

THE COMBI-TARGETING CONCEPT: SYNTHESIS OF STABLE
NITROSOUREAS DESIGNED TO INHIBIT THE EPIDERMAL
GROWTH FACTOR RECEPTOR (EGFR)

*Juozas Domarkas, Fabienne Dudouit, Christopher Williams, Qiu Qiyu, Ranjita Banerjee,
Fouad Brahimi, Bertrand Jacques Jean-Claude**

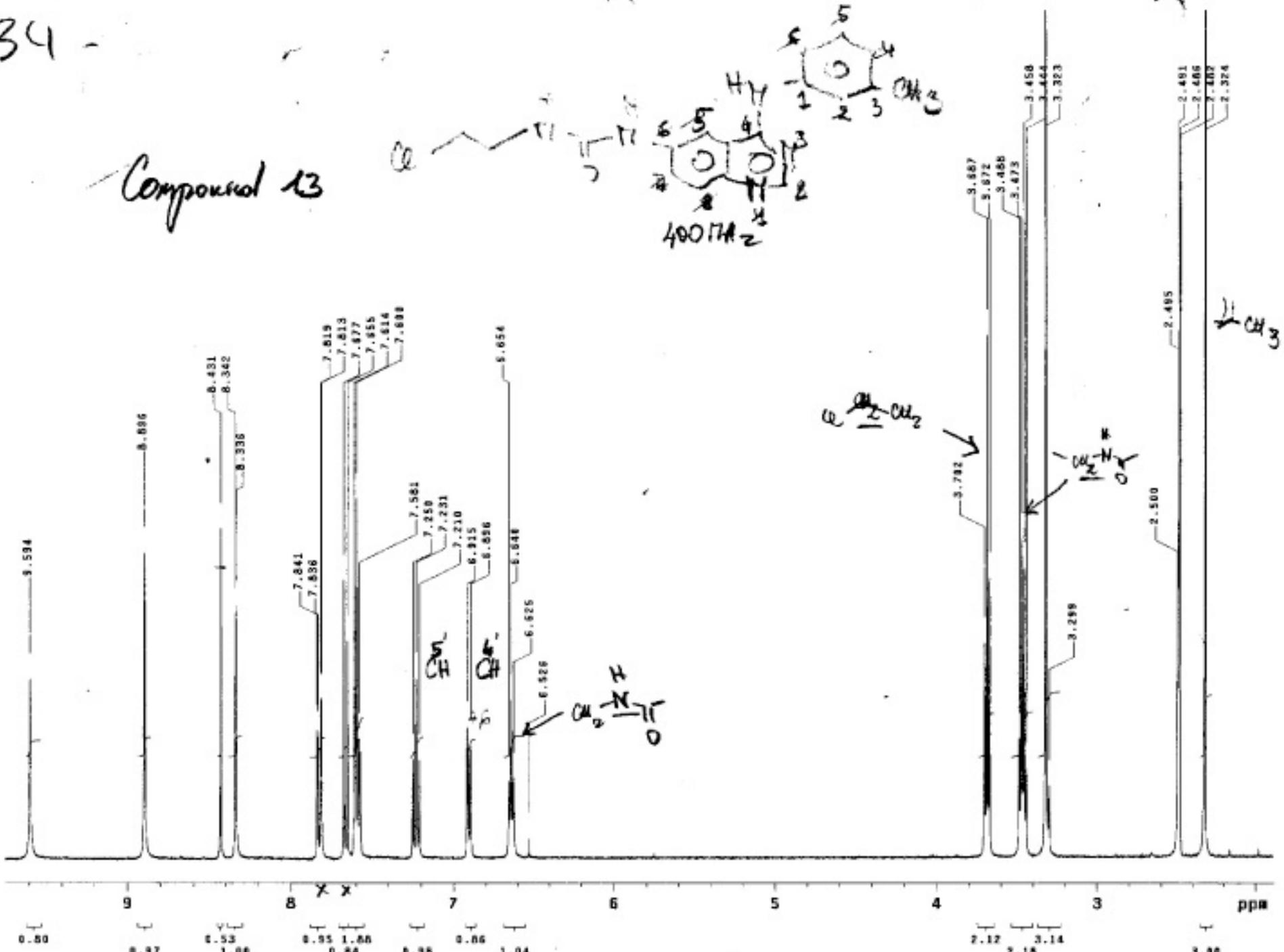
*Cancer Drug Research Laboratory, Department of Medicine, Division of Medical Oncology,
McGill University Health Center/Royal Victoria Hospital, Montreal, H3A1A1, Quebec, Canada*

SUPPORTING INFORMATION:

^1H NMR spectra.....	S2
^{13}C NMR spectra.....	S14
MS spectra	S26
HRMS elemental composition.....	S38
HPLC chromatograms	S50

A34

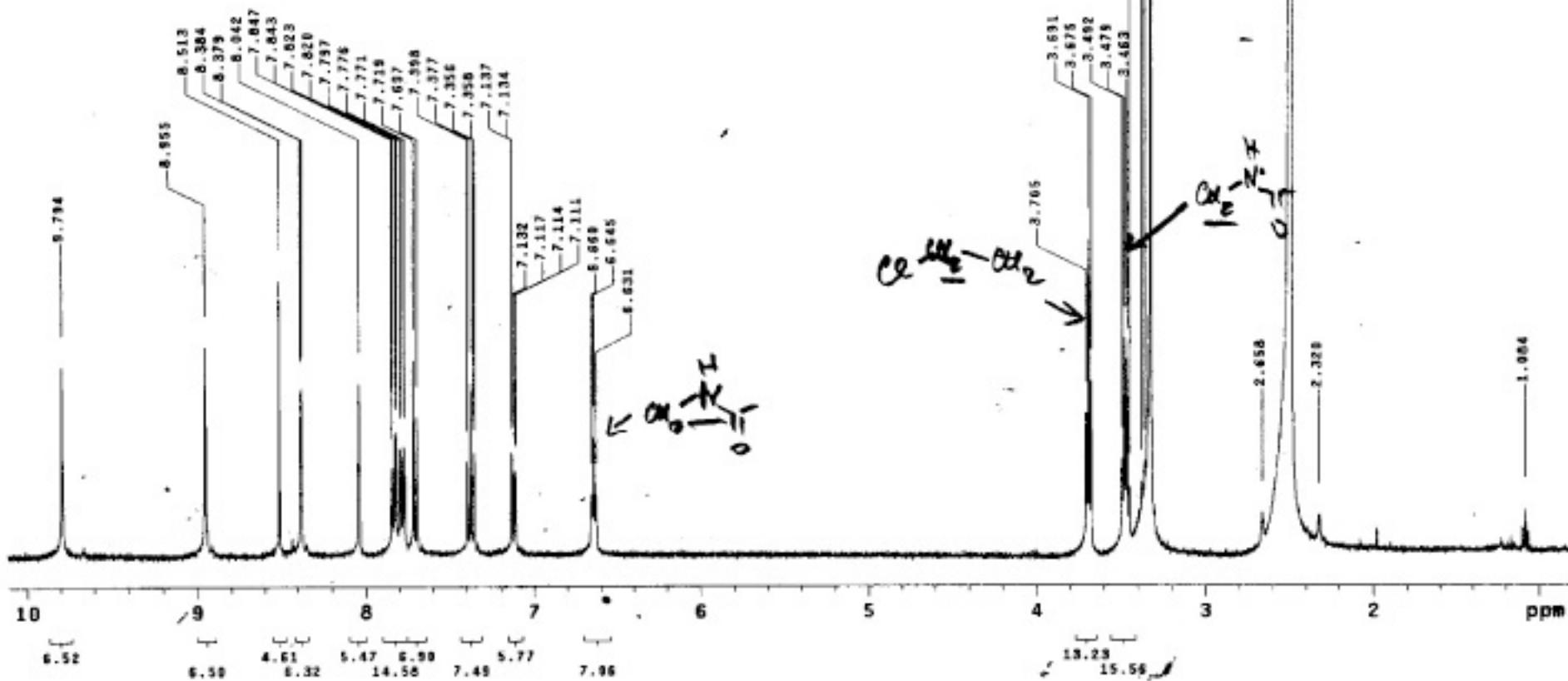
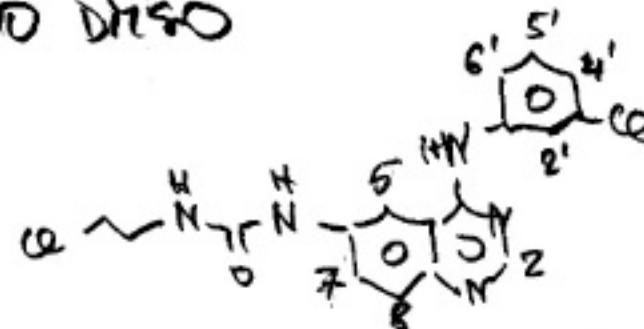
Compound 13



S2

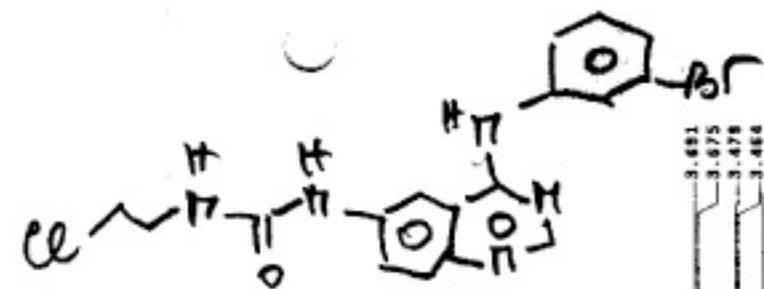
TDA36_col1 400 MHz

#14

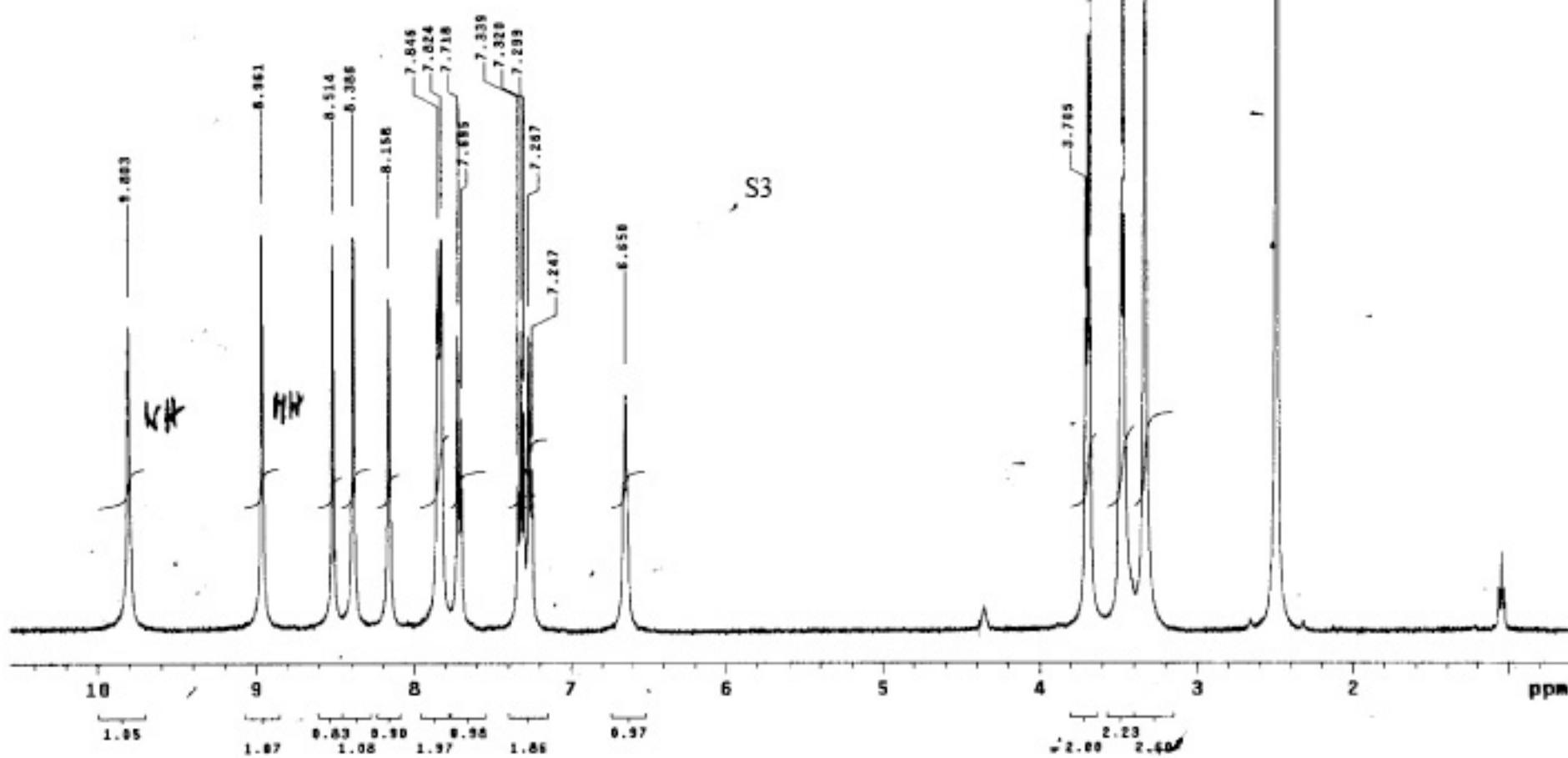


5DA¹³C rec

A40 #15



WCO



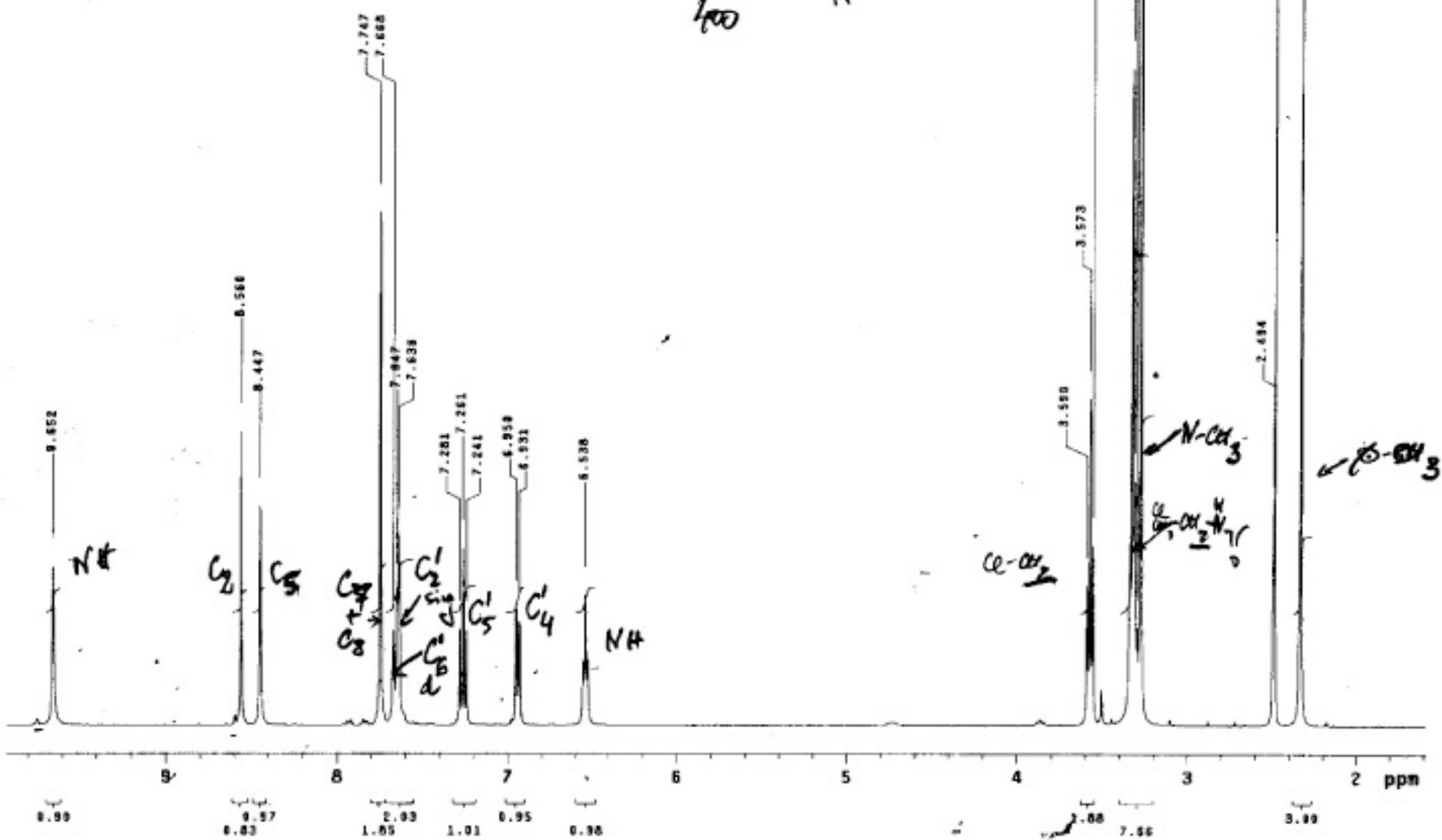
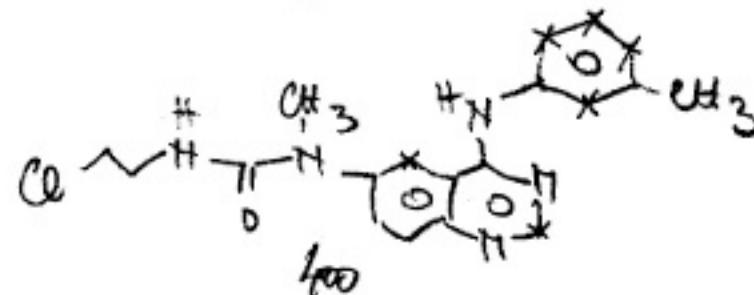
S4

JDA 42

400 Hz

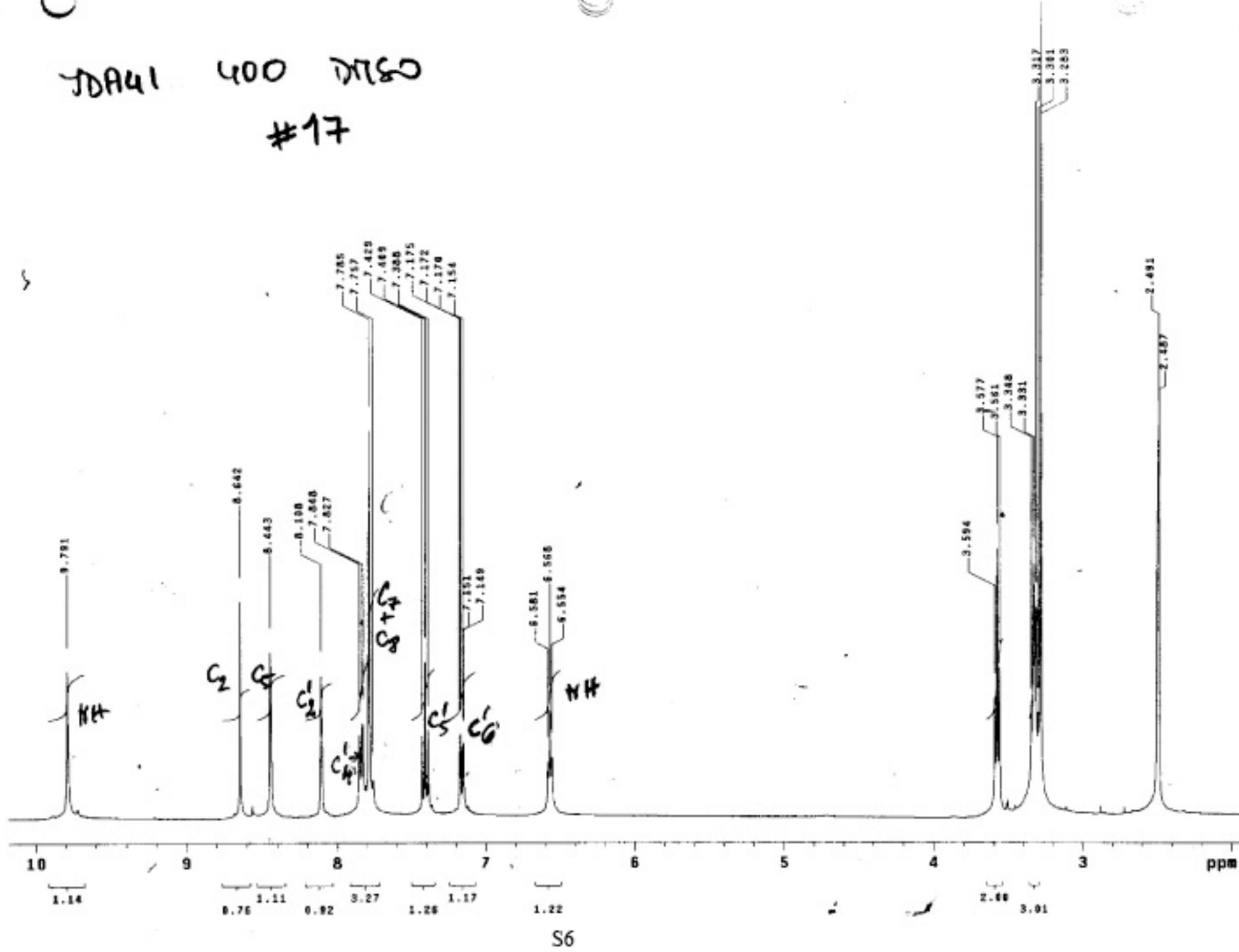
JDA 42

16



JDA41 400 MHz

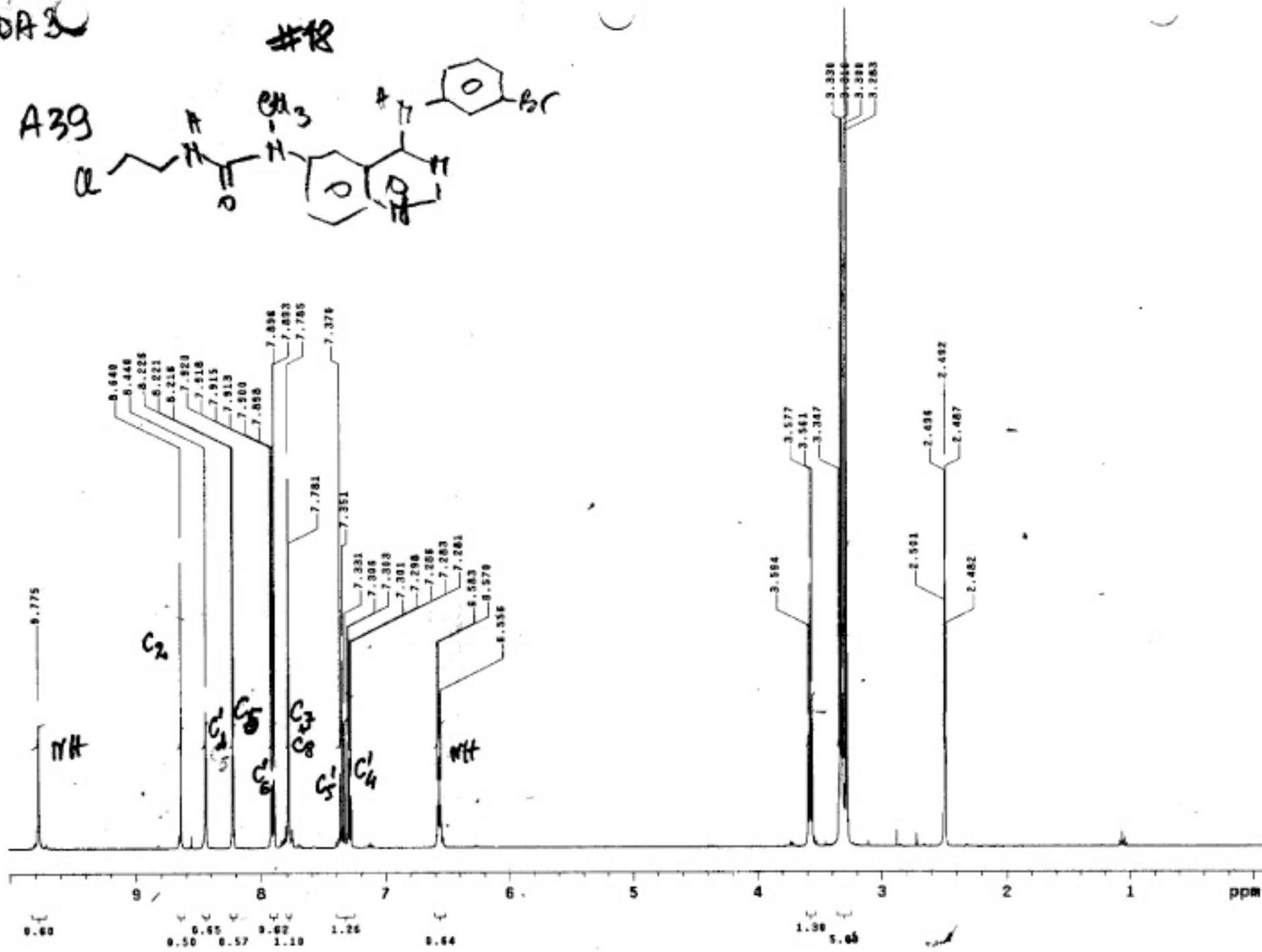
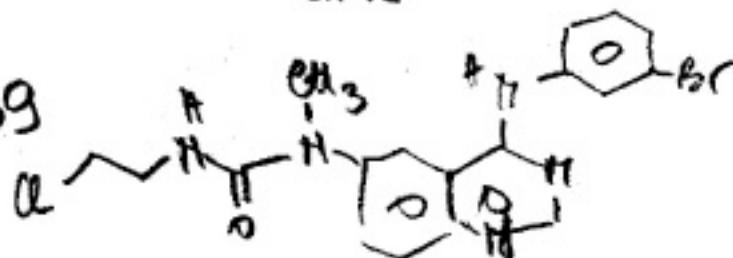
#17



四百三

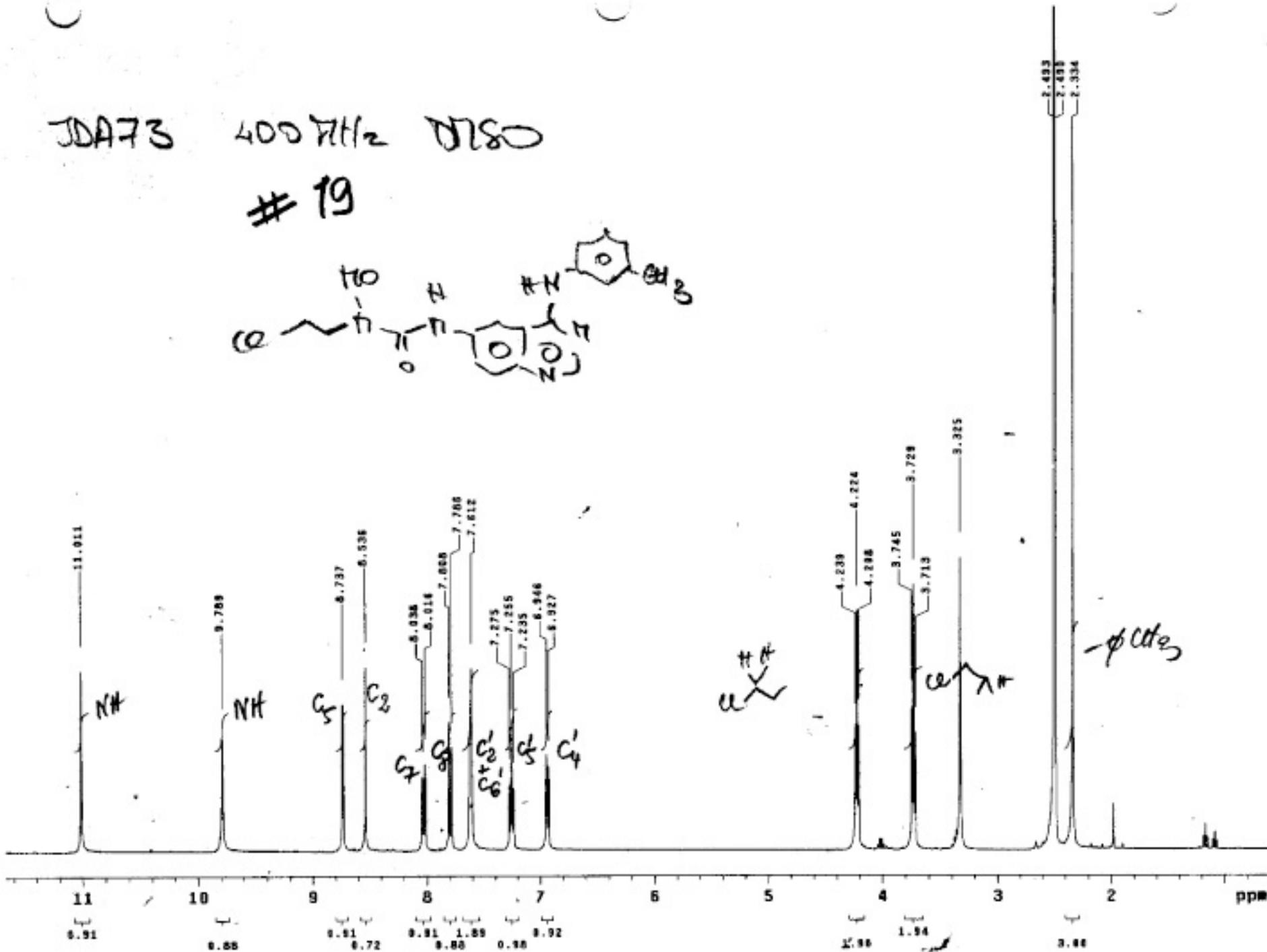
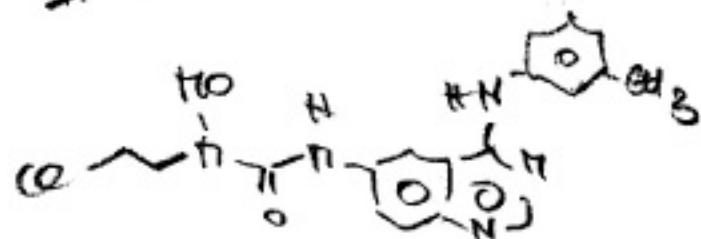
井18

A39



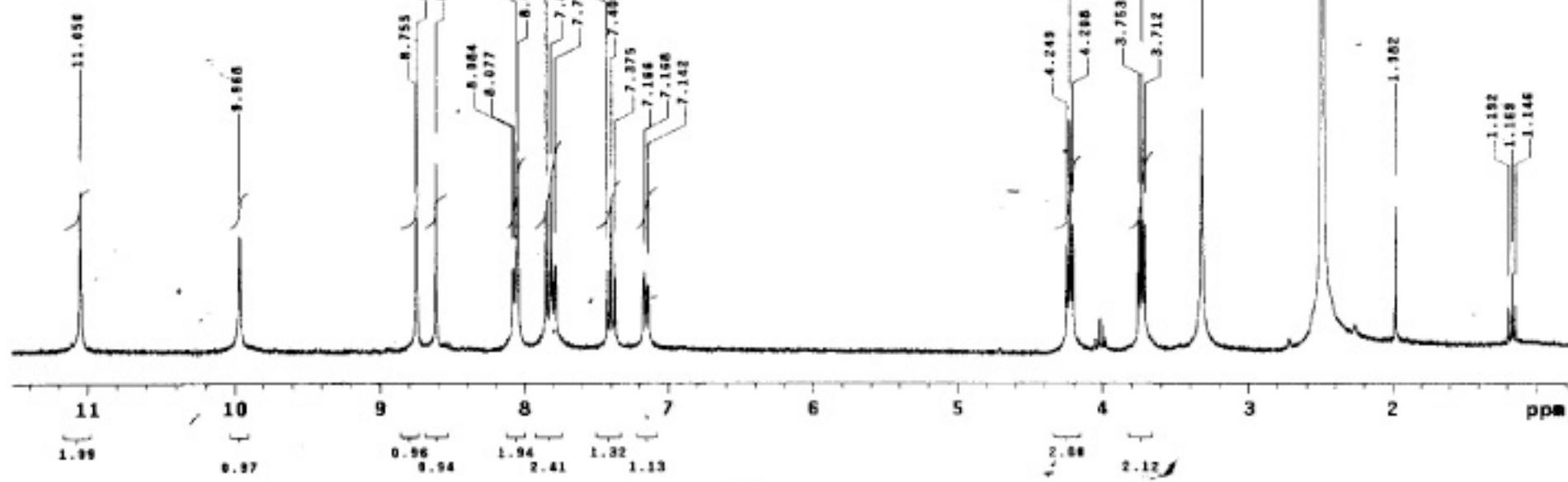
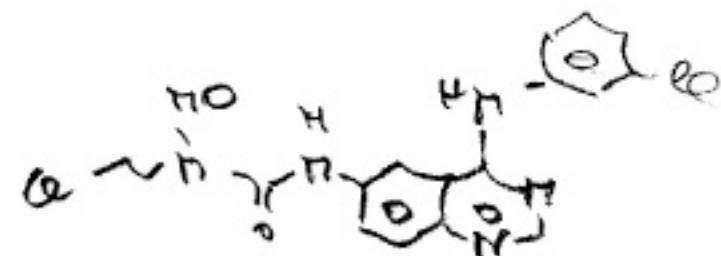
JDA73 400 MHz 8780

