Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Facile Synthesis of New *N*-Sulfonamidyl-4-thiazolidinone Derivatives and Biological Evaluation

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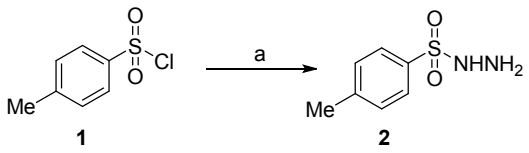
Experimental procedure for 4-methylbenzenesulfonohydrazide:

To the stirred solution of 4-methylbenzene-1-sulfonyl chloride (1 mmol) in THF (20 mL), hydrazine hydrate (1.5 mmol) was added dropwise at 0 °C temperature. The progress of the reaction was monitored by Thin Layer Chromatography using *n*-hexane:ethyl acetate (8:2) solvent system. After completion of reaction, mixture was slowly poured into 100 mL of ice water. A solid was formed thereafter. The precipitate was separated by filtration and washed successively with water and crystallized in ethanol to give desired product.



1 **2**

[a]Reagents and conditions: (a) hydrazine, 0 °C, THF.

Scheme S1: Synthesis of 4-methylbenzenesulfonohydrazide.

Table S1. Optimization of catalyst concentration:

Entries	Mol %	Solvent	Time (hr)	Temp (°C)	Yield[a] (%)
1	5	Solvent free	4	80	68
2	10	Solvent free	2.5	80	79
3	15	Solvent free	1.5	80	83
4	20	Solvent free	1	80	90
5	25	Solvent free	1	80	90

Reaction conditions: **1a** (1 mmol), **2** (1 mmol), **3** (1 mmol) at 80 °C for 1 hr. [a]Isolated yield.

Table S2. Recycling of the dried IL in the synthesis of 4-methyl-*N*-(4-oxo-2-phenylthiazolidin-3-yl)benzenesulfonamide.[a]

Entry	Run	Time (hr)	Yield (%)[b]
1	I	1	90
2	II	1	90
3	III	1	87
4	IV	1	86

[a]**Reaction conditions**: **1a** (1 mmol), **2** (1 mmol), **3** (1 mmol) and 20% [HDBU][HSO_4] at 80 °C. [b]Isolated yield.

Table S3. Recycling of the non-dried IL in the synthesis of 4-methyl-*N*-(4-oxo-2-phenylthiazolidin-3-yl)benzenesulfonamide.[a]

Entry	Run	Time (hr)	Yield (%)[b]
1	I	1	70
2	II	1	64
3	III	1	58
4	IV	1	52

[a]**Reaction conditions**: **1a** (1 mmol), **2** (1 mmol), **3** (1 mmol) and 20% [HDBU][HSO_4] at 80 °C. [b]Isolated yield.

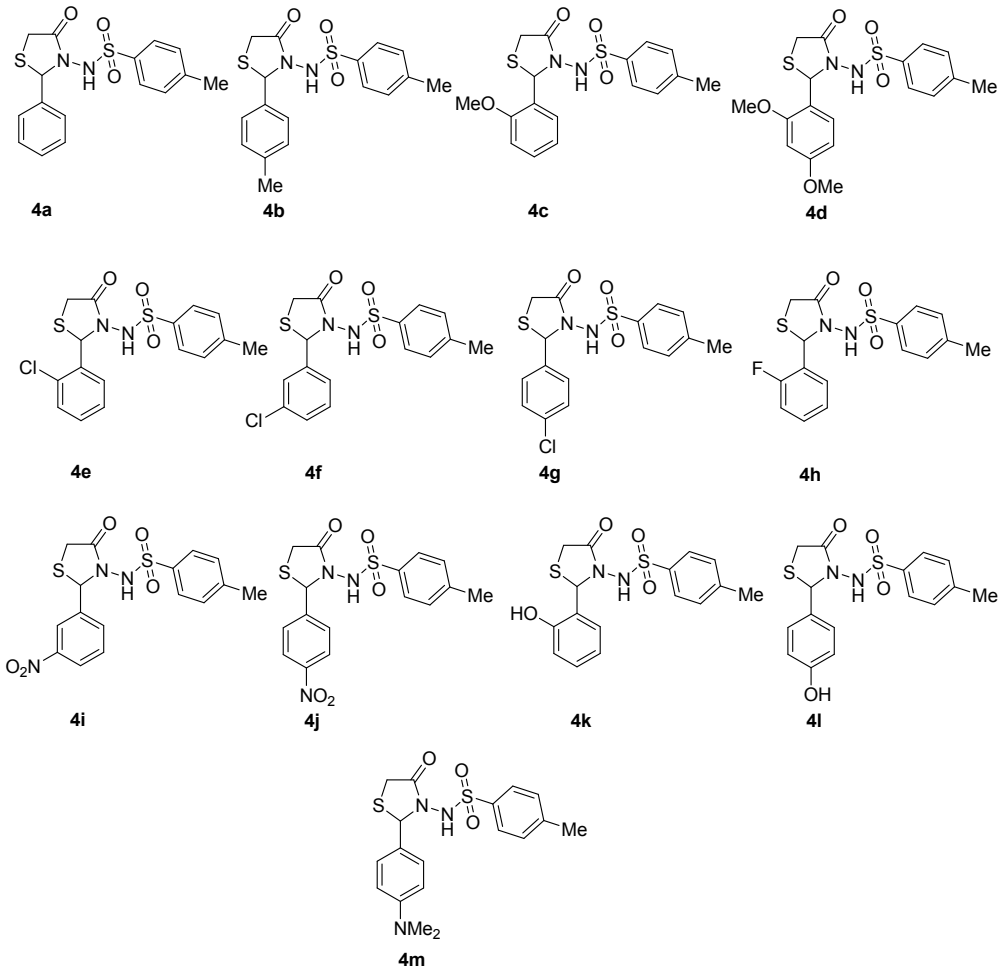


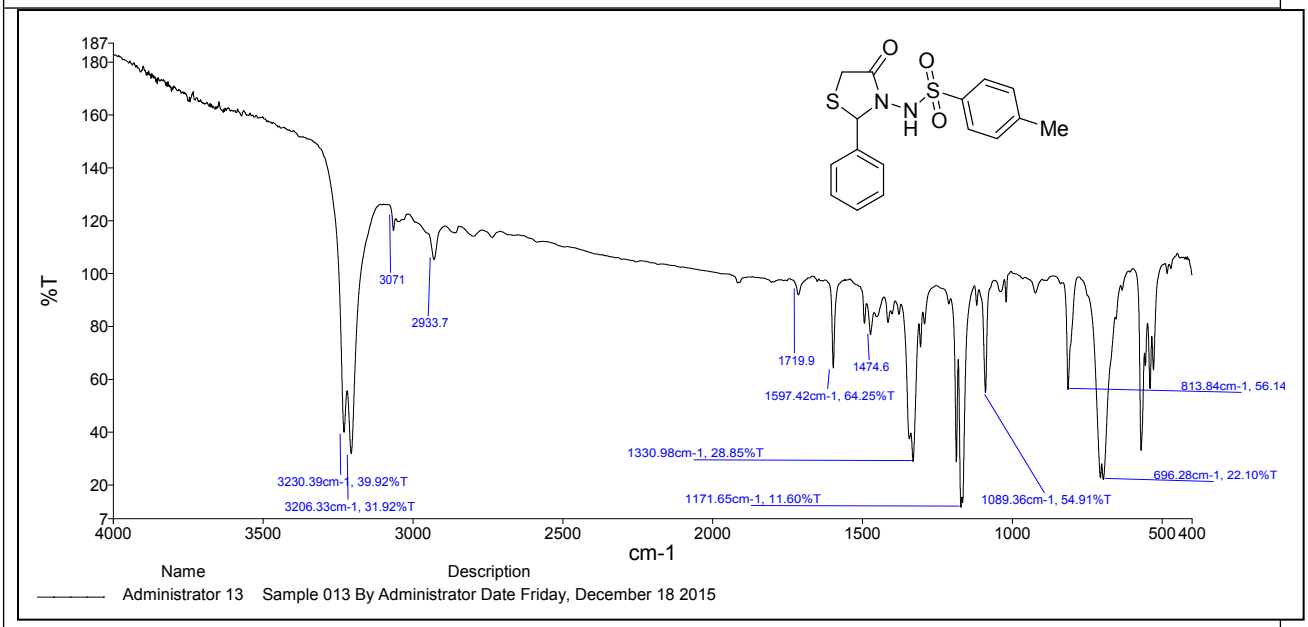
Figure S1. Structure of 4-methyl-*N*-(4-oxo-2-phenylthiazolidin-3-yl)benzenesulfonamide derivatives.

Table S4. Results of the per-residue interaction analysis for the 4-thiazolidinone derivatives.

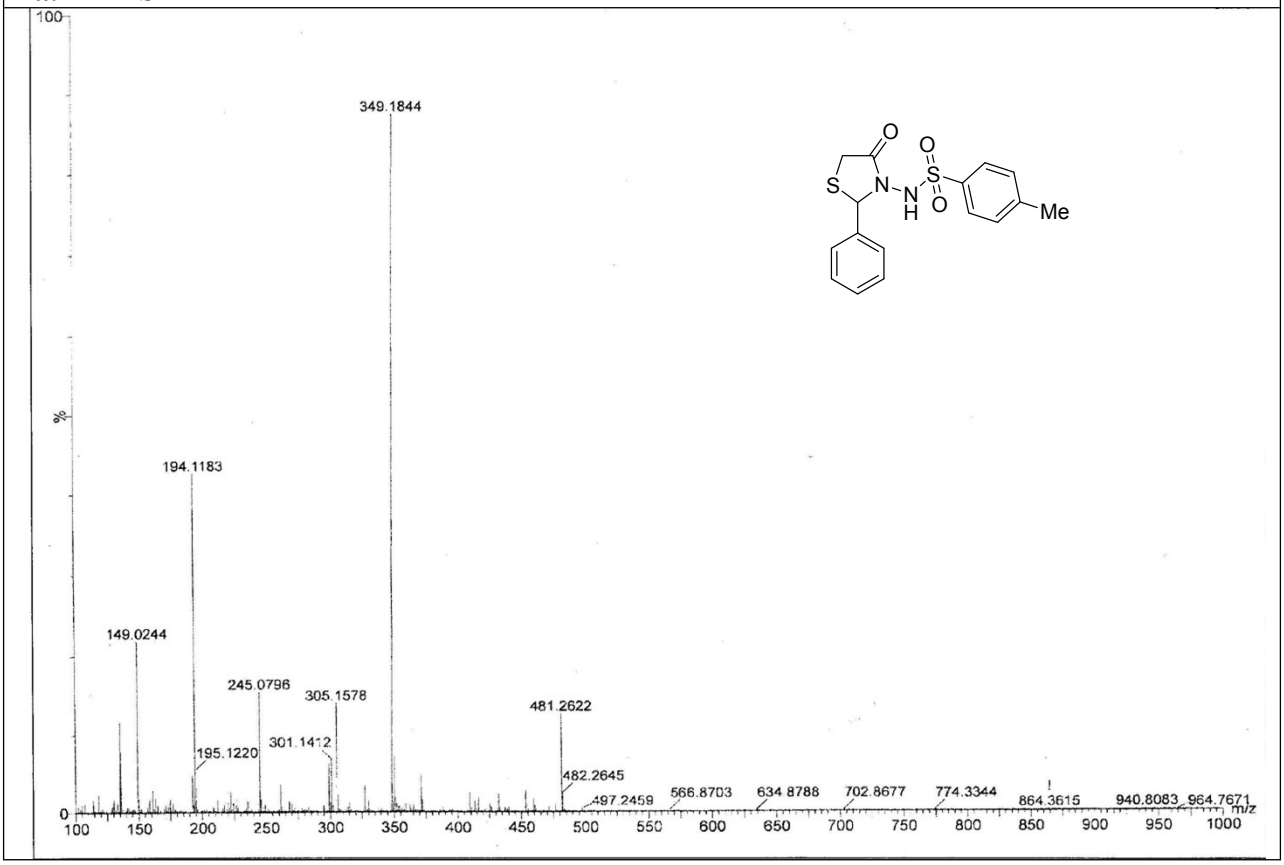
Comp. ID	Docking score	Binding energy	Per-residue interaction energy analysis		
			van der Waals (kcal/mol)	Electrostatic (kcal/mol)	π-π stacking
4d	-6.98	-43.42	Heme(-3.85), Val461(-2.93), Met460(-1.61), Thr459(-1.01), Cys422(-1.06), Val359(-1.35), Me358(-1.55), Leu356(-3.53), Thr295(-1.20), Ala291(-2.35), Phe290(-2.86), Ala288(-1.21), Ala287(-1.15), Met284(-1.13), Leu208(-1.22), Leu127(-1.32), Tyr116(-3.49), Phe110(-2.04), Met106(-2.15) and Tyr103(-4.70)	Heme(-16.96)	Phe110
4e	-7.04	-46.21	Heme(-2.24), Val461(-1.82), Met460(-2.01), Cys422(-1.72), Val359(-1.18), Met358(-1.11), Leu356(-2.23), Thr295(-1.06), Ala291(-2.38), Phe290(-2.37), Ala288(-1.72), Ala287(-1.29), Met284(-1.17), Leu208(-1.32), Leu130(-0.93), Leu127(-1.57), Phe110(-1.51), Met106(-1.55) and Tyr103(-1.94)	Heme(-21.78)	Tyr103
4g	-6.84	-41.49	Heme(-2.81), Val461(-1.30), Met460(-1.613), Cys422(-1.42), Val 359(-2.14), Met358(-1.17), Leu356(-1.07), Thr295(-1.41), Ala291(-2.48), Phe290(-1.18), Ala288(-1.35), Ala287(-1.48), Met284(-1.05), Leu208(-1.67), Leu130(-0.81), Leu127(-1.09), Tyr116(-2.73), Phe110(-	Heme(12.57), Tyr116(-1.19)	Tyr116

			1.55), Met106(-1.40) and Tyr103(-3.61)		
4h	-7.06	-48.81	Heme(-3.46), Val461(-2.12), Met460(-2.02), Cys422(-1.89), Val359(-1.08), Met358(-1.12), Leu356(-1.78), Ala291(-2.01), Phe290(-1.68), Ala288(-1.76), Met284(-1.20), Leu130(-0.95), Leu127(-1.55), Tyr116(-1.68), Phe110(-1.73), Met106(-1.33) and Tyr103(-1.78)	Heme(-23.30)	Tyr103
4k	-7.02	-45.81	Heme(-2.67), Val461(-1.80), Met460(-2.00), Cys422(-1.77), Val359(-1.02), Met358(-1.01), Leu356(-2.79), Thr295(-1.33), Ala291(-2.40), Phe290(-1.46), Ala288(-1.79), Met284(-1.24), Leu208(-1.00), Leu130(-0.89), Leu127(-1.62), Tyr116(-4.63), Phe110(-1.31), Met106(-1.40) and Tyr103(-1.11)	Heme(-18.78)	Tyr103 and Tyr116

