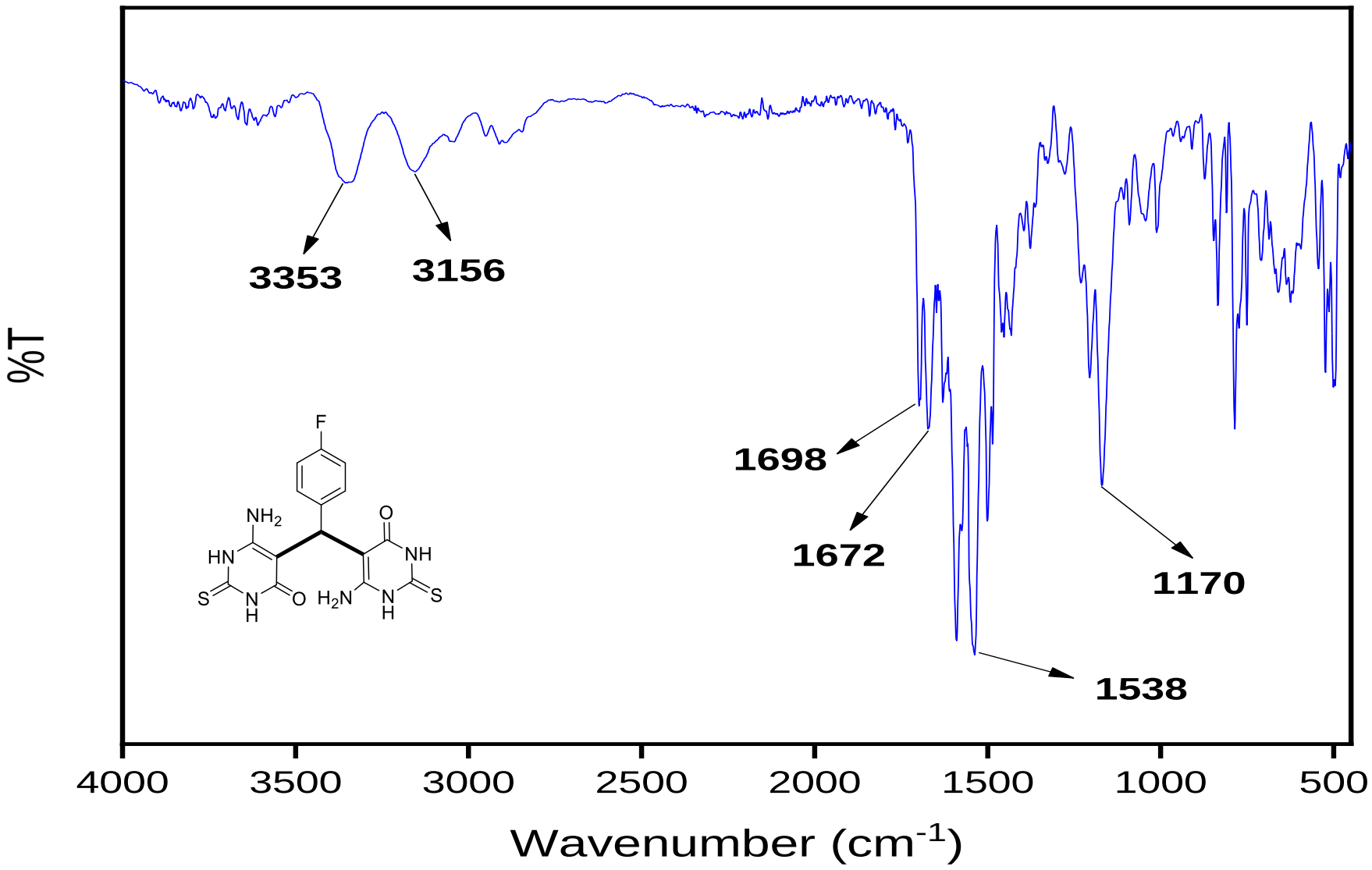

Figure S29. FT-IR spectra of compound **3c**.

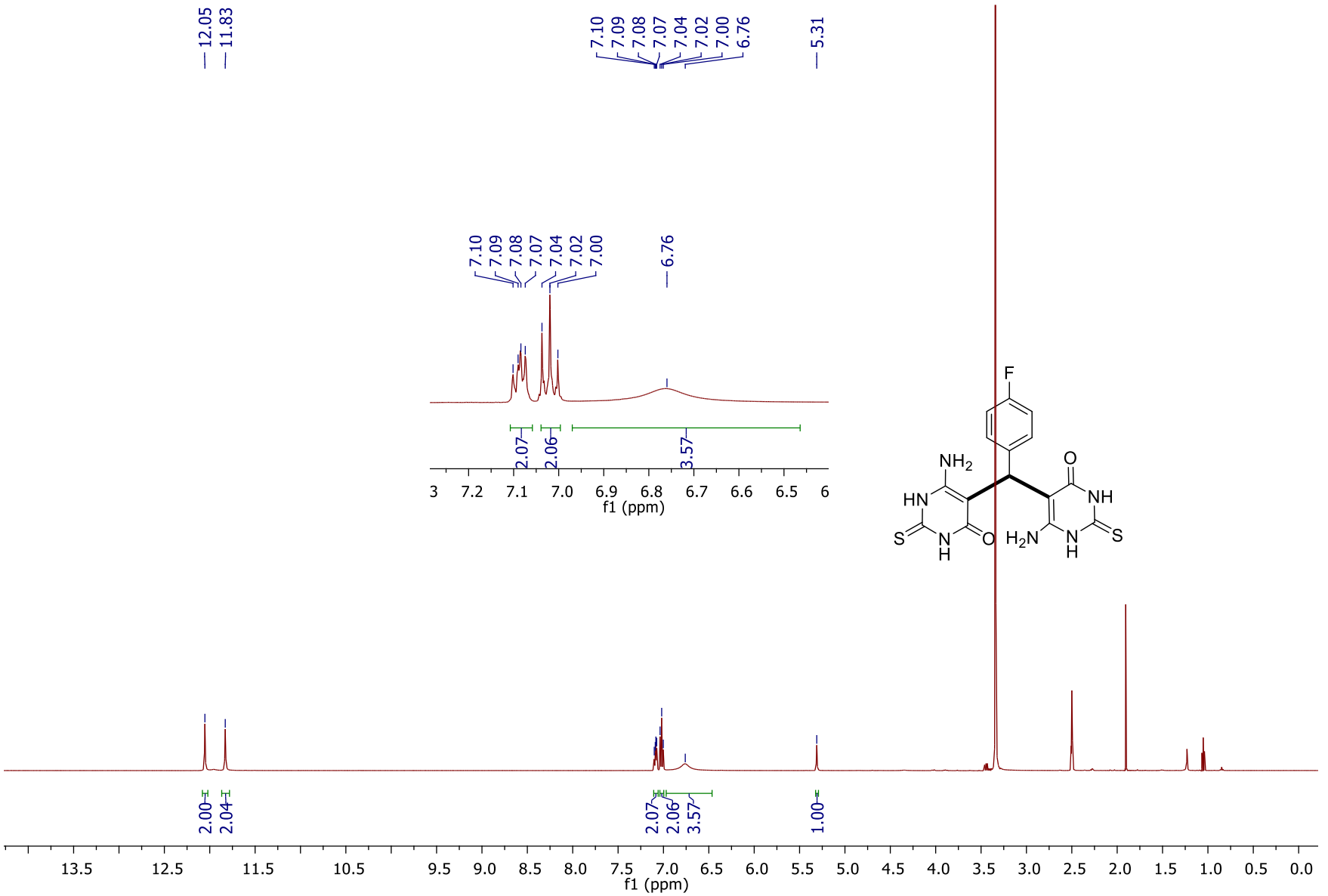

Figure S30. ^{1}H-NMR (500 MHz, DMSO-d_6) spectra of compound **3c**.

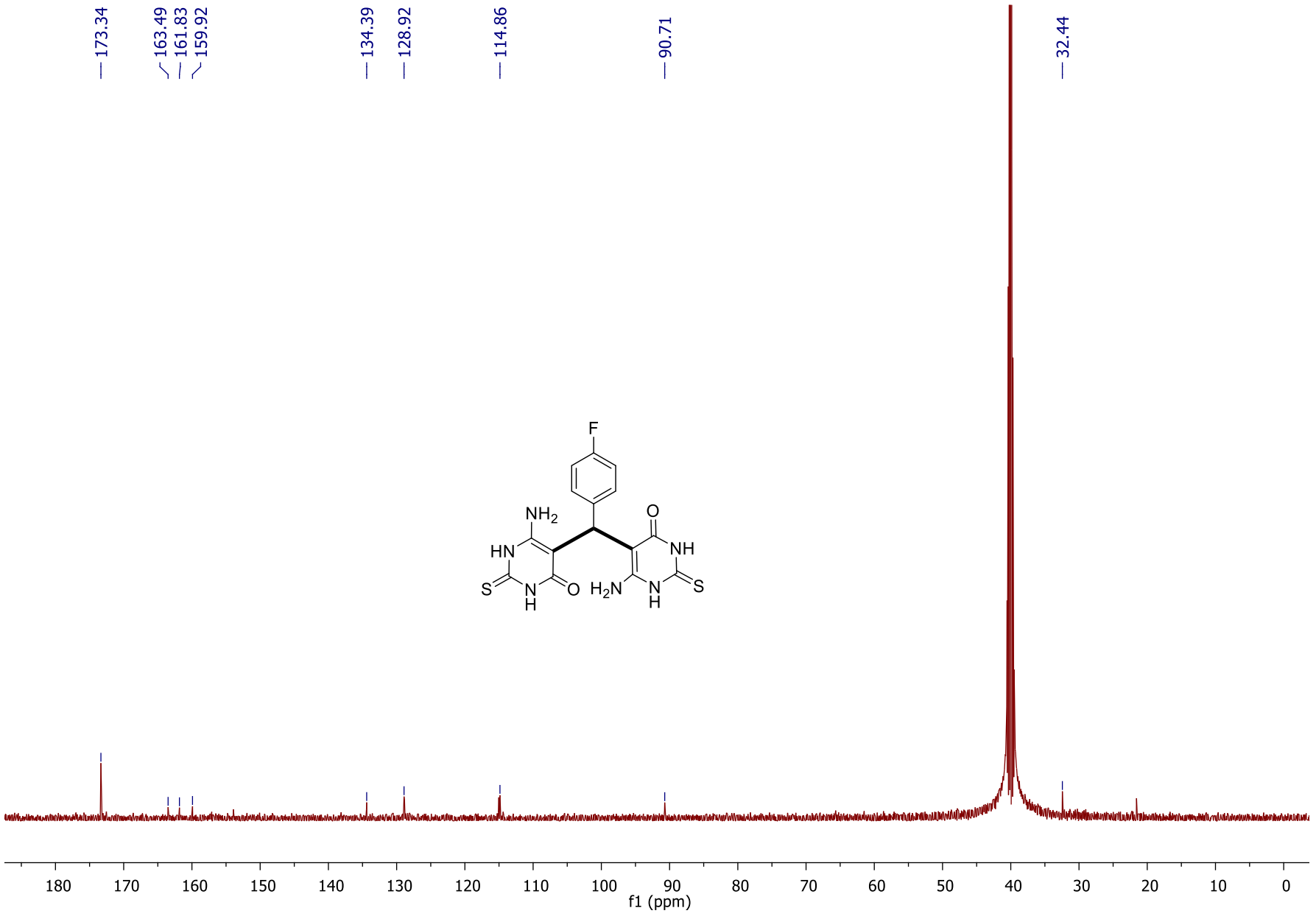

Figure S31. ^{13}C-NMR (126 MHz, DMSO-d_6) spectra of compound **3c**.

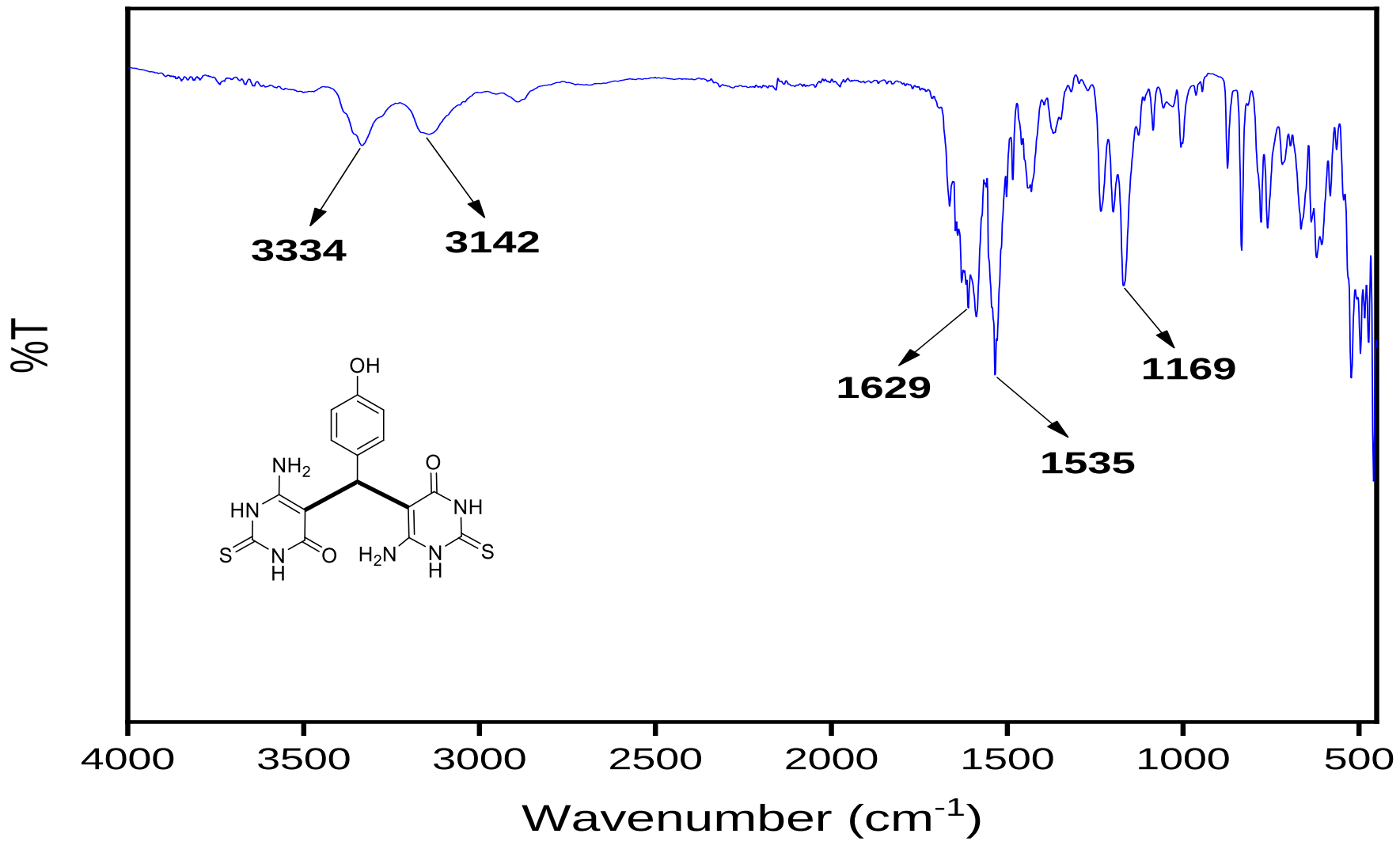

Figure S32. FT-IR spectra of compound **3d**.

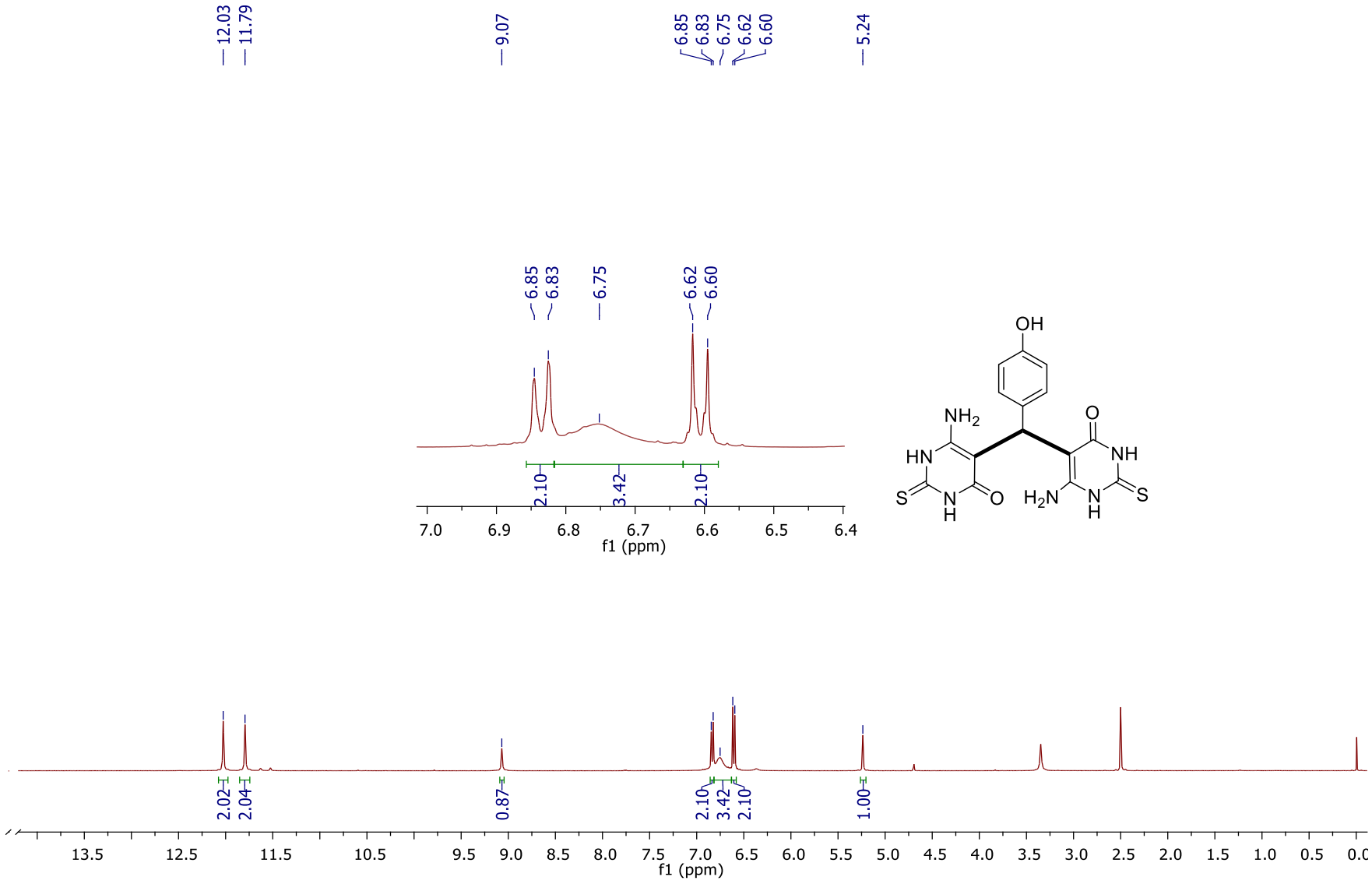

Figure S33. ^{1}H-NMR (400 MHz, DMSO-d_6) spectra of compound **3d**.

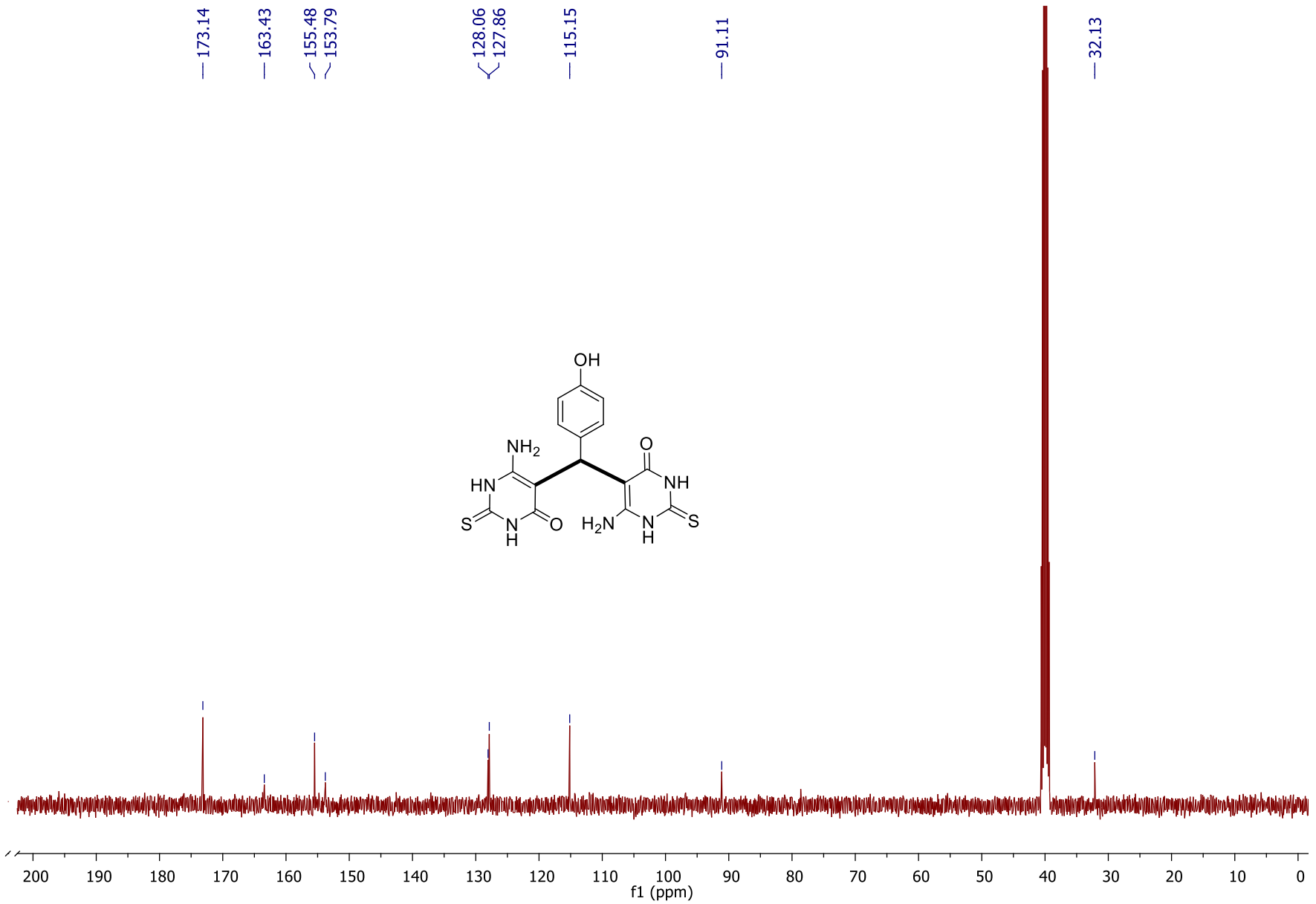

Figure S34. ^{13}C-NMR (101 MHz, DMSO-d_6) spectra of compound **3d**.

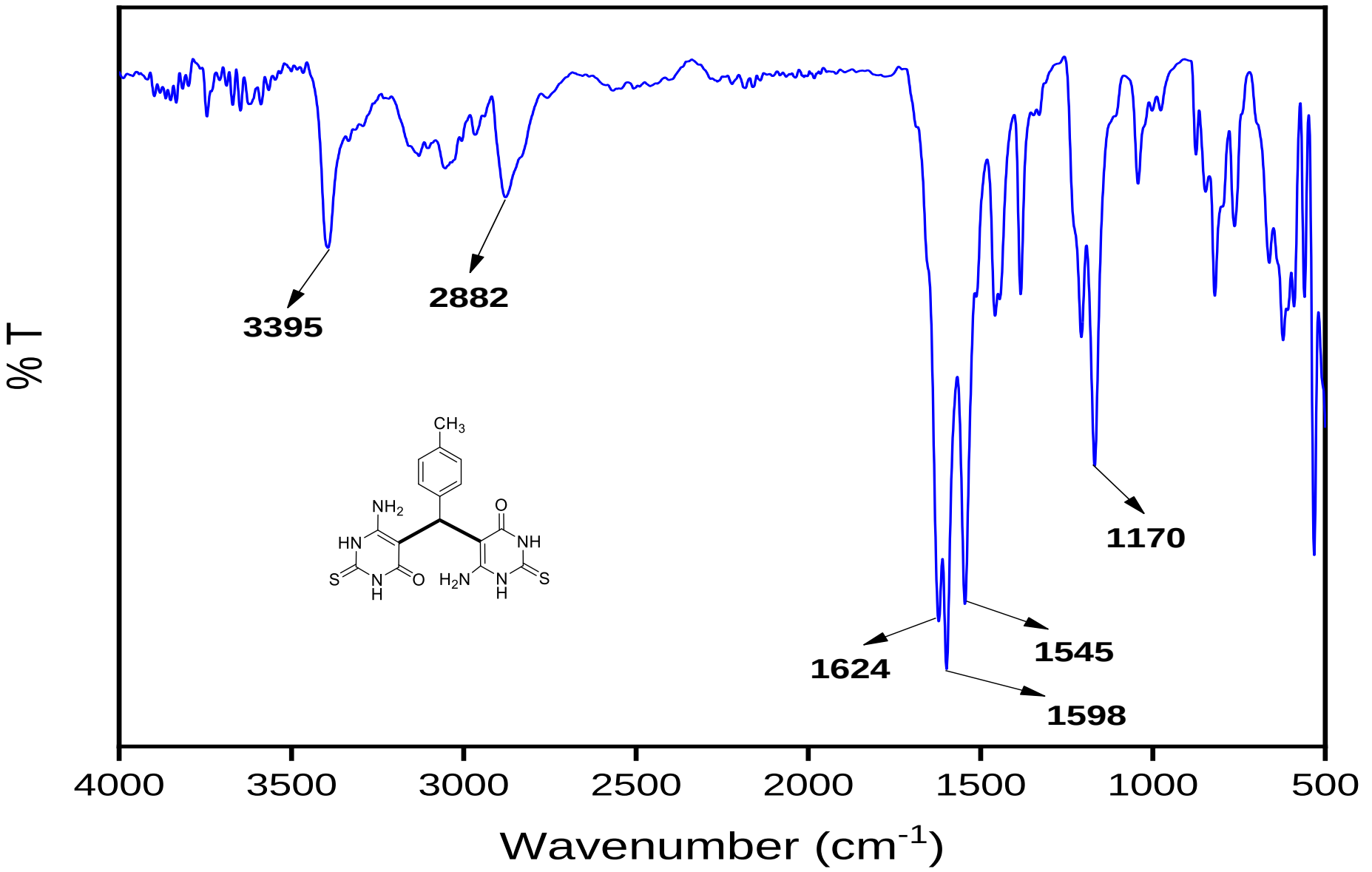

Figure S35. FT-IR spectra of compound **3e**.

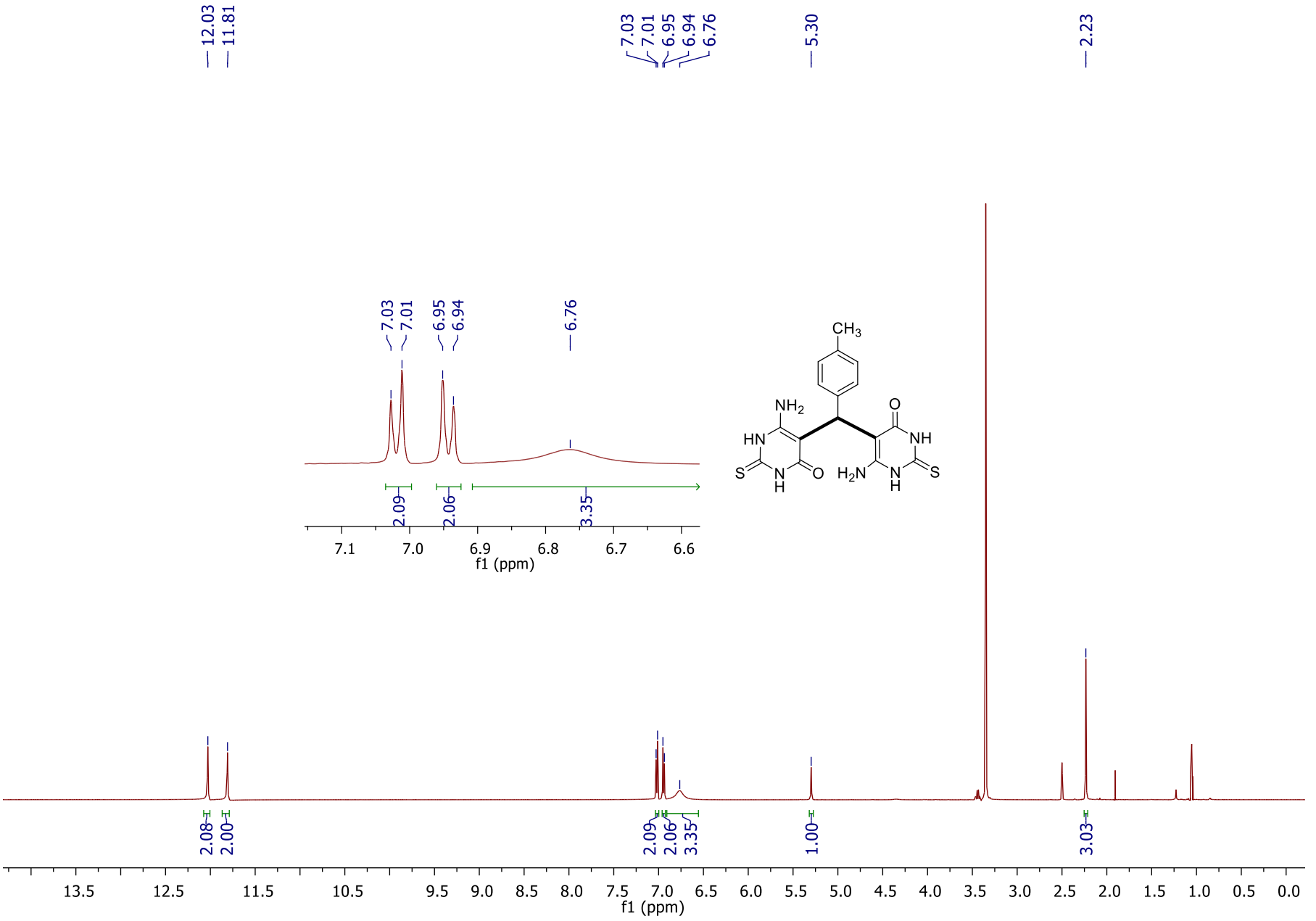

Figure S36. ^{1}H-NMR (500 MHz, DMSO-d_6) spectra of compound **3e**.

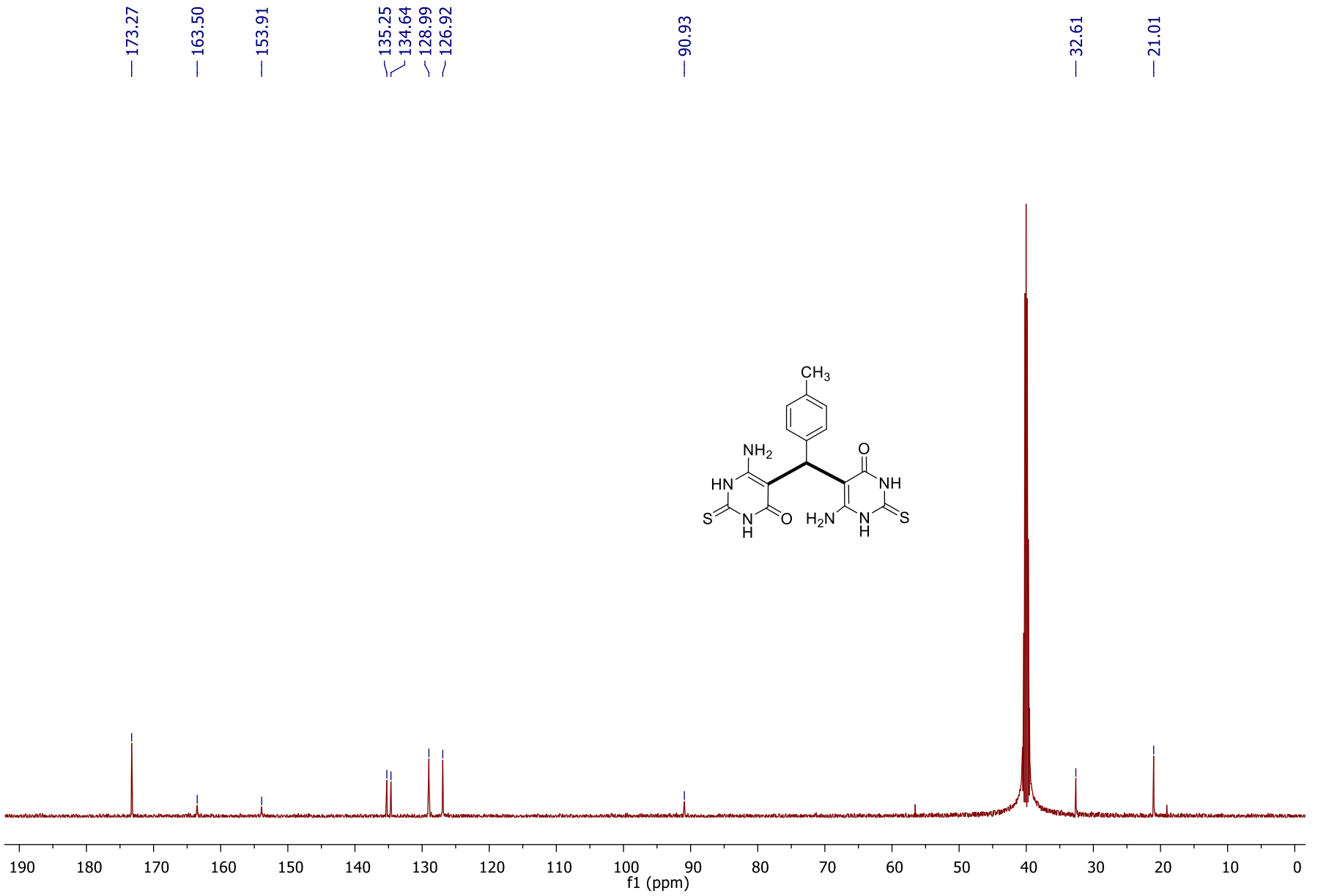

Figure S37. ^{13}C-NMR (126 MHz, DMSO-d_6) spectra of compound **3e**.

