Supplementary Information

Synthesis and characterization of magnetically recoverable 1-(Copperferritesiloxypropyl)-3-Methylimmidazolium Heteropolytungstate ionic liquid as a new nanocatalyst for the preparation of 1H-pyrazolo[1,2-b]phthalazine-5,10-diones

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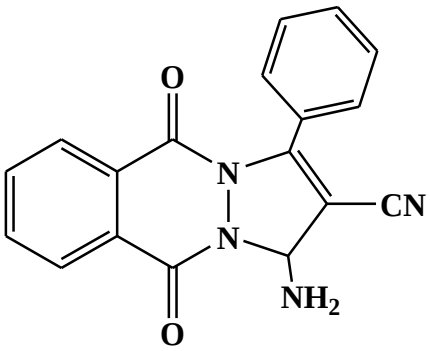
Methods

All Analytical thin layer chromatography was performed with E. Merck silica gel $60F_{254}$ aluminum sheets and was visualized with UV light. A 8400s Shimadzu spectrophotometer with KBr pellets have been used to record Fourier transform infrared (FT-IR spectra). The Melting point of products were measured by using the capillary tube method with a Bamstead electrothermal type 9200 melting points apparatus.

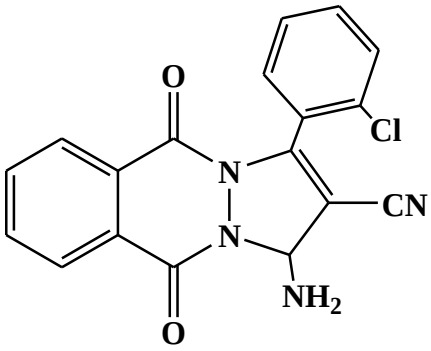


3-amino-1-(phenyl)-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-b]phthalazine-2-carbonitrile (4a)

vibration	**NH_2**	**=C-H**	**CN**	**C=O**	**C=C**	**C-N**
v (cm^{-1})	3397	3205	2196	1740	1668	1149
	3321				1602	1033

FT-IR band assignment

^{1}H NMR (DMSO) δ: 6.169 (s, 1H, Ar–CH), 6.363 (br s, 2H, NH_2), 7.397–7.484 (m, 5H, Ar–H), 7.831–7.911 (m, 2H), 8.231–8.273 (m, 2H); ^{13}C NMR (DMSO) δ: 59.173, 80.723, 113.725, 126.933, 127.935, 128.120, 128.773, 130.022, 134.337, 140.793, 158.231, 162.424, and 166.045.



3-amino-1-(2-chlorophenyl)-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-b]phthalazine-2-carbonitrile (4b)

vibration	**NH_2**	**=C-H**	**CN**	**C=O**	**C=C**	**C-N**
v (cm^{-1})	3392	3202	2196	1740	1670	1149
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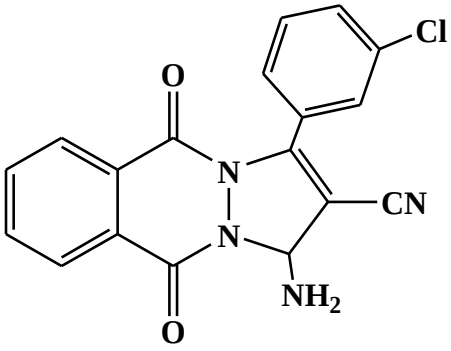
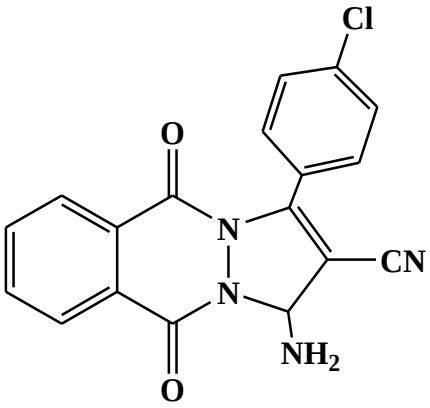
FT-IR band assignment



3-amino-1-(3-chlorophenyl)-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-b]phthalazine-2-carbonitrile (4c)

vibration	**NH_2**	**=C-H**	**CN**	**C=O**	**C=C**	**C-N**
v (cm^{-1})	3397 3346	3168	2190	1736	1681 1656 1598	1161 1033

