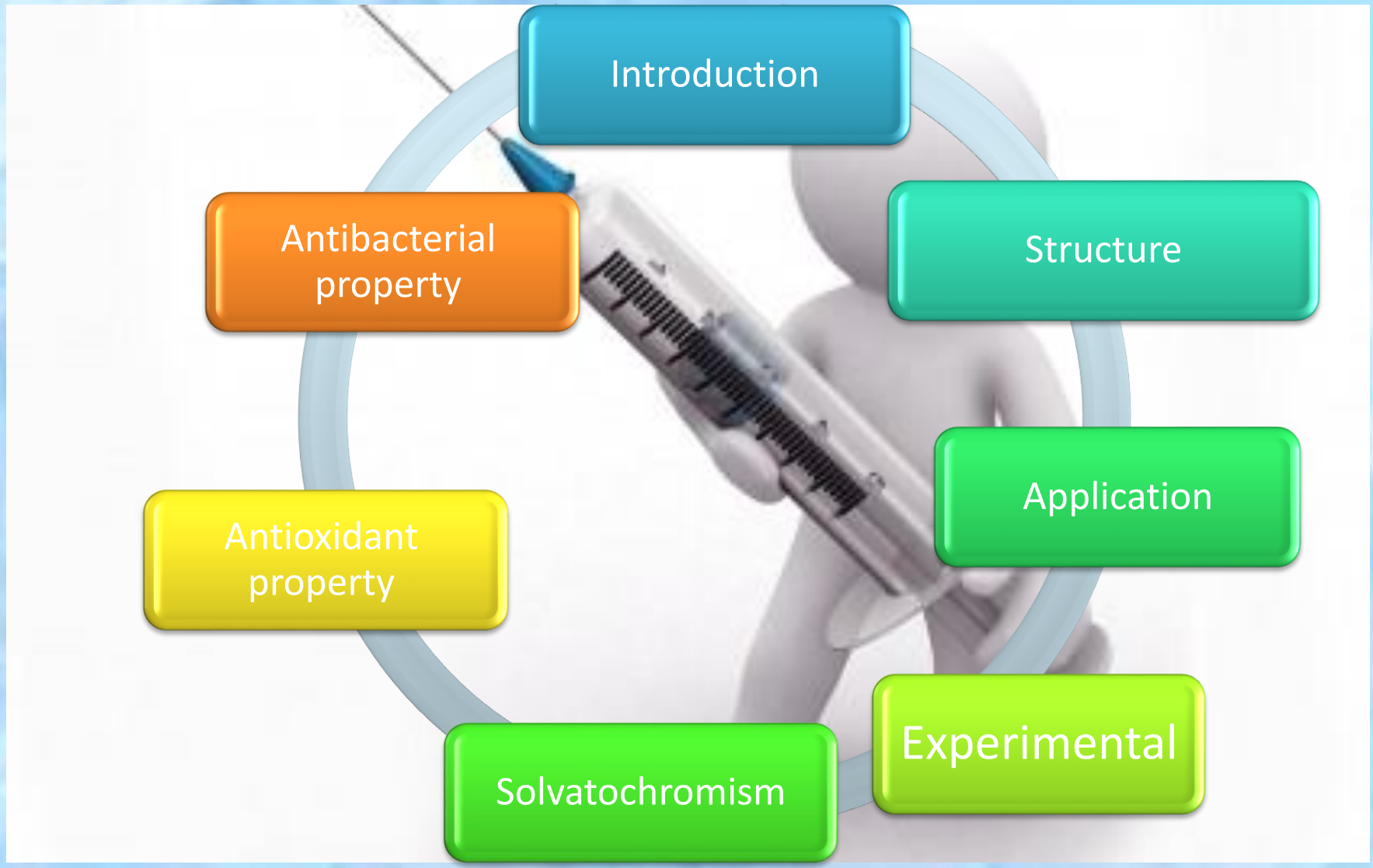

بسم الله الرحمن الرحيم

Title

Antioxidant , Antibacterial and Spectroscopy study of new schiff base 2,2`-(1,2,5-oxadiazole-3,4-diyl) bis (azan-1-yl-1-ylidene) bis (methan -1-yl-1-ylidene) bis (4 -phenyldiazenyl)phenol.

By:Zeinab Saki

Overview


Introduction
Structure
Application
Experimental
Solvatochromism
Antioxidant property
Antibacterial property

Introduction

A **Schiff base** (or **azomethine**), named after Hogo Schiff, is functional group that contains a C=N with the nitrogen atom connected to an aryl or alkyl group.

Y.Hamada, l. Takeuchi, Y. Lta, S. Matsui and T. Ita, Yakugaku Zasslzi, 101, 633(1981): chem.Abstr., 95, 18155;1981

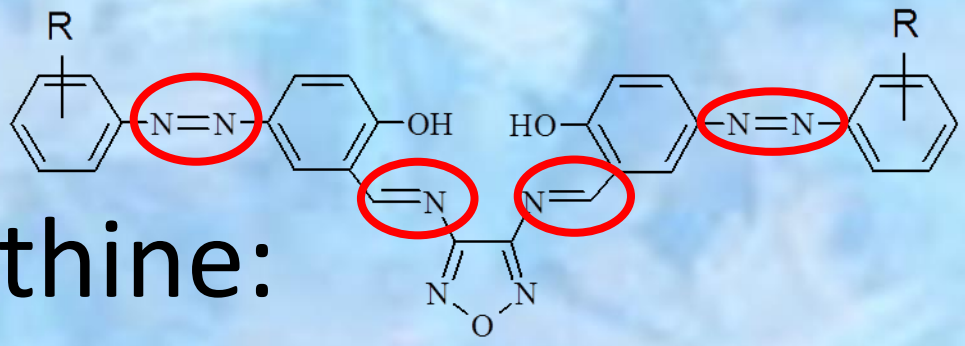
Structure

Azo : 'R-N=N-R

Schiff Base: $R_1R_2C=N-R_3$

Azo

Azomethine:



Applications

Anti Cancer

Anti Corrosion

Anti Microbe

Anti Tumor

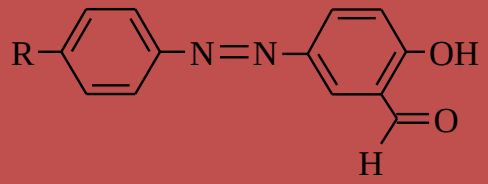
Pesticide

Effect on DNA

Y.Hamada, I. Takeuchi, Y. Lta, S. Matsui and T. Ita, Yakugaku Zasslzi, 101, 633(1981): chem.Abstr., 95, 18155;1981

