

In order to estimate predictive potential of an approach for an endpoint one should try to build up the model for several different splits into the training and validation sets. The training set should be used to build up the model. The validation set should be used to check up whether the model has predictive potential.

If you are using the CORAL software, the training set is structured into

First mode that is named balance of correlations:

Training set (+)

Invisible training set (-)

Calibration set (#)

Validation set (\*)

Second mode that is named classic scheme:

Training set (+)

Calibration set (#)

Validation set (\*).

In order to check that two splits are not identical, or to estimate how much these splits identical you can use program “MeasureOfIdentityOfTwoSplits.exe”.

Input for the program is two splits placed in files #TotalSet1.txt and #TotalSet2.txt in format

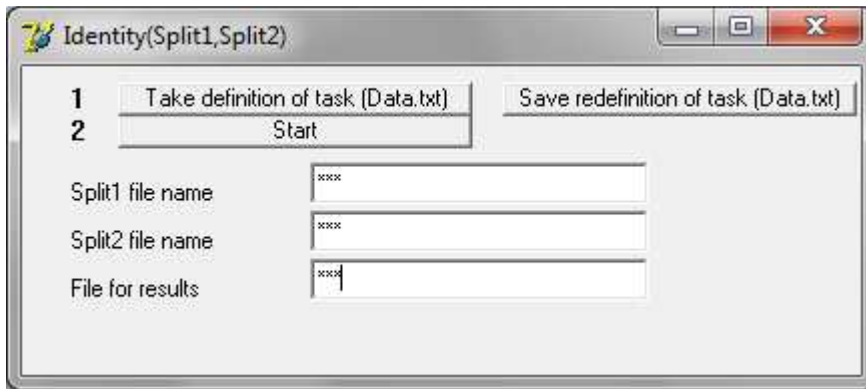
File #TotalSet1.txt, Split 1 (first)	File #TotalSet2.txt, Split 2 (second)
-1 [nH]1c2c(c3c1c(cc(c3C)N)[N+](O))Cccc2 2.360	*1 [nH]1c2c(c3c1c(cc(c3C)N)[N+](O))Cccc2 2.360
+2 [nH]1c2c(cc(c(c2)[N+](O))NC(=O)C)Ccccc12 -0.070	*2 [nH]1c2c(cc(c(c2)[N+](O))NC(=O)C)Ccccc12 -0.070
#3 [nH]1c2cc(c(N)cc2c2c1cccc2)[N+](=O)[O-] 0.910	*3 [nH]1c2cc(c(N)cc2c2c1cccc2)[N+](=O)[O-] 0.910
+4 [nH]1c2c(c3c1ccc(NC(C)=O)c3[N+](=O)[O-])Cccc2 -0.520	+4 [nH]1c2c(c3c1ccc(NC(C)=O)c3[N+](=O)[O-])Cccc2 -0.520
-5 [nH]1c2c(c3c1ccc(N)c3[N+](=O)[O-])Cccc2 -0.270	*5 [nH]1c2c(c3c1ccc(N)c3[N+](=O)[O-])Cccc2 -0.270
-6 n1(c2c(ccc(c2)[N+](O))c2c1cccc2)C 2.300	#6 n1(c2c(ccc(c2)[N+](O))c2c1cccc2)C 2.300
-7 n1(c2c(cc(c2)[N+](=O)[O-])c2c1cccc2)C 2.450	*7 n1(c2c(cc(c2)[N+](=O)[O-])c2c1cccc2)C 2.450
*8 n1(c2c(c3c1c(cc(c3C)[N+](O))C)Cccc2)C 2.230	-8 n1(c2c(c3c1c(cc(c3C)[N+](O))C)Cccc2)C 2.230
+9 [nH]1c2c(c3c1c(cc(c3C)[N+](=O)[O-])C)Cccc2 0.810	+9 [nH]1c2c(c3c1c(cc(c3C)[N+](=O)[O-])C)Cccc2 0.810
*10 [nH]1c2c(c3c1c(cc(c3C)[N+](=O)[O-])C)Cccc2 1.570	*10 [nH]1c2c(c3c1c(cc(c3C)[N+](=O)[O-])C)Cccc2 1.570
*11 [nH]1c2c(c3c1c(cc(c3C)[N+](O))C)Cccc2 0.280	+11 [nH]1c2c(c3c1c(cc(c3C)[N+](O))C)Cccc2 0.280
+12 c1c2c(ccc1[N+](O))c1c(cccc1)cc2 2.110	#12 c1c2c(ccc1[N+](O))c1c(cccc1)cc2 2.110
-13 n1cccc2c1c(ccc2)[N+](O) -1.240	-13 n1cccc2c1c(ccc2)[N+](O) -1.240
+14 n1cccc2c([N+](=O)[O-])Cccc12 -0.960	#14 n1cccc2c([N+](=O)[O-])Cccc12 -0.960
-15 c1(ccc2cccc3c4cccc4c1c23)[N+](O) -2.740	+15 c1(ccc2cccc3c4cccc4c1c23)[N+](O) -2.740
*16 c1(c(F)ccc(c1)F)[N+](=O)[O-] -0.790	-16 c1(c(F)ccc(c1)F)[N+](=O)[O-] -0.790
-17 c1([N+](O))c2ccc3c(cc(c4ccc(c1)N+)(=O)[O-])c2c34)[N+](O) -4.990	*17 c1([N+](O))c2ccc3c(cc(c4ccc(c1)N+)(=O)[O-])c2c34)[N+](O) -4.990
#18 c1(ccc(c(c1)C)[N+](=O)[O-])c1cccc1 -0.100	*18 c1(ccc(c(c1)C)[N+](=O)[O-])c1cccc1 -0.100
*19 C1c2cc(OC(C)=O)ccc2c2c1cc(cc2)[N+](O) -1.860	-19 C1c2cc(OC(C)=O)ccc2c2c1cc(cc2)[N+](O) -1.860
+20 c1nc2cc(ccc2[nH]1)[N+](=O)[O-] -1.830	+20 c1nc2cc(ccc2[nH]1)[N+](=O)[O-] -1.830
*21 C1c2cc(ccc2c2c1cc(cc2)[N+](O))C 2.360	*21 C1c2cc(ccc2c2c1cc(cc2)[N+](O))C 2.360
*22 c1c2c(ccc1)c1cccc1c(c2)[N+](O) -2.250	*22 c1c2c(ccc1)c1cccc1c(c2)[N+](O) -2.250
*23 c1(N)c2ccc3c(ccc4ccc(cc1)c2c34)[N+](O) -2.430	+23 c1(N)c2ccc3c(ccc4ccc(cc1)c2c34)[N+](O) -2.430
+24 c1c(ccc2c1n(nc2)C)[N+](O) -1.100	+24 c1c(ccc2c1n(nc2)C)[N+](O) -1.100
+25 c1(ccc2c3c1ccc1cccc(cc2)c31)[N+](=O)[O-] 2.760	-25 c1(ccc2c3c1ccc1cccc(cc2)c31)[N+](=O)[O-] 2.760
*26 c1cc(c2c([N+](O))c2ccc3c2c1c1c3cccc1)[N+](=O)[O-] 3.620	+26 c1cc(c2c([N+](O))c2ccc3c2c1c1c3cccc1)[N+](=O)[O-] 3.620
*27 c1(N)c([N+](O))c(ccc1)N -3.000	+27 c1(N)c([N+](O))c(ccc1)N -3.000
-28 C1(c2c(cc(cc2)[N+](O))c2cccc12)O 2.660	-28 C1(c2c(cc(cc2)[N+](O))c2cccc12)O 2.660
*29 n1c2c(ccc1)cc(cc2)[N+](=O)[O-] -1.080	-29 n1c2c(ccc1)cc(cc2)[N+](=O)[O-] -1.080
#30 C1c2c(c3c1cc(c3C)N)ccc(c2)[N+](O) 2.510	#30 C1c2c(c3c1cc(c3C)N)ccc(c2)[N+](O) 2.510
*31 c1(ccc([N+](=O)[O-])cc1c1cc([N+](O))ccc1 0.230	-31 c1(ccc([N+](=O)[O-])cc1c1cc([N+](O))ccc1 0.230
+32 c12c3C=C(c1cccc2cc1c3ccc2c1cccc2)[N+](=O)[O-] 0.860	+32 c12c3C=C(c1cccc2cc1c3ccc2c1cccc2)[N+](=O)[O-] 0.860
+33 c1(cc2ccc3c4c2c2c1ccc1ccc5ccc(cc3)c4c5c21)[N+](=O)[O-] 0.450	-33 c1(cc2ccc3c4c2c2c1ccc1ccc5ccc(cc3)c4c5c21)[N+](=O)[O-] 0.450
*34 C1c2cc(ccc2c2ccc([N+](=O)[O-])cc12)O 1.680	*34 C1c2cc(ccc2c2ccc([N+](=O)[O-])cc12)O 1.680
*35 c1(Cl)c(cc(cc1)[N+](=O)[O-])[N+](=O)[O-] 0.300	#35 c1(Cl)c(cc(cc1)[N+](=O)[O-])[N+](=O)[O-] 0.300
*36 c12c(cccc2)cc2c3c1ccc1c(ccc(cc2)c31)[N+](=O)[O-] 2.760	*36 c12c(cccc2)cc2c3c1ccc1c(ccc(cc2)c31)[N+](=O)[O-] 2.760
*37 C1c2c(c3c1cc(cc3)F)ccc([N+](O))c2 2.680	+37 C1c2c(c3c1cc(cc3)F)ccc([N+](O))c2 2.680
*38 C1(c2cc([N+](O))c(cc2c2ccc([N+](O))cc12)[N+](=O)[O-])O 3.410	-38 C1(c2cc([N+](O))c(cc2c2ccc([N+](O))cc12)[N+](=O)[O-])O 3.410
+39 c12c3cc4c(c1cccc2C(=C3)[N+](O))c1cccc1c4 0.670	*39 c12c3cc4c(c1cccc2C(=C3)[N+](O))c1cccc1c4 0.670
#40 C1c2cc(NC(=O)C(F)F)ccc2c2c1cc(cc2)[N+](=O)[O-] 2.810	-40 C1c2cc(NC(=O)C(F)F)ccc2c2c1cc(cc2)[N+](=O)[O-] 2.810
+41 c1c(ccc2c1cccc2)[N+](=O)[O-] -0.300	+41 c1c(ccc2c1cccc2)[N+](=O)[O-] -0.300
-42 C1c2c(ccc(c2)N)c2c1cc(cc2)[N+](=O)[O-] 1.560	+42 C1c2c(ccc(c2)N)c2c1cc(cc2)[N+](=O)[O-] 1.560
+43 c1c(c(C)cc2c1cccc2)[N+](=O)[O-] 0.000	*43 c1c(c(C)cc2c1cccc2)[N+](=O)[O-] 0.000
-44 C(=C)c1ccc(cc1)[N+](O) -1.210	*44 C(=C)c1ccc(cc1)[N+](O) -1.210
*45 c1(ccc([N+](=O)[O-])cc1c1cccc1 -0.300	#45 c1(ccc([N+](=O)[O-])cc1c1cccc1 -0.300
-46 n1cccc2c1c(cc(c2)OC)[N+](O) -1.210	+46 n1cccc2c1c(cc(c2)OC)[N+](O) -1.210
-47 c1(c2c(ccc1)cccc2)[N+](=O)[O-] -0.610	-47 c1(c2c(ccc1)cccc2)[N+](=O)[O-] -0.610
-48 C1c2c(c3c1cc(cc3)Br)ccc([N+](=O)[O-])c2 3.060	#48 C1c2c(c3c1cc(cc3)Br)ccc([N+](=O)[O-])c2 3.060
-49 n1c2c(cn1C)cc(cc2)[N+](O) -1.100	+49 n1c2c(cn1C)cc(cc2)[N+](O) -1.100
+50 c1c2c3c(c4cccc(cc1)[N+](O))c24)cccc3 3.010	+50 c1c2c3c(c4cccc(cc1)[N+](O))c24)cccc3 3.010

