



Quantum Intelligence, Inc.

Enhanced QID D² Drug **Toxicity** Model Using **BioSpice**

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BioCOMP

Commercial Impact

Biomedical significance of the cluster-based predictive modeling.

- Integrate knowledge source for drug candidates
- Assess and predict a new compound's toxicity and efficacy based on its structure or drug-gene association patterns.
- Increase Return of Investment (ROI)

Military Impact/Sponsorship

- QIS D² would significantly speed up the understanding of biological, chemical, genetic and medical signatures for biological agents and pathogens for homeland security and national defense.
- The potential military sponsors/users include Army, Navy, Air force, Chemical and Biological Defense (CBD), The Defense Threat Reduction Agency (DTRA), Defense Health Program under OSD.



Q15 Clustering Results: # of samples: 1265, # of clusters: 10, # of features: 96

- Cluster0 (# of samples: 17)
 - Structures (Total Lift: 2.01)
 - [Structures_Project_11 0.44/ 0.45][0.44]
 - C__C-1__C-2__H-1
 - C__H-1__H-1__H-1__D-1
 - C__C-1__C-1__C-1__C-1
 - C__C-1__C-2__D-1
 - O__C-2
 - Efficacy (Total Lift: 0.00)
 - [Standard Agents 0.29/ 0.12][0.29]
 - Toxicity (Total Lift: 1.58)
 - [Toxicity_Group 10 0.12/ 0.10][0.12]
 - Kidney, Ureter, Bladder - changes in tubules (including acute renal failure, acute tubular necrosis)
 - Related to Chronic Data - changes in testicular weight
 - Related to Chronic Data - death
 - Musculoskeletal - other changes
 - Kidney, Ureter, Bladder - urine volume increased
 - Blood - other hemolysis with or without anemia
 - Standard Agents (Total Lift: 0.29)
 - [Standard Agents 0.29/ 0.12][0.29]
 - Genes (Total Lift: 1.71)
 - Gene Group 0 -0.30/ 0.01 [0.30]
 - AA025939:nuclear transport factor 2 placental protein 15.GC16939.7537
 - AA041526:tinucleotide repeat containing 3.GC18900.9498
 - N35886:hypothetical protein MGC15563.GC14210.4908
 - AA053303:fasciculation and elongation protein zeta 2 zygii II.GC9744.10048
 - H40238:ESTs.GC12791.3389
 - AA043174:Rho guanine nucleotide exchange factor GEF 12.GC19164.9762
 - Other Molecular Targets (Total Lift: 0.00)
 - Members:
 - 14343.xxxx 70-43-9 Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)-, 6-chloropiperonyl ester,(+)-cis, trans- C18H21-ClO4 [0.0076]
 - ***79037 79037 13010-47-4 Urea, 1-(2-chloroethyl)-3-cyclohexyl-1-nitroso- C9H16-ClN3O2 [0.1228]
 - ***34462 34462 66-75-1 Uracil, 5-(bis[2-chloroethyl(amino)- C8H11-Cl2-N3-O2] [0.2163]
 - ***3088 3088 305-03-3 Butyric acid, 4-(p-bis[2-chloroethyl(aminophenyl)- C14H19-Cl2-N-O2] [0.2783]
 - ***261726.xxxx 41729-52-6 4H-imidazo[4,5-c]pyridin-4-one, 6-amino-1,5-dihydro- C6-H6-N4-O [0.2897]
 - 156216 189796 32164-26-4 Streptovaricin D C40-H51-N-O13 [0.2940]
- Cluster1 (# of samples: 44)
- Cluster2 (# of samples: 38)
- Cluster3 (# of samples: 572)
- Cluster4 (# of samples: 18)
- Cluster5 (# of samples: 472)
- Cluster6 (# of samples: 17)
- Cluster7 (# of samples: 16)
- Cluster8 (# of samples: 9)
- Cluster9 (# of samples: 62)

Drug Cluster 1