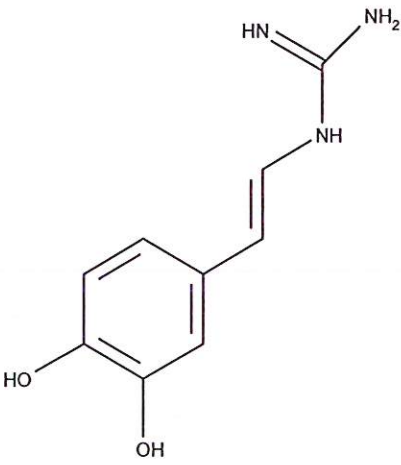


HBOI-85	
TUBASTRINE	
$C_9H_{11}N_3O_2$	193.20
<i>Tubastrea aurea</i>	
Sakai and Higa, 1987, <i>Chem. Lett.</i> , 1987, 127-128	

hplc (trace attached)

Method: Vydac C18 Protein and Peptide, 4.6 x 250mm, 10 μ
 flow 1 ml/min, detection: PDA: UV (extracted at 220 nm, black); ELSD (green dotted)
 A: H₂O:CH₃CN (95:5, v/v, 0.1% TFA), B: CH₃CN (0.1% TFA)
 t=0 min A: B (90:10, v/v), t=20 min (100%B) , t=28 min (100%B)

LC-MS (spectrum attached)

Method: Vydac C18 Protein and Peptide, 2.1x150 mm, flow 0.2 ml/min
 A: H₂O (0.1% formic acid), B: CH₃CN (0.1% formic acid)
 t= 0 min A: B (90:10, v/v), t=15 min (100%B), t=21 min (100%B), t=22.1 min A:B(90:10, v/v)
 using a linear gradient

¹H (600 MHz) CDCl₃ CD₃OD (Methanol-d₄) CDCl₃/CD₃OD

¹³C (150 MHz) CDCl₃ CD₃OD (Methanol-d₄) CDCl₃/CD₃OD

solubility CHCl₃/MeOH (9:1) MeOH DMSO

estimated purity __>90__%

sample weight _19.2__mg

For further information contact:

Amy E. Wright, PhD, HBOI@FAU, 5600 US 1, North, Fort Pierce, FL 34946
awrigh33@hboi.fau.edu, 772-242-2459

