*Supplementary Material for*

# Clinical development and informatics analysis of natural and semi-synthetic flavonoid drugs: a critical review

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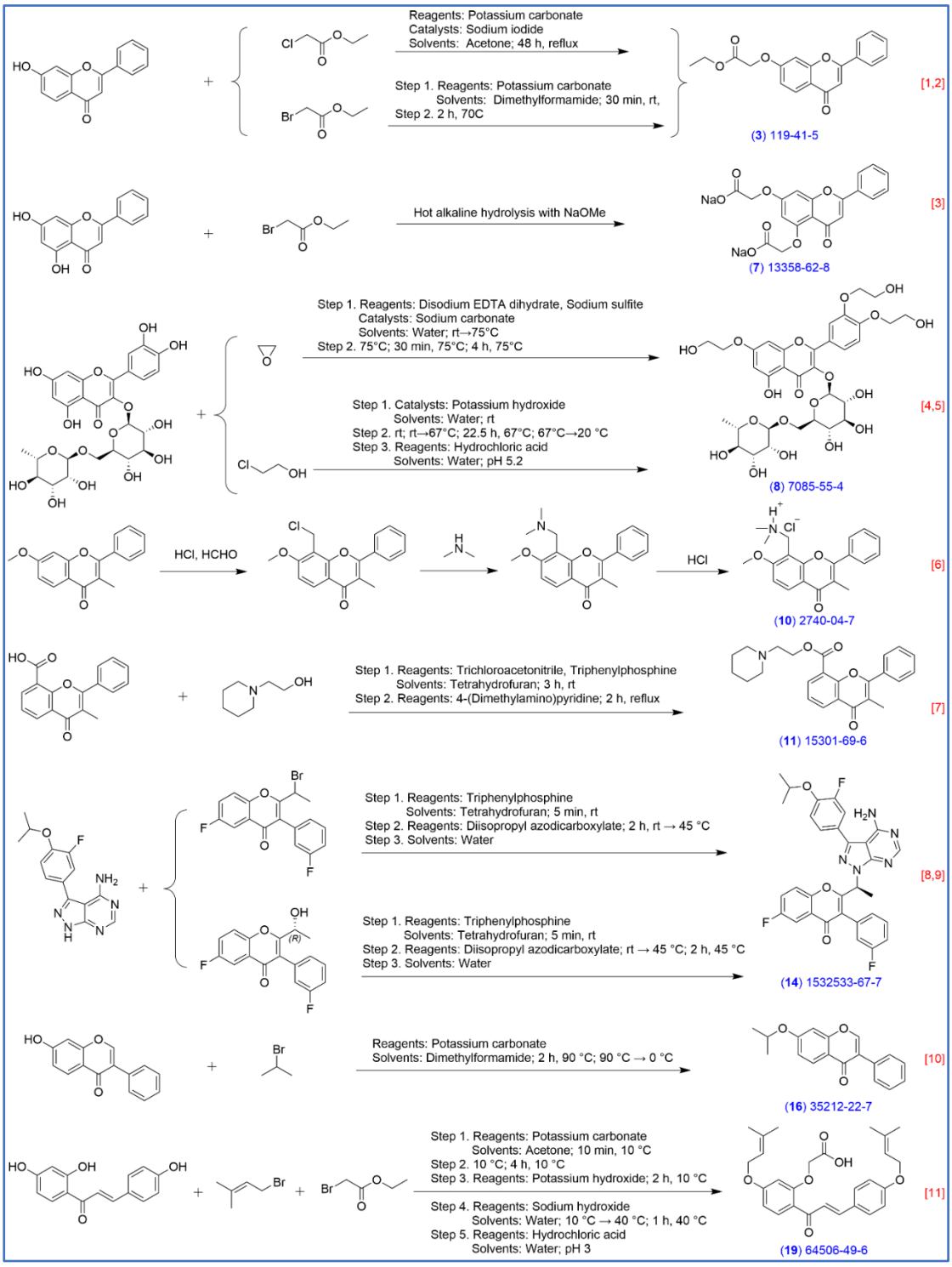
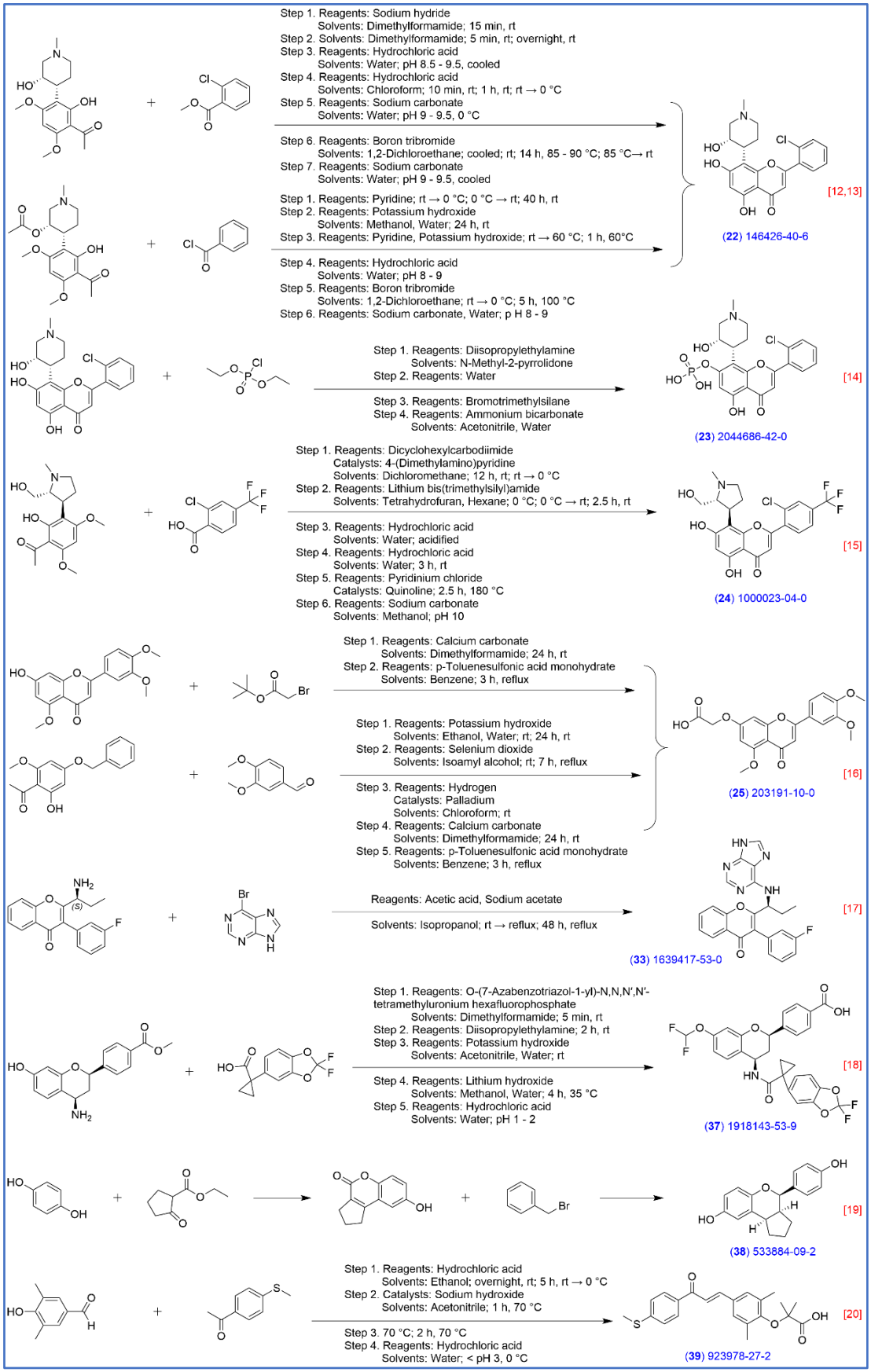
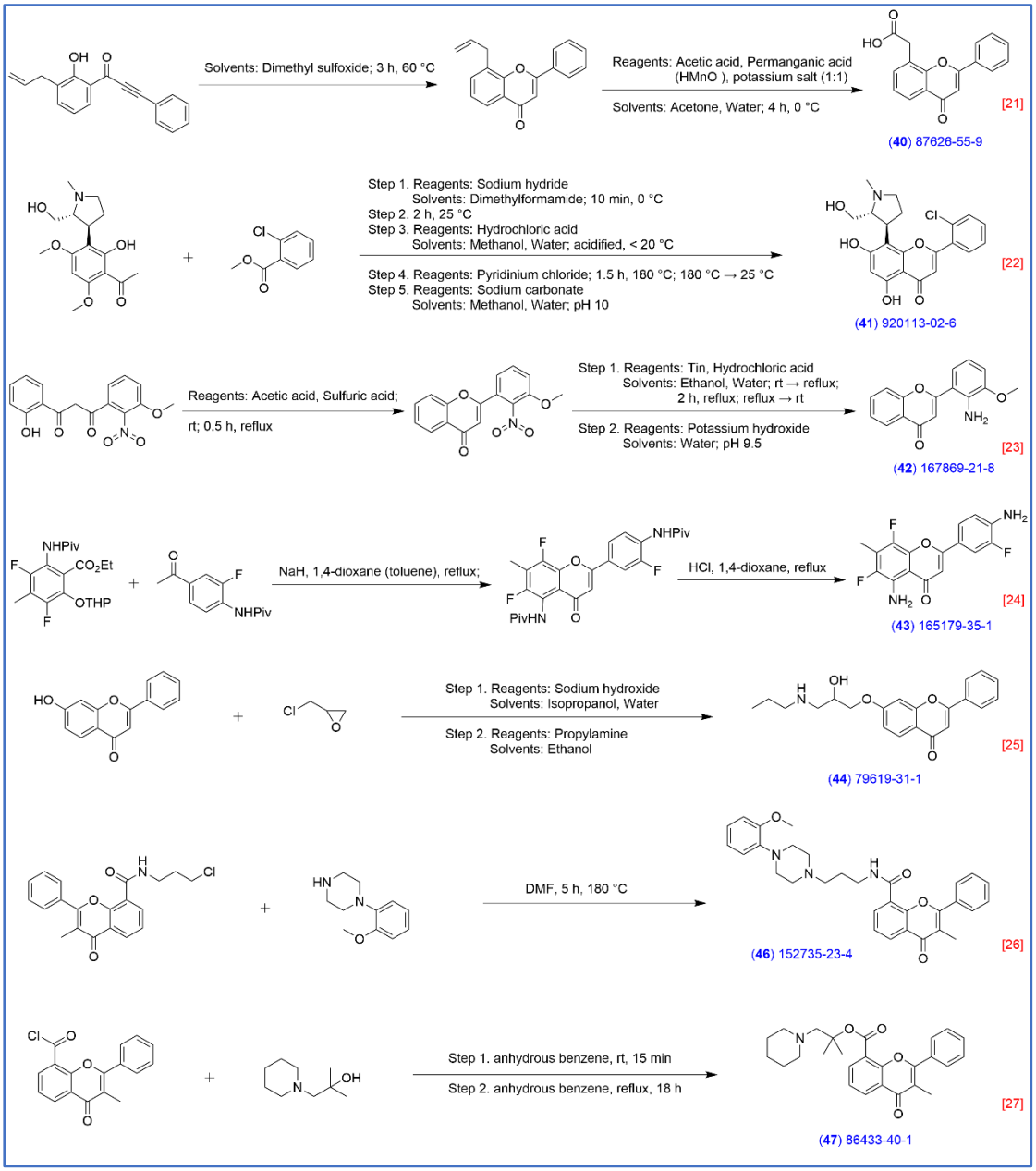


