

Supplementary material

Ksv															
Paracetamol	10.85*10 ²	18.85*10 ²	26.73*10 ²												
PS	26.10*10 ⁹	26.96*10 ⁹	28.92*10 ⁹												
Paracetamol in presence of Para PS	20 µg/mL NPS			40 µg/mL NPS			60 µg/mL NPS			80 µg/mL NPS			100 µg/mL NPS		
	81.50*10 ²	90.04*10 ²	92.98*10 ²	71.06*10 ²	80.33*10 ²	83.80*10 ²	93.25*10 ²	96.66*10 ²	97.00*10 ²	99.44*10 ²	103.28*10 ²	107.82*10 ²	68.62*10 ²	77.32*10 ²	91.64*10 ²
Kq															
Paracetamol	10.86*10 ¹¹	18.85*10 ¹¹	26.73*10 ¹¹												
PS	2.610*10 ¹⁹	2.696*10 ¹⁹	2.892*10 ¹⁹												
Paracetamol in presence of para PS	20 µg/mL NPS			40 µg/mL NPS			60 µg/mL NPS			80 µg/mL NPS			100 µg/mL NPS		
	8.150*10 ¹¹	9.004*10 ¹¹	9.298*10 ¹¹	7.106*10 ¹¹	8.033*10 ¹¹	8.380*10 ¹¹	9.325*10 ¹¹	9.666*10 ¹¹	9.700*10 ¹¹	9.944*10 ¹¹	10.328*10 ¹¹	10.782*10 ¹¹	6.862*10 ¹¹	7.732*10 ¹¹	9.164*10 ¹¹
LB Ka															
Paracetamol	4.551921822; 3.132872442; 5.35432237357469*10 ³														
PS	11.24429611; 5.798751749; 10.6179948191302*10 ⁹														
Paracetamol in presence of para PS	20 µg/mL NPS			40 µg/mL NPS			60 µg/mL NPS			80 µg/mL NPS			100 µg/mL NPS		
	5.277723495; 6.195815688; 2.07664142611306*10 ³	12.59097410; 14.39661043; 11.2539055704624*10 ³			020.8809456; 023.5698940; 037.41588817621; 021.7499952; 028.71401618; 031.61717336421; 052.9759303; 051.874205335; 055.8351210212859*10 ³										
DL n															
Paracetamol	1.78819022	1.73021132	1.791749338												
PS	0.56023568	0.57756137	0.445772612												
Paracetamol in presence of para PS	20 µg/mL NPS			40 µg/mL NPS			60 µg/mL NPS			80 µg/mL NPS			100 µg/mL NPS		
	0.80279504	0.76390832	0.501925209	0.65938781	0.61320849	0.61385452	0.50155226	0.47639489	0.36786548	0.48907587	0.439646554	0.406802014	0.28182517	0.292810682	0.29270159
Ka															
Paracetamol	8.365328499; 5.220222329; 24.48595235*10 ⁵														
PS	1.238268999; 5.3440683; 2.007335661*10 ⁴														
Paracetamol in presence of para PS	20 µg/mL NPS			40 µg/mL NPS			60 µg/mL NPS			80 µg/mL NPS			100 µg/mL NPS		
	1.56020261; 1.309456271; 1.670086633*10 ¹	3.946866252; 3.17087411; 4.675833089*10 ¹			1.70533223; 1.4516603; 1.6854661293*10 ¹			1.673119651; 1.166361028; 1.011372172*10 ¹			2.826682303; 3.327905611*1; 1.35427855*10 ⁰				
VH															
	ΔG 298.15			ΔG 303.15			ΔG 310.15								
PS	-40103.1972	-33915.3713	-25252.41501												
para	-30.8993174	-32.6298895	-35.05269049												
20 µg/mL NPS	-13.2496925	-10.9895972	-7.825463819												
40 µg/mL NPS	-9.11091696	-8.71195778	-8.153414916												
60 µg/mL NPS	-7.24489959	-6.36331378	-5.129093638												
80 µg/mL NPS	-6.84588725	-6.43518286	-5.860196719												
paracetamol in presence of para PS	100 µg/mL NPS	-3.02465605	-2.23479215	-1.128982692	paracetamol in presence of	100 µg/mL NPS	-50.1242403	-0.1579728							
	KJ/mol ⁻¹			KJ/mol ⁻¹			KJ/mol ⁻¹								
	ΔH			ΔS											
PS	-409.083257	-1.2375652													
para	-72.214	0.346													
20 µg/mL NPS	-148.019174	-0.4520191													
40 µg/mL NPS	-32.9008532	-0.0797918													
60 µg/mL NPS	-59.8138617	-0.1763172													
80 µg/mL NPS	-31.3361898	-0.0821409													
paracetamol in presence of para PS	100 µg/mL NPS	-50.1242403	-0.1579728												
	KJ/mol ⁻¹			KJ/mol ⁻¹			KJ/mol ⁻¹			KJ/mol ⁻¹					

