

Supplementary data

COA_flavocillin.pdf - Adobe Acrobat Reader (64-bit)

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General information of the substance

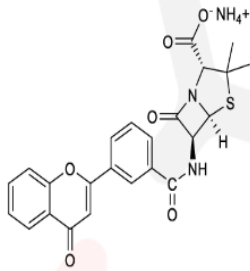
Product name: Flavocillin ammonium salt

CAS: N.A.

IUPAC name: (2R,5S,6S)-3,3-dimethyl-7-oxo-6-(3-(4-oxo-4H-chromen-2-yl)benzamido)-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid (ammonium salt 1:1)

Cat. No.: SACR042214-5

Physical and chemical properties



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Chemical structure of Flavocillin ammonium salt

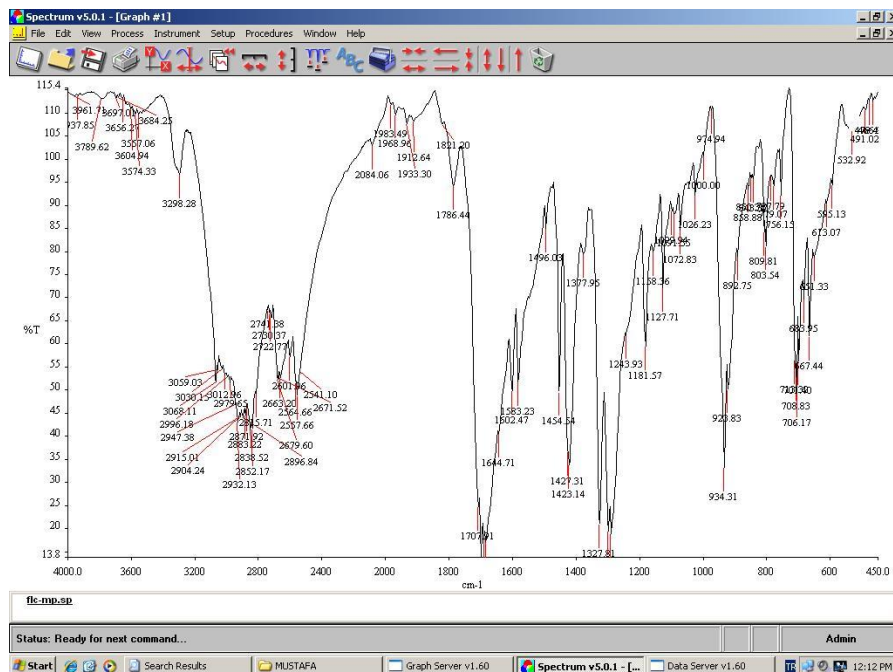


Figure 1 IR data for Flavocillin.

