Supporting information

A metal-organic framework based multifunctional catalytic platform for organic transformation and environmental remediation

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13	HRMS and ^{1}H-NMR spectra of 5-(2-thienyl)dipyrromethane	Figure S23, S24
14	TGA curves for iodine releasing profile during synthesis of 5-(2-thienyl)dipyrromethane and Histogram of %Yield vs reaction cycle	Figure S25 (a,b)
15	TEM image and EDAX pattern of I_2@Cd-MOF recovered after organic reaction	Figure S26 (a,b)
16	XRD patterns of Cd-MOF, Cd-MOF recovered after photocatalytic degradation of MB dye, I_2@Cd-MOF, recovered I_2@Cd-MOF after organic catalytic reaction	Figure S27 (a to d)
17	DRS spectra of Cd-MOF	Figure S28
18	TEM image and EDAX pattern of Cd-MOF recovered after photocatalytic dye degradation	Figure S29 (a, b)
19	Successive time dependent UV-vis spectra showing the photocatalytic degradation of MB under visible light irradiation from 2^{nd} to 4^{rth} cycles and under UV light irradiation	Figure S30(a to d)
20	Different reported MOFs used for the MB degradation	Table S2
21	Proposed mechanism for the MB degradation on the basis of peaks obtained in LC-MS	Figure S31
22	LC-MS spectra of MB degradation	Figure S32 to S34

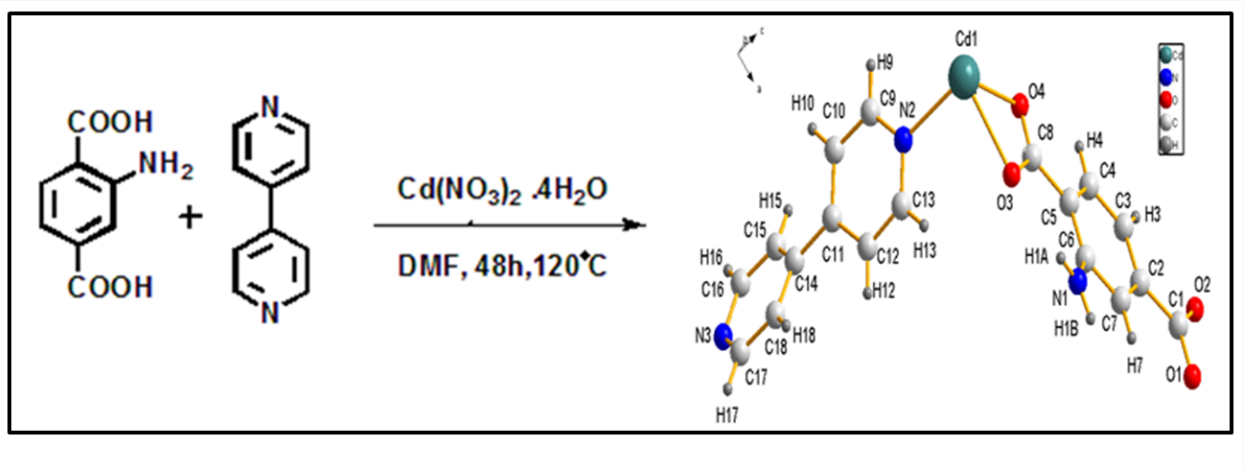


Figure S1. Synthesis scheme of Cd-MOF.

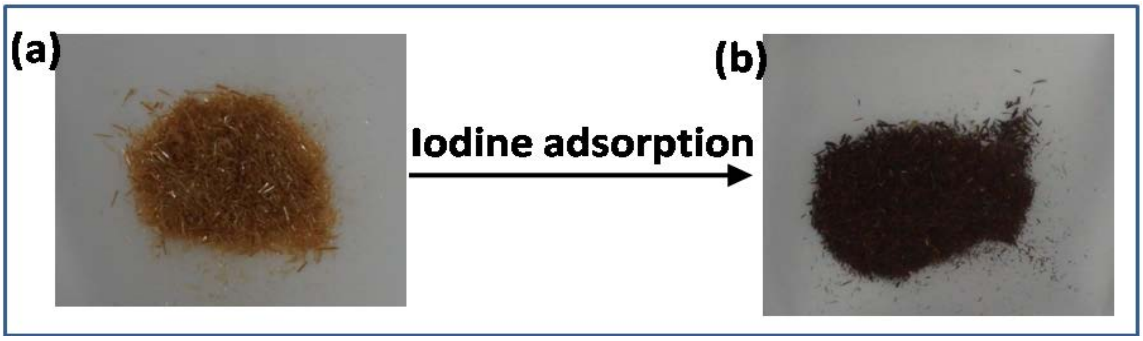


Figure S2. (a) Crystals of Cd-MOF and (b**)** Iodine@Cd-MOF.

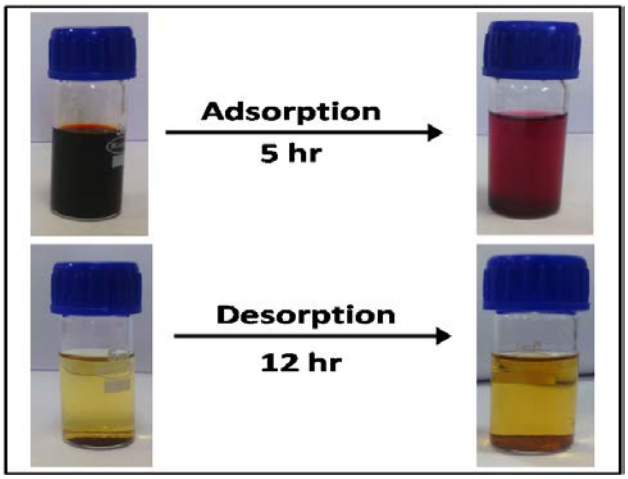


Figure S3. Iodine adsorption and desorption.

Table S1. Crystal data and structure refinement for Cd-MOF.

1.	Identification code	Cd-MOF
2.	Emperical Formula	$C_{18}H_8CdN_3O_4$
3.	Formula weight	442.67
4.	Temperature/K	150.00(10)
5.	Crystal System	Orthorhombic
6.	Space group	$P2_12_12$
7.	Unit Cell dimensions	a/Å=20.9793(4), **b/Å**=13.5240(4) **c/Å**=11.6673(3), **α/°** =90.00, **β/°** =90.00, **γ/°** =90.00
8.	Volume/ $Å^3$	3310.29(13)
9.	Z	4
10.	$P_{calc}g/cm^3$	0.888
11.	$\mu\ mm^{-1}$	0.674
12.	F(000)	868.0
13.	Crystal size/mm^3	0.354×0.151×0.128
14.	2θ range for data collection	3.88 to 56.56
15.	Index ranges	$-27 \leq h \leq 23, -17 \leq k \leq 11, -14 \leq l \leq 11$

16.	Reflection collected	7832
17.	Independent reflections	6201[R_{int}= 0.0211, R_{sigma}= 0.0516
18.	Goodness-of-fiton F^2	1.181
19.	Final R indexes[I>2σ(1)]	R_1= 0.0713, wR_2= 0.2217
20.	Final R indexes(all data)	R_1= 0.0753, wR_2= 0.2289
21.	Largest diff. peak/ hole/e$Å^{-3}$	1.66/-1.12
22.	Flack parameter	0.44 (7)

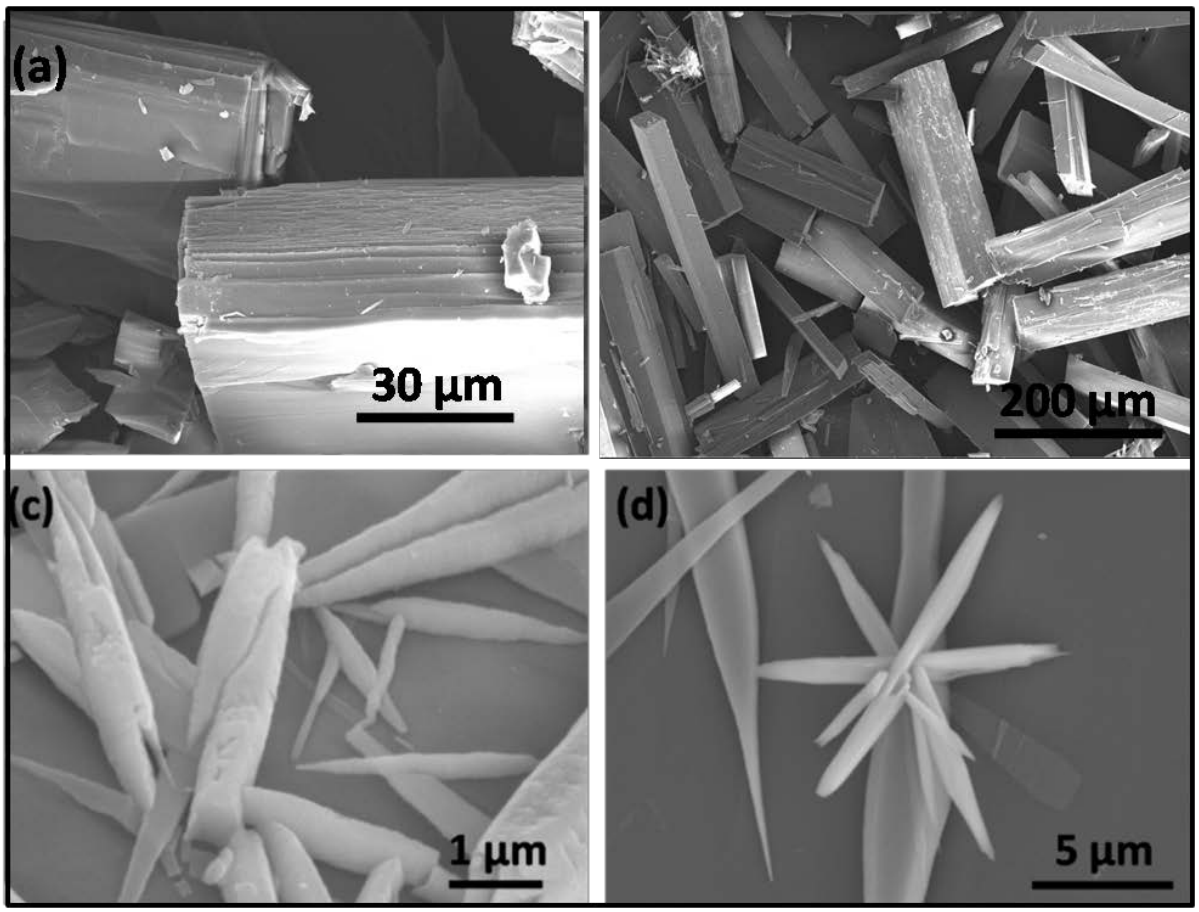


Figure S4. SEM images of Cd-MOF (a, b) and Iodine captured Cd-MOF (c,d).

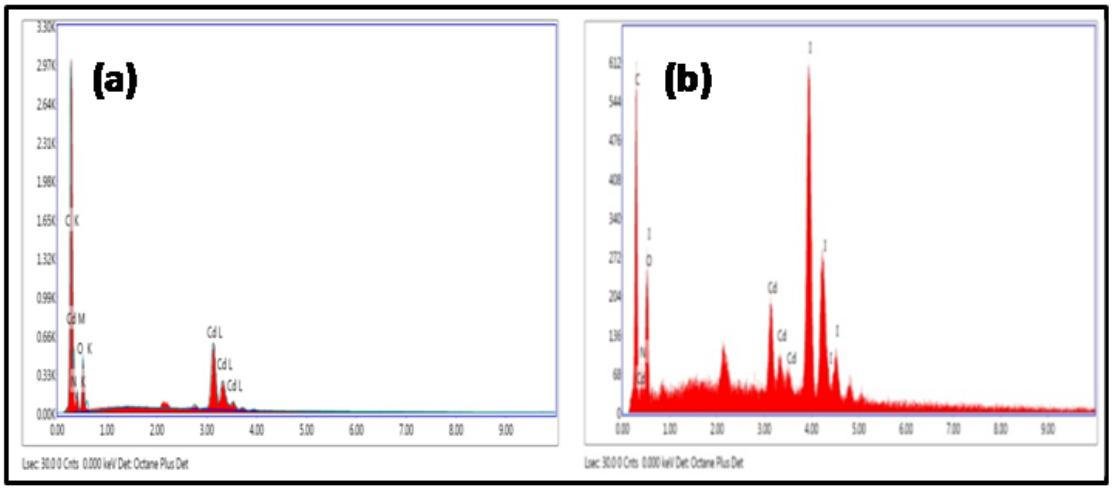


Figure S5. EDAX patterns of (a) Cd-MOF. (b) Iodine captured Cd-MOF.