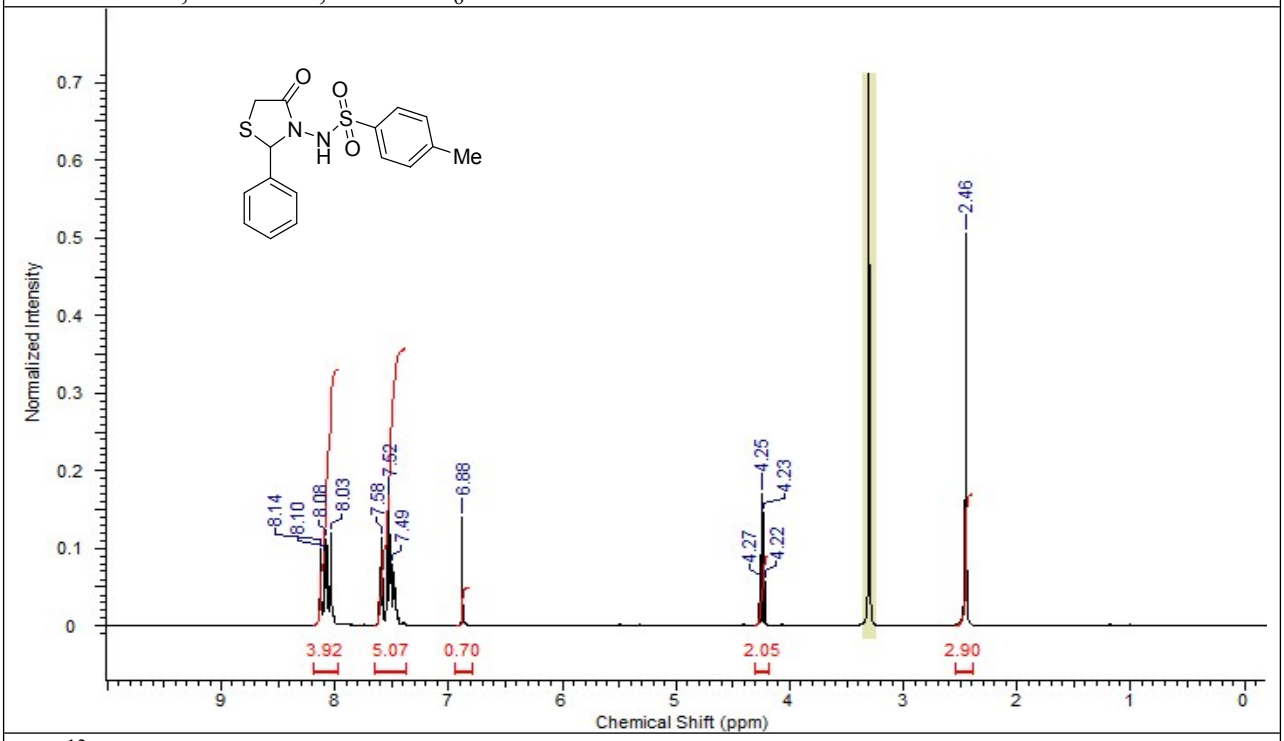
4a. FT-IR



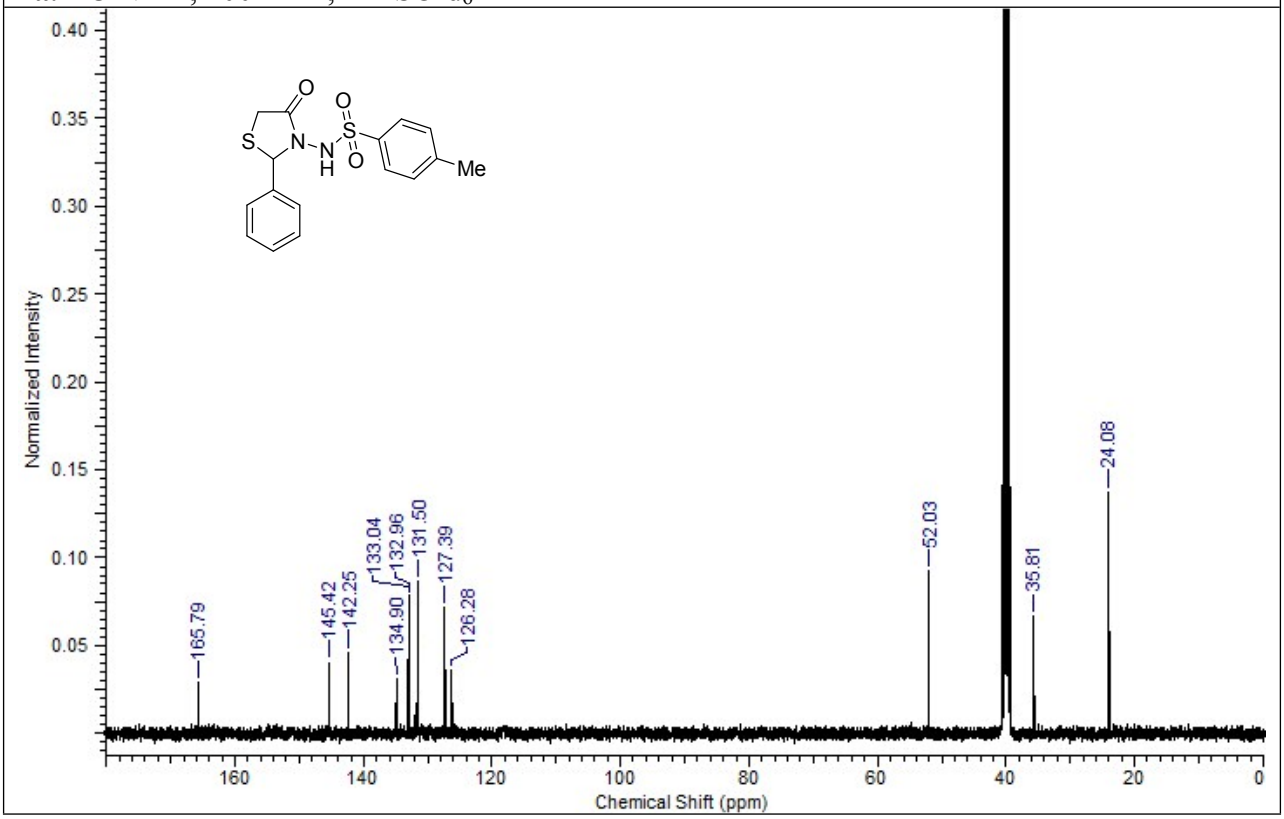
4a. HRMS



4a. ^{1}H NMR, 400 MHz, DMSO-d_6



4a. ^{13}C NMR, 100 MHz, DMSO-d_6



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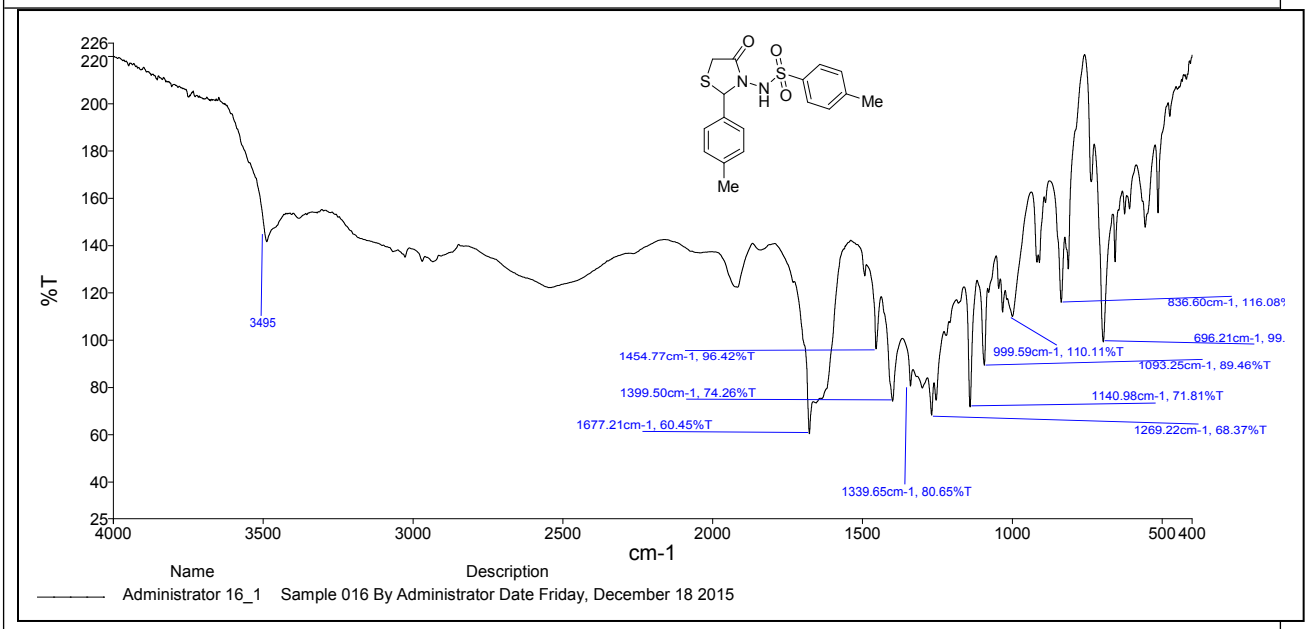

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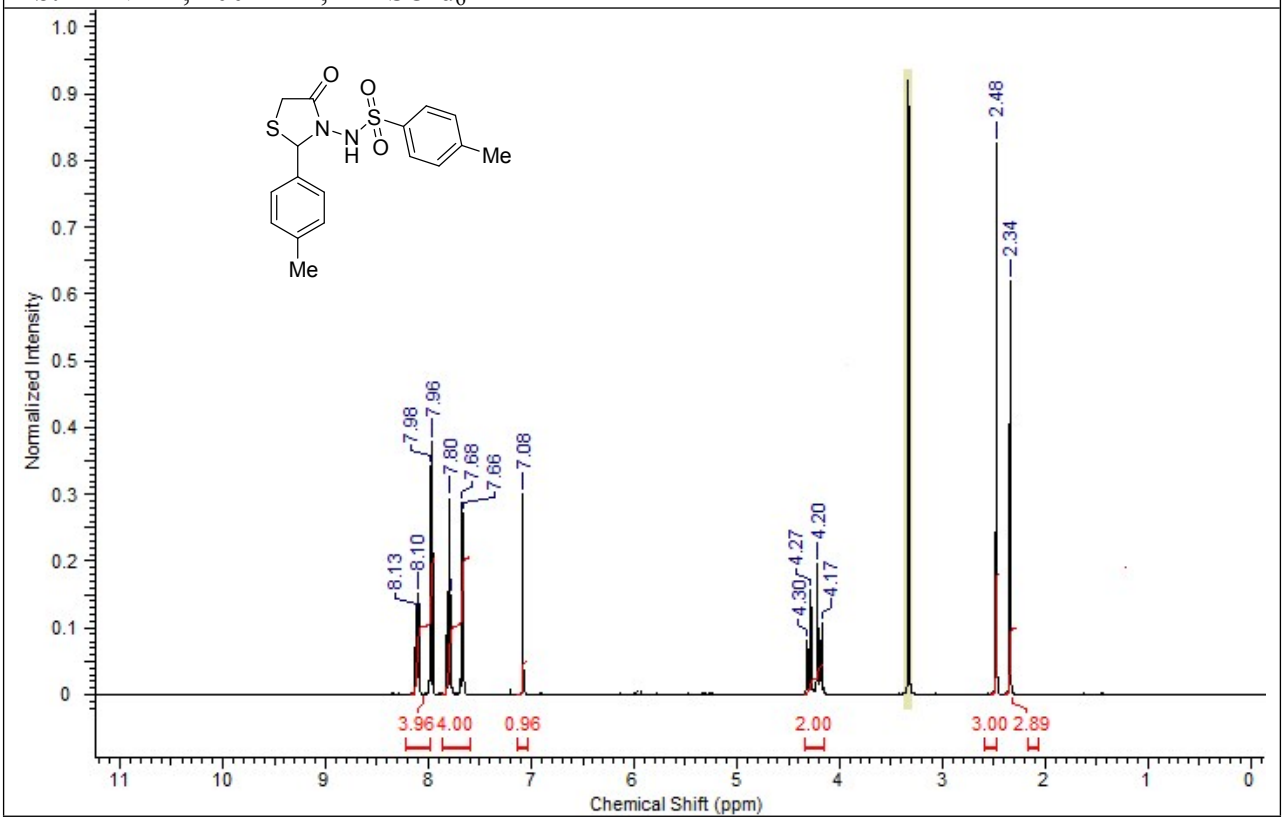

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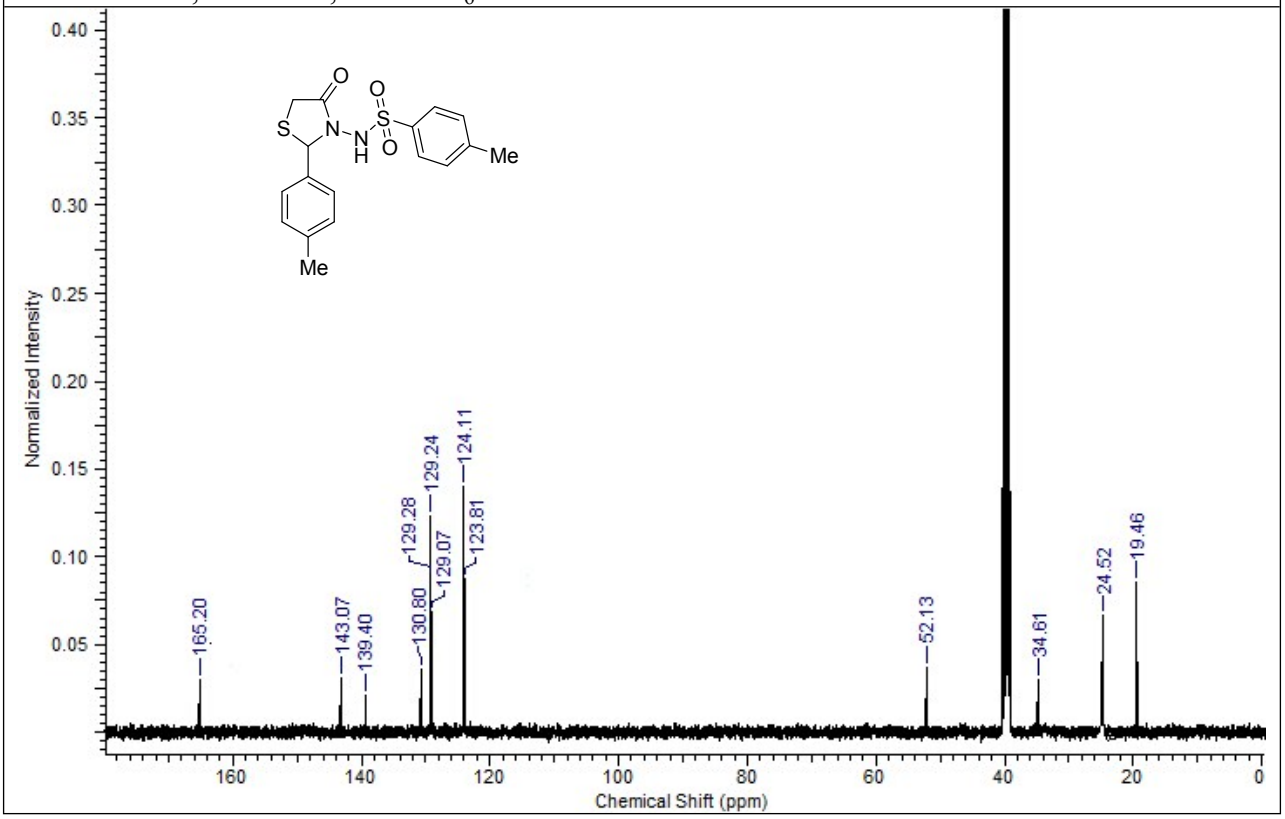

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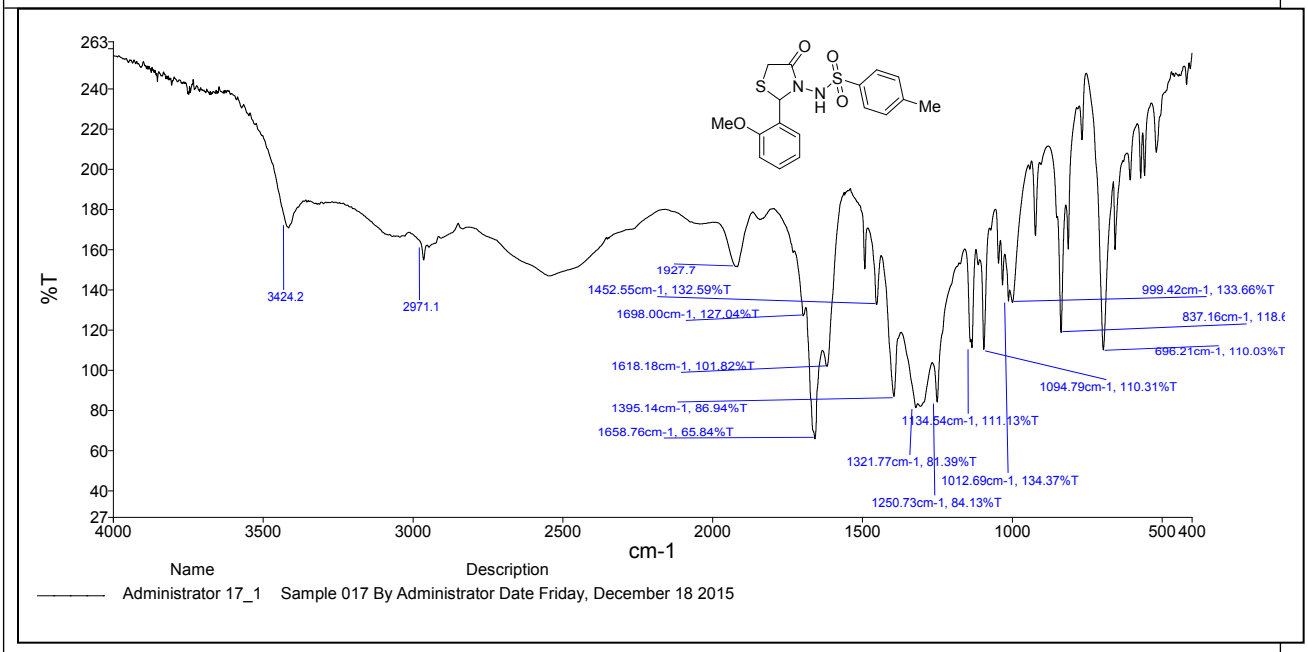

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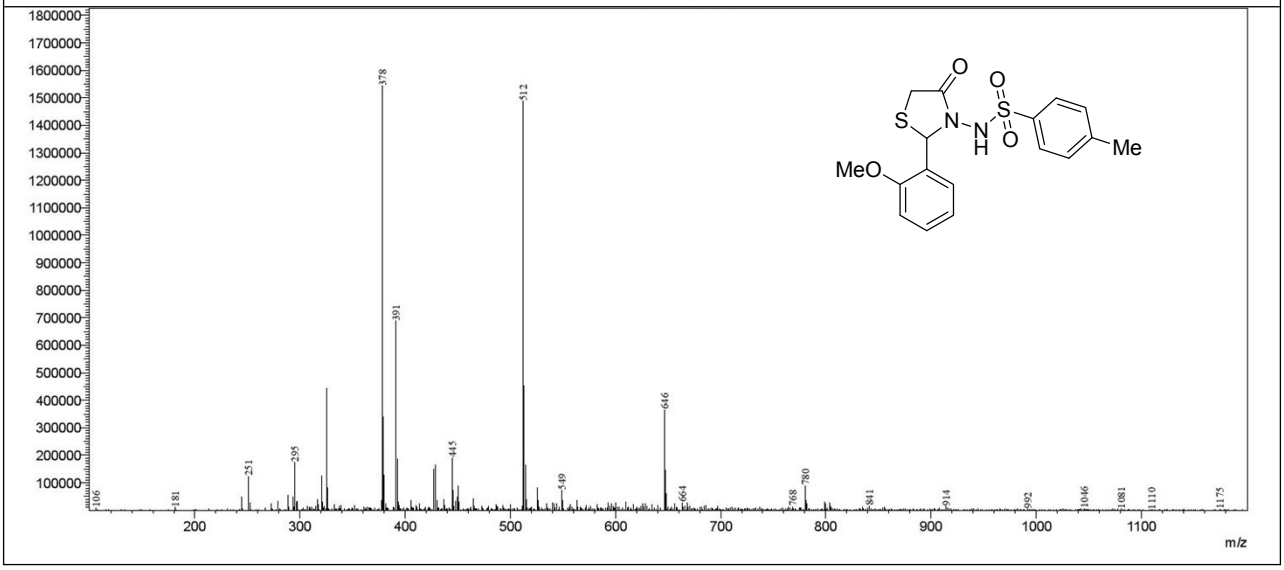
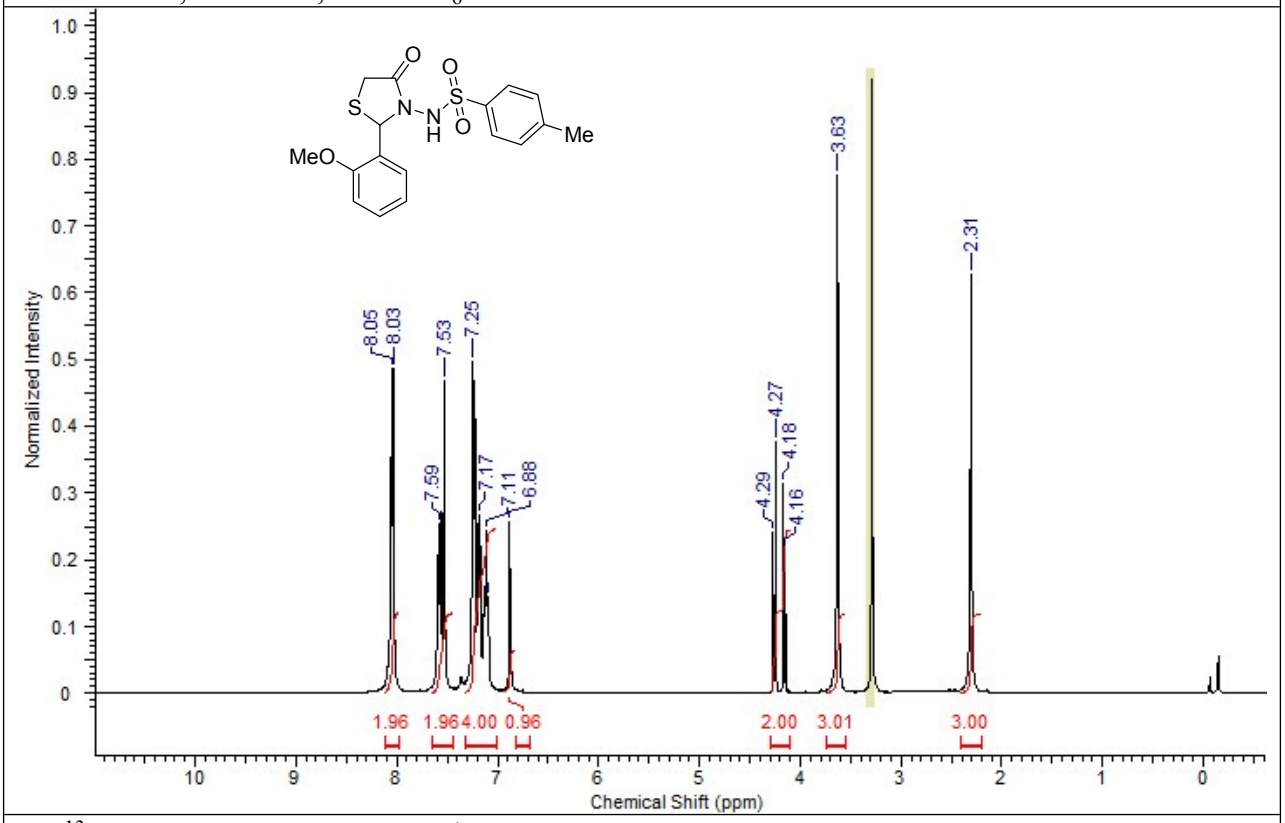


