descmng

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ADAPT Limitations?

- Fixed number of atoms.
- Storage space for descriptors is limited.
- Separate workareas are required for individual problems.
- Lack of automation.
- Stuck to *ares* & *hera*.
ADAPT Limitations

- **Storage Space**
  - Fixed upper limit.
  - We need to delete descriptors as we go along.
  - Descriptor storage is linked to workareas.

- Each type of model involves several steps.
Descriptor Manager (descmng)

- Carries out a number of ADAPT functions.
- No limits on descriptor number.
- No limits on number of molecules.
- Implements a number of recent items:
  - Tropsha set generation
  - Diversity Indices
  - KNN averaged predictions
descmng - Storage

- It can store all calculated descriptors.
- Implements descriptor reduction using correlation and identical testing.
- Can generate output files in *annlin*, *qnetin*, *dragon* or *pnn* formats.
- It can generate scrambled sets.
descmng - Analysis

- Performs multiple linear regression (multiple inputs possible).
- Generate diagnostics for outlier detection.
- Generates plots of predicted versus actual values.
Viewing Type I Models

![Model Statistics Viewer](image)

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<th>Residual</th>
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Viewing Type I Models
Viewing Type I Models
Automation

- Type I
  - Will run for varying descriptor lengths in one run.
  - Can automatically set the required validation number.
  - Runs committees and reports averaged RMS errors.
  - GUI available to review statistics, outliers and plots.
Automation

- Type II
  - Automatically process multiple CNN architectures.
  - For N neuron input layer, it will process architectures from N-(N-1)-1 to N-2-1.
  - Runs committees for each architecture and reports averaged RMS errors and averaged prediction values.