-51 c1c2c(ccc1[N+](=O)[O-])c1cccc1CC2 1.990	+51 c1c2c(ccc1[N+](=O)[O-])c1cccc1CC2 1.990
*52 c1(ccc([N+](O-))=O)cc1[N+](=O)[O-] 0.150	-52 c1(ccc([N+](O-))=O)cc1[N+](=O)[O-] 0.150
-53 c12c(cc3ccc4c5c(c(cc4)[N+](O-))=O)ccc1c35)CCCC2 0.900	-53 c12c(cc3ccc4c5c(c(cc4)[N+](O-))=O)ccc1c35)CCCC2 0.900
+54 c1c([N+](=O)[O-])cc2c3c1CCc1cc(ccc(C2)c31)[N+](=O)[O-] 3.500	+54 c1c([N+](=O)[O-])cc2c3c1CCc1cc(ccc(C2)c31)[N+](=O)[O-] 3.500
-55 c1c2c(ccc1[N+](=O)[O-])cc1cccc1c2 2.950	-55 c1c2c(ccc1[N+](=O)[O-])cc1cccc1c2 2.950
+56 c1c2c(ccc1[N+](=O)[O-])nc1ccc(cc1n2)[N+](O-)=O 2.750	+56 c1c2c(ccc1[N+](=O)[O-])nc1ccc(cc1n2)[N+](O-)=O 2.750
-57 c1(cccc2c(ccc12)[N+](O-))=O[N+](O-)=O 0.520	-57 c1(cccc2c(ccc12)[N+](O-))=O[N+](O-)=O 0.520
+58 c1c2ccc3c(ccc4c5c(c(c(c1)[N+](=O)[O-])c2c34)CCCC5)[N+](=O)[O-] 2.410	+58 c1c2ccc3c(ccc4c5c(c(c(c1)[N+](=O)[O-])c2c34)CCCC5)[N+](=O)[O-] 2.410
*59 c1([N+](O-))=O)c2ccc3cccc4c5c(c(c(c1)[N+](=O)[O-])c2c34)CCCC5 2.410	*59 c1([N+](O-))=O)c2ccc3cccc4c5c(c(c(c1)[N+](=O)[O-])c2c34)CCCC5 2.410
*60 C1c2c(c3c1cc([N+](O-))=O)ccc3ccc(c2)[N+](=O)[O-] 3.220	+60 C1c2c(c3c1cc([N+](O-))=O)ccc3ccc(c2)[N+](=O)[O-] 3.220
+61 O1=c2c(cc(c(c2)Cl)Cl)=Oc2c1cc([N+](=O)[O-])cc2 1.730	+61 O1=c2c(cc(c(c2)Cl)Cl)=Oc2c1cc([N+](=O)[O-])cc2 1.730
*62 c1(C)c2c(ccc1[N+](=O)[O-])cccc2 -0.700	-62 c1(C)c2c(ccc1[N+](=O)[O-])cccc2 -0.700
*63 c1c2c(ccc1[N+](O-))=O)nc1cccc1n2 2.060	*63 c1c2c(ccc1[N+](O-))=O)nc1cccc1n2 2.060
*64 c12[C@H]([C@H](C=Cc1cc1c3c2ccc2ccc(cc1)c32)[N+](O-))=O(O))O 2.800	+64 c12[C@H]([C@H](C=Cc1cc1c3c2ccc2ccc(cc1)c32)[N+](O-))=O(O))O 2.800
+65 c12c3C=C(c1cccc2cc1c3c2c(cc1)cccc2)[N+](=O)[O-] 0.260	+65 c12c3C=C(c1cccc2cc1c3c2c(cc1)cccc2)[N+](=O)[O-] 0.260
+66 C1c2cc(Cl)ccc2c2c1cc(cc2)[N+](O-)=O 3.110	-66 C1c2cc(Cl)ccc2c2c1cc(cc2)[N+](O-)=O 3.110
-67 c1(O)c(N)ccc([N+](=O)[O-])c1 -2.400	*67 c1(O)c(N)ccc([N+](=O)[O-])c1 -2.400
*68 C1(=O)c2c(c3c1cc([N+](=O)[O-])ccc3ccc([N+](O-))=O)c2 3.190	*68 C1(=O)c2c(c3c1cc([N+](=O)[O-])ccc3ccc([N+](O-))=O)c2 3.190
*69 c1(cc(cc2c1cccc2)[N+](=O)[O-])[N+](=O)[O-] -0.050	*69 c1(cc(cc2c1cccc2)[N+](=O)[O-])[N+](=O)[O-] -0.050
*70 c1(ccc(cc1)N)c1cc([N+](=O)[O-])ccc1 -1.520	*70 c1(ccc(cc1)N)c1cc([N+](=O)[O-])ccc1 -1.520
-71 c1(c(O)cc2c3c(ccc2)c2cccc2c13)[N+](=O)[O-] 2.260	*71 c1(c(O)cc2c3c(ccc2)c2cccc2c13)[N+](=O)[O-] 2.260
-72 c12c(cc3ccc4c5c(ccc4[N+](O-))=O)ccc1c35)cccc2 3.110	-72 c12c(cc3ccc4c5c(ccc4[N+](O-))=O)ccc1c35)cccc2 3.110
-73 C1c2c(c3c1cc(cc3)[N+](O-))=O)c(ccc2)[N+](=O)[O-] 3.200	+73 C1c2c(c3c1cc(cc3)[N+](O-))=O)c(ccc2)[N+](=O)[O-] 3.200
*74 N1C(=O)C(c2c1ccc(c2)[N+](=O)[O-])=O -0.940	-74 N1C(=O)C(c2c1ccc(c2)[N+](=O)[O-])=O -0.940
+75 c1cc(c2c3c1ccc1ccc(c(c4c2CCCC4)c31)[N+](O-))=O[N+](=O)[O-] 2.190	*75 c1cc(c2c3c1ccc1ccc(c(c4c2CCCC4)c31)[N+](O-))=O[N+](=O)[O-] 2.190
+76 C1c2cc([N+](=O)[O-])ccc2c2cccc12 1.430	*76 C1c2cc([N+](=O)[O-])ccc2c2cccc12 1.430
*77 c1(cc(N)ccc1)c1cccc1[N+](=O)[O-] -2.000	+77 c1(cc(N)ccc1)c1cccc1[N+](=O)[O-] -2.000
*78 c1ccc2c3c(ccc2)c2c(cc4c(c2)ccc(c4)[N+](=O)[O-])c13 2.760	*78 c1ccc2c3c(ccc2)c2c(cc4c(c2)ccc(c4)[N+](=O)[O-])c13 2.760
*79 c1(ccc(cc1)[N+](O-))=O)c1ccc(cc1)[N+](=O)[O-] 1.170	*79 c1(ccc(cc1)[N+](O-))=O)c1ccc(cc1)[N+](=O)[O-] 1.170
*80 c1(c(Cl)cccc1)[N+](=O)[O-] -1.720	+80 c1(c(Cl)cccc1)[N+](=O)[O-] -1.720
-81 c1(ccccc1N)c1cc([N+](O-))=O)ccc1 -1.520	*81 c1(ccccc1N)c1cc([N+](O-))=O)ccc1 -1.520
+82 c1(ccc(cc1)[N+](=O)[O-])ccc1ccc1C -0.230	*82 c1(ccc(cc1)[N+](=O)[O-])ccc1ccc1C -0.230
-83 O1=c2ccc(cc2=Oc2cccc12)[N+](O-)=O 1.790	-83 O1=c2ccc(cc2=Oc2cccc12)[N+](O-)=O 1.790
+84 c1ccc2cccc3c2c1c1c3c(ccc1)[N+](O-)=O 1.870	*84 c1ccc2cccc3c2c1c1c3c(ccc1)[N+](O-)=O 1.870
-85 c1([N+](=O)[O-])cc(ccc1)[N+](O-)=O 0.030	*85 c1([N+](=O)[O-])cc(ccc1)[N+](O-)=O 0.030
-86 [nH]1c2c(ccc(c2)[N+](=O)[O-])c2cccc12 1.010	*86 [nH]1c2c(ccc(c2)[N+](=O)[O-])c2cccc12 1.010
*87 C=Cc1ccc(cc1)[N+](=O)[O-] -1.300	+87 C=Cc1ccc(cc1)[N+](=O)[O-] -1.300
*88 c12c3ccc4cccc4c2cc2c(c1C=C3)[N+](=O)[O-])cccc2 0.040	+88 c12c3ccc4cccc4c2cc2c(c1C=C3)[N+](=O)[O-])cccc2 0.040
*89 c12c3C=C(c1cc1c(c2ccc3)cc2c(c1)cccc2)[N+](=O)[O-] 0.920	-89 c12c3C=C(c1cc1c(c2ccc3)cc2c(c1)cccc2)[N+](=O)[O-] 0.920
*90 o1c2c(ccc([N+](O-))=O)c2c2cccc12 1.450	*90 o1c2c(ccc([N+](O-))=O)c2c2cccc12 1.450
*91 c1([N+](O-))=O)ccc(cc1)C(=O)C -1.540	+91 c1([N+](O-))=O)ccc(cc1)C(=O)C -1.540
*92 n1(C)ccc2c1c(ccc2)[N+](O-)=O -1.000	*92 n1(C)ccc2c1c(ccc2)[N+](O-)=O -1.000
