

**Intralaboratory CV Analysis of BCOP -  
Data from Dr. Joseph Sina**

Substance	Cornea number	Concentration/ Incubation temp.	Opacity	Permeability	<i>In vitro</i> score <sup>1</sup>	Prediction
Dimethyl ethylimidazo pyridine	1	10%/32	11	0.044	11.66	
	2		-3	0.063	-2.06	
	3		5	0.068	6.02	
	4		-3	0.055	-2.18	
	mean		3	0.058	3.36	Mild
	SD		7	0.010	6.73	
	%CV		272	18.2	200.2	
Sodium bitartrate	1	20%/RT	16	0.002	16.03	
	2		8	0.008	8.12	
	3		6	0.020	6.30	
	4		17	0.000	17.00	
	mean		12	0.008	11.86	Mild
	SD		6	0.009	5.44	
	%CV		47	120.0	45.8	
Quinaldine (2-methylquinoline)	1	100%/32	17	0.211	20.17	
	2		23	0.250	26.75	
	3		22	0.507	29.61	
	mean		21	0.323	25.51	Moderate
	SD		3	0.161	4.84	
	%CV		16	49.8	19.0	
	N-Acetyl- <i>p</i> -anisidine	1	20%/RT	7	0.014	7.21
2			11	0.013	11.20	
3			-3	0.005	-2.93	
4			-2	0.000	-2.00	
mean			3	0.008	3.37	Mild
SD			7	0.007	6.94	
%CV			211	83.5	205.9	
1,3-Benzenedicarboxaldehyde	1	20%/32	11	0.019	11.29	
	2		1	0.006	1.09	
	3		10	0.091	11.37	
	4		9	0.051	9.77	
	mean		8	0.042	8.38	Mild
	SD		5	0.038	4.91	
	%CV		59	90.8	58.7	
	1	20%/RT	8	0.018	8.27	
	2		13	0.058	13.87	
	3		3	0.008	3.12	
	4		8	0.035	8.53	
	mean		8	0.030	8.45	Mild
	SD		4	0.022	4.39	
	%CV		51	73.6	52.0	
1	20%/32	24	0.217	27.26		
2		31	0.037	31.56		
3		23	0.255	26.83		
4		31	0.162	33.43		
mean		27	0.168	29.77	Moderate	
SD		4	0.095	3.24		
%CV		16	56.7	10.9		
Triethylammonium iodide	1	20%/RT	21	0.089	22.34	
	2		27	0.042	27.63	
	3		26	0.049	26.74	
	4		18	0.076	19.14	
	mean		23	0.064	23.96	Mild
	SD		4	0.022	3.96	
	%CV		18	34.7	16.5	

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Dicyclohexylcarbodiimide	1	20%/RT	23	0.010	23.15	
	2		22	0.032	22.48	
	3		16	0.037	16.56	
	4		18	0.034	18.51	
	mean		20	0.028	20.17	Mild
	SD		3	0.012	3.16	
	%CV		17	43.7	15.7	
L-Proline, N-carboxyanhydride	1	20%/RT	8	0.007	8.11	
	2		12	0.008	12.12	
	3		-5	0.009	-4.87	
	4		5	0.014	5.21	
	mean		5	0.010	5.14	Mild
	SD		7	0.003	7.25	
	%CV		145	32.7	141.0	
Substituted propanediol	1	20%/RT	50	1.538	73.07	
	2		52	1.552	75.28	
	3		48	2.428	84.42	
	4		46	1.625	70.38	
	mean		49	1.786	75.79	Severe
	SD		3	0.430	6.10	
	%CV		5	24.1	8.0	
3-Trichlorovinylaniline HCL	1	20%/32	398	0.001	398.02	
	2		404	0.001	404.02	
	3		406	0.000	406.00	
	4		408	0.002	408.03	
	mean		404	0.001	404.02	Severe
	SD		4	0.001	4.32	
	%CV		1	81.6	1.1	
Methyl chlorobenzyl butylthio propyl indolyl dimethylpropanoate	1	20%/RT	15	0.005	15.08	
	2		18	0.002	18.03	
	3		8	0.002	8.03	
	4		5	0.001	5.02	
	mean		12	0.003	11.54	Mild
	SD		6	0.002	6.04	
	%CV		52	69.3	52.4	
Nitropyridinone	1	20%/RT	11	0.043	11.65	
	2		12	0.035	12.53	
	3		5	0.025	5.38	
	4		6	0.002	6.03	
	mean		9	0.026	8.89	Mild
	SD		4	0.018	3.71	
	%CV		41	67.7	41.7	
	1	20%/32	-5	0.036	-4.46	
	2		2	0.027	2.41	
	3		-9	0.023	-8.66	
	4		-4	0.003	-3.96	
	mean		-4	0.022	-3.67	Mild
	SD		5	0.014	4.56	
	%CV		-114	62.6	-124.5	
alpha-Naphthyl-pyranone	1	20%/RT	1	0.026	1.39	
	2		12	0.020	12.30	
	3		-1	0.013	-0.81	
	4		11	0.018	11.27	
	mean		6	0.019	6.04	Mild
	SD		7	0.005	6.71	
	%CV		117	27.9	111.1	

