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Computer aided identification of toxicologically relevant substances by means of multiple analytical methods

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Appendix A

Test set data

Table A.1 contains the identification (*i.e.* retention) parameters obtained from five different chromatographic methods. The methods are described in Chapter 3, § 3.8.1.

Table A.1: Retention parameters for five chromatographic methods.

Substance name	Method				
	1 TLC	2 TLC	3 TLC	4 GC	5 HPLC
acebutolol	33	13	0	2811	311
aminophenazone	62	70	21	1895	243
amitriptyline	69	27	50	2194	440
amitriptyline M ¹ (=nortriptyline)	46	87	28	2215	400
amphetamine	43	12	26	1125	238
atenolol	22	14	0	2385	224
atropine	24	5	5	2190	287
benperidol	60	62	3	3433	371
bromazepam	63	73	6	2665	378
caffeine	52	59	3	1800	265
carbamazepine	56	79	2	2285	380
chlordiazepoxide	52	76	2	2797	357
chloroquine	46	4	14	2605	265
chlorphenarnine	46	12	35	1996	348
chlorpromazine	70	25	45	2495	452
clobazam	75	84	8	2558	484
clomipramine	72	26	53	2415	470
clonazepam	67	85	0	2823	451
clopenthixol	44	45	7	3400	456
clorazepic acid	68	83	3	2457	464
cocaine	77	35	45	2187	345
cocaine M (=benzoylecgonine)	2	22	0	2570	295
codeine	35	21	6	2375	250
demoxepam	41	81	0	2529	388
diamorphine	49	26	15	2615	327
diazepam	76	82	27	2428	520
diazepam M (=nordazepam)	69	82	3	2490	464
diphenhydramine	65	27	44	1870	390
dipyridamole	44	82	0	1640	387
disopyramide	60	9	7	2505	327
doxepin	63	24	48	2220	730
droperidol	58	71	2	3430	369
ephedrine	25	10	5	1365	218

1. M denotes a metabolite of the parent compound. If M has an international nonproprietary name (INN), the latter is given in brackets.

Table A.1: (continued)

Substance name	Method				
	1	2	3	4	5
ethosuximide	66	84	5	1205	284
flecainide	49	28	6	2250	410
flumazenil	61	76	3	2660	362
flunarizine	88	83	45	3035	571
flunitrazepam	74	80	10	2600	459
flupenthixol	46	50	6	3058	487
flurazepam	71	52	30	2780	392
glibenclamide	11	90	0	ND	623
gliclazide	9	84	0	1456	538
glutethimide	80	86	31	1830	430
haloperidol	76	51	11	2930	409
hydroxyzine	54	57	10	2849	435
imipramine	67	21	48	2230	437
imipramine M (=desipramine)	40	7	19	2235	423
ketamine	79	68	37	1840	294
ketazolam	74	83	14	2444	583
labetalol	29	32	0	1230	350
levomepromazine	76	32	47	2525	440
lidocaine	80	72	35	1870	278
loprazolam	40	26	1	3258	379
lorazepam	43	82	1	2410	422
maprotyline	36	6	18	2356	440
medazepam	78	79	41	2235	395
metamizole	2	85	0	1990	289
methadone	77	16	59	2145	441
methamphetamine	42	9	28	1175	246
methaqualone	78	79	36	2135	450
metoclopramide	51	17	1	2620	308
metoprolol	44	20	10	2035	317
mianserin	68	48	39	2210	390
midazolam	60	69	6	2575	386
morphine	20	18	0	2445	200
nifedipine	71	79	1	2170	503
nitrazepam	64	84	0	2740	430
opipramol	38	35	6	3050	387
orphenadrine	68	25	48	1935	416
oxazepam	45	82	0	2325	441
paracetamol	45	77	0	1665	234
pentazocine	70	34	16	2280	357
periciazine	51	46	4	3260	405
perphenazine	42	40	7	2207	438
pethidine	60	34	37	1754	334
phenazone	45	66	4	1850	303
pindolol	43	18	2	2245	277
pipamperone	43	33	1	3040	286
prazepam	81	84	36	2648	648
procainamide	39	17	1	2200	202
prochlorperazine	55	26	34	2955	462
promazine	62	18	38	2315	418
promethazine	65	30	36	2267	411
propoxyphene	82	50	58	2190	438
propranolol	49	21	6	2147	370

Table A.1: (continued)

Substance name	Method				
	1	2	3	4	5
propyphenazone	74	81	32	1920	422
quinidine	49	30	4	2790	316
quinine	45	26	2	2800	398
strychnine	32	8	8	3116	292
sulpiride	34	17	0	3102	240
temazepam	62	82	8	2595	466
terfenadine	74	45	13	3436	567
thioridazine	67	20	42	3115	504
tocainide	44	42	2	1714	251
trazodone	66	64	10	3330	358
triazolam	44	68	1	3080	452
trimethoprim	45	45	0	2558	345
verapamil	73	43	23	3150	454
zopicilone	47	42	4	3062	314

Appendix B

RP-HPLC *RI* Database

Table B.1 shows the *RI*s of 836 toxicologically relevant reference substances in alphabetical order. Besides the substance names, the CAS registration number and the calibration mixture used to calculate the *RI* are given. Characters A and B indicate whether calibration mixture A or B was used for the calculation. The method used to measure the *RI*s is described in Chapter 8.

Table B.1: RP-HPLC *RI* database of 836 toxicologically relevant substances.

Substance name	CAS no.	mixture	<i>RI</i>
acebutolol	37517-30-9	B	325
acecarbromal	77-66-7	A	429
acenocoumarol	152-72-7	A	563
acepromethazine	13461-01-3	B	406
acetazolamide	59-66-5	A	268
acetophenazine	2751-68-0	B	395
acetylcodeine	6703-27-1	B	336
acetylcysteine	616-91-1	A	149
acetylsalicylic acid	50-78-2	A	350
acitretin	55079-83-9	A	929
aconitine	302-27-2	B	432
adiphenine	64-95-9	B	422
alclometasone	67452-97-5	B	685
alcuronium	23214-96-2	A	354
alfentanil	71195-58-9	B	378
allobarbital	52-43-7	A	346
allyl-5-ethylbarbituric Acid,5-	2373-84-4	A	326
allyl-5-phenylbarbituric Acid,5-	115-43-5	A	396
alphacetylmethadol	17199-58-5	B	368
alphamethylfentanyl	79704-88-4	B	409
alphaprodine	77-20-3	A	363
alprazolam	28981-97-7	A	470
amdinocillin	32887-01-7	A	313
amiloride	2609-46-3	B	257
aminoacridine	90-45-9	B	320
aminophenazone	58-15-1	A	262
aminophenol,p-	123-30-8	A	41
aminopromazine	58-37-7	B	427
amiodarone	1951-25-3	B	683
amitriptyline	50-48-6	B	440
amitriptyline M (=nortriptyline)	72-69-5	B	430
amlodipine	88150-42-9	B	428
amobarbital	57-43-2	A	424
amoxapine	14028-44-5	B	398
amphetamine	300-62-9	B	244

