



Project Report on

"Analysis of NMR spectra of unknown compound"

Submitted By

M.Sc. SEM I Students (Roll No.1 to 6)

Guided By

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Submitted To

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Sir P.T.Science College, Modasa

SIR P.T.SCIENCE COLLEGE, MODASA
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Certificate

This is to certify that project report entitled "Analysis of NMR spectra of **Unknown Compound**" are carried out by students mentioned below. They have been satisfactorily completed their project work for academic year 2022-23. The project has been approved as it satisfies the academic requirement in respect of project work prescribed for the Master of Science. M.Sc-I

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SIR. P.T. SCIENCE COLLEGE
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(Dr. M. P. Gongiwala)

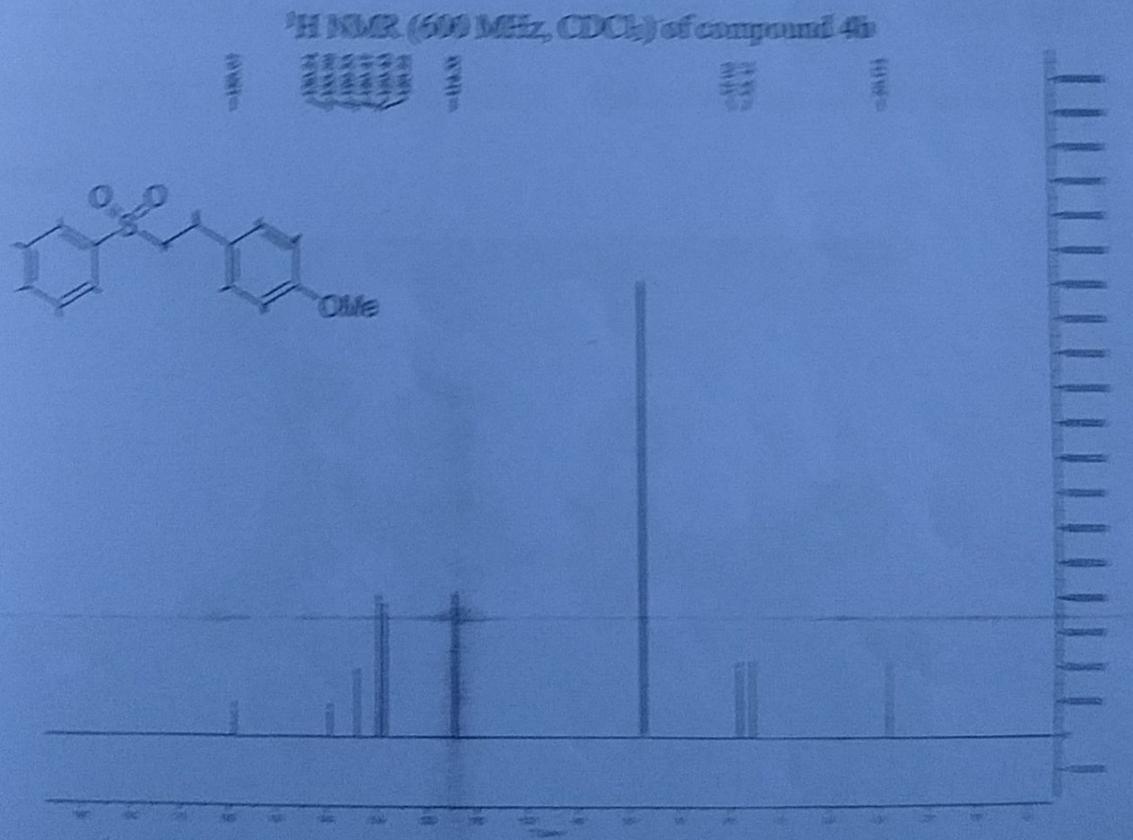
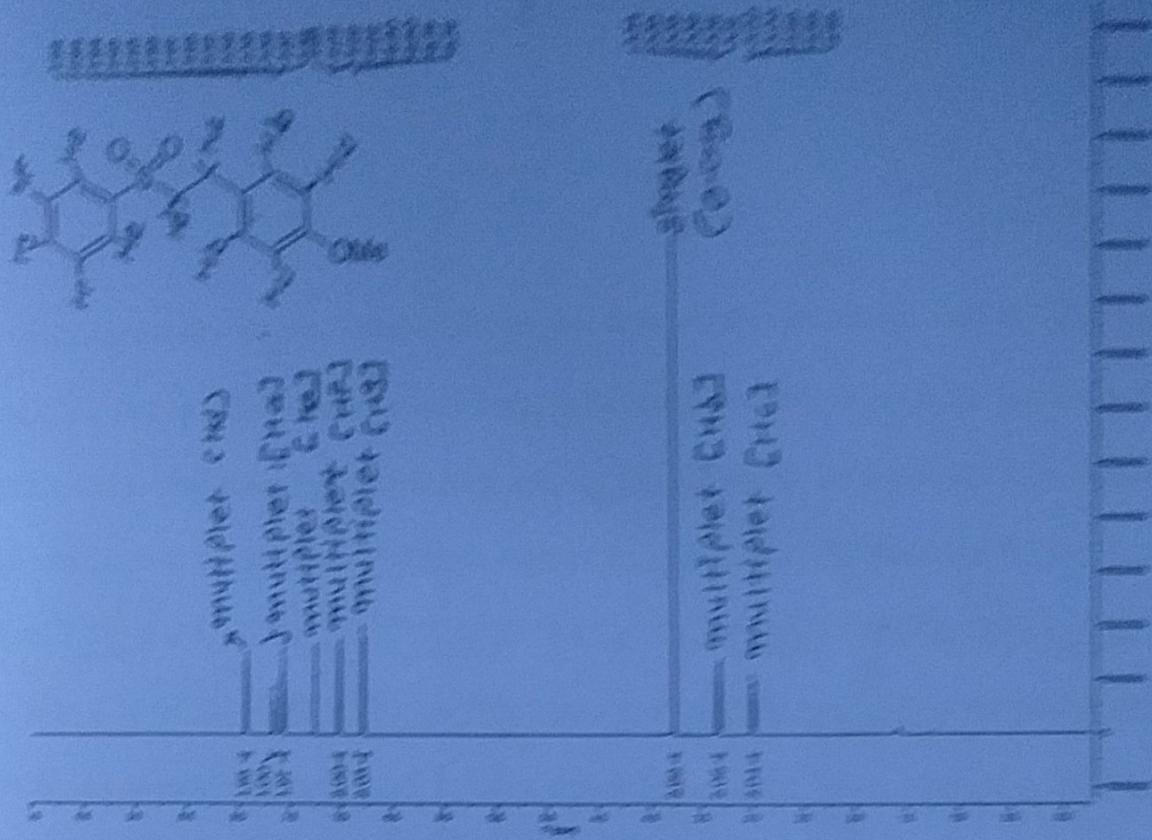
Table of Contents for Supporting Information

