

Supplemental Material: "Design and Characterization of a Functional Library for NMR Screening against Novel Protein Targets." K.A. Mercier, K. Germer, and R. Powers

	Mixture	Amino Acid	Carbohydrates	Co-factor	DNA/RNA	Drug	Fatty Acid/Lipid	Hormone	Metabolite	Neurotransmitter	Nucleotide	Protein Inhibitor	Substrate	Vitamin	MW	Cost	Heteratoms	clogP	aromatic rings	aliphatic rings
Adenosine 5'-triphosphate disodium salt (ATP)	1001										X		X		179.2	\$26.70	8	1.4	2	1
Cinoxacin						X						X			333.4	\$32.40	7	-1.4	1	2
Cycloheximide				X											99.17	\$17.40	6	-3.6	0	0
Sodium glycocholate hydrate (Bile salt)				X											86.03	\$26.40	4	-1.7	0	0
Cytidine 5'-triphosphate disodium salt (CTP)	1002										X		X		479.6	\$99.60	6	3.0	1	3
Cytochalasin B									X						179.2	\$10.60	6	-3.1	0	0
Doxycycline hyclate						X						X			230.3	\$8.90	3	2.8	2	0
L-Glutathione reduced				X											155.2	\$10.10	5	-3.7	0	1
Colchicine	1003					X									251.2	\$35.00	8	1.9	0	8
Nalidixic acid						X						X			311.4	\$73.30	4	0.7	1	4
Tetrahydropteridine				X											182.2	\$19.90	6	0.3	0	2
Acetylsalicylic acid (aspirin)	1004					X						X	X		162.3	\$8.45	3	-3.3	0	0
Biotin (vitamin H)				X									X	X	424.5	\$19.90	7	4.5	3	3
Thymidine 5'-triphosphate sodium salt (TTP)				X									X		478.1	\$50.50	19	-3.8	0	2
Methoxatin (PQQ)	1005			X											166.2	\$25.60	11	-0.7	0	2
Ouabain								X				X			387.4	\$16.20	9	2.1	1	3
Praziquantel						X									360.4	\$8.00	5	1.4	0	4
Uridine 5'-triphosphate trisodium salt dihydrate (UTP)											X		X		481.1	\$25.05	20	-4.6	0	2
Adenosine 3',5'-cyclic monophosphate (cyclic AMP)	1006										X		X		347.2	\$25.70	13	-3.2	1	2
Ethosuximide						X									165.2	\$14.80	3	0.9	1	0

L-Leucine (Leu)		X									X		256.3	\$14.60	3	3.2	2	0	
Neostigmine					X						X		429.4	\$144.60	13	-2.5	0	2	
Benzamidine hydrochloride hydrate	1007										X	X	122.1	\$13.70	4	5.1	0	1	
Guanosine 3',5'-cyclic monophosphate sodium salt (cyclic GMP)												X	X	519.2	\$29.05	22	-5.5	0	2
L-Isoleucine (Ile)		X											102.1	\$21.80	3	-0.9	0	0	
N-Phospho-Ile(O-ethyl)-Tyr(O-benzyl)-Gly dipotassium salt											X		116.2	\$28.20	1	5.1	0	0	
4-Aminobenzoic acid (PABA, vitamin H1)	1008			X								X	X	137.1	\$7.35	3	1.0	1	0
8-Methoxypsoralen					X								336.4	\$17.80	6	1.7	1	0	
Deoxyadenosyl cobalamin (Vitamin B12)				X								X	X	218.3	\$43.40	5	-3.1	0	1
MDL 28170											X		167.3	\$27.10	1	2.8	0	2	
Cantharidin	1009										X		217.3	\$90.90	5	0.9	0	1	
Coenzyme A sodium salt hydrate				X								X	399.4	\$11.95	7	1.2	1	3	
L-Arginine (Arg)		X										X	133.1	\$13.60	4	-7.0	3	2	
L-Carnitine inner salt (vitamin Bt)				X								X	X	147.1	\$8.80	5	-2.7	0	0
Calmidazolium chloride	1010										X		348.4	\$55.00	6	0.9	2	3	
L-Lysine (Lys)		X										X	149.2	\$9.10	4	-1.7	0	0	
Pantothenate (vitamin B5)				X								X	X	333.4	\$31.75	7	-0.7	1	2
Acetamide	1011										X	X	222.3	\$23.00	1	4.3	1	0	
b-Nicotinamide adenine dinucleotide phosphate (NADP+,NADPH)				X								X	251.3	\$12.30	4	2.4	1	1	
L-Histidine (His)		X										X	234.3	\$44.10	3	2.0	1	0	
S-(5'-Adenosyl)-L-methionine chloride		X		X									237.2	\$48.20	8	1.8	0	2	
b-Nicotinamide adenine dinucleotide (NAD+, NADH)	1012			X								X	665.4	\$50.50	23	-5.0	1	4	
Chymostatin											X		238.3	\$37.60	7	0.0	0	1	
L-Aspartic acid (Asp)		X										X	179.6	\$27.20	4	-7.0	0	0	
O-Phospho-L-serine		X											261.2	\$25.20	8	-3.6	1	0	
L-Alanine (Ala)	1013	X										X	174.2	\$12.00	5	-3.4	0	0	
O-Phospho-L-tyrosine		X											330.4	\$12.80	7	3.6	3	0	
Thiamine hydrochloride (Vitamin B1)				X									X	425.3	\$9.20	15	-5.0	1	1

