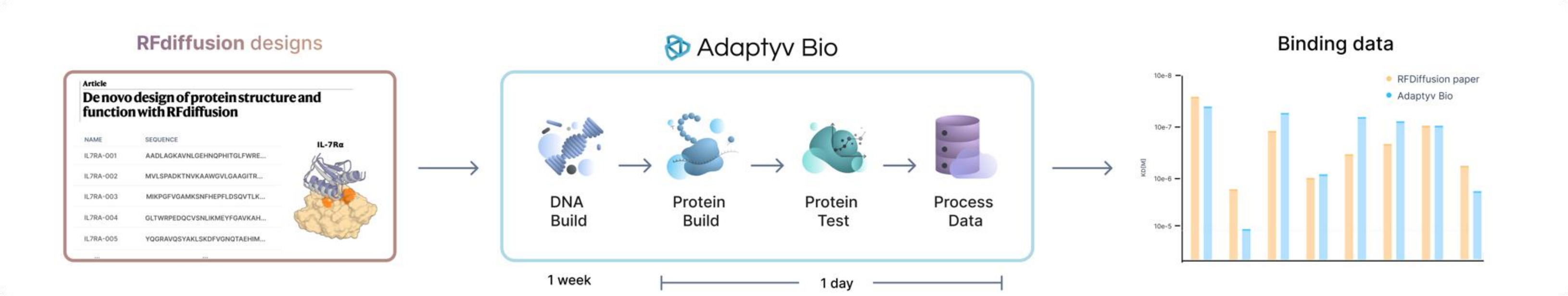
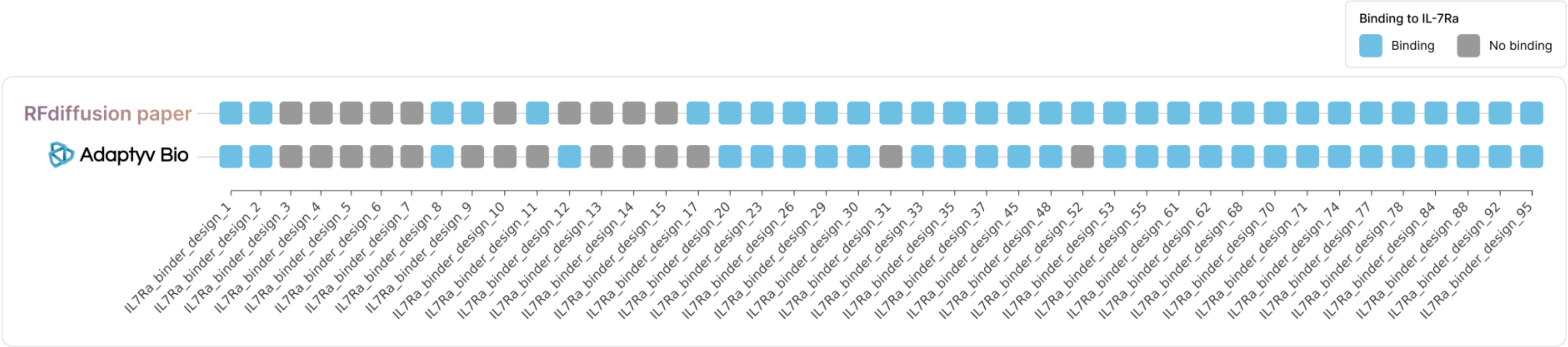
IL7a Case



De novo design of protein structure and function with RFdiffusion

NAME	SEQUENCE
IL7RA-001	AADLAGKAVNLGEHNQPHITGLFWRE...
IL7RA-002	MVLSPADKTNVKAAWGVLGAAGITR...
IL7RA-003	MIKPGFVGAMKSNFHEPFLDSQVTLK...
IL7RA-004	GLTWRPEDQCVSNLIKMEYFGAVKAH...
IL7RA-005	YQGRAVQSYAKLSKDFVGNQTAEHIM...
...	...

