Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

SUPPLEMENTAL INFORMATION

Antitumour activity and ERα molecular docking studies of newly synthesized D-homo fused steroidal tetrazoles

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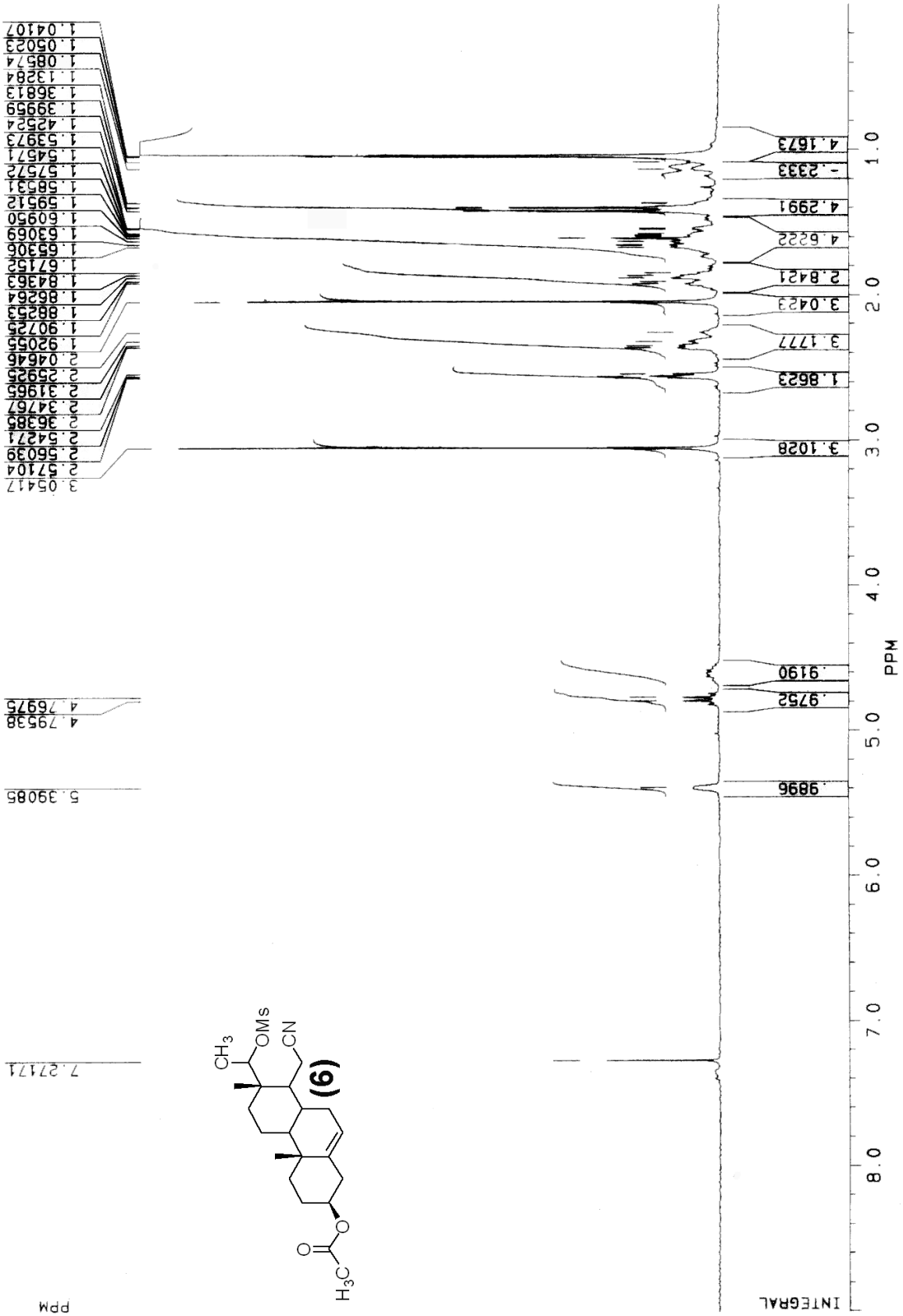
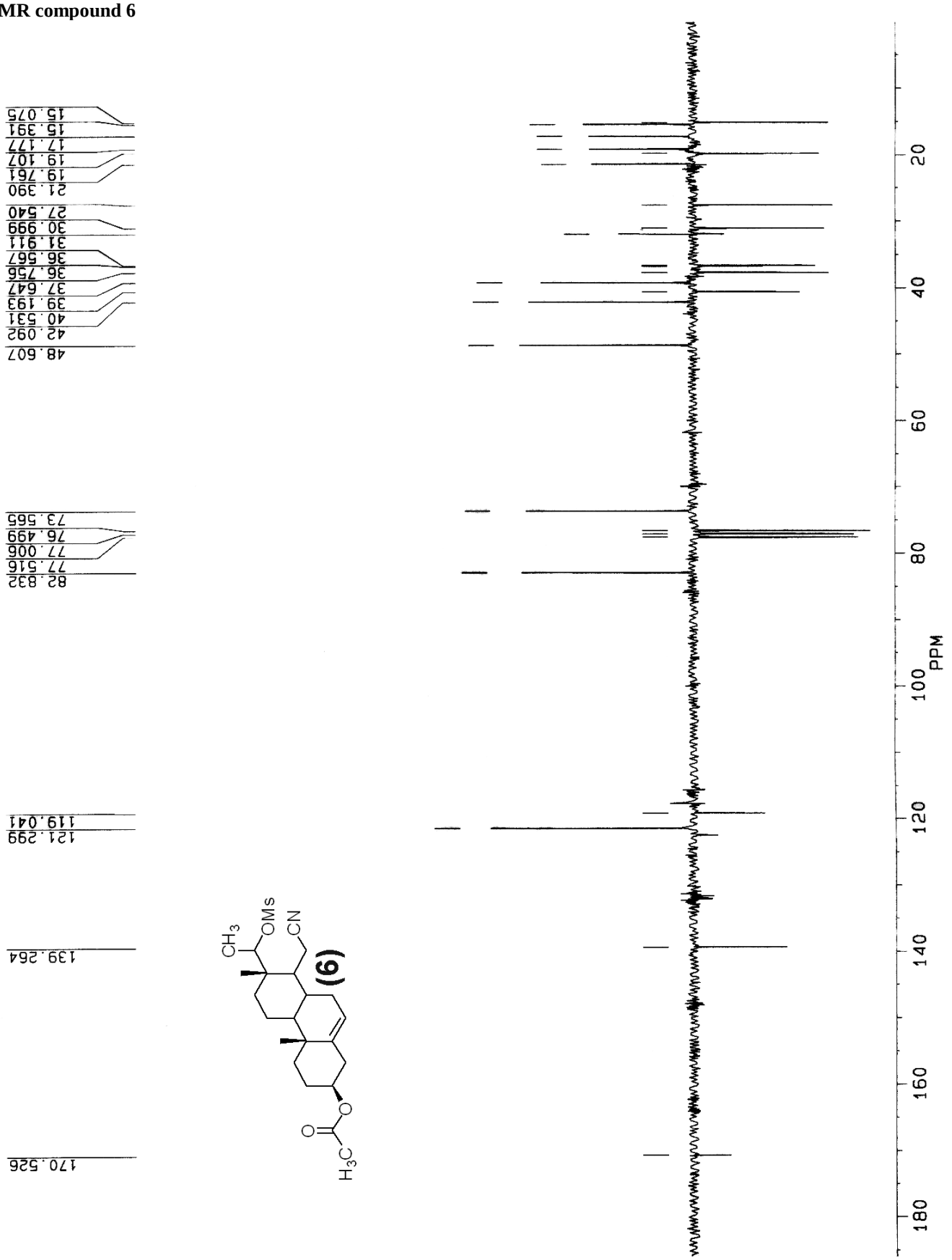
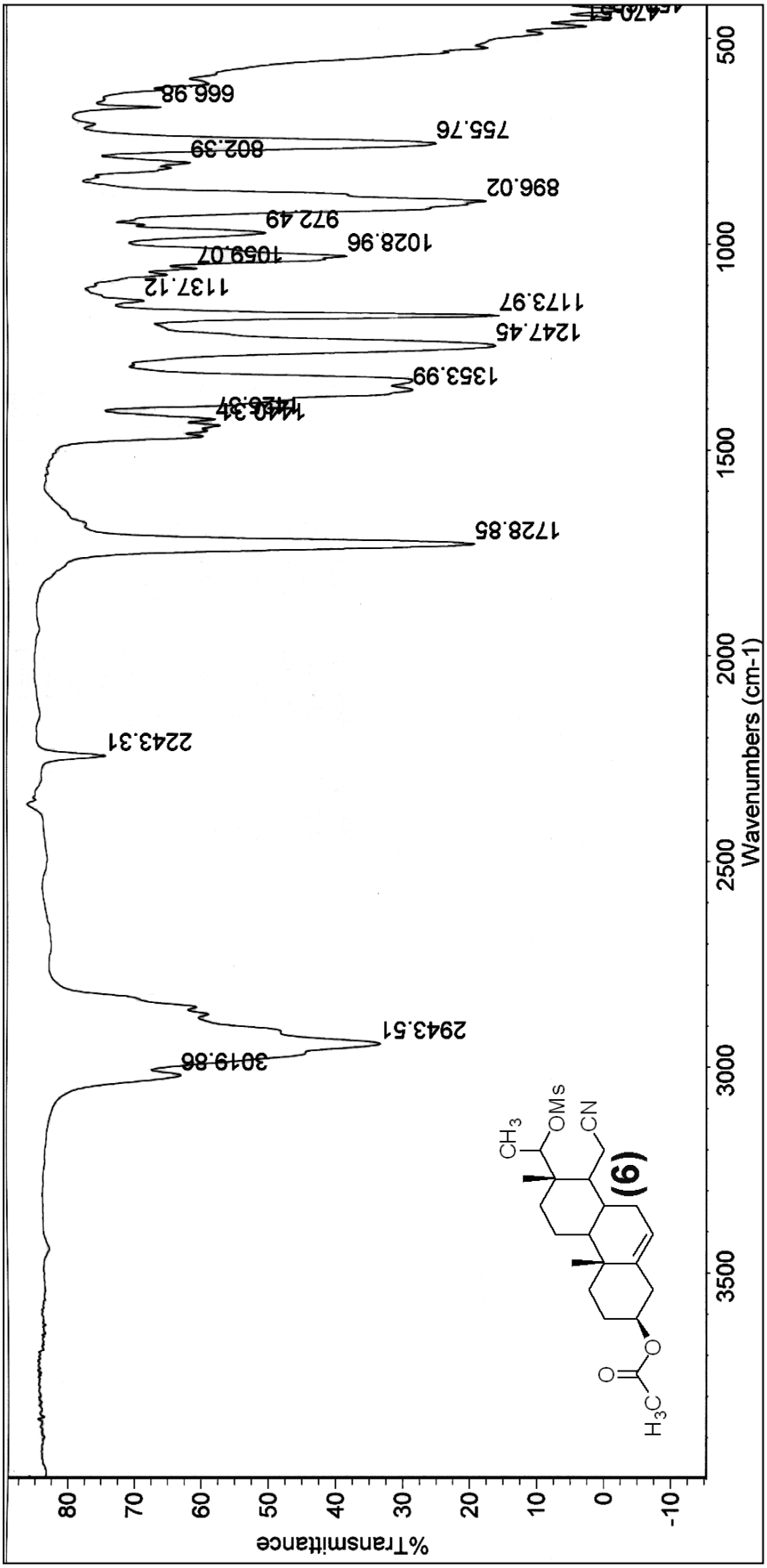
^{1}H NMR compound 6



