

(E)-1-(4-Ethoxycarbonylphenyl)-5-(3,4-dimethoxyphenyl)-3-(3,4-dimethoxystyryl)-2-pyrazoline: Synthesis, Characterization, DNA-Interaction and Evaluation of Activity Against Drug-Resistant Cell Lines

Dimitris Matiadis ¹, Barbara Mavroidi ¹, Angeliki Panagiotopoulou ¹,
Constantinos Methenitis ², Maria Pelecanou ¹, and Marina Sagnou ^{1,*}

¹ National Center for Scientific Research "Demokritos", Institute of Biosciences & Applications, Athens 153 10, Greece; matiadis@bio.demokritos.gr (D.M); bmavroidi@bio.demokritos.gr (B.M); apanagio@bio.demokritos.gr (A.P); pelmar@bio.demokritos.gr (M.P); sagnou@bio.demokritos.gr (M.S) *

² National and Kapodistrian University of Athens, Department of Chemistry, Athens 157 84, Greece; methenitis@chem.uoa.gr (C.M)

Supplementary Information

Contents

NMR spectra of 6	2
FT-IR spectrum	6
HRMS	7
UV-Vis spectra	8
HPLC	9

All presented data refer to the ethanol crystallized product

NMR spectra of **6**

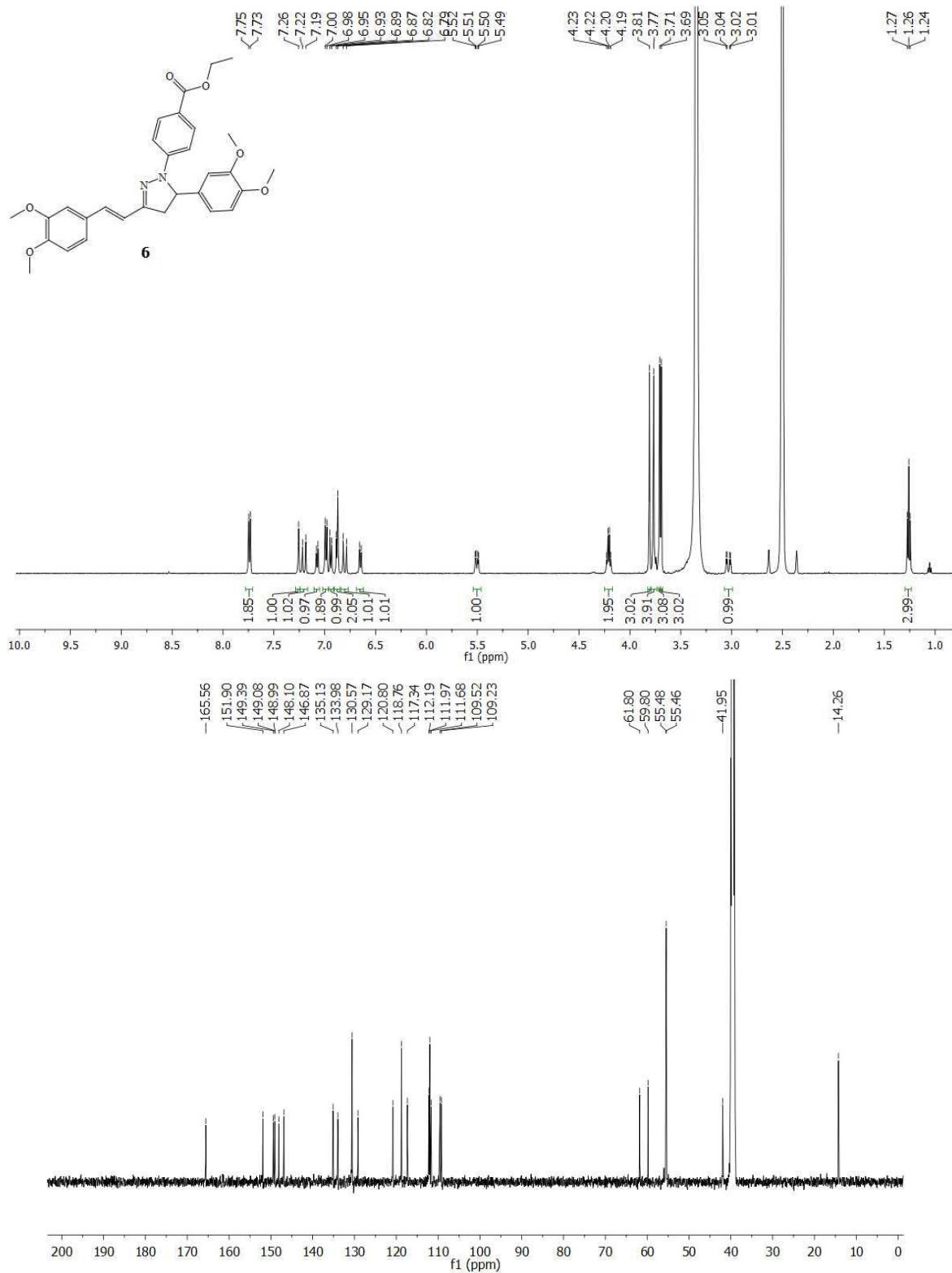


Figure S1. ¹H and ¹³C NMR of compound **6**.

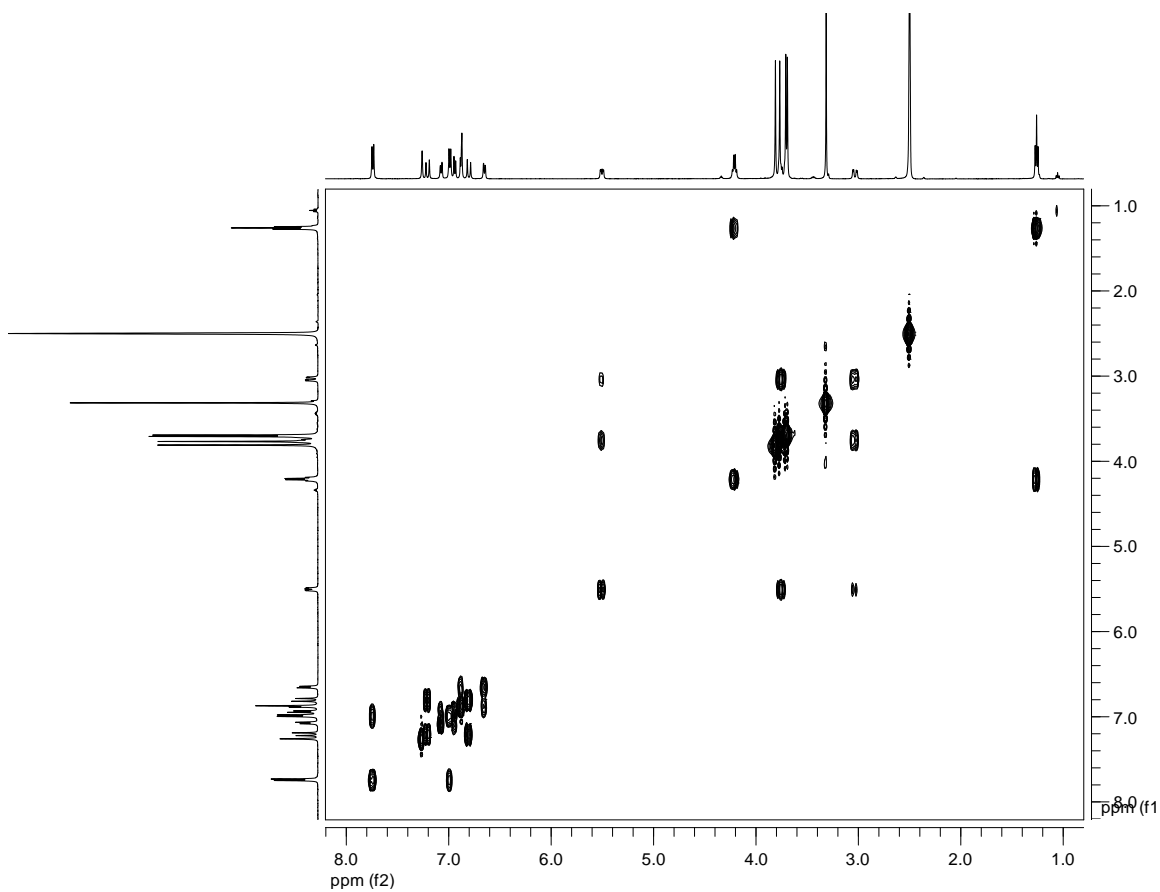


Figure S2. ^1H - ^1H COSY NMR spectrum of compound **6**.

