

Ultrasound assisted synthesis of 4-(benzyloxy)-N-(3-chloro-2-(substitutedphenyl)-4-oxoazetidin-1-yl) benzamide as challenging anti tubercular scaffold

Urja D. Nimbalkar¹, Julio A. Seijas², Rachna Borkute³, Manoj G. Damale ⁴, Jaiprakash N.

Sangshetti⁵, Dhiman Sarkar ³, Anna Pratima G. Nikalje*⁵

¹ Maulana Azad P. G. and Research Centre, Dr. Rafiq Zakaria Campus, Rauza Baug, Aurangabad 431001, India ; urjasatish@gmail.com

² Departamento de Química Orgánica, Facultad de Ciencias, Universidad of Santiago de Compostela, Alfonso X el Sabio, 27002 Lugo, Spain; julioa.seijas@usc.es

³Combichem-Bio Resource Centre, Division of Organic Chemistry, CSIR-National Chemical Laboratory, Pune 411008 , Maharashtra, India; rachnabrkt@gmail.com ; d.sarkar@ncl.res.in

⁴ Shreeyash College of Pharmacy, Aurangabad 431116, India; pharalink1985@gmail.com

⁵Department of Pharmaceutical Chemistry, Dr. Rafiq Zakaria Campus, Y. B. Chavan College of Pharmacy, Aurangabad 431001, M.S. India ; jnsangshetti@rediffmail.com

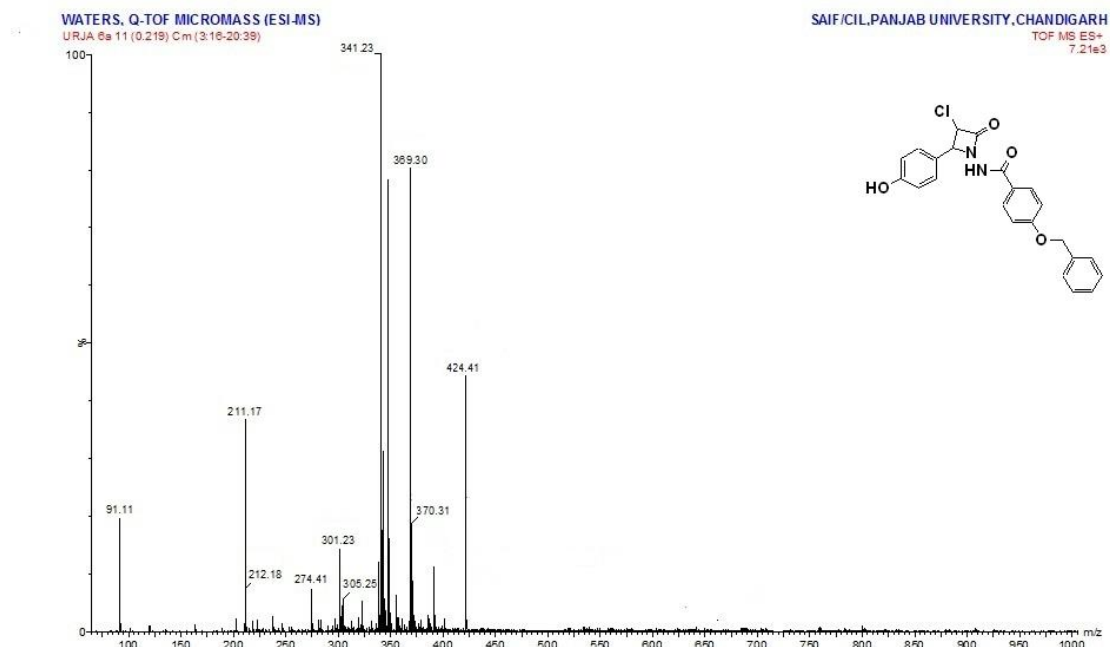
* Correspondence: annapratimanikalje@gmail.com ; Tel.: +91-9168929111

