

Supporting Information

Machine Learning-Assisted Prediction of Water Adsorption Isotherms and Cooling Performance

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Contents	Page Number
S1. Supplementary table data	2-33
S2. Structural characteristics of experimental adsorbents	34
S3. Machine learning algorithms and details	35-39
S4. Adsorption cooling performance calculation	40-42
S5. Supplementary results of machine learning	43-47

S1. Supplementary data in Excel file

Table S1. The literature source of 460 adsorbents used in this work

Ref. No.	Title	DOI	First author	Year
[1]	Liquid Phase Heteroepitaxial Growth of Moisture-Tolerant MOF-5 Isotype Thin Films and Assessment of the Sorption Properties by Quartz Crystal Microbalance	DOI: 10.1002/adfm.201302854	Suttipong Wannapaiboon	2013
[2]	Design of Hydrophilic Metal Organic Framework Water Adsorbents for Heat Reallocation	DOI: 10.1002/adma.201502418	Amandine Cadiau	2015
[3]	Enhancement of CO ₂ Adsorption and CO ₂ /N ₂ Selectivity on ZIF-8 via Postsynthetic Modification	DOI: 10.1002/Aic.13970	Zhijuan Zhang	2013
[4]	Dynamic Structural Behavior and Anion-Responsive Tunable Luminescence of a Flexible Cationic Metal-Organic Framework	DOI: 10.1002/anie.201206724	Biplab Manna	2013
[5]	A Water Stable Metal-Organic Framework with Optimal Features for CO ₂ Capture	DOI: 10.1002/anie.201302682	Qingyuan Yang	2013
[6]	Highly Hydrophobic Isorecticular Porous Metal-Organic Frameworks for the Capture of Harmful Volatile Organic Compounds	DOI: 10.1002/anie.201303484	Natalia M. Padial	2013
[7]	Ultra-Tuning of the Rare-Earth fcu-MOF Aperture Size for Selective Molecular Exclusion of Branched Paraffins	DOI: 10.1002/anie.201506345	Ayalew H. Assen	2015
[8]	A Robust Infinite Zirconium Phenolate Building Unit to Enhance the Chemical Stability of Zr MOFs	DOI: 10.1002/anie.201507058	Georges Mouchaham	2015
[9]	A Zeolite-Like Zinc Phosphonocarboxylate Framework and Its Transformation into Two- and Three-Dimensional Structures	DOI: 10.1002/asia.200700209	Zhenxia Chen	2007
[10]	Two Zn II Metal-Organic Frameworks with Coordinatively Unsaturated Metal Sites: Structures, Adsorption, and Catalysis	DOI: 10.1002/asia.201200601	Xiao-Ming Lin	2012
[11]	Chemical Property Change in a Metal-Organic Framework by Fluoro Functionality	DOI: 10.1002/bkcs.10087	Nakeun Ko	2015
[12]	Microporous Metal-Organic Framework Constructed from Heptanuclear Zinc Carboxylate Secondary Building Units	DOI: 10.1002/chem.200500963	Qian-Rong Fang	2006
[13]	A Porous Coordination Polymer with Accessible Metal Sites and its Complementary Coordination Action	DOI: 10.1002/chem.200802730	Hirotohi Sakamoto	2009
[14]	Flexible Metal-Organic Framework with Hydrophobic Pores	DOI: 10.1002/chem.201103078	Lin-Hua Xie	2011
[15]	A Robust Porous Metal-Organic Framework with a New Topology That Demonstrates Pronounced Porosity and High-Efficiency Sorption/Selectivity Properties of Small Molecules	DOI: 10.1002/chem.201103687	Huanhuan Li	2012
[16]	Decametalllic Co II -Cluster-Based Microporous Magnetic Framework with a Semirigid Multicoordinating Ligand	DOI: 10.1002/chem.201204458	Jumei Tian	2013
[17]	A New Synthetic Route to Microporous Silica with Well-Defined Pores by Replication of a Metal-Organic Framework	DOI: 10.1002/chem.201501599	Atsushi Kondo	2015
[18]	Topological Diversity, Adsorption and Fluorescence Properties of MOFs Based on a Tetracarboxylate Ligand	DOI: 10.1002/ejic.201000415	Ronny Gr�nker	2010
[19]	Two 3D Supramolecular Isomeric Mixed-Ligand Co II Frameworks - Guest-Induced Structural Variation, Magnetism, and Selective Gas Adsorption	DOI: 10.1002/ejic.201200851	Dan Liu	2012
[20]	On the Physical Adsorption of Vapors by Microporous Carbons	DOI: 10.1006/jcis.1995.1018	R. H. Bradley	1995
[21]	Comparison of Gaseous Molecular Adsorption Properties of Microporous Manganese Oxides and Crystalline Aluminosilicates	DOI: 10.1006/jcis.2000.7399	Z. M. Wang	2001
[22]	Activated Carbon Oxygen Content Influence on Water and Surfactant Adsorption	DOI: 10.1006/jcis.2001.8052	Phillip Pendleton	2002
[23]	Adsorption of toluene and toluene-water vapor mixture on almond shell based activated carbons	DOI: 10.1007/s10450-013-9540-5	Alicia Mart�nez de Yuso	2013
[24]	Synthesis, structures and properties of three new compounds based on multidentate ligand containing triazole and pyrimidine	DOI: 10.1007/s40242-015-5051-0	Lei L�	2015
[25]	Adsorption of water vapor by non-porous carbons	DOI: 10.1016/0008-6223(92)90080-g	P. J. M. Carrott	1992
[26]	Evaluation of confinement effects in zeolites under Henry's adsorption regime	DOI: 10.1016/j.apsusc.2009.12.067	Marc Pera-Titus	2010
[27]	CO ₂ adsorption and catalytic application of Co-MOF-74 synthesized by microwave heating	DOI: 10.1016/j.cattod.2011.08.019	Hye-Young Cho	2012
[28]	Adsorption/catalytic properties of MIL-125 and NH ₂ -MIL-125	DOI: 10.1016/j.cattod.2012.08.014	Se-Na Kim	2013
[29]	Adsorption characteristics of nanoporous carbon-silica composites synthesized from graphite oxide by a mechanochemical intercalation method	DOI: 10.1016/j.jcis.2007.04.016	Y. H. Chu	2007
[30]	Adsorption of water on three-dimensional pillared-layer metal organic frameworks	DOI: 10.1016/j.jcis.2007.05.090	Atsushi Kondo	2007
[31]	Syntheses, crystal structures, and water adsorption behaviors of jungle-gym-type porous coordination polymers containing nitro moieties	DOI: 10.1016/j.jssc.2009.07.048	Kazuhiro Uemura	2009
[32]	Simulations of model metal-organic frameworks for the separation of carbon dioxide	DOI: 10.1016/j.egypro.2011.01.090	Brad A. Wells	2011
[33]	Water adsorption-desorption property of stable porous supramolecular assembly composed of discrete tetranuclear iron(III) complex using π - π interactions	DOI: 10.1016/j.ica.2012.02.002	□	2012
[34]	Grafting of hydrophilic ethylene glycols or ethylenediamine on coordinatively unsaturated metal sites in MIL-100(Cr) for improved water adsorption characteristics	DOI: 10.1016/j.ica.2013.07.024	Martin Wickenheisser	2013
[35]	A 3D POM-MOF composite based on Ni(II) ion and 2,2'-bipyridyl-3,3'-dicarboxylic acid: Crystal structure and proton conductivity	DOI: 10.1016/j.jssc.2013.03.041	Meilin Wei	2013

[36]	Reversible flexible structural changes in multidimensional MOFs by guest molecules (I ₂ , NH ₃) and thermal stimulation	DOI: 10.1016/j.jssc.2015.02.014	Yang Chen	2015
[37]	Characterisation of metal organic frameworks for adsorption cooling	DOI: 10.1016/j.ijheatmasstransfer.2012.07.068	Ahmed Rezk	2012
[38]	Design, structure and properties of a novel 3D metal-organic framework constructed from N-donor ligand supporting Cd(II)-carboxylate layer	DOI: 10.1016/j.inoche.2006.02.029	Ming Xue	2006
[39]	Adsorption-desorption of water vapour on chars prepared from commercial wood charcoals, in relation to their chemical composition, surface chemistry and pore structure	DOI: 10.1016/j.jaap.2010.03.005	J. Pastor-Villegas	2010
[40]	Sulfation of metal-organic frameworks: Opportunities for acid catalysis and proton conductivity	DOI: 10.1016/j.jcat.2011.04.015	Maarten G	2011
[41]	Characterization of metal-organic frameworks by water adsorption	DOI: 10.1016/j.micromeso.2008.11.020	Pia Küsgens	2009
[42]	Effect of functional groups in MIL-101 on water sorption behavior	DOI: 10.1016/j.micromeso.2012.01.015	George Akiyama	2012
[43]	Bench-scale preparation of Cu ₃ (BTC) ₂ by ethanol reflux: Synthesis optimization and adsorption/catalytic applications	DOI: 10.1016/j.micromeso.2012.05.021	Jun Kim	2012
[44]	Thermogravimetric and adsorption studies of oxidized active carbons by using different probe molecules	DOI: 10.1016/s0040-6031(99)00375-5	Zuojiang Li	2000
[45]	Binary mixture adsorption of water and ethanol on silicalite	DOI: 10.1016/S0167-2991(02)80329-9	Y. Oumi	2002
[46]	Single-component gas phase adsorption and desorption studies using a tapered element oscillating microbalance	DOI: 10.1016/S1387-1811(02)00428-6	Arjan Giaya	2002
[47]	Defect Control To Enhance Proton Conductivity in a Metal-Organic Framework	DOI: 10.1021/acs.chemmater.5b00665	Jared M. Taylor	2015
[48]	Hydrostable and Nitril/Methyl-Functionalized Metal-Organic Framework for Drug Delivery and Highly Selective CO ₂ Adsorption	DOI: 10.1021/acs.inorgchem.5b00335	De-Yun Ma	2015
[49]	H ₂ O Adsorption/Desorption in MOF-74: Ab Initio Molecular Dynamics and Experiments	DOI: 10.1021/acs.jpcc.5b02069	Yunsong Li	2015
[50]	Solubility of Gases in Water Confined in Nanoporous Materials: ZSM-5, MCM-41, and MIL-100	DOI: 10.1021/acs.jpcc.5b06660	Linh Ngoc Ho	2015
[51]	Three-Dimensional Robust Porous Coordination Polymer with Schiff Base Site on the Pore Wall: Synthesis, Single-Crystal-to-Single-Crystal Reversibility, and Selective CO ₂ Adsorption	DOI: 10.1021/Cg2004672	Rajdip Dey	2011
[52]	Variable Water Adsorption in Amino Acid Derivative Based Homochiral Metal Organic Frameworks	DOI: 10.1021/Cg3008443	Tanay Kundu	2012
[53]	A CdSO ₄ -Type 3D Metal-Organic Framework Showing Coordination Dynamics on Cu ₂ +Axial Sites: Vapochromic Response and Guest Sorption Selectivity	DOI: 10.1021/Cg3017563	Guo-Bi Li	2013
[54]	A Series of Three-Dimensional Lanthanide Coordination Compounds with the Rutile Topology	DOI: 10.1021/Cg800204q	Xiaojun Zhao	2009
[55]	Immobilization of Alkali Metal Ions in a 3D Lanthanide-Organic Framework: Selective Sorption and H ₂ Storage Characteristics	DOI: 10.1021/Cm9014749	Sudip Mohapatra	2009
[56]	Investigation of Porous Ni-Based Metal-Organic Frameworks Containing Paddle-Wheel Type Inorganic Building Units via High-Throughput Methods	DOI: 10.1021/Ic200381f	Palanikumar Maniam	2011
[57]	A Vanadium (VO ₂ ⁺) Metal-Organic Framework: Selective Vapor Adsorption, Magnetic Properties, and Use as a Precursor for a Polyoxovanadate	DOI: 10.1021/Ic200463k	Prakash Kanoo	2011
[58]	Flexible and Hydrophobic Zn-Based Metal-Organic Framework	DOI: 10.1021/Ic200937u	Ines Maria Hauptvogel	2011
[59]	Bistable Dynamic Coordination Polymer Showing Reversible Structural and Functional Transformations	DOI: 10.1021/Ic301481p	Sanjog S	2012
[60]	Gas Storage in a Partially Fluorinated Highly Stable Three-Dimensional Porous Metal-Organic Framework	DOI: 10.1021/Ic302645rb	Atanu Santra	2013
[61]	Third-Generation Breathing Metal-Organic Framework with Selective, Stepwise, Reversible, and Hysteretic Adsorption Properties	DOI: 10.1021/Ic402095u	Suresh Sanda	2013
[62]	Stoichiometry-Controlled Two Flexible Interpenetrated Frameworks: Higher CO ₂ Uptake in a Nanoscale Counterpart Supported by Accelerated Adsorption Kinetics	DOI: 10.1021/Ic500234r	Nivedita Sikdar	2014
[63]	Conformation-Controlled Sorption Properties and Breathing of the Aliphatic Al-MOF [Al(OH)(CDC)]	DOI: 10.1021/Ic500288w	Felicita Niekpiel	2014
[64]	Effect of Water Adsorption on Retention of Structure and Surface Area of Metal-Organic Frameworks	DOI: 10.1021/Ic202325p	Paul M. Schoencker	2012
[65]	Zn(tbip) (H ₂ tbip= 5-tert-Butyl Isophthalic Acid): A Highly Stable Guest-Free Microporous Metal Organic Framework with Unique Gas Separation Capability	DOI: 10.1021/Ja057667b	Long Pan	2006
[66]	A Porous Framework Polymer Based on a Zinc(II) 4,4'-Bipyridine-2,6,2',6'-tetracarboxylate: Synthesis, Structure, and "Zeolite-Like" Behaviors	DOI: 10.1021/Ja060946u	Xiang Lin	2006
[67]	Reversible Water-Induced Magnetic and Structural Conversion of a Flexible Microporous Ni(II)/Fe(III) Ferromagnet	DOI: 10.1021/Ja069166b	Nobuhiro Yanai	2007
[68]	Explanation of the Adsorption of Polar Vapors in the Highly Flexible Metal Organic Framework MIL-53(Cr)	DOI: 10.1021/ja1023282	Sandrine Bourrelly	2010
[69]	A Sodalite-Type Porous Metal-Organic Framework with Polyoxometalate Templates: Adsorption and Decomposition of Dimethyl Methylphosphonate	DOI: 10.1021/Ja109659k	Feng-Ji Ma	2011
[70]	Super Flexibility of a 2D Cu-Based Porous Coordination Framework on Gas Adsorption in Comparison with a 3D Framework of Identical Composition: Framework Dimensionality-Dependent Gas Adsorptivities	DOI: 10.1021/Ja201170c	Atsushi Kondo	2011
[71]	Hydroxyl Group Recognition by Hydrogen-Bonding Donor and Acceptor Sites Embedded in a Layered Metal-Organic Framework	DOI: 10.1021/Ja203291n	Masaaki Sadakiyo	2011
[72]	Capture of Nerve Agents and Mustard Gas Analogues by Hydrophobic Robust MOF-5 Type Metal-Organic Frameworks	DOI: 10.1021/Ja2042113	Carmen Montoro	2011
[73]	Helical Water Chain Mediated Proton Conductivity in Homochiral Metal-Organic Frameworks with Unprecedented Zeoliticunh-Topology	DOI: 10.1021/Ja2078637	Subash Chandra Sahoo	2011
[74]	Enhancing Water Stability of Metal-Organic Frameworks via Phosphonate Monoester Linkers	DOI: 10.1021/Ja306812r	Jared M. Taylor	2012
[75]	Water Adsorption in Porous Metal-Organic Frameworks and Related Materials	DOI: 10.1021/Ja500330a	Hiroyasu Furukawa	2014
[76]	Adsorption Isotherms of Water, Propan-2-ol, and Methylbenzene Vapors on Grade 03 Silica Gel, Sorbonorit 4 Activated Carbon, and HiSiv 3000 Zeolite	DOI: 10.1021/je400517c	Józef Nastaj	2013

[77]	Uncommon Adsorption Isotherm of Methanol on a Hydrophobic Y-zeolite	DOI: 10.1021/Jp0103530	Istvan Halasz	2001
[78]	Molecular Understanding for the Adsorption of Water and Alcohols in Hydrophilic and Hydrophobic Zeolitic Metal–Organic Frameworks	DOI: 10.1021/Jp1033273	Anjaiah Nalaparaju	2010
[79]	Molecular Simulation of Water/Alcohol Mixtures' Adsorption and Diffusion in Zeolite 4A Membranes	DOI: 10.1021/Jp805923k	Jian Yang Wu	2009
[80]	Probing the Mechanism of Water Adsorption in Carbon Micropores with Multitemperature Isotherms and Water Preadsorption Experiments	DOI: 10.1021/la061140a	S. W. Rutherford	2006
[81]	CO ₂ /H ₂ O Adsorption Equilibrium and Rates on Metal–Organic Frameworks: HKUST-1 and Ni/DOBDC	DOI: 10.1021/La102359q	Jian Liu	2010
[82]	Electron Microscopic Study on Aerosol-Assisted Synthesis of Aluminum Organophosphonates Using Flexible Colloidal PS-b-PEO Templates	DOI: 10.1021/La302695q	Tatsuo Kimura	2012
[83]	Adjusting the Stability of Metal–Organic Frameworks under Humid Conditions by Ligand Functionalization	DOI: 10.1021/La304151r	Himanshu Jasuja	2012
[84]	Synthesis of Cobalt-, Nickel-, Copper-, and Zinc-Based, Water-Stable, Pillared Metal–Organic Frameworks	DOI: 10.1021/La503269f	Himanshu Jasuja	2014
[85]	Reversible Structural Change of Cu-MOF on Exposure to Water and Its CO ₂ Adsorptivity	DOI: 10.1021/la803818p	Yan Cheng	2009
[86]	Experimental Study of Water Adsorption on Activated Carbons	DOI: 10.1021/la980492h	Issa I. Salame	1999
[87]	A flexible interpenetrating coordination framework with a bimodal porous functionality	DOI: 10.1038/Nmat1827	Tapas Kumar Maji	2007
[88]	Selective guest sorption in an interdigitated porous framework with hydrophobic pore surfaces	DOI: 10.1039/B703502k	Satoshi Horike	2007
[89]	A cubic coordination framework constructed from benzobistriazolate ligands and zinc ions having selective gas sorption properties	DOI: 10.1039/B904280f	Shyam Biswas,	2009
[90]	Enhanced selectivity of CO ₂ from a ternary gas mixture in an interdigitated porous framework	DOI: 10.1039/C0cc00027b	Keiji Nakagawa	2010
[91]	A microporous luminescent metal–organic framework for highly selective and sensitive sensing of Cu ²⁺ in aqueous solution	DOI: 10.1039/C0cc00148a	Yunqing Xiao	2010
[92]	Construction of a trigonal bipyramidal cage-based metal–organic framework with hydrophilic pore surface via flexible tetrapodal ligands	DOI: 10.1039/C0cc02496a	Tian-Fu Liu	2010
[93]	Single-crystal-to-single-crystal transformations and selective adsorption of porous copper(ii) frameworks	DOI: 10.1039/C0cc04689b	Man-Sheng Chen	2011
[94]	Selective carbon dioxide uptake and crystal-to-crystal transformation: porous 3D framework to 1D chain triggered by conformational change of the spacer	DOI: 10.1039/C1cc05847a	Ritesh Haldar	2012
[95]	CO ₂ capture and conversion using Mg-MOF-74 prepared by a sonochemical method	DOI: 10.1039/C1cc02234b	Da-Ae Yang	2012
[96]	A microporous metal–organic framework with high stability for GC separation of alcohols from water	DOI: 10.1039/C2cc33023g	Tsolmon Borjigin	2012
[97]	Post-synthesis functionalization of MIL-101 using diethylenetriamine: a study on adsorption and catalysis	DOI: 10.1039/C2cc06608d	Se-Na Kim	2012
[98]	Controlled modification of the inorganic and organic bricks in an Al-based MOF by direct and post-synthetic synthesis routes	DOI: 10.1039/C2cc06620c	Tim Ahnfeldt	2012
[99]	Two ligand-functionalized Pb(ii) metal–organic frameworks: structures and catalytic performances	DOI: 10.1039/C2dt30935a	Xiao-Ming Lin	2012
[100]	Carbon dioxide adsorption by physisorption and chemisorption interactions in piperazine-grafted Ni ₂ (dobdc) (dobdc = 1,4-dioxido-2,5-benzenedicarboxylate)	DOI: 10.1039/C2dt31112g	Anita Das	2012
[101]	A robust microporous metal–organic framework constructed from a flexible organic linker for highly selective sorption of methanol over ethanol and water	DOI: 10.1039/C2jm15604k	Qian Huang	2012
[102]	Reversible solid-state hydration and dehydration process involving anion transfer in a self-assembled Cu ₂ system	DOI: 10.1039/C2ra21865h	T. Washizaki	2012
[103]	A charge-polarized porous metal–organic framework for gas chromatographic separation of alcohols from water	DOI: 10.1039/C3cc38260e	Jian-Ke Sun	2013
[104]	Polyoxometalate-based purely inorganic porous frameworks with selective adsorption and oxidative catalysis functionalities	DOI: 10.1039/C3cc40990b	Ding Liu	2013
[105]	Environmentally friendly synthesis of highly hydrophobic and stable MIL-53 MOF nanomaterials	DOI: 10.1039/C3cc42287a	Jia Liu	2013
[106]	An unusual highly connected 3D net with hydrophilic pore surface	DOI: 10.1039/C3cc26788a	Huabin Zhang	2013
[107]	Toxic gas removal – metal–organic frameworks for the capture and degradation of toxic gases and vapours	DOI: 10.1039/C3cs60475f	Elisa Barea	2014
[108]	Selective CO ₂ adsorption and proton conductivity in the two-dimensional Zn(ii) framework with protruded water molecules and flexible ether linkers	DOI: 10.1039/C3dt50896j	Won Ju Phang	2013
[109]	Zn(ii) coordination polymer of an in situ generated 4-pyridyl (4Py) attached bis(amido)phosphate ligand, [PO ₂ (NH ₄ Py) ₂] [–] showing preferential water uptake over aliphatic alcohols	DOI: 10.1039/C3dt51123e	Arvind K. Gupta,	2013
[110]	Postsynthetic tuning of hydrophilicity in pyrazolate MOFs to modulate water adsorption properties	DOI: 10.1039/C3cc40876k	Casey R. Wade	2013
[111]	Synthesis of reduced graphene oxide/phenolic resin-based carbon composite ultrafine fibers and their adsorption performance for volatile organic compounds and water	DOI: 10.1039/c3ta10545h	Yu Bai	2013
[112]	Water adsorption in MOFs: fundamentals and applications	DOI: 10.1039/C4cs00078a	Jérôme Canivet	2014
[113]	A highly stable multifunctional three-dimensional microporous framework: excellent selective sorption and visible photoluminescence	DOI: 10.1039/C4dt00230j	Yumei Huang	2014
[114]	Manufacture of dense CAU-10-H coatings for application in adsorption driven heat pumps: optimization and characterization	DOI: 10.1039/c5cc00789e	M. F. de Lange	2015
[115]	New layered copper 1,3,5-benzenetriphosphonates pillared with N-donor ligands: their synthesis, crystal structures, and adsorption properties	DOI: 10.1039/c5dt01137j	Atsushi Kondo	2015
[116]	Water stable triazolyl phosphonate MOFs: steep water uptake and facile regeneration	DOI: 10.1039/c5dt02651b	S. Begum	2015
[117]	Rational design of a pyrene based luminescent porous supramolecular framework: excimer emission and energy transfer	DOI: 10.1039/c5ra14267a	Komal Prasad	2015
[118]	Synthesis, Structure, and Properties of a Chiral Zinc(II) Metal-Organic Framework Featuring Linear Trinuclear Secondary Building Blocks	DOI: 10.1071/Ch12270	Zilu Chen	2012

[119]	A porous Cu(II)-MOF containing [PW12O40]3- and a large protonated water cluster: synthesis, structure, and proton conductivity	DOI: 10.1080/00958972.2014.957689	Meilin Wei	2014
[120]	Adsorption of Radon and Water Vapor on Commercial Activated Carbons	DOI: 10.1080/01496399508225610	Neguib M. Hassan	1995
[121]	Molecular Simulation Study on Adsorption and Diffusion Behavior of Ethanol/Water Molecules in NaA Zeolite Crystal	DOI: 10.1252/Jcej.37.67	Shin-ichi Furukawa	2004
[122]	Dependence of Water Vapour Adsorption on the Polarity of the Graphene Surfaces of Multi-wall Carbon Nanotubes	DOI: 10.1260/0263-6174.28.10.903	Robert Bradley	2010
[123]	Enhanced Adsorption of Methanol by Oxidised Nutshell Carbon	DOI: 10.1260/0263617001493422	Alan Bailey	2000
[124]	A Stable Polyoxometalate-Pillared Metal-Organic Framework for Proton-Conducting and Colorimetric Biosensing	DOI: 10.1002/chem.201501515	En-Long Zhou	2015
[125]	Protection of open-metal V(III) sites and their associated CO2/CH4/N2/O2/H2O adsorption properties in mesoporous V-MOFs	DOI: 10.1016/j.jcis.2015.06.036	Jiangfeng Yang	2015
[126]	Stability of an Al-Fumarate MOF and Its Potential for CO2 Capture from Wet Stream	DOI: 10.1021/acs.iecr.5b03509	Juliana A. Coelho	2016
[127]	A metal-organic framework constructed using a flexible tripodal ligand and tetranuclear copper cluster for sensing small molecules	DOI: 10.1039/c5dt00762c	Chaoyi Hou	2015
[128]	Enhancing the Water Capacity in Zr-based Metal-Organic Framework for Heat Pump and Atmospheric Water Generator Applications	DOI: 10.1021/acsanm.9b00416	A. Luna-Triguero	2019
[129]	A robust large-pore zirconium carboxylate metal-organic framework for energy-efficient water-sorption-driven refrigeration	□	Sujing Wang	2018
[130]	The porous metal-organic framework CUK-1 for adsorption heat allocation toward green applications of natural refrigerant water	DOI: 10.1021/acsami.9b02605	Ji Sun Lee	2019
[131]	A metal-organic framework for efficient waterbased ultra-low-temperature-driven cooling	DOI: 10.1038/s41467-019-10960-0	Dirk Lenzen	2019
[132]	Record Atmospheric Fresh Water Capture and Heat Transfer with a Material Operating at the Water Uptake Reversibility Limit	DOI: 10.1021/acscentsci.7b00186	Adam J. Rieth	2017
[133]	Tunable Water and CO2 Sorption Properties in Isostructural AzineBased Covalent Organic Frameworks through Polarity Engineering	DOI: 10.1021/acs.chemmater.5b02151	Linus Stegbauer	2015
[134]	Pd loaded amphiphilic COF as catalyst for multi-fold Heck reactions, C-C couplings and CO oxidation	DOI: 10.1038/srep10876	Dinesh Mullangi	2015
[135]	Pore surface engineering in porous, chemically stable covalent organic frameworks for water adsorption†	DOI: 10.1039/c5ta07998e	Bishnu P. Biswal	2015
[136]	Constructing Ultraporous Covalent Organic Frameworks in Seconds via an Organic Terracotta Process	DOI: 10.1021/jacs.6b08815	Suwendu Karak	2017
[137]	Microporous Cyanate Resins: Synthesis, Porous Structure, and Correlations with Gas and Vapor Adsorptions	DOI:10.1021/ma3008652	Hao Yu	2012
[138]	Nitrogen-Rich Covalent Triazine Frameworks as High-Performance Platforms for Selective Carbon Capture and Storage	DOI: 10.1021/acs.chemmater.5b03330	Stephan Hug	2015
[139]	Base-Free Aqueous-Phase Oxidation of 5-Hydroxymethylfurfural over Ruthenium Catalysts Supported on Covalent Triazine Frameworks	DOI:10.1002/essc.201501106.	Jens Artz	2015
[140]	A mixed-linker approach towards improving covalent triazine-based frameworks for CO2 capture and separation	DOI:10.1016/j.micromeso.2016.11.033	Subarna Dey	2017
[141]	Two linkers are better than one: enhancing CO2 capture and separation with porous covalent triazine-based frameworks from mixed nitrile linkers	DOI: 10.1039/c6ta07076k	Subarna Dey	2017
[142]	Preparation of covalent triazine frameworks with imidazolium cations embedded in basic sites and their application for CO2 capture	DOI: 10.1039/c6ta11226a	Kwangho Park	2017
[143]	A fluorine-containing hydrophobic covalent triazine framework with excellent selective CO2 capture performance	DOI: 10.1039/c7ta08913a	Guangbo Wang	2018
[144]	Mesoporous Conjugated Polycarbazole with High Porosity via Structure Tuning	DOI:10.1021/ma501330v	Qi Chen	2014
[145]	Adsorption performance and catalytic activity of porous conjugated polyporphyrins via carbazolebased oxidative coupling polymerization	DOI: 10.1039/c3py01430d	Li-Juan Feng	2014
[146]	Microporous Poly(Schiff Base) Constructed from Tetraphenyladamantane Units for Adsorption of Gases and Organic Vapors	DOI: 10.1002/marc.201400013	Guiyang Li	2014
[147]	Microporous polyimides with functional groups for the adsorption of carbon dioxide and organic vapors	DOI: 10.1039/c6ta04337b	Guiyang Li	2016
[148]	Evaluation of a robust, diimide-based, porous organic polymer (POP) as a high-capacity sorbent for representative chemical threats	DOI 10.1007/s10934-011-9468-7	Gregory W. Peterson	2012
[149]	Tailoring Pore Structure and Properties of Functionalized Porous Polymers by Cyclotrimerization	DOI:10.1021/ma500512j	Florian M. Wieser	2014
[150]	Microporous Organic Polyimides for CO2 and H2O Capture and Separation from CH4 and N2 Mixtures: Interplay between Porosity and Chemical Function	DOI: 10.1021/acs.chemmater.6b01949	Christoph Klumpen	2016
[151]	Reversible water capture by a charged metal-free porous polymer	DOI:10.1016/j.polymer.2017.05.071	J. Byun	2017
[152]	Epoxy-Functionalized Porous Organic Polymers via the Diels-Alder Cycloaddition Reaction for Atmospheric Water Capture	DOI:10.1002/ange.201800380	Yearin Byun	2018
[153]	New element organic frameworks via Suzuki coupling with high adsorption capacity for hydrophobic molecules	DOI: 10.1039/c003130e	Marcus Rose	2010
[154]	Guest-Responsive Reversible Swelling and Enhanced Fluorescence in a Super-Absorbent, Dynamic Microporous Polymer	DOI: 10.1002/chem.201103750	K. Venkata Rao	2012
[155]	Butanol Separation from Humid CO2-Containing Multicomponent Vapor Mixtures by Zeolitic Imidazolate Frameworks	DOI: 10.1021/acssuschemeng.7b02604	Souryadeep Bhattacharyya	2017
[156]	Separation of CO2 in a Solid Waste Management Incineration Facility Using Activated Carbon Derived from Pine Sawdust	DOI: 10.3390/en10060827	Inés Durán	2017
[157]	Rapid Cycling and Exceptional Yield in a Metal-Organic Framework Water Harvester	DOI: 10.1021/acscentsci.9b00745	Nikita Hanikel	2019
[158]	A copper (II)-paddlewheel metal-organic framework with exceptional hydrolytic stability and selective adsorption and detection ability of aniline in water	DOI: 10.1021/acsami.7b07920	Ya Chen	2017
[159]	Tuning water sorption in highly stable Zr (IV)-metal-organic frameworks through local functionalization of metal clusters	DOI: 10.1021/acsami.8b09333	Yong-Zheng Zhang	2018
[160]	Base-resistant ionic metal-organic framework as a porous ion-exchange sorbent	DOI: 10.1016/j.isci.2018.04.004	Aamod V. Desai	2018
[161]	Principles of designing extra-large pore openings and cages in zeolitic imidazolate frameworks	DOI: 10.1021/jacs.7b02272	Jingjing Yang	2017

