

Table 2: Clusters Results

Simple Model, use extracted features

Cluster 0 has 188 treatments:

- 1-octanol
- 2,5-furandimethanol
- 2-Oleoylglycerol
- 4-methylhistamine
- AK-7
- ANR-94
- AVL-292
- AZD9668
- BAM7
- BAN-ORL-24
- BAY-87-2243
- BI-2536
- BMS-536924
- BQ-788
- BRL-50481
- BVT-948
- CCG-50014
- CCG-63802
- CGP-53353
- CVT-10216
- CYM-50260
- CYM-50358
- CYM-5442
- CYM-5520
- DDR1-IN-1
- DG-172
- DMSO
- EI1
- FK-866
- FPS-ZM1
- GNF-5
- GNF-5837
- GSK-37647
- GSK2110183
- GSK3787
- GW-311616
- H2L-5765834
- IRL-2500
- IWP-L6
- JTE-607
- KH-CB19

- KU-55933
- L-proline
- LDN-27219
- LGK-974
- LOXO-101
- MCOPPB
- ME0328
- ML-323
- N-alpha-Methylhistamine-dihydrochloride
- N6-cyclopentyladenosine
- NNC-55-0396
- NQDI-1
- NS-11021
- NS-309
- NSC-625987
- NSC-632839
- NSC-663284
- NSC-95397
- NVP-AEW541
- PD-98059
- PF-03758309
- PF-04217903
- PF-05190457
- PF-431396
- PFI-1
- PP-2
- RGFP966
- RKI-1447
- RX-821002
- Ro-1138452
- SB-202190
- SGX523
- SU3327
- SirReal-2
- TC-S-7004
- TCN201
- TFC-007
- TG-003
- TG-02
- TUG-891
- VU591
- ZK-93423
- ZK811752
- ZM-336372
- acalabrutinib
- acetohexamide

- acetylcysteine
- afimoxifene
- alda-1
- aloxistatin
- alrestatin
- amiloride
- amlexanox
- amlodipine
- anandamide
- apatinib
- arundic-acid
- ascorbic-acid
- azacitidine
- azathioprine
- azeliragon
- baclofen
- batimastat
- benzamil
- bepridil
- bufexamac
- carzenide
- castanospermine
- cetilistat
- citric-acid
- conivaptan
- coumarin
- cycloheximide
- cyclosporine
- dalbavancin
- dalfampridine
- deferasirox
- delanzomib
- desonide
- dexamethasone
- diacerein
- dilazep
- droxinostat
- dyphylline
- edoxaban
- efaproxiral
- enilconazole
- ethoxzolamide
- ethyl-pyruvate
- felodipine
- filgotinib
- flindokalner

- fludarabine
- flufenamic-acid
- flupirtine
- fomepizole
- gabapentin-enacarbil
- glutamine-(l)
- glyburide
- guanidine
- halopemide
- ibudilast
- ibutamoren
- ibutilide
- ilomastat
- ingenol-mebutate
- isoflurane
- leflunomide
- lercanidipine
- lonafarnib
- meclofenamic-acid
- menadione
- methoxsalen
- miglitol
- minocycline
- misoprostol
- motesanib
- nialamide
- nilvadipine
- octreotide
- oxytocin
- ozagrel
- paliperidone
- pazopanib
- phenylbutazone
- picroton
- polydatin
- purvalanol-a
- quinidine
- quinine
- racecadotril
- rifamycin
- riociguat
- ryuvidine
- saclofen
- somatostatin
- sorbinil
- sotrastaurin

- spiroxatrine
- sulfasalazine
- sulfinpyrazone
- taladegib
- thioguanine
- thiostrepton
- torcitabine
- tranilast
- vitamin-E

Cluster 1 has 62 treatments:

- 4-CMTB
- 7-hydroxystaurosporine
- A205804
- AC-710
- AR-12
- AZ191
- AZD7762
- BAX-channel-blocker
- CC-401
- CP-724714
- CYT-997
- GK921
- GSK1070916
- KG-5
- KU-60019
- LDN-212854
- LY2109761
- M-25
- ME-0328
- ML-193
- ML-228
- NVP-ADW742
- NVP-HSP990
- PETCM
- PHA-793887
- PP-1
- PP-121
- RGB-286638
- SB-203580
- SRC-kinase-inhibitor-I
- TG-101348
- UNC1999
- UNC2025
- WH-4-023
- YC-1

- aminopurvalanol-a
- anisomycin
- arcyriaflavin-a
- briciclib
- brinzolamide
- buparlisib
- cediranib
- colchicine
- danusertib
- enflurane
- epoprostenol
- epothilone-b
- formononetin
- ganetespib
- geldanamycin
- hexestrol
- ixabepilone
- nafamostat
- olopatadine
- oxibendazole
- ponatinib
- puromycin
- ruxolitinib
- sacubitril
- trazodone
- trihexyphenidyl
- zamifenacin

