

Software News & Status

Alay Arya

Overview of ICAS 20.0

Integrated Computer Aided System (ICAS)



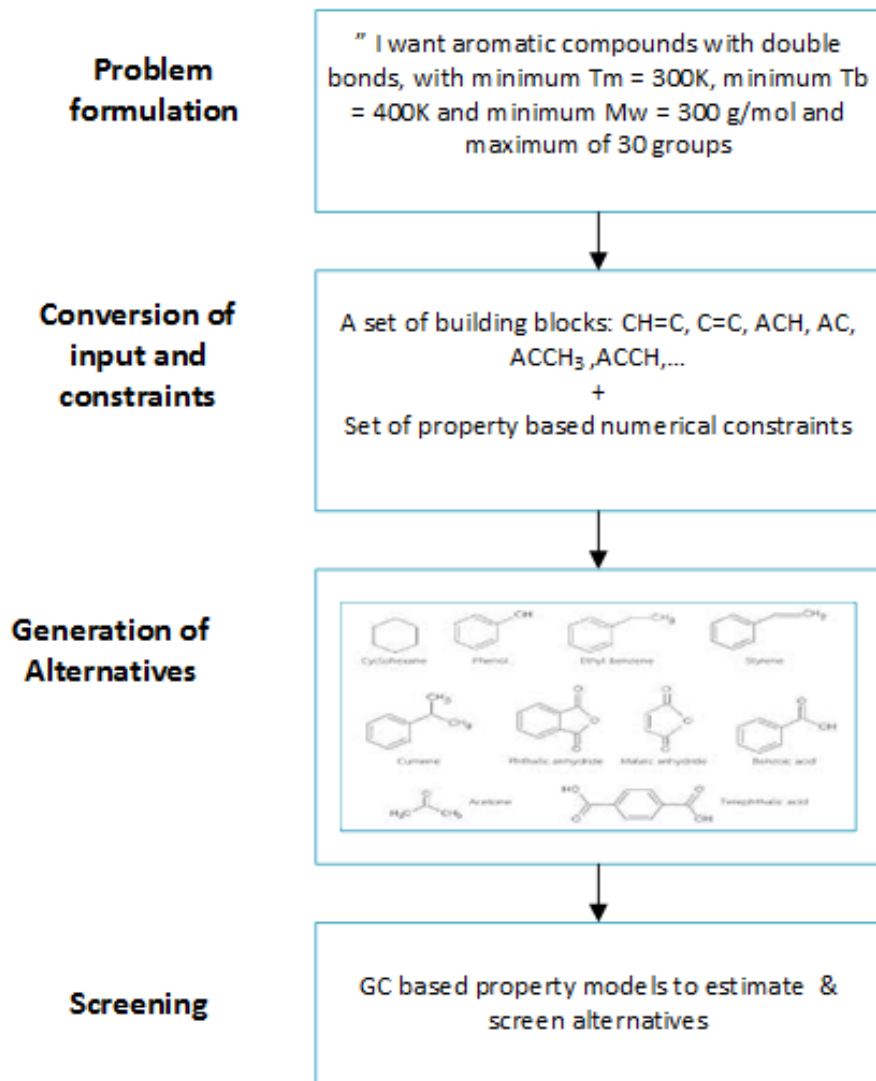
Task Manager

Use this manager to invoke the external tools connected to ICAS, or close it if no external tools are required

| | |
|---------------|--|
| ProCAMD | Computer Aided Molecular Design |
| ProPred | Component Property Prediction |
| ModFrame | Modelling Framework |
| TMS | Thermodynamic Model Selection |
| ReacDef | Define Reactions in the ICAS database |
| TML | Thermodynamic Model Parameter Estimation |
| CAPSS | Process Synthesis |
| BRIC | Batch Records in ICAS |
| PDS | Process Design Studio |
| SolventPro | Solvents selection tool |
| ProCAFD | Process Synthesis |
| ConvertSmiles | Converts Smiles to groups or atom-connectivity indices |

Close Manager

ProCAMD (Computer Aided Molecular Design)



- General problem control
- Non temperature dependent properties
- Temperature dependent properties
- Mixture properties
- Azeotrope/Miscibility calculations
- Biodegradation calculations

ProPred (Property Prediction)

ProPred - NoName

File Edit View Tools Help

Summary Marrero and Gani Constantinou and Gani Joback and Reid Wilson Polymers CI_MG Polymers VK Lipids Amino Acids

