

Supplementary Material

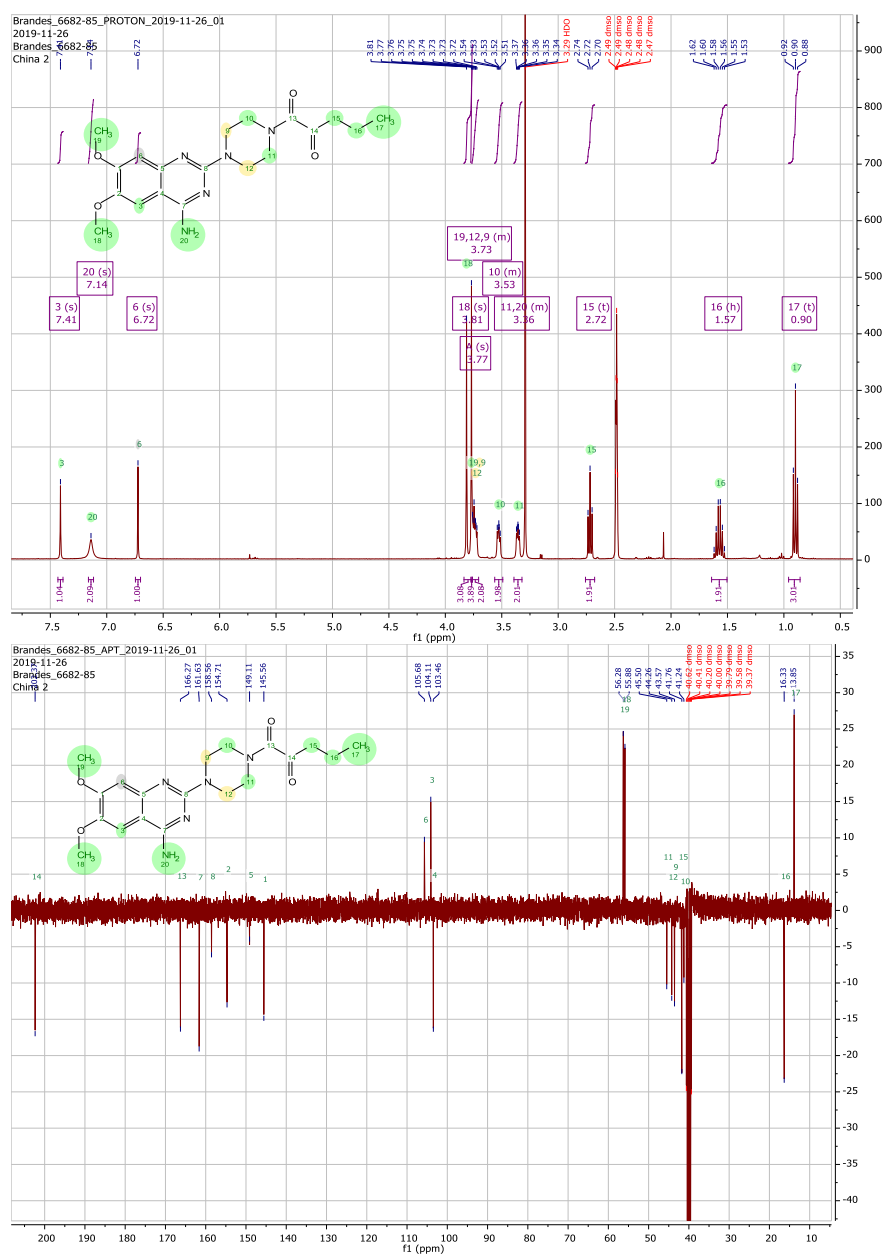
A hitherto unreported impurity in Terazosin – elucidation of the structure, synthesis and cytotoxicity