FT-IR band assignment

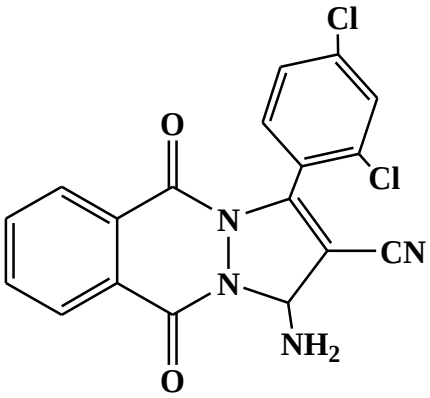


3-amino-1-(4-chlorophenyl)-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-b]phthalazine-2-carbonitrile (4d)

vibration	**NH_2**	**=C-H**	**CN**	**C-O**	**C=C**	**C-N**
v (cm^{-1})	3397 3379	3182	2187	1751	1674 1637 1483	1143 1026

FT-IR band assignment

^{1}H NMR (DMSO) δ: 6.179 (s, 1H, Ar–CH), 6.674 (br s, 2H, NH_2), 7.397–7.488 (m, 4H, Ar–H), 7.833–7.907 (m, 2H), 8.231–8.314 (m, 2H)



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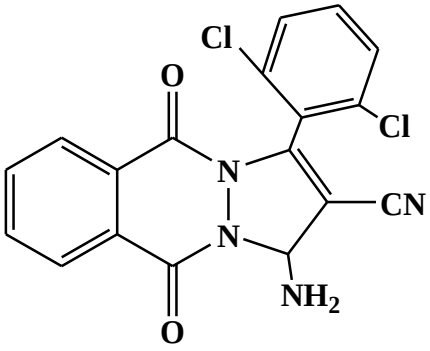
FT-IR band assignment



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vibration	**NH_2**	**=C-H**	**CN**	**C=O**	**C=C**	**C-N**
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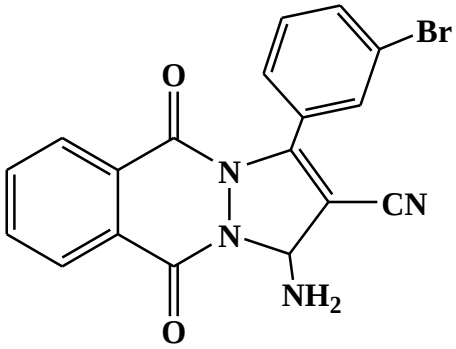
FT-IR band assignment



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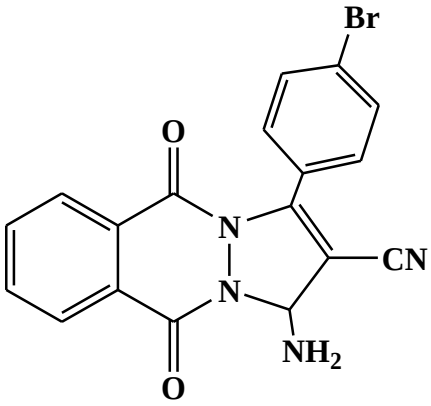
FT-IR band assignment



3-amino-1-(4-bromophenyl)-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-b]phthalazine-2-carbonitrile (4h)

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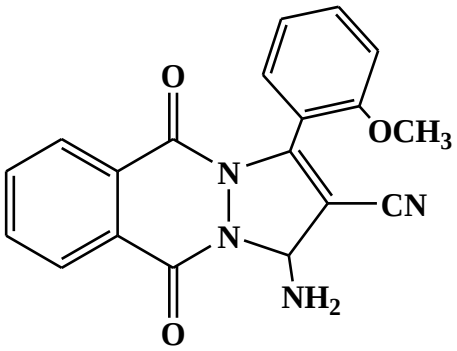
FT-IR band assignment



3-amino-1-(2-methoxyphenyl)-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-b]phthalazine-2-carbonitrile (4i)

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v (cm^{-1})	3397 3394	3209	2189	1746	1649 1596 1479	1151 1022

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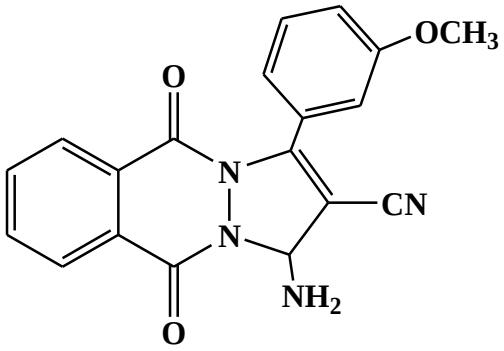
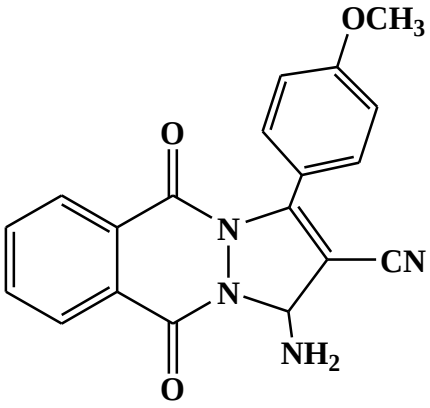