Property Values estimated by using methods included in ProPred

Compound Name : Acetamide, N-(3,4-dichlorophenyl)-2,2-difluoro
 Compound CAS : 000000-02-0
 Compound Smiles : FC(F)C(=O)Nc1ccc(Cl)c(Cl)c1
 Compound Formula : C8H5Cl2F2NO
 Mw (g/mol) : 240.03

Connectivity Index (CI) values:

zeroth-order (atomic) CI : 6.64
 first-order (bond) CI : 2.36

PC-Saft parameters:

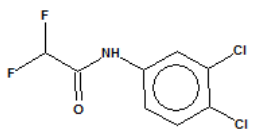
m : 6.941736
 sigma : 3.409378
 epsilon : 243.594962

Best estimates are suggested for each property according to developers' criteria. See detailed estimates through each method in the corresponding pages

WARNING:
 Accuracy of some estimated properties (e.g. Hansen parameters) might be poor if the melting point is far above 298 K

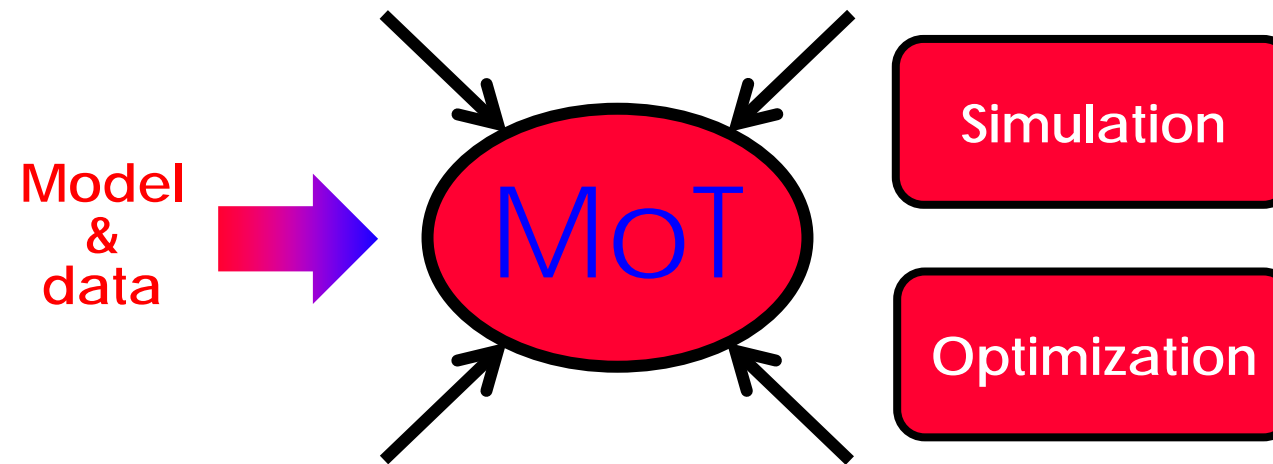
Primary Properties

| Property | Method | Unit | Est. Value | Exp. Value | Rel. Error | Abs. Error |
|----------------|--------|----------------------|------------|------------|------------|------------|
| Tm | MG | K | 406.93 | N/A | N/A | N/A |
| Tb | MG | K | 621.90 | N/A | N/A | N/A |
| Tc | JR | K | 812.19 | N/A | N/A | N/A |
| Pc | JR | bar | 32.10 | N/A | N/A | N/A |
| Vc | JR | cm ³ /mol | 544.50 | N/A | N/A | N/A |
| Zc | Wilson | | 0.250 | N/A | N/A | N/A |
| Gf[298K] | JR | kJ/mol | -345.82 | N/A | N/A | N/A |
| Hf[298K] | JR | kJ/mol | -482.95 | N/A | N/A | N/A |
| omega | MG | | 0.752 | N/A | N/A | N/A |
| Hv[298K] | ***** | kJ/mol | N/A | N/A | N/A | N/A |
| Hv[Tb] | JR | kJ/mol | 56.93 | N/A | N/A | N/A |
| Hfus | JR | kJ/mol | 27.38 | N/A | N/A | N/A |
| Vm[298K] | MG | cm ³ /mol | 165.21 | N/A | N/A | N/A |
| Sol_Par.[298K] | MG | MPa% | 19.10 | N/A | N/A | N/A |
| SurfTens | ***** | dyn/cm | N/A | N/A | N/A | N/A |
| HansenD_sol | MG | MPa% | 19.94 | N/A | N/A | N/A |
| HansenP_sol | MG | MPa% | 16.92 | N/A | N/A | N/A |
| HansenH_sol | MG | MPa% | 7.93 | N/A | N/A | N/A |
| Log(Kow) | MG | | 3.88 | 3.18 | 22.04 | 0.70 |
| Log(WS) | MG | Log(mg/L) | 1.72 | N/A | N/A | N/A |
| pKa | MG | | N/A | N/A | N/A | N/A |
| AiT | ***** | K | N/A | N/A | N/A | N/A |
| Fp | ***** | K | N/A | N/A | N/A | N/A |
| Viscosity | ***** | cp | N/A | N/A | N/A | N/A |
| THERM.COND | MG | mW/m-K | N/A | N/A | N/A | N/A |



