

# “Supporting Information”

## Probing the Anticancer Activity of Nucleoside Analogues: A QSAR Model Approach Using an Internally Consistent Training Set

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**Supporting Information:** Training set chemicals, their inhibitory activity against the cellular line L1210/0, and their classification (*a posteriori* probabilities) according to the final model (eq. 2)

| No. | Names  | IC <sub>50</sub> obs <sup>a</sup> | Prob  | Class <sup>b</sup> |
|-----|--|-----------------------------------|-------|--------------------|
|     | <b>cytostatic chemicals</b>  |                                   |       |                    |
| 1   | ((1R,2S)-2-((6-chloro-9H-purin-9-yl)methyl)cyclopentyl)methanol  | 52.49                             | 4.11  | -1                 |
| 2   | ((1R,2S)-2-(5-amino-7-chloro-3H-[1,2,3]triazolo[4,5-d]pyrimidin-3-yl)cyclohexyl)methanol                                     | 95.50                             | 55.24 | +1                 |
| 3   | ((1S,3R)-3-((6-(4-chlorophenyl)-9H-purin-9-yl)methyl)-2,3-dihydro-1H-inden-1-yl)methanol                                     | 8.44                              | 99.49 | +1                 |
| 4   | ((1S,3R)-3-((6-(4-methoxyphenyl)-9H-purin-9-yl)methyl)-2,3-dihydro-1H-inden-1-yl)methanol                                    | 17.60                             | 99.23 | +1                 |
| 5   | ((1S,3R)-3-((6-chloro-9H-purin-9-yl)methyl)-2,2,3-trimethylcyclopentyl)methanol  | 42.75                             | 6.65  | -1                 |
| 6   | ((1S,3R)-3-((6-phenyl-9H-purin-9-yl)methyl)-2,3-dihydro-1H-inden-1-yl)methanol   | 28.06                             | 89.46 | +1                 |
| 7   | ((1S,3R)-3-((6-p-tolyl-9H-purin-9-yl)methyl)-2,3-dihydro-1H-inden-1-yl)methanol  | 15.39                             | 96.18 | +1                 |
| 8   | (2-(2,6-diamino-9H-purin-9-yl)ethoxy)methylphosphonic acid   | 1.73                              | 88.62 | +1                 |
| 9   | (2-(2-amino-6-(cyclopropylamino)-9H-purin-9-yl)ethoxy)methylphosphonic acid  | 10.20                             | 85.85 | +1                 |
| 10  | (2-(2-amino-6-oxo-1,6-dihydropurin-9-yl)ethoxy)methylphosphonic acid   | 0.57                              | 91.25 | +1                 |
| 11  | (2-(6-amino-9H-purin-9-yl)ethoxy)methylphosphonic acid   | 7.45                              | 85.52 | +1                 |
| 12  | (2R,3R,4R,5R)-2-(6-amino-9H-purin-9-yl)-4-fluoro-5-(hydroxymethyl)-tetrahydrofuran-3-ol                                      | 5.94                              | 84.47 | +1                 |
| 13  | (2R,3S,4R,5R)-2-(6-amino-9H-purin-9-yl)-5-ethynyl-tetrahydrofuran-3,4-diol   | 1.20                              | 57.39 | +1                 |
| 14  | (2R,3S,4R,5R,E)-2-(6-amino-9H-purin-9-yl)-5-(2-tosylvinyl)-tetrahydrofuran-3,4-diol  | 54.00                             | 94.38 | +1                 |
| 15  | (2R,3S,4R,5R,Z)-2-(6-amino-9H-purin-9-yl)-5-(2-bromovinyl)-tetrahydrofuran-3,4-diol  | 104.00                            | 83.37 | +1                 |
| 16  | (2R,3S,4R,5R,Z)-2-(6-amino-9H-purin-9-yl)-5-(2-chlorovinyl)-tetrahydrofuran-3,4-diol   | 143.00                            | 84.34 | +1                 |
| 17  | (2R,3S,4R,5R,Z)-2-(6-amino-9H-purin-9-yl)-5-(2-iodovinyl)-tetrahydrofuran-3,4-diol   | 43.00                             | 81.04 | +1                 |
| 18  | (2R,3S,4R,5S)-2-(6-amino-9H-purin-9-yl)-5-(1-bromovinyl)-tetrahydrofuran-3,4-diol  | 25.00                             | 82.91 | +1                 |
| 19  | (2S,3R,4S,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxy-tetrahydrofuran-2-carbaldehyde   | 36.61                             | 67.55 | +1                 |
| 20  | (2S,3R,5R)-5-(6-amino-9H-purin-9-yl)-3-hydroxy-tetrahydrofuran-2-carbaldehyde  | 26.64                             | 70.46 | +1                 |