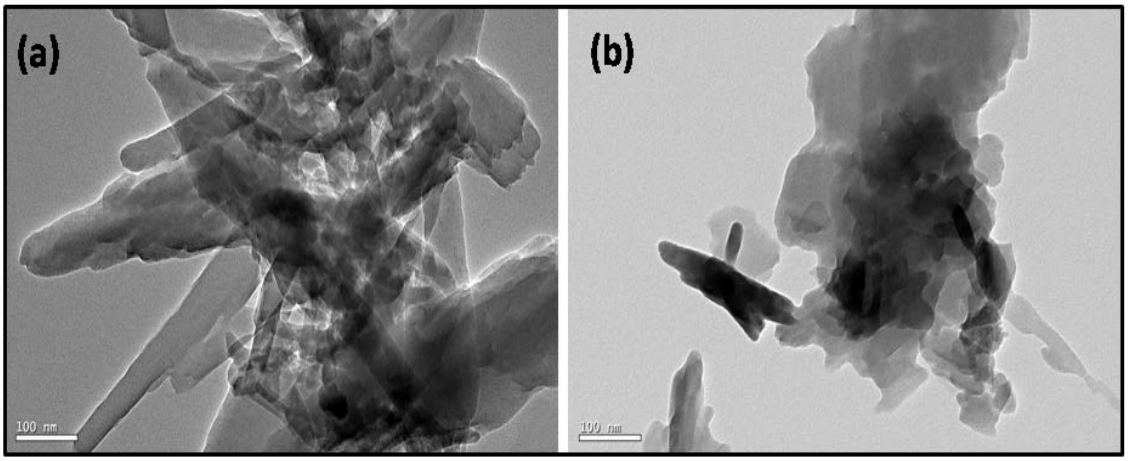
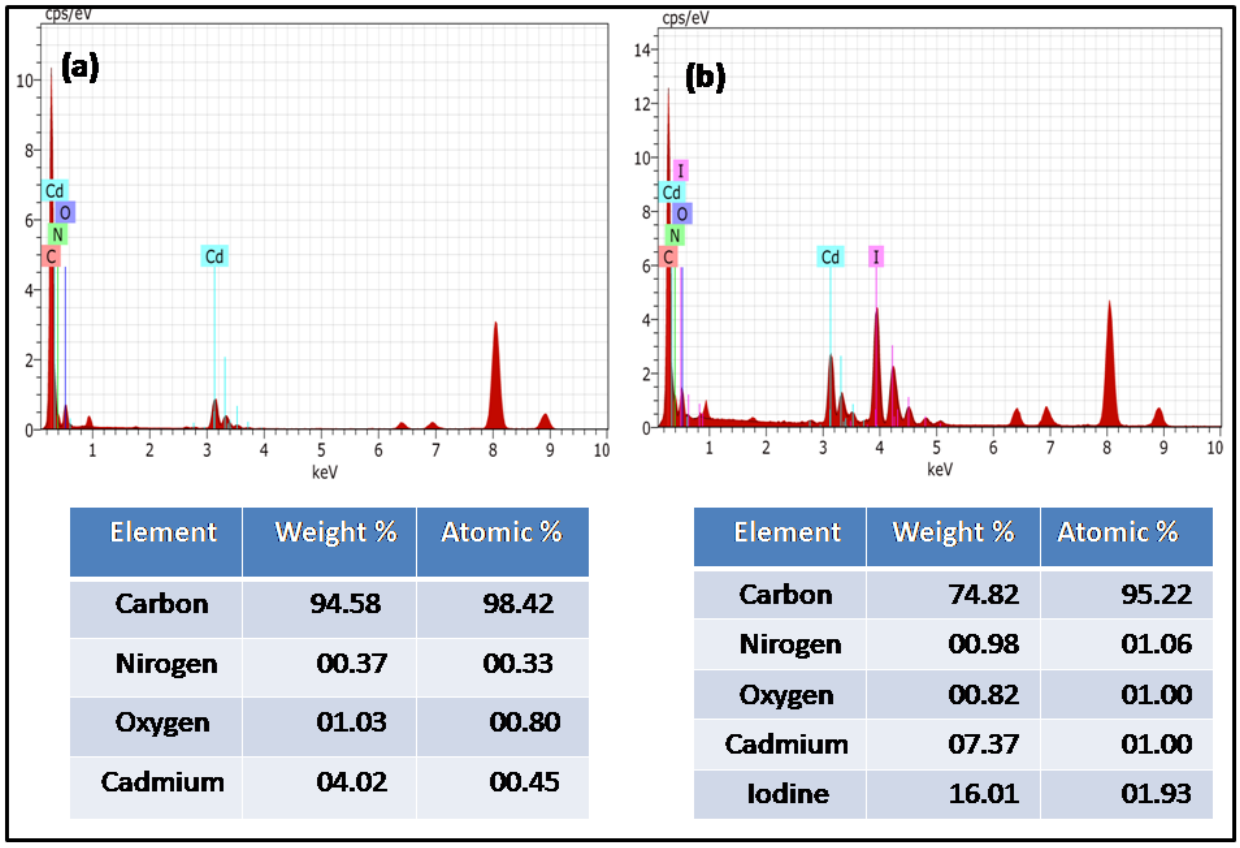


Figure S6. TEM images of (a) Cd-MOF. (b) Iodine captured Cd-MOF.



Element	Weight %	Atomic %
Carbon	94.58	98.42
Nirogen	00.37	00.33
Oxygen	01.03	00.80
Cadmium	04.02	00.45

Element	Weight %	Atomic %
Carbon	74.82	95.22
Nirogen	00.98	01.06
Oxygen	00.82	01.00
Cadmium	07.37	01.00
Iodine	16.01	01.93

Figure S7. EDAX patterens of (a) Cd-MOF. (b) Iodine captured Cd-MOF.

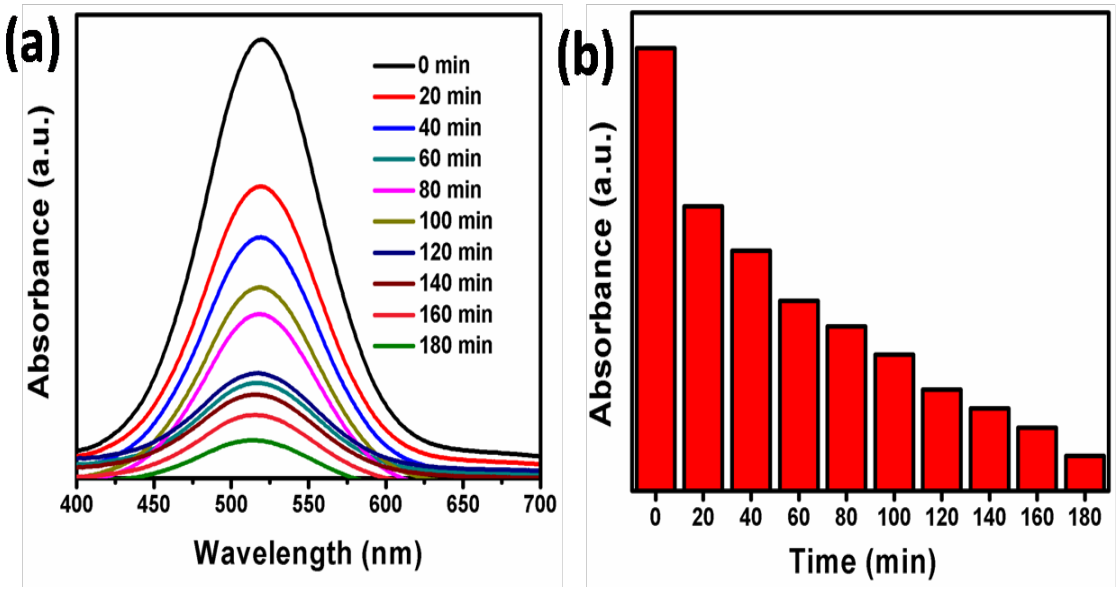


Figure S8. (a) UV-vis absorbance spectra of 0.1M hexane solution of iodine. (b) Histogram of 0.1M hexane solution of iodine.

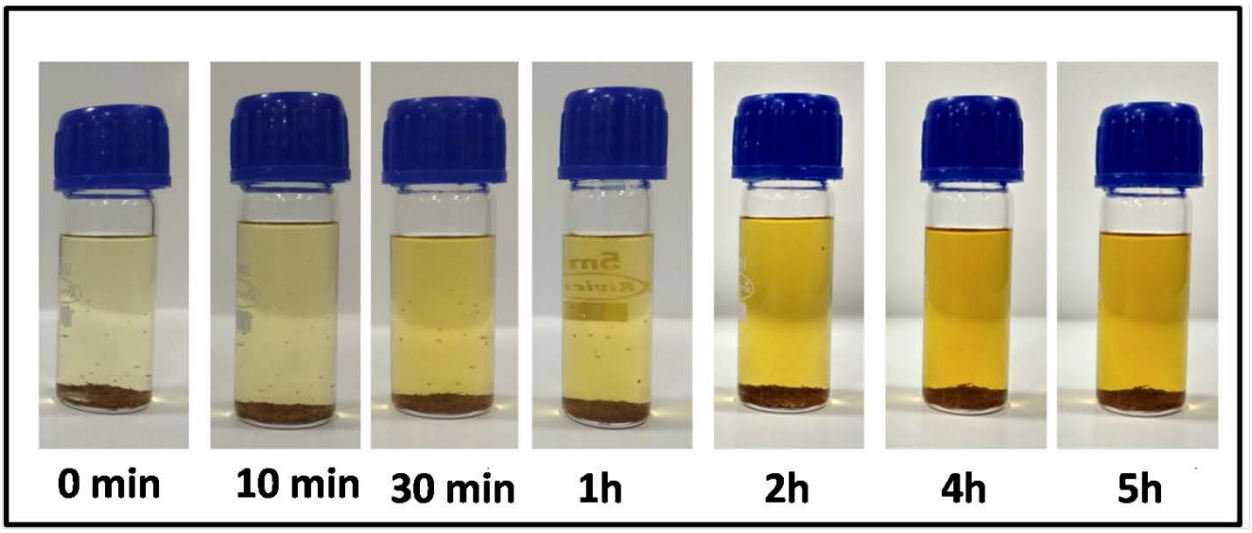


Figure S9: Photographs showing color change of ethanol sloution containing Iodine loaded MOF crystals .

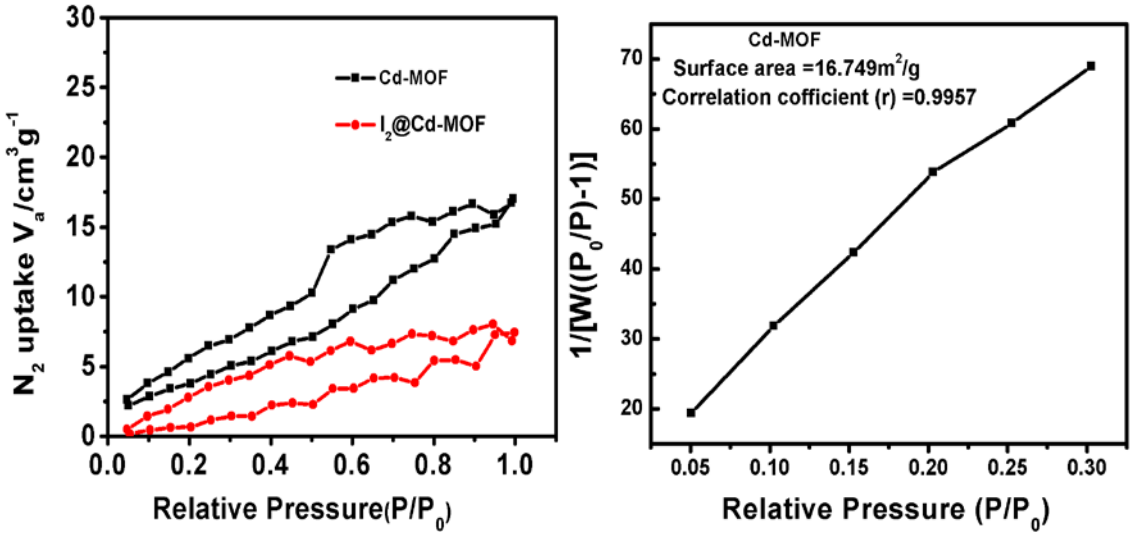


Figure S10. N_2 adsorption isotherms of Cd-MOF and Iodine loaded MOF (Iodine@Cd-MOF). On the basis of N_2 adsorption studies, BET surface area for Cd-MOF and I_2@Cd-MOF at 77K was found to be 16.749 m^2/g and 12.463 m^2/g respectively.

Measurements	Cd-MOF	I_2@Cd-MOF
Volume of N_2 gas adsorbed (cm^3g^{-1})	17.186	7.549
BET- Surface Area(m^2/g)	16.749	12.463
Pore Radius ($\mathring{A}$)	21.505	16.924

HRMS and ^{1}H-NMR data of various benzimidazole derivatives:

Figure S11. HRMS spectra of 2-phenyl-1H-benzo[d]imidazole in MeOH.