1.NMR-SPECTRA OF COMPOUND

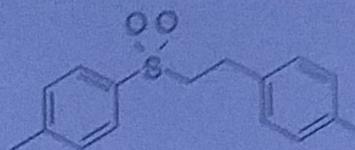
2.3D-STRUCTURE OF COMPOUND

3.PROPERTIES

4.GRAPHICAL INFORMATION

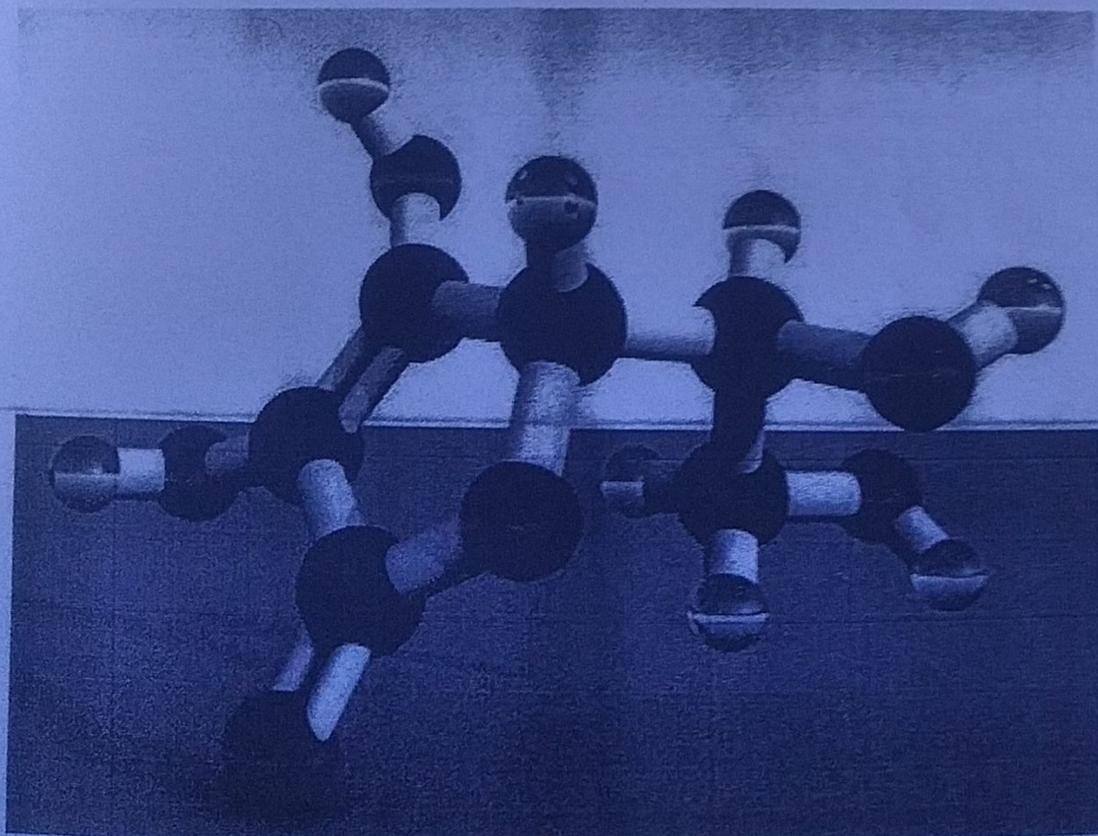


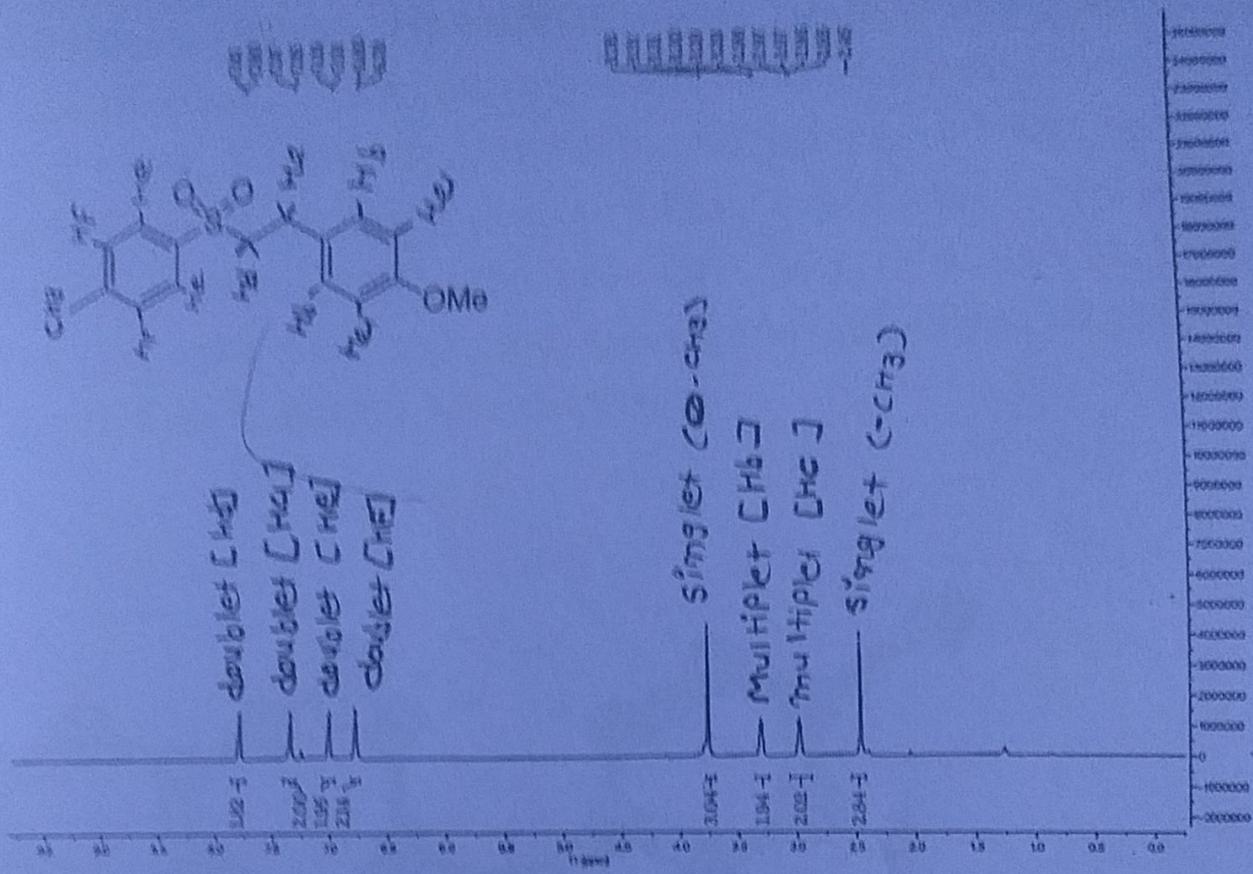
1-Methoxy-4-(2-tosylethyl)benzene (4c)



OMe

Prepared according to the *General Procedure* from 4-toluenesulfonyl fluoride (218 mg, 1.25 mmol, 2.5 equiv) and 4-vinylanisole (67 mg, 0.50 mmol, 1 equiv). After purification by automated flash column chromatography (from hexanes to 20% EtOAc in hexanes), the title compound **4c** was obtained as an off-white solid (51 mg, 0.18 mmol, 35%). $^1\text{H NMR}$ (600 MHz, CDCl_3), δ (ppm) 7.81 (d, $J = 7.9$ Hz, 2H), 7.36 (d, $J = 7.8$ Hz, 2H), 7.02 (d, $J = 8.1$ Hz, 2H), 6.79 (d, $J = 8.2$ Hz, 2H), 3.76 (s, 3H), 3.33 – 3.27 (m, 2H), 3.00 – 2.94 (m, 2H), 2.45 (s, 3H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3), δ (ppm) 158.6, 144.9, 136.2, 130.1, 129.6, 129.4, 128.2, 114.3, 58.0, 55.4, 28.1, 21.8. mp = 92 – 94 °C. FT-IR (cm^{-1} , neat, ATR), $\tilde{\nu} = 1511, 1494, 1247, 1145$. HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{19}\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 291.1055, found 291.1057. Spectral data agreed with those reported in the literature.²

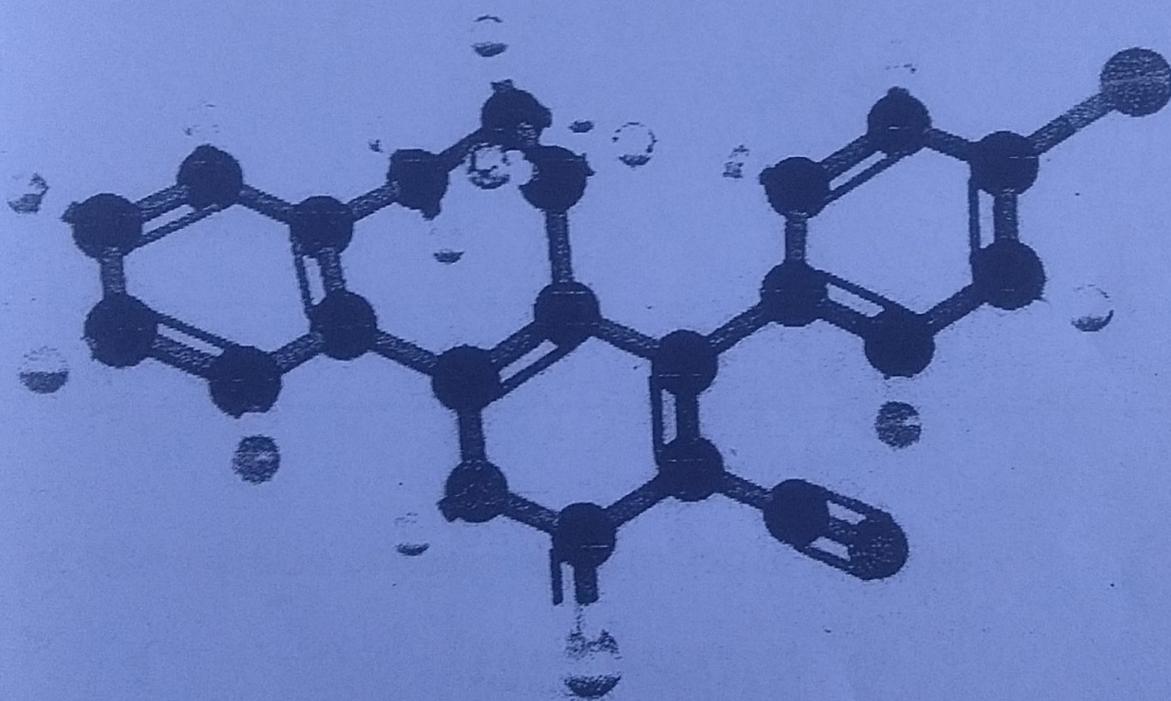




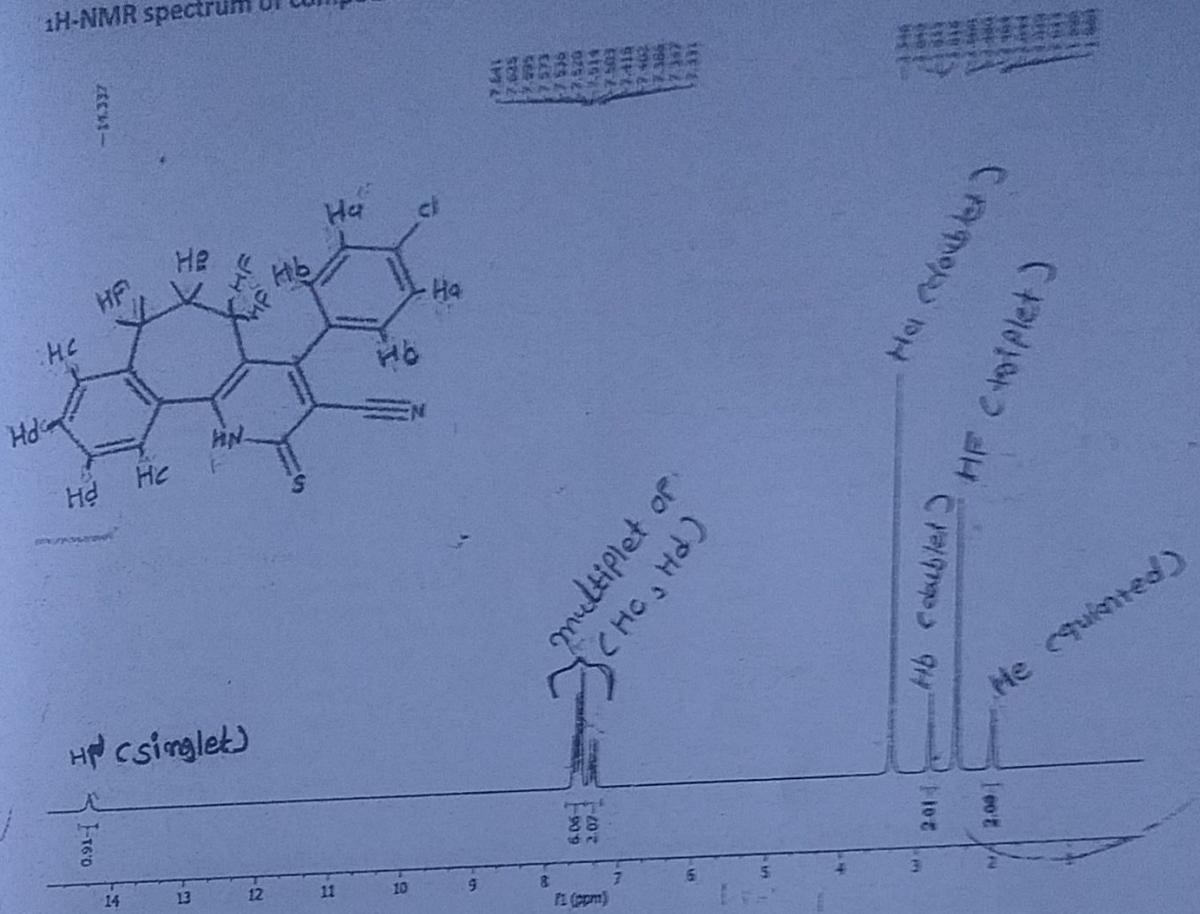
¹H NMR (600 MHz, CDCl₃) of compound 4c

2.1.1. 4-(4-Chlorophenyl)-2-thioxo-2,5,6,7-tetrahydro-1*H*-benzo[6,7]cyclohepta[1,2-*b*]pyridine-3-carbonitrile (3a).

