

Structure-guided approach identifies a novel class of HIV-1
Ribonuclease H inhibitors: Binding mode insights through
magnesium complexation and site-directed mutagenesis studies

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Francesca Esposito,² Enzo Tramontano^{2,4*} and Jacob Kongsted^{1*}

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DK-5230 Odense M, Denmark

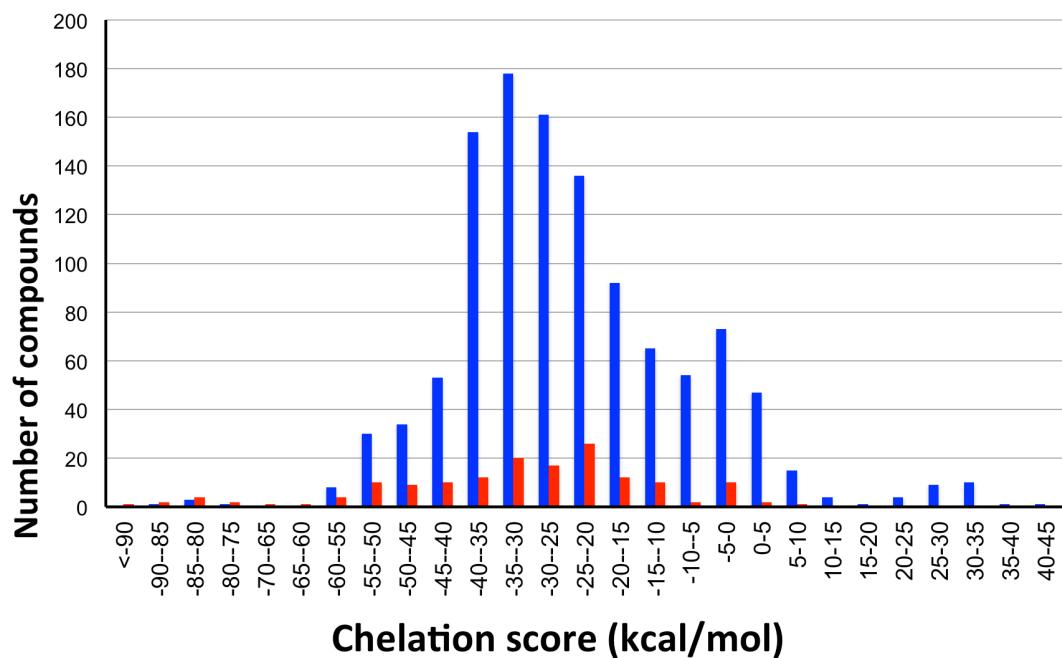
² Department of Life and Environmental Sciences, University of Cagliari, Italy

³ Dipartimento di Chimica e Tecnologie del Farmaco, Istituto Pasteur-Fondazione
Cenci Bolognetti, “Sapienza” Università di Roma, Roma, Italy

⁴ Istituto di Ricerca Genetica e Biomedica, Consiglio Nazionale delle Ricerche
(CNR), Monserrato(CA), Italy.

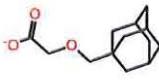
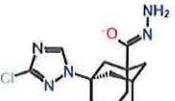
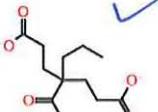
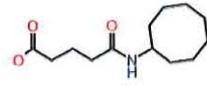
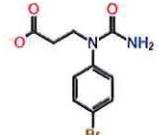
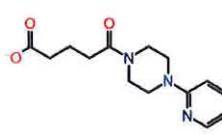
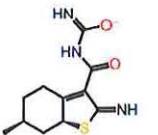
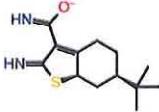
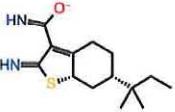
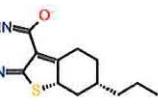
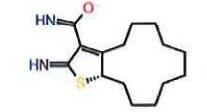
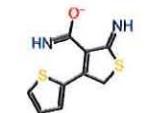
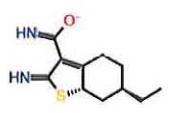
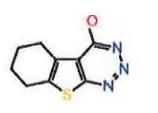
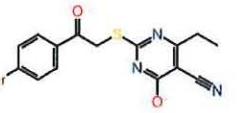
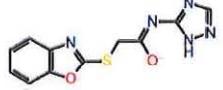
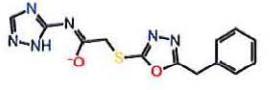
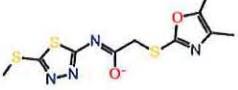
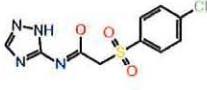
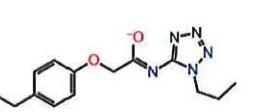
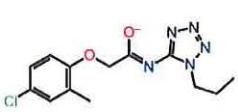
Supporting information

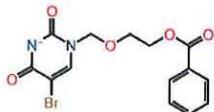
- S1. Comparison of frequency of compounds used for chelation calculation (n=1135, blue bar) and compounds selected from chelation calculation (n=180, red bar).



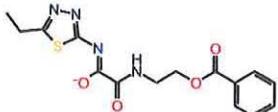
S2. List of compounds used for cluster analysis and its chelation score

①

			
Compound: ZINC12362958 XP GScore: None dE [kcal/mol]: -3.61 ORDER CLUSTER: 1	Compound: ZINC18161917 XP GScore: None dE [kcal/mol]: 1.03 ORDER CLUSTER: 1	Compound: ZINC45028182 XP GScore: None dE [kcal/mol]: -34.19 ORDER CLUSTER: 2	Compound: ZINC00475491 XP GScore: None dE [kcal/mol]: -34.61 ORDER CLUSTER: 3
			
Compound: ZINC01019453 XP GScore: None dE [kcal/mol]: -59.34 ORDER CLUSTER: 4	Compound: ZINC00152847 XP GScore: None dE [kcal/mol]: -36.47 ORDER CLUSTER: 4	Compound: ZINC02807453 XP GScore: None dE [kcal/mol]: -46.38 ORDER CLUSTER: 5	Compound: ZINC02807454 XP GScore: None dE [kcal/mol]: -43.8 ORDER CLUSTER: 5
			
Compound: ZINC00191631 XP GScore: None dE [kcal/mol]: -32.1 ORDER CLUSTER: 5	Compound: ZINC37858717 XP GScore: None dE [kcal/mol]: -25.16 ORDER CLUSTER: 5	Compound: ZINC37858768 XP GScore: None dE [kcal/mol]: -21.61 ORDER CLUSTER: 5	Compound: ZINC04651416 XP GScore: None dE [kcal/mol]: -10.58 ORDER CLUSTER: 5
			
