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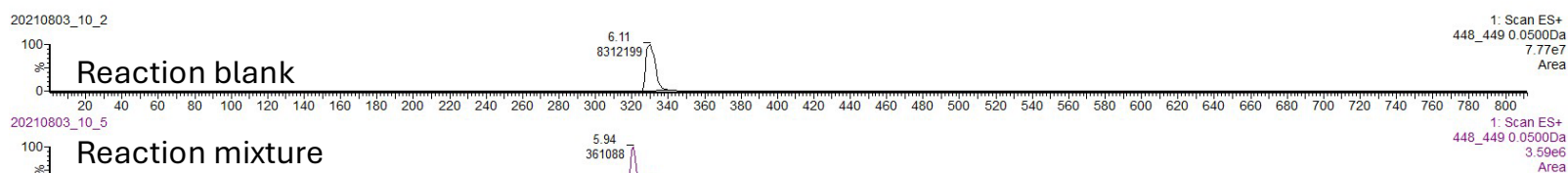
Model APIs

Aripiprazole LC-MS results

pH 2.7 LC-MS results of Aripiprazole

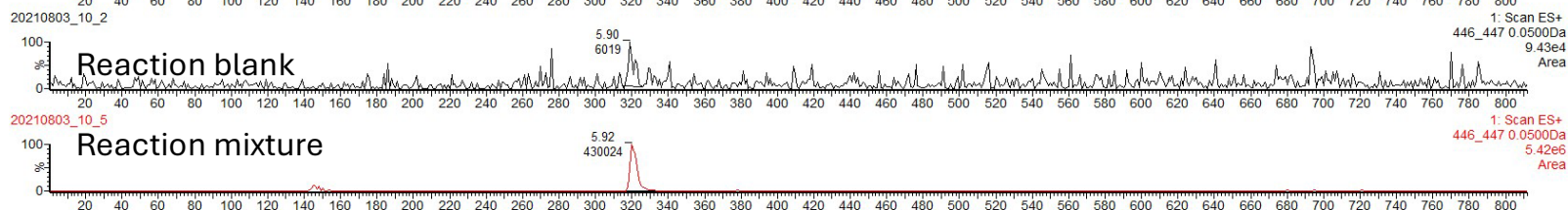
Drug

Aripiprazole
m/z: 448.1559



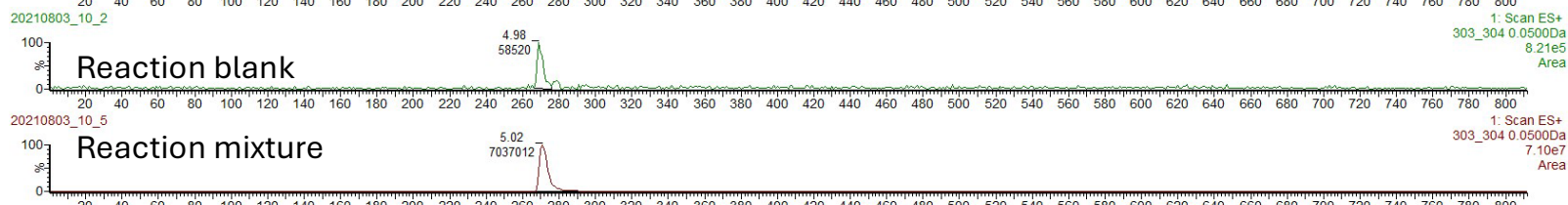
Metabolite

Dehydroaripiprazole
m/z: 446.1402



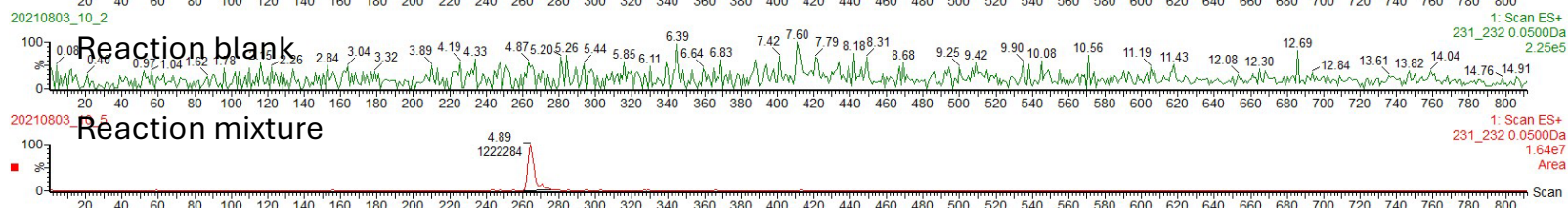
Metabolite

4-(2,3-Dichlorophenyl)-1-piperazinebutanol
m/z: 303.1031



Metabolite

2,3-Dichlorophenyl-piperazine
m/z: 231.0456

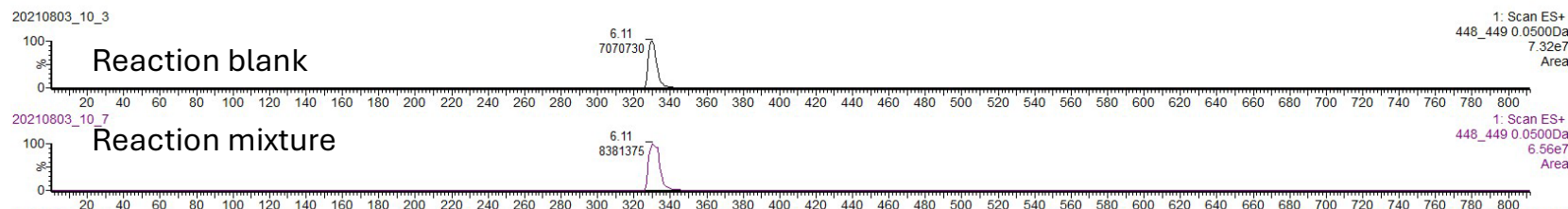


Supplementary Figure S1: Aripiprazole's reaction blanks and reaction mixture's metabolic profile at pH 2.7 (extracted ion chromatograms)

