Supporting Information

Construction of a series of metal-directed MOFs to explore their physical and chemical properties

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1. Synthesis of 5-Azidoisophthalic acid (5-N_3H_2IPA):

An aqueous solution of 5-aminoisophthalic (2g, 11mmol) was taken in a beaker, to which 4 mL of conc. HCl was added. The mixture was then cooled below 5°C using icebath. A solution of $NaNO_2$ (760mg, 11mmol in 10 mL water) was added dropwise. A pale-yellow precipitate was formed soon after the addition of $NaNO_2$ solution. The temperature of the mixture was maintained below 5°C for another half an hour. Then the reaction mixture was stirred at room temperature for 14 hours. The white precipitate was then filtered, washed with water and dried in vacuum at 50°C. The yield was found to be 83% with respect to 5-aminoisophthalic acid.

IR KBr(cm^{-1}): 3553(m), 3462(w), 3099(m), 2662(w), 2214(vw), 2122(s), 1811(vw), 1720(s), 1682(m), 1599(m), 1464(m), 1404(m), 1307(m), 1288(w), 1258(w), 1219(m), 1173(m), 1115(w), 931(w), 901(m)

2. Photocatalysis of dye solutions

In order to explore the catalytic properties of our compounds, solutions of methyl orange (20 ppm) and Rhodamine B (10ppm) were prepared. The dye solutions were taken in a cuvette and 2 drops of 30% H_2O_2 were added followed by the addition of *ca*. 5mg of compound. The change in the characteristic peaks of the dye solutions were monitored using UV-Vis spectrometer by collecting data periodically. It was noted that after 90 mins almost 70% of methyl orange and 60% of RhB were degraded and removed from the solution, whereas during the same span of time there was no significant change when no catalyst was used. After the process is done the MOF was collected and PXRD data was collected in order to check whether the MOF undergone any damage or distortion. The PXRD data confirms that the MOFs were intact and ready for reuse.

3. Reduction of 4-nitrophenol

In the reduction of 4- nitrophenol using $NaBH_4$, 2 mL of $NaBH_4$ (0.3 M) solution and 2 mL of 4-NP (0.1 mM) solution were added in a cuvette. The solution was sonicated for few mins and becomes yellowish due to the formation of 4-nitrophenolate ion. the change was also noted using a UV-Vis spectrometer as the formation of 4-nitrophenolate ion give rise to a new peak at 400.58nm. Now *ca* 5 mg of the compound was added in the solution and the change in the absorption at the peak 400.58nmwas monitored for the progress of the reaction.

4. Crystallographic data

Table SI-1: Crystal data and structure refinement information of Compound 1-7.

	Compound 1	Compound 2	Compound 3	Compound 4	Compound 5	Compound 6	Compound 7
Empirical Formula	$C_{43}H_{30}Cu_2\ N_{11}O_9$	$C_{26}H_{21}CoN_6O_4$	$C_{78}H_{63}N_{18}Ni_3O_{12}$	$C_{28}H_{18}CdN_8O_8$	$C_{55}H_{48}\ Mn_2N_{13}O_{10}$	$C_{21}H_{18}N_5O_6Zn$	$C_{20}H_{15}N_5O_4Zn$
Formula Wt	971.86	540.42	1620.59	706.90	1160.94	501.77	454.74
Crystal system	Triclinic	Triclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	*P*-1	*P*-1	*P*-1	$P2_{1/c}$	$P2_{1/c}$	$P2_{1/n}$	*C*2/c
a/Å	7.2638(3)	10.0002(10)	15.1952(7)	12.7472(15)	27.0142(14)	7.8286(3)	14.5651(8)
b/ Å	11.8595(5)	10.0870(10)	17.0749(9)	17.173(2)	10.0523(6)	17.0971(7)	15.7498(9)
c/ Å	13.0619(6)	13.5209(14)	17.2622(9)	13.6504(16)	20.5231(12)	16.1032(7)	16.6824(9)
α/°	72.350(2)	98.126(4)	115.355(2)	90	90	90	90
β/°	78.127(2)	94.279(4)	112.7570(10)	110.216(3)	111.045(2)	95.5120(10)	104.2180(14)
γ/°	76.793(2)	112.649(3)	92.171(2)	90	90	90	90
V/ Å3	1032.53(8)	1233.6(2)	3619.2(3)	2804.2(6)	5201.4(5)	2145.39(15)	3709.7(4)
Z	1	2	2	4	4	4	8
Reflections collected	41863	16189	51754	38491	81591	30194	28674
Unique reflections	6288	4975	21005	6119	19008	5364	5599
Obs.reflections	5598	2965	11321	4407	10708	4236	4041
R1	0.0396	0.0633	0.0792	0.0368	0.0941	0.0414	0.0466
wR2	0.1072	0.1539	0.1866	0.0738	0.2455	0.1125	0.1090
CCDC Nos.	1963350	1963351	1963352	1963353	1963354	1963355	1963356