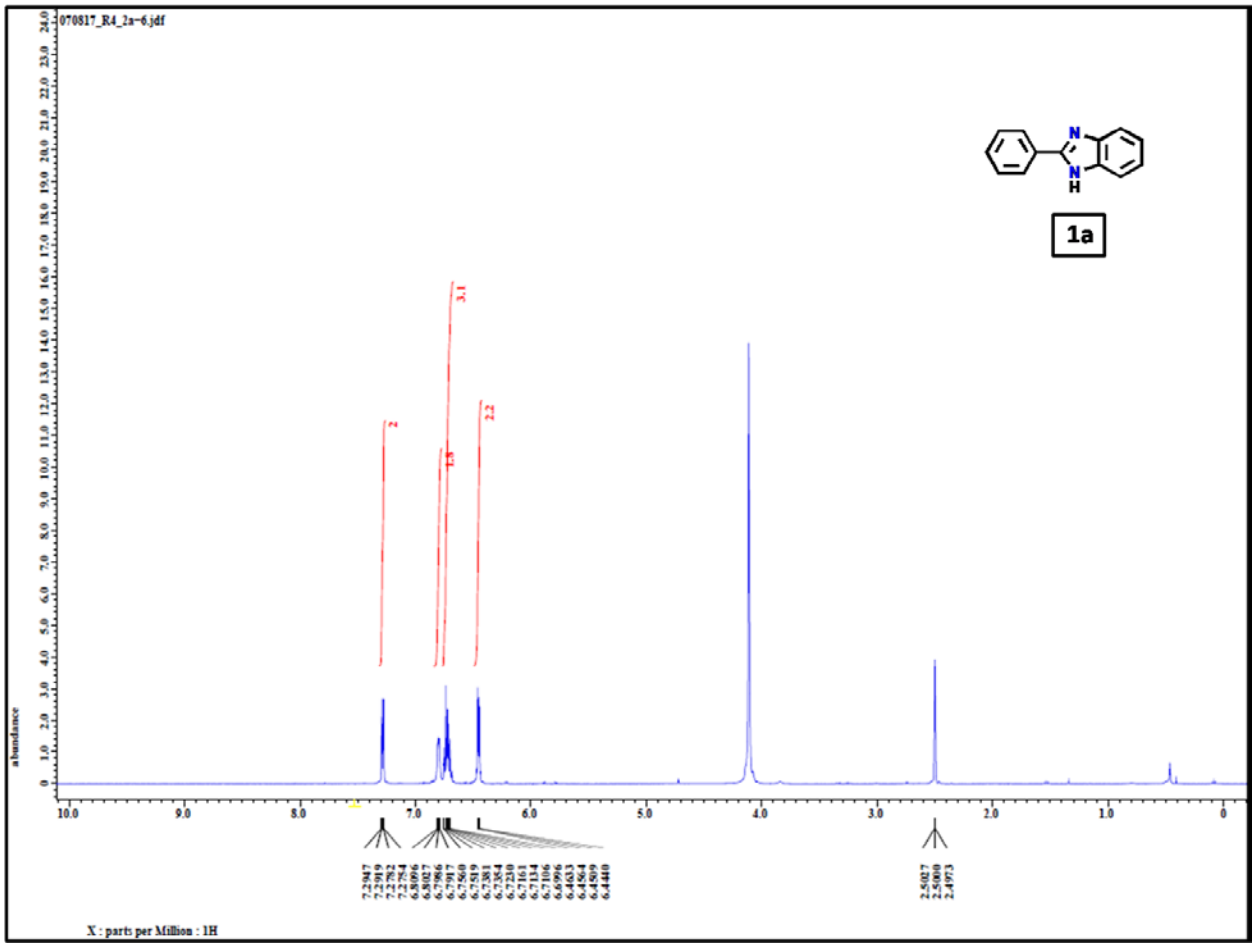


Figure S12. ^{1}H-NMR spectra of 2-phenyl-1H-benzo[d]imidazole in DMSO-d_6.

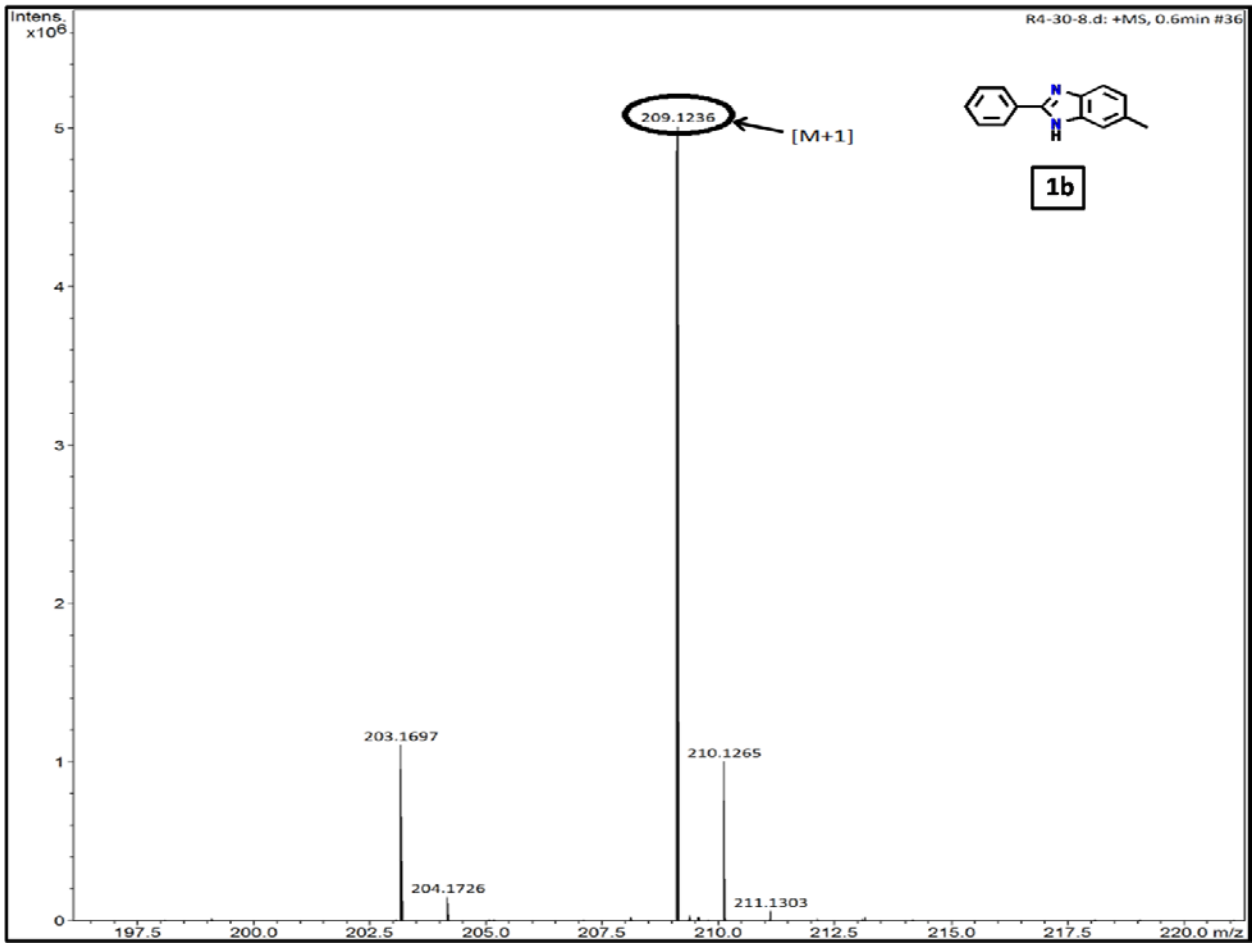


Figure S13. HRMS spectra of 6-methyl-2-phenyl-1H-benzo[d]imidazole in MeOH.

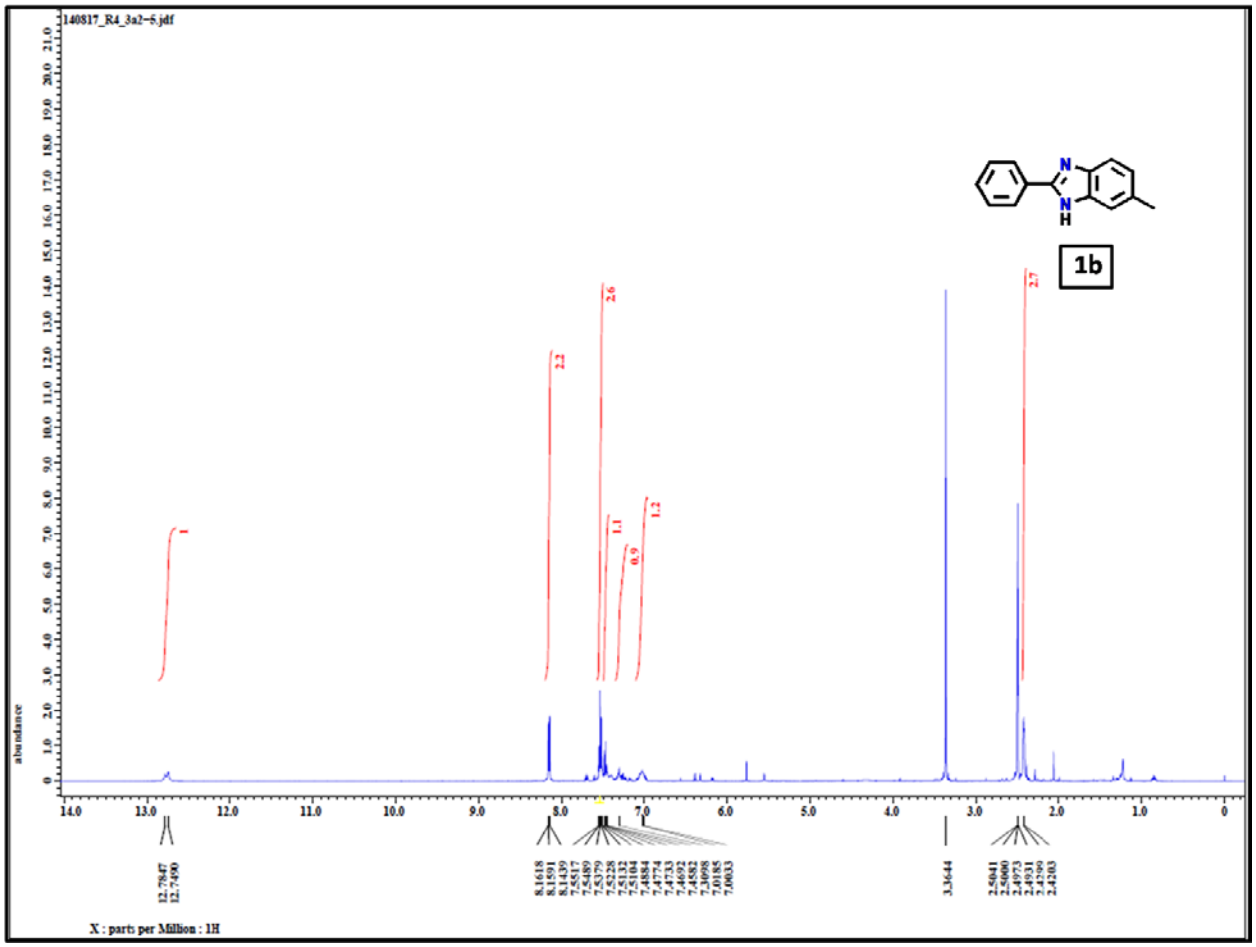


Figure S14. ^{1}H-NMR spectra of 6-methyl-2-phenyl-1H-benzo[d]imidazole in DMSO-d_6.

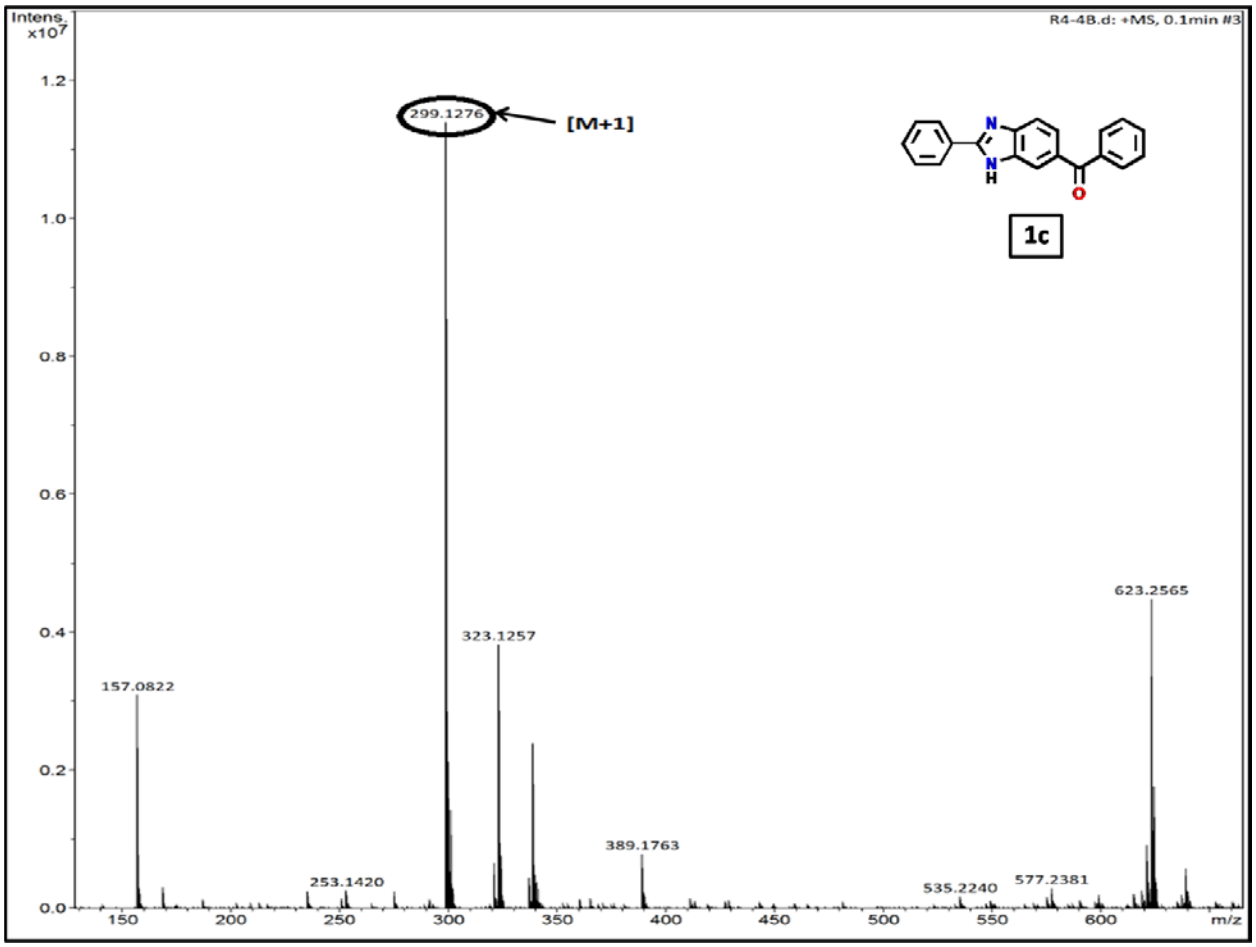


Figure S15. HRMS spectra of phenyl(2-phenyl-1H-benzo[d]imidazol-5-yl)methanone in MeOH.

