Hello Greg,

once the properties are stored in DW's main table, both Boolean .or. and .and. may be used for further analysis. In the example below, I extended the initial query for molecular weights greater than 110 (yielding mesitylene) to one that would accept molecules with a molecular weight of either less than 80 .or. greater than 110 by the instruction

if((TotalMolweight<80) || (TotalMolweight>110), "True", "False")

in an additional column (Data -> Add Calculated Values). As expected, the second query yields both benzene and mesitylene now.

It is possible to use multiple properties of different columns, too. DW's mathematics, including logic expressions, which may be used are presented on
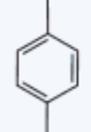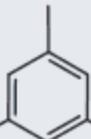
http://www.openmolecules.org/help/jep.html

Norwid

File Attachments
1) example.dwar, downloaded 643 times
2) boolean_or.png, downloaded 1241 times

example.dwar

File Edit Data Chemistry Database List Macro Help

Table

	Structure	Total Molweight	simple_if	Boolean .OR.
1		78.1136	False	True
2		92.1405	False	False
3		106.167	False	False
4		120.194	True	True

Add Calculated Values

Please enter a formula:

if((TotalMolweight<80) || (TotalMolweight>110), "True", "False")

[Add Variable] [TotalMolweight ▾]

☑ Overwrite existing column

Column to overwrite: [Boolean .OR. ▾]

[Help] [Cancel] [OK]