

SUPPORTING INFORMATION

Benzothiazole DNA gyrase inhibitors and their conjugates with siderophore mimics:

Design, synthesis and evaluation

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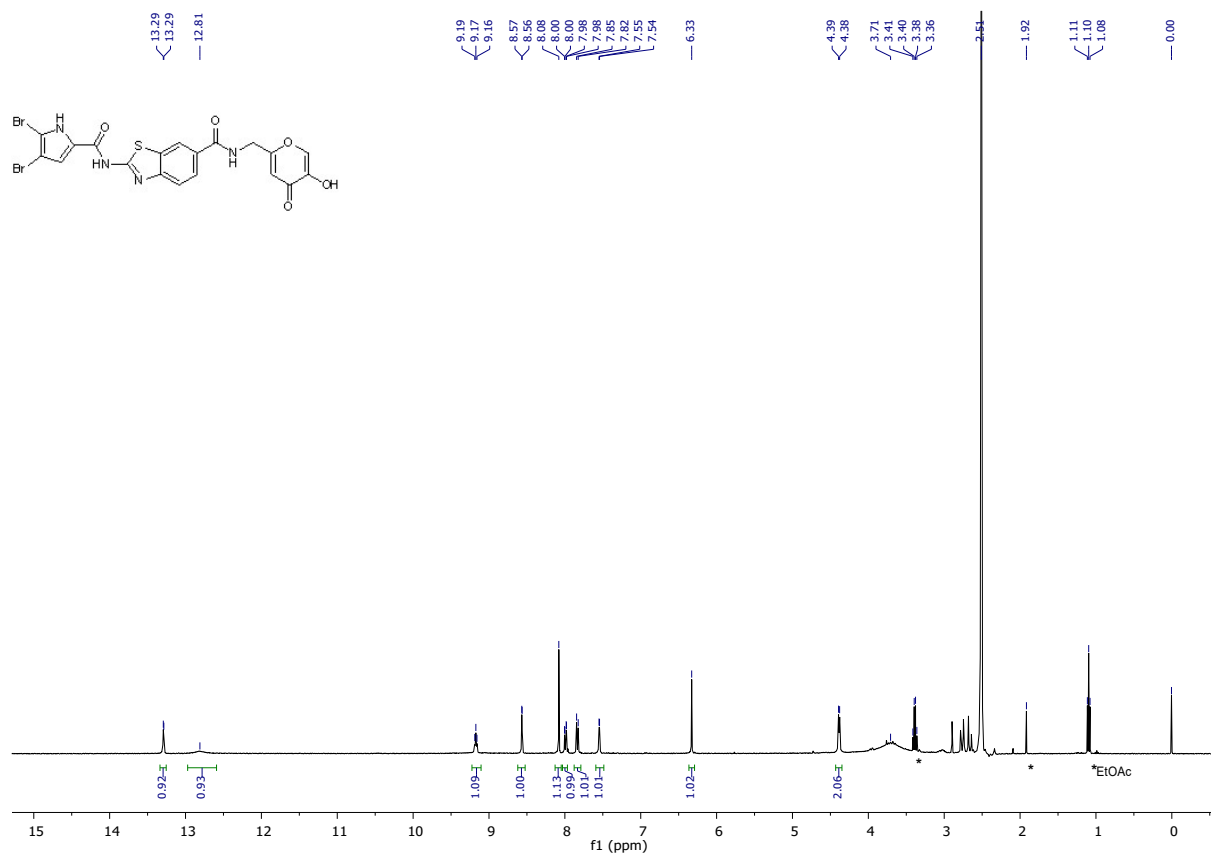
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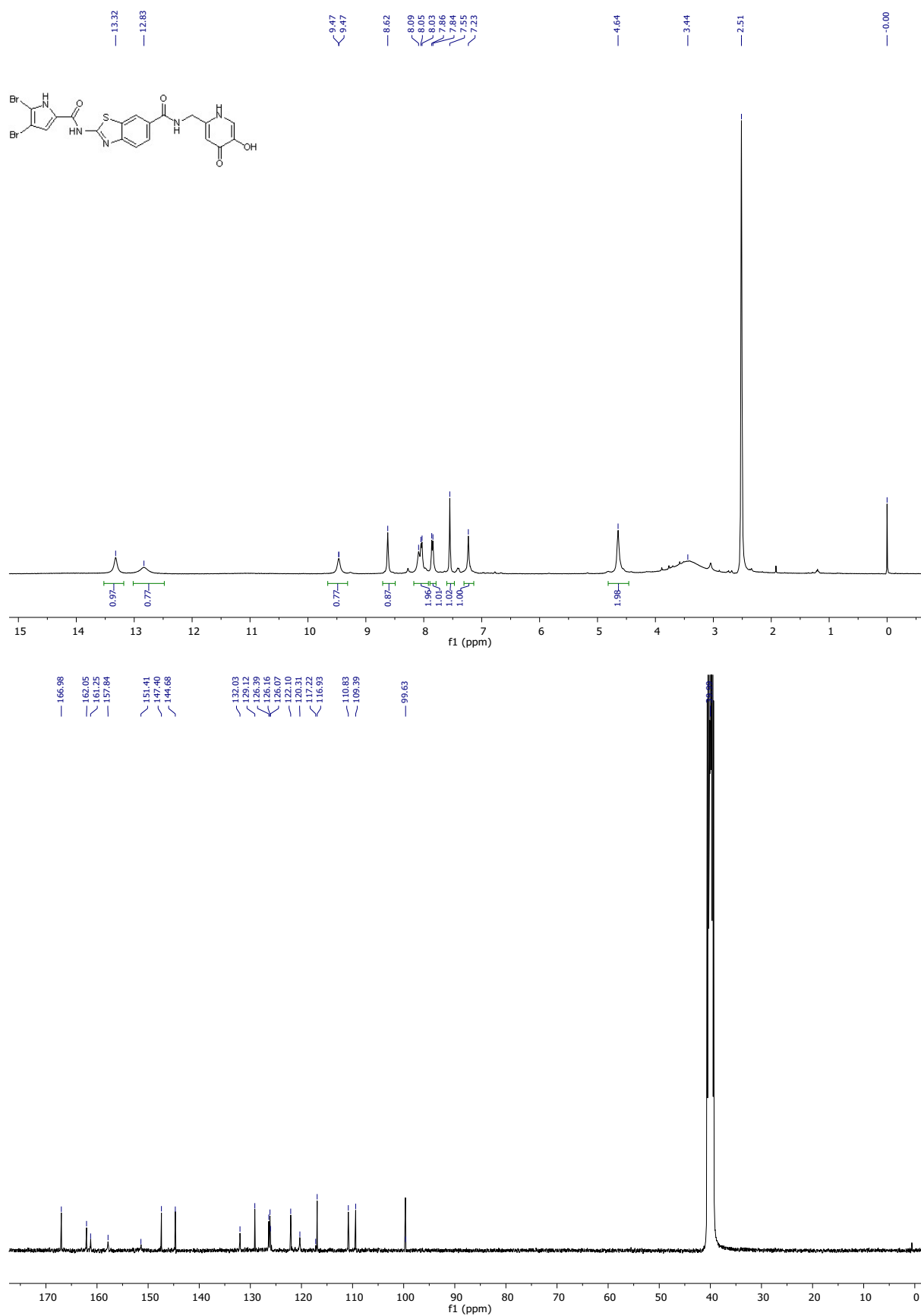
E-mail: tihomir.tomasic@ffa.uni-lj.si

