



Taming Computational Chemistry Data: ioChem-BD and Beyond

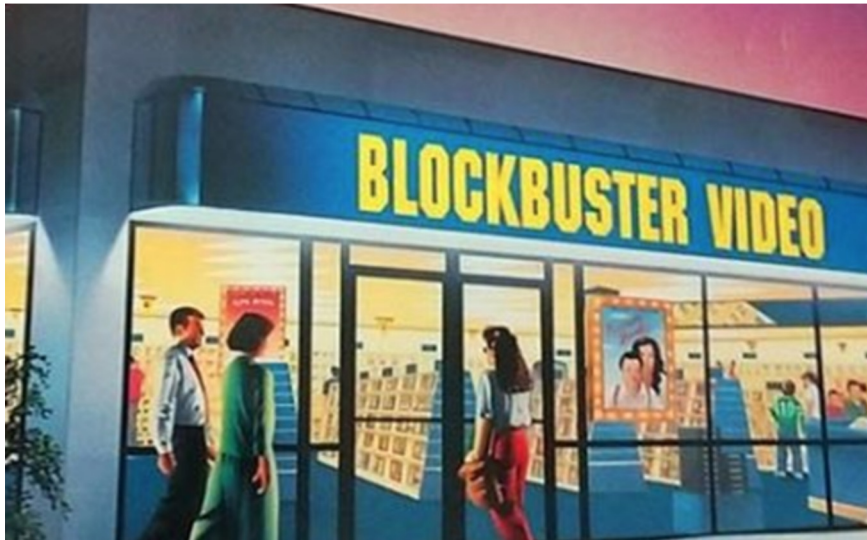
Carles Bo
Institute of Chemical Research of Catalonia (ICIQ)
Tarragona

Research Data Management in HPC
#HPC.NRW
14/5/2024

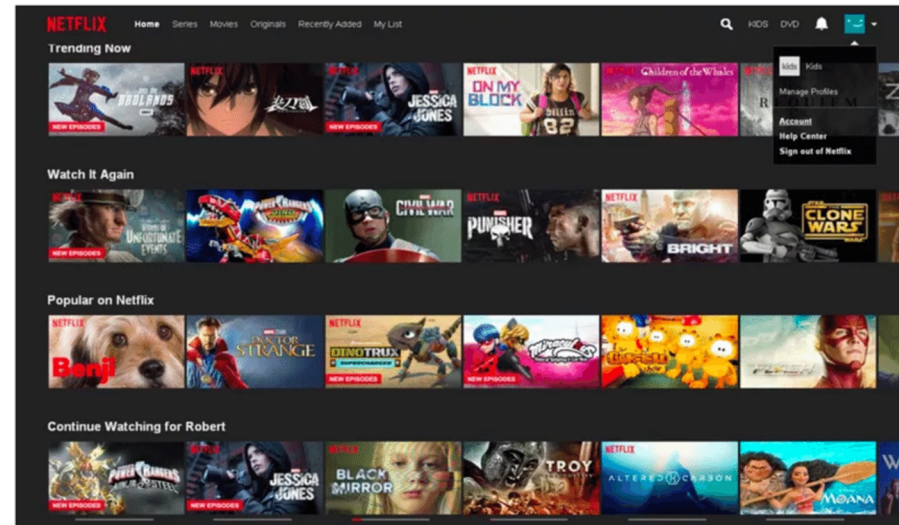


The **NETFLIX** disruption

HOW IT STARTED



HOW IT'S GOING



The **NETFLIX** disruption

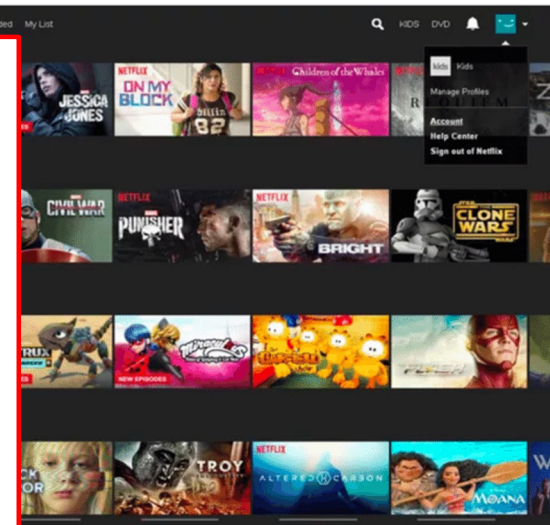
HOW IT STARTED



Killer features

- Online content (24/7)
- User-Friendly Interface
- Easy content search
- Categories and themes
- Flexibility and Portability
- Cost-Effective

HOW IT'S GOING

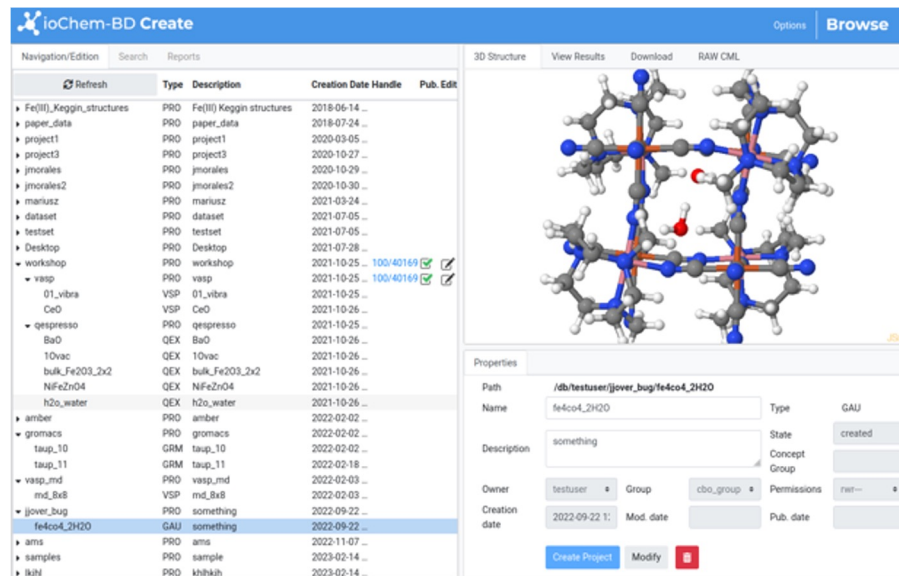


The ioChem-BD disruption

HOW IT STARTED



HOW IT'S GOING



The screenshot shows the ioChem-BD Create web interface. On the left, there is a table listing various projects and datasets. On the right, there is a 3D molecular structure visualization of a complex molecule, likely a protein-ligand complex. Below the structure, there are property fields for the selected project.

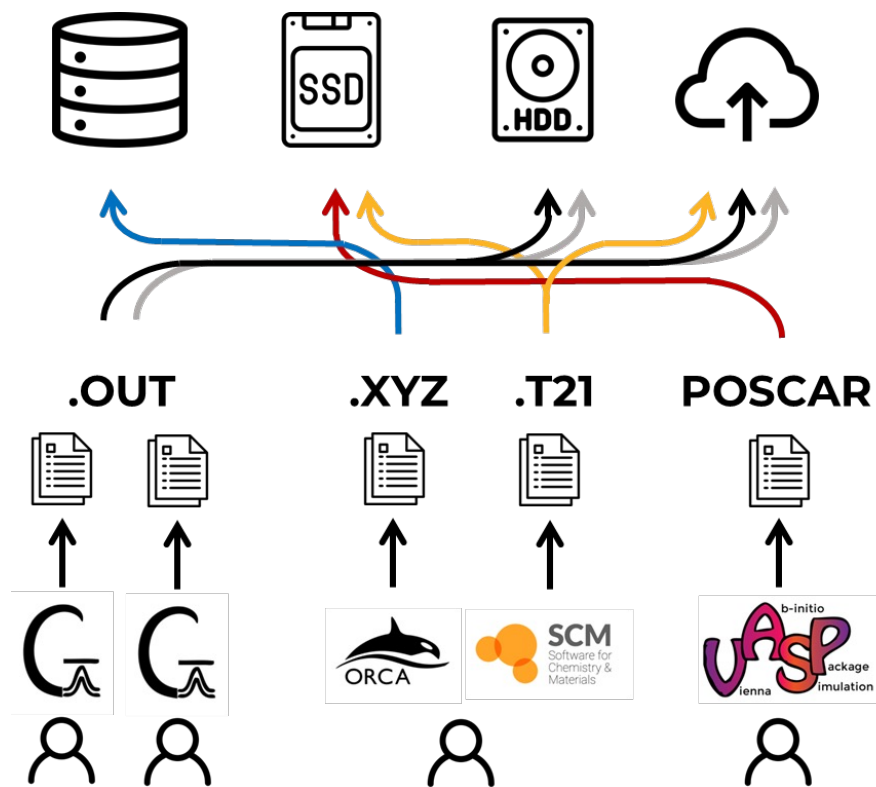
Type	Description	Creation Date	Handle	Pub. Edit
PRO	Fe(II) Keggin structures	2018-06-14
PRO	paper_data	2018-07-24
PRO	project1	2020-03-05
PRO	project3	2020-10-27
PRO	jmorales	2020-10-29
PRO	jmorales2	2020-10-30
PRO	marusz	2021-03-24
PRO	dataset	2021-07-05
PRO	testset	2021-07-05
PRO	Desktop	2021-07-28
PRO	workshop	2021-10-25	100/40169	✓
PRO	vasp	2021-10-25	100/40169	✓
VSP	01_vibra	2021-10-25
VSP	CoO	2021-10-26
QESPRESSO	qespresso	2021-10-25
QEX	BaO	2021-10-26
QEX	10vac	2021-10-26
QEX	bulk_Fe203_2x2	2021-10-26
QEX	NFeZnO4	2021-10-26
QEX	h2o_water	2021-10-26
PRO	amber	2022-02-02
PRO	gromacs	2022-02-02
GRM	taup_10	2022-02-02
GRM	taup_11	2022-02-18
PRO	vasp_md	2022-02-03
VSP	md_8x8	2022-02-03
PRO	something	2022-09-22
GAU	fe4co4_2H2O	2022-09-22
PRO	ams	2022-11-07
PRO	sample	2023-02-14
PRO	khkh	2023-02-14

Properties for the selected project:

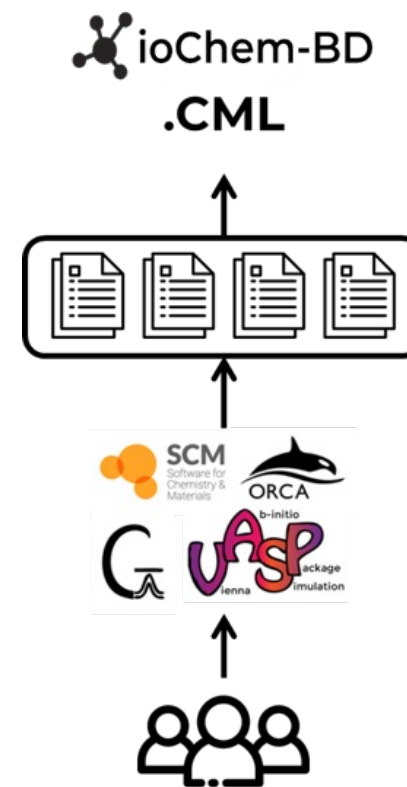
- Path: /db/testuser/jover_bug/fe4co4_2H2O
- Name: fe4co4_2H2O
- Type: GAU
- Description: something
- Owner: testuser
- Group: cbo_group
- Creation date: 2022-09-22 11:...