Aminophylline hydrate	1014					X						X			291.4	\$23.10	1	5.4	2	1
Phenylmethanesulfonyl fluoride (PMSF)												X			164.2	\$10.40	3	-3.1	1	0
Thiamine pyrophosphate (TPP)				X									X		425.3	\$10.50	15	-6.4	1	1
4-(2-Aminoethyl)benzenesulfonyl fluoride hydrochloride (AEBSF)	1015											X			203.2	\$25.35	5	1.6	1	0
erythro-9-(2-Hydroxy-3-nonyl)adenine hydrochloride												X			275.4	\$39.00	4	3.1	1	0
Tetrahydrofolate (Folic acid, vitamin M)				X									X	X	430.4	\$8.95	12	-3.5	1	2
4-Chloromercuribenzoic acid	1016											X			357.2	\$12.95	8	-3.7	1	0
6-Hydroxydopamine hydrochloride (6-hydroxyDOPA)				X											202.3	\$31.90	3	1.6	1	2
Ceftriaxone sodium salt						X						X			554.6	\$38.90	13	-2.7	0	3
L-Tyrosine (Tyr)		X											X		399.4	\$44.00	6	0.3	1	3
Allopurinol	1017											X			151.3	\$17.00	5	2.9	1	1
L-2-Aminoadipic acid												X	X		89.09	\$7.45	16	-1.4	2	1
L-Tryptophan (Trp)		X											X		181.2	\$9.10	26	-3.9	1	0
L-Serine (Ser)	1018	X											X		119.1	\$9.70	4	-2.4	0	0
Methyl 6,7-dimethoxy-4-ethyl-b-carboline-3-carboxylate						X						X			289.3	\$32.10	10	-1.7	0	2
Pepstatin A												X			354.4	\$11.40	6	-2.8	3	1
Pyridoxine (Vitamin B6)				X									X	X	172.1	\$37.40	7	-3.0	0	0
Daphnetin; 7,8-Dihydroxycoumarin	1019											X	X		527.5	\$29.30	11	0.9	2	3
Idazoxan hydrochloride												X			357.8	\$33.20	5	-0.3	1	1
Lorglumide sodium salt												X			115.1	\$9.60	3	-2.4	0	1
L-Threonine (Thr)		X											X		204.2	\$11.40	4	-1.6	1	1
Bepridil hydrochloride	1020											X			308.4	\$21.00	6	-0.3	1	0
Flavin adenine dinucleotide (FAD,FADH2)				X									X		276.2	\$21.80	7	0.6	1	0
L-Glutamic acid (Glu)		X											X		146.1	\$38.30	5	-3.4	0	0
Suramin						X									1291	\$54.70	35	0.0	8	0
4-Aminobenzamidine dihydrochloride	1021											X			135.2	\$5.00	3	-0.5	1	0
Indomethacin						X						X			348.2	\$14.70	13	-4.2	0	2
L-Glutamine (Gln)		X											X		307.3	\$14.20	10	-3.1	0	0

N-Phenylanthranilic acid												X			551.5	\$87.55	14	-0.9	2	0
Bay 11-7085	1022											X			121.1	\$18.10	3	-0.5	0	0
L-Methionine (Met)		X											X		321.2	\$22.85	6	4.8	2	1
Nicotinic acid (Niacin, vitamin B)				X									X	X	346.3	\$31.80	8	3.1	1	1
Penicillin G potassium salt (benzyl penicillin)						X							X		238.3	\$39.40	2	0.0	1	0
Estradiol	1023					X		X					X		288.4	\$29.00	3	3.2	1	3
L-Proline (Pro)		X											X		105.1	\$12.80	4	-2.7	0	0
Ranolazine dihydrochloride													X		197.2	\$73.40	3	1.6	1	2
Rifampicin						X									340.4	\$50.25	7	0.1	2	1
Diethylenetriaminepentaacetic acid	1024												X		268.4	\$47.00	2	3.7	2	3
Puromycin dihydrochloride hydrate					X	X							X		247.1	\$26.45	8	-1.7	1	0
Ribavirin						X							X		822.9	\$21.76	16	0.0	3	3
trans-4-Hydroxy-L-proline		X											X		131.1	\$11.30	4	-1.9	0	1
(±)-Epinephrine	1025							X		X			X		183.2	\$31.85	6	-2.1	2	0
2,3,5,6, Tetramethyl-P-Benzoquinone (Duroquinone)													X		164.2	\$21.35	2	2.3	0	1
Acetylthiocholine chloride													X		265.4	\$19.34	8	3.8	0	0
rac-Glycerol 3-phosphate disodium salt						X							X		316.4	\$17.50	8	0.6	0	1
4-Methylpyrazole hydrochloride	1026												X		82.1	\$19.95	2	0.5	0	1
a-Methyl-DL-tyrosine		X											X		240.3	\$14.70	8	0.0	0	2
Chelidamic acid													X		323.1	\$24.20	3	2.7	3	0
Lonidamine						X							X		457.4	\$56.70	7	5.7	1	0
6-Methoxy-1,2,3,4-tetrahydro-9H-pyrido[3,4-b]indole	1027												X		276.1	\$51.80	11	-4.2	0	0
g-Aminobutyric acid (GABA)						X							X		270.2	\$63.60	5	2.4	2	1
Naloxone hydrochloride dihydrate						X							X		230.3	\$33.30	3	2.8	2	1
Picotamide													X		310.3	\$79.00	7	-1.5	0	4
(-)-Tetramisole hydrochloride	1028					X							X		204.3	\$21.65	3	1.8	1	2
3'-Azido-3'-deoxythymidine						X							X		94.11	\$16.40	2	2.4	3	1
Atropine sulfate salt hydrate													X	X	282.3	\$29.16	7	-0.3	1	1
Captopril						X							X		236.3	\$33.40	3	2.4	2	1

