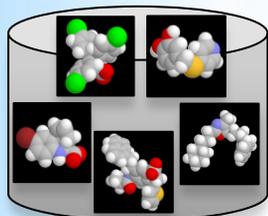


一歩先のインシリコ・スクリーニングと分子設計 創薬支援総合ソフトウェアmyPresto

機材も経験もなくとも未来の創薬に貢献できる世界の実現

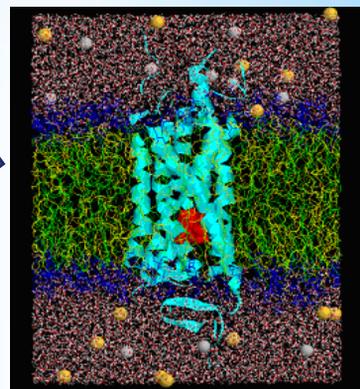
福西 快文

産業技術総合研究所 創薬分子プロファイリング研究センター



①4000万化合物データベース

②分子シミュレーション
GPU利用で30倍高速



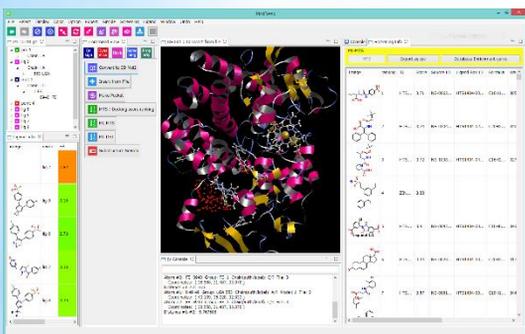
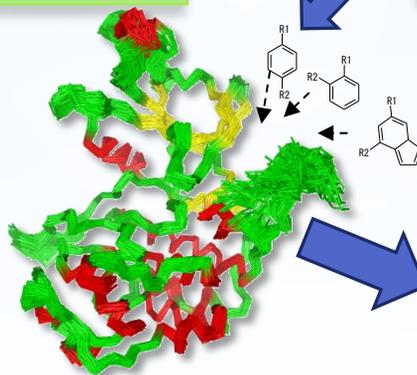
④薬物ドッキング
世界標準の10-100倍

③薬物結合部位予測

⑤薬物スクリーニング
：世界標準の10倍正確

⑥類似化合物探索

クラウド利用で
200万化合物スクリーニング
5000円 2時間（最短）
民間企業でのサービス利用可



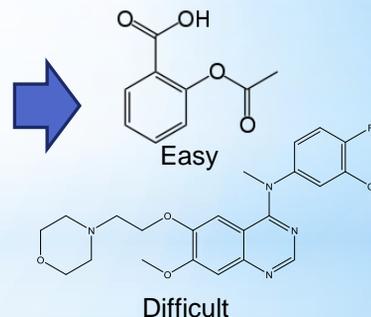
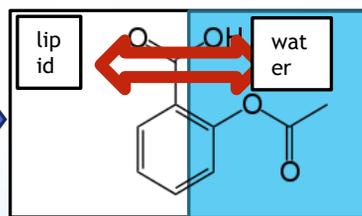
⑦分子設計

⑧溶解度など物性予測

⑨合成可能判定

GUI (専用市販品：数社から販売)の価格は、
通常市販品の1/10

ハード・ソフト一体商品・サービス有
ネットで試薬購入まで容易に
利用講習・指導サポートなど有



■ URL <http://presto.protein.osaka-u.ac.jp/myPresto4/>

http://www.jbic.or.jp/activity/st_pr_pj/mypresto/index_mypr.html

■ 謝辞:AMED・経済産業省・NEDOの創薬加速支援事業の一環として、大阪大学 中村春木教授・産総研 福西快文らの研究グループが研究開発を進めてきた無償・公開版の医薬品候補化合物を探索する次世代天然物化学技術研究組合のコンピュータシミュレーションソフトウェアです。国立大学法人大阪大学蛋白質研究所附属プロテオミクス総合研究センターのウェブサイトより、自由にダウンロードして利用できます。

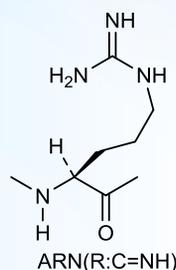
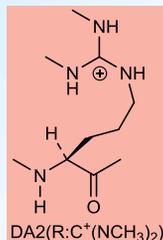
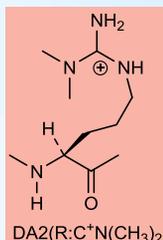
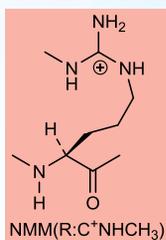
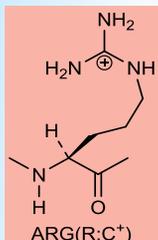
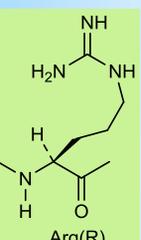
myPresto ver4.400で利用できるアミノ酸 (2016年1月現在)