[162]	Zr-and Hf-based metal-organic frameworks: tracking down the polymorphism	DOI: 10.1021/cg301691d	Volodymyr Bon	2013
[163]	The synergistic effect of oxygen and water on the stability of the isostructural family of metal-organic frameworks [Cr 3 (BTC) 2] and [Cu 3 (BTC) 2]	DOI: 10.1039/C7DT02957H	Zhuoming Zhang	2017
[164]	Stable Aluminum Metal-Organic Frameworks (Al-MOFs) for Balanced CO2 and Water Selectivity	DOI: 10.1021/acsami.7b17026	Haiwei Li	2018
[165]	High CO 2/N 2/O 2/CO separation in a chemically robust porous coordination polymer with low binding energy	DOI: 10.1039/C3SC52177J	Jingui Duan	2014
[166]	Stability and degradation mechanisms of metal-organic frameworks containing the Zr 6 O 4 (OH) 4 secondary building unit	DOI: 10.1039/C3TA10662D	Jared B. DeCoste	2013
[167]	A highly stable metal-organic framework with optimum aperture size for CO2 capture	DOI: 10.1002/aic.15837	Zhigang Hu	2017
[168]	UiO-67-type metal-organic frameworks with enhanced water stability and methane adsorption capacity	DOI: 10.1021/acs.inorgchem.5b02257	Sigurd Øien-Ødegaard	2016
[169]	Structural Stability of N-Alkyl-Functionalized Titanium Metal-Organic Frameworks in Aqueous and Humid Environments	DOI: 10.1021/acsami.7b15045	Matthew W. Logan	2017
[170]	A fine-tuned MOF for gas and vapor separation: A multipurpose adsorbent for acid gas removal, dehydration, and BTX sieving	DOI: 10.1016/j.chempr.2017.09.002	M. Infas H. Mohideen	2017
[171]	Antenna-protected metal-organic squares for water/ammonia uptake with excellent stability and regenerability	DOI: 10.1021/acssuschemeng.7b00460	Yang Chen	2017
[172]	Water-Stable Metal-Organic Framework with Three Hydrogen-Bond Acceptors: Versatile Theoretical and Experimental Insights into Adsorption Ability and Thermo-Hydrolytic Stability	DOI: 10.1021/acs.inorgchem.8b00078	Kornel Roztock	2018
[173]	Reticular chemistry in action: A hydrolytically stable MOF capturing twice its weight in adsorbed water	DOI: 10.1016/j.chempr.2017.11.005	Sk Md Towsif Abtab	2018
[174]	A fine-tuned metal-organic framework for autonomous indoor moisture control	DOI: 10.1021/jacs.7b04132	Rasha G. AbdulHalim	2017
[175]	Wide Control of Proton Conductivity in Porous Coordination Polymers	DOI: 10.1021/ja109810w	Akihito Shigematsu	2011
[176]	Structure-property relationships of water adsorption in metal-organic frameworks	DOI: 10.1039/C4NJ00076E	Je'ro'me Canivet	2014
[177]	Hydrolytically stable fluorinated metal-organic frameworks for energy-efficient dehydration	DOI: 10.1126/science.aam8310	Amandine Cadiou,	2017
[178]	Metal-organic frameworks with high working capacities and cyclic hydrothermal stabilities for fresh water production	DOI: 10.1016/j.ccej.2015.10.098	Seung-Ik Kim	2016
[179]	Highly porous and stable coordination polymers as water sorption materials	DOI: 10.1246/cl.2010.360	George Akiyama	2010
[180]	Water stabilization of Zr 6-based metal-organic frameworks via solvent-assisted ligand incorporation	DOI: 10.1039/C5SC01784J	Pravas Deria	2015
[181]	Water adsorption/desorption over metal-organic frameworks with ammonium group for possible application in adsorption heat transformation	DOI: 10.1016/j.ccej.2019.05.121	Hyung Jun An	2019
[182]	Ligand rigidification for enhancing the stability of metal-organic frameworks	DOI: 10.1021/jacs.9b02947	Xiu-Liang Lv	2019
[183]	Tailoring the water adsorption properties of MIL-101 metal-organic frameworks by partial functionalization	DOI: 10.1039/C4TA04907A	Nakeun Ko	2015
[184]	Precise control of pore hydrophilicity enabled by post-synthetic cation exchange in metal-organic frameworks	DOI: 10.1039/C8SC00112J	Ashley M. Wright	2018
[185]	Perfluoroalkane Functionalization of NU-1000 via Solvent-Assisted Ligand Incorporation: Synthesis and CO2 Adsorption Studies	DOI: 10.1021/ja408959g	Pravas Deria	2013
[186]	Pore-engineered metal-organic frameworks with excellent adsorption of water and fluorocarbon refrigerant for cooling applications	DOI: 10.1021/jacs.7b04872	Jian Zheng	2017
[187]	Experimental investigation of metal organic frameworks characteristics for water adsorption chillers	DOI: 10.1177/0954406212456469	Ahmed Rezk	2013
[188]	A Tunable Bimetallic MOF-74 for Adsorption Chiller Applications	DOI: 10.1002/ejic.201800042	Jian Liu	2018
[189]	Controlled modification of the inorganic and organic bricks in an Al-based MOF by direct and post-synthetic synthesis routes	DOI: 10.1039/C2CE06620C	Tim Ahnfeldt	2012
[190]	Zr (IV) and Hf (IV) based metal-organic frameworks with reo-topology	DOI: 10.1039/C2CC34246D	Volodymyr Bon	2012
[191]	CAU-3: A new family of porous MOFs with a novel Al-based brick:[Al 2 (OCH 3) 4 (O 2 CX-CO 2)](X= aryl)	DOI: 10.1039/C2DT12005D	Helge Reinsch	2012
[192]	Impact of alkyl-functionalized BTC on properties of copper-based metal-organic frameworks	DOI: 10.1021/cg300518k	Yang Cai	2012
[193]	Tuning the adsorption properties of UiO-66 via ligand functionalization	DOI: 10.1021/la3035352	Gregory E. Cmarik	2012
[194]	Evaluation of the highly stable metal-organic framework MIL-53(Al)-TDC (TDC = 2,5-thiophenedicarboxylate) as a new and promising adsorbent for heat transformation applications	DOI: 10.1039/C8TA04407D	Niels Tannert	2018
[195]	Tunable Metal-Organic Frameworks Enable High-Efficiency Cascaded Adsorption Heat Pumps	DOI: 10.1021/jacs.8b09655	Adam J. Rieth	2018
[196]	Kinetic water stability of an isostructural family of zinc-based pillared metal-organic frameworks	DOI: 10.1021/la304204k	Himanshu Jasuja	2013
[197]	Pore Surface Tailored SOD-Type Metal-Organic Zeolites	DOI: 10.1002/adma.201004028	Jie-Peng Zhang ,	2011
[198]	MOF/polymer composite synthesized using a double solvent method offers enhanced water and CO 2 adsorption properties	DOI: 10.1039/C8CC05428B	Li Peng	2018
[199]	Enhancing the Water Stability of Al-MIL-101-NH2 via Postsynthetic Modification	DOI: 10.1002/chem.201404654	Thomas Wittmann	2014
[200]	Functionalization of Zr-based MOFs with alkyl and perfluoroalkyl groups: the effect on the water sorption behavior	DOI: 10.1039/C5SDT02908B	C. Yu	2015
[201]	Synthesis of cobalt-, nickel-, copper-, and zinc-based, water-stable, pillared metal-organic frameworks	DOI: 10.1021/la503269f	Himanshu Jasuja	2014
[202]	New Functionalized Flexible Al-MIL-53-X (X = -Cl, -Br, -CH3, -NO2, -(OH)2) Solids: Syntheses, Characterization, Sorption, and Breathing Behavior	DOI: 10.1021/ic201219g	Shyam Biswas	2011

[203]	A new Al-MOF based on a unique column-shaped inorganic building unit exhibiting strongly hydrophilic sorption behaviour	DOI: 10.1039/C2CC34909D	Helge Reinsch	2012
[204]	Single-crystal and humidity-controlled powder diffraction study of the breathing effect in a metal-organic framework upon water adsorption/desorption	DOI: 10.1039/C6CC02908F	Javier Ariñez-Soriano	2016
[205]	Crystals for sustainability-structuring Al-based MOFs for the allocation of heat and cold	DOI: 10.1039/C4CE01073F	M. F. de Lange	2015
[206]	Variable water adsorption in amino acid derivative based homochiral metal organic frameworks	DOI: 10.1021/cg3008443	Tanay Kundu	2012
[207]	Rational Tuning of Water Vapor and CO ₂ Adsorption in Highly Stable Zr-Based MOFs	DOI: 10.1021/jp308657x	Himanshu Jasuja	2012
[208]	Synthesis, Water Adsorption, and Proton Conductivity of Solid-Solution-Type Metal-Organic Frameworks Al(OH)(bdc-OH) _x (bdc-NH ₂) _{1-x}	DOI: 10.1002/asia.201301673	Tepei Yamada	2014
[209]	Alcohol and water adsorption in zeolitic imidazolate frameworks	DOI: 10.1039/C3CC39116G	Ke Zhang	2013
[210]	Water stable triazolyl phosphonate MOFs: steep water uptake and facile regeneration	DOI: 10.1039/C5DT02651B	S. Begum	2015
[211]	MOFs as adsorbents for low temperature heating and cooling applications	DOI: 10.1021/ja808444z	Stefan K. Henninger	2009
[212]	Structural stability of BTTB-based metal-organic frameworks under humid conditions	DOI: 10.1039/C4TA01372G	Jagadeswara R. Karra	2015
[213]	Water vapor sorption in hybrid pillared square grid materials	DOI: 10.1021/jacs.7b01682	Daniel O'Nolan	2017
[214]	Relating pore hydrophilicity with vapour adsorption capacity in a series of amino acid based metal organic frameworks	DOI: 10.1039/C3CE41083H	Tanay Kundu	2013
[215]	Systematic ligand modulation enhances the moisture stability and gas sorption characteristics of quaternary metal-organic frameworks	DOI: 10.1021/jacs.5b00365	Lujia Liu	2015
[216]	Tailoring of network dimensionality and porosity adjustment in Zr- and Hf-based MOFs	DOI: 10.1039/C3CE41121D	Volodymyr Bon	2013
[217]	MIL-91(Ti), a small pore metal-organic framework which fulfils several criteria: an upscaled green synthesis, excellent water stability, high CO ₂ selectivity and fast CO ₂ transport	DOI: 10.1039/C5TA09349J	Virginie Benoit	2016
[218]	Sorption and breathing properties of difluorinated MIL-47 and Al-MIL-53 frameworks	DOI: 10.1016/j.micromeso.2013.07.030	Shyam Biswas	2013
[219]	A soft copper (II) porous coordination polymer with unprecedented aqua bridge and selective adsorption properties	DOI: 10.1002/chem.201201820	Elsa Quartapelle Procopio,	2012
[220]	Single- and double-layer structures and sorption properties of two microporous metal-organic frameworks with flexible tritopic ligand	DOI: 10.1021/cg301559s	Liqin Han	2013
[221]	Study of hydrothermal stability and water sorption characteristics of 3-dimensional Zn-based trimesate	DOI: 10.1021/jp4036327	Tadeja Birsa Čelic	2013
[222]	Dynamic porous metal-organic frameworks: synthesis, structure and sorption property	DOI: 10.1039/C2CE26533H	Chao Hou	2012
[223]	Partially fluorinated MIL-47 and Al-MIL-53 frameworks: influence of functionalization on sorption and breathing properties	DOI: 10.1039/C3CP44204G	Shyam Biswas	2013
[224]	Hydrolytic stability in hemilabile metal-organic frameworks	DOI: 10.1038/s41557-018-0104-x	Lauren N. McHugh	2018
[225]	A porous framework polymer based on a Zinc (II) 4, 4'-bipyridine-2, 6, 2', 6'-tetracarboxylate: Synthesis, structure, and "zeolite-like" behaviors	DOI: 10.1021/ja060946u	Xiang Lin	2006
[226]	Nanochannels of two distinct cross-sections in a porous Al-based coordination polymer	10.1021/ja802589u	Angiolina Comotti,	2008
[227]	Salt metathesis in three dimensional metal-organic frameworks (MOFs) with unprecedented hydrolytic regenerability	DOI: 10.1039/C3CC41842A	Tanay Kundu	2013
[228]	Solution mediated phase transformation (RHO to SOD) in porous Co-imidazolate based zeolitic frameworks with high water stability	DOI: 10.1039/C2CC36651G	Bishnu P. Biswal	2012
[229]	Porous metal-organic frameworks with high stability and selective sorption for CO ₂ over N ₂	DOI: 10.1016/j.micromeso.2013.01.020	Chao Hou	2013
[230]	A microporous metal-organic framework with high stability for GC separation of alcohols from water	DOI: 10.1039/C2CC33023G	Tsolmon Borjigin	2012
[231]	Porous high-valence metal-organic framework featuring open coordination sites for effective water adsorption	DOI: 10.1021/acs.inorgchem.8b03042	Cong Wang	2019
[232]	Third-generation breathing metal-organic framework with selective, stepwise, reversible, and hysteretic adsorption properties	DOI: 10.1021/ic402095u	Suresh Sanda	2013
[233]	Highly Water-Stable Lanthanide-Oxalate MOFs with Remarkable Proton Conductivity and Tunable Luminescence	DOI: 10.1002/adma.201701804	Kun Zhang	2017
[234]	Modulation of Water Vapor Sorption by a Fourth-Generation Metal-Organic Material with a Rigid Framework and Self-Switching Pores	DOI: 10.1021/jacs.8b07290	Shi-Yuan Zhang	2018
[235]	Selective separation of water, methanol, and ethanol by a porous coordination polymer built with a flexible tetrahedral ligand	DOI: 10.1021/ja306401j	Akihito Shigematsu	2012
[236]	Highly selective water adsorption in a lanthanum metal-organic framework	DOI: 10.1002/chem.201403241	Raoul Plessius	2014
[237]	Multiple Functions of Gas Separation and Vapor Adsorption in a New MOF with Open Tubular Channels	DOI: 10.1021/acsami.0c21554	Yong-Zhi Li	2021
[238]	A Hydrolytically Stable Vanadium(IV) Metal-Organic Framework with Photocatalytic Bacteriostatic Activity for Autonomous Indoor Humidity Control	DOI: 10.1002/anie.201914762	Dou Ma	2020
[239]	Collective Breathing in an Eightfold Interpenetrated Metal-Organic Framework: From Mechanistic Understanding towards Threshold Sensing Architectures	DOI: 10.1002/ange.201914198	Kornel Roztocki	2020
[240]	Rational design of a robust aluminum metal-organic framework for multi-purpose water-sorption-driven heat allocations	DOI: 10.1038/s41467-020-18968-7	Kyung Ho Cho	2020
[241]	Nanoporous Water-Stable Zr-Based Metal-Organic Frameworks for Water Adsorption	DOI: 10.1021/acsanm.1c00638	Lifeng Yang	2021
[242]	Defective Zr-Fumarate MOFs Enable High-Efficiency Adsorption Heat Allocations	DOI: 10.1021/acsami.0c15901	Kyung Ho Cho	2021

[243]	Integrated High Water Affinity and Size Exclusion Effect on Robust Cu-Based Metal–Organic Framework for Efficient Ethanol–Water Separation	DOI: 10.1021/acssuschemeng.0c08256	Lu Wang	2021
[244]	A Porous Covalent Organic Framework with Voided Square Grid Topology for Atmospheric Water Harvesting	DOI: 10.1021/jacs.9b13094	Ha L. Nguyen	2020
[245]	Functionally graded membranes from nanoporous covalent organic frameworks for highly selective water permeation	DOI: 10.1039/C7TA09596A	Hao Yang	2018

Table S2. The fitting parameters of water adsorption isotherm of 460 adsorbents by universal adsorption isotherm model

No.	ID No.	Adsorbent	Species	Ref. No.	T_fit (K)	a1	b1	c1	a2	b2	c2	a3	b3	c3	Wsat (g/g)	chi-square	reduced chi-square
1	M-1	[(Ni(L6)2]4H2O)n	MOF	[229]	298	0.510662	5234.837	270.0865	0.489338	4257.473	1298.778	0	1	1	0.118849	0.01615301	4.75E-04
2	M-2	(H2dab)[Zn2(ox)3]	MOF	[71]	298	0.306957	8766.317	1603.352	0.049921	86008.91	232.158	0.643123	808.8088	92.00176	0.234775	0.01123785	2.74E-04
3	M-3	[Zn(L)(H2O)2](NO3)2*2H2O)n	MOF	[4]	298	0.52882	626.3419	279.071	0.150542	4965.846	1028.225	0.320638	2227.108	174.7954	0.108096	0.00890053	5.24E-04
4	M-4	[Cd(L'1)(Cl)](H2O)	MOF	[206]	298	0.23332	894.2387	458.8756	0.76668	349.8843	14.82106	0	1	1	0.408752	0.03237045	0.00231218
5	M-5	[Cd(L'2)(Cl)](H2O)	MOF	[206]	298	0.653642	4820.121	1504.807	0.346358	5435.722	510.5705	0	1	1	0.09618	0.01682548	9.90E-04
6	M-6	[Cd(L'2)(Br)2](H2O)3	MOF	[206]	298	0.51479	849.6784	439.9004	0.48521	5625.533	1452.515	0	1	1	0.033113	0.01692648	0.00130204
7	M-7	[Cd(L'3)(Cl)](H2O)2	MOF	[206]	298	0.486496	3741.888	2280.979	0.513504	4772.443	75.20946	0	1	1	0.104072	0.02426504	0.00202209
8	M-8	[Cd(mpto)2.CH3CH2OH]n	MOF	[24]	298	0.856283	1144.64	454.4525	0.143717	12466.96	3158.51	0	1	1	0.00313	0.01715695	9.53E-04
9	M-9	[Co(L)(PIN)]dioxane	MOF	[222]	298	0.504974	1299.791	723.4581	0.431863	2064.6	78.72741	0.063163	6285.649	1445.445	0.173416	0.02700116	0.00150006
10	M-10	[Co2(BDC)2(BPNO)]*H2BDC*2MeOH	MOF	[19]	298	0.500489	2285.762	1094.925	0.499511	11358.58	1681.481	0	1	1	0.08074	0.01231925	8.80E-04
11	M-11	[Co3(ndc)-(HCOO)3(mu3-OH)(H2O)]n	MOF	[15]	298	0.821781	3773.782	1411.814	0.178219	4302.689	92.83301	0	1	1	0.241479	0.01060292	0.0011781
12	M-12	[Co4L3(u3-OH)(H2O)3](SO4)0.5	MOF	[210]	298	0.457018	4467.489	2219.253	0.542982	5982.605	59.36753	0	1	1	0.19396	0.0144575	0.00103268
13	M-13	[Cu(INA)2(NH3)2(H2O)2]	MOF	[36]	298	0.519577	626.1485	284.1374	0.480423	3819.02	1462.802	0	1	1	0.02194	0.01485276	0.00123773
14	M-14	[Cu(INA)2]	MOF	[36]	298	0.520865	1277.909	402.0382	0.479135	4331.69	1731.428	0	1	1	0.066653	0.00560449	4.67E-04
15	M-15	[Cu(INAIP)]*2H2O	MOF	[93]	298	0.503767	6593.571	221.4058	0.496233	6833.148	1840.676	0	1	1	0.133666	0.00721822	6.56E-04
16	M-16	[Cu2(H2btp)(H2O)2(12-bis(4-pyridl)ethylene)]	MOF	[115]	303	0.526565	1906.299	800.4013	0.473435	6631.287	1498.19	0	1	1	0.091301	0.00767242	2.84E-04
17	M-17	[Cu2(H2btp)(H2O)2(13-bis(4-pyridl)propane)]	MOF	[115]	303	0.530884	2336.677	966.9342	0.469116	6735.408	1482.661	0	1	1	0.068456	0.0074342	7.43E-04
18	M-18	[Cu2(H2btp)(H2O)2(bipyridine)]	MOF	[115]	303	0.506145	2900.827	1029.683	0.493855	5786.118	1569.181	0	1	1	0.046108	0.0072867	2.91E-04
19	M-19	[Cu2(pzdc)2(pyz)]*2H2O	MOF	[30]	303	0.969259	4226.324	2810.954	0.209982	10597.37	28.83339	0	1	1	0.144907	0.02906739	0.00581348
20	M-20	[La3L4(H2O)6]-Cl	MOF	[210]	298	0.570808	3404.587	30.17457	0.429192	3995.195	2684.724	0	1	1	0.27352	0.01959506	0.00103132
21	M-21	[Mn(mpto)2.CH3CH2OH]2	MOF	[24]	298	0.522038	1549.688	232.4576	0.477962	2187.135	599.34	0	1	1	0.053901	0.00162296	1.01E-04
22	M-22	[Ni(dipn)]2[Ni(dipn)(H2O)][Fe(CN)6]2.2H2O	MOF	[67]	298	0.523824	961.6951	469.8777	0.476176	5895.676	1873.033	0	1	1	0.196248	0.02129363	7.89E-04
23	M-23	[Ni(pca)(bdc)0.5(H2O)2]	MOF	[59]	298	0.496969	1161.827	434.6495	0.503031	4663.914	2023.556	0	1	1	0.158619	0.01961132	0.00108952
24	M-24	[Ni8(L5)6]	MOF	[6]	298	0.153115	338.3301	2140.756	0.846885	868.308	109.3566	0	1	1	1.052699	0.00904644	7.54E-04
25	M-25	[Ni8(L5-CF3)6]	MOF	[6]	298	0.93668	457.9261	60.32911	0.06332	2919.346	1166.59	0	1	1	0.857637	8.02E-04	4.72E-05
26	M-26	[Ni8(L5-CH3)6]	MOF	[107]	298	0.366774	804.6751	853.1446	0.633226	891.7756	35.15321	0	1	1	0.630968	0.02119443	7.85E-04
27	M-27	[PbL2]*2DMF*6H2O	MOF	[99]	298	0.499445	431.3161	100.718	0.330314	4031.836	1819.959	0.170242	1236.091	11.16846	0.215335	0.00783151	0.00130525
28	M-28	[PbL2]*DMF*2H2O	MOF	[99]	298	0.455572	1675.621	762.8275	0.157796	9482.9	27.94876	0.386632	8758.604	658.7146	0.048438	0.00981114	0.00163519
29	M-29	[Zn(NO2-BDC)(dmbpy).5](C2H6O)(H2O)	MOF	[48]	298	0.558257	1596.695	448.4559	0.276337	1872.877	1050.049	0.165406	1960.921	30.96552	0.169732	0.02116387	8.47E-04
30	M-30	[Zn2(ip)2(bpy)2]*DMF)n	MOF	[88]	298	0.504148	2996.081	161.3552	0.374465	5613.251	1623.944	0.121387	4307.901	94.6146	0.042329	0.01508728	0.00301746
31	M-31	[Zn3(TCPB)2*2H2O]*2H2O*4DMF	MOF	[10]	298	0.483444	3179.553	1151.034	0.243495	580.1572	201.7043	0.273061	5453.091	17.87949	0.104953	0.00387811	5.54E-04
32	M-32	[Zn4O(micapz)3]n on [Zn4O(dmcapz)3]n	MOF	[1]	298	0.804632	698.7384	175.8002	0.195368	2478.516	567.755	0	1	1	0.13255	0.00197556	3.29E-04
33	M-33	{(H2PIP)0.5[VO(CEP)]*H2O}	MOF	[57]	298	0.503332	2896.618	811.8085	0.496668	3484.221	79.21435	0	1	1	0.060483	0.0030137	3.35E-04
34	M-34	{[Cu(azpy)(glut)](H2O)2}	MOF	[51]	298	0.566442	3077.898	107.2347	0.256673	3030.451	960.1884	0.176886	376.1818	50.48967	0.165398	0.01478491	0.00164277
35	M-35	{[Cu2(4-pmpmd)2(CH3OH)4(opd)2]*2H2O}	MOF	[53]	298	0.330916	248.803	44.55468	0.669084	2450.532	460.1328	0	1	1	0.224113	0.01444006	0.00144401

36	M-36	{[Cu2(pzdc)2(bpy)]*4H2O}	MOF	[30]	303	0.500825	5064.406	1742.309	0.041599	45100.44	110.4454	0.457577	8888.133	603.8811	0.167213	0.00381672	4.24E-04
37	M-37	{[Cu4(OH)2(tec)2-(bpy)2]·11H2O}	MOF	[127]	298	0.330531	1082.349	306.7249	0.669469	4115.438	1159.243	0	1	1	0.08087	0.00661317	8.27E-04
38	M-38	{[Dy(ox)(Bpybc)(H2O)]*OH*13H2O}n	MOF	[103]	298	0.503903	1201.382	187.0009	0.496097	4107.045	1445.385	0	1	1	0.238927	0.00966116	0.00107346
39	M-39	{[Ni(bpe)2(N(CN)2)](N(CN)2)}n	MOF	[87]	298	0.377542	811.145	238.2205	0.622458	4343.966	1760.858	0	1	1	0.077416	0.03856806	8.38E-04
40	M-40	{[Zn-(C10H2O8)0.5(C10S2N2H8)]*5H2O}n	MOF	[61]	298	0.455391	1382.875	509.8604	0.544609	7415.456	399.4682	0	1	1	0.08575	0.01013948	7.80E-04
41	M-41	{[Zn(oxo-pba)2(bpy)]4H2O}n	MOF	[117]	298	0.637025	684.3635	160.378	0.362975	4842.724	2068.992	0	1	1	0.077068	0.02040387	0.00136026
42	M-42	{[Zn2(bpdc)2(azpy)]*2H2O*2DMF}n	MOF	[62]	298	0.314243	4533.593	1551.743	0.685757	1087.168	369.6797	0	1	1	0.080016	0.00862457	6.63E-04
43	M-43	{[Zn2(bpdc)2(azpy)]*2H2O*2DMF}n Nanoscale	MOF	[62]	298	0.477293	969.86	415.0624	0.522707	4705.219	1861.323	0	1	1	0.096342	0.01848627	0.00168057
44	M-44	{[Zn3(bpdc)3(azpy)]*4H2O*2DEF}n	MOF	[62]	298	0.452338	482.8178	81.43422	0.547662	3632.904	1693.692	0	1	1	0.111684	0.02216496	0.001705
45	M-45	{[Zn4O(bfbpdc)3-(bpy)0.5(H2O)]*(3DMF)(H2O)}n	MOF	[60]	298	0.029183	869.2451	224.5988	0.970817	276.6266	20.43725	0	1	1	0.407887	0.00108437	8.34E-05
46	M-46	{[ZnL(HCO2)(H2O)]*DMF}	MOF	[109]	298	0.659379	1761.468	378.391	0.198253	4444.955	3335.9	0.142368	2029.932	35.62504	0.470142	0.00817563	6.81E-04
47	M-47	1 C76H116N14O42Zn3	MOF	[118]	298	0.501983	867.3542	472.6359	0.026441	3765.455	63.39667	0.471576	5001.142	1714.793	0.168687	0.02524824	7.21E-04
48	M-48	13R(Co)	MOF	[234]	298	0.640873	932.4805	289.5853	0.359127	3635.083	1114.012	0	1	1	0.015587	0.00949731	6.78E-04
49	M-49	1-LiCl	MOF	[112]	298	0.607952	3437.951	649.652	0.203173	6897.542	40.74488	0.188875	4886.074	6.52728	0.229565	0.01639451	0.00409863
50	M-50	23R(Co)	MOF	[234]	298	0.79326	505.7056	69.95749	0.20674	1895.939	692.9192	0	1	1	0.052796	0.01000746	5.56E-04
51	M-51	2D [Cu(bpy)2(OTf)2]n	MOF	[70]	303	0.672567	4696.213	954.583	0.021929	166112.3	233.4801	0.305504	528.2632	42.9281	0.177634	0.00331925	2.77E-04
52	M-52	33R(Co)	MOF	[234]	298	0.560974	1340.934	68.54631	0.439026	2710.92	922.7126	0	1	1	0.041072	0.00556062	3.48E-04
53	M-53	3S(Co)	MOF	[234]	298	0.624739	936.7449	111.9363	0.375261	2346.342	1001.279	0	1	1	0.027462	0.00840965	5.26E-04
54	M-54	43R(Co)	MOF	[234]	298	0.427069	3334.722	1131.89	0.572931	997.1203	326.9824	0	1	1	0.019246	0.01555107	0.00111079
55	M-55	Al(OH)-(1,4-NDC)	MOF	[226]	298	0.372883	1775.189	721.4617	0.627117	1870.424	62.05933	0	1	1	0.158218	0.00397948	2.21E-04
56	M-56	AlaZnBr	MOF	[227]	298	0.495244	836.3366	172.6985	0.504756	2622.13	1000.698	0	1	1	0.066466	0.01345469	0.00103498
57	M-57	AlaZnCl	MOF	[227]	298	0.499809	560.6638	170.0564	0.500191	4465.553	824.8671	0	1	1	0.159732	0.01195512	8.54E-04
58	M-58	AlaZnOAc	MOF	[214]	298	0.501634	312.99	49.70892	0.196867	6745.649	2434.339	0.301499	263.5642	10.13563	0.280444	0.01355115	7.97E-04
59	M-59	ALFFIVE-1-Ni	MOF	[177]	308	0.179548	3427.491	1949.645	0.820452	9870.539	294.1314	0	1	1	0.233664	0.03279483	0.00182193
60	M-60	Aluminum fumarate	MOF	[126]	288	0.506178	3856.701	867.6701	0.408293	4585.964	59.43055	0.08553	9470.881	1251.102	0.440096	0.00951903	0.00105767
61	M-61	Basolite™ F300(Fe)	MOF	[187]	293	0.702736	2928.745	523.2538	0.297264	5287.008	2382.407	0	1	1	0.375685	0.00460621	3.84E-04
62	M-62	BIT-66(V)	MOF	[238]	298	0.748827	1250.022	42.72423	0.047293	97683.99	173.3818	0.20388	129.3036	10.84913	0.704999	0.02030529	8.83E-04
63	M-63	BIT-72(Al)	MOF	[164]	283	0.640122	1237.503	919.3266	0.359878	1609.403	34.93199	0	1	1	0.52676	0.02783257	0.00309251
64	M-64	BIT-73(Al)	MOF	[164]	283	0.473024	1134.681	756.595	0.526976	1620.782	35.66584	0	1	1	0.467809	0.01229347	0.00136594
65	M-65	BIT-74(Al)	MOF	[164]	283	0.489695	1380.483	738.6405	0.011839	42449.02	59.62863	0.498467	2261.408	79.89422	0.577498	0.01352542	0.00270508
66	M-66	Blucher-101408	MOF	[107]	298	0.645251	717.158	175.8046	0.354749	556.1822	31.91108	0	1	1	0.741299	0.0020904	9.95E-05
67	M-67	Bu-FeCr	MOF	[112]	298	0.518268	779.8054	307.3632	0.481732	4052.882	1589.797	0	1	1	0.043052	0.02957144	0.00246429
68	M-68	BUT-155(Cu)	MOF	[158]	298	0.345575	3250.295	136.9656	0.654425	3854.049	1928.157	0	1	1	0.42961	0.01857296	7.14E-04
69	M-69	BUT-46A(Zr)	MOF	[159]	298	0.840141	1843.742	102.0156	0.159859	3443.272	2124.786	0	1	1	0.503352	0.00241368	1.61E-04
70	M-70	BUT-46B(Zr)	MOF	[159]	298	0.490504	1536.385	57.83868	0.132986	2971.123	1652.917	0.37651	1543.975	19.95696	0.484661	0.00249597	1.31E-04
71	M-71	BUT-46F(Zr)	MOF	[159]	298	0.287531	1983.241	753.0703	0.712469	2139.437	64.70286	0	1	1	0.574709	0.00551788	2.90E-04
72	M-72	BUT-46W(Zr)	MOF	[159]	298	0.659375	2759.009	188.4812	0.340625	3290.434	1755.627	0	1	1	0.599538	0.01111326	5.29E-04
73	M-73	C10H4O12Eu2	MOF	[91]	298	0.55939	2903.706	985.3003	0.44061	7794.129	1868.902	0	1	1	0.098133	0.00544059	1.94E-04
74	M-74	C115.5H202N14O43Zn4	MOF	[92]	298	0.536308	1109.726	435.3952	0.463692	4798.04	1082.293	0	1	1	0.088443	0.01023167	0.00113685
75	M-75	C11H15BrN2O4Zn	MOF	[73]	298	0.501868	1511.161	491.198	0.017552	40960.77	434.0118	0.480581	6446.472	1545.676	0.061531	0.00726914	3.30E-04
76	M-76	C11H15ClN2O4Zn	MOF	[73]	298	0.615534	2081.81	120.8613	0.384466	3292.065	1503.1	0	1	1	0.133025	0.0568803	0.00203144
77	M-77	C12H17ClN2O3Cd	MOF	[52]	303	0.273736	391.0387	96.47974	0.120947	1543.931	525.3683	0.605317	393.3542	10.5173	0.419649	0.04289651	0.00214483
78	M-78	C15H27N2O10Dy	MOF	[54]	298	0.979598	5309.281	1284.24	0.020402	116271.6	167.3794	0	1	1	0.111031	0.00604608	4.32E-04

79	M-79	C15H27N2O10Er	MOF	[54]	298	0.9487	4501.377	1190.851	0.0513	51123.33	72.00131	0	1	1	0.149247	0.0092179	6.58E-04
80	M-80	C15H27N2O10Ho	MOF	[54]	298	0.947979	5259.546	1202.063	0.052021	13437.33	2153.641	0	1	1	0.104644	7.71E-04	5.14E-05
81	M-81	C15H27N2O10Tb	MOF	[54]	298	0.517475	5236.31	889.5998	0.482525	7913.84	1240.819	0	1	1	0.104723	0.00110943	1.58E-04
82	M-82	C15H27N2O10Tm	MOF	[54]	298	0.507653	2863.366	629.0747	0.492347	5442.666	1198.521	0	1	1	0.116477	0.0012386	8.26E-05
83	M-83	C18H21Br2N4O9Cd2	MOF	[52]	303	0.405929	837.1194	336.6141	0.594071	4843.006	1778.07	0	1	1	0.03345	0.02032987	9.24E-04
84	M-84	C24H40N2O16Cl2Cd3	MOF	[38]	298	0.822274	6225.138	1780.069	0.177726	207.1526	79.21355	0	1	1	0.087345	0.01981637	3.20E-04
85	M-85	C26H24Br2Cu2N8O3	MOF	[102]	298	0.999076	9467.483	1700.204	0.000923	16086.43	117.1451	1.74E-08	9624.564	71.83435	0.075073	0.0032134	5.36E-04
86	M-86	C28H24CoN10	MOF	[94]	298	0.506454	524.605	153.2857	0.493546	4093.691	2243.338	0	1	1	0.076317	0.01915821	0.00127721
87	M-87	C32H24Cu3N6O12	MOF	[13]	288	0.741871	4788.26	2042.183	0.038326	130613.5	4749.623	0.219803	5193.839	173.7663	0.180299	0.0244773	5.97E-04
88	M-88	C32H46N4O8Zn	MOF	[101]	298	0.546794	1084.812	262.3904	0.003935	8337.619	53.52271	0.44927	4186.954	1403.056	0.006019	0.02217844	0.00221784
89	M-89	C4H8HoKO12 Dehydrated	MOF	[55]	298	0.535648	8553.543	526.2685	0.464352	8536.52	2623.427	0	1	1	0.187247	0.03887798	0.00259187
90	M-90	C55H52Fe4N20O18	MOF	[33]	298	0.758574	5585.69	2306.928	0.241426	9051.161	141.4404	0	1	1	0.101851	0.02953675	0.00210977
91	M-91	C62H44N2O8Zn2	MOF	[58]	298	0.619108	154.4522	0.792987	0.380892	2106.844	1003.895	0	1	1	0.279552	0.00632615	3.95E-04
92	M-92	C62H50Cd3K2N2O26	MOF	[106]	298	0.505015	2225.925	507.9046	0.494985	5073.836	1281.53	0	1	1	0.145102	0.01362427	4.01E-04
93	M-93	C9H11ClN2O4Cd	MOF	[52]	303	0.504267	4800.661	1920.095	0.495733	5462.21	563.8127	0	1	1	0.094969	0.04048639	0.00119078
94	M-94	CALF-25	MOF	[74]	298	0.647108	804.2719	283.0545	0.352892	3973.336	1539.357	0	1	1	0.072361	0.018209	0.00121393
95	M-95	CAU-1(AI)-(OH)2	MOF	[205]	298	0.713448	2493.458	362.3371	0.286552	5542.192	2724.161	0	1	1	0.310129	0.00588334	2.67E-04
96	M-96	CAU-1(AI)-NH2	MOF	[189]	298	0.082898	3051.135	4586.231	0.917102	1918.052	249.4663	0	1	1	0.376916	0.00506479	2.30E-04
97	M-97	CAU-1(AI)-NHCH3	MOF	[189]	298	0.503736	2283.802	174.7008	0.266861	2798.515	1502.954	0.229403	2416.838	41.66872	0.511945	0.0059868	3.52E-04
98	M-98	CAU-1(AI)-NHCOCH3	MOF	[189]	298	0.505685	2676.094	475.1216	0.494315	4587.841	2164.997	0	1	1	0.242911	0.00944627	4.50E-04
99	M-99	CAU-10-CH3	MOF	[112]	298	0.606472	1639.047	371.7382	0.151009	6239.894	1724.632	0.242519	2014.032	24.71852	0.180798	0.00514792	3.03E-04
100	M-100	CAU-10-H	MOF	[112]	298	0.374274	2911.799	1262.177	0.350639	4243.646	5.816306	0.275087	4499.975	6.17744	0.379873	0.36291498	0.0259225
101	M-101	CAU-10-NH2	MOF	[112]	298	0.501692	4082.048	784.2965	0.498308	7757.765	2433.145	0	1	1	0.226555	0.0049774	2.07E-04
102	M-102	CAU-10-NO2	MOF	[112]	298	0.5019	2666.301	168.1114	0.4981	3056.374	564.6944	0	1	1	0.174018	0.00713932	3.76E-04
103	M-103	CAU-10-OCH3	MOF	[112]	298	0.293463	3724.138	1352.805	0.706537	3330.578	33.81504	0	1	1	0.087649	0.01874362	0.00156197
104	M-104	CAU-10-OH	MOF	[112]	298	0.556738	3495.599	1781.102	0.167066	4366.106	55.06857	0.276196	5140.368	50.62285	0.295798	0.02669268	8.90E-04
105	M-105	CAU-10-pydc	MOF	[2]	303	0.471067	5733.005	650.6848	0.017647	10624.48	55.69884	0.511286	5988.54	2115.588	0.389493	0.00562562	2.96E-04
106	M-106	CAU-13	MOF	[63]	298	0.546533	2663.44	1553.063	0.453467	3868.919	61.20036	0	1	1	0.137491	0.0177353	0.00104325
107	M-107	CAU-1-NH2	MOF	[98]	298	0.501819	2054.022	163.3519	0.061664	5606.069	1196.815	0.436517	1634.777	365.8726	0.391084	0.00214636	9.76E-05
108	M-108	CAU-1-NHCH3	MOF	[98]	298	0.81102	2370.665	172.8617	0.18898	2113.495	4194.553	0	19744.46	27.41727	0.698689	0.02544292	8.21E-04
109	M-109	CAU-1-NHCOCH3	MOF	[98]	298	0.728752	2717.906	698.9819	0.047404	6171.319	139.2509	0.223843	7095.983	3347.987	0.251244	0.00607442	2.64E-04
110	M-110	CAU-23	MOF	[131]	298	0.745529	3212.707	55.6809	0.254471	2219.412	1254.928	0	1	1	0.407314	0.02150413	7.42E-04
111	M-111	CAU-3(AI)	MOF	[191]	298	0.353234	1149.786	64.45253	0.226674	2273.881	1628.989	0.420092	1168.05	16.05594	0.493741	0.01008637	4.39E-04
112	M-112	CAU-3(AI)-NH2	MOF	[191]	298	0.687306	979.1474	88.95147	0.312694	3199.662	1501.351	0	1	1	0.521111	0.02035233	7.54E-04
113	M-113	CAU-6(AI)	MOF	[203]	298	0.501704	11133.89	1101.168	0.498296	2907.121	1825.468	0	1	1	0.358976	0.02086948	9.07E-04
114	M-114	CAU-8(AI)	MOF	[205]	298	0.906368	1883.343	974.4826	0.093632	35489.67	57.93996	0	1	1	0.158484	0.05532487	0.0032544
115	M-115	Cd (II)-MOF [Cd(L)(DMF)]	MOF	[113]	298	0.521397	2364.367	1094.986	0.478603	8172.391	1567.734	0	1	1	0.141479	0.01135994	4.37E-04
116	M-116	Cd(BTTB)	MOF	[212]	298	0.506559	1416.187	328.9653	0.493441	4375.635	2191.944	0	1	1	0.242902	0.01752124	0.00109508
117	M-117	Cd2(sdb)2(pcih)2	MOF	[172]	298	0.509802	2727.822	1145.908	0.490198	3845.803	233.9403	0	1	1	0.178928	0.00511331	2.43E-04
118	M-118	Cd3L2	MOF	[220]	298	0.504193	1488.334	732.4625	0.012049	10340.31	1496.223	0.483758	8468.114	2818.72	0.118513	0.02056017	0.00158155
119	M-119	CID-3	MOF	[90]	298	0.575182	1414.131	596.9599	0.424818	1262.943	59.77037	0	1	1	0.097375	0.01269015	7.05E-04
120	M-120	Co(BTTB)(AZPY)	MOF	[212]	298	0.263347	1563.054	1312.838	0.736653	1409.006	161.6176	0	1	1	0.207404	0.01361648	9.08E-04
121	M-121	Co(BTTB)(BPY)	MOF	[212]	298	0.546868	433.3997	78.92365	0.25028	2660.979	1126.198	0.202852	675.7011	128.4626	0.025354	0.02480307	0.00248031

