

## Supplementary Material

To refine thiostrepton aspherical scattering factors from the invariom database were used. The data to parameter ratio did not increase with respect to a refinement with the independent atom model (IAM). A substantial number of model compounds were used (see Table 3). Several new model compounds were calculated and included in the database, since they were missing prior to refinement. In case the calculation of new model compounds that provide invarioms is necessary, a systematic analysis of the chemical environments of each particular atom is recommended in order to avoid time-consuming quantum chemical calculations.

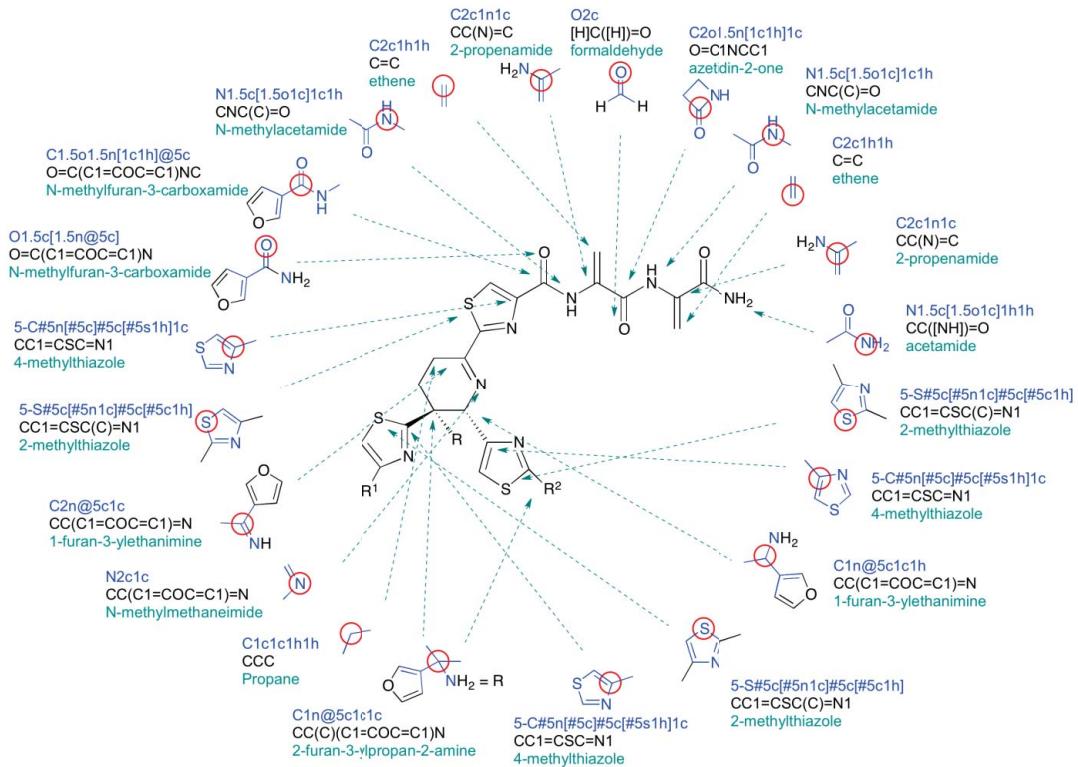


Fig. S1. Holstein plot for the dehydroalanine tail region of thiostrepton. Remaining parts of the molecule are marked with the letter R (for rest). Invariom names, including next-nearest neighbors in parentheses, are given in blue, IUPAC nomenclature in green and letters in black color contain the SMILES name for each invariom model compound used. Arrows point to the specific region of the molecule and the red circle surrounds the atom of interest.

Holstein plots are useful to illustrate how to select the most suited (smallest) model compounds for a particular chemical environment. Such plots show the main molecular structure surrounded by the respective model compounds (Figure 8). These compounds provide the electron density distribution that is converted to scattering factors of the invariom database.

Table 3: Aspherical atomic scattering factors used for invariom refinement of thiostrepton. Invariom names and corresponding model compounds from the invariom database are listed for all atoms together with respective IUPAC names, sorted by atomic number.

<b>Atom</b>	<b>Invariom Name</b>	<b>Model Compound</b>
S(21Z3)	5-S#5c[#5n1c]#5c[#5c1h]	2-methylthiazole
S(21Z3_-)	5-S#5c[#5n1c]#5c[#5c1h]	2-methylthiazole
S(23X6)	S1c1c	dimethylsulfide
S(25Z3)	5-S#5c[#5n1c]#5c[#5c1h]	2-methylthiazole
S(26X3)	5-S#5c[#5n1c]#5c[#5c1h]	2-methylthiazole
S(26X3_-)	5-S#5c[#5n1c]#5c[#5c1h]	2-methylthiazole
S(33Z3)	5-S#5c[#5n1c]#5c[#5c1h]	2-methylthiazole
S(33Z3_-)	5-S#5c[#5n1c]#5c[#5c1h]	2-methylthiazole
S(01Z3)	5-S#5c[#5n1c]#5c[#5c1h]	2-methylthiazole
S(03X6)	S1c1c	dimethylsulfide
S(05Z3)	5-S#5c[#5n1c]#5c[#5c1h]	2-methylthiazole
S(06X3)	5-S#5c[#5n1c]#5c[#5c1h]	2-methylthiazole
S(06X3_-)	5-S#5c[#5n1c]#5c[#5c1h]	2-methylthiazole
S(13Z3)	5-S#5c[#5n1c]#5c[#5c1h]	2-methylthiazole
S(13Z3_-)	5-S#5c[#5n1c]#5c[#5c1h]	2-methylthiazole
O(21Z7)	O1.5c[1.5n@5c]	furan-3-carboxamide
O(21Z7_-)	O1.5c[1.5n@5c]	furan-3-carboxamide
O(22TG1)	O1c1h	methanol
O(22T)	O1.5c[1.5n1c]	acetamide
O(23X7)	O1.5c[1.5n1c]	acetamide
O(24X7)	O1c1h	methanol
O(24X4)	O1c1h	methanol
O(25Z7)	O1.5c[1.5n@5c]	furan-3-carboxamide
O(26X10)	O1c1c	dimethylether
O(27J12)	O2c	formaldehyde
O(27J16)	O1c1h	methanol
O(27J15)	O1c1h	methanol
O(28I)	O1.5c[1.5n1c]	acetamide
O(29A)	O1.5c[1.5n1c]	acetamide
O(30U)	O1.5c[1.5n1c]	acetamide
O(31A)	O1.5c[1.5n1c]	acetamide
O(33Z7)	O1.5c[1.5n@5c]	furan-3-carboxamide

