

Supporting Information

Undecaprenyl Diphosphate Synthase Inhibitors: Antibacterial Drug Leads

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Figure S1: Correlation of pIC₅₀ with docking scores

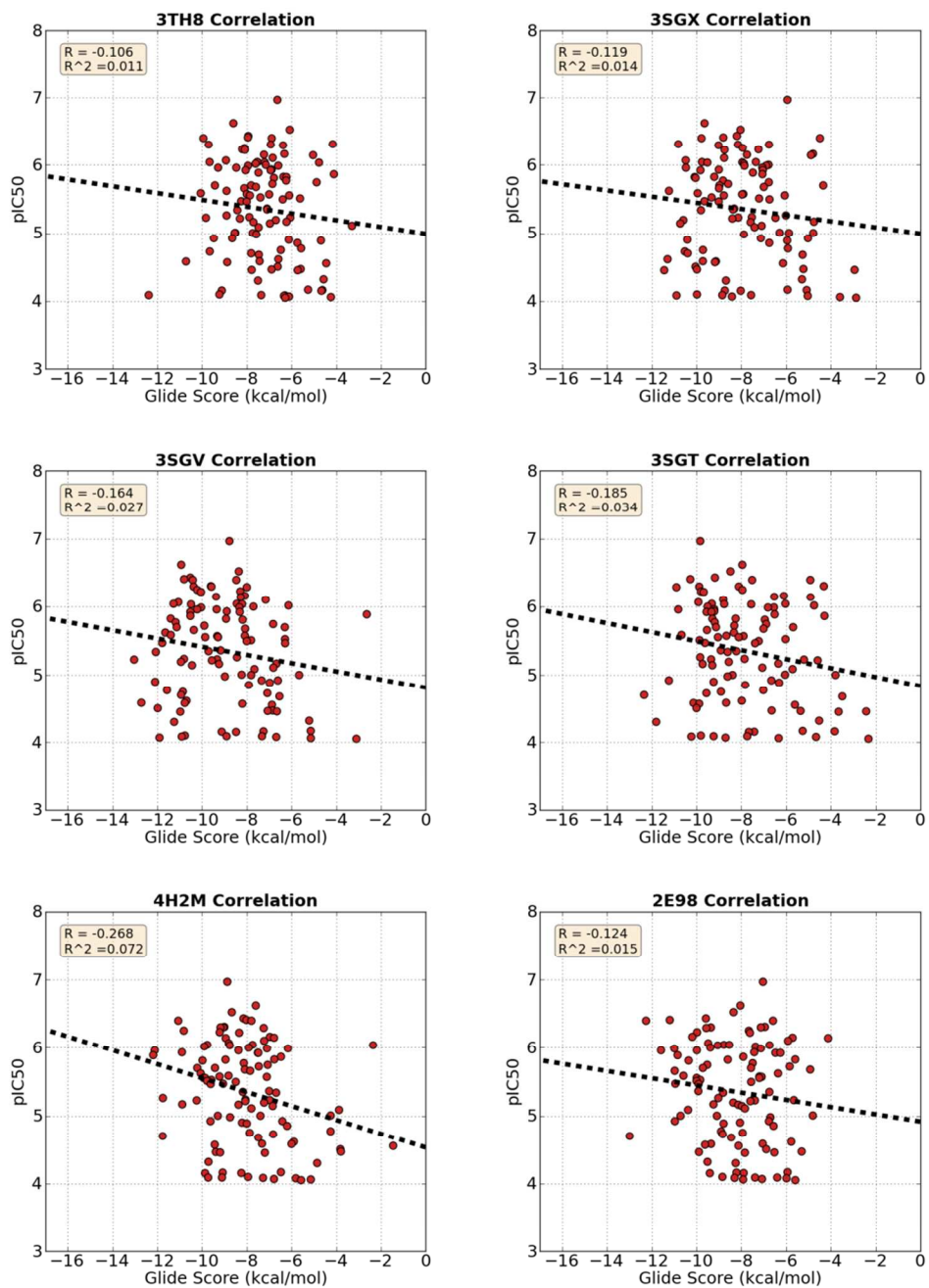