市販ソフトにより画面上で選択・置換可能

 Standard structure

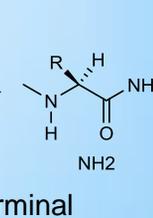
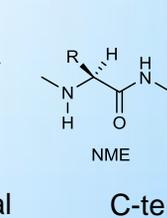
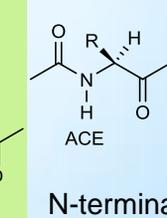
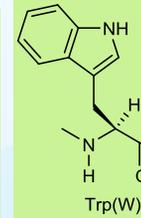
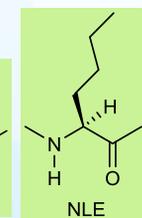
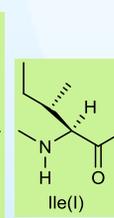
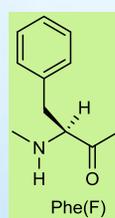
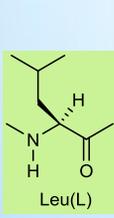
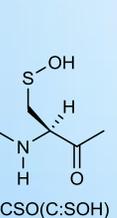
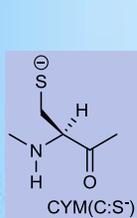
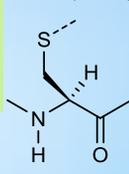
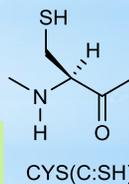
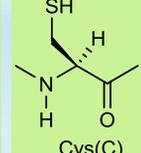
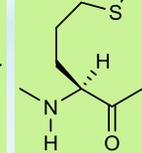
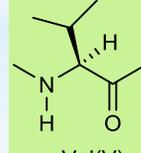
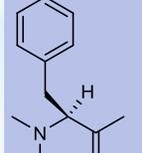
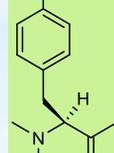
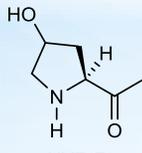
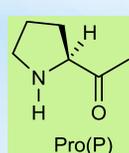
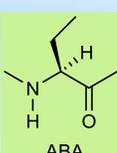
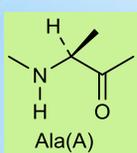
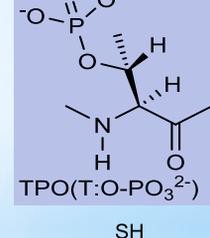
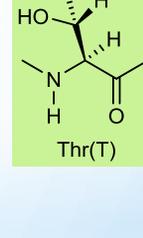
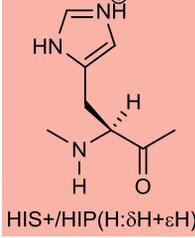
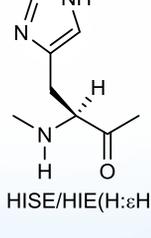
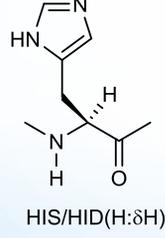
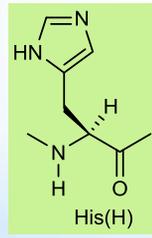
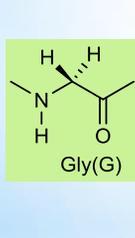
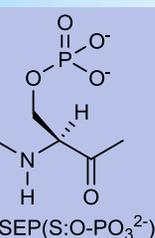
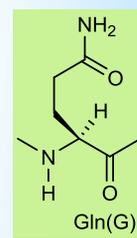
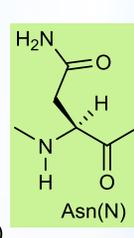
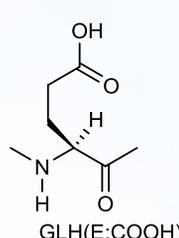
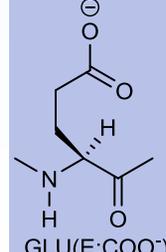
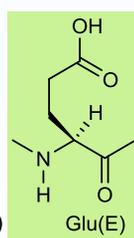
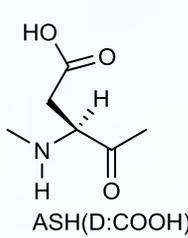
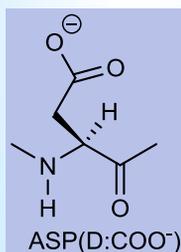
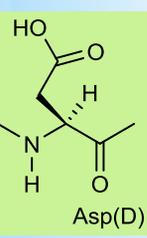
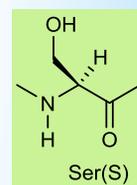
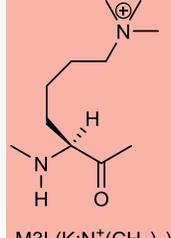
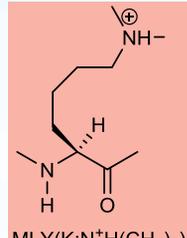
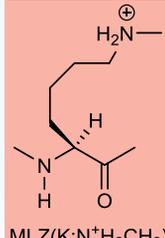
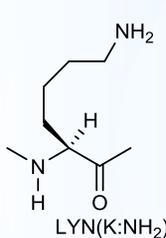
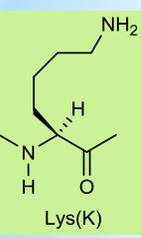
 Negative charge