| 21  | (3R,4R,5R,6R)-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-5-fluoro-6-methoxy-tetrahydro-2H-pyran-3,4-diyl diacetate          | 55.00                             | 98.70 | +1                 |
| 22  | (3R,4R,5R,6R)-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-5-fluoro-6-methoxy-tetrahydro-2H-pyran-3,4-diyl dihexanoate        | 40.00                             | 80.32 | +1                 |
| 23  | (3R,4R,5R,6R)-5-fluoro-5-(5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-6-methoxy-tetrahydro-2H-pyran-3,4-diyl diacetate | 34.00                             | 99.17 | +1                 |
| 24  | (E)-1-((2-hydroxyethoxy)methyl)-6-(3-(2-methoxyphenyl)-3-oxoprop-1-enyl)pyrimidine-2,4(1H,3H)-dione                          | 15.16                             | 28.39 | -1                 |
| 25  | (E)-1-((2-hydroxyethoxy)methyl)-6-(3-(4-methoxyphenyl)-3-oxoprop-1-enyl)pyrimidine-2,4(1H,3H)-dione                          | 33.49                             | 55.90 | +1                 |

|    |  |        |       |    |
|----|--|--------|-------|----|
| 26 | (E)-1-((2-hydroxyethoxy)methyl)-6-(3-oxo-3-phenylprop-1-enyl)pyrimidine-2,4(1H,3H)-dione   | 43.31  | 31.00 | -1 |
| 27 | (E)-1-((2-hydroxyethoxy)methyl)-6-(3-oxo-3-p-tolylprop-1-enyl)pyrimidine-2,4(1H,3H)-dione  | 27.91  | 39.81 | -1 |
| 28 | (E)-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-2,4-dioxo-1,2,3,4-tetrahydropyrimidine-5-carbaldehyde oxime              | 15.49  | 43.22 | -1 |
| 29 | (E)-3,4-bis(benzyloxy)-5-(2-(6-chloro-7H-purin-7-yl)ethylidene)furan-2(5H)-one   | 4.10   | 98.62 | +1 |
| 30 | (E)-6-(3-oxo-3-p-tolylprop-1-enyl)pyrimidine-2,4(1H,3H)-dione  | 182.24 | 19.39 | -1 |
| 31 | (Z)-1-(2-(3,4-bis(benzyloxy)-5-oxofuran-2(5H)-ylidene)ethyl)-5-(trifluoromethyl)pyrimidine-2,4(1H,3H)-dione                                  | 2.00   | 99.91 | +1 |
| 32 | (Z)-1-(2-(3,4-bis(benzyloxy)-5-oxofuran-2(5H)-ylidene)ethyl)-5-bromopyrimidine-2,4(1H,3H)-dione  | 7.50   | 98.28 | +1 |
| 33 | (Z)-1-(2-(3,4-bis(benzyloxy)-5-oxofuran-2(5H)-ylidene)ethyl)-5-chloropyrimidine-2,4(1H,3H)-dione   | 12.20  | 98.33 | +1 |
| 34 | (Z)-1-(2-(3,4-bis(benzyloxy)-5-oxofuran-2(5H)-ylidene)ethyl)-5-fluoropyrimidine-2,4(1H,3H)-dione   | 5.10   | 98.41 | +1 |
| 35 | (Z)-1-(2-(3,4-bis(benzyloxy)-5-oxofuran-2(5H)-ylidene)ethyl)-5-iodopyrimidine-2,4(1H,3H)-dione   | 7.50   | 98.15 | +1 |
| 36 | (Z)-1-(2-(3,4-bis(benzyloxy)-5-oxofuran-2(5H)-ylidene)ethyl)pyrimidine-2,4(1H,3H)-dione  | 12.90  | 92.70 | +1 |
| 37 | (Z)-1-(2-(3,4-dihydroxy-5-oxofuran-2(5H)-ylidene)ethyl)-5-fluoropyrimidine-2,4(1H,3H)-dione  | 5.18   | 80.05 | +1 |
| 38 | (Z)-1-(6-amino-9H-purin-9-yl)-2-(3,4-dimethoxy-5-oxofuran-2(5H)-ylidene)ethylphosphonic acid   | 11.42  | 94.56 | +1 |
| 39 | (Z)-3,4-bis(benzyloxy)-5-(2-(6-chloro-9H-purin-9-yl)ethylidene)furan-2(5H)-one   | 11.60  | 99.26 | +1 |
| 40 | (Z)-5-(2-(6-(1H-pyrrol-1-yl)-9H-purin-9-yl)ethylidene)-3,4-bis(benzyloxy)furan-2(5H)-one   | 110.00 | 99.54 | +1 |
| 41 | (Z)-5-(2-(6-chloro-9H-purin-9-yl)ethylidene)-3,4-dimethoxyfuran-2(5H)-one  | 14.01  | 92.07 | +1 |
| 42 | (Z)-5-(2-(6-chloro-9H-purin-9-yl)ethylidene)-3-methoxy-4-(4-nitrobenzyloxy)furan-2(5H)-one   | 13.09  | 99.08 | +1 |
| 43 | (Z)-5-(2-(6-chloro-9H-purin-9-yl)ethylidene)-4-methoxy-3-(4-nitrobenzyloxy)furan-2(5H)-one   | 13.59  | 99.04 | +1 |
| 44 | (Z)-dimethyl 1-(6-chloro-9H-purin-9-yl)-2-(3,4-dimethoxy-5-oxofuran-2(5H)-ylidene)ethylphosphonate   | 37.73  | 91.50 | +1 |
| 45 | 1-((2R,3S,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-ethynylpyrimidine-2,4(1H,3H)-dione                                  | 167.77 | 59.39 | +1 |
| 46 | 1-((2R,3S,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione                                   | 24.40  | 54.06 | +1 |
| 47 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-2,4-dioxo-1,2,3,4-tetrahydropyrimidine-5-carbaldehyde                        | 1.07   | 59.11 | +1 |
| 48 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-((E)-2-iodovinyl)pyrimidine-2,4(1H,3H)-dione                               | 63.92  | 76.67 | +1 |
