Marvin Beans Examples

The examples having bolded links below contain additional description of the example.

1. MarvinSketch
    a. MarvinSketch Simple Bean:
    Creates a MarvinSketch bean and shows getting and setting molecules.
    b. MarvinSketch Images:
    Creates an image from the contents of the MarvinSketch canvas.
    c. Structure Display Parameters:
    Example of R-group visibility parameters.
    d. Structure Templates:
    Customizing structure templates used in MarvinSketch.
    e. Text Box:
    Creating a text box containing formatted text.
2. MarvinView
    a. MarvinView Simple Bean:
    Creates a single-cell MarvinView bean component.
    b. MarvinView In JTable:
    Loads multiple molecules from a file and displays them in a JTable using MarvinView as the renderer of Molecule cells.
    c. MarvinView Table View:
    Displays a molecule file in MarvinView using a scrollable molecule table. Molecules are loaded dynamically and cached automatically, hence arbitrary size files are supported.
    d. Lower level ways for creating molecule tables.
    In these examples, all molecules are loaded in advance, hence the table size is limited by the available memory.
        i. Table View with Parameters:
        Loads multiple molecules from a file into memory, then displays them using MarvinView's scrollable multi-cell molecule matrix mode.
        ii. CustomMenuExample: Customize the menu of MarvinView.
        iii. MViewPopupExample: A viewer example with a customized popup menu.
        iv. MViewExampleWithCheckbox: Demonstrates the handling of action and item events.
        v. MViewSaveProperties: Demonstrates how to save Marvin properties.
3. Swing Components
    - JFileChooser accessory component:
    Marvin as a custom accessory component of a file chooser to provide preview to molecule files.
    - DialogLauncher.java.txt:
    Launches a sketcher or a viewer from a dialog window.
4. Events
    - SketchEventTest.java.txt Shows the fired events of the sketcher.
    - ViewEventTest.java.txt This viewer example logs the fired events of the viewer.
    - MolChangedEventExample.java.txt: Howto listen the modifying of the structure in the editor.
5. SimpleConverter.java.txt: Converts the specified molecule file into the required file format.

6. JSP Image Generation: A JSP example to create an image from a molecule structure and display it in the browser.
7. Excelsheet Generation: A JSP example to create an Excel Sheet with Marvin generated structure images and structure data.
8. Calculator Plugins
    - Using Calculator Plugins via API: general overview that shows how calculator plugins can be used via API.
    - Plugin API usage examples can be found in the API doc headers of the corresponding plugin classes.
        - ElementalAnalyserPlugin
        - IUPACNamingPlugin
        - Protonation
            - pKaPlugin
            - MajorMicrospeciesPlugin
            - IsoelectricPointPlugin
        - Partitioning
            - logPPlugin
            - logDPlugin
            - HLBPlugin
        - Charge
            - ChargePlugin
            - IonChargePlugin
            - PolarizabilityPlugin
            - OrbitalElectronegativityPlugin
        - Isomers
            - TautomerizationPlugin
            - StereoisomerPlugin
            - StereoAnalysis
        - Conformation
            - ConformerPlugin
            - MolecularDynamicsPlugin
            - AlignmentPlugin
        - Geometry
            - TopologyAnalyserPlugin
            - GeometryPlugin
            - TPSAPlugin
            - MSAPlugin
        - Solubility Prediction
            - SolubilityCalculator
        - NMR Prediction
            - NMRCalculator
        - Other
            - HuckelAnalysisPlugin
            - RefractivityPlugin
            - HBDAPlugin
            - ResonancePlugin
            - StructuralFrameworksPlugin
    - Concurrent plugin examples: examples which show concurrent usage of calculator plugins.

- Custom plugin implementation: custom calculator plugin implementation and test application.