1-Carbamoylmethyl-3-carbamoyl-1,4-dihydropyrimidine	1029					X						X		184.2	\$47.70	1	1.1	3	1
Chlorzoxazone						X						X		104.2	\$9.90	2	-4.4	0	0
DL-p-Chlorophenylalanine						X						X		253.3	\$71.35	5	1.7	1	0
Melatonin								X				X	X	172.2	\$13.30	2	2.5	1	1
(±)-2,3-Dichloro-a-methylbenzylamine hydrochloride	1030											X		190.1	\$48.50	3	2.7	1	0
(±)-Thalidomide						X						X		258.2	\$39.10	6	0.5	1	2
7,7-Dimethyl-(5Z,8Z)-eicosadienoic acid												X		328.4	\$38.50	4	-1.4	0	0
Genistein						X						X	X	352.8	\$42.00	6	1.2	1	1
(1R,2S)-(-)-Ephedrine	1031							X					X	165.2	\$29.10	2	0.9	1	0
3,5-Dinitrocatechol												X		433	\$27.80	6	-0.3	1	0
Choline bromide												X		607.7	\$68.05	13	0.1	2	1
D-(+)-Maltose monohydrate			X										X	253.2	\$30.10	9	-3.8	1	1
(±)-Norepinephrine (+)-bitartrate salt	1032									X			X	169.2	\$44.25	4	-1.0	1	0
3-Amino-2,3-dihydrobenzoic acid hydrochloride												X		202.1	\$63.60	8	-5.7	1	1
Methiothepin mesylate salt												X		454.4	\$18.30	13	-0.5	3	3
Sucrose			X										X	342.3	\$9.90	11	-3.1	0	2
3-Indoleacetic acid	1033							X				X		175.2	\$26.65	6	1.4	1	0
3-Isobutyl-1-methylxanthine												X		222.2	\$19.10	6	1.4	0	2
Acetylcholine						X				X			X	180.2	\$5.72	4	1.0	1	0
Alaproclate hydrochloride												X		374.5	\$79.70	5	0.4	0	5
Carbetapentane citrate salt	1034											X		260.3	\$24.70	3	3.2	2	1
D-(+)-Glucose			X										X	342.3	\$9.80	11	-4.4	0	2
Dopamine hydrochloride										X			X	543.5	\$22.80	12	0.4	2	3
N-Acetyl-L-tryptophan 3,5-bis(trifluoromethyl)benzyl ester												X		245.3	\$13.60	3	-1.0	0	1
3-Indoleacetic acid	1035					X						X		175.2	\$26.65	6	1.4	1	0
Lipoic acid						X							X	131.2	\$9.10	3	-1.8	0	0
Sodium DL-lactate													X	487.6	\$14.45	8	-0.5	0	4
(±)-a-Lipoamide	1036					X							X	205.3	\$10.20	4	1.5	0	1
3-Aminopropionitrile fumarate salt												X	X	143.2	\$122.85	3	-1.9	0	1

