**Table 1** Results from the cluster evaluation methods on ECFP4 dataset

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **random\_state** | **n\_clusters** | **davies\_bouldin\_index** | **silhouette\_coefficient** | **calinski\_harabasz\_score** |
| 0 | 1538 | 0.873563 | 0.242808 | 99,35024 |
|  | 1539 | 0.856085 | 0.246215 | 98,66799 |
|  | 1540 | 0.790692 | 0.251960 | 104,2044 |
|  | 1541 | 0.810197 | 0.250200 | 104,4831 |
|  | 1542 | 0.792110 | 0.258222 | 106,4714 |
|  | 1543 | 0.775540 | 0.254884 | 105,3599 |
| 2 | 1538 | 0.788215 | 0.247295 | 104,8728 |
|  | 1539 | 0.786949 | 0.251080 | 105,5336 |
|  | 1540 | 0.784626 | 0.252434 | 105,8447 |
|  | 1541 | 0.785582 | 0.250113 | 105,3581 |
|  | 1542 | 0.812825 | 0.245408 | 102,2498 |
|  | 1543 | 0.834923 | 0.239133 | 99,94494 |
| 4 | 1538 | 0.825557 | 0.244235 | 101,7465 |
|  | 1539 | 0.799516 | 0.248618 | 104,5228 |
|  | 1540 | 0.843299 | 0.249028 | 104,7029 |
|  | 1541 | 0.840442 | 0.247939 | 102,2129 |
|  | 1542 | 0.892754 | 0.244232 | 101,4642 |
|  | 1543 | 0.849038 | 0.242902 | 102,0121 |
| 6 | 1538 | 0.778138 | 0.248952 | 105,7446 |
|  | 1539 | 0.822352 | 0.246682 | 101,4978 |
|  | 1540 | 0.811149 | 0.244980 | 101,786 |
|  | 1541 | 0.801316 | 0.248261 | 103,4933 |
|  | 1542 | 0.799196 | 0.248676 | 103,5811 |
|  | 1543 | 0.781607 | 0.250484 | 105,5944 |

**Table 2** Results from the cluster evaluation methods on ECFP6 dataset

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **random\_state** | **n\_clusters** | **davies\_bouldin\_index** | **silhouette\_coefficient** | **calinski\_harabasz\_score** |
| 0 | 1538 | 0.954781 | 0.234569 | 83,32759 |
|  | 1539 | 0.835329 | 0.242227 | 85,87328 |
|  | 1540 | 0.826768 | 0.247456 | 86,794 |
|  | 1541 | 0.790843 | 0.247583 | 87,87604 |
|  | 1542 | 0.819672 | 0.248138 | 88,72124 |
|  | 1543 | 0.830326 | 0.250047 | 88,27771 |
| 2 | 1538 | 0.810635 | 0.246738 | 88,68926 |
|  | 1539 | 0.796226 | 0.245550 | 87,4181 |
|  | 1540 | 0.807626 | 0.247628 | 88,53765 |
|  | 1541 | 0.796788 | 0.249031 | 87,84735 |
|  | 1542 | 0.806408 | 0.253548 | 89,06318 |
|  | 1543 | 0.834433 | 0.249829 | 87,0495 |
| 4 | 1538 | 0.857205 | 0.241561 | 85,41344 |
|  | 1539 | 0.826208 | 0.247317 | 86,38929 |
|  | 1540 | 0.816317 | 0.248962 | 88,52012 |
|  | 1541 | 0.825234 | 0.243793 | 85,7419 |
|  | 1542 | 0.843209 | 0.249170 | 87,49144 |
|  | 1543 | 0.880278 | 0.241908 | 84,60391 |
| 6 | 1538 | 0.793804 | 0.242120 | 87,51725 |