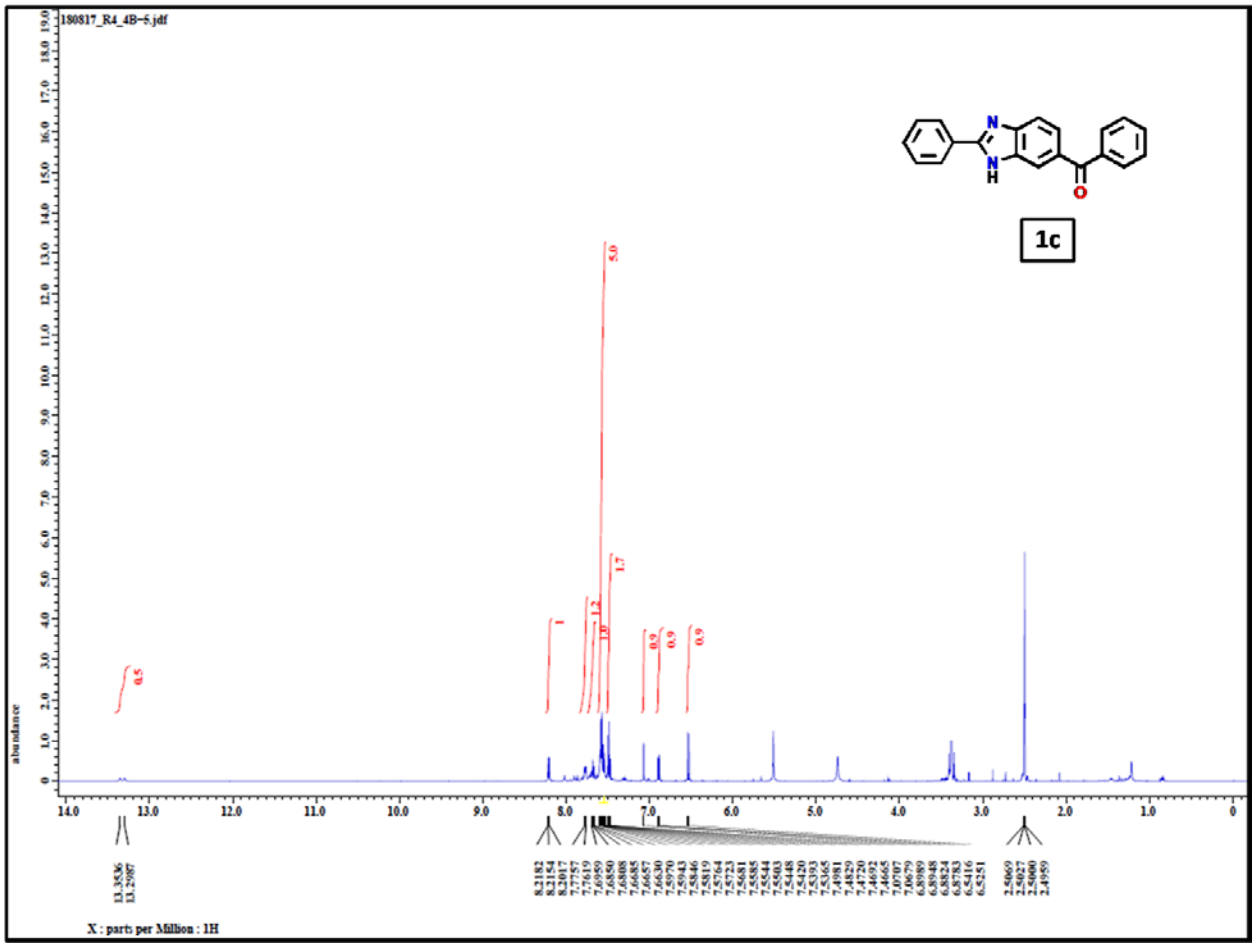


Figure S16. ^{1}H-NMR spectra of phenyl(2-phenyl-1H-benzo[d]imidazol-5-yl)methanone in DMSO-d_6.

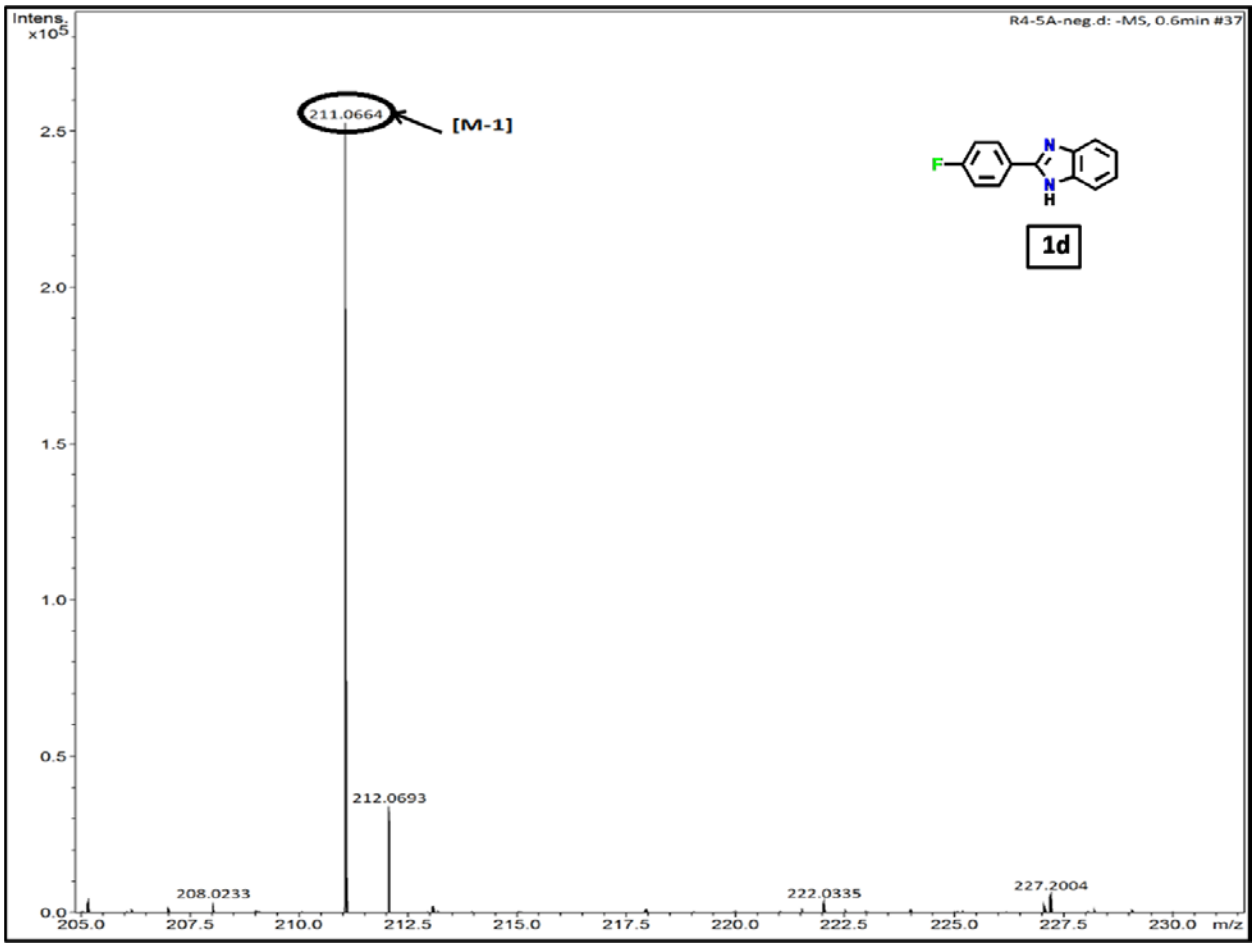


Figure S17. HRMS spectra of 2-(4-fluorophenyl)-1H-benzo[d]imidazole in MeOH.

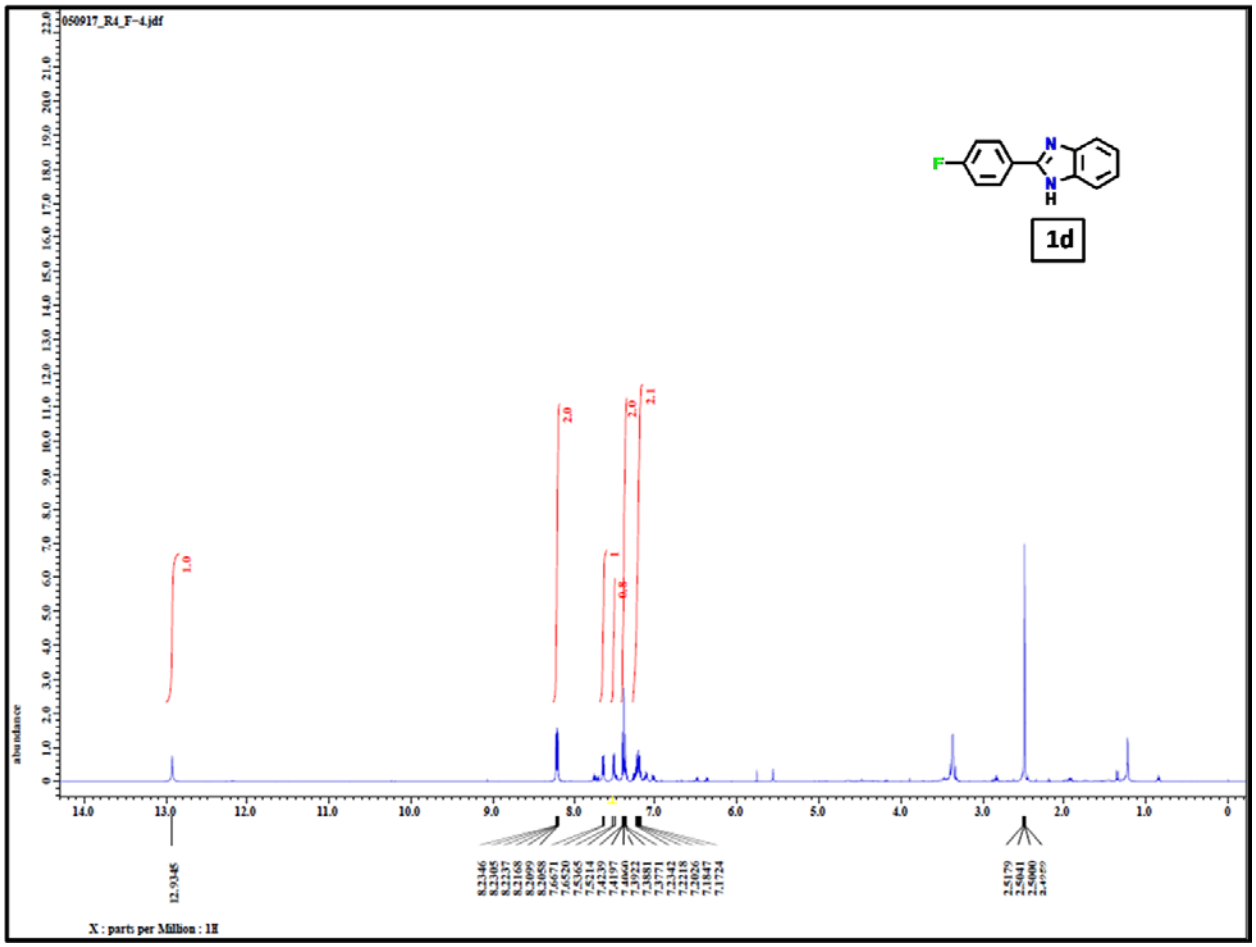


Figure S18. ^{1}H-NMR spectra of 2-(4-fluorophenyl)-1H-benzo[d]imidazole in DMSO-d_6.