<b>Atom</b>	<b>Invariom Name</b>	<b>Model Compound</b>
O(33Z7_)	O1.5c[1.5n@5c]	furan-3-carboxamide
O(34U)	O2c	formaldehyde
O(34U_)	O2c	formaldehyde
O(35PYT)	O1.5c[1.5n1c]	acetamide
O(35PYT_)	O1.5c[1.5n1c]	acetamide
O(01Z7)	O1.5c[1.5n@5c]	furan-3-carboxamide
O(02TG1)	O1c1h	methanol
O(02T)	O1.5c[1.5n1c]	acetamide
O(03X7)	O1.5c[1.5n1c]	acetamide
O(04X7)	O1c1h	methanol
O(04X4)	O1c1h	methanol
O(05Z7)	O1.5c[1.5n@5c]	furan-3-carboxamide
O(06X10)	O1c1c	dimethylether
O(06X1_)	O1c1c	dimethylether
O(07J12)	O2c	formaldehyde
O(07J15)	O1c1h	methanol
O(07J16)	O1c1h	methanol
O(08I)	O1.5c[1.5n1c]	acetamide
O(09A)	O1.5c[1.5n1c]	acetamide
O(10U)	O1.5c[1.5n1c]	acetamide
O(11A)	O1.5c[1.5n1c]	acetamide
O(13Z7)	O1.5c[1.5n@5c]	furan-3-carboxamide
O(13Z7_)	O1.5c[1.5n@5c]	furan-3-carboxamide
O(14U)	O2c	formaldehyde
O(14U_)	O2c	formaldehyde
O(15PYT)	O1.5c[1.5n1c]	acetamide
O(15PYT_)	O1.5c[1.5n1c]	acetamide
O(40O1)	O1.5c[1.5n1h]	N,N-dimethylformamid
O(41O1)	O2c	formaldehyde
O(42O1)	O1.5c[1.5n1h]	N,N-dimethylformamid
O(42O1_)	O1.5c[1.5n1h]	N,N-dimethylformamid
O(43O1)	O1.5c[1.5n1h]	N,N-dimethylformamid
O(43O1_)	O1.5c[1.5n1h]	N,N-dimethylformamid
O(44O1)	O1.5c[1.5n1h]	N,N-dimethylformamid
O(45O1)	O2c	formaldehyde
O(45O1_)	O2c	formaldehyde
O(47O1)	O1.5c[1.5n1h]	N,N-dimethylformamid
O(49O1)	O2c	formaldehyde
O(49O1_)	O2c	formaldehyde
O(50O10)	O1c1c	dimethylether
O(51O1)	O1c1c	dimethylether
O(52O12)	O1c1c	dimethylether
O(53O1)	O1c1c	dimethylether
O(53O10)	O1c1c	dimethylether
O(55O1)	O1c1c	dimethylether
O(54O1)	O1c1c	dimethylether

Atom	Invariom Name	Model Compound
O(60O1)	O1h1h	water
O(60O2)	O1h1h	water
N(21Z1)	5-N#5c[#5s1c]#5c[#5c1c]	2,4-dimethylthiazole
N(21Z1_)	5-N#5c[#5s1c]#5c[#5c1c]	2,4-dimethylthiazole
N(22T)	N1.5c[1.5o@5c]1c1h	N-methylfuran-3-carboxamide
N(23X)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(23X1)	N2c1c	N-methylmethaneimide
N(24X1)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(25Z1)	5-N#5c[#5s1c]#5c[#5c1c]	2,4-dimethylthiazole
N(26X7)	N1.5c[1.5o@5c]1c1h	N-methylfuran-3-carboxamide
N(26X1)	5-N#5c[#5s1c]#5c[#5c1c]	2,4-dimethylthiazole
N(26X1_)	5-N#5c[#5s1c]#5c[#5c1c]	2,4-dimethylthiazole
N(27J1)	6-N#6c[#6c1c]#6c[#6c1c]	2,6-dimethylpyridine
N(28I)	N1c1c1h	dimethylamine
N(29A9)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(30U)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(31A)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(32#7)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(32#1)	N2c1c	N-methylmethaneimide
N(32#1_)	N2c1c	N-methylmethaneimide
N(32#7_)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(33Z1)	5-N#5c[#5s1c]#5c[#5c1c]	2,4-dimethylthiazole
N(33Z1_)	5-N#5c[#5s1c]#5c[#5c1c]	2,4-dimethylthiazole
N(34U1)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(34U1_)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(35PYT)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(35PATT)	N1.5c[1.5o1c]1h1h	acetamide
N(35PYT_)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(35PBTT)	N1.5c[1.5o1c]1h1h	acetamide
N(01Z1)	5-N#5c[#5s1c]#5c[#5c1c]	2,4-dimethylthiazole
N(02T)	N1.5c[1.5o@5c]1c1h	N-methylfuran-3-carboxamide
N(03X)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(03X1)	N2c1c	N-methylmethaneimide
N(04X1)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(05Z1)	5-N#5c[#5s1c]#5c[#5c1c]	2,4-dimethylthiazole
N(06X7)	N1.5c[1.5o@5c]1c1h	N-methylfuran-3-carboxamide
N(06X1)	5-N#5c[#5s1c]#5c[#5c1c]	2,4-dimethylthiazole
N(06X7_)	N1.5c[1.5o@5c]1c1h	N-methylfuran-3-carboxamide
N(06X1_)	5-N#5c[#5s1c]#5c[#5c1c]	2,4-dimethylthiazole
N(07J1)	6-N#6c[#6c1c]#6c[#6c1c]	2,6-dimethylpyridine
N(08I)	N1c1c1h	dimethylamine
N(09A)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(10U)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(11A)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(12#7)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(12#1)	N2c1c	N-methylmethaneimide