Table S1: Physical characterization of 4-(benzyloxy)-N-(3-chloro-2-(substituted phenyl)-4-oxoazetidin-1-yl) benzamide **6a-j**

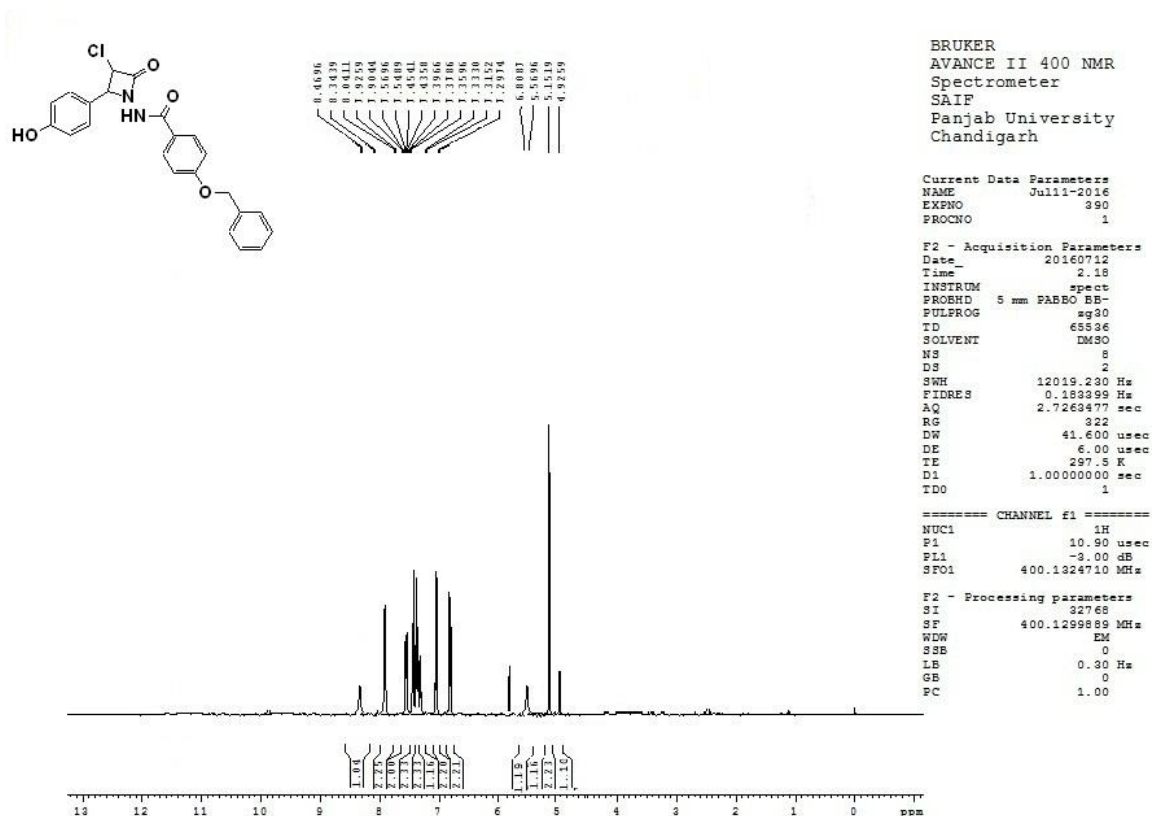
Code No.	Structure	Molecular Formula	Mol. Wt.	Yield (%)	M.P.(°C)
6a	4-Hydroxyphenyl	C ₂₃ H ₁₉ ClN ₂ O ₄	422.86	88	175
6b	4-Methoxyphenyl	C ₂₄ H ₂₁ ClN ₂ O ₄	436.89	82	170
6c	4-Fluorophenyl	C ₂₃ H ₁₈ ClFN ₂ O ₃	424.85	80	144
6d	4-Chlorophenyl	C ₂₃ H ₁₈ Cl ₂ N ₂ O ₃	441.31	79	152
6e	3-Nitrophenyl	C ₂₃ H ₁₈ ClN ₃ O ₅	451.86	80	198
6f	3,4-Dimethoxyphenyl	C ₂₅ H ₂₃ ClN ₂ O ₅	466.91	79	182
6g	4-Hydroxy-3-methoxyphenyl	C ₂₄ H ₂₁ ClN ₂ O ₅	452.89	86	164
6h	3-Ethoxy-4-hydroxyphenyl	C ₂₅ H ₂₃ ClN ₂ O ₅	466.91	81	156
6i	4-Benzyloxyphenyl	C ₃₀ H ₂₅ ClN ₂ O ₄	512.98	78	180
6j	Thiophen-2-yl	C ₂₁ H ₁₇ ClN ₂ O ₃ S	412.89	79	172

