

The Influence of a 1,1-Diarylvinyli Moiety on the Photochromism of Naphthopyrans

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Supplementary Information

Crystal data and structure refinement for 1-[2,2-bis-(4-dimethylaminophenyl)vinyli]-3-phenyl-1*H*-naphtho[2,1-*b*]pyran **14**

Measurements were carried out at 150 K on a Bruker-Nonius Apex X8 diffractometer equipped with an Apex II CCD detector and using graphite monochromated Mo-K α radiation from a FR591 rotating anode generator. The structure was solved by direct methods and refined using SHELXL-97. Compound **14** crystallises in the chiral space group $P2_12_12_1$. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms could be located in a difference Fourier map but, in the final stages of the refinement, they were placed in calculated positions and refined using a riding model. In the absence of significant anomalous scattering effects, the absolute configuration could not be confirmed from the diffraction data and Friedel pairs were merged. An arbitrary choice of enantiomer has been made.

The structure has been deposited at the Cambridge Crystallographic Data Centre and information on the structure can be obtained by quoting the CCDC at:

<http://www.ccdc.cam.ac.uk/deposit>

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Table S1. Crystal data and structure refinement for compound 14.

Formula	C ₃₇ H ₃₄ N ₂ O	
Formula weight	522.66	
Size	0.19 x 0.11 x 0.05 mm	
Crystal morphology	Colourless fragment	
Temperature	150K	
Wavelength	0.71073 Å [Mo-K _α]	
Crystal system	Orthorhombic	
Space group	P2 ₁ 2 ₁ 2 ₁	
Unit cell dimensions	$a = 10.9909(10)$ Å	$\alpha = 90^\circ$
	$b = 13.0053(11)$ Å	$\beta = 90^\circ$
	$c = 20.0553(18)$ Å	$\gamma = 90^\circ$
Volume	2866.7(4) Å ³	
Z	4	
Density (calculated)	1.211 Mg/m ³	
Absorption coefficient	0.072 mm ⁻¹	
<i>F</i> (000)	1112	
Data collection range	2.57 ≤ θ ≤ 27.94°	
Index ranges	-13 ≤ h ≤ 14, -14 ≤ k ≤ 17, -25 ≤ l ≤ 26	
Reflections collected	27053	
Independent reflections	3842 [$R(\text{int}) = 0.0786$]	
Observed reflections	2744 [$I > 2\sigma(I)$]	
Absorption correction	multi-scan	
Max. and min. transmission	0.9964 and 0.8278	
Refinement method	Full	
Data / restraints / parameters	3114 / 0 / 365	
Goodness of fit	1.063	
Final <i>R</i> indices [$I > 2\sigma(I)$]	$R_1 = 0.0431$, $wR_2 = 0.0957$	
<i>R</i> indices (all data)	$R_1 = 0.0669$, $wR_2 = 0.1087$	
Largest diff. peak and hole	0.190 and -0.182 e.Å ⁻³	

Table 2. Atomic co-ordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) with standard uncertainties (s.u.s) in parentheses. U_{eq} is defined as $1/3$ of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
O(4)	8371.3(16)	8420.9(16)	1240.2(9)	322(5)
C(31)	7239(3)	7247(2)	577.9(13)	251(6)
C(1)	6230(2)	9238(2)	1957.3(14)	255(6)
C(13)	7839(3)	10224(2)	2664.6(13)	257(6)
C(2)	6229(3)	8365(2)	1454.5(14)	266(6)
N(57)	1710(2)	8224.1(19)	3834.3(12)	334(6)
C(52)	3428(3)	10363(2)	3014.5(13)	274(6)
C(3)	7206(2)	8035(2)	1113.4(13)	256(6)
C(61)	3952(2)	11518(2)	1599.4(13)	253(6)
C(56)	3287(2)	8955(2)	2247.8(13)	252(6)
C(14)	7558(2)	9516(2)	2132.7(13)	246(6)
C(6)	9759(2)	9326(2)	1923.9(14)	306(7)
C(64)	2951(3)	13307(2)	945.8(14)	306(7)
C(36)	8363(3)	6937(2)	290.5(14)	296(7)
C(65)	2203(3)	12559(2)	1245.9(15)	320(7)
C(33)	6208(3)	6042(2)	-171.7(14)	329(7)
C(12)	6919(3)	10708(2)	3062.3(14)	293(7)
C(32)	6165(3)	6777(2)	332.5(14)	287(7)
C(66)	2683(3)	11701(2)	1561.3(14)	295(7)
C(11)	7212(3)	11412(2)	3549.5(14)	329(7)
C(5)	8511(2)	9098(2)	1773.6(13)	270(6)
N(67)	2472(3)	14141(2)	593.9(13)	402(7)
C(55)	2635(3)	8377(2)	2715.3(14)	273(6)
C(53)	2796(3)	9791(2)	3496.0(14)	284(7)
C(41)	4450(2)	10540(2)	1876.0(13)	247(6)
C(10)	8444(3)	11677(3)	3676.3(15)	377(8)
C(59)	1305(3)	7179(3)	3658.3(18)	418(8)
C(9)	9356(3)	11214(2)	3312.3(15)	364(8)
C(54)	2385(2)	8786(2)	3354.6(13)	260(6)
C(7)	10026(3)	10002(2)	2420.8(14)	304(7)
C(51)	3706(2)	9952(2)	2382.6(13)	240(6)
C(34)	7327(3)	5743(2)	-449.7(14)	345(7)
C(35)	8394(3)	6199(2)	-214.4(15)	346(7)
C(8)	9089(3)	10486(2)	2805.2(14)	282(7)
C(69)	1163(3)	14167(3)	443.7(18)	465(9)
C(62)	4695(3)	12309(2)	1342.2(14)	305(7)
C(63)	4232(3)	13175(2)	1027.0(15)	318(7)
C(68)	3272(3)	14786(3)	188.5(17)	457(9)
C(40)	5555(2)	10164(2)	1675.4(13)	261(6)
C(58)	1985(3)	8380(3)	4538.6(15)	495(10)

Table 3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O(4)	19.4(10)	46.5(13)	30.8(11)	-10.7(10)	0.8(9)	-2.4(10)
C(31)	25.9(15)	28.9(15)	20.5(13)	4.4(12)	-1.2(12)	0.5(13)
C(1)	19.6(14)	31.9(16)	24.9(14)	-0.7(14)	1.7(11)	-3.2(12)
C(13)	28.4(15)	28.3(15)	20.5(13)	4.0(13)	0.1(12)	1.3(13)
C(2)	22.2(14)	30.0(16)	27.5(14)	1.1(14)	1.0(12)	-4.5(13)
N(57)	39.5(14)	32.6(14)	28.2(13)	1.5(11)	7.2(12)	-1.9(12)
C(52)	26.8(15)	27.5(15)	28.0(14)	-4.8(13)	-2.1(12)	-0.6(13)
C(3)	19.8(14)	31.1(16)	25.9(14)	4.5(13)	0.3(12)	-3.2(12)
C(61)	23.2(14)	27.7(15)	25.2(14)	-1.9(13)	-1.8(12)	-0.9(12)
C(56)	24.3(14)	30.9(16)	20.4(13)	-3.7(12)	-0.8(11)	3.5(13)
C(14)	20.0(14)	29.6(15)	24.1(14)	4.9(12)	0.4(11)	0.0(12)
C(6)	21.0(15)	40.7(19)	30.0(15)	-1.7(15)	0.6(12)	3.7(13)
C(64)	33.9(17)	29.0(16)	29.0(15)	-2.8(14)	-1.1(13)	1.3(14)
C(36)	26.4(16)	34.6(17)	27.8(15)	2.4(13)	1.6(13)	0.5(14)
C(65)	25.3(15)	33.7(17)	36.9(17)	2.0(14)	-0.4(14)	1.4(13)
C(33)	35.1(17)	37.2(18)	26.5(15)	1.6(15)	-0.9(13)	-6.4(15)
C(12)	31.2(16)	31.0(17)	25.5(14)	4.7(13)	2.4(12)	2.0(13)
C(32)	24.9(15)	36.5(17)	24.8(14)	1.8(14)	0.4(12)	-0.8(14)
C(66)	23.5(15)	34.7(16)	30.2(15)	1.7(14)	4.1(13)	-1.8(13)
C(11)	40.9(18)	31.6(17)	26.3(15)	3.3(14)	2.7(14)	3.4(14)
C(5)	24.0(15)	36.4(16)	20.7(14)	-0.9(13)	-0.6(12)	-0.5(13)
N(67)	40.9(16)	33.1(15)	46.5(15)	10.4(13)	-5.9(13)	-0.2(13)
C(55)	25.1(14)	27.4(15)	29.3(15)	-1.2(13)	-0.4(12)	0.6(13)
C(53)	29.2(16)	33.8(16)	22.1(14)	-3.1(13)	2.4(12)	1.6(13)
C(41)	23.9(14)	27.5(16)	22.6(14)	-2.8(12)	1.3(11)	-3.4(12)
C(10)	48(2)	35.7(18)	29.3(16)	-4.9(14)	-8.1(15)	-0.5(16)
C(59)	40.4(19)	39.5(19)	45(2)	3.1(16)	10.3(16)	-3.9(16)
C(9)	35.5(17)	40.0(19)	33.8(17)	-3.4(15)	-7.7(14)	-1.9(15)
C(54)	20.1(14)	32.9(16)	25.1(14)	4.2(13)	-0.8(11)	3.9(12)
C(7)	24.5(14)	37.7(19)	29.2(15)	-0.7(15)	-3.6(12)	-1.7(13)
C(51)	18.8(13)	29.4(16)	23.7(14)	2.0(13)	-0.3(11)	2.6(12)
C(34)	47.7(19)	31.7(17)	24.0(15)	-2.7(13)	0.7(14)	-0.9(15)
C(35)	35.4(18)	37.5(18)	30.7(16)	1.0(15)	6.7(14)	5.1(15)
C(8)	28.5(15)	30.5(17)	25.6(15)	3.1(13)	-3.3(12)	-0.9(13)
C(69)	41(2)	47(2)	51(2)	9.0(18)	-9.4(16)	10.5(17)
C(62)	22.2(15)	34.8(17)	34.5(17)	-2.8(14)	-0.4(13)	-3.6(13)
C(63)	28.9(16)	29.3(17)	37.3(17)	1.9(14)	0.1(13)	-6.1(14)
C(68)	62(2)	36.9(19)	38.6(18)	5.9(16)	7.8(17)	0.9(18)
C(40)	25.4(15)	31.0(16)	21.7(14)	0.5(13)	2.0(11)	-1.8(12)
C(58)	55(2)	66(2)	28.2(17)	6.8(17)	3.1(15)	-13(2)

Table 4. Hydrogen atom co-ordinates ($\times 10^3$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^2$) with s.u.s in parentheses.

	x	y	z	U_{eq}
H(1)	5805.	9003.	2371.	31.
H(2)	5478.	8026.	1375.	32.
H(52)	3674.	11045.	3117.	33.
H(56)	3451.	8661.	1824.	30.
H(6)	10394.	9008.	1678.	37.
H(36)	9101.	7235.	444.	36.
H(65)	1345.	12646.	1232.	38.
H(33)	5475.	5740.	-329.	40.
H(12)	6089.	10539.	2988.	35.
H(32)	5401.	6968.	516.	34.
H(66)	2142.	11220.	1759.	35.
H(11)	6583.	11723.	3804.	40.
H(55)	2359.	7706.	2603.	33.
H(53)	2642.	10083.	3922.	34.
H(10)	8638.	12169.	4009.	45.
H(59a)	847.	7201.	3239.	63.
H(59b)	783.	6909.	4014.	63.
H(59c)	2016.	6731.	3605.	63.
H(9)	10180.	11385.	3402.	44.
H(7)	10854.	10156.	2515.	37.
H(34)	7357.	5239.	-792.	41.
H(35)	9154.	6004.	-401.	41.
H(69a)	950.	13577.	163.	70.
H(69b)	967.	14805.	208.	70.
H(69c)	699.	14135.	861.	70.
H(62)	5552.	12246.	1387.	37.
H(63)	4774.	13685.	863.	38.
H(68a)	3917.	15073.	470.	69.
H(68b)	2799.	15347.	-10.	69.
H(68c)	3637.	14370.	-167.	69.
H(40)	5944.	10521.	1321.	31.
H(58a)	2827.	8174.	4627.	74.
H(58b)	1432.	7963.	4810.	74.
H(58c)	1880.	9108.	4651.	74.

Table 5. Interatomic distances (Å) with s.u.s in parentheses.

O(4)-C(5)	1.394(3)	O(4)-C(3)	1.399(3)
C(31)-C(32)	1.417(4)	C(31)-C(36)	1.422(4)
C(31)-C(3)	1.485(4)	C(1)-C(2)	1.519(4)
C(1)-C(40)	1.523(4)	C(1)-C(14)	1.544(4)
C(13)-C(12)	1.433(4)	C(13)-C(14)	1.443(4)
C(13)-C(8)	1.443(4)	C(2)-C(3)	1.344(4)
N(57)-C(54)	1.418(4)	N(57)-C(58)	1.459(4)
N(57)-C(59)	1.473(4)	C(52)-C(53)	1.403(4)
C(52)-C(51)	1.409(4)	C(61)-C(62)	1.411(4)
C(61)-C(66)	1.417(4)	C(61)-C(41)	1.492(4)
C(56)-C(55)	1.399(4)	C(56)-C(51)	1.402(4)
C(14)-C(5)	1.383(4)	C(6)-C(7)	1.361(4)
C(6)-C(5)	1.435(4)	C(64)-N(67)	1.397(4)
C(64)-C(65)	1.409(4)	C(64)-C(63)	1.427(4)
C(36)-C(35)	1.395(4)	C(65)-C(66)	1.387(4)
C(33)-C(32)	1.392(4)	C(33)-C(34)	1.405(4)
C(12)-C(11)	1.377(4)	C(11)-C(10)	1.420(4)
N(67)-C(68)	1.462(4)	N(67)-C(69)	1.470(4)
C(55)-C(54)	1.415(4)	C(53)-C(54)	1.412(4)
C(41)-C(40)	1.369(4)	C(41)-C(51)	1.512(4)
C(10)-C(9)	1.378(4)	C(9)-C(8)	1.420(4)
C(7)-C(8)	1.433(4)	C(34)-C(35)	1.396(4)
C(62)-C(63)	1.388(4)		

Table 6. Angles between interatomic vectors ($^{\circ}$) with s.u.s in parentheses.

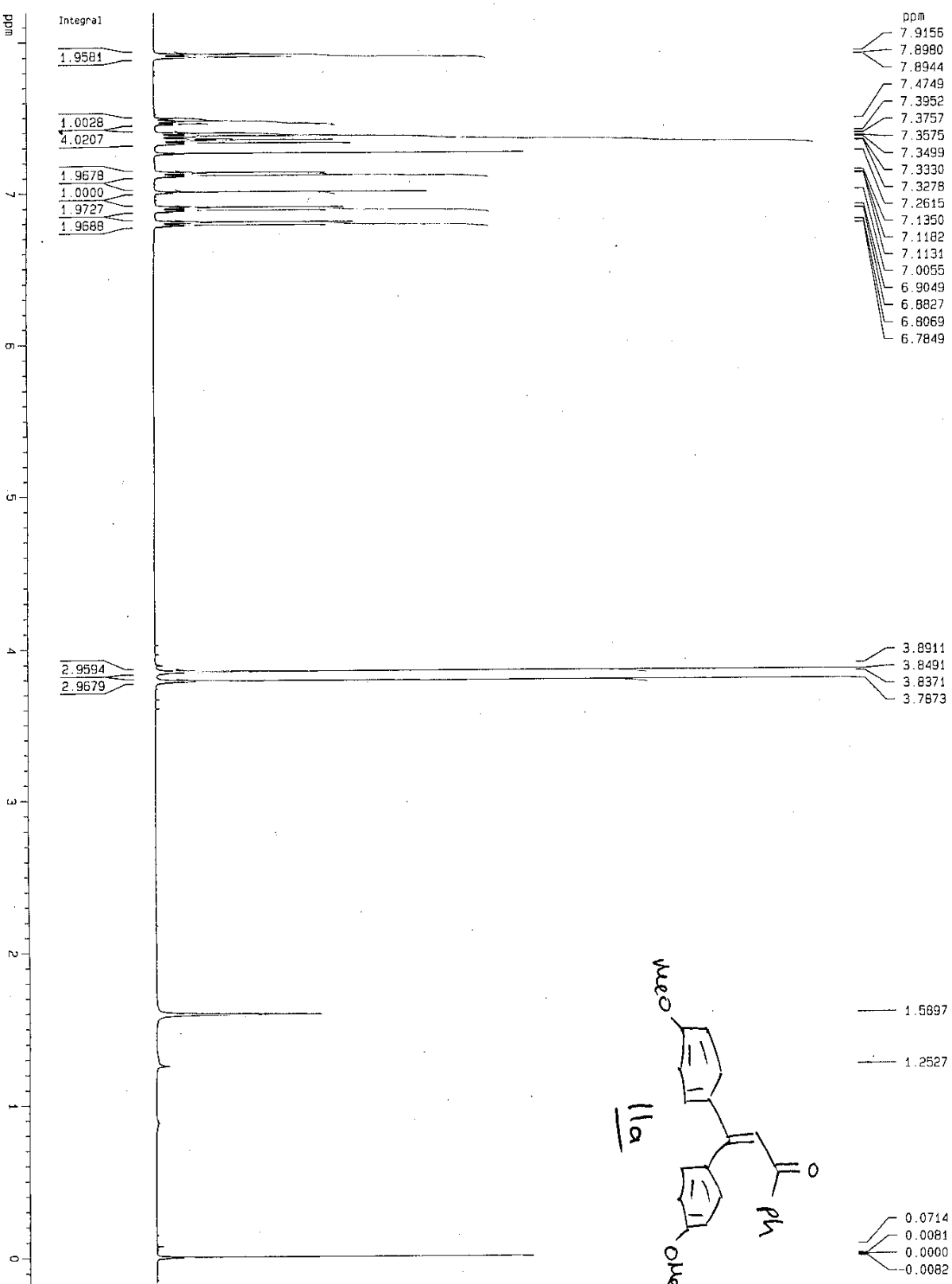
C(5)-O(4)-C(3)	117.9(2)	C(32)-C(31)-C(36)	117.4(2)
C(32)-C(31)-C(3)	121.9(3)	C(36)-C(31)-C(3)	120.7(2)
C(2)-C(1)-C(40)	110.2(2)	C(2)-C(1)-C(14)	109.0(2)
C(40)-C(1)-C(14)	111.1(2)	C(12)-C(13)-C(14)	122.7(3)
C(12)-C(13)-C(8)	117.3(2)	C(14)-C(13)-C(8)	119.9(2)
C(3)-C(2)-C(1)	125.2(2)	C(54)-N(57)-C(58)	118.5(3)
C(54)-N(57)-C(59)	118.1(2)	C(58)-N(57)-C(59)	115.0(3)
C(53)-C(52)-C(51)	121.6(3)	C(2)-C(3)-O(4)	121.6(2)
C(2)-C(3)-C(31)	127.4(3)	O(4)-C(3)-C(31)	110.9(2)
C(62)-C(61)-C(66)	115.3(3)	C(62)-C(61)-C(41)	123.1(2)
C(66)-C(61)-C(41)	121.6(2)	C(55)-C(56)-C(51)	122.4(3)
C(5)-C(14)-C(13)	118.3(2)	C(5)-C(14)-C(1)	120.4(2)
C(13)-C(14)-C(1)	121.3(2)	C(7)-C(6)-C(5)	119.6(3)
N(67)-C(64)-C(65)	122.1(3)	N(67)-C(64)-C(63)	121.5(3)
C(65)-C(64)-C(63)	116.4(3)	C(35)-C(36)-C(31)	120.7(3)
C(66)-C(65)-C(64)	121.9(3)	C(32)-C(33)-C(34)	120.5(3)
C(11)-C(12)-C(13)	121.4(3)	C(33)-C(32)-C(31)	121.3(3)
C(65)-C(66)-C(61)	122.3(3)	C(12)-C(11)-C(10)	120.8(3)
C(14)-C(5)-O(4)	124.3(2)	C(14)-C(5)-C(6)	122.2(3)
O(4)-C(5)-C(6)	113.4(2)	C(64)-N(67)-C(68)	120.0(3)
C(64)-N(67)-C(69)	119.4(3)	C(68)-N(67)-C(69)	117.5(3)
C(56)-C(55)-C(54)	120.3(3)	C(52)-C(53)-C(54)	120.7(3)
C(40)-C(41)-C(61)	121.3(2)	C(40)-C(41)-C(51)	119.7(3)
C(61)-C(41)-C(51)	118.9(2)	C(9)-C(10)-C(11)	119.5(3)
C(10)-C(9)-C(8)	121.3(3)	C(53)-C(54)-C(55)	117.9(3)
C(53)-C(54)-N(57)	120.5(2)	C(55)-C(54)-N(57)	121.5(3)
C(6)-C(7)-C(8)	121.5(3)	C(56)-C(51)-C(52)	117.0(3)
C(56)-C(51)-C(41)	121.1(2)	C(52)-C(51)-C(41)	122.0(3)
C(35)-C(34)-C(33)	118.9(3)	C(36)-C(35)-C(34)	121.2(3)
C(9)-C(8)-C(7)	122.0(3)	C(9)-C(8)-C(13)	119.6(3)
C(7)-C(8)-C(13)	118.4(3)	C(63)-C(62)-C(61)	123.1(3)
C(62)-C(63)-C(64)	120.7(3)	C(41)-C(40)-C(1)	127.2(2)

Table 7. Torsion angles ($^{\circ}$) with s.u.s in parentheses.

C(40)-C(1)-C(2)-C(3)	109.4(3)	C(14)-C(1)-C(2)-C(3)	-12.8(4)
C(1)-C(2)-C(3)-O(4)	5.9(4)	C(1)-C(2)-C(3)-C(31)	-174.5(3)
C(5)-O(4)-C(3)-C(2)	5.5(4)	C(5)-O(4)-C(3)-C(31)	-174.1(2)
C(32)-C(31)-C(3)-C(2)	3.8(4)	C(36)-C(31)-C(3)-C(2)	-176.3(3)
C(32)-C(31)-C(3)-O(4)	-176.6(3)	C(36)-C(31)-C(3)-O(4)	3.3(4)
C(12)-C(13)-C(14)-C(5)	179.4(3)	C(8)-C(13)-C(14)-C(5)	0.6(4)
C(12)-C(13)-C(14)-C(1)	0.3(4)	C(8)-C(13)-C(14)-C(1)	-178.5(3)
C(2)-C(1)-C(14)-C(5)	9.4(4)	C(40)-C(1)-C(14)-C(5)	-112.2(3)
C(2)-C(1)-C(14)-C(13)	-171.6(2)	C(40)-C(1)-C(14)-C(13)	66.8(3)
C(32)-C(31)-C(36)-C(35)	0.2(4)	C(3)-C(31)-C(36)-C(35)	-179.8(3)
N(67)-C(64)-C(65)-C(66)	176.2(3)	C(63)-C(64)-C(65)-C(66)	-4.6(4)
C(14)-C(13)-C(12)-C(11)	-177.4(3)	C(8)-C(13)-C(12)-C(11)	1.4(4)
C(34)-C(33)-C(32)-C(31)	0.3(4)	C(36)-C(31)-C(32)-C(33)	-0.2(4)
C(3)-C(31)-C(32)-C(33)	179.8(3)	C(64)-C(65)-C(66)-C(61)	-0.3(5)
C(62)-C(61)-C(66)-C(65)	4.9(4)	C(41)-C(61)-C(66)-C(65)	-173.4(3)
C(13)-C(12)-C(11)-C(10)	-0.4(4)	C(13)-C(14)-C(5)-O(4)	-178.7(2)
C(1)-C(14)-C(5)-O(4)	0.4(4)	C(13)-C(14)-C(5)-C(6)	1.6(4)
C(1)-C(14)-C(5)-C(6)	-179.3(3)	C(3)-O(4)-C(5)-C(14)	-8.6(4)
C(3)-O(4)-C(5)-C(6)	171.1(3)	C(7)-C(6)-C(5)-C(14)	-2.2(5)
C(7)-C(6)-C(5)-O(4)	178.0(3)	C(65)-C(64)-N(67)-C(68)	-168.6(3)
C(63)-C(64)-N(67)-C(68)	12.2(4)	C(65)-C(64)-N(67)-C(69)	-9.3(4)
C(63)-C(64)-N(67)-C(69)	171.5(3)	C(51)-C(56)-C(55)-C(54)	-0.7(4)
C(51)-C(52)-C(53)-C(54)	-1.8(4)	C(62)-C(61)-C(41)-C(40)	-25.8(4)
C(66)-C(61)-C(41)-C(40)	152.4(3)	C(62)-C(61)-C(41)-C(51)	154.8(3)
C(66)-C(61)-C(41)-C(51)	-27.0(4)	C(12)-C(11)-C(10)-C(9)	-0.8(5)
C(11)-C(10)-C(9)-C(8)	0.9(5)	C(52)-C(53)-C(54)-C(55)	0.2(4)
C(52)-C(53)-C(54)-N(57)	-177.8(3)	C(56)-C(55)-C(54)-C(53)	1.0(4)
C(56)-C(55)-C(54)-N(57)	178.9(3)	C(58)-N(57)-C(54)-C(53)	-33.4(4)
C(59)-N(57)-C(54)-C(53)	179.9(3)	C(58)-N(57)-C(54)-C(55)	148.7(3)
C(59)-N(57)-C(54)-C(55)	2.1(4)	C(5)-C(6)-C(7)-C(8)	0.7(4)
C(55)-C(56)-C(51)-C(52)	-0.9(4)	C(55)-C(56)-C(51)-C(41)	177.6(3)
C(53)-C(52)-C(51)-C(56)	2.1(4)	C(53)-C(52)-C(51)-C(41)	-176.4(3)
C(40)-C(41)-C(51)-C(56)	-61.8(4)	C(61)-C(41)-C(51)-C(56)	117.5(3)
C(40)-C(41)-C(51)-C(52)	116.6(3)	C(61)-C(41)-C(51)-C(52)	-64.0(3)
C(32)-C(33)-C(34)-C(35)	-0.3(4)	C(31)-C(36)-C(35)-C(34)	-0.3(4)
C(33)-C(34)-C(35)-C(36)	0.3(4)	C(10)-C(9)-C(8)-C(7)	179.7(3)
C(10)-C(9)-C(8)-C(13)	0.1(4)	C(6)-C(7)-C(8)-C(9)	-178.2(3)
C(6)-C(7)-C(8)-C(13)	1.4(4)	C(12)-C(13)-C(8)-C(9)	-1.3(4)
C(14)-C(13)-C(8)-C(9)	177.6(3)	C(12)-C(13)-C(8)-C(7)	179.1(3)
C(14)-C(13)-C(8)-C(7)	-2.0(4)	C(66)-C(61)-C(62)-C(63)	-4.7(4)
C(41)-C(61)-C(62)-C(63)	173.6(3)	C(61)-C(62)-C(63)-C(64)	-0.1(5)
N(67)-C(64)-C(63)-C(62)	-176.0(3)	C(65)-C(64)-C(63)-C(62)	4.8(4)
C(61)-C(41)-C(40)-C(1)	173.9(2)	C(51)-C(41)-C(40)-C(1)	-6.8(4)
C(2)-C(1)-C(40)-C(41)	109.8(3)	C(14)-C(1)-C(40)-C(41)	-129.3(3)

The following supplementary pages contain ^1H NMR, ^{13}C NMR, infrared and mass spectra of compounds **11a – 11c**, **13a – 13c**, **14**, **16a** and **16b**. ^1H NMR spectra of compounds **12a – c** only are provided as these materials were used directly in subsequent reactions to obtain the target naphthopyrans.

SK-3-25
 PROTON: ColChem CDC13 (D: \u) Suresh 13



Current Data Parameters
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 EXPNO 10
 PROCNO 1

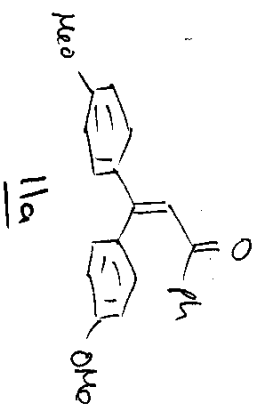
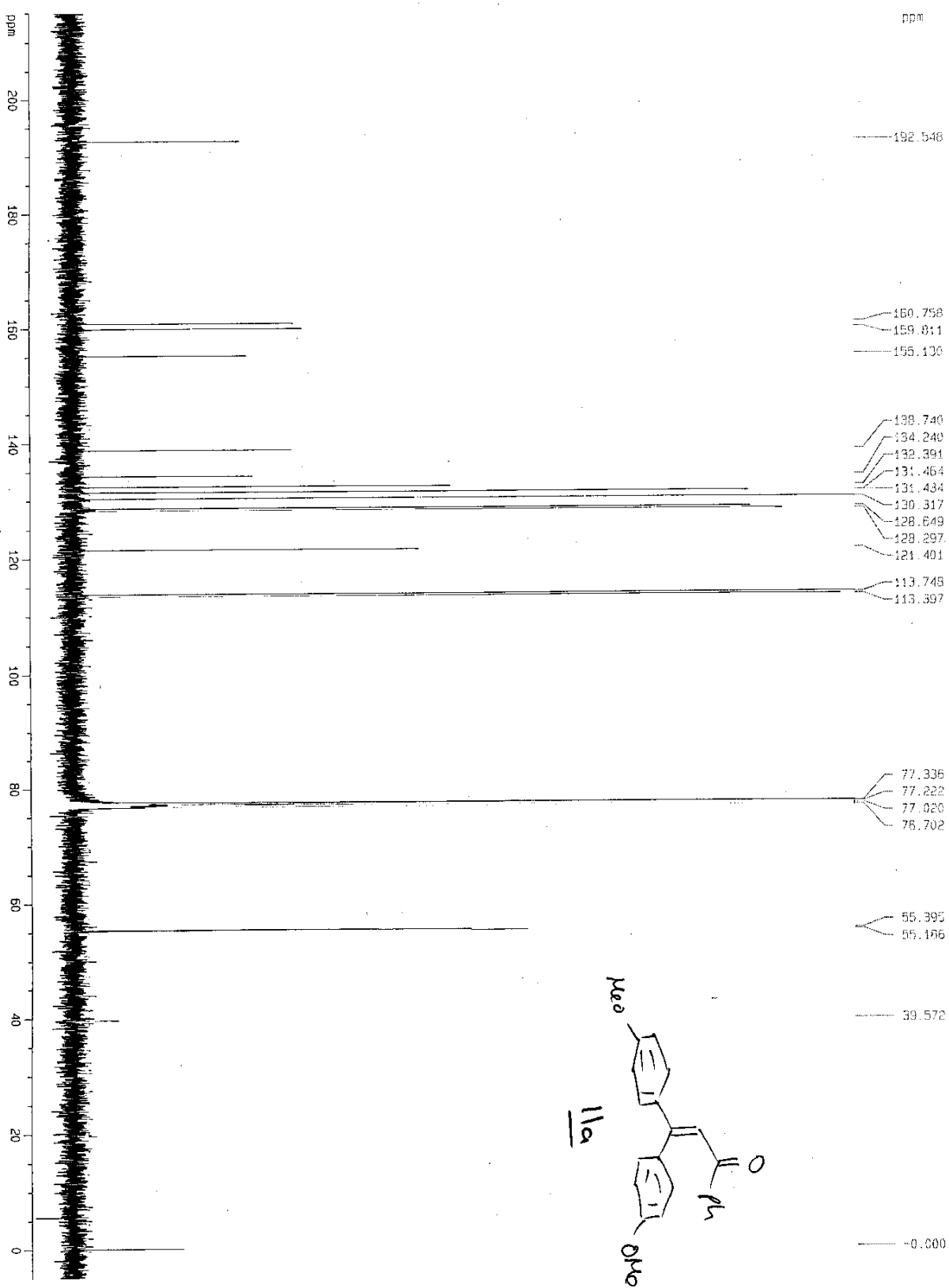
F2 - Acquisition Parameters
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 Time 13.19
 INSTRUM spect
 PROBHD 5 mm QNP 1H/15
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SMH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 322.5
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.25 usec
 PL1 2.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300088 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 CY 19.00 cm
 F1P 8.190 ppm
 F1 3277.09 Hz
 F2P -0.164 ppm
 F2 -65.47 Hz
 PPMCM 0.27846 ppm/cm
 HZCM 111.41887 Hz/cm

SK-3-25-CARBON
 C13CPD CDCl3 {D: \u} Suresh 3



Current Data Parameters
 NAME SK-3-25-CARBON
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080218
 Time 20.31
 INSTNUM spect
 PROBHD 5 mm GNP 1H/15
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 4000
 DS 4
 SMH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 20642.5
 DW 20.850 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

CHANNEL f1
 NUC1 13C
 P1 8.00 usec
 PL1 4.00 dB
 SF01 100.6227898 MHz

CHANNEL f2
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PL2 2.00 dB
 PL12 20.00 dB
 PL13 21.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127705 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 30.00 cm
 CY 19.00 cm
 F1P 215.000 ppm
 F1 21631.75 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCM 7.33333 ppm/cm
 HZCM 737.82697 Hz/cm

ACCURATE MASS MEASUREMENT REPORT

YOUR REFERENCE: SK-3-25

OUR REFERENCE: LEEHER059

Instrument: MAT900 XLT

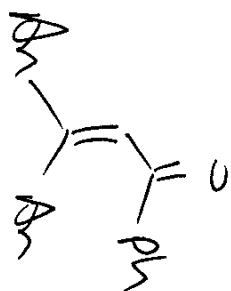
Ionisation Mode: Electrospray (positive)

Reference compound: Polyethylenimine

Ion identity: $[M+H]^+$

Calculated mass (of ion): 345.1485

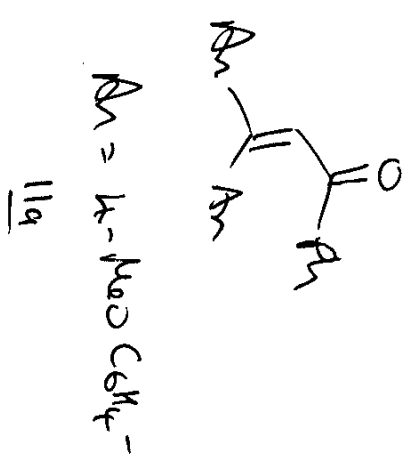
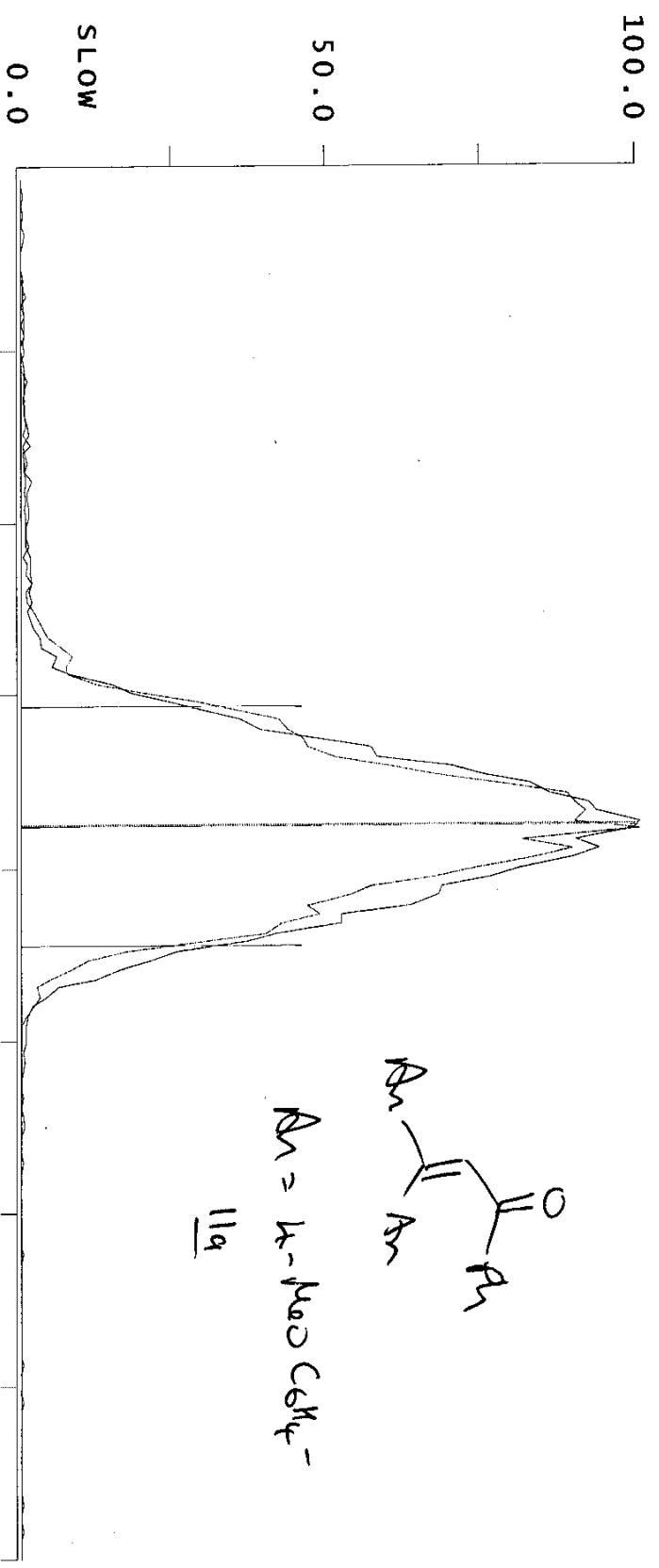
Measured mass (of ion): 345.1489



11a

Peak Register Display

Copy result to ULIST



REG 1/2:	345.148935	REG 1/3:	REG 2/3:
MASS	:	319.32411	345.14341
REF MASS	:	319.32922	362.37142
PEAK WIDTH [ppm]	:	86.65248	86.67676

Active Register: 1 0.30 1.00

N REG RCOPY2 RCOPY3 LIMIT CENTER SPREAD ERASE RESUME PAGE
 PEAK:

SK-3-25 MW=344?

