Supporting Information

Bromo-cyclobutenaminones as new covalent MurA inhibitors

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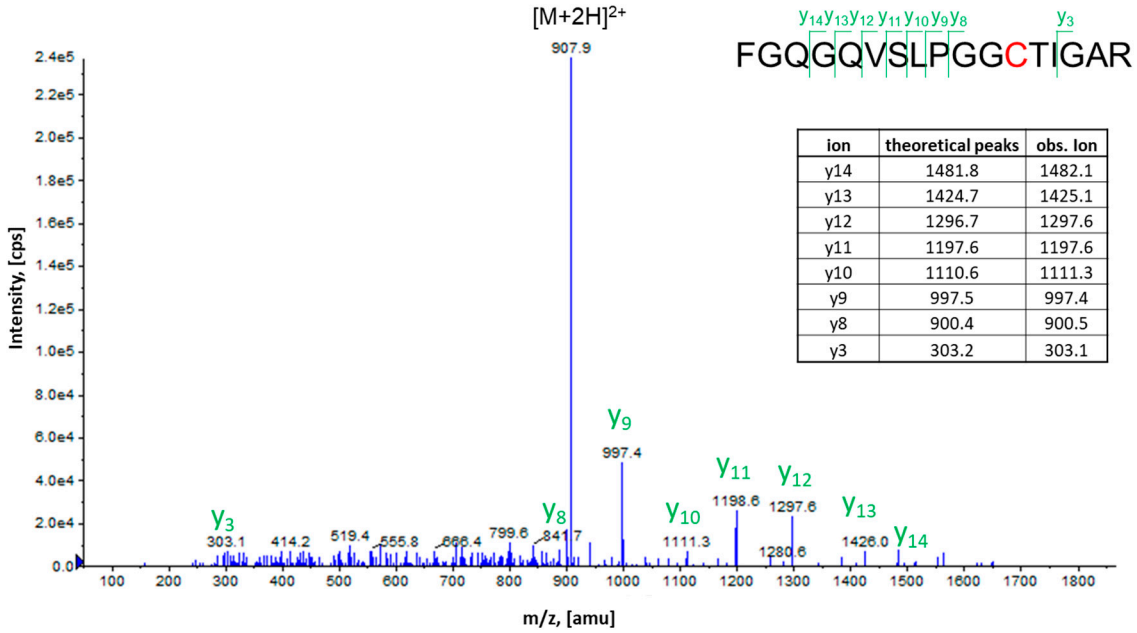
Table of contents

Table S1. Results of time-dependent IC_{50} measurements of 17b

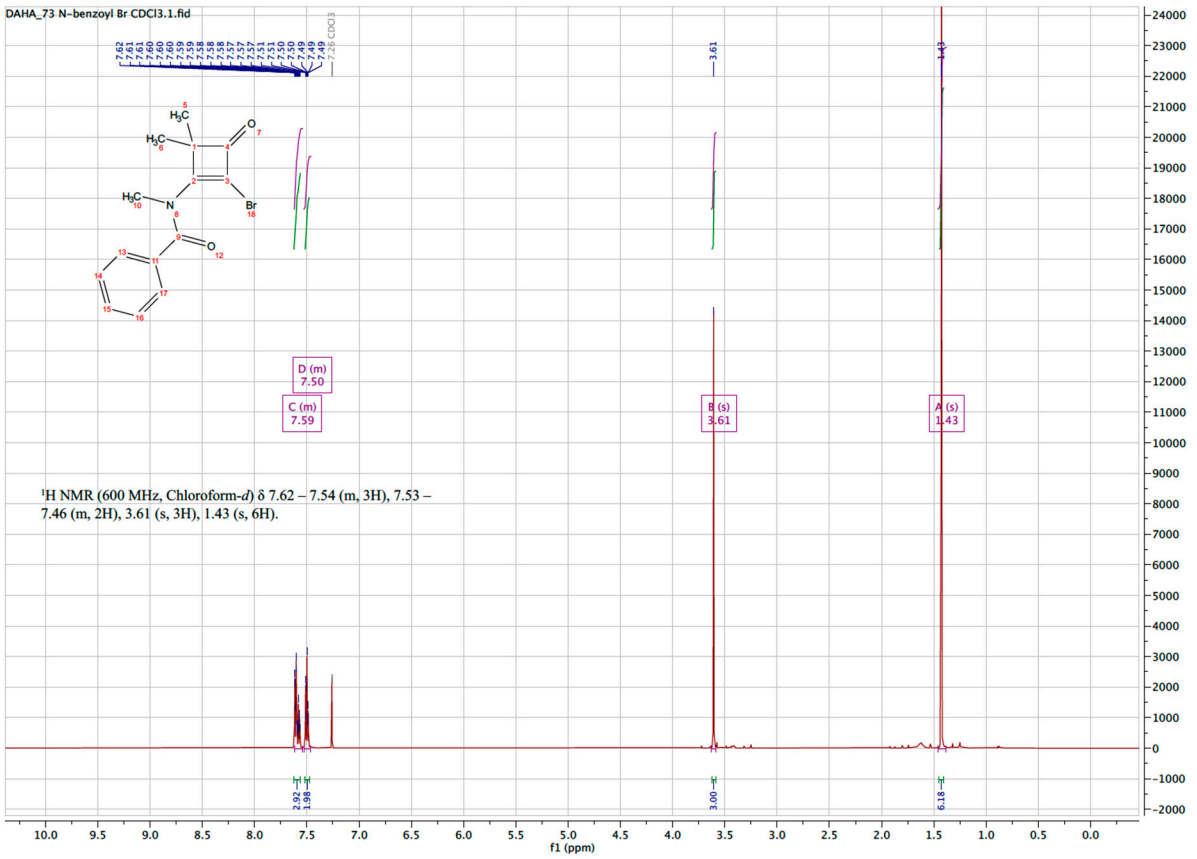
Preincubation time	IC_{50} (μM)
0 min	356 ± 29
15 min	149 ± 15
30 min	128 ± 10