Table B.1: (continued)

Substance name	CAS no.	mixture	<i>RI</i>
ampyrone	83-07-8	A	264
anethole	104-46-1	A	637
antazoline	91-75-8	B	383
apomorphine	58-00-4	B	348
apraclonidine	66711-07-4	B	231
aprindine	37640-71-4	B	433
aprindine M (desethyl-)		B	379
aprobarbital	77-02-1	A	357
apronal	528-92-7	A	396
arecoline	63-75-2	B	79
articaïne	23964-58-1	B	307
astemizole	68844-77-9	B	383
astemizole M (Nor-)		B	361
atenolol	29122-68-7	B	243
atropine	51-55-8	B	306
atropine methonitrate	52-88-0	B	299
azaperone	1649-18-9	A	319
azathioprine	446-86-6	B	323
azelastine	58581-89-8	B	429
BBO T	7128-64-5	A	340
baclofen	1134-47-0	B	271
bambuterol	81732-65-2	B	353
bambuterol monocarbamate		B	304
bamethan	3703-79-5	B	250
bamipine	4945-47-5	B	468
barbital	57-44-3	A	308
beclomethasone	4419-39-0	B	444
benactyzine	302-40-9	B	382
benazepril		B	427
bendroflumethiazide	73-48-3	A	508
benperidol	2062-84-2	A	393
benserazide	322-35-0	B	35
benzbromarone	3562-84-3	A	860
benzetimide	14051-33-3	B	372
benzocaine	94-09-7	B	404
benzocetamine	17243-39-9	B	380
benzoic acid	65-85-0	A	360
benzophenone	119-61-9	A	592
benzquinamide M (desacetyl-)		B	299
benzquinamide M (desacetyldesethyl-)		B	276
benzquinamide M (nor-)		B	256
betaxolol	63659-18-7	A	386
bezafibrate	41859-67-0	A	513
bezitramide	15301-48-1	B	564
bifonazole	60628-96-8	B	484
bioallethrin	584-79-2	B	936
bisacodyl	603-50-9	B	531
bisoprolol	66722-44-9	A	358
brallobarbital	561-86-4	A	371
bromazepam	1812-30-2	A	397
bromazine	118-23-0	B	444
bromhexine	3572-43-8	B	417
bromhexine M (=ambroxol)	18683-91-5	B	342

Table B.1: (continued)

Substance name	CAS no.	mixture	<i>RI</i>
bromisoval	496-67-3	A	365
bromisoval M1		A	312
bromisoval M2		A	211
bromisoval M3		A	237
bromocriptine	25614-03-3	B	456
bromolysergide,2-	478-84-2	B	382
bromoxynil	1689-84-5	B	421
bromperidol	10457-90-6	A	434
brotizolam	57801-81-7	A	484
brucine	357-57-3	B	312
budesonide	51333-22-3	A	530
buflovedil	55837-25-7	B	347
buphenine	447-41-6	B	370
bupivacaine	2180-92-9	B	366
bupivacaine M (4-HO-)		B	310
bupivacaine M (=mepivacaine M)		B	285
bupranolol	14556-46-8	A	391
buprenorphine	52485-79-7	B	397
buprenorphine M (nor-)		B	359
buspirone	36505-84-7	A	369
busulfan	55-98-1	A	368
butacaine	149-16-6	B	392
butalbital	77-26-9	A	394
butallylonal	1142-70-7	A	423
butaperazine	653-03-2	B	464
butetamate	14007-64-8	B	390
butobarbital	77-28-1	A	384
buzepide	3691-21-2	B	381
caffeine	58-08-2	A	305
camylofine	54-30-8	A	459
cannabidiol	13956-29-1	A	990
cannabinol	521-35-7	A	1080
captan	133-06-2	A	563
captodiamine	486-17-9	B	561
captopril	62571-86-2	A	316
carazolol	57775-29-8	A	381
carbamazepine	298-46-4	B	418
carbamazepine M (dihydro-HO-)		B	355
carbimazole	22232-54-8	A	318
carbinoxamine	486-16-8	B	359
carbromal	77-65-6	A	410
carfenazine	2622-30-2	B	419
carnidazole	42116-76-7	B	376
cefaclor	70356-03-5	A	268
cefamandole	34444-01-4	A	358
cefoxitin	35607-66-0	A	338
ceftriaxone	73384-59-5	B	239
cetrimide	8044-71-1	B	56
chloramphenicol	56-75-7	A	390
chlordane	57-74-9	A	1017
chlordiazepoxide	58-25-3	A	363
chlorhexidine	55-56-1	B	398
chlorobenzilate	510-15-6	A	825

Table B.1: (continued)

Substance name	CAS no.	mixture	<i>RI</i>
chloroquine	54-05-7	B	282
chlorphenamine	132-22-9	B	356
chlorphenesin carbamate	886-74-8	B	387
chlorphenprocoumon,p-		A	671
chlorpromazine	50-53-3	B	456
chlorpropamide	94-20-2	B	450
chlorpropham	101-21-3	A	618
chlorprothixene	113-59-7	B	459
chlortalidone	77-36-1	A	367
chlorzoxazone	95-25-0	B	397
cilastatin	82009-34-5	A	316
cilazapril	92077-78-6	A	420
cimetidine	51481-61-9	B	251
cinchonidine	485-71-2	B	306
cinchonine	118-10-5	B	304
cinnamoylcocaine	521-67-5	B	392
cinnarizine	298-57-7	B	560
cinoxacin	28657-80-9	A	532
ciprofloxacin	85721-33-1	A	318
cisapride	81098-60-4	B	431
citalopram	59729-33-8	B	403
clemastine	15686-51-8	B	501
clemizole	442-52-4	B	420
clenbuterol	37148-27-9	B	326
clenbuterol M1 (HO-)		B	297
clenbuterol M2		B	346
clenbuterol M3		B	419
clidinium Bromide	3485-62-9	A	379
clindamycin	18323-44-9	B	354
clobazam	22316-47-8	A	488
clocinizine	298-55-5	B	615
clomethiazole	533-45-9	B	395
clomipramine	303-49-1	B	462
clomipramine M1 (nor-)		B	459
clomipramine M2 (8-HO-)		B	410
clomipramine M3 (8-HO-nor-)		B	404
clomipramine M4 (2-HO-)		B	397
clomipramine M5 (10-HO-)		B	389
clomipramine M6 (-N-oxide)		B	478
clonazepam	1622-61-3	A	465
clonazepam M (7-acetamido-)	41993-30-0	A	366
clonazepam M (7-amino-)	4959-17-5	A	345
clonidine	4205-90-7	B	258
clopamide	636-54-4	A	377
clopenthixol	982-24-1	B	448
clorazepic acid	23887-31-2	A	475
clozapine	5786-21-0	B	368
clozapine M (-N-oxide)		B	357
clozapine M (nor-)		B	390
cocaine	50-36-2	B	348
cocaine M (=benzoylecgonine)	519-09-5	B	313
cocaine M	18717-72-1	B	352
codeine	76-57-3	B	266