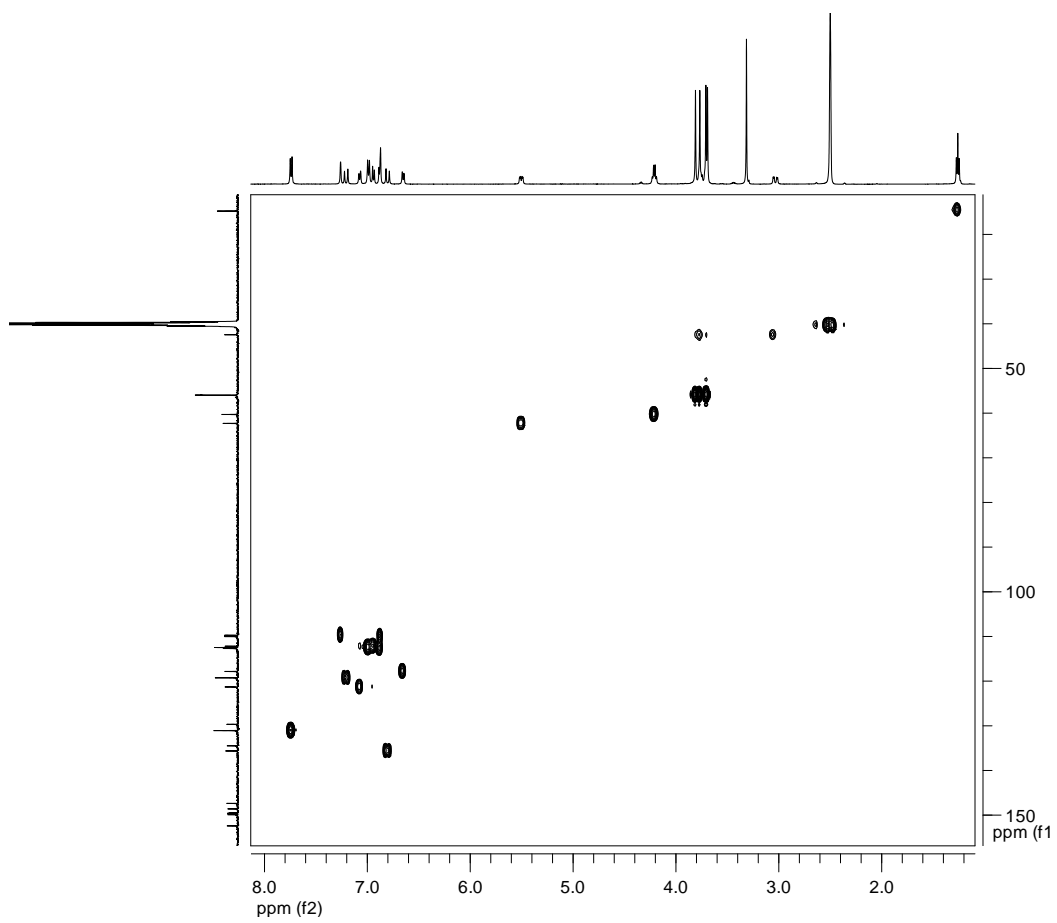


Figure S3. HSQC NMR spectrum of compound **6**.

