Annexure B

Applications of PCCA for finding class-specific features

EYE-RELATED SIDE EFFECTS

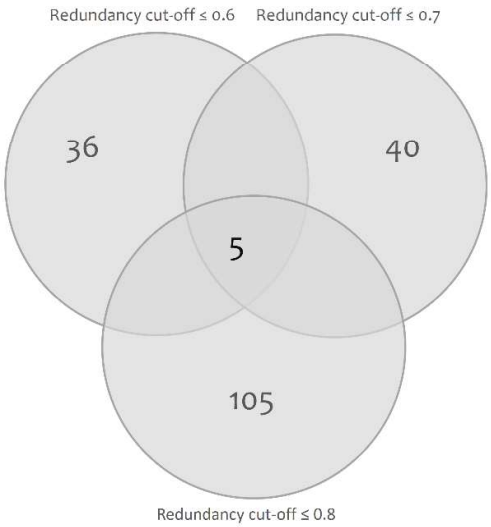

Figure B.1 : Identification of 2D features linked to Eye-related side effects class that were consistently found among the top sets at different cut-offs of redundancy using PCCA. Sets with Top 5 best performance were shortlisted for redundancy cut-off of ≤0.6 and ≤0.7, whereas those with Top25 best performances were used for the cut-off of ≤0.8. This yielded a total of 5 features consistently associated with Eye-related side effects (See Table 8.4).

Table B.1 : 'Eye' Class: Best sets (Top 5) of 2D Chemical features and their performance with redundancy cut-off of ≤0.6. For mapping the index listed in the table corresponding to 2D features, please refer to Table 3.2.

Feature set	Performance
80,39,183,249,2,89,207,234,200,166	0.6869
11,187,158,33,257,80,234,188,77,271	0.6869
257,45,155,123,219,190,250,178,270,169	0.6866
161,29,241,164,227,259,18,207,124,123	0.6866
160,89,123,192,98,32,181,227,4,241	0.6865

Table B.2 : 'Eye' Class: Best sets (Top 5) of 2D Chemical features and their performance with redundancy cut-off of ≤0.7. For mapping the index listed in the table corresponding to 2D features, please refer to Table 3.2.

Feature set	Performance
236,189,266,18,241,8,44,110,170,269	0.5744
172,3,267,121,268,204,164,1,65,159	0.5743
258,183,45,202,157,4,7,112,16,2	0.5734
1,15,2,92,159,194,205,195,131,165	0.5727
2,77,167,177,131,79,168,194,174,27	0.5727

Table B.3 : 'Eye' Class: Best sets (Top 25) of 2D Chemical features and their performance with redundancy cut-off of ≤0.8. For mapping the index listed in the table corresponding to 2D features, please refer to Table 3.2.

Feature set	Performance
252,208,265,175,99,104,51,124,193,266	0.6192
234,201,104,206,27,265,166,25,175,196	0.6192
210,258,240,125,109,102,255,269,160,173	0.6192
271,210,259,125,27,104,5,167,69,237	0.6192
45,133,265,53,139,183,9,14,28,104	0.6192
104,48,157,2,133,213,165,181,15,195	0.6192
27,54,194,48,104,269,161,253,245,181	0.6192
104,207,176,15,4,239,60,188,162,252	0.6192
181,4,104,251,162,183,28,156,125,225	0.6192
165,141,185,9,16,95,133,168,27,104	0.6192
207,266,235,196,171,104,91,54,258,133	0.6192
127,244,11,62,210,104,2,220,207,166	0.6192
196,171,48,69,27,53,250,164,162,240	0.6191
185,141,169,125,170,193,59,179,104,207	0.6191
69,8,99,145,104,182,237,59,197,127	0.6191
213,176,51,91,193,104,225,255,99,188	0.6191
167,30,157,252,213,171,104,179,19,15	0.6191
15,245,213,220,208,26,206,104,125,194	0.6191

177,99,207,15,270,19,90,104,268,228	0.6191
132,256,225,77,178,213,76,155,220,255	0.6191
266,53,26,104,124,2,182,5,159,148	0.6191
187,27,104,166,180,206,271,190,210,8	0.6191
242,240,125,102,253,196,45,176,109,255	0.6191
171,183,104,235,193,169,46,241,188,95	0.6191
235,225,104,208,23,132,54,265,258,159	0.6191