|  | 1539 | 0.847735 | 0.237897 | 84,73237 |
|  | 1540 | 0.801734 | 0.243219 | 88,53812 |
|  | 1541 | 0.860465 | 0.246811 | 86,41212 |
|  | 1542 | 0.817537 | 0.246957 | 86,69276 |
|  | 1543 | 0.832878 | 0.238163 | 85,27536 |

**Table 3** Results from the cluster evaluation methods on FCFP4 dataset

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **random\_state** | **n\_clusters** | **davies\_bouldin\_index** | **silhouette\_coefficient** | **calinski\_harabasz\_score** |
| 0 | 1538 | 0.752112 | 0.297457 | 137,3523 |
|  | 1539 | 0.711814 | 0.304011 | 142,8809 |
|  | 1540 | 0.710910 | 0.303451 | 141,6864 |
|  | 1541 | 0.751813 | 0.298608 | 136,9351 |
|  | 1542 | 0.766257 | 0.299320 | 136,4681 |
|  | 1543 | 0.716984 | 0.306077 | 142,4918 |
| 2 | 1538 | 0.730184 | 0.300353 | 142,0791 |
|  | 1539 | 0.713257 | 0.306918 | 141,9025 |
|  | 1540 | 0.729202 | 0.306197 | 144,0288 |
|  | 1541 | 0.738489 | 0.307894 | 142,5825 |
|  | 1542 | 0.747987 | 0.303741 | 137,6714 |
|  | 1543 | 0.708586 | 0.306516 | 142,903 |
| 4 | 1538 | 0.746620 | 0.295070 | 135,6059 |
|  | 1539 | 0.713368 | 0.300062 | 141,1683 |
|  | 1540 | 0.722871 | 0.304117 | 143,3174 |
|  | 1541 | 0.756163 | 0.297963 | 136,544 |
|  | 1542 | 0.769154 | 0.299184 | 138,5593 |
|  | 1543 | 0.714802 | 0.305369 | 144,7779 |
| 6 | 1538 | 0.746620 | 0.295070 | 135,6059 |
|  | 1539 | 0.713368 | 0.300062 | 141,1683 |
|  | 1540 | 0.722871 | 0.304117 | 143,3174 |
|  | 1541 | 0.756163 | 0.297963 | 136,544 |
|  | 1542 | 0.769154 | 0.299184 | 138,5593 |
|  | 1543 | 0.714802 | 0.305369 | 144,7779 |

**Table 4** Results from the cluster evaluation methods on FCFP6 dataset

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **random\_state** | **n\_clusters** | **davies\_bouldin\_index** | **silhouette\_coefficient** | **calinski\_harabasz\_score** |
| 0 | 1538 | 0.760583 | 0.290645 | 114,1657 |
|  | 1539 | 0.752842 | 0.290091 | 113,2827 |
|  | 1540 | 0.748744 | 0.286224 | 113,3527 |
|  | 1541 | 0.752535 | 0.291900 | 113,3673 |
|  | 1542 | 0.748551 | 0.294830 | 112,8462 |
|  | 1543 | 0.750473 | 0.295263 | 117,4277 |
| 2 | 1538 | 0.728304 | 0.293291 | 116,4701 |
|  | 1539 | 0.733484 | 0.293390 | 116,4989 |
|  | 1540 | 0.729350 | 0.293108 | 116,2927 |
|  | 1541 | 0.728099 | 0.295928 | 116,9726 |
|  | 1542 | 0.793083 | 0.295663 | 116,3453 |
|  | 1543 | 0.723490 | 0.297354 | 116,08 |
| 4 | 1538 | 0.728446 | 0.299695 | 117,4072 |
|  | 1539 | 0.728751 | 0.293677 | 116,6708 |
|  | 1540 | 0.781823 | 0.289678 | 111,3704 |