5. Powder XRD pattern comparison

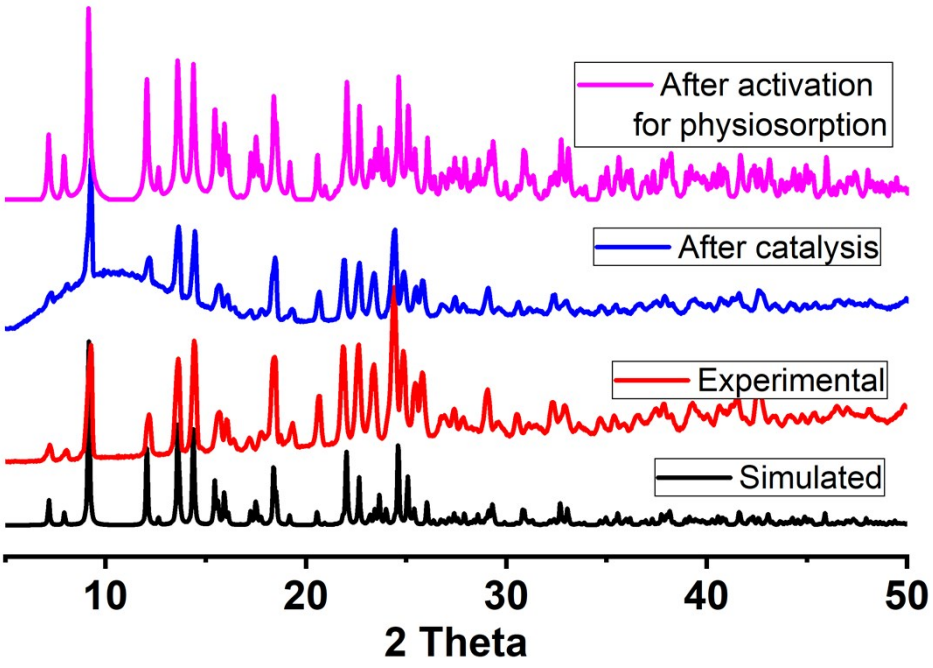


Figure S1: PXRD pattern of compound **1.**

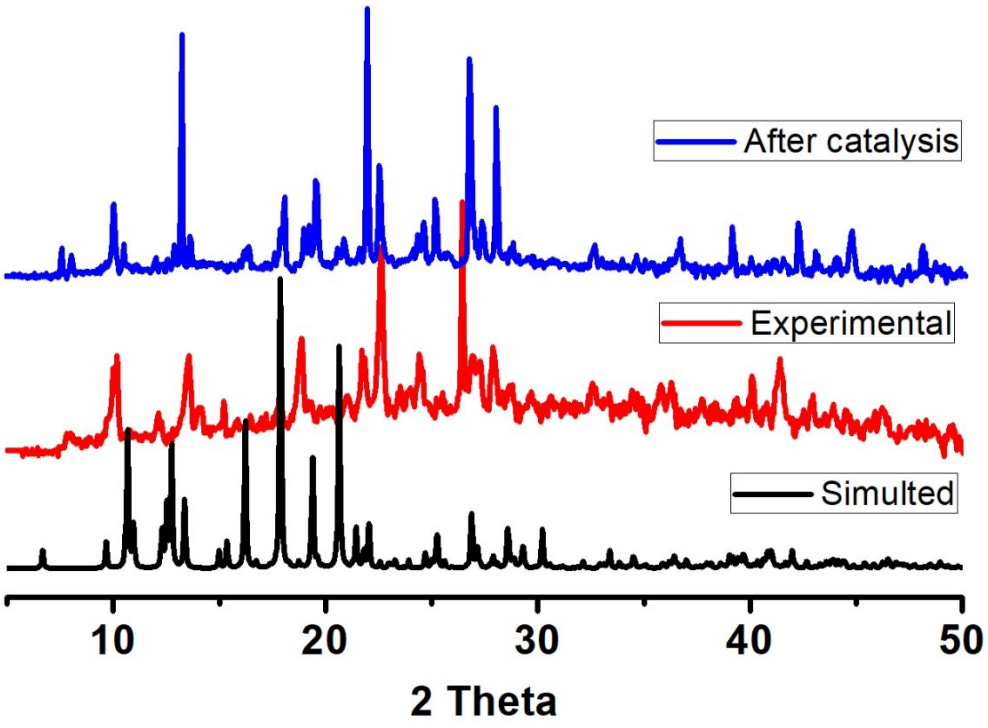


Figure S2: PXRD pattern of compound **2.**

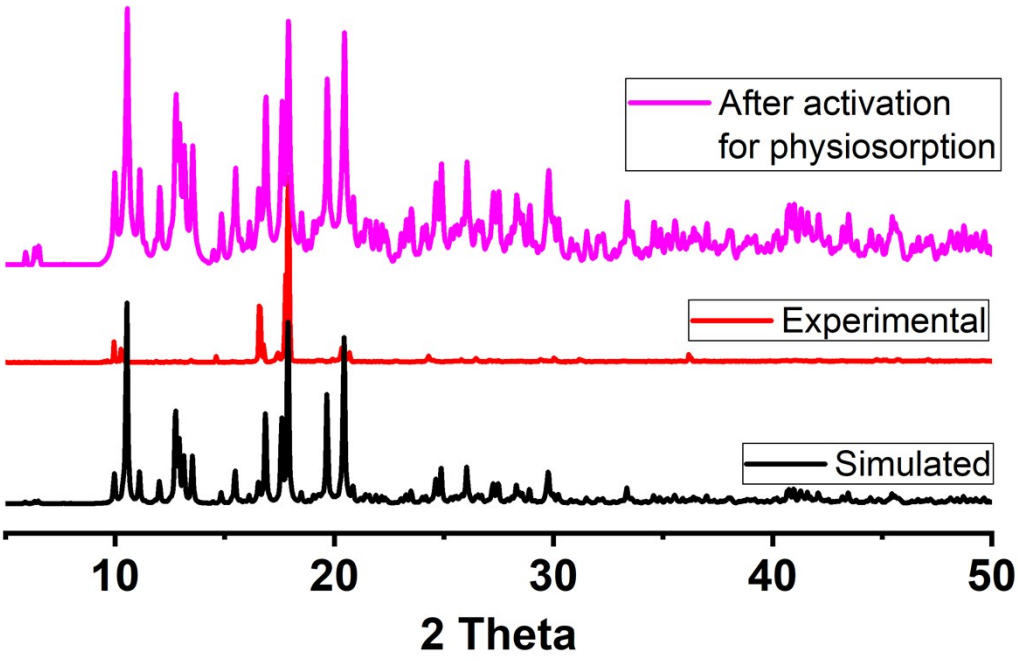


Figure S3:PXRD pattern of compound **3.**

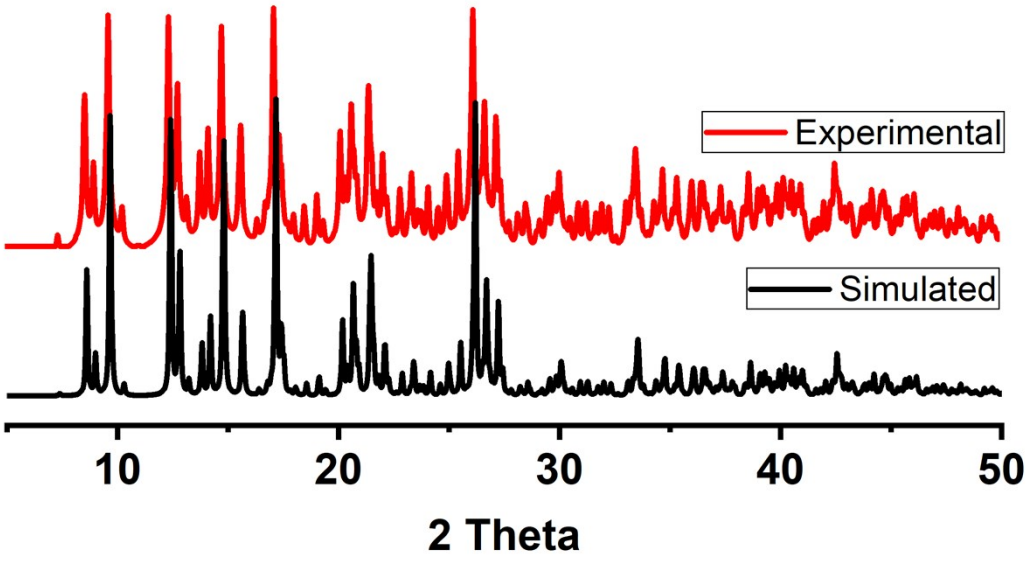


Figure S4: PXRD pattern of compound**4.**