19



20065 11150 300 MHz

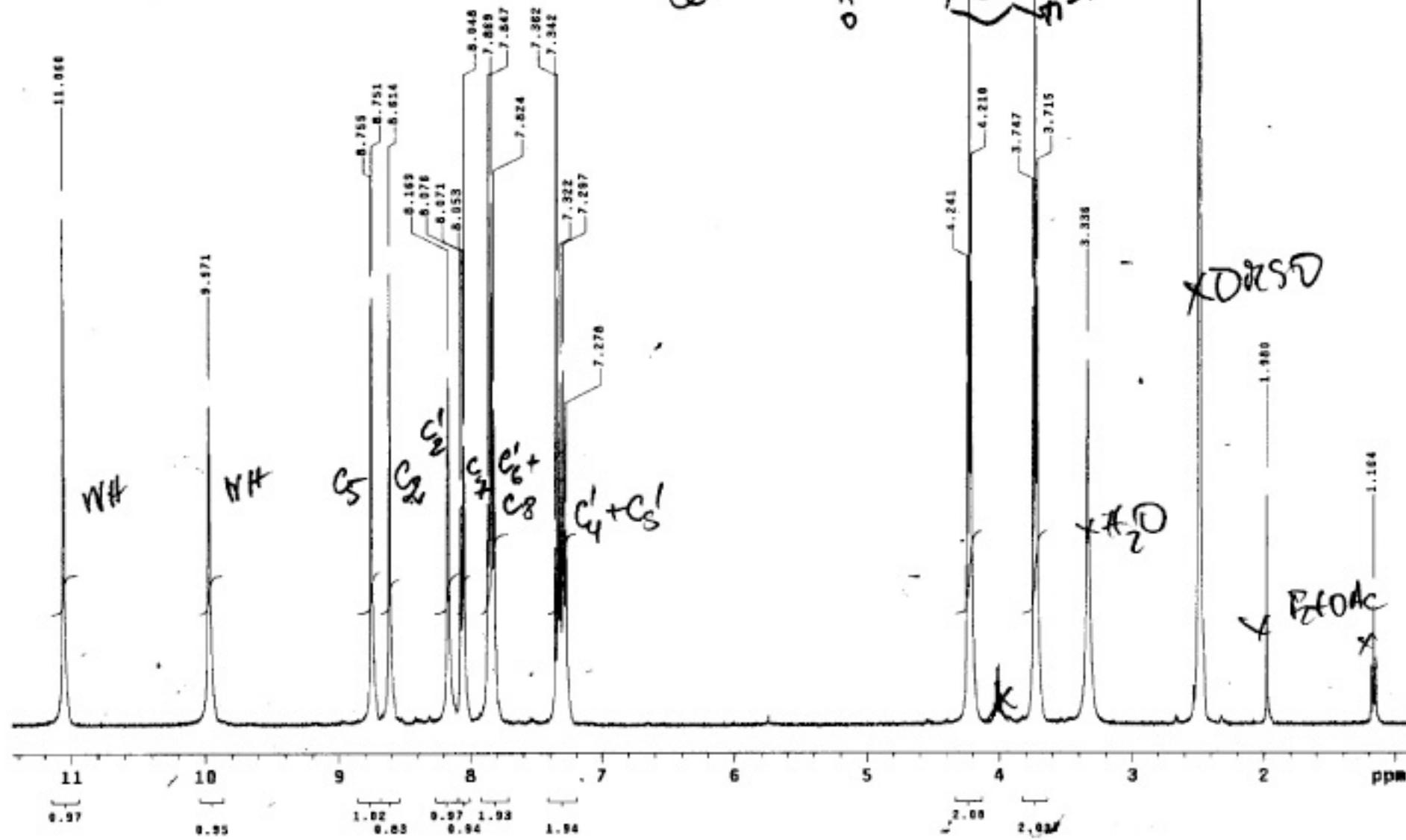
#20



TDAc

A66

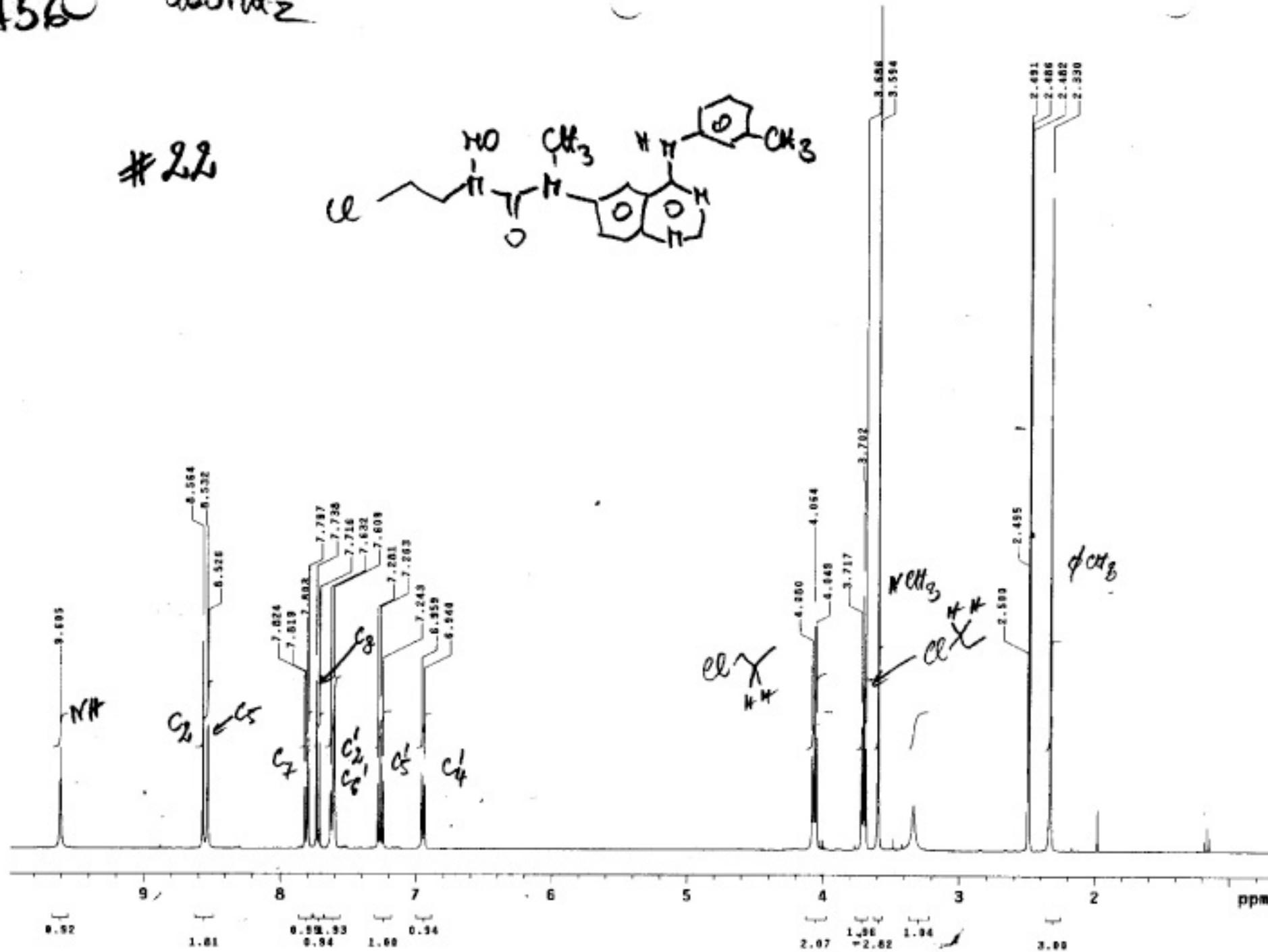
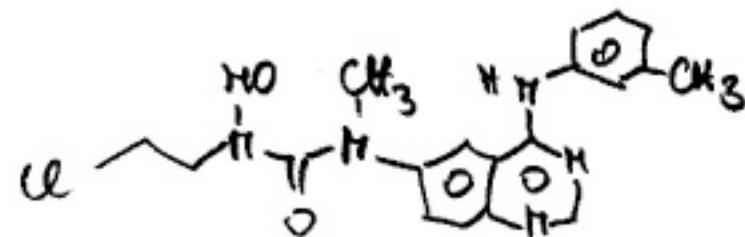
#21



—A560

Goodwill

井 22

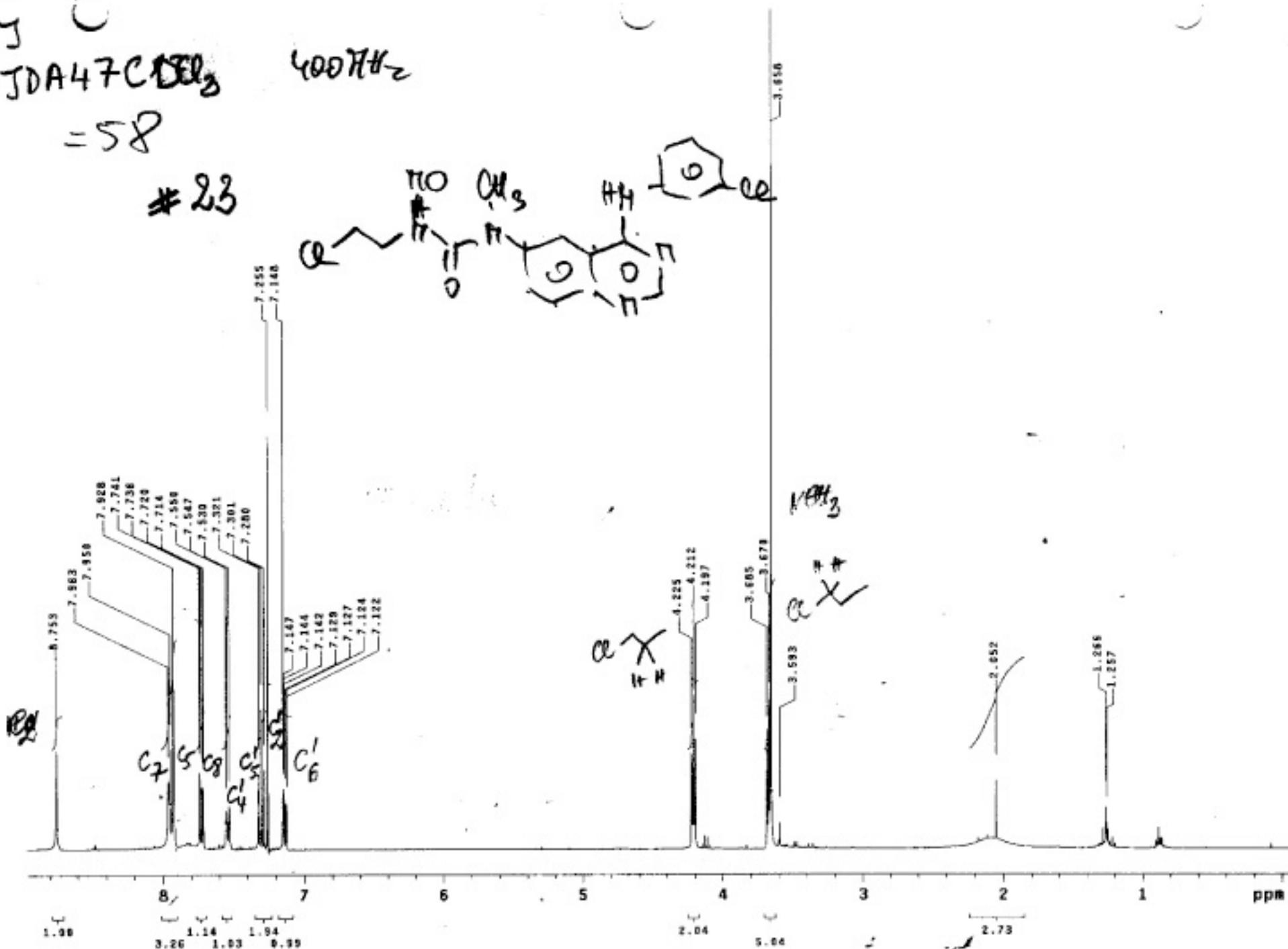
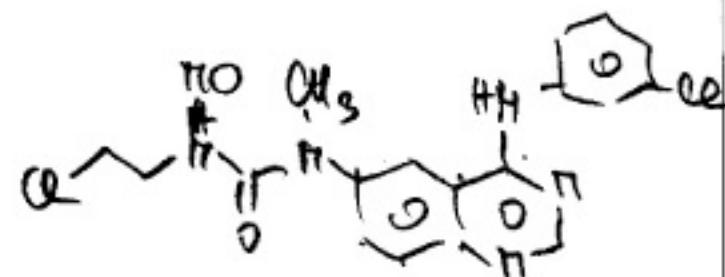


J
JDA47 CDCl₃

400 Hz

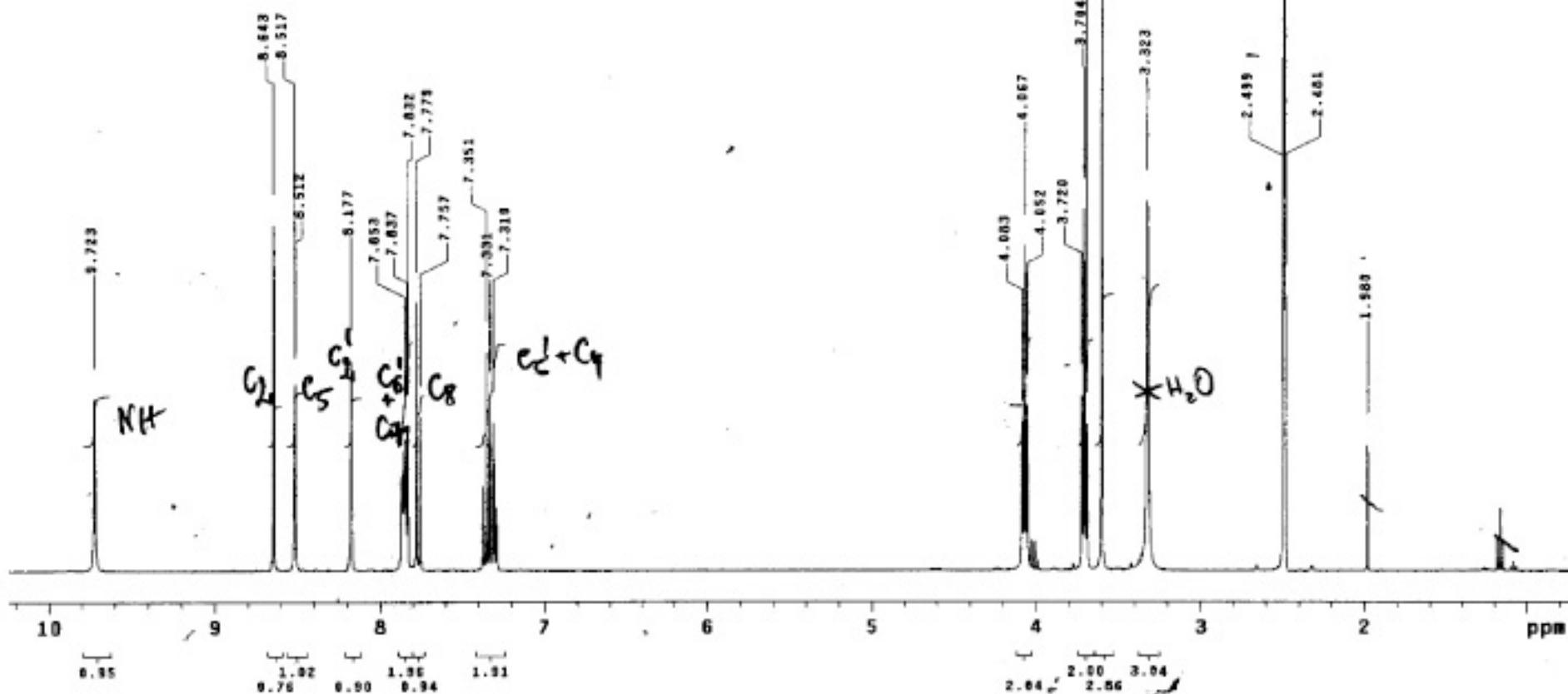
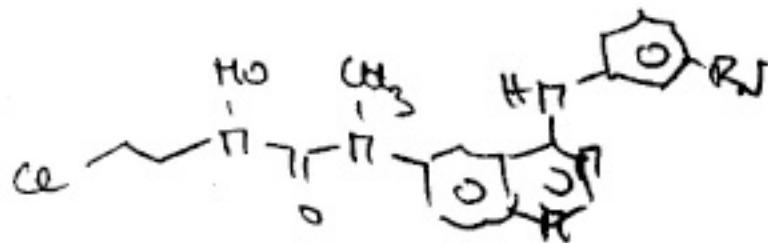
= 58

* 23



A52-2 DR280 400

#24

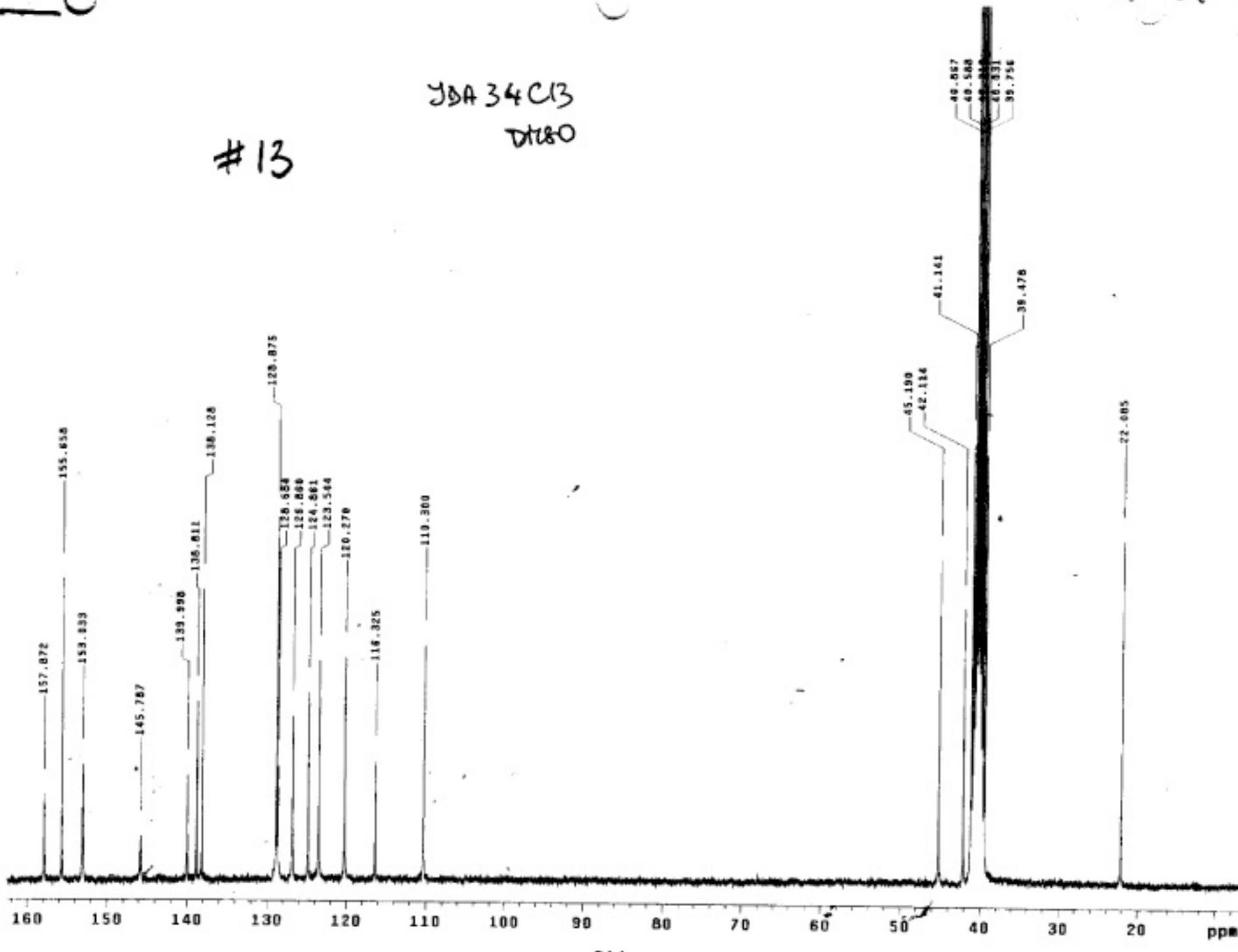


05 04 04

JDA 34C13

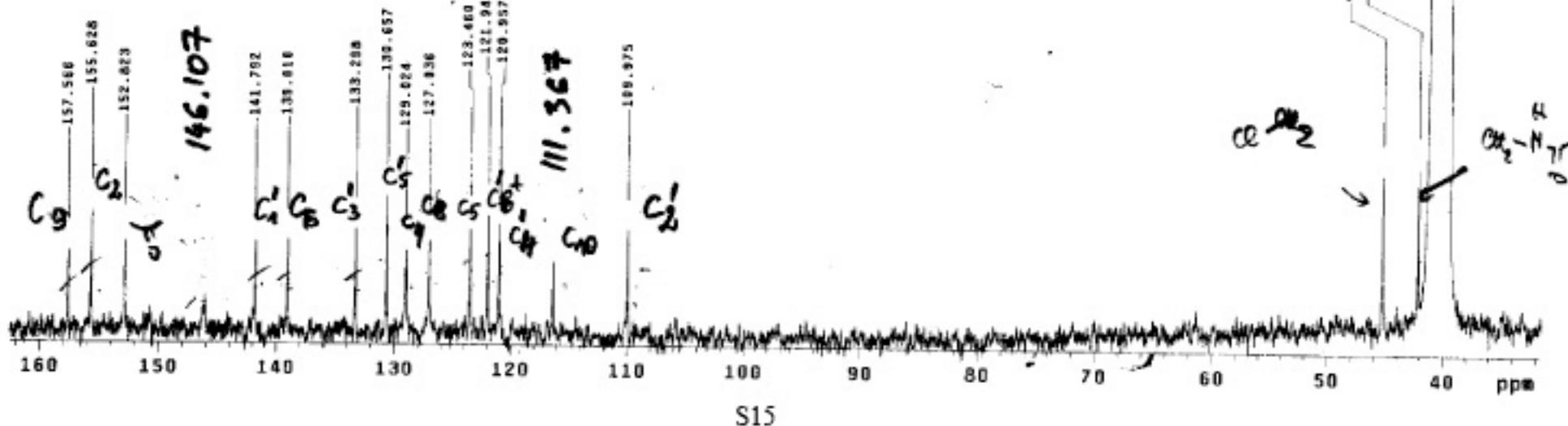
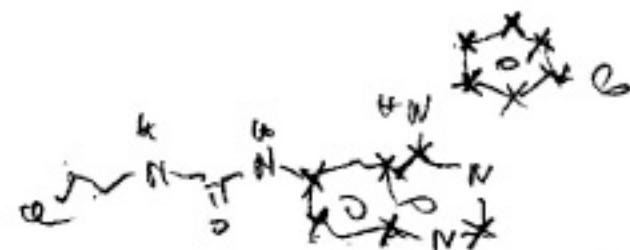
D₂O

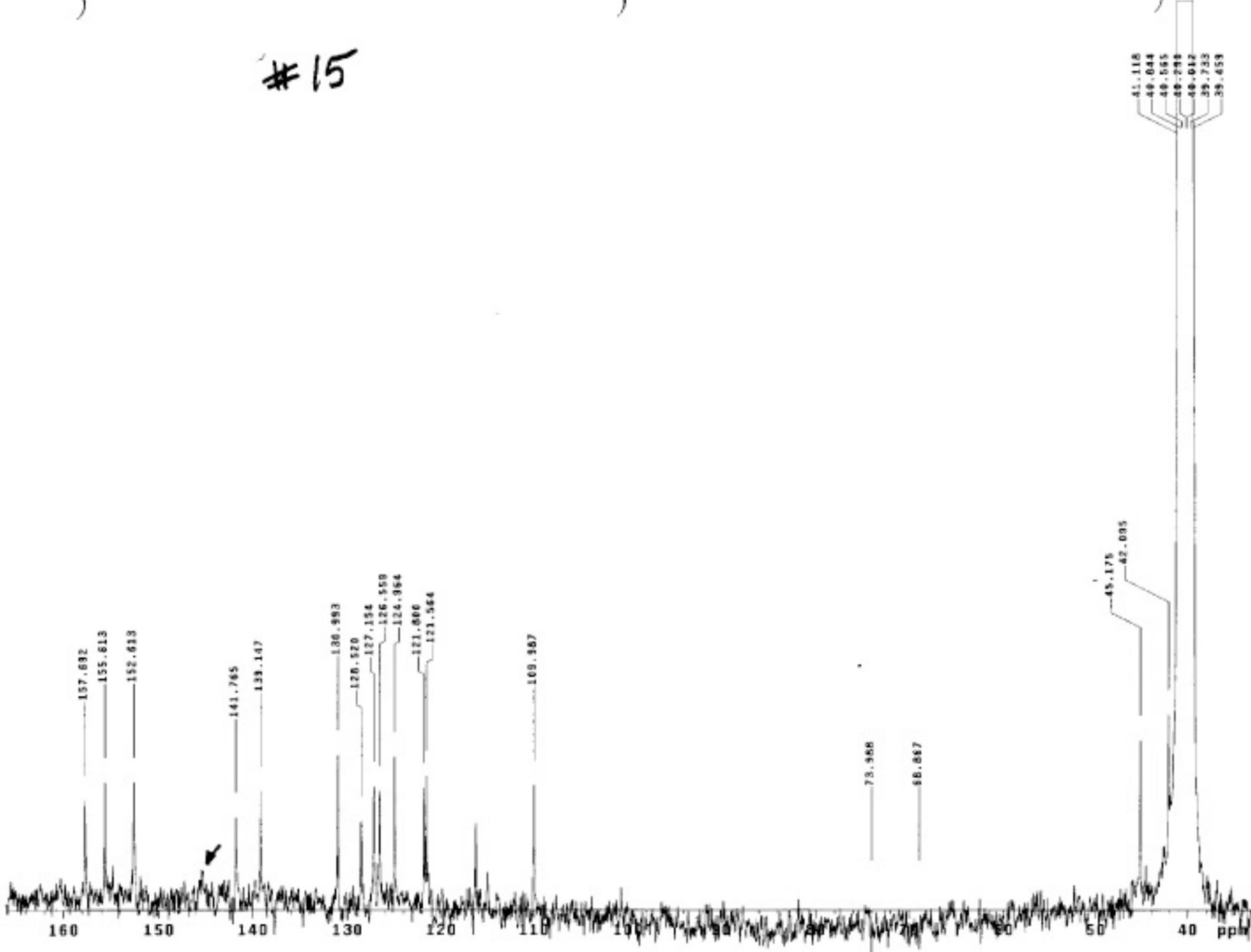
#13



TDR36. col1 C13 DMSO 300

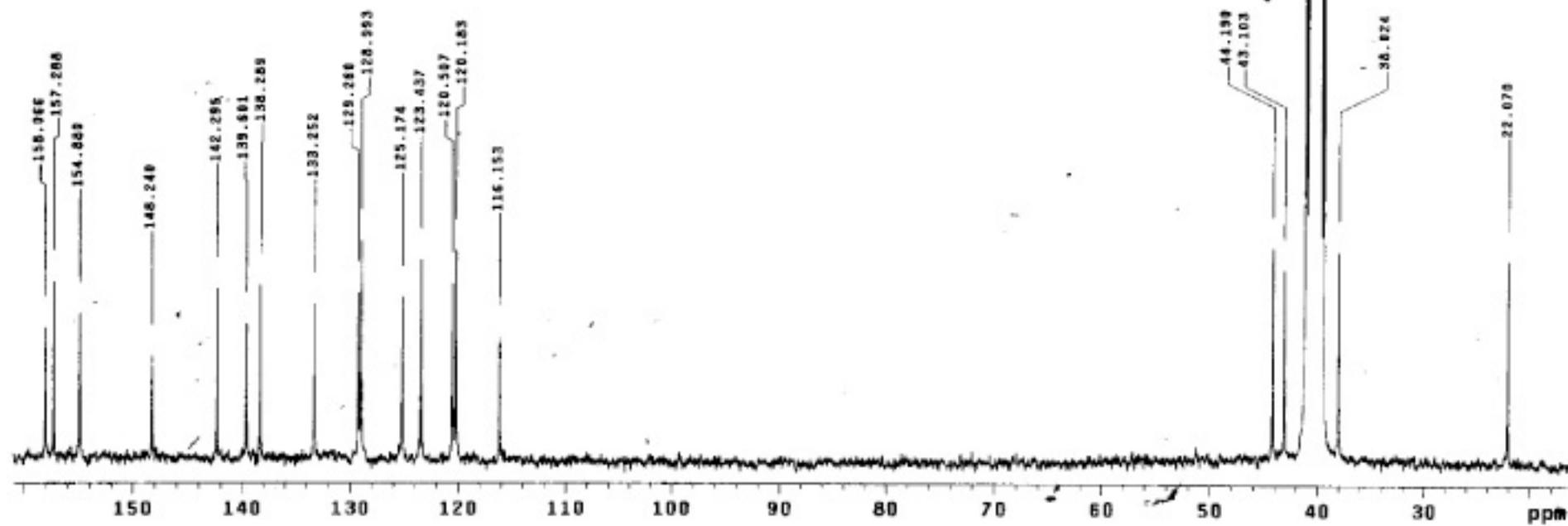
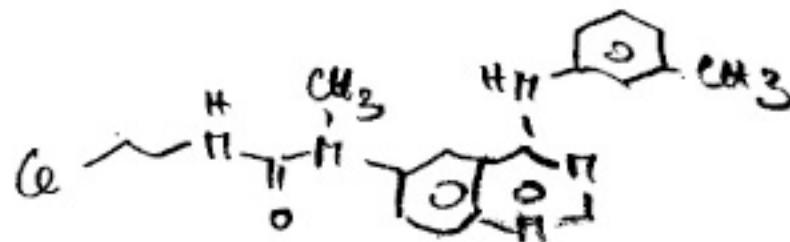
#14





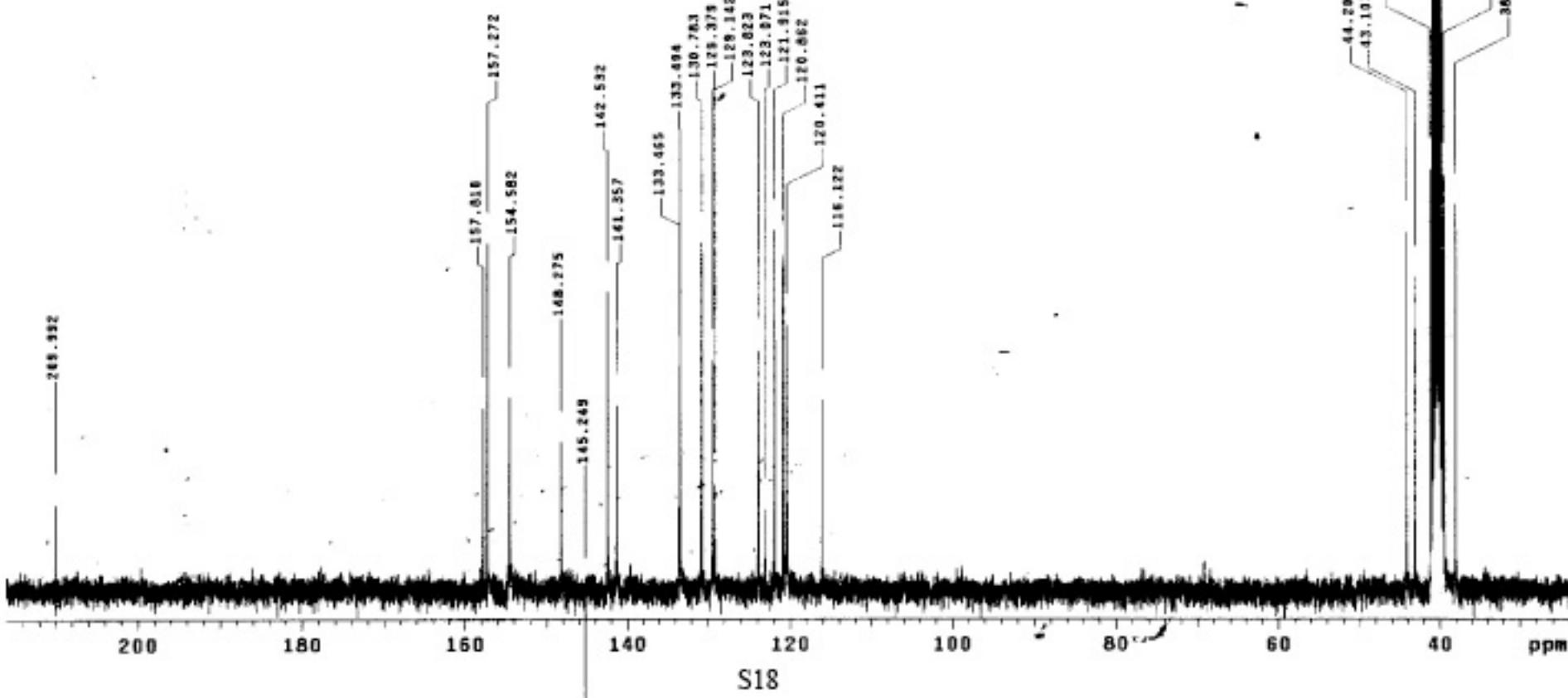
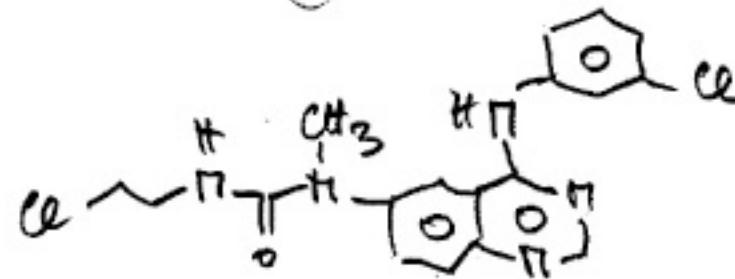
A92C13
J0A92C13