Date: 1/28/13

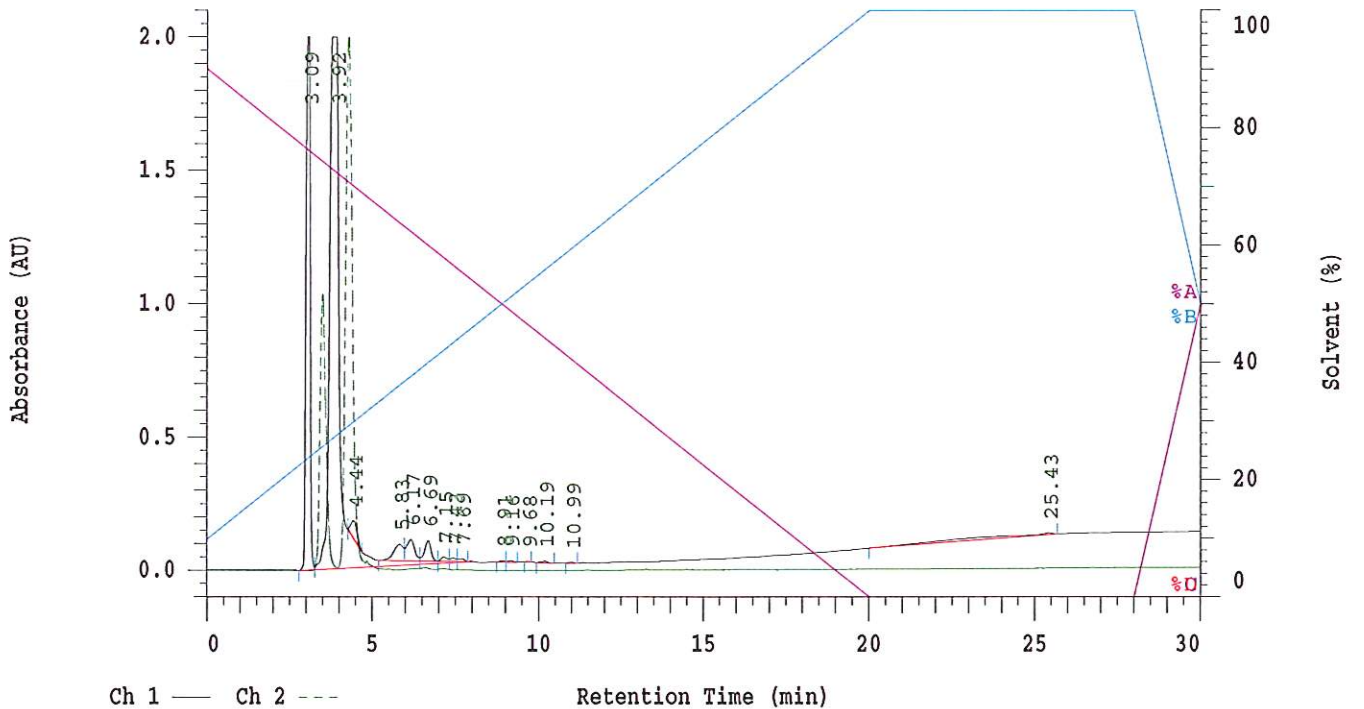
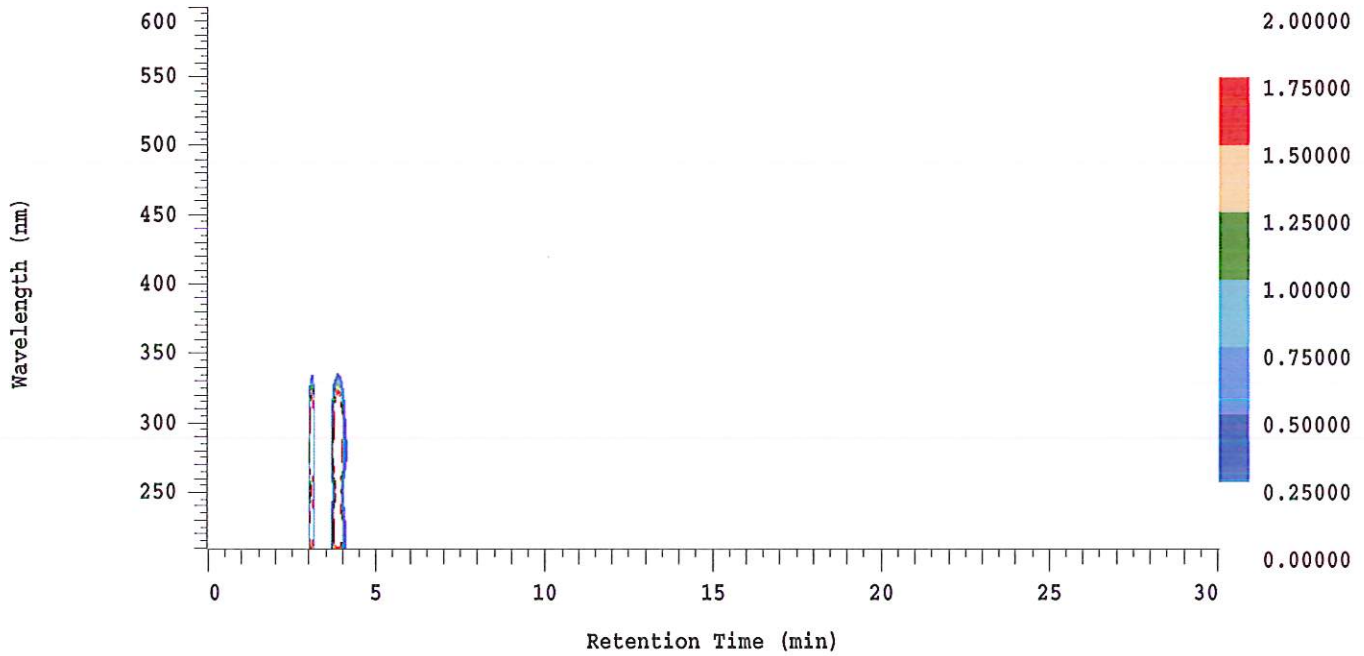
D-2000 Elite HPLC System Manager Report