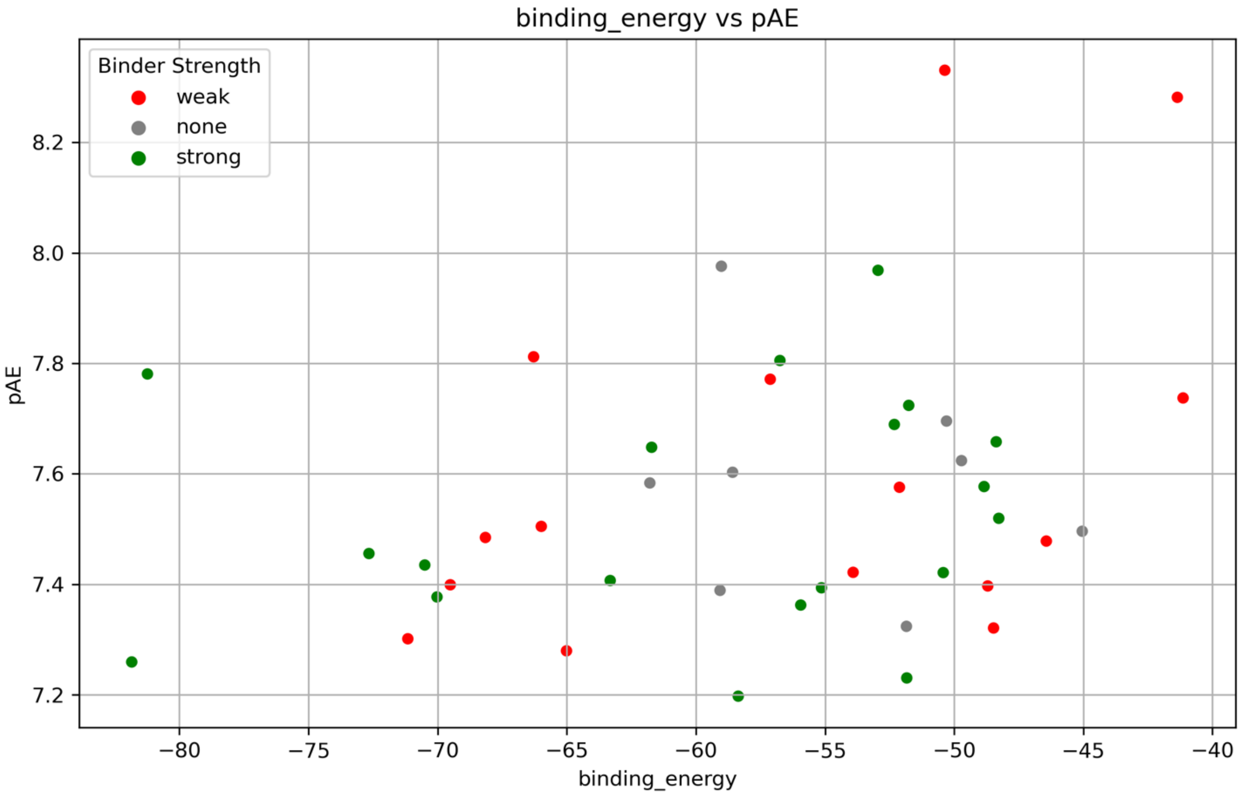


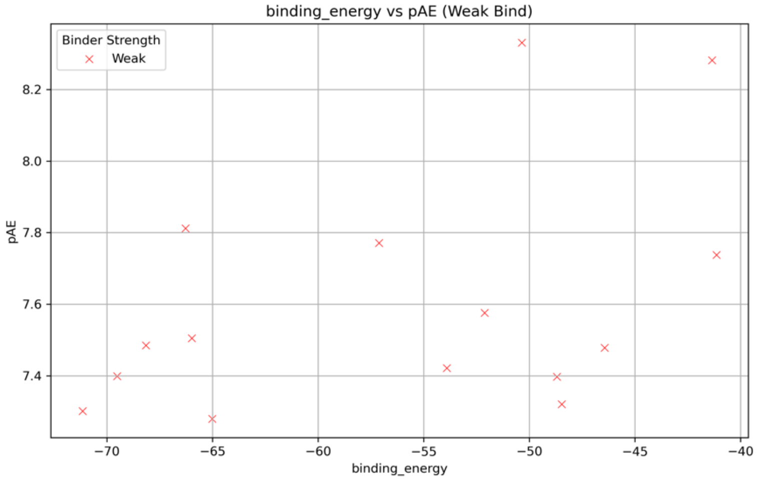
	RFdiffusion paper	Adaptyv Bio
IL7Ra_binder_design_1	🟦	🟦
IL7Ra_binder_design_2	🟦	🟦
IL7Ra_binder_design_3	⬛	⬛
IL7Ra_binder_design_4	⬛	⬛
IL7Ra_binder_design_5	⬛	⬛
IL7Ra_binder_design_6	⬛	⬛
IL7Ra_binder_design_7	⬛	⬛
IL7Ra_binder_design_8	🟦	🟦
IL7Ra_binder_design_9	🟦	⬛
IL7Ra_binder_design_10	⬛	⬛
IL7Ra_binder_design_11	🟦	⬛
IL7Ra_binder_design_12	⬛	🟦
IL7Ra_binder_design_13	⬛	⬛
IL7Ra_binder_design_14	⬛	⬛
IL7Ra_binder_design_15	⬛	⬛
IL7Ra_binder_design_17	🟦	⬛
IL7Ra_binder_design_20	🟦	🟦
IL7Ra_binder_design_23	🟦	🟦
IL7Ra_binder_design_26	🟦	🟦
IL7Ra_binder_design_29	🟦	🟦
IL7Ra_binder_design_30	🟦	🟦
IL7Ra_binder_design_31	🟦	⬛
IL7Ra_binder_design_33	🟦	🟦
IL7Ra_binder_design_35	🟦	🟦
IL7Ra_binder_design_37	🟦	🟦
IL7Ra_binder_design_45	🟦	🟦
IL7Ra_binder_design_48	🟦	🟦
IL7Ra_binder_design_52	🟦	⬛
IL7Ra_binder_design_53	🟦	🟦
IL7Ra_binder_design_55	🟦	🟦
IL7Ra_binder_design_61	🟦	🟦
IL7Ra_binder_design_62	🟦	🟦
IL7Ra_binder_design_68	🟦	🟦
IL7Ra_binder_design_70	🟦	🟦
IL7Ra_binder_design_71	🟦	🟦
IL7Ra_binder_design_74	🟦	🟦
IL7Ra_binder_design_77	🟦	🟦
IL7Ra_binder_design_78	🟦	🟦
IL7Ra_binder_design_84	🟦	🟦
IL7Ra_binder_design_88	🟦	🟦
IL7Ra_binder_design_92	🟦	🟦
IL7Ra_binder_design_95	🟦	🟦

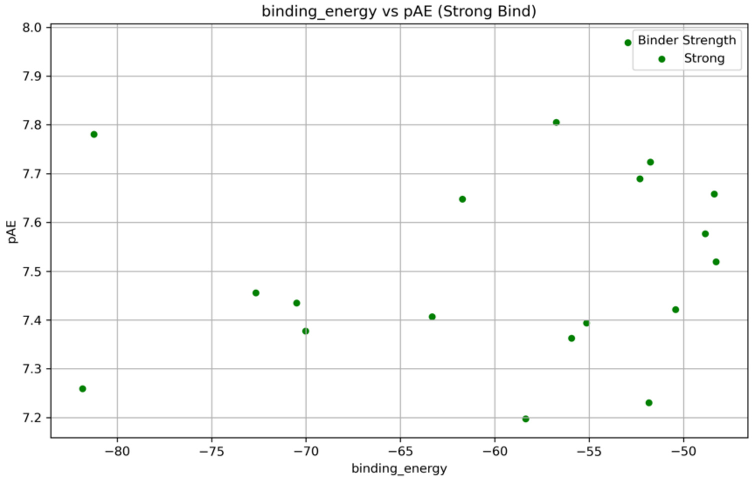
32 Protein:
Baker (B/U): 22/10
Adaptyv (B/U): 18/14

Original Paper: https://www.nature.com/articles/s41586-023-06415-8
Adaptyv_bio_Analysis: https://www.adaptyvbio.com/blog/rfdiff_il7ra
Data: https://github.com/adaptyvbio/rfdiff_il7ra