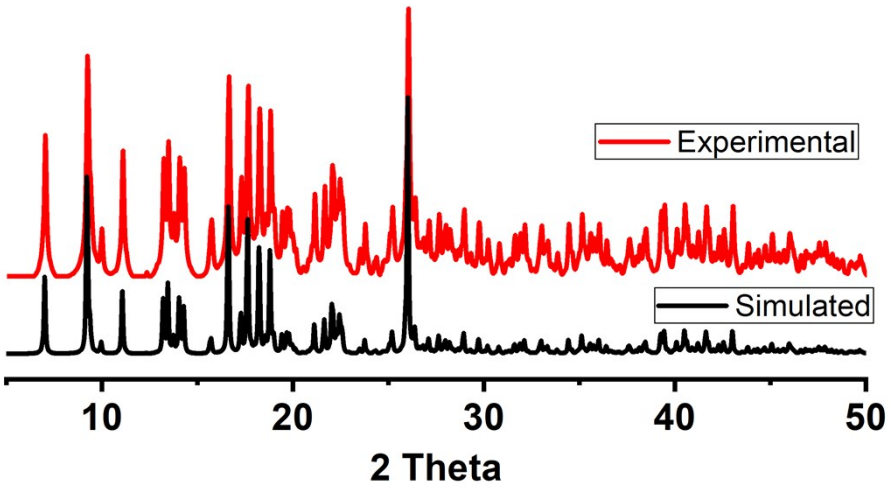


Figure S5: PXRD pattern of compound **5.**

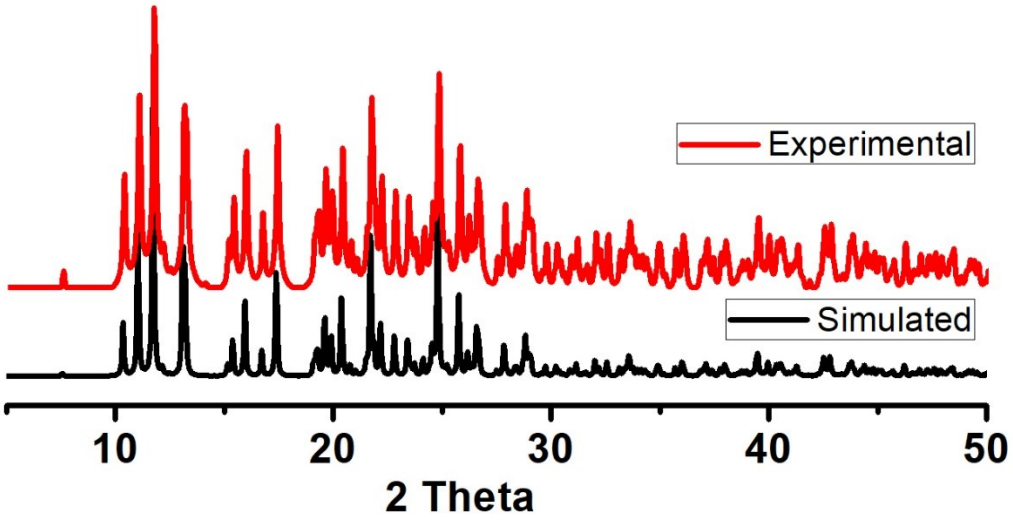


Figure S6: PXRD pattern of compound **6.**

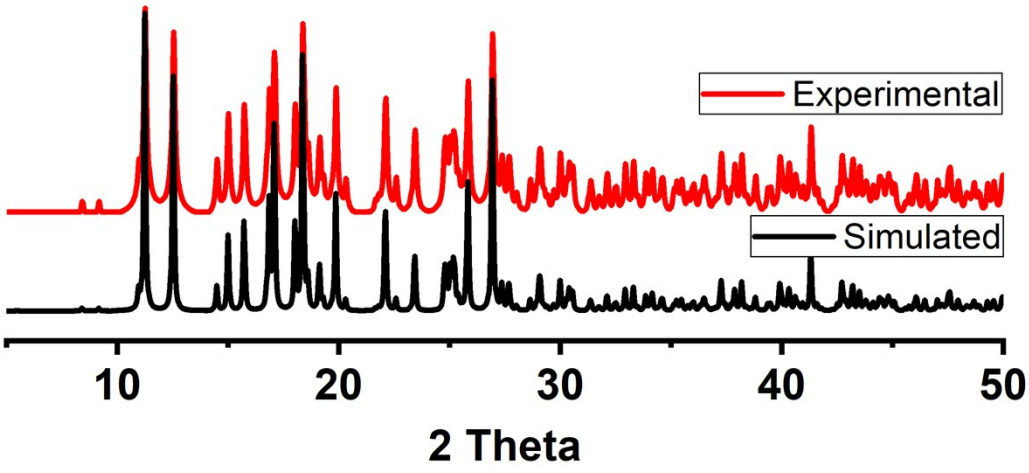


Figure S7: PXRD pattern of compound **7.**

6. IR data

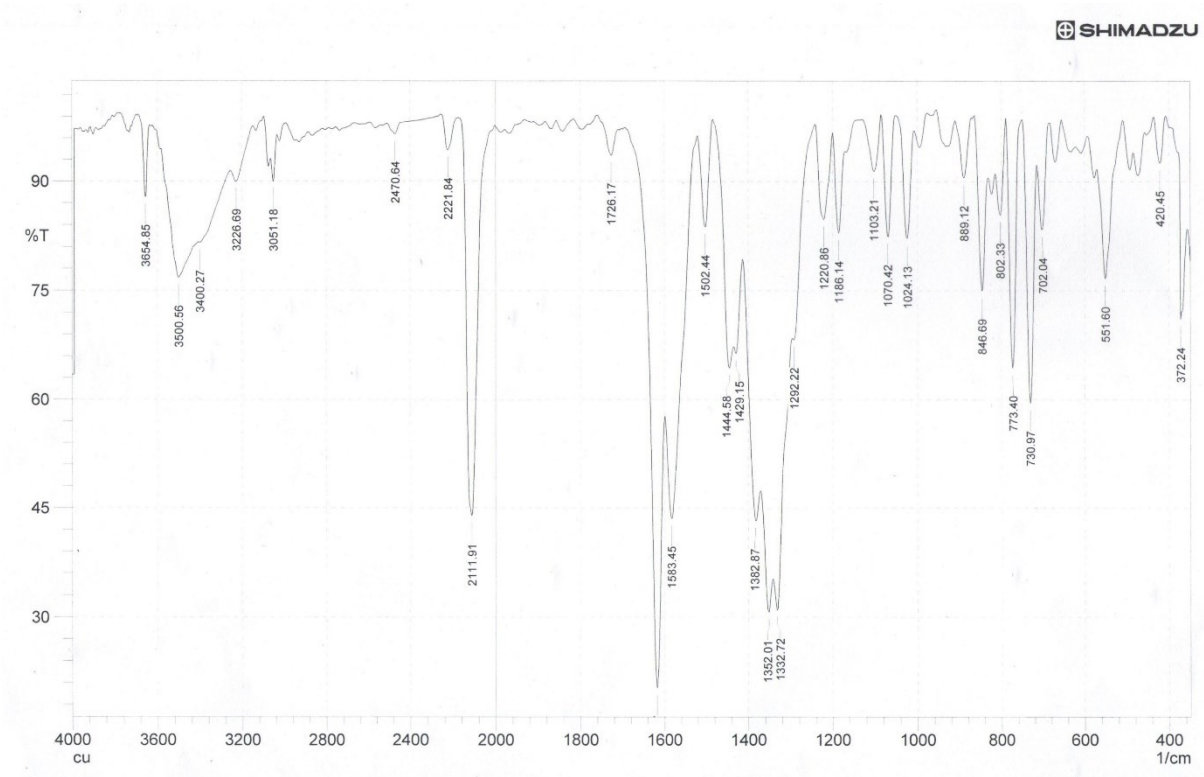


Figure S8: IR spectra of compound **1.**

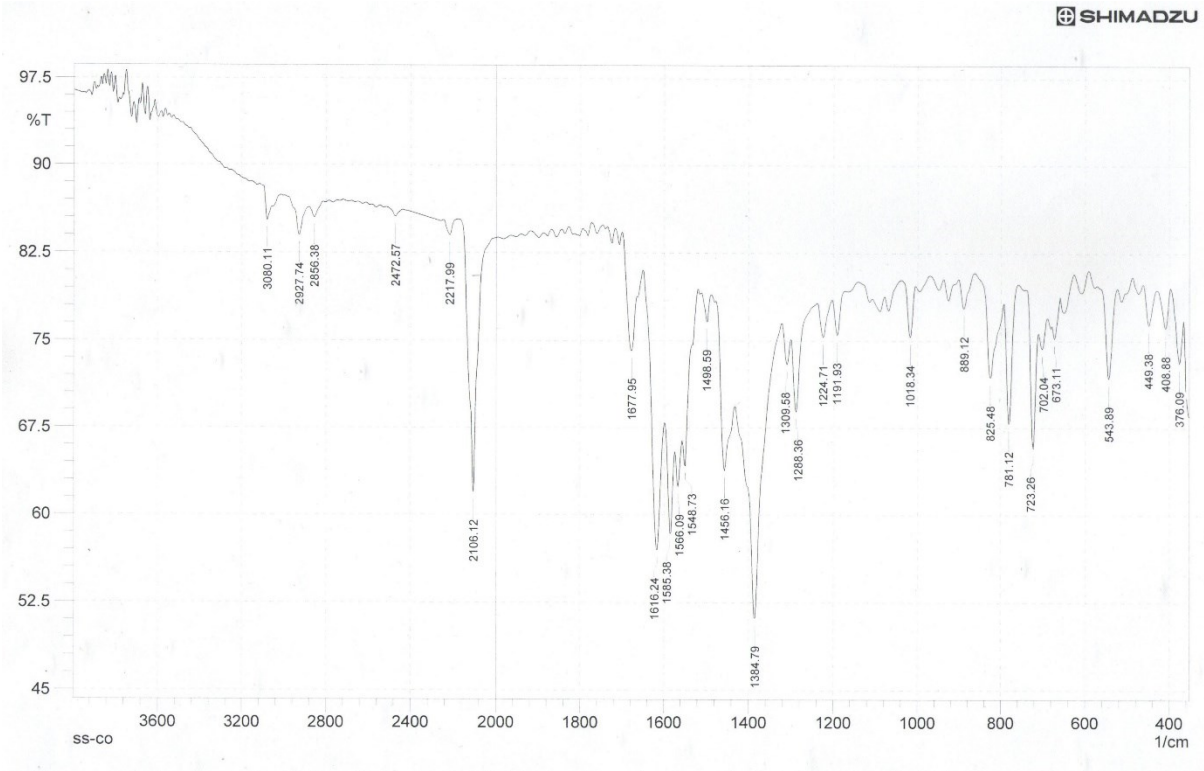