Experimental

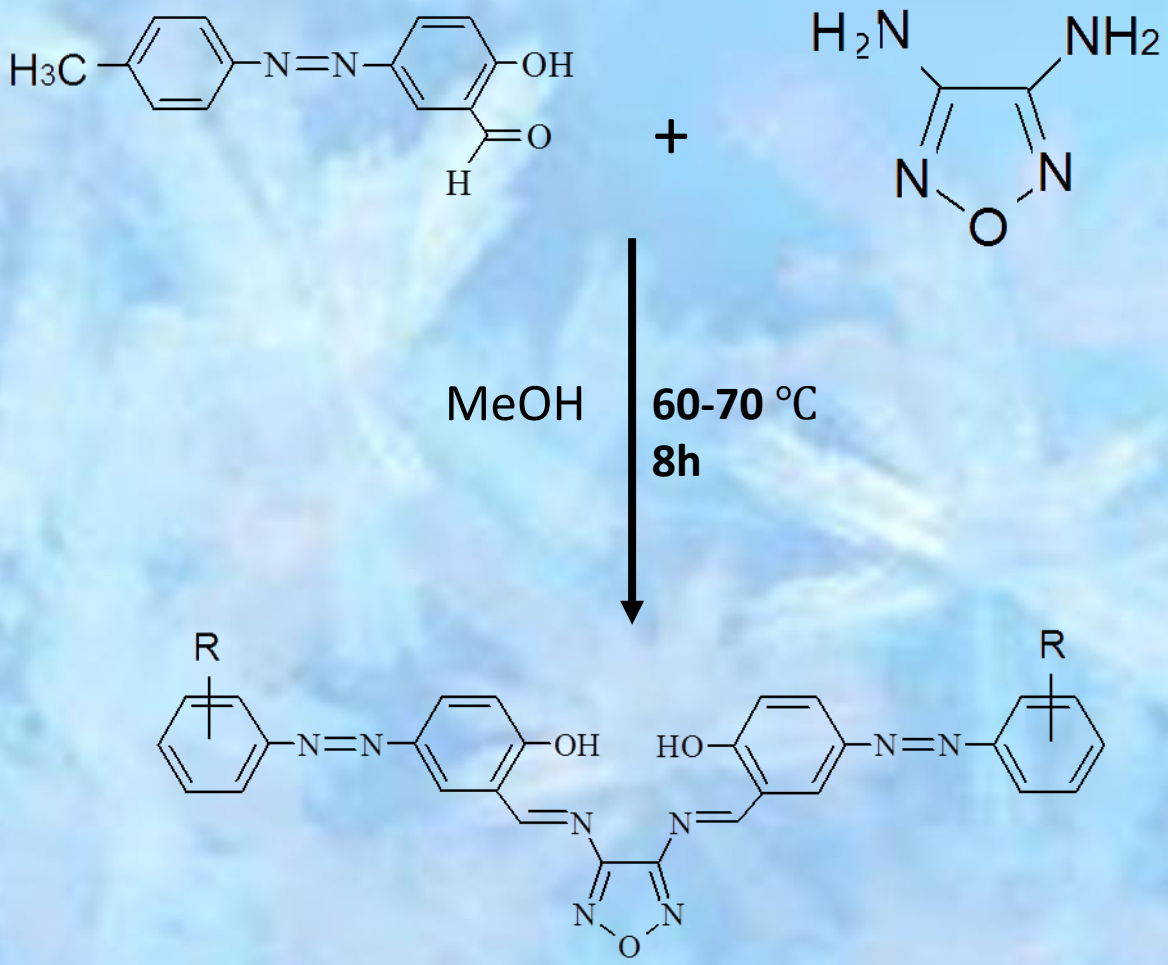
Properties of Reactants



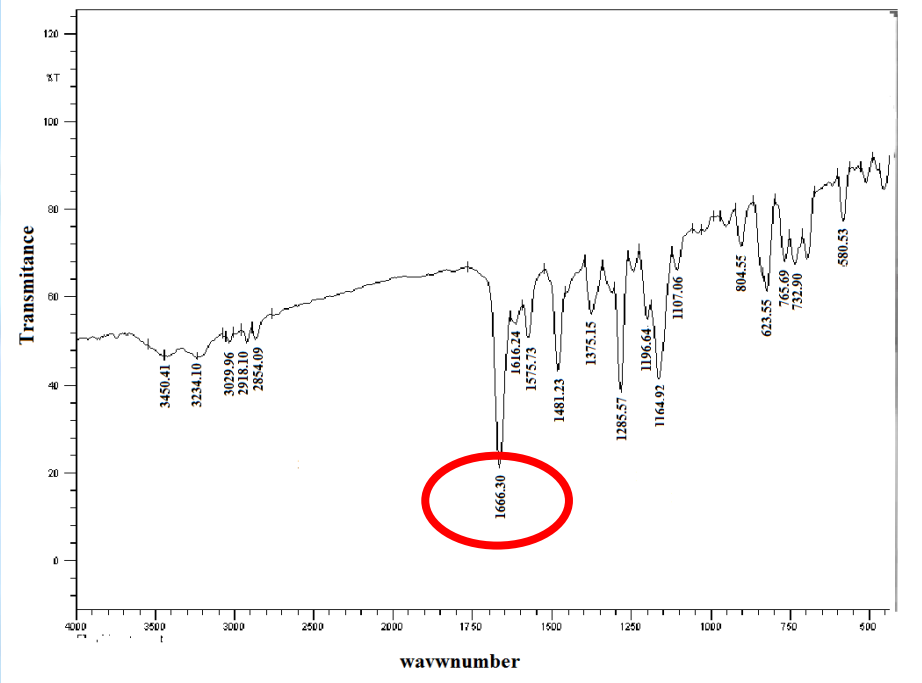
R= **a**= H , **b**= CH_3 , **c**= 3,5 Di-Me, **d**= NO2 ,**e**= Et , **f**=Iso-pro , **g**=O-Me

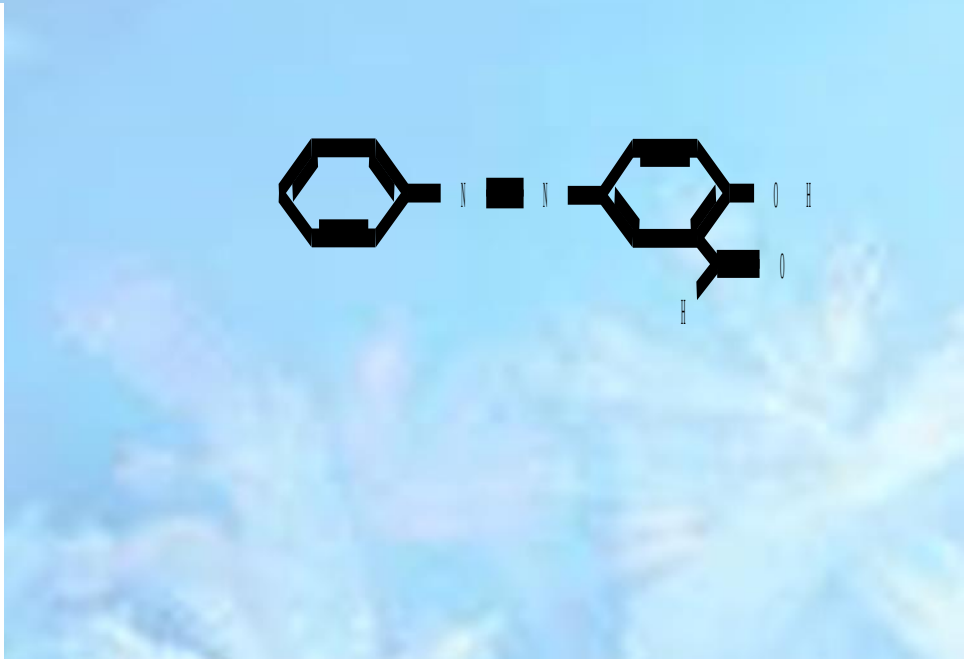
Compound	Color	M.p(°C)	Randman(%)
1a	Brown	123	**55**
1b	Dark brown	134	**44**
1c	Brown	130	**50**
1d	Yellow	185	**93.7**
1e	Brown	125	**60**
1f	Brown	128	**45**
1g	Orange	138	**40**