Analyzed: 01/24/2013 08:35 PM

Reported: 01/25/2013 08:02 AM

Sample Name: HBOI-85

Sample Description: HBOI-85



Acquisition Method: NIH_30min_UV220_wELSD_TFA

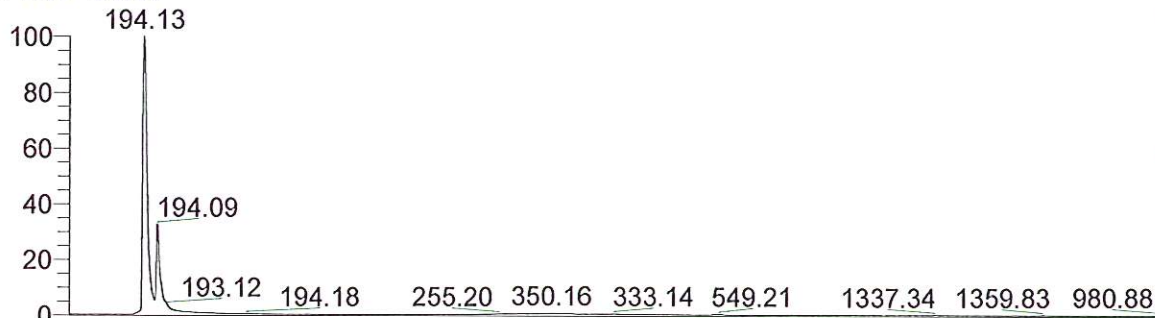
Column Type: Vydac C18

Pump A Solvent A: H2O/5% ACN TFA 0.1%

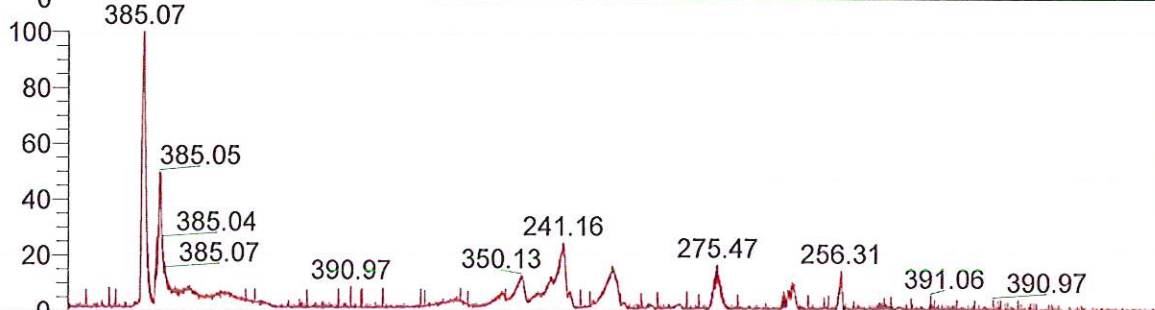
Pump A Solvent B: ACN TFA 0.1%

Method Description:

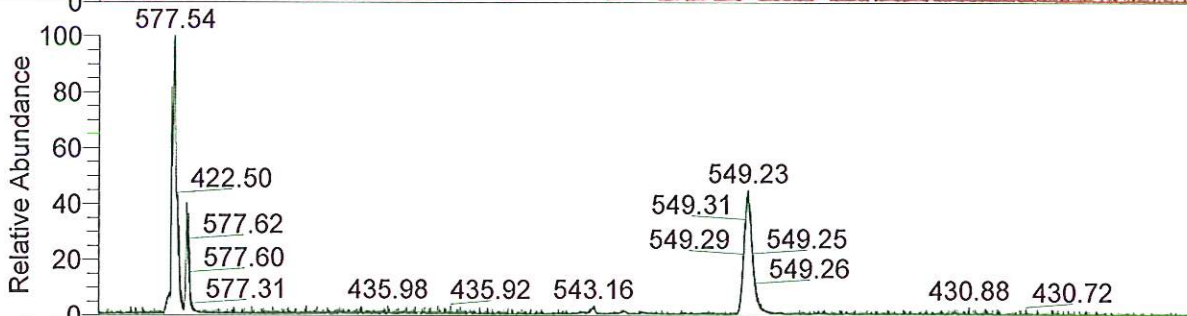
RT: 0.00 - 24.99



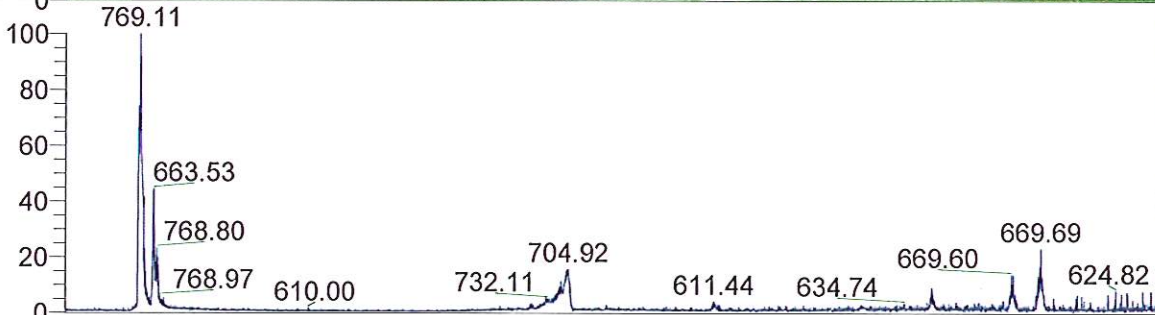
NL: 2.13E7
TIC F: ITMS + c ESI Full ms [125.00-2000.00] MS
BG_HB_85_Tubastrine_1301
24113506



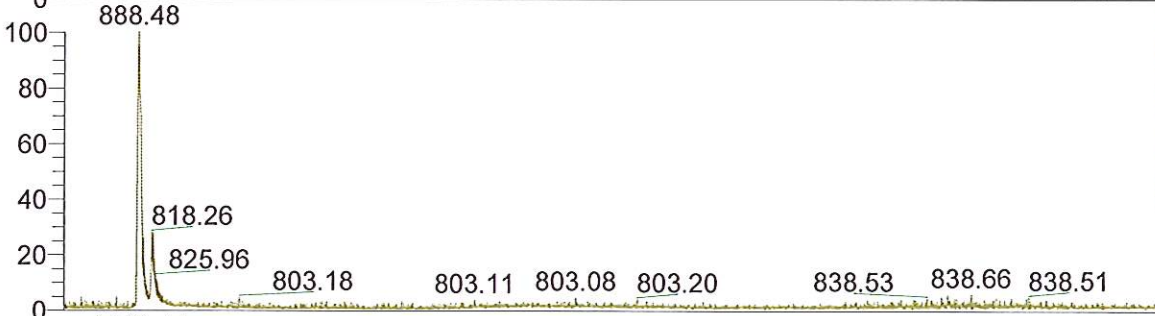
NL: 1.03E5
Base Peak m/z=
200.00-400.00 F: ITMS + c
ESI Full ms [125.00-2000.00]
MS
BG_HB_85_Tubastrine_1301
24113506