Table B.1: (continued)

Substance name	CAS no.	mixture	<i>RI</i>
colchicine	64-86-8	B	382
coniine	458-88-8	B	214
cotinine	486-56-6	B	215
crotarbital	1952-67-6	A	361
crothamide	6168-76-9	B	366
cryptopine	482-74-6	B	350
cyclizine	82-92-8	A	405
cyclobarbital	52-31-3	A	384
cyclopentobarbital	76-68-6	A	391
cyclopentolate	512-15-2	B	353
cyproteron	2098-66-0	A	670
decamethonium	156-74-1	B	56
demoxepam	963-39-3	A	416
deoxyephedrine, (+/-)	4846-07-5	B	260
depropine	604-51-3	B	471
dexetimide	21888-98-2	B	371
dextromethorphan	125-71-3	B	377
dextromoramide	3 357-56-2	B	440
dextropropoxyphene	125-73-5	B	325
diamocaine	27112-37-4	B	326
diamorphine	561-27-3	B	340
diamorphine M (=6-MAM)	59833-14-6	B	286
diazepam	439-14-5	A	528
diazepam M (nor-)	1088-11-5	A	470
diazoxide	364-98-7	A	368
dibenzepin	4498-32-2	B	361
dibenzepin M (bisnor-5-desmethyl-)		B	336
dibenzepin M (5-desmethyl-)		B	330
dibenzepin M (dinor-)		B	325
dibenzepin M (nor-5-desmethyl-)		B	353
dibenzepin M (nor-)		B	347
dichlorophenoxy acetic acid, 2,4-	94-75-7	A	437
diclofenac	15307-86-5	A	616
dicoumarol	66-76-2	A	599
diethylcarbamazine	90-89-1	B	219
diethylstilbestrol	56-53-1	A	592
diflunisal	22494-42-4	A	508
dihydralazine	484-23-1	B	39
dihydrocodeine	125-28-0	B	261
dihydroergotamine	511-12-6	B	411
dihydroergotamine M (8'-HO-)		B	393
dihydromorphine	509-60-4	B	237
diisopromine	5966-41-6	B	457
dimethoxy-4-ethylamphetamine,2,5-	22004-32-6	B	371
dimethoxy-4-methylamphetamine,2,5-	15588-95-1	B	340
dimethoxyphenethylamine,3,4-	120-20-7	B	342
dimethyl-POPOP	3073-87-8	A	925
dimethylaminobenzaldehyde,p-	100-10-7	A	426
dimetindene	5636-83-9	B	338
dimpylate / diazinon	333-41-5	A	618
diphenhydramine	58-73-1	B	393
diphenylamine	122-39-4	B	650
dipipanone	467-83-4	B	500

Table B.1: (continued)

Substance name	CAS no.	mixture	<i>RI</i>
diprophylline	479-18-5	B	275
dipyridamole	58-32-2	B	393
disopyramide	3737-09-5	B	345
disulfiram	97-77-8	B	741
dobutamine	34368-04-2	B	308
domperidone	57808-66-9	B	377
dopexamine	86197-47-9	B	289
dothiepin	113-53-1	B	428
dothiepin M (-sulfoxide)		B	420
dothiepin M (nor-)	1154-09-2	B	320
dothiepin M (nor-, -sulfoxide)		B	323
doxazosin	74191-85-8	B	403
doxepin	1668-19-5	B	404
doxifluridine	3094-09-5	B	242
doxorubicin	23214-92-8	A	370
droperidol	548-73-2	B	385
dropropizine	17692-31-8	B	240
econazole	27220-47-9	B	526
emepromium	27892-33-7	B	420
emetine	483-18-1	B	310
enalapril	75847-73-3	A	201
encainide	66778-36-7	B	363
enilconazole	35554-44-0	B	425
ephedrine	299-42-3	B	221
ephedrine M (=phenylpropanolamine)	492-41-1	B	174
epinephrine	51-43-4	B	301
epirubicin	56420-45-2	A	379
epithiazide	1764-85-8	A	457
ergometrine	60-79-7	B	292
ergosine	561-94-4	B	397
ergotamine	113-15-5	B	416
estazolam	29975-16-4	B	445
estrone	53-16-7	A	544
etacrynic acid	58-54-8	A	521
ethinylestradiol	57-63-6	B	539
ethoheptazine	77-15-6	B	359
ethosuximide	77-67-8	A	301
ethyl-2-(p-tolyl)malonamide,2-	68692-83-1	A	338
ethyl-5-p-tolylbarbituric Acid,5-	52584-39-1	A	414
ethylmorphine	76-58-4	B	291
ethylpiperidyl benzilate	3567-12-2	B	384
ethynodiol diacetate	297-76-7	B	549
eticyclidine	2201-15-2	B	351
etilefrine	709-55-7	B	118
etofylline	519-37-9	A	289
etomidate	33125-97-2	B	475
etonitazene	911-65-9	B	406
etorphine	14521-96-1	B	344
etoxeridine	469-82-9	B	349
famatidine	76824-35-6	B	233
felodipine	72509-76-3	B	640
fenbufen	36330-85-5	A	520
fencamfamine	1209-98-9	B	354

Table B.1: (continued)