D-Sorbitol			X			X					X	X		274.2	\$72.60	5	0.2	3	3
Hydrocortisone (cortisol)						X		X				X		206.3	\$206.28	2	3.7	1	0
3-Indoleacetic acid	1037						X					X		175.2	\$15.55	6	1.4	1	0
Caffeine						X						X		652.3	\$78.00	9	5.4	4	1
Phenylbutazone												X		174.2	\$13.58	4	1.8	1	0
a-Lactose monohydrate	1038		X									X		255.7	\$33.90	4	3.1	1	0
Betaine hydrochloride		X						X				X	X	330.2	\$11.30	10	-0.1	0	2
Progesterone								X				X		116.1	\$25.10	4	0.0	0	1
Serotonin hydrochloride								X		X		X		482.4	\$10.70	1	2.2	0	5
3-(1-Naphthyl)-D-alanine	1039	X												215.3	\$50.60	3	-0.4	2	0
Histamine		X								X		X		182.2	\$8.30	4	0.6	1	0
Sodium citrate tribasic dihydrate												X		211.1	\$14.60	9	-1.7	0	0
(-)-Cotinine	1040							X						176.22	\$52.55	3	-0.3	1	1
Porphobilinogen												X		312.4	\$17.25	6	3.4	1	3
Sodium succinate dibasic							X					X		157.4	\$27.52	5	2.8	1	1
Vasopressin						X		X		X				1084	\$123.80	29	0.0	2	2
1-Octen-3-ol	1041						X					X		128.2	\$20.50	1	2.4	0	0
N-Vanillynonanamide												X		185.1	\$10.85	8	-3.7	0	0
Phospho(enol)pyruvate potassium salt												X		184.2	\$28.00	6	0.1	0	0
12-Hydroxydodecanoic acid	1042						X							216.3	\$23.30	6	3.2	0	0
Adenine (Vitamine B4, 6-Aminopurine)				X						X		X	X	329.2	\$17.20	12	-2.5	1	3
Sodium pyruvate												X		138.1	\$0.00	3	0.3	1	0
D-(+)-Gluconic acid-lactone	1043		X									X		180.2	\$15.00	6	-2.2	0	1
D-Panthenol (R)-(+)-2,4-Dihydroxy-N-(3-hydroxypropyl)-3,3-dimethylbutyramide)				X								X	X	182.2	\$14.80	6	-2.0	0	0
Eserine (Physostigmine)						X						X		272.4	\$20.40	2	3.8	1	3
Menadione (2-Methyl-1,4-naphthoquinone, vitamin k3)				X									X	447.6	\$21.30	6	-1.7	1	1
Lithium acetoacetate	1044						X							138	\$55.80	6	-1.3	0	0
N-Acetyl-L-tryptophanamide												X		309.3	\$24.90	6	-2.0	3	1
Novobiocin sodium salt											X	X		213.2	\$25.90	3	4.3	2	0
3,5-Diiodo-L-tyrosine dihydrate	1045											X	X	122.2	\$13.50	2	2.4	2	0

3-Iodo-L-tyrosine		X									X	X		307.1	\$22.60	3	-1.2	1	1
Cyclo(His-Pro)		X											X	234.3	\$51.00	6	-1.9	0	3
(±)-Carnitine chloride	1046					X						X		176.2	\$8.41	4	-4.8	0	0
N-p-Tosyl-L-phenylalanine chloromethyl ketone											X			624.6	\$44.70	13	-3.5	2	1
Theophylline (2,6-dihydroxy-1,3dimethylpurine						X					X			182.2	\$19.90	6	-0.8	0	2
1-(4-Chlorobenzyl)-5-methoxy-2-methylindole-3-acetic acid	1047										X			343.8	\$79.60	4	1.8	0	0
Buspirone hydrochloride						X						X		194.2	\$9.10	6	0.0	0	2
4-Deoxypyridoxine hydrochloride	1048			X									X	153.2	\$38.00	3	0.7	1	0
5-Bromo-4-chloro-3-indolylb-D-galactopyranoside			X									X		408.6	\$38.40	4	5.3	3	2
6,7-Dimethyl-5,6,7,8-tetrahydropterine hydrochloride				X										195.2	\$10.80	6	2.9	1	1
Guanosine 5'-triphosphate sodium salt hydrate (GTP)										X		X		291.4	\$77.40	5	1.6	2	1
Boc-L-phenylalaninol	1049	X												294.4	\$27.10	3	1.4	1	0
Ellipticine					X	X					X			277.4	\$110.50	6	2.0	1	1
Sepiapterin				X								X		176.2	\$19.80	3	0.8	1	1
Mitoxantrone dihydrochloride	1050				X	X								243.2	\$33.70	6	6.4	1	2
N-Succinyl-Ala-Ala-Pro-Phe p-nitroanilide												X		177.2	\$12.00	2	3.0	1	0
N-tert-Butyl-a-phenylnitrone											X	X		241.3	\$67.70	2	-0.6	0	0
Thioctic acid				X								X	X	206.3	\$13.60	4	2.4	0	1
Aztreonam	1051					X								249.3	\$77.15	4	2.3	1	0
Chelerythrine chloride											X			183.1	\$63.90	6	-1.6	0	1
D-(+)-Neopterin				X								X		335.5	\$17.70	6	2.7	2	0
[Hydroxy(tosyloxy)iodo]benzene	1052											X		390.2	\$23.00	4	2.2	2	0
2-Chloro-5,5-dimethyl-1,3-cyclohexanedione											X			174.6	\$42.00	3	1.2	0	1
Phosphoramidon disodium salt											X			376.4	\$48.75	7	1.0	2	0
Xanthtoxin L-Methionine sulfoximine											X			180.2	\$40.30	10	-0.5	2	3