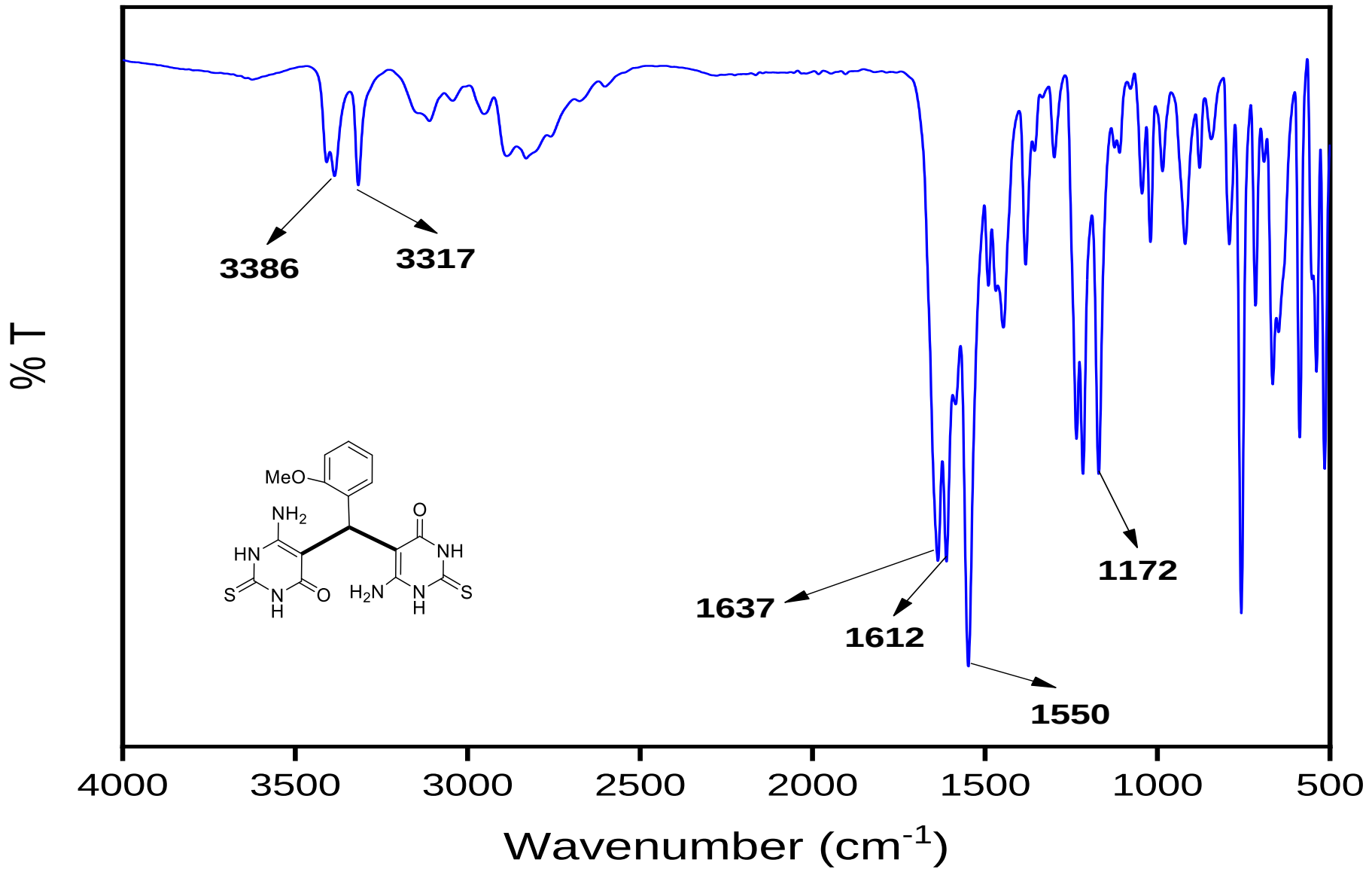

Figure S38. FT-IR spectra of compound **3f**.

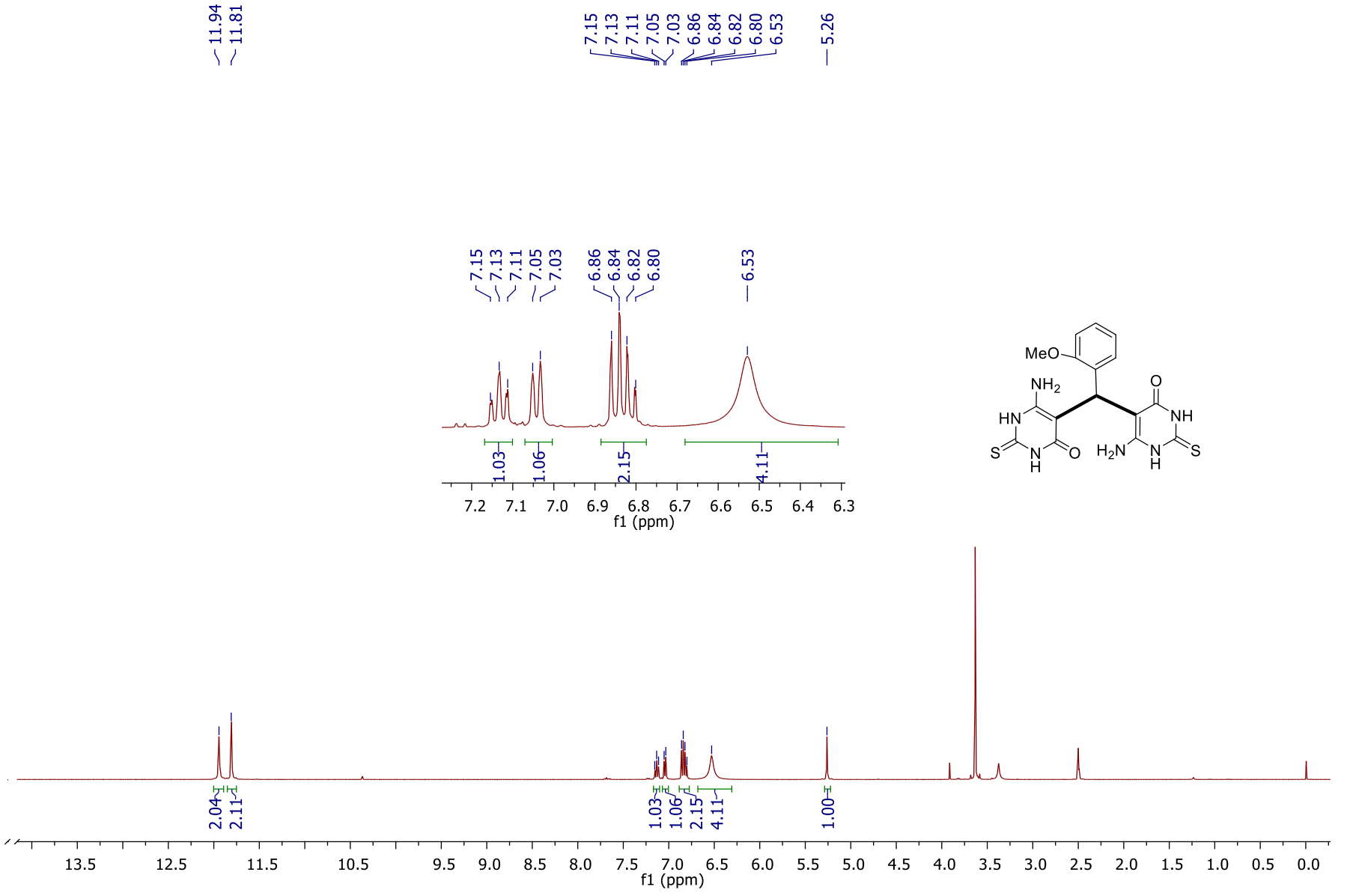

Figure S39. ^{1}H-NMR (400 MHz, DMSO-d_6) spectra of compound **3f**.

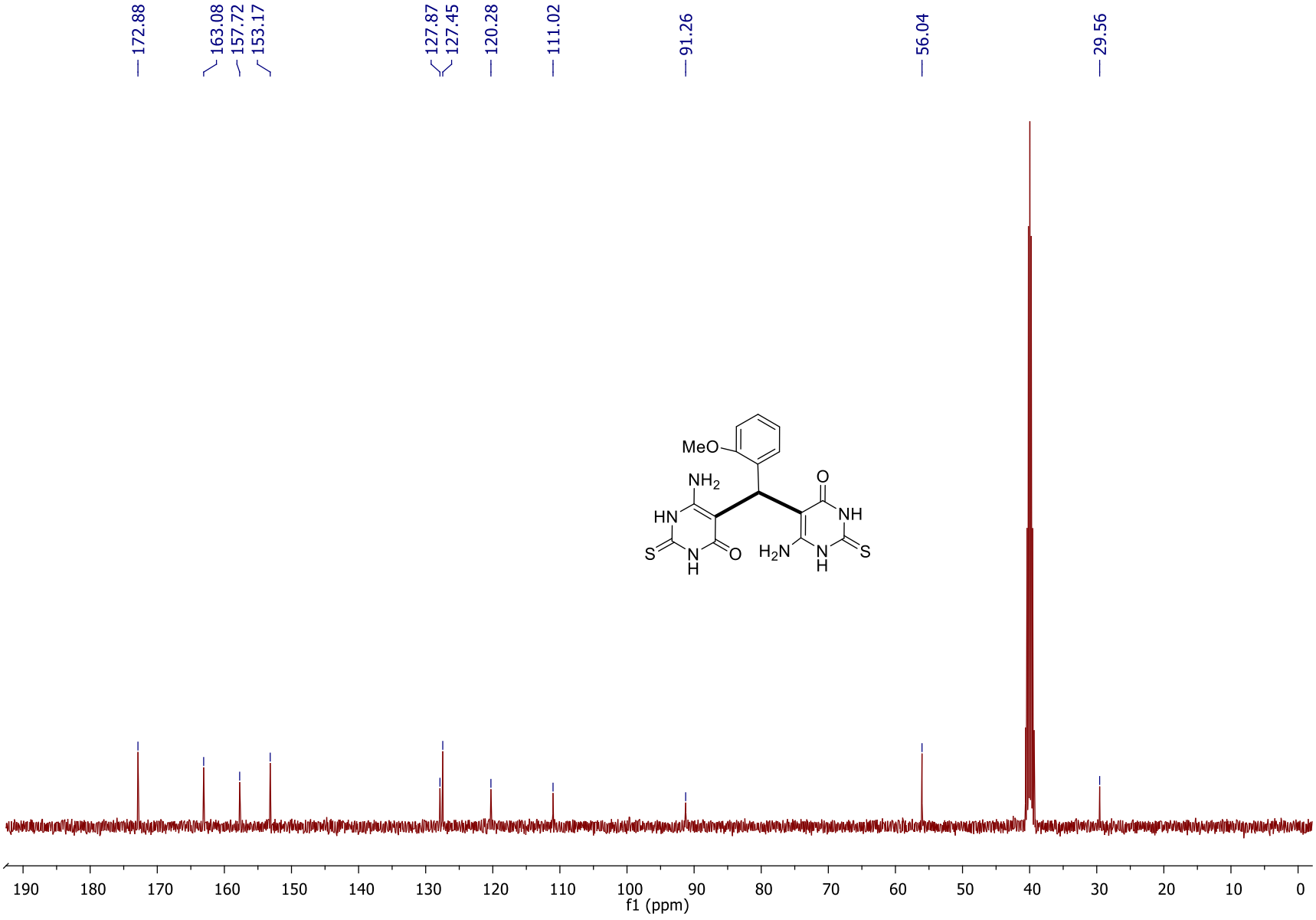

Figure S40. ^{13}C-NMR (101 MHz, DMSO-d_6) spectra of compound **3f**.

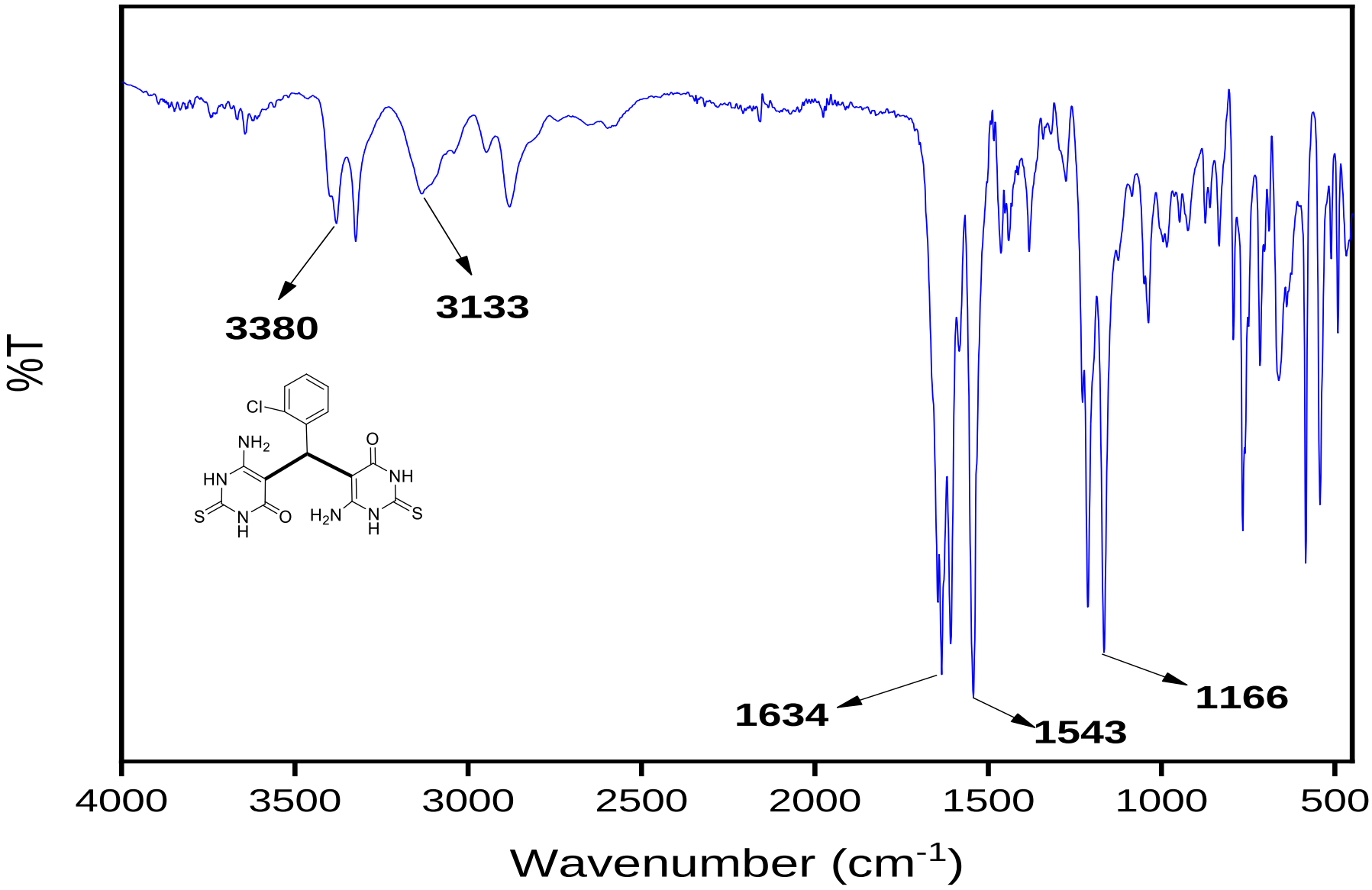

Figure S41. FT-IR spectra of compound **3g**.

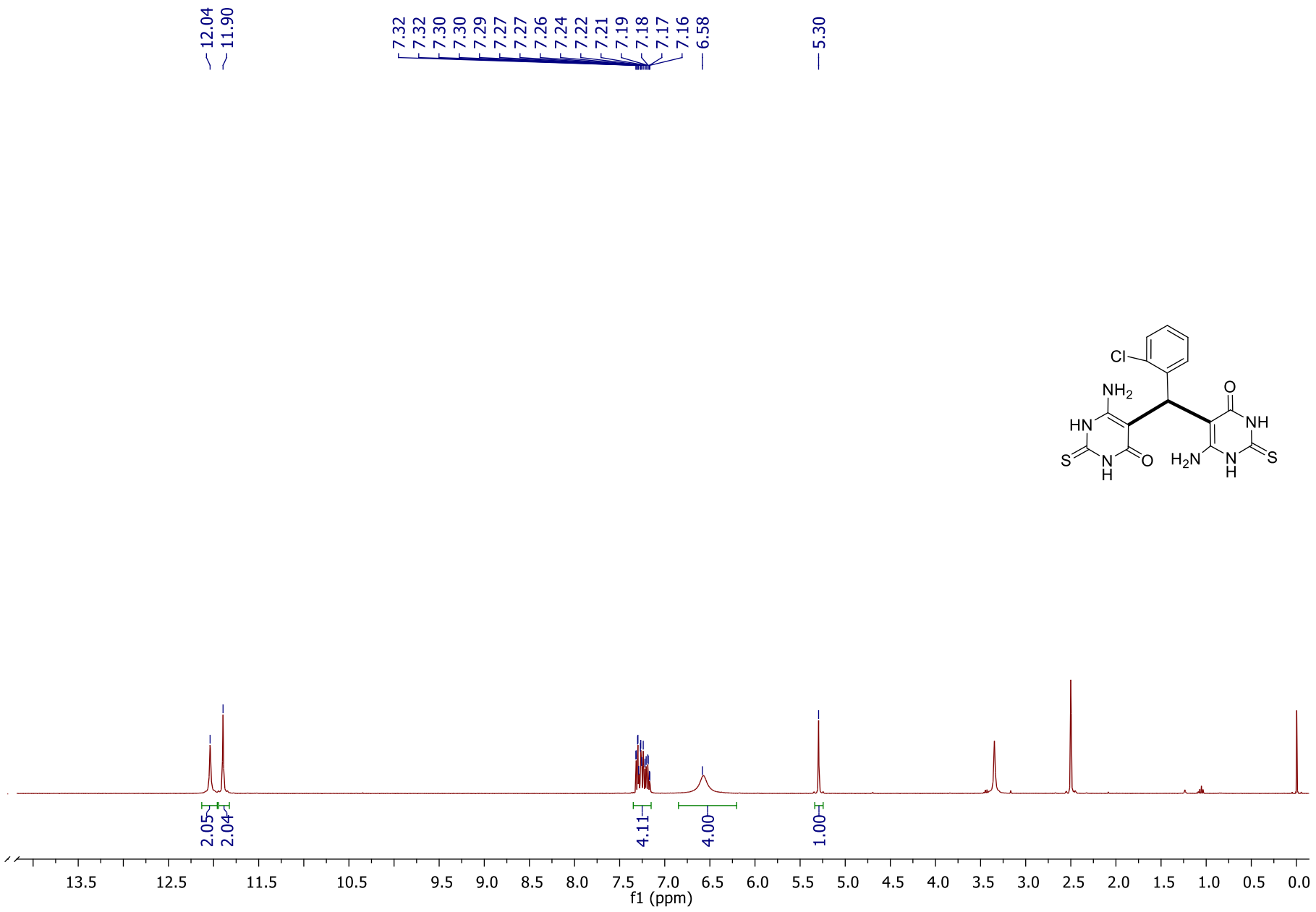

Figure S42. ^{1}H-NMR (400 MHz, DMSO-d_6) spectra of compound **3g**.

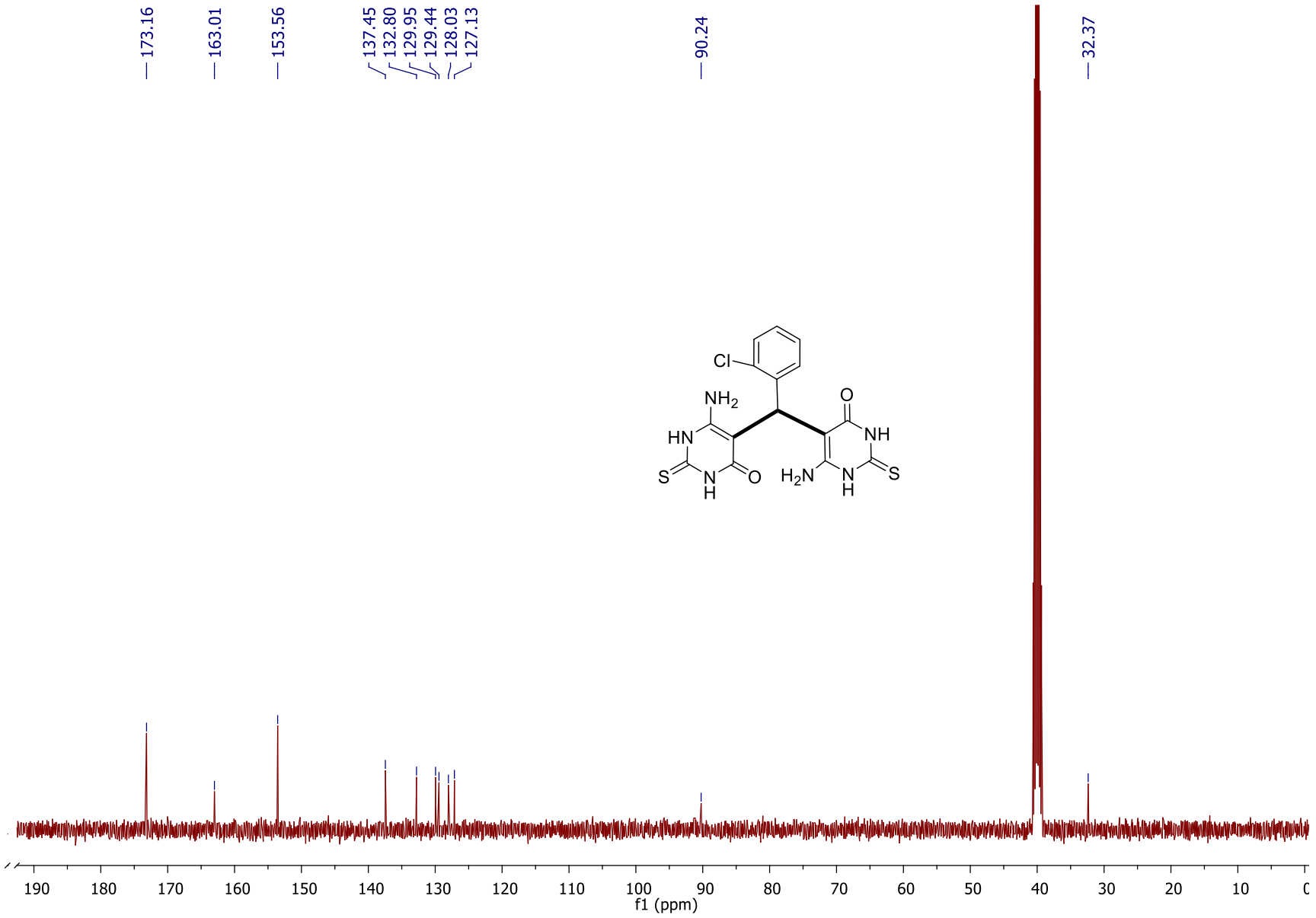

Figure S43. ^{13}C-NMR (101 MHz, DMSO-d_6) spectra of compound **3g**.

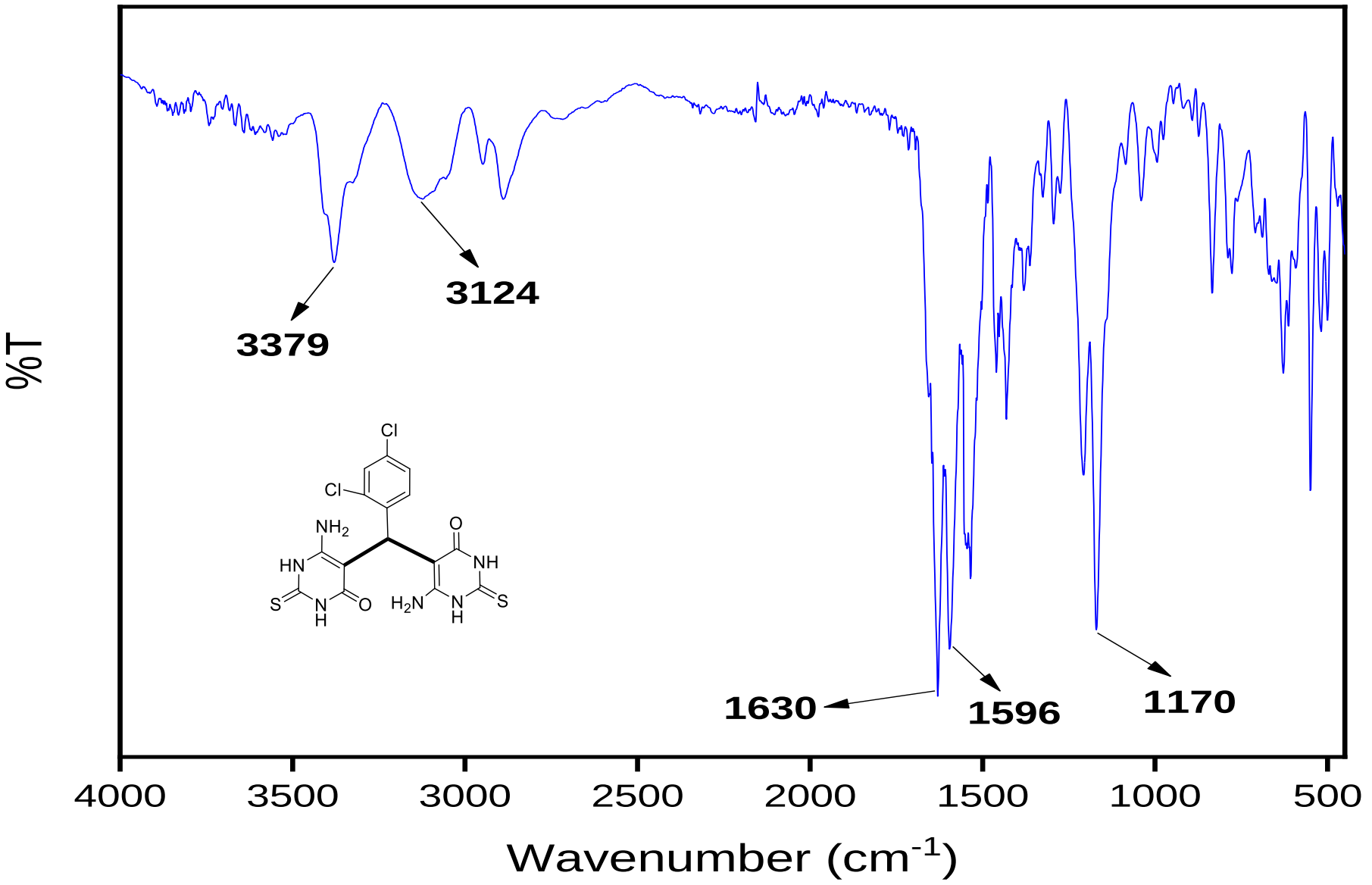

Figure S44. FT-IR spectra of compound **3h**.

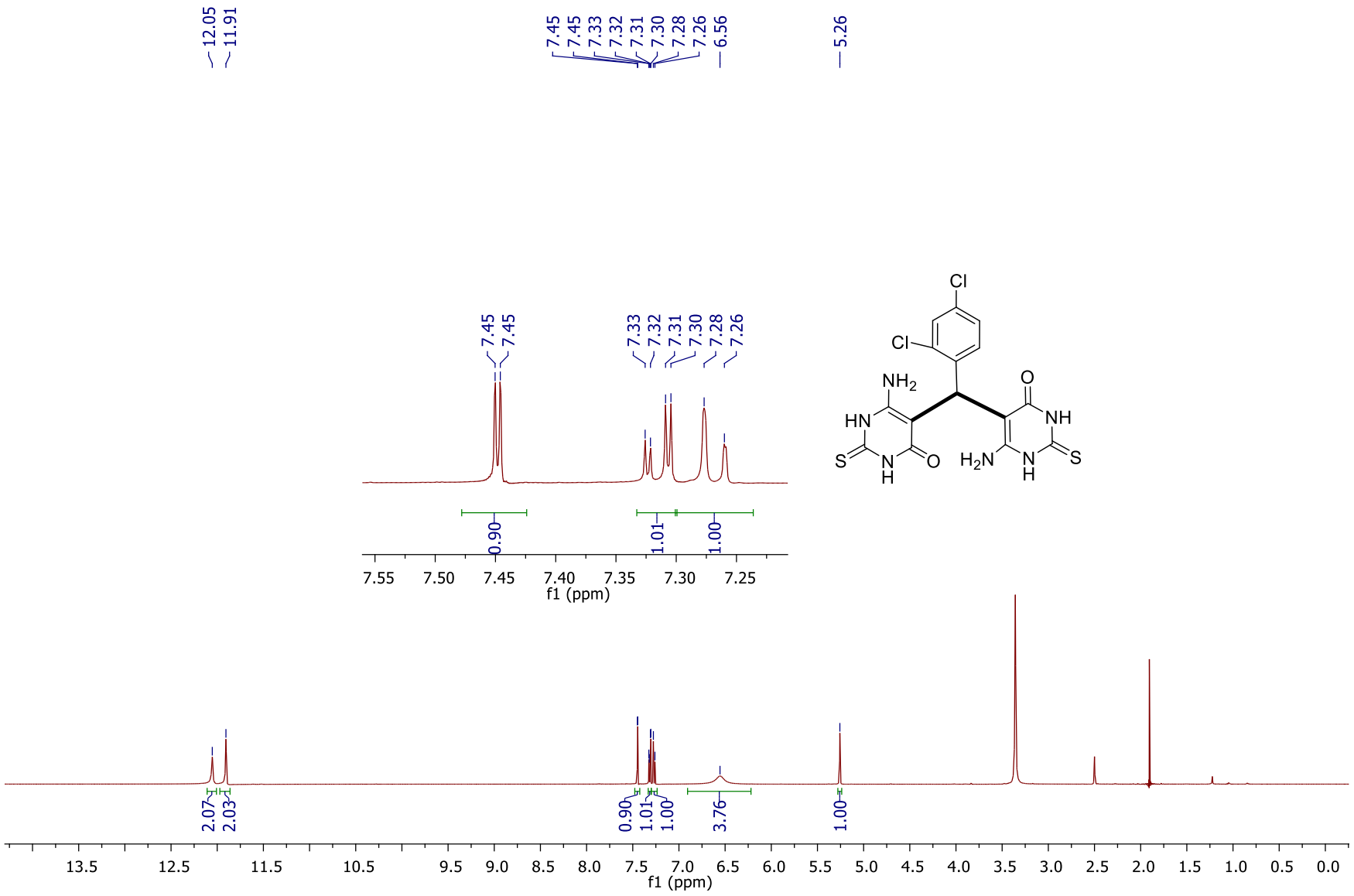

Figure S45. ^{1}H-NMR (400 MHz, DMSO-d_6) spectra of compound **3h**.

