# Supplementary Materials

**Table S1.** Active compounds included in the enriched dataset.
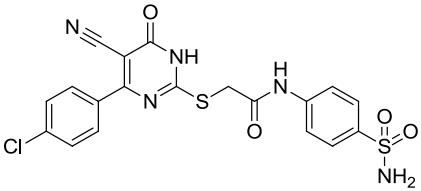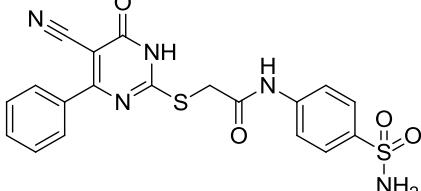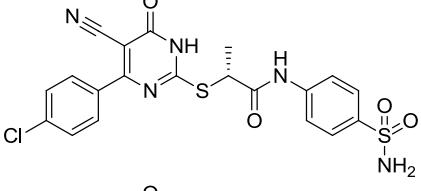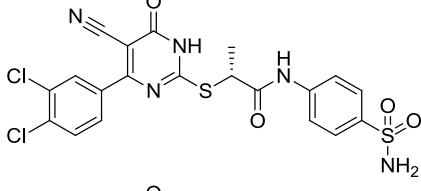
| # | | IC$_{50}$ (µM) | # | | IC$_{50}$ (µM) |
|---|---|---|---|---|---|
| 1 |  | 8.8 | 2 |  | 12.1 |
| 3 |  | 0.48 | 4 |  | 0.75 |
| 5 |  | 0.71 | 6 |  | 0.65 |
| 7 |  | 7.4 | 8 |  | 4 |
| 9 |  | 14 | 10 |  | 10 |
| 11 |  | 4 | 12 |  | 2 |
| 13 |  | 2 | 14 |  | 2 |
| 15 |  | 2 | 16 |  | 12 |
| 17 |  | 2 | 18 |  | 3 |
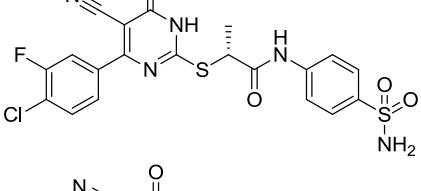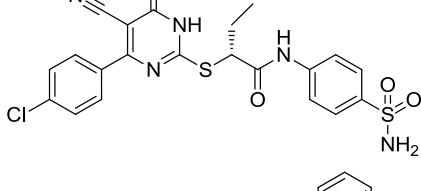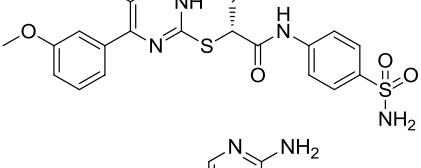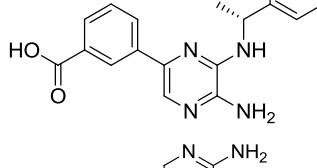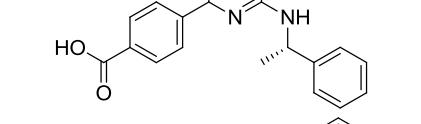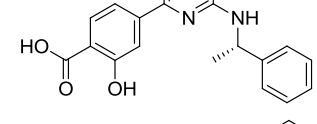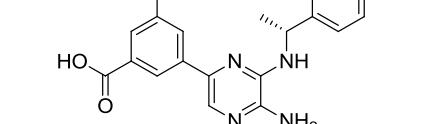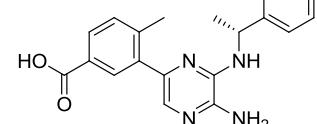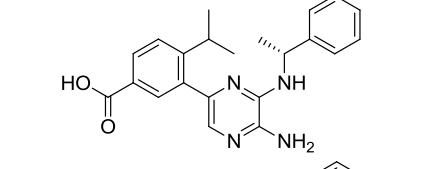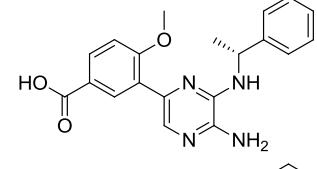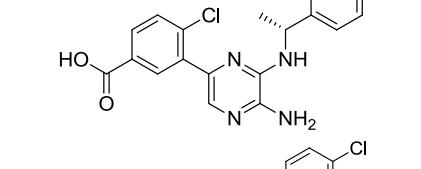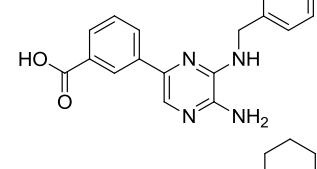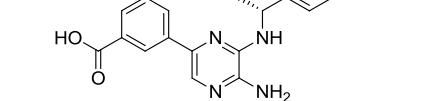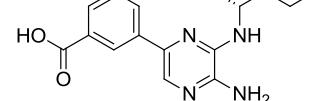
**Table S1.** *Cont.*

| # | | IC$_{50}$ (µM) | # | | IC$_{50}$ (µM) |
|---|---|---|---|---|---|
| 19 | | 7 | 20 | | 4.6 |
| 21 | | 1.6 | 22 | | 12 |
| 23 | | 5.6 | 24 | | 5.6 |
| 25 | | 0.87 | 26 | | 3.7 |
| 27 | | 0.58 | 28 | | 1.0 |
| 29 | | 7.4 | 30 | | 0.27 |
| 31 | | 2.3 | 32 | | 0.5 |
| 33 | | 3.1 | 34 | | 6.8 |
| 35 | | 0.45 | 36 | | 0.64 |
| 37 | | 2.1 | 38 | | 0.18 |

