

Database-driven Traceability of Reagents and Stock Solutions

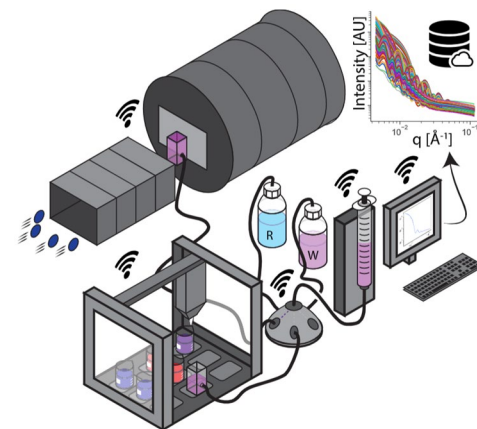
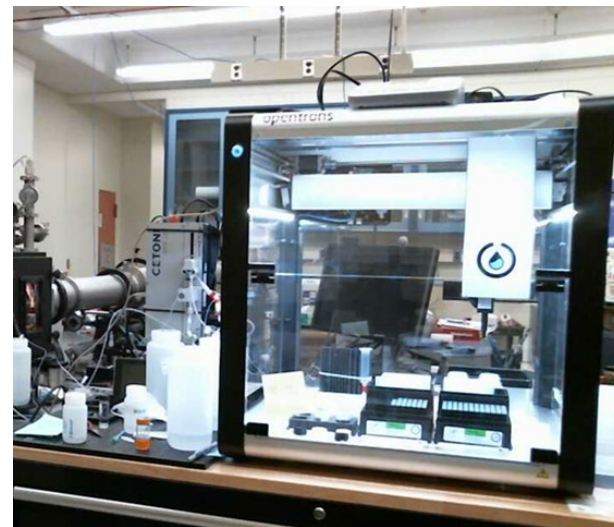
By Aaron Tian

Mentored by Dr. Peter Beaucage



Chemical Mixing Robot

- Developed by MML and NCNR
- Automatically create complex liquids
 - Personal care, biopharmacy, COVID vaccines
- Analyze structure with SANS / SAXS
 - Phase stability mapping
- Train ML network for scattering data processing



Sample Preparation

- Current process very manual
 - Target composition
 - Weigh out reagents
 - Write down quantities
 - Type back into robot
- Human Error
 - Typing/clicking
- Lack of traceability



Goals

Web app and Database(s)

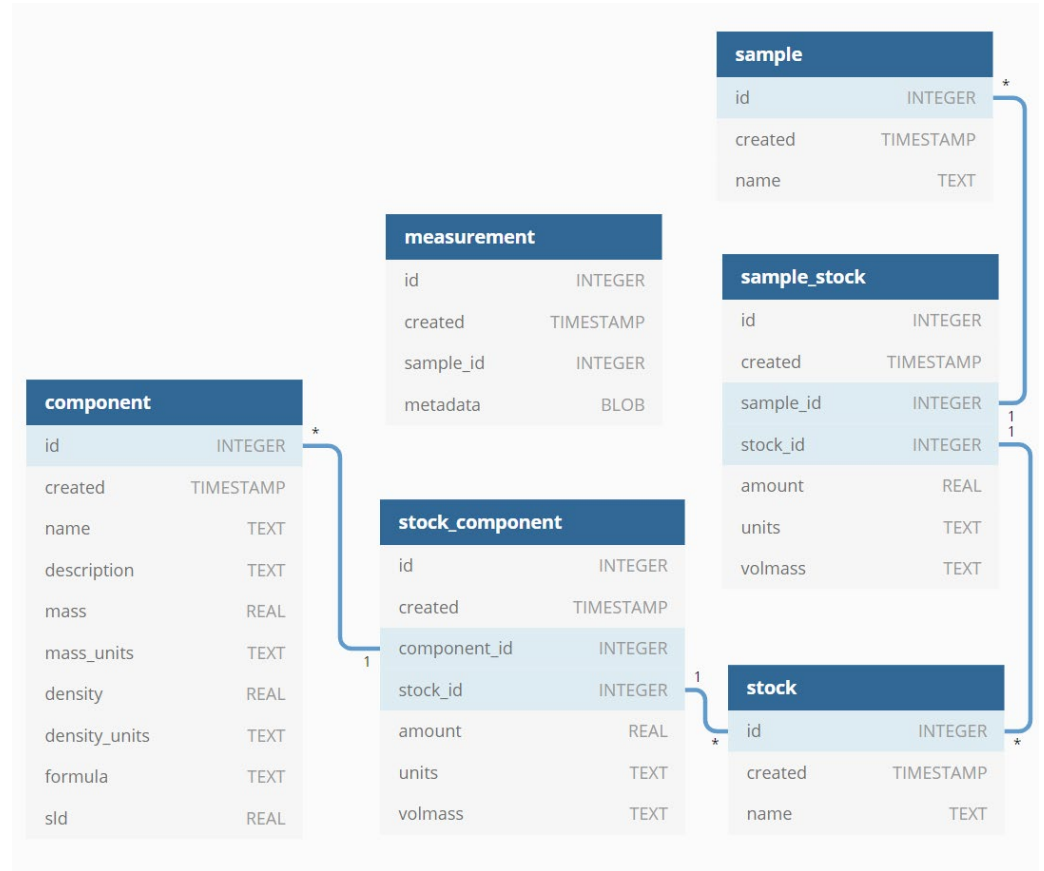
- Remove manual input in robot
 - Barcode scanning
- Centralized database view
 - Create, update entries
 - Detailed information
- Integration with already existing codebase
 - Remote entry
 - Chemistry abstractions