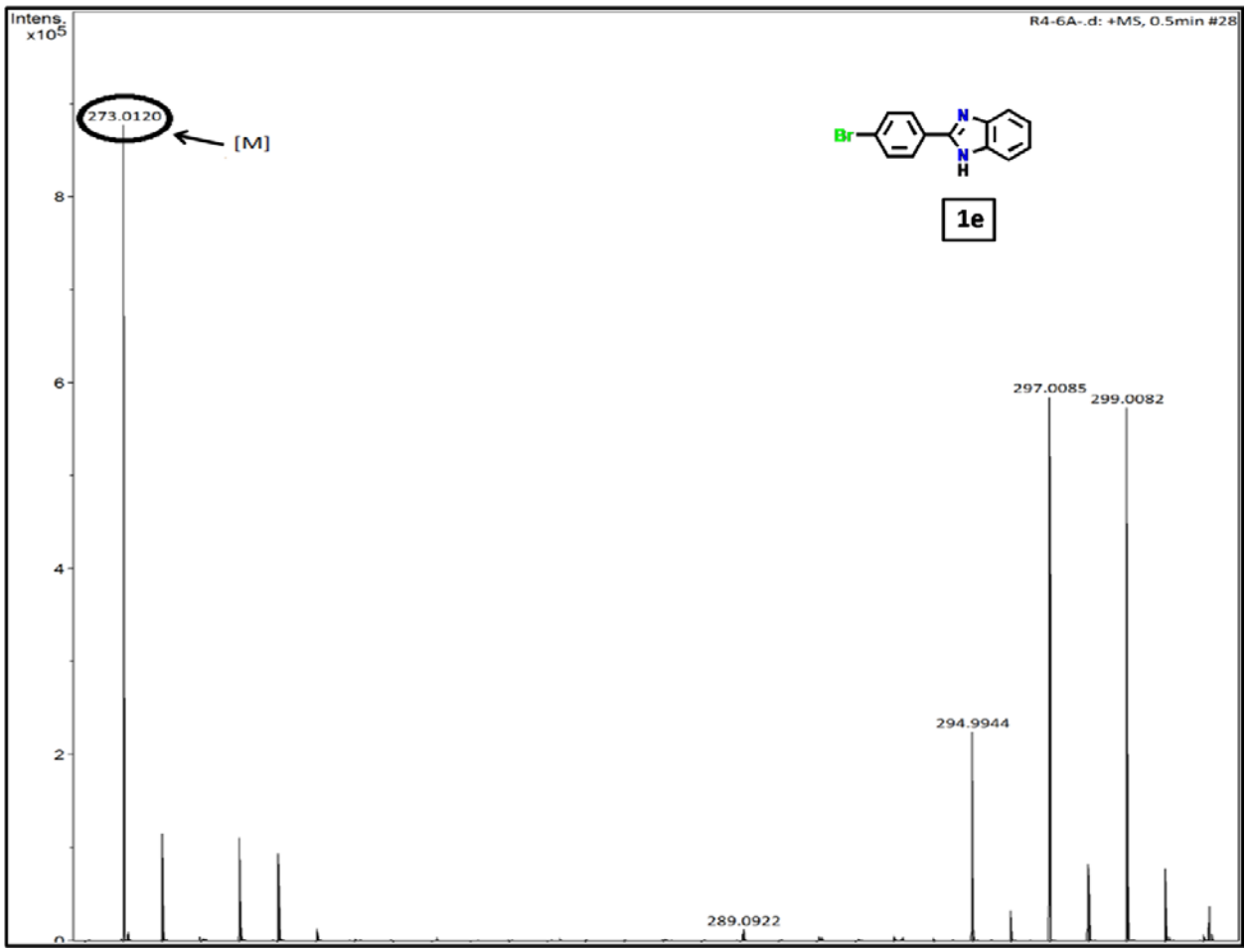


Figure S19. HRMS spectra of 2-(4-bromophenyl)-1H-benzo[d]imidazole in MeOH.

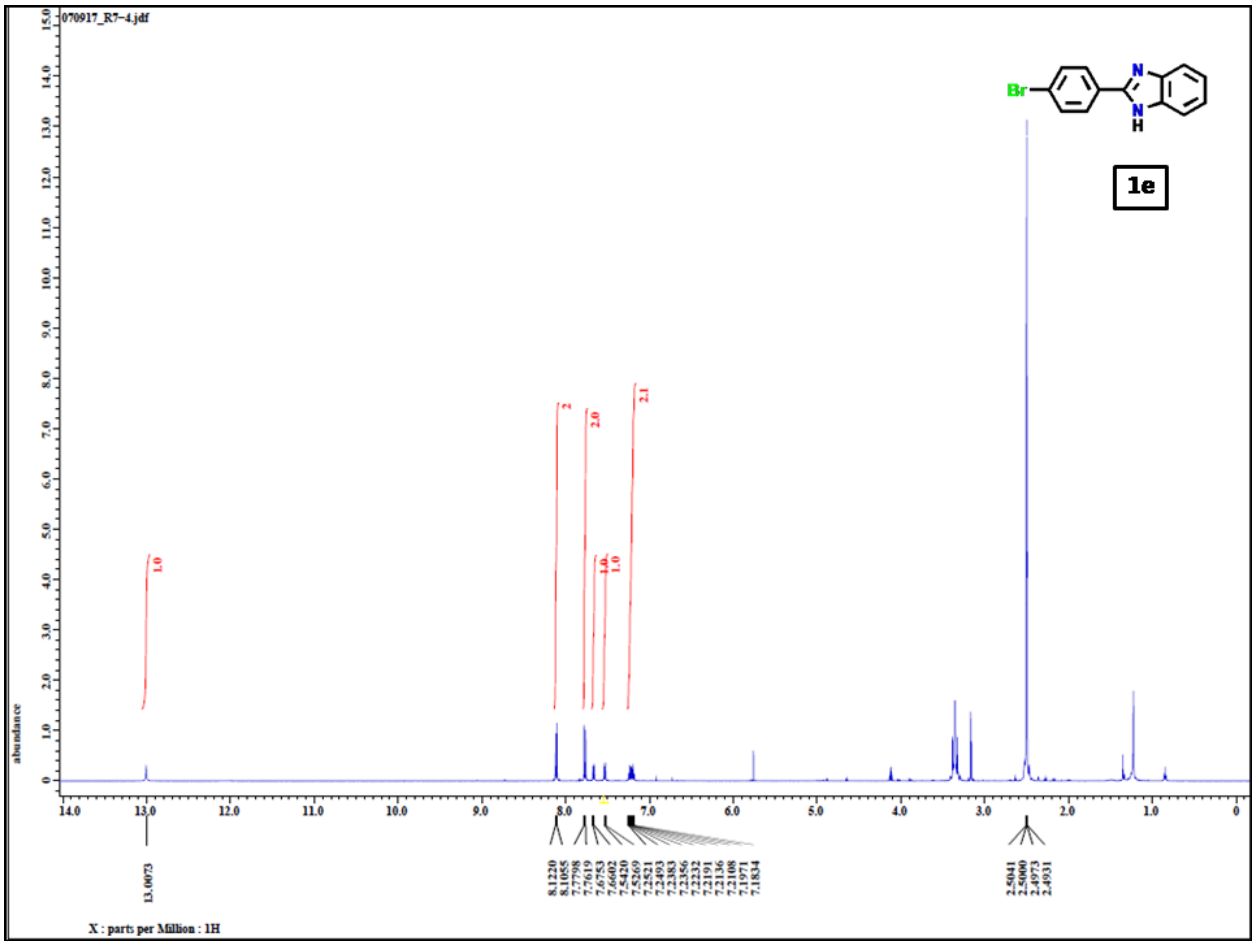


Figure S20. ^{1}H-NMR spectra of 2-(4-bromophenyl)-1H-benzo[d]imidazole in DMSO-d_6.

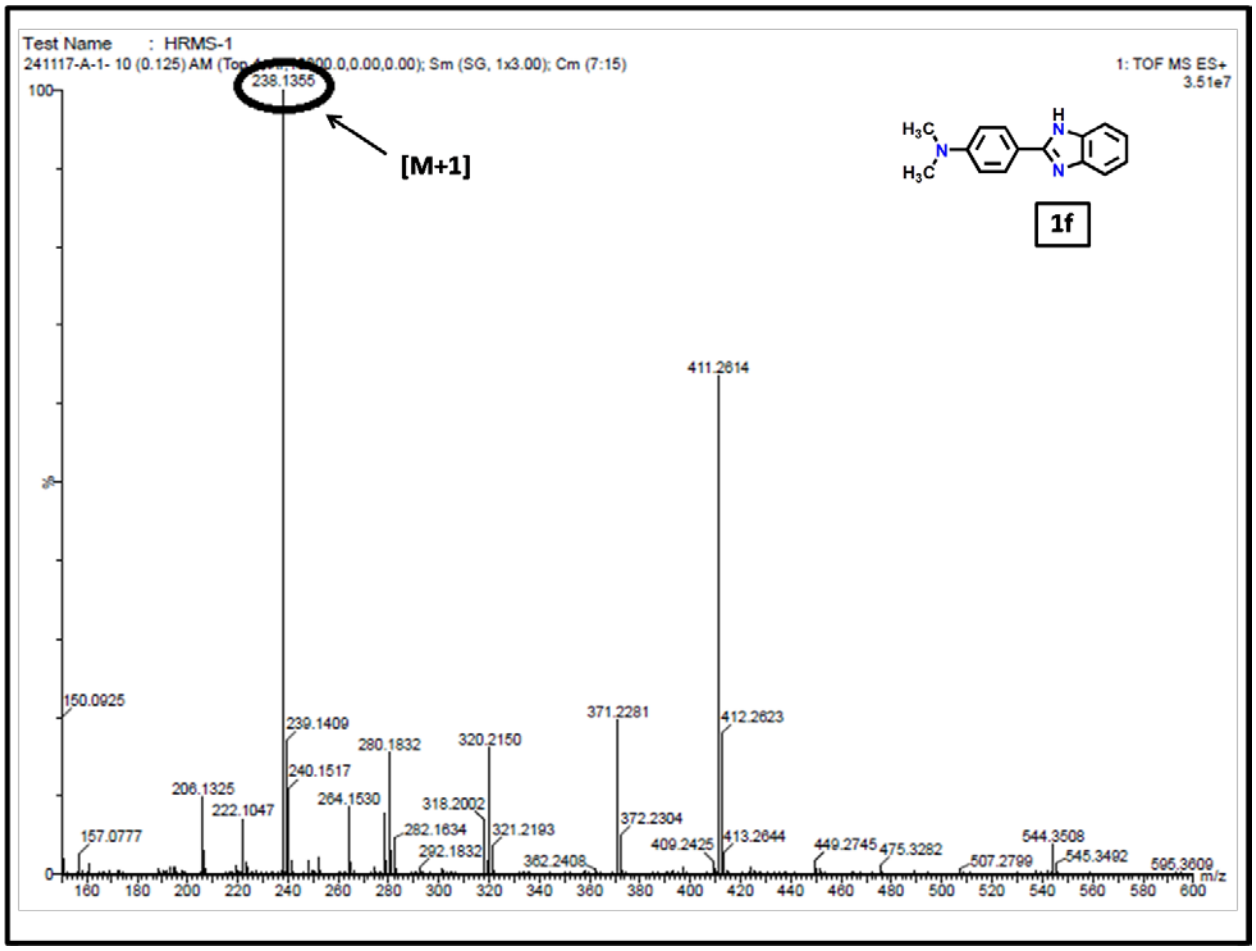


Figure S21. HRMS spectra of 4-(1H-benzo[d]imidazol-2-yl)-N,N-dimethylbenzenamine in MeOH.

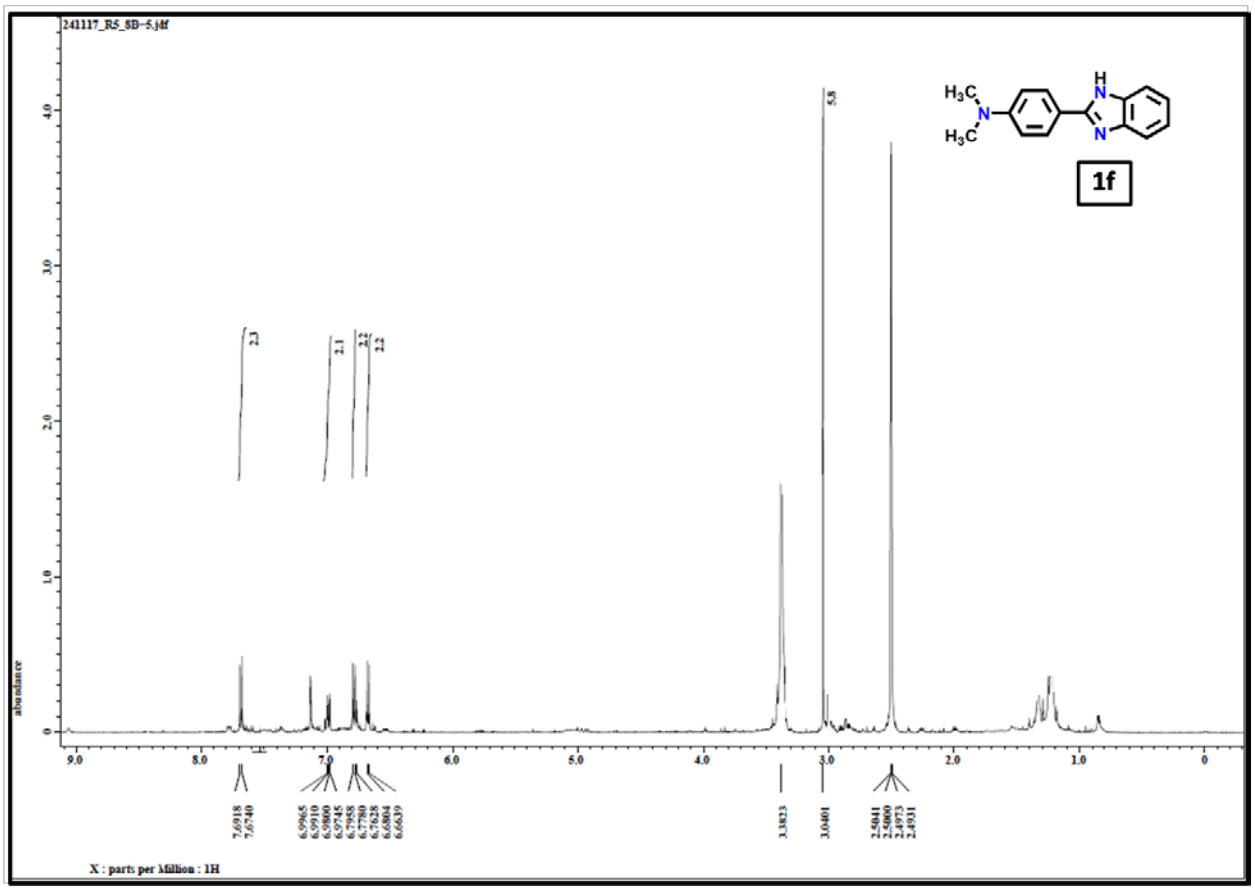


Figure S22. ^{1}H-NMR spectra of 4-(1H-benzo[d]imidazol-2-yl)-N,N-dimethylbenzenamine in DMSO-d_6.