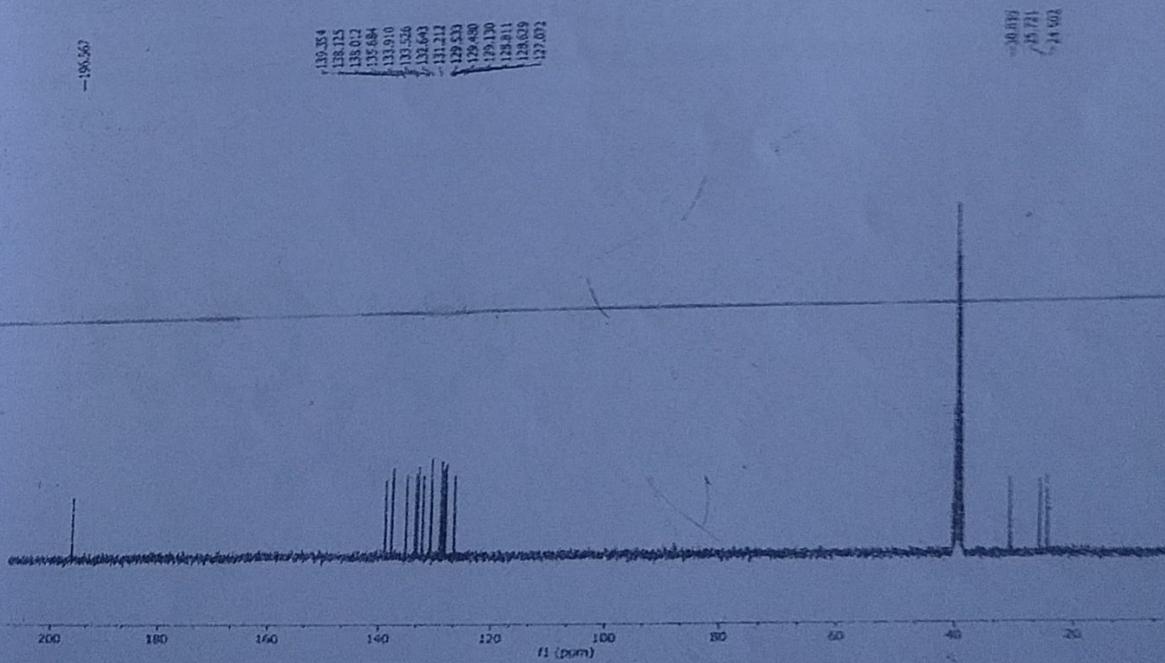
Yellow solid (dioxane, 74%); m.p. 198-200 °C; IR (ν cm^{-1}): 3335 (NH), 2210 (CN); $^1\text{H-NMR}$ (DMSO- d_6): δ 2.01 (quint, $J = 6.4$ Hz, 2H, CH_2), 2.48 (t, $J = 6.4$ Hz, 2H, CH_2), 2.83 (t, $J = 6.4$ Hz, 2H, CH_2), 7.32 (d, $J = 6.4$ Hz, 1H, ArH), 7.40 (t, $J = 6.4$ Hz, 1H, ArH), 7.50-7.53 (m, 3H, ArH), 7.58 (d, $J = 8.8$ Hz, 2H, ArH), 7.63 (d, $J = 6.4$ Hz, 1H, ArH), 14.33 (s, 1H, NH); $^{13}\text{C-NMR}$ (DMSO- d_6): δ 24.5, 25.7, 30.8, 127.0, 128.6, 128.8, 129.1, 129.4, 129.5, 131.2, 132.6, 133.5, 133.9, 135.6, 138.0, 138.1, 139.3, 196.5; Anal. calcd for $\text{C}_{21}\text{H}_{15}\text{ClN}_2\text{S}$ (362.8): C, 69.51; H, 4.17; N, 7.72; found: C, 69.35; H, 4.01; N, 7.90%.



3. NMR spectral data
¹H-NMR spectrum of compound 3a (DMSO-d₆ 400 MHz).

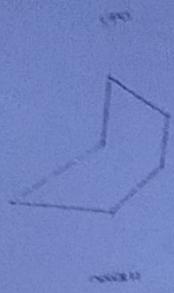
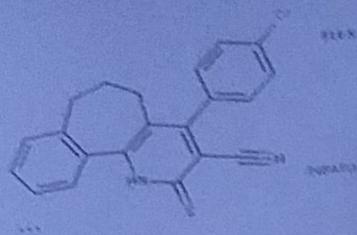


¹³C-NMR spectrum of compound 3a (DMSO-d₆ 100 MHz).



Molecule 1

11 0 0 0



SMILES: CN1C=NC2=C(C(=N1)C#N)C(=O)C2c3ccccc3OC

Physicochemical Properties	
Formula	C ₂₂ H ₁₈ N ₂ O ₂ S
Molecular weight	358.39 g/mol
Num. heavy atoms	25
Num. arom. heavy atoms	18
Fraction Csp ³	0.14
Num. rotatable bonds	3
Num. H-bond acceptors	1
Num. H-bond donors	1
Molar Refractivity	104.85
TPSA	71.07 Å ²
Lipophilicity	
Log P _{ov} (LOGP)	3.23
Log P _{ov} (OLOGP)	4.56
Log P _{ov} (MLOGP)	6.69
Log P _{ov} (MLOGP)	3.80
Log P _{ov} (SILICOS-IT)	7.62
Consensus Log P _{ov}	5.06

Log S (ESOL)
Solubility
Class

Log S (Aq)
Solubility
Class

Log S (SILICOS-IT)
Solubility
Class

GI absorption
BBB permeant
P-gp substrate
CYP1A2 inhibitor
CYP2C19 inhibitor
CYP2C9 inhibitor
CYP2D6 inhibitor
CYP3A4 inhibitor
Log K_o (SML permeant)

Lipinski
Chose
Veber
Egan
Muegge
Bioavailability Score

PAINS
Brenk
Leadlikeness
Synthetic accessibility

Water solubility
5.43
1.35e-03 mg/ml, 3.72e-08

Moderately soluble
5.79
5.51e-04 mg/ml, 1.52e-08

Moderately soluble
-0.85
8.07e-07 mg/ml, 2.22e-09

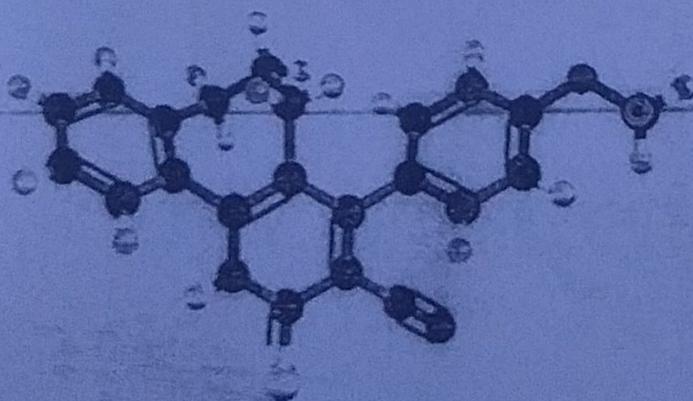
Poorly soluble
Pharmacokinetics
High
No
Yes
Yes
Yes
No
Yes
-5.28 cm/s

Druglikeness
Yes, 0 violation
No, 1 violation, WLOGP>5.1
Yes
No, 1 violation, WLOGP>5.1
Yes

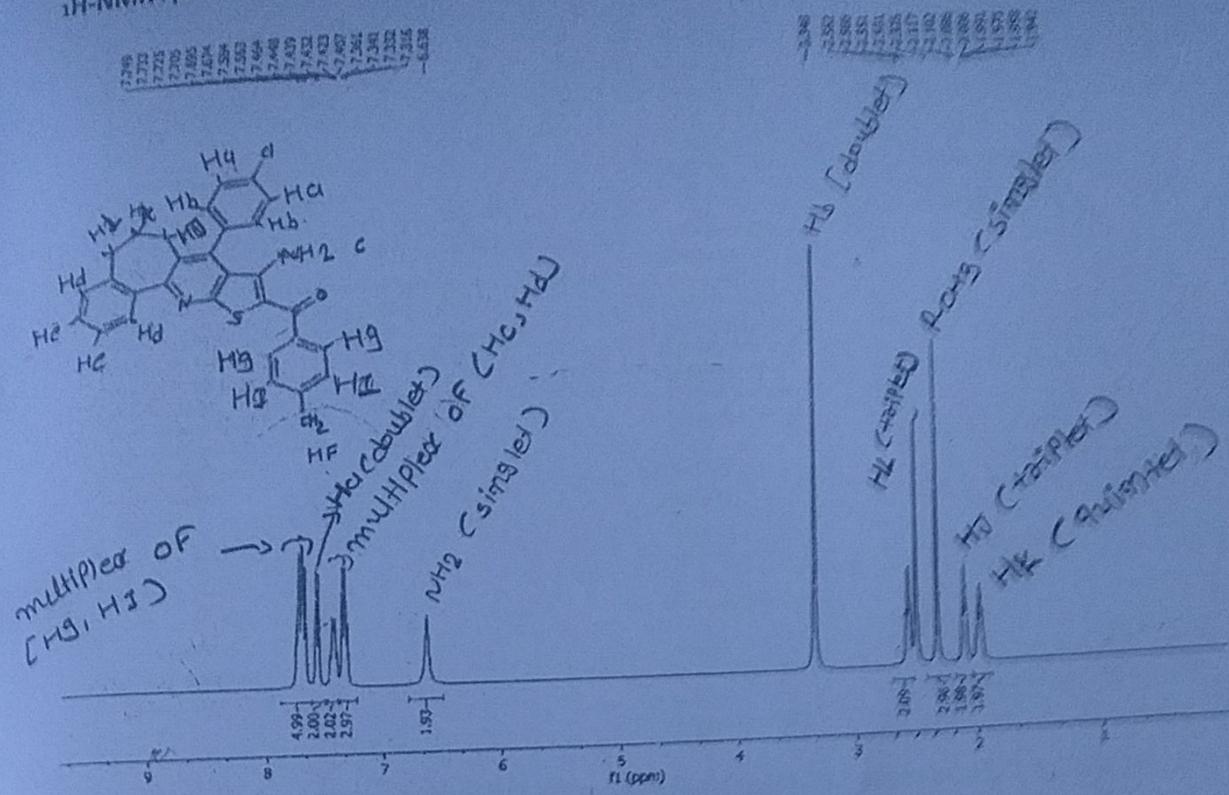
0.56
Medicinal Chemistry
0 alert
1 alert thiocarbonyl_group
No, 2 violations, MW>350, 1
3.10

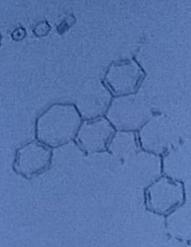
2.1.2. 4-(4-Methoxyphenyl)-2-thioxo-2,5,6,7-tetrahydro-1H-benzo[6,7]cyclohepta[1,2-b]pyridine-3-carbonitrile (3b).

Yellow solid (dioxane / ethanol mixture, 77%); m.p. 230-231 °C; IR (u cm⁻¹): 3327 (NH), 2211 (CN); ¹H-NMR (DMSO-d₆): δ 2.02 (quint, J = 6.4 Hz, 2H, CH₂), 2.52 (t, J = 6.4 Hz, 2H, CH₂), 2.82 (t, J = 6.4 Hz, 2H, CH₂), 3.81 (s, 3H, p-OCH₃), 7.04 (d, J = 8.4 Hz, 2H, ArH), 7.30 (d, J = 6.4 Hz, 1H, ArH), 7.39 (t, J = 6.4 Hz, 1H, ArH), 7.50-7.56 (m, 3H, ArH), 7.62 (d, J = 6.4 Hz, 1H, ArH), 14.20 (s, 1H, NH); Anal. calcd for C₂₂H₁₈N₂O₂S (358.4): C, 73.72; H, 5.06; N, 7.82; found: C, 73.57; H, 5.13; N, 7.69%.



¹H-NMR spectrum of compound 5c (DMSO-d₆ 400 MHz).