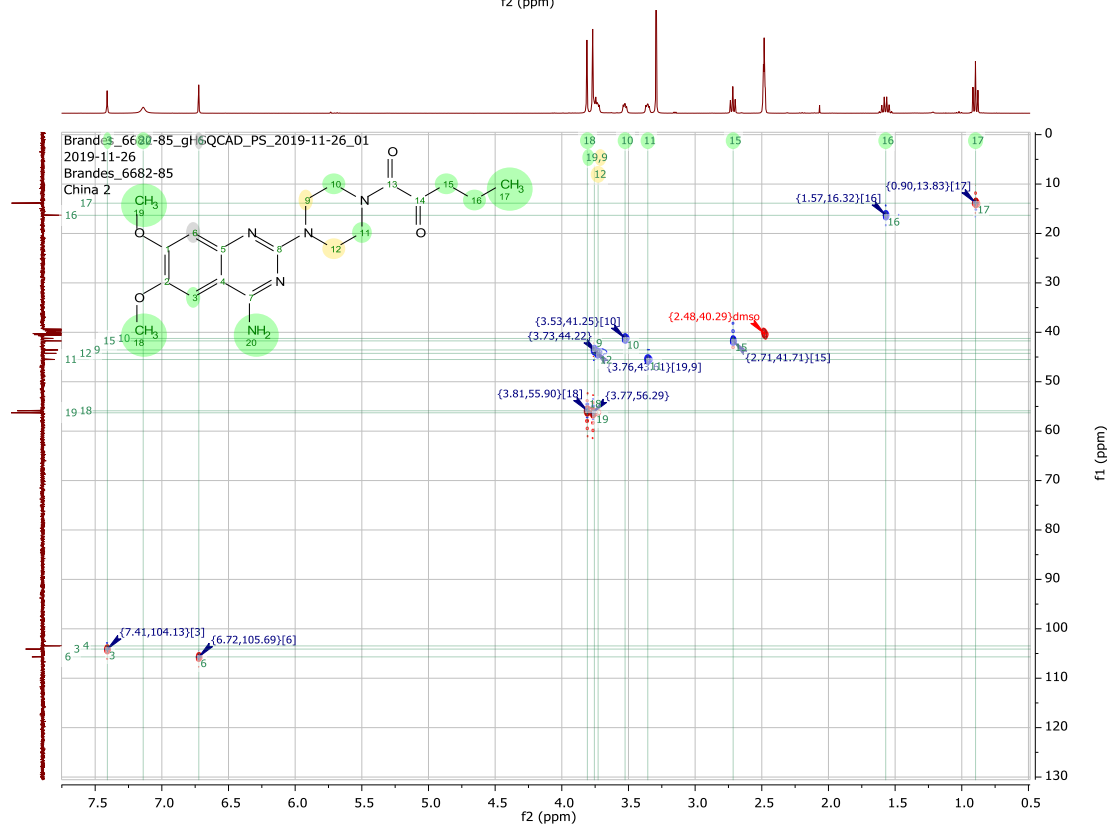
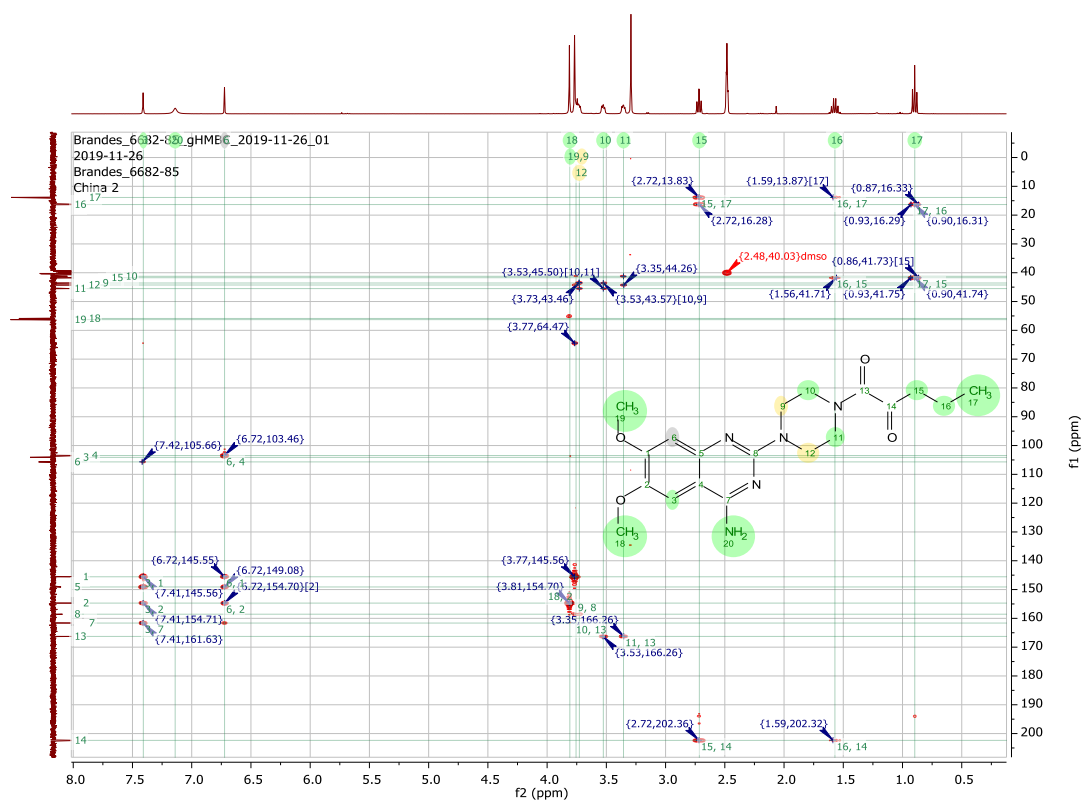
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