#16



JDR41C13

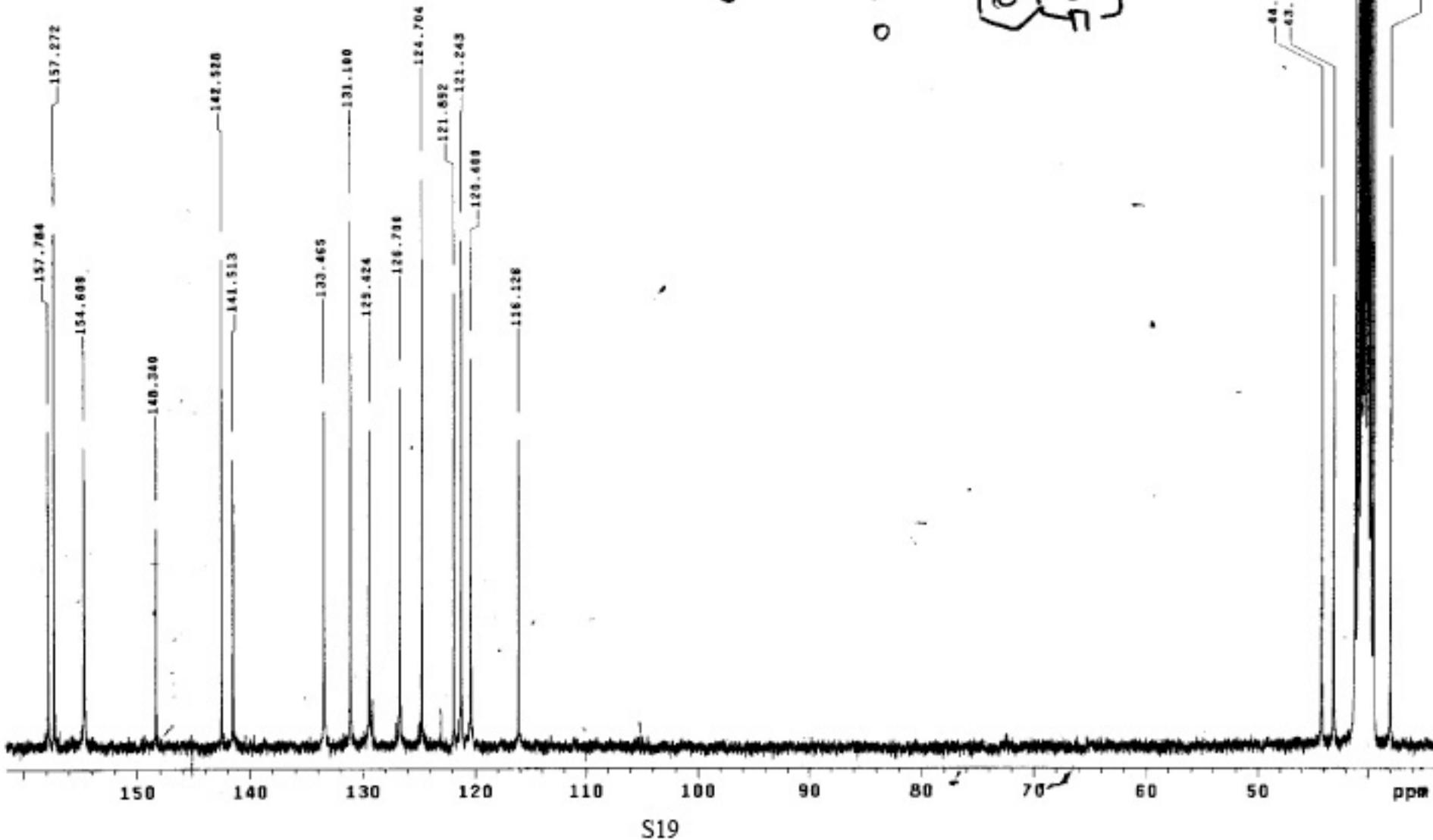
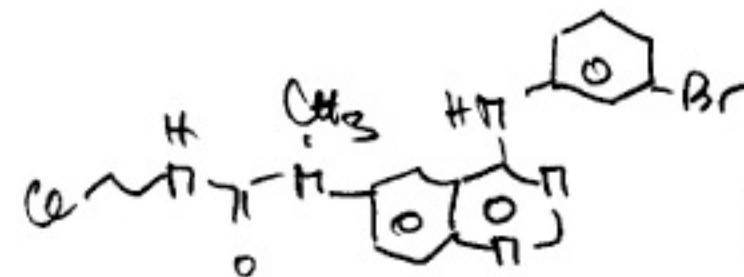
#17



JDA 3-2C13

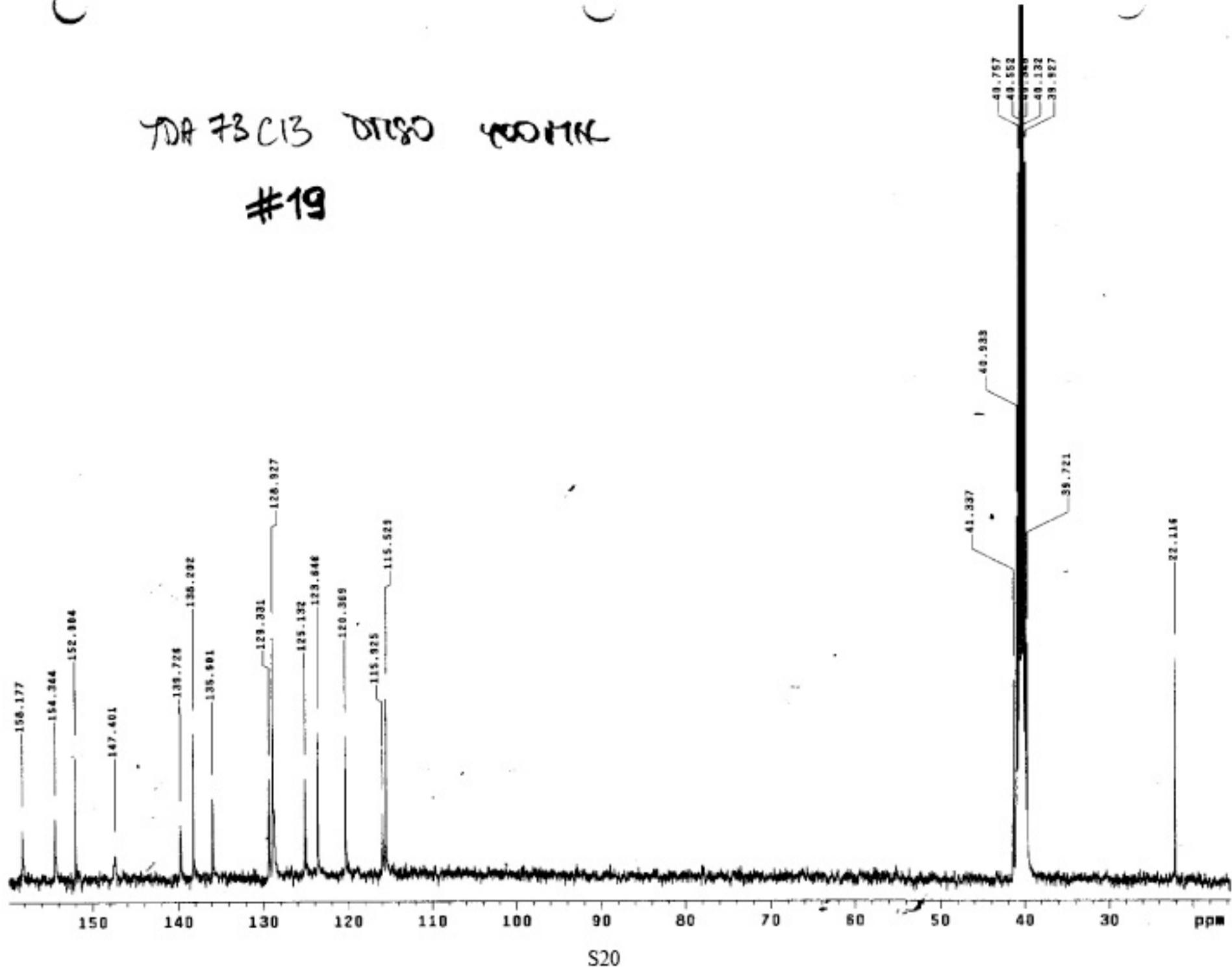
A39-2C13

#18



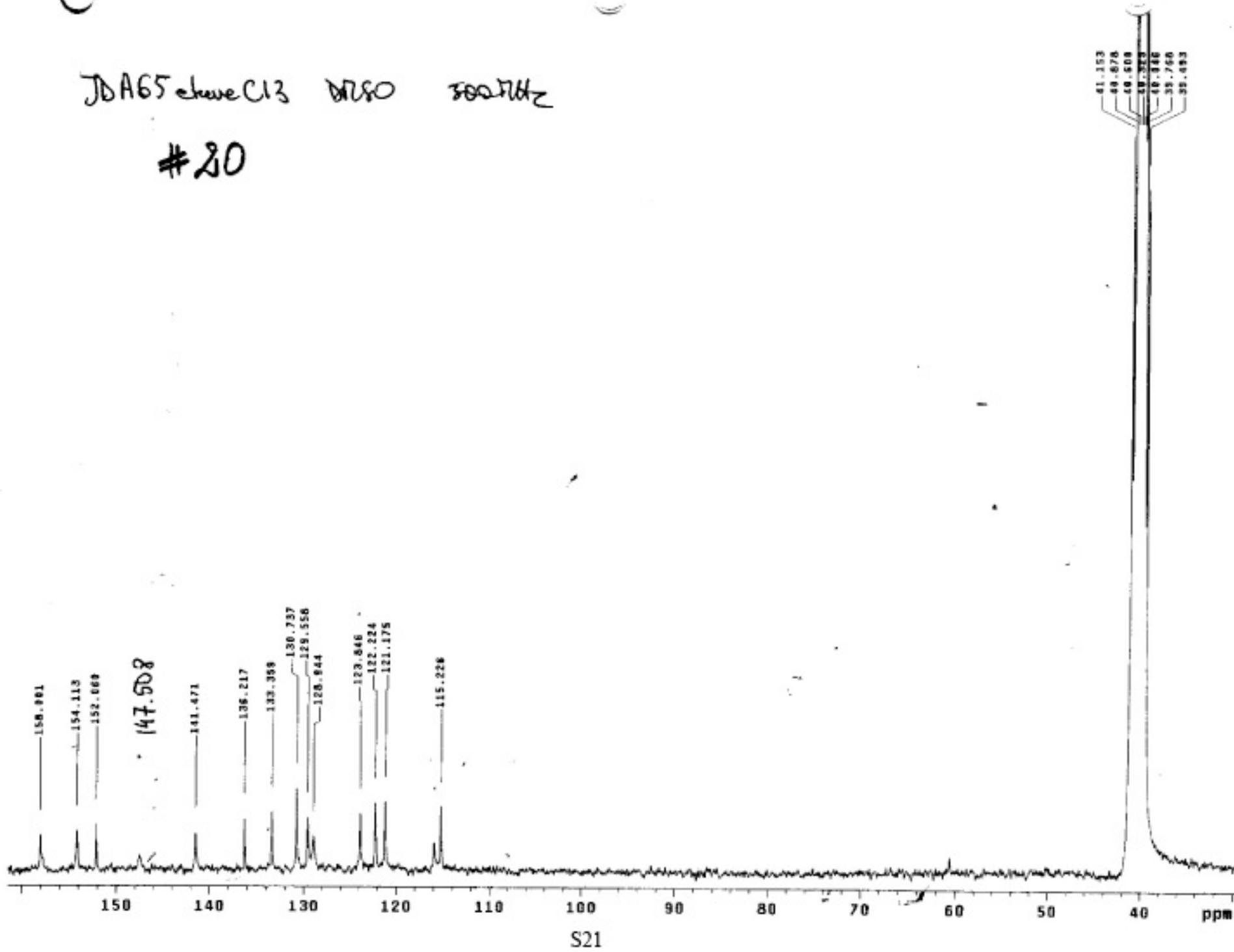
TDA 73C13 D1180 400MHz

#19



JD A65 chive C13 8780 300MHz

#20



JD066 #21 C13, 09/03/06

Pulse Sequence: s2pul

Solvent: DMSO

Ambient temperature

Mercury-300 "m300"

Relax. delay 3.000 sec

Pulse 45.9 degrees

Acq. time 1.815 sec

Width 18761.7 Hz

2608 repetitions

DBSERVI C13, 75.4492276 MHz

DECOUPLED H1, 300.0578578 MHz

Power 44 dB

continuously on

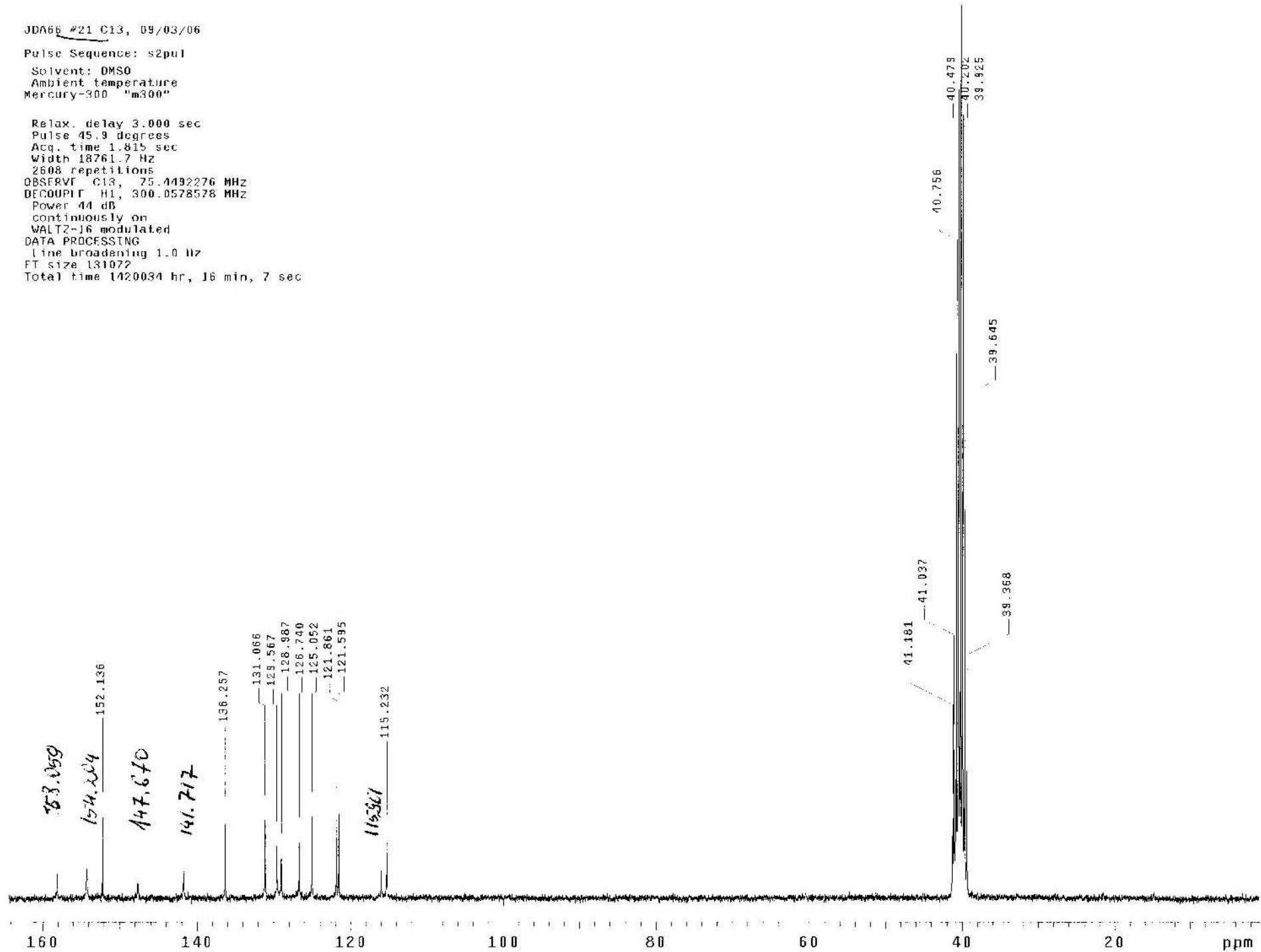
WALTZ-16 modulated

DATA PROCESSING

line broadening 1.0 Hz

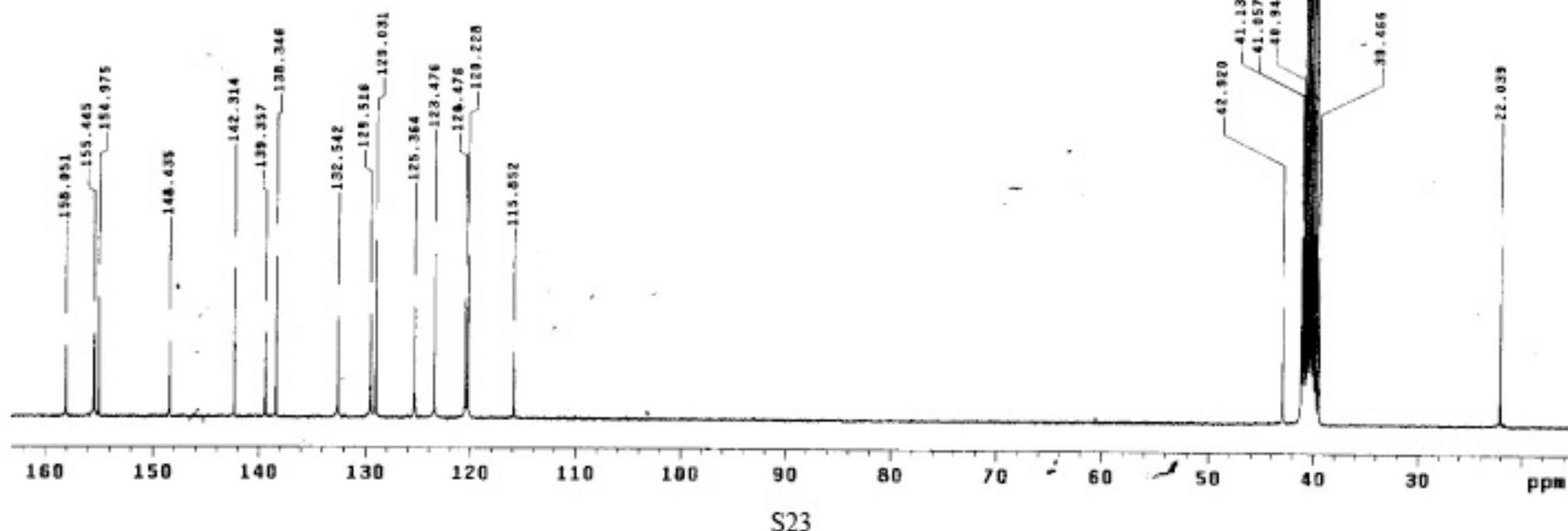
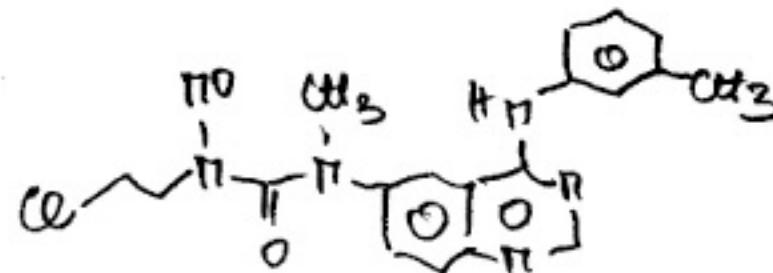
FT size 131072

Total time 1420034 hr, 16 min, 7 sec



ASG C13

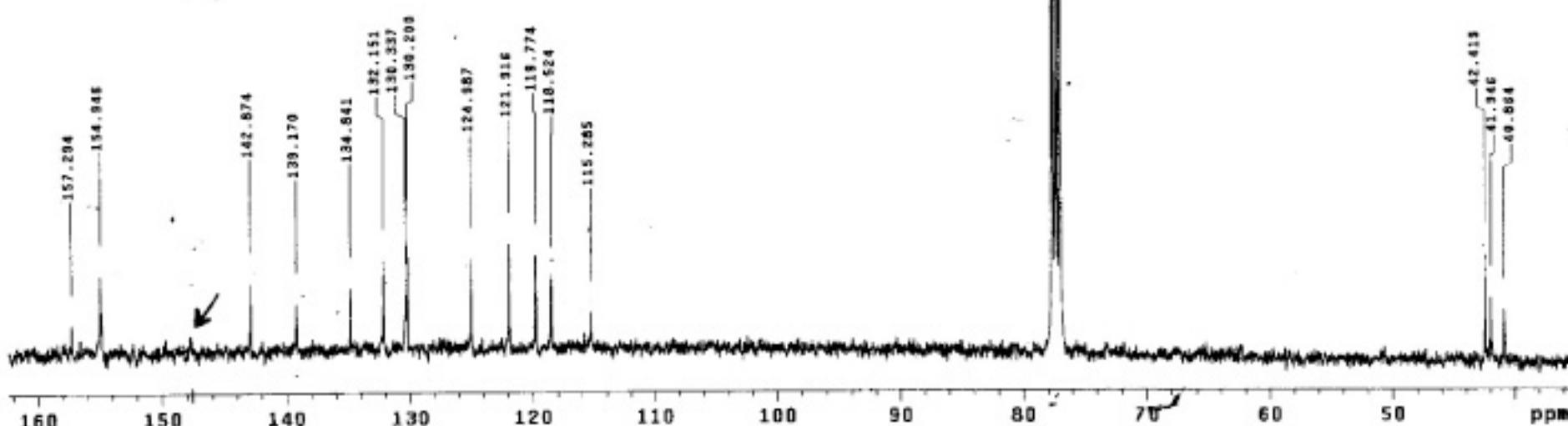
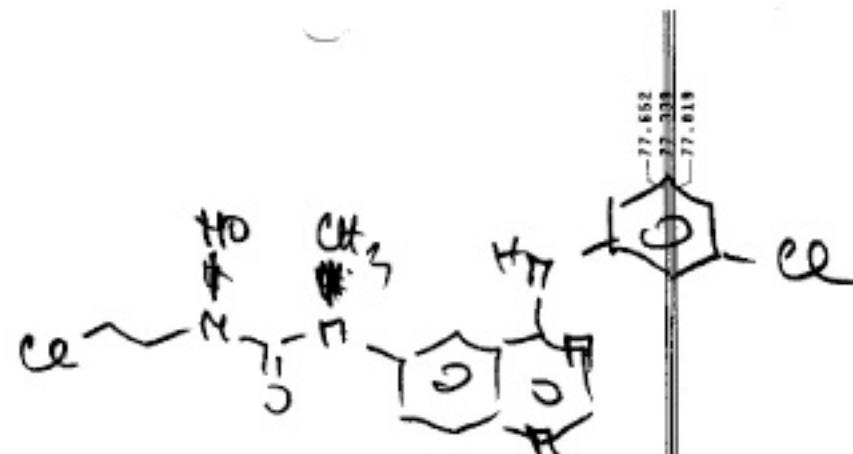
#22



S23

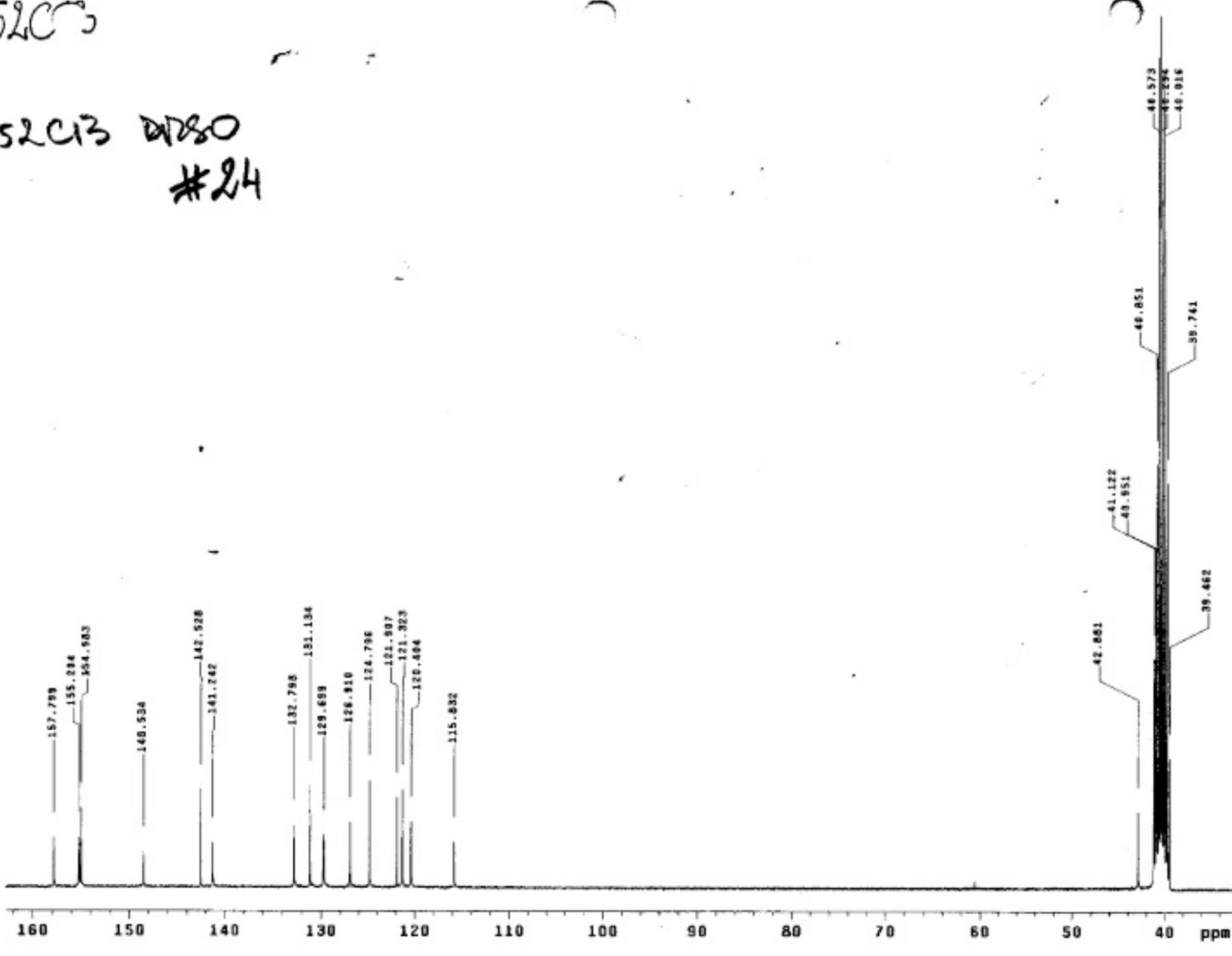
JDA47C13 CDCl₃
400

23

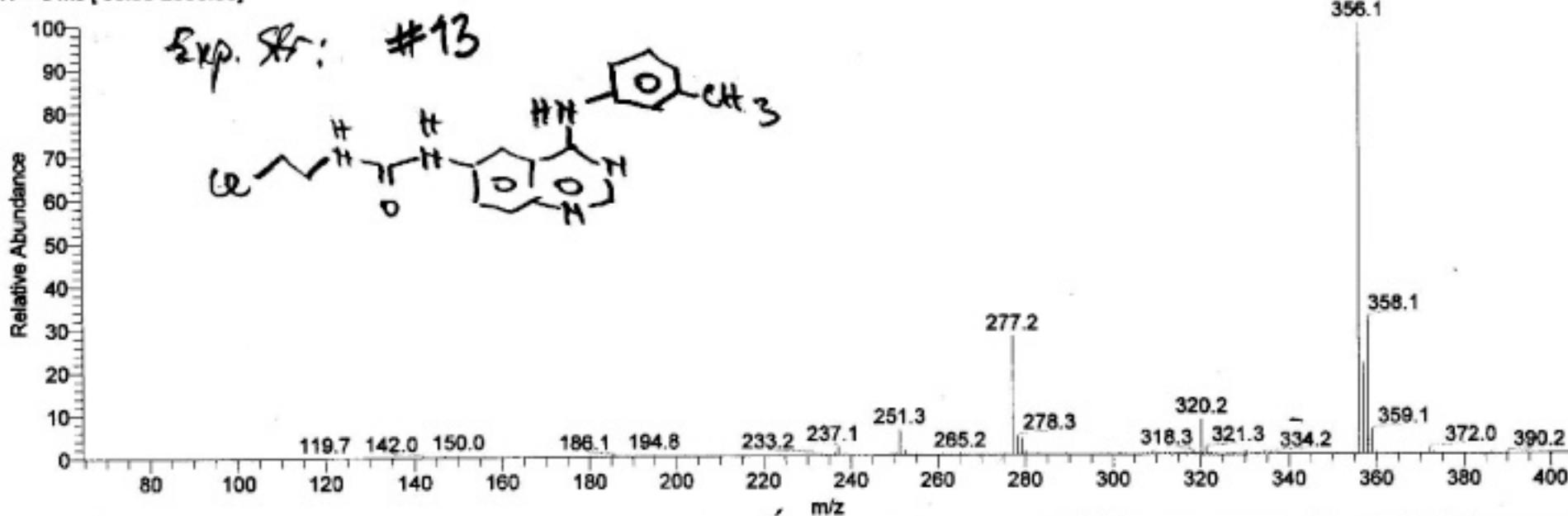


A52C13

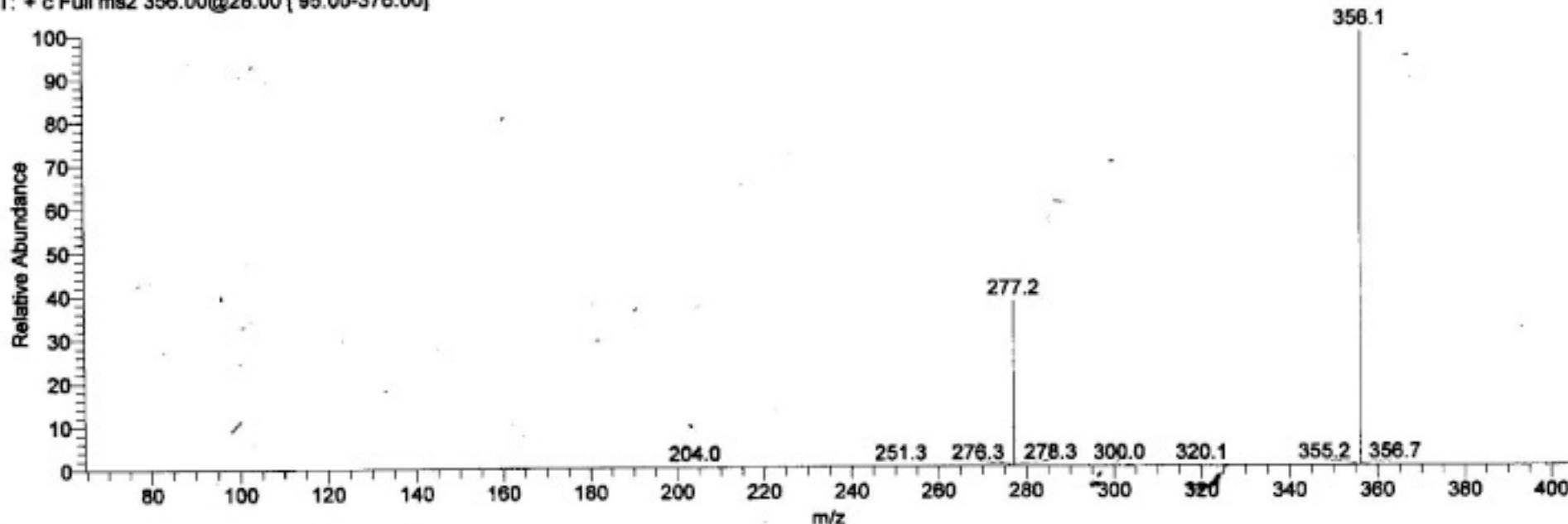
A52C13 D1280
#24



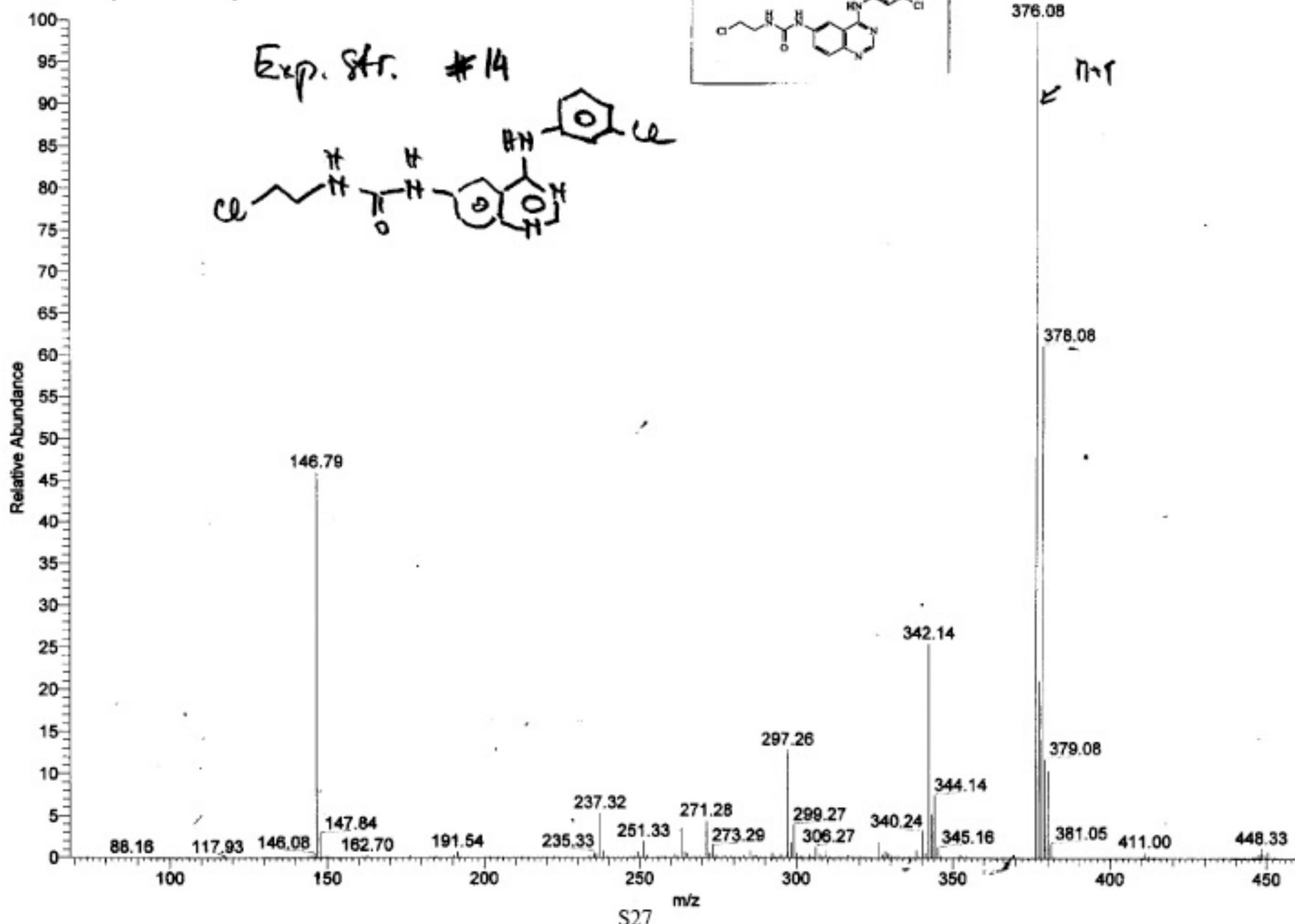
020425_06Aif_DOMARKAS_JDA34 #22-26 RT: 0.71-0.84 AV: 5 NL: 8.35E8
T: + c ms [50.00-2000.00]