Substance name	CAS no.	mixture	<i>RI</i>
fendiline	13042-18-7	B	493
fenethylline	3736-08-1	B	366
fenfluramine	458-24-2	B	371
fenocyclidine	21500-98-1	B	362
fenopropfen	31879-05-7	A	574
fenoterol	13392-18-2	B	287
fempiverinium	125-60-0	B	363
fentanyl	437-38-7	B	373
fenyramidol	553-69-5	B	282
flecainide	54143-55-4	B	419
fluanisone	1480-19-9	A	423
flubendazole	31430-15-6	B	454
fluconazole	86386-73-4	B	340
flucytosine	2022-85-0	A	72
flufenamic acid	530-78-9	A	671
flumazenil	78755-81-4	A	387
flumazenil M (=RO-15-3890)		A	322
flunarizine	52468-60-7	B	581
flunitrazepam	1622-62-4	A	483
flunitrazepam M (3-HO-)	67739-71-3	A	451
flunitrazepam M (nor-)	2558-30-7	A	441
flunitrazepam M (nor-) Hy	344-80-9	A	569
fluorofentanyl, p-	1506-86-1	B	405
fluorometholone	426-13-1	B	470
fluorouracil	51-21-8	A	70
flupenthixol	2709-56-0	B	475
fluphenazine	69-23-8	B	462
flurazepam	17617-23-1	A	397
flurbiprofen	5104-49-4	A	585
flurbiprofen M1		A	466
flurbiprofen M2		A	471
fluspirilene	1841-19-6	B	538
flutamide	13311-84-7	B	611
flutropium bromide	63516-07-4	B	391
fluvoxamine	5439-18-3	B	430
furazolidone	67-45-8	A	336
furosemide	60568-05-0	A	435
fusidic acid M (3-keto-)		A	695
gallopamil	16662-47-8	A	460
gallopamil M (=D-517)		A	441
gallopamil M (nor-)		A	455
gelsemine	509-15-9	B	290
gestodene	60282-87-3	B	560
glafenine	3820-67-5	A	372
glibenclamide	10238-21-8	A	637
gliclazide	21187-98-4	A	536
glipizide	29094-61-9	B	478
glisoxepid	25046-79-1	B	469
glutethimide	77-21-4	B	436
glymidine	339-44-4	A	390
granisetron	109889-09-	B	359
guaifenesin	93-14-1	B	328
guanoxan	2165-19-7	B	295

Table B.1: (continued)

Substance name	CAS no.	mixture	<i>RI</i>
halofantrine	69756-53-2	B	800
halofantrine M (desbutyl-)		B	618
haloperidol	52-86-8	B	421
haloperidol M (reduced)		B	397
haloxazolam	59128-97-1	A	400
harman	486-84-0	B	319
harmine	442-51-3	B	339
heptabarbital	509-86-4	A	416
heptachlor	76-44-8	A	1072
heptachlor epoxide	1024-57-3	A	940
hexachlorophene	70-30-4	A	936
hexafluorenum Bromide	317-52-2	A	413
hexamidine	659-40-5	B	345
hexestrol	5635-50-7	A	618
hexobarbital	56-29-1	A	419
hexylresorcinol	136-77-6	B	579
homatropine	87-00-3	B	272
homatropine methylbromide	80-49-9	B	262
homofenazine	3833-99-6	B	405
hydralazine	86-54-4	B	193
hydrochlorothiazide	58-93-5	A	294
hydrocodone	125-29-1	B	286
hydrocortisone	50-23-7	A	403
hydromorphone	466-99-9	B	240
hydroxychloroquine	118-42-3	B	280
hydroxymorphinan,3(+)-	1531-12-0	B	319
hydroxyprogesterone	68-96-2	B	1054
hydroxyzine	68-88-2	B	437
ibomal	545-93-7	A	379
ibopamine	66195-31-1	B	409
ibuprofen	15687-27-1	A	616
ibuprofen M1		A	389
ibuprofen M2		A	405
idarubicin	58957-92-9	A	410
imipenem	74431-23-5	A	135
imipramine	50-49-7	N	437
imipramine M (Des-)	50-47-5	B	424
impurity HPLC system		A/B	837
indometacin	53-86-1	A	607
iproniazid	54-92-2	B	249
isocarboxazid	59-63-2	B	392
isoconazole	27523-40-6	B	536
isoetharine	530-08-5	B	222
isomet hadone	466-40-0	B	443
isoprenaline	7683-59-2	B	79
isopropamide iodide	71-81-8	B	379
isothebaine	568-21-8	B	329
isothipendyl	482-15-5	B	390
isoxsuprine	395-28-8	B	353
isradipine	75695-93-1	B	632
itraconazole	84625-61-6	B	725
ketamine	6740-88-1	A	311
ketanserin	74050-98-9	B	376

Table B.1: (continued)

Substance name	CAS no.	mixture	<i>RI</i>
ketanserin M (=ketanserinol)		B	363
ketazolam	27223-35-4	A	577
ketobemidone	469-79-4	B	294
ketoconazole	65277-42-1	B	439
ketoprofen	22071-15-4	A	495
ketotifen	34580-13-7	B	373
labetalol	36894-69-6	A	365
lacidipine	103890-78-4	A	900
levallorphan	152-02-3	B	356
levarterenol	51-41-2	B	17
levocabastine	79516-68-0	B	431
levodopa	59-92-7	A	65
levomepromazine	60-99-1	B	435
levophenacetylmorphan	10061-32-2	B	414
lidocaine	137-58-6	B	288
lidoflazine	3416-26-0	B	530
lisinopril	83915-83-7	A	271
lisuride	18016-80-3	B	383
loperamide	53179-11-6	B	510
loprazolam	61197-73-7	B	388
loratadine	79794-75-5	B	523
lorazepam	846-49-1	B	444
lorcainide	59729-31-6	B	425
lorcainide M (=N-methyllofazepam)		B	397
lormetazepam	848-75-9	A	487
loxapine	1977-10-2	B	407
lysergide	50-37-3	B	362
maprotyline	10262-69-8	B	438
maprotyline M (nor-)		B	428
mazindol	22232-71-9	B	357
mebendazole	31431-39-7	B	438
mebeverine	3625-06-7	B	448
mebhydrolin	524-81-2	B	411
meclofenamic acid	644-62-2	A	653
mecloqualone	340-57-8	B	482
meclozine	569-65-3	B	587
meconin	569-31-3	B	358
medazepam	2898-12-6	A	405
medazepam M (nor-)		A	388
medrogestone	977-79-7	B	835
mefenamic acid	61-68-7	A	661
mefenorex	17243-57-1	B	342
mefloquine	51773-92-3	B	462
melitracen	5118-29-6	B	465
melperone	3575-80-2	A	360
melperone M (=FG-5155)		A	342
mepacrine	83-89-6	B	345
mephesisin	59-47-2	B	364
mephentermine	100-92-5	B	294
mepindolol	23694-81-7	B	321
mepivacaine	96-88-8	B	296
mepyramine	91-84-9	B	349
mequitazine	29216-28-2	B	448