ModFrame (Modelling Framework)

MoT (Modelling Testbed)

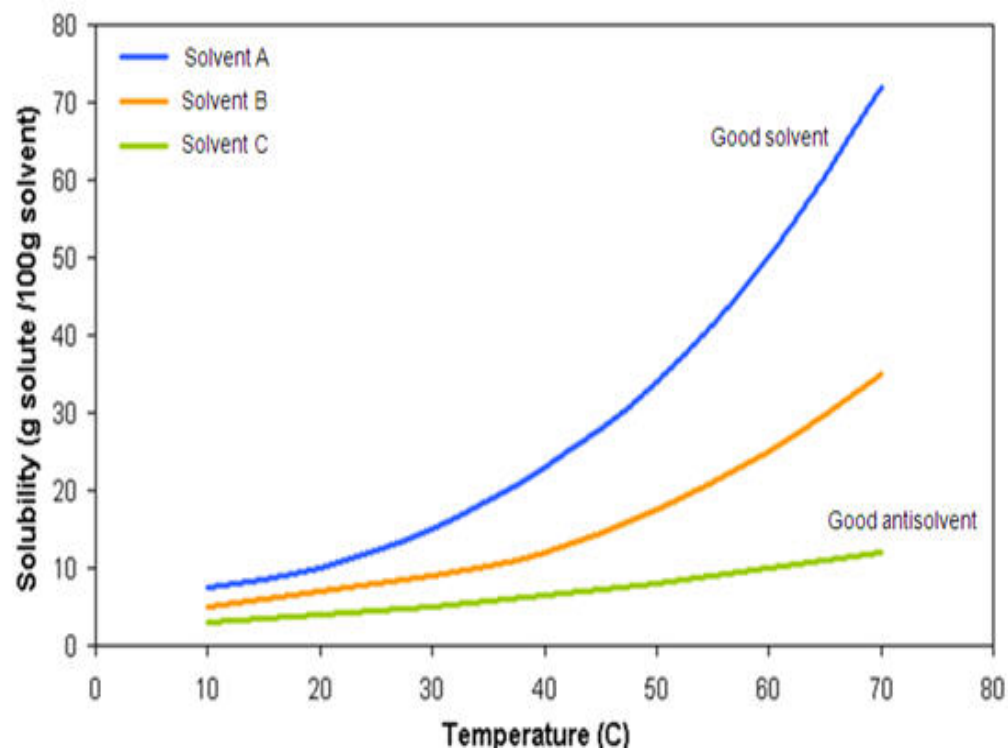


- Steady state simulation & optimization
- Dynamic simulation (open/closed loop) & optimization
- Parameter estimation

PDS (Process Design Studio)



- Design and analysis problems related to vapor-liquid separation processes for
 - Non-reactive systems
 - Reactive systems (element-based calculations)
- Types of calculations:
 - Standard (non-reactive)
 - Binodal, residue, azeotrope, driving force based distillation design, equilibrium based distillation design.
 - Element-based (reactive)
 - PT-flash, bubble point, ternary phase diagrams, distillation design.