Figure S9: IR spectra of compound **2.**

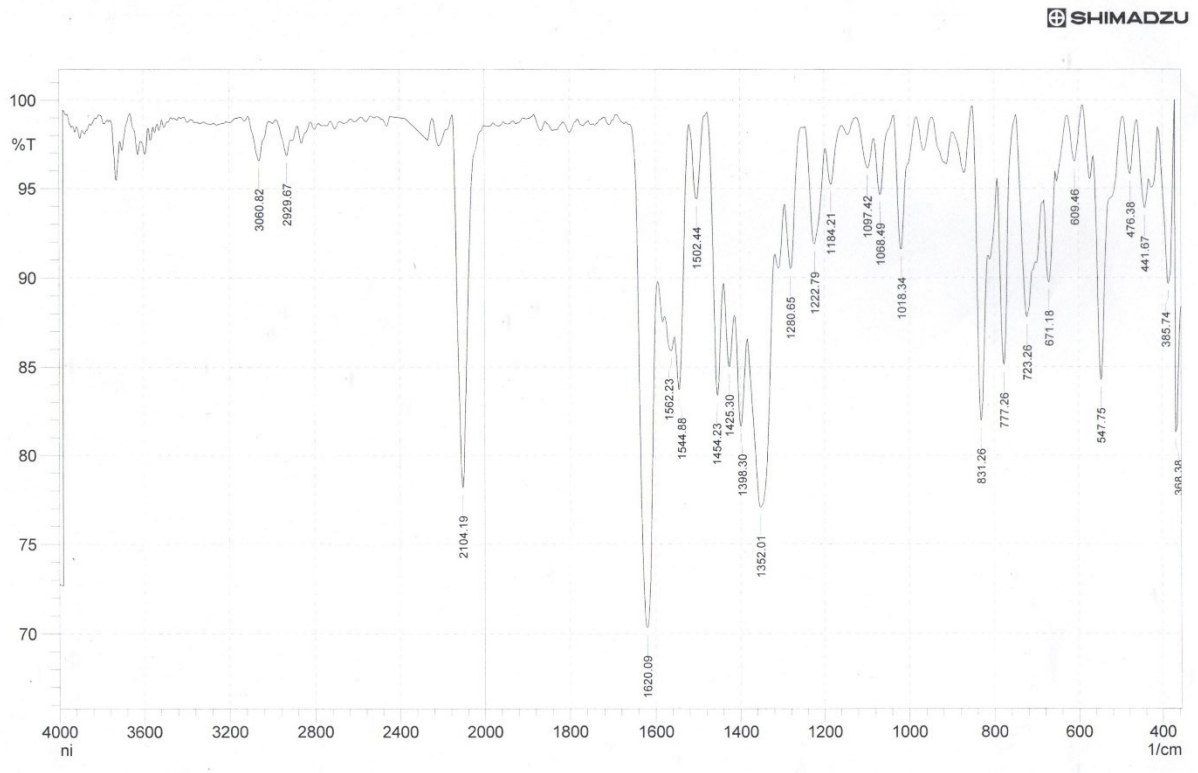


Figure S10: IR spectra of compound **3.**

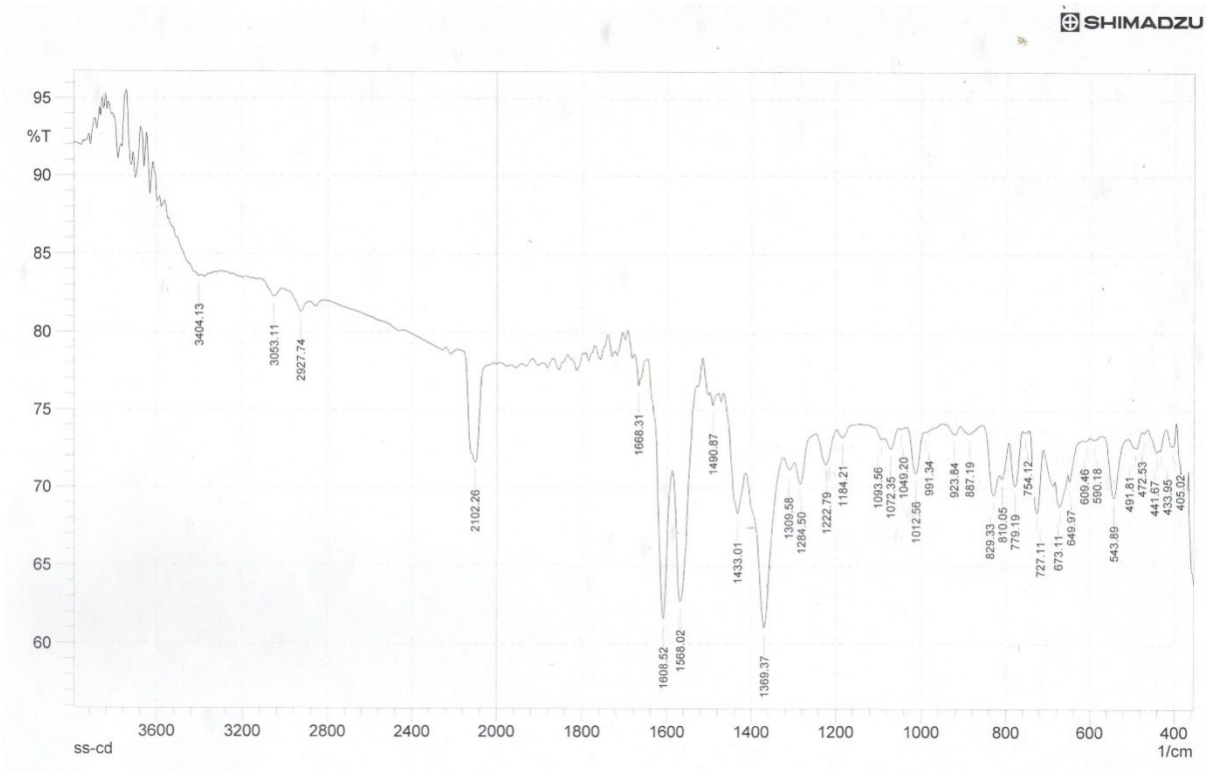


Figure S11: IR spectra of compound **4.**

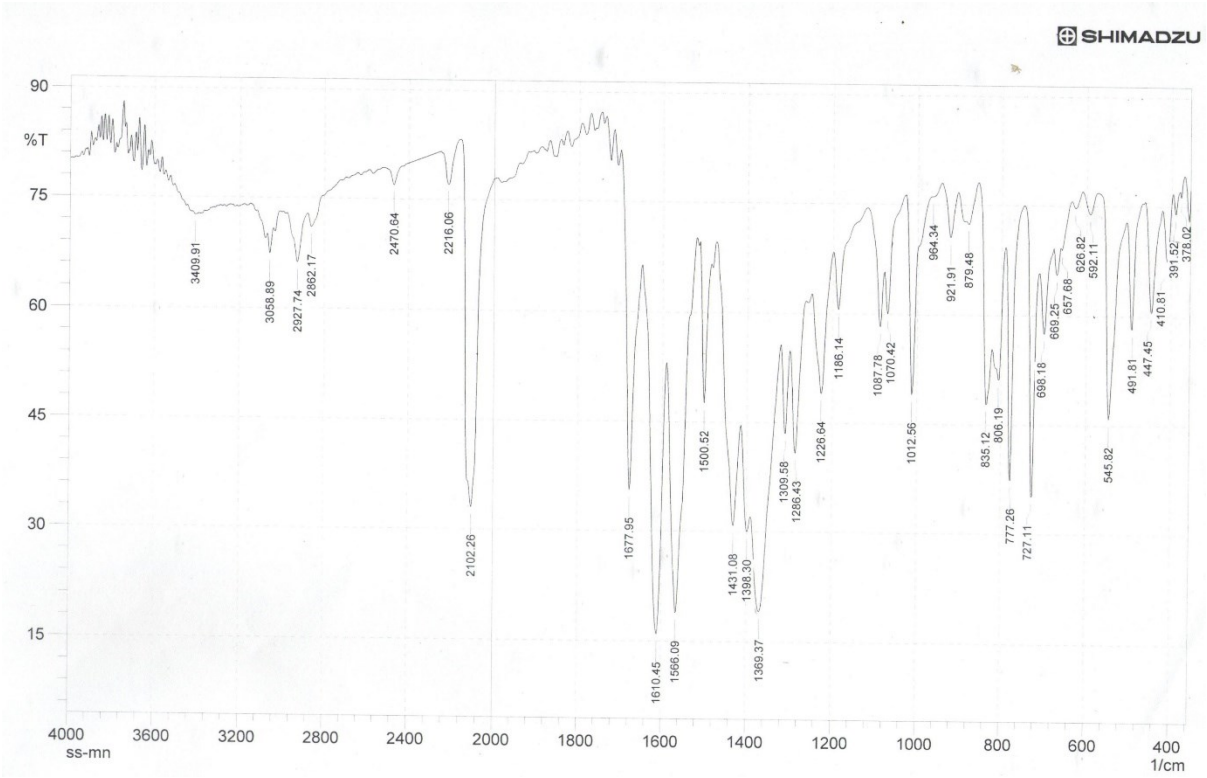


Figure S12: IR spectra of compound **5.**

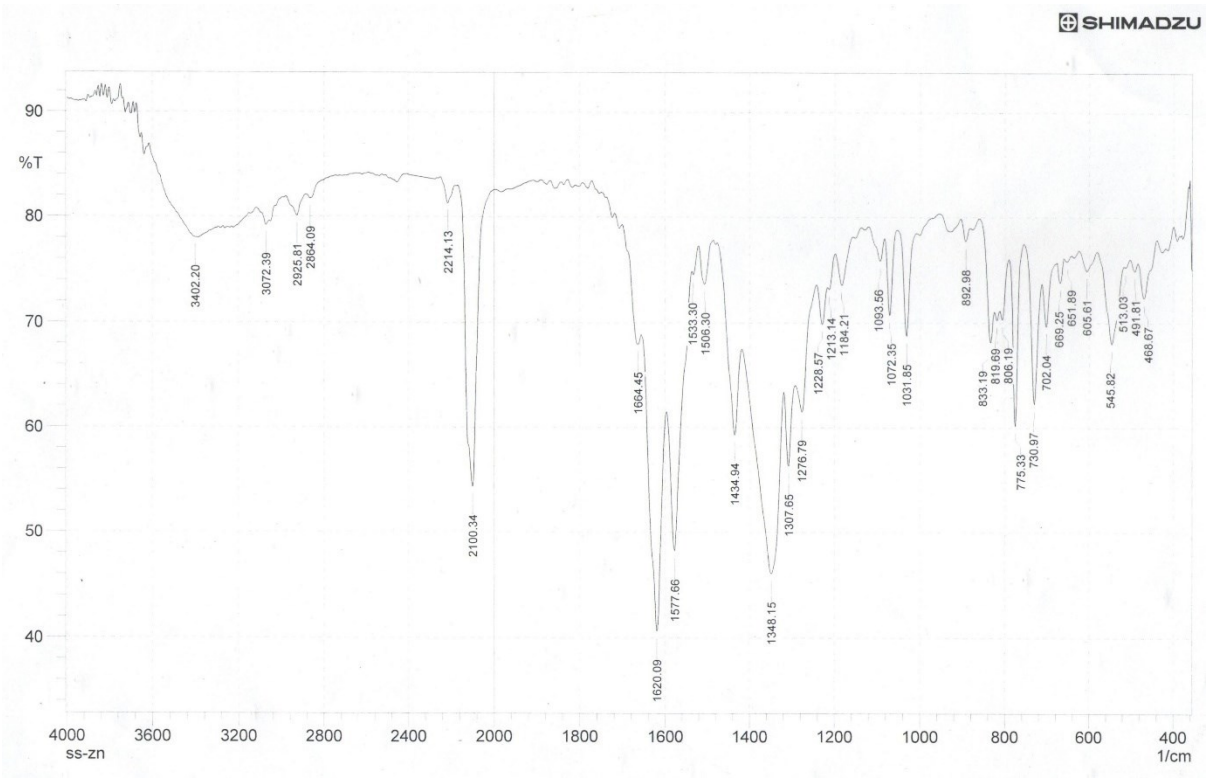


Figure S13: IR spectra of compound **6.**