122	M-122	Co(BTTB)(DMBPY)	MOF	[201]	298	0.917255	427.8484	64.20248	0.082745	2904.861	971.7103	0	1	1	0.196984	0.00981734	6.14E-04
123	M-123	Co ₂ C12(BTDD)	MOF	[132]	298	0.273219	4808.701	1962.336	0.726781	3061.117	14.96877	0	1	1	0.940152	0.00961169	4.81E-04
124	M-124	Co ₂ C12BBTA	MOF	[195]	298	0.499194	6161.346	2294.562	0.500806	10300.21	436.274	0	1	1	0.420166	0.02148556	0.00119364
125	M-125	Cobalt Triazolyl Phosphonate MOF	MOF	[116]	298	0.5014	6166.038	260.8109	0.4986	4465.786	2064.498	0	1	1	0.196583	0.02107313	0.00150522
126	M-126	Cobalt Triazolyl Phosphonate MOF (95%RH)	MOF	[116]	298	0.432101	3951.04	2060.999	0.102313	28273.95	39.52983	0.465586	6068.82	76.04365	0.245199	0.01409047	0.00100646
127	M-127	Cobalt Triazolyl Phosphonate MOF (Activated at 403K)	MOF	[116]	298	0.504975	983.1542	391.3612	0.495025	4870.004	1307.119	0	1	1	0.358866	0.02044212	7.86E-04
128	M-128	Co-CUK-1	MOF	[130]	303	0.208709	3634.849	1436.989	0.791291	5183.317	68.01181	0	1	1	0.298332	0.01365012	5.46E-04
129	M-129	Co-MOF-74(M)	MOF	[27]	298	0.000667	4018.014	247.3233	1.60E-06	48202.63	67.38384	0.999332	8789.76	1708.746	0.766851	0.01539949	0.00384987
130	M-130	Co-MOF-74(S)	MOF	[27]	298	0.933003	8420.789	1283.271	0.066997	42876.19	4.29E+09	0	15082.77	20.61553	0.970423	0.00941796	0.00235449
131	M-131	CoNlm	MOF	[228]	293	0.467512	1400.989	186.4208	0.532488	1746.068	1916.384	0	1	1	0.135527	0.05119941	0.00255997
132	M-132	CPO-27-Ni	MOF	[100]	298	0.50284	7727.53	3311.866	0.49716	11849.33	1588.03	0	1	1	0.527958	0.02108168	5.55E-04
133	M-133	Cr ₃ (BTC) ₂	MOF	[163]	298	0.504831	3705.142	649.094	0.495169	5788.528	1386.7	0	1	1	0.432001	0.00310316	2.22E-04
134	M-134	Cr-MIL(101)	MOF	[112]	298	0.341587	1982.734	68.23827	0.542525	1491.399	123.1261	0.115887	4689.158	626.6896	1.339039	0.02517602	4.84E-04
135	M-135	Cr-MIL-101-NO ₂	MOF	[112]	298	0.667705	1974.481	111.778	0.185165	2915.03	2382.041	0.14713	1555.775	34.49866	0.753398	0.0546236	0.00121386
136	M-136	Cr-soc-MOF-1	MOF	[173]	298	0.502124	1073.715	105.5002	0.482359	831.9149	59.91381	0.015518	13171.37	36.30194	1.929962	0.00238872	1.59E-04
137	M-137	Cu(mtpm)C12	MOF	[235]	298	0.506227	2159.327	1042.898	0.493773	9215.365	2549.023	0	1	1	0.027911	0.01576224	9.27E-04
138	M-138	Cu ₂ (dmcapz) ₂	MOF	[219]	298	0.822334	2552.065	131.669	0.177666	5305.265	4742.901	0	1	1	0.221849	0.0102823	5.41E-04
139	M-139	Cu ₂ (pzdC) ₂ bpe	MOF	[30]	303	0.766861	6530.514	2227.074	0.233139	6986.812	142.6348	0	1	1	0.210506	0.00961237	0.00106804
140	M-140	Cu ₂ C12BBTA	MOF	[195]	298	0.335964	2707.957	675.0195	0.487296	9105.138	708.516	0.17674	9541.63	14.11635	0.341945	0.02113923	0.00162609
141	M-141	Cu ₆ (Trz) ₁₀ (H ₂ O) ₄ [H ₂ SiW ₁₂ O ₄₀] ₈ H ₂ O	MOF	[124]	298	0.369886	512.321	108.9123	0.630114	3538.78	1073.463	0	1	1	0.092745	0.00809855	5.78E-04
142	M-142	CuBTC	MOF	[11]	298	0.675464	4814.229	1658.316	0.1742	9456.902	49.39552	0.150336	815.954	79.79317	0.525288	0.00744981	2.40E-04
143	M-143	CuEBTC	MOF	[192]	293	0.274882	1559.018	278.4578	0.735876	6519.399	1372.227	0	64123.47	186.7339	0.188646	0.00590674	5.37E-04
144	M-144	CuMBTC	MOF	[192]	293	0.379367	1951.31	99.68637	0.620633	5817.342	1963.163	0	1	1	0.189056	0.00657126	5.05E-04
145	M-145	Cu-MOF	MOF	[85]	303	0.47193	10605.24	2264.053	0.52807	15773.37	90.22378	2.00E-09	12837.05	73.31952	0.06957	0.0013389	6.69E-04
146	M-146	Cu-Tria	MOF	[243]	298	0.506382	10368.86	296.7121	0.493618	7730.738	2026.499	0	1	1	0.189956	0.05699737	0.00356234
147	M-147	DETA-MIL-101	MOF	[97]	298	0.607507	1267.653	494.3548	0.392493	8539.519	2462.506	0	1	1	0.105643	0.02090345	0.00209035
148	M-148	DMOF	MOF	[64]	298	0.503404	2839.256	535.3779	0.496596	3306.321	178.4745	0	1	1	0.094165	0.00431072	5.39E-04
149	M-149	DMOF(Zn)-A	MOF	[83]	298	0.928374	2940.752	318.7314	0.071626	2236.423	1131.182	0	1	1	0.292403	0.00470859	3.62E-04
150	M-150	DMOF(Zn)-Br	MOF	[83]	298	0.807842	2570.243	987.6379	0.192158	7163.595	1090.241	0	1	1	0.056451	0.00918496	5.74E-04
151	M-151	DMOF(Zn)-N	MOF	[83]	298	0.891788	3351.314	1423.911	0.022785	46375.13	1086.105	0.085427	11490.24	68.77548	0.021774	0.02082558	0.0026032
152	M-152	DMOF(Zn)-NH ₃	MOF	[64]	298	0.508263	1341.638	377.4531	0.491737	5547.413	1232.355	0	1	1	0.112755	0.011978	0.0011978
153	M-153	DMOF-Cl ₂	MOF	[83]	298	0.631632	2345.277	33.17692	0.368368	2549.349	1194.274	0	1	1	0.073706	0.00420671	7.01E-04
154	M-154	DMOF-NO ₂	MOF	[83]	298	0.633592	1947.788	129.9575	0.366408	6801.995	2546.332	0	1	1	0.129396	0.01657255	6.91E-04
155	M-155	DMOF-OH	MOF	[83]	298	0.902182	3543.636	1301.761	0.097818	1271.661	37.48507	0	1	1	0.057282	0.00907017	0.00151169
156	M-156	DMOF-TM(Co)	MOF	[201]	298	0.090816	4021.189	1604.002	0.909184	2569.524	182.029	0	1	1	0.369453	0.00443186	3.41E-04
157	M-157	DMOF-TM(Cu)	MOF	[201]	298	0.159965	2646.829	1066.883	0.840035	1530.472	123.0975	0	1	1	0.383207	0.00693193	4.95E-04
158	M-158	DMOF-TM(Ni)	MOF	[201]	298	0.207422	2684.934	1106.816	0.792578	1949.313	162.5383	0	1	1	0.362781	0.00285258	2.04E-04
159	M-159	DMOF-TM1(Zn)	MOF	[196]	298	0.667818	2019.031	126.2855	0.332182	2977.4	603.5558	0	1	1	0.272351	0.00480677	4.01E-04
160	M-160	DMOF-TM2(Zn)	MOF	[196]	298	0.921714	3371.946	211.7989	0.078286	1227.579	456.233	0	1	1	0.414926	0.00419673	3.82E-04
161	M-161	DUT-10(Zn)	MOF	[18]	298	0.314576	384.9323	89.42328	0.227271	1895.238	539.187	0.458152	230.1206	41.89914	0.446058	0.00511756	0.00102351
162	M-162	DUT-4	MOF	[41]	298	0.986261	1015.7	374.6411	0.013739	5830.375	1941.031	0	28667.8	40.31983	0.672343	0.0378782	0.00291371
163	M-163	DUT-51(Zr)	MOF	[190]	298	0.219275	1952.882	673.5299	0.780725	1094.815	112.1042	0	1	1	0.547637	0.00512867	2.56E-04

164	M-164	DUT-52(Zr)	MOF	[216]	298	0.393348	2756.75	1306.62	0.29511	201.3502	69.74464	0.311542	2577.099	98.74416	0.28068	0.01545755	7.73E-04
165	M-165	DUT-53(Hf)	MOF	[216]	298	0.58255	1690.564	994.6235	0.41745	2509.04	62.78436	0	1	1	0.199289	0.024091	0.00114719
166	M-166	DUT-67	MOF	[75]	298	0.503223	2572.146	359.7785	0.231963	6710.328	1063.468	0.264813	3421.127	49.97068	0.505598	0.01158343	4.83E-04
167	M-167	DUT-67(Hf)	MOF	[162]	298	0.500243	2208.876	268.3965	0.499757	3779.809	1247.496	0	1	1	0.280351	0.00823291	4.57E-04
168	M-168	DUT-68(Hf)	MOF	[162]	298	0.406801	2230.142	48.8466	0.593199	3715.708	1344.496	0	1	1	0.275936	0.00742026	2.75E-04
169	M-169	DUT-68(Zr)	MOF	[162]	298	0.375257	2250.23	55.96516	0.624743	3433.105	1402.658	0	1	1	0.342094	0.00881618	3.67E-04
170	M-170	DUT-69(Hf)	MOF	[162]	298	0.500491	1493.04	862.378	0.499509	5378.798	1213.53	0	1	1	0.184688	0.01392542	6.05E-04
171	M-171	DUT-69(Zr)	MOF	[162]	298	0.991949	2693.188	1537.377	0.008051	4644.066	127.496	0	1	1	0.221023	0.03325509	0.00144587
172	M-172	DUT-84(Zr)	MOF	[216]	298	0.778632	2143.329	969.5693	0.221368	3741.428	1326.341	0	1	1	0.125666	0.0167259	0.00119471
173	M-173	ED-ZIF-8	MOF	[3]	298	0.495424	1903.182	221.7082	0.504576	3617.912	754.2025	0	1	1	0.0032	0.0088483	0.00110604
174	M-174	Et-MnCr	MOF	[112]	298	0.512585	2359.228	1193.12	0.487415	3249.845	428.1259	0	1	1	0.1018	0.04433905	0.00170535
175	M-175	FeFIV1E-1-Ni	MOF	[177]	308	0.704895	7574.122	3073.259	0.067486	9765.54	113.2924	0.227619	13096.82	502.8588	0.257916	0.01685931	9.37E-04
176	M-176	HKUST-1-F	MOF	[11]	298	0.707847	94.94752	6.889319	0.292153	6392.671	2062.858	0	1	1	1.001542	0.15578135	0.00370908
177	M-177	HV-MOF-1(Er)	MOF	[231]	298	0.510172	1291.848	577.5289	0.489828	4701.221	1292.941	0	1	1	0.097572	0.00964097	6.03E-04
178	M-178	IPM-MOF-201(Ni)	MOF	[160]	298	0.507667	940.793	481.3307	0.492333	5230.643	1680.261	0	1	1	0.201533	0.01663662	7.92E-04
179	M-179	ISE-1(Ni)	MOF	[211]	313	0.317471	3352.105	518.875	0.682529	7566.331	2024.367	0	1	1	0.14361	0.01209501	0.00134389
180	M-180	JUC-110	MOF	[96]	298	0.55939	2903.706	985.3003	0.44061	7794.129	1868.902	0	1	1	0.098133	0.00544059	1.94E-04
181	M-181	JUK-8(Zn)	MOF	[239]	298	0.641759	1462.478	33.2039	0.266362	5871.28	3005.084	0.091879	41394.71	10879.19	0.242198	0.10320437	0.00412817
182	M-182	kag-MOF-1(Zn)	MOF	[170]	298	1	6455.272	1505.02	6.88E-15	412399.1	618.1548	0	1	1	0.119363	0.01617028	0.00147003
183	M-183	KMF-1(Al)	MOF	[240]	303	0.278685	4712.993	1585.448	0.721315	5012.989	59.44821	0	1	1	0.433045	0.00424844	2.36E-04
184	M-184	La(py2dc)L5	MOF	[236]	298	0.295391	954.179	304.1234	0.704609	3812.225	1373.619	0	1	1	0.018265	0.0085916	7.16E-04
185	M-185	LA^1-Zr6^12-shp	MOF	[182]	298	0.339518	4907.364	1884.863	0.660482	1292.343	276.9442	0	1	1	0.351303	0.015376	9.04E-04
186	M-186	LA^1-Zr6^8-csq	MOF	[182]	298	0.870251	1126.099	234.6506	0.129749	2864.75	3443.152	0	1	1	0.38428	0.02590304	0.00136332
187	M-187	LA^1-Zr6^8-flu	MOF	[182]	298	0.768701	772.8882	123.7483	0.231299	3425.356	1361.13	0	1	1	0.198209	0.01344395	7.91E-04
188	M-188	LA^2-Zr6^12-shp	MOF	[182]	298	0.638104	1218.969	117.5587	0.36841	4462.436	1874.588	0	6180.757	8.157055	1.005081	0.03521449	0.00234763
189	M-189	LA^2-Zr6^8-csq	MOF	[182]	298	0.098366	3584.241	1404.212	0.901634	652.5199	60.0177	0	1	1	1.449598	0.00573394	3.19E-04
190	M-190	LA^3-Zr6^8-flu	MOF	[182]	298	0.810676	745.6139	80.80403	0.189324	3304.372	1040.572	0	1	1	0.745239	0.02059581	0.00102979
191	M-191	Lanthanum Triazolyl Phosphonate MOF	MOF	[116]	298	0.391869	3807.986	3049.19	0.608131	3453.771	114.7683	0	1	1	0.274053	0.07768506	0.00369929
192	M-192	LB^1-Zr6^8-flu	MOF	[182]	298	0.964052	1222.552	377.2726	0.067399	10206.43	1552.432	0	24624.56	7190.373	0.199008	0.01534443	9.03E-04
193	M-193	LB^2-Zr6^8-csq	MOF	[182]	298	0.805986	1260.831	68.80899	0.079677	726.5926	62.64983	0.114337	3678.79	1452.062	1.298984	0.03078334	0.00205222
194	M-194	LB^2-Zr6^8-scu	MOF	[182]	298	0.518139	1173.967	46.42733	0.1719	7241.4	1928.605	0.309962	2037.57	697.3091	0.751842	0.00834751	4.91E-04
195	M-195	LB^3-Zr6^8-flu	MOF	[182]	298	0.140481	6687.757	3697.47	0.859519	1654.715	191.176	0	1	1	0.720353	0.00555066	3.47E-04
196	M-196	LC^1-Zr6^12-fcu	MOF	[182]	298	0.856626	1783.823	203.7619	0.143374	3416.459	2055.012	0	1	1	0.323389	0.00165443	9.19E-05
197	M-197	LC^2-Zr6^12-fcu	MOF	[182]	298	0.420019	1707.372	294.3917	0.048798	6259.656	973.6299	0.531182	2137.145	62.70482	0.428422	0.00580368	2.76E-04
198	M-198	LC^3-Zr6^8-beu	MOF	[182]	298	0.257995	3609.593	1107.155	0.742005	1401.769	104.1468	0	1	1	0.27832	0.00931592	4.05E-04
199	M-199	MAF-4.23-7.77	MOF	[197]	298	0.498412	1785.7	364.6631	0.501588	2160.178	156.7604	0	1	1	0.44734	0.003578	1.38E-04
200	M-200	MAF-4.49-7.51	MOF	[197]	298	0.50182	874.4354	210.2788	0.49818	1370.429	305.242	0	1	1	0.431208	0.00126124	5.26E-05
201	M-201	MAF-4.76-7.24	MOF	[197]	298	0.498468	577.5718	189.657	0.501532	269.4487	75.02069	0	1	1	0.393276	0.00693721	3.02E-04
202	M-202	MAF-7(Zn)	MOF	[197]	298	0.725857	2834.968	85.4277	0.274143	2533.703	881.1636	0	1	1	0.434546	0.00539214	2.00E-04
203	M-203	Me-FeCr	MOF	[112]	298	0.512656	1547.773	79.80626	0.14004	5347.658	2413.772	0.347303	2408.546	270.4415	0.212827	0.01070166	3.15E-04
204	M-204	MFU-4	MOF	[89]	298	0.700605	3827.166	558.8586	0.299395	2871.42	1533.005	0	1	1	0.431396	0.00509063	8.48E-04
205	M-205	Mg-CPO-27	MOF	[112]	298	0.500029	7164.554	2738.928	0.499971	27513.22	160.2618	0	1	1	0.637304	0.00603418	6.70E-04
206	M-206	Mg-CUK-1	MOF	[130]	303	0.328581	2467.215	681.0256	0.671419	3546.614	117.994	0	1	1	0.363863	0.02610647	0.00137402

207	M-207	Mg-MOF-74©	MOF	[95]	298	0.304278	2608.44	1411.766	0.317609	15783.49	54.55677	0.378112	9380.373	758.9617	0.662248	0.02104185	4.57E-04
208	M-208	MIL-100	MOF	[37]	293	0.743355	3033.496	482.5422	0.078796	931.2175	58.43063	0.177849	4999.503	2782.73	0.365318	0.00434744	4.83E-04
209	M-209	MIL-100(Al)	MOF	[178]	298	0.4913	2062.239	276.7578	0.197285	3036.409	78.62595	0.311415	5140.737	1801.042	0.658446	0.03040174	0.00178834
210	M-210	MIL-100(Cr)	MOF	[50]	298	0.731382	985.567	360.0925	0.268618	4171.3	2201.736	0	1	1	0.708955	0.01880449	0.00208939
211	M-211	MIL-100(Cr(X=Cl))	MOF	[179]	298	0.644131	2511.886	378.3194	0.226958	7218.792	1938.229	0.128911	3430.666	121.5384	0.599269	0.02005018	9.55E-04
212	M-212	MIL-100(Cr(X=SO4))	MOF	[179]	298	0.526002	2558.143	304.3808	0.183556	8954.215	1962.857	0.290442	3822.426	250.3033	0.607773	0.01299275	5.65E-04
213	M-213	MIL-100(Cr)-DEG	MOF	[34]	293	0.791778	1061.739	1795.842	0.444717	2486.561	370.0798	0	14507.87	20.22559	0.560718	0.00795079	8.83E-04
214	M-214	MIL-100(Cr)-EG	MOF	[34]	293	0.684451	2084.654	756.5853	0.142003	2550.358	43.19899	0.173545	5469.522	2616.464	0.429676	0.00834059	0.00104257
215	M-215	MIL-100(Cr)-EN	MOF	[34]	293	0.713852	2163.905	843.5579	0.141109	3005.126	337.7383	0.145039	6349.314	2008.047	0.368281	0.00642222	8.03E-04
216	M-216	MIL-100(Cr)-TEG	MOF	[34]	293	0.685031	1879.206	785.5674	0.104018	6624.063	1734.369	0.210951	2665.568	170.0879	0.330679	0.00804615	8.05E-04
217	M-217	MIL-100(Fe)	MOF	[41]	298	0.621864	2408.045	365.0629	0.093203	8461.044	526.4078	0.284933	2447.375	1011.061	0.824966	0.01702265	0.00130943
218	M-218	MIL-100V	MOF	[125]	298	0.434562	1847.247	433.7706	0.565438	6178.951	1912.118	0	1	1	0.151153	0.00654863	6.55E-04
219	M-219	MIL-101(Al)-NH2	MOF	[199]	298	0.507893	2155.121	502.0777	0.000878	29645.11	102.0575	0.491229	6063.808	3389.427	0.268538	0.02766176	0.00138309
220	M-220	MIL-101(Al)-URPh	MOF	[199]	298	0.504792	1836.967	481.5588	0.495208	4927.123	2192.562	0	1	1	0.325854	0.00983351	4.47E-04
221	M-221	MIL-101(Cr)-pCOOH	MOF	[183]	298	0.634841	1928.81	366.4655	0.247902	2418.404	28.38242	0.117257	4691.697	3381.855	1.031695	0.01510037	8.39E-04
222	M-222	MIL-101(Cr)-pMal	MOF	[183]	298	0.490238	1920.3	1188.625	0.509762	2213.925	221.2802	0	1	1	0.701877	0.01835266	8.74E-04
223	M-223	MIL-101(Cr)-pUR2	MOF	[183]	298	0.460782	1788.156	106.698	0.328099	1225.028	57.80958	0.211119	3072.14	1398.303	0.68424	0.01167794	7.79E-04
224	M-224	MIL-101-NH2	MOF	[42]	298	0.323691	1473.737	1091.141	0.305998	2074.554	74.57307	0.370311	2482.963	32.62592	1.052714	0.04300037	0.00119445
225	M-225	MIL-101-SO3H	MOF	[42]	298	0.565383	2945.146	557.4294	0.251749	5187.709	3339.362	0.182868	2457.896	16.57479	0.745162	0.02119939	5.30E-04
226	M-226	MIL-101V	MOF	[125]	298	0.514902	3332.318	1339.494	0.256263	902.618	43.78099	0.228835	10109.71	1273.782	0.25369	0.00625235	5.68E-04
227	M-227	MIL-125	MOF	[28]	298	0.456981	2482.835	102.7297	0.317129	2280.338	3.657329	0.225891	1650.258	1089.354	0.28895	0.00410394	3.16E-04
228	M-228	MIL-125(Ti)-NH3 ⁺ +Cl-	MOF	[181]	293	0.393348	3222.779	1549.529	0.606652	4002.788	55.48829	0	1	1	0.58048	0.00675389	4.82E-04
229	M-229	MIL-125(Ti)-NHCyp	MOF	[169]	308	0.504632	2127.473	680.7324	0.495368	4680.151	1386.264	0	1	1	0.110675	0.00879604	8.80E-04
230	M-230	MIL-125(Ti)-NHMe	MOF	[169]	308	0.462828	3317.081	178.2343	0.537172	3389.008	1277.408	0	1	1	0.294219	0.00675069	4.82E-04
231	M-231	MIL-125-NH2	MOF	[112]	298	0.492814	4139.952	133.5502	0.507186	4372.903	1195.19	0	1	1	0.368255	0.00848237	5.65E-04
232	M-232	MIL-160	MOF	[2]	303	0.417007	5602.208	1692.244	0.010332	124668.1	175.4971	0.572661	6303.936	526.3767	0.497066	0.00682446	3.10E-04
233	M-233	MIL-163	MOF	[8]	298	0.62787	1353.897	190.1964	0.37213	2540.055	2235.248	0	1	1	0.583277	0.02114975	6.04E-04
234	M-234	MIL-47(V)-F	MOF	[223]	323	0.123015	4665.792	1464.924	0.876985	1403.93	203.0093	0	1	1	0.179958	0.00362707	2.42E-04
235	M-235	MIL-47(V)-F2	MOF	[218]	293	0.502379	1095.14	246.4745	0.292277	1414.428	27.29647	0.205343	1712.651	684.5472	0.175171	0.00926737	5.79E-04
236	M-236	MIL-53(Al)-(OH)0.34(NH2)0.66	MOF	[208]	298	0.49824	6283.572	3130.779	0.50176	6656.634	2954.007	0	1	1	0.103621	0.03633657	0.00227104
237	M-237	MIL-53(Al)-(OH)0.53(NH2)0.47	MOF	[208]	298	0.50908	253.1494	43.29441	0.49092	6240.829	2796.482	0	1	1	0.209207	0.01274881	6.71E-04
238	M-238	MIL-53(Al)-(OH)0.68(NH2)0.32	MOF	[208]	298	0.660194	443.6292	117.6896	0.339806	8016.379	2625.033	0	1	1	0.441262	0.0070403	3.06E-04
239	M-239	MIL-53(Al)-(OH)2	MOF	[202]	298	0.706559	851.3172	282.7144	0.293441	8205.895	2664.164	0	1	1	0.401615	0.02520695	0.00105029
240	M-240	MIL-53(Al)-Br	MOF	[202]	298	0.390753	522.2401	121.6543	0.609247	3012.039	1198.4	0	1	1	0.10345	0.03227673	0.00189863
241	M-241	MIL-53(Al)-CH3	MOF	[202]	298	0.332006	735.2095	249.5307	0.667994	4527.531	1049.091	0	1	1	0.113056	0.0056009	3.50E-04
242	M-242	MIL-53(Al)-Cl	MOF	[202]	298	0.697429	4797.332	1312.309	0.001366	19959.63	35.21033	0.301205	664.5786	215.4774	0.136664	0.00637459	4.55E-04
243	M-243	MIL-53(Al)-F	MOF	[223]	323	0.4948	436.3747	84.13191	0.054353	6348.469	1761.96	0.450847	1138.488	128.0168	0.064325	5.26E-04	4.05E-05
244	M-244	MIL-53(Al)-F2	MOF	[218]	293	0.256529	293.396	112.2513	0.743471	1254.531	316.0496	0	1	1	0.234428	0.00514577	2.57E-04
245	M-245	MIL-53(Al)ht	MOF	[105]	298	0.906468	5198.046	454.6547	0.093532	1794.978	741.2177	0	1	1	0.082386	0.00181373	9.55E-05
246	M-246	MIL-53(Al)it	MOF	[105]	298	0.495934	1103.995	89.40362	0.504066	2054.801	1138.514	0	1	1	0.169374	0.0131529	6.58E-04
247	M-247	MIL-53(Al)-NH2	MOF	[176]	298	0.747711	6640.441	2674.838	0.022806	10590.39	66.48122	0.229483	9430.376	325.2914	0.084718	0.01584956	0.00144087
248	M-248	MIL-53(Al)-NO2	MOF	[202]	298	0.353262	990.202	487.0898	0.646738	7128.806	1319.493	0	1	1	0.122393	0.01232508	7.70E-04
249	M-249	MIL-53(Al)-OH	MOF	[175]	298	0.651331	538.0821	86.51005	0.348669	5198.504	2179.032	0	1	1	0.390638	0.0048294	1.93E-04

250	M-250	MIL-53(Al)-TDC	MOF	[194]	298	0.591613	1268.627	1331.969	0.479048	2517.43	86.55613	0	17910.84	25.13513	0.535171	0.02853157	0.00150166
251	M-251	MIL-53(Cr)	MOF	[68]	298	0.780831	52.0721	46.33583	0.219169	5010.95	464.5444	0	1	1	0.326576	0.22028366	0.03146909
252	M-252	MIL-53(Fe)-(COOH) ₂	MOF	[175]	298	0.355945	490.1338	384.9797	0.644055	8163.521	2363.662	0	1	1	0.147994	0.02127309	0.00125136
253	M-253	MIL-53(Ga)	MOF	[176]	298	0.498912	6803.662	3154.177	0.501088	9571.371	148.6663	0	1	1	0.062017	0.0058068	5.28E-04
254	M-254	MIL-53(Ga)-NH ₂	MOF	[176]	298	0.548667	534.6001	143.3098	0.451333	6416.233	2992.1	0	1	1	0.171048	0.03015203	0.00177365
255	M-255	MIL-68(In)	MOF	[176]	298	0.071354	999.0263	429.5969	0.928646	1336.567	19.64387	0	1	1	0.300081	0.01703466	0.00106467
256	M-256	MIL-68(In)-NH ₂	MOF	[176]	298	0.7676	1998.915	37.705	0.2324	2133.297	833.9159	0	1	1	0.332354	0.00832915	3.97E-04
257	M-257	MIL-91(Ti)	MOF	[217]	298	0.505564	4330.91	2797.727	0.494436	11874.37	882.4846	0	1	1	0.209607	0.01660419	7.91E-04
258	M-258	MIP-200	MOF	[129]	303	0.53283	4237.455	123.2385	0.46717	8273.98	4010.785	0	1	1	0.424402	0.02253365	9.39E-04
259	M-259	Mn ₂ (Gd-H-DOTA-4AmP)(H ₂ O) ₇	MOF	[204]	298	0.276375	531.5643	96.09803	0.723625	4671.6	1834.66	0	1	1	0.280111	0.02378695	0.00169907
260	M-260	Mn ₂ Cl ₂ (BTDD)	MOF	[132]	298	0.302483	477.9604	116.7864	0.697517	4544.661	1924.591	0	1	1	0.360883	0.0255045	0.0017003
261	M-261	MOF-1(Ce,Eu)	MOF	[233]	298	0.69108	1600.959	558.3068	0.30892	7762.754	1918.685	0	1	1	0.062526	0.00634177	3.17E-04
262	M-262	MOF-303(Al)	MOF	[157]	303	0.508353	5080.664	202.9002	0.491647	5478.487	2340.013	0	1	1	0.427712	0.0183572	4.48E-04
263	M-263	MOF-74(Ni)-BPP	MOF	[186]	298	0.320171	3509.614	199.8216	0.679829	4065.848	2096.239	0	1	1	0.733469	0.01688704	0.00120622
264	M-264	MOF-74(Ni)-TPP	MOF	[186]	298	0.818534	1598.128	256.8818	0.181466	7835.326	1917.151	0	1	1	0.891861	0.00736671	4.91E-04
265	M-265	MOS-1(Co)	MOF	[171]	298	0.511117	3812.635	656.8152	0.488883	8374.288	1102.98	0	1	1	0.315437	0.00308133	3.08E-04
266	M-266	MOS-2(Co)	MOF	[171]	298	0.621184	3324.605	1080.775	0.378816	8788.933	1214.002	0	1	1	0.144878	0.00270646	3.38E-04
267	M-267	MOS-3(Co)	MOF	[171]	298	0.510144	2192.276	1016.12	8.96E-07	46199.63	87.78811	0.489855	7712.262	1484.597	0.130331	0.0103277	0.00206554
268	M-268	MUF-77(Zn)-butyl	MOF	[215]	298	0.901684	447.3653	49.19317	0.098316	499.4139	17.72988	0	1	1	0.226977	0.00878852	4.39E-04
269	M-269	MUF-77(Zn)-decyl	MOF	[215]	298	0.264917	0.696998	867.9431	0.847617	294.2208	58.75272	0	9200.818	12.86373	0.140886	0.00669688	4.46E-04
270	M-270	MUF-77(Zn)-ethyl	MOF	[215]	298	0.508455	554.3279	42.00971	0.491545	491.3864	101.7306	0	1	1	0.253011	0.00552182	2.12E-04
271	M-271	MUF-77(Zn)-hexyl	MOF	[215]	298	0.082821	1223.212	439.1074	0.917179	273.9079	43.71072	0	1	1	0.142063	0.01257319	5.47E-04
272	M-272	MUF-77(Zn)-methyl	MOF	[215]	298	0.211065	505.4844	243.6987	0.788935	823.8007	25.39946	0	1	1	0.199194	0.00564913	2.82E-04
273	M-273	MUF-77(Zn)-octyl	MOF	[215]	298	0.090783	1851.078	562.6628	0.909217	397.6711	80.02301	0	1	1	0.107961	0.00352268	1.76E-04
274	M-274	MUF-7a(Zn)	MOF	[215]	298	0.747071	1844.755	162.1853	0.252929	296.8932	113.3357	0	1	1	0.1602	0.01102679	6.13E-04
275	M-275	NBu ₄	MOF	[112]	298	0.505808	816.536	424.3487	0.494192	4027.483	1900.835	0	1	1	0.010976	0.04427806	0.00368984
276	M-276	NENU-11	MOF	[69]	298	0.500213	4840.618	429.3322	0.499787	5931.22	1371.319	0	1	1	0.024384	0.01425679	2.59E-04
277	M-277	Ni(BTTB)	MOF	[212]	298	0.512401	2532.927	951.8299	0.487599	5660.017	2033.345	0	1	1	0.011727	0.01321904	0.0013219
278	M-278	Ni(dpip) ₂ .5DMF	MOF	[237]	298	0.511184	2899.455	539.038	0.488816	3103.751	1456.731	0	1	1	0.197664	0.01480613	5.92E-04
279	M-279	Ni ₂ Zn ₇₅ -MOF-74	MOF	[188]	298	0.496317	5253.587	560.9479	0.503683	5780.76	1520.251	0	1	1	0.51525	0.00683867	5.70E-04
280	M-280	Ni ₂ Cl ₂ (BTDD)	MOF	[132]	298	0.66111	2803.983	40.85867	0.33889	4417.011	2109.289	0	1	1	0.735604	0.01204018	5.47E-04
281	M-281	Ni ₂ Cl ₂ BBTA	MOF	[195]	298	0.508996	5027.303	1947.814	0.491004	10268.8	418.5787	0	1	1	0.403992	0.05047138	0.0029689
282	M-282	Ni ₃ C ₈ H ₁₁ N ₁₈ O ₂₉	MOF	[56]	298	0.510934	746.8534	314.7162	0.489066	4205.262	1329.151	0	1	1	0.255224	0.02322476	9.68E-04
283	M-283	Ni ₅₀ Zn ₅₀ -MOF-74	MOF	[188]	298	0.502967	5759.136	1603.408	0.497033	6048.783	515.7612	0	1	1	0.534689	0.0037092	3.09E-04
284	M-284	Ni ₇₅ Zn ₂₅ -MOF-74	MOF	[188]	298	0.502608	5221.225	1480.664	0.497392	5140.046	543.2289	0	1	1	0.558835	0.00509761	3.64E-04
285	M-285	Ni ₈ (L1)6	MOF	[6]	298	0.670325	248.7041	141.9782	0.329675	5884.062	1523.122	0	1	1	0.400567	0.03571427	0.00210084
286	M-286	Ni ₈ (L2)6	MOF	[6]	298	0.496607	237.8638	84.15512	0.193921	2743.507	178.1743	0.309472	2826.315	1076.274	0.606962	0.01319217	7.76E-04
287	M-287	Ni ₈ (L3)6	MOF	[6]	298	0.48553	217.653	108.3299	0.049965	5782.932	2918.78	0.464505	2078.159	166.5243	0.927167	0.01107563	6.15E-04
288	M-288	Ni ₈ (L4)6	MOF	[6]	298	0.289546	177.4771	81.38462	0.50945	1920.717	88.64337	0.201004	1770.304	666.5864	0.878911	0.00774963	4.56E-04
289	M-289	Ni ₈ (L5-(CF ₃) ₂) ₆	MOF	[6]	298	0.936497	427.3448	59.79	0.063503	2676.745	1196.518	0	1	1	0.851119	0.00172831	7.51E-05
290	M-290	Ni ₈ (L5-(CH ₃) ₂) ₆	MOF	[6]	298	0.287433	832.9993	1239.585	0.712567	850.7145	44.89623	0	1	1	0.636498	0.02303556	8.86E-04
291	M-291	Ni-CUK-1	MOF	[130]	303	0.213688	2757.722	1528.498	0.786312	5105.776	146.7415	0	1	1	0.308396	0.00392554	1.35E-04
292	M-292	Ni-DOBDC	MOF	[81]	298	0.463666	5400.988	3628.447	1.85E-05	122772.2	172.9244	0.536315	9750.556	255.9781	0.699552	0.02234932	0.00372489

