v2.0

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-added 130 Smarts from Kenny, P.; Montanari, C. & Prokopczyk, I. ClogPalk: a method for predicting alkane/water partition coefficient Journal of Computer-Aided Molecular Design, Springer Netherlands, 2013, 27, 389-402

 -smarts/literature\_noHs\_noRec.smarts changed

 -smarts/literature\_noHs\_rec.smarts changed

-recomputed benchmark sets (substructure\_search\_set) from ZINC lead-like and everything as of Feb. 12th, 2011.

 -substructure\_search\_set/literature\_noHs\_noRec.smarts.lead-like.benchmarkset changed

 -substructure\_search\_set/literature\_noHs\_noRec.smarts.everything.benchmarkset changed

 -substructure\_search\_set/literature\_noHs\_rec.smarts.lead-like.benchmarkset changed

 -substructure\_search\_set/literature\_noHs\_rec.smarts.everything.benchmarkset changed

-benchmark sets (molecule\_search\_set, worst-case, zinc) are of version 1.1

v1.1:

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-corrected hann.smarts\_0 ([Br,Cl,I][CX4,CH,CH2] -> [Br,Cl,I][CX4;CH,CH2])

-corrected hann.smarts\_39 (N=NC(S)N -> N=NC(=S)N)

-corrected hann.smarts\_62 ([nH1]ncoc1=O -> [nH1]1ncoc1=O)

-corrected hann.smarts\_96 ([$(NH2)!:c],$([NH1]([CX4])!:c),$([NH0]([CX4])([CX4])!:c)] -> [$([NH2]!:c),$([NH1]([CX4])!:c),$([NH0]([CX4])([CX4])!:c)])

-corrected hann.smarts\_109 ([$(C(=O)(~c)~c);!$([$(c1(=O)ccn([C,c])cc1),$(c1(=O)n([C,c])cccc1)])] -> [$(c(=O)(~c)~c);!$([$(c1(=O)ccn([C,c])cc1),$(c1(=O)n([C,c])cccc1)])])

-corrected daylight\_examples.smarts\_211 ([$([$(\*-[NX2-]-[NX2+]#[NX1]),$(\*-[NX2]=[NX2+]=[NX1-])]),$([$([NX1-]=[NX2+]=[NX1-]),$( -> [$([$(\*-[NX2-]-[NX2+]#[NX1]),$(\*-[NX2]=[NX2+]=[NX1-])]),$([$([NX1-]=[NX2+]=[NX1-]),$([NX1]#[NX2+]-[NX1-2])])])

-removed daylight\_examples.smarts\_44 (parsing error)

-added daylight\_examples.smarts\_264 (smarts: 'c')

-added daylight\_examples.smarts\_265 (smarts: '[2H]')

-added literature references

-benchmark sets (molecule\_search\_set, substructure\_search\_set, worst-case, zinc) are of version 1.0

v1.0:

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smarts and benchmarksets as described in:

Ehrlich, H.-C. & Rarey, M. Systematic benchmark of substructure search in molecular graphs - From Ullmann to VF2. J Cheminform, Center for Bioinformatics, University of Hamburg, Bundestraße 43, 20146 Hamburg, Germany. rarey@zbh.uni-hamburg.de., 2012, 4, 13