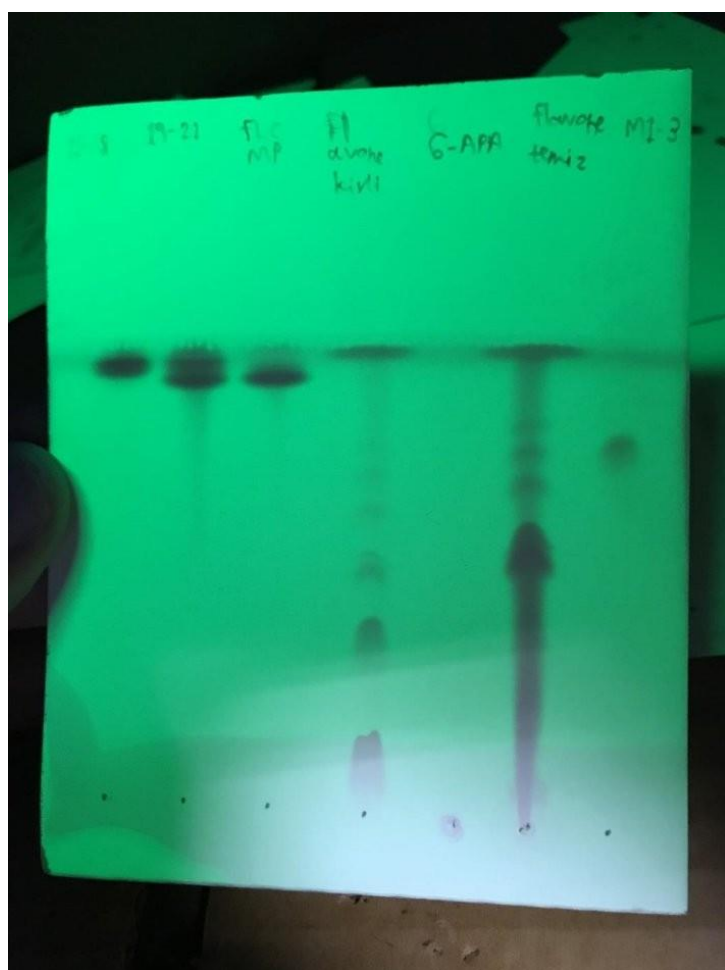


Figure 2 TLC Chromatogram of Flavocillin (FLC-MP) indicating new product formation compared to Flavones, Chalcone (M1-3) and 6-Amino Penicillanic Acid (6-APA).

