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Correlation between structure, retention, property, and activity of biologically relevant 1,7-bis(aminoalkyl)diazachrysene derivatives

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Supplementary material

Table S1. Calculated values of molecular descriptors for 1,7-DAAC derivatives

	Potential Energy	mol MW	dipole	SASA	FOSA	FISA	PISA	volume	donorHB	accptHB	dip^2/V	ACxDN^.5/SA
1	-274.414276	542.723	0.009	969.242	731.866	30.444	206.932	1776.743	2	11.40	0.000000	0.016634
2	-189.468185	510.724	0.149	985.352	744.563	34.84	205.95	1773.132	2	8.00	0.000013	0.011482
3	-274.440399	514.669	0.005	890.513	662.602	30.063	197.848	1649.552	2	11.40	0.000000	0.018104
4	-222.01857	482.67	0.992	915.581	678.579	34.405	202.598	1648.193	2	8.00	0.000598	0.012357
5	-670.298157	430.595	0.042	845.992	484.846	155.588	205.559	1491.322	6	6.00	0.000001	0.017372
6	-383.594299	458.648	0.019	912.036	668.647	36.598	206.791	1626.261	2	8.00	0.000000	0.012405
7	-289.893219	514.756	0.036	994.48	760.769	30.211	203.5	1824.276	2	8.00	0.000001	0.011376
8	-284.123413	510.724	0.016	956.319	729.651	28.314	198.354	1743.99	2	8.00	0.000000	0.011831
9	-251.555008	538.778	0.048	1035.647	799.562	29.005	207.08	1870.619	2	8.00	0.000001	0.010924
10	-323.668671	486.702	0.606	921.872	690.837	28.832	202.203	1696.963	2	8.00	0.000216	0.012273
11	-407.078094	430.595	0.083	836.61	600.023	35.425	201.162	1501.284	2	8.00	0.000005	0.013523
12	-715.206482	374.488	2.502	728.819	357.226	152.095	219.498	1263.75	6	6.00	0.004955	0.020165
13	-622.905334	402.541	0.048	784.37	421.186	155.384	207.801	1372.714	6	6.00	0.000002	0.018737

	glob	QPpolrz	QPlogPC16	QPlogPoct	QPlogPw	QPlogPo/w	QPlogS	CIQPlogS	QPlogHERG	QPPCaco	QPlogBB
1	0.731952	60.506	17.431	28.408	15.619	4.450	-5.408	-4.811	-8.308	316.958	0.379
2	0.719009	60.353	17.605	26.451	12.332	5.823	-6.978	-5.404	-8.513	287.950	0.309
3	0.758174	56.614	15.891	27.212	15.806	3.678	-4.388	-4.255	-7.841	319.604	0.530
4	0.73701	56.605	16.167	25.283	12.579	5.045	-6.069	-4.839	-8.206	290.698	0.456
5	0.746185	47.787	16.367	27.404	16.262	3.184	-4.041	-4.018	-8.072	20.619	-1.226
6	0.733297	54.483	16.047	24.453	12.173	4.894	-5.681	-4.278	-8.286	277.102	0.304
7	0.726044	59.808	17.928	26.165	11.423	6.181	-6.49	-5.404	-8.388	318.574	0.135
8	0.732698	60.398	17.042	26.571	12.607	5.684	-6.789	-5.394	-8.255	332.049	0.527
9	0.708941	64.265	18.647	27.754	12.421	6.476	-7.876	-5.961	-8.682	327.072	0.373
10	0.74635	55.984	16.472	24.973	11.671	5.398	-5.529	-4.839	-8.053	328.313	0.292
11	0.757909	50.712	14.577	23.290	12.386	4.130	-4.689	-3.722	-7.861	284.295	0.467
12	0.775627	41.381	14.055	25.459	16.934	1.863	-2.751	-2.952	-7.662	22.253	-0.807
13	0.761548	44.346	15.124	26.318	16.569	2.474	-3.336	-3.481	-7.834	20.711	-1.028

