2021-2 학기 파란학기 도전과제 최종성과 발표

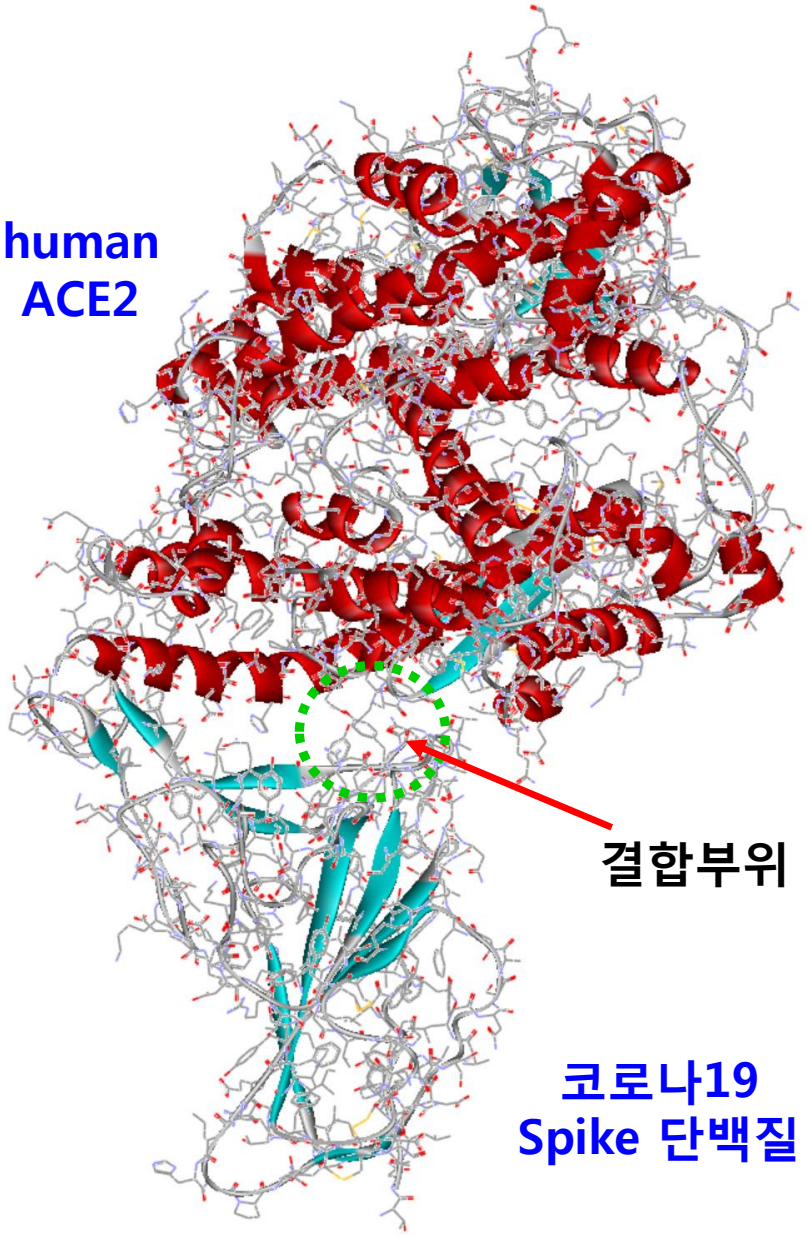
도킹 모의실험을 통한 가상 스크리닝으로 코로나19 치료제 후보물질 찾기

지도교수: 응용화학생명공학과 최준원 교수님

아주대학교 응용화학생명공학과

201920382 박찬엽

표적단백질의 3차원 좌표 준비



PDB website에서 다운로드

http://www.rcsb.org

ID number: 6M0J

도킹 모의실험을 위한 ZINC15 화합물 선별

ZINC15 웹페이지에서 608,000 개 다운로드

https://zinc15.docking.org/

3차원 좌표 제공 구매 가능 전하량 0

LogP (up to)	200	250	300	325	350	375	400	425	450	500	>500	Totals, by LogP
-1	425	399	411	191	215	131	53	61	57	60	183	2,003
0	1,425	1,290	2,322	1,479	1,414	812	364	200	134	103	162	9,543
1	3,607	5,460	10,572	8,260	7,967	4,739	2,215	966	640	551	285	44,977
2	3,437	9,248	21,404	21,102	15,307	14,501	7,043	4,185	2,966	2,551	912	101,744
2.5	744	3,995	15,033	14,798	13,262	12,556	7,188	5,119	3,833	3,557	1,203	80,085
3	284	2,691	12,207	12,649	12,342	17,032	9,821	7,368	5,968	6,149	2,064	86,511
3.5	56	1,339	8,158	10,376	9,424	15,506	9,156	9,258	7,868	8,572	3,132	79,713
4	14	334	3,964	5,976	10,359	11,816	12,819	10,235	9,446	10,864	4,643	75,827
4.5	0	81	1,446	2,521	5,117	7,001	8,819	9,102	8,977	11,892	4,671	54,956
5	0	25	437	923	2,005	3,388	4,499	5,799	6,638	11,253	7,214	34,967
>5	0	0	110	315	998	1,959	3,199	5,168	7,029	18,662	30,791	37,440
												608K

