**MLP Molecule Data Frame:**

<bound method NDFrame.head of mean\_fit\_time mean\_score\_time mean\_test\_score mean\_train\_score \

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1 4.800167 0.036709 0.920184 0.920281

2 2.312350 0.037515 0.920070 0.920254

3 7.829425 0.087833 0.920381 0.920373

4 6.129715 0.081834 0.920265 0.920207

5 3.013615 0.080423 0.920548 0.920619

6 3.420096 0.044920 0.920382 0.920373

7 4.332071 0.043115 0.920361 0.920396

8 2.589487 0.045322 0.920202 0.920365

9 21.012889 0.164638 0.920352 0.920371

10 8.712488 0.144184 0.920316 0.920402

11 8.975071 0.144599 0.920429 0.920192

12 15.474558 0.047745 0.929566 0.929821

13 26.643264 0.044134 0.920870 0.920913

14 9.276273 0.044928 0.928911 0.928966

15 180.320963 0.164036 0.929049 0.929281

16 29.813496 0.145998 0.919740 0.919727

17 20.614830 0.150008 0.929273 0.929211

18 42.006998 0.057553 0.930067 0.930049

19 52.213274 0.056951 0.926221 0.926283

20 14.582386 0.054144 0.929386 0.929325

21 394.402412 0.319450 0.928994 0.928853

22 58.707949 0.281156 0.919991 0.920051

23 56.549452 0.272124 0.929723 0.929814

24 23.634061 0.057976 0.929695 0.930010

25 19.412232 0.053544 0.927758 0.927847

26 9.044857 0.055748 0.928853 0.928997

27 254.383294 0.271924 0.930083 0.930271

28 54.762254 0.189304 0.927322 0.927424

29 32.462943 0.227606 0.929555 0.929776

30 63.769210 0.078008 0.930144 0.930354

31 24.387933 0.074198 0.928272 0.928363

32 13.397434 0.079813 0.929530 0.929661

33 465.362269 0.493714 0.930198 0.930472

34 90.619205 0.378013 0.928306 0.928361

35 39.929402 0.435582 0.930166 0.930345

36 20.066372 0.040909 0.929742 0.930036

37 13.899570 0.041109 0.928601 0.928689

38 8.246935 0.039915 0.929029 0.929387

39 158.066929 0.123328 0.930190 0.930778

40 30.657541 0.118917 0.928667 0.928804

41 16.501690 0.118917 0.930042 0.930633

42 37.628625 0.047936 0.930041 0.930106

43 14.870953 0.050543 0.929391 0.929368

44 9.117049 0.048337 0.929446 0.929604

45 344.349200 0.224196 0.930085 0.931069

46 59.133880 0.216377 0.929324 0.929524

47 29.945046 0.413701 0.929881 0.930562

param\_mlpclassifier\_\_activation param\_mlpclassifier\_\_hidden\_layer\_sizes \

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4 identity 100

5 identity 100

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7 identity (10, 10)

8 identity (10, 10)

9 identity (100, 100)

10 identity (100, 100)

11 identity (100, 100)

12 logistic 10

13 logistic 10

14 logistic 10

15 logistic 100

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18 logistic (10, 10)

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22 logistic (100, 100)

23 logistic (100, 100)

24 tanh 10

25 tanh 10

26 tanh 10

27 tanh 100

28 tanh 100

29 tanh 100

30 tanh (10, 10)

31 tanh (10, 10)

32 tanh (10, 10)

33 tanh (100, 100)

34 tanh (100, 100)

35 tanh (100, 100)

36 relu 10

37 relu 10

38 relu 10

39 relu 100

40 relu 100

41 relu 100

42 relu (10, 10)

43 relu (10, 10)

44 relu (10, 10)

45 relu (100, 100)

46 relu (100, 100)