5,5-Diphenylhydantoin	1053					X								252.3	\$17.00	18	-1.7	2	0
L-Leucine-b-naphthylamide		X									X			149.2	\$9.10	4	-3.2	0	0
Sodium creatine phosphate dibasic tetrahydrate											X			90.08	\$35.25	3	-0.7	0	0
Warfarin						X								308.3	\$12.00	10	1.7	2	2
Adenosine 5'-monophosphoric acid (AMP)	1054									X		X		505.2	\$26.80	18	-4.6	1	2
Ethidium Bromide					X									141.2	\$16.75	3	0.4	0	1
Sodium oxamate											X	X		88.06	\$26.00	3	-0.9	0	0
1-Methylimidazole	1055	X									X			82.1	\$18.60	2	1.3	0	0
2-Fluoroaniline											X			111.1	\$13.30	3	-3.4	1	1
3,4-Dimethylaniline											X			621.9	\$35.30	9	0.5	3	1
Dansylcadaverine											X			308.4	\$19.10	7	2.2	2	0
1-Aminocyclopropanecarboxylic acid	1056										X			101.1	\$38.50	5	-1.1	2	0
Pentaethylene glycol						X								278.3	\$29.30	7	0.1	0	2
Phenylpyruvic acid								X			X			168	\$85.40	7	-1.0	0	0
Tyramine		X									X			137.2	\$7.60	7	-1.5	4	1
2-Chloro-1,3,2-dioxaphospholane	1057					X								387.4	\$16.20	9	2.1	1	3
Acridine Orange base					X						X			225.2	\$44.95	2	2.8	0	2
Oxacillin						X								261.2	\$22.70	10	0.2	0	2
Tubercidin					X	X				X				266.3	\$23.10	3	1.4	1	0
3-Aminopyridine	1058									X		X		186.2	\$30.75	6	-0.2	0	0
Lithium potassium acetyl phosphate											X			131.2	\$8.80	3	-1.7	0	0
S-(-)-Carbidopa						X					X			418.9	\$34.50	12	-1.8	0	3
Triethylenetetramine						X								146.2	\$14.50	4	-2.4	0	0
2-Amino-5-methylthiazole	1059										X			114.2	\$17.90	3	0.7	0	1
3,4-Dimethylphenol											X			121.2	\$16.50	4	-1.3	2	0
Bisbenzimidazole H 33258					X									356.1	\$17.30	7	2.6	2	2
Cytidine 5'-monophosphate (CMP)									X		X			481.1	\$27.10	20	-4.8	0	2
2-Amino-4-methylphenol	1060										X			123.2	\$17.40	2	0.7	1	0
2-Aminopyridine									X					94.11	\$10.80	2	0.3	2	0
Inosine 5'-monophosphate disodium salt									X		X			286.2	\$26.70	1	9.4	3	1
2-Aminophenol	1061										X			109.1	\$17.60	12	1.1	1	0

2-Ethylimidazole		X									X		96.13	\$15.60	1	0.8	1	0
Kaempferol										X	X		189.2	\$9.10	2	6.8	2	2
2-Ketoglutaric acid	1062	X									X		146.1	\$16.70	4	-1.6	0	0
2-Methylimidazole		X									X		82.1	\$6.70	2	-0.8	1	1
Bromophenol Blue											X		371.5	\$36.30	7	1.2	1	3
Uridine 5'-monophosphate									X		X		324.2	\$65.20	2	12.5	0	0
2'-Deoxyadenosine 5'-monophosphate (dAMP)	1063								X		X		331.2	\$15.90	12	-2.7	1	2
Cordycepin					X				X				466.4	\$27.80	10	2.1	4	0
Netropsin dihydrochloride hydrate					X								123.1	\$10.50	3	0.8	1	0
2-Aminofluorene	1064				X								181.2	\$35.00	1	2.9	2	1
2'-Deoxyadenosine 3'-monophosphate sodium salt									X				315.2	\$72.80	11	-2.0	1	2
Didecyldimethylammonium bromide						X							393.4	\$31.00	13	-2.1	0	0
2-Cyclohexen-1-one	1065										X		96.13	\$19.60	7	-1.8	0	4
Cyclohexylamine											X		261.1	\$27.80	7	0.8	0	1
Picrotin										X			414.4	\$15.90	8	3.7	2	3
(-)-Bilobalide	1066									X			310.30	\$75.80	7	-1.0	0	4
Metergoline					X					X			356.6	\$51.60	4	5.3	2	2
Pseudothiohydantoin									X		X		186.2	\$28.90	3	-2.2	1	2
Ureidosuccinic acid		X											176.1	\$6.95	4	-0.4	0	1
2-Aminothiazol	1067	X									X		100.1	\$15.90	2	0.1	0	0
2-Hydroxyethyl disulfide											X		154.3	\$35.80	7	-1.0	0	0
Androsterone						X					X		188.2	\$7.10	2	4.4	1	2
Dimethyl 2-oxoglutarate		X									X		224.2	\$25.10	7	2.1	3	1
1-Methylhistamine dihydrochloride	1068							X					125.2	\$72.70	3	-1.0	0	1
2',3'-Dideoxyadenosine									X	X			235.2	\$48.90	3	0.5	0	4
DL-Thiorphan					X					X			301.4	\$39.60	4	2.4	1	0
2,3-diphosphoglycerate pentasodium salt	1069										X		261	\$25.05	12	-5.1	0	0
Hydralazine hydrochloride											X		297.7	\$38.80	4	-0.7	1	0
N-Propyl-1,3-propanediamine						X							351.9	\$14.30	13	2.9	0	1
Pyridoxal 5'-phosphate				X							X		169.2	\$16.60	4	-0.8	1	0
(-)-Perillic acid	1070										X	X	166.22	\$46.10	2	2.8	0	1