*93 c1c2ccc3cccc4c5c(c(c(c1)[N+](=O)[O-])c2c34)cccc5 1.590	*93 c1c2ccc3cccc4c5c(c(c(c1)[N+](=O)[O-])c2c34)cccc5 1.590
-94 c12C=C[C@H]([C@H](C=Cc1cc1c3c2ccc2ccc(cc1)c32)[N+](O-))=O(O))O 3.080	-94 c12C=C[C@H]([C@H](C=Cc1cc1c3c2ccc2ccc(cc1)c32)[N+](O-))=O(O))O 3.080
*95 c1c2CCc3cccc4CCc(cc1[N+](=O)[O-])c2c34 1.580	*95 c1c2CCc3cccc4CCc(cc1[N+](=O)[O-])c2c34 1.580
*96 c1(ccc2c3c1ccc1ccc(c(c4c2ccc4)c31)[N+](O-))=O 2.950	*96 c1(ccc2c3c1ccc1ccc(c(c4c2ccc4)c31)[N+](O-))=O 2.950
+97 c1ccc2c(cc3c4c(ccc3)ccc1c24)[N+](O-)=O 3.390	-97 c1ccc2c(cc3c4c(ccc3)ccc1c24)[N+](O-)=O 3.390
-98 c1c([N+](O-))=O)c(cc2c([N+](O-))=O)cccc12)[N+](O-)=O 1.510	+98 c1c([N+](O-))=O)c(cc2c([N+](O-))=O)cccc12)[N+](O-)=O 1.510
-99 c1(ccc2ccc3c(ccc4ccc1c2c34)[N+](O-))=O[N+](O-)=O[N+](O-)=O 4.990	*99 c1(ccc2ccc3c(ccc4ccc1c2c34)[N+](O-))=O[N+](O-)=O[N+](O-)=O 4.990
*100 C1c2cc(OC)ccc2c2c1cc(ccc2)[N+](O-)=O 2.790	+100 C1c2cc(OC)ccc2c2c1cc(ccc2)[N+](O-)=O 2.790
*101 c1nccc2c([N+](O-))=O)ccc12 -1.550	-101 c1nccc2c([N+](O-))=O)ccc12 -1.550
*102 C=1(c2cccc3cccc(C1)c23)[N+](O-)=O 1.770	-102 C=1(c2cccc3cccc(C1)c23)[N+](O-)=O 1.770
-103 c1(cccc(c1)N)c1cccc(c1)[N+](O-)=O -1.700	+103 c1(cccc(c1)N)c1cccc(c1)[N+](O-)=O -1.700
*104 c1(c2ccc3cccc4c5c(c(cc1)c2c34)CCCC5)[N+](O-)=O 0.780	*104 c1(c2ccc3cccc4c5c(c(cc1)c2c34)CCCC5)[N+](O-)=O 0.780
*105 C1(c2cc([N+](=O)[O-])cc(c2c2c([N+](=O)[O-])cc(cc12)[N+](O-))=O[N+](=O)[O-])=O 2.930	*105 C1(c2cc([N+](=O)[O-])cc(c2c2c([N+](=O)[O-])cc(cc12)[N+](O-))=O[N+](=O)[O-])=O 2.930
*106 c1c2ccc3cccc4ccc(cc1[N+](O-))=O)c2c34 3.310	-106 c1c2ccc3cccc4ccc(cc1[N+](O-))=O)c2c34 3.310
*107 c1c2ccc3cccc4c5c(c(c(c1)[N+](O-))=O)c2c34)CCCC5 0.700	*107 c1c2ccc3cccc4c5c(c(c(c1)[N+](O-))=O)c2c34)CCCC5 0.700
*108 c12c3c(c(cc1ccc2)[N+](O-))=O)ccc2 0.590	*108 c12c3c(c(cc1ccc2)[N+](O-))=O)ccc2 0.590
+109 c1(ccc2c3c1c(cc1cccc(cc2)c31)[N+](O-))=O 1.890	*109 c1(ccc2c3c1c(cc1cccc(cc2)c31)[N+](O-))=O 1.890
*110 c1cc(c2c3c(ccc2)c2c(cccc2)c13)[N+](O-)=O 3.670	*110 c1cc(c2c3c(ccc2)c2c(cccc2)c13)[N+](O-)=O 3.670
-111 c1cc(c2ccc3ccc4c5c3c2c1c1ccc(cc4)c51)[N+](O-)=O[N+](=O)[O-] 3.600	*111 c1cc(c2ccc3ccc4c5c3c2c1c1ccc(cc4)c51)[N+](O-)=O[N+](=O)[O-] 3.600
*112 C(=O)c1ccc([N+](O-))=O)cc1 -1.640	*112 C(=O)c1ccc([N+](O-))=O)cc1 -1.640
*113 C1Cc2c([N+](=O)[O-])ccc3c2c1ccc3 1.000	*113 C1Cc2c([N+](=O)[O-])ccc3c2c1ccc3 1.000
*114 c1(ccccc1N)c1ccc(cc1)[N+](=O)[O-] -1.700	-114 c1(ccccc1N)c1ccc(cc1)[N+](=O)[O-] -1.700
-115 C1C=Cc2cc([N+](O-))=O)ccc12 0.080	*115 C1C=Cc2cc([N+](O-))=O)ccc12 0.080
*116 c1(ccc(F)cc1)[N+](=O)[O-] -0.230	+116 c1(ccc(F)cc1)[N+](=O)[O-] -0.230
+117 c12c(cc3ccc4c(ccc5c4c3c1cc5)[N+](O-))=O)CCCC2 0.300	-117 c12c(cc3ccc4c(ccc5c4c3c1cc5)[N+](O-))=O)CCCC2 0.300
-118 c1(c([N+](O-))=O)cc([N+](=O)[O-])cc1c1c([N+](=O)[O-])cccc1 -0.190	+118 c1(c([N+](O-))=O)cc([N+](=O)[O-])cc1c1c([N+](=O)[O-])cccc1 -0.190
+119 n1(c2c(en1)cc(cc2)[N+](=O)[O-])C -0.820	-119 n1(c2c(en1)cc(cc2)[N+](=O)[O-])C -0.820
+120 c1(c2c3c(c4cc(ccc1[N+](O-))=O)c24)[N+](O-)=O)cccc3)[N+](=O)[O-] 3.160	+120 c1(c2c3c(c4cc(ccc1[N+](O-))=O)c24)[N+](O-)=O)cccc3)[N+](=O)[O-] 3.160
-121 c1cccc2c3cc(c4cccc4c3ccc12)[N+](=O)[O-] 1.750	*121 c1cccc2c3cc(c4cccc4c3ccc12)[N+](=O)[O-] 1.750
+122 c1ccc(c(c1)C)c1ccc([N+](O-))=O)c(c1)C -0.840	-122 c1ccc(c(c1)C)c1ccc([N+](O-))=O)c(c1)C -0.840
*123 c1(ccc(c1F)F)[N+](O-)=O -1.660	*123 c1(ccc(c1F)F)[N+](O-)=O -1.660
*124 c1c2ccc3cccc4CCc(cc1[N+](=O)[O-])c2c34 3.270	+124 c1c2ccc3cccc4CCc(cc1[N+](=O)[O-])c2c34 3.270
+125 c1(cccc2c1nc1c(n2)cc(cc1)[N+](O-))=O[N+](=O)[O-] 2.020	-125 c1(cccc2c1nc1c(n2)cc(cc1)[N+](O-))=O[N+](=O)[O-] 2.020
*126 c1(ccc(c(c1)[N+](O-))=O)[N+](O-)=O[N+](=O)[O-]c1cccc(c1)[N+](O-)=O 1.920	-126 c1(ccc(c(c1)[N+](O-))=O)[N+](O-)=O[N+](=O)[O-]c1cccc(c1)[N+](O-)=O 1.920
-127 C=1c2cccc3c(ccc(C1)c23)[N+](=O)[O-] 1.910	*127 C=1c2cccc3c(ccc(C1)c23)[N+](=O)[O-] 1.910
*128 N(c1ccc(cc1[N+](=O)[O-])[N+](O-))=O[N+](O-)=O[N+](O-)=O -0.070	-128 N(c1ccc(cc1[N+](=O)[O-])[N+](O-))=O[N+](O-)=O[N+](O-)=O -0.070
*129 COc1cccc1[N+](O-)=O -2.700	+129 COc1cccc1[N+](O-)=O -2.700
*130 C/C(c1cccc1)=O=C/c1ccc([N+](=O)[O-])cc1 -1.150	-130 C/C(c1cccc1)=O=C/c1ccc([N+](=O)[O-])cc1 -1.150
-131 C(c1cccc1[N+](O-))=O -1.920	*131 C(c1cccc1[N+](O-))=O -1.920
-132 O1=c2cc(c(c2=Oc2c1cc(Cl)c(c2)Cl)Cl)[N+](=O)[O-]C1 -1.400	+132 O1=c2cc(c(c2=Oc2c1cc(Cl)c(c2)Cl)Cl)[N+](=O)[O-]C1 -1.400
+133 c1c2ccc3ccc(cc4CCc(cc1[N+](=O)[O-])c2c34)[N+](O-)=O 4.250	-133 c1c2ccc3ccc(cc4CCc(cc1[N+](=O)[O-])c2c34)[N+](O-)=O 4.250