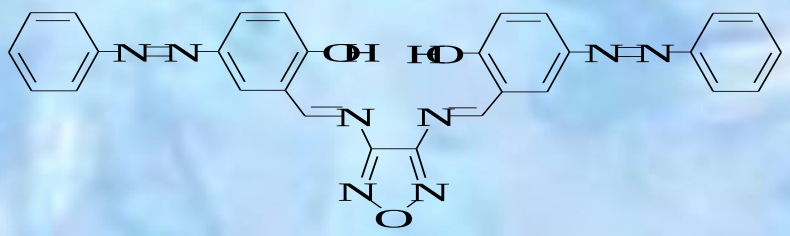
Synthesis of Schiff Base

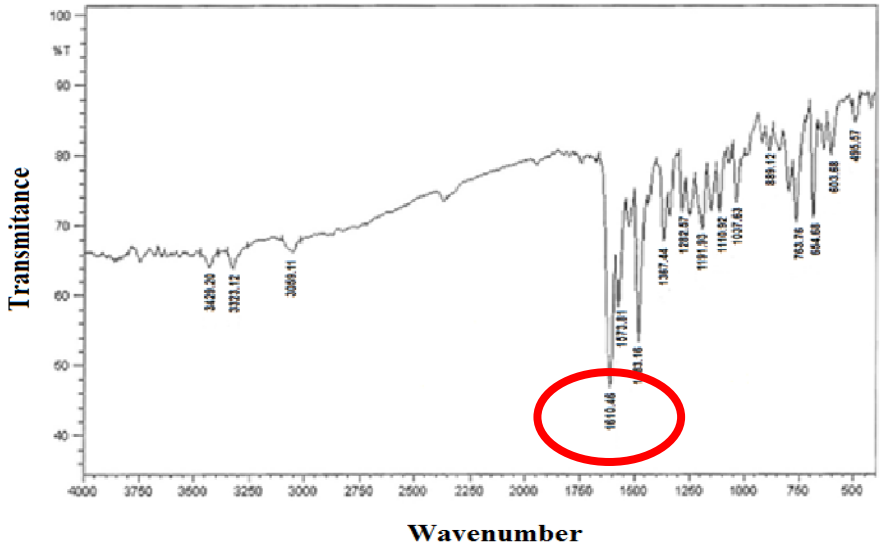


FT-IR spectrum

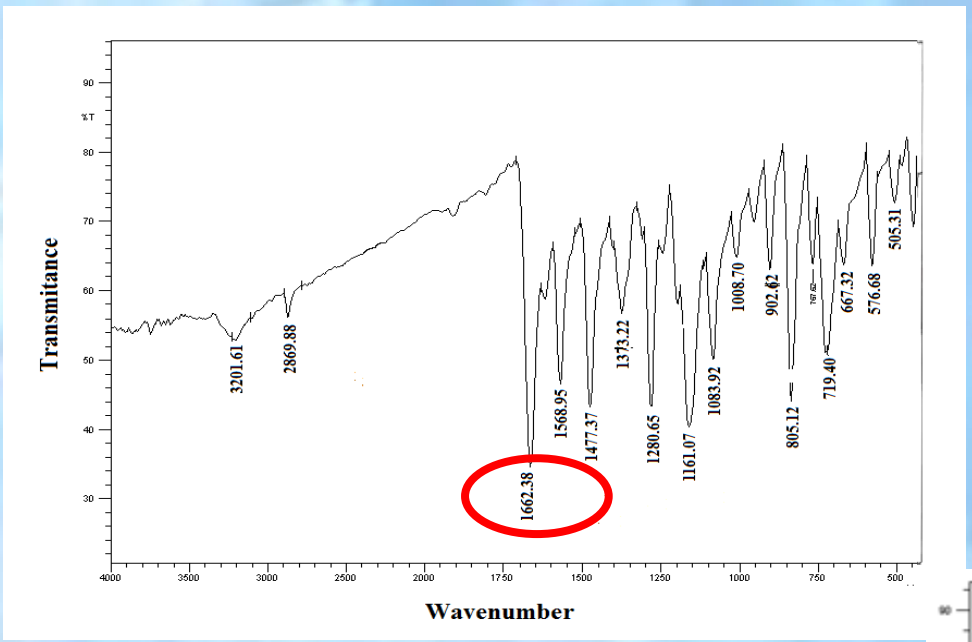


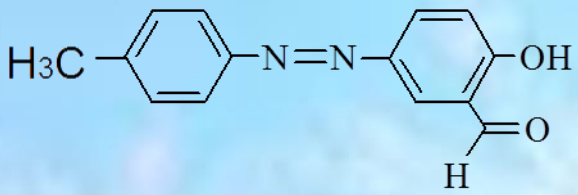


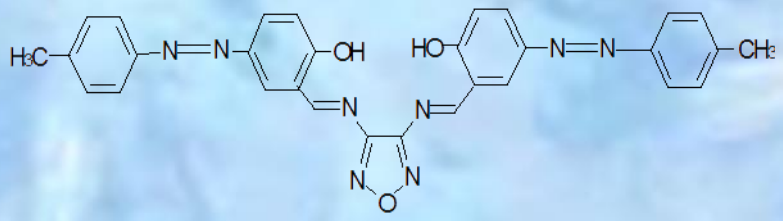


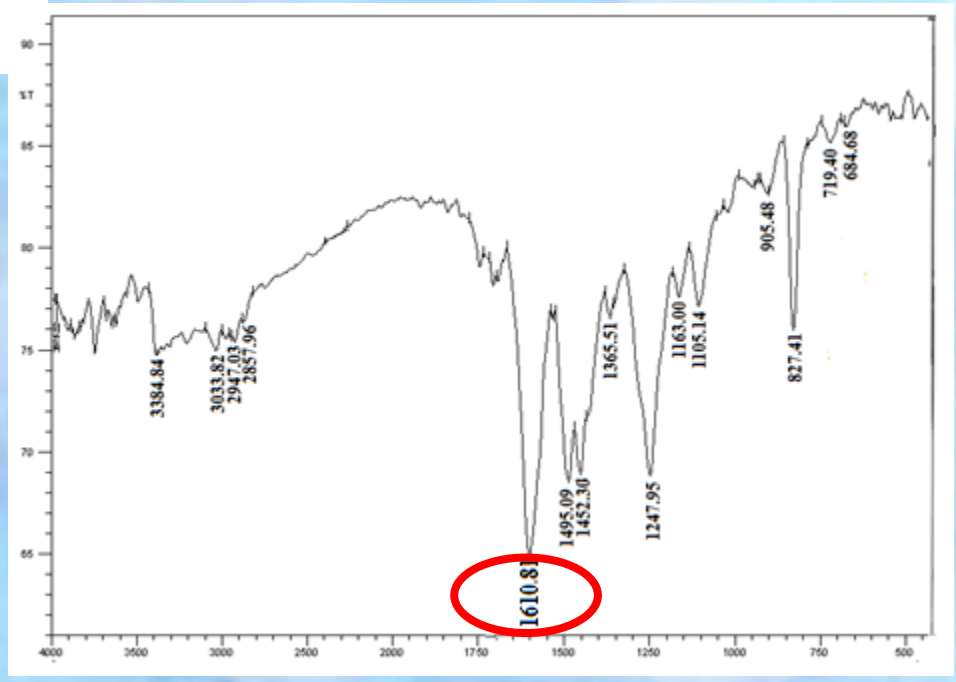


FT-IR spectrum





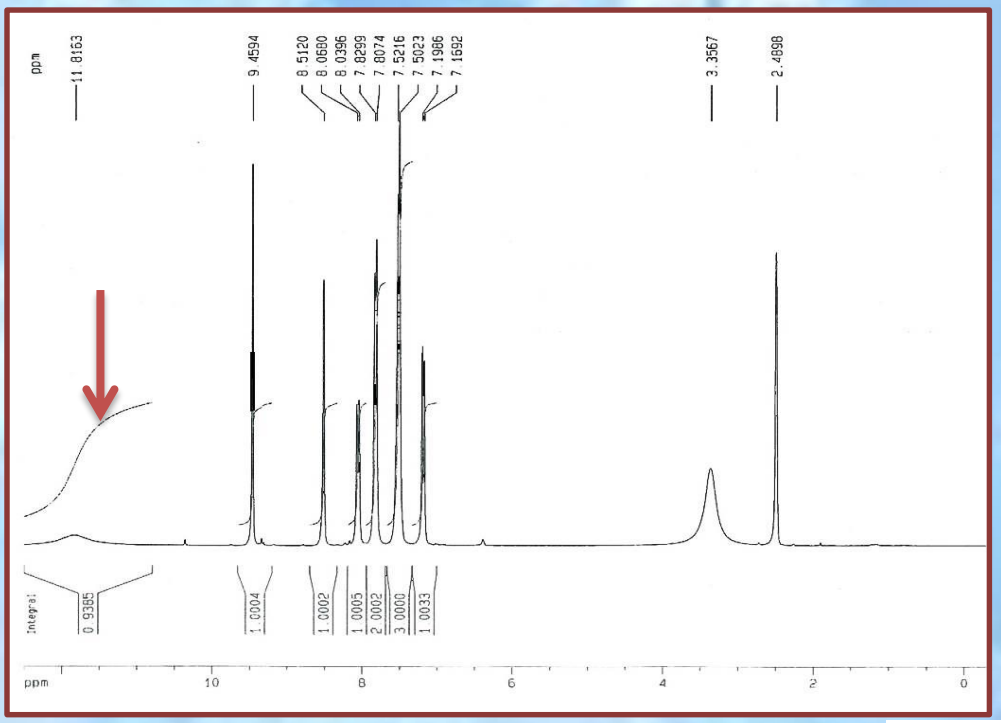




FT-IR

compound	OH	Ar-H	CH=N	C=N	N=N	C=C	C-N	Ar-O	N-O
4a	3429	3068	2910,2826	1610	1573	1483	1284	1110	1037
4b	3442	3033	2947,2857	1600	1575	1485	1296	1163	1018
4c	3442	3058	2918,2852	1610	1581	1483	1280	1143	1033
4d	3417	3099	2925,2854	1635	1521	1481	1288	1149	1037
4e	3465	3039	2958,2869	1604	1521	1479	1280	1153	1045
4f	3460	3035	2964,2871	1606	1525	1481	1284	1153	1037
4g	3461	3035	2939,2840	1654	1583	1473	1278	1147	1033

^1H NMR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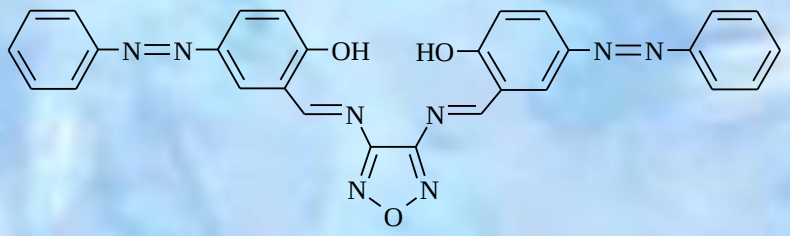
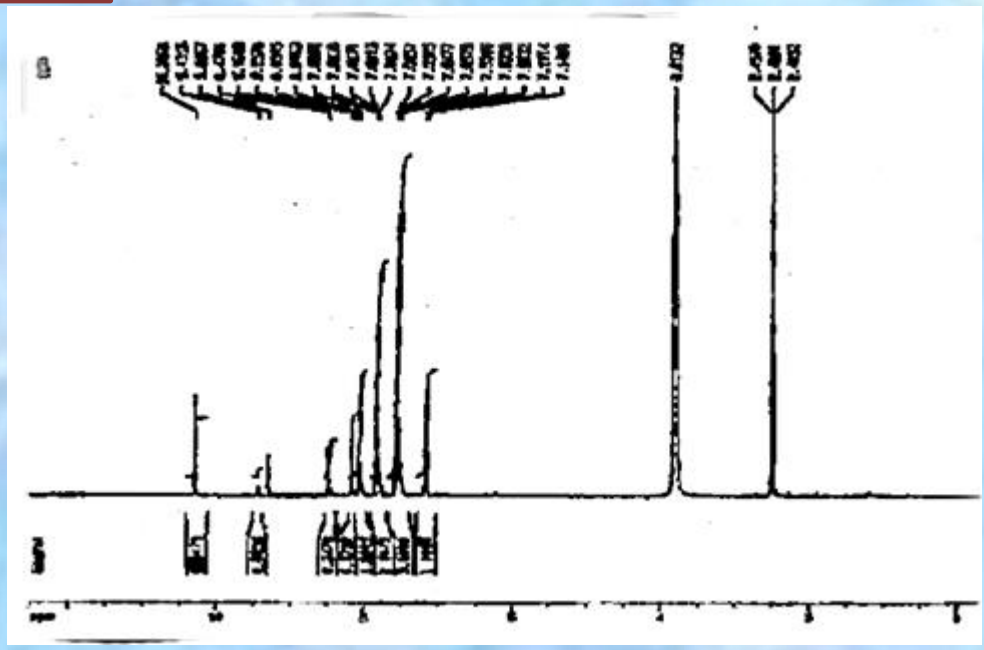
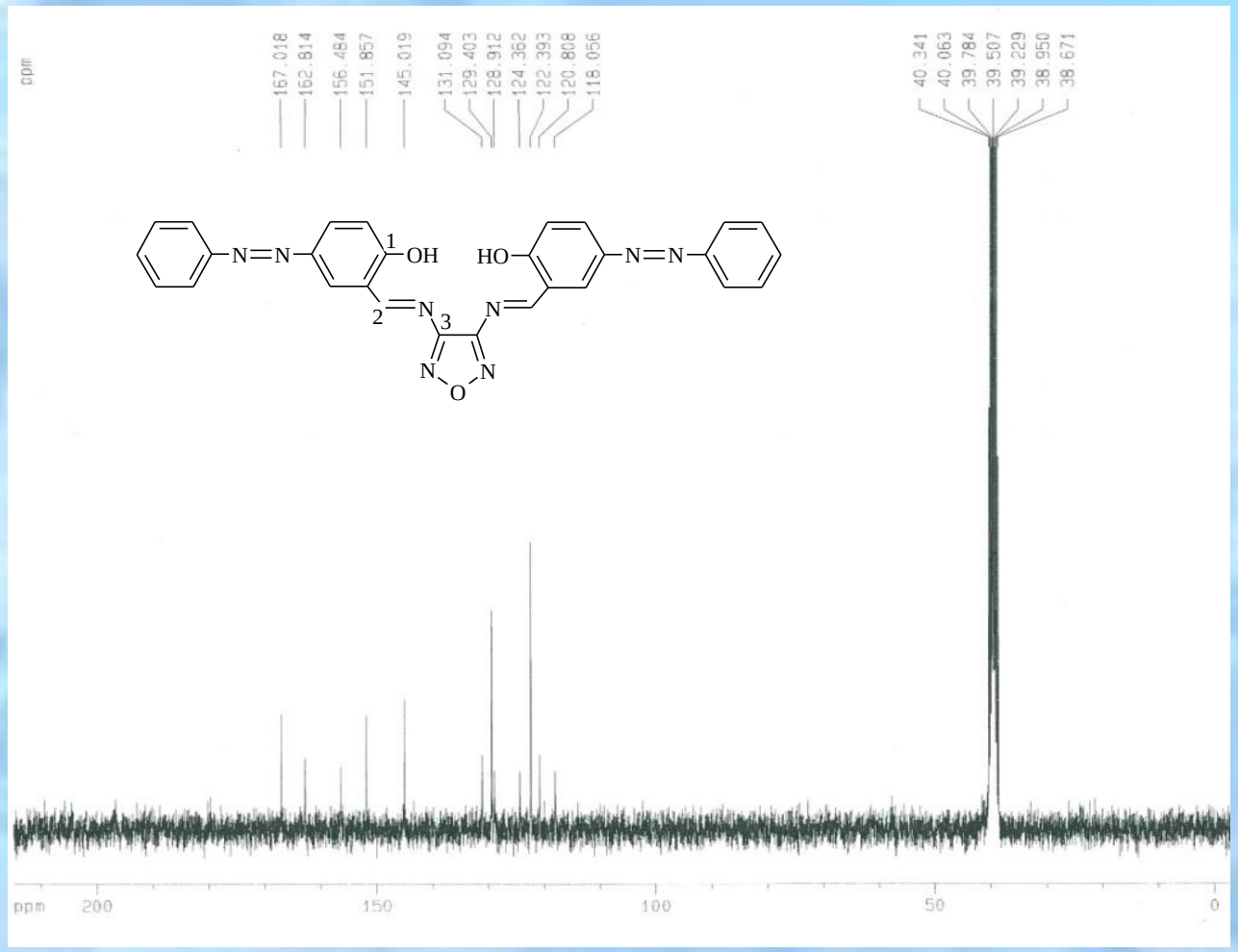
9.4594
8.5120
8.0680
8.0396
7.8299
7.8074
7.5216
7.5023
7.1986
7.1692
3.3567
2.4898
Integral
0.9385
1.0004
1.0002
1.0005
2.0002
3.0000
1.0033
ppm
10
8
6
4
2
0

