Supporting Information for:

Effective BPA degradation from water: the integration of bimetallic UiO-66 Ce-Zr

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S1. Experimental details

Section S1.

Materials

Zirconium oxychloride octahydrate (ZrOCl$_2$8H$_2$O), terephthalic acid (BDC), methanol, ethanol, acetone, N-dimethylformamide (DMF), and bisphenol A (BPA) were some of the chemicals we bought from Sigma Aldrich. All chemicals used in this work are of analytical-grade purity and did not require additional purification.

Analytical instruments

To obtain powder X-ray diffraction (PXRD) patterns, a Bruker D2 phaser diffractometer with a Linex eye detector and a Cu-Kα1 radiation anode (λ = 1.5418 Å) was used. Data were recorded in the 2–40° 2θ range with a step scan of 0.02°. A Shimadzu IRTracer-100 spectrometer and KBr pellets were used to obtain Fourier transform infrared (FT-IR) spectra in the 4000-500 cm^{-1} range, which helped identify the unique bands of each material. Nitrogen adsorption-desorption isotherms were measured by a volumetric method using a Micromeritics ASAP 2020 gas sorption analyzer. The sample mass employed was 65.0 mg. Free space correction measurements were performed using ultra-high purity He gas (UHP grade 5, 99.999% pure). Nitrogen isotherms were measured using UHP-grade Nitrogen. All nitrogen analyses were performed using a liquid nitrogen bath at 77 K. Oil-free vacuum pumps were used to prevent contamination of sample or feed gases. UV-Vis diffuse reflectance spectra were used to determine the band gap energies of all materials, following David and Mott's proposed method based on the Kubelka-Munk equation.[1]

Kubelka-Munk function for the Tauc plot graphic.

$$F(R_\infty) = \frac{K}{S} = \frac{(1 - R_\infty)^2}{2R_\infty} \qquad (1)$$

$$R_\infty = \frac{R_{sample}}{R_{standard}} \qquad (2)$$

$$E_g = hv - \frac{(F(R_\infty)hv)^\gamma}{\beta} \qquad (3)$$

Where,

R: reflectance

$\gamma = 2$ for direct allowed transitions

β: semiconductor absorption coefficient

h: Planck's constant

ν: photon's frequency

E_g: band gap energy.

Micrographs were obtained using scanning electron microscopy (SEM) with a JSM-JEOL 7600F microscope to characterize the morphology and size of the prepared samples. X-ray photoelectron spectroscopy (XPS) analyses were conducted using a Thermo Scientific K-alpha X-ray photoelectron spectrometer set to 72 W with a hemispherical analyzer and a monochromator. Survey scans were recorded with a spot size of 400 μm and a fixed pass energy of 200 eV, while high-resolution scans were collected at a pass energy of 20 eV. The spectra were charged and corrected by setting the mainline of the carbon 1s spectrum (adventitious carbon) to 284.8 eV. Spectra analysis was performed using CasaXPS software (version 2.3.14). The Shirley method was used to subtract spectral backgrounds, and the same CasaXPS program carried out curve-fitting procedures and elemental quantifications.

Photocatalytic tests for Bisphenol A degradation
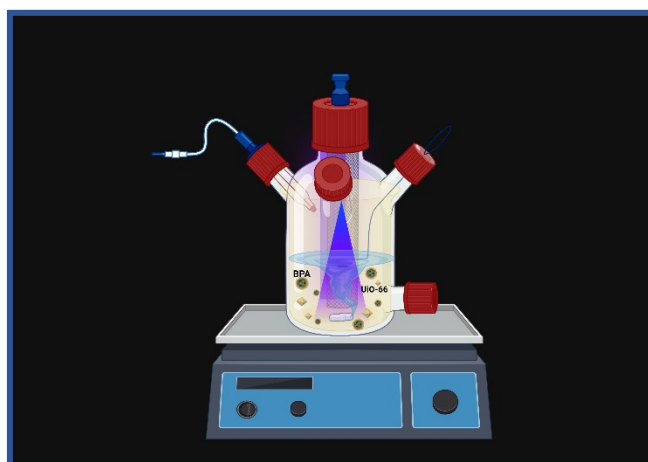
Figure S1. Schematic representation of the photocatalytic process.

Scavenger tests

Figure S2. Schematic representation of the scavenger.

Reusability

The reusability of MOFs UiO-66 was tested for three cycles using ethanol as desorbing agent.

Kinetic degradation experiments

Table S1. Kinetics Models for the BPA Degradation		
Kinetic model	Equation	Parameter
PFO model	$$C = C_0 e^{-k_{p1}t}$$	C: is the concentration of the contaminant at time t (mg·L) C_o: Initial concentration of the contaminant. (mg·L) k_{p1}: pseudo-first-order rate constant for the kinetic model (mg·L-1·min-1)
PSO model	$$C = \frac{C_0}{1 + k_{p2}tC_0}$$	C: is the concentration of the contaminant at time t (mg·L) C_o: Initial concentration of the contaminant. (mg·L) k_{p2}: pseudo-second-order rate constant for the kinetic model (mg·L-1·min-1)

S2. Results and Discussions

Synthesis of MOF UiO-66

PXRD
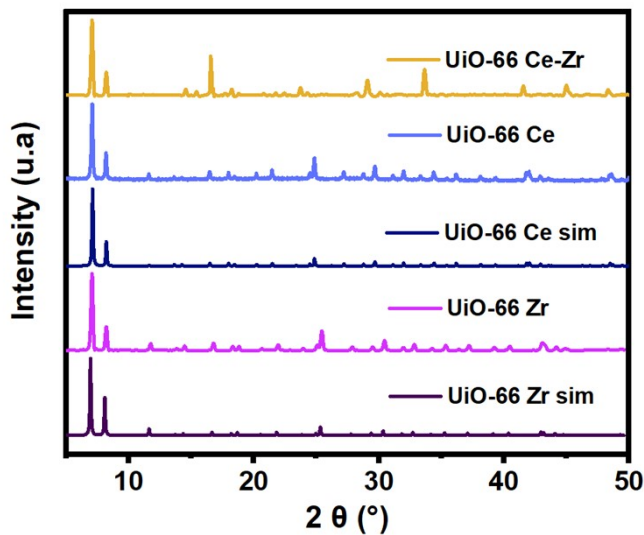
Figure S3. PXRD patterns of MOF UiO-66 Zr simulated, MOF UiO-66 Zr as-synthetized, MOF UiO-66 Ce simulated, MOF UiO-66 Ce as-synthetized and MOF UiO-66 Ce-Zr as-synthetized,
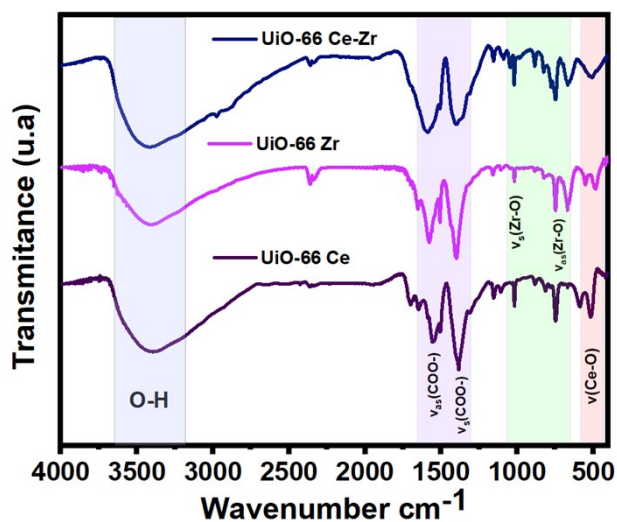
FT-IR

Figure S4. FTIR spectra of synthesized MOFs UiO-66 Ce, UiO-66 Zr and UiO-66 Ce-Zr