Atom	Invariom Name	Model Compound
N(12#7_)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(12#1_)	N2c1c	N-methylmethaneimide
N(13Z1)	5-N#5c[#5s1c]#5c[#5c1c]	2,4-dimethylthiazole
N(13Z1_)	5-N#5c[#5s1c]#5c[#5c1c]	2,4-dimethylthiazole
N(14U)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(14U_)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(15PYT)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(15PATT)	N1.5c[1.5o1c]1h1h	acetamide
N(15PYT_)	N1.5c[1.5o1c]1c1h	N-methylacetamide
N(15PBTT)	N1.5c[1.5o1c]1h1h	acetamide
N(40O1)	N1.5c[1.5o1h]1c1c	N,N-dimethylformamid
N(41O1)	N1.5c[1.5o1h]1c1c	N,N-dimethylformamid
N(42O1)	N1.5c[1.5o1h]1c1c	N,N-dimethylformamid
N(42O1_)	N1.5c[1.5o1h]1c1c	N,N-dimethylformamid
N(43O1)	N1.5c[1.5o1h]1c1c	N,N-dimethylformamid
N(43O1_)	N1.5c[1.5o1h]1c1c	N,N-dimethylformamid
N(44O1)	N1.5c[1.5o1h]1c1c	N,N-dimethylformamid
N(45O1)	N1.5c[1.5o1h]1c1c	N,N-dimethylformamid
N(45O1_)	N1.5c[1.5o1h]1c1c	N,N-dimethylformamid
N(47O1)	N1.5c[1.5o1h]1c1c	N,N-dimethylformamid
N(49O1)	N1.5c[1.5o1h]1c1c	N,N-dimethylformamid
N(49O1_)	N1.5c[1.5o1h]1c1c	N,N-dimethylformamid
C(21Z2)	5-C#5s[#5c]#5n[#5c]1c	2-methylthiazole
C(21Z4)	5-C#5s[#5c]#5c[#5n1c]1h	4-methylthiazole
C(21Z5)	5-C#5n[#5c]#5c[#5s1h]1c	4-methylthiazole
C(21Z6)	C1.5o1.5n[1c1h]@5c	N-methylfuran-3-carboxamide
C(21Z2_)	5-C#5s[#5c]#5n[#5c]1c	2-methylthiazole
C(21Z4_)	5-C#5s[#5c]#5c[#5n1c]1h	4-methylthiazole
C(21Z5_)	5-C#5n[#5c]#5c[#5s1h]1c	4-methylthiazole
C(21Z6_)	C1.5o1.5n[1c1h]@5c	N-methylfuran-3-carboxamide
C(22TG2)	C1c1h1h1h	ethane
C(22TB)	C1o1c1c1h	2-propanol
C(22TA)	C1n1c1c1h	2-aminopropane
C(22T)	C1.5o1.5n[1c1h]1c	N-methylacetamide
C(23X41)	C1c1h1h1h	ethane
C(23X31)	C2c1c1h	propene
C(23X21)	C2c1n1c	2-propenamide
C(23X2)	C2n1s[1c]1c	methyleneethanethioimidate
C(23X4)	C1s[1c]1c1h1h	ethylmethylsulfane
C(23X5)	C1n1c1c1h	2-aminopropane
C(23X6)	C1.5o1.5n[1c1h]1c	N-methylacetamide
C(24X8)	C1c1h1h1h	ethane
C(24X6)	C1o1c1c1h	2-propanol
C(24X5)	C1c1h1h1h	ethane
C(24X3)	C1o1c1c1c	isobutanol
C(24X2)	C1n@5c1c1h	1-furan-3-ylethanamine

Atom	Invariom Name	Model Compound
C(25Z2)	5-C#[5s[#5c]#5n[#5c]1c	2-methylthiazole
C(25Z4)	5-C#[5s[#5c]#5c[#5n1c]1h	4-methylthiazole
C(25Z5)	5-C#5n[#5c]#5c[#5s1h]1c	4-methylthiazole
C(25Z6)	C1.5o1.5n[1c1h]@5c	N-methylfuran-3-carboxamide
C(26X4)	5-C#[5s[#5c]#5c[#5n1c]1h	4-methylthiazole
C(26X5)	5-C#5n[#5c]#5c[#5s1h]1c	4-methylthiazole
C(26X2)	5-C#[5s[#5c]#5n[#5c]1c	2-methylthiazole
C(26X6)	C1n@5c1c1h	1-furan-3-ylethanamine
C(26X9)	C1c1h1h1h	ethane
C(26X8)	C1o1c1c1h	2-propanol
C(26X5_)	5-C#5n[#5c]#5c[#5s1h]1c	4-methylthiazole
C(26X4_)	5-C#[5s[#5c]#5c[#5n1c]1h	4-methylthiazole
C(26X2_)	5-C#[5s[#5c]#5n[#5c]1c	2-methylthiazole
C(27J11)	C2o1o@6c	benzoic acid
C(27J14)	C1c1h1h1h	ethane
C(27J13)	C1o@6c1c1h	<i>S</i> -1-phenylethanol
C(27J2A)	6-C#[6c[#6c1c]#6c[#6c1h]1c	1,2-dimethylbenzene
C(27J3)	6-C#[6c[#6n1c]#6c[#6c1c]1h	2,4-dimethylpyridine
C(27J2)	6-C#6n[#6c]#6c[#6c1h]1c	2-methylpyridine
C(27J9)	6-C#6n[#6c]#6c[#6c1c]1c	2,3-dimethylpyridine
C(27J10)	6-C#[6n1c]#6c[#6c1c]1c	2,3,4-trimethylpyridine
C(27J5)	C2c@6c1h	styrene
C(27J6)	C2c1c1h	propene
C(27J8)	C1o@6c1c1h	<i>S</i> -1-phenylethanol
C(27J7)	C1n1c1c1h	2-aminopropane
C(28ID)	C1c1h1h1h	ethane
C(28IG1)	C1c1c1h1h	propane
C(28IG2)	C1c1h1h1h	ethane
C(28IB)	C1c1c1c1h	2-methylpropane
C(28IA)	C1n1c1c1h	2-aminopropane
C(28I)	C1.5o1.5n[1c1h]1c	N-methylacetamide
C(29AB)	C1c1h1h1h	ethane
C(29AA)	C1n1c1c1h	2-aminopropane
C(29A)	C1.5o1.5n[1c1h]1c	N-methylacetamide
C(30UB)	C2c1h1h	ethene
C(30UA)	C2c1n1c	2-propenamide
C(30U)	C1.5o1.5n[1c1h]1c	N-methylacetamide
C(31AB)	C1c1h1h1h	ethane
C(31AA)	C1n1c1c1h	2-aminopropane
C(31A)	C1.5o1.5n[1c1h]1c	N-methylacetamide
C(32#6)	C1n@5c1c1h	1-furan-3-ylethanamine
C(32#5)	C1n@5c1c1c	2-furan-3-ylpropan-2-amine
C(32#4)	C1c1c1h1h	propane
C(32#3)	C1c1c1h1h	propane
C(32#2)	C2n@5c1c	1-furan-3-ylethanimine
C(32#2_)	C2n@5c1c	1-furan-3-ylethanimine

