**IOKR**

**TOPOLOGICAL FINGERPRINTS IOKR**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | SUBSET  1 | SUBSET  2 | SUBSET  3 | SUBSET  4 | SUBSET  5 | AVERAGE |
| TOP 1 | 26.21 | 27.67 | 24.27 | 23.30 | 23.79 | **25.05** |
| TOP 3 | 27.18 | 32.04 | 25.73 | 27.18 | 25.24 | **27.47** |
| TOP 5 | 27.67 | 32.04 | 25.73 | 27.67 | 25.73 | **27.77** |
| TOP 10 | 28.16 | 33.01 | 25.73 | 29.61 | 27.18 | **28.74** |
| TOP 25 | 30.10 | 33.98 | 29.61 | 32.04 | 30.58 | **31.26** |

**MACC FINGERPRINTS IOKR**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | SUBSET  1 | SUBSET  2 | SUBSET  3 | SUBSET  4 | SUBSET  5 | AVERAGE |
| TOP 1 | 36.41 | 37.38 | 35.92 | 36.41 | 36.89 | **36.60** |
| TOP 3 | 48.06 | 46.12 | 43.69 | 47.09 | 45.63 | **46.12** |
| TOP 5 | 55.83 | 51.94 | 47.57 | 51.46 | 51.46 | **51.65** |
| TOP 10 | 63.11 | 59.71 | 58.25 | 57.28 | 59.71 | **59.61** |
| TOP 25 | 77.18 | 73.30 | 71.36 | 72.82 | 73.30 | **73.59** |

**ESTATE FINGERPRINTS IOKR**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | SUBSET  1 | SUBSET  2 | SUBSET  3 | SUBSET  4 | SUBSET  5 | AVERAGE |
| TOP 1 | 33.98 | 29.13 | 28.64 | 33.98 | 31.55 | **31.46** |
| TOP 3 | 37.38 | 36.41 | 35.92 | 42.23 | 39.32 | **38.25** |
| TOP 5 | 41.26 | 38.83 | 39.32 | 44.66 | 45.15 | **41.84** |
| TOP 10 | 47.09 | 44.66 | 44.17 | 49.03 | 50.49 | **47.09** |
| TOP 25 | 61.17 | 58.74 | 59.71 | 60.68 | 63.59 | **60.78** |

**DAYLIGHT FINGERPRINTS IOKR**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | SUBSET  1 | SUBSET  2 | SUBSET  3 | SUBSET  4 | SUBSET  5 | AVERAGE |
| TOP 1 | 28.16 | 31.55 | 27.18 | 27.67 | 29.61 | **28.83** |
| TOP 3 | 34.47 | 34.95 | 30.10 | 35.44 | 33.98 | **33.79** |
| TOP 5 | 37.86 | 37.86 | 31.07 | 37.86 | 35.92 | **36.11** |
| TOP 10 | 41.26 | 39.32 | 33.50 | 42.72 | 38.83 | **39.13** |
| TOP 25 | 49.03 | 46.60 | 41.26 | 49.51 | 48.54 | **46.99** |

**KLEKOTA-ROTH FINGERPRINTS IOKR**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | SUBSET  1 | SUBSET  2 | SUBSET  3 | SUBSET  4 | SUBSET  5 | AVERAGE |
| TOP 1 | 30.58 | 32.52 | 29.13 | 30.58 | 30.58 | **30.68** |
| TOP 3 | 33.98 | 38.83 | 33.50 | 37.38 | 34.95 | **35.73** |
| TOP 5 | 36.41 | 39.81 | 38.35 | 39.81 | 38.83 | **38.64** |
| TOP 10 | 44.66 | 45.15 | 42.72 | 42.72 | 41.75 | **43.4** |
| TOP 25 | 55.34 | 52.91 | 48.06 | 54.37 | 52.43 | **52.62** |