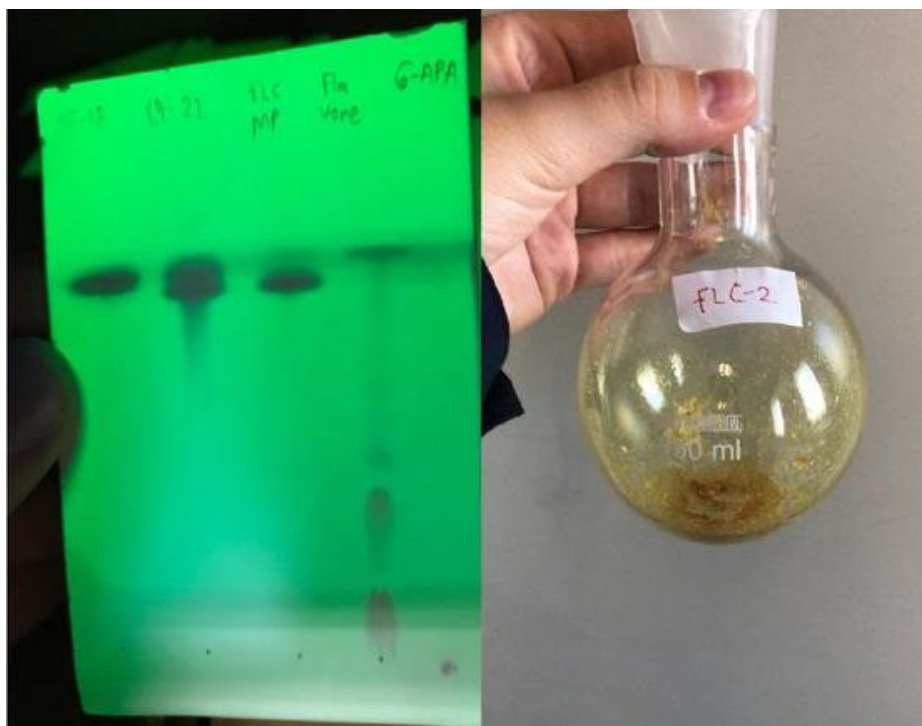
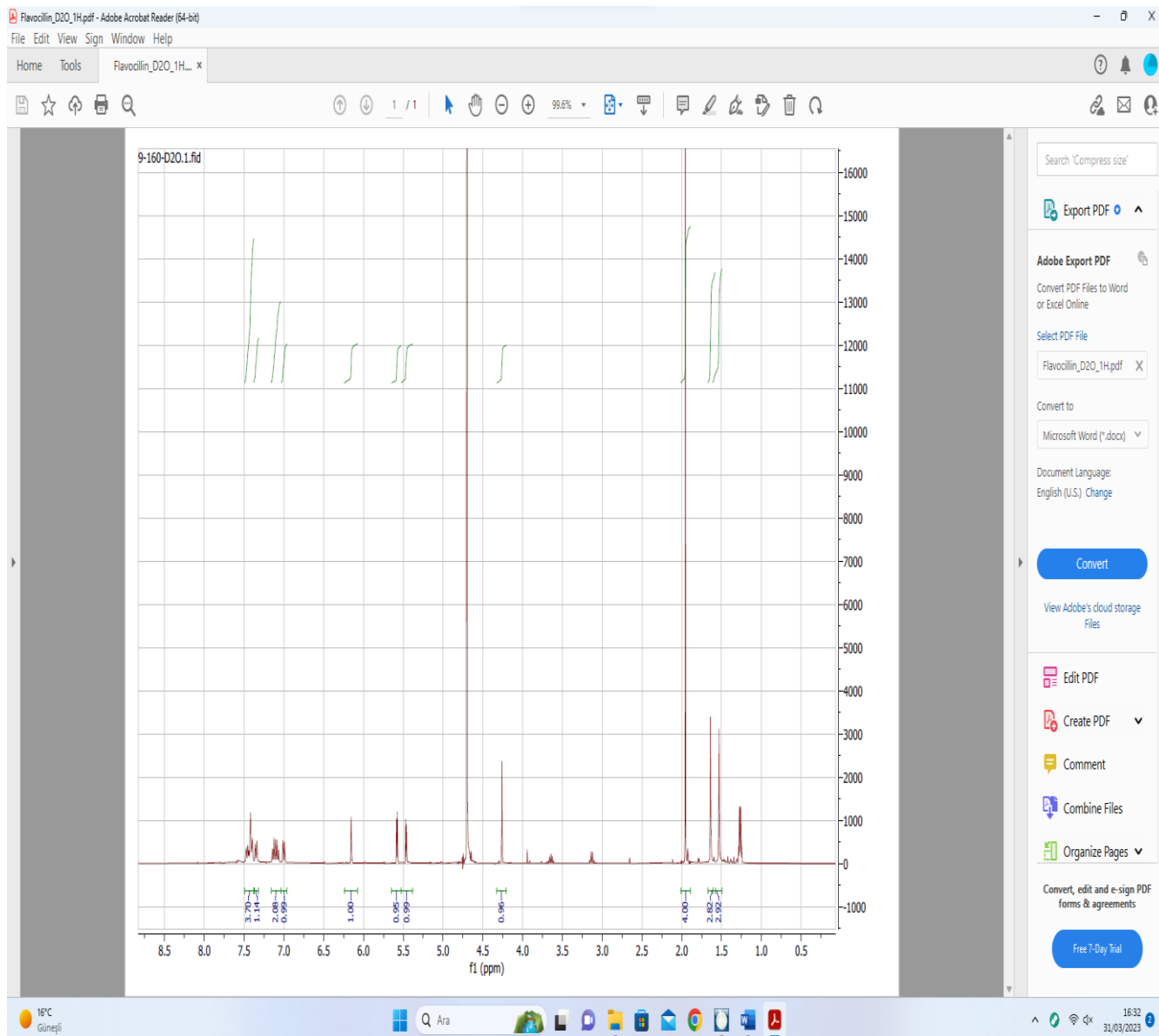