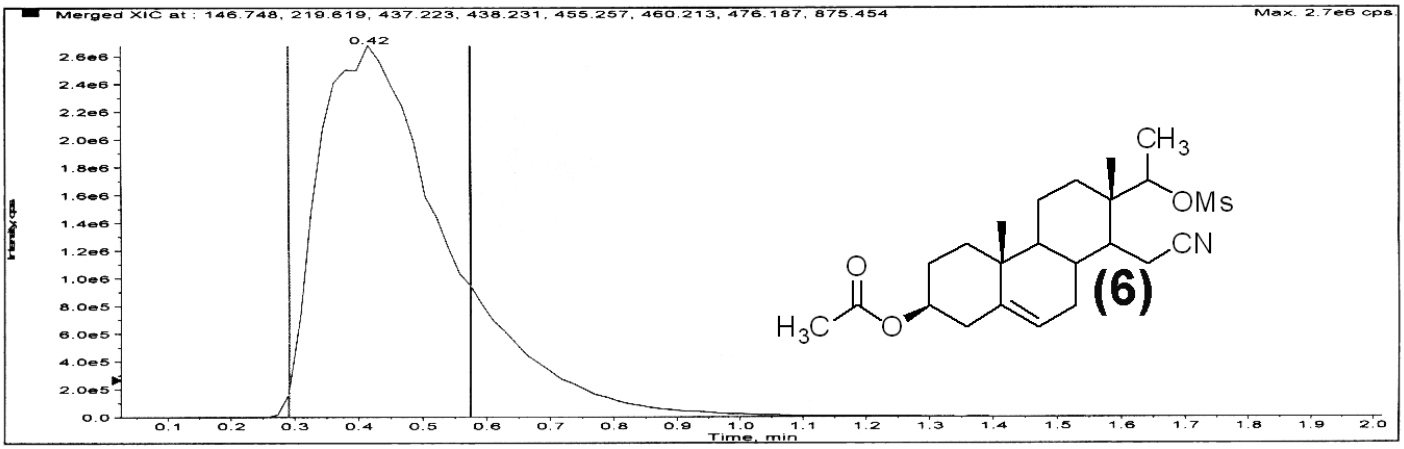
^{13}C NMR compound 6



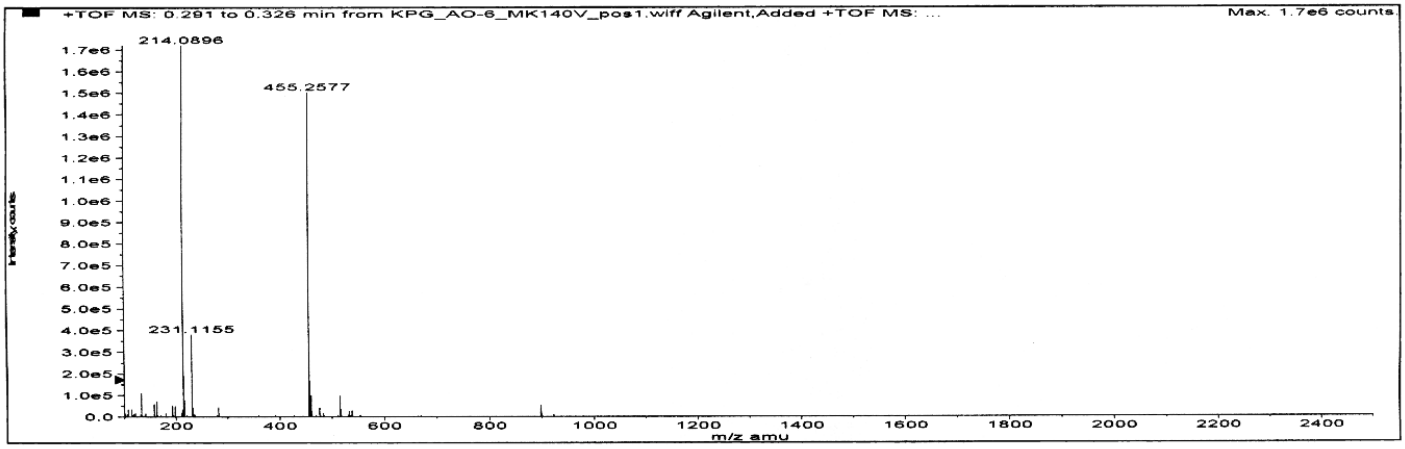
IR compound 6

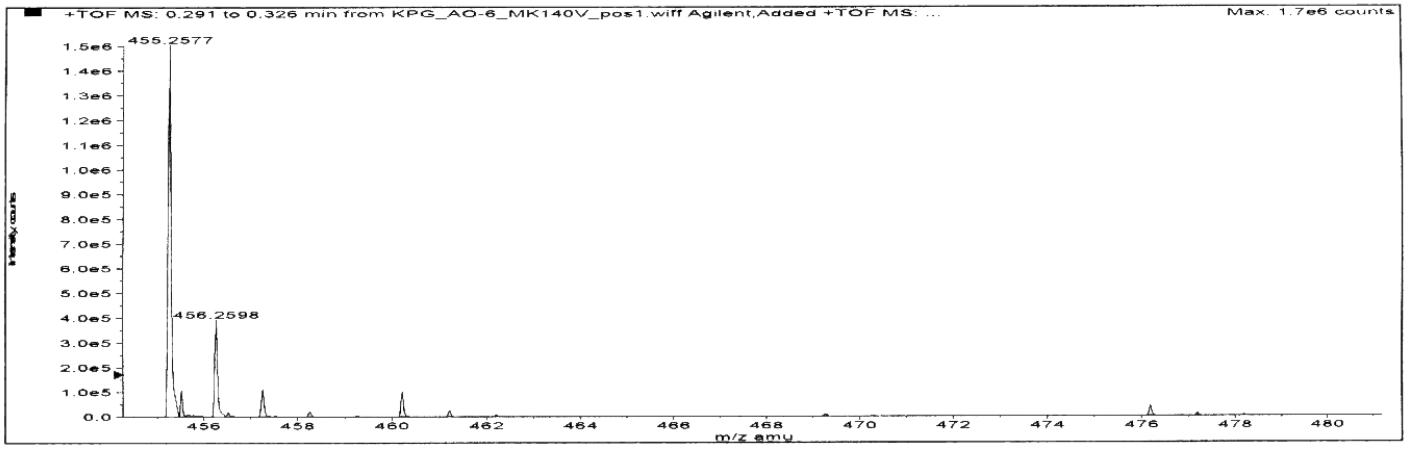


HRMS compound 6



Merged XIC, Period# : 1 Experiment# : 1

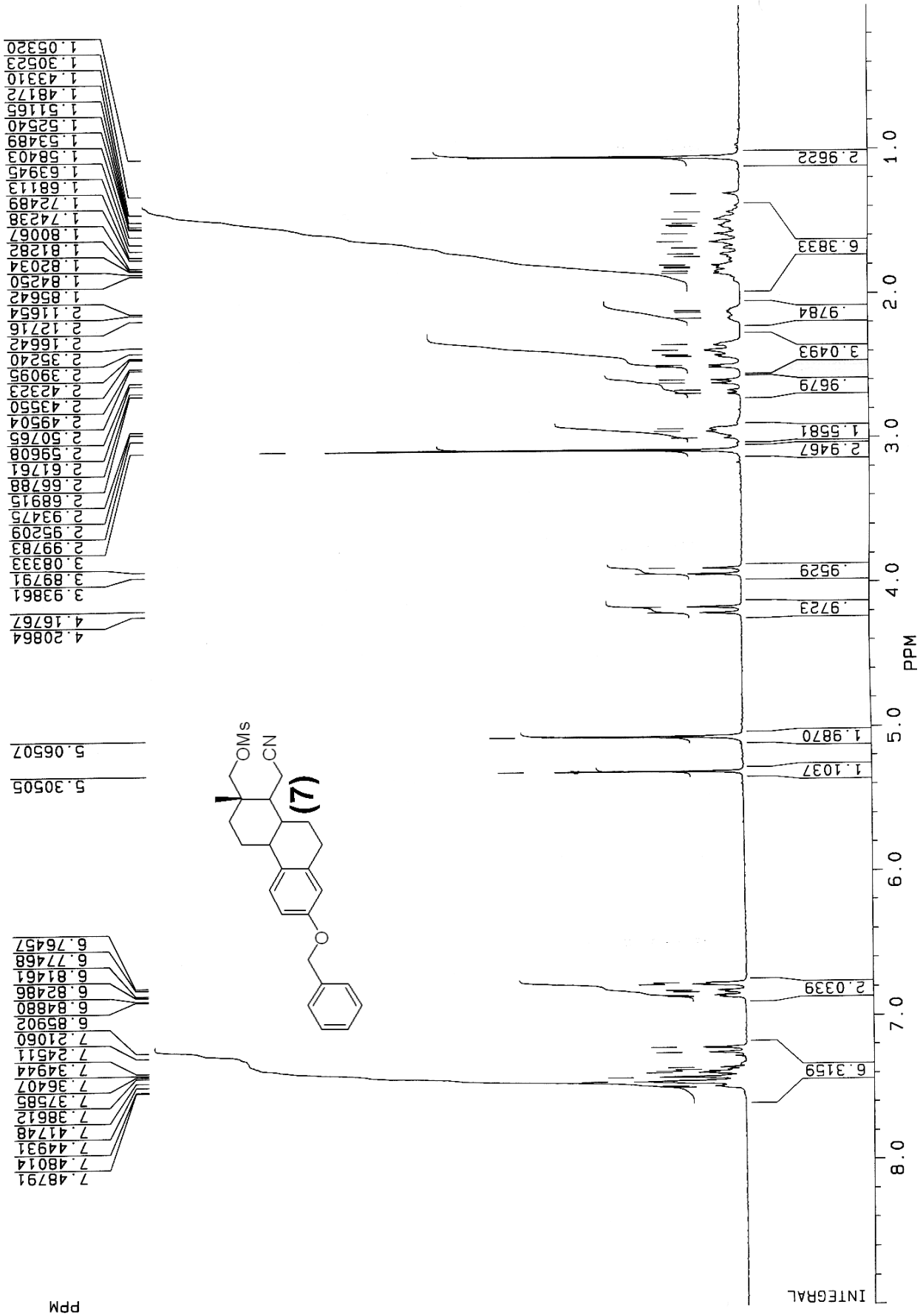




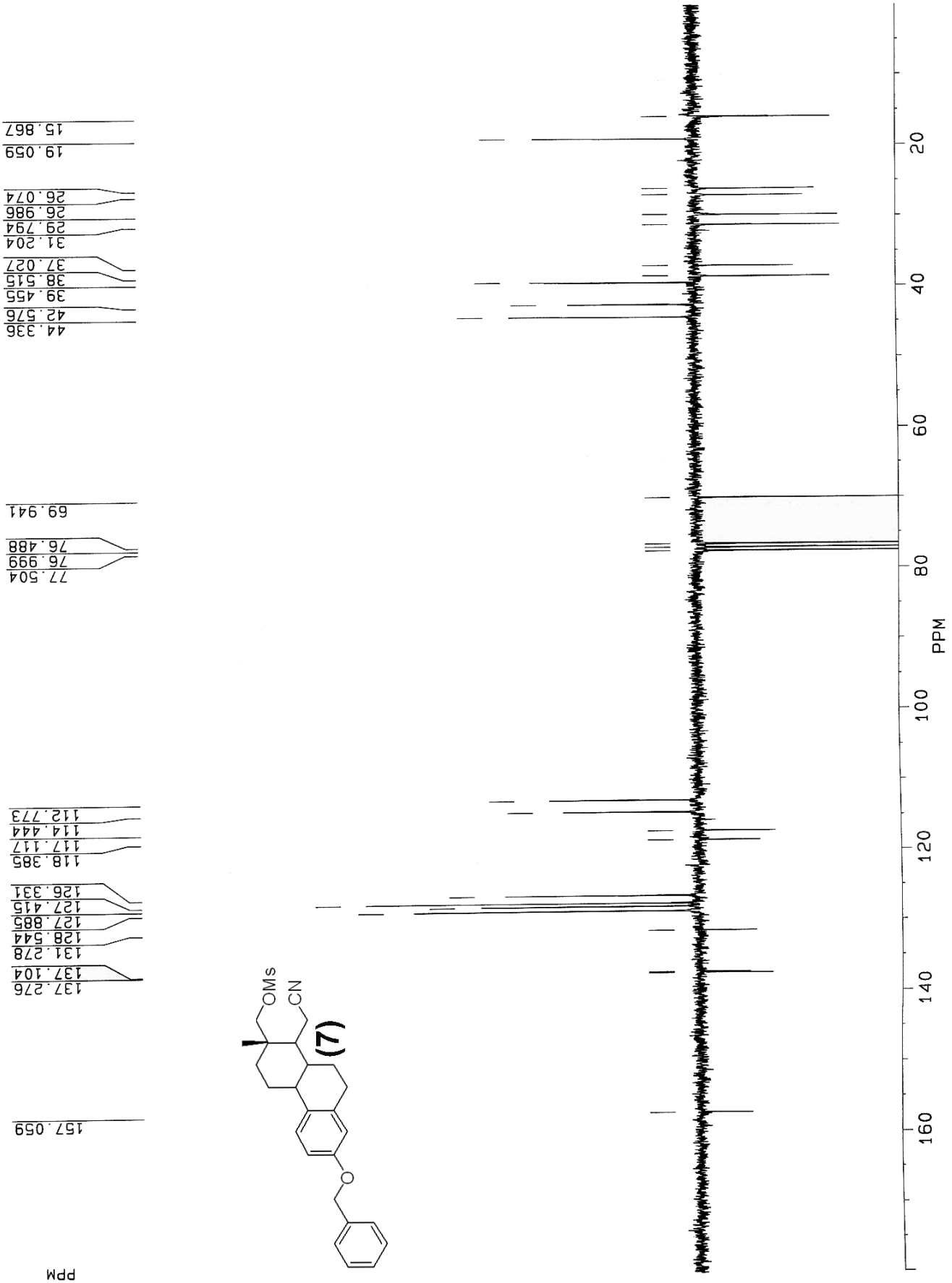
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C23H35NO5S	--	437.22359	0.42	3.75659 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+NH4]+	1506511.36	455.25742	455.25771	0.28895	0.63	--
[M+Na]+	101743.68	460.21282	460.21217	-0.64697	-1.41	--
[M+K]+	41807.72	476.18675	476.18622	-0.52749	-1.11	--