SEM-EDS

10000X   30000X

Element	Weight %	Atomic %
C K	70.39	80.8
O K	20.73	17.86
Zr L	8.87	1.34
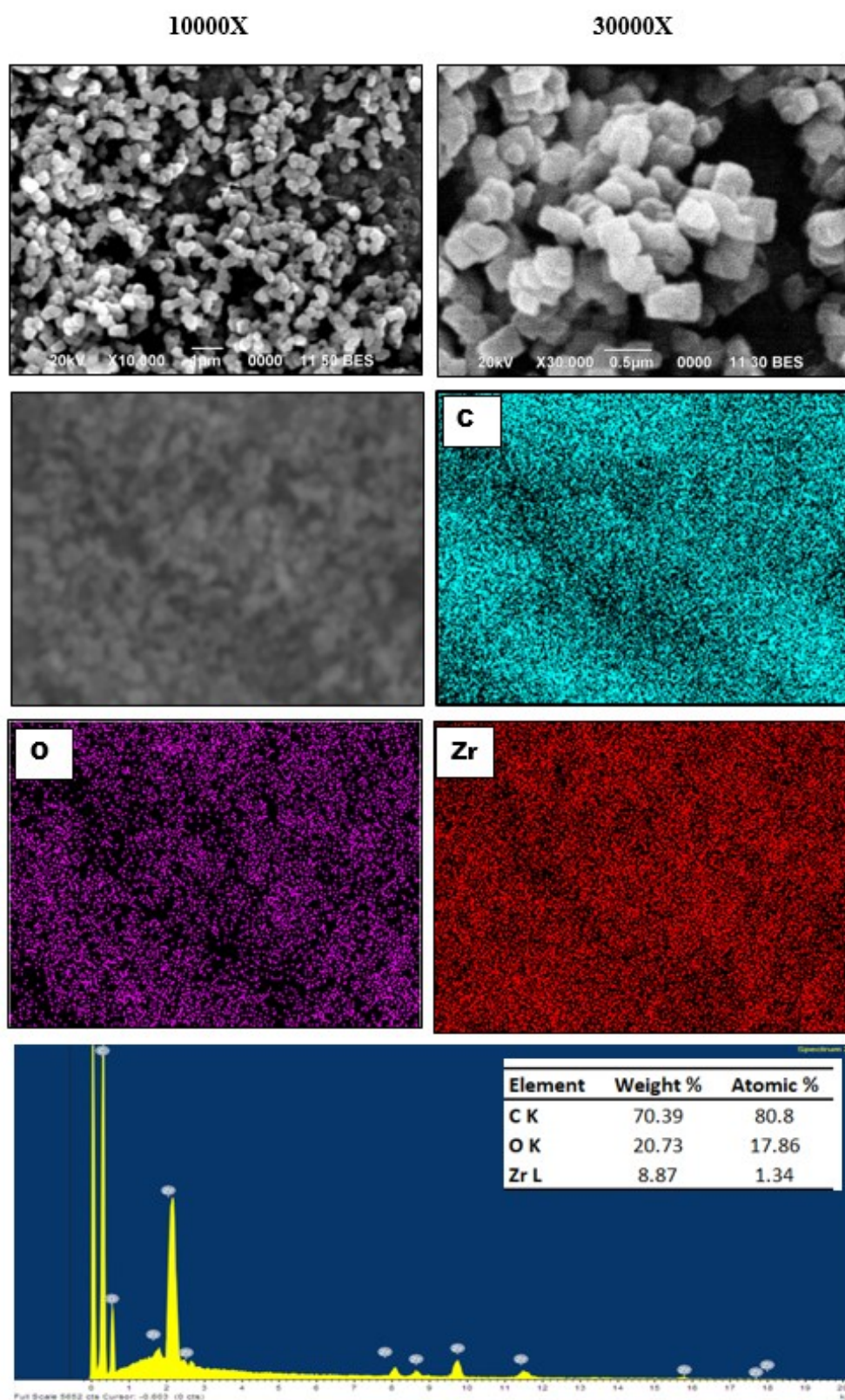
Figure S5. SEM images and SEM-EDS mapping for MOF UiO-66 Zr
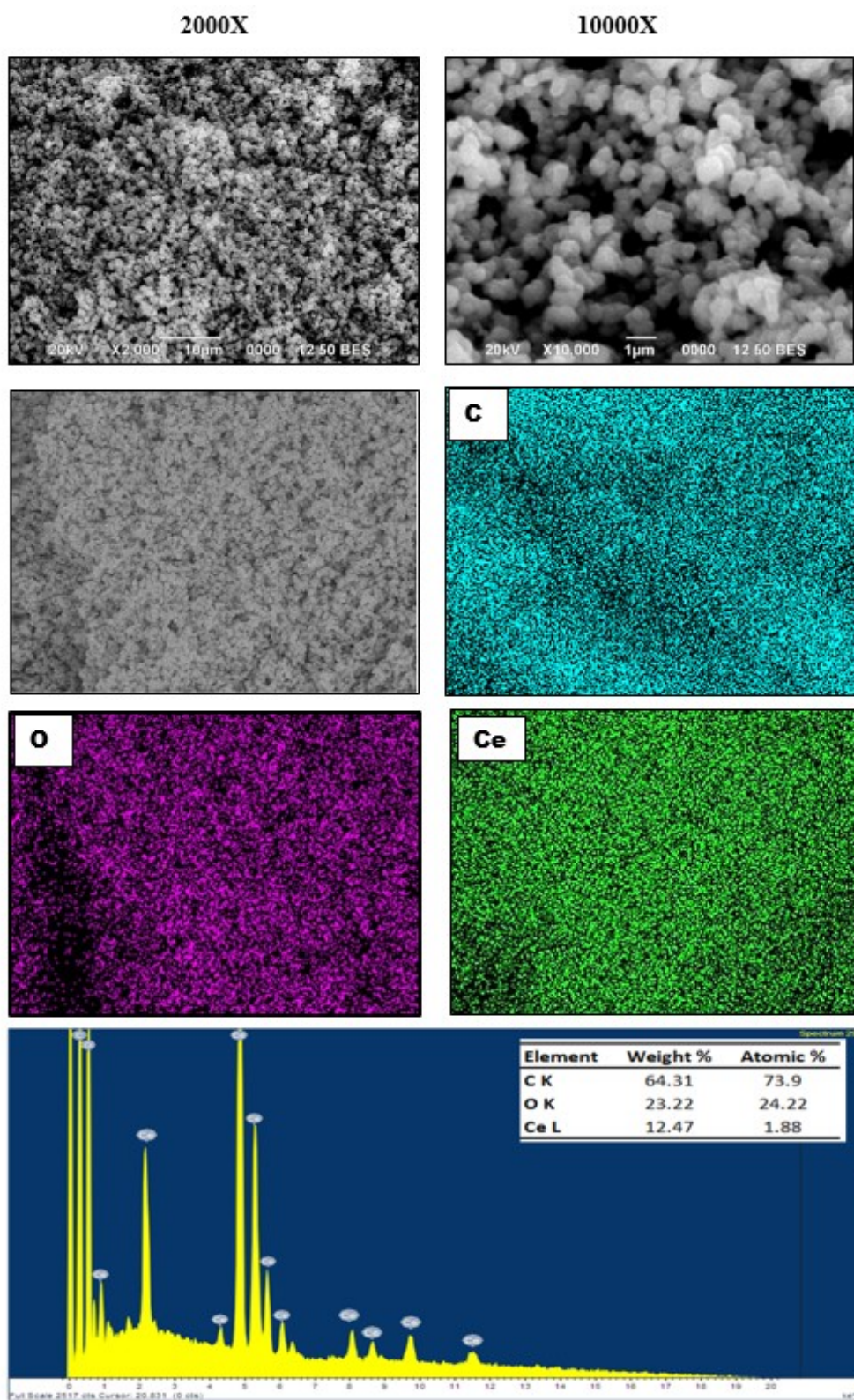
Figure S6. SEM images and SEM-EDS mapping for MOF UiO-66 Ce