Figure S1. The MS/MS spectrum of 17b modified MurA enzyme peptide [104-120] together with the annotation of the peaks

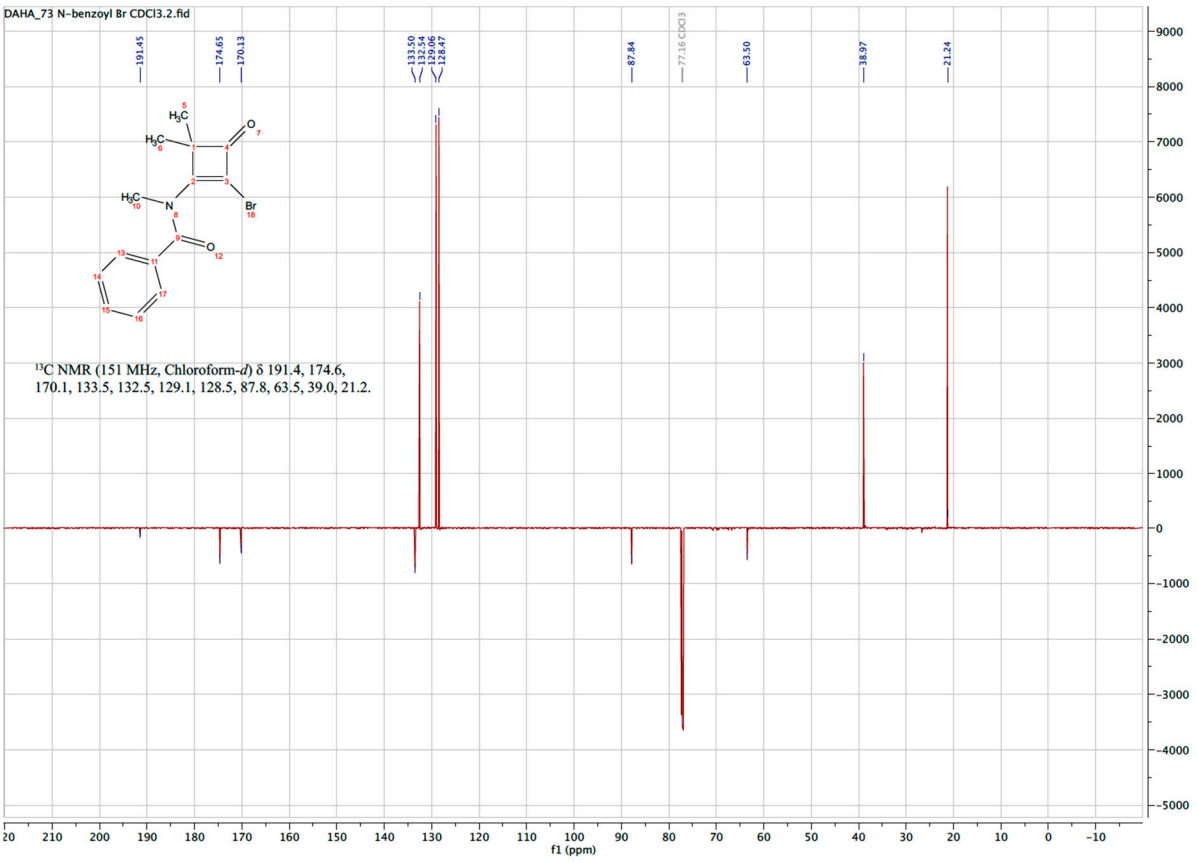


ion	theoretical peaks	obs. Ion
y14	1481.8	1482.1
y13	1424.7	1425.1
y12	1296.7	1297.6
y11	1197.6	1197.6
y10	1110.6	1111.3
y9	997.5	997.4
y8	900.4	900.5
y3	303.2	303.1

NMR, LC-MS and HRMS data of key compound 17a

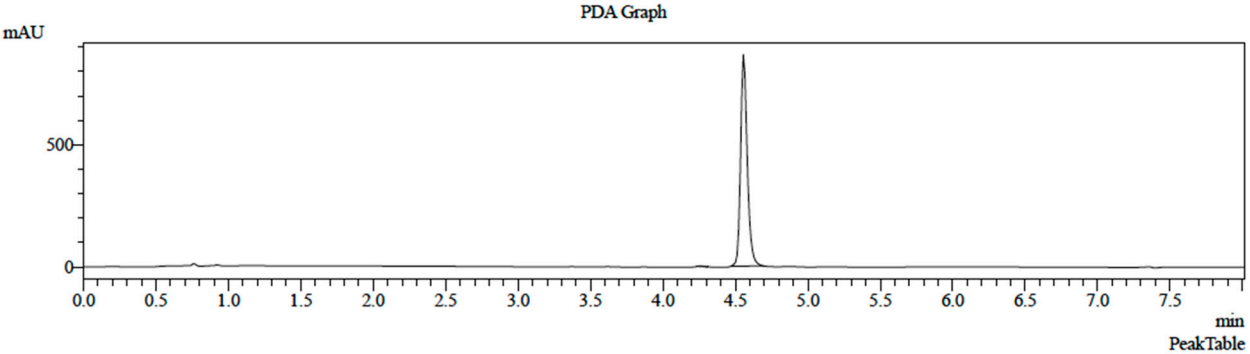


^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.62 – 7.54 (m, 3H), 7.53 – 7.46 (m, 2H), 3.61 (s, 3H), 1.43 (s, 6H).