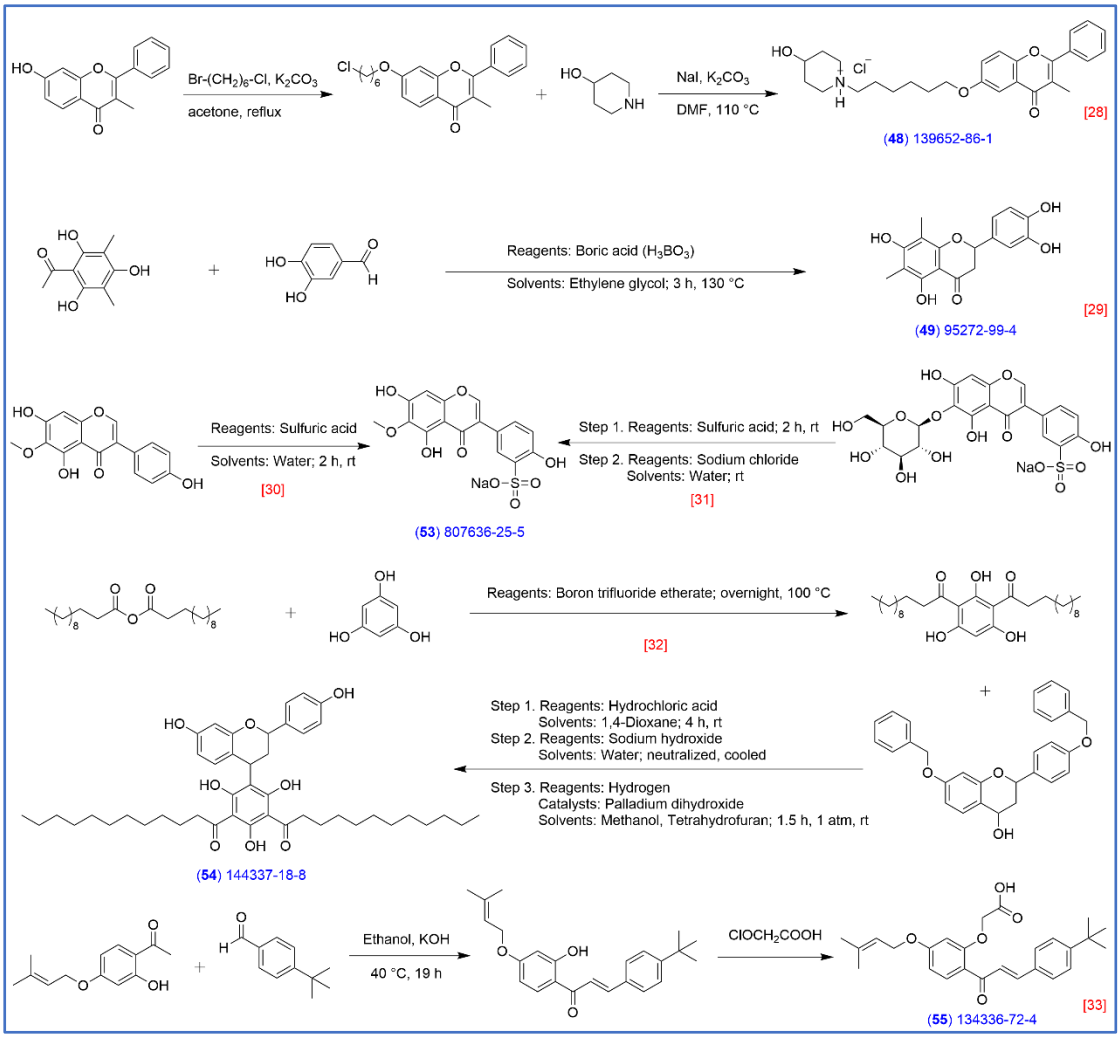

**Scheme S1.** The semi-synthetic routes and reference for flavonoid-derived drug molecules **3**, **7**, **8**, **10**, **11**, **14**, **16**, and **19**.




**Scheme S2.** The semi-synthetic routes and reference for flavonoid-derived drug candidates **22-25**, **33**, and **37-39**.




**Scheme S3.** The semi-synthetic routes and reference for flavonoid-derived drug candidates **40**-**44**, **46**, and **47**.




**Scheme S4.** The semi-synthetic routes and reference for flavonoid-derived drug candidates **48**, **49**, and **53-55**.