pH 4.5 LC-MS results of Aripiprazole

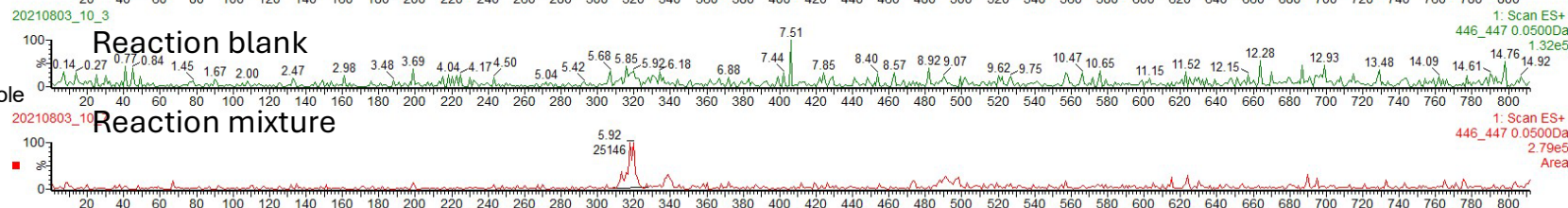
Drug

Aripiprazole
m/z: 448.1559



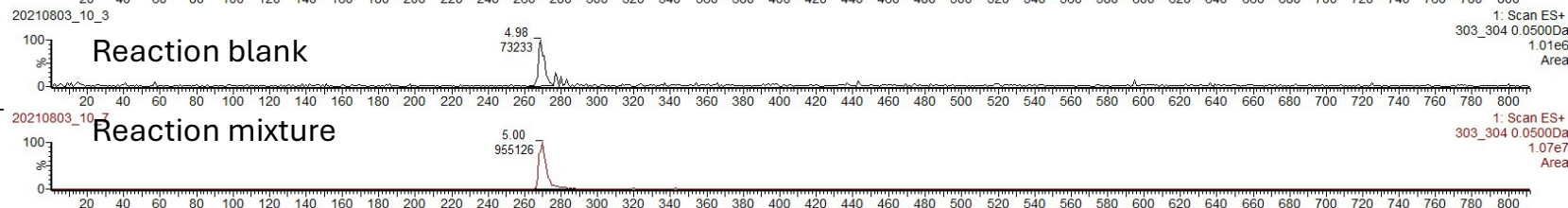
Metabolite

Dehydroariprazole
m/z: 446.1402



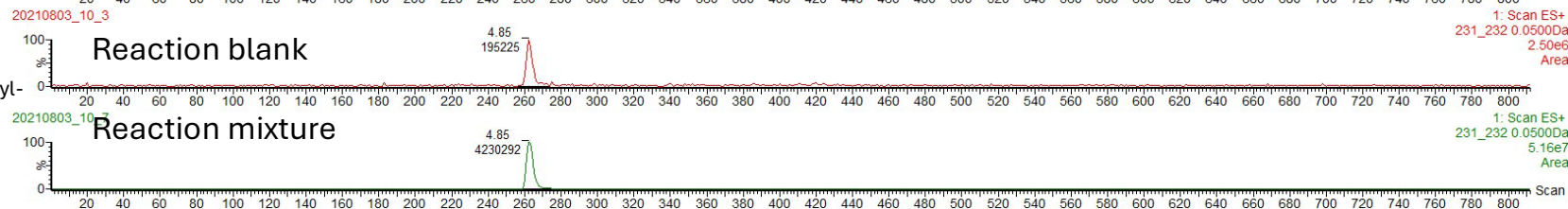
Metabolite

4-(2,3-
Dichlorophenyl)-1-
piperazinebutanol
m/z: 303.1031



Metabolite

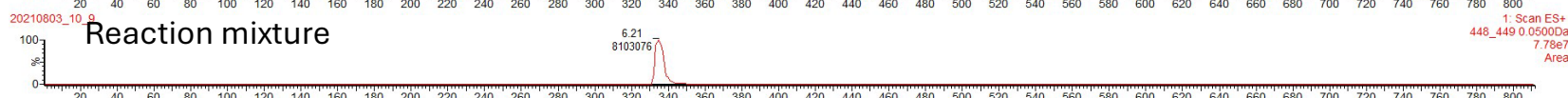
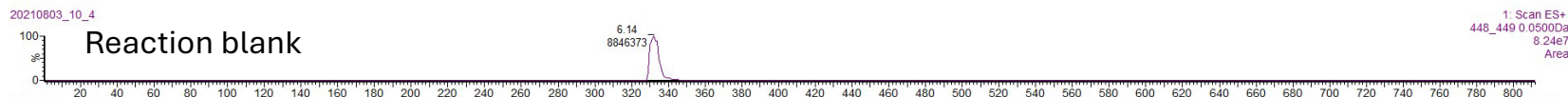
2,3-Dichlorophenyl-
piperazine
m/z: 231.0456



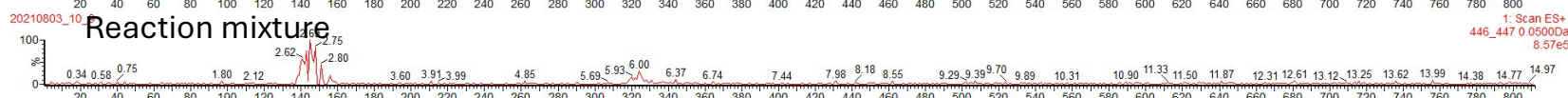
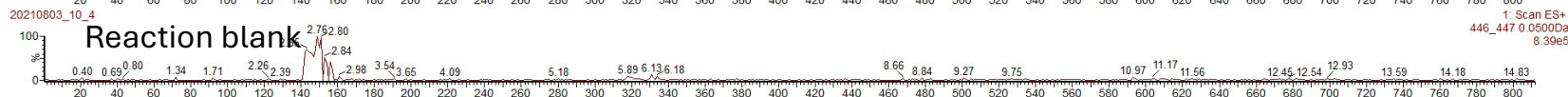
Supplementary Figure S2: Aripiprazole's reaction blank's and reaction mixture's metabolic profile at pH 4.5 (extracted ion chromatograms)

pH 7.4 LC-MS results of Aripiprazole

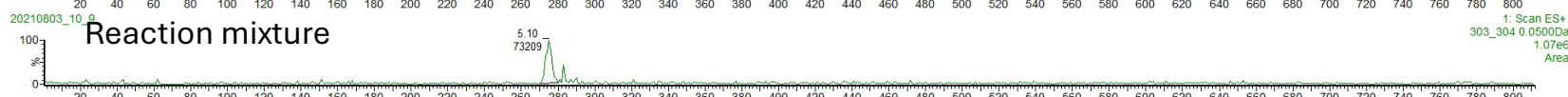
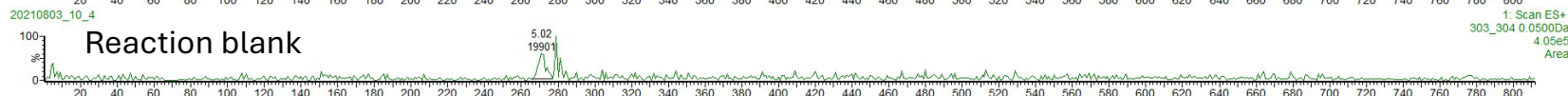
Drug
Aripiprazole
m/z: 448.1559



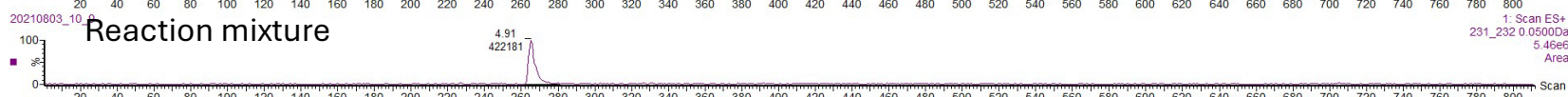
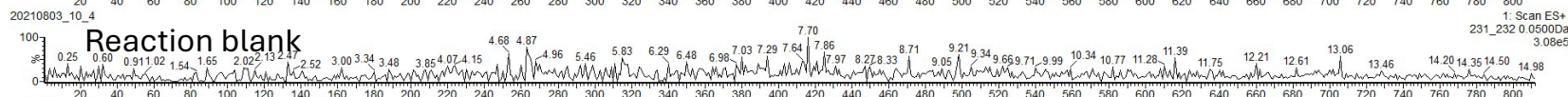
Metabolite
Dehydroariprazole
m/z: 446.1402



Metabolite
4-(2,3-Dichlorophenyl)-1-piperazinebutanol
m/z: 303.1031

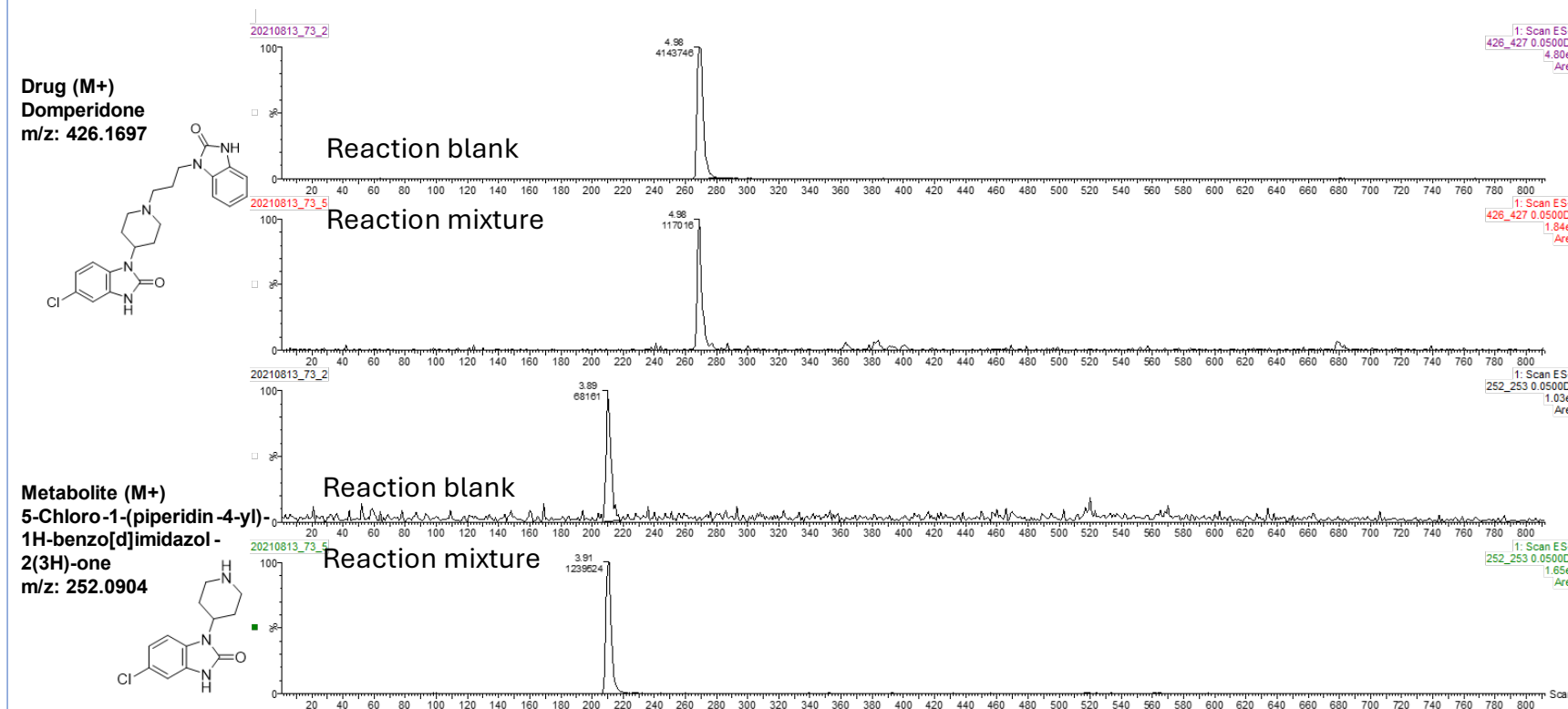


Metabolite
2,3-Dichlorophenyl-piperazine
m/z: 231.0456



Supplementary Figure S3: Aripiprazole's reaction blank's and reaction mixture's metabolic profile at pH 7.4 (extracted ion chromatograms)