4c. ^{1}H NMR, 400 MHz, DMSO-d_6



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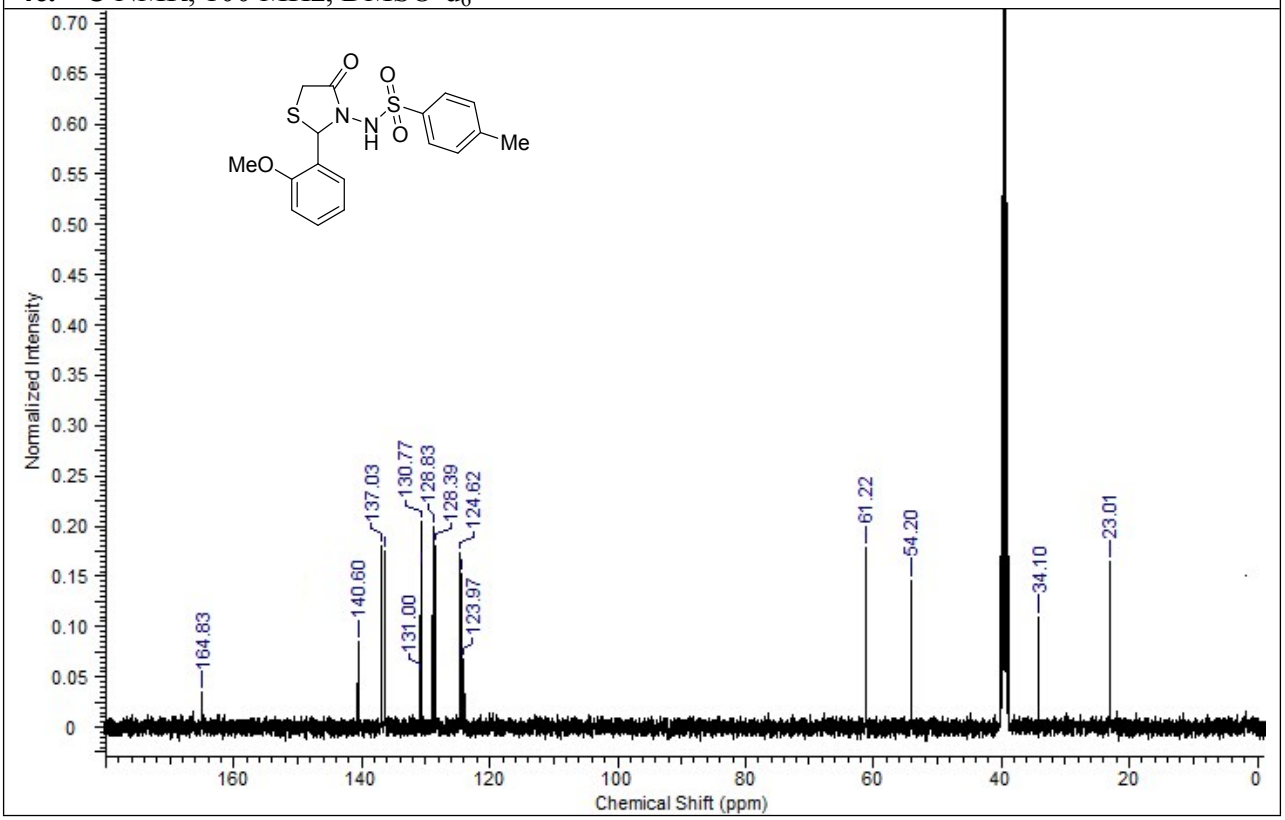

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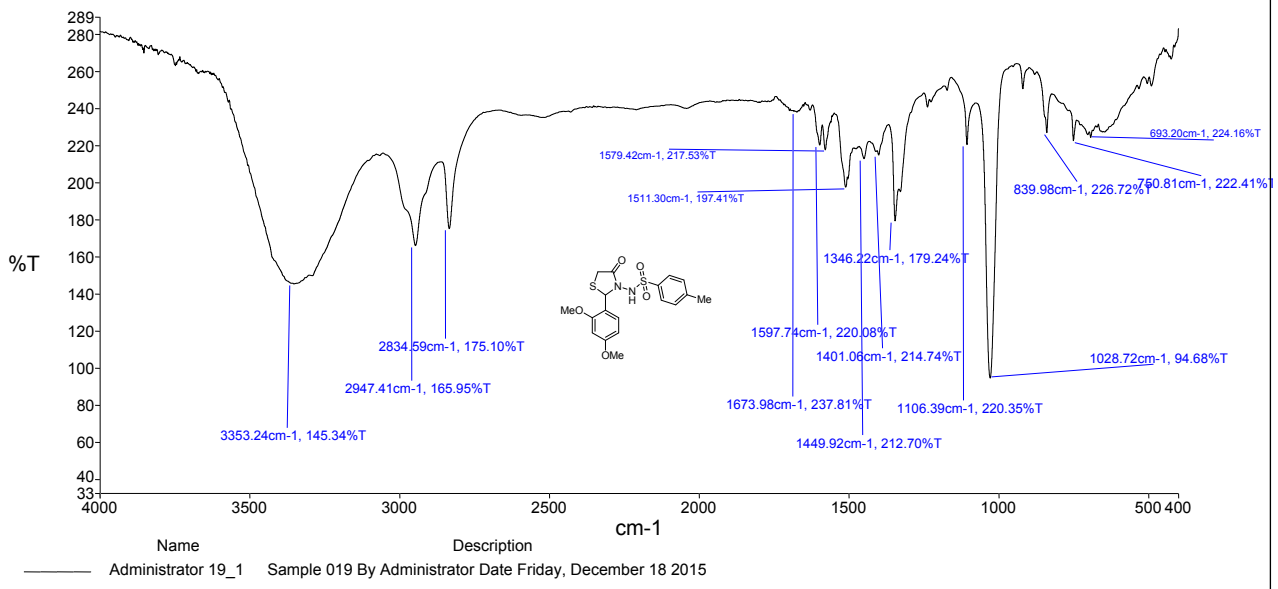

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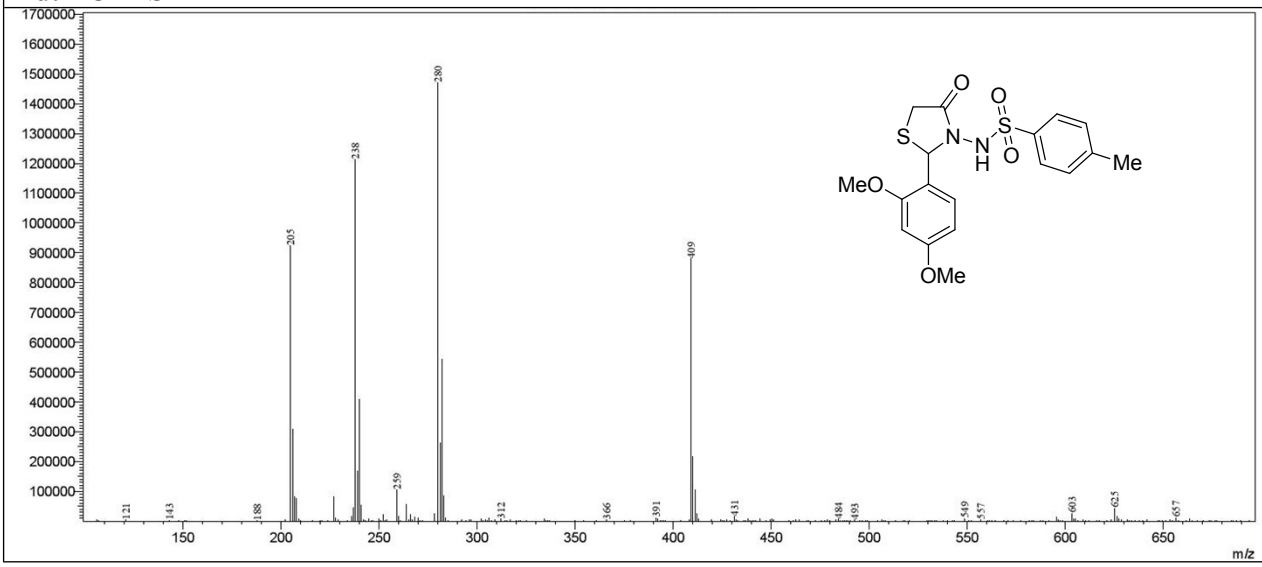
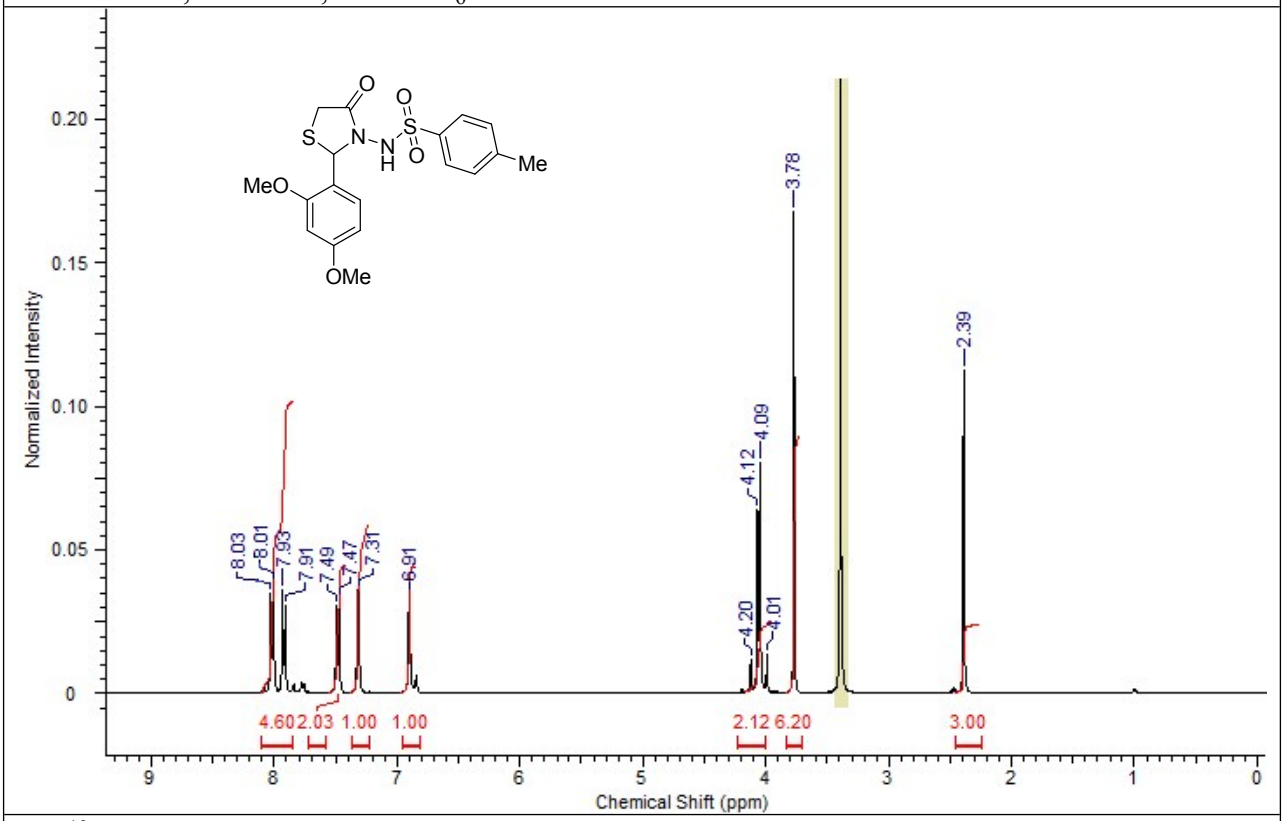
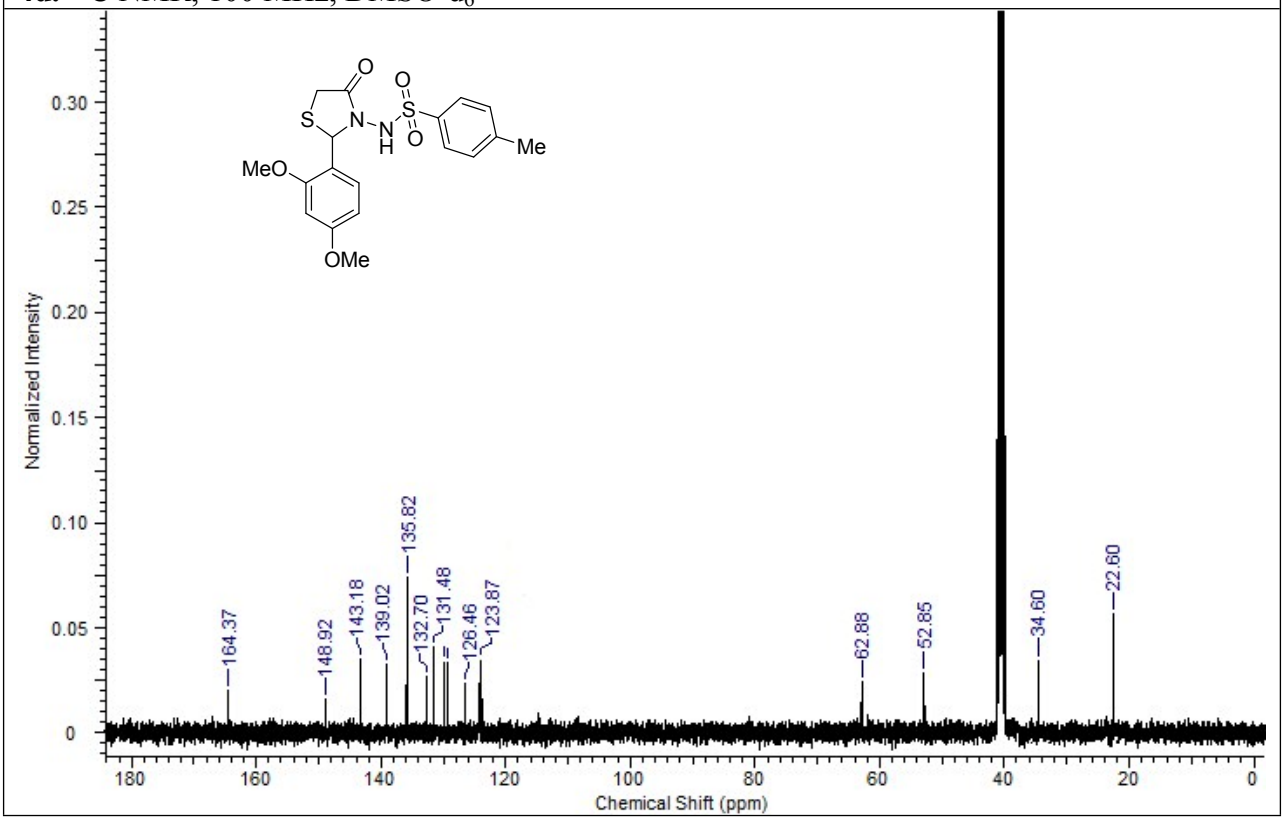


