MOF-BAM DATABASE USER INTERFACE - http://mofdb-bam.de/

A quick introduction on how to get started with using the tool

The web version of the MOF-BAM database consists of three sections:

- 1. Search parameters of MOFs
- 2. Search parameters of Organics
- 3. Results
- 4. Exporting



MOF Database

1. The search parameters of MOFs are divided in:

Number of components: amount of metals (any, 0 - 3), amount of linkers (any, 0 - 3). It allows also including organic molecules that are not linkers, like structure directing agents, charge compensating ions, capping agents, etc., selecting the option "Allow MOFs with Non-Linker organics". Also the instruction "Keep order when searching for Used Organics" (see section XX)

Search parameters: The drop-down menu allows to select the search parameter and its value. Included parameters are MOF name, CSD reference code, porous properties like accessible surface area (ASA gravimetric and volumetric), pore volume, density, crystallographic properties, estimated hydrogen total uptake at 77 K and 100 bar, presence of open metal sites (OMS), specific metals, and price of linkers per gram. The total uptakes are estimated from the porous properties by following the procedure reported in https://doi.org/10.1016/j.ijhydene.2020.10.265.

It is possible to add (or delete, if needed) search parameters combining these parameters with the option "Add search parameter". Finally, the button "Reset search parameters" cleans all the search fields, and the button "Search" looks for matches within the database. The results from the search appear in section 3.a.

2. The search parameters of Organics

This field allows to look among organic components within MOF structures, even if they are linkers or not. It is possible to look for organics from their name (total name or fragments), CAS number, molar mass, their price $(\mathbf{\xi}/\mathbf{g})$, and the presence of specific chemical moieties (including carbonyl, amine, azolates, fluor,...).

3. Results

Results are divided for MOFs structures (3.a) and organics (3.b). Both tables can be sorted by any attribute by clicking on the appropriate column header.

<u>3.a</u>: Found MOFs, the interface provides the CSD reference, MOF name (if available), porous and crystalline properties, density, gravimetric hydrogen excess in saturation, gravimetric and volumetric total uptakes at 77 K and 100 bar, metallic and organic composition, and the potential presence or not of OMS. It is also possible to select one or many structures from the results field to export or to select their organic components as a search criteria in 2.

MOF Name	~						Search
OMS?	✓ Yes					~	Remove
Rel. Price [€/g]	~			to 26			Remove
		Add search pa	arameter	Reset search pa	rameters		
Organic by MOF	• 1249	Add search pa	arameter	Reset search pa	rameters		Search
ound MOFs							630 Results
CSD Reference	Org	anic 1			Organic 2		Organi ^
ABUWOJ	1,4-Benzen	edicarboxylate					
ACIBOE	1,3,5-Benzen	netricarboxylate					
ADODAA	4-carboxyl	atopyrazolate					
AFEKAX	4,4'-B	ipyridine					
AGIREP	1,3,5-Benzen	netricarboxylate					
AMILOY	2,6-Naphtale	nedicarboxylate					
AMILUE	2,6-Naphtale	nedicarboxylate					-
4							
Use selected Org	ganics as Organic 1 🗸]				Show used	Organics
ound Organics							# Results
	CAS	IUPAC Name	Alt. Names	Mol. Mass [g/mol]	SMILES (Cambridge)	SMILES (Canonical	l) Linker?
	Export selected M	DEs			Download CS	/ File	
	Export selected Pit	013			Download C5	v ine	

3.b: Found Organics: The organic compounds matching the search parameters in section "2." appear here. For example, cheaper linkers than 10 €/g.

Rel. Price [€/g] ▼ to 10													
			Add search para	meter Reset search parameters									
Found Organics	•	Alt. Names	Mol. Mass [g/mol]	SMILES (Cambridge)	SMILES (Canonical)	275 Results							
99-32-1	4-	Oxo-4H-pyran-2,6-dicarboxylate	184.1	0=C1C=C(0C(=C1)C(=0)0)C(=0)0	OC(=0)cloc(cc(=0)cl)C(=0)0	Yes							
99-31-0		5-amineisophthalate	181.15	NC=1C=C(C=C(C(=0)0)C1)C(=0)0	Nclcc(cc(c1)C(=0)0)C(=0)0	Yes							
99-05-8		3-aminebenzoate	137.14	NC=1C=C(C(=0)0)C=CC1	Nclcccc(cl)C(=0)0	Yes							
98-97-5		pyrazine-2-carboxylate	124.1	N1=C(C=NC=C1)C(=O)O	OC(=O)cloncen1	Yes							
96404-79-4		2-formyltriphenylene	256.3	C(=0)C1=CC=2C3=CC=CC=C3C3=CC=C3C2C=C1	C(=0)C1=CC=2C3=CC=CC=C3C3=CC=CC=C3C2C=C1	No							
96404-79-4		triphenylene-2-carbaldehyde	256.3	C1=C(C=CC=2C3=CC=CC=C3C3=CC=CC=C3C12)C=O	0=Cc1ccc2c(c1)c1ccccc1c1c2cccc1	No							
4	·		336.34	et alter en plet alare erler en plet alare er		U *							
	Export selected MDFs Download CSV File												

4. Exporting

Exportation buttons allow to export the MOF structures results into a csv file. After the selection is made (Selecting no MOFs will automatically result in all results in the MOF table to be exported), it is necessary to click on "Export selected MOFs". This will generate a file containing the information on both the selected MOFs and the organics associated with them. Once the file is ready the "Download CSV File" button will turn clickable and upon its use the generated file will be downloaded. The file contains the following fields:

Identifiers of the structure: csd_ref, name, as identifiers of the structure.