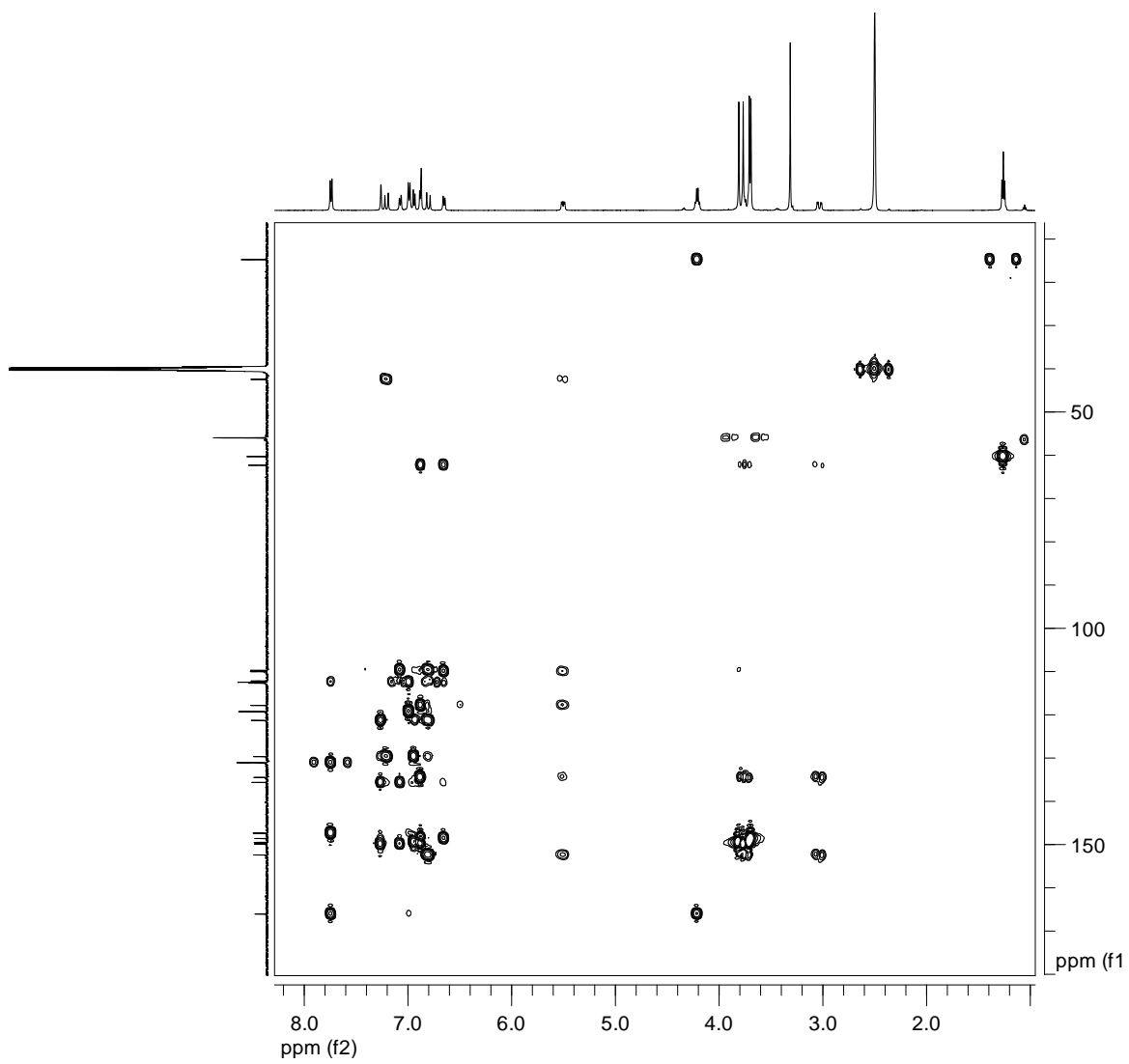