S2: Mass, ^1H NMR and ^{13}C NMR and elemental analysis of representative derivatives.

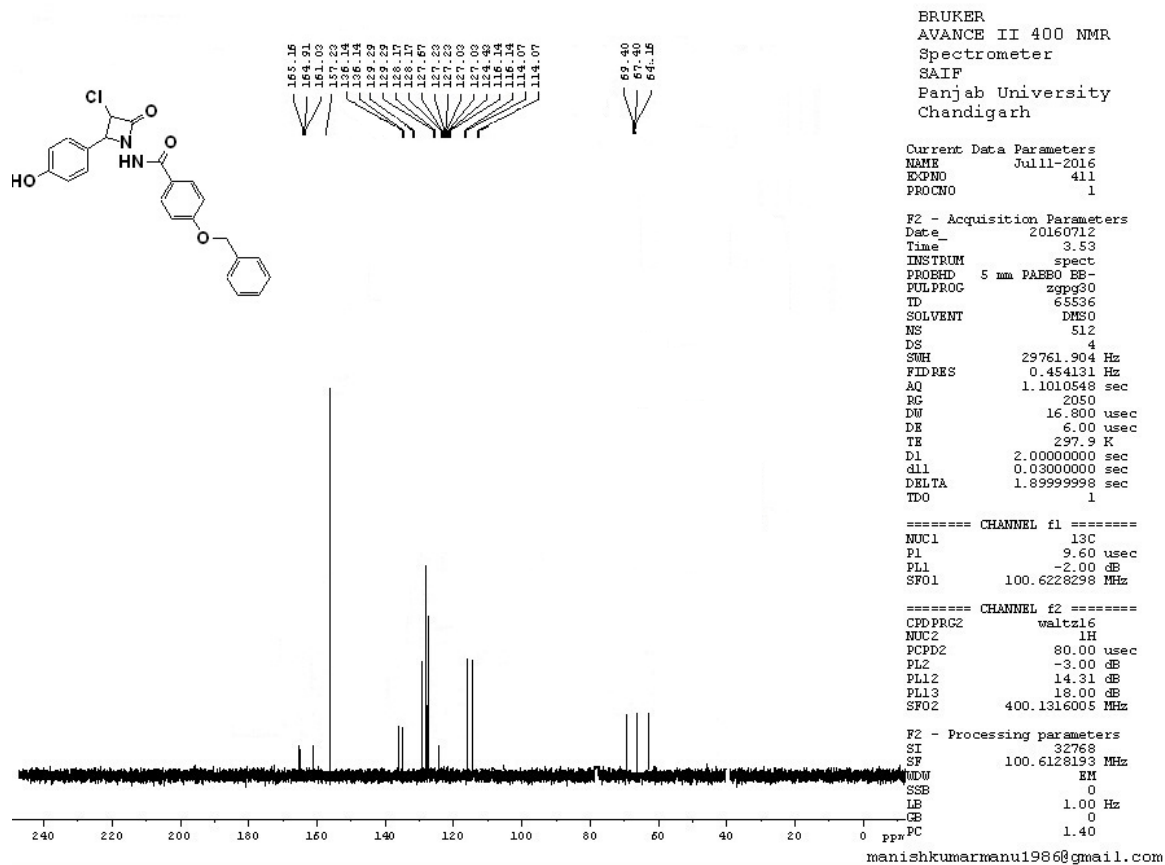
Mass Spectra: 6a) 4-(benzyloxy)-N-(3-chloro-2-(4-hydroxyphenyl)-4-oxoazetidin-1-yl) benzamide:



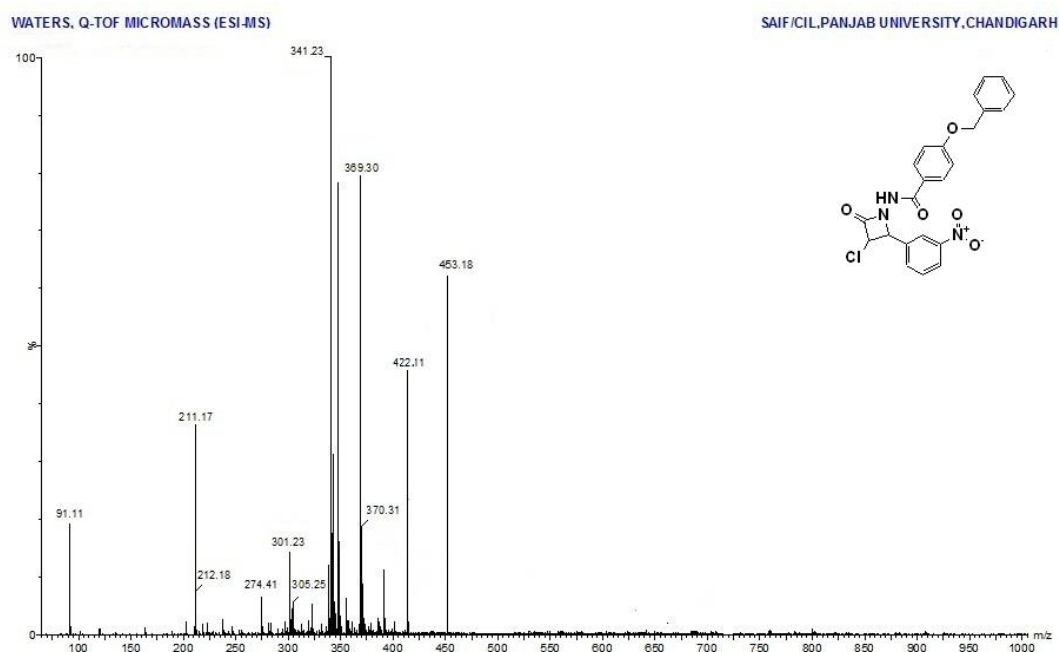
^1H NMR Spectra: 6a) 4-(benzyloxy)-N-(3-chloro-2-(4-hydroxyphenyl)-4-oxoazetidin-1-yl) benzamide:



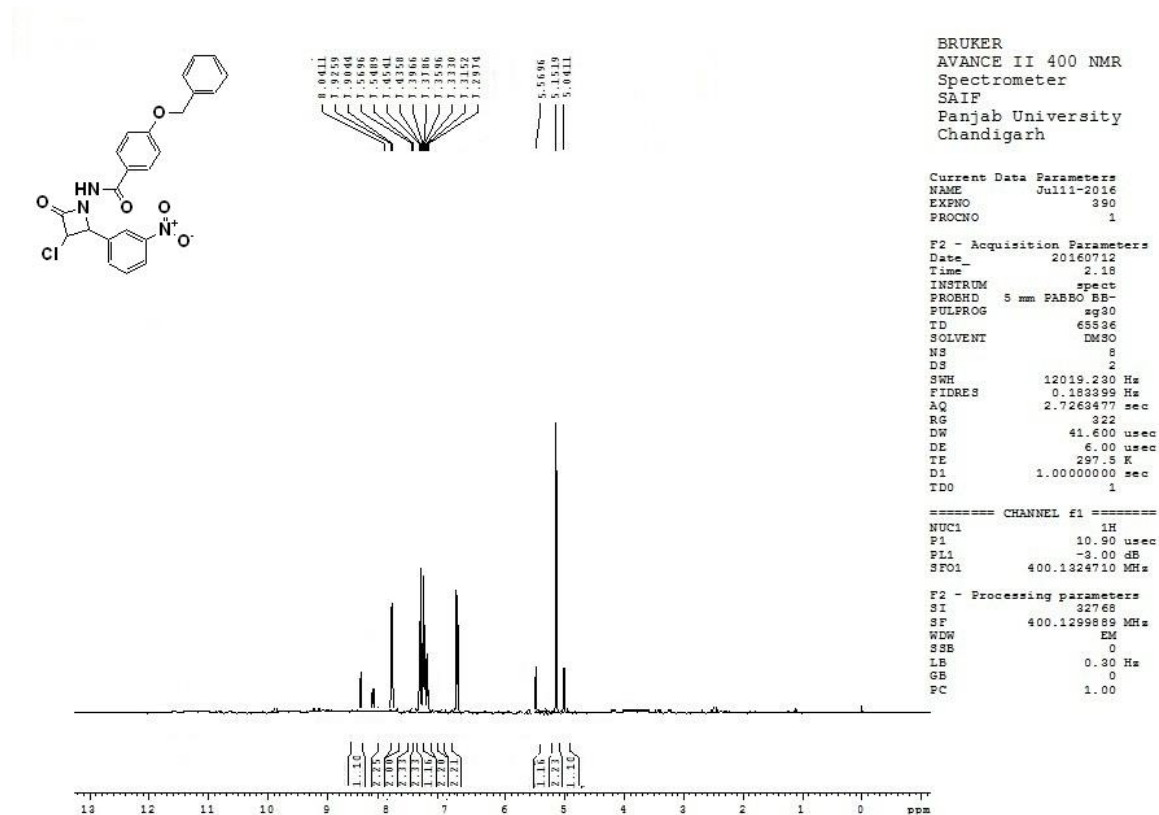
¹³C NMR Spectra: 6a) 4-(benzyloxy)-N-(3-chloro-2-(4-hydroxyphenyl)-4-oxoazetidin-1-yl)benzamide:



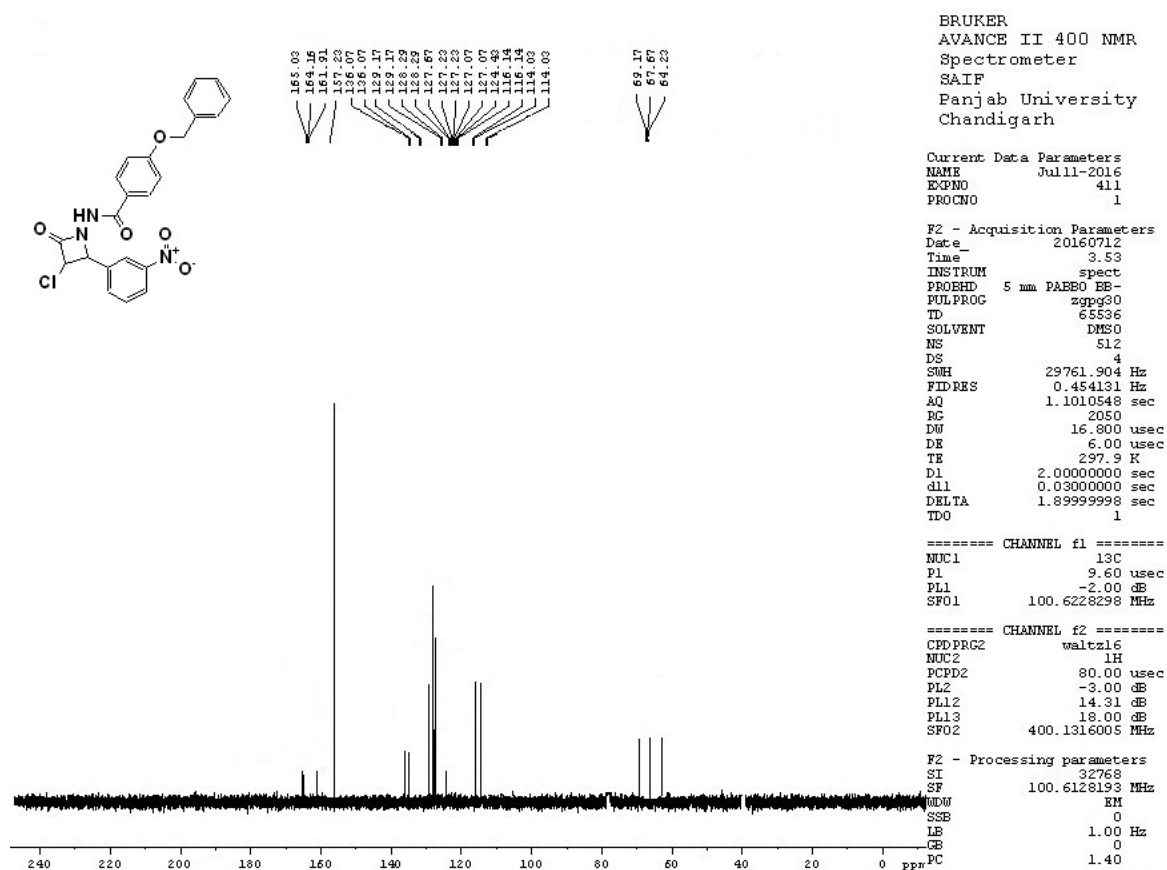
Mass Spectra 6e): 4-(benzyloxy)-N-(3-chloro-2-(3-nitrophenyl)-4-oxoazetidin-1-yl)benzamide



¹H NMR Spectra 6e): 4-(benzyloxy)-N-(3-chloro-2-(3-nitrophenyl)-4-oxoazetidin-1-yl) benzamide

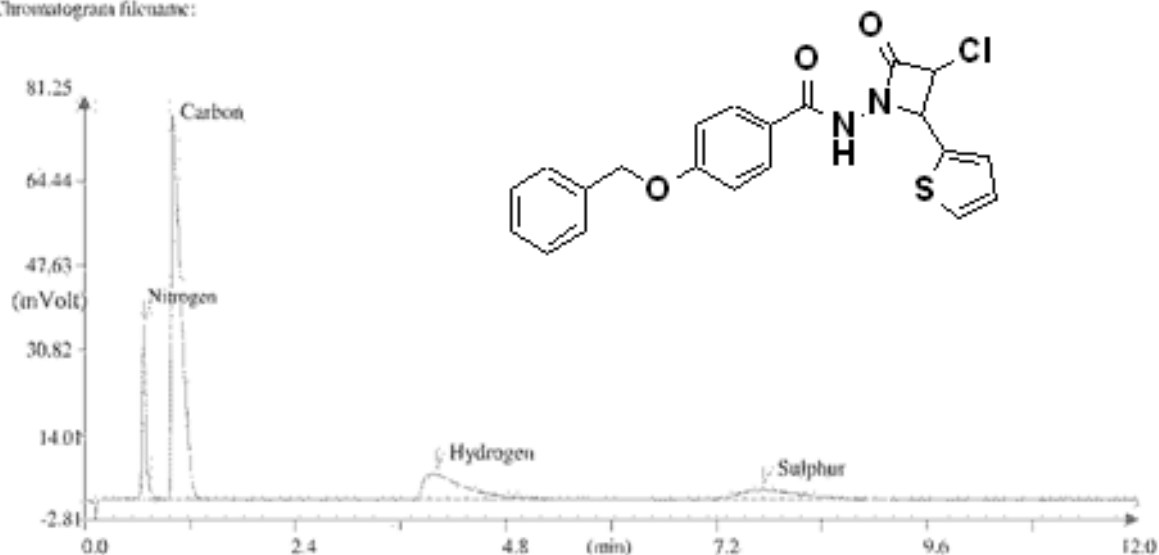


¹³C NMR Spectra 6e): 4-(benzyloxy)-N-(3-chloro-2-(3-nitrophenyl)-4-oxoazetidin-1-yl) benzamide



