ELECTRONIC SUPPLEMENTARY INFORMATION

Designing Expanded and Contracted Porphyrin-Azulene Based Photosensitizers for Photodynamic Therapy

Swati Singh Rajput,[a] Samarth Razdan,[a,#], Tejendra Banana,[a,#] Neelam Chandravanshi,[a] and Md Mehboob Alam [a,b*]

[a] Department of Chemistry, Indian Institute of Technology Bhilai, Durg, Chhattisgarh – 491001, India, E-mail: mehboob@iitbhilai.ac.in

[b] Department of Chemistry, and Department of Materials Science and Metallurgical Engineering, Indian Institute of Technology Bhilai, Chhattisgarh 491001, India

[#]These authors have equal contributions

E-mail: mehboob@iitbhilai.ac.in

Table of contents

S1: The terms involved in the calculation of the rate of intersystem crossing (k_{ISC}).

The rate of intersystem crossing (k_{ISC}) for $S_a \rightarrow T_b$ transition is given as,

$$k_{ISC} = 2^{\frac{N}{2}+1}\left|\langle S_a|\widehat{H_{SO}}|T_b\rangle\right|^2 \int_0^\infty \sqrt{\sqrt{(U^2+V^2)}}\, e^{K_1} \cos\left(\frac{\theta}{2}+K_2\right) dt \qquad (1)$$

where N is the number of vibrational modes, $\langle S_a|\widehat{H_{SO}}|T_b\rangle$ is the corresponding SOCME. The integrand is calculated using the frequency matrices of singlet and triplet states $(\mathbf{\Omega_S}, \mathbf{\Omega_T})$, and corresponding Duschinsky (J) and displacement (D) matrices. U and V are scalars given by

$$U + iV = det(\mathbf{U'} + i\mathbf{V'}) \qquad (2)$$

The matrices U′ and V′ are given as $U' = \mathbf{s_T^{-1}\Omega_S\Omega_T E}$ and $V' = -\mathbf{s_T^{-1}\Omega_S\Omega_T C}$, where $\mathbf{s_T} = \sin(\omega_T)_n t$, $(\omega_T)_n$ is the n-th vibrational frequency of triplet state. The E and C matrices are obtained as

$$(\mathbf{P} + i\mathbf{Q})^{-1} = \mathbf{C} + i\mathbf{E} \qquad (3)$$

where, $\mathbf{P} = \mathbf{J^\dagger \Omega_T^2 J} + \mathbf{\Omega_S^2}$, $\mathbf{Q} = (\mathbf{J^\dagger \Omega_T b_T \Omega_S} - \mathbf{\Omega_S J^\dagger \Omega_T b_T^{-1} J})$ and $\mathbf{b_T} = \tan\left(\frac{(\omega_T)_n t}{2}\right)$. The term K_1 and K_2 in Eq. 1 are given as

$$K_1 = F + \frac{1}{2} Tr\mathbf{\Omega_s} \qquad (4)$$

$$K_2 = H + t\Delta E_{ab} \qquad (5)$$

Where, ΔE_{ab} is the energy gap between S_a and T_b and the scalars F and H are obtained from

$$F = -\mathbf{D^\dagger \Omega_T b_T J A' J^\dagger \Omega_T b_T D} \qquad (6)$$

$$H = -\mathbf{D^\dagger \Omega_T b_T J B' J^\dagger \Omega_T b_T D} - \mathbf{D^\dagger \Omega_T b_T D} \qquad (7)$$

The $\mathbf{A'}$ and $\mathbf{B'}$ matrices are obtained from

$$\mathbf{A'} + i\mathbf{B'} = (\mathbf{J^\dagger \Omega_T} i\mathbf{b_T J} + \mathbf{\Omega_S})^{-1} \qquad (8)$$

S2: This includes the optimized cartesian coordinates for the excited states of all Pr-az systems considered in this work, that are optimized at B3LYP/6-311+G(d,p) level of theory using Gaussian 16 program.

Pr-1,2-HP-s1

N	3.819732	-0.904374	0.098509
N	0.874034	-1.739350	-0.053259
N	0.050840	0.977362	-0.121250
N	2.942897	1.803732	0.041152
C	5.051593	-0.319161	0.215904
C	6.012294	-1.374837	0.229413
C	5.330780	-2.563739	0.097561
C	3.937157	-2.267736	0.011433
C	2.888908	-3.174517	-0.165935
C	1.517915	-2.944793	-0.234684
C	0.559207	-3.991853	-0.506832
C	-0.668208	-3.408004	-0.475371
C	-0.444558	-2.005545	-0.165338
C	-1.470907	-0.996949	-0.030042
C	-1.168156	0.397661	-0.089499
C	-2.160741	1.445145	-0.146386
C	-1.458957	2.649352	-0.219131
C	-0.073512	2.359984	-0.183812
C	0.981399	3.269085	-0.163554
C	2.355078	3.022533	-0.046676
C	3.350935	4.088991	0.019388
C	4.552793	3.478807	0.156015
C	4.283434	2.045692	0.163366
C	5.266717	1.064191	0.259806
H	7.078753	-1.233375	0.315575
H	5.746937	-3.559101	0.060850
H	3.198379	-4.208677	-0.275437
H	0.798053	-5.024337	-0.718295
H	-1.612476	-3.874012	-0.696870
H	-1.862076	3.648654	-0.262777
H	0.686437	4.311255	-0.219860
H	3.139460	5.147676	-0.030114
H	5.529433	3.933679	0.240136
H	6.295999	1.390631	0.351456
H	2.960253	-0.367566	0.053798
H	0.920349	0.456371	-0.069339
C	-3.556206	1.133564	-0.105641
C	-4.519176	2.169766	-0.226102
C	-3.870222	-0.246222	0.086452
C	-5.894553	2.129672	-0.160648
H	-4.102691	3.157789	-0.399210
C	-5.121709	-0.870953	0.280031
C	-2.845935	-1.280391	0.150639
C	-6.759139	1.018128	0.072582
H	-6.396461	3.082474	-0.295918

C	-6.423792	-0.294185	0.273239
C	-4.868976	-2.276965	0.511465
C	-3.523219	-2.525275	0.440498
H	-7.819056	1.253355	0.096343
H	-7.243338	-0.987301	0.442056
H	-5.639875	-3.004475	0.728359
H	-3.052068	-3.473308	0.634326

Pr-1,2-PH-s1

N	3.607536	-1.224471	0.089163
N	0.585993	-1.618113	-0.096136
N	0.176517	1.185322	-0.112029
N	3.142670	1.585608	0.101476
C	4.909103	-0.826272	0.249630
C	5.708951	-2.019349	0.226612
C	4.871446	-3.083430	0.023780
C	3.527667	-2.585913	-0.068902
C	2.373489	-3.318424	-0.307398
C	1.044845	-2.877077	-0.371538
C	-0.050612	-3.752607	-0.733004
C	-1.182331	-3.004130	-0.653767
C	-0.766033	-1.675907	-0.224210
C	-1.631792	-0.547339	-0.029336
C	-1.112938	0.779243	-0.094156
C	-1.927215	1.962122	-0.188225
C	-1.059955	3.061328	-0.257881
C	0.257240	2.574767	-0.186553
C	1.436556	3.334209	-0.136506
C	2.743001	2.892248	0.013053
C	3.889454	3.789674	0.118833
C	4.977238	2.999324	0.278936
C	4.489592	1.622126	0.257168
C	5.324076	0.496804	0.349547
H	6.782662	-2.036782	0.335669
H	5.140115	-4.125873	-0.058169
H	2.527603	-4.379209	-0.473281
H	0.042521	-4.786156	-1.034802
H	-2.182865	-3.308673	-0.914417
H	-1.329401	4.103178	-0.334136
H	1.289663	4.406997	-0.194463
H	3.845570	4.868765	0.077984
H	6.009904	3.296472	0.394246
H	6.387064	0.667883	0.469645
H	2.834954	-0.569483	0.052732
H	0.965195	0.549798	-0.040015
C	-3.323586	1.813708	-0.197514
C	-3.885903	0.483804	0.017588
C	-4.389636	2.740435	-0.345952
C	-3.057189	-0.669707	0.186682
C	-5.293188	0.630167	0.003674

H	-4.288817	3.802215	-0.514160
C	-5.571308	2.030339	-0.240703
C	-3.601963	-1.894078	0.701509
C	-6.304664	-0.355769	0.166137
H	-6.569320	2.441220	-0.319136
C	-4.900905	-2.313721	0.853650
H	-2.860006	-2.600403	1.053084
C	-6.130131	-1.660660	0.534595
H	-7.325572	-0.016419	0.013091
H	-5.012182	-3.304411	1.285181
H	-7.025956	-2.263015	0.649131

SP-1,2-HP-s1

C	-2.103980	3.308795	-0.679899
C	-0.747282	3.168073	-0.422445
C	-2.755333	2.111358	-0.248603
C	-0.547085	1.890612	0.185615
N	-1.786743	1.335432	0.335701
C	-4.010398	1.528502	-0.562289
H	-4.760947	2.126756	-1.062498
C	-4.196740	0.141555	-0.437188
C	-5.082162	-0.803566	-1.068447
N	-3.211809	-0.604122	0.156733
C	-4.533409	-2.060548	-0.916794
C	-3.298390	-1.920857	-0.185759
C	-2.169422	-2.767813	-0.040155
H	-2.242537	-3.800685	-0.354306
C	-0.912063	-2.216957	0.269639
C	0.452093	-2.609786	0.062251
N	-0.882526	-0.873754	0.598940
C	1.251162	-1.455531	0.165630
C	0.340559	-0.374558	0.451571
C	0.600549	1.025549	0.347533
B	-2.072214	-0.024358	0.971552
O	-2.248275	-0.021144	2.394896
H	-3.008538	0.490664	2.682559
H	0.769214	-3.601367	-0.220851
H	0.029755	3.859939	-0.705577
H	-2.579234	4.132718	-1.190738
H	-5.970632	-0.551031	-1.627653
H	-4.910020	-2.982514	-1.333860
C	2.637061	-1.137810	-0.020602
C	3.582321	-2.176319	-0.242993
C	2.968110	0.261550	0.028321
C	4.944428	-2.131093	-0.428221
H	3.154084	-3.174889	-0.255524
C	4.216799	0.899867	-0.119398
C	1.966867	1.327983	0.190806
C	5.821078	-1.001228	-0.461112
H	5.429046	-3.092321	-0.567033

C	5.505871	0.321671	-0.327974
C	3.990889	2.328928	-0.037720
C	2.650706	2.585340	0.136572
H	6.870196	-1.234149	-0.616797
H	6.328568	1.028551	-0.392775
H	4.778034	3.068706	-0.101511
H	2.194454	3.555389	0.259984

SP-1,2-PH-s1

C	-1.418867	3.354408	-0.737448
C	-0.113689	2.960508	-0.497597
C	-2.281157	2.314974	-0.263679
C	-0.143366	1.680469	0.150152
N	-1.473582	1.383715	0.332836
C	-3.636299	1.996365	-0.542423
H	-4.265604	2.728325	-1.030716
C	-4.075565	0.671990	-0.406781
C	-5.157098	-0.088061	-1.000779
N	-3.249691	-0.243958	0.180241
C	-4.872755	-1.421407	-0.840987
C	-3.605790	-1.530547	-0.146487
C	-2.677810	-2.570917	-0.026204
H	-2.955371	-3.575419	-0.316071
C	-1.314581	-2.264985	0.245687
C	-0.079690	-2.908633	-0.016638
N	-1.013420	-0.954631	0.588157
C	0.937469	-1.922412	0.076382
C	0.279689	-0.690134	0.408433
C	0.822933	0.626406	0.322136
B	-2.011090	0.109054	0.981530
O	-2.159023	0.143229	2.407680
H	-2.772818	0.817736	2.709031
H	0.041374	-3.934643	-0.327929
H	0.771177	3.481609	-0.826100
H	-1.736306	4.237330	-1.271572
H	-5.990297	0.334536	-1.542250
H	-5.437974	-2.253401	-1.233961
C	2.322301	-1.834021	-0.141476
C	2.972891	-0.516067	-0.053364
C	3.316194	-2.807542	-0.442505
C	2.254094	0.707436	0.190500
C	4.346335	-0.732854	-0.303692
H	3.144712	-3.867166	-0.559537
C	4.525549	-2.151344	-0.540531
C	2.903117	1.970307	0.346314
C	5.418068	0.204663	-0.359746
H	5.481874	-2.607810	-0.759946
C	4.221714	2.335610	0.217858
H	2.242210	2.773932	0.651870
C	5.362970	1.551134	-0.133357