3-amino-1-(3-methoxyphenyl)-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-b]phthalazine-2-carbonitrile (4j)

vibration	**NH_2**	**=C-H**	**CN**	**C=O**	**C=C**	**C-N**
v (cm^{-1})	3397 3350	3182	2190	1749	1656 1604 1477	1141 1039

FT-IR band assignment

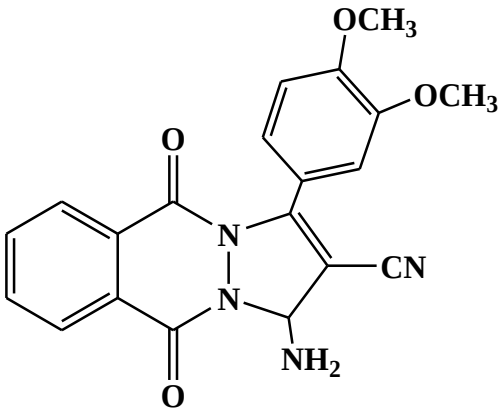


3-amino-1-(4-methoxyphenyl)-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-b]phthalazine-2-carbonitrile (4k)

vibration	**NH_2**	**=C-H**	**CN**	**C=O**	**C=C**	**C-N**
v (cm^{-1})	3397 3373	3184	2192	1740	1654 1604 1510	1164 1033

FT-IR band assignment

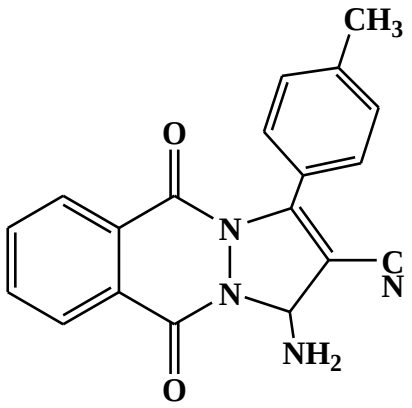
^{1}H NMR (DMSO) δ: 3.892 (s, 3H, O–CH_3), 6.174 (s, 1H, Ar–CH), 6.663 (br s, 2H, NH_2), 7.419–7.489 (m, 4H, Ar–H), 7.843–7.932 (m, 2H), 8.283–8.371 (m, 2H)



3-amino-1-(3,4-dimethoxyphenyl)-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-b]phthalazine-2-carbonitrile (4l)

vibration	**NH_2**	**=C-H**	**CN**	**C=O**	**C=C**	**C-N**
v (cm^{-1})	3397 3377	3178	2190	1736	1674 1604 1514	1141 1031

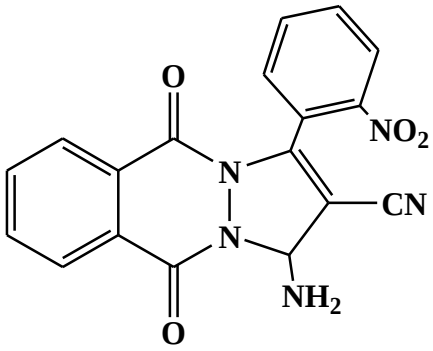
FT-IR band assignment



3-amino-1-(4-p-tolyl)-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-b]phthalazine-2-carbonitrile (4m)

vibration	**NH_2**	**=C-H**	**CN**	**C=O**	**C=C**	**C-N**
v (cm^{-1})	3397 3425	3220	2196	1740	1677 1600	1145 1031

FT-IR band assignment

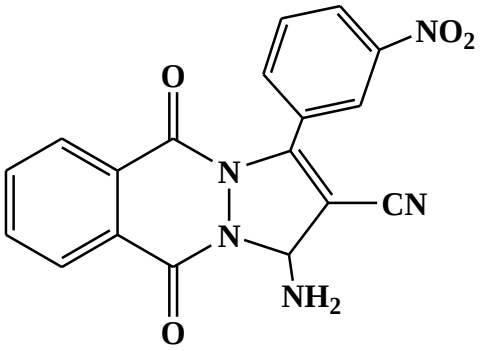


3-amino-1-(2-nitrophenyl)-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-b]phthalazine-2-carbonitrile (4n)

vibration	**NH_2**	**=C-H**	**CN**	**C=O**	**C=C**	**C-N**
v (cm^{-1})	3397 3469	3207	2194	1742	1683 1595 1521	1149 1039