020425_06Aif_DOMARKAS_JDA34 #42-49 RT: 1.07-1.15 AV: 8 NL: 5.56E7
T: + c Full ms2 356.00@28.00 [95.00-376.00]



020429_03Aif_DOMARKAS_JDA36 #60-83 RT: 2.00-2.68 AV: 24 NL: 2.26E7
T: + c Full ms [50.00-2000.00]

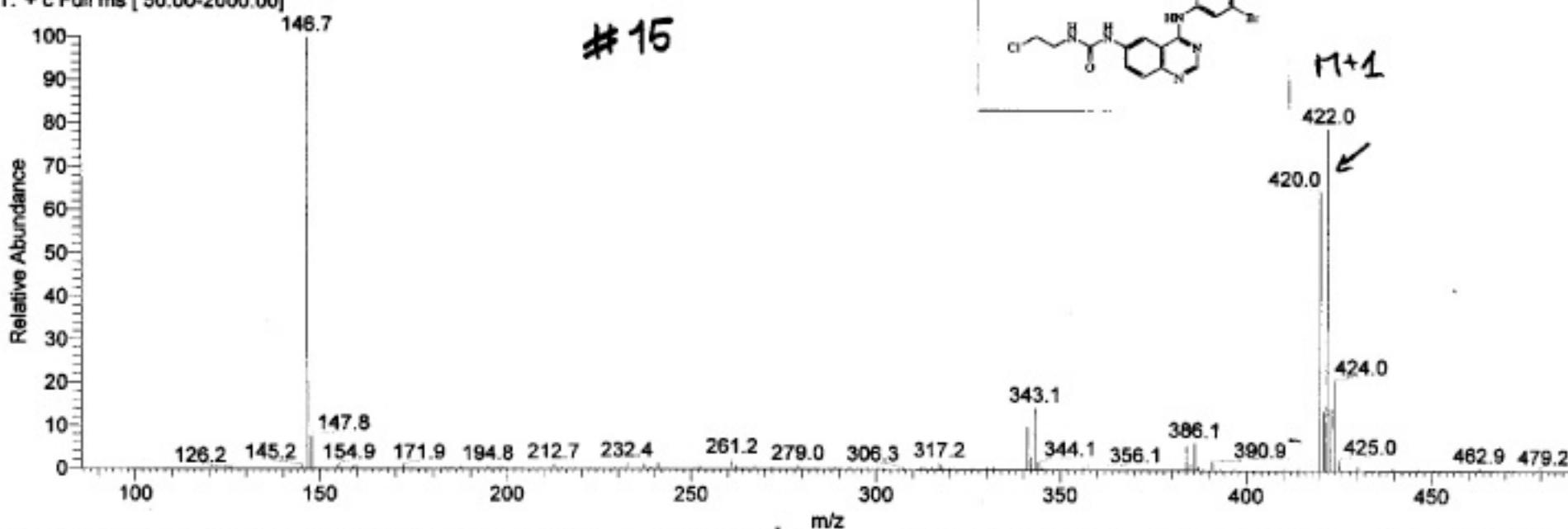


D:\Users\...\030227_04Aif_DOMARKAS_JDA40
APCI

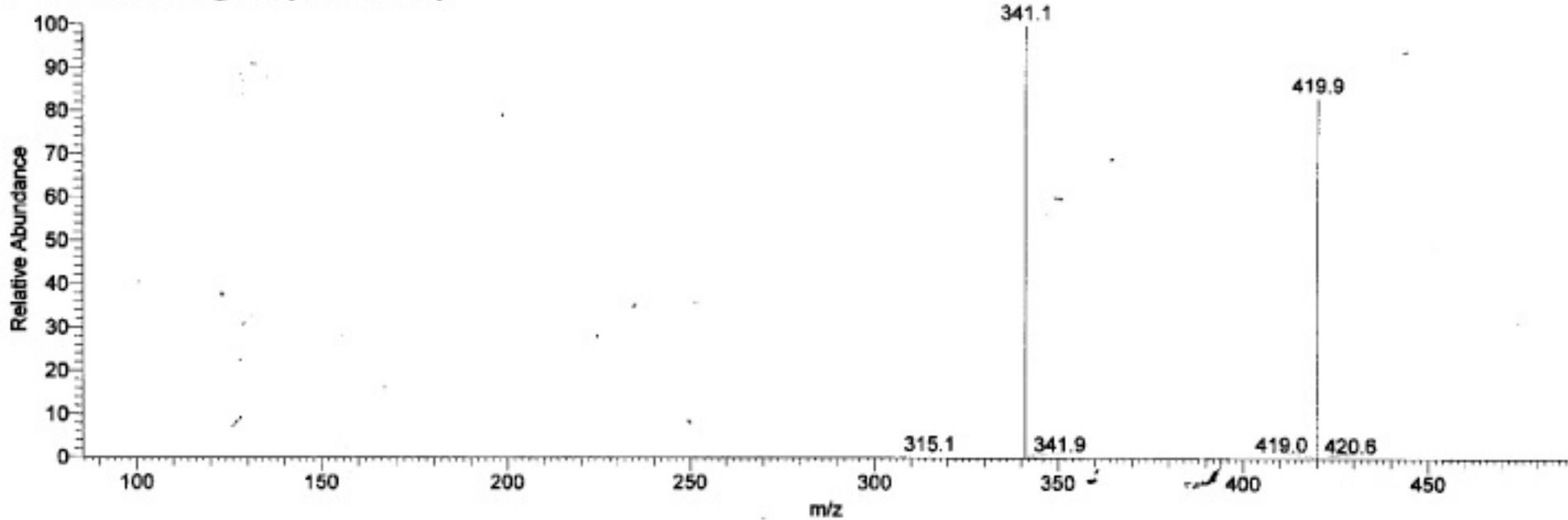
02/27/2003 03:31 PM

BERTRAND/DOMARKAS #JDA40

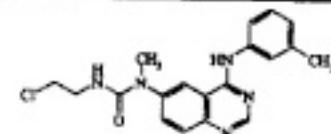
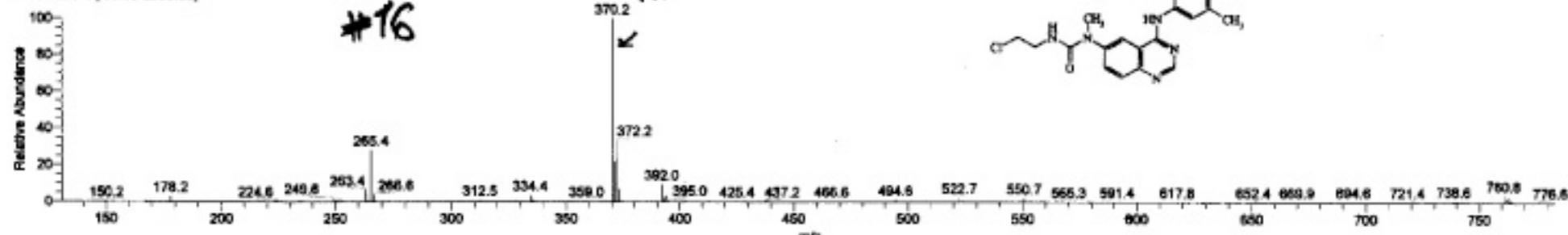
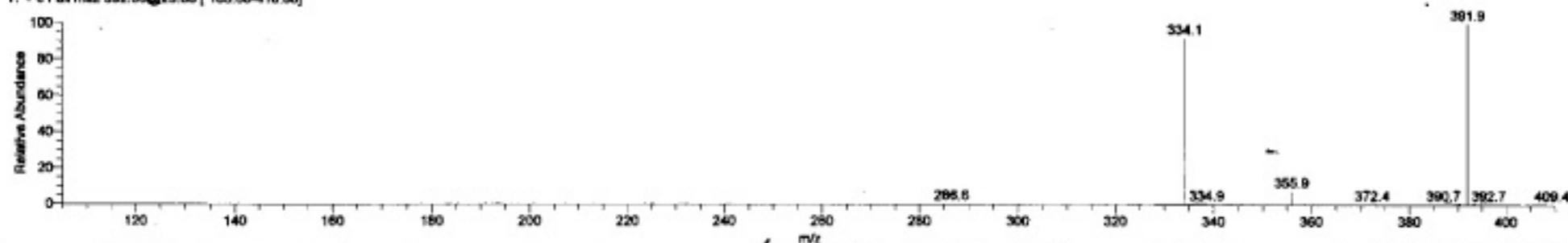
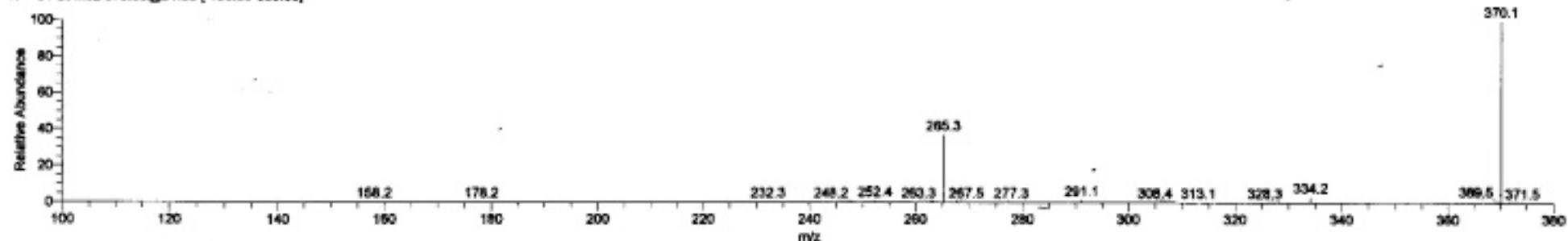
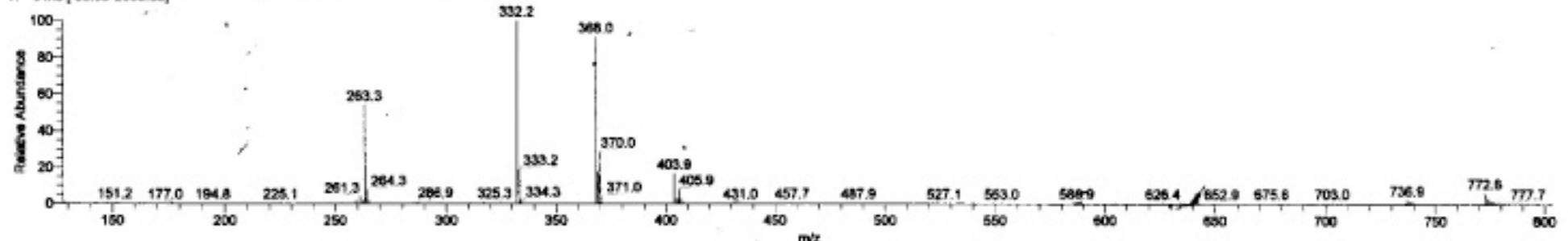
030227_04Aif_DOMARKAS_JDA40 #98-101 RT: 6.01-6.09 AV: 4 NL: 9.71E6
T: + c Full ms [50.00-2000.00]



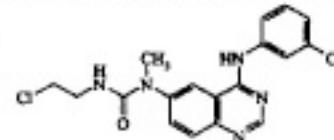
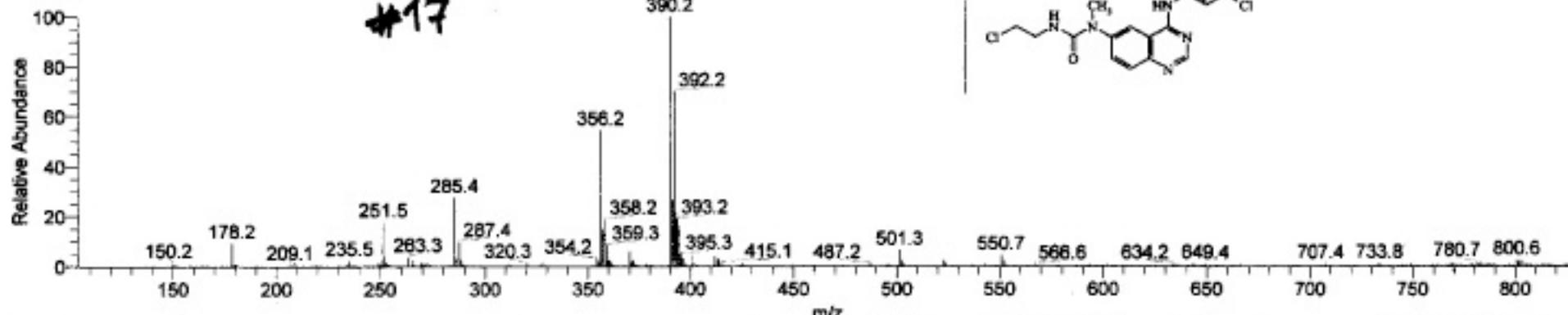
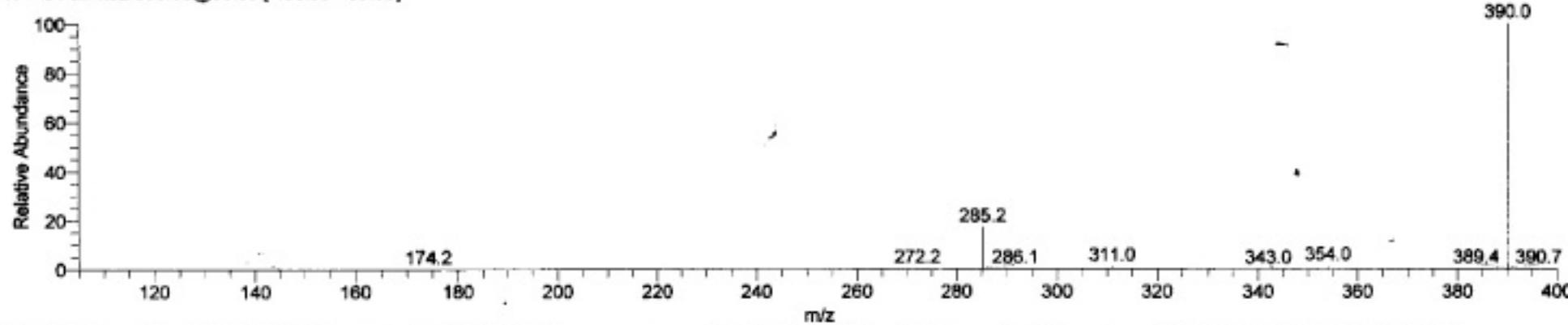
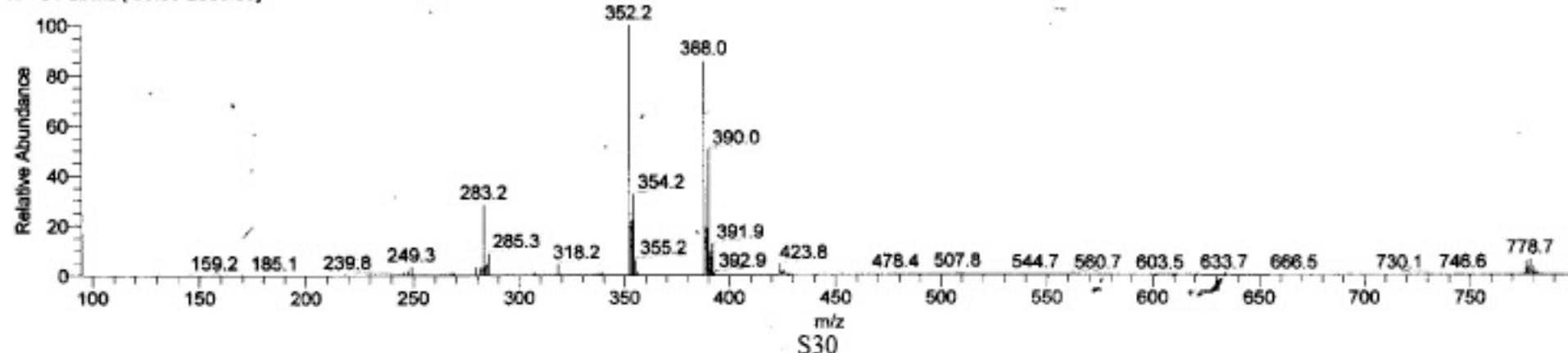
030227_04Aif_DOMARKAS_JDA40 #84-93 RT: 5.84-5.95 AV: 10 NL: 9.85E6
T: + c Full ms2 420.00@28.00 [115.00-430.00]



ESI

030226_03EI_DOMARKAS_JDA41 #48-54 RT: 1.27-1.44 AV: 7 NL: 1.05E7
T: + c Full ms [50.00-2000.00]030226_03EI_DOMARKAS_JDA41 #39-45 RT: 1.96-1.21 AV: 7 NL: 7.11E5
T: + c Full ms2 392.00@25.00 | 105.00-410.00030226_03EI_DOMARKAS_JDA41 #61 RT: 7.89 AV: 1 NL: 1.42E7
T: + c Full ms2 370.00@31.00 | 100.00-380.00030226_03EI_DOMARKAS_JDA41 #12-18 RT: 0.34-0.45 AV: 5 NL: 8.47E5
T: - c ms [50.00-2000.00]

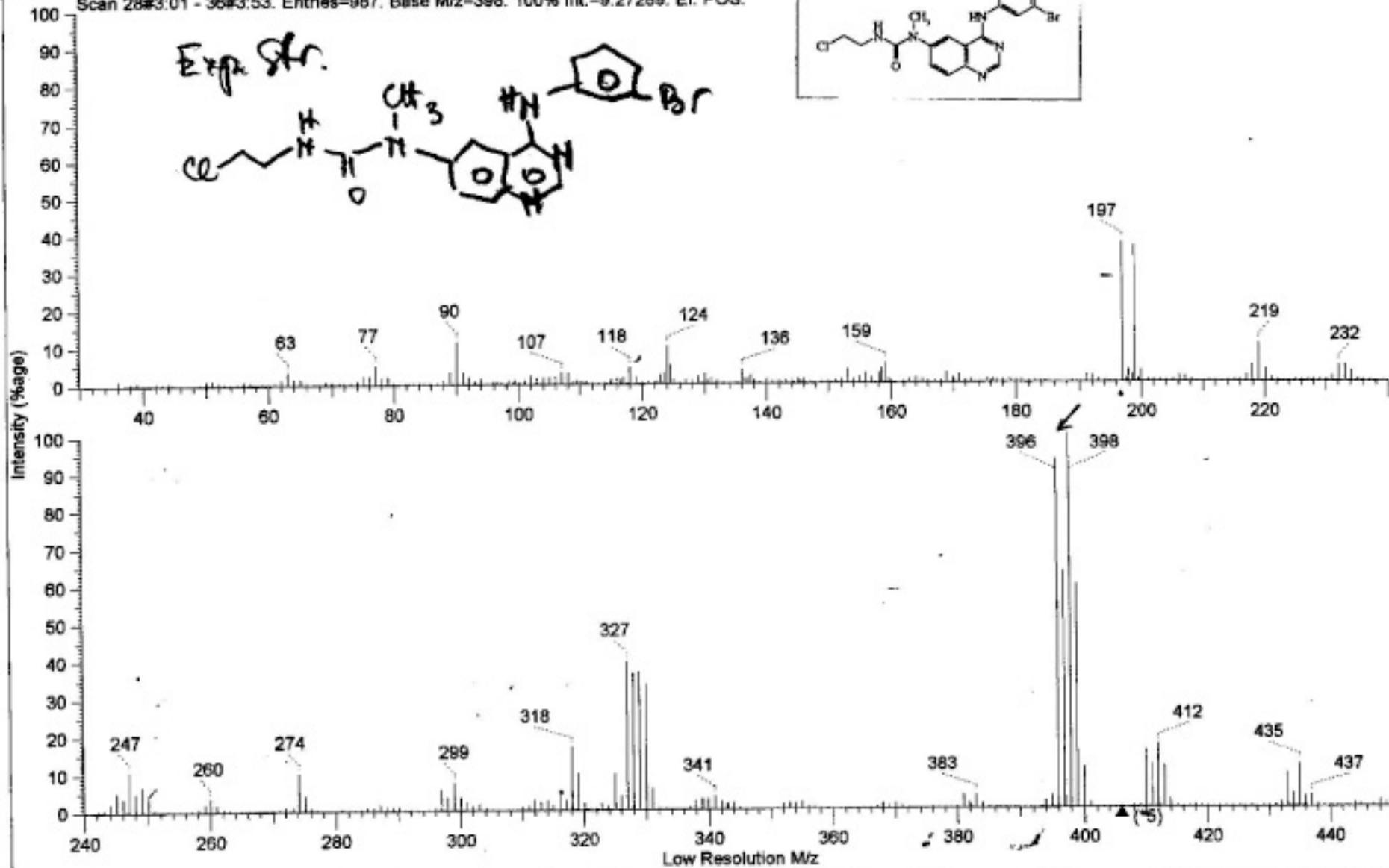
ESI

030226_04EI_DOMARKAS_JDA42 #18-22 RT: 0.60-0.74 AV: 5 NL: 1.71E7
T: + c Full ms [50.00-2000.00]030226_04EI_DOMARKAS_JDA42 #33-38 RT: 0.94-1.01 AV: 6 NL: 4.86E7
T: + c Full ms2 390.00@30.00 [105.00-400.00]030226_04EI_DOMARKAS_JDA42 #54-59 RT: 1.33-1.46 AV: 6 NL: 2.82E6
T: - c Full ms [50.00-2000.00]

File Name : E:\Data\ELCDATA\EVEI_CI_DATA2002\020503-02-E.ms2
 Creation Date/Time : 5/3/02 at 9:44:46
 File Type : Lo-Res Data - Ctd (Magnet)
 File Source : Acquired on MASPEC II system [II32/A111]
 File Title : BERTRAND/DOMARKAS #JDA39
 Operator : NADIM
 Instrument : MS25RFA

18

SCAN GRAPH. Flagging=Nominal M/z. Filter=[Range:35-19680.].Highlighting=Base Peak.
 Scan 28#3:01 - 36#3:53. Entries=987. Base M/z=398. 100% Int.=9.27289. EI. POS.

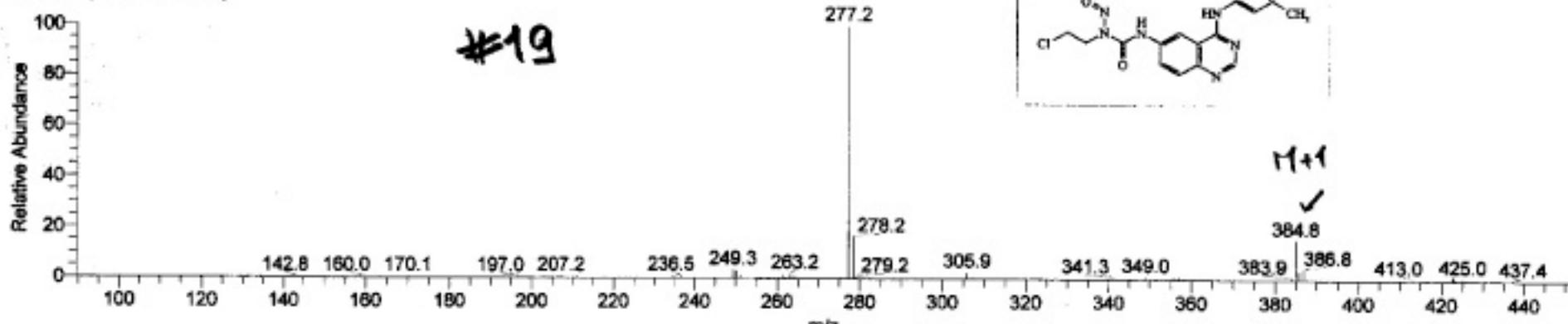


D:\Users\... 0312_02EI_DOMARKAS_JDA73
ESI

03/12/2003 10:52 AM

BERTRAND/DOMARKAS #JDA73

030312_02EI_DOMARKAS_JDA73 #14-17 RT: 0.45-0.53 AV: 4 NL: 6.12E7
T: + c ms [50.00-2000.00]

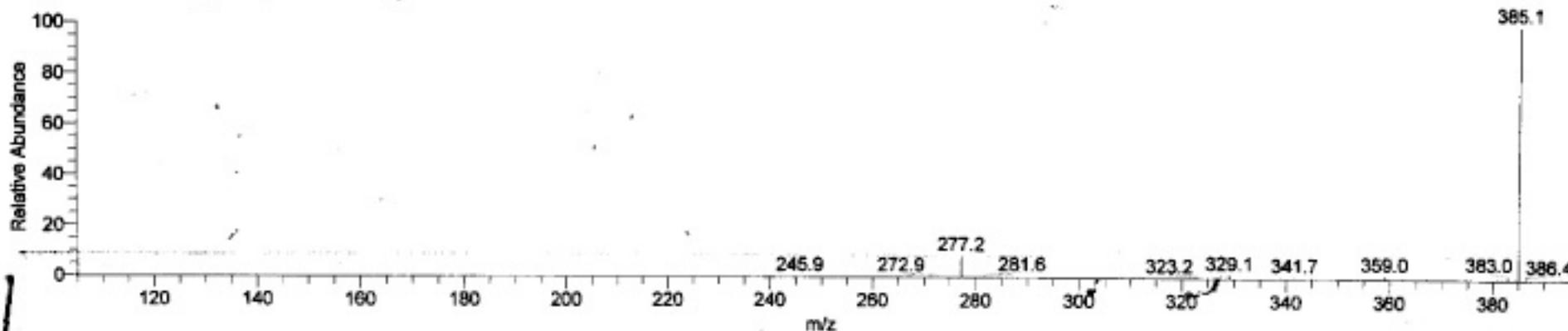


030312_02EI_DOMARKAS_JDA73#14-17 RT: 0.45-0.53 AV: 4
T: + c ms [50.00-2000.00]

m/z= 89.7-452.9

m/z	Intensity	Relative
249.3	1970536.3	3.22
250.2	1841170.5	3.01
277.2	61236264.0	100.00
278.2	10033336.0	16.38
384.8	9620522.5	15.71
385.8	1912317.0	3.12
386.8	2583000.3	4.22

030312_02EI_DOMARKAS_JDA73 #50-52 RT: 1.30-1.34 AV: 3 NL: 5.54E4
T: + c Full ms2 385.00@27.00 [105.00-396.00]

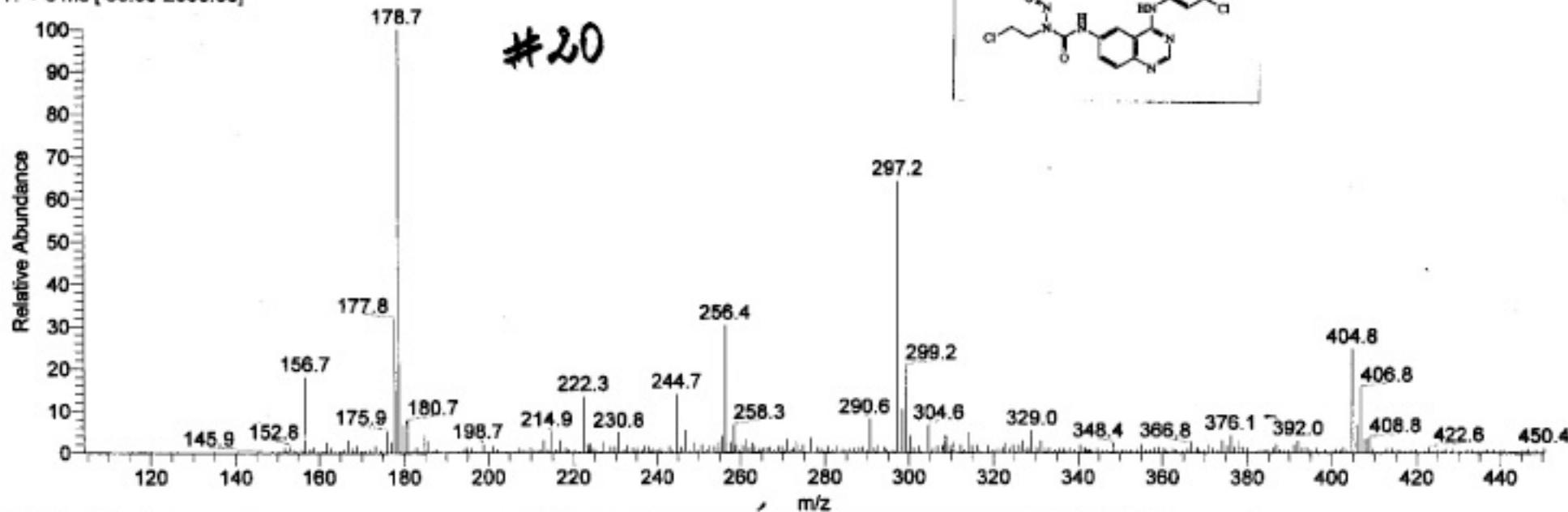


D:\Users\...\030325_07EI_DOMARKAS_JDA65
ESI

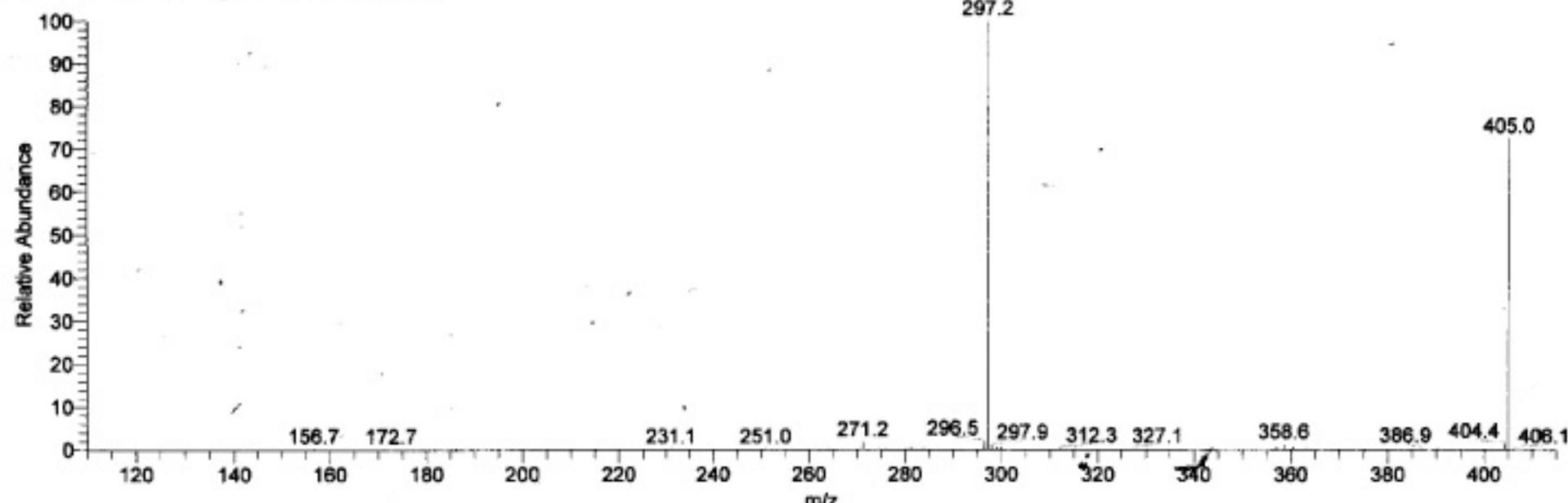
03/25/2003 12:05 PM

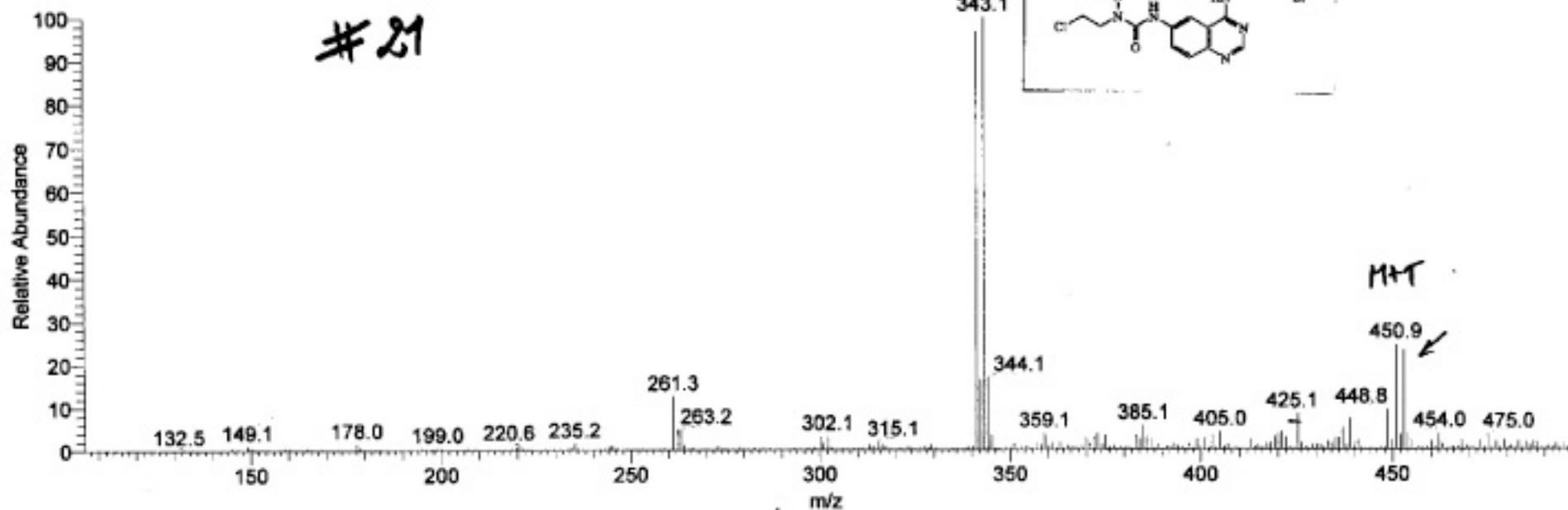
BERTRAND/DOMARKAS #JDA65

030325_07EI_DOMARKAS_JDA65 #26-28 RT: 0.75-0.81 AV: 3 NL: 1.57E7
T: + c ms [50.00-2000.00]