4d. ^{1}H NMR, 400 MHz, DMSO-d_6



4d. ^{13}C NMR, 100 MHz, DMSO-d_6



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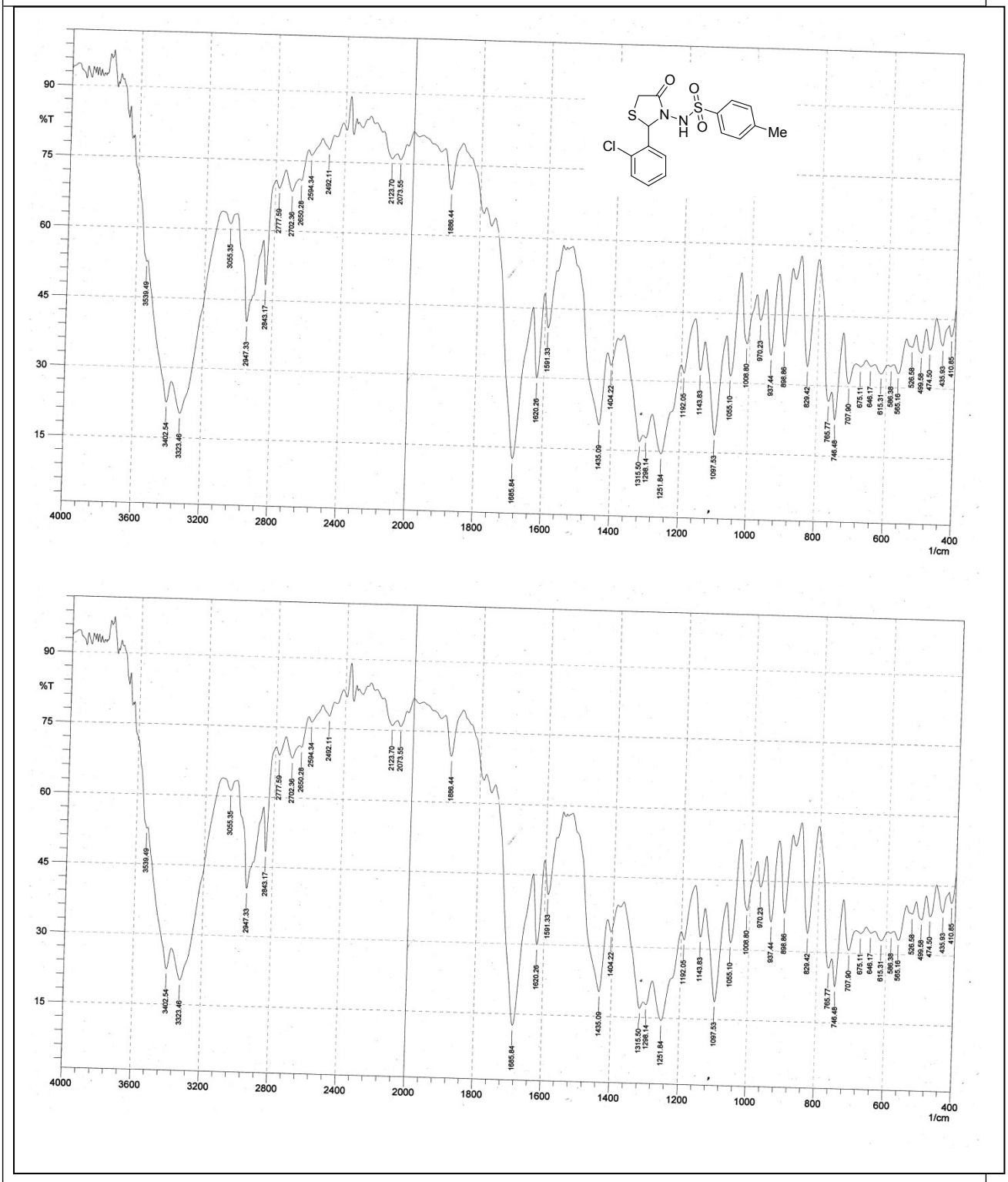
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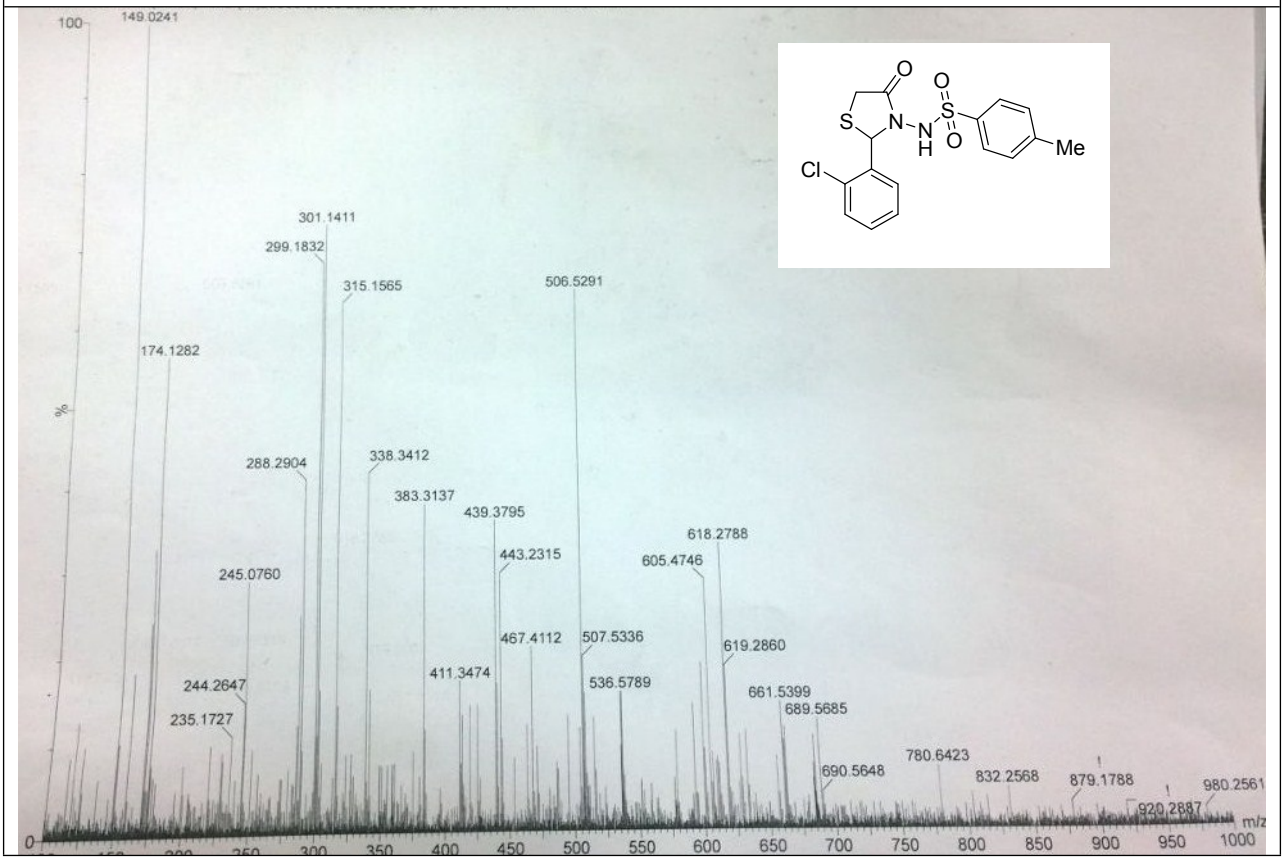
4e. HRMS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690.5648
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980.2561
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m/z
%
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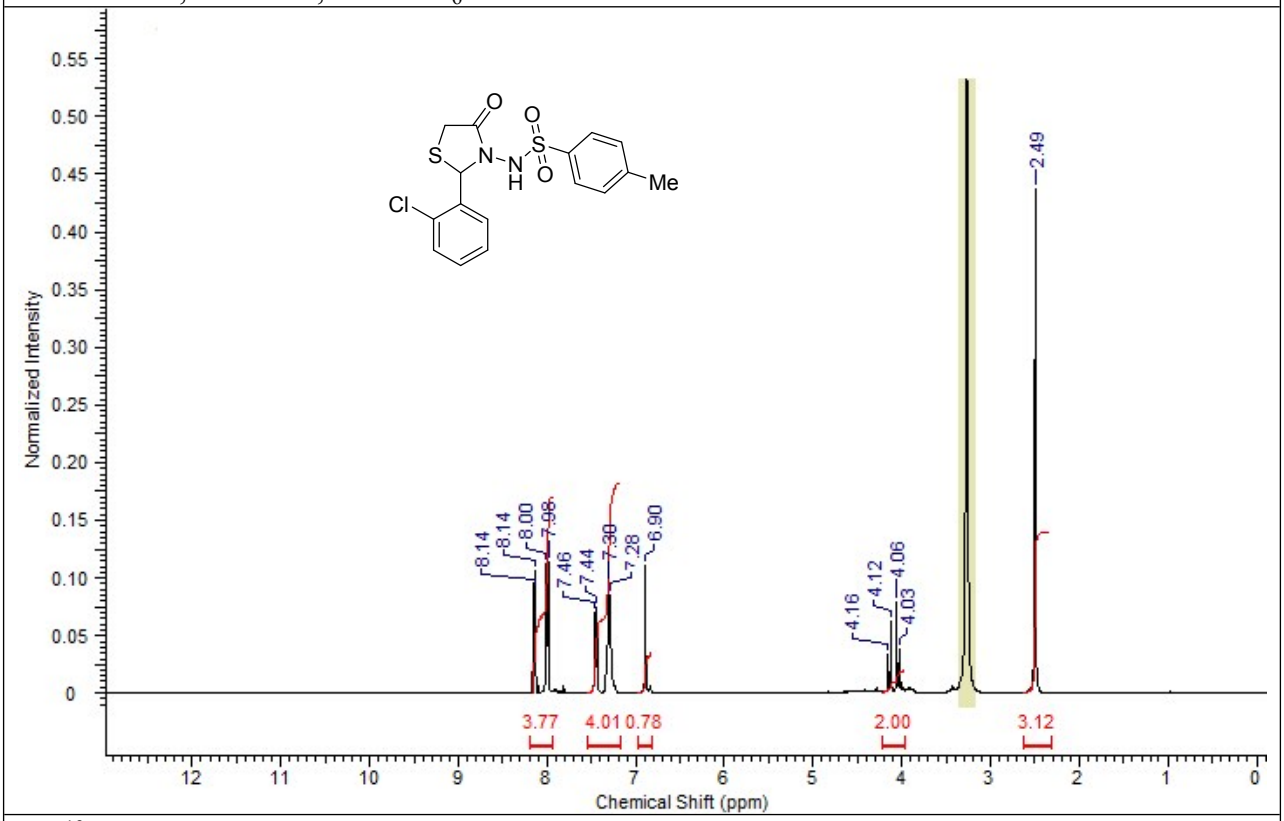
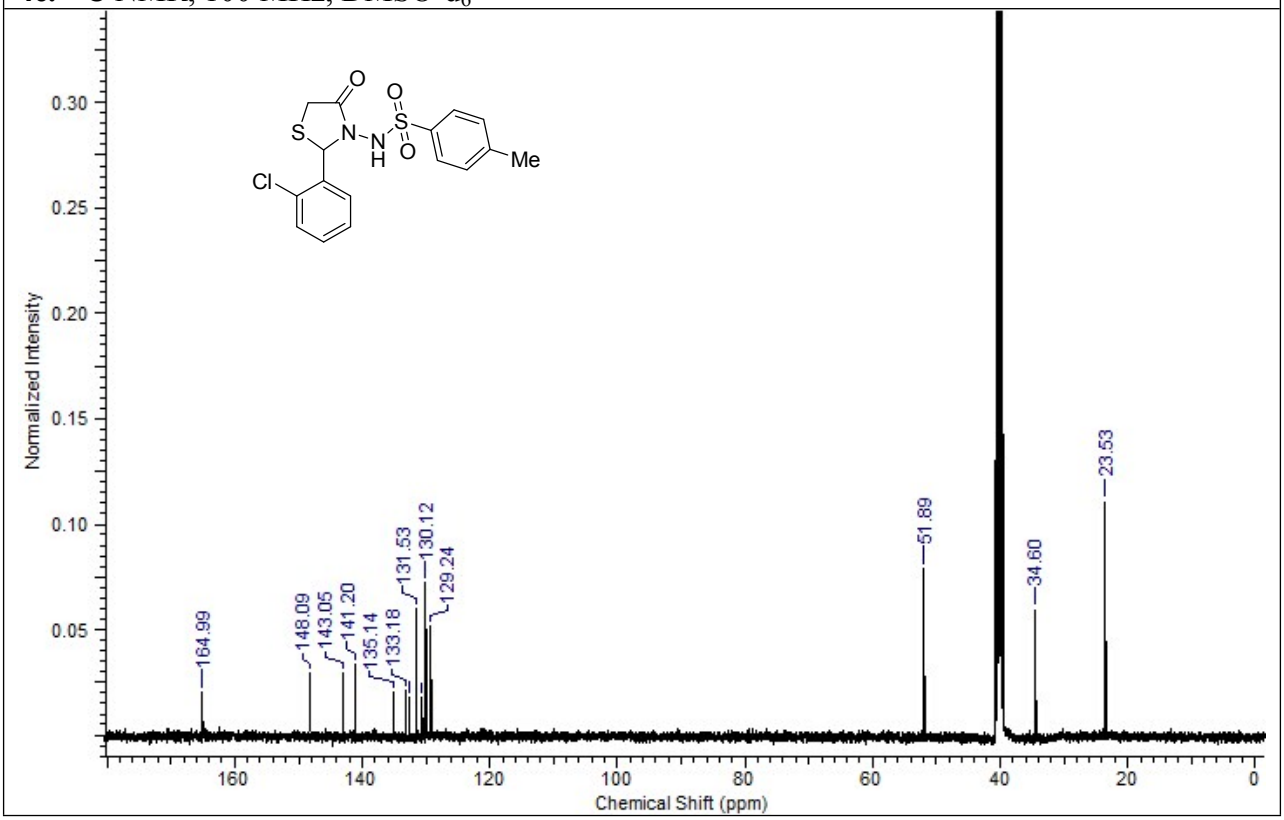
Cl

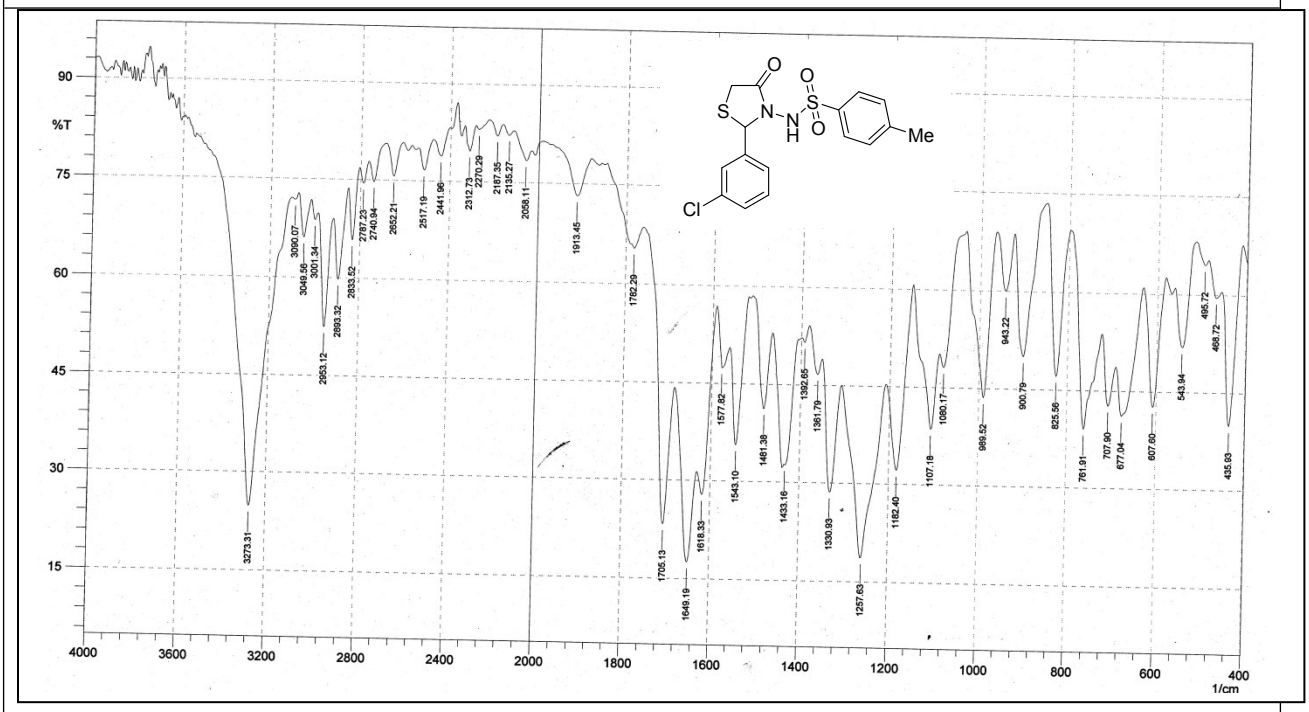
4e. ^{1}H NMR, 400 MHz, DMSO-d_6



4e. ^{13}C NMR, 100 MHz, DMSO-d_6



4f. FT-IR



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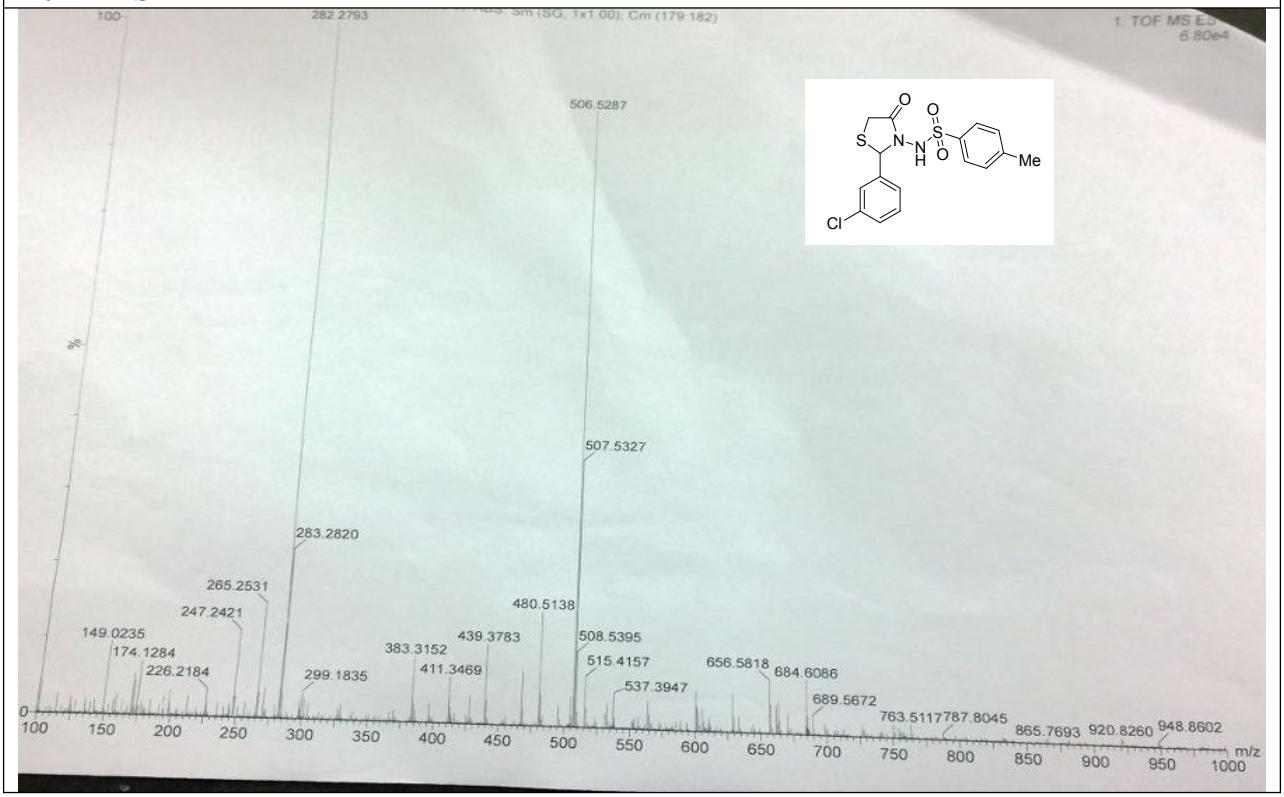

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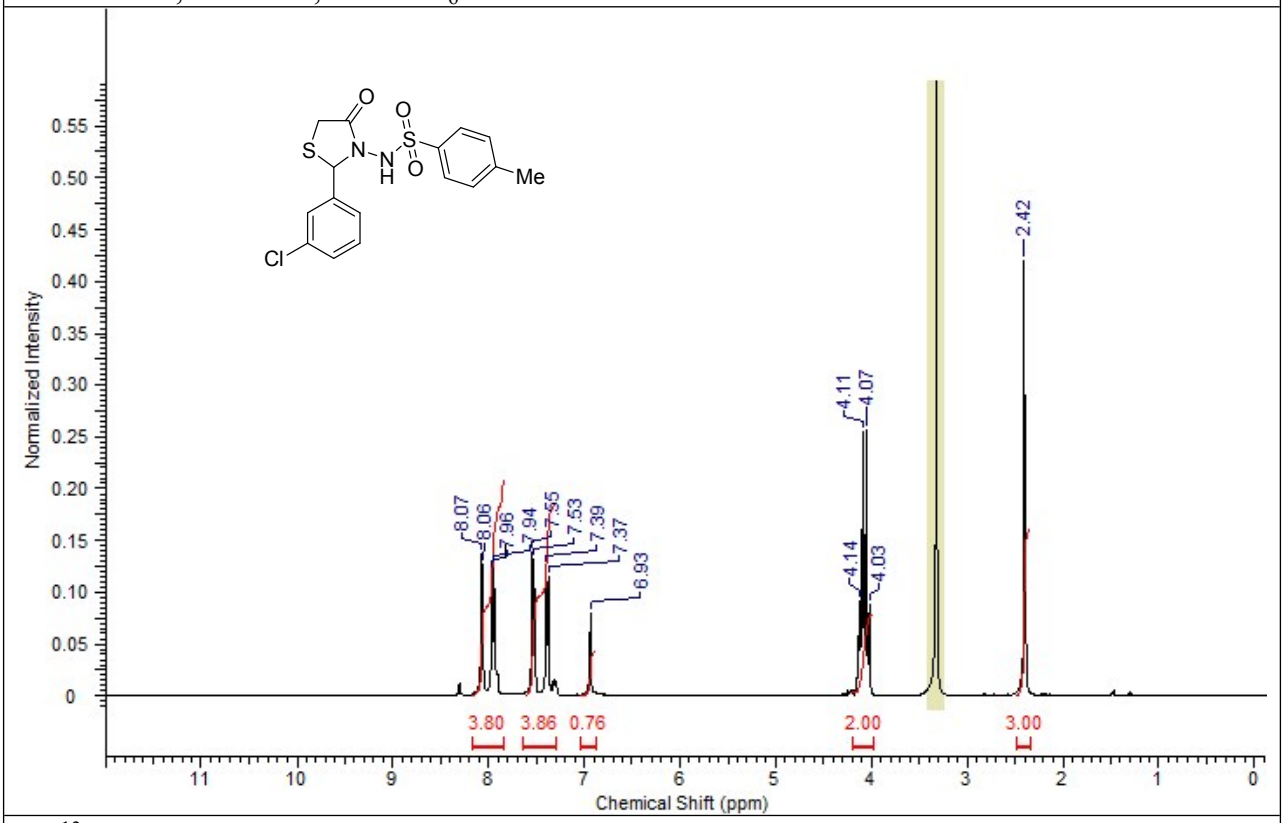