| 49 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-(2,4,5-trimethyl-3,6-dioxocyclohexa-1,4-dienyl)pyrimidine-2,4(1H,3H)-dione | 174.30 | 60.40 | +1 |
| 50 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-(3-methyl-1,4-dioxo-1,4-dihydronaphthalen-2-yl)pyrimidine-2,4(1H,3H)-dione | 68.78  | 54.26 | +1 |
| 51 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-(hydroxymethyl)pyrimidine-2,4(1H,3H)-dione                                 | 9.18   | 57.33 | +1 |
| 52 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-(trifluoromethyl)pyrimidine-2,4(1H,3H)-dione                               | 0.02   | 97.58 | +1 |
| 53 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-iodopyrimidine-2,4(1H,3H)-dione  | 172.83 | 86.08 | +1 |
| 54 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-nitropyrimidine-2,4(1H,3H)-dione   | 0.13   | 83.44 | +1 |
| 55 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-thiocyanatopyrimidine-2,4(1H,3H)-dione                                     | 78.87  | 86.70 | +1 |
| 56 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-vinylpyrimidine-2,4(1H,3H)-dione   | 14.20  | 49.05 | NC |
| 57 | 1-(2-(3,4-bis(benzyloxy)-5-oxo-2,5-dihydrofuran-2-yl)-2-hydroxyethyl)-5-(trifluoromethyl)pyrimidine-2,4(1H,3H)-dione                         | 50.15  | 99.82 | +1 |
| 58 | 1-(2-(3,4-bis(benzyloxy)-5-oxo-2,5-dihydrofuran-2-yl)-2-hydroxyethyl)-5-fluoropyrimidine-2,4(1H,3H)-dione                                    | 140.04 | 98.27 | +1 |
| 59 | 1-(2-(3,4-bis(benzyloxy)-5-oxo-2,5-dihydrofuran-2-yl)-2-hydroxyethyl)pyrimidine-2,4(1H,3H)-dione   | 157.18 | 91.29 | +1 |
| 60 | 1-(2-amino-6-thioxo-1,6-dihydropurin-9-yl)propan-2-yl acetate  | 128.00 | 27.63 | -1 |
| 61 | 1-(6-chloro-2-fluoro-9H-purin-9-yl)propan-2-yl acetate   | 37.00  | 55.75 | +1 |
| 62 | 1-(6-chloro-2-iodo-9H-purin-9-yl)propan-2-yl acetate   | 13.00  | 71.05 | +1 |
| 63 | 2-((2,6-dichloro-9H-purin-9-yl)methoxy)ethyl acetate   | 39.33  | 61.28 | +1 |
| 64 | 2-((2-amino-6-thioxo-1,6-dihydropurin-9-yl)methoxy)ethyl acetate   | 3.20   | 51.95 | NC |
| 65 | 2-((2-fluoro-6-mercapto-9H-purin-9-yl)methoxy)ethanol  | 170.00 | 80.57 | +1 |

|     |   |        |       |    |
|-----|---|--------|-------|----|
| 66  | 2-((2-fluoro-6-mercapto-9H-purin-9-yl)methoxy)ethyl acetate   | 40.00  | 75.52 | +1 |
| 67  | 2-((6-chloro-2-iodo-9H-purin-9-yl)methoxy)ethyl acetate   | 8.60   | 82.69 | +1 |
| 68  | 2-((6-chloro-9H-purin-9-yl)methoxy)ethyl acetate  | 162.56 | 36.35 | -1 |
| 69  | 2'-Deoxy-5,5'',5'''-trifluoro-5'-O-1'',3'',2''-dioxaphosphacyclohex-2''-yluridine 2''-oxide   | 0.01   | 99.39 | +1 |
| 70  | 2'-Deoxy-5-fluoro-5''-hydroxy-5'-O-1'',3'',2''-dioxaphosphacyclohex-2''-yluridine 2''-oxide   | 0.84   | 96.31 | +1 |
| 71  | 2'-Deoxy-5-fluoro-5'-O-1'',3'',2''-dioxaphosphacyclohex-2''-yluridine 2''-oxide   | 0.75   | 95.94 | +1 |
| 72  | 2-amino-9-((2-hydroxyethoxy)methyl)-1H-purin-6(9H)-one  | 57.73  | 22.11 | -1 |
| 73  | 2-amino-9-((2-hydroxyethoxy)methyl)-8-iodo-1H-purin-6(9H)-one   | 111.08 | 68.42 | +1 |
| 74  | 2-amino-9-((2R,3R,4R,5R)-4-fluoro-3-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-1H-purin-6(9H)-one                                    | 17.53  | 83.80 | +1 |
| 75  | 5-(6-amino-9H-purin-9-yl)-3,4-dihydroxy-tetrahydrofuran-2-carbaldehyde oxime  | 6.47   | 61.43 | +1 |
| 76  | 4-amino-1-((2R,3R,4R,5R)-4-fluoro-3-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidin-2(1H)-one                                    | 159.05 | 87.37 | +1 |
| 77  | 4-amino-1-((2R,3S,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidin-2(1H)-one   | 0.70   | 57.50 | +1 |
| 78  | 4-amino-1-((2R,3S,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidin-2(1H)-one   | 53.51  | 58.20 | +1 |
| 79  | 5-((E)-2-bromovinyl)-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione                           | 80.75  | 72.11 | +1 |
| 80  | 5-(1-chlorovinyl)-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione                              | 1.66   | 91.48 | +1 |