D_2O


N=N
OH
HO
N=N
N
N
N
N
O



^{13}C NMR


ppm
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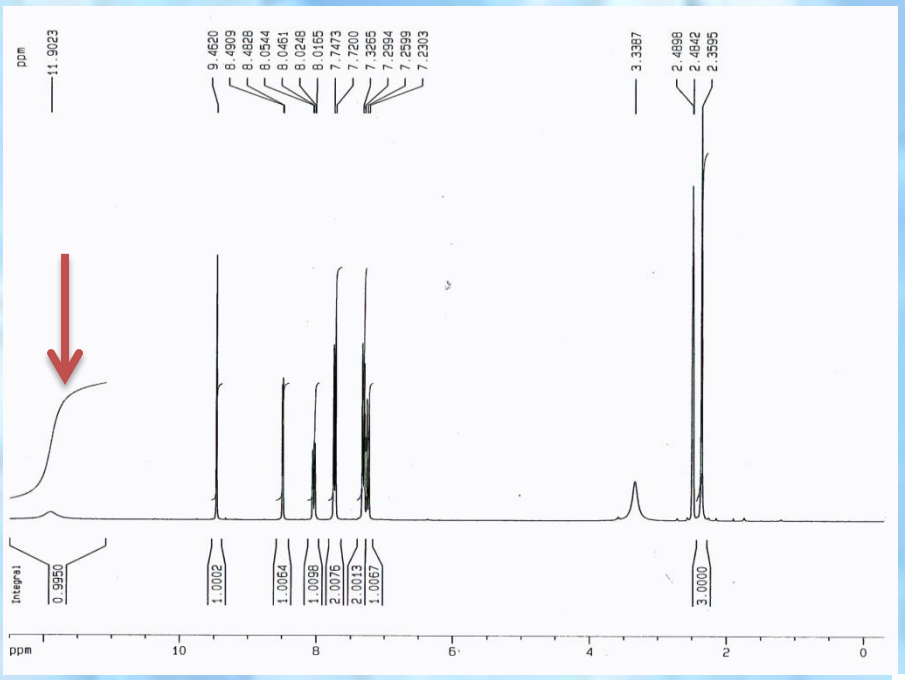
162.814
156.484
151.857
145.019
131.094
129.403
128.912
124.362
122.393
120.808
118.056
40.341
40.063
39.784
39.507
39.229
38.950
38.671
OH
HO
N=N
N
O
1
2
3
ppm
200
150
100
50
0

^1H NMR

D2O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8.0461
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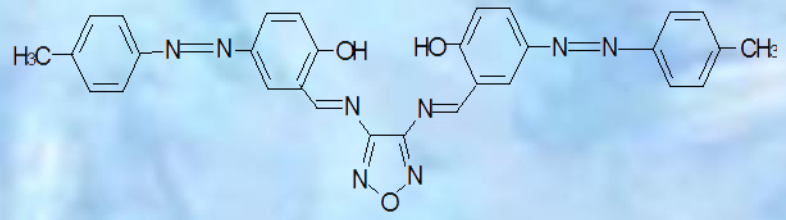
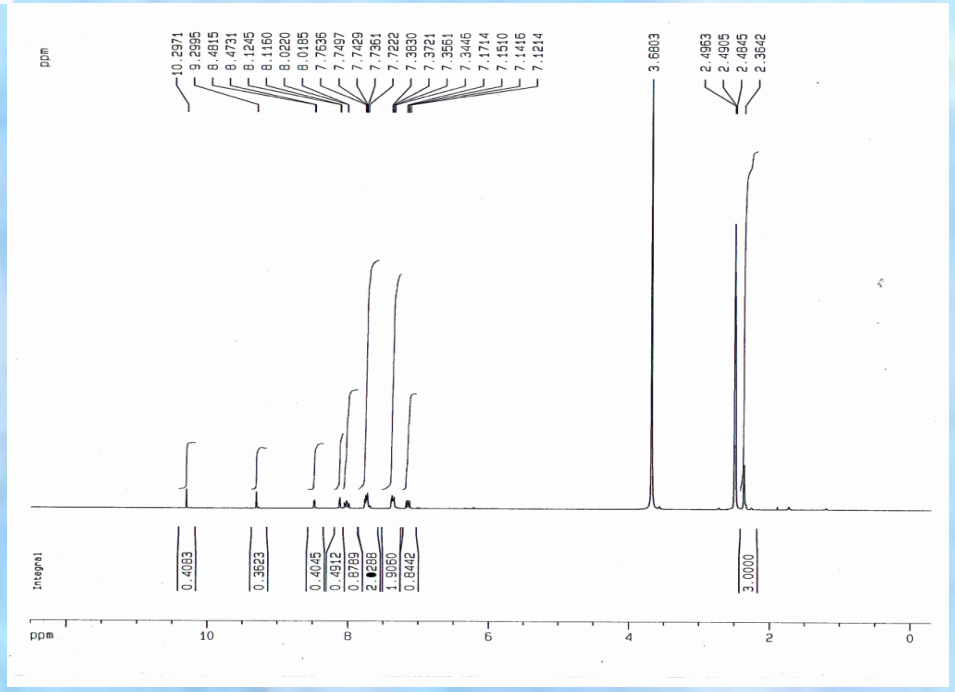
7.3265
7.2994
7.2599
7.2303
3.3387
2.4898
2.4842
2.3595
Integral
0.9950
1.0002
1.0064
1.0098
2.0076
2.0013
1.0067
3.0000
ppm
10
8
6
4
2
0


H3C
N=N
OH
HO
N=N
CH3
N=N
N=N
N
N
O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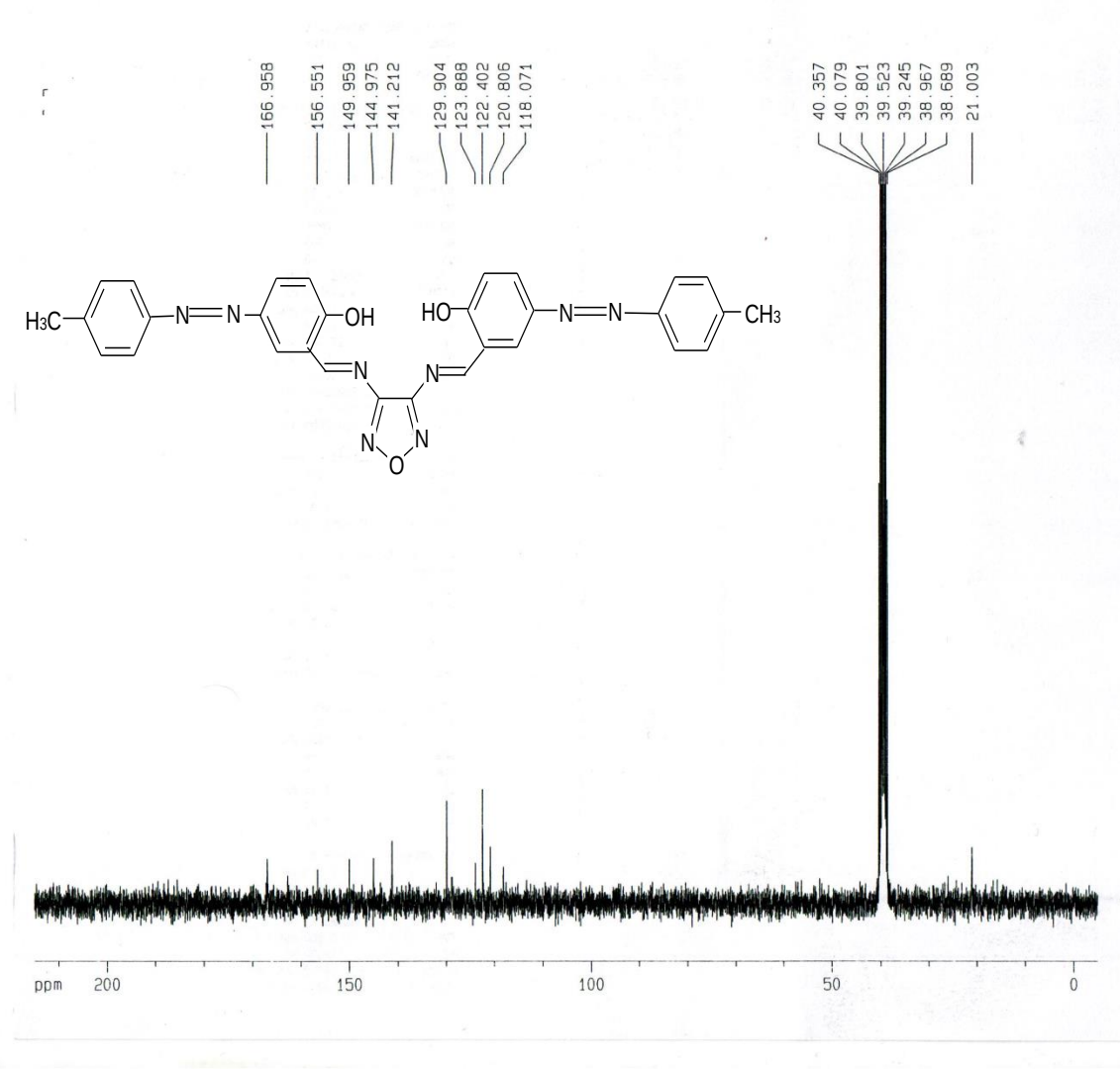
8.4815
8.4731
8.1245
8.1160
8.0220
8.0185
7.7636
7.7497
7.7429
7.7361
7.7222
7.3830
7.3721
7.3561
7.3446
7.1714
7.1510
7.1416
7.1214
3.6803
2.4963
2.4905
2.4845
2.3642
Integral
0.4083
0.3623
0.4045
0.4912
0.8789
2.0288
1.9060
0.8442
3.0000
ppm
10
8
6
4
2
0