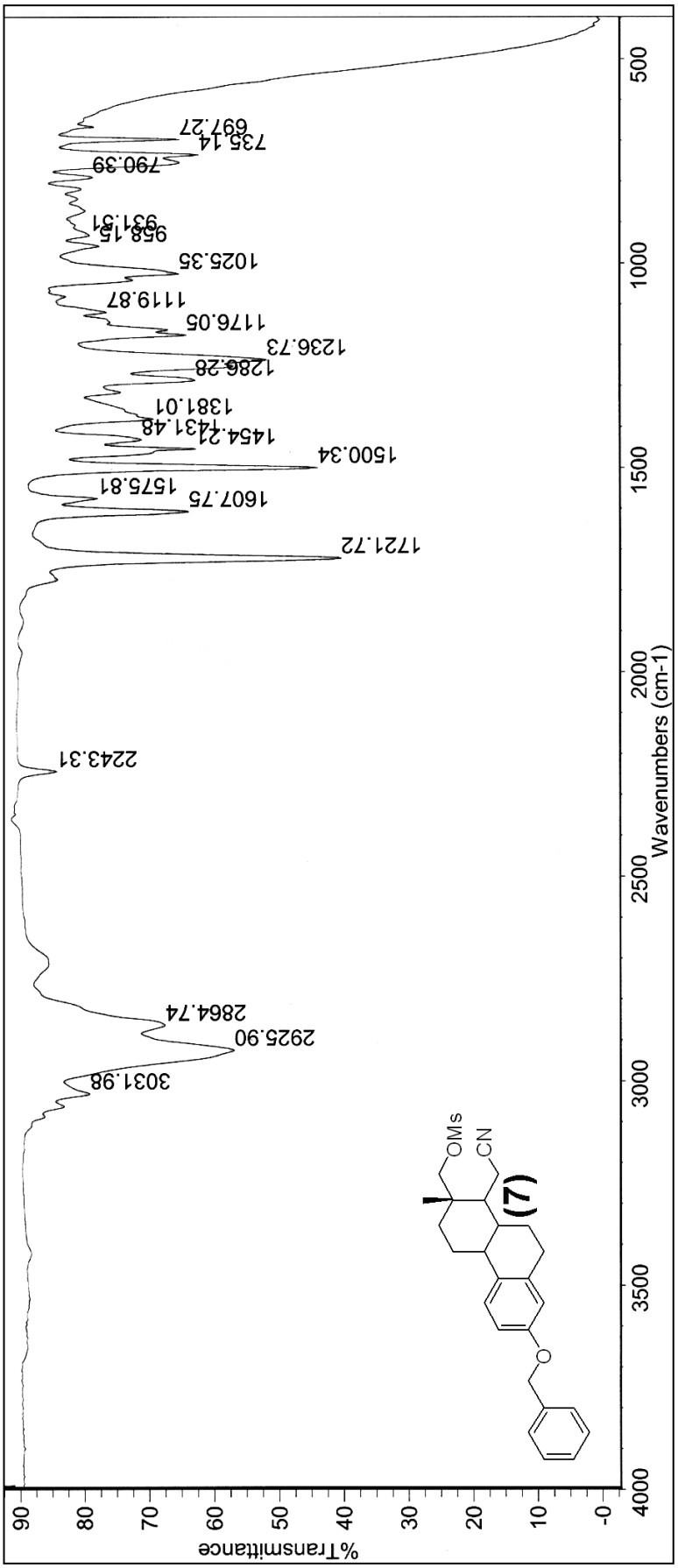
^{1}H NMR compound 7



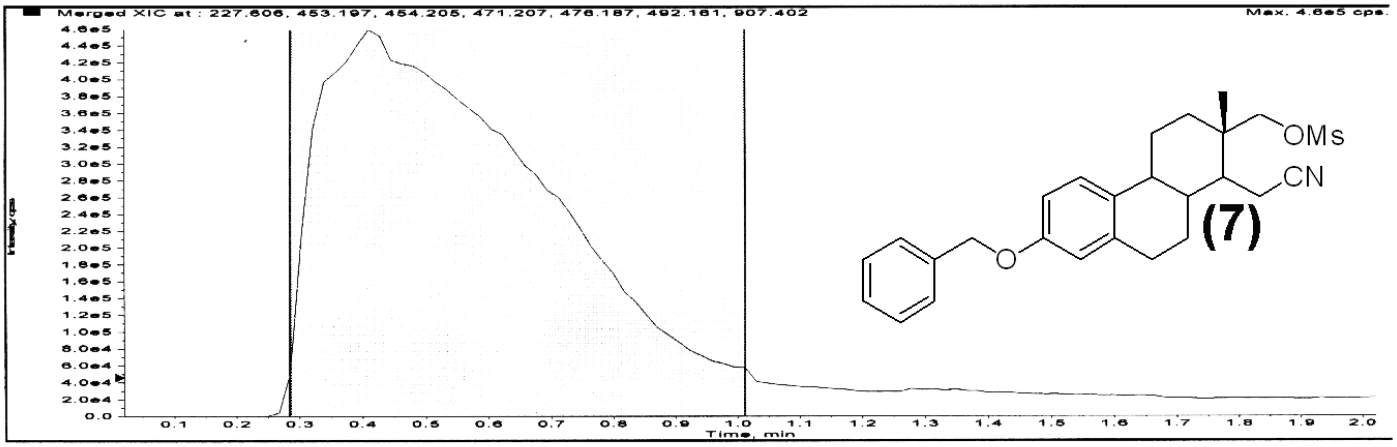
^{13}C NMR compound 7



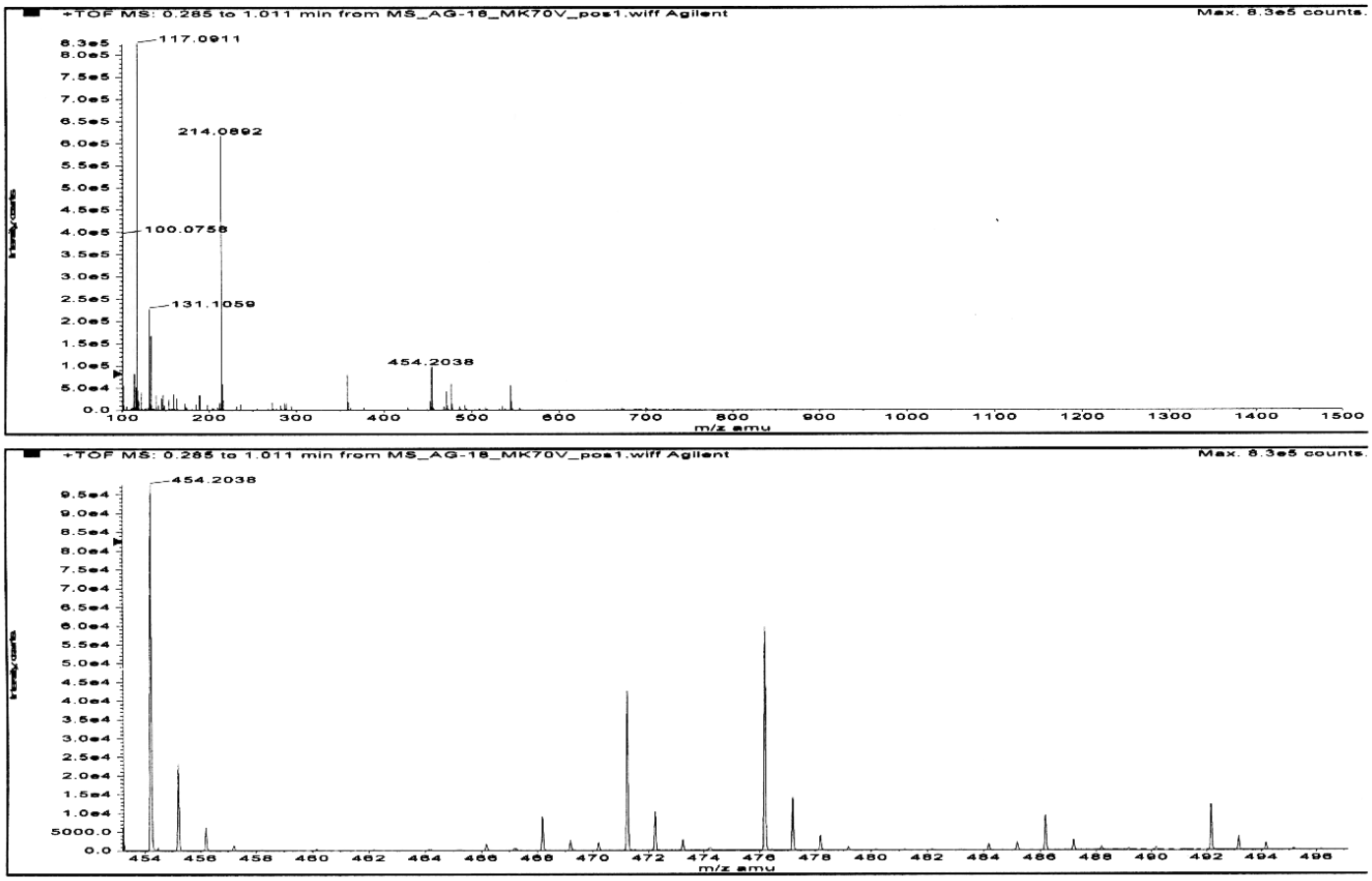
IR compound 7



HRMS compound 7



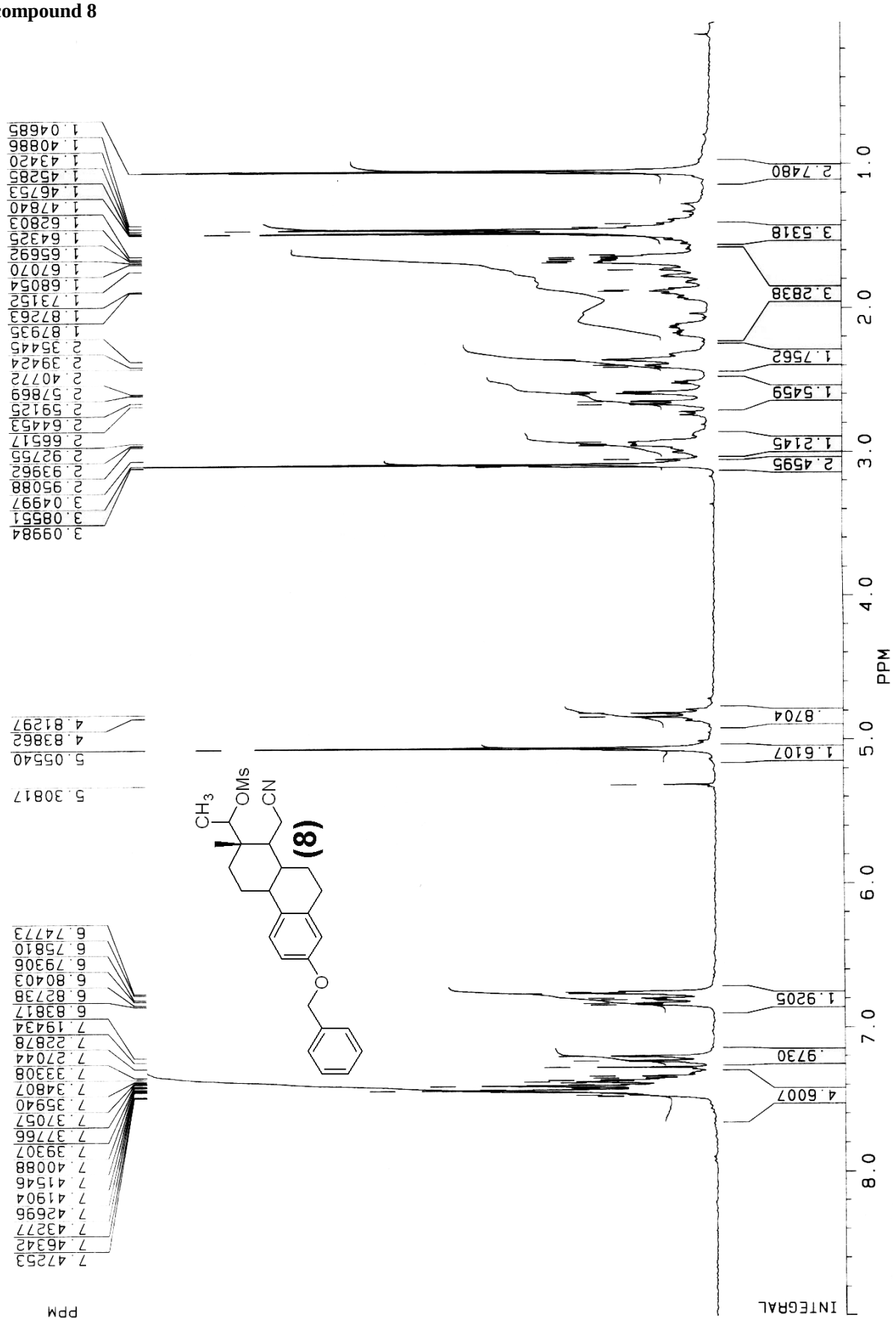
Merged XIC, Period# : 1 Experiment# : 1



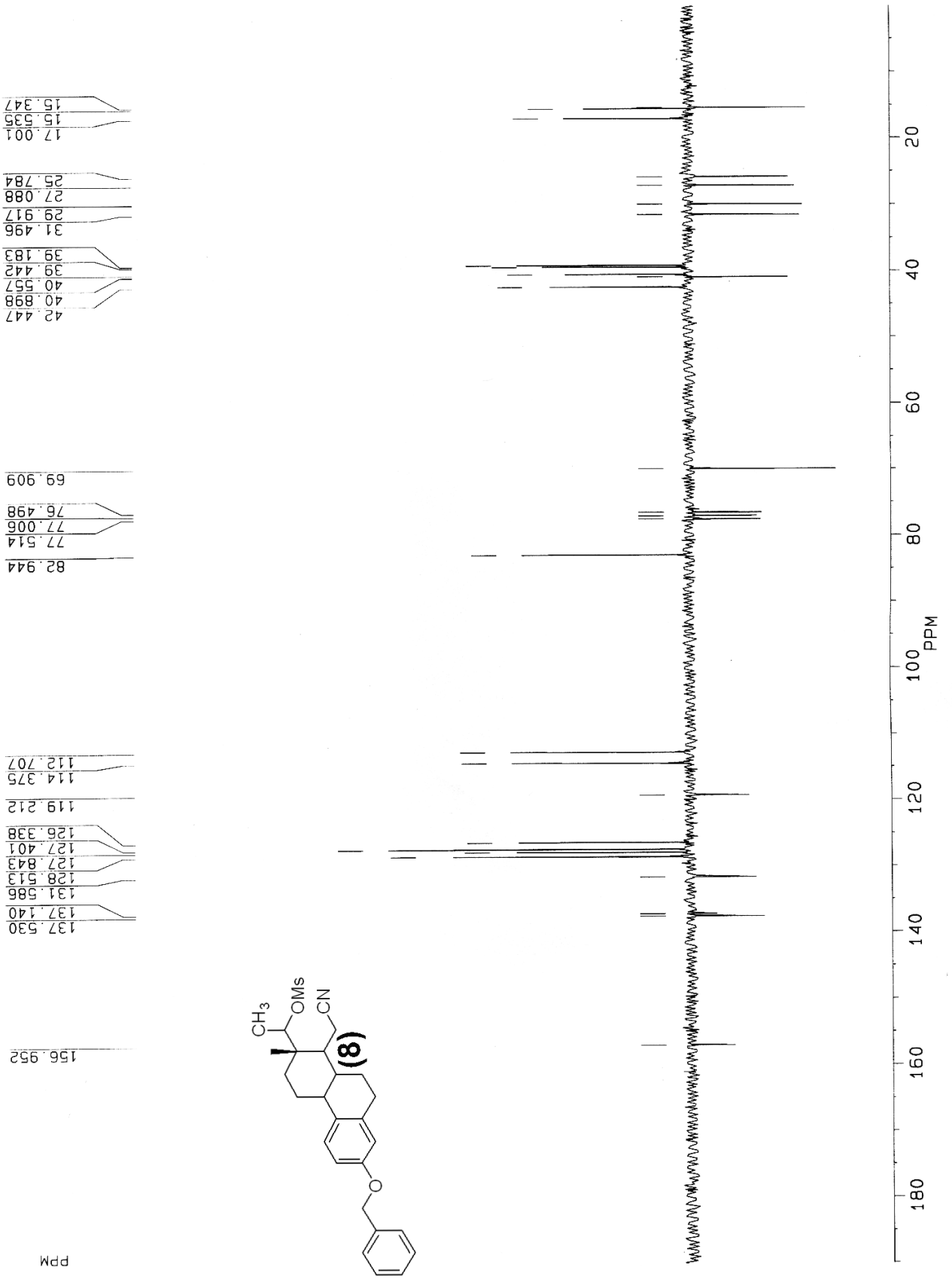
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C26H31NO4S	--	453.19738	0.41	1.10939 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H]+	97819.58	454.20466	454.20379	-0.87045	-1.92	--
[M+H2O]+	43592.36	471.20740	471.23037	22.97597	48.76	--
[M+Na]+	63483.87	476.18660	476.18609	-0.50555	-1.06	--
[M+K]+	13153.07	492.16054	492.16071	0.17467	0.35	--