8). Elemental analysis 6j

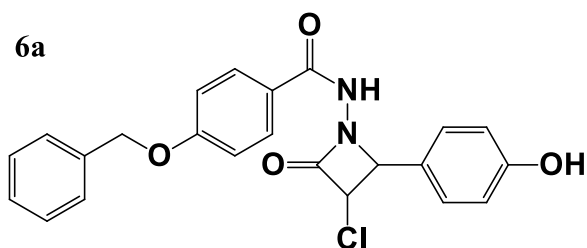
Method name: CHNS method
 Analysed: 07/01/2017 14:08
 Printed: 07-01-2017 15:05
 Sample ID: S
 Analysis type: Unknown
 Chromatogram filename:



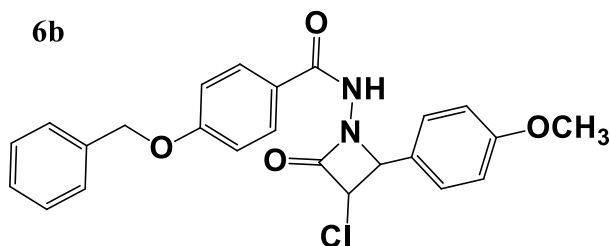
Element Name	% Element	Ret. Time	Area	BC	Area ratio	K factor
Nitrogen	7.9455	0.70	766724	RS	7.47289	0.220309E+07
Carbon	63.9767	1.07	5729644	RS	1.00000	0.475253E+07
Hydrogen	3.6536	4.00	1488423	RS	3.84947	3.141951E+08
Totals	82.5258		7985340			