| 81  | 5-(4,5-dimethyl-3,6-dioxocyclohexa-1,4-dienyl)-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione | 111.78 | 68.99 | +1 |
| 82  | 5-(6-amino-9H-purin-9-yl)-3,4-dihydroxy-tetrahydrofuran-2-carbaldehyde oxime  | 37.47  | 73.85 | +1 |
| 83  | 5-(6-amino-9H-purin-9-yl)-3-hydroxy-tetrahydrofuran-2-carbaldehyde oxime  | 17.41  | 74.72 | +1 |
| 84  | 5-(azidomethyl)-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione                                | 123.57 | 77.38 | +1 |
| 85  | 5-bromo-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione  | 84.66  | 85.04 | +1 |
| 86  | 5-ethyl-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione  | 33.17  | 42.62 | -1 |
| 87  | 5-ethynyl-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione                                      | 0.36   | 53.23 | +1 |
| 88  | 5-fluoro-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione                                       | 0.00   | 82.32 | +1 |
| 89  | 5-fluoropyrimidine-2,4(1H,3H)-dione   | 0.31   | 50.08 | NC |
| 90  | acetic ((Z)-methyl 1-(6-amino-9H-purin-9-yl)-2-(3,4-dimethoxy-5-oxofuran-2(5H)-ylidene)ethylphosphonic thioanhydride                      | 2.26   | 83.89 | +1 |
| 91  | N-((1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5-yl)methyl)-2-iodoacetamide    | 107.48 | 87.44 | +1 |
|     | <b>Non-cytostatic chemical</b>  |        |       |    |
| 92  | ((1R,2R)-2-((6-amino-9H-purin-9-yl)methyl)cyclopentyl)methanol  | >200   | 1.43  | -1 |
| 93  | ((1R,2R)-2-(6-amino-9H-purin-9-yl)cyclopentyl)methanol  | >200   | 10.31 | -1 |
| 94  | ((1R,2S)-2-((7-amino-3H-[1,2,3]triazolo[4,5-d]pyrimidin-3-yl)methyl)cyclopentyl)methanol  | >200   | 2.33  | -1 |
| 95  | ((1R,2S)-2-(2,6-diamino-9H-purin-9-yl)cyclohexyl)methanol   | >200   | 21.88 | -1 |
| 96  | ((1R,2S)-2-(2-amino-6-chloro-9H-purin-9-yl)cyclohexyl)methanol  | >200   | 44.68 | -1 |
| 97  | ((1R,2S)-2-(5,7-diamino-3H-[1,2,3]triazolo[4,5-d]pyrimidin-3-yl)cyclohexyl)methanol   | >200   | 28.98 | -1 |
| 98  | ((1R,2S,4r)-4-(6-(cyclopropylamino)-9H-purin-9-yl)cyclopentane-1,2-diyl)dimethanol  | >200   | 3.06  | -1 |
| 99  | ((1R,2S,4r)-4-(6-(isopropylamino)-9H-purin-9-yl)cyclopentane-1,2-diyl)dimethanol  | >200   | 3.10  | -1 |
| 100 | ((1R,2S,4r)-4-(6-amino-9H-purin-9-yl)cyclopentane-1,2-diyl)dimethanol   | >200   | 9.70  | -1 |
| 101 | ((1S,2R,3R,4R)-4-(7-amino-3H-[1,2,3]triazolo[4,5-d]pyrimidin-3-yl)cyclopentane-1,2,3-triyl)trimethanol                                    | >200   | 25.21 | -1 |
| 102 | ((1S,2S)-2-(6-chloro-9H-purin-9-yl)cyclopentyl)methanol   | >200   | 20.82 | -1 |
| 103 | ((1S,3R)-3-((6-(cyclopropylamino)-9H-purin-9-yl)methyl)-2,3-dihydro-1H-inden-1-yl)methanol  | >200   | 11.32 | -1 |
| 104 | ((1S,3R)-3-((6-(propylamino)-9H-purin-9-yl)methyl)-2,3-dihydro-1H-inden-1-yl)methanol   | >200   | 7.12  | -1 |
| 105 | ((1S,3R)-3-((6-amino-9H-purin-9-yl)methyl)-2,2,3-trimethylcyclopentyl)methanol  | >200   | 2.87  | -1 |

|     |   |      |       |    |
|-----|---|------|-------|----|
| 106 | ((1S,3R)-3-((6-amino-9H-purin-9-yl)methyl)-2,3-dihydro-1H-inden-1-yl)methanol                                     | >200 | 16.41 | -1 |
| 107 | ((1S,3R)-3-((6-ethoxy-9H-purin-9-yl)methyl)-2,3-dihydro-1H-inden-1-yl)methanol                                    | >200 | 16.60 | -1 |
| 108 | ((1S,3R)-3-((6-methoxy-9H-purin-9-yl)methyl)-2,3-dihydro-1H-inden-1-yl)methanol                                   | >200 | 18.09 | -1 |
| 109 | ((1S,3R)-3-((7-amino-3H-[1,2,3]triazolo[4,5-d]pyrimidin-3-yl)methyl)-2,2,3-trimethylcyclopentyl)methanol          | >200 | 4.36  | -1 |
| 110 | ((3aR,4R,5R,6aS)-5-(6-amino-9H-purin-9-yl)-hexahydro-1H-cyclopenta[c]furan-4-yl)methanol                          | >200 | 13.53 | -1 |
| 111 | ((3aR,4R,5R,6aS)-5-(6-chloro-9H-purin-9-yl)-hexahydro-1H-cyclopenta[c]furan-4-yl)methanol                         | >200 | 29.98 | -1 |
| 112 | (1S)-1-(3-((6-amino-9H-purin-9-yl)methyl)-2,2-dimethylcyclobutyl)ethanol  | >200 | 6.17  | -1 |
| 113 | (1S)-1-(3-((7-amino-6,7-dihydro-[1,2,3]triazolo[4,5-d]pyrimidin-3-yl)methyl)-2,2-dimethylcyclobutyl)ethanol       | >200 | 5.34  | -1 |
