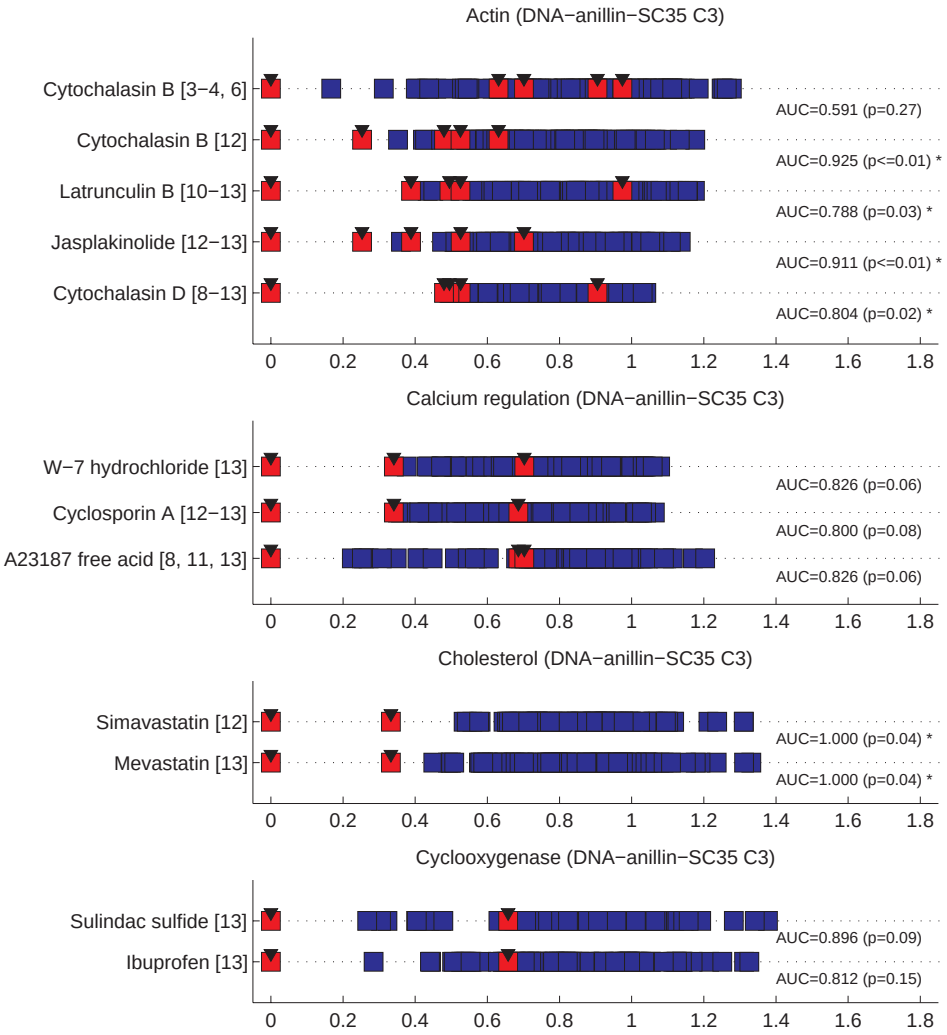
Supplementary Data 1: Drug screening performance for all compounds

For each d-profile, the drug screening performance was measured on the **a)** DNA-SC35-anillin, **b)** DNA-p53-cFos, **c)** DNA-pp38-pERK, and **d)** DNA-microtubule-actin marker sets. The d-profile was used as the reference profile (the first  at 0) and its similarities to all other d-profiles (d-profiles belonged to the same category as the reference compounds,  ; and d-profiles from other categories, ) were measured and ranked. The area under receiver operating characteristic curve (AUC) was calculated based on the ranking (see Methods). * d-profiles with statistically significant AUC values ($P < 0.05$).

Supplementary Data 1

a)



Supplementary Data 1 (cont.)

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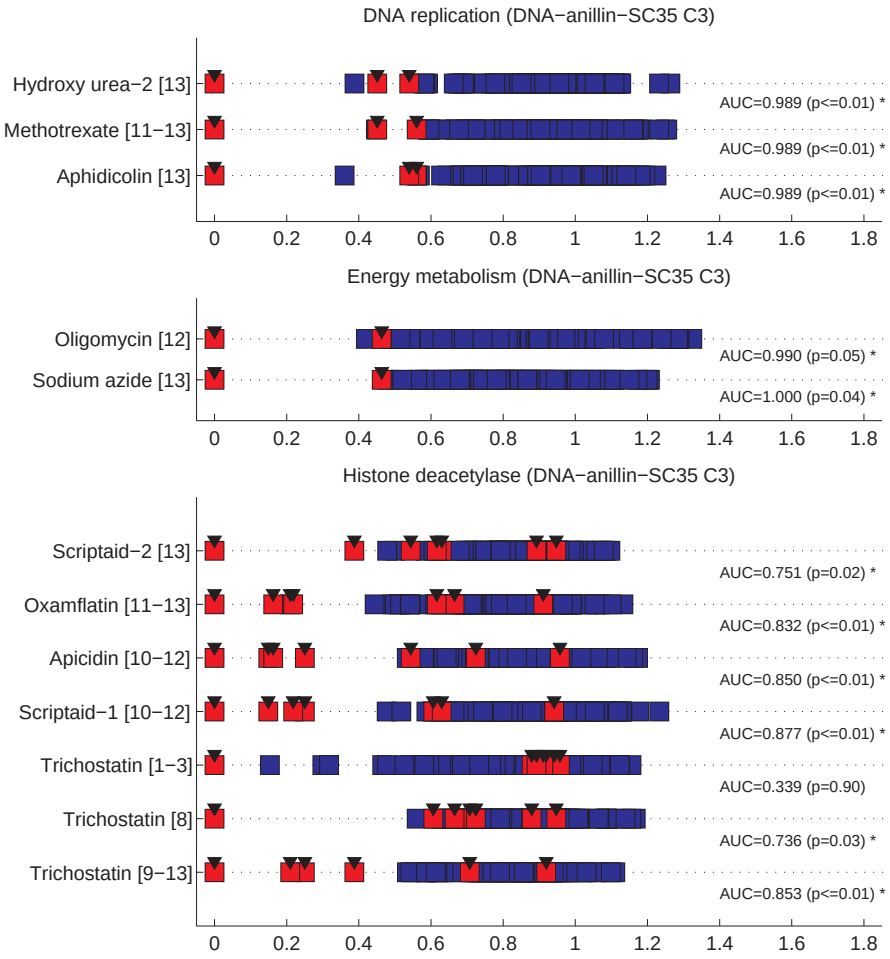

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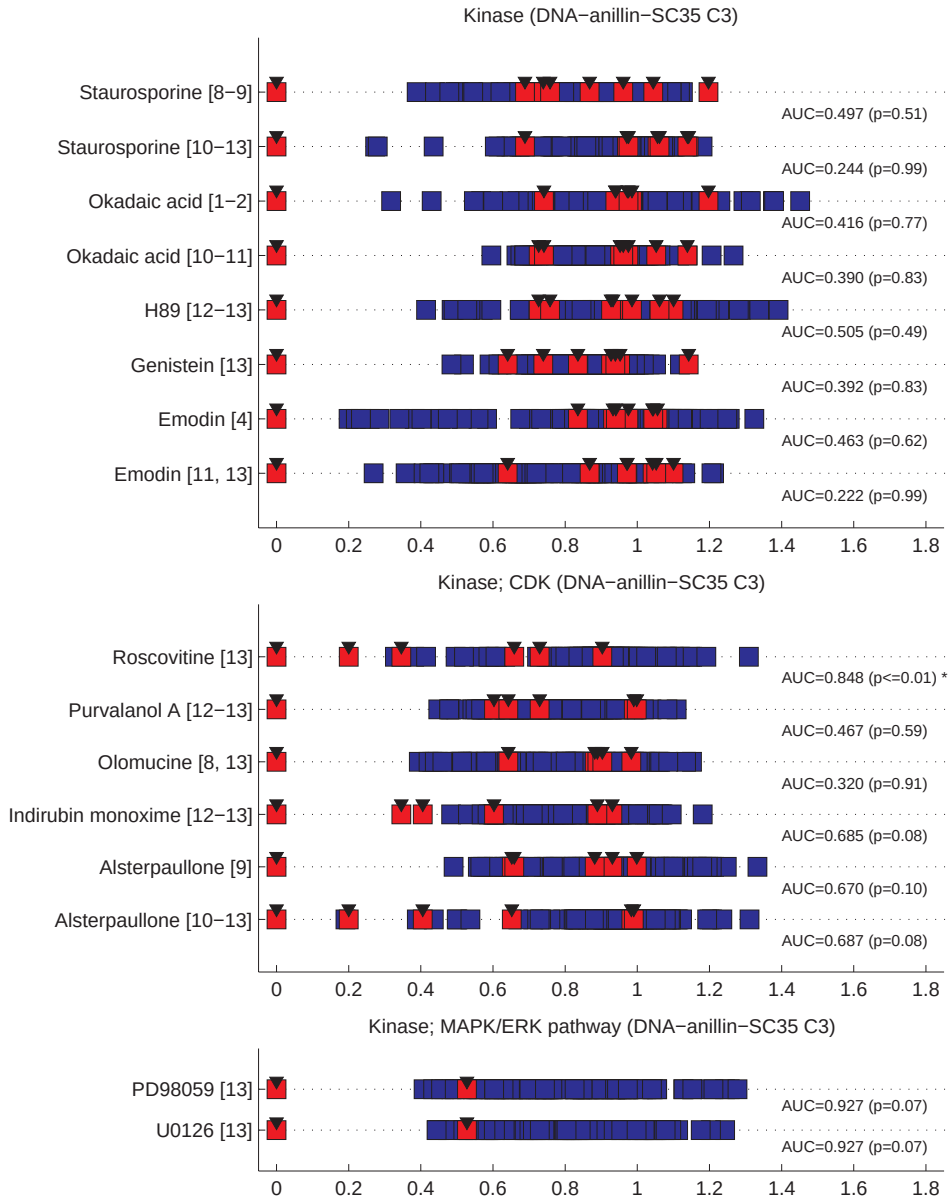

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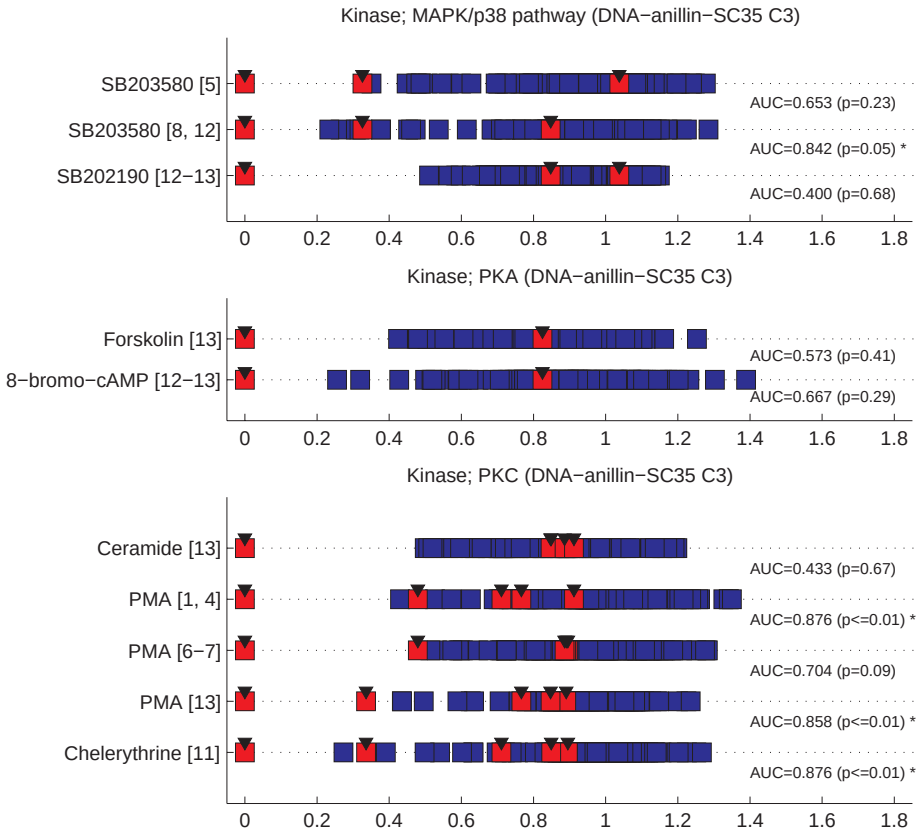

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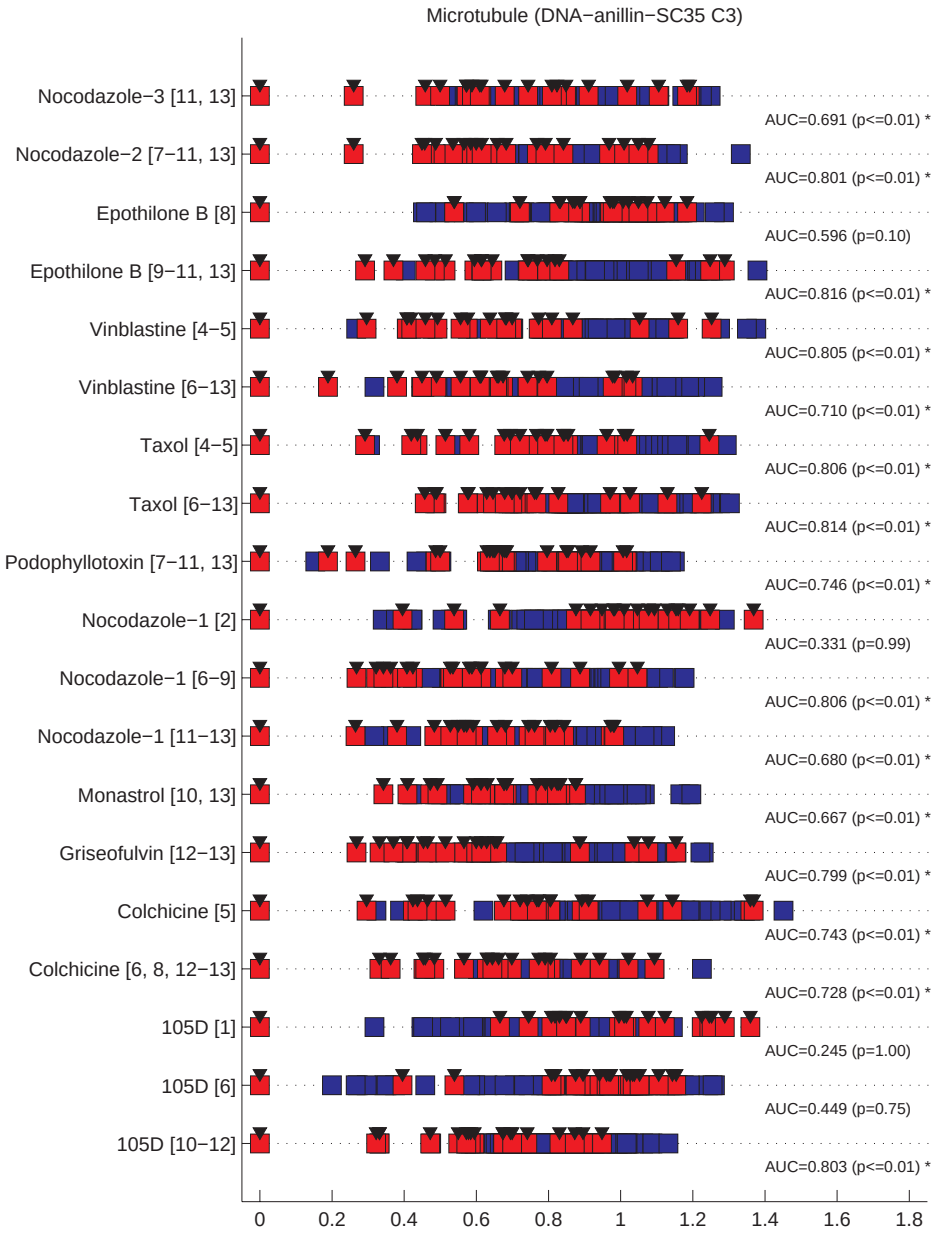

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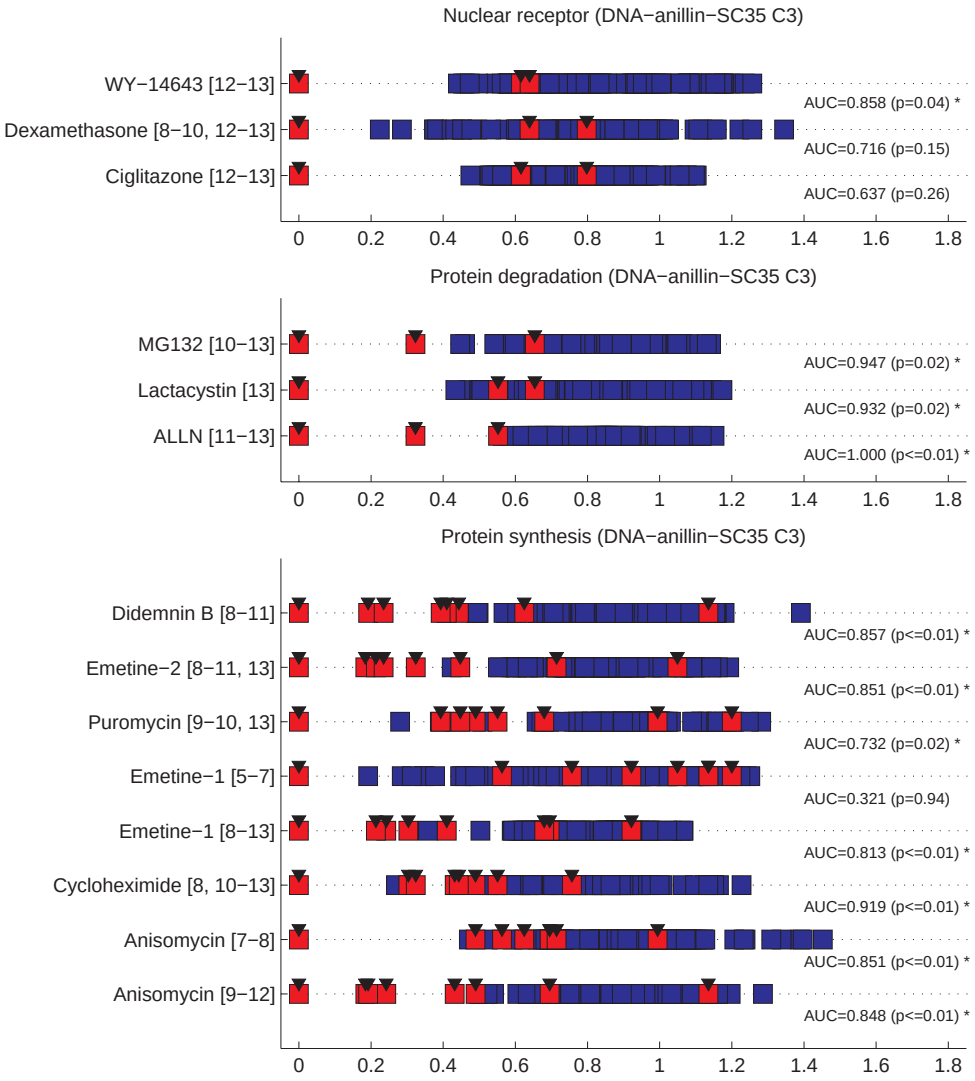

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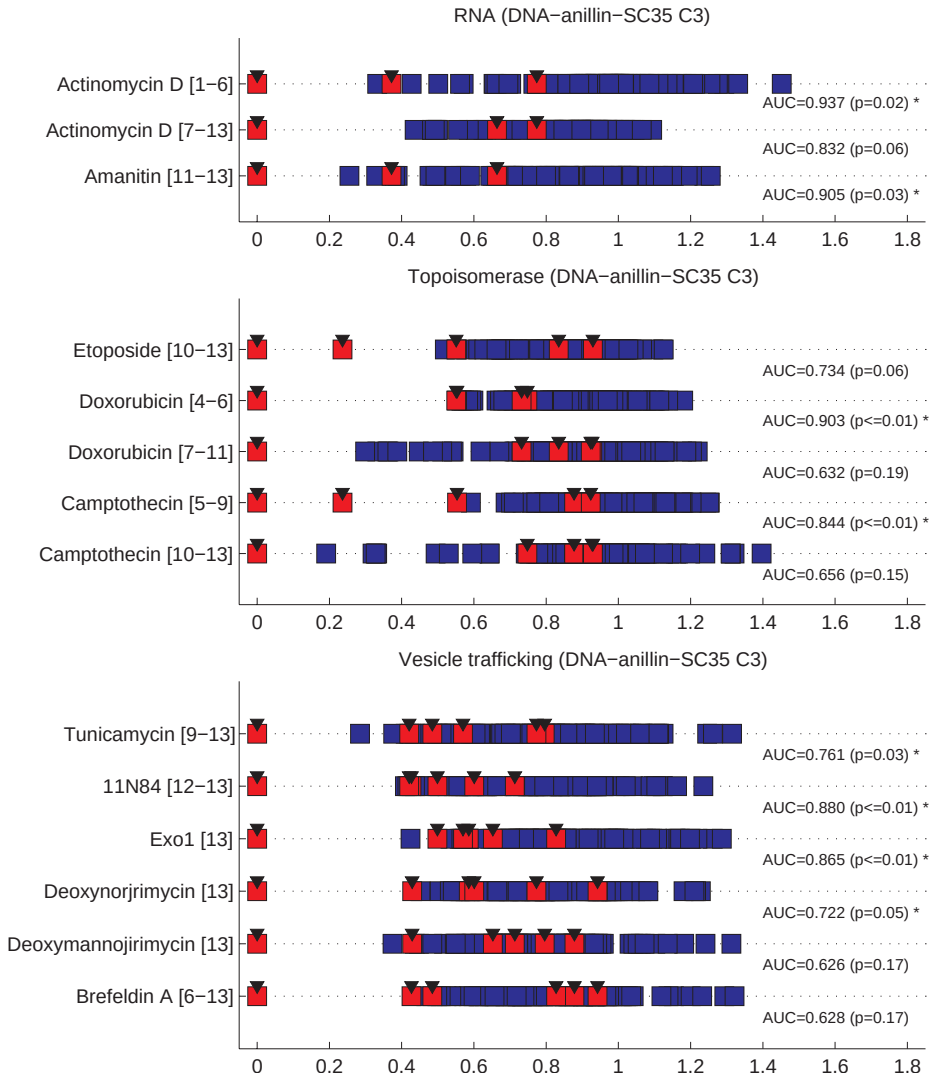

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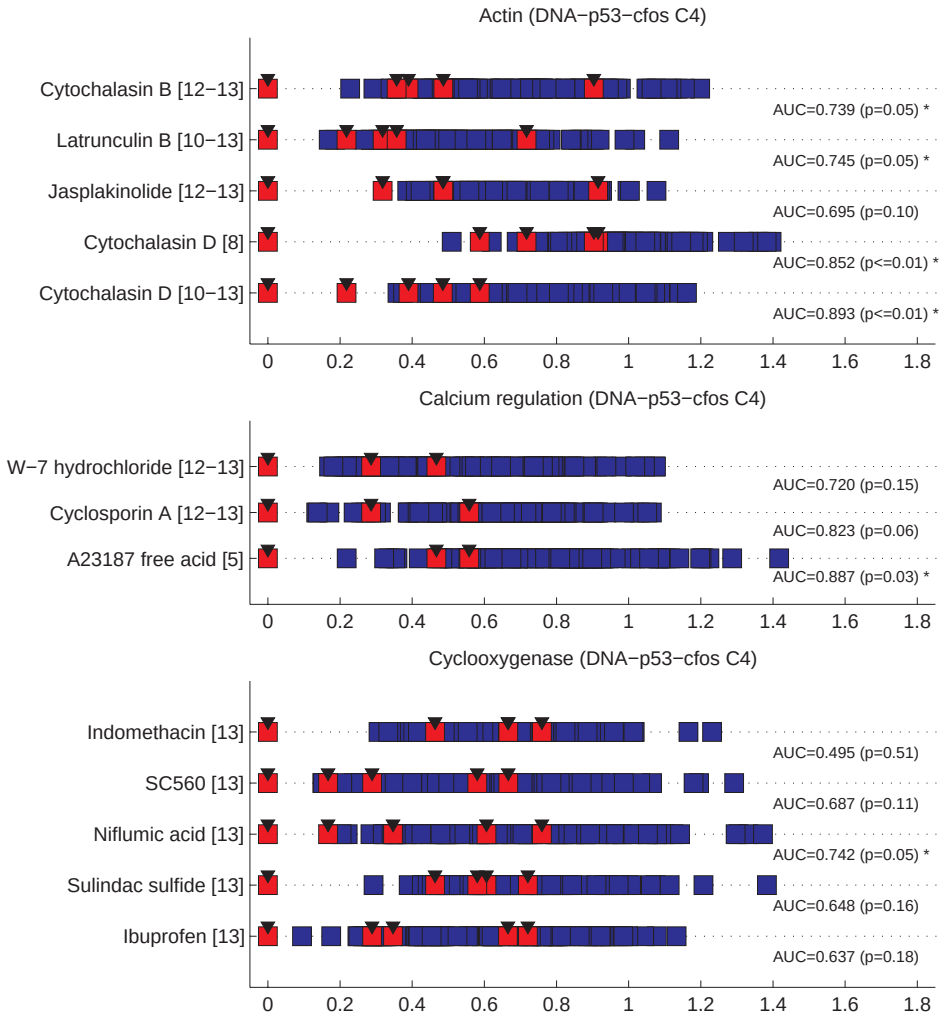

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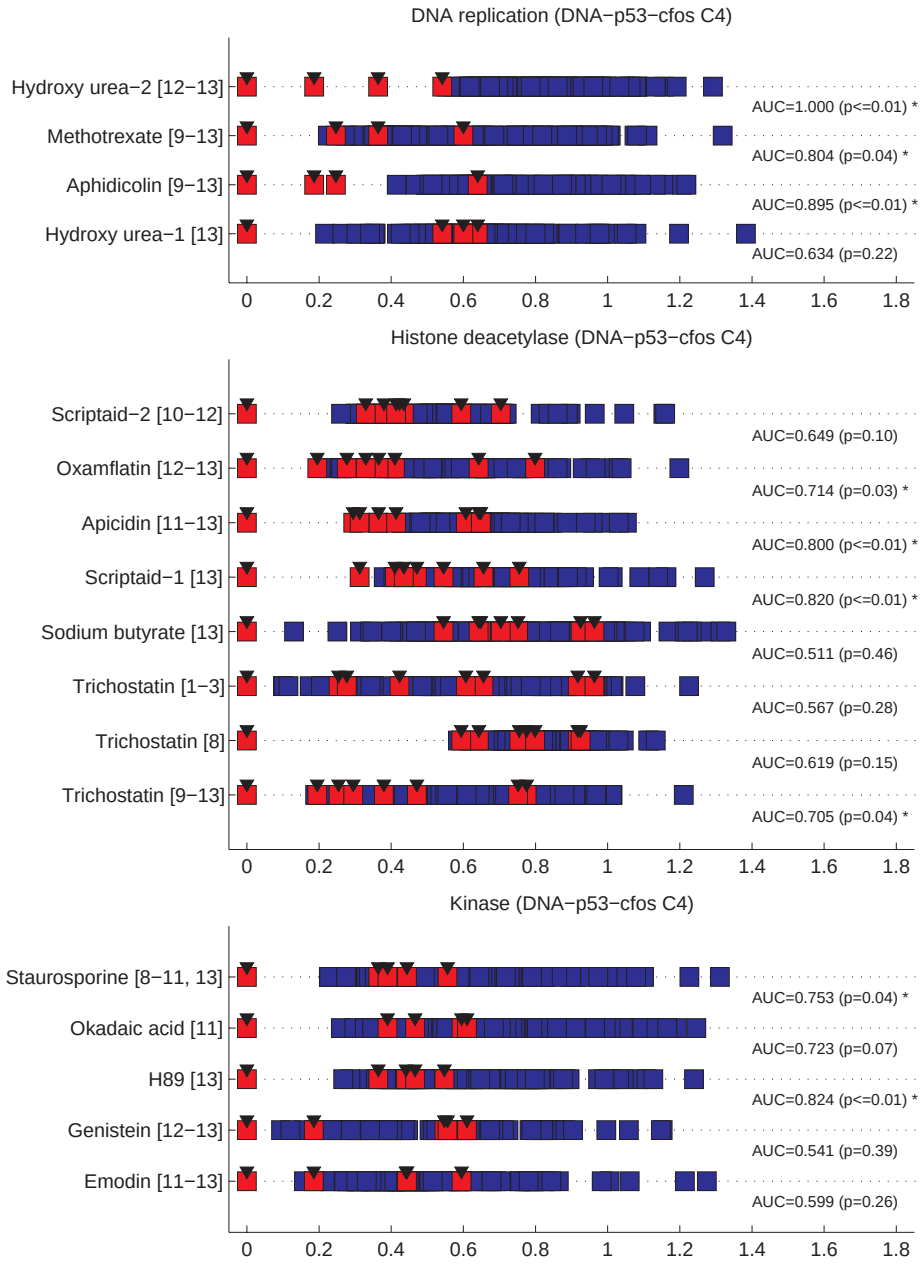