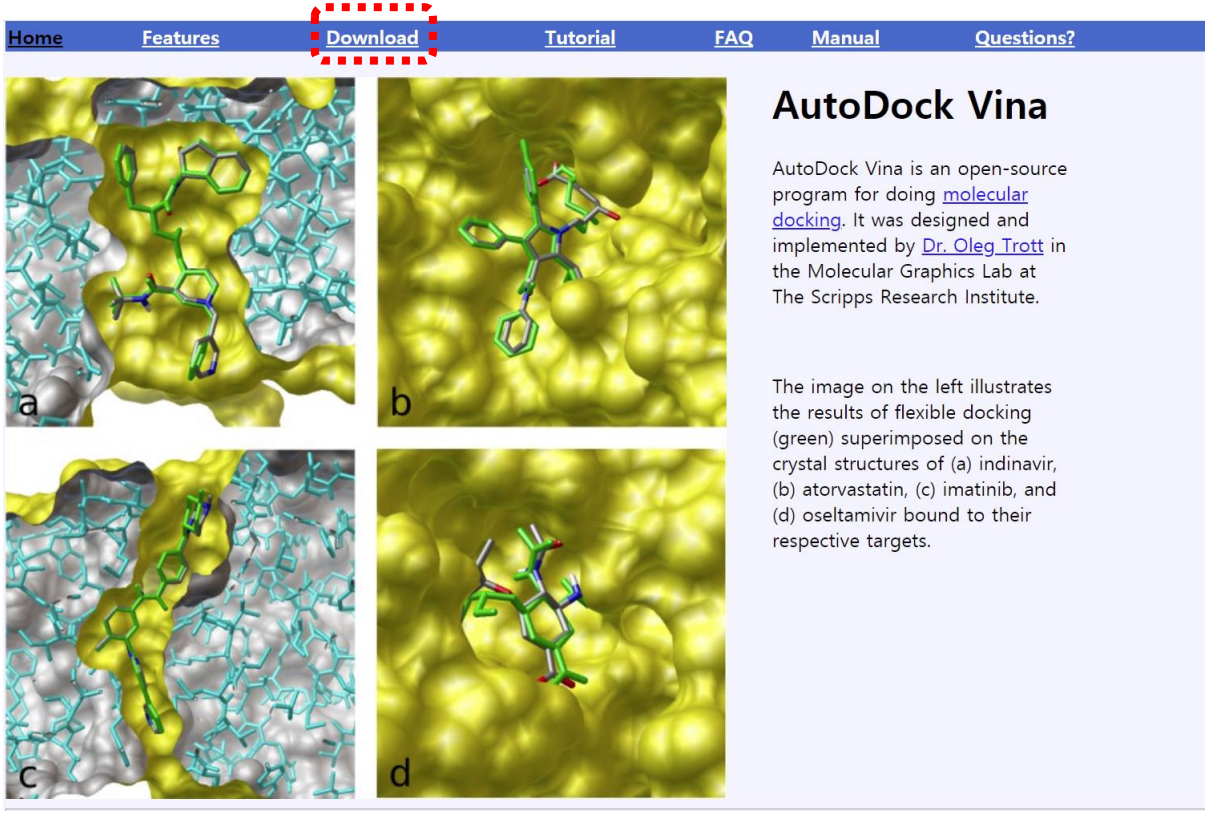
"5의 법칙"

- **-5 < LogP < 5**
- **수소결합 받개 수 < 10**
- **수소결합 주개 수 < 5**
- **자유회전 공유결합 수 < 10**
- **200 < 분자량 < 500**