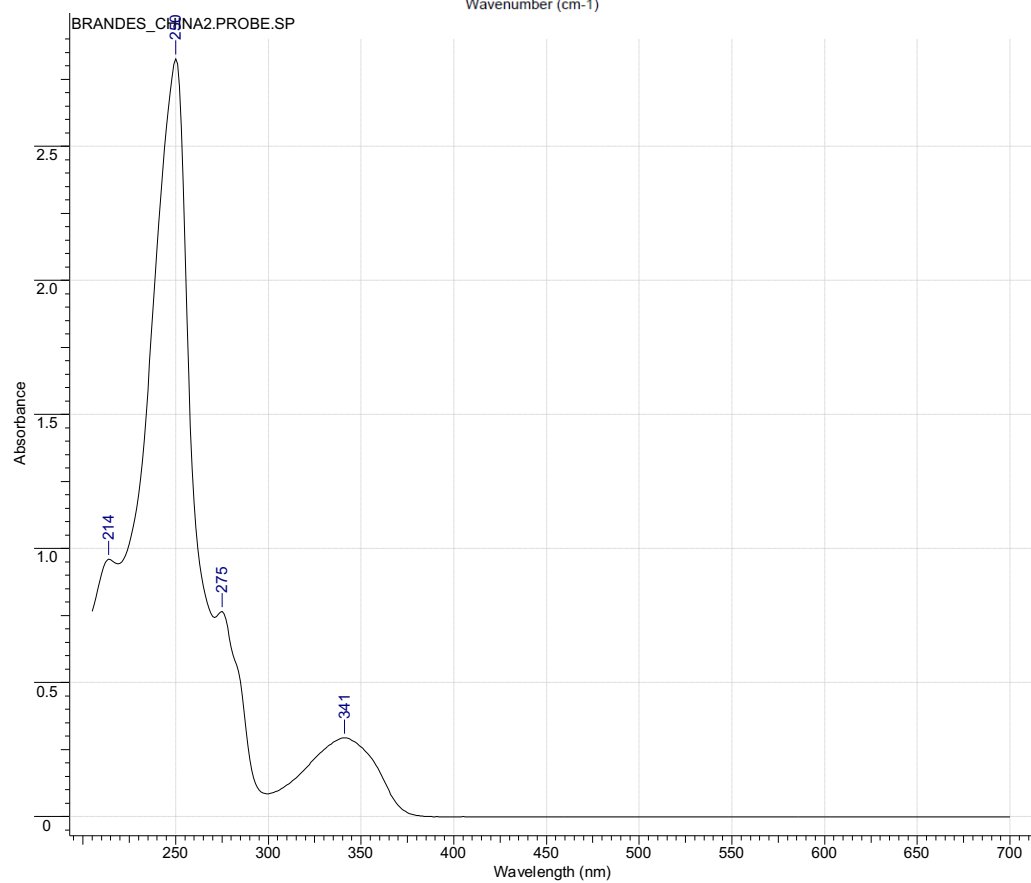
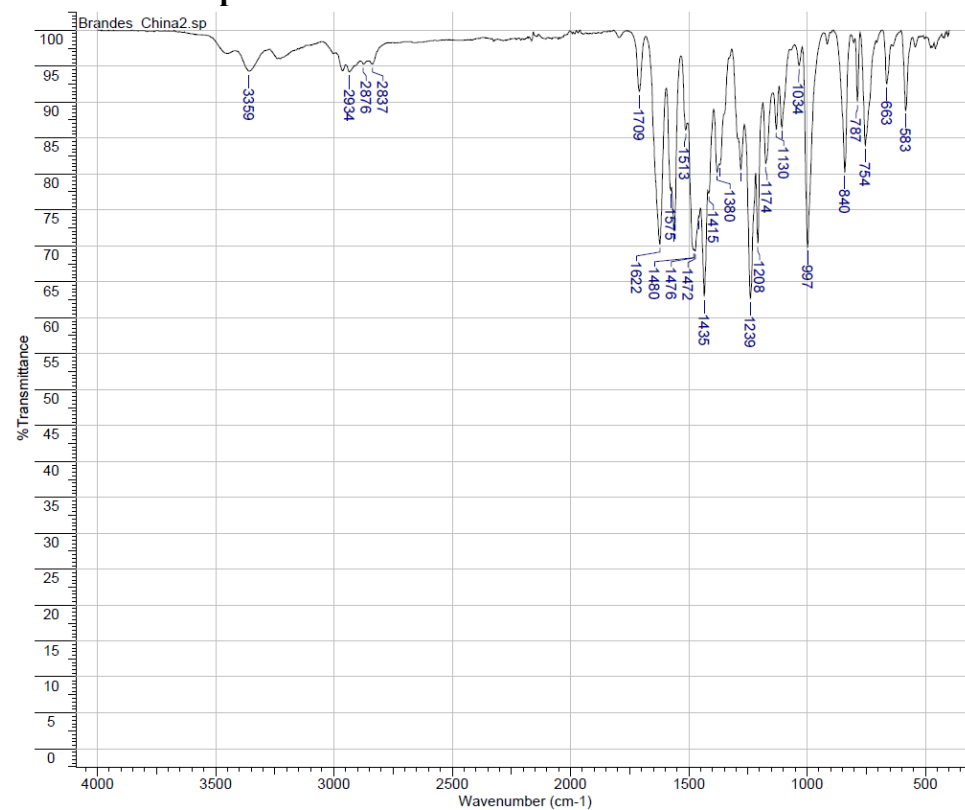
² Furtwangen University, Medical and Life Sciences Faculty, Jakob-Kienzle Str. 17, D-78054 Villingen-Schwenningen, Germany