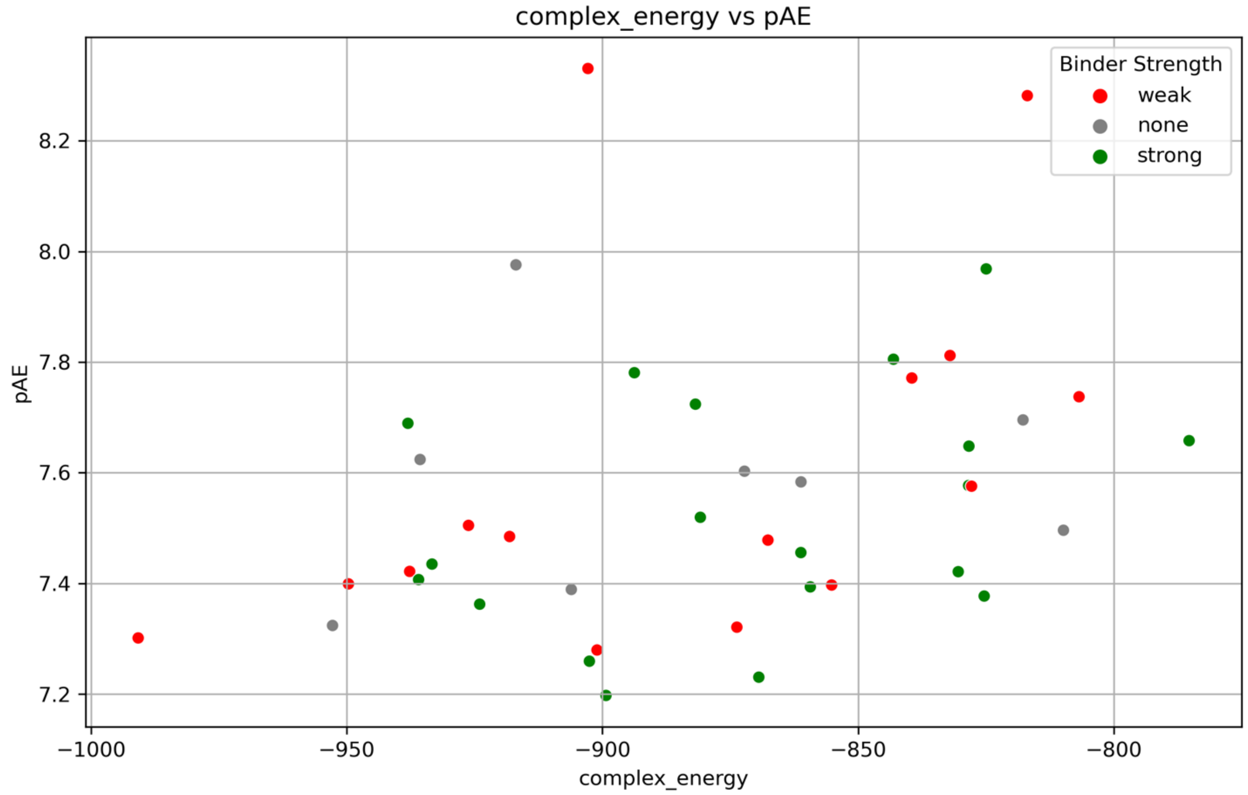
Binding Energy vs pAE

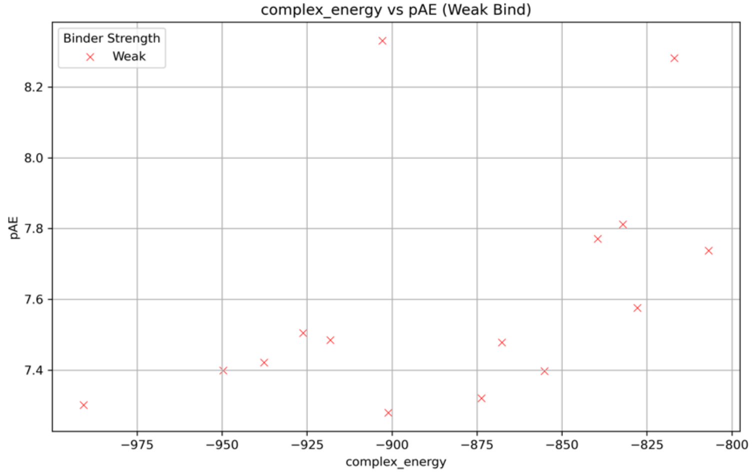


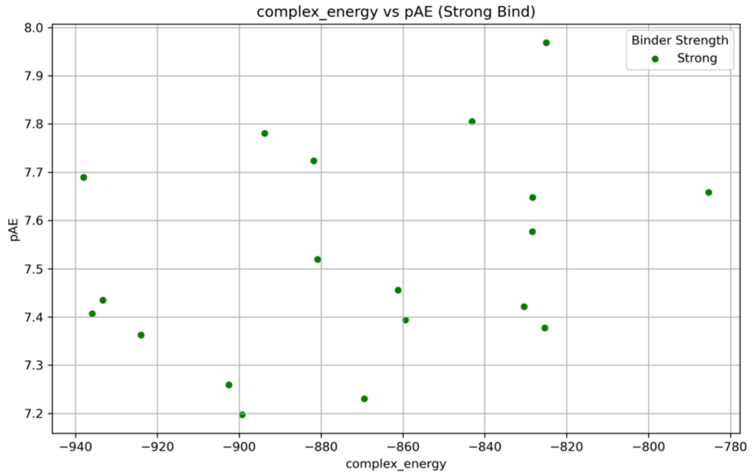




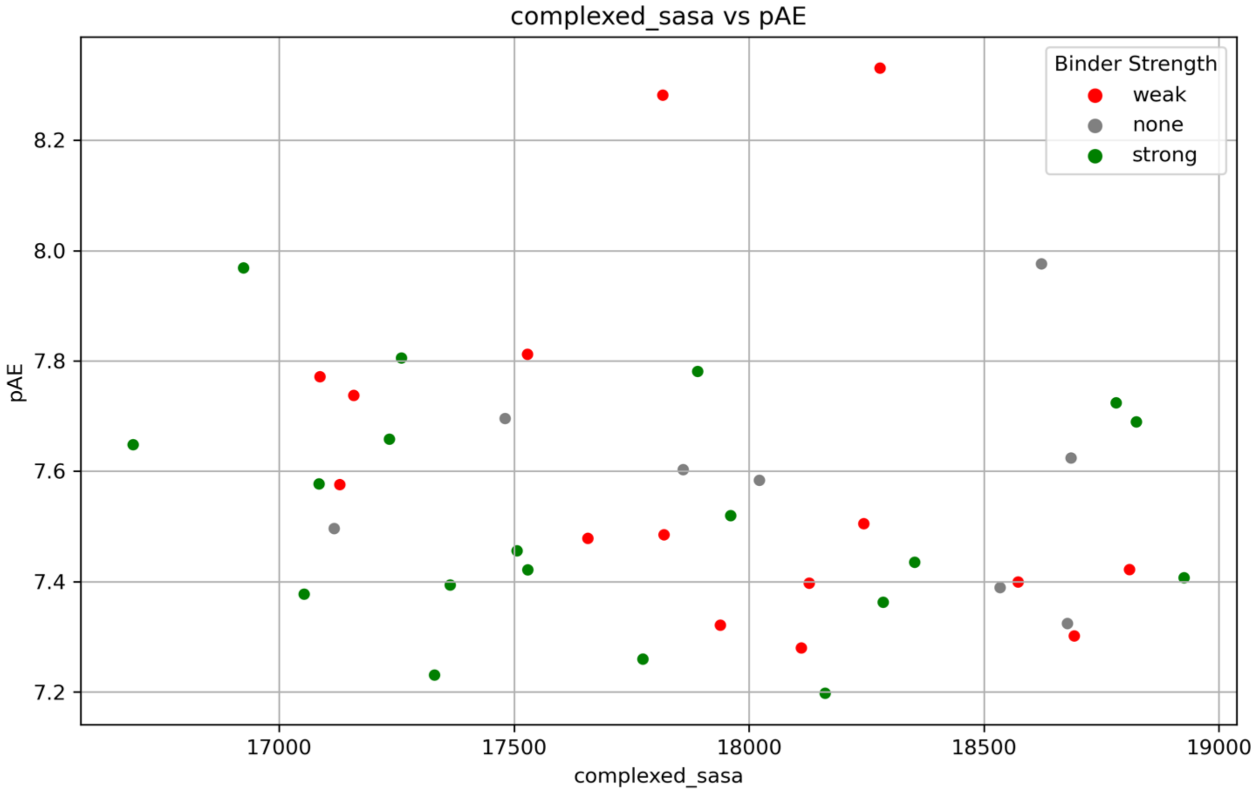
Complex Energy vs pAE



