

Supplementary Material I: The benchmark dataset consisted of 726 combinations, of which 121 were positive combinations and 605 were negative combinations.

Index	Drug #1	Drug #2	Positive or Negative
1	D00236	D02487	Positive
2	D00475	D00570	Positive
3	D00848	D02272	Positive
4	D00217	D03182	Positive
5	D00340	D00626	Positive
6	D00023	D00165	Positive
7	D01024	D03820	Positive
8	D00251	D00340	Positive
9	D00554	D01294	Positive
10	D00340	D00627	Positive
11	D00683	D02212	Positive
12	D00593	D00945	Positive
13	D00432	D00650	Positive
14	D00485	D00970	Positive
15	D00340	D00400	Positive
16	D00340	D00362	Positive
17	D00554	D00950	Positive
18	D00267	D00809	Positive
19	D00126	D00847	Positive
20	D00615	D06412	Positive
21	D01450	D02149	Positive
22	D00455	D01203	Positive
23	D00454	D00823	Positive
24	D00358	D00551	Positive
25	D00340	D01204	Positive
26	D00340	D02082	Positive
27	D00679	D01453	Positive
28	D00113	D00469	Positive
29	D00944	D08996	Positive
30	D00340	D01302	Positive
31	D00842	D02095	Positive
32	D01413	D03799	Positive
33	D00105	D00953	Positive
34	D00126	D00511	Positive
35	D00217	D00847	Positive
36	D00554	D03917	Positive
37	D00400	D06412	Positive
38	D00516	D01302	Positive

39	D00480	D02101	Positive
40	D00554	D00953	Positive
41	D00615	D00887	Positive
42	D00603	D02076	Positive
43	D00340	D00459	Positive
44	D00335	D00944	Positive
45	D00340	D00357	Positive
46	D00480	D00848	Positive
47	D00182	D00575	Positive
48	D00109	D00847	Positive
49	D00088	D02216	Positive
50	D00615	D00627	Positive
51	D00554	D05205	Positive
52	D00336	D00944	Positive
53	D00554	D04104	Positive
54	D00235	D00272	Positive
55	D00272	D00604	Positive
56	D00503	D00809	Positive
57	D00049	D00434	Positive
58	D00211	D00346	Positive
59	D00095	D02086	Positive
60	D00217	D02101	Positive
61	D00246	D05277	Positive
62	D00186	D02216	Positive
63	D01066	D03048	Positive
64	D00687	D01708	Positive
65	D00554	D02367	Positive
66	D00340	D00523	Positive
67	D00944	D06645	Positive
68	D00182	D00554	Positive
69	D00340	D00634	Positive
70	D00340	D00623	Positive
71	D00105	D00950	Positive
72	D00603	D00653	Positive
73	D01066	D06236	Positive
74	D00554	D05209	Positive
75	D00088	D00222	Positive
76	D00105	D03917	Positive
77	D00340	D00405	Positive
78	D00594	D00944	Positive
79	D00340	D00386	Positive
80	D00593	D00596	Positive
81	D00511	D01002	Positive

82	D00340	D00483	Positive
83	D00118	D01984	Positive
84	D01340	D02227	Positive
85	D00738	D02388	Positive
86	D00340	D06412	Positive
87	D00059	D00558	Positive
88	D00615	D01204	Positive
89	D00383	D00619	Positive
90	D00109	D00302	Positive
91	D00690	D01373	Positive
92	D00358	D00553	Positive
93	D00596	D00944	Positive
94	D00217	D00482	Positive
95	D00340	D00443	Positive
96	D00217	D02227	Positive
97	D00400	D00615	Positive
98	D00480	D00511	Positive
99	D00972	D01402	Positive
100	D00126	D00485	Positive
101	D00282	D01637	Positive
102	D00105	D05209	Positive
103	D00615	D00620	Positive
104	D02069	D03860	Positive
105	D00419	D00904	Positive
106	D00944	D00945	Positive
107	D07132	D08249	Positive
108	D00217	D01355	Positive
109	D00186	D00292	Positive
110	D00434	D01966	Positive
111	D00665	D05649	Positive
112	D00109	D00402	Positive
113	D00340	D00649	Positive
114	D00340	D00620	Positive
115	D00188	D00939	Positive
116	D00994	D02069	Positive
117	D00676	D00970	Positive
118	D00049	D00359	Positive
119	D00340	D00621	Positive
120	D00340	D07992	Positive
121	D00217	D05632	Positive
122	D00023	D00217	Negative
123	D00023	D00335	Negative
124	D00023	D00848	Negative