H	6.391498	-0.212480	-0.603044
H	4.431622	3.381679	0.419567
H	6.298447	2.096718	-0.209674

NCP-1,2-HP-s1

H	-7.141078	-1.158520	-0.308808
H	-5.872897	-3.529197	-0.291721
H	-3.287552	-4.270305	0.064579
H	-0.708271	-4.877763	0.750297
H	1.980429	3.677362	0.024032
H	-0.654816	4.369292	0.181735
H	-3.088164	5.144408	0.211183
H	-6.260310	1.455655	-0.107067
H	-3.028957	-0.402764	0.036851
H	-0.905749	0.633436	0.232464
C	-5.089266	-0.307407	-0.155538
C	-6.077630	-1.332065	-0.249611
C	-5.426119	-2.547916	-0.237033
C	-4.024607	-2.306354	-0.149896
C	-2.980386	-3.235301	-0.053370
C	-1.617921	-2.953879	-0.018939
C	-0.571053	-3.848853	0.436484
C	0.400017	-1.938188	0.066827
C	1.475864	-0.974171	0.040208
C	1.207148	0.432561	0.044070
C	2.219786	1.457511	-0.000062
C	1.548750	2.689430	0.044062
C	0.163935	2.431878	0.114330
C	-0.917577	3.317660	0.156634
C	-2.288246	3.029920	0.138631
C	-3.296406	4.085353	0.157782
C	-4.227789	2.037644	0.027818
C	-5.242467	1.084987	-0.079723
N	-3.875817	-0.934446	-0.117099
N	0.005563	1.054767	0.116664
N	-2.877868	1.799486	0.068410
N	0.597694	-3.262910	0.500806
C	-0.930672	-1.729149	-0.275018
H	-1.332295	-0.885082	-0.810103
C	-4.499187	3.469670	0.089283
H	-5.481996	3.918612	0.074259
C	3.604580	1.103113	-0.054466
C	4.595438	2.124469	-0.120287
C	3.885953	-0.293026	-0.026152
C	5.965883	2.038466	-0.169406
H	4.203147	3.137056	-0.135194
C	5.125287	-0.978069	-0.060452
C	2.841184	-1.303038	0.035310
C	6.805044	0.881061	-0.169349
H	6.492448	2.986533	-0.216000

C	6.438551	-0.437597	-0.123074
C	4.837496	-2.399063	-0.016801
C	3.485994	-2.600967	0.039071
H	7.870983	1.083347	-0.213519
H	7.243986	-1.167070	-0.134483
H	5.597977	-3.168733	-0.025681
H	2.956602	-3.536625	0.097721

NCP-1,2-PH-s1

H	-6.887374	-1.931768	-0.336194
H	-5.301534	-4.091051	-0.184116
H	-2.643974	-4.433634	0.243594
H	-0.070942	-4.584475	1.146163
H	1.454795	4.118686	0.107650
H	-1.230059	4.436472	0.199982
H	-3.754212	4.885855	0.152613
H	-6.387876	0.788442	-0.235766
H	-2.926393	-0.579541	0.008922
H	-0.953697	0.673774	0.196803
H	4.376827	3.784311	0.039089
H	6.642341	2.385349	-0.027287
H	2.897085	-2.824778	-0.342029
H	7.378784	-0.073646	-0.072896
H	5.038770	-3.559892	-0.469334
H	7.068866	-2.400981	-0.250658
C	-4.976280	-0.784745	-0.210515
C	-5.810733	-1.951389	-0.263016
C	-4.999389	-3.054446	-0.180179
C	-3.638386	-2.613148	-0.092024
C	-2.488273	-3.372175	0.076466
C	-1.171643	-2.887902	0.128405
C	-0.042145	-3.592968	0.707292
C	0.717192	-1.639647	0.122276
C	1.661715	-0.556607	0.015604
C	1.168379	0.784937	0.034187
C	1.997800	1.958788	0.025663
C	1.158321	3.081632	0.091049
C	-0.167385	2.619634	0.134583
C	-1.360300	3.360959	0.159858
C	-2.670679	2.901437	0.103855
C	-3.813899	3.808495	0.092056
C	-4.450304	1.650802	-0.063964
C	-5.329854	0.562721	-0.180980
C	3.391060	1.785298	-0.003684
C	3.934318	0.427267	-0.052693
C	4.465148	2.708639	0.006955
C	3.094610	-0.727754	-0.070636
C	5.347760	0.562488	-0.075193
C	5.639919	1.977869	-0.030157
C	3.640002	-2.045593	-0.258146

C	6.354947	-0.435446	-0.114875
C	4.937551	-2.488541	-0.321222
C	6.174444	-1.786800	-0.218424
N	-3.685995	-1.232119	-0.139303
N	-0.113379	1.230346	0.114300
N	-3.090782	1.595090	0.014738
N	1.049914	-2.872511	0.718688
C	-0.636965	-1.633987	-0.247656
H	-1.124425	-0.906257	-0.876355
C	-4.917504	3.034117	-0.014766
H	-5.951850	3.343864	-0.059849

S-5,6-HP-s1

C	-3.113781	-3.393302	-0.288244
C	-2.460425	-4.614647	-0.569109
C	-1.102213	-4.360430	-0.655910
C	-0.901778	-2.978539	-0.433238
N	-2.138418	-2.418133	-0.236459
H	-2.389803	-1.462675	0.000403
H	-2.956467	-5.565978	-0.684668
H	-0.319866	-5.072655	-0.863211
C	0.349244	-2.310396	-0.362889
C	1.607567	-2.912682	-0.297704
C	2.563504	-1.892931	-0.140364
C	1.856502	-0.650220	-0.134565
N	0.535111	-0.932213	-0.270450
H	1.792387	-3.973929	-0.326562
C	1.708789	1.796911	-0.403535
C	2.259351	3.024963	-0.944749
C	1.202077	3.848089	-1.167181
H	1.212370	4.848507	-1.575894
C	2.471892	0.629668	-0.074681
C	0.017378	3.123245	-0.752846
N	0.345731	1.863907	-0.333322
C	-4.421524	2.473130	0.389177
C	-2.512237	3.478646	-0.325529
C	-3.531465	4.478299	-0.187633
H	-5.617746	4.345214	0.489898
H	-3.375005	5.524512	-0.402624
C	-5.450878	0.145656	0.665350
C	-6.716382	-0.547950	0.892945
C	-6.483682	-1.858111	0.648435
C	-5.076287	-1.960675	0.298555
N	-4.468431	-0.722878	0.328956
H	-7.644121	-0.072650	1.178106
H	-7.177261	-2.685446	0.696303
C	-1.218298	3.787658	-0.722359
C	-4.667825	3.881723	0.271551
C	-5.402791	1.550578	0.717145
N	-3.098631	2.278009	0.038270

C	-4.470157	-3.165322	-0.020960
H	-5.105571	-4.043450	-0.041149
H	-6.346333	2.015870	0.981326
H	-1.136683	4.827802	-1.022146
H	-0.135285	-0.164753	-0.321823
H	-2.648232	1.376768	0.021715
H	3.295492	3.211378	-1.176701
C	3.881277	0.649516	0.243578
C	4.488233	1.863911	0.709991
C	4.612359	-0.578887	0.208802
C	5.801321	2.180593	0.962109
H	3.786799	2.661429	0.922518
C	6.002095	-0.845061	0.341309
C	3.961863	-1.860735	-0.009885
C	6.986379	1.397970	0.829300
H	5.964301	3.192727	1.321580
C	7.073869	0.057800	0.562170
C	6.177654	-2.271364	0.182541
C	4.953672	-2.881138	-0.016046
H	7.919179	1.924476	1.005684
H	8.069419	-0.377713	0.545028
H	7.137877	-2.768588	0.222374
H	4.775189	-3.937477	-0.152295

S-5,6-PH-s1

C	-2.693108	-3.554131	0.374959
C	-1.876245	-4.685455	0.643129
C	-0.565077	-4.264170	0.679655
C	-0.544348	-2.863629	0.442428
N	-1.848065	-2.464979	0.285775
H	-2.223081	-1.553652	0.039608
H	-2.246351	-5.689261	0.784610
H	0.307937	-4.868431	0.866749
C	0.610414	-2.054054	0.346187
C	1.941213	-2.494377	0.250670
C	2.766287	-1.368176	0.106696
C	1.903365	-0.233302	0.141709
N	0.623523	-0.671017	0.277315
H	2.240675	-3.529344	0.244918
C	1.435277	2.212008	0.370114
C	1.830760	3.530203	0.808080
C	0.678366	4.238262	0.958418
H	0.565800	5.264257	1.278633
C	2.341412	1.122887	0.106551
C	-0.403410	3.348818	0.603961
N	0.083066	2.103471	0.283831
C	-4.739589	2.085397	-0.446587
C	-2.963499	3.355363	0.169241
C	-4.092581	4.210374	-0.004700
H	-6.161798	3.779159	-0.624183

H	-4.064474	5.279001	0.144968
C	-5.481966	-0.361640	-0.601257
C	-6.651889	-1.219248	-0.776768
C	-6.248607	-2.478599	-0.494612
C	-4.831065	-2.387489	-0.175471
N	-4.385584	-1.096657	-0.254994
H	-7.637720	-0.876215	-1.056620
H	-6.830583	-3.389121	-0.499635
C	-1.709365	3.843816	0.529626
C	-5.158679	3.449015	-0.402320
C	-5.608647	1.022595	-0.709671
N	-3.402089	2.070984	-0.114271
C	-4.066388	-3.508183	0.153770
H	-4.586830	-4.457117	0.210754
H	-6.604996	1.357644	-0.977544
H	-1.760291	4.903050	0.763463
H	-0.135390	0.006140	0.339142
H	-2.845678	1.232747	-0.052755
H	2.832824	3.857104	1.027278
C	3.720458	1.275453	-0.161470
C	4.623291	0.147057	-0.232301
C	4.500527	2.464892	-0.446322
C	5.916592	0.650967	-0.508104
C	4.181743	-1.204632	-0.060904
C	5.800134	2.087345	-0.648220
H	4.112973	3.465087	-0.543979
C	7.142647	-0.056371	-0.638800
C	5.030441	-2.334544	-0.067427
H	6.624851	2.742296	-0.895479
C	7.347485	-1.408744	-0.519942
H	8.016934	0.552814	-0.850291
C	6.396817	-2.433833	-0.255752
H	4.528351	-3.283045	0.101005
H	8.370858	-1.750259	-0.646444
H	6.803448	-3.438729	-0.205171

Hx-2,3-HP-s1

C	7.838143	-1.996166	0.421411
H	8.888643	-1.826137	0.602167
C	7.219888	-3.181922	0.132656
H	8.043080	0.716281	0.851018
C	7.025368	0.394733	0.663349
C	6.231311	2.813833	0.781750
C	6.834643	-0.967656	0.441087
C	5.018675	3.392679	0.623774
C	6.020115	1.372072	0.629827
H	7.177003	3.297652	0.982770
C	5.816562	-2.923511	-0.029983
C	4.826135	-3.851426	-0.332282
C	4.066770	2.299749	0.389794