Porous properties: asa_grav [m²/g], asa_vol [m²/cm³], av_vf, pore_volume [cm³/g],

density [g/cm³]

Hydrogen uptake: nexc [wt. %], uptake_grav [wt. %], uptake_vol [g H2/L],

Composition: metal1, metal2, metal3, cas1, norm_name1, name1, mol_mass1 [g/mol], smile_cam1, smile_can1, linker1, vendor_name1, max_amount1 [g], rel_price1 [€/g], min_purity1, cas2, norm_name2, name2, mol_mass2 [g/mol], smile_cam2, smile_can2, linker2, vendor_name2, max_amount2 [g], rel_price2 [€/g], min_purity2, cas3, norm_name3, name3, mol_mass3 [g/mol], smile_cam3, smile_can3, linker3, vendor_name3, max_amount3 [g], rel_price3 [€/g], min_purity3

Structural/crystalline parameters: oms, lcd [Å...], pld [Å ...], LFPD [Å ...], symmetry_space_group, cell_length_a, cell_length_b, cell_length_c, cell_angle_alpha, cell_angle_beta, cell_angle_gamma, cell_volume [Å³].

Example 1:

We want to search structures using the same linkers than material PCN-250. In the Structure search fields (1.), select "MOF Name", and type "PCN-250", then click on "Search".

Collapse Parameter Section													
Amount of Metals: Any v to 0 v Allow MOFs with Non-Linker Organics	Amount of Linkers: Any 💙 to 1 💙												
MOF Name PCN-250	Add search parameter Reset search parameters	Search											
Organic Name 🗸	Add search parameter Reset search parameters	Search											

Found MOFs					-			-	1 Results
CSD Reference	Name	ASA [m²/g]	ASA [m²/cm³]	AV_VF	Pore Volume [cm³/g]	Density [g/cm³]	nexc [wt. %]	Uptake [wt. %]	Uptake [g H2
TOWPEC	PCN-250'	1671.76	1486.62	0.68	0.76	0.89	3.42	4.73	44.16
4									
4									•

Now, select the structure with left click over it in the results field "3.a" and then, click on "Show Used organics". An internal ID, assigned to this linker, will appear in the search field "2." labeled as "Organic by MOF". Click on "Search" button, and the information about this linker appears in the results box "3.b". It is possible to check the information about a linker by double-clicking anywhere on its row in the results field. Clicking anywhere next to the opened information panel will close it again.



Now, reset search parameters in the structure search (1.), and click on "Use selected organic as" after selecting the position "Organic 1" in the drop-down menu rightwards. If the option "keep order when searching for Used Organics" is not selected in the field "1.", then structures where the linker is in position 2 or 3 (if any) would also be displayed.

	Collapse P	arameter Section	
Amount of Metals: Any v to 0 v Allow MOFs with Non-Linker Organics		Amount of Linkers: Any v to 1 v	
Organic 1 🗸 496	Add search parameter	Reset search parameters	Search
Organic by MOF 🗸 1716	Add search parameter	Reset search parameters	Search
Saved MOS			Dr. Develo

Found MOFs								2	1 Result
CSD Reference	Name 🔻	ASA [m²/g]	ASA [m ² /cm ³]	AV_VF	Pore Volume [cm³/g]	Density [g/cm³]	nexc [wt. %]	Uptake [wt. %]	Upta 🔺
TOWPEC	PCN-250'	1671.76	1486.62	0.68	0.76	0.89	3.42	4.73	
OFODET	JUC-64	1161.73	1340.43	0.52	0.45	1.15	2.75	3.36	
UBIBUF	FJI-9	3087.55	2339.26	0.75	0.98	0.76	5.21	6.62	
DAPHOU	FJI-8	3056.76	2401.47	0.74	0.94	0.79	5.18	6.48	
VALXOY	CPM-200-V/Mg	1910.51	1484.63	0.68	0.88	0.78	3.73	5.29	
VALXIS	CPM-200-In/Ni	1671.71	1485.32	0.69	0.78	0.89	3.42	4.79	
VALXEO	CPM-200-In/Mn	1802.51	1503.01	0.68	0.82	0.83	3.59	5.02	
									- F

The structure DACYUE uses a mixture of linkers. By clicking on it and on "Show used Organics", it would include this organic compound in the results field "3.b". First, we need to Reset search parameters on fields "1." and "2.".