Compound: ZINC38142834 XP GScore: None dE [kcal/mol]: -2.57 ORDER CLUSTER: 5	Compound: ZINC00259051 XP GScore: None dE [kcal/mol]: -2.51 ORDER CLUSTER: 5	Compound: ZINC08763102 XP GScore: None dE [kcal/mol]: -21.09 ORDER CLUSTER: 6	Compound: ZINC01016895 XP GScore: None dE [kcal/mol]: 1.12 ORDER CLUSTER: 7
			
Compound: ZINC19849744 XP GScore: None dE [kcal/mol]: -3.66 ORDER CLUSTER: 8	Compound: ZINC19849690 XP GScore: None dE [kcal/mol]: -2.88 ORDER CLUSTER: 8	Compound: ZINC08334000 XP GScore: None dE [kcal/mol]: -0.94 ORDER CLUSTER: 8	Compound: ZINC19851980 XP GScore: None dE [kcal/mol]: -0.48 ORDER CLUSTER: 8
			
Compound: ZINC85388658 XP GScore: None dE [kcal/mol]: -12.35 ORDER CLUSTER: 9	Compound: ZINC00386315 XP GScore: None dE [kcal/mol]: -8.81 ORDER CLUSTER: 9	Compound: ZINC02592664 XP GScore: None dE [kcal/mol]: -2.18 ORDER CLUSTER: 9	Compound: ZINC02472023 XP GScore: None dE [kcal/mol]: -22.42 ORDER CLUSTER: 10



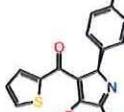
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ORDER CLUSTER: 11



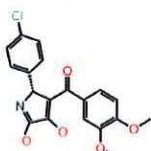
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dE [kcal/mol]: -13.91
ORDER CLUSTER: 11



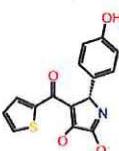
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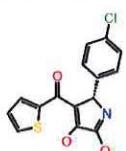
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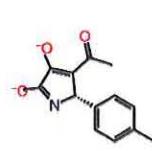
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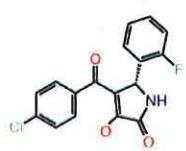
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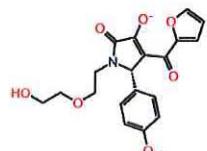
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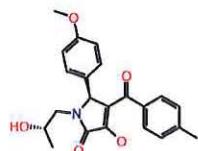
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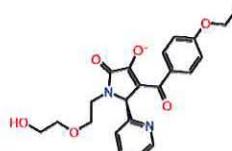
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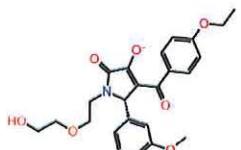
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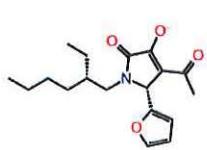
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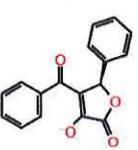
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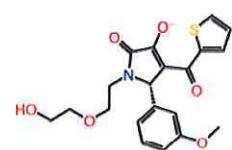
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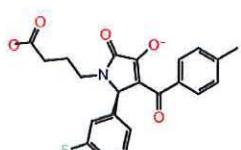
Compound: ZINC19923586
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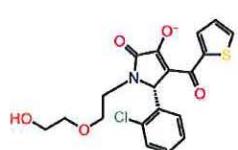
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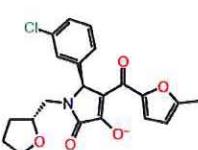
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ORDER CLUSTER: 13



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ORDER CLUSTER: 13



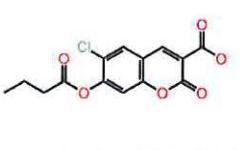
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ORDER CLUSTER: 13



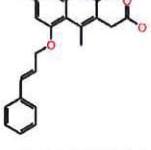
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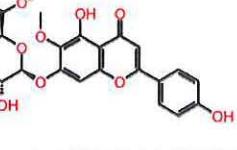
Compound: ZINC26522544
XP GScore: None
dE [kcal/mol]: -43.6
ORDER CLUSTER: 14



Compound: ZINC37637282
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ORDER CLUSTER: 14



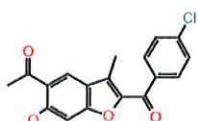
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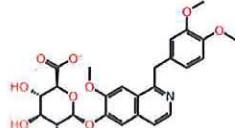
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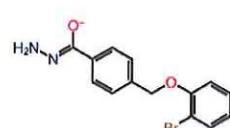
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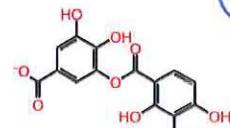
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dE [kcal/mol]: -19.91
ORDER CLUSTER: 17



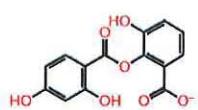
Compound: ZINC77286738
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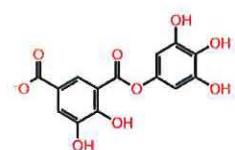
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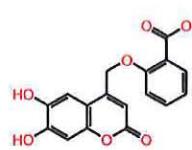
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XP GScore: None
dE [kcal/mol]: None
ORDER CLUSTER: 19



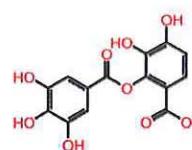
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dE [kcal/mol]: None
ORDER CLUSTER: 19



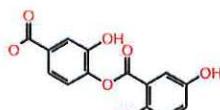
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dE [kcal/mol]: None
ORDER CLUSTER: 19



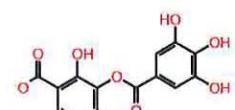
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dE [kcal/mol]: None
ORDER CLUSTER: 19



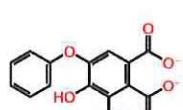
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dE [kcal/mol]: None
ORDER CLUSTER: 19



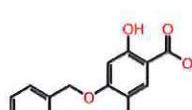
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dE [kcal/mol]: None
ORDER CLUSTER: 19



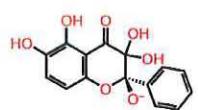
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dE [kcal/mol]: None
ORDER CLUSTER: 19



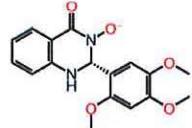
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ORDER CLUSTER: 19