293	M-293	Ni-MOF	MOF	[198]	298	1	490.8316	1653.848	0.388157	2658.252	70.53188	0	8749.555	449.4651	0.449167	0.01422168	6.46E-04
294	M-294	NU-1000(Zr)	MOF	[185]	298	0.602408	1000.758	445.6731	0.501022	554.0378	83.67076	0	30949.46	43.43242	1.37234	0.0076781	9.60E-04
295	M-295	NU-1000(Zr)-SALI-1	MOF	[185]	298	0.544869	799.7138	282.6519	0.093915	4231.759	751.0957	0.361216	445.4653	47.70256	0.865542	0.00284893	4.75E-04
296	M-296	NU-1000(Zr)-SALI-7	MOF	[185]	298	0.492511	880.0559	332.2543	0.077041	4967.567	430.4169	0.430448	342.1594	85.37631	0.457813	0.00356125	5.09E-04
297	M-297	NU-1000(Zr)-SALI-9	MOF	[185]	298	0.513506	955.2464	1254.92	0.793625	315.7282	199.7835	0	3912.165	70.81256	0.36091	0.002716	3.88E-04
298	M-298	NU-1000(Zr)-TFA	MOF	[241]	298	0.132879	2639.07	1817.63	0.867121	1037.2	63.53054	0	1	1	1.276978	0.0050816	2.67E-04
299	M-299	NU-901(Zr)-TFA	MOF	[241]	298	0.190143	2931.194	1838.219	0.809857	1490.835	87.05099	0	1	1	0.563327	0.00579749	3.05E-04
300	M-300	NU-905(Zr)-TFA	MOF	[241]	298	0.687692	2217.696	38.0205	0.312308	1790.152	713.5145	0	1	1	0.727495	0.0065702	3.46E-04
301	M-301	PCP-1(La)	MOF	[165]	298	0.599049	976.6407	384.0573	0.400951	4048.833	1425.569	0	1	1	0.098091	0.0127391	9.80E-04
302	M-302	Pip-CPO-27-Ni	MOF	[100]	298	0.723051	7695.038	3314.398	0.276949	14944.16	52.62422	0	1	1	0.283069	0.04154519	0.00109329
303	M-303	PZOF-2	MOF	[75]	298	0.470192	733.0653	60.1039	0.529808	666.3301	18.35891	0	1	1	0.690592	0.01043864	4.18E-04
304	M-304	pretreated a-Al	MOF	[114]	298	0.357451	3330.099	1303.38	0.12571	7192.665	2089.708	0.516839	4457.374	41.84832	0.007948	0.02265757	0.0011925
305	M-305	pretreated m-Al	MOF	[114]	298	0.504771	3324.861	1108.809	0.111448	9448.807	823.1938	0.383781	4015.047	32.45811	0.007443	0.00441064	2.76E-04
306	M-306	SALI-5(Zr)	MOF	[180]	298	0.870559	483.1285	128.7548	0.129441	3023.826	854.322	0	1	1	0.707883	0.00816754	4.08E-04
307	M-307	SALI-9(Zr)	MOF	[180]	298	0.785107	425.8059	140.4082	0.214893	2205.144	748.5094	0	1	1	0.409866	0.00720631	4.00E-04
308	M-308	SALI-9'(Zr)	MOF	[180]	298	0.876307	492.3257	131.7443	0.123693	1420.264	363.7307	0	1	1	0.758279	0.00434963	1.98E-04
309	M-309	SALI-BA(Zr)	MOF	[180]	298	0.496579	581.2383	133.3765	0.143759	1901.379	558.6194	0.359662	323.1126	69.67271	0.984661	0.00799793	4.21E-04
310	M-310	SIFSIX-14-Cu-i	MOF	[213]	298	0.431901	3394.729	786.6951	0.568099	7986.518	2067.468	0	1	1	0.155253	0.00191972	1.48E-04
311	M-311	SIFSIX-1-Cu	MOF	[213]	298	1	5666.709	1162.962	5.28E-13	48826.01	8146.468	0	1	1	0.150846	0.00362192	2.41E-04
312	M-312	SIFSIX-2-Cu-i	MOF	[213]	298	0.398925	602.3592	125.4379	0.601075	4045.21	1692.344	0	1	1	0.24888	0.0141204	9.41E-04
313	M-313	SIFSIX-3-Ni	MOF	[213]	298	0.511637	4036.45	1101.127	0.488363	7590.076	1651.183	0	1	1	0.161107	0.00429479	2.86E-04
314	M-314	SIM-1	MOF	[112]	298	0.876079	2589.978	1178.642	0.01076	65711.2	103.0298	0.113161	3816.495	23.17886	0.131592	0.02305409	0.00144088
315	M-315	S-MIL-53(Al)	MOF	[40]	298	0.180971	659.7659	197.7328	0.344961	2134.581	180.5296	0.474068	281.9265	16.34491	1.058074	0.00470578	2.94E-04
316	M-316	SNU-80	MOF	[14]	298	0.489874	1018.897	576.3313	0.510126	5310.178	1394.158	0	1	1	0.009374	0.05031222	0.00359373
317	M-317	STAM-17(Cu)-Oet	MOF	[224]	298	0.502219	5311.898	2095.945	0.497781	8385.955	214.9846	0	1	1	0.14928	0.01540725	6.42E-04
318	M-318	TAF-1a	MOF	[16]	298	0.661688	2125.17	869.9973	0.338312	7356.384	1998.595	0	1	1	0.01201	0.01669351	0.00104334
319	M-319	ThrZnOAc	MOF	[214]	298	0.850538	3590.431	242.7135	0.149462	3269.49	1290.109	0	1	1	0.15033	0.00394372	3.29E-04
320	M-320	Ti(pyradine-2-carboxylic acid)	MOF	[11]	298	0.412089	1205.446	213.2038	0.107568	2242.851	135.0045	0.480343	4324.569	917.964	0.180256	0.02120926	0.00132558
321	M-321	TUC-110(Cd)	MOF	[230]	298	0.506	2859.611	941.7649	0.494	7399.133	2150.367	0	1	1	0.098072	0.00550509	2.20E-04
322	M-322	UiO-66	MOF	[75]	298	0.609352	2542.912	79.2177	0.023064	6798.648	2200.589	0.367584	3133.564	899.0752	0.425506	0.00439239	1.69E-04
323	M-323	UiO-66(Hf)-(OH)2	MOF	[167]	273	0.502726	2935.445	1144.013	0.497274	8011.228	1662.3	0	1	1	0.284202	0.00796101	3.06E-04
324	M-324	UiO-66(Zr)-(C2H5)2	MOF	[200]	298	0.962837	9.47E-05	172.964	0.777507	2580.42	1285.282	0	74948.49	105.4182	0.175134	0.01046799	4.76E-04
325	M-325	UiO-66(Zr)-(CF3)2	MOF	[200]	298	0.530349	2269.567	956.4353	0.469651	2659.431	178.613	0	1	1	0.182363	0.00821527	3.42E-04
326	M-326	UiO-66(Zr)-(CH3)2	MOF	[200]	298	0.507615	1436.711	396.2563	0.095347	8911.998	1273.573	0.397038	3454.164	511.0291	0.275174	0.00230323	9.60E-05
327	M-327	UiO-66(Zr)-(COOH)2	MOF	[5]	303	0.304515	482.9366	169.4011	0.695485	4417.716	1790.378	0	1	1	0.24748	0.01428671	0.00142867
328	M-328	UiO-66(Zr)-(OH)2	MOF	[167]	273	0.572813	3014.195	1093.717	0.427187	7685.855	1050.216	0	1	1	0.308957	0.00741897	3.09E-04
329	M-329	UiO-66(Zr)-1,4-Napthyl	MOF	[193]	298	0.500631	1812.277	573.3056	0.029026	8876.233	60.83095	0.470343	4789.8	619.4786	0.287955	0.01699119	0.00130701
330	M-330	UiO-66(Zr)-2,5-(oMe)2	MOF	[193]	298	0.881427	3658.677	873.2672	0.118573	9208.459	953.4753	0	1	1	0.466774	0.00202611	1.13E-04
331	M-331	UiO-66(Zr)-C2F5	MOF	[200]	298	0.360367	366.2452	160.9424	0.103466	5861.669	1510.152	0.536167	1694.643	422.4785	0.240609	0.01185242	6.97E-04
332	M-332	UiO-66(Zr)-CF3	MOF	[200]	298	0.503813	2766.147	332.5817	0.496187	2890.063	1182.274	0	1	1	0.267913	0.012038	4.15E-04
333	M-333	UiO-66(Zr)-CH3	MOF	[207]	298	0.876991	2897.709	588.6617	0.123009	5067.306	3286.791	0	1	1	0.309088	0.00747308	6.79E-04
334	M-334	UiO-66(Zr)-NH3 ⁺ 3+Cl-	MOF	[181]	293	0.596734	3594.697	663.9573	0.403266	7212.262	2376.918	0	1	1	0.604926	0.00192659	1.01E-04
335	M-335	UiO-66(Zr)-NO2	MOF	[193]	298	0.731527	4526.341	1381.286	0.268473	4516.622	254.2	0	1	1	0.391304	0.0049899	3.12E-04

336	M-336	UiO-66(Zr ⁴⁺) with high concentration stearic acid	MOF	[47]	298	0.387829	2890.318	128.1624	0.478125	4581.301	2021.578	0.134046	4116.138	29.13452	0.52282	0.02055129	3.21E-04
337	M-337	UiO-66(Zr ⁴⁺) with metal/ligand ratio 6:3	MOF	[47]	298	0.428496	2875.092	66.43074	0.458954	4888.714	2098.83	0.11255	3605.445	29.96738	0.420137	0.03175891	5.99E-04
338	M-338	UiO-66D(Zr)	MOF	[200]	298	0.47645	893.9073	119.1353	0.048441	4615.599	1528.09	0.475109	883.4783	18.98614	0.33316	0.00775528	3.53E-04
339	M-339	UiO-66D(Zr)-(CF ₃) ₂	MOF	[200]	298	0.493219	367.2997	71.72049	0.0136	29568.3	46.67037	0.493182	359.2959	17.89431	0.280178	0.00623405	2.71E-04
340	M-340	UiO-66-NH ₂	MOF	[64]	298	0.517083	4380.525	400.6071	0.482917	5589.41	2044.634	0	1	1	0.384388	0.00422706	3.25E-04
341	M-341	UiO-67(Zr)	MOF	[166]	298	0.540402	1761.414	90.43108	0.108289	6392.706	1695.509	0.351309	1874.926	508.7158	0.284822	4.58E-04	6.54E-05
342	M-342	UiO-67(Zr)-BIPY	MOF	[166]	298	0.166954	3374.338	188.5673	0.784811	3333.149	1813.846	0.048235	27203.59	5852.568	0.210456	0.02180251	0.00311464
343	M-343	UiO-67(Zr)-BN	MOF	[168]	303	0.126903	998.0223	592.4379	0.028481	7179.357	30.54931	0.844616	1545.697	14.71387	0.493011	0.03731303	0.00219488
344	M-344	UMCM-1	MOF	[64]	298	0.499287	573.3889	125.8854	0.999998	694.8533	2029.496	0	6139.003	36.93433	0.262395	0.0026725	8.91E-04
345	M-345	untreated a-Al	MOF	[114]	298	0.545565	3351.159	787.3222	0.454435	9012.839	1956.067	0	1	1	0.003825	0.00297384	2.12E-04
346	M-346	untreated m-Al	MOF	[114]	298	0.465261	3002.816	1507.113	0.010671	4304.017	169.2416	0.524068	4514.5	28.4181	0.009671	0.02643508	8.53E-04
347	M-347	ValZnCl	MOF	[227]	298	0.594207	294.2315	131.2806	0.405793	2453.74	1119.102	0	1	1	0.124496	0.01990543	0.00124409
348	M-348	ValZnOAc	MOF	[214]	298	0.768919	611.1979	72.2377	0.231081	3753.314	2040.305	0	1	1	0.284638	0.0062802	3.49E-04
349	M-349	Y-fum-fcu-MOF	MOF	[7]	298	0.56522	4156.195	1258.508	0.172976	5729.898	304.3069	0.261804	6464.649	83.5495	0.372251	0.00541576	2.26E-04
350	M-350	Y-shp-MOF-5	MOF	[174]	298	0.856175	1078.945	137.7689	0.143825	6472.962	1354.712	0	1	1	0.502226	0.00247961	1.55E-04
351	M-351	ZIF-412(Zn)	MOF	[161]	298	0.820696	582.6233	110.0614	0.179304	2737.658	1207.38	0	1	1	0.071962	0.00617102	3.43E-04
352	M-352	ZIF-71(Zn)	MOF	[209]	308	0.485101	1466.007	413.4958	0.514899	7667.267	2113.854	0	1	1	0.007619	0.05903531	0.00491961
353	M-353	ZIF-8	MOF	[58]	298	0.386877	3.605498	671.4135	0.005877	24280.38	34.09344	0.607246	148.9765	25.36475	0.140004	0.12547041	0.0078419
354	M-354	ZIF-8_50-90_50	MOF	[155]	308	0.520056	524.1085	45.27914	0.470153	738.1826	68.96281	0.00979	27373.47	432.225	0.373885	0.0017727	5.06E-05
355	M-355	ZIF-8_55-71_45	MOF	[155]	308	0.64032	773.776	333.8122	0.045613	5283.365	62.98759	0.314067	4709.558	1068.19	0.014188	0.04078682	0.00509835
356	M-356	ZIF-8_70-90_30	MOF	[155]	308	0.332585	492.7528	51.49542	0.027251	15442.53	114.2819	0.640163	366.6848	16.73294	0.074435	0.00385246	2.27E-04
357	M-357	ZIF-90(Zn)	MOF	[209]	308	0.150075	1039.357	373.8904	0.849925	2695.763	162.9264	0	1	1	0.332063	0.00443987	2.47E-04
358	M-358	Zn(BTTB)	MOF	[212]	298	0.623584	727.4595	187.9098	0.376416	2841.032	975.8172	0	1	1	0.209057	0.01292671	8.62E-04
359	M-359	Zn(BTTB)(AZPY)	MOF	[212]	298	0.547865	1749.233	471.0811	0.452135	1514.386	117.9161	0	1	1	0.190481	0.00478803	3.42E-04
360	M-360	Zn(BTTB)(BDC)	MOF	[212]	298	0.398726	1021.803	284.5386	0.068091	47861.05	91.20061	0.533183	3597.996	1161.4	0.089574	0.00722661	9.03E-04
361	M-361	Zn(BTTB)(BPY)	MOF	[212]	298	0.500428	528.936	91.18816	0.499572	762.1553	66.84877	0	1	1	0.252617	0.00482664	2.84E-04
362	M-362	Zn(BTTB)(DMBPY)	MOF	[201]	298	0.941159	424.7759	57.12816	0.058841	2569.625	780.3566	0	1	1	0.210438	0.01138207	7.11E-04
363	M-363	Zn(DM)0.5(AT)	MOF	[232]	298	0.429791	1341.784	492.4026	0.570209	7848.846	525.2286	0	1	1	0.085284	0.00869773	4.83E-04
364	M-364	Zn(II)-MOF [Zn(HPyImDC)(DMA)] _n	MOF	#N/A	298	0.507281	1884.824	945.2224	0.492719	8797.816	2746.489	0	1	1	0.064361	0.02076277	8.31E-04
365	M-365	Zn(L)(tdca)*1.5DMF	MOF	[119]	298	0.499966	4088.22	616.9256	0.4867	6576.537	1904.097	0.013334	28676.39	40.25674	0.068253	0.00941698	5.23E-04
366	M-366	Zn(NDI-H)	MOF	[110]	293	0.816913	2001.684	86.46705	0.183087	2044.068	766.6184	0	1	1	0.427152	0.00276507	2.51E-04
367	M-367	Zn(NDI-NHEt)	MOF	[110]	293	0.407534	2005.041	732.101	0.592466	1936.2	54.70427	0	1	1	0.290714	0.00744827	4.66E-04
368	M-368	Zn(NDI-SEt)	MOF	[112]	293	0.438776	1273.661	477.548	0.304453	3642	245.1882	0.25677	6475.792	1477.958	0.283436	0.01011043	4.60E-04
369	M-369	Zn(NDI-SO ₂ Et)	MOF	[112]	293	0.566983	2776.583	1162.496	0.433017	2579.297	195.028	0	1	1	0.214494	0.00978313	5.44E-04
370	M-370	Zn(NDI-SOEt)	MOF	[112]	293	0.438776	1273.661	477.548	0.304453	3642	245.1882	0.25677	6475.792	1477.958	0.283436	0.01011043	4.60E-04
371	M-371	Zn(NO ₃) ₂ *6H ₂ O	MOF	[12]	293	0.985361	6524.086	1352.529	0.014639	91592.69	1.72E+14	0	1	1	0.165408	0.00432446	6.18E-04
372	M-372	Zn ₂ (bptc)	MOF	[225]	298	0.242704	2274.707	188.4351	0.757296	4533.692	643.3204	0	1	1	0.1519	0.00521929	2.27E-04
373	M-373	Zn ₂ C ₁₄ N ₂ O ₈ H ₄	MOF	[66]	298	0.644464	4614.064	540.5646	0.343052	2338.016	312.1533	0.012484	13056.81	60.46827	0.178903	0.00580891	2.77E-04
374	M-374	Zn ₂ Co ₃ (MFU-4l)	MOF	[184]	298	0.868554	2229.267	36.12001	0.131446	1539.829	870.8675	0	1	1	1.078923	0.00268569	2.07E-04
375	M-375	Zn ₃ (TCPB) ₂ (H ₂ O) ₂	MOF	[108]	298	0.505488	358.5125	254.6445	0.494512	3893.094	1472.996	0	1	1	0.080967	0.04515646	0.00282228
376	M-376	Zn ₃ Co ₂ (MFU-4l)	MOF	[184]	298	0.498693	1960.296	75.84075	0.088647	1956.18	1134.933	0.41266	1912.625	37.0963	0.933303	0.00319145	2.90E-04
377	M-377	Zn ₃ L ₂	MOF	[220]	298	0.819108	1709.701	512.0237	0.180892	7356.975	2903.214	0	1	1	0.197481	0.01191099	7.44E-04
378	M-378	Zn ₄ O(dmcapz) ₃	MOF	[72]	298	0.501181	401.6259	311.0816	0.498819	498.5091	86.04612	0	1	1	0.386253	0.03468625	8.89E-04

379	M-379	Zn5(MFU-4I)	MOF	[184]	298	0.690055	1045.504	59.92128	0.309945	1017.364	3.271531	0	1	1	1.04	0.00514324	4.29E-04
380	M-380	Zn-BTTB-DMBPY	MOF	[84]	298	0.937923	535.0298	10.87049	0.062077	2611.036	1023.103	0	1	1	0.212146	2.12E-04	3.54E-05
381	M-381	ZnCo4(MFU-4I)	MOF	[184]	298	0.500988	788.9504	196.9154	0.416848	2768.105	93.40769	0.082164	38750.37	16949.77	0.733665	0.00695068	6.32E-04
382	M-382	Zn-MOF-74(cycle 1)	MOF	[49]	298	0.248079	2335.718	778.4186	0.094536	14127.16	36.30765	0.657384	9894.046	2235.856	0.304731	0.01754745	6.75E-04
383	M-383	Zn-Trimesate	MOF	[221]	303	0.509155	3659.72	2045.334	0.490845	10926.03	2179.467	0	1	1	0.191241	0.01591952	8.84E-04
384	M-384	Zr-Fum HT	MOF	[242]	303	0.501892	4898.313	1644.63	0.019614	13858.06	95.52634	0.478494	5736.287	251.4275	0.421503	0.00952017	4.33E-04
385	M-385	Zr-MOF-801-P	MOF	[75]	298	0.506838	4461.036	1482.833	0.493162	6298.696	258.8384	0	1	1	0.353338	0.00571732	2.60E-04
386	M-386	Zr-MOF-801-SC	MOF	[75]	298	0.496899	6060.586	180.8317	0.503101	3248.116	964.524	0	1	1	0.277296	0.00584813	3.66E-04
387	M-387	Zr-MOF-802	MOF	[75]	298	0.539938	2232.916	923.7017	0.460062	7002.563	1567.614	0	1	1	0.085072	0.0106349	5.60E-04
388	M-388	Zr-MOF-804	MOF	[75]	298	0.695395	2239.42	119.5774	0.247545	2475.471	1064.086	0.05706	12721.92	2336.141	0.339164	0.01684772	8.02E-04
389	M-389	Zr-MOF-805	MOF	[75]	298	0.504792	2433.999	411.5314	0.172137	2990.924	72.41521	0.323072	3462.959	1297.696	0.332925	0.00363472	1.73E-04
390	M-390	Zr-MOF-806	MOF	[75]	298	0.504591	3116.499	986.3802	0.495409	7906.258	1333.443	0	1	1	0.266152	0.01269104	5.08E-04
391	M-391	Zr-MOF-808	MOF	[75]	298	0.494796	2864.039	126.8056	0.182665	4284.108	3294.859	0.322539	2692.613	29.19263	0.572069	0.01288774	4.77E-04
392	M-392	Zr-MOF-841	MOF	[75]	298	0.339695	3016.221	645.8683	0.660305	3445.717	15.97044	0	1	1	0.48299	0.02876344	0.00136969
393	C-1	2,5-DhaTab	COF	[135]	298	0.097381	1566.607	745.6322	0.902619	512.335	45.08477	0	1	1	0.567901	0.00388094	2.16E-04
394	C-2	2,3-DhaTph	COF	[135]	298	0.547371	915.8813	384.4404	0.452629	3581.024	917.427	0	1	1	0.144552	0.02149095	0.00143273
395	C-3	2,5-DhaTph	COF	[135]	298	0.837135	994.4528	97.88871	0.162865	691.8936	2295.39	0	1	1	0.16939	0.01244947	8.30E-04
396	C-4	AB-COF	COF	[133]	298	0.681521	3361.615	63.35843	0.318479	3012.831	539.7694	0	1	1	0.347584	0.00517381	1.67E-04
397	C-5	Ad2L1	COF	[140]	293	0.497577	386.2955	48.09814	0.502423	924.1279	333.8558	0	1	1	0.279405	0.05356133	0.00111586
398	C-6	Ad2L2	COF	[140]	293	0.618822	477.4786	111.1531	0.381178	1439.428	564.5594	0	1	1	0.14943	0.04424278	0.00119575
399	C-7	Ad2L3	COF	[140]	293	0.609821	537.8645	127.6498	0.132817	3683.9	947.1684	0.257362	1243.038	220.6713	0.229107	0.01266511	2.81E-04
400	C-8	Ad3L1	COF	[140]	293	0.645825	563.8632	108.6725	0.268967	1124.015	167.518	0.085208	2955.58	715.4997	0.415802	0.00538049	1.25E-04
401	C-9	Ad3L2	COF	[140]	293	0.620702	446.2351	79.66079	0.379298	1096.919	341.9286	0	1	1	0.374514	0.03720836	8.65E-04
402	C-10	Ad3L3	COF	[140]	293	0.507137	552.5921	84.4648	0.492863	1019.82	280.9918	0	1	1	0.545552	0.02360688	4.14E-04
403	C-11	Ad4L1	COF	[140]	293	0.887182	1211.685	312.8256	0.112818	3557.648	846.3142	0	1	1	0.447004	0.00868395	1.50E-04
404	C-12	Ad4L2	COF	[140]	293	0.501524	481.3115	86.57941	0.498476	870.4368	250.8065	0	1	1	0.686162	0.02750222	3.99E-04
405	C-13	Ad4L3	COF	[140]	293	0.834413	1416.01	364.4511	0.116752	4318.374	1096.1	0.048835	479.5628	53.94949	0.522857	0.00310065	5.96E-05
406	C-14	ATFG-COF	COF	[133]	298	0.367549	322.9185	136.5887	0.632451	3967.628	1197.45	0	1	1	0.290484	0.01701856	4.86E-04
407	C-15	bipy -CTF500	COF	[138]	298	0.500448	1972.095	655.1905	0.499552	3581.488	1369.043	0	1	1	0.422224	0.02337568	3.65E-04
408	C-16	bpim -CTF -300	COF	[142]	298	0.505268	1170.08	663.672	0.251719	167.4877	56.2371	0.243013	6070.865	1042.515	0.153404	0.05440536	7.56E-04
409	C-17	bpim -CTF -400	COF	[142]	298	0.504849	2306.9	979.0922	0.495151	4723.95	2068.517	0	1	1	0.300465	0.04082749	3.14E-04
410	C-18	bpim -CTF -500	COF	[142]	298	0.734716	1945.152	523.0528	0.265284	3166.627	2222.782	0	1	1	0.486059	0.02156582	2.25E-04
411	C-19	CE-1	COF	[137]	293	0.511117	599.1868	158.7074	0.488883	2276.583	930.4716	0	1	1	0.267784	0.02292345	0.00163739
412	C-20	CE-2	COF	[137]	293	0.50187	1118.955	313.5736	0.49813	3572.46	1469	0	1	1	0.066125	0.01678645	0.00119903
413	C-21	CE-3	COF	[137]	293	0.518177	1147.807	303.0739	0.481823	2978.738	1304.4	0	1	1	0.069853	0.01844045	0.00131718
414	C-22	COF-432	COF	[244]	298	0.318342	1427.349	720.1676	0.681658	2636.028	32.64642	0	1	1	0.289395	0.00544728	2.48E-04
415	C-23	CTF-a	COF	[139]	292.5	0.504674	869.4397	139.6679	0.495326	1150.113	472.6623	0	1	1	1.313891	0.01680125	3.43E-04
416	C-24	CTF-b	COF	[139]	292.5	0.822395	2168.86	712.633	0.177605	6044.253	1074.53	0	1	1	0.541573	0.00952645	2.98E-04
417	C-25	CTF-c	COF	[139]	292.5	0.498085	1259.645	288.1291	0.501915	1944.77	762.9849	0	1	1	0.869319	0.01453854	4.15E-04
418	C-26	CTF-d	COF	[140]	292.5	0.592695	618.9742	216.5458	0.070502	2791.944	495.8614	0.336803	338.4606	32.05491	0.726657	0.02696523	8.17E-04
419	C-27	DCBP -CTF - 1	COF	[143]	293	0.508802	880.9977	214.7088	0.206646	1926.34	702.2331	0.284551	335.5909	27.93984	0.49843	0.01077566	1.71E-04
420	C-28	F -DCBP -CTF - 1	COF	[143]	293	0.496482	339.8585	84.65792	0.415297	1288.885	450.8813	0.088221	3802.596	861.4808	0.192556	0.07550609	0.00279652
421	C-29	MM1	COF	[141]	293	0.505477	1033.195	235.1752	0.289609	1972.942	591.979	0.204913	568.929	87.22596	0.493741	0.00687421	1.81E-04

422	C-30	MM2	COF	[141]	293	0.725247	1922.253	629.5268	0.211499	4411.921	1610.25	0.063254	2356.408	63.01398	0.419974	0.00862063	2.61E-04
423	C-31	MM3	COF	[141]	293	0.606634	721.6107	165.2136	0.104894	1901.395	446.6941	0.288472	453.6314	56.58749	0.753041	0.00650856	1.45E-04
424	C-32	MM4	COF	[141]	293	0.082199	5020.221	1124.864	0.917801	1424.182	460.6111	0	1	1	0.371208	0.01024817	3.11E-04
425	C-33	pym-CTF500	COF	[138]	298	0.391001	1489.865	679.6906	0.608999	7853.384	2917.171	0	1	1	0.210234	0.03849364	6.01E-04
426	C-34	TPAnq	COF	[136]	298	0.642224	1850.638	932.9408	0.043538	3234.226	69.29447	0.314238	2591.731	29.4195	0.3565	0.01732093	0.00144341
427	C-35	TP-Azo	COF	[135]	298	0.500414	974.5745	341.9585	0.354917	1430.138	48.70908	0.144669	2843.705	911.2126	0.394341	0.00629376	5.72E-04
428	C-36	TP-Azo	COF	[136]	298	0.606939	1240.382	406.9566	0.393061	1424.388	79.33931	0	1	1	0.394341	0.02187967	0.00145864
429	C-37	TPBD	COF	[135]	298	0.499158	1977.516	1181.988	0.500842	1864.832	85.13109	0	1	1	0.133563	0.01910326	0.00127355
430	C-38	TPBD	COF	[136]	298	0.506635	1192.139	677.1365	0.493365	1965.686	132.3464	0	1	1	0.133563	0.01831041	0.00122069
431	C-39	TPBD-(NO ₂) ₂	COF	[135]	298	0.502913	1318.535	269.126	0.497087	2185.923	1358.432	0	1	1	0.078553	0.01883444	0.00117715
432	C-40	TPBD-(NO ₂) ₂	COF	[136]	298	0.331444	630.0225	225.7134	0.30281	2607.866	19.74372	0.365746	2219.427	861.162	0.078553	0.01071439	8.93E-04
433	C-41	TPBD-(OMe) ₂	COF	[135]	298	0.845741	1318.981	392.9424	0.154259	4340.698	1398.792	0	1	1	0.13026	0.01082577	7.22E-04
434	C-42	TPBD-(OMe) ₂	COF	[136]	298	0.979023	1325.062	450.04	0.020977	6736.508	445.1613	0	1	1	0.13026	0.02868125	0.00191208
435	C-43	TPBD-Me ₂	COF	[135]	298	0.845741	1318.981	392.9424	0.154259	4340.698	1398.792	0	1	1	0.13026	0.01082577	7.22E-04
436	C-44	TPBD-Me ₂	COF	[136]	298	0.827992	1252.969	514.2285	0.172008	1696.073	39.69077	0	1	1	0.13026	0.01968716	0.00131248
437	C-45	TPBpy	COF	[136]	298	0.349302	1613.412	594.0984	0.650698	2183.442	99.77114	0	1	1	0.76505	0.00234467	1.56E-04
438	C-46	TPHZ	COF	[245]	298	0.506901	3442.974	364.2581	0.493099	2836.812	1565.033	0	1	1	0.391853	0.016265	9.04E-04
439	C-47	TPPa-1	COF	[135]	298	0.628114	2706.175	1232.613	0.371886	4031.365	22.97711	0	1	1	0.41232	0.01366714	0.00105132
440	C-48	TPPa-1*	COF	[136]	298	0.451068	635.3058	218.1973	0.548932	3643.702	509.6672	0	1	1	0.41232	0.01572563	0.00104838
441	C-49	TPPa-2	COF	[135]	298	0.899988	2109.976	1045.081	0.100012	2907.45	60.12731	0	1	1	0.202156	0.0273045	0.00170653
442	C-50	TPPa-2*	COF	[136]	298	0.294951	784.3398	228.3629	0.705049	3177.031	703.9923	0	1	1	0.202156	0.00595121	3.97E-04
443	C-51	TPPa-F ₄	COF	[135]	298	0.178853	2025.356	872.9894	0.821147	1060.011	136.7955	0	1	1	0.179023	0.0028341	1.89E-04
444	C-52	TPPa-NO ₂	COF	[135]	298	0.178853	2025.356	872.9894	0.821147	1060.011	136.7955	0	1	1	0.179023	0.0028341	1.89E-04
445	C-53	TPPa-NO ₂	COF	[136]	298	0.48326	787.5587	262.9427	0.51674	4001.624	664.6495	0	1	1	0.179023	0.00952487	6.35E-04
446	C-54	TPTph	COF	[136]	298	0.161812	1684.692	1436.232	0.838188	1143.002	151.763	0	1	1	0.327808	0.00487247	3.25E-04
447	C-55	TPTta	COF	[136]	298	0.457327	551.9909	132.6649	0.542673	2962.693	782.2186	0	1	1	0.334507	0.00798899	5.33E-04
448	C-56	trzn-COF	COF	[134]	298	0.50475	860.4851	384.5944	0.49525	3956.809	1517.122	0	1	1	0.068892	0.03098193	6.74E-04
449	Z-1	CBV-901	Zeolite	[77]	294	0.312592	3317.455	102.0243	0.687408	7485.203	2008.658	0	1	1	1.21E-05	0.01400746	0.00200107
450	Z-2	H _{0.34} Na _{0.06} Al _{10.4} Si _{47.6} O ₉₆	Zeolite	[21]	298	0.506298	1536.745	487.5242	0.493702	4866.792	1000.129	0	1	1	0.153272	0.0058525	5.85E-04
451	Z-3	HiSiv 3000 Zeolite	Zeolite	[76]	293	0.507345	3117.671	872.903	0.492655	8183.668	2936.886	0	1	1	0.030593	0.01136684	7.58E-04
452	Z-4	K ₆ Na ₆ Al ₁₁ O ₄₈	Zeolite	[21]	298	0.668746	13322.04	4495.86	0.331254	12024.44	16.3652	0	1	1	0.259865	0.16826934	0.01051683
453	Z-5	MCM-41	Zeolite	[50]	298	0.7702	771.5722	108.0828	0.2298	2425.47	1261.032	0	1	1	0.560662	0.00851225	0.00106403
454	Z-6	NaX	Zeolite	[128]	298	0.320478	5676.816	2530.857	0.679522	14229.34	1022.596	0	1	1	0.331483	0.00206617	1.29E-04
455	Z-7	Na-ZSM-5	Zeolite	[50]	298	0.248079	2335.718	778.4186	0.094536	14127.16	36.30765	0.657384	9894.046	2235.856	0.304731	0.01754745	6.75E-04
456	Z-8	Zeolite 13X	Zeolite	[43]	298	0.296552	4649.157	1951.07	0.703448	5804.545	304.662	0	1	1	0.320663	0.23781279	0.01080967
457	Z-9	Zeolite 4A	Zeolite	[79]	298	0.50418	7411.187	2067.505	0.49582	16069.26	1934.26	0	1	1	0.286452	0.0024327	1.87E-04
458	Z-10	Zeolite Na-A	Zeolite	[121]	298	0.497849	7178.515	1488.82	0.502151	9281.592	111.5377	0	1	1	0.253694	0.03041288	0.00304129
459	Z-11	Zn ₂ (pbc) ₂ *H ₂ ma*H ₃ O*2H ₂ O	Zeolite	[9]	298	0.727554	3107.02	1298.294	0.250151	8283.224	679.561	0.022295	17390.28	24.27352	0.147544	0.00841441	0.0021036
460	Z-12	ZSM-5	Zeolite	[65]	298	0.524857	2341.584	363.3627	0.475143	5047.698	1523.547	0	1	1	0.01095	0.01631197	0.0016312

Chi-square (χ^2) and reduced chi-square (χ^2/ν) are statistical indicators that commonly used to judge the goodness of curve fitting. According to the rule of thumb, a "good" fitting has χ^2/ν less than 1, and smaller χ^2 usually means smaller fitting error with the reasonable fitting parameters.