Amount of Met	Imount of Metals: Any to Imount of Linkers: Any to Imount of Linkers: Any to Imount of Linkers: I														
Organic 1		~	767		A	dd search parameter Reset sear	ch parameters	Search							
Orace in her M			700												
Organic by MOF Y Add search parameter Reset search parameters															
Found MOFs								6 Results							
CSD Reference]	Metal 1	Metal 2	Metal 3	OMS?	Organic 1	Organic 2 v	Organic 3							
DACYUE		Mg			Yes	3,3',5,5'-Azobenzenetetracarboxylate	1,3-dimethylimidazoleidin-2-one								
DADLOM		Mn			Yes	4',4'',4'''-Nitrilotribiphenyl-4-carboxylate	1,3-dimethylimidazoleidin-2-one								
REGRIG		Zn			Yes	1,3,5-Benzenetricarboxylate 1,3-dimethylimidazoleidin-2-one									
ROCZIU		Cd			Yes	pyridine-4-carboxamide 1,3-dimethylimidazoleidin-2-one									
RODBAP		Cd			Yes	5-(4-pyridyl)tetrazol	1,3-dimethylimidazoleidin-2-one								
UJUPUM		Zn			Yes	5-Methyltetrazole	oxalonitrile	1,3-dimethylimidazoleidin-2-one							

Example 2:

Now, let us search for MOF structures with higher volumetric area than 2,000 m²/cm³, with OMS, and using a cheaper linker than $1 \notin$ /g. The interface gives 164 MOF structures fulfilling this criteria.

MOF Database

				Collapse Paran	neter Section									
Amount of Met	tals: 1	✓ to 2 ✓	•	A	Amount of Linker	s: 1 🗸	to 2 🗸							
Allow MOFs	v MOFs with Non-Linker Organics													
ASA [m²/cm3	s] v	2000			to				Search					
OMS?	✓ Yes ✓ Re £/a] ✓ to 1 Re													
Rel. Price [€/	Add search parameter Reset search parameters													
	Add search parameter Reset search parameters													
Organic Nam	e 🗸								Search					
	Add search parameter Reset search parameters													
Found MOFs								16	54 Results					
CSD Reference	ASA [m²/g]	A [m ² /g] ASA [m ² /cm ³] AV_VF Pore Volume [cm ³ /g] Density [g/cm ³] nexc [wt. %] Uptake [wt. %] Uptake [g H ₂ /L												
ACIBOE	1873.86	2063.01	0.66	0.6	1.1	3.68	4.46	51.42						
AGIREP	2253.69	2250.02	0.69	0.69	1.0	4.16	5.07	53.29						
ARADEE	2211.32	2613.25	0.65	0.55	1.18	4.11	4.77	59.24						
ATAFIK	1722.65	2093.15	0.64	0.53	1.22	3.48	4.13	52.35						
BABREE	2623.96	2356.63	0.68	0.76	0.9	4.63	5.6	53.28						
BODPAN	2370.57	2105.25	0.72	0.82	0.89	4.31	5.54	52.07						
BUKMUO	3400.71	2895.4	0.71	0.83	0.85	5.6	6.57	59.87						
Use selected	Organics as	Organic 1 🗸						Show used O	rganics					
									<u> </u>					
CAS v				Alt. Names		Mol. Mass	s [g/mol]	27	5 Results					
99-32-1			4-0xo-4	H-pyran-2,6-dicarboxylate	2	18	4.1	0	=C1C					
99-31-0			5	amineisophthalate		181	.15	N	C=1C					
99-05-8				3-aminebenzoate		137	.14		NC					
98-97-5			руг	azine-2-carboxylate		12	4.1		N					
96404-79-4			2-	formyltriphenylene		25	6.3	C(=0)C1=0	CC=2					
96404-79-4			triphe	nylene-2-carbaldehyde		25	6.3	C1=C(C=C	C=2C					
964-68-1		Be	nzophen	ene-para,para-dicarboxyla	ate	270	.24	C(=0)(C =0	C=C(
	Fx	port selected M	OFs			Dowr	nload CSV File							
	LA	port bereeted i			L	2011								

To export this data, click first on "Export Selected MOFs", and then on "Download CSD File". It will generate a .csv file using comma as data delimiters. In some regions importing this file in other programs like EXCEL may require the user to set the appropriate delimiter for the columns to be displayed properly (for EXCEL

see <u>https://support.microsoft.com/en-us/office/import-or-export-text-txt-or-csv-files-5250ac4c-663c-47ce-937b-339e391393ba</u>).