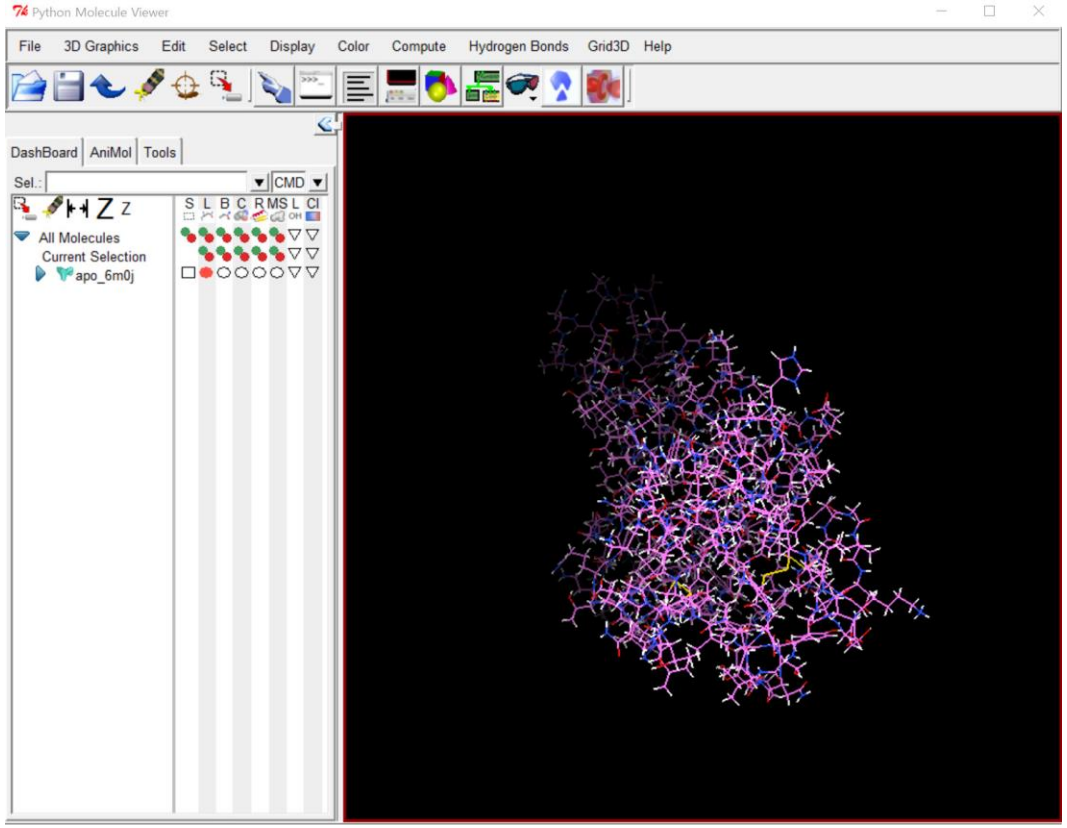
AutoDock Vina 프로그램 다운로드 및 설치

웹페이지에서 설치 파일 다운로드

http://vina.scripps.edu/

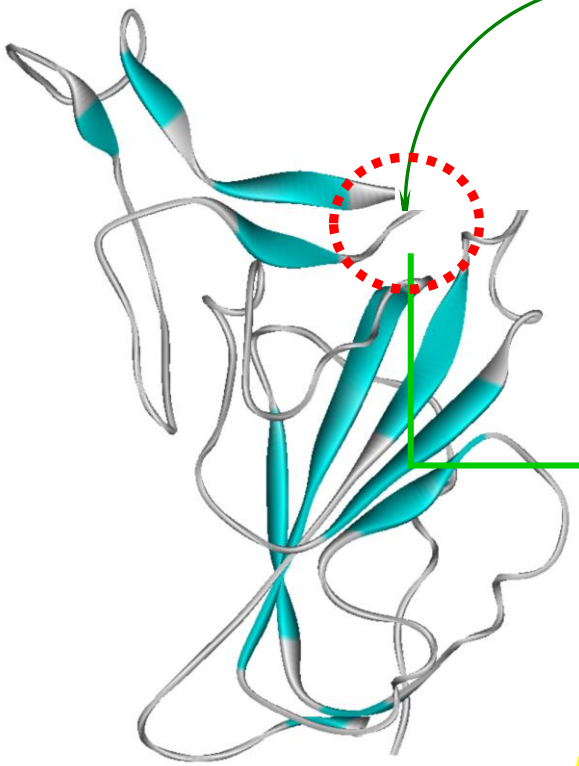


PC에 설치한 후 **Spike** 단백질 불러오기



가상 스크리닝 진행상황

도킹 모의실험



Spike 단백질

ZINC15 화합물
274,905 개

강한 결합물질 선별
(낮은 결합에너지)

1	화합물 ID	결합에너지 (kcal/mol)
2	ZINC000032102996	-23.36
3	ZINC000001168101	-23.33
4	ZINC000096118264	-23.09
5	ZINC000006781821	-23.03
6	ZINC000000602116	-23.02
7	ZINC000005004011	-23.01
8	ZINC000006579671	-22.94
9	ZINC000000498541	-22.94
10	ZINC000004910575	-22.91
11	ZINC000000008121	-22.9