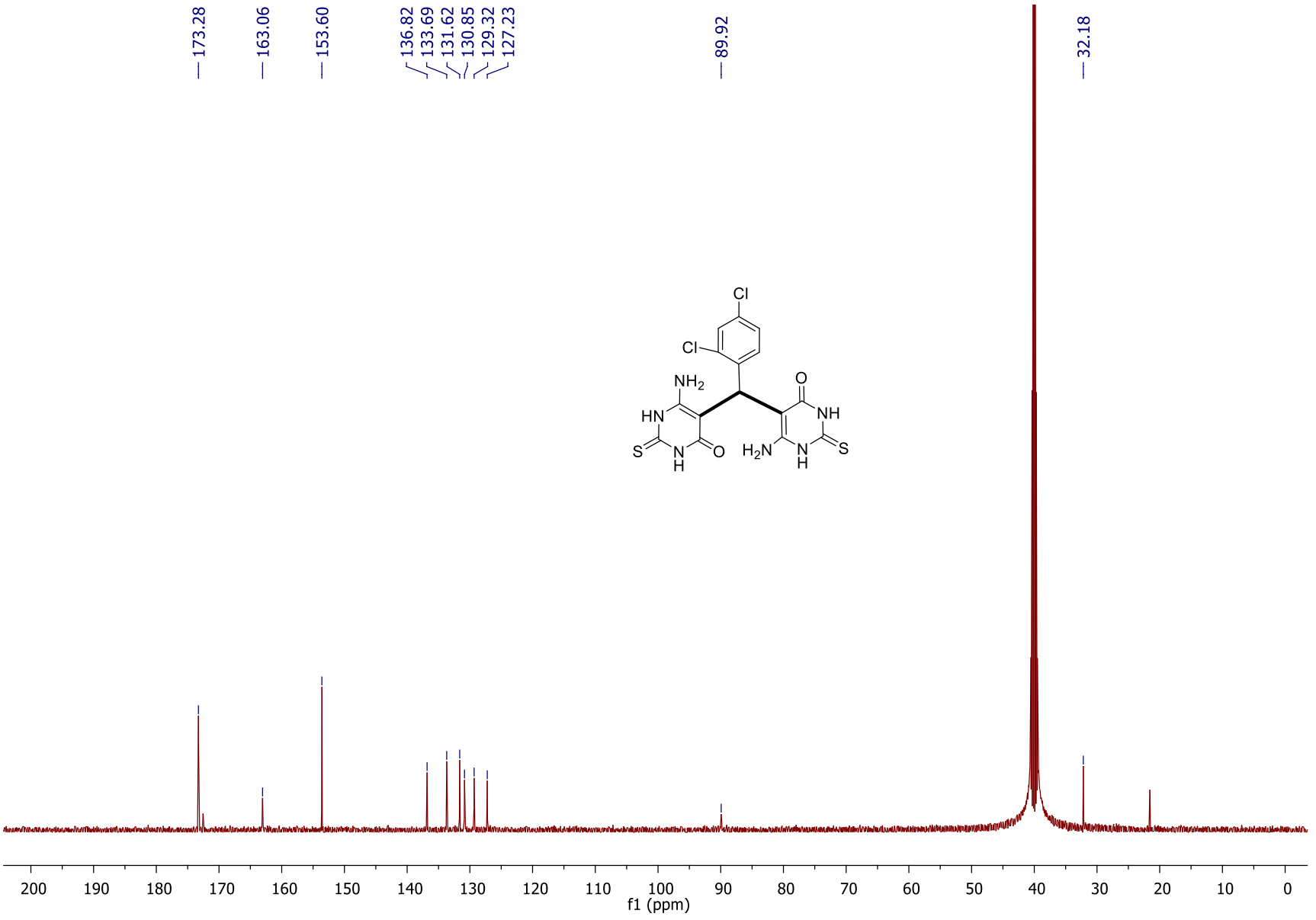

Figure S46. ^{13}C-NMR (101 MHz, DMSO-d_6) spectra of compound **3h**.

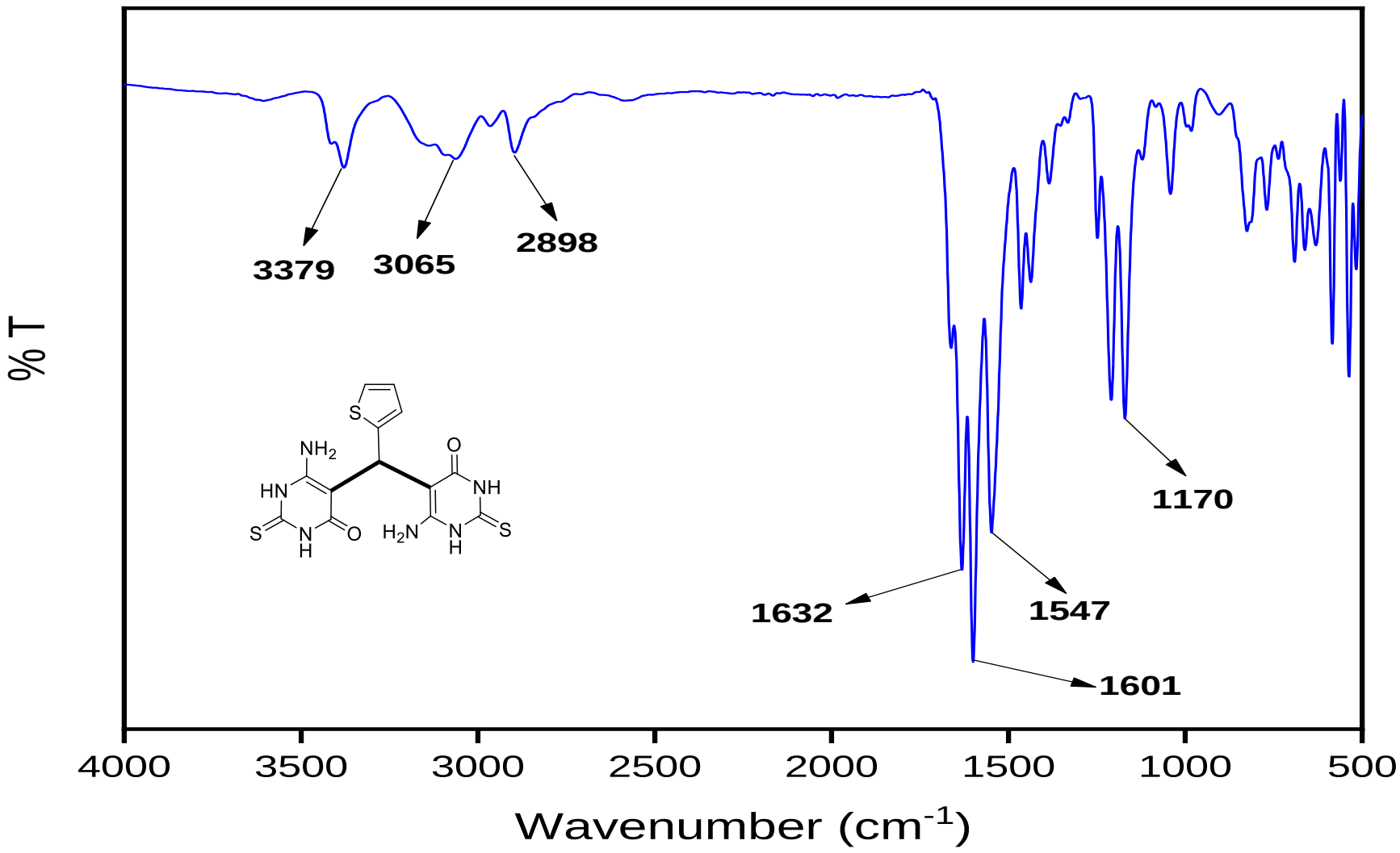

Figure S47. FT-IR spectra of compound **3i**.

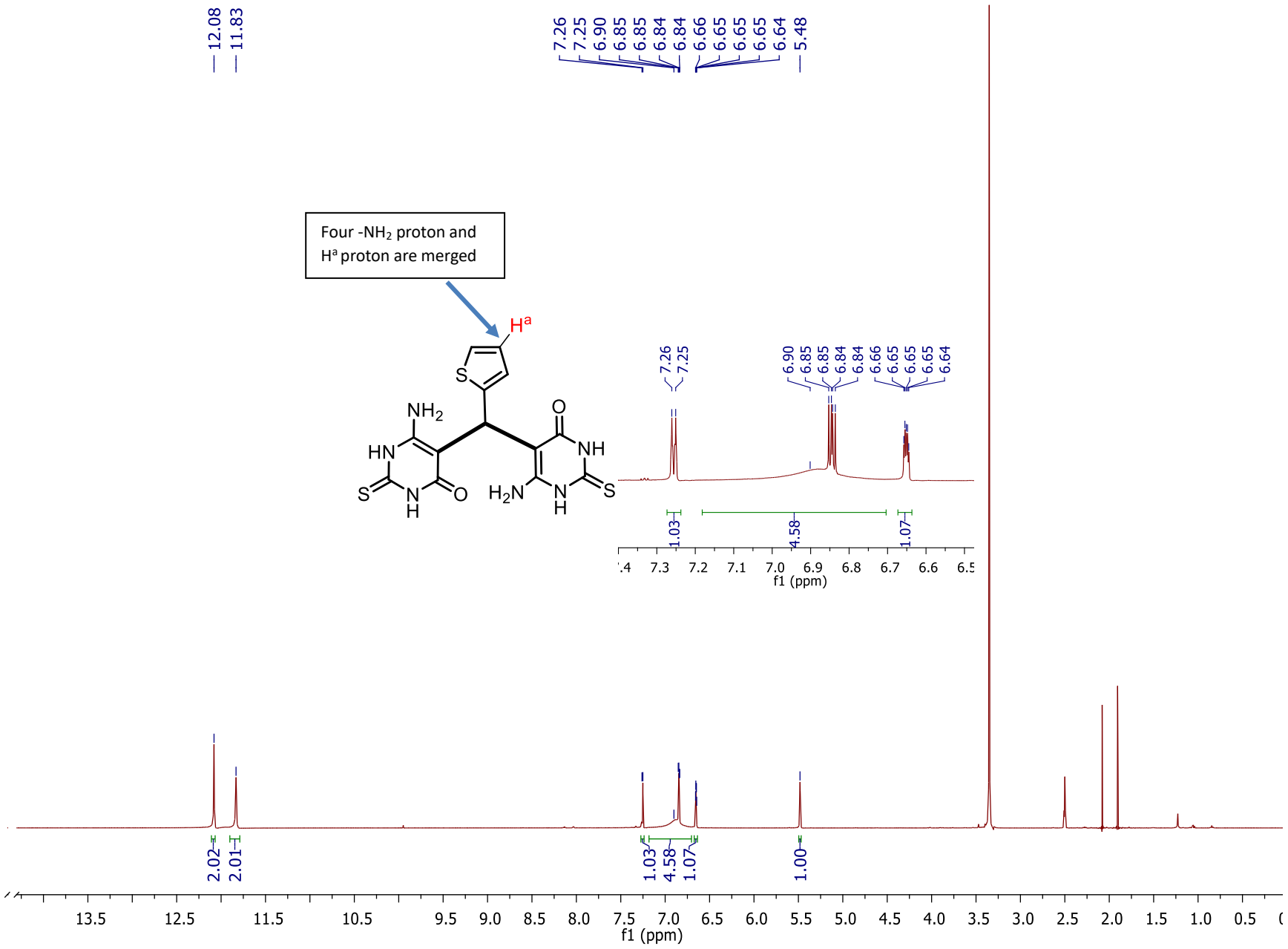

Figure S48. ^{1}H-NMR (500 MHz, DMSO-d_6) spectra of compound **3i**.

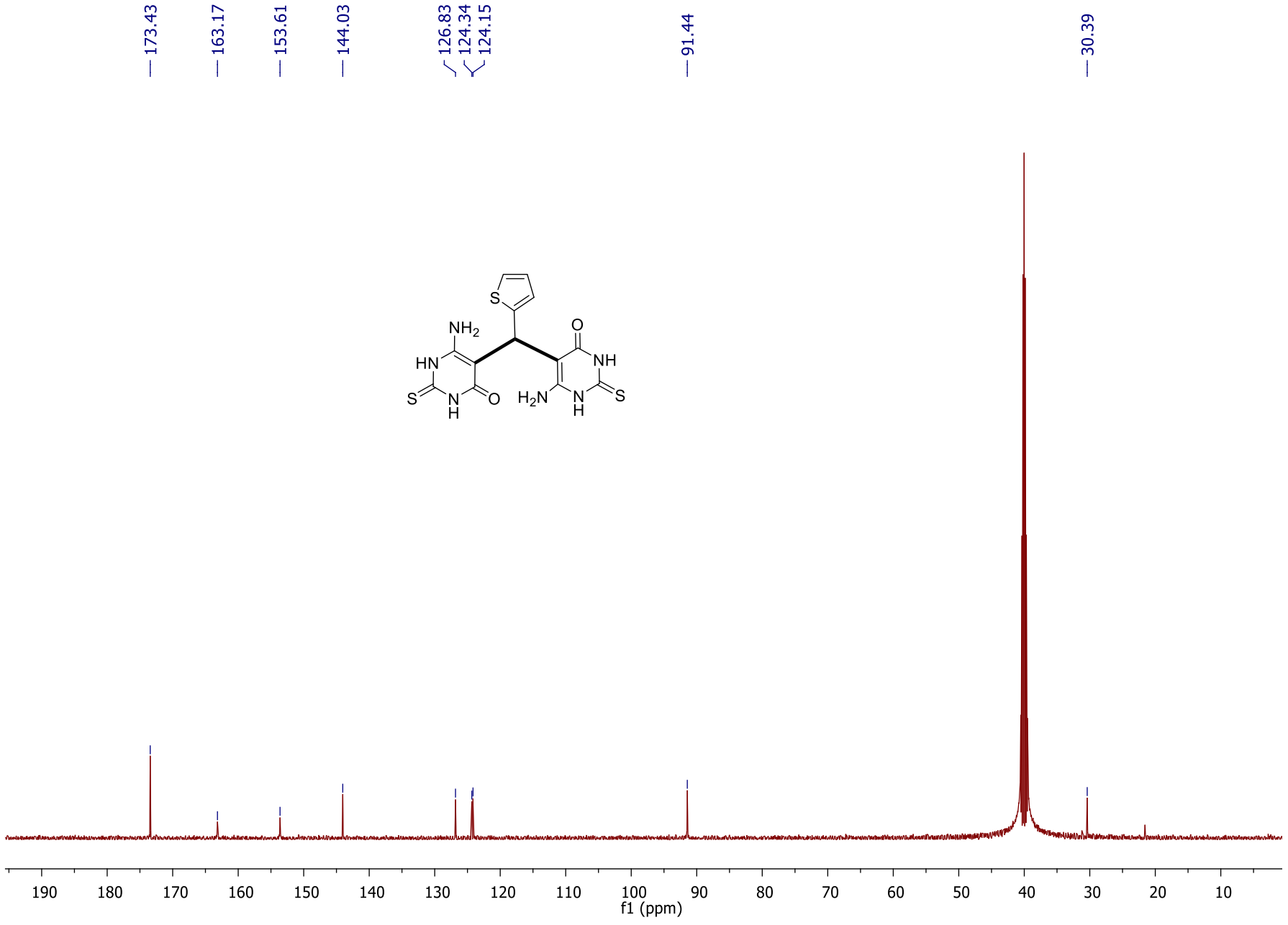

Figure S49. ^{13}C-NMR (126 MHz, DMSO-d_6) spectra of compound **3i**.

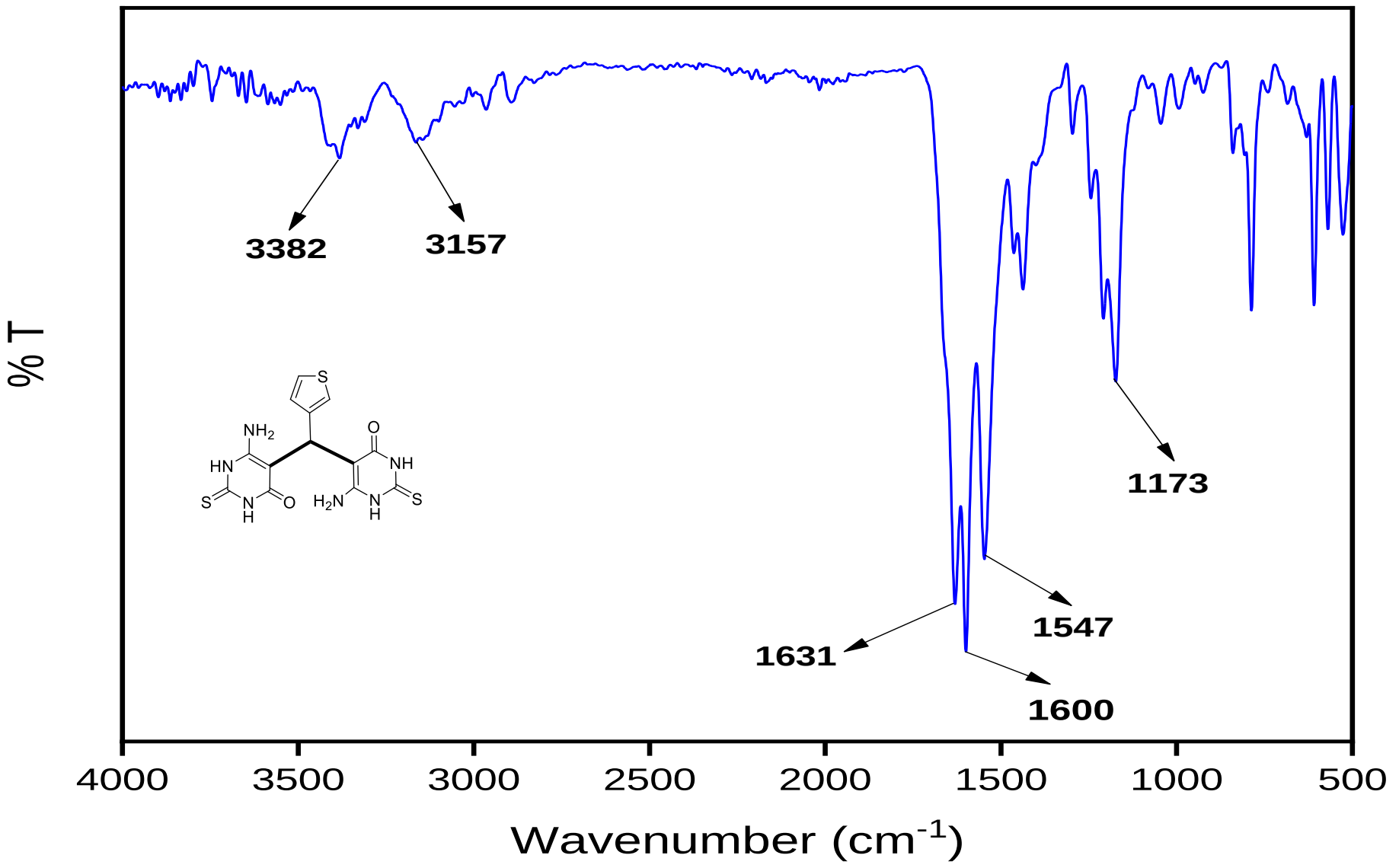

Figure S50. FT-IR spectra of compound **3j**.

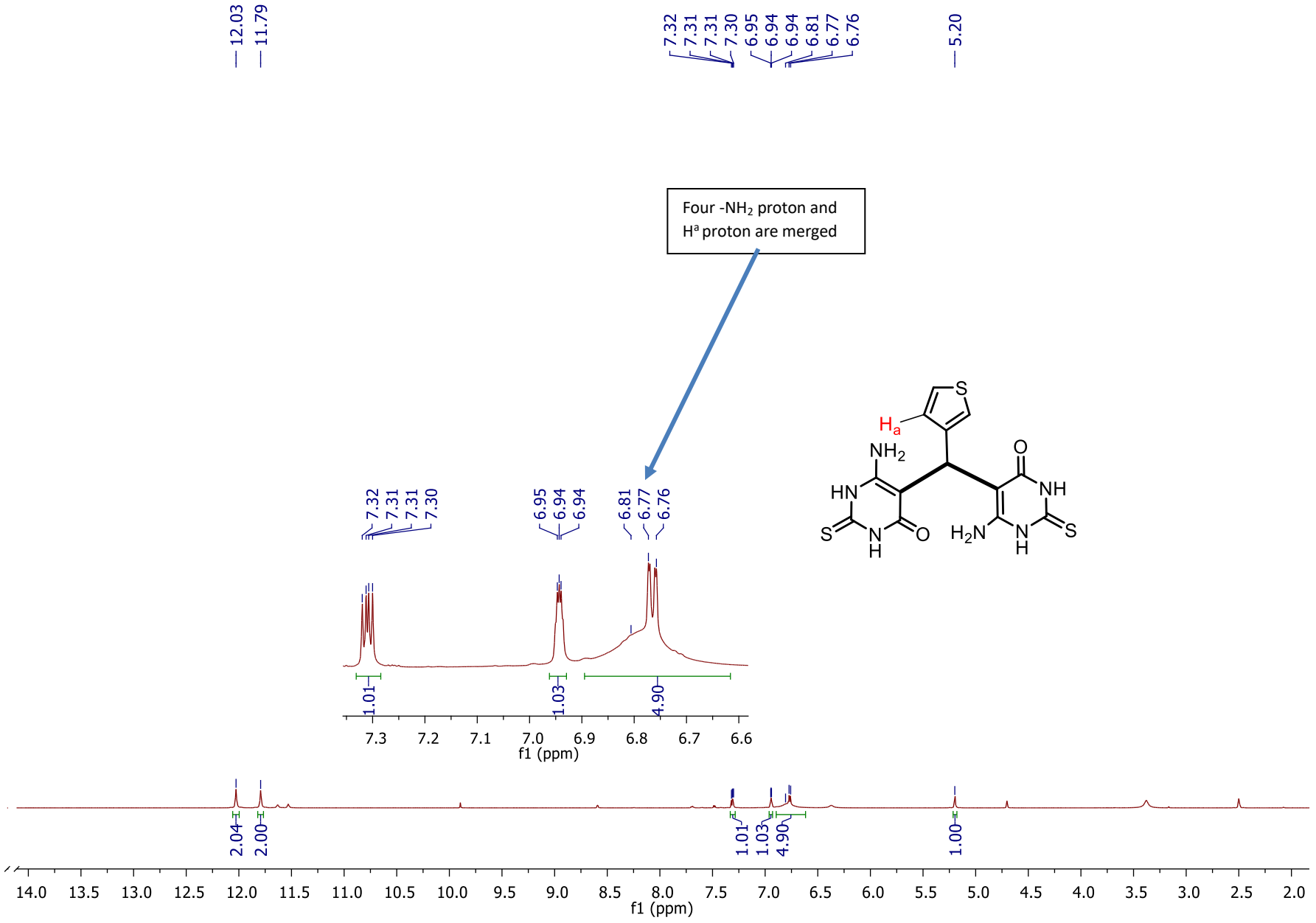

Figure S51. ^{1}H-NMR (400 MHz, DMSO-d_6) spectra of compound **3j**.

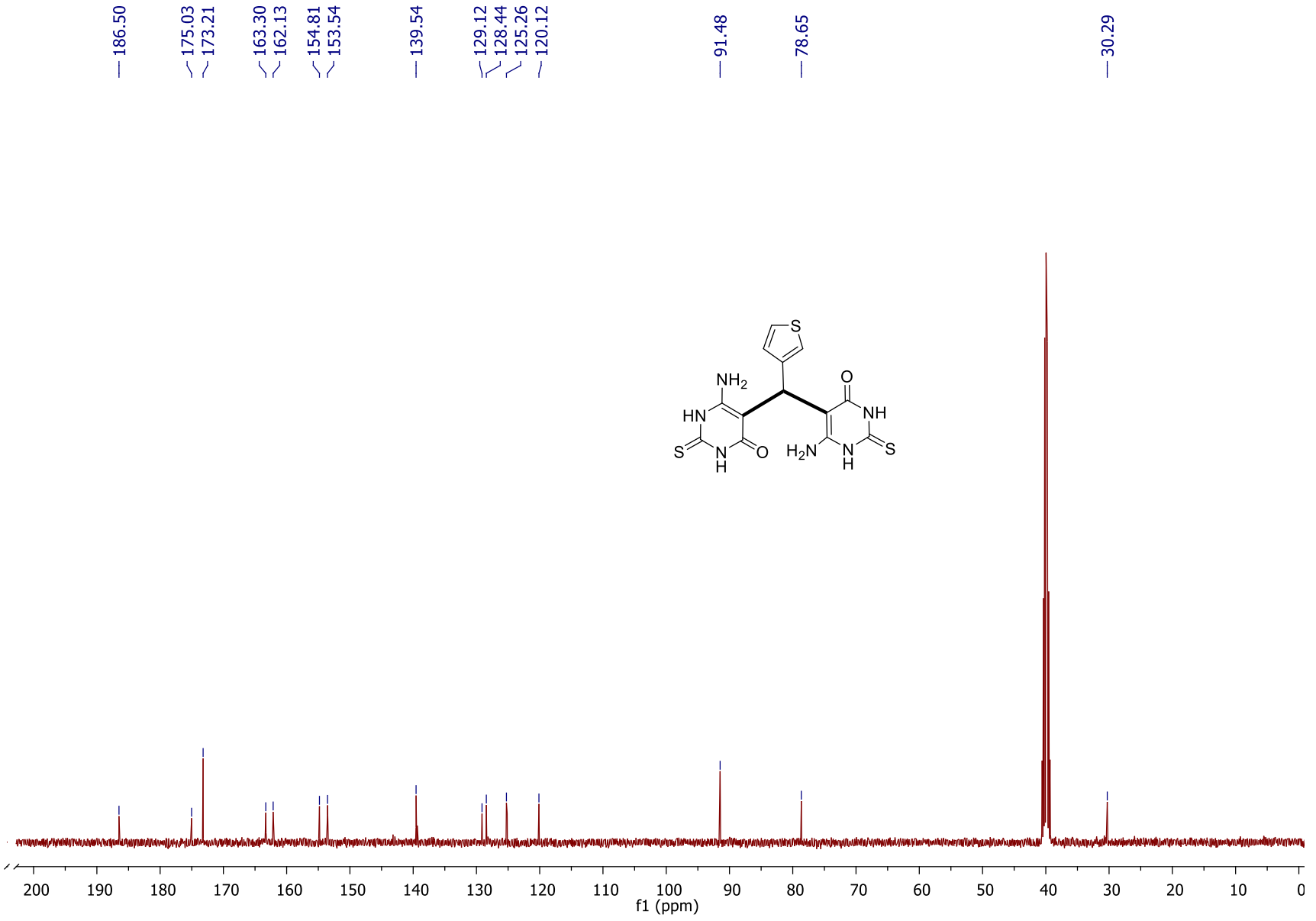

Figure S52. ^{13}C-NMR (101 MHz, DMSO-d_6) spectra of compound **3j**.

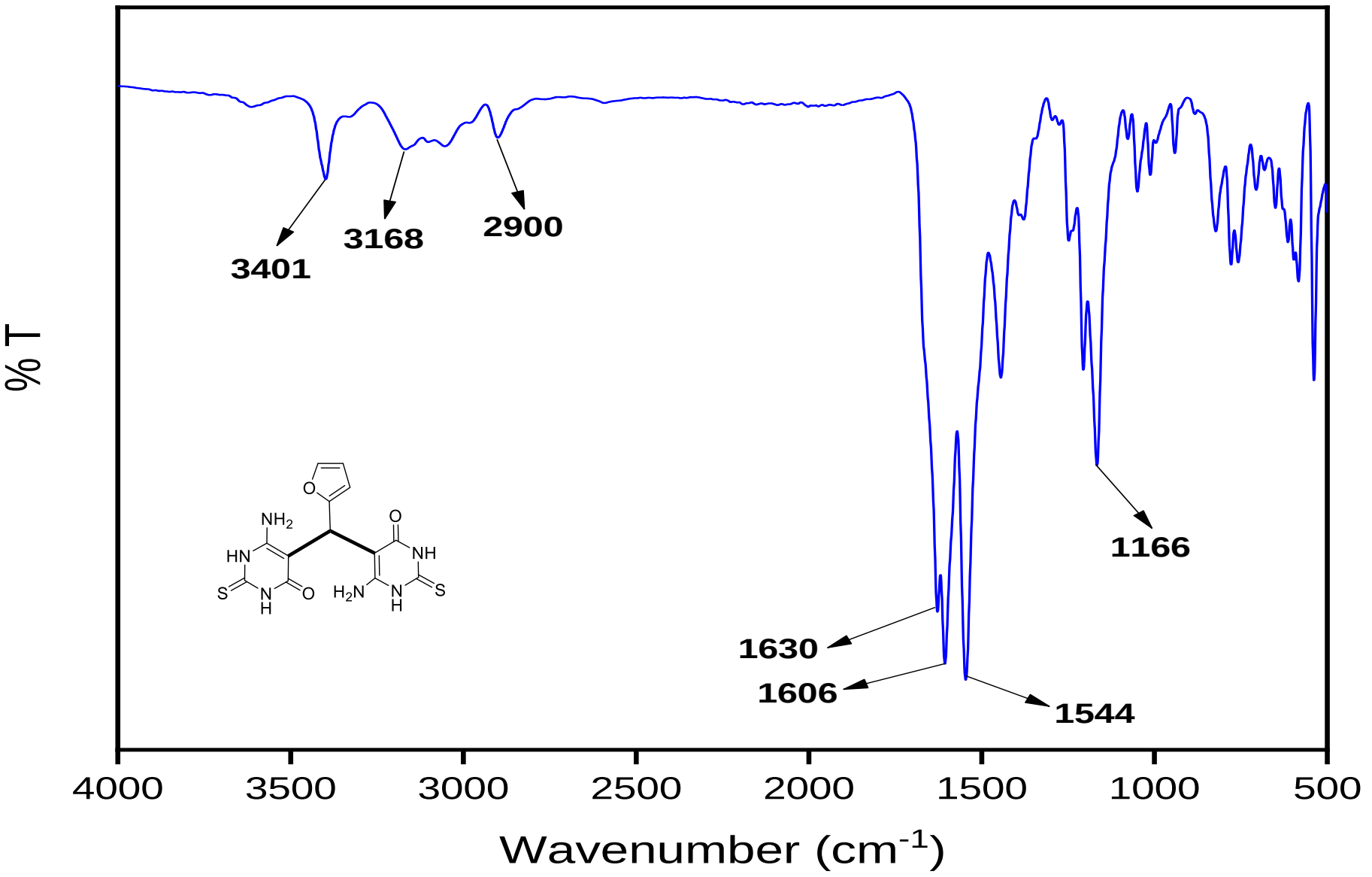

Figure S53. FT-IR spectra of compound **3k**.

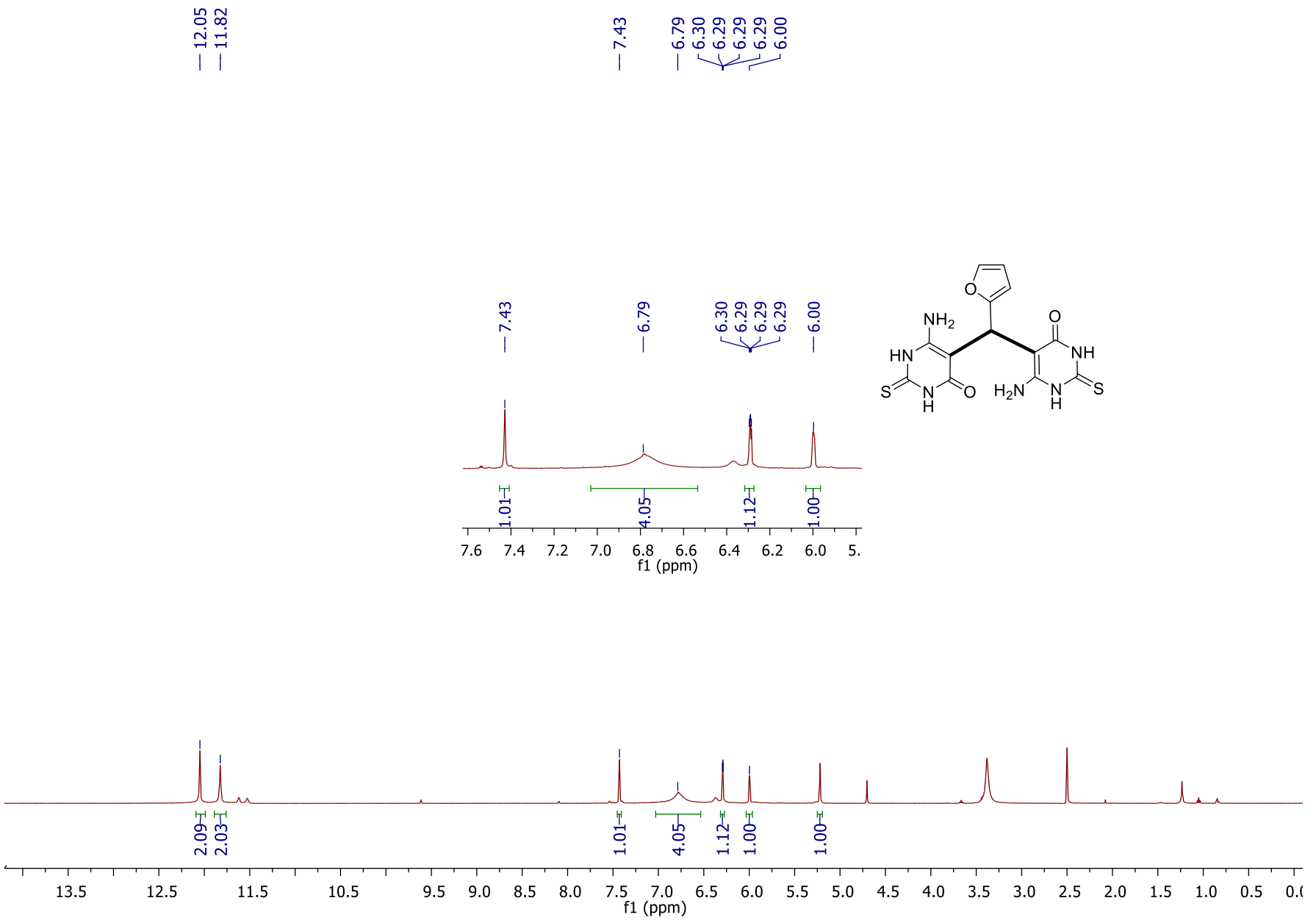

Figure S54. ^{1}H-NMR (500 MHz, DMSO-d_6) spectra of compound **3k**.