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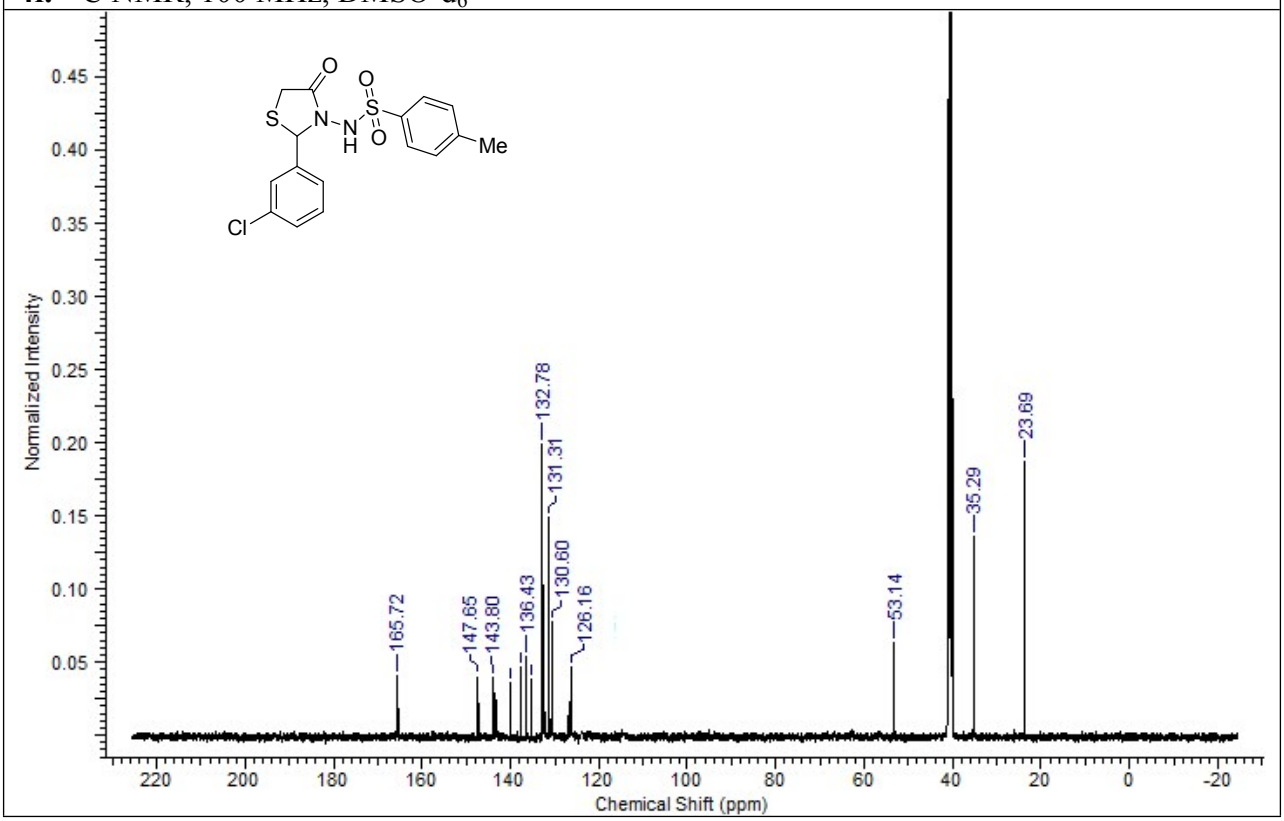

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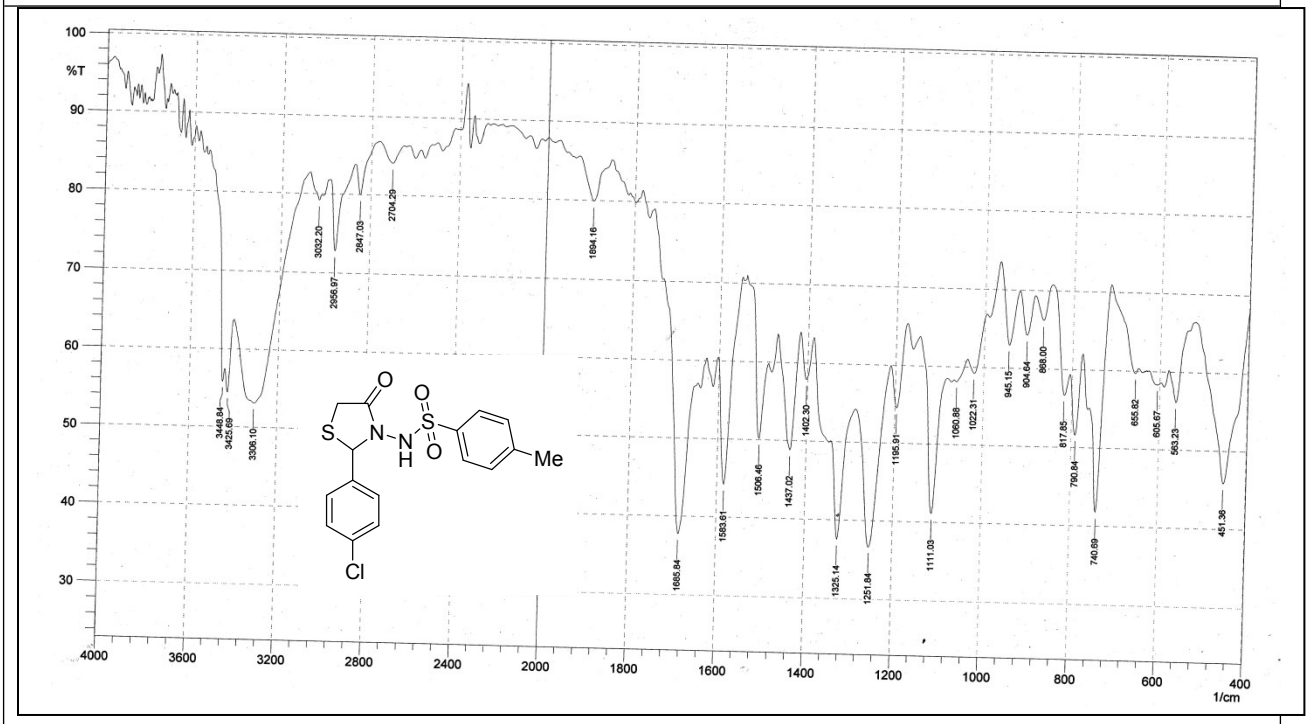

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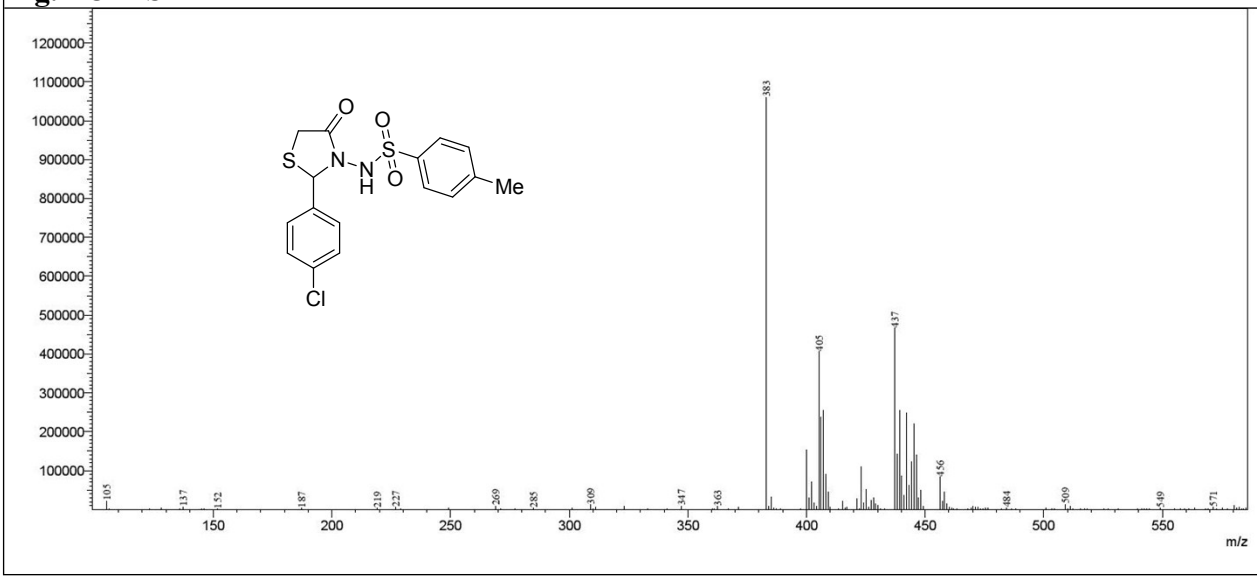
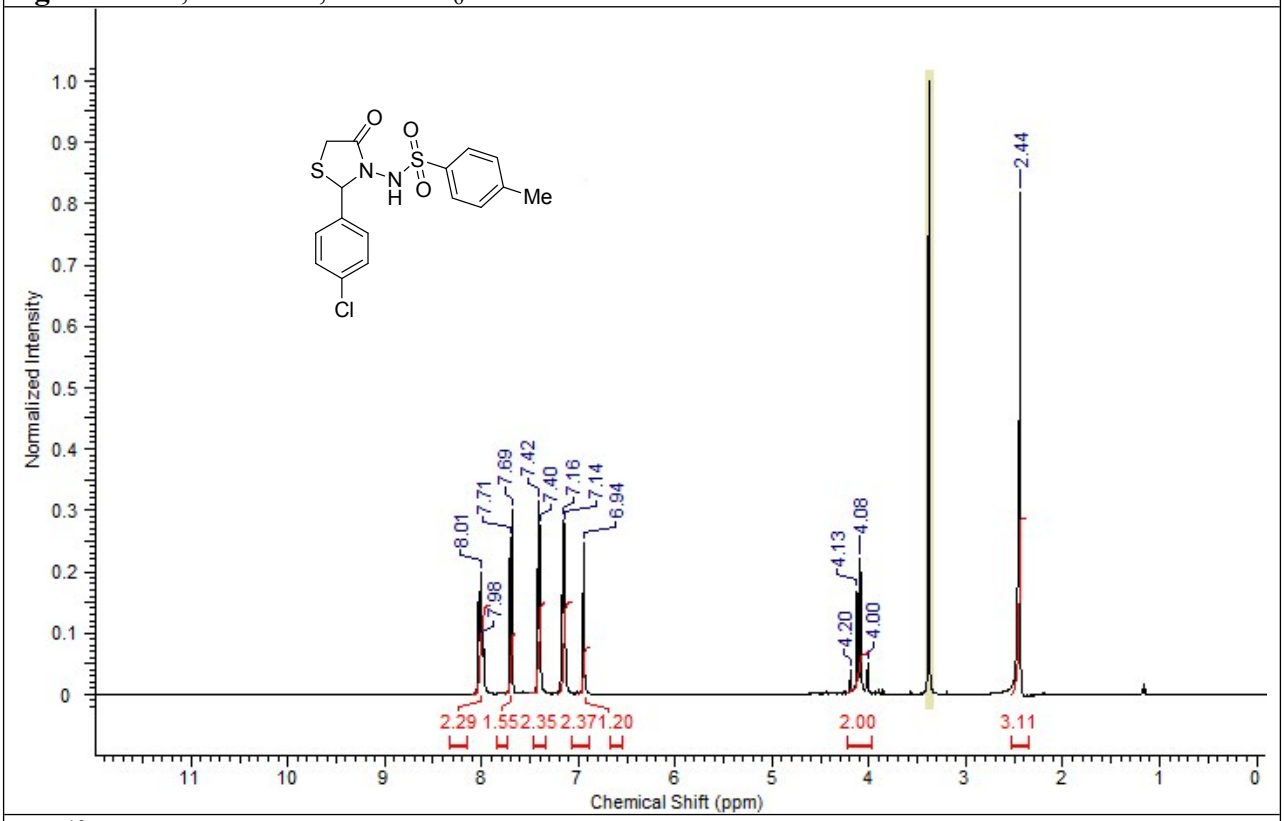


4g. ^{1}H NMR, 400 MHz, DMSO-d_6



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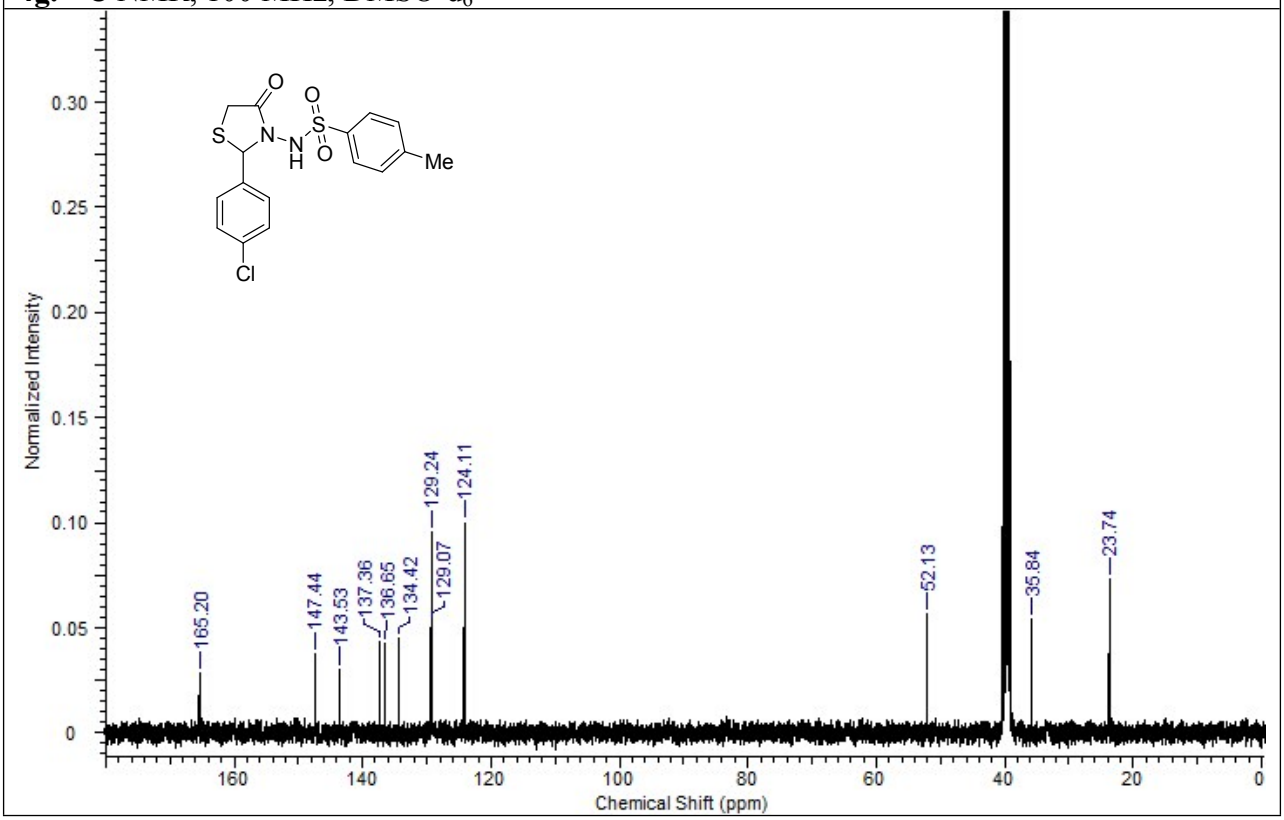

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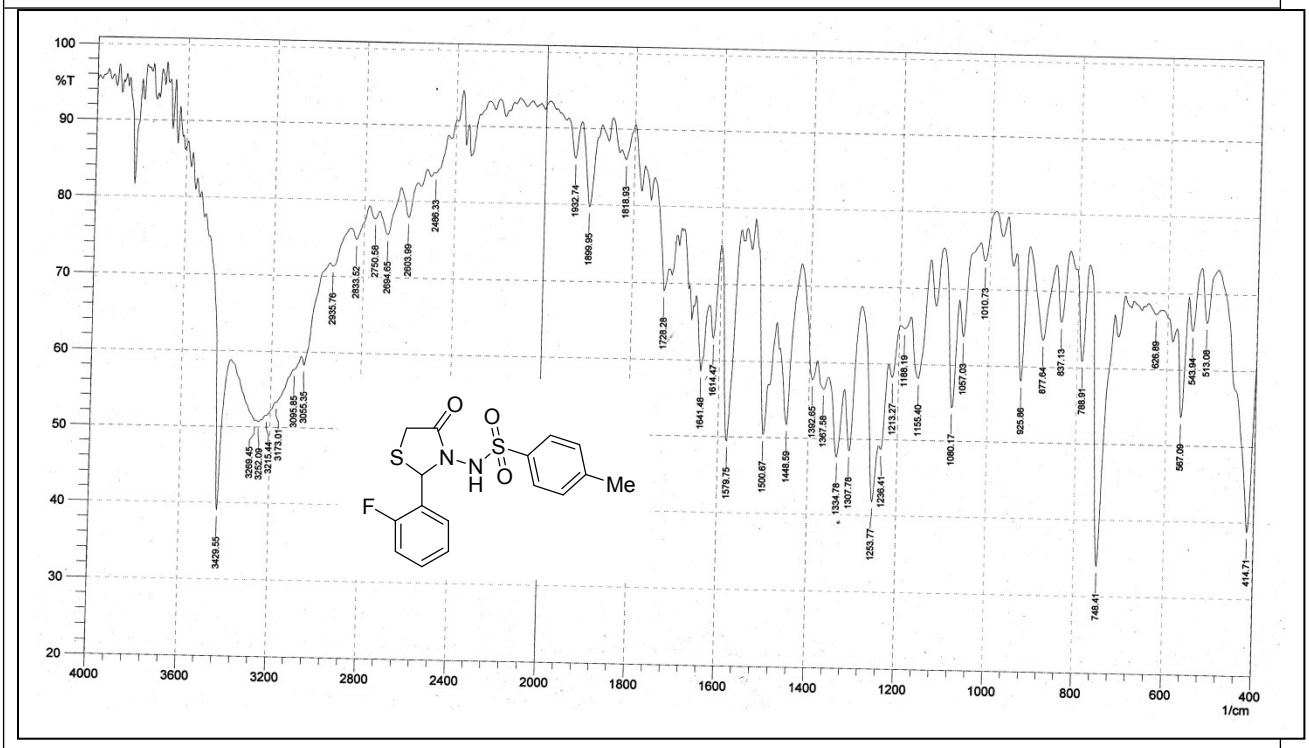

