**Two experiments with IOKR dividing the results into category products. Then, these 10 batches were combined (two experiments of 5 subsets each) to average the results. Saccharides are predicted with higher accuracy than the other categories.**

**FIRST EXPERIMENT**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | TOP 1 | TOP 3 | TOP 5 | TOP 10 | TOP 25 |
| ALKALOID | 80.00% (4 out of 5)  62.50% (5 out of 8)  33.33% (1 out of 3)  75.00% (3 out of 4)  33.33% (3 out of 9) | 80.00% (4 out of 5)  62.50% (5 out of 8)  66.67% (2 out of 3)  75.00% (3 out of 4)  33.33% (3 out of 9) | 80.00% (4 out of 5)  75.00% (6 out of 8)  66.67% (2 out of 3)  75.00% (3 out of 4)  33.33% (3 out of 9) | 80.00% (4 out of 5)  75.00% (6 out of 8)  66.67% (2 out of 3)  75.00% (3 out of 4)  33.33% (3 out of 9) | 80.00% (4 out of 5)  87.50% (7 out of 8)  66.67% (2 out of 3)  75.00% (3 out of 4)  55.56% (5 out of 9) |
| NRP | 32.10% (26 out of 81)  30.51% (18 out of 59)  34.78% (24 out of 69)  26.32% (15 out of 57)  25.81% (16 out of 62) | 39.51% (32 out of 81)  38.98% (23 out of 59)  43.48% (30 out of 69)  35.09% (20 out of 57)  33.87% (21 out of 62) | 44.44% (36 out of 81)  44.07% (26 out of 59)  44.93% (31 out of 69)  36.84% (21 out of 57)  38.71% (24 out of 62) | 50.62% (41 out of 81)  49.15% (29 out of 59)  50.72% (35 out of 69)  47.37% (27 out of 57)  51.61% (32 out of 62) | 66.67% (54 out of 81)  66.10% (39 out of 59)  69.57% (48 out of 69)  68.42% (39 out of 57)  67.74% (42 out of 62) |
| NUCLEOSIDE | ---  0.00% (0 out of 1)  ---  ---  --- | ---  0.00% (0 out of 1)  ---  ---  --- | ---  0.00% (0 out of 1)  ---  ---  --- | ---  0.00% (0 out of 1)  ---  ---  --- | ---  0.00% (0 out of 1)  ---  ---  --- |
| OTHERS | 43.75% (14 out of 32)  53.85% (14 out of 26)  37.93% (11 out of 29)  22.73% (5 out of 22)  51.72% (15 out of 29) | 50.00% (16 out of 32)  57.69% (15 out of 26)  37.93% (11 out of 29)  27.27% (6 out of 22)  51.72% (15 out of 29) | 53.12% (17 out of 32)  65.38% (17 out of 26)  44.83% (13 out of 29)  31.82% (7 out of 22)  51.72% (15 out of 29) | 53.12% (17 out of 32)  65.38% (17 out of 26)  44.83% (13 out of 29)  40.91% (9 out of 22)  58.62% (17 out of 29) | 62.50% (20 out of 32)  80.77% (21 out of 26)  55.17% (16 out of 29)  50.00% (11 out of 22)  65.52% (19 out of 29) |
| POLYKETIDE | 39.66% (23 out of 58)  38.36% (28 out of 73)  32.81% (21 out of 64)  31.58% (24 out of 76)  36.21% (21 out of 58) | 53.45% (31 out of 58)  42.47% (31 out of 73)  46.88% (30 out of 64)  38.16% (29 out of 76)  46.55% (27 out of 58) | 58.62% (34 out of 58)  49.32% (36 out of 73)  54.69% (35 out of 64)  38.16% (29 out of 76)  55.17% (32 out of 58) | 70.69% (41 out of 58)  57.53% (42 out of 73)  70.31% (45 out of 64)  48.68% (37 out of 76)  58.62% (34 out of 58) | 82.76% (48 out of 58)  75.34% (55 out of 73)  84.38% (54 out of 64)  69.74% (53 out of 76)  77.59% (45 out of 58) |
| RIPP | 60.00% (3 out of 5)  33.33% (3 out of 9)  38.46% (5 out of 13)  41.67% (5 out of 12)  41.67% (5 out of 12) | 60.00% (3 out of 5)  33.33% (3 out of 9)  38.46% (5 out of 13)  50.00% (6 out of 12)  41.67% (5 out of 12) | 60.00% (3 out of 5)  33.33% (3 out of 9)  38.46% (5 out of 13)  66.67% (8 out of 12)  41.67% (5 out of 12) | 80.00% (4 out of 5)  33.33% (3 out of 9)  61.54% (8 out of 13)  66.67% (8 out of 12)  50.00% (6 out of 12) | 80.00% (4 out of 5)  33.33% (3 out of 9)  69.23% (9 out of 13)  75.00% (9 out of 12)  66.67% (8 out of 12) |