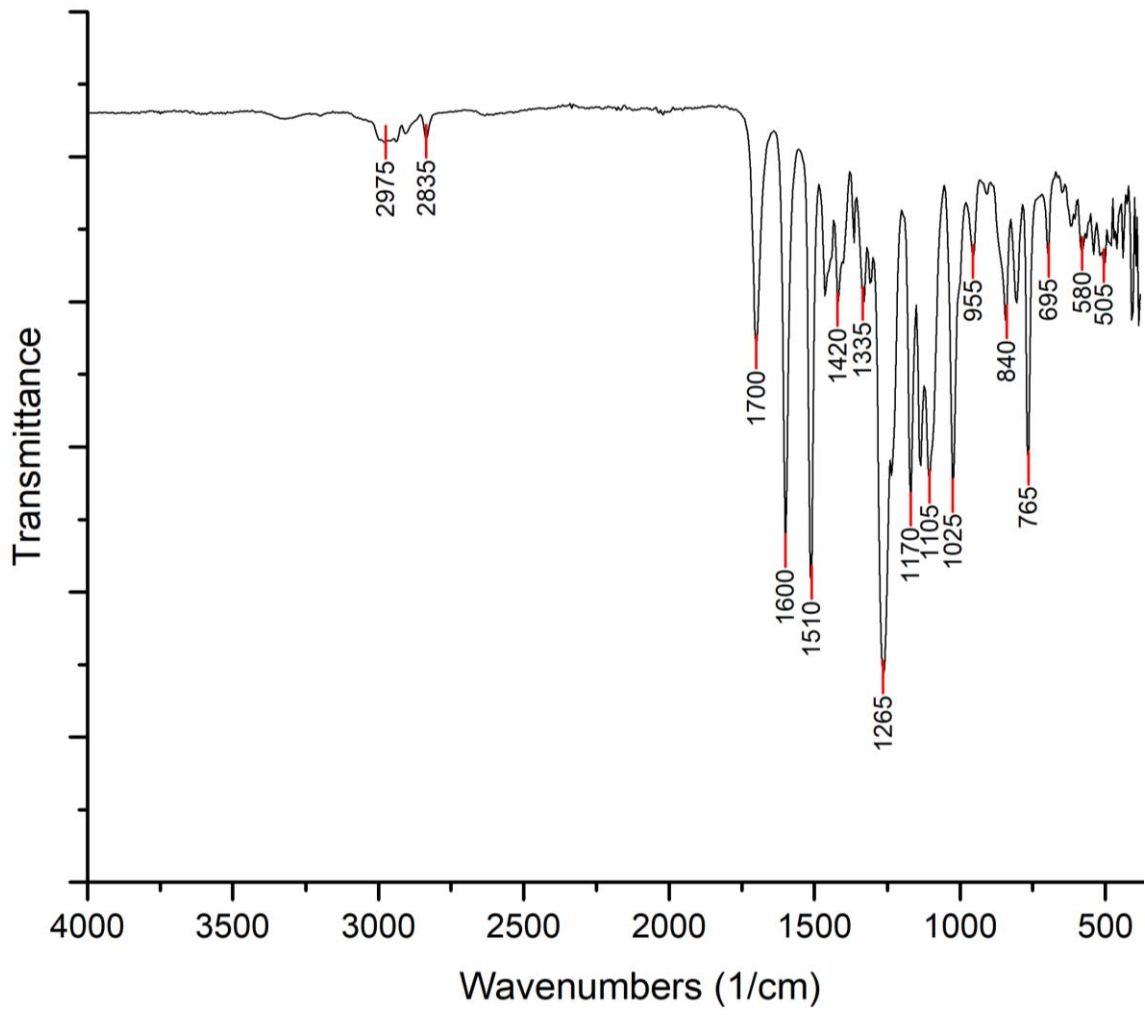