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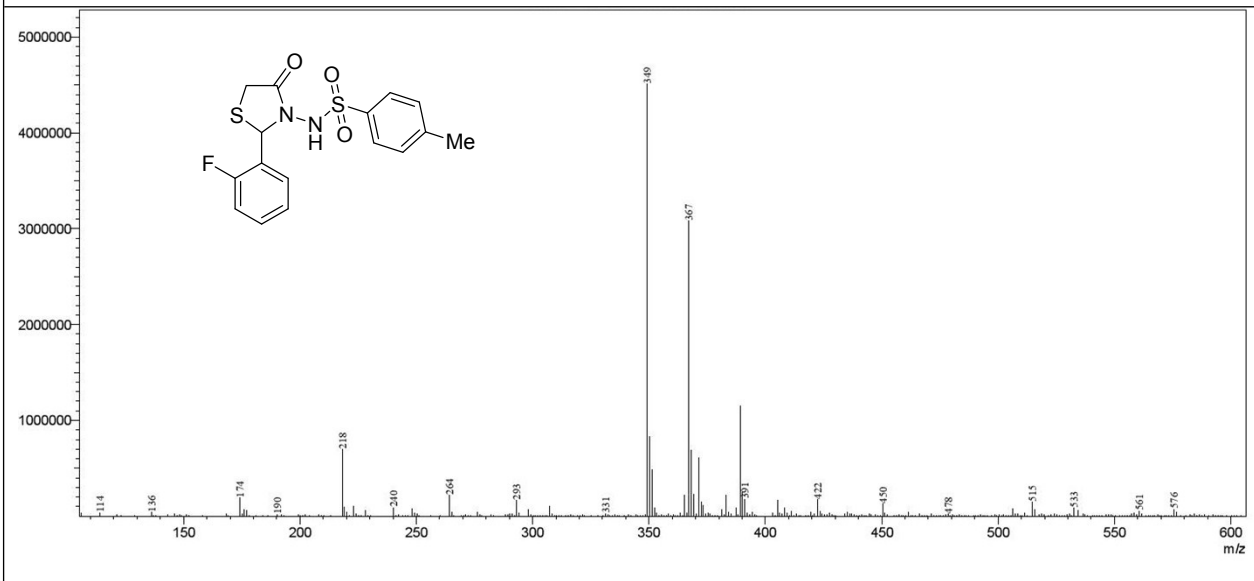
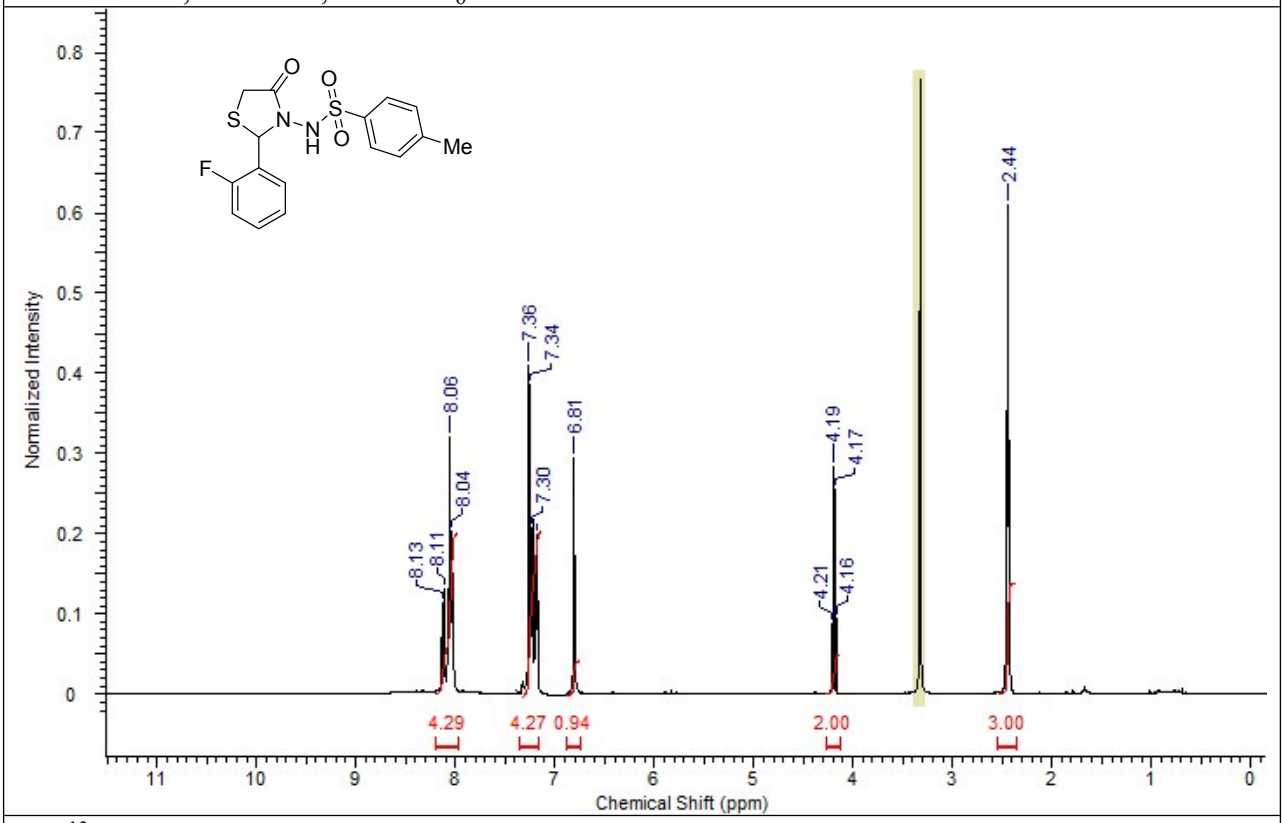


4h. ^{1}H NMR, 400 MHz, DMSO-d_6



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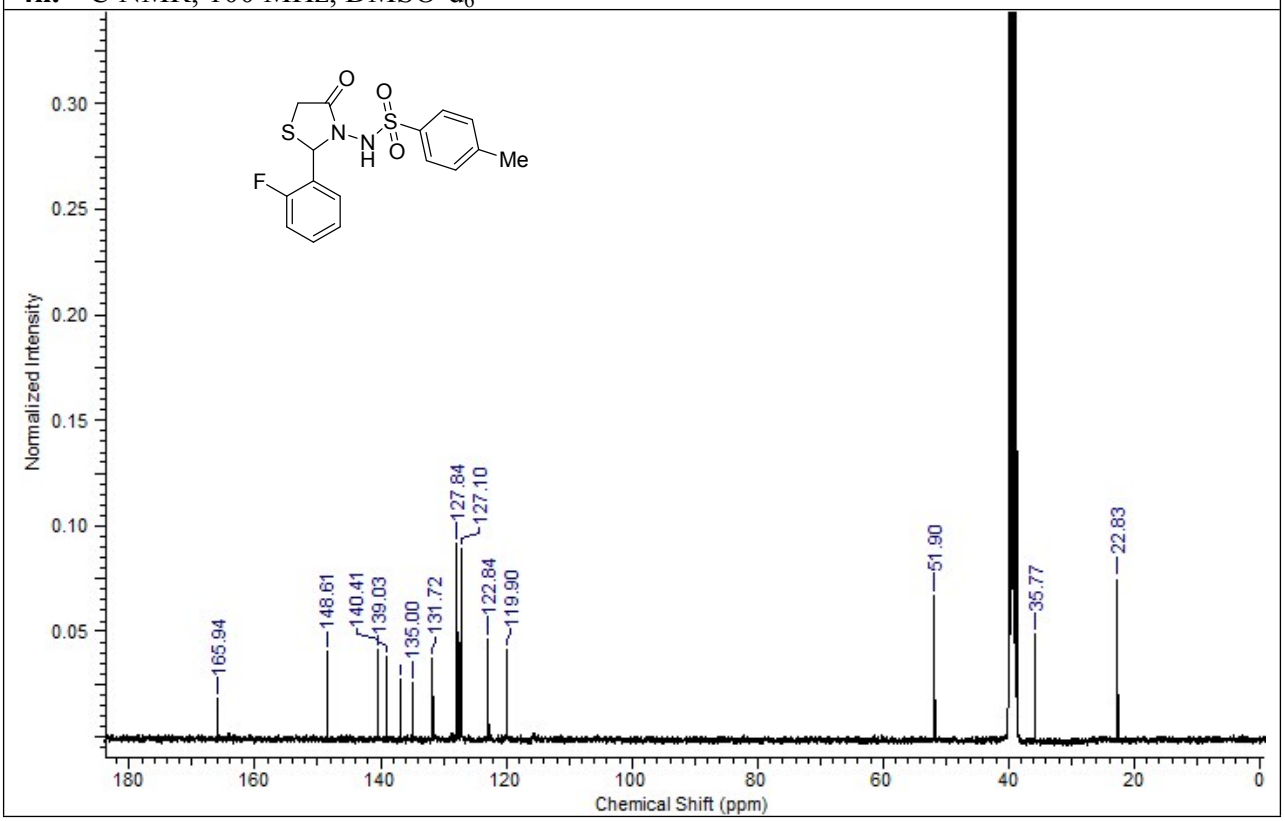

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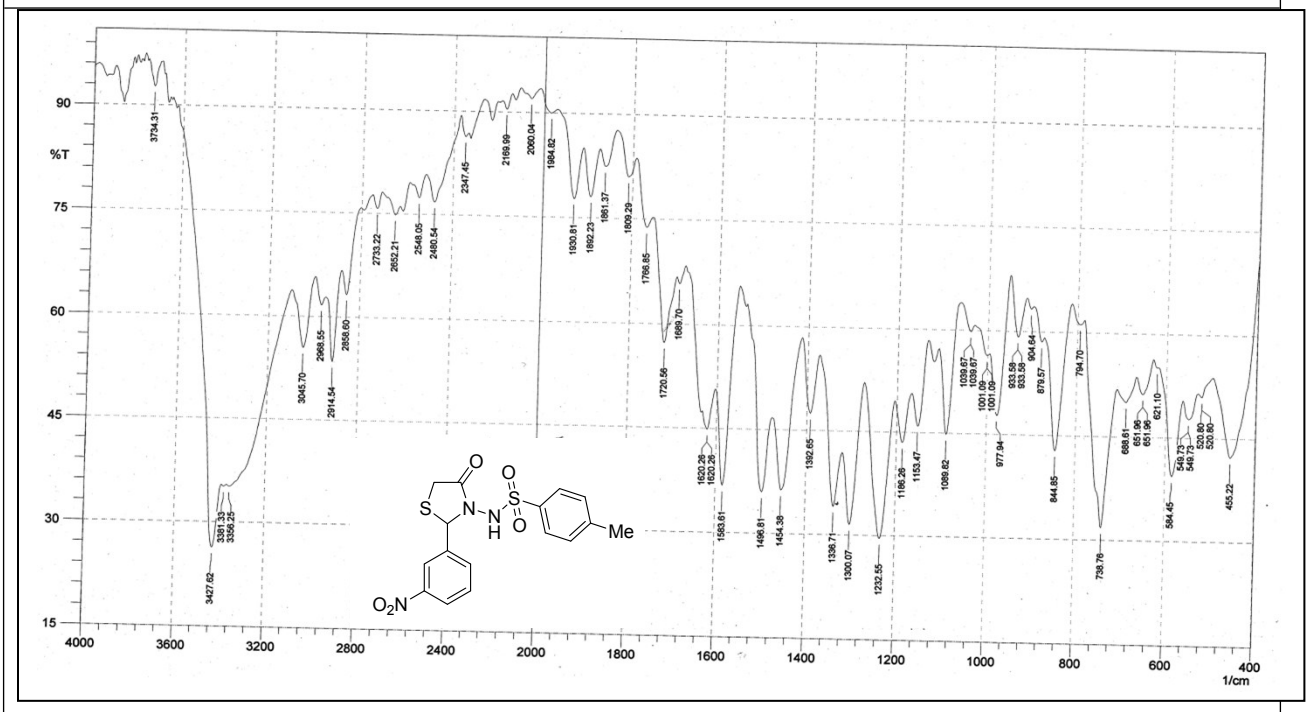

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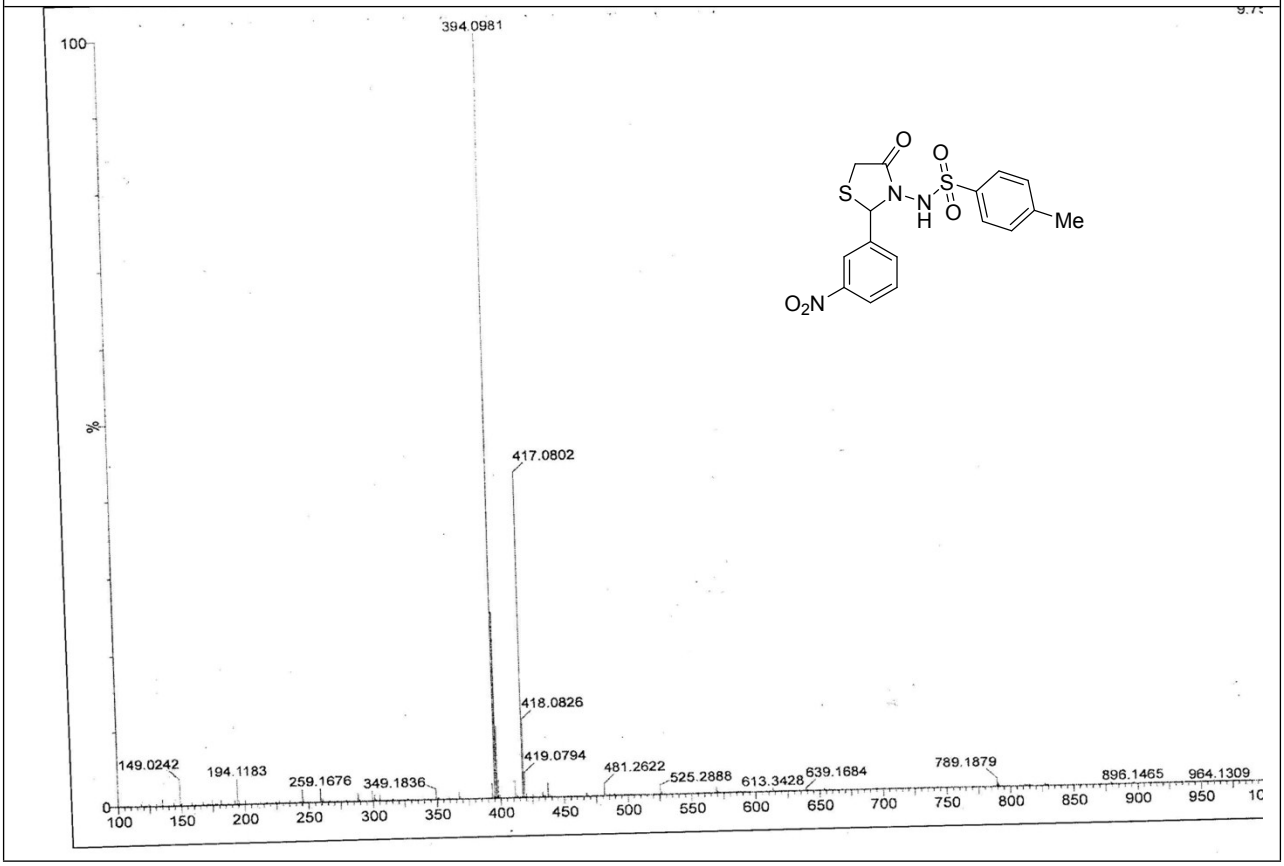
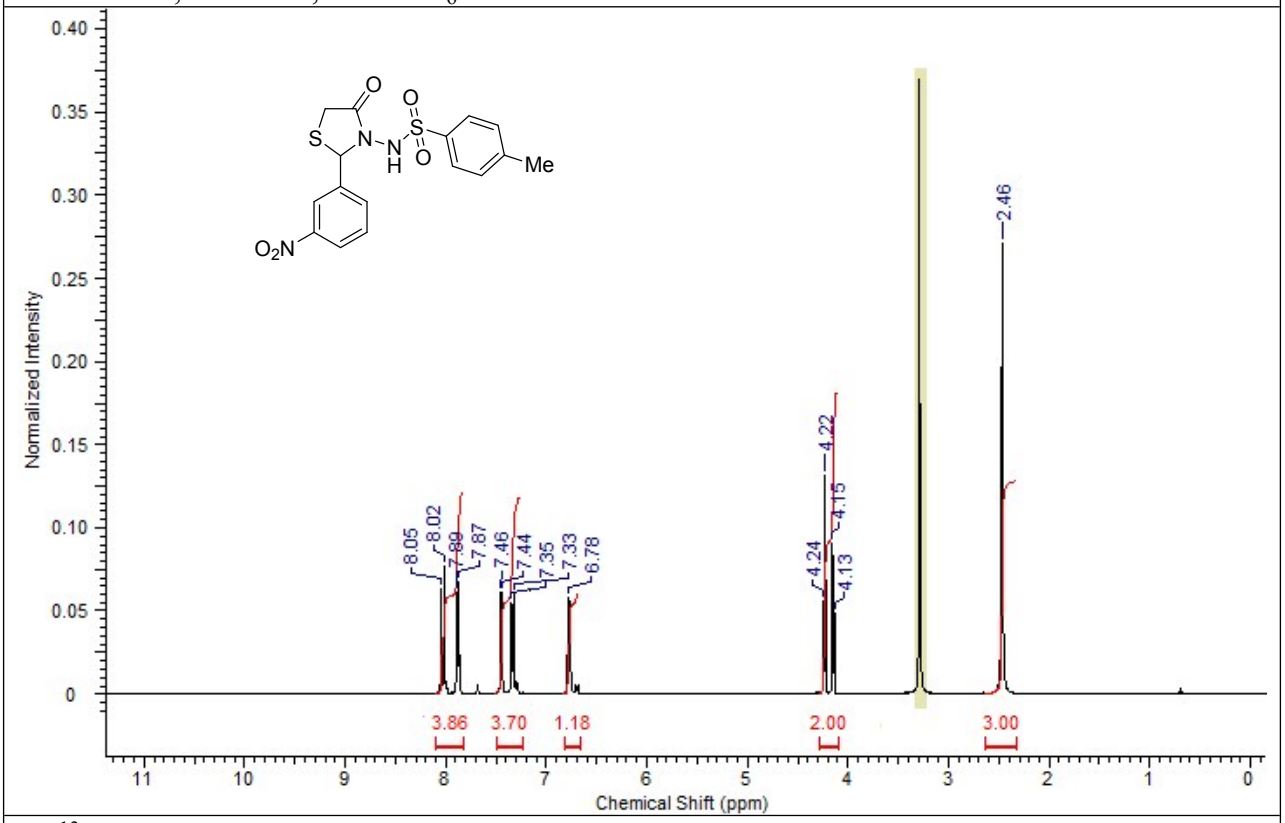
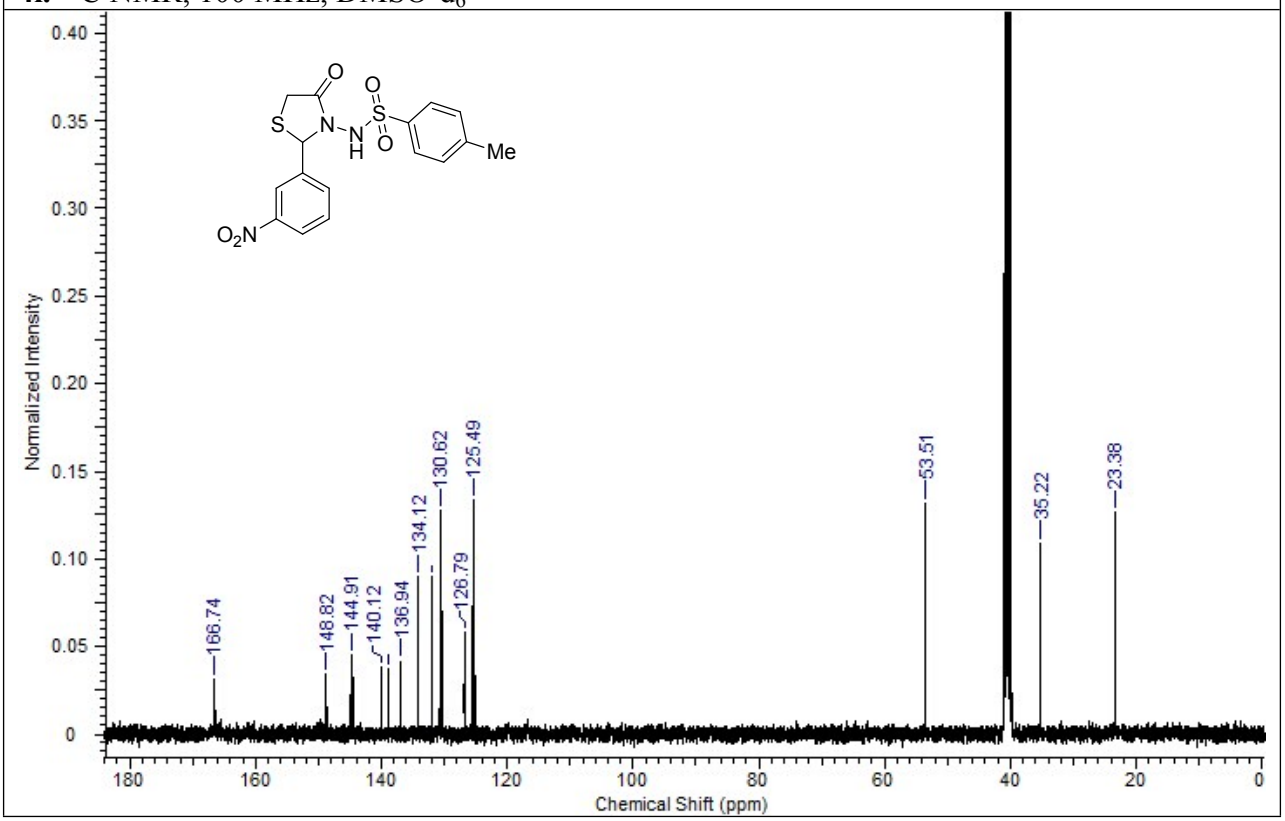