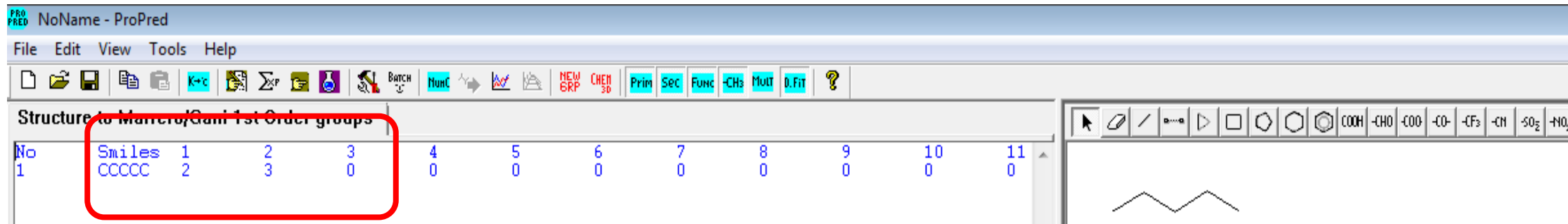
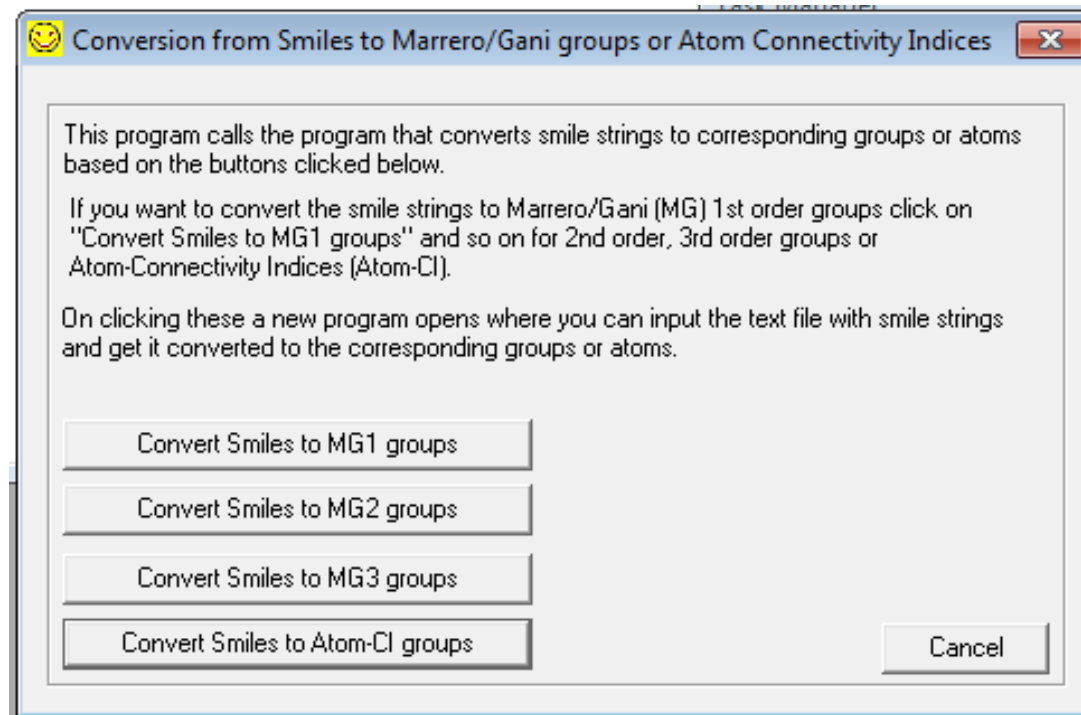
- KT-UNIFAC
- NRTL-SAC : Regression Analysis
- PC-SAFT
- PC-SAFT Parameter Estimation : GC method
- Solvent Design
- Model Comparison
- Compare two models solubility curves (Binary system)
- Compare two models solubility curves (Ternary system)
- Database Manager