| SACCHARIDE | 69.23% (9 out of 13)  71.43% (10 out of 14)  70.00% (7 out of 10)  60.00% (9 out of 15)  66.67% (12 out of 18) | 76.92% (10 out of 13)  71.43% (10 out of 14)  70.00% (7 out of 10)  80.00% (12 out of 15)  66.67% (12 out of 18) | 84.62% (11 out of 13)  71.43% (10 out of 14)  80.00% (8 out of 10)  80.00% (12 out of 15)  66.67% (12 out of 18) | 84.62% (11 out of 13)  71.43% (10 out of 14)  80.00% (8 out of 10)  86.67% (13 out of 15)  77.78% (14 out of 18) | 92.31% (12 out of 13)  71.43% (10 out of 14)  80.00% (8 out of 10)  100.00% (15 out of 15)  94.44% (17 out of 18) |
| TERPENE | 41.67% (5 out of 12)  62.50% (10 out of 16)  33.33% (6 out of 18)  20.00% (4 out of 20)  47.37% (9 out of 19) | 41.67% (5 out of 12)  68.75% (11 out of 16)  55.56% (10 out of 18)  30.00% (6 out of 20)  52.63% (10 out of 19) | 50.00% (6 out of 12)  68.75% (11 out of 16)  66.67% (12 out of 18)  55.00% (11 out of 20)  68.42% (13 out of 19) | 58.33% (7 out of 12)  75.00% (12 out of 16)  72.22% (13 out of 18)  75.00% (15 out of 20)  84.21% (16 out of 19) | 83.33% (10 out of 12)  75.00% (12 out of 16)  88.89% (16 out of 18)  90.00% (18 out of 20)  100.00% (19 out of 19) |

**SECOND EXPERIMENT**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | TOP 1 | TOP 3 | TOP 5 | TOP 10 | TOP 25 |
| ALKALOID | 80.00% (4 out of 5)  100.00% (3 out of 3)  42.86% (3 out of 7)  57.14% (4 out of 7)  28.57% (2 out of 7) | 80.00% (4 out of 5)  100.00% (3 out of 3)  57.14% (4 out of 7)  71.43% (5 out of 7)  42.86% (3 out of 7) | 80.00% (4 out of 5)  100.00% (3 out of 3)  57.14% (4 out of 7)  71.43% (5 out of 7)  42.86% (3 out of 7) | 80.00% (4 out of 5)  100.00% (3 out of 3)  57.14% (4 out of 7)  71.43% (5 out of 7)  42.86% (3 out of 7) | 80.00% (4 out of 5)  100.00% (3 out of 3)  71.43% (5 out of 7)  85.71% (6 out of 7)  42.86% (3 out of 7) |
| NRP | 20.97% (13 out of 62)  30.65% (19 out of 62)  22.73% (15 out of 66)  30.00% (21 out of 70)  36.76% (25 out of 68) | 35.48% (22 out of 62)  41.94% (26 out of 62)  30.30% (20 out of 66)  40.00% (28 out of 70)  41.18% (28 out of 68) | 40.32% (25 out of 62)  46.77% (29 out of 62)  34.85% (23 out of 66)  45.71% (32 out of 70)  42.65% (29 out of 68) | 45.16% (28 out of 62)  53.23% (33 out of 62)  40.91% (27 out of 66)  55.71% (39 out of 70)  50.00% (34 out of 68) | 61.29% (38 out of 62)  67.74% (42 out of 62)  62.12% (41 out of 66)  71.43% (50 out of 70)  64.71% (44 out of 68) |
| NUCLEOSIDE | ---  ---  ---  ---  0.00% (0 out of 1) | ---  ---  ---  ---  0.00% (0 out of 1) | ---  ---  ---  ---  0.00% (0 out of 1) | ---  ---  ---  ---  0.00% (0 out of 1) | ---  ---  ---  ---  0.00% (0 out of 1) |
| OTHERS | 12.50% (3 out of 24)  46.43% (13 out of 28)  40.00% (12 out of 30)  29.17% (7 out of 24)  37.50% (12 out of 32) | 29.17% (7 out of 24)  50.00% (14 out of 28)  56.67% (17 out of 30)  41.67% (10 out of 24)  40.62% (13 out of 32) | 29.17% (7 out of 24)  53.57% (15 out of 28)  63.33% (19 out of 30)  41.67% (10 out of 24)  43.75% (14 out of 32) | 33.33% (8 out of 24)  64.29% (18 out of 28)  63.33% (19 out of 30)  50.00% (12 out of 24)  50.00% (16 out of 32) | 54.17% (13 out of 24)  64.29% (18 out of 28)  76.67% (23 out of 30)  79.17% (19 out of 24)  65.62% (21 out of 32) |
