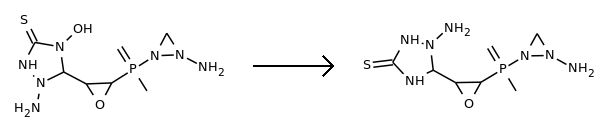
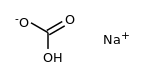
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 Export Results

| **Rank** | **Product** | **Probability** | **Max. Score** | **Molecular Weight** | **Predict impurities** | **Predict regio-selectivities** |
| --- | --- | --- | --- | --- | --- | --- |
| 1 | C=P1(C)C2OC2C2N(NC(=O)NN3CN31)NC(=S)N2O | 0.5259 | -66.449 | 319.3 |  |  |
| 2 | C=P(C)(C1OC1C1N(NC(=O)O)NC(=S)N1O)N1CN1N | 0.1114 | -68.001 | 337.3 |  |  |
| 3 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1CN1NC(=O)O | 0.0996 | -68.112 | 337.3 |  |  |
| 4 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1CN1N(C=O)CO | 0.0415 | -68.988 | 351.3 |  |  |
| 5 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1CN1N(CO)C(=O)O | 0.0238 | -69.544 | 367.3 |  |  |
| 6 | C=P(C)(C1OC1C1N(NC)NC(=S)N1O)N1CN1N | 0.0238 | -69.546 | 307.3 |  |  |
| 7 | C=P1(C)C2OC2C2N(NC(=O)[N+]3(N)CN31)NC(=S)N2O | 0.0217 | -69.634 | 320.3 |  |  |
| 8 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1CN1NC | 0.0205 | -69.691 | 307.3 |  |  |
| 9 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1C[N+]1(N)C(=O)O | 0.0193 | -69.752 | 338.3 |  |  |
| 10 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1CN1NCO | 0.0142 | -70.062 | 323.3 |  |  |
| 11 | C=P(C)(C1OC1C1N(NC=O)NC(=S)N1O)N1CN1N | 0.0139 | -70.080 | 321.3 |  |  |
| 12 | C=P(C)(C1OC1C1N(NCO)NC(=S)N1O)N1CN1N | 0.0139 | -70.082 | 323.3 |  |  |
| 13 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1CN1NC=O | 0.0116 | -70.265 | 321.3 |  |  |
| 14 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1C[N+]1(C)N | 0.0096 | -70.450 | 308.3 |  |  |
| 15 | C=P(C)(C1OC1C1N(NC[O-])NC(=S)N1O)N1CN1N | 0.0084 | -70.589 | 322.3 |  |  |
| 16 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1CN1NC[O-] | 0.0075 | -70.703 | 322.3 |  |  |
| 17 | C=P1(C)C2OC2C2N(NC(=O)N(CO)N3CN31)NC(=S)N2O | 0.0061 | -70.912 | 349.3 |  |  |
| 18 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1CN1N(C)CO | 0.0054 | -71.019 | 337.3 |  |  |
| 19 | O=CO | 0.0039 | -71.357 | 46.0 |  |  |
| 20 | O=C[O-] | 0.0030 | -71.628 | 45.0 |  |  |
| 21 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1C[N+]1(N)CO | 0.0028 | -71.697 | 324.3 |  |  |
| 22 | C=P(C)(C1OC1C1NNC(=S)N1O)N1CN1NC(N)=O | 0.0025 | -71.801 | 321.3 |  |  |
| 23 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1CN1N(C[O-])CO | 0.0022 | -71.913 | 352.3 |  |  |
| 24 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1CN1N(CO)CO | 0.0019 | -72.089 | 353.3 |  |  |
| 25 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1C[N+]1(N)C[O-] | 0.0018 | -72.140 | 323.3 |  |  |
| 26 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1C[N+]1(N)C=O | 0.0015 | -72.277 | 322.3 |  |  |
| 27 | C=P1(C)C2OC2C2N(NC[N+]3(N)CN31)NC(=S)N2O | 0.0008 | -72.933 | 306.3 |  |  |
| 28 | C=P(C)(C1OC1C1NNC(=S)N1O)N1CN1N | 0.0005 | -73.349 | 278.3 |  |  |
| 29 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1C[N+]12NC2=O | 0.0004 | -73.757 | 320.3 |  |  |
| 30 | C=P(C)(C1OC1C1NNC(=S)N1O)N1C[N+]1(N)C(N)=O | 0.0002 | -74.450 | 322.3 |  |  |
| 31 | C=P(C)(C1OC1C1N(O)C2NN1N2C(=O)O)N1CN1N | 0.0001 | -74.970 | 305.2 |  |  |
| 32 | C=P(C)(C1OC1C1N(O)C2NN1N2C=O)N1CN1N | 0.0001 | -75.337 | 289.2 |  |  |