After separating the fields, the selection looks like this:

	0	D		F	0 0	6 J G	1	JK	1.	##	NO		0 0		T	U	Y		X Y Z	AA AD	AC AD	AE AF	AG	AR	A A	AK	AL AM	AN	AD AD	AP AD	AR	AL .	AT	AU K	N AW
1 cad rel name	414 98.4	ara_vol a	v_vi pr	pre_voi der	aits (nes	c fut, upt	ake i up	Aake i metal	metal2	metal3 on	a led[A.]	p46[A.] I	FPO(2 symmetric	cell_leng c	ell_leng o	ell leng o	el_ang cel	Lang cel	Lang cell voli carl	norm_n/name1	mol_ma_smile_c	is sende_ci bekert	Vendor_ r	nas_arti rel	price min_p	uri cas2	norm_ni name	2 mol_	ma smile_ci st	nile_o. linker2	vendor_ r	mag_am r	el_price m	n puri cast	3 horm_ni
2 KOZNY	1904.6	2076.2	0.63	9.61	105	3.82	4.59	50.36 Zh		Ye	s 6.57	5.25	6.52 P28o	15.22	9.85	10.27	90 1	02.04	90 2679.1 100-25	0 14-Benz ["Benze	 N6.10 C1 +CC 	- OCI+Ok Yes	AmBrei	1000 0	0215 0.1	15.64-10-6	Formate ['Yorr	541 45	103 CI+O(O C	+OIO Yes	AllaAes	2500	0.0192	0.95	
5 12UUUL	2254.4	2447.8	0.67	0.62	109	4.57	4.95	59.00 Zn	Sn	Ye	8.09	5.66	8.00 P4/mbm	22.9	22.9	9.25	90	90	90 4098.7							64-19-6	Formate ['Yonr	541 46	103 CI+O(O C	+0)0 Yes	Allahaz	2500	0.0182	0.95	
4 APJADEE	228.3	2613.3	0.65	0.55	1.10	4.0	4.77	59.24 Cd		Ve Ve	s 5.90	5.29	5.90 C2A	21.79	11.63	13.51	90	93.82	90 4087.6 554-95	-C 125-Ber ["125-9	1 210.14 Ct(+CC	OCI+OX Yes	AmBrei	1000 0.	0909 0.1	90 95-94-7	benzotti ["L2.1	44 10	3.94 NINENCC	ScCc2x Yes	BLD Ph	1000	0.123	0.99	
\$ ZAPLOV	2548.5	2258.4	0.65	0.61	105	4.03	4.77	62.61 Zn		Ye	s 759	4.25	7.53 Prom	23.94	27.32	22.59	90	90	90 14291 554-95	-C 13,5-Ber ["13,5-ti	1 210.14 C11+CC	(OCI+O) Yes	AmBrec	1000 0.	0999 0.1	93 95-94-7	benzotri ["#44	eci 111	9.14 NIN-NC of	occ2ci Yes	BLDPh	1000	6.123	0.99	
6 FORDAM	2717.2	261	0.73	0.92	0.9	4.75	6.0	5191 Zh		Ye	r 18.97	6.01	18.91 Fm-3m	39.97	38.93	29.93	90	90	90 62669 121-95	bergene ["13-Ee	NE.14 CII+CO	OCI+OX Yes	AFFERES	5000	0.098 0.1	99 200-57-1	14-01220 ["[4-	531 15	ES MECCAC	ICN2C Yes	TCIChe	500	0.125	0.98	
P HVSAI DMOF	1126.3	2005.4	0.65	0.5	100	3.75	451	5114 Zh		Ye	8.01	5.43	7.95 H/mom	15.06	15.06	19.24	90	90	90 4365 900-25	0 (4-Elenz ["Elenza	HED CUCC	OCI+OX Yes	AmBrei	1000 0	0275 0.1	95 250-57-5	14-diaza ["[4-	141 15	E2 NECCK C	KINDC Yes	TCIChe	500	0.525	0.90	
B VOPINELOP	2207.0	2008.7	0.67	0.71	0.99	100	0.00	bund an			8 8.10		eter Linem	1.10	91.01	3.0	- 22		30 23007 00-25	o 74-Deut I. Deute	ALL CHUCK	COLLOG THE	Ambres	1010 0	0275 0.	10 200-01-1	Le-mara Le-	<u></u>	E2 NULLING	R. PECL, YPE	TUICHE	000	0.025	0.00	
IN WAFFING	2340.3	2017.6	0.66	0.72	0.95	1.04	4.00	50.35 Eh		10	5 0.00	7.04	2.00 Permon	12.06	12.05	847			90 4367 000-25 90 2228 4 100-25	14-Denz [Denze	HED CH-CC	DOLLON Ves	AmBrec	1000 0	0210 0.1	PS 200-57-5	Le-chapp (Le-	NAC 15	E2 NECCH C	CAUC Yes	TOUChe	500	6 104	0.99	