FT-IR band assignment

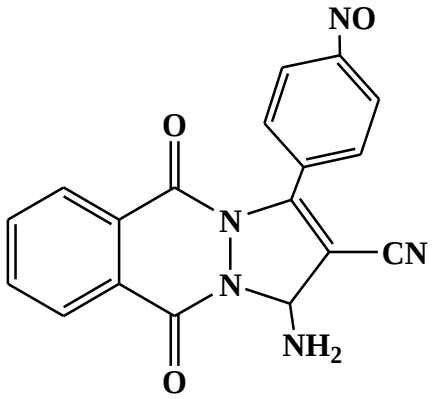
^{1}H NMR (DMSO) δ: 6.425 (s, 1H, Ar–CH), 6.819 (br s, 2H, NH_2), 7.395–7.489 (m, 4H, Ar–H), 7.891–7.962 (m, 2H), 8.281–8.375 (m, 2H)



3-amino-1-(3-nitrophenyl)-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-b]phthalazine-2-carbonitrile (4o)

vibration	**NH_2**	**=C-H**	**CN**	**C=O**	**C=C**	**C-N**
v (cm^{-1})	3397 3433	3201	2192	1740	1666 1531	1145 1035

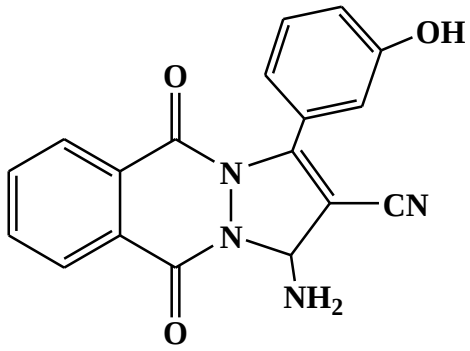
FT-IR band assignment



3-amino-1-(4-nitrophenyl)-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-b]phthalazine-2-carbonitrile (4p)

vibration	**NH_2**	**=C-H**	**CN**	**C=O**	**C=C**	**C-N**
v (cm^{-1})	3397 3404	3176	2185	1748	1674 1523	1143 1026

FT-IR band assignment

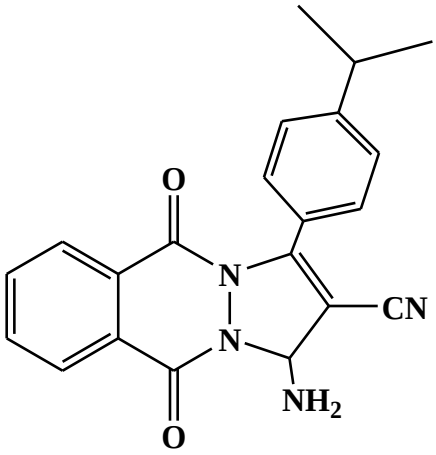


3-amino-1-(3-hydroxyphenyl)-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-b]phthalazine-2-carbonitrile (4q)

vibration	**NH_2**	**=C-H**	**CN**	**C=O**	**C=C**	**C-N**
v (cm^{-1})	3397 3311	3195	2192	1732	1654 1585 1458	1149 1041

FT-IR band assignment

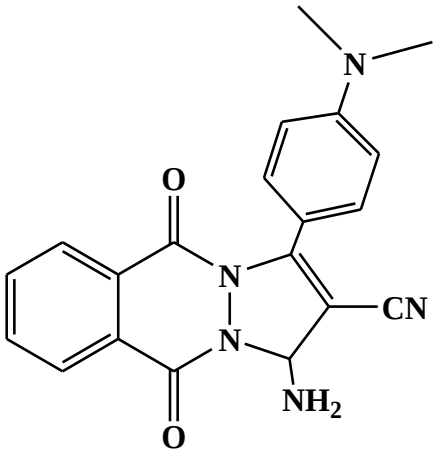
^{1}H NMR (DMSO) δ: 6.146 (s, 1H, Ar–CH), 6.564–6.726 (m, 4H, Ar–H), 7.39 (br s, 2H, NH_2), 7.829–7.898 (m, 2H), 8.218–8.291 (m, 2H), 10.621 (br s, 1H, OH)



3-amino-1-(4-(isopropyl)phenyl)-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-b]phthalazine-2-carbonitrile (4r)

vibration	**NH_2**	**=C-H**	**CN**	**C=O**	**C=C**	**C-N**
v (cm^{-1})	3397 3367	3178	2187	1742	1652	1143 1031