Table B.1: (continued)

Substance name	CAS no.	mixture	<i>RI</i>
mercaptapurine, 6-	50-44-2	A	187
mescaline	54-04-6	B	272
metaclozepam	84031-17-4	A	451
metaclozepam M (didesmethyl-)		A	425
metaclozepam M (nor-)		A	393
metamizole	68-89-3	B	316
metaraminol	54-49-9	B	84
methadone	76-99-3	B	440
methadone intermediate (=pre methadone)	125-79-1	B	399
methadone M (=EDDP)	467-85-6	B	439
methamphetamine	537-46-2	B	262
methanthelinium bromide	53-46-3	B	418
methapyrilene	91-80-5	B	342
methaqualone	72-44-6	B	459
metharbital	50-11-3	A	435
methazolamide	554-57-4	B	304
methenolone	153-00-4	B	809
methformin	657-24-9	B	60
methionine	63-68-3	A	422
methocarbamol	532-03-6	A	345
methohexital	151-83-7	A	503
methotrexate	59-05-2	A	292
methoxsalen	298-81-7	A	457
methoxyamphetamine, 4-	23239-32-9	B	274
methoxychlor	72-43-5	A	900
methoxyphenamine	93-30-1	B	303
methscopolamine bromide	155-41-9	B	284
methyl salicylate	119-36-8	A	480
methyl phenidate	113-45-1	B	328
methyl-3,4-methylenedioxyamphetamine	42542-10-9	B	278
methyl-5-phenylbarbituric acid, 5-	76-94-8	A	354
methyl dopa	555-30-6	B	69
methylenedioxy-5-methoxyamphetamine, 3,4-	64638-02-4	B	306
methylergometrine	113-42-8	B	320
methylphenobarbital	115-38-8	A	435
methylphenyl)-5-phenylhydantoin, 5-(51169-17-6	A	470
methylpiperidyl benzilate	3321-80-0	B	377
methylprednisolon	83-43-2	A	426
methylprimidone, 4-	59026-32-3	A	362
methypylon	125-64-4	A	347
metipranolol	22664-55-7	A	379
metixene	4969-02-2	B	451
metoclopramide	364-62-5	B	324
metomidate	5377-20-8	B	424
metoprolol	37350-58-6	B	326
metronidazole	443-48-1	B	257
metryrosine	672-87-7	A	61
mexazolam	31868-18-5	A	345
mexiletine	31828-71-4	B	329
mianserin	24219-97-4	B	391
mianserine M1 (8-HO-)		B	335
mianserine M2 (Nor-)		B	388
mianserine M3 (=Mianderin-N-oxide)		B	417

Table B.1: (continued)

Substance name	CAS no.	mixture	<i>RI</i>
miconazole	22916-47-8	A	584
midazolam	59467-70-8	A	399
minoxidil	38304-91-5	B	297
mitotane	53-19-0	A	1026
moclobemide	71320-77-9	B	295
moperone	1050-79-9	B	406
moroxydine	3731-59-7	B	39
morphine	57-27-2	B	200
morphine M (-3-glucuronide)		B	69
moxalactam	64952-97-2	A	316
moxaverine	10539-19-2	B	414
mupirocin	12650-69-0	A	459
nadolol	42200-33-9	B	288
nafcilline sodium	985-16-0	A	470
nalbuphine	20594-83-6	B	295
nalorphine	62-67-9	B	260
naphazoline	835-31-4	B	320
naproxen	22204-53-1	A	488
narceine	131-28-2	B	360
narcobarbital	125-55-3	A	452
narcophin	6055-90-9	B	368
nealbarbital	561-83-1	A	417
nedocromil	69049-73-6	A	318
neostigmine	59-99-4	B	253
neostigmine	59-99-4	B	248
nialamide	51-12-7	B	334
nicardipine	55985-32-5	B	450
niclosamide	50-65-7	B	723
nicodicodine	808-24-2	B	334
nicomorphine	639-48-5	B	375
nicotinamide	98-92-0	B	168
nicotine	54-11-5	B	69
nicotiny alcohol	100-55-0	B	55
nifedipine	21829-25-4	B	527
nifedipine M		B	505
nifenazone	2139-47-1	B	310
niflumic acid	4394-00-7	A	595
nifuratel	4936-47-4	A	432
niketamide	59-26-7	B	304
nimodipine	66085-59-4	B	668
nimodipine M		B	653
nisoldipine	63675-72-9	B	690
nitrazepam	146-22-5	A	448
nitrendipine	39562-70-4	B	625
nitrendipine M (=BAY-M-4786)		B	598
nitrofurantoin	67-20-9	A	319
nitrofurantoin M (HO-Methyl-)		A	320
nitrofurazone	59-87-0	A	316
nomifensine	24526-64-5	B	349
norethisterone	68-22-4	A	536
norfloxacin	70458-96-7	A	315
norgestrel	797-63-7	B	591
norpipanone	561-48-8	B	466

Table B.1: (continued)