Representative analytical data (NMR spectra, HRMS spectra, HPLC chromatograms)

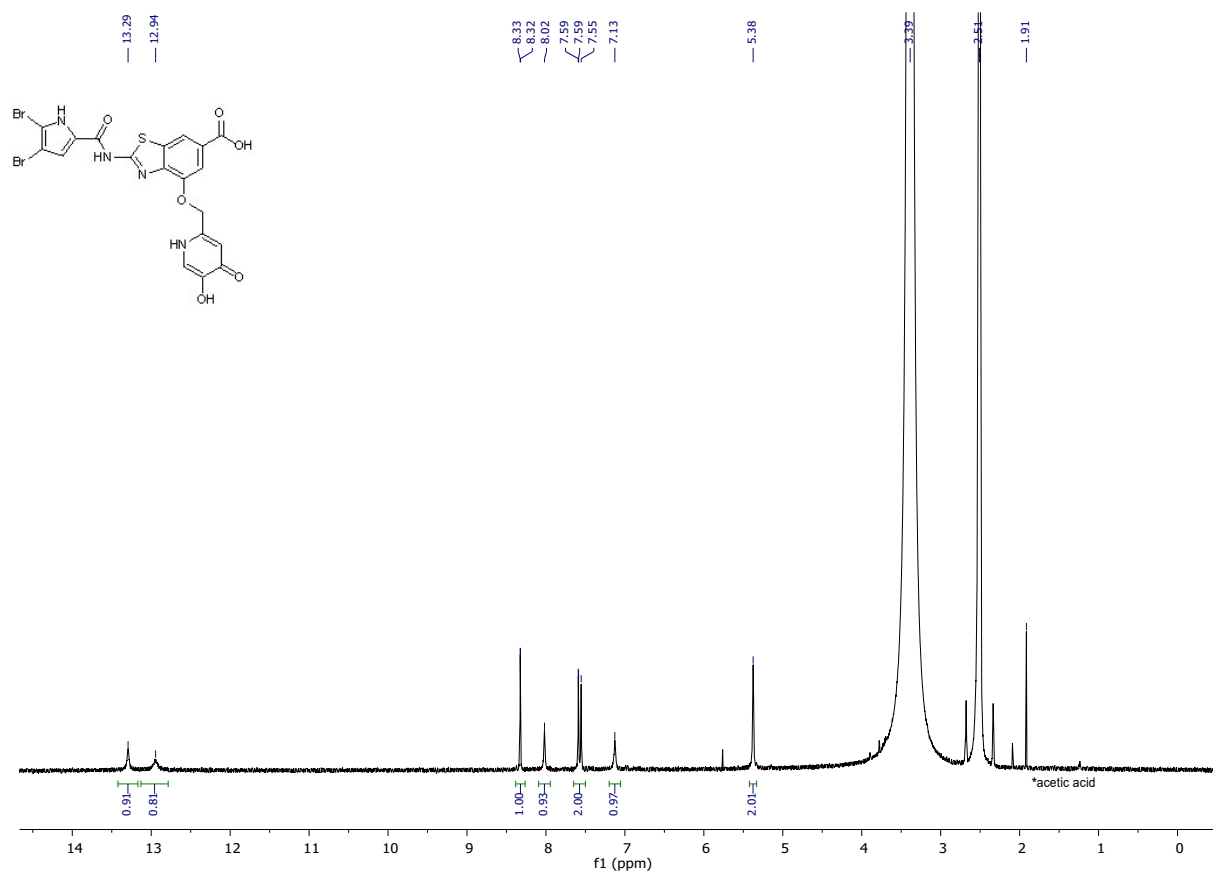
^1H NMR spectrum of 2-(4,5-dibromo-1*H*-pyrrole-2-carboxamido)-*N*-((5-hydroxy-4-oxo-4*H*-pyran-2-yl)methyl)benzo[*d*]thiazole-6-carboxamide (**10**).



