

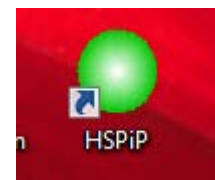


Introductory HSPiP Software and DOSS Training Workshop

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Finding the Program



- Open HSPiP by looking under “All Programs” then “Hansen-Solubility” then “HSPiP”
- When it opens the main page will pop up

File Dist. Diff. Adh./Visc. ForceFit Teas HPLC IGC GC Temp. Evap. FindMols Grid DPC SMILES Help

No.	Solvent	δD	δP	δH	Score	RED	MVol	CAS	SMILES
1	Acetaldehyde	14.7	12.5	7.9			56.5	75-07-0	CC([H])=O
2	Acetaldoxime	16.3	4	20.2			61.2	107-29-9	C/C=N/O
3	Acetamide	17.3	18.7	19.3			59	60-35-5	CC(N)=O
4	Acetanilide	20.6	14.4	13.5			131	103-84-4	CC(=O)N...
5	Acetic Acid	14.5	8	13.5			57.6	64-19-7	CC(O)=O
6	Acetic Anhydride	16	11.7	10.2			95	108-24-7	CC(OC(C)...
7	Acetone	15.5	10.4	7			73.8	67-64-1	CC(C)=O
8	Acetonecyanhydrin	16.6	12.2	15.5			91.8	75-86-5	CC(C)(OC)...
9	Acetonemethyloxime	14.7	4.6	4.6			96.7	3376-35-0	CC(=NOC)C
10	Acetonitrile	15.3	18	6.1			52.9	75-05-8	CC#N
11	Acetophenone	18.8	9	4			117.4	98-86-2	CC(C1=C...
12	Acetoxime	16.3	3.7	10.9			80.2	127-06-0	CC(=NO)C
765	1-Acetoxy-1,3-Butadiene	16.1	4.4	8.3			118.4	1515-76-0	CC(=O)O...
1116	Acetyl Salicylic Acid	19	6.9	9.7			149.4	50-78-2	CC(=O)O...
785	2-Acetyl Thiophene	19.1	12.2	9.3			108	88-15-3	CC(C1=C...

HSPIP Master Data

P O DIY QSAR 3DO

Donor/Acceptor Genetic Algorithm Hide Unused
 MVol Correction Show Selected Save as hsd
 Sphere Rad. Chk ESC Alert DC-Rad 4.0 Limit

Search_Text

"Inside" Font Size: Medium Info: Both only

Total Compounds = 1235

Show Master Dataset

Wire Frame 3D Reset D-Min 12.5 P&H-Max 25

Creating a Sphere Experimentally

- Use 30-40 solvents in realistic application
- Score results as 0 (ineffective) or 1 (effective)



Solvent Optimizer Function

- Create a blend targeting the solute's exact HSP value
- Before optimizing, assess limitations of the application
 - EHS considerations, physical properties that enhance performance, cost
- Create custom solvent list

Seeing the Bigger Picture

What if there was a database of solvents with:

- Environmental Health and Safety Information
- Physical Properties Data
- Cost and Suppliers
- Solubility Theory Data

Wouldn't life be much easier?



Doss

Database of
Safer Solvents

Criteria for Solvents

- Commercially available without inquiry
- Has an accurate SDS
 - Matches with Pharos database hazards
- According to most current research isn't a:
 - Carcinogen (GHS category, 1A, 1B, or 2)
 - Reproductive toxin (GHS category, 1A, 1B, or 2)
 - Mutagen (GHS category, 1A, 1B, or 2)
 - Halogenated

Disclaimers

- Avoiding misuse of the tool
 - Choose a solvent appropriate for your environment
- Cost
 - Bulk costs aren't as reliable, will likely be cheaper
 - Companies are not accountable to prices displayed



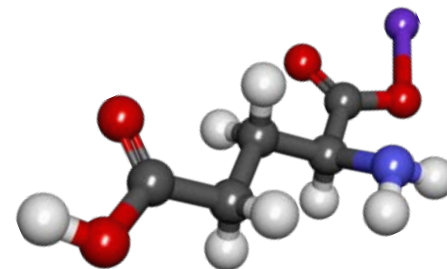
Gathering Reliable Data: EHS Information

- Finding recently updated SDS
 - GHS Categories (Health and Environment)
 - Glove type
- Access to toxicology databases
 - Pharos Database
 - ToxPlanet
 - TURI Library Resource Guide



Gathering Reliable Data: Physical Properties

- Finding Literature Values
 - MPt, BPt, Flash Point, Viscosity (cP), Vapor Pressure (mmHg, temp.), MVol, density, refractive index, and water solubility
- Curating data from:
 - SciFinder Scholar
 - Updated SDS
 - Chemical Distributor



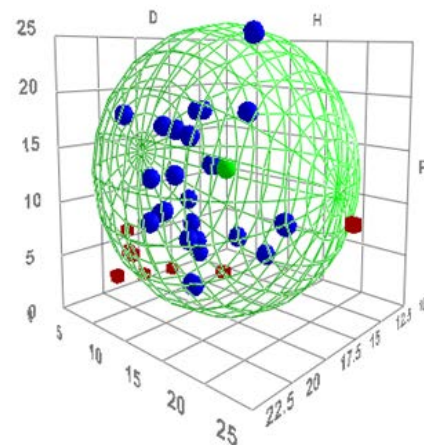
Gathering Reliable Data: Cost

- Lab Bench Cost
 - \$/g (based on website price)
 - Average of 2-5 online prices
- Industrial Cost
 - \$/lb. (based on kg or larger)
 - Molbase.com
- Reaching out to manufacturers, getting a contact



Gathering Reliable Data: Solubility Theory

- Hansen Solubility Parameters
 - HSPiP Database Match
 - SMILES Code Generated
 - Manufacturer Determined (TDS)
- Kamlet-Taft Parameters
 - Literature search
 - Experimental Determination



Database of Safer Solvents Goals

Goal #1: Reliable, useful data in one spot to aide in the selection of a better solvent.

Goal #2: Increase communication between solvent users and solvent makers.

Goal #3: Introduce “unusual” chemicals as viable options.

Goal #4: Database will be sustained by TURI students.

DOSS

Database of
Safer Solvents

DOSS.TURI.org

Vetting Solvent Blends

- For most effective blends determine overall safety and cost and choose best blends
- Follow up with realistic experimental testing

Case Study: PET

A company is creating parts by using a polyethylene terephthalate (PET) mold that needs to be dissolved. The company is currently using toluene at room temperature to dissolve the PET mold. The workers are wearing proper gloves and eye protection, but no masks and has no ventilation equipment.

Find a solvent or create a solvent blend using HSPiP that can optimally dissolve the PET mold and is safer for the workers to use.

Case Study: PET

PET: (18.2, 6.4, 6.6) Radius: 8

- Toluene (18, 1.4, 2); RED is 0.85
- Make sure your solvents are liquid at room temperature
- Make sure the blends are miscible

Blends or solvents will be judged on TURP criteria:

- Highest Effectiveness (lowest RED)
- Lowest Health and Safety Effects (Low inhalation toxicity, Flammability)
- Lowest Cost (<\$1/g)

Email your best option to Abigail_Giarrosso@student.uml.edu

	Group 1	Group 2	Group 3	Group 4	Group 5
Solvent Blend					
HSP					
RED					
Cost (\$/g)					
GHS Hazards					
	Group 6	Group 7	Group 8	Group 9	Group 10
Solvent Blend					
HSP					
RED					
Cost (\$/g)					
GHS Hazards					

Contact Information

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www.doss.turi.org

Email with any questions!