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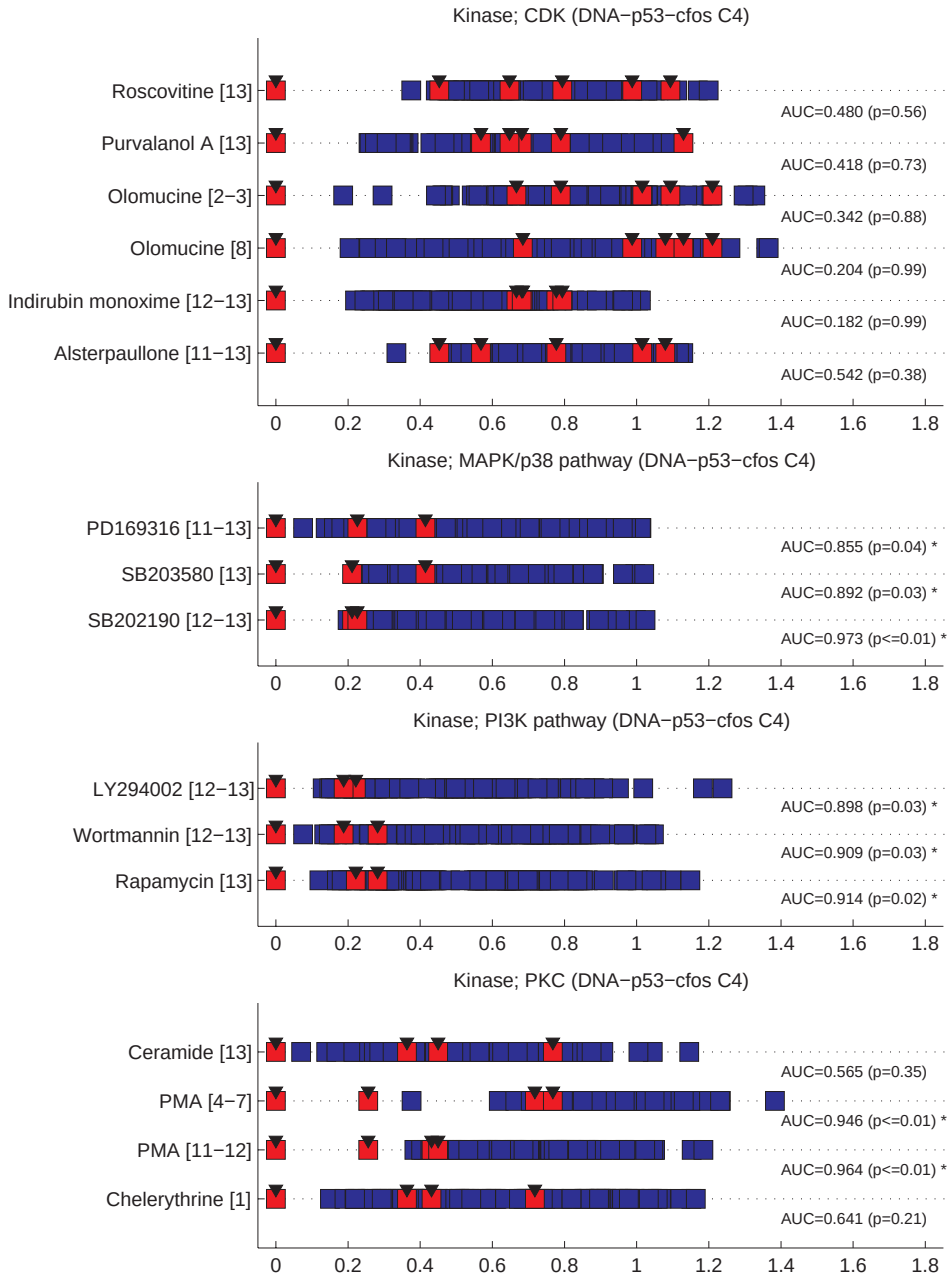

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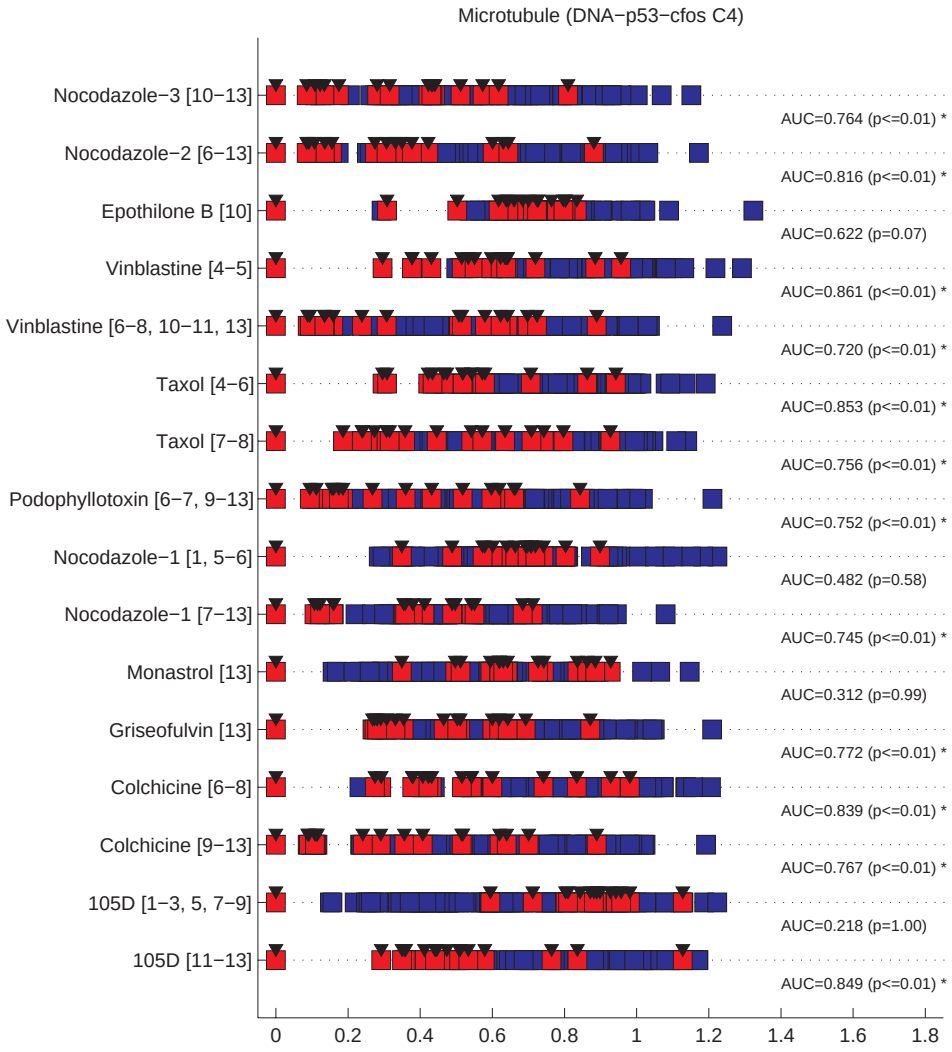

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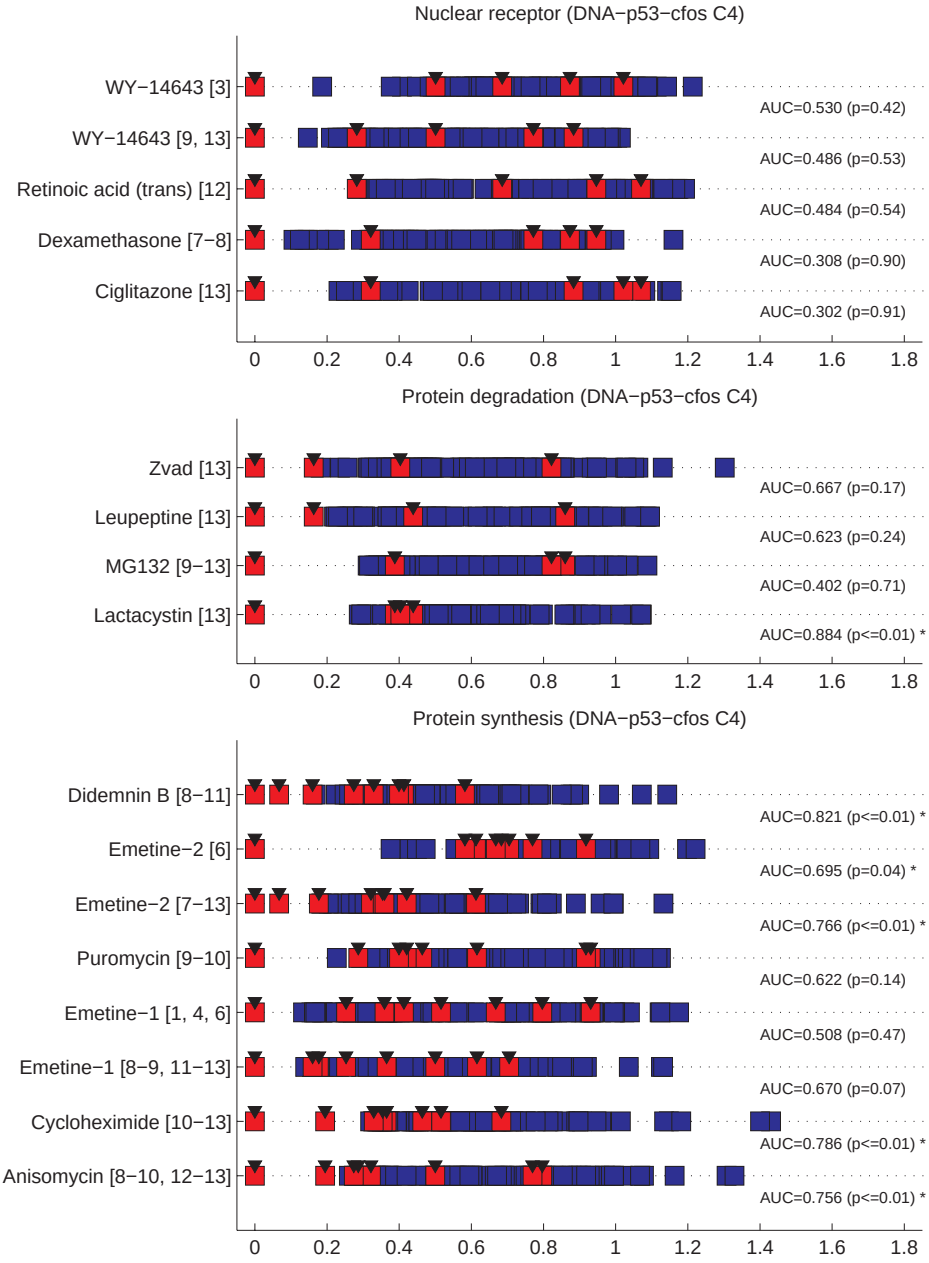

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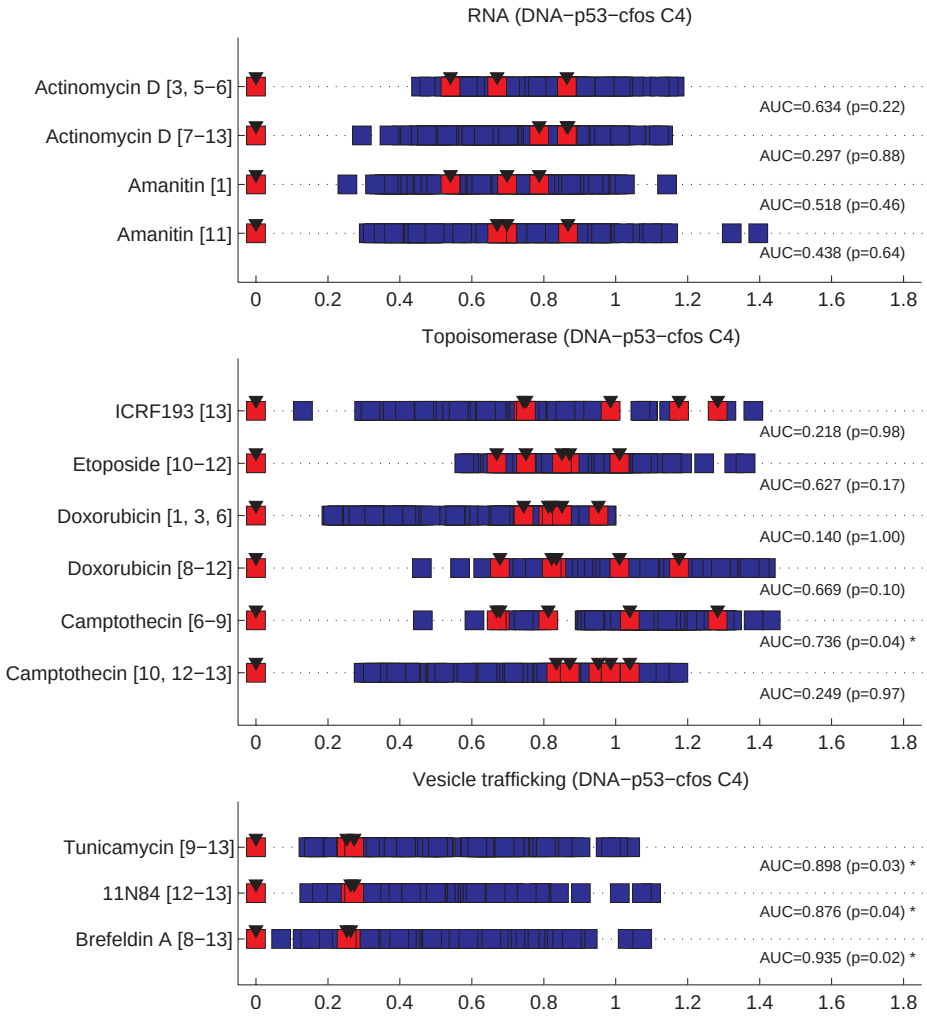

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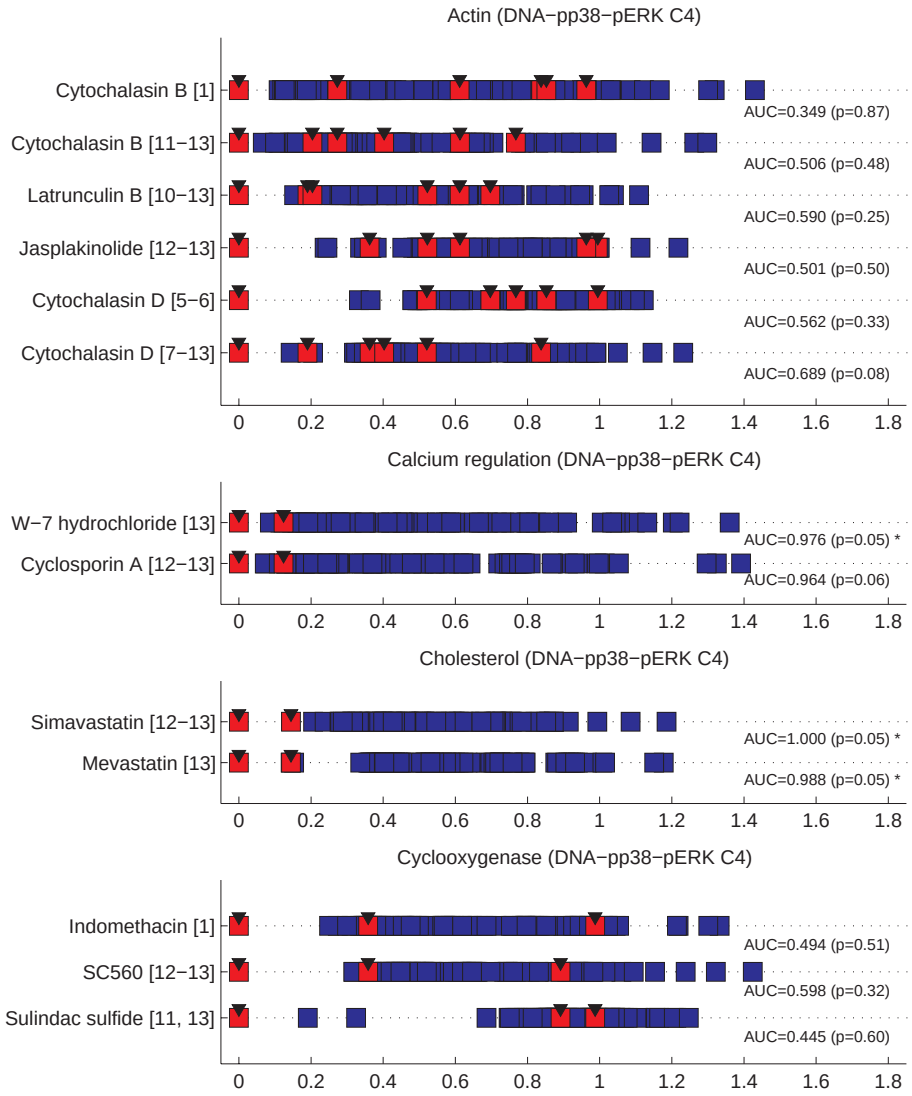

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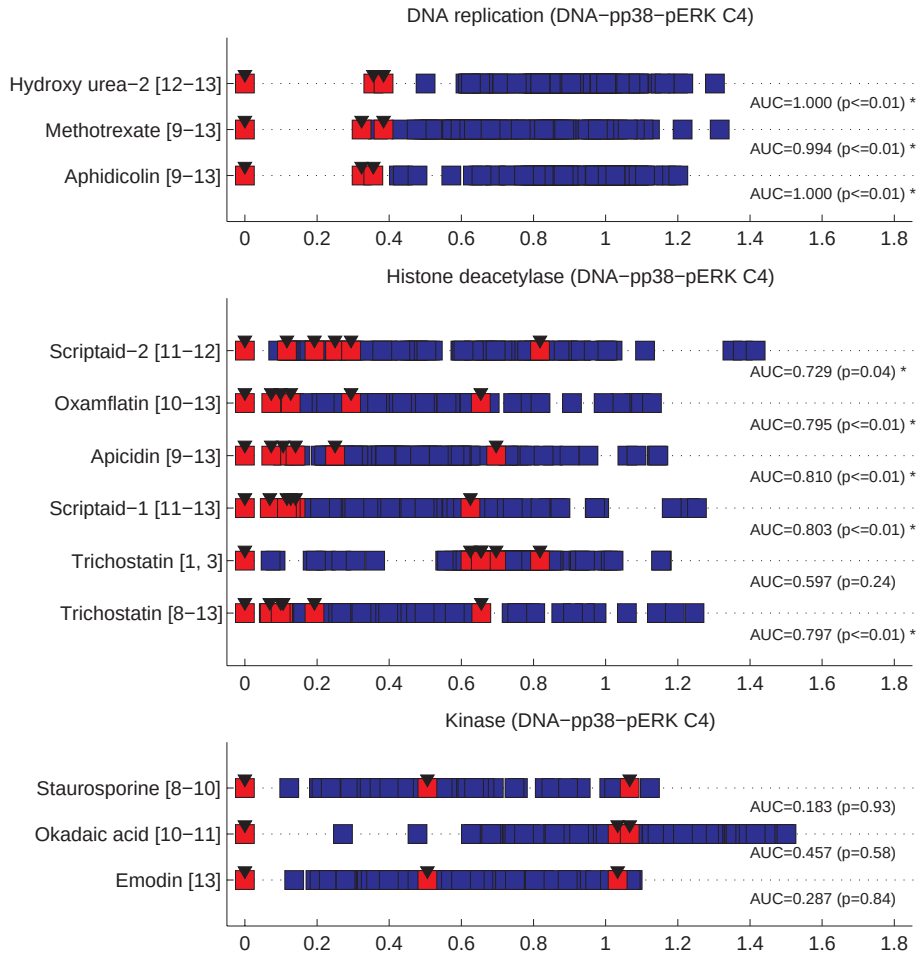

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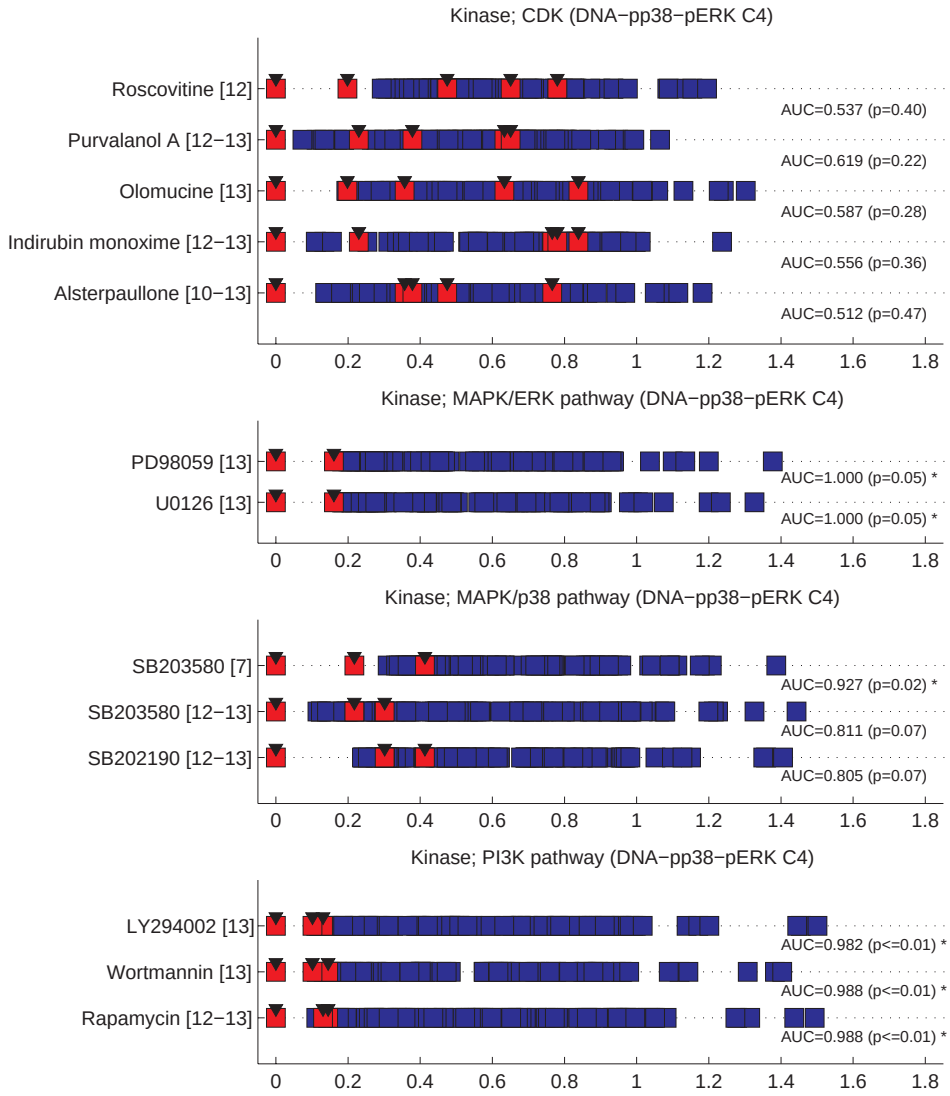

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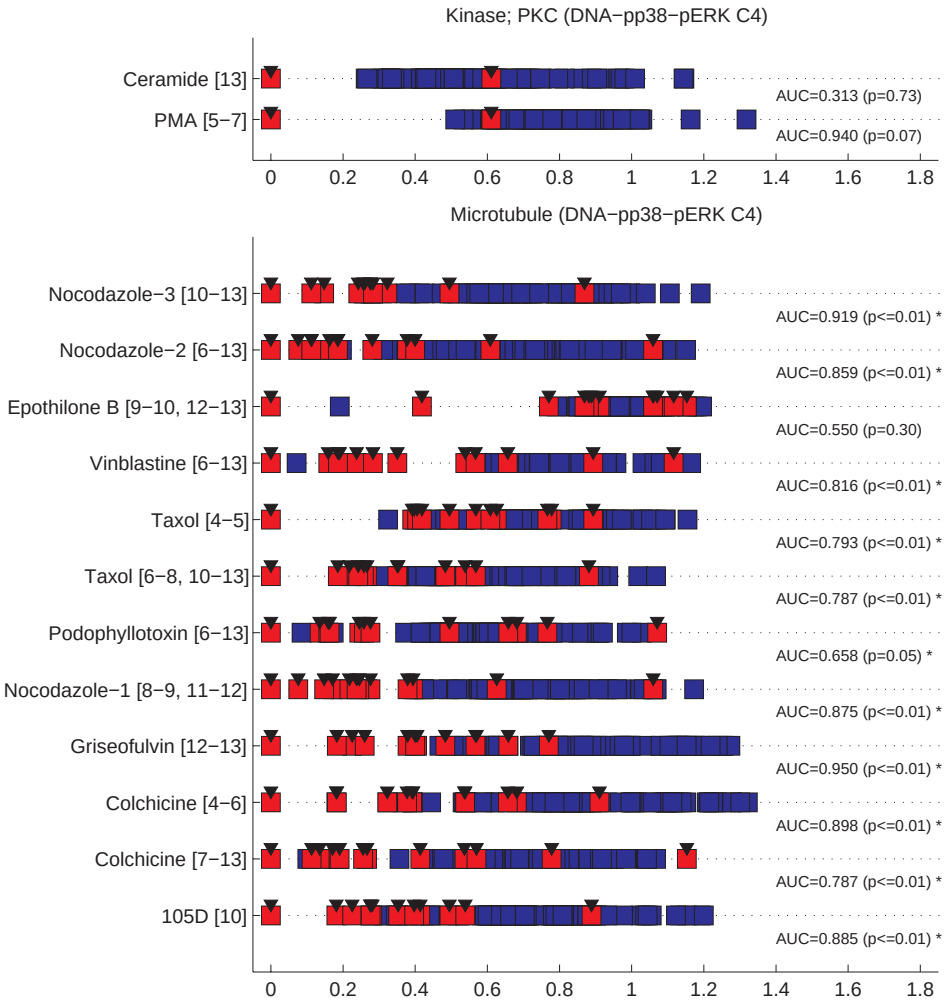

