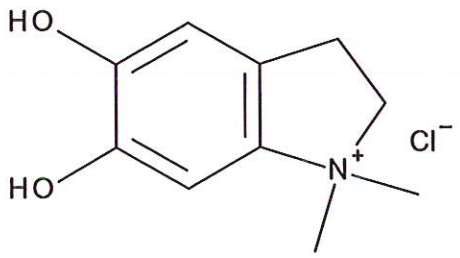
HARBOR BRANCH

FLORIDA ATLANTIC UNIVERSITY

HBOI-28	
	
DIHYDROXY-DIMETHYL-INDOLINIUM CHLORIDE	
$C_{10}H_{14}ClNO_2$	215.67
Dercitus sp.	
Kohmoto, McConnell, and Wright, 1988, *Experientia*. 44: 85-86	

☑ hplc (trace attached)

Method: Vydac C18 Protein and Peptide, 4.6 x 250mm, 10µ
flow 1 ml/min, detection: PDA: UV (extracted at 220 nm, black); ELSD (green dotted)
A: H_2O:CH_3CN (95:5, v/v, 0.1%TFA), B: CH_3CN (0.1% TFA)
t=0 min A:B (90:10, v/v), t=20 min (100%B) , t=28 in (100%B)

☑ LC-MS (spectrum attached) Does not ionize well

Method: Vydac C18 Protein and Peptide, 2.1x150 mm, flow 0.2 ml/min
A: H_2O (0.1% formic acid), B: CH_3CN (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) ☐ $CDCL_3$ ☑ CD_3OD (Methanol-d_4) ☐ $CDCl_3/CD_3OD$

☑ ^{13}C (150 MHz) ☐ $CDCL_3$ ☑ CD_3OD (Methanol-d_4) ☐ $CDCl_3/CD_3OD$

☑ solubility ☐ $CHCl_3$/MeOH (9:1) ☑ MeOH ☐ DMSO

☑ estimated purity _>90_%

☑ sample weight _19.6_mg

For further information contact:
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awrigh33@hboi.fau.edu, 772-242-2459