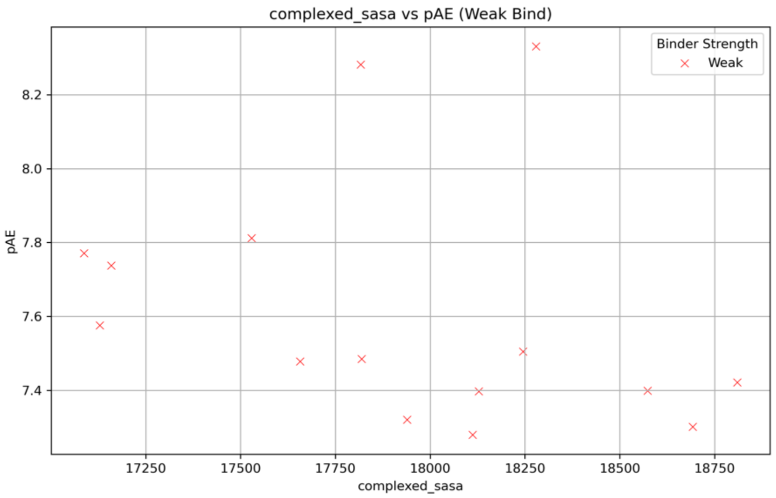




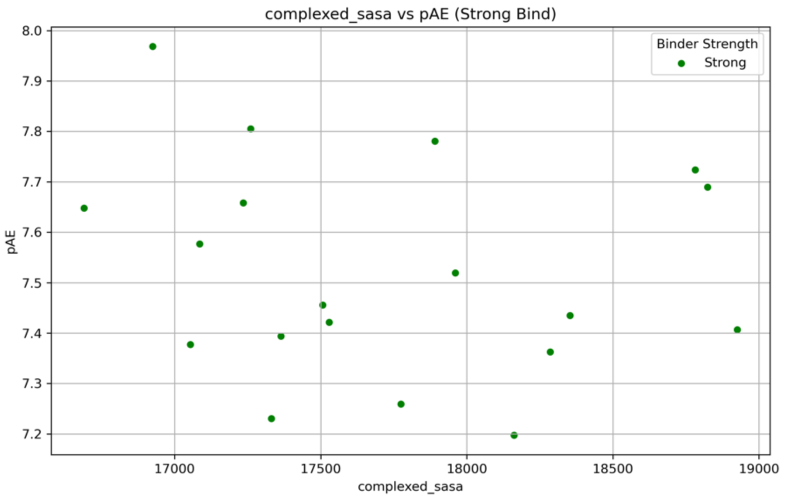
Complex SASA vs pAE



complexed_sasa vs pAE

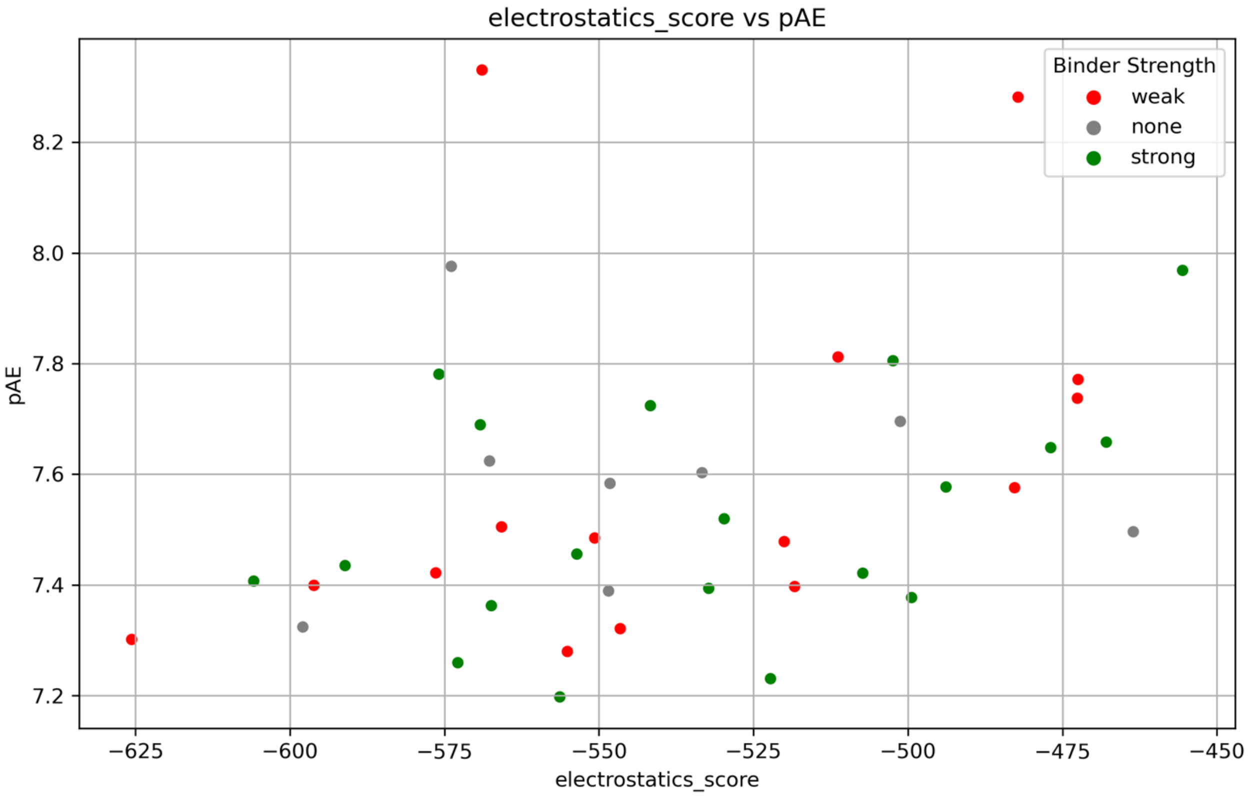


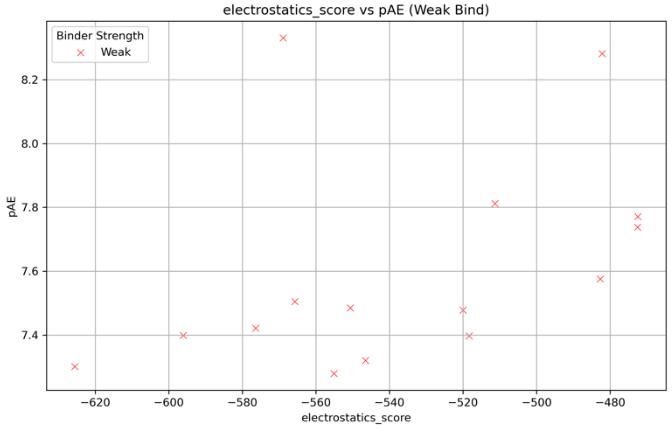
complexed_sasa vs pAE (Weak Bind)