|  | 1541 | 0.734250 | 0.294063 | 116,0924 |
|  | 1542 | 0.790425 | 0.290949 | 112,0203 |
|  | 1543 | 0.737153 | 0.295538 | 115,6392 |
| 6 | 1538 | 0.723127 | 0.296530 | 117,6796 |
|  | 1539 | 0.780241 | 0.289901 | 113,1207 |
|  | 1540 | 0.721637 | 0.297483 | 118,52 |
|  | 1541 | 0.743881 | 0.292632 | 117,0701 |
|  | 1542 | 0.739413 | 0.300785 | 117,577 |
|  | 1543 | 0.756148 | 0.293328 | 114,0998 |

**Table 5** Results from the cluster evaluation methods on MACCS Keys dataset

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **random\_state** | **n\_clusters** | **davies\_bouldin\_index** | **silhouette\_coefficient** | **calinski\_harabasz\_score** |
| 0 | 1538 | 0.571658 | 0.286861 | 312,3626 |
|  | 1539 | 0.573828 | 0.289092 | 315,3002 |
|  | 1540 | 0.548826 | 0.298700 | 332,7179 |
|  | 1541 | 0.549431 | 0.301358 | 338,1443 |
|  | 1542 | 0.579768 | 0.284430 | 309,9345 |
|  | 1543 | 0.551123 | 0.292183 | 323,9784 |
| 2 | 1538 | 0.560277 | 0.293218 | 329,4285 |
|  | 1539 | 0.550871 | 0.296962 | 337,0563 |
|  | 1540 | 0.565730 | 0.287885 | 319,6373 |
|  | 1541 | 0.569997 | 0.286438 | 318,4997 |
|  | 1542 | 0.557282 | 0.290723 | 318,5938 |
|  | 1543 | 0.576439 | 0.286484 | 322,9323 |
| 4 | 1538 | 0.578157 | 0.284462 | 305,189 |
|  | 1539 | 0.545709 | 0.297757 | 332,8769 |
|  | 1540 | 0.545311 | 0.302842 | 331,3942 |
|  | 1541 | 0.562070 | 0.290244 | 319,5191 |
|  | 1542 | 0.549739 | 0.299186 | 335,8125 |
|  | 1543 | 0.560445 | 0.293318 | 321,6108 |
| 6 | 1538 | 0.551146 | 0.296710 | 329,3317 |
|  | 1539 | 0.573105 | 0.280035 | 306,0804 |
|  | 1540 | 0.574675 | 0.286281 | 309,2146 |
|  | 1541 | 0.576455 | 0.283806 | 304,4873 |
|  | 1542 | 0.567399 | 0.287396 | 315,9356 |
|  | 1543 | 0.581973 | 0.284724 | 312,7237 |

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Molecular Selection Results | | | | | | | | | |
| CHEMBL1082345  CHEMBL1082350  CHEMBL1082464  CHEMBL1082653  CHEMBL1082716  CHEMBL1082996  CHEMBL1082997  CHEMBL1083032  CHEMBL1083287  CHEMBL1083916  CHEMBL1084972  CHEMBL1085305  CHEMBL1085306  CHEMBL1085333  CHEMBL1085552  CHEMBL1085595  CHEMBL1085596  CHEMBL1086039  CHEMBL1090  CHEMBL1162974  CHEMBL1182947  CHEMBL1185242  CHEMBL1194345  CHEMBL1197118  CHEMBL1202081  CHEMBL1202082  CHEMBL1202083  CHEMBL1202084  CHEMBL1202087  CHEMBL1202088  CHEMBL1202091  CHEMBL1202092  CHEMBL1202094  CHEMBL122206  CHEMBL1229644  CHEMBL1229855  CHEMBL1230015  CHEMBL1230044  CHEMBL1233461  CHEMBL1236897  CHEMBL1243372  