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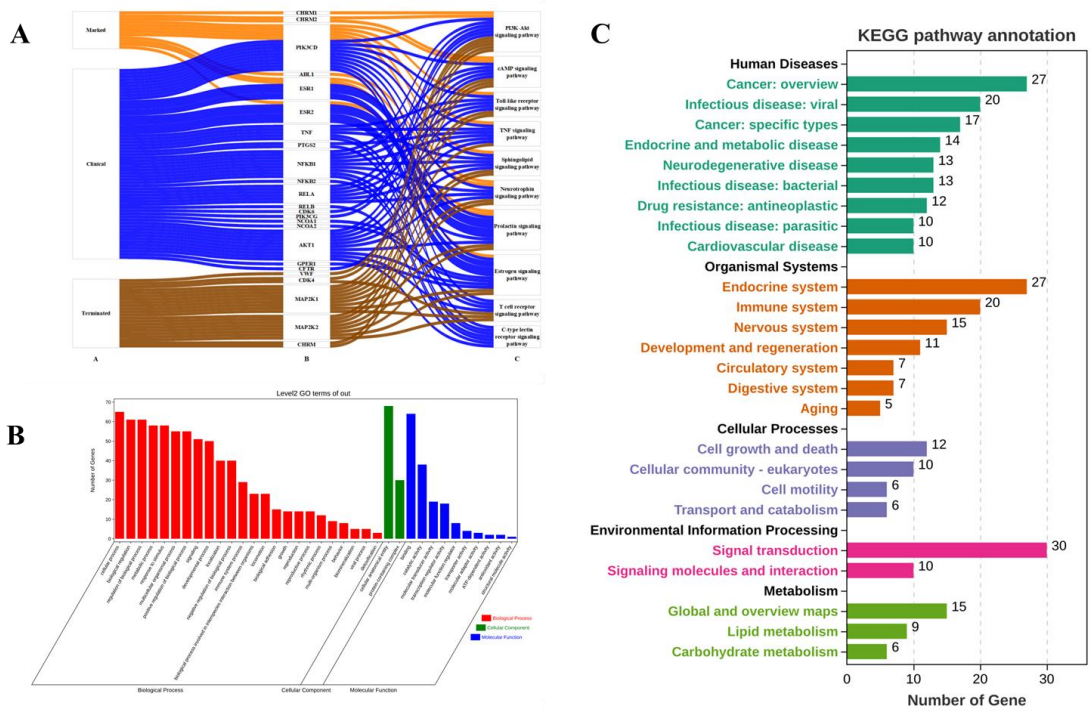


**Figure S1.** Bioinformatic analysis for flavonoid-based marketed drugs (**1**–**4** and **6**–**19**) and clinical candidates (**20**–**51** and **53**–**55**). (A) Sankey diagram of drug-target-pathway. (B) Bar graph of GO pathway annotation analysis. (C) Bar plot of KEGG pathway annotation analysis.

**Table S1.** The original structural and physicochemical parameters of flavonoid-based drugs (**1**–**4** and **6**–**19**) and candidates (**20**–**51** and **53**–**55**).

| NO. | CAS | SMILLES | MW | H-Donors | H-Acceptors | cLogP | cLogS | Rotatable Bonds | Polar Surface Area | sp3-Atoms | total C | sp3/total C | Aromatic Rings | Total Surface Area | Relative PSA | Stereo Centers | nSteo/MW | Small Rings | Hetero-Rings | Hetero-Rings/Rings | RngAr/Rings | Shape Index | Molecular Flexibility | Molecular Complexity |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **1** | 22368-21-4 | COC1=CC(C(OC2=CC(O)=C(C(O)=C23)OC)=CC3=O)=CC=C1OC | 344.32 | 2 | 7 | 2.47 | -3.21 | 4 | 94.45 | 9 | 18 | 0.5000 | 2 | 251.46 | 0.31512 | 0 | 0.0000 | 3 | 1 | 0.33 | 0.67 | 0.56 | 0.29 | 0.88 |
| **2** | 520-27-4 | O[C@H]([C@H]1O)[C@@H](O[C@@H](OC[C@@H](O[C@H]2OC3=CC(OC(C4=CC=C(C(O)=C4)OC)=CC5=O)=C5C(O)=C3)[C@H]([C@@H]([C@H]2O)O)O)[C@@H]1O)C | 608.55 | 8 | 15 | -0.63 | -2.97 | 7 | 234.29 | 27 | 28 | 0.9643 | 2 | 409.06 | 0.43475 | 10 | 0.0164 | 5 | 3 | 0.60 | 0.40 | 0.51 | 0.35 | 0.95 |
| **3** | 119-41-5 | O=C(OCC)COC1=CC=C2C(C=C(C3=CC=CC=C3)OC2=C1)=O | 324.33 | 0 | 5 | 3.27 | -3.97 | 6 | 61.83 | 6 | 19 | 0.3158 | 2 | 249.51 | 0.22476 | 0 | 0.0000 | 3 | 1 | 0.33 | 0.67 | 0.63 | 0.35 | 0.80 |
| **4** | 21967-41-9 | OC1=C(C2=O)C(OC(C3=CC=CC=C3)=C2)=CC(O[C@H]4[C@H](O)[C@H]([C@@H]([C@H](O4)C(O)=O)O)O)=C1O | 446.36 | 6 | 11 | 0.00 | -2.72 | 4 | 183.21 | 14 | 21 | 0.6667 | 2 | 296.83 | 0.45373 | 5 | 0.0112 | 4 | 2 | 0.50 | 0.50 | 0.47 | 0.20 | 0.93 |
| **6** | 27740-01-8 | O[C@H]1[C@@H](O[C@H](C(O)=O)[C@@H](O)[C@@H]1O)OC2=CC(OC(C3=CC=C(C=C3)O)=CC4=O)=C4C(O)=C2O | 462.36 | 7 | 12 | -0.35 | -2.43 | 4 | 203.44 | 15 | 21 | 0.7143 | 2 | 303.18 | 0.48743 | 5 | 0.0108 | 4 | 2 | 0.50 | 0.50 | 0.48 | 0.20 | 0.93 |
| **7** | 13358-62-8 | O=C(COC1=C2C(OC(C3=CC=CC=C3)=CC2=O)=CC(OCC(O[Na])=O)=C1)O[Na] | 414.28 | 0 | 8 | -2.66 | -3.33 | 7 | 125.02 | 7 | 19 | 0.3684 | 2 | 261.5 | 0.3408 | 0 | 0.0000 | 3 | 1 | 0.33 | 0.67 | 0.48 | 0.35 | 0.87 |
| **8** | 7085-55-4 | O=C1C(O[C@@H]([C@@H]([C@@H](O)[C@@H]2O)O)O[C@@H]2CO[C@H](O[C@@H](C)[C@H](O)[C@H]3O)[C@@H]3O)=C(C4=CC(OCCO)=C(OCCO)C=C4)OC5=CC(OCCO)=CC(O)=C15 | 742.68 | 10 | 19 | -1.99 | -2.72 | 15 | 293.21 | 36 | 33 | 1.0909 | 2 | 510.27 | 0.43906 | 10 | 0.0135 | 5 | 3 | 0.60 | 0.40 | 0.40 | 0.41 | 0.99 |