47 relu (100, 100)

param\_mlpclassifier\_\_solver \

0 lbfgs

1 sgd

2 adam

3 lbfgs

4 sgd

5 adam

6 lbfgs

7 sgd

8 adam

9 lbfgs

10 sgd

11 adam

12 lbfgs

13 sgd

14 adam

15 lbfgs

16 sgd

17 adam

18 lbfgs

19 sgd

20 adam

21 lbfgs

22 sgd

23 adam

24 lbfgs

25 sgd

26 adam

27 lbfgs

28 sgd

29 adam

30 lbfgs

31 sgd

32 adam

33 lbfgs

34 sgd

35 adam

36 lbfgs

37 sgd

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43 sgd

44 adam

45 lbfgs

46 sgd

47 adam

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47 {'mlpclassifier\_\_activation': 'relu', 'mlpclas... 10

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1 0.919017 ... 0.920110 0.920262

2 0.919620 ... 0.919532 0.920289

3 0.919730 ... 0.919876 0.920455

4 0.919470 ... 0.919955 0.920234

5 0.919539 ... 0.920548 0.920684

6 0.919707 ... 0.919876 0.920459

7 0.919762 ... 0.919855 0.920589

8 0.919201 ... 0.920004 0.920443

9 0.919625 ... 0.919876 0.920474

10 0.919610 ... 0.919432 0.920576

11 0.919501 ... 0.919745 0.919975

12 0.928390 ... 0.930291 0.930100

13 0.919666 ... 0.921156 0.920878

14 0.927124 ... 0.929746 0.929185

15 0.927985 ... 0.929583 0.929716

16 0.918667 ... 0.919545 0.919678

17 0.928036 ... 0.929492 0.929016

18 0.929810 ... 0.930405 0.930160

19 0.926701 ... 0.928303 0.927693

20 0.928058 ... 0.929991 0.929343

21 0.928123 ... 0.929552 0.929120

22 0.918768 ... 0.919862 0.920041

23 0.928445 ... 0.930330 0.930471

24 0.929047 ... 0.929930 0.929915

25 0.926538 ... 0.927880 0.927709

26 0.928202 ... 0.929367 0.929049

27 0.929068 ... 0.930486 0.930199

28 0.926262 ... 0.927239 0.927286

29 0.928350 ... 0.929472 0.929438

30 0.929366 ... 0.930563 0.930130

31 0.927315 ... 0.928712 0.928013

32 0.929284 ... 0.930171 0.929878

33 0.929697 ... 0.930866 0.930387

34 0.927036 ... 0.928928 0.928078

35 0.929339 ... 0.930993 0.930498

36 0.928821 ... 0.930291 0.929738

37 0.927958 ... 0.929035 0.928481

38 0.928214 ... 0.929868 0.929130

39 0.929113 ... 0.931168 0.930670

40 0.927788 ... 0.929491 0.928685

41 0.928903 ... 0.930642 0.930621

42 0.929054 ... 0.930518 0.929724

43 0.928026 ... 0.930095 0.929346

44 0.929018 ... 0.929905 0.929605

45 0.929028 ... 0.931191 0.930657

46 0.928497 ... 0.929898 0.929552

47 0.929858 ... 0.930323 0.930535

split3\_test\_score split3\_train\_score split4\_test\_score \

0 0.919519 0.920548 0.919962

1 0.919694 0.920440 0.919601

2 0.919302 0.920168 0.919678

3 0.919585 0.920550 0.919971

4 0.919613 0.920344 0.919627

5 0.920253 0.920918 0.919886

6 0.919542 0.920577 0.920013

7 0.919549 0.920583 0.919741

8 0.919254 0.920386 0.920151

9 0.919638 0.920504 0.919902