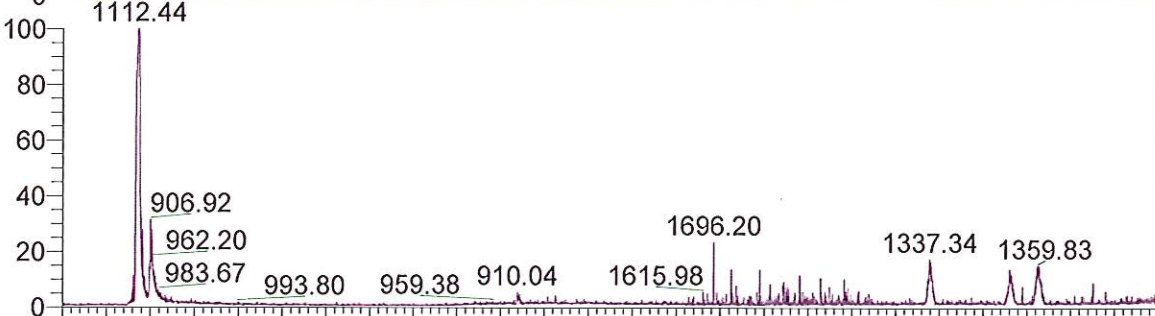
NL: 8.30E4
Base Peak m/z=
400.00-600.00 F: ITMS + c
ESI Full ms [125.00-2000.00]
MS
BG_HB_85_Tubastrine_1301
24113506



NL: 2.57E4
Base Peak m/z=
600.00-800.00 F: ITMS + c
ESI Full ms [125.00-2000.00]
MS
BG_HB_85_Tubastrine_1301
24113506