Database Schema

- Component
- Stock
- Sample
- Measurement

Helper Tables

- Stock Component
- Sample Stock



Number of entries per page: 10

Submit

Toggle Unified View:

29 total entries [Export CSV](#) [JSON](#)

[Send JSONs to component/send_json](#)

ethanol | ID:29

created on 2021-07-22 18:43:32

[Edit](#) [Export Individual Component](#) [Individual JSON](#)

Ethanol

Mass	0.0
Mass Units	gram / milliliter
Density	0.789
Density Units	gram / milliliter
Formula	C2H5OH
SLD	-3.448567970839845e-07

PEO5 | ID:28

created on 2021-07-22 18:43:32

[Edit](#) [Export Individual Component](#) [Individual JSON](#)

Polymer Source #P40189-EG2OH, PEO, a,w-bis(hydroxy)-terminated, 5 kDa

Mass	0.0
Mass Units	None
Density	0.0
Density Units	None
Formula	
SLD	0.0

HFblend | ID:20

22 18:43:31

[Full Component](#) [Individual JSON](#)

Handle binary solvent mixing do not use

	0.0
	gram / milliliter
	0.9
	gram / milliliter
	C4H10O2
	4.778769076797411e-08

<< first

< prev

1

2

3

next >

last >>

Number of entries per page:

Toggle Unified View:

Sort By:

29 total entries [Export CSV](#) [JSON](#)

[Send JSONs to component/send_json](#)

ID	Created	Name	Description	Mass	Mass Units	Density	Density Units	Formula	SLD	
1	2021-07-22 18:43:29	H2O	Water	0.0	gram / milliliter	1.0	gram / milliliter	H2O	-5.605201447588935e-07	Edit CSV JSON
2	2021-07-22 18:43:29	D2O	Heavy Water	0.0	gram / milliliter	1.11	gram / milliliter	D2O	6.39286252368673e-06	Edit CSV JSON
3	2021-07-22 18:43:29	EtOH	Ethanol	0.0	gram / milliliter	0.789	gram / milliliter	C2H5OH	-3.448567970839845e-07	Edit CSV JSON
4	2021-07-22 18:43:30	EtOH-d6	Deuterated Ethanol	0.0	gram / milliliter	0.892	gram / milliliter	C2D5OD	6.097571735265915e-06	Edit CSV JSON
5	2021-07-22 18:43:30	polymer	Generic Polymer	0.0	None	0.0	None		0.0	Edit CSV JSON
6	2021-07-22 18:43:30	SDS	Sodium Dodecyl Sulfate	0.0	gram / milliliter	1.01	gram / milliliter	NaC12H25SO4	3.36521864733921e-07	Edit CSV JSON
7	2021-07-22 18:43:30	CTAB	Cetrimonium bromide	0.0	None	0.0	None	C19H42BrN	0.0	Edit CSV JSON
8	2021-07-22 18:43:30	F127	Pluronic F127	0.0	None	0.0	None	C572H1146O259	0.0	Edit CSV JSON
9	2021-07-22 18:43:30	P188	Poloxamer 188	0.0	gram / milliliter	1.25	gram / milliliter		0.0	Edit CSV JSON
10	2021-07-22 18:43:30	particle	Generic Particle	0.0	None	0.0	None		0.0	Edit CSV JSON
11	2021-07-22 18:43:30	nanoparticle	Generic Nanoparticle	0.0	None	0.0	None		0.0	Edit CSV JSON
12	2021-07-22 18:43:30	hexane	Hexane	0.0	kilogram / meter ** 3	855.0	kilogram / meter ** 3	C6H14	-5.713474681683418e-07	Edit CSV JSON
13	2021-07-22 18:43:31	SiO2	Silica	0.0	None	0.0	None	SiO2	0.0	Edit CSV JSON
14	2021-07-22 18:43:31	NaCl	Sodium Chloride	0.0	None	0.0	None	NaCl	0.0	Edit CSV JSON
15	2021-07-22 18:43:31	hexanes	Hexanes	0.0	kilogram / meter ** 3	855.0	kilogram / meter ** 3	C6H14	-5.713474681683418e-07	Edit CSV JSON
16	2021-07-22 18:43:31	THF	Tetrahydrofuran	0.0	gram / milliliter	0.889	gram / milliliter	C4H8O	0.0	Edit CSV JSON
17	2021-07-22 18:43:31	PS40-PEO35	Poly(styrene)-b-poly(ethylene oxide), 40kDa - 35 kDa	0.0	gram / milliliter	1.085	gram / milliliter		0.0	Edit CSV JSON