030325_07EI_DOMARKAS_JDA65 #34-36 RT: 0.95-0.99 AV: 3 NL: 3.20E5
T: + c Full ms2 405.00@25.00 [110.00-415.00]



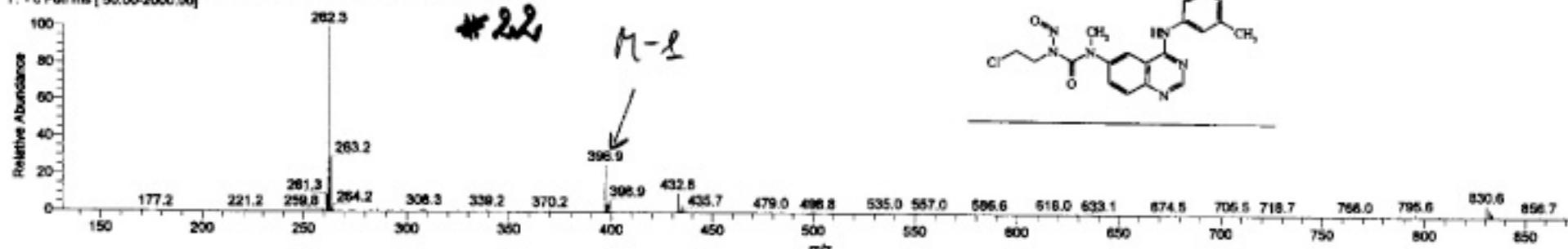
030311_07EI_DOMARKAS_JDA66 #5-7 RT: 0.15-0.21 AV: 3 NL: 2.94E7
T: + c ms [50.00-2000.00]

030311_07EI_DOMARKAS_JDA66#5-7 RT: 0.15-0.21 AV: 3

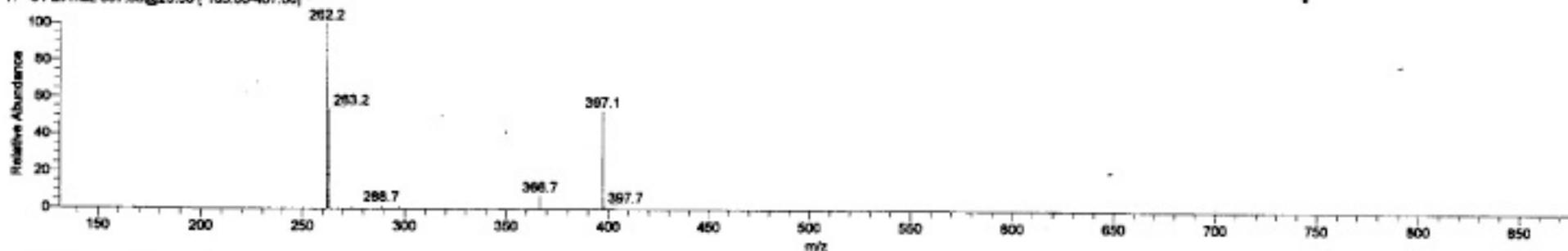
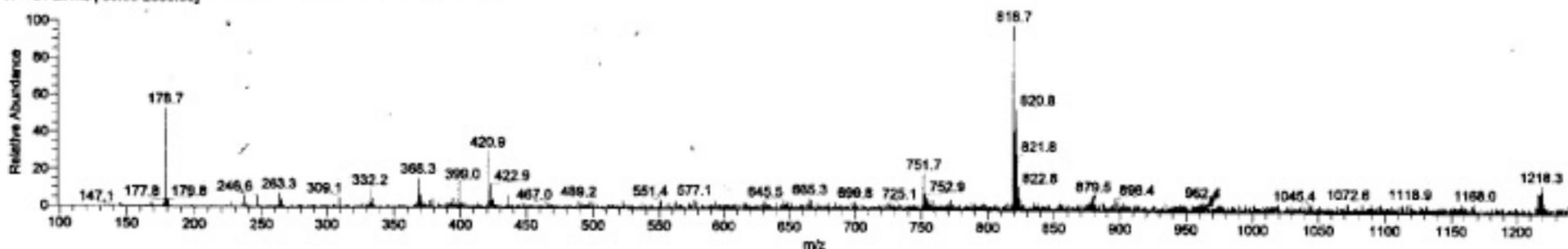
T: + c ms [50.00-2000.00]

m/z= 106.4-496.8

m/z	Intensity	Relative
261.3	3671818.3	12.47
341.1	28464248.0	96.67
342.1	4783479.0	16.25
343.1	29443616.0	100.00
344.1	4952343.3	16.82
450.9	7178803.0	24.38
453.0	6818951.7	23.16

030325_04EI_DOMARKAS_JDA56 #19-21 RT: 0.45-0.50 AV: 3 NL: 8.42E6
T: + c Full ms [50.00-2000.00]

m/z	Intensity	Relative
261.3	781268.3	9.28
262.3	8415081.0	100.00
263.2	2490768.0	29.60
396.9	2135298.3	25.37
398.9	542671.0	6.45
432.8	863498.3	10.26
830.6	555154.7	6.60

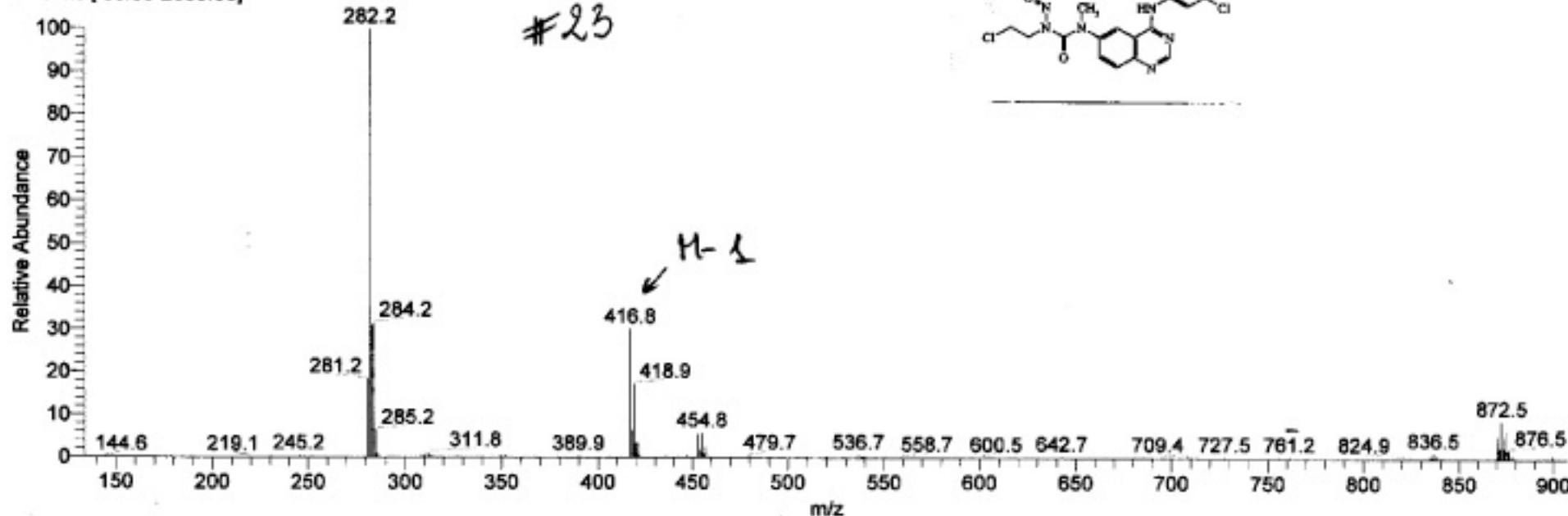
030325_04EI_DOMARKAS_JDA56 #16-18 RT: 0.39-0.43 AV: 3 NL: 1.92E6
T: + c Full ms2 397.00@25.00 / 105.00-407.00]030325_04EI_DOMARKAS_JDA56 #31-34 RT: 0.80-0.88 AV: 4 NL: 2.84E6
T: + c Full ms [50.00-2000.00]

D:\Users\LM\25_03EI_DOMARKAS_JDA58
ESI

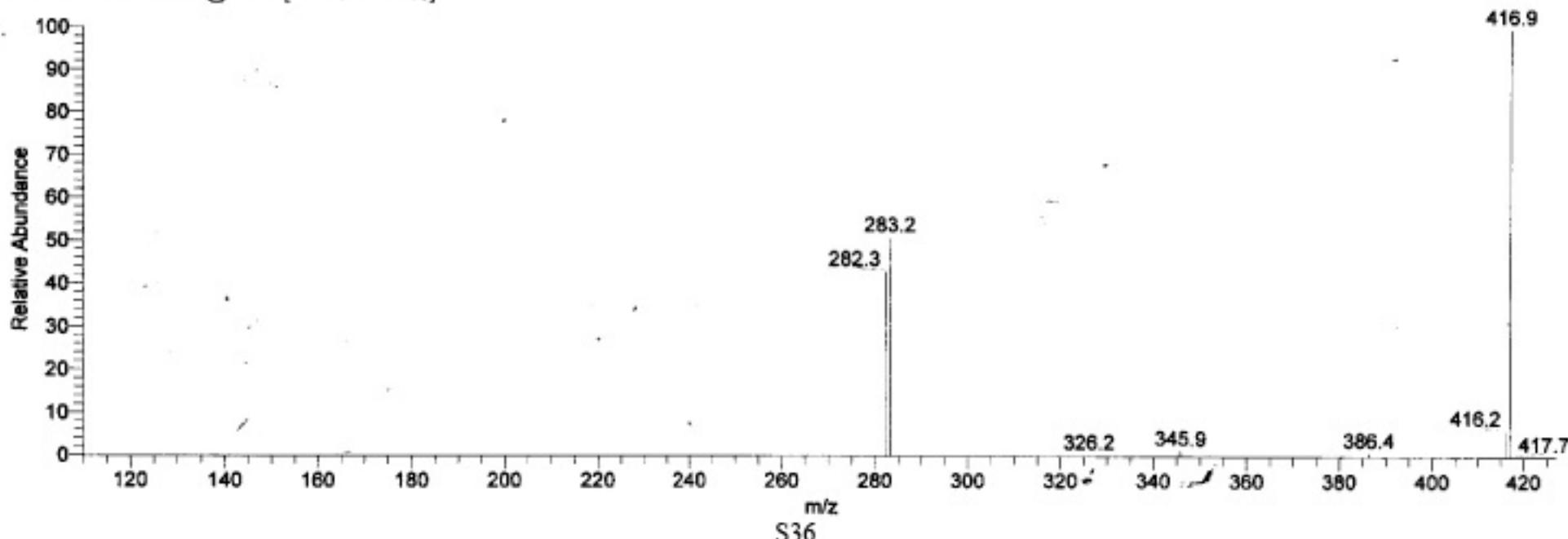
03/25/2003 11:06:06 AM

BERTRAND/DOMARKAS #JDA58

030325_03EI_DOMARKAS_JDA58 #8-11 RT: 0.20-0.28 AV: 4 NL: 1.54E7
T: - c ms [50.00-2000.00]



030325_03EI_DOMARKAS_JDA58 #25-28 RT: 0.59-0.65 AV: 4 NL: 5.73E4
T: - c Full ms2 417.00@21.00 [110.00-427.00]

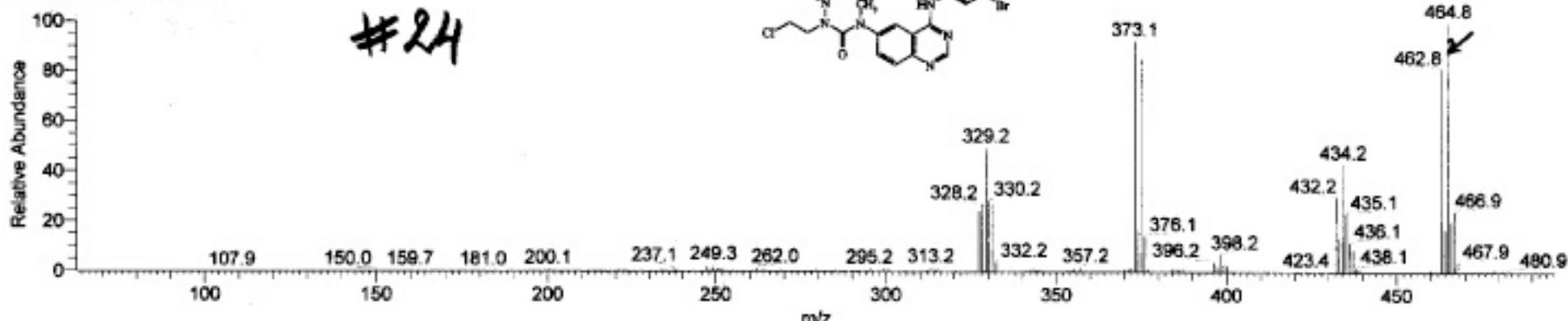


D:\Users\... 020617_01Aif_DOMARKAS_JDA52
APCI MEOH

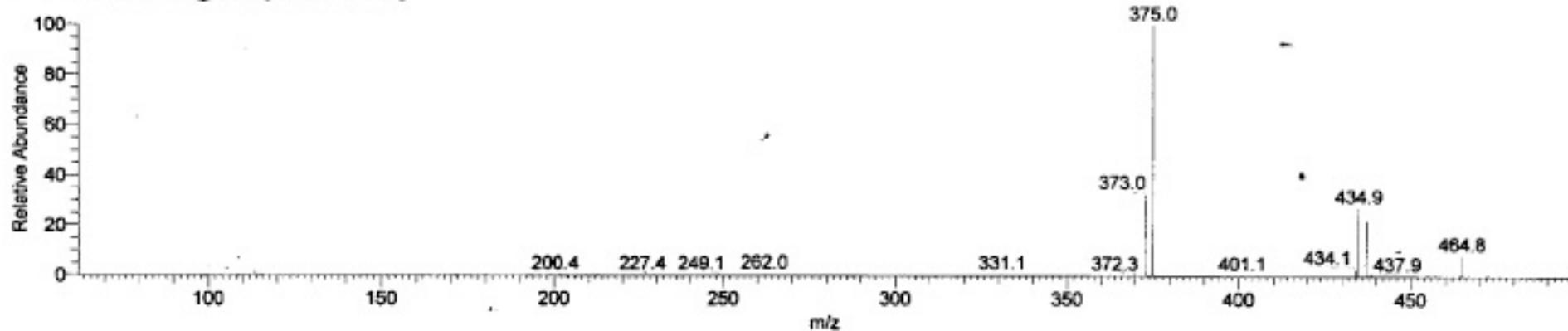
06/17/2002 10:47 AM

BERTRAND/DOMARKAS #JDA52

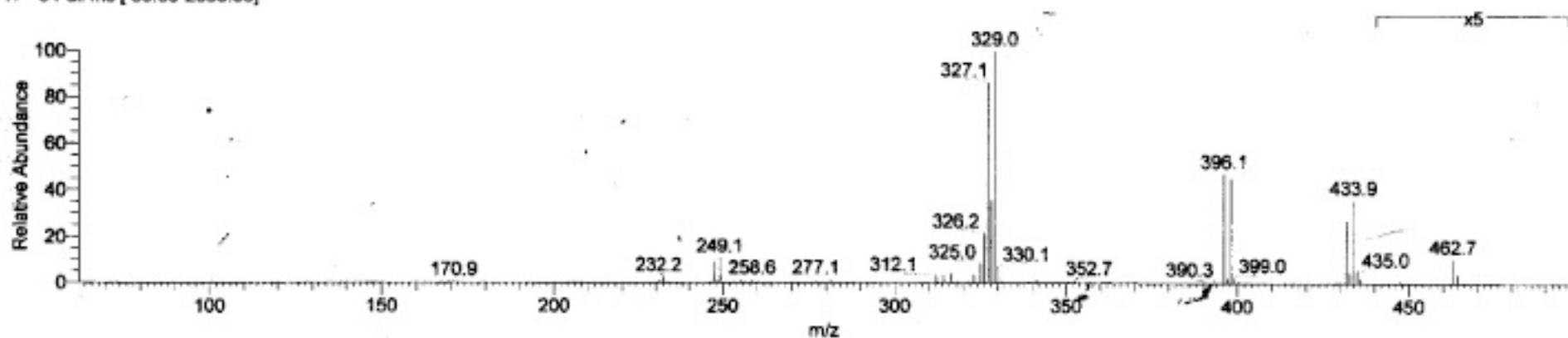
020617_01Aif_DOMARKAS_JDA52 #17-18 RT: 0.48-0.51 AV: 2 NL: 1.49E7
T: + c ms [50.00-2000.00]



020617_01Aif_DOMARKAS_JDA52 #42-45 RT: 0.84-0.88 AV: 4 NL: 3.29E7
T: + c Full ms2 455.00@20.00 | 125.00-485.00



020617_01Aif_DOMARKAS_JDA52 #65-67 RT: 1.27-1.32 AV: 3 NL: 2.82E5
T: - c Full ms [50.00-2000.00]



Elemental Composition #13

Date : 2-AUG-2003

Heteroatom Max: 44 Ion: Both Even and Odd
 Limits:

Mass	mDa	PPM	Calc. Mass	DBE	Elemental Composition						
					-4.2	0	0	3	0	0	0
356.127670		10.9		32.9	200	400	7	4	3	1	
					C	H	N	O	Cl	Br	
356.127670	-2.5	-7.1	356.125133	7.0	15	21	4	4	1		
	-2.0	-5.8	356.125620	2.5	12	24	5	3	2		
	-1.7	-4.7	356.125983	16.5	19	14	7	1			
	-1.6	-4.4	356.126108	-2.0	9	27	6	2	3		
	-0.3	-1.	356.127326	16.0	21	16	4	2			
	-0.2	-0.6	356.127450	-2.5	11	29	3	3	3		
	0.1	0.4	356.127813	11.5	18	19	5	1	1		
	0.6	1.8	356.128300	7.0	15	22	6			2	
	2.0	5.5	356.129643	6.5	17	24	3	1	2		
	2.1	5.8	356.129726	0.5	11	27	5	3			1
	2.5	6.9	356.130130	2.0	14	27	4		3		
	2.5	7.1	356.130213	-4.0	8	30	6	2	1	1	

- 1 -

Elemental Composition #14

Date : 2-AUG-2003

Heteroatom Max: 44 Ion: Both Even and Odd
 Limits:

			-4.2	0	0	3	0	0	0	
			39.9	200	400	7	4	3	1	
Mass	mDa	PPM	Calc. Mass	DBE	C	H	N	O	Cl	Br
376.073120	7.4									
-2.6	-6.9	376.070511	7.0	14	18	4	4	2		
-2.2	-6.0	376.070874	21.0	21	8	6	2			
-2.1	-5.6	376.070998	2.5	11	21	5	3	3		
-1.8	-4.7	376.071361	16.5	18	11	7	1	1		
-0.9	-2.4	376.072216	20.5	23	10	3	2			
-0.4	-1.1	376.072704	16.0	20	13	4	2	1		
0.1	0.2	376.073191	11.5	17	16	5	1	2		
0.2	0.4	376.073274	5.5	11	19	7	3			1
0.6	1.5	376.073678	7.0	14	19	6		3		
1.5	4.0	376.074617	5.0	13	21	4	4			1
1.8	4.7	376.074896	25.0	26	8	4				
1.9	5.1	376.075021	6.5	16	21	3	1	3		
2.0	5.3	376.075104	0.5	10	24	5	3	1	1	
2.5	6.6	376.075591	-4.0	7	27	6	2	2		1

Elemental Composition

Date : 2-AUG-2003

Heteroatom Max: 44 Ion: Both Even and Odd
 Limits:

			-4.2	0	0	3	0	0	0	
			39.9	200	400	7	4	3	1	
Mass	mDa	PPM	Calc. Mass	DBE	C	H	N	O	Cl	Br
420.022780		7.4								
-3.0	-7.1	420.019787	31.5	30	2	3	1			
-2.8	-6.6	420.019994	7.0	14	18	4	4	1	1	
-2.5	-6.0	420.020274	27.0	27	5	4		1		
-2.3	-5.5	420.020481	2.5	11	21	5	3	2	1	
-1.9	-4.6	420.020844	16.5	18	11	7	1			
-1.8	-4.3	420.020969	-2.0	8	24	6	2	3	1	
-0.6	-1.4	420.022187	16.0	20	13	4	2			
-0.5	-1.1	420.022311	-2.5	10	26	3	3	3	1	
-0.1	-0.3	420.022674	11.5	17	16	5	1	1	1	
0.4	0.9	420.023151	7.0	14	19	6		2	1	
1.7	4.1	420.024504	6.5	16	21	3	1	2	1	
2.0	4.8	420.024805	18.5	18	7	7	4	1		
2.2	5.3	420.024991	2.0	13	24	4		3	1	

Elemental Composition #16

Date : 2-AUG-2003

Heteroatom Max: 44 Ion: Both Even and Odd
 Limits:

			-4.2	0	0	3	0	0	0	
			39.9	200	400	7	4	3	1	
Mass	mDa.	PPM	Calc. Mass	DBE	C	H	N	O	Cl	Br
370.143450	-2.7	-7.2	370.140783	7.0	16	23	4	4	1	
	-2.2	-5.9	370.141270	2.5	13	26	5	3	2	
	-1.8	-4.9	370.141633	16.5	20	16	7	1		
	-1.7	-4.6	370.141758	-2.0	10	29	6	2	3	
	-0.5	-1.3	370.142976	16.0	22	18	4	2		
	-0.3	-0.9	370.143100	-2.5	12	31	3	3	3	
	0.0	0.0	370.143463	11.5	19	21	5	1	1	
	0.5	1.4	370.143950	7.0	16	24	6		2	
	1.8	5.0	370.145293	6.5	18	26	3	1	2	
	1.9	5.2	370.145376	0.5	12	29	5	3		1
	2.3	6.3	370.145780	2.0	15	29	4		3	
	2.4	6.5	370.145863	-4.0	9	32	6	2	1	1

Heteroatom Max: 38 Ion: Both Even and Odd
 Limits:

			-4.7	1	0	0	0	0	0
Mass	mDa	PPM	Calc. Mass	DBE	C	H	N	O	Cl
390.088960		4.1		39.7	100	200	10	6	4
-1.5	-3.7	390.087504	6.5	17	22	1	5	2	
-1.5	-3.7	390.087498	12.0	16	16	8		2	
-1.1	-2.8	390.087866	20.5	24	12	3	3		
-1.	-2.5	390.087991	2.0	14	25	2	4	3	
-0.6	-1.6	390.088354	16.0	21	15	4	2	1	
-0.5	-1.2	390.088478	-2.5	11	28	3	3	4	
-0.1	-0.3	390.088841	11.5	18	18	5	1	2	
0.2	0.6	390.089209	20.0	26	14		4		
0.4	0.9	390.089328	7.0	15	21	6		3	
0.7	1.9	390.089696	15.5	23	17	1	3	1	
0.9	2.2	390.089821	-3.0	13	30		4	4	
1.2	3.1	390.090184	11.0	20	20	2	2	2	
1.6	4.1	390.090546	25.0	27	10	4			

Elemental Composition #18

Date : 2-AUG-2003

Heteroatom Max: 44 Ion: Both Even and Odd
 Limits:

			-4.2	0	0	3	0	0	0	
			39.9	200	400	7	4	3	1	
Mass	mDa	PPM	Calc. Mass	DBE	C	H	N	O	Cl	Br
434.038210		7.4								
-2.8	-6.4	434.035437	31.5	31	4	3	1			
-2.6	-5.9	434.035644	7.0	15	0	4	4	1	1	
-2.3	-5.3	434.035924	27.0	28	7	4		1		
-2.1	-4.8	434.036131	2.5	12	13	5	3	2	1	
-1.7	-4.0	434.036494	16.5	19	13	7			1	
-1.6	-3.7	434.036619	-2.0	9	26	6	2	3	1	
-0.4	-0.9	434.037837	16.0	21	15	4	2		1	
-0.2	-0.6	434.037961	-2.5	11	28	3	3	3	1	
0.1	0.3	434.038124	11.5	18	18	5	1	1	1	
0.6	1.4	434.038811	7.0	15	21	6		2	1	
1.9	4.5	434.040154	6.5	17	23	3	1	2	1	
2.2	5.2	434.040455	18.5	19	9	7	4	1		
2.4	5.6	434.040641	2.0	14	26	4		3	1	

Elemental Composition

Date : 2-AUG-2003

Heteroatom Max: 44 Ion: Both Even and Odd
Limits:

Mass	mDa	PPM	Calc. Mass	DBE ^a	C	H	N	O	C1	Br
385.118090		7.4		-4.2 39.9	0 200	0 400	3 7	0 4	0 3	0 1
385.118090	-2.7	-7.1	385.115359	10.0	20	24	3			1
	-2.3	-6.0	385.115784	3.5	12	23	6	4	2	
	-1.8	-4.7	385.116271	-1.0	9	26	7	3	3	
	-0.6	-1.6	385.117490	17.0	21	15	5	3		
	-0.5	-1.2	385.117614	-1.5	11	28	4	4	3	
	-0.1	-0.3	385.117977	12.5	18	18	6	2	1	
	0.4	1.	385.118464	8.0	15	21	7	1	2	
	1.2	3.2	385.119319	12.0	20	20	3	3	1	
	1.7	4.5	385.119807	7.5	17	23	4	2	2	
	1.8	4.7	385.119890	1.5	11	26	6	4		1
	2.1	5.4	385.120170	21.5	24	13	6			
	2.2	5.7	385.120294	3.0	14	26	5	1	3	
	2.3	5.9	385.120377	-3.0	8	29	7	3	1	1

Elemental Composition #20

Date : 2-AUG-2003

Heteroatom Max: 44 Ion: Both Even and Odd
 Limits:

			-4.2	0	0	3	0	0	0	
			39.9	200	400	7	4	3	1	
Mass	mDa	PPM	Calc. Mass	DBE	C	H	N	O	Cl	Br
405.063230	-2.5	-6.2	405.060737	10.0	19	21	3		1	1
	-2.2	-5.4	405.061037	22.0	21	7	7	3		
	-2.1	-5.1	405.061162	3.5	11	20	6	4	3	
	-0.9	-2.1	405.062380	21.5	23	9	4	4		
	-0.4	-0.9	405.062867	17.0	20	12	5	3	1	
	0.1	0.3	405.063354	12.5	17	15	6	2	2	
	0.6	1.5	405.063842	8.0	14	18	7	1	3	
	1.5	3.6	405.064697	12.0	19	17	3	3	2	
	1.8	4.5	405.065060	26.0	26	7	5	1		
	2.0	4.8	405.065184	7.5	16	20	4	2	3	
	2.0	5.0	405.065267	1.5	10	23	6	4	1	1
	2.3	5.7	405.065547	21.5	23	10	6		1	
	2.5	6.2	405.065755	-3.0	7	26	7	3	2	1

- 1 -

Elemental Composition #24

Date : 2-AUG-2003

Heteroatom Max: 44 Ion: Both Even and Odd

Limits:

			-4.2	0	0	3	0	0	0	
			39.9	200	400	7	4	3	1	
Mass	mDa	PPM	Calc. Mass	DBE	C	H	N	O	Cl	Br
449.012890	7.4									
-2.9	-6.5	449.009950	32.5	30	1	4	2			
-2.8	-6.3	449.010075	14.0	20	14	3	3	3		
-2.5	-5.5	449.010438	28.0	27	4	5	1	1		
-2.2	-5.0	449.010645	3.5	11	20	6	4	2		1
-2.0	-4.4	449.010925	23.5	24	7	6		2		
-1.8	-3.9	449.011132	-1.0	8	23	7	3	3		1
-0.6	-1.4	449.012267	23.0	26	9	3	1	2		
-0.5	-1.2	449.012351	17.0	20	12	5	3			1
-0.4	-0.9	449.012475	-1.5	10	25	4	4	3		1
-0.1	-0.3	449.012755	18.5	23	12	4		3		
-0.1	-0.1	449.012838	12.5	17	15	6	2	1		1
0.4	1.	449.013325	8.0	14	18	7	1	2		1
1.3	2.9	449.014180	12.0	19	17	3	3	1		1
1.8	4.0	449.014668	7.5	16	20	4	2	2		1
2.1	4.8	449.015031	21.5	23	10	6				1
2.3	5.0	449.015155	3.0	13	23	5	1	3		1

Elemental Composition #22

Date : 2-AUG-2003

Heteroatom Max: 44 Ion: Both Even and Odd
 Limits:

Mass	mDa	PPM	Calc. Mass	DBE	Elemental Composition						
					-4	-2	0	2	3	0	0
399.133550		7.4			-4.2	0	0	3	0	0	0
					39.9	200	400	7	4	3	1
Mass	mDa	PPM	Calc. Mass	DBE	C	H	N	O	Cl	Br	
399.133550	-2.5	-6.4	399.131009	10.0	21	26	3				1
	-2.1	-5.3	399.131434	3.5	13	25	6	4	2		
	-1.6	-4.1	399.131921	-1.0	10	28	7	3	3		
	-0.4	-1.0	399.133140	17.0	22	17	5	3			
	-0.3	-0.7	399.133264	-1.5	12	30	4	4	3		
	0.1	0.2	399.133627	12.5	19	20	6	2	1		
	0.6	1.4	399.134114	8.0	16	23	7	1	2		
	1.4	3.6	399.134970	12.0	21	22	3	3	1		
	1.9	4.8	399.135457	7.5	18	25	4	2	2		
	2.0	5.0	399.135540	1.5	12	28	6	4			1
	2.3	5.7	399.135820	21.5	25	15	6				
	2.4	6.0	399.135944	3.0	15	28	5	1	3		
	2.5	6.2	399.136027	-3.0	9	31	7	3	1		1

Elemental Composition #23

Date : 2-ADG-2003

Heteroatom Max: 44 Ion: Both Even and Odd
 Limits:

				-4.2	0	0	3	0	0	0
				39.9	200	400	7	4	3	1
Mass	mDa	PPM	Calc. Mass	DRR	C	H	N	O	Cl	Br
419.079000	-2.6	-6.2	419.076387	10.0	20	23	3		1	1
	-3.3	-5.5	419.076687	22.0	22	9	7	3		
	-2.2	-5.2	419.076812	3.5	12	22	6	4	3	
	-1.	-2.3	419.078030	21.5	24	11	4	4		
	-0.5	-1.2	419.078517	17.0	21	14	5	3	1	
	0.0	0.0	419.079004	12.5	18	17	6	2	2	
	0.5	1.2	419.079492	8.0	15	20	7	1	3	
	1.3	3.2	419.080347	12.0	20	19	3	3	2	
	1.7	4.1	419.080710	26.0	27	9	5	1		
	1.8	4.4	419.080834	7.5	17	22	4	2	3	
	1.9	4.6	419.080917	1.5	11	25	6	4	1	1
	2.2	5.2	419.081197	21.5	24	12	6		1	
	2.4	5.7	419.081405	-3.0	8	28	7	3	2	1

- 1 -

Elemental Composition #24

Date : 2-AUG-2003

Heteroatom Max: 44 Ion: Both Even and Odd
 Limits:

			-4.2	0	0	3	0	0	0	
			39.9	200	400	7	4	3	1	
Mass	mDa	PPM	Calc. Mass	DBE	C	H	N	O	Cl	Br
463.028640	7.4									
-3.0	-6.6	463.025600	32.5	31	3	4	2			
-2.9	-6.3	463.025725	14.0	21	16	3	3	3		
-2.6	-5.5	463.026088	28.0	28	6	5	1	1		
-2.3	-5.1	463.026295	3.5	12	12	6	4	2	1	
-2.1	-4.5	463.026575	23.5	25	9	6		2		
-1.9	-4.0	463.026782	-1.0	9	25	7	3	3	1	
-0.7	-1.6	463.027918	33.0	27	11	3	1	2		
-0.6	-1.4	463.028001	17.0	21	14	5	3		1	
-0.5	-1.1	463.028125	-1.5	11	27	4	4	3	1	
-0.2	-0.5	463.028405	18.5	24	14	4		3		
-0.2	-0.3	463.028488	12.5	18	17	6	2	1	1	
0.3	0.7	463.028975	8.0	15	20	7	1	2	1	
1.2	2.6	463.029831	12.0	20	19	3	3	1	1	
1.7	3.6	463.030318	7.5	17	22	4	2	2	1	
2.0	4.4	463.030681	21.5	24	12	6			1	
2.2	4.7	463.030805	3.0	14	25	5	1	3	1	
3.4	7.3	463.032023	21.0	26	14	3	1		1	