Benzamide												X	X		120.2	\$21.25	2	0.7	1	0
D(+)-Galactosamine hydrochloride			X										X		178.1	\$9.50	6	1.4	0	0
3-Quinolinecarboxylic acid	1071					X									173.2	\$26.40	3	-0.4	3	1
Aldosterone								X					X		287.2	\$21.94	3	-0.1	2	0
Alizarin Yellow R													X		136.1	\$24.60	5	0.6	1	1
Ampicillin						X							X		290.4	\$6.95	8	0.1	0	0
Clofibrate	1072					X							X		230.1	\$30.60	5	1.7	1	1
Furosemide						X							X		103.1	\$11.20	3	-2.8	0	0
Ibuprofen						X									204.2	\$34.25	4	1.8	1	2
Naproxen						X							X		223.3	\$29.85	4	2.8	1	0
Bromocresol Green	1073													X	670	\$11.40	7	1.9	0	0
Digitoxin			X			X							X		174.2	\$14.30	2	3.6	0	1
Methyl 4-hydroxyphenylacetate														X	314.3	\$59.60	6	3.1	2	1
Phenol Red														X	308.4	\$19.95	4	2.4	2	1
6,9-Diamino-2-ethoxyacridine-DL-lactate monohydrate	1074					X									253.3	\$21.40	4	3.4	3	0
Ciprofloxacin						X							X		277.2	\$19.30	5	2.4	1	0
Cyclo(His-Pro)			X						X						281.3	\$39.70	5	-0.3	0	2
N-Acetylneuraminic acid			X											X	291.4	\$50.20	5	1.9	1	0
3-Chlorophenol	1075													X	268.3	\$32.50	9	0.0	0	2
6,9-Diamino-2-ethoxyacridine-DL-lactate monohydrate						X									169.2	\$51.00	4	-0.6	1	0
Orange II sodium salt														X	598.7	\$23.20	12	-3.6	0	6
Phosphocholine chloride calcium salt tetrahydrate								X						X	543.5	\$130.65	14	1.5	1	3
3-Chlorophenol	1076													X	128.6	\$11.60	2	0.3	3	0
Acetazolamide						X							X		146.2	\$8.14	3	-3.5	0	0
Benzylamine														X	366.5	\$85.60	3	6.0	2	1
Methotrexate				X											454.4	\$32.90	13	-0.5	3	3
Diethylstilbestrol	1077					X		X							761	\$23.50	11	0.0	0	8
Doxorubicin hydrochloride					X	X								X	444.4	\$18.80	10	-0.5	1	3
Psoralen					X	X									321.4	\$47.20	5	4.7	2	2
Tolbutamide						X								X	270.4	\$20.60	13	-0.5	0	6

(±)-Verapamil hydrochloride	1078					X						X	X		491.1	\$54.10	4	0.6	1	1
Diclofenac sodium salt						X						X			326.6	\$38.40	1	4.3	0	0
Estriol								X	X				X		314.4	\$10.60	-	-0.7	-	-
Amoxicillin	1079					X						X			365.4	\$14.00	2	-1.8	1	0
Bestatin hydrochloride												X			308.4	\$21.00	3	-2.9	0	0
Dansylglycin						X							X		178.1	\$66.60	4	1.2	1	1
Diaminobiotin									X						296.2	\$34.90	5	4.6	2	0
5-Hydroxyindole-3-acetic acid	1080								X						191.2	\$15.00	3	2.2	1	0
Benzoic acid													X		107.2	\$8.10	1	3.6	1	0
H-7 dihydrochloride												X			211.7	\$18.40	3	1.4	1	0
Resveratrol												X	X		244.2	\$18.10	9	-2.9	0	2
1,3-Dimethyluric acid	1081								X		X				196.2	\$12.90	6	-0.3	1	0
Chlortetracycline hydrochloride						X									169.6	\$11.90	5	1.7	1	1
Flutamide						X						X			294.3	\$25.00	7	0.7	1	1
Kynurenic acid													X		161.2	\$16.95	5	-2.5	0	0
(-)-Arctigenin	1082											X			358.39	\$38.00	6	1.5	2	1
5-Phenylvaleric acid													X		178.2	\$19.30	3	2.4	0	3
Agmatine sulfate salt		X								X			X		342.3	\$12.15	7	1.0	1	2
Diminazene aceturate					X	X									311.4	\$19.50	8	-0.9	1	1
Podophyllotoxin	1083					X									225.2	\$157.60	5	-2.8	0	1
Roscovitine												X			226.2	\$47.00	6	2.0	1	0
Silibinin													X		138	\$58.40	3	-0.5	0	0
tert-Butyl carbazate		X				X									132.2	\$14.40	4	0.3	0	0
4-Hydroxy-3-methoxyphenylglycol sulfate potassium salt	1084														264.3	\$40.60	8	-1.5	1	0
Carisoprodol						X			X						427.5	\$48.90	12	-1.2	0	3
Ethylenediaminetetraacetic acid												X			783.5	\$32.10	26	-3.4	2	4
Mycophenolic acid						X									387.5	\$34.80	7	2.6	0	0
5α-Androstane-3,17-dione	1085								X				X		302.5	\$29.10	2	3.7	0	4
Lumicolchicine									X						382.5	\$102.20	6	3.6	2	0
PTH-tryptophan		X													471.5	\$39.20	12	0.0	2	2
Sodium cacodylate trihydrate													X		258.1	\$12.24	10	-2.4	0	0