H	5.162123	-4.874304	-0.461913
H	4.788999	4.443280	0.692369
C	2.152594	4.841090	-0.232394
N	4.718427	1.098571	0.415819
C	2.692259	2.329891	0.178530
C	1.832066	3.423824	-0.037767
C	0.976921	5.463402	-0.487847
N	5.635818	-1.576115	0.169535
C	3.452633	-3.606115	-0.472428
C	-0.049995	4.427626	-0.439532
H	3.132065	5.289602	-0.213298
N	2.874382	-2.391033	-0.326391
N	0.501657	3.214002	-0.167182
C	2.452363	-4.624482	-0.771830
C	1.535738	-2.581940	-0.488947
C	0.655365	-1.494563	-0.365897
C	-1.406741	4.640685	-0.655552
C	1.255234	-3.986978	-0.781654
H	0.810840	6.510690	-0.698294
C	-0.740622	-1.483699	-0.320559
H	2.212465	1.358543	0.148806
N	-1.421997	-0.260728	-0.229910
N	-2.345347	2.373994	-0.262655
C	-2.447220	3.706719	-0.593910
C	-1.671491	-2.564054	-0.280408
H	1.129905	-0.525554	-0.263630
C	-2.710172	-0.544826	-0.121511
H	2.649056	-5.671243	-0.957166
H	-1.465528	1.875258	-0.118546
C	-2.934022	-1.990065	-0.141903
C	-3.803032	0.387398	-0.003044
C	-3.582525	1.783074	-0.253729
H	-1.713497	5.653151	-0.895920
H	4.741620	-1.085234	0.118016
H	0.295226	-4.424333	-1.000807
C	-3.823608	3.965694	-0.834582
H	-1.449164	-3.616969	-0.306588
C	-4.518589	2.795380	-0.630735
H	-4.225098	4.920805	-1.137434
H	7.674444	-4.156355	0.036152
H	-5.573322	2.644648	-0.783050
C	-5.101695	-0.140656	0.322399
C	-6.124600	0.725798	0.852310
C	-5.318230	-1.548453	0.233091
C	-7.457694	0.514123	1.090487
H	-5.772459	1.707988	1.139207
C	-6.508710	-2.322255	0.342188
C	-4.232030	-2.487235	-0.022723
C	-8.268104	-0.641445	0.896152
H	-7.984933	1.370647	1.502162

C	-7.840226	-1.901442	0.575338
C	-6.135643	-3.702320	0.134308
C	-4.774798	-3.802086	-0.066371
H	-9.330189	-0.510895	1.075915
H	-8.596095	-2.680617	0.522284
H	-6.839261	-4.524242	0.146918
H	-4.214731	-4.710347	-0.232828

Hx-2,3-PH-s1

C	-7.598182	-2.481961	0.320267
H	-8.661254	-2.402762	0.490070
C	-6.879452	-3.609479	0.026062
H	-8.035353	0.188661	0.784535
C	-6.991687	-0.039638	0.600843
C	-6.416703	2.438901	0.777954
C	-6.685630	-1.374819	0.363447
C	-5.256682	3.127129	0.647536
C	-6.078006	1.028875	0.594638
H	-7.402756	2.833172	0.980375
C	-5.502276	-3.231560	-0.115678
C	-4.428860	-4.074268	-0.414003
C	-4.213478	2.131490	0.395624
H	-4.676050	-5.119817	-0.559755
H	-5.122441	4.192041	0.742568
C	-2.498055	4.843806	-0.100588
N	-4.757310	0.874894	0.384910
C	-2.845402	2.280724	0.191555
C	-2.073445	3.448855	0.025337
C	-1.370365	5.565416	-0.312353
N	-5.434303	-1.880679	0.098303
C	-3.086090	-3.710415	-0.527979
C	-0.269659	4.609552	-0.307650
H	-3.508280	5.216784	-0.065670
N	-2.613964	-2.448465	-0.357215
N	-0.731124	3.343780	-0.103642
C	-1.995401	-4.635937	-0.826998
C	-1.266632	-2.524642	-0.500144
C	-0.468977	-1.374549	-0.358130
C	1.068150	4.931739	-0.495859
C	-0.860088	-3.898786	-0.809509
H	-1.282694	6.631817	-0.466041
C	0.920345	-1.273617	-0.281332
H	-2.288080	1.353161	0.128505
N	1.492576	0.009807	-0.228313
N	2.183231	2.725002	-0.232825
C	2.181188	4.078028	-0.475781
C	1.934530	-2.272777	-0.191581
H	-1.009421	-0.438690	-0.276108
C	2.792745	-0.176730	-0.115287
H	-2.100523	-5.692095	-1.032049

H	1.351450	2.143558	-0.113216
C	3.144740	-1.600228	-0.075200
C	3.802904	0.860411	-0.035983
C	3.465564	2.240324	-0.250820
H	1.299593	5.976454	-0.675500
H	-4.580698	-1.321006	0.063496
H	0.139320	-4.239911	-1.023011
C	3.531971	4.462059	-0.684552
H	1.777238	-3.336296	-0.147990
C	4.318777	3.337759	-0.551878
H	3.856534	5.464306	-0.919558
H	-7.249541	-4.617231	-0.086301
H	5.381563	3.279969	-0.703938
C	4.488400	-2.033750	0.088338
C	4.792898	-3.435257	0.077462
C	5.448161	-1.006596	0.272730
C	5.981310	-4.090268	0.259602
H	3.937892	-4.077839	-0.106163
C	6.843669	-1.100536	0.544072
C	5.104152	0.412502	0.240415
C	7.283884	-3.569224	0.528635
H	5.928460	-5.173270	0.196698
C	7.654879	-2.257009	0.657794
C	7.335815	0.243182	0.719061
C	6.315015	1.140524	0.547582
H	8.068080	-4.310152	0.646374
H	8.703966	-2.068312	0.871242
H	8.359040	0.486009	0.973245
H	6.396055	2.205694	0.683776

Pr-1,2-HP-t1

N	3.802676	-0.922886	0.128099
N	0.855903	-1.765957	-0.042072
N	0.059620	0.982955	-0.193413
N	2.941842	1.826518	0.013112
C	5.032436	-0.330618	0.265133
C	5.989375	-1.367747	0.313745
C	5.306528	-2.576441	0.183631
C	3.933867	-2.283315	0.066378
C	2.867638	-3.209270	-0.138135
C	1.522638	-2.993745	-0.223916
C	0.554567	-4.031756	-0.524545
C	-0.660981	-3.438547	-0.521212
C	-0.433458	-2.026461	-0.188038
C	-1.479341	-0.996250	-0.069094
C	-1.165948	0.397369	-0.140169
C	-2.151278	1.424512	-0.163613
C	-1.438733	2.660703	-0.244652
C	-0.078078	2.363328	-0.242243
C	0.993065	3.291330	-0.227267

C	2.357497	3.057203	-0.097935
C	3.363432	4.113224	-0.029426
C	4.557008	3.495441	0.134457
C	4.277714	2.063294	0.155929
C	5.246367	1.067620	0.290311
H	7.053623	-1.223619	0.419089
H	5.729793	-3.569090	0.168933
H	3.192025	-4.237904	-0.260135
H	0.789416	-5.065818	-0.732389
H	-1.604901	-3.895566	-0.761111
H	-1.846025	3.658746	-0.268663
H	0.689117	4.330756	-0.293166
H	3.163111	5.173164	-0.094185
H	5.534980	3.944941	0.230286
H	6.276503	1.386830	0.400882
H	2.936878	-0.401034	0.065349
H	0.931893	0.475736	-0.137698
C	-3.528099	1.117098	-0.074354
C	-4.506585	2.209291	-0.128887
C	-3.846972	-0.228581	0.081621
C	-5.860262	2.167064	-0.024280
H	-4.076289	3.193398	-0.278995
C	-5.139489	-0.871296	0.271607
C	-2.838974	-1.270368	0.096325
C	-6.744880	1.050673	0.176510
H	-6.362515	3.127972	-0.101428
C	-6.407960	-0.286675	0.307596
C	-4.881108	-2.286641	0.438127
C	-3.548691	-2.537127	0.339628
H	-7.800343	1.294518	0.233905
H	-7.236575	-0.975038	0.459402
H	-5.650984	-3.022418	0.630603
H	-3.087756	-3.499848	0.479850

Pr-1,2-PH-t1

N	3.585208	-1.236454	0.166090
N	0.562977	-1.649658	-0.091438
N	0.187398	1.169565	-0.279061
N	3.148444	1.604762	0.059557
C	4.878864	-0.831468	0.384444
C	5.676668	-2.005973	0.421232
C	4.841330	-3.090055	0.189300
C	3.525662	-2.597384	0.027279
C	2.359230	-3.341134	-0.296320
C	1.060192	-2.923865	-0.405204
C	-0.026583	-3.776307	-0.856476
C	-1.148062	-3.023593	-0.808026
C	-0.747068	-1.706315	-0.288390
C	-1.650408	-0.555174	-0.087794
C	-1.116744	0.759514	-0.199488

C	-1.922441	1.924947	-0.229203
C	-1.029634	3.057060	-0.328289
C	0.251698	2.554428	-0.331882
C	1.460212	3.342449	-0.294828
C	2.748221	2.929671	-0.097287
C	3.901626	3.816793	0.024249
C	4.970961	3.026953	0.267306
C	4.474136	1.648734	0.277790
C	5.292234	0.508577	0.463438
H	6.743897	-2.021388	0.580419
H	5.119977	-4.131305	0.133651
H	2.541805	-4.390187	-0.506423
H	0.075117	-4.800503	-1.185801
H	-2.140353	-3.309020	-1.116258
H	-1.297399	4.101628	-0.358598
H	1.297469	4.410587	-0.392759
H	3.871583	4.893779	-0.058706
H	5.998597	3.323249	0.422461
H	6.348800	0.676409	0.636090
H	2.805712	-0.595042	0.090527
H	0.978855	0.548896	-0.191448
C	-3.296629	1.785969	-0.119804
C	-3.851901	0.491868	0.081307
C	-4.379913	2.777703	-0.139922
C	-3.044539	-0.670097	0.131096
C	-5.292959	0.681553	0.180768
H	-4.247355	3.840885	-0.278449
C	-5.548931	2.111493	0.029839
C	-3.624076	-1.971072	0.544122
C	-6.305368	-0.279486	0.316673
H	-6.539248	2.547114	0.050407
C	-4.908927	-2.357931	0.706266
H	-2.891733	-2.720792	0.813880
C	-6.151717	-1.634139	0.514490
H	-7.325598	0.094486	0.270332
H	-5.042629	-3.380656	1.050062
H	-7.056483	-2.227948	0.594475

SP-1,2-HP-t1

C	-2.098345	3.323530	-0.654551
C	-0.741838	3.181337	-0.389468
C	-2.750341	2.121553	-0.242674
C	-0.546318	1.895425	0.202299
N	-1.772922	1.335603	0.338627
C	-3.988068	1.535224	-0.578051
H	-4.733771	2.134482	-1.085463
C	-4.186722	0.142455	-0.457854
C	-5.070785	-0.792179	-1.097331
N	-3.206612	-0.604834	0.136482
C	-4.531819	-2.055871	-0.937790

C	-3.305140	-1.922179	-0.197780
C	-2.178527	-2.775759	-0.031454
H	-2.252678	-3.811634	-0.335339
C	-0.913759	-2.220041	0.286511
C	0.440335	-2.619651	0.081484
N	-0.888060	-0.881074	0.611607
C	1.251407	-1.442602	0.188244
C	0.344437	-0.380035	0.465521
C	0.614427	1.015372	0.377317
B	-2.069885	-0.029577	0.969210
O	-2.283498	-0.016449	2.387048
H	-3.033227	0.519399	2.658096
H	0.759214	-3.613494	-0.191362
H	0.035195	3.880624	-0.652327
H	-2.572000	4.155360	-1.154161
H	-5.952806	-0.534339	-1.664194
H	-4.913335	-2.976031	-1.354096
C	2.623106	-1.120149	-0.005032
C	3.580617	-2.195255	-0.247646
C	2.954066	0.247325	0.037514
C	4.926144	-2.142634	-0.431489
H	3.141485	-3.187724	-0.268032
C	4.234305	0.904807	-0.133229
C	1.970691	1.304563	0.196897
C	5.816310	-1.010464	-0.461634
H	5.414895	-3.101586	-0.580653
C	5.496107	0.326539	-0.338062
C	3.995615	2.337543	-0.069096
C	2.668632	2.583318	0.111407
H	6.864069	-1.246544	-0.615314
H	6.325033	1.026466	-0.415807
H	4.776920	3.081506	-0.152475
H	2.204348	3.552093	0.217363