Compound: None
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dE [kcal/mol]: None
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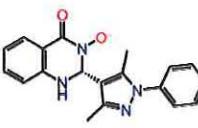
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dE [kcal/mol]: None
ORDER CLUSTER: 20



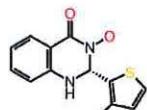
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ORDER CLUSTER: 21



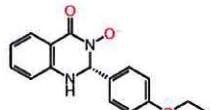
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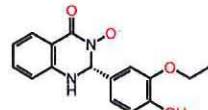
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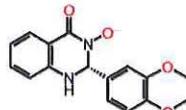
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dE [kcal/mol]: -41.43
ORDER CLUSTER: 21



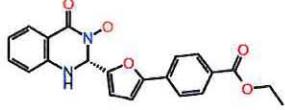
Compound: ZINC00374685
XP GScore: None
dE [kcal/mol]: -37.97
ORDER CLUSTER: 21



Compound: ZINC00375077
XP GScore: None
dE [kcal/mol]: -37.05
ORDER CLUSTER: 21



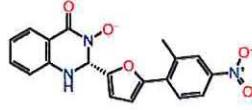
Compound: ZINC00079918
XP GScore: None
dE [kcal/mol]: -35.19
ORDER CLUSTER: 21



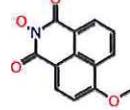
Compound: ZINC01012036
XP GScore: None
dE [kcal/mol]: -34.19
ORDER CLUSTER: 21



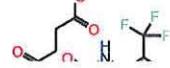
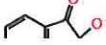
Compound: ZINC00373588
XP GScore: None
dE [kcal/mol]: -22.05
ORDER CLUSTER: 21

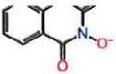
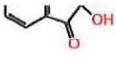
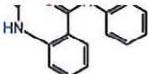
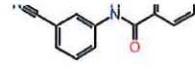
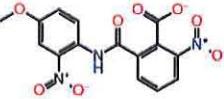
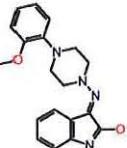
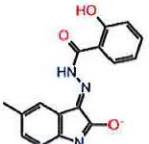
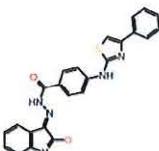
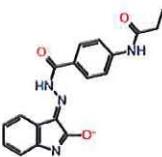
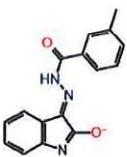
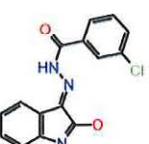
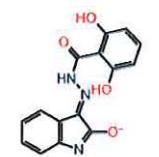
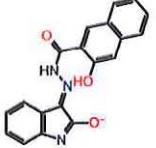
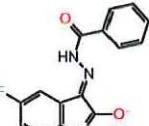
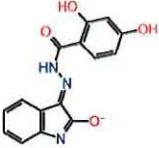
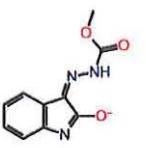
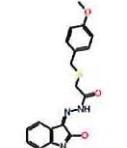
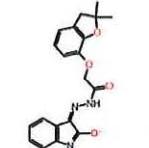
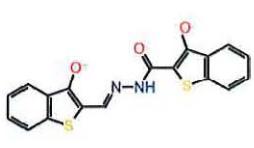
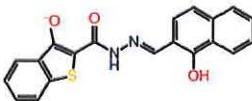
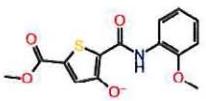
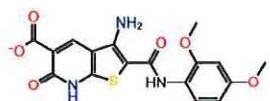
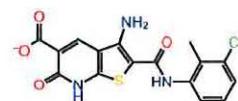


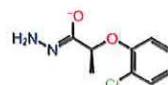
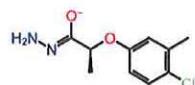
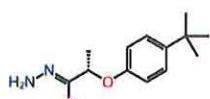
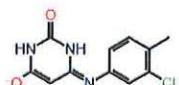
Compound: ZINC00651709
XP GScore: None
dE [kcal/mol]: -20.69
ORDER CLUSTER: 21



Compound: ZINC02857491
XP GScore: None
dE [kcal/mol]: -56.28
ORDER CLUSTER: 21



			
Compound: ZINC00507434 XP GScore: None dE [kcal/mol]: -50.47 ORDER CLUSTER: 21	Compound: ZINC00388306 XP GScore: None dE [kcal/mol]: -51.6 ORDER CLUSTER: 22	Compound: ZINC00991839 XP GScore: None dE [kcal/mol]: -51.01 ORDER CLUSTER: 22	Compound: ZINC00038659 XP GScore: None dE [kcal/mol]: -44.92 ORDER CLUSTER: 22
			
Compound: ZINC08397431 XP GScore: None dE [kcal/mol]: -32.02 ORDER CLUSTER: 22	Compound: ZINC00046712 XP GScore: None dE [kcal/mol]: -26.97 ORDER CLUSTER: 23	Compound: ZINC13564422 XP GScore: None dE [kcal/mol]: -24.74 ORDER CLUSTER: 23	Compound: ZINC00632016 XP GScore: None dE [kcal/mol]: -23.92 ORDER CLUSTER: 23
			
Compound: ZINC05903864 XP GScore: None dE [kcal/mol]: -23.91 ORDER CLUSTER: 23	Compound: ZINC18158953 XP GScore: None dE [kcal/mol]: -23.46 ORDER CLUSTER: 23	Compound: ZINC05731671 XP GScore: None dE [kcal/mol]: -22.82 ORDER CLUSTER: 23	Compound: ZINC06557787 XP GScore: None dE [kcal/mol]: -22.78 ORDER CLUSTER: 23
			
Compound: ZINC05093953 XP GScore: None dE [kcal/mol]: -22.59 ORDER CLUSTER: 23	Compound: ZINC18122388 XP GScore: None dE [kcal/mol]: -22.12 ORDER CLUSTER: 23	Compound: ZINC15018524 XP GScore: None dE [kcal/mol]: -22.1 ORDER CLUSTER: 23	Compound: ZINC05731666 XP GScore: None dE [kcal/mol]: -19.46 ORDER CLUSTER: 23
			
Compound: ZINC05729674 XP GScore: None dE [kcal/mol]: -14.9 ORDER CLUSTER: 23	Compound: ZINC05432928 XP GScore: None dE [kcal/mol]: -14.52 ORDER CLUSTER: 23	Compound: ZINC05408234 XP GScore: None dE [kcal/mol]: -12.65 ORDER CLUSTER: 23	Compound: ZINC00704088 XP GScore: None dE [kcal/mol]: -36.0 ORDER CLUSTER: 24
			
