

Table A.1 – DOE scheme and results

Run order	Design Order	Arg, mM	Succ,mM	HDMB, %	pH	R, U1-GHB	R, GHB-IBO	R, IBO-U2	R., U3-PY	N, GHB (10 ⁵)	N, IBO (10 ⁵)	N, PY (10 ⁵)
1	12	0	0	0	0	1.39	0.92	2.05	0.94	2.52	1.93	1.64
2	14	-1	0	0	1	1.17	0.60	2.92	1.34	0.73	4.44	1.69
3	19	-1	0	1	0	1.08	0.69	2.05	1.21	2.43	0.79	3.61
4	18	1	0	1	0	1.51	0.00	2.66	0.87	2.17	2.17	3.97
5	13	0	-1	0	-1	1.10	1.01	1.63	2.00	2.74	1.90	3.33
6	3	0	0	1	-1	1.07	0.99	1.73	-1.11	2.49	1.75	2.18
7	4	-1	1	0	0	1.05	0.75	1.76	1.00	3.16	2.33	2.01
8	20	0	0	-1	1	0.93	0.00	3.16	1.59	2.09	2.09	2.48
9	11	1	0	-1	0	1.43	0.61	2.37	1.96	3.10	1.37	2.57
10	6	0	1	0	1	0.93	0.00	2.67	1.39	1.90	2.09	3.55
11	23	0	0	0	0	1.42	0.97	2.44	1.71	3.01	2.26	3.69
12	15	0	0	-1	-1	1.31	0.87	1.94	1.55	2.25	1.53	2.99
13	22	-1	-1	0	0	1.04	0.76	1.84	1.92	2.64	1.17	4.37
14	16	0	-1	1	0	1.03	0.79	1.87	1.75	2.95	1.77	4.83
15	25	0	1	1	0	1.40	0.88	1.84	1.46	3.51	2.08	2.88
16	26	1	1	0	0	1.20	0.88	4.74	2.00	3.20	1.99	3.46
17	2	-1	0	-1	0	1.03	0.77	2.06	1.12	2.74	1.55	2.96
18	24	1	0	0	1	0.88	0.41	1.95	1.49	0.69	0.52	3.40
19	27	0	0	0	0	1.15	0.62	2.24	1.63	2.61	0.97	5.52
20	5	0	0	1	1	1.03	0.00	3.08	1.57	1.83	1.83	5.23
21	21	0	-1	0	1	1.22	0.65	2.98	1.53	1.99	3.22	2.50
22	17	1	-1	0	0	1.15	0.88	1.74	1.93	3.37	1.78	3.44
23	9	0	1	-1	0	1.13	0.70	2.37	1.52	2.12	1.60	1.23
24	8	0	-1	-1	0	1.22	0.75	2.19	1.56	2.31	1.21	1.07
25	7	1	0	0	-1	1.15	0.93	1.91	1.59	2.86	1.96	4.13
26	10	-1	0	0	-1	1.10	1.40	1.36	1.93	3.34	2.08	3.00
27	1	0	1	0	-1	1.08	1.07	1.45	1.89	2.78	1.53	2.10

Fig A.1 – Interaction profilers for GHB, IBO and PY at two extrema values.