Atom	Invariom Name	Model Compound
C(32#3_)	C1c1c1h1h	propane
C(32#4_)	C1c1c1h1h	propane
C(32#5_)	C1n@5c1c1c	2-furan-3-ylpropan-2-amine
C(32#6_)	C1n@5c1c1h	1-furan-3-ylethanamine
C(33Z2)	5-C#[5s][#5c]#5n[#5c]1c	2-methylthiazole
C(33Z5)	5-C#[5n][#5c]#5c[#5s1h]1c	4-methylthiazole
C(33Z6)	C1.5o1.5n[1c1h]@5c	N-methylfuran-3-carboxamide
C(33Z4)	5-C#[5s][#5c]#5c[#5n1c]1h	4-methylthiazole
C(33Z2_)	5-C#[5s][#5c]#5n[#5c]1c	2-methylthiazole
C(33Z5_)	5-C#[5n][#5c]#5c[#5s1h]1c	4-methylthiazole
C(33Z6_)	C1.5o1.5n[1c1h]@5c	N-methylfuran-3-carboxamide
C(33Z4_)	5-C#[5s][#5c]#5c[#5n1c]1h	4-methylthiazole
C(34UA)	C2c1n1c	2-propenamide
C(34UB)	C2c1h1h	ethene
C(34U)	C2o1.5n[1c1h]1c	azetidin-2-one
C(34UA_)	C2c1n1c	2-propenamide
C(34UB_)	C2c1h1h	ethene
C(34U_)	C1.5o1.5n[1c1h]1c	N-methylacetamide
C(35PYTA)	C2c1n1c	2-propenamide
C(35PYTB)	C2c1h1h	ethene
C(35PYT)	C1.5o1.5n[1h1h]1c	acetamide
C(35PATA)	C2c1n1c	2-propenamide
C(35PBTB)	C2c1h1h	ethene
C(35PYT_)	C1.5o1.5n[1h1h]1c	acetamide
C(01Z4)	5-C#[5s][#5c]#5c[#5n1c]1h	4-methylthiazole
C(01Z2)	5-C#[5s][#5c]#5n[#5c]1c	2-methylthiazole
C(01Z5)	5-C#[5n][#5c]#5c[#5s1h]1c	4-methylthiazole
C(01Z6)	C1.5o1.5n[1c1h]@5c	N-methylfuran-3-carboxamide
C(02TG2)	C1c1h1h1h	ethane
C(02TB)	C1o1c1c1h	2-propanol
C(02TA)	C1n1c1c1h	2-aminopropane
C(02T)	C1.5o1.5n[1c1h]1c	N-methylacetamide
C(03X41)	C1c1h1h1h	ethane
C(03X31)	C2c1c1h	propene
C(03X21)	C2c1n1c	2-propenamide
C(03X2)	C2n1s[1c]1c	methyleneethioimidate
C(03X4)	C1s[1c]1c1h1h	ethylmethylsulfane
C(03X5)	C1n1c1c1h	2-aminopropane
C(03X6)	C1.5o1.5n[1c1h]1c	N-methylacetamide
C(04X8)	C1c1h1h1h	ethane
C(04X6)	C1o1c1c1h	2-propanol
C(04X5)	C1c1h1h1h	ethane
C(04X3)	C1o1c1c1c	isobutanol
C(04X2)	C1n@5c1c1h	1-furan-3-ylethanamine
C(05Z2)	5-C#[5s][#5c]#5n[#5c]1c	2-methylthiazole
C(05Z5)	5-C#[5n][#5c]#5c[#5s1h]1c	4-methylthiazole