NOSE-RELATED SIDE EFFECTS

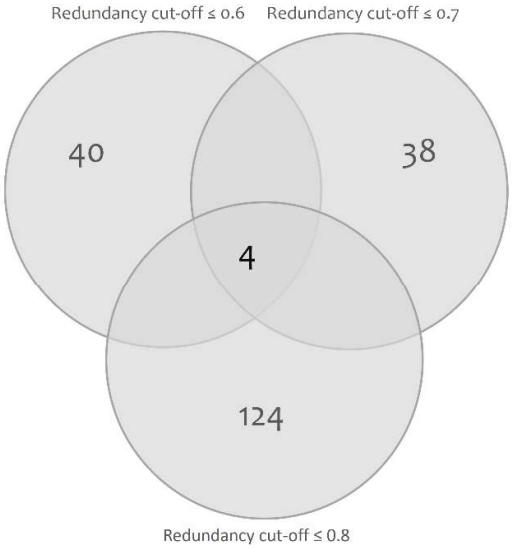

Figure B.2 : Identification of 2D features linked to Nose-related side effects class that were consistently found among the top sets at different cut-offs of redundancy using PCCA. Top 5 sets with best performance were shortlisted for redundancy cut-off of ≤0.6 and ≤0.7, whereas Top25 sets were used for the cut-off of ≤0.8. This yielded a total of 4 features consistently associated with Nose-related side effects (See Table 8.5).

Table B.4 : 'Nose' Class: Best sets (Top 5) of 2D Chemical features and their performance with redundancy cut-off of ≤0.6. For mapping the index listed in the table corresponding to 2D features, please refer to Table 3.2.

Feature set	**Performance**
179,137,255,154,194,26,79,219,186,44	0.6529
2,167,24,44,89,124,22,129,193,255	0.6522
193,111,47,44,14,110,266,112,15,269	0.6502
237,79,86,44,29,5,168,193,254,269	0.6502
156,258,254,264,20,44,269,224,194,87	0.6502

Table B.5 : 'Nose' Class: Best sets (Top 5) of 2D Chemical features and their performance with redundancy cut-off of ≤0.7. For mapping the index listed in the table corresponding to 2D features, please refer to Table 3.2.

Feature set	Performance
14,31,258,238,86,45,161,50,194,13	0.6115
18,184,257,32,61,266,174,240,166,31	0.6115
53,182,138,209,205,259,183,252,31,195	0.6110
89,175,98,31,234,174,188,203,157,266	0.6110
183,192,4,241,103,180,31,203,144,77	0.6110

Table B.6 : 'Nose' Class: Best sets (Top 25) of 2D Chemical features and their performance with redundancy cut-off of ≤0.8. For mapping the index listed in the table corresponding to 2D features, please refer to Table 3.2.

Feature set	Performance
105,242,166,68,103,147,194,195,265,251	0.5870
182,10,7,52,132,262,204,179,15,75	0.5868
187,156,251,3,262,29,1,123,169,219	0.5868
168,172,26,241,218,20,237,156,240,174	0.5867
174,124,204,27,155,219,179,140,197,84	0.5866
75,99,108,181,98,86,206,186,10,218	0.5866
121,53,108,267,254,50,259,80,184,174	0.5866
196,179,131,266,207,193,4,22,227,124	0.5866
10,168,112,11,93,192,144,1,80,50	0.5866
266,262,219,243,192,10,168,53,82,58	0.5866
47,68,243,104,27,5,112,205,254,268	0.5866
184,10,1,131,7,94,16,11,170,224	0.5866
196,236,124,45,174,254,24,22,92,265	0.5866
171,44,97,197,218,26,14,195,187,138	0.5866
208,137,10,83,183,77,104,197,131,87	0.5866
249,45,32,22,68,25,207,209,97,163	0.5866
178,44,186,90,269,89,24,22,212,93	0.5866
238,5,101,111,14,174,81,129,2,4	0.5866

132,188,265,224,243,266,154,77,244,15	0.5866
18,208,44,132,121,265,68,75,202,269	0.5866
132,90,86,207,18,205,16,105,154,235	0.5866
31,99,233,47,269,10,243,18,202,158	0.5866
101,1,244,45,24,195,20,241,203,172	0.5866
235,170,95,15,192,1,242,97,25,112	0.5866
13,267,18,259,94,239,89,53,129,58	0.5866