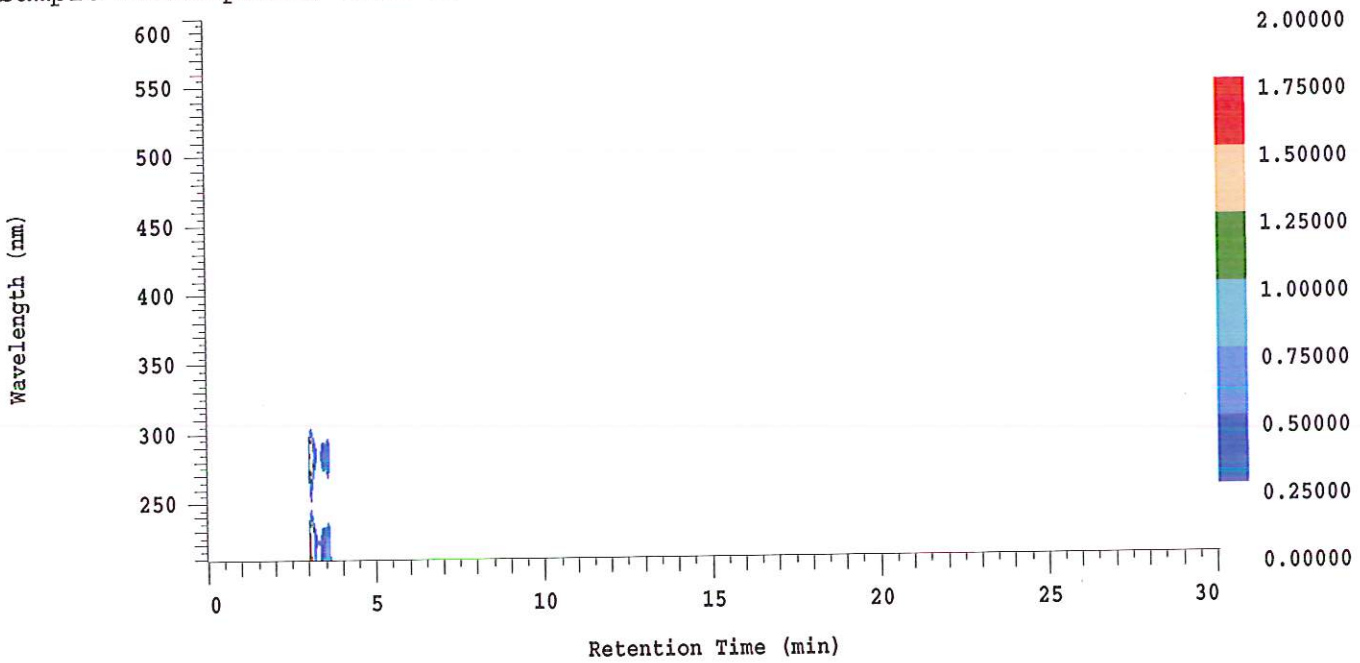
Date: 1/28/13

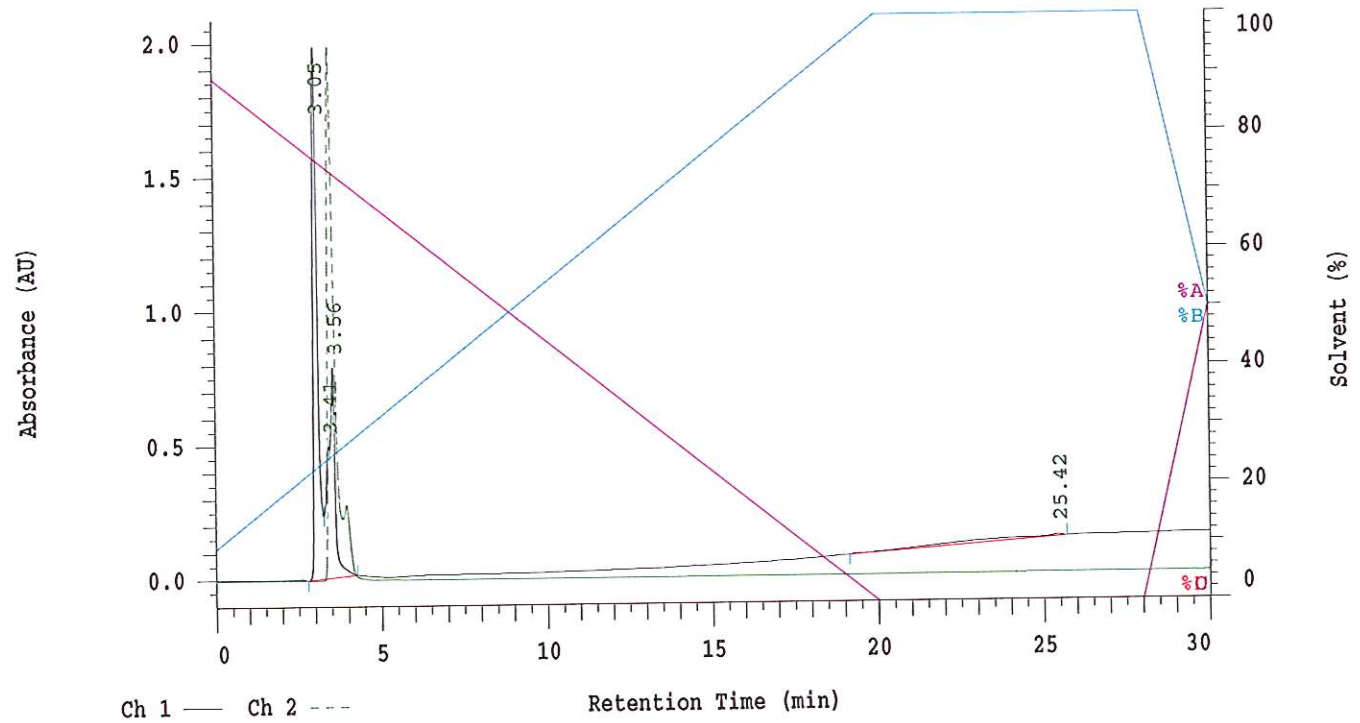
D-2000 Elite HPLC System Manager Report

