Sample File: NCTRER, truncated to 3 records:

```
 20 22  0  0  0  0  0  0  0  0  1 V2000
    5.3203   -2.3043    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.9874   -2.3043    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.3209   -3.4565    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.9880   -3.4565    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.3329   -2.3043    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.9880   -1.1522    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.3209   -1.1522    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.9874    0.0000    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.0000   -2.3043    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.9874   -4.6086    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    5.3203   -4.6086    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.9754   -3.4565    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    7.3083   -3.4565    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    7.9748   -2.3043    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.3077   -2.3043    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.9628   -3.4565    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.3077   -4.6086    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    7.9748   -4.6086    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.2957   -3.4565    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    5.9754   -1.1522    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  1 12  1  0  0  0  0
  1 20  2  0  0  0  0
  2  3  2  0  0  0  0
  2  7  1  0  0  0  0
  3  4  1  0  0  0  0
  3 10  1  0  0  0  0
  4  5  2  0  0  0  0
  5  6  1  0  0  0  0
  5  9  1  0  0  0  0
  6  7  2  0  0  0  0
  7  8  1  0  0  0  0
 10 11  1  0  0  0  0
 11 12  2  0  0  0  0
 12 13  1  0  0  0  0
 13 14  1  0  0  0  0
 13 18  2  0  0  0  0
 14 15  2  0  0  0  0
 15 16  1  0  0  0  0
 16 17  2  0  0  0  0
 16 19  1  0  0  0  0
 17 18  1  0  0  0  0
M  END
>  <DSSTox_RID>
22308

>  <DSSTox_CID>
2308

>  <DSSTox_Generic_SID>
22308
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> <DSSTox_FileID>
1_NCTRER_v4a

> <STRUCTURE_Formula>
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> <STRUCTURE_MolecularWeight>
270.2369

> <STRUCTURE_ChemicalType>
defined organic

> <STRUCTURE_TestedForm_DefinedOrganic>
parent

> <STRUCTURE_Shown>
tested chemical

> <TestSubstance_ChemicalName>
genistein

> <TestSubstance_CASRN>
446-72-0

> <TestSubstance_Description>
single chemical compound

> <ChemicalNote>
blank

> <STRUCTURE_ChemicalName_IUPAC>
5,7-dihydroxy-3-(4-hydroxyphenyl)-4H-chromen-4-one

> <STRUCTURE_SMILES>
O=C(C(C(C=C3)=CC=C3O)=CO2)C1=C2C=C(O)C=C1O

> <STRUCTURE_Parent_SMILES>
O=C(C(C(C=C3)=CC=C3O)=CO2)C1=C2C=C(O)C=C1O

> <STRUCTURE_InChI>
InChI=1/C15H10O5/c16-9-3-1-8(2-4-9)11-7-20-13-6-10(17)5-12(18)14(13)15(11)19/h1-7,16-18H

> <StudyType>
Receptor Binding

> <Endpoint>
Estrogen Receptor Relative Binding Affinity

> <Species>
rat

> <ChemClass_ERB>
Phytoestrogens Isoflavones

> <ER_RBA>
0.436

> <LOG_ER_RBA>
-0.36

> <ActivityCategory_ER_RBA>
active medium

> <Mean_ER_RBA_ChemClass>
0.019

> <ActivityCategory_Rationale_ChemClass_ERB>
Isoflavones are relatively weak binders, RBA optimized when OH groups in 7,4' positions approx correspond to 4,4' OH positions in DES, a more frequent coincidence than in flavones and flavanones.

> <F1_Ring>
1

> <F2_AromaticRing>
1

> <F3_PhenolicRing>
1

> <F4_Heteroatom>
0

> <F5_Phenol3nPhenyl>
1

> <F6_OtherKeyFeatures>
0

> <LOGP>
2.84

> <Note_NCTRER>
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 18 20 0 0 1 0 0 0 0 0 1 V2000
    7.9737   -2.3040   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    7.3073   -3.4560   0.0000 O   0 0 0 0 0 0 0 0 0 0 0 0
    5.9746   -3.4560   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    5.3196   -2.3040   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    5.9746   -1.1520   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    7.3073   -1.1520   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    7.9737   0.0000   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    9.3064   0.0000   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    9.9615   -1.1520   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    9.3064   -2.3040   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
   11.2942   -1.1520   0.0000 O   0 0 0 0 0 0 0 0 0 0 0 0
    3.9868   -2.3040   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    3.3205   -3.4560   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0