Table.1 The analysed fluorescence data; ster volmer, double log, vant hoff's, ΔG, ΔH and ΔS

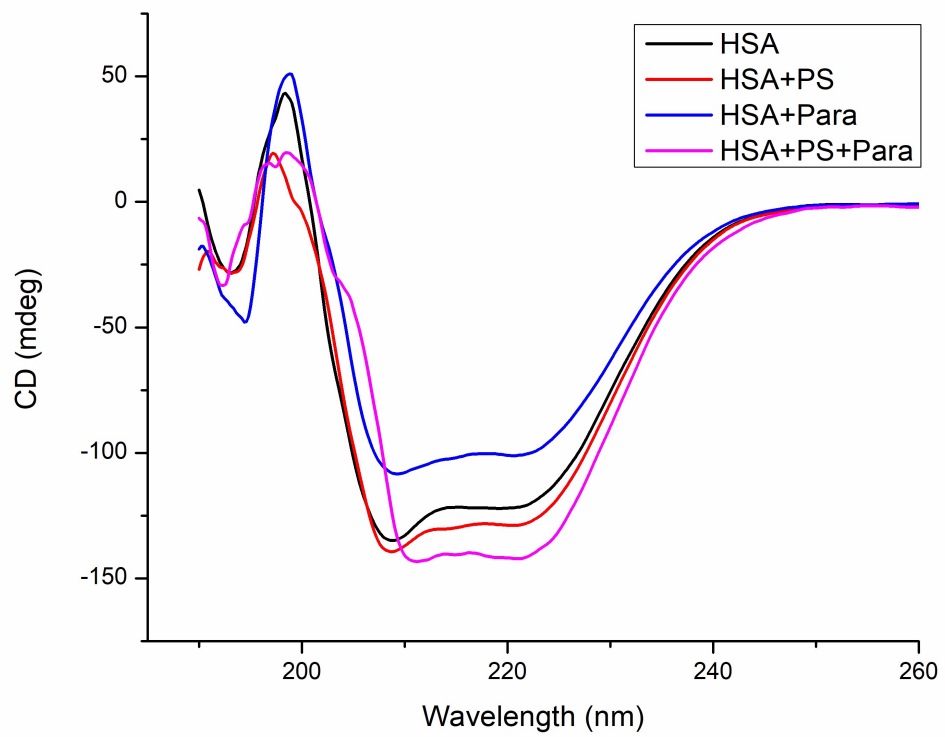


Fig.1 CD spectrum of control, NPS, paracetamol, NPS-paracetamol interacted HSA