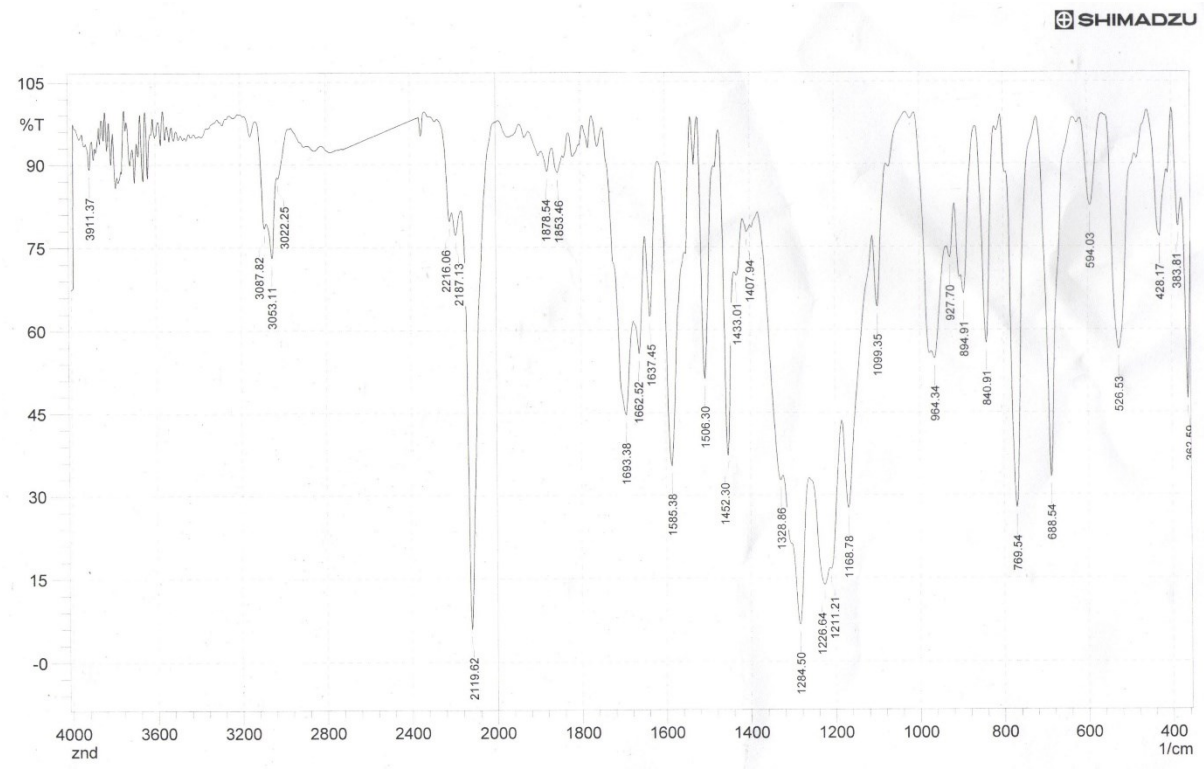


Figure S14: IR spectra of compound **7.**

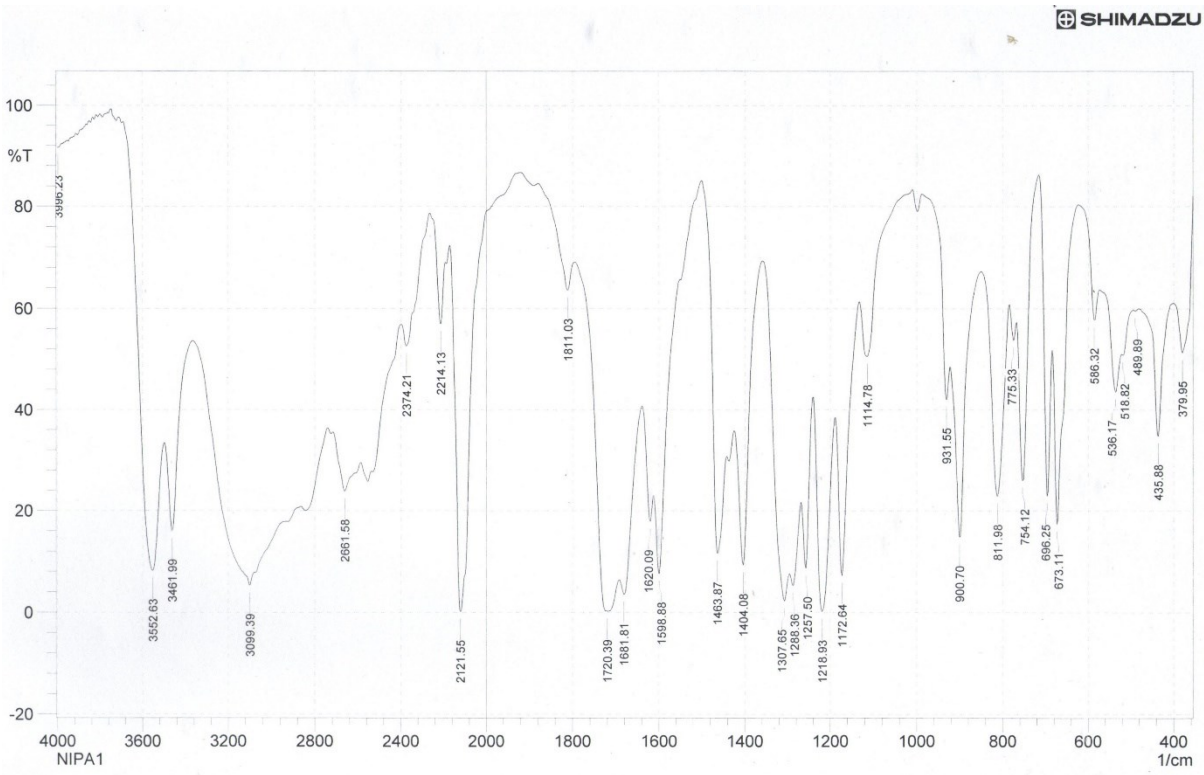


Figure S15: IR spectra of **5-N_3IPA.**

7. Rate law study of photocatalysis:

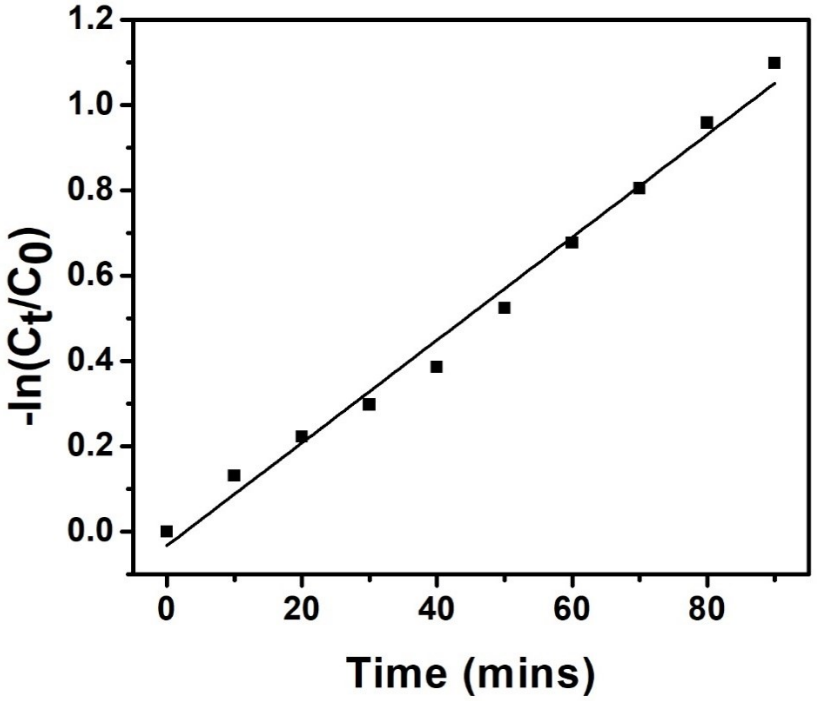


Figure S16: Rate law study of photodegradation of methyl orange in presence of compound **2.**

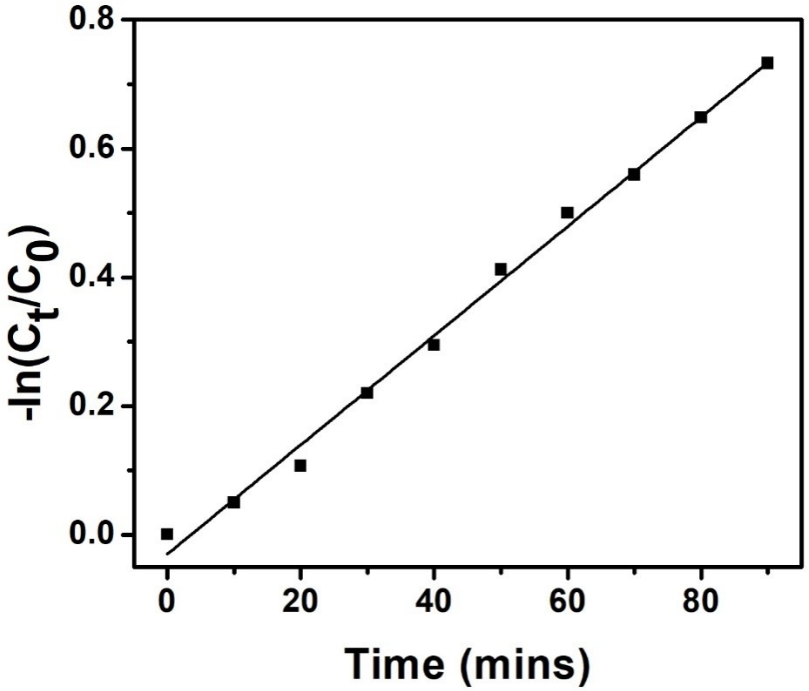