	QPPMDCK	QPlogKp	IP(eV)	EA(eV)	#metab	QPlogKhsa	HumanOral Absorption	PercentHumanOral Absorption	PSA	#ringatoms
1	174.884	-4.517	7.574	0.786	11	0.654	1	84.809	69.344	30
2	157.650	-4.601	7.514	0.728	9	1.329	1	79.138	51.262	28
3	176.463	-4.734	7.603	0.818	11	0.433	1	80.350	69.311	30
4	159.277	-4.797	7.539	0.756	9	1.089	3	87.620	51.153	28
5	9.121	-6.636	7.578	0.790	11	0.477	1	56.150	95.164	18
6	151.241	-4.631	7.514	0.729	9	0.943	3	100.000	51.345	18
7	175.848	-4.140	7.575	0.789	9	1.303	1	82.021	49.942	18
8	183.902	-4.700	7.535	0.754	9	1.345	1	79.436	50.161	30
9	180.924	-4.490	7.510	0.725	9	1.588	1	83.952	50.299	30
10	181.666	-4.312	7.529	0.748	9	1.057	3	90.630	49.567	18
11	155.489	-4.821	7.539	0.756	9	0.714	3	95.045	51.032	18
12	9.904	-6.907	7.510	0.734	11	0.108	1	49.013	94.982	18
13	9.165	-6.816	7.515	0.729	11	0.277	1	52.032	95.194	18

	#in56	#noncon	#nonHatm	SemiEmpirical Energy	HOMO Energy	LUMO Energy	Molecular Electronegativity	Molecular Hardness	Total Electrophilic Superdelocalizability
1	30	8	40	766.174089	-17.774800	-10.724080	-14.249440	3.525360	-6.370627
2	28	8	38	821.073683	-17.722707	-10.672542	-14.197624	3.525082	-5.935597
3	30	8	38	801.65964	-18.257156	-11.205441	-14.731298	3.525857	-5.943151
4	28	8	36	856.801267	-18.207581	-11.155055	-14.681318	3.526263	-5.510060
5	18	0	32	798.597815	-17.424272	-10.377774	-13.901023	3.523249	-5.006495
6	18	0	34	834.484788	-17.783673	-10.732885	-14.258279	3.525394	-5.255678
7	18	0	38	806.530736	-17.722482	-10.673716	-14.198099	3.524383	-5.953988
8	30	10	38	836.252058	-18.162211	-11.109101	-14.635656	3.526555	-5.880234
9	30	10	40	801.304236	-17.692581	-10.642167	-14.167374	3.525207	-6.306551
10	18	0	36	841.562262	-18.191852	-11.139563	-14.665708	3.526144	-5.531808
11	18	0	32	870.795144	-18.284008	-11.229898	-14.756953	3.527055	-4.841858
12	18	0	28	870.447405	-18.322360	-11.249193	-14.785776	3.536584	-4.199296
13	18	0	30	832.47818	-17.913961	-10.861478	-14.387719	3.526242	-4.589031

	Total Nucleophilic Superdelocalizability	Total Radical Superdelocalizability	Total Atom Self Polarizability	Mopac dipole
1	30.176227	11.902800	-29.456165	0.042
2	29.296652	11.680527	-28.498795	0.070
3	25.876282	9.966565	-27.935461	0.003
4	24.978075	9.734007	-26.974090	3.061
5	24.333649	9.663577	-23.891312	0.373
6	24.159081	9.451702	-25.446067	0.155
7	29.242213	11.644113	-28.525738	0.251
8	28.400080	11.259923	-28.530090	0.024
9	33.076505	13.384977	-30.053052	0.108
10	24.966061	9.717127	-27.001955	2.975
11	20.449979	7.804060	-23.917497	0.653
12	17.265542	6.533123	-20.819987	0.045
13	20.215550	7.813260	-22.361069	0.230