BeStSel analysis result of CD spectrum

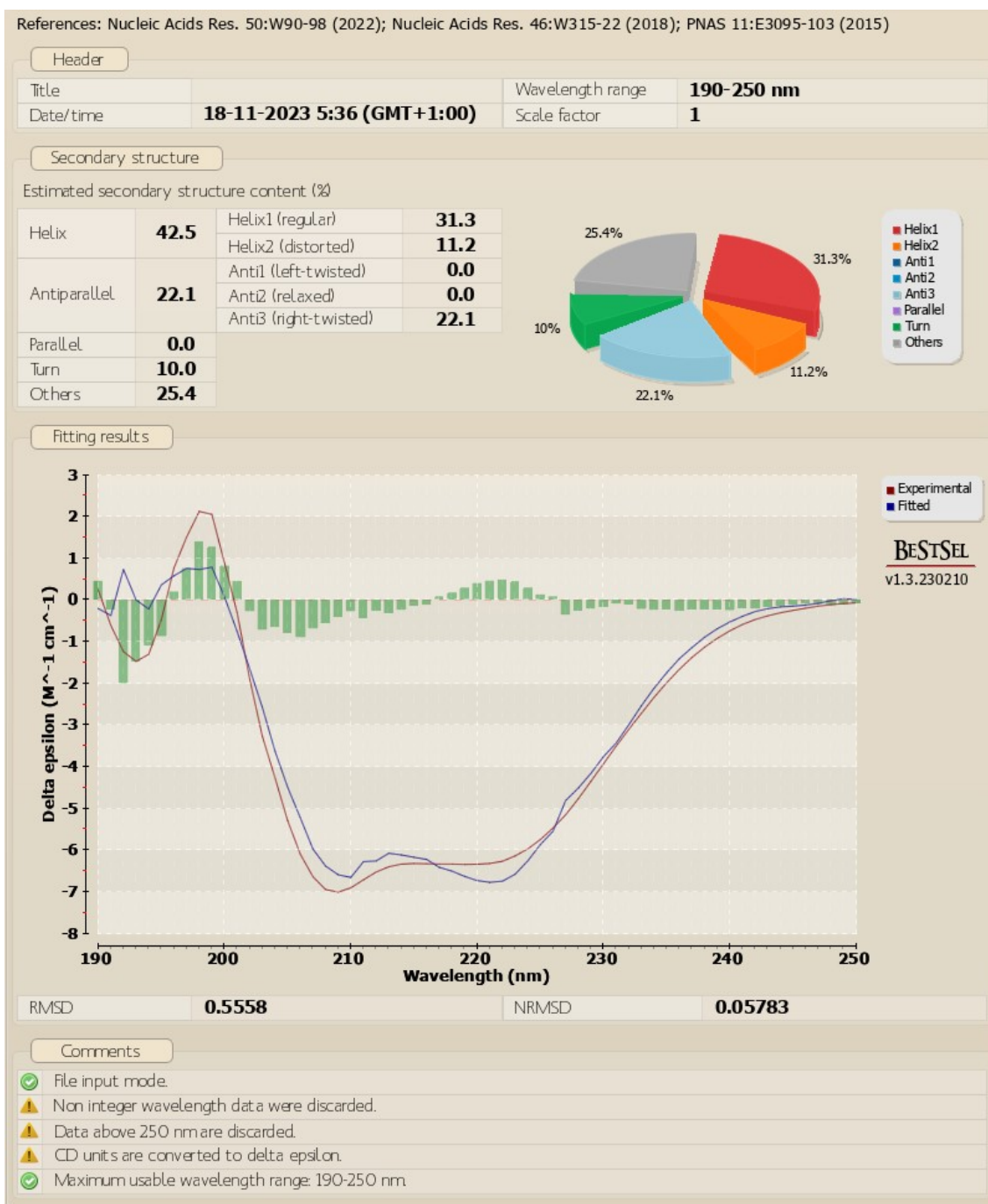


Fig.2 Control. Untreated HSA

References: Nucleic Acids Res. 50:W90-98 (2022); Nucleic Acids Res. 46:W315-22 (2018); PNAS 11:E3095-103 (2015)