| 33 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1C[N+]12CN2 | 0.0001 | -75.387 | 306.3 |  |  |
| 34 | C=P1(C)C2OC2C2N(N)NC(N2O)N(C(=O)O)N2CN21 | 0.0001 | -75.553 | 305.2 |  |  |
| 35 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1C[N+]12C(=O)N2CO | 0.0001 | -75.698 | 350.3 |  |  |
| 36 | C[P+](C)(C1OC1C1N(N)NC(=S)N1O)N1CN1N | 0.0000 | -75.818 | 294.3 |  |  |
| 37 | C=P(C)(C1OC1C1N(O)CNN1N)N1CN1N | 0.0000 | -75.871 | 263.2 |  |  |
| 38 | C=P1(C)C2OC2C2N(N)NC(N2O)N(C=O)N2CN21 | 0.0000 | -76.151 | 289.2 |  |  |
| 39 | [O-]CO | 0.0000 | -77.525 | 47.0 |  |  |
| 40 | [O-] | 0.0000 | -77.673 | 16.0 |  |  |
| 41 | C=P(C)(C1OC1C1NNC(NC(=O)O)N1O)N1CN1N | 0.0000 | -77.687 | 307.3 |  |  |
| 42 | CP(C1OC1C1N(N)NC(=S)N1O)N1CN1N | 0.0000 | -77.781 | 279.3 |  |  |
| 43 | C=P(C)(C(O)CC1N(N)NC(=S)N1O)N1CN1N | 0.0000 | -77.829 | 295.3 |  |  |
| 44 | C=P(C)(C1OC1C1N2NC(N2)N1O)N1CN1N | 0.0000 | -78.455 | 261.2 |  |  |
| 45 | C=P(C)(C1OC1C1N(O)C2NN1N2CO)N1CN1N | 0.0000 | -78.546 | 291.3 |  |  |
| 46 | C=P(C)(C1OC1C1N(NC([O-])O)NC(=S)N1O)N1CN1N | 0.0000 | -78.582 | 338.3 |  |  |
| 47 | C=P(C)(C1OC1C1N(O)C2NN1N2C[O-])N1CN1N | 0.0000 | -78.800 | 290.2 |  |  |
| 48 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1C[N+]1(N)C([O-])O | 0.0000 | -78.895 | 339.3 |  |  |
| 49 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1CN1NC([O-])O | 0.0000 | -78.903 | 338.3 |  |  |
| 50 | C=P1(C)C2OC2C2N(N)NC(N2O)N(CO)N2CN21 | 0.0000 | -78.991 | 291.3 |  |  |
| 51 | C=P1(C)C2OC2C2N(N)NC(NN3CN31)N2O | 0.0000 | -79.010 | 261.2 |  |  |
| 52 | C=P1(C)C2OC2C2N(N)NC(N2O)[N+](CO)(C(=O)O)N2CN21 | 0.0000 | -79.418 | 336.3 |  |  |
| 53 | C=P1(C)C2OC2C2N(N)NC(N2O)N(C[O-])N2CN21 | 0.0000 | -79.495 | 290.2 |  |  |
| 54 | C=P(C)(C1=C(C2N(N)NC(=S)N2O)O1)N1CN1N | 0.0000 | -80.496 | 291.3 |  |  |
| 55 | C=P(C)(C(O)=CC1N(N)NC(=S)N1O)N1CN1N | 0.0000 | -81.130 | 293.3 |  |  |
| 56 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1CN1N(CO)C([O-])O | 0.0000 | -81.183 | 368.3 |  |  |
| 57 | C=P(C)(C1OC1C1NNC(N)N1O)N1CN1N | 0.0000 | -81.353 | 263.2 |  |  |
| 58 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1C[N+]1(N)C(O)O | 0.0000 | -84.068 | 340.3 |  |  |
| 59 | C=P(C)(C1OC1C1N(NC(O)O)NC(=S)N1O)N1CN1N | 0.0000 | -84.162 | 339.3 |  |  |
| 60 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1CN1NC(O)O | 0.0000 | -84.523 | 339.3 |  |  |
| 61 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1CN1N(CO)C(O)O | 0.0000 | -85.386 | 369.3 |  |  |
| 62 | C=P1(C)C2OC2C2N(NCNN3CN31)NC(=S)N2O | 0.0000 | -85.617 | 305.3 |  |  |
| 63 | C=P1(C)C2OC2C2N(NC(=S)N2O)NC([O-])[N+]2(N)CN21 | 0.0000 | -85.874 | 321.3 |  |  |
| 64 | C[O-] | 0.0000 | -85.961 | 31.0 |  |  |
| 65 | C=P(C)(C1OC1C1NNC(NC([O-])O)N1O)N1CN1N | 0.0000 | -87.302 | 308.3 |  |  |
| 66 | C=P(C)(C1OC1C1N(O)C2NN1N2C([O-])O)N1CN1N | 0.0000 | -87.416 | 306.2 |  |  |
| 67 | C=P1(C)C2OC2C2N(N)NC(N2O)N(C([O-])O)N2CN21 | 0.0000 | -88.029 | 306.2 |  |  |
| 68 | C=P1(C)C2OC2C2N(NC(=S)N2O)NC(O)[N+]2(N)CN21 | 0.0000 | -88.205 | 322.3 |  |  |
| 69 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1C[N+]12C([O-])N2CO | 0.0000 | -88.264 | 351.3 |  |  |
| 70 | C=P(C)(C1OC1C1N(N)NC(=S)N1O)N1C[N+]12NC2[O-] | 0.0000 | -88.992 | 321.3 |  |  |
| 71 | [O-]C(O)O | 0.0000 | -89.445 | 63.0 |  |  |

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