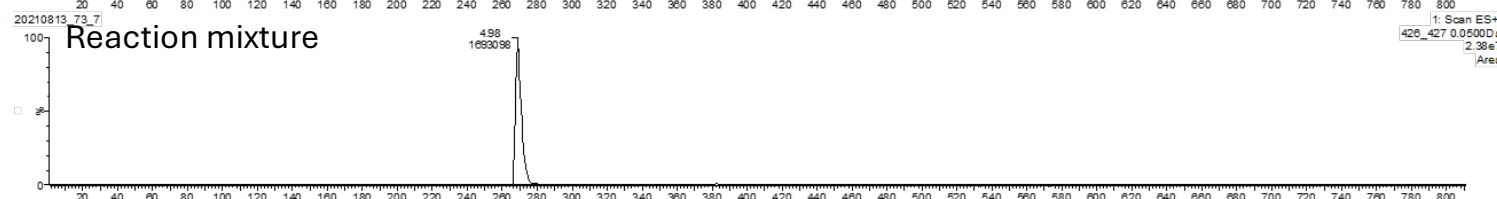
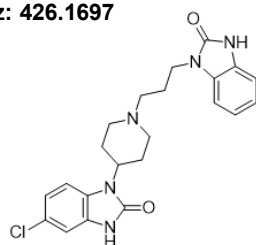
pH 2.7 LC-MS results of Domperidone



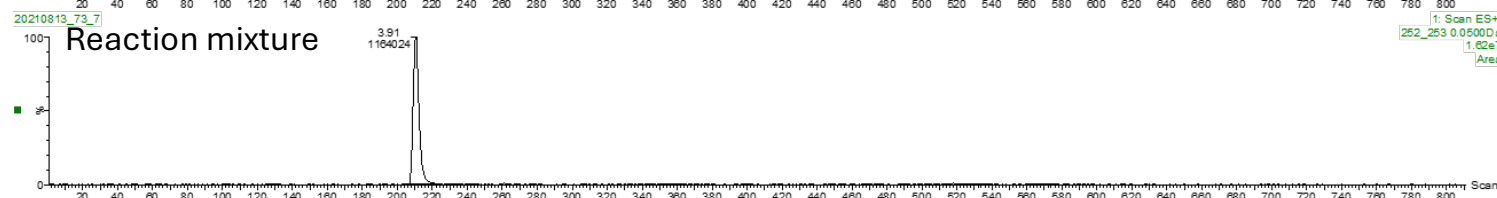
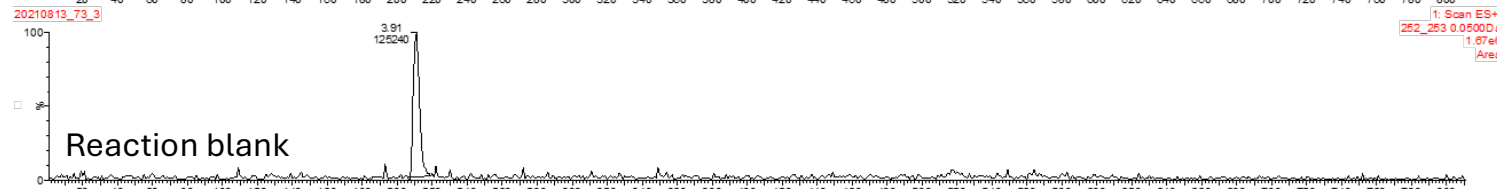
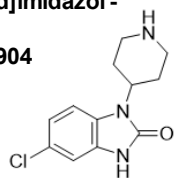
Supplementary Figure S4: Domperidone's reaction blank's and reaction mixture's metabolic profile at pH 2.7 (extracted ion chromatograms)

pH 4.5 LC-MS results of Domperidone

Drug (M+)
Domperidone
m/z: 426.1697



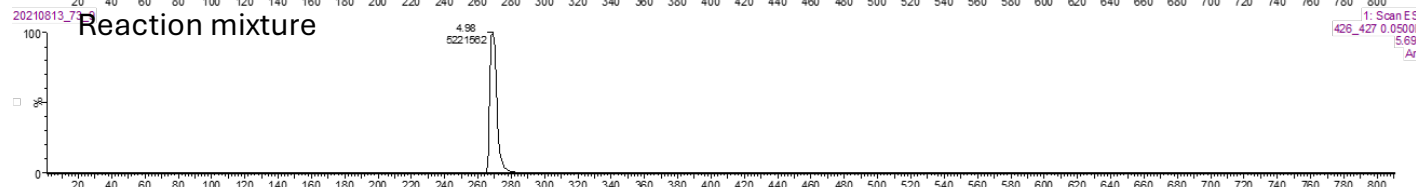
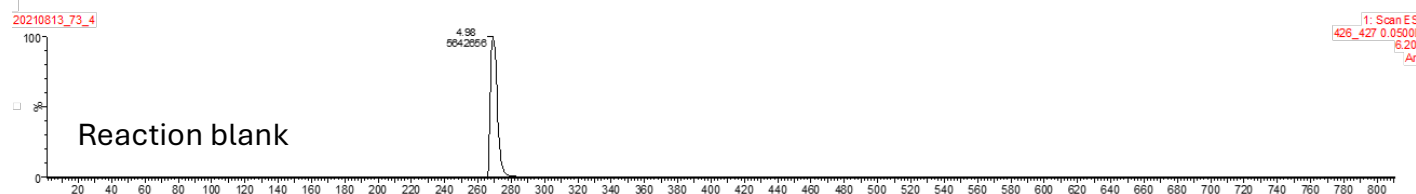
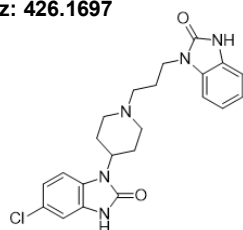
Metabolite (M+)
5-Chloro-1-(piperidin-4-yl)-
1H-benzo[d]imidazol-
2(3H)-one
m/z: 252.0904



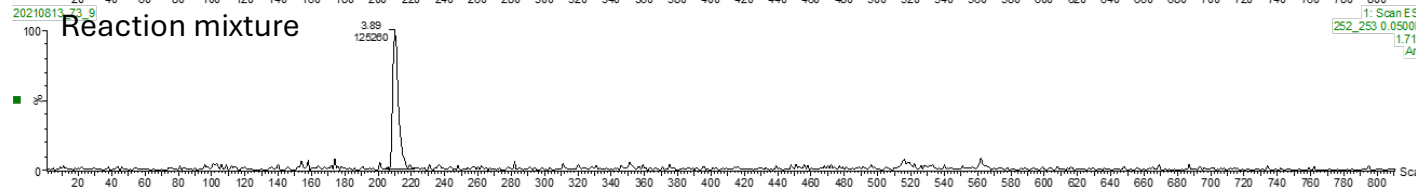
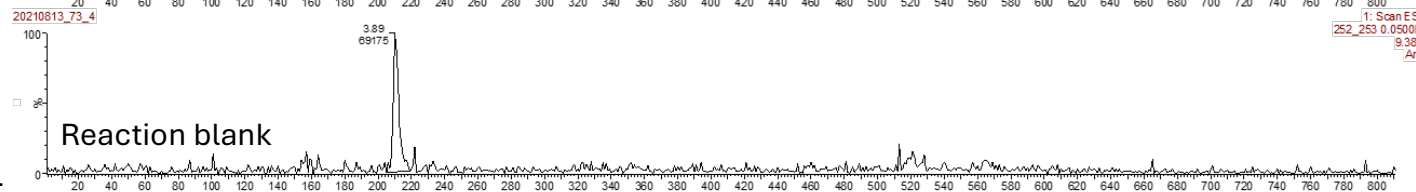
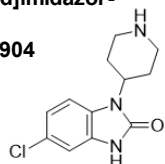
Supplementary Figure S5: Domperidone's reaction blank's and reaction mixture's metabolic profile at pH 4.5 (extracted ion chromatograms)