125	D00023	D01002	Negative
126	D00023	D01966	Negative
127	D00023	D02388	Negative
128	D00049	D00634	Negative
129	D00049	D00665	Negative
130	D00049	D00676	Negative
131	D00049	D01302	Negative
132	D00049	D02082	Negative
133	D00049	D03182	Negative
134	D00059	D00236	Negative
135	D00059	D00282	Negative
136	D00059	D00480	Negative
137	D00059	D00553	Negative
138	D00059	D00679	Negative
139	D00059	D00729	Negative
140	D00059	D00945	Negative
141	D00059	D02076	Negative
142	D00059	D02483	Negative
143	D00068	D00145	Negative
144	D00068	D00292	Negative
145	D00068	D00346	Negative
146	D00068	D00604	Negative
147	D00068	D00743	Negative
148	D00068	D00823	Negative
149	D00068	D02101	Negative
150	D00068	D03799	Negative
151	D00068	D05649	Negative
152	D00088	D00626	Negative
153	D00088	D00665	Negative
154	D00088	D00944	Negative
155	D00088	D06412	Negative
156	D00094	D00402	Negative
157	D00094	D00419	Negative
158	D00094	D00945	Negative
159	D00094	D01302	Negative
160	D00094	D01413	Negative
161	D00095	D00386	Negative
162	D00095	D00649	Negative
163	D00095	D00809	Negative
164	D00095	D01966	Negative
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176	D00109	D01450	Negative
177	D00109	D01708	Negative
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182	D00113	D00604	Negative
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184	D00113	D01066	Negative
185	D00113	D02149	Negative
186	D00113	D02216	Negative
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191	D00118	D05632	Negative
192	D00118	D08127	Negative
193	D00126	D00165	Negative
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196	D00126	D00475	Negative
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202	D00145	D01413	Negative
203	D00145	D01450	Negative
204	D00145	D05632	Negative
205	D00145	D08996	Negative
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207	D00165	D00222	Negative
208	D00165	D00383	Negative
209	D00165	D01112	Negative
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213	D00165	D05649	Negative
214	D00182	D00405	Negative
215	D00182	D01204	Negative
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217	D00182	D04104	Negative
218	D00182	D05632	Negative
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222	D00186	D00634	Negative
223	D00186	D00687	Negative
224	D00186	D00823	Negative
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227	D00186	D01450	Negative
228	D00186	D01637	Negative
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232	D00186	D03048	Negative
233	D00186	D05277	Negative
234	D00186	D08249	Negative
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237	D00188	D00848	Negative
238	D00188	D00972	Negative
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260	D00222	D00397	Negative
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262	D00222	D00455	Negative
263	D00222	D00523	Negative
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277	D00236	D00634	Negative
278	D00236	D00653	Negative
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280	D00246	D00516	Negative
281	D00246	D00604	Negative
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286	D00246	D05209	Negative
287	D00251	D00282	Negative
288	D00251	D00554	Negative
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292	D00251	D00887	Negative
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318	D00302	D00953	Negative
319	D00302	D01373	Negative
320	D00302	D02367	Negative
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322	D00335	D00516	Negative
323	D00335	D00558	Negative
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325	D00335	D02227	Negative
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328	D00336	D00650	Negative
329	D00336	D00738	Negative
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331	D00340	D01689	Negative
332	D00340	D07132	Negative
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334	D00346	D00485	Negative
335	D00346	D00676	Negative
336	D00346	D02227	Negative
337	D00357	D00402	Negative
338	D00357	D00469	Negative
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343	D00357	D02272	Negative
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348	D00358	D01066	Negative
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357	D00362	D00904	Negative
358	D00362	D00970	Negative
359	D00362	D01355	Negative
360	D00362	D02149	Negative
361	D00362	D03917	Negative
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396	D00419	D01002	Negative
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398	D00419	D05277	Negative
399	D00432	D00570	Negative
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404	D00434	D00516	Negative
405	D00434	D00626	Negative
406	D00434	D00627	Negative
407	D00434	D00994	Negative
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455	D00483	D00615	Negative
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487	D00551	D08205	Negative
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492	D00553	D02227	Negative
493	D00553	D05209	Negative
494	D00553	D08205	Negative
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496	D00554	D02483	Negative
497	D00554	D07132	Negative
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523	D00603	D08249	Negative
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536	D00615	D07132	Negative
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538	D00619	D00620	Negative
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543	D00620	D06645	Negative
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563	D00634	D03860	Negative
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571	D00653	D01294	Negative
572	D00653	D05205	Negative
573	D00653	D06236	Negative
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575	D00665	D00809	Negative
576	D00665	D01373	Negative
577	D00665	D02227	Negative
578	D00665	D02367	Negative
579	D00665	D02483	Negative
580	D00665	D08249	Negative
581	D00676	D00953	Negative
582	D00676	D00980	Negative
583	D00676	D01708	Negative
584	D00676	D02227	Negative
585	D00679	D02082	Negative
586	D00679	D02272	Negative
587	D00679	D06412	Negative
588	D00679	D06645	Negative
589	D00687	D00970	Negative
590	D00687	D01373	Negative
591	D00687	D02212	Negative
592	D00687	D03048	Negative
593	D00690	D00980	Negative
594	D00690	D01002	Negative
595	D00690	D01413	Negative
596	D00690	D03860	Negative
597	D00690	D03917	Negative