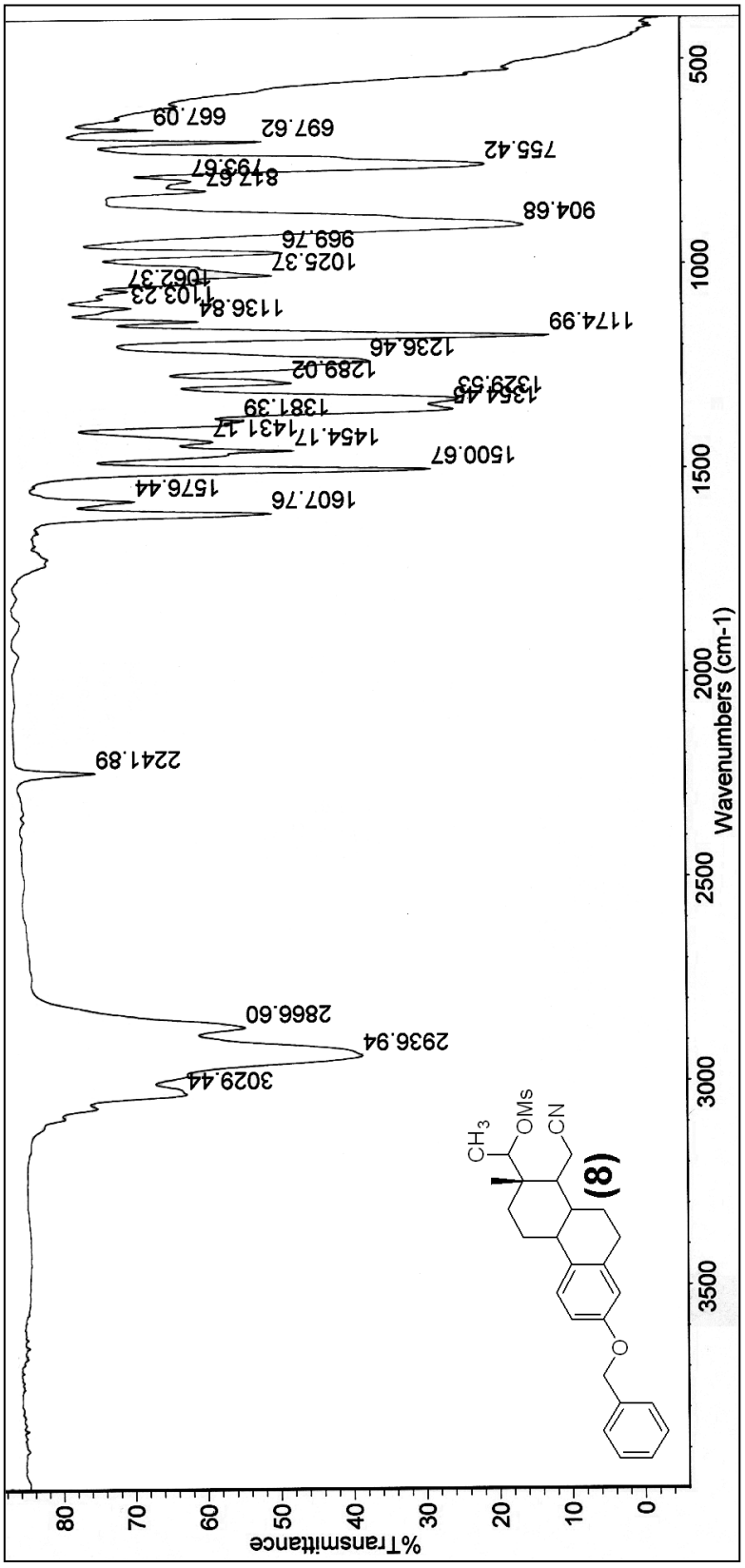
1H NMR compound 8



^{13}C NMR compound 8



IR compound 8



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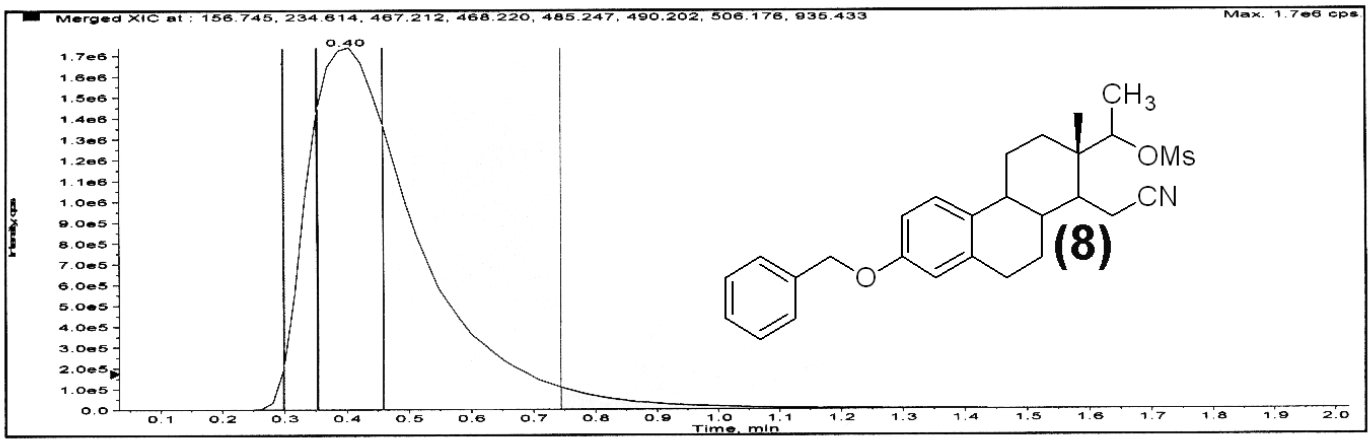
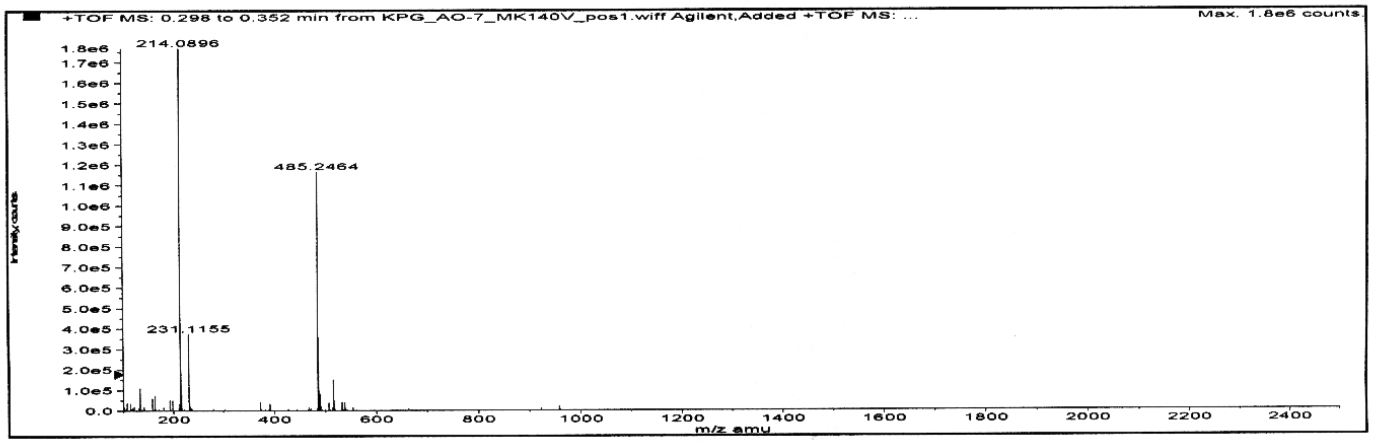
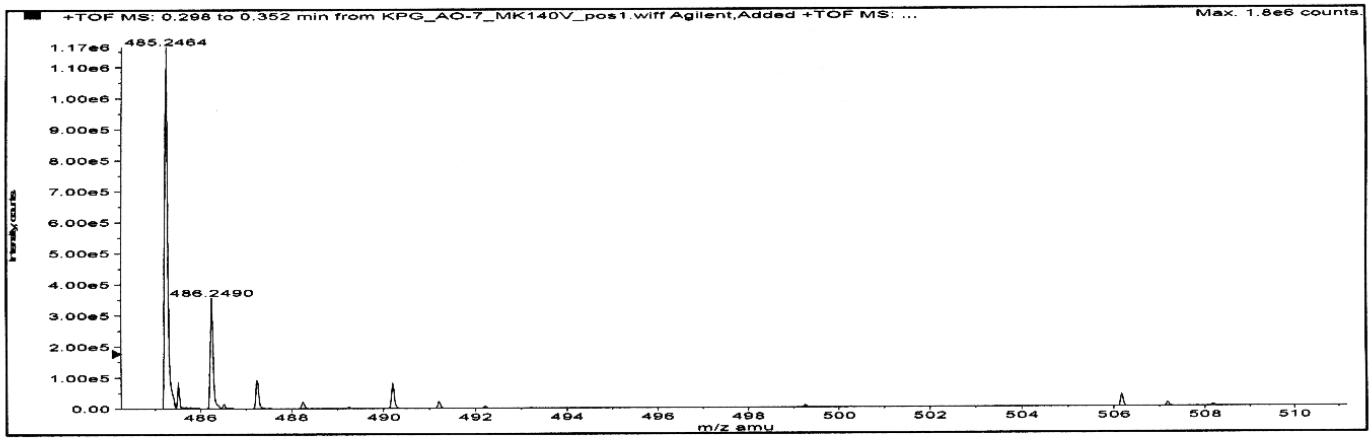