SP-1,2-PH-t1

C	-1.424449	3.373425	-0.689760
C	-0.119924	2.982925	-0.444621
C	-2.285088	2.320477	-0.244180
C	-0.148690	1.687521	0.177810
N	-1.468828	1.379331	0.345504
C	-3.624223	1.994470	-0.545998
H	-4.251521	2.727282	-1.036399
C	-4.068707	0.662291	-0.424805
C	-5.147161	-0.089275	-1.031382
N	-3.247580	-0.251969	0.159268
C	-4.871305	-1.425188	-0.869618
C	-3.610388	-1.540155	-0.166643
C	-2.685422	-2.578779	-0.035612
H	-2.959599	-3.586026	-0.319351
C	-1.309691	-2.265836	0.247568

C	-0.088326	-2.910958	-0.015461
N	-1.019109	-0.959906	0.591962
C	0.945010	-1.902774	0.087139
C	0.282170	-0.687315	0.413405
C	0.830932	0.621858	0.347696
B	-2.013135	0.096562	0.979683
O	-2.195378	0.134321	2.401643
H	-2.787547	0.831725	2.694013
H	0.035453	-3.937862	-0.322657
H	0.763622	3.517893	-0.751284
H	-1.742463	4.266563	-1.206405
H	-5.974178	0.338225	-1.578370
H	-5.439141	-2.253986	-1.265340
C	2.320260	-1.806342	-0.120830
C	2.959947	-0.509803	-0.034515
C	3.330690	-2.804395	-0.425547
C	2.251152	0.694292	0.188144
C	4.366582	-0.743240	-0.287422
H	3.142703	-3.861456	-0.544669
C	4.533124	-2.170031	-0.519025
C	2.910708	1.993812	0.304231
C	5.421303	0.182406	-0.359974
H	5.486345	-2.634103	-0.735685
C	4.216138	2.343707	0.158143
H	2.252395	2.800724	0.602038
C	5.368158	1.545747	-0.174112
H	6.398194	-0.236106	-0.590684
H	4.434162	3.394779	0.327415
H	6.302092	2.089737	-0.269110

NCP-1,2-HP-t1

H	-7.109275	-1.149418	-0.458451
H	-5.850583	-3.537407	-0.333204
H	-3.269655	-4.268250	0.305642
H	-0.711866	-4.878736	0.911500
H	1.950524	3.671859	0.107913
H	-0.648788	4.365962	0.263066
H	-3.105465	5.169613	0.198262
H	-6.248407	1.445961	-0.240322
H	-3.010947	-0.435510	0.086840
H	-0.911574	0.601231	0.255241
C	-5.071490	-0.317119	-0.209213
C	-6.051425	-1.324450	-0.337044
C	-5.400294	-2.558689	-0.271026
C	-4.023821	-2.314637	-0.119106
C	-2.954279	-3.258418	0.058921
C	-1.619707	-2.993550	0.018755
C	-0.566580	-3.868084	0.545043
C	0.391664	-1.959665	0.073501
C	1.484789	-0.979759	0.043973

C	1.204531	0.418802	0.079575
C	2.208243	1.428599	0.051430
C	1.521563	2.682491	0.121921
C	0.154418	2.411748	0.184238
C	-0.929252	3.318965	0.216733
C	-2.299729	3.058743	0.160090
C	-3.308116	4.109893	0.139786
C	-4.231732	2.062558	-0.022172
C	-5.228293	1.087283	-0.161338
N	-3.860536	-0.952127	-0.095191
N	-0.009768	1.036943	0.153641
N	-2.889783	1.822781	0.070800
N	0.581842	-3.271617	0.609620
C	-0.903949	-1.773891	-0.316991
H	-1.294902	-0.951611	-0.892719
C	-4.508016	3.492240	0.023088
H	-5.488886	3.941799	-0.032657
C	3.581423	1.085060	-0.029141
C	4.587491	2.158941	-0.074534
C	3.870418	-0.271613	-0.057389
C	5.940447	2.069857	-0.143028
H	4.180482	3.163978	-0.049241
C	5.151628	-0.969292	-0.136281
C	2.838308	-1.292680	-0.008919
C	6.802218	0.917755	-0.194024
H	6.466261	3.021359	-0.163484
C	6.431831	-0.420510	-0.191000
C	4.850617	-2.388949	-0.133451
C	3.508548	-2.595242	-0.056207
H	7.864770	1.129441	-0.243078
H	7.247434	-1.139313	-0.238551
H	5.607705	-3.161566	-0.177230
H	2.992157	-3.539573	-0.008753

NCP-1,2-PH-t1

H	-6.816545	-1.928880	-0.719370
H	-5.245582	-4.093409	-0.376017
H	-2.655636	-4.395133	0.494863
H	-0.148321	-4.566236	1.424186
H	1.393542	4.099562	0.242089
H	-1.236155	4.414511	0.424991
H	-3.775872	4.907739	0.187749
H	-6.349373	0.778659	-0.562011
H	-2.902731	-0.589960	0.011444
H	-0.947060	0.615036	0.406862
H	4.329070	3.800729	-0.030301
H	6.596864	2.466297	-0.370655
H	2.950856	-2.876305	0.049584
H	7.336962	0.009773	-0.610668
H	5.071824	-3.559659	-0.376708

H	7.050639	-2.328737	-0.682717
C	-4.934609	-0.788970	-0.406722
C	-5.753682	-1.943168	-0.533392
C	-4.944356	-3.057264	-0.353270
C	-3.620897	-2.608570	-0.140143
C	-2.459549	-3.373470	0.181511
C	-1.166930	-2.932324	0.214125
C	-0.078165	-3.603393	0.929240
C	0.715090	-1.674696	0.260627
C	1.694525	-0.569826	0.152167
C	1.177361	0.758345	0.218484
C	1.987735	1.912909	0.175252
C	1.113341	3.057712	0.264415
C	-0.175506	2.571869	0.345980
C	-1.389507	3.343604	0.339344
C	-2.686324	2.930037	0.186376
C	-3.825851	3.832235	0.096431
C	-4.441754	1.681439	-0.176423
C	-5.299209	0.564243	-0.402487
C	3.365335	1.750187	0.031500
C	3.902387	0.442333	-0.066589
C	4.449884	2.728043	-0.079046
C	3.086955	-0.718919	0.002986
C	5.341258	0.609591	-0.263170
C	5.609077	2.040609	-0.252575
C	3.663570	-2.079591	-0.103767
C	6.324901	-0.362592	-0.468334
C	4.935999	-2.481773	-0.337047
C	6.158967	-1.733258	-0.515160
N	-3.651870	-1.236652	-0.200112
N	-0.126389	1.190477	0.325090
N	-3.115853	1.607188	0.025575
N	0.987538	-2.870223	0.999288
C	-0.564120	-1.689222	-0.226013
H	-0.997043	-0.983881	-0.917488
C	-4.914385	3.063148	-0.136264
H	-5.938665	3.378740	-0.272932

S-5,6-HP-t1

C	-3.172329	-3.326854	-0.530372
C	-2.612758	-4.510765	-1.039511
C	-1.232248	-4.311931	-1.166046
C	-0.950352	-3.015242	-0.725186
N	-2.133821	-2.429338	-0.371269
H	-2.294339	-1.518016	0.043874
H	-3.168239	-5.403520	-1.282817
H	-0.501540	-5.011958	-1.538242
C	0.338419	-2.376220	-0.551044
C	1.549989	-2.973620	-0.278603
C	2.505172	-1.925084	-0.096741

C	1.814825	-0.696413	-0.280615
N	0.506488	-0.999818	-0.557981
H	1.713932	-4.033631	-0.171838
C	1.653809	1.737924	-0.677512
C	2.206538	2.848088	-1.454355
C	1.174155	3.686804	-1.704608
H	1.189563	4.622522	-2.245167
C	2.424605	0.571208	-0.222762
C	0.001446	3.093479	-1.082688
N	0.340811	1.866565	-0.503400
C	-4.179176	2.520263	0.688812
C	-2.427044	3.505527	-0.345128
C	-3.379246	4.504117	-0.055300
H	-5.337411	4.382116	0.972985
H	-3.261666	5.547989	-0.302828
C	-5.236118	0.191909	1.017558
C	-6.488916	-0.483947	1.346523
C	-6.354646	-1.762721	0.927343
C	-5.007330	-1.876487	0.387793
N	-4.342133	-0.676176	0.467047
H	-7.349412	-0.014349	1.801257
H	-7.077609	-2.564431	0.976102
C	-1.183830	3.772986	-0.978508
C	-4.438928	3.908678	0.608510
C	-5.121063	1.578265	1.156203
N	-2.939433	2.312352	0.121981
C	-4.496567	-3.061226	-0.131732
H	-5.184115	-3.896559	-0.205819
H	-5.987698	2.052072	1.605535
H	-1.161794	4.767689	-1.414160
H	-0.181179	-0.274814	-0.716331
H	-2.488161	1.413738	0.045385
H	3.231993	2.945203	-1.774082
C	3.794057	0.621089	0.180546
C	4.402076	1.909333	0.475400
C	4.489030	-0.601485	0.370300
C	5.683460	2.233443	0.827591
H	3.722081	2.750578	0.440487
C	5.884998	-0.869420	0.724081
C	3.868269	-1.863268	0.213661
C	6.837775	1.418583	1.018357
H	5.852972	3.293771	0.996601
C	6.915125	0.035798	0.980469
C	6.046133	-2.304521	0.750672
C	4.853346	-2.903823	0.455711
H	7.754467	1.950809	1.251074
H	7.888746	-0.400941	1.189965
H	6.979029	-2.803741	0.974770
H	4.660922	-3.966415	0.405687

S-5,6-PH-t1

C	-2.734042	-3.534071	0.556188
C	-1.982193	-4.643970	0.991560
C	-0.643910	-4.257631	1.049950
C	-0.568418	-2.915095	0.646597
N	-1.841575	-2.493525	0.376580
H	-2.155395	-1.604920	0.001163
H	-2.394147	-5.611585	1.234080
H	0.196689	-4.857151	1.360486
C	0.612338	-2.109637	0.468585
C	1.906493	-2.539722	0.246341
C	2.726089	-1.380502	0.088103
C	1.869411	-0.261520	0.235957
N	0.602601	-0.723717	0.455830
H	2.203618	-3.572213	0.163763
C	1.400827	2.181527	0.541921
C	1.821594	3.458498	1.109997
C	0.692080	4.185357	1.278329
H	0.595747	5.187322	1.671718
C	2.308237	1.084929	0.208728
C	-0.407365	3.360325	0.806285
N	0.077225	2.112116	0.400834
C	-4.593130	2.125138	-0.656434
C	-2.910270	3.391878	0.164145
C	-3.993713	4.242778	-0.127719
H	-5.990227	3.803988	-0.984744
H	-3.988386	5.310671	0.028048
C	-5.359227	-0.333852	-0.830072
C	-6.528530	-1.177062	-1.065496
C	-6.190583	-2.421866	-0.660292
C	-4.804864	-2.344765	-0.218644
N	-4.317053	-1.071684	-0.339293
H	-7.474858	-0.833010	-1.457770
H	-6.797578	-3.315926	-0.659192
C	-1.674466	3.868378	0.680881
C	-5.017756	3.471612	-0.656082
C	-5.438388	1.044966	-1.003669
N	-3.302217	2.110683	-0.170786
C	-4.099993	-3.454537	0.250191
H	-4.658958	-4.377707	0.354471
H	-6.390089	1.385938	-1.398203
H	-1.755905	4.906243	0.990829
H	-0.169321	-0.083079	0.595754
H	-2.743800	1.278877	-0.056504
H	2.829235	3.734789	1.372964
C	3.670701	1.247019	-0.104071
C	4.546641	0.126142	-0.289332
C	4.460921	2.449235	-0.343964
C	5.871414	0.657576	-0.606490
C	4.113004	-1.200227	-0.177169