We conducted chi-square goodness-of-fit test1 for each fitting, and provided statistical indicators including the chi-square (χ^2) and reduced chi-square (χ^2/ν) that commonly used to judge the goodness of curve fitting in Table S1. According to the rule of thumb, a "good"

fitting has χ^2 less than 1, and smaller χ^2 usually means smaller fitting error with the reasonable fitting parameters. 2-3 All adsorption isotherms fitted in our study ($\chi^2 < 0.03$) has decent fitting. Concretely, their formulas are $\chi^2 = \sum_i N r_i^2$ and $\chi^2 = \chi^2 / (N - N_{\text{vars}})$. Where, r is the residual array returned by the objective function (likely to be (data-model)/uncertainty for data modelling usages), N is the number of data points, and N_{vars} is number of variable parameters. 4

1	Cochran, W. G., The χ^2 test of goodness of fit. The Annals of Mathematical Statistics 1952, 23 (3), 315-345.
2	Chi-square: testing for goodness of fit. http://maxwell.ucsc.edu/~drip/133/ch4.pdf .
3	Chi square distribution (X2) and least squares fitting. https://www.asc.ohio-state.edu/gan.1/teaching/spring04/Chapter6.pdf .
4	LMFIT: Non-Linear Least-Squares Minimization and Curve-Fitting for Python. https://lmfit.github.io/lmfit-py/ .

Table S3. The structural characteristics, isotherm features and cooling performance of 460 adsorbents

No.	ID No.	Adsorbent	Species	Ref. No.	Sa (m ² /g)	Notes	Va (cm ³ /g)	Notes	Dp (Å)	Notes	Wsat (g/g)	alpha	KH (mol/(kg Pa))	SCE (kJ/kg)	COPc
1	M-1	[(Ni(L6)2)4H2O]n	MOF	[229]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.118848812	0.15	0.002038923	244.391545	0.684779
2	M-2	(H2dab)[Zn2(ox)3]	MOF	[71]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.234775319	0.75	0.01634968	91.90013099	0.49548
3	M-3	[{Zn(L)(H2O)2}(NO3)2*2H2O]n	MOF	[4]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.108095778	0.45	0.000614281	34.99503361	0.335109
4	M-4	[Cd(L'1)(Cl)](H2O)	MOF	[206]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.408752142	0.85	1.39E-08	1.782178078	0.026616
5	M-5	[Cd(L'2)(Cl)](H2O)	MOF	[206]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.096180068	0.15	0.004260882	189.1566586	0.64594
6	M-6	[Cd(L'2)2(Br)2](H2O)3	MOF	[206]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.033113269	0.05	0.00166598	32.13181146	0.31271
7	M-7	[Cd(L'3)(Cl)](H2O)2	MOF	[206]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.10407219	0.15	0.003212751	202.1890104	0.663299
8	M-8	[Cd(mpto)2.CH3CH2OH]n	MOF	[24]	25.8	s1	n.d.	n.d.	n.d.	n.d.	0.003130305	0.55	4.00E-05	0.328357983	0.005015
9	M-9	[Co(L)(PIN)]dioxane	MOF	[222]	244	s1	n.d.	n.d.	n.d.	n.d.	0.173415552	0.45	0.001586381	38.64672411	0.354834
10	M-10	[Co2(BDC)2(BPNO)]*H2BDC*2MeOH	MOF	[19]	n.d.	n.d.	n.d.	n.d.	5.8	d2	0.080739885	0.05	0.00547091	53.17553037	0.386808
11	M-11	[Co3(ndc)-(HCOO)3(mu3-OH)(H2O)]n	MOF	[15]	1386	s1	0.58	v1	13.6	d2	0.241479318	0.15	0.006215665	404.7922898	0.750943
12	M-12	[Co4L3(u3-OH)(H2O)3](SO4)0.5	MOF	[210]	n.d.	n.d.	n.d.	n.d.	18	d1	0.193959876	0.05	0.00690667	387.0751406	0.719742
13	M-13	[Cu(INA)2(NH3)2(H2O)2]	MOF	[36]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.021940066	0.75	0.000380002	16.2645392	0.194844
14	M-14	[Cu(INA)2]	MOF	[36]	164.4	s1	n.d.	n.d.	4.99	d2	0.066652985	0.55	0.001954751	50.21096296	0.407579
15	M-15	[Cu(INAIP)]*2H2O	MOF	[93]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.133665825	0.05	0.010385545	269.3413181	0.661989
16	M-16	[Cu2(H2btp)(H2O)2(12-bis(4-pyridyl)ethylene)]	MOF	[115]	2.8	s1	0.095	v1	13.4	d2	0.091300699	0.05	0.007084607	103.8410682	0.546155
17	M-17	[Cu2(H2btp)(H2O)2(13-bis(4-pyridyl)propane)]	MOF	[115]	3	s1	0.083	v1	14	d2	0.068456308	0.05	0.005550609	88.8935706	0.515441
18	M-18	[Cu2(H2btp)(H2O)2(bipyridine)]	MOF	[115]	1.1	s1	0.047	v1	11.2	d2	0.046107966	0.05	0.002687605	67.76960875	0.464619
19	M-19	[Cu2(pzdc)2(pyz)]*2H2O	MOF	[30]	n.d.	n.d.	n.d.	n.d.	6	d2	0.144906921	0.05	0.007663396	113.163315	0.552948
20	M-20	[La3L4(H2O)6]-Cl	MOF	[210]	n.d.	n.d.	n.d.	n.d.	19	d1	0.273519548	0.25	0.008693749	543.598237	0.783822
21	M-21	[Mn(mpto)2.CH3CH2OH]2	MOF	[24]	86.2	s1	n.d.	n.d.	n.d.	n.d.	0.053901013	0.55	1.27E-06	10.78692331	0.140194
22	M-22	[Ni(dipn)]2[Ni(dipn)(H2O)][Fe(CN)6]2.2H2O	MOF	[67]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.196247646	0.05	0.011755152	164.1711497	0.630437
23	M-23	[Ni(pca)(bdc)0.5(H2O)2]	MOF	[59]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.158619042	0.05	0.006548765	122.8788389	0.588285
24	M-24	[Ni8(L5)6]	MOF	[6]	2215	s1	n.d.	n.d.	n.d.	n.d.	1.052699405	0.75	0.002279367	81.95477544	0.525993
25	M-25	[Ni8(L5-CF3)6]	MOF	[6]	1985	s1	n.d.	n.d.	n.d.	n.d.	0.857636874	0.85	0.000475773	58.79207534	0.455622
26	M-26	[Ni8(L5-CH3)6]	MOF	[107]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.63096808	0.65	4.28E-05	37.87200629	0.356707
27	M-27	[PbL2]*2DMF*6H2O	MOF	[99]	n.d.	n.d.	n.d.	n.d.	13	d3	0.215334642	0.85	0.00392194	100.0820709	0.560398
28	M-28	[PbL2]*DMF*2H2O	MOF	[99]	n.d.	n.d.	n.d.	n.d.	13	d3	0.048438421	0.05	0.010531939	37.55421838	0.325028
29	M-29	[Zn(NO2-BDC)(dmbpy).5](C2H6O)(H2O)	MOF	[48]	925	s1	n.d.	n.d.	9	d2	0.169732315	0.45	0.000103889	35.01476648	0.337526
30	M-30	[Zn2(ip)2(bpy)2]*DMF]n	MOF	[88]	300	s1	n.d.	n.d.	6	d2	0.042328796	0.25	0.001621206	55.70652581	0.42598
31	M-31	[Zn3(TCPB)2*2H2O]*2H2O*4DMF	MOF	[10]	573	s1	n.d.	n.d.	4.3	d2	0.104953428	0.15	0.000547097	135.5492877	0.612592

32	M-32	[Zn4O(mipcapz)3]n on [Zn4O(dmcapz)3]n	MOF	[1]	640	s1	0.279	v1	n.d.	n.d.	0.132550096	0.75	1.24E-06	15.17396785	0.186262
33	M-33	{(H2PIP)0.5[VO(CEP)]*H2O}	MOF	[57]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.060483089	0.25	4.43E-05	103.6625882	0.567284
34	M-34	{[Cu(azpy)(glut)](H2O)2}	MOF	[51]	131	s2	n.d.	n.d.	7.8	d3	0.165397762	0.25	0.000178399	134.3022291	0.62155
35	M-35	{[Cu2(4-pmpmd)2(CH3OH)4(opd)2]*2H2O}	MOF	[53]	n.d.	n.d.	n.d.	n.d.	6.48	d3	0.224113296	0.35	6.57E-07	66.90129388	0.482612
36	M-36	{[Cu2(pzdc)2(bpy)]*4H2O}	MOF	[30]	n.d.	n.d.	n.d.	n.d.	9	d2	0.167213489	0.05	0.052007339	251.5986206	0.625414
37	M-37	{[Cu4(OH)2(tci)2-(bpy)2]-11H2O}	MOF	[127]	n.d.	n.d.	n.d.	n.d.	12.54	d1	0.080869713	0.15	0.001295986	91.75020143	0.536578
38	M-38	{[Dy(ox)(Bpybc)(H2O)]*OH*13H2O}n	MOF	[103]	n.d.	n.d.	n.d.	n.d.	8.4	d3	0.238927337	0.65	0.004719372	184.8290916	0.666508
39	M-39	{[Ni(bpe)2(N(CN)2)](N(CN)2)}n	MOF	[87]	n.d.	n.d.	n.d.	n.d.	6.78	d3	0.077415888	0.05	0.003035346	74.25676527	0.489677
40	M-40	{[Zn-(C10H2O8)0.5(C10S2N2H8)]*5H2O}n	MOF	[61]	n.d.	n.d.	n.d.	n.d.	12.7	d3	0.085750301	0.05	0.007078219	116.5875137	0.563153
41	M-41	{[Zn(oxo-pba)2(bpy)]4H2O}n	MOF	[117]	n.d.	n.d.	n.d.	n.d.	6.2	d3	0.077068032	0.75	0.002379007	40.8470216	0.363401
42	M-42	{[Zn2(bpdc)2(azpy)]*2H2O*2DMF}n	MOF	[62]	235	s1	n.d.	n.d.	8.2	d3	0.080015806	0.65	0.001483579	42.58878309	0.374685
43	M-43	{[Zn2(bpdc)2(azpy)]*2H2O*2DMF}n Nanoscale	MOF	[62]	385	s1	n.d.	n.d.	n.d.	n.d.	0.096342137	0.05	0.004007365	81.39887313	0.507954
44	M-44	{[Zn3(bpdc)3(azpy)]*4H2O*2DEF}n	MOF	[62]	200	s1	n.d.	n.d.	11.9	d2	0.111684322	0.85	0.002539602	83.44261205	0.520716
45	M-45	{[Zn4O(bfpdc)3-(bpy)0.5(H2O)]*(3DMF)(H2O)}n	MOF	[60]	1450	s1	0.59	v1	10.76	d3	0.407886883	0.85	8.50E-17	0.001206392	1.86E-05
46	M-46	{[ZnL(HCO2)(H2O)]*DMF}	MOF	[109]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.47014202	0.45	0.007288208	114.3613406	0.572207
47	M-47	1 C76H116N14O4Zn3	MOF	[118]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.16868733	0.05	0.006906125	153.6930774	0.629675
48	M-48	13R(Co)	MOF	[234]	293	s1	n.d.	n.d.	8	d3	0.01558669	0.65	7.94E-05	8.424957964	0.113165
49	M-49	1-LiCl	MOF	[112]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.229565198	0.15	8.65E-05	369.9474249	0.789692
50	M-50	23R(Co)	MOF	[234]	267	s1	n.d.	n.d.	8	d3	0.052795943	0.85	1.30E-06	3.810883125	0.055128
51	M-51	2D [Cu(bpy)2(OTf)2]n	MOF	[70]	740	s1	0.295	v1	n.d.	n.d.	0.177633584	0.85	0.002066215	181.6967976	0.651021
52	M-52	33R(Co)	MOF	[234]	241	s1	n.d.	n.d.	8	d3	0.04107238	0.55	4.46E-05	17.08438872	0.203308
53	M-53	3S(Co)	MOF	[234]	281	s1	n.d.	n.d.	8	d3	0.027462335	0.65	2.74E-05	7.967755823	0.10796
54	M-54	43R(Co)	MOF	[234]	203	s1	n.d.	n.d.	8	d3	0.019245782	0.65	9.58E-05	11.16916114	0.144085
55	M-55	Al(OH)-(1,4-NDC)	MOF	[226]	546	s2	0.22	v1	7.7	d3	0.158218396	0.45	8.55E-06	19.26289588	0.223077
56	M-56	AlaZnBr	MOF	[227]	n.d.	n.d.	n.d.	n.d.	12.5	d3	0.066465981	0.75	0.000117443	31.22294345	0.313421
57	M-57	AlaZnCl	MOF	[227]	n.d.	n.d.	n.d.	n.d.	12.5	d3	0.159731829	0.15	0.000853233	162.1537853	0.650628
58	M-58	AlaZnOAc	MOF	[214]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.280444314	0.85	0.00713702	72.88050576	0.481896
59	M-59	ALFFIVE-1-Ni	MOF	[177]	258	s1	0.1	v1	n.d.	n.d.	0.233663825	0.05	0.026746109	88.92110119	0.398061
60	M-60	Aluminum fumarate	MOF	[126]	971	s1	0.85	v1	n.d.	n.d.	0.440095924	0.15	0.011482308	844.6210082	0.789254
61	M-61	Basolite™ F300(Fe)	MOF	[187]	1600	s1	n.d.	n.d.	n.d.	n.d.	0.375684758	0.25	0.01095934	415.0791308	0.753676
62	M-62	BIT-66(V)	MOF	[238]	1417	s1	0.87	v1	25.8	d2	0.704999042	0.65	0	0	0
63	M-63	BIT-72(Al)	MOF	[164]	1618	s1	0.59	v1	6.2	d2	0.52676009	0.55	0.000185884	104.975028	0.58272
64	M-64	BIT-73(Al)	MOF	[164]	1511	s1	0.56	v1	6.6	d2	0.467808602	0.55	2.17E-05	38.64130744	0.359655
65	M-65	BIT-74(Al)	MOF	[164]	1394	s1	0.51	v1	5.7	d2	0.577498058	0.95	2.27E-05	46.18274622	0.381472
66	M-66	Blucher-101408	MOF	[107]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.741298882	0.75	1.51E-19	0.00126029	1.94E-05
67	M-67	Bu-FeCr	MOF	[112]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.043051862	0.75	0.000991085	32.27076728	0.316541
68	M-68	BUT-155(Cu)	MOF	[158]	2070	s1	0.82	v1	16	d3	0.429609977	0.25	0.015935927	660.4018117	0.790437
69	M-69	BUT-46A(Zr)	MOF	[159]	1550	s1	0.69	v1	16	d2	0.503352285	0.45	0.004052011	93.5754297	0.542443
70	M-70	BUT-46B(Zr)	MOF	[159]	1403	s1	0.65	v1	16	d2	0.484661122	0.55	0.001699436	71.17081725	0.490843
71	M-71	BUT-46F(Zr)	MOF	[159]	1563	s1	0.71	v1	16	d2	0.574709137	0.45	4.46E-05	72.08761696	0.495827
72	M-72	BUT-46W(Zr)	MOF	[159]	1565	s1	0.71	v1	16	d2	0.599537928	0.35	0.007436412	370.9997729	0.755631
73	M-73	C10H4O12Eu2	MOF	[91]	n.d.	n.d.	n.d.	n.d.	5	d2	0.098132796	0.05	0.00844423	124.1585886	0.569333
74	M-74	C115.5H202N14O43Zn4	MOF	[92]	n.d.	n.d.	n.d.	n.d.	13	d3	0.088442571	0.15	0.001494187	83.90308156	0.51963

75	M-75	C11H15BrN2O4Zn	MOF	[73]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.061531331	0.05	0.004376032	57.2374011	0.423612
76	M-76	C11H15ClN2O4Zn	MOF	[73]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.133025064	0.45	0.001337287	64.58007002	0.465153
77	M-77	C12H17ClN2O3Cd	MOF	[52]	n.d.	n.d.	n.d.	n.d.	9.8	d3	0.419649263	0.85	1.84E-07	5.708314941	0.080407
78	M-78	C15H27N2O10Dy	MOF	[54]	n.d.	n.d.	n.d.	n.d.	10.4	d3	0.111030943	0.05	0.007780646	210.8278398	0.652504
79	M-79	C15H27N2O10Er	MOF	[54]	n.d.	n.d.	n.d.	n.d.	10.4	d3	0.149247219	0.15	0.003833682	199.3886719	0.639189
80	M-80	C15H27N2O10Ho	MOF	[54]	n.d.	n.d.	n.d.	n.d.	10.4	d3	0.1046435	0.05	0.006562572	197.7588699	0.639269
81	M-81	C15H27N2O10Tb	MOF	[54]	n.d.	n.d.	n.d.	n.d.	10.4	d3	0.104723288	0.05	0.015105402	203.4483648	0.631472
82	M-82	C15H27N2O10Tm	MOF	[54]	n.d.	n.d.	n.d.	n.d.	10.4	d3	0.116477282	0.15	0.004104866	171.6248229	0.640156
83	M-83	C18H21Br2N4O9Cd2	MOF	[52]	n.d.	n.d.	n.d.	n.d.	12	d3	0.033449637	0.05	0.001602757	32.8162842	0.316744
84	M-84	C24H40N2O16Cl2Cd3	MOF	[38]	n.d.	n.d.	0.07	v1	8.4	d3	0.087344716	0.05	0.0096956	122.9032834	0.565323
85	M-85	C26H24Br2Cu2N8O3	MOF	[102]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.075072844	0.05	0.015360811	77.72244428	0.442243
86	M-86	C28H24CoN10	MOF	[94]	137	s1	n.d.	n.d.	6	d2	0.076316731	0.85	0.002686532	50.31384925	0.407484
87	M-87	C32H24Cu3N6O12	MOF	[13]	445	s1	n.d.	n.d.	9.8	d3	0.180298956	0.15	0.011385625	302.4159028	0.696246
88	M-88	C32H46N4O8Zn	MOF	[101]	n.d.	n.d.	n.d.	n.d.	7.21	d2	0.006018712	0.65	0.000134851	4.409979568	0.062953
89	M-89	C4H8HoKO12 Dehydrated	MOF	[55]	69.1	s2	0.1042	v1	3.6	d3	0.187247233	0.05	0.078178121	280.0398751	0.623073
90	M-90	C55H52Fe4N20O18	MOF	[33]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.101850663	0.05	0.038169416	154.8574297	0.588597
91	M-91	C62H44N2O8Zn2	MOF	[58]	960	s1	0.43	v1	10.5	d2	0.279552409	0.95	0.000227962	70.21550206	0.478647
92	M-92	C62H50Cd3K2N2O26	MOF	[106]	8.27	s1	n.d.	n.d.	12.7	d2	0.145102154	0.05	0.004364069	161.8883029	0.635714
93	M-93	C9H11ClN2O4Cd	MOF	[52]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.094968809	0.05	0.00428737	187.9388568	0.641538
94	M-94	CALF-25	MOF	[74]	385	s1	n.d.	n.d.	4.6	d2	0.072361431	0.75	0.001088709	39.07052038	0.357576
95	M-95	CAU-1(AI)-(OH)2	MOF	[205]	n.d.	n.d.	0.5	v1	n.d.	n.d.	0.310128925	0.35	0.008928379	190.1852621	0.656108
96	M-96	CAU-1(AI)-NH2	MOF	[189]	1530	s1	0.64	v1	n.d.	n.d.	0.376915556	0.45	0.001787251	28.61109453	0.288509
97	M-97	CAU-1(AI)-NHCH3	MOF	[189]	1340	s1	0.53	v1	n.d.	n.d.	0.511944778	0.35	0.002603728	150.9910586	0.637406
98	M-98	CAU-1(AI)-NHCOCH3	MOF	[189]	680	s1	0.3	v1	n.d.	n.d.	0.242910944	0.35	0.009655912	254.7433161	0.697165
99	M-99	CAU-10-CH3	MOF	[112]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.180798213	0.45	0.00362674	51.16807952	0.410392
100	M-100	CAU-10-H	MOF	[112]	600	s1	0.26	v1	7	d2	0.379872893	0.15	0.001643033	721.4898298	0.674541
101	M-101	CAU-10-NH2	MOF	[112]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.226554684	0.05	0.017249242	355.0448259	0.701687
102	M-102	CAU-10-NO2	MOF	[112]	440	s1	0.18	v1	n.d.	n.d.	0.174018131	0.35	1.08E-05	109.4997264	0.580612
103	M-103	CAU-10-OCH3	MOF	[112]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.08764921	0.25	0.000678289	187.4066947	0.672536
104	M-104	CAU-10-OH	MOF	[112]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.295797726	0.15	0.006996717	553.0821416	0.771535
105	M-105	CAU-10-pydc	MOF	[2]	926	s1	0.43	v1	n.d.	n.d.	0.389492976	0.05	0.028410281	741.5351953	0.750945
106	M-106	CAU-13	MOF	[63]	380	s1	0.15	v1	n.d.	n.d.	0.137490639	0.25	0.001513944	243.239401	0.707645
107	M-107	CAU-1-NH2	MOF	[98]	1530	s1	0.64	v2	n.d.	n.d.	0.391083518	0.45	0.001922594	56.09412936	0.435188
108	M-108	CAU-1-NHCH3	MOF	[98]	1340	s1	0.53	v1	n.d.	n.d.	0.698688689	0.35	0.005191766	84.00343164	0.508946
109	M-109	CAU-1-NHCOCH3	MOF	[98]	680	s1	0.3	v2	n.d.	n.d.	0.251244285	0.25	0.00609345	250.1433779	0.693255
110	M-110	CAU-23	MOF	[131]	1250	s1	n.d.	n.d.	7.6	d1	0.407314336	0.25	0.000708567	696.2947146	0.81822
111	M-111	CAU-3(AI)	MOF	[191]	1550	s1	0.64	v1	27	d3	0.493741224	0.65	0.001951062	100.1215015	0.567208
112	M-112	CAU-3(AI)-NH2	MOF	[191]	1250	s1	0.53	v1	n.d.	n.d.	0.521111149	0.65	0.003985377	198.7946441	0.688933
113	M-113	CAU-6(AI)	MOF	[203]	620	s1	0.25	v1	10	d3	0.358975538	0.05	0.029889773	271.5210072	0.620676
114	M-114	CAU-8(AI)	MOF	[205]	n.d.	n.d.	0.25	v1	n.d.	n.d.	0.158483704	0.35	0.000224092	84.21774925	0.489641
115	M-115	Cd (II)-MOF [Cd(L)(DMF)]	MOF	[113]	231.31	s1	n.d.	n.d.	6	d2	0.141478998	0.05	0.016454304	167.1307411	0.609184
116	M-116	Cd(BTTB)	MOF	[212]	415	s1	0.19	v1	5.41	d1	0.242901624	0.55	0.009116248	166.5491619	0.638305
117	M-117	Cd2(sdb)2(pcih)2	MOF	[172]	n.d.	n.d.	0.22	v1	4.4	d2	0.1789279	0.25	0.000656838	302.8577775	0.737085

118	M-118	Cd3L2	MOF	[220]	417	s1	n.d.	n.d.	8	d3	0.118513324	0.05	0.008351457	80.30956068	0.478567
119	M-119	CID-3	MOF	[90]	n.d.	n.d.	n.d.	n.d.	8.1	d2	0.097374879	0.55	7.53E-07	7.520685862	0.10268
120	M-120	Co(BTTB)(AZPY)	MOF	[212]	805	s1	0.39	v1	4.94	d1	0.207403947	0.55	0.00027953	31.96160392	0.318211
121	M-121	Co(BTTB)(BPY)	MOF	[212]	843	s1	0.4	v1	4.06	d1	0.025354391	0.85	3.93E-05	6.135896265	0.085535
122	M-122	Co(BTTB)(DMBPY)	MOF	[201]	809	s1	0.29	v1	4.41	d1	0.1969837	0.85	6.34E-05	17.26904522	0.206065
123	M-123	Co2Cl2(BTDD)	MOF	[132]	1912	s1	n.d.	n.d.	22	d1	0.940151904	0.25	0.02067297	394.7013481	0.740726
124	M-124	Co2Cl2BBTA	MOF	[195]	n.d.	n.d.	n.d.	n.d.	13	d3	0.420166302	0.05	0.046623597	334.2649349	0.619611
125	M-125	Cobalt Triazolyl Phosphonate MOF	MOF	[116]	n.d.	n.d.	n.d.	n.d.	13	d2	0.196582842	0.05	0.007390575	387.8221934	0.719557
126	M-126	Cobalt Triazolyl Phosphonate MOF (95%RH)	MOF	[116]	n.d.	n.d.	n.d.	n.d.	13	d2	0.245199239	0.05	0.005260183	346.3998946	0.692578
127	M-127	Cobalt Triazolyl Phosphonate MOF (Activated at 403K)	MOF	[116]	n.d.	n.d.	n.d.	n.d.	13	d2	0.358866014	0.05	0.010019359	339.4228543	0.741293
128	M-128	Co-CUK-1	MOF	[130]	510	s1	0.26	v1	13.4	d1	0.298331923	0.15	0.001781923	659.3493398	0.772757
129	M-129	Co-MOF-74(M)	MOF	[27]	1314	s1	0.51	v1	12	d2	0.766850514	0.05	0.123083147	719.3156332	0.678394
130	M-130	Co-MOF-74(S)	MOF	[27]	1327	s1	0.52	v1	12	d2	0.970422594	0.05	0.19466153	1044.147082	0.702799
131	M-131	CoNIm	MOF	[228]	1858	s2	n.d.	n.d.	22	d3	0.135527089	0.55	0.001629634	62.47238286	0.461862
132	M-132	CPO-27-Ni	MOF	[100]	n.d.	n.d.	n.d.	n.d.	11	d2	0.527958385	0.05	0.057233196	369.9022978	0.596592
133	M-133	Cr3(BTC)2	MOF	[163]	1330	s1	n.d.	n.d.	n.d.	n.d.	0.432000606	0.15	0.02221205	781.2631847	0.781152
134	M-134	Cr-MIL(101)	MOF	[112]	3124	s1	1.58	v1	34	d2	1.339038707	0.45	0.000621212	342.5308983	0.760114
135	M-135	Cr-MIL-101-NO2	MOF	[112]	2146	s1	1.19	v1	34	d2	0.753398389	0.45	0.006618339	142.7775207	0.62335
136	M-136	Cr-soc-MOF-1	MOF	[173]	4549	s1	2.1	v1	17	d3	1.929962287	0.65	-6.08E-18	7.88143E-06	1.08E-07
137	M-137	Cu(mtpm)Cl2	MOF	[235]	n.d.	n.d.	n.d.	n.d.	8	d3	0.027910947	0.05	0.002139203	24.77237221	0.256409
138	M-138	Cu2(dmcapz)2	MOF	[219]	539	s1	0.227	v1	9.7	d3	0.221848832	0.35	0.002795129	35.67145895	0.325593
139	M-139	Cu2(pzdc)2bpe	MOF	[30]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.210505749	0.05	0.021809068	357.8961819	0.687506
140	M-140	Cu2Cl2BBTA	MOF	[195]	n.d.	n.d.	n.d.	n.d.	13	d3	0.341944558	0.05	0.078677512	304.5282629	0.62508
141	M-141	Cu6(Trz)10(H2O)4[H2SiW12O40]·8H2O	MOF	[124]	n.d.	n.d.	n.d.	n.d.	5.65	d1	0.092744533	0.85	0.000657997	84.48507112	0.52653
142	M-142	CuBTC	MOF	[11]	1507	s1	n.d.	n.d.	n.d.	n.d.	0.525287501	0.05	0.026023397	586.7583512	0.741763
143	M-143	CuEBTC	MOF	[192]	1434	s1	0.65	v1	9	d3	0.188646382	0.05	0.020566787	263.4772354	0.67541
144	M-144	CuMBTC	MOF	[192]	1471	s1	0.79	v1	9	d3	0.189056047	0.45	0.013618273	186.2139304	0.637249
145	M-145	Cu-MOF	MOF	[85]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.069570294	0.05	0.00449114	24.46800139	0.214536
146	M-146	Cu-Tria	MOF	[243]	188	s1	n.d.	n.d.	n.d.	n.d.	0.189956067	0.05	0.018556048	134.4517953	0.507672
147	M-147	DETA-MIL-101	MOF	[97]	1560	s1	1.1	v1	n.d.	n.d.	0.105642838	0.05	0.00648769	52.24933351	0.395748
148	M-148	DMOF	MOF	[64]	1960	s1	0.58	v1	7.5	d3	0.094164738	0.25	2.42E-06	123.3603331	0.602449
149	M-149	DMOF(Zn)-A	MOF	[83]	760	s1	0.33	v1	4.8	d1	0.292402997	0.25	8.97E-05	248.3684541	0.719762
150	M-150	DMOF(Zn)-Br	MOF	[83]	1315	s1	0.53	v1	5	d1	0.056451417	0.05	0.002547972	64.70821965	0.460136
151	M-151	DMOF(Zn)-N	MOF	[83]	1420	s1	0.57	v1	5.7	d1	0.021773607	0.05	0.000480639	26.28742886	0.267752
152	M-152	DMOF(Zn)-NH3	MOF	[64]	2010	s1	0.58	v1	7.5	d3	0.112754557	0.05	0.004454562	112.9839806	0.571517
153	M-153	DMOF-Cl2	MOF	[83]	1175	s1	0.45	v1	3.8	d2	0.073706417	0.35	0.000198323	25.46447003	0.271684
154	M-154	DMOF-NO2	MOF	[83]	1310	s1	0.53	v1	6.2	d2	0.129395754	0.45	0.006055571	61.02883856	0.434332
155	M-155	DMOF-OH	MOF	[83]	1130	s1	0.54	v1	7.5	d2	0.057281764	0.15	0.001124812	74.03798631	0.492034
156	M-156	DMOF-TM(Co)	MOF	[201]	1052	s1	0.49	v1	3.5	d1	0.369453451	0.35	0.001491607	83.61835257	0.521703
157	M-157	DMOF-TM(Cu)	MOF	[201]	1041	s1	0.46	v1	3.5	d1	0.383206667	0.55	0.000291137	57.36511394	0.445332
158	M-158	DMOF-TM(Ni)	MOF	[201]	1095	s1	0.48	v1	3.5	d1	0.362781316	0.45	0.000438275	73.3302995	0.497794
159	M-159	DMOF-TM1(Zn)	MOF	[196]	1210	s1	0.53	v1	7.5	d3	0.272351339	0.45	1.74E-05	94.83029402	0.554382
160	M-160	DMOF-TM2(Zn)	MOF	[196]	1050	s1	0.51	v1	3.5	d3	0.414926163	0.25	8.83E-09	697.6739125	0.828863