| 114 | (1S)-1-(3-(2-(6-amino-9H-purin-9-yl)ethyl)-2,2-dimethylcyclobutyl)ethanol   | >200 | 0.69  | -1 |
| 115 | (1S)-1-(3-(2-(7-amino-3H-[1,2,3]triazolo[4,5-d]pyrimidin-3-yl)ethyl)-2,2-dimethylcyclobutyl)ethanol               | >200 | 1.25  | -1 |
| 116 | (2R,3R,4R,5S)-2-(6-amino-9H-purin-9-yl)-5-(dihydroxymethyl)-tetrahydrofuran-3,4-diol                              | >200 | 63.85 | +1 |
| 117 | (2R,3S,4R,5R,E)-2-(6-amino-9H-purin-9-yl)-5-(2-fluorovinyl)-tetrahydrofuran-3,4-diol                              | >200 | 85.37 | +1 |
| 118 | (2S,3S,5S)-5-(4-amino-2,5-difluorophenyl)-2-(hydroxymethyl)-2-methyl-tetrahydrofuran-3-ol                         | >200 | 48.25 | NC |
| 119 | (2S,3S,5S)-5-(4-amino-2-fluorophenyl)-2-(hydroxymethyl)-2-methyl-tetrahydrofuran-3-ol                             | >200 | 36.56 | -1 |
| 120 | (2S,4S,5R)-5-(6-amino-9H-purin-9-yl)-4-hydroxy-tetrahydrofuran-2-carbaldehyde                                     | >200 | 27.23 | -1 |
| 121 | (3-((2,6-diamino-9H-purin-9-yl)methyl)-2,2-dimethylcyclobutyl)methanol  | >200 | 5.75  | -1 |
| 122 | (3-((2-amino-6-chloro-9H-purin-9-yl)methyl)-2,2-dimethylcyclobutyl)methanol                                       | >200 | 15.61 | -1 |
| 123 | (3-((5,7-diamino-3H-[1,2,3]triazolo[4,5-d]pyrimidin-3-yl)methyl)-2,2-dimethylcyclobutyl)methanol                  | >200 | 8.10  | -1 |
| 124 | (3-((5-amino-7-chloro-3H-[1,2,3]triazolo[4,5-d]pyrimidin-3-yl)methyl)-2,2-dimethylcyclobutyl)methanol             | >200 | 22.49 | -1 |
| 125 | (3-((6-amino-9H-purin-9-yl)methyl)cyclopentyl)methanol  | >200 | 2.06  | -1 |
| 126 | (E)-2-((5-(2-bromovinyl)-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methoxy)ethyl acetate                            | >200 | 19.80 | -1 |
| 127 | (E)-5-(2-bromovinyl)-1-((2-hydroxyethoxy)methyl)pyrimidine-2,4(1H,3H)-dione                                       | >200 | 30.73 | -1 |
| 128 | (E)-6-(3-(4-methoxyphenyl)-3-oxoprop-1-enyl)pyrimidine-2,4(1H,3H)-dione   | >200 | 26.29 | -1 |
| 129 | (E)-6-(3-oxo-3-phenylprop-1-enyl)pyrimidine-2,4(1H,3H)-dione  | >200 | 12.69 | -1 |
| 130 | (Z)-1-(2-(3,4-dihydroxy-5-oxofuran-2(5H)-ylidene)ethyl)-5-(trifluoromethyl)pyrimidine-2,4(1H,3H)-dione            | >200 | 98.79 | -1 |
| 131 | (Z)-1-(2-(3,4-dihydroxy-5-oxofuran-2(5H)-ylidene)ethyl)pyrimidine-2,4(1H,3H)-dione                                | >200 | 36.98 | -1 |
| 132 | (Z)-1-(2-(3-benzyl-4-hydroxy-5-oxofuran-2(5H)-ylidene)ethyl)pyrimidine-2,4(1H,3H)-dione                           | >200 | 37.12 | -1 |
| 133 | (Z)-5-(2-(6-amino-9H-purin-9-yl)ethylidene)-3,4-dimethoxyfuran-2(5H)-one  | >200 | 75.73 | +1 |
| 134 | (Z)-dimethyl 2-(3,4-dimethoxy-5-oxofuran-2(5H)-ylidene)ethylphosphonate   | >200 | 0.44  | -1 |
| 135 | (Z)-O-methyl O-hydrogen 1-(6-amino-9H-purin-9-yl)-2-(3,4-dimethoxy-5-oxofuran-2(5H)-ylidene)ethylphosphonothioate | >200 | 93.98 | +1 |
| 136 | 1-(((1R,2R)-2-(hydroxymethyl)cyclopentyl)methyl)pyrimidine-2,4(1H,3H)-dione                                       | >200 | 1.40  | -1 |
| 137 | 1-(((1R,3S)-3-(hydroxymethyl)-1,2,2-trimethylcyclopentyl)methyl)-5-iodopyrimidine-2,4(1H,3H)-dione                | >200 | 33.83 | -1 |
| 138 | 1-(((1R,3S)-3-(hydroxymethyl)-1,2,2-trimethylcyclopentyl)methyl)pyrimidine-2,4(1H,3H)-dione                       | >200 | 11.65 | -1 |
| 139 | 1-(((1R,3S)-3-(hydroxymethyl)-2,3-dihydro-1H-inden-1-yl)methyl)-5-methylpyrimidine-2,4(1H,3H)-dione               | >200 | 14.21 | -1 |
| 140 | 1-(((1R,3S)-3-(hydroxymethyl)-2,3-dihydro-1H-inden-1-yl)methyl)pyrimidine-2,4(1H,3H)-dione                        | >200 | 14.09 | -1 |
| 141 | 1-(((1S,2R)-2-(hydroxymethyl)cyclopentyl)methyl)-5-iodopyrimidine-2,4(1H,3H)-dione                                | >200 | 10.48 | -1 |
| 142 | 1-(((1R,2R)-2-(hydroxymethyl)cyclopentyl)-5-iodopyrimidine-2,4(1H,3H)-dione                                       | >200 | 32.91 | -1 |
| 143 | 1-(((1R,2R)-2-(hydroxymethyl)cyclopentyl)pyrimidine-2,4(1H,3H)-dione  | >200 | 5.66  | -1 |