Figure S1(continued): Correlation of pIC₅₀ with docking scores

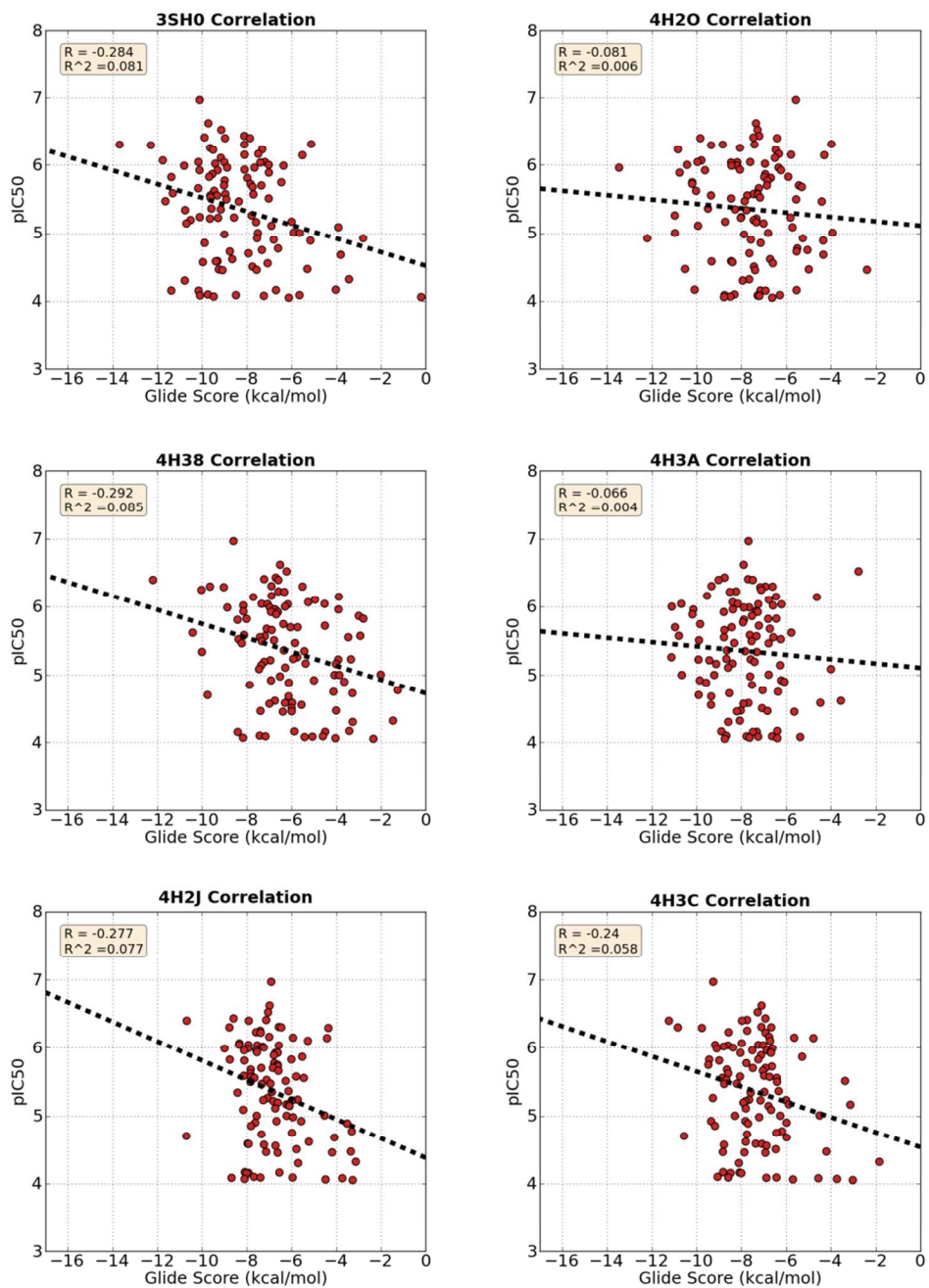
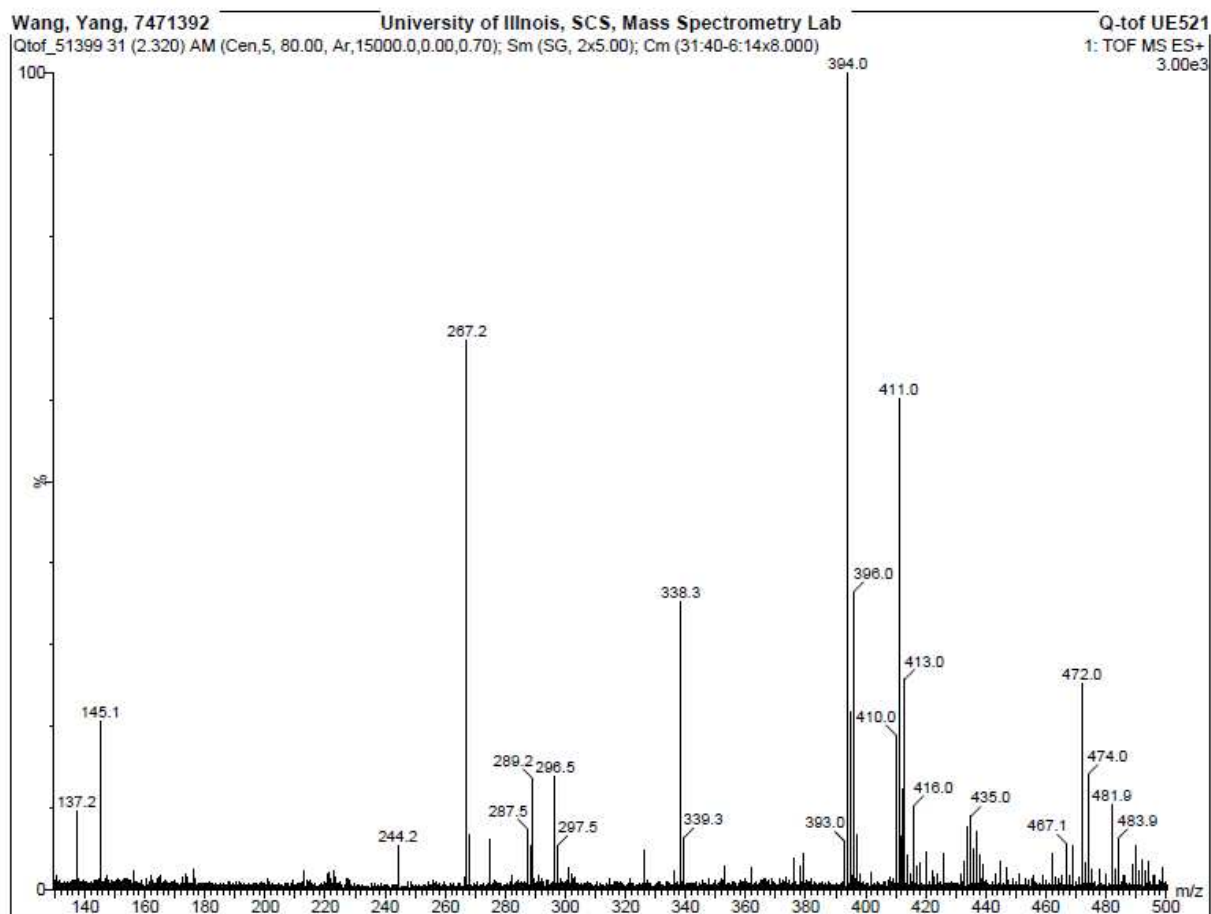