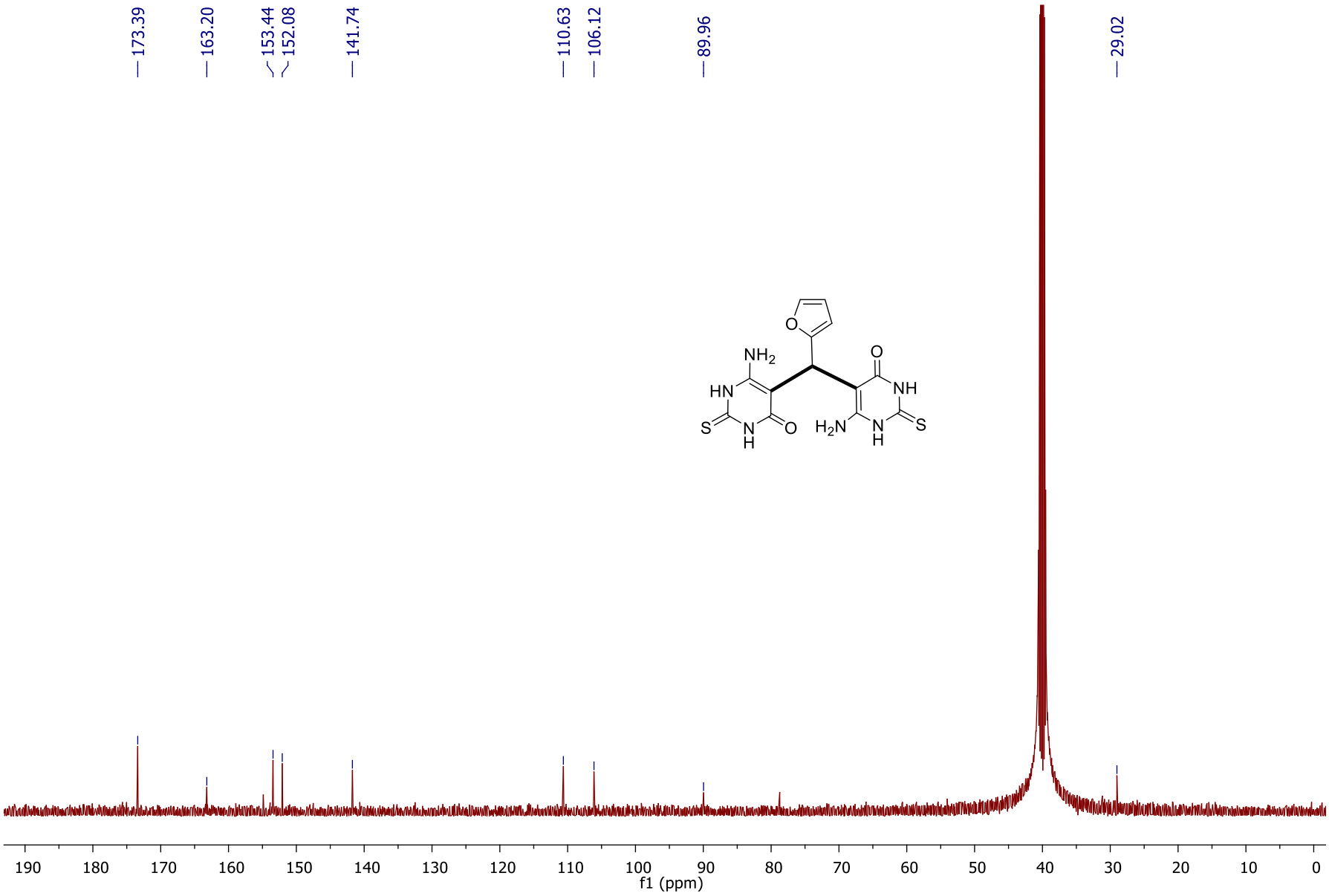

Figure S55. ^{13}C-NMR (126 MHz, DMSO-d_6) spectra of compound **3k.**

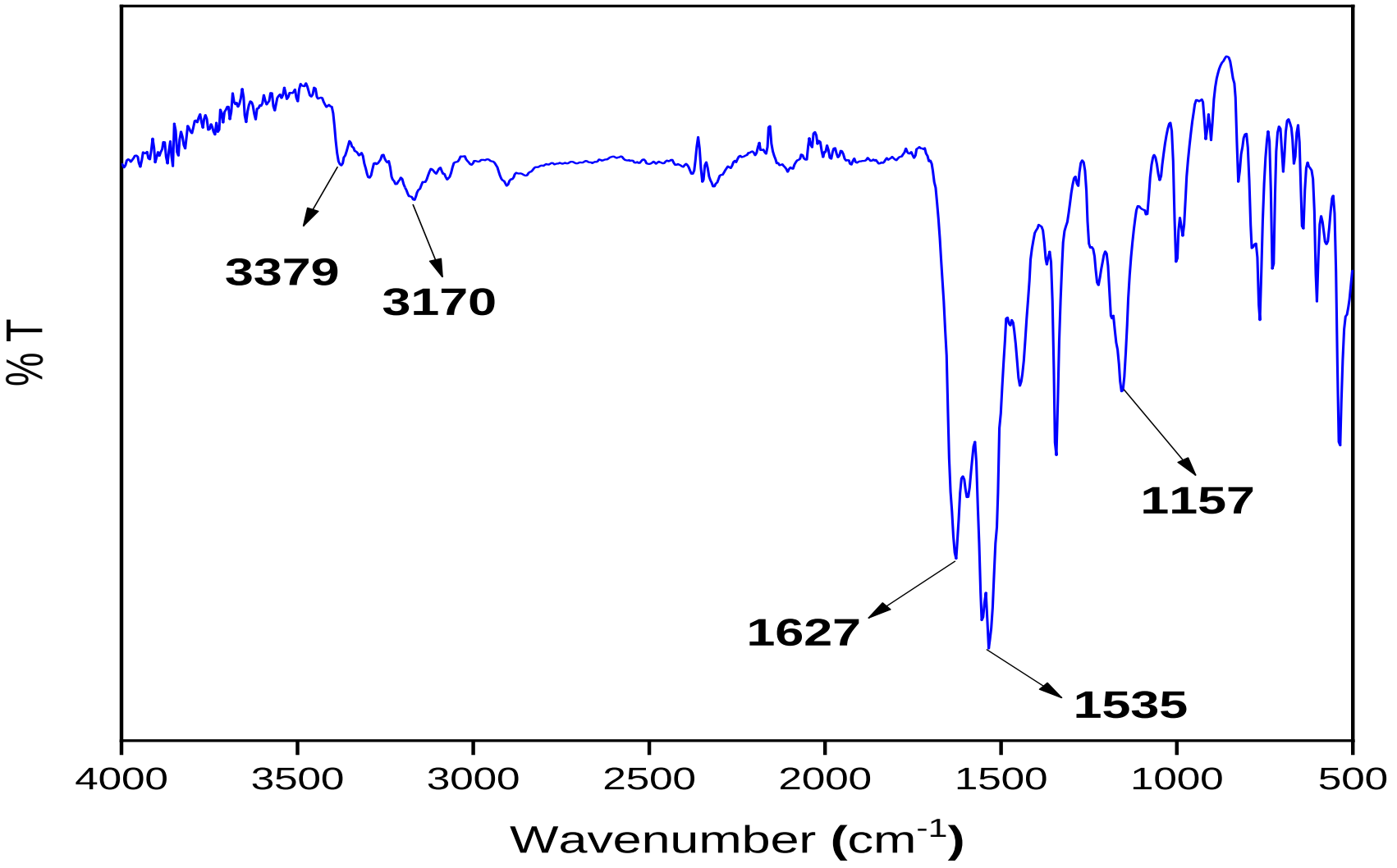

Figure S56. FT-IR spectra of compound **3l**.

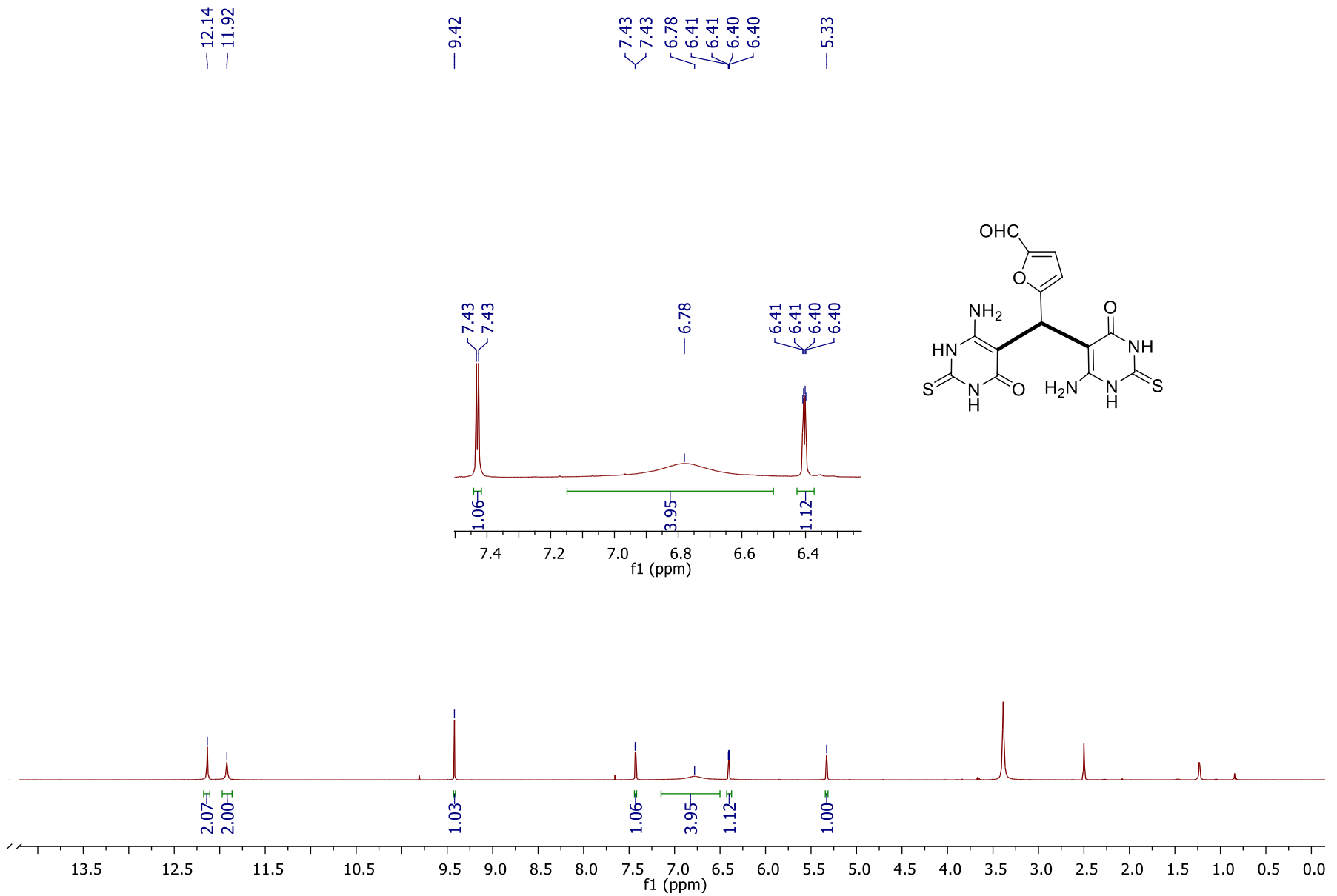

Figure S57. ^{1}H-NMR (400 MHz, DMSO-d_6) spectra of compound **3l**.

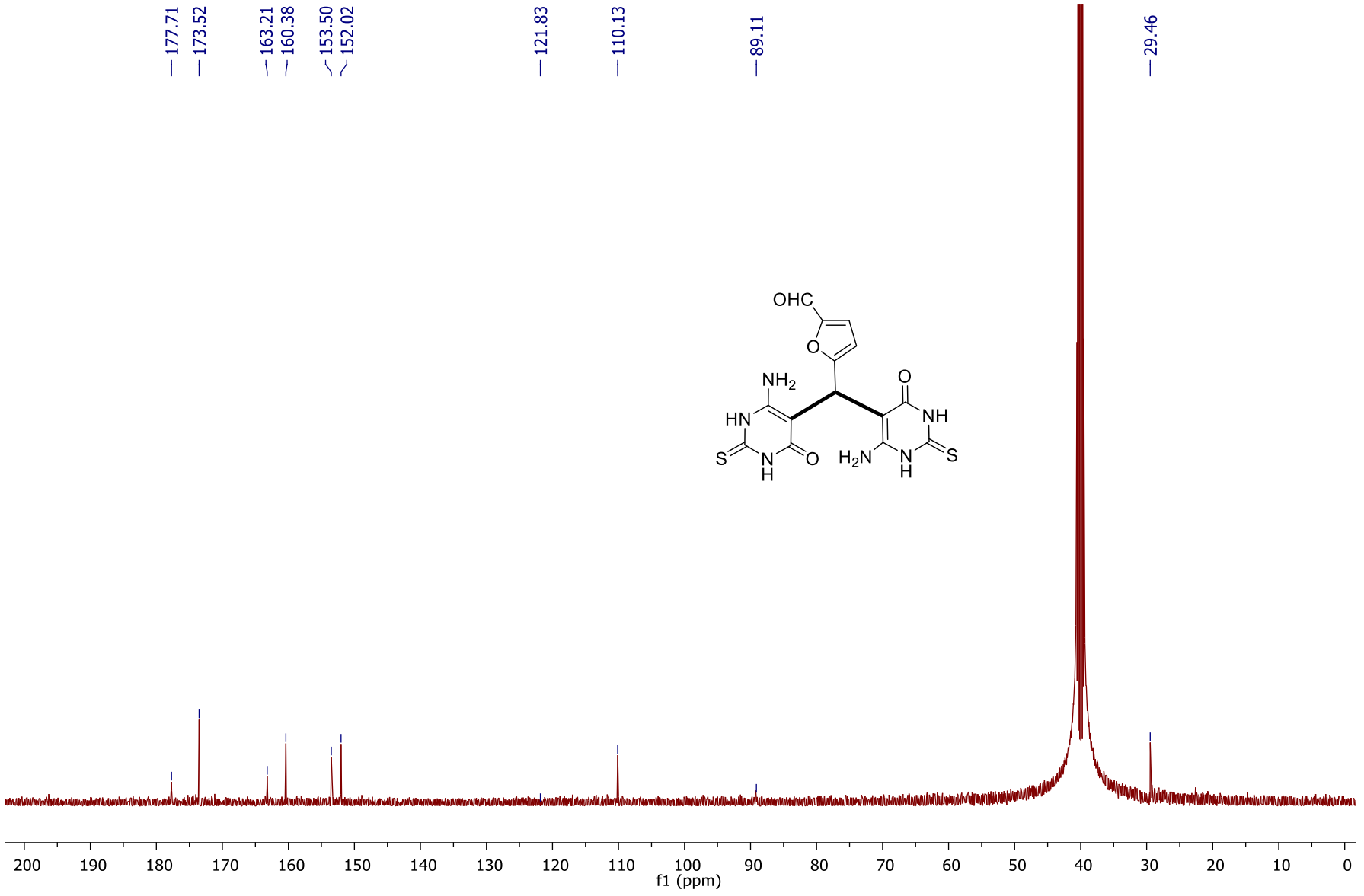

Figure S58. ^{13}C-NMR (101 MHz, DMSO-d_6) spectra of compound **3l**.

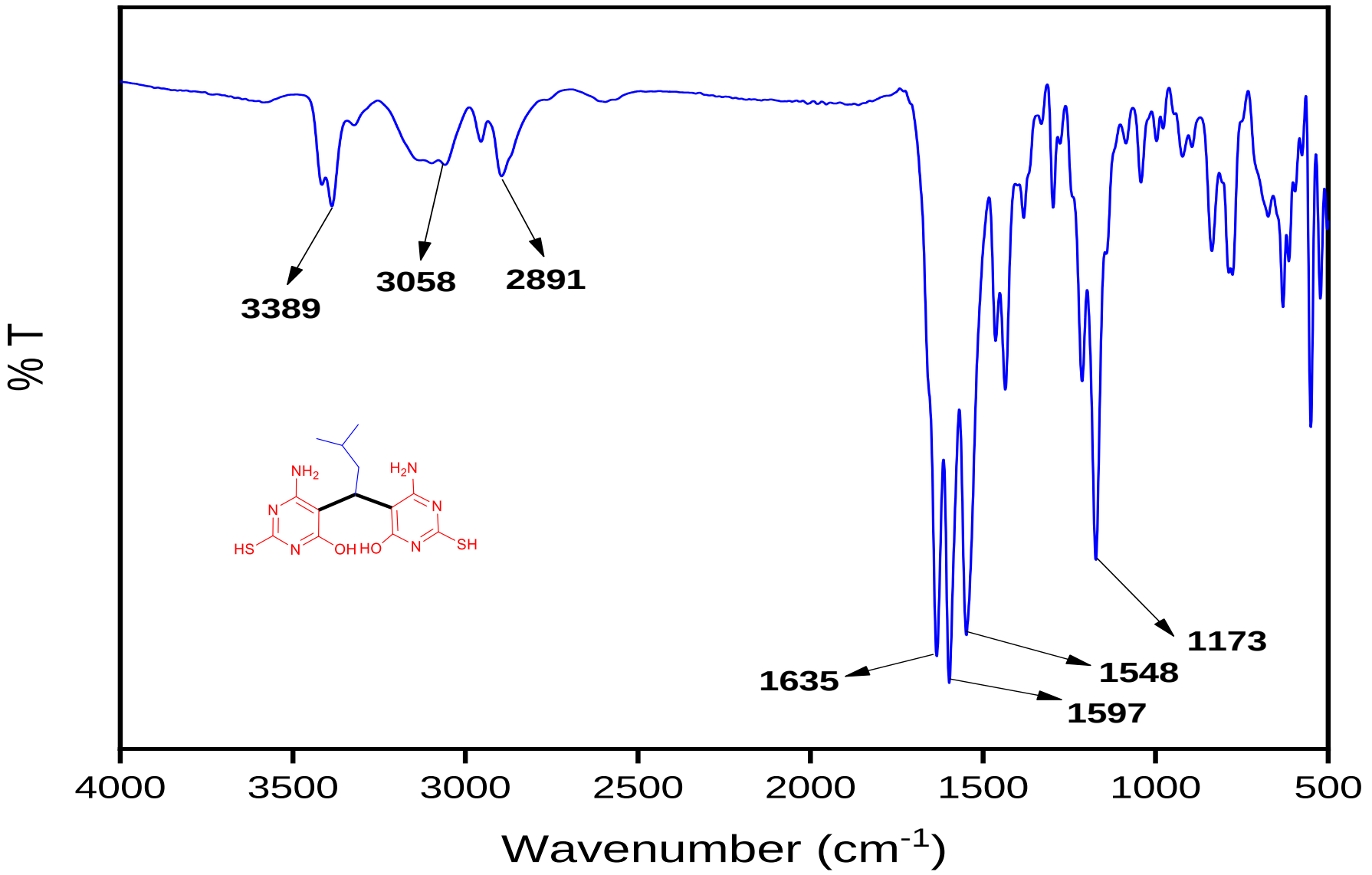

Figure S59. FT-IR spectra of compound **3o**.

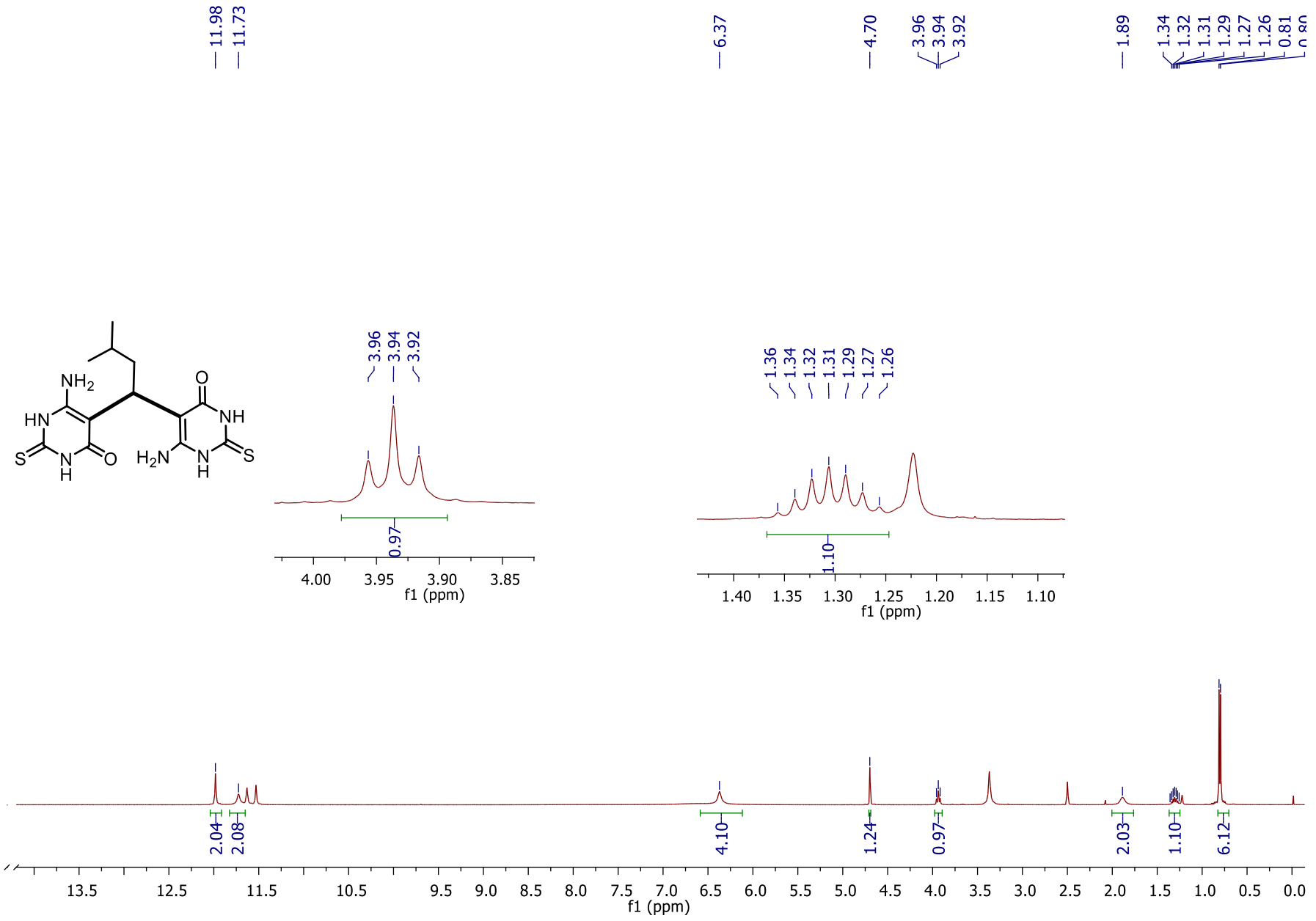

Figure S60. ^{1}H-NMR (400 MHz, DMSO-d_6) spectra of compound **3o**.

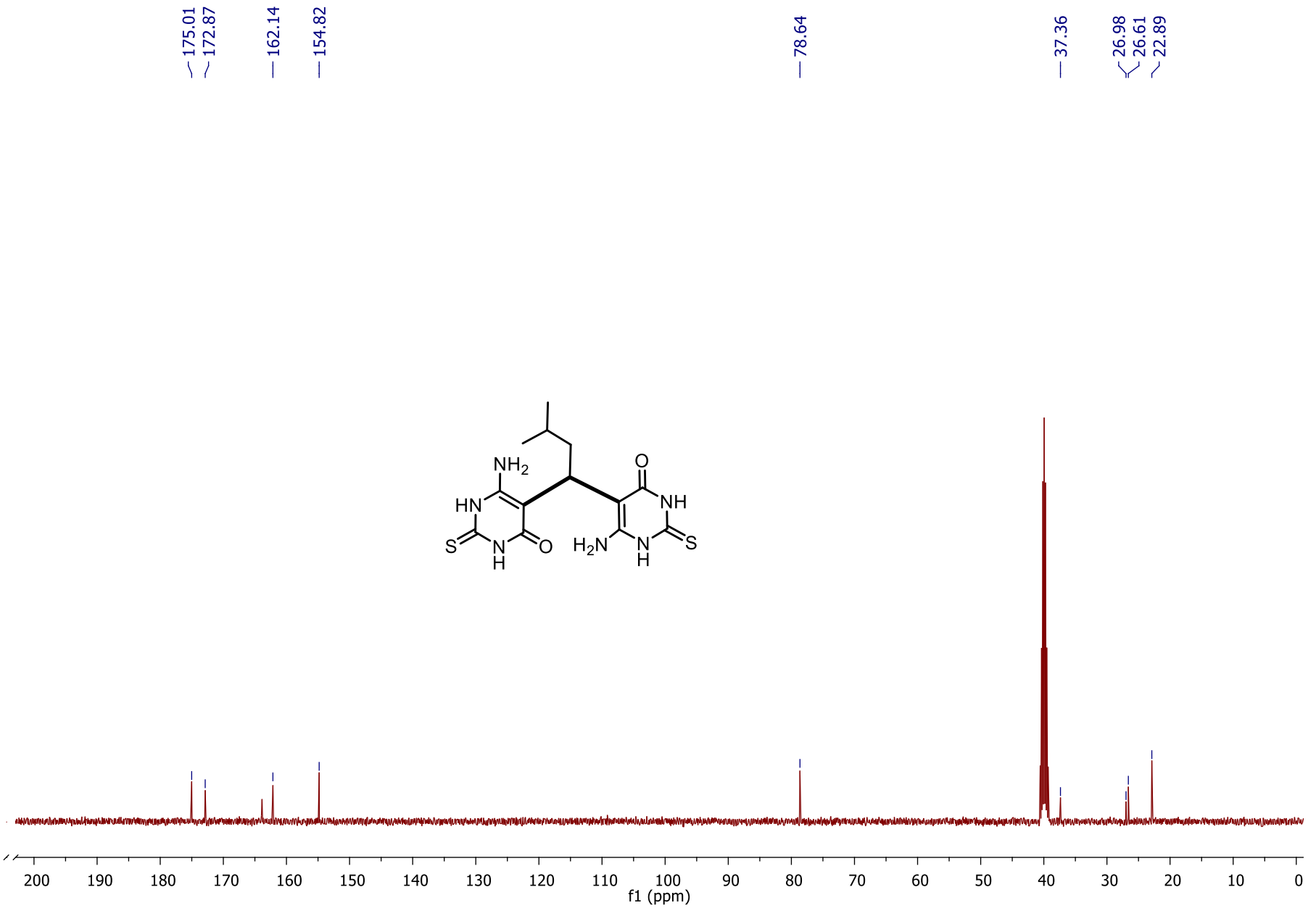

Figure S61. ^{13}C-NMR (101 MHz, DMSO-d_6) spectra of compound **3o**.

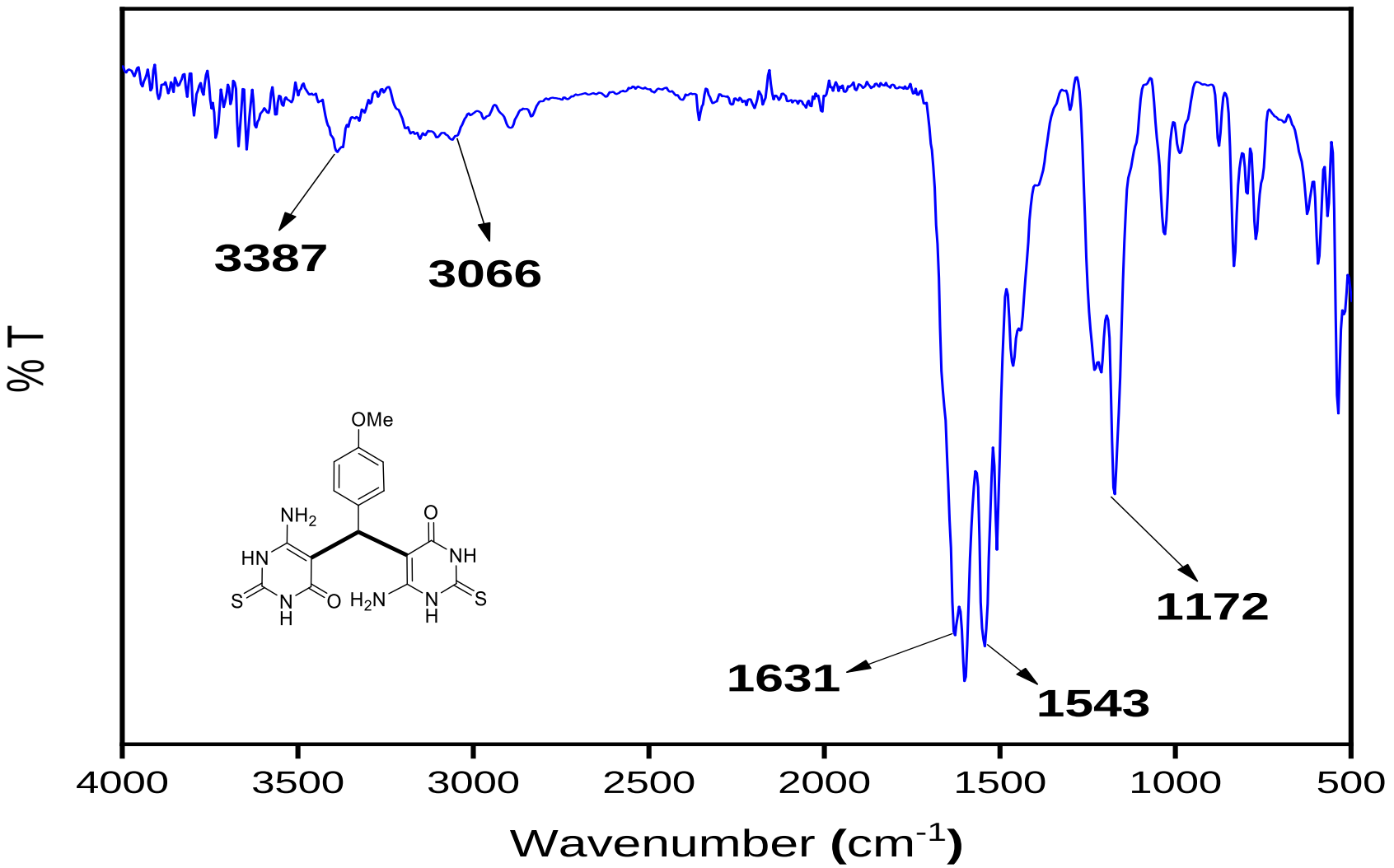

Figure S62. FT-IR spectra of compound **3p**.

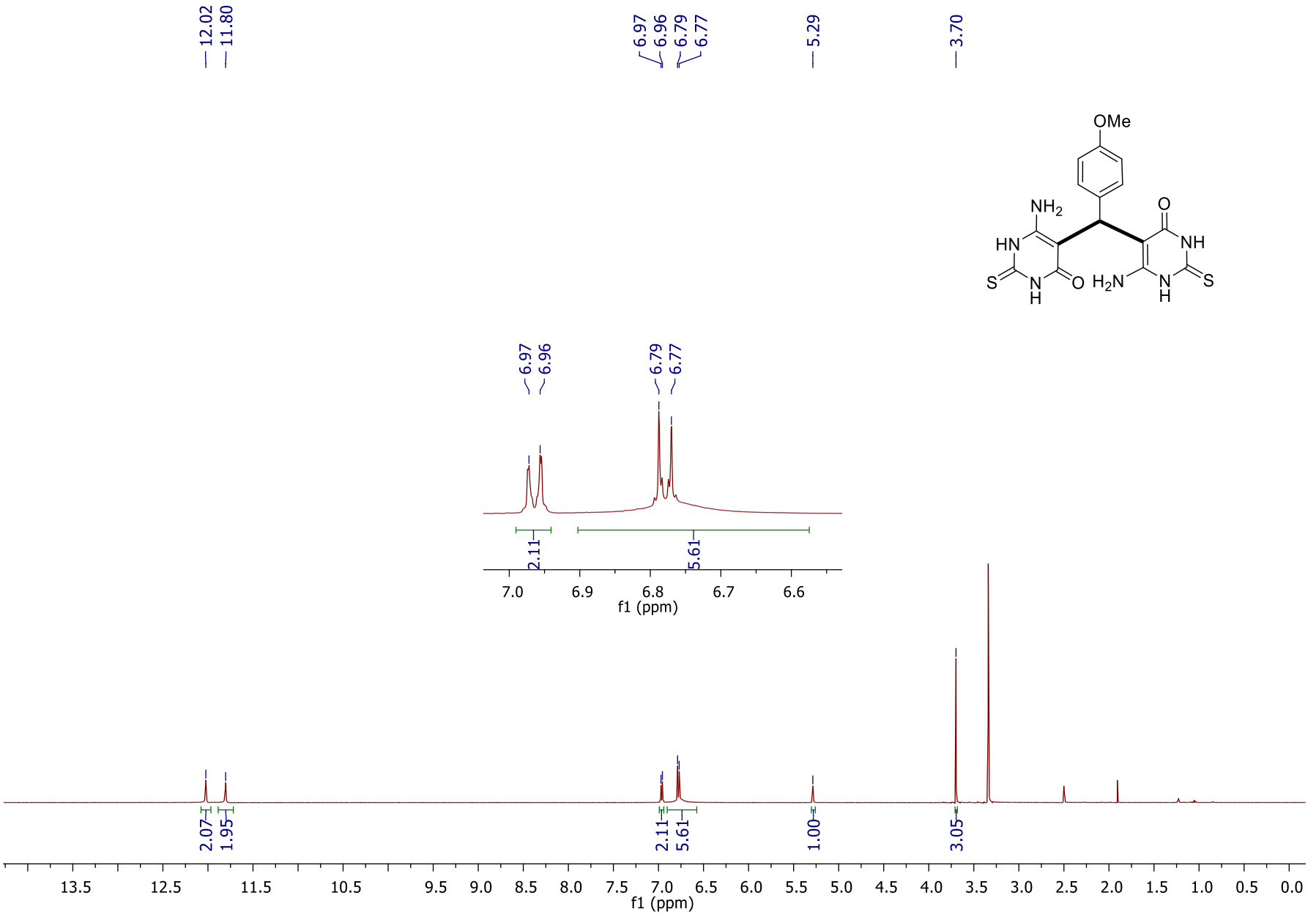

Figure S63. ^{1}H-NMR (500 MHz, DMSO-d_6) spectra of compound **3p**.