^{13}C NMR


166.958
156.551
149.959
144.975
141.212
129.904
123.888
122.402
120.806
118.071
40.357
40.079
39.801
39.523
39.245
38.967
38.689
21.003
H3C
N=N
OH
HO
N=N
CH3
N
N
N
N
O
ppm
200
150
100
50
0

^1H NMR

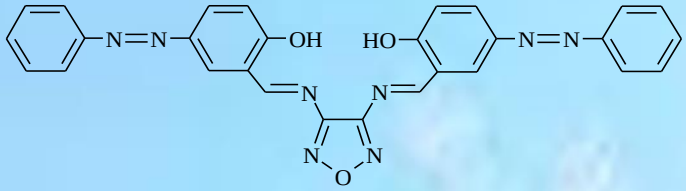
compound	OH	CH=N	Ar-H	R
4a	11.57	10.35	8.19 – 7.17	-
4b	11.82	9.46	8.51 – 7.16	1.68
4c	11.81	9.40	8.02 – 7.09	2.28
4d	11.89	10.58	8.36 -7.22	-
4e	11.87	10.35	8.48-7.18	2.48

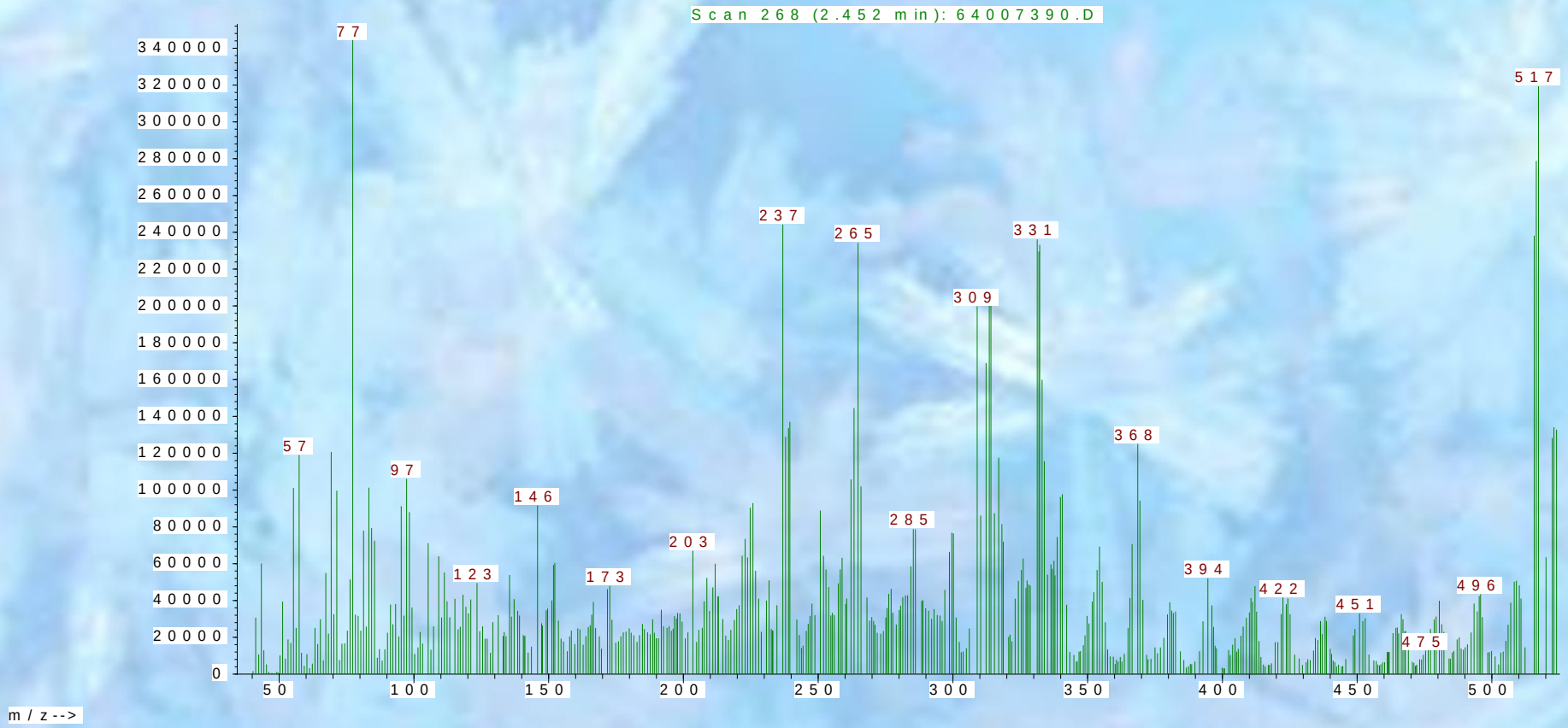
^{13}C NMR

number	C_1	C_2	C_3	Ar	Subs.
4a	167.02	162.81	156.48	151.86, 145.02, 131.128, 124.40, 124.36, 122.39, 120.80, 118.05, 110.91	-
4b	167.00	162.58	156.46	149.02, 145.10, 140.10, 140.62, 131.34, 128.69, 124.30, 122.30, 120.78, 118.00	97.20
4c	167.10	162.75	156.38	152.04, 145.17, 138.63, 132.54, 129.02, 124.32, 120.80, 120.30, 117.03	88.20
4d	167.42	163.80	156.72	152.12, 149.96,143.68, 129.78, 126.79, 124.08, 122.44, 122.08, 117.08	-
4e	167.05	163.80	156.45	151.78, 150.25, 144.88, 128.87, 127.22, 124.05, 122.47, 120.77,118.15	23.64