Heron

LEE59HE2 99 (1.932) Cm (96:101)

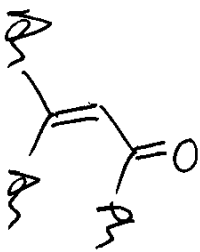
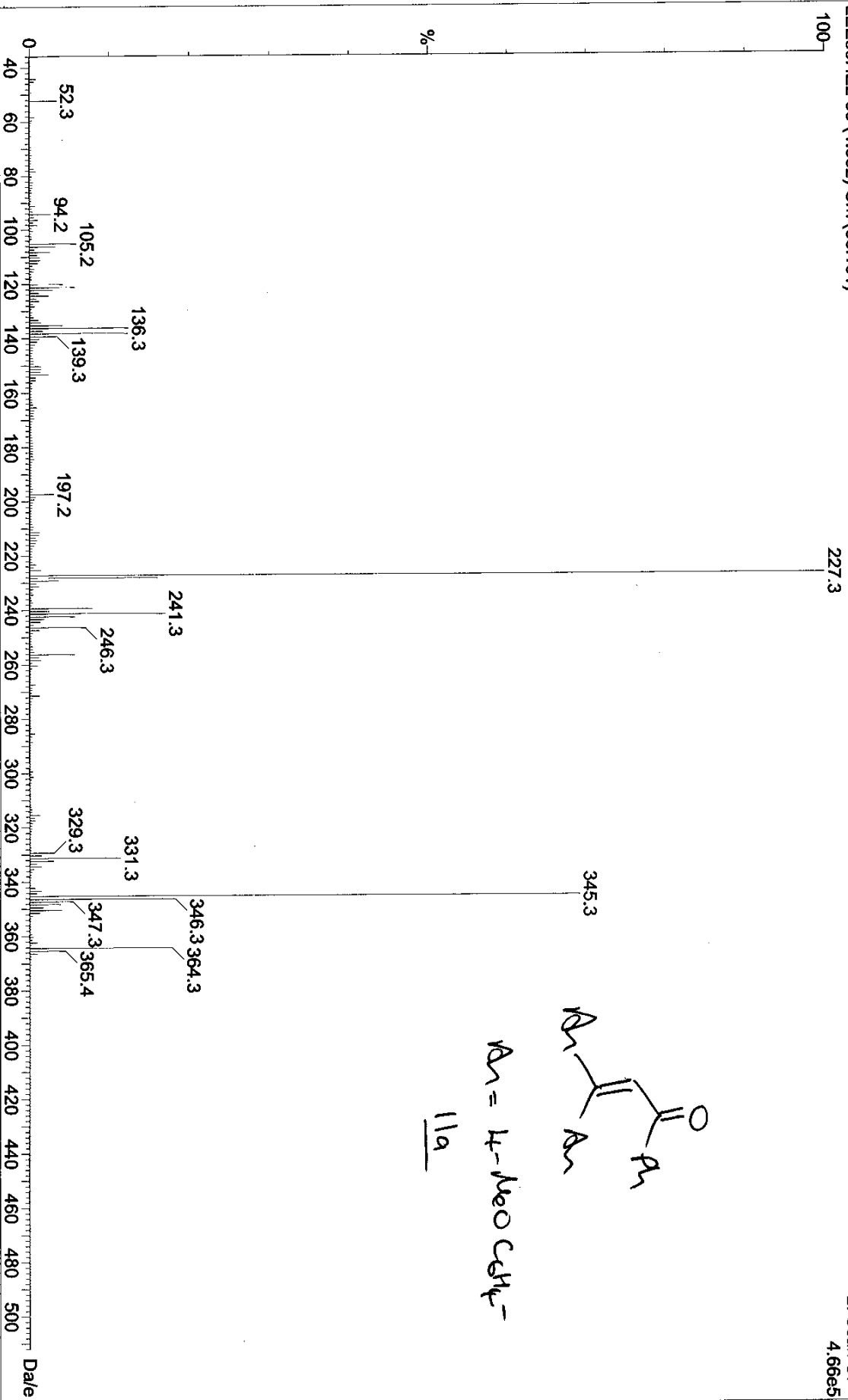
EP SRC National Centre Swansea

QUATTRO

04-Mar-2008

21:43:16

CI+(NH3)
2: Scan CI+
4.66e5



Van = 4-MeO C₆H₄-

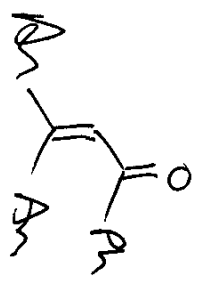
11a

Date

Isotope: Min. ... Max.
 12 C 0....50
 1 H 0....80
 14 N 0....10
 16 O 0....10
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -2.. 100
 PIts: 100

N-Rule: Do not use
 Charge: 1

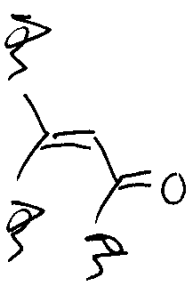
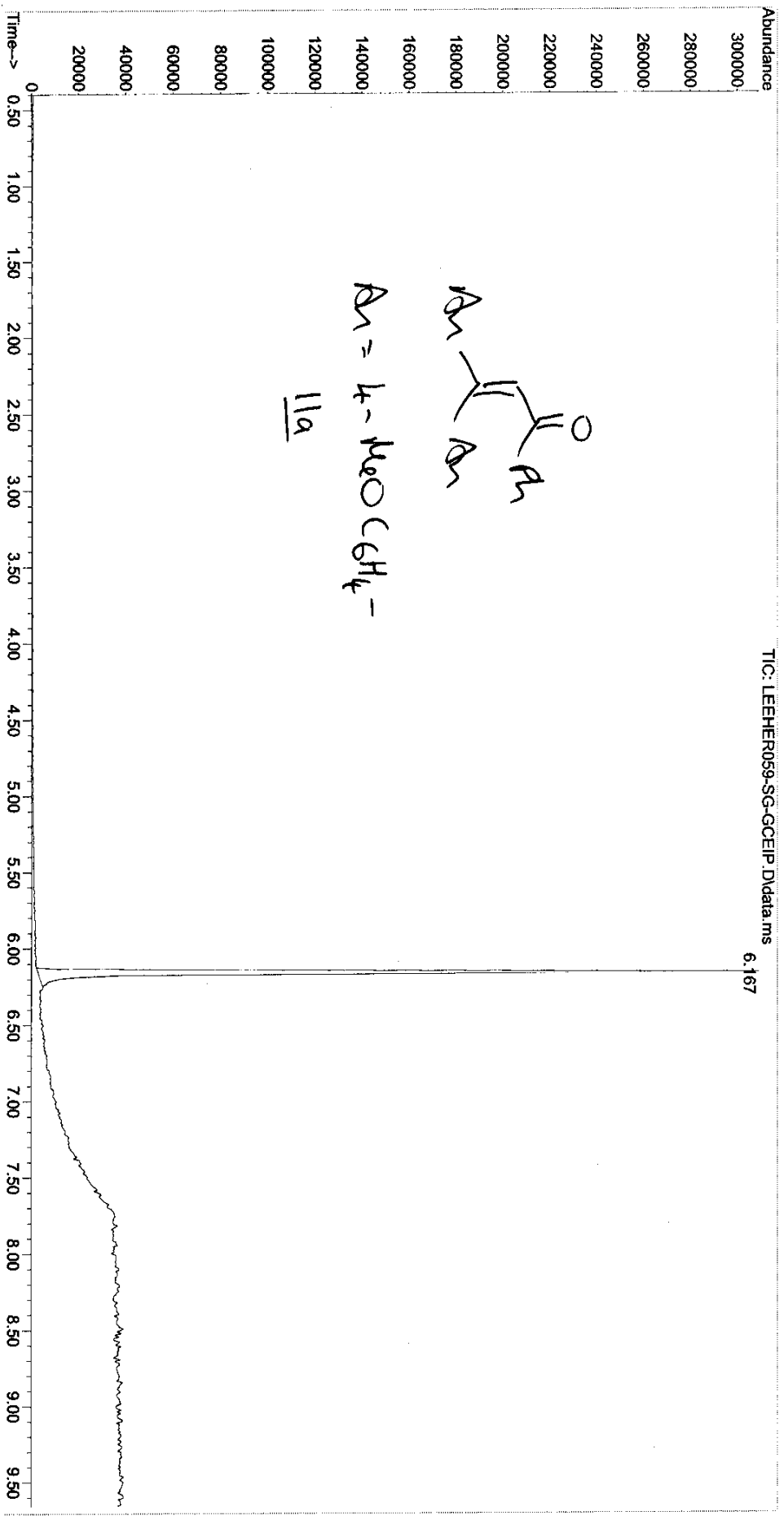
Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
345.1489	345.1490	-0.3	1.0	C ₉ H ₂₃ O ₆ N ₅
	345.1485	1.2	13.5	C ₂₃ H ₂₁ O ₃
	345.1477	3.6	1.5	C ₇ H ₂₁ O ₈ N ₈
	345.1504	-4.1	6.0	C ₁₀ H ₉ O ₅ N ₉
	345.1504	-4.2	0.5	C ₁₁ H ₂₅ O ₁₀ N ₂



Ar = 4- MeO C₆H₄-

11a

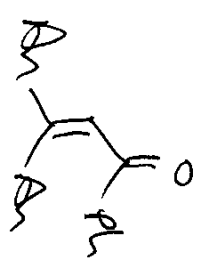
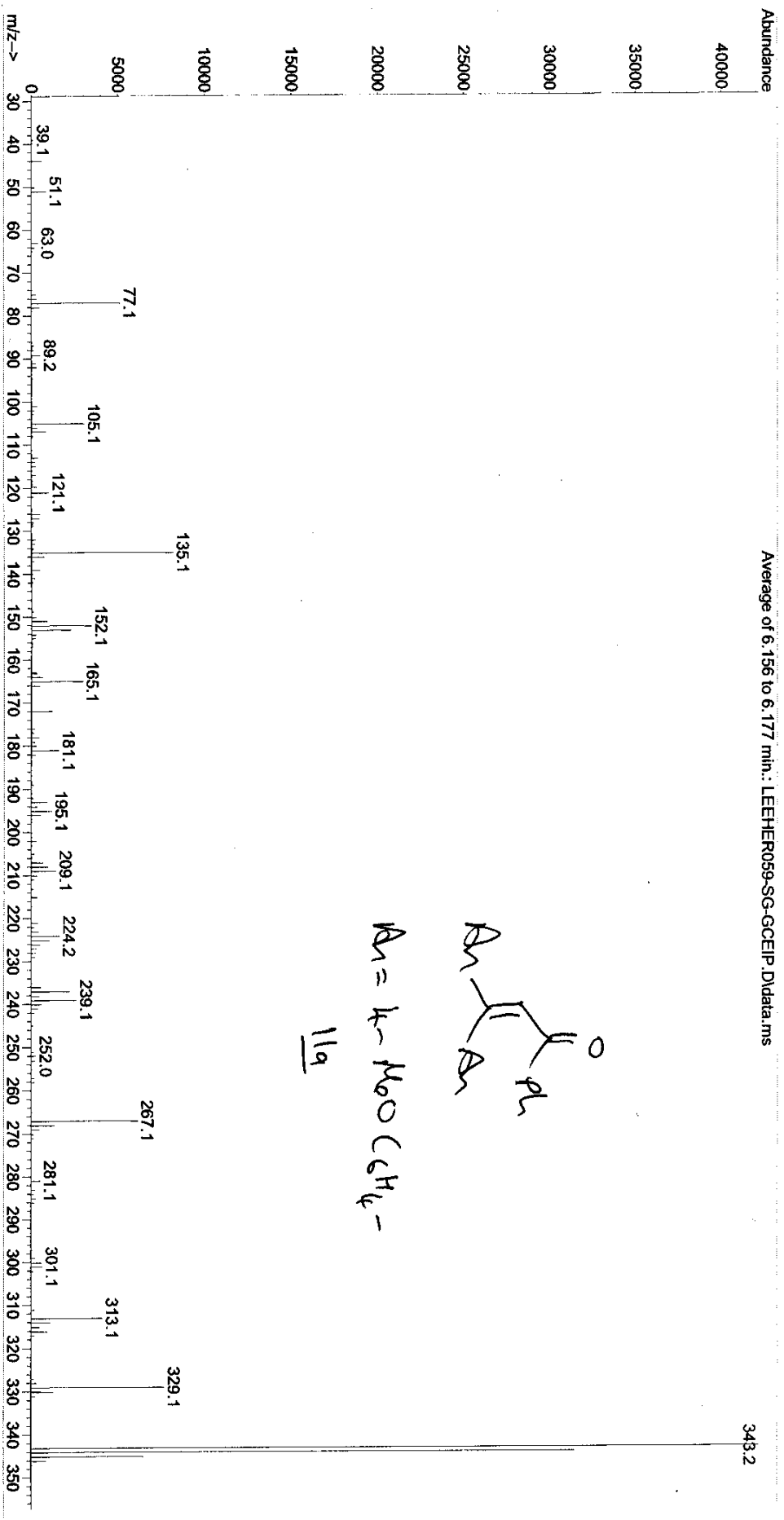
File : C:\msdchem\1\DATA\20080226\LEHER059-SG-GCEIP.D
Operator : AFT
Acquired : 26 Feb 2008 15:34 using AcqMethod nms_eipos-ptv.M
Instrument : Agilent GCMS
Sample Name : SK-3-25 MW=344?
Misc Info : Heron
Vial Number: 12



AN = 4-MeO C₆H₄-
IIa

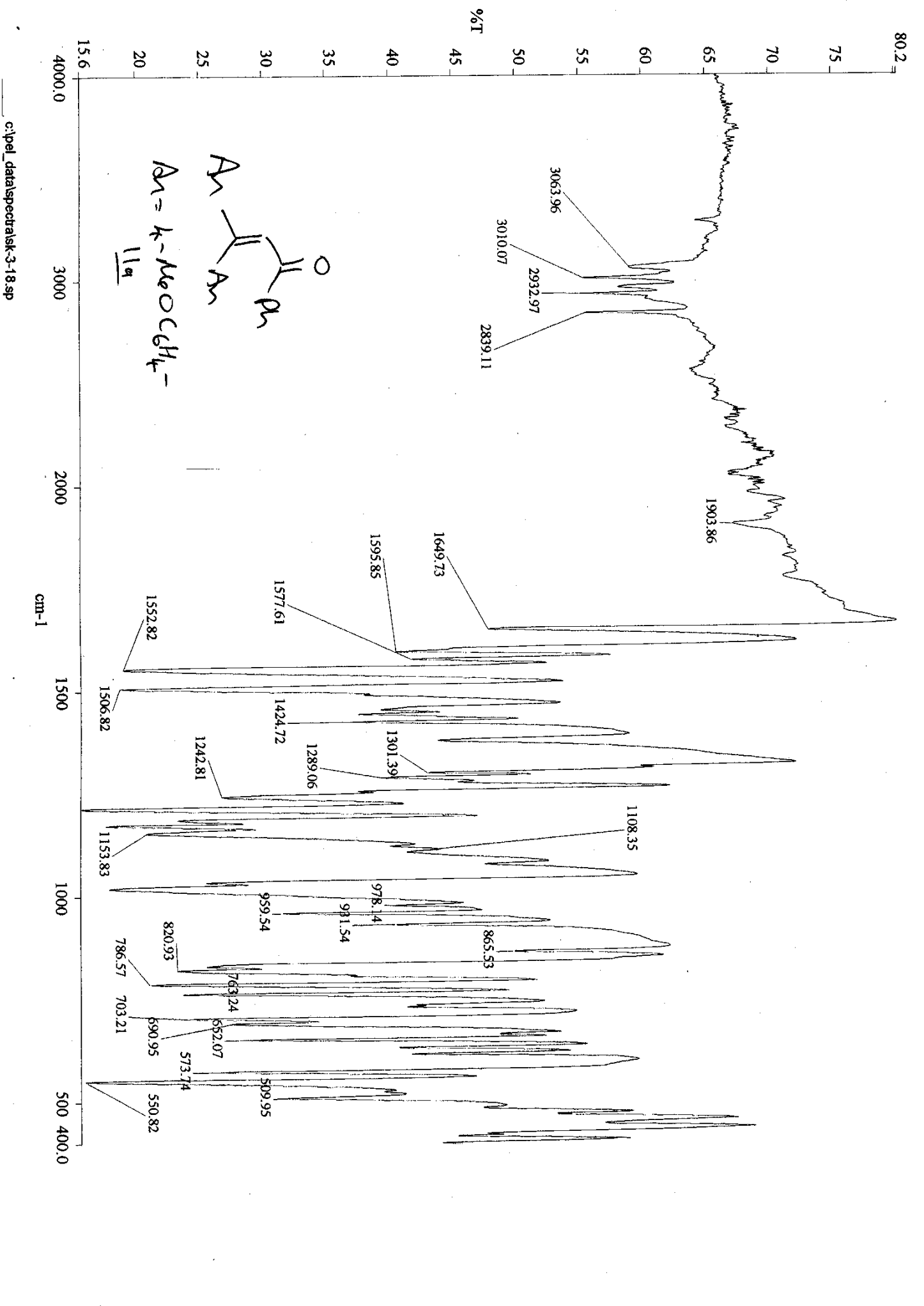
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 Operator : AET
 Acquired : 26 Feb 2008 15:34 using AcqMethod nms_eipos-pltv.M
 Instrument : Agilent GCMS
 Sample Name : SK-3-25 MW=344?
 Misc Info : Heron
 Vial Number: 12

Average of 6.156 to 6.177 min.: LEEHER059-SG-GCEIP.D\data.ms



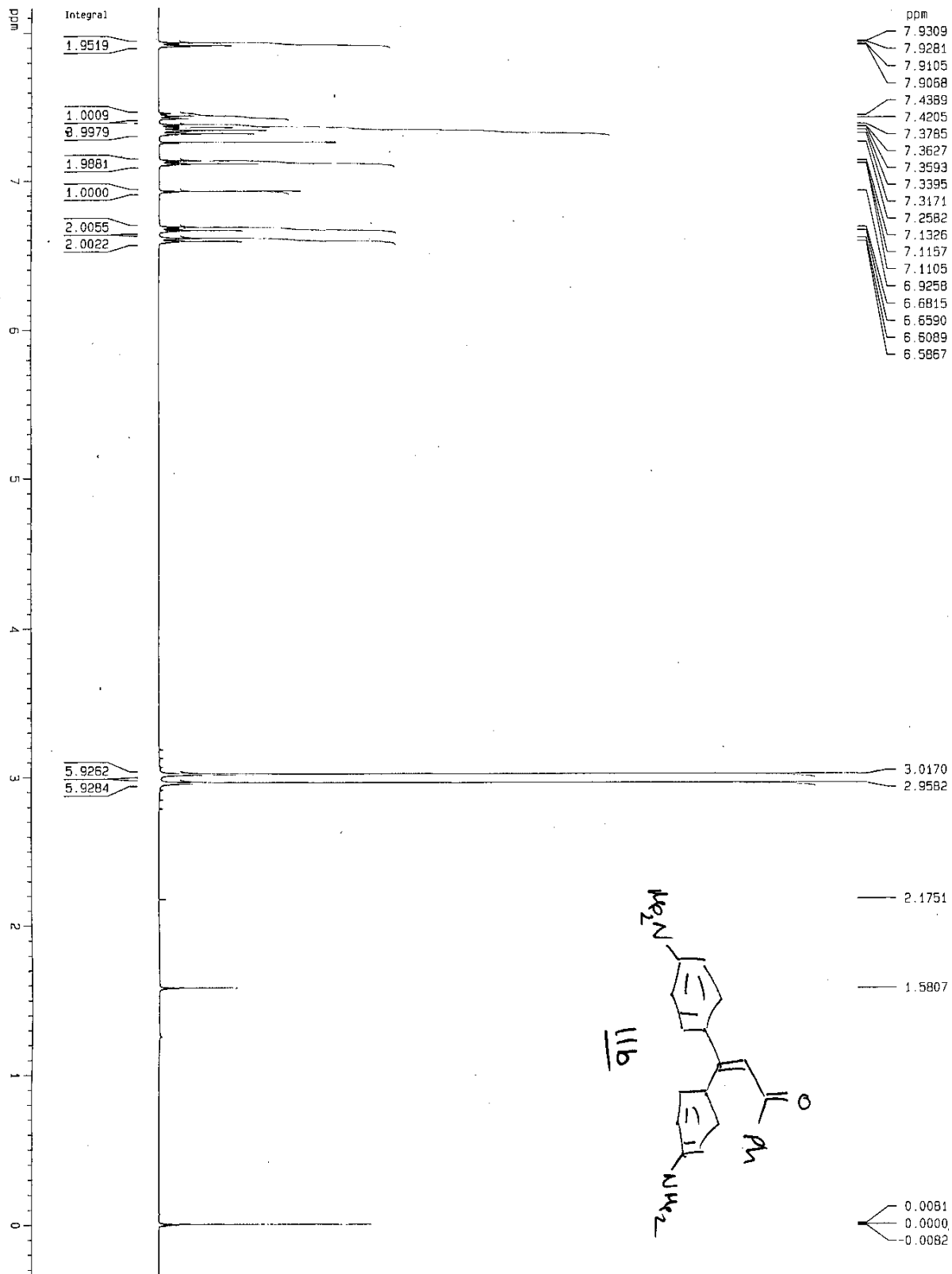
Ph = 4-PhCOCH₂-

119



c:\pel_data\spectra\sk-3-18.sp

SK-3-26 (1)
 PROTON, CoiChem CDC13 {D: \u} Suresh 14



Current Data Parameters

NAME	SK-3-26-1
EXPNO	10
PROCNO	1

F2 - Acquisition Parameters

Date_	20080218
Time	13:26
INSTRUM	spect
PROBHD	5 mm QNP 1H/15
PULPROG	zg30
TD	65536
SOLVENT	CDC13
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9564243 sec
RG	256
DM	60.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec

==== CHANNEL f1 =====

NUC1	1H
P1	10.25 usec
PL1	2.00 dB
SFO1	400.1324710 MHz

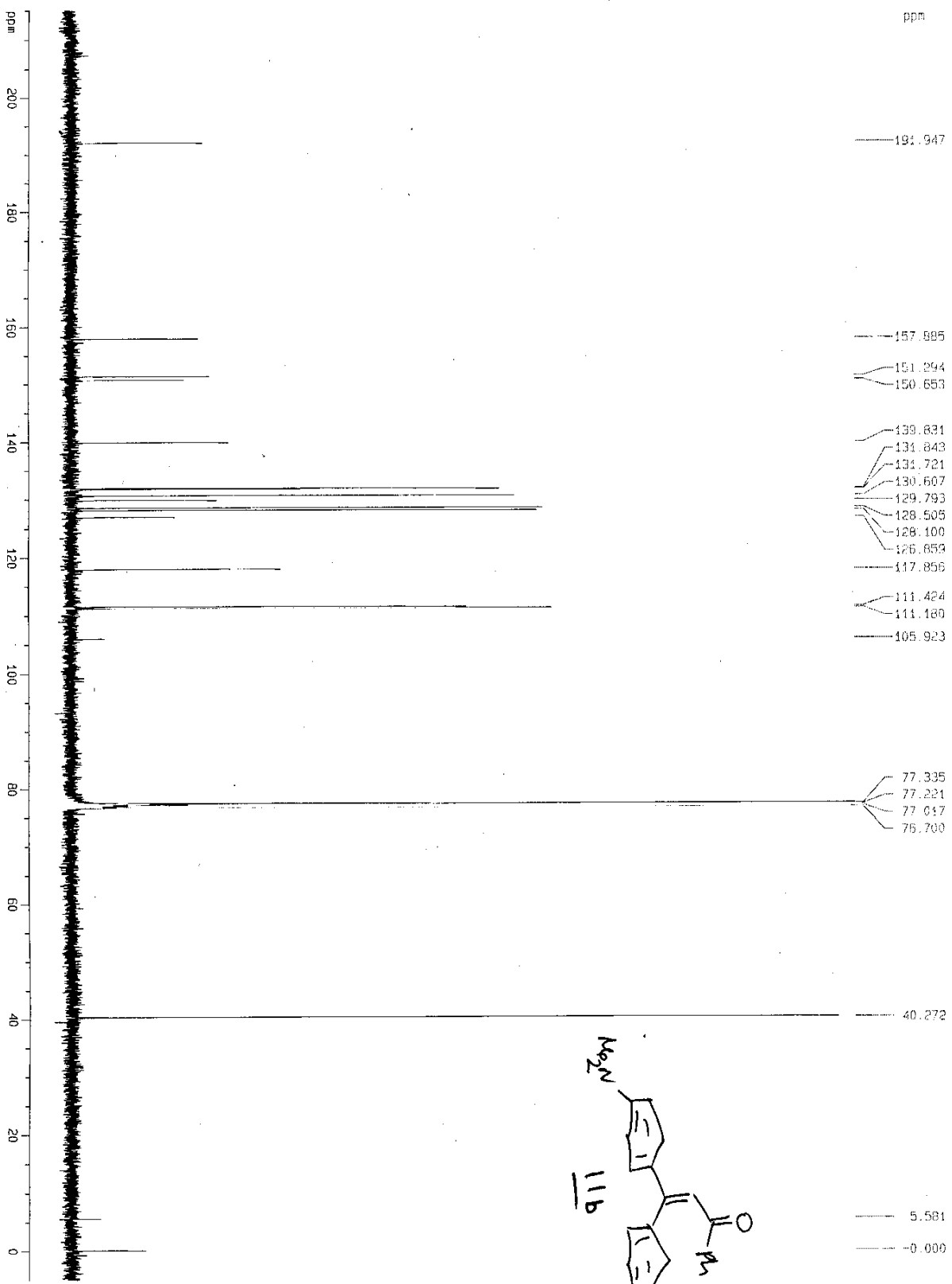
F2 - Processing parameters

SI	32768
SF	400.1300101 MHz
KCW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters.