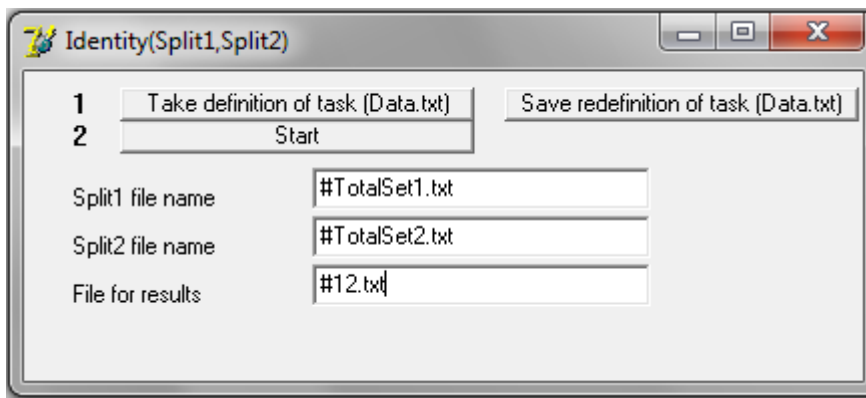
*134 c1(ccc(c(c1)Cl)F)[N+](=O)[O-] -1.210	-134 c1(ccc(c(c1)Cl)F)[N+](=O)[O-] -1.210
*135 c1(cc(c2ccc3cccc4c3c2c1cc4)[N+](O)=O)O 3.870	*135 c1(cc(c2ccc3cccc4c3c2c1cc4)[N+](O)=O)O 3.870
-136 c1c([N+](O)=O)(c2c3c(ccc2)c2c(cccc2)c13)[N+](=O)[O-] 2.620	-136 c1c([N+](O)=O)(c2c3c(ccc2)c2c(cccc2)c13)[N+](=O)[O-] 2.620
*137 n1c2c(en1C)ccc([N+](=O)[O-])c2 -0.410	*137 n1c2c(en1C)ccc([N+](=O)[O-])c2 -0.410
+138 c1(Cl)cc(c(cc1)N)[N+](O)=O -2.000	*138 c1(Cl)cc(c(cc1)N)[N+](O)=O -2.000
*139 c1([N+](=O)[O-])c2c(ccc1)cccc2[N+](O)=O 0.900	+139 c1([N+](=O)[O-])c2c(ccc1)cccc2[N+](O)=O 0.900
+140 c1(c(Cl)c(Cl)ccc1)[N+](=O)[O-] -1.510	#140 c1(c(Cl)c(Cl)ccc1)[N+](=O)[O-] -1.510
*141 O1=c2c(=Oc3c1cc(c(c3)[N+](=O)[O-])Cl)cc(c(c2)Cl)Cl -0.530	+141 O1=c2c(=Oc3c1cc(c(c3)[N+](=O)[O-])Cl)cc(c(c2)Cl)Cl -0.530
+142 CCOc1cccc1[N+](=O)[O-] -2.220	+142 CCOc1cccc1[N+](=O)[O-] -2.220
#143 c1(c(Cl)ccc(c1)Cl)[N+](=O)[O-] -1.540	*143 c1(c(Cl)ccc(c1)Cl)[N+](=O)[O-] -1.540
-144 c1(cccc(c1)N)c1ccc(cc1)[N+](=O)[O-] 0.250	#144 c1(cccc(c1)N)c1ccc(cc1)[N+](=O)[O-] 0.250
+145 c1(ccc(N)cc1)c1ccc([N+](=O)[O-])cc1 0.190	+145 c1(ccc(N)cc1)c1ccc([N+](=O)[O-])cc1 0.190
*146 c1([nH]c2c(n1)cc(cc2)[N+](O)=O)C -0.510	#146 c1([nH]c2c(n1)cc(cc2)[N+](O)=O)C -0.510
+147 C1=Cc2c(ccc3cccc1c23)[N+](=O)[O-] 1.770	*147 C1=Cc2c(ccc3cccc1c23)[N+](=O)[O-] 1.770
-148 c1c([N+](=O)[O-])ccc2nc3cc([N+](O)=O)[O-])ccc3nc12 4.340	+148 c1c([N+](=O)[O-])ccc2nc3cc([N+](O)=O)[O-])ccc3nc12 4.340
+149 [nH]1c2c(en1)cccc2[N+](=O)[O-] 0.110	+149 [nH]1c2c(en1)cccc2[N+](=O)[O-] 0.110
*150 c1c2c3c(c4ccc(cc1[N+](=O)[O-])c24)[N+](=O)[O-])cccc3 2.320	-150 c1c2c3c(c4ccc(cc1[N+](=O)[O-])c24)[N+](=O)[O-])cccc3 2.320
-151 C1Cc2ccc(c3cccc1c23)[N+](=O)[O-] 0.580	+151 C1Cc2ccc(c3cccc1c23)[N+](=O)[O-] 0.580
*152 c1([nH]c2c(n1)cccc2[N+](=O)[O-] 0.000	*152 c1([nH]c2c(n1)cccc2[N+](=O)[O-] 0.000
*153 COc1c(cc([N+](O)=O)cc1[N+](=O)[O-]) -1.890	*153 COc1c(cc([N+](O)=O)cc1[N+](=O)[O-]) -1.890
*154 N1c2c(CC1)ccc(c2)[N+](O)=O -0.480	#154 N1c2c(CC1)ccc(c2)[N+](O)=O -0.480
*155 c1(ccc2c3c1ccc1ccc(c(c2)c31)O)[N+](O)=O 1.340	*155 c1(ccc2c3c1ccc1ccc(c(c2)c31)O)[N+](O)=O 1.340
+156 C1c2c(ccc(c2)NC(=O)C)c2ccc(cc12)[N+](=O)[O-] 2.850	*156 C1c2c(ccc(c2)NC(=O)C)c2ccc(cc12)[N+](=O)[O-] 2.850
*157 c1(ccc2c3c1ccc1ccc(cc2)c31)O)[N+](O)=O 1.490	+157 c1(ccc2c3c1ccc1ccc(cc2)c31)O)[N+](O)=O 1.490
-158 Nc1c(Br)ccc(cc1[N+](=O)[O-])[N+](=O)[O-] -1.320	-158 Nc1c(Br)ccc(cc1[N+](=O)[O-])[N+](=O)[O-] -1.320
+159 c1c2ccc3c(ccc4c5c(c(c1)[N+](O)=O)c2c34)cccc5[N+](=O)[O-] 1.990	-159 c1c2ccc3c(ccc4c5c(c(c1)[N+](O)=O)c2c34)cccc5[N+](=O)[O-] 1.990
#160 c1c([N+](O)=O)(c2c3c1ccc1ccc(cc2)c31)O)[N+](=O)[O-] 4.580	*160 c1c([N+](O)=O)(c2c3c1ccc1ccc(cc2)c31)O)[N+](=O)[O-] 4.580
*161 c1([N+](=O)[O-])cc(c2ccc3cccc4c3c2c1cc4)[N+](O)=O 5.040	+161 c1([N+](=O)[O-])cc(c2ccc3cccc4c3c2c1cc4)[N+](O)=O 5.040
-162 c1ccc2c3c(ccc2)c2cc([N+](=O)[O-])ccc2c13 4.050	+162 c1ccc2c3c(ccc2)c2cc([N+](=O)[O-])ccc2c13 4.050
*163 c1(cc(OC(=O)C)c2ccc3cccc4c3c2c1cc4)[N+](=O)[O-] 4.220	-163 c1(cc(OC(=O)C)c2ccc3cccc4c3c2c1cc4)[N+](=O)[O-] 4.220
+164 c1(ccc2ccc3c4c(ccc3[N+](O)=O)ccc1c24)[N+](O)=O 5.060	*164 c1(ccc2ccc3c4c(ccc3[N+](O)=O)ccc1c24)[N+](O)=O 5.060
*165 COc1ccc(cc1)[N+](O)=O -2.700	#165 COc1ccc(cc1)[N+](O)=O -2.700
-166 c1(c([N+](O)=O)cc(cc1)[N+](O)=O)F 1.200	+166 c1(c([N+](O)=O)cc(cc1)[N+](O)=O)F 1.200
*167 c1(cccc2c1nc1c(n2)cccc1)[N+](O)=O 0.870	*167 c1(cccc2c1nc1c(n2)cccc1)[N+](O)=O 0.870
*168 [nH]1c2c(en1)ccc(c2)[N+](=O)[O-] 0.660	*168 [nH]1c2c(en1)ccc(c2)[N+](=O)[O-] 0.660
*169 c1(ccc(c1)[N+](=O)[O-])[N+](O)=O)c1ccc(cc1)[N+](O)=O 2.600	*169 c1(ccc(c1)[N+](=O)[O-])[N+](O)=O)c1ccc(cc1)[N+](O)=O 2.600
-170 c1c2c3c(c4cccc(c(c1)[N+](=O)[O-])c24)ccc(c3)[N+](=O)[O-] 5.020	+170 c1c2c3c(c4cccc(c(c1)[N+](=O)[O-])c24)ccc(c3)[N+](=O)[O-] 5.020
*171 O1=c2c(=Oc3cc(c(cc13)Cl)Cl)c(Cl)c(Cl)c(c2Cl)[N+](=O)[O-] -0.330	*171 O1=c2c(=Oc3cc(c(cc13)Cl)Cl)c(Cl)c(Cl)c(c2Cl)[N+](=O)[O-] -0.330
-172 C1c2c(C=C1)ccc(c2)[N+](O)=O 0.960	#172 C1c2c(C=C1)ccc(c2)[N+](O)=O 0.960
*173 c1(cccc2nc3c(c(ccc3[N+](=O)[O-])nc12)[N+](O)=O 1.260	+173 c1(cccc2nc3c(c(ccc3[N+](=O)[O-])nc12)[N+](O)=O 1.260
+174 n1c2c(en1C)cccc2[N+](=O)[O-] 0.230	+174 n1c2c(en1C)cccc2[N+](=O)[O-] 0.230
+175 C/(C1ccc([N+](=O)[O-])cc1)O)=C/c1ccc([N+](=O)[O-])cc1 -1.420	-175 C/(C1ccc([N+](=O)[O-])cc1)O)=C/c1ccc([N+](=O)[O-])cc1 -1.420
-176 c1cc([N+](O)=O)c2c3c4c(cc2)ccc2c4c4c(cc2)ccc(c4c13)[N+](O)=O 4.330	+176 c1cc([N+](O)=O)c2c3c4c(cc2)ccc2c4c4c(cc2)ccc(c4c13)[N+](O)=O 4.330