ConvertSmiles

MG1 Groups for *n*-Pentane

No. of CH₃ group = 2

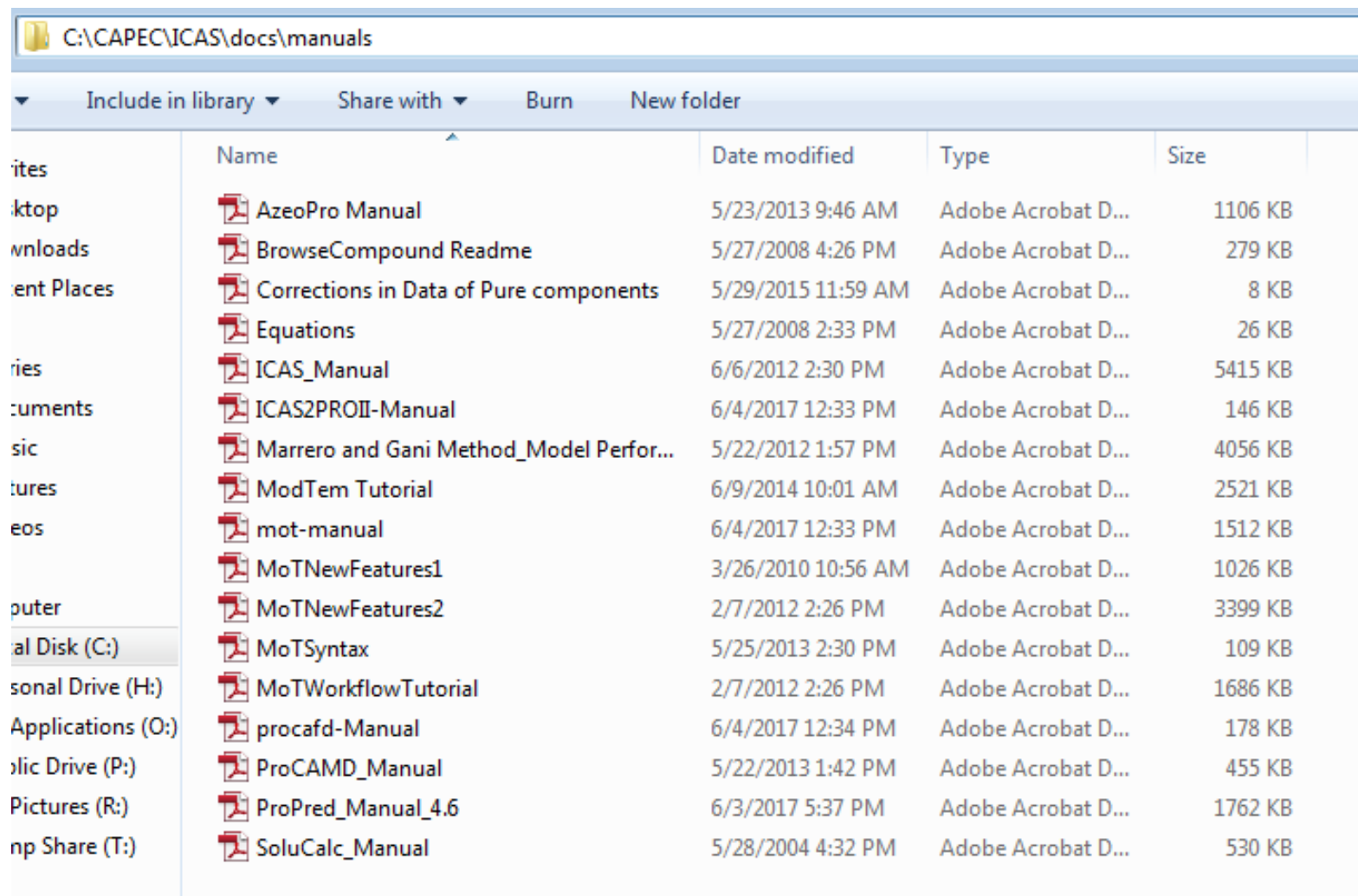
No. of CH₂ group = 3



Structure to Marrero/Gani 1st Order groups

| No | Smiles | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
|----|--------|---|---|---|---|---|---|---|---|---|----|----|
| 1 | CCCCC | 2 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

Location of Manuals



The screenshot shows a Windows File Explorer window with the address bar set to `C:\CAPEC\ICAS\docs>manuals`. The window displays a list of files, all of which are Adobe Acrobat PDF documents. The files are listed in a table with columns for Name, Date modified, Type, and Size. The left sidebar shows the navigation pane with 'Local Disk (C:)' selected.