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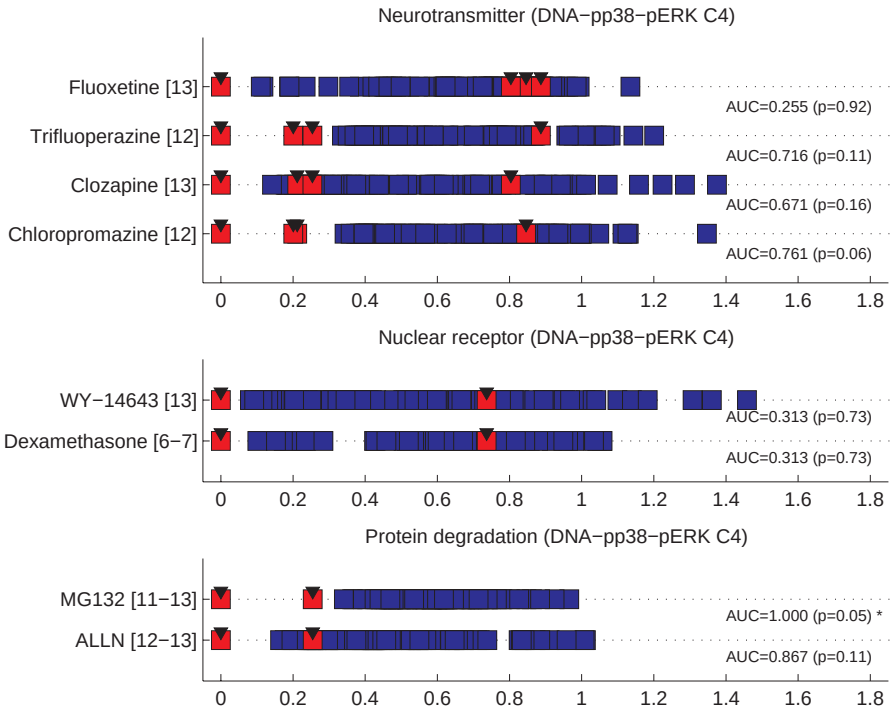

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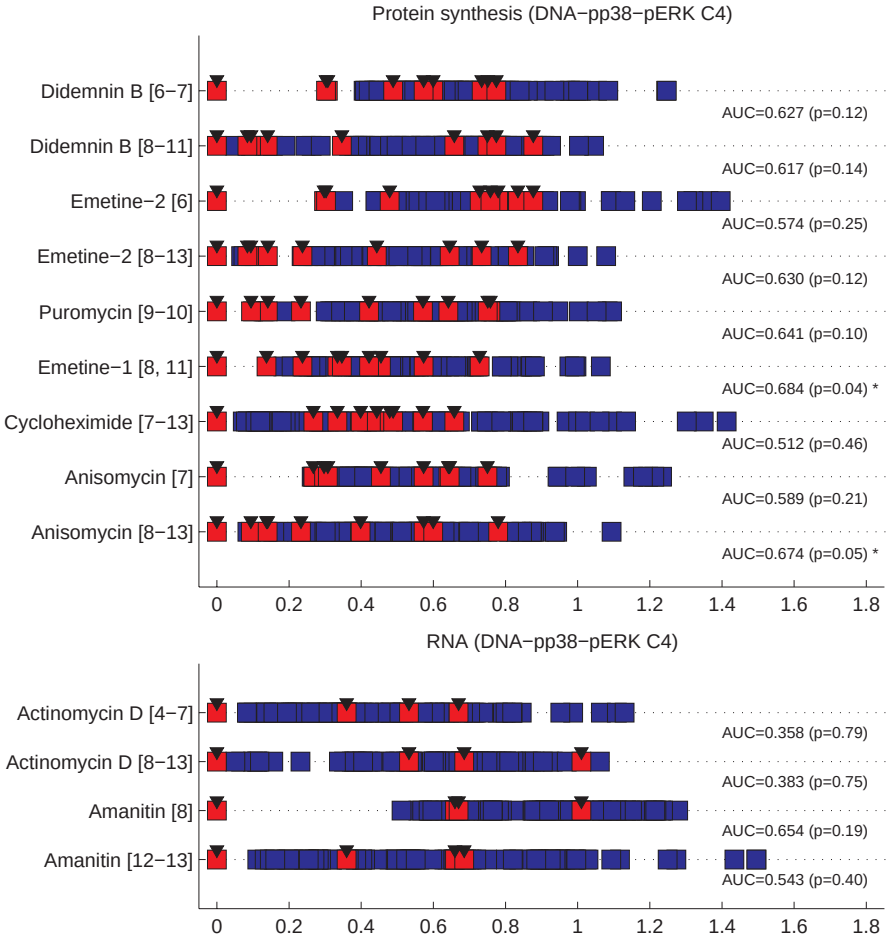

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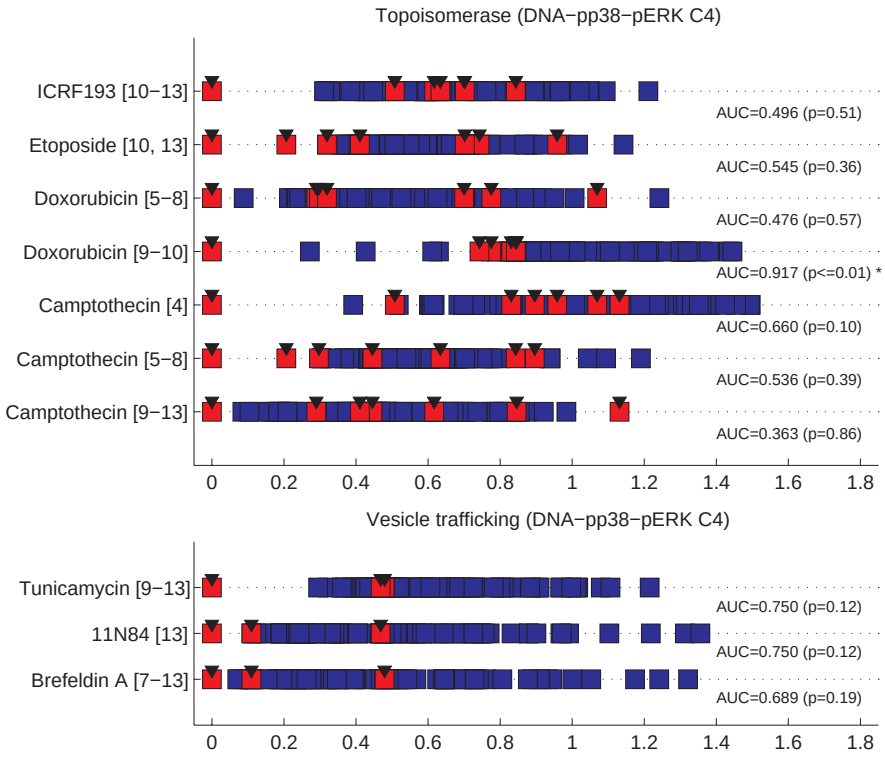

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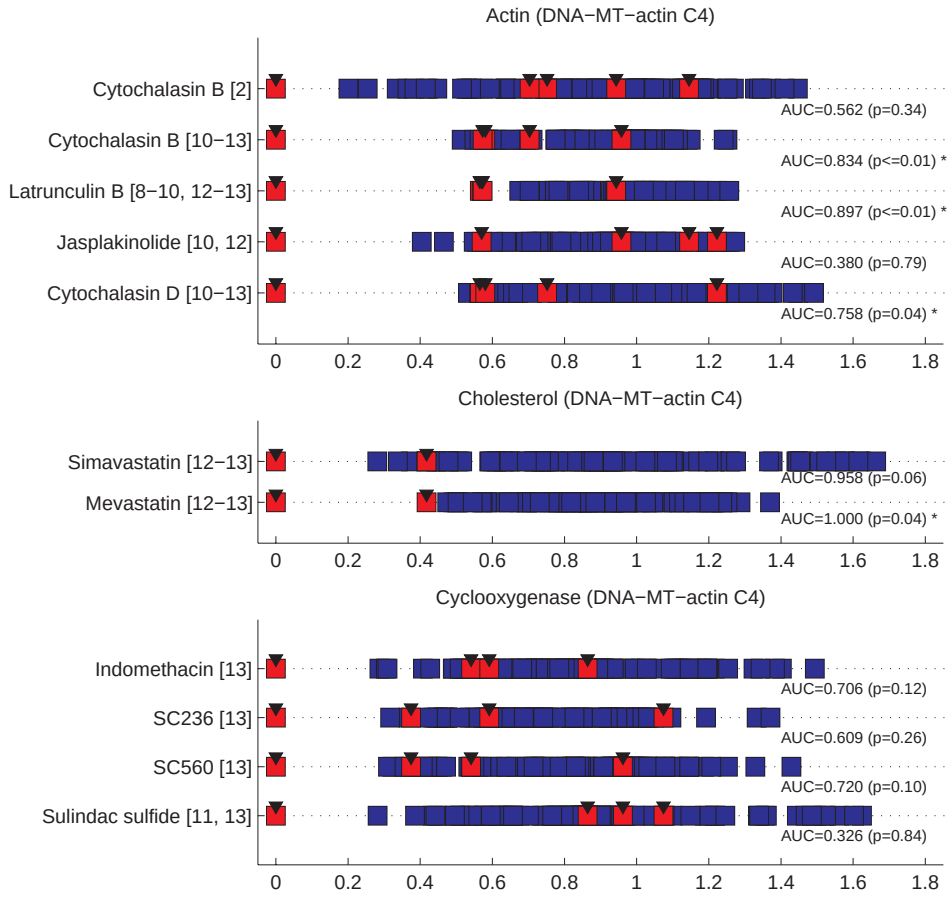

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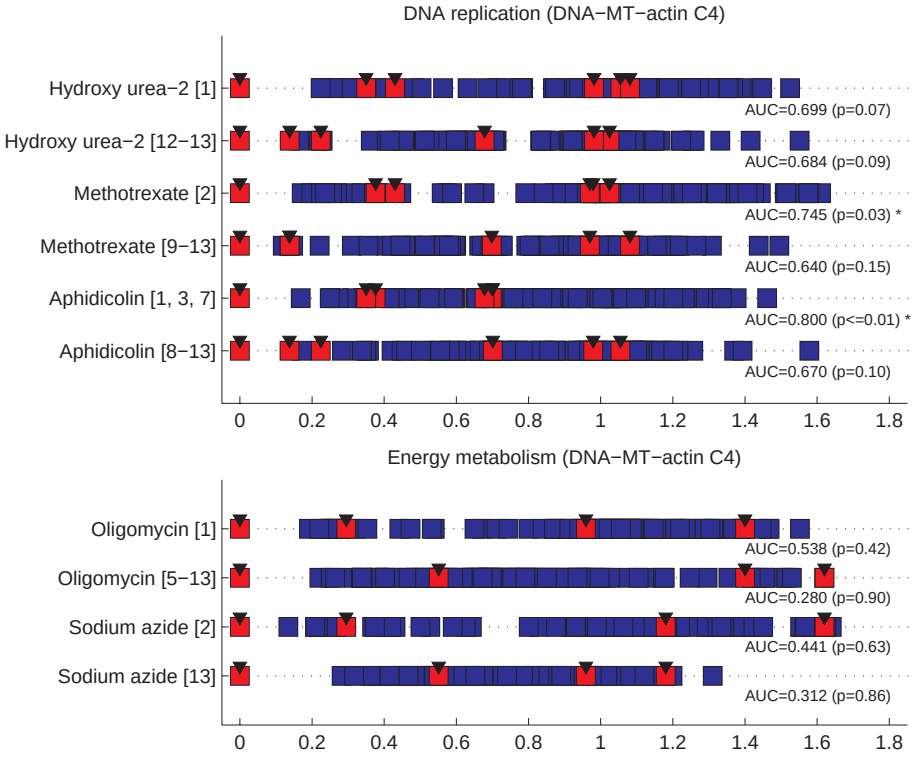

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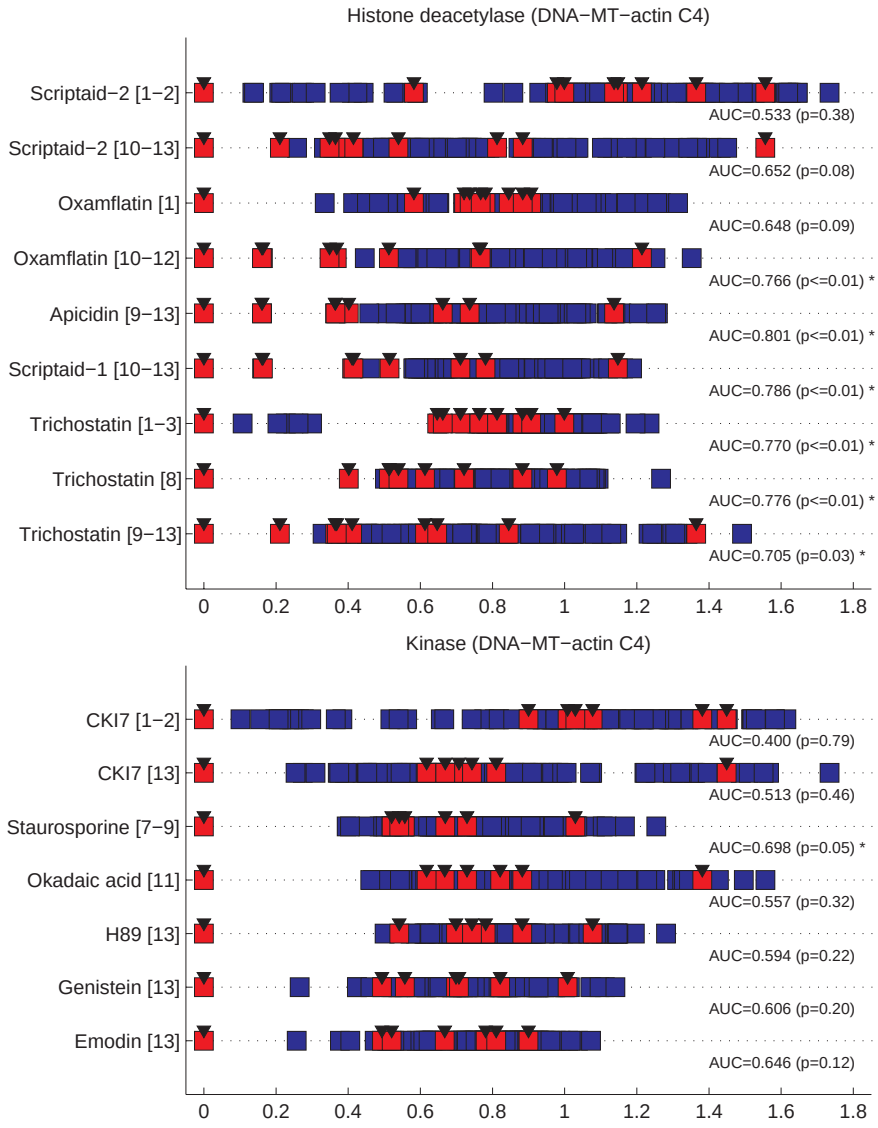

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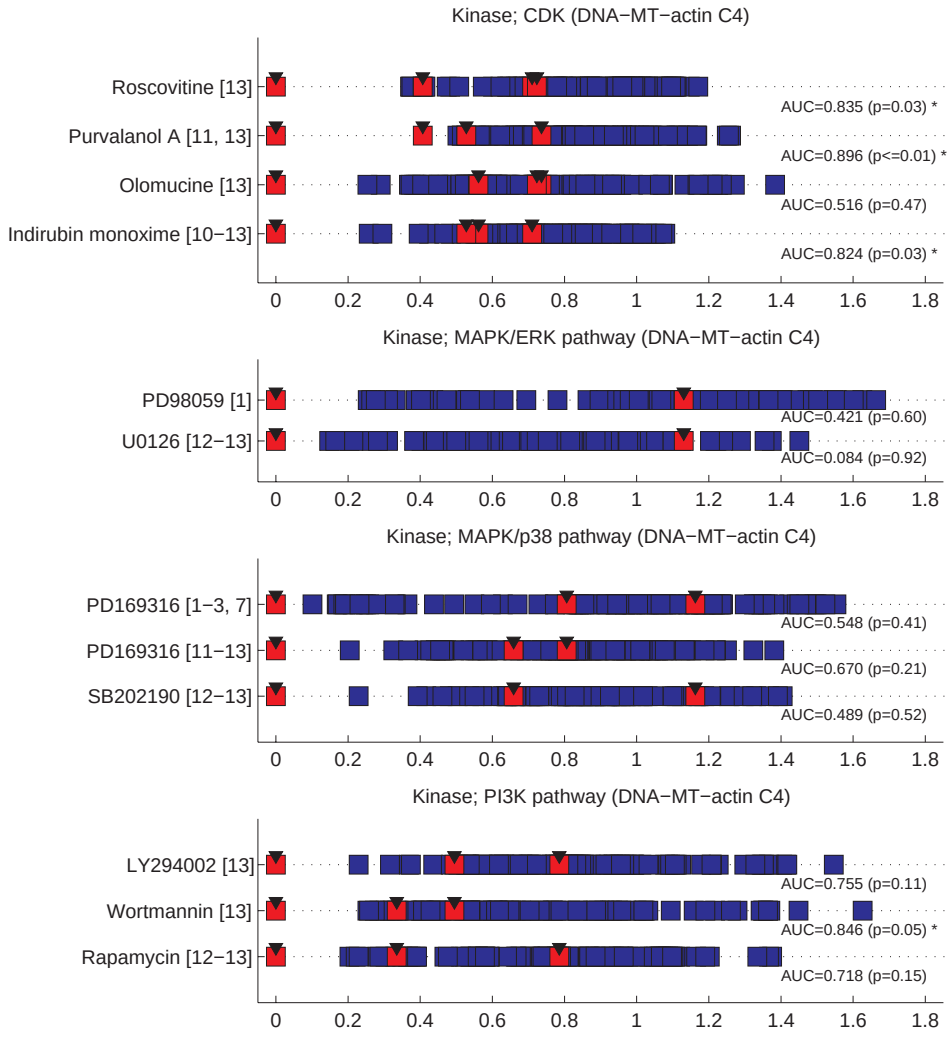

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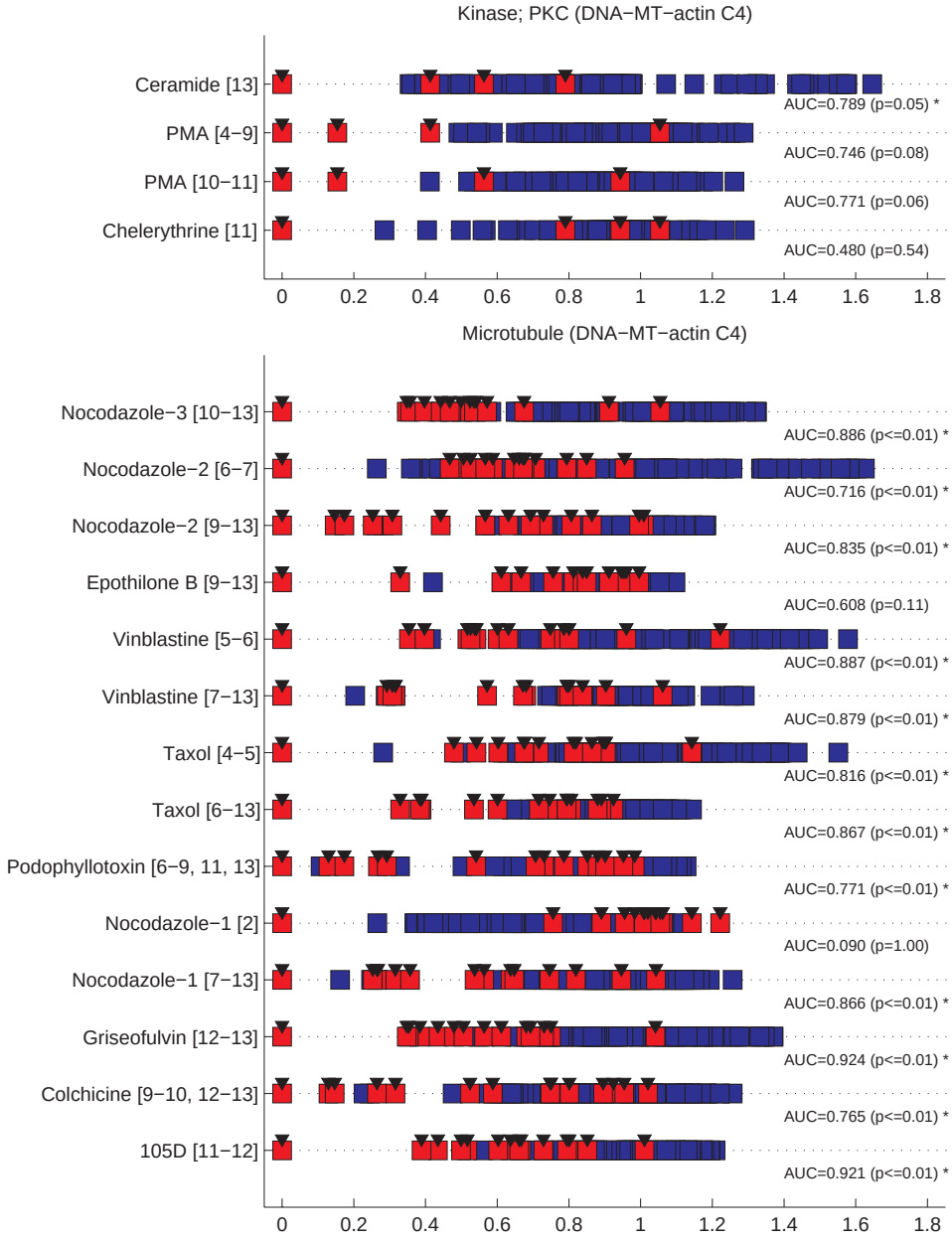

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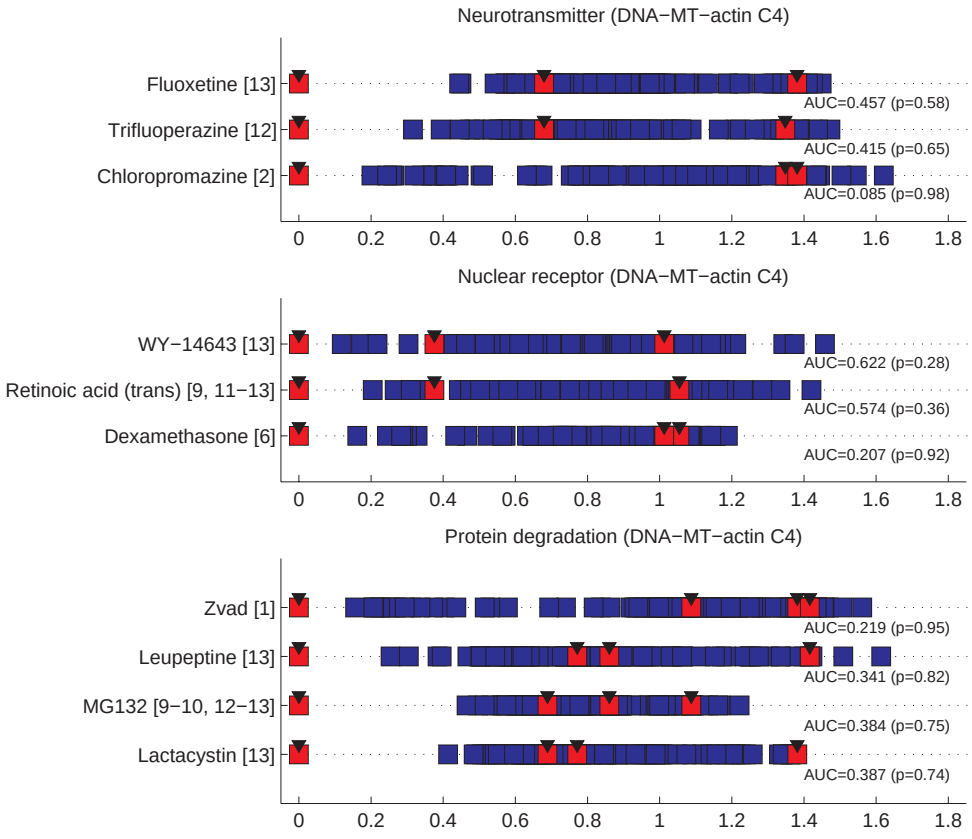
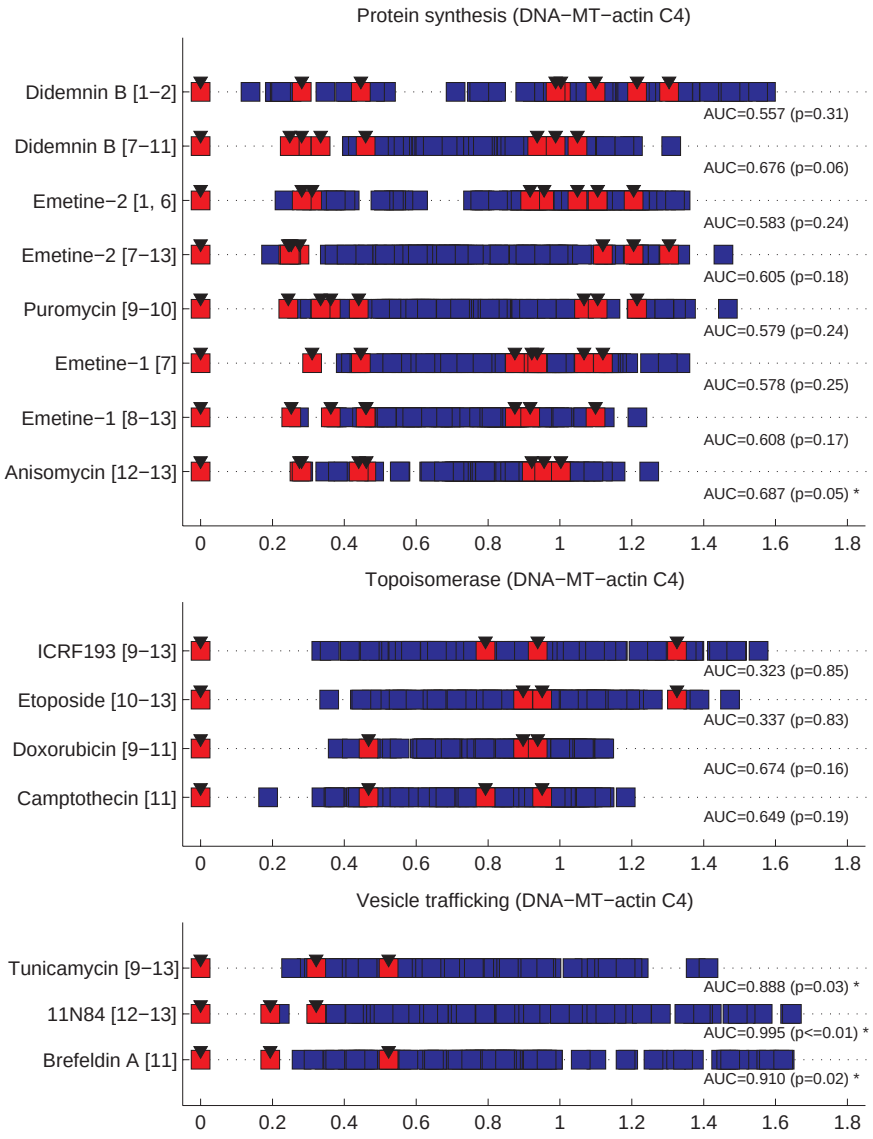


Supplementary Data 1 (cont.)

d)



Supplementary Data 2: Category prediction for all compounds

The category of a novel d-profile can be inferred from its closest characterized d-profiles. The five most similar d-profiles to the d-profiles of all compounds on the **a)** DNA-SC35-anillin, **b)** DNA-p53-cFos, **c)** DNA-pp38-pERK, and **d)** DNA-microtubule-actin marker sets are listed along with their similarity scores (see Methods).