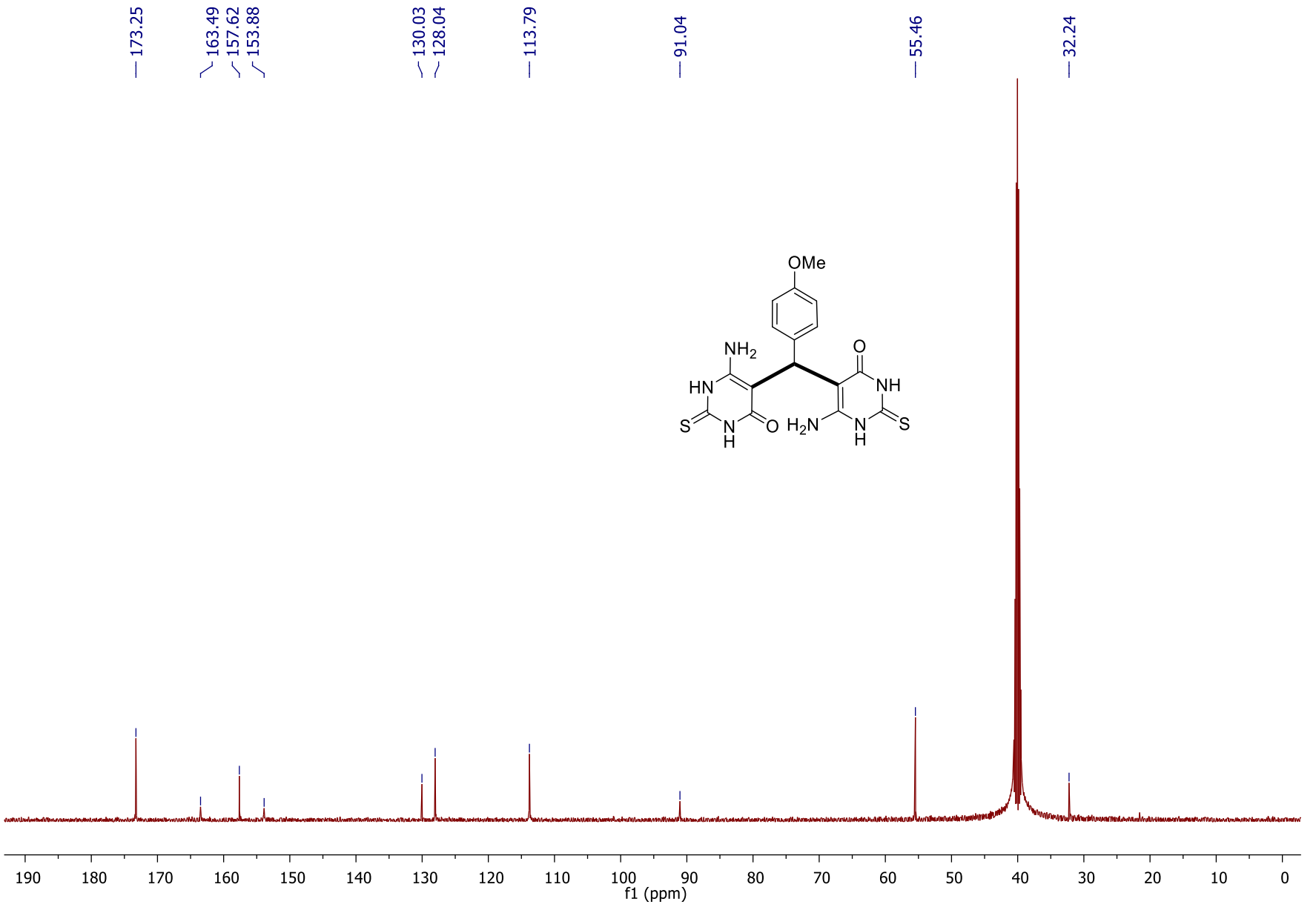

Figure S64. ^{13}C-NMR (126 MHz, DMSO-d_6) spectra of compound **3p**.

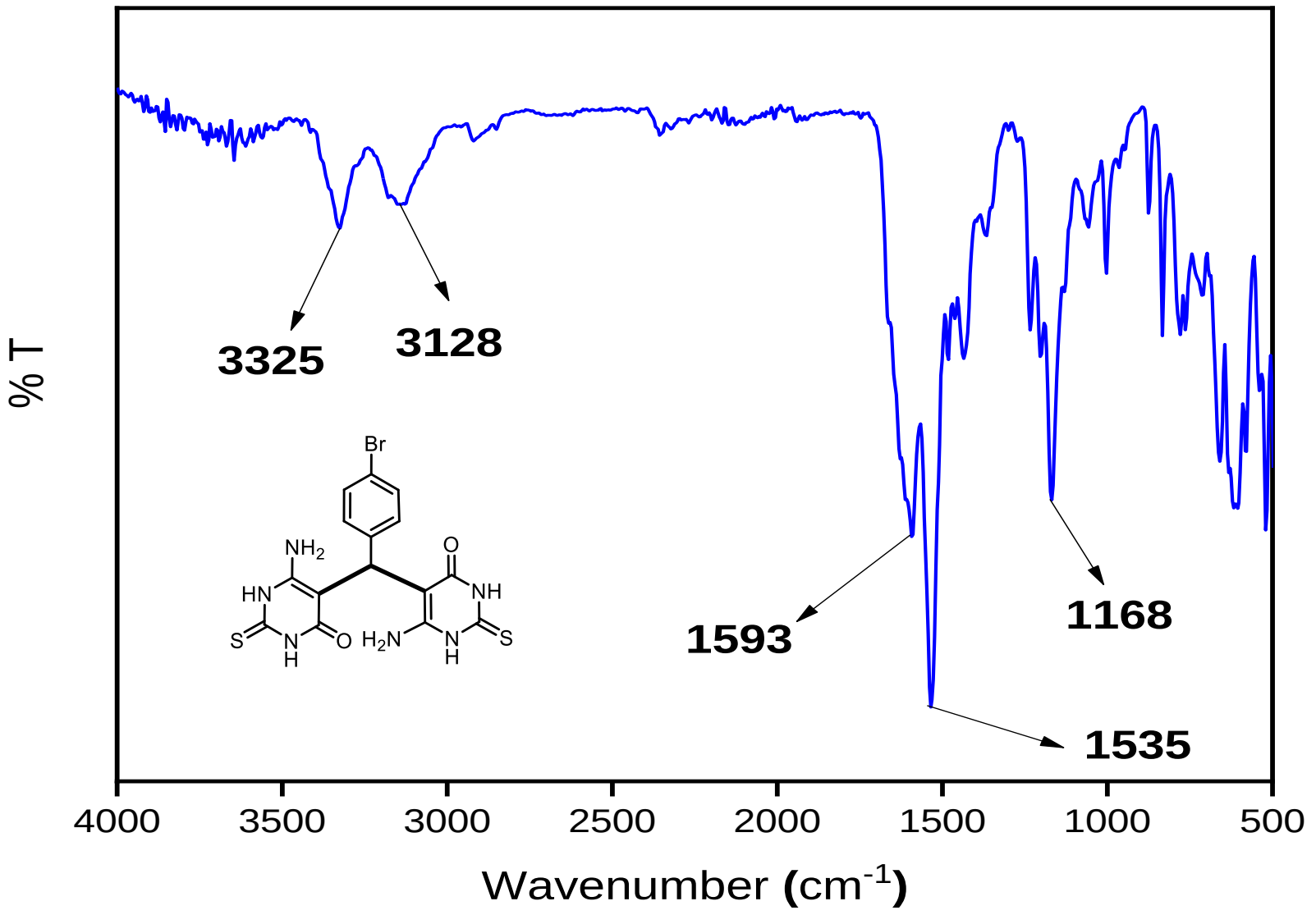

Figure S65. FT-IR spectra of compound **3q**.

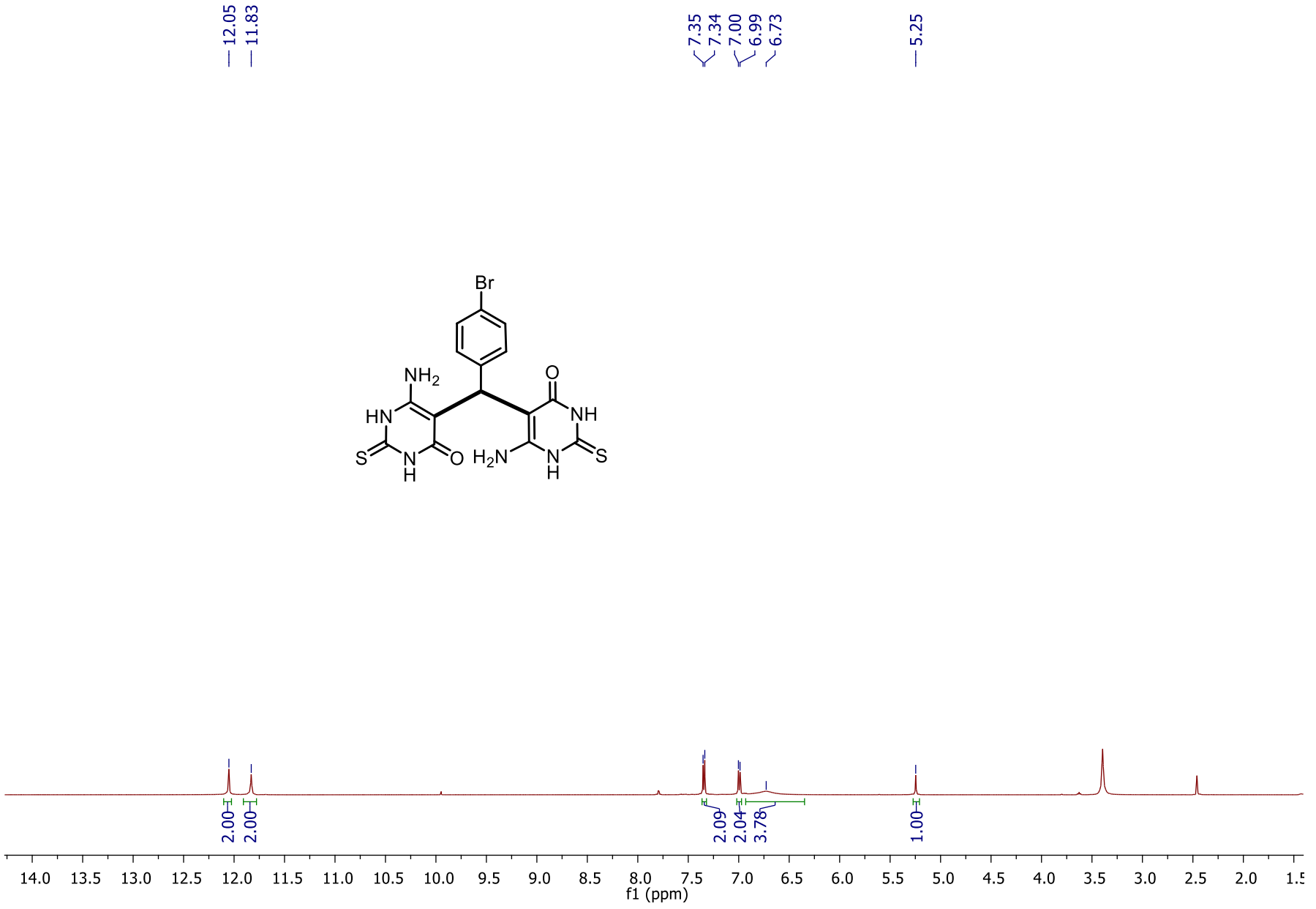

Figure S66. ^{1}H-NMR (500 MHz, DMSO-d_6) spectra of compound **3q**.

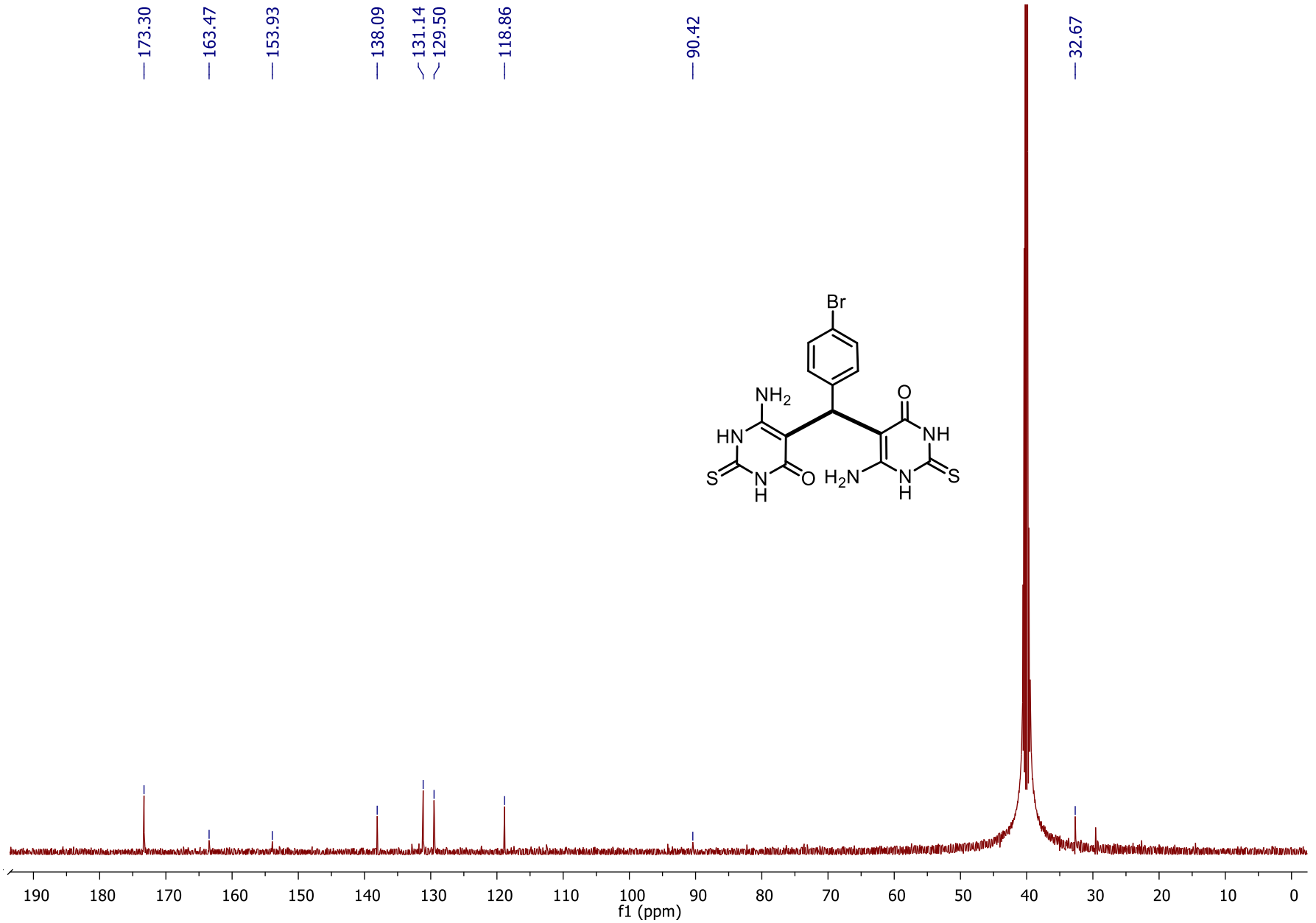

Figure S67. ^{13}C-NMR (126 MHz, DMSO-d_6) spectra of compound **3q**.

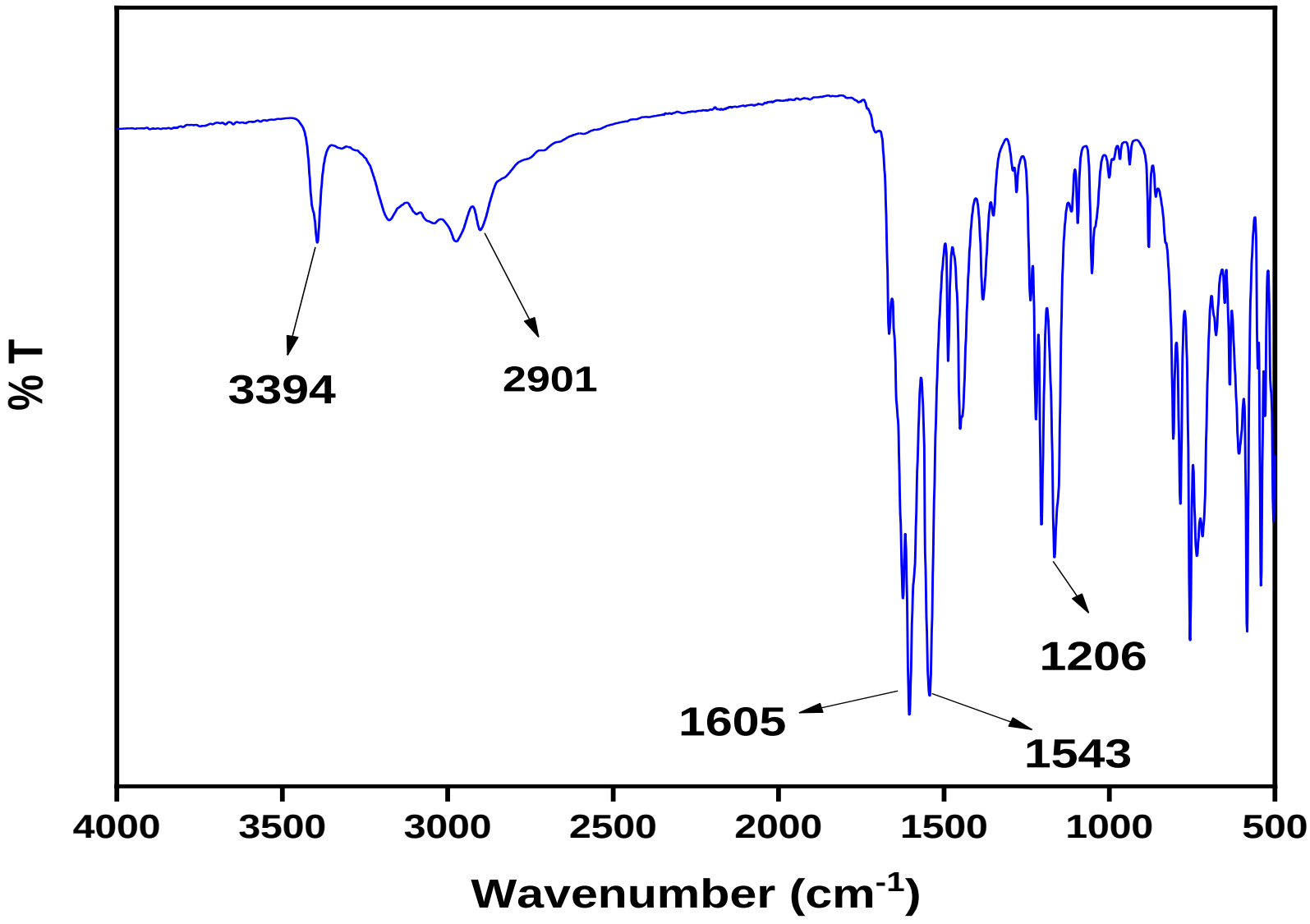

Figure S68. FT-IR spectra of compound **3r**.

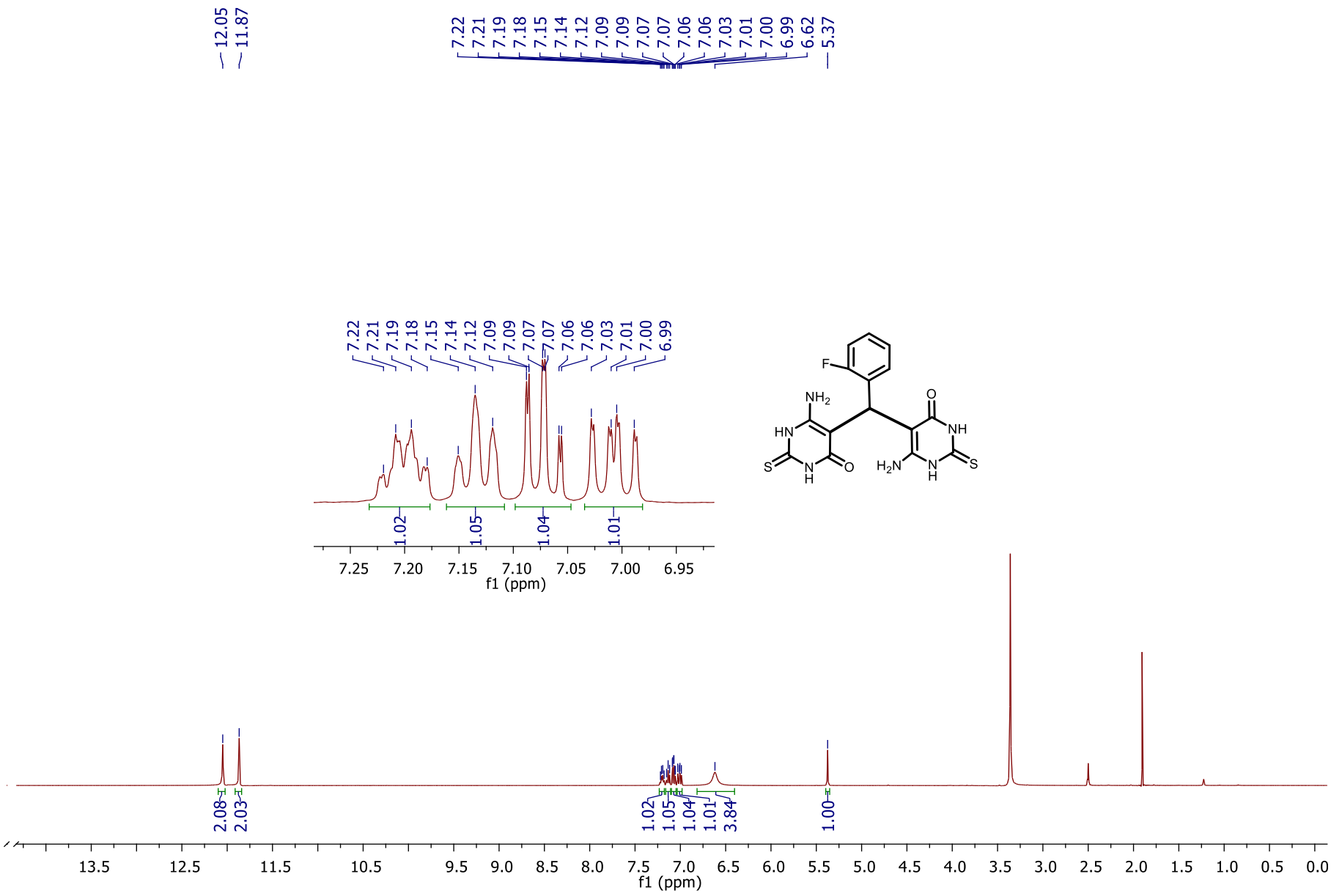

Figure S69. ^{13}C-NMR (126 MHz, DMSO-d_6) spectra of compound **3r**.

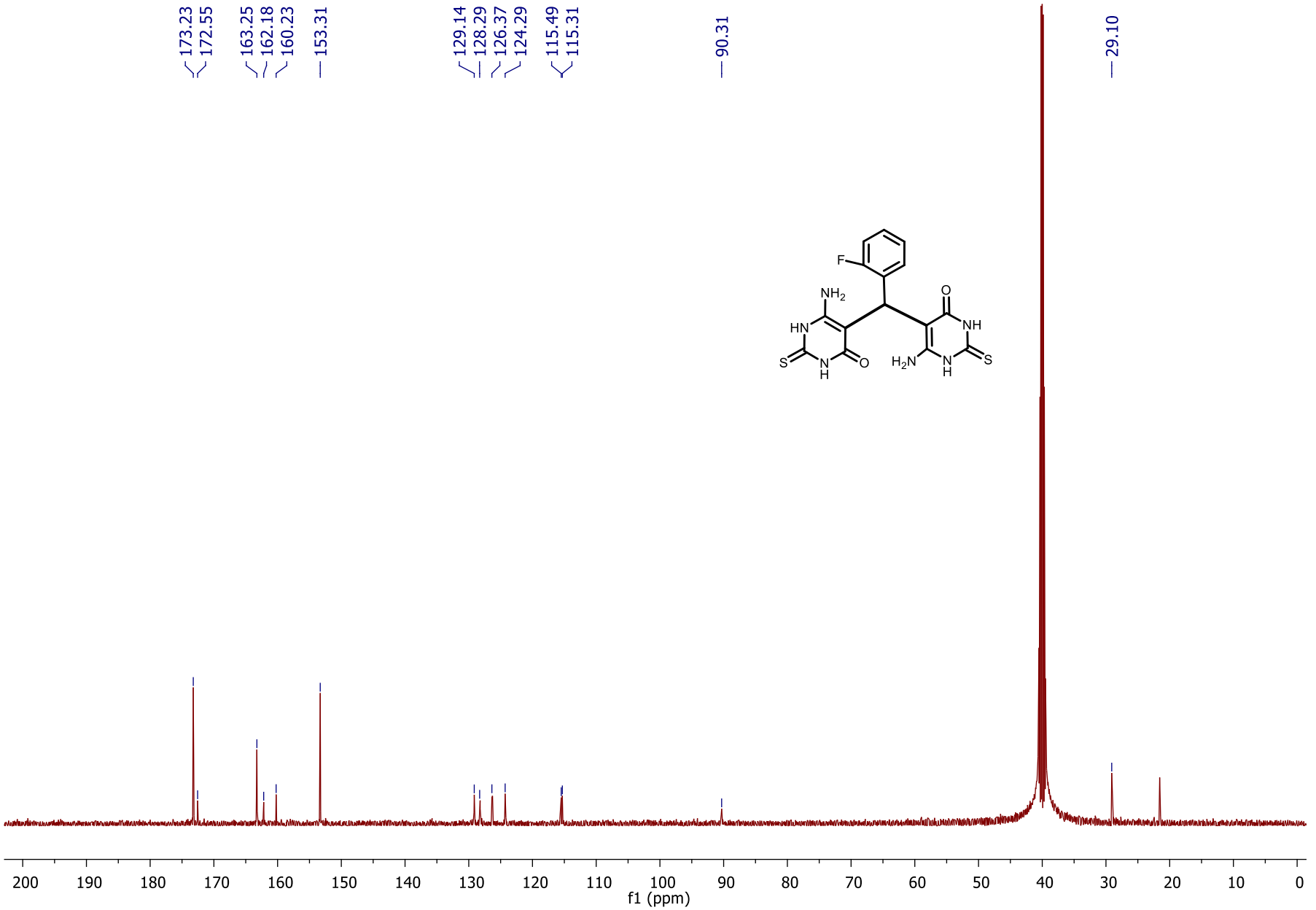

Figure S70. ^{13}C-NMR (126 MHz, DMSO-d_6) spectra of compound **3r**.

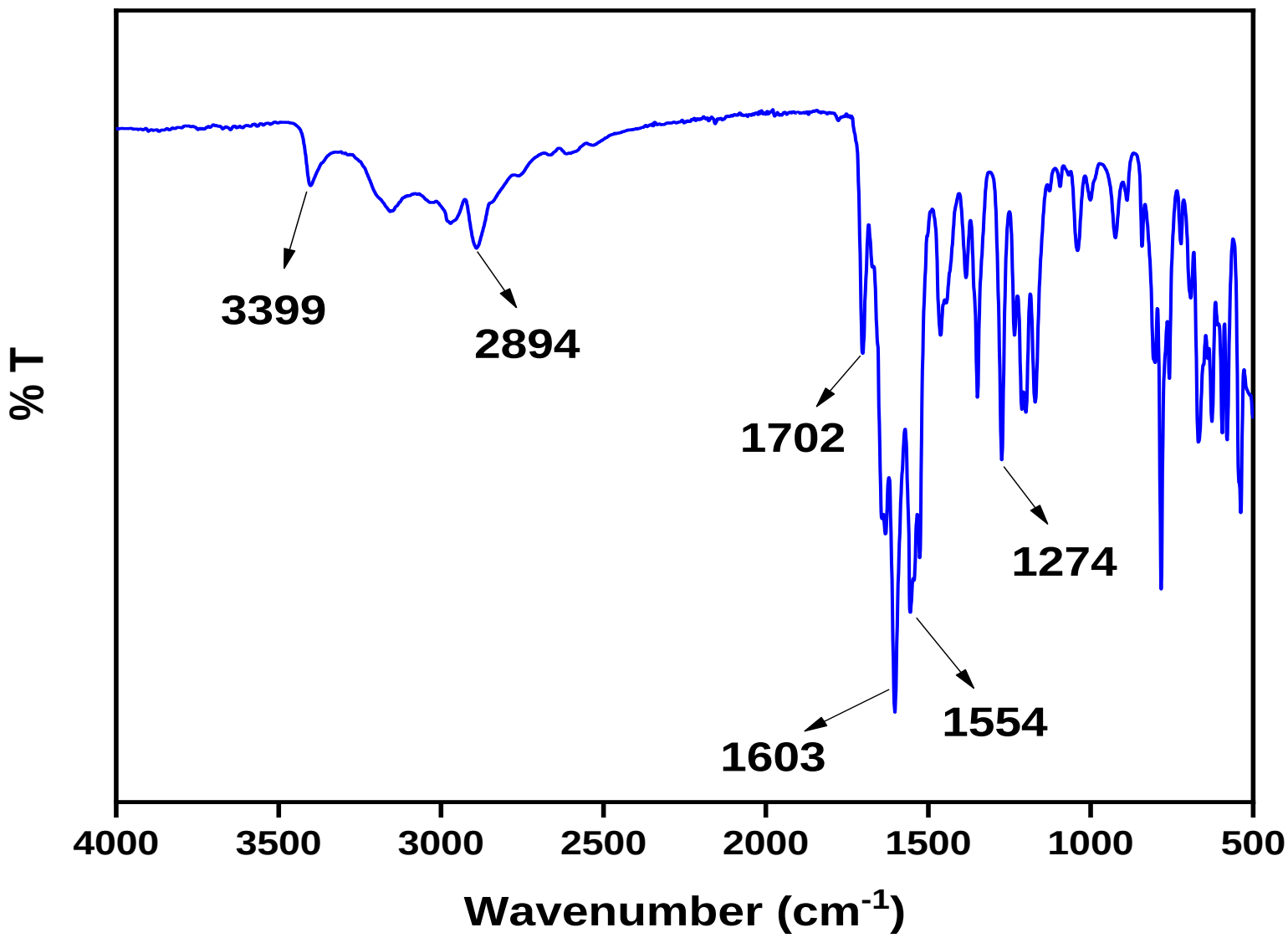
3399
2894
1702
1274
1603
1554
% T
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)

Figure S71. FT-IR spectra of compound **3s**.