 Positive charge



AMBER name:
ARN, LYN, GLH,
ASH, HID, HIE,
HIP, CYM

“HIS” in
myPresto: HIS,
HISE, HIS+



myPresto ver4.400で利用・購入できる化合物（2016年1月現在）

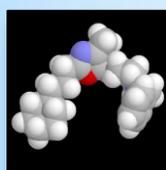
現在は、2015年版が配布中。市販ソフトにより画面上で選択・購買リストファイル作成

Vender name	Year				
	2015	2014	2013	2008	2006
Ambinter				120764	101720
AMRI				195420	
ACB Blocks(Fragment)	1291	1292	1292		
Alinda	186836	254092			
AnalytiCon(Fragment)	222	218	204		
AnalytiConMACROx	1118	1027			
AnalytiConMEGx	5130	4579	4855	1092	522
AnalytiConMEGxp				2799	2066
AnalytiConNATx	26282	25498	24264	19080	9640
Aronis					45746
ART-CHEM				185637	164136
ASDI				105587	42578
Asinex	402046	426345	426345	233540	236765
Asinex(Fragment)	23191	10412	3479	9315	
AsinexPlatinum	16240			126615	132155
AsinexSynergy				10740	
Aurora				24647	59164
Bahrain				998	998
Bellen(Fragment)	2911	2911			
BioBioPha(Natural)	3283	2910	2675		
BioMar	128				
Bionet	52025	47191	41618	46384	43410
Bionet(Fragment)	25906	20584	13127		
ButtPark	21926	21926	21926	17273	14212
CBI	125594	125230			
ChemOvation	3121	3143	3143	2922	
Chem-X-Infinity	11650	11825	13148	332	
Chem-X-Infinity(Fragment)	1156	727	700	2400	
Cerep					29230
Chemstar				60081	60081
ChemT&I				844248	641842
Enamine	2089786	2056024	1883713	952314	506809
Enamine(Fragment)	42044	157022	153444		
EvoBlocks(Fragment)	944	944	700		
Florida				30910	30419
FSSI		102509			
He.Co.				7087	6136
Innovapharm		324568			
Intermed	32037	50295			
Labotest	80096	81805	82296	107737	97794
LifeChemicals	392633	378162	333920	267020	147680
LifeChemicals(Fragment)		32877	30042		

現在は、2015年版が配布中。市販ソフトにより画面上で選択・購買リストファイル作成

- 続き -

Maybridge	54228	54575	54768	56839	58854
Maybridge(Fragment)	8956	8915	9273		
MDD				31254	31255
MDPI		11189	19749	10649	10649
Menai	5005	5005	5210	5017	
Menai(Fragment)	402	402	402		
MolMall	14415				
OTAVA	279563	263086	254048	118173	62091
OTAVA(Fragment)	11719	8748	7810		
Peakdale			14636	6072	8548
Peakdale				6257	6572
Pharmeks	396620	396620	376899	276367	228630
Pharmeks(Natural)	49587	49587	44840	31720	29038
Princeton	1160008	1012682	416068	873993	517484
RareChemicals	11279	11279	11279	15245	9375
SALOR	174978	142206	186899	142876	137428
ScientificExchange	47833	47843	47733	43964	34569
SPECS	207973	199969	199969	199270	151570
SPECS(Natural)	866	456	456	335	
Synthon Labs		32706	49727		
TimTec	130361	128078	1066286	308111	198599
UOS	565990	540678	457256	700730	331710
VillaPharma				4612	
Vitas-M	1319150	1321860	1163246	311813	220970
Vitas-M(Natural)				24694	24694
Vitas-M(Fragment)	18909	18909	8315		
WuxiAppTec	104245	93892	81983		
WuxiAppTec(Fragment)		1155	908		
WuxiAppTec(Natural)	1417	4565	4689		
Zelinsky	386127	386127	385559		
Toal number of entities	8497227	8884648	7908899	6542933	4435139
Nonredundant Total Number	5,150,322	5,026,965	4,740,609	4,206,460	
Number of New chemical entiries	229,015	157,820	195,377		



【化合物情報書式】

- ・3次元化された立体構造(Sybyl mol2 file)
- ・溶解度(LogS)/脂溶性(LogP)などの物性値付
- ・市販ソフトにより画面に合成容易性が表示可能