Figure S17: Rate law study of photodegradation of rhodamine B in presence of compound **2.**

8. Absorption spectra of solutions of methyl orange solution.

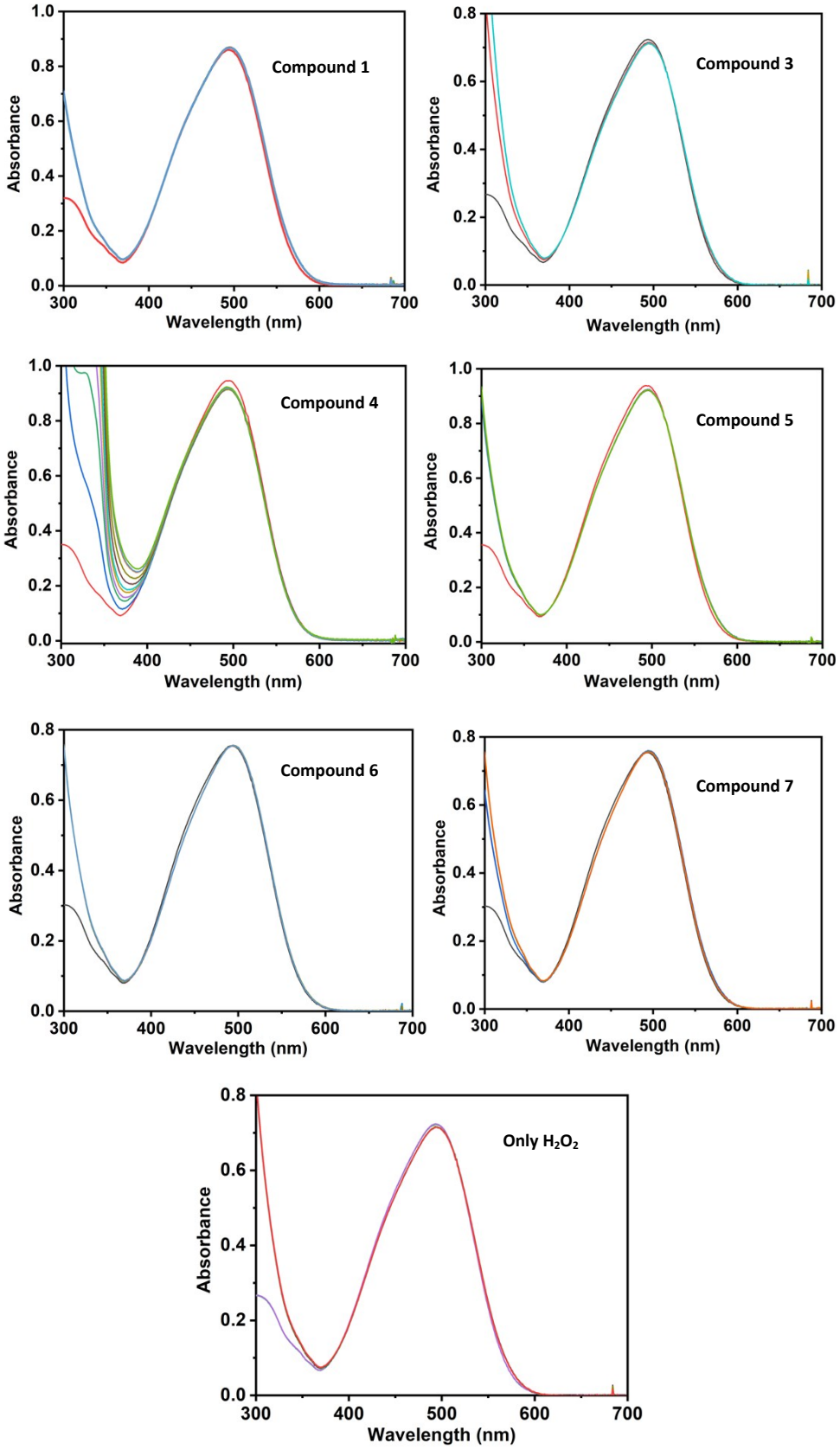


Figure S18: Absorption spectra of methyl orange solution in presence of H_2O_2 compound **1** and compound **3-7** under exposure of UV light at room temperature.