¹H NMR, ¹³C (APT) NMR as well as representative 2D NMR spectra of 2:

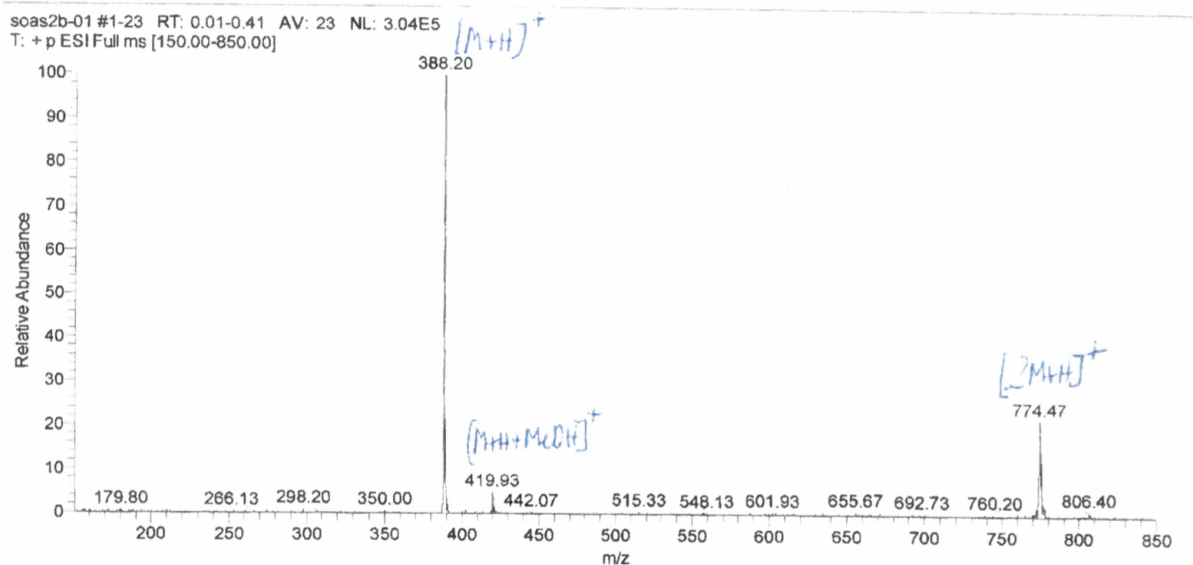




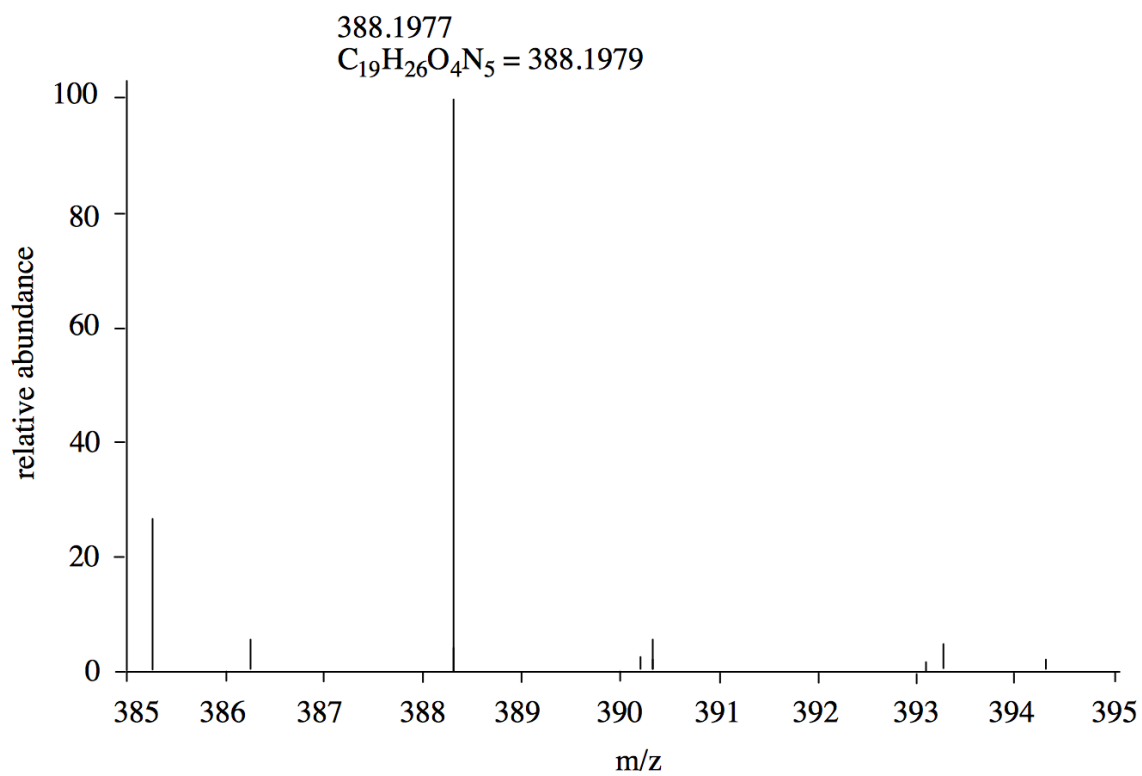
IR and UV/vis spectra of 2



ESI-MS (isolated material):