[Upload CSY](#)

Name

Description

Mass

Mass Units

Density

Density Units

Formula

SLD (Optional)

Save

This will link a stock and component(s) together. If the specified stock (ID) does not already exist a new stock in the stock table will be created using the provided stock name. If a link with the same IDs are found information will be overwritten.

Number of components:

[Upload CSV](#)

Stock Name (for stock entry, will not be used if the stock already exists)

Stock ID

Total Quantity

g/ml

Components	Component Fraction (%)
<input type="text" value="select an option..."/>	<input type="text"/>
<input type="text" value="select an option..."/>	<input type="text"/>
<input type="text" value="select an option..."/>	<input type="text"/>
<input type="text" value="select an option..."/>	<input type="text"/>
<input type="text" value="select an option..."/>	<input type="text"/>

Mixture | ID:1

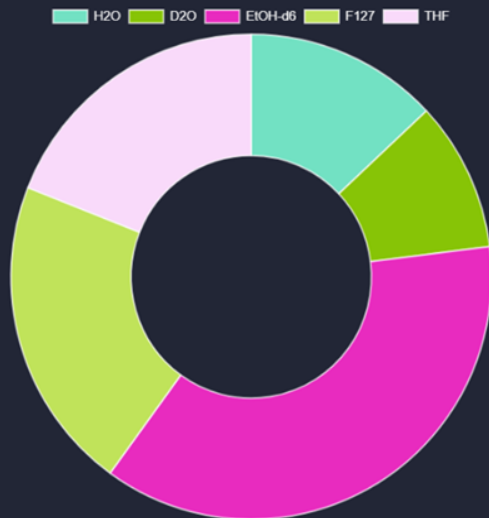
created on 2021-07-23 03:33:44

Component ID	Component Name	Amount	Units	Volmass	
1	H2O	11.05	g	mass	Edit
2	D2O	8.5	g	mass	Edit
4	EtOH-d6	31.45	g	mass	Edit
8	F127	17.85	g	mass	Edit
16	THF	16.15	g	mass	Edit

Numbers displayed in chart are in g or ml.

[Export Individual Stock](#)

[Individual JSON](#)



Data upload/export

NIST Upload Component CSV
[Back](#)

CSV file upload for rapid entry. Format is NAME, DESCRIPTION, MASS, MASS UNITS, DENSITY, DENSITY UNITS, FORMULA, SLD (LEAVE BLANK IF OPTIONAL).

