

Drug Discovery in the Sandbox

Presented by Miklos Vargyas

US UGM 2010 Boston



ChemAxon
Solutions for Cheminformatics

Acknowledgements

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Gábor Imre



Ödön Farkas

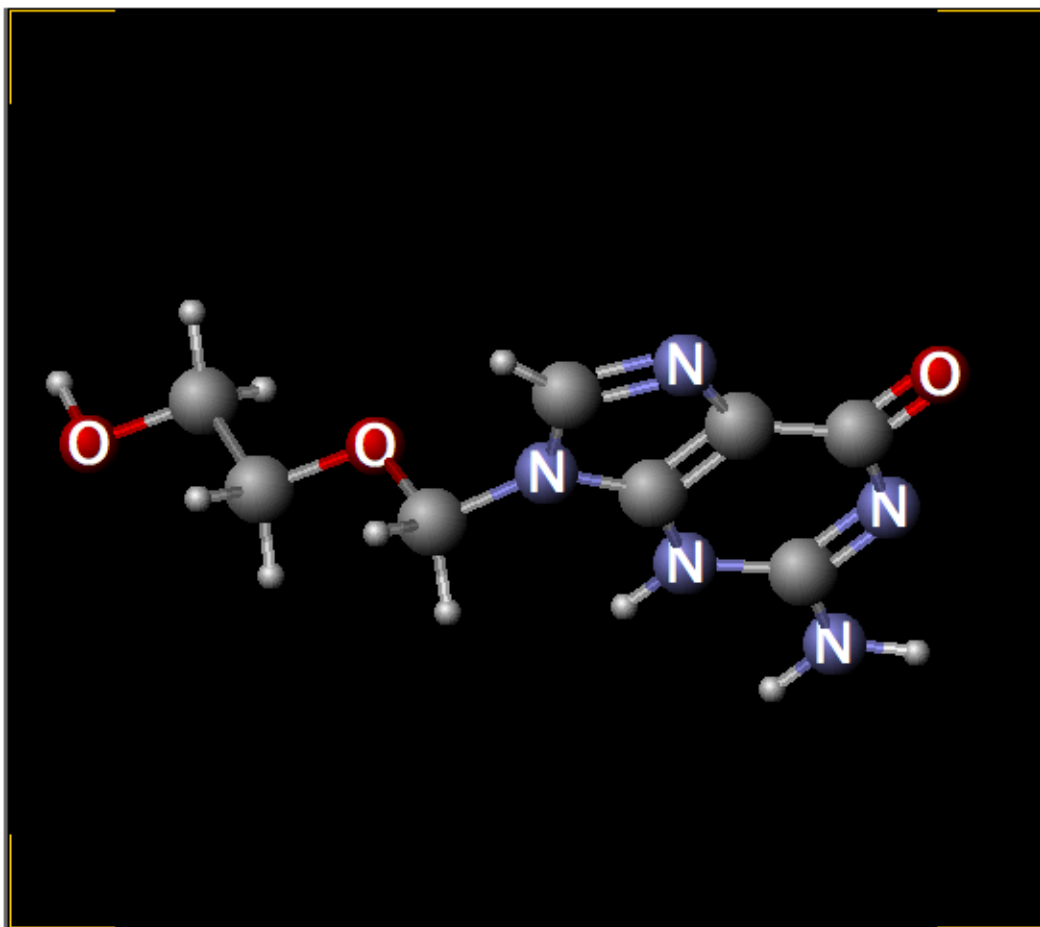


László Antal



3D structure generation

Resulted 3D structure:



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in SDF format

Calculated properties:

Molecular volume:		183.98 Å ³
Min. projected 2D area:		35.38 Å ²
Max. projected 2D area:		66.81 Å ²