161	M-161	DUT-10(Zn)	MOF	[18]	423	s1	n.d.	n.d.	n.d.	n.d.	0.446058142	0.95	9.72E-07	22.55451977	0.252539
162	M-162	DUT-4	MOF	[41]	1360	s1	0.79	v1	8.5	d3	0.672343272	0.95	0.000823923	15.70506832	0.189898
163	M-163	DUT-51(Zr)	MOF	[190]	2106	s1	1.08	v1	18.8	d3	0.547636507	0.65	1.21E-05	43.06143018	0.384251
164	M-164	DUT-52(Zr)	MOF	[216]	1399	s1	0.54	v1	8.59	d3	0.28067997	0.35	0.001357	119.0378562	0.600199
165	M-165	DUT-53(Hf)	MOF	[216]	1097	s1	0.31	v1	11.23	d3	0.199288625	0.35	0.000163768	57.93356849	0.44657
166	M-166	DUT-67	MOF	[75]	1560	s1	0.6	v1	16.6	d2	0.505598453	0.25	0.018507217	672.0653808	0.792777
167	M-167	DUT-67(Hf)	MOF	[162]	810	s1	0.33	v1	14.2	d3	0.280350685	0.35	0.003129004	221.4389629	0.692896
168	M-168	DUT-68(Hf)	MOF	[162]	749	s1	0.34	v1	27.7	d3	0.275935938	0.45	0.004302448	239.4854195	0.700934
169	M-169	DUT-68(Zr)	MOF	[162]	891	s1	0.41	v1	27.7	d3	0.342093711	0.45	0.005221806	289.0388968	0.726155
170	M-170	DUT-69(Hf)	MOF	[162]	450	s1	0.22	v1	5	d3	0.184688473	0.05	0.006924653	228.7773881	0.687758
171	M-171	DUT-69(Zr)	MOF	[162]	560	s1	0.31	v1	5	d3	0.221022976	0.15	0.004700978	259.8788597	0.716532
172	M-172	DUT-84(Zr)	MOF	[216]	637	s1	0.27	v1	11.14	d3	0.125666464	0.25	0.000950547	111.6348964	0.583
173	M-173	ED-ZIF-8	MOF	[3]	1428	s1	0.75	v1	45.3	d2	0.00319995	0.45	3.79E-06	2.557843662	0.037669
174	M-174	Et-MnCr	MOF	[112]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.101799909	0.25	0.000333063	117.4037656	0.594017
175	M-175	FeFFIVE-1-Ni	MOF	[177]	324	s1	0.13	v1	n.d.	n.d.	0.257916281	0.05	0.022228266	200.8358409	0.564867
176	M-176	HKUST-1-F	MOF	[11]	1404	s1	n.d.	n.d.	n.d.	n.d.	1.001541909	0.95	0.038725709	441.1414588	0.755847
177	M-177	HV-MOF-1(Er)	MOF	[231]	165	s2	n.d.	n.d.	24	d3	0.097572329	0.15	0.002384043	95.28692971	0.544049
178	M-178	IPM-MOF-201(Ni)	MOF	[160]	n.d.	n.d.	n.d.	n.d.	12.78	d3	0.201533186	0.05	0.009351735	181.436369	0.652963
179	M-179	ISE-1(Ni)	MOF	[211]	n.d.	n.d.	0.51	v1	n.d.	n.d.	0.143610089	0.05	0.016553794	206.9903153	0.633611
180	M-180	JUC-110	MOF	[96]	n.d.	n.d.	n.d.	n.d.	4.5	d3	0.098132796	0.05	0.00844423	124.1585886	0.569333
181	M-181	JUK-8(Zn)	MOF	[239]	n.d.	n.d.	0.256	v1	n.d.	n.d.	0.242198111	0.55	0.006677376	75.12669829	0.46169
182	M-182	kag-MOF-1(Zn)	MOF	[170]	210	s1	0.12	v1	4.6	d2	0.119362769	0.05	0.017474965	219.7146197	0.640487
183	M-183	KMF-1(Al)	MOF	[240]	1130	s1	0.473	v1	6	d1	0.433044779	0.15	0.00776528	954.9207482	0.790149
184	M-184	La(pyzdc)L5	MOF	[236]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.018265018	0.15	0.000388575	19.58521693	0.223622
185	M-185	LA ¹ -Zr6 ⁸ -shp	MOF	[182]	2486	s1	0.94	v1	n.d.	n.d.	0.351302766	0.55	0.009852715	184.4959473	0.659784
186	M-186	LA ¹ -Zr6 ⁸ -csq	MOF	[182]	3150	s1	2.18	v1	47	d3	0.384279556	0.65	0.002897549	42.98577117	0.373423
187	M-187	LA ¹ -Zr6 ⁸ -flu	MOF	[182]	2850	s1	1.31	v1	38.6	d3	0.198209087	0.75	0.000996825	60.29242151	0.456328
188	M-188	LA ² -Zr6 ⁸ -shp	MOF	[182]	2250	s1	0.89	v1	n.d.	n.d.	1.005080877	0.65	0.018805314	403.9030564	0.759292
189	M-189	LA ² -Zr6 ⁸ -csq	MOF	[182]	n.d.	n.d.	2	v1	47	d3	1.449597515	0.75	0.003704031	192.9619343	0.693791
190	M-190	LA ³ -Zr6 ⁸ -flu	MOF	[182]	2950	s1	1.01	v1	n.d.	n.d.	0.745239108	0.75	0.001110195	183.036369	0.6854
191	M-191	Lanthanum Triazolyl Phosphonate MOF	MOF	[116]	n.d.	n.d.	n.d.	n.d.	19	d2	0.274052974	0.25	0.00782489	527.0717077	0.780758
192	M-192	LB ¹ -Zr6 ⁸ -flu	MOF	[182]	2450	s1	0.94	v1	n.d.	n.d.	0.199008226	0.55	0.002539228	13.46820074	0.162707
193	M-193	LB ² -Zr6 ⁸ -csq	MOF	[182]	n.d.	n.d.	1.41	v1	n.d.	n.d.	1.298983642	0.65	0.004447036	204.5770852	0.695957
194	M-194	LB ² -Zr6 ⁸ -scu	MOF	[182]	n.d.	n.d.	0.96	v1	n.d.	n.d.	0.751842036	0.65	0.021613987	294.9654987	0.715589
195	M-195	LB ³ -Zr6 ⁸ -flu	MOF	[182]	2542	s1	0.9	v1	n.d.	n.d.	0.720352848	0.55	0.009459818	95.72159088	0.520056
196	M-196	LC ¹ -Zr6 ¹² -fcu	MOF	[182]	n.d.	n.d.	0.92	v1	34.5	d3	0.323389425	0.45	0.002214991	55.08762301	0.430904
197	M-197	LC ² -Zr6 ¹² -fcu	MOF	[182]	2105	s1	0.61	v1	n.d.	n.d.	0.428422204	0.45	0.002186347	49.13060003	0.405293
198	M-198	LC ³ -Zr6 ⁸ -bcu	MOF	[182]	n.d.	n.d.	0.54	v1	n.d.	n.d.	0.278320185	0.55	0.000946916	104.0551203	0.572245
199	M-199	MAF-4.23-7.77	MOF	[197]	1870	s1	0.64	v1	11	d3	0.447340455	0.45	6.05E-09	14.15835417	0.175577
200	M-200	MAF-4.49-7.51	MOF	[197]	1870	s1	0.65	v1	11	d3	0.431208293	0.65	4.84E-11	1.635449317	0.02447
201	M-201	MAF-4.76-7.24	MOF	[197]	1870	s1	0.64	v1	11	d3	0.393276192	0.85	7.08E-19	0.000692219	1.06E-05
202	M-202	MAF-7(Zn)	MOF	[197]	1874	s1	0.67	v1	11.2	d3	0.434546172	0.35	0.000184945	120.4967732	0.598557
203	M-203	Me-FeCr	MOF	[112]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.212827269	0.55	0.002907439	50.93160935	0.40949

204	M-204	MFU-4	MOF	[89]	1611	s2	0.42	v2	n.d.	n.d.	0.431395604	0.15	0.002873624	727.587416	0.803644
205	M-205	Mg-CPO-27	MOF	[112]	1400	s1	0.65	v1	11	d2	0.637303559	0.05	0.040571103	385.2081257	0.543273
206	M-206	Mg-CUK-1	MOF	[130]	580	s1	0.28	v1	13.4	d1	0.363863092	0.25	2.82E-05	651.7679263	0.80893
207	M-207	Mg-MOF-74©	MOF	[95]	1525	s1	0.62	v1	11	d2	0.662247648	0.05	0.106317381	468.0017962	0.621697
208	M-208	MIL-100	MOF	[37]	1600	s1	n.d.	n.d.	n.d.	n.d.	0.365317629	0.25	0.005779545	376.6774509	0.754769
209	M-209	MIL-100(Al)	MOF	[178]	1786	s1	n.d.	n.d.	n.d.	n.d.	0.658446269	0.45	0.017986044	416.9656052	0.754424
210	M-210	MIL-100(Cr)	MOF	[50]	1871	s1	1.02	v1	29	d2	0.708954908	0.65	0.013727033	261.9154981	0.715029
211	M-211	MIL-100(Cr)(X=Cl)	MOF	[179]	1522	s1	0.7	v1	n.d.	n.d.	0.599268672	0.35	0.02222327	526.9740731	0.76766
212	M-212	MIL-100(Cr)(X=SO4)	MOF	[179]	1452	s1	0.7	v1	n.d.	n.d.	0.607772954	0.25	0.020658407	627.0892687	0.776529
213	M-213	MIL-100(Cr)-DEG	MOF	[34]	580	s1	0.5	v1	12	d2	0.560718126	0.95	0.003874057	258.989567	0.721359
214	M-214	MIL-100(Cr)-EG	MOF	[34]	710	s1	0.47	v1	12	d2	0.429676274	0.35	0.007795488	247.5506616	0.704831
215	M-215	MIL-100(Cr)-EN	MOF	[34]	640	s1	0.42	v1	15	d2	0.368280986	0.25	0.007610811	300.4707369	0.731105
216	M-216	MIL-100(Cr)-TEG	MOF	[34]	680	s1	0.53	v1	12	d2	0.33067934	0.35	0.005527477	168.8632131	0.652871
217	M-217	MIL-100(Fe)	MOF	[41]	1549	s1	0.82	v2	29	d2	0.824965936	0.35	0.050045808	495.1573266	0.774234
218	M-218	MIL-100V	MOF	[125]	1203	s1	0.74	v1	11	d1	0.151153239	0.05	0.011109941	146.2239133	0.600936
219	M-219	MIL-101(Al)-NH2	MOF	[199]	3363	s1	1.67	v1	25	d2	0.268537763	0.05	0.013253166	187.0994974	0.634269
220	M-220	MIL-101(Al)-URPh	MOF	[199]	1555	s1	0.83	v1	18	d2	0.325853744	0.05	0.014617907	259.2670519	0.696145
221	M-221	MIL-101(Cr)-pCOOH	MOF	[183]	2380	s1	1.26	v1	n.d.	n.d.	1.031695125	0.35	0.009594675	178.161549	0.650415
222	M-222	MIL-101(Cr)-pMal	MOF	[183]	1670	s1	0.89	v1	n.d.	n.d.	0.701876868	0.45	0.001526432	250.3061516	0.724302
223	M-223	MIL-101(Cr)-pUR2	MOF	[183]	1330	s1	0.64	v1	n.d.	n.d.	0.684240433	0.45	0.002653547	168.3696437	0.66371
224	M-224	MIL-101-NH2	MOF	[42]	2509	s1	1.27	v1	34	d2	1.052714347	0.35	0.000650685	156.1672883	0.652839
225	M-225	MIL-101-SO3H	MOF	[42]	1920	s1	0.94	v1	34	d2	0.745162373	0.35	0.016504721	637.35741	0.78774
226	M-226	MIL-101V	MOF	[125]	2705	s1	1.4	v1	21	d1	0.25368951	0.05	0.015633053	216.7337424	0.655796
227	M-227	MIL-125	MOF	[28]	1510	s1	0.68	v1	n.d.	n.d.	0.288950349	0.35	0.00014124	33.70686477	0.330806
228	M-228	MIL-125(Ti)-NH3 ⁺ 3+Cl-	MOF	[181]	1388	s1	0.5	v1	n.d.	n.d.	0.58048035	0.15	0.006177663	1163.163919	0.824205
229	M-229	MIL-125(Ti)-NHCyp	MOF	[169]	510	s1	n.d.	n.d.	n.d.	n.d.	0.110675333	0.15	0.002965627	123.4084975	0.591184
230	M-230	MIL-125(Ti)-NHMe	MOF	[169]	1047	s1	n.d.	n.d.	n.d.	n.d.	0.294219129	0.25	0.002839648	461.3758881	0.77633
231	M-231	MIL-125-NH2	MOF	[112]	1220	s1	0.55	v1	12	d2	0.368255172	0.15	0.005869273	765.9392798	0.794908
232	M-232	MIL-160	MOF	[2]	1070	s1	0.398	v1	5	d3	0.497065962	0.05	0.022823571	785.5035913	0.75618
233	M-233	MIL-163	MOF	[8]	170	s1	n.d.	n.d.	12	d3	0.583277316	0.55	0.008726954	220.1102004	0.69671
234	M-234	MIL-47(V)-F	MOF	[223]	1078	s1	0.36	v1	n.d.	n.d.	0.179957959	0.55	0.00124439	37.15322309	0.346872
235	M-235	MIL-47(V)-F2	MOF	[218]	987	s2	0.34	v1	n.d.	n.d.	0.175171482	0.55	2.98E-06	9.892535296	0.130471
236	M-236	MIL-53(Al)-(OH)0.34(NH2)0.66	MOF	[208]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.103620557	0.05	0.012190174	126.947947	0.553286
237	M-237	MIL-53(Al)-(OH)0.53(NH2)0.47	MOF	[208]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.209207472	0.95	0.011649567	127.1804523	0.577926
238	M-238	MIL-53(Al)-(OH)0.68(NH2)0.32	MOF	[208]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.441262358	0.85	0.0210926	174.8655031	0.616747
239	M-239	MIL-53(Al)-(OH)2	MOF	[202]	n.d.	n.d.	0.07	v1	n.d.	n.d.	0.401615004	0.05	0.016750369	135.9203296	0.576266
240	M-240	MIL-53(Al)-Br	MOF	[202]	n.d.	n.d.	0.14	v1	n.d.	n.d.	0.103450142	0.85	0.000691525	74.58038546	0.501163
241	M-241	MIL-53(Al)-CH3	MOF	[202]	n.d.	n.d.	0.32	v1	n.d.	n.d.	0.11305649	0.15	0.00195386	144.4666307	0.621864
242	M-242	MIL-53(Al)-Cl	MOF	[202]	n.d.	n.d.	0.32	v1	n.d.	n.d.	0.136663898	0.05	0.005048064	175.535755	0.645652
243	M-243	MIL-53(Al)-F	MOF	[223]	1137	s1	0.48	v1	n.d.	n.d.	0.06432521	0.85	0.000476907	5.820082364	0.081204
244	M-244	MIL-53(Al)-F2	MOF	[218]	467	s2	0.16	v1	n.d.	n.d.	0.234427734	0.55	5.99E-11	1.133443664	0.017103
245	M-245	MIL-53(Al)ht	MOF	[105]	1489	s1	0.56	v1	8.5	d2	0.082386233	0.15	0.000120408	180.7882354	0.64292
246	M-246	MIL-53(Al)it	MOF	[105]	1031	s1	0.72	v1	34	d2	0.169374264	0.65	0.000343061	61.12676919	0.459948

247	M-247	MIL-53(Al)-NH ₂	MOF	[176]	940	s1	0.37	v1	13	d3	0.084718069	0.05	0.017301746	96.58332732	0.497821
248	M-248	MIL-53(Al)-NO ₂	MOF	[202]	n.d.	n.d.	0.34	v1	n.d.	n.d.	0.122392945	0.05	0.016223691	155.2897837	0.602883
249	M-249	MIL-53(Al)-OH	MOF	[175]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.390637719	0.85	0.013033841	195.4223901	0.666354
250	M-250	MIL-53(Al)-TDC	MOF	[194]	1150	s1	0.48	v1	8.2	d3	0.535170719	0.35	0.001052167	120.215751	0.600785
251	M-251	MIL-53(Cr)	MOF	[68]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.326575715	0.95	0.000107455	208.1859909	0.724336
252	M-252	MIL-53(Fe)-(COOH) ₂	MOF	[175]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.1479941	0.05	0.01606069	125.905817	0.551948
253	M-253	MIL-53(Ga)	MOF	[176]	1230	s1	0.47	v1	20	d3	0.062017173	0.05	0.006416549	39.04264063	0.315881
254	M-254	MIL-53(Ga)-NH ₂	MOF	[176]	210	s1	n.d.	n.d.	20	d3	0.171047963	0.05	0.008667994	91.26476175	0.515177
255	M-255	MIL-68(In)	MOF	[176]	1110	s1	0.42	v1	16	d3	0.30008142	0.55	1.33E-09	0.358164907	0.005475
256	M-256	MIL-68(In)-NH ₂	MOF	[176]	850	s1	0.3	v1	16	d3	0.332353762	0.45	5.31E-05	43.5901619	0.384085
257	M-257	MIL-91(Ti)	MOF	[217]	403	s1	0.16	v1	4	d3	0.209607405	0.05	0.013831509	138.459618	0.51613
258	M-258	MIP-200	MOF	[129]	1000	s1	0.4	v1	13	d1	0.424401855	0.15	0.018988887	740.3292455	0.762049
259	M-259	Mn ₂ (Gd-H-DOTA-4AmP)(H ₂ O) ₇	MOF	[204]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.280110766	0.05	0.01528369	317.1163332	0.720073
260	M-260	Mn ₂ Cl ₂ (BTDD)	MOF	[132]	n.d.	n.d.	n.d.	n.d.	22	d1	0.360882982	0.05	0.01885729	381.7181369	0.740529
261	M-261	MOF-1(Ce,Eu)	MOF	[233]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.062526094	0.05	0.003599382	35.13815773	0.325561
262	M-262	MOF-303(Al)	MOF	[157]	1119	s1	0.58	v1	n.d.	n.d.	0.427711981	0.15	0.02196392	838.1722224	0.771215
263	M-263	MOF-74(Ni)-BPP	MOF	[186]	n.d.	n.d.	0.88	v1	17	d2	0.733469402	0.25	0.033654197	1224.028801	0.813555
264	M-264	MOF-74(Ni)-TPP	MOF	[186]	n.d.	n.d.	1.14	v1	23	d2	0.891860901	0.55	0.029286854	232.8770426	0.664676
265	M-265	MOS-1(Co)	MOF	[171]	1112	s1	n.d.	n.d.	13.9	d3	0.315436918	0.05	0.049592169	530.1423733	0.724976
266	M-266	MOS-2(Co)	MOF	[171]	76	s1	n.d.	n.d.	7.6	d3	0.144877543	0.05	0.017666396	196.1439553	0.633992
267	M-267	MOS-3(Co)	MOF	[171]	27	s1	n.d.	n.d.	7.5	d3	0.130331485	0.05	0.014951392	158.0908908	0.60755
268	M-268	MUF-77(Zn)-butyl	MOF	[215]	3250	s1	1.21	v1	13.6	d2	0.22697701	0.85	1.51E-70	9.96158E-22	1.53E-23
269	M-269	MUF-77(Zn)-decyl	MOF	[215]	1170	s1	0.48	v1	n.d.	n.d.	0.140885942	0.95	2.16E-06	1.807600536	0.027001
270	M-270	MUF-77(Zn)-ethyl	MOF	[215]	3600	s1	1.55	v1	18.5	d2	0.253010792	0.85	9.54E-35	1.61E-09	2.48E-11
271	M-271	MUF-77(Zn)-hexyl	MOF	[215]	2170	s1	1	v1	11.2	d2	0.142063255	0.85	1.75E-09	0.363051074	0.005551
272	M-272	MUF-77(Zn)-methyl	MOF	[215]	3600	s1	1.85	v1	21.1	d2	0.199193613	0.75	9.17E-16	0.002158333	3.32E-05
273	M-273	MUF-77(Zn)-octyl	MOF	[215]	1570	s1	0.65	v1	n.d.	n.d.	0.10796083	0.85	1.40E-07	2.20771866	0.032774
274	M-274	MUF-7a(Zn)	MOF	[215]	4450	s1	2.16	v1	n.d.	n.d.	0.160199745	0.45	1.06E-18	0.104754255	0.001609
275	M-275	NBu ₄	MOF	[112]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.010976246	0.05	0.000341323	8.194537252	0.110064
276	M-276	NENU-11	MOF	[69]	572	s1	0.39	v1	n.d.	n.d.	0.024384263	0.15	0.001349376	52.27691461	0.406816
277	M-277	Ni(BTTB)	MOF	[212]	391	s1	0.2	v1	4.3	d1	0.011726874	0.05	0.000666446	14.42598124	0.175385
278	M-278	Ni(dpip) ₂ .5DMF	MOF	[237]	1441.6	s2	n.d.	n.d.	10	d2	0.197664336	0.25	0.002108145	218.11357	0.693512
279	M-279	Ni ₂ SZn ₇₅ -MOF-74	MOF	[188]	1160	s1	n.d.	n.d.	n.d.	n.d.	0.515249846	0.15	0.029444318	1077.480297	0.782353
280	M-280	Ni ₂ Cl ₂ (BTDD)	MOF	[132]	1762	s1	n.d.	n.d.	22	d1	0.735604073	0.35	0.018294763	342.6475701	0.727413
281	M-281	Ni ₂ Cl ₂ BBTA	MOF	[195]	n.d.	n.d.	n.d.	n.d.	13	d3	0.403991923	0.05	0.037662587	348.3243835	0.639495
282	M-282	Ni ₃ C ₈ H ₁₁ N ₁₈ O ₂₉	MOF	[56]	n.d.	n.d.	0.68	v1	16	d2	0.255224043	0.15	0.004646201	213.2775156	0.692518
283	M-283	Ni ₅₀ Zn ₅₀ -MOF-74	MOF	[188]	1190	s1	n.d.	n.d.	n.d.	n.d.	0.534689238	0.05	0.033994188	1117.262464	0.77231
284	M-284	Ni ₇₅ Zn ₂₅ -MOF-74	MOF	[188]	1200	s1	n.d.	n.d.	n.d.	n.d.	0.558835134	0.15	0.023377778	1161.846223	0.790105
285	M-285	Ni ₈ (L1) ₆	MOF	[6]	205	s1	0.52	v1	n.d.	n.d.	0.40056716	0.95	0.016535198	266.7627015	0.714806
286	M-286	Ni ₈ (L2) ₆	MOF	[6]	990	s1	0.52	v1	n.d.	n.d.	0.606961946	0.95	0.001137476	231.9240613	0.720997
287	M-287	Ni ₈ (L3) ₆	MOF	[6]	1770	s1	1.21	v1	n.d.	n.d.	0.927167251	0.45	0.004850478	58.01875029	0.43524
288	M-288	Ni ₈ (L4) ₆	MOF	[6]	1920	s1	0.97	v1	n.d.	n.d.	0.878911391	0.45	1.27E-05	50.74636807	0.420877
289	M-289	Ni ₈ (L5-(CF ₃) ₂) ₆	MOF	[6]	2195	s1	n.d.	n.d.	n.d.	n.d.	0.851119016	0.85	0.000427627	52.32601802	0.429101

290	M-290	NI8(L5-(CH3)2)6	MOF	[6]	1985	s1	n.d.	n.d.	n.d.	n.d.	0.636497655	0.75	0.000417473	65.08192028	0.478136
291	M-291	Ni-CUK-1	MOF	[130]	520	s1	0.26	v1	13.4	d1	0.308395558	0.15	0.001274309	667.3326275	0.777564
292	M-292	Ni-DOBDC	MOF	[81]	639	s1	0.362	v1	11	d2	0.699551835	0.05	0.064024574	308.2504254	0.581344
293	M-293	Ni-MOF	MOF	[198]	1960	s1	0.71	v1	n.d.	n.d.	0.449166682	0.35	0.002833942	182.9383077	0.671073
294	M-294	NU-1000(Zr)	MOF	[185]	2320	s1	1.4	v1	31	d2	1.372340473	0.95	6.79E-08	11.9812527	0.148279
295	M-295	NU-1000(Zr)-SALI-1	MOF	[185]	1710	s1	1	v1	30	d2	0.865541944	0.85	0.000432018	163.0544263	0.668355
296	M-296	NU-1000(Zr)-SALI-7	MOF	[185]	900	s1	0.6	v1	28	d2	0.457813455	0.85	2.36E-05	87.35618259	0.542306
297	M-297	NU-1000(Zr)-SALI-9	MOF	[185]	870	s1	0.6	v1	28	d2	0.360910484	0.85	0.000445225	65.39769937	0.478563
298	M-298	NU-1000(Zr)-TFA	MOF	[241]	1880	s1	n.d.	n.d.	31	d3	1.276977692	0.65	0.004628426	169.0447211	0.665899
299	M-299	NU-901(Zr)-TFA	MOF	[241]	1980	s1	n.d.	n.d.	11	d3	0.563326647	0.55	0.003487522	116.5683284	0.592184
300	M-300	NU-905(Zr)-TFA	MOF	[241]	2055	s1	n.d.	n.d.	20	d3	0.727495102	0.45	3.04E-05	73.74400379	0.501098
301	M-301	PCP-1(La)	MOF	[165]	n.d.	n.d.	0.1218	v1	n.d.	n.d.	0.098090909	0.65	0.001527379	63.8798226	0.463227
302	M-302	Pip-CPO-27-Ni	MOF	[100]	46.7	s1	n.d.	n.d.	n.d.	n.d.	0.283069114	0.05	0.023520852	213.2309208	0.563202
303	M-303	PIZOF-2	MOF	[75]	2080	s1	0.88	v1	17.6	d2	0.690592468	0.75	1.09E-55	3.66366E-15	5.64E-17
304	M-304	pretreated a-Al	MOF	[114]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.007948468	0.15	0.000209154	15.28612377	0.184089
305	M-305	pretreated m-Al	MOF	[114]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.007442734	0.15	0.000348414	12.80169428	0.159792
306	M-306	SALI-5(Zr)	MOF	[180]	1270	s1	0.85	v1	29	d2	0.707883074	0.85	0.000211074	105.07945	0.585803
307	M-307	SALI-9(Zr)	MOF	[180]	900	s1	0.63	v1	27.5	d2	0.409866405	0.85	3.14E-05	49.72577109	0.417965
308	M-308	SALI-9'(Zr)	MOF	[180]	1190	s1	0.87	v1	29.6	d2	0.758279452	0.85	9.09E-10	2.063701248	0.030625
309	M-309	SALI-BA(Zr)	MOF	[180]	2005	s1	1.21	v1	27.8	d2	0.984661111	0.85	2.05E-06	34.24522391	0.336257
310	M-310	SIFSIX-14-Cu-i	MOF	[213]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.15525335	0.05	0.015474454	213.4524517	0.640764
311	M-311	SIFSIX-1-Cu	MOF	[213]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.150845573	0.05	0.012161796	309.6073399	0.692807
312	M-312	SIFSIX-2-Cu-i	MOF	[213]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.248879786	0.75	0.007667268	221.4568828	0.689958
313	M-313	SIFSIX-3-Ni	MOF	[213]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.161107122	0.05	0.017303676	263.7653439	0.668803
314	M-314	SIM-1	MOF	[112]	470	s1	0.23	v1	6	d2	0.131592032	0.25	0.00086942	154.9884358	0.639486
315	M-315	S-MIL-53(Al)	MOF	[40]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	1.058074498	0.85	9.14E-16	3.511118691	0.051031
316	M-316	SNU-80	MOF	[14]	456	s1	0.18	v1	7	d3	0.009373608	0.05	0.000403634	9.868657881	0.128921
317	M-317	STAM-17(Cu)-Oet	MOF	[224]	58.42	s1	n.d.	n.d.	n.d.	n.d.	0.149279745	0.05	0.08360182	291.74787	0.664821
318	M-318	TAF-1a	MOF	[16]	268.5	s1	n.d.	n.d.	4.6	d2	0.012010011	0.05	0.000711319	11.09546314	0.141545
319	M-319	ThrZnOAc	MOF	[214]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.150330381	0.25	0.000370772	296.944778	0.732054
320	M-320	Ti(pyridine-2-carboxylic acid)	MOF	[11]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.180255949	0.15	0.001169572	162.7801125	0.648136
321	M-321	TUC-110(Cd)	MOF	[230]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.09807167	0.05	0.007944081	121.8747257	0.56592
322	M-322	UiO-66	MOF	[75]	1290	s1	0.49	v1	8.4	d2	0.425506024	0.35	0.001898017	203.5160111	0.683939
323	M-323	UiO-66(Hf)-(OH)2	MOF	[167]	920	s1	0.4	v1	5.85	d2	0.284201897	0.05	0.031992992	378.2207674	0.703265
324	M-324	UiO-66(Zr)-(C2H5)2	MOF	[200]	340	s1	0.16	v1	n.d.	n.d.	0.17513366	0.95	0.000869281	84.58484969	0.527454
325	M-325	UiO-66(Zr)-(CF3)2	MOF	[200]	630	s1	0.3	v1	n.d.	n.d.	0.182363484	0.35	0.0001871	84.15112733	0.526943
326	M-326	UiO-66(Zr)-(CH3)2	MOF	[200]	790	s1	0.35	v1	n.d.	n.d.	0.27517369	0.25	0.007535298	211.9908991	0.683437
327	M-327	UiO-66(Zr)-(COOH)2	MOF	[5]	415	s1	0.21	v1	n.d.	n.d.	0.247479533	0.05	0.011545638	268.7785778	0.706726
328	M-328	UiO-66(Zr)-(OH)2	MOF	[167]	1230	s1	0.56	v1	5.85	d2	0.308956621	0.05	0.038777015	464.3982396	0.73298
329	M-329	UiO-66(Zr)-1,4-Naphthyl	MOF	[193]	757	s1	0.4	v1	n.d.	n.d.	0.287955402	0.15	0.015378566	361.650391	0.748549
330	M-330	UiO-66(Zr)-2,5-(oMe)2	MOF	[193]	868	s1	0.38	v1	n.d.	n.d.	0.466773732	0.15	0.022078061	708.4522855	0.780965
331	M-331	UiO-66(Zr)-C2F5	MOF	[200]	570	s1	0.26	v1	n.d.	n.d.	0.24060938	0.85	0.002878941	57.73430123	0.442156
332	M-332	UiO-66(Zr)-CF3	MOF	[200]	815	s1	0.36	v1	n.d.	n.d.	0.267912625	0.35	0.001239155	231.372879	0.706516

333	M-333	UiO-66(Zr)-CH3	MOF	[207]	1065	s1	0.51	v1	n.d.	n.d.	0.309088479	0.25	0.003275969	307.6785912	0.735035
334	M-334	UiO-66(Zr)-NH3 ⁺ 3+Cl-	MOF	[181]	1007	s1	0.35	v1	n.d.	n.d.	0.604925638	0.05	0.035006001	912.2861638	0.778297
335	M-335	UiO-66(Zr)-NO2	MOF	[193]	792	s1	0.42	v1	n.d.	n.d.	0.391303918	0.15	0.013732541	749.25377	0.783768
336	M-336	UiO-66(Zr ⁴⁺) with high concentration stearic acid	MOF	[47]	n.d.	n.d.	0.574	v1	6.5	d2	0.522819782	0.35	0.0191929	604.9641854	0.778948
337	M-337	UiO-66(Zr ⁴⁺) with metal/ligand ratio 6:3	MOF	[47]	n.d.	n.d.	0.45	v1	6	d2	0.420137117	0.35	0.016744609	407.4134749	0.745029
338	M-338	UiO-66D(Zr)	MOF	[200]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.333159849	0.65	0.000930261	26.20326487	0.278065
339	M-339	UiO-66D(Zr)-(CF3)2	MOF	[200]	2180	s1	0.88	v1	n.d.	n.d.	0.280177712	0.85	-1.52E-18	6.22653E-15	9.43E-17
340	M-340	UiO-66-NH2	MOF	[64]	1040	s1	0.57	v1	6	d2	0.384387735	0.15	0.020005424	753.2742416	0.774049
341	M-341	UiO-67(Zr)	MOF	[166]	2145	s1	n.d.	n.d.	n.d.	n.d.	0.284821904	0.45	0.004334139	71.81078578	0.485387
342	M-342	UiO-67(Zr)-BIPY	MOF	[166]	2385	s1	n.d.	n.d.	n.d.	n.d.	0.21045566	0.25	0.007074058	291.4848083	0.701282
343	M-343	UiO-67(Zr)-BN	MOF	[168]	1416	s1	0.548	v1	n.d.	n.d.	0.493011054	0.55	3.71E-07	38.3419324	0.359435
344	M-344	UMCM-1	MOF	[64]	6010	s1	2.41	v1	32	d2	0.26239535	0.75	0.003248938	125.8332028	0.606103
345	M-345	untreated a-Al	MOF	[114]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.003825435	0.05	0.000330135	4.861868435	0.068396
346	M-346	untreated m-Al	MOF	[114]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.009671484	0.15	0.000100468	18.37818195	0.212825
347	M-347	ValZnCl	MOF	[227]	n.d.	n.d.	n.d.	n.d.	12.2	d3	0.124495805	0.85	0.000274072	46.99103631	0.402669
348	M-348	ValZnOAc	MOF	[214]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.284637869	0.75	0.003615879	82.8577724	0.522207
349	M-349	Y-fum-fcu-MOF	MOF	[7]	691	s1	0.28	v1	8	d2	0.372250645	0.05	0.006403716	741.8168169	0.772592
350	M-350	Y-shp-MOF-5	MOF	[174]	1550	s1	0.63	v1	n.d.	n.d.	0.502225621	0.65	0.01050338	138.6355934	0.615912
351	M-351	ZIF-412(Zn)	MOF	[161]	1520	s1	n.d.	n.d.	38.1	d2	0.071961578	0.75	0.00011276	13.06847681	0.164724
352	M-352	ZIF-71(Zn)	MOF	[209]	1183	s1	0.39	v1	n.d.	n.d.	0.007619033	0.05	0.000653415	5.608540073	0.077815
353	M-353	ZIF-8	MOF	[58]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.140004414	0.95	2.55E-07	1.078235066	0.016251
354	M-354	ZIF-8_50-90_50	MOF	[155]	1350	s1	0.61	v1	n.d.	n.d.	0.373884826	0.75	0	3.58025E-13	5.42E-15
355	M-355	ZIF-8_55-71_45	MOF	[155]	630	s1	0.29	v1	n.d.	n.d.	0.014188257	0.15	0.000148019	10.74388039	0.139182
356	M-356	ZIF-8_70-90_30	MOF	[155]	1310	s1	0.61	v1	n.d.	n.d.	0.07443547	0.85	0	0	0
357	M-357	ZIF-90(Zn)	MOF	[209]	1280	s1	0.49	v1	n.d.	n.d.	0.332062752	0.35	2.85E-10	44.52722532	0.381984
358	M-358	Zn(BTTB)	MOF	[212]	447	s1	0.25	v1	4.47	d1	0.209056821	0.75	0.000301107	82.63420981	0.528013
359	M-359	Zn(BTTB)(AZPY)	MOF	[212]	647	s1	0.36	v1	4.94	d1	0.19048136	0.55	1.39E-07	12.78831989	0.16194
360	M-360	Zn(BTTB)(BDC)	MOF	[212]	441	s1	0.21	v1	4.24	d1	0.08957362	0.15	0.000750907	69.94579776	0.478739
361	M-361	Zn(BTTB)(BPY)	MOF	[212]	841	s1	0.38	v1	4.06	d1	0.252616617	0.75	2.03E-38	1.22855E-10	1.89E-12
362	M-362	Zn(BTTB)(DMBPY)	MOF	[201]	749	s1	0.27	v1	4.41	d1	0.210438246	0.85	9.17E-06	9.72448197	0.128815
363	M-363	Zn(DM)0.5(AT)	MOF	[232]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.085283941	0.05	0.018943593	112.7324539	0.550825
364	M-364	Zn(II)-MOF [Zn(HPyImDC)(DMA)]n	MOF	#N/A	185.6	s1	n.d.	n.d.	4.425	d1	0.064361385	0.05	0.004616737	52.5483783	0.398597
365	M-365	Zn(L)(tdca)*1.5DMF	MOF	[119]	n.d.	n.d.	n.d.	n.d.	6.6	d3	0.068252503	0.05	0.00365508	91.75801363	0.516871
366	M-366	Zn(NDI-H)	MOF	[110]	1460	s1	n.d.	n.d.	16	d3	0.427152275	0.45	2.61E-05	36.91795936	0.348209
367	M-367	Zn(NDI-NHEt)	MOF	[110]	1236	s1	n.d.	n.d.	n.d.	n.d.	0.29071397	0.45	2.65E-05	51.38917832	0.420916
368	M-368	Zn(NDI-SEt)	MOF	[112]	888	s1	n.d.	n.d.	16	d2	0.283435813	0.25	0.010958513	333.5540272	0.737165
369	M-369	Zn(NDI-SO2Et)	MOF	[112]	764	s1	n.d.	n.d.	16	d2	0.214493776	0.35	0.000972599	141.4450738	0.626629
370	M-370	Zn(NDI-SOEt)	MOF	[112]	927	s1	n.d.	n.d.	16	d2	0.283435813	0.25	0.010958513	333.5540272	0.737165
371	M-371	Zn(NO3)2*6H2O	MOF	[12]	n.d.	n.d.	0.17	v1	17.3	d3	0.165407999	0.05	0.024637759	316.8461966	0.681538
372	M-372	Zn2(bptc)	MOF	[225]	313	s1	0.15	v1	n.d.	n.d.	0.151899763	0.15	0.000414928	248.2029807	0.69968
373	M-373	Zn2C14N2O8H4	MOF	[66]	312.7	s1	0.146	v1	5.2	d2	0.178903355	0.15	0.000171657	269.9743786	0.711337
374	M-374	Zn2Co3(MFU-4l)	MOF	[184]	3544	s1	n.d.	n.d.	16.2	d2	1.078922814	0.45	6.59E-05	47.89550743	0.404057
375	M-375	Zn3(TCPB)2(H2O)2	MOF	[108]	284	s1	n.d.	n.d.	4.3	d2	0.080967226	0.85	0.00161864	66.16957195	0.472633

