Screening a Panel of Topical Ophthalmic Medications against MMP-2 and MMP-9 to Investigate Their Potential in Keratoconus Management

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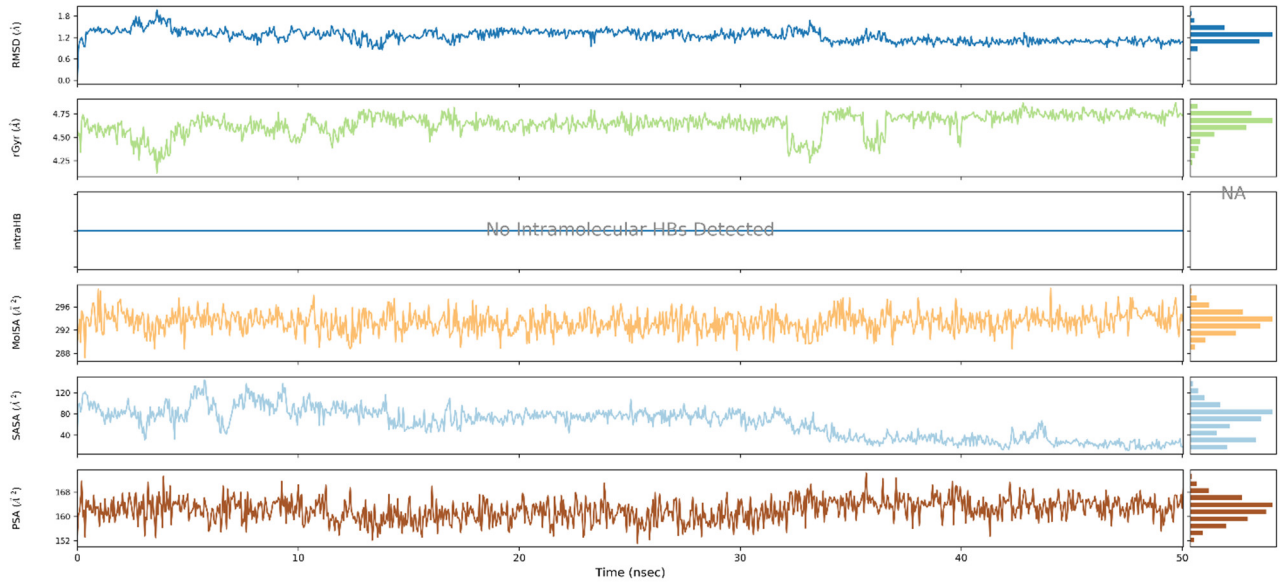


Figure S1. Atenolol properties throughout 50 ns simulation in complex with MMP-2.