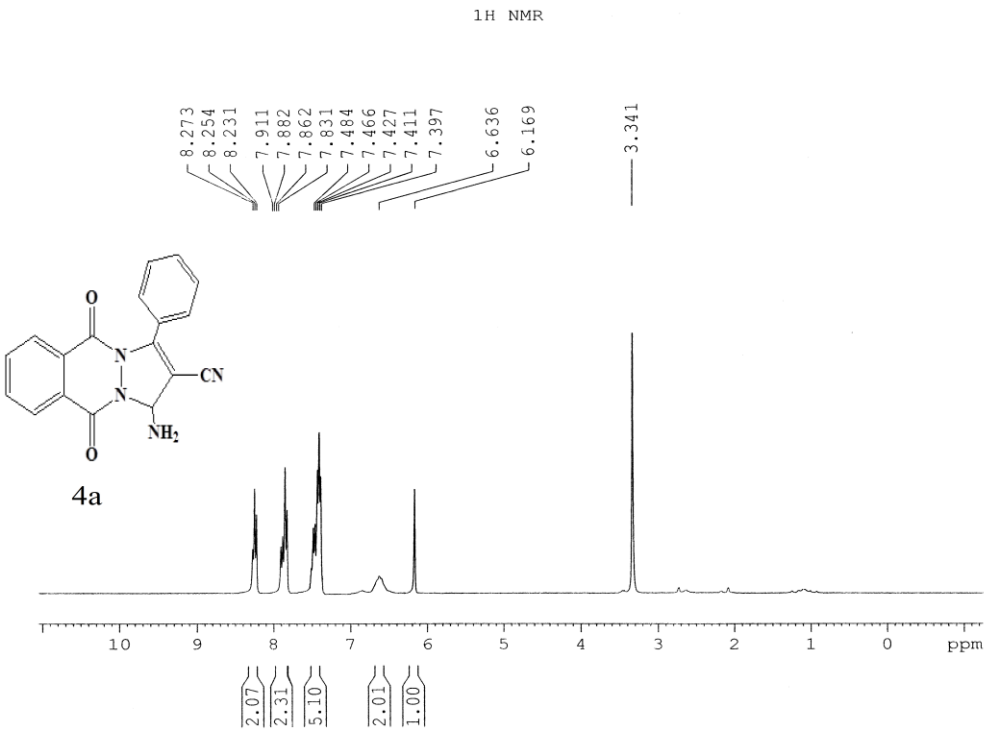
FT-IR band assignment



3-amino-1-(4-(dimethylamino)phenyl)-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-b]phthalazine-2-carbonitrile (4s)

vibration	**NH_2**	**=C-H**	**CN**	**C=O**	**C=C**	**C-N**
v (cm^{-1})	3397 3380	3205	2204	1748	1612 1521	1197

FT-IR band assignment

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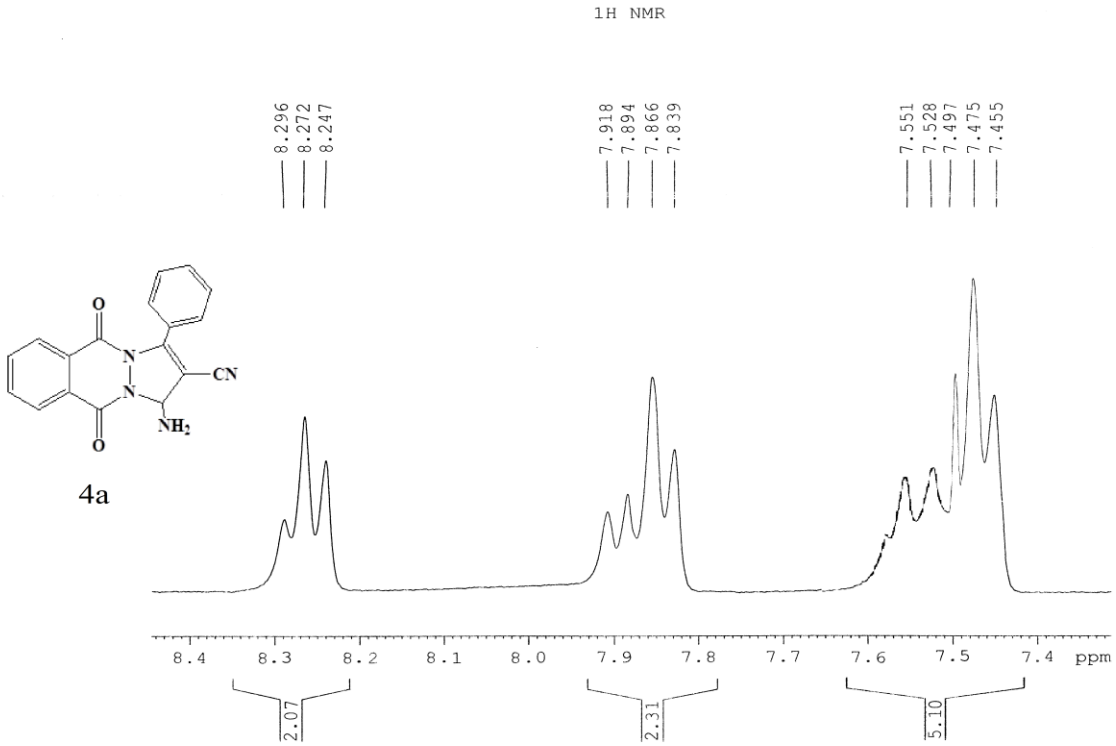