10 0.919861 0.920478 0.920076

11 0.920182 0.920821 0.920210

12 0.929027 0.929648 0.928042

13 0.920054 0.921092 0.920470

14 0.928883 0.929472 0.927955

15 0.928135 0.929210 0.928153

16 0.919288 0.919925 0.919492

17 0.928966 0.929698 0.928035

18 0.929635 0.929938 0.928113

19 0.926763 0.928022 0.919557

20 0.928862 0.929791 0.928370

21 0.928244 0.928590 0.928047

22 0.919245 0.920185 0.919881

23 0.929843 0.930112 0.928899

24 0.928943 0.930063 0.928402

25 0.927199 0.927974 0.927263

26 0.927604 0.928627 0.928453

27 0.929531 0.930472 0.929175

28 0.926285 0.927477 0.926881

29 0.929061 0.929571 0.928674

30 0.929695 0.930572 0.928783

31 0.926898 0.928629 0.927908

32 0.928420 0.929218 0.928130

33 0.929282 0.930456 0.928709

34 0.926953 0.928378 0.928183

35 0.929211 0.929978 0.928986

36 0.928716 0.930016 0.928577

37 0.928273 0.928733 0.927224

38 0.927761 0.928919 0.927668

39 0.929158 0.930889 0.929266

40 0.927508 0.928884 0.927533

41 0.929145 0.930637 0.929215

42 0.929192 0.930135 0.929307

43 0.929186 0.929478 0.928056

44 0.928639 0.929538 0.928730

45 0.929147 0.931311 0.928845

46 0.928653 0.929721 0.928208

47 0.929136 0.930244 0.928387

split4\_train\_score std\_fit\_time std\_score\_time std\_test\_score \

0 0.920477 0.089803 0.001375 0.001195

1 0.920371 0.168636 0.000499 0.001208

2 0.920432 0.058014 0.001625 0.001081

3 0.920493 0.021946 0.001360 0.001189

4 0.920430 0.155583 0.002433 0.001209

5 0.920639 0.190095 0.000759 0.001041

6 0.920460 0.093111 0.001725 0.001206

7 0.920438 0.220691 0.002537 0.001271

8 0.920597 0.088554 0.002794 0.001164

9 0.920495 0.739248 0.001944 0.001190

10 0.920617 0.392162 0.002793 0.001163

11 0.920774 1.197598 0.004288 0.001073

12 0.930321 0.762412 0.002422 0.001473

13 0.921017 0.333550 0.001435 0.001175

14 0.928903 0.477242 0.002791 0.001308

15 0.929347 0.875092 0.008451 0.001305

16 0.919803 0.625065 0.005951 0.001033

17 0.929066 3.291362 0.007611 0.001399

18 0.930382 2.779854 0.001860 0.001378

19 0.920685 16.178531 0.003196 0.003520

20 0.929656 1.369532 0.000897 0.001309

21 0.929023 0.780678 0.018689 0.001146

22 0.920106 0.373077 0.003149 0.001180

23 0.930504 5.609420 0.007782 0.000958

24 0.930492 3.418753 0.003877 0.001323

25 0.928076 0.344173 0.001859 0.001156

26 0.929335 0.955228 0.003391 0.001058

27 0.930591 9.361143 0.020087 0.001150

28 0.927656 2.393227 0.004367 0.001361

29 0.930240 7.051770 0.009035 0.001384

30 0.930784 0.215022 0.002645 0.001227

31 0.928123 1.088809 0.003171 0.001282

32 0.930139 0.782298 0.004466 0.001275

33 0.930933 22.206998 0.010118 0.001323

34 0.928778 4.364407 0.009529 0.001293