Clustering based on VAE embedding

Cluster 0 has 207 treatments:

- gabapentin-enacarbil
- DMSO
- amlodipine
- hexestrol
- quinine
- LOXO-101
- brinzolamide
- NS-11021
- GNF-5837
- apatinib
- ethoxzolamide
- ascorbic-acid
- BAN-ORL-24

- flupirtine
- ZK811752
- dexamethasone
- DDR1-IN-1
- H2L-5765834
- thiostrepton
- arcylriaflavin-a
- CYM-5520
- fludarabine
- alda-1
- meclofenamic-acid
- GNF-5
- NS-309
- AK-7
- BVT-948
- SirReal-2
- MCOPPB
- ozagrel
- CYM-5442
- CVT-10216
- TCN201
- fomepizole
- benzamil
- lercanidipine
- 4-CMTB
- ML-228
- ML-193
- M-25
- azeliragon
- CYM-50260
- JTE-607
- ilomastat
- RX-821002
- TUG-891
- acetylcysteine
- NSC-625987
- dalfampridine
- NSC-95397
- alrestatin
- PF-03758309
- IRL-2500
- PF-04217903
- FK-866
- amlexanox
- GW-311616
- amiloride

- DG-172
- misoprostol
- conivaptan
- spiroxatrine
- diacerein
- glyburide
- ANR-94
- TFC-007
- trihexyphenidyl
- epoprostenol
- sacubitril
- BQ-788
- SB-202190
- GSK2110183
- GSK3787
- BAM7
- GSK-37647
- desonide
- aloxistatin
- azathioprine
- ZK-93423
- EI1
- NVP-HSP990
- nialamide
- arundic-acid
- torcitabine
- dyphylline
- quinidine
- halopemide
- sulfinpyrazone
- ML-323
- racecadotril
- BRL-50481
- bufexamac
- anandamide
- thioguanine
- IWP-L6
- edoxaban
- lonafarnib
- ibutamoren
- somatostatin
- L-proline
- zamifenacin
- YC-1
- ME-0328
- NSC-663284



- CYM-50358
- trazodone
- sulfasalazine
- 2,5-furandimethanol
- dilazep
- felodipine
- paliperidone
- purvalanol-a
- Ro-1138452
- sorbinil
- TC-S-7004
- saclofen
- BAY-87-2243
- ibudilast
- 2-Oleoyleglycerol
- RGFP966
- azacitidine
- N6-cyclopentyladenosine
- filgotinib
- guanidine
- coumarin
- ZM-336372
- citric-acid
- CCG-63802
- ibutilide
- batimastat
- glutamine-(l)
- PD-98059
- enilconazole
- N-alpha-Methylhistamine-dihydrochloride
- nilvadipine
- AC-710
- PETCM
- nafamostat
- taladegib
- acetohexamide
- minocycline
- riociguat
- CP-724714
- ganetespib
- AZ191
- octreotide
- 1-octanol
- acalabrutinib
- rifamycin
- pazopanib

- RKI-1447
- vitamin-E
- ethyl-pyruvate
- picrotin
- SGX523
- ME0328
- AZD9668
- NQDI-1
- carzenide
- KU-55933
- NVP-AEW541
- leflunomide
- KH-CB19
- PF-05190457
- formononetin
- ruxolitinib
- LGK-974
- enflurane
- PFI-1
- sotrastaurin
- oxytocin
- afimoxifene
- FPS-ZM1
- flindokalner
- motesanib
- geldanamycin
- CGP-53353
- 7-hydroxystaurosporine
- efaproxiral
- SB-203580
- bepridil
- phenylbutazone
- deferasirox
- isoflurane
- CCG-50014
- PF-431396
- baclofen
- flufenamic-acid
- LY2109761
- olopatadine
- castanospermine
- A205804
- VU591
- dalbavancin
- CC-401
- ingenol-mebutate

- menadione
- cetilistat
- methoxsalen
- cyclosporine
- TG-003
- miglitol
- tranilast
- 4-methylhistamine
- LDN-27219
- droxinostat

Cluster 1 has 43 treatments:

- ryuvudine
- NNC-55-0396
- WH-4-023
- PP-1
- AVL-292
- BMS-536924
- PP-121
- GSK1070916
- CYT-997
- AR-12
- KG-5
- ponatinib
- puromycin
- SRC-kinase-inhibitor-I
- buparlisib
- NVP-ADW742
- danusertib
- PHA-793887
- BI-2536
- epothilone-b
- briciclib
- UNC1999
- GK921
- AZD7762
- KU-60019
- BAX-channel-blocker
- SU3327
- PP-2
- ixabepilone
- LDN-212854
- aminopurvalanol-a
- polydatin
- cycloheximide
- colchicine

- RGB-286638
- delanzomib
- cediranib
- TG-02
- NSC-632839
- oxibendazole
- TG-101348
- anisomycin
- UNC2025