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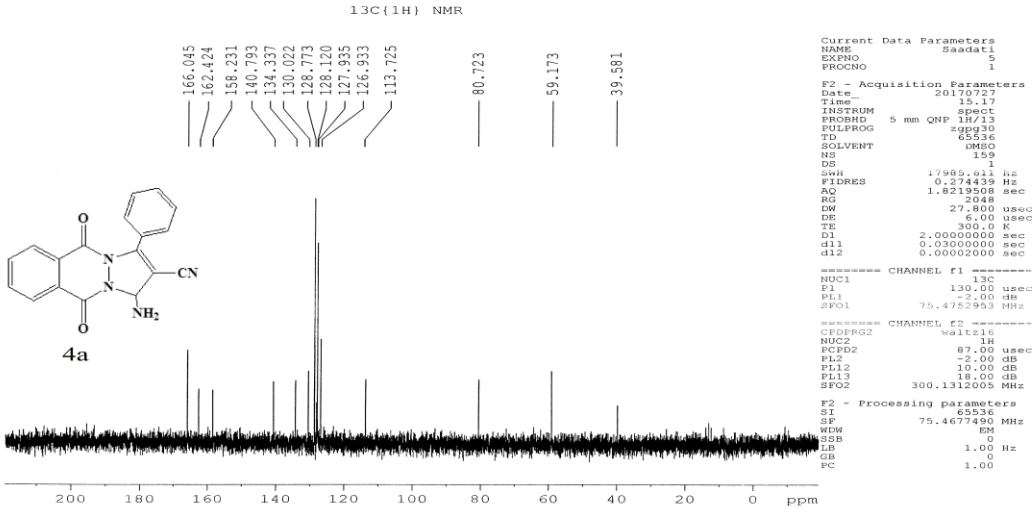
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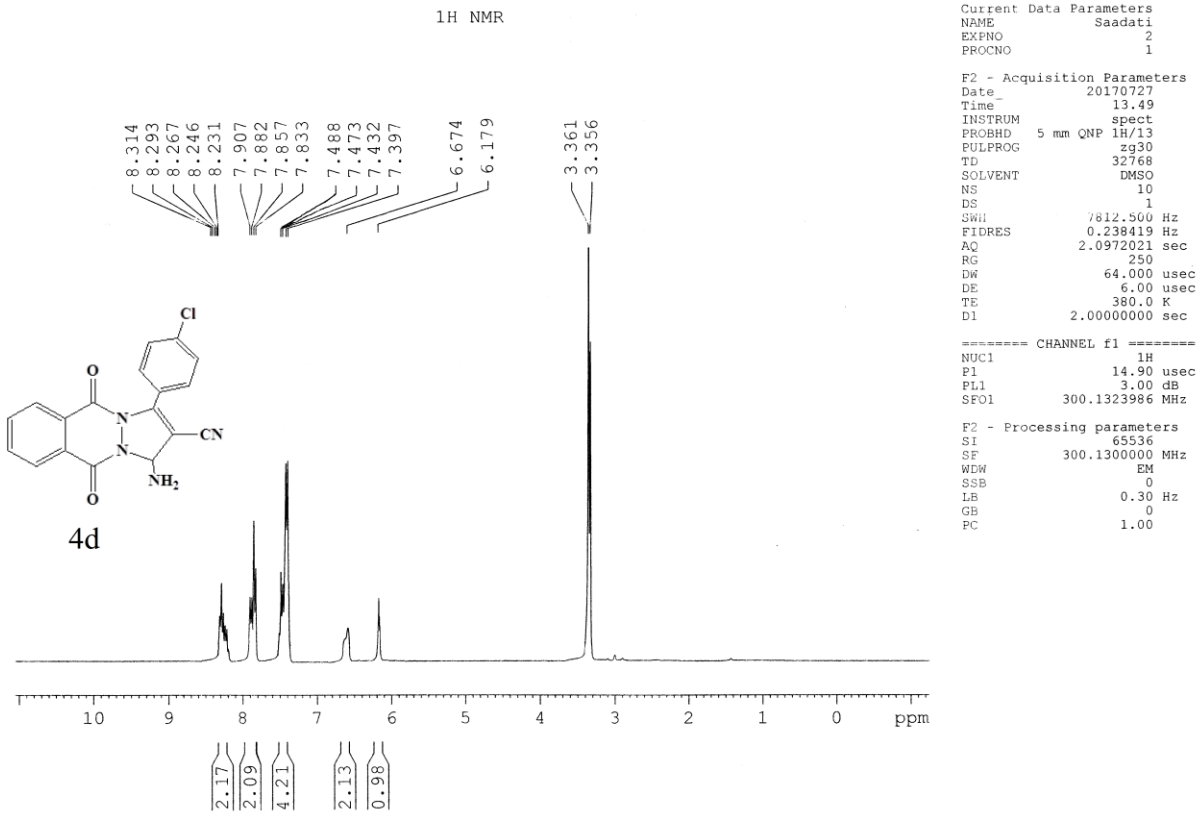
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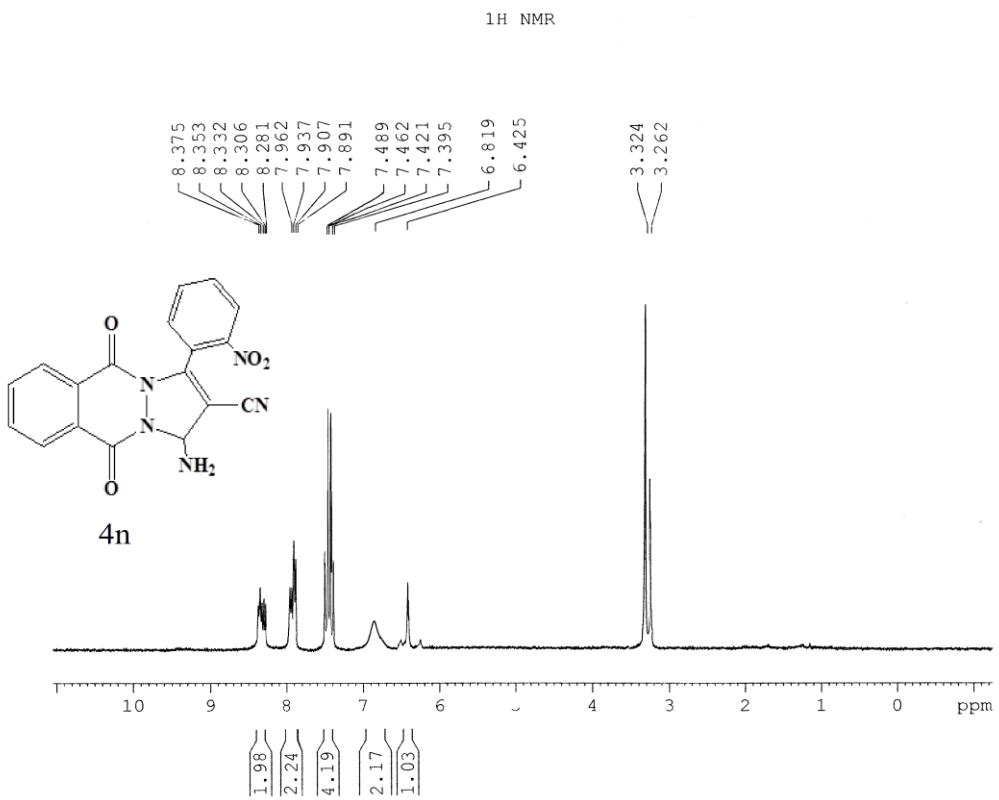