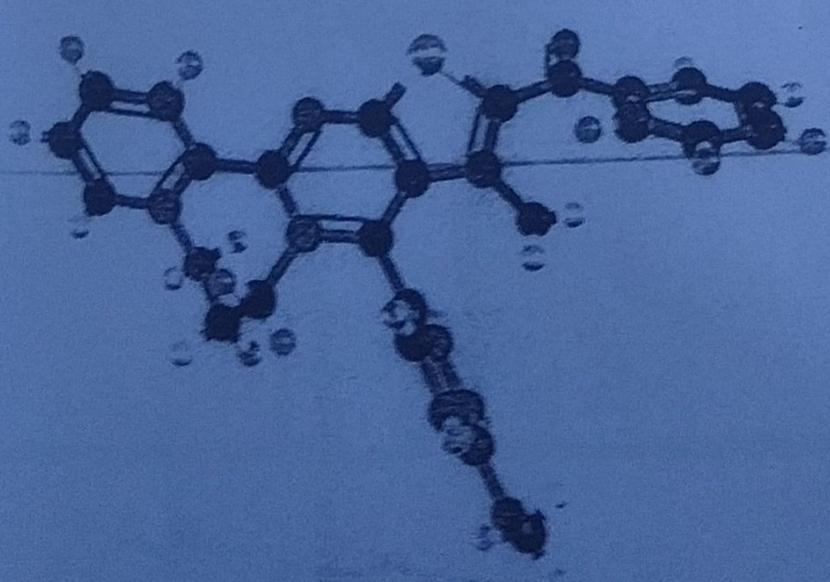
5e



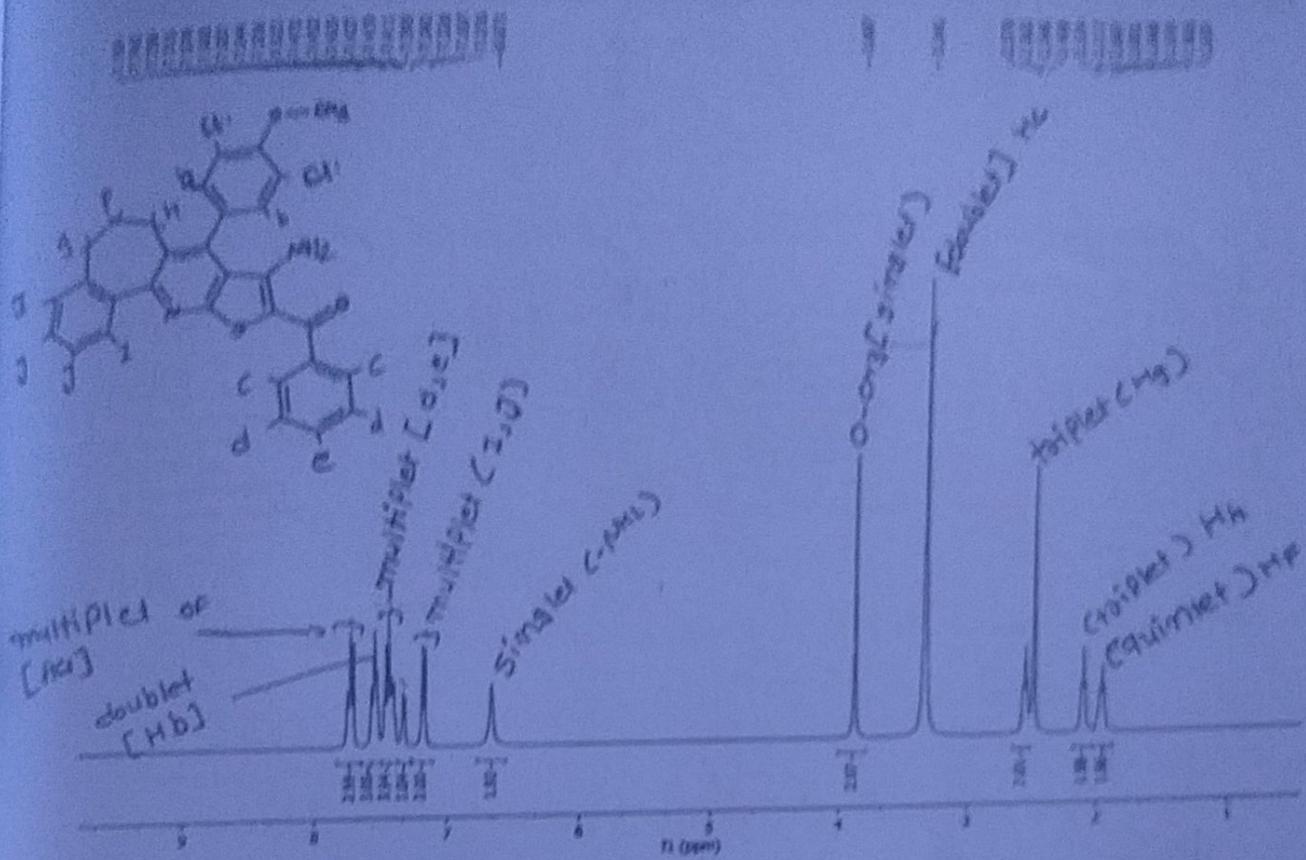
5e

Physicochemical Properties		ADMET	
Formula	C ₃₀ H ₂₄ N ₂ O ₂ S	Log S (ESOL)	-1.64
Molecular weight	476.53 g/mol	Solubility	1.17e-09 mg/ml, 2.31e-09 mol/l
Num. heavy atoms	28	Class	Poorly soluble
Num. rotatable bonds	27	Log S (Mj)	-10.91
Fraction Csp ³	0.13	Solubility	2.64e-06 mg/ml, 4.58e-11 mol/l
Num. H-bond acceptors	4	Class	None-to
Num. H-bond donors	3	Log S (SILICOS-IT)	-11.49
Molar Refractivity	148.80	Solubility	1.91e-09 mg/ml, 2.1e-12 mol/l
TPSA	83.43 Å ²	Class	Insoluble
Log P _{ow} (ALOGP)	4.50	Pharmacokinetics	
Log P _{ow} (XLOGP3)	3.47	GI absorption	Low
Log P _{ow} (MLOGP)	7.60	BBB permeant	No
Log P _{ow} (MLOGP)	4.61	P-gp substrate	No
Log P _{ow} (SILICOS-IT)	8.49	CYP1A2 inhibitor	Yes
Consensus Log P _{ow}	6.75	CYP2C19 inhibitor	Yes
		CYP2C9 inhibitor	No
		CYP2D6 inhibitor	No
		CYP3A4 inhibitor	No
		Log K _p (skin permeation)	-3.40 cm ² /s
		Druglikeness	
		Lipinski	No, 2 violations, MW>500, HLOGP>4.15
		Chao	No, 3 violations, MW>400, HLOGP>6.6, MR>130
		Veber	Yes
		Egan	No, 1 violation, HLOGP>6.6
		Muegge	No, 1 violation, XLOGP3>4
		Bioavailability Score	0.17
		Medicinal Chemistry	
		PAINS	0 alert
		Brenk	0 alert
		Leadlikeness	No, 2 violations, MW>350, XLOGP3>3.5
		Synthetic accessibility	3.22

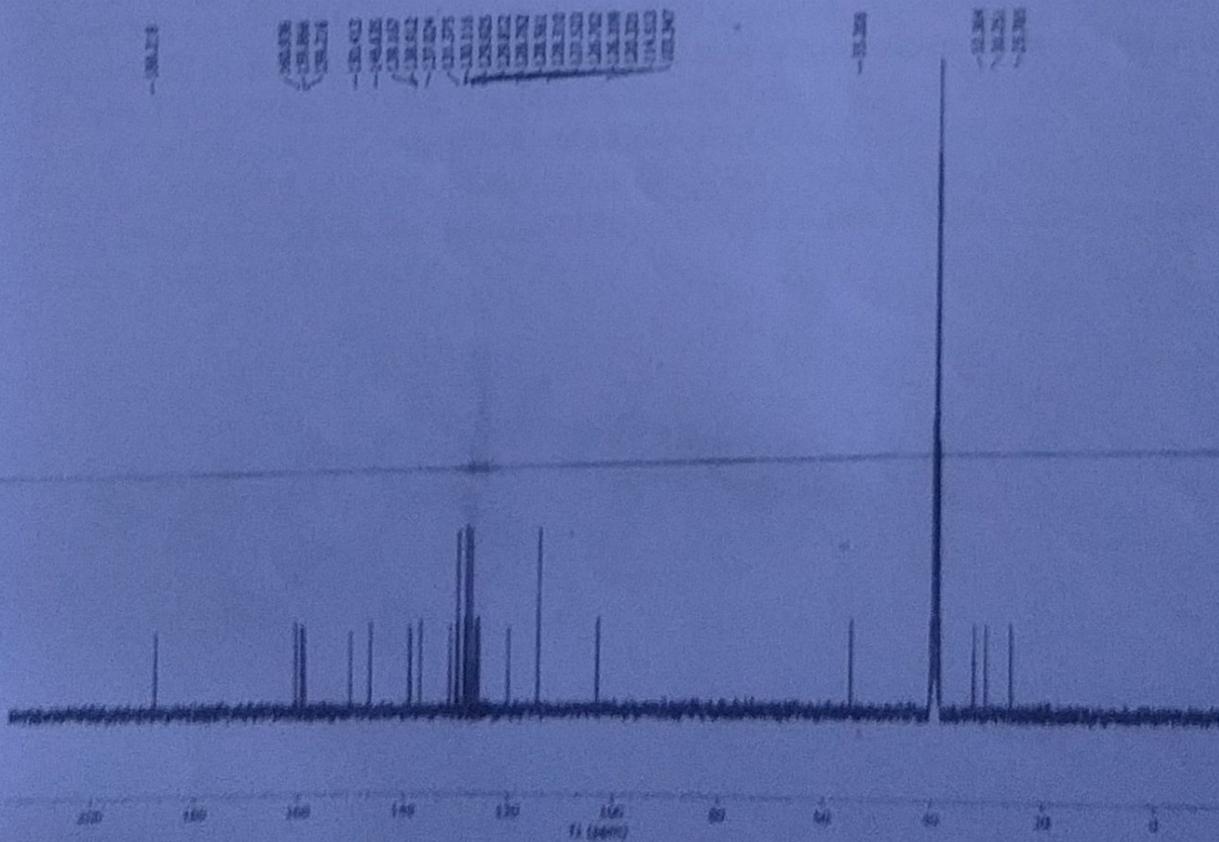
(9-Amino-8-(4-methoxyphenyl)-6,7-dihydro-5H-benzo[6,7]cyclohepta[1,2-b]thieno[3,2-e]pyridin-10-yl)(phenyl)methanone (5e).
 Yellow solid (dioxane, 90%); m.p. 280-281 °C; IR (ν cm⁻¹): 3415, 3242 (NH₂), 1633 (CO); ¹H-NMR (DMSO-d₆): δ 1.97 (quint, J = 6.4 Hz, 2H, CH₂), 2.11 (t, J = 6.4 Hz, 2H, CH₂), 2.56 (t, J = 6.4 Hz, 2H, CH₂), 3.88 (s, 3H, p-OCH₃), 6.67 (br s, 2H, NH₂), 7.18 (d, J = 8.4 Hz, 2H, ArH), 7.33 (d, J = 6.4 Hz, 1H, ArH), 7.41-7.47 (m, 4H, ArH), 7.52-7.57 (m, 3H, ArH), 7.71-7.75 (m, 3H, ArH); ¹³C-NMR (DMSO-d₆): δ 25.7, 30.2, 32.3, 55.2, 103.3, 114.5, 120.3, 126.1, 126.7, 127.5, 128.3, 128.5, 128.7, 129.8, 129.9, 130.1, 131.3, 137.0, 138.9, 139.1, 146.6, 150.4, 159.2, 159.8, 160.9, 188.2; Anal. calcd for C₃₀H₂₄N₂O₂S (476.5): C, 75.61; H, 5.08; N, 5.88; found: C, 75.49; H, 4.92; N, 6.04%.