| POLYKETIDE | 39.44% (28 out of 71)  37.68% (26 out of 69)  34.92% (22 out of 63)  42.86% (30 out of 70)  33.93% (19 out of 56) | 49.30% (35 out of 71)  46.38% (32 out of 69)  44.44% (28 out of 63)  44.29% (31 out of 70)  41.07% (23 out of 56) | 56.34% (40 out of 71)  53.62% (37 out of 69)  53.97% (34 out of 63)  44.29% (31 out of 70)  48.21% (27 out of 56) | 67.61% (48 out of 71)  65.22% (45 out of 69)  61.90% (39 out of 63)  61.43% (43 out of 70)  58.93% (33 out of 56) | 76.06% (54 out of 71)  78.26% (54 out of 69)  80.95% (51 out of 63)  71.43% (50 out of 70)  75.00% (42 out of 56) |
| RIPP | 70.00% (7 out of 10)  33.33% (4 out of 12)  45.45% (5 out of 11)  14.29% (1 out of 7)  18.18% (2 out of 11) | 70.00% (7 out of 10)  50.00% (6 out of 12)  54.55% (6 out of 11)  42.86% (3 out of 7)  18.18% (2 out of 11) | 70.00% (7 out of 10)  58.33% (7 out of 12)  54.55% (6 out of 11)  42.86% (3 out of 7)  36.36% (4 out of 11) | 70.00% (7 out of 10)  66.67% (8 out of 12)  54.55% (6 out of 11)  57.14% (4 out of 7)  54.55% (6 out of 11) | 70.00% (7 out of 10)  75.00% (9 out of 12)  63.64% (7 out of 11)  57.14% (4 out of 7)  72.73% (8 out of 11) |
| SACCHARIDE | 64.71% (11 out of 17)  50.00% (8 out of 16)  70.00% (7 out of 10)  66.67% (8 out of 12)  60.00% (9 out of 15) | 64.71% (11 out of 17)  62.50% (10 out of 16)  80.00% (8 out of 10)  75.00% (9 out of 12)  60.00% (9 out of 15) | 64.71% (11 out of 17)  75.00% (12 out of 16)  80.00% (8 out of 10)  83.33% (10 out of 12)  66.67% (10 out of 15) | 70.59% (12 out of 17)  81.25% (13 out of 16)  90.00% (9 out of 10)  83.33% (10 out of 12)  66.67% (10 out of 15) | 94.12% (16 out of 17)  100.00% (16 out of 16)  100.00% (10 out of 10)  91.67% (11 out of 12)  80.00% (12 out of 15) |
| TERPENE | 23.53% (4 out of 17)  18.75% (3 out of 16)  31.58% (6 out of 19)  75.00% (12 out of 16)  47.06% (8 out of 17) | 29.41% (5 out of 17)  43.75% (7 out of 16)  57.89% (11 out of 19)  81.25% (13 out of 16)  52.94% (9 out of 17) | 52.94% (9 out of 17)  50.00% (8 out of 16)  63.16% (12 out of 19)  81.25% (13 out of 16)  64.71% (11 out of 17) | 70.59% (12 out of 17)  56.25% (9 out of 16)  84.21% (16 out of 19)  87.50% (14 out of 16)  70.59% (12 out of 17) | 76.47% (13 out of 17)  68.75% (11 out of 16)  94.74% (18 out of 19)  87.50% (14 out of 16)  82.35% (14 out of 17) |

**AVERAGE**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | TOP 1 | TOP 3 | TOP 5 | TOP 10 | TOP 25 |
| ALKALOID | **55.17%** (32 out of 58) | **62.07%** (36 out of 58) | **63.79%** (37 out of 58) | **63.79%** (37 out of 58) | **72.41%** (42 out of 58) |
| NRP | **29.27%** (192 out of 656) | **38.11%** (250 out of 656) | **42.07%** (276 out of 656) | **49.54%** (325 out of 656) | **66.62%** (437 out of 656) |
| NUCLEOSIDE | **0%** (0 out of 2) | **0%** (0 out of 2) | **0%** (0 out of 2) | **0%** (0 out of 2) | **0%** (0 out of 2) |
| OTHERS | **38.41%** (106 out of 276) | **44.93%** (124 out of 276) | **48.55%** (134 out of 276) | **52.90%** (146 out of 276) | **65.58%** (181 out of 276) |
| POLYKETIDE | **36.78%** (242 out of 658) | **45.14%** (297 out of 658) | **50.91%** (335 out of 658) | **61.85%** (407 out of 658) | **76.90%** (506 out of 658) |
| RIPP | **39.22%** (40 out of 102) | **45.10%** (46 out of 102) | **50.00%** (51 out of 102) | **58.82%** (60 out of 102) | **66.67%** (68 out of 102) |
| SACCHARIDE | **64.29%** (90 out of 140) | **70.00%** (98 out of 140) | **74.29%** (104 out of 140) | **78.57%** (110 out of 140) | **90.71%** (127 out of 140) |
| TERPENE | **39.41%** (67 out of 170) | **51.18%** (87 out of 170) | **62.35%** (106 out of 170) | **74.12%** (126 out of 170) | **85.29%** (145 out of 170) |