<b>Atom</b>	<b>Invariom Name</b>	<b>Model Compound</b>
C(05Z6)	C1.5o1.5n[1c1h]@5c	N-methylfuran-3-carboxamide
C(06X5)	5-C#[5s[#5c]#5c[#5n1c]1h	4-methylthiazole
C(06X4)	5-C#[5n[#5c]#5c[#5s1h]1c	4-methylthiazole
C(06X2)	5-C#[5s[#5c]#5n[#5c]1c	2-methylthiazole
C(06X6)	C1n@5c1c1h	1-furan-3-ylethanamine
C(06X9)	C1c1h1h1h	ethane
C(06X8)	C1o1c1c1h	2-propanol
C(06X4_)	5-C#[5n[#5c]#5c[#5s1h]1c	4-methylthiazole
C(06X2_)	5-C#[5s[#5c]#5n[#5c]1c	2-methylthiazole
C(06X6_)	C1n@5c1c1h	1-furan-3-ylethanamine
C(06X5_)	5-C#[5n[#5c]#5c[#5s1h]1c	4-methylthiazole
C(06X8_)	C1o1c1c1h	2-propanol
C(06X9_)	C1c1h1h1h	ethane
C(05Z4)	5-C#[5s[#5c]#5c[#5n1c]1h	4-methylthiazole
C(07J11)	C2o1o@6c	benzoic acid
C(07J2)	6-C#[6n[#6c]#6c[#6c1h]1c	2-methylpyridine
C(07J3)	6-C#[6c[#6n1c]#6c[#6c1c]1h	2,4-dimethylpyridine
C(07J14)	C1c1h1h1h	ethane
C(07J13)	C1o@6c1c1h	S-1-phenylethanol
C(07J4)	6-C#[6c[#6c1c]#6c[#6c1h]1c	1,2-dimethylbenzene
C(07J6)	C2c1c1h	propene
C(07J5)	C2c@6c1h	styrene
C(07J10)	6-C#[6n1c]#6c[#6c1c]1c	2,3,4-trimethylpyridine
C(07J9)	6-C#[6n[#6c]#6c[#6c1c]1c	2,3-dimethylpyridine
C(07J8)	C1o@6c1c1h	S-1-phenylethanol
C(07J7)	C1n1c1c1h	2-aminopropane
C(08ID)	C1c1h1h1h	ethane
C(08IG1)	C1c1c1h1h	propane
C(08IG2)	C1c1h1h1h	ethane
C(08IB)	C1c1c1c1h	2-methylpropane
C(08IA)	C1n1c1c1h	2-aminopropane
C(08I)	C1.5o1.5n[1c1h]1c	N-methylacetamide
C(09AB)	C1c1h1h1h	ethane
C(09AA)	C1n1c1c1h	2-aminopropane
C(09A)	C1.5o1.5n[1c1h]1c	N-methylacetamide
C(10UB)	C2c1h1h	ethene
C(10UA)	C2c1n1c	2-propenamide
C(10U)	C1.5o1.5n[1c1h]1c	N-methylacetamide
C(11AB)	C1c1h1h1h	ethane
C(11AA)	C1n1c1c1h	2-aminopropane
C(11A)	C1.5o1.5n[1c1h]1c	N-methylacetamide
C(12#6)	C1n@5c1c1h	1-furan-3-ylethanamine
C(12#5)	C1n1c1c1c	aminoisobutane
C(12#4)	C1c1c1h1h	propane
C(12#3)	C1c1c1h1h	propane
C(12#2)	C2n@5c1c	1-furan-3-ylethanimine

Atom	Invariom Name	Model Compound
C(12#2_)	C2n@5c1c	1-furan-3-ylethanamine
C(12#6_)	C1n@5c1c1h	1-furan-3-ylethanamine
C(12#5_)	C1n1c1c1c	aminoisobutane
C(12#4_)	C1c1c1h1h	propane
C(12#3_)	C1c1c1h1h	propane
C(13Z2)	5-C#[5s[#5c]#5n[#5c]1c	2-methylthiazole
C(13Z5)	5-C#[5n[#5c]#5c[#5s1h]1c	4-methylthiazole
C(13Z6)	C1.5o1.5n[1c1h]@5c	N-methylfuran-3-carboxamide
C(13Z4)	5-C#[5s[#5c]#5c[#5n1c]1h	4-methylthiazole
C(13Z2_)	5-C#[5s[#5c]#5n[#5c]1c	2-methylthiazole
C(13Z5_)	5-C#[5n[#5c]#5c[#5s1h]1c	4-methylthiazole
C(13Z6_)	C1.5o1.5n[1c1h]@5c	N-methylfuran-3-carboxamide
C(13Z4_)	5-C#[5s[#5c]#5c[#5n1c]1h	4-methylthiazole
C(14UB)	C2c1h1h	ethene
C(14UA)	C2c1n1c	2-propenamide
C(14U)	C2o1.5n[1c1h]1c	azetidin-2-one
C(14UA_)	C2c1n1c	2-propenamide
C(14UB_)	C2c1h1h	ethene
C(14U_)	C2o1.5n[1c1h]1c	azetidin-2-one
C(15PYTB)	C2c1h1h	ethene
C(15PYTA)	C2c1n1c	2-propenamide
C(15PYT)	C1.5o1.5n[1h1h]1c	acetamide
C(15PATA)	C2c1n1c	2-propenamide
C(15PBTB)	C2c1h1h	ethene
C(15PYT_-)	C1.5o1.5n[1h1h]1c	acetamide
C(40O2)	C1n1h1h1h	methylamine
C(40O1)	C1n1h1h1h	methylamine
C(40O3)	C1.5o1.5n[1c1c]1h	<i>N,N</i> -dimethylformamid
C(41O1)	C1n1h1h1h	methylamine
C(41O2)	C1n1h1h1h	methylamine
C(41O3)	C1.5o1.5n[1c1c]1h	<i>N,N</i> -dimethylformamid
C(42O3)	C1.5o1.5n[1c1c]1h	<i>N,N</i> -dimethylformamid
C(42O1)	C1n1h1h1h	methylamine
C(42O2)	C1n1h1h1h	methylamine
C(42O1_)	C1n1h1h1h	methylamine
C(42O2_)	C1n1h1h1h	methylamine
C(42O3_)	C1.5o1.5n[1c1c]1h	<i>N,N</i> -dimethylformamid
C(43O3)	C1.5o1.5n[1c1c]1h	<i>N,N</i> -dimethylformamid
C(43O1)	C1n1h1h1h	methylamine
C(43O2)	C1n1h1h1h	methylamine
C(43O1_)	C1n1h1h1h	methylamine
C(43O3_)	C1.5o1.5n[1c1c]1h	<i>N,N</i> -dimethylformamid
C(43O2_)	C1n1h1h1h	methylamine
C(44O1)	C1n1h1h1h	methylamine
C(44O2)	C1n1h1h1h	methylamine
C(44O3)	C1.5o1.5n[1c1c]1h	<i>N,N</i> -dimethylformamid