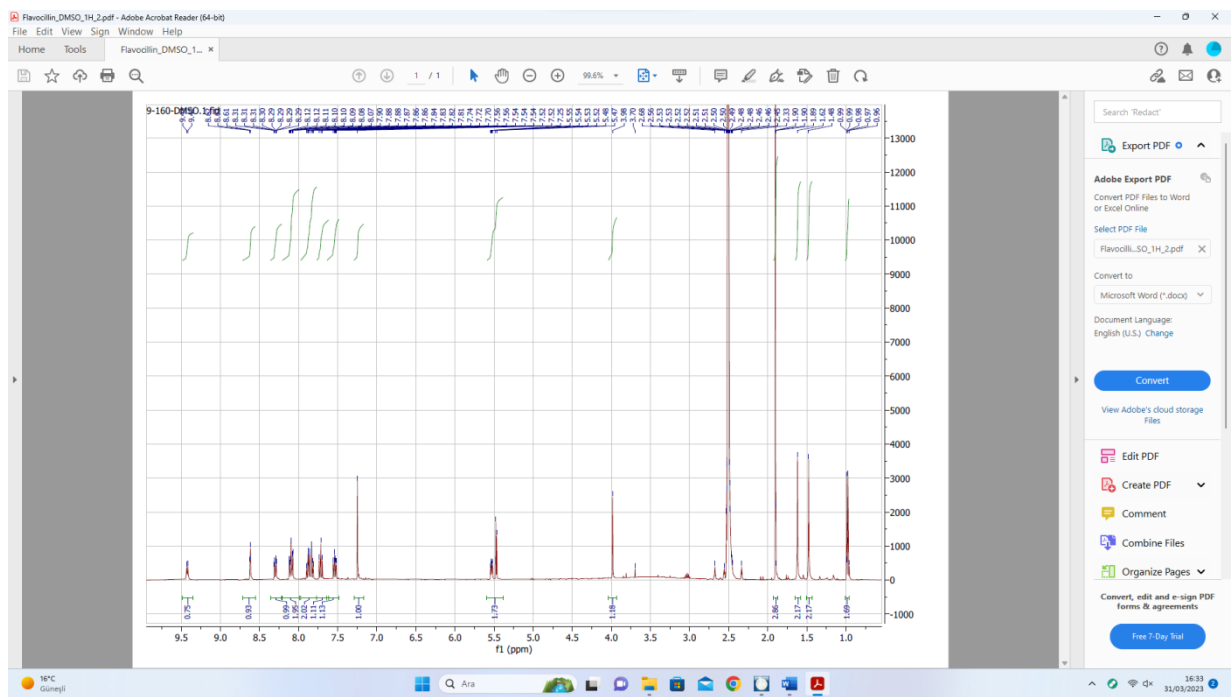