376	M-376	Zn3Co2(MFU-4l)	MOF	[184]	3037	s1	n.d.	n.d.	16.1	d2	0.933303071	0.45	0.000282771	52.24349474	0.423973
377	M-377	Zn3L2	MOF	[220]	535	s1	n.d.	n.d.	4.5	d3	0.197481147	0.45	0.004433582	64.81524624	0.454888
378	M-378	Zn4O(dmcapz)3	MOF	[72]	840	s1	0.45	v2	6	d2	0.386252684	0.85	3.28E-12	0.080497121	0.001237
379	M-379	Zn5(MFU-4l)	MOF	[184]	3525	s1	n.d.	n.d.	16.5	d2	1.039999981	0.65	3.01E-53	1.31827E-12	2.03E-14
380	M-380	Zn-BTTB-DMBPY	MOF	[84]	749	s1	0.269	v1	4.41	d2	0.212145729	0.85	4.92E-05	11.8378722	0.152073
381	M-381	ZnCo4(MFU-4l)	MOF	[184]	3091	s1	n.d.	n.d.	n.d.	n.d.	0.73366512	0.35	0.000656516	20.80644276	0.202642
382	M-382	Zn-MOF-74(cycle 1)	MOF	[49]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.30473112	0.05	0.031166149	230.8498698	0.590683
383	M-383	Zn-Trimesate	MOF	[221]	n.d.	n.d.	n.d.	n.d.	5	d1	0.191240619	0.05	0.018725034	194.4920496	0.603192
384	M-384	Zr-Fum HT	MOF	[242]	1020	s1	0.553	v1	7.5	d2	0.421503274	0.05	0.015726677	845.2241909	0.769347
385	M-385	Zr-MOF-801-P	MOF	[75]	990	s1	0.45	v1	7.4	d2	0.353337839	0.05	0.00936137	721.2660121	0.763867
386	M-386	Zr-MOF-801-SC	MOF	[75]	690	s1	0.27	v1	7.4	d2	0.277295605	0.05	0.000755354	514.6543682	0.757147
387	M-387	Zr-MOF-802	MOF	[75]	20	s1	0.01	v1	5.6	d2	0.085072421	0.05	0.007261338	102.6440109	0.541456
388	M-388	Zr-MOF-804	MOF	[75]	1145	s1	0.46	v1	7.2	d2	0.339163933	0.45	0.001944916	79.70880276	0.498225
389	M-389	Zr-MOF-805	MOF	[75]	1230	s1	0.48	v1	9.5	d2	0.332925229	0.35	0.002111432	226.7492798	0.701004
390	M-390	Zr-MOF-806	MOF	[75]	2220	s1	0.85	v1	12.6	d2	0.266152366	0.05	0.034186061	385.5856762	0.707297
391	M-391	Zr-MOF-808	MOF	[75]	2060	s1	0.84	v1	18.4	d2	0.572069429	0.35	0.00789984	180.9596289	0.651969
392	M-392	Zr-MOF-841	MOF	[75]	1390	s1	0.53	v1	9.2	d2	0.482990008	0.25	5.80E-05	945.0075276	0.829717
393	C-1	2,5-DhaTab	COF	[135]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.567901494	0.85	7.83E-06	14.61304946	0.180901
394	C-2	2,3-DhaTph	COF	[135]	659	s1	n.d.	n.d.	20	d1	0.144551587	0.65	0.00041687	103.0331066	0.570247
395	C-3	2,5-DhaTph	COF	[135]	1112	s1	n.d.	n.d.	20	d1	0.169390323	0.65	0.000540108	16.48609631	0.197687
396	C-4	AB-COF	COF	[133]	1125	s1	0.47	v1	13	d1	0.347584161	0.25	8.42E-06	671.1610043	0.812696
397	C-5	Ad2L1	COF	[140]	918	s1	0.86	v1	n.d.	n.d.	0.279405316	0.85	5.81E-11	0.465652999	0.007105
398	C-6	Ad2L2	COF	[140]	1316	s1	2.2	v1	n.d.	n.d.	0.14942995	0.85	4.17E-07	6.729213013	0.093111
399	C-7	Ad2L3	COF	[140]	747	s1	0.45	v1	n.d.	n.d.	0.22910699	0.75	0.000237689	47.13325851	0.403283
400	C-8	Ad3L1	COF	[140]	1199	s1	0.8	v1	n.d.	n.d.	0.415801945	0.75	2.43E-05	37.40452045	0.353965
401	C-9	Ad3L2	COF	[140]	1093	s1	0.96	v1	n.d.	n.d.	0.374513785	0.85	1.61E-10	0.899916072	0.013629
402	C-10	Ad3L3	COF	[140]	1328	s1	0.93	v1	n.d.	n.d.	0.545551611	0.75	2.48E-12	0.355808179	0.005442
403	C-11	Ad4L1	COF	[140]	1617	s1	0.9	v1	n.d.	n.d.	0.447003907	0.55	0.00020576	78.67474522	0.51755
404	C-12	Ad4L2	COF	[140]	1885	s1	1.52	v1	n.d.	n.d.	0.686162376	0.85	7.84E-14	0.101408424	0.001558
405	C-13	Ad4L3	COF	[140]	1341	s1	0.74	v1	n.d.	n.d.	0.522857307	0.55	0.001471305	119.0154178	0.601344
406	C-14	ATFG-COF	COF	[133]	520	s1	0.5	v1	13	d1	0.290484138	0.15	0.004381974	304.3131807	0.737196
407	C-15	bipy -CTF500	COF	[138]	1548	s1	0.71	v1	8	d1	0.422223944	0.35	0.005425682	380.6369248	0.760904
408	C-16	bpim -CTF -300	COF	[142]	2.4	s1	n.d.	n.d.	n.d.	n.d.	0.153404013	0.95	0.003928976	97.45636464	0.553248
409	C-17	bpim -CTF -400	COF	[142]	786	s1	0.34	v1	n.d.	n.d.	0.300465211	0.05	0.013141475	345.9798338	0.732702
410	C-18	bpim -CTF -500	COF	[142]	1556	s1	0.75	v1	n.d.	n.d.	0.486059199	0.45	0.006409464	232.2339939	0.704478
411	C-19	CE-1	COF	[137]	960	s1	0.97	v1	8.2	d1	0.267784288	0.75	0.00021895	93.92493256	0.557279
412	C-20	CE-2	COF	[137]	588	s1	0.47	v1	7.8	d1	0.066125386	0.65	0.000991074	46.19345187	0.393252
413	C-21	CE-3	COF	[137]	540	s1	0.43	v1	8.6	d1	0.069852695	0.65	0.000484562	39.56496389	0.361041
414	C-22	COF-432	COF	[244]	895	s1	0.43	v1	8	d1	0.289395193	0.35	8.19E-06	19.67652681	0.226311
415	C-23	CTF-a	COF	[139]	2439	s1	1.96	v1	n.d.	n.d.	1.313891234	0.65	2.62E-07	24.20830575	0.248805
416	C-24	CTF-b	COF	[139]	1179	s1	0.64	v1	n.d.	n.d.	0.54157319	0.35	0.009833301	439.895921	0.771788
417	C-25	CTF-c	COF	[139]	2071	s1	1.36	v1	n.d.	n.d.	0.869318557	0.55	0.000127126	191.7524444	0.693208
418	C-26	CTF-d	COF	[140]	1683	s1	2.63	v1	n.d.	n.d.	0.726657285	0.85	1.12E-06	42.50852025	0.38347

419	C-27	DCBP -CTF - 1	COF	[143]	2437	s1	1.48	v1	n.d.	n.d.	0.498429618	0.85	1.45E-05	38.3829128	0.359984
420	C-28	F -DCBP -CTF - 1	COF	[143]	1574	s1	1.5	v1	n.d.	n.d.	0.192555556	0.85	0.000101702	31.988639	0.319657
421	C-29	MM1	COF	[141]	1800	s1	1.11	v1	n.d.	n.d.	0.493740584	0.75	4.35E-06	43.17636987	0.384947
422	C-30	MM2	COF	[141]	1360	s1	0.67	v1	n.d.	n.d.	0.419973752	0.35	0.005136968	239.9667126	0.709356
423	C-31	MM3	COF	[141]	1884	s1	1.52	v1	n.d.	n.d.	0.753041074	0.85	7.01E-08	11.43494435	0.145711
424	C-32	MM4	COF	[141]	1407	s1	0.78	v1	n.d.	n.d.	0.371207711	0.55	0.001455256	82.68271154	0.52433
425	C-33	pym -CTF500	COF	[138]	208	s1	n.d.	n.d.	8	d1	0.210234255	0.05	0.016987929	165.2863258	0.596458
426	C-34	TpAnq	COF	[136]	1027	s1	n.d.	n.d.	16.3	d1	0.356499502	0.35	0.000253824	152.7583722	0.649648
427	C-35	Tp-Azo	COF	[135]	942	s1	n.d.	n.d.	27	d1	0.394341285	0.55	0.000154082	60.33304239	0.458657
428	C-36	Tp-Azo	COF	[136]	3038	s1	n.d.	n.d.	25.8	d1	0.475918112	0.55	1.31E-08	6.760601533	0.093413
429	C-37	TpBD	COF	[135]	341	s1	n.d.	n.d.	24	d1	0.133562917	0.45	0.00030153	47.00917362	0.399847
430	C-38	TpBD	COF	[136]	1400	s1	n.d.	n.d.	21.8	d1	0.562804979	0.45	1.05E-05	39.90507756	0.366507
431	C-39	TpBD-(NO2)2	COF	[135]	90	s1	n.d.	n.d.	22	d1	0.078553477	0.55	0.000373503	33.5644726	0.327626
432	C-40	TpBD-(NO2)2	COF	[136]	769	s1	n.d.	n.d.	16.3	d1	0.365770733	0.35	0.000129639	86.24556679	0.536998
433	C-41	TpBD-(OMe)2	COF	[135]	365	s1	n.d.	n.d.	23	d1	0.130259926	0.55	0.000880845	36.2138149	0.341846
434	C-42	TpBD-(OMe)2	COF	[136]	1343	s1	n.d.	n.d.	16.3	d1	0.353788093	0.55	0.000329729	34.06640836	0.330667
435	C-43	TpBD-Me2	COF	[135]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.130259926	0.55	0.000880845	36.2138149	0.341846
436	C-44	TpBD-Me2	COF	[136]	3109	s1	n.d.	n.d.	16.3	d1	0.356562456	0.55	4.92E-07	19.13486487	0.222694
437	C-45	TpBpy	COF	[136]	2336	s1	n.d.	n.d.	24.2	d1	0.76505039	0.45	4.63E-06	47.23832005	0.402801
438	C-46	TpHZ	COF	[245]	422	s1	0.56	v1	7	d2	0.391853224	0.25	0.004351858	574.9706571	0.795138
439	C-47	TpPa-1	COF	[135]	984	s1	n.d.	n.d.	18	d1	0.412319505	0.15	0.002494176	662.2930877	0.805649
440	C-48	TpPa-1*	COF	[136]	1432	s1	n.d.	n.d.	14.8	d1	0.508653291	0.25	4.30E-05	501.106808	0.80199
441	C-49	TpPa-2	COF	[135]	460	s1	n.d.	n.d.	15	d1	0.202156405	0.35	0.000519744	133.82654	0.622558
442	C-50	TpPa-2*	COF	[136]	538	s1	n.d.	n.d.	10.6	d1	0.305756585	0.25	0.000182719	270.8286477	0.733202
443	C-51	TpPa-F4	COF	[135]	529	s1	n.d.	n.d.	17	d1	0.17902296	0.65	2.63E-05	17.10378571	0.204206
444	C-52	TpPa-NO2	COF	[135]	457	s1	n.d.	n.d.	16	d1	0.17902296	0.65	2.63E-05	17.10378571	0.204206
445	C-53	TpPa-NO2	COF	[136]	850	s1	n.d.	n.d.	13.2	d1	0.47810461	0.15	0.000487634	476.9598602	0.790072
446	C-54	TpTph	COF	[136]	1020	s1	n.d.	n.d.	25.8	d1	0.327807584	0.65	0.000417368	34.6091601	0.335351
447	C-55	TpTta	COF	[136]	825	s1	n.d.	n.d.	8.6	d1	0.33450653	0.75	0.000229351	197.5226404	0.695374
448	C-56	trzn-COF	COF	[134]	408.5	s1	0.21	v1	23	d1	0.068891992	0.65	0.001436592	53.77525984	0.425676
449	Z-1	CBV-901	Zeolite	[77]	n.d.	n.d.	0.31	v1	7.4	d2	1.21E-05	0.05	1.40E-06	0.019953808	0.000307
450	Z-2	H0.34Na0.06Al0.4Si47.6O96	Zeolite	[21]	340	s1	0.24	v1	4	d2	0.153272444	0.15	0.002359705	162.2739977	0.641957
451	Z-3	HiSiv 3000 Zeolite	Zeolite	[76]	282	s1	0.1	v2	15.2	d1	0.030592954	0.05	0.001984272	35.4244324	0.324841
452	Z-4	K6Na6Al12O48	Zeolite	[21]	756	s1	0.57	v1	4	d2	0.259864592	0.05	0.011373219	81.7462776	0.352926
453	Z-5	MCM-41	Zeolite	[50]	882	s1	0.63	v1	34	d2	0.560661512	0.75	0.001047751	114.0616838	0.598007
454	Z-6	NaX	Zeolite	[128]	1010	s1	0.31	v1	10.5	d1	0.33148317	0.05	0.012784433	143.0370418	0.446221
455	Z-7	Na-ZSM-5	Zeolite	[50]	366	s1	0.18	v1	6	d2	0.30473112	0.05	0.031166149	230.8498698	0.590683
456	Z-8	Zeolite 13X	Zeolite	[43]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.32066269	0.05	0.007294272	692.446057	0.761198
457	Z-9	Zeolite 4A	Zeolite	[79]	n.d.	n.d.	n.d.	n.d.	11.4	d2	0.286451781	0.05	0.025731054	214.9120287	0.548309
458	Z-10	Zeolite Na-A	Zeolite	[121]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.253694094	0.05	0.072963424	298.2305533	0.638711
459	Z-11	Zn2(pbc)2*Hdma*H3O*2H2O	Zeolite	[9]	213	s2	n.d.	n.d.	n.d.	n.d.	0.14754382	0.05	0.015317173	155.6442235	0.608756
460	Z-12	ZSM-5	Zeolite	[65]	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.010949513	0.35	0.000386052	10.49976448	0.13574

n.d. represents "no data" .

For Sa notes: s1 represents BET surface area; s2 represents Langmuir surface area.

For Va notes: v1 represents pore volume based on N2 adsorption, v2 represents pore volume measured basing on H2O adsorption.

For Dp notes: d1 represents average pore diameter, d2 represents dominant pore size obtained according to pore size distribution, d3 represents largest cavity diameter.

Table S4. Predicted indexes of 148 adsorbents by machine learning model (RF)

No.	ID No.	Adsorbent	Species	Ref. No.	Sa (m ² /g)	Va (cm ³ /g)	Dp (Å)	pre_Wsat (g/g)	pre_alpha	pre_KH (mol/(kg Pa))	pre_SCE (kJ/kg)	pre_COPc
1	M-11	[Co ₃ (ndc)-(HCOO) ₃ (mu-3-OH)(H ₂ O)] _n	MOF	[15]	1386	0.58	13.6	0.24951872	0.15	0.006224053	314.8829045	0.720123487
2	M-16	[Cu ₂ (H ₂ btp)(H ₂ O) ₂ (1,2-bis(4-pyridyl)ethylene)]	MOF	[115]	2.8	0.095	13.4	0.090635131	0.05	0.004043664	96.54617395	0.537984378
3	M-17	[Cu ₂ (H ₂ btp)(H ₂ O) ₂ (1,3-bis(4-pyridyl)propane)]	MOF	[115]	3	0.083	14	0.067709975	0.05	0.003879242	82.34883969	0.474862355
4	M-18	[Cu ₂ (H ₂ btp)(H ₂ O) ₂ (bipyridine)]	MOF	[115]	1.1	0.047	11.2	0.046674019	0.05	0.000750604	69.73859333	0.3854835
5	M-45	{[Zn ₄ O(bfbpdc)3-(bpy)0.5(H ₂ O)]*(3DMF)(H ₂ O)} _n	MOF	[60]	1450	0.59	10.76	0.372540217	0.85	0.006609505	195.5540098	0.592205984
6	M-55	Al(OH)-(1,4-NDC)	MOF	[226]	546	0.22	7.7	0.157690736	0.45	3.29818E-05	32.73527481	0.267158089
7	M-62	BIT-66(V)	MOF	[238]	1417	0.87	25.8	0.674484598	0.55	0.000924331	72.19338132	0.446554383
8	M-63	BIT-72(Al)	MOF	[164]	1618	0.59	6.2	0.520796067	0.55	0.000291971	60.72468358	0.458470082
9	M-64	BIT-73(Al)	MOF	[164]	1511	0.56	6.6	0.453146089	0.55	0.003178957	135.4313782	0.589893227
10	M-65	BIT-74(Al)	MOF	[164]	1394	0.51	5.7	0.421491088	0.45	0.010070306	245.8792651	0.64068368
11	M-68	BUT-155(Cu)	MOF	[158]	2070	0.82	16	0.550826573	0.25	0.010413134	714.0419027	0.786163381
12	M-69	BUT-46A(Zr)	MOF	[159]	1550	0.69	16	0.501991463	0.45	0.001356185	116.6765037	0.5534372
13	M-70	BUT-46B(Zr)	MOF	[159]	1403	0.65	16	0.542716204	0.55	0.011816176	186.9381021	0.624245196
14	M-71	BUT-46F(Zr)	MOF	[159]	1563	0.71	16	0.575758956	0.45	0.001860886	120.8260602	0.558518665
15	M-72	BUT-46W(Zr)	MOF	[159]	1565	0.71	16	0.596168957	0.35	0.00048022	81.38156111	0.514960872
16	M-89	C ₄ H ₈ HoKO ₁₂ Dehydrated	MOF	[55]	69.1	0.1042	3.6	0.187157489	0.05	0.045571523	273.1156377	0.63362781
17	M-91	C ₆ H ₄ N ₂ O ₈ Zn ₂	MOF	[58]	960	0.43	10.5	0.253092486	0.95	0.000868563	97.4652781	0.443779024
18	M-100	CAU-10-H	MOF	[112]	600	0.26	7	0.210878327	0.15	0.000500401	288.7913133	0.712780266
19	M-111	CAU-3(Al)	MOF	[191]	1550	0.64	27	0.503413121	0.65	0.000378804	61.10058763	0.457526726
20	M-113	CAU-6(Al)	MOF	[203]	620	0.25	10	0.327849971	0.05	0.017162068	264.6829384	0.660493601
21	M-116	Cd(BTTB)	MOF	[212]	415	0.19	5.41	0.241100856	0.55	0.002547661	70.69559122	0.396411402
22	M-120	Co(BTTB)(AZPY)	MOF	[212]	805	0.39	4.94	0.208230708	0.55	0.003243943	90.78455706	0.50444312
23	M-121	Co(BTTB)(BPY)	MOF	[212]	843	0.4	4.06	0.033107459	0.75	0.003152568	59.788674	0.344544818
24	M-122	Co(BTTB)(DMBPY)	MOF	[201]	809	0.29	4.41	0.194826543	0.85	1.32895E-05	23.93524263	0.212486514
25	M-128	Co-CUK-1	MOF	[130]	510	0.26	13.4	0.293089478	0.15	0.001598389	404.6388848	0.745449686
26	M-129	Co-MOF-74(M)	MOF	[27]	1314	0.51	12	0.581900113	0.05	0.085969477	541.4166558	0.630079955
27	M-130	Co-MOF-74(S)	MOF	[27]	1327	0.52	12	0.730318251	0.05	0.106895179	559.2655415	0.633839703
28	M-134	Cr-MIL(101)	MOF	[112]	3124	1.58	34	1.294077592	0.45	0.001534661	216.8688525	0.672933563
29	M-135	Cr-MIL-101-NO ₂	MOF	[112]	2146	1.19	34	0.813584943	0.45	0.003534228	150.5795635	0.601864215
30	M-136	Cr-soc-MOF-1	MOF	[173]	4549	2.1	17	1.929653256	0.75	0.000119965	212.5105115	0.669381297
31	M-138	Cu ₂ (dmcapz) ₂	MOF	[219]	539	0.227	9.7	0.222083742	0.35	0.001958672	115.1230474	0.524895284
32	M-143	CuEBTC	MOF	[192]	1434	0.65	9	0.205768957	0.05	0.00238856	239.1782526	0.652859354
33	M-144	CuMBTC	MOF	[192]	1471	0.79	9	0.207238333	0.05	0.006545307	277.1515846	0.66085683
34	M-148	DMOF	MOF	[64]	1960	0.58	7.5	0.096476321	0.25	0.000481642	151.5177996	0.572663938

35	M-149	DMOF(Zn)-A	MOF	[83]	760	0.33	4.8	0.289369046	0.35	0.000481108	92.48347303	0.527792948
36	M-150	DMOF(Zn)-Br	MOF	[83]	1315	0.53	5	0.061518844	0.35	0.003628163	73.60828348	0.426118439
37	M-151	DMOF(Zn)-N	MOF	[83]	1420	0.57	5.7	0.034977535	0.05	0.000127082	39.44716306	0.231325
38	M-152	DMOF(Zn)-NH3	MOF	[64]	2010	0.58	7.5	0.111401352	0.05	0.001941017	147.8355781	0.592069944
39	M-153	DMOF-Cl2	MOF	[83]	1175	0.45	3.8	0.074636585	0.35	0.001164568	59.45790027	0.380008761
40	M-154	DMOF-NO2	MOF	[83]	1310	0.53	6.2	0.130028213	0.45	0.004132799	86.47111627	0.498233964
41	M-155	DMOF-OH	MOF	[83]	1130	0.54	7.5	0.076392066	0.15	0.000792655	84.25750695	0.389528352
42	M-156	DMOF-TM(Co)	MOF	[201]	1052	0.49	3.5	0.369958762	0.35	0.001549415	124.585621	0.583953256
43	M-157	DMOF-TM(Cu)	MOF	[201]	1041	0.46	3.5	0.38255236	0.55	0.001210008	82.11540595	0.478470767
44	M-158	DMOF-TM(Ni)	MOF	[201]	1095	0.48	3.5	0.363541936	0.45	0.001434098	79.32536156	0.440588286
45	M-159	DMOF-TM1(Zn)	MOF	[196]	1210	0.53	7.5	0.272091276	0.45	7.73409E-06	41.94777085	0.322973119
46	M-160	DMOF-TM2(Zn)	MOF	[196]	1050	0.51	3.5	0.41420566	0.25	0.001105497	651.4632752	0.777766251
47	M-162	DUT-4	MOF	[41]	1360	0.79	8.5	0.490154175	0.55	0.003003968	118.720018	0.573726553
48	M-163	DUT-51(Zr)	MOF	[190]	2106	1.08	18.8	0.561614348	0.65	0.000879168	58.25226878	0.430095058
49	M-164	DUT-52(Zr)	MOF	[216]	1399	0.54	8.59	0.270214523	0.35	0.000719113	132.8698834	0.530917978
50	M-165	DUT-53(Hf)	MOF	[216]	1097	0.31	11.23	0.199770179	0.35	0.000753169	104.2959145	0.532993431
51	M-166	DUT-67	MOF	[75]	1560	0.6	16.6	0.504997046	0.25	0.007689695	655.6014828	0.782689143
52	M-167	DUT-67(Hf)	MOF	[162]	810	0.33	14.2	0.286009356	0.45	0.002471801	96.47403211	0.425973447
53	M-168	DUT-68(Hf)	MOF	[162]	749	0.34	27.7	0.284947589	0.45	0.003017055	111.4112898	0.517710974
54	M-169	DUT-68(Zr)	MOF	[162]	891	0.41	27.7	0.34236205	0.45	0.003671658	144.8560679	0.605538247
55	M-170	DUT-69(Hf)	MOF	[162]	450	0.22	5	0.182964385	0.15	0.000780182	233.4986197	0.685463791
56	M-171	DUT-69(Zr)	MOF	[162]	560	0.31	5	0.213884399	0.15	0.000161455	283.0259905	0.704729046
57	M-172	DUT-84(Zr)	MOF	[216]	637	0.27	11.14	0.138362356	0.35	5.24619E-05	50.43254566	0.328518308
58	M-173	ED-ZIF-8	MOF	[3]	1428	0.75	45.3	0.079480738	0.95	0.004927734	96.62050942	0.44530983
59	M-182	kag-MOF-1(Zn)	MOF	[170]	210	0.12	4.6	0.119742128	0.05	0.008131168	164.4107911	0.598592305
60	M-183	KMF-1(Al)	MOF	[240]	1130	0.473	6	0.432039995	0.15	0.004663643	639.8048207	0.795003791
61	M-186	LA ¹ -Zr6 ⁸ -csq	MOF	[182]	3150	2.18	47	0.393603212	0.65	0.001377992	85.81792939	0.480007165
62	M-187	LA ¹ -Zr6 ⁸ -flu	MOF	[182]	2850	1.31	38.6	0.234264781	0.75	5.33039E-05	33.11356145	0.273189966
63	M-199	MAF-4.23-7.77	MOF	[197]	1870	0.64	11	0.415833165	0.55	0.003671321	147.1084682	0.594253079
64	M-200	MAF-4.49-7.51	MOF	[197]	1870	0.65	11	0.427889064	0.55	0.00367132	149.3782905	0.593929469
65	M-201	MAF-4.76-7.24	MOF	[197]	1870	0.64	11	0.415833165	0.55	0.003671321	147.1084682	0.594253079
66	M-202	MAF-7(Zn)	MOF	[197]	1874	0.67	11.2	0.434262982	0.35	0.00529625	243.5243755	0.687150912
67	M-205	Mg-CPO-27	MOF	[112]	1400	0.65	11	0.638881405	0.05	0.026434324	840.1181417	0.705159799
68	M-206	Mg-CUK-1	MOF	[130]	580	0.28	13.4	0.36002771	0.25	0.001176993	610.7910158	0.751140847
69	M-207	Mg-MOF-74	MOF	[95]	1525	0.62	11	0.659733295	0.05	0.042000019	547.4956388	0.597875254
70	M-210	MIL-100(Cr)	MOF	[50]	1871	1.02	29	0.717571608	0.65	0.008493215	151.6632102	0.601994416
71	M-213	MIL-100(Cr)-DEG	MOF	[34]	580	0.5	12	0.414898058	0.35	0.002852496	194.8096466	0.67739585
72	M-214	MIL-100(Cr)-EG	MOF	[34]	710	0.47	12	0.42687522	0.35	0.005101	202.5155396	0.689732694
73	M-215	MIL-100(Cr)-EN	MOF	[34]	640	0.42	15	0.359748986	0.35	0.00560422	261.9542019	0.680752921
74	M-216	MIL-100(Cr)-TEG	MOF	[34]	680	0.53	12	0.332861284	0.35	0.001673317	144.1137544	0.602960339
75	M-217	MIL-100(Fe)	MOF	[41]	1549	0.82	29	0.831269175	0.35	0.006993703	251.7732251	0.657045977
76	M-218	MIL-100V	MOF	[125]	1203	0.74	11	0.165296484	0.35	0.01044834	200.3882269	0.557774774
77	M-219	MIL-101(Al)-NH2	MOF	[199]	3363	1.67	25	0.276163646	0.05	0.003884156	379.7603801	0.706928059

78	M-220	MIL-101(Al)-URPh	MOF	[199]	1555	0.83	18	0.335659036	0.05	0.008327194	522.090608	0.712135555
79	M-224	MIL-101-NH2	MOF	[42]	2509	1.27	34	1.049898489	0.45	0.000139467	85.69115407	0.541487267
80	M-225	MIL-101-SO3H	MOF	[42]	1920	0.94	34	0.752328015	0.35	0.011016428	397.1485264	0.72357068
81	M-226	MIL-101V	MOF	[125]	2705	1.4	21	0.273064751	0.05	0.007336733	458.3991198	0.713951849
82	M-231	MIL-125-NH2	MOF	[112]	1220	0.55	12	0.370744936	0.15	0.001319363	655.0996777	0.761496126
83	M-232	MIL-160	MOF	[2]	1070	0.398	5	0.375054105	0.05	0.009720631	564.8764743	0.741874528
84	M-245	MIL-53(Al)ht	MOF	[105]	1489	0.56	8.5	0.1106706	0.05	0.002936971	132.7091141	0.580310166
85	M-246	MIL-53(Al)it	MOF	[105]	1031	0.72	34	0.235053064	0.65	0.000182862	71.97743111	0.485264458
86	M-247	MIL-53(Al)-NH2	MOF	[176]	940	0.37	13	0.111487594	0.05	0.009212304	150.156807	0.57529795
87	M-250	MIL-53(Al)-TDC	MOF	[194]	1150	0.48	8.2	0.390831341	0.35	0.000911103	93.6371178	0.53293766
88	M-253	MIL-53(Ga)	MOF	[176]	1230	0.47	20	0.098515589	0.05	0.007288339	135.6566489	0.568885779
89	M-255	MIL-68(In)	MOF	[176]	1110	0.42	16	0.30176478	0.55	0.002275906	95.89965888	0.472007539
90	M-256	MIL-68(In)-NH2	MOF	[176]	850	0.3	16	0.33086807	0.45	0.000595992	76.45041234	0.390114215
91	M-257	MIL-91(Ti)	MOF	[217]	403	0.16	4	0.211999733	0.05	0.020037195	302.7632102	0.65686031
92	M-258	MIP-200	MOF	[129]	1000	0.4	13	0.422486987	0.15	0.016003478	640.6507308	0.776882257
93	M-268	MUF-77(Zn)-butyl	MOF	[215]	3250	1.21	13.6	0.24197643	0.85	0.003041738	89.12011291	0.505742449
94	M-270	MUF-77(Zn)-ethyl	MOF	[215]	3600	1.55	18.5	0.271524053	0.75	0.003352474	135.3841803	0.590401012
95	M-271	MUF-77(Zn)-hexyl	MOF	[215]	2170	1	11.2	0.139323695	0.85	0.00577935	109.6876333	0.518403189
96	M-272	MUF-77(Zn)-methyl	MOF	[215]	3600	1.85	21.1	0.217927835	0.75	0.001600345	91.34753506	0.497726356
97	M-277	Ni(BTTB)	MOF	[212]	391	0.2	4.3	0.014994921	0.05	0.001517826	18.85713016	0.253990829
98	M-291	Ni-CUK-1	MOF	[130]	520	0.26	13.4	0.299307085	0.15	0.001361331	443.0044427	0.757004006
99	M-292	Ni-DOBDC	MOF	[81]	639	0.362	11	0.514127935	0.05	0.043203375	589.5520791	0.621897843
100	M-294	NU-1000(Zr)	MOF	[185]	2320	1.4	31	1.032751135	0.75	0.000312041	74.65595726	0.495878478
101	M-295	NU-1000(Zr)-SALI-1	MOF	[185]	1710	1	30	0.85008459	0.75	0.002328516	125.7127841	0.570357104
102	M-296	NU-1000(Zr)-SALI-7	MOF	[185]	900	0.6	28	0.436277795	0.85	0.00052576	68.02446053	0.456290224
103	M-297	NU-1000(Zr)-SALI-9	MOF	[185]	870	0.6	28	0.354930087	0.85	0.000767613	65.72177359	0.36875401
104	M-303	PIZOF-2	MOF	[75]	2080	0.88	17.6	0.686767031	0.75	0.000492699	65.06657036	0.451336442
105	M-306	SALI-5(Zr)	MOF	[180]	1270	0.85	29	0.618263604	0.85	0.005450689	177.0553796	0.629126723
106	M-307	SALI-9(Zr)	MOF	[180]	900	0.63	27.5	0.403002865	0.85	0.000121931	110.2837833	0.583672804
107	M-308	SALI-9(Zr)	MOF	[180]	1190	0.87	29.6	0.679793914	0.85	0.001320842	158.07622	0.598943682
108	M-309	SALI-BA(Zr)	MOF	[180]	2005	1.21	27.8	0.945049254	0.85	0.007646528	176.237861	0.591872315
109	M-314	SIM-1	MOF	[112]	470	0.23	6	0.131705849	0.35	0.000493221	78.59399429	0.50489559
110	M-316	SNU-80	MOF	[14]	456	0.18	7	0.009249037	0.05	0.018177824	101.2628876	0.256217943
111	M-322	UiO-66	MOF	[75]	1290	0.49	8.4	0.42493345	0.35	0.001035108	140.7162198	0.605627942
112	M-323	UiO-66(Hf)-(OH)2	MOF	[167]	920	0.4	5.85	0.285866656	0.05	0.00229884	424.5606883	0.713143264
113	M-328	UiO-66(Zr)-(OH)2	MOF	[167]	1230	0.56	5.85	0.312104671	0.05	0.00283963	539.3887043	0.748510797
114	M-340	UiO-66-NH2	MOF	[64]	1040	0.57	6	0.386400563	0.15	0.012404728	632.4070428	0.768391886
115	M-344	UMCM-1	MOF	[64]	6010	2.41	32	0.275598201	0.85	0.00176389	101.4474128	0.512819114
116	M-349	Y-fum-fcu-MOF	MOF	[7]	691	0.28	8	0.343403216	0.05	0.003042732	635.6276127	0.739290341
117	M-358	Zn(BTTB)	MOF	[212]	447	0.25	4.47	0.20369296	0.75	0.00012173	100.432305	0.485530293
118	M-359	Zn(BTTB)(AZPY)	MOF	[212]	647	0.36	4.94	0.191637331	0.55	0.003282272	81.91009358	0.500479542
119	M-360	Zn(BTTB)(BDC)	MOF	[212]	441	0.21	4.24	0.089425375	0.05	0.000602022	111.7589389	0.548679661
120	M-361	Zn(BTTB)(BPY)	MOF	[212]	841	0.38	4.06	0.247242539	0.75	0.002106975	111.539838	0.552127395

121	M-362	Zn(BTTB)(DMBPY)	MOF	[201]	749	0.27	4.41	0.207141293	0.85	0.000104112	57.99341168	0.354420011
122	M-373	Zn2C14N2O8H4	MOF	[66]	312.7	0.146	5.2	0.179712435	0.15	0.008308243	273.253582	0.678269255
123	M-378	Zn4O(dmcapz)3	MOF	[72]	840	0.45	6	0.354870117	0.75	0.000114592	113.8339806	0.560816242
124	M-380	Zn-BTTB-DMBPY	MOF	[84]	749	0.269	4.41	0.211270567	0.85	9.75632E-05	34.6289003	0.343717623
125	M-384	Zr-Fum HT	MOF	[242]	1020	0.553	7.5	0.415148428	0.15	0.008491119	702.7812801	0.780178843
126	M-385	Zr-MOF-801-P	MOF	[75]	990	0.45	7.4	0.352231002	0.15	0.005382607	598.5436157	0.768710935
127	M-386	Zr-MOF-801-SC	MOF	[75]	690	0.27	7.4	0.27008494	0.05	0.00057885	370.2304643	0.712318529
128	M-387	Zr-MOF-802	MOF	[75]	20	0.01	5.6	0.084818536	0.05	0.002835949	98.1101677	0.52200308
129	M-388	Zr-MOF-804	MOF	[75]	1145	0.46	7.2	0.338986061	0.45	0.003965923	159.9588229	0.618724459
130	M-389	Zr-MOF-805	MOF	[75]	1230	0.48	9.5	0.337840949	0.35	0.000910883	106.5955013	0.553469925
131	M-390	Zr-MOF-806	MOF	[75]	2220	0.85	12.6	0.267134771	0.05	0.016359846	262.4387094	0.652968862
132	M-391	Zr-MOF-808	MOF	[75]	2060	0.84	18.4	0.573868155	0.35	0.009819092	374.5037641	0.728567496
133	M-392	Zr-MOF-841	MOF	[75]	1390	0.53	9.2	0.481943765	0.25	0.002072541	566.8002898	0.783816038
134	C-4	AB-COF	COF	[133]	1125	0.47	13	0.348029897	0.25	0.006541188	461.5690599	0.753445043
135	C-14	ATFG-COF	COF	[133]	520	0.5	13	0.292517069	0.25	0.00224043	379.8108419	0.746984045
136	C-15	bipy -CTF500	COF	[138]	1548	0.71	8	0.426992511	0.35	0.000916257	97.4978498	0.555580333
137	C-19	CE-1	COF	[137]	960	0.97	8.2	0.298752536	0.75	0.00046685	78.96493589	0.489121476
138	C-20	CE-2	COF	[137]	588	0.47	7.8	0.094549019	0.35	0.000424959	75.90570676	0.496575648
139	C-21	CE-3	COF	[137]	540	0.43	8.6	0.086502789	0.35	0.000425951	63.46249372	0.48597969
140	C-22	COF-432	COF	[244]	895	0.43	8	0.2935057	0.35	0.000481202	93.1078138	0.537633275
141	C-46	TpHZ	COF	[245]	422	0.56	7	0.379123632	0.35	0.002119662	169.719018	0.633003019
142	C-56	trzn-COF	COF	[134]	408.5	0.21	23	0.068768591	0.35	0.001093217	63.31739479	0.429395162
143	Z-2	H0.34Na0.06Al0.4Si47.6O96	Zeolite	[21]	340	0.24	4	0.15335972	0.05	0.003189983	170.2615093	0.631546445
144	Z-3	HiSiv 3000 Zeolite	Zeolite	[76]	282	0.1	15.2	0.038703178	0.35	0.001634238	55.04164738	0.383277662
145	Z-4	K6Na6Al12O48	Zeolite	[21]	756	0.57	4	0.182682269	0.05	0.020857254	269.6208504	0.655765652
146	Z-5	MCM-41	Zeolite	[50]	882	0.63	34	0.551029723	0.75	0.000720482	85.12147326	0.397144345
147	Z-6	NaX	Zeolite	[128]	1010	0.31	10.5	0.325366906	0.05	0.033186679	417.3203987	0.693416411
148	Z-7	Na-ZSM-5	Zeolite	[50]	366	0.18	6	0.303698863	0.05	0.017477747	323.698955	0.672911956

