**User Guides for QSAR/QSPR and PCM workflow**

The workflow has been developed and successfully tested on Windows systems. The user could download the workflow from https://github.com/cdmbi/PCM

On Windows:

(1): download the PCM-master.zip

(2): extract or uncompress the .zip file

(3): cd PCM-master

(4): type the series

python Run\_Program.py ExampleData Result [0] [0] [0] PLS 10-folds No 0.15 20 100

**Table S1** List of molecular descriptors

|  |  |  |
| --- | --- | --- |
| Index | Descriptors | Number of descriptors |
| 0 | All descriptors | 615 |
| 1 | Constitutional descriptors | 30 |
| 2 | Topological descriptors | 25 |
| 3 | Connectivity descriptors | 44 |
| 4 | Kappa shape descriptors | 7 |
| 5 | E-state descriptors | 237 |
| 6 | Moreau-Broto autocorrelation descriptors | 32 |
| 7 | Moran autocorrelation descriptors | 32 |
| 8 | Geary autocorrelation descriptors | 32 |
| 9 | Charge descriptors | 25 |
| 10 | Molecular property descriptors | 6 |
| 11 | MOE-type descriptors | 60 |

Table S2 List of protein sequences descriptors

|  |  |  |
| --- | --- | --- |
| Index | Descriptors | Number of descriptors |
| 0 | All descriptors | 2049 |
| 1 | Amino acid composition | 20 |
| 2 | Dipeptide composition | 400 |
| 3 | Tripeptide composition | 8000 |
| 4 | Normalized Moreau-Broto autocorrelation | 240 |
| 5 | Moran autocorrelation | 240 |
| 6 | Geary autocorrelation | 240 |
| 7 | Composition, Transition, Distribution | 147 |
| 8 | Conjoint triad features | 343 |
| 9 | Sequence order coupling number | 60 |
| 10 | Quasi-sequence order descriptors | 100 |
| 11 | Pseudo amino acid composition | 50 |