Analyzed: 01/24/2013 07:57 PM Reported: 01/25/2013 08:02 AM

Sample Name: HBOI-28

Sample Description: HBOI-28





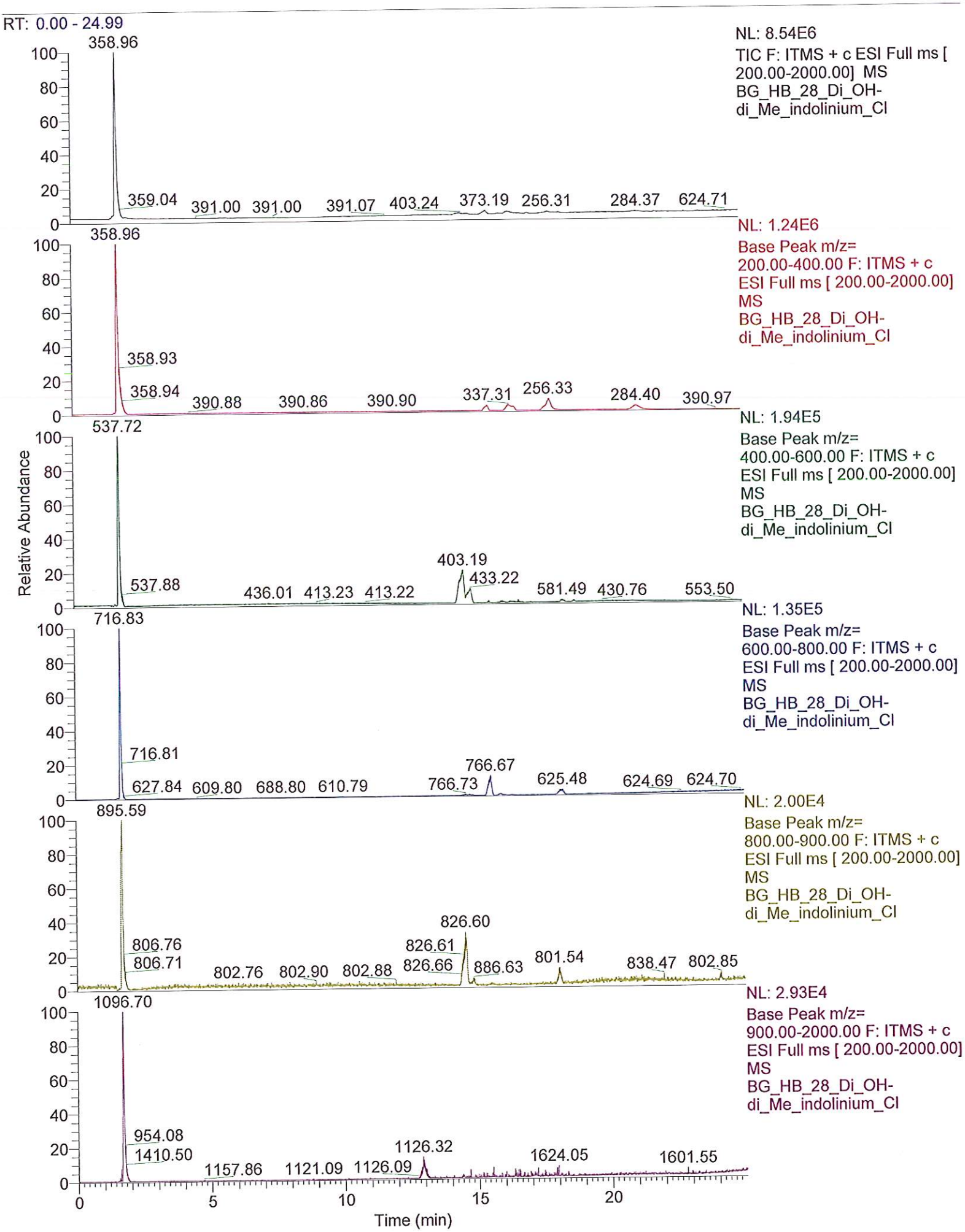
Ch 1 —— Ch 2 ---

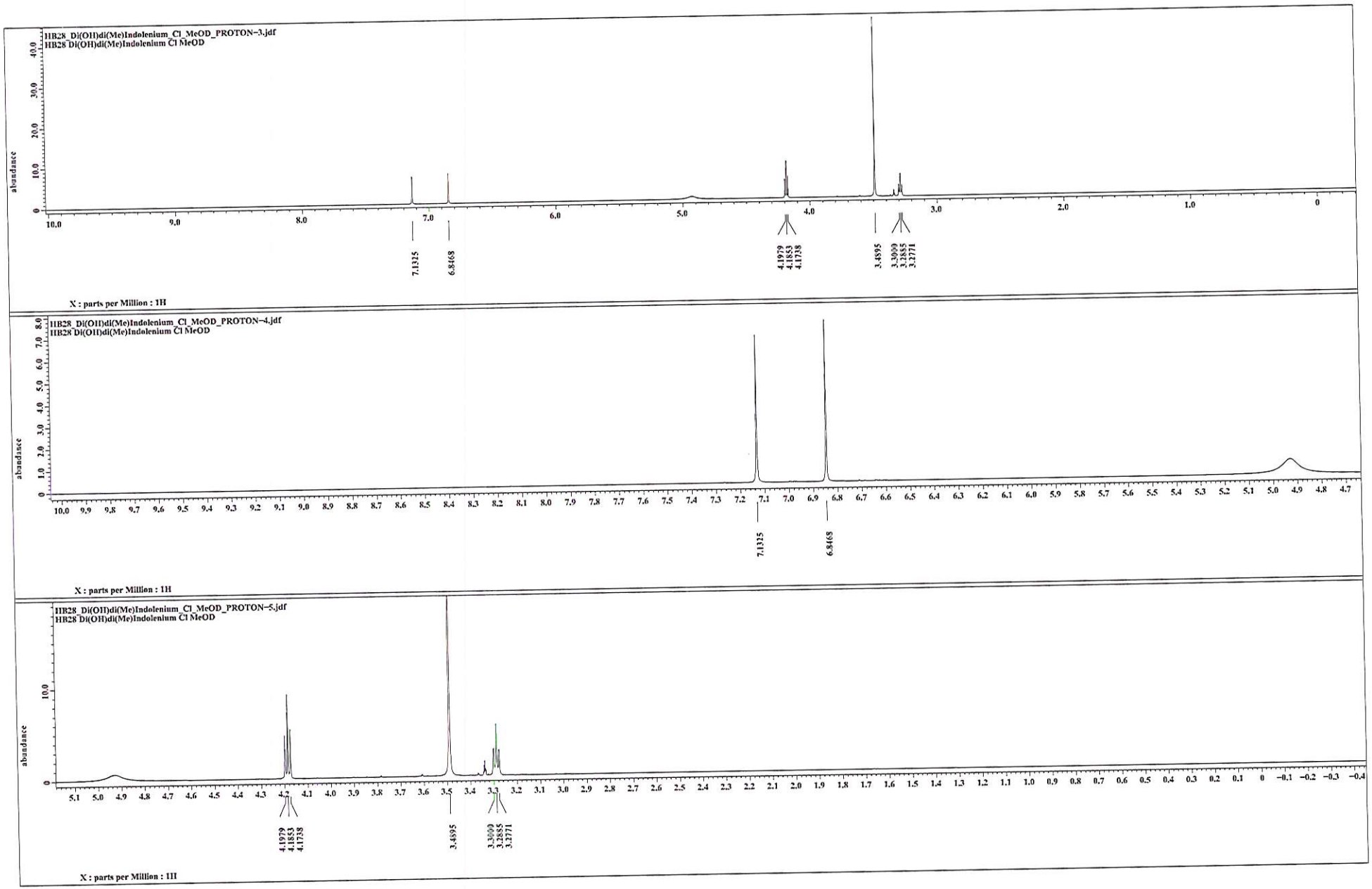
Acquisition Method: NIH_30min_UV220_wELSD_TFA