Supplementary Data 2a: DNA-SC35-Anillin Marker Set

d-Profile	*Major annotated activity*	*Similarity*
105D (10-12)	**Microtubule**	
Nocodazole-1 (6-9)	Microtubule	0.322
Colchicine (6, 8, 12-13)	Microtubule	0.332
Griseofulvin (12-13)	Microtubule	0.332
Monastrol (10, 13)	Microtubule	0.472
11N84 (12-13)	Vesicle trafficking	0.475
105D (6)	**Microtubule**	
Emodin (4)	Kinase	0.200
SB203580 (8, 12)	Kinase; MAPK/p38 pwy.	0.265
A23187 free acid (8, 11, 13)	Calcium regulation	0.271
Chloropromazine (4, 6)	Neurotransmitter	0.296
Emetine-1 (5-7)	Protein synthesis	0.345
105D (1)	**Microtubule**	
Okadaic acid (1-2)	Kinase	0.318
Deoxymannojirimycin (13)	Vesicle trafficking	0.448
Deoxynorjrimycin (13)	Vesicle trafficking	0.453
Amanitin (11-13)	RNA	0.504
PMA (1, 4)	Kinase; PKC	0.527
11N84 (12-13)	**Vesicle trafficking**	
Cyclosporin A (12-13)	Calcium regulation	0.409
Monastrol (10, 13)	Microtubule	0.416
Tunicamycin (9-13)	Vesicle trafficking	0.421
Brefeldin A (6-13)	Vesicle trafficking	0.427
W-7 hydrochloride (13)	Calcium regulation	0.437
8-bromo-cAMP (12-13)	**Kinase; PKA**	
Amanitin (11-13)	RNA	0.256
Camptothecin (10-13)	Topoisomerase	0.320
Actinomycin D (1-6)	RNA	0.428
Alsterpaullone (10-13)	Kinase; CDK	0.500
Deoxymannojirimycin (13)	Vesicle trafficking	0.517
A23187 free acid (8, 11, 13)	**Calcium regulation**	
Dexamethasone (8-10, 12-13)	Nuclear receptor	0.224
Chloropromazine (4, 6)	Neurotransmitter	0.252
Emodin (4)	Kinase	0.258
105D (6)	Microtubule	0.271
SB203580 (8, 12)	Kinase; MAPK/p38 pwy.	0.307
Actinomycin D (7-13)	**RNA**	
Alsterpaullone (10-13)	Kinase; CDK	0.436
Indirubin monoxime (12-13)	Kinase; CDK	0.484
Purvalanol A (12-13)	Kinase; CDK	0.484
Didemnin B (8-11)	Protein synthesis	0.492
Camptothecin (10-13)	Topoisomerase	0.494
Actinomycin D (1-6)	**RNA**	
Camptothecin (10-13)	Topoisomerase	0.332
Amanitin (11-13)	RNA	0.372
8-bromo-cAMP (12-13)	Kinase; PKA	0.428
Alsterpaullone (10-13)	Kinase; CDK	0.501
Roscovitine (13)	Kinase; CDK	0.562
ALLN (11-13)	**Protein degradation**	
MG132 (10-13)	Protein degradation	0.323
Austocystin (12)	Unknown	0.520
Lactacystin (13)	Protein degradation	0.552
Doxorubicin (4-6)	Topoisomerase	0.565
Etoposide (10-13)	Topoisomerase	0.579
Alsterpaullone (10-13)	**Kinase; CDK**	
Camptothecin (10-13)	Topoisomerase	0.191
Roscovitine (13)	Kinase; CDK	0.200
Amanitin (11-13)	RNA	0.389
Indirubin monoxime (12-13)	Kinase; CDK	0.406
Actinomycin D (7-13)	RNA	0.436
Alsterpaullone (9)	**Kinase; CDK**	
H89 (12-13)	Kinase	0.491
Amanitin (11-13)	RNA	0.558
SB203580 (5)	Kinase; MAPK/p38 pwy.	0.565
Dexamethasone (8-10, 12-13)	Nuclear receptor	0.573
Emodin (4)	Kinase	0.584

d-Profile	*Major annotated activity*	*Similarity*
Amanitin (11-13)	**RNA**	
8-bromo-cAMP (12-13)	Kinase; PKA	0.256
Camptothecin (10-13)	Topoisomerase	0.329
Actinomycin D (1-6)	RNA	0.372
Roscovitine (13)	Kinase; CDK	0.382
Alsterpaullone (10-13)	Kinase; CDK	0.389
Anisomycin (9-12)	**Protein synthesis**	
Emetine-2 (8-11, 13)	Protein synthesis	0.184
Didemnin B (8-11)	Protein synthesis	0.192
Emetine-1 (8-13)	Protein synthesis	0.242
Austocystin (12)	Unknown	0.292
Cycloheximide (8, 10-13)	Protein synthesis	0.432
Anisomycin (7-8)	**Protein synthesis**	
Concentramide (6)	Unknown	0.348
Lactacystin (13)	Protein degradation	0.471
Cycloheximide (8, 10-13)	Protein synthesis	0.489
Brefeldin A (6-13)	Vesicle trafficking	0.524
Emetine-1 (5-7)	Protein synthesis	0.563
Aphidicolin (13)	**DNA replication**	
Doxorubicin (7-11)	Topoisomerase	0.361
Hydroxy urea-2 (13)	DNA replication	0.540
Methotrexate (11-13)	DNA replication	0.560
Sodium azide (13)	Energy metabolism	0.562
Purvalanol A (12-13)	Kinase; CDK	0.569
Apicidin (10-12)	**Histone deacetylase**	
Scriptaid-1 (10-12)	Histone deacetylase	0.149
Oxamflatin (11-13)	Histone deacetylase	0.163
Trichostatin (9-13)	Histone deacetylase	0.251
U0126 (13)	Kinase; MAPK/ERK pwy.	0.533
Scriptaid-2 (13)	Histone deacetylase	0.544
Austocystin (12)	**Unknown**	
Emetine-1 (8-13)	Protein synthesis	0.233
Emetine-2 (8-11, 13)	Protein synthesis	0.282
Anisomycin (9-12)	Protein synthesis	0.292
Cycloheximide (8, 10-13)	Protein synthesis	0.413
Didemnin B (8-11)	Protein synthesis	0.415
Brefeldin A (6-13)	**Vesicle trafficking**	
11N84 (12-13)	Vesicle trafficking	0.427
Cyclosporin A (12-13)	Calcium regulation	0.468
Tunicamycin (9-13)	Vesicle trafficking	0.485
Ceramide (13)	Kinase; PKC	0.499
W-7 hydrochloride (13)	Calcium regulation	0.508
Camptothecin (10-13)	**Topoisomerase**	
Alsterpaullone (10-13)	Kinase; CDK	0.191
8-bromo-cAMP (12-13)	Kinase; PKA	0.320
Roscovitine (13)	Kinase; CDK	0.328
Amanitin (11-13)	RNA	0.329
Actinomycin D (1-6)	RNA	0.332
Camptothecin (5-9)	**Topoisomerase**	
Etoposide (10-13)	Topoisomerase	0.236
Doxorubicin (4-6)	Topoisomerase	0.553
Hydroxy urea-2 (13)	DNA replication	0.592
ALLN (11-13)	Protein degradation	0.688
Methotrexate (11-13)	DNA replication	0.703
Ceramide (13)	**Kinase; PKC**	
Brefeldin A (6-13)	Vesicle trafficking	0.499
Mevastatin (13)	Cholesterol	0.508
Sodium azide (13)	Energy metabolism	0.520
11N84 (12-13)	Vesicle trafficking	0.527
Purvalanol A (12-13)	Kinase; CDK	0.556
Chelerythrine (11)	**Kinase; PKC**	
Staurosporine (10-13)	Kinase	0.273
PMA (13)	Kinase; PKC	0.336
Puromycin (9-10, 13)	Protein synthesis	0.391
Didemnin B (8-11)	Protein synthesis	0.498
Anisomycin (9-12)	Protein synthesis	0.541

Supplementary Data 2a: DNA-SC35-Anillin Marker Set

d-Profile	*Major annotated activity*	*Similarity*
Chloropromazine (4, 6)	**Neurotransmitter**	
Cytochalasin B (3-4, 6)	Actin	0.167
Emetine-1 (5-7)	Protein synthesis	0.192
Emodin (4)	Kinase	0.220
A23187 free acid (8, 11, 13)	Calcium regulation	0.252
Dexamethasone (8-10, 12-13)	Nuclear receptor	0.286
Ciglitazone (12-13)	**Nuclear receptor**	
W-7 hydrochloride (13)	Calcium regulation	0.475
Monastrol (10, 13)	Microtubule	0.529
Cyclosporin A (12-13)	Calcium regulation	0.529
Tunicamycin (9-13)	Vesicle trafficking	0.534
Ibuprofen (13)	Cyclooxygenase	0.539
Colchicine (6, 8, 12-13)	**Microtubule**	
105D (10-12)	Microtubule	0.332
Nocodazole-1 (6-9)	Microtubule	0.363
Griseofulvin (12-13)	Microtubule	0.453
Nocodazole-3 (11, 13)	Microtubule	0.458
Nocodazole-1 (11-13)	Microtubule	0.484
Colchicine (5)	**Microtubule**	
Vinblastine (4-5)	Microtubule	0.296
Sulindac sulfide (13)	Cyclooxygenase	0.323
Staurosporine (8-9)	Kinase	0.389
Nocodazole-1 (6-9)	Microtubule	0.424
Taxol (4-5)	Microtubule	0.437
Concentramide (6)	**Unknown**	
Anisomycin (7-8)	Protein synthesis	0.348
Lactacystin (13)	Protein degradation	0.446
Emodin (11, 13)	Kinase	0.483
Cycloheximide (8, 10-13)	Protein synthesis	0.484
Mevastatin (13)	Cholesterol	0.488
Cycloheximide (8, 10-13)	**Protein synthesis**	
Emodin (11, 13)	Kinase	0.269
Emetine-1 (8-13)	Protein synthesis	0.304
Emetine-2 (8-11, 13)	Protein synthesis	0.324
Austocystin (12)	Unknown	0.413
Anisomycin (9-12)	Protein synthesis	0.432
Cyclosporin A (12-13)	**Calcium regulation**	
W-7 hydrochloride (13)	Calcium regulation	0.341
Cytochalasin B (12)	Actin	0.352
Jasplakinolide (12-13)	Actin	0.361
Olomucine (8, 13)	Kinase; CDK	0.394
11N84 (12-13)	Vesicle trafficking	0.409
Cytochalasin B (12)	**Actin**	
Jasplakinolide (12-13)	Actin	0.253
Cyclosporin A (12-13)	Calcium regulation	0.352
Olomucine (8, 13)	Kinase; CDK	0.421
Tunicamycin (9-13)	Vesicle trafficking	0.427
W-7 hydrochloride (13)	Calcium regulation	0.471
Cytochalasin B (3-4, 6)	**Actin**	
Chloropromazine (4, 6)	Neurotransmitter	0.167
Emetine-1 (5-7)	Protein synthesis	0.313
Emodin (4)	Kinase	0.402
A23187 free acid (8, 11, 13)	Calcium regulation	0.406
Dexamethasone (8-10, 12-13)	Nuclear receptor	0.433
Cytochalasin D (8-13)	**Actin**	
Cytochalasin B (12)	Actin	0.480
Latrunculin B (10-13)	Actin	0.495
Cyclosporin A (12-13)	Calcium regulation	0.499
Jasplakinolide (12-13)	Actin	0.526
Cycloheximide (8, 10-13)	Protein synthesis	0.544
Deoxymannojirimycin (13)	**Vesicle trafficking**	
Dexamethasone (8-10, 12-13)	Nuclear receptor	0.375
Deoxynorjrimycin (13)	Vesicle trafficking	0.429
Cyclosporin A (12-13)	Calcium regulation	0.436
105D (1)	Microtubule	0.448
Cytochalasin B (3-4, 6)	Actin	0.485

d-Profile	*Major annotated activity*	*Similarity*
Deoxynorjrimycin (13)	**Vesicle trafficking**	
Deoxymannojirimycin (13)	Vesicle trafficking	0.429
105D (1)	Microtubule	0.453
Forskolin (13)	Kinase; PKA	0.505
Trichostatin (9-13)	Histone deacetylase	0.533
Oxamflatin (11-13)	Histone deacetylase	0.542
Dexamethasone (8-10, 12-13)	**Nuclear receptor**	
A23187 free acid (8, 11, 13)	Calcium regulation	0.224
Chloropromazine (4, 6)	Neurotransmitter	0.286
Deoxymannojirimycin (13)	Vesicle trafficking	0.375
105D (6)	Microtubule	0.375
Emodin (4)	Kinase	0.383
Didemnin B (8-11)	**Protein synthesis**	
Anisomycin (9-12)	Protein synthesis	0.192
Emetine-2 (8-11, 13)	Protein synthesis	0.235
Puromycin (9-10, 13)	Protein synthesis	0.393
Emetine-1 (8-13)	Protein synthesis	0.410
Austocystin (12)	Unknown	0.415
Doxorubicin (7-11)	**Topoisomerase**	
Trichostatin (1-3)	Histone deacetylase	0.299
Podophyllotoxin (7-11, 13)	Microtubule	0.333
Aphidicolin (13)	DNA replication	0.361
Nocodazole-1 (11-13)	Microtubule	0.363
Hydroxy urea-2 (13)	DNA replication	0.388
Doxorubicin (4-6)	**Topoisomerase**	
Etoposide (10-13)	Topoisomerase	0.551
Camptothecin (5-9)	Topoisomerase	0.553
ALLN (11-13)	Protein degradation	0.565
Okadaic acid (1-2)	Kinase	0.567
PMA (1, 4)	Kinase; PKC	0.573
Emetine-1 (8-13)	**Protein synthesis**	
Emetine-2 (8-11, 13)	Protein synthesis	0.213
Austocystin (12)	Unknown	0.233
Anisomycin (9-12)	Protein synthesis	0.242
Cycloheximide (8, 10-13)	Protein synthesis	0.304
Emodin (11, 13)	Kinase	0.358
Emetine-1 (5-7)	**Protein synthesis**	
Chloropromazine (4, 6)	Neurotransmitter	0.192
Emodin (4)	Kinase	0.285
Cytochalasin B (3-4, 6)	Actin	0.313
105D (6)	Microtubule	0.345
A23187 free acid (8, 11, 13)	Calcium regulation	0.349
Emetine-2 (8-11, 13)	**Protein synthesis**	
Anisomycin (9-12)	Protein synthesis	0.184
Emetine-1 (8-13)	Protein synthesis	0.213
Didemnin B (8-11)	Protein synthesis	0.235
Austocystin (12)	Unknown	0.282
Cycloheximide (8, 10-13)	Protein synthesis	0.324
Emodin (11, 13)	**Kinase**	
Cycloheximide (8, 10-13)	Protein synthesis	0.269
Emetine-1 (8-13)	Protein synthesis	0.358
PD98059 (13)	Kinase; MAPK/ERK pathwa	0.408
Emetine-2 (8-11, 13)	Protein synthesis	0.424
Austocystin (12)	Unknown	0.425
Emodin (4)	**Kinase**	
105D (6)	Microtubule	0.200
Chloropromazine (4, 6)	Neurotransmitter	0.220
SB203580 (8, 12)	Kinase; MAPK/p38 pathwa	0.234
A23187 free acid (8, 11, 13)	Calcium regulation	0.258
Emetine-1 (5-7)	Protein synthesis	0.285

Supplementary Data 2a: DNA-SC35-Anillin Marker Set

d-Profile	*Major annotated activity*	*Similarity*
Epothilone B (9-11, 13)	**Microtubule**	
Taxol (4-5)	Microtubule	0.291
Griseofulvin (12-13)	Microtubule	0.370
Sulindac sulfide (13)	Cyclooxygenase	0.405
Vinblastine (4-5)	Microtubule	0.459
Taxol (6-13)	Microtubule	0.485
Epothilone B (8)	**Microtubule**	
Chloropromazine (4, 6)	Neurotransmitter	0.452
SB203580 (8, 12)	Kinase; MAPK/p38 pwy.	0.461
Emetine-1 (5-7)	Protein synthesis	0.498
Emodin (4)	Kinase	0.514
Nocodazole-1 (2)	Microtubule	0.539
Etoposide (10-13)	**Topoisomerase**	
Camptothecin (5-9)	Topoisomerase	0.236
Genistein (13)	Kinase	0.519
Doxorubicin (4-6)	Topoisomerase	0.551
MG132 (10-13)	Protein degradation	0.553
ALLN (11-13)	Protein degradation	0.579
Exo1 (13)	**Vesicle trafficking**	
Forskolin (13)	Kinase; PKA	0.424
11N84 (12-13)	Vesicle trafficking	0.499
Ibuprofen (13)	Cyclooxygenase	0.535
Emodin (11, 13)	Kinase	0.561
PD98059 (13)	Kinase; MAPK/ERK pwy.	0.565
Forskolin (13)	**Kinase; PKA**	
Exo1 (13)	Vesicle trafficking	0.424
11N84 (12-13)	Vesicle trafficking	0.478
U0126 (13)	Kinase; MAPK/ERK pwy.	0.480
Deoxynorjrimycin (13)	Vesicle trafficking	0.505
Tunicamycin (9-13)	Vesicle trafficking	0.519
Genistein (13)	**Kinase**	
Monastrol (10, 13)	Microtubule	0.485
Etoposide (10-13)	Topoisomerase	0.519
Doxorubicin (4-6)	Topoisomerase	0.591
Nocodazole-1 (6-9)	Microtubule	0.615
MG132 (10-13)	Protein degradation	0.624
Griseofulvin (12-13)	**Microtubule**	
Nocodazole-1 (6-9)	Microtubule	0.268
105D (10-12)	Microtubule	0.332
Epothilone B (9-11, 13)	Microtubule	0.370
Sulindac sulfide (13)	Cyclooxygenase	0.403
Vinblastine (4-5)	Microtubule	0.407
H89 (12-13)	**Kinase**	
Roscovitine (13)	Kinase; CDK	0.414
Amanitin (11-13)	RNA	0.485
Alsterpaullone (9)	Kinase; CDK	0.491
8-bromo-cAMP (12-13)	Kinase; PKA	0.529
Alsterpaullone (10-13)	Kinase; CDK	0.537
Hydroxy urea-2 (13)	**DNA replication**	
Doxorubicin (7-11)	Topoisomerase	0.388
Methotrexate (11-13)	DNA replication	0.451
Aphidicolin (13)	DNA replication	0.540
Trichostatin (1-3)	Histone deacetylase	0.581
Doxorubicin (4-6)	Topoisomerase	0.584
Ibuprofen (13)	**Cyclooxygenase**	
Tunicamycin (9-13)	Vesicle trafficking	0.285
WY-14643 (12-13)	Nuclear receptor	0.441
U0126 (13)	Kinase; MAPK/ERK pwy.	0.444
Monastrol (10, 13)	Microtubule	0.502
W-7 hydrochloride (13)	Calcium regulation	0.507
Indirubin monoxime (12-13)	**Kinase; CDK**	
Roscovitine (13)	Kinase; CDK	0.346
Alsterpaullone (10-13)	Kinase; CDK	0.406
Actinomycin D (7-13)	RNA	0.484
Camptothecin (10-13)	Topoisomerase	0.531
Emodin (11, 13)	Kinase	0.568

d-Profile	*Major annotated activity*	*Similarity*
Jasplakinolide (12-13)	**Actin**	
Cytochalasin B (12)	Actin	0.253
Cyclosporin A (12-13)	Calcium regulation	0.361
Latrunculin B (10-13)	Actin	0.388
W-7 hydrochloride (13)	Calcium regulation	0.474
Puromycin (9-10, 13)	Protein synthesis	0.509
Lactacystin (13)	**Protein degradation**	
Emodin (11, 13)	Kinase	0.433
Concentramide (6)	Unknown	0.446
Austocystin (12)	Unknown	0.463
Anisomycin (7-8)	Protein synthesis	0.471
Cycloheximide (8, 10-13)	Protein synthesis	0.500
Latrunculin B (10-13)	**Actin**	
Jasplakinolide (12-13)	Actin	0.388
Cyclosporin A (12-13)	Calcium regulation	0.435
Mevastatin (13)	Cholesterol	0.450
Cytochalasin D (8-13)	Actin	0.495
Cytochalasin B (12)	Actin	0.526
Methotrexate (11-13)	**DNA replication**	
Doxorubicin (7-11)	Topoisomerase	0.447
Hydroxy urea-2 (13)	DNA replication	0.451
Aphidicolin (13)	DNA replication	0.560
105D (1)	Microtubule	0.591
Doxorubicin (4-6)	Topoisomerase	0.593
Mevastatin (13)	**Cholesterol**	
Simavastatin (12)	Cholesterol	0.333
Latrunculin B (10-13)	Actin	0.450
Concentramide (6)	Unknown	0.488
Cyclosporin A (12-13)	Calcium regulation	0.491
Purvalanol A (12-13)	Kinase; CDK	0.498
MG132 (10-13)	**Protein degradation**	
ALLN (11-13)	Protein degradation	0.323
Vinblastine (6-13)	Microtubule	0.447
Podophyllotoxin (7-11, 13)	Microtubule	0.461
Trichostatin (1-3)	Histone deacetylase	0.542
Doxorubicin (7-11)	Topoisomerase	0.544
Monastrol (10, 13)	**Microtubule**	
Nocodazole-1 (6-9)	Microtubule	0.342
Griseofulvin (12-13)	Microtubule	0.409
11N84 (12-13)	Vesicle trafficking	0.416
Sulindac sulfide (13)	Cyclooxygenase	0.422
105D (10-12)	Microtubule	0.472
Nocodazole-1 (11-13)	**Microtubule**	
Podophyllotoxin (7-11, 13)	Microtubule	0.265
Trichostatin (1-3)	Histone deacetylase	0.317
Doxorubicin (7-11)	Topoisomerase	0.363
Vinblastine (6-13)	Microtubule	0.380
Oligomycin (12)	Energy metabolism	0.419
Nocodazole-1 (6-9)	**Microtubule**	
Griseofulvin (12-13)	Microtubule	0.268
105D (10-12)	Microtubule	0.322
Monastrol (10, 13)	Microtubule	0.342
Colchicine (6, 8, 12-13)	Microtubule	0.363
Vinblastine (4-5)	Microtubule	0.408
Nocodazole-1 (2)	**Microtubule**	
Emodin (4)	Kinase	0.340
SB203580 (8, 12)	Kinase; MAPK/p38 pwy.	0.377
105D (6)	Microtubule	0.395
A23187 free acid (8, 11, 13)	Calcium regulation	0.409
Chloropromazine (4, 6)	Neurotransmitter	0.422
Nocodazole-2 (7-11, 13)	**Microtubule**	
Nocodazole-3 (11, 13)	Microtubule	0.260
Vinblastine (6-13)	Microtubule	0.449
Taxol (6-13)	Microtubule	0.457
Podophyllotoxin (7-11, 13)	Microtubule	0.487
Nocodazole-1 (6-9)	Microtubule	0.535

Supplementary Data 2a: DNA-SC35-Anillin Marker Set

d-Profile	*Major annotated activity*	*Similarity*
Nocodazole-3 (11, 13)	**Microtubule**	
Nocodazole-2 (7-11, 13)	Microtubule	0.260
Colchicine (6, 8, 12-13)	Microtubule	0.458
Podophyllotoxin (7-11, 13)	Microtubule	0.500
Oligomycin (12)	Energy metabolism	0.516
Trichostatin (1-3)	Histone deacetylase	0.527
Okadaic acid (10-11)	**Kinase**	
105D (1)	Microtubule	0.595
Simavastatin (12)	Cholesterol	0.665
Aphidicolin (13)	DNA replication	0.676
Nocodazole-3 (11, 13)	Microtubule	0.687
Hydroxy urea-2 (13)	DNA replication	0.687
Okadaic acid (1-2)	**Kinase**	
105D (1)	Microtubule	0.318
PMA (1, 4)	Kinase; PKC	0.430
Nocodazole-1 (2)	Microtubule	0.547
Doxorubicin (4-6)	Topoisomerase	0.567
Methotrexate (11-13)	DNA replication	0.600
Oligomycin (12)	**Energy metabolism**	
Nocodazole-1 (11-13)	Microtubule	0.419
Sodium azide (13)	Energy metabolism	0.463
Trichostatin (1-3)	Histone deacetylase	0.478
Doxorubicin (7-11)	Topoisomerase	0.487
PD98059 (13)	Kinase; MAPK/ERK pwy.	0.494
Olomucine (8, 13)	**Kinase; CDK**	
Cyclosporin A (12-13)	Calcium regulation	0.394
Cytochalasin B (12)	Actin	0.421
W-7 hydrochloride (13)	Calcium regulation	0.432
Cytochalasin B (3-4, 6)	Actin	0.439
Emetine-1 (5-7)	Protein synthesis	0.447
Oxamflatin (11-13)	**Histone deacetylase**	
Apicidin (10-12)	Histone deacetylase	0.163
Trichostatin (9-13)	Histone deacetylase	0.210
Scriptaid-1 (10-12)	Histone deacetylase	0.218
U0126 (13)	Kinase; MAPK/ERK pwy.	0.444
Amanitin (11-13)	RNA	0.494
PD98059 (13)	**Kinase; MAPK/ERK pwy.**	
Emodin (11, 13)	Kinase	0.408
Podophyllotoxin (7-11, 13)	Microtubule	0.434
Vinblastine (6-13)	Microtubule	0.456
Trichostatin (1-3)	Histone deacetylase	0.465
Nocodazole-1 (11-13)	Microtubule	0.485
PMA (13)	**Kinase; PKC**	
Chelerythrine (11)	Kinase; PKC	0.336
Puromycin (9-10, 13)	Protein synthesis	0.435
Staurosporine (10-13)	Kinase	0.436
Didemnin B (8-11)	Protein synthesis	0.496
Emetine-2 (8-11, 13)	Protein synthesis	0.589
PMA (6-7)	**Kinase; PKC**	
Olomucine (8, 13)	Kinase; CDK	0.514
Dexamethasone (8-10, 12-13)	Nuclear receptor	0.533
Chloropromazine (4, 6)	Neurotransmitter	0.575
Anisomycin (7-8)	Protein synthesis	0.593
105D (6)	Microtubule	0.597
PMA (1, 4)	**Kinase; PKC**	
Okadaic acid (1-2)	Kinase	0.430
105D (1)	Microtubule	0.527
Doxorubicin (4-6)	Topoisomerase	0.573
Methotrexate (11-13)	DNA replication	0.626
Dexamethasone (8-10, 12-13)	Nuclear receptor	0.690
Podophyllotoxin (7-11, 13)	**Microtubule**	
Trichostatin (1-3)	Histone deacetylase	0.153
Vinblastine (6-13)	Microtubule	0.189
Nocodazole-1 (11-13)	Microtubule	0.265
Doxorubicin (7-11)	Topoisomerase	0.333
PD98059 (13)	Kinase; MAPK/ERK pwy.	0.434

d-Profile	*Major annotated activity*	*Similarity*
Puromycin (9-10, 13)	**Protein synthesis**	
Staurosporine (10-13)	Kinase	0.280
Chelerythrine (11)	Kinase; PKC	0.391
Didemnin B (8-11)	Protein synthesis	0.393
PMA (13)	Kinase; PKC	0.435
Emetine-2 (8-11, 13)	Protein synthesis	0.447
Purvalanol A (12-13)	**Kinase; CDK**	
Cyclosporin A (12-13)	Calcium regulation	0.448
Scriptaid-2 (13)	Histone deacetylase	0.479
Sodium azide (13)	Energy metabolism	0.479
Actinomycin D (7-13)	RNA	0.484
Mevastatin (13)	Cholesterol	0.498
Roscovitine (13)	**Kinase; CDK**	
Alsterpaullone (10-13)	Kinase; CDK	0.200
Camptothecin (10-13)	Topoisomerase	0.328
Indirubin monoxime (12-13)	Kinase; CDK	0.346
Amanitin (11-13)	RNA	0.382
H89 (12-13)	Kinase	0.414
SB202190 (12-13)	**Kinase; MAPK/p38 pwy.**	
Tunicamycin (9-13)	Vesicle trafficking	0.510
11N84 (12-13)	Vesicle trafficking	0.564
Cyclosporin A (12-13)	Calcium regulation	0.586
Griseofulvin (12-13)	Microtubule	0.598
WY-14643 (12-13)	Nuclear receptor	0.629
SB203580 (8, 12)	**Kinase; MAPK/p38 pwy.**	
Emodin (4)	Kinase	0.234
105D (6)	Microtubule	0.265
A23187 free acid (8, 11, 13)	Calcium regulation	0.307
Chloropromazine (4, 6)	Neurotransmitter	0.318
Nocodazole-1 (2)	Microtubule	0.377
SB203580 (5)	**Kinase; MAPK/p38 pwy.**	
105D (6)	Microtubule	0.351
A23187 free acid (8, 11, 13)	Calcium regulation	0.448
Emodin (4)	Kinase	0.475
Dexamethasone (8-10, 12-13)	Nuclear receptor	0.478
Chloropromazine (4, 6)	Neurotransmitter	0.487
Scriptaid-1 (10-12)	**Histone deacetylase**	
Apicidin (10-12)	Histone deacetylase	0.149
Oxamflatin (11-13)	Histone deacetylase	0.218
Trichostatin (9-13)	Histone deacetylase	0.250
Amanitin (11-13)	RNA	0.477
U0126 (13)	Kinase; MAPK/ERK pwy.	0.518
Scriptaid-2 (13)	**Histone deacetylase**	
Trichostatin (9-13)	Histone deacetylase	0.388
Purvalanol A (12-13)	Kinase; CDK	0.479
Actinomycin D (7-13)	RNA	0.501
Apicidin (10-12)	Histone deacetylase	0.544
Indirubin monoxime (12-13)	Kinase; CDK	0.585
Simavastatin (12)	**Cholesterol**	
Mevastatin (13)	Cholesterol	0.333
Concentramide (6)	Unknown	0.526
Cyclosporin A (12-13)	Calcium regulation	0.534
Cytochalasin B (12)	Actin	0.543
Latrunculin B (10-13)	Actin	0.559
Sodium azide (13)	**Energy metabolism**	
Oligomycin (12)	Energy metabolism	0.463
Purvalanol A (12-13)	Kinase; CDK	0.479
Cyclosporin A (12-13)	Calcium regulation	0.513
Ceramide (13)	Kinase; PKC	0.520
Aphidicolin (13)	DNA replication	0.562