Atom	Invariom Name	Model Compound
C(45O2)	C1n1h1h1h	methylamine
C(45O1)	C1n1h1h1h	methylamine
C(45O3)	C1.5o1.5n[1c1c]1h	<i>N,N</i> -dimethylformamid
C(45O3_-)	C1.5o1.5n[1c1c]1h	<i>N,N</i> -dimethylformamid
C(45O2_-)	C1n1h1h1h	methylamine
C(45O1_-)	C1n1h1h1h	methylamine
C(47O1)	C1n1h1h1h	methylamine
C(47O2)	C1n1h1h1h	methylamine
C(47O3)	C1.5o1.5n[1c1c]1h	<i>N,N</i> -dimethylformamid
C(49O2)	C1n1h1h1h	methylamine
C(49O1)	C1n1h1h1h	methylamine
C(49O3)	C1.5o1.5n[1c1c]1h	<i>N,N</i> -dimethylformamid
C(49O1_-)	C1n1h1h1h	methylamine
C(49O2_-)	C1n1h1h1h	methylamine
C(49O3_-)	C1.5o1.5n[1c1c]1h	<i>N,N</i> -dimethylformamid
C(50O10)	C1c1h1h1h	ethane
C(50O20)	C1o1c1h1h	ethanol
C(50O30)	C1o1c1h1h	ethanol
C(50O40)	C1c1h1h1h	ethane
C(51O1)	C1c1h1h1h	ethane
C(51O2)	C1o1c1h1h	ethanol
C(51O3)	C1o1c1h1h	ethanol
C(51O4)	C1c1h1h1h	ethane
C(52O12)	C1c1h1h1h	ethane
C(52O42)	C1c1h1h1h	ethane
C(52O22)	C1o1c1h1h	ethanol
C(52O32)	C1o1c1h1h	ethanol
C(53O4)	C1c1h1h1h	ethane
C(53O3)	C1o1c1h1h	ethanol
C(53O2)	C1o1c1h1h	ethanol
C(53O1)	C1c1h1h1h	ethane
C(53O40)	C1c1h1h1h	ethane
C(53O30)	C1o1c1h1h	ethanol
C(53O10)	C1c1h1h1h	ethane
C(53O20)	C1o1c1h1h	ethanol
C(55O1)	C1c1h1h1h	ethane
C(55O2)	C1o1c1h1h	ethanol
C(55O3)	C1o1c1h1h	ethanol
C(55O4)	C1c1h1h1h	ethane
C(54O1)	C1c1h1h1h	ethane
C(54O2)	C1o1c1h1h	ethanol
C(54O3)	C1o1c1h1h	ethanol
C(54O4)	C1c1h1h1h	ethane
H(21Z4L)	H@5c	cyclopentadienyl anion
H(21Z4_-)	H@5c	cyclopentadienyl anion
H(22T0H)	H1n[1.5c1c]	N-methyformamide

<b>Atom</b>	<b>Invariom Name</b>	<b>Model Compound</b>
H(22TGA,B,C)	H1c[1c1h1h]	ethane
H(22TGD)	H1o[1c]	methanol
H(22TBF)	H1c[1o1c1c]	2-propanol
H(22TAE)	H1c[1n1c1c]	2-aminopropane
H(23X0I)	H1n[1.5c1c]	N-methyformamide
H(23X4A,B,C)	H1c[1c1h1h]	ethane
H(23X3)	H1c[2c1c]	propene
H(23X4F)	H1c[1s1c1h]	ethanethiol
H(23X4G)	H1c[1s1c1h]	ethanethiol
H(23X5E)	H1c[1n1c1c]	2-aminopropane
H(24X1K)	H1n[1.5c1c]	N-methyformamide
H(24X8F,G,H)	H1c[1c1h1h]	ethane
H(24X7E)	H1o[1c]	methanol
H(24X6E)	H1c[1o1c1c]	2-propanol
H(24X4J)	H1o[1c]	methanol
H(24X5F,H,I)	H1c[1c1h1h]	ethane
H(24X2B)	H1c[1n@5c1c]	1-furan-3-ylethanamine
H(25Z4N)	H@5c	cyclopentadienyl anion
H(26X7F)	H1n[1.5c1c]	N-methyformamide
H(26X4M)	H@5c	cyclopentadienyl anion
H(26X6F)	H1c[1n@5c1c]	1-furan-3-ylethanamine
H(26X9D,E,F)	H1c[1c1h1h]	ethane
H(26X8I)	H1c[1o1c1c]	2-propanol
H(26X4_)	H@5c	cyclopentadienyl anion
H(27J1A)	H1o[1c]	methanol
H(27J1B)	H1o[1c]	methanol
H(27J1C,D,E)	H1c[1c1h1h]	ethane
H(27J1F)	H1c[1o@6c1c]	<i>S</i> -1-phenylethanol
H(27J3D)	H@6c	benzene
H(27J5J)	H1c[2c@6c]	styrene
H(27J6G)	H1c[2c1c]	propene
H(27J8J)	H1c[1o@6c1c]	<i>S</i> -1-phenylethanol
H(27J7G)	H1c[1n1c1c]	2-aminopropane
H(28I0J)	H1n[1c1c]	dimethylamine
H(28IDD,E,F)	H1c[1c1h1h]	ethane
H(28IGA)	H1c[1c1c1h]	propane
H(28IGB)	H1c[1c1c1h]	propane
H(28IGC,D,E)	H1c[1c1h1h]	ethane
H(28IBG)	H1c[1c1c1c]	2-methylpropane
H(28IAF)	H1c[1n1c1c]	2-aminopropane
H(29A9G)	H1n[1.5c1c]	N-methyformamide
H(29ABH,L,M)	H1c[1c1h1h]	ethane
H(29AAG)	H1c[1n1c1c]	2-aminopropane
H(30U0K)	H1n[1.5c1c]	N-methyformamide
H(30UBA)	H1c[2c1h]	ethene
H(30UBB)	H1c[2c1h]	ethene