250X   **3000X**
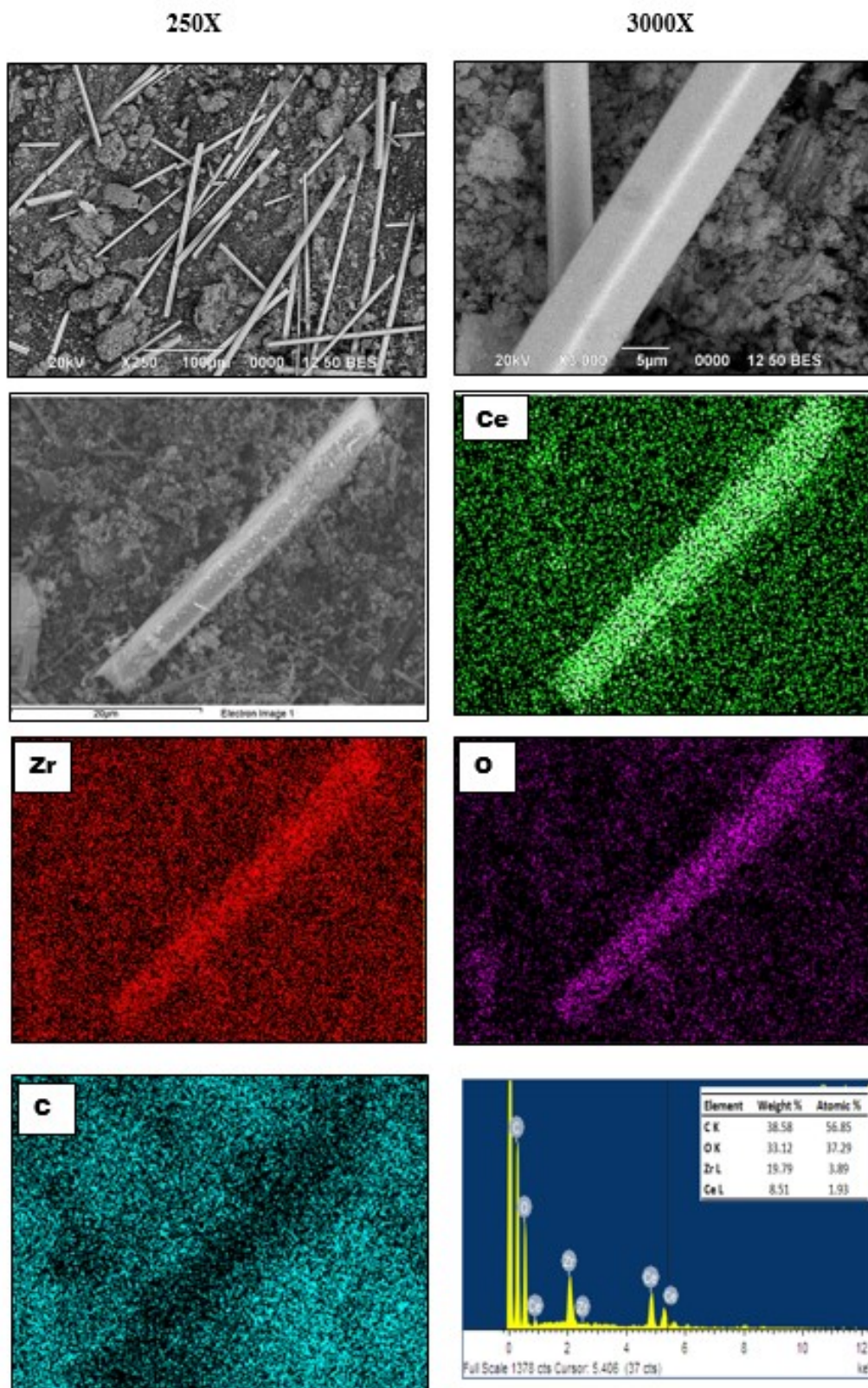
Figure S7. SEM images and SEM-EDS mapping for MOF UiO-66 Ce-Zr

Nitrogen adsorption-desorption
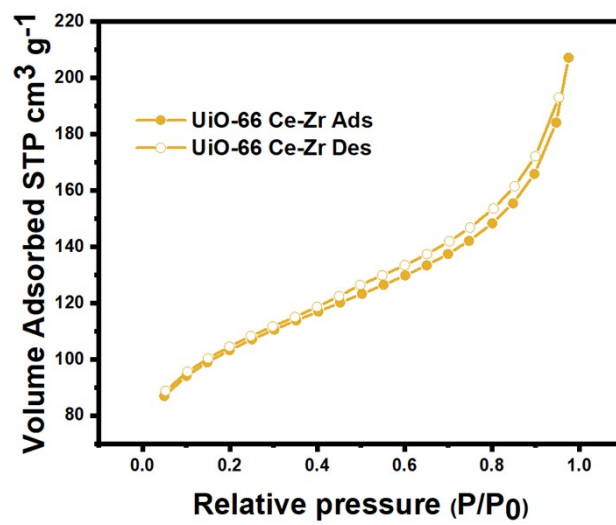
Figure S8. Nitrogen isotherm MOF UiO-66 Ce-Zr: adsorption (Ads) and desorption (Des).

Electrochemical characterization

a) Plot of $(F(R\infty) \cdot h\nu)^2$ versus Energy (eV) for UiO-66 Ce, UiO-66 Ce-Zr, and UiO-66 Zr, with E_g: 3.08 eV, E_g: 3.2 eV, and E_g: 4.05 eV respectively.

b) Plot of $C^{-2}/10^9 cm^2 F^{-2}$ versus Potencial (V vs Ag/Ag/Cl)(3M NaCl) for UiO-66 Ce at 1500 Hz, 2000 Hz, 2500 Hz with values 0.86, 0.89, 0.88.

c) Band diagram of Potencial (V) vs. NHE for UiO-66 Ce with E_g = 3.2 eV, showing −0.671, $O_2/·O_2$ −0.33, $H_2O/·OH$ +2.32, +2.41, BPA, O_2.
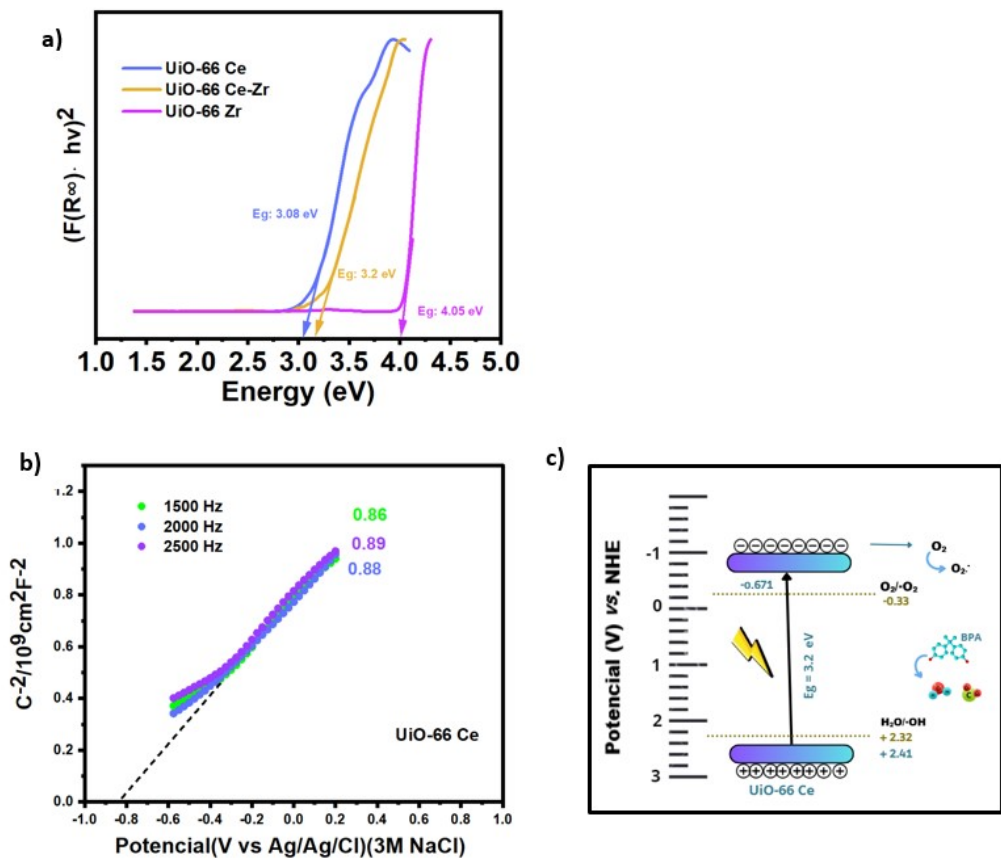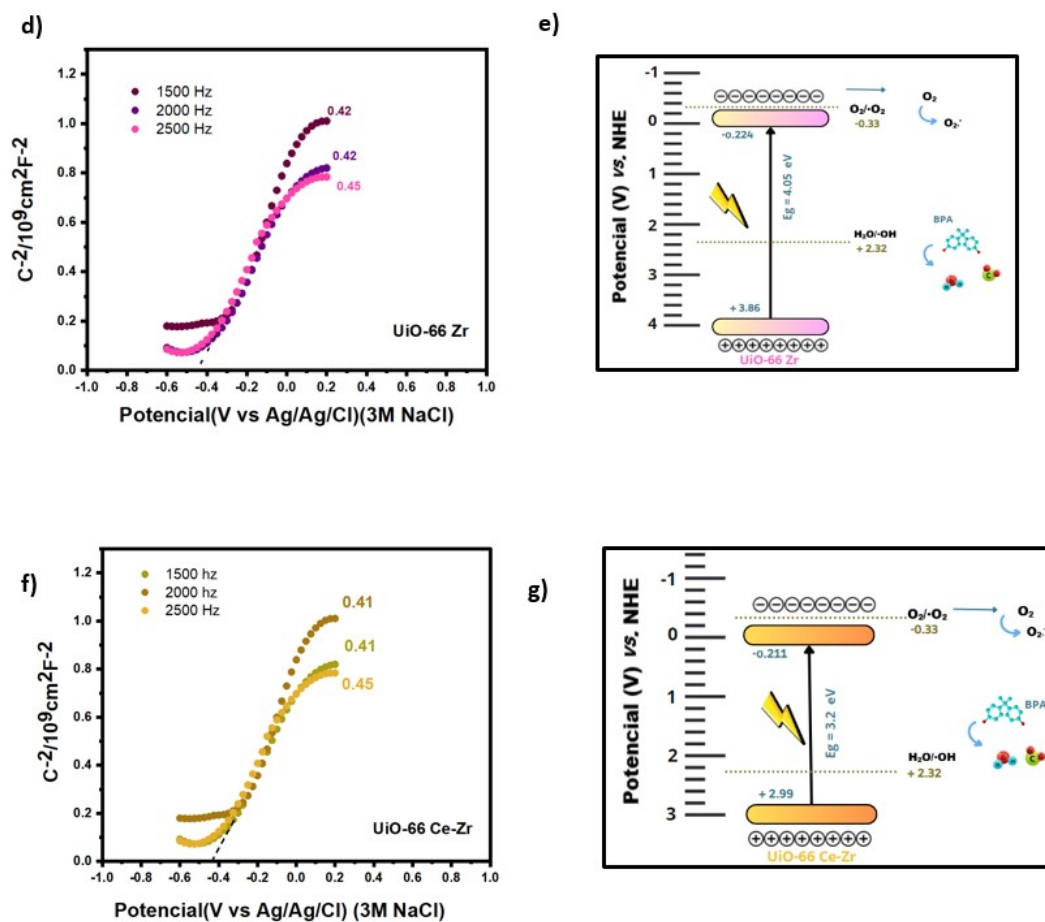
Figure S9 (a) Tauc plots representation and estimated band-gap (Eg) values MOFs UiO-66, **(b)-(c)** Mott-Schottky curves of prepared at different frequencies (1500, 2000, 2500 Hz) – and electronic band structure of the MOF UiO-66 Ce, **(d)-(e)** Mott-Schottky curves of prepared at different frequencies (1500, 2000, 2500 Hz) – and electronic band structure of the MOF UiO-66 Zr and **(f)-(g)** Mott-Schottky curves of prepared at different frequencies (1500, 2000, and 2500 Hz) – and electronic band structure of the MOF UiO-66 Ce-Zr.