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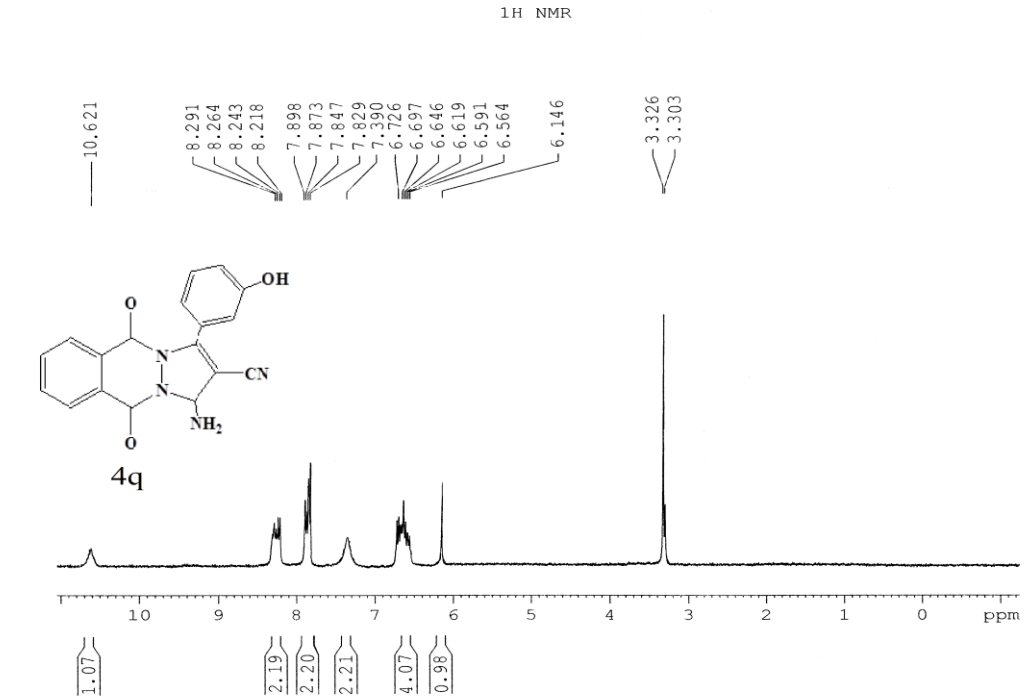
P1                     14.90 usec
PL1                     3.00 dB
SFO1           300.1323986 MHz