Compound: ZINC00704090 XP GScore: None dE [kcal/mol]: -26.98 ORDER CLUSTER: 24	Compound: ZINC00480526 XP GScore: None dE [kcal/mol]: -19.17 ORDER CLUSTER: 24	Compound: ZINC02694784 XP GScore: None dE [kcal/mol]: -49.35 ORDER CLUSTER: 24	Compound: ZINC02293585 XP GScore: None dE [kcal/mol]: -47.77 ORDER CLUSTER: 24

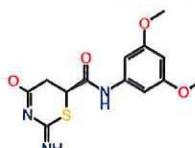
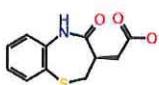


Compound: ZINC00262568
XP GScore: None
dE [kcal/mol]: 6.07
ORDER CLUSTER: 25

Compound: ZINC00369784
XP GScore: None
dE [kcal/mol]: -18.26
ORDER CLUSTER: 26

Compound: ZINC00374953
XP GScore: None
dE [kcal/mol]: -17.59
ORDER CLUSTER: 26

Compound: ZINC00370112
XP GScore: None
dE [kcal/mol]: -16.63
ORDER CLUSTER: 26



Compound: ZINC00374052
XP GScore: None
dE [kcal/mol]: -22.3
ORDER CLUSTER: 27

Compound: ZINC20031542
XP GScore: None
dE [kcal/mol]: -37.8
ORDER CLUSTER: 28

Compound: ZINC00208967
XP GScore: None
dE [kcal/mol]: -35.68
ORDER CLUSTER: 28

Compound: ZINC00185284
XP GScore: None
dE [kcal/mol]: -34.7
ORDER CLUSTER: 28

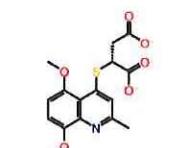
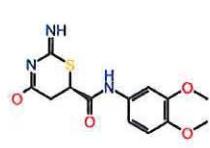
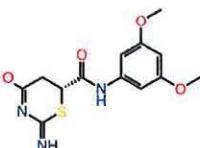


Compound: ZINC00216229
XP GScore: None
dE [kcal/mol]: -34.45
ORDER CLUSTER: 28

Compound: ZINC00216235
XP GScore: None
dE [kcal/mol]: -34.25
ORDER CLUSTER: 28

Compound: ZINC00216226
XP GScore: None
dE [kcal/mol]: -31.22
ORDER CLUSTER: 28

Compound: ZINC00190868
XP GScore: None
dE [kcal/mol]: -29.84
ORDER CLUSTER: 28

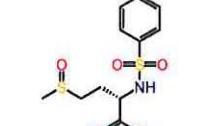
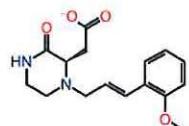


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XP GScore: None
dE [kcal/mol]: -28.11
ORDER CLUSTER: 28

Compound: ZINC00185281
XP GScore: None
dE [kcal/mol]: -26.64
ORDER CLUSTER: 28

Compound: ZINC72309484
XP GScore: None
dE [kcal/mol]: -86.9
ORDER CLUSTER: 28

Compound: ZINC16385868
XP GScore: None
dE [kcal/mol]: -77.8
ORDER CLUSTER: 28

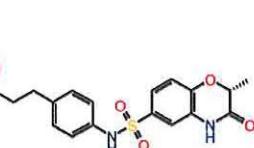
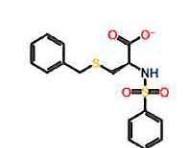
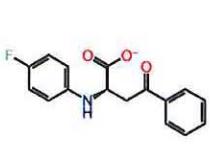


Compound: ZINC04502202
XP GScore: None
dE [kcal/mol]: -54.79
ORDER CLUSTER: 29

Compound: ZINC04195890
XP GScore: None
dE [kcal/mol]: -42.83
ORDER CLUSTER: 30

Compound: ZINC03281818
XP GScore: None
dE [kcal/mol]: -27.56
ORDER CLUSTER: 30

Compound: ZINC49537596
XP GScore: None
dE [kcal/mol]: -54.82
ORDER CLUSTER: 30

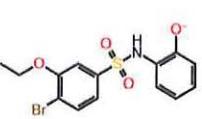
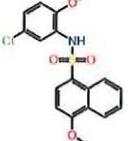
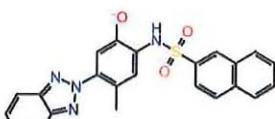
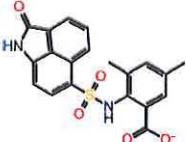
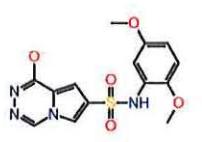
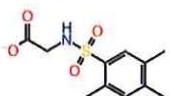
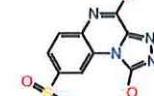
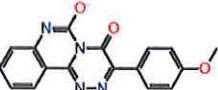
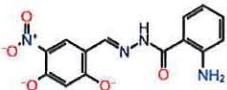
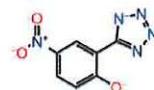
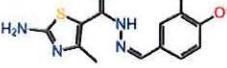
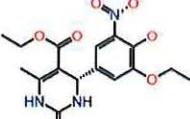
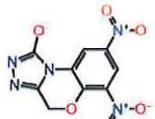
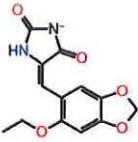
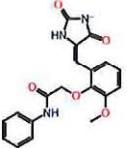
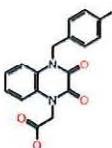
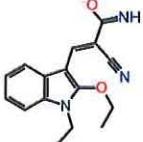
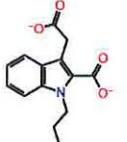
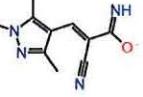
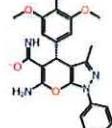


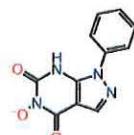
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XP GScore: None
dE [kcal/mol]: -52.43
ORDER CLUSTER: 30

Compound: ZINC04197488
XP GScore: None
dE [kcal/mol]: -46.16
ORDER CLUSTER: 30

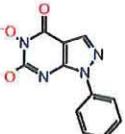
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XP GScore: None
dE [kcal/mol]: -38.39
ORDER CLUSTER: 30