2-Fluoro-2-deoxy-D-glucose 6-phosphate barium salt	1086								X		X					262.1	\$29.40	6	1.6	0	0
AY 9944											X					391.4	\$52.50	4	6.4	2	1
Cimetidine						X						X	X			252.3	\$37.60	12	-1.2	0	2
N-tert-Butyldimethylsilyl-N-methyltrifluoroacetamide																293.4	\$26.05	3	-0.4	0	1
6-Phosphogluconic acid trisodium salt	1087						X						X			336.6	\$55.95	2	9.2	0	0
Haloperidol metabolite I									X							111.1	\$18.37	3	-1.0	0	1
Nitrendipine						X						X				612.6	\$22.20	13	2.9	2	2
Resorufin acetate													X			228.2	\$57.00	3	-0.5	3	0
(±)-Camphor	1088					X							X			152.2	\$16.30	3	7.9	0	0
Amantadine hydrochloride						X										195.2	\$24.10	4	-1.7	1	0
Oxolinic acid						X						X				194.2	\$37.40	5	-0.3	1	0
Tyrphostin 25												X				202.2	\$44.50	2	2.8	0	0
(±)-Propranolol hydrochloride	1089					X							X			259.3	\$21.60	10	-1.9	0	3
Adrenochrome								X	X							312.3	\$26.90	7	0.3	1	0
Astemizole						X						X	X			266.3	\$23.70	7	6.1	1	0
Homovanillic acid									X				X			160.2	\$28.10	4	1.0	2	0
Cefoxitin	1090					X						X				554.6	\$38.90	18	-1.6	0	4
Cephalexin hydrate						X										348.4	\$87.20	5	-3.5	4	1
Cyproheptadine hydrochloride						X						X				323.2	\$21.50	12	-3.3	0	1
N-(1H-Benzotriazol-1-ylphenylmethyl)benzamide						X										184.2	\$70.70	4	1.9	0	1
1-Octanol	1091						X					X	X			130.2	\$20.00	8	2.6	1	0
Aflatoxin B1													X			130.2	\$30.20	4	-1.8	0	0
Daunorubicin hydrochloride						X						X	X			1580	\$16.25	37	0.0	2	7
p-Aminohippuric acid		X														218.2	\$15.00	6	-4.5	0	0
(-)-Bicuculline methiodide	1092											X				382.39	\$31.40	7	4.1	4	2
3-Hydroxy-DL-kynurenine									X							224.2	\$38.70	23	0.0	3	1
7-Deazaguanine											X	X				216.2	\$21.10	5	-1.1	0	1
trans-4-(Aminomethyl)cyclohexanecarboxylic acid		X										X				157.2	\$25.10	3	-1.8	0	1

5-Fluoro-5'-deoxyuridine	1093				X						X	X			246.2	\$34.50	6	1.0	2	0
5-Hydroxyisophthalic acid					X										182.1	\$14.00	11	0.9	1	1
Chloramphenicol					X						X	X			274.8	\$50.40	7	3.0	1	0
Dipyrene					X						X				198.2	\$9.60	7	2.7	3	0
3-Hydroxy-4-methoxyphenethylamine hydrochloride	1094								X						167.2	\$37.80	3	0.6	1	0
DL-4-Hydroxy-3-methoxymandelic acid									X						199.6	\$24.80	3	-0.8	1	0
Mecamylamine hydrochloride					X						X				232.3	\$41.60	4	1.0	1	1
Nifedipine					X						X				348.4	\$34.50	7	3.4	1	1
3-Indoleacrylic acid	1095										X				187.2	\$35.90	2	2.8	0	2
Clindamycin hydrochloride					X						X				242.7	\$28.30	6	-2.6	1	0
Sulindac Sulfide									X		X				340.4	\$31.80	4	-1.8	2	1
Taxifolin											X	X			304.3	\$36.00	7	0.9	2	1
4-Hydroxytamoxifen	1096										X	X			387.5	\$44.80	1	6.2	3	0
N-Acetylprocainamide hydrochloride									X			X			309.4	\$42.00	7	3.4	1	4
Tamoxifen					X						X	X			371.5	\$43.30	2	6.8	3	0
2,6-Diisopropylphenol	1097				X						X	X			178.3	\$15.70	1	3.9	1	0
4-Guanidinobutyric acid		X							X		X				159.2	\$27.40	6	-4.1	1	0
Tyrphostin 1											X				184.2	\$28.80	3	-1.8	1	0
Atenolol	1098				X						X				288.4	\$23.70	8	-1.3	0	1
Methotrexate hydrate					X						X				330.2	\$163.10	10	1.7	1	2
Nadolol					X						X				232.2	\$14.80	5	-1.1	1	1
Procaine hydrochloride					X						X				314.5	\$13.20	2	3.8	0	4
Clonidine hydrochloride	1099				X							X			783.5	\$45.15	28	-4.9	0	3
Prednisolone					X	X	X				X	X			236.3	\$16.40	4	2.5	1	0
Ranitidine hydrochloride					X						X				413.5	\$90.00	4	1.2	2	1
Timolol maleate salt					X										316.4	\$35.20	8	1.6	0	2
(-)-Scopolamine hydrobromide trihydrate	1100				X						X				303.4	\$34.90	5	0.3	1	3
Camptothecin											X				196.2	\$35.40	12	-3.6	2	0
Myristic acid						X									328.4	\$30.80	5	3.7	3	1
Acycloguanosine	1101										X	X	X		225.2	\$49.30	7	2.6	1	0
Antipyrine					X										1300	\$39.00	28	0.2	1	6
Ceftriaxone sodium salt					X						X				347.4	\$38.30	8	-1.8	1	2

