

| COMPARISON OF INForm AND CAD/Chem Feature | CAD/Chem v5.1.3 | INForm v2 |
|---|-----------------|-----------|
| Data loading | | |
| Cut and paste from spreadsheet (e.g. 1-2-3, Excel) | ✓ | ✓ |
| Import tab-delimited file | ✓ | ✓ |
| Data allowed in text form (e.g. wet, dry) as well as numerical form | | ✓ |
| Quick Select for assigning inputs and outputs | ✓ | ✓ |
| Statistical analysis | ✓ | ✓ |
| Graphical analysis | ✓ | ✓ |
| 'Belief' function for user to specify reliability of data | ✓ | Not yet |
| | | |
| Training | | |
| | | |
| Backpropagation neural networks (Multi-layer perceptron) | ✓ | ✓ |
| Accelerated backpropagation | ✓ | |
| Functional Link Nets | ✓ | |
| Automatic network architecture selection | ✓ | ✓ |
| Ability to design own network (select network parameters) | ✓ | ✓ |
| Separate models for each property | ✓ | ✓ |
| Optional interactive training | ✓ | ✓ |
| Ability to determine one single model for ALL properties | | ✓ |
| Redesign of networks after data points removed for validation | | ✓ |
| Smart Stop to prevent overtraining | ✓ | ✓ |
| Smart Stop as default option | | ✓ |
| ANOVA statistics to assess quality of model | ✓ | ✓ |
| Ability to define output scripts (e.g. cost) | ✓ | ✓ (*) |
| | | |
| Using the Model | | |
| | | |
| Guided evolutionary simulated annealing (GESA) optimization | ✓ | |
| Flexible tolerance method optimization | ✓ | |
| Genetic algorithms with full user control of parameters | | ✓ |
| Global minimum and maximum values set as constraints in optimization by default (avoids going outside range of validity of model) | | ✓ |
| | | |
| Ability to set range of desirable parameters for 'tent' function | | ✓ |
| Ability to change Minimum and Maximum values for desirability functions (within Global minimum and maximum values) | | ✓ |
| Ability to 'batch predict' a range of formulations | | ✓ |
| Log for data | ✓ | |
| 2D and 3D graphs | ✓ | ✓ |

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|---|--|---|---|
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| Graphs | | | |
| Optional time stamps on plots | | | ✓ |
| Easy zoom and rescale facility on 2D plots | | | ✓ |
| Ability to use 2 y axes on 2D plots (to plot two different variables) | | | ✓ |
| Calculation of slope and intercept for regression line on 2D plots | | | ✓ |
| Ability to overlay actual points on 3D graph of model | | ✓ | ✓ |
| Contour plots | | | |
| | | | |
| Spreadsheets | | | |
| Ability to save all spreadsheets/reports as tab-delimited files | | | ✓ |
| | | | |

(*) Scripting is easier to use in **INForm** than in CAD/Chem.