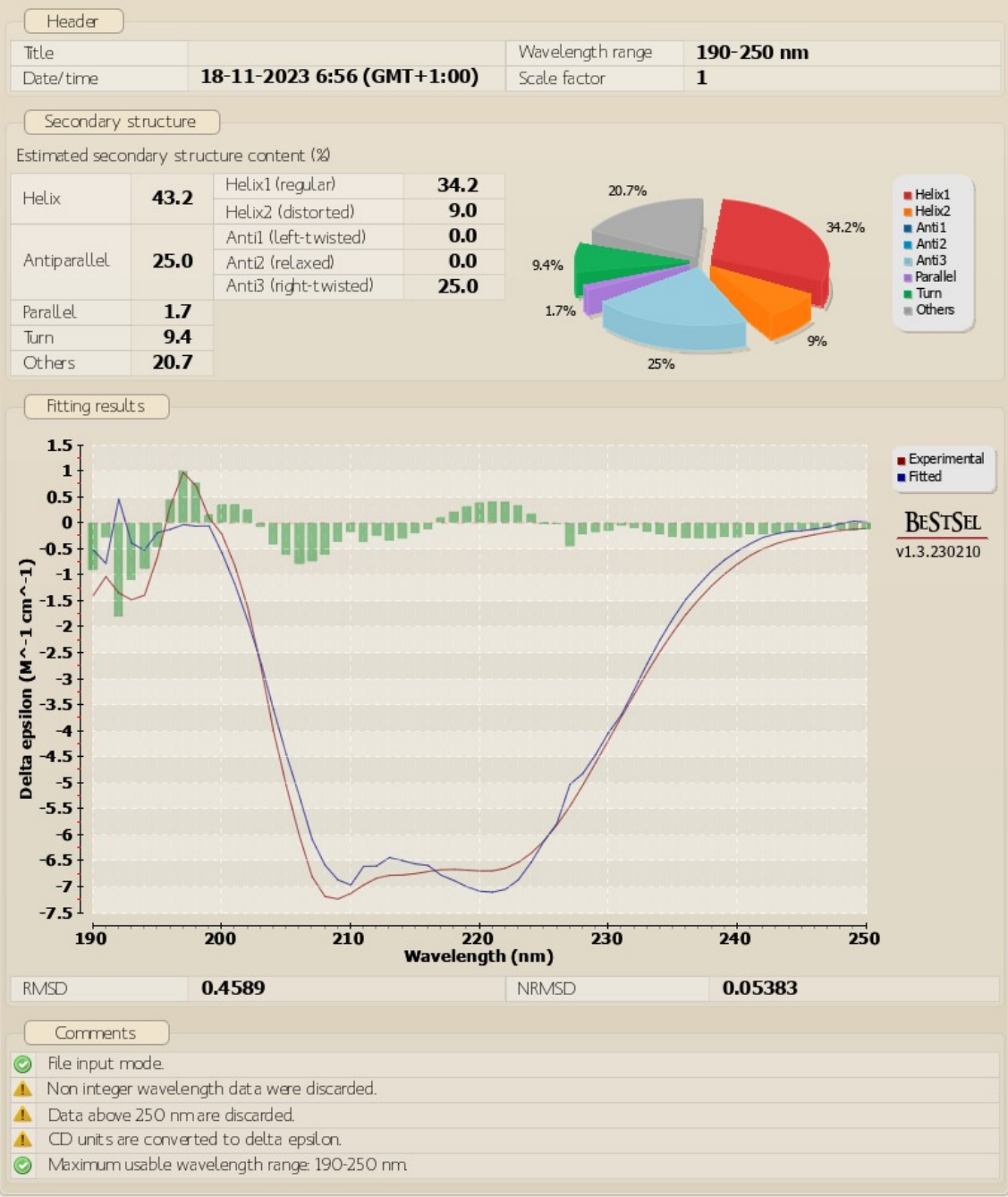


Fig.3 PS interacted HSA

References: Nucleic Acids Res. 50:W90-98 (2022); Nucleic Acids Res. 46:W315-22 (2018); PNAS 11:E3095-103 (2015)