# WADEAVOA	1042-2	2078.8	0.64	0.50	100	3.73	4.47	60.0 70			745	6.14	7 05 DAlese	14.90	14.00	45.2		- 40	50 4500 E 100-11	14 East CEast	NED CH-CC	OCI-ON Ves	AmBen	2010 0	018 01	10 250 57.0	14-diate Pla-		IS A MADOCK C	Carlos Ver	TOChe	500	0.005	0.94	
IE VAREAVIS	1975.1	2025.4	0.65	0.65	106	3.85	4.50	\$107 Zn		Ye.	7.96	5.43	7.05 M/mcm	16.02	15.00	19.24	90		90 43451 100-25	14-Benz C'Elenze	NED CHICK	DCI+OX Yes	Artillee	1010 0	6275 0.1	18 280.67.5	14-diara C'14-	lar II	2 MOCCA C	TACK Yes	TCIChe	500	0.126	0.90	
13 VAREAVOS	1200	2112.5	0.65	0.62	106	3.64	4.62	6130 20		Ye.	8.62	5.51	0.02 M/mcm	15.06	15.06	19.75	90	90	90 4368.2 100.25	1 14-Bent C'Bente	NE12 CH-CC	OCI+ON Ver	Amilian	1010 0	0775 01	15 200.57.5	14-diata f"14-	141 18	2.2 MICCA C	CADC Yes	TCIChe	500	0.026	0.98	
H OMOVE TIMOF	1016.1	2048.3	0.62	0.55	1.10	3.6	4.27	50.35 Zn		Ye	6 6.41	4.66	6.41 1-424	\$8.76	18.76	10	90	90	90 6334.5 4282-3	5- Thiophe ("2.5-mi	172.16 SICI+C	COCI+Ob Yes	AmBeel	1000 0	2393 0.1	97.288-36-6	12.3-tria ["trial	04 63	07 NIN-NC of	unefek Yes	BLDPh	500	0.6846	0.98	
15 HOVPU JUC-66	21011	20416	0.65	0.67	0.97	2.97	4.87	49.75 Zn		Ye	7.90	5.40	7.91 P21212	13.82	2164	\$2.53	90	90	90 3630.2 490-5	5.34 Puris (*3.4-Pu	# 107.12 NI+CC	a OCI+Ok Yes	Chemen	1000 0.	0053 01	100-97-0	12574# [*125	7. 140	22 CINICK C	ROCK Yes	Allahox	5000	0.0142	0.99	
16 CUOFILO	2219.3	2398.9	0.64	0.64	0.99	4.12	4.89	60.76 Zn		Ye	5 5.87	4.6	5.82 C2/o	38.03	9.65	9.87	90	97.49	90 2590.3 103-35	2 4.4'-ethe ["4.4'-et	\$ 268.27 C(+CC	- OCI+Ox Yes	ELD Ph.	500 0.	5968 0.1	95 288-88-6	12,4-114 ("12,4	41 68	106 NIN-Ch of	non(nii Yes	Carbory	10000	0.0102		
17 NIMQAD	3578.6	20517	0.77	1.10	0.65	5.33	7.24	5114 Cu		Ye	18.6	6.65	11.6 Fm-3m	40.09	40.09	40.09	90	90	90 64446 618-83	7 5-Hydroi (*6-Hyd	112.14 OC+1C	· Ocloc(o-Yes	ELD Ph	510 0	1058 0.1	98 290-37-5	Paradra ['Par	ale 80	109 NI=CC+ nt	oonoo' Yes	AK5d	100	0.5048		
N JORVET	2395.6	2012.3	0.66	0.79	0.84	4.54	5.48	49.67 2n		Ye	s 10.62	4.73	10.82 C2/c	40.43	18.12	25.35	90 t	23.89	90 21456 530-85	8 4,4'-metl ["4,4'-m	< 388.39 C(Ct+C	(OC(=O): Yes	AmBeel	500 0.	2546 0.1	99 1455-77-	0,5-diam (*3,5-	Ša 99	9.12 NCI-NIT N	CtsNff Yes	BLD Ph.	500	0.42	0.90	
19 IVENEA	3474.9	2003	0.82	1.4	0.59	5.7	0.09	61,47 Ou		Ye	8 22.61	7.45	22.6 Fm-3m	46.95	46.15	46.35	(H)	90	90 98291 653-26	444'-Bpg["44'-B	116.10 NI+CC	 nloostoc Yes 	Chemes	1000	0.276	1 99-39-0	6-amino (16-ar	nin 301	1.15 NC+1C+ N	olooje+Yes	Carbozy	10000	0.0613		
20 FAVEALML-88	2209.4	2445.2	0.65	0.59	109	4.15	4.06	05.73 Fe		Ye	4 6.89	5.1	6.09 P-62o	11.50	11.10	14.59	90	90	120 1580.6 190-17-	Fumaratic ["Tumar	1 1H.00 C(VC+C	a OCI+OV Yes	AmBeel	1000 0.	0096 0.1	99									
at PEZKE	2893.9	2365.9	0.71	0.87	0.82	4.97	6.85	63.57 Fe		Ye	I 862	8.1	8.82 P-620	12.97	12.87	12.68	90	90	120 2110 110-17-1	E fumaratic ("Tumar	HL08 CIVC+C	LOCI-OX Yes	AmBeel	1000 0.	0095 0.1	99									