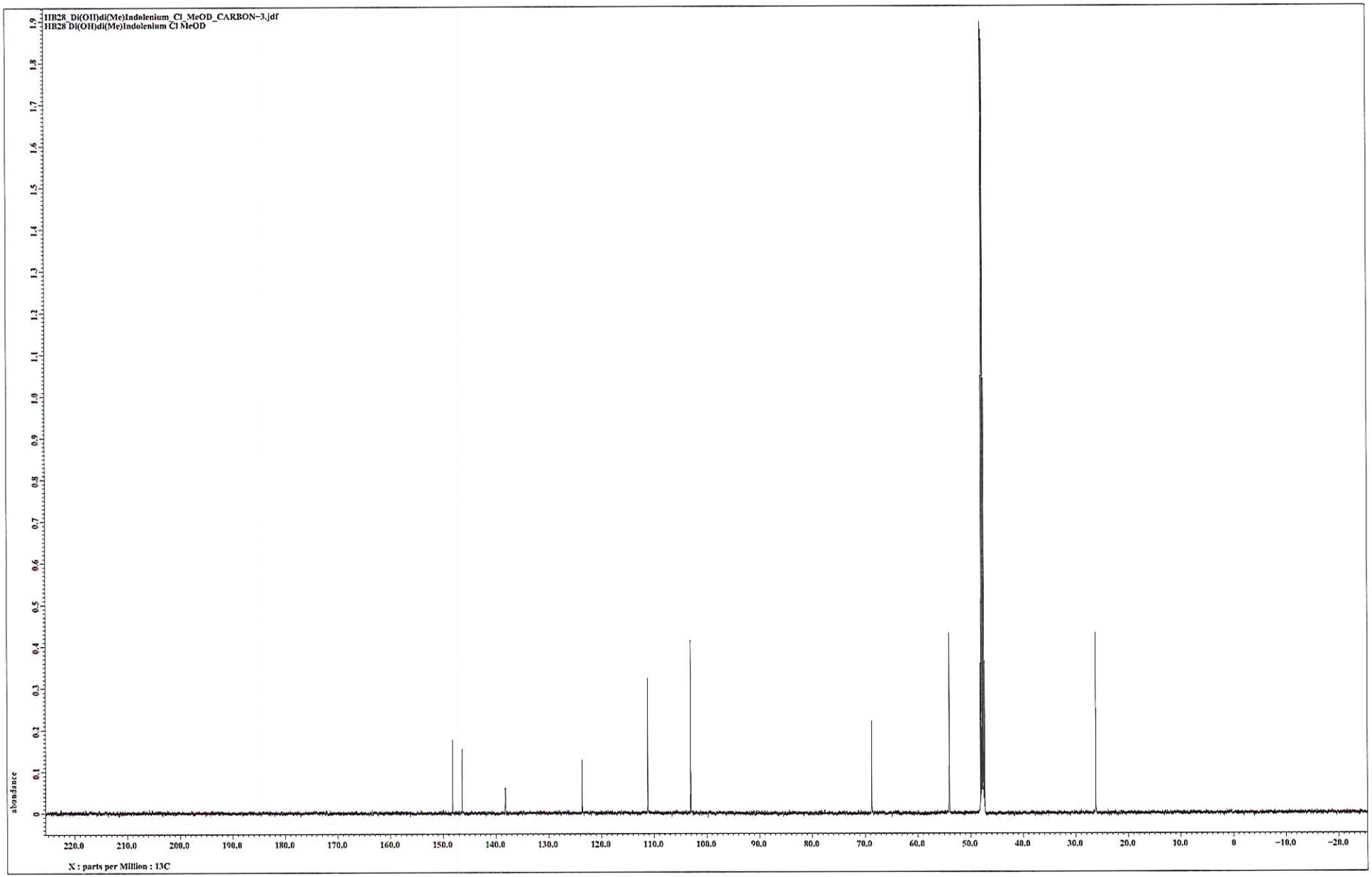
Column Type: Vydac C18

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: 8.54E6
TIC F: ITMS + c ESI Full ms [200.00-2000.00] MS BG_HB_28_Di_OH-di_Me_indolinium_Cl
358.96
359.04 391.00 391.00 391.07 403.24 373.19 256.31 284.37 624.71
NL: 1.24E6
Base Peak m/z= 200.00-400.00 F: ITMS + c ESI Full ms [200.00-2000.00] MS BG_HB_28_Di_OH-di_Me_indolinium_Cl
358.96
358.93 358.94 390.88 390.86 390.90 337.31 256.33 284.40 390.97
NL: 1.94E5
Base Peak m/z= 400.00-600.00 F: ITMS + c ESI Full ms [200.00-2000.00] MS BG_HB_28_Di_OH-di_Me_indolinium_Cl
537.72
537.88 436.01 413.23 413.22 403.19 433.22 581.49 430.76 553.50
NL: 1.35E5
Base Peak m/z= 600.00-800.00 F: ITMS + c ESI Full ms [200.00-2000.00] MS BG_HB_28_Di_OH-di_Me_indolinium_Cl
716.83
716.81 627.84 609.80 688.80 610.79 766.67 766.73 625.48 624.69 624.70
NL: 2.00E4
Base Peak m/z= 800.00-900.00 F: ITMS + c ESI Full ms [200.00-2000.00] MS BG_HB_28_Di_OH-di_Me_indolinium_Cl