Supplementary Data 2a: DNA-SC35-Anillin Marker Set

d-Profile	*Major annotated activity*	*Similarity*
Staurosporine (10-13)	**Kinase**	
Chelerythrine (11)	Kinase; PKC	0.273
Puromycin (9-10, 13)	Protein synthesis	0.280
PMA (13)	Kinase; PKC	0.436
Didemnin B (8-11)	Protein synthesis	0.605
Colchicine (6, 8, 12-13)	Microtubule	0.616
Staurosporine (8-9)	**Kinase**	
Colchicine (5)	Microtubule	0.389
Sulindac sulfide (13)	Cyclooxygenase	0.439
Vinblastine (4-5)	Microtubule	0.479
Griseofulvin (12-13)	Microtubule	0.497
Nocodazole-1 (6-9)	Microtubule	0.504
Sulindac sulfide (13)	**Cyclooxygenase**	
Vinblastine (4-5)	Microtubule	0.267
Taxol (4-5)	Microtubule	0.305
Colchicine (5)	Microtubule	0.323
Griseofulvin (12-13)	Microtubule	0.403
Epothilone B (9-11, 13)	Microtubule	0.405
Taxol (6-13)	**Microtubule**	
Nocodazole-2 (7-11, 13)	Microtubule	0.457
Epothilone B (9-11, 13)	Microtubule	0.485
Vinblastine (6-13)	Microtubule	0.490
Vinblastine (4-5)	Microtubule	0.576
105D (10-12)	Microtubule	0.578
Taxol (4-5)	**Microtubule**	
Epothilone B (9-11, 13)	Microtubule	0.291
Sulindac sulfide (13)	Cyclooxygenase	0.305
Vinblastine (4-5)	Microtubule	0.419
Colchicine (5)	Microtubule	0.437
Griseofulvin (12-13)	Microtubule	0.514
Trichostatin (9-13)	**Histone deacetylase**	
Oxamflatin (11-13)	Histone deacetylase	0.210
Scriptaid-1 (10-12)	Histone deacetylase	0.250
Apicidin (10-12)	Histone deacetylase	0.251
Scriptaid-2 (13)	Histone deacetylase	0.388
Deoxynorjrimycin (13)	Vesicle trafficking	0.533
Trichostatin (8)	**Histone deacetylase**	
Cytochalasin D (8-13)	Actin	0.560
Scriptaid-1 (10-12)	Histone deacetylase	0.606
Cytochalasin B (12)	Actin	0.616
Dexamethasone (8-10, 12-13)	Nuclear receptor	0.626
Cycloheximide (8, 10-13)	Protein synthesis	0.641
Trichostatin (1-3)	**Histone deacetylase**	
Podophyllotoxin (7-11, 13)	Microtubule	0.153
Doxorubicin (7-11)	Topoisomerase	0.299
Nocodazole-1 (11-13)	Microtubule	0.317
Vinblastine (6-13)	Microtubule	0.317
PD98059 (13)	Kinase; MAPK/ERK pwy.	0.465

d-Profile	*Major annotated activity*	*Similarity*
Tunicamycin (9-13)	**Vesicle trafficking**	
Ibuprofen (13)	Cyclooxygenase	0.285
W-7 hydrochloride (13)	Calcium regulation	0.377
Cyclosporin A (12-13)	Calcium regulation	0.411
11N84 (12-13)	Vesicle trafficking	0.421
Cytochalasin B (12)	Actin	0.427
U0126 (13)	**Kinase; MAPK/ERK pwy.**	
Oxamflatin (11-13)	Histone deacetylase	0.444
Ibuprofen (13)	Cyclooxygenase	0.444
Tunicamycin (9-13)	Vesicle trafficking	0.451
W-7 hydrochloride (13)	Calcium regulation	0.474
Forskolin (13)	Kinase; PKA	0.480
Vinblastine (6-13)	**Microtubule**	
Podophyllotoxin (7-11, 13)	Microtubule	0.189
Trichostatin (1-3)	Histone deacetylase	0.317
Nocodazole-1 (11-13)	Microtubule	0.380
MG132 (10-13)	Protein degradation	0.447
Nocodazole-2 (7-11, 13)	Microtubule	0.449
Vinblastine (4-5)	**Microtubule**	
Sulindac sulfide (13)	Cyclooxygenase	0.267
Colchicine (5)	Microtubule	0.296
Griseofulvin (12-13)	Microtubule	0.407
Nocodazole-1 (6-9)	Microtubule	0.408
Taxol (4-5)	Microtubule	0.419
W-7 hydrochloride (13)	**Calcium regulation**	
Cyclosporin A (12-13)	Calcium regulation	0.341
Tunicamycin (9-13)	Vesicle trafficking	0.377
Olomucine (8, 13)	Kinase; CDK	0.432
11N84 (12-13)	Vesicle trafficking	0.437
Cytochalasin B (12)	Actin	0.471
WY-14643 (12-13)	**Nuclear receptor**	
Ibuprofen (13)	Cyclooxygenase	0.441
Emodin (4)	Kinase	0.454
Emetine-1 (5-7)	Protein synthesis	0.461
SB203580 (8, 12)	Kinase; MAPK/p38 pwy.	0.474
Tunicamycin (9-13)	Vesicle trafficking	0.497

Supplementary Data 2b: DNA-p53-cFos Marker Set

d-Profile	*Major annotated activity*	*Similarity*
105D (11-13)	**Microtubule**	
Colchicine (6-8)	Microtubule	0.292
Nocodazole-2 (6-13)	Microtubule	0.350
Colchicine (9-13)	Microtubule	0.356
Podophyllotoxin (6-7, 9-13)	Microtubule	0.360
Dexamethasone (7-8)	Nuclear receptor	0.373
105D (1-3, 5, 7-9)	**Microtubule**	
Chelerythrine (1)	Kinase; PKC	0.150
Emetine-1 (1, 4, 6)	Protein synthesis	0.157
A23187 free acid (5)	Calcium regulation	0.218
Concentramide (13)	Unknown	0.241
Olomucine (8)	Kinase; CDK	0.249
11N84 (12-13)	**Vesicle trafficking**	
LY294002 (12-13)	Kinase; PI3K pwy.	0.148
Austocystin (12-13)	Unknown	0.177
Emetine-2 (7-13)	Protein synthesis	0.183
SB202190 (12-13)	Kinase; MAPK/p38 pwy.	0.199
Emetine-1 (8-9, 11-13)	Protein synthesis	0.217
A23187 free acid (5)	**Calcium regulation**	
105D (1-3, 5, 7-9)	Microtubule	0.218
SC560 (13)	Cyclooxygenase	0.322
Olomucine (8)	Kinase; CDK	0.335
Niflumic acid (13)	Cyclooxygenase	0.353
Emetine-1 (1, 4, 6)	Protein synthesis	0.359
Actinomycin D (7-13)	**RNA**	
Puromycin (9-10)	Protein synthesis	0.294
Staurosporine (8-11, 13)	Kinase	0.371
Camptothecin (10, 12-13)	Topoisomerase	0.405
Cytochalasin B (12-13)	Actin	0.428
MG132 (9-13)	Protein degradation	0.452
Actinomycin D (3, 5-6)	**RNA**	
Doxorubicin (1, 3, 6)	Topoisomerase	0.459
Olomucine (2-3)	Kinase; CDK	0.482
Concentramide (13)	Unknown	0.497
Methotrexate (9-13)	DNA replication	0.524
Chelerythrine (1)	Kinase; PKC	0.536
Alsterpaullone (11-13)	**Kinase; CDK**	
Camptothecin (10, 12-13)	Topoisomerase	0.334
Roscovitine (13)	Kinase; CDK	0.453
Sulindac sulfide (13)	Cyclooxygenase	0.460
MG132 (9-13)	Protein degradation	0.497
H89 (13)	Kinase	0.503
Amanitin (11)	**RNA**	
Emetine-1 (1, 4, 6)	Protein synthesis	0.314
Niflumic acid (13)	Cyclooxygenase	0.325
105D (1-3, 5, 7-9)	Microtubule	0.330
U0126 (12-13)	Kinase; MAPK/ERK pwy.	0.354
SC560 (13)	Cyclooxygenase	0.355
Amanitin (1)	**RNA**	
Chelerythrine (1)	Kinase; PKC	0.254
Zvad (13)	Protein degradation	0.331
Doxorubicin (1, 3, 6)	Topoisomerase	0.344
PD169316 (11-13)	Kinase; MAPK/p38 pwy.	0.357
Wortmannin (12-13)	Kinase; PI3K pwy.	0.358
Anisomycin (8-10, 12-13)	**Protein synthesis**	
Cycloheximide (10-13)	Protein synthesis	0.195
Okadaic acid (11)	Kinase	0.261
Didemnin B (8-11)	Protein synthesis	0.274
Staurosporine (8-11, 13)	Kinase	0.275
Vinblastine (6-8, 10-11, 13)	Microtubule	0.282
Aphidicolin (9-13)	**DNA replication**	
Hydroxy urea-2 (12-13)	DNA replication	0.186
Methotrexate (9-13)	DNA replication	0.247
Doxorubicin (1, 3, 6)	Topoisomerase	0.415
Retinoic acid (trans) (12)	Nuclear receptor	0.468
Emetine-1 (1, 4, 6)	Protein synthesis	0.496

d-Profile	*Major annotated activity*	*Similarity*
Apicidin (11-13)	**Histone deacetylase**	
Trichostatin (9-13)	Histone deacetylase	0.295
Scriptaid-1 (13)	Histone deacetylase	0.313
Oligomycin (7-10, 12-13)	Energy metabolism	0.364
Oxamflatin (12-13)	Histone deacetylase	0.365
Scriptaid-2 (10-12)	Histone deacetylase	0.413
Austocystin (12-13)	**Unknown**	
Didemnin B (8-11)	Protein synthesis	0.084
Emetine-1 (8-9, 11-13)	Protein synthesis	0.102
Emetine-2 (7-13)	Protein synthesis	0.107
11N84 (12-13)	Vesicle trafficking	0.177
LY294002 (12-13)	Kinase; PI3K pwy.	0.179
Austocystin (3)	**Unknown**	
Olomucine (2-3)	Kinase; CDK	0.315
WY-14643 (3)	Nuclear receptor	0.360
Emetine-2 (6)	Protein synthesis	0.480
Camptothecin (6-9)	Topoisomerase	0.486
PMA (4-7)	Kinase; PKC	0.578
Brefeldin A (8-13)	**Vesicle trafficking**	
Ceramide (13)	Kinase; PKC	0.070
LY294002 (12-13)	Kinase; PI3K pwy.	0.130
Emetine-1 (1, 4, 6)	Protein synthesis	0.134
SC560 (13)	Cyclooxygenase	0.151
Emetine-1 (8-9, 11-13)	Protein synthesis	0.192
Camptothecin (10, 12-13)	**Topoisomerase**	
Trichostatin (1-3)	Histone deacetylase	0.299
Trichostatin (9-13)	Histone deacetylase	0.311
Puromycin (9-10)	Protein synthesis	0.318
Podophyllotoxin (6-7, 9-13)	Microtubule	0.318
Vinblastine (6-8, 10-11, 13)	Microtubule	0.325
Camptothecin (6-9)	**Topoisomerase**	
Olomucine (2-3)	Kinase; CDK	0.464
Austocystin (3)	Unknown	0.486
WY-14643 (3)	Nuclear receptor	0.607
Etoposide (10-12)	Topoisomerase	0.669
Doxorubicin (8-12)	Topoisomerase	0.678
Ceramide (13)	**Kinase; PKC**	
Brefeldin A (8-13)	Vesicle trafficking	0.070
Emetine-1 (8-9, 11-13)	Protein synthesis	0.139
Emetine-1 (1, 4, 6)	Protein synthesis	0.168
LY294002 (12-13)	Kinase; PI3K pwy.	0.215
Emodin (11-13)	Kinase	0.216
Chelerythrine (1)	**Kinase; PKC**	
105D (1-3, 5, 7-9)	Microtubule	0.150
Emetine-1 (1, 4, 6)	Protein synthesis	0.190
Concentramide (13)	Unknown	0.217
Wortmannin (12-13)	Kinase; PI3K pwy.	0.218
Leupeptine (13)	Protein degradation	0.220
Ciglitazone (13)	**Nuclear receptor**	
Colchicine (6-8)	Microtubule	0.232
Nocodazole-2 (6-13)	Microtubule	0.252
Oligomycin (7-10, 12-13)	Energy metabolism	0.279
Nocodazole-3 (10-13)	Microtubule	0.299
Nocodazole-1 (7-13)	Microtubule	0.309
Clozapine (13)	**Neurotransmitter**	
Tunicamycin (9-13)	Vesicle trafficking	0.146
LY294002 (12-13)	Kinase; PI3K pwy.	0.213
Wortmannin (12-13)	Kinase; PI3K pwy.	0.276
Brefeldin A (8-13)	Vesicle trafficking	0.295
Cyclosporin A (12-13)	Calcium regulation	0.300

Supplementary Data 2b: DNA-p53-cFos Marker Set

d-Profile	*Major annotated activity*	*Similarity*
Colchicine (9-13)	**Microtubule**	
Vinblastine (6-8, 10-11, 13)	Microtubule	0.088
Nocodazole-2 (6-13)	Microtubule	0.091
Trichostatin (1-3)	Histone deacetylase	0.100
Dexamethasone (7-8)	Nuclear receptor	0.107
Nocodazole-3 (10-13)	Microtubule	0.108
Colchicine (6-8)	**Microtubule**	
Ciglitazone (13)	Nuclear receptor	0.232
Nocodazole-2 (6-13)	Microtubule	0.274
105D (11-13)	Microtubule	0.292
Vinblastine (4-5)	Microtubule	0.378
Nocodazole-1 (7-13)	Microtubule	0.380
Concentramide (13)	**Unknown**	
Leupeptine (13)	Protein degradation	0.128
WY-14643 (9, 13)	Nuclear receptor	0.197
Wortmannin (12-13)	Kinase; PI3K pwy.	0.198
Doxorubicin (1, 3, 6)	Topoisomerase	0.209
Chelerythrine (1)	Kinase; PKC	0.217
Cycloheximide (10-13)	**Protein synthesis**	
Anisomycin (8-10, 12-13)	Protein synthesis	0.195
Scriptaid-2 (10-12)	Histone deacetylase	0.319
Austocystin (12-13)	Unknown	0.324
Staurosporine (8-11, 13)	Kinase	0.327
Didemnin B (8-11)	Protein synthesis	0.329
Cyclosporin A (12-13)	**Calcium regulation**	
Wortmannin (12-13)	Kinase; PI3K pwy.	0.134
PD169316 (11-13)	Kinase; MAPK/p38 pwy.	0.138
Tunicamycin (9-13)	Vesicle trafficking	0.170
SC560 (13)	Cyclooxygenase	0.238
LY294002 (12-13)	Kinase; PI3K pwy.	0.259
Cytochalasin B (12-13)	**Actin**	
Staurosporine (8-11, 13)	Kinase	0.228
Anisomycin (8-10, 12-13)	Protein synthesis	0.293
Didemnin B (8-11)	Protein synthesis	0.340
Puromycin (9-10)	Protein synthesis	0.343
Latrunculin B (10-13)	Actin	0.357
Cytochalasin D (10-13)	**Actin**	
Latrunculin B (10-13)	Actin	0.218
Nocodazole-1 (1, 5-6)	Microtubule	0.359
Didemnin B (8-11)	Protein synthesis	0.375
Cytochalasin B (12-13)	Actin	0.390
Austocystin (12-13)	Unknown	0.399
Cytochalasin D (8)	**Actin**	
Nocodazole-1 (1, 5-6)	Microtubule	0.509
Olomucine (2-3)	Kinase; CDK	0.620
Okadaic acid (11)	Kinase	0.690
105D (11-13)	Microtubule	0.716
Latrunculin B (10-13)	Actin	0.717
Dexamethasone (7-8)	**Nuclear receptor**	
Colchicine (9-13)	Microtubule	0.107
Nocodazole-3 (10-13)	Microtubule	0.125
Nocodazole-1 (7-13)	Microtubule	0.138
Nocodazole-2 (6-13)	Microtubule	0.147
Vinblastine (6-8, 10-11, 13)	Microtubule	0.178
Didemnin B (8-11)	**Protein synthesis**	
Emetine-2 (7-13)	Protein synthesis	0.067
Austocystin (12-13)	Unknown	0.084
Emetine-1 (8-9, 11-13)	Protein synthesis	0.160
Latrunculin B (10-13)	Actin	0.169
11N84 (12-13)	Vesicle trafficking	0.225

d-Profile	*Major annotated activity*	*Similarity*
Doxorubicin (8-12)	**Topoisomerase**	
Olomucine (2-3)	Kinase; CDK	0.461
Nocodazole-1 (1, 5-6)	Microtubule	0.567
Austocystin (3)	Unknown	0.623
WY-14643 (3)	Nuclear receptor	0.632
Camptothecin (6-9)	Topoisomerase	0.678
Doxorubicin (1, 3, 6)	**Topoisomerase**	
Concentramide (13)	Unknown	0.209
Wortmannin (12-13)	Kinase; PI3K pwy.	0.210
PD169316 (11-13)	Kinase; MAPK/p38 pwy.	0.215
SB202190 (12-13)	Kinase; MAPK/p38 pwy.	0.226
WY-14643 (9, 13)	Nuclear receptor	0.227
Emetine-1 (8-9, 11-13)	**Protein synthesis**	
Austocystin (12-13)	Unknown	0.102
Ceramide (13)	Kinase; PKC	0.139
Emodin (11-13)	Kinase	0.158
Didemnin B (8-11)	Protein synthesis	0.160
LY294002 (12-13)	Kinase; PI3K pwy.	0.170
Emetine-1 (1, 4, 6)	**Protein synthesis**	
Brefeldin A (8-13)	Vesicle trafficking	0.134
105D (1-3, 5, 7-9)	Microtubule	0.157
SC560 (13)	Cyclooxygenase	0.164
Ceramide (13)	Kinase; PKC	0.168
LY294002 (12-13)	Kinase; PI3K pwy.	0.186
Emetine-2 (7-13)	**Protein synthesis**	
Didemnin B (8-11)	Protein synthesis	0.067
Austocystin (12-13)	Unknown	0.107
Emetine-1 (8-9, 11-13)	Protein synthesis	0.177
11N84 (12-13)	Vesicle trafficking	0.183
Latrunculin B (10-13)	Actin	0.186
Emetine-2 (6)	**Protein synthesis**	
PMA (4-7)	Kinase; PKC	0.376
PMA (11-12)	Kinase; PKC	0.428
WY-14643 (3)	Nuclear receptor	0.449
Scriptaid-2 (10-12)	Histone deacetylase	0.474
Austocystin (3)	Unknown	0.480
Emodin (11-13)	**Kinase**	
Emetine-1 (8-9, 11-13)	Protein synthesis	0.158
Genistein (12-13)	Kinase	0.185
Ceramide (13)	Kinase; PKC	0.216
LY294002 (12-13)	Kinase; PI3K pwy.	0.230
Austocystin (12-13)	Unknown	0.243
Epothilone B (10)	**Microtubule**	
Sulindac sulfide (13)	Cyclooxygenase	0.293
Taxol (4-6)	Microtubule	0.308
Griseofulvin (13)	Microtubule	0.503
Actinomycin D (7-13)	RNA	0.537
Didemnin B (8-11)	Protein synthesis	0.553
Etoposide (10-12)	**Topoisomerase**	
Methotrexate (9-13)	DNA replication	0.579
Aphidicolin (9-13)	DNA replication	0.591
Actinomycin D (3, 5-6)	RNA	0.598
105D (1-3, 5, 7-9)	Microtubule	0.640
SC560 (13)	Cyclooxygenase	0.656
Filopodine (12-13)	**Unknown**	
SB202190 (12-13)	Kinase; MAPK/p38 pwy.	0.122
11N84 (12-13)	Vesicle trafficking	0.219
Emetine-2 (7-13)	Protein synthesis	0.219
PD169316 (11-13)	Kinase; MAPK/p38 pwy.	0.231
LY294002 (12-13)	Kinase; PI3K pwy.	0.238
Genistein (12-13)	**Kinase**	
Ibuprofen (13)	Cyclooxygenase	0.095
Rapamycin (13)	Kinase; PI3K pwy.	0.121
Monastrol (13)	Microtubule	0.157
Emodin (11-13)	Kinase	0.185
LY294002 (12-13)	Kinase; PI3K pwy.	0.194

Supplementary Data 2b: DNA-p53-cFos Marker Set

d-Profile	*Major annotated activity*	*Similarity*
Griseofulvin (13)	**Microtubule**	
Podophyllotoxin (6-7, 9-13)	Microtubule	0.268
Taxol (7-8)	Microtubule	0.273
Nocodazole-3 (10-13)	Microtubule	0.281
Colchicine (9-13)	Microtubule	0.291
Trichostatin (1-3)	Histone deacetylase	0.300
H89 (13)	**Kinase**	
Oxamflatin (12-13)	Histone deacetylase	0.267
Trichostatin (9-13)	Histone deacetylase	0.287
Anisomycin (8-10, 12-13)	Protein synthesis	0.334
Camptothecin (10, 12-13)	Topoisomerase	0.357
Staurosporine (8-11, 13)	Kinase	0.364
Hydroxy urea-1 (13)	**DNA replication**	
Genistein (12-13)	Kinase	0.217
Ibuprofen (13)	Cyclooxygenase	0.264
Rapamycin (13)	Kinase; PI3K pwy.	0.303
Monastrol (13)	Microtubule	0.318
Sodium butyrate (13)	Histone deacetylase	0.341
Hydroxy urea-2 (12-13)	**DNA replication**	
Aphidicolin (9-13)	DNA replication	0.186
Methotrexate (9-13)	DNA replication	0.364
Hydroxy urea-1 (13)	DNA replication	0.541
Doxorubicin (1, 3, 6)	Topoisomerase	0.555
U0126 (12-13)	Kinase; MAPK/ERK pwy.	0.575
Ibuprofen (13)	**Cyclooxygenase**	
Genistein (12-13)	Kinase	0.095
Rapamycin (13)	Kinase; PI3K pwy.	0.176
Emetine-1 (1, 4, 6)	Protein synthesis	0.248
Sodium butyrate (13)	Histone deacetylase	0.251
Monastrol (13)	Microtubule	0.263
Indirubin monoxime (12-13)	**Kinase; CDK**	
11N84 (12-13)	Vesicle trafficking	0.219
Emetine-2 (7-13)	Protein synthesis	0.245
SB202190 (12-13)	Kinase; MAPK/p38 pwy.	0.262
W-7 hydrochloride (12-13)	Calcium regulation	0.266
Tunicamycin (9-13)	Vesicle trafficking	0.296
Indomethacin (13)	**Cyclooxygenase**	
Griseofulvin (13)	Microtubule	0.307
Nocodazole-3 (10-13)	Microtubule	0.334
Podophyllotoxin (6-7, 9-13)	Microtubule	0.341
Nocodazole-2 (6-13)	Microtubule	0.341
Trichostatin (1-3)	Histone deacetylase	0.343
Jasplakinolide (12-13)	**Actin**	
Latrunculin B (10-13)	Actin	0.318
Tunicamycin (9-13)	Vesicle trafficking	0.386
Indirubin monoxime (12-13)	Kinase; CDK	0.407
Clozapine (13)	Neurotransmitter	0.410
Trichostatin (9-13)	Histone deacetylase	0.416
Lactacystin (13)	**Protein degradation**	
Genistein (12-13)	Kinase	0.288
Emetine-2 (7-13)	Protein synthesis	0.295
Monastrol (13)	Microtubule	0.295
Rapamycin (13)	Kinase; PI3K pwy.	0.310
Indirubin monoxime (12-13)	Kinase; CDK	0.312
Latrunculin B (10-13)	**Actin**	
Didemnin B (8-11)	Protein synthesis	0.169
Emetine-2 (7-13)	Protein synthesis	0.186
Austocystin (12-13)	Unknown	0.204
Cytochalasin D (10-13)	Actin	0.218
LY294002 (12-13)	Kinase; PI3K pwy.	0.268
Leupeptine (13)	**Protein degradation**	
Concentramide (13)	Unknown	0.128
Zvad (13)	Protein degradation	0.163
Chelerythrine (1)	Kinase; PKC	0.220
Rapamycin (13)	Kinase; PI3K pwy.	0.224
WY-14643 (9, 13)	Nuclear receptor	0.230

d-Profile	*Major annotated activity*	*Similarity*
LY294002 (12-13)	**Kinase; PI3K pwy.**	
Brefeldin A (8-13)	Vesicle trafficking	0.130
11N84 (12-13)	Vesicle trafficking	0.148
SC560 (13)	Cyclooxygenase	0.153
Tunicamycin (9-13)	Vesicle trafficking	0.163
Emetine-1 (8-9, 11-13)	Protein synthesis	0.170
Methotrexate (9-13)	**DNA replication**	
Emetine-1 (1, 4, 6)	Protein synthesis	0.224
Aphidicolin (9-13)	DNA replication	0.247
Ceramide (13)	Kinase; PKC	0.271
Brefeldin A (8-13)	Vesicle trafficking	0.278
Chelerythrine (1)	Kinase; PKC	0.293
Mevastatin (12)	**Cholesterol**	
11N84 (12-13)	Vesicle trafficking	0.256
LY294002 (12-13)	Kinase; PI3K pwy.	0.262
Emodin (11-13)	Kinase	0.308
Genistein (12-13)	Kinase	0.310
Cycloheximide (10-13)	Protein synthesis	0.345
MG132 (9-13)	**Protein degradation**	
Vinblastine (6-8, 10-11, 13)	Microtubule	0.313
Nocodazole-3 (10-13)	Microtubule	0.316
Trichostatin (9-13)	Histone deacetylase	0.331
Dexamethasone (7-8)	Nuclear receptor	0.335
Trichostatin (1-3)	Histone deacetylase	0.341
Monastrol (13)	**Microtubule**	
Genistein (12-13)	Kinase	0.157
Rapamycin (13)	Kinase; PI3K pwy.	0.169
Emetine-2 (7-13)	Protein synthesis	0.215
11N84 (12-13)	Vesicle trafficking	0.234
Austocystin (12-13)	Unknown	0.247
Niflumic acid (13)	**Cyclooxygenase**	
SC560 (13)	Cyclooxygenase	0.167
Olomucine (8)	Kinase; CDK	0.204
Emetine-1 (1, 4, 6)	Protein synthesis	0.221
105D (1-3, 5, 7-9)	Microtubule	0.284
ICRF193 (13)	Topoisomerase	0.318
Nocodazole-1 (7-13)	**Microtubule**	
Nocodazole-2 (6-13)	Microtubule	0.107
Colchicine (9-13)	Microtubule	0.115
Nocodazole-3 (10-13)	Microtubule	0.122
Dexamethasone (7-8)	Nuclear receptor	0.138
Vinblastine (6-8, 10-11, 13)	Microtubule	0.159
Nocodazole-1 (1, 5-6)	**Microtubule**	
Latrunculin B (10-13)	Actin	0.285
Olomucine (2-3)	Kinase; CDK	0.296
Doxorubicin (1, 3, 6)	Topoisomerase	0.318
Didemnin B (8-11)	Protein synthesis	0.342
Monastrol (13)	Microtubule	0.349
Nocodazole-2 (6-13)	**Microtubule**	
Nocodazole-3 (10-13)	Microtubule	0.085
Colchicine (9-13)	Microtubule	0.091
Nocodazole-1 (7-13)	Microtubule	0.107
Vinblastine (6-8, 10-11, 13)	Microtubule	0.136
Dexamethasone (7-8)	Nuclear receptor	0.147
Nocodazole-3 (10-13)	**Microtubule**	
Nocodazole-2 (6-13)	Microtubule	0.085
Colchicine (9-13)	Microtubule	0.108
Nocodazole-1 (7-13)	Microtubule	0.122
Dexamethasone (7-8)	Nuclear receptor	0.125
Vinblastine (6-8, 10-11, 13)	Microtubule	0.134
Okadaic acid (11)	**Kinase**	
Anisomycin (8-10, 12-13)	Protein synthesis	0.261
Podophyllotoxin (6-7, 9-13)	Microtubule	0.298
Trichostatin (1-3)	Histone deacetylase	0.327
Puromycin (9-10)	Protein synthesis	0.335
Nocodazole-3 (10-13)	Microtubule	0.348