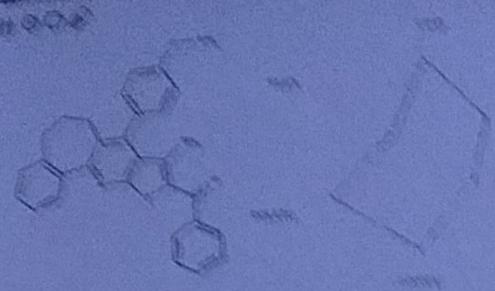
¹H-NMR spectrum of compound 5e (DMSO-d₆ 400 MHz).



¹³C-NMR spectrum of compound 5e (DMSO-d₆ 100 MHz).



Molecule 1

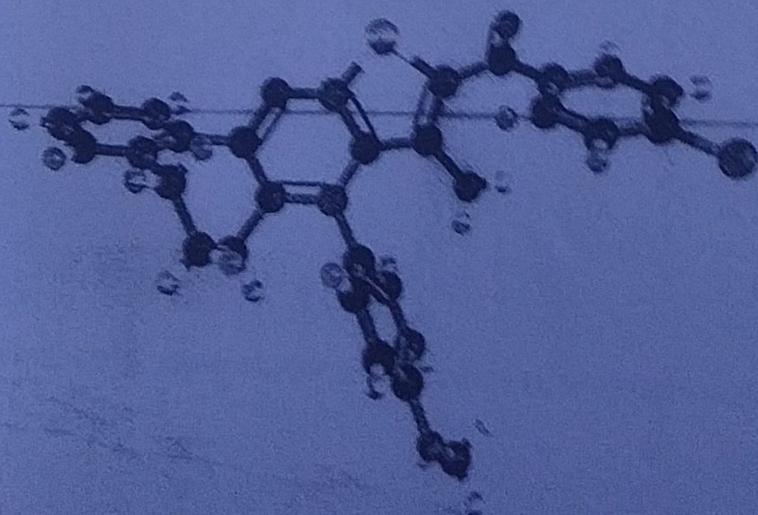


SMILES: COc1ccc(cc1)C(=O)Nc2c3ccccc3c4ccccc24

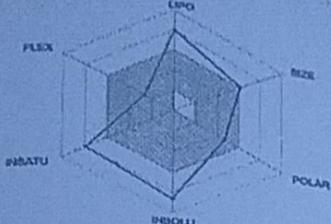
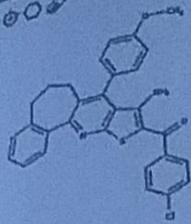
Physicochemical Properties		Molecular Weight	
Formula	C ₂₀ H ₁₅ N ₂ O ₂	297.34 (g/mol)	297.34
Molecular weight	478.50 (g/mol)	297.34 (g/mol)	297.34
Num. heavy atoms	36	297.34 (g/mol)	297.34
Num. arom. heavy atoms	27	297.34 (g/mol)	297.34
Fraction Csp ³	0.10	297.34 (g/mol)	297.34
Num. rotatable bonds	4	297.34 (g/mol)	297.34
Num. H-bond acceptors	3	297.34 (g/mol)	297.34
Num. H-bond donors	1	297.34 (g/mol)	297.34
Molar Refractivity	143.55	297.34 (g/mol)	297.34
TPSA	52.48 (Å ²)	297.34 (g/mol)	297.34
Lipophilicity		Molecular Weight	
Log P _{ov} (ALOGP)	4.44	297.34 (g/mol)	297.34
Log P _{ov} (XLOGP3)	7.66	297.34 (g/mol)	297.34
Log P _{ov} (MLOGP)	3.46	297.34 (g/mol)	297.34
Log P _{ov} (MLCGP)	4.20	297.34 (g/mol)	297.34
Log P _{ov} (SILICOS-IT)	7.32	297.34 (g/mol)	297.34
Chromophore Log P _{ov}	3.26	297.34 (g/mol)	297.34

2.2.8. (9-Amino-8-(4-methoxyphenyl)-6,7-dihydro-5H-benzo[6,7]cyclohepta[1,2-b]thieno[3,2-e]pyridin-10-yl)(4-chlorophenyl)methanone (50),

Yellow solid (dioxane, 91%); m.p. 180-182 °C; IR (ν cm⁻¹): 3423, 3247 (NH₂), 1627 (CO); ¹H-NMR (DMSO-d₆): δ 1.97 (quint, J = 6.4 Hz, 2H, CH₂), 2.14 (t, J = 6.4 Hz, 2H, CH₂), 2.55 (t, J = 6.4 Hz, 2H, CH₂), 3.88 (s, 3H, p-OCH₃), 6.72 (br s, 2H, NH₂), 7.19 (d, J = 8.4 Hz, 2H, ArH), 7.32 (d, J = 6.4 Hz, 1H, ArH), 7.40-7.45 (m, 4H, ArH), 7.60 (d, J = 8.4 Hz, 2H, ArH), 7.72 (d, J = 6.4 Hz, 1H, ArH), 7.79 (d, J = 8.4 Hz, 2H, ArH); ¹³C-NMR (DMSO-d₆): δ 25.6, 30.4, 32.2, 55.3, 103.0, 114.7, 120.5, 126.2, 126.7, 128.6, 128.7, 128.8, 129.3, 129.7, 130.0, 130.1, 135.9, 139.1, 139.3, 139.4, 146.4, 150.9, 159.4, 159.7, 161.0, 187.4; Anal. calcd for C₃₀H₂₃ClN₂O₂S (511.0): C, 70.51; H, 4.54; N, 5.48; found: C, 70.63; H, 4.62; N, 5.33%.



Molecule 1



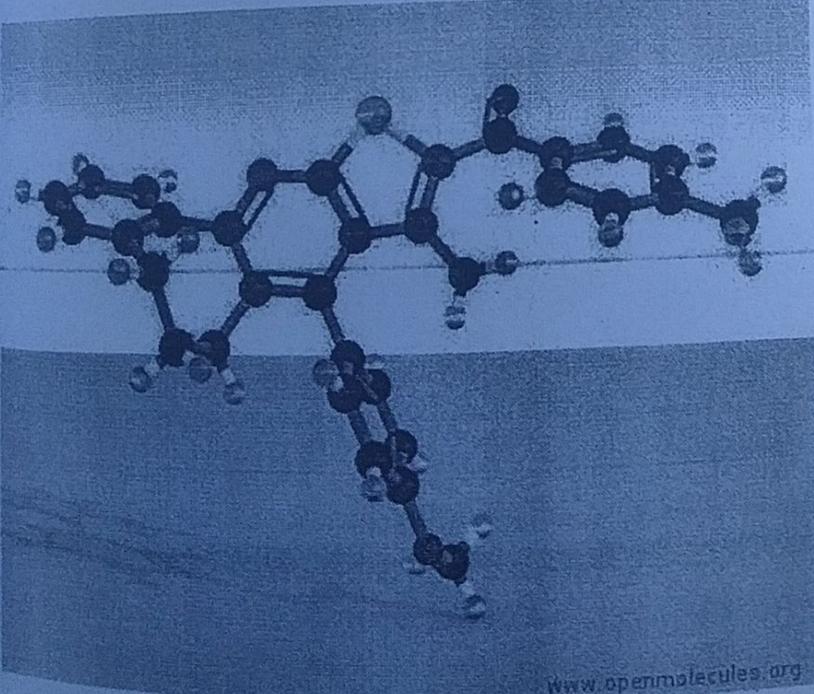
SMILES COc1ccc(cc1)c1c2CCc3c(c2nc2c1c(N)c(s2)C(=O)c1ccc(cc1)Cl)cc
cc3

Physicochemical Properties	
Formula	C30H23ClN2O2S
Molecular weight	511.03 g/mol
Num. heavy atoms	36
Num. arom. heavy atoms	27
Fraction Csp3	0.13
Num. rotatable bonds	4
Num. H-bond acceptors	3
Num. H-bond donors	1
Molar Refractivity	148.90
TPSA	93.45 Å²
Lipophilicity	
Log <i>P</i> _{ov} (LOGP)	4.55
Log <i>P</i> _{ov} (XLOGP3)	8.47
Log <i>P</i> _{ov} (WLOGP)	7.60
Log <i>P</i> _{ov} (MLOGP)	4.68
Log <i>P</i> _{ov} (SILICOS-IT)	8.46
Consensus Log <i>P</i> _{ov}	6.75

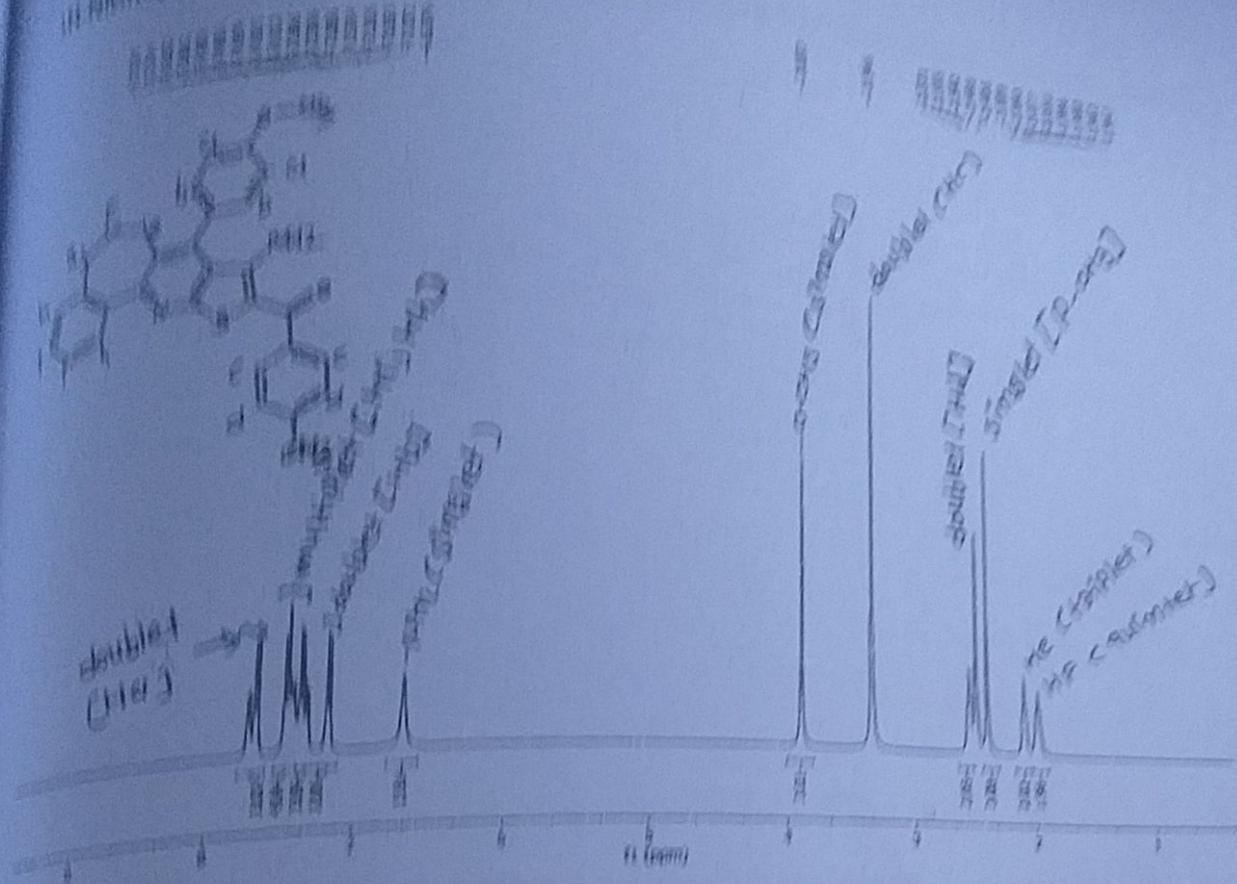
Log S (ESOL)	-8.64
Solubility Class	Poorly soluble
Log S (Aii)	1.18e-09 mg/ml ; 2.31e-09 mol/l
Solubility Class	Insoluble
Log S (SILICOS-IT)	-11.49
Solubility Class	Insoluble
GI absorption	Insoluble
BBB permeant	Low
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C9 inhibitor	Yes
CYP2C19 inhibitor	Yes
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log <i>K</i> _p (skin permeation)	-3.40 cm/s
Drug-likeness	
Lipinski	No; 2 violations: MW>500, MLOGP>4.15
Chose	No; 3 violations: MW>480, WLOGP>5.6, MFF>130
Veber	Yes
Egan	No; 1 violation: WLOGP>5.88
Muegge	No; 1 violation: XLOGP3>5
Bioavailability Score	0.17
Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	0 alert
Synthetic accessibility	No; 2 violations: MW>350, XLOGP3>3.5

2.2.9. (9-Amino-8-(4-methoxyphenyl)-6,7-dihydro-5H-benzo[6,7]cyclohepta[1,2-b]thieno[3,2-e]pyridin-10-yl)(p-tolyl)methanone (5g).