The ioChem-BD disruption

HOW IT STARTED



HOW IT'S GOING



Journal	Journal	Journal	Journal paper report				
/db/	41	/db/	/db/malvares/quintet/turbo				
	42		Atom	X	Y	Z	
1	43	1	1	N	0.0045	0.0019	-0.0695
2	44	2	2	Sc	1.1440	1.6738	-0.1053
3	45	3	3	Sc	0.9089	-1.8060	-0.0320
4	46	4	4	Sc	-2.0200	0.1475	-0.0691
5	47	5	5	C	-1.7648	-2.9982	-2.1960
6	48	6	6	C	-0.5818	-2.7742	-2.9878
7	49	7	7	C	-0.7688	-1.5586	-3.7370
8	50	8	8	C	-2.0630	-1.0356	-3.4115
9	51	9	9	C	-2.6833	-1.9219	-2.4587
10	52	10	10	C	-3.5577	-1.4382	-1.4369
11	53	11	11	C	-3.5150	-2.0918	-0.1667
12	54	12	12	C	-2.5985	-3.1650	0.0962
13	55	13	13	C	-1.6841	-3.5913	-0.9087
14	56	14	14	C	-0.3853	-4.0172	-0.4597
15	57	15	15	C	0.8018	-3.8618	-1.2532
16	58	16	16	C	0.7068	-3.1442	-2.5092
17	59	17	17	C	1.8079	-2.3128	-2.8626
18	60	18	18	C	1.6309	-1.1049	-3.6130
19	61		19	C	0.3247	-0.6831	-4.0160
20	62		20	C	0.0640	0.7188	-4.0583
21	63		21	C	-1.2322	1.2405	-3.7209
22	64		22	C	-2.2893	0.3669	-3.3498
23	65		23	C	-3.2116	0.8336	-2.3463
24	66		24	C	-3.9194	-0.0385	-1.4401
25	67		25	C	-4.1896	0.7049	-0.2026
26	68		26	C	-4.0402	0.0375	1.0894
27	69		27	C	-3.7316	-1.3663	1.0706
28	70		28	C	-2.9229	-2.0020	2.0881
29	71		29	C	-2.2349	-3.1067	1.4868
30	72		30	C	-0.9308	-3.4757	1.9265
31	73		31	C	-0.0154	-3.9757	0.9279
32	74		32	C	1.4165	-3.8169	1.0141
33	75		33	C	1.9502	-3.7634	-0.3547
34	76		34	C	2.9872	-2.7951	-0.6792
35	77		35	C	2.9073	-2.1201	-1.9415
36	78		36	C	3.4045	-0.7805	-2.1361
37	79		37	C	2.6137	-0.1578	-3.1632
38	80		38	C	2.3076	1.2323	-3.1183
39	81		39	C	1.0498	1.6635	-3.6140
40	82		40	C	0.3652	2.7785	-3.0054

From hundreds of pages...

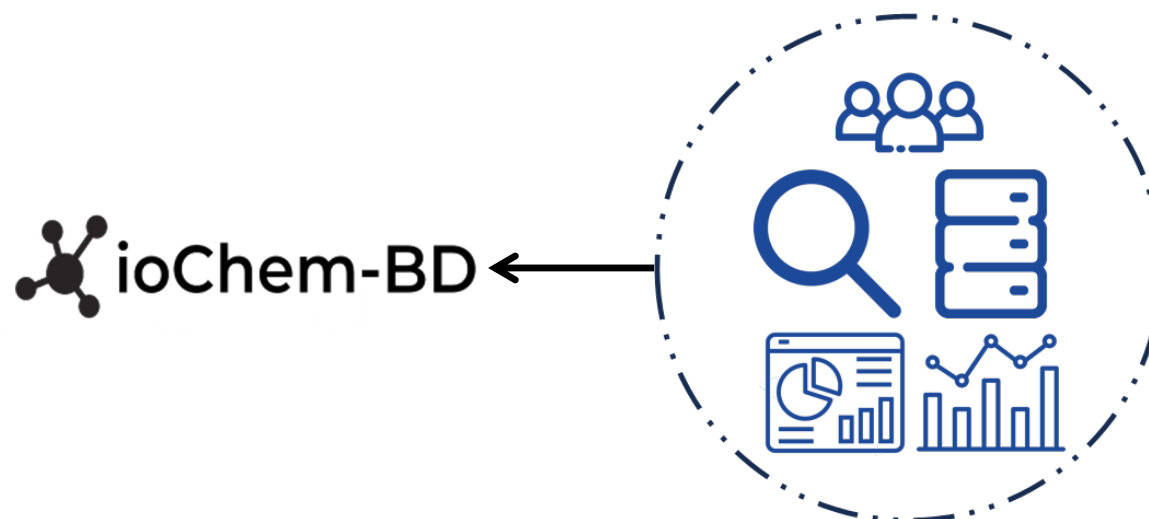
Journal paper supporting information in traditional format

... to a single link:

<https://doi.org/10.19061/iochem-bd-1-129>

R&D Challenges

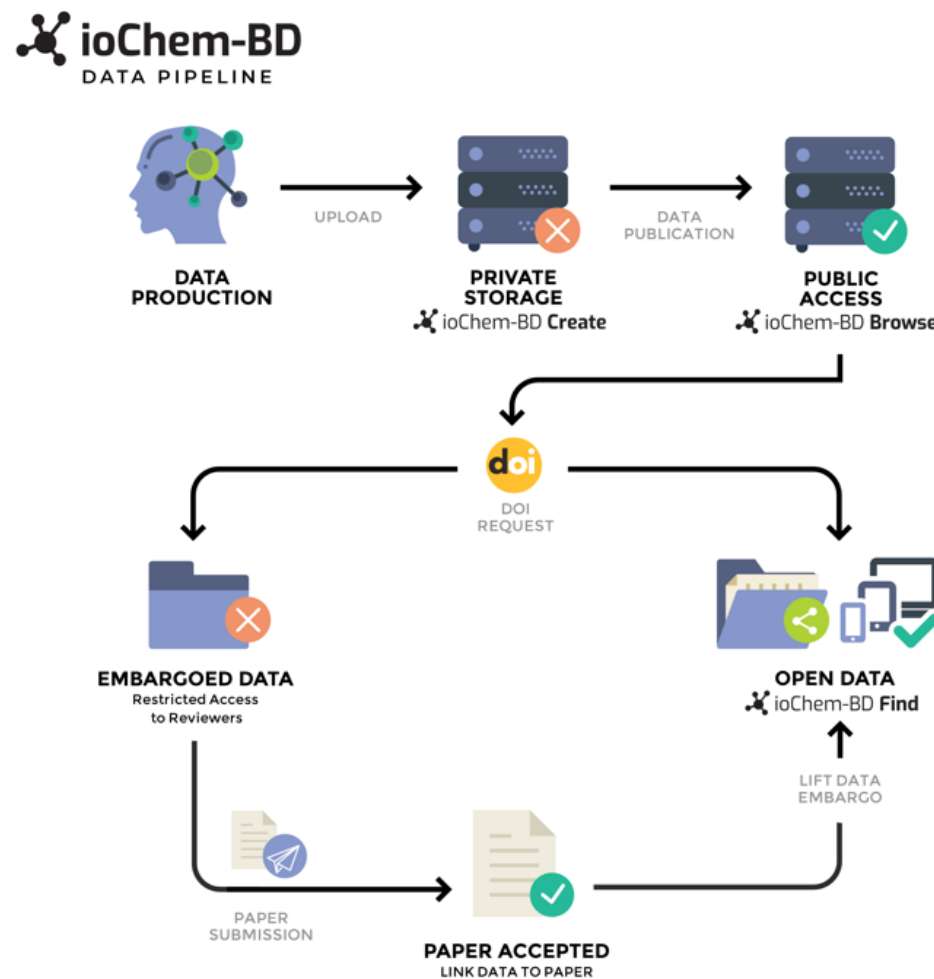
- Share
- Search
- Store
- Visualize
- Analyse



Findable, **A**ccessible, **I**nteroperable and **R**eusable data
FAIR data for new collaborative Data-Driven research

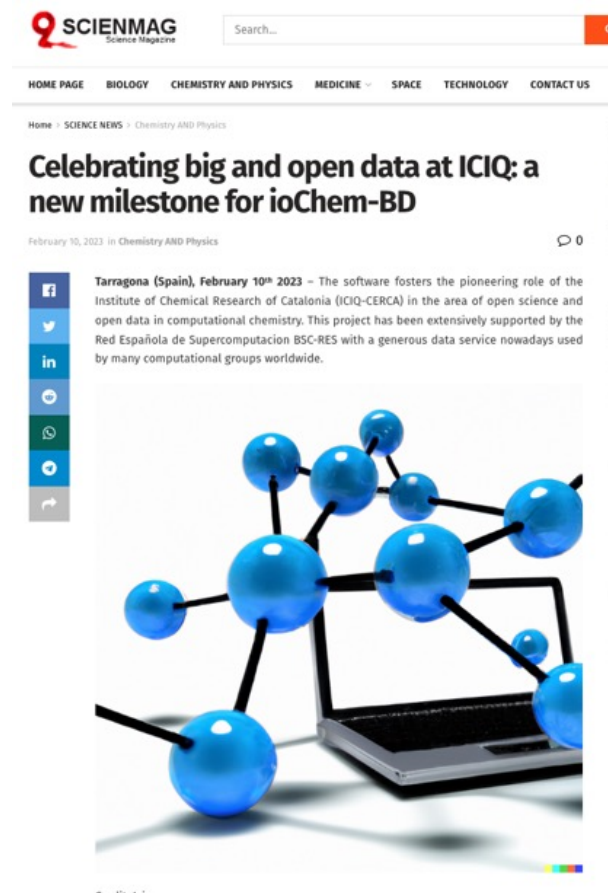
R&D Solutions

- Storage reduction
- Data Organization
- Easy retrieval
- Profitable data
- Adaption to standards



About the platform

- Manage private/public data
- 10+ years' experience
- International Acceptance
- Agreements with companies



About the platform

2011

It all started as a distributed digital repository of CompChem and material science results.