pH 7.4 LC-MS results of Domperidone

Drug (M+)
Domperidone
m/z: 426.1697

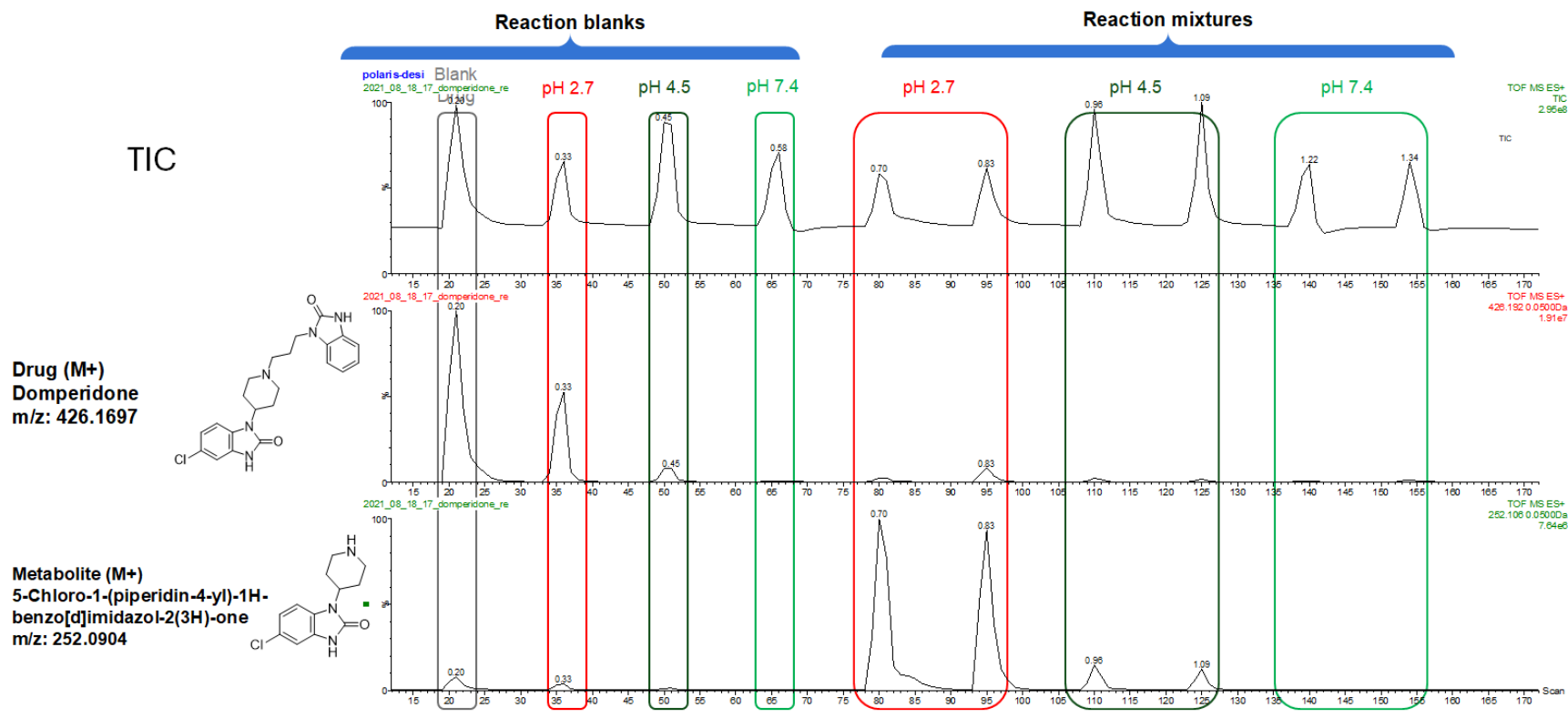


Metabolite (M+)
5-Chloro-1-(piperidin-4-yl)-
1H-benzo[d]imidazol-
2(3H)-one
m/z: 252.0904



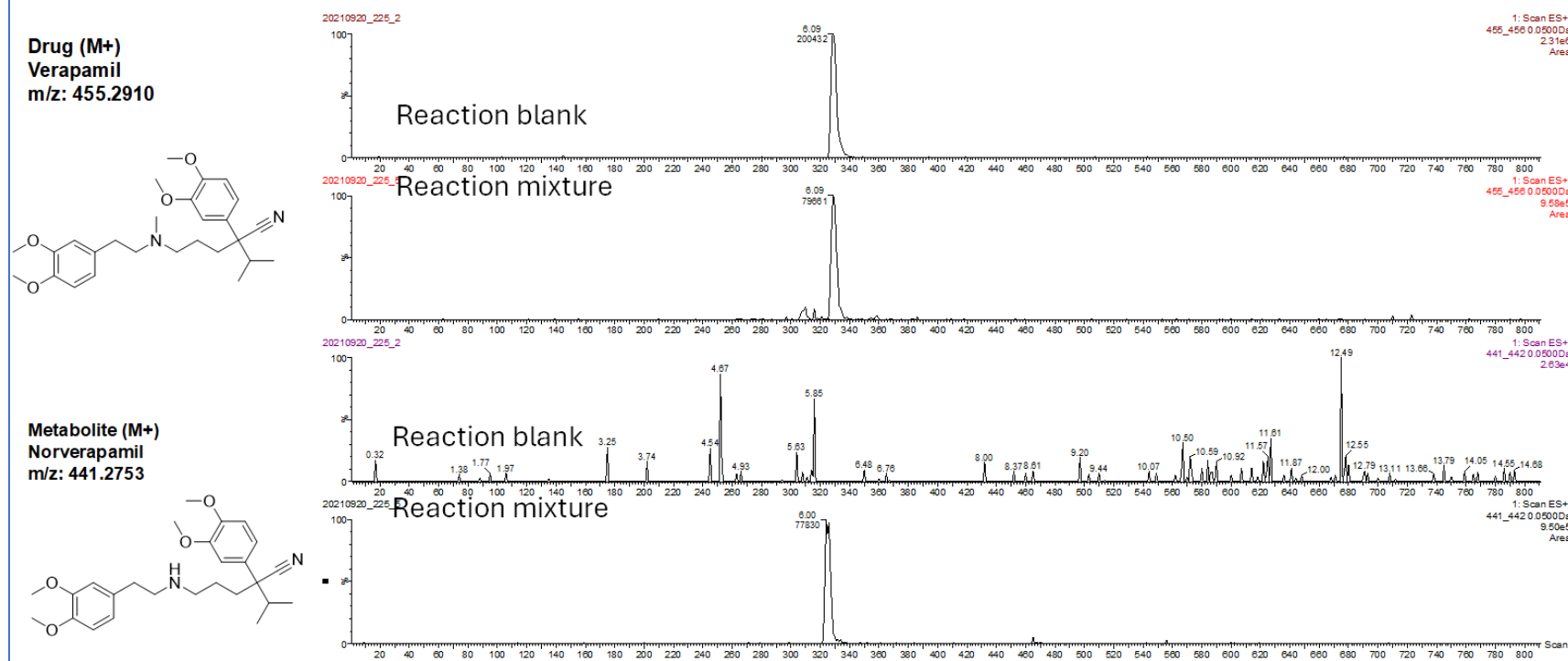
Supplementary Figure S6: Domperidone's reaction blank's and reaction mixture's metabolic profile at pH 7.4 (extracted ion chromatograms)

LA-REIMS Sample Chromatogram - Domperidone



Supplementary Figure S7: Extracted LA-REIMS chromatograms of Domperidone

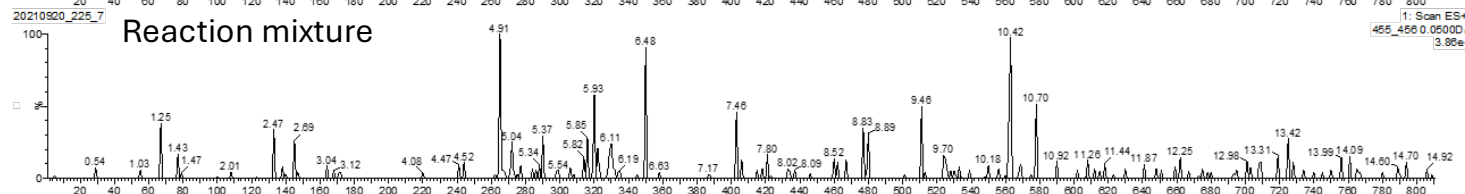
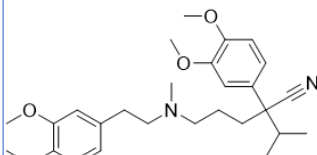
pH 2.7 LC-MS results of Verapamil