Figure S4. HMBC NMR spectrum of compound **6**.

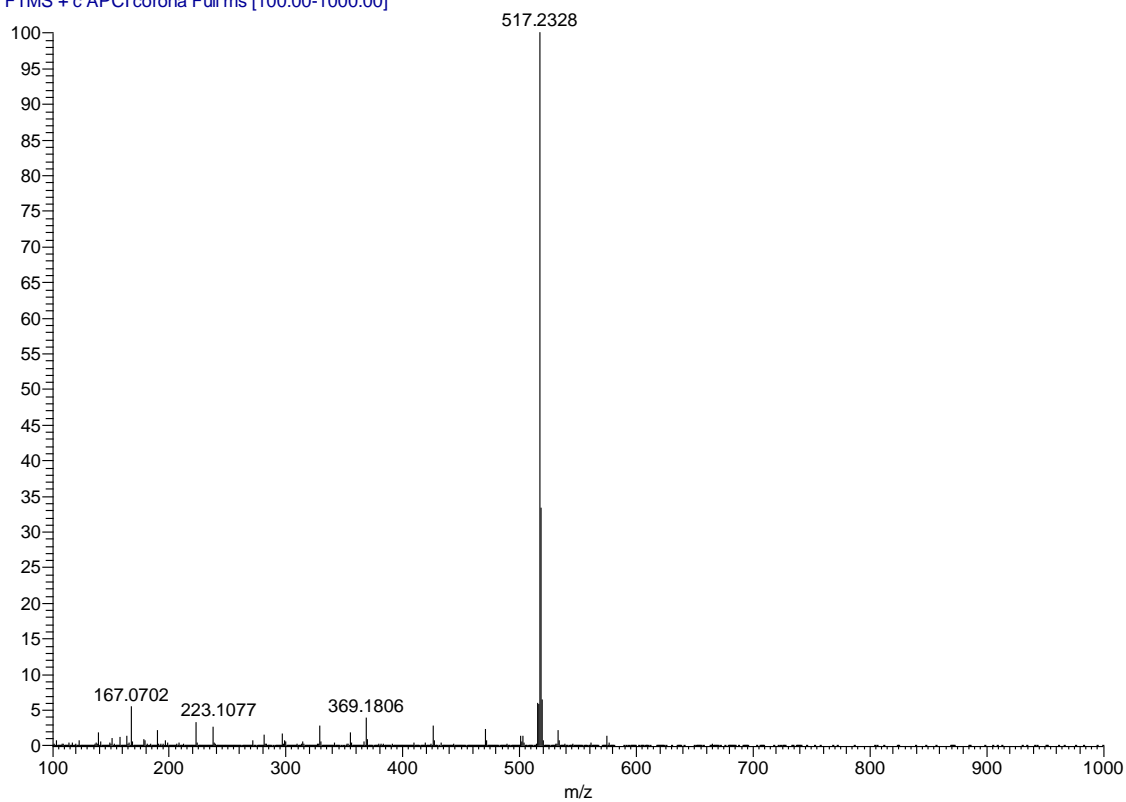
FTIR spectrum of 6



HRMS

Scan for compound 6

DM102 #15-23 RT: 0.11-0.17 AV: 9 NL: 1.20E8
T: FTMS + c APCI corona Full ms [100.00-1000.00]



Elemental composition

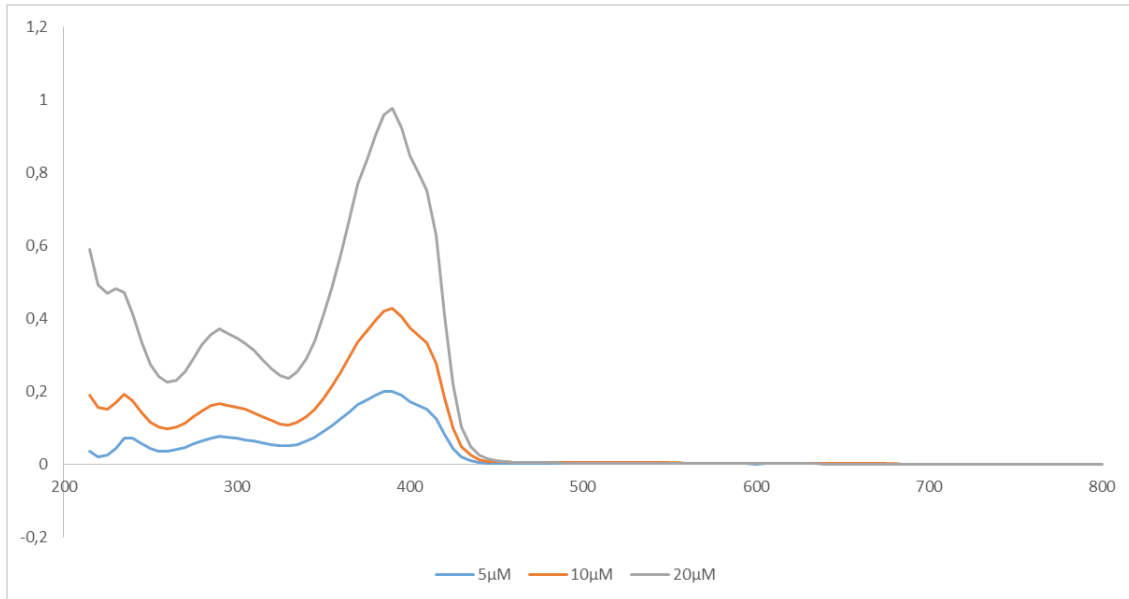
Single mass

Mass:

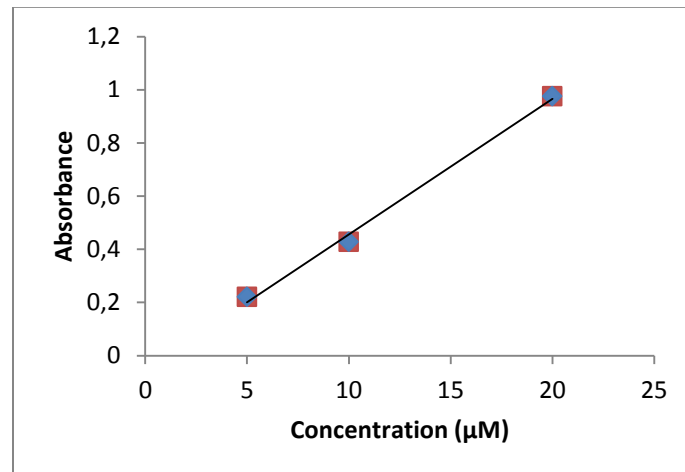
Max. results:

Idx	Formula	RDB	Delta ppm
1	C ₃₀ H ₃₃ O ₆ N ₂	15.5	-0.954

UV-Vis spectra and Absorbance Vs Concentration graph

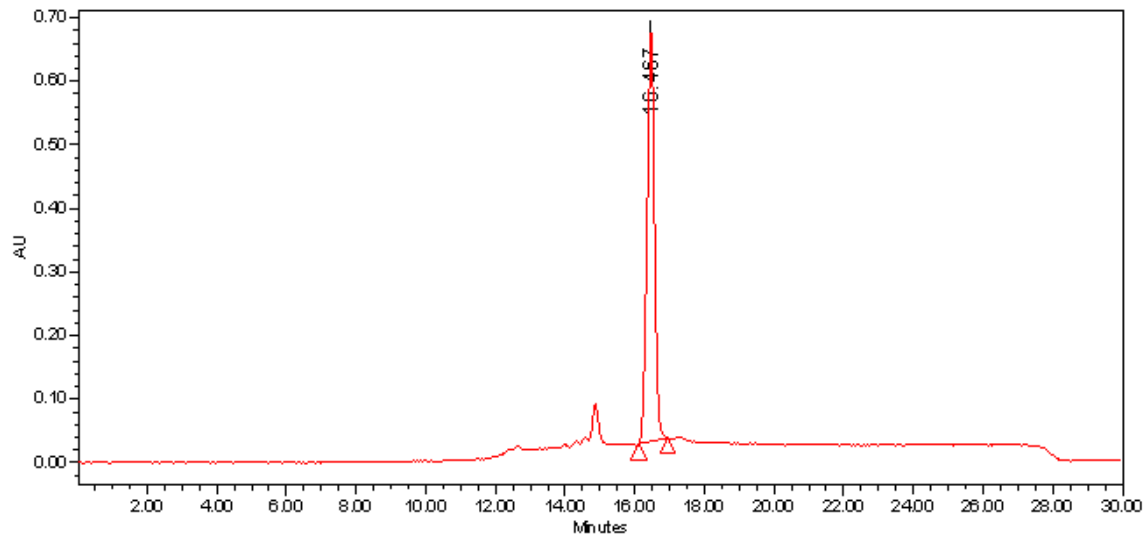


Concentration (μM)	Absorbance
5	0.22
10	0.43
20	0.97



$$\epsilon = 45166,67 \quad \log \epsilon = 4,65$$

HPLC trace and peak quantitation



Peak Results

	Name	RT	Area	Height	Amount	Units
1		16.467	9633756	642423		