

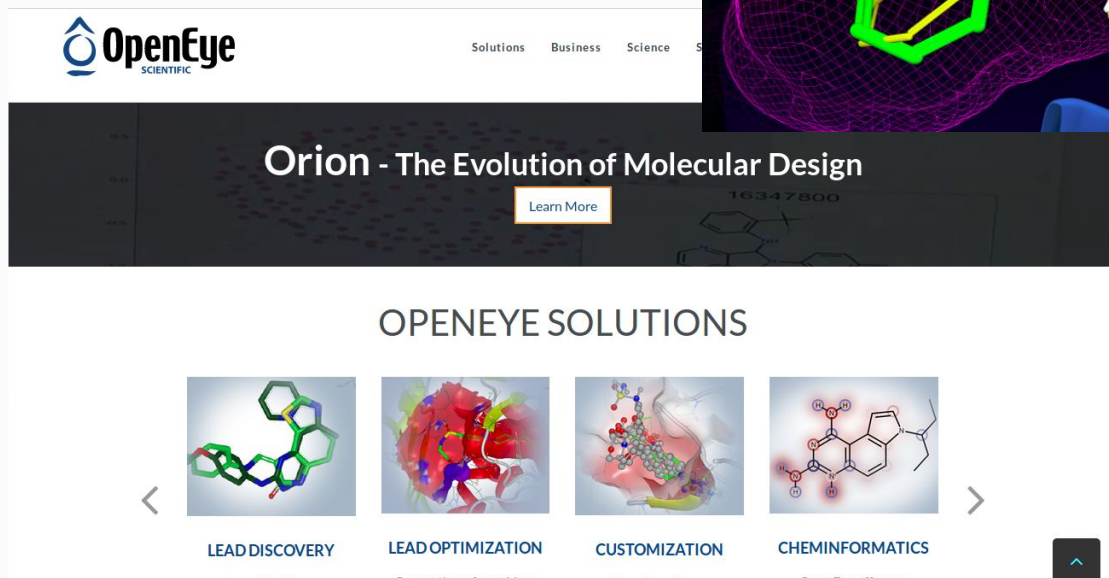
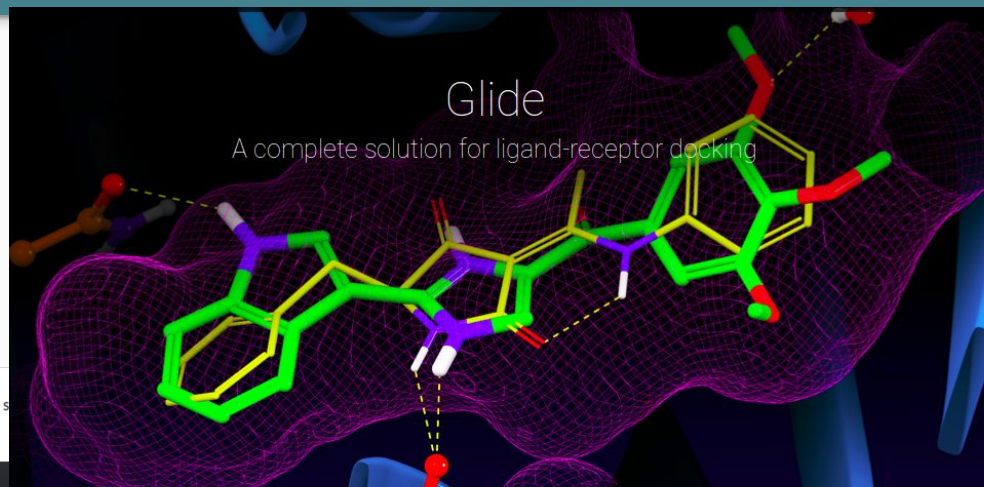
# Binding site characteristics in structure-based virtual screening: evaluation of current docking tools