CHEMBL1275853  CHEMBL1276590  CHEMBL1276591  CHEMBL1276619  CHEMBL1276650  CHEMBL1287844  CHEMBL1287902  CHEMBL1288231  CHEMBL1288288  CHEMBL1431  CHEMBL148954  CHEMBL153096  CHEMBL1614729  CHEMBL1650403  CHEMBL1650404  CHEMBL1650406  CHEMBL1650409  CHEMBL1650410  CHEMBL1650411  CHEMBL1650412  CHEMBL1650413  CHEMBL1650414  CHEMBL1650415  CHEMBL1650416  CHEMBL1650417  CHEMBL1650418  CHEMBL1650419  CHEMBL1650420  CHEMBL1650421  CHEMBL1650424  CHEMBL1650429  CHEMBL1650430  CHEMBL1650431  CHEMBL1650435  CHEMBL1650436  CHEMBL1650439  CHEMBL1650443  CHEMBL1650446  CHEMBL1650447  CHEMBL1651764  CHEMBL1651766  CHEMBL1651767  CHEMBL1672127  CHEMBL1682974  CHEMBL1682979  CHEMBL1682981  CHEMBL1682985  CHEMBL1683086  CHEMBL1683087  CHEMBL1683088  CHEMBL1683089  CHEMBL1683090  CHEMBL1683092  CHEMBL1683096  CHEMBL1683101  CHEMBL1683102  CHEMBL370677  CHEMBL370755  CHEMBL371057  CHEMBL371143  CHEMBL371480  CHEMBL371521  CHEMBL371585  CHEMBL371907  CHEMBL372004  CHEMBL372078  CHEMBL372391  CHEMBL372472  CHEMBL37260  CHEMBL372746  CHEMBL373148  CHEMBL373268  CHEMBL3734769  CHEMBL3734964  CHEMBL3735129  CHEMBL3735329  CHEMBL3735433  CHEMBL3735843  CHEMBL3735852  CHEMBL3735917  CHEMBL3735925  CHEMBL3736137  CHEMBL3736190  CHEMBL3736423  CHEMBL3736511  CHEMBL374032  CHEMBL374688  CHEMBL37536  CHEMBL375442  CHEMBL375508  CHEMBL375745  CHEMBL376359  CHEMBL37748  CHEMBL377724  CHEMBL378048  CHEMBL378597  CHEMBL378673  CHEMBL379086  CHEMBL379260  CHEMBL379261  CHEMBL379702  CHEMBL3797299  CHEMBL37980  CHEMBL3799074  CHEMBL3799388  CHEMBL3800380  CHEMBL380240  CHEMBL380496  CHEMBL3804996  CHEMBL3805154  CHEMBL3805226  CHEMBL3805294  CHEMBL3805353  CHEMBL3805400  CHEMBL3805629  CHEMBL3805696  CHEMBL3806023  CHEMBL3806052  CHEMBL3806157  CHEMBL3806164  CHEMBL3806216  CHEMBL3806239  CHEMBL3806310  CHEMBL380681  CHEMBL381145  CHEMBL381340  CHEMBL3813856  CHEMBL381530  CHEMBL381806  CHEMBL382045  CHEMBL382127  CHEMBL382382  CHEMBL382674  CHEMBL383841  CHEMBL384816  CHEMBL385517  CHEMBL385711  CHEMBL386380  CHEMBL386812  CHEMBL387333  CHEMBL387552  CHEMBL388475  CHEMBL388900  CHEMBL3890161  CHEMBL389138  CHEMBL389151  CHEMBL389244  CHEMBL389537  CHEMBL389599  CHEMBL389600  CHEMBL389624  CHEMBL389803  CHEMBL389804  CHEMBL389848  CHEMBL3901191 | CHEMBL1683106  CHEMBL1683107  CHEMBL1683109  CHEMBL1683112  CHEMBL1683113  CHEMBL1683115  CHEMBL1683119  CHEMBL1683123  CHEMBL1683124  CHEMBL1683125  CHEMBL1683127  CHEMBL1683130  CHEMBL1683131  CHEMBL1683132  CHEMBL1683134  