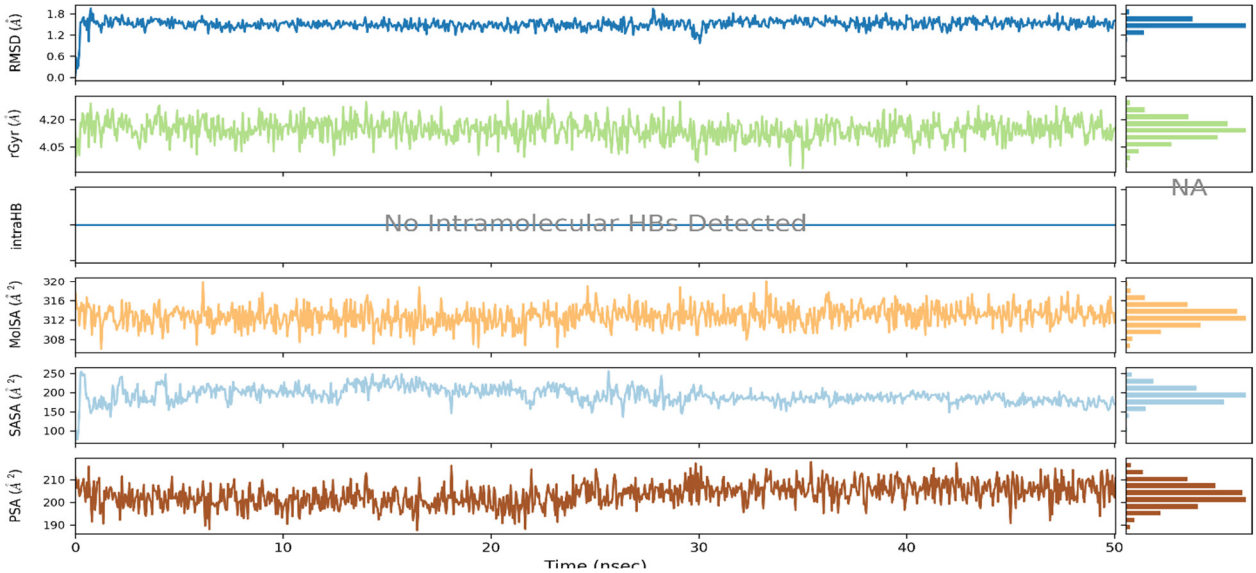


Figure S2. Ampicillin properties throughout 50 ns simulation in complex with MMP-9.

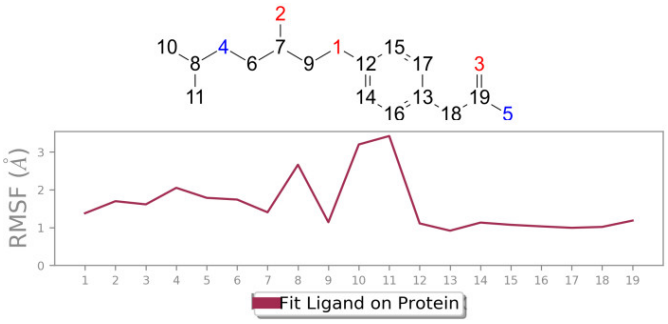


Figure S3. RMSF of atenolol throughout 50 ns simulation in complex with MMP-2.

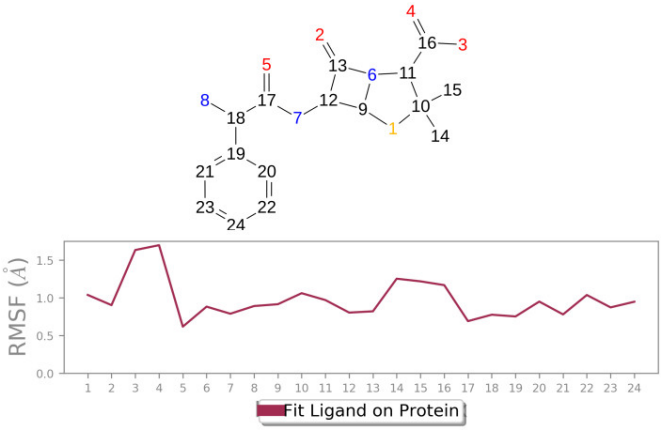


Figure S4. RMSF of ampicillin throughout 50 ns simulation in complex with MMP-9.

Table S1. Fit values of the full library on MMP-9 pharmacophore.

Serial	Compound	Fit value	Serial	Compound	Fit value
1	Acetazolamide	2.67	17	Ganciclovir	2.65
2	Acyclovir	2.62	18	Indomethacin	2.82
3	Ampicillin	3.76	19	Ketorolac	2.61
4	Atenolol	3.22	20	Levocabastine	2.60
5	Atropine	3.41	21	Lincomycin	3.76
6	Aztreonam	4.13	22	Lornoxicam	3.14
7	Betaxolol	3	23	Methazolamide	2.97
8	Brinzolamide	2.78	24	Methotrexate	3.66
9	Bromfenac	3.08	25	Nadolol	3.69
10	Carteolol	2.96	26	Pilocarpine	2.92
11	Cephalexine	4.06	27	Pindolol	2.94
12	Ciprofloxacin	2.59	28	Prednisolone	3.53
13	Dexamethasone	3.63	29	Propranolol	2.95
14	Diclofenac	2.90	30	Quinidine	3.06
15	Dorzolamide	2.79	31	Tizanidine	2.84
16	Fluconazole	2.54	32	Voriconazole	3.45