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# Introducción

- **FRED (OpenEyeScientific Software)**
- **Glide (Schrödinger, Inc.)**



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LEAD DISCOVERY

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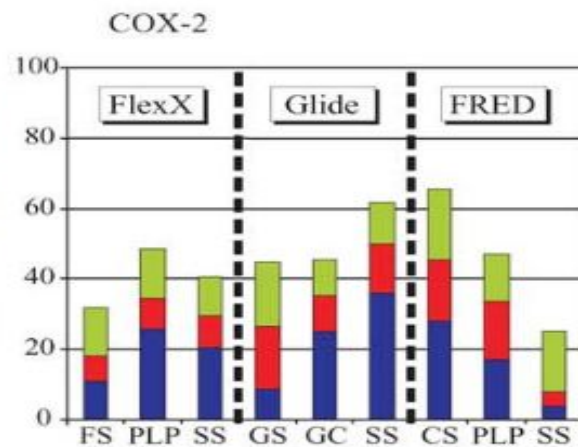
CHEMINFORMATICS

The image is a screenshot of the OpenEye Scientific website. It features a dark banner for "Orion - The Evolution of Molecular Design" with a "Learn More" button. Below the banner, there is a section titled "OPENEYE SOLUTIONS" with four icons representing different services: Lead Discovery, Lead Optimization, Customization, and Cheminformatics. The icons are arranged in a row with navigation arrows on either side.

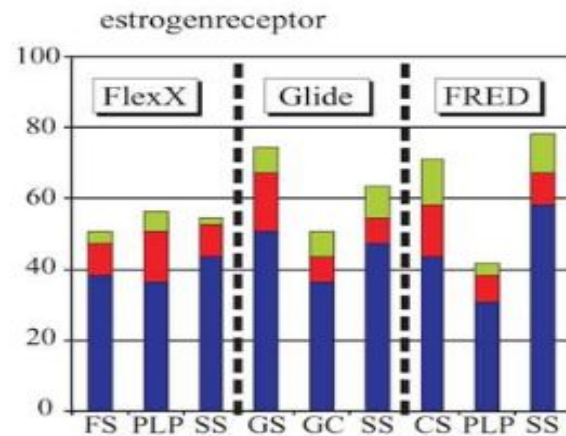
**Table 1** Number and origin of active compounds used in this docking study [20]

Number of compounds	Target	Origin
128	Cyclooxygenase 2	[38, 39, 40]
55	Estrogen receptor	[41, 42, 43]
72	p38 MAP kinase	Roche, [44]
36	Gyrase B	Roche
67	Thrombin	[45, 46]
43	Gelatinase A and general MMP	WDI, PDB, [47]
51	Neuraminidase	PDB, Roche

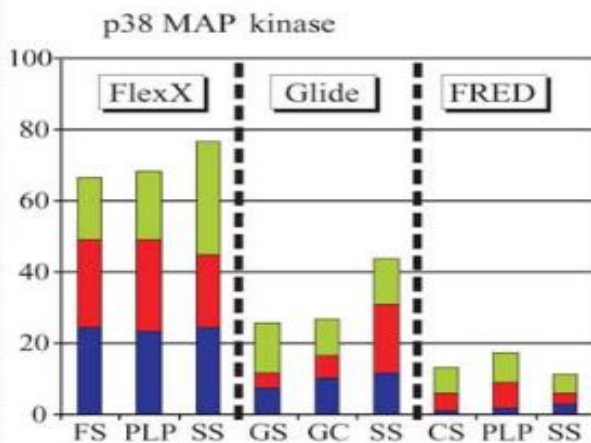
Percent inhibitors at 2%, 5% and 10% of database



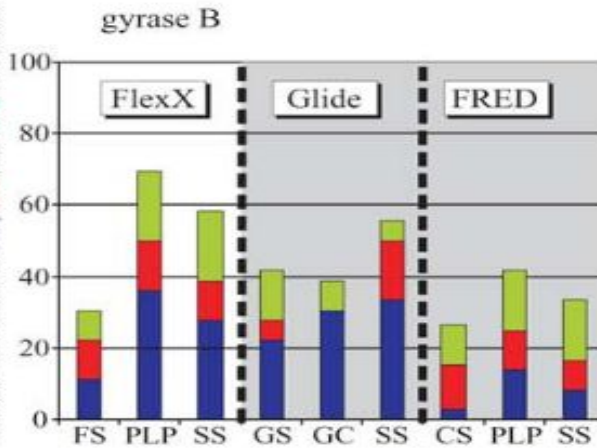
Percent inhibitors at 2%, 5% and 10% of database