BPA degradation analysis
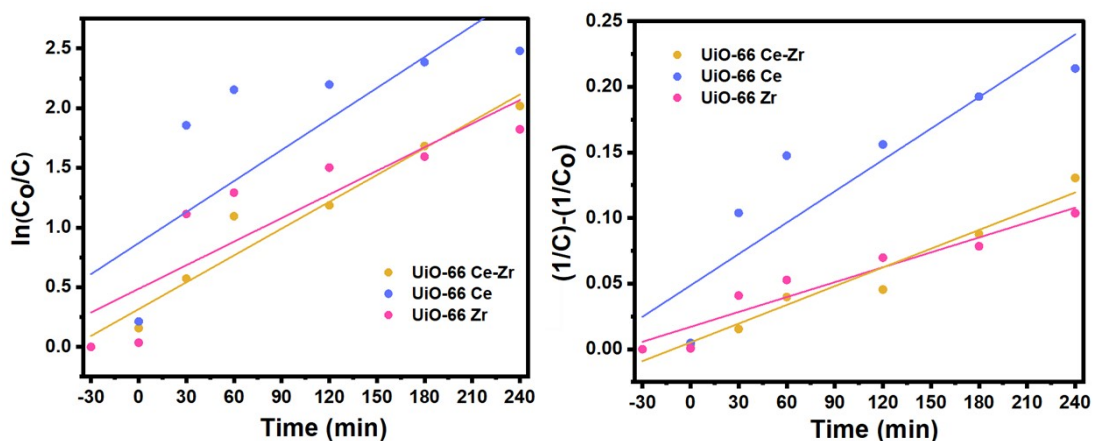
Figure S10. Kinetic studies without and with the lamp of the MOFs UiO-66

Model	Parameter	Material		
		UiO-66 Ce	**UiO-66 Zr**	**UiO-66 Ce-Zr**
	C_0 $(mg \cdot L)$	49.7843	49.8012	49.8012
PFO model	k_1 $(mg \cdot L^{-1} \cdot min^{-1})$	0.00866	0.00621	0.00749
	R^2	0.664	0.731	0.955
	C_0 $(mg \cdot L)$	49.7843	49.8012	49.8012
PSO model	k_1 $(mg \cdot L^{-1} \cdot min^{-1})$	0.000813	0.000335	0.000476
	R^2	0.84	0.92	0.960

Table S2. Parameters of the kinetic models.

Table S3. Comparative Table of Different Materials for BPA Degradation

Photocatalyst	BPA concentration (mg/L)	Reaction time (min)	Degradation efficiency (%)	References
UiO-66 Ce-Zr	50	240	84	This work
UiO-66-NH$_2$	5	120	16.2	[2]
Bi$_2$MoO$_6$/MIL-88B(Fe)	20	120	54	[3]
Bi$_{12}$O$_{17}$Cl$_2$/MIL-100(Fe)	20	300	57.4	[4]
UiO-66 Zr	10	120	66	[5]
Mpg-C$_3$N$_4$	20	180	52.1	[6]
2% N,B-TiO$_2$	5	120	79	[7]
BiOI/ZIF-8	10	180	82.5	[8]

Material characterization after BPA degradation

SEM analysis
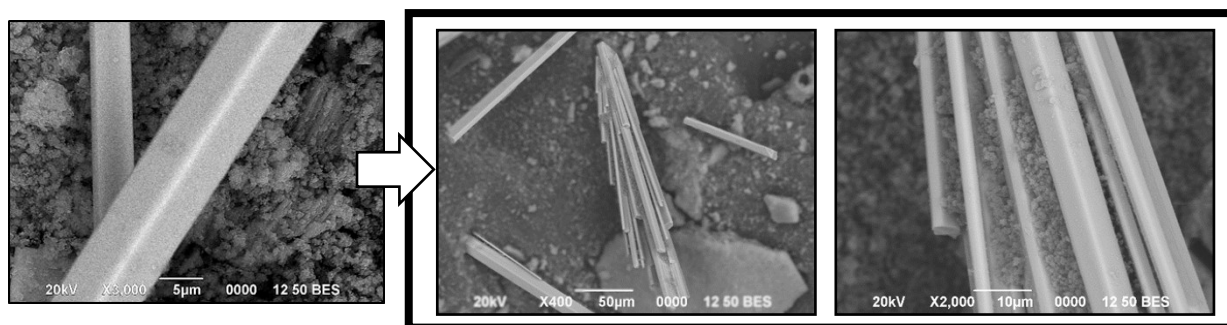
Before   **After**
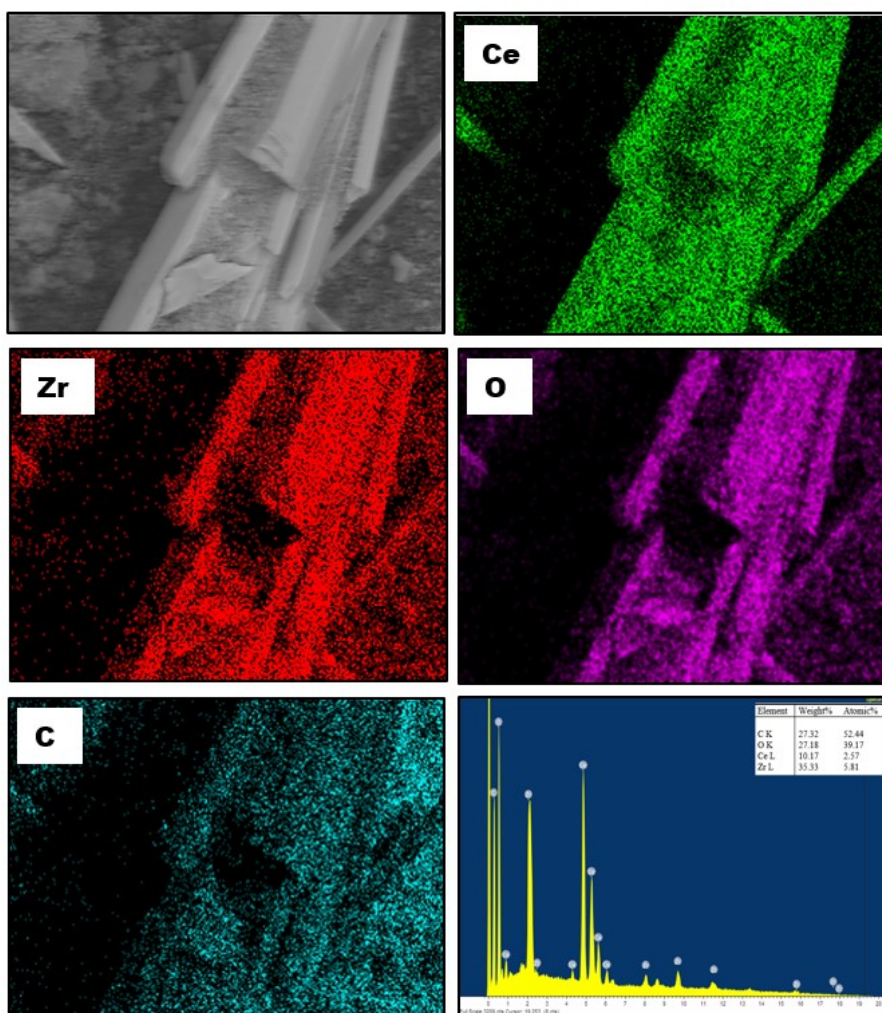
Figure S11. SEM images and SEM MOF UiO-66 Ce-Zr before and after the degradation.