Initial set of web services

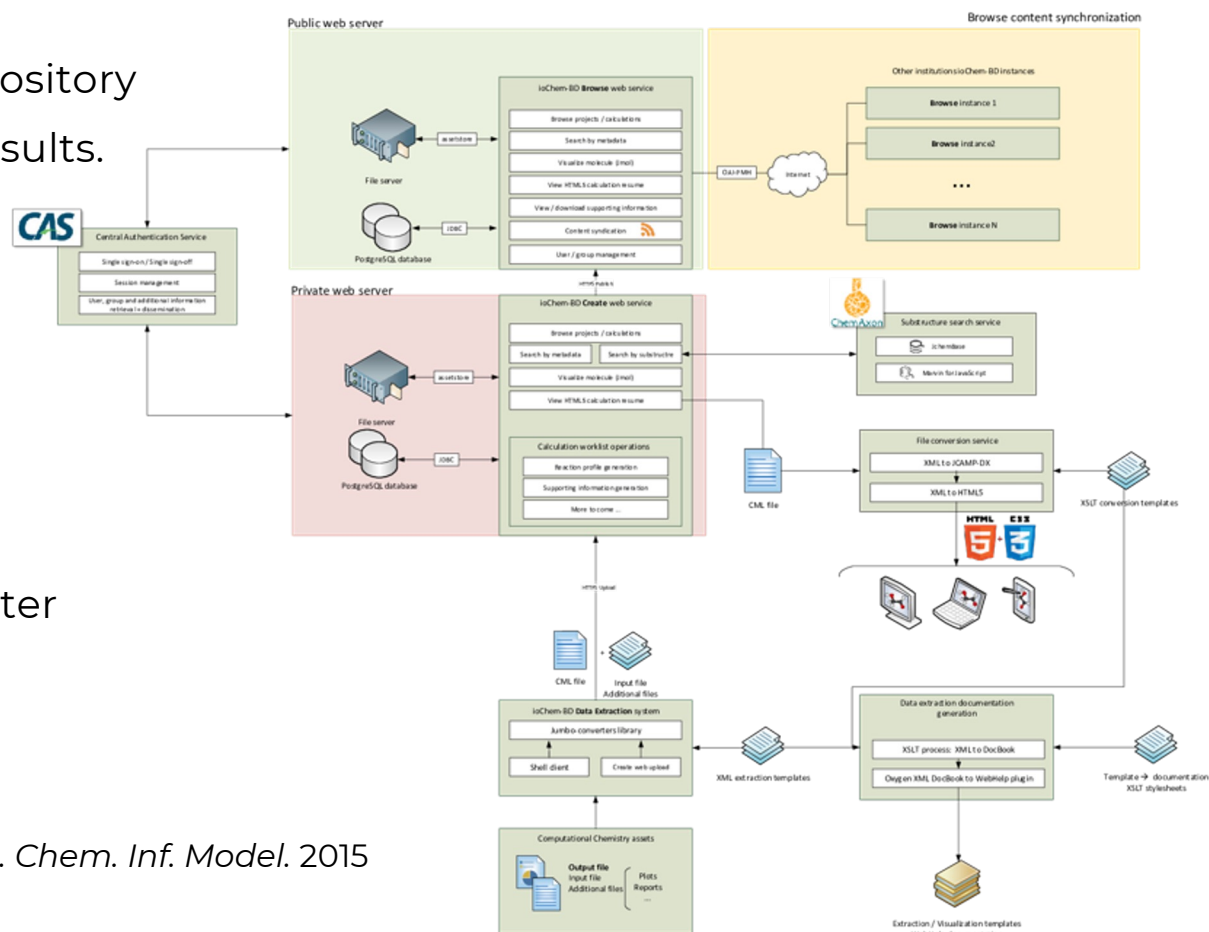
- Private space (Create module)
- Public portal (Browse module)
- Identity portal (CAS)

2017

Central node with all public assets:

- Main service Find module
- Barcelona Supercomputer Center

www.iochem-bd.org

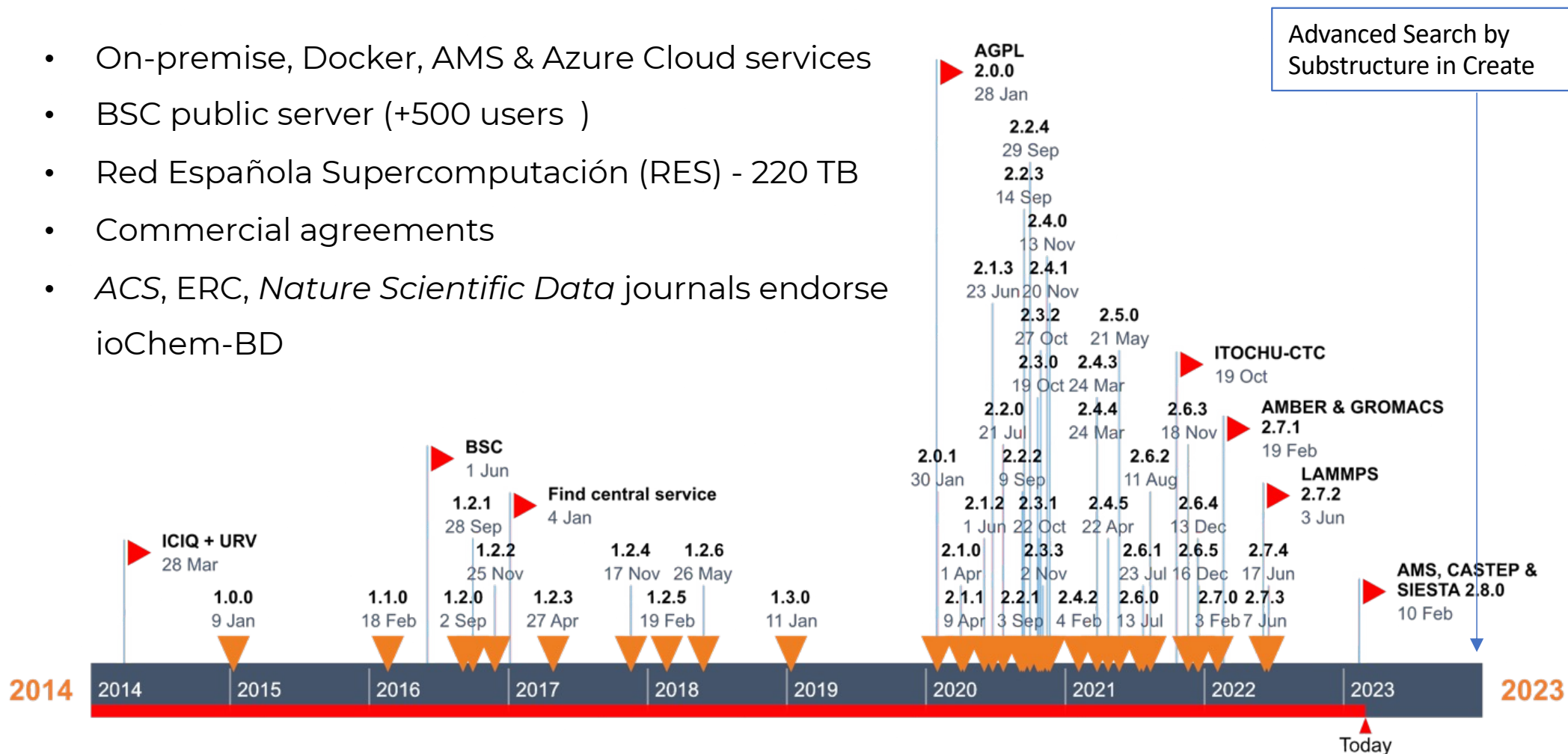


Álvarez-Moreno, de Graaf, López, Maseras, Poblet, Bo, *J. Chem. Inf. Model.* 2015

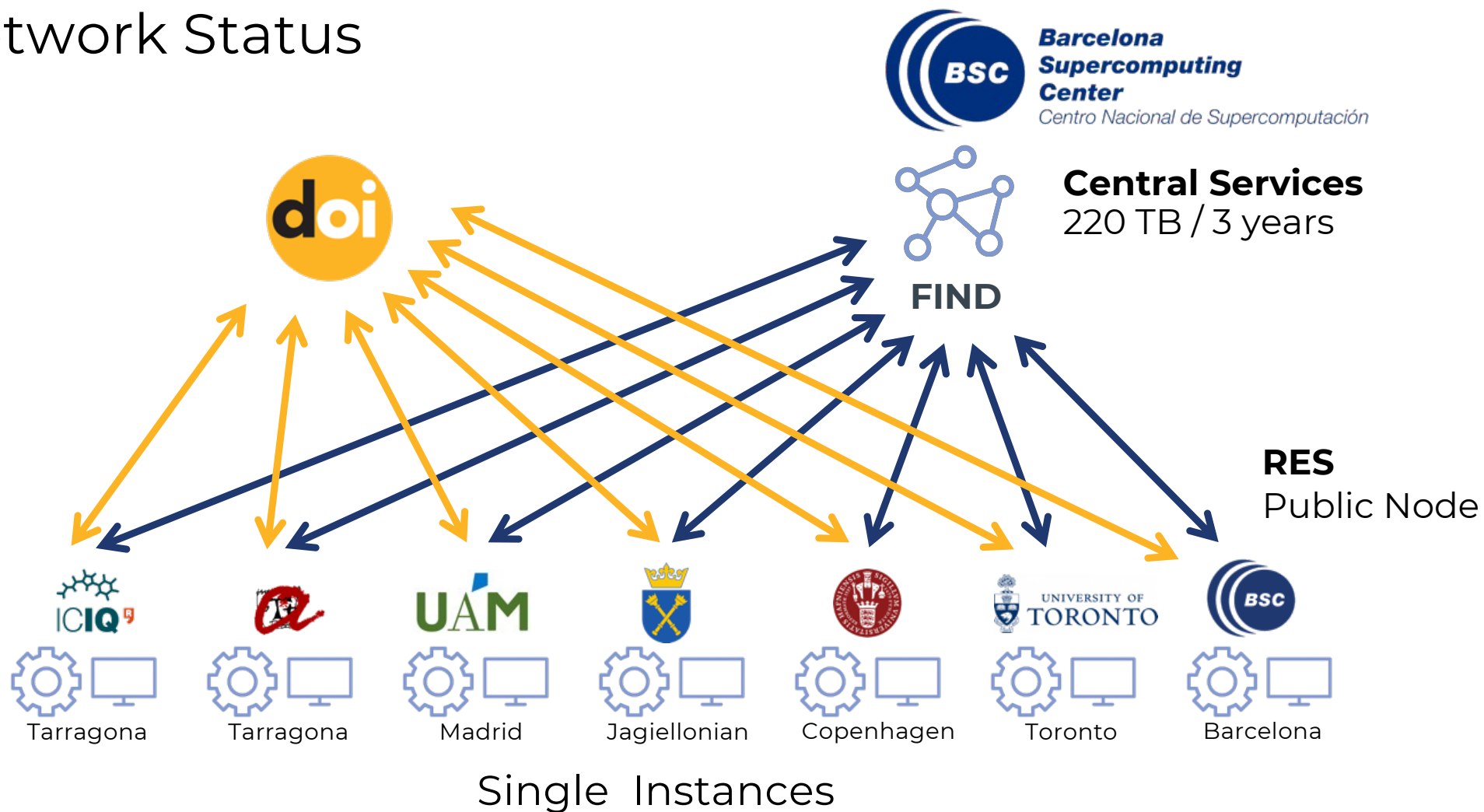
Bo, Maseras, López, *Nat. Catal.* 2018

Today

- On-premise, Docker, AMS & Azure Cloud services
- BSC public server (+500 users)
- Red Española Supercomputación (RES) - 220 TB
- Commercial agreements
- *ACS, ERC, Nature Scientific Data* journals endorse ioChem-BD