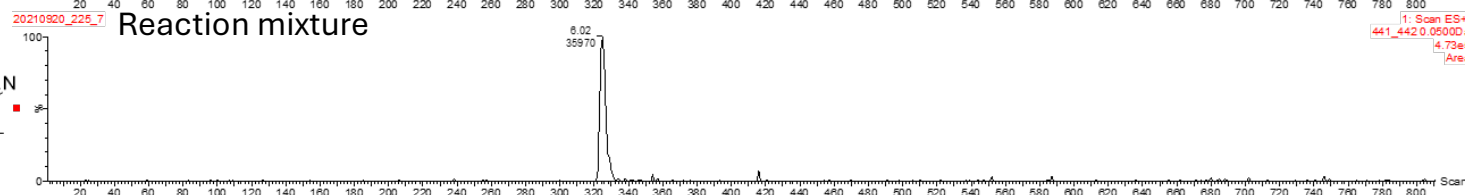
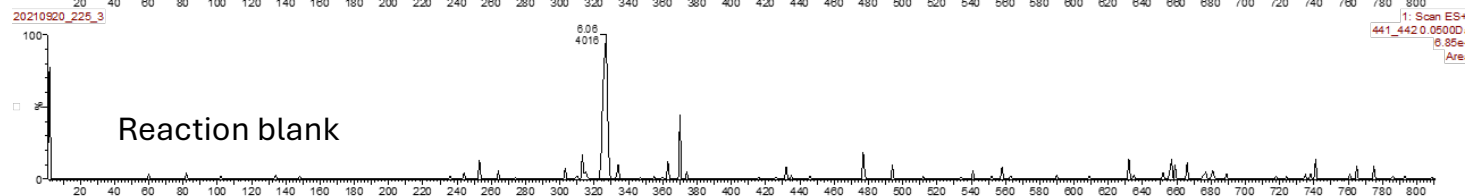
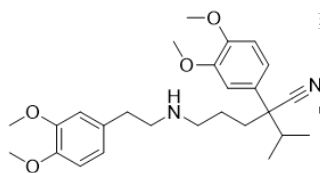
Supplementary Figure S8: Verapamil's reaction blank's and reaction mixture's metabolic profile at pH 2.7 (extracted ion chromatograms)

pH 4.5 LC-MS results of Verapamil

Drug (M+)
Verapamil
m/z: 455.2910



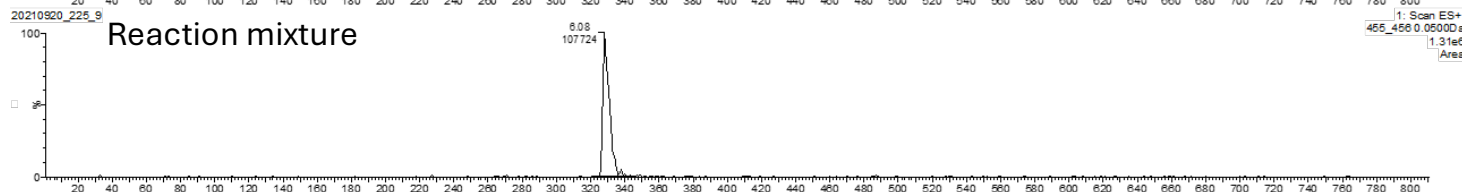
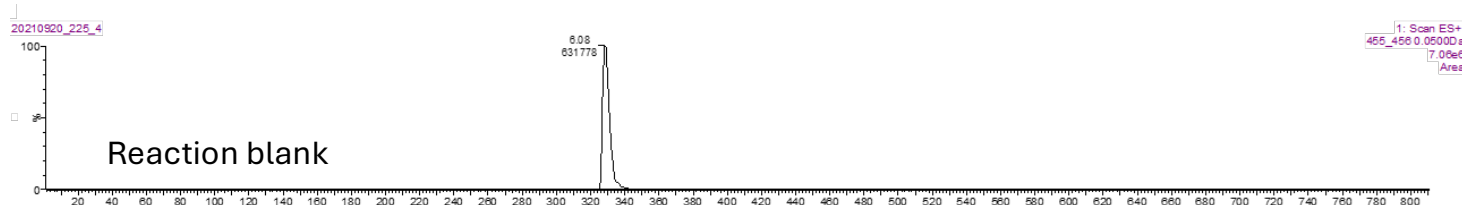
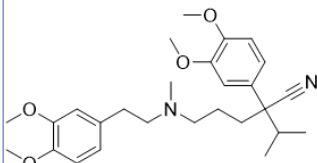
Metabolite (M+)
Norverapamil
m/z: 441.2753



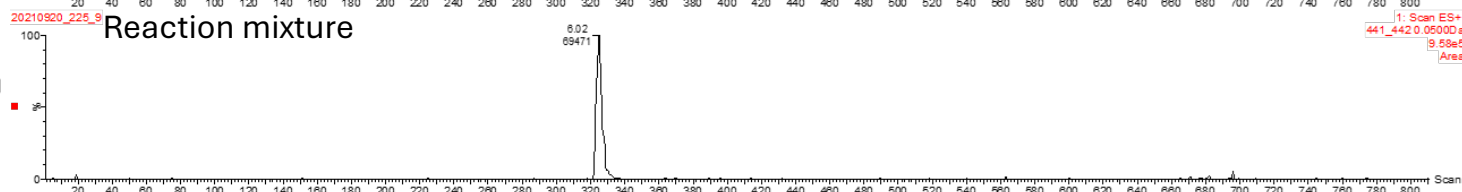
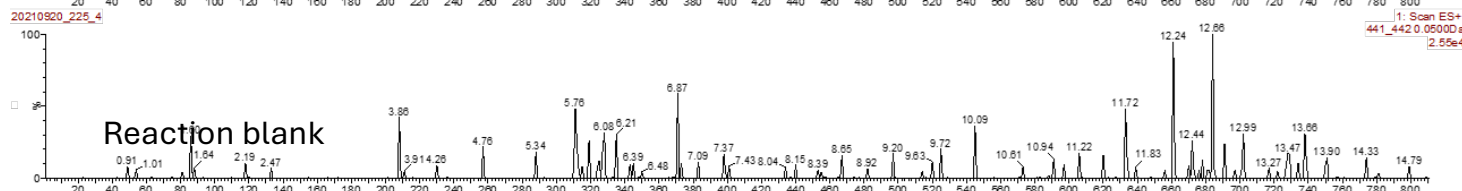
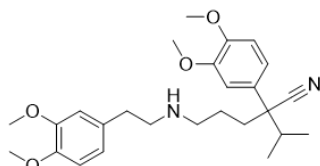
Supplementary Figure S9: Verapamil's reaction blank's and reaction mixture's metabolic profile at pH 4.5 (extracted ion chromatograms)

