

Supplementary data
In silico* Evaluation of Savirin Derivatives As Inhibitors of the *agr* Quorum Sensing System of *Staphylococcus aureus
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Table S1. Medicinal chemistry evaluation of the molecules

Molecule	PAINS alerts	Brenk alerts	Leadlikeness violations	Synthetic Accessibility
Savirin	0	0	1	3.20
1	0	0	2	3.66
2	0	0	1	3.42
3	0	0	2	3.57
4	0	1	1	3.42
5	0	0	2	3.66
6	0	0	2	3.42
7	0	0	1	3.48
8	0	0	1	3.48
9	0	0	2	3.39
10	0	3	2	3.60
11	0	0	2	3.56
12	0	1	1	3.32
13	0	0	1	3.41
14	0	0	2	3.26
15	0	1	1	3.53
16	0	0	2	3.22
17	0	0	1	3.46
18	0	0	1	3.43
19	0	0	1	3.35
20	0	2	1	3.40
21	0	0	2	3.52

table S1. (continued).

Molecule	PAINS alerts	Brenk alerts	Leadlikeness violations	Synthetic Accessibility
22	0	1	1	3.28
23	0	0	1	3.40
24	0	0	1	3.29
25	0	1	1	3.51
26	0	0	2	3.19
27	0	0	1	3.34
28	0	0	1	3.34
29	0	0	1	3.34
30	0	2	1	3.37

Table S2. Water solubility evaluation of the molecules

Molecule	ESOL Log S	ESOL Solubility (mg/ml)	ESOL Solubility (mol/l)	ESOL Class	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
Savirin	-4.65	8.19E-03	2.22E-05	Moderately soluble	-5.37	1.58E-03	4.28E-06	Moderately soluble	-6.14	2.69E-04	7.31E-07	Poorly soluble
1	-5.03	3.83E-03	9.31E-06	Moderately soluble	-5.59	1.05E-03	2.55E-06	Moderately soluble	-5.39	1.69E-03	4.11E-06	Moderately soluble
2	-4.34	1.75E-02	4.55E-05	Moderately soluble	-5.05	3.38E-03	8.82E-06	Moderately soluble	-4.94	4.39E-03	1.15E-05	Moderately soluble
3	-4.85	5.57E-03	1.40E-05	Moderately soluble	-5.53	1.17E-03	2.94E-06	Moderately soluble	-5.42	1.53E-03	3.85E-06	Moderately soluble
4	-4.51	1.18E-02	3.08E-05	Moderately soluble	-5.2	2.41E-03	6.27E-06	Moderately soluble	-4.72	7.26E-03	1.89E-05	Moderately soluble
5	-4.95	4.81E-03	1.13E-05	Moderately soluble	-5.92	5.11E-04	1.20E-06	Moderately soluble	-5.34	1.96E-03	4.59E-06	Moderately soluble
6	-5.1	3.09E-03	7.99E-06	Moderately soluble	-5.72	7.33E-04	1.90E-06	Moderately soluble	-5.58	1.03E-03	2.65E-06	Moderately soluble
7	-4.46	1.44E-02	3.49E-05	Moderately soluble	-5.35	1.83E-03	4.43E-06	Moderately soluble	-4.65	9.25E-03	2.24E-05	Moderately soluble
8	-4.04	3.74E-02	9.08E-05	Moderately soluble	-4.8	6.51E-03	1.58E-05	Moderately soluble	-4.87	5.60E-03	1.36E-05	Moderately soluble
9	-4.89	5.08E-03	1.29E-05	Moderately soluble	-5.84	5.72E-04	1.45E-06	Moderately soluble	-5.38	1.65E-03	4.20E-06	Moderately soluble
10	-5	4.14E-03	1.00E-05	Moderately soluble	-6.41	1.59E-04	3.85E-07	Poorly soluble	-4.65	9.17E-03	2.22E-05	Moderately soluble
11	-4.88	5.42E-03	1.32E-05	Moderately soluble	-5.57	1.10E-03	2.68E-06	Moderately soluble	-6.21	2.53E-04	6.14E-07	Poorly soluble
12	-4.64	8.70E-03	2.27E-05	Moderately soluble	-5.78	6.36E-04	1.66E-06	Moderately soluble	-5.77	6.57E-04	1.71E-06	Moderately soluble
13	-4.72	7.67E-03	1.92E-05	Moderately soluble	-5.53	1.17E-03	2.94E-06	Moderately soluble	-6.24	2.29E-04	5.75E-07	Poorly soluble
14	-4.86	5.33E-03	1.39E-05	Moderately soluble	-6	3.83E-04	9.97E-07	Poorly soluble	-5.55	1.09E-03	2.82E-06	Moderately soluble
15	-4.65	9.52E-03	2.23E-05	Moderately soluble	-5.66	9.29E-04	2.18E-06	Moderately soluble	-6.16	2.92E-04	6.85E-07	Poorly soluble

