

Mapping pilicide anti-virulence effect in *E. coli*, a comprehensive structure-activity study

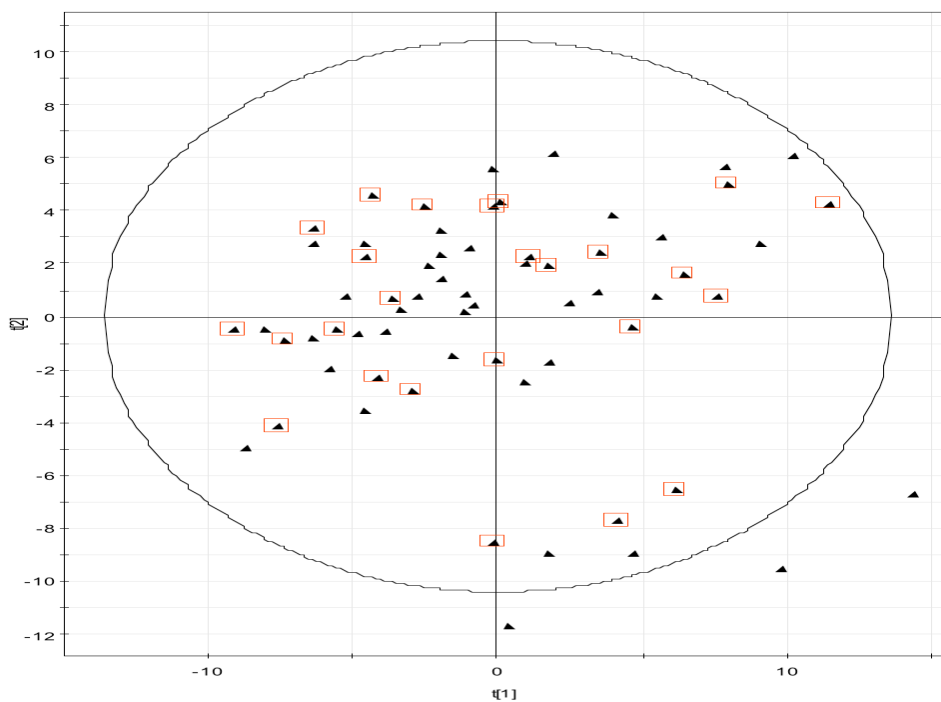
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Supporting Information

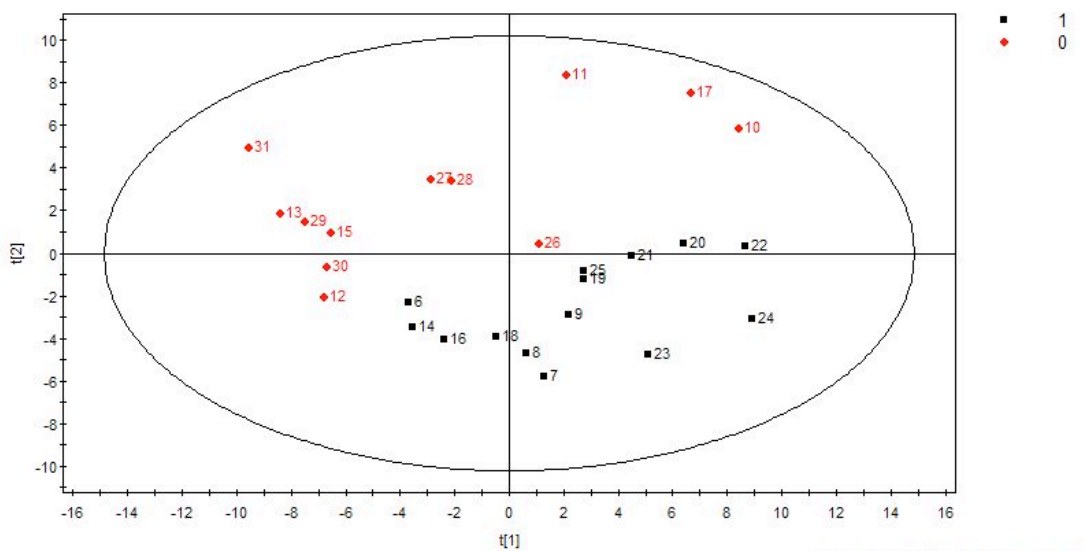
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Score plot showing the 24 di-substituted derivatives that was chosen by the D-optimal design (red boxes):



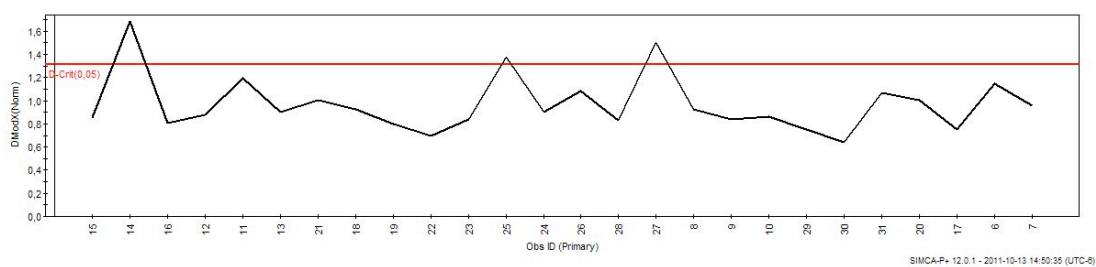
Score

Plot from the PCA of all 24 di-substituted compounds in the training set (red = inactive, black = active):