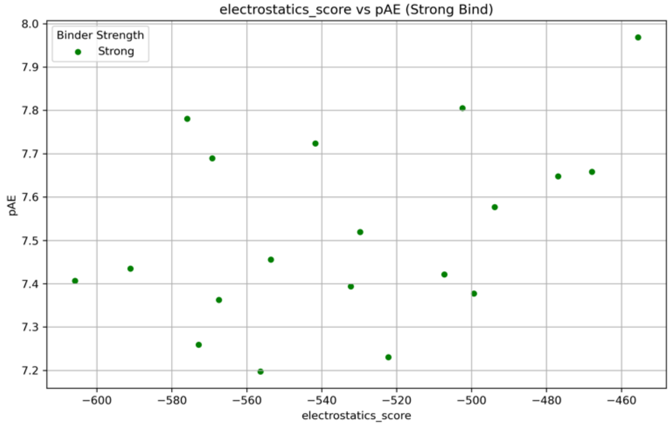


complexed_sasa vs pAE (Strong Bind)

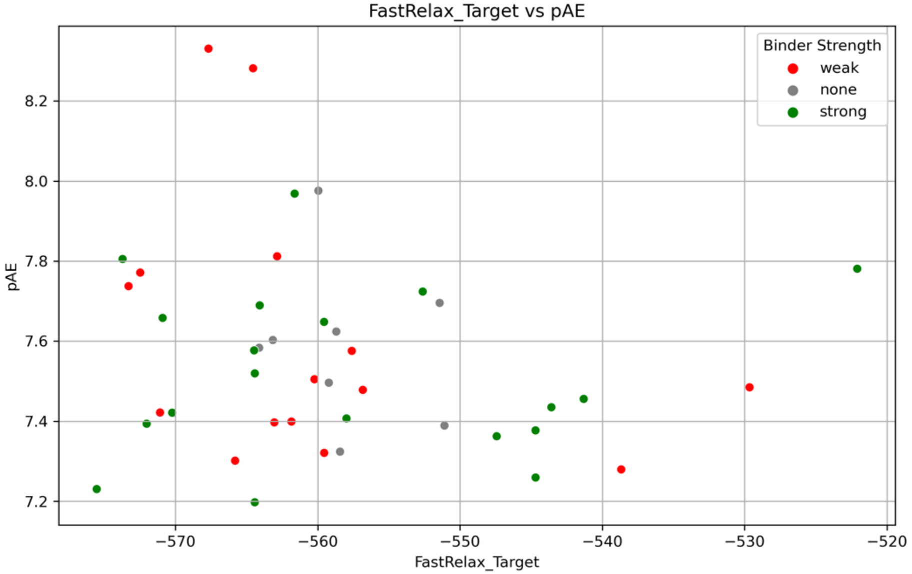
Electrostatic vs pAE

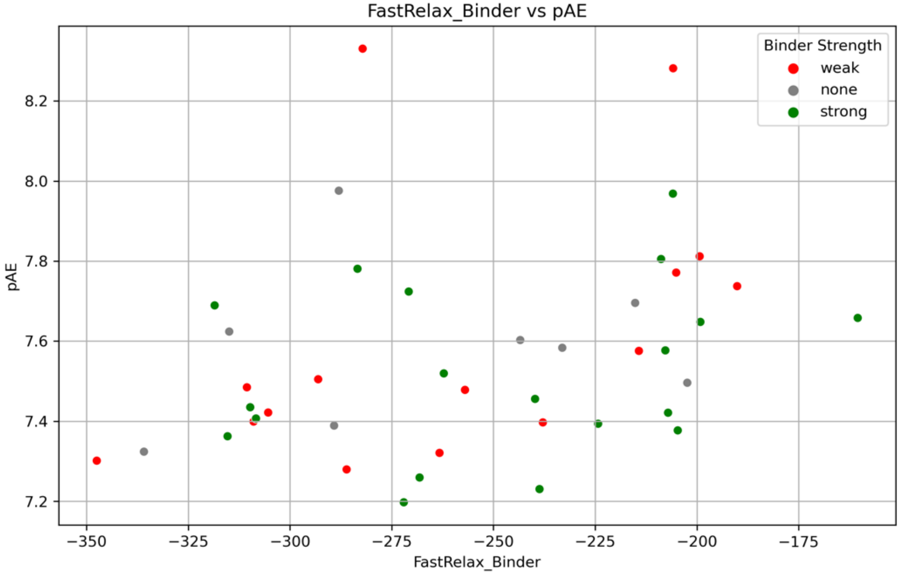


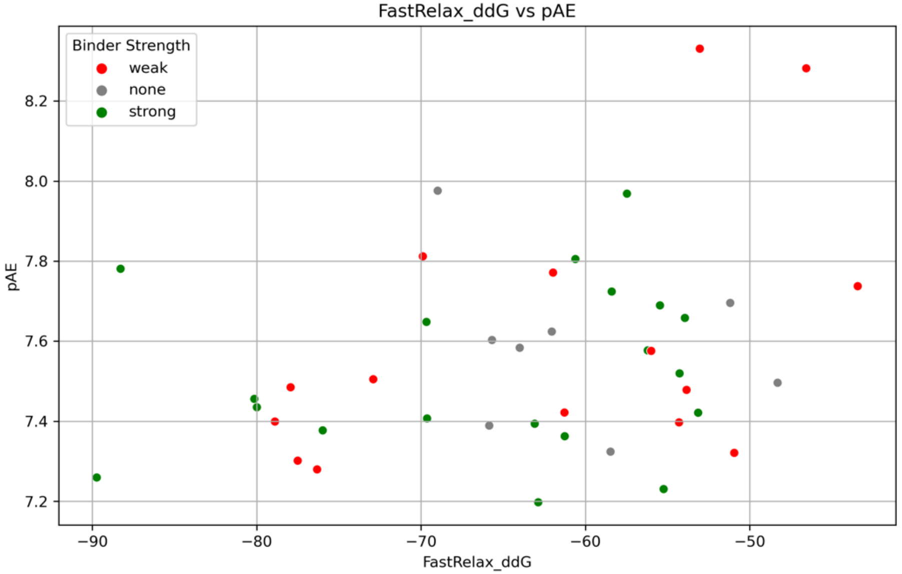




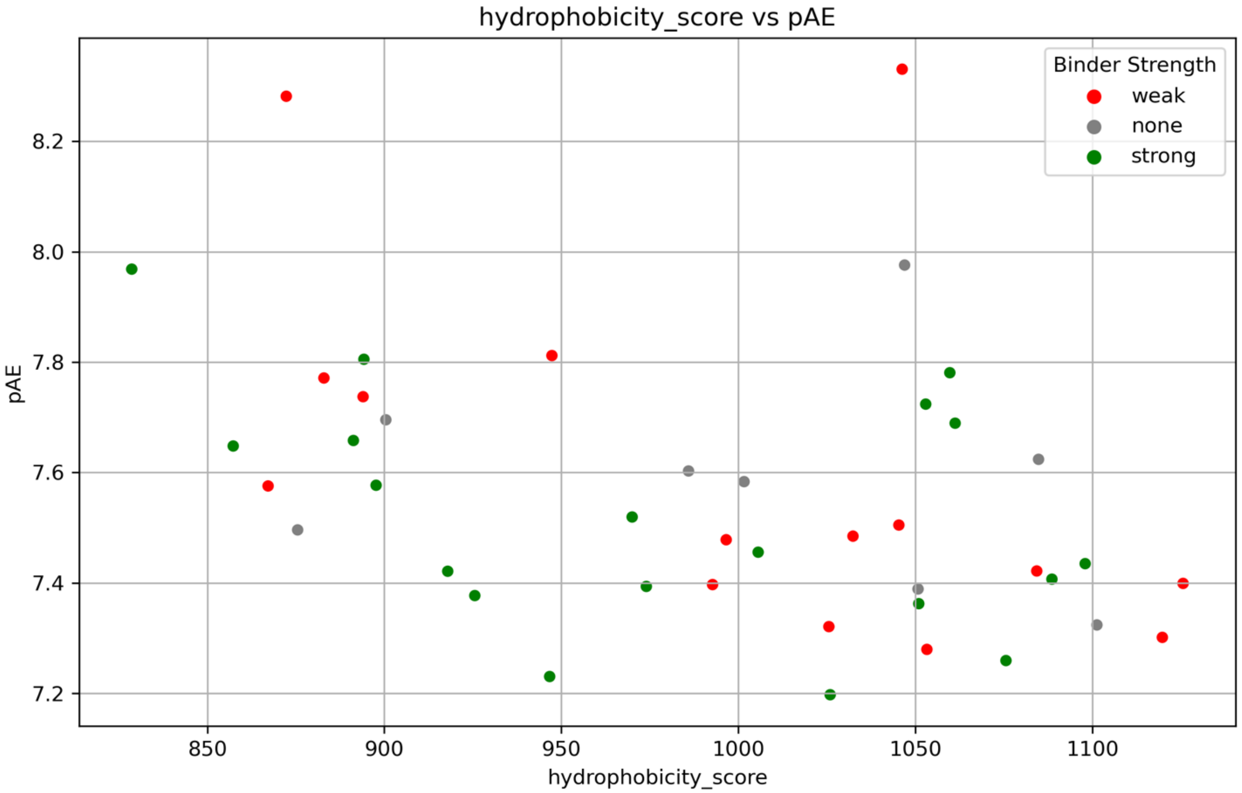
ddG vs pAE

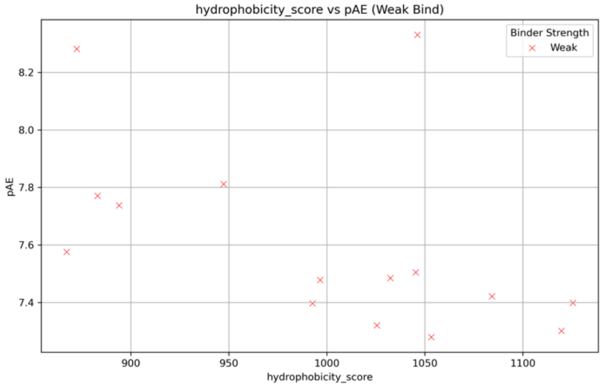

FastRelax_Target vs pAE
Binder Strength
weak
none
strong