pH 7.4 LC-MS results of Verapamil

Drug (M+)
Verapamil
m/z: 455.2910

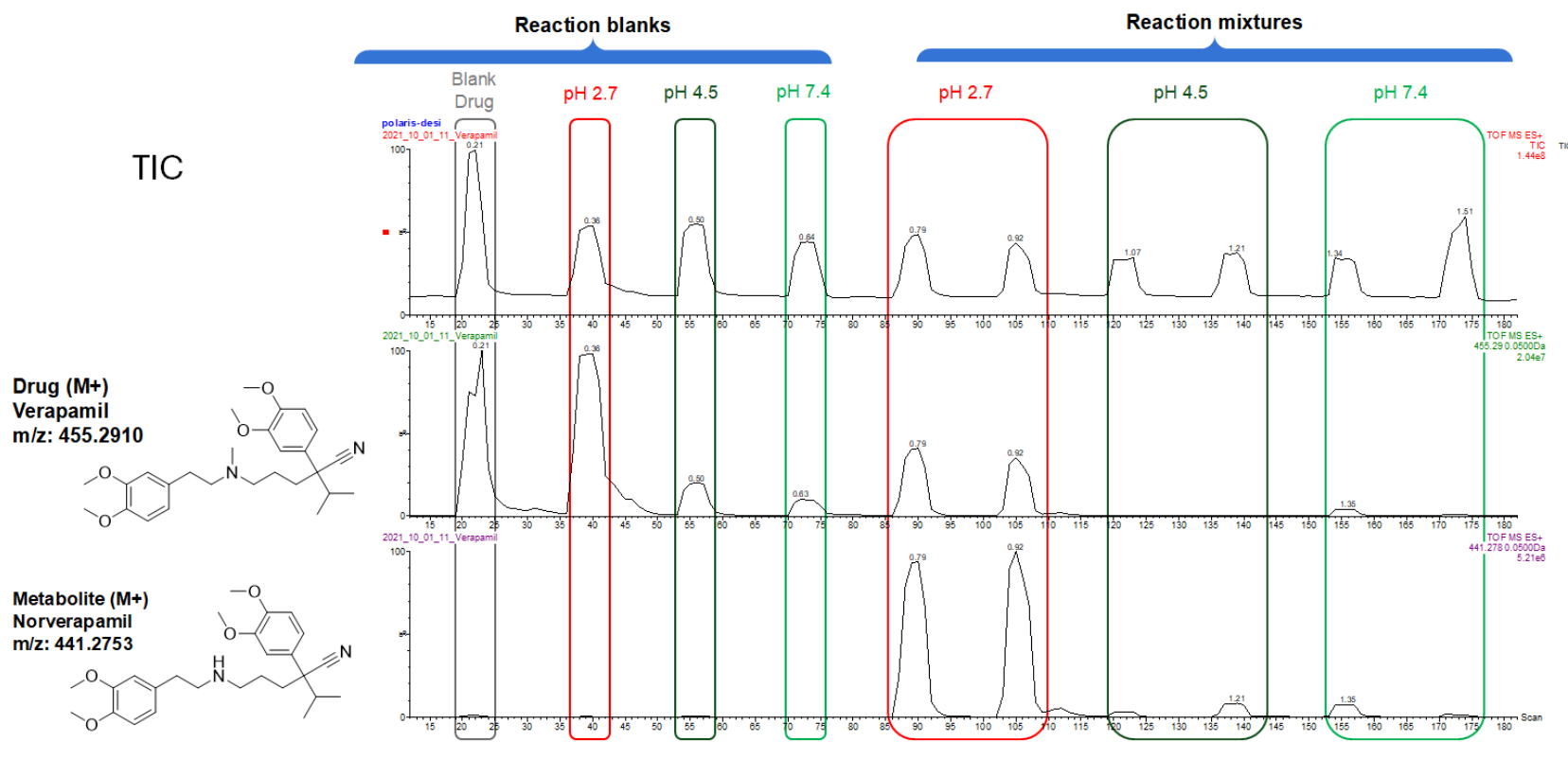


Metabolite (M+)
Norverapamil
m/z: 441.2753



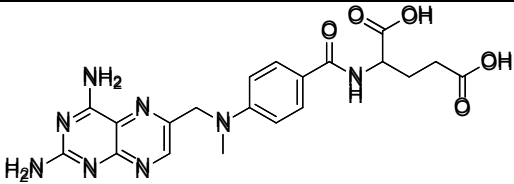
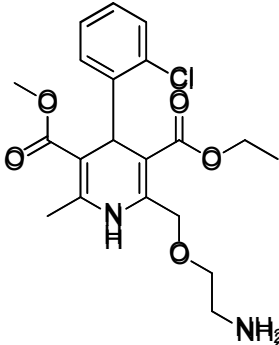
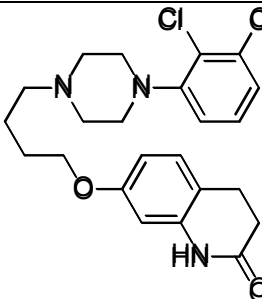
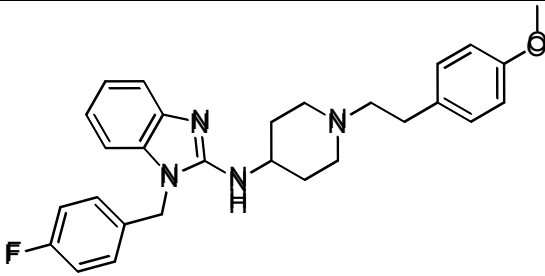
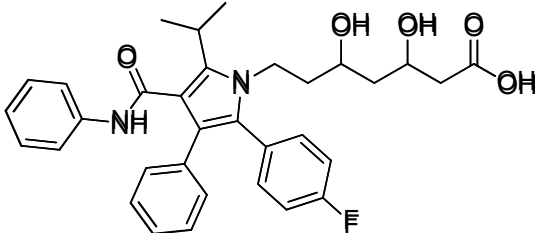
Supplementary Figure S10: Verapamil's reaction blank's and reaction mixture's metabolic profile at pH 7.4 (extracted ion chromatograms)

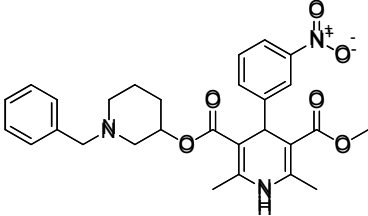
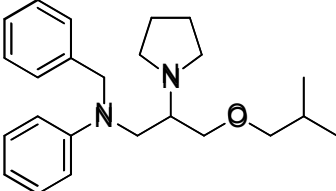
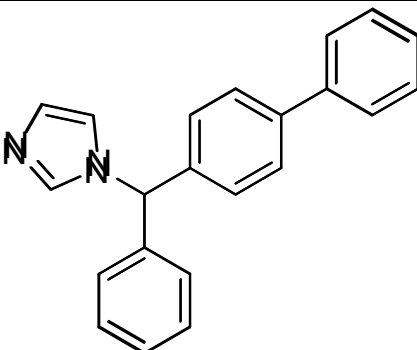
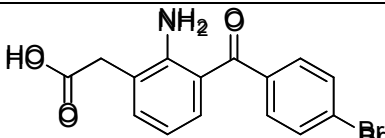
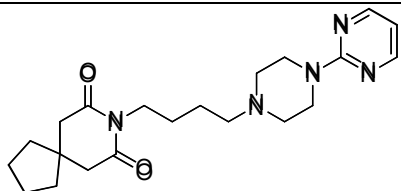
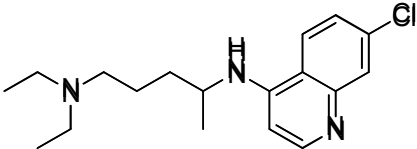
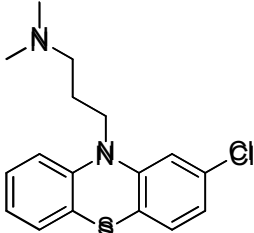
LA-REIMS Sample Chromatogram - Verapamil

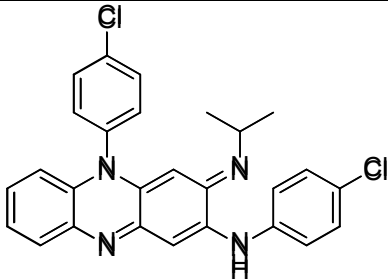
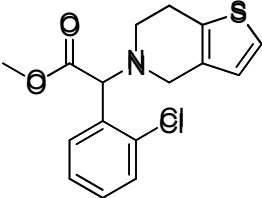
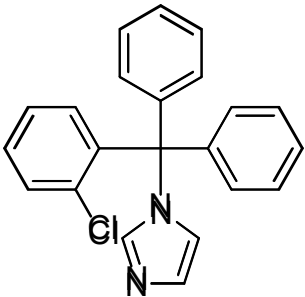
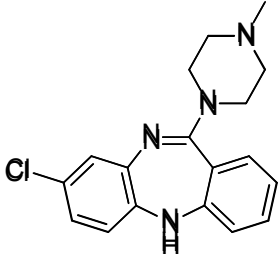
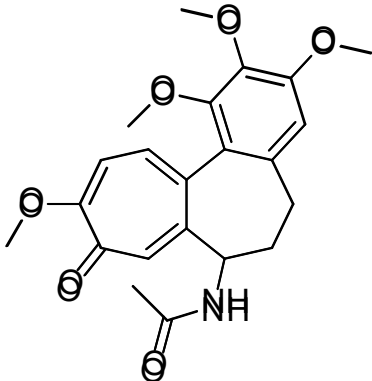
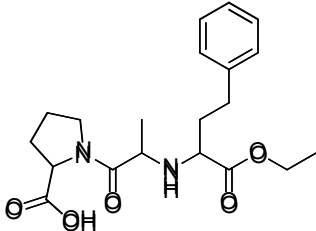


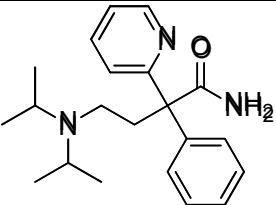
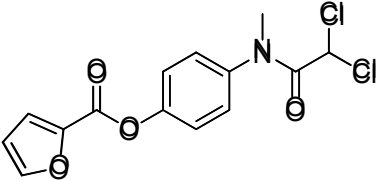
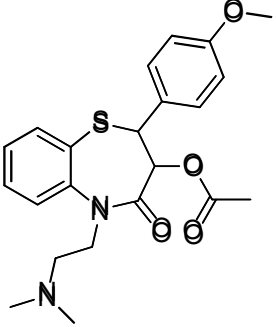
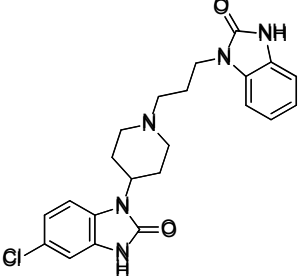
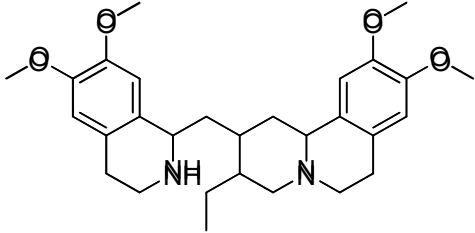
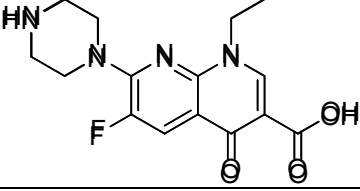
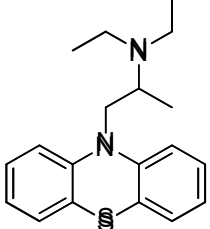
Supplementary Figure S11: Extracted LA-REIMS chromatograms of Verapamil