CX	30.00 cm
CY	19.00 cm
F1P	8.164 ppm
F1	3266.53 Hz
F2P	-0.351 ppm
F2	-140.49 Hz
PMWCM	0.28383 ppm/cm
HZCM	113.56744 Hz/cm

SK-3-26-CARBON
 C13CPD CDC13 (D: \u) Sureash 4



ppm

194.947
 157.585
 151.294
 150.653
 139.831
 134.843
 134.721
 130.607
 129.793
 128.505
 128.100
 126.859
 117.856
 111.424
 111.180
 105.923
 77.335
 77.221
 77.017
 76.700

40.272
 5.581
 0.000

Current Data Parameters
 NAME SK-3-26-CARBON
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080219
 Time 0.23
 INSTRUM spect
 PROBHD 5 mm DNP 1H/15
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 4000
 DS 4
 SMH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 R6 14536.5
 DW 20.850 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 4.00 dB
 SF01 100.6227898 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 POPD2 80.00 usec
 PL2 2.00 dB
 PL12 20.00 dB
 PL13 21.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127712 MHz
 MDW FM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR parameters
 CX 30.00 cm
 CY 19.00 cm
 F1P 215.000 ppm
 F1 21631.75 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPKCM 7.33333 ppm/cm
 HZCM 737.82697 Hz/cm

EPSRC National Mass Spectrometry Service Centre

ACCURATE MASS MEASUREMENT REPORT

YOUR REFERENCE: SK-3-26

OUR REFERENCE: LEEHER060

Instrument: MAT900 XLT

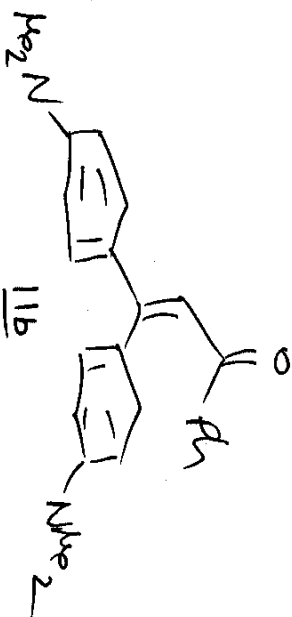
Ionisation Mode: Electrospray (positive)

Reference compound: Polyethylenimine

Ion identity: $[M+H]^+$

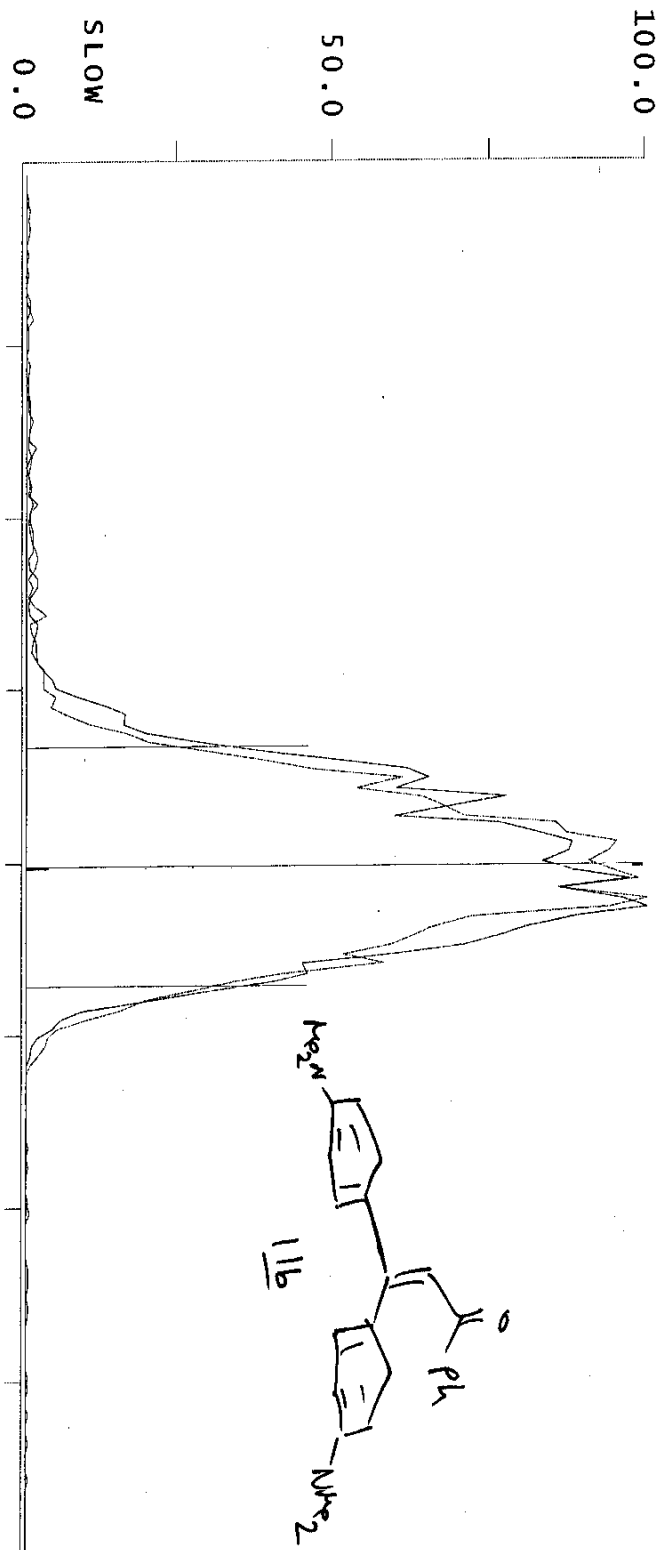
Calculated mass (of ion): 371.2118

Measured mass (of ion): 371.2117



Peak Register Display

Copy result to ULIST



REG 1/2:	371.211720	REG 1/3:	REG 2/3:
MASS	:	362.37200	371.21232
REF MASS	:	362.37142	362.37142
PEAK WIDTH [ppm]	:	86.65401	86.67356

Active Register: 1 0.30 1.00

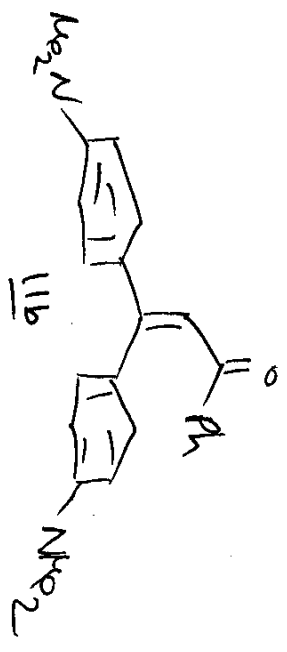
N REG RCOPY2 RCOPY3 LIMIT CENTER SPREAD ERASE RESUME PAGE

PEAK:

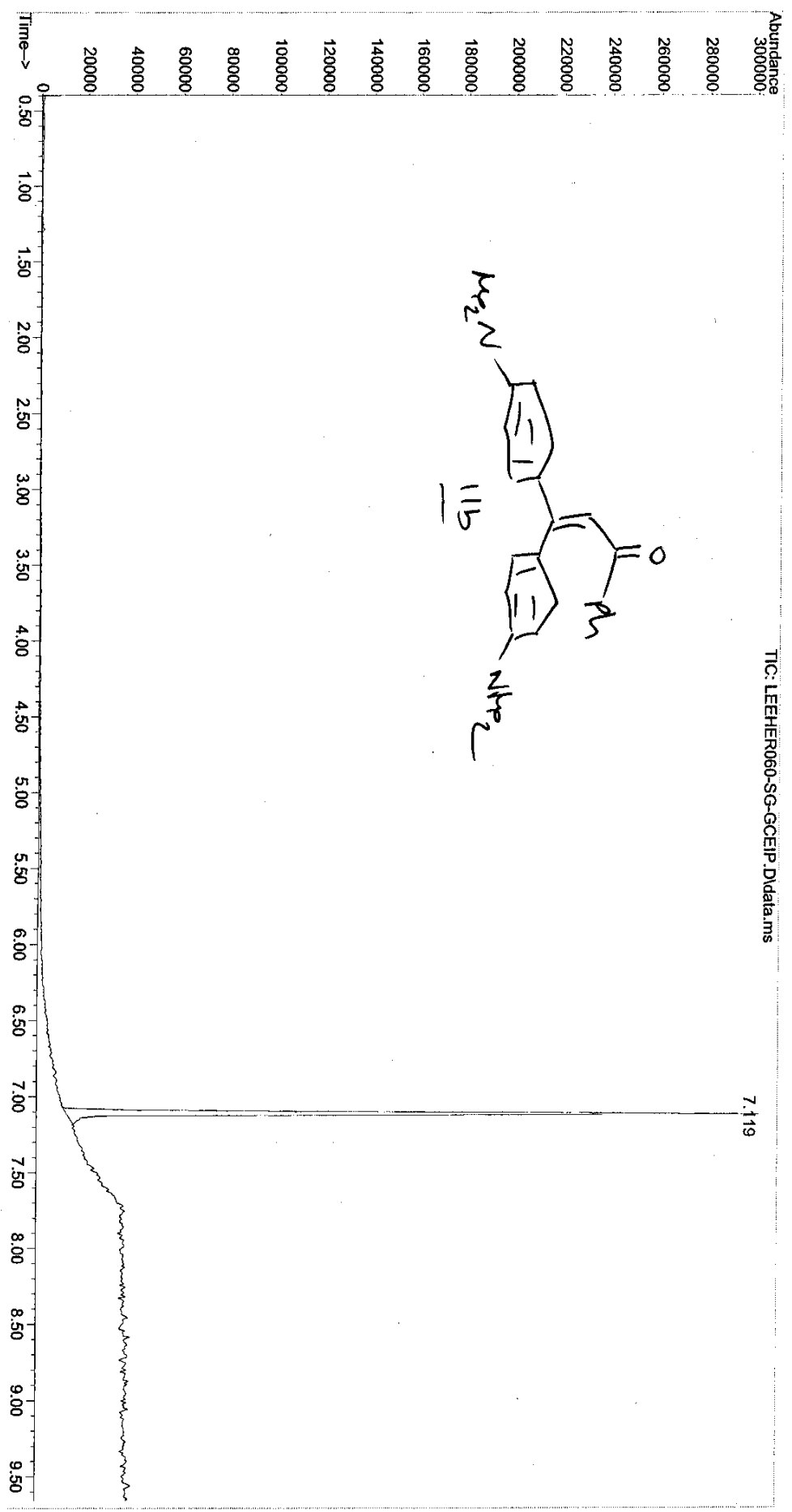
Isotope: Min. ... Max.
 12 C 0.....50
 1 H 0.....80
 14 N 0.....10
 16 O 0.....10
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -2.. 100
 Fits: 100

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
371.2117	371.2118	-0.2	13.5	C ₂₅ H ₂₇ O ₂ N ₂
	371.2123	-1.6	1.0	C ₁₁ H ₇ O ₂ N ₇
	371.2110	2.1	1.5	C ₉ H ₂₇ O ₆ N ₁₀
	371.2104	3.4	14.0	C ₂₃ H ₂₅ N ₅

N-Rule: Do not use
 Charge: 1



File : C:\msdchem\1\DATA\20080226\LEEHER060-SG-GCEIP.D
Operator : AET
Acquired : 26 Feb 2008 15:45 using AcqMethod nms_eipos-ptv.M
Instrument : Agilent GCMS
Sample Name: SK-3-26 MW=370?
Misc Info : Heron
Vial Number: 13



SK-3-26 MW=370?

Heron

LEE60HE2 111 (2.152) Cm (100:111)

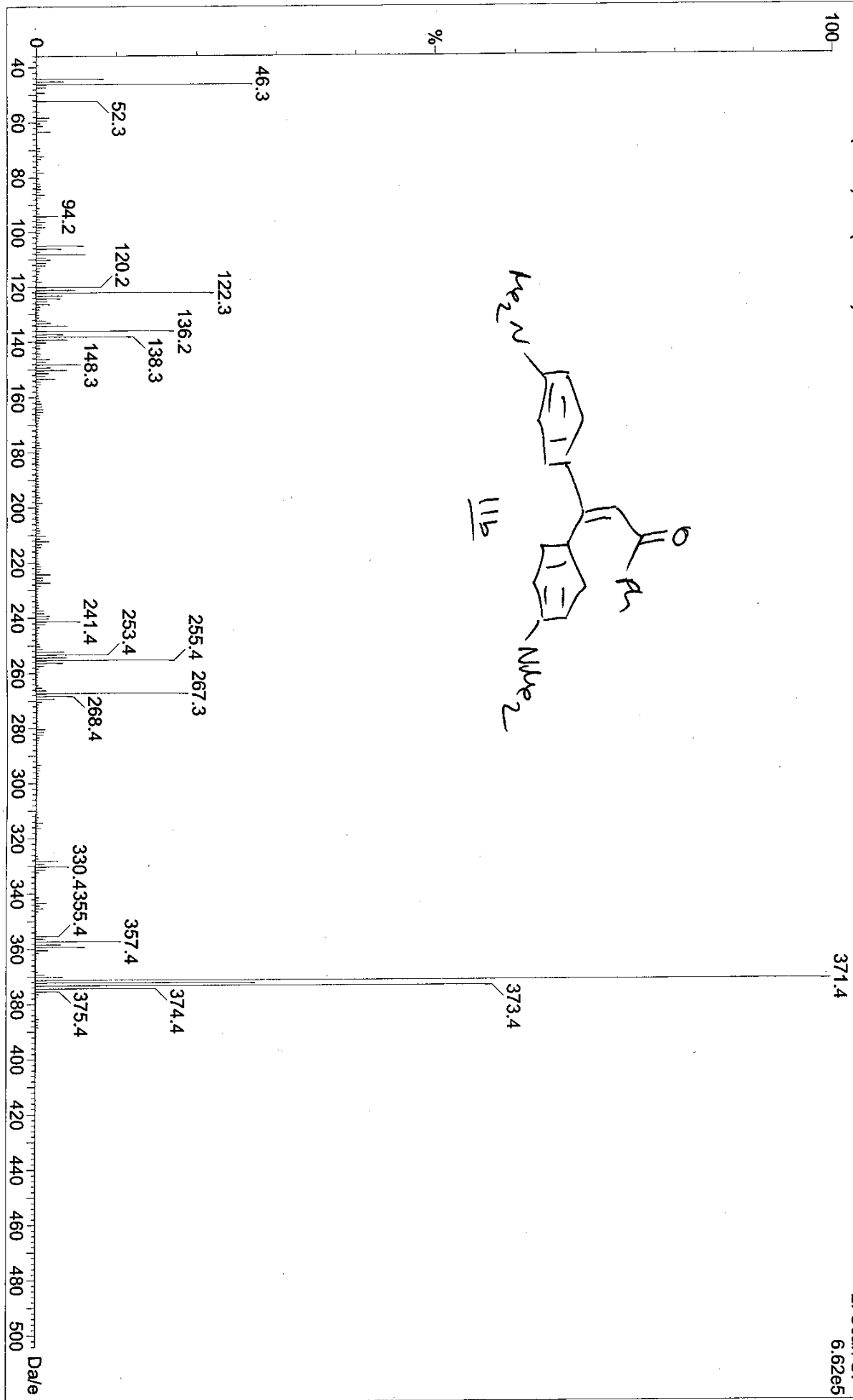
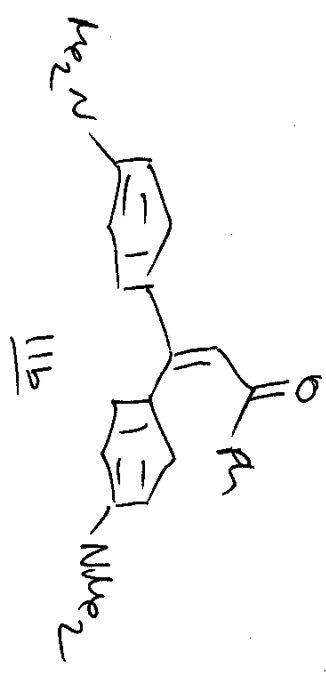
EPSRC National Centre Swansea
QUATTRO

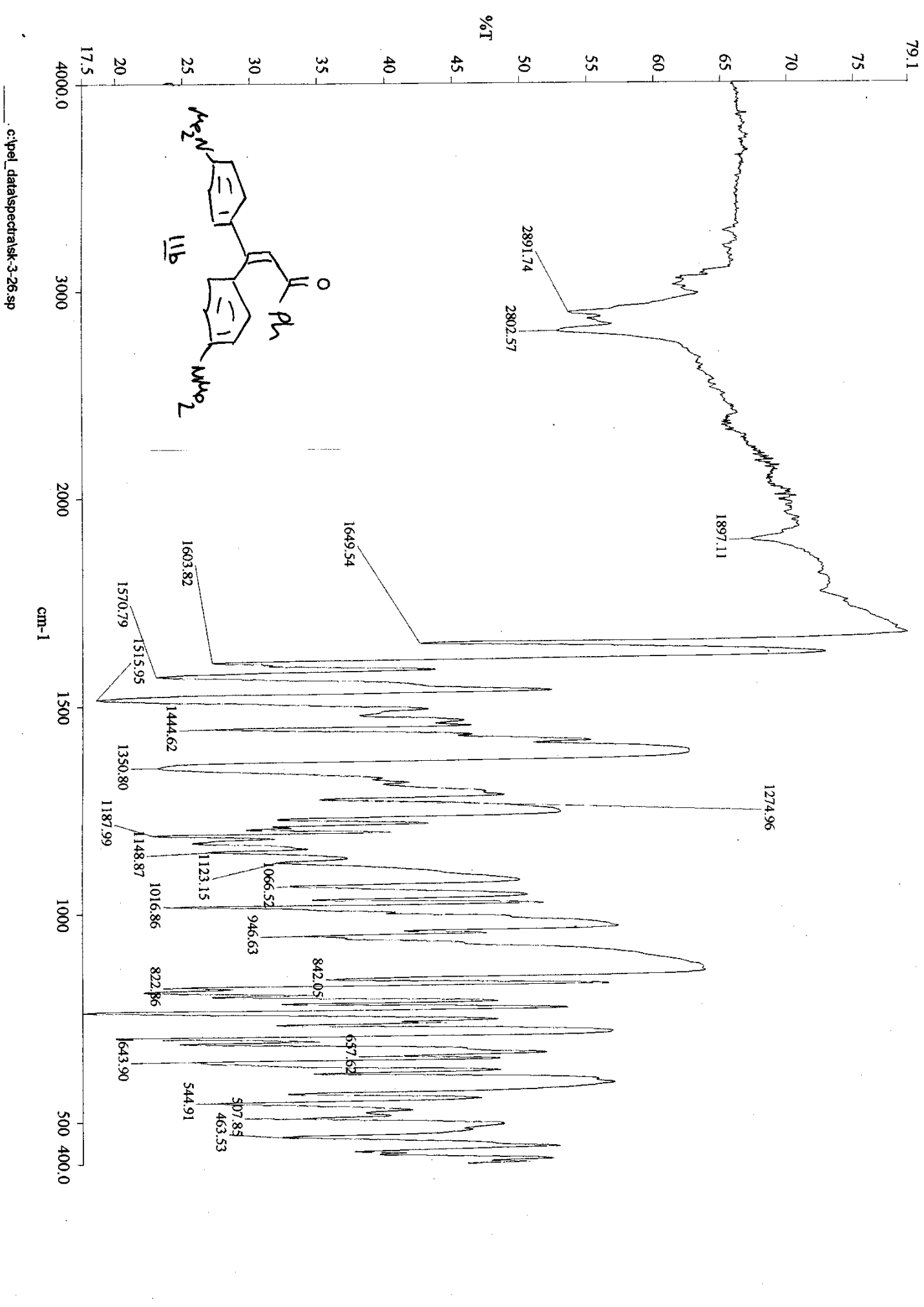
04-Mar-2008 21:48:44

CH+(NH3)

2: Scan CH+

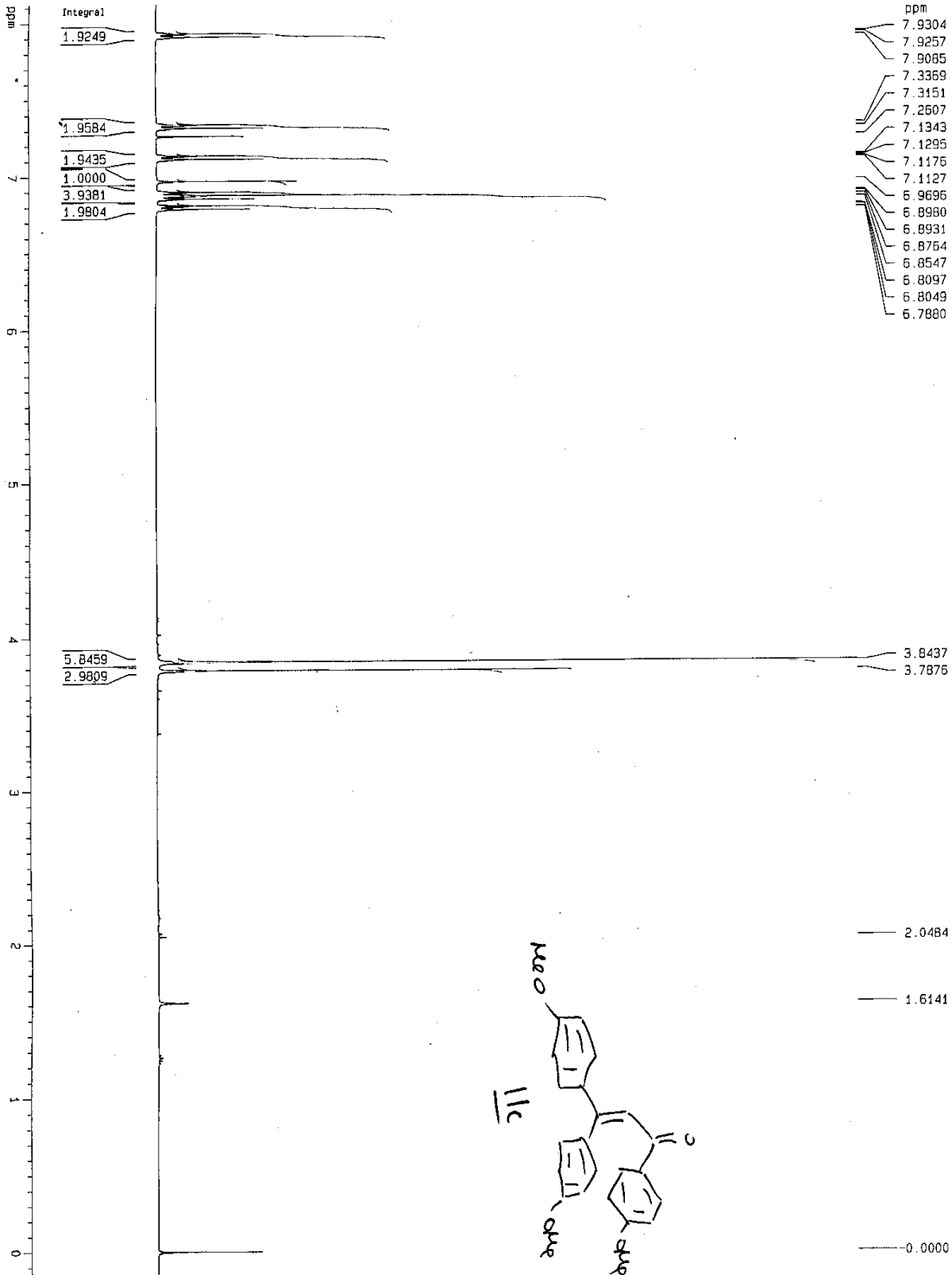
6.62e5





c:\pel_data\spectra\sk-3-26.sp

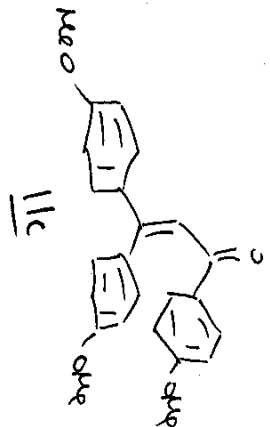
SK-3-27-co1umned
 PROTON.CO1Chem CDC13 {D: \U} Suresh 21



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 7.9085
 7.3369
 7.3151
 7.2507
 7.1343
 7.1295
 7.1176
 7.1127
 6.9696
 6.8980
 6.8931
 6.8764
 6.8547
 6.8097
 6.8049
 6.7880

3.8437
 3.7876
 2.0484
 1.6141
 0.0000

Integral
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 1.9584
 1.9435
 1.0000
 3.9381
 1.9804



Current Data Parameters
 NAME SK-3-27-co1umned
 EXPNO 10
 PROCNO 1

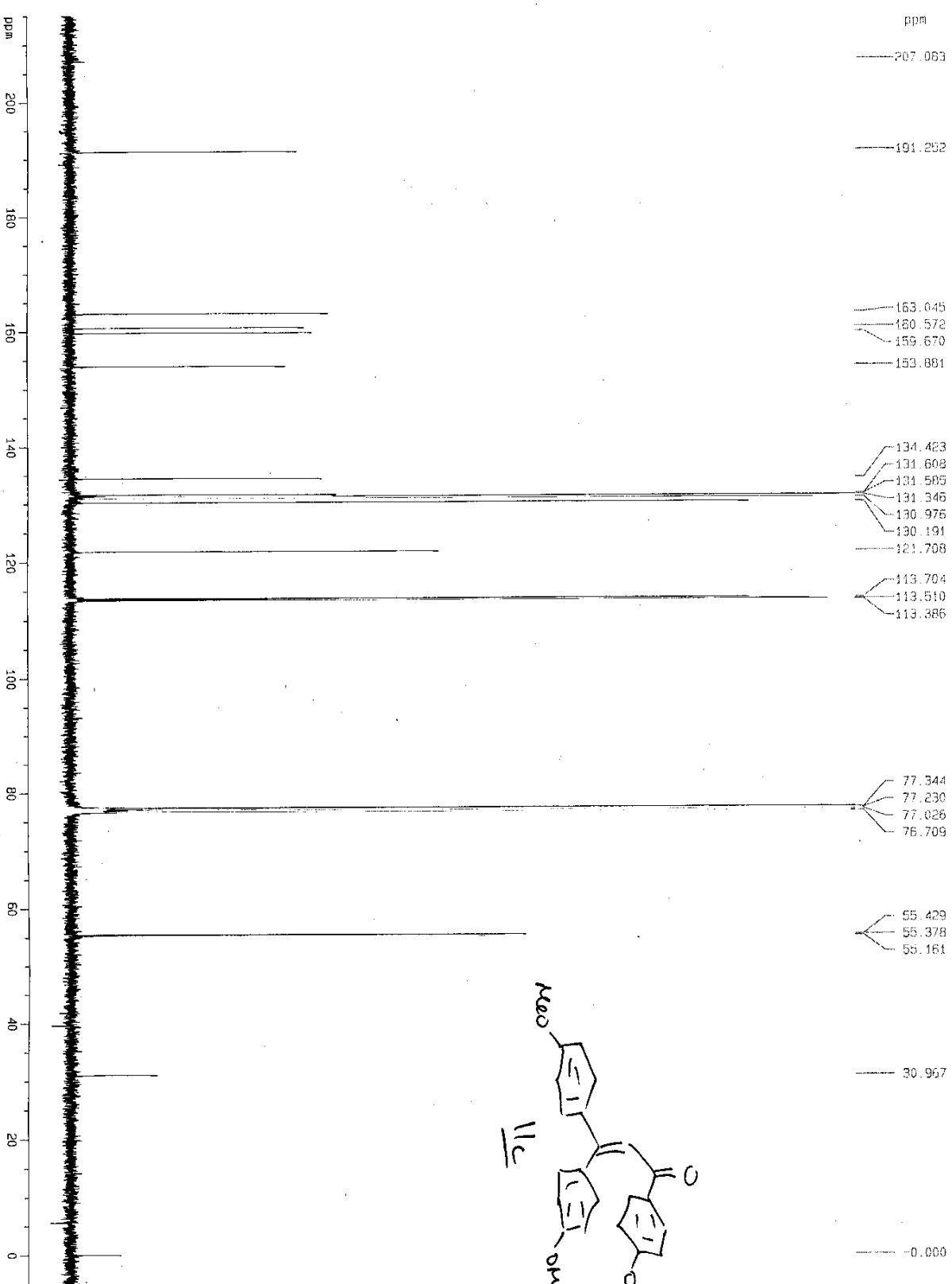
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 Time 15:41
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 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SMH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 181
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.25 usec
 PL1 2.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.130093 MHz
 MDN EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 CY 19.00 cm
 F4P B.120 ppm
 F1 3248.99 Hz
 F2P -0.142 ppm
 F2 -56.75 Hz
 PPMCM 0.27539 ppm/cm
 HZCM 110.19111 Hz/cm

SK-3-27-carbon
 C13CPD CDCl3 (D: \u) Suresh 6



Current Data Parameters
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 EXPNO 10
 PROCNO 1

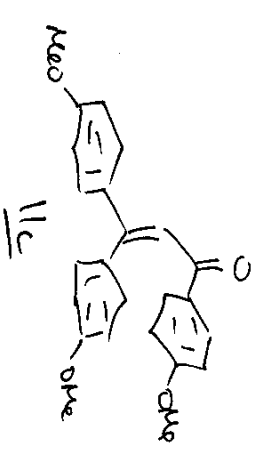
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 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 4000
 DS 4
 SMH 23980.814 HZ
 FIDRES 0.365818 HZ
 AQ 1.3664756 sec
 R6 16384
 DW 20.850 usec
 DE 6.00 usec
 TE 300.0 K
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 d11 0.03000000 sec
 d12 0.00002000 sec

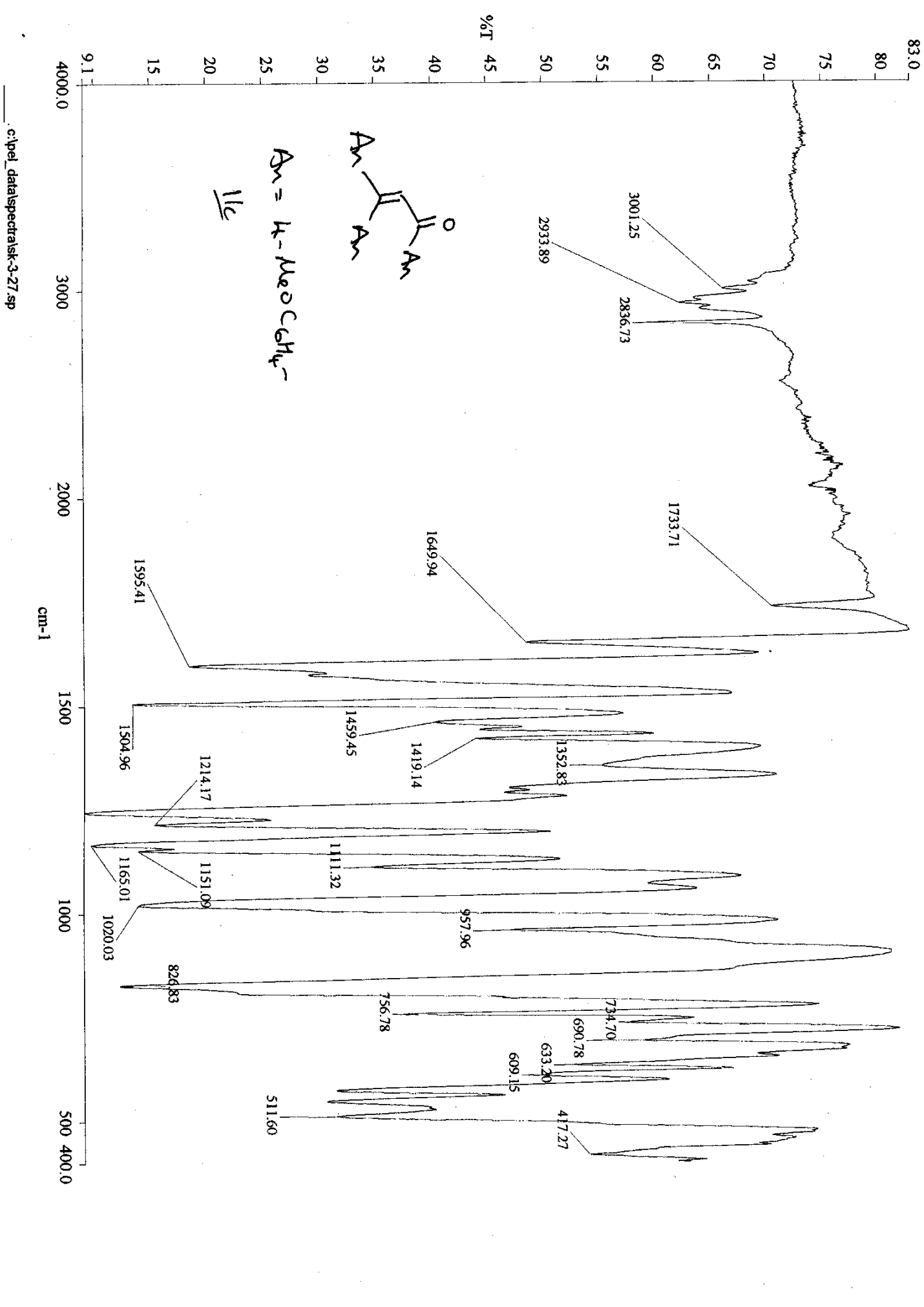
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 PL1 4.00 dB
 SF01 100.6227898 MHz

==== CHANNEL f2 =====
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 NUC2 1H
 PCPD2 80.00 usec
 PL2 2.00 dB
 PL12 20.00 dB
 PL13 21.00 dB
 SF02 400.1316005 MHz

F2 - Processing Parameters
 SI 32768
 SF 100.6127709 MHz
 MDW EM
 SSB 0
 LB 1.00 HZ
 GB 0
 PC 1.40

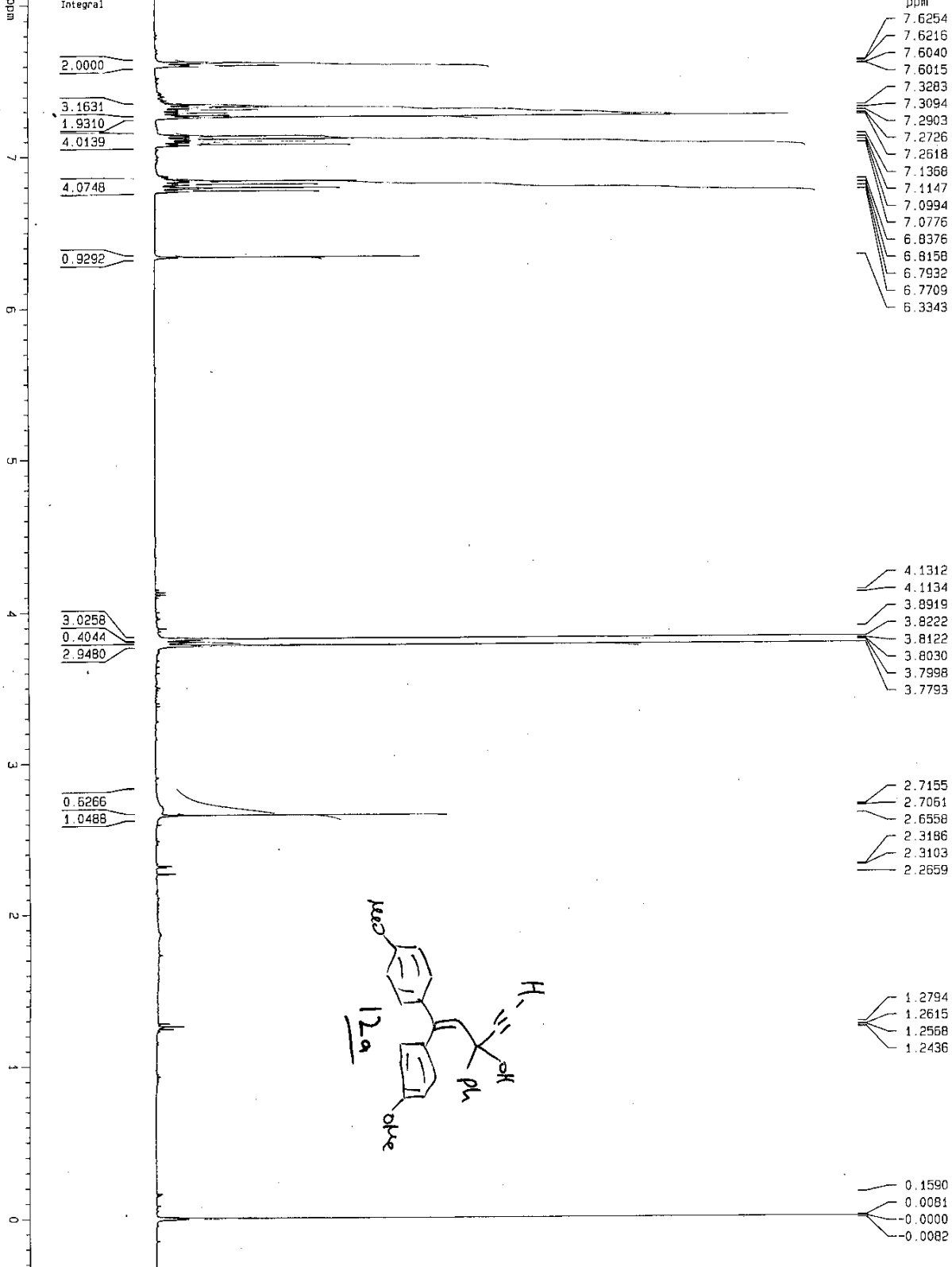
1D NMR plot parameters
 CX 30.00 cm
 CY 19.00 cm
 F1P 215.000 ppm
 F1 21631.75 HZ
 F2P -5.000 ppm
 F2 -503.06 HZ
 PPMCM 7.33333 ppm/cm
 HZCM 737.82697 HZ/cm





c:\pel_data\spectra\sk-3-27.sp

sk-3-28-pure alkyno1
 PROTON.C01chem C0C13 [D: \u] Suresh 7



ppm
 7.6254
 7.6216
 7.6040
 7.6015
 7.3283
 7.3094
 7.2903
 7.2726
 7.2618
 7.1368
 7.1147
 7.0994
 7.0776
 6.8376
 6.8158
 6.7932
 6.7709
 6.3343