| 144 | 1-(((1R,2S,4R)-2,4-bis(hydroxymethyl)cyclopentyl)-5-iodopyrimidine-2,4(1H,3H)-dione                               | >200 | 45.21 | -1 |
| 145 | 1-(((1R,2S,4R)-2,4-bis(hydroxymethyl)cyclopentyl)pyrimidine-2,4(1H,3H)-dione                                      | >200 | 11.03 | -1 |
| 146 | 1-(((1r,3R,4S)-3,4-bis(hydroxymethyl)cyclopentyl)-5-iodopyrimidine-2,4(1H,3H)-dione                               | >200 | 24.62 | -1 |
| 147 | 1-((2-hydroxyethoxy)methyl)-5-iodopyrimidine-2,4(1H,3H)-dione   | >200 | 24.72 | -1 |
| 148 | 1-((2-hydroxyethoxy)methyl)-5-methylpyrimidine-2,4(1H,3H)-dione   | >200 | 5.37  | -1 |

|     |  |      |       |    |
|-----|--|------|-------|----|
| 149 | 1-((2-hydroxyethoxy)methyl)-5-nitropyrimidine-2,4(1H,3H)-dione   | >200 | 30.22 | -1 |
| 150 | 1-((2-hydroxyethoxy)methyl)pyridine-2,4(1H,3H)-dione   | >200 | 0.55  | -1 |
| 151 | 1-((2-hydroxyethoxy)methyl)pyrimidine-2,4(1H,3H)-dione   | >200 | 1.65  | -1 |
| 152 | 1-((2R,3R,4R,5R)-4-fluoro-3-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione                       | >200 | 86.74 | +1 |
| 153 | 1-((2R,3S,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-(3,3-dimethylbut-1-ynyl)pyrimidine-2,4(1H,3H)-dione | >200 | 24.98 | -1 |
| 154 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-2,4-dioxo-1,2,3,4-tetrahydropyrimidine-5-carbonitrile        | >200 | 69.73 | +1 |
| 155 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-(3-hydroxyprop-1-ynyl)pyrimidine-2,4(1H,3H)-dione          | >200 | 43.65 | -1 |
| 156 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-(3-methoxyprop-1-ynyl)pyrimidine-2,4(1H,3H)-dione          | >200 | 19.48 | -1 |
| 157 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-(4-hydroxybut-1-ynyl)pyrimidine-2,4(1H,3H)-dione           | >200 | 14.35 | -1 |
| 158 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-(5-hydroxypent-1-ynyl)pyrimidine-2,4(1H,3H)-dione          | >200 | 18.05 | -1 |
| 159 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-(methylsulfinyl)pyrimidine-2,4(1H,3H)-dione                | >200 | 93.07 | +1 |
| 160 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-(methylsulfonylmethyl)pyrimidine-2,4(1H,3H)-dione          | >200 | 41.59 | -1 |
| 161 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-(methylthio)pyrimidine-2,4(1H,3H)-dione                    | >200 | 86.82 | +1 |
| 162 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-(pent-1-ynyl)pyrimidine-2,4(1H,3H)-dione                   | >200 | 7.22  | -1 |
| 163 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-(phenylethynyl)pyrimidine-2,4(1H,3H)-dione                 | >200 | 56.64 | +1 |
| 164 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-(prop-1-ynyl)pyrimidine-2,4(1H,3H)-dione                   | >200 | 17.24 | -1 |
| 165 | 1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-5-propylpyrimidine-2,4(1H,3H)-dione                          | >200 | 15.65 | -1 |
| 166 | 1-((3-(hydroxymethyl)cyclopentyl)methyl)-5-iodopyrimidine-2,4(1H,3H)-dione   | >200 | 17.92 | -1 |
| 167 | 1-((3-(hydroxymethyl)cyclopentyl)methyl)pyrimidine-2,4(1H,3H)-dione  | >200 | 2.94  | -1 |
| 168 | 1-(2-amino-6-chloro-9H-purin-9-yl)propan-2-yl acetate  | >200 | 22.69 | -1 |
| 169 | 1-(2-amino-6-fluoro-9H-purin-9-yl)propan-2-ol  | >200 | 3.73  | -1 |
| 170 | 1-(2-fluoro-6-mercapto-9H-purin-9-yl)propan-2-ol   | >200 | 19.06 | -1 |
| 171 | 1-(6-amino-2-iodo-9H-purin-9-yl)propan-2-ol  | >200 | 10.53 | -1 |
| 172 | 1-(6-amino-2-iodo-9H-purin-9-yl)propan-2-yl acetate  | >200 | 31.37 | -1 |
| 173 | 1-(6-chloro-2-iodo-9H-purin-9-yl)propan-2-ol   | >200 | 30.85 | -1 |
| 174 | 2-((2-amino-6-chloro-9H-purin-9-yl)methoxy)ethanol   | >200 | 41.98 | -1 |
| 175 | 2-((2-amino-6-chloro-9H-purin-9-yl)methoxy)ethyl acetate   | >200 | 41.71 | -1 |
| 176 | 2-((2-iodo-6-methoxy-9H-purin-9-yl)methoxy)ethanol   | >200 | 35.07 | -1 |
| 177 | 2-((6-(dimethylamino)-9H-purin-9-yl)methoxy)ethanol  | >200 | 4.26  | -1 |
| 178 | 2-((6-amino-2-iodo-9H-purin-9-yl)methoxy)ethanol   | >200 | 56.65 | +1 |