table S2. (continued).

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
16	-4.81	6.02E-03	1.56E-05	Moderately soluble	-5.47	1.30E-03	3.37E-06	Moderately soluble	-6.4	1.53E-04	3.96E-07	Poorly soluble
17	-4.51	1.28E-02	3.11E-05	Moderately soluble	-5.66	8.93E-04	2.16E-06	Moderately soluble	-5.47	1.38E-03	3.36E-06	Moderately soluble
18	-4.09	3.33E-02	8.09E-05	Moderately soluble	-5.11	3.18E-03	7.73E-06	Moderately soluble	-5.69	8.38E-04	2.04E-06	Moderately soluble
19	-4.59	1.00E-02	2.55E-05	Moderately soluble	-5.58	1.04E-03	2.64E-06	Moderately soluble	-6.2	2.47E-04	6.27E-07	Poorly soluble
20	-4.7	8.19E-03	1.98E-05	Moderately soluble	-6.15	2.89E-04	7.00E-07	Poorly soluble	-5.48	1.37E-03	3.32E-06	Moderately soluble
21	-4.88	5.42E-03	1.32E-05	Moderately soluble	-5.57	1.10E-03	2.68E-06	Moderately soluble	-6.21	2.53E-04	6.14E-07	Poorly soluble
22	-4.3	1.93E-02	5.04E-05	Moderately soluble	-5.21	2.37E-03	6.17E-06	Moderately soluble	-5.77	6.57E-04	1.71E-06	Moderately soluble
23	-4.72	7.67E-03	1.92E-05	Moderately soluble	-5.53	1.17E-03	2.94E-06	Moderately soluble	-6.24	2.29E-04	5.75E-07	Poorly soluble
24	-4.51	1.18E-02	3.08E-05	Moderately soluble	-5.43	1.43E-03	3.71E-06	Moderately soluble	-5.55	1.09E-03	2.82E-06	Moderately soluble
25	-4.65	9.52E-03	2.23E-05	Moderately soluble	-5.66	9.29E-04	2.18E-06	Moderately soluble	-6.16	2.92E-04	6.85E-07	Poorly soluble
26	-4.81	6.02E-03	1.56E-05	Moderately soluble	-5.47	1.30E-03	3.37E-06	Moderately soluble	-6.4	1.53E-04	3.96E-07	Poorly soluble
27	-4.51	1.28E-02	3.11E-05	Moderately soluble	-5.66	8.93E-04	2.16E-06	Moderately soluble	-5.47	1.38E-03	3.36E-06	Moderately soluble
28	-4.09	3.33E-02	8.09E-05	Moderately soluble	-5.11	3.18E-03	7.73E-06	Moderately soluble	-5.69	8.38E-04	2.04E-06	Moderately soluble
29	-4.59	1.00E-02	2.55E-05	Moderately soluble	-5.58	1.04E-03	2.64E-06	Moderately soluble	-6.2	2.47E-04	6.27E-07	Poorly soluble
30	-4.7	8.19E-03	1.98E-05	Moderately soluble	-6.15	2.89E-04	7.00E-07	Poorly soluble	-5.48	1.37E-03	3.32E-06	Moderately soluble