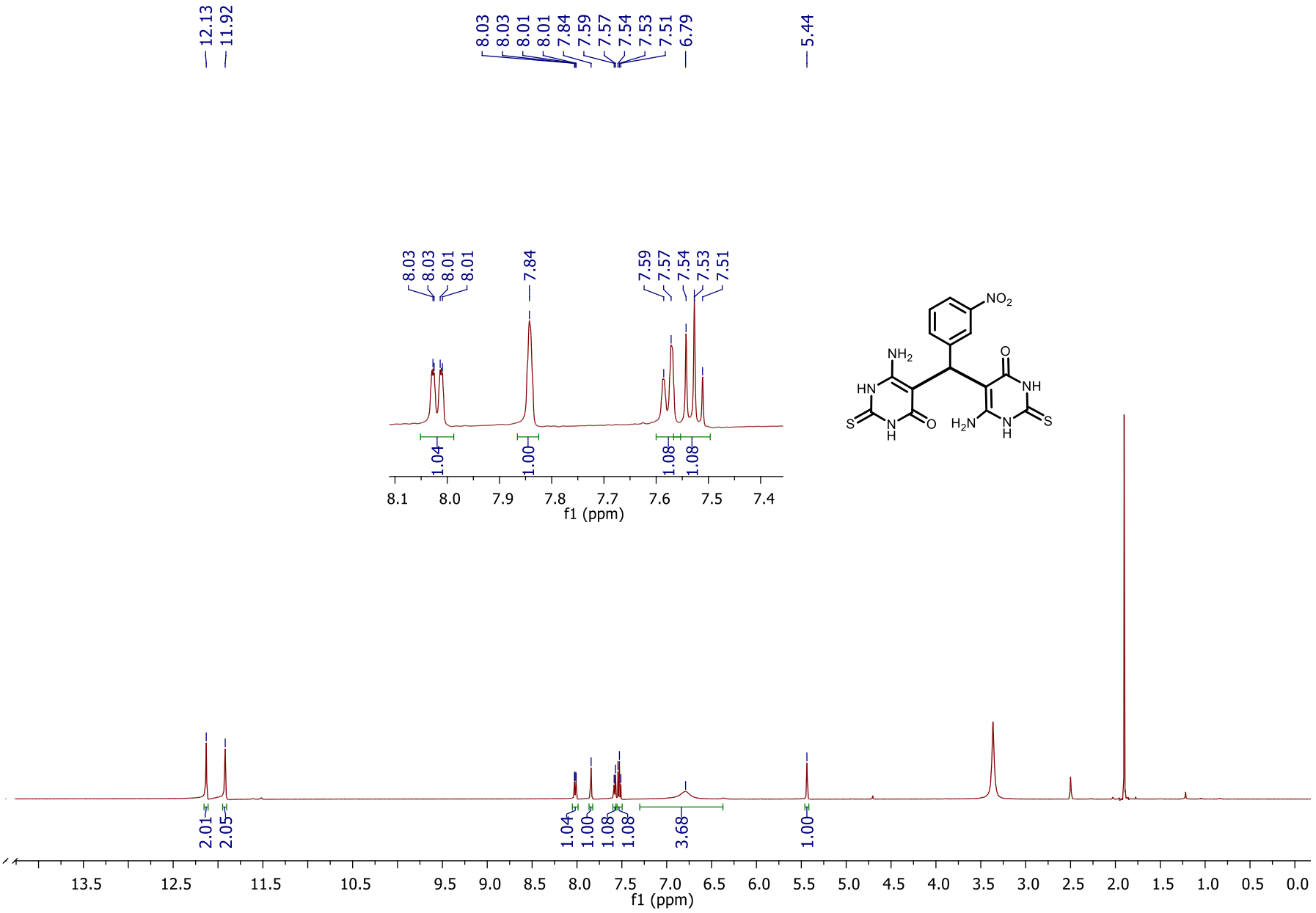

Figure S72. ^{13}C-NMR (126 MHz, DMSO-d_6) spectra of compound **3s**.

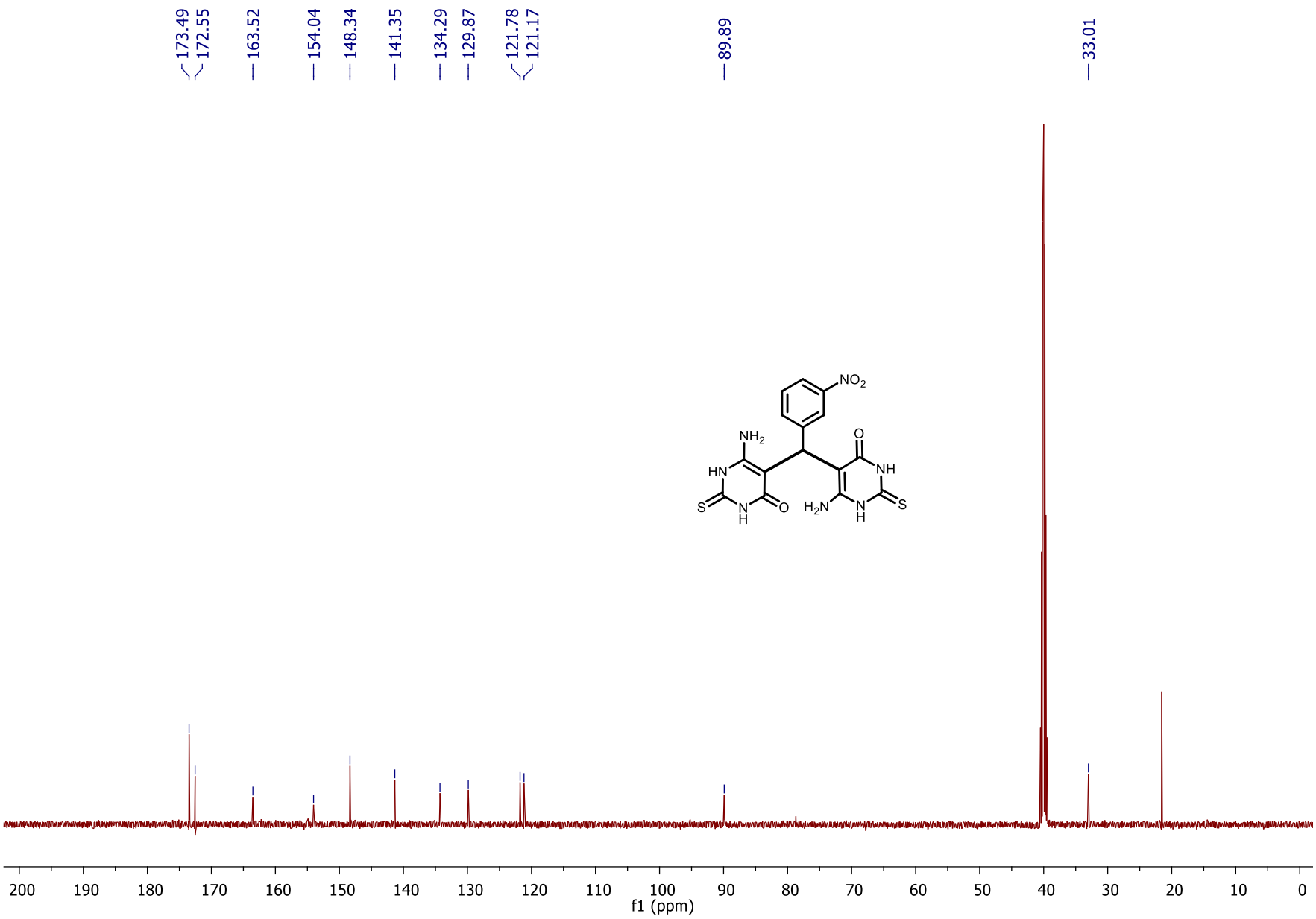
173.49
172.55
163.52
154.04
148.34
141.35
134.29
129.87
121.78
121.17
89.89
33.01
NO2
NH2
HN
S
N
H
O
O
NH
H2N
N
H
S
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Figure S73. ^{13}C-NMR (126 MHz, DMSO-d_6) spectra of compound **3s**.

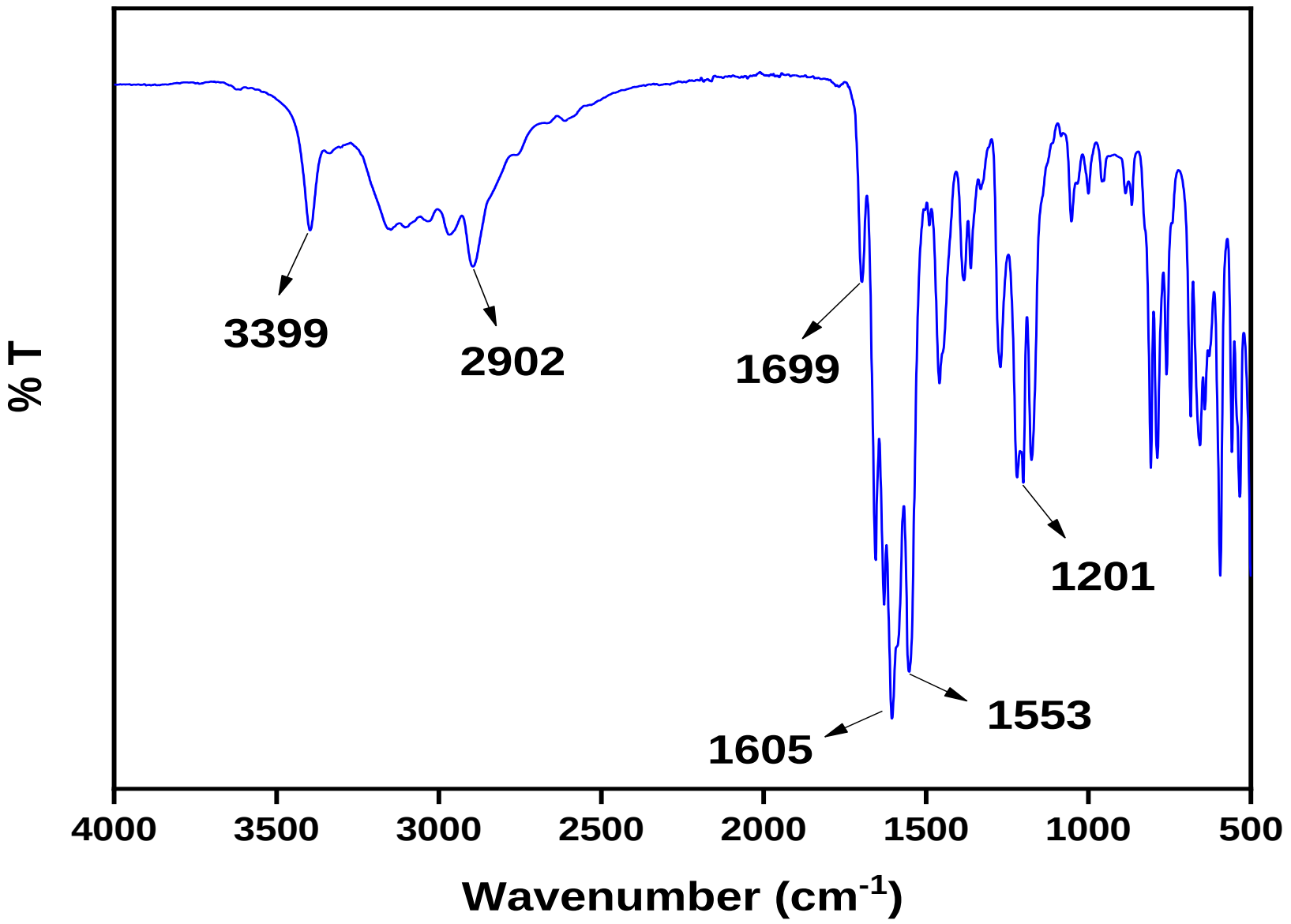

Figure S74. FT-IR spectra of compound **3t**.

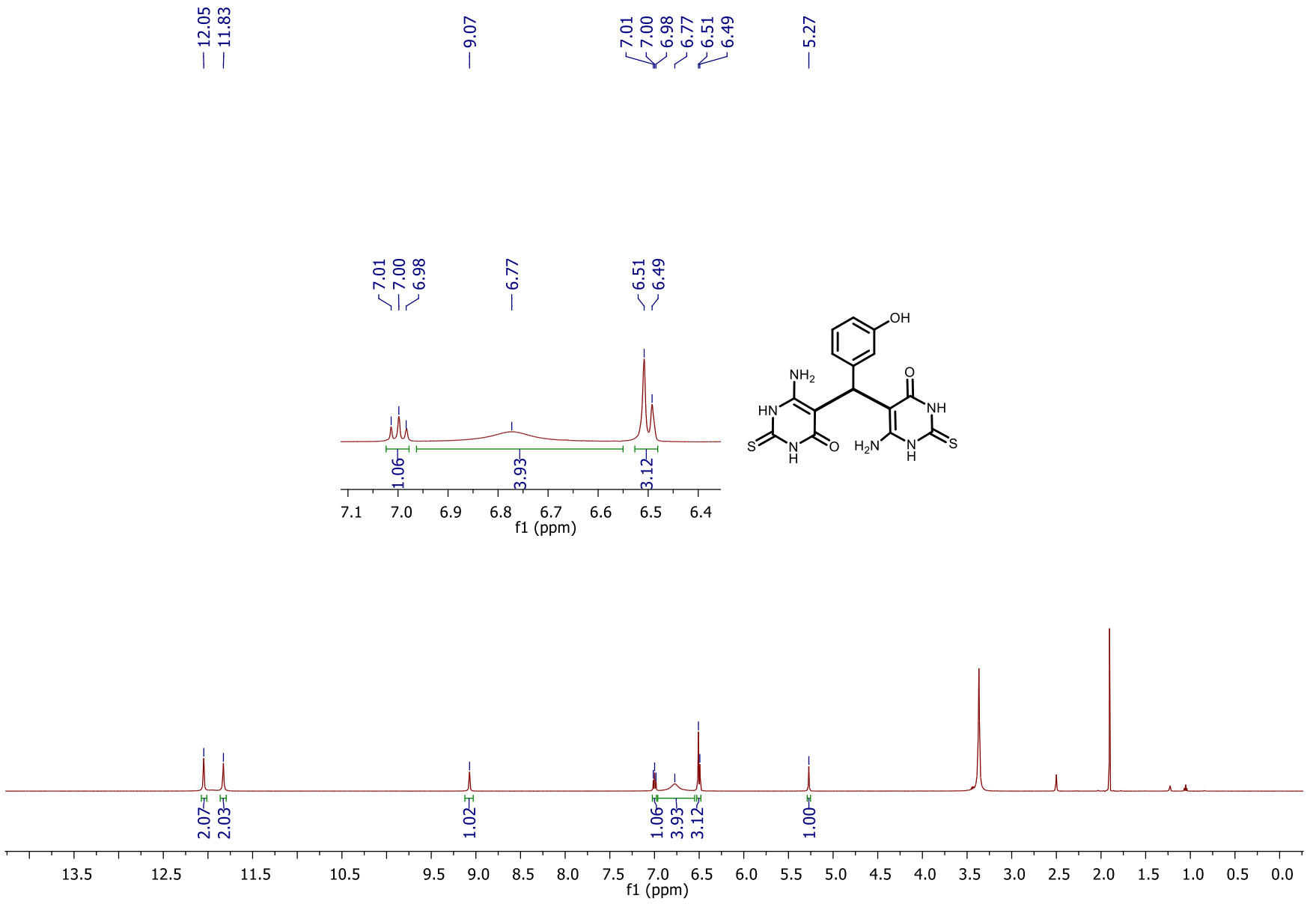

Figure S75. ^{13}C-NMR (126 MHz, DMSO-d_6) spectra of compound **3t**.

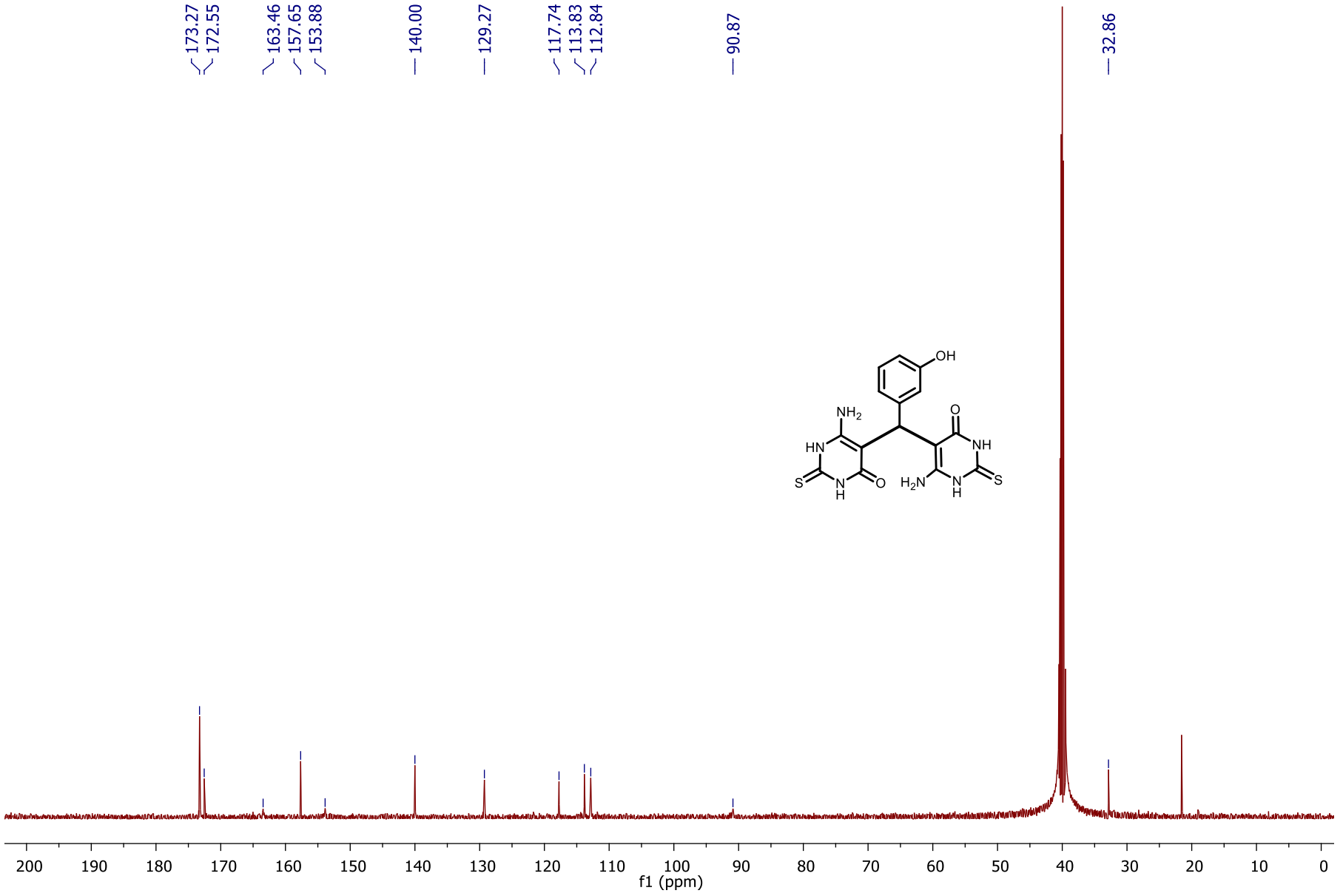

Figure S76. ^{13}C-NMR (126 MHz, DMSO-d_6) spectra of compound **3t**.

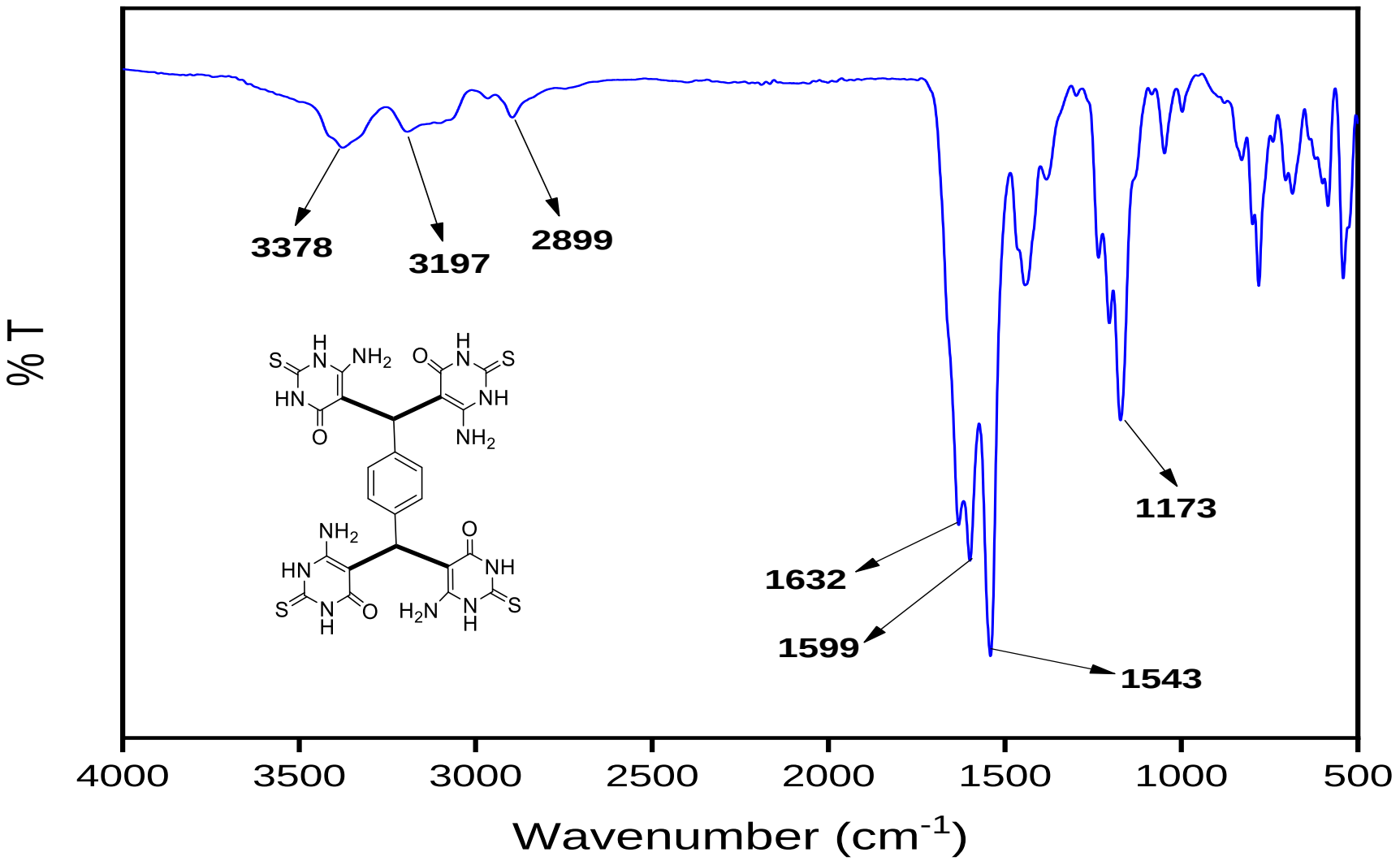

Figure S78. FT-IR spectra of compound **4a**.

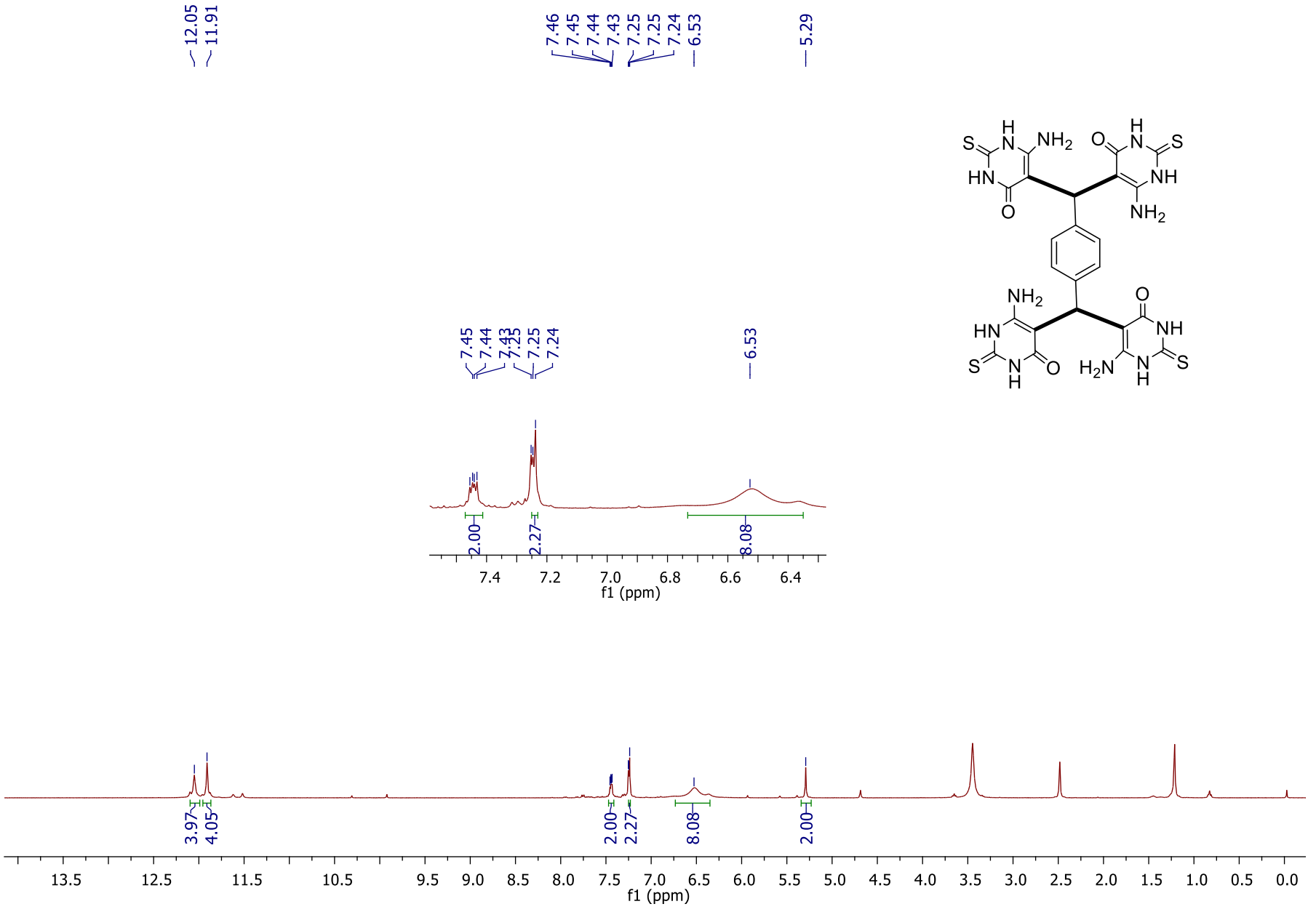

Figure S79. ^{1}H-NMR (400 MHz, DMSO-d_6) spectra of compound **4a**.

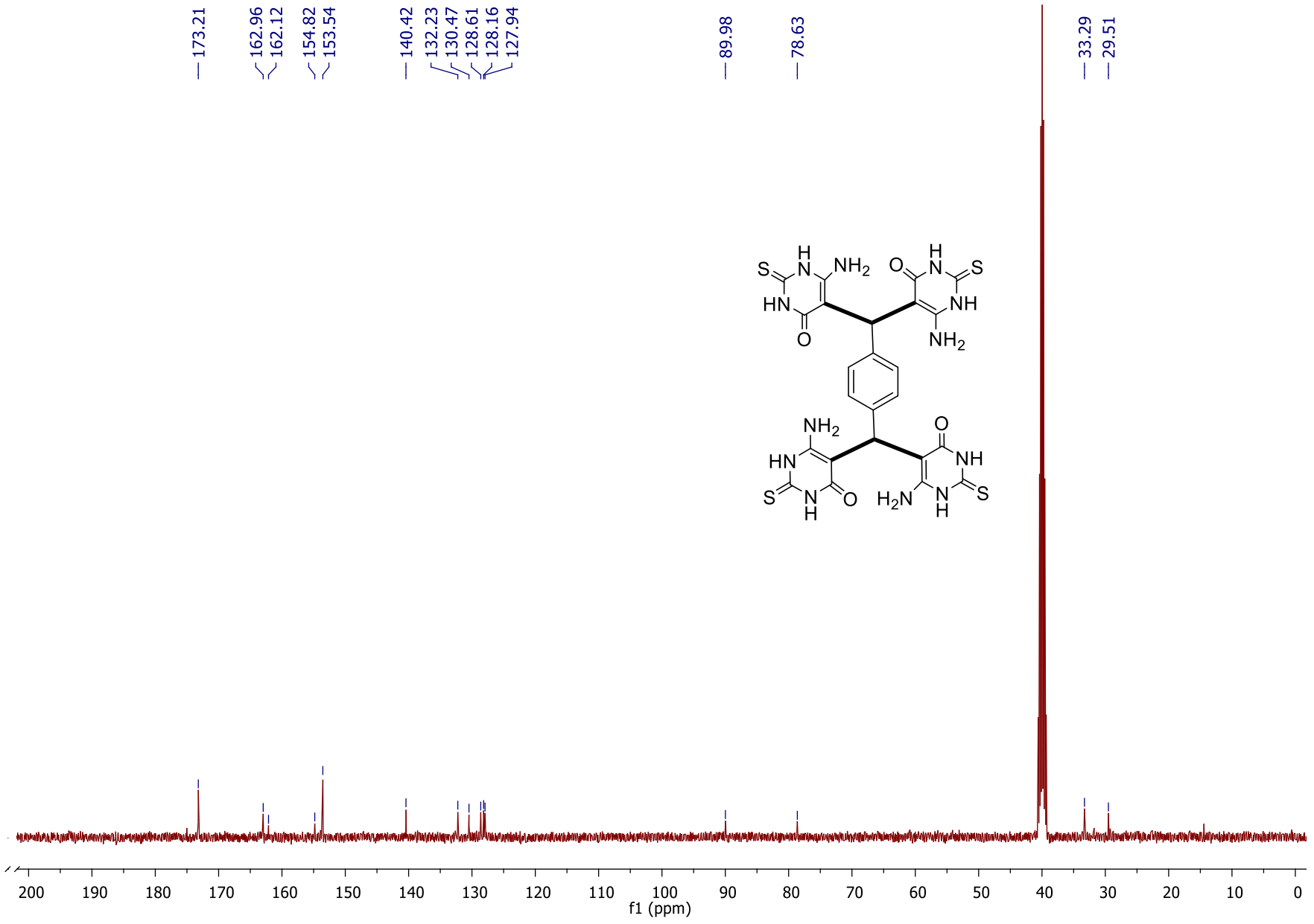

Figure S80. ^{13}C-NMR (101 MHz, DMSO-d_6) spectra of compound **4a**.

10. Listing S6. Cartesian coordinates of the components, stable intermediates and transition states of the reaction pathways depicted in Figures 1, 2 and S1 optimized at the r^{2}SCAN-3c/CPCM(water) level. The listing format follows the ones of the standard XYZ file: number of atoms, title, coordinates. The title contains the name followed by the charge and multiplicity.