Merged XIC, Period# : 1 Experiment# : 1

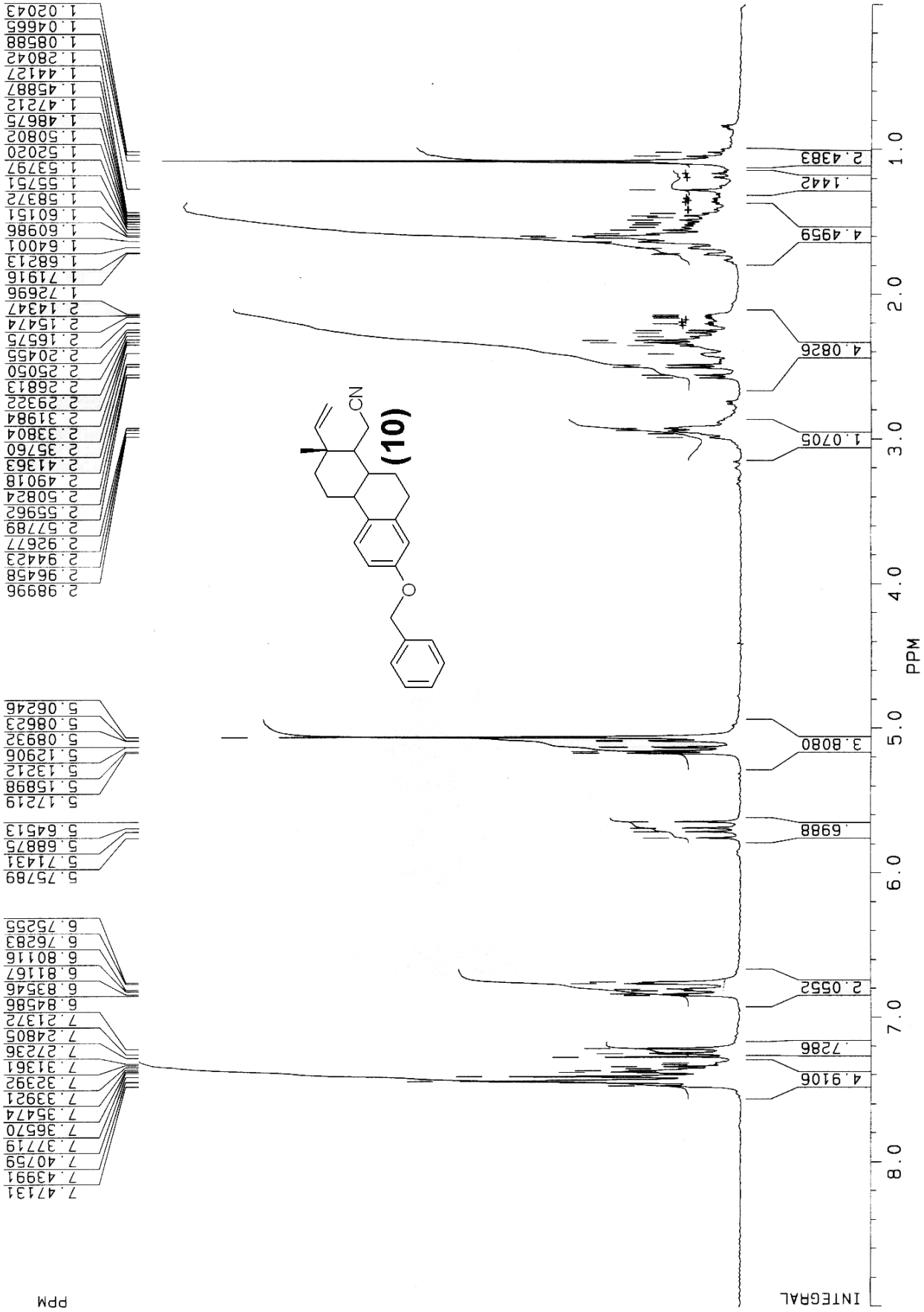




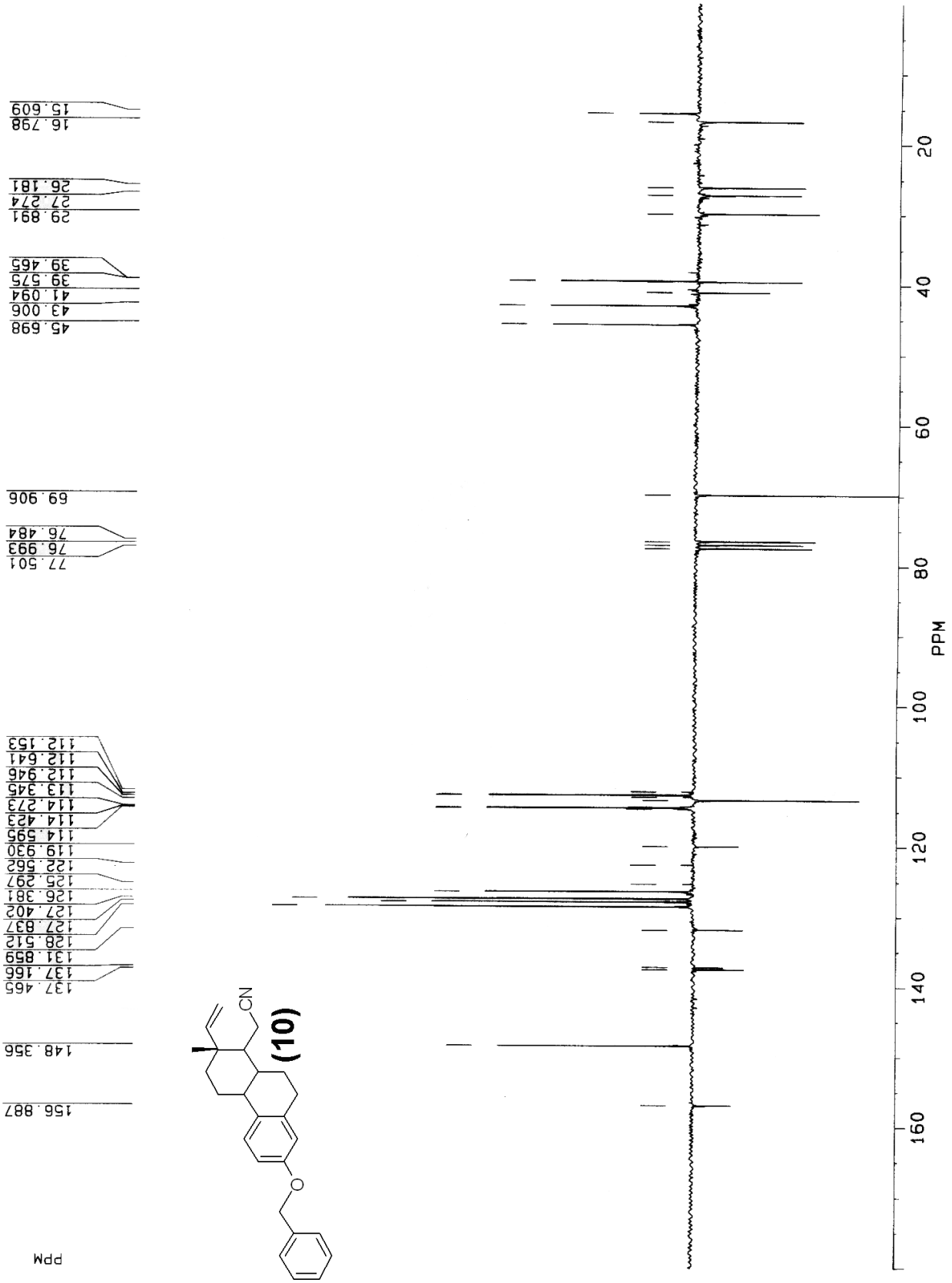
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C27H33NO4S	--	467.21303	0.40	2.17886 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+NH4]+	1190903.28	485.24685	485.24641	-0.44412	-0.92	--
[M+Na]+	83346.34	490.20225	490.20169	-0.55585	-1.13	--
[M+K]+	41684.97	506.17619	506.17534	-0.84262	-1.66	--