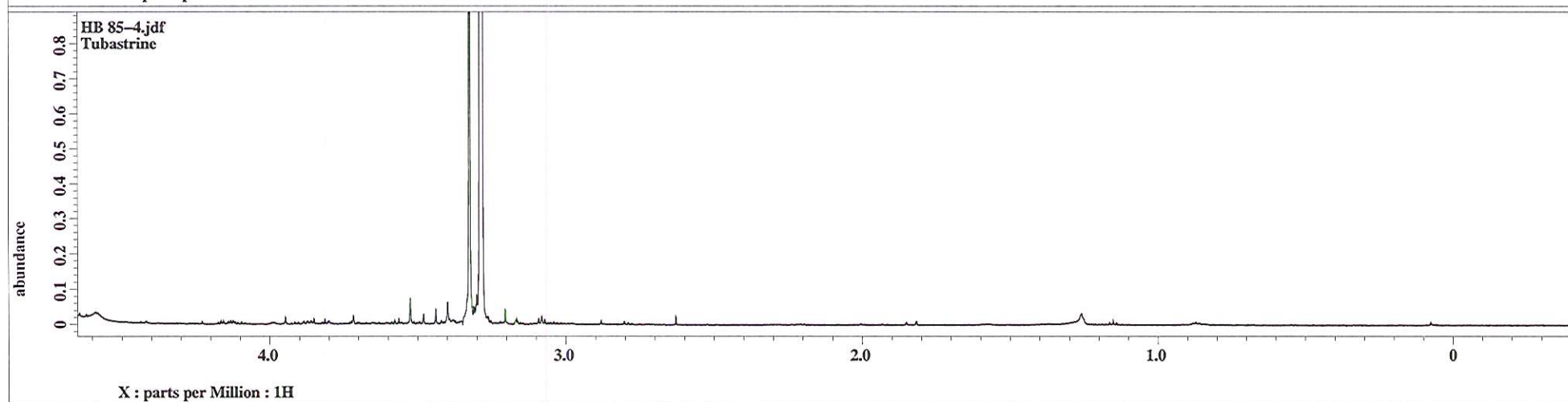
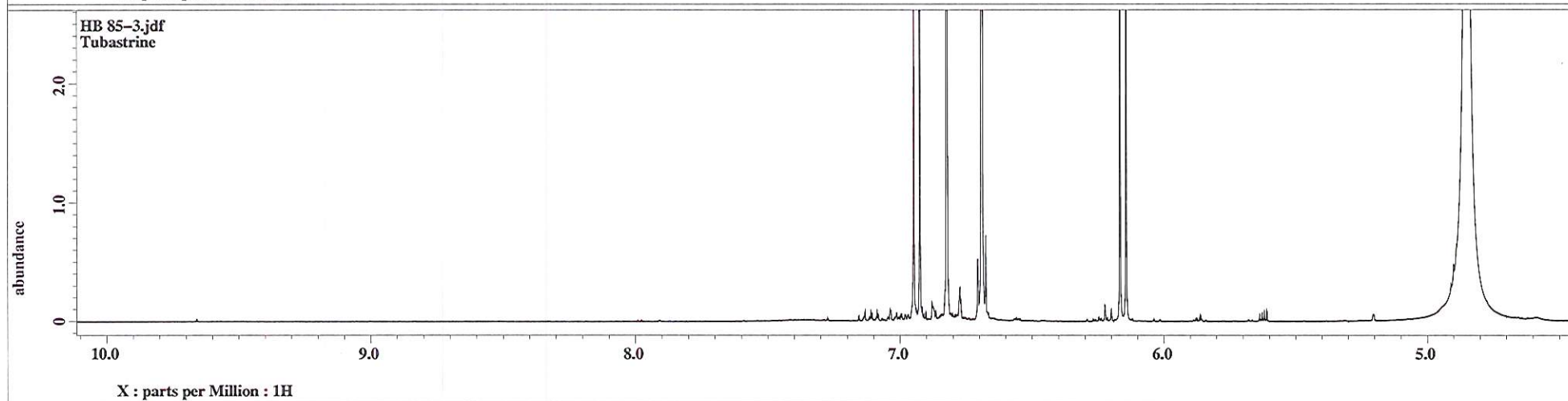
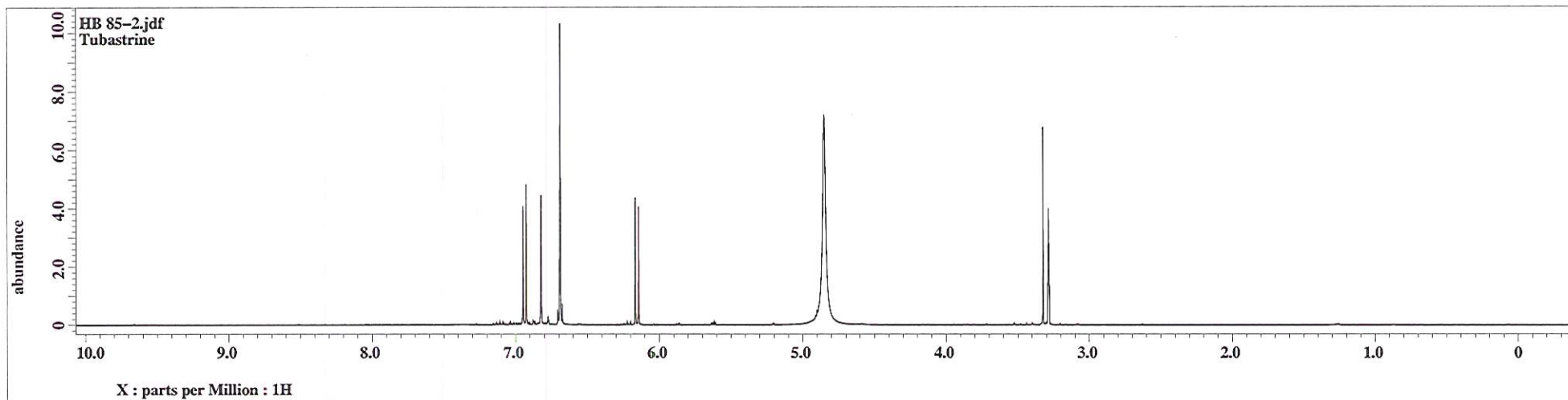


NL: 1.58E4
Base Peak m/z=
800.00-900.00 F: ITMS + c
ESI Full ms [125.00-2000.00]
MS
BG_HB_85_Tubastrine_1301
24113506