4i. ^{1}H NMR, 400 MHz, DMSO-d_6



4i. ^{13}C NMR, 100 MHz, DMSO-d_6



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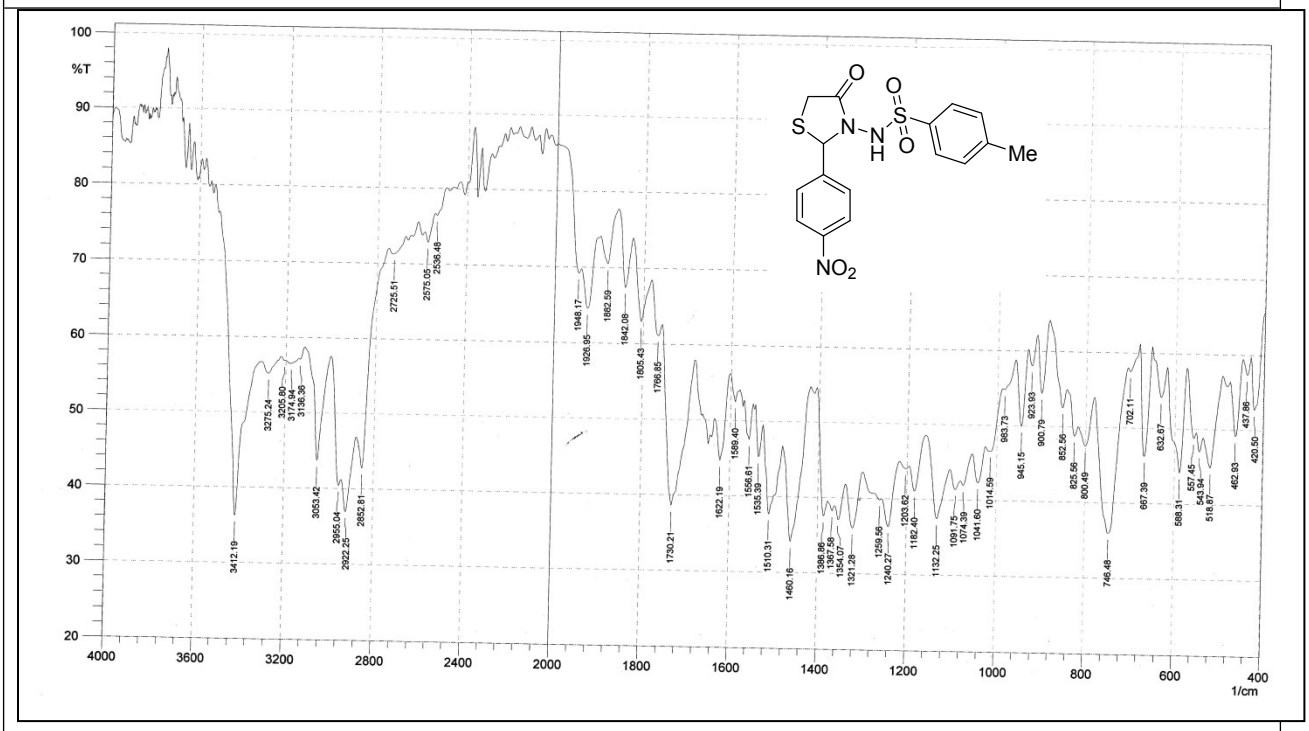

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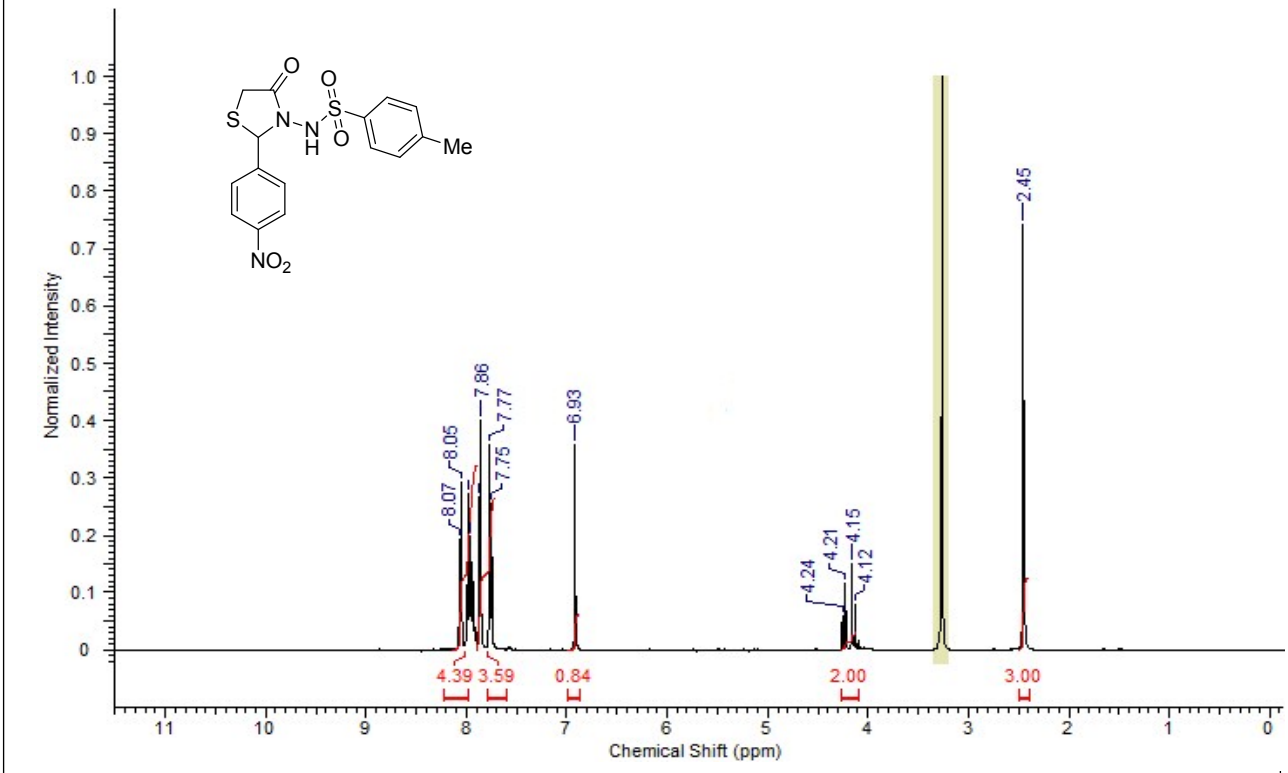
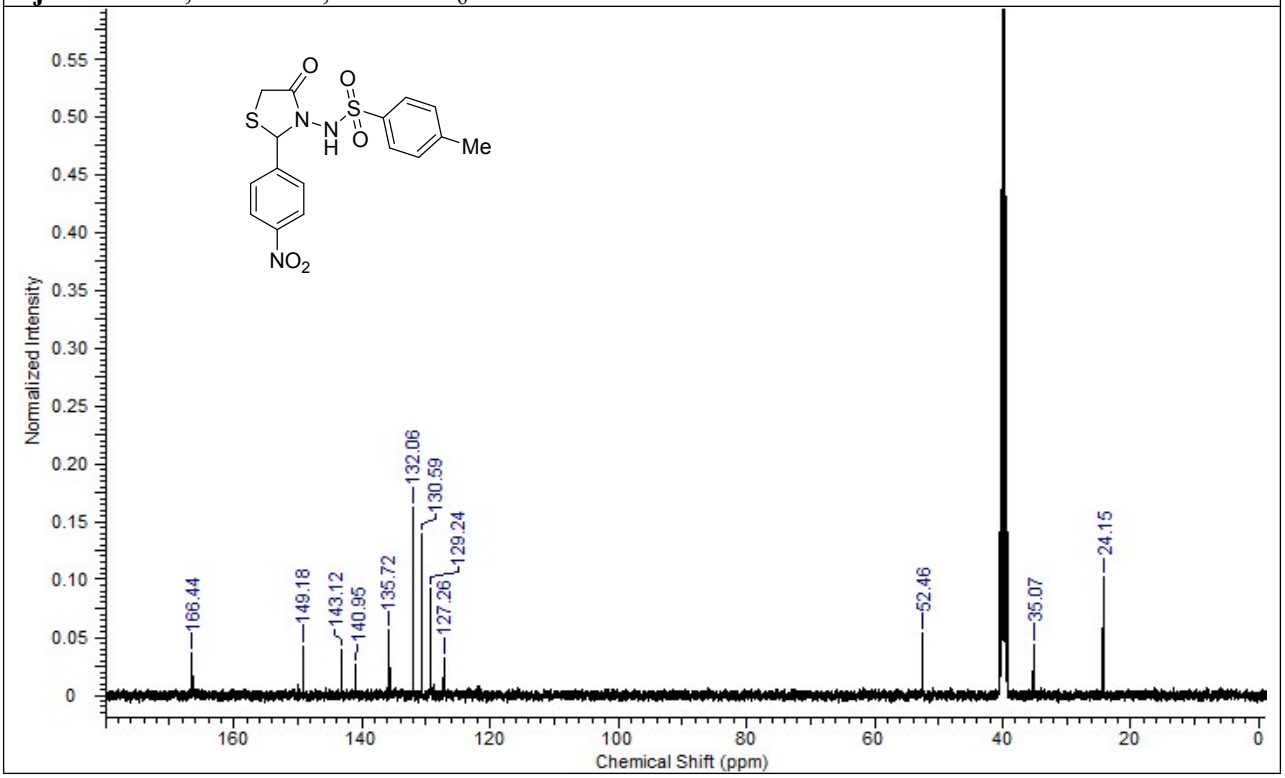
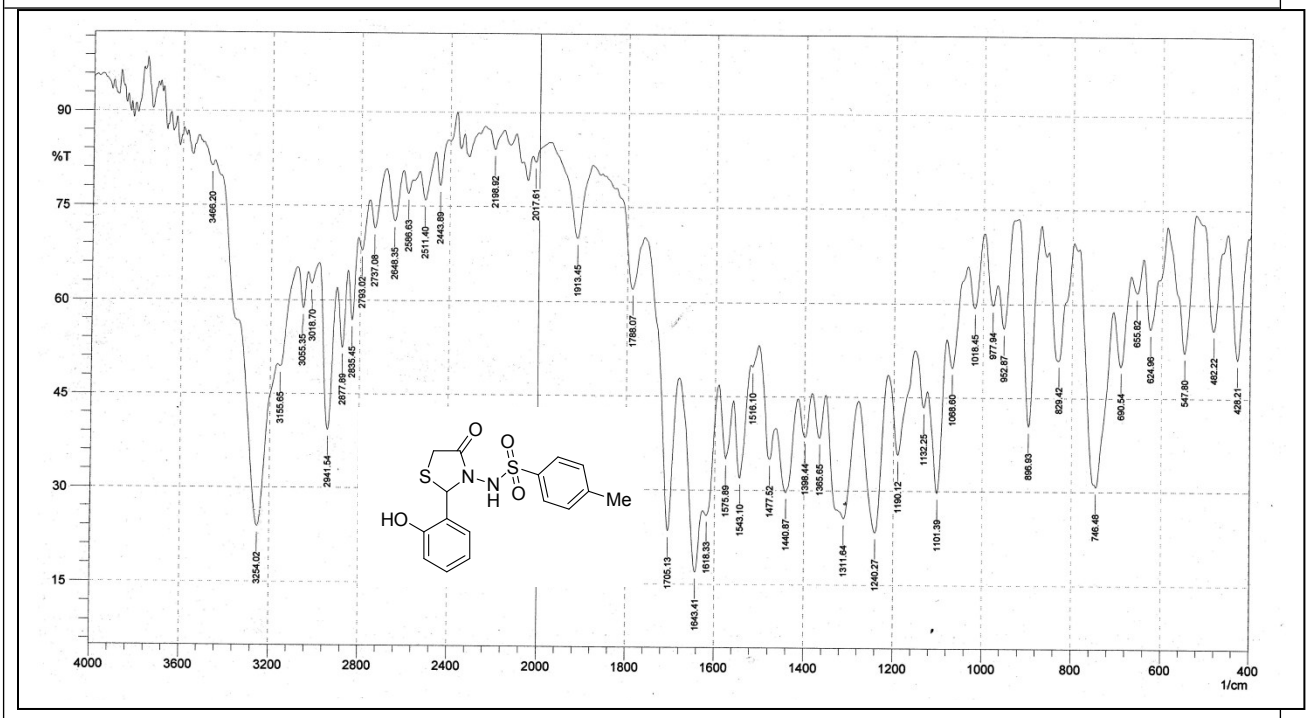