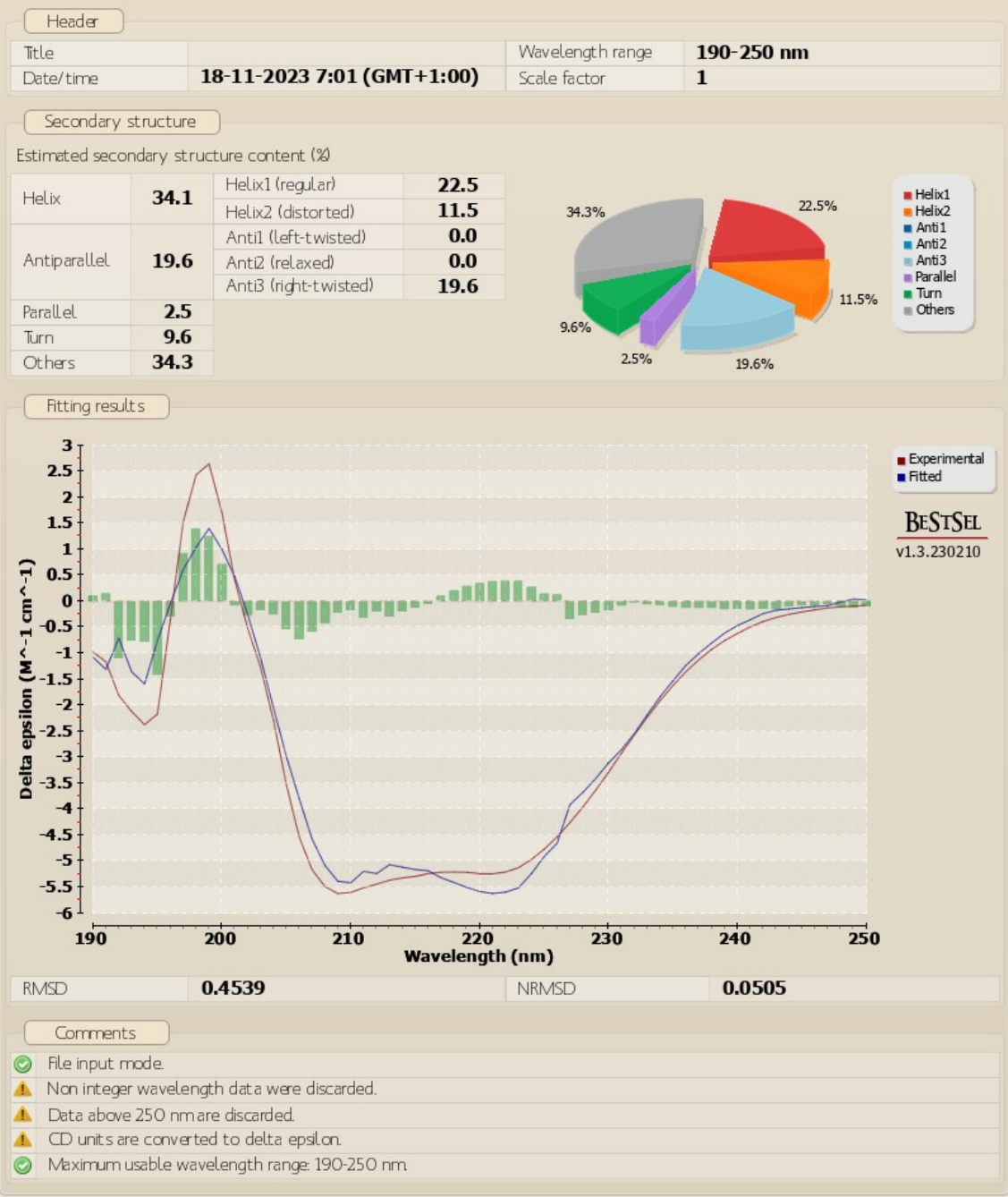


Fig.4 Para interacted HSA

References: Nucleic Acids Res. 50:W90-98 (2022); Nucleic Acids Res. 46:W315-22 (2018); PNAS 11:E3095-103 (2015)