**Table S1.** *Cont.*

| # | | IC$_{50}$ (µM) | # | | IC$_{50}$ (µM) |
|---|---|---|---|---|---|
| **39** | | 4.0 | **40** | | 4.0 |
| **41** | | 11 | **42** | | 11 |
| **43** | | 13 | **44** | | 5.5 |
| **45** | | 3.9 | **46** | | 5.0 |
| **47** | | 9.5 | **48** | | 3.8 |
| **49** | | 2.2 | **50** | | 3.5 |
| **51** | | 4.1 | **52** | | 13 |
| **53** | | 5.6 | **54** | | 6.6 |
| **55** | | 7.4 | **56** | | 3.3 |
| **57** | | 2.1 | **58** | | 0.36 |
| **59** | | 0.35 | **60** | | 0.03 |

**Table S1.** *Cont.*

| # | | IC$_{50}$ (μM) | # | | IC$_{50}$ (μM) |
|---|---|---|---|---|---|
| **61** | | 0.24 | **62** | | 2.6 |
| **63** | | 0.23 | **64** | | 0.37 |
| **65** | | 0.10 | **66** | | 0.17 |
| **67** | | 0.06 | **68** | | 0.09 |
| **69** | | 0.10 | **70** | | 0.06 |
| **71** | | 0.108 | **72** | | 0.085 |
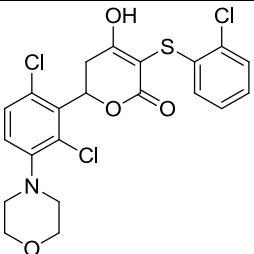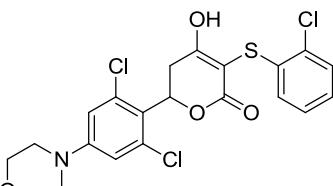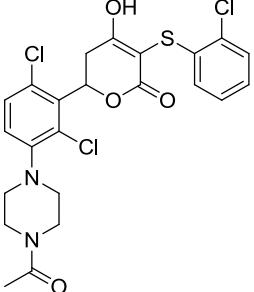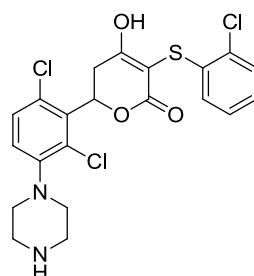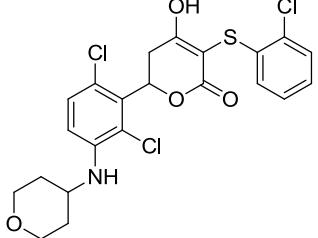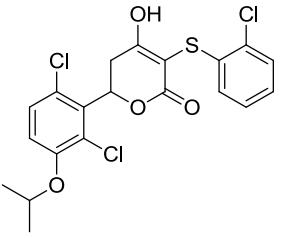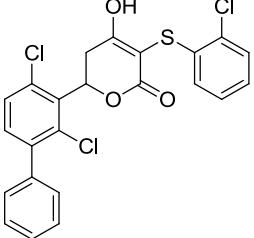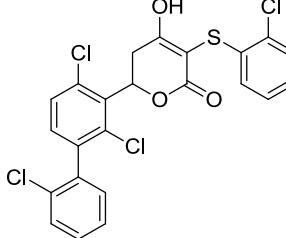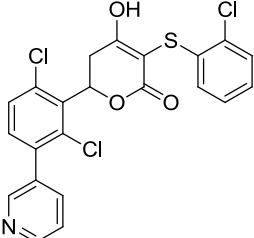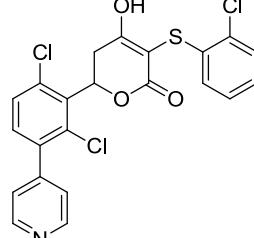
**Table S1.** *Cont.*

| # | | IC$_{50}$ (µM) | # | | IC$_{50}$ (µM) |
|---|---|---|---|---|---|
| **73** | | 1.1 | **74** | | 0.12 |
| **75** | | 0.37 | **76** | | 0.64 |
| **77** | | 0.17 | **78** | | 3.5 |
| **79** | | 1.8 | **80** | | 0.3 |
| **81** | | 0.04 | **82** | | 0.13 |
| **83** | | 0.12 | **84** | | 0.006 |

**Table S1.** *Cont.*

| # | | IC$_{50}$ (µM) | # | | IC$_{50}$ (µM) |
|---|---|---|---|---|---|
| **85** |  | 0.09 | **86** |  | 0.03 |
| **87** |  | 0.025 | **88** |  | 0.015 |
| **89** |  | 0.46 | **90** |  | 0.035 |
| **91** |  | 0.030 | **92** |  | 0.49 |
| **93** |  | 0.87 | | | |