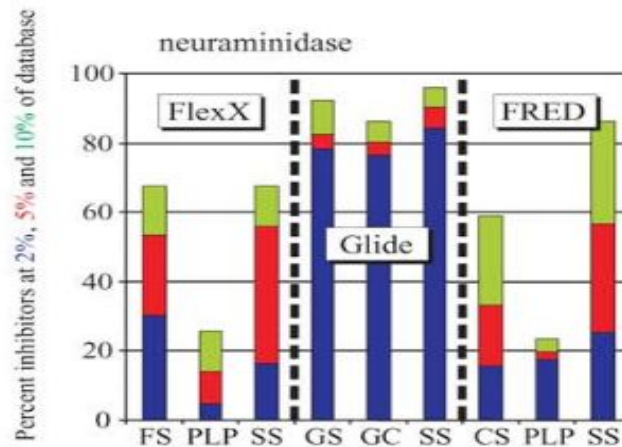
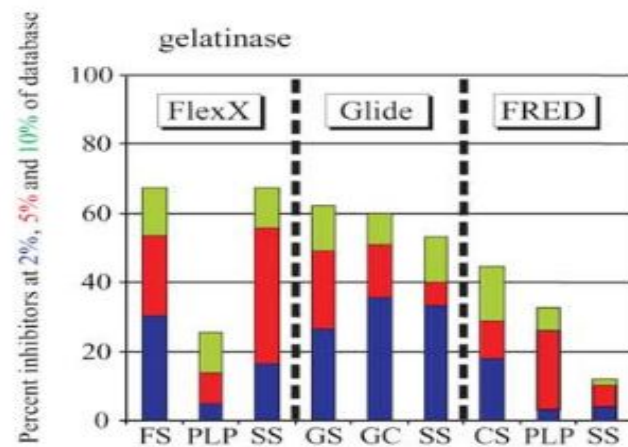
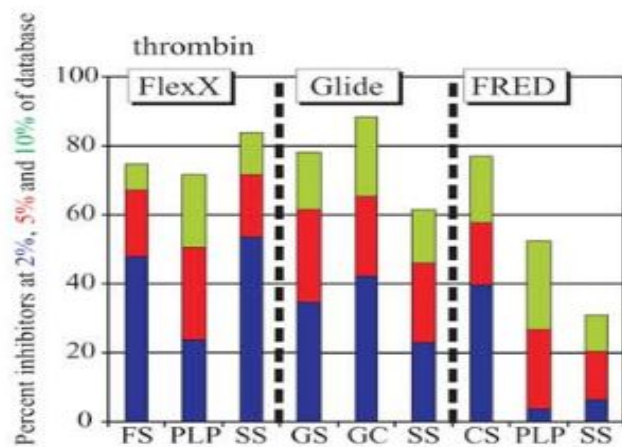


Percent inhibitors at 2%, 5% and 10% of database



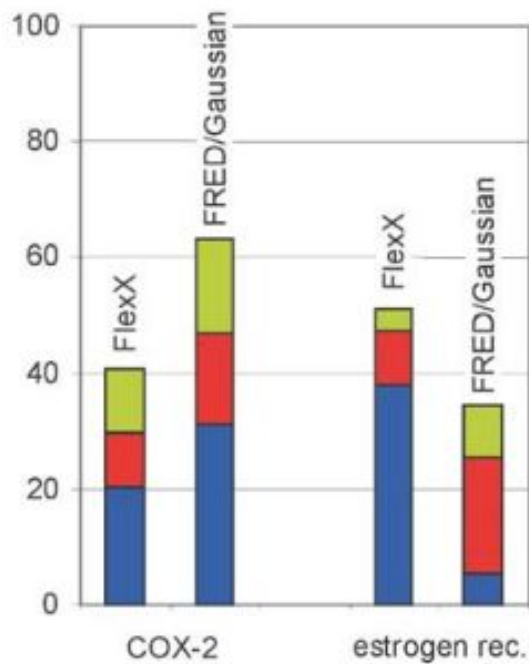
Percent inhibitors at 2%, 5% and 10% of database