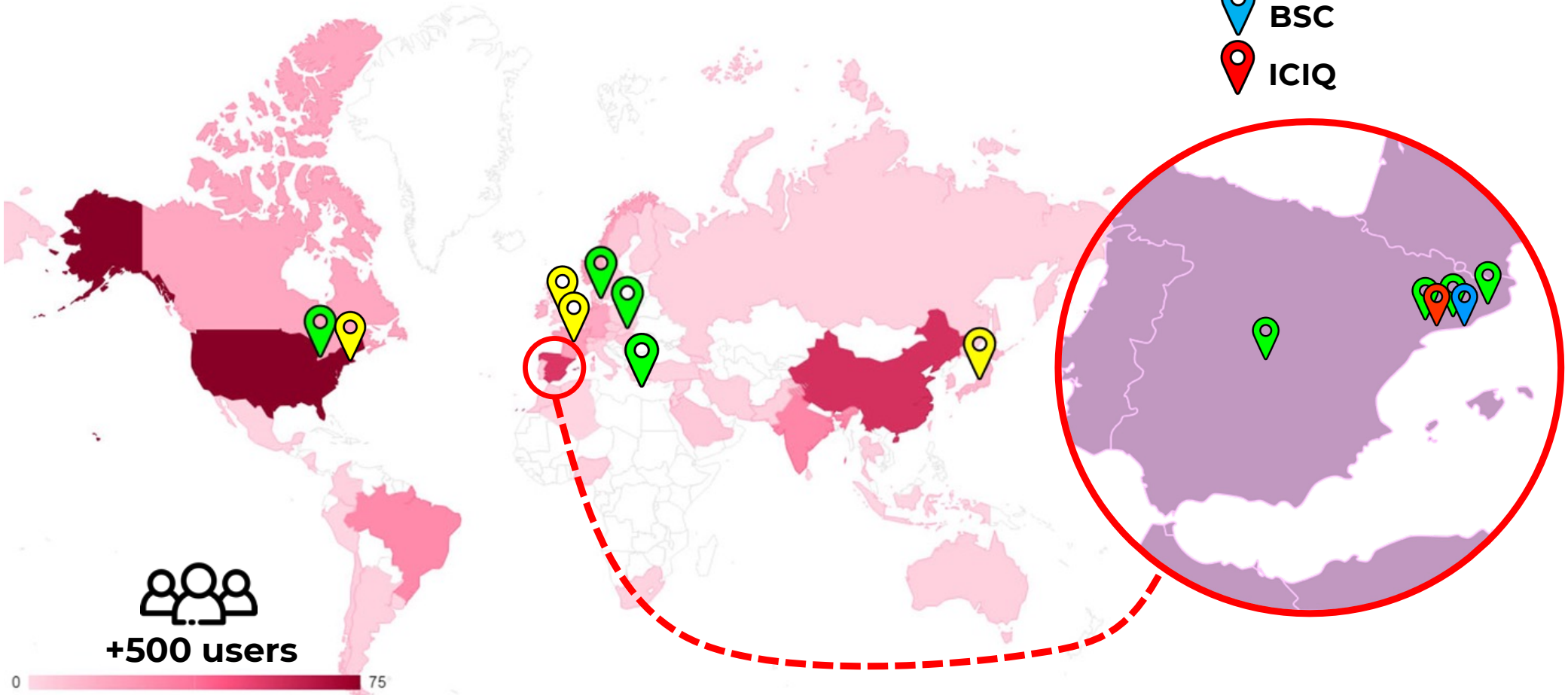


Network Status



Current Status

-  Universities
-  Commercial
-  BSC
-  ICIQ



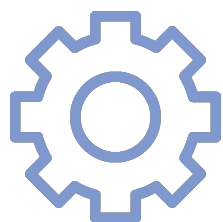
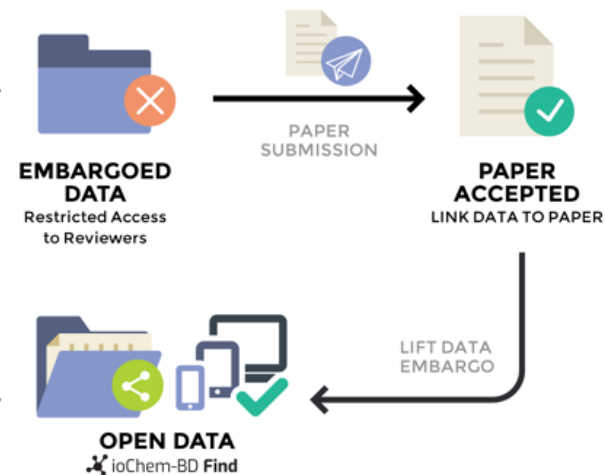
ioChem-BD DATA PIPELINE



UPLOAD



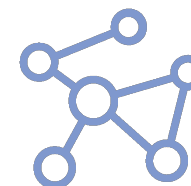
DATA PUBLICATION



CREATE



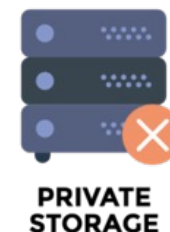
BROWSE



FIND



... the entry point



Web service / Desktop App, user-oriented, aimed at handling and managing your files on a daily basis

Features:

- Private storage area (private server, logged users only)
- Compact and intuitive interface design: Single page application (SPA)
- Multiple visualization tools: JSmol, JCamp-DX and HighCharts
- Search by metadata / Users / Groups
- Reports-generation tools

External services:

- Shell client interface for task automation
- REST API interface enables remote interaction and process automation (experimental)

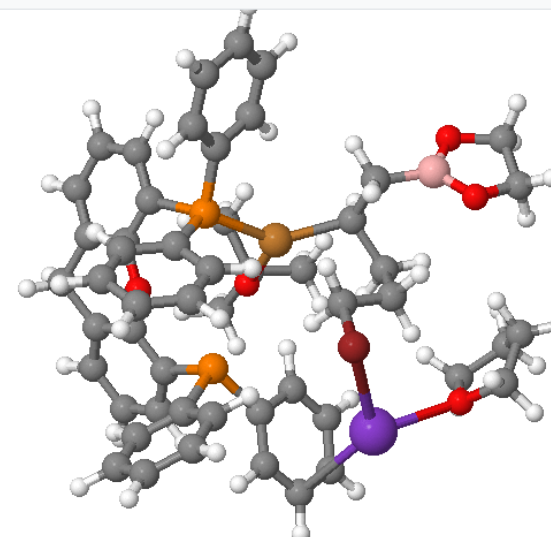
Navigation/Edition Search Reports

3D Structure View Results Download RAW CML

Refresh

Type Description Creation Date Handle Pub. Edit

	Type	Description	Creation Date	Handle	Pub. Edit
▼ Fe(III)_Keggin_structures	PRO	Fe(III) Keggin structures	2018-06-14 11:09		
▶ kimik2222	PRO	-	2018-03-07 15:35		
▶ Aromatic_Amination_of_Lactones	PRO	Aromatic_Amination_of_Lactones	2018-06-14 11:07		
gaussian_calc	GAU	-	2016-10-24 16:03		
calc	GAU	calc	2017-02-14 16:44		
calc1	GAU	calc1	2017-08-04 09:48		
K-Br-C4-1THF-I5	GAU	K-Br-C4-1THF-I5	2017-12-23 10:57		
upload_sni	GAU	uploadsni	2017-12-23 10:59		
upload_sni2	GAU	uploadsni2	2017-12-23 11:07		
upload_sni3	GAU	uploadsni3	2017-12-23 11:08		
upload_sni4	GAU	uploadsni4	2017-12-23 11:08		
▼ Mo(I)_hydrogen_generation_	PRO	Mo(I)_hydrogen_generation	2018-06-14 11:10		
cucurb	GAU	cucurb	2017-09-04 11:48		
calc1_2	GAU	calc1	2017-09-06 11:06		
hexenol2	GAU	hexenol2	2018-04-12 18:33		
sample2	ADF	sample2	2018-10-15 19:15		
▼ Ni_catalyzed_aryl_borylation_RM	PRO	Ni_catalyzed_aryl_borylation_RM	2018-06-14 11:11		
adf	ADF	adf	2015-07-13 19:12		
ts_bp-uff	GAU	ts_bp-uff	2015-07-08 18:40		
g09	GAU	g09	2015-07-09 19:13		
vasp_demo	VSP	vasp_demp	2015-07-09 20:02		
geomopt2012	ADF	geomopt2012	2015-07-09 20:03		
adf1	ADF	adf1	2015-07-13 20:31		
gaussian1	GAU	gaussian1	2015-07-13 20:32		
vasp1	VSP	vasp1	2015-07-13 20:32		
opt10	VSP	opt10	2015-07-13 20:35		
freq	ADF	freq	2015-07-13 20:39		
sample2	GAU	sample	2015-07-23 19:45		
sample3	GAU	sample	2015-07-23 19:48		
sample4	GAU	sample	2015-07-23 19:50		
sample	GAU	sample	2015-07-23 19:45		
demoGaussian	GAU	test	2015-11-04 11:18		



