Publication data

NOE table *.pdf*

#	Atom 1	Atom 2	NMR
1	Ser HN	Ser Ha	3.0
2	Leu HN	Ser Ha	2.2
3	Asp HN	Leu Ha	2.7
4	Asp HN	Asp Ha	2.5

Tabula*

NOE constraints *.csv*

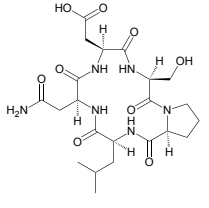
```
#,Atom 1,Atom 2,NMR,
1,Ser HN,Ser Ha,3.0,
2,Leu HN,Ser Ha,2.2,
3,Asp HN,Leu Ha,2.7,
4,Asp HN,Asp Ha,2.5,
```

Python script*

NOE constraints matching topology

```
#,Atom 1,Atom 2,NMR,
1,1,3,3.0,
2,1,3,2.2,
3,4,5,2.7,
4,2,4,2.5,
```

Molecular structure image *.pdf*



OSRA*

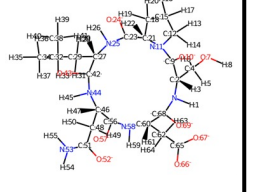
SMILES

```
N2[C@@]([H])(CO)
C(=O)N1[C@@]([H
])(CCC1)C(=O)N[C
@@]([H])(CC(C)C)
C(=O)N[C@@]([H])
(CC(=O)N)C(=O)N[
C@@]([H])(CC(=O
)O)C2(=O)
```

Parametrised molecule

.pdb file

RDKit



Annotated 2d structure with atom #

OR

Amino acid sequence

HHAHS

PepLibGen

Openbabel → PDB4Amber → Tleap

Parametrisation of natural cyclic peptides