<b>Atom</b>	<b>Invariom Name</b>	<b>Model Compound</b>
H(31A0L)	H1n[1.5c1c]	N-methylformamide
H(31ABQ,R,S)	H1c[1c1h1h]	ethane
H(31AAH)	H1c[1n1c1c]	2-aminopropane
H(32#7H)	H1n[1.5c1c]	N-methylformamide
H(32#6H)	H1c[1n@5c1c]	1-furan-3-ylethanamine
H(32#4O)	H1c[1c1c1h]	propane
H(32#4P)	H1c[1c1c1h]	propane
H(32#3E)	H1c[1c1c1h]	propane
H(32#3F)	H1c[1c1c1h]	propane
H(32#3E_)	H1c[1c1c1h]	propane
H(32#3F_)	H1c[1c1c1h]	propane
H(32#4O_)	H1c[1c1c1h]	propane
H(32#4P_)	H1c[1c1c1h]	propane
H(32#6_)	H1c[1n@5c1c]	1-furan-3-ylethanamine
H(32#7_)	H1n[1.5c1c]	N-methylformamide
H(33Z4Q)	H@5c	cyclopentadienyl anion
H(33Z4_-)	H@5c	cyclopentadienyl anion
H(34U1Q)	H1n[1.5c1c]	N-methylformamide
H(34UBA)	H1c[2c1h]	ethene
H(34UBB)	H1c[2c1h]	ethene
H(34U1_-)	H1n[1.5c1c]	N-methylformamide
H(34U3A_-)	H1c[2c1h]	ethene
H(34U3B_-)	H1c[2c1h]	ethene
H(35PYT0)	H1n[1.5c1c]	N-methylformamide
H(35PATB)	H1c[2c1h]	ethene
H(35PBTB)	H1c[2c1h]	ethene
H(35PATT)	H1n[1.5c1h]	formamide
H(35PBTT)	H1n[1.5c1h]	formamide
H(35PYT_-)	H1n[1.5c1c]	N-methylformamide
H(35PAB_-)	H1c[2c1h]	ethene
H(35PBB_-)	H1c[2c1h]	ethene
H(35PAT_-)	H1n[1.5c1h]	formamide
H(35PBT_-)	H1n[1.5c1h]	formamide
H(01Z4T)	H@5c	cyclopentadienyl anion
H(02T0A)	H1n[1.5c1c]	N-methylformamide
H(02TG)	H1o[1c]	methanol
H(02TGA,B,C)	H1c[1c1h1h]	ethane
H(02TB)	H1c[1o1c1c]	2-propanol
H(02TAA)	H1c[1n1c1c]	2-aminopropane
H(03X0B)	H1n[1.5c1c]	N-methylformamide
H(03X4A,B,C)	H1c[1c1h1h]	ethane
H(03X3)	H1c[2c1c]	propene
H(03X4D,E)	H1c[1s1c1h]	ethanethiol
H(03X5A)	H1c[1n1c1c]	2-aminopropane
H(04X1C)	H1n[1.5c1c]	N-methylformamide
H(04X8A,B,C)	H1c[1c1h1h]	ethane

<b>Atom</b>	<b>Invariom Name</b>	<b>Model Compound</b>
H(04X7A)	H1o[1c]	methanol
H(04X6A)	H1c[1o1c1c]	2-propanol
H(04X5B,C,D)	H1c[1c1h1h]	ethane
H(04X4E)	H1o[1c]	methanol
H(04X2A)	H1c[1n@5c1c]	1-furan-3-ylethanamine
H(06X7B)	H1n[1.5c1c]	N-methylformamide
H(06X5K)	H@5c	cyclopentadienyl anion
H(06X6B)	H1c[1n@5c1c]	1-furan-3-ylethanamine
H(06X9A,B,C)	H1c[1c1h1h]	ethane
H(06X8D)	H1c[1o1c1c]	2-propanol
H(06X7_)	H1n[1.5c1c]	N-methylformamide
H(06X6)	H1c[1n@5c1c]	1-furan-3-ylethanamine
H(06X5_)	H@5c	cyclopentadienyl anion
H(06X8B)	H1c[1o1c1c]	2-propanol
H(06X9A_,B_,C_)	H1c[1c1h1h]	ethane
H(05Z4R)	H@5c	cyclopentadienyl anion
H(07J3A)	H@6c	benzene
H(07J1A)	H1o[1c]	methanol
H(07J1B,C,D)	H1c[1c1h1h]	ethane
H(07J1E)	H1c[1o@6c1c]	<i>S</i> -1-phenylethanol
H(07J6C)	H1c[2c1c]	propene
H(07J5G)	H1c[2c@6c]	styrene
H(07J1)	H1o[1c]	methanol
H(07J8E)	H1c[1o@6c1c]	<i>S</i> -1-phenylethanol
H(07J7C)	H1c[1n1c1c]	2-aminopropane
H(08I0C)	H1n[1c1c]	dimethylamine
H(08IDA,B,C)	H1c[1c1h1h]	ethane
H(08IGA)	H1c[1c1c1h]	propane
H(08IGB)	H1c[1c1c1h]	propane
H(08IGC,D,E)	H1c[1c1h1h]	ethane
H(08IBB)	H1c[1c1c1c]	2-methylpropane
H(08IAB)	H1c[1n1c1c]	2-aminopropane
H(09A0D)	H1n[1.5c1c]	N-methylformamide
H(09ABC,D,E)	H1c[1c1h1h]	ethane
H(09AAC)	H1c[1n1c1c]	2-aminopropane
H(10U0E)	H1n[1.5c1c]	N-methylformamide
H(10UBY,Z)	H1c[2c1h]	ethene
H(11A0F)	H1n[1.5c1c]	N-methylformamide
H(11ABI,J,K)	H1c[1c1h1h]	ethane
H(11AAD)	H1c[1n1c1c]	2-aminopropane
H(12#7D)	H1n[1.5c1c]	N-methylformamide
H(12#6D)	H1c[1n@5c1c]	1-furan-3-ylethanamine
H(12#4H,I)	H1c[1c1c1h]	propane
H(12#3B,C)	H1c[1c1c1h]	propane
H(12#6_)	H1c[1n@5c1c]	1-furan-3-ylethanamine
H(12#7_)	H1n[1.5c1c]	N-methylformamide