JSm

Properties

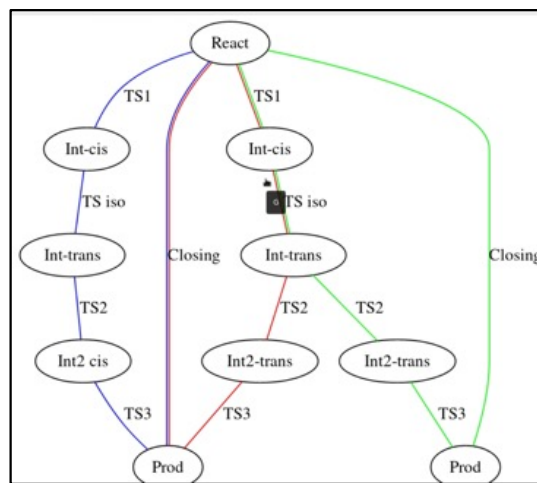
Path	/db/testuser/Fe(III)_Keggin_structures/upload_sni3		
Name	upload_sni3	Type	GAU
Description	uploadsni3	State	created
Owner	testuser	Group	cbo_group
Creation date	2017-12-23 11:08	Mod. date	
		Permissions	rw----
		Pub. date	
	<input type="button" value="Create Project"/> <input type="button" value="Modify"/> <input type="button" value="Delete"/>		

ioChem-BD Create

Navigation: Edit, Search, Reports

3D Structure | View Results | Download | RAW CML

Refresh	Type	Description	Creation Date	Handle	Pub. Edit
Fe(II)_Keggin_structures	PRO	Fe(II) Keggin structures	2018-05-14...		
paper_data	PRO	paper_data	2018-07-24...		
project1	PRO	project1	2020-03-05...		
project3	PRO	project3	2020-10-27...		
project5	PRO	project5	2020-10-29...		
project6	PRO	project6	2020-10-30...		
project7	PRO	project7	2021-03-24...		
project8	PRO	project8	2021-03-24...		
project9	PRO	project9	2021-03-24...		
project10	PRO	project10	2021-03-24...		
project11	PRO	project11	2021-03-24...		
project12	PRO	project12	2021-03-24...		
project13	PRO	project13	2021-03-24...		
project14	PRO	project14	2021-03-24...		
project15	PRO	project15	2021-03-24...		
project16	PRO	project16	2021-03-24...		
project17	PRO	project17	2021-03-24...		
project18	PRO	project18	2021-03-24...		
project19	PRO	project19	2021-03-24...		
project20	PRO	project20	2021-03-24...		
project21	PRO	project21	2021-03-24...		
project22	PRO	project22	2021-03-24...		
project23	PRO	project23	2021-03-24...		
project24	PRO	project24	2021-03-24...		
project25	PRO	project25	2021-03-24...		
project26	PRO	project26	2021-03-24...		
project27	PRO	project27	2021-03-24...		
project28	PRO	project28	2021-03-24...		
project29	PRO	project29	2021-03-24...		
project30	PRO	project30	2021-03-24...		
project31	PRO	project31	2021-03-24...		
project32	PRO	project32	2021-03-24...		
project33	PRO	project33	2021-03-24...		
project34	PRO	project34	2021-03-24...		
project35	PRO	project35	2021-03-24...		
project36	PRO	project36	2021-03-24...		
project37	PRO	project37	2021-03-24...		
project38	PRO	project38	2021-03-24...		
project39	PRO	project39	2021-03-24...		
project40	PRO	project40	2021-03-24...		
project41	PRO	project41	2021-03-24...		
project42	PRO	project42	2021-03-24...		
project43	PRO	project43	2021-03-24...		
project44	PRO	project44	2021-03-24...		
project45	PRO	project45	2021-03-24...		
project46	PRO	project46	2021-03-24...		
project47	PRO	project47	2021-03-24...		
project48	PRO	project48	2021-03-24...		
project49	PRO	project49	2021-03-24...		
project50	PRO	project50	2021-03-24...		



ioChem-BD Create

Navigation: Edit, Search, Reports

3D Structure | View Results | Download | RAW CML

Choose geometry file:

Properties

Path: /db/malvarez/moldorb/moldorb

Name: moldorb

Type: MOL

State: created

Description: moldorb

Owner: malvarez

Creation date: 2023-02-28 10:25

Mod. date: 2023-02-28 10:25

Pub. date: 2023-02-28 10:25

ioChem-BD Create

Navigation: Edit, Search, Reports

3D Structure | View Results | Download | RAW CML

Choose geometry file:

Properties

Path: /db/malvarez/moldorb/moldorb

Name: moldorb

Type: MOL

State: created

Description: moldorb

Owner: malvarez

Creation date: 2023-02-28 10:25

Mod. date: 2023-02-28 10:25

Pub. date: 2023-02-28 10:25

ATOM INFO

Atomic coordinates [Å]

MOLECULAR INFO

Charge / Multiplicity: 0/1

Polarizable Continuum Model (PCM)

Model: PCM (using non-symmetric T-matrix)

Atomic radii UFF

Solvent: Water

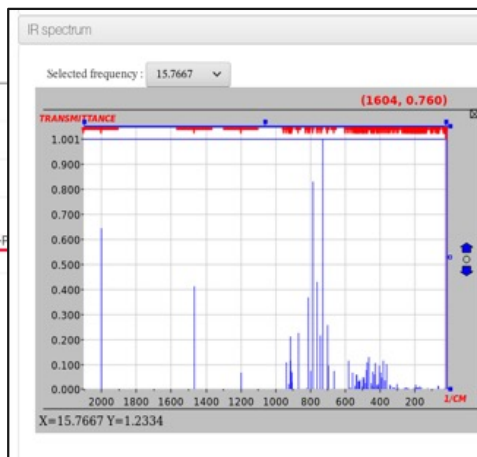
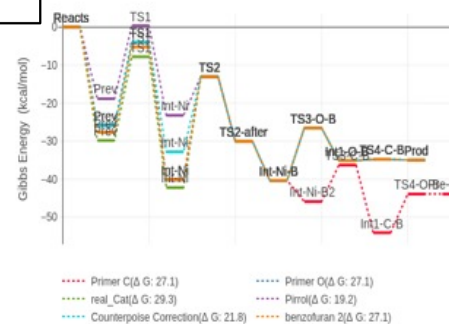
Rp(=): 78.333300

Rp(=)Co: 1.777644

JOB

Energies

Energy	Value	Units
SCF Done:	-2874.33514339	Eh
Zero-point correction	0.123406	Eh
Thermal correction to Energy	0.184510	Eh
Thermal correction to Enthalpy	0.184510	Eh
Thermal correction to Gibbs Free Energy	0.017264	Eh
Sum of electronic and zero-point Energies	-2874.211733	Eh
Sum of electronic and thermal Energies	-2874.150611	Eh
Sum of electronic and thermal Enthalpies	-2874.149460	Eh
Sum of electronic and thermal Free Energies	-2874.117637	Eh



Choose orbital file:

15 Alpha 16a 1.979 0.000

Properties

Path: /db/malvarez/moldorb/orbitals/casscf

Name: casscf

Type: MOL

State: created

Description: casscf

Owner: malvarez

Creation date: 2023-02-28 10:25

Mod. date: 2023-02-28 10:25

Pub. date: 2023-02-28 10:25

Create Shell client

- Command line tool (Unix-like OSes)
- Operates ioChem-BD Create module
- Provides repository specific commands
- Integrable inside scripts for:
 - Large batch uploads or
 - Automatic upload after content creation



```
$ . $HOME/shell/start-rep-shell
$ cpro -n metOH-oxidation -d metOH-oxidation
$ cdpro metOH-oxidation
$ cpro -n MoO2 -d MoO2
$ cdpro MoO2
$ cpro -n metOH -d metOH
$ cdpro metOH
$ cpro -n freq -d freq
$ cdpro freq
$ loadvasp -i INCAR2 -o OUTCAR2 -n opt2 -d opt2 -kp KPOINTS
-dc DOSCAR
$ exit-rep
```

```
#!/bin/bash
#` -pe smp* 12
#$ -N test
#$ -cwd

input=input.in  output=output.out

/home/programs/bin/gaussian09.sh C01 :math: $input $output
. $HOME/shell/start-rep-shell
loadgauss -i $input -o $output -n $output -d $output -auto
exit-rep
```

launch_and_upload.sh

Create REST API



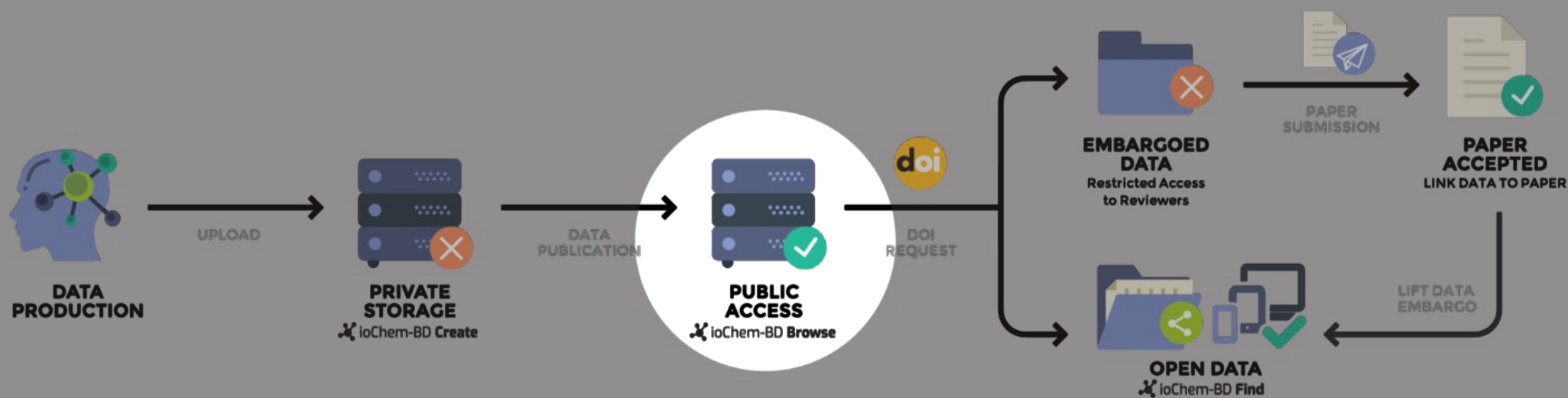
- Representational state transfer API (REST)
- Service is:
 - Stateless
 - Extensible
 - Service-oriented
 - Bundled with a uniform interface
- Enables querying and modifying data from a command line or automated service.
- Machine oriented
- Can be easily extended with new endpoints

The screenshot shows the Swagger API interface for the 'Create REST API 1.0'. The header includes the Swagger logo and the text 'Create REST API 1.0'. Below the header, there is a section for 'calculation' with several endpoints listed, each with a method (GET or POST) and a description. The endpoints are:

- POST /create-rest/api/calculation: Creates a new calculation
- GET /create-rest/api/calculation/{calcId}: Find calculation by ID
- GET /create-rest/api/calculation/{calcId}/file: Returns all files related to a calculation
- POST /create-rest/api/calculation/{calcId}/file: Add a new file to an existing calculation
- GET /create-rest/api/calculation/{calcId}/file/{fileId}: Retrieve a file from a calculation
- GET /create-rest/api/calculation/{calcId}/geometry: Returns the calculation (final) geometry as a download
- POST /create-rest/api/calculation/{calcId}/query: Query calculation fields

Below the 'calculation' section, there is a 'health-check' section with a 'Health check endpoint' and a 'project' section with 'Operations related to projects'.

ioChem-BD DATA PIPELINE



Data flow along the different modules: Browse

ioChem-BD **Browse** ... *the open repository*



**PUBLIC
ACCESS**

Open web portal where content published from the Create module is displayed.

