

Table 10. UPPS Catalyst pharmacophore output

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Summary of parameters:
HyposReported      10
Spacing            250
MinPoints          4
MinSubsetPoints    4
SuperpositionError      1
Misses             1
FeatureMisses       1
CompleteMisses     0.0e+00
ToleranceFactor     1
CheckSuperposition  1
WeightVariation     0.3
MappingCoeff       0.0e+00
Mem                60
IdealHBondGeomOnly  0.0e+00
VariableWeight      1
VariableTolerance   1

Constraints on numbers of features:
Name:  HYDROPHOBIC      NegIonizable  Total
Min:   0                0              3
Max:   5                5              10

Best records in pass 3.
dumping score for hypothesis 1

Definition:          HYDROPHOBIC      HYDROPHOBIC      HYDROPHOBIC      NegIonizable      NegIonizable
Weights:            1.58288            1.58288            2.05774            3.00747            2.05774
Tolerances:         1.60              1.75              1.45              1.30              1.45
Coords: X           0.01              0.94              -2.36            1.74              -1.72
      : Y            2.19              1.34              0.90             -0.57            -1.68
      : Z           -1.86              5.86              1.96            -6.74            -3.30
      :              o                  o                  o                  o                  o

HYDROPHOBIC o
HYDROPHOBIC o      7.8
HYDROPHOBIC o      4.7
NegIonizable o      5.9
NegIonizable o      4.5

Maximum Fit: 10.2887

Name  Fit  Cnf/Enan  Mapping  Est  Act  Error  Unc
629  8.79 203 + [26 6 16 39 35 ] 0.69 0.5 + 1.4 2
608  8.70 133 + [26 42 30 1 2 ] 0.85 0.68 + 1.2 2
628  8.22 23 - [3 * 17 43 38 ] 2.6 0.92 + 2.8 2
625  8.05 33 - [8 42 17 27 32 ] 3.9 1 + 3.8 2
675  8.00 224 - [57 * 9 34 33 ] 4.3 1.1 + 3.8 2
676  7.89 110 - [3 * 14 34 29 ] 5.6 1.3 + 4.4 2
640  7.84 32 + [3 26 18 40 35 ] 6.2 1.8 + 3.5 2
626  7.76 3 - [10 * 17 32 27 ] 7.5 2 + 3.8 2
680  8.03 169 - [3 * 14 37 32 ] 4 3.3 + 1.2 2
681  8.70 88 + [30 6 16 39 43 ] 0.87 3.3 - 3.8 2
622  8.22 125 - [27 45 33 11 16 ] 2.6 4.5 - 1.7 2
621  8.19 198 - [27 * 45 11 16 ] 2.8 4.6 - 1.7 2
294  7.75 177 - [4 * 32 22 17 ] 7.7 6.8 + 1.1 2
228  7.84 132 + [4 * 30 15 20 ] 6.2 7.8 - 1.3 2
618  7.86 92 - [3 * 14 36 31 ] 6 10 - 1.7 2
646  8.01 16 - [17 * 25 40 45 ] 4.2 12 - 2.8 2
364  7.75 127 - [* 42 30 1 2 ] 7.6 13 - 1.8 2
642  7.20 184 + [* 25 17 36 41 ] 27 13 + 2 2
633  7.20 116 + [* 41 17 26 31 ] 27 22 + 1.3 2
632  6.64 52 + [19 * 41 31 * ] 99 27 + 3.6 2
641  7.46 239 - [* 6 16 39 35 ] 15 34 - 2.3 2
620  6.71 55 - [* 41 33 1 2 ] 85 35 + 2.4 2
300  6.75 146 + [* * 32 1 2 ] 76 48 + 1.6 2
614  7.49 38 - [* 41 29 2 1 ] 14 67 - 4.9 2
674  7.22 118 + [23 * 37 17 12 ] 26 69 - 2.6 2
663  6.68 33 + [26 * 23 7 1 ] 89 87 + 1 2
601  6.92 59 + [* 20 25 2 1 ] 52 90 - 1.7 2
619  7.04 89 + [* 41 31 1 2 ] 39 120 - 3.2 2
11  6.10 198 + [20 * * 2 1 ] 340 200 + 1.7 2
461  6.10 30 + [25 * * 1 2 ] 340 500 - 1.5 2
2  6.25 236 + [22 * * 2 1 ] 240 660 - 2.7 2
652  6.72 15 + [* * 3 40 35 ] 82 1000 - 12 2
673  5.20 52 + [7 45 15 * * ] 2700 1000 + 2.7 2
*****
Mirror image used. To turn this option off, put
catHypo.forceAbsoluteStereochemistry=1 in the .Catalyst file.
*****
totalcost=164.991 RMS=1.41992 correl=0.889633
Cost components: Error=129.067 Weight=1.14327 Config=33.2403 Tolerance=1.54001
Fixed Cost:
totalcost=131.314 RMS=0 correl=0
Cost components: Error=95.8005 Weight=1.12499 Config=33.2403 Tolerance=1.14801
dumping score for the null hypothesis:
totalcost=255.268 RMS=3.10881 correl=1.79494e-08
Cost components: Error=255.268 Weight=0 Config=0 Mapping=0 Tolerance=0

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