Substance name	CAS no.	mixture	<i>RI</i>
noscapine	128-62-1	B	368
octopamine	104-14-3	B	157
ofloxacin	82419-36-1	A	314
opipramol	315-72-0	B	377
orciiprenaline	586-06-1	B	151
orientalidine	23943-90-0	A	336
ornidazole	16773-42-5	A	331
orphenadrine	83-98-7	B	418
oxatomide	60607-34-3	B	461
oxazepam	604-75-1	A	441
oxazepam M Hy (=ACB)	719-59-5	A	660
oxazolam	24143-17-7	A	339
oxcarbazepine	28721-07-5	A	396
oxomemazine	3689-50-7	B	363
oxprenolol	6452-71-7	B	354
oxybuprocaine	99-43-4	A	405
oxycodone	76-42-6	B	277
oxymorphone	76-41-5	B	217
oxypertine	153-87-7	B	402
oxyphenbutazone	129-20-4	B	501
oxyphencyclimine	125-53-1	B	424
oxyphenonium bromide	50-10-2	B	424
oxytetracycline	79-57-2	B	299
PCM	2201-40-3	B	343
papaverine	58-74-2	B	363
paracetamol	103-90-2	A	264
paroxetine	61869-08-7	B	426
pezazine	60-89-9	A	443
pemoline	2152-34-3	A	307
penbutolol	38363-40-5	A	451
penfluridol	26864-56-2	B	659
pentaerithritol tetranitrate	78-11-5	A	663
pentazocine	359-83-1	B	372
pentetrazol	54-95-5	B	290
pentobarbital	76-74-4	A	424
pentolinium	144-44-5	B	48
pentoxifylline	6493-05-6	A	355
perazine	84-97-9	B	403
periciazine	2622-26-6	B	410
perphenazine	58-39-9	B	428
pethidine	57-42-1	B	345
pethidine M (nor-)	77-17-8	B	344
pethidine intermediate A	3627-62-1	A	298
pethidine intermediate B		A	349
phenacetin	62-44-2	A	377
phenazocine	127-35-5	B	409
phenazone	60-80-0	A	333
phencyclidine	77-10-1	B	375
phendimetrazine	634-03-7	B	263
phenelzine	51-71-8	B	184
phenformin	114-86-3	B	250
phenindamine	82-88-2	B	397
pheniramine	86-21-5	B	283

Table B.1: (continued)

Substance name	CAS no.	mixture	<i>RI</i>
phenmetrazine	134-49-6	B	258
phenobarbital	50-06-6	A	379
phenolphthalein	77-09-8	A	436
phenomorphan	468-07-5	B	436
phenoperidine	562-26-5	A	434
phenothiazine	92-84-2	B	665
phenoxybenzamine	59-96-1	B	396
phenprocoumon	435-97-2	A	616
phentolamine	50-60-2	B	368
phenyl salicylate	118-55-8	A	666
phenylbutazone	50-33-9	A	672
phenylcyclohexylamine, 1-	2201-24-3	B	323
phenylephrine	59-42-7	B	80
phenylmercury Borate	102-98-7	A	427
phenyltoloxamine	92-12-6	B	415
phenytoin	57-41-0	A	431
phenytoin M (4-HO-phenyl-)		A	377
pholcodine	509-67-1	B	65
pholedrine	370-14-9	B	205
physostigmine	57-47-6	B	296
pimozide	2062-78-4	B	504
pinacidil	85371-64-8	B	336
pinacidil M (-N-oxide)		A	361
pindolol	13523-86-9	B	300
pipamperone	1893-33-0	B	299
pipazetate	2167-85-3	B	385
pipemidic acid	51940-44-4	A	298
piperidine, 1-(4-methyl-1-phenylcyclohexyl)	19420-52-1	B	398
piperidolate	82-98-4	B	429
piperocaine	136-82-3	B	357
piperonal	120-57-0	A	386
pipotiazine	39860-99-6	B	431
pipradrol	467-60-7	B	355
pirenzepine	28797-61-7	B	293
pirenzepine M (nor-)		B	373
pirenzepine M (-desamide)		B	291
piretanide	55837-27-9	A	497
piribedil	3605-01-4	B	328
piritramide	302-41-0	B	377
piroxicam	36322-90-4	A	431
piroxicam M (5-HO-)		A	446
pirprofen	31793-07-4	A	540
pitofenone	54063-52-4	B	384
pizotifen	15574-96-6	B	435
podophyllotoxin	518-28-5	B	440
pralidoxime mesylate	154-97-2	A	46
pramoxine	140-65-8	B	415
prazepam	2955-38-6	A	648
praziquantel	55268-74-1	B	498
prazosin	19216-56-9	B	352
prednisolon	50-24-8	A	401
prednison	53-03-2	B	250
prenoxdiazine	982-43-4	B	452

Table B.1: (continued)

Substance name	CAS no.	mixture	<i>RI</i>
primidone	125-33-7	A	322
primidone M (=PEMA)	80866-90-6	A	298
(nor-) Probenecid	57-66-9	A	526
procainamide	51-06-9	B	208
procaine	59-46-1	B	264
prochlorperazine	58-38-8	B	450
proclonol	14088-71-2	B	894
procyclidine	77-37-2	B	406
profenamine	522-00-9	B	444
progesterone	57-83-0	A	672
proguanil	500-92-5	B	379
prolintane	493-92-5	B	370
promazine	58-40-2	B	407
promethazine	60-87-7	B	409
propafenone	54063-53-5	B	433
propafenone M (5-HO-)		B	387
propafenone M (nor-)		B	388
propantheline bromide	50-34-0	B	454
propantheline M (=xanthanoic acid)		A	499
properidine	561-76-2	A	374
propiomazine	362-29-8	B	440
propoxyphene	469-62-5	B	442
propranolol	525-66-6	B	377
propranolol M (4-HO-)		B	335
propyl p-Hydroxybenzoate	94-13-3	A	473
propyphenazone	479-92-5	A	441
prothipendyl	303-69-5	B	388
protiptyline	438-60-8	B	418
proxiphylline	603-00-9	B	293
prozapine	3426-08-2	B	455
pseudoephedrine	90-82-4	B	237
psilocin	520-53-6	B	240
pyrantel	15686-83-6	B	299
pyridostigmine bromide	101-26-8	A	65
pyrithydione	77-04-3	A	329
pyroxidine hydrochloride	58-56-0	B	65
pyrrobutamine	91-82-7	B	477
quinidine	56-54-2	B	322
quinine	130-95-0	B	327
remoxipride		B	334
remoxipride M (=FLA-838)		B	341
remoxipride M (=NCM-001)		B	364
remoxipride M (=NCM-009)		B	316
reposal	3625-25-0	A	434
rescinnamine	24815-24-5	B	496
reserpine	50-55-5	B	467
resorcinol	108-46-3	B	243
rimiterol	32953-89-2	B	150
rolicyclidine	2201-39-0	B	363
roxatidine acetate	78628-28-1	B	320
saccharin	81-07-2	A	291
salbutamol	18559-94-9	A	220
salicylaldehyde	90-02-8	A	379

Table B.1: (continued)