*177 c1(N)c(cc(N)cc1)[N+](O)=O -1.110	-177 c1(N)c(cc(N)cc1)[N+](O)=O -1.110
-178 Cc1nc2c(cc1)cccc2[N+](=O)[O-] -2.700	+178 Cc1nc2c(cc1)cccc2[N+](=O)[O-] -2.700
*179 c1([N+](=O)[O-])c2ccc3c(ccc4ccc(cc1)c2c34)[N+](O)=O 5.390	*179 c1([N+](=O)[O-])c2ccc3c(ccc4ccc(cc1)c2c34)[N+](O)=O 5.390
+180 c1ccc(c2cccc3c2c1c3c(ccc1)[N+](O)=O)[N+](O)=O 5.090	*180 c1ccc(c2cccc3c2c1c3c(ccc1)[N+](O)=O)[N+](O)=O 5.090
*181 c1(ccc(c(c1)[N+](O)=O)[N+](=O)[O-])F -1.840	-181 c1(ccc(c(c1)[N+](O)=O)[N+](=O)[O-])F -1.840
+182 N1c2c(CC1)cc(cc2)[N+](=O)[O-] -0.170	+182 N1c2c(CC1)cc(cc2)[N+](=O)[O-] -0.170
+183 c1c2c(ccc1[N+](=O)[O-])cc1)O)=C/c1ccc(cc1)c1c2cccc1 4.090	-183 c1c2c(ccc1[N+](=O)[O-])cc1)O)=C/c1ccc(cc1)c1c2cccc1 4.090
*184 [nH]1c2c(cc(cc2)[N+](=O)[O-])c2c1cccc2 1.180	*184 [nH]1c2c(cc(cc2)[N+](=O)[O-])c2c1cccc2 1.180
+185 c1(cccc(c1)[N+](O)=O)c1cccc1 -1.580	*185 c1(cccc(c1)[N+](O)=O)c1cccc1 -1.580
*186 c1(c([N+](O)=O)ccc1)c1cccc1 -2.100	-186 c1(c([N+](O)=O)ccc1)c1cccc1 -2.100
*187 c1(c(ccc2c1cccc2)C)[N+](=O)[O-] -0.290	#187 c1(c(ccc2c1cccc2)C)[N+](=O)[O-] -0.290
*188 C/(c1ccc(cc1)[N+](O)=O)=C/c1ccc(cc1)N 0.530	*188 C/(c1ccc(cc1)[N+](O)=O)=C/c1ccc(cc1)N 0.530
+189 C(=C/c1ccc(Cl)ccc1)/c1ccc(cc1)[N+](O)=O 0.950	-189 C(=C/c1ccc(Cl)ccc1)/c1ccc(cc1)[N+](O)=O 0.950
*190 C(=C/c1ccc(cc1)Cl)/c1ccc([N+](=O)[O-])cc1 1.170	*190 C(=C/c1ccc(cc1)Cl)/c1ccc([N+](=O)[O-])cc1 1.170
*191 C(=C/c1ccc(cc1)C#N)/c1ccc([N+](=O)[O-])cc1 1.600	*191 C(=C/c1ccc(cc1)C#N)/c1ccc([N+](=O)[O-])cc1 1.600
-192 C(=C/c1ccc(C#N)cc1)/c1ccc(cc1)[N+](=O)[O-] 1.170	+192 C(=C/c1ccc(C#N)cc1)/c1ccc(cc1)[N+](=O)[O-] 1.170
+193 C/(c1ccc([N+](=O)[O-])cc1)=C/c1cc(OC)ccc1 0.920	#193 C/(c1ccc([N+](=O)[O-])cc1)=C/c1cc(OC)ccc1 0.920
*194 C(=C/c1ccc(OC)cc1)/c1ccc(cc1)[N+](=O)[O-] 0.560	*194 C(=C/c1ccc(OC)cc1)/c1ccc(cc1)[N+](=O)[O-] 0.560
+195 C(=C/c1ccc([N+](=O)[O-])cc1)/c1ccc(cc1)[N+](=O)[O-] 1.900	-195 C(=C/c1ccc([N+](=O)[O-])cc1)/c1ccc(cc1)[N+](=O)[O-] 1.900
-196 C(=C/c1ccc([N+](O)=O)cc1)/c1ccc(cc1)[N+](=O)[O-] 1.990	#196 C(=C/c1ccc([N+](O)=O)cc1)/c1ccc(cc1)[N+](=O)[O-] 1.990
*197 C/(c1ccc([N+](=O)[O-])cc1)=C/c1ccc(C#N)ccc1 1.010	*197 C/(c1ccc([N+](=O)[O-])cc1)=C/c1ccc(C#N)ccc1 1.010
*198 C/(c1ccc(cc1)[N+](O)=O)=C/c1ccc(cc1)C#N 0.940	*198 C/(c1ccc(cc1)[N+](O)=O)=C/c1ccc(cc1)C#N 0.940
*199 c1c(ccc(SC)c1)[N+](O)=O -1.010	*199 c1c(ccc(SC)c1)[N+](O)=O -1.010
+200 c1c(ccc(SCC)c1)[N+](O)=O -0.740	-200 c1c(ccc(SCC)c1)[N+](O)=O -0.740
+201 c1c(ccc(SCCC)c1)[N+](O)=O -0.720	#201 c1c(ccc(SCCC)c1)[N+](O)=O -0.720
-202 S(c1ccc(cc1)[N+](=O)[O-])CCCC -0.360	*202 S(c1ccc(cc1)[N+](=O)[O-])CCCC -0.360
+203 c1c(ccc(SCC=C)c1)[N+](O)=O 0.610	-203 c1c(ccc(SCC=C)c1)[N+](O)=O 0.610
*204 [N+](c1ccc(SCc2cccc2)cc1)=O)[O-] 0.450	*204 [N+](c1ccc(SCc2cccc2)cc1)=O)[O-] 0.450
*205 c1cc(ccc1[N+](=O)[O-])Sc1cccc1 0.450	*205 c1cc(ccc1[N+](=O)[O-])Sc1cccc1 0.450
+206 S(c1ccc(cc1)N)c1ccc([N+](=O)[O-])cc1 -0.740	#206 S(c1ccc(cc1)N)c1ccc([N+](=O)[O-])cc1 -0.740
*207 c1ccc2c3c1cc(c1ccc(c4c2CCCC4)c31)[N+](O)=O 2.230	-207 c1ccc2c3c1cc(c1ccc(c4c2CCCC4)c31)[N+](O)=O 2.230
-208 c12c([C@H](CCC2)O)cc2ccc3c4c(c(cc3)[N+](=O)[O-])ccc1c24 1.200	*208 c12c([C@H](CCC2)O)cc2ccc3c4c(c(cc3)[N+](=O)[O-])ccc1c24 1.200
*209 c12c3ccc4ccc(c5ccc(cc2[C@@H](O)(CCC1)c3c45)[N+](=O)[O-] 1.200	-209 c12c3ccc4ccc(c5ccc(cc2[C@@H](O)(CCC1)c3c45)[N+](=O)[O-] 1.200
*210 c1ccc2c3c1cc(c1ccc(c4c2cccc4)c31)[N+](=O)[O-] 2.990	+210 c1ccc2c3c1cc(c1ccc(c4c2cccc4)c31)[N+](=O)[O-] 2.990
*211 c1([N+](=O)[O-])c2c(c(c3cccc4c5c(c(cc1)c2c34)cccc5)CC(=O)[O-])CC(=O)[O-] 2.030	*211 c1([N+](=O)[O-])c2c(c(c3cccc4c5c(c(cc1)c2c34)cccc5)CC(=O)[O-])CC(=O)[O-] 2.030
-212 c1([N+](=O)[O-])c2ccc3cccc4c5c(c(c1)[N+](=O)[O-])c2c34)cccc5 3.930	*212 c1([N+](=O)[O-])c2ccc3cccc4c5c(c(c1)[N+](=O)[O-])c2c34)cccc5 3.930
*213 c1(ccc(c(c1)CC)[N+](O)=O)c1cccc1 -1.270	-213 c1(ccc(c(c1)CC)[N+](O)=O)c1cccc1 -1.270
+214 c1(ccc(c(c1)C(C)C)[N+](O)=O)c1cccc1 -1.390	+214 c1(ccc(c(c1)C(C)C)[N+](O)=O)c1cccc1 -1.390
*215 c1(cc(CC)c1[N+](=O)[O-])c1(C)CCc1cccc1 -1.510	+215 c1(cc(CC)c1[N+](=O)[O-])c1(C)CCc1cccc1 -1.510
-216 c1(cc(C(C)C)c([N+](O)=O)c(c1)C(C)C)c1cccc1 -1.960	#216 c1(cc(C(C)C)c([N+](O)=O)c(c1)C(C)C)c1cccc1 -1.960
*217 c1(ccc(cc1)[N+](=O)[O-])c1c(cccc1)CC -1.600	-217 c1(ccc(cc1)[N+](=O)[O-])c1c(cccc1)CC -1.600
*218 c1(ccc(cc1)[N+](=O)[O-])c1ccc(cc1)C -0.660	#218 c1(ccc(cc1)[N+](=O)[O-])c1ccc(cc1)C -0.660
-219 c1(ccc(cc1)[N+](=O)[O-])c1ccc(cc1)CC -0.980	+219 c1(ccc(cc1)[N+](=O)[O-])c1ccc(cc1)CC -0.980