| 179 | 2,8-diamino-9-((2-hydroxyethoxy)methyl)-1H-purin-6(9H)-one   | >200 | 34.92 | -1 |
| 180 | 2-acetamido-3-(2-(2-(6-amino-9H-purin-9-yl)ethyl)-3,4-dimethoxy-5-oxo-2,5-dihydrofuran-2-ylthio)propanoic acid               | >200 | 56.66 | +1 |
| 181 | 2-amino-1-((2-hydroxyethoxy)methyl)pyrimidin-4(1H)-one   | >200 | 1.57  | -1 |
| 182 | 2-amino-8-(dimethylamino)-9-((2-hydroxyethoxy)methyl)-1H-purin-6(9H)-one   | >200 | 44.44 | -1 |
| 183 | 2-amino-8-bromo-9-((2-hydroxyethoxy)methyl)-1H-purin-6(9H)-one   | >200 | 65.51 | +1 |
| 184 | 2-amino-8-chloro-9-((2-hydroxyethoxy)methyl)-1H-purin-6(9H)-one  | >200 | 65.78 | +1 |
| 185 | 2-amino-8-hydroxy-9-((2-hydroxyethoxy)methyl)-1H-purin-6(9H)-one   | >200 | 40.79 | -1 |
| 186 | 2-amino-9-((1R,3S)-3-(3-hydroxypropyl)-2,2-dimethylcyclobutyl)-1H-purin-6(9H)-one  | >200 | 2.17  | -1 |
| 187 | 2-amino-9-((1S,2R)-2-(hydroxymethyl)cyclohexyl)-9H-purin-6-ol  | >200 | 29.45 | -1 |
| 188 | 2-amino-9-((2-hydroxyethoxy)methyl)-1H-purin-6(9H)-one   | >200 | 29.74 | -1 |

|     |   |      |       |    |
|-----|---|------|-------|----|
| 189 | 2-amino-9-((2-hydroxyethoxy)methyl)-7-(piperidin-1-yl)-8,9-dihydro-1H-purin-6(7H)-one   | >200 | 17.40 | -1 |
| 190 | 2-amino-9-((2-hydroxyethoxy)methyl)-8-(methylamino)-1H-purin-6(9H)-one  | >200 | 40.12 | -1 |
| 191 | 2-amino-9-((3-(hydroxymethyl)-2,2-dimethylcyclobutyl)methyl)-1H-purin-6(9H)-one   | >200 | 7.15  | -1 |
| 192 | 3-(((1R,3S)-3-(hydroxymethyl)-1,2,2-trimethylcyclopentyl)methyl)-3H-[1,2,3]triazolo[4,5-d]pyrimidin-7(6H)-one                                     | >200 | 4.86  | -1 |
| 193 | 3-(((1S,2R)-2-(hydroxymethyl)cyclopentyl)methyl)-3H-[1,2,3]triazolo[4,5-d]pyrimidin-7(6H)-one   | >200 | 3.22  | -1 |
| 194 | 3-(((1R,2R,3R,4S)-2,3,4-tris(hydroxymethyl)cyclopentyl)-3H-[1,2,3]triazolo[4,5-d]pyrimidin-7(6H)-one  | >200 | 17.34 | -1 |
| 195 | 3-(((1S,3R)-3-(2-amino-6-chloro-9H-purin-9-yl)-2,2-dimethylcyclobutyl)propan-1-ol   | >200 | 4.43  | -1 |
| 196 | 3-(((1S,3R)-3-(5,7-diamino-3H-[1,2,3]triazolo[4,5-d]pyrimidin-3-yl)-2,2-dimethylcyclobutyl)propan-1-ol  | >200 | 3.43  | -1 |
| 197 | 3-(((1S,3R)-3-(5-amino-7-chloro-3H-[1,2,3]triazolo[4,5-d]pyrimidin-3-yl)-2,2-dimethylcyclobutyl)propan-1-ol                                       | >200 | 8.04  | -1 |
| 198 | 3-(((S)-1-hydroxyethyl)-2,2-dimethylcyclobutyl)methyl)-3H-[1,2,3]triazolo[4,5-d]pyrimidin-7(6H)-one   | >200 | 8.37  | -1 |
| 199 | 3-((3-(hydroxymethyl)cyclopentyl)methyl)-3H-[1,2,3]triazolo[4,5-d]pyrimidin-7(6H)-one   | >200 | 3.83  | -1 |
| 200 | 4-(1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5-yl)but-3-ynyl 4-methylbenzenesulfonate | >200 | 95.35 | +1 |
| 201 | 5-(6-amino-9H-purin-9-yl)-3,4-dihydroxy-tetrahydrofuran-2-carbaldehyde O-ethyl oxime  | >200 | 33.37 | -1 |
| 202 | 4-(6-amino-9H-purin-9-yl)-2,3-dihydroxycyclopentanecarbaldehyde O-methyl oxime  | >200 | 42.32 | -1 |
| 203 | 4-amino-1-(((1R,3S)-3-(hydroxymethyl)-2,3-dihydro-1H-inden-1-yl)methyl)pyrimidin-2(1H)-one  | >200 | 20.95 | -1 |
| 204 | 4-amino-1-((2-hydroxyethoxy)methyl)-5-nitropyrimidin-2(1H)-one  | >200 | 38.52 | -1 |
| 205 | 4-amino-1-((2-hydroxyethoxy)methyl)pyrimidin-2(1H)-one  | >200 | 2.36  | -1 |
| 206 | 5-((E)-2-chlorovinyl)-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione                                  | >200 | 69.30 | +1 |
| 207 | 5-((Z)-hex-1-enyl)-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione                                     | >200 | 5.66  | -1 |
| 208 | 5-(1,3-dithiolan-2-yl)-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione                                 | >200 | 60.29 | +1 |
| 209 | 5-(1,4-dimethoxy-3-methylnaphthalen-2-yl)-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione              | >200 | 34.80 | -1 |
| 210 | 5-(2-(6-amino-9H-purin-9-yl)ethyl)-5-hydroxy-3,4-dimethoxyfuran-2(5H)-one   | >200 | 63.31 | +1 |
| 211 | 5-(2-(6-chloro-9H-purin-9-yl)ethyl)-5-hydroxy-3,4-dimethoxyfuran-2(5H)-one  | >200 | 86.68 | +1 |