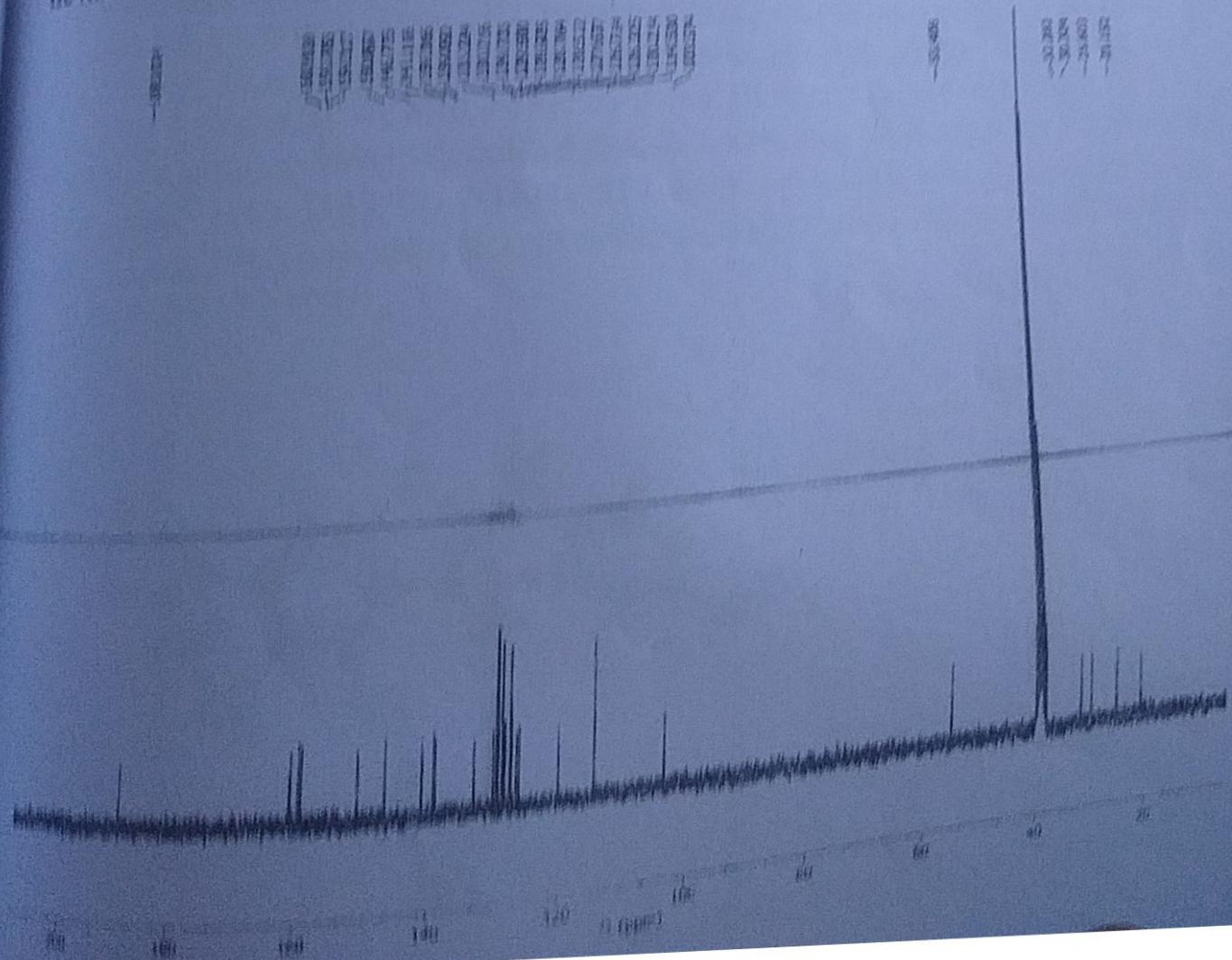
Yellow solid (dioxane, 89%); m.p. 250-253 °C; IR (u cm⁻¹): 3444, 3227 (NH₂), 1631 (CO); ¹H-NMR (DMSO-d₆): δ 1.98 (quint, *J* = 6.4 Hz, 2H, CH₂), 2.09 (t, *J* = 6.4 Hz, 2H, CH₂), 2.40 (s, 3H, *p*-CH₃), 2.55 (t, *J* = 6.4 Hz, 2H, CH₂), 3.89 (s, 3H, *p*-OCH₃), 6.67 (br s, 2H, NH₂), 7.18 (d, *J* = 8.4 Hz, 2H, ArH), 7.32 (d, *J* = 6.4 Hz, 1H, ArH), 7.36 (d, *J* = 8.0 Hz, 2H, ArH), 7.41-7.43 (m, 2H, ArH), 7.46 (d, *J* = 8.4 Hz, 2H, ArH), 7.67 (d, *J* = 8.4 Hz, 2H, ArH), 7.72 (d, *J* = 6.4 Hz, 1H, ArH); ¹³C-NMR (DMSO-d₆): δ 21.1, 25.6, 30.3, 32.2, 55.4, 103.5, 114.5, 120.2, 126.3, 126.7, 127.6, 128.5, 128.7, 128.9, 129.5, 129.7, 130.2, 133.2, 139.0, 139.3, 141.1, 146.7, 150.8, 159.3, 159.7, 160.9, 188.8; Anal. calcd for C₃₁H₂₆N₂O₂S (490.6): C, 75.89; H, 5.34; N, 5.71; found: C, 75.80; H, 5.47; N, 5.92%.



¹H NMR spectrum of compound 5g (DMSO-d₆ 400 MHz)



¹³C NMR spectrum of compound 5g (DMSO-d₆ 100 MHz)



Molecule 4

Log S (S.A.)
 Solubility
 Class

Log S (A)
 Solubility
 Class

Log S (S.LICOS-IT)
 Solubility
 Class

Water Solubility
 4.87
 5.66e-07 mg/ml 1.0e-09 mol/L
 6.00e-07 mg/ml
 10.50
 1.45e-02 mg/ml 2.25e-04 mol/L
 Insoluble
 10.77
 0.27e-02 mg/ml 3.85e-02 mol/L
 Insoluble

Pharmacokinetics
 GI absorption: Low
 BBB penetration: No
 P-gp substrate: Yes
 CYP1A2 inhibitor: Yes
 CYP2C19 inhibitor: No
 CYP2C8 inhibitor: No
 CYP2D6 inhibitor: No
 CYP3A4 inhibitor: No
 Leo K_p (skin permeability): 3.02 cm/s

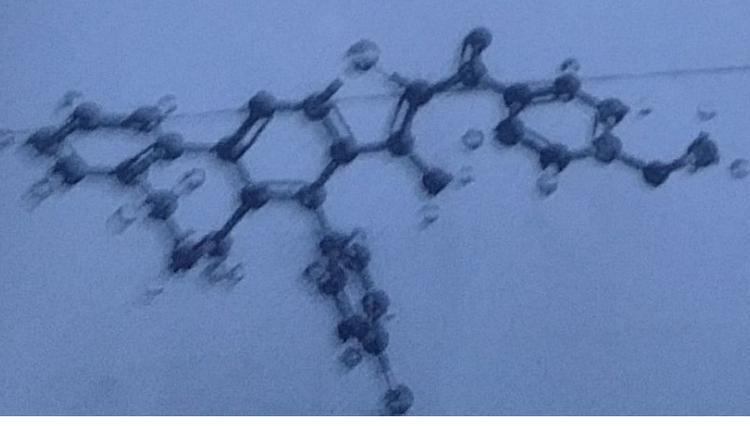
Drugbank
 Yes 1 molecule: WL0001415
 No 2 molecules: MW-480, WL0001415
 681-120
 Yes
 No 1 molecule: WL0001415
 No 1 molecule: WL0001415
 0.55

Molecular Chemistry
 0.000
 0.000
 No 2 molecules: MW-480, WL0001415
 0.80

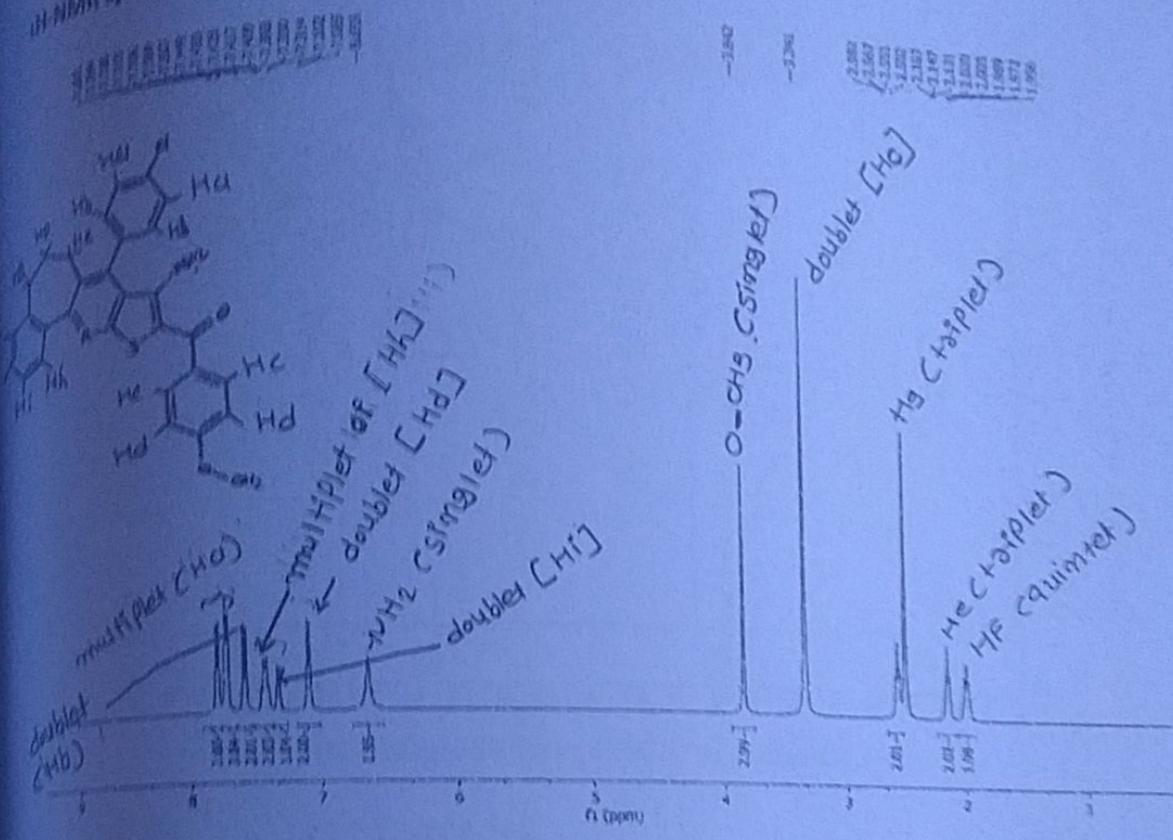
Pharmacological Properties

Weight	323.42
Molar Weight	323.42
Topological Polar Surface Area	49.50
Hydrogen Bond Donor Count	2
Hydrogen Bond Acceptor Count	2
Rotatable Bond Count	0
TPSA	49.50
QED	0.27
Rule of Five	Yes
Rule of Three	Yes
Rule of Two	Yes
Rule of One	Yes