*220 c1(ccc([N+](O-)=O)cc1)c1ccc(C(C)C)cc1 -1.960	-220 c1(ccc([N+](O-)=O)cc1)c1ccc(C(C)C)cc1 -1.960
+221 c1(ccc([N+](O-)=O)cc1)c1ccc(cc1)CCCC -1.140	+221 c1(ccc([N+](O-)=O)cc1)c1ccc(cc1)CCCC -1.140
*222 c1(ccc(cc1)[N+](O-)=O)c1ccc(cc1)C -0.810	*222 c1(ccc(cc1)[N+](O-)=O)c1ccc(cc1)C -0.810
#223 c1(ccc([N+](O-)=O)cc1)c1ccc(cc1)C -1.840	*223 c1(ccc([N+](O-)=O)cc1)c1ccc(cc1)C -1.840
*224 c1(ccc(cc1)[N+](O-)=O)cc1ccc(cc1)C(C)C(C)C(C)C -1.930	#224 c1(ccc(cc1)[N+](O-)=O)cc1ccc(cc1)C(C)C(C)C(C)C(C)C -1.930
*225 c1(ncc(cc1)[N+](O-)=O)c1ccc(cc1)C -0.540	-225 c1(ncc(cc1)[N+](O-)=O)c1ccc(cc1)C -0.540
#226 c1(ccc([N+](O-)=O)cc1)c1ccc(C(C)C(C)C)cc1 -1.700	*226 c1(ccc([N+](O-)=O)cc1)c1ccc(C(C)C(C)C)cc1 -1.700
-227 C1c2c(c3c1cc(cc3)[N+](O-)=O)ccc(c2)C(C)C(C)C -0.430	-227 C1c2c(c3c1cc(cc3)[N+](O-)=O)ccc(c2)C(C)C(C)C -0.430
+228 C1c2c(c3c1cc([N+](O-)=O)cc3)ccc([C@@H]1([C@H]3(C[C@H]4(C[C@H](C3)(C[C@H]1(C4))))))c2 -1.030	+228 C1c2c(c3c1cc([N+](O-)=O)cc3)ccc([C@@H]1([C@H]3(C[C@H]4(C[C@H](C3)(C[C@H]1(C4))))))c2 -1.030
+229 [nH]1c2c(c3c1c([N+](O-)=O)ccc3)cccc2 -0.830	*229 [nH]1c2c(c3c1c([N+](O-)=O)ccc3)cccc2 -0.830
#230 C(=C)c1ccc(cc1)[N+](O-)=O/c1ccc(C)cc1 0.260	#230 C(=C)c1ccc(cc1)[N+](O-)=O/c1ccc(C)cc1 0.260
*231 C/c1ccc(CC)cc1=C/c1ccc([N+](O-)=O)cc1 -0.420	*231 C/c1ccc(CC)cc1=C/c1ccc([N+](O-)=O)cc1 -0.420
#232 C/c1ccc(C(C)C)cc1=C/c1ccc([N+](O-)=O)cc1 -1.000	*232 C/c1ccc(C(C)C)cc1=C/c1ccc([N+](O-)=O)cc1 -1.000
*233 C/c1ccc(cc1)C(C)C(C)C=C/c1ccc(cc1)[N+](O-)=O -1.460	#233 C/c1ccc(cc1)C(C)C(C)C=C/c1ccc(cc1)[N+](O-)=O -1.460
+234 C(=C)c1ccc([N+](O-)=O)cc1/c1ccc(cc1)[C@@H](CC)C -0.640	*234 C(=C)c1ccc([N+](O-)=O)cc1/c1ccc(cc1)[C@@H](CC)C -0.640
+235 [n+](c2c(c(cc1)[N+](O-)=O)ccc2)[O-] 1.980	+235 [n+](c2c(c(cc1)[N+](O-)=O)ccc2)[O-] 1.980
+236 c1cccc2cc3c(ccc3)c([N+](O-)=O)[O-]c12 -0.400	+236 c1cccc2cc3c(ccc3)c([N+](O-)=O)[O-]c12 -0.400
+237 c12cccc1c(c1c3c2ccc2cccc(CC1)c32)[N+](O-)=O 0.300	-237 c12cccc1c(c1c3c2ccc2cccc(CC1)c32)[N+](O-)=O 0.300
-238 c1cc2c(cc1)C(c1c3c(ccc1)ccc(c23)[N+](O-)=O)O 3.750	#238 c1cc2c(cc1)C(c1c3c(ccc1)ccc(c23)[N+](O-)=O)O 3.750
+239 c1ccc2C(=O)c3cccc4c3c(c2c1)cc(c4)[N+](O-)=O 2.200	*239 c1ccc2C(=O)c3cccc4c3c(c2c1)cc(c4)[N+](O-)=O 2.200
-240 c1ccc2C(=O)c3cccc4c3c(c2c1)ccc4[N+](O-)=O 5.320	*240 c1ccc2C(=O)c3cccc4c3c(c2c1)ccc4[N+](O-)=O 5.320
+241 c1c([N+](O-)=O)[O-]ccc2c(c1)c1c3c(C2=O)cccc3ccc1 4.930	+241 c1c([N+](O-)=O)[O-]ccc2c(c1)c1c3c(C2=O)cccc3ccc1 4.930
-242 c1ccc2c(c3c4c(C2=O)cccc4ccc3)c1[N+](O-)=O 0.780	+242 c1ccc2c(c3c4c(C2=O)cccc4ccc3)c1[N+](O-)=O 0.780
*243 c1cc2c(cc1)[N+](O-)=O)C(c1c3c(ccc1)ccc(c23)[N+](O-)=O)O 4.620	+243 c1cc2c(cc1)[N+](O-)=O)C(c1c3c(ccc1)ccc(c23)[N+](O-)=O)O 4.620
*244 c1c(cc2C(=O)c3cccc4c3c(c2c1)ccc4[N+](O-)=O)O 4.670	+244 c1c(cc2C(=O)c3cccc4c3c(c2c1)ccc4[N+](O-)=O)O 4.670
-245 c1ccc2C(=O)c3c4c(c2c1)[N+](O-)=O)ccc(c4ccc3)[N+](O-)=O 3.520	#245 c1ccc2C(=O)c3c4c(c2c1)[N+](O-)=O)ccc(c4ccc3)[N+](O-)=O 3.520
-246 n1c2c(ccc1)c1c(c(ccc1)[N+](O-)=O)cc2 2.080	*246 n1c2c(ccc1)c1c(c(ccc1)[N+](O-)=O)cc2 2.080
-247 c1c2c(ncc1)c1cc([N+](O-)=O)ccc1cc2 -0.160	+247 c1c2c(ncc1)c1cc([N+](O-)=O)ccc1cc2 -0.160
-248 c1c2c(ncc1)c1c(c(ccc1)[N+](O-)=O)cc2 2.270	-248 c1c2c(ncc1)c1c(c(ccc1)[N+](O-)=O)cc2 2.270
#249 c1ccc(c2c3cccc3ncc12)[N+](O-)=O 1.400	#249 c1ccc(c2c3cccc3ncc12)[N+](O-)=O 1.400
#250 c1cccc2c3c(cccc3ncc12)[N+](O-)=O 0.130	+250 c1cccc2c3c(cccc3ncc12)[N+](O-)=O 0.130
#251 c1c2c(ccc1)c1c(ccc(c1)[N+](O-)=O)nc2 2.210	+251 c1c2c(ccc1)c1c(ccc(c1)[N+](O-)=O)nc2 2.210
-252 c1c2c(ccc1)c1c(ccc(c1)[N+](O-)=O)nc2 2.010	+252 c1c2c(ccc1)c1c(ccc(c1)[N+](O-)=O)nc2 2.010
+253 [n+](c2c2c3c(cccc3ccc12)[N+](O-)=O)O -0.140	+253 [n+](c2c2c3c(cccc3ccc12)[N+](O-)=O)O -0.140
*254 [n+](c2c(ccc1)c1c(ccc(c1)[N+](O-)=O)cc2)[O-] 1.560	*254 [n+](c2c(ccc1)c1c(ccc(c1)[N+](O-)=O)cc2)[O-] 1.560
-255 [n+](c2c(ccc1)c1c(ccc(c1)[N+](O-)=O)cc2)O 0.960	*255 [n+](c2c(ccc1)c1c(ccc(c1)[N+](O-)=O)cc2)O 0.960
*256 c1cc[n+](O-)=O)cc2c3c(cccc3[N+](O-)=O)cc12 1.180	-256 c1cc[n+](O-)=O)cc2c3c(cccc3[N+](O-)=O)cc12 1.180
-257 c1cc[n+](O-)=O)cc2c3c(ccc3[N+](O-)=O)cc3ccc12 2.230	+257 c1cc[n+](O-)=O)cc2c3c(ccc3[N+](O-)=O)cc3ccc12 2.230
-258 c1c2c([n+](cc1)[O-])c1c(ccc1)[N+](O-)=O)cc2 1.210	#258 c1c2c([n+](cc1)[O-])c1c(ccc1)[N+](O-)=O)cc2 1.210