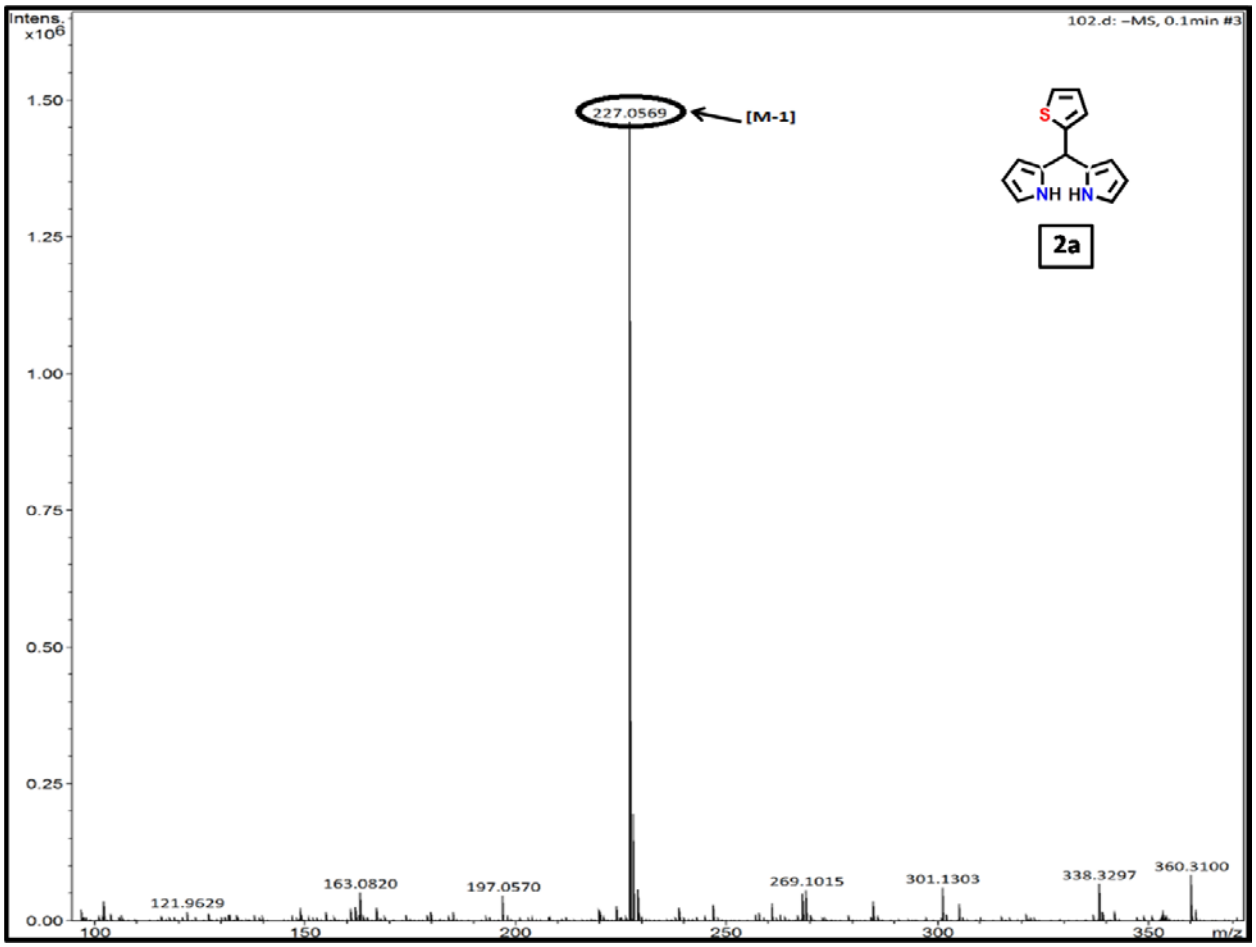


Figure S23. HRMS spectra of 5-(2-thienyl)dipyrromethane in MeOH.

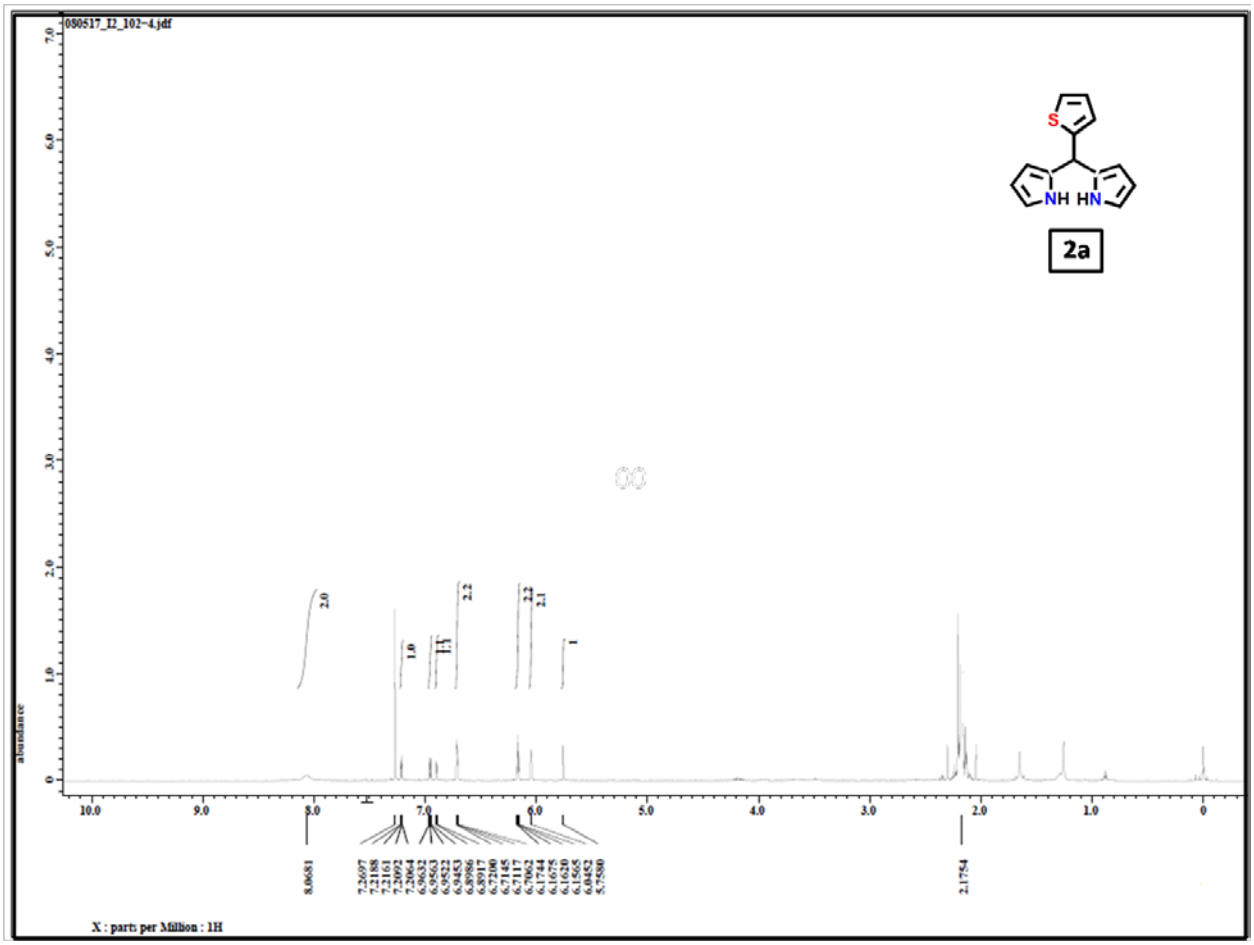


Figure S24. ^{1}H-NMR spectra of 5-(2-thienyl)dipyrromethane in $CDCl_3$.

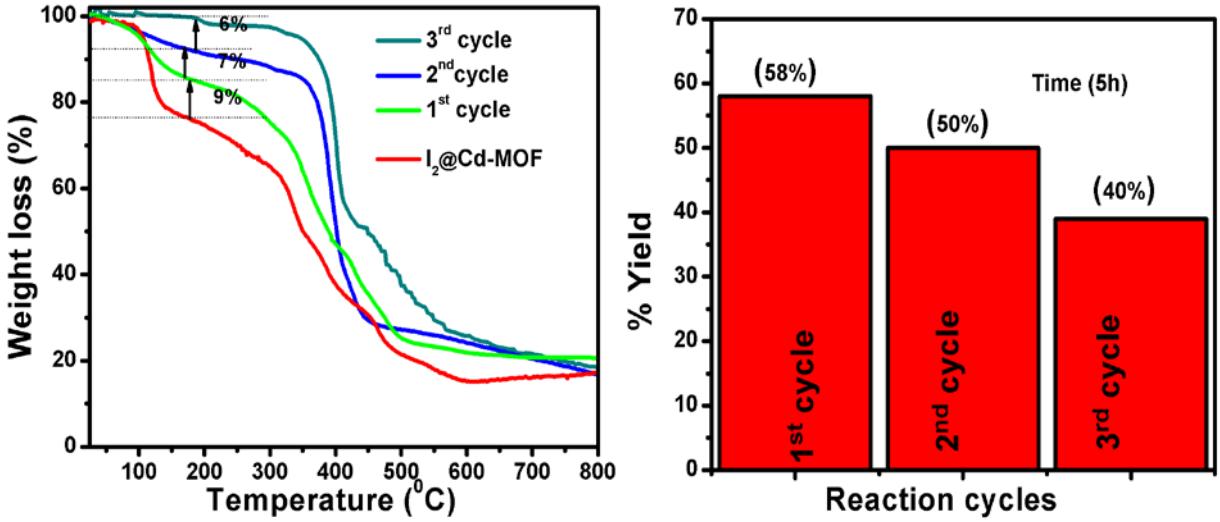
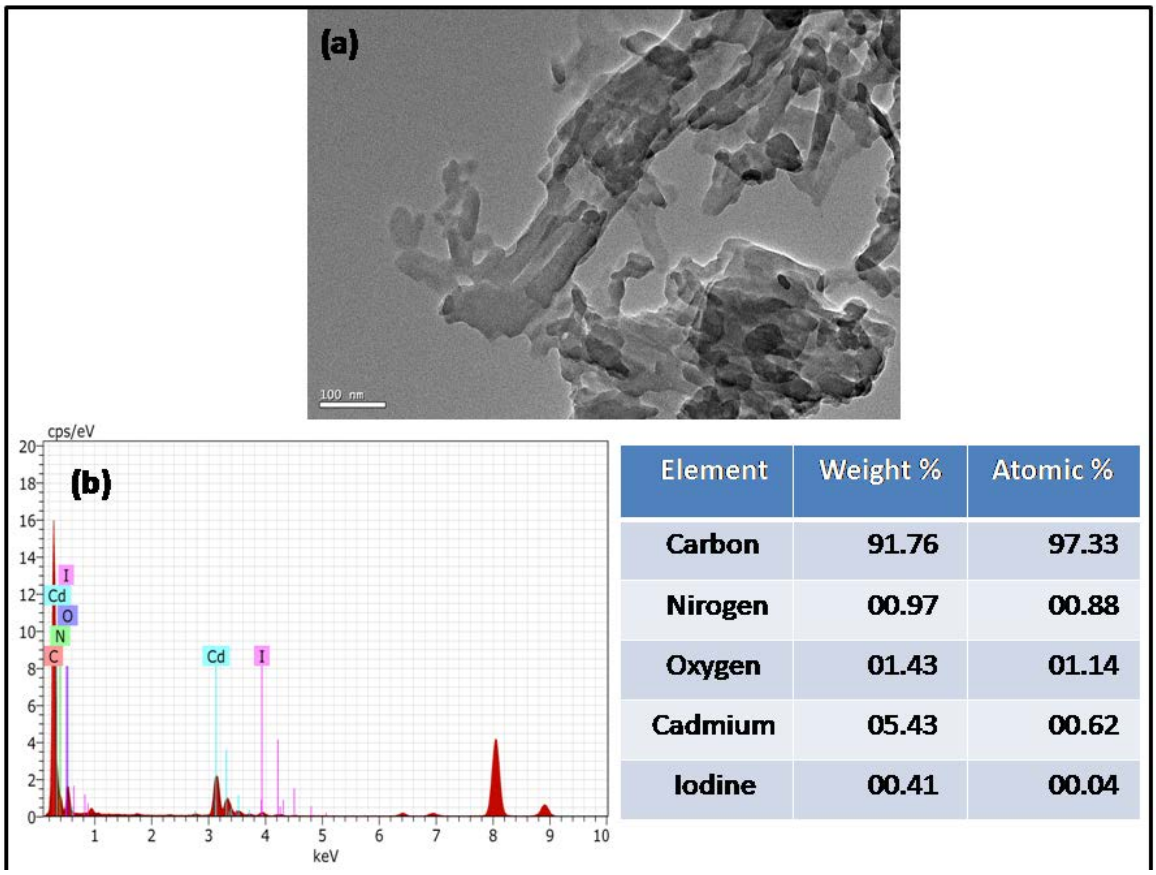


Figure S25. (a) TGA curve for Iodine releasing profile during the synthesis of 5-(2-thienyl)dipyrromethane. **(b)** % Yield in each consecutive cycles during synthesis of 5-(2-thenyl)dipyrromethane.