Compound: ZINC15108384
XP GScore: None
dE [kcal/mol]: -35.76
ORDER CLUSTER: 30

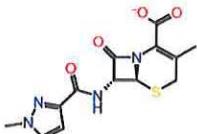
			
Compound: ZINC12417073 XP GScore: None dE [kcal/mol]: -35.71 ORDER CLUSTER: 30	Compound: ZINC32601987 XP GScore: None dE [kcal/mol]: -23.71 ORDER CLUSTER: 30	Compound: ZINC35592618 XP GScore: None dE [kcal/mol]: -19.82 ORDER CLUSTER: 30	Compound: ZINC00717638 XP GScore: None dE [kcal/mol]: -17.11 ORDER CLUSTER: 30
			
Compound: ZINC60360593 XP GScore: None dE [kcal/mol]: -46.02 ORDER CLUSTER: 30	Compound: ZINC75874141 XP GScore: None dE [kcal/mol]: -20.45 ORDER CLUSTER: 30	Compound: ZINC00216006 XP GScore: None dE [kcal/mol]: -36.21 ORDER CLUSTER: 31	Compound: ZINC02150471 XP GScore: None dE [kcal/mol]: -35.73 ORDER CLUSTER: 32
			
Compound: ZINC12810395 XP GScore: None dE [kcal/mol]: -13.05 ORDER CLUSTER: 32	Compound: ZINC04114736 XP GScore: None dE [kcal/mol]: -25.85 ORDER CLUSTER: 33	Compound: ZINC19938708 XP GScore: None dE [kcal/mol]: -51.14 ORDER CLUSTER: 34	Compound: ZINC17154752 XP GScore: None dE [kcal/mol]: -40.72 ORDER CLUSTER: 34
			
Compound: ZINC06131978 XP GScore: None dE [kcal/mol]: -18.68 ORDER CLUSTER: 34	Compound: ZINC00674226 XP GScore: Nonc dE [kcal/mol]: -33.33 ORDER CLUSTER: 35	Compound: ZINC36042410 XP GScore: None dE [kcal/mol]: -23.6 ORDER CLUSTER: 35	Compound: ZINC02150493 XP GScore: None dE [kcal/mol]: -16.72 ORDER CLUSTER: 35
			
Compound: ZINC00474054 XP GScore: None dE [kcal/mol]: -23.9 ORDER CLUSTER: 36	Compound: ZINC00661401 XP GScore: None dE [kcal/mol]: -21.83 ORDER CLUSTER: 36	Compound: ZINC09087212 XP GScore: None dE [kcal/mol]: -21.17 ORDER CLUSTER: 36	Compound: ZINC49455234 XP GScore: None dE [kcal/mol]: -46.73 ORDER CLUSTER: 37
			
Compound: ZINC00448075 XP GScore: None dE [kcal/mol]: -2.26 ORDER CLUSTER: 38	Compound: ZINC00269788 XP GScore: None dE [kcal/mol]: -81.89 ORDER CLUSTER: 38	Compound: ZINC00373991 XP GScore: None dE [kcal/mol]: -0.18 ORDER CLUSTER: 39	Compound: ZINC58903464 XP GScore: None dE [kcal/mol]: -60.8 ORDER CLUSTER: 40



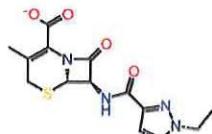
Compound: ZINC01686082
XP GScore: None
dE [kcal/mol]: -103.62
ORDER CLUSTER: 41



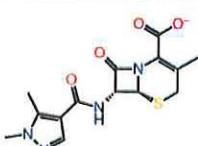
Compound: ZINC01686082
XP GScore: None
dE [kcal/mol]: -103.62
ORDER CLUSTER: 41



Compound: ZINC02735297
XP GScore: None
dE [kcal/mol]: -33.4
ORDER CLUSTER: 42



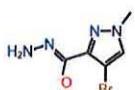
Compound: ZINC02735291
XP GScore: None
dE [kcal/mol]: -31.71
ORDER CLUSTER: 42



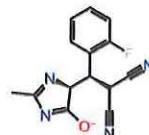
Compound: ZINC02739550
XP GScore: None
dE [kcal/mol]: -31.41
ORDER CLUSTER: 42



Compound: ZINC02739502
XP GScore: None
dE [kcal/mol]: -26.91
ORDER CLUSTER: 42



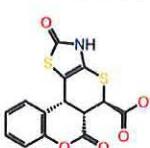
Compound: ZINC01019011
XP GScore: None
dE [kcal/mol]: -10.55
ORDER CLUSTER: 43



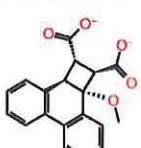
Compound: ZINC00214264
XP GScore: None
dE [kcal/mol]: -5.61
ORDER CLUSTER: 44



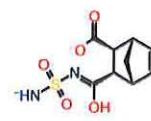
Compound: ZINC33331372
XP GScore: None
dE [kcal/mol]: -34.22
ORDER CLUSTER: 45



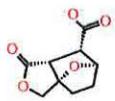
Compound: ZINC33331372
XP GScore: None
dE [kcal/mol]: -34.22
ORDER CLUSTER: 45



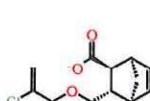
Compound: ZINC16958095
XP GScore: None
dE [kcal/mol]: -59.33
ORDER CLUSTER: 46



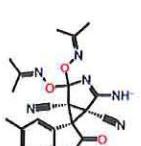
Compound: ZINC19594458
XP GScore: None
dE [kcal/mol]: -59.7
ORDER CLUSTER: 47



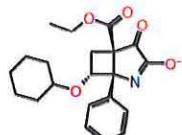
Compound: ZINC04568228
XP GScore: None
dE [kcal/mol]: -34.53
ORDER CLUSTER: 47



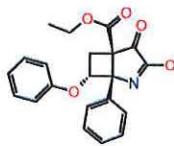
Compound: ZINC00143290
XP GScore: None
dE [kcal/mol]: -20.48
ORDER CLUSTER: 47



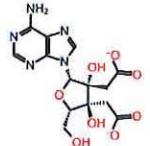
Compound: ZINC33821869
XP GScore: None
dE [kcal/mol]: -14.45
ORDER CLUSTER: 48