35 0.930922 5.421511 0.020810 0.001283

36 0.930484 3.411452 0.000983 0.001423

37 0.929071 0.161814 0.002103 0.001120

38 0.930168 0.593104 0.000993 0.001524

39 0.931218 0.400917 0.002615 0.001285

40 0.929012 0.826426 0.002339 0.001386

41 0.931416 3.848513 0.003784 0.001286

42 0.930744 0.081448 0.000763 0.001170

43 0.929668 0.230294 0.001866 0.001344

44 0.930373 1.514349 0.001175 0.000871

45 0.931227 0.818769 0.003209 0.001363

46 0.929848 3.222991 0.004969 0.001172

47 0.931249 10.585809 0.149619 0.001122

std\_train\_score

0 0.000303

1 0.000361

2 0.000336

3 0.000294

4 0.000313

5 0.000300

6 0.000308

7 0.000308

8 0.000357

9 0.000298

10 0.000343

11 0.000539

12 0.000392

13 0.000288

14 0.000433

15 0.000374

16 0.000346

17 0.000327

18 0.000280

19 0.002812

20 0.000376

21 0.000287

22 0.000247

23 0.000759

24 0.000417

25 0.000327

26 0.000414

27 0.000270

28 0.000249

29 0.000321

30 0.000340

31 0.000414

32 0.000623

33 0.000304

34 0.000378

35 0.000415

36 0.000301

37 0.000342

38 0.000523

39 0.000273

40 0.000268

41 0.000450

42 0.000436

43 0.000238

44 0.000540

45 0.000281

46 0.000347

47 0.000442

[48 rows x 23 columns]>

Test set score: 0.93 Best parameters: {'mlpclassifier\_\_activation': 'tanh', 'mlpclassifier\_\_hidden\_layer\_sizes': (100,100), 'mlpclassifier\_\_solver': 'lbfgs'}

**kNN Molecule Data Frame:**

<bound method NDFrame.head of mean\_fit\_time mean\_score\_time mean\_test\_score mean\_train\_score \

0 0.807989 28.115727 0.899674 1.000000

1 0.681019 27.513103 0.899674 1.000000

2 0.829836 14.216610 0.898265 1.000000

3 0.826422 14.224471 0.898265 1.000000

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27 0.827400 25.090176 0.916400 1.000000

28 0.827602 97.992603 0.915204 0.940363

29 0.828411 98.010282 0.915482 1.000000

param\_kneighborsclassifier\_\_n\_neighbors param\_kneighborsclassifier\_\_p \

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1 1 1

2 1 2

3 1 2

4 1 3

5 1 3

6 2 1

7 2 1

8 2 2

9 2 2

10 2 3

11 2 3

12 3 1

13 3 1

14 3 2

15 3 2

16 3 3

17 3 3

18 4 1

19 4 1

20 4 2

21 4 2

22 4 3

23 4 3

24 5 1

25 5 1

26 5 2

27 5 2

28 5 3

29 5 3

param\_kneighborsclassifier\_\_weights \

0 uniform

1 distance

2 uniform

3 distance

4 uniform

5 distance

6 uniform

7 distance

8 uniform

9 distance

10 uniform

11 distance

12 uniform

13 distance

14 uniform

15 distance

16 uniform

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23 distance

24 uniform

25 distance

26 uniform

27 distance

28 uniform

29 distance

params rank\_test\_score \

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2 0.897933 ... 0.898673 1.000000