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Cyclic peptide	1	20%/32	5	0.087	6.31	
	2		2	0.086	3.29	
	3		-5	0.057	-4.15	
	4		5	0.025	5.38	
	mean		2	0.064	2.71	Mild
	SD		5	0.029	4.74	
	%CV		270	46.0	175.1	
Chloroquinoliny methyl ester carboxylic acid	1	20%/RT	38	0.246	41.69	
	2		39	0.325	43.88	
	3		50	0.378	55.67	
	4		25	0.409	31.14	
	mean		38	0.340	43.09	Moderate
	SD		10	0.071	10.06	
	%CV		27	21.0	23.4	
7-Chloroquinaldine	1	20%/RT	4	0.002	4.03	
	2		8	0.000	8.00	
	3		3	0.000	3.00	
	4		6	0.000	6.00	
	mean		5	0.001	5.26	Mild
	SD		2	0.001	2.21	
	%CV		42	200.0	42.1	
	1	20%/32	7	0.044	7.66	
	2		14	0.029	14.44	
	3		8	0.057	8.86	
	4		11	0.043	11.65	
	mean		10	0.043	10.65	Mild
	SD		3	0.011	3.03	
	%CV		32	26.5	28.4	
alpha-Pyranone, 7,7-dioxide	1	20%/RT	0	0.045	0.68	
	2		0	0.072	1.08	
	3		6	0.136	8.04	
	4		2	0.090	3.35	
	mean		2	0.086	3.29	Mild
	SD		3	0.038	3.38	
	%CV		141	44.6	102.9	
Methyl boronic acid	1	20%/RT	10	0.144	12.16	
	2		21	0.143	23.15	
	3		28	0.164	30.46	
	4		19	0.114	20.71	
	mean		20	0.141	21.62	Mild
	SD		7	0.021	7.55	
	%CV		38	14.6	34.9	
	1	20%/32	20	0.305	24.58	
	2		14	0.164	16.46	
	3		21	0.383	26.75	
	4		28	0.303	32.55	
	mean		21	0.289	25.08	Moderate
	SD		6	0.091	6.66	
	%CV		28	31.6	26.6	
1,1-Diphenyl prolinol (sulfate salt)	1	20%/RT	11	1.730	36.95	
	2		17	0.790	28.85	
	3		7	1.144	24.16	
	4		10	2.405	46.08	
	mean		11	1.517	34.01	Severe
	SD		4	0.707	9.62	
	%CV		37	46.6	28.3	
4-(2-Quinolylmethoxy)aniline	1	20%/32	23	0.000	23.00	
	2		-3	0.000	-3.00	
	3		-6	0.001	-5.99	
	4		-3	0.019	-2.72	
	mean		3	0.005	2.83	Mild
	SD		14	0.009	13.53	