Atom	Invariom Name	Model Compound
H(12#4H_)	H1c[1c1c1h]	propane
H(12#4I_)	H1c[1c1c1h]	propane
H(12#3B_)	H1c[1c1c1h]	propane
H(12#3C_)	H1c[1c1c1h]	propane
H(14U0G)	H1n[1.5c1c]	N-methyformamide
H(14UBP)	H1c[2c1h]	ethene
H(14UBT)	H1c[2c1h]	ethene
H(14U_)	H1n[1.5c1c]	N-methyformamide
H(14UBP_)	H1c[2c1h]	ethene
H(14UBT_)	H1c[2c1h]	ethene
H(15PYT)	H1n[1.5c1h]	formamide
H(15PATB)	H1c[2c1h]	ethene
H(15PBTB)	H1c[2c1h]	ethene
H(15PATT)	H1n[1.5c1h]	formamide
H(15PBTT)	H1n[1.5c1h]	formamide
H(15PYT_)	H1n[1.5c1h]	formamide
H(15PAB_)	H1c[2c1h]	ethene
H(15PBB_)	H1c[2c1h]	ethene
H(15PAT_)	H1n[1.5c1h]	formamide
H(15PBT_)	H1n[1.5c1h]	formamide
H(40O2A,B,C)	H1c[1n1h1h]	methylamine
H(40O1A,B,C)	H1c[1n1h1h]	methylamine
H(40O3)	H1c[1.5o1.5n]	<i>N,N</i> -dimethylformamid
H(41O1U,V,W)	H1c[1n1h1h]	methylamine
H(41O2F,G,H)	H1c[1n1h1h]	methylamine
H(41O3H)	H1c[2o1.5n]	formamide
H(42O3I)	H1c[1.5o1.5n]	<i>N,N</i> -dimethylformamid
H(42O1X,Y,Z)	H1c[1n1h1h]	methylamine
H(42O2I,J,K)	H1c[1n1h1h]	methylamine
H(42O1A,B,C)	H1c[1n1h1h]	methylamine
H(42O2A,B,C)	H1c[1n1h1h]	methylamine
H(42O3)	H1c[1.5o1.5n]	<i>N,N</i> -dimethylformamid
H(43O3)	H1c[1.5o1.5n]	<i>N,N</i> -dimethylformamid
H(43O1A,B,C)	H1c[1n1h1h]	methylamine
H(43O2A,B,C)	H1c[1n1h1h]	methylamine
H(43O1A_-,B_-,C_)	H1c[1n1h1h]	methylamine
H(43O3_-)	H1c[1.5o1.5n]	<i>N,N</i> -dimethylformamid
H(43O2A_-,B_-,C_-)	H1c[1n1h1h]	methylamine
H(44O1A,B,C)	H1c[1n1h1h]	methylamine
H(44O2A,B,C)	H1c[1n1h1h]	methylamine
H(44O3)	H1c[1.5o1.5n]	<i>N,N</i> -dimethylformamid
H(45O2R,S,T)	H1c[1n1h1h]	methylamine
H(45O1G,H,I)	H1c[1n1h1h]	methylamine
H(45O3)	H1c[2o1.5n]	formamide
H(45O3_-)	H1c[2o1.5n]	formamide
H(45O2A,B,C)	H1c[1n1h1h]	methylamine

<b>Atom</b>	<b>Invariom Name</b>	<b>Model Compound</b>
H(45O1A,B,C)	H1c[1n1h1h]	methylamine
H(47O1A,B,C)	H1c[1n1h1h]	methylamine
H(47O2A,B,C)	H1c[1n1h1h]	methylamine
H(47O3)	H1c[1.5o1.5n]	<i>N,N</i> -dimethylformamid
H(49O2A,B,C)	H1c[1n1h1h]	methylamine
H(49O1A,B,C)	H1c[1n1h1h]	methylamine
H(49O3)	H1c[2o1.5n]	formamide
H(49O1A <sub>-</sub> ,B <sub>-</sub> ,C <sub>-</sub> )	H1c[1n1h1h]	methylamine
H(49O2A <sub>-</sub> ,B <sub>-</sub> ,C <sub>-</sub> )	H1c[1n1h1h]	methylamine
H(49O3 <sub>-</sub> )	H1c[2o1.5n]	formamide
H(50O1A,B,C)	H1c[1c1h1h]	ethane
H(50O2A,B)	H1c[1o1c1h]	ethanol
H(50O3A,B)	H1c[1o1c1h]	ethanol
H(50O4A,B,C)	H1c[1c1h1h]	ethane
H(51O1A,B,C)	H1c[1c1h1h]	ethane
H(51O2A,B)	H1c[1o1c1h]	ethanol
H(51O3A,B)	H1c[1o1c1h]	ethanol
H(51O4,A,B)	H1c[1c1h1h]	ethane
H(52O1A,B,C)	H1c[1c1h1h]	ethane
H(52O4A,B,C)	H1c[1c1h1h]	ethane
H(52O2A,B)	H1c[1o1c1h]	ethanol
H(52O3A,B)	H1c[1o1c1h]	ethanol
H(53O4A,B,C)	H1c[1c1h1h]	ethane
H(53O3A,B)	H1c[1o1c1h]	ethanol
H(53O2A,B)	H1c[1o1c1h]	ethanol
H(53O1A,B,C)	H1c[1c1h1h]	ethane
H(53O4A <sub>-</sub> ,B <sub>-</sub> ,C <sub>-</sub> )	H1c[1c1h1h]	ethane
H(53O3A <sub>-</sub> ,B <sub>-</sub> )	H1c[1o1c1h]	ethanol
H(53O1A <sub>-</sub> ,B <sub>-</sub> ,C <sub>-</sub> )	H1c[1c1h1h]	ethane
H(53O2A <sub>-</sub> ,B <sub>-</sub> )	H1c[1o1c1h]	ethanol
H(55O1A,B,C)	H1c[1c1h1h]	ethane
H(55O2A,B)	H1c[1o1c1h]	ethanol
H(55O3A,B)	H1c[1o1c1h]	ethanol
H(55O4A,B,C)	H1c[1c1h1h]	ethane
H(54O1A,B,C)	H1c[1c1h1h]	ethane
H(54O2A,B)	H1c[1o1c1h]	ethanol
H(54O3A,B)	H1c[1o1c1h]	ethanol
H(54O4A,B,C)	H1c[1c1h1h]	ethane
H(60O1,2,3,4)	H1o[1h]	water
H(13Z4Q)	H@5c	cyclopentadienyl anion
H(13Z4 <sub>-</sub> )	H@5c	cyclopentadienyl anion