```
    1.9878   -3.4560    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.3327   -2.3040    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.9878   -1.1520    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.3205   -1.1520    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.0000   -2.3040    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  1  6  2  0  0  0  0
  1 10  1  0  0  0  0
  2  3  1  0  0  0  0
  3  4  1  0  0  0  0
  4  5  1  0  0  0  0
  4 12  1  6  0  0  0
  5  6  1  0  0  0  0
  6  7  1  0  0  0  0
  7  8  2  0  0  0  0
  8  9  1  0  0  0  0
  9 10  2  0  0  0  0
  9 11  1  0  0  0  0
 12 13  2  0  0  0  0
 12 17  1  0  0  0  0
 13 14  1  0  0  0  0
 14 15  2  0  0  0  0
 15 16  1  0  0  0  0
 15 18  1  0  0  0  0
 16 17  2  0  0  0  0
M  END
>  <DSSTox_RID>
22309

>  <DSSTox_CID>
2309

>  <DSSTox_Generic_SID>
22309

>  <DSSTox_FileID>
2_NCTRER_v4a

>  <STRUCTURE_Formula>
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>  <STRUCTURE_MolecularWeight>
242.2699

>  <STRUCTURE_ChemicalType>
defined organic

>  <STRUCTURE_TestedForm_DefinedOrganic>
parent

>  <STRUCTURE_Shown>
tested chemical

>  <TestSubstance_ChemicalName>
equol

>  <TestSubstance_CASRN>
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531-95-3

> <TestSubstance_Description>
single chemical compound

> <ChemicalNote>
stereochem

> <STRUCTURE_ChemicalName_IUPAC>
(3S)-3-(4-hydroxyphenyl)chroman-7-ol

> <STRUCTURE_SMILES>
Oc1ccc(cc1)[C@@H]2Cc3ccc(O)cc3OC2

> <STRUCTURE_Parent_SMILES>
Oc1ccc(cc1)[C@@H]2Cc3ccc(O)cc3OC2

> <STRUCTURE_InChI>
InChI=1/C15H14O3/c16-13-4-1-10(2-5-13)12-7-11-3-6-14(17)8-15(11)18-9-12/h1-6,8,12,16-17H,7,9H2/t12-/m1/s1

> <StudyType>
Receptor Binding

> <Endpoint>
Estrogen Receptor Relative Binding Affinity

> <Species>
rat

> <ChemClass_ERB>
Phytoestrogens Isoflavones

> <ER_RBA>
0.151

> <LOG_ER_RBA>
-0.82

> <ActivityCategory_ER_RBA>
active medium

> <Mean_ER_RBA_ChemClass>
0.019

> <ActivityCategory_Rationale_ChemClass_ERB>
Isoflavones are relatively weak binders, RBA optimized when OH groups in 7,4' positions approx correspond to 4,4' OH positions in DES, a more frequent coincidence than in flavones and flavanones.