Supplementary Data 2b: DNA-p53-cFos Marker Set

d-Profile	*Major annotated activity*	*Similarity*
Oligomycin (7-10, 12-13)	**Energy metabolism**	
Ciglitazone (13)	Nuclear receptor	0.279
Nocodazole-3 (10-13)	Microtubule	0.295
Nocodazole-2 (6-13)	Microtubule	0.317
Nocodazole-1 (7-13)	Microtubule	0.321
Dexamethasone (7-8)	Nuclear receptor	0.358
Oxamflatin (12-13)	**Histone deacetylase**	
Trichostatin (9-13)	Histone deacetylase	0.195
Podophyllotoxin (6-7, 9-13)	Microtubule	0.228
Colchicine (9-13)	Microtubule	0.236
Vinblastine (6-8, 10-11, 13)	Microtubule	0.256
Nocodazole-2 (6-13)	Microtubule	0.261
Olomucine (8)	**Kinase; CDK**	
Niflumic acid (13)	Cyclooxygenase	0.204
105D (1-3, 5, 7-9)	Microtubule	0.249
Emetine-1 (1, 4, 6)	Protein synthesis	0.258
SC560 (13)	Cyclooxygenase	0.302
Chelerythrine (1)	Kinase; PKC	0.315
Olomucine (2-3)	Kinase; CDK	
WY-14643 (3)	Nuclear receptor	0.186
Nocodazole-1 (1, 5-6)	Microtubule	0.296
Austocystin (3)	Unknown	0.315
Doxorubicin (1, 3, 6)	Topoisomerase	0.444
Doxorubicin (8-12)	Topoisomerase	0.461
PD169316 (11-13)	**Kinase; MAPK/p38 pwy.**	
Wortmannin (12-13)	Kinase; PI3K pwy.	0.075
Cyclosporin A (12-13)	Calcium regulation	0.138
Tunicamycin (9-13)	Vesicle trafficking	0.161
W-7 hydrochloride (12-13)	Calcium regulation	0.181
LY294002 (12-13)	Kinase; PI3K pwy.	0.214
PMA (11-12)	**Kinase; PKC**	
Emetine-1 (1, 4, 6)	Protein synthesis	0.384
Methotrexate (9-13)	DNA replication	0.403
Brefeldin A (8-13)	Vesicle trafficking	0.410
W-7 hydrochloride (12-13)	Calcium regulation	0.418
Emetine-2 (6)	Protein synthesis	0.428
PMA (4-7)	**Kinase; PKC**	
Emetine-2 (6)	Protein synthesis	0.376
Austocystin (3)	Unknown	0.578
Olomucine (8)	Kinase; CDK	0.618
WY-14643 (3)	Nuclear receptor	0.664
Scriptaid-2 (10-12)	Histone deacetylase	0.707
Podophyllotoxin (6-7, 9-13)	**Microtubule**	
Vinblastine (6-8, 10-11, 13)	Microtubule	0.094
Trichostatin (1-3)	Histone deacetylase	0.102
Colchicine (9-13)	Microtubule	0.112
Nocodazole-2 (6-13)	Microtubule	0.156
Nocodazole-1 (7-13)	Microtubule	0.160
Puromycin (9-10)	**Protein synthesis**	
Staurosporine (8-11, 13)	Kinase	0.227
Anisomycin (8-10, 12-13)	Protein synthesis	0.287
Actinomycin D (7-13)	RNA	0.294
Camptothecin (10, 12-13)	Topoisomerase	0.318
Nocodazole-3 (10-13)	Microtubule	0.320
Purvalanol A (13)	**Kinase; CDK**	
Trichostatin (9-13)	Histone deacetylase	0.257
Vinblastine (6-8, 10-11, 13)	Microtubule	0.259
Nocodazole-2 (6-13)	Microtubule	0.274
Colchicine (9-13)	Microtubule	0.276
Taxol (7-8)	Microtubule	0.301
Rapamycin (13)	**Kinase; PI3K pwy.**	
Genistein (12-13)	Kinase	0.121
Monastrol (13)	Microtubule	0.169
Ibuprofen (13)	Cyclooxygenase	0.176
Zvad (13)	Protein degradation	0.182
U0126 (12-13)	Kinase; MAPK/ERK pwy.	0.201

d-Profile	*Major annotated activity*	*Similarity*
Retinoic acid (trans) (12)	**Nuclear receptor**	
WY-14643 (9, 13)	Nuclear receptor	0.283
Leupeptine (13)	Protein degradation	0.285
Ibuprofen (13)	Cyclooxygenase	0.318
Emetine-1 (1, 4, 6)	Protein synthesis	0.331
Concentramide (13)	Unknown	0.341
Roscovitine (13)	**Kinase; CDK**	
Camptothecin (10, 12-13)	Topoisomerase	0.375
H89 (13)	Kinase	0.443
Alsterpaullone (11-13)	Kinase; CDK	0.453
Puromycin (9-10)	Protein synthesis	0.475
Actinomycin D (7-13)	RNA	0.480
ICRF193 (13)	**Topoisomerase**	
Sodium butyrate (13)	Histone deacetylase	0.131
Ibuprofen (13)	Cyclooxygenase	0.301
Emodin (11-13)	Kinase	0.303
Genistein (12-13)	Kinase	0.314
Niflumic acid (13)	Cyclooxygenase	0.318
SB202190 (12-13)	**Kinase; MAPK/p38 pwy.**	
Filopodine (12-13)	Unknown	0.122
11N84 (12-13)	Vesicle trafficking	0.199
SB203580 (13)	Kinase; MAPK/p38 pwy.	0.211
LY294002 (12-13)	Kinase; PI3K pwy.	0.216
Emetine-2 (7-13)	Protein synthesis	0.218
SB203580 (13)	**Kinase; MAPK/p38 pwy.**	
SB202190 (12-13)	Kinase; MAPK/p38 pwy.	0.211
11N84 (12-13)	Vesicle trafficking	0.231
Monastrol (13)	Microtubule	0.256
Emetine-2 (7-13)	Protein synthesis	0.266
Austocystin (12-13)	Unknown	0.277
SC560 (13)	**Cyclooxygenase**	
Brefeldin A (8-13)	Vesicle trafficking	0.151
LY294002 (12-13)	Kinase; PI3K pwy.	0.153
Emetine-1 (1, 4, 6)	Protein synthesis	0.164
Niflumic acid (13)	Cyclooxygenase	0.167
W-7 hydrochloride (12-13)	Calcium regulation	0.219
Scriptaid-1 (13)	**Histone deacetylase**	
Apicidin (11-13)	Histone deacetylase	0.313
Brefeldin A (8-13)	Vesicle trafficking	0.379
SC560 (13)	Cyclooxygenase	0.406
Oxamflatin (12-13)	Histone deacetylase	0.410
Niflumic acid (13)	Cyclooxygenase	0.432
Scriptaid-2 (10-12)	**Histone deacetylase**	
Didemnin B (8-11)	Protein synthesis	0.261
Nocodazole-1 (7-13)	Microtubule	0.300
Emodin (11-13)	Kinase	0.303
Emetine-2 (7-13)	Protein synthesis	0.304
Cycloheximide (10-13)	Protein synthesis	0.319
Sodium butyrate (13)	**Histone deacetylase**	
ICRF193 (13)	Topoisomerase	0.131
Ibuprofen (13)	Cyclooxygenase	0.251
Genistein (12-13)	Kinase	0.313
Hydroxy urea-1 (13)	DNA replication	0.341
Niflumic acid (13)	Cyclooxygenase	0.348
Staurosporine (8-11, 13)	**Kinase**	
Puromycin (9-10)	Protein synthesis	0.227
Cytochalasin B (12-13)	Actin	0.228
Anisomycin (8-10, 12-13)	Protein synthesis	0.275
Nocodazole-3 (10-13)	Microtubule	0.275
Vinblastine (6-8, 10-11, 13)	Microtubule	0.277
Sulindac sulfide (13)	**Cyclooxygenase**	
Epothilone B (10)	Microtubule	0.293
Griseofulvin (13)	Microtubule	0.390
Staurosporine (8-11, 13)	Kinase	0.427
H89 (13)	Kinase	0.433
Taxol (4-6)	Microtubule	0.443

Supplementary Data 2b: DNA-p53-cFos Marker Set

d-Profile	*Major annotated activity*	*Similarity*
Taxol (7-8)	**Microtubule**	
Podophyllotoxin (6-7, 9-13)	Microtubule	0.186
Vinblastine (6-8, 10-11, 13)	Microtubule	0.238
Colchicine (9-13)	Microtubule	0.241
Trichostatin (1-3)	Histone deacetylase	0.241
Griseofulvin (13)	Microtubule	0.273
Taxol (4-6)	**Microtubule**	
Vinblastine (4-5)	Microtubule	0.296
Epothilone B (10)	Microtubule	0.308
Nocodazole-2 (6-13)	Microtubule	0.422
Nocodazole-3 (10-13)	Microtubule	0.434
Sulindac sulfide (13)	Cyclooxygenase	0.443
Trichostatin (9-13)	**Histone deacetylase**	
Vinblastine (6-8, 10-11, 13)	Microtubule	0.189
Oxamflatin (12-13)	Histone deacetylase	0.195
Colchicine (9-13)	Microtubule	0.233
Podophyllotoxin (6-7, 9-13)	Microtubule	0.245
Purvalanol A (13)	Kinase; CDK	0.257
Trichostatin (8)	**Histone deacetylase**	
Cytochalasin D (10-13)	Actin	0.585
Scriptaid-2 (10-12)	Histone deacetylase	0.594
Tunicamycin (9-13)	Vesicle trafficking	0.615
Emetine-2 (6)	Protein synthesis	0.627
Apicidin (11-13)	Histone deacetylase	0.643
Trichostatin (1-3)	**Histone deacetylase**	
Colchicine (9-13)	Microtubule	0.100
Podophyllotoxin (6-7, 9-13)	Microtubule	0.102
Vinblastine (6-8, 10-11, 13)	Microtubule	0.115
Nocodazole-2 (6-13)	Microtubule	0.174
Nocodazole-3 (10-13)	Microtubule	0.205
Tunicamycin (9-13)	**Vesicle trafficking**	
Clozapine (13)	Neurotransmitter	0.146
Wortmannin (12-13)	Kinase; PI3K pwy.	0.152
PD169316 (11-13)	Kinase; MAPK/p38 pwy.	0.161
LY294002 (12-13)	Kinase; PI3K pwy.	0.163
Cyclosporin A (12-13)	Calcium regulation	0.170
U0126 (12-13)	**Kinase; MAPK/ERK pwy.**	
Tunicamycin (9-13)	Vesicle trafficking	0.174
Rapamycin (13)	Kinase; PI3K pwy.	0.201
Wortmannin (12-13)	Kinase; PI3K pwy.	0.257
W-7 hydrochloride (12-13)	Calcium regulation	0.259
Genistein (12-13)	Kinase	0.268

d-Profile	*Major annotated activity*	*Similarity*
Vinblastine (6-8, 10-11, 13)	**Microtubule**	
Colchicine (9-13)	Microtubule	0.088
Podophyllotoxin (6-7, 9-13)	Microtubule	0.094
Trichostatin (1-3)	Histone deacetylase	0.115
Nocodazole-3 (10-13)	Microtubule	0.134
Nocodazole-2 (6-13)	Microtubule	0.136
Vinblastine (4-5)	**Microtubule**	
Taxol (4-6)	Microtubule	0.296
Nocodazole-2 (6-13)	Microtubule	0.377
Colchicine (6-8)	Microtubule	0.378
Nocodazole-3 (10-13)	Microtubule	0.431
Oligomycin (7-10, 12-13)	Energy metabolism	0.500
W-7 hydrochloride (12-13)	**Calcium regulation**	
Wortmannin (12-13)	Kinase; PI3K pwy.	0.170
PD169316 (11-13)	Kinase; MAPK/p38 pwy.	0.181
Emetine-1 (1, 4, 6)	Protein synthesis	0.187
Tunicamycin (9-13)	Vesicle trafficking	0.208
LY294002 (12-13)	Kinase; PI3K pwy.	0.217
Wortmannin (12-13)	**Kinase; PI3K pwy.**	
PD169316 (11-13)	Kinase; MAPK/p38 pwy.	0.075
Cyclosporin A (12-13)	Calcium regulation	0.134
WY-14643 (9, 13)	Nuclear receptor	0.147
Tunicamycin (9-13)	Vesicle trafficking	0.152
W-7 hydrochloride (12-13)	Calcium regulation	0.170
WY-14643 (9, 13)	**Nuclear receptor**	
Wortmannin (12-13)	Kinase; PI3K pwy.	0.147
Concentramide (13)	Unknown	0.197
Tunicamycin (9-13)	Vesicle trafficking	0.211
Doxorubicin (1, 3, 6)	Topoisomerase	0.227
Leupeptine (13)	Protein degradation	0.230
WY-14643 (3)	**Nuclear receptor**	
Olomucine (2-3)	Kinase; CDK	0.186
Austocystin (3)	Unknown	0.360
Nocodazole-1 (1, 5-6)	Microtubule	0.376
Doxorubicin (1, 3, 6)	Topoisomerase	0.408
Emetine-2 (6)	Protein synthesis	0.449
Zvad (13)	**Protein degradation**	
Leupeptine (13)	Protein degradation	0.163
Rapamycin (13)	Kinase; PI3K pwy.	0.182
Concentramide (13)	Unknown	0.218
Genistein (12-13)	Kinase	0.236
Monastrol (13)	Microtubule	0.257

Supplementary Data 2c: DNA-pp38-pERK Marker Set

d-Profile	*Major annotated activity*	*Similarity*
105D (10)	**Microtubule**	
Colchicine (4-6)	Microtubule	0.182
Griseofulvin (12-13)	Microtubule	0.225
Nocodazole-1 (8-9, 11-12)	Microtubule	0.276
Nocodazole-3 (10-13)	Microtubule	0.277
Nocodazole-2 (6-13)	Microtubule	0.281
11N84 (13)	**Vesicle trafficking**	
Brefeldin A (7-13)	Vesicle trafficking	0.110
Cytochalasin B (11-13)	Actin	0.110
Cycloheximide (7-13)	Protein synthesis	0.117
Scriptaid-1 (11-13)	Histone deacetylase	0.123
Trichostatin (8-13)	Histone deacetylase	0.155
8-bromo-cAMP (13)	**Kinase; PKA**	
Hydroxy urea-2 (12-13)	DNA replication	0.623
SC560 (12-13)	Cyclooxygenase	0.735
Fluoxetine (13)	Neurotransmitter	0.742
Emodin (13)	Kinase	0.786
Actinomycin D (8-13)	RNA	0.789
Actinomycin D (8-13)	**RNA**	
Didemnin B (8-11)	Protein synthesis	0.051
Emetine-2 (8-13)	Protein synthesis	0.067
Puromycin (9-10)	Protein synthesis	0.100
Indirubin monoxime (12-13)	Kinase; CDK	0.111
Purvalanol A (12-13)	Kinase; CDK	0.113
Actinomycin D (4-7)	**RNA**	
Scriptaid-1 (11-13)	Histone deacetylase	0.083
Trichostatin (8-13)	Histone deacetylase	0.084
Doxorubicin (5-8)	Topoisomerase	0.088
Brefeldin A (7-13)	Vesicle trafficking	0.102
Cyclosporin A (12-13)	Calcium regulation	0.132
ALLN (12-13)	**Protein degradation**	
Camptothecin (9-13)	Topoisomerase	0.164
Brefeldin A (7-13)	Vesicle trafficking	0.177
Emodin (13)	Kinase	0.195
Alsterpaullone (10-13)	Kinase; CDK	0.201
Actinomycin D (4-7)	RNA	0.216
Alsterpaullone (10-13)	**Kinase; CDK**	
Emodin (13)	Kinase	0.137
Camptothecin (9-13)	Topoisomerase	0.138
Scriptaid-1 (11-13)	Histone deacetylase	0.180
Brefeldin A (7-13)	Vesicle trafficking	0.184
W-7 hydrochloride (13)	Calcium regulation	0.187
Amanitin (12-13)	**RNA**	
Rapamycin (12-13)	Kinase; PI3K pwy.	0.112
Concentramide (1, 4-5)	Unknown	0.128
Wortmannin (13)	Kinase; PI3K pwy.	0.133
LY294002 (13)	Kinase; PI3K pwy.	0.147
Concentramide (8, 13)	Unknown	0.148
Amanitin (8)	**RNA**	
Concentramide (8, 13)	Unknown	0.455
WY-14643 (13)	Nuclear receptor	0.512
Concentramide (1, 4-5)	Unknown	0.514
Doxorubicin (5-8)	Topoisomerase	0.559
SB203580 (12-13)	Kinase; MAPK/p38 pwy.	0.569
Anisomycin (8-13)	**Protein synthesis**	
Camptothecin (9-13)	Topoisomerase	0.085
Emetine-2 (8-13)	Protein synthesis	0.094
Emetine-1 (8, 11)	Protein synthesis	0.138
Didemnin B (8-11)	Protein synthesis	0.141
Actinomycin D (8-13)	RNA	0.156
Anisomycin (7)	**Protein synthesis**	
Latrunculin B (10-13)	Actin	0.263
Trichostatin (8-13)	Histone deacetylase	0.267
Cycloheximide (7-13)	Protein synthesis	0.267
W-7 hydrochloride (13)	Calcium regulation	0.274
Oligomycin (6-13)	Energy metabolism	0.287

d-Profile	*Major annotated activity*	*Similarity*
Aphidicolin (9-13)	**DNA replication**	
Methotrexate (9-13)	DNA replication	0.323
Austocystin (11-12)	Unknown	0.339
Hydroxy urea-2 (12-13)	DNA replication	0.356
Doxorubicin (9-10)	Topoisomerase	0.427
Etoposide (10, 13)	Topoisomerase	0.438
Apicidin (9-13)	**Histone deacetylase**	
Oxamflatin (10-13)	Histone deacetylase	0.073
Trichostatin (8-13)	Histone deacetylase	0.106
Actinomycin D (4-7)	RNA	0.136
Scriptaid-1 (11-13)	Histone deacetylase	0.140
Cytochalasin B (11-13)	Actin	0.154
Austocystin (11-12)	**Unknown**	
Methotrexate (9-13)	DNA replication	0.267
Aphidicolin (9-13)	DNA replication	0.339
Etoposide (10, 13)	Topoisomerase	0.353
Camptothecin (5-8)	Topoisomerase	0.459
Hydroxy urea-2 (12-13)	DNA replication	0.465
Brefeldin A (7-13)	**Vesicle trafficking**	
Scriptaid-1 (11-13)	Histone deacetylase	0.071
Cyclosporin A (12-13)	Calcium regulation	0.073
Cycloheximide (7-13)	Protein synthesis	0.086
Actinomycin D (4-7)	RNA	0.102
Trichostatin (8-13)	Histone deacetylase	0.104
Camptothecin (9-13)	**Topoisomerase**	
Anisomycin (8-13)	Protein synthesis	0.085
Emetine-2 (8-13)	Protein synthesis	0.104
Alsterpaullone (10-13)	Kinase; CDK	0.138
ALLN (12-13)	Protein degradation	0.164
Actinomycin D (4-7)	RNA	0.173
Camptothecin (5-8)	**Topoisomerase**	
Etoposide (10, 13)	Topoisomerase	0.206
Doxorubicin (5-8)	Topoisomerase	0.297
Anisomycin (7)	Protein synthesis	0.305
Actinomycin D (4-7)	RNA	0.306
Oligomycin (6-13)	Energy metabolism	0.333
Camptothecin (4)	**Topoisomerase**	
Colchicine (4-6)	Microtubule	0.392
ICRF193 (10-13)	Topoisomerase	0.508
105D (10)	Microtubule	0.519
Cytochalasin D (5-6)	Actin	0.602
Griseofulvin (12-13)	Microtubule	0.606
Ceramide (13)	**Kinase; PKC**	
Brefeldin A (7-13)	Vesicle trafficking	0.263
Cytochalasin B (11-13)	Actin	0.268
Actinomycin D (4-7)	RNA	0.309
ALLN (12-13)	Protein degradation	0.317
Trichostatin (8-13)	Histone deacetylase	0.323
Chloropromazine (12)	**Neurotransmitter**	
Trifluoperazine (12)	Neurotransmitter	0.201
Clozapine (13)	Neurotransmitter	0.212
Concentramide (8, 13)	Unknown	0.335
Cytochalasin B (1)	Actin	0.343
SB203580 (12-13)	Kinase; MAPK/p38 pwy.	0.360
Clozapine (13)	**Neurotransmitter**	
SB203580 (12-13)	Kinase; MAPK/p38 pwy.	0.142
Concentramide (8, 13)	Unknown	0.168
Concentramide (1, 4-5)	Unknown	0.173
Cycloheximide (7-13)	Protein synthesis	0.179
Cytochalasin B (1)	Actin	0.183

Supplementary Data 2c: DNA-pp38-pERK Marker Set

d-Profile	*Major annotated activity*	*Similarity*
Colchicine (7-13)	**Microtubule**	
Dexamethasone (6-7)	Nuclear receptor	0.101
Nocodazole-2 (6-13)	Microtubule	0.113
Podophyllotoxin (6-13)	Microtubule	0.136
Nocodazole-1 (8-9, 11-12)	Microtubule	0.171
Trichostatin (1, 3)	Histone deacetylase	0.188
Colchicine (4-6)	**Microtubule**	
105D (10)	Microtubule	0.182
Griseofulvin (12-13)	Microtubule	0.183
Nocodazole-3 (10-13)	Microtubule	0.322
ICRF193 (10-13)	Topoisomerase	0.324
Cytochalasin D (5-6)	Actin	0.365
Concentramide (8, 13)	**Unknown**	
WY-14643 (13)	Nuclear receptor	0.067
Scriptaid-2 (11-12)	Histone deacetylase	0.107
Cycloheximide (7-13)	Protein synthesis	0.115
SB203580 (12-13)	Kinase; MAPK/p38 pwy.	0.135
Amanitin (12-13)	RNA	0.148
Concentramide (1, 4-5)	**Unknown**	
WY-14643 (13)	Nuclear receptor	0.030
Cycloheximide (7-13)	Protein synthesis	0.070
Scriptaid-2 (11-12)	Histone deacetylase	0.081
SB203580 (12-13)	Kinase; MAPK/p38 pwy.	0.091
Cytochalasin B (1)	Actin	0.108
Cycloheximide (7-13)	**Protein synthesis**	
Concentramide (1, 4-5)	Unknown	0.070
Cyclosporin A (12-13)	Calcium regulation	0.072
WY-14643 (13)	Nuclear receptor	0.081
Brefeldin A (7-13)	Vesicle trafficking	0.086
W-7 hydrochloride (13)	Calcium regulation	0.086
Cyclosporin A (12-13)	**Calcium regulation**	
Cycloheximide (7-13)	Protein synthesis	0.072
Brefeldin A (7-13)	Vesicle trafficking	0.073
Scriptaid-1 (11-13)	Histone deacetylase	0.111
W-7 hydrochloride (13)	Calcium regulation	0.124
Trichostatin (8-13)	Histone deacetylase	0.131
Cytochalasin B (11-13)	**Actin**	
Trichostatin (8-13)	Histone deacetylase	0.066
Scriptaid-1 (11-13)	Histone deacetylase	0.100
11N84 (13)	Vesicle trafficking	0.110
Brefeldin A (7-13)	Vesicle trafficking	0.112
Actinomycin D (4-7)	RNA	0.142
Cytochalasin B (1)	Actin	
Concentramide (1, 4-5)	Unknown	0.108
WY-14643 (13)	Nuclear receptor	0.110
Cycloheximide (7-13)	Protein synthesis	0.119
LY294002 (13)	Kinase; PI3K pwy.	0.120
SB203580 (12-13)	Kinase; MAPK/p38 pwy.	0.125
Cytochalasin D (7-13)	**Actin**	
Mevastatin (13)	Cholesterol	0.143
Latrunculin B (10-13)	Actin	0.190
Simavastatin (12-13)	Cholesterol	0.205
ICRF193 (10-13)	Topoisomerase	0.319
Oligomycin (6-13)	Energy metabolism	0.325
Cytochalasin D (5-6)	**Actin**	
105D (10)	Microtubule	0.333
Colchicine (4-6)	Microtubule	0.365
Nocodazole-2 (6-13)	Microtubule	0.481
ICRF193 (10-13)	Topoisomerase	0.481
Nocodazole-1 (8-9, 11-12)	Microtubule	0.493
Dexamethasone (6-7)	**Nuclear receptor**	
Colchicine (7-13)	Microtubule	0.101
Nocodazole-2 (6-13)	Microtubule	0.152
Podophyllotoxin (6-13)	Microtubule	0.174
Nocodazole-1 (8-9, 11-12)	Microtubule	0.191
Trichostatin (1, 3)	Histone deacetylase	0.224

d-Profile	*Major annotated activity*	*Similarity*
Didemnin B (8-11)	**Protein synthesis**	
Actinomycin D (8-13)	RNA	0.051
Emetine-2 (8-13)	Protein synthesis	0.085
Puromycin (9-10)	Protein synthesis	0.094
Purvalanol A (12-13)	Kinase; CDK	0.135
Anisomycin (8-13)	Protein synthesis	0.141
Didemnin B (6-7)	**Protein synthesis**	
Emetine-2 (6)	Protein synthesis	0.303
Anisomycin (7)	Protein synthesis	0.308
Etoposide (10, 13)	Topoisomerase	0.407
SB202190 (12-13)	Kinase; MAPK/p38 pwy.	0.410
W-7 hydrochloride (13)	Calcium regulation	0.412
Doxorubicin (9-10)	**Topoisomerase**	
Okadaic acid (10-11)	Kinase	0.272
Aphidicolin (9-13)	DNA replication	0.427
Hydroxy urea-2 (12-13)	DNA replication	0.612
MG132 (11-13)	Protein degradation	0.630
Etoposide (10, 13)	Topoisomerase	0.743
Doxorubicin (5-8)	**Topoisomerase**	
Actinomycin D (4-7)	RNA	0.088
Scriptaid-1 (11-13)	Histone deacetylase	0.214
Trichostatin (8-13)	Histone deacetylase	0.222
Apicidin (9-13)	Histone deacetylase	0.234
Oxamflatin (10-13)	Histone deacetylase	0.236
Emetine-1 (8, 11)	**Protein synthesis**	
Anisomycin (8-13)	Protein synthesis	0.138
Camptothecin (9-13)	Topoisomerase	0.184
Emodin (13)	Kinase	0.207
Emetine-2 (8-13)	Protein synthesis	0.237
11N84 (13)	Vesicle trafficking	0.239
Emetine-2 (8-13)	**Protein synthesis**	
Actinomycin D (8-13)	RNA	0.067
Purvalanol A (12-13)	Kinase; CDK	0.074
Didemnin B (8-11)	Protein synthesis	0.085
Anisomycin (8-13)	Protein synthesis	0.094
Camptothecin (9-13)	Topoisomerase	0.104
Emetine-2 (6)	**Protein synthesis**	
Anisomycin (7)	Protein synthesis	0.297
Didemnin B (6-7)	Protein synthesis	0.303
Oligomycin (6-13)	Energy metabolism	0.350
SB203580 (7)	Kinase; MAPK/p38 pwy.	0.440
W-7 hydrochloride (13)	Calcium regulation	0.440
Emodin (13)	**Kinase**	
Alsterpaullone (10-13)	Kinase; CDK	0.137
ALLN (12-13)	Protein degradation	0.195
Emetine-1 (8, 11)	Protein synthesis	0.207
Camptothecin (9-13)	Topoisomerase	0.229
11N84 (13)	Vesicle trafficking	0.233
Epothilone B (9-10, 12-13)	**Microtubule**	
Sulindac sulfide (11, 13)	Cyclooxygenase	0.191
Taxol (4-5)	Microtubule	0.419
Griseofulvin (12-13)	Microtubule	0.770
PMA (5-7)	Kinase; PKC	0.793
MG132 (11-13)	Protein degradation	0.827
Etoposide (10, 13)	**Topoisomerase**	
Camptothecin (5-8)	Topoisomerase	0.206
Actinomycin D (4-7)	RNA	0.319
Doxorubicin (5-8)	Topoisomerase	0.319
Austocystin (11-12)	Unknown	0.353
Oxamflatin (10-13)	Histone deacetylase	0.356
Filopodine (12-13)	**Unknown**	
Scriptaid-2 (11-12)	Histone deacetylase	0.114
Cyclosporin A (12-13)	Calcium regulation	0.150
PD98059 (13)	Kinase; MAPK/ERK pwy.	0.166
Concentramide (1, 4-5)	Unknown	0.189
Scriptaid-1 (11-13)	Histone deacetylase	0.194