| Name | Date modified | Type | Size |
|---|--------------------|--------------------|---------|
| AzeoPro Manual | 5/23/2013 9:46 AM | Adobe Acrobat D... | 1106 KB |
| BrowseCompound Readme | 5/27/2008 4:26 PM | Adobe Acrobat D... | 279 KB |
| Corrections in Data of Pure components | 5/29/2015 11:59 AM | Adobe Acrobat D... | 8 KB |
| Equations | 5/27/2008 2:33 PM | Adobe Acrobat D... | 26 KB |
| ICAS_Manual | 6/6/2012 2:30 PM | Adobe Acrobat D... | 5415 KB |
| ICAS2PROII-Manual | 6/4/2017 12:33 PM | Adobe Acrobat D... | 146 KB |
| Marrero and Gani Method_Model Perfor... | 5/22/2012 1:57 PM | Adobe Acrobat D... | 4056 KB |
| ModTem Tutorial | 6/9/2014 10:01 AM | Adobe Acrobat D... | 2521 KB |
| mot-manual | 6/4/2017 12:33 PM | Adobe Acrobat D... | 1512 KB |
| MoTNewFeatures1 | 3/26/2010 10:56 AM | Adobe Acrobat D... | 1026 KB |
| MoTNewFeatures2 | 2/7/2012 2:26 PM | Adobe Acrobat D... | 3399 KB |
| MoTSyntax | 5/25/2013 2:30 PM | Adobe Acrobat D... | 109 KB |
| MoTWorkflowTutorial | 2/7/2012 2:26 PM | Adobe Acrobat D... | 1686 KB |
| procafd-Manual | 6/4/2017 12:34 PM | Adobe Acrobat D... | 178 KB |
| ProCAMD_Manual | 5/22/2013 1:42 PM | Adobe Acrobat D... | 455 KB |
| ProPred_Manual_4.6 | 6/3/2017 5:37 PM | Adobe Acrobat D... | 1762 KB |
| SoluCalc_Manual | 5/28/2004 4:32 PM | Adobe Acrobat D... | 530 KB |

Updates in ICAS 20.0

- ProPred with Amino-Acid compounds

ProPred - NoName

File Edit View Tools Help

Summary | Marrero and Gani | Constantinou and Gani | Joback and Reid | Wilson | Polymers CI_MG | Polymers VK | Lipids | **Amino Acids**

Prediction of Amino Acid property values

AminoAcids Examples

Compound Name: L-Serine
Compound CAS : 000056-45-1
Compound Smiles : OCC(N)C(=O)O
Compound Formula : C3H7NO3
Mw (g/mol) : 105.09

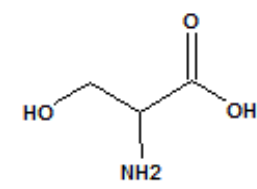
NOTE:
The primary properties of Amino Acid

Primary Properties

| Property | Unit | Est. Value(*) | Exp. Value | Rel. Error | Abs. Error |
|----------|-----------|---------------|------------|------------|------------|
| Tm | K | 514.19 | 495.15 | 3.85 | 19.04 |
| Log(Ws) | Log(mg/L) | 5.13 | 5.63 | 8.88 | 0.50 |
| Log(Kow) | | -3.10 | -3.07 | 1.10 | 0.03 |

Est. Value(*) is the predicted property value obtained from step wise regression method (Multilevel Estimation)

Important Note: If HCl group exists in Smiles/Compound, it should be selected separately by right clicking on b



Updates in ICAS 20.0, cont...



- ProPred Bug fixes
- MOT Model Library
- ProCAMD Bug fixes

ICAS Future Plan

Visual C++ 6.0 (1998)
Compiler

ICAS Program

Access Database (1998)

ICAS Database



Visual C++ 2015
Compiler

ICAS Program

Access Database (2010/2013)
OR better Platform

ICAS Database

- ProPred has already been upgraded and now compatible with Visual C++ 2015.
- ProCAMD and SolventPro are next ones to be upgraded like ProPred.

ICAS Future Plan, cont...



- **Compatibility**
 - ✓ Move towards upgrading old tools to newer development systems, thus improving compatibility with new Windows systems and user experience.
- **Database Manager**
 - ✓ Move to a new search engine – faster search.
 - ✓ Update of interface.
- **Review of Tools**
 - ✓ Functionalities, tests and removal of redundant files.
- **Manuals**
 - ✓ Review and updates of all tools' manuals.
- **Potential Bugs Fixing**