PXRD analysis
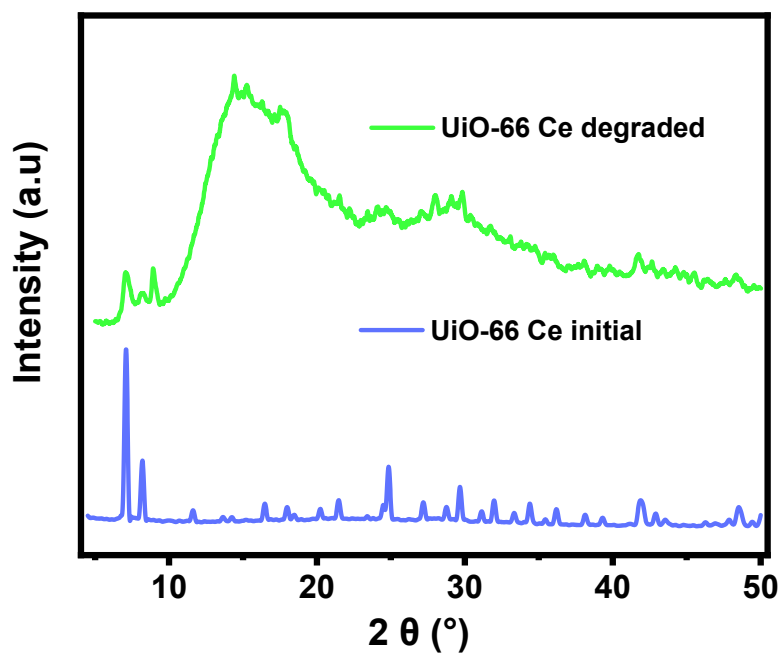
Figure S12. PXRD pattern of MOF UiO-66 Ce initial (blue line) and MOF UiO-66 Ce after degradation (green line).
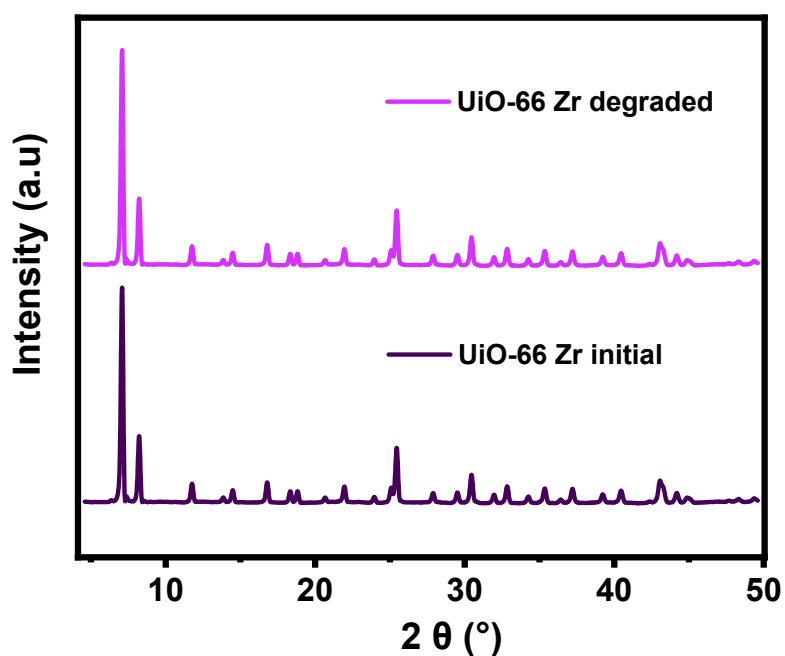
Figure S13. PXRD pattern of MOF UiO-66 Zr initial (dark purple line) and MOF UiO-66 Zr after degradation (purple line).
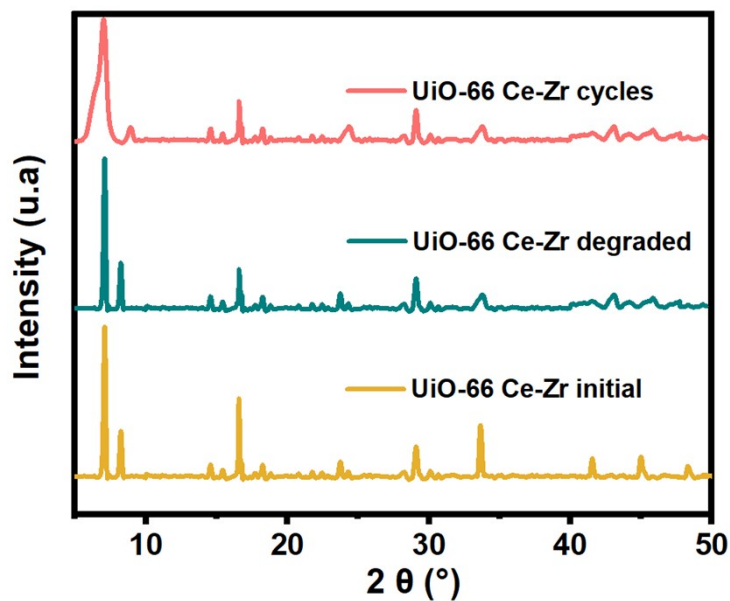
Figure S14. PXRD patterns MOF UiO-66 Ce-Zr initial (yellow line), MOF UiO-66 Ce-Zr degraded (green line) and MOF UiO-66 Ce-Zr after three cycles (red line).

Nitrogen adsorption-desorption after degradation
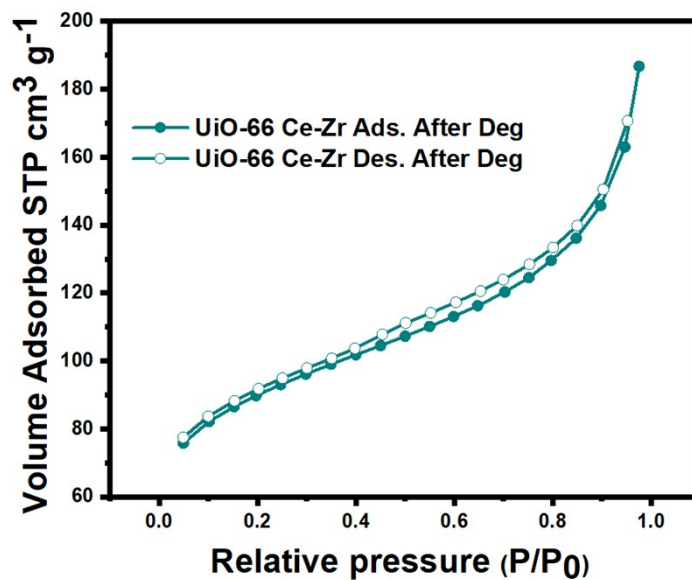
Figure S15. Nitrogen isotherm MOF UiO-66 Ce-Zr: adsorption (Ads) and desorption (Des) after the degradation.