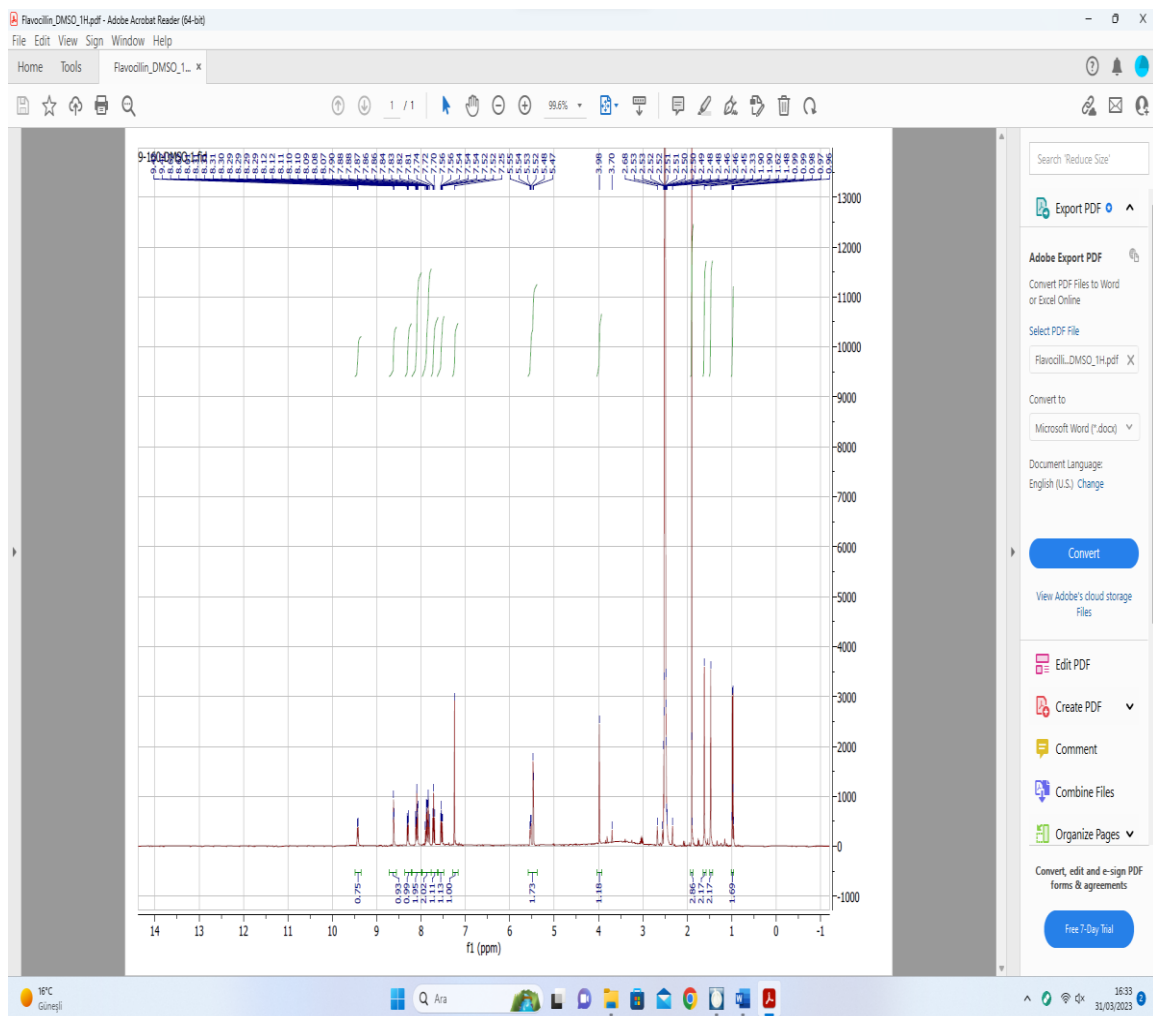
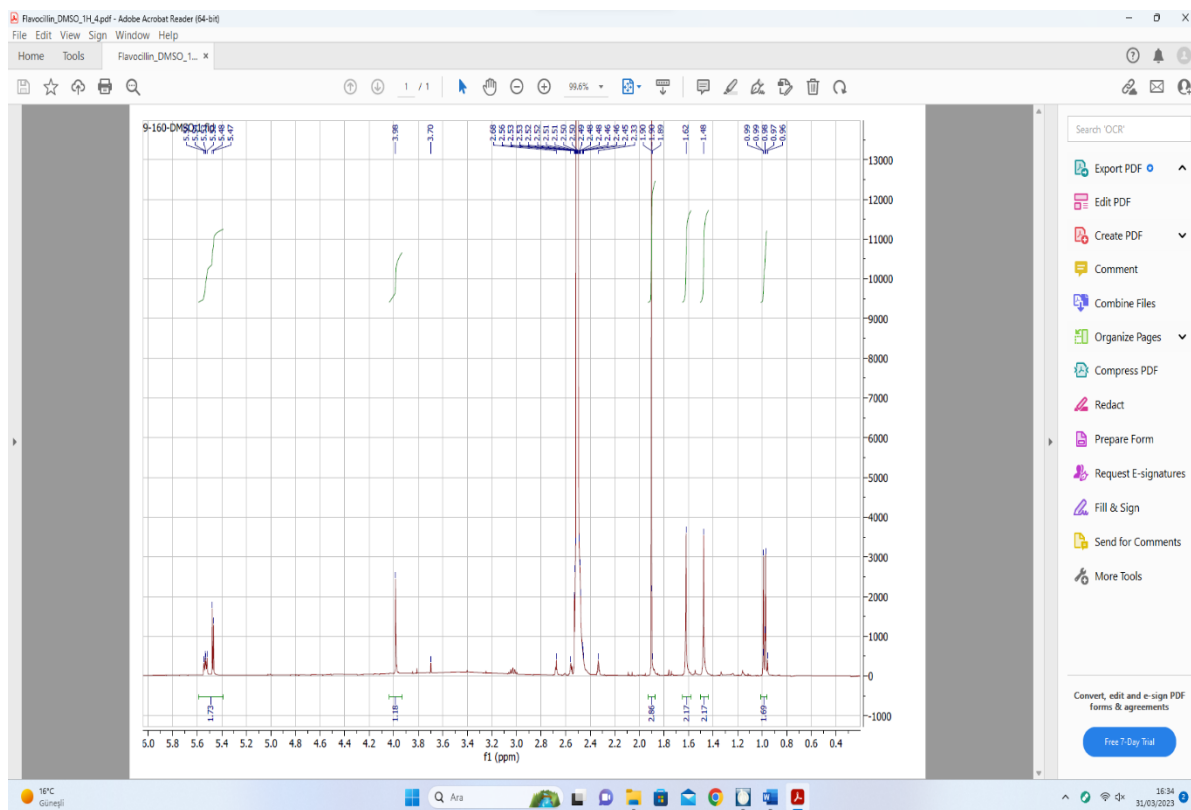