RR PICZNEDI	2093.7	2305.8	0.71	0.87	0.82	4.97	6.85	53.57 Fe		Ye	8.62	8.1	8.62 P-62e	13.87	13.87	12.66	90	90	120 2110 150-17-	fumatati (Tumar	THEOD CIVELO	A OCI+OV Yes	Amilieet	1000 0	0095 0.1	99									
20 CMQ/194	3799.2	2013	0.85	152	0.56	6.09	0.60	63.21 C4		70	0 20.26	8.97	15.77 Pd-385	40.94	48.94	40.94	- 100	- 90	30 117225 100-97	0 73/2/146 1.73/2/1	90.22 CIN2C	N CINZCK Yes	Allanes	5000 0	0142 0.1	19									
24 EKOPE	1040	2002.7	0.61	0.51	122	3.09	4.05	50.78 51	04	10	5 6.82	5.54	6.81 P43252	17,49	17.49	10.21	90	- 90	90 4044 121-95	Denzene [1]3-Ere	REN CHICK	OCHOR Yes	Allahos	5000	100 0.	55									
as perman	10,00.0	2032.7	0.6.7	0.11	100	3.65	2.00	52.49 DA	0.0			2.5	SORE D.O.	22.4	1000	70.00			10 4223 K1-35	berners [13-me	NEW CRUCE	COLLEGE Ver	Alladara	5000											
an MARIA	1178.6	2784.0	0.71	0.04	0.04		100	62.49 0.0		10	1 1.10	8.00	6.44 PO1101	47.4		10.07			80 10770 School	bennere [Loue	NEH CHICK	COLON Ves	Allahas	5000	0.040 0.0										
In FUVCIC lambdad	0162-0	2494.6	0.75	0.84	0.92	4.5		6164 70		94	12.00	7.14	10 DE (0.01)	16.17	05.17	26.12	90		90 10227 100.21	h 14.Benz C'Esnas	NET CH-CC	ODI+ON Ves	Amilland	1000 0	0745 01	10									
28 KUNFIEL ML-DOE	2108	2297.7	0.74	102	0.72	6.54	6.82	52.74 Fe			3.09	0.3	3.09 PESime	14.42	14.42	17.3	90	90	120 2014 4 100-25	0 14-Benz C'Benze	HED CHACE	OCI+Oh Yes	Amiliant	1000 0	0275 0.1	Wi I									
30 LAGVER	2762.2	2238.7	0.64	0.65	0.99	4.10	4.95	515 Co		Ye	c 7.33	5.01	7.33 C24	33.23	9.73	10.29	90	93.68	90 5238.6 100-25	0 14-Benz l'Benze	KEID CH-CC	+ OCI+Ox Yes	Amilieec	1010 0	0215 01	15									
as PICTIG	2227.9	2131.7	0.65	0.68	0.96	4.12	6.02	50.52 Zn		94	7.19	5.2	7.17 C24e	21.22	9.77	18.22	90	93.60	90 5998.9 100.25	14.Banz C'Elenza	NED CH-CC	+ OCI+Oh Yes	Amiliani	1000 0	02% 01	15									
52 PEZIEA	9530.9	2266.2	0.76	1.10	0.64	6.76	7.55	52.41 Cr		¥e.	10.50	9.9	10.50 P63/mm	15.63	15.60	15.96	90	90	\$20 2275 100-25	0 14-Benz ("Benze	4 16.13 Ct+CC	OCI+Ok Yes	AmBeet	1000 0	02% 0.1	95									
00 SEFEOV	2419.2	2400.5	0.67	0.65	100	4.37	5.15	55.71 Zn		Ye	5.66	5.15	5.65 P212121	10.3	11.82	20.37	90	90	90 2400.0 100-25	0 14-Benz ("Benze	< N6.13 C1+CC	+ OCI+Ox Yes	AmBrei	1000 0	0275 0.1	16									
34 TAGYALCPM-20	3328.7	2474.9	0.60	0.95	0.74	5.51	6.64	62.91 Mg		Ye	£ 7.19	5.47	7.19 P3c1	22.81	22.81	96.81	90	90	120 7674.6 103-25	0 14-Benz ["Benze	< H6.13 CI +CC	+ OCI+Ox Yes	AmBee:	1000 0	0215 0.1	95									
35 UFENAV	4090.6	3008.4	0.74	0.98	0.75	6.45	7.57	61.01 Zn		Ye	4 7.29	5.26	7.ff Co	03.24	9.72	10.42	90	90.54	90 5950.9 100-25	0 14-Benz ("Benze	#6.13 Ctj+CC	OC(+O): Yes	AmDrei	1000 0	02% 0.	95									