CHEMBL1683135  CHEMBL1683138  CHEMBL1683139  CHEMBL1683142  CHEMBL1683144  CHEMBL1683145  CHEMBL1683476  CHEMBL1683477  CHEMBL1683478  CHEMBL1683479  CHEMBL1683482  CHEMBL1683484  CHEMBL1683486  CHEMBL1683557  CHEMBL1683558  CHEMBL1683560  CHEMBL1683561  CHEMBL1683563  CHEMBL1683564  CHEMBL1683566  CHEMBL1683567  CHEMBL1683568  CHEMBL1683569  CHEMBL1683572  CHEMBL1683977  CHEMBL1683979  CHEMBL1683981  CHEMBL1683983  CHEMBL1683988  CHEMBL1683991  CHEMBL1683995  CHEMBL1684000  CHEMBL1688415  CHEMBL1688416  CHEMBL1688418  CHEMBL1688419  CHEMBL1688423  CHEMBL1688425  CHEMBL169962  CHEMBL170051  CHEMBL171033  CHEMBL171290  CHEMBL171430  CHEMBL1724888  CHEMBL172631  CHEMBL172730  CHEMBL17347  CHEMBL1744354  CHEMBL175872  CHEMBL1779688  CHEMBL1779689  CHEMBL1779691  CHEMBL1779692  CHEMBL1779696  CHEMBL1779705  CHEMBL1779706  CHEMBL1779710  CHEMBL1779713  CHEMBL177980  CHEMBL179289  CHEMBL180000  CHEMBL1808463  CHEMBL1808464  CHEMBL1808468  CHEMBL1808473  CHEMBL1808474  CHEMBL1808475  CHEMBL1809262  CHEMBL1812728  CHEMBL1812733  CHEMBL1812734  CHEMBL1812736  CHEMBL1812900  CHEMBL1812902  CHEMBL1812903  CHEMBL1812905  CHEMBL1812909  CHEMBL1812911  CHEMBL1814760  CHEMBL1819090  CHEMBL182168  CHEMBL182544  CHEMBL390194  CHEMBL390221  CHEMBL390241  CHEMBL390418  CHEMBL390513  CHEMBL390776  CHEMBL391037  CHEMBL391047  CHEMBL391048  CHEMBL3911786  CHEMBL391252  CHEMBL391269  CHEMBL391307  CHEMBL391332  CHEMBL391559  CHEMBL391634  CHEMBL391645  CHEMBL391929  CHEMBL392524  CHEMBL3926320  CHEMBL392696  CHEMBL392924  CHEMBL3932825  CHEMBL393336  CHEMBL393611  CHEMBL393947  CHEMBL3941804  CHEMBL3942715  CHEMBL3942843  CHEMBL3944427  CHEMBL394507  CHEMBL394594  CHEMBL394662  CHEMBL394834  CHEMBL394836  CHEMBL395004  CHEMBL3950517  CHEMBL395166  CHEMBL3952691  CHEMBL3952716  CHEMBL395546  CHEMBL395696  CHEMBL395798  CHEMBL395919  CHEMBL3959221  CHEMBL396136  CHEMBL396195  CHEMBL396789  CHEMBL397010  CHEMBL397070  CHEMBL397144  CHEMBL397242  CHEMBL397893  CHEMBL3981442  CHEMBL398661  CHEMBL399189  CHEMBL399499  CHEMBL399525  CHEMBL399615  CHEMBL399693  CHEMBL399726  CHEMBL399791  CHEMBL400338  CHEMBL400359  CHEMBL400532  CHEMBL400533  CHEMBL400624  CHEMBL400752  CHEMBL400761  CHEMBL400841  CHEMBL400911  CHEMBL400954  CHEMBL401057  CHEMBL401378  CHEMBL401542  CHEMBL401971  CHEMBL401972  CHEMBL402111  CHEMBL402151  CHEMBL402236  CHEMBL402466  CHEMBL402496  CHEMBL402573  CHEMBL402645  CHEMBL402819  CHEMBL403156  CHEMBL403160  CHEMBL403449  