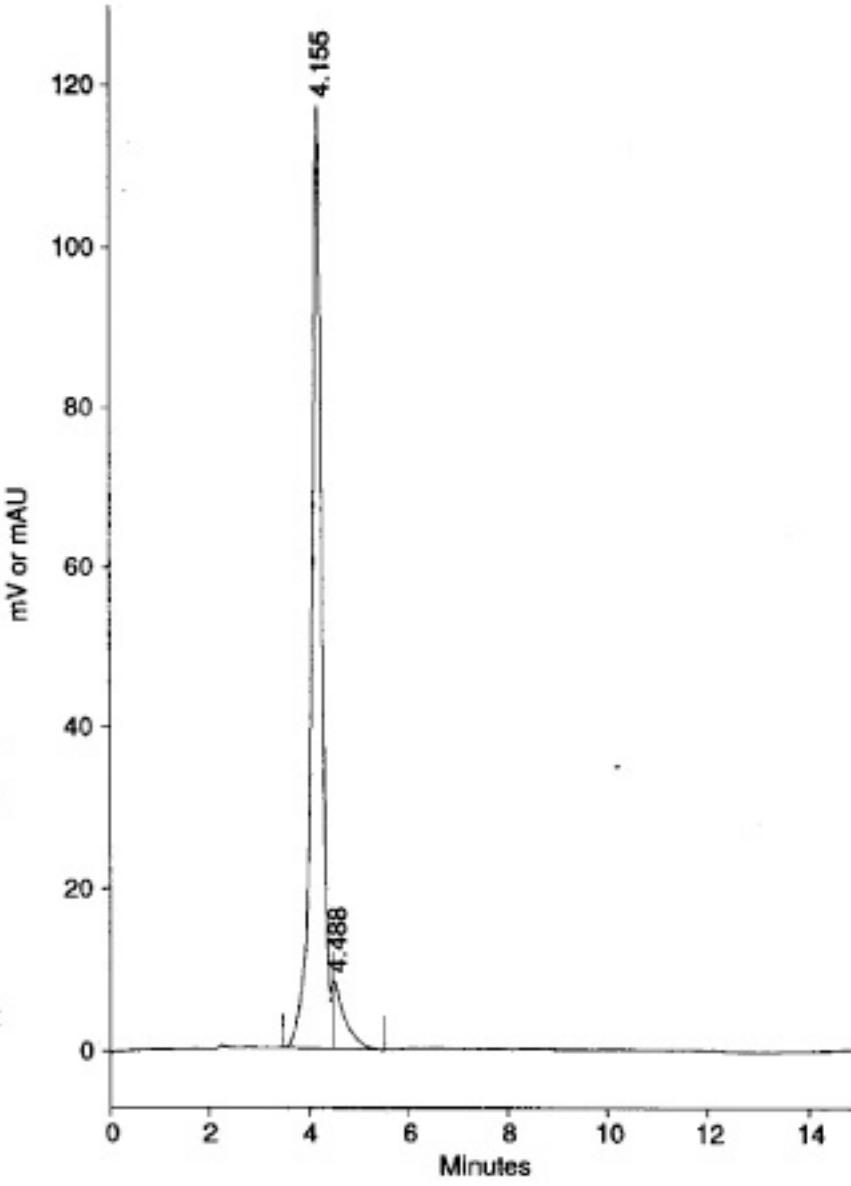
- 1 -

Analysis Report

Name: n jda34isOHb2-26
Type: Sample
Injection Volume: 10.0 μ L

Acquisition Log
Column Pressure (PSI): 1343
Noise (microAU): 4e+01
Run-Time Messages: None

Signal 1: UV3000 A 254 nm
Calculation Type: Area Percent (Area)



Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	4.155	1684813	117198	92.46	Fused
Unident0002	4.488	137454	8352	7.54	Fused
Totals		1822267	125550	100.00	

System: Bertrand on Comm Port 1
Acquisition Method: C:\TSP\SYSTEMUVFLUO\Methods\jda isoh.AQM

PC1000 Ver 3.5 Test Rel 17
02-06-03 12:09:28

Mode: Acquired Data
Original Results: C:\TSP\SYSTEM\UVFLUO\Results\fd152 isohn.RES

Reported On: 02-26-03 15:01:46

Page 1

Analysis Report

Name: fd152 isohn
Type: Sample
Injection Volume: 10.0 μ L

Acquisition Log

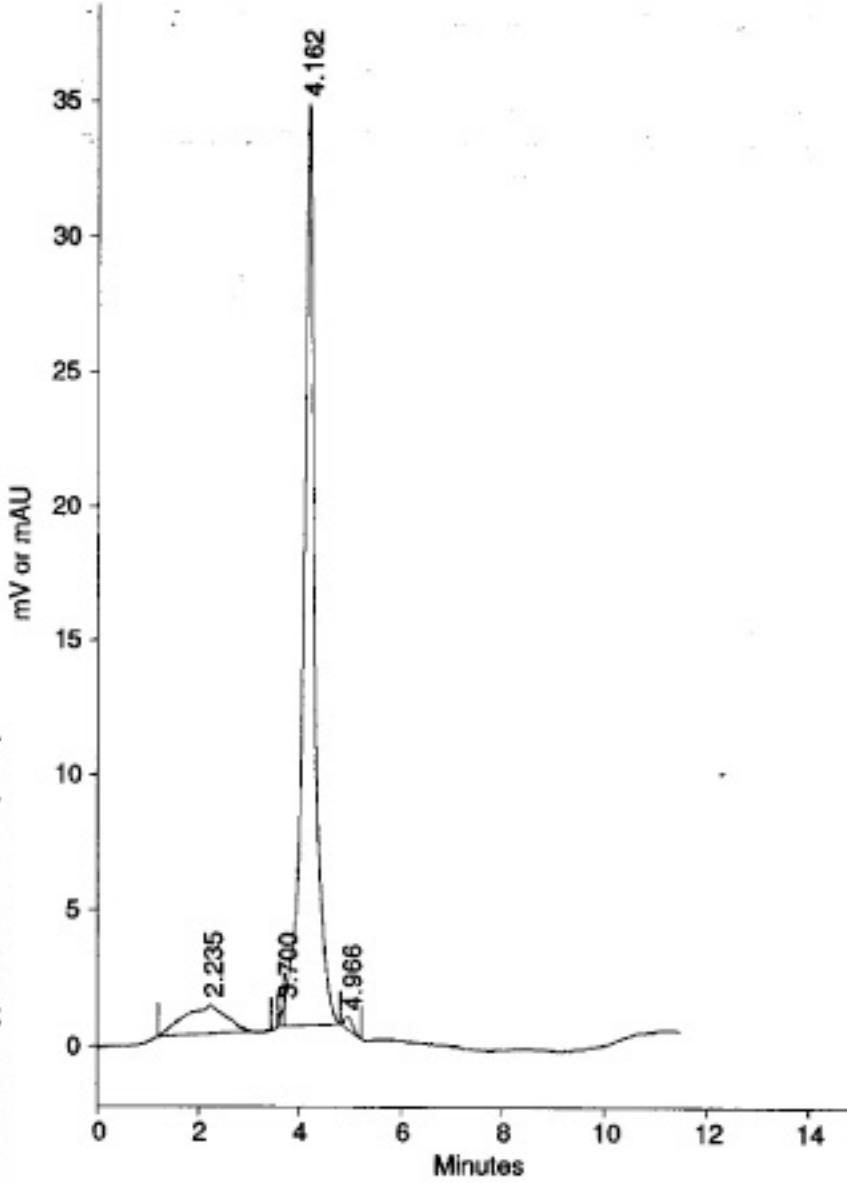
Column Pressure (PSI): 1333
Noise (microAU): 26+01
Run-Time Messages: None

Pump Flow Stability: 1.3

Column Temperature (C): N/A

Drift (microAU/min): 9e+01

Signal 1: UV3000 A 254 nm
Calculation Type: Area Percent (Area)



S51

Vial: C11
Injection: 1 of 1
Injected On: 02-26-03 14:50:08

100% Sample

#14
PrOH: C₆CN 70:30

n j fd152 isohn,Inj1, UV3000 A 254nm

Component	RT(min)	Area	Height	Area%	Peak Type
Unident001	2.235	59167	1052	9.86	Resolved
Unident002	3.700	3172	773	0.53	Fused
Unident003	4.162	532380	34165	88.76	Fused
Unident004	4.966	5104	480	0.85	Fused
Totals		599823	36470	100.00	

System: Bertrand on Comm Port 1
Acquisition Method: C:\TSP\SYSTEM\UVFLUO\Methods\fd152 isohn.AQM
Calculation Method: C:\TSP\SYSTEM\UVFLUO\Methods\DEFAULT.CAM

Analyst: <GUEST>
PC1000 Ver 3.5 Test Rel 17
02-06-03 12:09:28
08-28-00 09:43:20

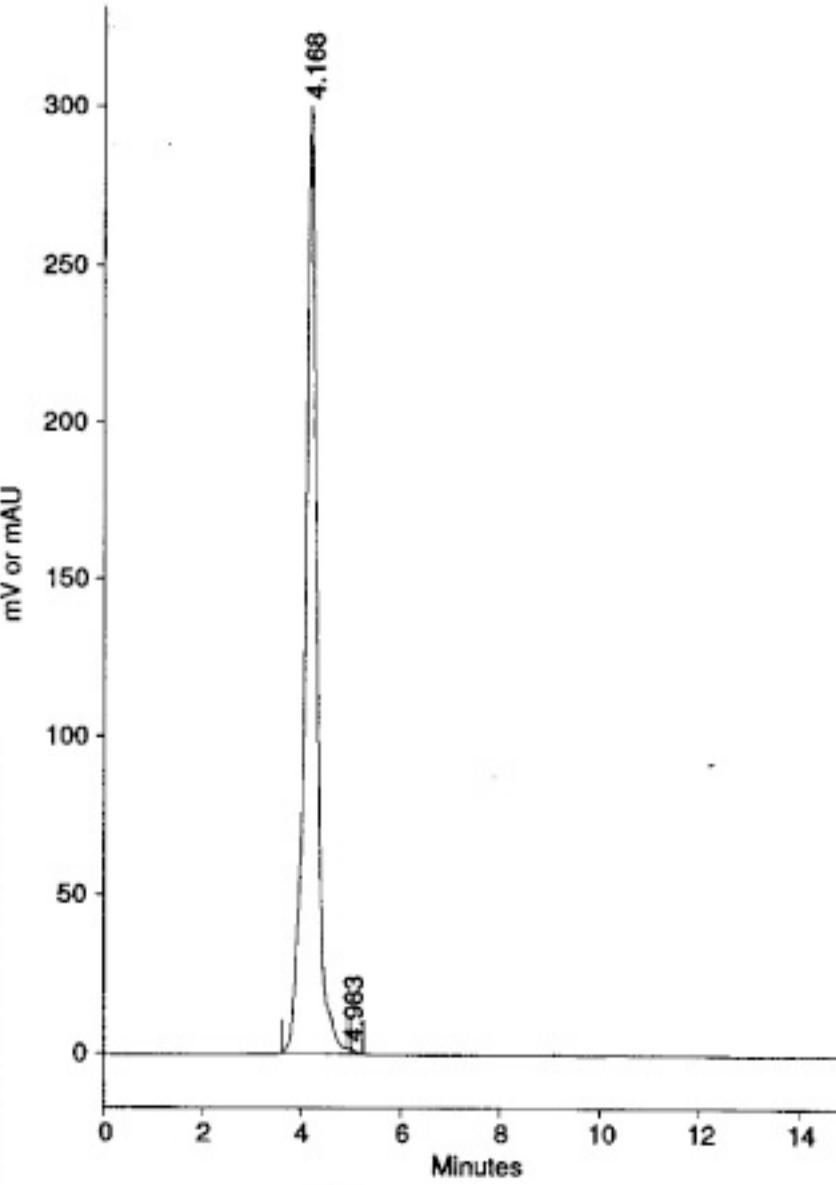
Page 17
02-06-03 12:09:28
08-28-00 09:43:20

Analysis Report

Name: n jda40 isoh1
Type: Sample
Injection Volume: 15.0 μ L

Acquisition Log
Column Pressure (PSI): 328
Noise (microAU): 2e+01
Run-Time Messages: None

Signal 1: UV3000 A 254 nm
Calculation Type: Area Percent (Area)



S52

Vial: A04
Injection: 1 of 1
Injected On: 11-20-02 13:47:26

#15

iPrOH:CH₃CN 70:30

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	4.168	4853764	300203	99.99	Fused
Unident0002	4.983	245	75	5.05e-03	Fused
Totals		4854009	300278	100.00	

System: Bertrand on Comm Port 1
Acquisition Method: C:\TSP\SYSTEMUVFLUO\Methods\nicole.AQM
Calculation Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.CAM
Report Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.RPM

PC1000 Ver 3.5 Test Rel 170
01-17-03 14:38:44
08-28-00 09:43:20
08-28-00 09:43:20

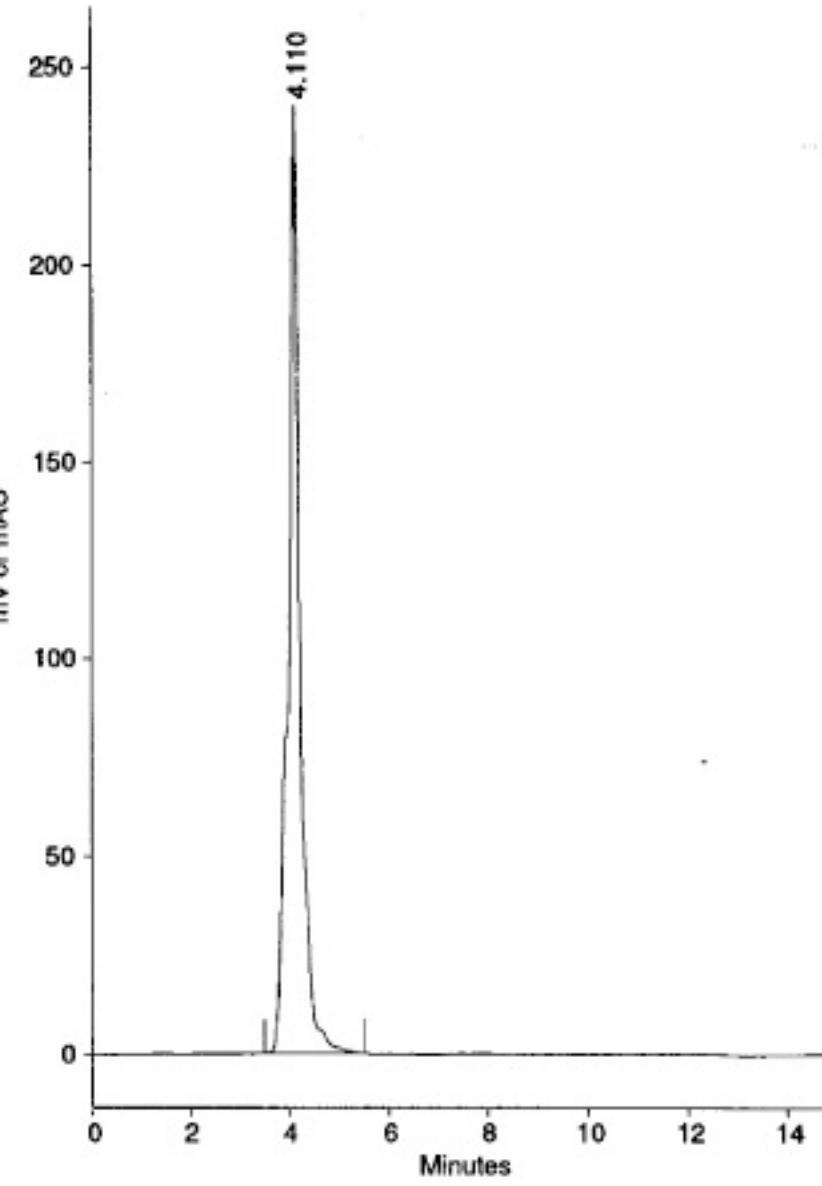
Mode: Acquired Data
Original Results: C:\TSP\SYSTEM\UVFLUO\Da\jda42.lsoh.RES

Analysis Report

Name: jda42.lsoh
Type: Sample
Injection Volume: 15.0 μ L

Acquisition Log
Column Pressure (PSI): 307
Noise (microAU): 2e+01
Run-Time Messages: None

Signal 1: UV3000 A 254 nm
Calculation Type: Area Percent (Area)



System: Bertrand on Comm Port 1
Acquisition Method: C:\TSP\SYSTEM\UVFLUO\Methods\nicole.AQM
Calculation Method: C:\TSP\SYSTEM\UVFLUO\Methods\DEFAULT.CAM
Report Method: C:\TSP\SYSTEM\UVFLUO\Methods\DEFAULT.RPM

Analyst: <GUEST>

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	4.110	3974549	239858	100.00	Resolved
Totals		3974549	239858	100.00	

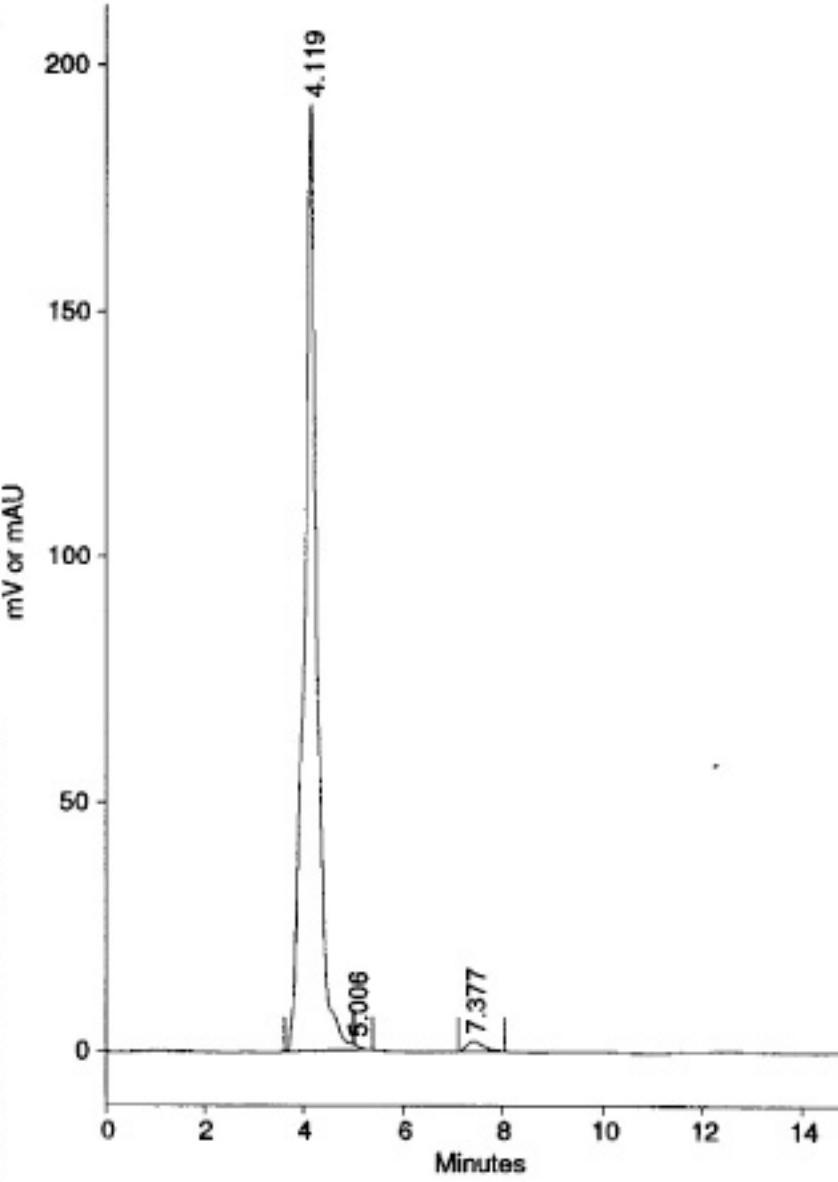
PC1000 Ver 3.5 Test Rel 17
01-17-03 14:38:44
08-28-00 09:43:20
08-28-00 09:43:20

Analysis Report

Name: n jda41 isoh1
Type: Sample
Injection Volume: 15.0 μ L

Acquisition Log
Column Pressure (PSI): 331
Noise (microAU): 2e+01
Run-Time Messages: None

Signal 1: UV3000 A 254 nm
Calculation Type: Area Percent (Area)



Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	4.119	3386050	192124	96.66	Fused
Unident0002	5.006	29	53	8.45e-04	Fused
Unident0003	7.377	46455	1903	1.35	Resolved
Totals		3432534	194080	100.00	

System: Bertrand on Comm Port 1
Acquisition Method: C:\TSP\SYSTEMUVFLUO\Methods\nicole.AQM
Calculation Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.CAM
Report Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.RPM

Analyst: <GUEST>

PC1000 Ver 3.5 Test Ref 17
01-17-03 14:38:44
08-28-00 09:43:20
08-28-00 09:43:20

Mode: Acquired Data
Original Results: C:\TSP\SYSTEM\UVFLUO\Results\jda39_isOH2-26.RES
Notes:

Page 1
Reported On: 02-26-03 16:47:09

Analysis Report

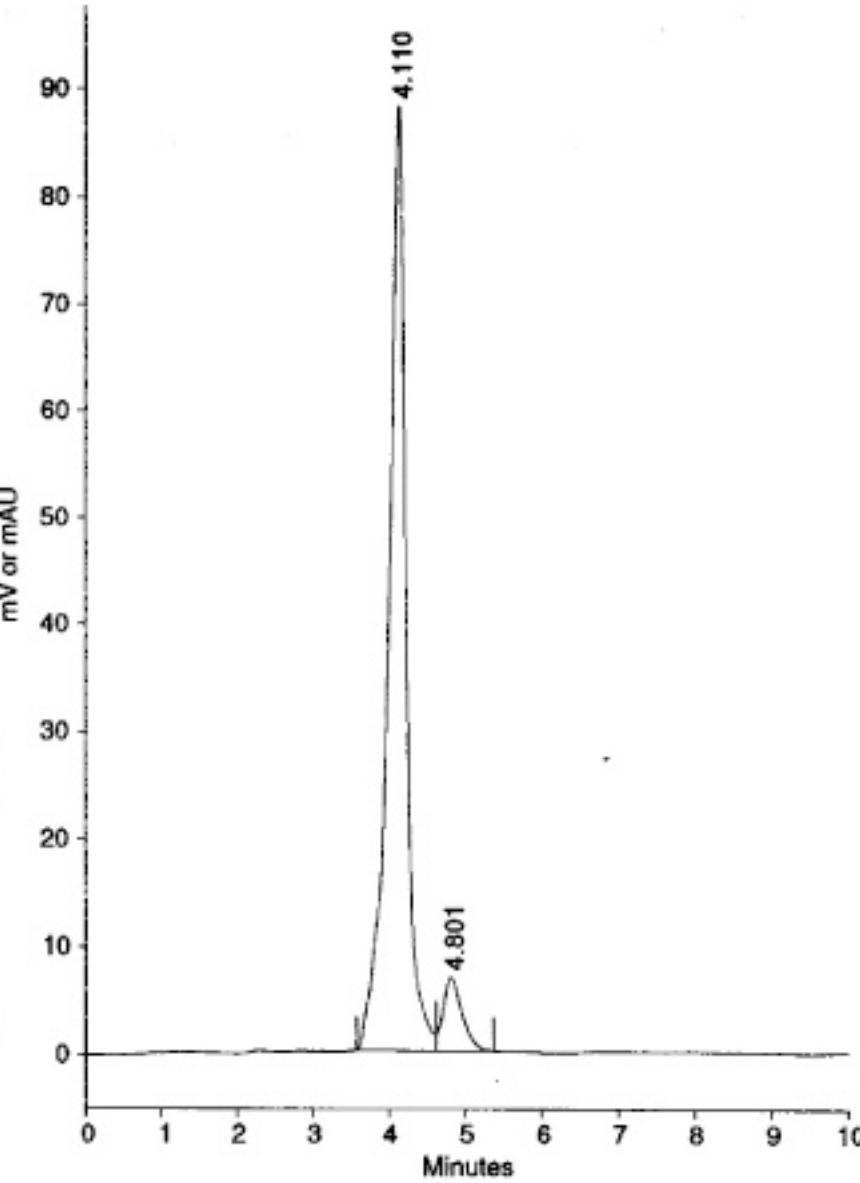
Name: n_jda39_isOH2-26
Type: Sample
Injection Volume: 10.0 μ L

Acquisition Log

Column Pressure (PSI): 1334
Noise (microAU): 2e+01
Run-Time Messages: None

Signal 1: UV3000 A 254 nm

Calculation Type: Area Percent (Area)



S55

#18

PrOH: CH₃CN 70:30

n jda39_isOH2-26, Inj1, UV3000 A 254nm

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	4.110	1387479	88125	92.24	Fused
Unident0002	4.801	116734	6796	7.76	Fused
Totals		1504213	94921	100.00	

System: Bertrand on Compaq Port 1
Acquisition Method: C:\TSP\SYSTEM\UVFLUO\Methods\nicole_jda_isoh.AQM
Analyst: <GUEST>

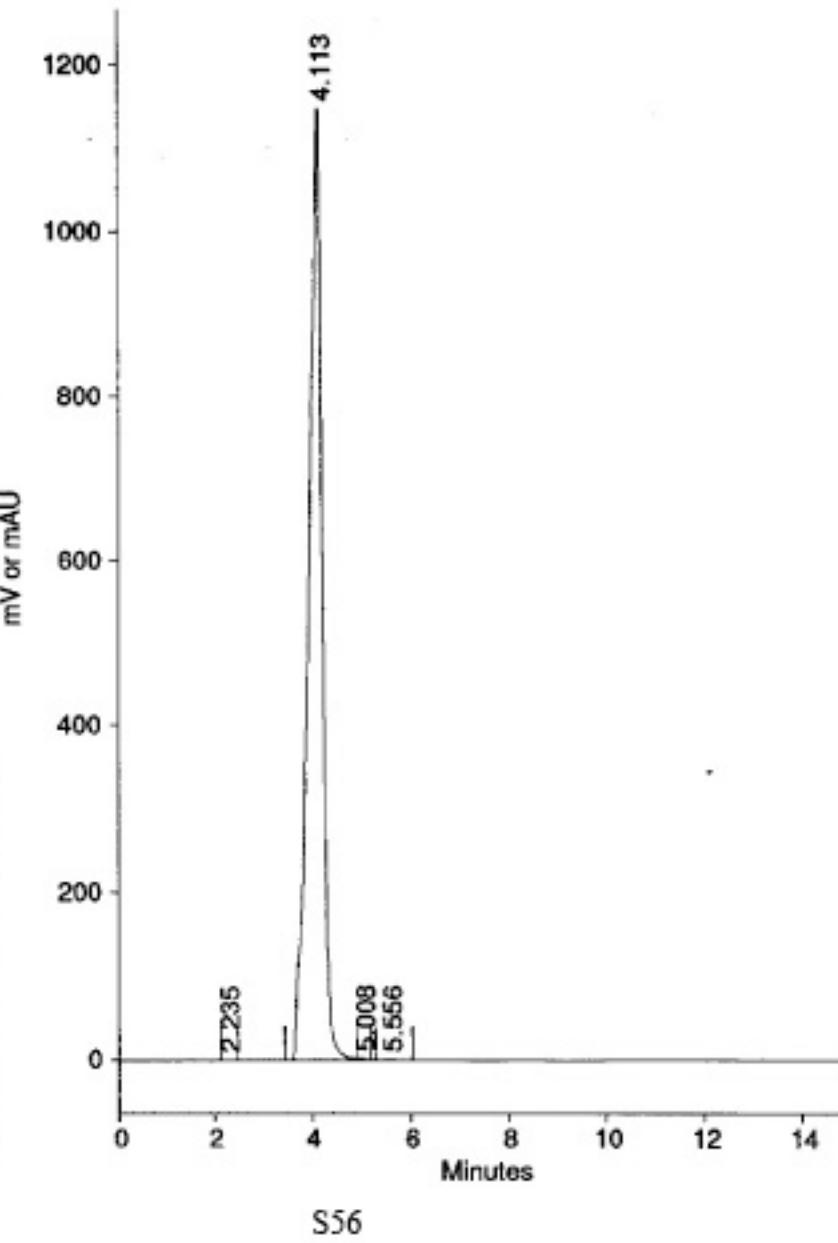
PC1000 Ver 3.5 Test Rel 17
02-26-03 16:06:32

Analysis Report

Name: n\jda73\isoh2-26
Type: Sample
Injection Volume: 10.0 μ L

Acquisition Log
Column Pressure (PSI): 1384
Noise (microAU): 2e+01
Run-Time Messages: None

Signal 1: UV3000 A 254 nm
Calculation Type: Area Percent (Area)



Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	2.235	4132	451	0.02	Resolved
Unident0002	4.113	21467761	1148411	99.90	Fused
Unident0003	5.008	4383	524	0.02	Fused
Unident0004	5.556	13973	770	0.07	Fused
Totals		21490249	1150156	100.00	

System: Bertrand on Comm Port 1
Acquisition Method: C:\TSP\SYSTEMUVFLUO\Methods\jda_isoh.AQM
Calculation Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.CAM

Analyst: <GUEST>
PC1000 Ver 3.5 Test Rel 17
02-06-03 12:09:28
08-28-00 09:43:20

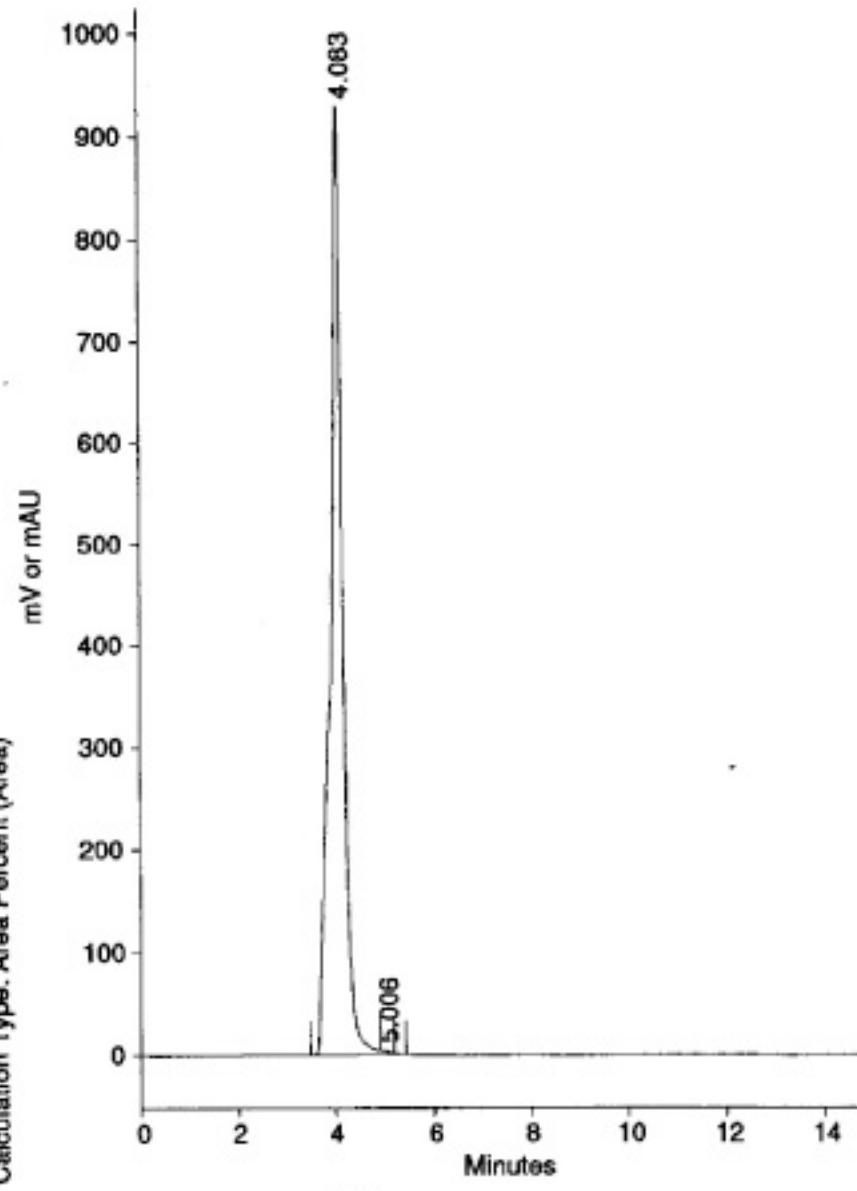
Injection: 1 of 1
Injected On: 02-26-03 14:01:44

Analysis Report

Name: n jda65 isOH
Type: Sample
Injection Volume: 15.0 μ L

Acquisition Log
Column Pressure (PSI): 318
Noise (microAU): 2e+01
Run-Time Messages: None

Signal 1: UV3000 A 254 nm
Calculation Type: Area Percent (Area)



S57

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	4.063	15846176	929743	99.95	Fused
Unident0002	5.006	7421	837	0.05	Fused
Totals		15853597	930580	100.00	

System: Bertrand on Comm Port 1
Acquisition Method: C:\TSP\SYSTEM\UVFLUO\Methods\nicole.ACM
Calculation Method: C:\TSP\SYSTEM\UVFLUO\Methods\DEFAULT.CAM
Report Method: C:\TSP\SYSTEM\UVFLUO\Methods\DEFAULT.RPM

Analyst: <GUEST>

PC1000 Ver 3.5 Test Rel 17
01-17-03 14:38:44
08-28-00 09:43:20
08-28-00 09:43:20

Analysis Report

Name: n jda66 isoh2-26
Type: Sample
Injection Volume: 10.0 μ L

Injection: 1 of 1
Injected On: 02-26-03 13:13:16

Acquisition Log

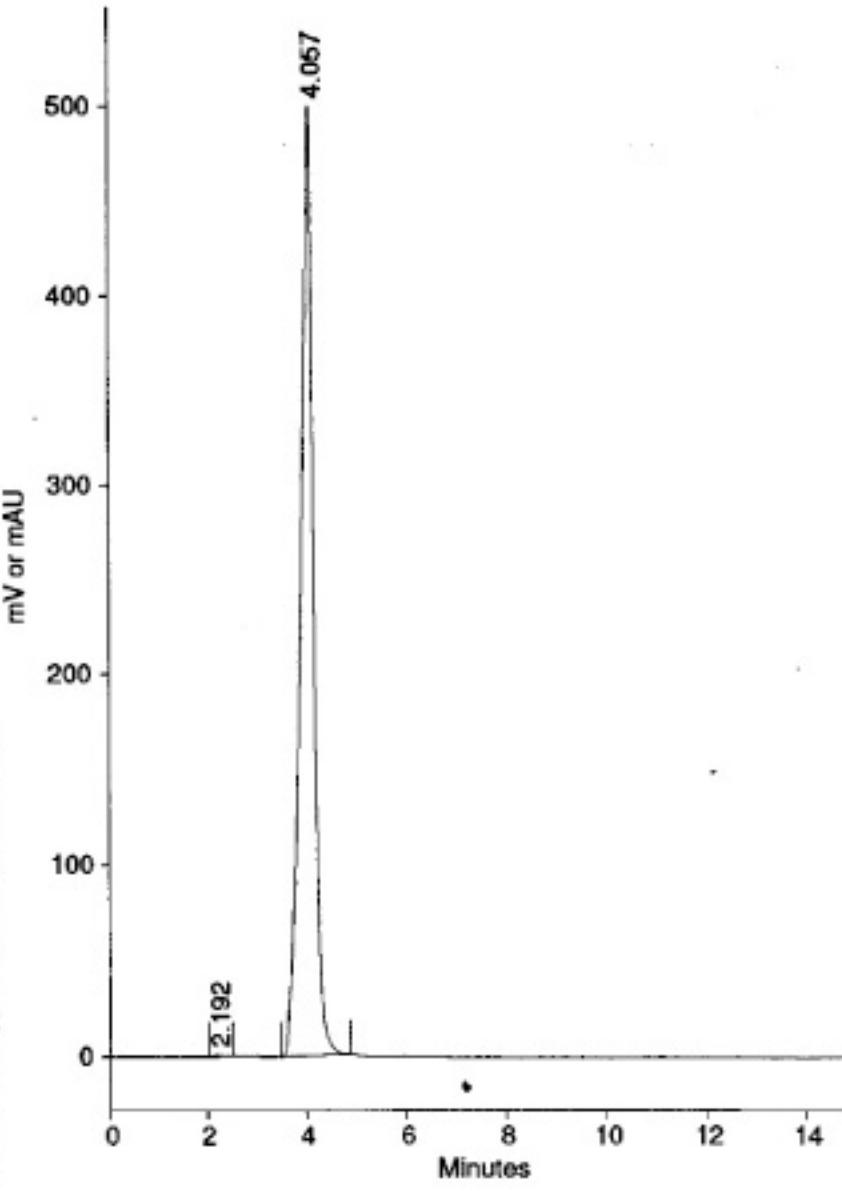
Column Pressure (PSI): 1624
Noise (microAU): 2e+01
Run-Time Messages: None