COMPONENTS

```
14
Substrate (1), charge 0, mult 1
S -0.43723 -4.42884 -3.04785
N 0.09431 -5.54043 1.77080
O 3.10210 -7.47197 -1.39364
N -0.03185 -5.13965 -0.51015
C 0.36445 -5.24889 -1.81135
C 0.58611 -5.78734 0.54306
N 1.43126 -6.05238 -2.02299
C 1.66966 -6.60184 0.29048
C 2.14924 -6.77327 -1.03089
H -0.80669 -5.10267 1.89069
H 0.43222 -6.09600 2.54087
H 1.75034 -6.15438 -2.97908
H -0.82759 -4.53703 -0.33854
H 2.16251 -7.12167 1.10249

14
benzaldehyde, charge 0, mult 1
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C -3.38605 -0.44717 0.00000
C -2.12473 -1.03976 0.00000
C -0.97074 -0.25050 -0.00000
C -1.07583 1.13192 -0.00000
C -2.34273 1.73272 -0.00000
C -2.49240 3.19442 0.00000
O -1.56449 3.98936 0.00000
H -3.54333 3.55448 -0.00000
H -4.47414 1.41458 -0.00000
H -4.27893 -1.06532 0.00000
H -2.03662 -2.12275 0.00000
H 0.00768 -0.72216 -0.00000
H -0.18952 1.76000 -0.00000

3
H2O, charge 0, mult 1
O 0.10848 0.00000 -0.16188
H 1.07032 0.00000 -0.09648
H -0.17879 0.00000 0.75836

39
3b product, charge 0, mult 1
S -1.19542 -9.53646 -4.00928
N -0.99657 -5.62466 -0.96085
O 3.07448 -7.45594 -2.66858
N -0.90728 -7.42839 -2.39873
C -0.30618 -8.39084 -3.15153
C -0.23160 -6.47798 -1.65678
N 1.04454 -8.33696 -3.15994
C 1.16115 -6.46568 -1.65511
C 1.84459 -7.39174 -2.48527
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H 1.53374 -9.01304 -3.73465
H -1.92048 -7.43983 -2.39338
C 4.26777 -5.22422 0.14931
C 5.35239 -5.72533 0.86944
C 5.32624 -7.02373 1.36769
C 4.19931 -7.81601 1.14806
C 3.12104 -7.31558 0.42795
C 3.14635 -6.01713 -0.09264
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H 1.22632 -5.27182 0.07125
H 4.29925 -4.20251 -0.21858
H 6.21870 -5.09199 1.04097
H 6.17122 -7.41477 1.92767
H 4.15956 -8.82847 1.54106
H 2.24629 -7.94117 0.26484
S 2.45897 0.05583 -3.17463
C 2.28577 -1.48667 -2.51915
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H 0.84547 -1.02238 -1.16754
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N 3.72551 -4.74122 -3.03513
O 0.35795 -3.14568 -0.05288
C 2.05302 -4.09713 -1.42006
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19
PTSA, charge 0, mult 1
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O -1.71491 -0.02223 0.83370
S -0.68636 -1.04068 1.08074
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O -1.29289 -2.51084 0.66706
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C -0.21994 -1.76604 5.55338
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H 0.41737 -1.09538 7.48523

18
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H -1.00100 -2.12829 7.54203
H 0.41100 -1.06777 7.50046

20
PTSA prot., charge 1, mult 1
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H 0.69058 -1.12225 7.35790
H 0.46111 -0.20457 -0.28022

15
Cu, charge 0, mult 2
Cu 0.27385 2.02227 2.20614
Cl 0.19022 3.42490 0.38779
Cl 0.35126 0.61684 4.02411
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H -2.50295 2.21438 1.52342
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H -0.85977 3.21500 4.16979
H -0.94144 4.15542 2.94940
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O 2.59435 2.61533 2.56256
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INTERMEDIATES

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47
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47
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C -1.83654 3.89470 0.11273
C -1.67189 5.10642 -0.76071
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C -3.10627 3.51275 0.56712
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H -4.27033 2.08840 1.68192
H -3.97220 4.11636 0.30551

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O 2.57604 -7.77334 -1.35626
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N 1.10190 -6.18656 -2.03436
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C 6.67413 -6.97541 -0.16511
C 5.97078 -7.33408 0.98494
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C 2.83179 -5.23168 0.62773
O 2.73586 -4.83854 1.97993
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H 6.67751 -5.76072 -1.94385
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H 6.39228 -8.05746 1.67718
H 4.17914 -7.05470 2.14214
H 2.22012 -4.02344 2.04112

48
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C 3.75643 -0.79106 -3.03887
C 2.86934 -1.10465 -2.00998
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H 1.30461 2.93724 -1.21695
O -1.48255 1.92312 2.52769
S -0.83464 0.77058 1.88943
O 0.63187 1.20996 1.34799
O -1.55113 0.09282 0.79154
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C 0.42344 -2.26455 5.04575
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C 0.47791 -2.58470 3.68182
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C -0.03008 -0.99656 5.42105
C 0.09782 -1.66662 2.71455
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48
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N -2.46563 -0.14144 -2.41270
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C 3.42972 -0.50455 -3.73538
C 2.64414 0.01355 -2.70828
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C 0.82571 1.65354 -1.94413
O 1.36382 1.38469 -0.51156
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C -1.39679 -1.19229 5.04753
C 0.66366 -1.89849 3.29616
C -1.55648 -0.96568 3.68721
H 1.46003 -2.16943 2.61051
C -0.51828 -1.32485 2.83197
H -2.46660 -0.51901 3.30029
H 0.58912 -2.83824 7.23229
H -1.01337 -2.11460 7.52485
H 0.43019 -1.09641 7.47752
H 1.07051 0.47136 -0.12982

26
I7, charge 1, mult 1
S -2.72435 -7.94647 -1.13622
N 0.11379 -4.81036 1.38983
O 2.17077 -8.30947 -1.18295
N -1.05424 -6.32680 0.13853
C -1.21456 -7.42198 -0.68295
C 0.13567 -5.82234 0.54835
N -0.06110 -8.02762 -1.06215
C 1.36397 -6.42923 0.07768
C 1.24622 -7.65855 -0.73058
H -0.75513 -4.38226 1.68233
H 0.95512 -4.46692 1.82842
H -0.14857 -8.83738 -1.66787
H -1.91705 -5.91270 0.47902
C 4.82732 -5.10685 -0.31414
C 6.16877 -5.40130 -0.48367
C 6.62785 -6.69767 -0.24543
C 5.74174 -7.69723 0.16362
C 4.39113 -7.42454 0.29079
C 3.90830 -6.12366 0.03366
C 2.54238 -5.72929 0.21604
H 2.43786 -4.67544 0.47351
H 4.46574 -4.09360 -0.46897
H 6.86325 -4.62135 -0.77990
H 7.68429 -6.92556 -0.35608
H 6.11314 -8.69284 0.38641
H 3.71067 -8.19404 0.63174

40
I8, charge 1, mult 1
S -2.75935 -7.57605 -0.90221
N 0.16618 -4.77846 1.88626
O 2.12043 -7.78735 -1.32163
N -1.03234 -6.16655 0.53456
C -1.22961 -7.11412 -0.44292
C 0.17058 -5.68872 0.93528
N -0.09629 -7.63893 -0.96869
C 1.38210 -6.22030 0.33969
C 1.22016 -7.27180 -0.68212
H -0.69994 -4.41442 2.26059
H 1.01558 -4.45128 2.31913
H -0.20884 -8.32854 -1.70469
H -1.87827 -5.79874 0.95901
C 4.83663 -4.80379 0.23558
C 6.17240 -4.99576 -0.07181
C 6.65631 -6.28937 -0.26653
C 5.80106 -7.38743 -0.14216
C 4.45483 -7.20267 0.11919
C 3.94126 -5.89851 0.28460
C 2.57581 -5.58109 0.59263
H 2.49361 -4.61667 1.09258
H 4.46199 -3.80068 0.42623
H 6.84214 -4.14387 -0.13800
H 7.70781 -6.44632 -0.48996
H 6.19368 -8.39407 -0.24931
H 3.80364 -8.05835 0.23311
S 3.24618 -0.99057 -0.69002
C 2.81253 -2.38592 -1.52709
H 4.62376 -2.63230 -2.39996
H 0.90502 -2.49560 -0.84693
N 3.69870 -3.04036 -2.33311
N 1.58519 -2.95049 -1.44487
C 3.41283 -4.21268 -3.00512
C 1.16423 -4.13435 -2.10276
H 5.35090 -4.40166 -3.66457
N 4.40494 -4.74403 -3.73387
O 0.00946 -4.53431 -1.89712
C 2.14596 -4.75291 -2.90799
H 4.26783 -5.64791 -4.15765
H 1.90450 -5.67526 -3.42041

40
I9, charge 1, mult 1
S -2.06749 -9.50698 -0.07697
N 0.41719 -5.80602 2.07251
O 1.61280 -7.15909 -2.36063
N -0.63013 -7.49228 0.91676
C -0.87256 -8.32771 -0.13332
C 0.33146 -6.50228 0.93392
N -0.07186 -8.12843 -1.20633
C 1.13422 -6.31320 -0.19092
C 0.95170 -7.17636 -1.30211
H -0.24125 -5.94092 2.82490
H 1.09389 -5.07133 2.19018
H -0.20663 -8.73342 -2.00819
H -1.20256 -7.64521 1.73860
C 4.56396 -4.75993 0.41623
C 5.88317 -5.13509 0.64673
C 6.26503 -6.46723 0.49994
C 5.31634 -7.41704 0.13282
C 3.99554 -7.04001 -0.10214
C 3.60917 -5.70592 0.02633
C 2.18392 -5.23483 -0.23152
H 1.96279 -4.51924 0.56443
H 4.27131 -3.72023 0.55606
H 6.60967 -4.38778 0.95297
H 7.29411 -6.76384 0.68190
H 5.60128 -8.46014 0.02810
H 3.26919 -7.79620 -0.38101
S 4.53023 -0.60111 -2.34926
C 3.58586 -1.93398 -2.09077
H 4.82214 -3.18801 -3.11193
H 2.08623 -0.98024 -1.10413
N 3.96418 -3.17942 -2.56700
N 2.39497 -1.89382 -1.42345
C 3.25934 -4.31820 -2.42363
C 1.55198 -2.96146 -1.16294
H 4.45196 -5.46622 -3.60114
N 3.62632 -5.41320 -3.01563
O 0.48854 -2.79622 -0.59921
C 2.03697 -4.33526 -1.56367
H 3.03721 -6.24546 -2.85306
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H 1.23594 -4.77416 -2.16866

40
I10, charge 1, mult 1
S -1.65333 -9.12790 -3.90820
N -0.02412 -6.93315 0.23186
O 1.90000 -5.77386 -4.00328
N -0.67105 -7.86419 -1.77188
C -0.64712 -8.05337 -3.12666
C 0.13597 -6.99853 -1.08165
N 0.27206 -7.28125 -3.77373
C 1.08774 -6.22350 -1.78454
C 1.11106 -6.39952 -3.15396
H -0.70324 -7.50336 0.71552
H 0.59170 -6.37352 0.80155
H 0.32688 -7.36657 -4.78386
H -1.34557 -8.42885 -1.26555
C 3.46573 -5.25179 1.00643
C 4.37763 -5.84650 1.87049
C 4.78449 -7.16416 1.66113
C 4.26988 -7.88254 0.58660
C 3.35472 -7.28723 -0.28122
C 2.95257 -5.96545 -0.08117
C 1.96871 -5.25764 -1.01004
H 1.27118 -4.71072 -0.35489
H 3.14996 -4.22323 1.16857
H 4.77021 -5.28208 2.71151
H 5.49703 -7.62847 2.33682
H 4.57796 -8.91041 0.41818
H 2.96152 -7.85484 -1.12149
S 4.16724 -0.32844 -3.72404
C 3.55770 -1.72258 -3.01523
H 5.33056 -2.69140 -2.99395
H 1.62834 -1.10765 -2.86899
N 4.35575 -2.79396 -2.73552
N 2.25510 -1.88195 -2.68198
C 3.93209 -3.97901 -2.16516
C 1.69120 -3.01666 -2.07341
H 5.83989 -4.72226 -2.25117
N 4.87449 -4.91561 -2.03161
O 0.49118 -3.00519 -1.79385
C 2.58003 -4.12417 -1.83287
H 4.66730 -5.78282 -1.55965
H 2.37531 -5.05817 -3.51149

29
I11, charge 0, mult 2
C 2.55651 -0.20980 -2.01854
C 2.85186 -1.26220 -2.87436
C 2.27950 -2.51387 -2.65214
C 1.41054 -2.72110 -1.57557
C 1.10844 -1.67802 -0.71706
C 1.68367 -0.41468 -0.93897
C 1.39817 0.70508 -0.06593
O 0.63394 0.61702 0.90589
H 1.89095 1.66213 -0.29784
H 2.99522 0.77247 -2.17637
H 3.52569 -1.11158 -3.71213
H 2.51130 -3.33793 -3.32125
H 0.97376 -3.70223 -1.41457
H 0.43932 -1.81986 0.12782
Cu 0.23596 2.11098 2.20390
Cl -0.10870 3.64889 0.51967
Cl 0.54087 0.62226 3.96518
O -2.11685 1.46992 2.09893
H -2.17190 0.54224 2.36288
H -2.34880 1.46518 1.16127
O -0.26222 3.55782 3.58138
H -0.71461 3.14413 4.33210
H -0.91037 4.16084 3.18665
H 2.86419 3.18053 1.53771
O 2.55520 2.73811 2.33875
H 3.13294 1.96946 2.43039
O -0.61120 -2.17510 2.43591
H -0.27526 -1.32893 2.77361
H -1.56875 -2.06267 2.45284

43
I12, charge 0, mult 2
S -0.19065 1.65547 -3.88249
N -2.52068 0.79889 0.42193
O -1.73841 -2.85734 -2.55113
N -1.40695 1.01662 -1.59951
C -0.91975 0.58827 -2.79889
C -2.03348 0.19707 -0.67841
N -1.06731 -0.73360 -3.04126
C -2.15765 -1.14903 -0.95402
C -1.67680 -1.68138 -2.17485
H -2.21889 1.74143 0.63535
H -2.75468 0.21807 1.22463
H -0.71206 -1.08574 -3.92230
H -1.25740 1.99627 -1.37254
H -2.64409 -1.80845 -0.24601
C 2.46034 -0.21055 -2.08270
C 2.72787 -1.24832 -2.96370
C 2.28321 -2.53627 -2.66767
C 1.57248 -2.79578 -1.49138
C 1.28968 -1.76657 -0.61095
C 1.73416 -0.46524 -0.90778
C 1.43294 0.65153 -0.04452
O 0.74112 0.54044 0.98356
H 1.83133 1.63506 -0.33710
H 2.79794 0.79989 -2.29711
H 3.28081 -1.05879 -3.87845
H 2.49342 -3.34914 -3.35749
H 1.23528 -3.80483 -1.27473
H 0.72677 -1.94949 0.30017
Cu 0.28505 2.06729 2.18789
Cl -0.19910 3.49863 0.44195
Cl 0.22068 0.59956 3.97123
O -2.70469 -0.71951 2.97255
H -3.47478 -0.81581 3.54628
H -2.07361 -0.18838 3.48619
O -0.34381 3.52700 3.46275
H -0.82901 3.13964 4.20802
H -0.97065 4.11869 3.01795
H 2.85811 3.10050 1.65901
O 2.48096 2.68111 2.44376
H 3.05278 1.92001 2.61083
O -0.38606 -2.45676 2.41224
H 0.14827 -1.69566 2.68014
H -1.28995 -2.12313 2.52967

43
I13, charge 0, mult 2
S -2.19653 2.35707 -4.30440
N -2.89237 0.77501 0.32703
O -0.69739 -2.04760 -2.69609
N -2.44519 1.41999 -1.83560
C -1.95327 1.22830 -3.11271
C -2.26788 0.56912 -0.79561
N -1.29844 0.04967 -3.31994
C -1.28924 -0.52540 -0.94468
C -1.08738 -0.94421 -2.36840
H -3.48765 1.58623 0.44990
H -2.70084 0.22253 1.17352
H -1.03680 -0.16176 -4.27778
H -2.99981 2.26212 -1.70894
H -1.56508 -1.39971 -0.34860
C 2.00950 -0.39407 -1.85340
C 3.10383 -1.13213 -2.29539
C 3.48447 -2.28722 -1.61563
C 2.77061 -2.69404 -0.48985
C 1.67560 -1.95652 -0.04735
C 1.28332 -0.80430 -0.73205
C 0.10567 0.03109 -0.26830
O -0.09448 0.02360 1.08415
H 0.23233 1.04685 -0.67759
H 1.71826 0.51327 -2.37963
H 3.66419 -0.80016 -3.16495
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H 4.34069 -2.86326 -1.95539
H 3.06997 -3.58852 0.04965
H 1.13294 -2.27405 0.83689
Cu 0.43561 1.52780 2.14878
Cl -0.32268 3.21914 0.73234
Cl 0.19415 0.27194 4.13523
O -2.82090 -0.29911 2.97878
H -3.51467 0.14733 3.47985
H -1.99005 -0.05549 3.42837
O 1.17913 3.03229 3.35172
H 0.93434 2.84745 4.27180
H 0.73429 3.86307 3.12250
H 3.01796 1.93120 1.07039
O 2.66196 1.17301 1.55268
H 2.70030 0.44548 0.91481
O -1.14989 -2.47046 1.91019
H -0.74445 -1.59225 1.75685
H -1.97686 -2.24497 2.35575

43
I14, charge 0, mult 2
S -4.56065 -0.35236 -4.22479
N -2.26766 2.21317 -0.66574
O -0.63189 -2.13351 -1.84329
N -3.20598 0.88057 -2.28828
C -3.32863 -0.21589 -3.08830
C -2.21024 1.06664 -1.34834
N -2.39804 -1.17417 -2.87819
C -1.22547 0.08604 -1.19685
C -1.35151 -1.12402 -1.93842
H -3.02881 2.85692 -0.82313
H -1.72124 2.38423 0.17863
H -2.47431 -2.02654 -3.42110
H -3.91391 1.59417 -2.41651
H -0.56280 -2.81093 -0.16470
C 1.65710 0.35086 -2.12334
C 2.85911 -0.03572 -2.70661
C 3.68954 -0.94894 -2.05763
C 3.30840 -1.46118 -0.82045
C 2.10447 -1.07218 -0.23492
C 1.26723 -0.17233 -0.88779
C -0.04271 0.31482 -0.29259
O -0.30723 -0.19847 1.03952
H 0.07891 1.39300 -0.14152
H 1.01105 1.06297 -2.63314
H 3.14889 0.37762 -3.66892
H 4.62816 -1.25421 -2.51176
H 3.95059 -2.16922 -0.30313
H 1.82566 -1.47388 0.73295
Cu 0.39065 0.41550 2.82815
Cl 1.88553 1.93068 1.95916
Cl -1.36772 -0.69105 3.81716
O -1.19927 3.23477 1.84082
H -0.24690 3.06984 1.94392
H -1.59387 2.72890 2.56376
O 0.82600 1.19501 4.68508
H 0.02752 1.18074 5.23528
H 1.08000 2.12752 4.60751
H 1.70808 -1.70319 4.04986
O 1.87097 -1.32343 3.17606
H 2.77974 -0.99687 3.21983
O -0.56540 -2.84119 0.81618
H -0.45114 -1.19105 1.01680
H -1.45028 -3.14897 1.05219

28
I15, charge 0, mult 1
S -3.76309 2.50796 -2.88217
N -2.34216 0.28135 1.32022
O 0.99578 2.05364 -1.60934
N -2.81806 1.38516 -0.65511
C -2.54135 2.01820 -1.82781
C -1.86681 0.95134 0.25361
N -1.22624 2.21474 -2.06966
C -0.52567 1.18628 -0.00836
C -0.15895 1.82359 -1.23028
H -3.32434 0.32211 1.54845
H -1.68881 0.13156 2.07922
H -0.97441 2.67543 -2.93622
H -3.79950 1.21928 -0.46602
C 2.60717 -0.74452 0.58338
C 3.18928 -1.97731 0.29509
C 2.38867 -3.05542 -0.07360
C 1.00556 -2.89483 -0.15579
C 0.42586 -1.66254 0.12956
C 1.22261 -0.57765 0.50591
C 0.61877 0.76498 0.88000
O 0.17357 0.76284 2.25597
H 1.40557 1.52404 0.76531
H 3.23293 0.09998 0.86499
H 4.26812 -2.09315 0.35250
H 2.83997 -4.01685 -0.30288
H 0.37755 -3.73144 -0.44978
H -0.65150 -1.54328 0.05081
H 0.87217 0.35486 2.78489

28
I16, charge 0, mult 1
S -4.27359 2.89668 -2.32664
N -1.70975 0.06119 0.87626
O 0.60422 3.18910 -1.82173
N -2.78430 1.29025 -0.81628
C -2.83490 2.34727 -1.66748
C -1.64214 0.81368 -0.15594
N -1.64069 2.95678 -1.93383
C -0.36276 1.28954 -0.71324
C -0.38398 2.54327 -1.50316
H -2.67177 -0.14753 1.14269
H -0.41581 -0.35850 2.26439
H -1.66771 3.76923 -2.53981
H -3.68231 0.91013 -0.53982
C 2.53348 -0.69268 0.52799
C 2.98430 -1.90735 1.03062
C 2.19066 -3.04636 0.90942
C 0.94529 -2.96477 0.28279
C 0.47286 -1.74745 -0.18281
C 1.25501 -0.58770 -0.04956
C 0.85631 0.71063 -0.56111
O 0.10814 -0.52236 3.07583
H 1.68279 1.32353 -0.92174
H 3.16013 0.19297 0.59850
H 3.96193 -1.96895 1.49938
H 2.54748 -4.00061 1.28642
H 0.34005 -3.85826 0.16028
H -0.49350 -1.69442 -0.67107
H 0.97782 -0.77769 2.74673

39
I17, charge 0, mult 1
S -4.90609 2.19930 2.67361
N -1.37942 -1.19860 1.71096
O -0.78474 3.30592 0.25565
N -2.87864 0.52944 2.23633
C -3.39343 1.77111 2.08325
C -1.65878 0.04856 1.72262
N -2.61069 2.65950 1.40587
C -0.76501 1.08095 1.16737
C -1.34718 2.41551 0.88270
H -2.14123 -1.75461 2.10002
H -2.99393 3.58521 1.25287
H -3.48948 -0.14580 2.68103
C 2.59751 -0.06911 -0.00522
C 3.61796 -1.00821 0.04678
C 3.63156 -1.95864 1.06538
C 2.62215 -1.95813 2.03057
C 1.57770 -1.04929 1.95831
C 1.53631 -0.09758 0.92287
C 0.53339 0.93813 0.77831
H 0.90298 1.81215 0.24002
H 2.60735 0.69776 -0.77625
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H 4.41264 -0.98587 -0.69313
H 4.43595 -2.68683 1.12062
H 2.65115 -2.67731 2.84419
H 0.79890 -1.06104 2.70902
S 1.11460 2.47625 -3.42484
C 0.22481 1.17180 -2.83524
H 1.64309 -0.20719 -3.26450
H -1.38994 2.23514 -2.23319
N 0.71939 -0.09977 -2.86238
N -1.00859 1.29839 -2.29684
C 0.05994 -1.19559 -2.33987
C -1.77906 0.25672 -1.71871
H 1.67396 -2.42410 -2.66177
N 0.69224 -2.37834 -2.43343
O -2.86212 0.55603 -1.19841
C -1.19193 -1.02752 -1.78652
H 0.30380 -3.16768 -1.94159
H -1.71245 -1.86919 -1.34851

39
I18, charge 0, mult 1
S -4.23094 2.19906 3.89348
N -2.00022 -1.41974 1.21593
O -0.39010 3.07609 0.91526
N -2.94060 0.38623 2.41003
C -3.03822 1.67505 2.80329
C -1.97241 -0.15272 1.52485
N -2.12505 2.51310 2.26955
C -1.02554 0.78062 1.01157
C -1.11263 2.15248 1.34134
H -2.78440 -1.89131 1.66258
H -2.17036 3.48845 2.53443
H -3.62518 -0.24915 2.79964
C 2.48774 0.04122 -0.05788
C 3.66183 -0.57476 0.36638
C 3.61853 -1.53672 1.37247
C 2.39601 -1.86747 1.95381
C 1.22107 -1.25206 1.52887
C 1.25345 -0.29552 0.51024
C 0.01485 0.41736 0.00161
H 0.36989 1.36546 -0.41973
H 2.52985 0.79996 -0.83742
H 4.61045 -0.29636 -0.08445
H 4.53241 -2.01941 1.70771
H 2.35490 -2.60971 2.74661
H 0.27130 -1.51899 1.97966
S 0.83641 1.69020 -4.98958
C 0.19518 0.88978 -3.68492
H 1.55051 -0.62867 -3.76126
H -1.43436 2.07540 -3.43559
N 0.77775 -0.27298 -3.20429
N -0.93705 1.28381 -3.03956
C 0.32777 -0.97444 -2.14224
C -1.52742 0.64864 -1.94793
H 1.53493 -2.58816 -2.45793
N 0.81110 -2.16312 -1.89117
O -2.62212 0.99255 -1.54800
C -0.67582 -0.36734 -1.24869
H 0.49797 -2.67198 -1.07504
H -1.30615 -1.14235 -0.79157

39
I19, charge 0, mult 1
S -4.75630 0.95830 3.49059
N -2.08688 -1.16323 -0.10064
O -0.17424 2.45005 2.40158
N -3.16620 -0.05273 1.60132
C -3.33199 0.86328 2.59255
C -2.02515 -0.18443 0.82499
N -2.26958 1.67263 2.79581
C -0.96337 0.68191 1.02283
C -1.05641 1.64763 2.07527
H -2.82608 -1.84881 -0.04519
H -2.34129 2.35908 3.53756
H -3.95208 -0.67086 1.43911
C 2.72934 -0.00187 0.24035
C 3.78253 -0.78389 0.69953
C 3.55699 -1.76515 1.66571
C 2.27322 -1.95126 2.16794
C 1.21626 -1.16524 1.70727
C 1.43171 -0.18806 0.73496
C 0.31784 0.71346 0.21310
H 0.68906 1.73219 0.39097
H 2.90684 0.76223 -0.51411
H 4.78293 -0.62609 0.30602
H 4.37940 -2.37736 2.02485
H 2.08750 -2.71052 2.92262
H 0.21709 -1.31622 2.10772
S -0.65299 0.90481 -5.75500
C -0.37885 0.84261 -4.09372
H 0.22129 -1.08678 -4.08156
H -0.90447 2.75740 -3.67991
N 0.06463 -0.28780 -3.47874
N -0.57331 1.89398 -3.26567
C 0.29599 -0.40713 -2.12019
C -0.36038 1.90722 -1.87141
H 0.90026 -2.34349 -2.39119
N 0.62840 -1.65646 -1.70173
O -0.58520 2.95403 -1.25735
C 0.10081 0.67946 -1.29023
H 1.11761 -1.73268 -0.81884
H -1.24325 -1.48568 -0.55213

42
I20, charge 0, mult 1
S 4.02750 -4.26975 -2.11268
S -5.67175 -1.78271 -1.52385
Cl 1.24358 4.49070 2.65571
N 0.66076 -0.61864 -2.08190
N -1.73868 -3.53592 0.94950
O 1.35539 -3.20899 1.86129
O -1.60328 0.87106 -0.89497
C -0.16615 -1.10314 0.76663
C 1.75117 2.18553 1.29246
C 1.42463 0.90442 0.84769
C 0.84491 2.86917 2.08769
C 0.20728 0.31772 1.18116
C -0.37043 2.30138 2.45719
C -0.67626 1.02706 2.00078
C -1.54848 -1.25503 0.13998
C -2.21155 -0.29107 -0.62176
C -2.26421 -2.46462 0.31012
N -3.44862 -0.45380 -1.12302
N -3.51324 -2.64521 -0.18670
C -4.02140 -1.62539 -0.85952
N 2.19768 -2.31310 -2.00739
C 2.77998 -3.27627 -1.31347
C 1.25187 -1.58719 -1.35629
N 2.55516 -3.62001 -0.04406
C 0.90649 -1.84777 -0.00904
C 1.62027 -2.88957 0.57506
H 3.95549 -3.64427 -3.30049
H -5.88179 -3.03029 -1.06924
H 1.03696 -0.42143 -2.99623
H 0.05985 0.07582 -1.65883
H -0.89182 -3.46983 1.49221
H -2.36293 -4.29620 1.17034
H -2.69365 2.82045 -3.15997
H -2.19417 1.43338 -1.47611
H -0.23894 -1.61798 1.73286
H 2.70021 2.63645 1.02159
H 2.14314 0.36718 0.23588
H -1.06373 2.84386 3.09169
H -1.62615 0.57799 2.28228
O -3.15022 2.47534 -2.38115
H 1.90459 -3.97263 2.10235
H -3.84811 1.91184 -2.74158

42
I21, charge 0, mult 1
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S 4.04712 -4.22682 -2.17548
S -5.73426 -1.51285 -1.48617
Cl 1.38816 4.42481 2.79415
N 0.84126 -0.43474 -2.01642
N -1.88399 -3.38678 1.01307
O 1.21083 -3.35594 1.73119
O -1.48231 0.91146 -1.05406
C -0.14143 -1.08200 0.73932
C 1.89221 2.09570 1.46927
C 1.53571 0.83824 0.98235
C 0.95248 2.83132 2.17420
C 0.25694 0.32468 1.18352
C -0.32626 2.33763 2.41210
C -0.66053 1.08531 1.91553
C -1.52506 -1.17475 0.10689
C -2.06293 -0.14393 -0.69623
C -2.31598 -2.31724 0.31904
N -3.38350 -0.33769 -1.13539
N -3.59928 -2.44692 -0.15425
C -4.08010 -1.45633 -0.84779
N 2.29252 -2.20624 -2.01135
C 2.79781 -3.24278 -1.36512
C 1.34298 -1.48805 -1.35378
N 2.49063 -3.67378 -0.14063
C 0.92316 -1.83108 -0.04395
C 1.55701 -2.94780 0.48752
H 4.07163 -3.50456 -3.30904
H -5.98467 -2.73645 -0.98829
H 1.19169 -0.24276 -2.94173
H 0.12783 0.17515 -1.62101
H -0.94981 -3.46212 1.38448
H -2.51039 -4.16654 1.13497
H -3.29603 2.16307 -3.53055
H -2.58610 1.99914 -2.17996
H -0.22982 -1.61312 1.69532
H 2.88963 2.48830 1.30011
H 2.27915 0.25992 0.44190
H -1.04748 2.91975 2.97659
H -1.65934 0.69485 2.09667
O -3.44472 2.23849 -2.58043
H 1.71557 -4.15933 1.93776
H -3.77366 0.40770 -1.71838

42
I22, charge 0, mult 1
S 3.98979 -4.27770 -2.16241
S -5.75523 -1.38801 -1.50812
Cl 1.45863 4.41971 2.79852
N 0.85770 -0.42356 -2.01064
N -1.93419 -3.33610 0.99843
O 1.15097 -3.35953 1.73173
O -1.45821 0.94979 -1.07909
C -0.15470 -1.05988 0.73522
C 1.93042 2.08053 1.47955
C 1.55462 0.82973 0.99014
C 0.99834 2.83448 2.17526
C 0.26450 0.34055 1.17975
C -0.29178 2.36546 2.40127
C -0.64517 1.11927 1.90238
C -1.53695 -1.12939 0.09737
C -2.04889 -0.08547 -0.71272
C -2.34607 -2.25567 0.30840
N -3.37984 -0.25930 -1.14750
N -3.63126 -2.35953 -0.17171
C -4.10396 -1.36212 -0.86770
N 2.27448 -2.22335 -2.00286
C 2.75557 -3.27119 -1.35637
C 1.33477 -1.48873 -1.34913
N 2.43337 -3.69899 -0.13459
C 0.90084 -1.82700 -0.04262
C 1.51050 -2.95632 0.49012
H 4.03408 -3.55381 -3.29434
H -6.03087 -2.62672 -1.02518
H 1.21306 -0.23868 -2.93554
H 0.14662 0.19347 -1.62033
H -1.01138 -3.41228 1.39737
H -2.58130 -4.09247 1.15523
H -5.48426 -5.08573 -0.72578
H -4.82714 -3.91584 0.01548
H -0.25521 -1.58788 1.69176
H 2.93670 2.45388 1.31952
H 2.29192 0.23679 0.45718
H -1.00708 2.96163 2.95856
H -1.65277 0.74798 2.07482
O -5.65145 -4.44113 -0.02737
H 1.63946 -4.17264 1.93925
H -3.76238 0.48424 -1.72148

42
I23, charge 0, mult 1
S 3.92420 -4.32431 -2.17283
S -5.77587 -1.27468 -1.58846
Cl 1.50885 4.37589 2.85395
N 0.89184 -0.39244 -2.00215
N -2.02482 -3.28985 0.95346
O 1.03705 -3.40612 1.68600
O -1.42897 0.99653 -1.08461
C -0.18110 -1.05166 0.71727
C 1.95388 2.03896 1.52235
C 1.56053 0.80047 1.01582
C 1.02648 2.80590 2.21008
C 0.25779 0.33695 1.18081
C -0.27623 2.36148 2.41197
C -0.64719 1.12729 1.89636
C -1.55878 -1.08592 0.06699
C -2.05062 -0.02355 -0.73887
C -2.38150 -2.19234 0.26939
N -3.38368 -0.14525 -1.18426
N -3.65555 -2.21663 -0.25857
C -4.19859 -1.20367 -0.98094
N 2.26025 -2.22918 -2.00430
C 2.70236 -3.30124 -1.36965
C 1.32980 -1.48148 -1.35276
N 2.34636 -3.74360 -0.16226
C 0.86615 -1.83095 -0.05954
C 1.43332 -2.98799 0.46040
H 4.00907 -3.57947 -3.28879
H -6.13422 -3.77807 -0.69416
H 1.26067 -0.20315 -2.92085
H 0.18651 0.23077 -1.61388
H -1.10902 -3.38047 1.36811
H -2.68730 -4.02689 1.13958
H -5.35278 -5.09088 -0.64273
H -4.25081 -3.04988 -0.12832
H -0.29835 -1.58634 1.66810
H 2.96993 2.39288 1.38123
H 2.29399 0.19714 0.48940
H -0.98795 2.96724 2.96344
H -1.66468 0.77545 2.05053
O -5.59439 -4.32719 -0.10276
H 1.49748 -4.23710 1.88694
H -3.74084 0.62055 -1.74375

TRANSITION STATES

47
TS1, charge 0, mult 1
S -2.57701 0.73911 -2.35078
N -1.43151 -2.93570 0.77709
O 1.31948 -2.23245 -3.00097
N -1.81981 -1.22779 -0.72734
C -1.57357 -0.50969 -1.86962
C -1.03661 -2.25993 -0.28862
N -0.47825 -0.89653 -2.57882
C 0.19601 -2.49970 -0.92781
C 0.41351 -1.92803 -2.23322
H -2.20479 -2.59237 1.34235
H -0.84031 -3.66528 1.14756
H -0.31013 -0.42077 -3.45843

H -2.60207 -0.93137 -0.13860
H 0.73211 -3.41182 -0.69125
C 3.28081 -0.79972 -1.10509
C 4.56124 -1.08841 -1.56003
C 5.28469 -2.12913 -0.98282
C 4.73206 -2.88040 0.05827
C 3.45909 -2.59411 0.52492
C 2.72703 -1.54765 -0.05690
C 1.40110 -1.19540 0.41943
O 1.05188 -1.58357 1.61792
H 0.94241 -0.28555 0.02502
H 2.71000 0.01211 -1.54836
H 4.99374 -0.50309 -2.36575
H 6.28403 -2.35802 -1.34208
H 5.30193 -3.68992 0.50458
H 3.02392 -3.17393 1.33298
H 0.22819 -1.09884 1.96697
H -0.00255 1.58144 1.49327
H 0.10724 3.66374 0.15976
O -3.10929 -0.80141 1.80859
C -0.91166 2.12123 1.24921
C -0.85683 3.29688 0.50333
O -0.85430 -0.37035 2.81531
H -0.94755 5.67213 -0.66837
S -2.26811 0.13281 2.63797
C -2.14381 1.65314 1.68765
C -2.01653 4.01068 0.19416
C -1.95966 5.26042 -0.63824
H -2.26570 5.04590 -1.66968
O -2.90179 0.46947 3.93682
C -3.31714 2.35113 1.40044
C -3.24500 3.52295 0.66077
H -2.64091 6.02409 -0.25042
H -4.27769 1.98384 1.75159
H -4.15793 4.06985 0.43725

29
TS1a, charge 1, mult 1
S -4.24246 0.20180 -3.09061
N -2.16705 2.06242 0.96867
O -0.28783 -1.87477 -1.01010
N -3.02714 1.03526 -0.88429
C -3.07161 0.11666 -1.91100
C -2.10798 1.05691 0.11943
N -2.10486 -0.83565 -1.87738
C -1.16939 -0.02622 0.21050
C -1.10293 -0.97257 -0.91080
H -2.87444 2.78117 0.88551
H -1.55287 2.12119 1.76590
H -2.10802 -1.52168 -2.62522
H -3.74503 1.75237 -0.91767
H -1.44325 -0.87981 1.31100
C 1.82586 0.57239 -0.48532
C 3.11123 0.41817 -0.99247
C 3.98176 -0.50985 -0.42271
C 3.56073 -1.27800 0.65935
C 2.27392 -1.12754 1.17200
C 1.40339 -0.20759 0.59313
C 0.03147 0.04036 1.14528
O -0.43105 -1.07521 2.06048
H 0.03975 0.96122 1.73446
H 1.14632 1.29385 -0.93440
H 3.43198 1.02182 -1.83662
H 4.98434 -0.63311 -0.82216
H 4.23411 -2.00234 1.10878
H 1.94811 -1.73496 2.01011
H -0.53710 -0.75626 2.97616

48
TS2, charge 1, mult 1
S -5.37673 -0.13165 -2.50174
N -1.92269 3.23024 -1.45697
O -0.59698 -0.93486 -3.32835
N -3.39097 1.53731 -1.92009
C -3.77010 0.31074 -2.40780
C -2.09944 1.96940 -1.81294
N -2.74481 -0.47903 -2.80748
C -1.02243 1.04988 -2.04022
C -1.37162 -0.16328 -2.78442
H -2.70769 3.83569 -1.26121
H -0.99480 3.56999 -1.24253
H -2.98456 -1.36669 -3.23529
H -4.14698 2.15331 -1.64048
H -1.05016 0.35234 -0.60214
C 2.18080 0.88846 -3.78172
C 3.26442 0.07001 -4.09450
C 3.68383 -0.90398 -3.19360
C 3.01789 -1.05577 -1.97654
C 1.93322 -0.24504 -1.66824
C 1.50087 0.72547 -2.57579
C 0.36435 1.65883 -2.24912
O 0.68826 2.40415 -1.01143
H 0.29688 2.42025 -3.03941
H 1.85592 1.65224 -4.48418
H 3.78375 0.20009 -5.03972
H 4.53095 -1.54055 -3.43330
H 3.34390 -1.81160 -1.26754
H 1.41676 -0.38399 -0.72210
H 1.54767 2.83931 -1.13665
O -1.87998 1.55340 2.02170
S -0.77974 0.68674 1.62462
O 0.54783 1.45279 1.30176
O -1.08253 -0.19202 0.36726
C 0.73949 -3.23065 5.93593
C 0.34940 -2.26667 4.85634
H 1.93110 -2.87471 3.52025
C 1.08798 -2.20465 3.66432
H -1.32003 -1.44446 5.94167
C -0.73731 -1.40294 5.02592
C 0.76176 -1.30409 2.66512
C -1.08866 -0.48886 4.04111
H 1.33667 -1.26066 1.74504
C -0.32726 -0.45669 2.87690
H -1.93206 0.18007 4.17528
H 1.04294 -4.19247 5.51218
H -0.07871 -3.39031 6.64199
H 1.59709 -2.83752 6.49593
H 0.60250 1.82243 0.30220

40
TS3, charge 1, mult 1
S -4.93995 -3.70009 0.42614
N -2.56191 0.10975 2.46390
O -0.64554 -2.07722 -1.34033
N -3.52584 -1.66112 1.38097
C -3.61742 -2.68104 0.47052
C -2.47090 -0.79661 1.49884
N -2.56403 -2.78228 -0.37676
C -1.35668 -0.95014 0.63467
C -1.44096 -1.94951 -0.40680
H -3.38736 0.18140 3.04160
H -1.79509 0.72130 2.69017
H -2.62143 -3.48685 -1.10427
H -4.29820 -1.59279 2.03480
C 2.04795 0.70764 0.92964
C 3.41323 0.48112 0.97312
C 3.90808 -0.80970 0.78450
C 3.02746 -1.86963 0.56821
C 1.66004 -1.64719 0.50783
C 1.14590 -0.34770 0.67550
C -0.26831 -0.03135 0.69970
H -0.47153 0.89919 1.22614
H 1.65911 1.70894 1.10285
H 4.09274 1.30591 1.16538
H 4.97821 -0.99229 0.82304
H 3.41147 -2.87822 0.44767
H 0.99117 -2.48458 0.35527
S 2.02697 4.74344 -1.22115
C 1.02704 3.40640 -1.29122
H 2.42162 2.21141 -2.16284

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H -0.60045 4.27188 -0.44276
N 1.46436 2.21799 -1.82740
N -0.24744 3.40019 -0.82214
C 0.70687 1.08384 -1.90845
C -1.14380 2.31495 -0.86433
H 2.17187 -0.01425 -2.82656
N 1.23006 0.00213 -2.46120
O -2.29724 2.46489 -0.47154
C -0.58209 1.08111 -1.34251
H 0.72155 -0.87135 -2.37063
H -1.26951 0.31042 -1.65952

40
TS4, charge 1, mult 1
S -3.87361 -3.75854 -2.72402
N -2.67260 -1.17029 1.33679
O -0.18888 -0.48266 -2.67112
N -3.10276 -2.29390 -0.63263
C -2.91790 -2.62531 -1.94385
C -2.34392 -1.37896 0.06153
N -1.90174 -1.95893 -2.55420
C -1.29609 -0.72390 -0.58948
C -1.08328 -1.02403 -1.94299
H -3.41364 -1.68900 1.78456
H -2.09597 -0.59514 1.93040
H -1.73281 -2.16061 -3.53380
H -3.85331 -2.78386 -0.15868
C 0.81127 0.53542 2.30093
C 1.60428 0.03524 3.32690
C 1.98352 -1.30698 3.32715
C 1.55888 -2.14453 2.30032
C 0.76208 -1.64410 1.27127
C 0.38964 -0.29835 1.26052
C -0.46387 0.30011 0.14998
H -1.17316 0.98064 0.64319
H 0.51757 1.58361 2.30007
H 1.92469 0.69239 4.13033
H 2.60265 -1.69800 4.12944
H 1.84591 -3.19211 2.29567
H 0.43175 -2.30442 0.47269
S 2.32029 5.12908 -2.07038
C 1.55114 3.73455 -1.58820
H 3.27341 2.74212 -1.19915
H -0.35388 4.39198 -1.84324
N 2.26456 2.63320 -1.17056
N 0.20115 3.58657 -1.57254
C 1.73575 1.44188 -0.77741
C -0.49819 2.45946 -1.14453
H 3.58305 0.62807 -0.48460
N 2.58136 0.48458 -0.46541
O -1.71738 2.49111 -1.08481
C 0.29976 1.25062 -0.83771
H 2.24384 -0.41186 -0.14254
H 0.19643 0.54482 -1.88991

43
TS5, charge 0, mult 2
S -1.98277 2.55322 -4.13812
N -2.70878 0.82224 0.44489
O -0.77122 -2.02319 -2.74124
N -2.26315 1.52089 -1.70682
C -1.81507 1.34904 -2.99517
C -2.12998 0.59748 -0.71073
N -1.26263 0.13509 -3.26389
C -1.29515 -0.54452 -0.94937
C -1.10969 -0.91647 -2.34917
H -3.20184 1.68836 0.61883
H -2.62072 0.18355 1.24023
H -1.01222 -0.05086 -4.22910
H -2.72201 2.40628 -1.51677
H -1.44909 -1.38984 -0.28190
C 1.99899 -0.61400 -2.03874
C 2.94583 -1.47338 -2.58580
C 3.30159 -2.63779 -1.90846
C 2.71420 -2.93232 -0.67823
C 1.77029 -2.07260 -0.12734
C 1.40145 -0.90985 -0.80954
C 0.41748 0.05929 -0.24453
O 0.26084 0.07434 1.05614
H 0.45778 1.03353 -0.75005
H 1.72353 0.29797 -2.56477
H 3.40840 -1.23236 -3.53868
H 4.04068 -3.31116 -2.33351
H 2.99763 -3.83447 -0.14316
H 1.32827 -2.30231 0.83610
Cu 0.31596 1.68676 2.15335
Cl -0.16517 3.24245 0.50836
Cl 0.15507 0.37291 4.08143
O -2.80709 -0.47495 3.03098
H -3.59052 -0.18185 3.51235
H -2.04972 -0.11671 3.52902
O 0.48323 3.28898 3.43104
H 0.08260 3.07532 4.28781
H -0.02230 4.03755 3.07831
H 2.86907 2.27493 1.16507
O 2.66564 1.69417 1.91048
H 2.90165 0.81299 1.59041
O -0.97117 -2.43514 1.93273
H -0.49747 -1.59056 1.83096
H -1.79242 -2.16303 2.36660

43
TS6, charge 0, mult 2
S -4.50789 0.01444 -4.29983
N -2.45180 1.33044 -0.00176
O -0.06347 -1.57522 -2.93174
N -3.30157 0.59433 -2.00265
C -3.25536 -0.07908 -3.20082
C -2.31618 0.56532 -1.06389
N -2.13009 -0.80481 -3.40530
C -1.18229 -0.31900 -1.21587
C -1.02234 -0.92788 -2.54188
H -3.25919 1.92259 0.13425
H -1.77286 1.23485 0.75191
H -2.05523 -1.29167 -4.29178
H -4.13041 1.15790 -1.84205
H -1.56292 -1.38021 -0.42132
C 2.30706 0.23744 -1.52045
C 3.55058 -0.30754 -1.83552
C 3.88335 -1.58569 -1.39565
C 2.96670 -2.31544 -0.63735
C 1.72473 -1.77067 -0.32499
C 1.38210 -0.49156 -0.77422
C 0.06706 0.14989 -0.39183
O -0.23699 -0.05757 0.98279
H 0.16756 1.22965 -0.57824
H 2.05263 1.24054 -1.85588
H 4.26382 0.27242 -2.41484
H 4.85503 -2.00999 -1.63231
H 3.22294 -3.31034 -0.28334
H 1.02036 -2.34483 0.27087
Cu 0.57956 0.86940 2.45568
Cl 0.71957 2.96211 1.41944
Cl -0.63389 -0.50979 3.93376
O -2.37185 2.41297 3.10344
H -1.60770 2.83297 2.68240
H -2.00406 1.58461 3.44852
O 1.39224 1.76229 4.12161
H 0.87202 1.49702 4.89656
H 1.27769 2.72257 4.04471
H 3.31112 0.56807 2.18073
O 2.62883 -0.11174 2.26495
H 2.65753 -0.59029 1.42123
O -1.57269 -2.06742 0.64326
H -0.99914 -1.29304 1.08377
H -2.46457 -2.01801 1.02365

28
TS7, charge 0, mult 1
S -4.17375 2.47836 -2.53287
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N -1.81406 0.06152 1.18224
O 0.66973 2.88736 -1.66127
N -2.80840 1.12349 -0.68658
C -2.77988 2.04087 -1.69130
C -1.70311 0.73735 0.07451
N -1.56821 2.59115 -1.95199
C -0.42634 1.20976 -0.36616
C -0.34425 2.27188 -1.31606
H -2.77123 -0.16672 1.43350
H -0.55860 0.57369 2.00157
H -1.52604 3.28621 -2.68753
H -3.72378 0.78264 -0.41885
C 2.46207 -0.92055 0.90684
C 2.95010 -2.22068 0.91995
C 2.21453 -3.24487 0.32552
C 0.99509 -2.96019 -0.28877
C 0.50030 -1.66250 -0.29627
C 1.22213 -0.63042 0.31621
C 0.76975 0.77267 0.28063
O 0.36071 1.06342 2.12518
H 1.58874 1.48798 0.20851
H 3.04242 -0.11731 1.35642
H 3.90879 -2.43415 1.38343
H 2.59754 -4.26147 0.32782
H 0.43146 -3.75333 -0.77149
H -0.43868 -1.44235 -0.79339
H 0.92298 0.44617 2.62017

39
TS8, charge 0, mult 1
S -4.47627 2.35013 3.53576
N -1.80092 -1.38935 1.54317
O -0.71768 3.11578 0.44541
N -2.89353 0.46676 2.49836
C -3.19143 1.78203 2.59357
C -1.86506 -0.10806 1.71536
N -2.39845 2.61213 1.87509
C -0.96162 0.82922 1.09920
C -1.30574 2.22421 1.07362
H -2.55698 -1.86799 2.03098
H -2.60480 3.60251 1.91006
H -3.51566 -0.16301 2.98909
C 2.51708 -0.12214 -0.01513
C 3.67473 -0.82270 0.30007
C 3.64578 -1.80206 1.28994
C 2.45275 -2.06438 1.96128
C 1.29068 -1.36933 1.64300
C 1.30366 -0.38604 0.64428
C 0.14984 0.46553 0.26708
H 0.51050 1.35072 -0.25883
H 2.55007 0.65142 -0.77982
H 4.59998 -0.59868 -0.22323
H 4.54780 -2.35301 1.54147
H 2.42486 -2.81983 2.74189
H 0.36580 -1.59051 2.16077
S 0.69185 2.00890 -4.82627
C 0.11629 1.06682 -3.57182
H 1.56275 -0.34889 -3.75636
H -1.54262 2.16646 -3.17456
N 0.76083 -0.08832 -3.19153
N -1.01118 1.35701 -2.87272
C 0.34705 -0.90444 -2.18017
C -1.54867 0.59865 -1.82158
H 1.74619 -2.35061 -2.57059
N 0.95792 -2.06243 -2.00640
O -2.63440 0.89898 -1.34271
C -0.68881 -0.45763 -1.31120
H 0.68980 -2.65408 -1.23333
H -1.19238 -1.22377 -0.72323

39
TS9, charge 0, mult 1
S -4.52395 0.97631 4.04914
N -2.16772 -1.15413 0.14141
O -0.15564 2.55229 2.33425
N -3.18944 -0.03538 1.96455
C -3.22465 0.88118 2.96260
C -2.13086 -0.20404 1.05716
N -2.15655 1.70543 3.02640
C -1.05409 0.69505 1.15361
C -1.03897 1.69537 2.14701
H -3.06859 -1.62218 0.08175
H -2.14912 2.40245 3.76044
H -3.97686 -0.66881 1.90853
C 2.52769 0.08481 0.06312
C 3.63783 -0.66271 0.43996
C 3.50427 -1.68782 1.37636
C 2.25729 -1.94943 1.93730
C 1.14614 -1.19489 1.56258
C 1.26965 -0.17761 0.61567
C 0.08281 0.66185 0.17454
H 0.45843 1.68944 0.09901
H 2.63440 0.88259 -0.67063
H 4.60987 -0.44289 0.00701
H 4.37046 -2.27321 1.67197
H 2.14615 -2.74104 2.67329
H 0.17652 -1.39335 2.01173
S 0.84212 1.16213 -5.58796
C 0.34576 0.87017 -4.02764
H 1.18369 -0.97822 -3.94747
H -0.69549 2.59208 -3.76871
N 0.68011 -0.30213 -3.38119
N -0.41968 1.73093 -3.30732
C 0.31577 -0.62647 -2.11720
C -0.85113 1.56254 -1.98936
H 1.08704 -2.51406 -2.23490
N 0.58193 -1.83423 -1.68083
O -1.52484 2.43402 -1.46498
C -0.44182 0.31583 -1.29602
H 0.30258 -2.09765 -0.74472
H -1.39110 -0.33423 -1.00046

42
TS10, charge 0, mult 1
S 4.42162 -3.53733 -2.08285
S -5.29572 -0.81262 -1.51425
Cl 1.75472 5.14762 2.84996
N 1.17901 0.22423 -1.97936
N -1.45687 -2.71478 0.99072
O 1.63646 -2.58786 1.84215
O -1.10752 1.65414 -0.93944
C 0.23731 -0.36501 0.80571
C 2.24936 2.83653 1.49093
C 1.89666 1.57626 1.00823
C 1.32333 3.55149 2.23419
C 0.63499 1.04026 1.25225
C 0.06220 3.03485 2.51444
C -0.26862 1.78034 2.02146
C -1.13949 -0.46263 0.15979
C -1.71695 0.54810 -0.62131
C -1.91479 -1.63037 0.33191
N -2.99581 0.39579 -1.10908
N -3.17733 -1.76208 -0.16758
C -3.64521 -0.73897 -0.84822
N 2.65004 -1.52965 -1.94550
C 3.17519 -2.54395 -1.27993
C 1.70387 -0.80359 -1.29253
N 2.89232 -2.94346 -0.03892
C 1.30514 -1.11672 0.03043
C 1.95979 -2.21137 0.58343
H 4.41970 -2.84724 -3.23654
H -5.55011 -2.05373 -1.06451
H 1.53775 0.41341 -2.90205
H 0.50112 0.86475 -1.57711
H -0.56759 -2.73187 1.46438
H -2.09467 -3.47735 1.15573
H -2.78245 2.50057 -3.20630
H -1.91742 2.29900 -1.71336
H 0.14062 -0.89600 1.76112
H 3.23337 3.24707 1.28908
```