**PUBCHEM FINGERPRINTS IOKR**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | SUBSET  1 | SUBSET  2 | SUBSET  3 | SUBSET  4 | SUBSET  5 | AVERAGE |
| TOP 1 | 32.52 | 34.95 | 32.04 | 33.98 | 35.44 | **33.79** |
| TOP 3 | 41.26 | 42.23 | 35.92 | 39.81 | 41.26 | **40.10** |
| TOP 5 | 43.69 | 44.66 | 38.83 | 42.23 | 46.12 | **43.11** |
| TOP 10 | 51.46 | 49.03 | 46.60 | 47.57 | 52.91 | **49.51** |
| TOP 25 | 61.17 | 56.31 | 56.31 | 62.14 | 63.59 | **59.90** |

**CDKIT FINGERPRINTS IOKR**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | SUBSET  1 | SUBSET  2 | SUBSET  3 | SUBSET  4 | SUBSET  5 | AVERAGE |
| TOP 1 | 36.41 | 37.38 | 35.44 | 33.50 | 35.44 | **35.63** |
| TOP 3 | 43.69 | 43.69 | 42.23 | 44.17 | 45.63 | **43.88** |
| TOP 5 | 50.97 | 49.03 | 48.54 | 49.03 | 49.51 | **49.42** |
| TOP 10 | 60.68 | 57.77 | 54.37 | 57.28 | 57.28 | **57.48** |
| TOP 25 | 73.79 | 71.36 | 67.48 | 71.36 | 69.90 | **70.78** |

**SUMMARY FINGERPRINTS IOKR**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | CDKIT | DAYLIGHT | ESTATE | KLEKOTA-ROTH | MACC | PUBCHEM | TOPOLOGICAL |
| TOP 1 | **35.63** | 28.83 | 31.46 | 30.68 | 36.60 | 33.79 | 25.05 |
| TOP 3 | **43.88** | 33.79 | 38.25 | 35.73 | 46.12 | 40.10 | 27.47 |
| TOP 5 | **49.42** | 36.11 | 41.84 | 38.64 | 51.65 | 43.11 | 27.77 |
| TOP 10 | **57.48** | 39.13 | 47.09 | 43.4 | 59.61 | 49.51 | 28.74 |
| TOP 25 | **70.78** | 46.99 | 60.78 | 52.62 | 73.59 | 59.90 | 31.26 |

**NEURAL NETWORK**

**TOPOLOGICAL FINGERPRINTS NEURAL NETWORK**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | SUBSET  1 | SUBSET  2 | SUBSET  3 | SUBSET  4 | SUBSET  5 | AVERAGE |
| TOP 1 | 18.45 | 27.67 | 20.39 | 20.39 | 20.87 | **21.55** |
| TOP 3 | 27.67 | 39.32 | 35.44 | 29.13 | 33.50 | **33.01** |
| TOP 5 | 33.01 | 45.15 | 41.75 | 36.89 | 37.38 | **38.84** |
| TOP 10 | 45.63 | 54.85 | 52.91 | 47.09 | 43.69 | **48.83** |
| TOP 25 | 62.62 | 68.93 | 68.93 | 60.19 | 60.68 | **64.27** |

**MACC FINGERPRINTS NEURAL NETWORK**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | SUBSET  1 | SUBSET  2 | SUBSET  3 | SUBSET  4 | SUBSET  5 | AVERAGE |
| TOP 1 | 23.30 | 17.96 | 23.30 | 22.82 | 18.45 | **21.17** |
| TOP 3 | 32.52 | 32.04 | 34.95 | 30.58 | 26.70 | **31.36** |
| TOP 5 | 38.83 | 35.44 | 38.83 | 39.81 | 34.95 | **37.57** |
| TOP 10 | 44.66 | 46.60 | 50.97 | 50.00 | 45.63 | **47.57** |
| TOP 25 | 64.56 | 64.08 | 66.99 | 66.02 | 62.62 | **64.85** |