9. Absorption spectra of solutions of rhodamine B solution.

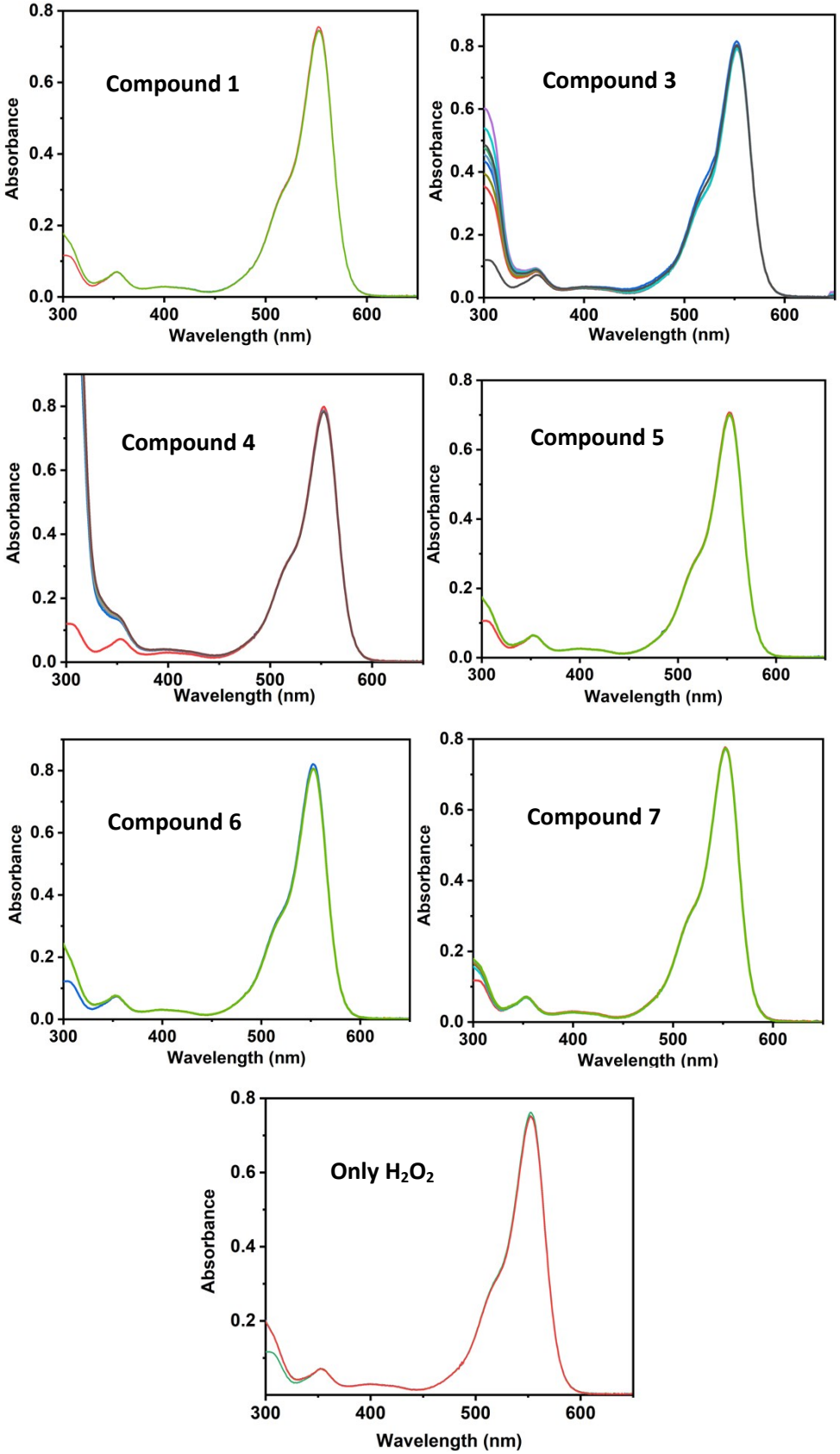


Figure S19: Absorption spectra of methyl orange solution in presence of H_2O_2 compound **1** and compound **3-7** under exposure of UV light at room temperature.

10. Reduction of 4- nitrophenol

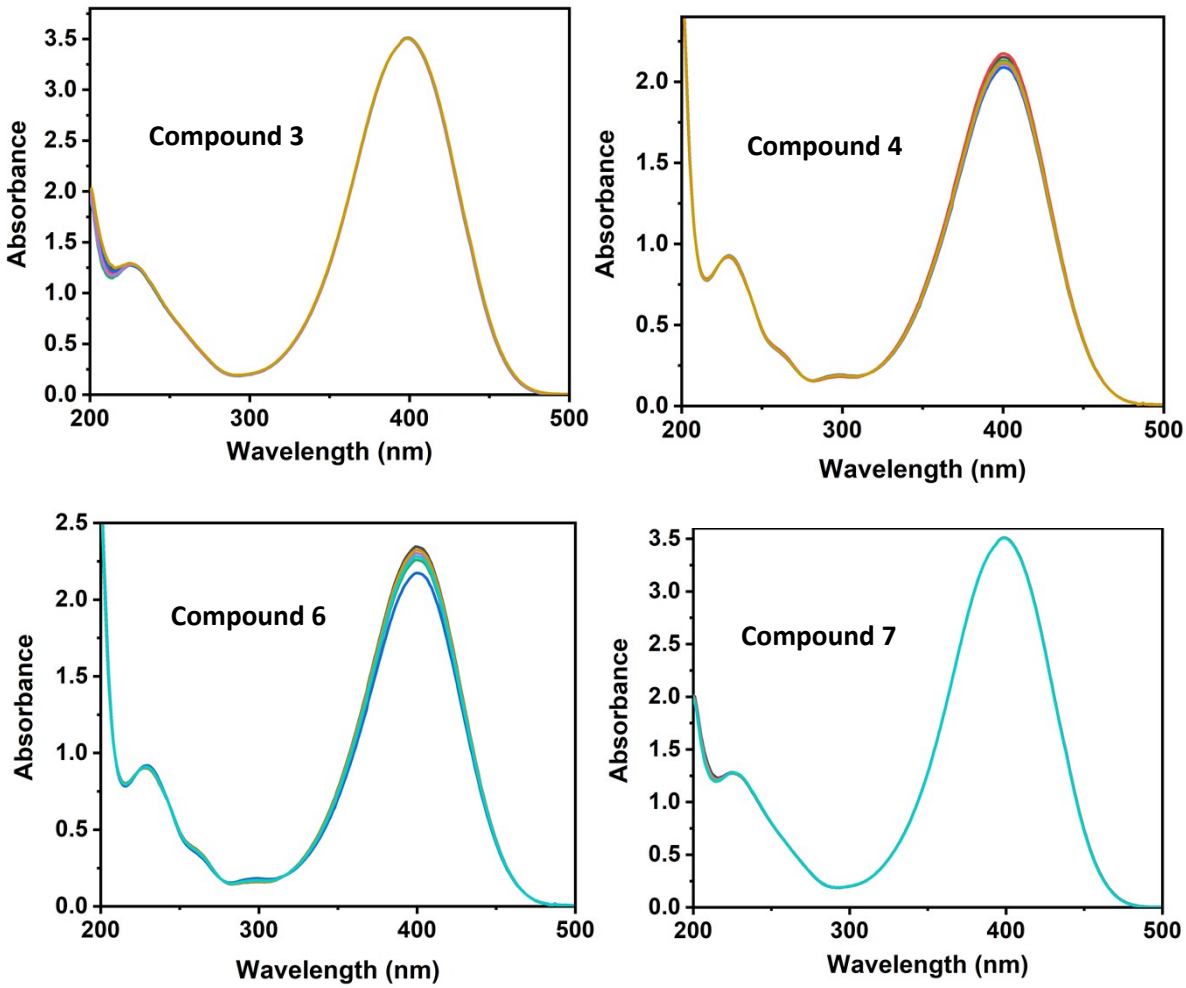


Figure S20: Reduction of 4-NP in presence of NaBH4 using compound **3**-**4** and compound **6**-**7.**