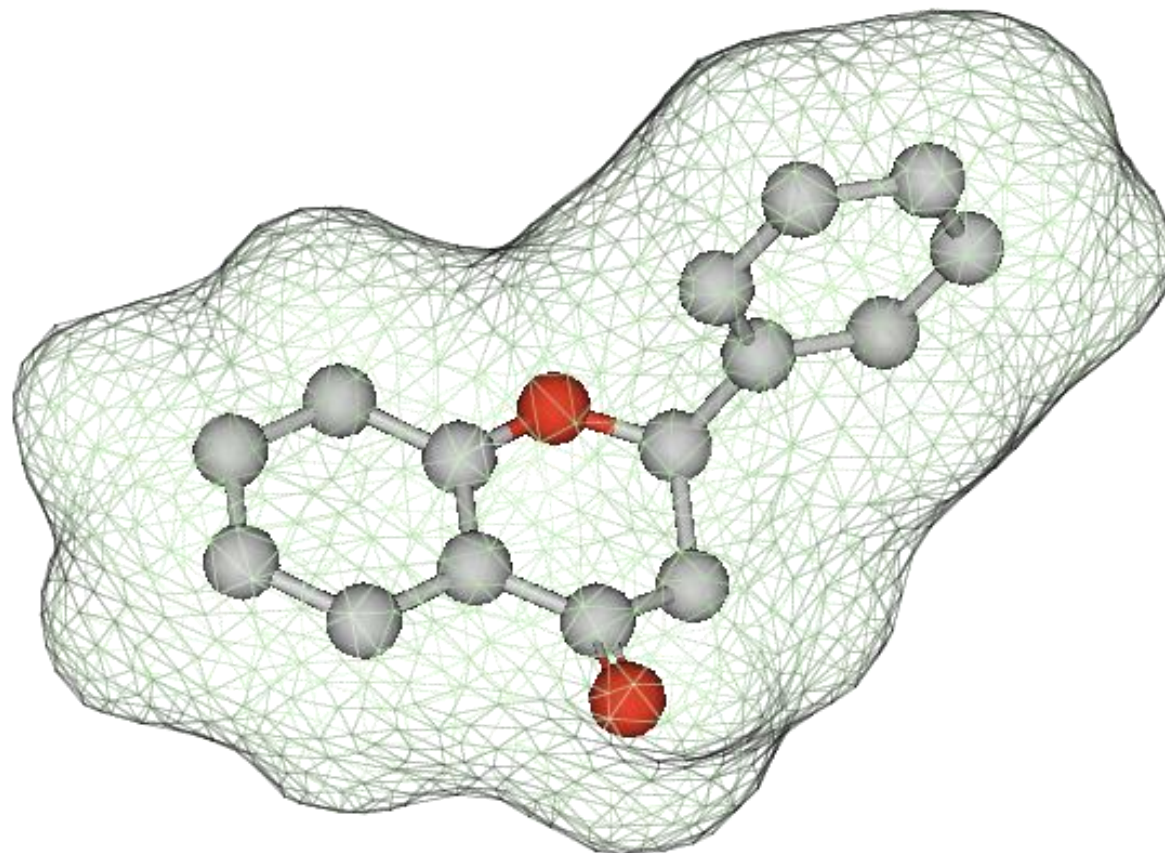
ForceField trends on **MMFFTest_0.sdf**

Number of molecules: 737

Number of conformers: 737

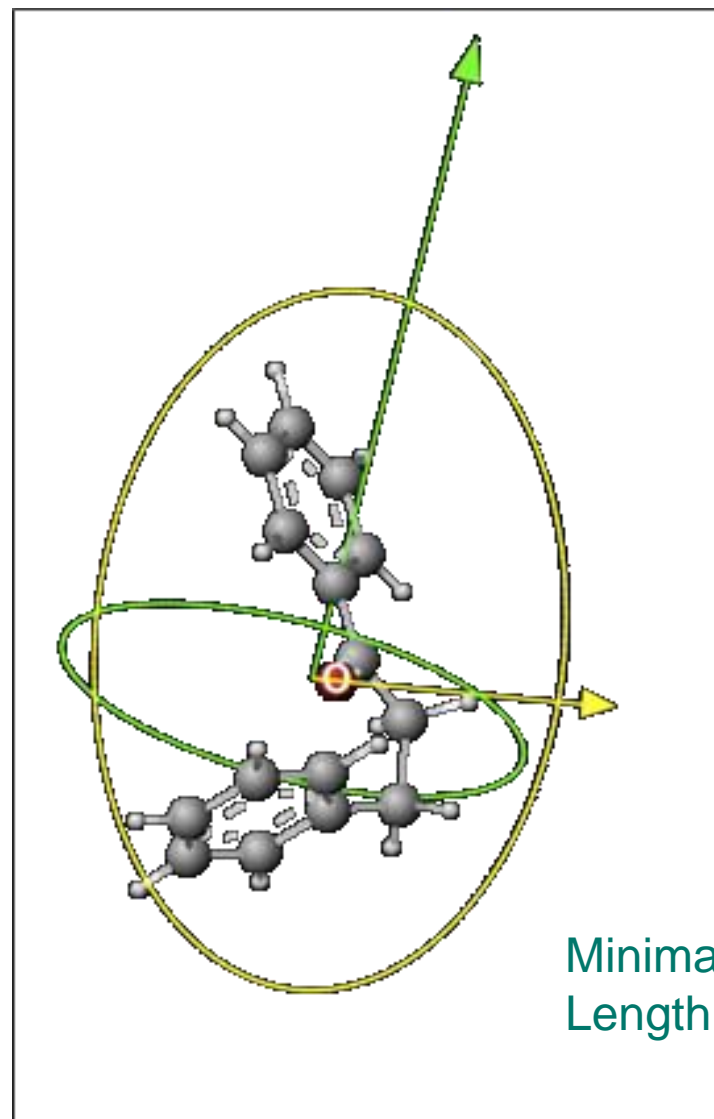
Date	Speed (ms)	Accuracy (A)	Local geometry warning count	NonConverged count	Comment
8-11-2009-21-47-33	60	0.129	21	1	before5.2Dreiding
8-11-2009-21-53-39	31	0.110	10	0	after5.2Dreiding
9-11-2009-18-51-12	11	0.001	0	0	MMFF
14-4-2010-16-13-32	104	0.281	24	0	Generate3D
15-4-2010-16-20-15	108	0.407	29	0	Generate3D(piff.chem.elte.hu)
17-6-2010-13-4-27	10419	0.400	20	0	Gen3DwithMMFF(piff.chem.elte.hu)
25-6-2010-15-48-46	15	0.000	0	0	test
3-8-2010-11-43-8	9	0.111	10	0	newDreiding
3-8-2010-11-48-10	3	0.002	0	0	MMFF