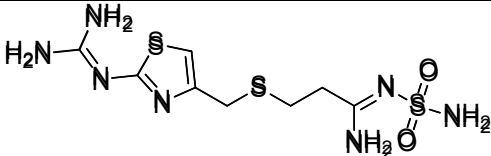
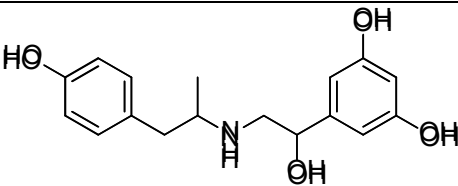
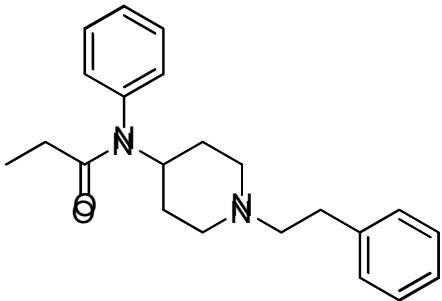
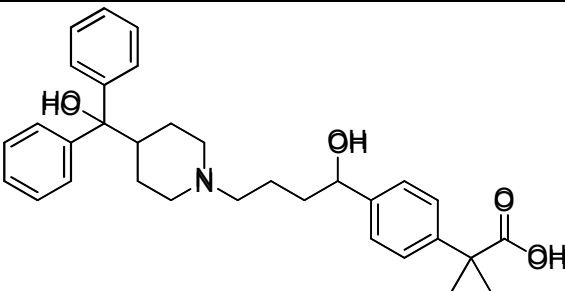
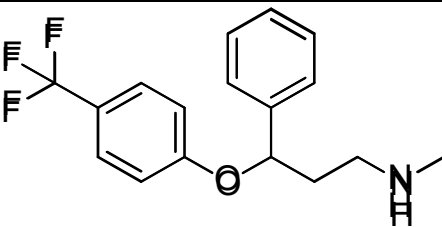
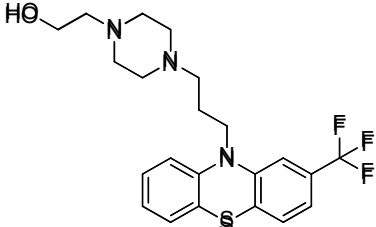
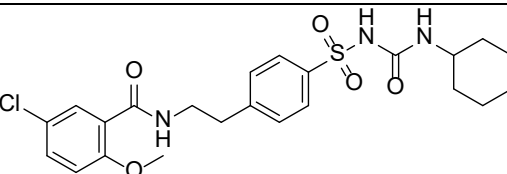
Used APIs and measured conversion rates on pH 4.5

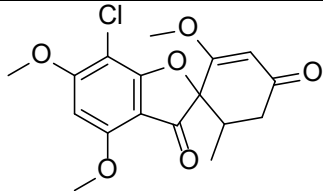
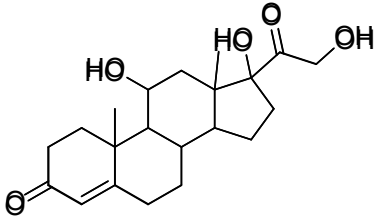
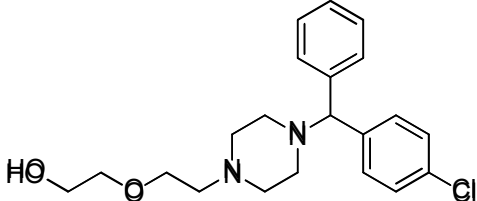
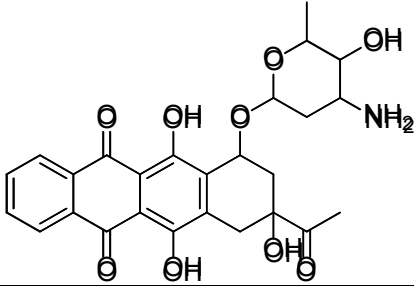
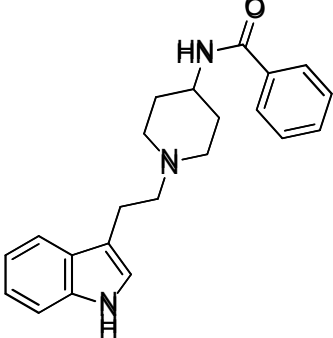
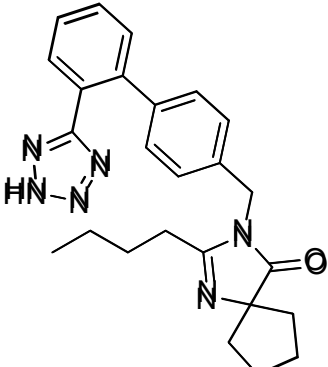
API name	Structures	Measured conversion rates on pH4.5(%)		
		LC-UV	LC-MS	LA-REIMS
Amodiaquine		100.00	100.00	99.41
Amlodipine		100.00	99.92	100.00
Aripiprazole		17.20	0.00	40.25
Astemizole		100.00	100.00	99.88
Atorvastatin		100.00	95.82	83.23

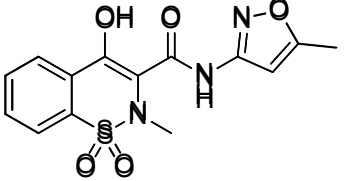
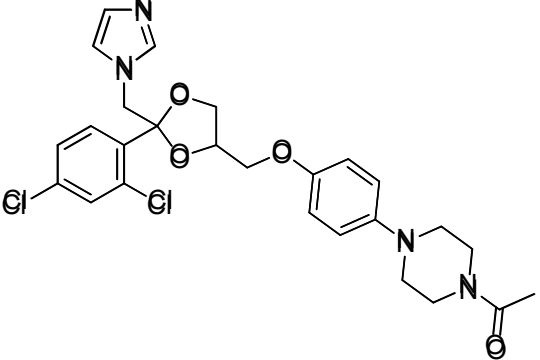
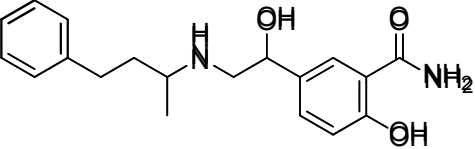
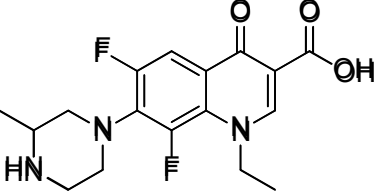
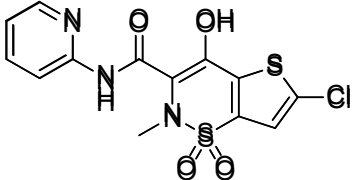
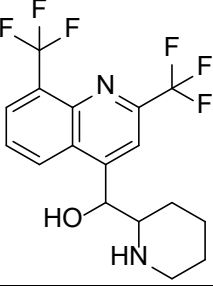
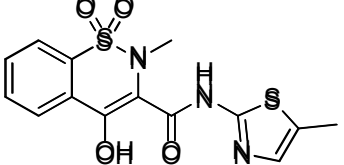
Benidipin		100.00	98.62	98.04
Bepiridil		100.00	95.82	99.13
Bifonazole		0.00	0.00	0.00
Bromfenac		100.00	100.00	99.87
Buspirone		67.69	38.12	68.04
Chloroquine		96.55	92.60	95.91
Chlorpromazine		71.18	57.02	79.22

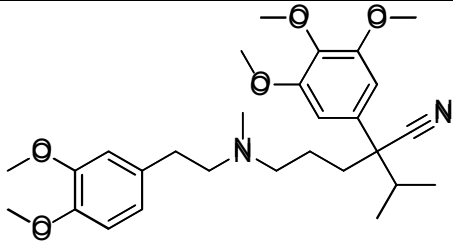
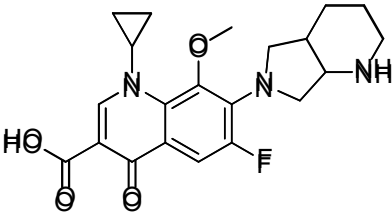
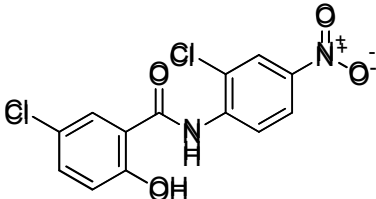
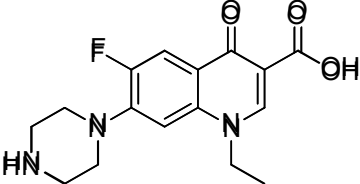
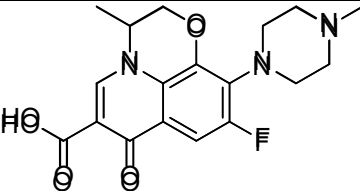
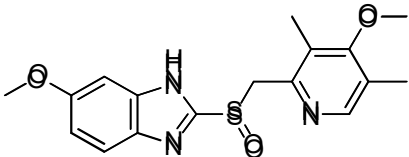
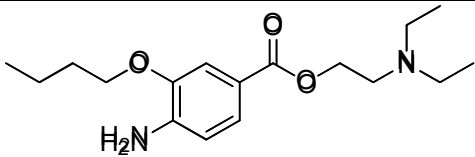
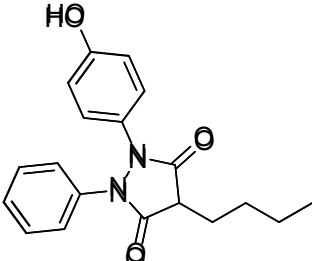
Chlofazimine		88.04	98.07	73.41
Clopidogrel		23.34	21.15	24.04
Clotrimazole		0.00	6.87	0.00
Clozapine		92.88	80.45	89.72
Colchicine		0.00	10.13	14.73
Enalapril		0.00	4.17	6.00