06 CLAYON	N62.6	2299.4	0.69	0.40	144	3.41	3.99	69.02 Cd		Ye	5.67	4.4	5.67 P212121	8.37	8.0	20.95	90	90	90 178.2 07-69-	 (Sartaa)-LJanab 	< 150.1 C[[C89	HO[CBH] Yes	ABCR	25000 1	1029 0.1	33									
ST OYEFER	4736.8	2199.2	0.94	102	0.45	7.23	10.23	52.68 Cr	Cu	Ye	E H.33	11.45	H.01 P63m	20.77	20.77	2105	- 90	90	120 7866.9 59-67-	s pyridne- ["pyrdn	6 15315 CICPO	TOCI+OX Yes	AmBrec	500 0.	0292: 0.1	10									
38 OVERCE	2942.9	2225.9	0.73	0.92	0.79	5.03	6.33	53.4 C/	Cd	74	8 9.45	7.58	9.45 P-4250	20.61	20.61	22.16	90	90	90 94918 59-67-	pyridne- ("pyrdin	4 123.12 CICS-C	OCI+OX Yes	Amiliaec	510 0	0292 0.1	98									
as concent	1102.3	2000.2	0.69	0.40	140	3.84	14	62.5 0.6		10	8 872		S.F.C. Pretent	0.91	10.00	2103		- 22	30 1736 4 133-37	a zocanji rama	e meno Ciroli	OCIUC YES	Cattory	10000 0	0.001										
at FOutsta	MOTO	2033.2	0.67	0.55	1.04	245	4.00	BLOT CO	70		8.47		8 TH 874 The	40.70	80.71	10.745		- 22	00 4117 0 00 0F	1245 B Cheson	TRAIN CANCE	OCLOS Ver	AmBrei	1010 0	0000 01	8									
42 LABPEC	144.3	2022.1	0.62	0.51	123	3.98	4.00	5142 20	en.		7.02	4.82	6.99 Phoa	11.05	10.0	22.94	90	90	50 82187 69.05	1245.B ("hence	254 16 CallCo	+ OCI+OX Yes	Amiliani	1010 0	0115 0.1										
45 WONRAD	1121.0	25511	0.57	0.2	19	2.71	3.09	6054 C4			8.27	4.23	4.8 Ama2	12.75	15.60	15.44	90	90	90 2917 03-05-	1245.8 Chenne	254 16 C+ 9CH	1 OCI+Ok Ver	Amilian	1010 0	0716 01	10									
44 JOYFOD	2292.3	2309	0.71	0.71	1.01	42	5.85	64.92 Cu		Ye	6.50	6.27	6.06 P285	12.69	7.8	17.23	90	23.06	90 1029.7 298-80	C 12.4-miai ["12.4-m	62.06 NRI-C	N officially Yes	Cathors	10000 0.	0602										
45 NEGZUV	15.67	2102.0	0.62	0.45	1.41	3.22	0.77	65.00 V	Zn	Ye	6.53	5.76	6.53 Phon	24.60	10.04	17.3	90	90	90 7701.3 288-88	C 12.4-min [12.4-m	68.06 MIN-C	A officially Yes	Cathors	10000 0.	0602										
45 VOHDON	1773.3	2534.1	0.7	0.49	142	3.85	4.15	6182 Cd		Ye	\$ 5.72	4.44	5.72 P212121	8.41	9.81	2102	90	90	90 1733.3 147-75	7 (25,35)-: ["D-Tar	150:09 C(=O))	0 O[C@@ Yes	Cattors	10000 0	0413										
AT IGAGUU	0427.9	2294.4	0.77	121	0.63	5.00	7.71	62.86 Cr	Cu	Ye	s N.25	12.97	16.25 (P63/mol	29.72	29.72	26.29	(90)	90	120 20115 150-13	0 4-amino ["4-amia	137.15 NCI-C	C OCI+Ok Yes	Gleenhar	1000 0	05% 0.1	99									
48 INEVAJ polyMOI	0493.0	2372.7	0.78	1.21	0.64	5.96	7.77	54.12 Cu			£ 13.76	6.60	53.76 Himmm	26.22	28.22	44.81	(90)	90	90 20801 99-214	6-amino [16-amia	18115 NC+IC	 Noloc(or Yes 	Carbosy	10000 0	0613										
45 QIVGES	3529.7	2658.6	0.68	0.8	0.85	5.27	6.21	56.16 Cu		Ye	8 6.44	4.4	6.26 P2We	22.55	11.46	21.06	90 1	05.65	90 5442 1453-8	2- pyridine- ['Isonic	122.10 C(C+C	If NC(+O): Yes	Hotel Ha	10000 0	0671										
10 PIOCZAM	2064	2335	0.64	0.57	1.0	3.92	4.61	54.7 Cd		Ye	5.60	4.29	5.45 P296	862	21.12	13.75	90	9113	90 2670.5 1453-0	2- pyridne- ["Isonio	< 122.13 C(C1+C	I NCI+Ok Yes	Helei Hit	10000 0	0671										