Features:

- DOIs and permanent storage for users' published datasets
- Easy navigation across dataset collections
- Allows browsing by term and facet navigation
- Same visualization tools as Create: JSmol, JCamp-DX and HighCharts
- Search by multiple administrative and descriptive metadata fields
- Dspace allows easy content syndication, data replication and data harvesting

External services:






- Data services to offer public data to third party services and social networks.
- Multiple services and connectors: REST API, RDF, OAI-PMH



Welcome to the ioChem-BD repository of
Institute of Chemical Research of Catalonia!

Communities in Browse

Choose a community to browse its collections.

	Bo Research Group
	Llobet Research Group
	Lloret-Fillol Research Group
	López Research Group
	Maseras Research

Discover

Author

García Muelas, Rodrigo	5547
Besora, Maria	3924
Fako, Edvin	1935
González Fabra, Joan	1656
Li, Qiang	1038
Navarro-Ruiz, Javier	573
Cornu, Damien	571

Subject

Palladium	3179
Platinum	3064
Ruthenium	2743
Methanol	2493
Principal Component Analysis	2018
Nickel	1858
Alcohols	1795

Date Issued

2017	1
------	---

Method

DFT	5580
RB3LYP	4160
RwB97XD	785
UB3LYP	737
RB97D3	683

Collections in this community

[Alkali-Driven Disassembly and Reassembly of Molecular Niobium Oxide in Water](#) DOI: [10.19061/iochem-bd-1-88](#)

Alkali counterions for polyoxometalate (POM) clusters control solubility with distinct periodic trends, but evidence for alkali control over speciation is ambiguous. Here we show that a simple Nb-POM, $[\text{Nb}_{10}\text{O}_{28}]^{6-}$ ($\{\text{Nb}_{10}\}$), converts to oligomers of $(\text{H}_x\text{Nb}_{24}\text{O}_{72})^{(24-x)-}$ ($\{\text{Nb}_{24}\}$) upon adding only alkali chloride salts, even in buffered neutral solutions.

This dataset derived results are published in:

Manuscript title: Alkali-Driven Disassembly and Reassembly of Molecular Niobium Oxide in Water

Journal: J. Am. Chem. Soc.

DOI: [10.1021/jacs.8b05015](#)

[Al\(x\)Cr\(y\)_Keggin_oxos](#) DOI: [10.19061/iochem-bd-1-23](#)

This dataset derived results are published in:

Manuscript title: Crystallizing Elusive Chromium Polycations.

Journal: Chem

DOI: [10.1016/j.chempr.2016.11.006](#)

[A Metal-Free Synthesis of N-Aryl Carbamates under Ambient Conditions](#) DOI: [10.19061/iochem-bd-1-3](#)

This dataset derived results are published in:

Manuscript title: A Metal-Free Synthesis of N-Aryl Carbamates under Ambient Conditions

Journal: Angew. Chem. Int. Ed.

DOI: [10.1002/anie.201504956](#)

[Analysis of the interaction between Keplerate nanocapsules and their anionic ligands](#) DOI: [10.19061/iochem-bd-1-33](#)

This dataset derived results are published in:

Manuscript title: Anions coordinating anions: Analysis of the interaction between anionic Keplerate nanocapsules and their anionic ligands

Journal: PCCP

DOI: [10.1039/C6CP08511C](#)

U@C82_U@C74 collection home page

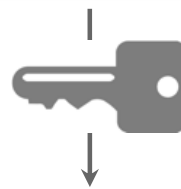
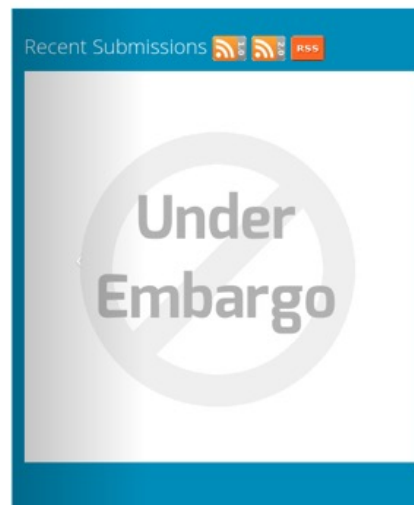
Share - copy and redistribute the material in any medium or format. Adapt - remix, transform, and build upon the material for any purpose, even commercially. The licensor cannot revoke these freedoms as long as you follow the license terms.

Please use this identifier to cite or link to this collection: DOI: 10.19061/chem-bd-2-14

No other publication derived

View as [Tree](#) [List](#) Search:

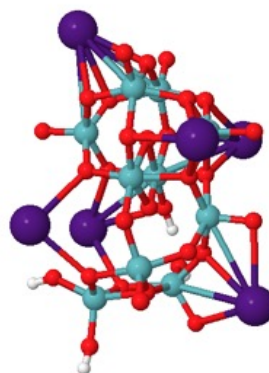
Preview	Title	Issue Date	Author(s)	Program	Calculation type	Method(s)	Basis Set	Ener
Under embargo	/U@C74/U@C74_opt_U@C74_1_triplet	30-Jan-2017	Roser, Morales	ADF; 2013; 01	Geometry optimization	DFT	TZP	-23. ER
Under embargo	/U@C82/U@C82_opt_U@C82_5_A Quintet	30-Jan-2017	Roser, Morales	ADF; 2013; 01	Geometry optimization	DFT	TZP	-26. ER
Under embargo	/U@C82/U@C82_opt_U@C82_5_A triplet	30-Jan-2017	Roser, Morales	ADF; 2013; 01	Geometry optimization	DFT	TZP	-26. ER
Under embargo	/U@C82/U@C82_opt_U@C82_5_B Quintet	30-Jan-2017	Roser, Morales	ADF; 2013; 01	Geometry optimization	DFT	TZP	-26. ER



Reviewers link

Institute of Chemical Research of Catalonia / Bo Research Group
/ Alkali-Driven Disassembly and Reassembly of Molecular Niobium Oxide in Water

Geometry:



Actions:

[View data](#)

[Download geometry](#)

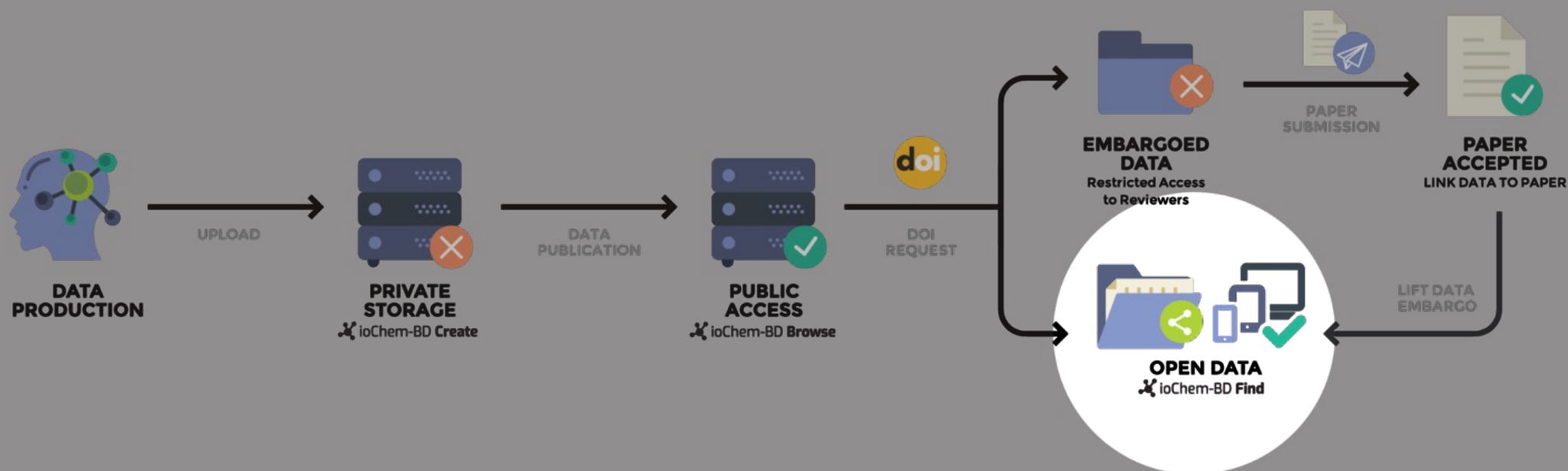
Files in This Item:

File	Size	Format	
NB10_Cs_C1_EHFN.in	3.11 kB	Gaussian Input format	Download
output.cml	588.98 kB	Chemical Markup Language	Download

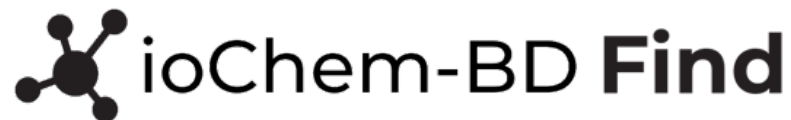
Referenced by:

Manuscript title: Alkali-Driven Disassembly and Reassembly of Molecular Niobium Oxide in Water
Journal: J. Am. Chem. Soc.
DOI: 10.1021/jacs.8b05015

ioChem-BD DATA PIPELINE



Data flow along the different modules: Find



... or the distributed database



Central point and search engine

Features:

- Fed by ioChem-BD distributed nodes whenever a new item/collection is published
- Advanced indexing of chemical data and metadata (InChi, smiles)
- Fast search engine implemented over Apache Solr and RDKit frameworks
- Search by chemical substructure similarity, chemical elements or any text term