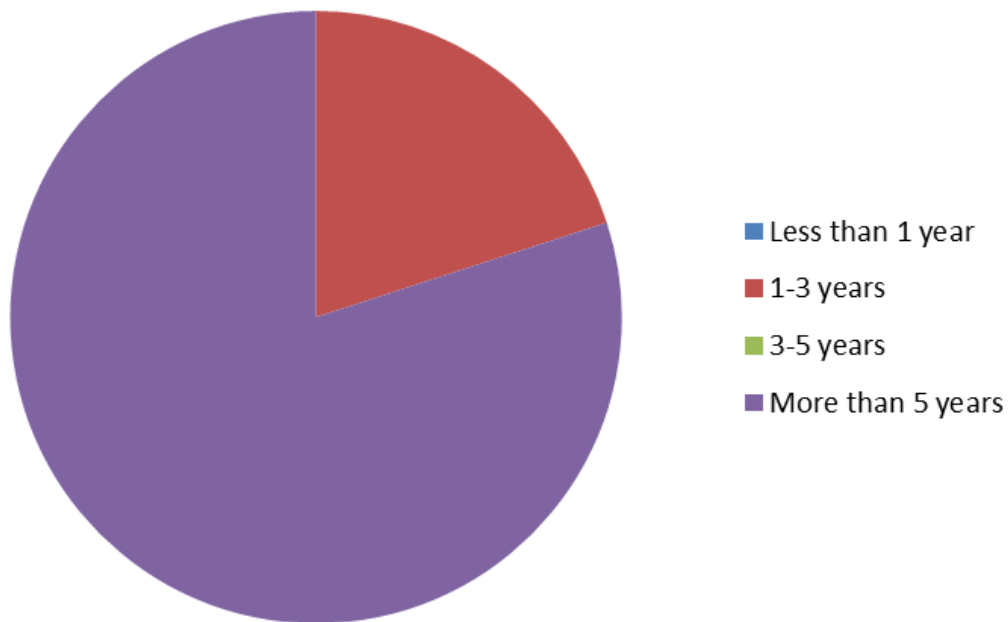
Questionnaire about ICAS

- How long have ICAS tools been used in your company/institution?
- How often do you use any of the ICAS tools?
- I don't know/don't understand how to use this tool (bad manual, difficult interface etc).
- I don't need its functionality in my work.
- The functionality is too poor to use in my work.
- How often do you encounter any issues with any tool (i.e. errors, crashes etc.)?
- What issues that could cause you not using the tools?

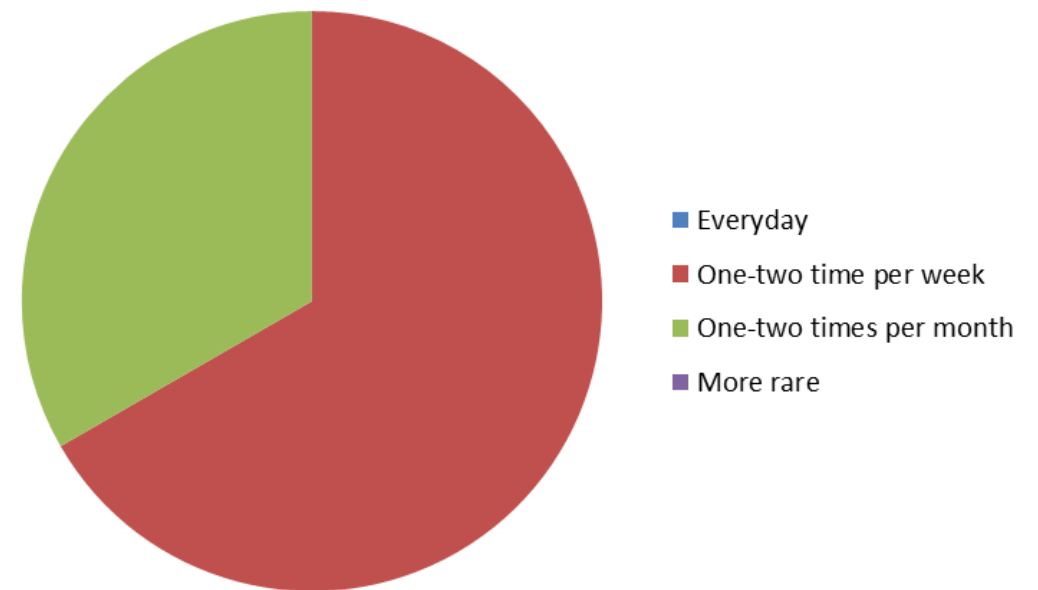
Not enough data to show statistics
(Received only partial responses from 6 companies)

Questionnaire Results

How long have ICAS tools been used in your company/institution?



How often do you use any of the ICAS tools?



Thank You