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600	D00729	D02487	Negative
601	D00729	D06412	Negative
602	D00729	D08205	Negative
603	D00738	D00743	Negative
604	D00738	D00944	Negative
605	D00738	D08127	Negative
606	D00743	D00847	Negative
607	D00743	D00981	Negative
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609	D00743	D02095	Negative
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616	D00842	D02076	Negative
617	D00847	D00939	Negative
618	D00847	D00945	Negative
619	D00847	D02076	Negative
620	D00847	D02082	Negative
621	D00848	D00980	Negative
622	D00848	D00981	Negative
623	D00848	D01984	Negative
624	D00887	D00970	Negative
625	D00887	D02367	Negative
626	D00887	D05277	Negative
627	D00904	D00953	Negative
628	D00904	D02060	Negative
629	D00904	D05205	Negative
630	D00904	D08996	Negative
631	D00939	D00994	Negative
632	D00939	D01302	Negative
633	D00939	D01453	Negative
634	D00939	D01637	Negative
635	D00939	D02367	Negative
636	D00944	D01204	Negative
637	D00944	D02212	Negative
638	D00944	D03860	Negative
639	D00944	D05205	Negative
640	D00944	D07132	Negative

641	D00945	D00953	Negative
642	D00945	D00980	Negative
643	D00945	D01402	Negative
644	D00950	D00972	Negative
645	D00950	D01413	Negative
646	D00950	D05209	Negative
647	D00950	D08127	Negative
648	D00950	D08996	Negative
649	D00953	D00970	Negative
650	D00953	D01002	Negative
651	D00970	D01066	Negative
652	D00970	D02101	Negative
653	D00970	D08127	Negative
654	D00972	D01373	Negative
655	D00972	D02101	Negative
656	D00980	D00994	Negative
657	D00980	D01204	Negative
658	D00983	D01204	Negative
659	D00983	D01294	Negative
660	D00983	D01689	Negative
661	D00983	D02194	Negative
662	D00983	D07132	Negative
663	D00994	D01302	Negative
664	D01002	D01637	Negative
665	D01002	D02095	Negative
666	D01002	D08205	Negative
667	D01002	D08249	Negative
668	D01066	D01112	Negative
669	D01066	D01453	Negative
670	D01066	D07992	Negative
671	D01112	D01302	Negative
672	D01112	D01689	Negative
673	D01112	D02095	Negative
674	D01112	D06412	Negative
675	D01203	D01355	Negative
676	D01204	D01302	Negative
677	D01204	D02086	Negative
678	D01204	D02216	Negative
679	D01204	D03860	Negative
680	D01294	D01984	Negative
681	D01294	D02060	Negative
682	D01294	D06236	Negative
683	D01294	D07132	Negative

684	D01302	D01453	Negative
685	D01302	D05277	Negative
686	D01302	D06236	Negative
687	D01302	D08131	Negative
688	D01340	D08205	Negative
689	D01355	D01453	Negative
690	D01402	D02487	Negative
691	D01450	D05205	Negative
692	D01453	D02060	Negative
693	D01637	D02082	Negative
694	D01637	D02227	Negative
695	D01689	D02194	Negative
696	D01689	D02483	Negative
697	D01689	D05209	Negative
698	D01689	D06645	Negative
699	D01708	D07132	Negative
700	D01708	D07992	Negative
701	D01708	D08996	Negative
702	D01966	D05632	Negative
703	D01984	D03820	Negative
704	D02076	D02086	Negative
705	D02082	D03048	Negative
706	D02082	D05209	Negative
707	D02095	D03860	Negative
708	D02095	D05649	Negative
709	D02101	D06645	Negative
710	D02149	D06412	Negative
711	D02216	D02367	Negative
712	D02272	D04104	Negative
713	D02272	D05632	Negative
714	D02367	D02487	Negative
715	D02367	D06645	Negative
716	D02367	D08131	Negative
717	D02388	D03182	Negative
718	D02483	D08127	Negative
719	D02487	D03182	Negative
720	D03182	D03820	Negative
721	D03182	D05277	Negative
722	D03182	D05649	Negative
723	D03182	D08205	Negative
724	D05277	D07992	Negative
725	D06236	D07992	Negative
726	D06645	D08205	Negative