Supplementary Data 2c: DNA-pp38-pERK Marker Set

d-Profile	*Major annotated activity*	*Similarity*
Fluoxetine (13)	**Neurotransmitter**	
Indirubin monoxime (12-13)	Kinase; CDK	0.111
Actinomycin D (8-13)	RNA	0.118
Purvalanol A (12-13)	Kinase; CDK	0.189
Didemnin B (8-11)	Protein synthesis	0.190
Puromycin (9-10)	Protein synthesis	0.190
Griseofulvin (12-13)	**Microtubule**	
Colchicine (4-6)	Microtubule	0.183
105D (10)	Microtubule	0.225
Nocodazole-3 (10-13)	Microtubule	0.260
Nocodazole-1 (8-9, 11-12)	Microtubule	0.379
Nocodazole-2 (6-13)	Microtubule	0.400
Hydroxy urea-2 (12-13)	**DNA replication**	
Aphidicolin (9-13)	DNA replication	0.356
Methotrexate (9-13)	DNA replication	0.384
Austocystin (11-12)	Unknown	0.465
SC560 (12-13)	Cyclooxygenase	0.501
Doxorubicin (9-10)	Topoisomerase	0.612
ICRF193 (10-13)	**Topoisomerase**	
Nocodazole-2 (6-13)	Microtubule	0.311
105D (10)	Microtubule	0.312
Cytochalasin D (7-13)	Actin	0.319
Colchicine (4-6)	Microtubule	0.324
Staurosporine (8-10)	Kinase	0.328
Indirubin monoxime (12-13)	**Kinase; CDK**	
Fluoxetine (13)	Neurotransmitter	0.111
Actinomycin D (8-13)	RNA	0.111
Puromycin (9-10)	Protein synthesis	0.135
Didemnin B (8-11)	Protein synthesis	0.155
Purvalanol A (12-13)	Kinase; CDK	0.230
Indomethacin (1)	**Cyclooxygenase**	
Concentramide (8, 13)	Unknown	0.235
Clozapine (13)	Neurotransmitter	0.250
PD98059 (13)	Kinase; MAPK/ERK pwy.	0.274
Concentramide (1, 4-5)	Unknown	0.287
SB203580 (12-13)	Kinase; MAPK/p38 pwy.	0.300
Jasplakinolide (12-13)	**Actin**	
Simavastatin (12-13)	Cholesterol	0.238
Didemnin B (8-11)	Protein synthesis	0.245
Indirubin monoxime (12-13)	Kinase; CDK	0.336
Emetine-2 (8-13)	Protein synthesis	0.347
Actinomycin D (8-13)	RNA	0.352
Latrunculin B (10-13)	**Actin**	
Mevastatin (13)	Cholesterol	0.153
Cytochalasin D (7-13)	Actin	0.190
Cytochalasin B (11-13)	Actin	0.204
Trichostatin (8-13)	Histone deacetylase	0.243
ALLN (12-13)	Protein degradation	0.250
LY294002 (13)	**Kinase; PI3K pwy.**	
Wortmannin (13)	Kinase; PI3K pwy.	0.101
Cycloheximide (7-13)	Protein synthesis	0.112
Cytochalasin B (1)	Actin	0.120
Scriptaid-2 (11-12)	Histone deacetylase	0.121
Concentramide (1, 4-5)	Unknown	0.128
Methotrexate (9-13)	**DNA replication**	
Austocystin (11-12)	Unknown	0.267
Aphidicolin (9-13)	DNA replication	0.323
SC560 (12-13)	Cyclooxygenase	0.368
Hydroxy urea-2 (12-13)	DNA replication	0.384
PD98059 (13)	Kinase; MAPK/ERK pwy.	0.434
Mevastatin (13)	**Cholesterol**	
Cytochalasin D (7-13)	Actin	0.143
Simavastatin (12-13)	Cholesterol	0.144
Latrunculin B (10-13)	Actin	0.153
Oligomycin (6-13)	Energy metabolism	0.336
Anisomycin (7)	Protein synthesis	0.359

d-Profile	*Major annotated activity*	*Similarity*
MG132 (11-13)	**Protein degradation**	
ALLN (12-13)	Protein degradation	0.255
Staurosporine (8-10)	Kinase	0.341
Actinomycin D (4-7)	RNA	0.364
Camptothecin (9-13)	Topoisomerase	0.368
Latrunculin B (10-13)	Actin	0.394
Nocodazole-1 (8-9, 11-12)	**Microtubule**	
Nocodazole-2 (6-13)	Microtubule	0.076
Nocodazole-3 (10-13)	Microtubule	0.148
Colchicine (7-13)	Microtubule	0.171
Dexamethasone (6-7)	Nuclear receptor	0.191
Taxol (6-8, 10-13)	Microtubule	0.217
Nocodazole-2 (6-13)	**Microtubule**	
Nocodazole-1 (8-9, 11-12)	Microtubule	0.076
Nocodazole-3 (10-13)	Microtubule	0.112
Colchicine (7-13)	Microtubule	0.113
Dexamethasone (6-7)	Nuclear receptor	0.152
Podophyllotoxin (6-13)	Microtubule	0.163
Nocodazole-3 (10-13)	**Microtubule**	
Nocodazole-2 (6-13)	Microtubule	0.112
Nocodazole-1 (8-9, 11-12)	Microtubule	0.148
Taxol (6-8, 10-13)	Microtubule	0.242
Colchicine (7-13)	Microtubule	0.256
Griseofulvin (12-13)	Microtubule	0.260
Okadaic acid (10-11)	**Kinase**	
Doxorubicin (9-10)	Topoisomerase	0.272
Aphidicolin (9-13)	DNA replication	0.479
Hydroxy urea-2 (12-13)	DNA replication	0.627
Griseofulvin (12-13)	Microtubule	0.634
Cytochalasin D (5-6)	Actin	0.647
Oligomycin (6-13)	**Energy metabolism**	
Staurosporine (8-10)	Kinase	0.123
Actinomycin D (4-7)	RNA	0.157
Trichostatin (8-13)	Histone deacetylase	0.161
Brefeldin A (7-13)	Vesicle trafficking	0.195
Scriptaid-1 (11-13)	Histone deacetylase	0.208
Olomucine (13)	**Kinase; CDK**	
LY294002 (13)	Kinase; PI3K pwy.	0.195
W-7 hydrochloride (13)	Calcium regulation	0.197
Roscovitine (12)	Kinase; CDK	0.198
Cycloheximide (7-13)	Protein synthesis	0.200
Wortmannin (13)	Kinase; PI3K pwy.	0.214
Oxamflatin (10-13)	**Histone deacetylase**	
Apicidin (9-13)	Histone deacetylase	0.073
Trichostatin (8-13)	Histone deacetylase	0.099
Scriptaid-1 (11-13)	Histone deacetylase	0.127
Actinomycin D (4-7)	RNA	0.137
Cytochalasin B (11-13)	Actin	0.160
PD98059 (13)	**Kinase; MAPK/ERK pwy.**	
U0126 (13)	Kinase; MAPK/ERK pwy.	0.161
Filopodine (12-13)	Unknown	0.166
Cyclosporin A (12-13)	Calcium regulation	0.184
Cytochalasin B (1)	Actin	0.201
Scriptaid-2 (11-12)	Histone deacetylase	0.206
PMA (5-7)	**Kinase; PKC**	
Didemnin B (6-7)	Protein synthesis	0.511
Emetine-2 (6)	Protein synthesis	0.534
Mevastatin (13)	Cholesterol	0.555
Cytochalasin D (7-13)	Actin	0.582
Simavastatin (12-13)	Cholesterol	0.610
Podophyllotoxin (6-13)	**Microtubule**	
Trichostatin (1, 3)	Histone deacetylase	0.085
Colchicine (7-13)	Microtubule	0.136
Vinblastine (6-13)	Microtubule	0.159
Nocodazole-2 (6-13)	Microtubule	0.163
Dexamethasone (6-7)	Nuclear receptor	0.174

Supplementary Data 2c: DNA-pp38-pERK Marker Set

d-Profile	*Major annotated activity*	*Similarity*
Puromycin (9-10)	**Protein synthesis**	
Didemnin B (8-11)	Protein synthesis	0.094
Actinomycin D (8-13)	RNA	0.100
Purvalanol A (12-13)	Kinase; CDK	0.129
Indirubin monoxime (12-13)	Kinase; CDK	0.135
Emetine-2 (8-13)	Protein synthesis	0.141
Purvalanol A (12-13)	**Kinase; CDK**	
Emetine-2 (8-13)	Protein synthesis	0.074
Actinomycin D (8-13)	RNA	0.113
Puromycin (9-10)	Protein synthesis	0.129
Didemnin B (8-11)	Protein synthesis	0.135
Anisomycin (8-13)	Protein synthesis	0.171
Rapamycin (12-13)	**Kinase; PI3K pwy.**	
Amanitin (12-13)	RNA	0.112
LY294002 (13)	Kinase; PI3K pwy.	0.131
Wortmannin (13)	Kinase; PI3K pwy.	0.145
Concentramide (1, 4-5)	Unknown	0.153
Concentramide (8, 13)	Unknown	0.153
Roscovitine (12)	**Kinase; CDK**	
Olomucine (13)	Kinase; CDK	0.198
Oligomycin (6-13)	Energy metabolism	0.293
W-7 hydrochloride (13)	Calcium regulation	0.305
Anisomycin (7)	Protein synthesis	0.311
ALLN (12-13)	Protein degradation	0.331
SB202190 (12-13)	**Kinase; MAPK/p38 pwy.**	
Wortmannin (13)	Kinase; PI3K pwy.	0.239
Amanitin (12-13)	RNA	0.241
Cycloheximide (7-13)	Protein synthesis	0.243
Concentramide (1, 4-5)	Unknown	0.254
LY294002 (13)	Kinase; PI3K pwy.	0.255
SB203580 (12-13)	**Kinase; MAPK/p38 pwy.**	
Concentramide (1, 4-5)	Unknown	0.091
WY-14643 (13)	Nuclear receptor	0.115
Cycloheximide (7-13)	Protein synthesis	0.124
Cytochalasin B (1)	Actin	0.125
Concentramide (8, 13)	Unknown	0.135
SB203580 (7)	**Kinase; MAPK/p38 pwy.**	
Cycloheximide (7-13)	Protein synthesis	0.310
Concentramide (1, 4-5)	Unknown	0.331
W-7 hydrochloride (13)	Calcium regulation	0.333
Cytochalasin B (1)	Actin	0.341
Cyclosporin A (12-13)	Calcium regulation	0.346
SC560 (12-13)	**Cyclooxygenase**	
PD98059 (13)	Kinase; MAPK/ERK pwy.	0.317
Alsterpaullone (10-13)	Kinase; CDK	0.318
Indomethacin (1)	Cyclooxygenase	0.358
Clozapine (13)	Neurotransmitter	0.360
Methotrexate (9-13)	DNA replication	0.368
Scriptaid-1 (11-13)	**Histone deacetylase**	
Trichostatin (8-13)	Histone deacetylase	0.069
Brefeldin A (7-13)	Vesicle trafficking	0.071
Actinomycin D (4-7)	RNA	0.083
Cytochalasin B (11-13)	Actin	0.100
Cycloheximide (7-13)	Protein synthesis	0.107
Scriptaid-2 (11-12)	**Histone deacetylase**	
Concentramide (1, 4-5)	Unknown	0.081
WY-14643 (13)	Nuclear receptor	0.092
Concentramide (8, 13)	Unknown	0.107
Filopodine (12-13)	Unknown	0.114
Scriptaid-1 (11-13)	Histone deacetylase	0.117
Simavastatin (12-13)	**Cholesterol**	
Mevastatin (13)	Cholesterol	0.144
Cytochalasin D (7-13)	Actin	0.205
Jasplakinolide (12-13)	Actin	0.238
Latrunculin B (10-13)	Actin	0.279
Oligomycin (6-13)	Energy metabolism	0.281

d-Profile	*Major annotated activity*	*Similarity*
Staurosporine (8-10)	**Kinase**	
Oligomycin (6-13)	Energy metabolism	0.123
Actinomycin D (4-7)	RNA	0.205
Trichostatin (8-13)	Histone deacetylase	0.212
Oxamflatin (10-13)	Histone deacetylase	0.238
Apicidin (9-13)	Histone deacetylase	0.240
Sulindac sulfide (11, 13)	**Cyclooxygenase**	
Epothilone B (9-10, 12-13)	Microtubule	0.191
Taxol (4-5)	Microtubule	0.325
MG132 (11-13)	Protein degradation	0.686
ICRF193 (10-13)	Topoisomerase	0.748
Didemnin B (8-11)	Protein synthesis	0.751
Taxol (6-8, 10-13)	**Microtubule**	
Nocodazole-2 (6-13)	Microtubule	0.185
Nocodazole-1 (8-9, 11-12)	Microtubule	0.217
Dexamethasone (6-7)	Nuclear receptor	0.230
Nocodazole-3 (10-13)	Microtubule	0.242
Podophyllotoxin (6-13)	Microtubule	0.258
Taxol (4-5)	**Microtubule**	
Sulindac sulfide (11, 13)	Cyclooxygenase	0.325
Colchicine (4-6)	Microtubule	0.392
105D (10)	Microtubule	0.397
Griseofulvin (12-13)	Microtubule	0.405
Epothilone B (9-10, 12-13)	Microtubule	0.419
Trichostatin (8-13)	**Histone deacetylase**	
Cytochalasin B (11-13)	Actin	0.066
Scriptaid-1 (11-13)	Histone deacetylase	0.069
Actinomycin D (4-7)	RNA	0.084
Oxamflatin (10-13)	Histone deacetylase	0.099
Brefeldin A (7-13)	Vesicle trafficking	0.104
Trichostatin (1, 3)	**Histone deacetylase**	
Vinblastine (6-13)	Microtubule	0.071
Podophyllotoxin (6-13)	Microtubule	0.085
Colchicine (7-13)	Microtubule	0.188
Nocodazole-2 (6-13)	Microtubule	0.197
Dexamethasone (6-7)	Nuclear receptor	0.224
Trifluoperazine (12)	**Neurotransmitter**	
Chloropromazine (12)	Neurotransmitter	0.201
Clozapine (13)	Neurotransmitter	0.254
Brefeldin A (7-13)	Vesicle trafficking	0.335
WY-14643 (13)	Nuclear receptor	0.351
Concentramide (8, 13)	Unknown	0.356
Tunicamycin (9-13)	**Vesicle trafficking**	
Latrunculin B (10-13)	Actin	0.295
ALLN (12-13)	Protein degradation	0.323
Purvalanol A (12-13)	Kinase; CDK	0.361
Puromycin (9-10)	Protein synthesis	0.365
Anisomycin (7)	Protein synthesis	0.369
U0126 (13)	**Kinase; MAPK/ERK pwy.**	
PD98059 (13)	Kinase; MAPK/ERK pwy.	0.161
Scriptaid-2 (11-12)	Histone deacetylase	0.183
Cyclosporin A (12-13)	Calcium regulation	0.184
Cycloheximide (7-13)	Protein synthesis	0.187
Filopodine (12-13)	Unknown	0.195
Vinblastine (6-13)	**Microtubule**	
Trichostatin (1, 3)	Histone deacetylase	0.071
Podophyllotoxin (6-13)	Microtubule	0.159
Nocodazole-2 (6-13)	Microtubule	0.186
Colchicine (7-13)	Microtubule	0.191
Dexamethasone (6-7)	Nuclear receptor	0.236
W-7 hydrochloride (13)	**Calcium regulation**	
Cycloheximide (7-13)	Protein synthesis	0.086
Brefeldin A (7-13)	Vesicle trafficking	0.115
Cyclosporin A (12-13)	Calcium regulation	0.124
Concentramide (1, 4-5)	Unknown	0.133
WY-14643 (13)	Nuclear receptor	0.140

Supplementary Data 2c: DNA-pp38-pERK Marker Set

d-Profile	*Major annotated activity*	*Similarity*
Wortmannin (13)	**Kinase; PI3K pwy.**	
LY294002 (13)	Kinase; PI3K pwy.	0.101
Cycloheximide (7-13)	Protein synthesis	0.113
Amanitin (12-13)	RNA	0.133
Concentramide (1, 4-5)	Unknown	0.144
Rapamycin (12-13)	Kinase; PI3K pwy.	0.145

d-Profile	*Major annotated activity*	*Similarity*
WY-14643 (13)	**Nuclear receptor**	
Concentramide (1, 4-5)	Unknown	0.030
Concentramide (8, 13)	Unknown	0.067
Cycloheximide (7-13)	Protein synthesis	0.081
Scriptaid-2 (11-12)	Histone deacetylase	0.092
Cytochalasin B (1)	Actin	0.110

Supplementary Data 2d: DNA-Microtubule-Actin Marker Set

d-Profile	*Major annotated activity*	*Similarity*
105D (11-12)	**Microtubule**	
Taxol (6-13)	Microtubule	0.389
Griseofulvin (12-13)	Microtubule	0.435
Nocodazole-3 (10-13)	Microtubule	0.499
Vinblastine (5-6)	Microtubule	0.517
ICRF193 (9-13)	Topoisomerase	0.560
11N84 (12-13)	**Vesicle trafficking**	
Brefeldin A (11)	Vesicle trafficking	0.194
Oligomycin (5-13)	Energy metabolism	0.220
Tunicamycin (9-13)	Vesicle trafficking	0.322
Wortmannin (13)	Kinase; PI3K pwy.	0.324
Filopodine (12-13)	Unknown	0.326
Actinomycin D (9-13)	**RNA**	
Camptothecin (11)	Topoisomerase	0.337
Puromycin (9-10)	Protein synthesis	0.339
Anisomycin (12-13)	Protein synthesis	0.347
Emetine-2 (7-13)	Protein synthesis	0.360
Roscovitine (13)	Kinase; CDK	0.373
Actinomycin D (7-8)	**RNA**	
Camptothecin (11)	Topoisomerase	0.188
Emetine-2 (7-13)	Protein synthesis	0.196
Puromycin (9-10)	Protein synthesis	0.268
Emetine-1 (8-13)	Protein synthesis	0.274
Roscovitine (13)	Kinase; CDK	0.372
Anisomycin (12-13)	**Protein synthesis**	
Emetine-2 (7-13)	Protein synthesis	0.275
Didemnin B (7-11)	Protein synthesis	0.281
Chelerythrine (11)	Kinase; PKC	0.286
Actinomycin D (9-13)	RNA	0.347
Camptothecin (11)	Topoisomerase	0.382
Aphidicolin (8-13)	**DNA replication**	
Methotrexate (9-13)	DNA replication	0.138
Austocystin (10-13)	Unknown	0.148
WY-14643 (13)	Nuclear receptor	0.172
Hydroxy urea-2 (12-13)	DNA replication	0.224
U0126 (12-13)	Kinase; MAPK/ERK pwy.	0.283
Aphidicolin (1, 3, 7)	**DNA replication**	
Concentramide (1-2, 4, 6-8)	Unknown	0.142
PD169316 (1-3, 7)	Kinase; MAPK/p38 pwy.	0.169
Oligomycin (1)	Energy metabolism	0.249
CKI7 (1-2)	Kinase	0.252
TPEN (1)	Metal homeostasis	0.273
Apicidin (9-13)	**Histone deacetylase**	
Oxamflatin (10-12)	Histone deacetylase	0.161
Scriptaid-1 (10-13)	Histone deacetylase	0.161
Trichostatin (9-13)	Histone deacetylase	0.364
Scriptaid-2 (10-13)	Histone deacetylase	0.365
SC560 (13)	Cyclooxygenase	0.367
Austocystin (10-13)	**Unknown**	
Aphidicolin (8-13)	DNA replication	0.148
Hydroxy urea-2 (12-13)	DNA replication	0.188
Etoposide (10-13)	Topoisomerase	0.214
PD169316 (11-13)	Kinase; MAPK/p38 pwy.	0.254
Methotrexate (9-13)	DNA replication	0.265
Austocystin (1)	**Unknown**	
Didemnin B (1-2)	Protein synthesis	0.171
Filopodine (1-2)	Unknown	0.207
Scriptaid-2 (1-2)	Histone deacetylase	0.212
Oligomycin (1)	Energy metabolism	0.267
Methotrexate (2)	DNA replication	0.281
Brefeldin A (11)	**Vesicle trafficking**	
11N84 (12-13)	Vesicle trafficking	0.194
Simavastatin (12-13)	Cholesterol	0.281
Oligomycin (5-13)	Energy metabolism	0.314
Puromycin (9-10)	Protein synthesis	0.345
LY294002 (13)	Kinase; PI3K pwy.	0.369

d-Profile	*Major annotated activity*	*Similarity*
Camptothecin (11)	**Topoisomerase**	
Actinomycin D (7-8)	RNA	0.188
Actinomycin D (9-13)	RNA	0.337
Emetine-1 (8-13)	Protein synthesis	0.370
Emetine-2 (7-13)	Protein synthesis	0.373
Roscovitine (13)	Kinase; CDK	0.376
Ceramide (13)	**Kinase; PKC**	
11N84 (12-13)	Vesicle trafficking	0.355
W-7 hydrochloride (13)	Calcium regulation	0.361
Brefeldin A (11)	Vesicle trafficking	0.375
Leupeptine (13)	Protein degradation	0.396
CKI7 (13)	Kinase	0.396
Chelerythrine (11)	**Kinase; PKC**	
Anisomycin (12-13)	Protein synthesis	0.286
Jasplakinolide (10, 12)	Actin	0.404
Didemnin B (7-11)	Protein synthesis	0.499
Brefeldin A (11)	Vesicle trafficking	0.559
Actinomycin D (9-13)	RNA	0.568
Chloropromazine (2)	**Neurotransmitter**	
Cytochalasin B (2)	Actin	0.201
CKI7 (1-2)	Kinase	0.245
PD169316 (1-3, 7)	Kinase; MAPK/p38 pwy.	0.259
PD98059 (1)	Kinase; MAPK/ERK pwy.	0.264
Oligomycin (1)	Energy metabolism	0.320
CKI7 (13)	**Kinase**	
Leupeptine (13)	Protein degradation	0.254
Filopodine (12-13)	Unknown	0.267
Wortmannin (13)	Kinase; PI3K pwy.	0.274
Indomethacin (13)	Cyclooxygenase	0.309
11N84 (12-13)	Vesicle trafficking	0.371
CKI7 (1-2)	**Kinase**	
PD169316 (1-3, 7)	Kinase; MAPK/p38 pwy.	0.101
Zvad (1)	Protein degradation	0.156
Methotrexate (2)	DNA replication	0.198
Didemnin B (1-2)	Protein synthesis	0.207
Sodium azide (2)	Energy metabolism	0.208
Colchicine (9-10, 12-13)	**Microtubule**	
Podophyllotoxin (6-9, 11, 13)	Microtubule	0.129
Nocodazole-2 (9-13)	Microtubule	0.147
Trichostatin (1-3)	Histone deacetylase	0.227
Dexamethasone (6)	Nuclear receptor	0.244
Nocodazole-1 (7-13)	Microtubule	0.265
Concentramide (1-2, 4, 6-8)	**Unknown**	
Aphidicolin (1, 3, 7)	DNA replication	0.142
TPEN (1)	Metal homeostasis	0.294
PD169316 (1-3, 7)	Kinase; MAPK/p38 pwy.	0.337
Oligomycin (1)	Energy metabolism	0.366
Nocodazole-1 (2)	Microtubule	0.368
Cytochalasin B (10-13)	**Actin**	
Indirubin monoxime (10-13)	Kinase; CDK	0.515
PD169316 (1-3, 7)	Kinase; MAPK/p38 pwy.	0.550
Emetine-2 (1, 6)	Protein synthesis	0.564
Latrunculin B (8-10, 12-13)	Actin	0.573
Cytochalasin D (10-13)	Actin	0.581
Cytochalasin B (2)	**Actin**	
Chloropromazine (2)	Neurotransmitter	0.201
PD98059 (1)	Kinase; MAPK/ERK pwy.	0.254
Oxamflatin (1)	Histone deacetylase	0.335
PD169316 (1-3, 7)	Kinase; MAPK/p38 pwy.	0.365
CKI7 (1-2)	Kinase	0.384
Cytochalasin D (10-13)	**Actin**	
PD98059 (1)	Kinase; MAPK/ERK pwy.	0.533
CKI7 (1-2)	Kinase	0.564
Latrunculin B (8-10, 12-13)	Actin	0.565
Methotrexate (2)	DNA replication	0.574
Zvad (1)	Protein degradation	0.579