Element	Weight %	Atomic %
Carbon	91.76	97.33
Nirogen	00.97	00.88
Oxygen	01.43	01.14
Cadmium	05.43	00.62
Iodine	00.41	00.04

Figure S26. TEM image (a) and EDAX pattern (b) of I_2@Cd-MOF recovered after organic reaction.

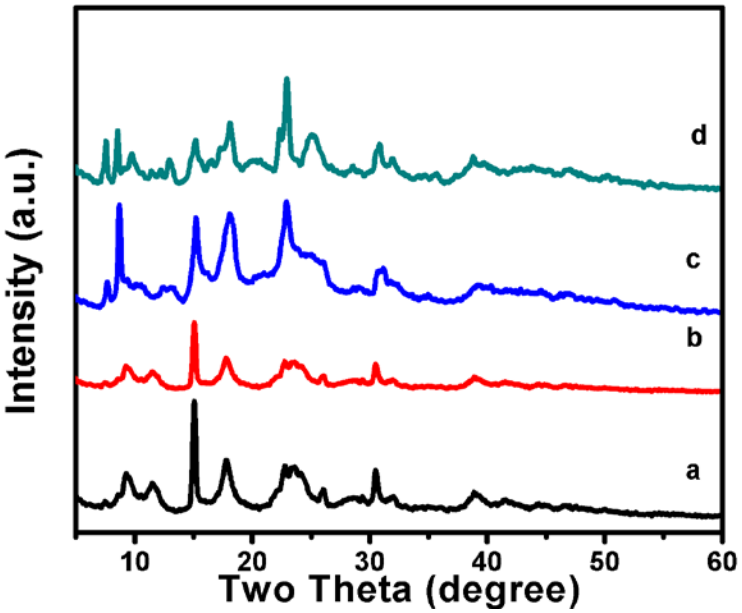


Figure S27. XRD patterns of (a) Cd-MOF. (b) Cd-MOF recovered after photocatalytic degradation of MB dye. (c) I_2@Cd-MOF. (d) I_2@Cd-MOF recovered after organic catalytic reaction.

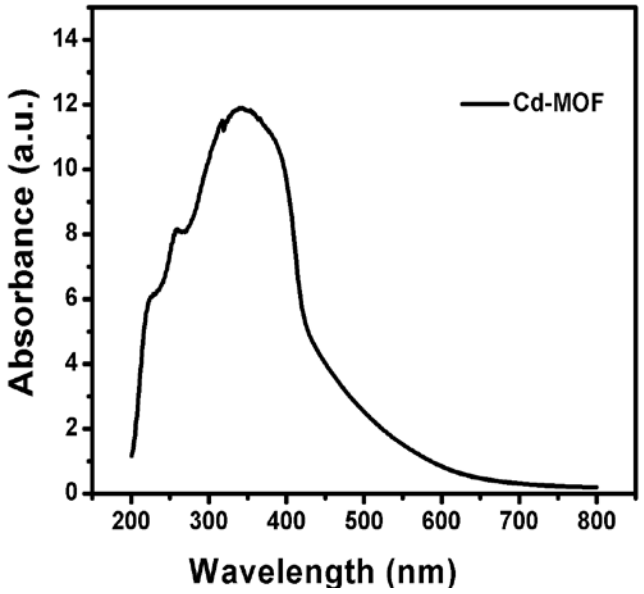
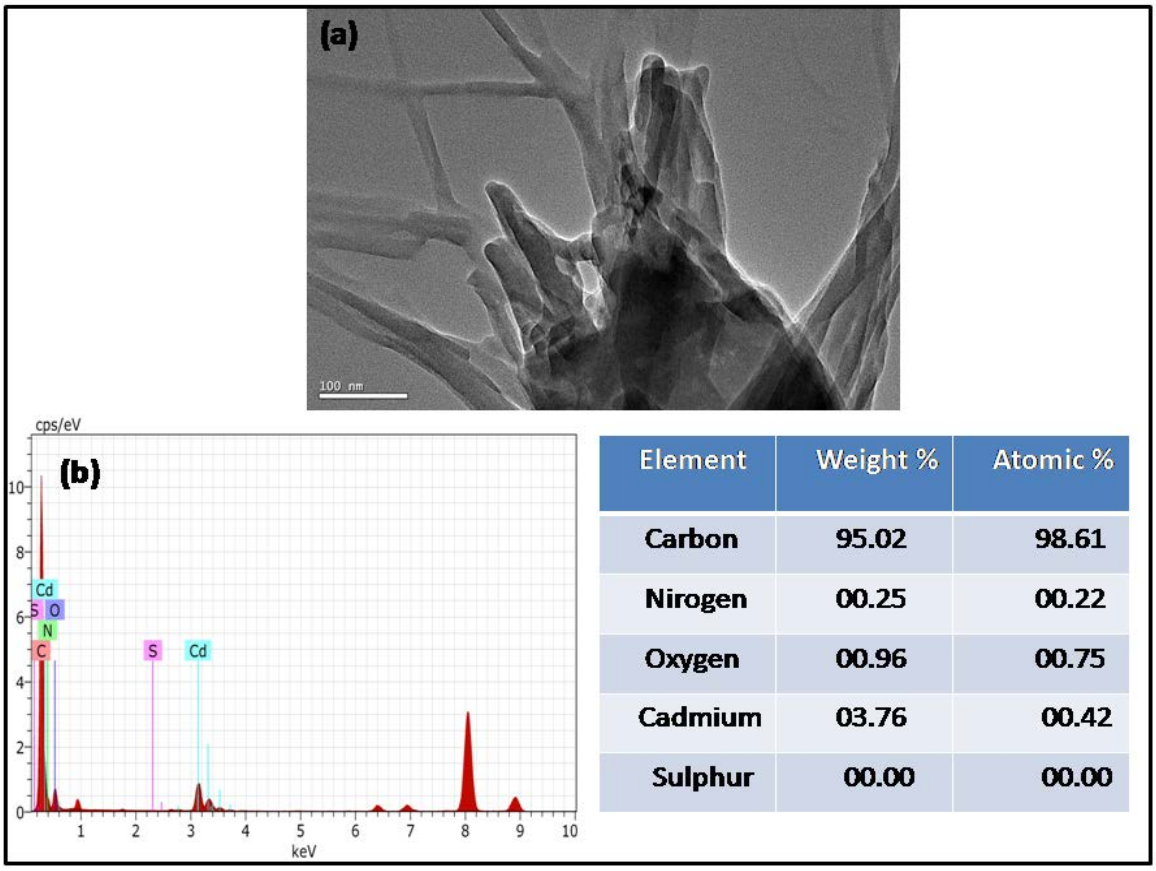


Figure S28. DRS spectra of Cd-MOF.



Element	Weight %	Atomic %
Carbon	95.02	98.61
Nirogen	00.25	00.22
Oxygen	00.96	00.75
Cadmium	03.76	00.42
Sulphur	00.00	00.00

Figure S29. TEM image (a) and EDAX pattern (b) of Cd-MOF recovered after photocatalytic dye degradation.

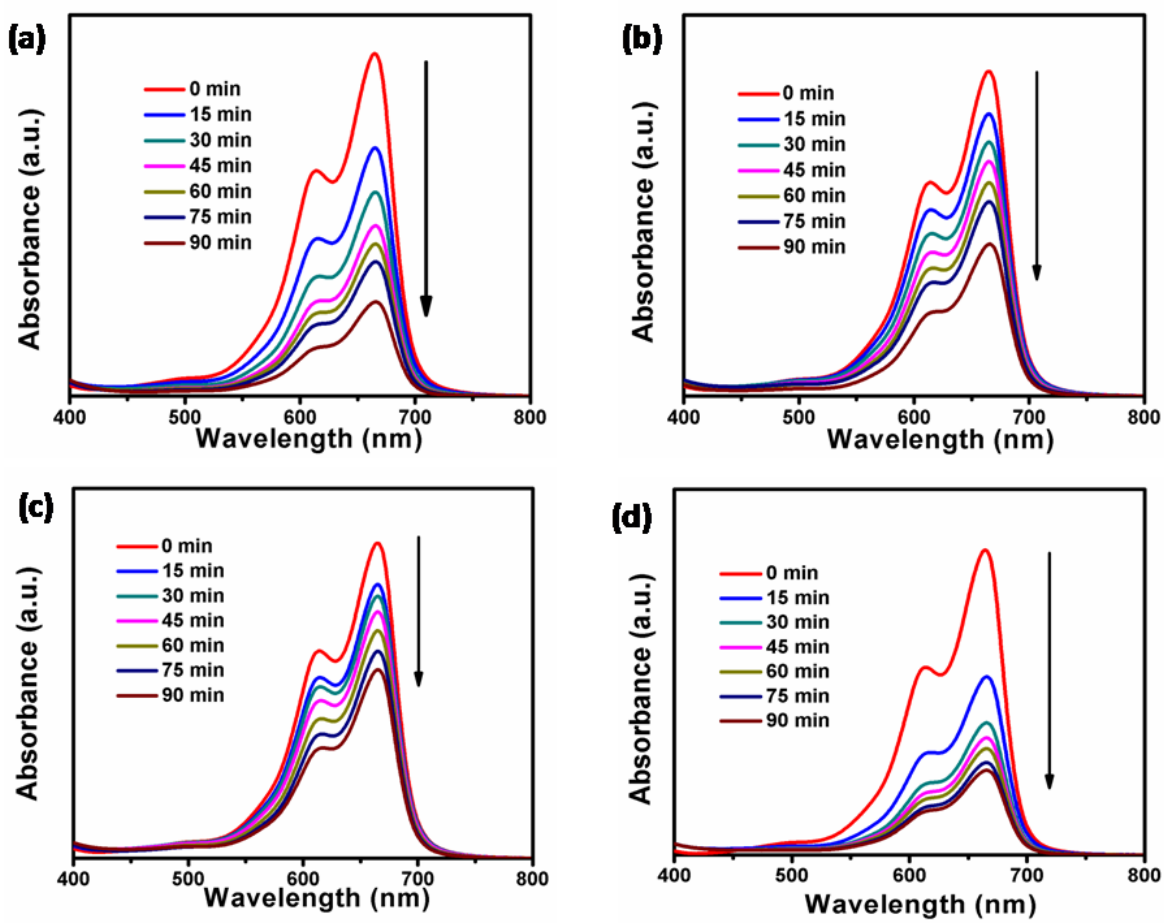


Figure S30. Successive time dependent UV-vis spectra showing the photocatalytic degradation of MB (a to c) under visible light irradiation from 2nd to 4^{rth} cycles. (d) under UV light irradiation.

TableS2. Different reported MOFs used for the MB degradation.

MOF	**Light source**	**%Degradation Efficiency**	**Time (min)**	**Reference**
[Cu(ONCP)(4,4'-H_2BPDA)0.5(H_2O) (4,4'-H_2BPDA)]$_n$	500watt Tungsten lamp	71.61	300	Y. Liu, S. Xie, H. Li, X. Wang, *ChemCatChem*, 2014, **6**, 2522-2526.
[Zn(TBTC)(2,6pydc)]$_n$	500watt Xenon lamp	80	270	M. Saranya, R. Ramachandran, P. Kollu, S. K. Jeong, A. N. Grace, *RSC Adv.*, 2015, **5**, 15831-15840.
[Co_2(1,4'-BDC)(NCP)$_2$]$_n$.4H_2O	500watt Tungsten lamp	62.75	300	C.-B. Liu, H.-Y. Sun, X.-Y. Li, H.-Y. Bai, Y. Cong, A. Ren, G.-B. Che, *Inorg. Chem.Commun.*,2014, **47**, 80-83
[Zn (4 bpah)(1,3-bdc)](H_2O)	UV	40	240	C.-B. Liu, Y. Cong, H.-Y. Sun, G.-B. Che, *Inorg. Chem.Commun.*, 2014, **47**, 71-74.
[Cu(3-dpye)(3-npa)(H_2O)].3(H_2O)	UV	70	240	H.-Y. Sun, C.-B. Liu, Y. Cong, M.-H. Yu, H.-Y. Bai, G.-B. Che, *Inorg. Chem. Commun.*, 2013, **35**, 130-134.