XPS analysis
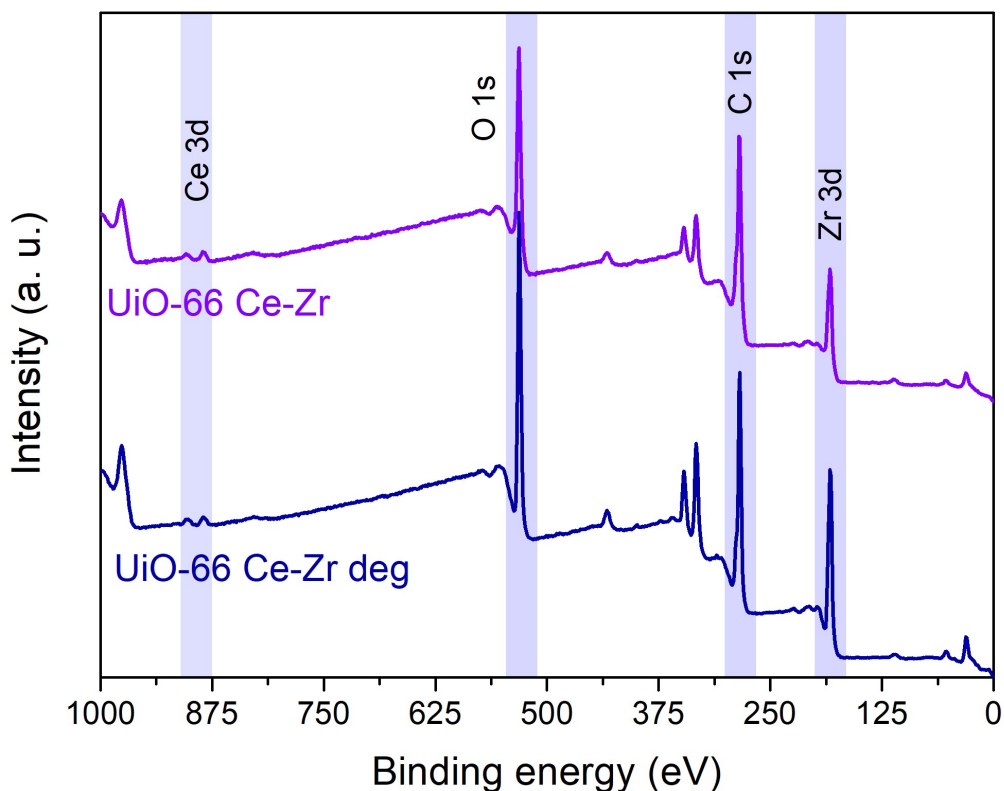
Figure S16. Survey spectra of MOF UiO-66 Ce-Zr, before and after the BPA photodegradation.

Table S4. XPS survey data (atomic percentage) of the different elements in UiO-66 Ce-Zr.

Samples	Elements (At. %)				
	C 1s	O 1s	Ce 3d	Zr 3d	N 1s
UiO-66 Ce-Zr	66.6	28.6	0.2	3.0	0.3
UiO-66 Ce-Zr deg	60.4	33.1	0.2	5.6	0.9

Table S5. The peak-fitting results of C 1s high-resolution signal of UiO-66 Ce-Zr.

Samples	Assignment	E_B (eV)	FWHM (eV)	At. %
UiO-66 Ce-Zr	**C1s** $_{C=C\ aromatic}$	284.7	1.6	64.5
	C1s $_{C-OH}$	286.1	1.7	15.5
	C1s $_{O-C=O}$	288.4	1.7	16.5

	C1s $_{\pi-\pi*}$	289.9	1.8	3.5
UiO-66 Ce-Zr deg	**C1s** $_{C=C\ aromatic}$	284.6	1.5	64.9
	C1s $_{C-OH}$	285.6	1.5	21.0
	C1s $_{O-C=O}$	288.6	1.5	10.7
	C1s $_{\pi-\pi*}$	289.6	1.6	3.4

Table S6. The peak-fitting results of O 1s high-resolution signal of UiO-66 Ce-Zr.

Samples	Assignment	E_B (eV)	FWHM (eV)	At. %
UiO-66 Ce-Zr	**O 1s** $_{Ce-O,\ Zr-O}$	530.1	1.8	14.9
	O 1s $_{O-H,\ C-O}$	531.7	1.9	64.0
	O 1s $_{C=O}$	533.3	1.9	21.1
UiO-66 Ce-Zr deg	**O 1s** $_{Ce-O,\ Zr-O}$	530.1	1.8	19.0
	O 1s $_{O-H,\ C-O}$	531.5	1.9	66.2
	O 1s $_{C=O}$	532.7	1.9	14.8

Table S7. The peak-fitting results of Ce 3d high-resolution signal of UiO-66 Ce-Zr.

Samples	Assignment	E_B (eV)	FWHM (eV)	At. %
UiO-66 Ce-Zr	**Ce 3d$_{5/2}$ (v^0)**	882.5	4.0	19.5
	Ce 3d$_{5/2}$ (v^1)	886.1	4.0	40.3
	Ce 3d$_{3/2}$ (u^0)	901.0	4.0	12.8
	Ce 3d$_{3/2}$ (u^1)	904.7	4.0	27.4
UiO-66 Ce-Zr deg	**Ce 3d$_{5/2}$ (v^0)**	882.2	3.5	24.7
	Ce 3d$_{5/2}$ (v^1)	885.8	3.5	35.9
	Ce 3d$_{3/2}$ (u^0)	900.7	3.5	15.8
	Ce 3d$_{3/2}$ (u^1)	904.4	3.5	23.6

Table S8. The peak-fitting results of Zr 3p high-resolution signal of UiO-66 Ce-Zr.

Samples	Assignment	E_B (eV)	FWHM (eV)	At. %
UiO-66 Ce-Zr	**Zr 3d$_{5/2}$**	182.6	1.9	51.6
	Zr 3d$_{3/2}$	184.9	1.9	48.4

UiO-66 Ce-Zr deg	Zr 3d$_{5/2}$	182.5	1.9	61.4
	Zr 3d$_{3/2}$	184.8	1.9	38.6

DFT and docking simulations results analysis
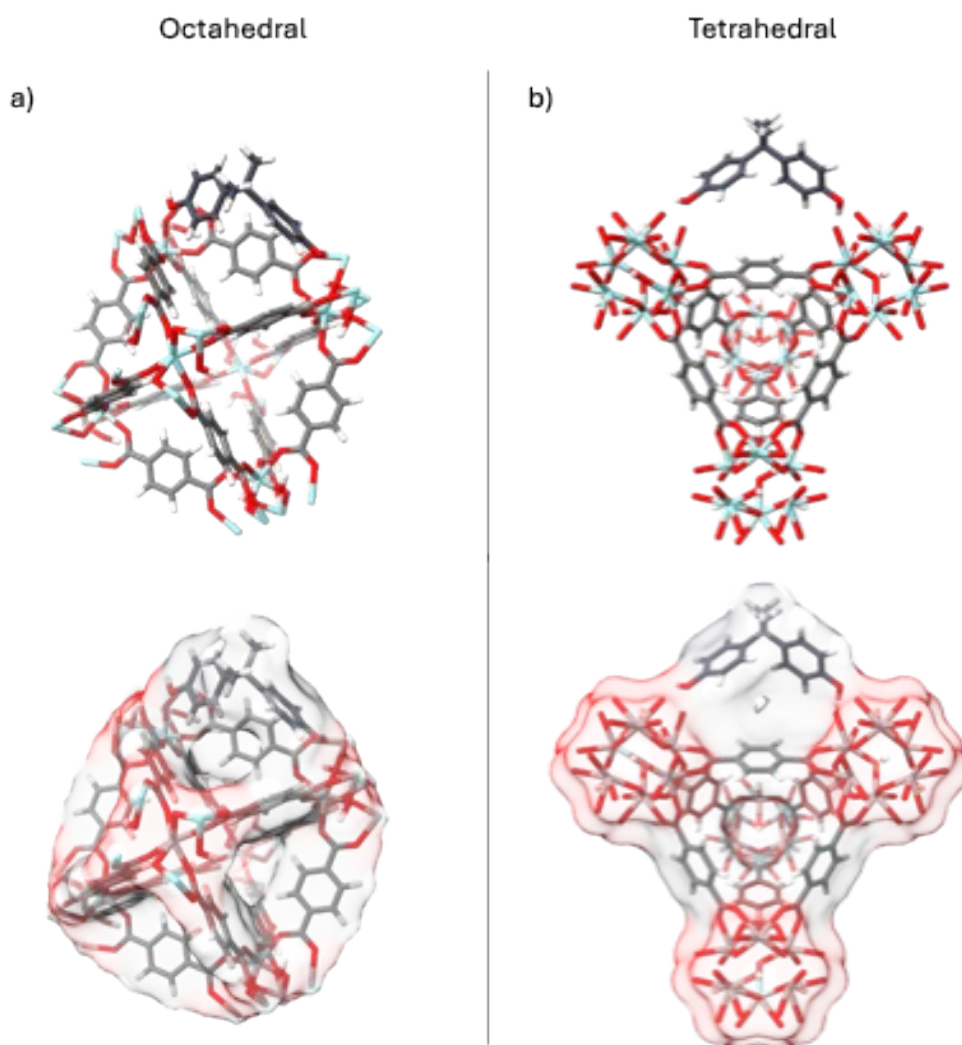
Figure S17. Structural representation of MOF/BPA interactions. (a) Proposed interaction between BPA and UiO-66 in octahedral pore. (b) Proposed interaction between BPA and UiO-66 in tetrahedral pore.

Table S9. Total parameters of volumes calculated with VolMol.

Total Volumes calculated (Å^3)		
	UiO-66	**BPA**
Van der Waals volume	2939.96	207.184
Probe excluded void volume	488.056	13.752
Molecular volume (vdw + probe excluded void)	3428.016	220.936
Molecular volume with isolated cavities	3441.32	220.936
Small probe core volume	11.304	0
Small probe shell volume	146.648	0
Small probe occupied volume (core + shell)	157.952	0
Large probe shell volume	7560.68	1323.584

Table S10. Energies reported by DFT study and calculation of binding energy.