+259 c1(cccc2c3c(cccc3)[n+](O-)=O)cc12)[N+](O-)=O 2.260	*259 c1(cccc2c3c(cccc3)[n+](O-)=O)cc12)[N+](O-)=O 2.260
*260 c1c([N+](O-)=O)ccc2c1c[n+](c1c2cccc1)[O-] 1.710	*260 c1c([N+](O-)=O)ccc2c1c[n+](c1c2cccc1)[O-] 1.710
*261 c1cc([N+](O-)=O)cc2c1c[n+](c1c2cccc1)[O-] 2.180	*261 c1cc([N+](O-)=O)cc2c1c[n+](c1c2cccc1)[O-] 2.180
*262 c1cccc2c3c(cccc3[n+](O-)=O)cc12)[N+](O-)=O -0.020	-262 c1cccc2c3c(cccc3[n+](O-)=O)cc12)[N+](O-)=O -0.020
*263 c1(cc[n+](O-)=O)cc2c3c(cccc3[N+](O-)=O)ccc12)[N+](O-)=O 3.470	-263 c1(cc[n+](O-)=O)cc2c3c(cccc3[N+](O-)=O)ccc12)[N+](O-)=O 3.470
*264 c1([N+](O-)=O)cc[n+](c2c1ccc1c2cccc1[N+](O-)=O)O -3.200	+264 c1([N+](O-)=O)cc[n+](c2c1ccc1c2cccc1[N+](O-)=O)O -3.200
+265 c1(C)ccc(cc1)[N+](O-)=O)cc12)[N+](O-)=O -1.220	#265 c1(C)ccc(cc1)[N+](O-)=O)cc12)[N+](O-)=O -1.220
#266 c1(c(cccc1[N+](O-)=O)O-)[N+](O-)=O)C -1.700	+266 c1(c(cccc1[N+](O-)=O)O-)[N+](O-)=O)C -1.700
-267 C1c2c(cccc2N)c2cccc([N+](O-)=O)cc12 1.750	+267 C1c2c(cccc2N)c2cccc([N+](O-)=O)cc12 1.750
*268 C1c2c(NC(=O)C)cccc2c2c1cc(cc2)[N+](O-)=O 1.410	*268 C1c2c(NC(=O)C)cccc2c2c1cc(cc2)[N+](O-)=O 1.410
*269 c1cc2c3C=C[C@@H]([C@H](C3cc3c2c2c1cc(cc2cc3)[N+](O-)=O)O)O) 2.820	*269 c1cc2c3C=C[C@@H]([C@H](C3cc3c2c2c1cc(cc2cc3)[N+](O-)=O)O)O) 2.820
*270 c1cc2c3C[C@H](O)[C@H](C=Cc3cc3c2c2c1cc(cc2cc3)[N+](O-)=O)O) 2.730	*270 c1cc2c3C[C@H](O)[C@H](C=Cc3cc3c2c2c1cc(cc2cc3)[N+](O-)=O)O) 2.730
*271 c12cccc2cc2c3c1ccc1cc(cc(cc2)c31)[N+](O-)=O 3.240	-271 c12cccc2cc2c3c1ccc1cc(cc(cc2)c31)[N+](O-)=O 3.240
-272 o1c2c(c3c1ccc(c3)[N+](O-)=O)cc(cc2)[N+](O-)=O 2.370	-272 o1c2c(c3c1ccc(c3)[N+](O-)=O)cc(cc2)[N+](O-)=O 2.370
#273 o1c2c(c3c1ccc(c3)[N+](O-)=O)cc2 -0.370	-273 o1c2c(c3c1ccc(c3)[N+](O-)=O)cc2 -0.370
#274 o1c2ccc(cc2c2c1cccc2)[N+](O-)=O 1.780	-274 o1c2ccc(cc2c2c1cccc2)[N+](O-)=O 1.780
*275 o1c2c(c3c1cccc3[N+](O-)=O)cccc2 1.100	#275 o1c2c(c3c1cccc3[N+](O-)=O)cccc2 1.100
+276 o1c2c(c3c1cc(cc3)[N+](O-)=O)ccc(c2)[N+](O-)=O 2.360	*276 o1c2c(c3c1cc(cc3)[N+](O-)=O)ccc(c2)[N+](O-)=O 2.360
-277 C1c2ccc([N+](O-)=O)cc2c2cccc12 0.870	-277 C1c2ccc([N+](O-)=O)cc2c2cccc12 0.870
+278 C1(=O)c2c(c3c1cc([N+](O-)=O)O-)[N+](O-)=O)ccc2 2.490	*278 C1(=O)c2c(c3c1cc([N+](O-)=O)O-)[N+](O-)=O)ccc2 2.490
#279 c12ccc(cc2c2c(c(o1)=O)cccc2)[N+](O-)=O 1.150	+279 c12ccc(cc2c2c(c(o1)=O)cccc2)[N+](O-)=O 1.150
*280 c12sc3c(c2cc(cc1)[N+](O-)=O)cccc3 2.440	+280 c12sc3c(c2cc(cc1)[N+](O-)=O)cccc3 2.440
-281 c12cc(ccc1c1c(s2)cccc1)[N+](O-)=O 2.660	+281 c12cc(ccc1c1c(s2)cccc1)[N+](O-)=O 2.660
*282 c12oc(c3c(c2ccc(c1)[N+](O-)=O)O-)[N+](O-)=O)cccc3=O 1.490	#282 c12oc(c3c(c2ccc(c1)[N+](O-)=O)O-)[N+](O-)=O)cccc3=O 1.490
-283 c1c2c(ccc1[N+](O-)=O)O-)[N+](O-)=O)cccc3CCCCc3c1CC2 -1.200	-283 c1c2c(ccc1[N+](O-)=O)O-)[N+](O-)=O)cccc3CCCCc3c1CC2 -1.200
-284 c12c(cc3CCc4c5c(ccc4)[N+](O-)=O)O-)[N+](O-)=O)CCCCc3CCCC2 0.600	+284 c12c(cc3CCc4c5c(ccc4)[N+](O-)=O)O-)[N+](O-)=O)CCCCc3CCCC2 0.600
#285 c12ccc(cc2CCc2cc3CCCCc3cc12)[N+](O-)=O 0.240	*285 c12ccc(cc2CCc2cc3CCCCc3cc12)[N+](O-)=O 0.240
+286 Nc1ccc(c(c1)[N+](O-)=O)O-)[N+](O-)=O)ccc1 2.510	-286 Nc1ccc(c(c1)[N+](O-)=O)O-)[N+](O-)=O)ccc1 2.510
-287 Nc1c([N+](O-)=O)O-)[N+](O-)=O)ccc(N)cc2cc1 2.560	+287 Nc1c([N+](O-)=O)O-)[N+](O-)=O)ccc(N)cc2cc1 2.560
-288 Nc1ccc(cc1[N+](O-)=O)O-)[N+](O-)=O)O-)[N+](O-)=O)N 2.490	*288 Nc1ccc(cc1[N+](O-)=O)O-)[N+](O-)=O)O-)[N+](O-)=O)N 2.490
+289 c12c3c(ccc2cc(cc1)[N+](O-)=O)O-)[N+](O-)=O)ccc2c1cccc2c3 2.740	-289 c12c3c(ccc2cc(cc1)[N+](O-)=O)O-)[N+](O-)=O)ccc2c1cccc2c3 2.740
*290 c12ccc(cc2CCc2cc3c4c(Cc3cc12)cccc4)[N+](O-)=O 2.790	#290 c12ccc(cc2CCc2cc3c4c(Cc3cc12)cccc4)[N+](O-)=O 2.790
+291 c1(ccc([N](O-)=O)O)c(c1)Cl)c1ccc([N](O-)=O)O)c(c1)Cl 1.950	-291 c1(ccc([N](O-)=O)O)c(c1)Cl)c1ccc([N](O-)=O)O)c(c1)Cl 1.950
#292 c1(ccc(N)c(c1)Cl)c1ccc([N](O-)=O)O)c(c1)Cl 1.900	-292 c1(ccc(N)c(c1)Cl)c1ccc([N](O-)=O)O)c(c1)Cl 1.900
+293 c1(cc(Cl)c(NC(C)=O)cc1)c1ccc(Cl)c([N](O-)=O)O)cc1 2.660	+293 c1(cc(Cl)c(NC(C)=O)cc1)c1ccc(Cl)c([N](O-)=O)O)cc1 2.660
+294 c1(cc(Cl)c(N)c(c1)[N](O-)=O)O)c1ccc([N](O-)=O)O)c(c1)Cl 4.820	*294 c1(cc(Cl)c(N)c(c1)[N](O-)=O)O)c1ccc([N](O-)=O)O)c(c1)Cl 4.820
#295 c1(ccc2c3c1ccc1c(ccc(c31)c1c2cccc1)[N](O-)=O)[N](O-)=O 5.450	#295 c1(ccc2c3c1ccc1c(ccc(c31)c1c2cccc1)[N](O-)=O)[N](O-)=O 5.450