^{13}C NMR (151 MHz, Chloroform-*d*) δ 191.4, 174.6, 170.1, 133.5, 132.5, 129.1, 128.5, 87.8, 63.5, 39.0, 21.2.

PDA Graph



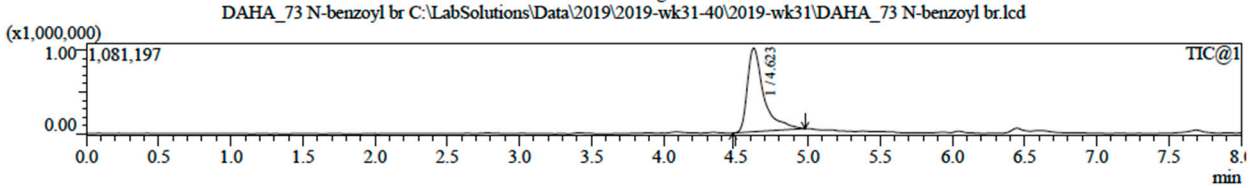
PeakTable

PDA Ch1 254nm 4nm

Peak#	Name	Ret. Time	Area	Area %
1		4.250	5177	0.188
2		4.551	2752417	99.812

MS Chromatogram

DAHA_73 N-benzoyl br C:\LabSolutions\Data\2019\2019-wk31-40\2019-wk31\DAHA_73 N-benzoyl br.lcd



MS Spectrum Graph

#:1 Ret.Time:Averaged 4.610-4.630(Scan#:462-464)
BG Mode:Calc 4.480<->4.980(449<->499)
Mass Peaks:8 Base Peak:310.00(406224) Polarity:Pos Segment1 - Event1