> <F1_Ring>
1

> <F2_AromaticRing>
1

> <F3_PhenolicRing>

1

> <F4_Heteroatom>
0

> <F5_Phenol3nPhenyl>
1

> <F6_OtherKeyFeatures>
0

> <LOGP>
3.67

$$$$

 19 21 0 0 0 0 0 0 0 0 1 V2000
    5.3205   -2.3044   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    5.9756   -1.1522   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    7.3086   -1.1522   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    7.9751   0.0000   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    9.3080   0.0000   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    9.9632   -1.1522   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    9.3080   -2.3044   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    7.9751   -2.3044   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    7.3086   -3.4566   0.0000 O   0 0 0 0 0 0 0 0 0 0 0 0
    5.9756   -3.4566   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
   11.2961   -1.1522   0.0000 O   0 0 0 0 0 0 0 0 0 0 0 0
    5.3205   0.0000   0.0000 O   0 0 0 0 0 0 0 0 0 0 0 0
    3.9875   -2.3044   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    3.3211   -3.4566   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    1.9881   -3.4566   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    1.3329   -2.3044   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    1.9881   -1.1522   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    3.3211   -1.1522   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 0
    0.0000   -2.3044   0.0000 O   0 0 0 0 0 0 0 0 0 0 0 0
  1 2 1 0 0 0 0
  1 10 2 0 0 0 0
  1 13 1 0 0 0 0
  2 3 1 0 0 0 0
  2 12 2 0 0 0 0
  3 4 1 0 0 0 0
  3 8 2 0 0 0 0
  4 5 2 0 0 0 0
  5 6 1 0 0 0 0
  6 7 2 0 0 0 0
  6 11 1 0 0 0 0
  7 8 1 0 0 0 0
  8 9 1 0 0 0 0
  9 10 1 0 0 0 0
 13 14 2 0 0 0 0
 13 18 1 0 0 0 0
 14 15 1 0 0 0 0
 15 16 2 0 0 0 0
 16 17 1 0 0 0 0

```
 16 19  1  0  0  0  0
 17 18  2  0  0  0  0
M  END
>  <DSSTox_RID>
22310

>  <DSSTox_CID>
2310

>  <DSSTox_Generic_SID>
22310

>  <DSSTox_FileID>
3_NCTRER_v4a

>  <STRUCTURE_Formula>
C15H10O4

>  <STRUCTURE_MolecularWeight>
254.2375

>  <STRUCTURE_ChemicalType>
defined organic

>  <STRUCTURE_TestedForm_DefinedOrganic>
parent

>  <STRUCTURE_Shown>
tested chemical

>  <TestSubstance_ChemicalName>
daidzein

>  <TestSubstance_CASRN>
486-66-8

>  <TestSubstance_Description>
single chemical compound

>  <STRUCTURE_ChemicalName_IUPAC>
7-hydroxy-3-(4-hydroxyphenyl)-4H-chromen-4-one

>  <STRUCTURE_SMILES>
O=C1C(C3=CC=C(O)C=C3)=COC2=C1C=CC(O)=C2

>  <STRUCTURE_Parent_SMILES>
O=C1C(C3=CC=C(O)C=C3)=COC2=C1C=CC(O)=C2

>  <STRUCTURE_InChI>
InChI=1/C15H10O4/c16-10-3-1-9(2-4-10)13-8-19-14-7-11(17)5-6-12(14)15(13)18/h1-
8,16-17H

>  <StudyType>
Receptor Binding

>  <Endpoint>
Estrogen Receptor Relative Binding Affinity
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> <Species>
rat

> <ChemClass_ERB>
Phytoestrogens Isoflavones

> <ER_RBA>
0.022

> <LOG_ER_RBA>
-1.65

> <ActivityCategory_ER_RBA>
active medium

> <Mean_ER_RBA_ChemClass>
0.019

> <ActivityCategory_Rationale_ChemClass_ERB>
Isoflavones are relatively weak binders, RBA optimized when OH groups in 7,4' positions approx correspond to 4,4' OH positions in DES, a more frequent coincidence than in flavones and flavanones.

> <F1_Ring>
1

> <F2_AromaticRing>
1

> <F3_PhenolicRing>
1

> <F4_Heteroatom>
0

> <F5_Phenol3nPhenyl>
1

> <F6_OtherKeyFeatures>
0

> <LOGP>
2.55

$$$$