C	5.748708	2.090964	-0.633344
H	4.080442	3.458462	-0.337387
C	7.051592	-0.043801	-0.850812
C	4.960781	-2.365226	-0.322329
H	6.561039	2.766499	-0.865251
C	7.252604	-1.417523	-0.852428
H	7.925001	0.567532	-1.066350
C	6.296793	-2.444578	-0.608298
H	4.456074	-3.315143	-0.183714
H	8.260428	-1.757542	-1.066747
H	6.697246	-3.453595	-0.662234

Hx-2,3-HP-t1

C	7.721820	-1.970170	0.673987
H	8.752028	-1.812000	0.953313
C	7.123396	-3.170842	0.276996
H	7.887422	0.731736	1.213623
C	6.883939	0.419817	0.946187
C	6.072845	2.822182	1.129692
C	6.729314	-0.974201	0.644227
C	4.868983	3.397617	0.919636
C	5.896069	1.385822	0.898949
H	6.997393	3.305194	1.413612
C	5.771758	-2.902842	0.006278
C	4.785395	-3.832687	-0.437265
C	3.937160	2.311307	0.577809
H	5.147518	-4.848724	-0.561686
H	4.622709	4.442477	1.020319
C	2.073547	4.887265	-0.189563
N	4.591902	1.112521	0.588394
C	2.578829	2.344498	0.280027
C	1.725465	3.475329	0.016064
C	0.918807	5.523917	-0.501758
N	5.563004	-1.564136	0.240717
C	3.463724	-3.610003	-0.712992
C	-0.127422	4.513691	-0.485781
H	3.059819	5.320023	-0.140047
N	2.850303	-2.358523	-0.600388
N	0.425089	3.270029	-0.155941
C	2.489025	-4.597911	-1.137254
C	1.574208	-2.549687	-0.897402
C	0.658514	-1.423850	-0.831612
C	-1.444247	4.693093	-0.788960
C	1.304835	-3.942463	-1.252762
H	0.781716	6.570189	-0.735895
C	-0.704173	-1.447404	-0.653594
H	2.093287	1.379645	0.195253
N	-1.400686	-0.238463	-0.593726
N	-2.370384	2.410706	-0.381500
C	-2.497766	3.717062	-0.787024

C	-1.608531	-2.567623	-0.434335
H	1.121116	-0.444829	-0.881106
C	-2.663877	-0.565390	-0.329088
H	2.690483	-5.642705	-1.326863
H	-1.478824	1.960311	-0.182210
C	-2.840996	-2.022573	-0.217408
C	-3.747934	0.346453	-0.147341
C	-3.575418	1.763826	-0.482033
H	-1.754806	5.692481	-1.077722
H	4.675874	-1.073851	0.132902
H	0.360249	-4.348074	-1.579019
C	-3.826575	3.908343	-1.170104
H	-1.337324	-3.609849	-0.403121
C	-4.499202	2.687594	-0.990164
H	-4.244180	4.833603	-1.536812
H	7.594081	-4.137874	0.185385
H	-5.529122	2.481438	-1.228845
C	-5.010660	-0.191643	0.341699
C	-5.992446	0.708201	0.823219
C	-5.168428	-1.612528	0.377844
C	-7.292695	0.483451	1.269650
H	-5.681351	1.742086	0.870855
C	-6.366144	-2.423902	0.706922
C	-4.144403	-2.514993	0.086283
C	-8.038470	-0.691786	1.366918
H	-7.815757	1.381580	1.586930
C	-7.619449	-2.001356	1.110249
C	-5.987526	-3.793074	0.560380
C	-4.656670	-3.849689	0.205933
H	-9.060968	-0.576663	1.712549
H	-8.354144	-2.784601	1.278791
H	-6.648276	-4.632026	0.725991
H	-4.081116	-4.751604	0.045866

Hx-2,3-PH-t2

C	-7.499631	-2.440516	0.553259
H	-8.545124	-2.360404	0.808038
C	-6.799785	-3.594737	0.189323
H	-7.892258	0.232925	1.061317
C	-6.861941	0.005970	0.810326
C	-6.270797	2.471820	1.008439
C	-6.588246	-1.367950	0.528760
C	-5.118355	3.155221	0.831050
C	-5.958728	1.060614	0.773666
H	-7.241343	2.866879	1.274120
C	-5.467286	-3.223051	-0.055775
C	-4.396832	-4.078488	-0.462904
C	-4.087885	2.162630	0.501112
H	-4.670223	-5.122376	-0.581085
H	-4.969687	4.216984	0.942215

C	-2.401581	4.913297	-0.070493
N	-4.636470	0.904852	0.486507
C	-2.735713	2.318629	0.234880
C	-1.966401	3.524886	0.052056
C	-1.276714	5.645393	-0.290271
N	-5.368741	-1.870847	0.159726
C	-3.097275	-3.742276	-0.709960
C	-0.171913	4.707459	-0.298647
H	-3.414415	5.279949	-0.029028
N	-2.601461	-2.437028	-0.597508
N	-0.646036	3.416314	-0.085417
C	-2.026466	-4.640237	-1.109781
C	-1.312456	-2.509290	-0.872782
C	-0.505581	-1.300440	-0.820767
C	1.151250	5.001618	-0.512187
C	-0.909240	-3.878400	-1.214389
H	-1.201715	6.712945	-0.442662
C	0.844566	-1.187460	-0.622733
H	-2.167984	1.401648	0.128043
N	1.455263	0.064762	-0.590498
N	2.237820	2.768441	-0.293807
C	2.271419	4.127898	-0.529890
C	1.833670	-2.231513	-0.359410
H	-1.060118	-0.373164	-0.908669
C	2.741739	-0.157644	-0.321921
H	-2.127607	-5.700120	-1.295496
H	1.387292	2.215986	-0.192650
C	3.023598	-1.597869	-0.164726
C	3.760356	0.814730	-0.162793
C	3.494892	2.244806	-0.374306
H	1.394191	6.044169	-0.696453
H	-4.517574	-1.318529	0.060630
H	0.071779	-4.196742	-1.530479
C	3.606478	4.468837	-0.774327
H	1.628370	-3.287566	-0.294901
C	4.370671	3.296289	-0.684670
H	3.964655	5.463802	-0.991730
H	-7.189833	-4.597405	0.103300
H	5.428369	3.209026	-0.861032
C	4.356715	-2.090860	0.164877
C	4.574576	-3.490262	0.269813
C	5.311335	-1.094606	0.357551
C	5.733033	-4.181381	0.584577
H	3.707815	-4.110576	0.071678
C	6.726483	-1.227803	0.769217
C	5.034060	0.310746	0.227252
C	7.015369	-3.712943	0.907744
H	5.629600	-5.263287	0.587658
C	7.450106	-2.391105	0.997370
C	7.230777	0.088582	0.898353

C	6.234225	0.999356	0.584425
H	7.756050	-4.475874	1.123457
H	8.489482	-2.247775	1.283173
H	8.238825	0.333360	1.203840
H	6.343862	2.070974	0.635790

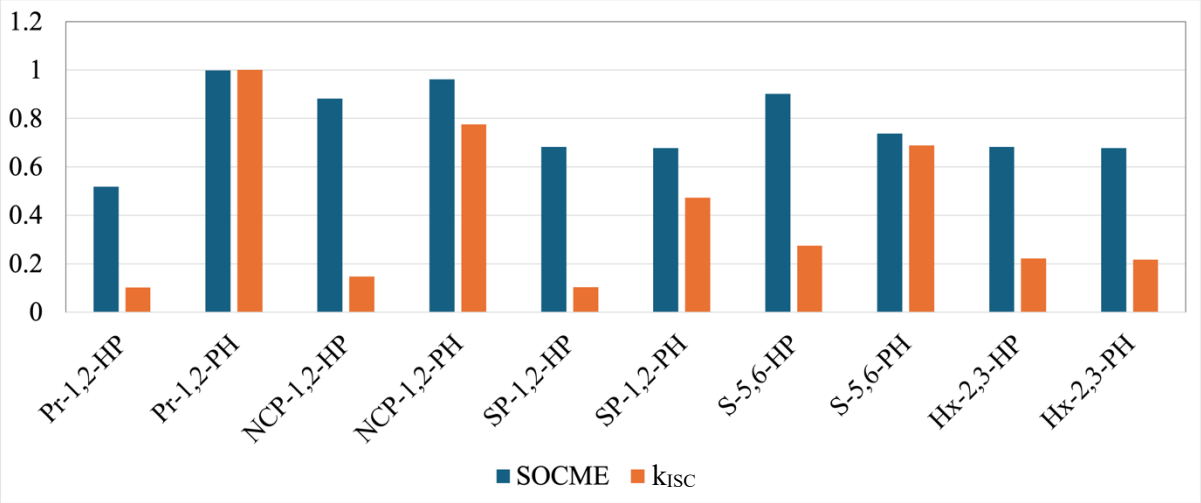
S3: Singlet and triplet states energies(eV) and spin orbit coupling (cm^{-1}) of all the system.

System	S_1	T_1	T_2	$S_1<\hat{H}_{SO}>T_n$
Pr-1,2-HP	1.103	0.54	1.519	0.062
Pr-1,2-PH	1.116	0.547	1.292	0.119
NCP-1,2-HP	1.133	0.649	1.343	0.105
NCP-1,2-PH	1.172	0.664	1.409	0.114
SP-1,2-HP	1.148	0.142	1.585	0.081
SP-1,2-PH	1.145	0.211	1.478	0.081
S-5,6-HP	1.103	0.299	1.363	0.107
S-5,6-PH	1.14	0.321	1.317	0.088
Hx-2,3-HP	0.822	0.519	0.862	0.081
Hx-2,3-PH	0.894	0.528	0.892	0.081

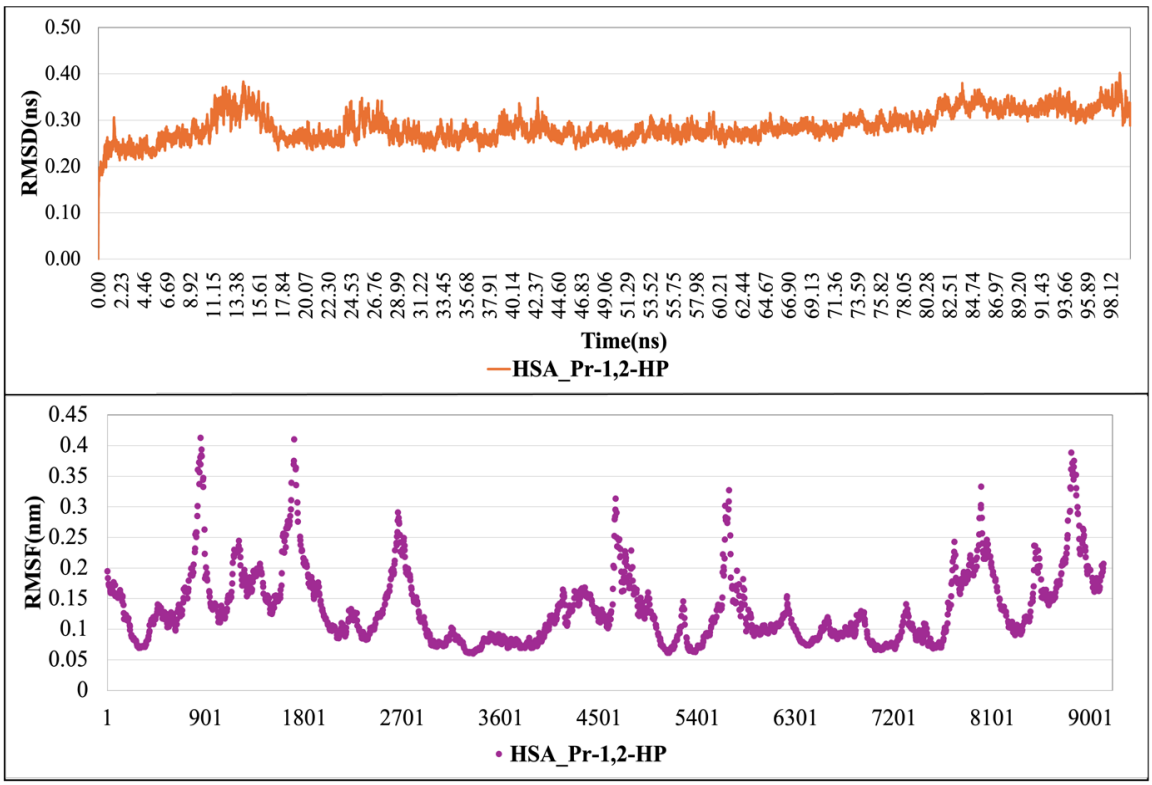
S4: Spin orbit coupling matrix element (cm^{-1}) and k_{ISC} (s^{-1}) of all the system.