Mass Spetroscopy

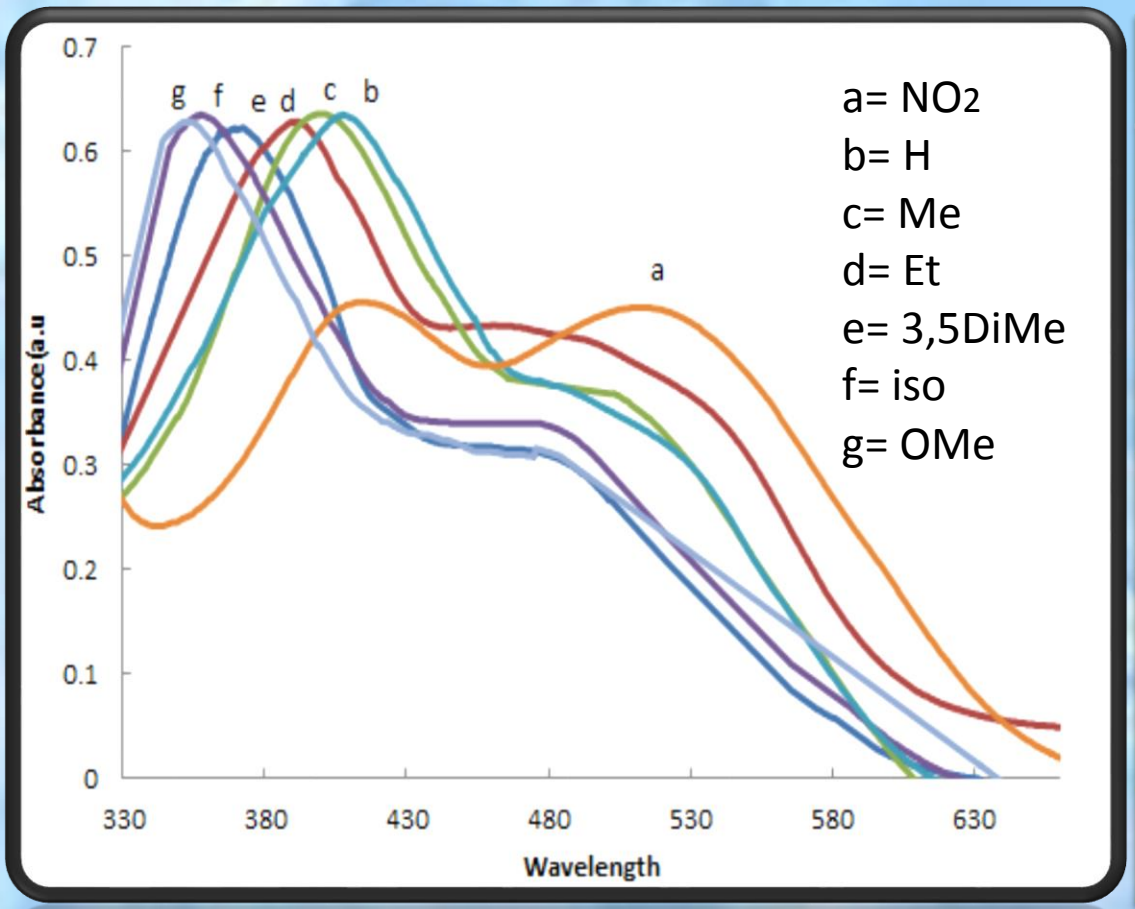
m/Z=516 ⟶ $C_{28}H_{20}N_8O_3$





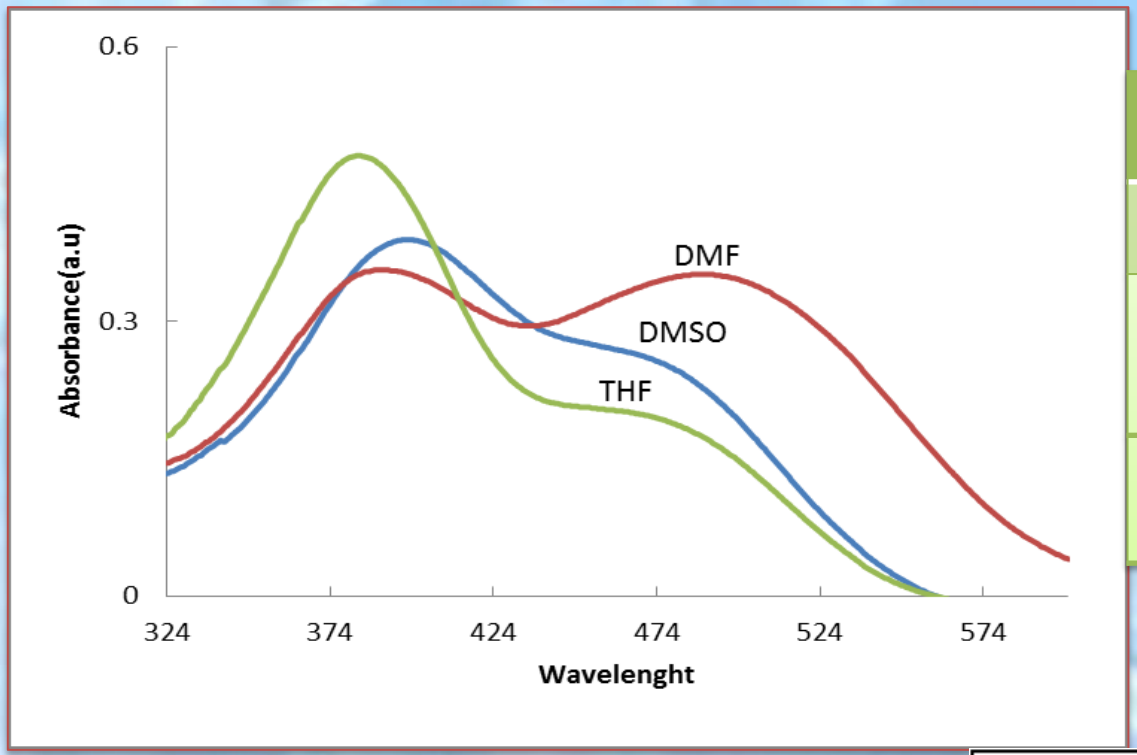

Solvatochromism
1
2
3
4
5
6

Effect of Substition

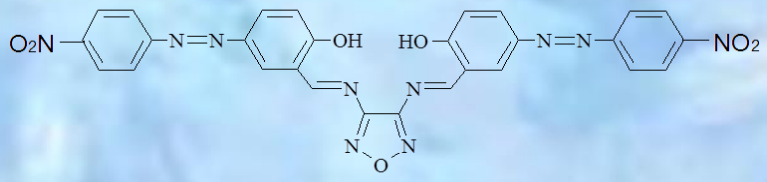


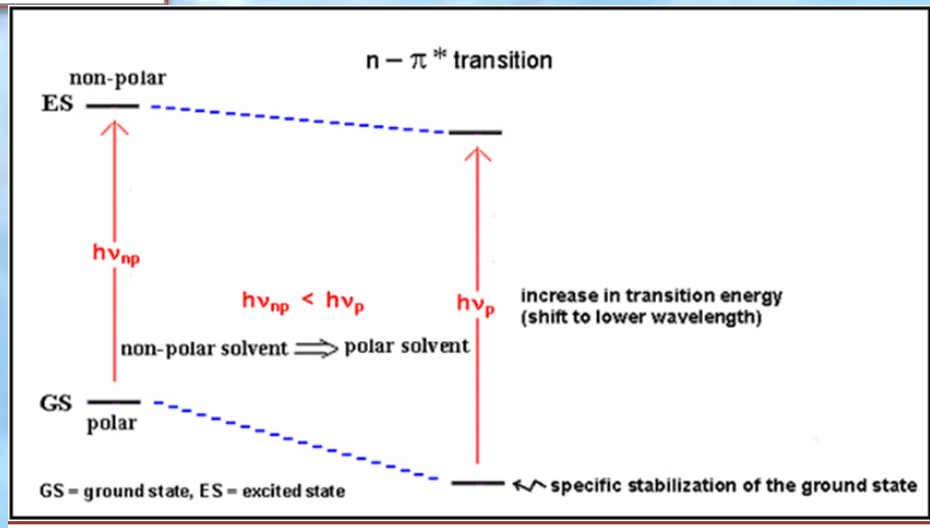
compound	DMF
a	416(A=0.634), 510(A=0.451)
b	398(A=0.634), 498(A= 0.357)
c	372(A=0.623), 490(A=0.350)
d	400(A=0.451), 508(A= 0.401)
e	389(A= 0.629). 485(A=0.334)
f	369(A=0.621), 482(A=0.332)
g	360(A= 0.619), 480(A=0.332)

Effect of Solvent

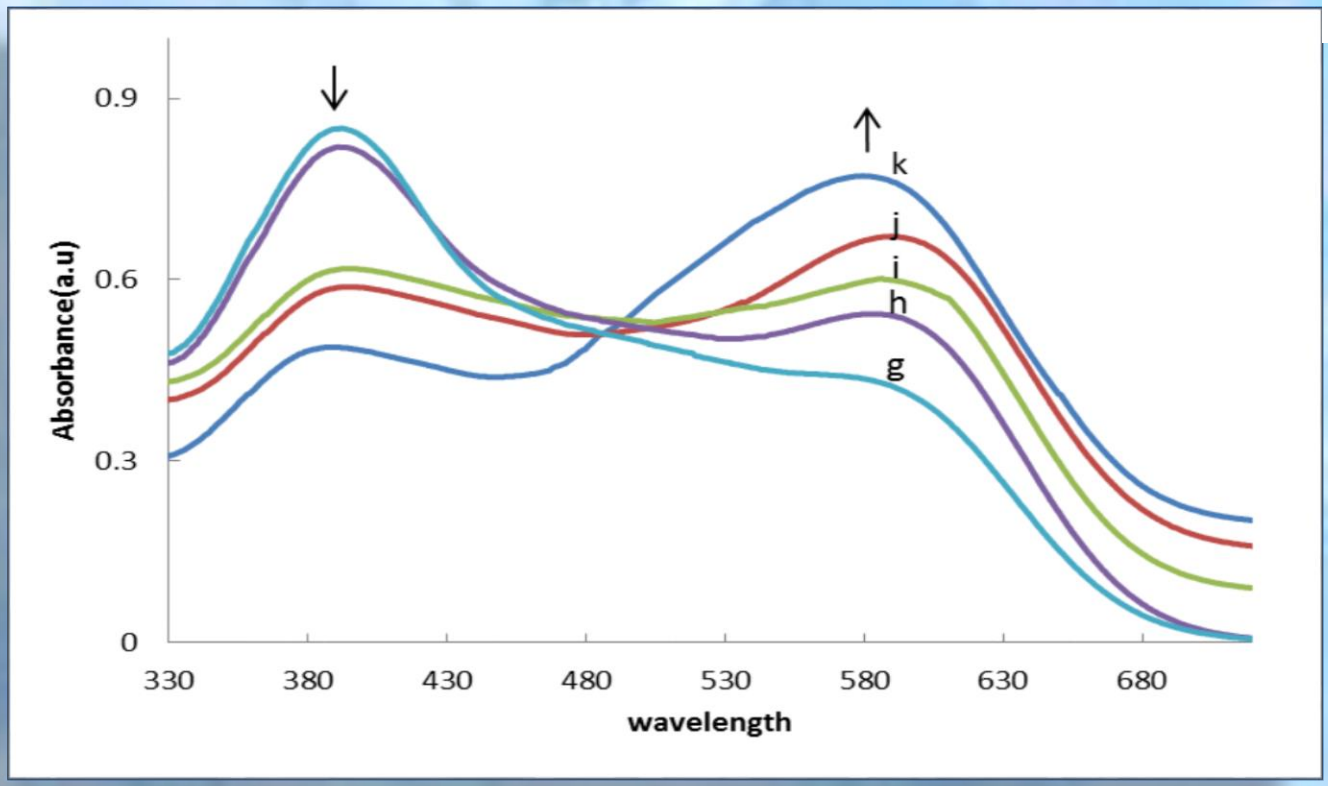


compound	4d
DMF	416(A=0.634), 510(A=0.451)
DMSO	393(A= 0.386) ,477(A=0.252),
THF	382(A=0.481), 466(A=0.200)