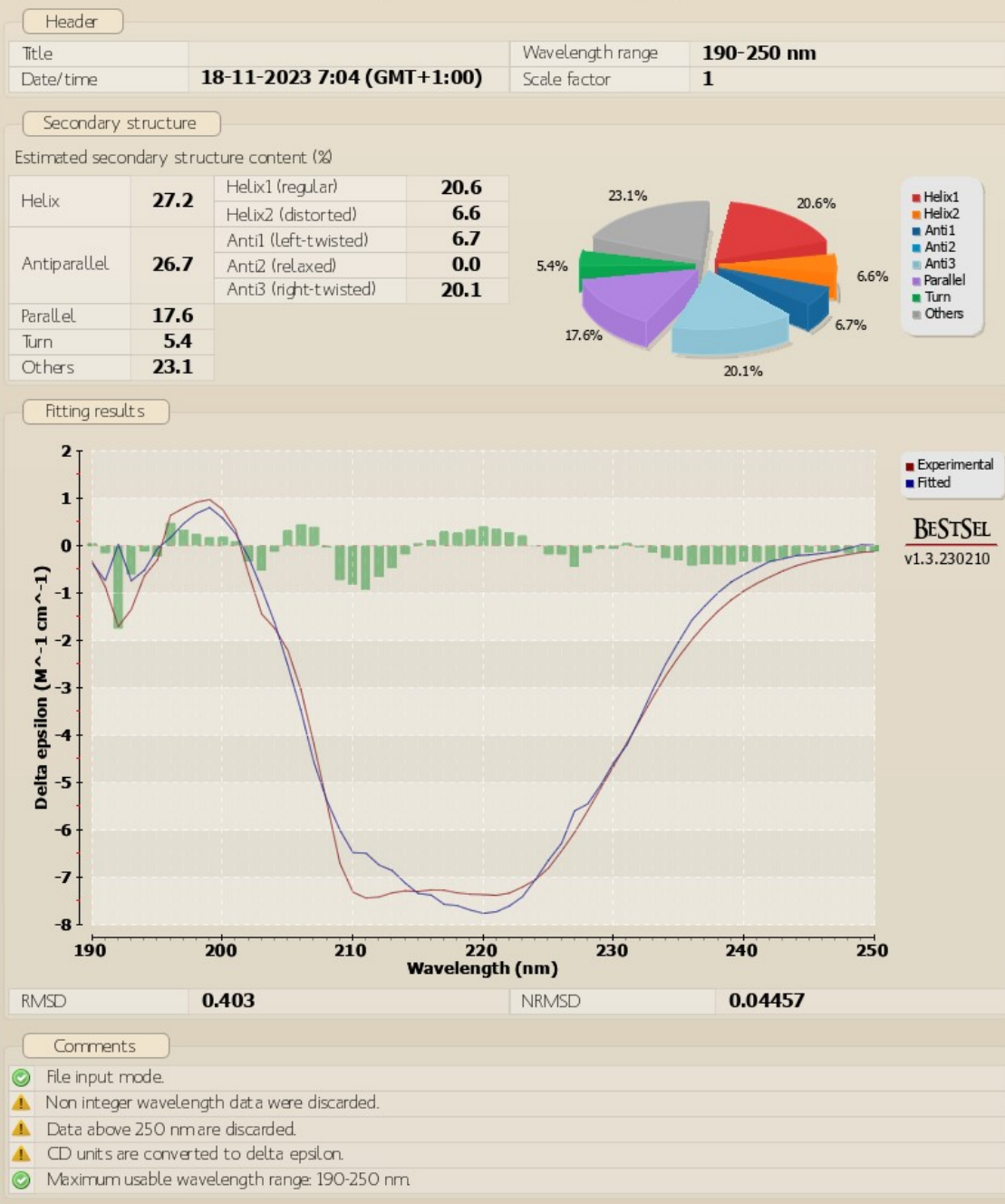


Fig.5 NPS-Paracetamol interacted HSA

BeStSel secondary structure tabularised

	control	PS	Para	PS Para
alpha				
Helix	42.5	43.2	34.1	27.2
beta				
sheets	22.1	26.7	22.1	44.3
Turn	10	9.4	9.6	5.4
Others	25.4	20.7	34.3	23.1