Figure 3 TLC chromatogram of the Flavocillin purified by column chromatography (FLC-MP , on the left) and Flavocillin powder.

H-NMR, C-NMR, LC-MS and COSY analysis results confirming 97% pure Flavocillin ammonium salt:

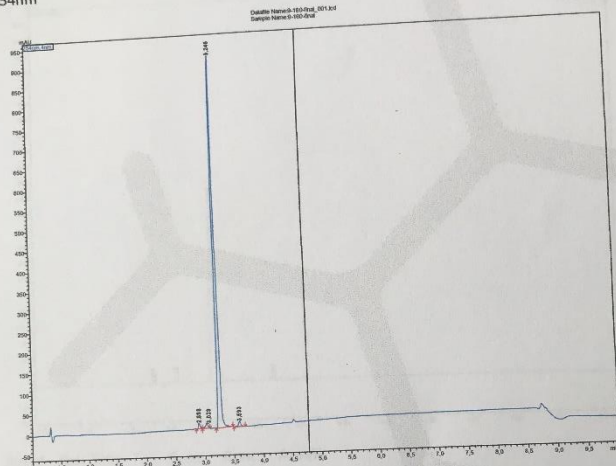






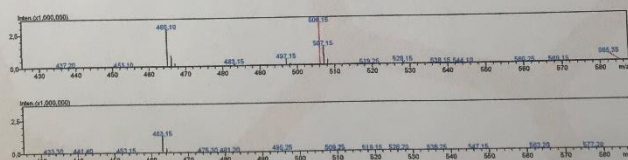


254nm

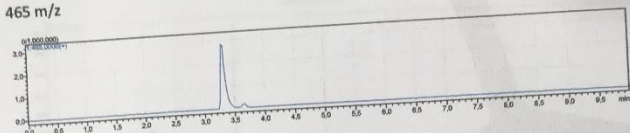


Peak#	Ret. Time	Area	Conc.	Area%
1	2,898	25199	0,000	1,239
2	3,029	30331	0,000	1,492
3	3,246	1946710	0,000	95,750
4	3,593	30872	0,000	1,518
Total		2033112	0,000	100,000

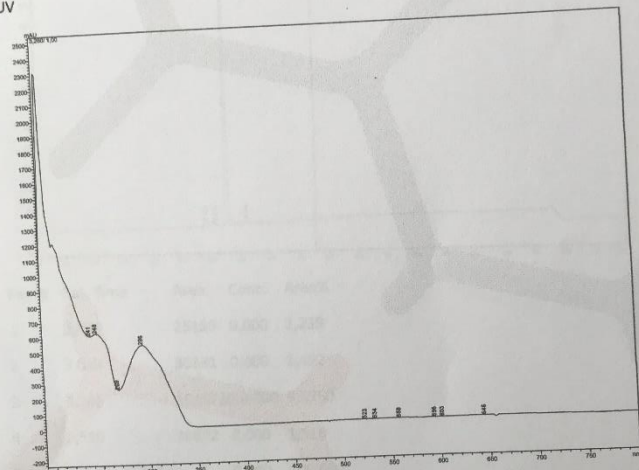
Peak at 3.246 min positive and negative mode