HRMS (isolated material)



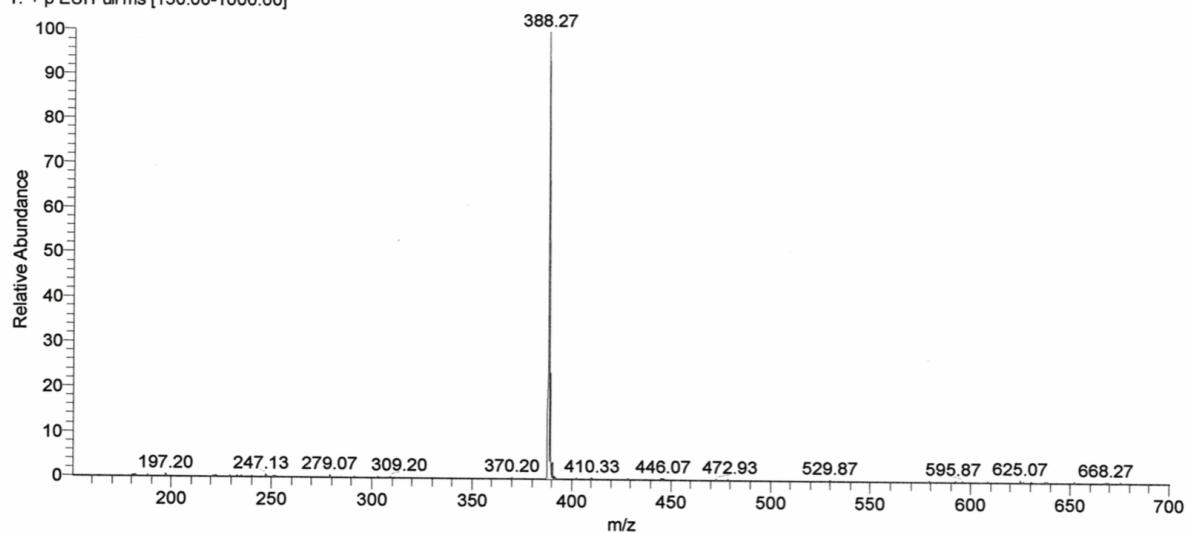
ESI-MS (synthesized material)

C:\Xcalibur\data\terazosin-01
MeOH

12/11/2013 11:23:25 AM

10459/1308B100

terazosin-01 #1-19 RT: 0.00-0.32 AV: 19 NL: 1.08E7
T: + p ESI Full ms [150.00-1000.00]