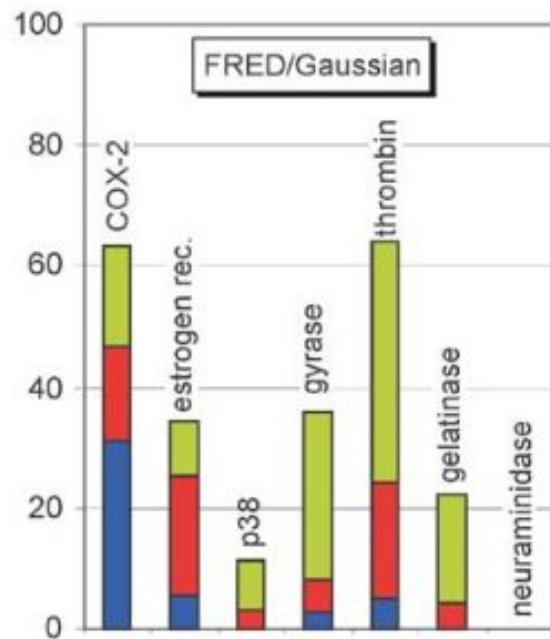
Percent inhibitors at 2%, 5% and 10% of database

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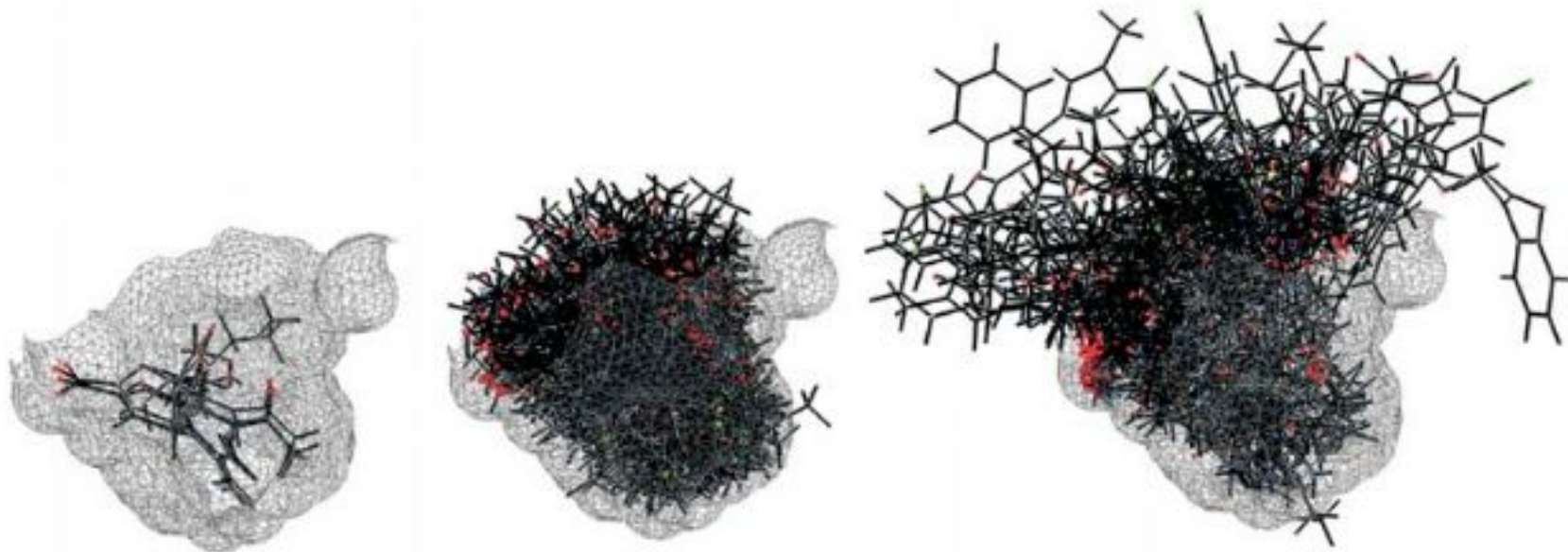


Percent inhibitors at 2%, 5% and 10% of database

B







Receptor	Average no. of rotors	Average no. of heavy atoms	FRED average docking time (s)	Glide average docking time (s)
COX-2	4.1	24.7	5	134
Estrogen rec.	4.2	26.7	15	290
p38 MAP kinase	4.7	26.6	9	133
Gyrase B	5.6	27.5	13	144
Thrombin	9.7	32.2	15	562
gel-A	9.9	30.6	13	513
Neuraminidase	6.5	21.1	8	207
WDI subset	5.6	24.2	13	400



# Conclusiones