4.1312
 4.1134
 3.8919
 3.8222
 3.8122
 3.8030
 3.7998
 3.7793

2.7155
 2.7051
 2.6558
 2.3186
 2.3103
 2.2659

1.2794
 1.2615
 1.2558
 1.2436

0.1590
 0.0081
 0.0000
 -0.0082

Integral
 2.0000
 3.1631
 1.9310
 4.0139
 4.0748

0.9292

3.0258
 0.4044
 2.9480

0.6266
 1.0488

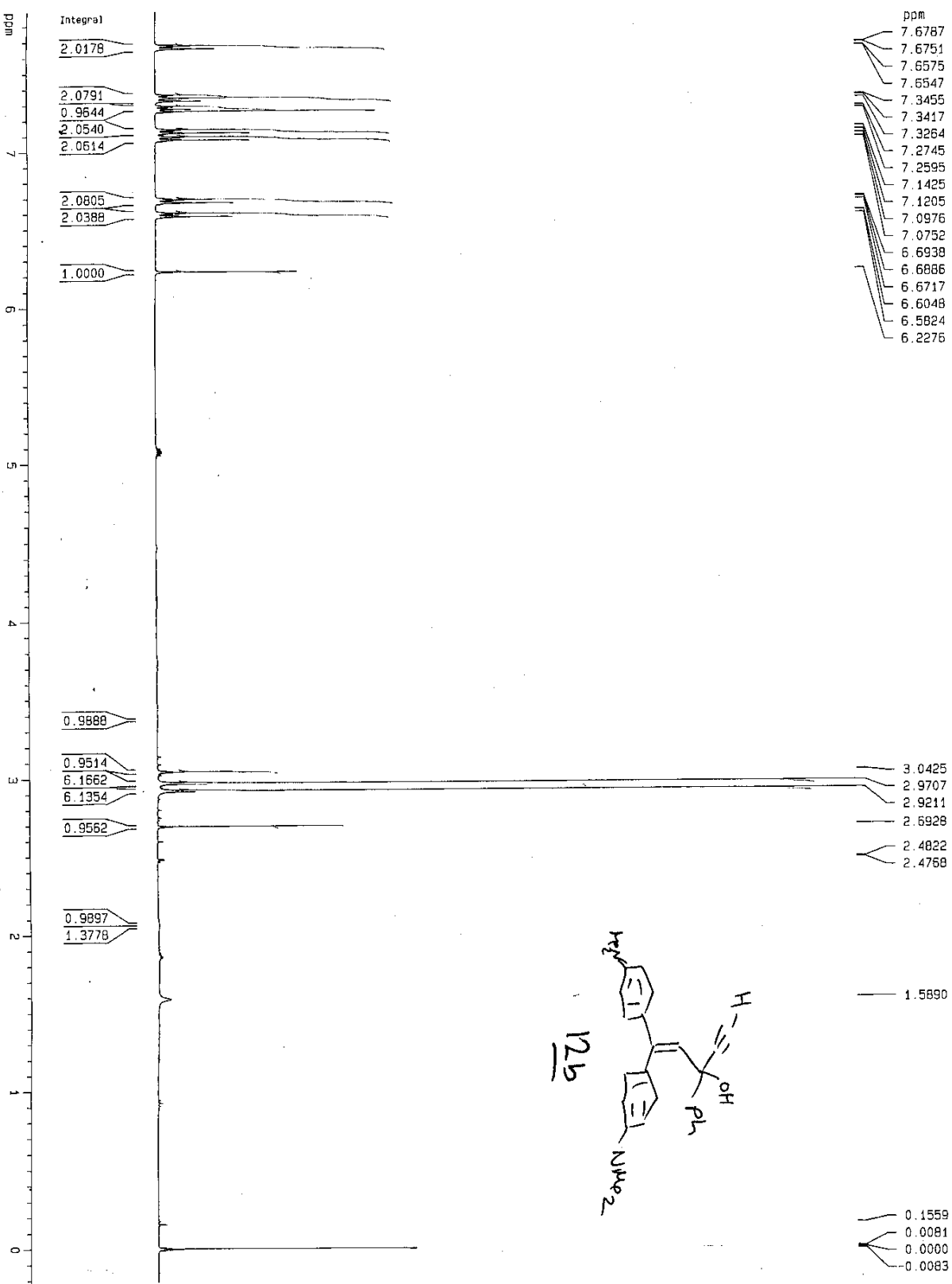
Current Data Parameters
 NAME sk-3-28-pure
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080221
 Time 9.58
 INSTRUM spect
 PROBRD 5 mm QNP 1H/15
 PULPROG zg30
 TD 65536
 SOLVENT C0C13
 NS 16
 DS 2
 SWH 8278.146 HZ
 FIDRES 0.126314 HZ
 AQ 3.9584243 sec
 RG 362
 DM 60.400 usec
 DE 5.00 usec
 TE 300.0 K
 D1 1.00000000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.25 usec
 PL1 2.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.130098 MHz
 WDW EM
 SSB 0
 LB 0.30 HZ
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 CY 19.00 cm
 F1P 8.052 ppm
 F1 3221.77 HZ
 F2P -0.325 ppm
 F2 -130.01 HZ
 PPMCM 0.27922 ppm/cm
 HZCM 111.72581 HZ/cm



Current Data Parameters
 NAME SK-3-40
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080305
 Time 15.35
 INSTRUM spect
 PROBHD 5 mm QNP 1H/15
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 228.1
 DM 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.25 usec
 PL1 2.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.130095 MHz
 MVM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 CY 19.00 cm
 F1P 7.889 ppm
 F1 3156.55 Hz
 F2P -0.212 ppm
 F2 -84.73 Hz
 PPMCM 0.27002 ppm/cm
 HZCM 108.04254 Hz/cm

SK-3-34 - ALKYNOL
 PROTON, Co1Chem CDC13 {D: \u} Suresh 4

ppm
 7.5396
 7.5228
 7.5174
 7.2618
 7.1410
 7.1189
 7.0828
 7.0610
 6.8543
 6.8489
 6.8374
 6.8312
 6.8251
 6.8087
 6.7947
 6.7725
 6.3306

3.8458
 3.8168
 3.8107
 3.7984
 3.7955
 3.7802
 3.7573
 3.7127
 3.6899
 3.5238

2.7503
 2.7362
 2.6446
 2.6363
 2.5832
 2.2781

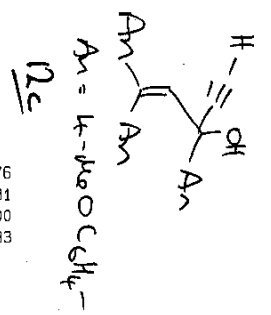
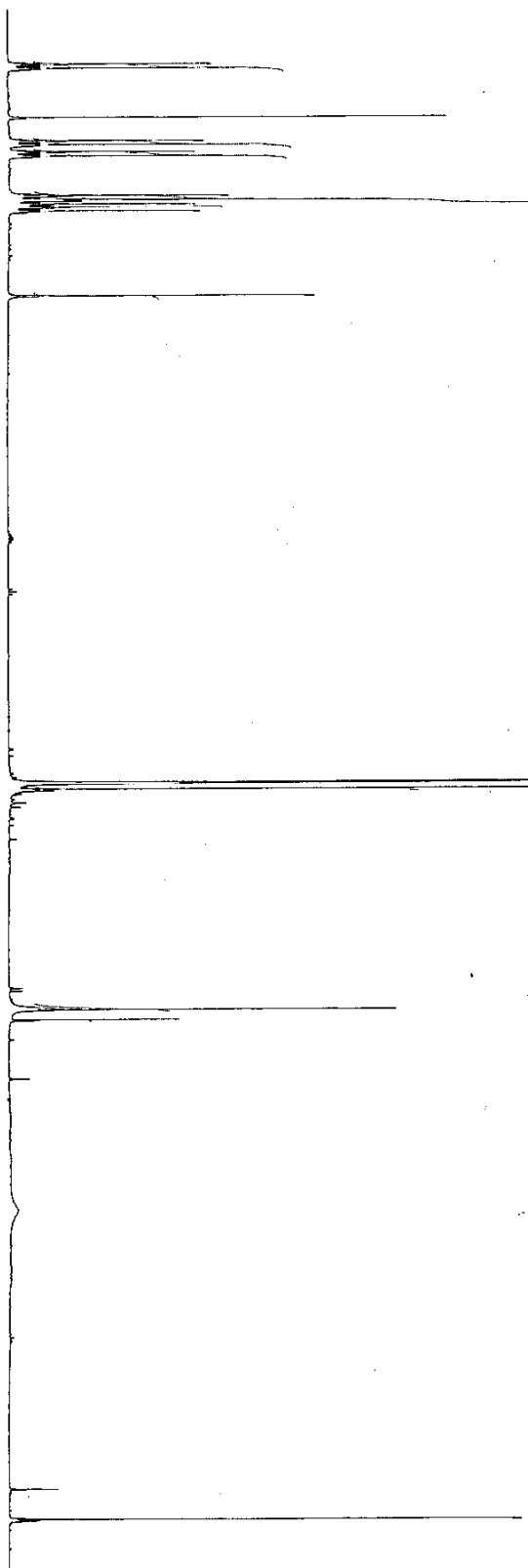
0.1576
 0.0081
 0.0000
 -0.0083

Integral
 2.0117
 2.0716
 2.0327
 6.3285
 1.0000

6.1346
 3.0880

0.7029
 1.0766
 0.4561

ppm
 7
 6
 5
 4
 3
 2
 1
 0



Current Data Parameters:
 NAME SK-3-34
 EXPNO 10
 PROCNO 1

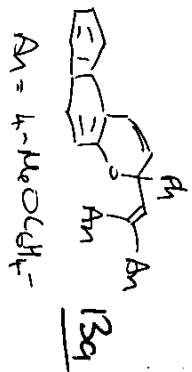
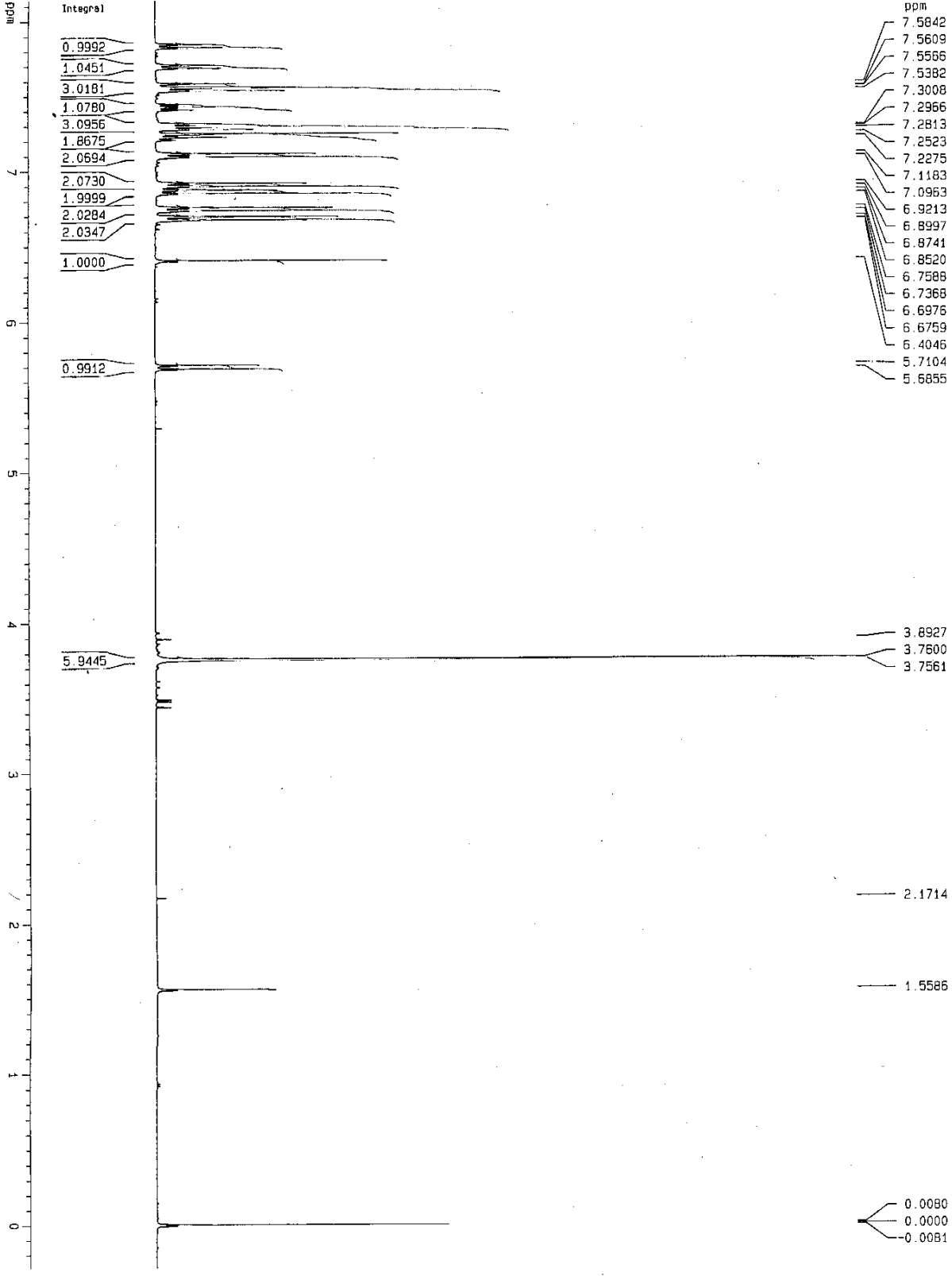
F2 - Acquisition Parameters
 Date_ 20080227
 Time 10.25
 INSTRUM spect
 PROBHD 5 mm QNP 1H/15
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SMH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 228.1
 DM 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.25 usec
 PL1 2.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.130087 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 CY 19.00 cm
 F1P 7.822 ppm
 F1 3129.82 Hz
 F2P -102.25 Hz
 F2 -102.25 Hz
 PPM1CM 0.26925 ppm/cm
 HZCM 107.73560 Hz/cm

sk-3-20-pure-proton
 PROTON: CoiChem CDCl3 {D: \u} Suresh 8



Current Data Parameters
 NAME sk-3-20-pure
 EXPNO 10
 PROCNO 1

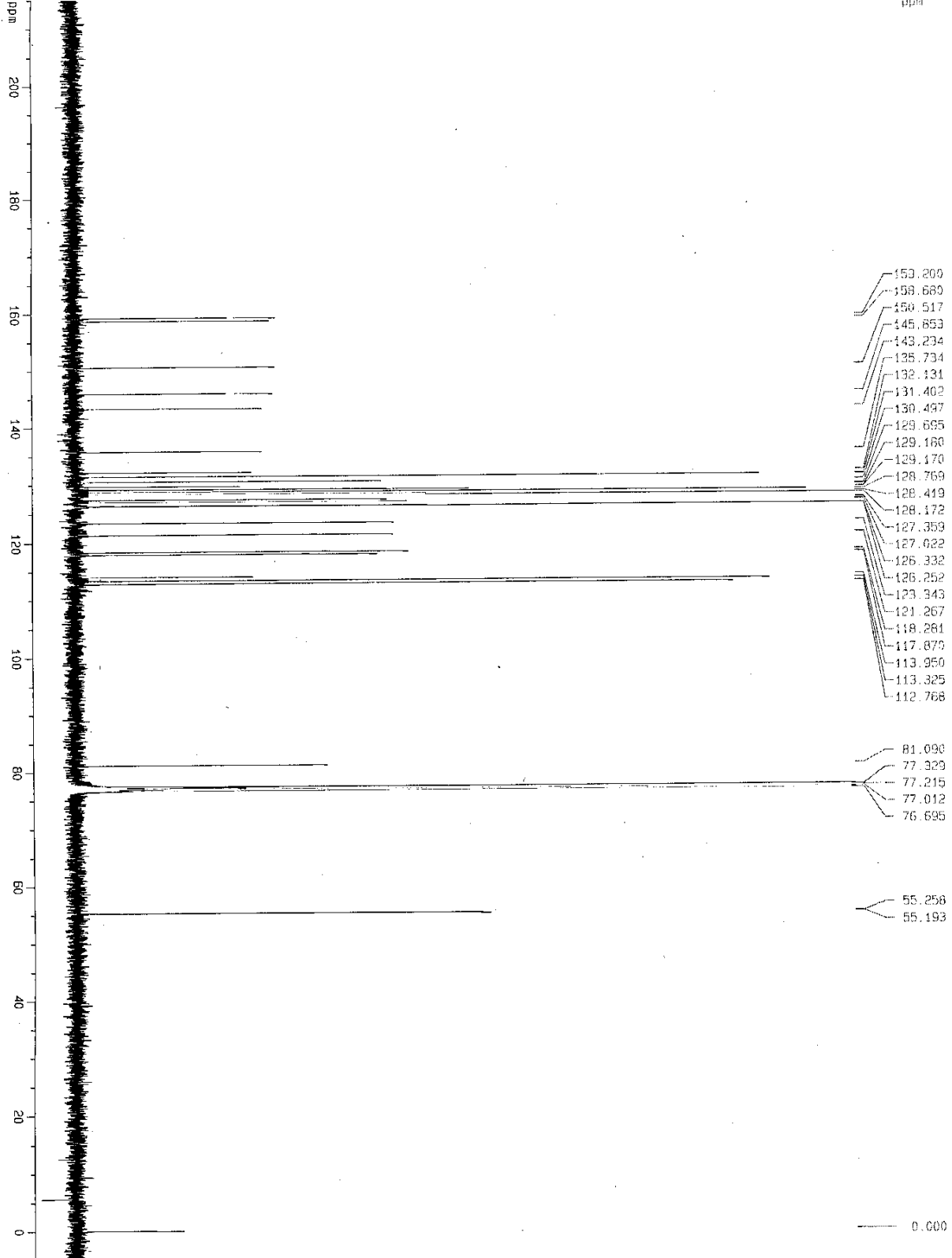
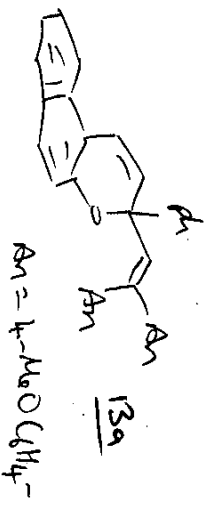
F2 - Acquisition Parameters
 Date_ 20080222
 Time 10.50
 INSTRUM spect
 PROBHD 5 mm QNP 1H/15
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 228.1
 DM 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.25 usec
 PL1 2.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300125 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 CY 19.00 cm
 F1P 8.135 ppm
 F1 3254.93 Hz
 F2P -0.288 ppm
 F2 -115.26 Hz
 PPMCM 0.28076 ppm/cm
 HZCM 112.33969 Hz/cm

SK-3-20-carbon
 C13CPD CDC13 (D: \u) Suresh 5



153.209
 150.660
 150.517
 145.853
 143.234
 135.734
 132.131
 131.402
 130.497
 129.695
 129.160
 129.170
 128.769
 128.419
 128.172
 127.359
 127.022
 126.332
 126.252
 123.343
 121.267
 118.281
 117.879
 113.950
 113.325
 112.768

81.090
 77.329
 77.215
 77.012
 76.696

55.258
 55.193

0.000

Current Data Parameters
 NAME SK-3-20-carbon
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080223
 Time 12.54

INSTRUM spect
 PROBHD 5 mm QNP 1H/15
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 5000

DS 4
 SMH 23986.814 HZ
 FIDRES 0.365918 HZ
 AQ 1.3684756 sec
 RG 20642.5
 DE 20.850 usec
 TE 300.0 K

D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

CHANNEL f1
 NUC1 13C
 P1 8.00 usec
 PL1 4.00 dB
 SF01 100.6227898 MHz

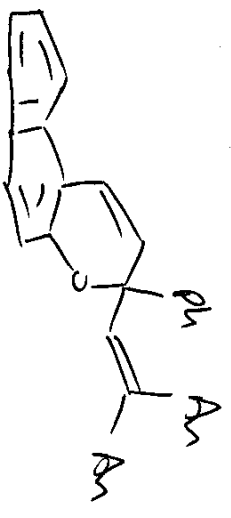
CHANNEL f2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 2.00 dB
 PL12 20.00 dB
 PL13 21.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127719 MHz
 WDW EM
 SSB 0
 LB 1.00 HZ
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 30.00 cm
 CY 19.00 cm
 FLIP 215.000 ppm
 F1 21631.75 HZ
 F2 -5.000 ppm
 F2 -503.06 HZ
 PPMKCH 7.33333 ppm/cm
 HZCM 737.82697 HZ/cm

EPSRC National Mass Spectrometry Service Centre
ACCURATE MASS MEASUREMENT REPORT

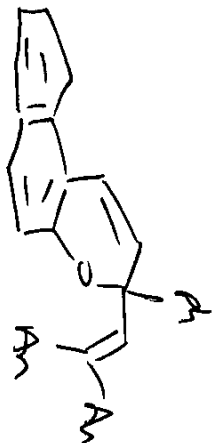
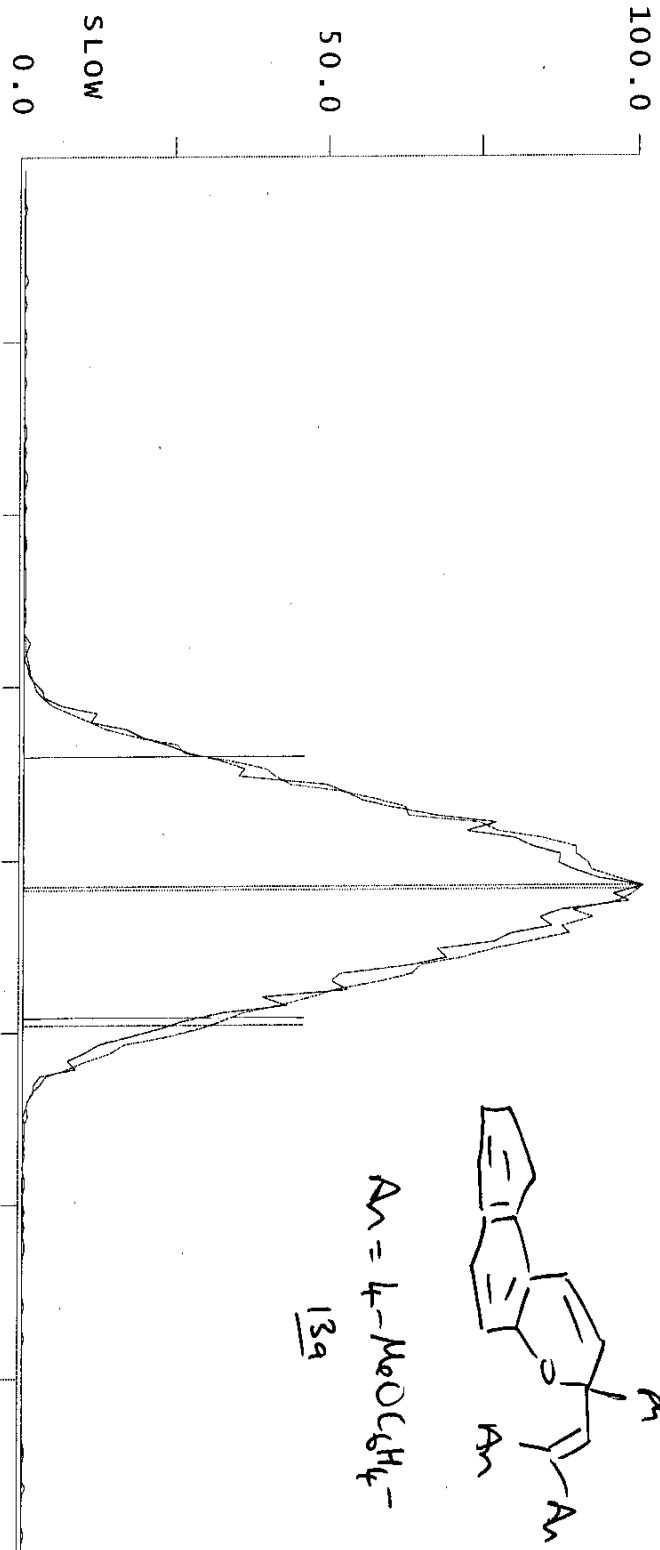
YOUR REFERENCE: SK-3-20
OUR REFERENCE: LEEHER061
Instrument: MAT 95 XP
Ionisation Mode: EI
Reference compound: Perfluorotributylamine
Ion identity: [M]⁺
Calculated mass (of ion): 496.2033
Measured mass (of ion): 496.2028



An = 4-MeO C₆H₄
13a

Peak Register Display

Copy result to ULIST



An = 4-MeOC₆H₄-
13a

REG 1/2:	496.202815	REG 1/3:	496.20716	REG 2/3:	501.97055
MASS	:	413.98058		496.20716	
REF MASS	:	413.97695		501.97055	
PEAK WIDTH [ppm]:		77.72298		75.44507	

Active Register: 2 0.30 1.00

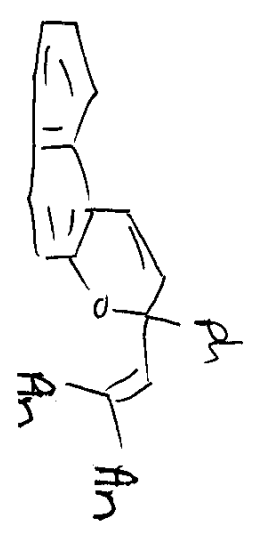
- N REG
- RCOPY1
- RCOPY3
- LIMIT
- CENTER
- SPREAD
- ERASE
- RESUME
- PAGE

Isotope:	Min. .. Max.
12 C	0.....60
1 H	0.....80
16 O	0.....12
14 N	0.....12

Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -2.. 100
 FIts: 100

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
496.2028	496.2025	0.7	10.0	C ₁₉ H ₂₈ O ₈ N ₈
	496.2033	-1.0	22.0	C ₃₅ H ₂₈ O ₁
	496.2020	1.7	22.5	C ₃₃ H ₂₆ O ₂ N ₃
	496.2038	-2.0	15.0	C ₂₆ H ₂₄ O ₄ N ₂
	496.2038	-2.0	9.5	C ₂₁ H ₃₀ O ₉ N ₅
	496.2011	3.4	5.0	C ₁₈ H ₃₂ O ₁₂ N ₄
	496.2011	3.4	10.5	C ₁₇ H ₂₆ O ₉ N ₁₁
	496.2006	4.4	23.0	C ₃₁ H ₂₄ O ₁ N ₆
	496.2051	-4.7	14.5	C ₂₂ H ₂₆ O ₅ N ₇
	496.2051	-4.7	9.0	C ₂₃ H ₃₂ O ₁₀ N ₂

N-Rule: Do not use
 Charge: 1



An = 4-MeO C₆H₄-

139

SK-3-20 MW=4967

Heron

LEE61HER 155 (2.867) Cm (154:155)

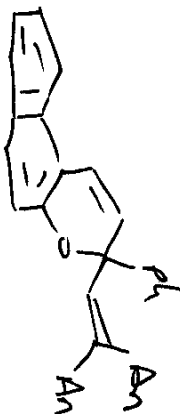
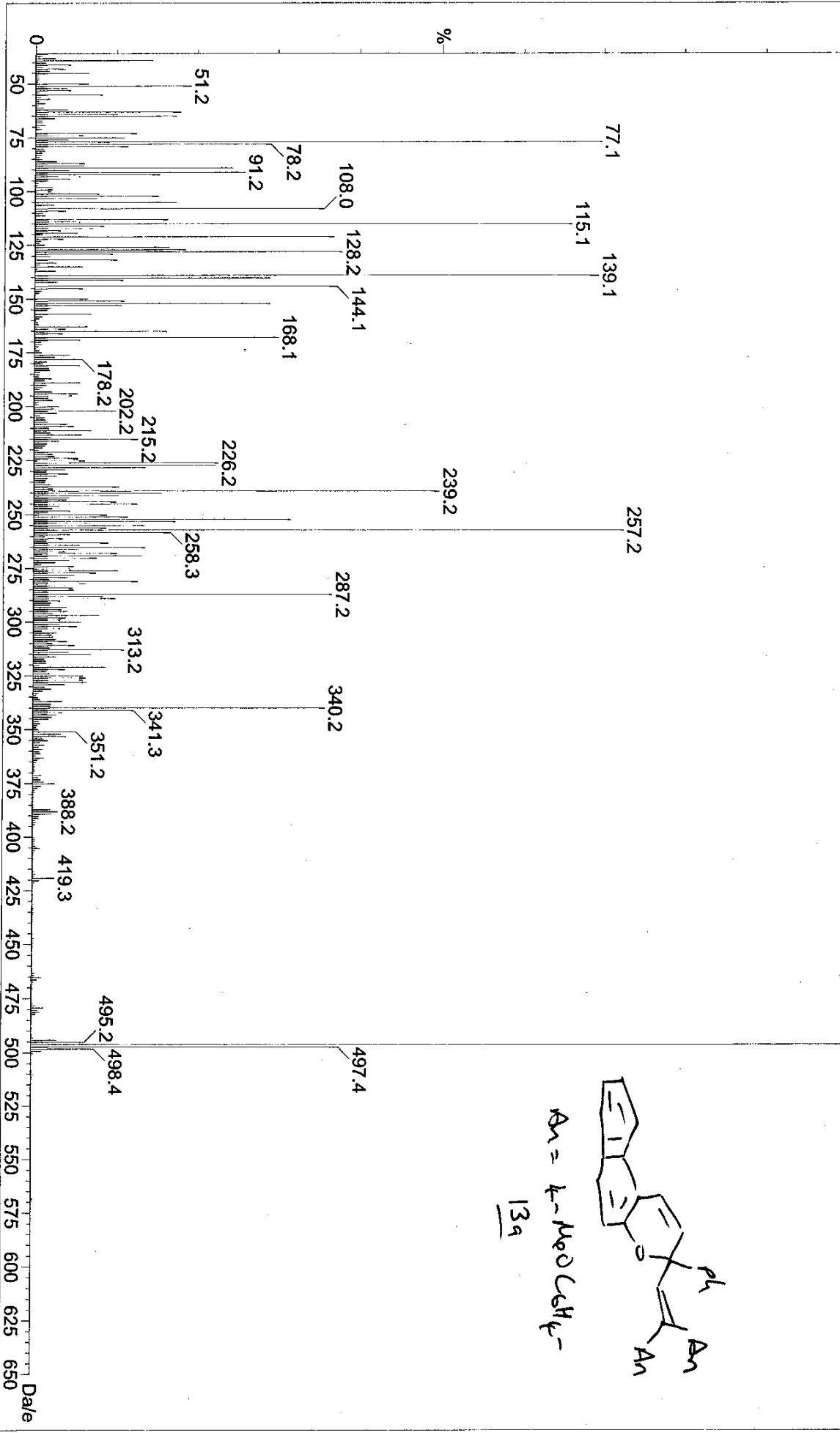
EPSRC National Centre Swansea
QUATTRO

10-Mar-2008 09:55:56

100%

496.3

Scan E1+
7.21e5



An = *p*-MeOC₆H₄-

139

Date

SK-3-20 MW=4967

EPSRC National Centre Swansea

10-Mar-2008 16:39:16

Heron

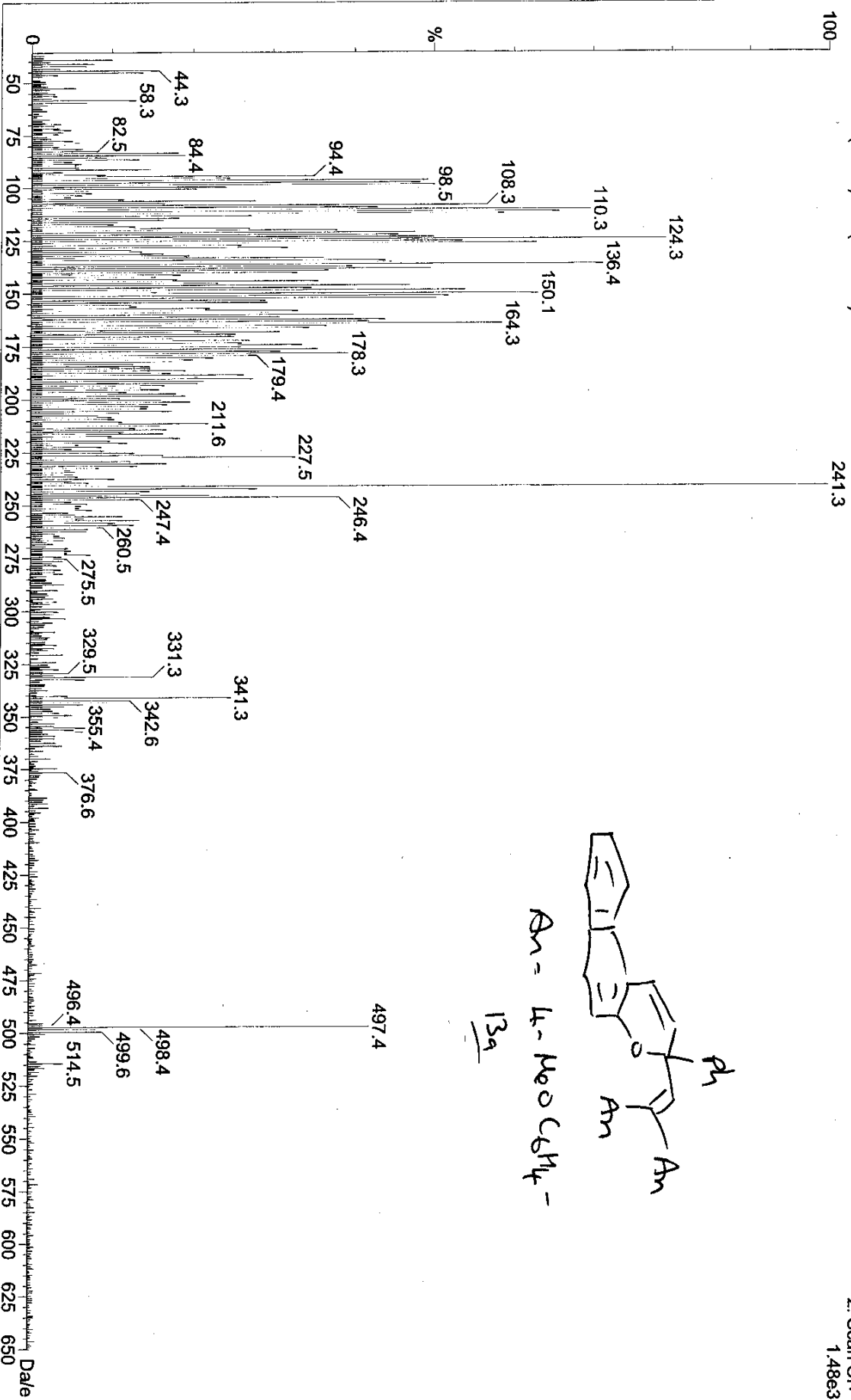
QUATTRO

CI+(NH3)

LEE61HE2 127 (2,445) Cm (126:127)