pAE
8.2
8.0
7.8
7.6
7.4
7.2
−570
−560
−550
−540
−530
−520
FastRelax_Target

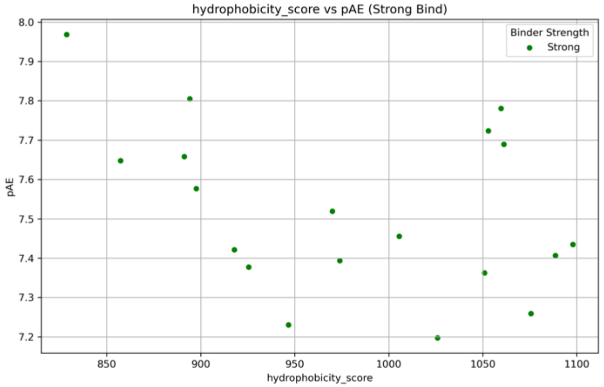

FastRelax_Binder vs pAE
Binder Strength
weak
none
strong
pAE
8.2
8.0
7.8
7.6
7.4
7.2
−350
−325
−300
−275
−250
−225
−200
−175
FastRelax_Binder


FastRelax_ddG vs pAE
Binder Strength
weak
none
strong
pAE
8.2
8.0
7.8
7.6
7.4
7.2
−90
−80
−70
−60
−50
FastRelax_ddG