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	%CV		494	186.9	479.0	
Sulfone amine	1	20%/RT	11	0.018	11.27	
	2		14	0.008	14.12	
	3		8	0.015	8.23	
	4		24	0.004	24.06	
	mean		14	0.011	14.42	Mild
	SD		7	0.006	6.86	
	%CV		49	56.9	47.6	
<i>p</i> -Nitrobenzyl 2-diazo acetoacetate	1	20%/RT	0	0.028	0.42	
	2		15	0.012	15.18	
	3		24	0.016	24.24	
	4		19	0.039	19.59	
	mean		15	0.024	14.86	Mild
	SD		10	0.012	10.31	
	%CV		71	51.5	69.4	
alpha-Pyranol, 7,7-dioxide	1	20%/RT	12	0.035	12.53	
	2		11	0.033	11.50	
	3		7	0.025	7.38	
	4		-1	0.014	-0.79	
	mean		7	0.027	7.65	Mild
	SD		6	0.010	6.05	
	%CV		82	35.6	79.1	
	1	20%/32	20	0.156	22.34	
	2		29	0.228	32.42	
	3		38	0.115	39.73	
	mean		29	0.166	31.50	Mild
	SD		9	0.057	8.73	
	%CV		31	34.4	27.7	
	Triethylamine hydroiodide	1	20%/RT	29	0.021	29.32
2			32	0.059	32.89	
3			33	0.064	33.96	
4			29	0.038	29.57	
mean			31	0.046	31.43	Moderate
SD			2	0.020	2.34	
%CV			7	43.6	7.4	
Substituted cephalosporanic acid	1	20%/RT	11	0.006	11.09	
	2		17	0.056	17.84	
	3		10	0.017	10.26	
	4		12	0.001	12.02	
	mean		13	0.020	12.80	Mild
	SD		3	0.025	3.44	
	%CV		25	124.6	26.8	
	1	20%/32	-3	0.006	-2.91	
	2		-6	0.000	-6.00	
	3		-6	0.010	-5.85	
	4		-3	0.012	-2.82	
	mean		-5	0.007	-4.40	Mild
	SD		2	0.005	1.77	
	%CV		-38	75.6	-40.2	

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4-Benzoxycarbonicamino-2-hydroxy-butanoic acid	1	20%/RT	392	0.001	392.02	
	2		395	0.006	395.09	
	3		397	0.008	397.12	
	4		399	0.000	399.00	
	mean		396	0.004	395.81	Severe
	SD		3	0.004	2.99	
	%CV		1	103.0	0.8	
N-Sulfonamido hydroxyacetophenone	1	20%/RT	4	0.006	4.09	
	2		3	0.040	3.60	
	3		12	0.026	12.39	
	4		-10	0.002	-9.97	
	mean		2	0.019	2.53	Mild
	SD		9	0.018	9.26	
	%CV		405	96.0	366.2	
	1	20%/32	-8	0.021	-7.69	
	2		-12	0.012	-11.82	
	3		-8	0.015	-7.78	
	4		4	0.001	4.02	
	mean		-6	0.012	-5.82	Mild
	SD		7	0.008	6.83	
	%CV		-115	68.4	-117.5	
Cyclic peptide	1	20%/32	7	0.011	7.17	
	2		4	0.007	4.11	
	3		10	0.013	10.20	
	4		10	0.017	10.26	
	mean		8	0.012	7.93	Mild
	SD		3	0.004	2.93	
	%CV		37	34.7	36.9	
4-Bromo-2,5-dimethylphenol	1	20%/32	54	4.006	114.09	
	2		54	4.708	124.62	
	3		61	5.000	136.00	
	4		76	4.914	149.71	
	mean		61	4.657	131.11	Severe
	SD		10	0.451	15.29	
	%CV		17	9.7	11.7	
2-Amino-3,6-dimethylphenol, hydrobromide salt	1	20%/32	162	0.252	165.78	
	2		141	0.228	144.42	
	3		138	0.294	142.41	
	4		145	0.272	149.08	
	mean		147	0.262	150.42	Severe
	SD		11	0.028	10.61	
	%CV		7	10.8	7.1	
Mixture of 2-chloromethyl-4,7-dimethylbenzoxazole and 2-bromomethyl dimethylbenzoxazole	1	20%/32	14	0.001	14.02	
	2		17	0.000	17.00	
	3		19	0.000	19.00	
	4		22	0.016	22.24	
	mean		18	0.004	18.06	Mild
	SD		3	0.008	3.46	
	%CV		19	184.6	19.1	