465 m/z



UV

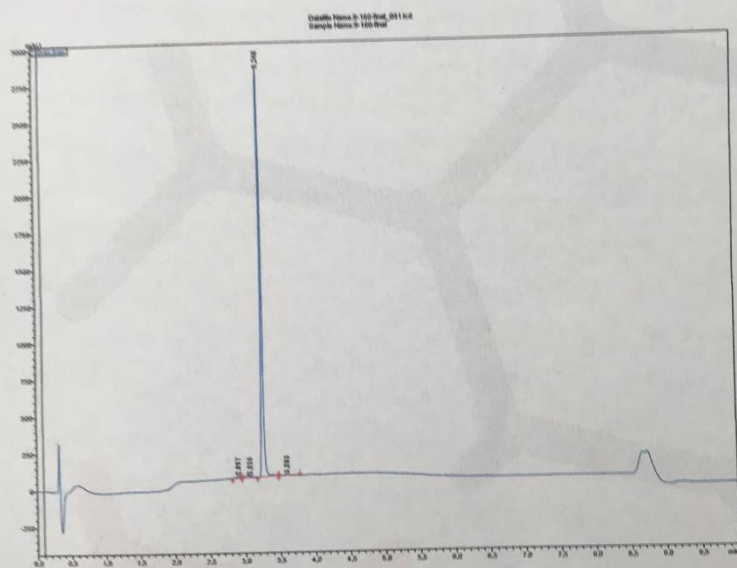


Flavocillin – analysis of the final product

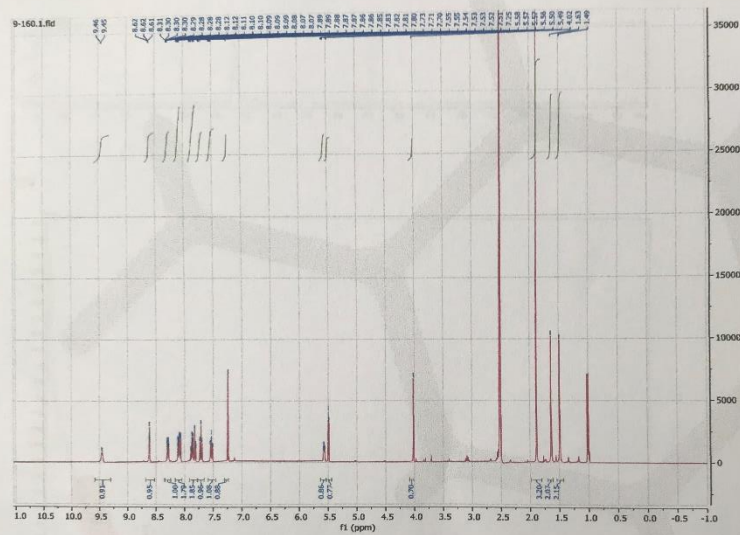
14.4.2022

Santiago Lab

210 nm

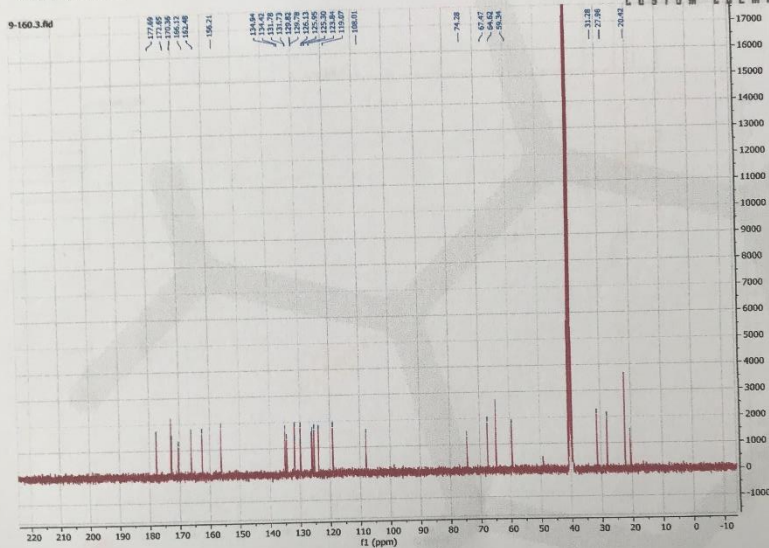


^1H NMR, DMSO

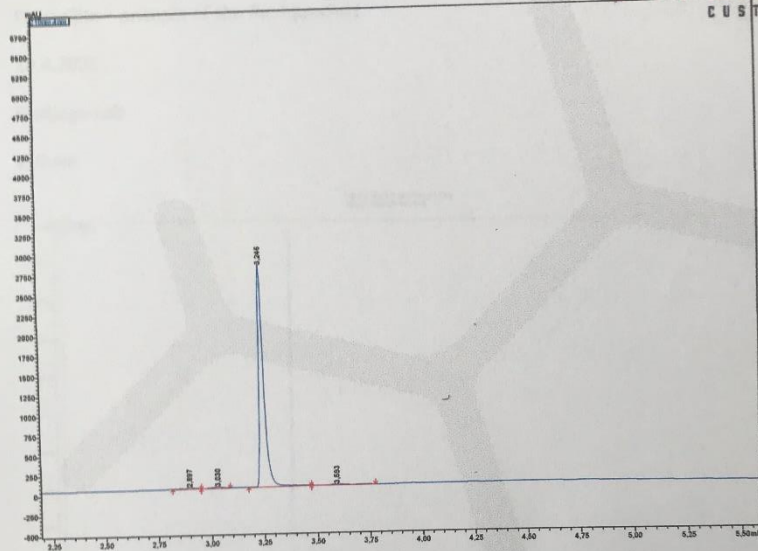


¹³C NMR, DMSO

9-160.3.fid

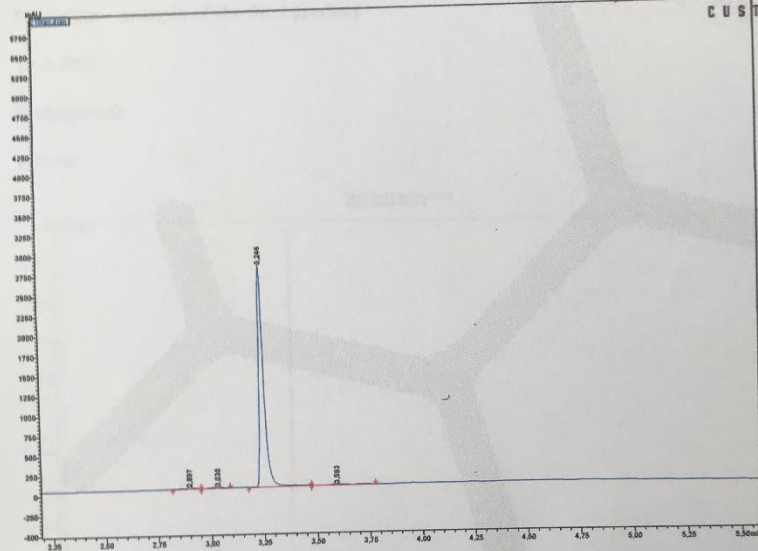


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 Sample Name: 28-183-Bref



Peak#	Ret. Time	Area	Conc.	Area%
1	2,897	48960	0,000	1,083
2	3,030	45527	0,000	1,007
3	3,246	4404544	0,000	97,402
4	3,593	22997	0,000	0,509
Total		4522028	0,000	100,000

DataFile Name: S-160-Ret_001.jud
 Sample Name: S-160-Ret



Peak#	Ret. Time	Area	Conc.	Area%
1	2,897	48960	0,000	1,083
2	3,030	45527	0,000	1,007
3	3,246	4404544	0,000	97,402
4	3,593	22997	0,000	0,509
Total		4522028	0,000	100,000