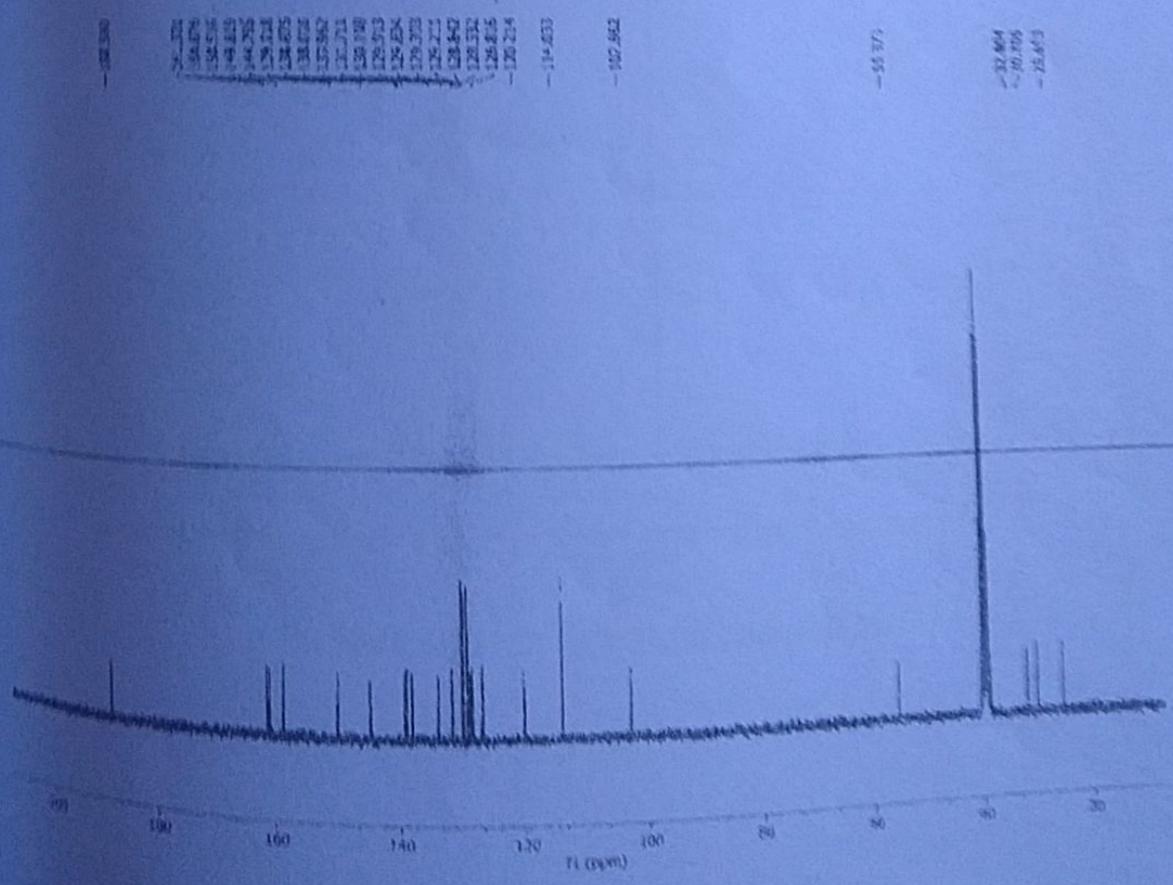
2,2,6,6-Tetramethylpiperidine-1-oxyl-4-(4-chlorophenyl)-6,7-dihydro-5H-benzo[6,7]cyclohepta[1,2-b]thieno[3,2-c]pyridin-10-yl(4-methoxyphenyl)methanone (5d).
 yellow solid (dioxane, 90%); m.p. 212-213 °C; IR (u cm⁻¹): 3423, 3237 (NH₂), 1629 (CO); ¹H-NMR (DMSO-d₆): δ 1.98 (quint, J = 6.4 Hz, 2H, CH₂), 2.56 (t, J = 6.4 Hz, 2H, CH₂), 3.84 (s, 3H, p-OCH₃), 6.65 (br s, 2H, NH₂), 7.09 (d, J = 6.8 Hz, 2H, ArH), 7.32 (d, J = 6.4 Hz, 3H, ArH), 7.39-7.44 (m, 2H, ArH), 7.57 (d, J = 8.4 Hz, 2H, ArH), 7.70-7.72 (m, 3H, ArH), 7.79 [d, J = 6.8 Hz, 2H, ArH]; ¹³C-NMR (DMSO-d₆): δ 25.6, 30.2, 32.0, 55.3, 102.8, 114.0, 120.2, 126.8, 128.5, 128.8, 129.2, 129.3, 129.8, 129.9, 130.1, 131.7, 133.9, 138.0, 138.8, 139.1, 144.7, 149.8, 158.5, 160.8, 161.3, 188.5; Anal. calcd for C₃₀H₂₃ClN₂O₂S (511.0): C, 70.51; H, 4.54; N, 5.48; found: C, 70.35; H, 4.42; N, 5.40%



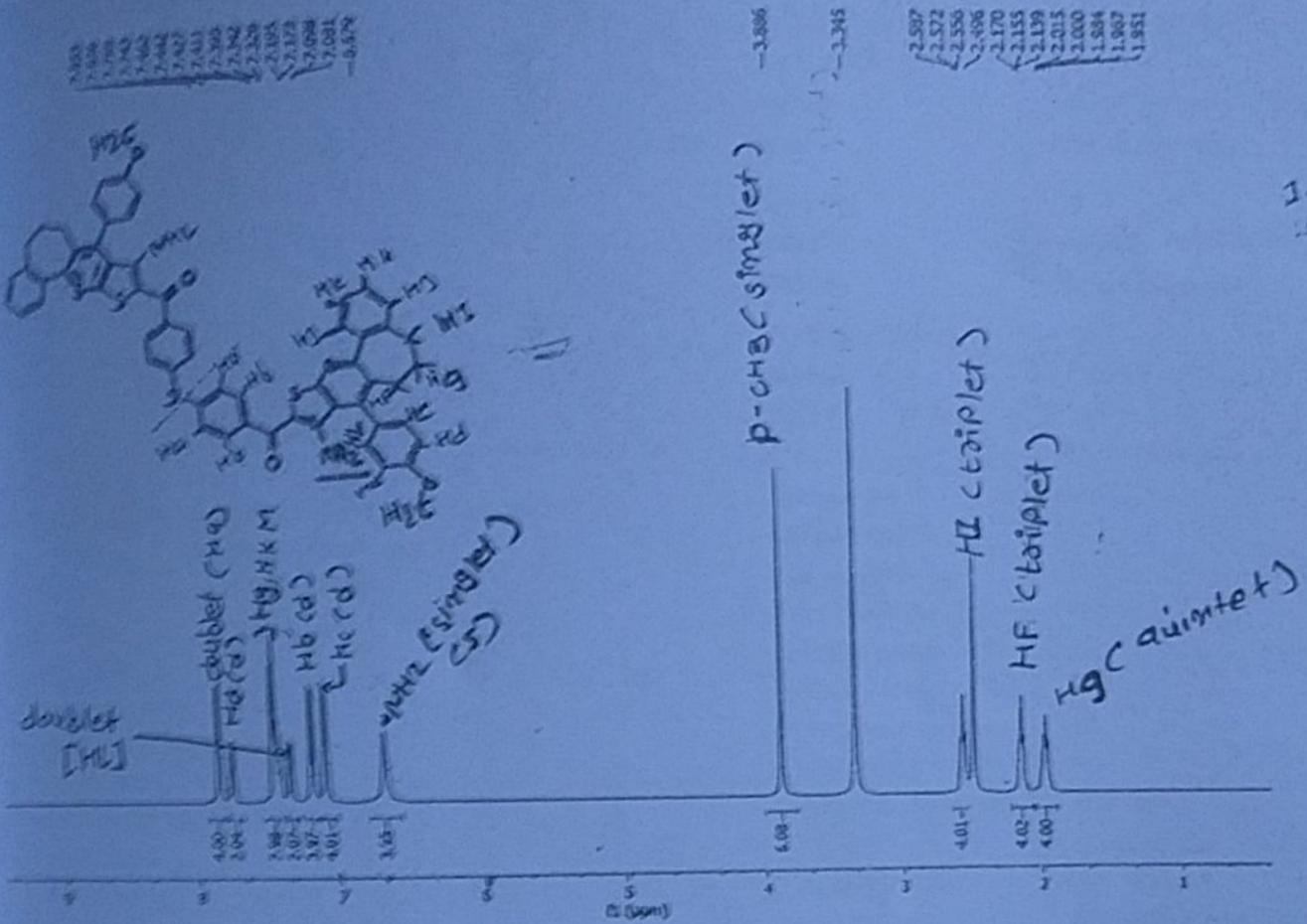
¹H-NMR spectrum of compound 5d (DMSO-d₆ 400 MHz).



