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Bisphenols affinity binding to hormonal and non-hormonal receptors, An in-silico study

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Endocrine disruptive chemicals (EDCs), such as xenoestrogen bisphenols, influence progenitor and mature cells in endocrine organs by mimicking endogenous hormones. Therefore, EDC toxodynamic signaling has long been thought to involve endocrine nuclear receptors. However, many EDC effects seem to be mediated by other classes of receptors. In this in silico study, we screened seven bisphenols for binding to Notch, the Notch negative regulatory domain, Sigma one, corticosteroid, androgen, mineralocorticoid and beta- estradiol receptors. The Galaxy Web server was used in this study for docking and optimizing proteins and minimizing energy. The crystal structures of the following receptors were downloaded as PDB files from the Protein Data Bank: Human Notch (ID: 5MWB), Notch (NRR) (ID:3ETO), Sigma one (ID: 5HK1), Estrogen beta (ID:1X7B), Androgen receptor (ID: 2PIR), Mineralocorticoid (ID 3 VHU) and Corticosteroid (ID: 4P6X) receptors. ByMOL software was used to visualize and optimize protein chain lengths. ByMOL and protein- ligand interaction profiler (PLIP) were used in the analysis of the results. The following chemical SDF files were downloaded from PubChem websites: Bisphenol A, Bisphenol B, Bisphenol C Bisphenol F Bisphenol S, Bisphenol AF Tetrabromobisphenol A, 17 beta-Estradiol, Corticosterone, Testosterone,

Dihydrotestosterone, Cortisol, Aldosterone. All the SDF files were converted to 3D structures and then to PDB files. The results of our computational study (figure 1) introduce evidence that bisphenol A and other congeners have the affinity to bind to hormonal and nonho.

Ligands	Binding Affinity in Kcal /mol						
	Notch Receptor	Notch RR	Sigma receptor	Estrogen B receptors	Corticosteroid receptor	*Mineralocorticoid receptor*	*Androgen receptors*
Bisphenol A	-12.869	-15.034	-18.135	-17.698	-20.499	-18.299	-14.465
Bisphenol B	-14.371	-15.495	-14.759	-19.808	-21.477	-19.347	-13.464
Bisphenol C	-12.385	-14.854	-17.418	-17.828	-19.687	-15.996	-13.116
Bisphenol F	-11.316	-12.599	-10.698	-16.776	-16.345	-15.856	-12.117
Bisphenol S	-12.303	-12.310	-14.761	-16.694	-16.848	-15.345	-11.434
Bisphenol AF	-17.594	-15.028	-16.058	-19.464	-23.330	-19.683	-15.885
Tetrabromobisphenol A	-16.229	-16.229	-17.376	-20.026	-24.094	-21.652	-16.138
17 B- Estradiol +	-12.602	-14.282	-18.750	-17.715	-21.965	-17.799	-13.719
Aldosterone						-17.066	
Dihydrotestosterone							-13.852
Cortisol					-24.872		
Testosterone							-13.588
Corticosterone					-24.250		

Table: Bisphenols binding affinity to hormonal and non-hormonal receptors

Biography

Husnia Marrif is a graduate of biomedical science division at the University of Saskatchewan. She was supervised by Professor Bernard juurlink in cell biology. Supported by fellowships from the thyroid foundation and Health Canada trained as post doc at McGill University. She served in several academic and government contracts. Her expertise in the area of cell Metabolism and Endocrinology. She founded Marrif Biotech Company in 2021 to focus on agents affecting pancreatic beta cell growth.