Supplementary Data 2d: DNA-Microtubule-Actin Marker Set

d-Profile	*Major annotated activity*	*Similarity*
Dexamethasone (6)	**Nuclear receptor**	
Nocodazole-1 (7-13)	Microtubule	0.162
Colchicine (9-10, 12-13)	Microtubule	0.244
Nocodazole-2 (9-13)	Microtubule	0.283
Vinblastine (7-13)	Microtubule	0.289
Trichostatin (1-3)	Histone deacetylase	0.300
Didemnin B (7-11)	**Protein synthesis**	
Emetine-2 (7-13)	Protein synthesis	0.248
Anisomycin (12-13)	Protein synthesis	0.281
Puromycin (9-10)	Protein synthesis	0.334
Actinomycin D (9-13)	RNA	0.421
Actinomycin D (7-8)	RNA	0.421
Didemnin B (1-2)	**Protein synthesis**	
Scriptaid-2 (1-2)	Histone deacetylase	0.139
Filopodine (1-2)	Unknown	0.154
Austocystin (1)	Unknown	0.171
Zvad (1)	Protein degradation	0.207
CKI7 (1-2)	Kinase	0.207
Doxorubicin (9-11)	**Topoisomerase**	
Actinomycin D (9-13)	RNA	0.382
Epothilone B (9-13)	Microtubule	0.421
Camptothecin (11)	Topoisomerase	0.467
Roscovitine (13)	Kinase; CDK	0.474
Emetine-1 (8-13)	Protein synthesis	0.518
Emetine-1 (8-13)	**Protein synthesis**	
Emetine-2 (7-13)	Protein synthesis	0.252
Actinomycin D (7-8)	RNA	0.274
Puromycin (9-10)	Protein synthesis	0.362
Camptothecin (11)	Topoisomerase	0.370
Emodin (13)	Kinase	0.377
Emetine-1 (7)	**Protein synthesis**	
Emetine-2 (1, 6)	Protein synthesis	0.310
Zvad (1)	Protein degradation	0.404
TPEN (1)	Metal homeostasis	0.419
Oxamflatin (1)	Histone deacetylase	0.433
Aphidicolin (1, 3, 7)	DNA replication	0.434
Emetine-2 (7-13)	**Protein synthesis**	
Actinomycin D (7-8)	RNA	0.196
Puromycin (9-10)	Protein synthesis	0.244
Didemnin B (7-11)	Protein synthesis	0.248
Emetine-1 (8-13)	Protein synthesis	0.252
Anisomycin (12-13)	Protein synthesis	0.275
Emetine-2 (1, 6)	**Protein synthesis**	
TPEN (1)	Metal homeostasis	0.234
Didemnin B (1-2)	Protein synthesis	0.282
Zvad (1)	Protein degradation	0.293
Emetine-1 (7)	Protein synthesis	0.310
PD169316 (1-3, 7)	Kinase; MAPK/p38 pwy.	0.329
Emodin (13)	**Kinase**	
Indirubin monoxime (10-13)	Kinase; CDK	0.257
Emetine-1 (8-13)	Protein synthesis	0.377
Tunicamycin (9-13)	Vesicle trafficking	0.406
Nocodazole-1 (2)	Microtubule	0.473
Genistein (13)	Kinase	0.494
Epothilone B (9-13)	**Microtubule**	
Taxol (6-13)	Microtubule	0.330
Doxorubicin (9-11)	Topoisomerase	0.421
Griseofulvin (12-13)	Microtubule	0.612
Actinomycin D (9-13)	RNA	0.623
105D (11-12)	Microtubule	0.667
Etoposide (10-13)	**Topoisomerase**	
Austocystin (10-13)	Unknown	0.214
Aphidicolin (8-13)	DNA replication	0.358
PD169316 (11-13)	Kinase; MAPK/p38 pwy.	0.443
Hydroxy urea-2 (12-13)	DNA replication	0.447
Methotrexate (9-13)	DNA replication	0.476

d-Profile	*Major annotated activity*	*Similarity*
Filopodine (12-13)	**Unknown**	
Wortmannin (13)	Kinase; PI3K pwy.	0.210
Sodium azide (13)	Energy metabolism	0.247
CKI7 (13)	Kinase	0.267
Scriptaid-2 (10-13)	Histone deacetylase	0.325
11N84 (12-13)	Vesicle trafficking	0.326
Filopodine (1-2)	**Unknown**	
Scriptaid-2 (1-2)	Histone deacetylase	0.112
Didemnin B (1-2)	Protein synthesis	0.154
Zvad (1)	Protein degradation	0.195
Sodium azide (2)	Energy metabolism	0.202
Austocystin (1)	Unknown	0.207
Fluoxetine (13)	**Neurotransmitter**	
Simavastatin (12-13)	Cholesterol	0.444
Brefeldin A (11)	Vesicle trafficking	0.451
Scriptaid-2 (10-13)	Histone deacetylase	0.543
SB202190 (12-13)	Kinase; MAPK/p38 pwy.	0.572
LY294002 (13)	Kinase; PI3K pwy.	0.573
Forskolin (13)	**Kinase; PKA**	
PD169316 (11-13)	Kinase; MAPK/p38 pwy.	0.326
Retinoic acid (trans) (9, 11-13)	Nuclear receptor	0.336
Austocystin (10-13)	Unknown	0.439
SC560 (13)	Cyclooxygenase	0.449
Sodium azide (13)	Energy metabolism	0.493
Genistein (13)	**Kinase**	
Nocodazole-1 (2)	Microtubule	0.266
Olomucine (13)	Kinase; CDK	0.424
Indirubin monoxime (10-13)	Kinase; CDK	0.424
Wortmannin (13)	Kinase; PI3K pwy.	0.462
Emodin (13)	Kinase	0.494
Griseofulvin (12-13)	**Microtubule**	
Nocodazole-3 (10-13)	Microtubule	0.348
Vinblastine (5-6)	Microtubule	0.354
Taxol (6-13)	Microtubule	0.384
105D (11-12)	Microtubule	0.435
Taxol (4-5)	Microtubule	0.479
H89 (13)	**Kinase**	
Nocodazole-3 (10-13)	Microtubule	0.501
Staurosporine (7-9)	Kinase	0.541
Scriptaid-2 (10-13)	Histone deacetylase	0.573
Olomucine (13)	Kinase; CDK	0.588
Filopodine (12-13)	Unknown	0.608
Hydroxy urea-2 (12-13)	**DNA replication**	
Methotrexate (9-13)	DNA replication	0.138
U0126 (12-13)	Kinase; MAPK/ERK pwy.	0.165
Austocystin (10-13)	Unknown	0.188
WY-14643 (13)	Nuclear receptor	0.218
Aphidicolin (8-13)	DNA replication	0.224
Hydroxy urea-2 (1)	**DNA replication**	
Didemnin B (1-2)	Protein synthesis	0.224
Zvad (1)	Protein degradation	0.225
PD169316 (1-3, 7)	Kinase; MAPK/p38 pwy.	0.243
Oligomycin (1)	Energy metabolism	0.265
Filopodine (1-2)	Unknown	0.289
ICRF193 (9-13)	**Topoisomerase**	
Oligomycin (5-13)	Energy metabolism	0.336
Nocodazole-2 (6-7)	Microtubule	0.359
Lactacystin (13)	Protein degradation	0.414
Vinblastine (5-6)	Microtubule	0.415
Sulindac sulfide (11, 13)	Cyclooxygenase	0.435
Indirubin monoxime (10-13)	**Kinase; CDK**	
Emodin (13)	Kinase	0.257
Tunicamycin (9-13)	Vesicle trafficking	0.295
Staurosporine (7-9)	Kinase	0.396
Genistein (13)	Kinase	0.424
Nocodazole-1 (2)	Microtubule	0.466

Supplementary Data 2d: DNA-Microtubule-Actin Marker Set

d-Profile	*Major annotated activity*	*Similarity*
Indomethacin (13)	**Cyclooxygenase**	
Rapamycin (12-13)	Kinase; PI3K pwy.	0.287
Leupeptine (13)	Protein degradation	0.305
CKI7 (13)	Kinase	0.309
Wortmannin (13)	Kinase; PI3K pwy.	0.408
PD169316 (11-13)	Kinase; MAPK/p38 pwy.	0.428
Jasplakinolide (10, 12)	**Actin**	
Chelerythrine (11)	Kinase; PKC	0.404
Brefeldin A (11)	Vesicle trafficking	0.466
LY294002 (13)	Kinase; PI3K pwy.	0.549
Anisomycin (12-13)	Protein synthesis	0.556
Latrunculin B (8-10, 12-13)	Actin	0.570
Lactacystin (13)	**Protein degradation**	
ICRF193 (9-13)	Topoisomerase	0.414
Oligomycin (5-13)	Energy metabolism	0.484
Olomucine (13)	Kinase; CDK	0.491
Puromycin (9-10)	Protein synthesis	0.507
Genistein (13)	Kinase	0.518
Latrunculin B (8-10, 12-13)	**Actin**	
Cytochalasin D (10-13)	Actin	0.565
Jasplakinolide (10, 12)	Actin	0.570
Cytochalasin B (10-13)	Actin	0.573
Indirubin monoxime (10-13)	Kinase; CDK	0.675
Chelerythrine (11)	Kinase; PKC	0.703
Leupeptine (13)	**Protein degradation**	
CKI7 (13)	Kinase	0.254
Indomethacin (13)	Cyclooxygenase	0.305
Wortmannin (13)	Kinase; PI3K pwy.	0.384
Ceramide (13)	Kinase; PKC	0.396
Filopodine (12-13)	Unknown	0.432
LY294002 (13)	**Kinase; PI3K pwy.**	
SB202190 (12-13)	Kinase; MAPK/p38 pwy.	0.229
Trifluoperazine (12)	Neurotransmitter	0.316
Brefeldin A (11)	Vesicle trafficking	0.369
Simavastatin (12-13)	Cholesterol	0.374
11N84 (12-13)	Vesicle trafficking	0.436
Methotrexate (9-13)	**DNA replication**	
WY-14643 (13)	Nuclear receptor	0.119
Aphidicolin (8-13)	DNA replication	0.138
Hydroxy urea-2 (12-13)	DNA replication	0.138
U0126 (12-13)	Kinase; MAPK/ERK pwy.	0.148
Rapamycin (12-13)	Kinase; PI3K pwy.	0.221
Methotrexate (2)	**DNA replication**	
PD169316 (1-3, 7)	Kinase; MAPK/p38 pwy.	0.171
CKI7 (1-2)	Kinase	0.198
Sodium azide (2)	Energy metabolism	0.220
Scriptaid-2 (1-2)	Histone deacetylase	0.225
Didemnin B (1-2)	Protein synthesis	0.236
Mevastatin (12-13)	**Cholesterol**	
Simavastatin (12-13)	Cholesterol	0.418
Trifluoperazine (12)	Neurotransmitter	0.475
PMA (4-9)	Kinase; PKC	0.492
11N84 (12-13)	Vesicle trafficking	0.500
SB202190 (12-13)	Kinase; MAPK/p38 pwy.	0.504
MG132 (9-10, 12-13)	**Protein degradation**	
Emetine-1 (8-13)	Protein synthesis	0.465
Actinomycin D (7-8)	RNA	0.497
W-7 hydrochloride (13)	Calcium regulation	0.515
Puromycin (9-10)	Protein synthesis	0.533
Purvalanol A (11, 13)	Kinase; CDK	0.562

d-Profile	*Major annotated activity*	*Similarity*
Nocodazole-1 (7-13)	**Microtubule**	
Dexamethasone (6)	Nuclear receptor	0.162
Trichostatin (1-3)	Histone deacetylase	0.248
Nocodazole-2 (9-13)	Microtubule	0.253
Colchicine (9-10, 12-13)	Microtubule	0.265
Podophyllotoxin (6-9, 11, 13)	Microtubule	0.267
Nocodazole-1 (2)	**Microtubule**	
Genistein (13)	Kinase	0.266
Concentramide (1-2, 4, 6-8)	Unknown	0.368
Olomucine (13)	Kinase; CDK	0.369
Rapamycin (12-13)	Kinase; PI3K pwy.	0.373
Wortmannin (13)	Kinase; PI3K pwy.	0.402
Nocodazole-2 (9-13)	**Microtubule**	
Colchicine (9-10, 12-13)	Microtubule	0.147
Podophyllotoxin (6-9, 11, 13)	Microtubule	0.174
Nocodazole-1 (7-13)	Microtubule	0.253
Trichostatin (1-3)	Histone deacetylase	0.262
Dexamethasone (6)	Nuclear receptor	0.283
Nocodazole-2 (6-7)	**Microtubule**	
Oligomycin (5-13)	Energy metabolism	0.264
ICRF193 (9-13)	Topoisomerase	0.359
11N84 (12-13)	Vesicle trafficking	0.378
Simavastatin (12-13)	Cholesterol	0.417
Ceramide (13)	Kinase; PKC	0.437
Nocodazole-3 (10-13)	**Microtubule**	
Griseofulvin (12-13)	Microtubule	0.348
Nocodazole-1 (7-13)	Microtubule	0.357
Vinblastine (5-6)	Microtubule	0.397
Dexamethasone (6)	Nuclear receptor	0.433
Nocodazole-2 (9-13)	Microtubule	0.442
Okadaic acid (11)	**Kinase**	
Oligomycin (5-13)	Energy metabolism	0.461
11N84 (12-13)	Vesicle trafficking	0.469
Simavastatin (12-13)	Cholesterol	0.503
Tunicamycin (9-13)	Vesicle trafficking	0.513
ICRF193 (9-13)	Topoisomerase	0.519
Oligomycin (5-13)	**Energy metabolism**	
11N84 (12-13)	Vesicle trafficking	0.220
Tunicamycin (9-13)	Vesicle trafficking	0.252
Nocodazole-2 (6-7)	Microtubule	0.264
Brefeldin A (11)	Vesicle trafficking	0.314
Puromycin (9-10)	Protein synthesis	0.336
Oligomycin (1)	**Energy metabolism**	
PD169316 (1-3, 7)	Kinase; MAPK/p38 pwy.	0.191
Didemnin B (1-2)	Protein synthesis	0.220
CKI7 (1-2)	Kinase	0.237
Filopodine (1-2)	Unknown	0.238
Aphidicolin (1, 3, 7)	DNA replication	0.249
Olomucine (13)	**Kinase; CDK**	
Wortmannin (13)	Kinase; PI3K pwy.	0.254
W-7 hydrochloride (13)	Calcium regulation	0.291
Nocodazole-1 (2)	Microtubule	0.369
Sodium azide (13)	Energy metabolism	0.373
Puromycin (9-10)	Protein synthesis	0.383
Oxamflatin (10-12)	**Histone deacetylase**	
Apicidin (9-13)	Histone deacetylase	0.161
Scriptaid-1 (10-13)	Histone deacetylase	0.164
Scriptaid-2 (10-13)	Histone deacetylase	0.348
Trichostatin (9-13)	Histone deacetylase	0.368
SC560 (13)	Cyclooxygenase	0.446
Oxamflatin (1)	**Histone deacetylase**	
Cytochalasin B (2)	Actin	0.335
Chloropromazine (2)	Neurotransmitter	0.414
Concentramide (1-2, 4, 6-8)	Unknown	0.423
Emetine-1 (7)	Protein synthesis	0.433
TPEN (1)	Metal homeostasis	0.452

Supplementary Data 2d: DNA-Microtubule-Actin Marker Set

d-Profile	*Major annotated activity*	*Similarity*
PD169316 (11-13)	**Kinase; MAPK/p38 pwy.**	
Retinoic acid (trans) (9, 11-13)	Nuclear receptor	0.205
Austocystin (10-13)	Unknown	0.254
Forskolin (13)	Kinase; PKA	0.326
Rapamycin (12-13)	Kinase; PI3K pwy.	0.367
PMA (10-11)	Kinase; PKC	0.412
PD169316 (1-3, 7)	**Kinase; MAPK/p38 pwy.**	
CKI7 (1-2)	Kinase	0.101
Aphidicolin (1, 3, 7)	DNA replication	0.169
Methotrexate (2)	DNA replication	0.171
TPEN (1)	Metal homeostasis	0.187
Oligomycin (1)	Energy metabolism	0.191
PD98059 (1)	**Kinase; MAPK/ERK pwy.**	
Cytochalasin B (2)	Actin	0.254
Chloropromazine (2)	Neurotransmitter	0.264
CKI7 (1-2)	Kinase	0.277
Methotrexate (2)	DNA replication	0.311
PD169316 (1-3, 7)	Kinase; MAPK/p38 pwy.	0.332
PMA (10-11)	**Kinase; PKC**	
PD169316 (11-13)	Kinase; MAPK/p38 pwy.	0.412
Indomethacin (13)	Cyclooxygenase	0.519
Forskolin (13)	Kinase; PKA	0.535
Retinoic acid (trans) (9, 11-13)	Nuclear receptor	0.556
Ceramide (13)	Kinase; PKC	0.563
PMA (4-9)	**Kinase; PKC**	
Ceramide (13)	Kinase; PKC	0.413
Mevastatin (12-13)	Cholesterol	0.492
Leupeptine (13)	Protein degradation	0.505
Indomethacin (13)	Cyclooxygenase	0.543
W-7 hydrochloride (13)	Calcium regulation	0.546
Podophyllotoxin (6-9, 11, 13)	**Microtubule**	
Trichostatin (1-3)	Histone deacetylase	0.107
Colchicine (9-10, 12-13)	Microtubule	0.129
Nocodazole-2 (9-13)	Microtubule	0.174
Nocodazole-1 (7-13)	Microtubule	0.267
Vinblastine (7-13)	Microtubule	0.292
Puromycin (9-10)	**Protein synthesis**	
Emetine-2 (7-13)	Protein synthesis	0.244
Actinomycin D (7-8)	RNA	0.268
Wortmannin (13)	Kinase; PI3K pwy.	0.305
Trichostatin (9-13)	Histone deacetylase	0.329
Scriptaid-2 (10-13)	Histone deacetylase	0.333
Purvalanol A (11, 13)	**Kinase; CDK**	
Roscovitine (13)	Kinase; CDK	0.407
Actinomycin D (7-8)	RNA	0.503
Actinomycin D (9-13)	RNA	0.515
Camptothecin (11)	Topoisomerase	0.516
Indirubin monoxime (10-13)	Kinase; CDK	0.528
Rapamycin (12-13)	**Kinase; PI3K pwy.**	
U0126 (12-13)	Kinase; MAPK/ERK pwy.	0.204
Methotrexate (9-13)	DNA replication	0.221
Hydroxy urea-2 (12-13)	DNA replication	0.229
Sodium azide (13)	Energy metabolism	0.282
Indomethacin (13)	Cyclooxygenase	0.287
Retinoic acid (trans) (9, 11-13)	**Nuclear receptor**	
PD169316 (11-13)	Kinase; MAPK/p38 pwy.	0.205
U0126 (12-13)	Kinase; MAPK/ERK pwy.	0.266
Austocystin (10-13)	Unknown	0.276
Methotrexate (9-13)	DNA replication	0.310
SC560 (13)	Cyclooxygenase	0.323
Roscovitine (13)	**Kinase; CDK**	
Actinomycin D (7-8)	RNA	0.372
Actinomycin D (9-13)	RNA	0.373
Camptothecin (11)	Topoisomerase	0.376
Emetine-1 (8-13)	Protein synthesis	0.407
Purvalanol A (11, 13)	Kinase; CDK	0.407

d-Profile	*Major annotated activity*	*Similarity*
SB202190 (12-13)	**Kinase; MAPK/p38 pwy.**	
LY294002 (13)	Kinase; PI3K pwy.	0.229
Trifluoperazine (12)	Neurotransmitter	0.393
Brefeldin A (11)	Vesicle trafficking	0.417
Simavastatin (12-13)	Cholesterol	0.462
Filopodine (12-13)	Unknown	0.482
SC236 (13)	**Cyclooxygenase**	
Sodium azide (13)	Energy metabolism	0.317
Rapamycin (12-13)	Kinase; PI3K pwy.	0.367
SC560 (13)	Cyclooxygenase	0.375
Austocystin (10-13)	Unknown	0.399
Methotrexate (9-13)	DNA replication	0.421
SC560 (13)	**Cyclooxygenase**	
U0126 (12-13)	Kinase; MAPK/ERK pwy.	0.311
Retinoic acid (trans) (9, 11-13)	Nuclear receptor	0.323
Methotrexate (9-13)	DNA replication	0.356
Apicidin (9-13)	Histone deacetylase	0.367
SC236 (13)	Cyclooxygenase	0.375
Scriptaid-1 (10-13)	**Histone deacetylase**	
Apicidin (9-13)	Histone deacetylase	0.161
Oxamflatin (10-12)	Histone deacetylase	0.164
Trichostatin (9-13)	Histone deacetylase	0.411
Scriptaid-2 (10-13)	Histone deacetylase	0.415
SC560 (13)	Cyclooxygenase	0.460
Scriptaid-2 (10-13)	**Histone deacetylase**	
Trichostatin (9-13)	Histone deacetylase	0.210
Wortmannin (13)	Kinase; PI3K pwy.	0.258
Filopodine (12-13)	Unknown	0.325
Puromycin (9-10)	Protein synthesis	0.333
Oxamflatin (10-12)	Histone deacetylase	0.348
Scriptaid-2 (1-2)	**Histone deacetylase**	
Filopodine (1-2)	Unknown	0.112
Sodium azide (2)	Energy metabolism	0.134
Didemnin B (1-2)	Protein synthesis	0.139
Zvad (1)	Protein degradation	0.209
Austocystin (1)	Unknown	0.212
Simavastatin (12-13)	**Cholesterol**	
Brefeldin A (11)	Vesicle trafficking	0.281
Oligomycin (5-13)	Energy metabolism	0.338
LY294002 (13)	Kinase; PI3K pwy.	0.374
Nocodazole-2 (6-7)	Microtubule	0.417
Mevastatin (12-13)	Cholesterol	0.418
Sodium azide (13)	**Energy metabolism**	
Filopodine (12-13)	Unknown	0.247
Rapamycin (12-13)	Kinase; PI3K pwy.	0.282
SC236 (13)	Cyclooxygenase	0.317
Wortmannin (13)	Kinase; PI3K pwy.	0.363
Olomucine (13)	Kinase; CDK	0.373
Sodium azide (2)	**Energy metabolism**	
Scriptaid-2 (1-2)	Histone deacetylase	0.134
Filopodine (1-2)	Unknown	0.202
CKI7 (1-2)	Kinase	0.208
Didemnin B (1-2)	Protein synthesis	0.209
Methotrexate (2)	DNA replication	0.220
Staurosporine (7-9)	**Kinase**	
Indirubin monoxime (10-13)	Kinase; CDK	0.396
Tunicamycin (9-13)	Vesicle trafficking	0.405
Trichostatin (9-13)	Histone deacetylase	0.453
Olomucine (13)	Kinase; CDK	0.487
Wortmannin (13)	Kinase; PI3K pwy.	0.497
Sulindac sulfide (11, 13)	**Cyclooxygenase**	
Taxol (4-5)	Microtubule	0.282
Oligomycin (5-13)	Energy metabolism	0.386
ICRF193 (9-13)	Topoisomerase	0.435
Nocodazole-2 (6-7)	Microtubule	0.442
11N84 (12-13)	Vesicle trafficking	0.447

Supplementary Data 2d: DNA-Microtubule-Actin Marker Set

d-Profile	*Major annotated activity*	*Similarity*
Taxol (6-13)	**Microtubule**	
Epothilone B (9-13)	Microtubule	0.330
Griseofulvin (12-13)	Microtubule	0.384
105D (11-12)	Microtubule	0.389
Nocodazole-3 (10-13)	Microtubule	0.535
Vinblastine (5-6)	Microtubule	0.601
Taxol (4-5)	**Microtubule**	
Sulindac sulfide (11, 13)	Cyclooxygenase	0.282
Griseofulvin (12-13)	Microtubule	0.479
ICRF193 (9-13)	Topoisomerase	0.498
Vinblastine (5-6)	Microtubule	0.542
105D (11-12)	Microtubule	0.603
TPEN (1)	**Metal homeostasis**	
PD169316 (1-3, 7)	Kinase; MAPK/p38 pwy.	0.187
Emetine-2 (1, 6)	Protein synthesis	0.234
Didemnin B (1-2)	Protein synthesis	0.253
Zvad (1)	Protein degradation	0.260
Oligomycin (1)	Energy metabolism	0.262
Trichostatin (9-13)	**Histone deacetylase**	
Scriptaid-2 (10-13)	Histone deacetylase	0.210
Puromycin (9-10)	Protein synthesis	0.329
Apicidin (9-13)	Histone deacetylase	0.364
Oxamflatin (10-12)	Histone deacetylase	0.368
Oligomycin (5-13)	Energy metabolism	0.379
Trichostatin (8)	**Histone deacetylase**	
Apicidin (9-13)	Histone deacetylase	0.402
Tunicamycin (9-13)	Vesicle trafficking	0.502
Oxamflatin (10-12)	Histone deacetylase	0.513
Scriptaid-1 (10-13)	Histone deacetylase	0.514
Scriptaid-2 (10-13)	Histone deacetylase	0.539
Trichostatin (1-3)	**Histone deacetylase**	
Podophyllotoxin (6-9, 11, 13)	Microtubule	0.107
Vinblastine (7-13)	Microtubule	0.204
Colchicine (9-10, 12-13)	Microtubule	0.227
Nocodazole-1 (7-13)	Microtubule	0.248
Nocodazole-2 (9-13)	Microtubule	0.262
Trifluoperazine (12)	**Neurotransmitter**	
LY294002 (13)	Kinase; PI3K pwy.	0.316
SB202190 (12-13)	Kinase; MAPK/p38 pwy.	0.393
Simavastatin (12-13)	Cholesterol	0.446
Mevastatin (12-13)	Cholesterol	0.475
W-7 hydrochloride (13)	Calcium regulation	0.488
Tunicamycin (9-13)	**Vesicle trafficking**	
Oligomycin (5-13)	Energy metabolism	0.252
Indirubin monoxime (10-13)	Kinase; CDK	0.295
Wortmannin (13)	Kinase; PI3K pwy.	0.315
11N84 (12-13)	Vesicle trafficking	0.322
Puromycin (9-10)	Protein synthesis	0.347

d-Profile	*Major annotated activity*	*Similarity*
U0126 (12-13)	**Kinase; MAPK/ERK pwy.**	
Methotrexate (9-13)	DNA replication	0.148
Hydroxy urea-2 (12-13)	DNA replication	0.165
Rapamycin (12-13)	Kinase; PI3K pwy.	0.204
WY-14643 (13)	Nuclear receptor	0.215
Retinoic acid (trans) (9, 11-13)	Nuclear receptor	0.266
Vinblastine (7-13)	**Microtubule**	
Trichostatin (1-3)	Histone deacetylase	0.204
Dexamethasone (6)	Nuclear receptor	0.289
Podophyllotoxin (6-9, 11, 13)	Microtubule	0.292
Nocodazole-2 (9-13)	Microtubule	0.308
Nocodazole-1 (7-13)	Microtubule	0.316
Vinblastine (5-6)	**Microtubule**	
Griseofulvin (12-13)	Microtubule	0.354
Nocodazole-3 (10-13)	Microtubule	0.397
ICRF193 (9-13)	Topoisomerase	0.415
105D (11-12)	Microtubule	0.517
Nocodazole-2 (6-7)	Microtubule	0.525
W-7 hydrochloride (13)	**Calcium regulation**	
Wortmannin (13)	Kinase; PI3K pwy.	0.287
Olomucine (13)	Kinase; CDK	0.291
Puromycin (9-10)	Protein synthesis	0.337
Filopodine (12-13)	Unknown	0.346
11N84 (12-13)	Vesicle trafficking	0.354
Wortmannin (13)	**Kinase; PI3K pwy.**	
Filopodine (12-13)	Unknown	0.210
Olomucine (13)	Kinase; CDK	0.254
Scriptaid-2 (10-13)	Histone deacetylase	0.258
CKI7 (13)	Kinase	0.274
W-7 hydrochloride (13)	Calcium regulation	0.287
WY-14643 (13)	**Nuclear receptor**	
Methotrexate (9-13)	DNA replication	0.119
Aphidicolin (8-13)	DNA replication	0.172
U0126 (12-13)	Kinase; MAPK/ERK pwy.	0.215
Hydroxy urea-2 (12-13)	DNA replication	0.218
Austocystin (10-13)	Unknown	0.272
Zvad (1)	**Protein degradation**	
CKI7 (1-2)	Kinase	0.156
Filopodine (1-2)	Unknown	0.195
Didemnin B (1-2)	Protein synthesis	0.207
Scriptaid-2 (1-2)	Histone deacetylase	0.209
PD169316 (1-3, 7)	Kinase; MAPK/p38 pwy.	0.213