2: Scan CI+

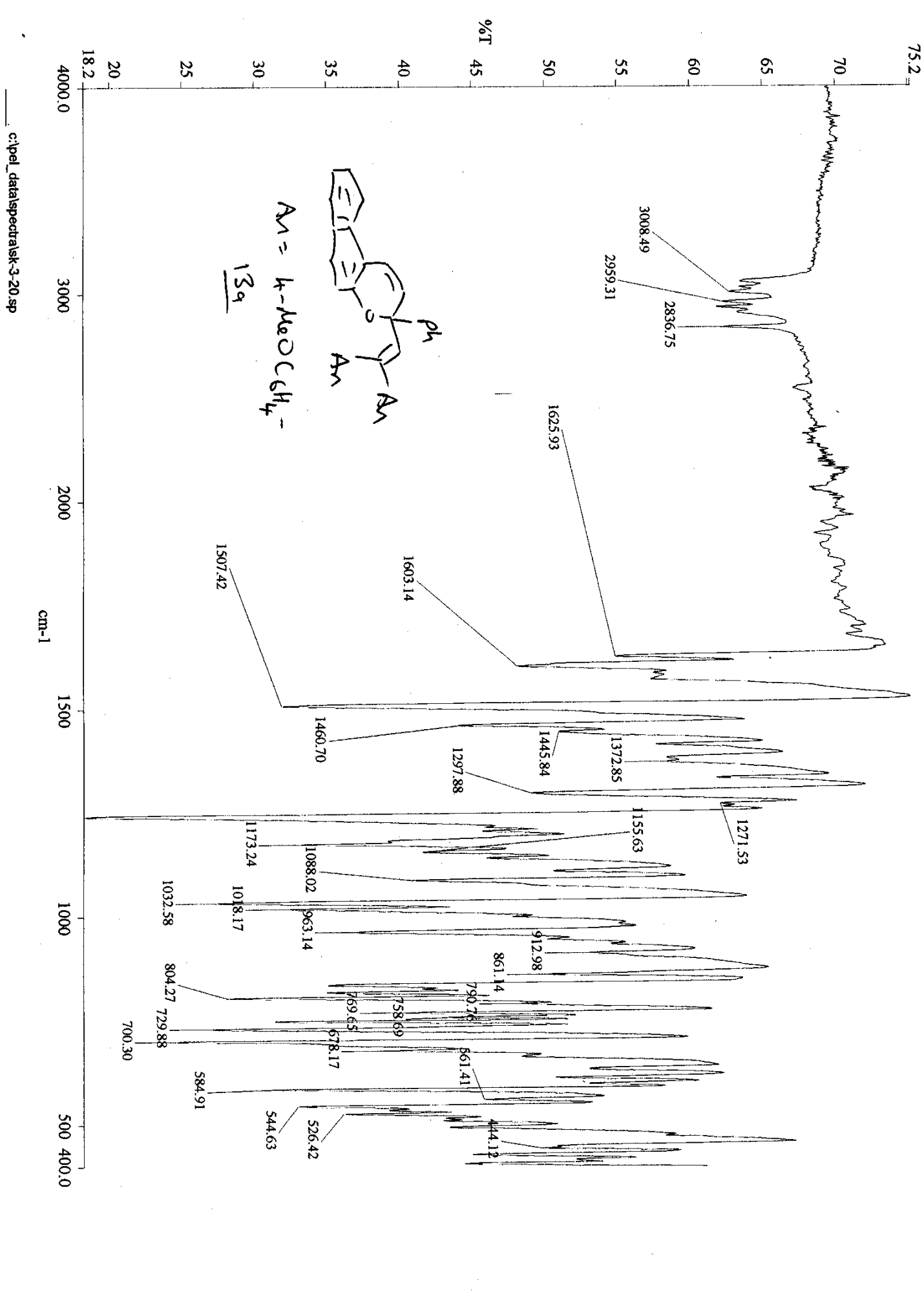
1.48e3



Am - C_6H_5

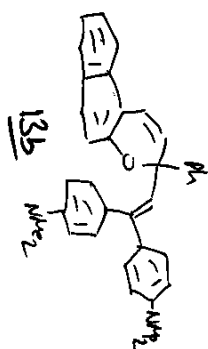
139

Date



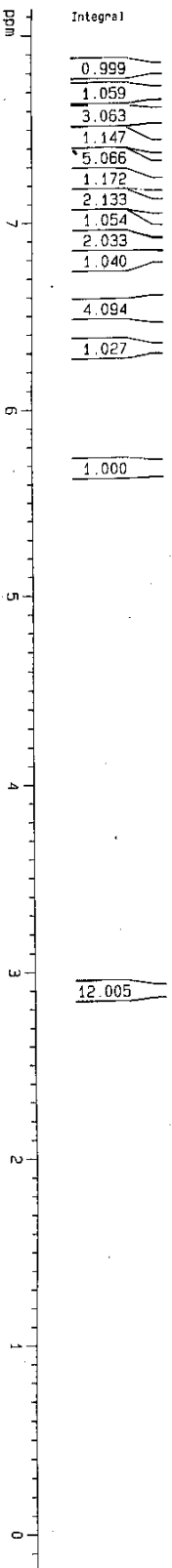
c:\pel_data\spectra\sk-3-20.sp

SK-3-42
 PROTON: CoIChem CDC13 {D: \u} Suresh 22



- 7.59007
- 7.58564
- 7.57194
- 7.56365
- 7.29282
- 7.28177
- 7.27847
- 7.27340
- 7.25683
- 7.10099
- 7.07904
- 6.95903
- 6.94703
- 6.89095
- 6.86946
- 6.82838
- 6.80330
- 6.57924
- 6.55718
- 6.52320
- 6.50156
- 6.33085
- 5.70616
- 5.68113

- 3.02551
- 2.98487
- 2.94144
- 2.90852
- 2.90189
- 2.87147
- 2.85957
- 2.85274
- 2.75187
- 2.17426
- 1.56382
- 0.94125
- 0.92732
- 0.00000



- 0.999
- 1.059
- 3.063
- 1.147
- 5.066
- 1.172
- 2.133
- 1.054
- 2.033
- 1.040
- 4.094
- 1.027
- 1.000

12.005

Current Data Parameters
 NAME SK-3-42
 EXPNO 10
 PROCNO 1

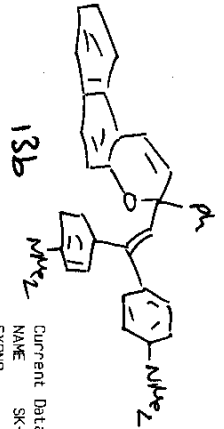
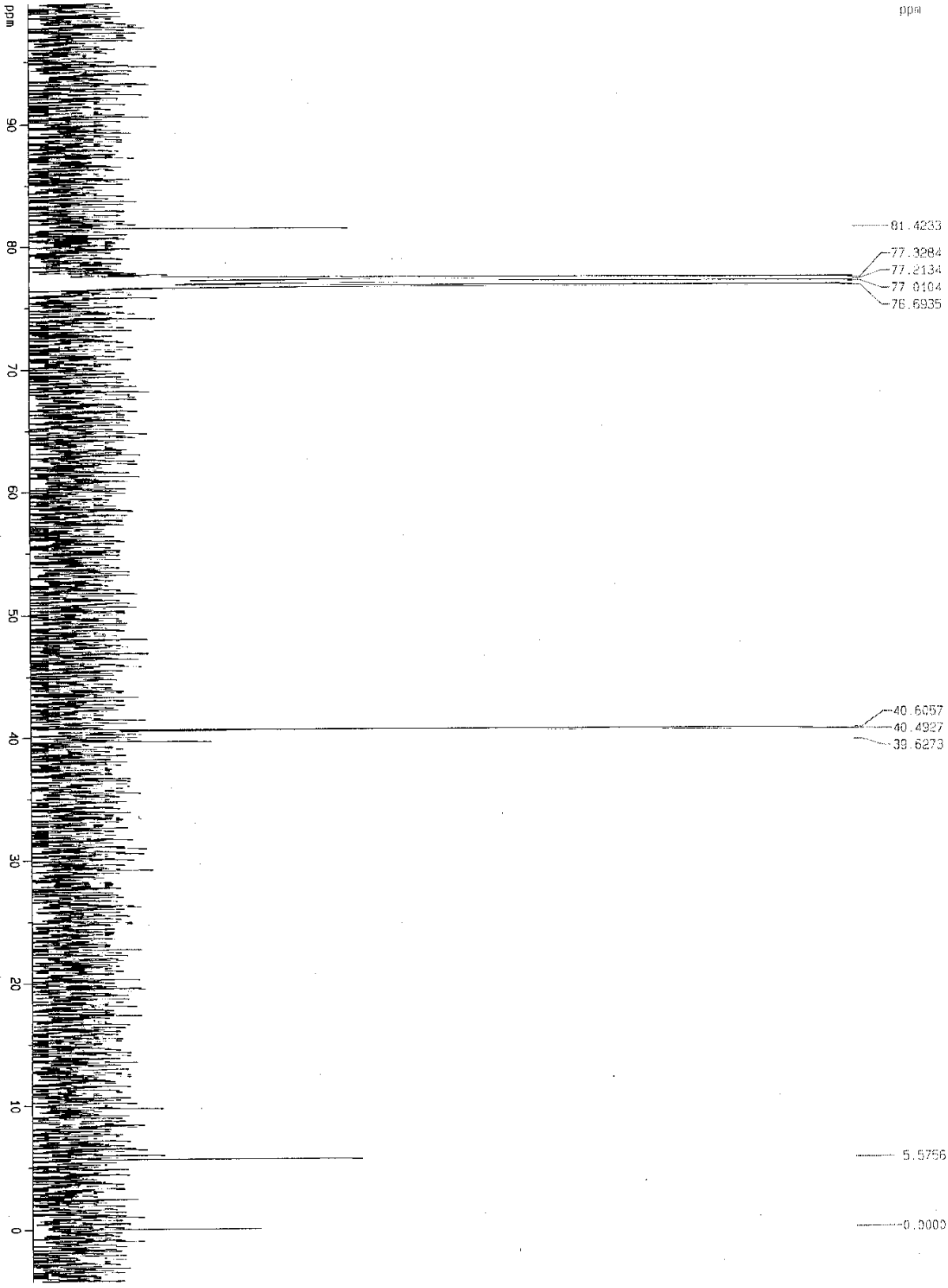
F2 - Acquisition Parameters
 Date_ 20080313
 Time 11.42
 INSTRUM spect
 PROBHD 5 mm QNP 1H/15
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 287.4
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.25 usec
 PL1 2.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300106 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 CY 19.00 cm
 F1P 8.139 ppm
 F1 3256.83 Hz
 F2P -0.191 ppm
 F2 -76.52 Hz
 PPMCM 0.27769 ppm/cm
 HZCM 111.11193 Hz/cm

SK-03-42-CARBON
 C13CPD CDC13 (D: \u) Suresh 18



Current Data Parameters
 NAME SK-3-42-CARBON
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080315
 Time 14.41

INSTRUM spect
 PROBHD 5 mm QNP 1H/15
 PULPROG zgpg30
 TD 65536
 TO 1024
 SOLVENT CDC13
 NS 4
 DS 4

SMH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 23170.5
 DW 20.850 usec
 DE 6.00 usec
 TE 300.0 K

D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

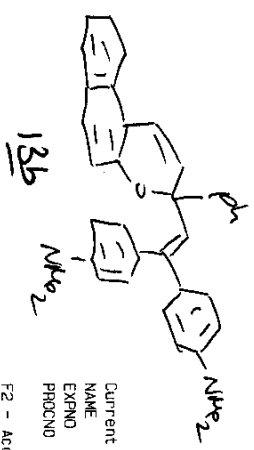
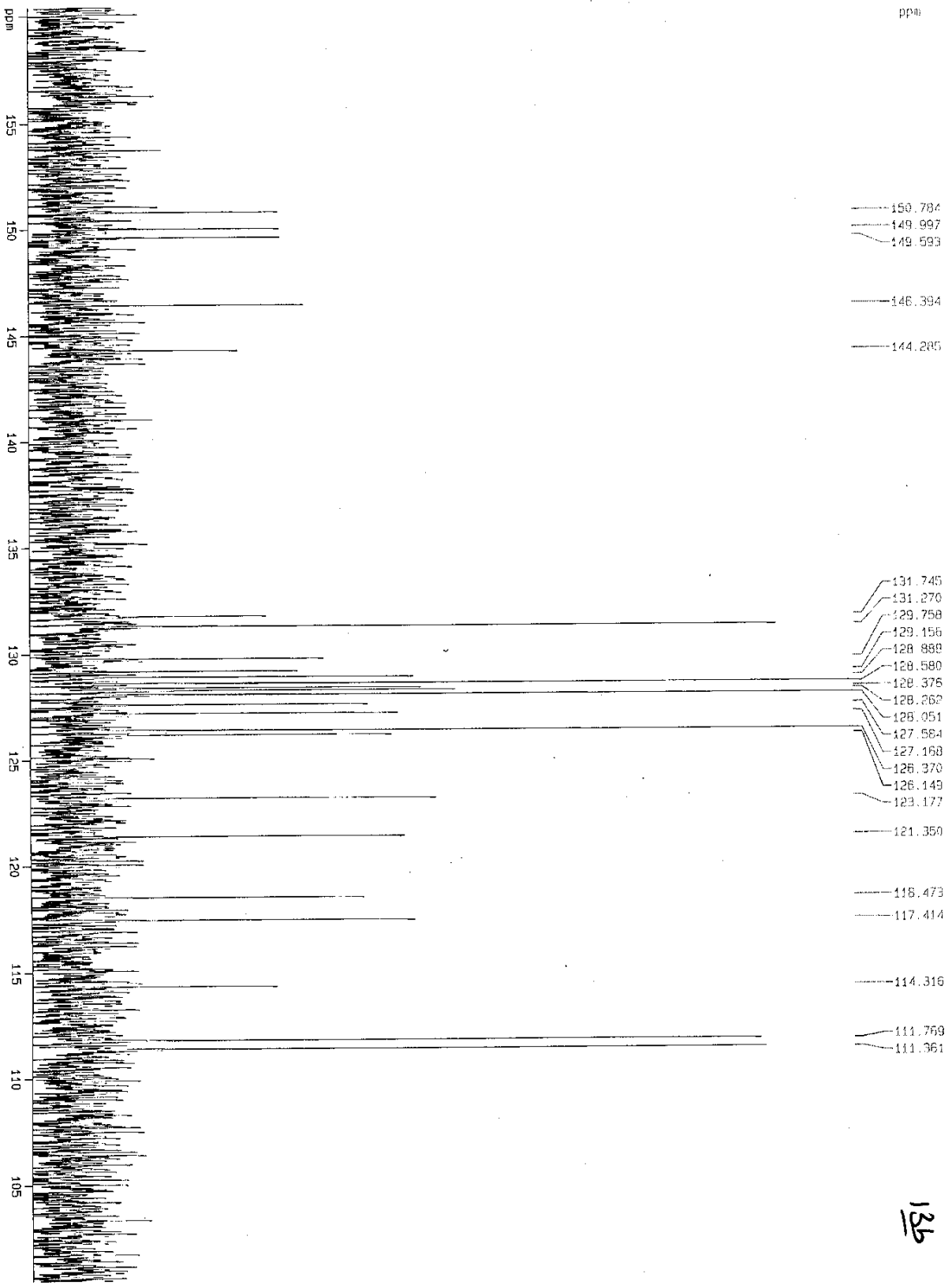
==== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 4.00 dB
 SF01 100.6227998 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 2.00 dB
 PL12 20.00 dB
 PL13 21.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127711 MHz
 WDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

10 NMR plot parameters
 CX 30.00 cm
 CY 19.00 cm
 F1P 99.697 ppm
 F1 10030.83 Hz
 F2P -4.232 ppm
 F2 -425.76 Hz
 PPMCM 3.46430 ppm/cm
 HZCM 348.55316 Hz/cm

SK-03-42-CARBON
 C13CPD CDC13 (D: \u) Suresh 18



Current Data Parameters
 NAME SK-3-42-CARBON
 EXPNO 10
 PROCNO 1

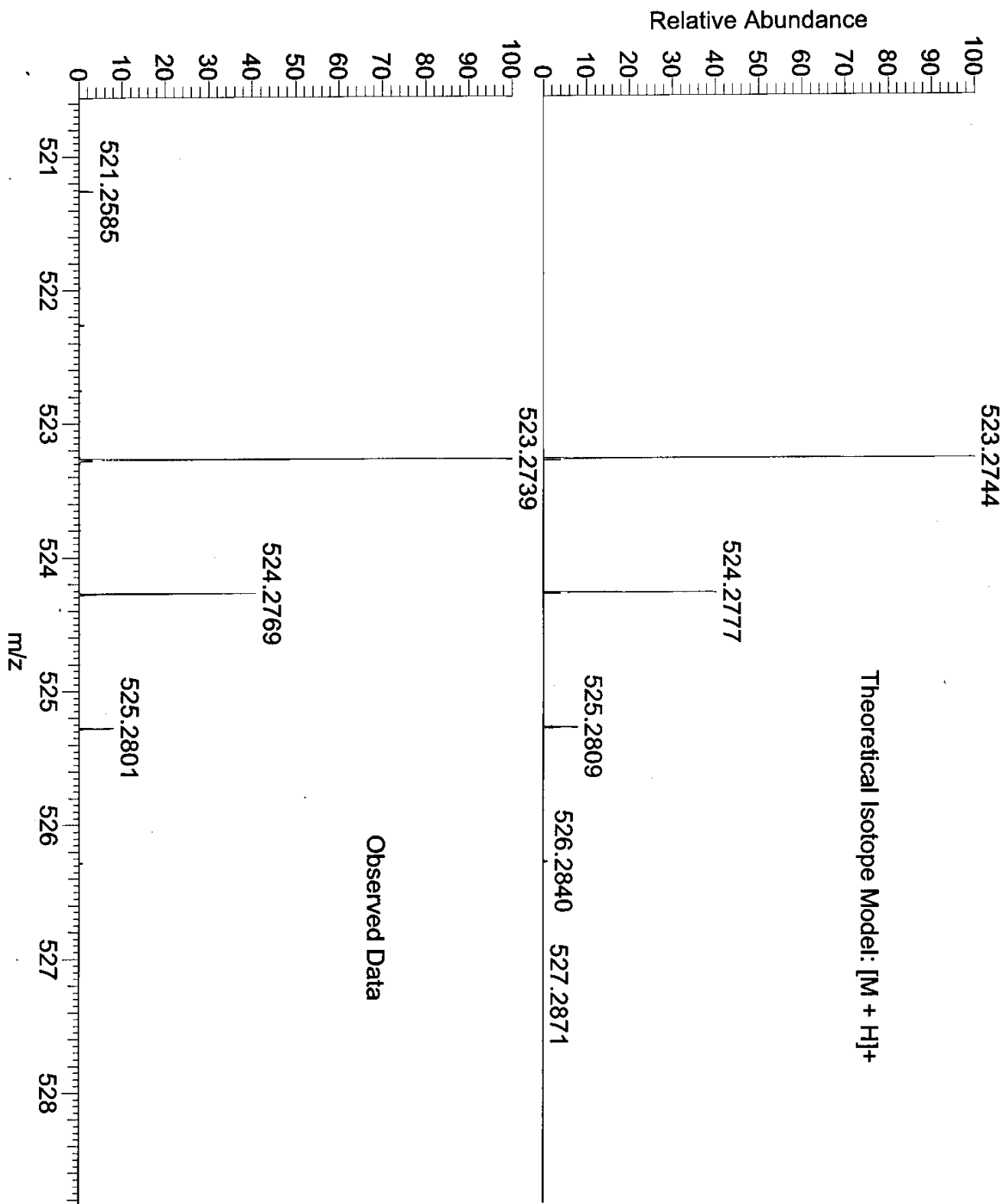
F2 - Acquisition Parameters
 Date_ 20080315
 Time 14.41
 INSTRUM spect
 PROBHD 5 mm QNP 1H/15
 PULPROG zgpg30
 TO 65636
 SOLVENT CDC13
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 23170.5
 DW 20.850 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 4.00 dB
 SF01 100.6227898 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PL2 2.00 dB
 PL12 20.00 dB
 PL13 21.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127711 MHz
 KGM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 30.00 cm
 CY 19.00 cm
 F1P 160.413 ppm
 F1 16139.41 Hz
 F2P 100.493 ppm
 F2 10110.86 Hz
 PPMCM 1.99728 ppm/cm
 HZCM 200.95158 Hz/cm



Theoretical Isotope Model: [M + H]⁺

Observed Data

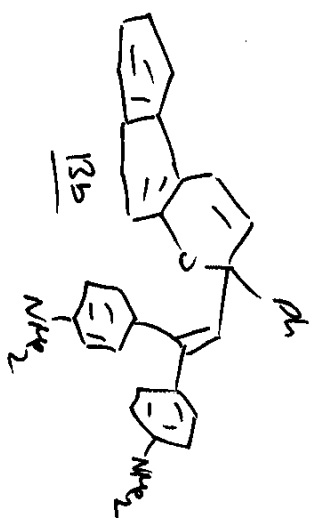
NL:
1.55E4

C₃₇ H₃₄ N₂ O₁ OH:

C₃₇ H₃₅ N₂ O₁

p (gss, s/p:40) Chrg 1

R: 100000 Res. Pwr. @FWHM



NL:
1.74E8

LEEHER082-OM-HNES#8-61

RT: 0.27-1.80 AV: 54 T: FTMS

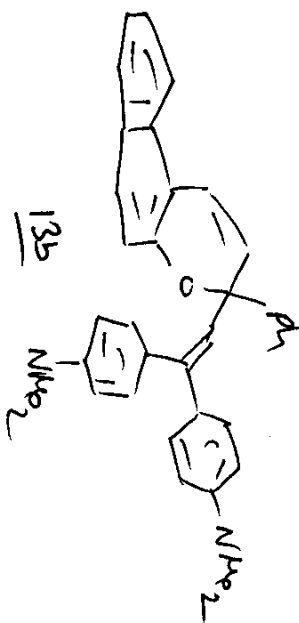
+ p NSI Full ms

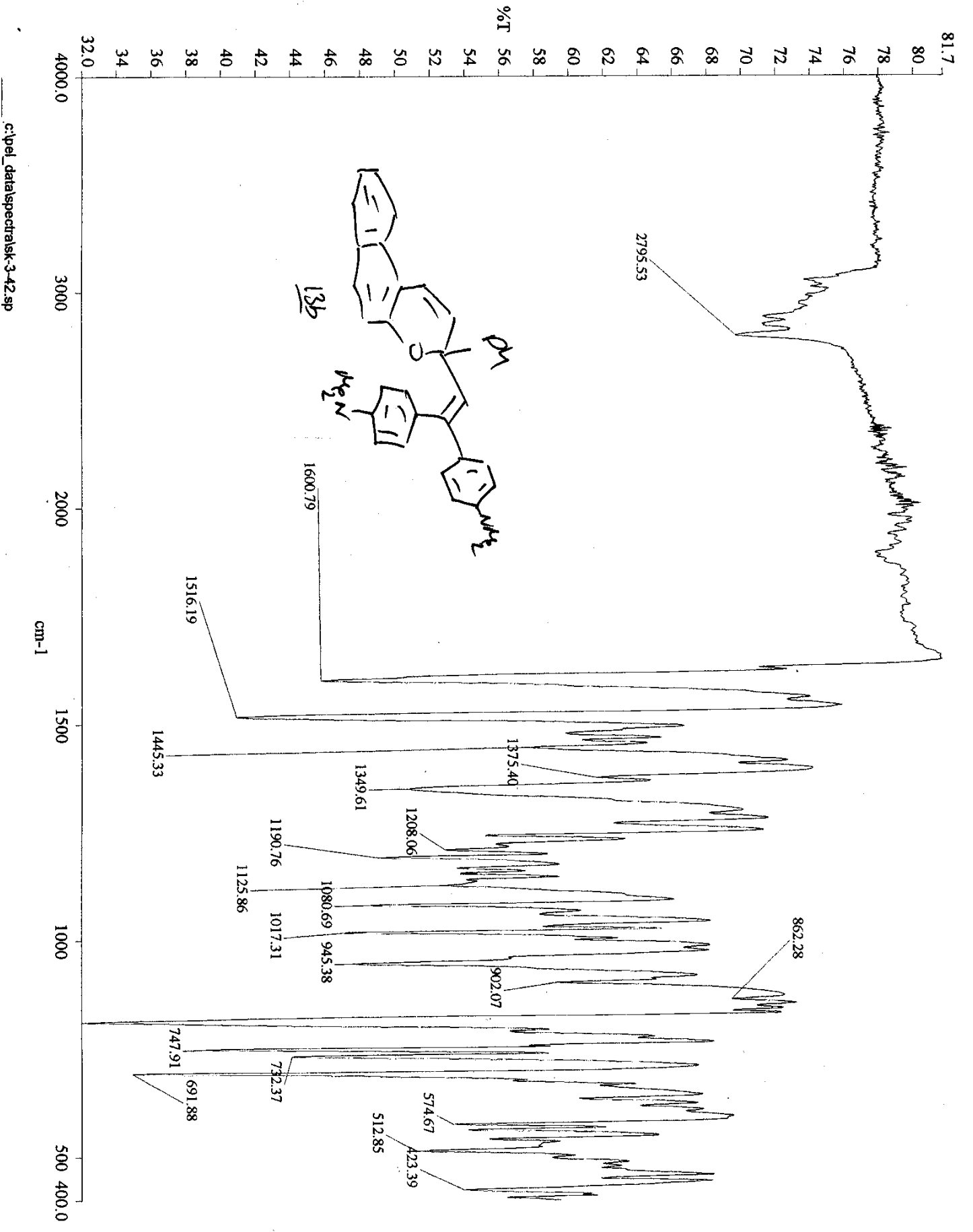
[120.00-2000.00]

Isotope: Min. ... Max.
 14 N 0....10
 16 O 0....15
 12 C 0....80
 1 H 0....110
 Tolerance Window: +- 5.00 ppm
 Dp/Ring Equiv: -2.. 100
 Filts: 100

N-Rule: Do not use
 Charge: 1

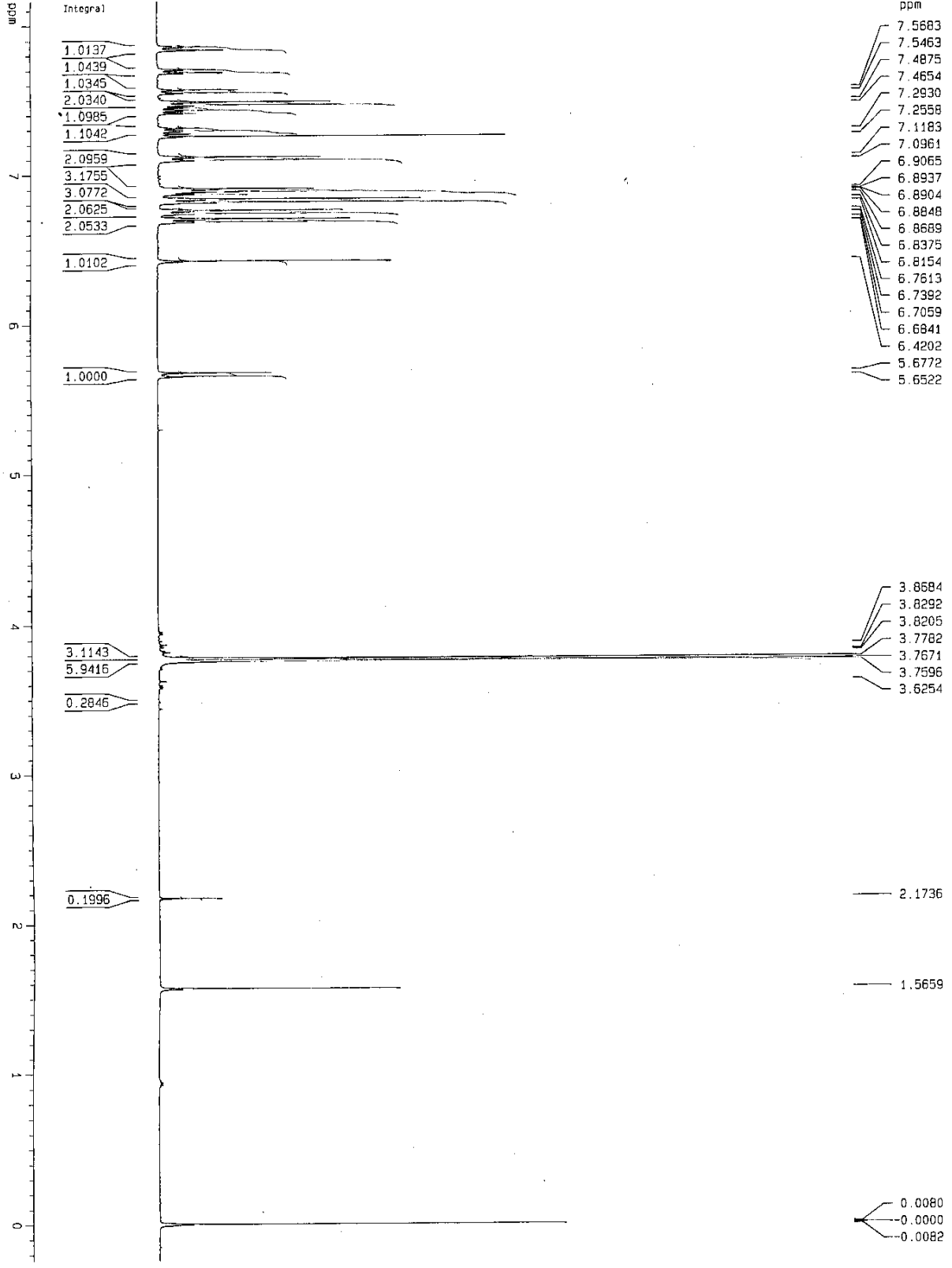
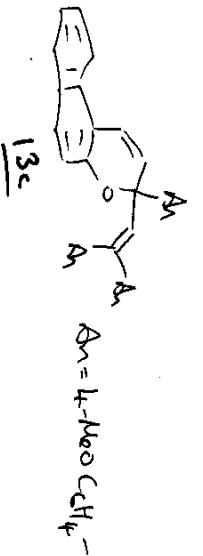
Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
523.2739	523.2736	0.6	4.0	C ₂₂ H ₄₁ O ₁₁ N ₃
	523.2736	0.7	9.5	C ₂₁ H ₃₅ O ₈ N ₁₀
	523.2744	-0.9	21.5	C ₃₇ H ₃₅ O ₁ N ₂
	523.2730	1.6	22.0	C ₃₅ H ₃₃ N ₅
	523.2749	-1.9	9.0	C ₂₃ H ₃₇ O ₇ N ₇
	523.2749	-1.9	3.5	C ₂₄ H ₄₉ O ₂
	523.2722	3.2	4.5	C ₂₀ H ₃₉ O ₁₀ N ₆
	523.2717	4.2	17.0	C ₃₄ H ₃₇ O ₂ N ₄
	523.2762	-4.5	8.5	C ₂₅ H ₃₉ O ₈ N ₄





PROTON, Co1Chem CDCl3 [D: \u] Suresh 3

SK-3-35



Current Data Parameters
 NAME SK-3-35
 EXPNO 20
 PROCNO 1

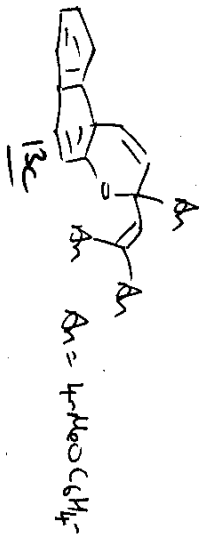
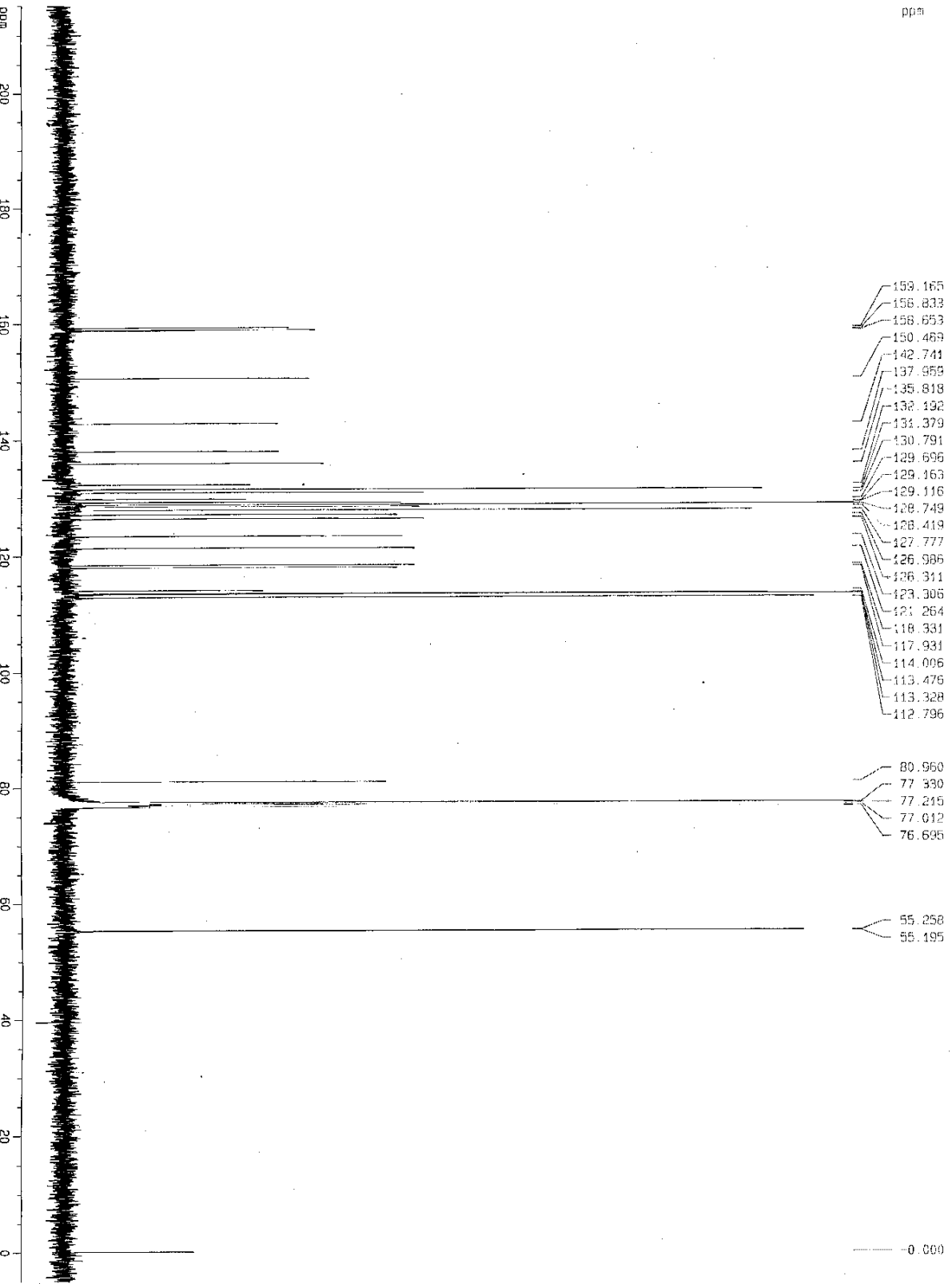
F2 - Acquisition Parameters
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 Time 16.44
 INSTRUM spect
 PROBD 5 mm QNP 1H/15
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 256
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.25 usec
 PL1 2.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300110 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 CY 19.00 cm
 F1P 8.161 ppm
 F1 3265.62 Hz
 F2P -0.238 ppm
 F2 -95.36 Hz
 PPMCM 0.27999 ppm/cm
 HZCM 112.03275 Hz/cm