System	SOCME	k_{ISC}
Pr-1,2-HP	0.062	5.18E+04
Pr-1,2-PH	0.119	5.04E+05
NCP-1,2-HP	0.105	7.44E+04
NCP-1,2-PH	0.114	3.91E+05
SP-1,2-HP	0.081	5.24E+04
SP-1,2-PH	0.081	2.38E+05
S-5,6-HP	0.107	1.38E+05
S-5,6-PH	0.088	3.47E+05
Hx-2,3-HP	0.081	1.12E+05
Hx-2,3-PH	0.081	1.10E+05

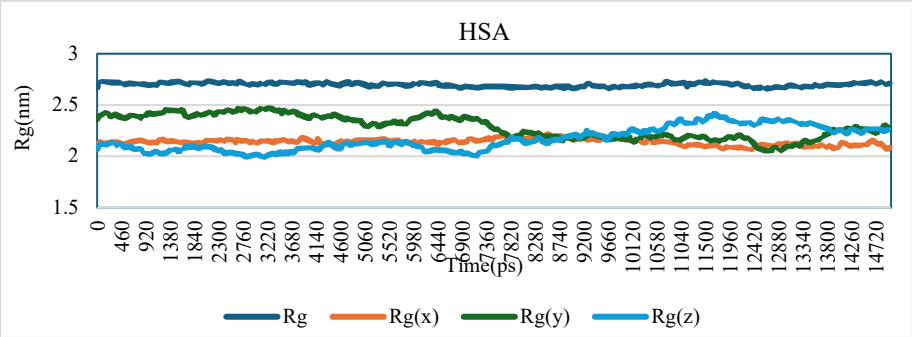
S5: Graph plotted between Spin orbit coupling matrix element (cm^{-1}) and k_{ISC} (s^{-1}) of all the system.

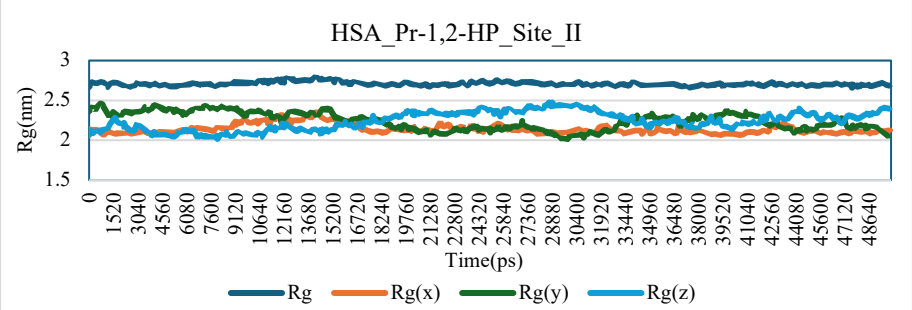


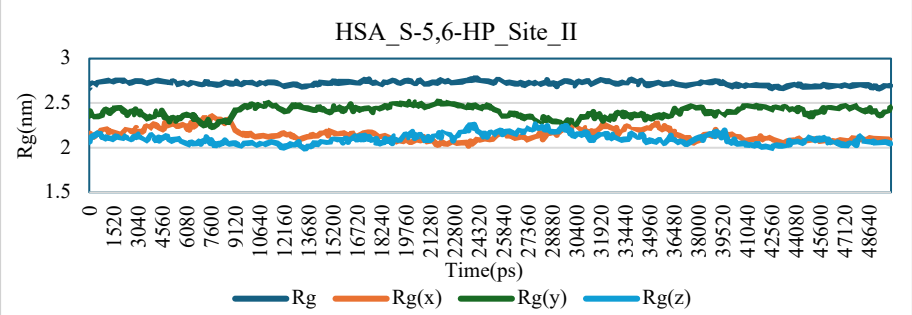
S6: RMSD and RMSF plot for HSA and Pr-1,2-HP system for 100 ns time scale.

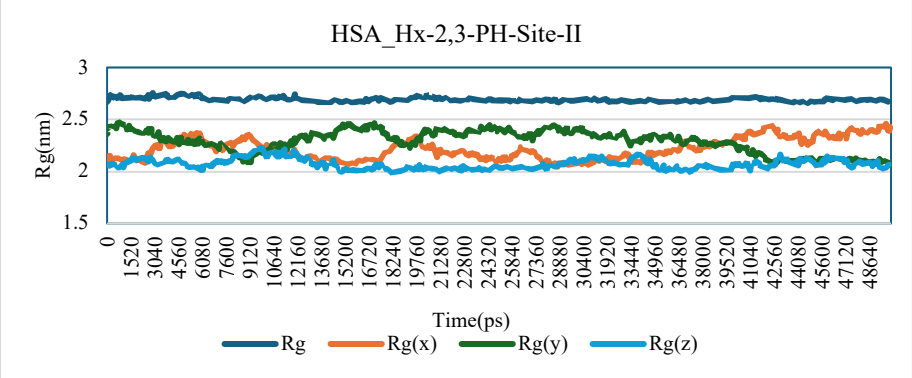


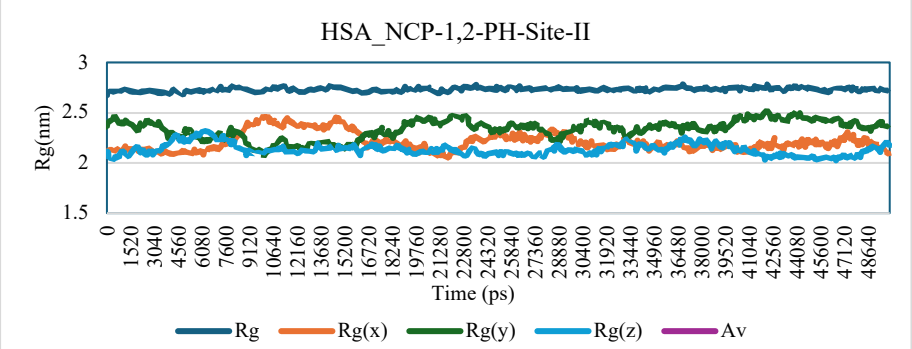
S7: Radius of gyration (R_g) of all Pr-az-HSA protein complexes (in nm).