Compound: ZINC07044829
XP GScore: None
dE [kcal/mol]: -27.79
ORDER CLUSTER: 49

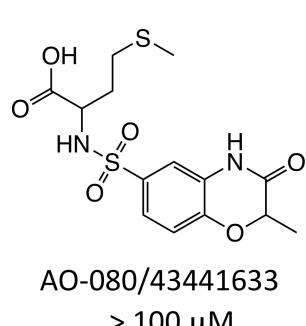
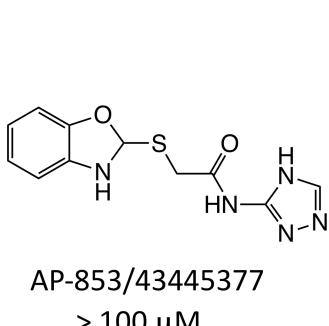
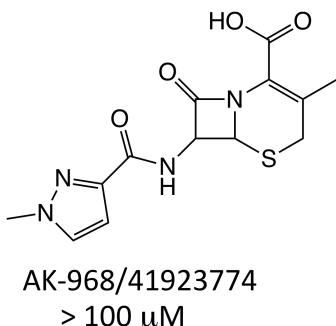
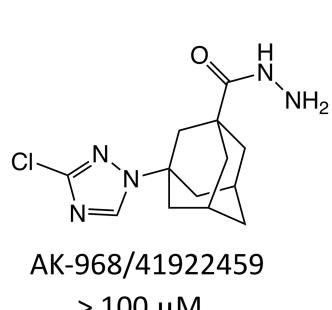
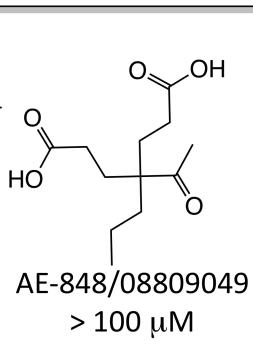
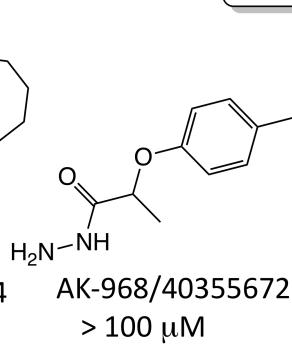
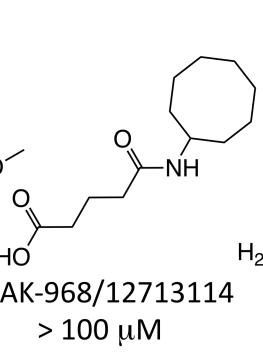
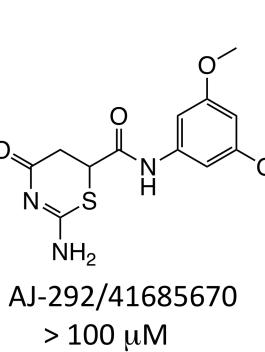
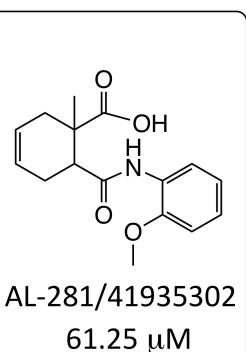
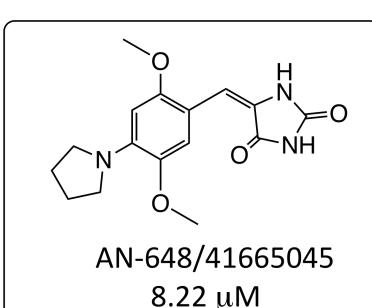
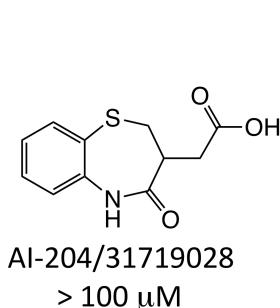
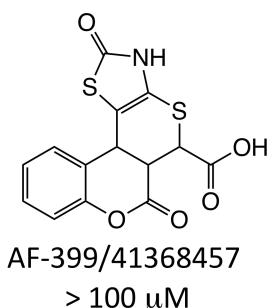
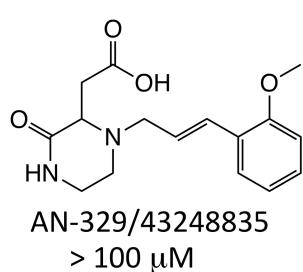
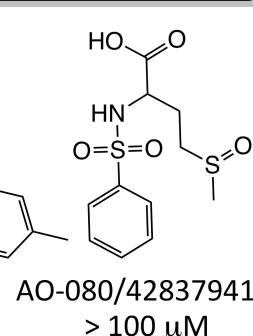
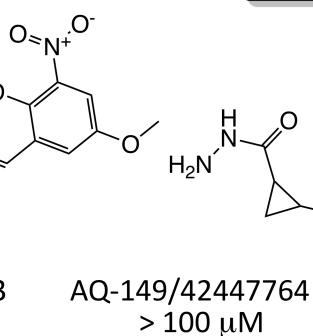
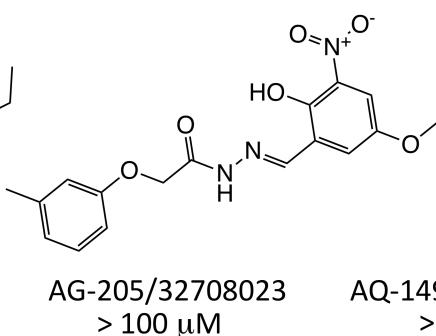
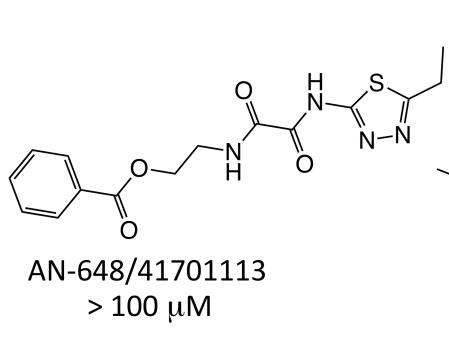
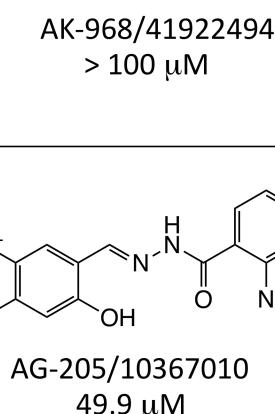
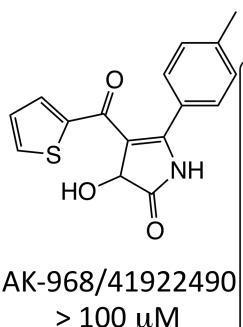
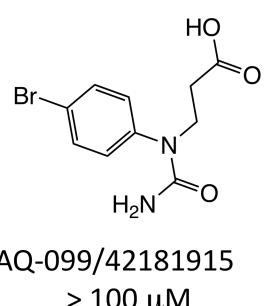
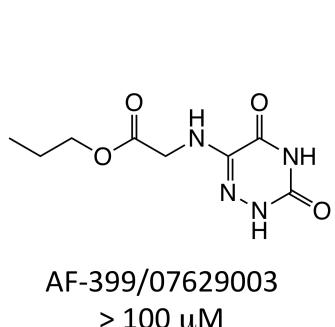
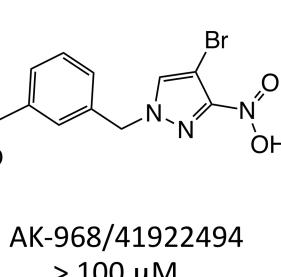
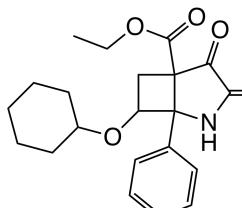
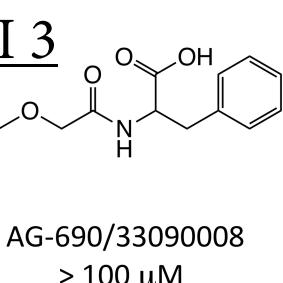
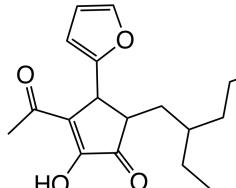