Choose File No file chosen

Upload

```
NAME,DESCRIPTION,MASS,MASS UNITS,DENSITY,DENSITY UNITS,FORMULA,SLD (LEAVE BLANK IF OPTIONAL)
H2O,Water,0.0,gram / milliliter,1.0,gram / milliliter,H2O,-5.605201447588935e-07
D2O,Heavy Water,0.0,gram / milliliter,1.11,gram / milliliter,D2O,6.39266252366673e-06
EtOH,Ethanol,0.0,gram / milliliter,0.789,gram / milliliter,C2H5OH,-3.448567970839845e-07
EtOH-d6,Deuterated Ethanol,0.0,gram / milliliter,0.892,gram / milliliter,C2D5OD,6.097571735265915e-06
polymer,Generic Polymer,0.0,None,0.0,None,,0.0
SDS,Sodium Dodecyl Sulfate,0.0,gram / milliliter,1.01,gram / milliliter,NaCl2H25SO4,3.36521864733921e-07
CTAB,Cetrimonium bromide,0.0,None,0.0,None,C19H42BrN,0.0
F127,Pluronic F127,0.0,None,0.0,None,C572H1146O259,0.0
P188,Poloxamer 188,0.0,gram / milliliter,1.25,gram / milliliter,,0.0
particle,Generic Particle,0.0,None,0.0,None,,0.0
nanoparticle,Generic Nanoparticle,0.0,None,0.0,None,,0.0
hexane,Hexane,0.0,kilogram / meter ** 3,655.0,kilogram / meter ** 3,C6H14,-5.713474681683418e-07
SiO2,Silica,0.0,None,0.0,None,SiO2,0.0
NaCl,Sodium Chloride,0.0,None,0.0,None,NaCl,0.0
hexanes,Hexanes,0.0,kilogram / meter ** 3,655.0,kilogram / meter ** 3,C6H14,-5.713474681683418e-07
THF,Tetrahydrofuran,0.0,gram / milliliter,0.889,gram / milliliter,C4H8O,0.0
PS40-PEO35,"Poly(styrene)-b-poly(ethylene oxide), 40kDa - 35 kDa",0.0,gram / milliliter,1.085,gram / milliliter,,0.0
PS20,Poly(styrene) 20kDa,0.0,gram / milliliter,1.05,gram / milliliter,C8H8,1.4121940630623668e-06
PEO2,"Poly(ethylene oxide), 2 kDa",0.0,gram / milliliter,1.12,gram / milliliter,C4H6O,9.57804033565141e-07
PB_H2O/HFblend,dummy entry to handle binary solvent mixing do not use,0.0,gram / milliliter,0.9,gram / milliliter,C4H10O2,4.778769076797411e-08
phenol,Phenol,0.0,gram / milliliter,1.07,gram / milliliter,C6H6O,1.5919015877457889e-06
benzyl_alcohol,Benzyl Alcohol,0.0,gram / milliliter,1.04,gram / milliliter,C7H8O,1.298304158486851e-06
phenol_solute,Phenol,0.0,gram / milliliter,1.07,gram / milliliter,C6H6O,1.5919015877457889e-06
benzyl_alcohol_solute,Benzyl Alcohol,0.0,gram / milliliter,1.04,gram / milliliter,C7H8O,1.298304158486851e-06
toluene,Toluene,0.0,gram / milliliter,0.867,gram / milliliter,C7H8,9.413275694813125e-07
PS40-PEO40,Polymer Source # P19463 PS-b-PEO,0.0,gram / milliliter,1.2,gram / milliliter,,0.0
PS6,"Polymer Source # P40034-S Polystyrene, narrow dispersity, 6 kDa",0.0,gram / milliliter,1.2,gram / milliliter,,0.0
PEO5,"Polymer Source #P40189-EG2OH, PEO, a,w-bis(hydroxy)-terminated, 5 kDa",0.0,None,0.0,None,,0.0
ethanol,Ethanol,0.0,gram / milliliter,0.789,gram / milliliter,C2H5OH,-3.448567970839845e-07
```

Remote Requests via JSON

```
req = requests.post('http://localhost:5000/component/send_json', json=data)
```

- Convert to JSON
 - Individual entry
 - Entire table
- Make post request
 - Python list of dictionaries

```
[  
  {  
    "density": 1.0,  
    "density_units": "gram / milliliter",  
    "description": "Water",  
    "formula": "H2O",  
    "id": 1,  
    "mass": 0.0,  
    "mass_units": "gram / milliliter",  
    "name": "H2O",  
    "sld": -5.605201447588935e-07  
  },  
  {  
    "density": 1.11,  
    "density_units": "gram / milliliter",  
    "description": "Heavy Water",  
    "formula": "D2O",  
    "id": 2,  
    "mass": 0.0,  
    "mass_units": "gram / milliliter",  
    "name": "D2O",  
    "sld": 6.39266252366673e-06  
  },  
  {  
    "density": 0.789,  
    "density_units": "gram / milliliter",  
    "description": "Ethanol",  
    "formula": "C2H5OH",  
    "id": 3,  
    "mass": 0.0,  
    "mass_units": "gram / milliliter",  
    "name": "EtOH",  
    "sld": -3.448567970839845e-07  
  },  
]
```

Barcode Generation / Label Printing

stock test | ID: 1

created on 2021-07-19 15:23:29

[Edit Detail](#) [Export Individual Stock](#) [Individual JSON](#)

Print Label



ID: 1

Type: Stock

Name: Stock Test

Last Printed: 2021-07-22 12:47:07.241765

Running on NIST hardware



Possible Future Steps

- Balance serial port interface
 - Further reduce manual input
- Javascript grids
 - More interactive tables
- CSV optimizations

Acknowledgements

- Dr. Peter Beaucage
- Dr. Tyler Martin
- CHRNS / NCNR



Questions?