Nanoarchitectonics and Molecular Docking of 4-(Dimethylamino)Pyridin-1-Ium 2-3 Methyl-4-Oxo-Pyri-Do[1,2-a]Pyrimidine-3-Carboxylate

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Table S1 Physicochemical Properties of the synthesized compounds.

Molecule	MW	#Heavy atoms	#Aromatic heavy atoms	Fraction Csp3	#Rotatable bonds	#H-bond acceptors	#H-bond donors	MR	TPSA
Fragment 1	203.17	15	10	0.1	1	4	0	51.45	74.5
Fragment 2	123.18	9	6	0.29	1	0	1	39.34	17.38
5	326.35	24	16	0.18	2	4	1	90.78	91.88

Table S2 Lipophilicity of the synthesized compounds.

Molecule	iLOGP	XLOGP3	WLOGP	MLOGP	Silicos-IT Log P	Consensus Log P
Fragment 1	0.9	0.91	-0.63	0.39	0.8	0.47
Fragment 2	1.53	1.34	0.57	0.49	0.9	0.96
5	1.92	1.89	-0.07	0.68	0.8	1.05

Table S3 Water Solubility of the synthesized compounds.

Molecule	ESOL Log S	ESOL Solubility (mg/ml)	ESOL Solubility (mol/l)	ESOL Class	Ali Log S	Ali Solubility (mg/ml)	Ali Solubility (mol/l)	Ali Class	Silicos-IT LogSw	Silicos-IT Solubility (mg/ml)	Silicos-IT Solubility (mol/l)	Silicos-IT class
Fragment 1	-2.1	1.61E+00	7.94E-03	Soluble	-2.06	1.77E+00	8.71E-03	Soluble	-2.18	1.35E+00	6.65E-03	Soluble
Fragment 2	-1.88	1.64E+00	1.33E-02	Very soluble	-1.31	6.08E+00	4.94E-02	Very soluble	-2.09	1.00E+00	8.15E-03	Soluble
5	-3.42	1.25E-01	3.84E-04	Soluble	-3.44	1.18E-01	3.61E-04	Soluble	-2.18	2.17E+00	6.65E-03	Soluble

Table S4 Pharmacokinetics Properties of the synthesized compounds.

Molecule	GI absorption	BBB permeant	Pgp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	log Kp (cm/s)
Fragment 1	High	No	No	Yes	No	No	No	No	-6.89
Fragment 2	High	No	No	No	No	No	No	No	-6.1
5	High	No	No	No	No	No	No	No	-6.95

Table S5 Druglikeness Properties of the synthesized compounds..

Molecule	Lipinski #violations	Ghose #violations	Veber #violations	Egan #violations	Muegge #violations	Bioavailability Score
Fragment 1	0	1	0	0	0	0.85
Fragment 2	0	2	0	0	1	0.55
5	0	0	0	0	0	0.55

Table S6 Medicinal Properties of the synthesized compounds.

Molecule	PAINS #alerts	Brenk #alerts	Leadlikeness #violations	Synthetic Accessibility
Fragment 1	0	0	1	1.67
Fragment 2	0	0	1	1.03
5	0	0	0	2.37