CHEMBL403553  CHEMBL403862  CHEMBL403882  CHEMBL403969  CHEMBL404159  CHEMBL404210  CHEMBL404220  CHEMBL404326  CHEMBL406219  CHEMBL4062977  CHEMBL4063983 | CHEMBL182861  CHEMBL183098  CHEMBL183418  CHEMBL184346  CHEMBL184380  CHEMBL184572  CHEMBL184624  CHEMBL184651  CHEMBL184808  CHEMBL185020  CHEMBL185067  CHEMBL185121  CHEMBL185244  CHEMBL1852708  CHEMBL185332  CHEMBL185482  CHEMBL186308  CHEMBL186406  CHEMBL186566  CHEMBL186610  CHEMBL186611  CHEMBL186787  CHEMBL187118  CHEMBL188043  CHEMBL188444  CHEMBL189046  CHEMBL189258  CHEMBL189645  CHEMBL190029  CHEMBL190183  CHEMBL190593  CHEMBL190752  CHEMBL191208  CHEMBL191327  CHEMBL191473  CHEMBL191486  CHEMBL191577  CHEMBL191805  CHEMBL191812  CHEMBL191823  CHEMBL191858  CHEMBL191866  CHEMBL192116  CHEMBL192425  CHEMBL192733  CHEMBL1929387  CHEMBL1929388  CHEMBL1929389  CHEMBL1929390  CHEMBL1929392  CHEMBL1929394  CHEMBL1929395  CHEMBL192980  CHEMBL193105  CHEMBL193106  CHEMBL193168  CHEMBL193802  CHEMBL193885  CHEMBL194993  CHEMBL1951417  CHEMBL1951418  CHEMBL1951419  CHEMBL1951420  CHEMBL1951422  CHEMBL1951424  CHEMBL1951427  CHEMBL1951428  CHEMBL1951431  CHEMBL1951432  CHEMBL1951433  CHEMBL1951434  CHEMBL1951435  CHEMBL1951436  CHEMBL1951437  CHEMBL1951438  CHEMBL1951439  CHEMBL1951440  CHEMBL1951597  CHEMBL1951599  CHEMBL1951601  CHEMBL1951602  CHEMBL1951603  CHEMBL1951604  CHEMBL1951605  CHEMBL1951608  CHEMBL1951610  CHEMBL1951612  CHEMBL1951613  CHEMBL195378  CHEMBL195420  CHEMBL195667  CHEMBL195721  CHEMBL195739  CHEMBL195804  CHEMBL195905  CHEMBL195984  CHEMBL196114  CHEMBL4064424  CHEMBL4068477  CHEMBL4071166  CHEMBL407293  CHEMBL4075351  CHEMBL4077174  CHEMBL4081741  CHEMBL4082445  CHEMBL4085550  CHEMBL4087191  CHEMBL4089584  CHEMBL4089615  CHEMBL4090906  CHEMBL4092983  CHEMBL4098218  CHEMBL4101425  CHEMBL410187  CHEMBL4105034  CHEMBL4111229  CHEMBL41114  CHEMBL4113723  CHEMBL411561  CHEMBL413797  CHEMBL415647  CHEMBL416008  CHEMBL424612  CHEMBL424687  CHEMBL424854  CHEMBL425347  CHEMBL425483  CHEMBL425585  CHEMBL425756  CHEMBL425905  CHEMBL426335  CHEMBL426469  CHEMBL427259  CHEMBL428747  CHEMBL428936  CHEMBL428937  CHEMBL429115  CHEMBL429258  CHEMBL429450  CHEMBL429653  CHEMBL429982  CHEMBL431885  CHEMBL432081  CHEMBL433572  CHEMBL437379  CHEMBL438258  CHEMBL438265  CHEMBL438520  CHEMBL438547  CHEMBL439067  CHEMBL439394  CHEMBL441559  CHEMBL442673  CHEMBL445437  CHEMBL451319  CHEMBL451619  CHEMBL452289  CHEMBL452290  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