| **9** | 118525-40-9 | OC1=C(OC2=C(C(O)=CC(O)=C2C1=O)C/C=C(C)/C)C3=CC=C(C=C3)OC | 368.38 | 3 | 6 | 4.13 | -4.04 | 4 | 96.22 | 9 | 21 | 0.4286 | 2 | 274.49 | 0.26354 | 0 | 0.0000 | 3 | 1 | 0.33 | 0.67 | 0.52 | 0.35 | 0.91 |
| **10** | 2740/4/7 | O=C1C2=C(OC(C3=CC=CC=C3)=C1C)C(C[N+](C)([H])C)=C(OC)C=C2.[Cl-] | 323.39 | 0 | 4 | 3.37 | -3.40 | 4 | 38.77 | 8 | 24 | 0.3333 | 2 | 253.29 | 0.14446 | 0 | 0.0000 | 3 | 1 | 0.33 | 0.67 | 0.46 | 0.33 | 0.89 |
| **11** | 15301-69-6 | O=C1C2=C(OC(C3=CC=CC=C3)=C1C)C(C(OCCN4CCCCC4)=O)=CC=C2 | 391.47 | 0 | 5 | 4.56 | -4.39 | 6 | 55.84 | 11 | 20 | 0.5500 | 2 | 303.32 | 0.16362 | 0 | 0.0000 | 4 | 2 | 0.50 | 0.50 | 0.55 | 0.38 | 0.88 |
| **12** | 520-26-3 | O=C1C(C(O)=CC(O[C@@H]2O[C@H](CO[C@H]3[C@H](O)[C@H](O)[C@@H](O)[C@H](C)O3)[C@@H](O)[C@H](O)[C@H]2O)=C4)=C4O[C@H](C5=CC=C(OC)C(O)=C5)C1 | 610.56 | 8 | 15 | -0.81 | -2.75 | 7 | 234.29 | 29 | 28 | 1.0357 | 2 | 410.61 | 0.43311 | 11 | 0.0180 | 5 | 3 | 0.60 | 0.40 | 0.51 | 0.35 | 0.95 |
| **13** | 22888-70-6 | O=C1[C@H](O)[C@@H](C2=CC=C(O[C@H](CO)[C@@H](C3=CC=C(O)C(OC)=C3)O4)C4=C2)OC5=CC(O)=CC(O)=C15 | 482.44 | 5 | 10 | 2.13 | -3.41 | 4 | 155.14 | 15 | 25 | 0.6000 | 3 | 331.3 | 0.3578 | 4 | 0.0083 | 5 | 2 | 0.40 | 0.60 | 0.46 | 0.32 | 0.94 |
| **14** | 1532533-67-7 | NC(N=CN=C12)=C2C(C3=CC=C(C(F)=C3)OC(C)C)=NN1[C@@H](C)C(OC4=CC=C(C=C4C5=O)F)=C5C6=CC=CC(F)=C6 | 571.56 | 1 | 8 | 5.28 | -8.55 | 6 | 105.15 | 7 | 31 | 0.2258 | 5 | 409.14 | 0.21531 | 1 | 0.0017 | 6 | 3 | 0.50 | 0.83 | 0.43 | 0.31 | 1.00 |
| **15** | 3681-99-0 | OC1=CC=C2C(OC=C(C3=CC=C(O)C=C3)C2=O)=C1[C@@H]([C@@H]([C@@H](O)[C@@H]4O)O)O[C@@H]4CO | 416.38 | 6 | 9 | -0.44 | -2.44 | 3 | 156.91 | 14 | 21 | 0.6667 | 2 | 282.84 | 0.39471 | 5 | 0.0120 | 4 | 2 | 0.50 | 0.50 | 0.50 | 0.33 | 0.95 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **16** | 35212-22-7 | CC(C)OC1=CC=C(C2=O)C(OC=C2C3=CC=CC=C3)=C1 | 280.32 | 0 | 3 | 3.36 | -4.31 | 3 | 35.53 | 5 | 18 | 0.2778 | 2 | 219 | 0.15087 | 0 | 0.0000 | 3 | 1 | 0.33 | 0.67 | 0.62 | 0.33 | 0.79 |
| **17** | 486-66-8 | OC1=CC=C(C2=O)C(OC=C2C3=CC=C(C=C3)O)=C1 | 254.24 | 2 | 4 | 1.97 | -3.02 | 1 | 66.76 | 3 | 15 | 0.2000 | 2 | 184.68 | 0.26662 | 0 | 0.0000 | 3 | 1 | 0.33 | 0.67 | 0.63 | 0.30 | 0.78 |
| **18** | 154-23-4 | O[C@@H]1[C@@H](C2=CC=C(O)C(O)=C2)OC3=CC(O)=CC(O)=C3C1 | 290.27 | 5 | 6 | 1.51 | -1.76 | 1 | 110.38 | 9 | 15 | 0.6000 | 2 | 200.03 | 0.37744 | 2 | 0.0069 | 3 | 1 | 0.33 | 0.67 | 0.52 | 0.28 | 0.82 |
| **19** | 64506-49-6 | O=C(O)COC1=CC(OC/C=C(C)/C)=CC=C1C(/C=C/C2=CC=C(OC/C=C(C)/C)C=C2)=O | 450.53 | 1 | 6 | 5.56 | -5.14 | 12 | 82.06 | 11 | 27 | 0.4074 | 2 | 371.11 | 0.18641 | 0 | 0.0000 | 2 | 0 | 0.00 | 1.00 | 0.64 | 0.52 | 0.77 |