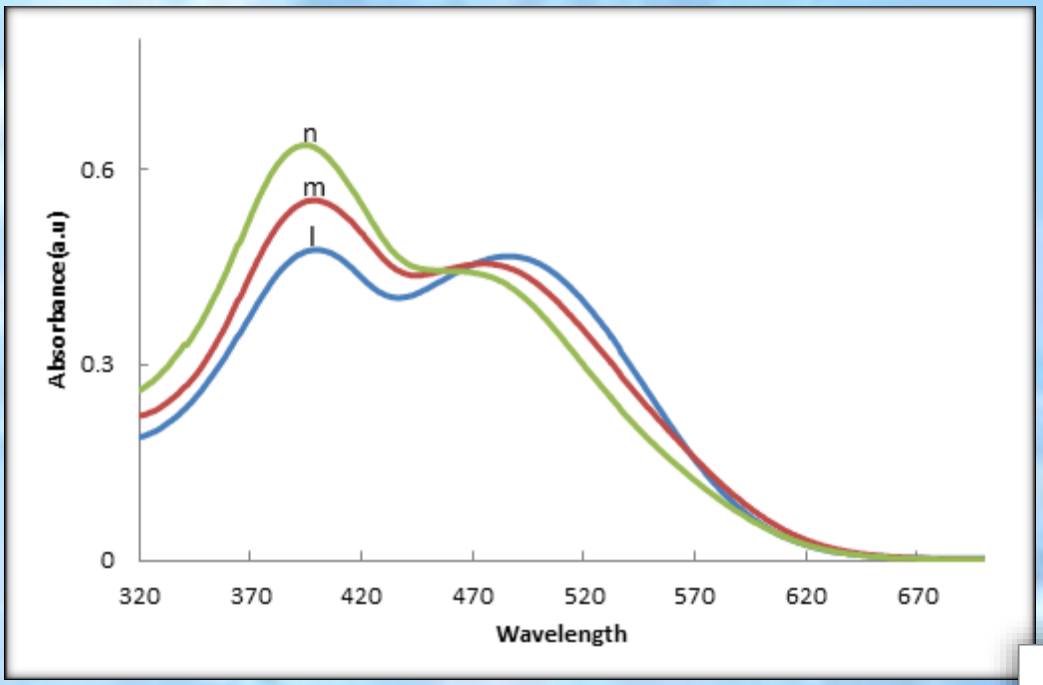


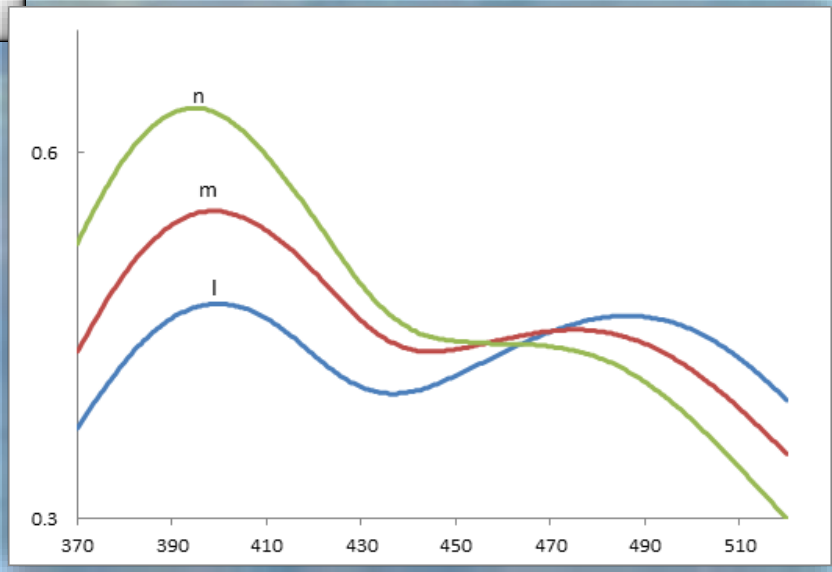


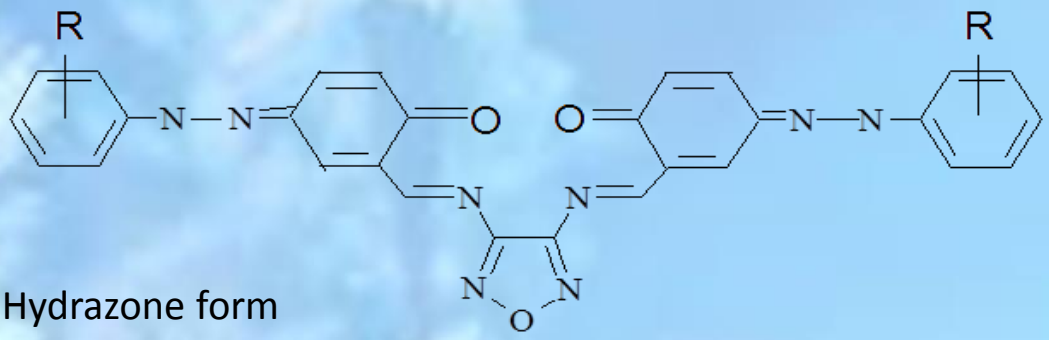
Effect of pH


0.9
0.6
0.3
0
Absorbance(a.u)
330
380
430
480
530
580
630
680
wavelength
k
j
i
h
g