11. Gas adsorption isotherms

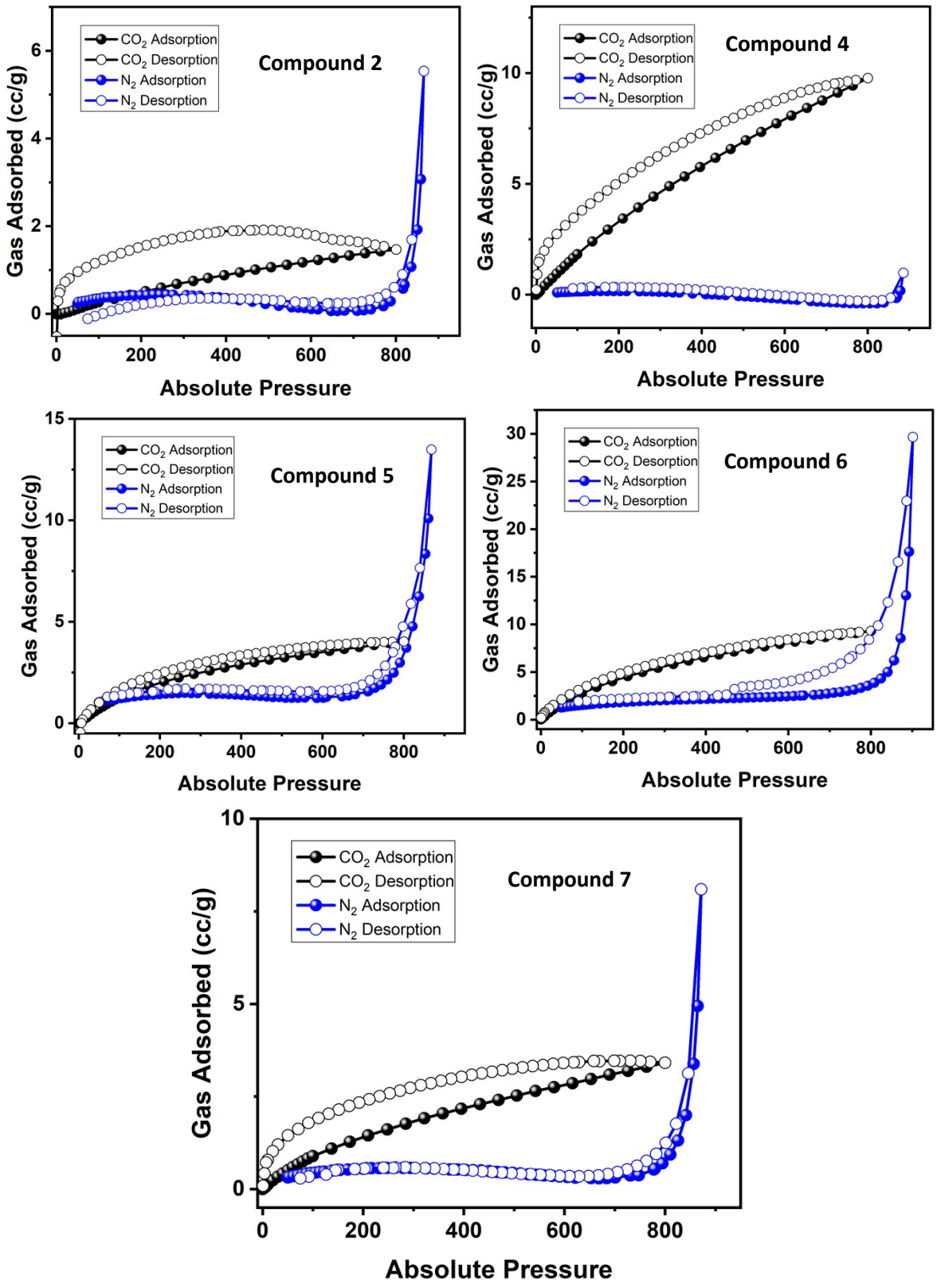
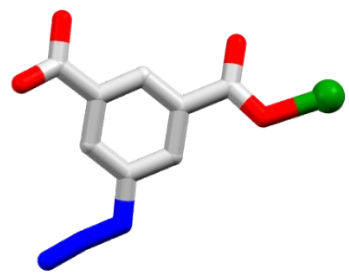
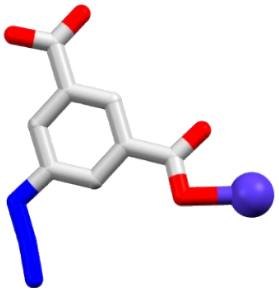


Figure S21: Gas adsorption isotherms of compound **2** and compounds **4**-**7**.

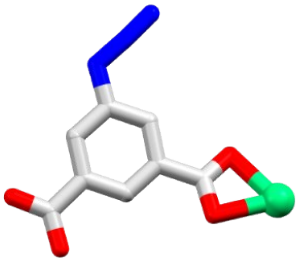
12. Coordination modes of carboxylic acid groups and the coordination geometry of the metal centres



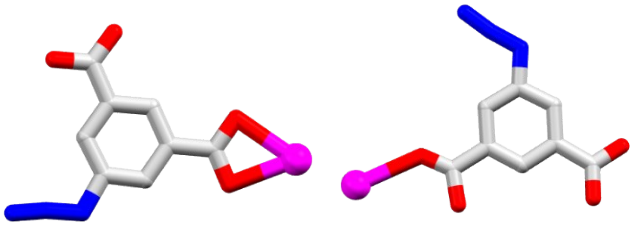
Compound **1**



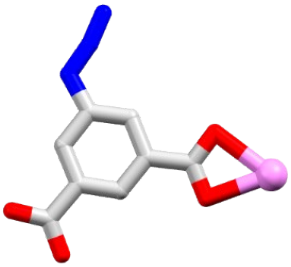
Compound **2**



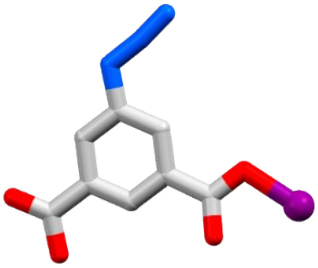
Compound **3**



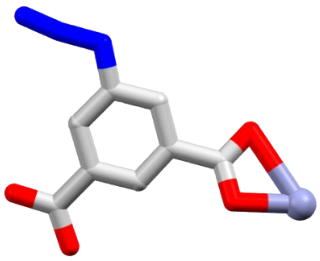
Compound **4**

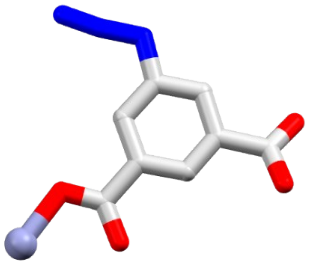


Compound **5**



Compound **6**





Compound **7**

Figure S22: Coordination modes of carboxylic acid groups adopted in compounds**1-7.**

Table SI-2: Detailed coordination geometry of the metal centres for compounds **1**-**7**.

Compounds	**Coordination mode of the carboxylic acid groups**	**Coordination geometry of the metal centers**
Compound **1**	monodentate, monodentate	square planner
Compound **2**	monodentate, monodentate	trigonal bipyramidal
Compound **3**	monodentate, monodentate monodentate, bidentate bidentate, bidentate	distorted octahedral
Compound **4**	monodentate, bidentate	pentagonal bipyramidal
Compound **5**	monodentate, bidentate	distorted octahedral
Compound **6**	monodentate, monodentate	tetrahedral
Compound **7**	monodentate, bidentate	distorted trigonal bipyramidal