895.59
806.76 806.71 802.76 802.90 802.88 826.60 826.61 826.66 886.63 801.54 838.47 802.85
NL: 2.93E4
Base Peak m/z= 900.00-2000.00 F: ITMS + c ESI Full ms [200.00-2000.00] MS BG_HB_28_Di_OH-di_Me_indolinium_Cl
1096.70
954.08 1410.50 1157.86 1121.09 1126.09 1126.32 1624.05 1601.55
Relative Abundance
Time (min)


HB28_Di(OH)di(Me)Indolenium_Cl_MeOD_PROTON-3.jdf
HB28 Di(OH)di(Me)Indolenium Cl MeOD
abundance
7.1325
6.8468
4.1979
4.1853
4.1738
3.4895
3.3009
3.2885
3.2771
X : parts per Million : 1H
HB28_Di(OH)di(Me)Indolenium_Cl_MeOD_PROTON-4.jdf
HB28 Di(OH)di(Me)Indolenium Cl MeOD
abundance
7.1325
6.8468
X : parts per Million : 1H
HB28_Di(OH)di(Me)Indolenium_Cl_MeOD_PROTON-5.jdf
HB28 Di(OH)di(Me)Indolenium Cl MeOD
abundance
4.1979
4.1853
4.1738
3.4895
3.3009
3.2885
3.2771
X : parts per Million : 1H


HB28_Di(OH)di(Me)Indolenium_Cl_MeOD_CARBON-3.jdf
HB28 Di(OH)di(Me)Indolenium Cl MeOD
abundance
X : parts per Million : 13C