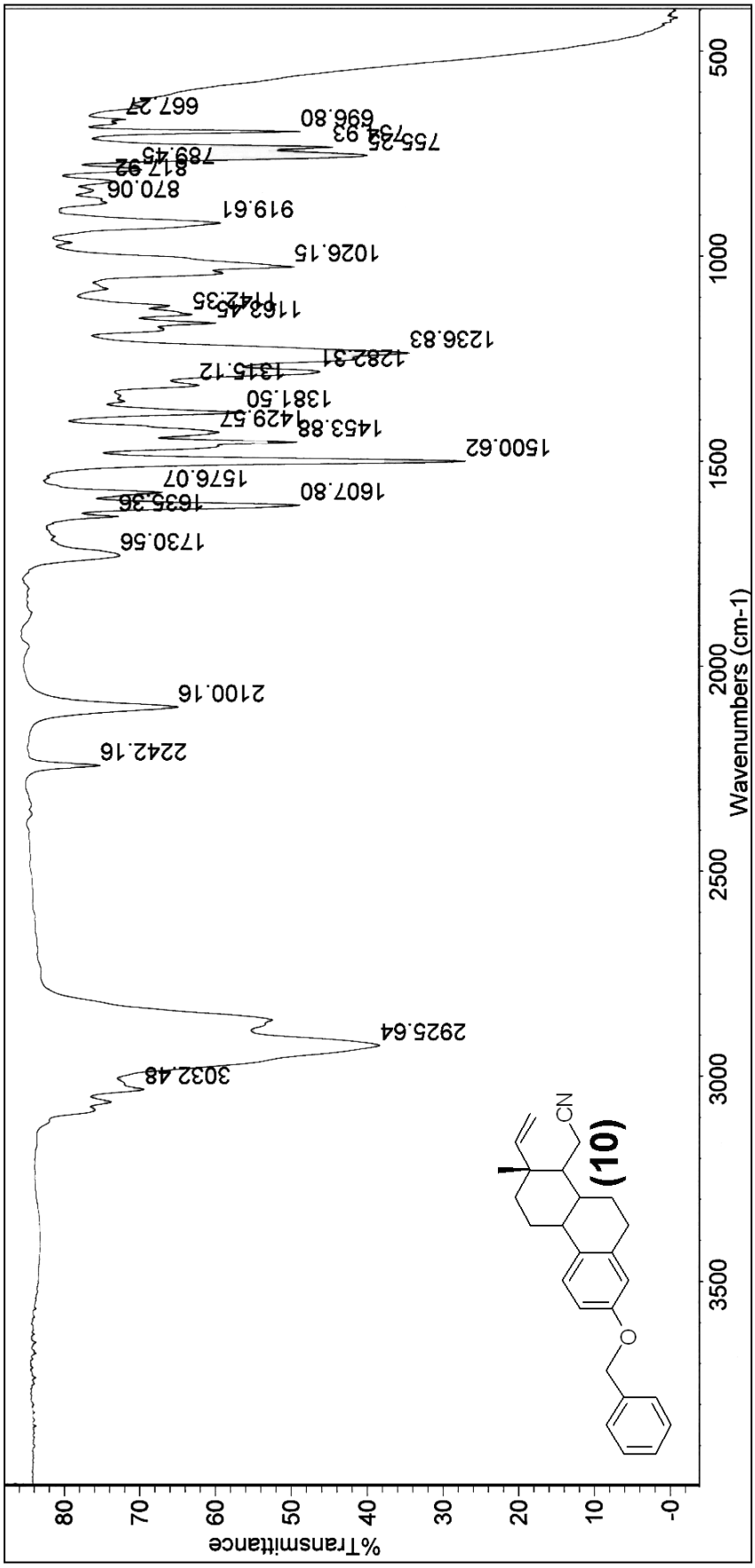
^{1}H NMR compound 10



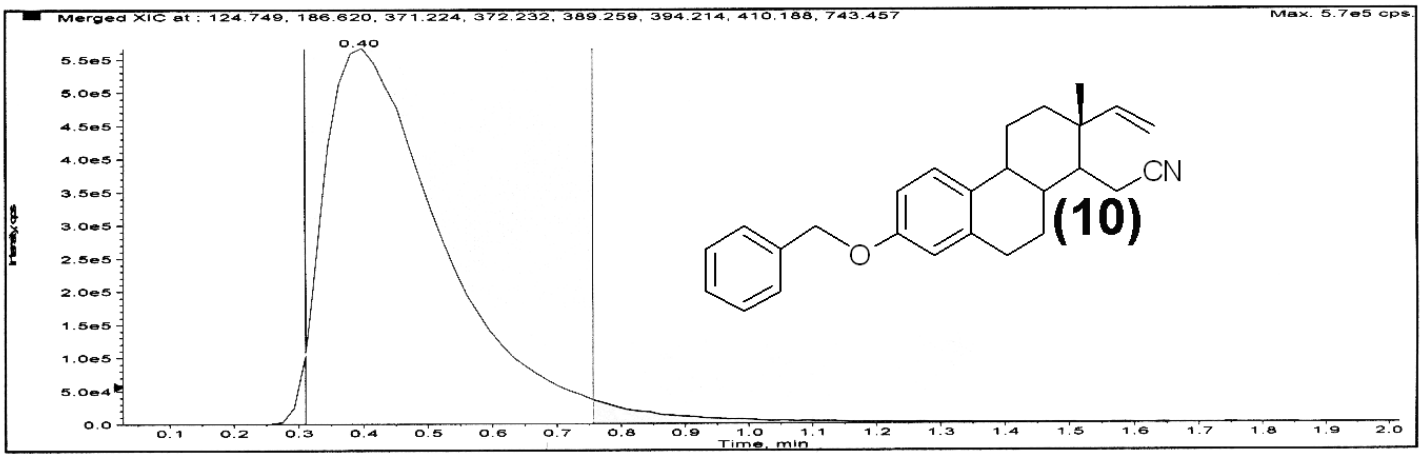
^{13}C NMR compound 10



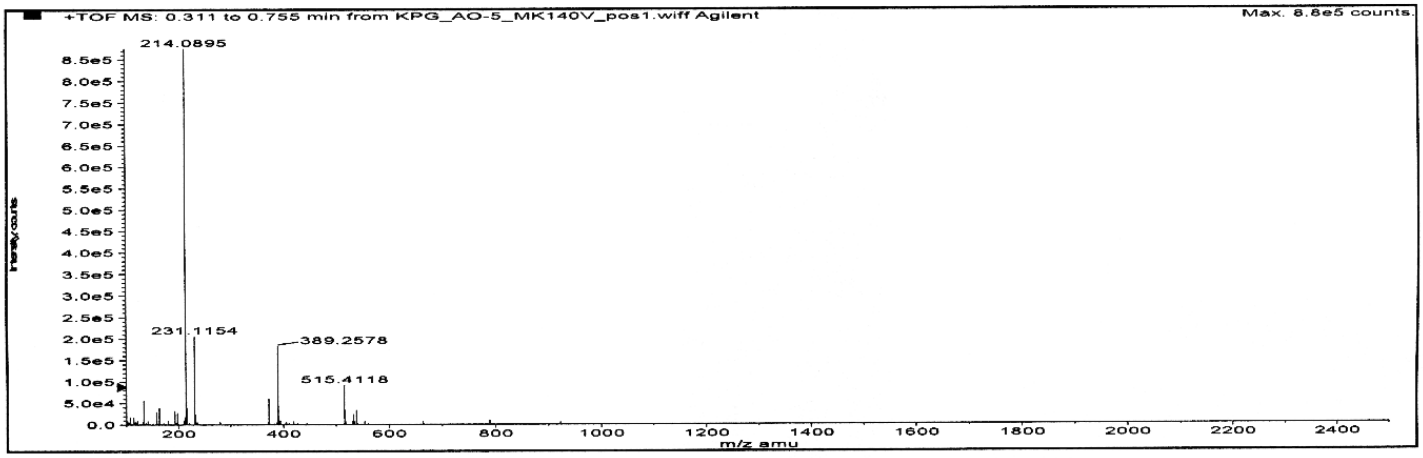
IR compound 10

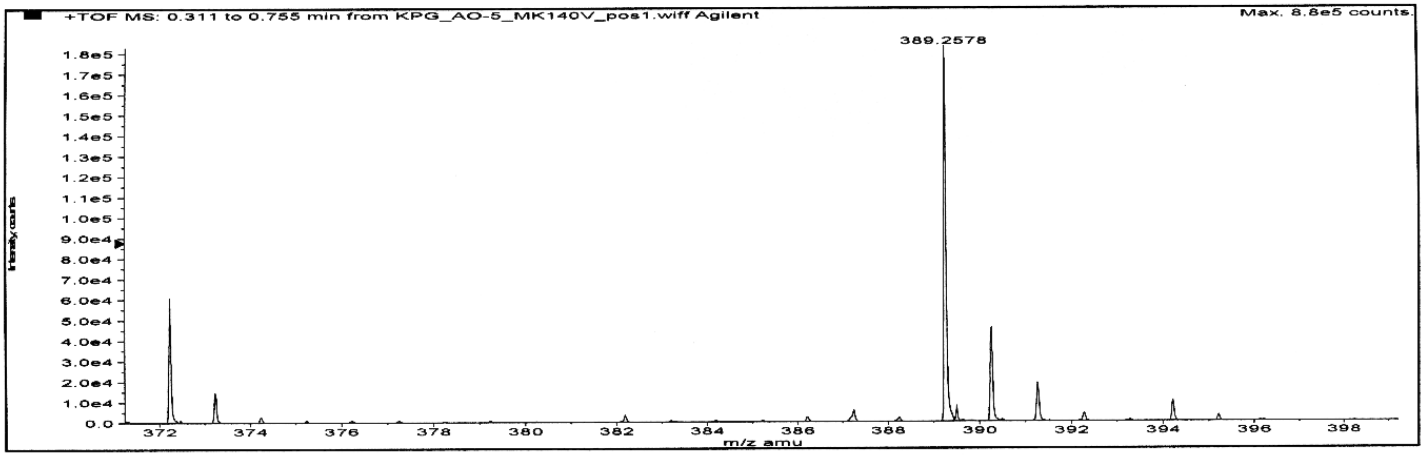


HRMS compound 10



Merged XIC, Period# : 1 Experiment# : 1

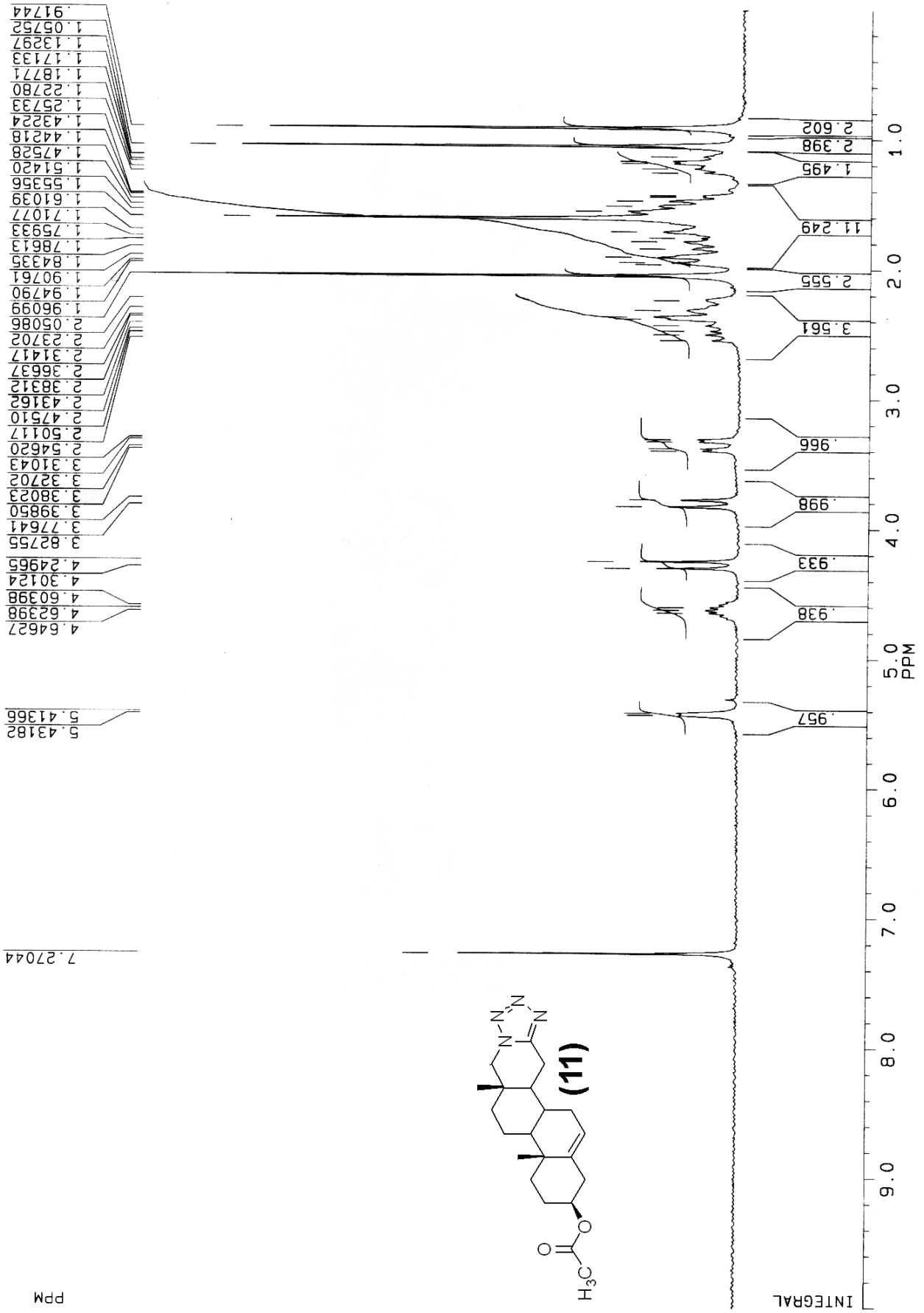




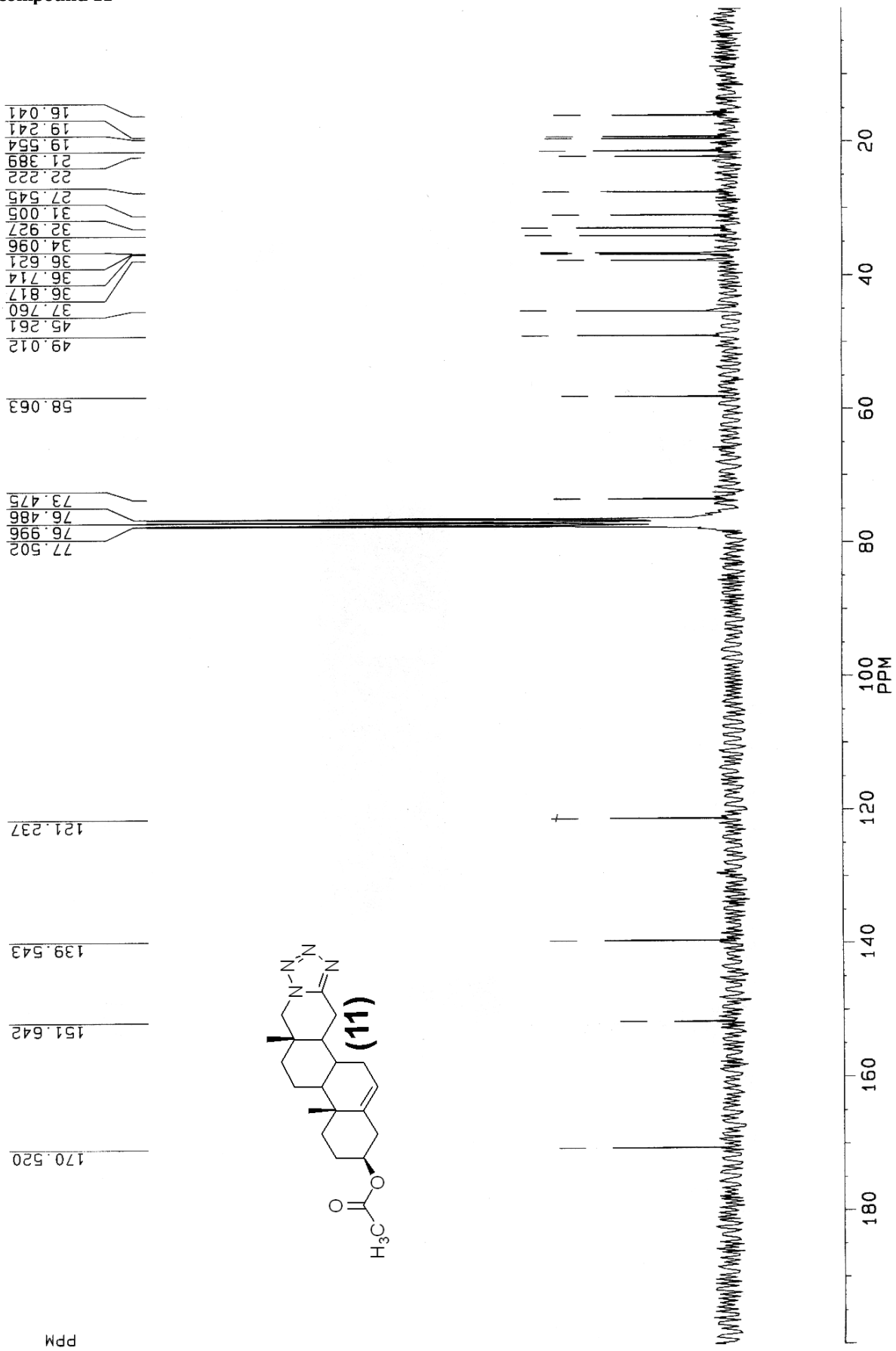
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C26H29NO	--	371.22491	0.40	7.32390 E6	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H]+	61058.33	372.23219	372.23144	-0.75094	-2.02	--
[M+NH4]+	186354.32	389.25874	389.25778	-0.95616	-2.46	--
[M+Na]+	10806.16	394.21414	394.21371	-0.42151	-1.07	--