Octahedral Pore					
E_i	**UiO-66**	**BPA**	→	**Adduct**	ΔE_i kcal/mol
SCF	-24059745	-458721.84		-24595311	-76843.426
Tetrahedral Pore					
E_i	**UiO-66**	**BPA**	→	**Adduct**	ΔE_i kcal/mol
SCF	-21792178	-458721.84		-22213412	37487.5007

Table S11. Total parameters of surface areas calculated with VolMol.
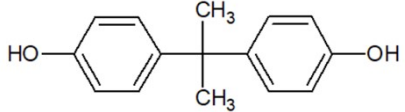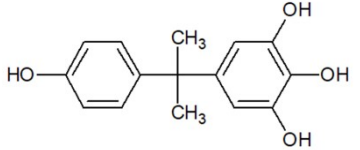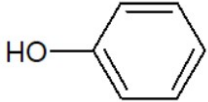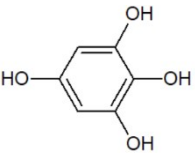
Total Surface Areas calculated (Å^2)		
	UiO-66	**BPA**
Van der Waals surface	2437.75147	232.359856
Small probe excluded surface	427.731376	0
Small probe accessible surface (similar to Lee-Richards surface)	69.34754	0
Molecular surface (both probes excluded surface)	2169.72376	220.33068
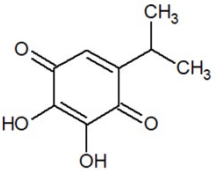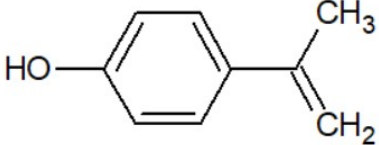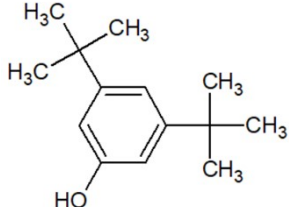
Table S12. Cavities data calculated with VolMol for UiO-66.

Cavity	Occupied Volume ($Å^3$)	Accessible Volume ($Å^3$)	Excluded Surface ($Å^2$)	Accessible Surface ($Å^2$)	Cavity Type	Cavity Center Cordinates ($Å$)		
						x	y	z
1	21.664	1.888	58.7557	11.348	Pocket	14.5	3.8	7.2
2	20.624	1.888	56.9695	10.8711	Pocket	10.8	10.4	7.2
3	19.784	1.896	54.6997	10.7459	Pocket	18.2	10.4	7.3
4	17.376	1.2	53.1163	8.67669	Pocket	14.5	8.1	1.2
5	17.216	1.136	44.1072	6.62316	Tunnel	14.5	8.6	10.7
6	16.328	1.104	42.7537	6.80827	Tunnel	14.5	12.9	4.6
7	15.888	1.08	41.4249	6.7227	Tunnel	18.4	6.2	4.4
8	15.768	1.088	41.3877	6.94111	Tunnel	10.6	6.2	4.4
9	4.544	0.008	15.1648	0.2035	Isolated	17.4	12.9	9.1
10	4.536	0.008	15.1648	0.2035	Isolated	11.6	12.9	9.1
11	4.224	0.008	15.0069	0.2035	Isolated	20	8.8	9.1

By-products analysis by UPLC-MS

Table S13. By.products analysis with diferen m/z.

Compound	Molecular Structure	Molecular formula	Molecular Mass (M)^a (g/mol)	(M-H) + - (m/z)	t_R (min)	Ref.
BPA		$C_{15}H_{16}O_2$	228.29	227.29	6.02 6.67	
5-[2-(4-hydroxyphenyl)propan-2-yl]benzene-1,2,3-triol		$C_{15}H_{16}O_4$	260.29	259.3	6.67	9
phenol		C_6H_6O	94.1	93.2	0.845	
benzene-1,2,3,5-tetrol		$C_6H_6O_4$	142.1	141.1	0.845	

2,3-dihydroxy-5-(propan-2-yl)cyclohexa-2,5-diene-1,4-dione		$C_9H_{10}O_4$	182.1	181.1	0.845 6.02 6.67	
(2Z)-but-2-enedioic acid		$C_4H_4O_4$	116.05	115.01	0.530	
4-(prop-1-en-2-yl)phenol		$C_9H_{10}O$	134.17	133	6.02 6.67	10
3,5-di-tert-butylphenol		$C_{14}H_{22}O$	206.32	205.12	0.845 6.02 6.67	11

Figure S18. Reaction pathway for the photocatalytic degradation of bisphenol A with UiO-66 Ce-Zr illuminated with UV light.

Toxicology in-silico study of degradation products

Molecule 1

SMILES   CC(c1ccc(cc1)O)(c1ccc(cc1)O)C

Physicochemical Properties

Property	Value
Formula	C15H16O2
Molecular weight	228.29 g/mol
Num. heavy atoms	17
Num. arom. heavy atoms	12
Fraction Csp3	0.20
Num. rotatable bonds	2
Num. H-bond acceptors	2
Num. H-bond donors	2
Molar Refractivity	69.44
TPSA	40.46 Å²

Lipophilicity

Property	Value
Log $P_{o/w}$ (iLOGP)	2.05
Log $P_{o/w}$ (XLOGP3)	3.32
Log $P_{o/w}$ (WLOGP)	3.42
Log $P_{o/w}$ (MLOGP)	3.20
Log $P_{o/w}$ (SILICOS-IT)	3.29
Consensus Log $P_{o/w}$	3.06

Water Solubility

Property	Value
Log S (ESOL)	-3.74
Solubility	4.18e-02 mg/ml ; 1.83e-04 mol/l
Class	Soluble
Log S (Ali)	-3.85
Solubility	3.25e-02 mg/ml ; 1.43e-04 mol/l
Class	Soluble
Log S (SILICOS-IT)	-4.59
Solubility	5.80e-03 mg/ml ; 2.54e-05 mol/l
Class	Moderately soluble

Pharmacokinetics

Property	Value
GI absorption	High
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-5.34 cm/s

Druglikeness

Property	Value
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

Medicinal Chemistry

Property	Value
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: MW<250
Synthetic accessibility	1.43

Molecule 1

⚦ ⊕ ⬡ ✏ Σ

SMILES Oc1ccc(cc1)C(c1cc(O)c(c(c1)O)O)(C)C

Physicochemical Properties

Formula	C15H16O4
Molecular weight	260.29 g/mol
Num. heavy atoms	19
Num. arom. heavy atoms	12
Fraction Csp3	0.20
Num. rotatable bonds	2
Num. H-bond acceptors	4
Num. H-bond donors	4
Molar Refractivity	73.48
TPSA	80.92 Å²

Lipophilicity

Log $P_{o/w}$ (iLOGP)	1.37
Log $P_{o/w}$ (XLOGP3)	3.30
Log $P_{o/w}$ (WLOGP)	2.83
Log $P_{o/w}$ (MLOGP)	2.01
Log $P_{o/w}$ (SILICOS-IT)	2.31
Consensus Log $P_{o/w}$	2.36

Water Solubility

Log S (ESOL)	-3.87
Solubility	3.53e-02 mg/ml ; 1.35e-04 mol/l
Class	Soluble
Log S (Ali)	-4.67
Solubility	5.50e-03 mg/ml ; 2.11e-05 mol/l
Class	Moderately soluble
Log S (SILICOS-IT)	-3.44
Solubility	9.43e-02 mg/ml ; 3.62e-04 mol/l
Class	Soluble

Pharmacokinetics

GI absorption	High
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	No
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	Yes
Log K_p (skin permeation)	-5.54 cm/s

Druglikeness

Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

Medicinal Chemistry

PAINS	1 alert: catechol_A
Brenk	1 alert: catechol
Leadlikeness	Yes
Synthetic accessibility	1.95

Molecule 1

⚦ ⊕ ⬡ ✏ Σ

SMILES Oc1ccccc1

Physicochemical Properties

Formula	C6H6O
Molecular weight	94.11 g/mol
Num. heavy atoms	7
Num. arom. heavy atoms	6
Fraction Csp3	0.00
Num. rotatable bonds	0
Num. H-bond acceptors	1
Num. H-bond donors	1
Molar Refractivity	28.46
TPSA	20.23 Å²

Lipophilicity

Log $P_{o/w}$ (iLOGP)	1.24
Log $P_{o/w}$ (XLOGP3)	1.46
Log $P_{o/w}$ (WLOGP)	1.39
Log $P_{o/w}$ (MLOGP)	1.45
Log $P_{o/w}$ (SILICOS-IT)	1.50
Consensus Log $P_{o/w}$	1.41