H 2.62968 1.01406 0.43739
H -0.64760 3.60108 3.10878
H -1.25397 1.37191 2.23434
O -2.91354 2.54289 -2.24727
H 2.15206 -3.38063 2.06251
H -3.25065 1.50285 -1.86285

42
TS11, charge 0, mult 1
S 4.59153 -3.11977 -2.27272
S -5.19679 -0.33764 -1.58374
Cl 1.97731 5.55493 2.69005
N 1.42724 0.70861 -2.11513
N -1.34209 -2.22882 0.91296
O 1.74906 -2.22713 1.62491
O -0.90583 2.04447 -1.19620
C 0.41807 0.05873 0.62770
C 2.47343 3.21818 1.37533
C 2.10972 1.96383 0.88573
C 1.53233 3.96541 2.06609
C 0.82273 1.46435 1.07001
C 0.24491 3.48645 2.28654
C -0.09636 2.23701 1.78728
C -0.96472 -0.02646 -0.00650
C -1.49058 1.00644 -0.82132
C -1.76642 -1.15591 0.21603
N -2.81917 0.82287 -1.24753
N -3.04822 -1.26635 -0.25965
C -3.55929 -0.27462 -0.96990
N 2.85810 -1.08062 -2.11112
C 3.34926 -2.12402 -1.46504
C 1.91221 -0.35457 -1.45637
N 3.03228 -2.55476 -0.24306
C 1.48213 -0.69727 -0.14967
C 2.10300 -1.82045 0.38260
H 4.62747 -2.39606 -3.40505
H -5.38420 -1.82974 -0.92598
H 1.76976 0.88859 -3.04585
H 0.69794 1.30887 -1.72992
H -0.41703 -2.29111 1.30849
H -1.98020 -2.98886 1.08629
H -5.04711 -3.58939 -0.88939
H -4.15676 -2.49193 -0.11808
H 0.32663 -0.46793 1.58582
H 3.47742 3.59934 1.21939
H 2.85411 1.37613 0.35680
H -0.47769 4.07758 2.83981
H -1.10181 1.85788 1.95494
O -5.11363 -2.83976 -0.27493
H 2.24519 -3.03587 1.83124
H -3.21391 1.55938 -1.82089

EXCPLICIT SOLVATION INTERMEDIATES

88
I15_20-H2O, charge 0, mult 1
S -3.37593 1.81619 -2.96852
N -2.14529 -0.13673 1.42538
O 1.04758 2.52451 -0.93611
N -2.60157 0.92985 -0.57177
C -2.29500 1.64240 -1.68501
C -1.70938 0.66250 0.44394
N -1.05655 2.18604 -1.69584
C -0.41436 1.18148 0.37990
C -0.07076 1.99043 -0.72437
H -3.13687 -0.31224 1.55319
H -1.56235 -0.18535 2.25233
H -0.79671 2.74076 -2.50372
H -3.52086 0.46488 -0.56396
C 2.22964 -0.56663 -0.15057
C 2.71551 -1.75656 -0.68312
C 2.24127 -2.97979 -0.20964
C 1.28975 -3.00273 0.80687
C 0.79723 -1.80995 1.33609
C 1.25666 -0.58156 0.85542
C 0.68443 0.74867 1.33098
O 0.16371 0.69752 2.66183
H 1.48715 1.49431 1.27565
H 2.59823 0.38594 -0.52270
H 3.46766 -1.72516 -1.46577
H 2.61129 -3.90946 -0.63339
H 0.91993 -3.95028 1.18873
H 0.05414 -1.84552 2.12459
H 0.78075 0.22200 3.26106
O -4.99401 -0.67512 -0.36488
H -5.33609 -0.40064 0.51091
H -5.71583 -0.55791 -0.99432
O 2.11965 4.10669 1.00587
H 2.50780 4.88888 0.59198
H 1.78499 3.56373 0.25434
O 1.38310 -0.96296 4.52431
H 0.53132 -1.45501 4.53155
H 1.43792 -0.55304 5.39687
O 4.17739 2.28680 1.71532
H 4.87772 2.77468 2.16713
H 3.50934 2.96773 1.48835
O -1.50483 2.80520 3.62307
H -1.11034 3.55671 3.12484
H -0.94448 2.05182 3.35985
O 5.57286 0.74724 -0.33158
H 5.09211 0.61105 -1.17342
H 5.00671 1.33035 0.20518
O -1.18034 -2.11314 4.48132
H -1.77840 -1.37826 4.66523
H -1.54921 -2.53257 3.67537
O -3.95607 2.68554 2.43545
H -4.51050 3.31132 2.91949
H -3.09399 2.67604 2.92979
O -2.16317 -3.50240 2.24143
H -2.46646 -3.15046 1.38197
H -2.87415 -4.09055 2.52315
O -5.07120 0.13835 2.23504
H -4.77156 1.05483 2.42163
H -5.49840 -0.17665 3.03942
O -3.04006 -2.73812 -0.40271
H -3.79262 -2.11275 -0.41704
H -3.37531 -3.54036 -0.82337
O 5.76364 -1.33815 1.57782
H 5.70009 -0.71104 0.82795
H 5.14306 -0.96613 2.23659
O -0.53597 4.86538 2.00638
H 0.33663 4.62440 1.64564
H -1.17713 4.68347 1.28983
O 4.43872 0.26646 -2.88764
H 3.55078 0.63891 -3.09067
H 5.02840 0.69409 -3.52003
O 3.96183 -0.06759 3.35948
H 3.09599 -0.46175 3.54489
H 3.78278 0.73596 2.83759
O 5.16773 -4.05529 1.31772
H 5.33191 -3.08894 1.35213
H 4.20668 -4.12493 1.32677
O 1.97432 1.42271 -3.42763
H 1.18104 0.88609 -3.63796
H 1.73201 1.88926 -2.60755
O -2.70041 4.16447 0.29368
H -3.23524 3.67391 0.94827
H -3.24869 4.92143 0.05418
O -0.75015 -1.75972 -1.81043
H -1.57164 -2.04636 -1.36426
H -0.11940 -1.61749 -1.09249
O -0.36236 -0.08445 -4.01935
H -0.57729 -0.62359 -3.22960
H -1.12817 0.49687 -4.12695

88
I16_20-H2O, charge 0, mult 1
S -3.87980 2.30225 -2.82096
N -1.59477 0.33761 1.15179

O 0.83209 3.12206 -1.71589
N -2.53963 1.08877 -0.87268
C -2.53347 2.00071 -1.87196
C -1.46683 0.84974 -0.01781
N -1.36638 2.70300 -2.04775
C -0.15758 1.29002 -0.52261
C -0.15952 2.44184 -1.43333
H -2.56880 0.14485 1.38643
H -0.12153 1.03642 2.41257
H -1.37299 3.42864 -2.75633
H -3.43509 0.63490 -0.64994
C 2.38293 -0.90665 1.05487
C 2.63568 -2.18949 1.52395
C 1.79760 -3.24258 1.16512
C 0.69071 -3.00395 0.34770
C 0.40492 -1.71676 -0.07719
C 1.24544 -0.64839 0.27816
C 1.02710 0.68604 -0.25402
O 0.48714 1.47471 3.03757
H 1.92434 1.22835 -0.55430
H 3.05601 -0.09116 1.30005
H 3.49994 -2.37004 2.15627
H 2.01130 -4.25027 1.51056
H 0.04803 -3.82533 0.04430
H -0.45154 -1.53685 -0.71848
H 0.85733 0.74415 3.56872
O -4.69347 -0.60562 0.04182
H -4.77032 -0.44876 1.01228
H -5.59132 -0.55872 -0.30959
O 1.88027 4.09941 0.74638
H 2.35498 4.92862 0.59859
H 1.66216 3.78069 -0.15133
O 1.41646 -0.89059 4.45605
H 0.67890 -1.37585 4.02322
H 1.16616 -0.83541 5.38653
O 3.86737 2.41643 1.85829
H 4.51423 3.06115 2.17290
H 3.12604 2.96227 1.52135
O -1.32660 3.31831 4.07524
H -1.07239 4.00987 3.42646
H -0.68538 2.60427 3.86958
O 5.33723 0.95912 -0.16376
H 4.77303 0.46624 -0.79552
H 4.72901 1.50988 0.36273
O -0.91725 -1.73171 3.21931
H -0.95541 -1.10509 2.47574
H -1.25832 -2.56519 2.83329
O -3.71947 2.56738 3.01957
H -4.38740 3.07857 3.49428
H -2.85966 2.78748 3.46907
O -2.15008 -3.95771 1.99076
H -2.50397 -3.58954 1.15656
H -2.93780 -4.17522 2.50429
O -4.54903 -0.08337 2.73088
H -4.22575 0.82436 2.92384
H -3.99840 -0.67121 3.26278
O -3.21567 -2.93116 -0.48002
H -3.76664 -2.13565 -0.30595
H -3.85429 -3.61106 -0.73392
O 5.98004 -0.80481 1.93944
H 5.75993 -0.19994 1.19755
H 5.29855 -0.60054 2.60839
O -0.64930 5.02472 1.91699
H 0.16848 4.67428 1.52059
H -1.37196 4.65853 1.36576
O 3.94418 -0.61632 -2.06086
H 3.23011 -0.15445 -2.55285
H 4.59546 -0.83742 -2.73746
O 4.03280 0.24548 3.81020
H 3.18314 -0.20476 3.95625
H 3.81251 1.01010 3.24887
O 5.88406 -3.15382 0.37057
H 5.84249 -2.39880 0.99283
H 5.15724 -3.72516 0.64184
O 1.97987 0.74913 -3.50060
H 1.06321 0.40108 -3.45029
H 1.91380 1.64905 -3.15390
O -2.86875 3.87067 0.62636
H -3.29122 3.41862 1.38444
H -3.52591 4.50691 0.31999
O -1.61746 -2.68698 -2.83864
H -2.15112 -2.74427 -2.01999
H -0.87663 -3.28601 -2.68312
O -0.68181 -0.11023 -3.41690
H -0.98706 -1.01828 -3.20137
H -1.13953 0.11335 -4.23610

88
TS7_20-H2O, charge 0, mult 1
S -3.97510 2.48020 -2.70501
N -1.76762 0.33894 1.25382
O 0.81462 2.98582 -1.67601
N -2.68529 1.24962 -0.72411
C -2.62773 2.12490 -1.75495
C -1.61095 0.93391 0.10602
N -1.42122 2.71730 -1.96298
C -0.31624 1.36387 -0.34022
C -0.22844 2.38645 -1.31395
H -2.74442 0.15971 1.47213
H -0.30721 1.08642 2.08811
H -1.35719 3.38541 -2.72124
H -3.59058 0.81599 -0.51787
C 2.38528 -0.97017 0.97208
C 2.74001 -2.31101 1.02759
C 1.91604 -3.27143 0.44291
C 0.74409 -2.88122 -0.20347
C 0.37870 -1.54186 -0.24215
C 1.18774 -0.57332 0.36358
C 0.87520 0.86952 0.28018
O 0.64968 1.37644 2.05513
H 1.75650 1.47940 0.08862
H 3.04311 -0.21901 1.40165
H 3.66887 -2.60565 1.50797
H 2.19570 -4.32089 0.47575
H 0.11013 -3.62504 -0.67729
H -0.52670 -1.24582 -0.76095
H 1.09261 0.74637 2.69356
O -4.80562 -0.58747 0.07031
H -4.96266 -0.43415 1.03287
H -5.67844 -0.60266 -0.34179
O 1.94931 4.15346 0.57738
H 2.27001 5.03949 0.36440
H 1.62886 3.78906 -0.27763
O 1.44205 -0.39676 3.95901
H 0.77657 -1.07349 3.68477
H 1.11115 -0.05513 4.80044
O 4.08692 2.57127 1.53155
H 4.81095 3.19080 1.68846
H 3.34391 3.13476 1.22613
O -1.39641 2.88335 4.22315
H -0.90662 3.39298 3.53641
H -0.85974 2.10079 4.39643
O 5.35742 0.61594 -0.22244
H 4.78773 0.16218 -0.87819
H 4.79093 1.27969 0.20977
O -0.74830 -1.77370 3.06908
H -1.01171 -1.12327 2.38880
H -0.97965 -2.63547 2.66588
O -3.83683 2.51975 3.01845
H -4.44577 3.06769 3.53082
H -2.97772 2.57572 3.50613
O -1.77405 -4.06654 1.76705
H -2.27387 -3.63310 1.04725
H -2.45847 -4.44024 2.33563
O -4.91520 -0.05403 2.75280
H -4.51793 0.82813 2.92193
H -4.40303 -0.66828 3.29312
O -3.26557 -2.88561 -0.40186
H -3.81020 -2.08887 -0.21178
H -3.91530 -3.57538 -0.59271

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O 6.03753 -0.78822 2.13504
H 5.81565 -0.40058 1.26229
H 5.39532 -0.36323 2.73886
O -0.43280 4.55487 2.23256
H 0.34778 4.33866 1.69091
H -1.19995 4.43553 1.63512
O 3.92382 -0.80308 -2.20418
H 3.16302 -0.28224 -2.54879
H 4.51405 -0.89358 -2.96183
O 4.17159 0.68266 3.71064
H 3.32341 0.21818 3.79669
H 4.00404 1.37431 3.04242
O 6.00965 -3.58544 2.25603
H 5.98965 -2.60491 2.22938
H 5.54133 -3.80670 3.06850
O 1.85693 0.72376 -3.21018
H 0.95531 0.34495 -3.28529
H 1.72482 1.54886 -2.71468
O -2.82982 4.07264 0.81782
H -3.28567 3.54549 1.50382
H -3.35857 4.87597 0.74034
O -1.88761 -2.62049 -2.88095
H -2.32945 -2.70431 -2.01121
H -1.22093 -3.31805 -2.88340
O -0.80136 -0.12753 -3.48308
H -1.15342 -1.01516 -3.25457
H -1.12299 0.03966 -4.37679

219
enol-3a_60-H2O, charge 0, mult 1
S 3.58484 -4.54015 -2.39114
S -5.49661 -1.93160 -1.88854
Cl 1.22419 4.53765 2.64604
N 0.89700 -0.37982 -2.00547
N -1.78387 -3.44591 1.06531
O 1.29059 -3.26565 1.75820
O -1.58229 0.86608 -0.97604
C -0.14941 -1.05382 0.73150
C 1.79603 2.19343 1.37564
C 1.46572 0.91787 0.91373
C 0.83322 2.92790 2.05036
C 0.20121 0.37685 1.13182
C -0.43953 2.41666 2.27828
C -0.74205 1.14042 1.82525
C -1.52476 -1.23553 0.08845
C -2.17565 -0.29345 -0.71287
C -2.22801 -2.44247 0.25714
N -3.39312 -0.49606 -1.25676
N -3.42295 -2.68484 -0.34344
C -3.93688 -1.69294 -1.06232
N 2.13194 -2.30530 -2.08340
C 2.59619 -3.37998 -1.47063
C 1.29846 -1.49691 -1.37522
N 2.38665 -3.72807 -0.20070
C 0.91866 -1.80777 -0.05050
C 1.55063 -2.92741 0.49002
H 3.60216 -3.83426 -3.53659
H -5.67106 -3.24175 -1.56638
H 1.04185 -0.32617 -3.00304
H 0.15841 0.19703 -1.62506
H -0.81030 -3.49221 1.33769
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