S3: Structures and IUPAC name of synthesised derivatives 6 a-j

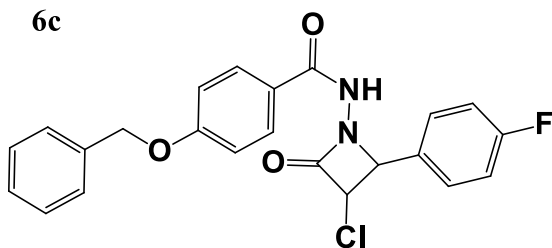
6a

4-(benzyloxy)-*N*-(3-chloro-2-(4-hydroxyphenyl)-4-oxoazetidin-1-yl)benzamide

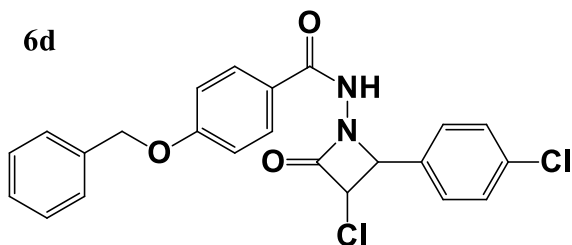
6b

4-(benzyloxy)-*N*-(3-chloro-2-(4-methoxyphenyl)-4-oxoazetidin-1-yl)benzamide

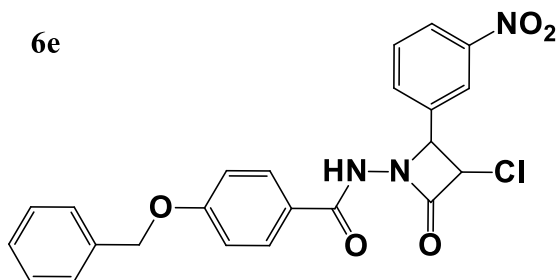
6c

4-(benzyloxy)-*N*-(3-chloro-2-(4-fluorophenyl)-4-oxoazetidin-1-yl)benzamide

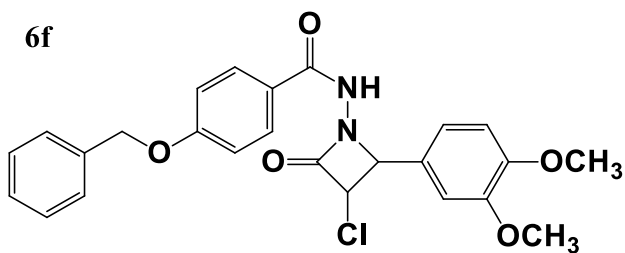
6d

4-(benzyloxy)-*N*-(3-chloro-2-(4-chlorophenyl)-4-oxoazetidin-1-yl)benzamide

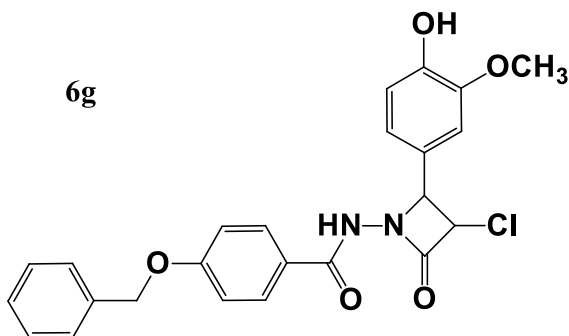
6e

4-(benzyloxy)-*N*-(3-chloro-2-(3-nitrophenyl)-4-oxoazetidin-1-yl)benzamide

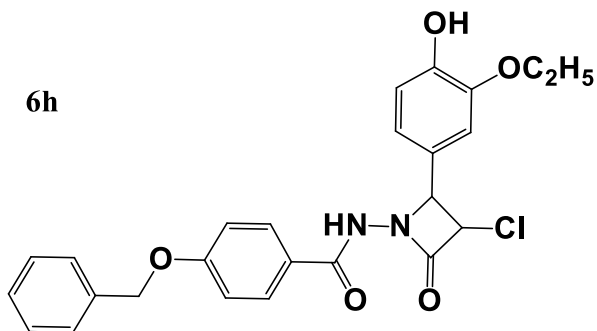
6f

4-(benzyloxy)-*N*-(3-chloro-2-(3,4-dimethoxyphenyl)-4-oxoazetidin-1-yl)benzamide

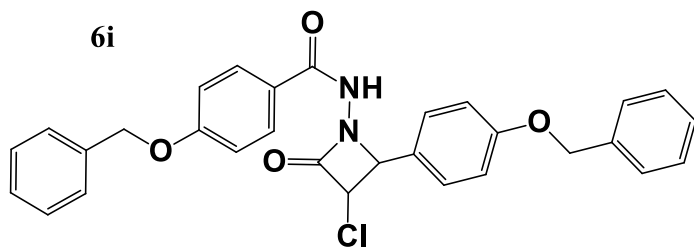
6g

4-(benzyloxy)-*N*-(3-chloro-2-(4-hydroxy-3-methoxyphenyl)-4-oxoazetidin-1-yl)benzamide

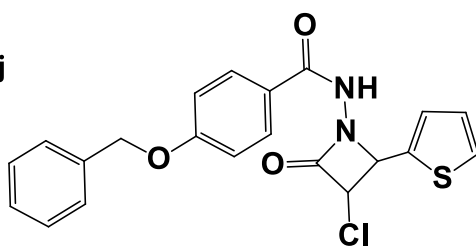
6h

4-(benzyloxy)-*N*-(3-chloro-2-(3-ethoxy-4-hydroxyphenyl)-4-oxoazetidin-1-yl)benzamide

6i

4-(benzyloxy)-*N*-(2-(4-(benzyloxy)phenyl)-3-chloro-4-oxoazetidin-1-yl)benzamide

6j

4-(benzyloxy)-*N*-(3-chloro-2-oxo-4-(thiophen-2-yl)azetidin-1-yl)benzamide