Column Temperature (C): N/A

Drift (micro AU/min): 1e+02
Pump Flow Stability: 19.8

Signal 1: UV3000 A 254 nm

Calculation Type: Area Percent (Area)



Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	2.192	9594	798	0.11	Resolved
Unident0002	4.057	8798894	499712	99.89	Resolved
Total's		8808488	500510	100.00	

System: Bertrand on Comm Port 1

Acquisition Method: C:\TSP\SYSTEMUVFLUO\METHODS\nicole jda isoh.AQM

Calculation Method: C:\TSP\SYSTEMUVFLUO\METHODS\DEFAULT.CAM

Report Method: C:\TSP\SYSTEMUVFLUO\METHODS\DEFAULT.RPM

Analyst: <GUEST>

PC1000 Ver 3.5 Test Rel 17
02-06-03 12:09:26
08-28-00 09:43:20
08-28-00 09:43:20

Mode: Acquired Data
Original Results: C:\TSP\SYSTEM\UVFLUO\Results\jda56 IsOH2-26.RES
Notes:

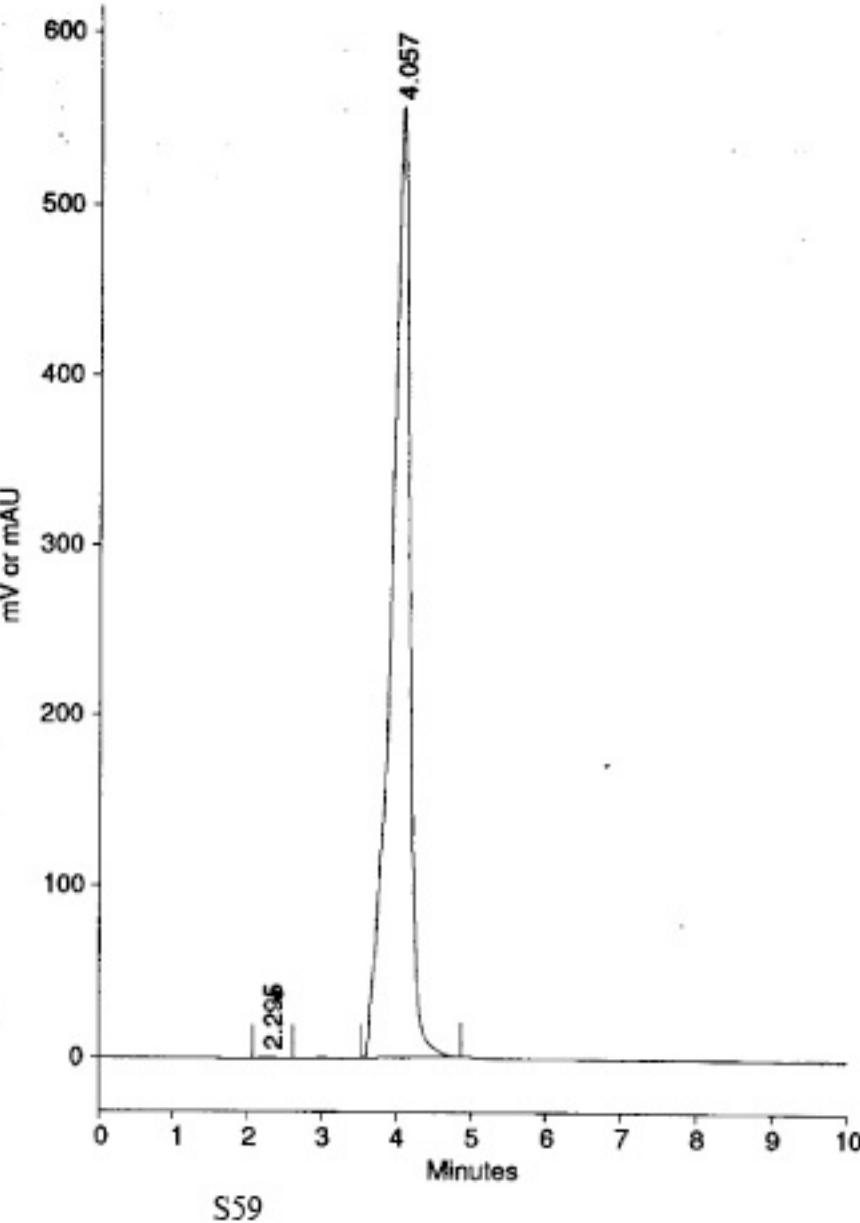
Page 1
Reported On: 02-26-03 16:48:16

Analysis Report

Name: n jda56 IsOH2-26
Type: Sample
Injection Volume: 10.0 μ L

Acquisition Log
Column Pressure (PSI): 1380
Noise (microAU): 2e+01
Run-Time Messages: None

Signal 1: UV3000 A 254 nm
Calculation Type: Area Percent (Area)



S59

Vial: C17
Injection: 1 of 1
Injected On: 02-26-03 16:37:47

Column Temperature (C): N/A
Drift (microAU/min): -1e+02
Pump Flow Stability: 5.0

#22 iPrOH: Et₃CN 70:30

n jda56 IsOH2-26, Inj1, UV3000 A 254nm

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	2.295	5742	441	0.06	Resolved
Unident0002	4.057	9630917	557190	99.94	Resolved
Totals		9636659	557631	100.00	

System: Bertrand on Comm Port 1
Acquisition Method: C:\TSP\SYSTEM\UVFLUO\Methods\jda Isoh.AQM
Analyst: <GUEST>
PC1000 Ver 3.5 Test Rel 17
02-26-03 16:06:32

Analysis Report

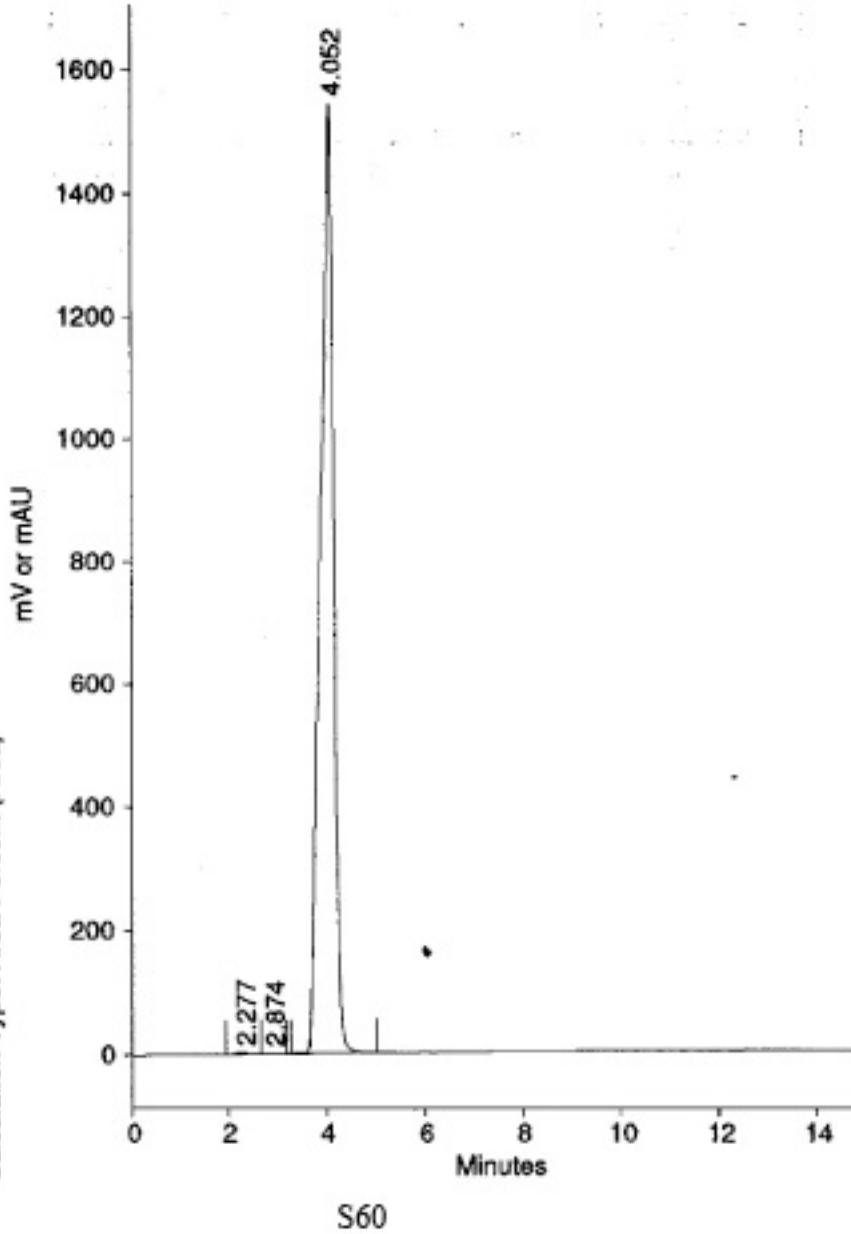
Name: jda58 isoh2-26
Type: Sample
Injection Volume: 10.0 μ L

Acquisition Log

Column Pressure (PSI): 1878
Noise (microAU): 1e+02
Run-Time Messages: None

Signal 1: UV3000 A 254 nm

Calculation Type: Area Percent (Area)



Vial: C03
Injected On: 02-26-03 12:40:54
Injection: 1 of 1

#23
iPrOH:CH₃CN 70:30

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	2.277	31773	1735	0.11	Fused
Unident0002	2.874	5638	401	0.02	Fused
Unident0003	4.052	28363563	1542290	99.87	Resolved
Totals		28400974	1544426	100.00	

System: Bertrand on Comm Port 1
Acquisition Method: C:\TSP\SYSTEM\UVFLUO\Methods\nicole.jda.isoh.AQM
Calculation Method: C:\TSP\SYSTEM\UVFLUO\Methods\DEFAULT.CAM
Report Method: C:\TSP\SYSTEM\UVFLUO\Methods\DEFAULT.RPM

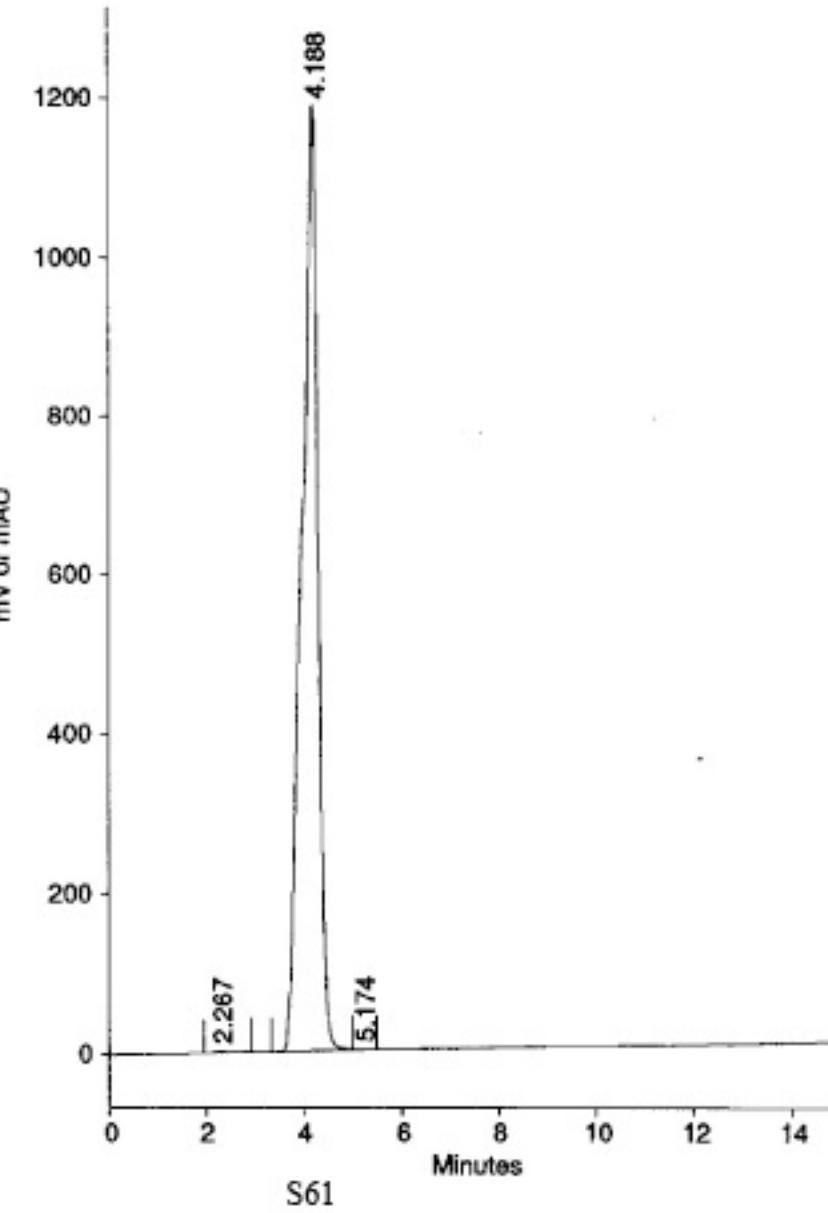
Analyst: <GUEST>
PC1000 Ver 3.5 Test Rel 17
02-06-03 12:09:28
08-28-00 09:43:20
08-28-00 09:43:20

Analysis Report

Name: n\jda52\isoh2-26
Type: Sample
Injection Volume: 10.0 μ L

Acquisition Log
Column Pressure (PSI): 1484
Noise (microAU): 9e+01
Run-Time Messages: None

Signal 1: UV3000 A 254 nm
Calculation Type: Area Percent (Area)



Vial: C02
Injected On: 02-26-03 12:24:43
Injection: 1 of 1

Column Temperature (C): N/A

Drift (microAU/min): 1e+03

Pump Flow Stability: 14.1

n\jda52\isoh2-26,Inj1,UV3000 A 254nm

#24

iPROH: Et₂CN 70:30

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	2.267	34724	2099	0.13	Resolved
Unident0002	4.188	26992152	1185894	99.85	Fused
Unident0003	5.174	4900	405	0.02	Fused
Totals		27031776	1188398	100.00	

System: Bertrand on Comm Port 1

Acquisition Method: C:\TSP\SYSTEMUVFLUO\Methods\nicole\jda isoh.AQM

Calculation Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.CAM

Report Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.RPM

Analyst: <GUEST>

PC1000 Ver 3.5 Test Rel 1

02-06-03 12:09:26

08-28-00 09:43:20

08-28-00 09:43:20

Analysis Report

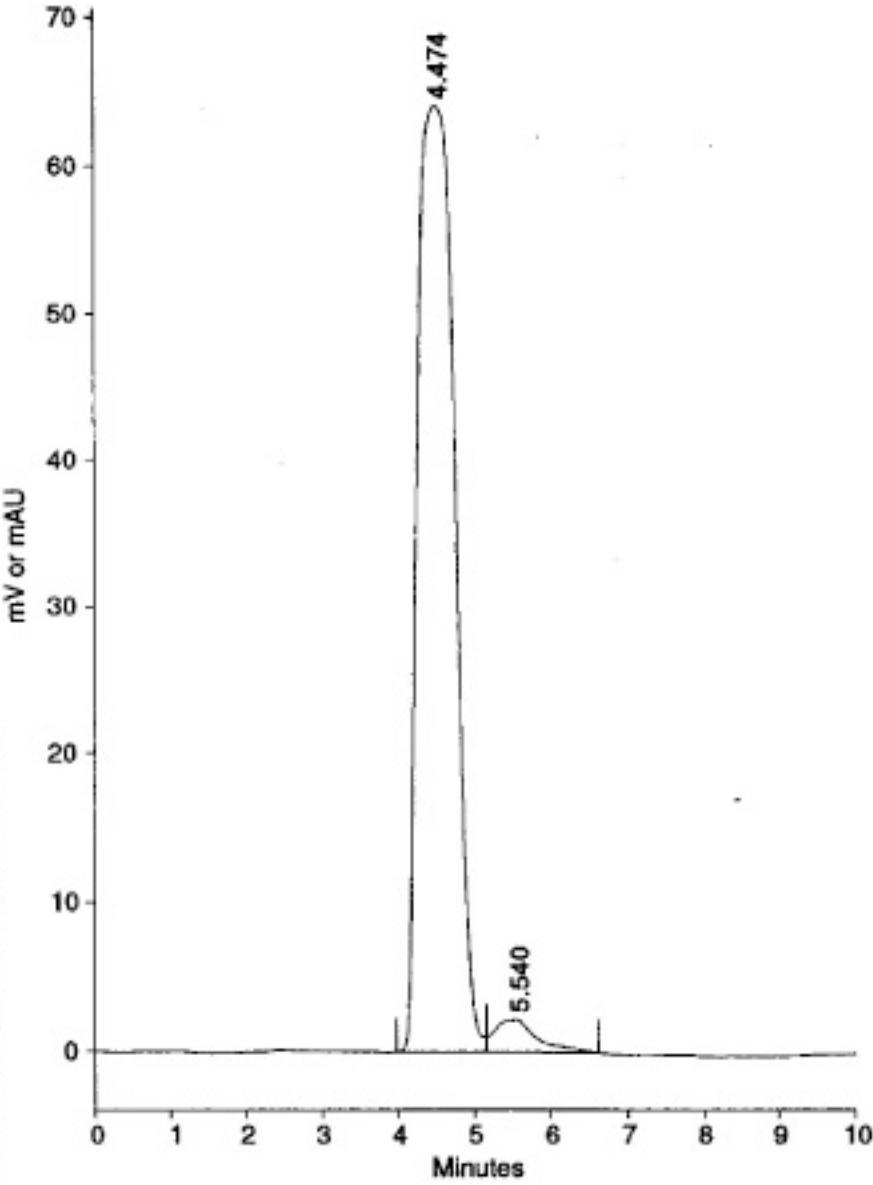
Name: jda34 dio 3-6
Type: Sample
Injection Volume: 10.0 uL

Acquisition Log

Column Pressure (PSI): 909
Noise (microAU): 20+01
Run-Time Messages: None

Signal 1: UV3000 A 254 nm

Calculation Type: Area Percent (Area)



Vial: C01
Injection: 1 of 1
Injected On: 03-06-03 14:46:20

13 iPrOH: dioxane 80:20
n jda34 dio 3-6,Inj1, UV3000 A 254nm —

Injection: 1 of 1
Injected On: 03-06-03 14:46:20

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	4.474	2130223	64147	96.10	Fused
Unident0002	5.540	86378	22223	3.90	Fused
Totals		2216601	66370	100.00	

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	4.474	2130223	64147	96.10	Fused
Unident0002	5.540	86378	22223	3.90	Fused
Totals		2216601	66370	100.00	

System: Bertrand on Comm Port 1
Acquisition Method: C:\TSP\SYSTEMUVFLUO\Methods\jda dioxane.AQM
Calculation Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.CAM
Report Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.RPM

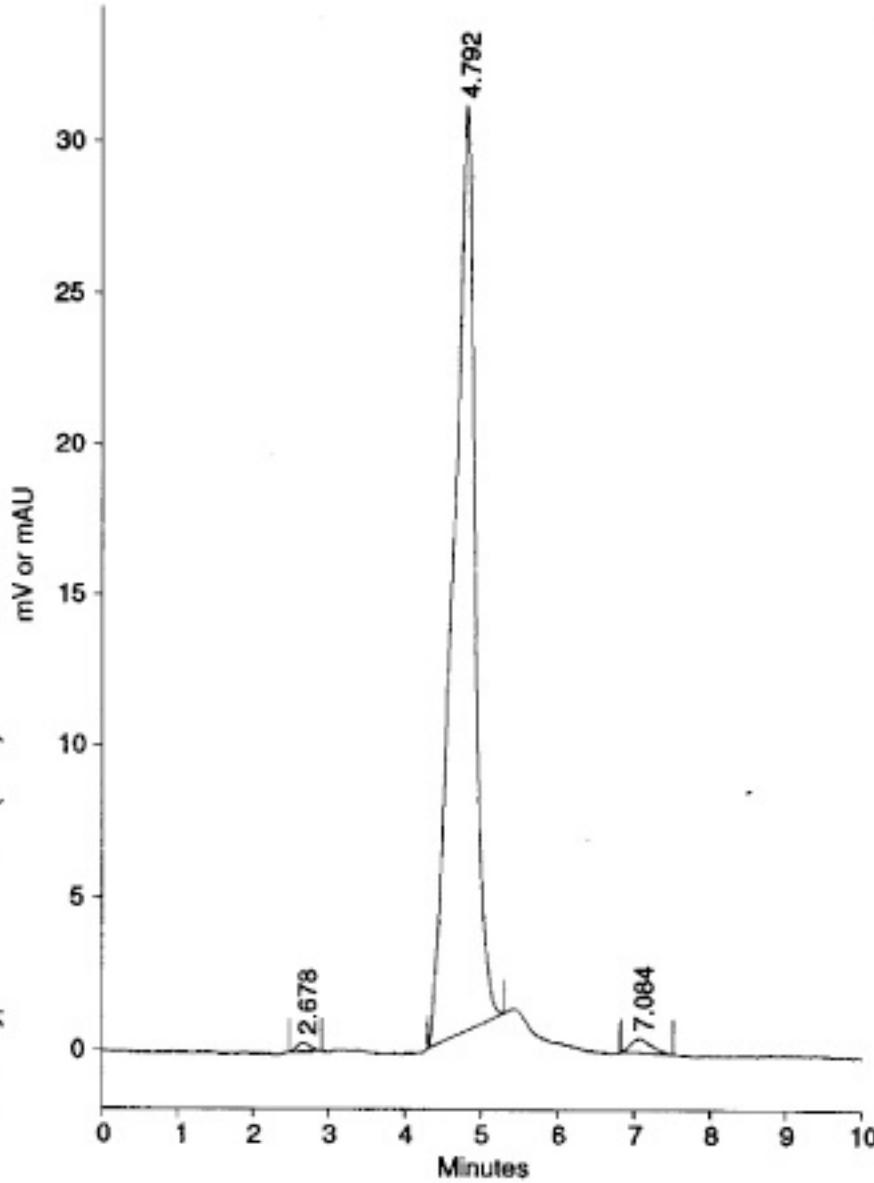
Page 17
03-06-03 14:08:52
08-28-00 09:43:20
08-28-00 09:43:20

Analysis Report

Name: n \ fd152met3-18
Type: Sample
Injection Volume: 10.0 μ L

Acquisition Log
Column Pressure (PSI): 1218
Noise (microAU): 1e+01
Run-Time Messages: None

Signal 1: UV3000 A 254 nm
Calculation Type: Area Percent (Area)



S63

Vial: C09
Injection: 1 of 1
Injected On: 03-18-03 16:50:48

#14
PROH: dioxane 80:20

n \ fd152met3-18,Inj1, UV3000 A 254nm —

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	2.678	3596	303	0.58	Resolved
Unident0002	4.792	604448	30555	98.02	Resolved
Unident0003	7.084	6635	462	1.40	Resolved
Totals		616669	31320	100.00	

System: Bertrand on Comm Port 1
Analyst: <GUEST
Acquisition Method: C:\Methods\nicole\ida\fd\methanol.AQM
Calculation Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.CAM
Report Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.RPM
PC1000 Ver 3.5 Test Rel 17
03-18-03 14:59:28
08-28-00 09:43:20
08-28-00 09:43:20

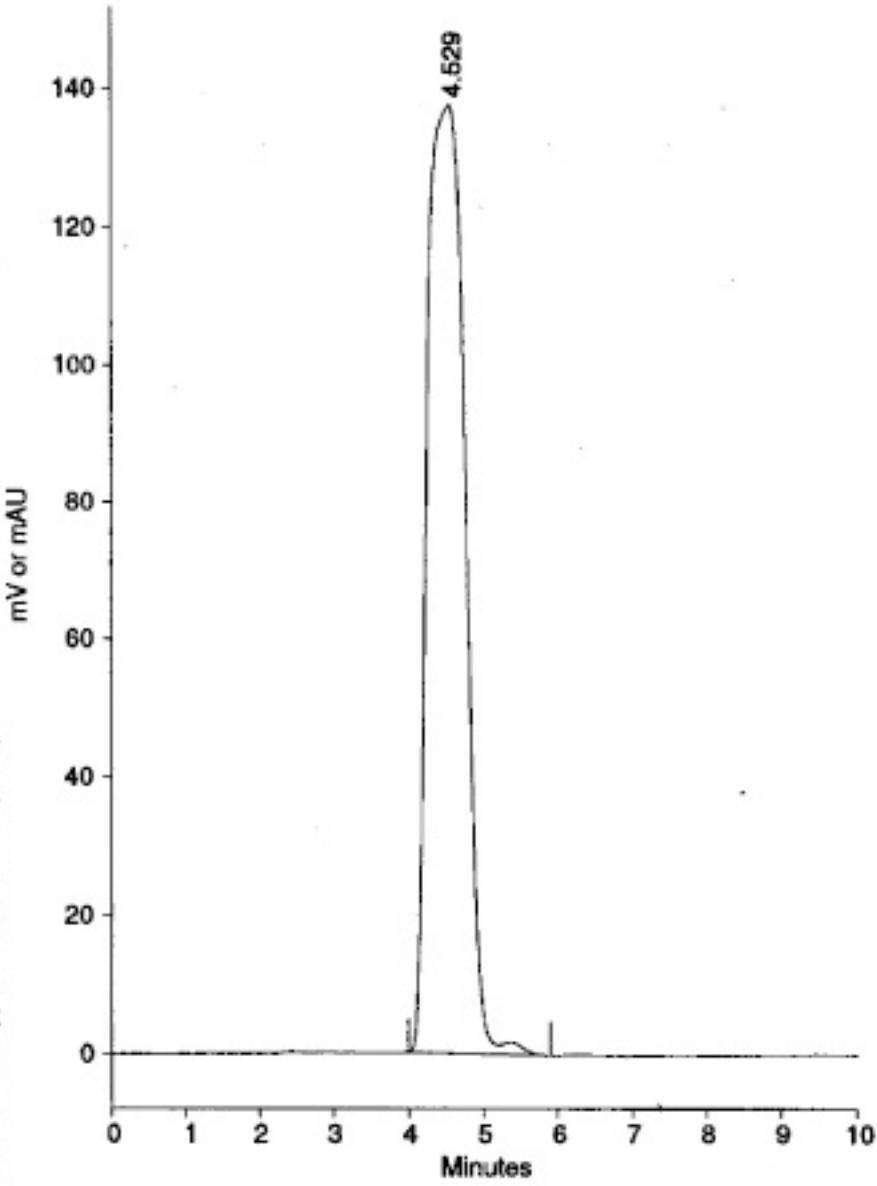
Analysis Report

Name: n jda40 DiAc 3-6
Type: Sample
Injection Volume: 10.0 μ L

Acquisition Log

Column Pressure (PSI): 881
Noise (microAU): 3e+01
Run-Time Messages: None

Signal 1: UV3000 A 254 nm
Calculation Type: Area Percent (Area)



Component
Unident0001
Totals

RT(min) Area Height Area% Peak Type
4.529 4783396 137421 100.00 Resolved

System: Bertrand on Comm Port 1
Acquisition Method: C:\TSP\SYSTEMUVFLUO\Methods\n jda dioxane.AQM
Calculation Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.CAM
Report Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.RPM

Analyst: <GUEST>
PC1000 Ver 3.5 Test Rel 10
03-06-03 14:08:52
08-28-00 09:43:20
08-28-00 09:43:20

#15
iPrOH: dioxane 80:20

Analysis Report

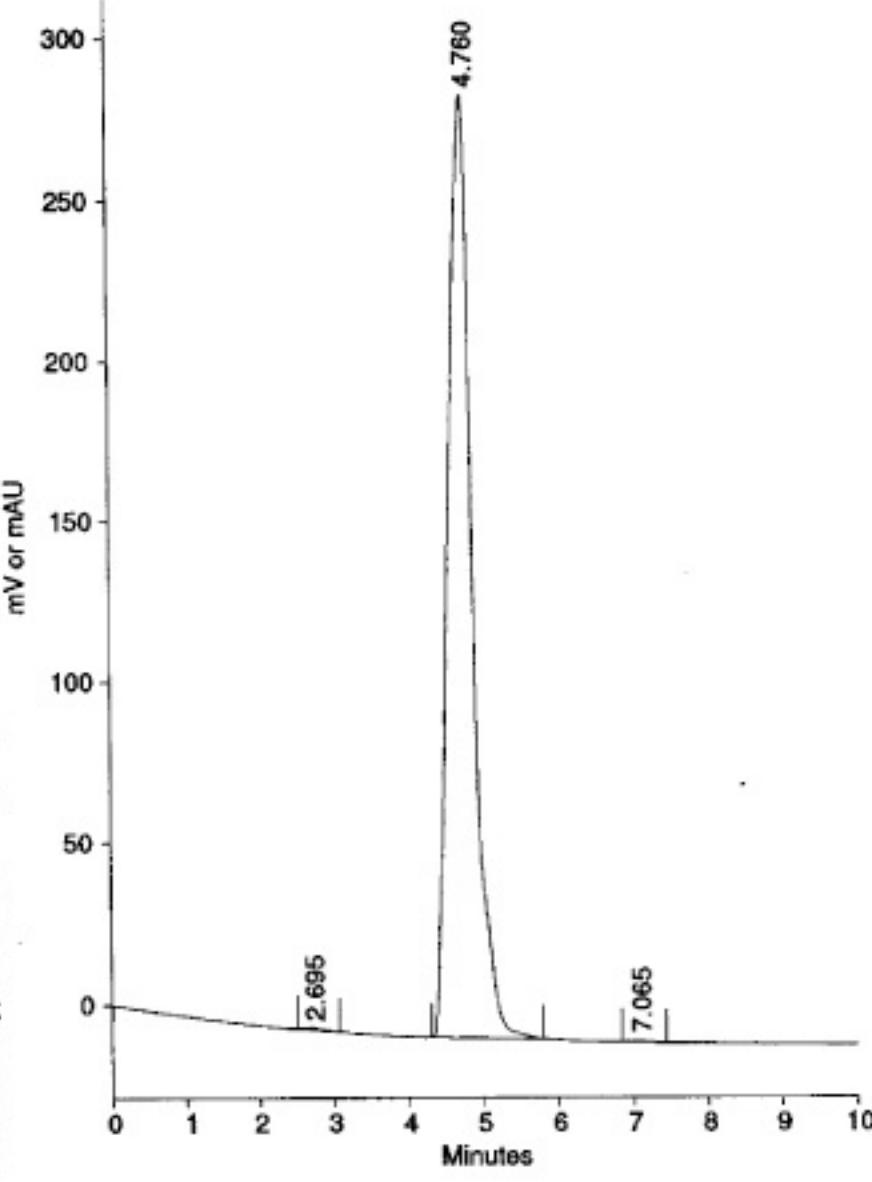
Name: n\fd127met3-18
Type: Sample
Injection Volume: 10.0 uL

Vial: C05
Injection: 1 of 1
Injected On: 03-18-03 16:06:07

Acquisition Log
Column Pressure (PSI): 896
Noise (microAU): 5e+02
Run-Time Messages: None

Column Temperature (C): N/A
Drift (microAU/min): -3e+03
Pump Flow Stability: 7.6

Signal 1: UV3000 A 254 nm
Calculation Type: Area Percent (Area)



Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	2.695	7714	660	0.12	Resolved
Unident0002	4.760	6542775	292563	99.79	Resolved
Unident0003	7.065	6295	393	0.10	Resolved
Totals		6556794	293616	100.00	

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	2.695	7714	660	0.12	Resolved
Unident0002	4.760	6542775	292563	99.79	Resolved
Unident0003	7.065	6295	393	0.10	Resolved
Totals		6556794	293616	100.00	

System: Bertrand on Comm Port 1
Acquisition Method: C:\Methods\nicole\ida\fd methanol.AQM
Calculation Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.CAM
Report Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.RPM