SK-3-35-CARBON
 C13CPD CDC13 (D: \u) Suresh S



Current Data Parameters
 NAME SK-3-35-CARBON
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080301
 Time 0.26

INSTRUM spect
 PROBRD 5 mm GNP 1H/13
 PULPROG zgpg30
 TO 65536
 SOLVENT CDC13
 NS 8000
 DS 4

SMH 23980.814 HZ
 FIDRES 0.365918 HZ
 AQ 1.3664756 sec
 RG 20642.5

DE 20.850 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 4.00 dB
 SFO1 100.6227698 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 2.00 dB
 PL12 20.00 dB
 PL13 21.00 dB
 SFO2 400.1316005 MHz

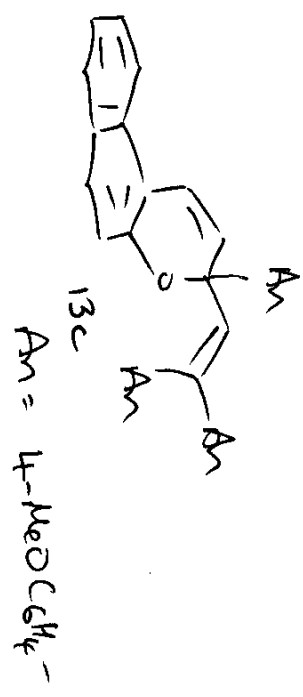
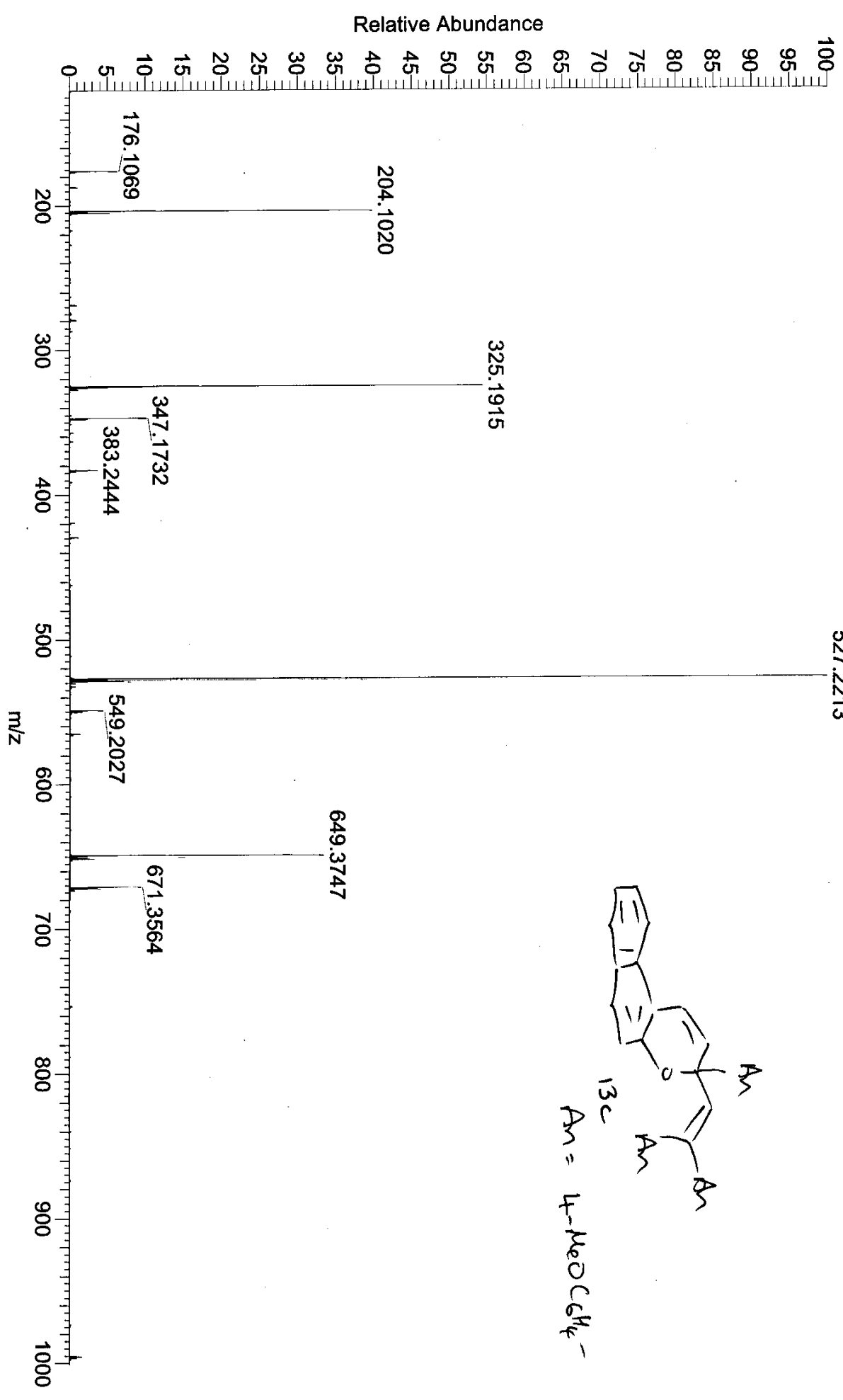
F2 - Processing parameters
 SI 32768
 SF 100.6127710 MHz
 MDW EM
 SSB 0
 LB 1.00 HZ
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 30.00 cm
 CY 19.00 cm
 F1P 215.000 ppm
 F1 21631.75 HZ
 F2P -5.000 ppm
 F2 -503.06 HZ
 PPMCM 7.33333 ppm/cm
 HZCM 737.82697 HZ/cm

SK-3-35 MW=526?
(DCM)/MeOH+NH4OAc
LEEHER083-OM-HNES #5-60 RT: 0.19-1.73 AV: 56 NL: 1.50E8
T: FTMS + p NSI Full ms [120.00-2000.00]

EPSRC National Centre Swansea
LTQ Orbitrap XL

Dr Heron
08/10/2008 15:32:41

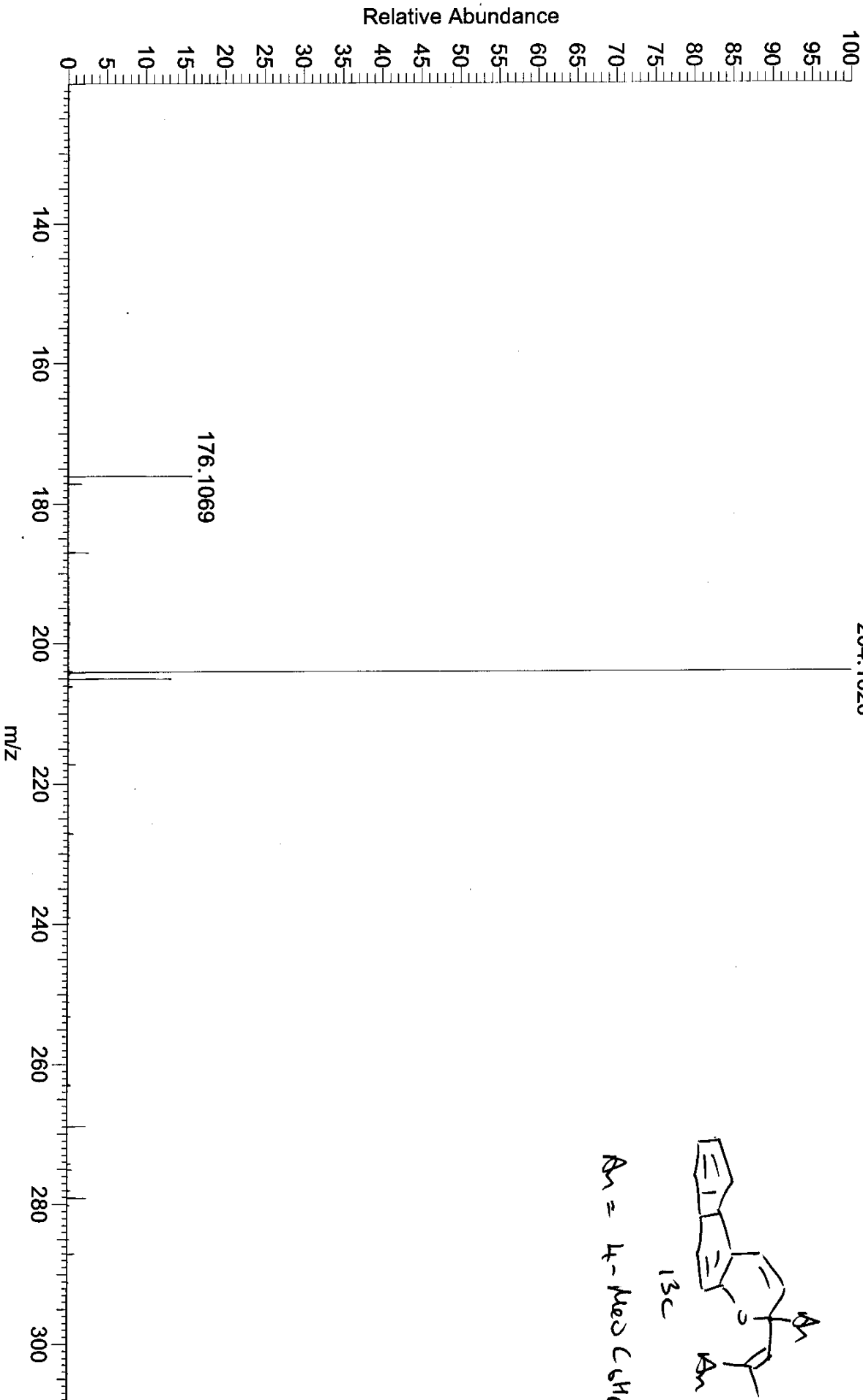


SK-3-35 MW=526?
(DCM)/MeOH/NH4OAc

EPSRC National Centre Swansea
LTQ Orbitrap XL

Dr Heron
08/10/2008 15:32:41

LEEHER083-OM-HNES #5-60 RT: 0.19-1.73 AV: 56 NL: 5.95E7
T: FTMS + p NSI Full ms [120.00-2000.00]

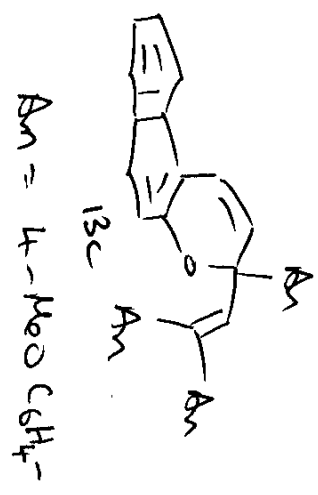
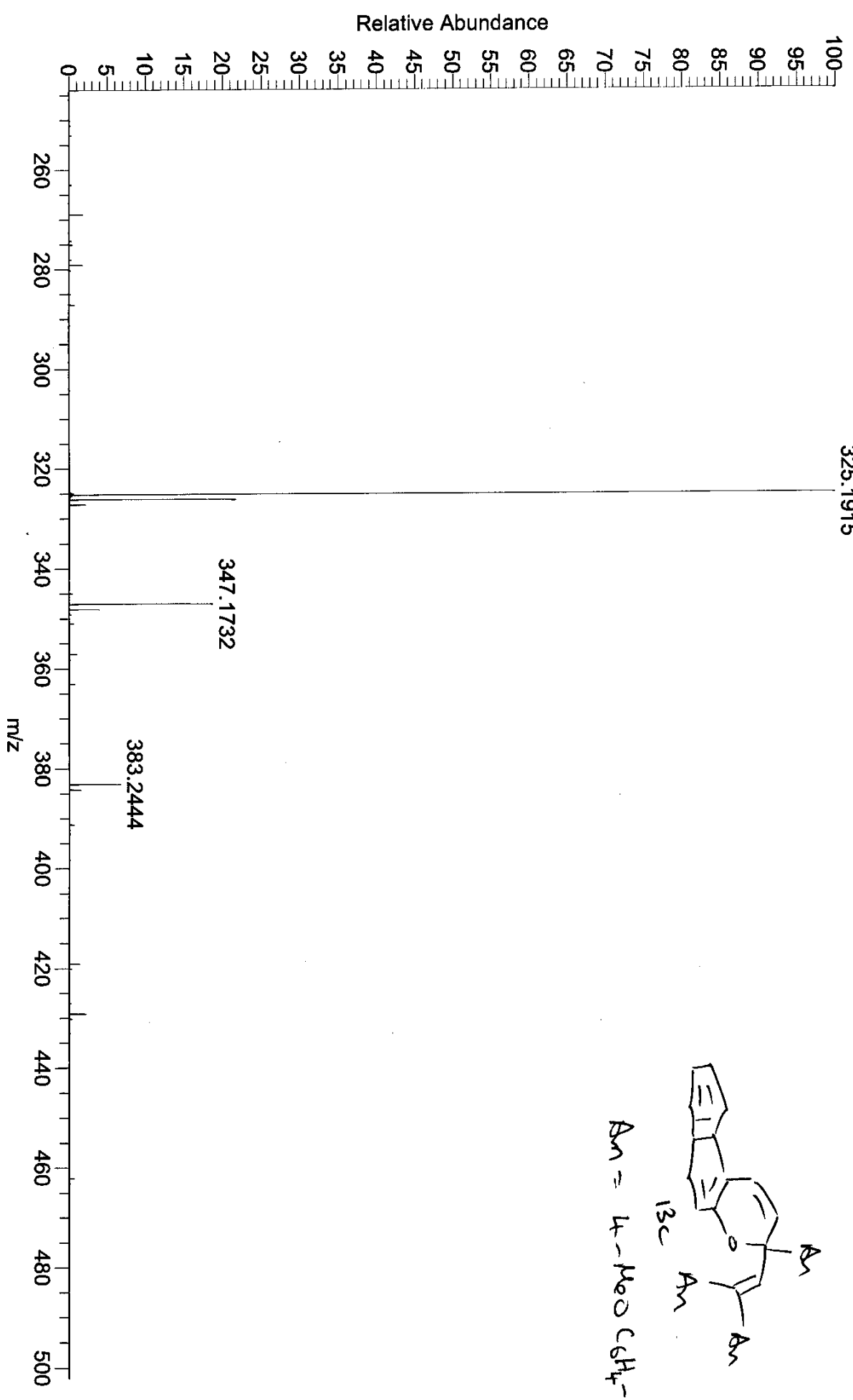


Ar = 4-Med C₆H₄-

SK-3-35 MW=526?
(DCM)/MeOH+NH4OAc
LEEHER083-OM-HNES #5-60 RT: 0.19-1.73 AV: 56 NL: 8.14E7
T: FTMS + p NSI Full ms [120.00-2000.00]

EPSRC National Centre-Swansea
LTQ Orbitrap XL

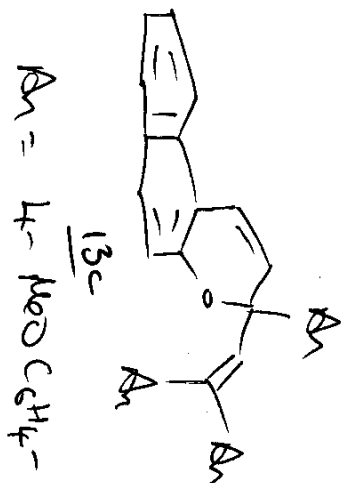
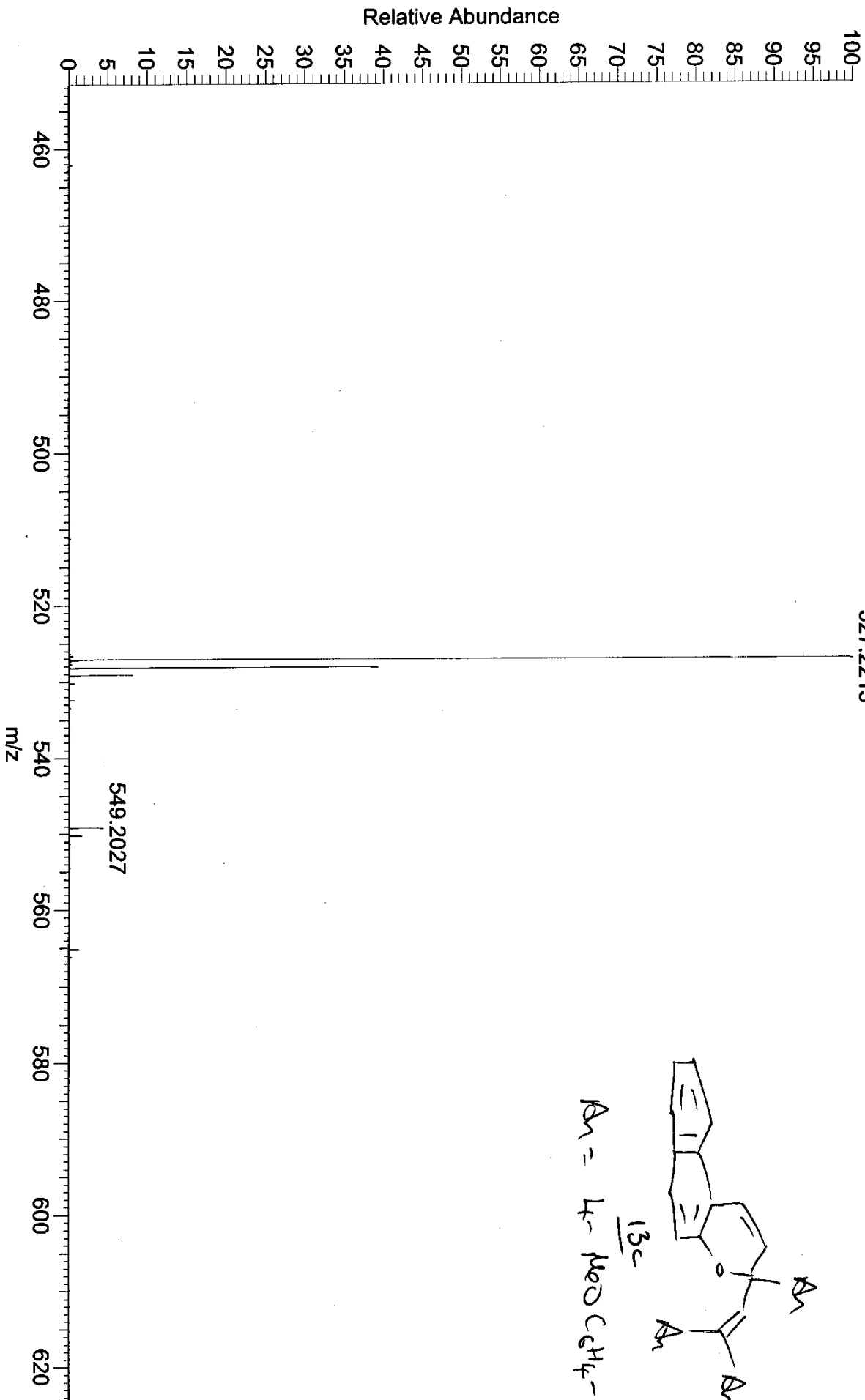
Dr Heron
08/10/2008 15:32:41



SK-3-35 MW=526? (DCM)/MeOH+NH4OAc
LEEHER083-OM-HNES #5-60 RT: 0.19-1.73 AV: 56 NL: 1.50E8
T: FTMS + p NSI Full ms [120.00-2000.00]

EPSRC National Centre Swansea
LTQ Orbitrap XL

Dr Heron
08/10/2008 15:32:41

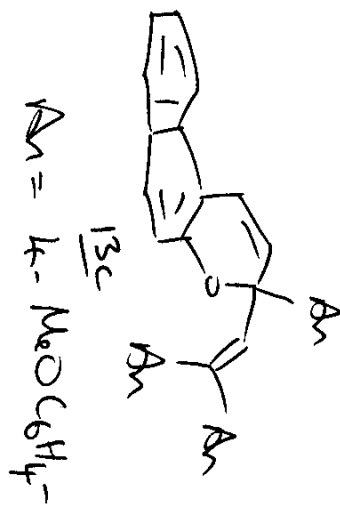
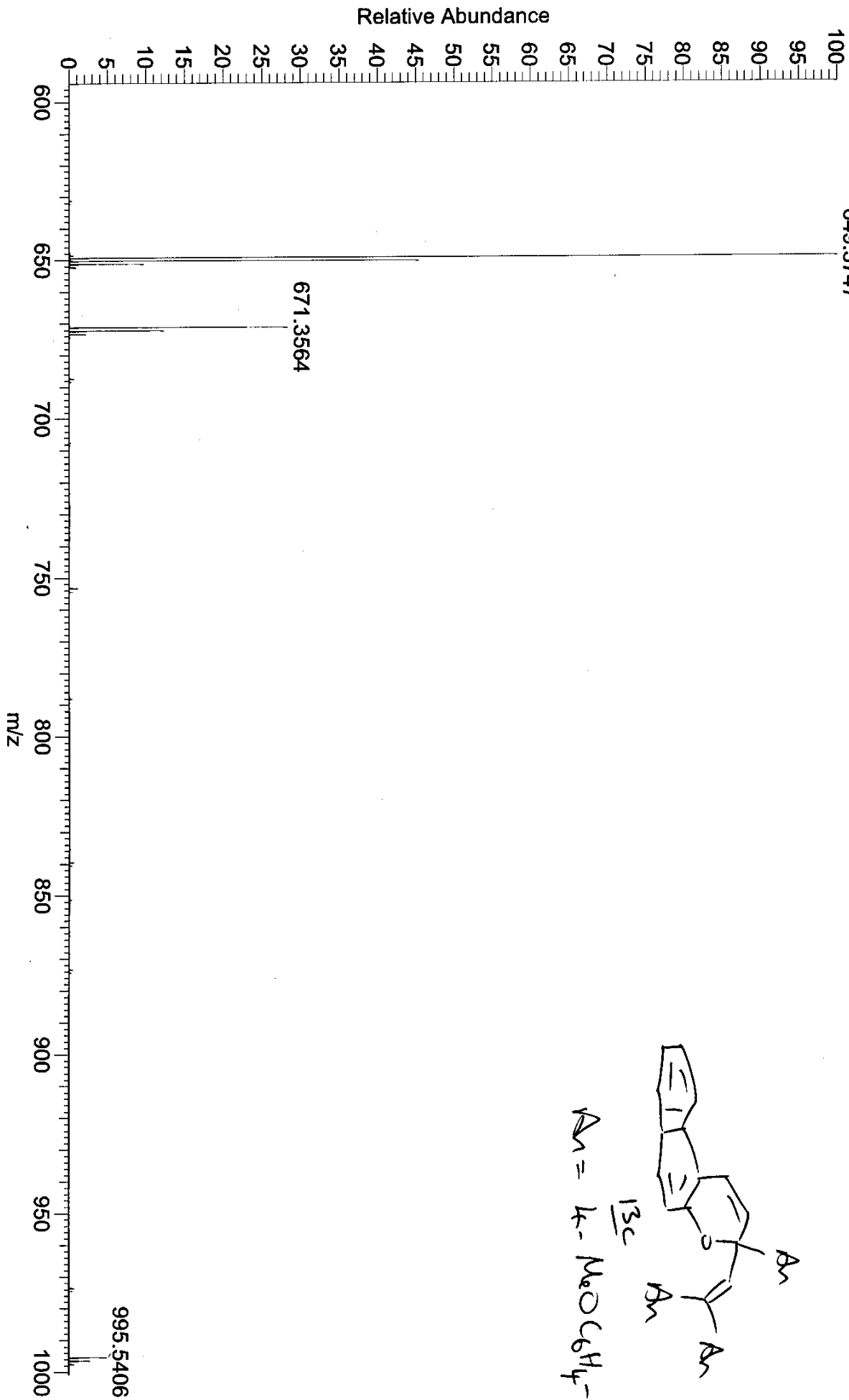


SK-3-35 MW=526?
(DCM)/MeOH+NH4OAc

EPSRC National Centre Swansea
LTQ Orbitrap XL

Dr Heron
08/10/2008 15:32:41

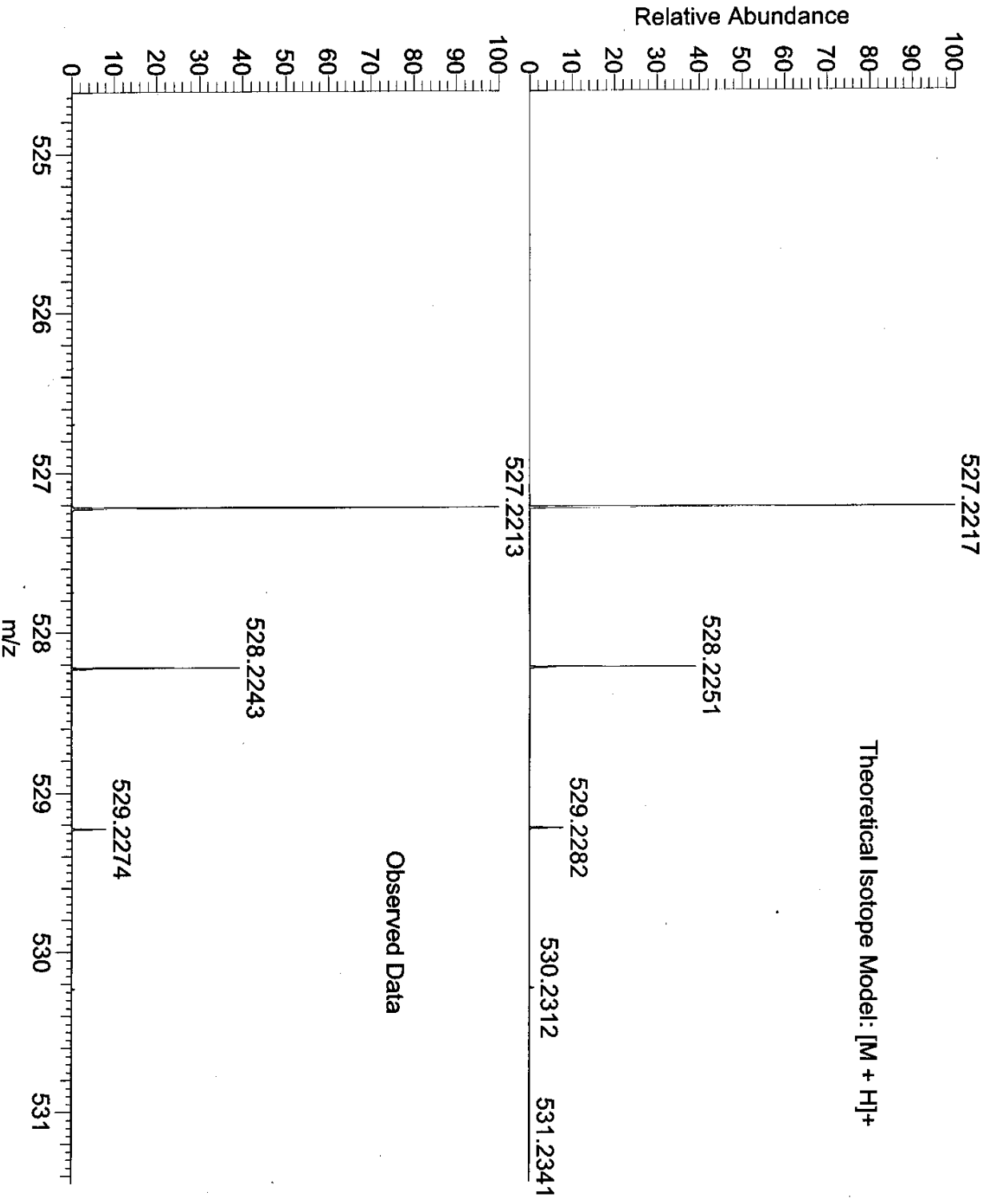
LEEHER083-OM-HNES #5-60 RT: 0.19-1.73 AV: 56 NL: 5.00E7
T: FTMS + p NSI Full ms [120.00-2000.00]



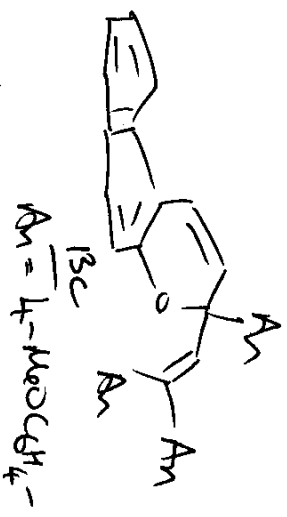
SK-3-35 MW=526?
(DCM)/MeOH+NH4OAc

EPSRC National Centre Swansea
LTQ Orbitrap XL

Dr Heron
08/10/2008 15:32:41



NL:
1.57E4
C₃₆ H₃₀ O₄ H:
C₃₆ H₃₁ O₄
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr. @FWHM

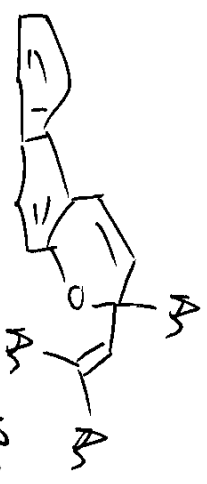


NL:
1.50E8
LEEHER083-OM-HNES#5-60
RT: 0.19-1.73 AV: 56 T: FTMS
+ p NSI Full ms
[120.00-2000.00]

Isotope: Min. ... Max.
 14 N 0...10
 16 O 0...15
 12 C 0...80
 1 H 0...110
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -2.. 100
 Fits: 100

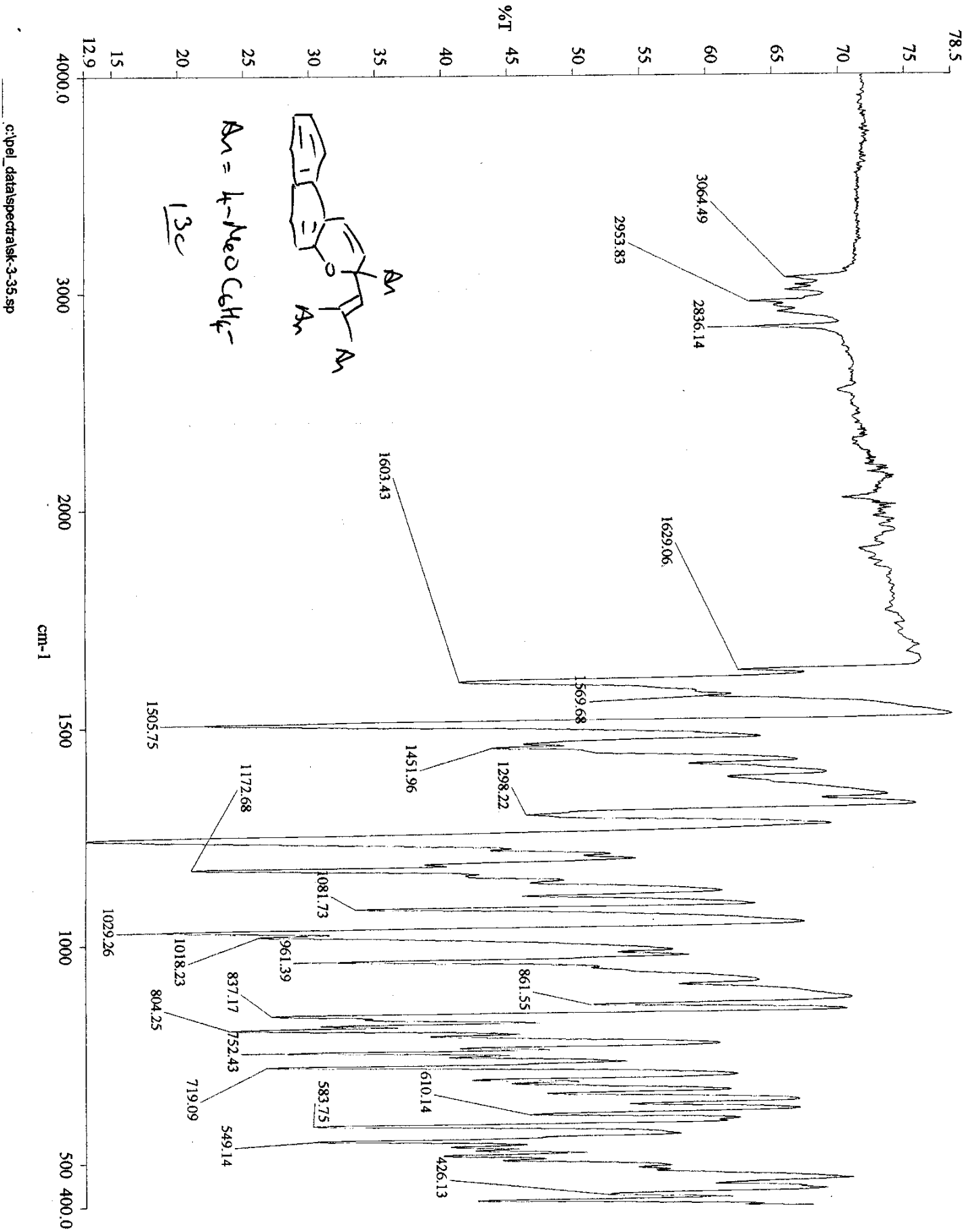
N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
527.2213	527.2217	-0.7	21.5	C ₃₆ H ₃₁ O ₄
	527.2209	0.8	4.0	C ₂₁ H ₃₇ O ₁₄ N ₁
	527.2209	0.9	9.5	C ₂₀ H ₃₁ O ₉ N ₈
	527.2222	-1.7	9.0	C ₃₂ H ₃₃ O ₁₀ N ₅
	527.2203	1.8	22.0	C ₁₄ H ₂₉ O ₃ N ₃
	527.2230	-3.3	26.5	C ₁₄ H ₂₇ N ₄
	527.2195	3.4	4.5	C ₁₉ H ₃₅ O ₁₃ N ₄
	527.2235	-4.2	14.0	C ₃₃ H ₂₉ O ₆ N ₉
	527.2235	-4.2	8.5	C ₃₄ H ₃₅ O ₁₁ N ₂
	527.2190	4.4	22.5	C ₃₂ H ₂₇ O ₂ N ₆