Water Solubility

Log S (ESOL)	-1.98
Solubility	9.91e-01 mg/ml ; 1.05e-02 mol/l
Class	Very soluble
Log S (Ali)	-1.49
Solubility	3.04e+00 mg/ml ; 3.23e-02 mol/l
Class	Very soluble
Log S (SILICOS-IT)	-1.73
Solubility	1.74e+00 mg/ml ; 1.85e-02 mol/l
Class	Soluble

Pharmacokinetics

GI absorption	High
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-5.84 cm/s

Druglikeness

Lipinski	Yes; 0 violation
Ghose	No; 3 violations: MW<160, MR<40, #atoms<20
Veber	Yes
Egan	Yes
Muegge	No; 2 violations: MW<200, Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry

PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: MW<250
Synthetic accessibility	1.00

Molecule 1

SMILES   Oc1cc(O)c(c(c1)O)O

Physicochemical Properties

Formula	C6H6O4
Molecular weight	142.11 g/mol
Num. heavy atoms	10
Num. arom. heavy atoms	6
Fraction Csp3	0.00
Num. rotatable bonds	0
Num. H-bond acceptors	4
Num. H-bond donors	4
Molar Refractivity	34.53
TPSA	80.92 Å²

Lipophilicity

Log $P_{o/w}$ (iLOGP)	0.37
Log $P_{o/w}$ (XLOGP3)	0.82
Log $P_{o/w}$ (WLOGP)	0.51
Log $P_{o/w}$ (MLOGP)	-0.40
Log $P_{o/w}$ (SILICOS-IT)	-0.06
Consensus Log $P_{o/w}$	0.25

Water Solubility

Log S (ESOL)	-1.68
Solubility	2.96e+00 mg/ml ; 2.08e-02 mol/l
Class	Very soluble
Log S (Ali)	-2.10
Solubility	1.13e+00 mg/ml ; 7.92e-03 mol/l
Class	Soluble
Log S (SILICOS-IT)	-0.07
Solubility	1.20e+02 mg/ml ; 8.47e-01 mol/l
Class	Soluble

Pharmacokinetics

GI absorption	High
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	Yes
Log K_p (skin permeation)	-6.58 cm/s

Druglikeness

Lipinski	Yes; 0 violation
Ghose	No; 3 violations: MW<160, MR<40, #atoms<20
Veber	Yes
Egan	Yes
Muegge	No; 1 violation: MW<200
Bioavailability Score	0.55

Medicinal Chemistry

PAINS	1 alert: catechol_A
Brenk	2 alerts: catechol, hydroquinone
Leadlikeness	No; 1 violation: MW<250
Synthetic accessibility	1.02

Molecule 1

SMILES   CC(C1=CC(=O)C(=C(C1=O)O)O)C

Physicochemical Properties

Formula	C9H10O4
Molecular weight	182.17 g/mol
Num. heavy atoms	13
Num. arom. heavy atoms	0
Fraction Csp3	0.33
Num. rotatable bonds	1
Num. H-bond acceptors	4
Num. H-bond donors	2
Molar Refractivity	45.86
TPSA	74.60 Å²

Lipophilicity

Log $P_{o/w}$ (iLOGP)	1.17
Log $P_{o/w}$ (XLOGP3)	0.88
Log $P_{o/w}$ (WLOGP)	1.05
Log $P_{o/w}$ (MLOGP)	-0.95
Log $P_{o/w}$ (SILICOS-IT)	0.86
Consensus Log $P_{o/w}$	0.60

Water Solubility

Log S (ESOL)	-1.46
Solubility	6.35e+00 mg/ml ; 3.48e-02 mol/l
Class	Very soluble
Log S (Ali)	-2.03
Solubility	1.70e+00 mg/ml ; 9.31e-03 mol/l
Class	Soluble
Log S (SILICOS-IT)	-0.72
Solubility	3.48e+01 mg/ml ; 1.91e-01 mol/l
Class	Soluble

Pharmacokinetics

GI absorption	High
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-6.79 cm/s

Druglikeness

Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	No; 1 violation: MW<200
Bioavailability Score	0.85

Medicinal Chemistry

PAINS	1 alert: quinone_A
Brenk	1 alert: chinone_1
Leadlikeness	No; 1 violation: MW<250
Synthetic accessibility	2.87

Molecule 1

⚕ ⊕ ◯ ✎ Σ

SMILES OC(=O)/C=C\C(=O)O

Physicochemical Properties	
Formula	C4H4O4
Molecular weight	116.07 g/mol
Num. heavy atoms	8
Num. arom. heavy atoms	0
Fraction Csp3	0.00
Num. rotatable bonds	2
Num. H-bond acceptors	4
Num. H-bond donors	2
Molar Refractivity	24.41
TPSA	74.60 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	0.12
Log $P_{o/w}$ (XLOGP3)	-0.34
Log $P_{o/w}$ (WLOGP)	-0.29
Log $P_{o/w}$ (MLOGP)	-0.64
Log $P_{o/w}$ (SILICOS-IT)	-0.81
Consensus Log $P_{o/w}$	-0.39

Water Solubility	
Log S (ESOL)	-0.21
Solubility	7.10e+01 mg/ml ; 6.12e-01 mol/l
Class	Very soluble
Log S (Ali)	-0.76
Solubility	1.99e+01 mg/ml ; 1.72e-01 mol/l
Class	Very soluble
Log S (SILICOS-IT)	1.34
Solubility	2.52e+03 mg/ml ; 2.17e+01 mol/l
Class	Soluble

Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-7.25 cm/s

Druglikeness	
Lipinski	Yes; 0 violation
Ghose	No; 3 violations: MW<160, MR<40, #atoms<20
Veber	Yes
Egan	Yes
Muegge	No; 2 violations: MW<200, #C<5
Bioavailability Score	0.85

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: michael_acceptor_1
Leadlikeness	No; 1 violation: MW<250
Synthetic accessibility	1.80

Molecule 1

⚕ ⊕ ◯ ✎ Σ

SMILES CC(=C)c1ccc(cc1)O

Physicochemical Properties	
Formula	C9H10O
Molecular weight	134.18 g/mol
Num. heavy atoms	10
Num. arom. heavy atoms	6
Fraction Csp3	0.11
Num. rotatable bonds	1
Num. H-bond acceptors	1
Num. H-bond donors	1
Molar Refractivity	43.36
TPSA	20.23 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	1.84
Log $P_{o/w}$ (XLOGP3)	2.97
Log $P_{o/w}$ (WLOGP)	2.43
Log $P_{o/w}$ (MLOGP)	2.37
Log $P_{o/w}$ (SILICOS-IT)	2.32
Consensus Log $P_{o/w}$	2.38

Water Solubility	
Log S (ESOL)	-2.92
Solubility	1.61e-01 mg/ml ; 1.20e-03 mol/l
Class	Soluble
Log S (Ali)	-3.06
Solubility	1.17e-01 mg/ml ; 8.75e-04 mol/l
Class	Soluble
Log S (SILICOS-IT)	-2.62
Solubility	3.20e-01 mg/ml ; 2.39e-03 mol/l
Class	Soluble

Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-5.01 cm/s

Druglikeness	
Lipinski	Yes; 0 violation
Ghose	No; 1 violation: MW<160
Veber	Yes
Egan	Yes
Muegge	No; 2 violations: MW<200, Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: MW<250
Synthetic accessibility	1.07

Molecule 1

SMILES Oc1cc(cc1C(C)(C)C)C(C)C

Physicochemical Properties	
Formula	C13H20O
Molecular weight	192.30 g/mol
Num. heavy atoms	14
Num. arom. heavy atoms	6
Fraction Csp3	0.54
Num. rotatable bonds	2
Num. H-bond acceptors	1
Num. H-bond donors	1
Molar Refractivity	62.32
TPSA	20.23 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.75
Log $P_{o/w}$ (XLOGP3)	4.36
Log $P_{o/w}$ (WLOGP)	3.81
Log $P_{o/w}$ (MLOGP)	3.60
Log $P_{o/w}$ (SILICOS-IT)	3.58
Consensus Log $P_{o/w}$	3.62

Water Solubility	
Log S (ESOL)	-3.96
Solubility	2.09e-02 mg/ml ; 1.09e-04 mol/l
Class	Soluble
Log S (Ali)	-4.50
Solubility	6.08e-03 mg/ml ; 3.16e-05 mol/l
Class	Moderately soluble
Log S (SILICOS-IT)	-3.86
Solubility	2.67e-02 mg/ml ; 1.39e-04 mol/l
Class	Soluble

Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-4.38 cm/s

Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	No; 2 violations: MW<200, Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 2 violations: MW<250, XLOGP3>3.5
Synthetic accessibility	1.26

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