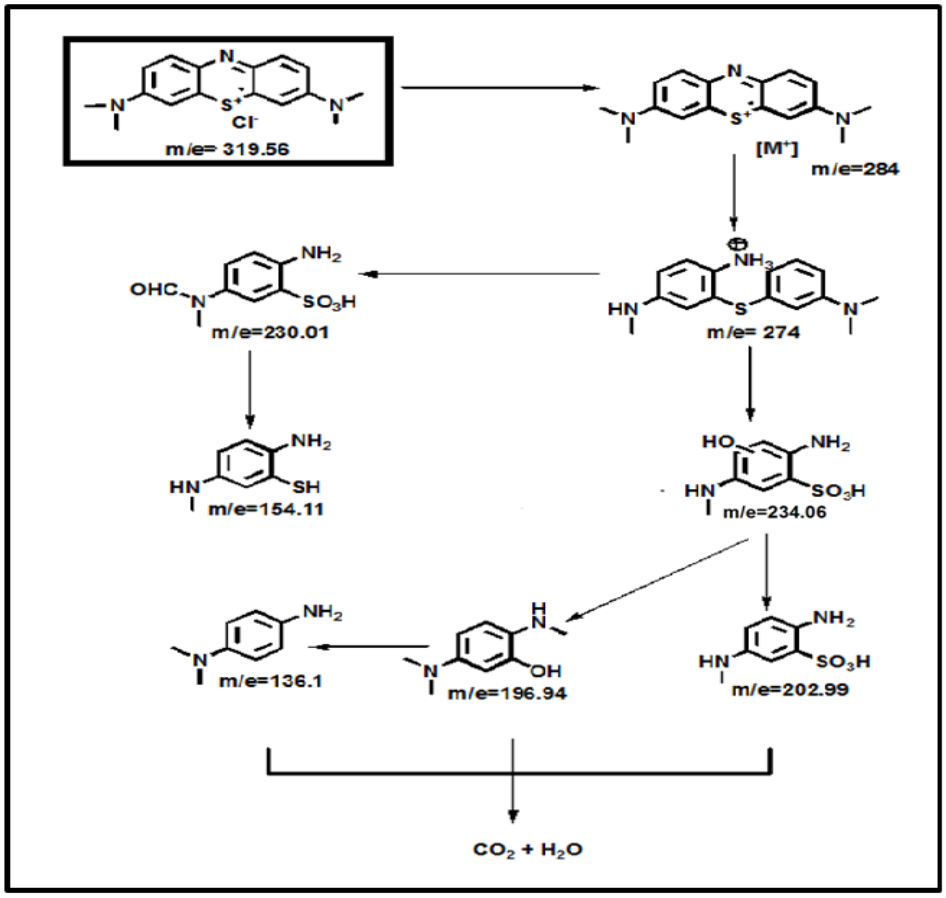


Figure S31. Proposed mechanism for the MB degradation on the basis of peaks obtained in LC-MS.

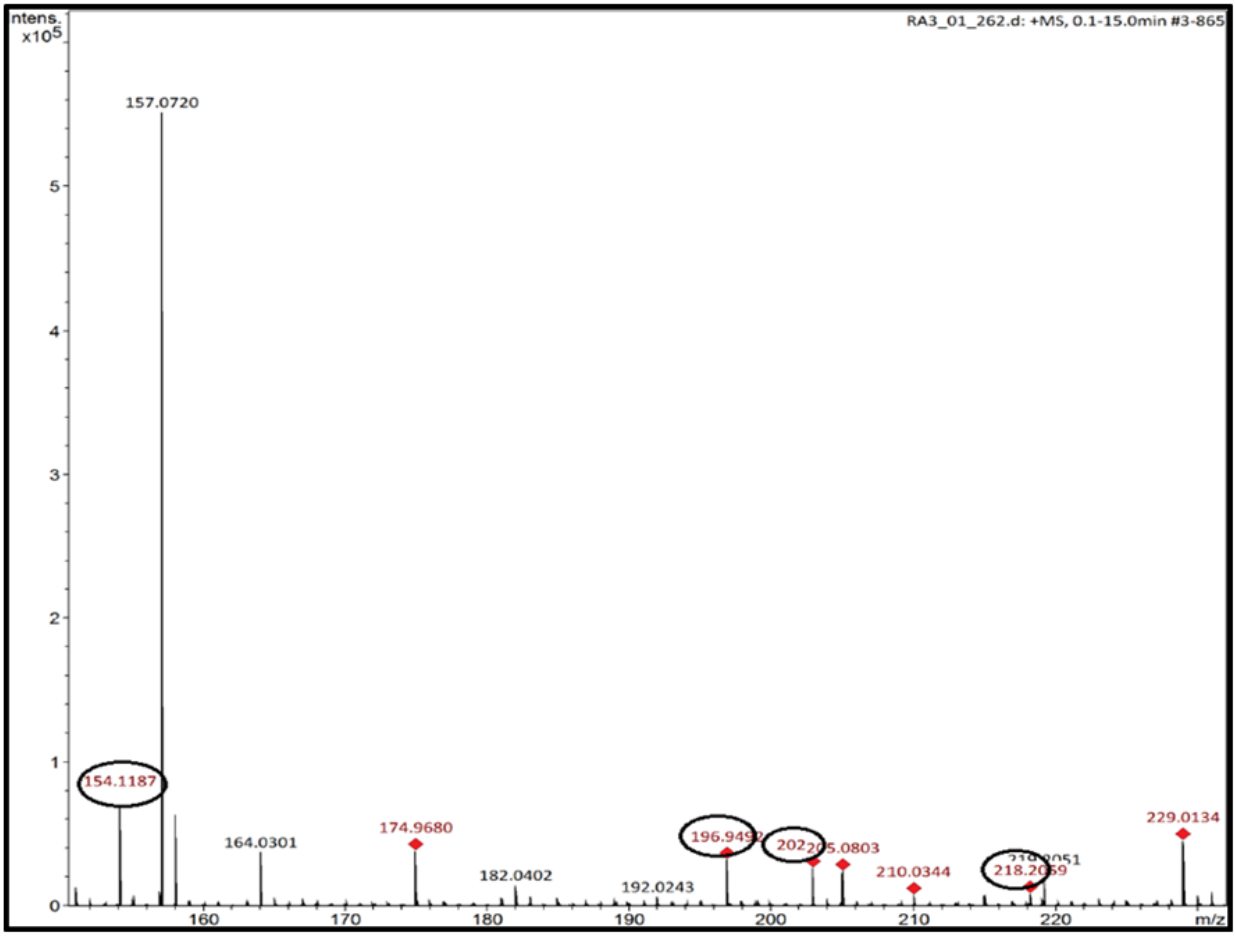


Figure S32. LC-MS spectra containing peaks in the range of 153 to 230.

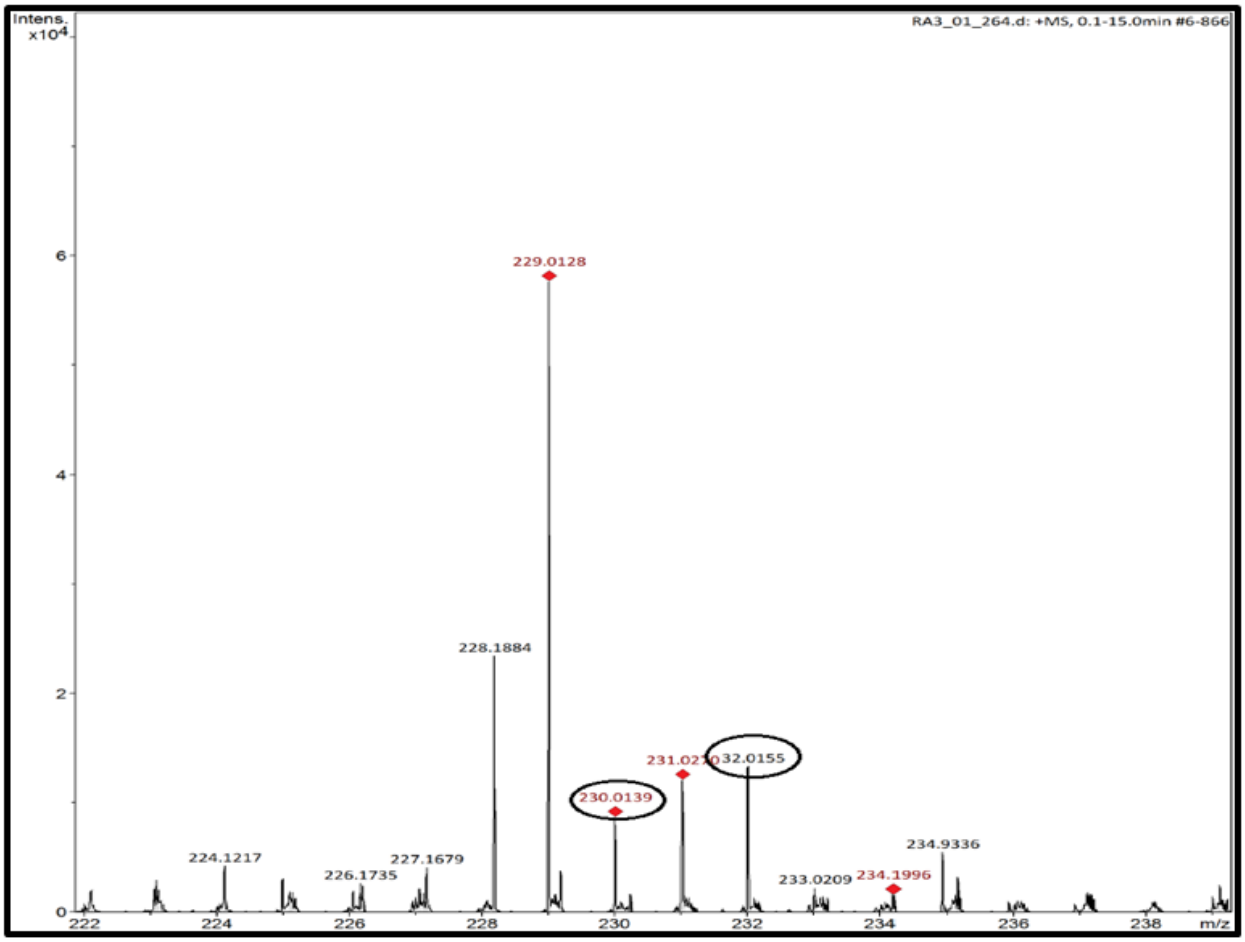


Figure S33. LC-MS spectra containing peaks in the range of 230 to 240.

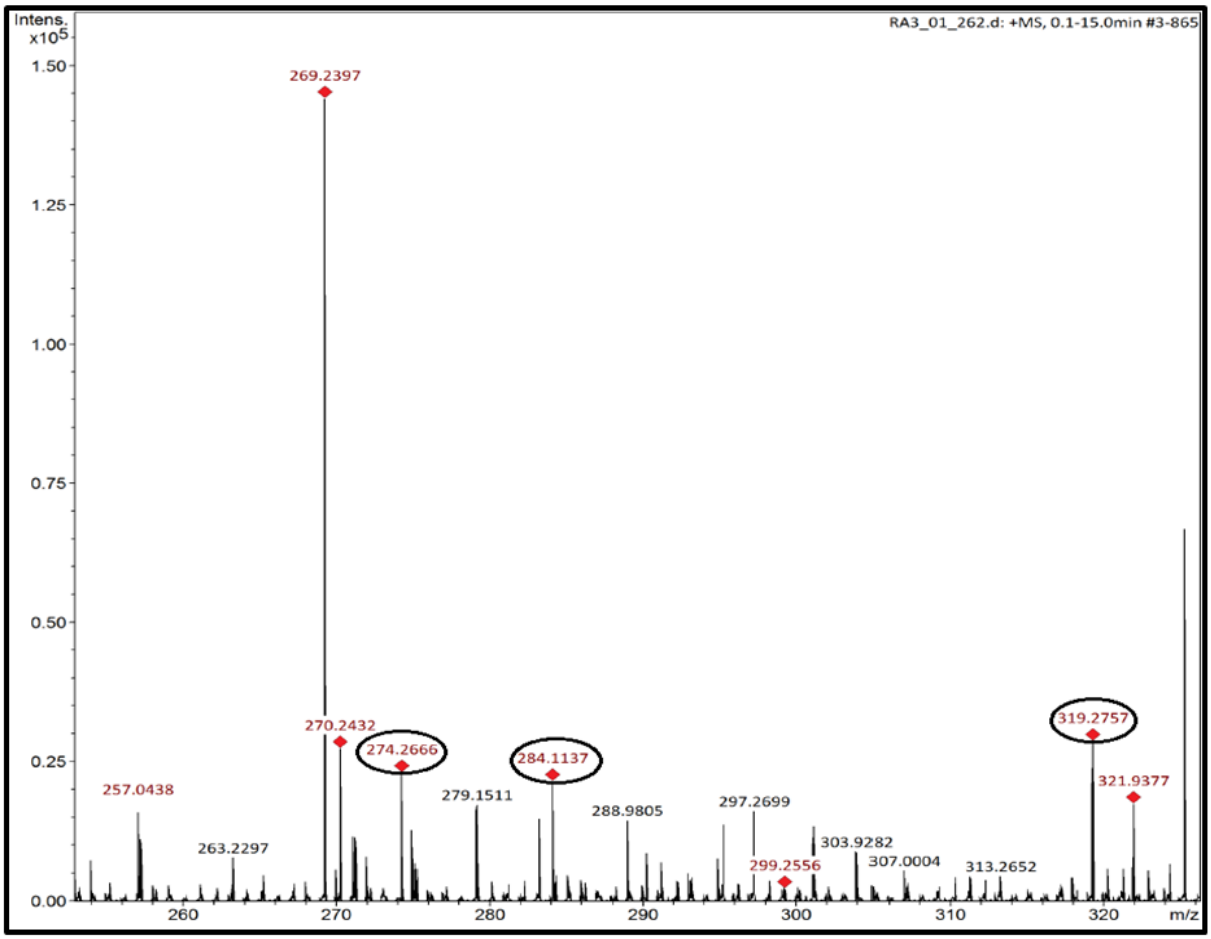


Figure S34. LC-MS spectra containing peaks in the range of 250 to 325.