<Insert table 1>

**Table 1**: Information on descriptor types in the congeneric amines data

|  |  |  |  |
| --- | --- | --- | --- |
| Type | Number of descriptors | Software used | Description |
| TS | 108 | 1. POLLY v. 2.3 [ ref] 2. MolconnZ, Version 4.05 [ref] | Both POLLY and MolconnZ can calculate a large number of topological indices from the SMILES LINE NOTATINs of molecular structure. |
| TC | 158 | 1. POLLY v. 2.3 2. MolconnZ, Version 4.05 3. TRIPLET | The TRIPLET software calculates the Triplet class of topological indices. |
| 3D | 3 | Sybyl v6.2 [ref] | Used for the calculaton of 3-D indices |
| QC | 6 | MOPAC v6.00 [ref] | Used for the calculation of quantum chemical descriptors |

Basak, S.C.; Grunwald, G.; Balaban, A. TRIPLET; Copyright of the Regents of the University of Minnesota, 1993. (**Subho: Please check that this is referred in the software section of the paper for TRIPLET CALCULATION**)

Sybyl Version 6.2. Tripos Associates, Inc.: St. Louis, MO, 1995.

Stewart, J.J.P. MOPAC Version 6.00, QCPE #455; Frank J. Seiler

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