Open your research to the world

ioChem-BD - The Computational Chemistry Results Repository



1

Central service



7

Connected nodes



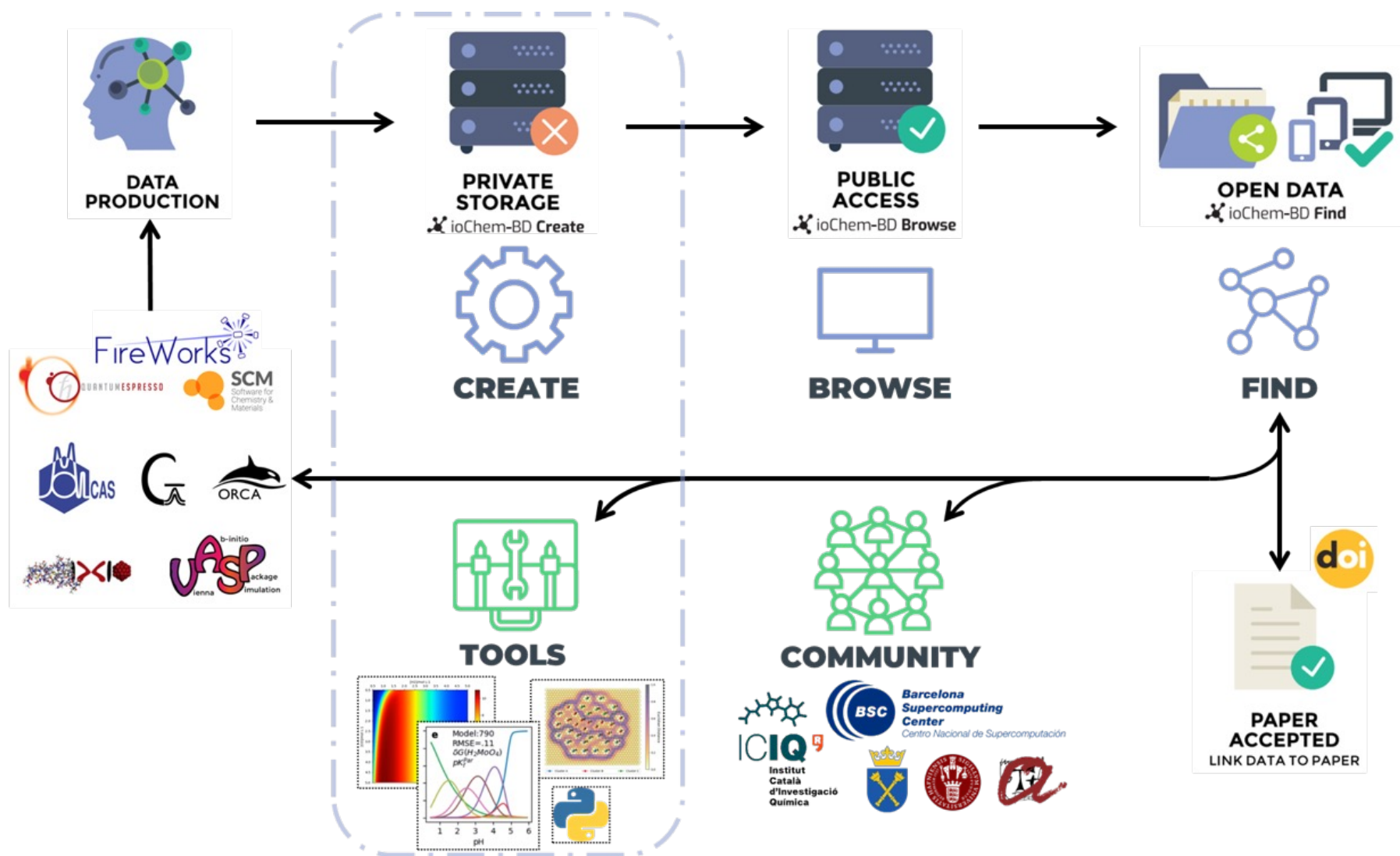
709

Collections available



360,290

Items indexed



Projects: Data to “papers”

Storage
 ioChem-BD **Browse**



Editing Webapp
AUTHOREA



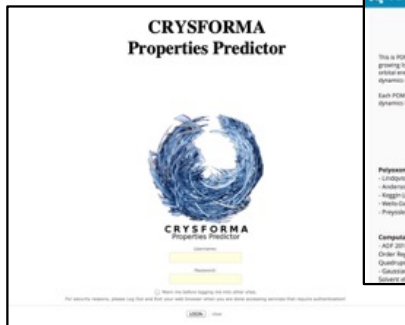
Wiley

 **QUARXiv -- Preprints for
Quantum Chemistry** ▾

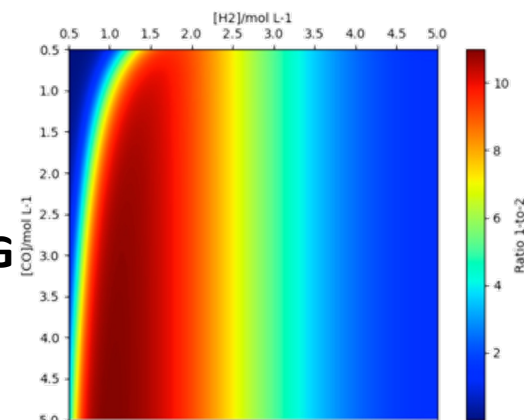
IJQC's Executable & Interactive Article

Preprints for Quantum Chemistry, by the Int. Journal of Quantum Chemistry

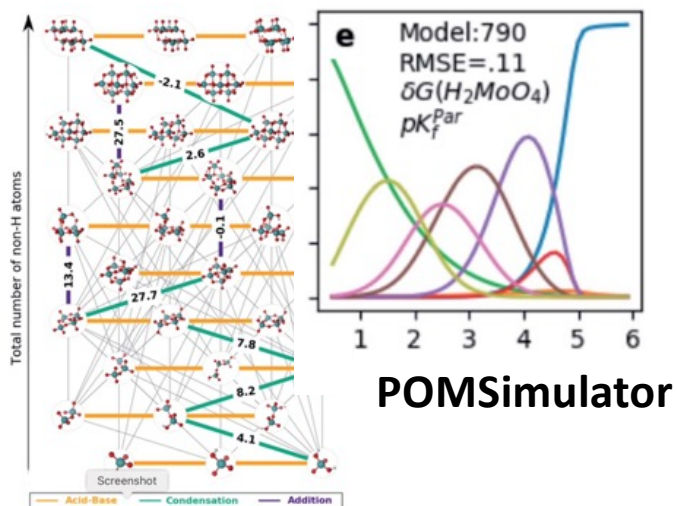
https://www.authorea.com/338280/SjnKeMOgx_Dw5IHUyE7iw



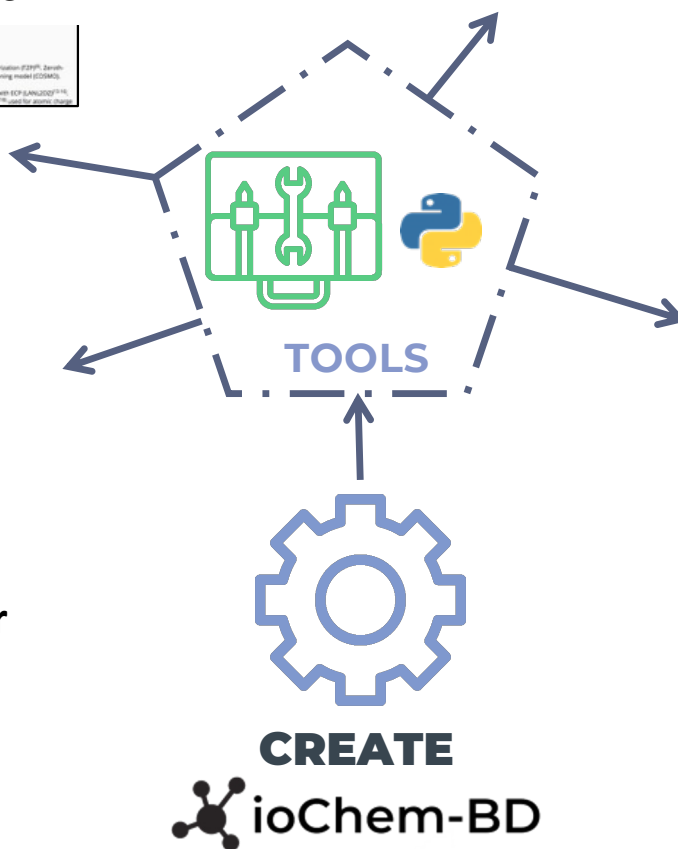
Catalytic Cycles
gTOFfee
amk-tools
OntoRXN / CRN-KG



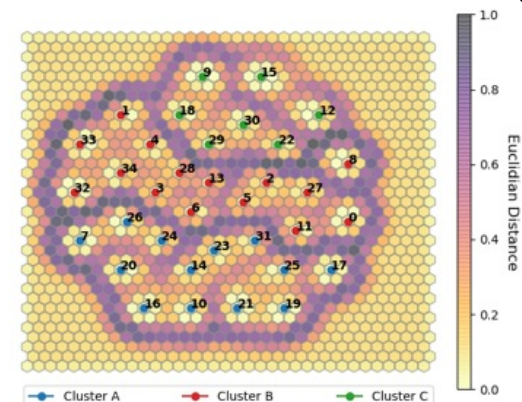
ACS Catal. **10**, 12627–12635 (2020)
ACS Phys. Chem. Au **2**, 3, 225–236 (2022)
J. Cheminformatics **14**:29 (2022)



Chem. Sci. **11**, 8448–8456 (2020)
J. Phys. Chem. A, **125**, 5212-5219 (2021)
Inorg.Chem., **61**, 13508–13518 (2022)
J. Am. Chem. Soc., **145**, 18920–18930 (2023)



AI – Machine Learning



Angew. Chem. Int. Ed. 2022, e202117839

CRYSFORMA Properties Predictor



CRYSFORMA
Properties Predictor

Username:

Password:

Warn me before logging me into other sites.

For security reasons, please Log Out and Exit your web browser when you are done accessing services that require authentication!

ioChem-BD Browse

POMsDB

This is POMsDB, a polyoxometalates (POMs) database which collects computational data on a growing list of POMs: optimized geometries, vibrational frequencies, atomic charges, molecular orbital energies, etc... Some data was combined to create all necessary files to run classical molecular dynamics simulations with GROMACS and NAMD.

Each POM contains downloadable content, such as outputs and a compressed file with the molecular dynamics files in ZIP format.