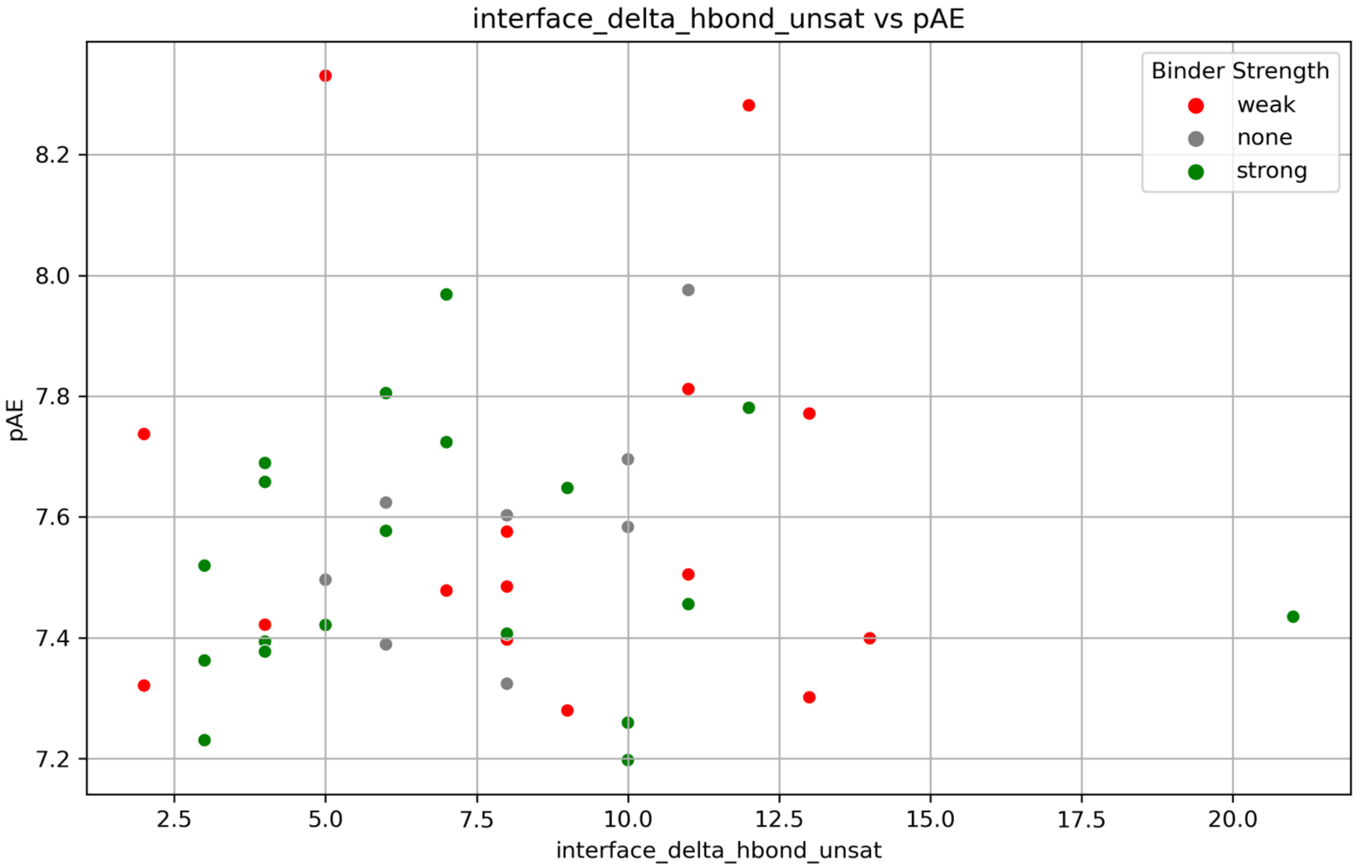
Hydrophobicity vs pAE





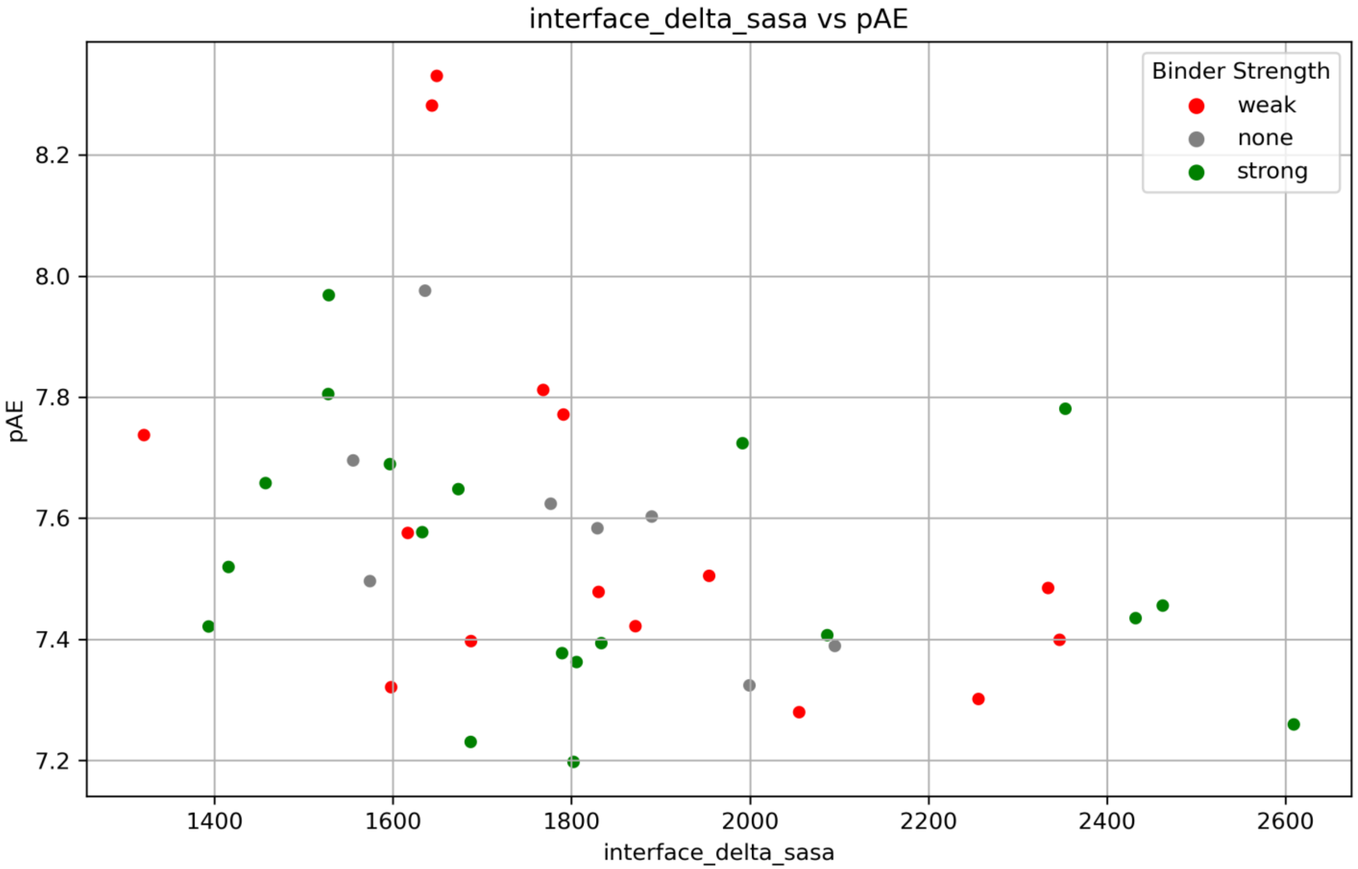


Interface delta Hbond unsat vs pAE

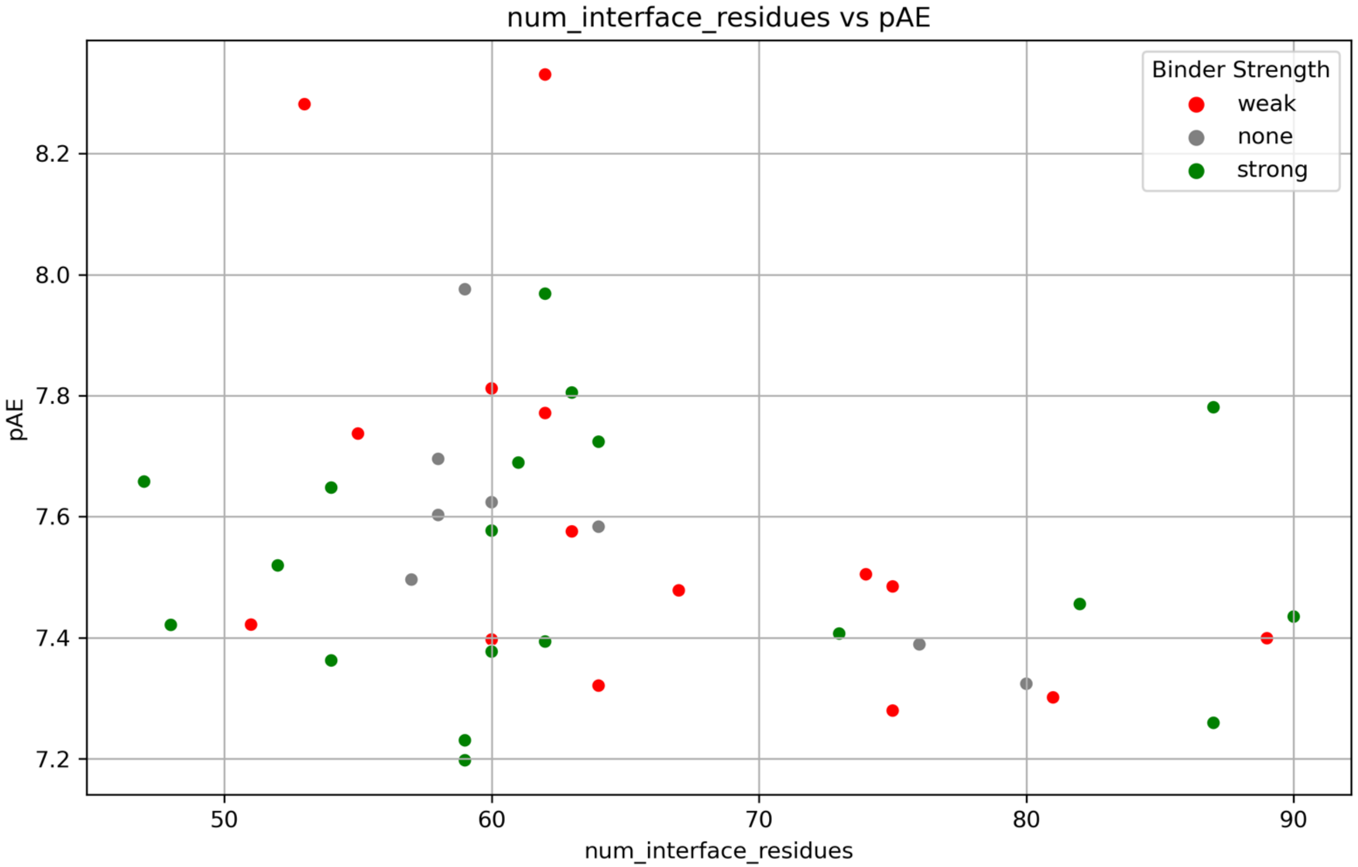


unsatisfied hydrogen bond donors or acceptors at the interface of a protein-protein complex. In other words, it measures