Analyst: <GUEST
PC1000 Ver 3.5 Test Rel 17

03-18-03 14:59:28
08-28-00 09:43:20
08-28-00 09:43:20

#16 ,PrOH:dioxane 80:20

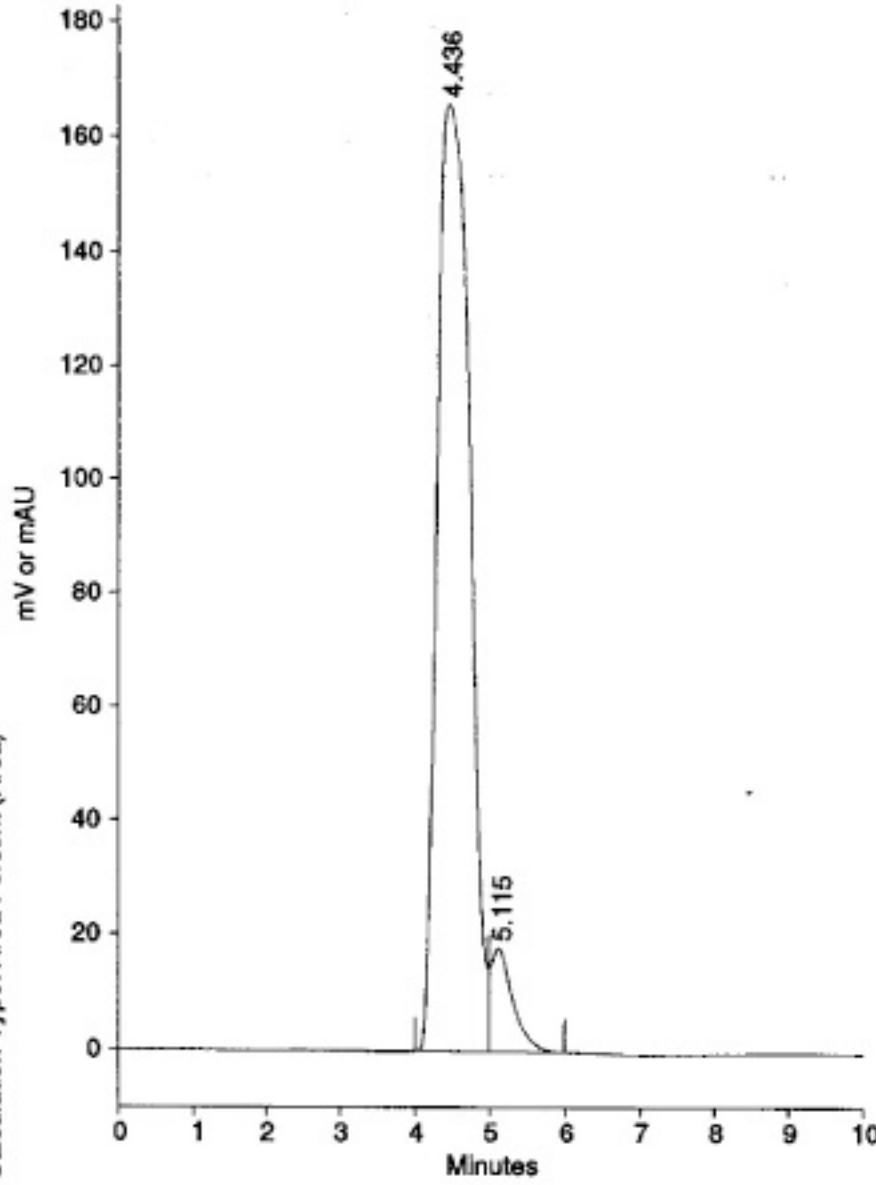
Analysis Report

Name: n jda41 DiAc 3-6
Type: Sample
Injection Volume: 10.0 uL

Acquisition Log

Column Pressure (PSI): 901
Noise (microAU): 2e+01
Run-Time Messages: None

Signal 1: UV3000 A 254 nm
Calculation Type: Area Percent (Area)



#17 iPrOH:dioxane 80:20

n jda41 DiAc 3-6,Inj1, UV3000 A 254nm

Vial: C05
Injection: 1 of 1
Injected On: 03-06-03 14:35:09

Pump Flow Stability: 3.7
Column Temperature (C): N/A
Drift (microAU/min): 1e+02

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	4.436	5010995	165922	93.24	Fused
Unident0002	5.115	363477	17998	6.76	Fused
Totals		5374472	183920	100.00	

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	4.436	5010995	165922	93.24	Fused
Unident0002	5.115	363477	17998	6.76	Fused
Totals		5374472	183920	100.00	

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	4.436	5010995	165922	93.24	Fused
Unident0002	5.115	363477	17998	6.76	Fused
Totals		5374472	183920	100.00	

System: Bertrand on Comm Port 1
Acquisition Method: C:\TSP\SYSTEM\UVFLUO\Methods\n jda dioxane.AQM
Calculation Method: C:\TSP\SYSTEM\UVFLUO\Methods\DEFAULT.CAM
Report Method: C:\TSP\SYSTEM\UVFLUO\Methods\DEFAULT.RPM

PC1000 Ver 3.5 Test Rel 17
03-06-03 14:08:52
08-26-00 09:43:20
08-26-00 09:43:20

Analysis Report

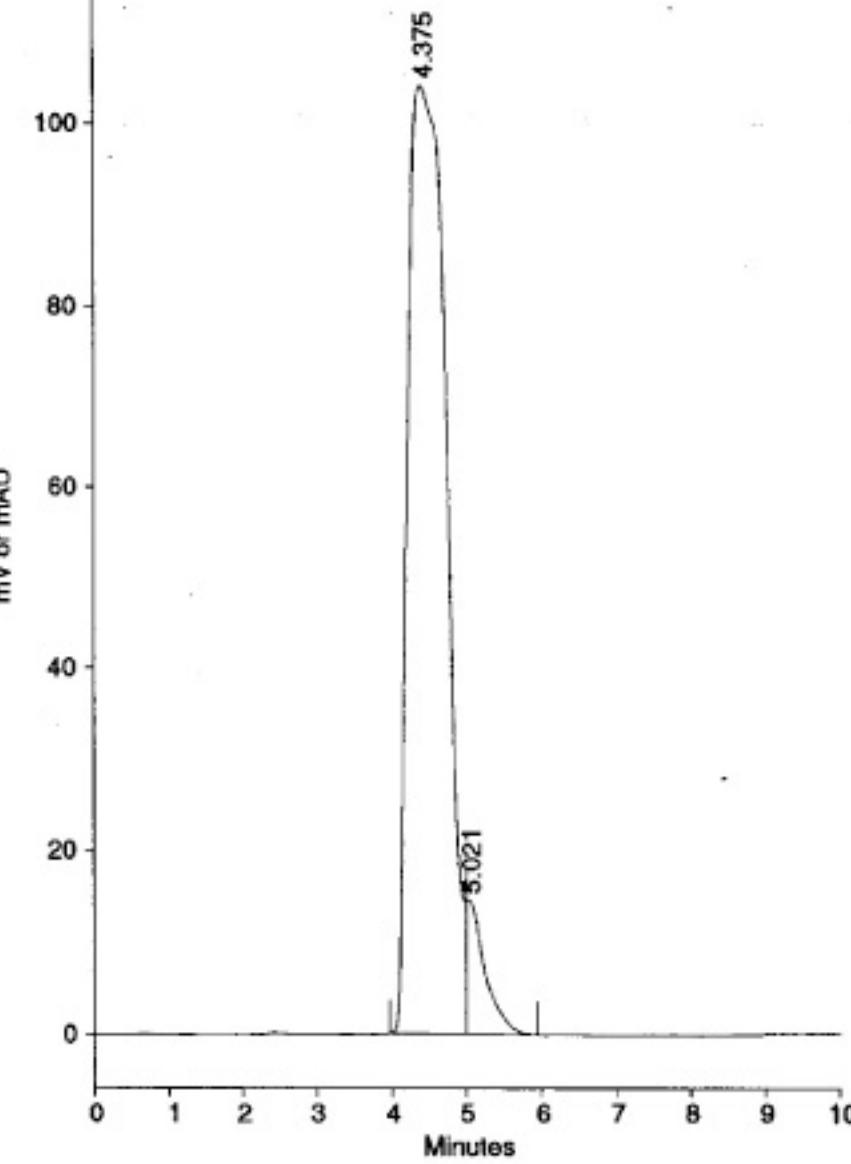
Name: jda39 dio 3-6
Type: Sample
Injection Volume: 10.0 μ L

Acquisition Log

Column Pressure (PSI): 919
Noise (microAU): 2e+01
Run-Time Messages: None

Signal 1: UV3000 A 254 nm

Calculation Type: Area Percent (Area)



n jda39 dio 3-6,Inj1, UV3000 A 254nm —

Vial: C03
Injection: 1 of 1
Injected On: 03-06-03 15:08:39

#18 NaOH:dioxane 80:20

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	4.375	3702872	103988	93.70	Fused
Unident0002	5.021	249013	14477	6.30	Fused
Totals		3951885	118465	100.00	

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	4.375	3702872	103988	93.70	Fused
Unident0002	5.021	249013	14477	6.30	Fused
Totals		3951885	118465	100.00	

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	4.375	3702872	103988	93.70	Fused
Unident0002	5.021	249013	14477	6.30	Fused
Totals		3951885	118465	100.00	

System: Bedrand on Comm Port 1
Analyst: <GUEST>
Acquisition Method: C:\TSP\SYSTEM\UVFLUO\Methods\jda dioxane.AQM
Calculation Method: C:\TSP\SYSTEM\UVFLUO\Methods\DEFAULT.CAM
Report Method: C:\TSP\SYSTEM\UVFLUO\Methods\DEFAULT.RPM

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03-06-03 14:08:52
03-28-00 09:43:20
03-28-00 09:43:20

Analysis Report

Name: jda73 dio 3-6
Type: Sample
Injection Volume: 10.0 μ L

Acquisition Log

Column Pressure (PSI): 909

Column Temperature (C): N/A

Drift (microAU/min): 7e+01

Run-Time Messages: None

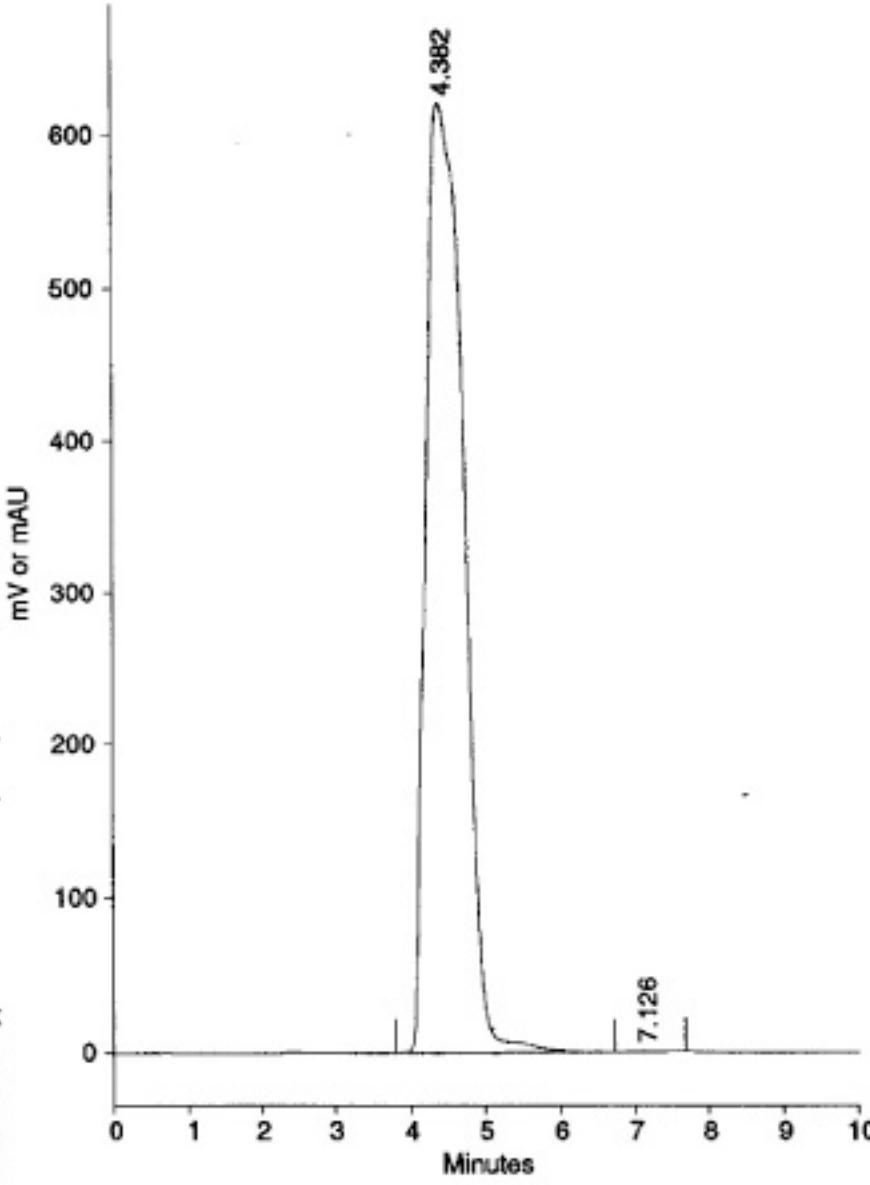
Noise (microAU): 2e+01

Pump Flow Stability: 4.3

Run-Time Messages: None

Signal 1: UV3000 A 254 nm

Calculation Type: Area Percent (Area)



S68

Vial: C14
Injection: 1 of 1
Injected On: 03-06-03 16:49:03

#19 iPrOH: dioxane 80:20

n jda73 dio 3-6,Inj1, UV3000 A 254nm

PC1000 Ver 3.5 Test Rel 17
03-06-03 14:08:52
08-28-00 09:43:20
08-28-00 09:43:20

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	4.382	21791152	620363	99.93	Fused
Unident0002	7.126	14219	663	0.07	Fused
Totals		21805371	621026	100.00	

System: Bertrand on Comm Port 1
Analyst: <GUEST>
Acquisition Method: C:\TSP\SYSTEMUVFLUO\Methods\jda dioxane.AQM
Calculation Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.CAM
Report Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.RPM

^{b3}
jda65 dio 3-6.RES

Analysis Report

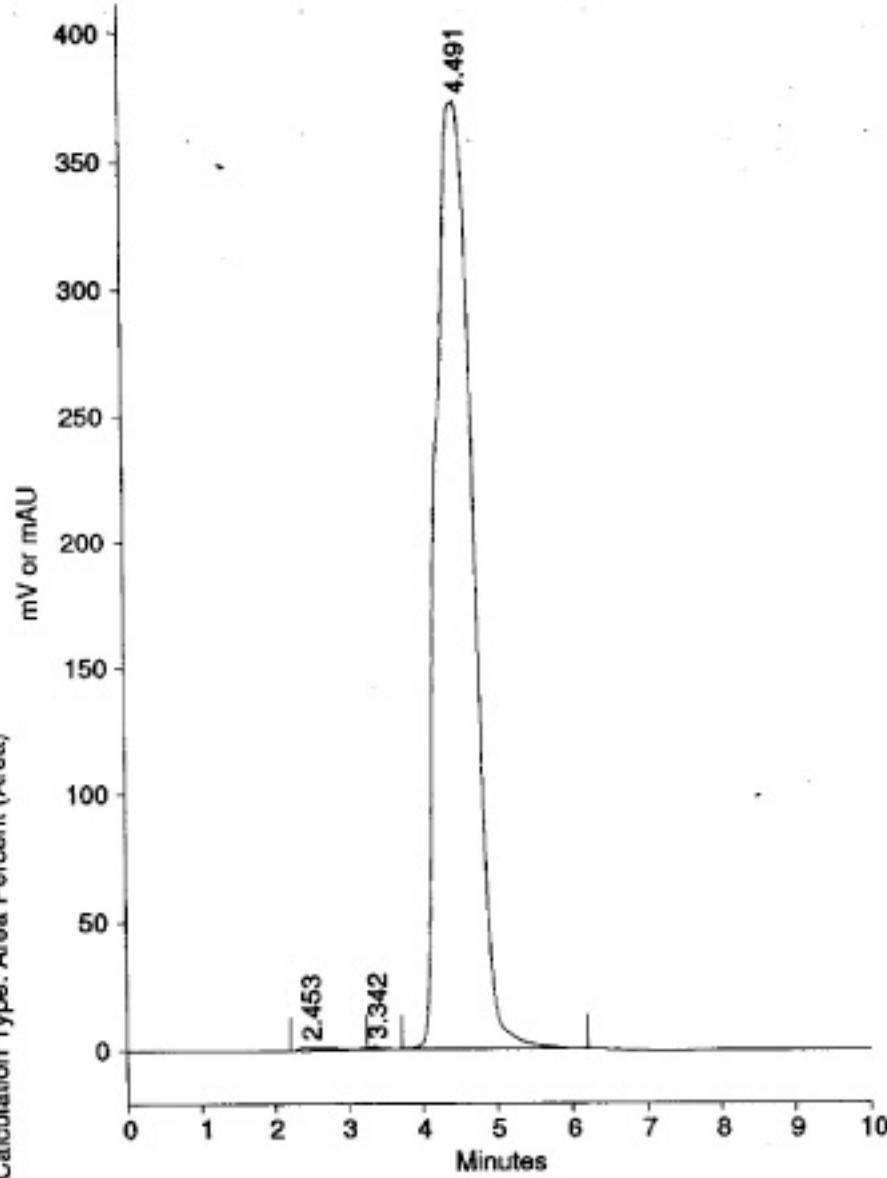
Name: jda65 dio 3-6
Type: Sample
Injection Volume: 10.0 μ L

Acquisition Log

Column Pressure (PSI): 932
Noise (microAU): 2e+01
Run-Time Messages: None

Signal 1: UV3000 A 254 nm

Calculation Type: Area Percent (Area)



Vial: C21
Injection: 1 of 1
Injected On: 03-06-03 18:07:09

#20 jda65 dio 3-6.Inj1, UV3000 A 254nm

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	2.453	37310	1172	0.30	Fused
Unident0002	3.342	10485	1042	0.08	Fused
Unident0003	4.491	12381363	372858	99.62	Fused
Totals		12429158	375072	100.00	

System: Bertrand on Comm Port 1
Acquisition Method: C:\TSP\SYSTEM\UVFLUO\Methods\jda_dioxane.AQM
Calculation Method: C:\TSP\SYSTEM\UVFLUO\Methods\DEFAULT.CAM
Report Method: C:\TSP\SYSTEM\UVFLUO\Methods\DEFAULT.RPM

Analyst: <GUEST>
PC1000 Ver 3.5 Test Rel 17
03-06-03 14:08:52
08-28-00 09:43:20
08-28-00 09:43:20

Analysis Report

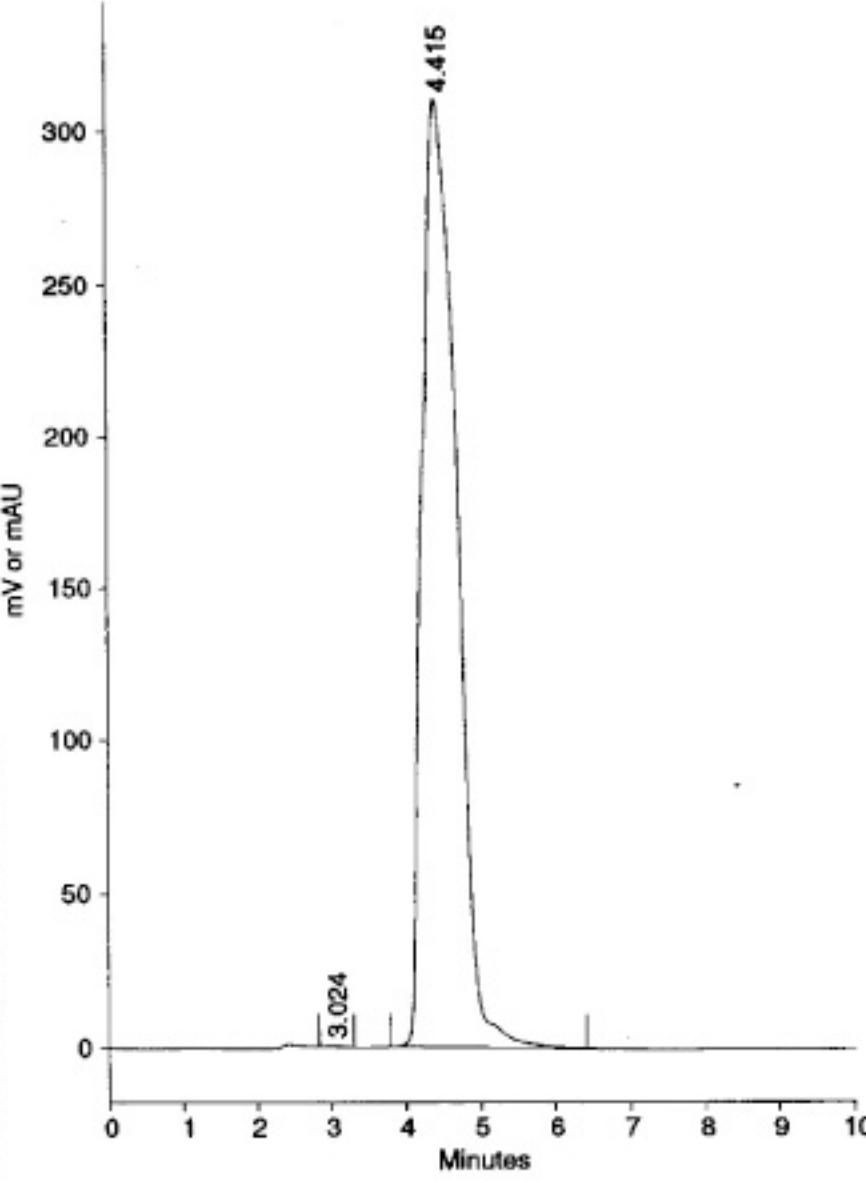
Name: jda66 dio 3-6
Type: Sample
Injection Volume: 10.0 μ L

Acquisition Log

Column Pressure (PSI): 923
Noise (microAU): 1e+01
Run-Time Messages: None

Signal 1: UV3000 A 254 nm

Calculation Type: Area Percent (Area)



S70

Vial: C08
Injected On: 03-06-03 15:42:07

#21 iPrOH:dioxane 80:20

n:jda66 dio 3-6,Inj1,UV3000 A 254nm

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	3.024	5029	506	0.05	Resolved
Unident0002	4.415	9853677	310253	99.95	Resolved
Totals		9858706	310759	100.00	

System: Bertrand on Comm Port 1
Acquisition Method: C:\TSP\SYSTEMUVFLUO\Methods\jda dioxane.AQM
Calculation Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.T.CAM
Report Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.RPM

Analyst: <GUEST>
PC1000 Ver 3.5 Test Rel 17
03-06-03 14:08:52
08-28-00 09:43:20
08-28-00 09:43:20

Analysis Report

Name: \data56 dio 3-6

Type: Sample

Injection Volume: 10.0 μ L

Acquisition Log

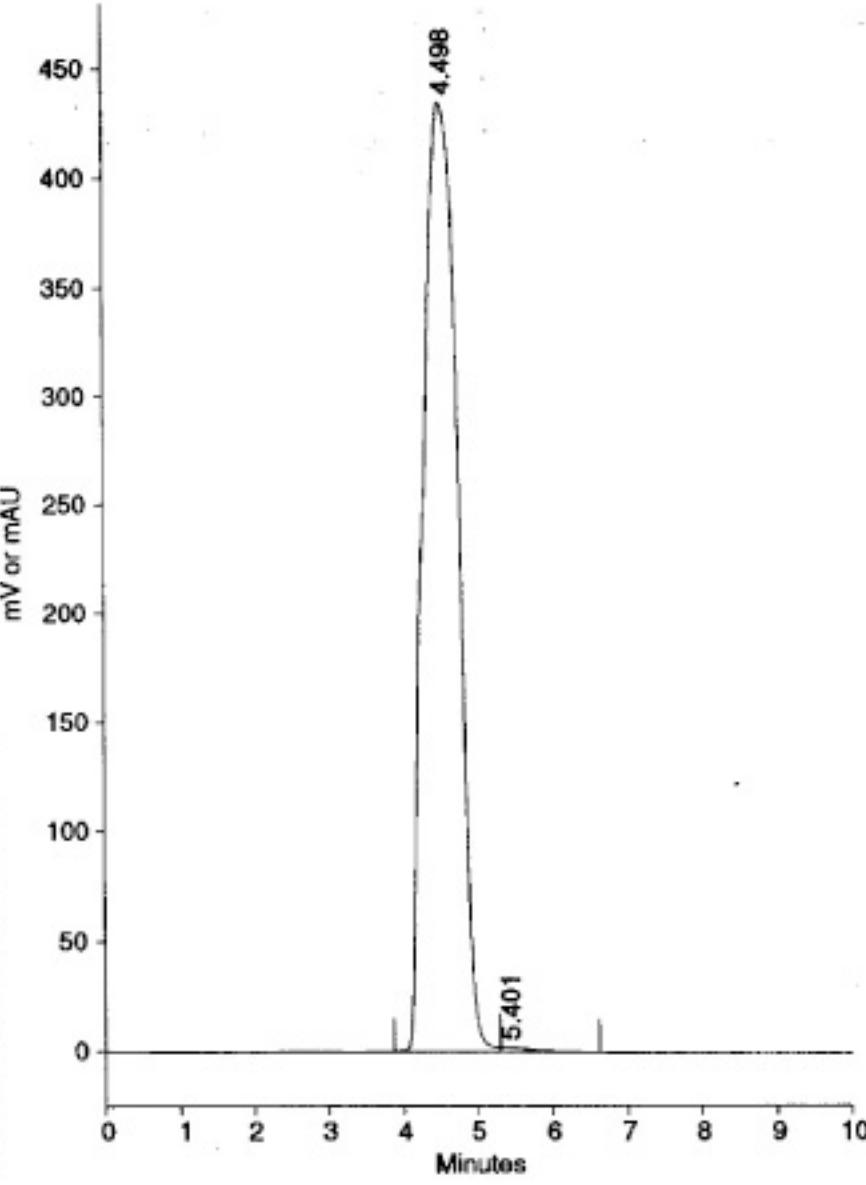
Column Pressure (PSI): 916

Noise (microAU): 4e+01

Run-Time Messages: None

Signal 1: UV3000 A 254 nm

Calculation Type: Area Percent (Area)



Vial: C20

Injection: 1 of 1

Injected On: 03-06-03 17:55:59

n \data56 dio 3-6,inj1, UV3000 A 254nm

#22 iPrOH:dioxane 80:20

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	4.498	14046871	434842	99.55	Fused
Unident0002	5.401	63991	2135	0.45	Fused
Totals		14110862	436977	100.00	

System: Bertrand on Comm Port 1

Analyst: <GUEST>

Acquisition Method: C:\TSP\SYSTEMUVFLUO\Methods\n\data dioxane.AQM

Calculation Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.CAM

Report Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.RPM

PCT1000 Ver 3.5 Test Rel 17

03-06-03 14:08:52

08-28-00 09:43:20

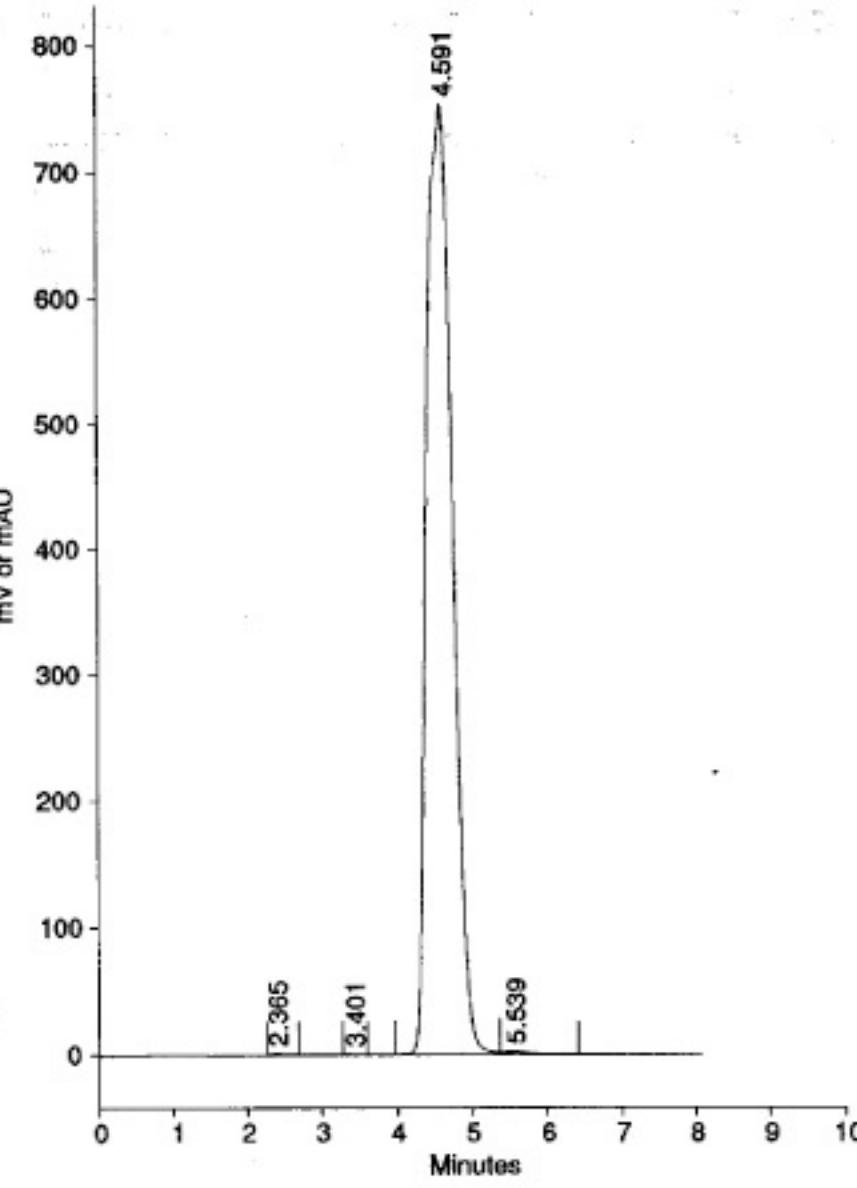
08-28-00 09:43:20

Analysis Report

Name: jda58 dio 3-6
Type: Sample
Injection Volume: 5.0 μ L

Acquisition Log
Column Pressure (PSI): 934
Noise (microAU): 3e+01
Run-Time Messages: None

Signal 1: UV3000 A 254 nm
Calculation Type: Area Percent (Area)



S72

#23

iP-Off: dioxane 80:20

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	2.365	12485	1116	0.07	Resolved
Unident0002	3.401	2363	316	0.01	Resolved
Unident0003	4.591	18181723	753550	99.57	Fused
Unident0004	5.539	62890	2352	0.34	Fused
Totals		18259461	757334	100.00	

System: Bertrand on Comm Port 1
Acquisition Method: C:\TSP\SYSTEM\UVFLUO\METHODS\jda_dioxane.ACM
Calculation Method: C:\TSP\SYSTEM\UVFLUO\METHODS\DEFAULT.CAM

Analyst: <GUEST>
PC1000 Ver 3.5 Test Rel 17
03-06-03 14:08:52
08-28-00 09:43:20

PC1000 Ver 3.5 Test Rel 17
03-06-03 14:08:52
08-28-00 09:43:20

Analysis Report

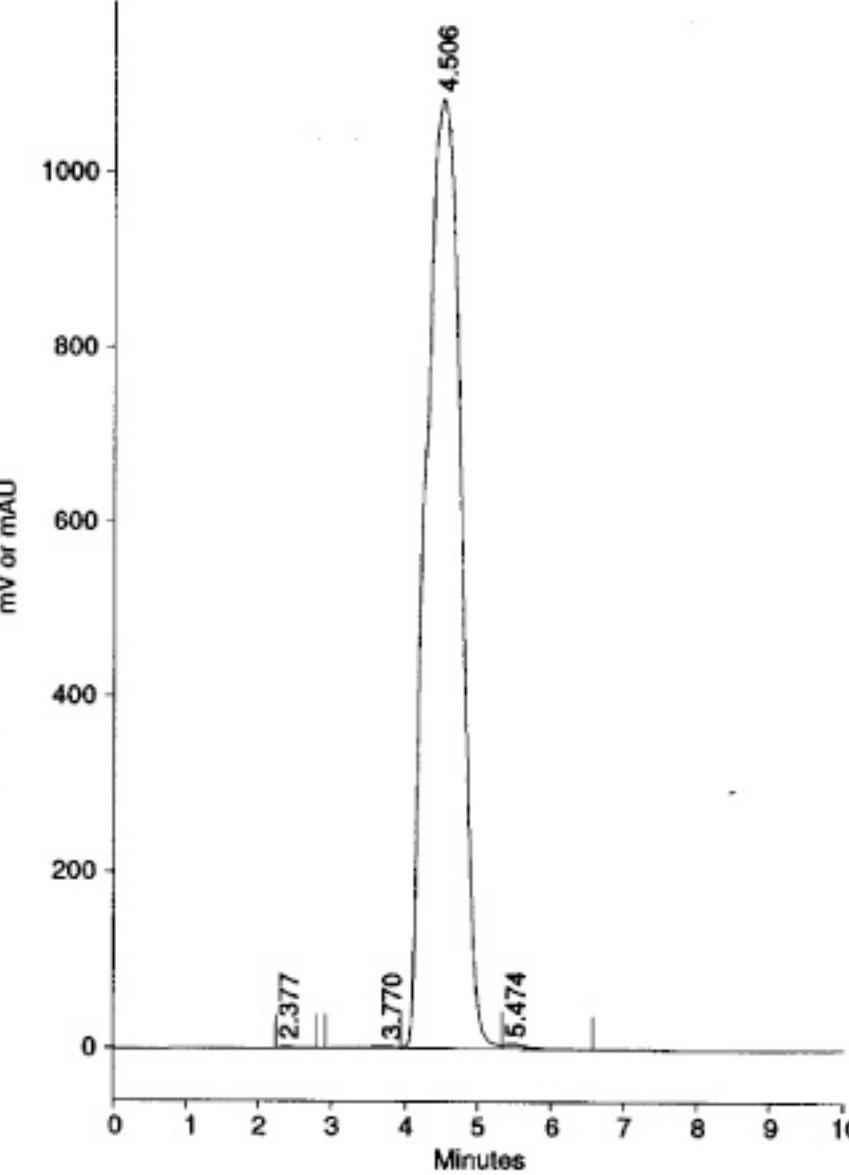
Name: n jda52 dio 3-6
Type: Sample
Injection Volume: 10.0 μ L

Acquisition Log

Column Pressure (PSI): 928
Noise (microAU): 3e+01
Run-Time Messages: None

Signal 1: UV3000 A 254 nm

Calculation Type: Area Percent (Area)



n jda52 dio 3-6,Inj1, UV3000 A 254nm

#24 ;PdOH: dioxane 80:20

Component	RT(min)	Area	Height	Area%	Peak Type
Unident0001	2.377	26175	1788	0.07	Resolved
Unident0002	3.770	72496	2301	0.20	Fused
Unident0003	4.506	35772263	1083909	99.36	Fused
Unident0004	5.474	132236	5714	0.37	Fused
Totals		36003170	1093712	100.00	

System: Bertrand on Comm Port 1

Analyst: <GUEST>
Acquisition Method: C:\TSP\SYSTEMUVFLUO\Methods\n jda_dioxane.AQM
Calculation Method: C:\TSP\SYSTEMUVFLUO\Methods\DEFAULT.CAM

PC1000 Ver 3.5 Test Rel 17
03-06-03 14:08:52
08-28-00 09:43:20