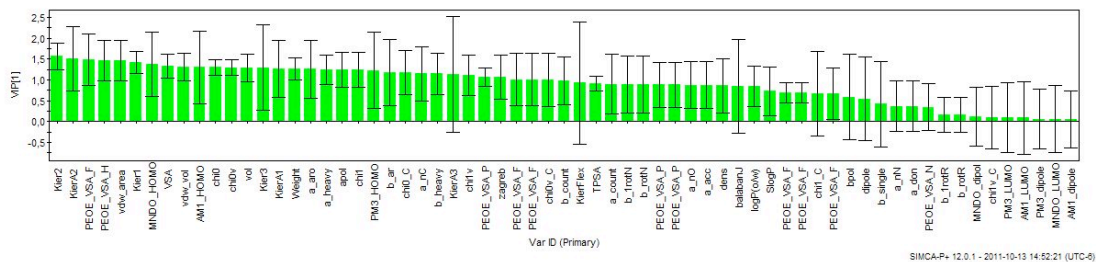


SIMCA-P+ 12.0.1 - 2011-10-13 14:33:38 (UTC-8)

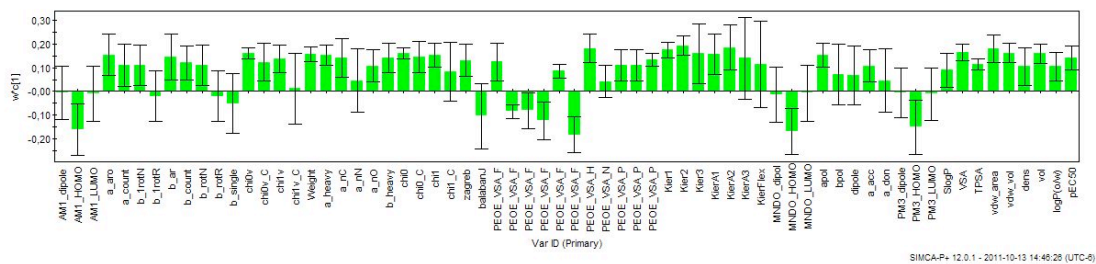
OPLS-DA DModX plot of all 24 di-substituted compounds in the training set:



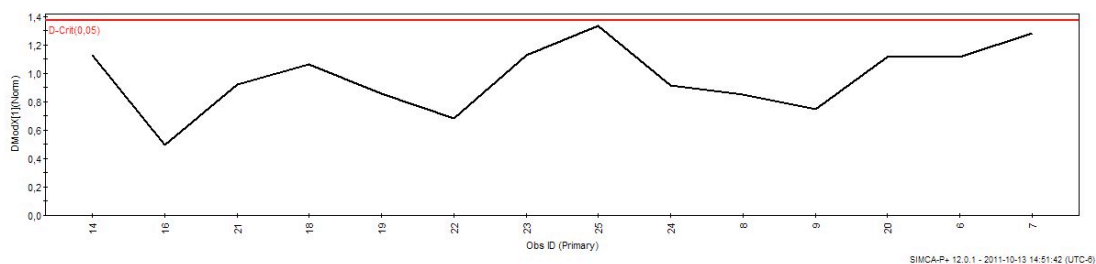
PLS Variable importance plot:



PLS Loading column plot:



PLS DModX plot of all 24 di-substituted compounds in the training set:



Descriptors used in all models:

Descriptors:

- 1 AM1_dipole
- 2 AM1_HOMO
- 3 AM1_LUMO
- 4 a_aro
- 5 a_count
- 6 b_1rotN
- 7 b_1rotR
- 8 b_ar
- 9 b_count
- 10 b_rotN
- 11 b_rotR
- 12 b_single
- 13 chi0v
- 14 chi0v_C
- 15 chi1v
- 16 chi1v_C
- 17 Weight
- 18 a_heavy
- 19 a_nC
- 20 a_nN
- 21 a_nO
- 22 b_heavy
- 23 chi0
- 24 chi0_C
- 25 chi1
- 26 chi1_C
- 27 zagreb
- 28 balabanJ
- 29 PEOE_VSA_FHYD

30 PEOE_VSA_FNEG
31 PEOE_VSA_FPNEG
32 PEOE_VSA_FPOL
33 PEOE_VSA_FPOS
34 PEOE_VSA_FPPOS
35 PEOE_VSA_HYD
36 PEOE_VSA_NEG
37 PEOE_VSA_PNEG
38 PEOE_VSA_POL
39 PEOE_VSA_POS
40 PEOE_VSA_PPOS
41 Kier1
42 Kier2
43 Kier3
44 KierA1
45 KierA2
46 KierA3
47 KierFlex
48 MNDO_dipole
49 MNDO_HOMO
50 MNDO_LUMO
51 apol
52 bpol
53 dipole
54 a_acc
55 a_don
56 PM3_dipole
57 PM3_HOMO
58 PM3_LUMO
59 SlogP
60 VSA

- 61 TPSA
- 62 vdw_area
- 63 vdw_vol
- 64 dens
- 65 vol
- 66 logP(o/w)