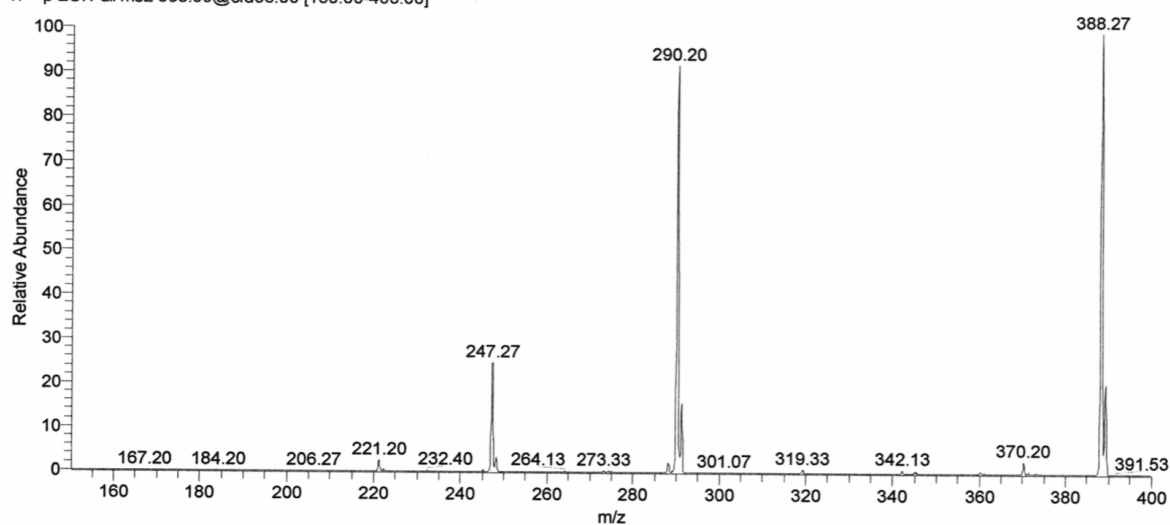
MSMS (synthesized material)

C:\Xcalibur\data\terazosin-02
MeOH

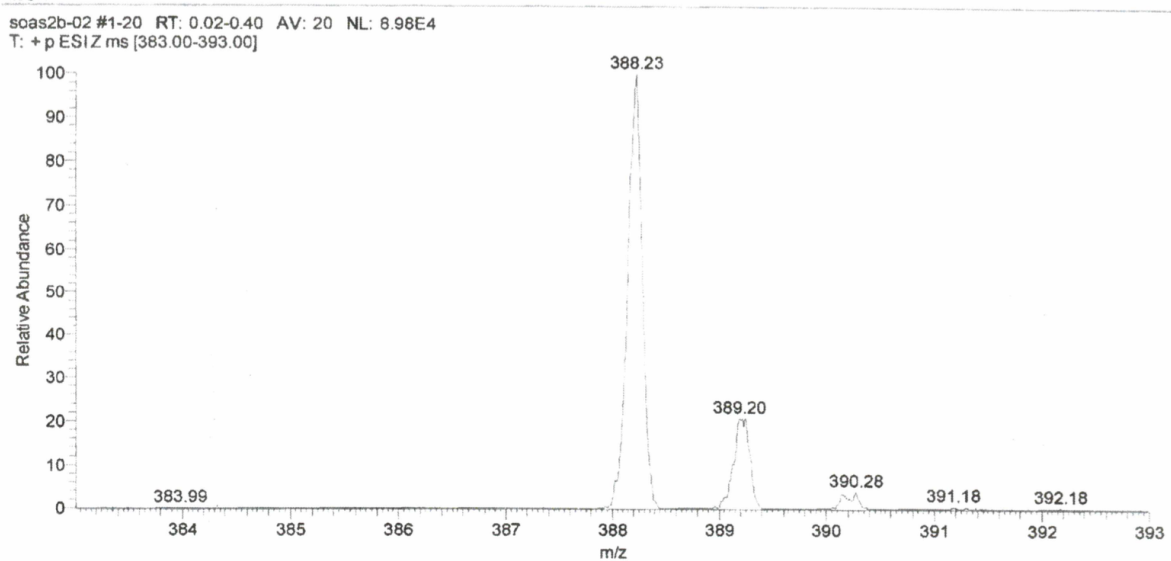
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10459/1308B100

terazosin-02 #1-29 RT: 0.01-0.36 AV: 29 NL: 2.42E7
T: + p ESI Full ms2 388.00@cid36.00 [150.00-400.00]



ESI-MS (synthesized material): zoom-spectrum



ESI-MS (simulated): zoom-spectrum

Isotopic abundances for $C_{19}H_{26}O_4N_5$

Neutral Mass	Fraction	Intensity
388.19847	0.7894159	100.00
389.19847	0.1810850	22.94
390.19847	0.0263604	3.34
391.19847	0.0028741	0.36
392.19847	0.0002521	0.003