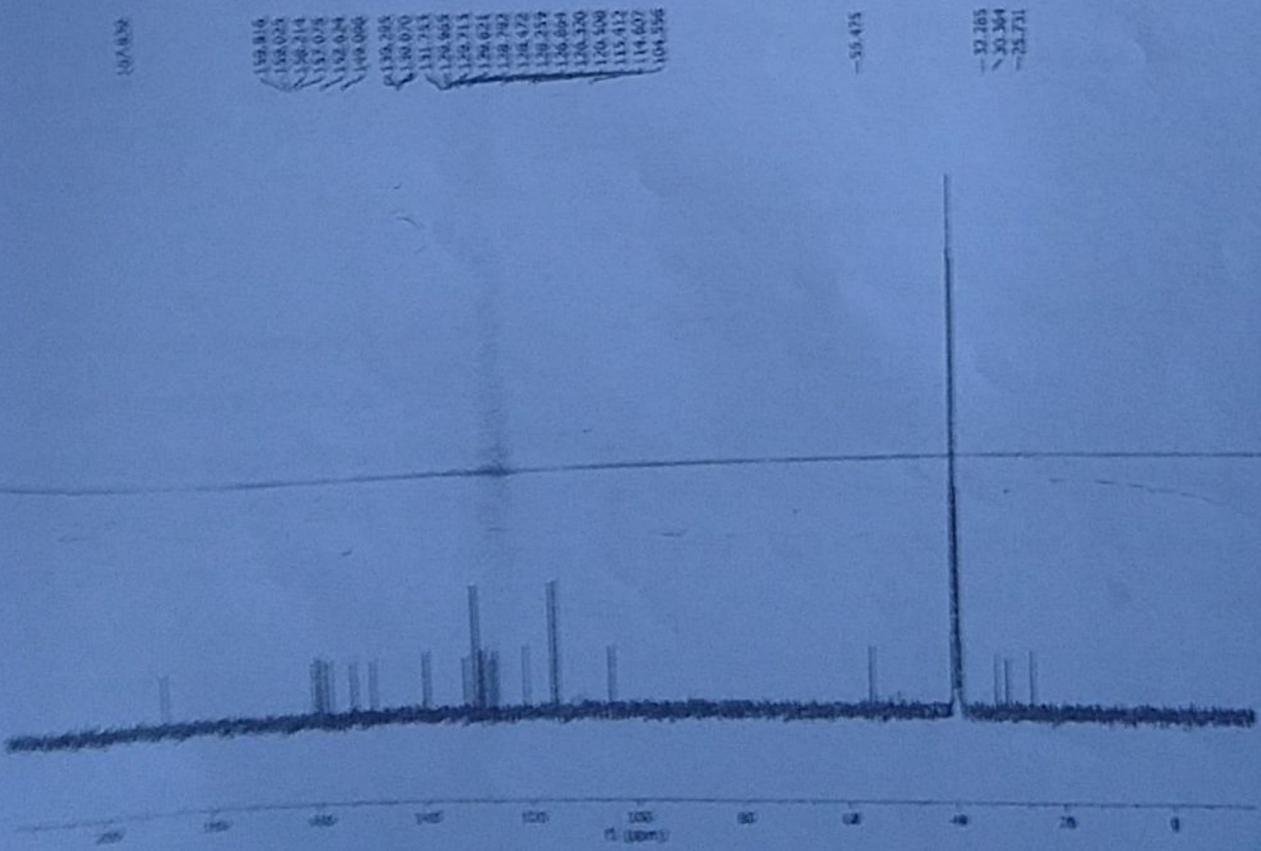
¹³C-NMR spectrum of compound 5d (DMSO-d₆ 100 MHz).



¹H-NMR spectrum of compound 8b (DMSO-d₆ 400 MHz).

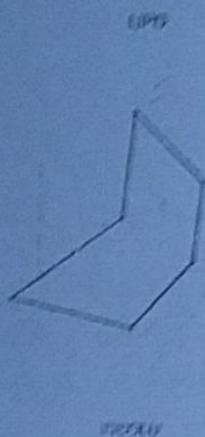
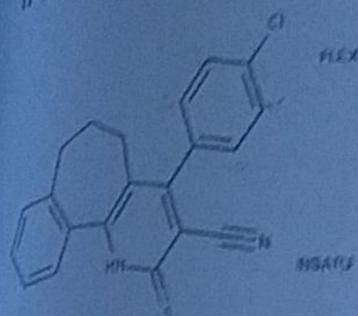


¹³C-NMR spectrum of compound 8b (DMSO-d₆ 100 MHz).



Molecule 1

II O O O



SMILES: NOc1c(=S)[nH]c2c1c1ccc(cc1)Cl/C/C=C/c1ccccc1

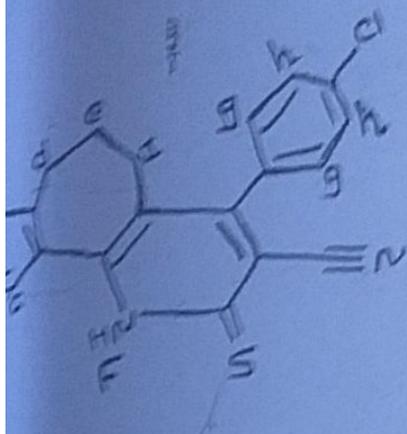
Physicochemical Properties

Formula	C ₂₁ H ₁₅ ClN ₂ S
Molecular weight	352.88 g/mol
Num. heavy atoms	25
Num. atom. heavy atoms	18
Fraction Csp ³	0.14
Num. rotatable bonds	1
Num. H-bond acceptors	1
Num. H-bond donors	1
Molar Refractivity	104.85
TPSA	71.67 Å ²
Lipophilicity	
Log P _{ow} (ILOGP) [⊕]	3.23
Log P _{ow} (XLOGP3) [⊕]	4.56
Log P _{ow} (MLOGP) [⊕]	6.09
Log P _{ow} (ALOGP) [⊕]	3.80
Log P _{ow} (SILICOS-IT) [⊕]	7.64
Consensus Log P _{ow}	5.06

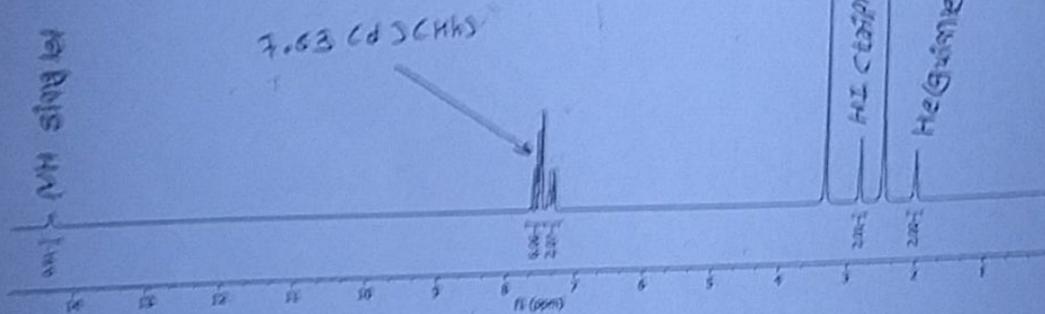
SIZE	Log S (ESOL) [⊕]	-5.40
	Solubility	1.36e-03 mg/ml, 2.72e-06 r
POLAR	Class [⊕]	Moderately soluble
	Log S (All) [⊕]	-5.79
POLAR	Solubility	5.41e-04 mg/ml, 1.08e-06 r
	Class [⊕]	Moderately soluble
POLAR	Log S (SILICOS-IT) [⊕]	-8.65
	Solubility	8.07e-07 mg/ml, 2.20e-06 r
POLAR	Class [⊕]	Fairly soluble
	Pharmacokinetics	
GI absorption [⊕]	High	
BBB permeant [⊕]	No	
P-gp substrate [⊕]	Yes	
CYP1A2 inhibitor [⊕]	Yes	
CYP2C19 inhibitor [⊕]	Yes	
CYP2C9 inhibitor [⊕]	Yes	
CYP2D6 inhibitor [⊕]	No	
CYP3A4 inhibitor [⊕]	Yes	
Log K _p (skin permeation) [⊕]	-5.28 cm/s	
Druglikeness		
Lipinski [⊕]	Yes (Violation)	
Ghose [⊕]	No (Violation: MWLOGP>5)	
Veber [⊕]	Yes	
Egan [⊕]	No (Violation: MWLOGP>5)	
Muegge [⊕]	Yes	
Bioavailability Score [⊕]	0.55	
Medicinal Chemistry		
PRING [⊕]	0 alert	
Brenk [⊕]	1 alert: thiocarbonyl_group	
Leadlikeness	No (2 violations: MW>350)	
Scaffold recoverability	3.00	

2.1.2. 4-(4-Methoxyphenyl)-2-thioxo-2,5,6,7-tetrahydro-1H-benzo[6,7]cyclohepta[1,2-b]pyridine-3-carbonitrile (3b).

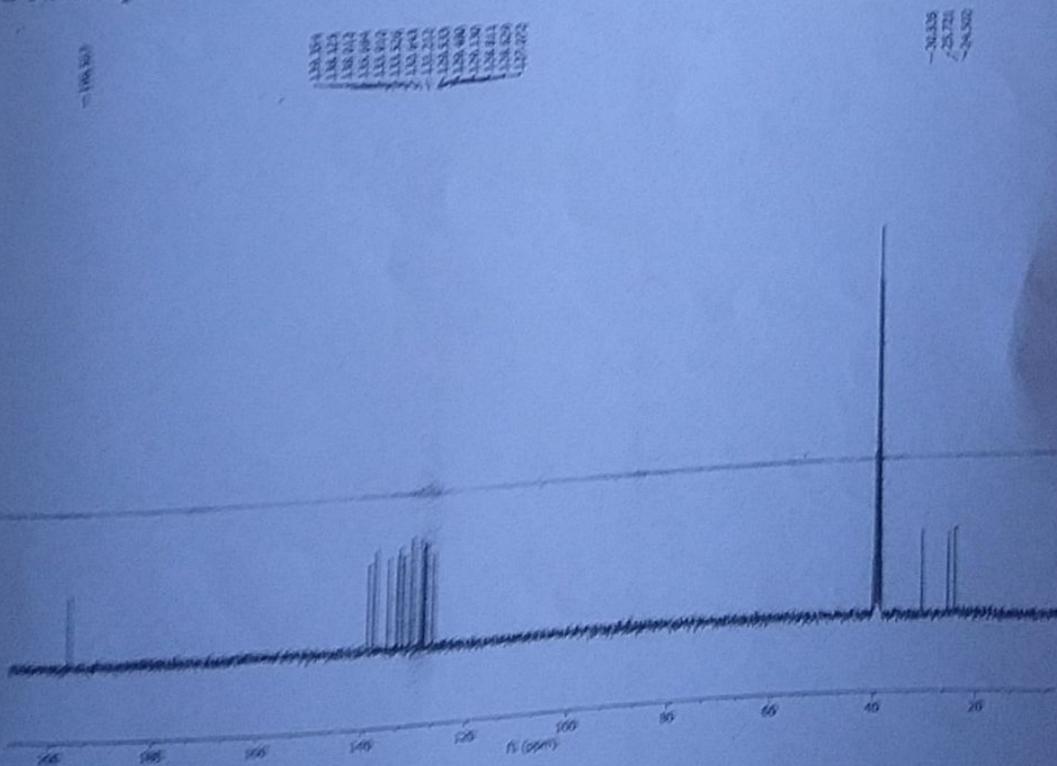
Yellow solid (dioxane / ethanol mixture, 77%); m.p. 230-231 °C; IR (ν cm⁻¹): 3327 (NH), 2211 (CN); ¹H-NMR (DMSO-*d*₆): δ 2.92 (quint, *J* = 6.4 Hz, 2H, CH₂), 2.52 (t, *J* = 6.4 Hz, 2H, CH₂), 2.82 (t, *J* = 6.4 Hz, 2H, CH₂), 3.81 (s, 3H, *p*-OCH₃), 7.04 (d, *J* = 8.4 Hz, 2H, ArH), 7.30 (d, *J* = 6.4 Hz, 1H, ArH), 7.39 (t, *J* = 6.4 Hz, 1H, ArH), 7.50-7.56 (m, 3H, ArH), 7.62 (d, *J* = 6.4 Hz, 1H, ArH), 14.20 (s, 1H, NH); Anal. calcd for C₂₂H₁₉N₂OS (358.4): C, 73.72; H, 5.06; N, 7.82; found: C, 73.57; H, 5.13; N, 7.69%.



7.50-7.53 (m) Hc
 7.58 - (doublet) Hd
 7.40 - (triplet) He



$^{13}\text{C-NMR}$ spectrum of compound 3a (DMSO- d_6 100 MHz).



$^1\text{H-NMR}$ spectrum of compound 3b (DMSO- d_6 400 MHz).