Polyoxometalates list:

- Lindqvist: M_6O_{14} M=Nb,W
- Anderson: M_7O_{24} M=Mo,W
- Keggin (alpha, beta, gamma, delta, epsilon): $XM_{12}O_{40}$
- Wells-Dawson: $X_2M_{14}O_{52}$ X=P;M=Mo,W
- Preyssler: $X_6M_{30}O_{112}$ X=P;M=W

Computational Details:

- ADF 2018 package⁽¹⁻³⁾; GGA density functional of Becke-Perdew
- Order Regular Approximation (ZORA)⁽⁷⁻⁹⁾ formalism in the relativistic
- Quadrupolar derived charges analysis⁽¹¹⁾ used for atomic charges
- Gaussian 16 package⁽¹²⁾; GGA density functional of Becke-Perdew
- Solvent effects incorporated self-consistently using the COSMO



Home

Tecnical Details

App SEPIA

Molecules available

Services

Team

Acknowledgements

Contact

» Welcome to SEPIA

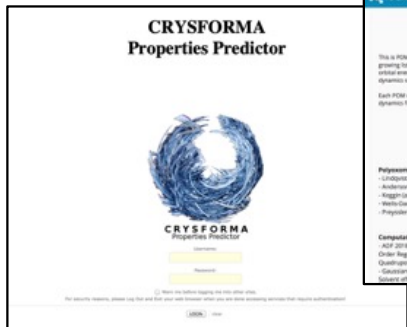
Environmental Impact Prediction Expert System SEPIA Database APP

(Sistema Experto para la Predicción del Impacto Ambiental – In Spanish)

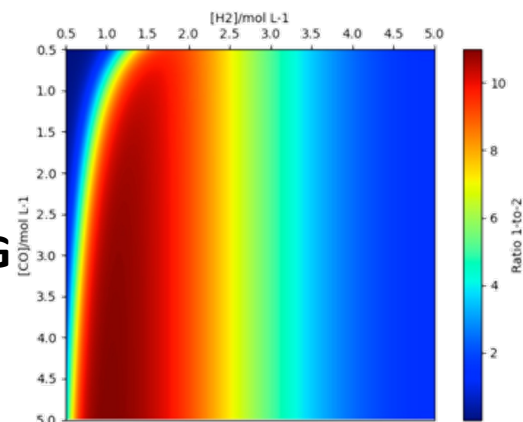
Is a powerful tool that can be used to perform risk assessment and in the development and design of new, safer pesticides.

Its main goal is to use state-of-the-art theoretical calculations to predict physico-chemical and ecotoxicological properties and to identify potential degradation products in different environments.

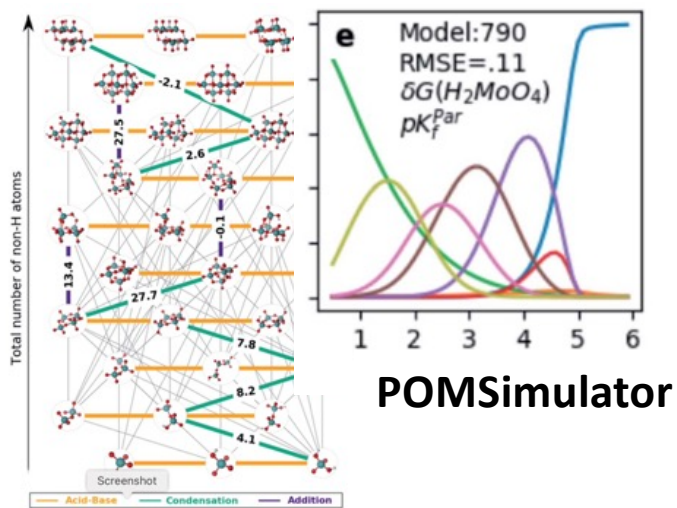
API co-crystals



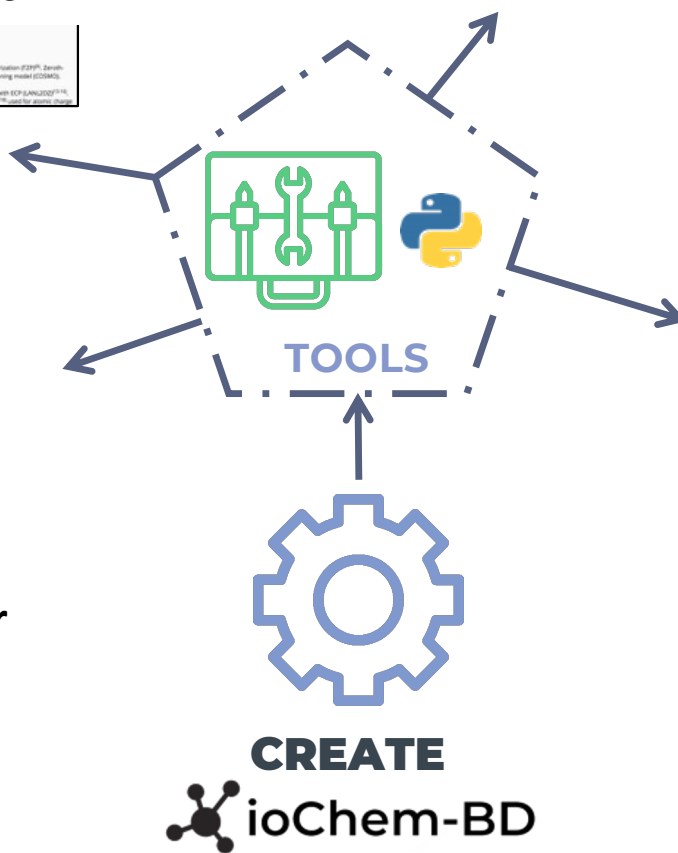
Catalytic Cycles
gTOFfee
amk-tools
OntoRXN / CRN-KG



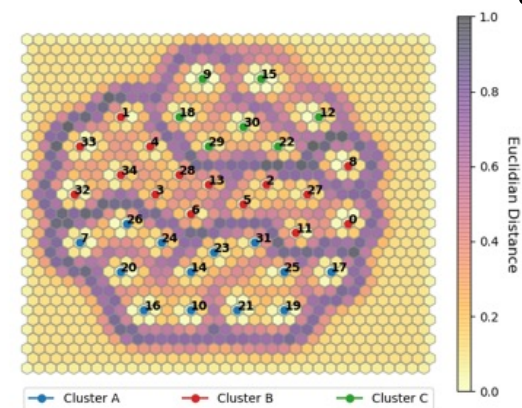
ACS Catal. **10**, 12627–12635 (2020)
ACS Phys. Chem. Au **2**, 3, 225–236 (2022)
J. Cheminformatics **14**:29 (2022)



Chem. Sci. **11**, 8448–8456 (2020)
J. Phys. Chem. A, **125**, 5212-5219 (2021)
Inorg.Chem., **61**, 13508–13518 (2022)
J. Am. Chem. Soc., **145**, 18920–18930 (2023)



AI – Machine Learning



Angew. Chem. Int. Ed. 2022, e202117839

Node configuration

Server running
Find module

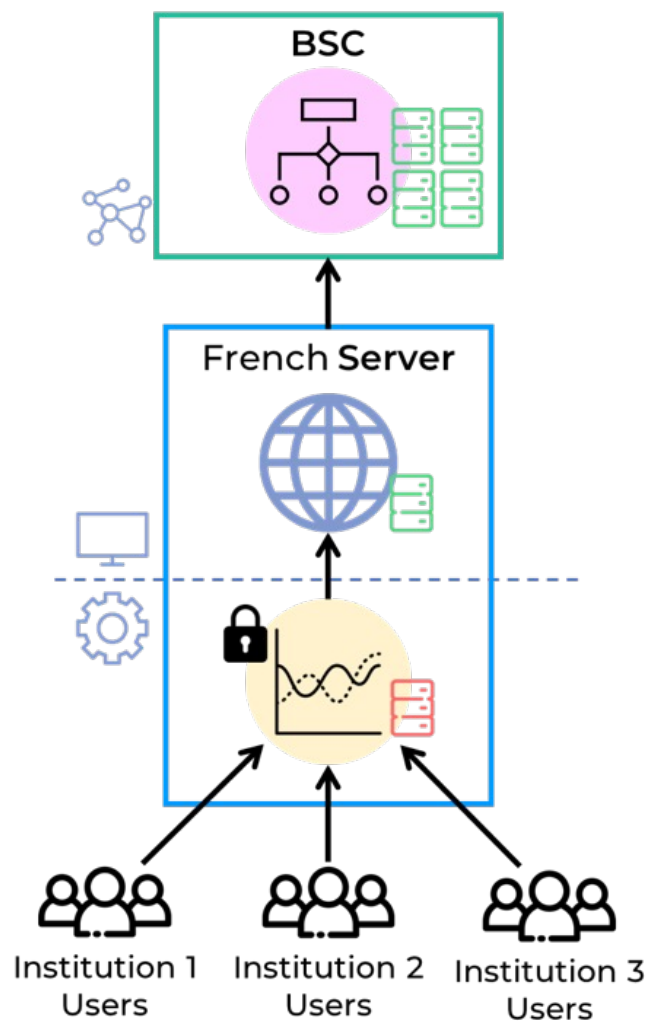
Server running
Browse module

 Public
Database

 Private
Database

 Credentials
Required

Public/Private
Boundary



ioChem-BD @BSC

Disk : Totals 20 Tb / Occ. 11 TB

Mem: 16Gb RAM

CPU: 8 cores Intel 2Ghz

Number of Users: 505

Number of Groups: 323

Datasets published: 331

Items published: 306619

Node configuration



Sign on to: ▼

- Create module
- Browse module
- Email updates
- Edit profile

Node name

Communities

University 1

University 2

- Research Group 2.1
- Research Group 2.2

University 3

- Research Group 3.1

Research Institute 1

Research Institute 2

Discover

Author

Name 1	3532
Name 2	2714
Name 3	1899
Name 4	1612

Year

2023	6001
2022	4732
2021	3003
2020	1866

Subject

Copper	8341
Graphene	7603
CO2 reduction	7881
Atom Catalyst	6392

Method

DFT	9612
RB3LYP	8613
RwB97XD	1501
PBE	1398

Concluding remarks:

ioChem-BD ...

..... is a stable and mature platform

.... and there is a lot beyond !!

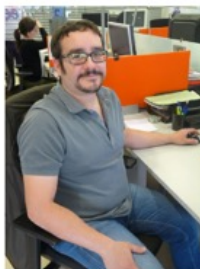
Team & Institutions



Núria Vendrell
Group Administrative
Coordinator



Martin Gumbau
System Manager



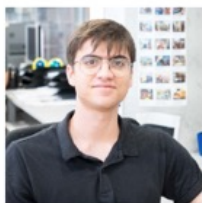
Moisés Álvarez
Programmer



Jair Wells Llanos
Technician



Aleix Mariné Tena
Technician



Marc Gruber López
Technician



**Dr. Mireia Segado
Centellas**
Postdoctoral Researcher



Dr. Diego Garay Ruiz
Postdoctoral Researcher



Alba Villar Yanez
PhD Student



Marco Nicaso
PhD Student



Jordi Bulls Casasnovas
PhD Student



Taming Computational Chemistry Data: ioChem-BD and Beyond