| 212 | 5-(2,5-dimethoxy-3,4,6-trimethylphenyl)-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione                | >200 | 43.01 | -1 |
| 213 | 5-(2,5-dimethoxy-3,4-dimethylphenyl)-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione                   | >200 | 56.14 | +1 |
| 214 | 5-(3,3-dimethylbut-1-ynyl)-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione                             | >200 | 22.37 | -1 |
| 215 | 5-(6-amino-9H-purin-9-yl)-4-hydroxy-tetrahydrofuran-2-carbaldehyde oxime  | >200 | 50.30 | NC |
| 216 | 5-(but-1-ynyl)-1-((2R,3S,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione                                  | >200 | 23.84 | -1 |
| 217 | 5-(but-1-ynyl)-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione   | >200 | 19.01 | -1 |
| 218 | 5-(but-3-en-1-ynyl)-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione                                    | >200 | 29.47 | -1 |
| 219 | 5-(ethynyloxy)-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione   | >200 | 41.61 | -1 |
| 220 | 5-(hept-1-ynyl)-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione  | >200 | 3.97  | -1 |
| 221 | 5-(hex-1-ynyl)-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione   | >200 | 6.32  | -1 |
| 222 | 5-amino-3-(((1R,3S)-3-(3-hydroxypropyl)-2,2-dimethylcyclobutyl)-3H-[1,2,3]triazolo[4,5-d]pyrimidin-7(6H)-one                                      | >200 | 3.88  | -1 |
| 223 | 5-amino-3-((1S,2R)-2-(hydroxymethyl)cyclohexyl)-3H-[1,2,3]triazolo[4,5-d]pyrimidin-7-ol   | >200 | 38.90 | -1 |
| 224 | 5-amino-3-((3-(hydroxymethyl)-2,2-dimethylcyclobutyl)methyl)-3H-[1,2,3]triazolo[4,5-d]pyrimidin-7(6H)-one   | >200 | 10.69 | -1 |
| 225 | 5-bromo-1-(((1R,3S)-3-(hydroxymethyl)-1,2,2-trimethylcyclopentyl)methyl)pyrimidine-2,4(1H,3H)-dione   | >200 | 20.72 | -1 |
| 226 | 5-bromo-1-((2-hydroxyethoxy)methyl)pyrimidine-2,4(1H,3H)-dione  | >200 | 27.33 | -1 |
| 227 | 5-chloro-1-((2-hydroxyethoxy)methyl)pyrimidine-2,4(1H,3H)-dione   | >200 | 29.44 | -1 |

|     |  |      |       |    |
|-----|--|------|-------|----|
| 228 | 5-fluoro-1-((2-hydroxyethoxy)methyl)pyrimidine-2,4(1H,3H)-dione                                      | >200 | 33.93 | -1 |
| 229 | 5-hexyl-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione   | >200 | 4.90  | -1 |
| 230 | 5-hydroxy-1-((2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione | >200 | 50.86 | NC |
| 231 | 9-(((1R,2R)-2-(hydroxymethyl)cyclopentyl)methyl)-9H-purin-6-ol                                       | >200 | 2.00  | -1 |
| 232 | 9-(((1R,3S)-3-(hydroxymethyl)-1,2,2-trimethylcyclopentyl)methyl)-1H-purin-6(9H)-one                  | >200 | 2.99  | -1 |
| 233 | 9-(((1R,3S)-3-(hydroxymethyl)-2,3-dihydro-1H-inden-1-yl)methyl)-9H-purin-6-ol                        | >200 | 20.30 | -1 |
| 234 | 9-(((1R,2R)-2-(hydroxymethyl)cyclopentyl)-9H-purin-6-ol  | >200 | 12.88 | -1 |
| 235 | 9-(((1R,3R,4S)-3,4-bis(hydroxymethyl)cyclopentyl)-1H-purin-6(9H)-one                                 | >200 | 5.83  | -1 |
| 236 | 9-((2-hydroxyethoxy)methyl)-9H-purin-6-ol  | >200 | 14.96 | -1 |
| 237 | 9-((3-((S)-1-hydroxyethyl)-2,2-dimethylcyclobutyl)methyl)-1H-purin-6(9H)-one                         | >200 | 6.23  | -1 |
| 238 | 9-((3-(hydroxymethyl)cyclopentyl)methyl)-1H-purin-6(9H)-one  | >200 | 2.32  | -1 |
| 239 | 9-((3aR,4R,5R,6aS)-4-(hydroxymethyl)-hexahydro-1H-cyclopenta[c]furan-5-yl)-1H-purin-6(9H)-one        | >200 | 9.47  | -1 |
| 240 | 9-(2-(3-((S)-1-hydroxyethyl)-2,2-dimethylcyclobutyl)ethyl)-1H-purin-6(9H)-one                        | >200 | 1.06  | -1 |
| 241 | acetic ((Z)-methyl 2-(3,4-dimethoxy-5-oxofuran-2(5H)-ylidene)ethylphosphonic) thioanhydride          | >200 | 1.07  | -1 |

<sup>a</sup>Observed inhibitory activity estimated as IC<sub>50</sub> (50% growth-inhibitory concentration in μM). Chemicals with IC<sub>50</sub> < 200 μM are considered cytostatic and those with IC<sub>50</sub> > 200 μM non-cytostatic.

<sup>b</sup>Values of +1 and -1 stand for compounds with and without cytotoxic activity, respectively, while NC refereeing to non-classified chemicals.