

Appendix I: Reasons for comparison of drugs not working

a) Cardiotoxic drugs dataset

Drug ID	Drug	ACD/I-Lab's Percepta (Probability of affecting Cardiovascular)	OpenTox (Cramer Extended)	HyQue-Cardiotoxicity
DB00016	epoetin alfa	NO SMILES	NO SMILES	0
DB05773	ado-trastuzumab emtansine	NO SMILES	NO SMILES	0.00
DB00734	risperidone	0.98	High (class III)	WON'T RUN
DB00433	prochlorperazine edisylate	0.73	High (class III)	WON'T RUN
DB01224	quetiapine fumarate	0.61	High (class III)	WON'T RUN
DB00482	celecoxib	0.83	High (class III)	WON'T RUN
DB00531	cyclophosphamide	0.08	High (class III)	WON'T RUN

b) Non-cardiotoxic drugs dataset

Drug ID	Drug	ACD/I-Lab's Percepta (Probability of affecting Cardiovascular)	OpenTox (Cramer Extended)	HyQue-Cardiotoxicity
DB00761	potassium chloride	ERROR	High (class III)	WON'T RUN
DB00281	lidocaine	0.63	High (class III)	WON'T RUN
DB00094	urofollitropin	NO SMILES	NO SMILES	0.00
DB00046	insulin Lispro	NO SMILES	NO SMILES	0.00
DB00040	glucagon	NO SMILES	NO SMILES	0.00