| **20** | 491-67-8 | O=C1C=C(C2=CC=CC=C2)OC3=CC(O)=C(O)C(O)=C13 | 270.24 | 3 | 5 | 2.34 | -2.86 | 1 | 86.99 | 4 | 15 | 0.2667 | 2 | 191.03 | 0.32634 | 0 | 0.0000 | 3 | 1 | 0.33 | 0.67 | 0.55 | 0.23 | 0.83 |
| **21** | 632-85-9 | O=C1C=C(C2=CC=CC=C2)OC3=C(OC)C(O)=CC(O)=C13 | 284.27 | 2 | 5 | 2.61 | -3.17 | 2 | 75.99 | 5 | 16 | 0.3125 | 2 | 206.94 | 0.28627 | 0 | 0.0000 | 3 | 1 | 0.33 | 0.67 | 0.48 | 0.27 | 0.86 |
| **22** | 146426-40-6 | ClC1=CC=CC=C1C(OC2=C(C(O)=CC(O)=C23)[C@H]([C@@H](C4)O)CCN4C)=CC3=O | 401.85 | 3 | 6 | 3.52 | -3.87 | 2 | 90.23 | 11 | 21 | 0.5238 | 2 | 281.79 | 0.23383 | 2 | 0.0050 | 4 | 2 | 0.50 | 0.50 | 0.46 | 0.27 | 0.93 |
| **23** | 2044686-42-0 | O=C1C=C(C2=CC=CC=C2Cl)OC3=C([C@H]4[C@@H](O)CN(C)CC4)C(OP(O)(O)=O)=CC(O)=C13 | 481.82 | 4 | 9 | -0.65 | -2.76 | 4 | 146.57 | 14 | 21 | 0.6667 | 2 | 321.91 | 0.32932 | 2 | 0.0042 | 4 | 2 | 0.50 | 0.50 | 0.41 | 0.33 | 0.95 |
| **24** | 1000023-04-0 | ClC1=CC(C(F)(F)F)=CC=C1C(OC2=C(C(O)=CC(O)=C23)[C@@H]([C@@H]4CO)CCN4C)=CC3=O | 469.84 | 3 | 6 | 4.27 | -4.65 | 4 | 90.23 | 12 | 22 | 0.5455 | 2 | 311.25 | 0.21169 | 2 | 0.0043 | 4 | 2 | 0.50 | 0.50 | 0.44 | 0.33 | 0.95 |
| **25** | 203191-10-0 | COC1=CC(C(OC2=CC(OCC(O)=O)=CC(OC)=C23)=CC3=O)=CC=C1OC | 386.36 | 1 | 8 | 2.22 | -3.59 | 7 | 100.52 | 10 | 20 | 0.5000 | 2 | 286.62 | 0.31114 | 0 | 0.0000 | 3 | 1 | 0.33 | 0.67 | 0.54 | 0.32 | 0.86 |
| **26** | 480-11-5 | OC1=C2C(OC(C3=CC=CC=C3)=CC2=O)=CC(O)=C1OC | 284.27 | 2 | 5 | 2.61 | -3.17 | 2 | 75.99 | 5 | 16 | 0.3125 | 2 | 206.94 | 0.28627 | 0 | 0.0000 | 3 | 1 | 0.33 | 0.67 | 0.57 | 0.27 | 0.85 |
| **27** | 528-48-3 | OC1=CC(C(OC2=CC(O)=CC=C2C3=O)=C3O)=CC=C1O | 286.24 | 4 | 6 | 1.84 | -2.79 | 1 | 107.22 | 5 | 15 | 0.3333 | 2 | 195.59 | 0.38577 | 0 | 0.0000 | 3 | 1 | 0.33 | 0.67 | 0.52 | 0.30 | 0.84 |
| **28** | 117-39-5 | OC1=CC(C(OC2=CC(O)=CC(O)=C2C3=O)=C3O)=CC=C1O | 302.24 | 5 | 7 | 1.49 | -2.49 | 1 | 127.45 | 6 | 15 | 0.4000 | 2 | 201.94 | 0.43845 | 0 | 0.0000 | 3 | 1 | 0.33 | 0.67 | 0.50 | 0.29 | 0.85 |
| **29** | 482-35-9 | OC(C=CC(C1=C(O[C@H]2[C@H](O)[C@H]([C@@H]([C@H](O2)CO)O)O)C(C3=C(O)C=C(C=C3O1)O)=O)=C4)=C4O | 464.38 | 8 | 12 | -0.35 | -2.19 | 4 | 206.6 | 17 | 21 | 0.8095 | 2 | 303.75 | 0.48672 | 5 | 0.0108 | 4 | 2 | 0.50 | 0.50 | 0.39 | 0.36 | 0.94 |
| **30** | 480-39-7 | O=C1C[C@@H](C2=CC=CC=C2)OC3=CC(O)=CC(O)=C13 | 256.26 | 2 | 4 | 2.50 | -2.94 | 1 | 66.76 | 5 | 15 | 0.3333 | 2 | 186.23 | 0.2644 | 1 | 0.0039 | 3 | 1 | 0.33 | 0.67 | 0.53 | 0.25 | 0.79 |
| **31** | 93602-28-9 | O=C1CC(C2=CC=C(O)C=C2)OC3=C1C(O)=CC(O)=C3 | 272.26 | 3 | 5 | 2.16 | -2.64 | 1 | 86.99 | 6 | 15 | 0.4000 | 2 | 192.58 | 0.32371 | 1 | 0.0037 | 3 | 1 | 0.33 | 0.67 | 0.55 | 0.25 | 0.80 |