Substance name	CAS no.	mixture	<i>RI</i>
salicylamide	65-45-2	A	327
salicylic acid	69-72-7	A	350
scopolamine	51-34-3	B	270
secbutabarbital	125-40-6	A	377
secobarbital	76-73-3	A	437
sertraline	79617-96-2	B	460
simvastatin	79902-63-9	A	814
sotalol	3930-20-9	B	226
spiperone	749-02-0	B	405
spironolactone	52-01-7	A	592
strophantin	11005-63-3	B	356
strychnine	57-24-9	B	302
sufentanil	56030-54-7	B	438
sulfamidine	57-68-1	A	333
sulfadoxine	2447-57-6	B	364
sulfalene	152-47-6	A	353
sulfamethoxypyridazine	80-35-3	A	335
sulfapyridine	144-83-2	A	312
sulfasalazine	599-79-1	A	433
sulfasomizole	632-00-8	A	443
sulfathiazole	72-14-0	A	310
sulfisomidine	515-64-0	A	290
sulforidazine	14759-06-9	A	421
sulindac	38194-50-2	A	488
sulpiride	15676-16-1	A	259
sulprostone	60325-46-4	A	435
sultiam	61-56-3	A	344
synephrin	94-07-5	B	52
TDE, p,p'-	72-54-8	A	1030
talbutal	115-44-6	A	403
tamoxifen	10540-29-1	B	592
temazepam	846-50-4	A	472
tenamfetamine	4764-17-4	B	266
tenoxicam	59804-37-4	B	366
terbinafine	91161-71-6	B	511
terbutaline	23031-25-6	B	225
terfenadin	50679-08-8	A	571
tertatolol	34784-64-0	A	381
testosterone	58-22-0	A	534
tetrabarbital	76-23-3	A	457
tetracaine	94-24-6	B	389
tetracycline	60-54-8	B	314
tetramisole	5036-02-2	B	261
tetrazepam	10379-14-3	A	511
thebacon	466-90-0	B	333
thebaine	115-37-7	B	340
thyldiamine	91-79-2	B	317
theobromine	83-67-0	B	262
theophylline	58-55-9	A	276
thialbarbital	467-36-7	A	480
thiamine hydrochloride	59-43-8	B	9
thiamylal	77-27-0	A	516
thiazinamium M (-sulfoxide)		A	326

Table B.1: (continued)

Substance name	CAS no.	mixture	<i>RI</i>
thiethylperazine	1420-55-9	B	487
thiobarbital	77-32-7	A	340
thiopental	76-75-5	A	485
thiopropazate	84-06-0	B	483
thiopropazine	316-81-4	B	427
thioridazine	50-52-2	B	490
tiapride	51012-32-9	B	278
tiaprofenic acid	33005-95-7	A	484
timolol	26839-75-8	B	317
tiotixene	5591-45-7	B	442
tizanidine	51322-75-9	A	247
tocainide	41708-72-9	B	247
tofenacin	15301-93-6	B	407
tolazamide	1156-19-0	B	452
tolazoline	59-98-3	B	225
tolbutamide	64-77-7	A	477
tolfenamic acid	13710-25-7	A	690
toliprolol	2933-94-0	A	340
tolmetin	26171-23-3	A	470
tolyfluanid	731-27-1	B	818
tramazoline	1082-57-1	B	341
tranlycypromine	155-09-9	B	230
trazodone	19794-93-5	B	378
triamcinolone	124-94-7	B	438
triamterene	396-01-0	B	298
triazolam	28911-01-5	A	476
trifluoperazine	117-89-5	B	480
trifluoperidol	749-13-3	A	459
triflupromazine	146-54-3	B	484
trifluridine	70-00-8	B	275
trihexyphenidyl	144-11-6	B	429
trimeprazine	84-96-8	B	420
trimethadione	127-48-0	A	286
trimethaphan camsylate	68-71-9	A	386
trimethobenzamide	138-56-7	B	347
trimethoprim	738-70-5	B	299
trimethoxyamphetamine	22199-17-3	B	290
trimipramine	739-71-9	B	454
tripelenamine	91-81-6	B	336
triprolidine	486-12-4	B	388
tropacocaine	537-26-8	B	332
tropicamide	1508-75-4	A	311
tropine	120-29-6	B	689
tubocurarine	57-95-4	B	321
umbelliferone	93-35-6	A	351
valnoctamide	4171-13-5	B	196
verapamil	52-53-9	B	447
viloxazine	46817-91-8	B	325
vinbarbital	125-42-8	A	379
vinclozolin	50471-44-8	A	672
vinylbital	2430-49-1	A	424
volazocine	15686-68-7	B	386
warfarin	81-81-2	A	546

Table B.1: (continued)

Substance name	CAS no.	mixture	<i>RI</i>
xamoterol	81801-12-9	B	239
xanthinol Nicotinate	437-74-1	B	215
xipamide	14293-44-8	A	488
xylometazoline	526-36-3	B	413
yohimbine	146-48-5	B	348
zopiclone	43200-80-2	A	331

Appendix C

Common RIs

Table C.1 shows the retention parameters of the substances the three different databases described in Chapter 9) have in common.

Table C.1: RIs for substances present in all three databases, with means, standard deviations and pK_{a1}

Substance	Table B.1	Bogusz	Hill	Mean	SD	pK_{a1}
acetylsalicylic acid	350	326	348	341	13.3	3.5
allobarbital	346	340	343	343	3.0	7.8
amitriptyline	440	446	430	439	8.1	9.4
amitriptyline M (=nortriptyline)	430	418	419	422	6.7	9.7
amobarbital	424	415	410	416	7.1	7.9
amoxapine	398	372	336	369	31.1	
amphetamine	244	241	242	242	1.5	9.9
aprobarital	357	347	355	353	5.3	8.0
atenolol	243	224	235	234	9.5	9.6
atropine	306	287	297	297	9.5	9.9
barbital	308	287	298	298	10.5	8.0
benzocaine	404	380	374	386	15.9	2.8
bromazepam	397	378	348	374	24.7	2.9
buprenorphine	397	386	384	389	7.0	8.1
buspirone	369	353	350	357	10.2	
caffeine	305	265	295	288	20.8	14.0
carbamazepine	418	380	399	399	19.0	
carbomal	410	400	398	403	6.4	
chlordiazepoxide	363	357	338	353	13.1	4.6
chloroquine	282	265	273	273	8.5	8.4
chlorphenamine †	356	342	264	320	49.6	9.1
chlorpromazine	456	466	438	453	14.2	9.3
cimetidine	251	229	236	239	11.2	6.8
clonazepam	465	451	443	453	11.1	1.5
clorazepic acid †	475	464	376	438	54.3	3.5
cocaine	348	336	327	337	10.5	8.6
cocaine M (=benzoylecgonine)	313	295	304	304	9.0	
codeine	266	243	258	256	11.7	8.2
colchicine	382	357	379	373	13.7	1.7
dextromethorphan	377	370	367	371	5.1	8.3
diamorphine	340	327	328	332	7.2	7.6
diamorphine M (=6-MAM)	286	276	274	279	6.4	
diazepam	528	529	458	505	40.7	2.7
diazepam M (=nordiazepam) †	470	464	377	437	52.0	3.5
diclofenac	616	630	614	620	8.7	
dihydrocodeine	261	237	245	248	12.2	8.8
diphenhydramine	393	385	372	383	10.6	9.0
dipyridamole	393	387	363	381	15.9	6.4