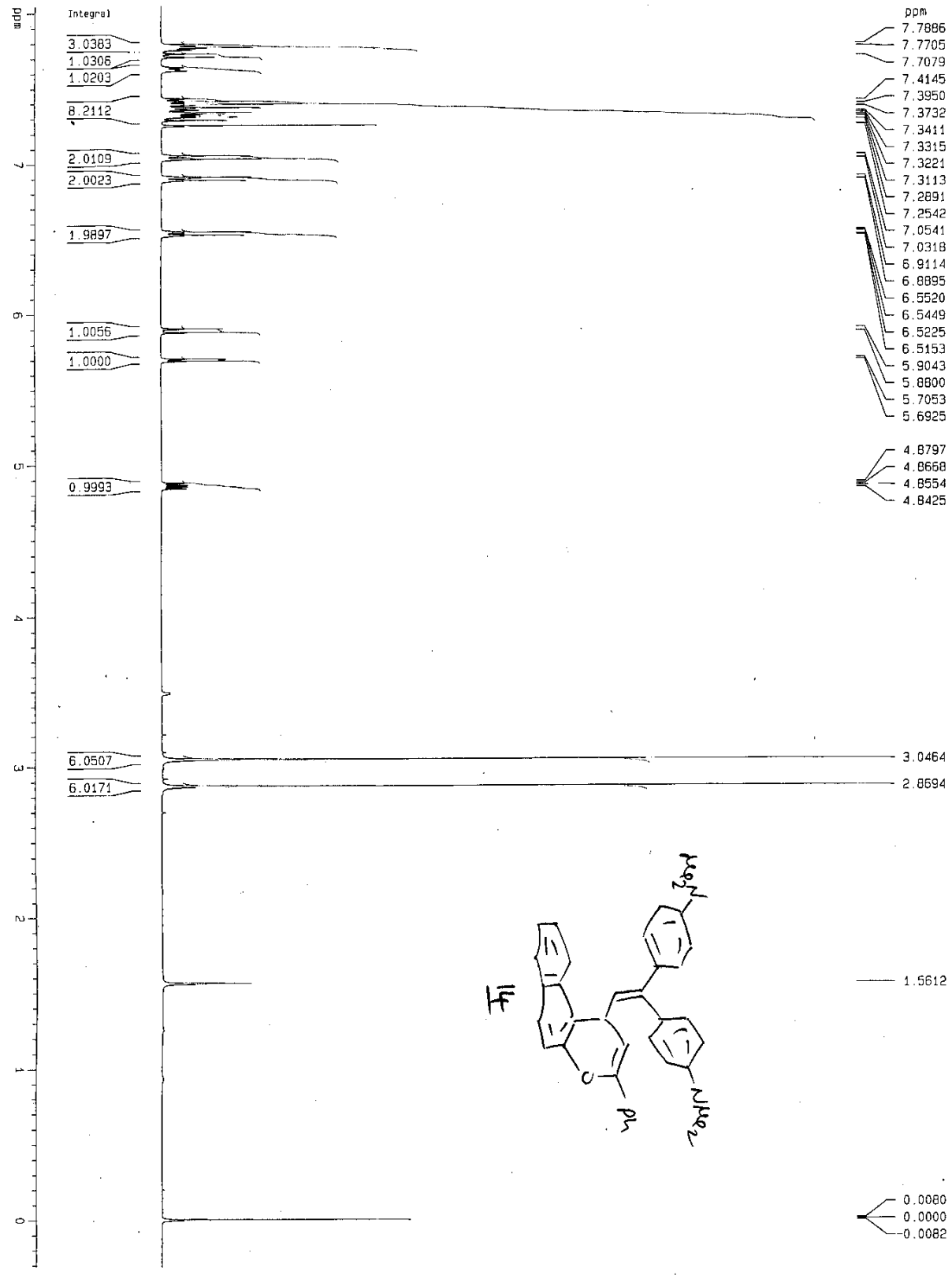
AN = 4-MeOC₆H₄-

13c



c:\pel_data\spectra\sk-3-35.sp

SK-3-31-b1 product
 PROTON COIChem CDC13 (D: \u) Suresh 17



Current Data Parameters
 NAME SK-3-31-D1product
 EXPNO 10
 PROCNO 1

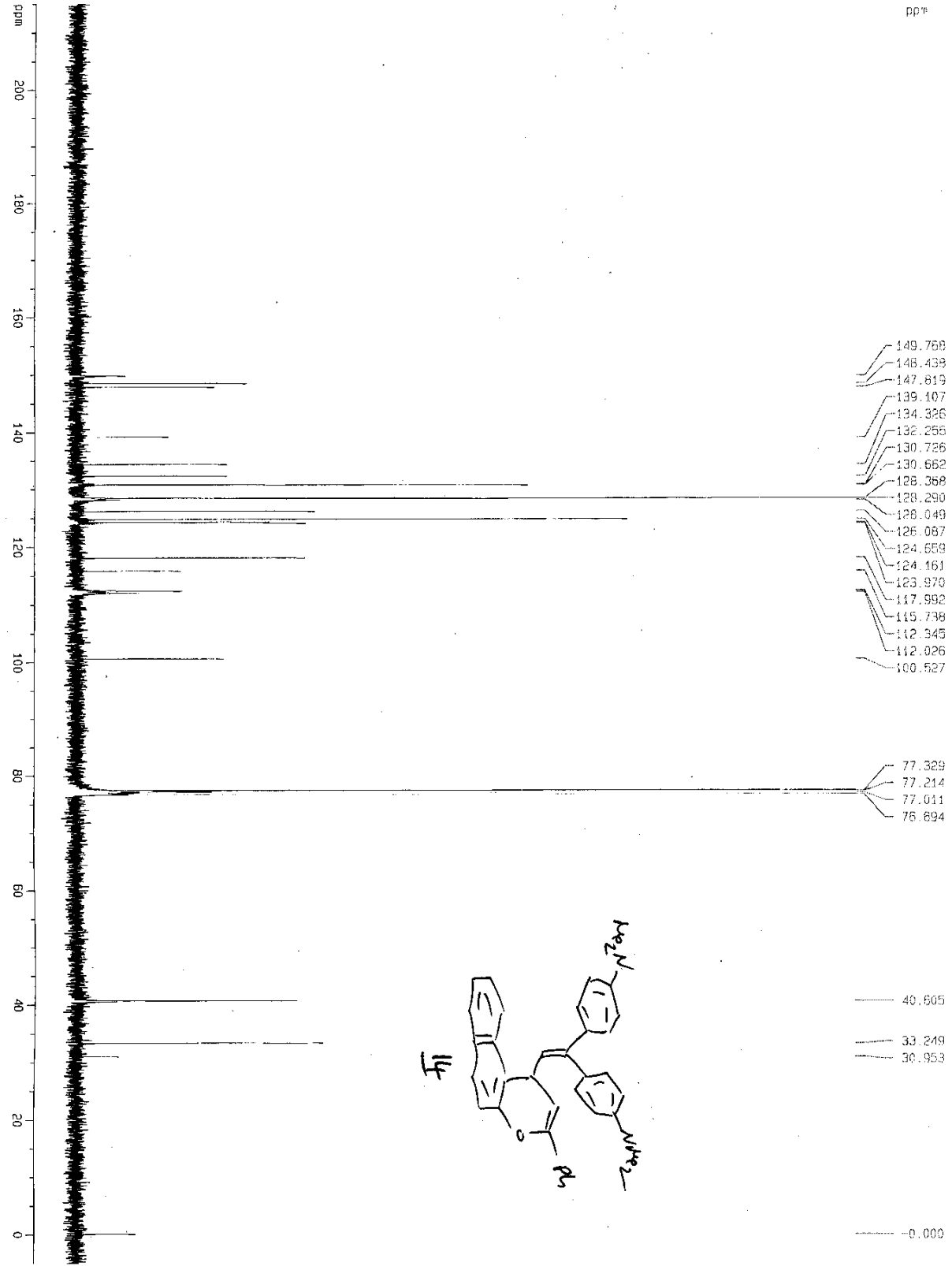
F2 - Acquisition Parameters
 Date_ 20080303
 Time 12.04
 INSTRUM spect
 PROBH0 5 mm QNP 1H/15
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8278.145 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 256
 DW 60.400 usec
 DE 5.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.25 usec
 PL1 2.00 dB
 SF01 400.1324710 MHz

F2 - Processing Parameters
 SI 32768
 SF 400.1300118 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 CY 19.00 cm
 F1P 8.044 ppm
 F1 3218.81 Hz
 F2P -0.309 ppm
 F2 -123.75 Hz
 PPM0M 0.27846 ppm/cm
 HZ0M 111.41897 Hz/cm

SK-3-31-biproduct-carbon
C13CPD CDC13 (D: \) Suresh 5



149.768
146.438
147.819
139.107
134.326
132.256
130.726
130.662
128.358
128.290
128.049
126.057
124.659
124.161
123.970
117.992
115.738
112.345
112.026
100.527

77.329
77.214
77.011
76.694

40.605
33.249
30.953

0.000

Current Data Parameters
NAME SK-3-31-biproduct-carbon
EXPNO 10

F2 - Acquisition Parameters
Date_ 20080304
Time 5.09
INSTRUM spect
PROBHD 5 mm QNP 1H/15
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 4056
DS 4
SWH 22960.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 2064.2 5
DM 20.860 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

CHANNEL: f1
NUC1 13C
P1 8.00 usec
PL1 4.00 dB
SFO1 100.6227888 MHz

CHANNEL: f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 20.00 dB
PL13 21.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127717 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

10 NMR plot parameters
CX 30.00 cm
CY 19.00 cm
FAP 215.000 ppm
F1 21531.75 Hz
F2 -5.000 ppm
PRNCK 7.33333 ppm/cm
HZCM 737.82689 Hz/cm

ACCURATE MASS MEASUREMENT REPORT

YOUR REFERENCE: SK-3-31-B1

OUR REFERENCE: LEEHER063

Instrument: MAT95 XP

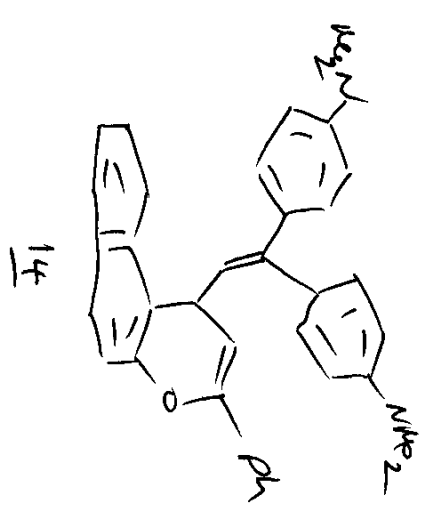
Ionisation Mode: Electrospray (positive)

Reference compound: Polyethylenimine

Ion identity: [M+H]⁺

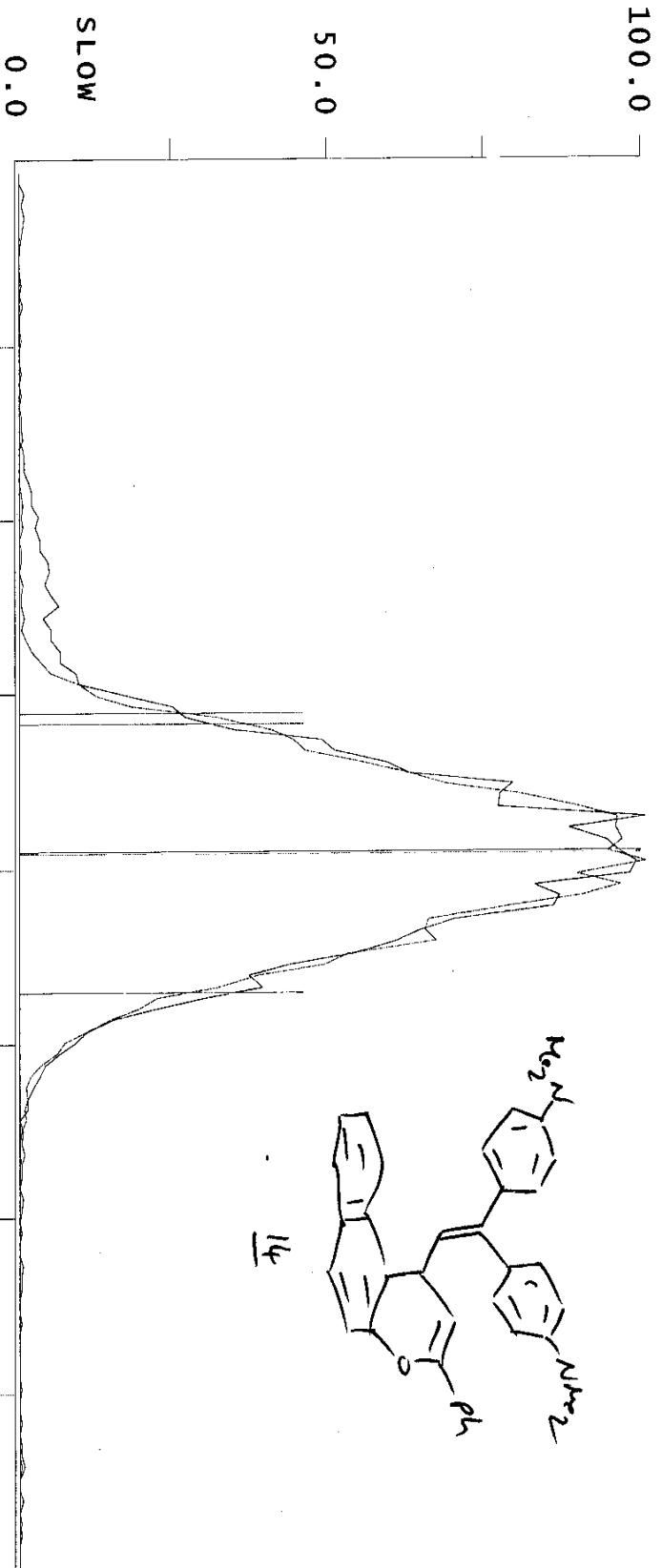
Calculated mass (of ion): 523.2744

Measured mass (of ion): 523.2747



Peak Register Display

Copy result
to ULIST



REG 1/2:	523.274654	REG 1/3:	REG 2/3:
MASS	:	491.49559	523.27208
REF MASS	:	491.49801	534.54021
PEAK WIDTH [ppm]:	:	80.00787	76.79719

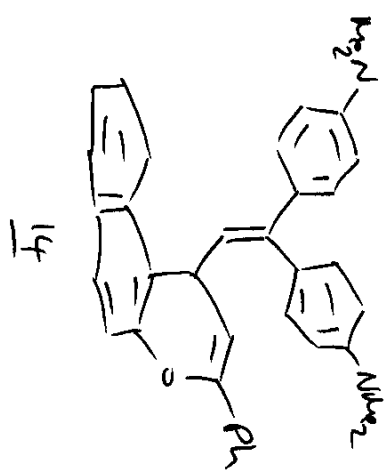
Active Register: 1 0.30 1.00

N REG RCOPY2 RCOPY3 LIMIT CENTER SPREAD ERASE RESUME PAGE
 PEAK:

Isotope: Min. ... Max.
 12 C 0....60
 1 H 0....90
 16 O 0....14
 14 N 0....14
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -2... 100
 Plts: 100

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
523.2747	523.2749	-0.4	14.5	C ₂₂ H ₃₁ O ₂ N ₁₄
	523.2749	-0.4	9.0	C ₂₃ H ₁₇ O ₁ N ₇
	523.2749	-0.4	3.5	C ₂₄ H ₄₃ O ₁₂
	523.2744	0.6	21.5	C ₂₇ H ₅ O ₁ N ₂
	523.2736	2.2	4.0	C ₂₂ H ₄₁ O ₁₁ N ₃
	523.2736	2.2	9.5	C ₂₁ H ₅ O ₆ N ₁₀
	523.2762	-2.9	14.0	C ₂₄ H ₃₃ O ₃ N ₁₁
	523.2762	-2.9	8.5	C ₂₆ H ₉ O ₈ N ₄
	523.2730	3.2	22.0	C ₃₅ H ₃ N ₅
	523.2722	4.7	4.5	C ₂₀ H ₃₉ O ₁₀ N ₆
	523.2722	4.8	10.0	C ₁₈ H ₃₃ O ₅ N ₁₃



SK-3-31-B1 MW=522

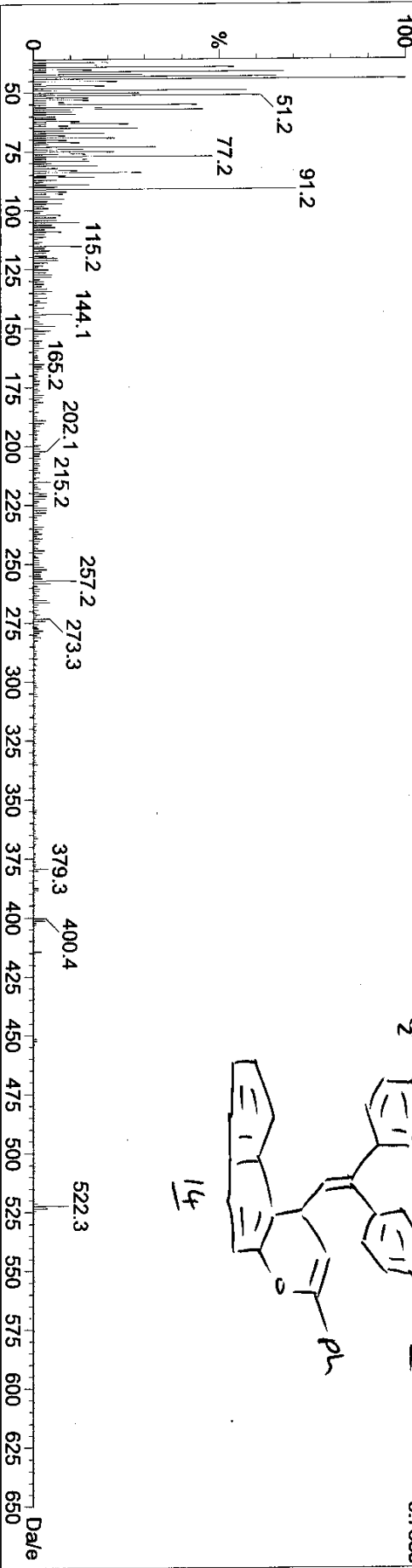
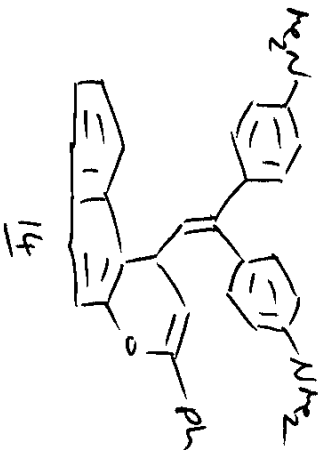
Heron

LEE63HER 134 (2.482) Cm (134)

EPSRC National Centre Swansea
QUATTRO

13-Mar-2008 12:34:56

Scan EI+
8.7863



SK-3-31-B1 MW=522

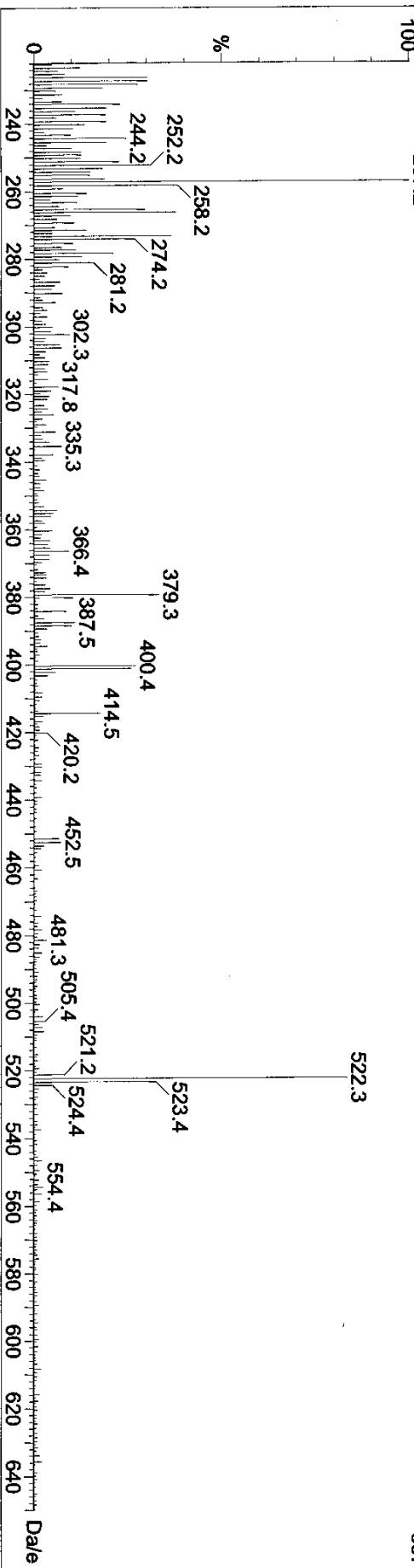
Heron

LEE63HER 134 (2.482) Cm (134)

EPSRC National Centre Swansea
QUATTRO

13-Mar-2008 12:34:56

Scan EI+
9.97



SK-3-31-B1 MW=522

Heron

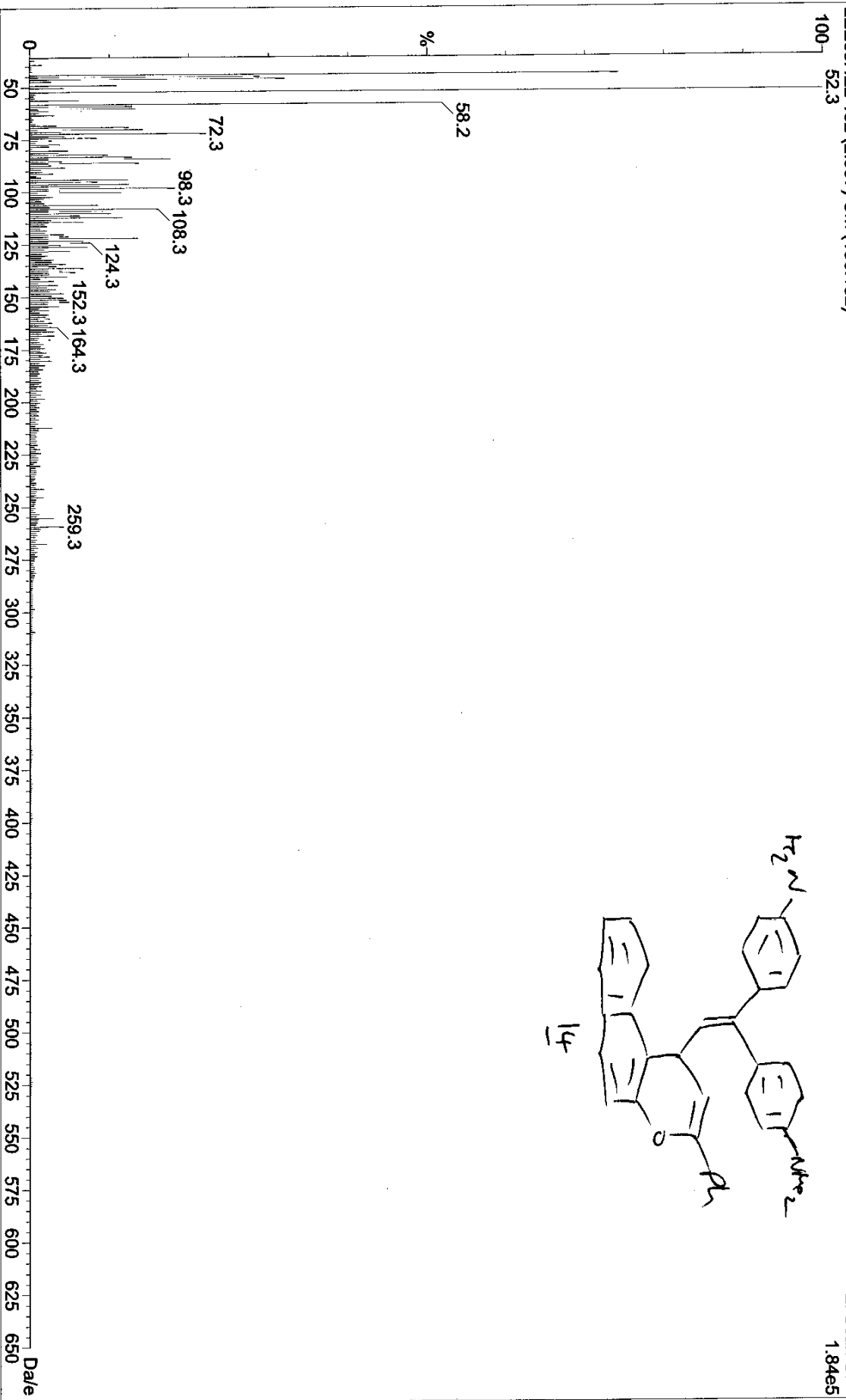
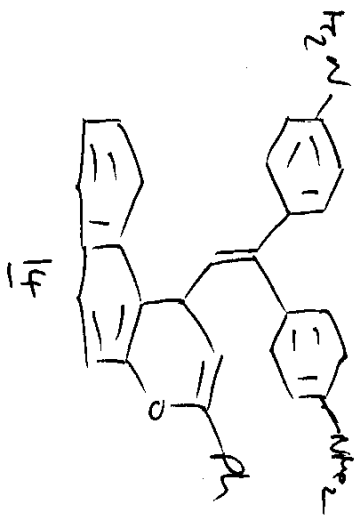
LEE63HE2 132 (2.537) Cm (130:132)

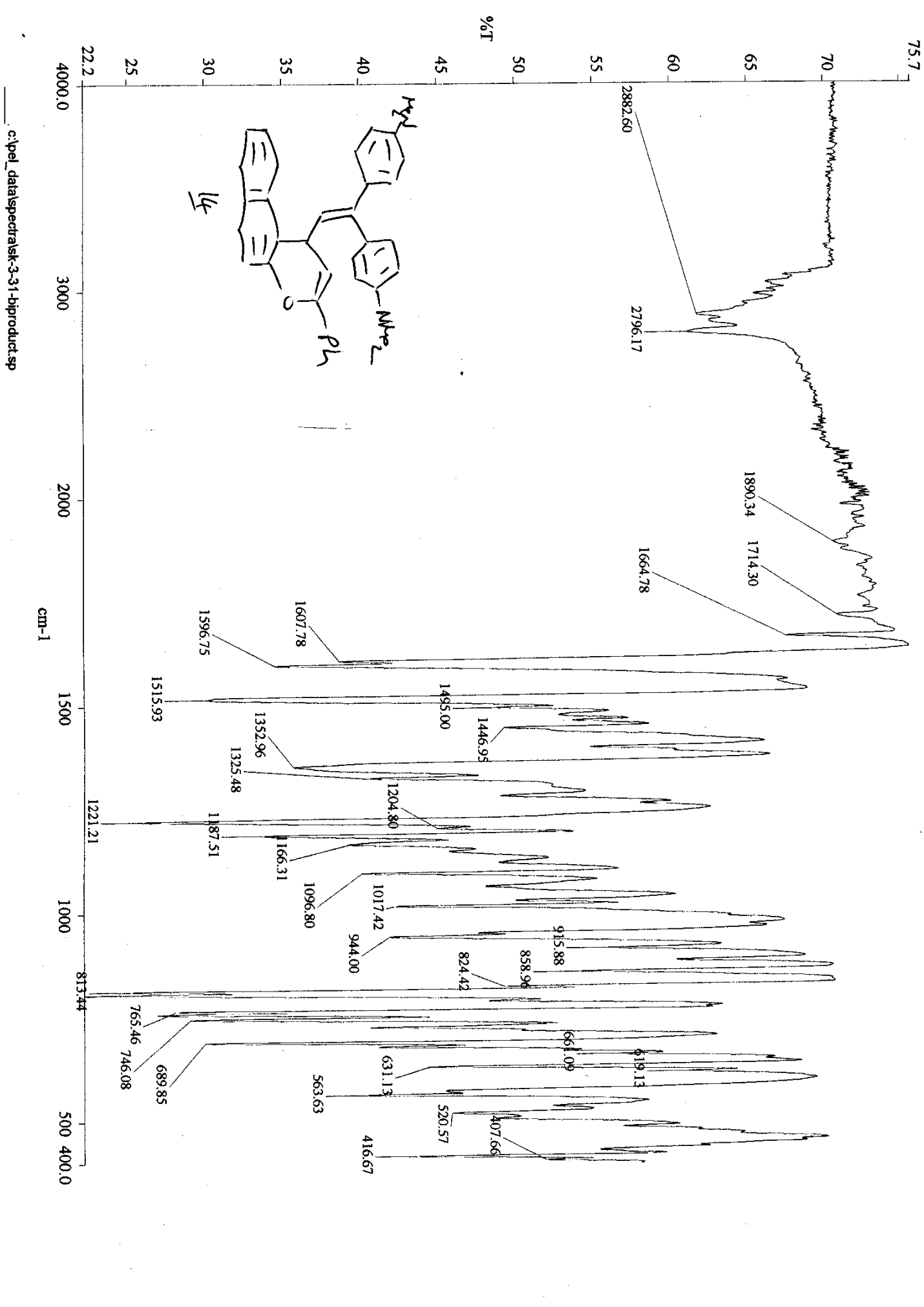
EPSRC National Centre Swansea
QUATTRO

13-Mar-2008

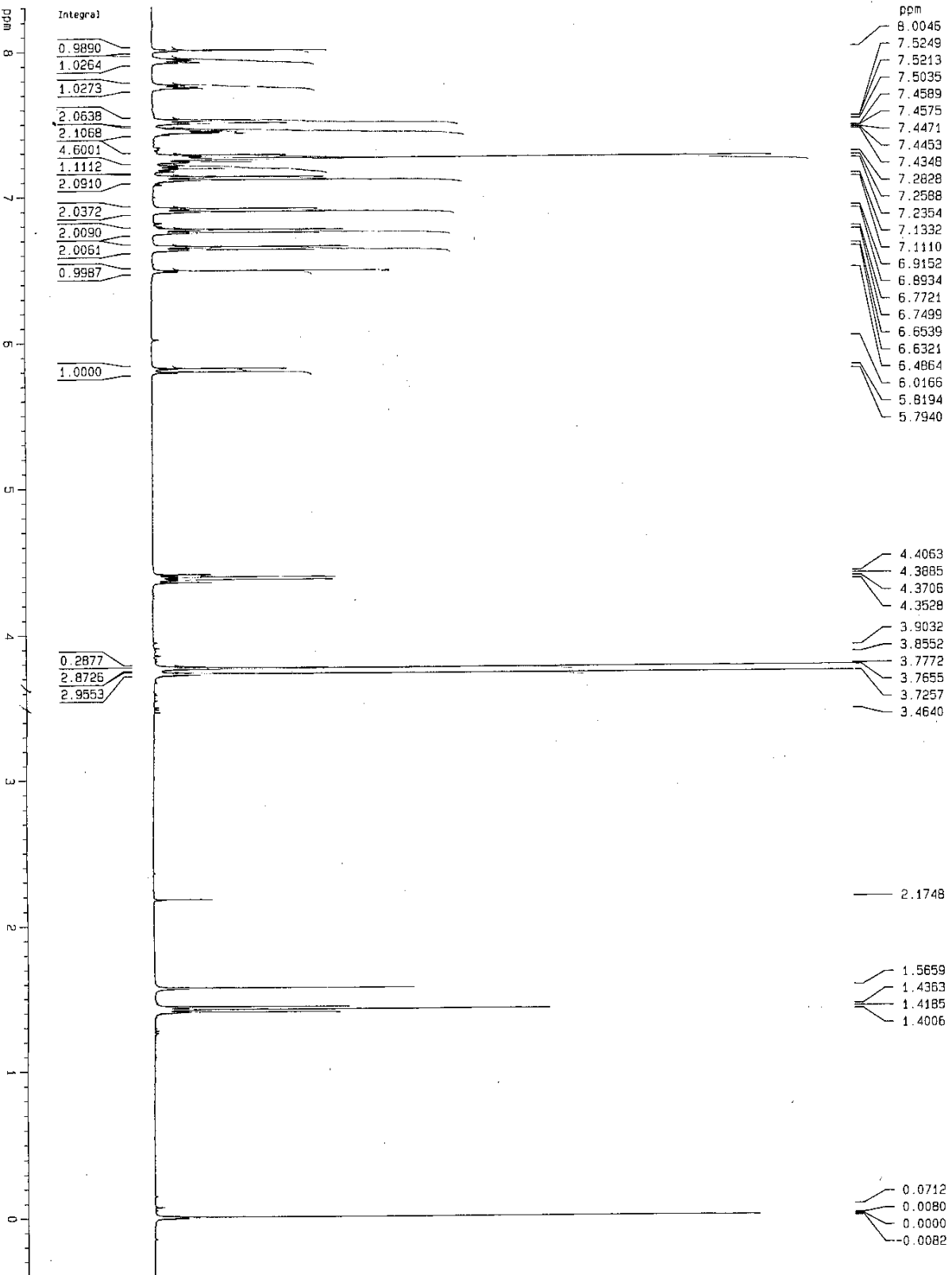
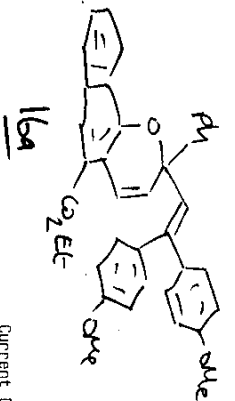
16:18:52
CI+(NH3)