| **32** | 10236-47-2 | O[C@H]([C@H]1O)[C@@H](O[C@@H](O[C@@H]2[C@H]([C@@H]([C@H](O[C@H]2OC3=CC4=C(C(C[C@H](O4)C5=CC=C(C=C5)O)=O)C(O)=C3)CO)O)O)[C@@H]1O)C | 580.54 | 8 | 14 | -0.74 | -2.73 | 6 | 225.06 | 27 | 27 | 1.0000 | 2 | 388.35 | 0.43219 | 11 | 0.0189 | 5 | 3 | 0.60 | 0.40 | 0.46 | 0.30 | 0.96 |
| **33** | 1639417-53-0 | FC1=CC(C2=C(OC3=CC=CC=C3C2=O)[C@H](CC)NC4=C5C(NC=N5)=NC=N4)=CC=C1 | 415.43 | 2 | 7 | 3.65 | -6.40 | 5 | 92.79 | 4 | 23 | 0.1739 | 4 | 306.73 | 0.26538 | 1 | 0.0024 | 5 | 3 | 0.60 | 0.80 | 0.39 | 0.30 | 0.95 |
| **34** | 446-72-0 | OC1=C(C2=O)C(OC=C2C3=CC=C(C=C3)O)=CC(O)=C1 | 270.24 | 3 | 5 | 1.63 | -2.73 | 1 | 86.99 | 4 | 15 | 0.2667 | 2 | 191.03 | 0.32634 | 0 | 0.0000 | 3 | 1 | 0.33 | 0.67 | 0.60 | 0.29 | 0.80 |
| **35** | 490-46-0 | OC1=CC([C@H]2OC3=CC(O)=CC(O)=C3C[C@H]2O)=CC=C1O | 290.27 | 5 | 6 | 1.51 | -1.76 | 1 | 110.38 | 9 | 15 | 0.6000 | 2 | 200.03 | 0.37744 | 2 | 0.0069 | 3 | 1 | 0.33 | 0.67 | 0.52 | 0.30 | 0.82 |
| **36** | 989-51-5 | O=C(O[C@H]1[C@@H](C2=CC(O)=C(O)C(O)=C2)OC3=CC(O)=CC(O)=C3C1)C4=CC(O)=C(O)C(O)=C4 | 458.37 | 8 | 11 | 2.05 | -2.16 | 4 | 197.37 | 13 | 22 | 0.5909 | 3 | 306.59 | 0.44959 | 2 | 0.0044 | 4 | 1 | 0.25 | 0.75 | 0.42 | 0.29 | 0.87 |
| **37** | 1918143-53-9 | FC1(OC2=CC(C3(CC3)C(N[C@H](C4)C5=CC=C(C=C5O[C@H]4C6=CC=C(C(O)=O)C=C6)OC(F)F)=O)=CC=C2O1)F | 559.47 | 2 | 8 | 6.02 | -6.40 | 7 | 103.32 | 13 | 28 | 0.4643 | 3 | 370.59 | 0.24458 | 2 | 0.0036 | 6 | 2 | 0.33 | 0.50 | 0.45 | 0.36 | 0.92 |

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| **38** | 533884-09-2 | [H][C@@]1(C2=CC(O)=CC=C2O[C@H]3C4=CC=C(C=C4)O)CCC[C@@]13[H] | 282.34 | 2 | 3 | 4.05 | -3.64 | 1 | 49.69 | 9 | 18 | 0.5000 | 2 | 207.5 | 0.17446 | 3 | 0.0106 | 4 | 1 | 0.25 | 0.50 | 0.57 | 0.24 | 0.85 |
| **39** | 923978-27-2 | CC(C)(OC1=C(C)C=C(/C=C/C(C2=CC=C(SC)C=C2)=O)C=C1C)C(O)=O | 384.50 | 1 | 4 | 4.27 | -5.66 | 7 | 88.9 | 9 | 22 | 0.4091 | 2 | 300.57 | 0.22181 | 0 | 0.0000 | 2 | 0 | 0.00 | 1.00 | 0.63 | 0.51 | 0.74 |
| **40** | 87626-55-9 | O=C1C2=CC=CC(CC(O)=O)=C2OC(C3=CC=CC=C3)=C1 | 280.28 | 1 | 4 | 2.86 | -3.72 | 3 | 63.6 | 3 | 17 | 0.1765 | 2 | 209.84 | 0.23437 | 0 | 0.0000 | 3 | 1 | 0.33 | 0.67 | 0.52 | 0.35 | 0.83 |
| **41** | 920113-02-6 | O=C1C=C(C2=CC=CC=C2Cl)OC3=C([C@H]4[C@H](CO)N(C)CC4)C(O)=CC(O)=C13 | 401.85 | 3 | 6 | 3.43 | -3.87 | 3 | 90.23 | 11 | 21 | 0.5238 | 2 | 281.79 | 0.23383 | 2 | 0.0050 | 4 | 2 | 0.50 | 0.50 | 0.43 | 0.29 | 0.94 |
| **42** | 167869-21-8 | NC1=C(C=CC=C1C(OC2=CC=CC=C23)=CC3=O)OC | 267.28 | 1 | 4 | 2.63 | -3.84 | 2 | 61.55 | 3 | 16 | 0.1875 | 2 | 202.76 | 0.23826 | 0 | 0.0000 | 3 | 1 | 0.33 | 0.67 | 0.55 | 0.26 | 0.82 |