S2. Structural characteristics of experimental adsorbents

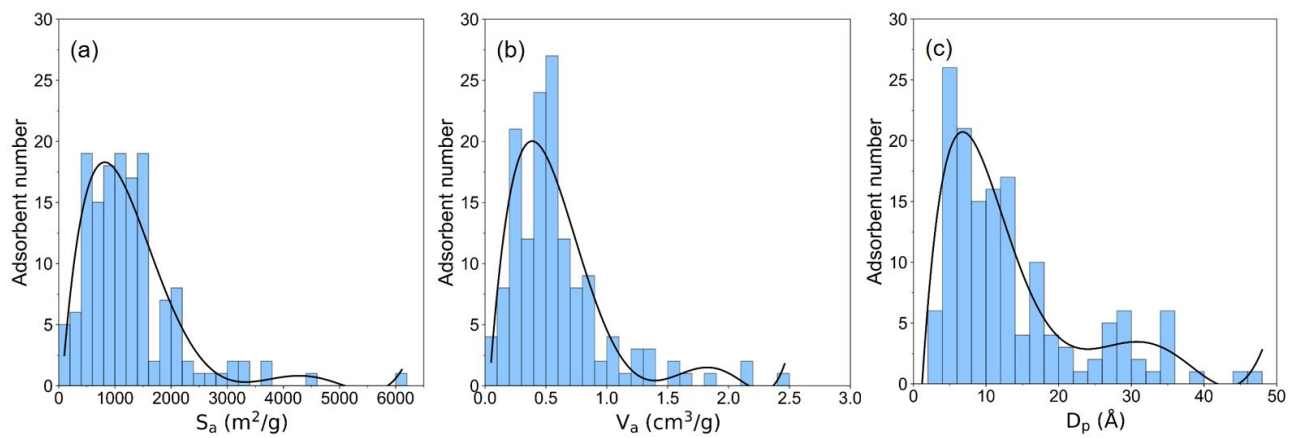


Figure S1. The distribution statistic of structural characteristics including (a) accessible surface area (S_a), (b) available pore volume (V_a) and (c) pore diameter (D_p) of 148 adsorbents

S3. Machine learning algorithms and details

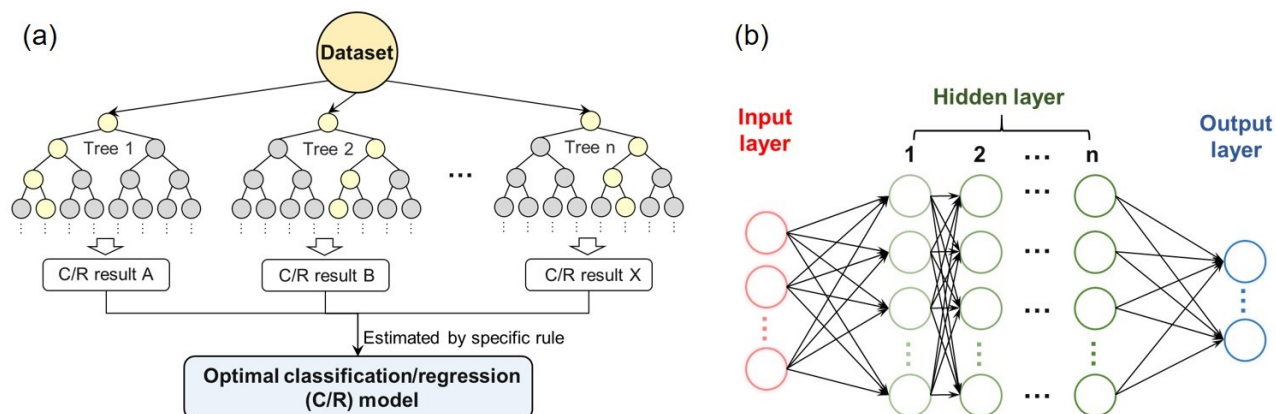


Figure S2. Schematic diagram of (a) random forest (RF) and (b) artificial neural network (ANN) model

Random forest (RF) algorithm

Firstly, it should be known that decision trees (DT) are a non-parametric supervised learning method used for classification and regression, which predicts the value of a target variable by learning simple decision rules inferred from the data features. Then, RF algorithm is originally inspired by the classic DT method, and it can be viewed as the improvement and optimization of DT. RF is an ensemble of DT that fits a number of classifying DT on various sub-samples of the dataset and uses averaging to improve the predictive accuracy and control over-fitting, overall, in a better prediction. Specifically, as Figure S2a shows, when training an RF model, multiple samples and several features are randomly selected and then the features with optimal segmentation were categorized as nodes for the establishment of DT. Repeating the process n times to build n DT, this is developing an uncorrelated forest. RF was estimated by a specific rule (usually average) based on the results of all trees, whose estimation on the whole group makes the model generalization ability stronger than any single tree. Tree indicators utilize numerical qualities randomly assigned to class names in an RF classifier, while a gathering of information parameters or self-assertively picks parameters at every node to grow a tree in an RF regression.¹

Artificial neural network (ANN) algorithm

Artificial neural network (ANN) is a bio-inspired algorithm developed by mimicking neural systems of organic life, which is one of the most widely applied examples of machine learning. Multi-layer perceptron (MLP) is a type of feedforward artificial neural network, which consists of an input layer, an output layer and at least one hidden layer (schematic diagram in Figure S2b). As with any other machine learning algorithm, the goal of ANN is to predict a response given a set of variables for either classification or regression. There can be one or more non-linear layers, called hidden layers, between the input and the output layer, and each hidden layer consists of multiple neurons (or nodes), In this fully connected network, every neuron is connected to all neurons of the next layer. Each neuron is assigned an activation function (a non-linear function) and a weight, which are applied to handle the weighted summation of the outputs of the preceding layer. The process is done until the output layer is reached, which consists of neurons with a linear (for regression) or step (for classification) activation function. It should be noted that the output of each node is applied to different weights into the summations that are received by the nodes in the next layer. The optimal weights are found using the backpropagation (BP) algorithm.² The weights of each node are initialized and then the prediction is tested for a single input or a set of inputs. The error of this prediction is then calculated (i.e. the loss function) and used to calculate the partial derivative of model error with respect to each weight in the network. The calculation of these derivatives is backpropagation and can be used in an optimization function that minimizes the loss function.³

Hyperparameter optimization and model setting

In this work, both ANN and RF models were deployed by the Scikit-learn module using Python codes.⁴ There are many so-called “hyper-parameters” which influence the final prediction effect of models. For example, the number of trees in a forest (`n_estimators`), the minimum number of samples required to split an internal node (`min_samples_split`) and being at a leaf node (`min_samples_leaf`) in trees are the most critical parameter affecting the RF model performance; the number of hidden layer and neurons in each layer (`hidden_layer_sizes`), the activation function for the hidden layer (`activation`) are the most key for ANN model. All hyper-parameters of RF and ANN Regressor were listed in Table S5, and their specific meanings can be found on the website of Scikit-learn (<https://scikit-learn.org/>). The key parameters (i.e., adjustable parameter in table) of models were optimized by grid-search (i.e.,

ergodic) within the given parameter range and five-fold cross-validation. During the process of hyper-parameters optimization, data were divided into five-folds, and four-fifths of the data were selected randomly as a training set while one-fifth of the data as a test set. The ML model was run five times for each group value of hyper-parameters by the five-fold cross-validation, in which the average determinate coefficient (R^2) of test sets in five-fold cross-validation was adopted to indicate the performance of the model built by different hyper-parameter groups. The hyper-parameter group with the maximum average R^2 will be the optimal hyper-parameters of learners for deploying models further.

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - p_i)^2}{\sum_{i=1}^n (y_i - \bar{p}_i)^2} \quad (\text{Eq. S1})$$

Where n , y_i , p_i , and \bar{p}_i refer to the number of data, target value, corresponding ML predicted value and average predicted value, respectively. It should be noted that all data used in models are normalized to eliminate the dimensional effects of data. Through testing in advance, it is determined that the linear normalization (MinMaxScaler) and mean normalization (StandardScaler) method are the best on RF and ANN, respectively. MinMaxScaler can scale the data between a given minimum and maximum value (0-1 in here), and the conversion formula is as follow.

$$x_{sca} = \frac{x - x_{\min}}{x_{\max} - x_{\min}} \quad (\text{Eq. S2})$$

Where x_{sca} , x , x_{\min} , x_{\max} are the scaled data, original data, minimum of data and maximum of data, respectively. For another, after StandardScaler processing, the data conform to the standard normal distribution (the mean is 0 and the standard deviation equals 1).

$$x_{sca} = \frac{x - x_{\text{mea}}}{x_{\text{std}}} \quad (\text{Eq. S3})$$

Where x_{mea} and x_{std} are the mean of data, the standard deviation of data, respectively.

ML models aiming to predict water adsorption isotherms using structure characteristics and adsorption pressure (ML S-I: one group data of [S_a , V_a , D_p , P] predict W), as well as predict adsorption cooling

performance using isotherm features as descriptors (ML I-P: one group data of $[W_{\text{sat}}, \alpha, K_H]$ predict SCE and COP_C) are expected to be realized. During the deployment of the model, 80% of samples in the available dataset were randomly chosen as the training dataset and the rest 20% served as the test dataset. The accuracy of models was assessed using R^2 , root mean squared error (RMSE) and mean absolute error (MAE). The calculation formula of RMSE and MAE are as follows.

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - p_i)^2} \quad (\text{Eq. S4})$$

$$\text{MAE} = \frac{1}{n} \sum_{i=1}^n |y_i - p_i| \quad (\text{Eq. S5})$$

Besides, the relative importance of descriptors for the prediction target of RF models is provided by the fitted attribute “feature_importances” in RF regressor, and they are computed as the mean and standard deviation of accumulation of the impurity decrease within each tree.

Table S5. The setting of random forest (RF) and artificial neural network (ANN) model

Model	Learner	Hyper-parameter		Parameter search mode	Data normalization
RF	Random Forest Regressor	Default parameter	max_depth=None, min_weight_fraction_leaf=0.0, max_features=1.0, max_leaf_nodes=None, min_impurity_decrease=0.0, bootstrap=True, oob_score=False, n_jobs=None, random_state=1, verbose=0, warm_start=False, ccp_alpha=0.0, max_samples=None	GridSearchCV(cv=5, scoring='r2', *)	MinMaxScaler([0,1])
		Adjustable parameter	n_estimators=[10, 20, 50, 100, 200, 300], criterion=['mse', 'mae'], min_samples_leaf=1-10, min_samples_split=2-10		

ANN	MLP Regressor	Default parameter	<pre> alpha=0.0001, batch_size='auto', learning_rate='constant', power_t=0.5, max_iter=10000, shuffle=True, random_state=1, tol=0.0001, verbose=False, warm_start=False, momentum=0.9, nesterovs_momentum=True, early_stopping=False, validation_fraction=0.1, beta_1=0.9, beta_2=0.999, epsilon=1e-08, n_iter_no_change=10, max_fun=15000 </pre>	GridSearchCV(cv=5, scoring='r2', *)	StandardScaler()
		Adjustable parameter	<pre> hidden_layer_sizes=[layers=1-6, neurons=2-50], activation=['identity', 'logistic', 'tanh', 'relu'], solver=['sgd', 'adam'], learning_rate_init=[0.1, 0.01, 0.001, 0.0001] </pre>		

S4. Adsorption cooling performance calculation

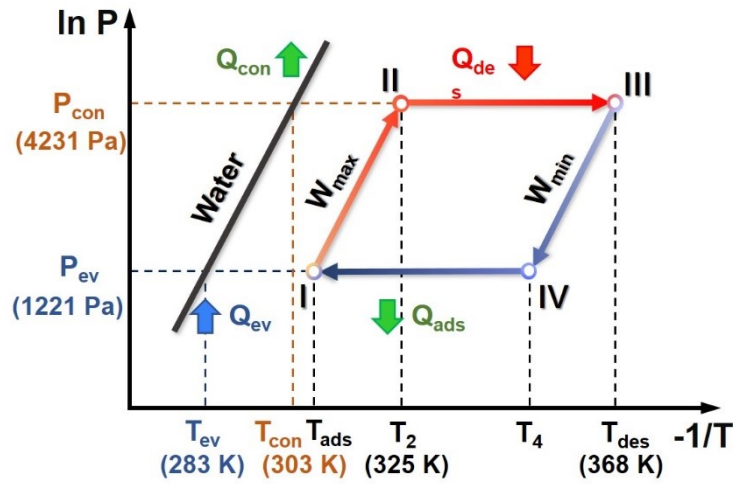


Figure S3. Diagram of the thermodynamic cycle for adsorption cooling. The cycle is consisting of four steps: isosteric heating (I-II), isobaric desorption (II-III), isosteric cooling (III-IV) and isobaric adsorption (IV-I).

As shown in Figure S3, the basic thermodynamic cycle consists of four steps: isosteric heating (I-II), isobaric desorption (II-III), isosteric cooling (III-IV) and isobaric adsorption (IV-I). The typical working conditions during the AC working process were adopted in this work.⁵⁻⁶ The evaporation temperature (T_{ev}) and condensation temperature (T_{con}) commonly used in the literature are 283 K and 303 K, respectively. The adsorption temperature (T_{ads}) is usually equal to T_{con} , which is close to the ambient temperature. The desorption temperature (T_{des}) is limited to the low-grade heat source, and it was fixed at 368 K in this work. T_2 is the minimum desorption temperature, which can be obtained according to the generalized Trouton's rule⁷, i.e. Evaporation pressure (P_{ev}) and condensation pressure (P_{con}) are the saturation pressure of ammonia at T_{ev} and T_{con} , respectively.

Based on the basic thermodynamic cycle diagram of AC, the cooling performance including the coefficient of performance for cooling (COP_C) and the specific cooling effects (SCE) of adsorbent/water working pairs can be calculated at typical cooling working conditions. SCE is the energy transferred for cooling by ammonia in the evaporator (i.e. Q_{ev}). COP_C describes the thermodynamic efficiency of AC that is defined as the output cooling capacity (i.e. Q_{ev}) divided

by the total heat input to the system (i.e. Q_{input} , and it approximately equals Q_{des}).

$$\text{SCE} = Q_{\text{ev}} \quad (\text{Eq. S6})$$

$$\text{COP}_c = \frac{\text{SCE}}{Q_{\text{input}}} = \frac{Q_{\text{ev}}}{Q_{\text{des}}} \quad (\text{Eq. S7})$$

Where Q_{ev} is the energy taken up in the evaporator, and Q_{input} is the heat energy from low-grade heat sources for desorption of adsorbent (Q_{des}).

$$Q_{\text{ev}} = \Delta W \Delta_{\text{vap}} H(T_{\text{ev}}) + \Delta W \int_{T_{\text{con}}}^{T_{\text{ev}}} C_p^{\text{ref}}(T) dT \quad (\text{Eq. S8})$$

$$\begin{aligned} Q_{\text{des}} &= Q_{\text{I-II}} + Q_{\text{II-III}} \\ &= \left[\int_{T_{\text{ads}}}^{T_2} C_p^{\text{ad}}(T) dT + W_{\text{max}} \int_{T_{\text{ads}}}^{T_2} C_p^{\text{ref}}(T) dT \right] + \left[\int_{T_2}^{T_{\text{des}}} C_p^{\text{ad}}(T) dT + \int_{T_2}^{T_{\text{des}}} W(T) C_p^{\text{ref}}(T) dT + \int_{W_{\text{max}}}^{W_{\text{min}}} \Delta_{\text{ads}} H(W) dW \right] \end{aligned} \quad (\text{Eq. S9})$$

Here, in the calculation of Q_{ev} , $\Delta W \Delta_{\text{ads}} H(T_{\text{ev}})$ and $\Delta W \int_{T_{\text{con}}}^{T_{\text{ev}}} C_p^{\text{ref}}(T) dT$ are latent heat and sensible heat taken up by the refrigerant (water in this work) in the evaporator. For the regeneration process of adsorbents

(i.e. steps of I-II and II-III), $\int_{T_{\text{ads}}}^{T_2} C_p^{\text{ad}}(T) dT$ and $\int_{T_2}^{T_{\text{des}}} C_p^{\text{ad}}(T) dT$ are the energy required for the adsorbent bed temperature changing from T_{ads} to T_{des} . Notably, we neglected the impact of heat exchanger and only

considered the effect of adsorbent. $W_{\text{max}} \int_{T_{\text{ads}}}^{T_2} C_p^{\text{ref}}(T) dT$ and $\int_{T_2}^{T_{\text{des}}} W(T) C_p^{\text{ad}}(T) dT$ are the energy required for

the temperature of refrigerant from T_{ads} to T_{des} . The last term $\int_{W_{\text{max}}}^{W_{\text{min}}} \Delta_{\text{ads}} H(W) dW$ is the heat adsorbed for ammonia desorption in the AC system. In the terms above, ΔW equals the difference of maximum water uptake (W_{max}) and minimum ammonia uptake (W_{min}).

$$\Delta W = W_{\text{max}} - W_{\text{min}} = W(T_{\text{ads}}, P_{\text{ev}}) - W(T_{\text{des}}, P_{\text{con}}) \quad (\text{Eq. S10})$$

Water equilibrium uptake (W) can be obtained from fitted isotherms by universal adsorption isotherm

model (UAIM) ⁸ as described in Eq. S11.

$$W = W_{\text{sat}} \sum_{i=1}^n \alpha_i \left\{ \frac{\left(\frac{P}{P_0} \exp\left(\frac{\varepsilon_i}{RT}\right) \right)^{\frac{RT}{m_i}}}{1 + \left(\frac{P}{P_0} \exp\left(\frac{\varepsilon_i}{RT}\right) \right)^{\frac{RT}{m_i}}} \right\}_i \quad (\text{Eq. S11})$$

In UAIM, W_{sat} is the saturation uptake of adsorbents. P and T represent the equilibrium pressure and temperature, and P_0 is the saturation pressure of water, R is the ideal gas constant. Additionally, α_i , ε_i , m_i and n are fitting parameters that are determined by the characteristic of adsorption isotherms given in Table S2. The vaporization enthalpy ($\Delta_{\text{vap}}H$, unit is kJ/kg) of water that is a function of temperature.⁹

$$\Delta_{\text{vap}}H = C1 \times \left(1 - \frac{T}{T_c} \right)^{C2 + C3 \times \frac{T}{T_c} + C4 \times \left(\frac{T}{T_c} \right)^2} \quad (\text{unit: kJ/mol}) \quad (\text{Eq. S12})$$

Table S6. Parameters for the evaporation enthalpy of ammonia in Eq. S12

Temperature range (K)	C1	C2	C3	C4	T_c
273.16-647.13 K	5.2053	0.3199	-0.212	0.25795	647.13

The average heat of adsorption ($\Delta_{\text{ads}}H_{\text{ave}}$) of adsorbents can be estimated as follows:

$$\Delta_{\text{ads}}H_{\text{ave}} = \frac{\int_{W_{\text{min}}}^{W_{\text{max}}} \Delta_{\text{ads}}H(W) dW}{W_{\text{max}} - W_{\text{min}}} \approx \frac{\int_0^{W_{\text{sat}}} \Delta_{\text{ads}}H(W) dW}{W_{\text{sat}}} \quad (\text{Eq. S13})$$

In Eq. S8, the enthalpy of adsorption ($\Delta_{\text{ads}}H$) is calculated using the predicted adsorption isotherms obtained by UAIM at varying temperatures according to the Clausius-Clapeyron equation shown in Eq. S16.

$$\Delta_{\text{ads}}H(W) = -R \frac{\partial(\ln p)}{\partial(1/T)} \quad (\text{Eq. S14})$$

In addition, C_p^{ref} and C_p^{ad} are the specific heat capacity of refrigerant and adsorbent, respectively. They are considered to be constant (C_p varies slightly with temperature used in fact) of 4.2 kJ/(kg·K) for water and 1 kJ/(kg·K) for adsorbents (reasonable value for a variety of adsorbents).⁵

Then, the formula for calculating SCE and COP_C can be obtained by substitution and simplification.

$$\text{SCE} = \Delta W \left[\Delta_{\text{vap}} H(T_{\text{ev}}) - C_{\text{p}}^{\text{ref}} (T_{\text{con}} - T_{\text{ev}}) \right] \quad (\text{Eq. S15})$$

$$\text{COP}_{\text{c}} = \frac{\Delta W \left[\Delta_{\text{vap}} H(T_{\text{ev}}) - C_{\text{p}}^{\text{ref}} (T_{\text{con}} - T_{\text{ev}}) \right]}{C_{\text{p}}^{\text{ad}} (T_{\text{des}} - T_{\text{ads}}) + C_{\text{p}}^{\text{ref}} \left[W_{\text{max}} (T_2 - T_{\text{ads}}) + \int_{T_2}^{T_{\text{des}}} W(T) dT \right] - \Delta W \Delta_{\text{ads}} H_{\text{ave}}} \quad (\text{Eq. S16})$$

S5. Supplementary results of machine learning

Table S7. The hyper-parameter setting and predictive effect of machine learning models (S-I) including random forest (RF) and artificial neural network (ANN)

Model	Aim	Hyper-parameter (adjustable)	Cross-validation R ²	Predictive effect								
				Trainin g R ²	Trainin g RMSE	Trainin g MAE	Test R ²	Test RMSE	Test MAE	R ²	RMSE	MAE
RF (S-I)	Predict uptake	criterion='mse', min_samples_leaf=1, min_samples_split=2, n_estimators=200	0.924	0.991	0.021	0.010	0.948	0.050	0.025	0.982	0.029	0.013
ANN (S-I)	Predict uptake	activation='relu', hidden_layer_sizes=(43, 43, 43), learning_rate_init=0.01, solver='adam'	0.894	0.922	0.060	0.041	0.915	0.065	0.044	0.921	0.061	0.041

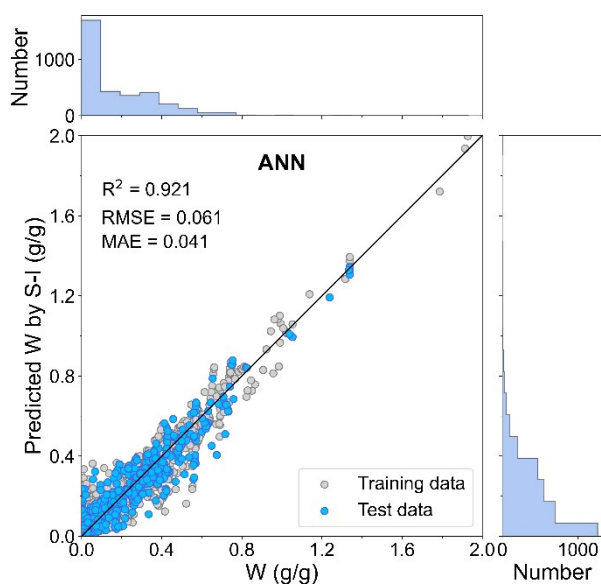


Figure S4. (a) The predicted results of water uptake (W) by artificial neural network models (ANN, S-I)

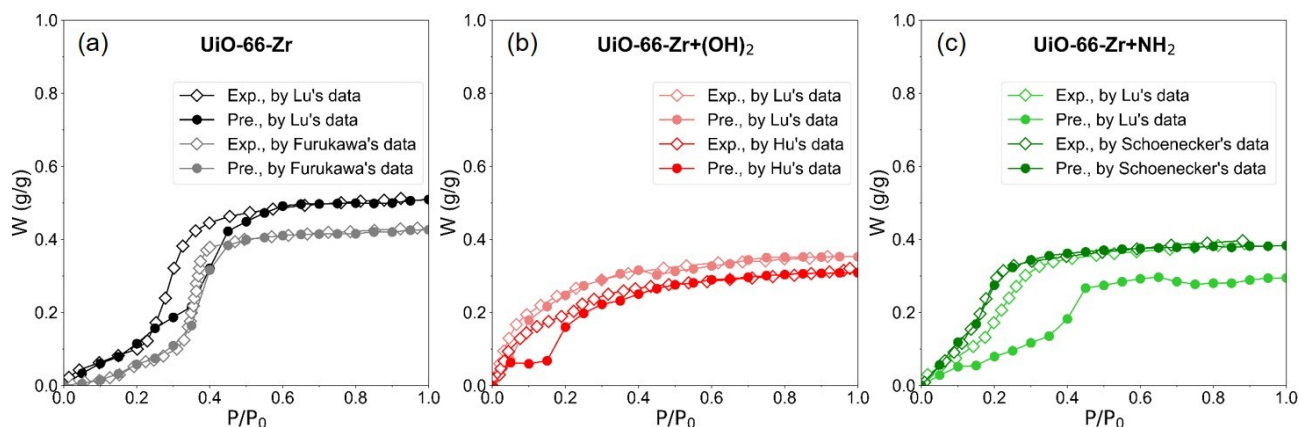


Figure S5. The experimental and predicted water adsorption isotherms of (a) UiO-66-Zr^{10,11}, (b) UiO-66-Zr+(OH)₂^{10,12}, (c) UiO-66-Zr+NH₂^{10,13} were reported by different research groups. In all figures, the diamond markers represent experimental data from our EWAID or scientific literature, the dots represent predicted data by random forest model (RF, S-I).

Table S8. The structural characteristics of adsorbents in Figure S5

No.	Adsorbent [Ref.]	Species	S _a (m ² /g)	V _a (cm ³ /g)	D _p (Å)
1	UiO-66-Zr (Lu's work) ¹⁰	MOF	1421	0.58	8.6
2	UiO-66-Zr (Furukawa's work) ¹¹	MOF	1290	0.49	8.4
3	UiO-66-Zr+(OH) ₂ (Lu's work) ¹⁰	MOF	1065	0.41	6.4
4	UiO-66-Zr+(OH) ₂ (Hu's work) ¹²	MOF	1230	0.56	5.9
5	UiO-66-Zr-NH ₂ (Lu's work) ¹⁰	MOF	1280	0.55	6.2
6	UiO-66-Zr+NH ₂ (Schoenecker's work) ¹³	MOF	1040	0.57	6.0

Table S9. The hyper-parameter setting and predictive effect of machine learning models (I-P) including random forest (RF) and neural network (NN)

Model	Aim	Hyper-parameter (adjustable)	Cross validation R ²	Predictive effect								
				Training R ²	Training RMSE	Training MAE	Test R ²	Test RMSE	Test MAE	R ²	RMSE	MAE
RF (I-P)	Predict SCE	criterion='mse', min_samples_leaf=1, min_samples_split=2, n_estimators=100	0.706	0.968	41.156	25.166	0.795	91.804	57.040	0.935	57.511	31.541

	Predict COP _C	criterion='mse', min_samples_leaf=1, min_samples_split=3, n_estimators=200	0.758	0.962	0.045	0.029	0.816	0.102	0.076	0.931	0.061	0.039
ANN (I-P)	Predict SCE	activation='logistic', hidden_layer_sizes=(45, 45), learning_rate_init=0.01, solver='adam'	0.745	0.832	94.520	62.510	0.798	91.519	59.849	0.827	93.927	61.978
	Predict COP _C	activation='logistic', hidden_layer_sizes=(48, 48, 48), learning_rate_init=0.01, solver='adam'	0.691	0.733	0.119	0.086	0.653	0.140	0.105	0.717	0.123	0.090

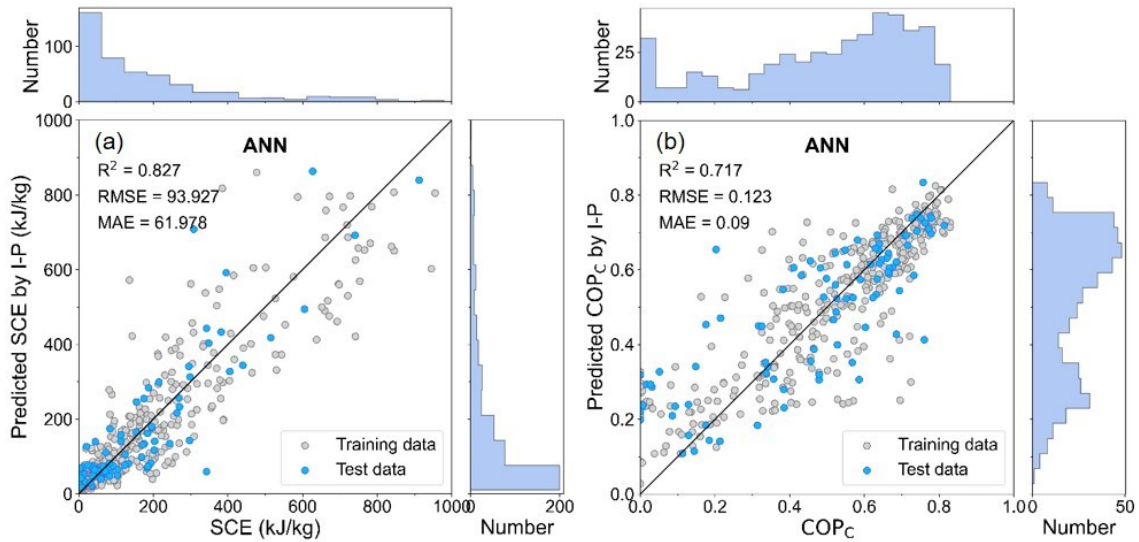


Figure S6. The predicted results of (a) specific cooling effect (SCE) and (b) coefficient of performance for cooling (COP_C) by artificial neural network models (ANN, I-P).

Table S10. The hyper-parameter setting and predictive effect of machine learning models (S-P) including random forest (RF) and artificial neural network (ANN)

Model	Aim	Hyper-parameter (adjustable)	Cross validation R ²	Predictive effect								
				Training R ²	Training RMSE	Training MAE	Test R ²	Test RMSE	Test MAE	R ²	RMSE	MAE
RF (S-P)	Predict SCE	criterion='mae', min_samples_leaf=2, min_samples_split=2, n_estimators=300	-0.039	0.630	146.277	100.430	0.030	264.071	219.760	0.488	176.621	124.619

	Predict COP _C	criterion='mse', min_samples_leaf=1, min_samples_split=3, n_estimators=50	0.113	0.834	0.096	0.075	0.082	0.258	0.211	0.646	0.144	0.102
ANN (S-P)	Predict SCE	activation='tanh', hidden_layer_sizes=(13, 13), learning_rate_init=0.000 1, solver='adam'	-0.027	0.752	123.097	80.034	-0.063	250.563	186.046	0.593	157.504	101.523
	Predict COP _C	activation='relu', hidden_layer_sizes=(24, 24), learning_rate_init=0.000 1, solver='adam'	0.001	0.744	0.128	0.087	-1.734	0.300	0.206	0.467	0.177	0.111

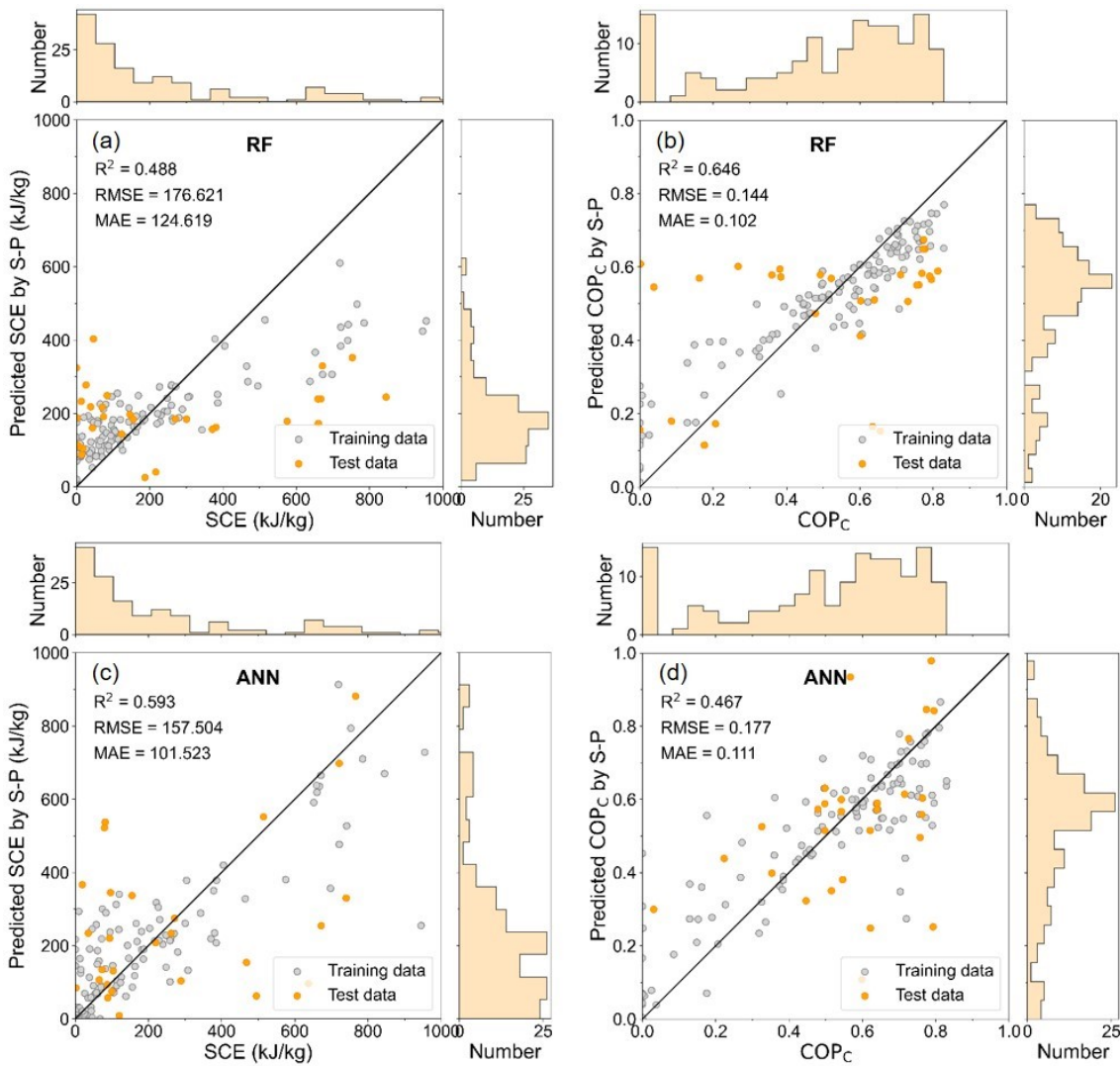


Figure S7. The predicted results of specific cooling effect (SCE) and coefficient of performance for cooling (COP_c) by machine learning models (S-P) including (a-b) random forest (RF) and (c-d) artificial neural network (ANN) model

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