Table 2. BeStSel predicted HAS secondary structure

Blind docking result

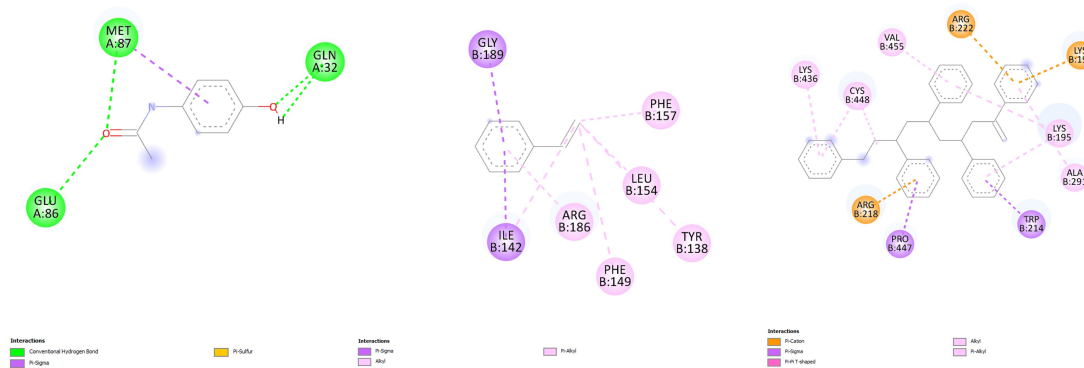


Fig.6 Blind docked

From left to right : paracetamol=-4.90 Kcal/mol, styrene=-4.25 Kcal/mol, pentamer=-7.55 Kcal/mol

Sudlow site I docked

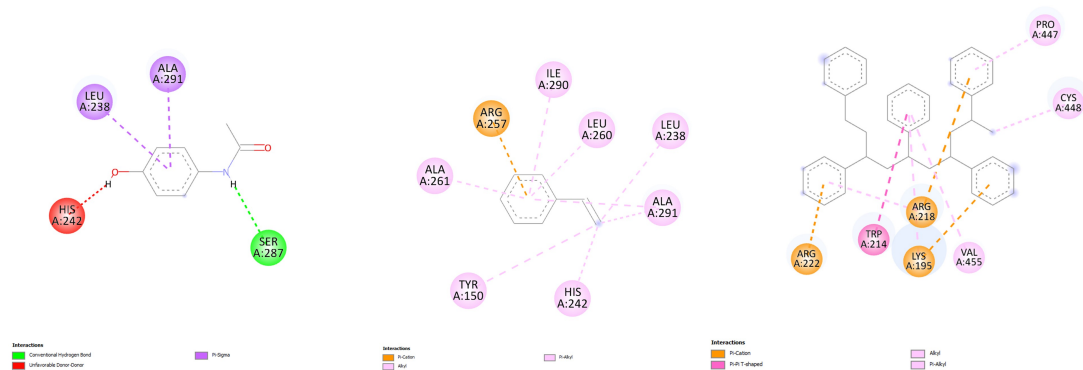


Fig.7 Sudlow site I docked

From left to right: paracetamol=-4.96 Kcal/mol, styrene=-4.25 Kcal/mol, pentamer=-6.46 Kcal/mol

Sudlow site II docked

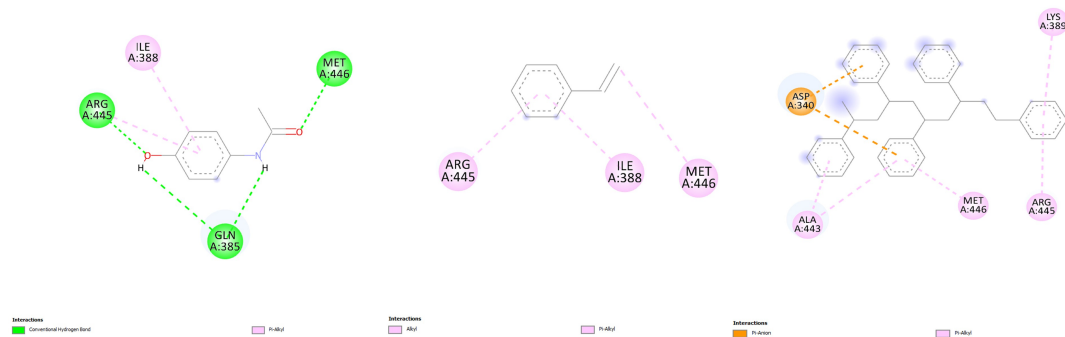


Fig.8 Sudlow site II docked

From left to right: paracetamol=-5.81 Kcal/mol, styrene=-4.36 Kcal/mol, pentamer=-5.81 Kcal/mol