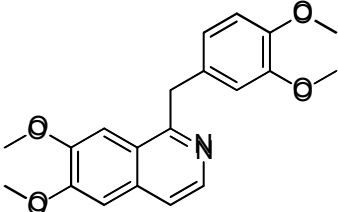
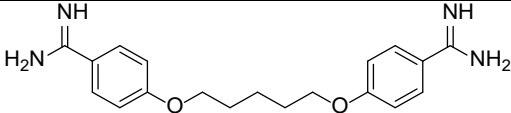
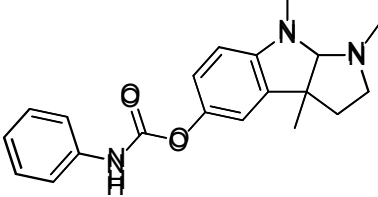
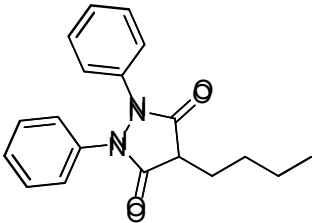
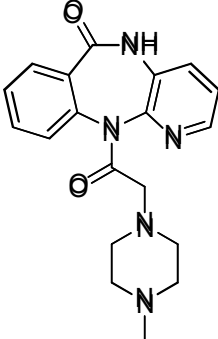
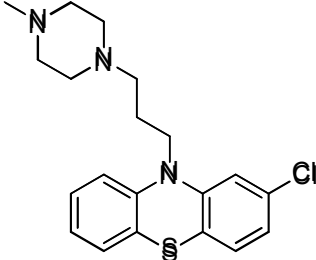
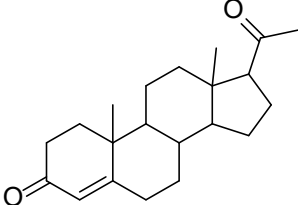
Disopyramide		4.81	13.75	11.82
Diloxandine		0.00	0.00	0.00
Dilthiazem		57.49	47.30	70.35
Domperidone		90.46	80.64	75.33
Emetan / emetine		76.17	94.64	82.65
Enoxacin		42.39	41.36	58.72
Ethopropazine		100.00	100.00	92.84

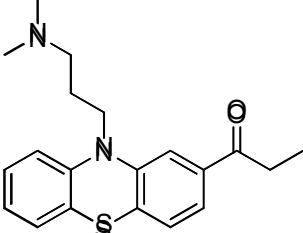
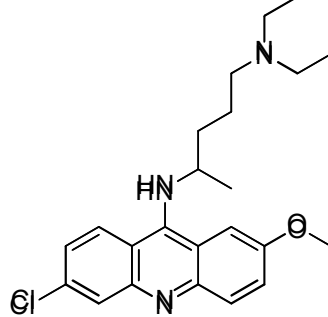
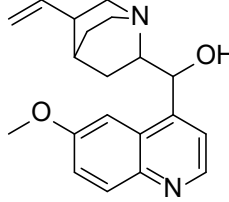
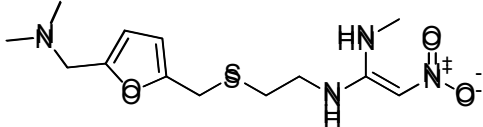
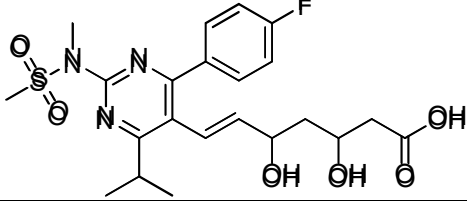
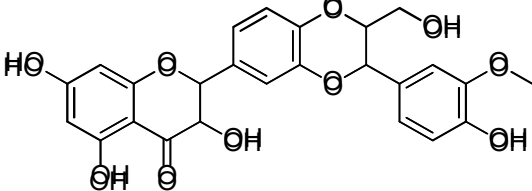
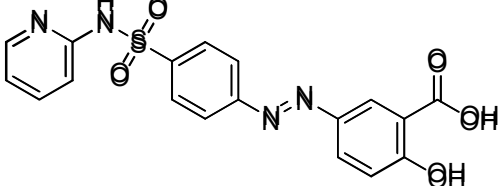
Famotidine		100.00	100.00	91.92
Fenoterol		100.00	100.00	100.00
Fentanyl		0.00	8.53	21.43
Fexofenadine		9.86	3.50	18.83
Fluoxetine		0.00	0.00	0.00
Fluphenazine		100.00	99.65	89.93
Glybenclamide		46.14	40.03	61.14

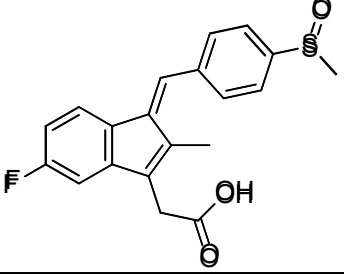
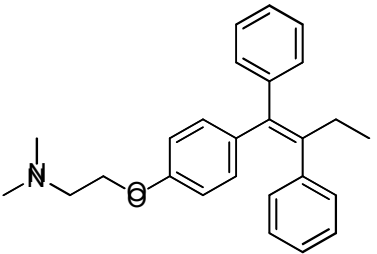
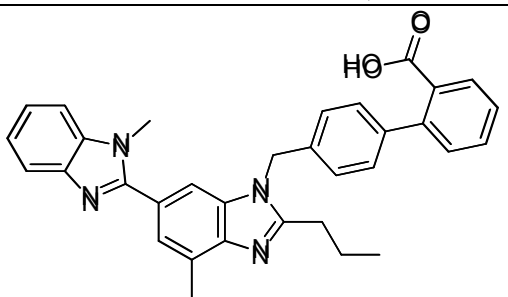
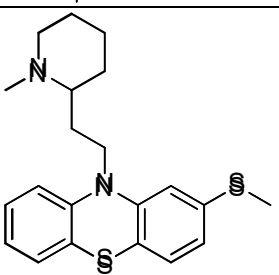
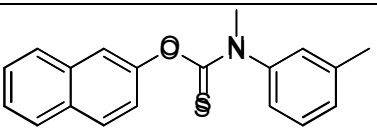
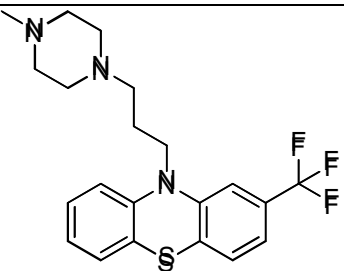
Griseofulvine		0.00	0.00	0.00
Hydrocortisone		26.59	24.31	20.17
Hydroxyzine		8.48	8.77	4.00
Idarubicin		100.00	99.33	99.99
Indoramine		100.00	99.96	100.00
Irbesartan		0.00	7.38	0.00

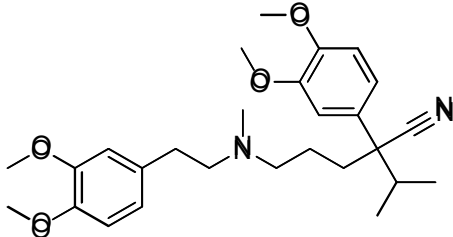
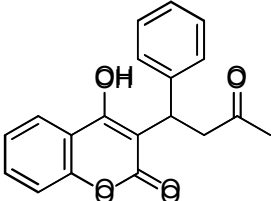
Isoxicam		100.00	98.55	99.90
Ketoconazole		100.00	96.78	98.58
Labetalol		83.38	75.54	83.96
Lomefloxacin		0.00	0.00	18.77
Lornoxicam		100.00	99.96	99.50
Mefloquine		0.00	1.57	0.00
Meloxicam		100.00	98.08	97.41

Gallopamil		100.00	85.93	81.55
Moxifloxacin		28.39	0.00	21.18
Nimesulide		0.00	0	0.00
Norfloxacin		38.17	21.37	44.81
Ofloxacin		79.60	96.04	99.16
Omeprazole		100.00	100	100.00
Oxybrupocaine		100.00	100	89.70
Oxyphenbutazone		100.00	99.54	86.79

Papaverine		0.00	4.96	0.00
Penamidine		0.00	0.00	0.00
Phenserine		100.00	100.00	92.21
Phenylbutazone		90.13	99.65	88.07
Pirenzepine		0.00	5.95	0.00
Prendisolone		0.00	0.00	10.07
Prochlorperazine		91.02	96.77	78.78
Progesterone		0.00	14.47	0.00

Propionylpromazine		100.00	99.92	99.49
Quinacrine		100.00	98.32	99.80
Quinine		0.00	5.78	0.00
Ranitidine		60.58	44.53	47.09
Rosuvastatin		0.00	0.20	0.00
Silibinin		88.19	94.67	91.01
Sulfasalazine		65.03	57.39	48.00

Sulindac		71.99	76.03	62.56
Tamoxifen		91.05	84.84	90.95
Telmisartan		0.00	0.00	0.00
Thioridazine		100.00	100.00	99.92
Tolnaftate		12.80	4.13	26.03
Trifluoperazine		100.00	99.88	99.70

Verapamil		100.00	99.89	99.98
Warfarin		100.00	99.79	96.14