Cimetidine						X						X	X		262.2	\$43.50	7	1.7	1	2
2,3,5-Triiodobenzoic acid	1102												X		499.8	\$29.40	10	-2.1	0	2
3,3',5-Triiodothyroacetic acid							X						X		621.9	\$35.30	0	0.0	0	1
Clenbuterol hydrochloride						X	X						X		423	\$38.60	8	2.6	1	1
Tetracycline						X						X			446.5	\$10.80	10	-1.5	1	3
4-Androstene-3,17-dione	1103							X					X		286.4	\$17.10	2	2.8	0	4
Carbamazepine						X							X		190.2	\$15.50	2	2.9	1	1
Amitriptyline hydrochloride	1104					X						X			365.4	\$14.00	2	0.0	1	0
Cromolyn sodium salt						X									234.3	\$51.00	6	-1.9	0	3
Sodium salicylate						X							X		116.1	\$13.50	4	-6.5	0	0
2,3,5-Triiodobenzoic acid	1105												X		499.8	\$29.40	10	-2.1	0	2
Amoxicillin						X						X			347.4	\$36.70	7	-0.3	1	2
Dobutamine hydrochloride													X		153.2	\$18.50	3	0.2	1	0
Pentoxifylline						X						X			685.9	\$101.75	14	0.0	0	0
3-Methoxytyramine hydrochloride	1106							X					X		167.2	\$31.10	3	0.6	1	0
5-Fluorocytosine					X					X					127.1	\$61.80	3	0.7	1	0
Acycloguanosine										X	X	X			135.1	\$23.50	5	-0.2	1	1
Aquocobalamin (Vitamin B12a)				X										X	458.6	\$31.00	7	4.5	0	2
Bithionol	1107					X									265.4	\$13.95	6	-4.7	1	4
Chlorpropamide						X	X								492.9	\$20.00	11	0.5	1	3
Cyclophosphamide monohydrate				X	X										295.5	\$27.80	1	6.0	1	3
Griseofulvin						X									345.2	\$24.25	13	-3.5	0	4
(+)-Pseudoephedrine hydrochloride	1108					X	X								165.2	\$30.20	2	0.9	1	0
Lidocaine hydrochloride						X						X			206.3	\$9.90	7	1.8	3	1
Minoxidil sulfate salt						X									444.5	\$23.70	10	1.1	2	1
(±)-Metoprolol (+)-tartrate salt	1109														267.4	\$13.80	4	1.5	1	0
Hydrochlorothiazide												X			362.5	\$13.70	5	1.7	0	4
N,N'-Dicyano-2,5-dimethylbenzoquinone-diimine						X									221.2	\$22.60	8	4.3	3	0
Sulfaphenazole												X			314.4	\$19.90	7	6.0	2	1
2-Acetamidophenol	1110							X							151.2	\$21.80	9	-1.1	0	3
5-Azacytidine										X	X				244.2	\$0.00	2	0.5	3	0
Brefeldin A						X		X							698	\$9.25	6	3.3	1	1

Ebselen												X			246.3	\$25.30	4	0.2	2	1
Acebutolol hydrochloride	1111					X						X			59.07	\$19.95	3	0.4	0	1
Molsidomine						X									320.3	\$38.20	6	4.6	1	0
Myriocin							X					X			214.3	\$25.00	2	5.6	0	0
N-Acetyl-D-galactosamine			X										X		472.4	\$45.30	11	4.4	2	1
1-Phenyl-1-cyclopropanecarboxylic acid	1112	X													162.2	\$10.20	8	-2.9	2	0
2-Pyridylacetic acid hydrochloride									X		X				137.1	\$29.00	3	-0.1	1	0
5-Aminosalicylic acid												X	X		153.1	\$12.80	4	1.1	1	0
1,7-Dimethylxanthine	1113								X				X		180.2	\$30.40	6	2.3	1	1
Dimethyl 4-methoxyisophthalate									X						281.3	\$36.70	7	0.9	2	0
Ethyl 3-pyridylacetate						X						X			292.2	\$18.60	10	-1.9	0	0