**CDKIT FINGERPRINTS NEURAL NETWORK**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | SUBSET  1 | SUBSET  2 | SUBSET  3 | SUBSET  4 | SUBSET  5 | AVERAGE |
| TOP 1 | 25.24 | 22.33 | 28.64 | 20.39 | 20.87 | **23.49** |
| TOP 3 | 34.47 | 30.58 | 36.89 | 30.58 | 32.52 | **33.01** |
| TOP 5 | 42.23 | 37.86 | 46.60 | 35.44 | 35.92 | **39.61** |
| TOP 10 | 52.91 | 48.06 | 60.19 | 45.15 | 45.15 | **50.29** |
| TOP 25 | 70.39 | 62.14 | 72.82 | 59.71 | 60.68 | **65.15** |

**KLEKOTA-ROTH FINGERPRINTS NEURAL NETWORK**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | SUBSET  1 | SUBSET  2 | SUBSET  3 | SUBSET  4 | SUBSET  5 | AVERAGE |
| TOP 1 | 21.36 | 24.27 | 23.30 | 19.42 | 18.45 | **21.36** |
| TOP 3 | 31.55 | 30.58 | 34.47 | 29.61 | 28.16 | **30.87** |
| TOP 5 | 35.92 | 34.95 | 41.26 | 33.98 | 33.98 | **36.02** |
| TOP 10 | 47.57 | 42.23 | 50.97 | 44.66 | 43.69 | **45.82** |
| TOP 25 | 63.59 | 60.19 | 65.05 | 55.34 | 56.80 | **60.19** |

**DAYLIGHT FINGERPRINTS NEURAL NETWORK**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | SUBSET  1 | SUBSET  2 | SUBSET  3 | SUBSET  4 | SUBSET  5 | AVERAGE |
| TOP 1 | 11.65 | 13.11 | 19.90 | 19.42 | 15.05 | **15.83** |
| TOP 3 | 21.36 | 22.82 | 26.70 | 27.18 | 20.39 | **23.69** |
| TOP 5 | 27.67 | 25.73 | 32.52 | 33.98 | 25.24 | **29.03** |
| TOP 10 | 36.89 | 34.47 | 42.72 | 40.78 | 31.55 | **37.28** |
| TOP 25 | 49.51 | 50.97 | 58.74 | 50.00 | 47.57 | **51.36** |

**PUBCHEM FINGERPRINTS NEURAL NETWORK**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | SUBSET  1 | SUBSET  2 | SUBSET  3 | SUBSET  4 | SUBSET  5 | AVERAGE |
| TOP 1 | 18.93 | 19.42 | 21.36 | 21.36 | 20.39 | **20.29** |
| TOP 3 | 33.01 | 32.52 | 32.04 | 32.04 | 30.58 | **32.04** |
| TOP 5 | 38.35 | 38.35 | 39.32 | 35.44 | 34.95 | **37.28** |
| TOP 10 | 46.12 | 49.03 | 52.91 | 46.12 | 46.60 | **48.16** |
| TOP 25 | 62.14 | 62.62 | 71.36 | 61.65 | 64.56 | **64.46** |

**ESTATE FINGERPRINTS NEURAL NETWORK**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | SUBSET  1 | SUBSET  2 | SUBSET  3 | SUBSET  4 | SUBSET  5 | AVERAGE |
| TOP 1 | 19.42 | 32.52 | 30.10 | 21.36 | 22.33 | **25.15** |
| TOP 3 | 26.21 | 42.72 | 38.35 | 31.07 | 28.16 | **33.30** |
| TOP 5 | 31.07 | 47.57 | 41.75 | 38.35 | 34.95 | **38.74** |
| TOP 10 | 45.15 | 54.37 | 52.43 | 47.09 | 45.15 | **48.84** |
| TOP 25 | 59.22 | 61.65 | 66.50 | 63.11 | 59.22 | **61.94** |