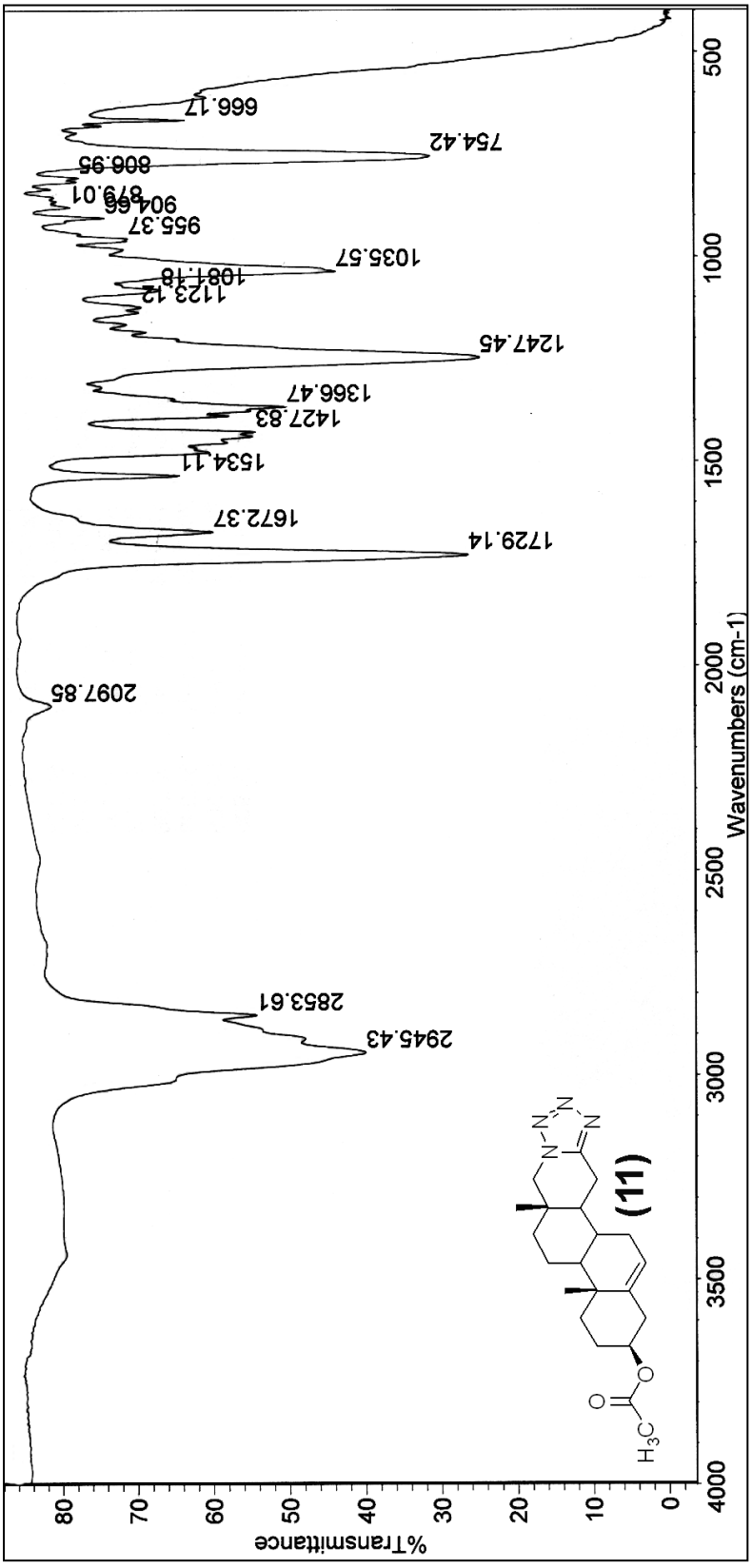
^{1}H-NMR compound 11



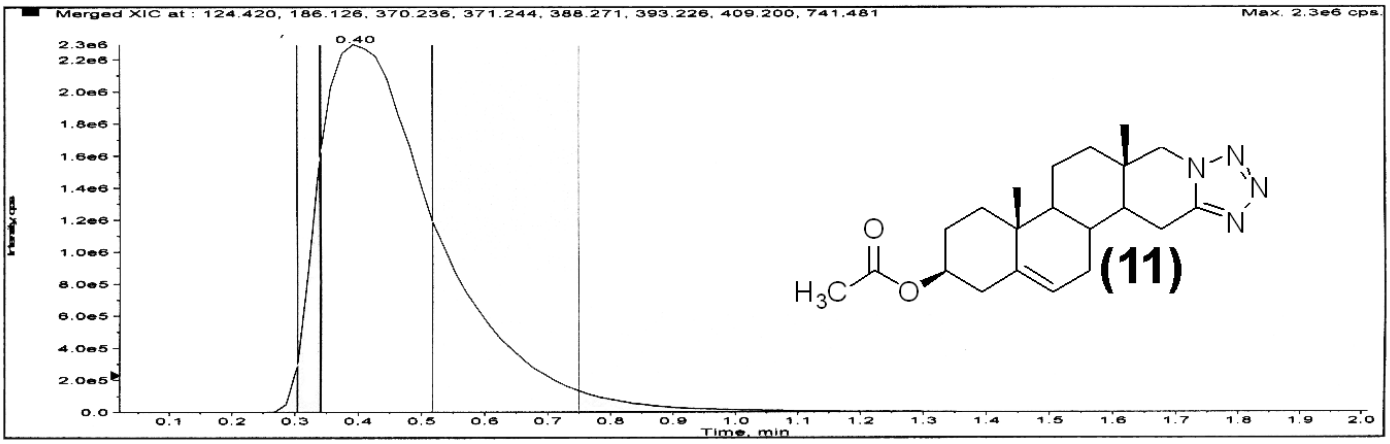
^{13}C NMR compound 11



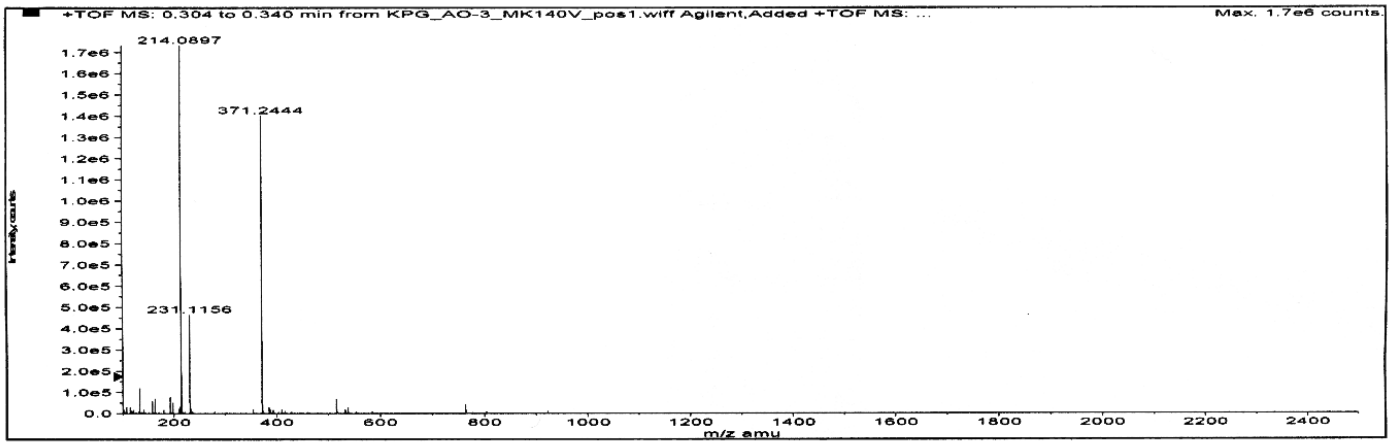
IR compound 11

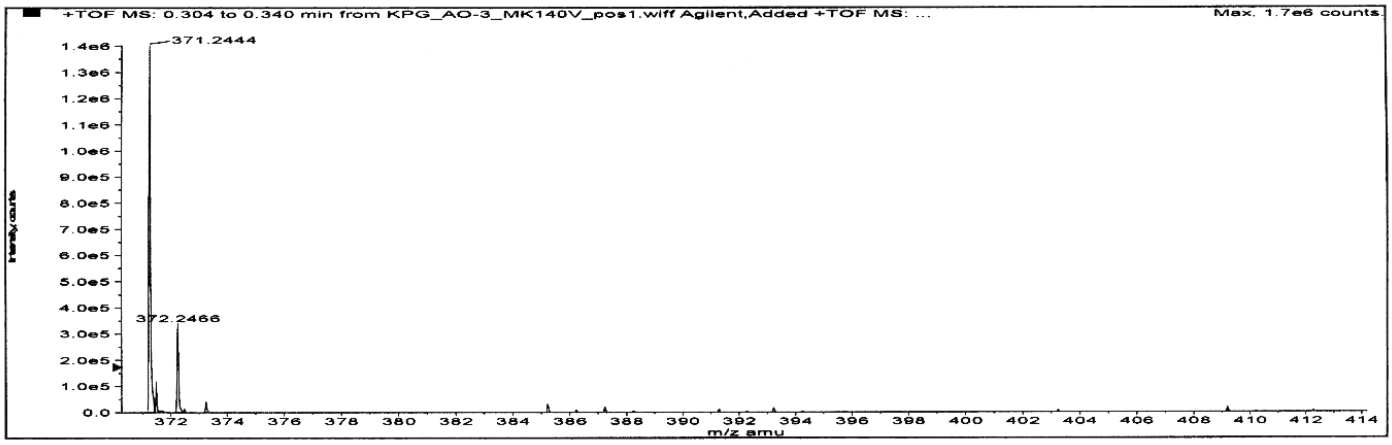


HRMS compound 11



Merged XIC, Period# : 1 Experiment# : 1

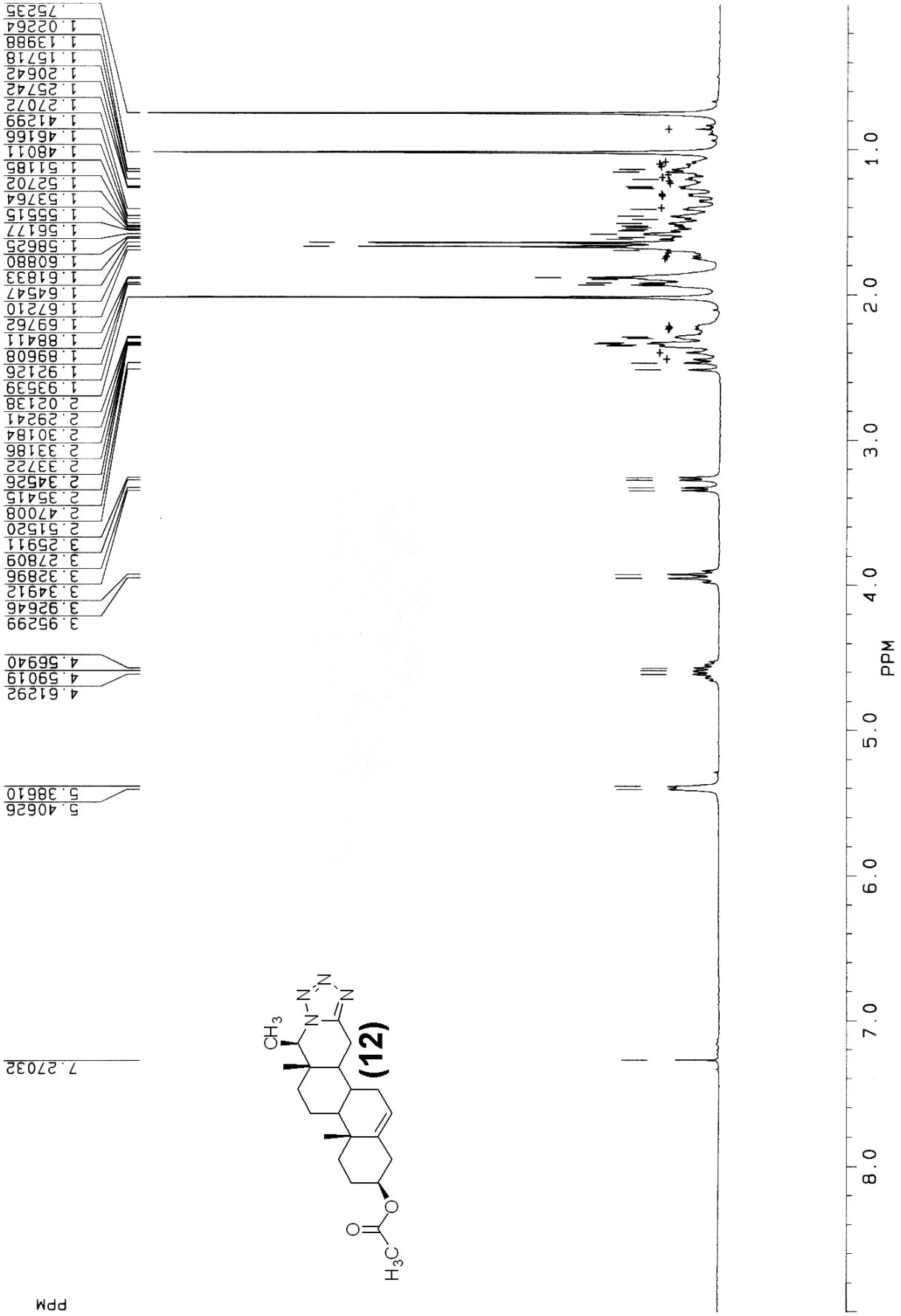




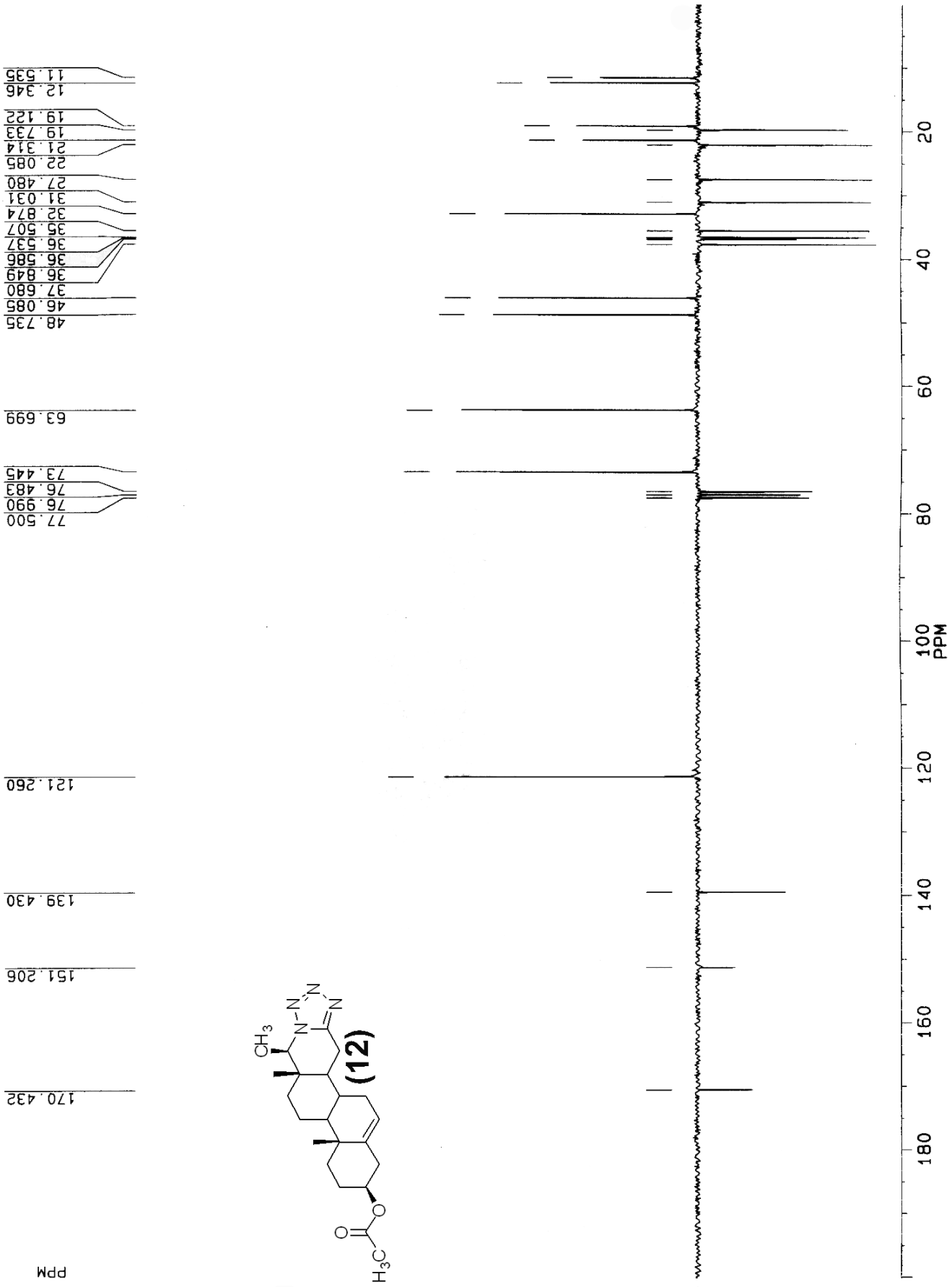
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C21H30N4O2	--	370.23688	0.40	3.03955 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H]+	1468803.43	371.24415	371.24438	0.22275	0.60	--
[M+Na]+	18249.65	393.22610	393.22639	0.29182	0.74	--
[M+K]+	19375.21	409.20003	409.20001	-0.02679	-0.07	--