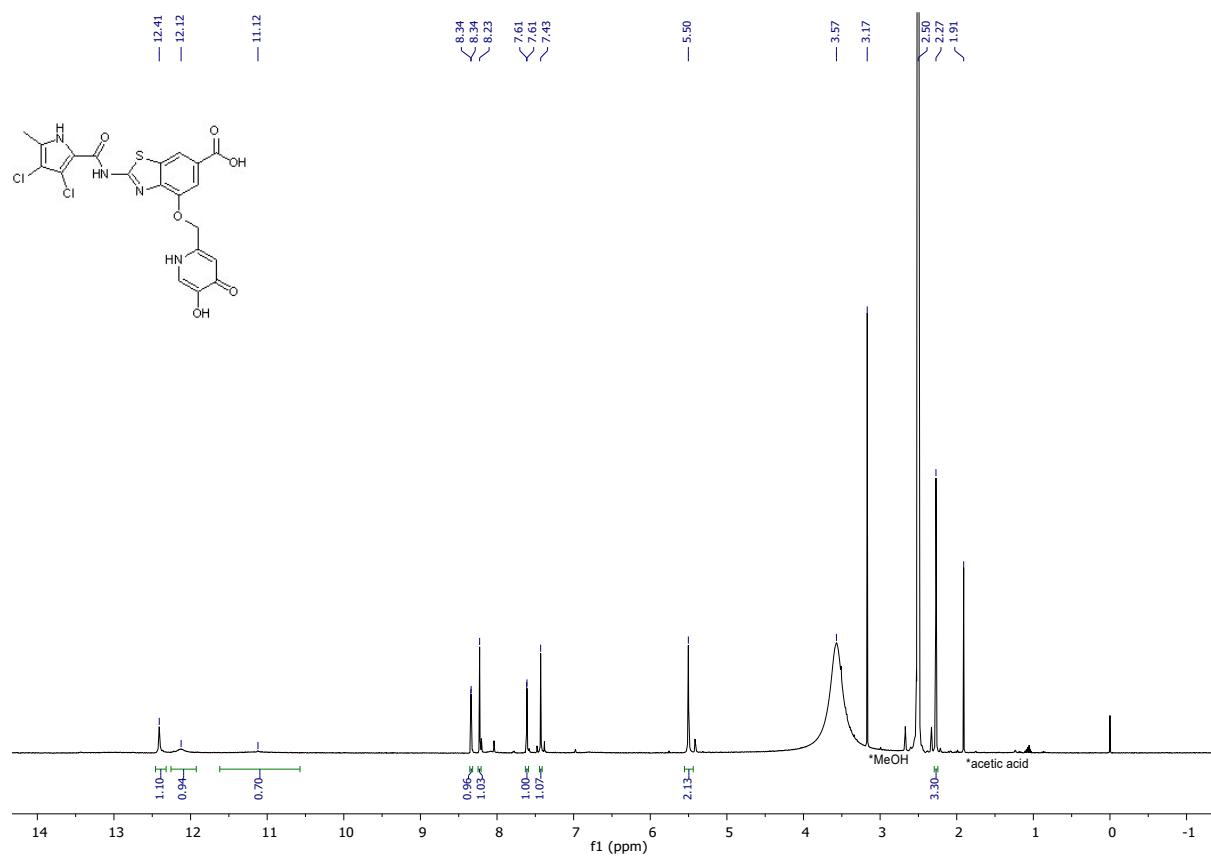
^1H and ^{13}C NMR spectrum of 2-(4,5-dibromo-1*H*-pyrrole-2-carboxamido)-*N*-((5-hydroxy-4-oxo-1,4-dihydropyridin-2-yl)methyl)benzo[*d*]thiazole-6-carboxamide (**12**).



^1H NMR spectrum of 2-(4,5-dibromo-1*H*-pyrrole-2-carboxamido)-4-((5-hydroxy-4-oxo-1,4-dihydropyridin-2-yl)methoxy)benzo[*d*]thiazole-6-carboxylic acid (**18a**).