Compound: ZINC04665024
XP GScore: None
dE [kcal/mol]: -15.76
ORDER CLUSTER: 49

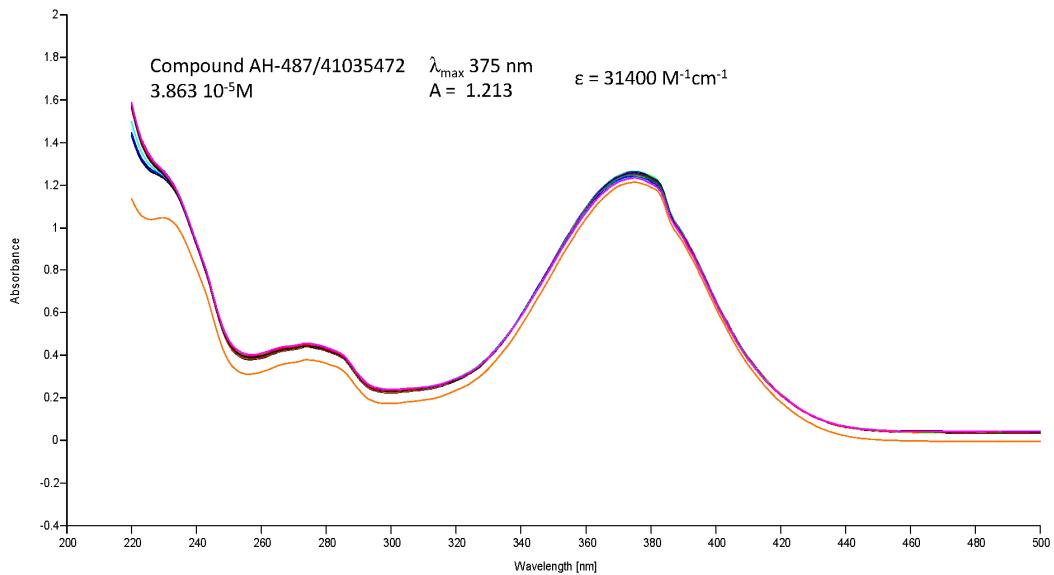


Compound: ZINC71613882
XP GScore: None
dE [kcal/mol]: -65.04
ORDER CLUSTER: 50

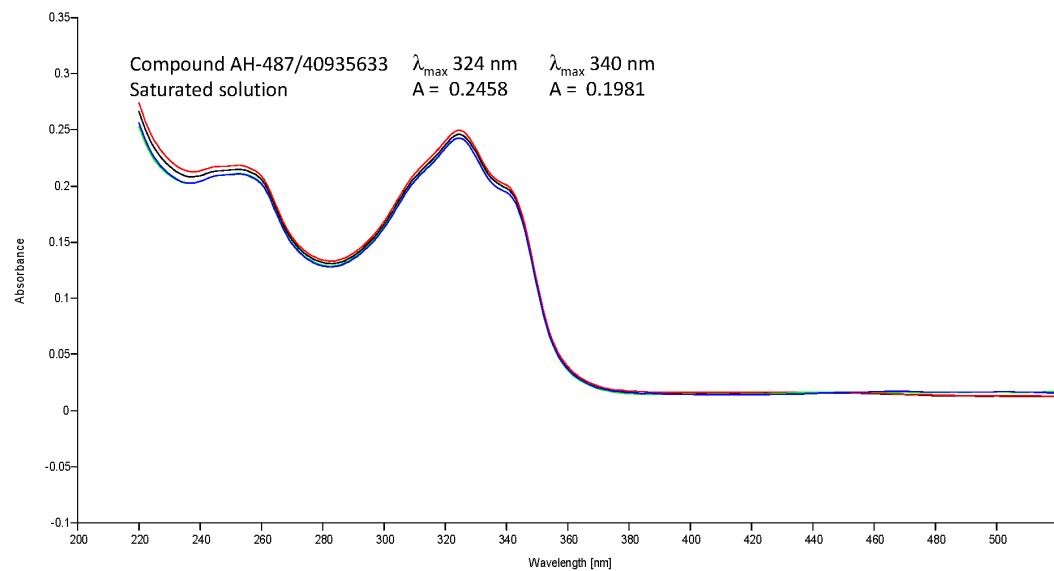
SI 3



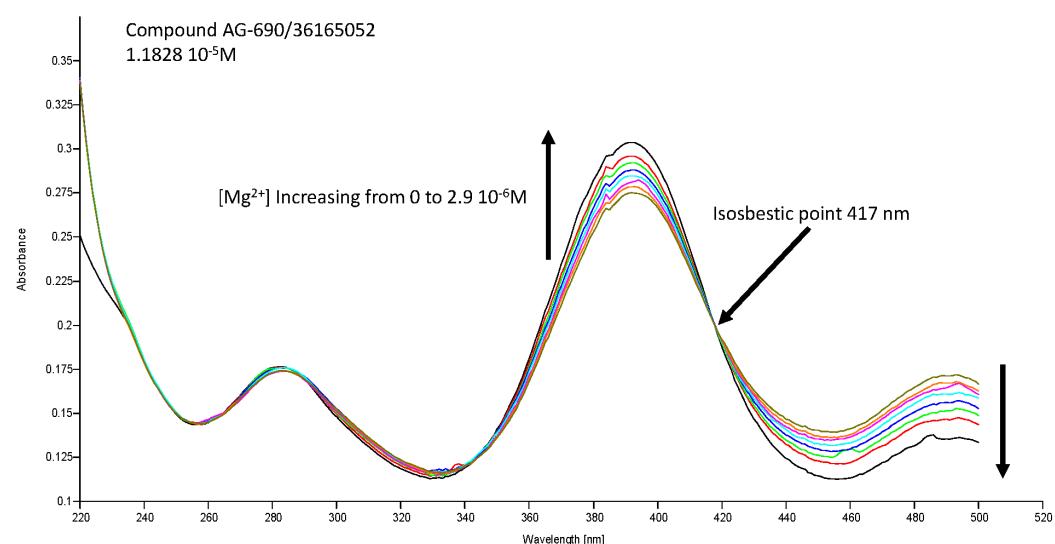
S4 UV-Vis Spectra of compound **AF**



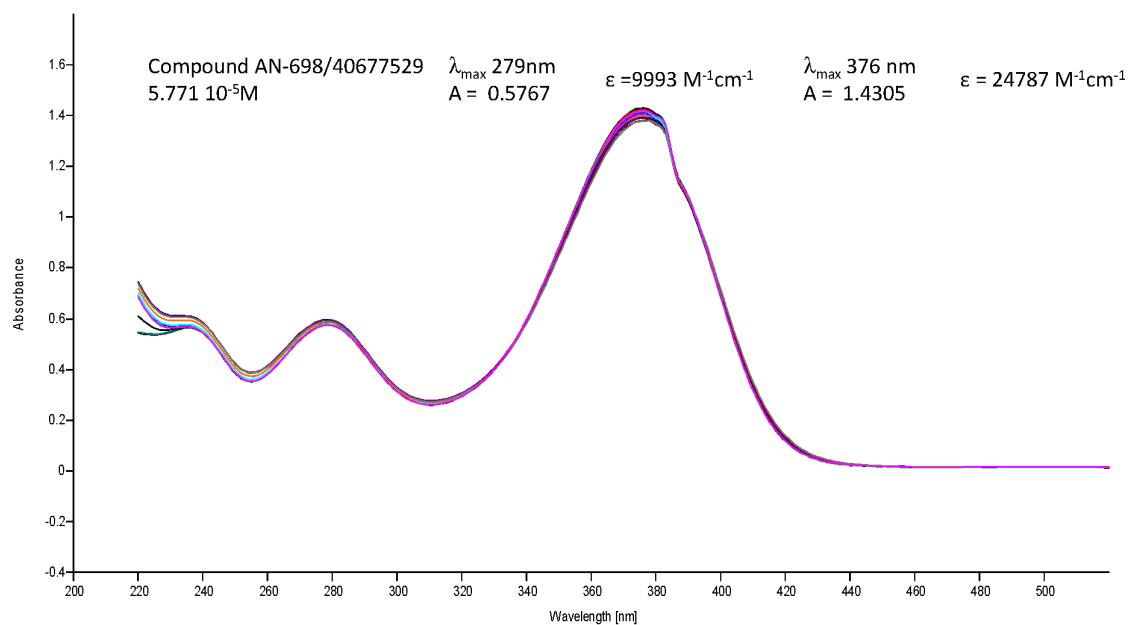