Molecular volume



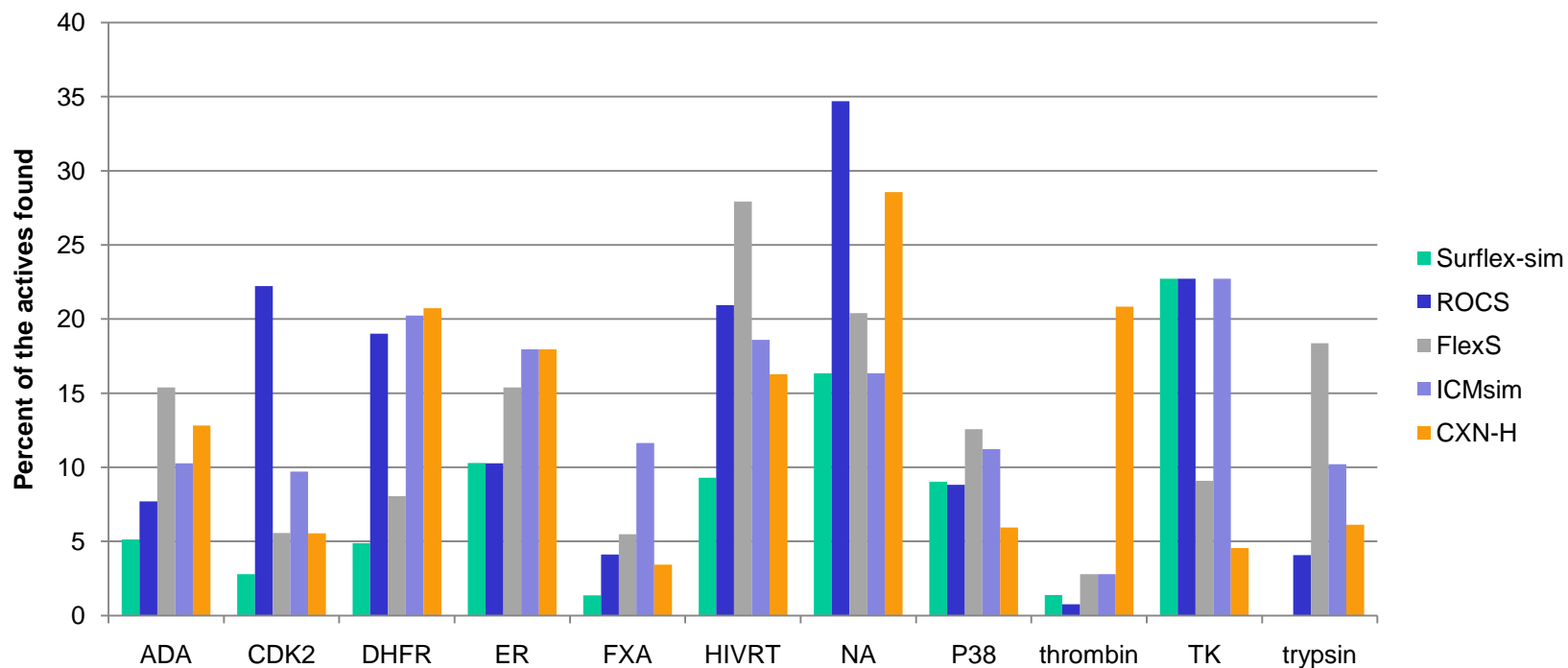
van der Waals volume = 204.55 Å³

Minimal projection area



Minimal projection area = 37.33 \AA^2
Length perpendicular to the max area = 7.01 \AA

3D screening



3D screening

average time per compound (s)

CXN-H	0.07
ROCS	0.5
FRED	1.0
ICMsim	2.4
Surflex-sim	6.7
FlexS	6.9
Surflex-dock	14.6
FLEXX	15.6
ICM	17.7

Intel Q6600 2.4 GHz

Intel Xeon 2.4 GHz

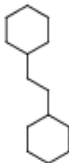
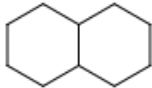
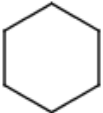
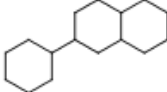
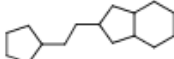
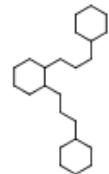
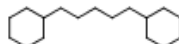
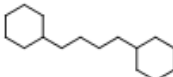
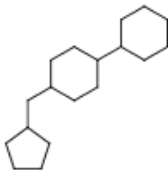
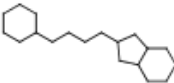
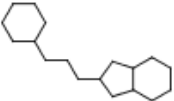
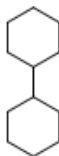
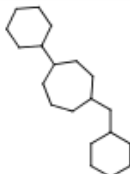
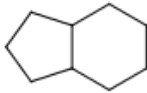
Chemical Clustering

Clusters view

All clusters **No singletons** **Only singletons** **Image size** **Columns** **Rows** **Show/hide**

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1-19

(1) Group ID: 1	(2) Group ID: 2	(3) Group ID: 3	(4) Group ID: 5	(5) Group ID: 7	(6) Group ID: 10	(7) Group ID: 12
						
Size: 6 (6 %)	Size: 3 (3 %)	Size: 17 (17 %)	Size: 2 (2 %)	Size: 3 (3 %)	Size: 2 (2 %)	Size: 2 (2 %)
(8) Group ID: 13	(9) Group ID: 14	(10) Group ID: 19	(11) Group ID: 20	(12) Group ID: 22	(13) Group ID: 24	(14) Group ID: 26
						
Size: 7 (7 %)	Size: 2 (2 %)	Size: 4 (4 %)	Size: 2 (2 %)	Size: 3 (3 %)	Size: 2 (2 %)	Size: 2 (2 %)
(15) Group ID: 29	(16) Group ID: 31	(17) Group ID: 37	(18) Group ID: 42	(19) Group ID: 44		
		