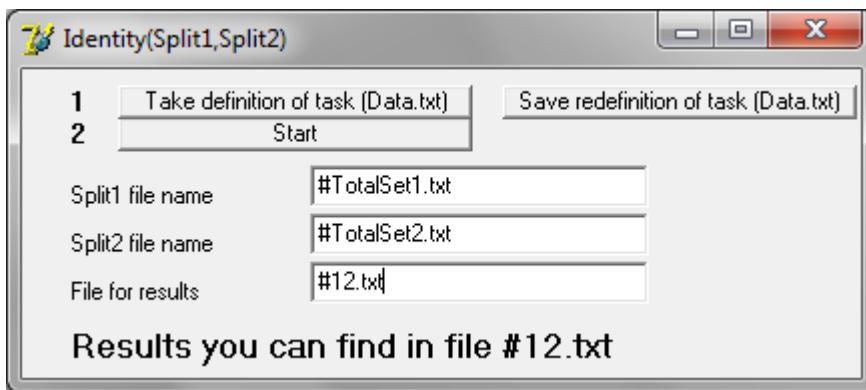
Run MeasureOfIdentityOfTwoSplits.exe  
You will see the following



Click button “Take definition of task”



Click button “start”



File 12.txt contains

```
First split is taken from file #TotalSet1.txt
Second split is taken from file #TotalSet2.txt

      : First   : Second   : Naverage : Identical: Identical %
Total set :      295:      295:      295:      85:   28.8
Training set :      72:      76:      74.00:      20:   27.0
Invisible training set :      74:      71:      72.50:      16:   22.1
Calibration set :      74:      74:      74.00:      23:   31.1
Validation set :      75:      74:      74.50:      26:   34.9

The column "first": how many compounds in the training set,
in the invisible training set, in the calibration set
and in the validation set, for the first split

The column "second": how many compounds in the training set,
in the invisible training set, in the calibration set
and in the validation set, for the second split

The column "Naverage" means  $(N1+N2) / 2$ ,
where N1 and N2 are the number of compounds which are distributed into X,
for split 1 and split 2; X can be (i) training set; (ii) invisible training set;
(iii) calibration set; and (iv) validation set.

The column "Identical" contains the numbers of compounds which are distributed
into the same set (i.e. training set; ..., validation set) for split 1 and split 2.

The column "Identical (%)" contains the percentage of compounds which are distributed
into the same set (i.e. training set; ..., validation set) for split 1 and split 2.
```

The same operations you can carry out with your splits placed in files with the similar files

#TotalSet1.txt

#TotalSet2.txt

#TotalSet3.txt

...

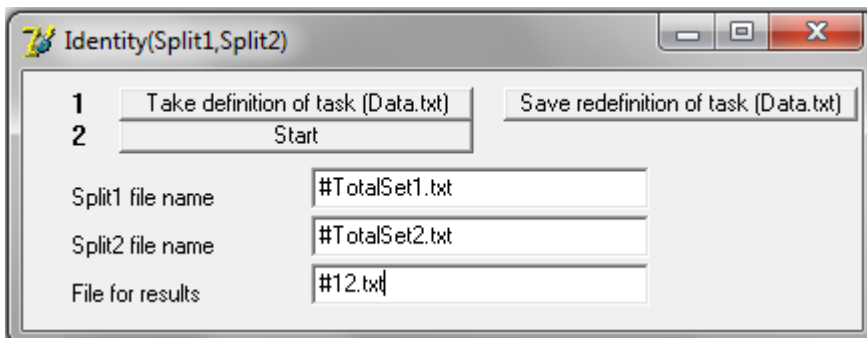
#TotalSet9.txt

#TotalSet10.txt

...

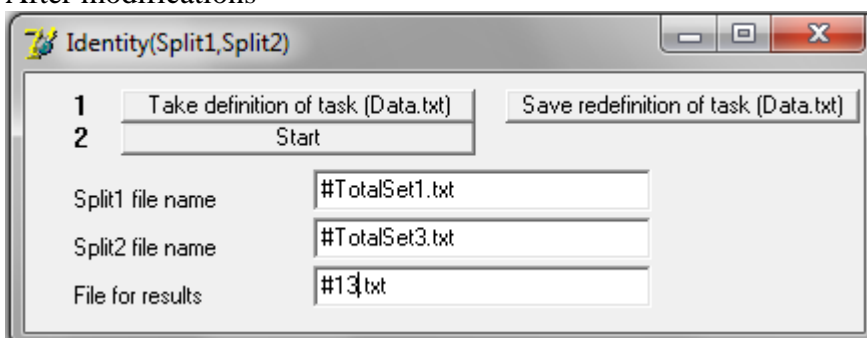
In order to compare #TotalSet1.txt and #TotalSet3.txt you can before click “Start” change status

Before modifications



The screenshot shows a window titled "Identity(Split1, Split2)". It contains two numbered steps: 1. "Take definition of task (Data.txt)" and 2. "Start". To the right of step 2 is a button labeled "Save redefinition of task (Data.txt)". Below the steps are three text input fields: "Split1 file name" with the value "#TotalSet1.txt", "Split2 file name" with the value "#TotalSet2.txt", and "File for results" with the value "#12.txt".

After modifications



The screenshot shows the same window "Identity(Split1, Split2)" after modifications. The "Split2 file name" field now contains "#TotalSet3.txt" and the "File for results" field now contains "#13.txt". The other elements, including the "Start" button and the "Save redefinition of task (Data.txt)" button, remain the same.

If you would like to use other names of the files, you can save these using buttons “Save redefinition of task”.

Pay attention, these files should be placed in the folder where you have placed program “MeasureOfIdentityOfTwoSplits.exe”.