51 XEYMAR	166.9	2239.5	0.66	0.49	124	3,41	4.01	56.14 Mn	CU	Ye	6.22	4.79	5.73 P2No	10	21.12	11.96	90	93.34	30 68322 1453-8	2 pyridine- ["Isonio	122.13 C(C)+C	R NCI+OX Yes	Hotel Ha	10000 0	0671										
S2 GOUVAB	1973.1	2097	0.63	0.6	106	3.85	4.55	50.71 Zh		74	\$ 4.95	4.07	4.96 1-420	10.25	16.36	7.56	90	90	90 21/2.7 504-17	e 5-animi [5-ino	E 144.16 NIL[+0	DICILC Yes	Chemes	1000 0.	0643 0.	98									
SO GLASSEP	K167.4	2105.4	0.62	0.54	100		10	Page Min		Ye	4.6	4.17	+ 00 1-42d		17.00	1.67			20 x240.0 504-17	o commit 2-mag	E PREMI ANCLUS	DICKLE YPE	Chemes	and 0.	0.41 0.1										
IS ACIDOE MORIC	1173.9	2263	0.64	0.00	11	3.00	144	8142 7n		Ye	4,60	7.05	8 10 1428	10.59	10.00	17.03	90		90 203.6 504-17	C 135 Ber C 135.0	E 200 M CHACK	I DOLLE YES	AmBaar	1010 0	Dalla 01	20									
TE ACADER	91657	2260	0.69	049		4.90	6.07	6129 70			10.92	0.00	7.90 D.sm	44.67	15.74	03.0	90		90 05000 554.00	(125.Ber (125.0	2 200 M CHUCC	COLON Yes	AmBrei	1010 0	0000 01	20									
TT DCCPA HOURT.	2370.6	2305.3	0.72	0.82	0.09	4.35	5.54	62.07 Cu		V.	13.15	6.66	13.13 Fm-3e	62.53	62.51	52.51	90	90	10 144708 154-95	C135-Ber (*135.0	230.14 CB+CC	OCI+ON Yes	Ardlen	1000 0	0000 0.1	NA NA									
M CEHAD	25593.2	2217.9	0.74	0.16	0.05	4.6	6.85	53.09 Zh		Ye	6 50.21	5.99	10.09 P41212	11.69	12.69	50.66	90	90	90 9499.3 574.95	C 135-Ber (*135-0	1 21014 CH-CE	OCI+OX Yes	Amilieed	1010 0	0909 01	12									
55 CIFMEL	2603.2	2748.4	0.75	0.98	0.78	5.06	7.08	57.99 Co		4	6 8.24	5.76	8.24 P213	14.65	14.65	14.65	90	90	90 2145.4 554.95	C 135-Ber ["135.n	4 21014 CH-CC	OCI+Ox Yes	AmBeel	1000 0	0909 01	10									
80 DEPHOM	2090	2294.0	0.61	0.54	100	3.96	4.62	52.45 Mn		Ye.	\$ 5.87	4.69	5.05 P2M	17.00	11.0	10.05	90 1	18.25	90 25610 554-95	C 13.5-Ber (*13.5-6	4 210.14 CE+CC	OCI+Oh Yes	AmBeec	1000 0.	0909 0.1	10									
61 DIHVE HKUST-	2305.0	2038.2	0.72	0.81	0.08	4.23	5.45	60.92 Cu		Ye	8 13.29	6.89	13.27 Fm-3m	26.3	26.0	26.3	90	90	80 10199 554-95	-C 13.5-Ber ["13.5-0	1 210.14 C1 +CC	OCI-Ox Yes	AmBrei	1000 0.	0909 0.1	98									
12 DIHVECHKUST-	2377.9	2096.7	0.71	0.81	0.88	4.32	6.52	51.48 Cu		Ye	£ 10.18	6.64	13.17 Fm-3m	28.32	26.72	28.22	90	90	90 18226 554-95	C 13,5-Ber ["13,5-0	210.14 CII+CO	OCI+OX Yes	AmBeec	1000 0.	0909 0.1	18									
65 DUPYER	2723.9	2168.1	0.72	0.92	0.8	4.76	6.13	52.01 Zn		Ye	9.90	6.47	9.92 P2M	16.6	25.92	17.44	90 1	07.38	90 6212.9 554-95	C 135-Ber ["135-0	210.14 Ctj+CC	OCI+OX Yes	AmBeet	1000 0.	0909 0.1	98									
64 EGATAI	2528.7	2426.3	0.7	0.73	0.96	4.51	5.40	55.09 Co	Zn	Ye	s 7.26	4.31	7.26 P213	14.15	14.15	94.15	90	90	90 2024.4 554-95	-C 13.5-Ber ["13.5-h	1 210.14 Cti+CC	(OC(+O)x Yes	AmBeet	1000 0.	0909 0.1	90									
#5 EXCENSION.																																			