3 0.897933 ... 0.898673 1.000000

4 0.897234 ... 0.896840 1.000000

5 0.897234 ... 0.896840 1.000000

6 0.901032 ... 0.903073 0.942805

7 0.899605 ... 0.899385 1.000000

8 0.901015 ... 0.902129 0.943883

9 0.897933 ... 0.898673 1.000000

10 0.899526 ... 0.901094 0.943818

11 0.897234 ... 0.896840 1.000000

12 0.911937 ... 0.913394 0.951468

13 0.912351 ... 0.914008 1.000000

14 0.910678 ... 0.912231 0.950581

15 0.910765 ... 0.912368 1.000000

16 0.909625 ... 0.910926 0.950335

17 0.909811 ... 0.911039 1.000000

18 0.909328 ... 0.911877 0.936730

19 0.912766 ... 0.913578 1.000000

20 0.910428 ... 0.911361 0.936538

21 0.911226 ... 0.912654 1.000000

22 0.910018 ... 0.910445 0.936197

23 0.909748 ... 0.911791 1.000000

24 0.915644 ... 0.917913 0.941759

25 0.916096 ... 0.918466 1.000000

26 0.915455 ... 0.916636 0.940461

27 0.915695 ... 0.916919 1.000000

28 0.913624 ... 0.915056 0.940338

29 0.913894 ... 0.915411 1.000000

split3\_test\_score split3\_train\_score split4\_test\_score \

0 0.899644 1.000000 0.899567

1 0.899644 1.000000 0.899567

2 0.898134 1.000000 0.897961

3 0.898134 1.000000 0.897961

4 0.897412 1.000000 0.898360

5 0.897412 1.000000 0.898360

6 0.899990 0.942700 0.901830

7 0.899644 1.000000 0.899567

8 0.899943 0.943574 0.901912

9 0.898134 1.000000 0.897961

10 0.898811 0.943339 0.901957

11 0.897412 1.000000 0.898360

12 0.913158 0.951672 0.912322

13 0.913766 1.000000 0.912851

14 0.910417 0.950380 0.911689

15 0.910696 1.000000 0.912001

16 0.909969 0.950152 0.911447

17 0.910152 1.000000 0.911613

18 0.910921 0.936649 0.910837

19 0.913449 1.000000 0.913083

20 0.910068 0.936127 0.911320

21 0.911433 1.000000 0.912261

22 0.909050 0.935963 0.910840

23 0.911372 1.000000 0.911369

24 0.915966 0.941917 0.916500

25 0.916685 1.000000 0.917290

26 0.915705 0.940452 0.916001

27 0.916097 1.000000 0.916248

28 0.915814 0.940297 0.915111

29 0.916152 1.000000 0.915306

split4\_train\_score std\_fit\_time std\_score\_time std\_test\_score \

0 1.000000 0.240691 1.305146 0.000263

1 1.000000 0.015684 0.268344 0.000263

2 1.000000 0.011947 0.187532 0.000321

3 1.000000 0.017201 0.133507 0.000321

4 1.000000 0.014564 0.661160 0.000516

5 1.000000 0.018767 0.610686 0.000516

6 0.942610 0.016486 0.346057 0.001064

7 1.000000 0.018736 0.379205 0.000263

8 0.943384 0.017442 0.209151 0.000903

9 1.000000 0.016717 0.220090 0.000321

10 0.943144 0.016426 0.931827 0.001311

11 1.000000 0.016711 0.836023 0.000516

12 0.951571 0.016749 0.345490 0.000653

13 1.000000 0.015106 0.346715 0.000690

14 0.950981 0.016454 0.247315 0.000701

15 1.000000 0.019551 0.270858 0.000697

16 0.950284 0.015784 1.011710 0.000960

17 1.000000 0.014534 1.024812 0.000984

18 0.937172 0.016598 0.398289 0.001000

19 1.000000 0.016117 0.368961 0.000644

20 0.936437 0.015282 0.279657 0.000526

21 1.000000 0.016074 0.294874 0.000677

22 0.936087 0.015327 1.146114 0.000918

23 1.000000 0.017299 1.147856 0.000966

24 0.942300 0.014760 0.360962 0.001020

25 1.000000 0.016043 0.413789 0.001009

26 0.941183 0.015873 0.300838 0.000497

27 1.000000 0.016892 0.279553 0.000508

28 0.940240 0.016554 1.210304 0.000934

29 1.000000 0.015992 1.213699 0.000934

std\_train\_score

0 0.000000

1 0.000000

2 0.000000

3 0.000000

4 0.000000

5 0.000000

6 0.000184

7 0.000000

8 0.000289

9 0.000000

10 0.000259

11 0.000000

12 0.000149

13 0.000000

14 0.000252

15 0.000000

16 0.000198

17 0.000000

18 0.000299

19 0.000000

20 0.000191

21 0.000000

22 0.000177

23 0.000000

24 0.000415

25 0.000000

26 0.000320

27 0.000000

28 0.000145

29 0.000000

[30 rows x 23 columns]>

Test set score: 0.92

Best parameters: {'kneighborsclassifier\_\_n\_neighbors': 5, 'kneighborsclassifier\_\_p': 1, 'kneighborsclassifier\_\_weights': 'distance'}