how many potential hydrogen bonds at the interface remain unformed or "unsatisfied," which can indicate suboptimal or incomplete interactions between the two proteins.

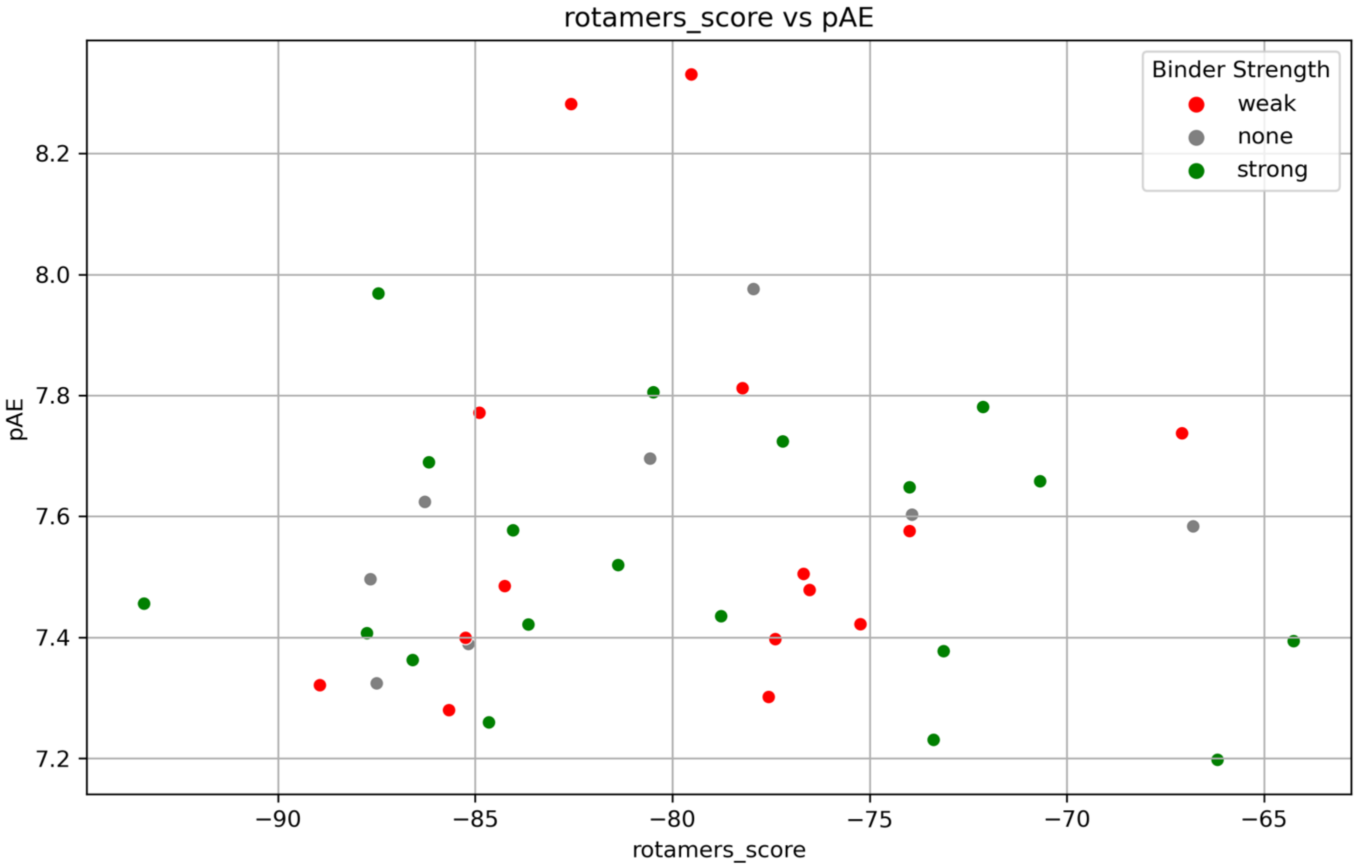
Interface delta SASA vs pAE



Num_Interface res vs pAE



Rotamer vs pAE



Total H-Bond Energy vs pAE