ABDOMEN-RELATED SIDE EFFECTS

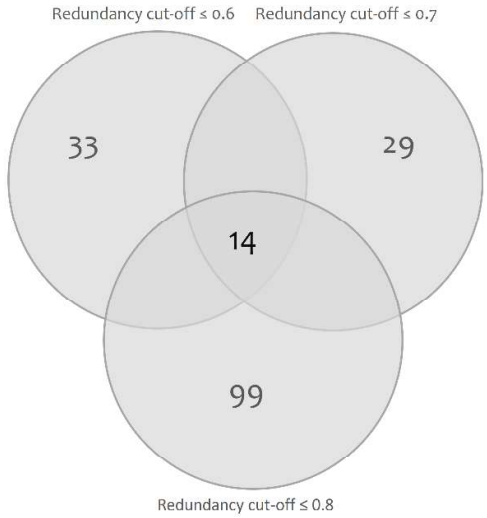

Figure B.3 : Identification of 2D features linked to Abdomen-related side effects class that were consistently found among the top sets at different cut-offs of redundancy using PCCA. Top 5 sets with best performance were shortlisted for redundancy cut-off of ≤0.6 and ≤0.7, whereas Top25 sets were used for the cut-off of ≤0.8. This yielded a total of 14 features consistently associated with Abdomen-related side effects (See Table 8.6).

Table B.7 : 'Abdomen' Class: Best sets (Top 5) of 2D Chemical features and their performance with redundancy cut-off of ≤0.6. For mapping the index listed in the table corresponding to 2D features, please refer to Table 3.2.

Feature set	**Performance**
240,38,167,253,269,217,128,237,100,49	0.6098
52,98,41,159,207,81,193,177,204,166	0.6098
194,223,185,266,269,1,232,75,38,188	0.6075
2,243,18,269,175,26,171,199,195,67	0.6075
3,201,88,183,64,248,24,265,93,261	0.6072

Table B.8 : 'Abdomen' Class: Best sets (Top 5) of 2D Chemical features and their performance with redundancy cut-off of ≤0.7. For mapping the index listed in the table corresponding to 2D features, please refer to Table 3.2.

Feature set	Performance
137,50,3,8,33,7,242,97,1,99	0.6171
147,218,8,137,68,200,186,193,171,266	0.6171
235,224,31,42,3,10,179,257,265,270	0.6171
266,76,31,39,254,188,32,205,118,208	0.6171
106,268,163,82,235,186,172,233,196,61	0.6166

Table B.9 : 'Abdomen' Class: Best sets (Top 25) of 2D Chemical features and their performance with redundancy cut-off of ≤0.9. For mapping the index listed in the table corresponding to 2D features, please refer to Table 3.2.

Feature set	Performance
166,3,13,212,184,15,203,75,25,132	0.6123
25,76,255,178,269,249,24,233,161,8	0.6122
53,181,126,20,173,197,203,206,251,238	0.6122
44,195,202,22,268,1,209,155,25,75	0.6122
234,3,45,25,138,164,31,258,124,158	0.6122
25,264,178,266,76,169,196,204,265,182	0.6122
183,8,25,178,155,180,269,99,179,76	0.6122
131,197,241,266,123,170,181,25,236,202	0.6122
61,187,196,241,123,233,108,7,25,76	0.6122
20,25,239,212,182,27,176,163,183,47	0.6122
190,44,25,249,58,267,131,13,77,20	0.6122
44,123,218,239,98,25,61,77,251,200	0.6122
258,16,25,154,249,239,255,10,212,50	0.6122
99,169,25,108,265,101,227,269,270,182	0.6122
241,268,238,93,44,172,25,68,239,158	0.6122
15,1,25,271,218,268,191,234,184,58	0.6122
176,197,25,101,178,258,2,265,31,269	0.6122

167,44,206,176,47,25,4,171,243,268	0.6122
154,27,93,196,25,26,200,123,31,186	0.6122
3,158,44,258,84,126,252,207,193,189	0.6122
270,236,61,53,204,25,205,173,29,271	0.6122
25,179,269,190,98,244,108,165,15,164	0.6122
236,204,25,31,7,188,257,205,242,10	0.6122
25,45,192,200,118,61,166,169,78,188	0.6122
1,196,202,118,3,124,93,25,241,18	0.6122

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