S5 UV-Vis Spectra of compound **AE**



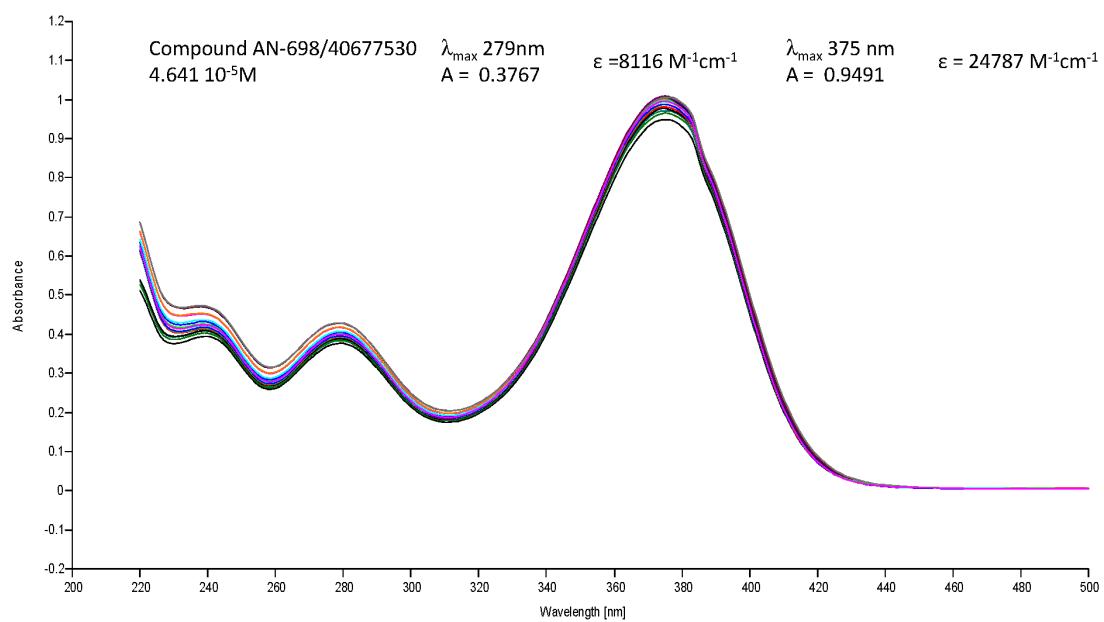
S6 UV-Vis Spectra of compound **AA**



S7 UV-Vis Spectra of compound **AC**



S8 UV-Vis Spectra of compound **AD**



S9. Comparison of binding modes of BPT in various site directed mutagenesis structural models with schematic representation of protein-ligand interactions.