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R-Hydroxy ester of benzoic acid compound	1	20%/32	-14	0.050	-13.25	
	2		-10	0.009	-9.87	
	3		-12	0.020	-11.70	
	4		-14	0.022	-13.67	
	mean		-13	0.025	-12.12	Mild
	SD		2	0.017	1.73	
	%CV		-15	69.2	-14.2	
<i>t</i> -Butyl-3-oxo-6-methoxyhexanoate	1	100%/32	7	0.008	7.12	
	2		17	0.000	17.00	
	3		19	0.191	21.87	
	mean		14	0.066	15.33	Mild
	SD		6	0.108	7.51	
	%CV		45	162.9	49.0	
	Methyl 3-oxo-6-methoxyhexanoate	1	100%/32	44	1.795	70.93
2			38	1.935	67.03	
3			34	0.824	46.36	
4			34	0.863	46.95	
mean			38	1.354	57.81	Severe
SD			5	0.593	12.99	
%CV			13	43.8	22.5	
+-Butyl-3R-hydroxy-6-methoxyhepanoate	1	100%/32	12	1.165	29.48	
	2		8	1.160	25.40	
	3		3	0.734	14.01	
	4		13	0.615	22.23	
	mean		9	0.919	22.78	Mild
	SD		5	0.286	6.56	
	%CV		51	31.1	28.8	
Aglycone; natural product	1	20%/32	14	0.005	14.08	
	2		3	0.016	3.24	
	3		11	0.000	11.00	
	4		17	0.005	17.08	
	mean		11	0.007	11.35	Mild
	SD		6	0.007	5.95	
	%CV		54	104.0	52.4	
Carbic anhydride	1	20%/32	192	0.000	192.00	
	2		185	0.000	185.00	
	3		209	0.000	209.00	
	4		221	0.000	221.00	
	mean		202	0.000	201.75	Severe
	SD		16	0.000	16.32	
	%CV		8	0.0	8.1	
3-Bromo-7-methyl-9-flurenone	1	20%/32	-2	0.019	-1.72	
	2		2	0.011	2.17	
	3		-6	0.009	-5.87	
	4		-5	0.007	-4.90	
	mean		-3	0.012	-2.58	Mild
	SD		4	0.005	3.62	
	%CV		-131	45.7	-140.6	
<i>tert</i> -Butyl-6-methoxy-3-S-(2-thiophenethio) hexanoate	1	100%/32	5	0.000	5.00	
	2		-3	0.000	-3.00	
	3		2	0.000	2.00	
	4		2	0.000	2.00	
	mean		2	0.000	1.50	Mild
	SD		3	0.000	3.32	
	%CV		221	0.0	221.1	
Cyanopyridinone	1	20%/32	-5	0.016	-4.76	
	2		-8	0.018	-7.73	
	3		-1	0.007	-0.90	
	4		-4	0.003	-3.96	
	mean		-5	0.011	-4.34	Mild
	SD		3	0.007	2.81	

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	%CV		-64	65.1	-64.8	
S-Hydroxy ester of benzoic acid compound	1	20%/32	12	0.021	12.32	
	2		18	0.000	18.00	
	3		20	0.000	20.00	
	4		33	0.000	33.00	
	mean		21	0.005	20.83	Mild
	SD		9	0.011	8.74	
	%CV		43	200.0	42.0	
Cyano methylpyridine	1	20%/32	8	0.037	8.56	
	2		17	0.025	17.38	
	3		21	0.013	21.20	
	4		15	0.000	15.00	
	mean		15	0.019	15.53	Mild
	SD		5	0.016	5.30	
	%CV		36	84.7	34.2	
Carbonitrile	1	20%/32	21	0.180	23.70	
	2		22	0.200	25.00	
	3		20	0.241	23.62	
	4		12	0.187	14.81	
	mean		19	0.202	21.78	
	SD		5	0.027	4.69	
	%CV		24	13.5	21.5	Mild
Abbreviations: CV = Coefficient of variation; RT = Room temperature; SD = Standard deviation.						
<sup>1</sup> <i>In Vitro</i> Score = Opacity + (15 x permeability value)						