Figure S5. High-resolution mass spectrum of compound 1



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

23 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-125 H: 0-250 N: 0-1 O: 3-5 S: 2-2 Cl: 1-1

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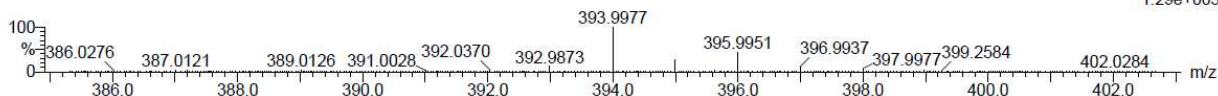
University of Illinois, SCS, Mass Spectrometry Lab

Q-tof UE521

Qtof_51399 32 (2.394) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70,LS 3); Sm (SG, 2x5.00); Cm (32:35)

1: TOF MS ES+

1.29e+003



Minimum:

-1.5

Maximum:

5.0

10.0

600.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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393.9977	393.9975	0.2	0.5	11.5	6.2	C17 H13 N O4 S2 Cl
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Figure S6. ¹H NMR of compound 4

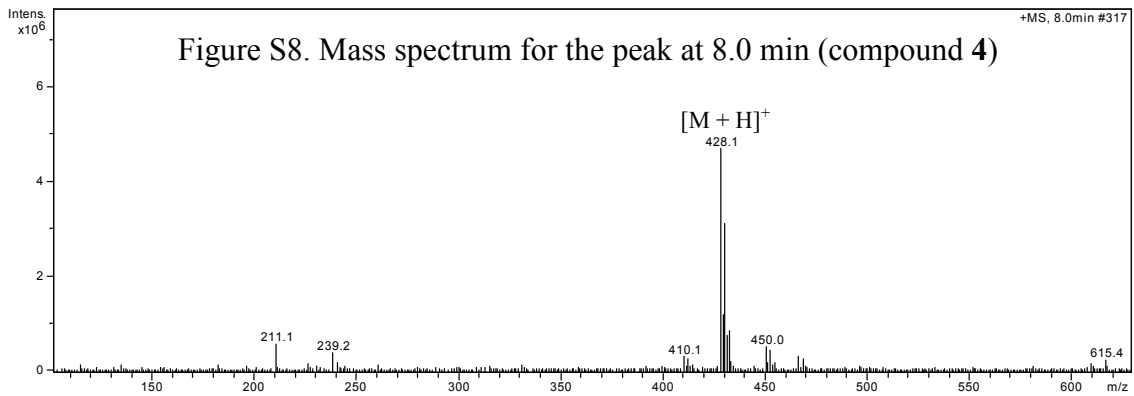
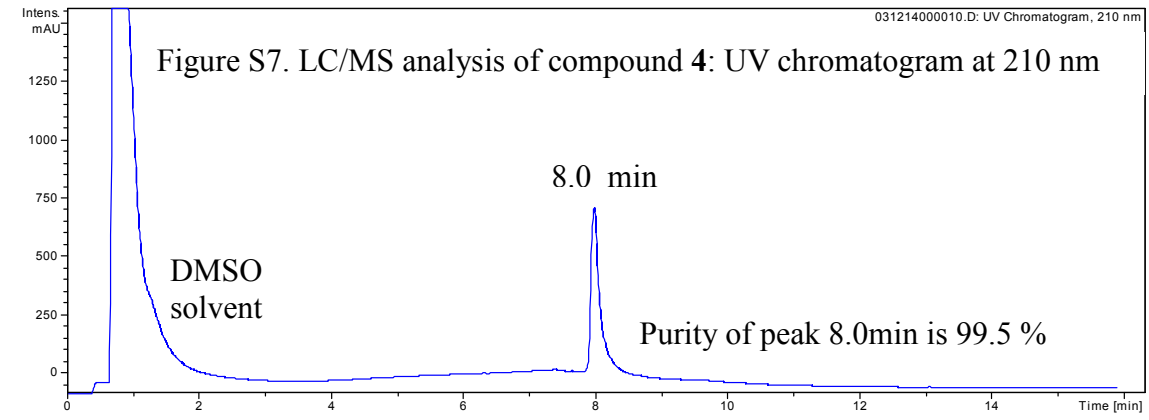
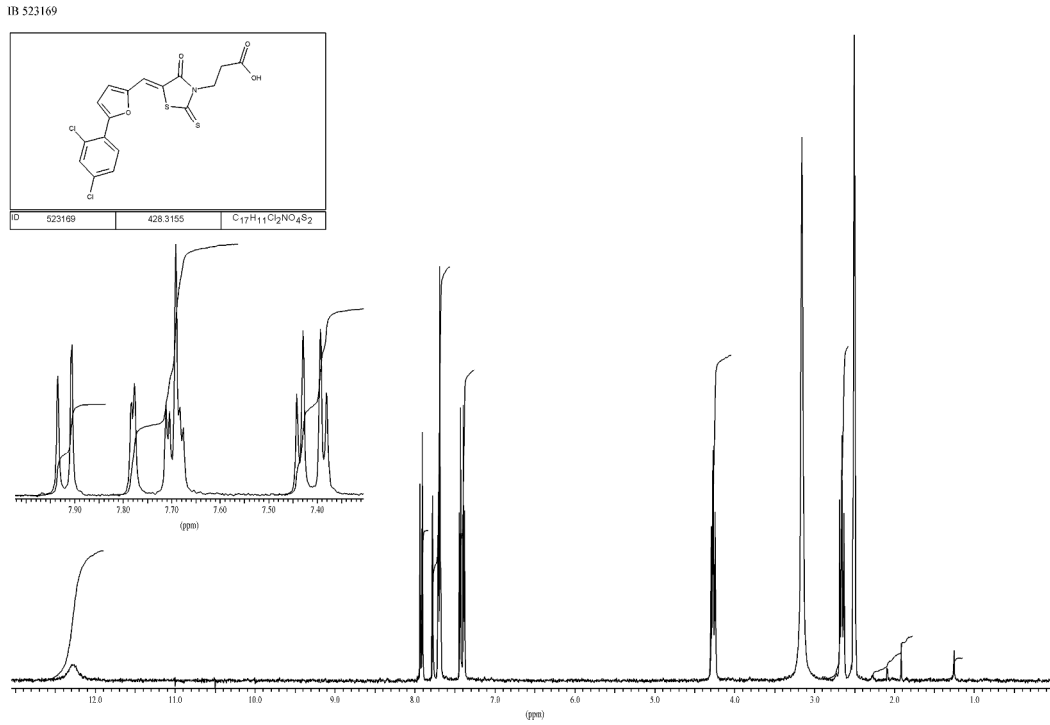
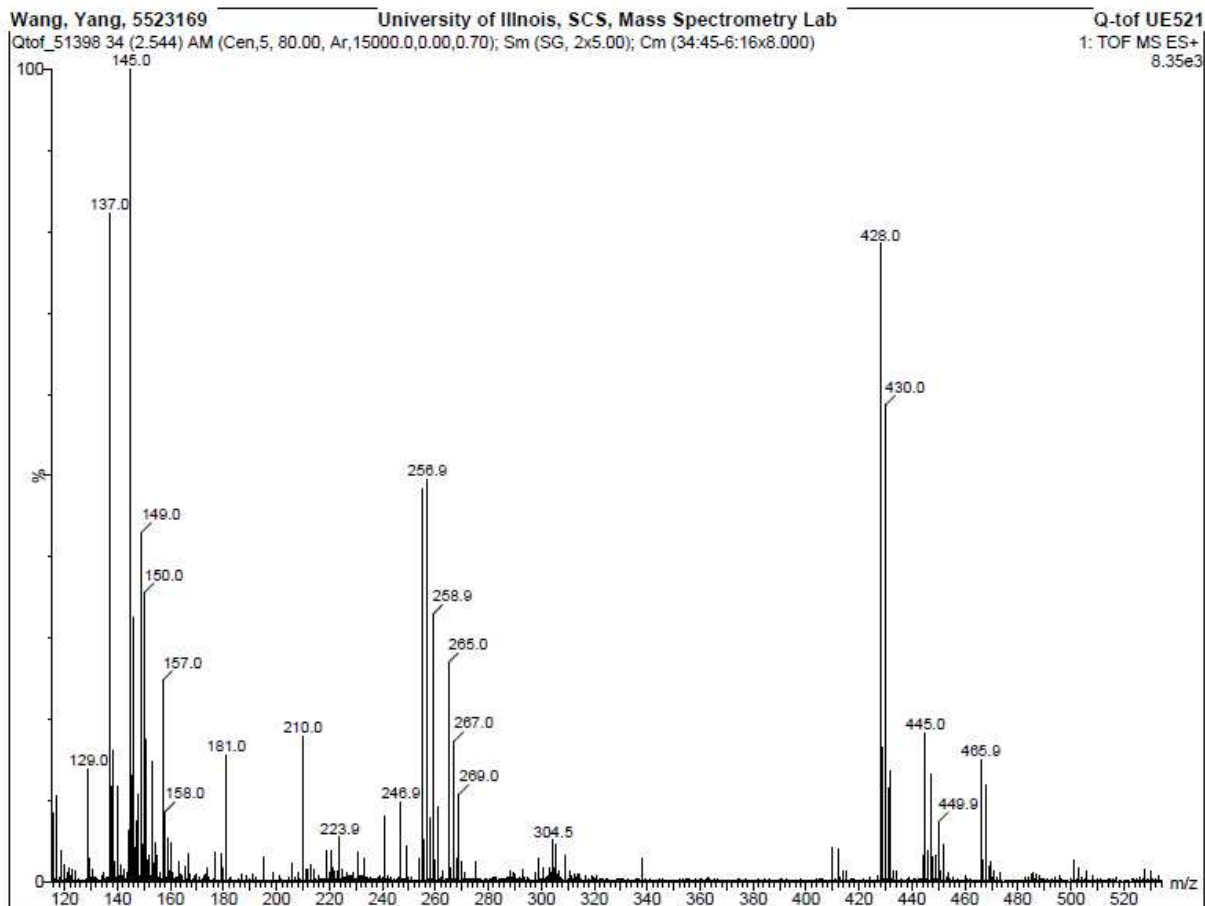


Figure S9. High-resolution mass spectrum of compound 4



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 600.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

22 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-125 H: 0-250 N: 0-1 O: 3-5 S: 2-2 Cl: 2-2

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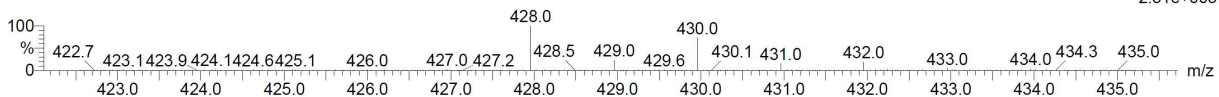
University of Illinois, SCS, Mass Spectrometry Lab

Q-tof UE521

Qtof_51398 35 (2.619) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70,LS 3); Sm (SG, 2x5.00); Cm (35:38)

1: TOF MS ES+

2.31e+003



Minimum:

Maximum:

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
427.9586	427.9585	0.1	0.2	11.5	2.2	C17 H12 N O4 S2 Cl2