| **43** | 165179-35-1 | NC(C(F)=C1C)=C2C(OC(C3=CC=C(C(F)=C3)N)=CC2=O)=C1F | 320.27 | 2 | 4 | 2.66 | -5.18 | 1 | 78.34 | 2 | 16 | 0.1250 | 2 | 220.33 | 0.24318 | 0 | 0.0000 | 3 | 1 | 0.33 | 0.67 | 0.52 | 0.25 | 0.91 |
| **44** | 79619-31-1 | OC(COC1=CC=C2C(OC(C3=CC=CC=C3)=CC2=O)=C1)CNCCC | 353.42 | 2 | 5 | 3.03 | -3.99 | 8 | 67.79 | 10 | 21 | 0.4762 | 2 | 279.59 | 0.20602 | 1 | 0.0028 | 3 | 1 | 0.33 | 0.67 | 0.65 | 0.44 | 0.80 |
| **45** | 3681-93-4 | OC1=CC=C(C(OC2=C3C(O)=CC(O)=C2[C@H]4[C@@H]([C@@H](O)[C@@H]([C@H](O4)CO)O)O)=CC3=O)C=C1 | 432.38 | 7 | 10 | -0.08 | -2.27 | 3 | 177.14 | 15 | 21 | 0.7143 | 2 | 289.19 | 0.43134 | 5 | 0.0116 | 4 | 2 | 0.50 | 0.50 | 0.45 | 0.30 | 0.97 |
| **46** | 152735-23-4 | O=C(C1=C2C(C(C(C)=C(C3=CC=CC=C3)O2)=O)=CC=C1)NCCCN4CCN(C5=CC=CC=C5OC)CC4 | 511.62 | 1 | 7 | 4.91 | -5.00 | 8 | 71.11 | 13 | 31 | 0.4194 | 3 | 397.1 | 0.16278 | 0 | 0.0000 | 5 | 2 | 0.40 | 0.60 | 0.55 | 0.48 | 0.91 |
| **47** | 86433-40-1 | CC(C)(CN1CCCCC1)OC(C(C=CC=C2C3=O)=C2OC(C4=CC=CC=C4)=C3C)=O | 419.52 | 0 | 5 | 5.30 | -4.88 | 6 | 55.84 | 13 | 26 | 0.5000 | 2 | 324.49 | 0.15295 | 0 | 0.0000 | 4 | 2 | 0.50 | 0.50 | 0.52 | 0.41 | 0.89 |
| **48** | 139652-86-1 | OC(CC1)CC[N+]1([H])CCCCCCOC2=CC(C3=O)=C(C=C2)OC(C4=CC=CC=C4)=C3C.[Cl-] | 435.56 | 1 | 5 | 5.54 | -4.95 | 9 | 59 | 16 | 27 | 0.5926 | 2 | 345.7 | 0.14374 | 0 | 0.0000 | 4 | 2 | 0.50 | 0.50 | 0.69 | 0.43 | 0.85 |
| **49** | 95272-99-4 | OC1=CC(C2OC(C(C)=C3O)=C(C(C2)=O)C(O)=C3C)=CC=C1O | 316.31 | 4 | 6 | 2.50 | -3.03 | 1 | 107.22 | 9 | 17 | 0.5294 | 2 | 223.45 | 0.33761 | 1 | 0.0032 | 3 | 1 | 0.33 | 0.67 | 0.52 | 0.25 | 0.87 |
| **50** | 578-86-9 | OC1=CC=C(C(C2)=O)C(O[C@@H]2C3=CC=C(C=C3)O)=C1 | 256.26 | 2 | 4 | 2.50 | -2.94 | 1 | 66.76 | 5 | 15 | 0.3333 | 2 | 186.23 | 0.26444 | 1 | 0.0039 | 3 | 1 | 0.33 | 0.67 | 0.58 | 0.28 | 0.78 |
| **51** | 132147-69-4 | O=C1C(C(O)=CC(O)=C2)=C2O[C@H](C3=CC=C(O)C=C3)[C@@H]1C | 286.28 | 3 | 5 | 2.43 | -2.80 | 1 | 86.99 | 7 | 16 | 0.4375 | 2 | 203.58 | 0.30622 | 2 | 0.0070 | 3 | 1 | 0.33 | 0.67 | 0.52 | 0.26 | 0.83 |
| **53** | 807636-25-5 | O=C(C(C1=CC(S(=O)(O[Na])=O)=C(O)C=C1)=COC2=CC(O)=C3OC)C2=C3O | 402.31 | 3 | 9 | -1.92 | -1.35 | 3 | 161.8 | 8 | 16 | 0.5000 | 2 | 245.12 | 0.45251 | 0 | 0.0000 | 3 | 1 | 0.33 | 0.67 | 0.48 | 0.42 | 0.92 |
| **54** | 144337-18-8 | OC1=C(C(CCCCCCCCCCC)=O)C(O)=C(C(CCCCCCCCCCC)=O)C(O)=C1C2CC(C3=CC=C(O)C=C3)OC4=CC(O)=CC=C24 | 730.98 | 5 | 8 | 11.79 | -9.78 | 24 | 144.52 | 31 | 45 | 0.6889 | 3 | 595.01 | 0.17072 | 2 | 0.0027 | 4 | 1 | 0.25 | 0.75 | 0.51 | 0.43 | 0.96 |
| **55** | 134336-72-4 | O=C(O)COC1=CC(OC/C=C(C)/C)=CC=C1C(/C=C/C2=CC=C(C(C)(C)C)C=C2)=O | 422.52 | 1 | 5 | 5.55 | -5.55 | 10 | 72.83 | 11 | 26 | 0.4231 | 2 | 345.31 | 0.17138 | 0 | 0.0000 | 2 | 0 | 0.00 | 1.00 | 0.58 | 0.50 | 0.76 |