F2 - Processing parameters
SI                        65536
SF             300.1300000 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
```

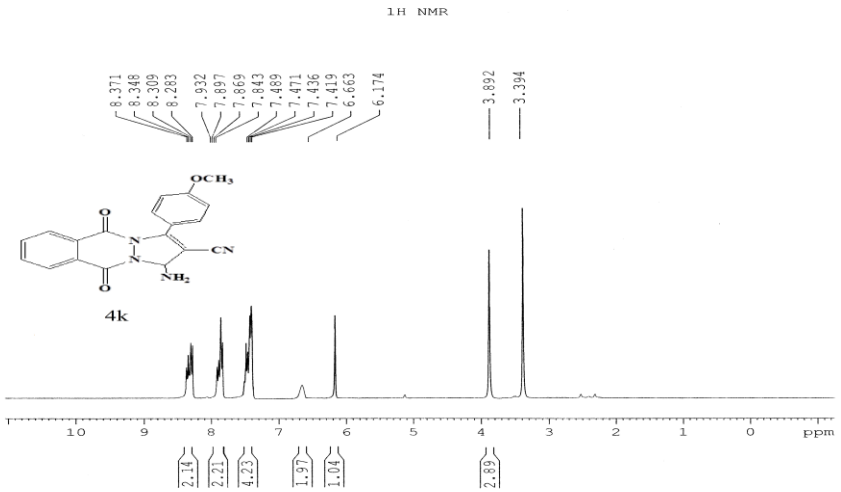



```
Current Data Parameters
NAME                  Saadati
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20170727
Time                   13.57
INSTRUM                spect
PROBHD    5 mm QNP 1H/13
PULPROG                zg30
TD                    32768
SOLVENT                DMSO
NS                        10
DS                         1
SWH                7812.500 Hz
FIDRES             0.238419 Hz
AQ                 2.0972021 sec
RG                       250
DW                    64.000 usec
DE                     6.00 usec
TE                    380.0 K
D1                 2.00000000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                     14.90 usec
PL1                     3.00 dB
SFO1           300.1323986 MHz

F2 - Processing parameters
SI                        65536
SF             300.1300000 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
```




```
Current Data Parameters
NAME                  Saadati
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_                20170727
Time                    14.21
INSTRUM                  spect
PROBHD    5 mm QNP 1H/13
PULPROG                 zg30
TD                     32768
SOLVENT                 DMSO
NS                        10
DS                         1
SWH                 7812.500 Hz
FIDRES              0.238419 Hz
AQ                  2.0972021 sec
RG                        250
DW                   64.000 usec
DE                    6.00 usec
TE                    380.0 K
D1                 2.00000000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                    14.90 usec
PL1                    3.00 dB
SFO1           300.1323986 MHz

F2 - Processing parameters
SI                        65536
SF                 300.1300000 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
```