2: Scan CI+
1.84e5





SK-3-33 -ester - pyran
 PROTON. CoiChem COC13 (D: VU) Suresh 9



Current Data Parameters
 NAME SK-3-33
 EXPNO 10
 PROCNO 1

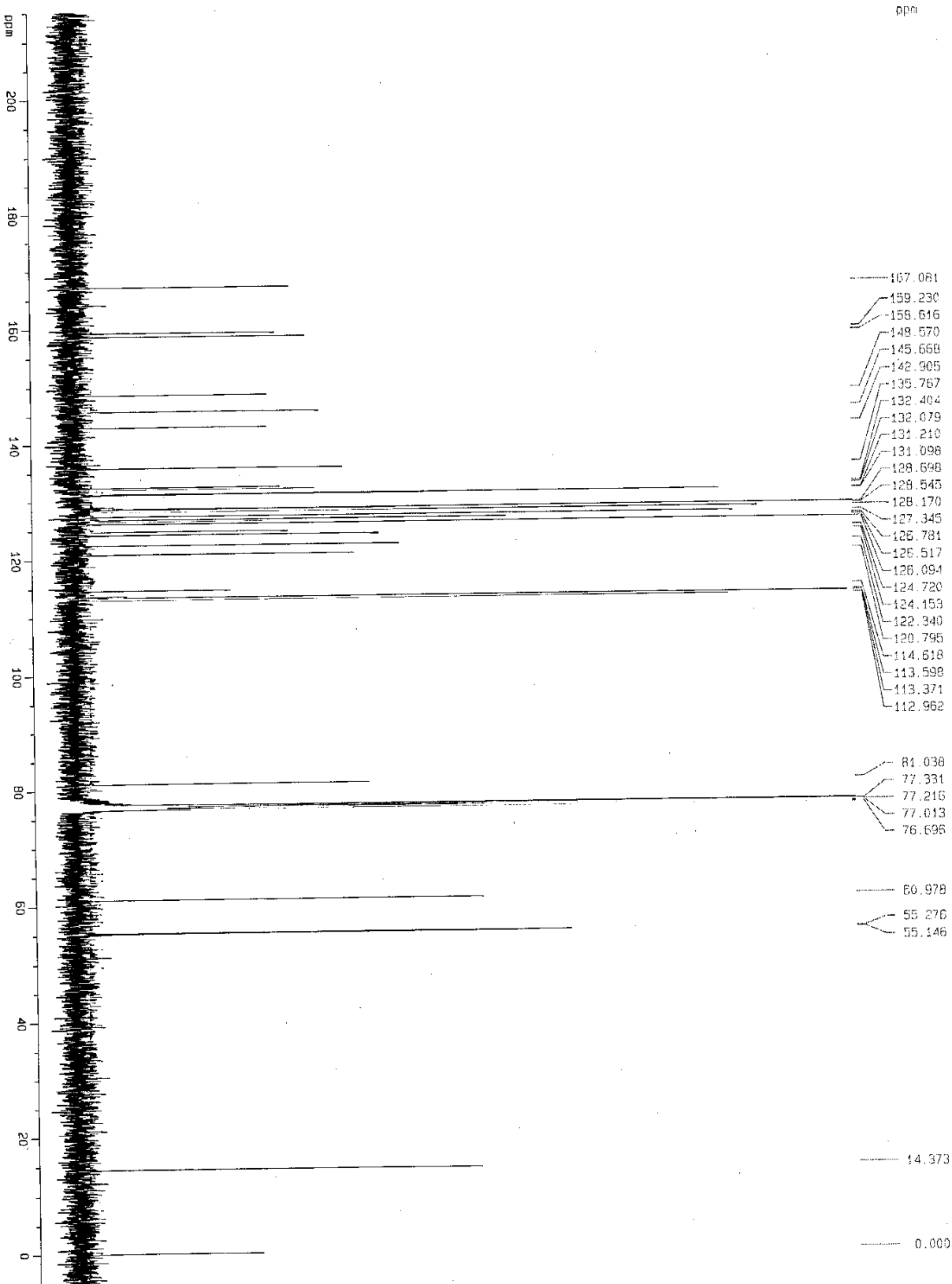
F2 - Acquisition Parameters
 Date_ 20080227
 Time 12.11
 INSTRUM spect
 PROBHD 5 mm GNP 1H/15
 PULPROG zg30
 TD 65536
 SOLVENT COC13
 NS 16
 DS 2
 SMH 8278.146 HZ
 FIDRES 0.186314 HZ
 AQ 3.9584243 sec
 RG 287.4
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 10.25 usec
 PL1 2.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.130098 MHz
 MDW EM
 SSB 0
 LB 0.30 HZ
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 CY 19.00 cm
 F1P 8.303 ppm
 F1 3322.08 HZ
 F2P -0.396 ppm
 F2 -158.61 HZ
 PPMCM 0.28996 ppm/cm
 HZCM 116.02295 HZ/cm

SK-3-33-carbon
 C13CPD CDC13 {D: \u} Suresh 8



- 167.061
- 159.230
- 158.616
- 149.570
- 145.668
- 142.905
- 135.767
- 132.404
- 132.079
- 131.210
- 131.098
- 128.698
- 128.545
- 128.170
- 127.345
- 125.781
- 125.517
- 126.094
- 124.720
- 124.159
- 122.340
- 120.795
- 114.818
- 113.598
- 113.371
- 112.962

- 81.038
- 77.331
- 77.216
- 77.013
- 76.695

- 60.978
- 55.276
- 55.146

- 14.373

- 0.000



Current Data Parameters
 NAME SK-3-33-carbon
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080228
 Time 7.13

INSTRUM spect
 PROCNO 5 mm QNP 1H/15
 PULPROG zgpg30
 TO 65536
 SOLVENT CDC13
 NS 6000
 DS 4

SMH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664795 sec
 RG 18390.4
 DW 20.850 usec
 DE 6.00 usec
 TE 300.0 K

D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 6.00 usec
 PL1 4.00 dB
 SFO1 100.6227898 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PL2 2.00 dB
 PL12 20.00 dB
 PL13 21.00 dB
 SFO2 400.1316005 MHz

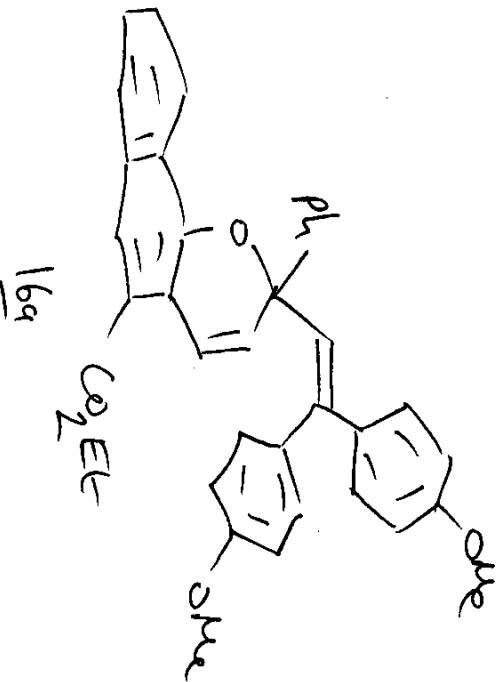
F2 - Processing parameters
 SI 32768
 SF 100.6127710 MHz
 WDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 30.00 cm
 CY 19.00 cm
 F1P 215.000 ppm
 F1 21631.75 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCM 7.33333 ppm/cm
 HZCM 737.82697 Hz/cm

EPSRC National Mass Spectrometry Service Centre

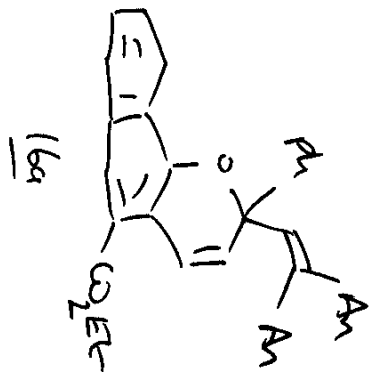
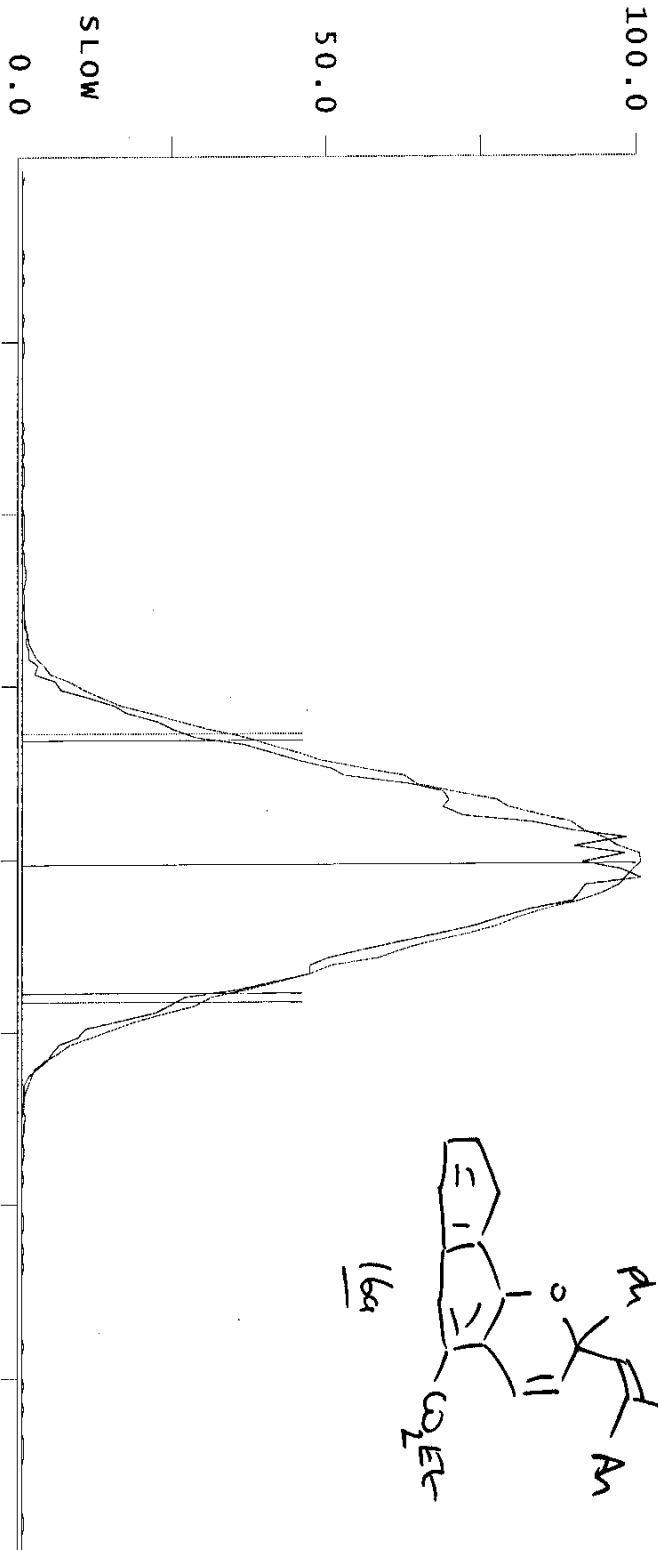
ACCURATE MASS MEASUREMENT REPORT

YOUR REFERENCE: SK-3-33
OUR REFERENCE: LEHHER062
Instrument: MAT 95 XP
Ionisation Mode: EI
Reference compound: Perfluorotributylamine
Ion identity: [M]⁺
Calculated mass (of ion): 568.2244
Measured mass (of ion): 568.2246



Peak Register Display

Copy result
to ULIST



An = 4-MeOC6H4-

MASS	:	501.97127	568.22536
REF MASS	:	501.97055	563.96739
PEAK WIDTH [ppm]	:	77.72241	73.14311

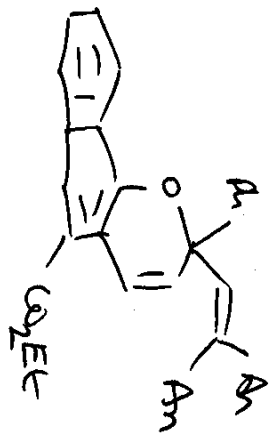
Active Register: 1 0.30 1.00

- N REG
- RCOPY2
- RCOPY3
- LIMIT
- CENTER
- SPREAD
- ERASE
- RESUME
- PAGE

Isotope: Min. .. Max.
 12 C 0....60
 1 H 0....80
 16 O 0....12
 14 N 0....12
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -2.. 100
 File: 100

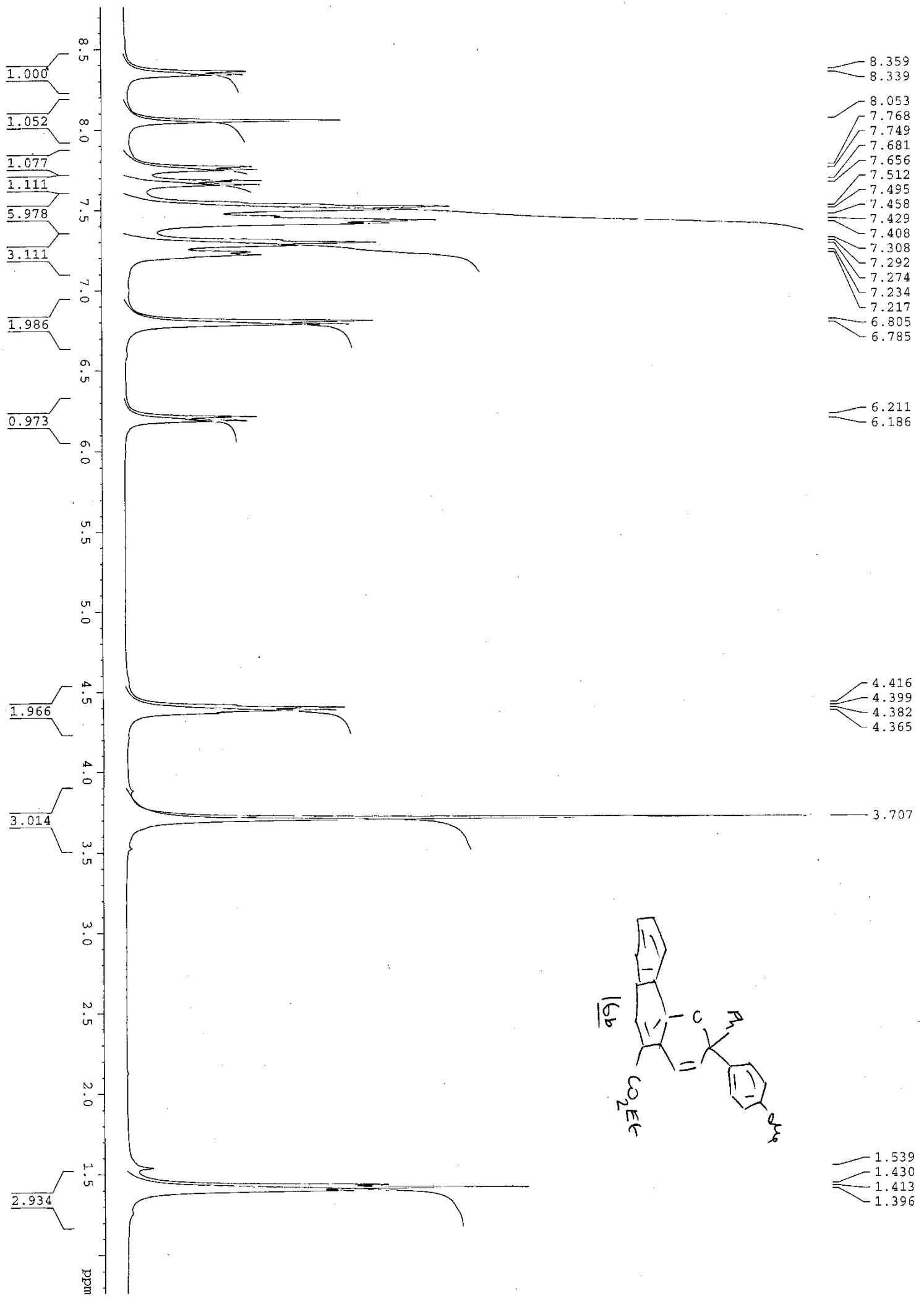
N-Rule: Do not use
 Charge: 1

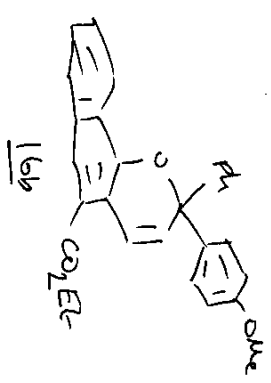
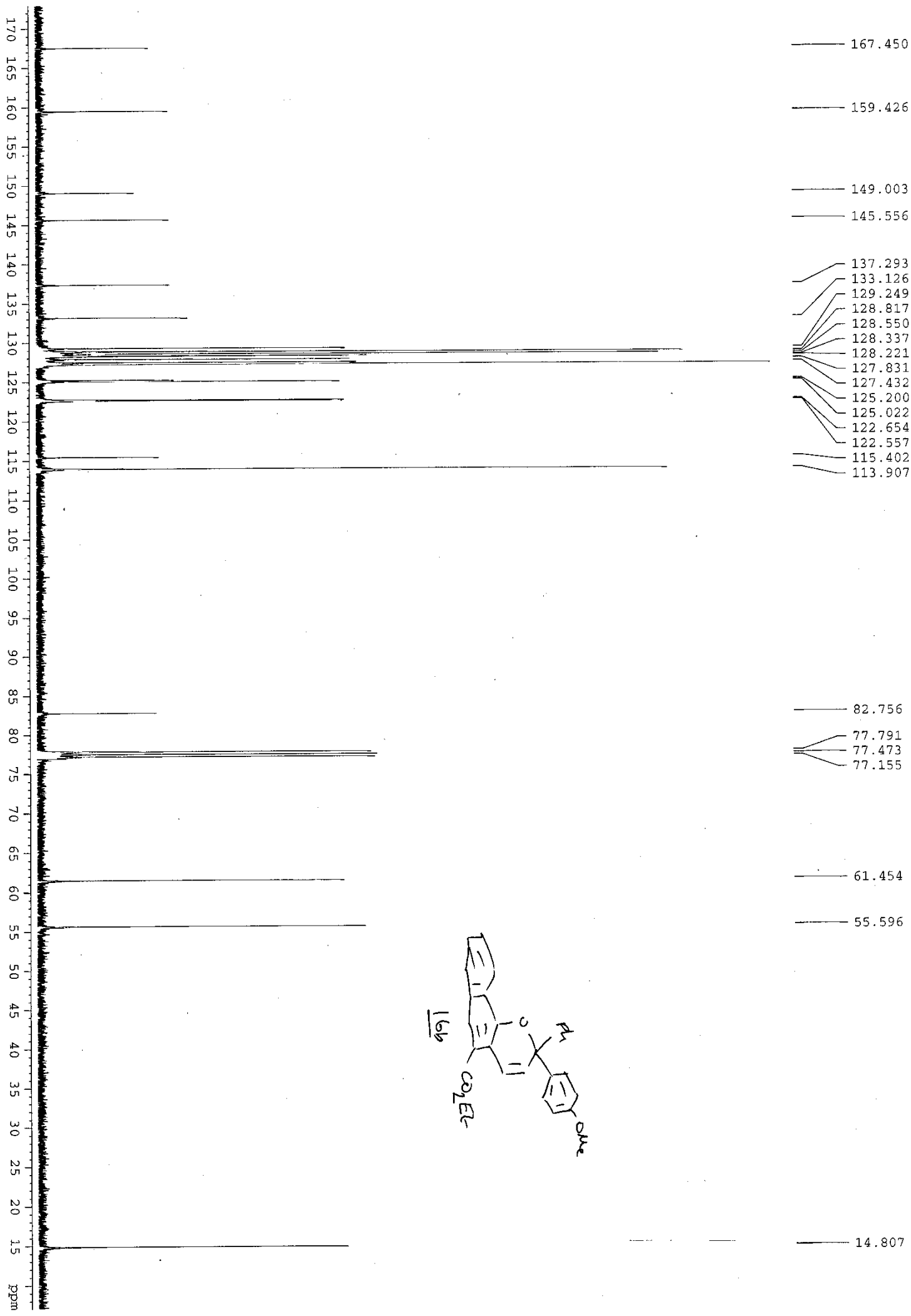
Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
568.2246	568.2244	0.3	23.0	C ₃₈ H ₃₂ O ₅
	568.2244	0.3	28.5	C ₃₇ H ₂₆ N ₇
	568.2249	-0.6	16.0	C ₃₅ H ₂₈ O ₆ N ₁₂
	568.2249	-0.6	10.5	C ₃₄ H ₃₄ O ₁₁ N ₅
	568.2236	1.8	11.0	C ₃₂ H ₃₂ O ₁₀ N ₈
	568.2258	-2.0	28.0	C ₃₉ H ₂₈ O ₁ N ₄
	568.2231	2.7	23.5	C ₃₆ H ₃₀ O ₄ N ₃
	568.2263	-2.9	15.5	C ₂₅ H ₃₀ O ₇ N ₉
	568.2263	-2.9	10.0	C ₂₆ H ₃₆ O ₁₂ N ₂
	568.2222	4.1	11.5	C ₂₀ H ₃₀ O ₉ N ₁₁
	568.2271	-4.4	27.5	C ₄₁ H ₃₀ O ₂ N ₁



AN = 4-Med C₆H₄-

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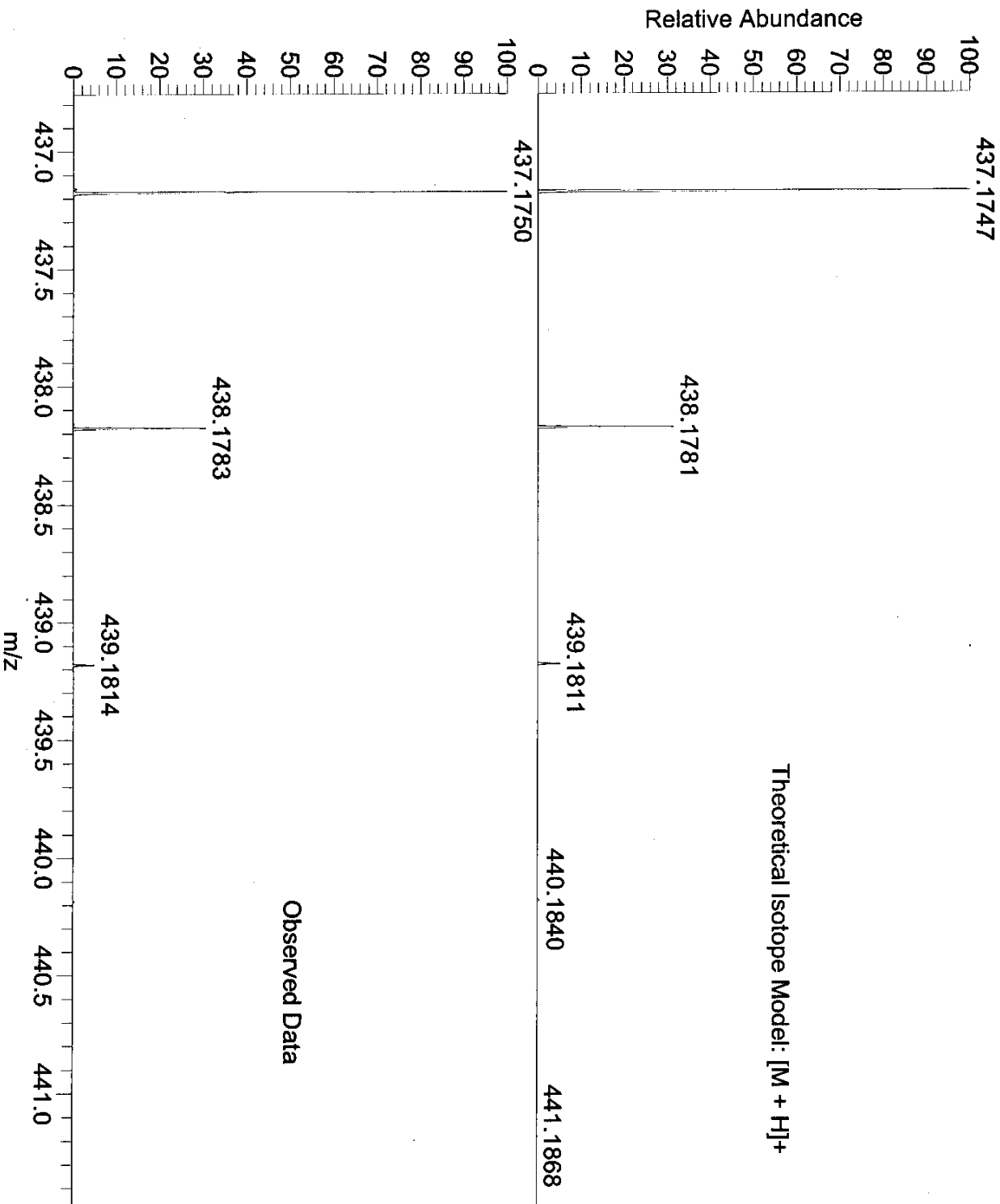


SK368 MW=436?
(DCM)/MeOH + NH4OAc

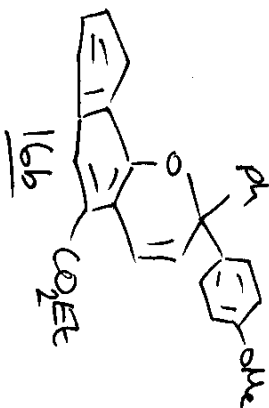
EPSRC National Centre Swansea
LTQ Orbitrap XL

Christopher S. Kershaw
12/02/2010 15:39:08

SM: 7G



NL:
1.70E4
C₂₉ H₂₄ O₄ H:
C₂₉ H₂₅ O₄
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr .@FWHM

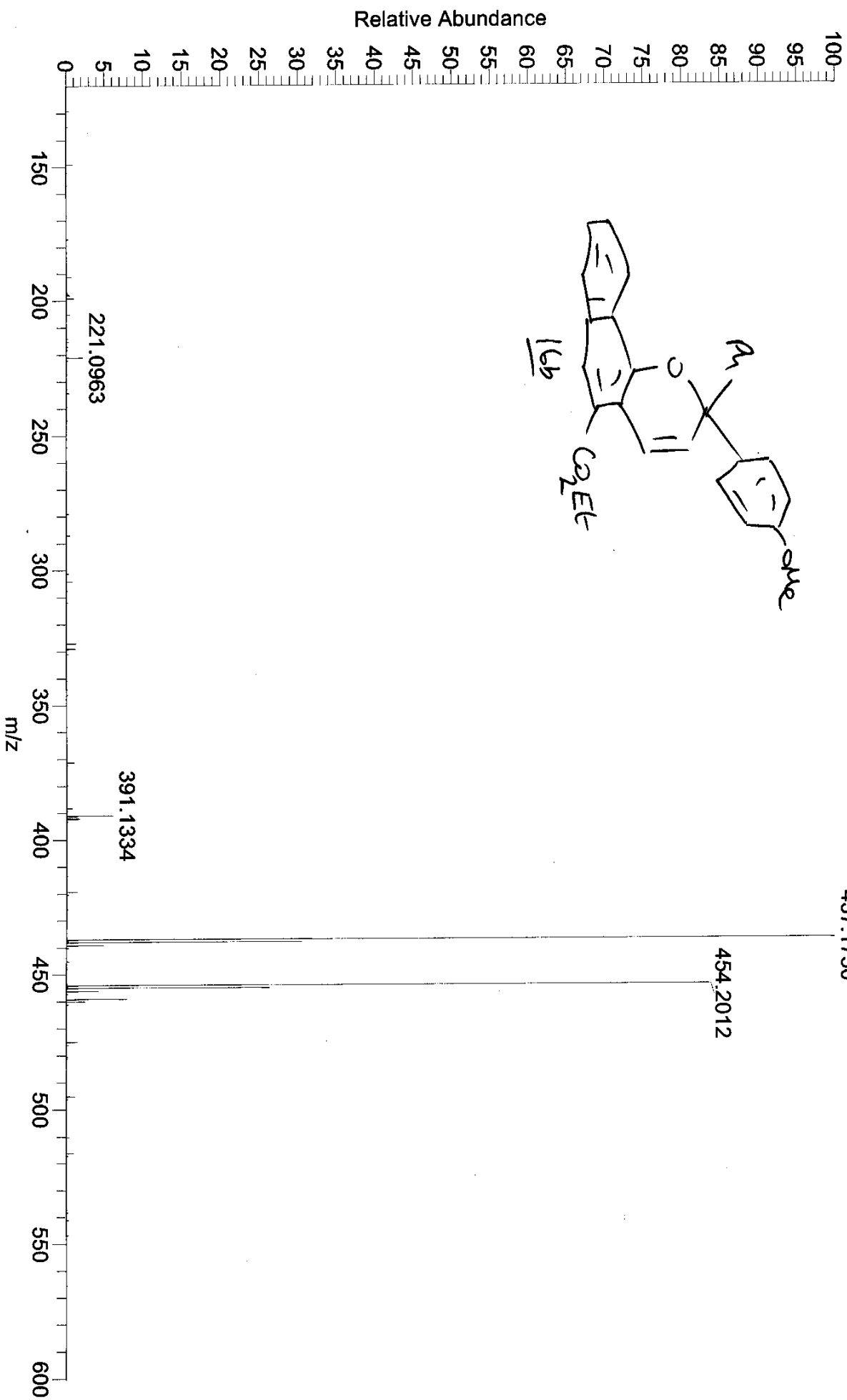


NL:
8.67E6
LEEHER112-OM-HNESP#9-13
RT: 0.87-1.19 AV: 5 T: FTMS
+ p NSI Full ms
[120.00-2000.00]

SK368 MW=436?
(DCM)/MeOH + NH4OAc
LEEHER112-OM-HNESP #9-13 RT: 0.87-1.19
T: FTMS + p NSI Full ms [120.00-2000.00]

EPSRC National Centre Swansea
LTQ Orbitrap XL

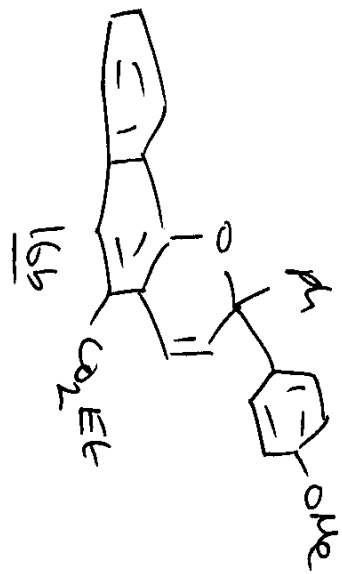
Christopher S. Kershaw
12/02/2010 15:39:08

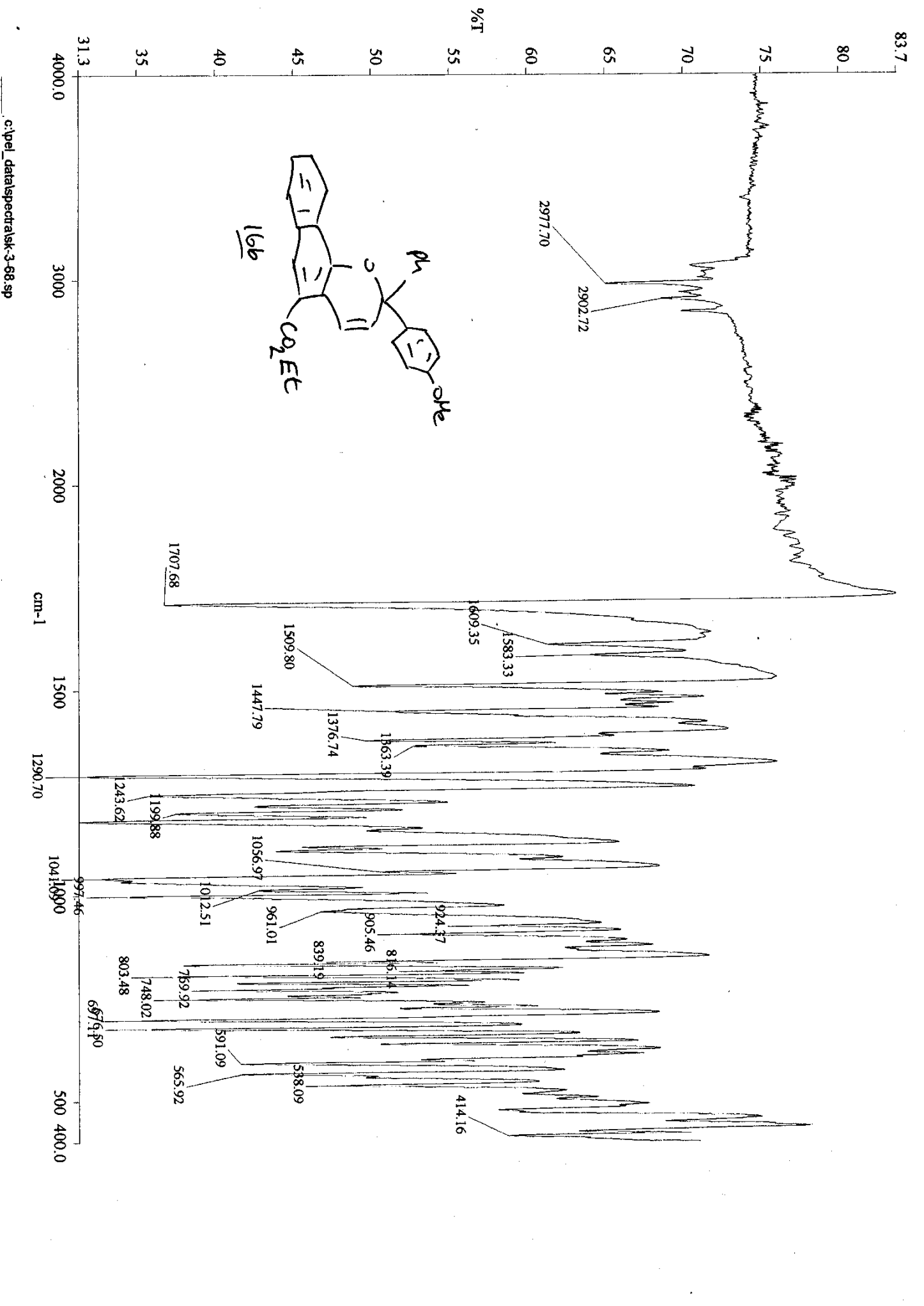


Isotope: Min. ... Max.
 14 N 0....10
 16 O 0....14
 12 C 0....60
 1 H 0....80
 23 Na 0....0
 Tolerance Window: +- 5.00 ppm
 Dp/Ring Equiv: -2.. 100
 Files: 200

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
437.1750	437.1752	-0.6	5.0	C ₁₅ H ₁₇ O ₁₀ N ₅
	437.1747	0.6	17.5	C ₂₉ H ₃₅ O ₄
	437.1761	-2.5	22.5	C ₃₀ H ₃₁ N ₄
	437.1739	2.5	0.0	C ₁₄ H ₃₁ O ₁₄ N ₁
	437.1739	2.5	5.5	C ₁₃ H ₃₅ O ₉ N ₈
	437.1766	-3.6	10.0	C ₁₆ H ₂₃ O ₆ N ₉
	437.1766	-3.6	4.5	C ₁₇ H ₂₉ O ₁₁ N ₂
	437.1734	3.7	18.0	C ₂₇ H ₃₃ O ₃ N ₃

N-Rule: Do not use
 Charge: 1





c:\pel_data\spectra\sk-3-68.sp