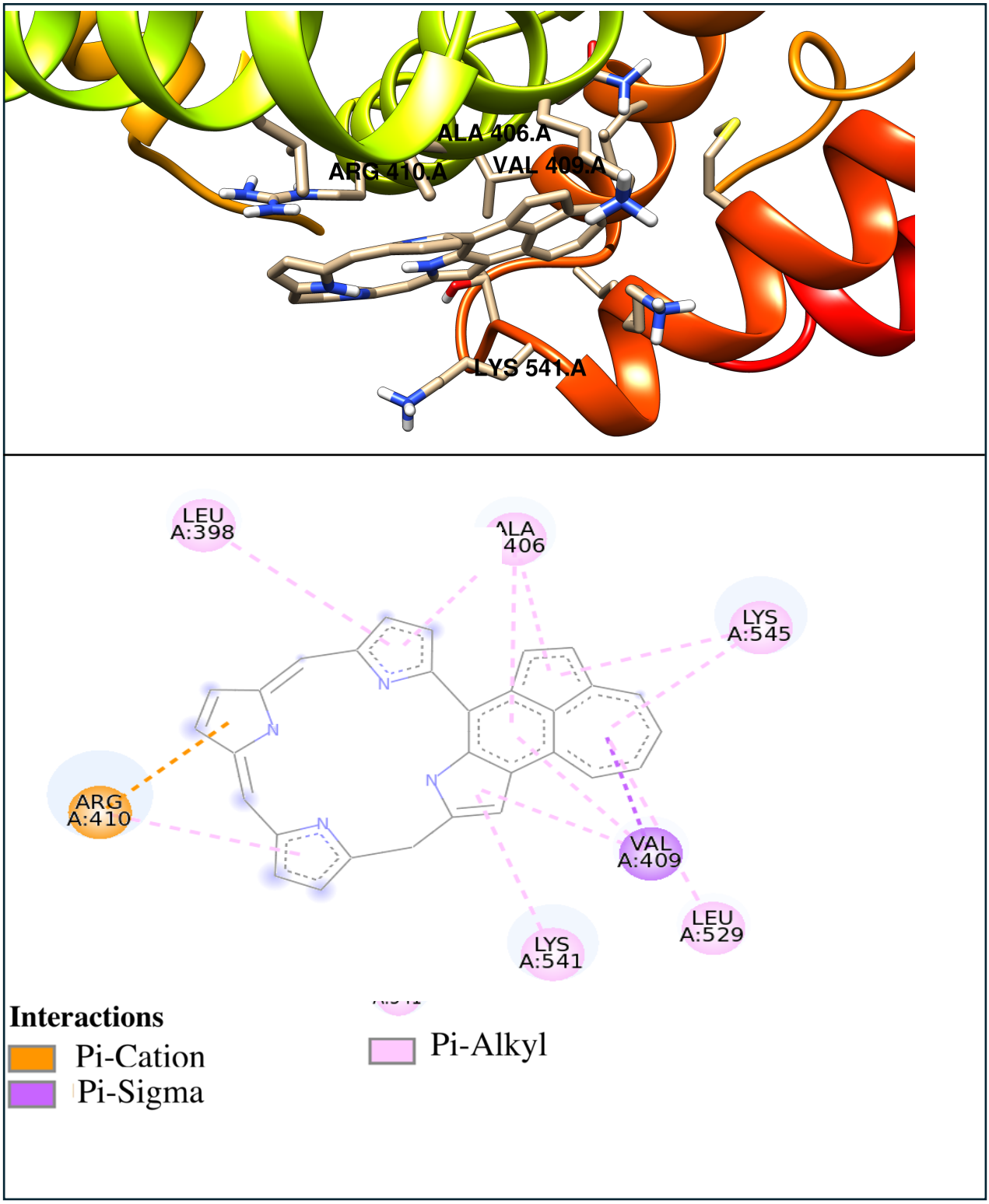




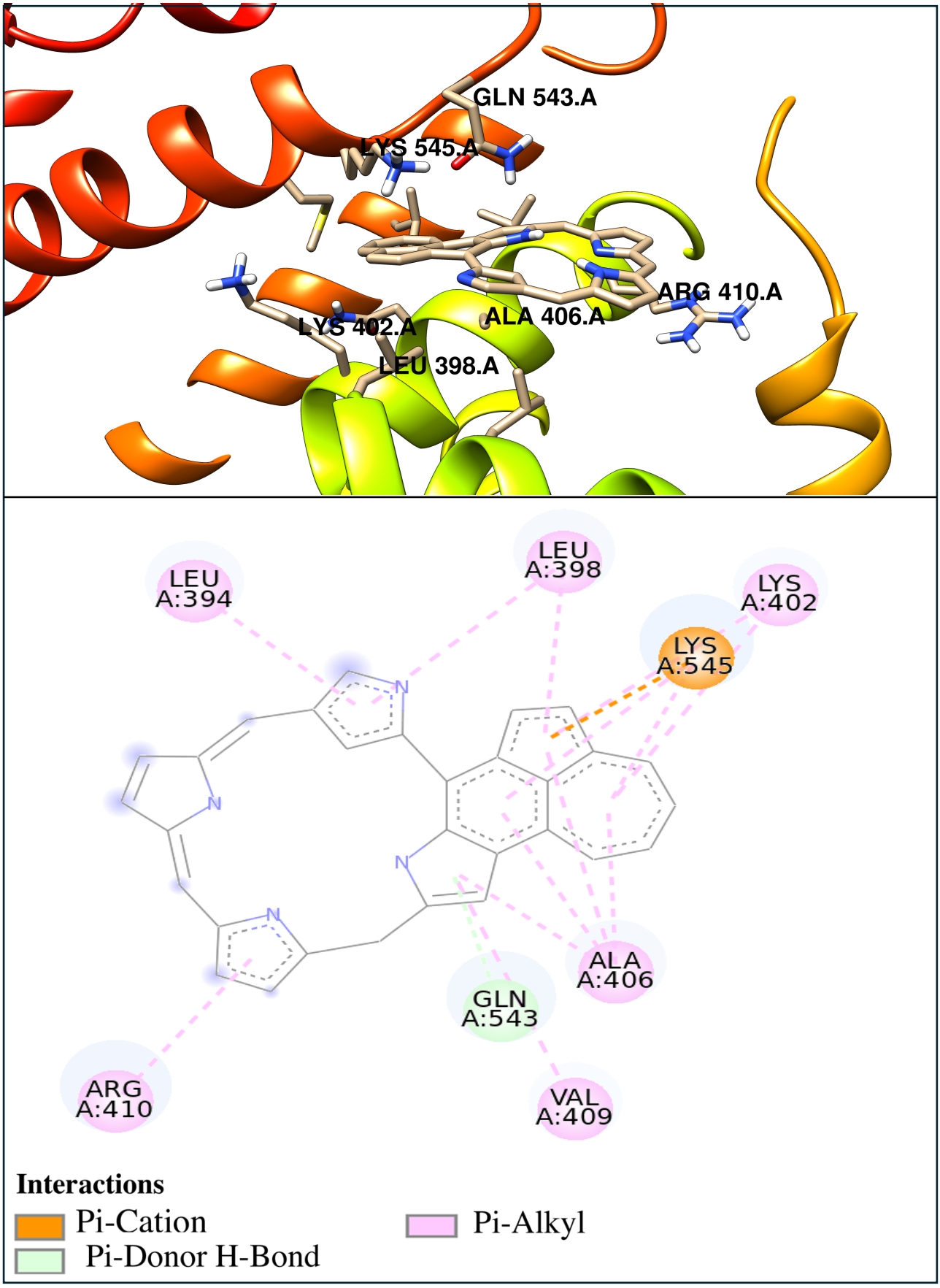


S8: Various non-covalent interactions between the Pr-az systems and the HSA protein observed after MD simulations.

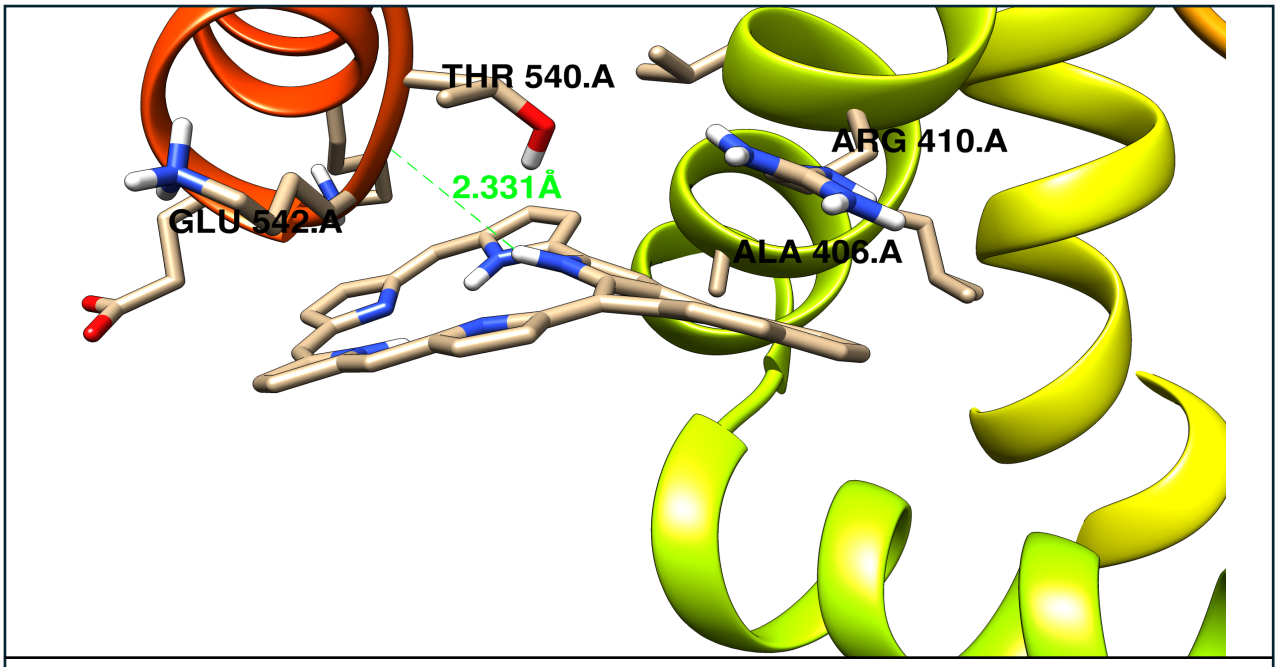
Pr-1,2-HP

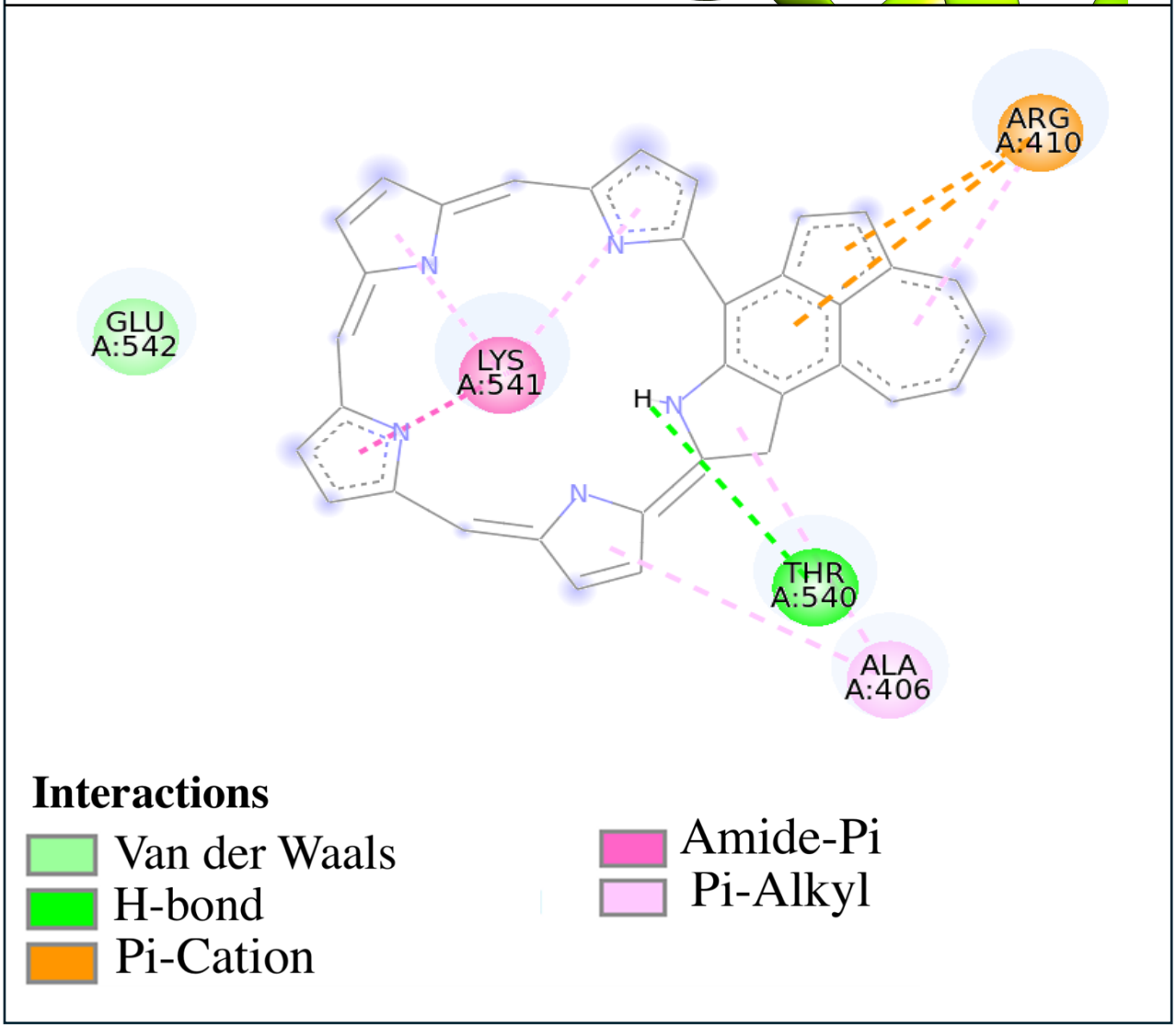


NCP-1,2-HP

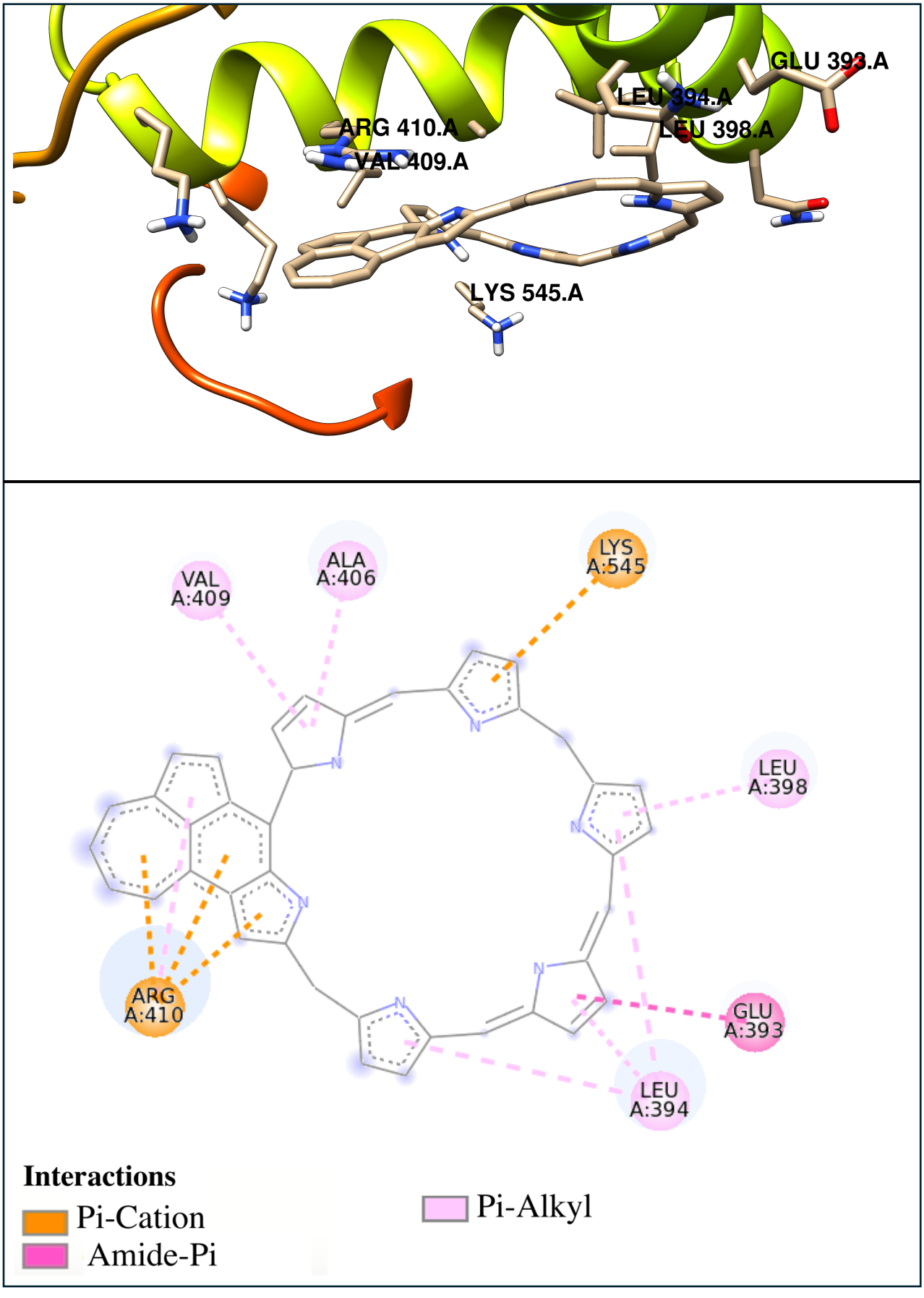

GLN 543.A
LYS 545.A
ARG 410.A
ALA 406.A
LYS 402.A
LEU 398.A
LEU A:394
LEU A:398
LYS A:402
LYS A:545
ALA A:406
GLN A:543
ARG A:410
VAL A:409
Interactions
Pi-Cation
Pi-Alkyl
Pi-Donor H-Bond

S-5,6-PH


THR 540.A
2.331Å
GLU 542.A
ARG 410.A
ALA 406.A


ARG
A:410
GLU
A:542
LYS
A:541
H
N
THR
A:540
ALA
A:406
Interactions
Van der Waals
H-bond
Pi-Cation
Amide-Pi
Pi-Alkyl

Hx-2,3-PH


GLU 393.A
LEU 394.A
LEU 398.A
ARG 410.A
VAL 409.A
LYS 545.A
VAL A:409
ALA A:406
LYS A:545
LEU A:398
ARG A:410
GLU A:393
LEU A:394
Interactions
Pi-Cation
Amide-Pi
Pi-Alkyl

S9: Molecular Docking and MD Simulation interaction results for DNA–Pr–1,2-HP systems.