Table C.1: (continued)

Substance	Table B.1	Bogusz	Hill	Mean	SD	pK_{a1}
disulfiram	741	730	731	734	6.1	
doxepin	404	401	379	395	13.7	9.0
ephedrine	221	224	231	225	5.1	9.6
ephedrine M (=phenylpropanolamine)	174	190	189	184	9.0	9.4
etacrynic acid	521	516	564	534	26.4	3.5
ethosuximide	301	284	297	294	8.9	9.5
ethylmorphine	291	283	289	288	4.2	8.2
fenoprofen	574	587	565	575	11.1	4.5
fentanyl	373	377	377	376	2.3	
flunitrazepam	483	459	480	474	13.1	1.8
fluphenazine †	462	480	391	444	47.1	3.9
furosemide	435	414	422	424	10.6	3.9
glibencamide	63	62	64	63	11.6	5.3
glipizide	478	464	493	478	14.5	
glutethimide	436	430	437	434	3.8	9.2
haloperidol	421	409	403	411	9.2	8.3
hexobarbital	419	404	416	413	7.9	8.2
hydrochlorothiazide	294	275	289	286	9.8	7.0
hydrocodone	286	262	268	272	12.5	8.3
hydromorphone	240	231	234	235	4.6	8.2
ibuprofen	616	650	620	629	18.6	4.4
imipramine	437	434	424	432	6.8	9.5
imipramine M (=desipramine)	424	421	414	420	5.1	10.5
indometacin	607	610	612	610	2.5	4.5
ketamine	311	294	293	299	10.1	7.5
lidocaine	288	285	282	285	3.0	7.9
lorazepam	444	422	423	430	12.4	1.3
lormetazepam	487	474	484	482	6.8	
loxapine	407	399	355	387	28.0	6.6
lysergide (=LSD)	362	358	342	354	10.6	7.5
meclozine	587	601	557	582	22.5	3.1
medazepam	405	395	355	385	26.5	6.2
mepivacaine	296	300	288	295	6.1	7.7
mescaline	272	255	258	262	9.1	3.6
metamizole (=dipyrone)	316	289	231	279	43.4	12.5
methadone	440	443	435	439	4.0	8.3
methadone M (=normethadone)	439	417	374	410	33.1	9.2
methamphetamine	262	255	259	259	3.5	10.1
methaqualone	459	455	435	450	12.9	2.5
methyl phenidate	328	316	311	318	8.7	8.8
methyl-3,4-methylenedioxyamphetamine	278	280	274	277	3.1	
metoprolol	326	317	313	319	6.7	9.7
morphine	200	198	212	203	7.6	8.0
nadolol	288	271	274	278	9.1	
nalorphine	260	237	243	247	11.9	7.8
naproxen	488	476	492	485	8.3	4.2
nicotinamide	168	146	92	135	39.1	3.3
nicotine	69	100	64	78	19.5	3.2
nifedipine	527	503	531	520	15.1	
niflumic acid	595	586	561	581	17.6	
nitrazepam	448	430	404	427	22.1	3.2
noscapine	368	354	339	354	14.5	6.2
oxazepam	441	441	422	435	11.0	1.7

Table C.1: (continued)

Substance	Table B.1	Bogusz	Hill	Mean	SD	pK_{a1}
oxycodone	277	260	262	266	9.3	8.9
oxyphenbutazone	501	503	516	507	8.1	4.7
papaverine	363	346	335	348	14.1	6.4
paracetamol (=acetaminophen)	264	234	257	252	15.7	9.5
pemoline	307	281	292	293	13.1	10.5
pentazocine	372	357	358	362	8.4	8.5
pentobarbital	424	405	409	413	10.0	8.0
pethidine	345	334	332	337	7.0	8.7
pethidine M (=norpethidine)	344	339	329	337	7.6	
phenacetin	377	356	371	368	10.8	2.2
phenazone	333	303	328	321	16.1	1.5
phencyclidine †	375	281	355	337	49.5	8.5
phenelzine †	184	377	193	251	108.9	
pheniramine	283	279	216	259	37.6	4.2
phenobarbital	379	357	366	367	11.1	7.4
phenylbutazone	672	651	687	670	18.1	4.4
phenytoin	431	415	413	420	9.9	8.3
prazepam	648	648	572	623	43.9	2.7
primidone	322	308	320	317	7.6	
probenecid	526	560	541	542	17.0	3.4
propoxyphene (=dextropropoxyphene)	442	438	409	430	18.0	6.3
propranolol	377	370	351	366	13.5	9.5
quinidine	322	316	261	300	33.6	4.2
quinine	327	308	276	304	25.8	4.1
reserpine	467	473	437	459	19.3	6.6
saccharin	291	254	295	280	22.6	1.6
salicylamide	327	305	319	317	11.1	8.2
salicylic acid	350	331	375	352	22.1	3.0
scopolamine (=hyoscine)	270	288	256	271	16.0	7.6
secbutabarbital (=butabarbital)	377	380	373	377	3.5	8.0
secobarbital	437	437	434	436	1.7	7.9
strychnine	302	292	296	297	5.0	2.3
temazepam	472	466	473	470	3.8	1.6
tetracaine	389	381	354	375	18.3	8.5
thebaine	340	324	316	327	12.2	8.2
theobromine	262	224	259	248	21.1	1
theophylline	276	239	270	262	19.9	1
thioridazine	490	504	454	483	25.8	9.5
tolbutamide	477	470	474	474	3.5	5.3
tranlycypromine	230	241	232	234	5.9	8.2
trifluoperazine †	480	491	396	456	52.0	8.1
trimethoprim	299	345	286	310	31.0	7.2
tripelenamine †	336	337	237	303	57.4	3.9
triprolidine (HCl) †	388	360	276	341	58.3	6.5
verapamil	447	454	437	446	8.5	
warfarin	546	555	538	546	8.5	5.0
yohimbine	348	333	318	333	15.0	
mean	382.6	373.9	364.5	373.5	16.1	
SD	109.5	112.4	111.0	109.8	14.9	