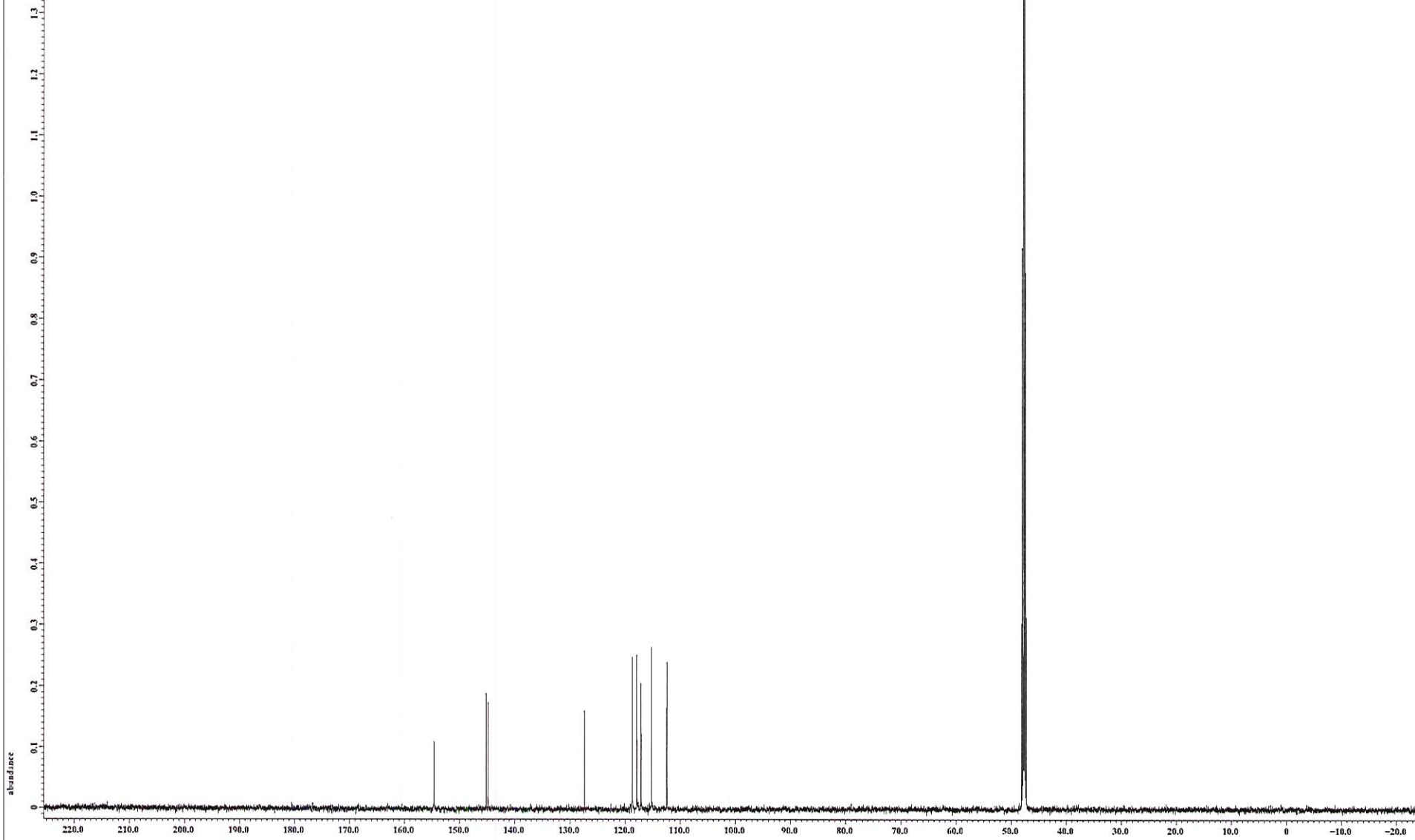


NL: 1.87E4
Base Peak m/z=
900.00-2000.00 F: ITMS + c
ESI Full ms [125.00-2000.00]
MS
BG_HB_85_Tubastrine_1301
24113506

Time (min)



HB85_Tubastrine_MeOD_CARON-3.jdf
HB85_Tubastrine MeOD



X : parts per Million : 13C