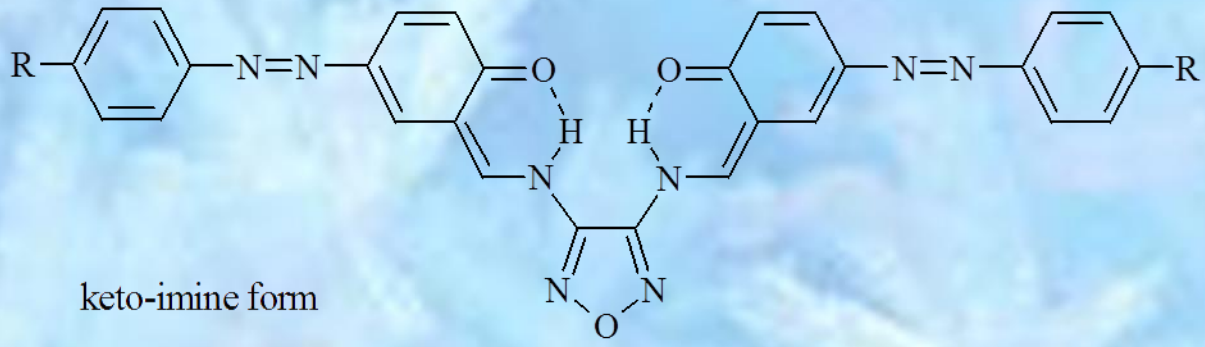
Effect of H2O



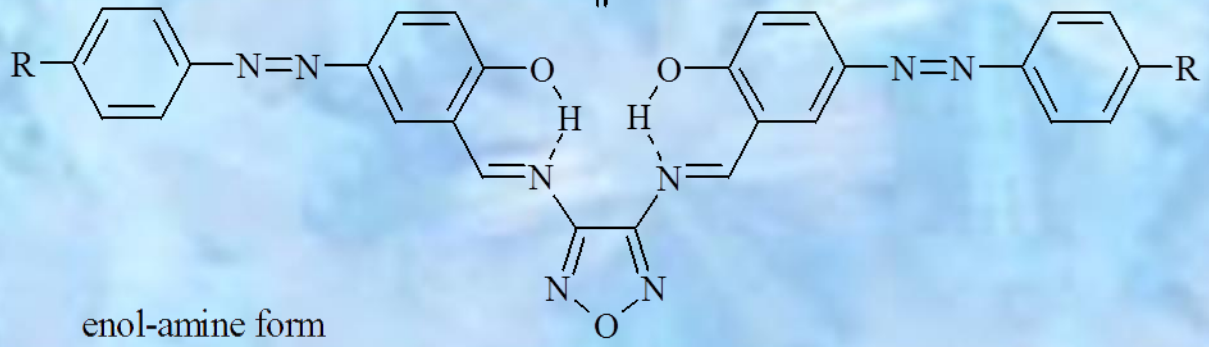




Hydrazone form



keto-imine form



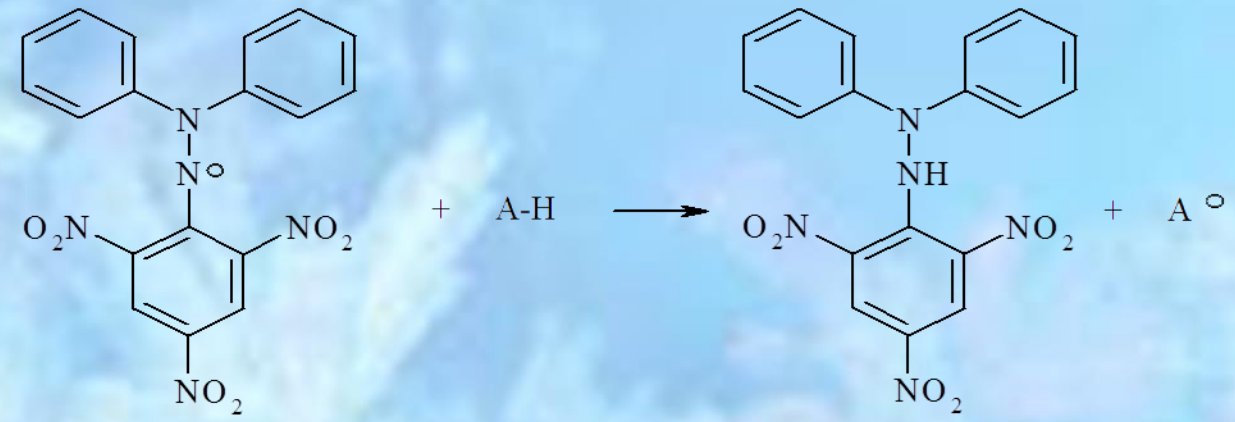
enol-amine form


Anti Microbial Properties
Anti Oxidant
Anti Bacterial

DPPH

1, 1-diphenyl-2-picryl-hydrazyl

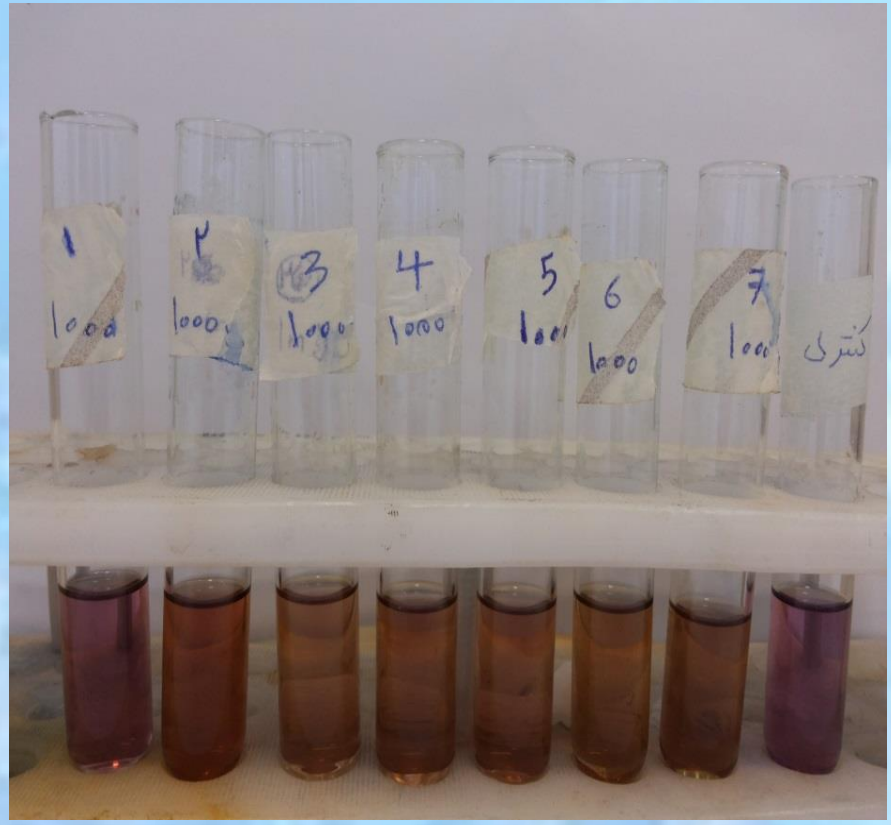
DPPH



DPPH
(purple, 517 nm)

DPPH-H
(colorless)

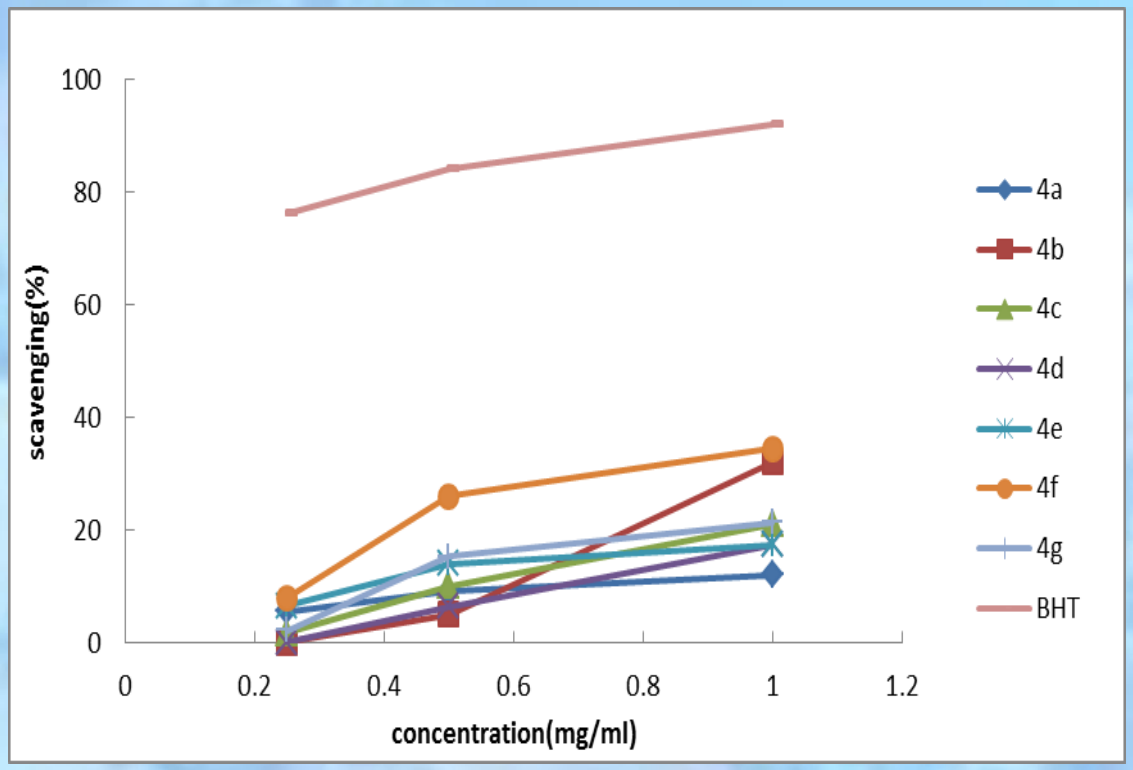
نمونه



Antioxidant activity

Number	C (mg/ml)	In(%)
4a	0.025	5.6
	0.050	0.9
	1.00	0.12
4b	0.025	0
	0.050	0.5
	1.00	0.32
4c	0.025	1.7
	0.050	0.10
	1.00	0.21
4d	0,025	0
	0.050	6.4
	1.00	17.4
4e	0.025	6.5
	0.050	0.14
	1.00	17.4
4f	0.025	8.0
	0.050	26.0
	1.00	34.5
4g	0.025	2.1
	0.050	15.2
	1.00	21.4
BHT	0.025	76.3
	0.050	84.3
	1.00	92.1

Antioxidant Activity Curve

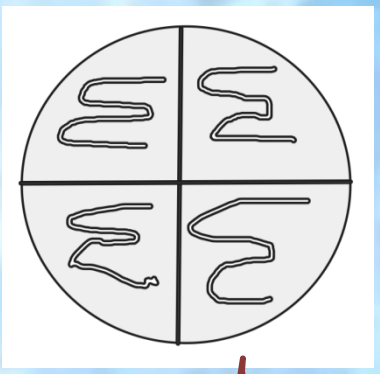


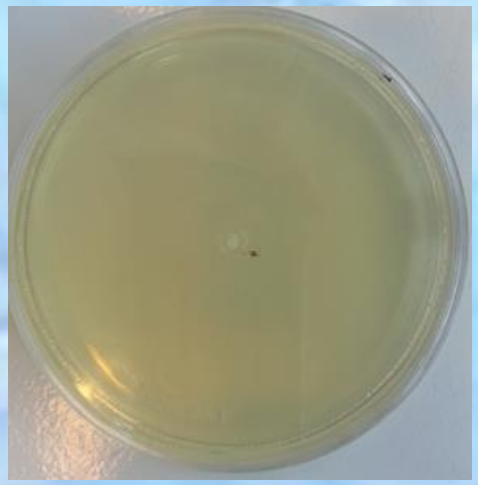
BHT> 4f > 4b > 4c > 4g > 4d > 4e > 4a

IC_{50}

compound	IC_{50} (mg/mL)
4a	5.6
4b	1.4
4c	2.1
4d	2.4
4e	3.3
4f	1.3
4g	2.2

disc diffusion method





Growth Inhibition

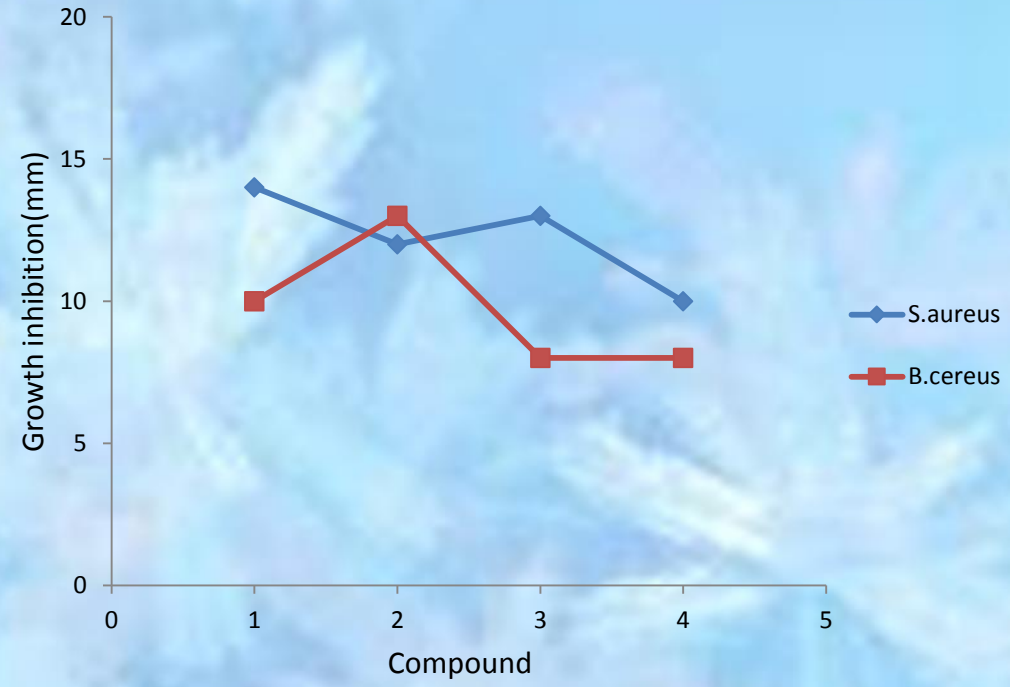
S.Aureus

B.Cereus

4f > 4e > 4b > 4c > 4a > 4d >4g

compound	C (µg/disc)	B.cereus	S.aureus
4a	30	10	11
4b	30	13	12
4c	30	8	13
4d	30	8	10
4e	30	12	13
4f	30	12	11
4g	30	9	9
Amikacin	30	25	21
DMSO		-	-

Compare of Bacteries




9
12
10
11


iso
Et
OMe
H

Conclusion

1.It looks that, substitution of electron donor groups on phenyl ring increases anti oxidant activity.

2. It looks that, *substitution of non polar groups on phenyl ring increases anti bacterial activities.*