Molecular Docking:

The crystal structure of calf thymus DNA, (PDB ID: 1BNA), was obtained from the Protein Data Bank. To prepare DNA for docking, water molecules were eliminated and necessary hydrogen atoms and partial charges were introduced. Molecular docking studies were conducted using the Autodock Vina (v4.2.6; MGLTools v.1.5.7) software. Docking results revealed that Pr-1,2-HP preferentially binds within the minor groove of the DNA helix as shown in the Fig 2. The ligand established stable interactions along this groove, suggesting a specific mode of interaction. The binding energy was calculated to be –12.15 kcal/mol, indicating a strong and favorable interaction between ligand and DNA. This negative binding energy reflects a thermodynamically stable complex**,** supporting the potential of Pr-1,2-HP to interact effectively with DNA through minor groove insertion.

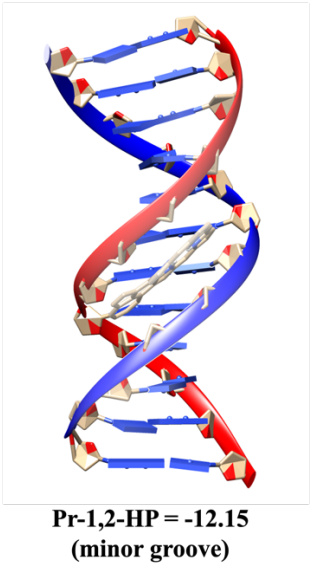


Figure 2: Docking results show the Pr-1,2-HP binding within the minor groove of DNA

Molecular Dynamics Simulation:

The molecular dynamics simulation of the DNA-Pr-1,2-HP complex was carried out for 25 ns using the AMBER99SB-ILDN force field with the TIP3P water model. The best docked pose of Pr-1,2-HP with DNA was used as the initial structure, and Mg^{+2} ions were added to neutralize the system. After energy minimization via the steepest descent algorithm, the system was heated from 50 K to 300 K over 100 ps in the NVT ensemble using a Berendsen thermostat, followed by 100 ps equilibration under the NPT ensemble at 300 K and 1 bar. The production run was conducted for 25 ns with a 2 fs time step, and periodic boundary conditions with a 10 Å cutoff were applied for long-range electrostatics.

A molecular dynamics simulation for 25 ns was performed on the DNA-Pr-1,2-HP complex using the docked structure with the lowest binding free energy as the starting point. RMSD values shown in top panel of Fig. 3 stabilized around 0.33 nm for DNA and 0.27 nm for the DNA-Pr-1,2-HP, indicating that the complex maintained structural stability throughout the simulation. Analysis of the trajectories confirmed that the DNA-Pr-1,2-HP complex remained

firmly bound within the DNA groove, supporting strong and stable interactions between the complex and DNA.

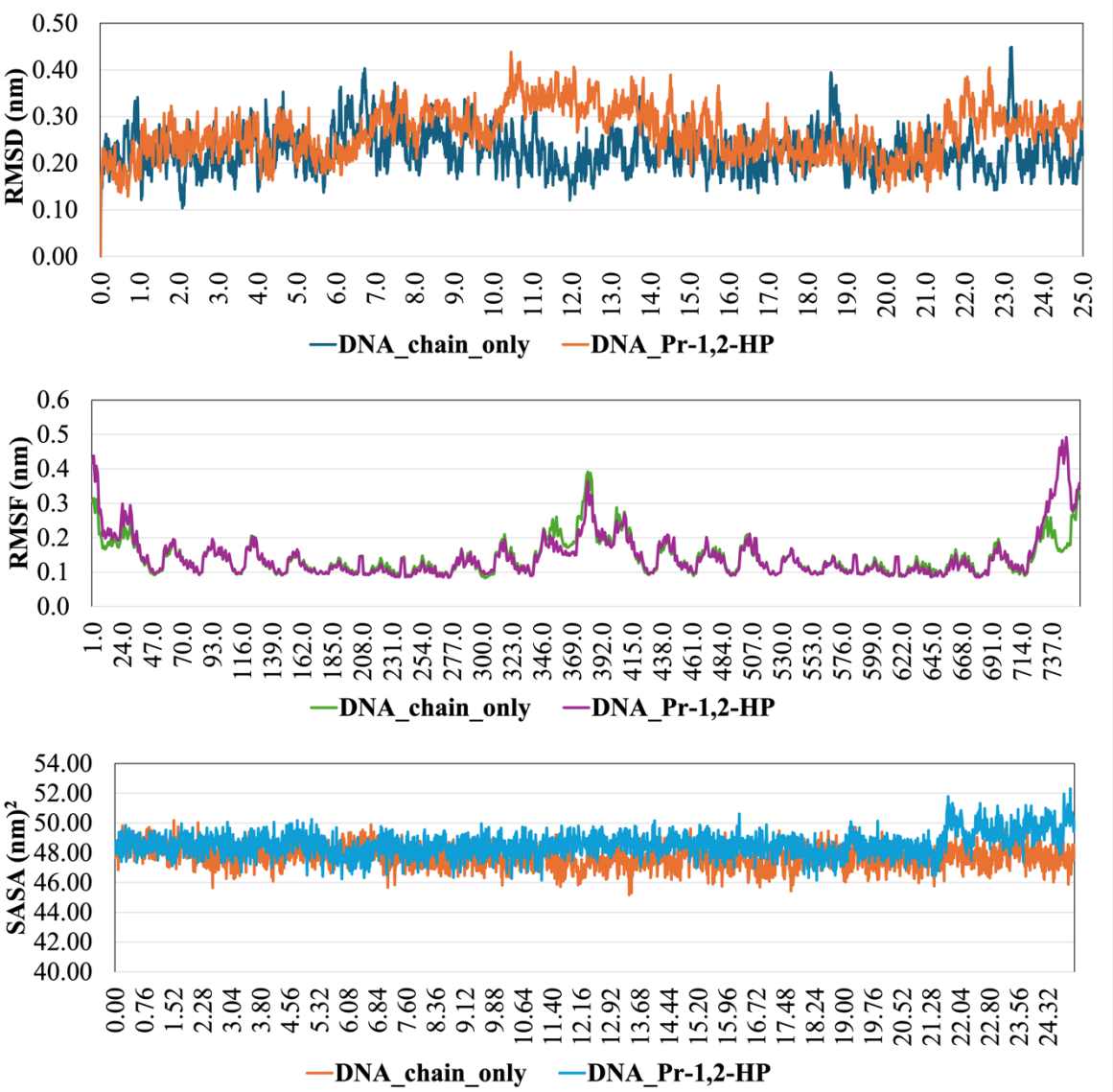


Figure 3: Plot showing the RMSD (top panel), RMSF (middle panel), and SASA (bottom panel) results for free DNA compared to the DNA-Pr-1,2-PH complex, calculated using the AMBER force field.

Further, root mean square fluctuation (RMSF) analysis (middle panel in Fig. 3) showed average values of 0.14 nm for DNA and 0.15 nm for the DNA-Pr-1,2-HP complex, indicating minimal atomic fluctuations and confirming the structural rigidity of complex during the simulation. The solvent-accessible surface area (SASA) of free DNA was approximately 47.74 nm^2, while DNA-Pr-1,2-HP complex showed a slightly higher SASA value of about 48.55 nm^2. This minor increase suggests that binding of the Pr-1,2-HP causes small changes in DNA exposure to the solvent, potentially reflecting slight conformational adjustments. After 21 ns of simulation, a sudden increase in the SASA of the complex was observed, which may indicate conformational changes exposing more surface area.

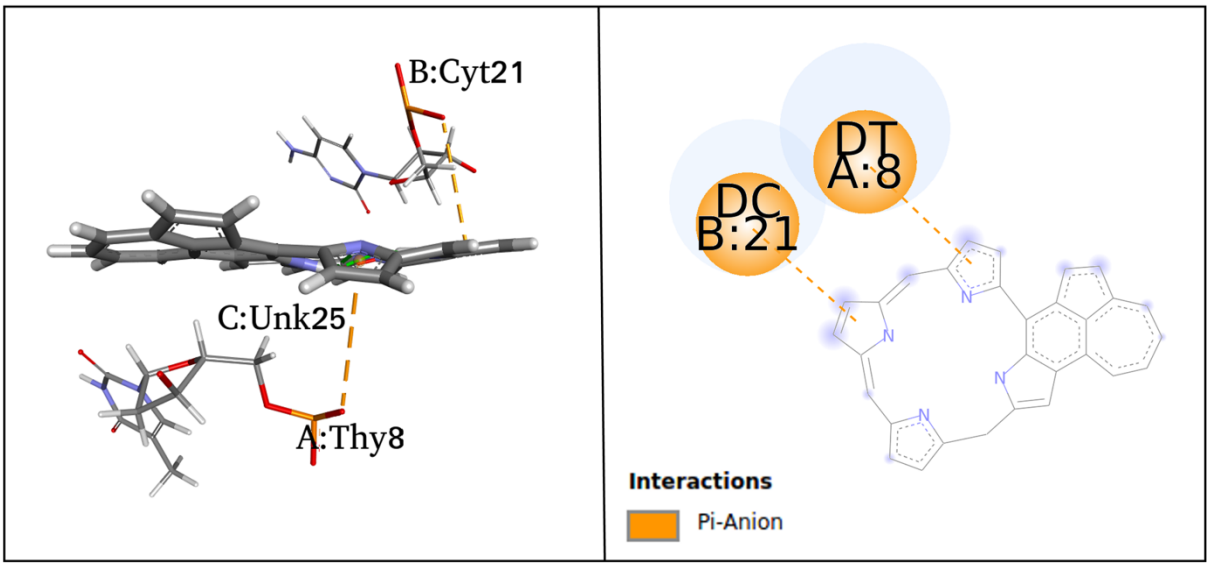


Figure 4: Image showing interaction of the Pr-1,2-HP with DNA near cytosine (Cyt) and thymine (Thy) bases after MD simulation.

Further analysis of the MD results revealed that the PS remains in close proximity to cytosine (CYT) and thymine (THY) part of DNA as shown in Fig. 4, exhibiting a π-interaction with these bases. Due to the lack of time and resources we are unable to repeat the whole study with DNA. However, it is clear from this small simulation with DNA that the proposed photosensitizers can interact with DNA but it does not lead to any DNA damage during the simulation time.