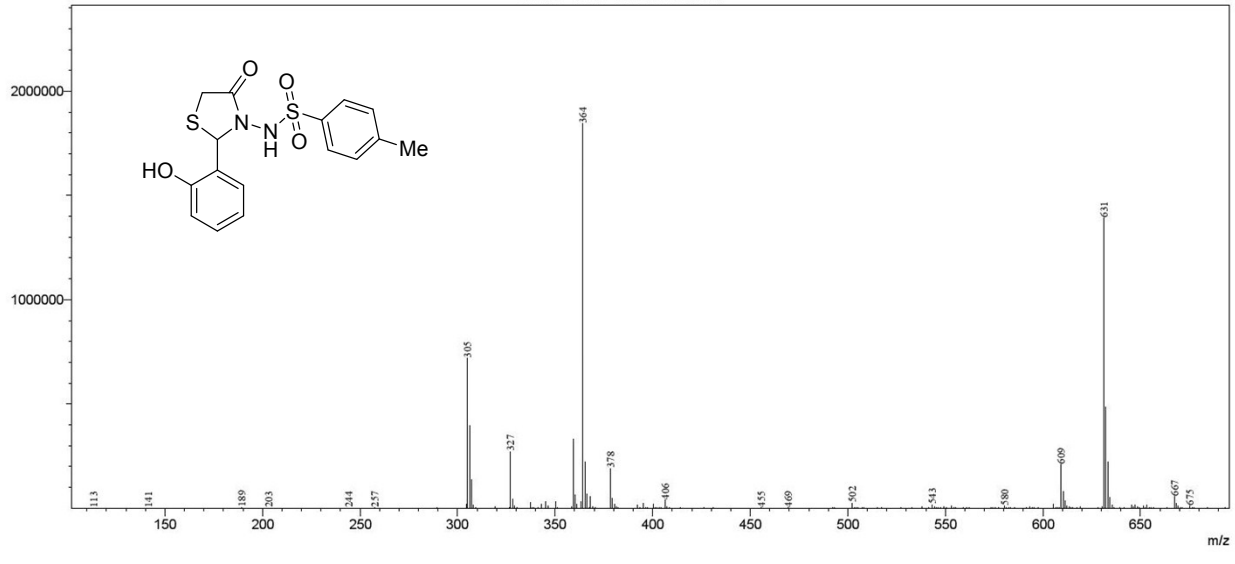
4j. ^{13}C NMR, 100 MHz, DMSO-d_6



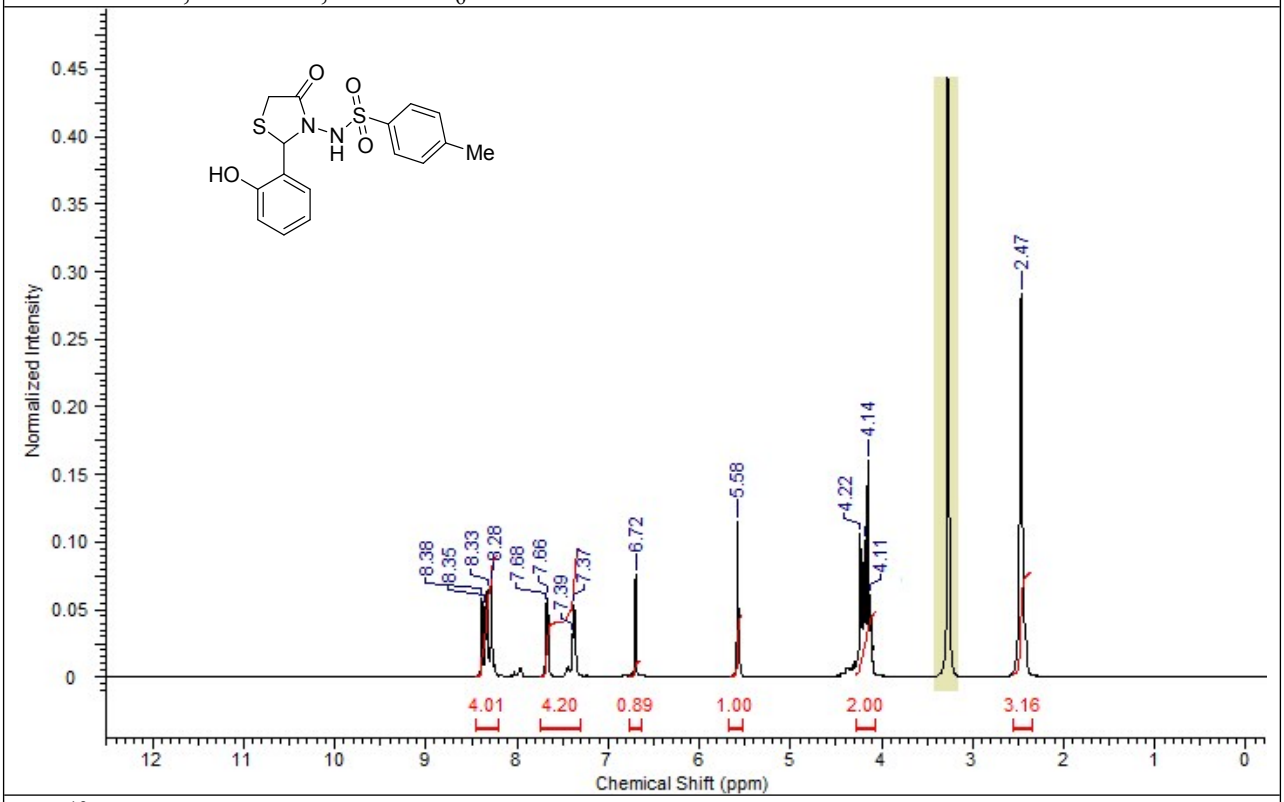
4k. FT-IR



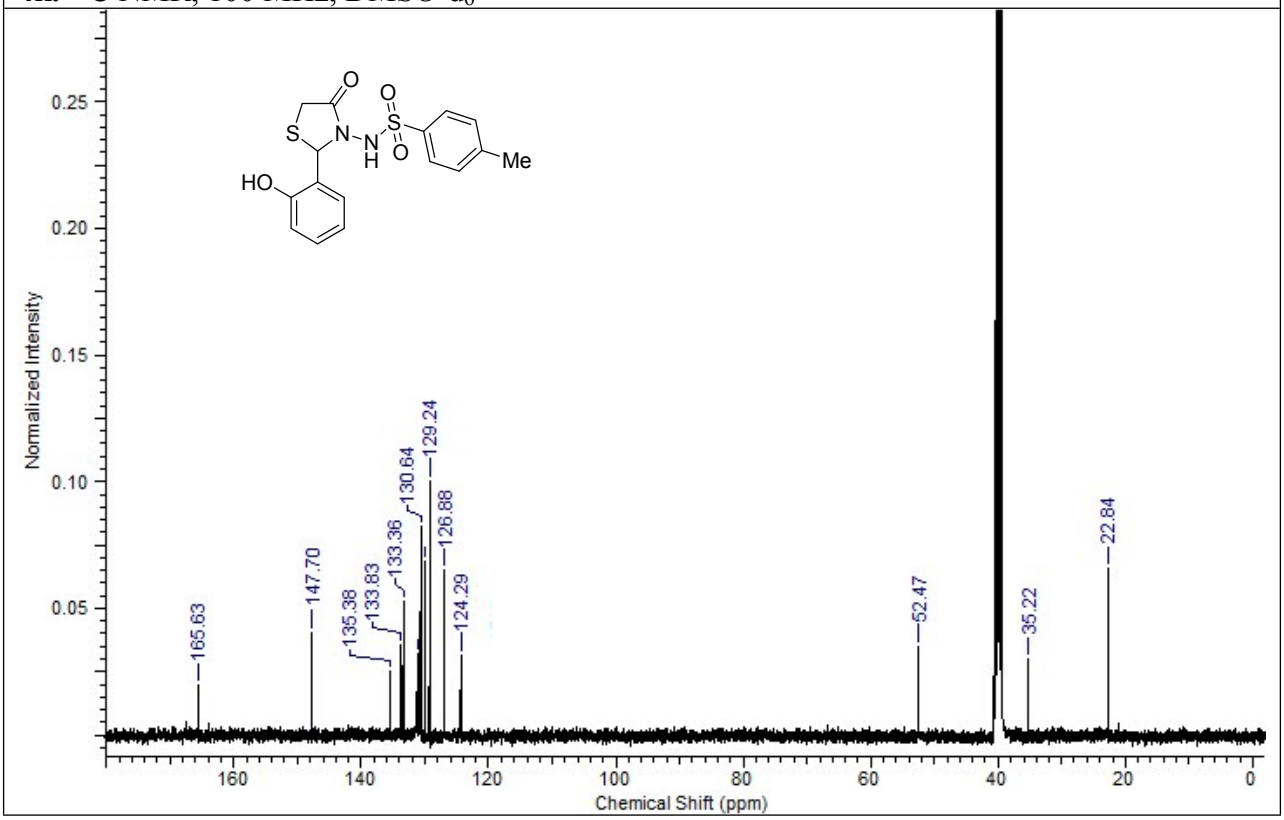
4k. LC-MS



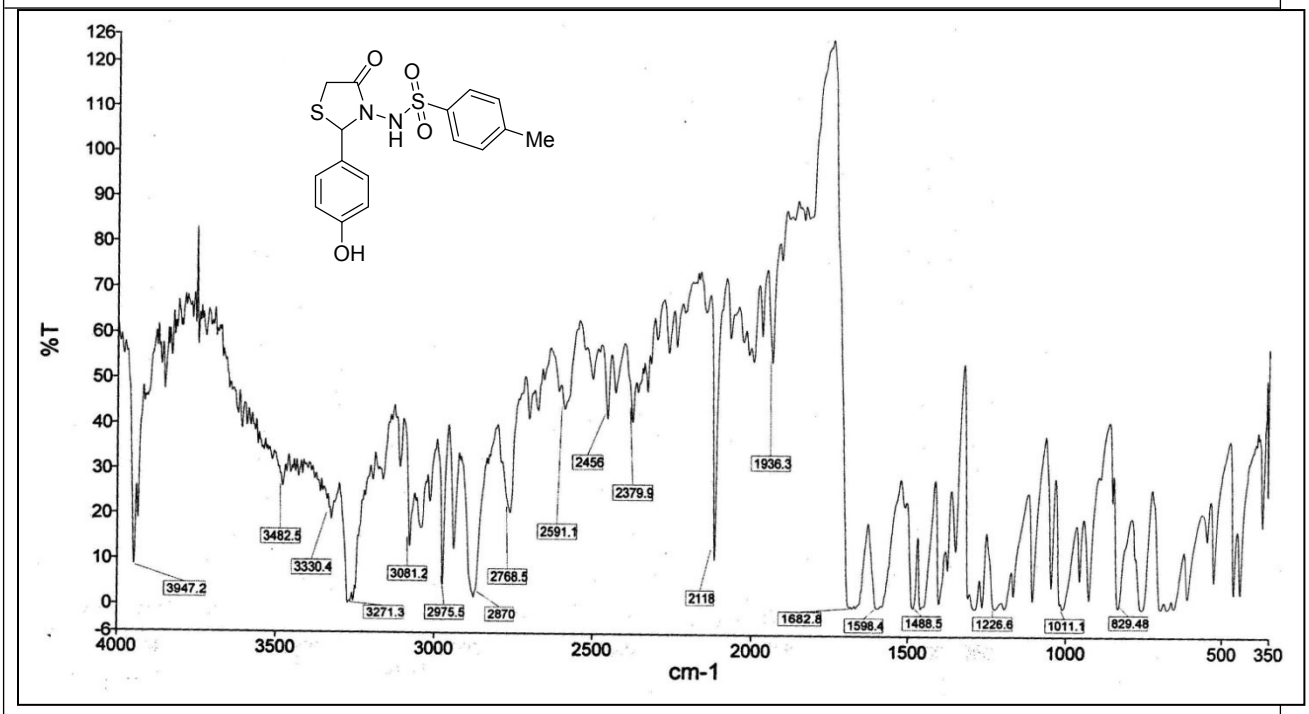
4k. ^{1}H NMR, 400 MHz, DMSO-d_6



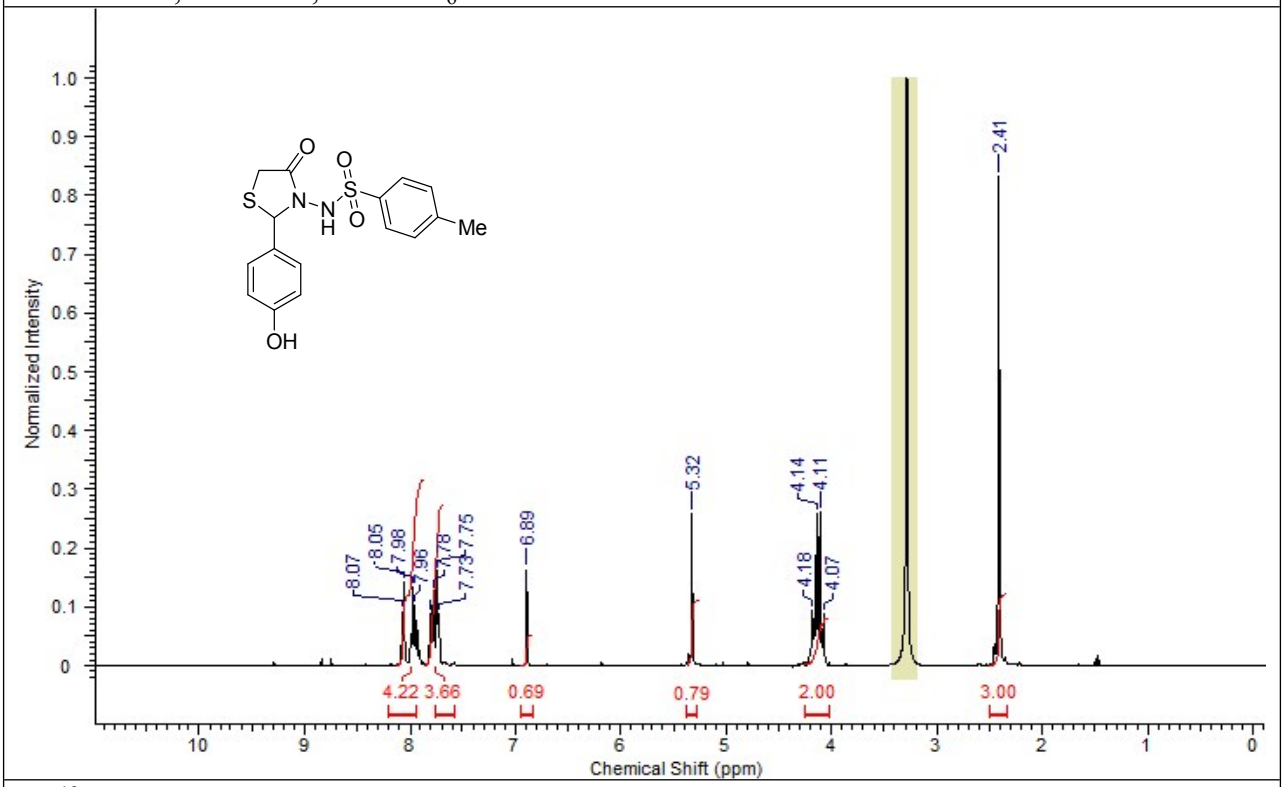
4k. ^{13}C NMR, 100 MHz, DMSO-d_6



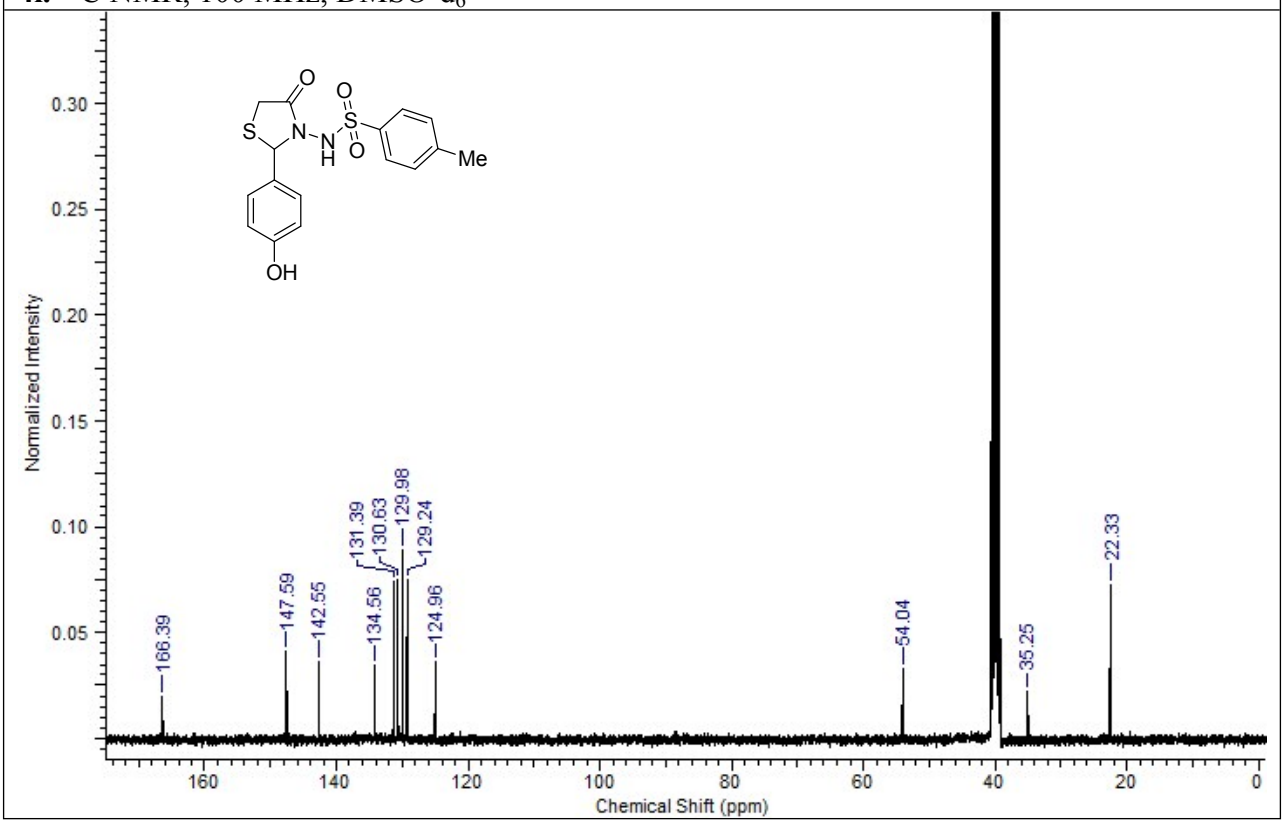
4l. FT-IR


%T
cm-1
3947.2
3482.5
3330.4
3271.3
3081.2
2975.5
2768.5
2870
2591.1
2456
2379.9
2118
1936.3
1682.8
1598.4
1488.5
1226.6
1011.1
829.48
Me
OH

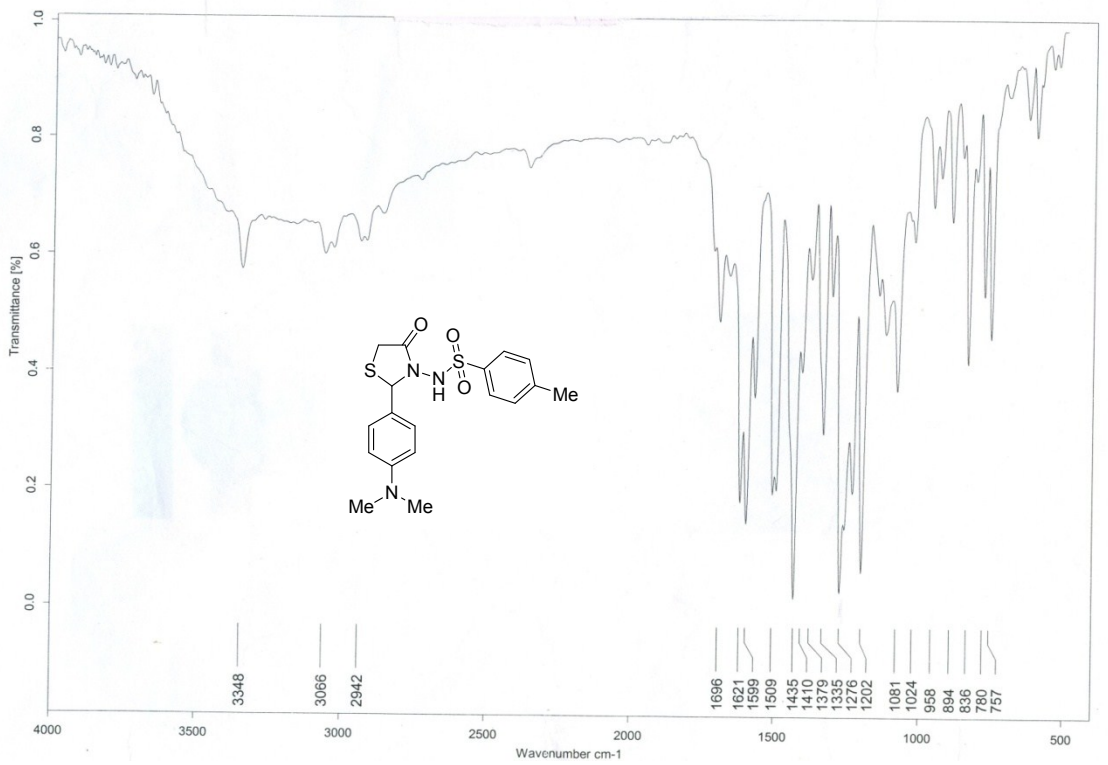
4l. ^{1}H NMR, 400 MHz, DMSO-d_6



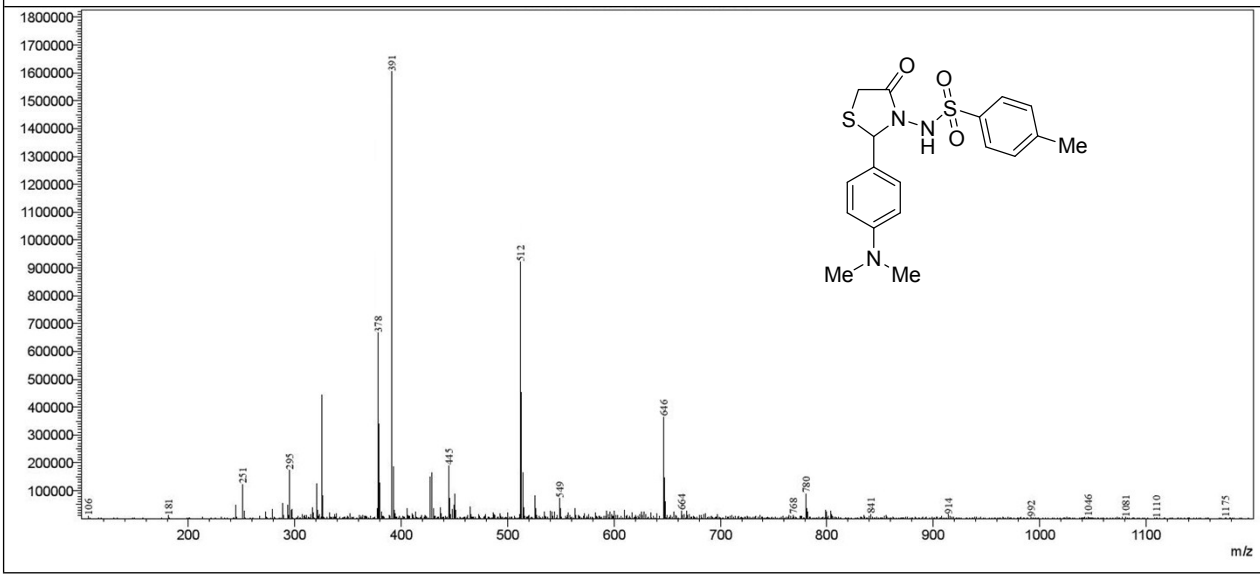
4l. ^{13}C NMR, 100 MHz, DMSO-d_6



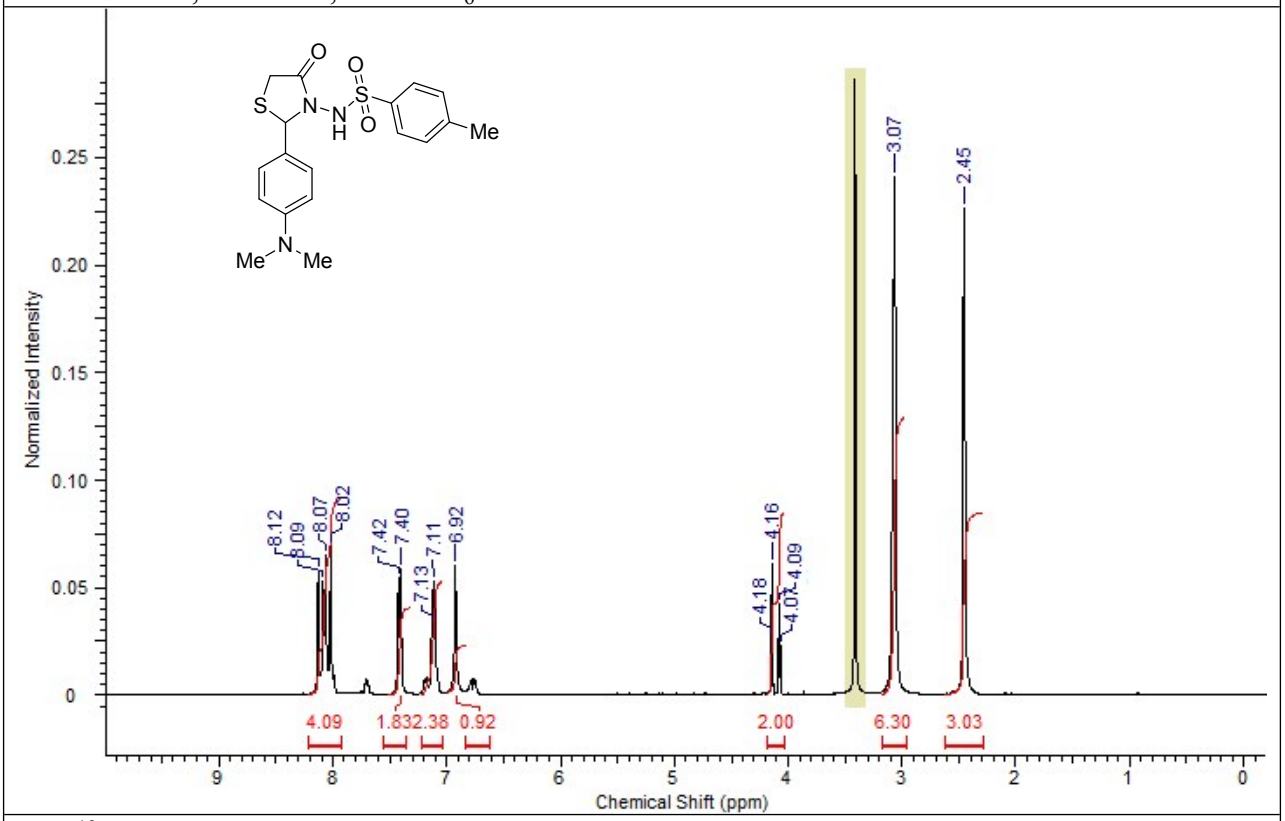
4m. FT-IR



4m. LC-MS



4m. ^{1}H NMR, 400 MHz, DMSO-d_6



4m. ^{13}C NMR, 100 MHz, DMSO-d_6