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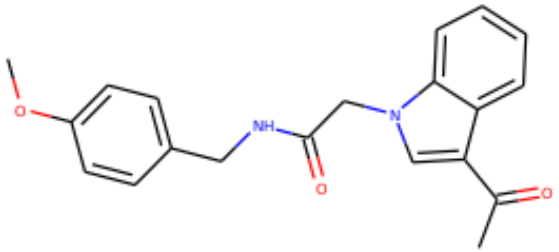
274897	ZINC000001557273	587.8
274898	ZINC000003849970	613.14
274899	ZINC000002107180	632.26
274900	ZINC000000487790	639.21
274901	ZINC000002111309	641.94
274902	ZINC000002121407	652.73
274903	ZINC000002138656	694.29
274904	ZINC000002138657	699.4
274905	ZINC000000488990	703.9
274906	ZINC000002418626	719.28

결합력이 가장 높은 화합별 선별 및 코로나19 치료제 후보물질 제안



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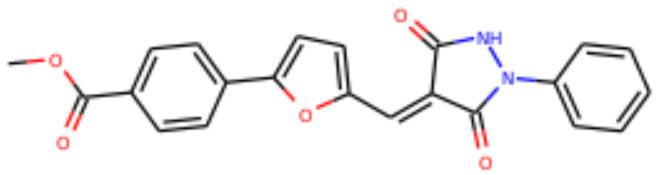

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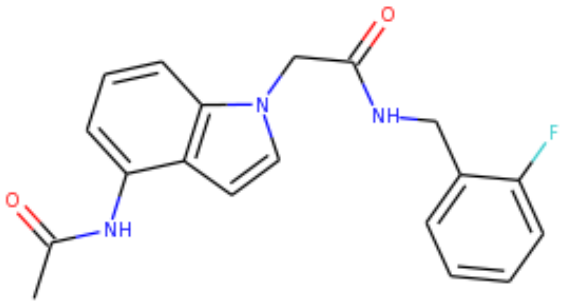
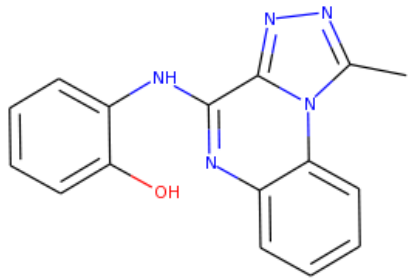
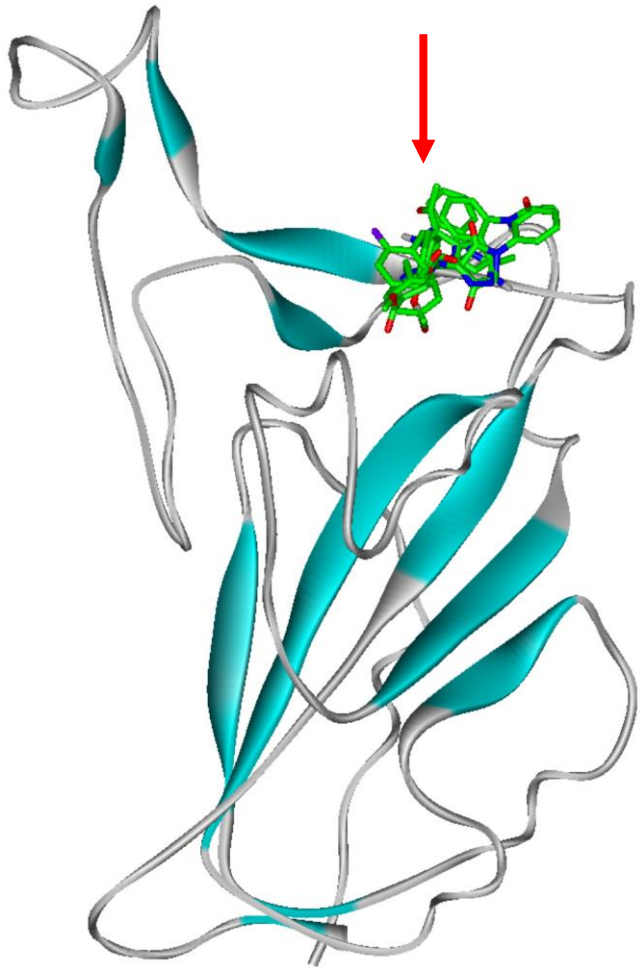


ZINC000096118264



ZINC000006781821

ACE2가 붙는 자리에
후보물질들이 결합한 모양



Spike 단백질