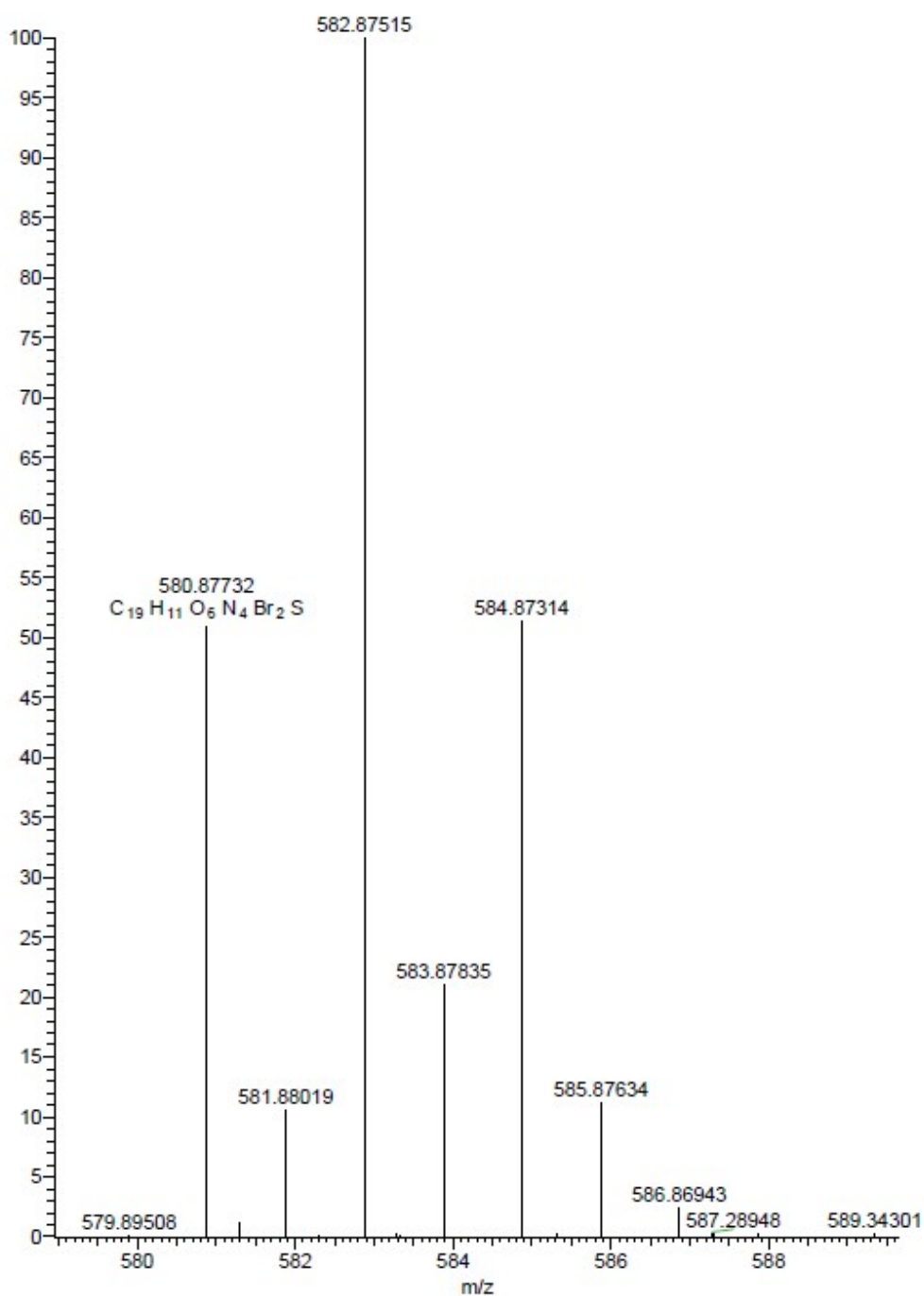


^1H NMR spectrum of 2-(3,4-dichloro-5-methyl-1*H*-pyrrole-2-carboxamido)-4-((5-hydroxy-4-oxo-1,4-dihydropyridin-2-yl)methoxy)benzo[*d*]thiazole-6-carboxylic acid (**18b**).



HRMS data for compound **18a**.

TGM-53
 TGM-53 #45-46 RT: 0.20-0.20 AV: 2 NL: 7.31E6
 T: FTMS - c ESI Full ms [150.0000-2000.0000]



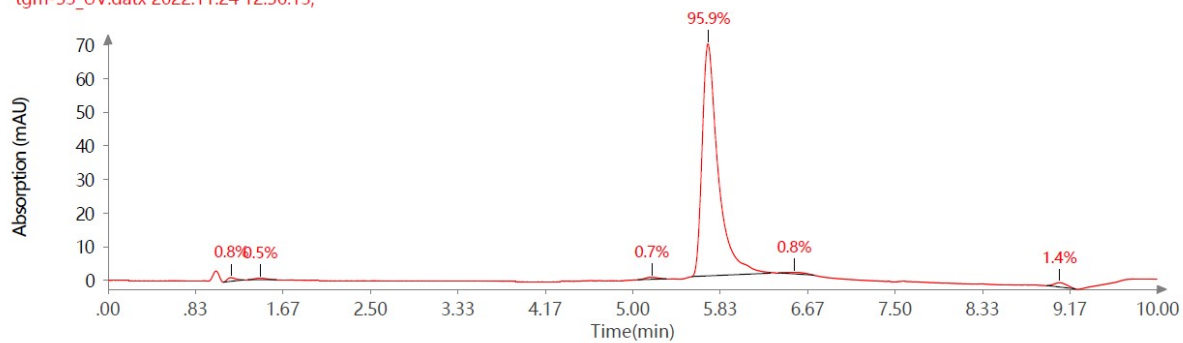
Elemental composition search on mass 580.87732

m/z= 575.87732-585.87732

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
580.87732	580.87715	0.29	15.5	C ₁₉ H ₁₁ O ₆ N ₄ Br ₂ S

HPLC traces for compound **18a**.

VWD: Signal A, 254 nm
tgm-53_UV.datx 2022.11.24 12:56:13;



HPLC traces for compound **18b**.

VWD: Signal A, 254 nm
LMD-266-iz_meoh_UV.datx 2020.01.13 10:20:35;