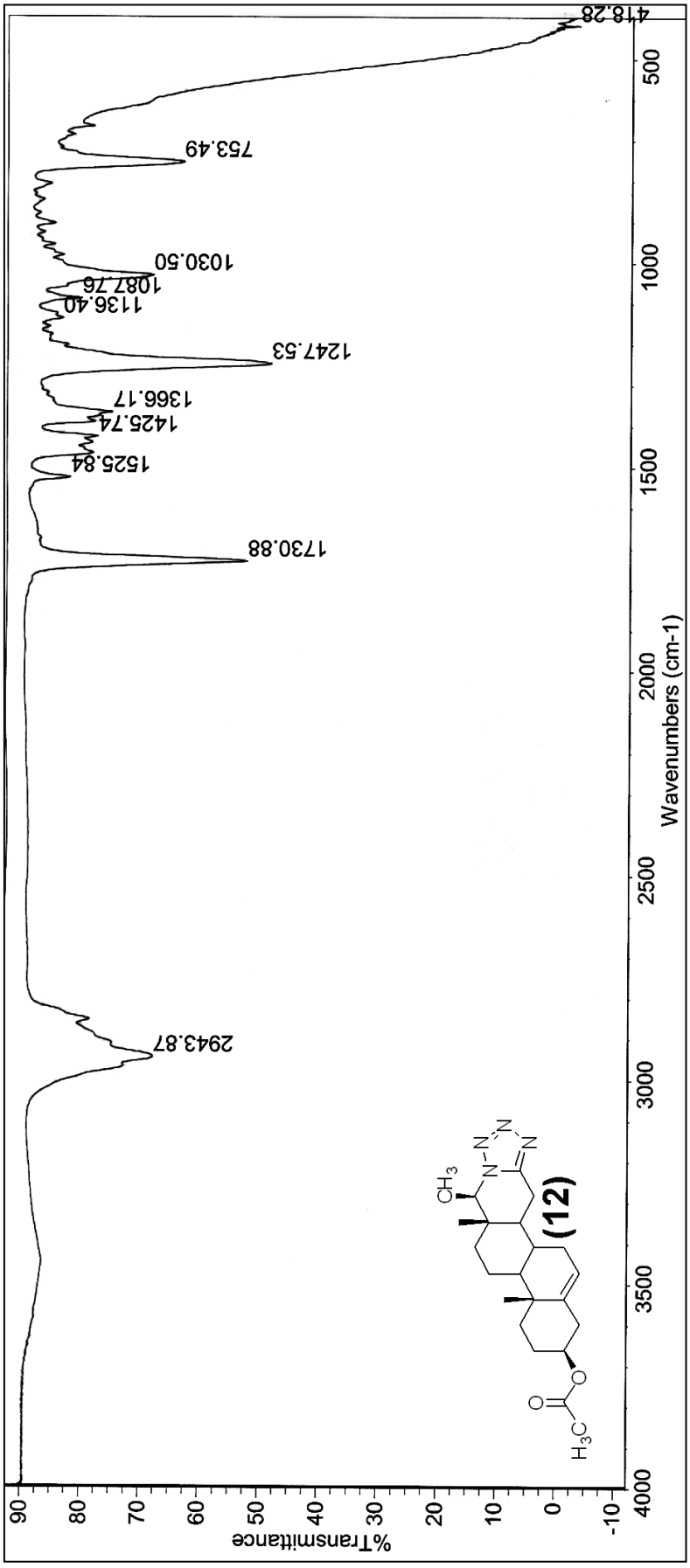
^{1}H NMR compound 12



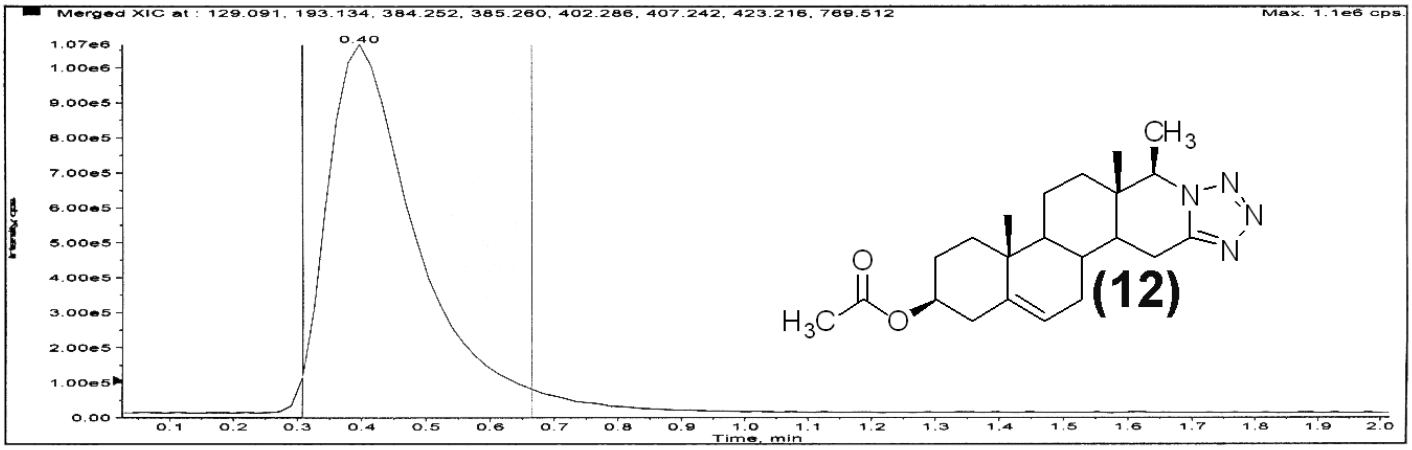
^{13}C NMR compound 12



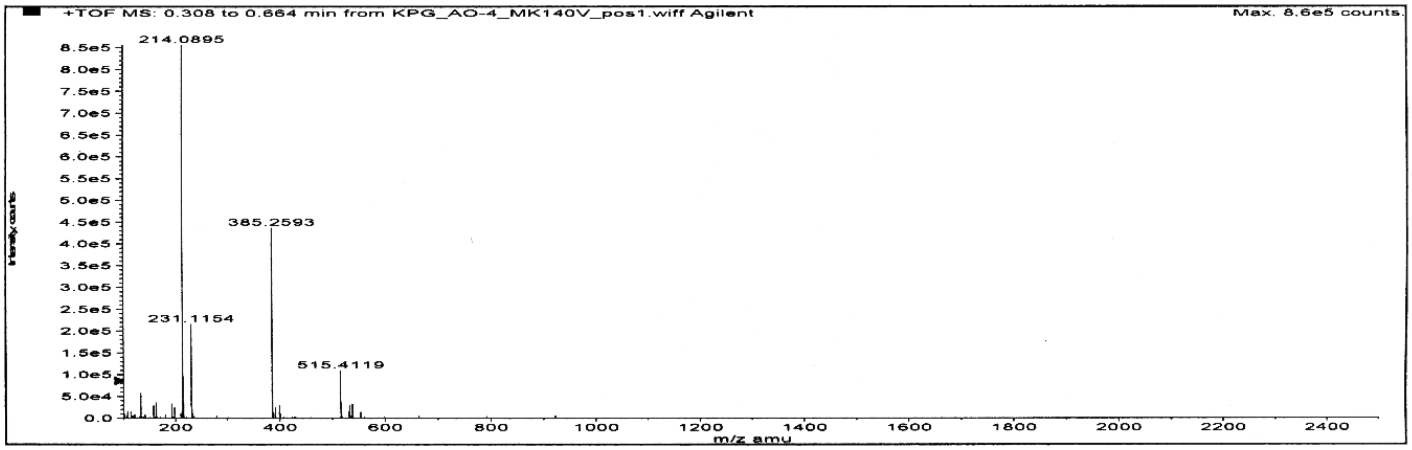
IR compound 12

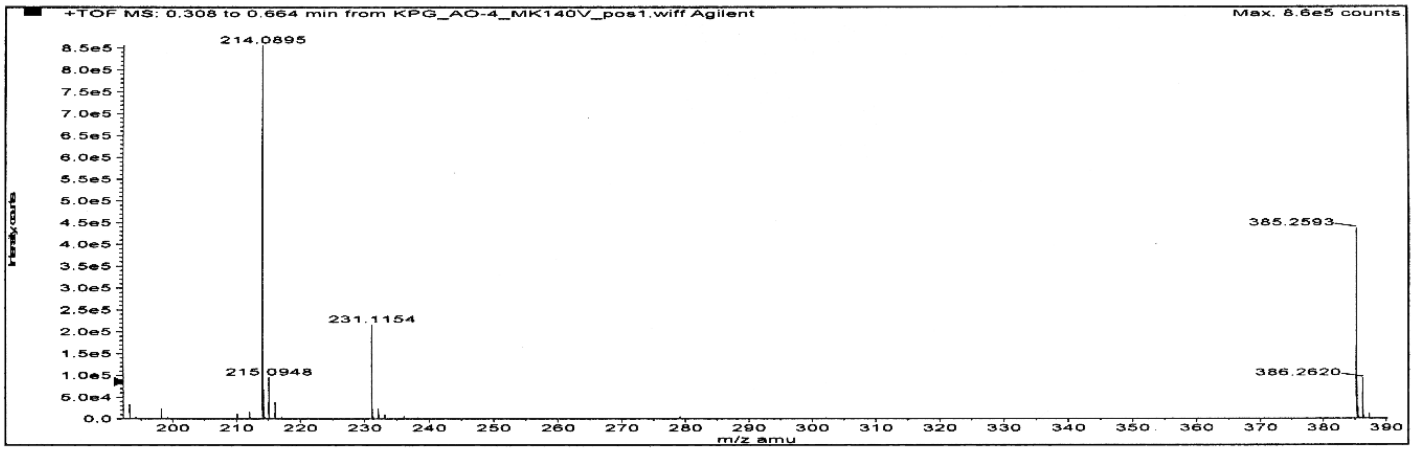


HRMS compound 12



Merged XIC, Period# : 1 Experiment# : 1

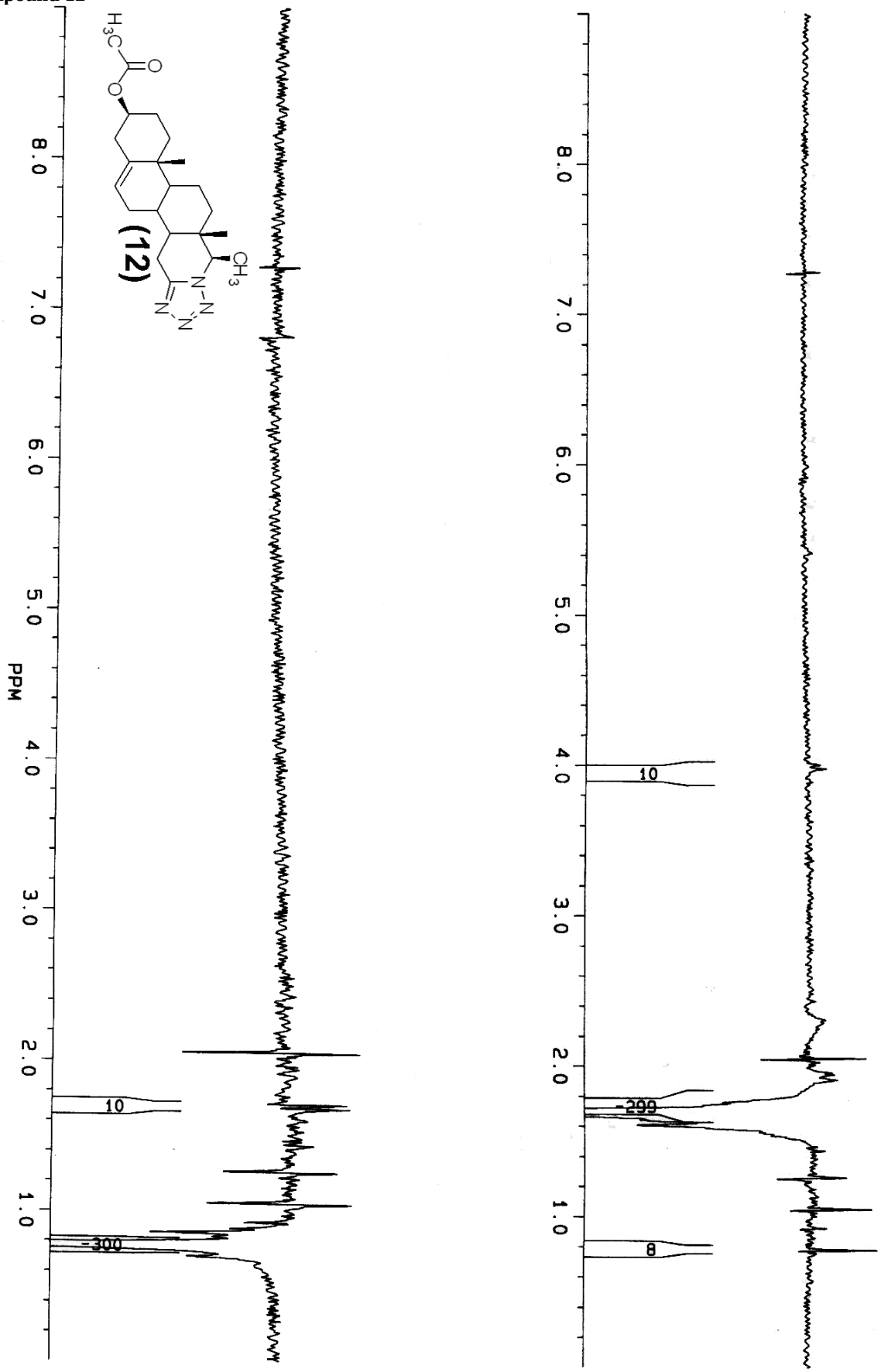




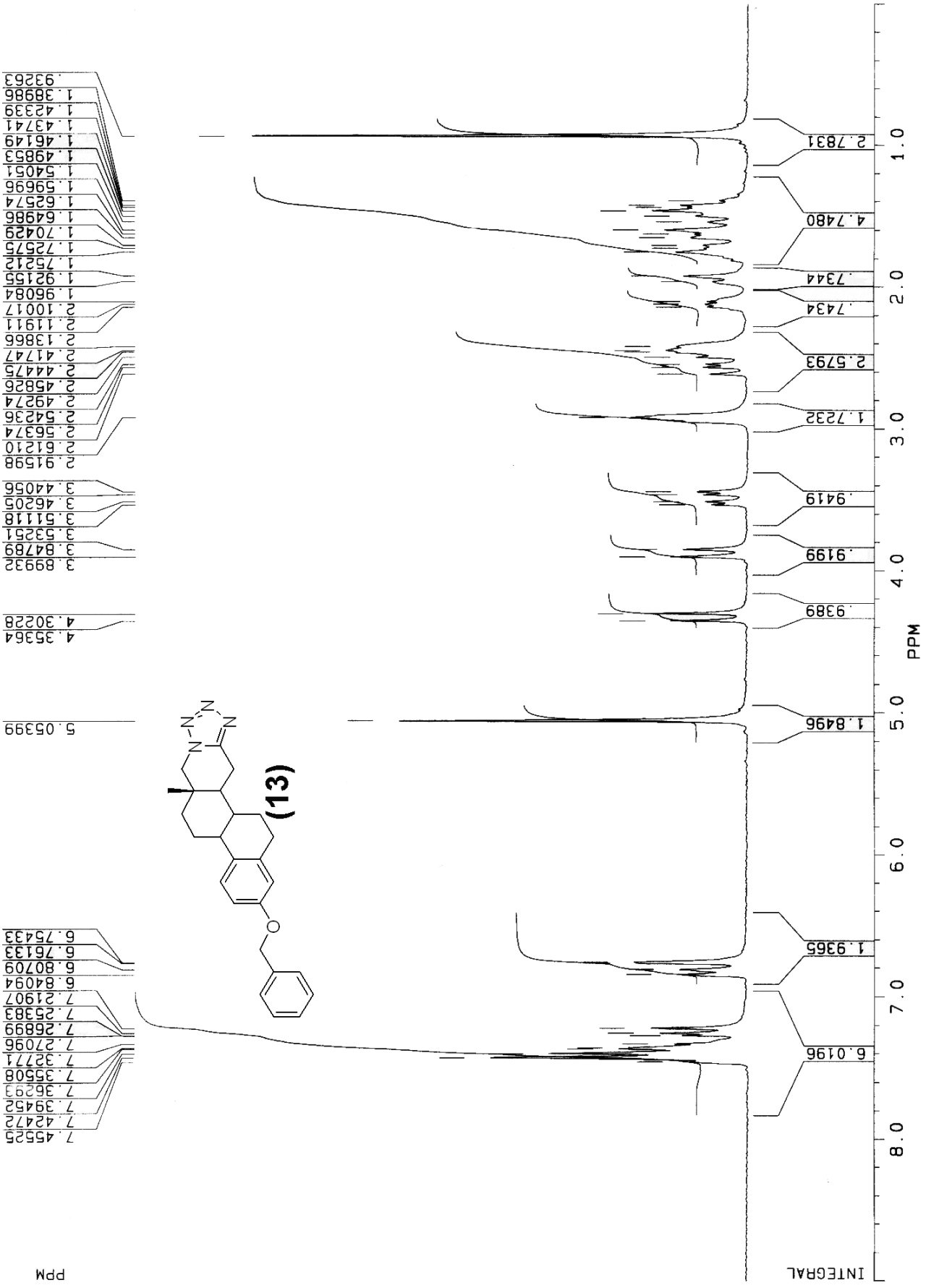
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C22H32N4O2	--	384.25253	0.40	1.02912 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+2H]2+	35683.33	193.13354	193.14292	9.38031	48.57	--
[M+H]+	437176.46	385.25980	385.25933	-0.46956	-1.22	--

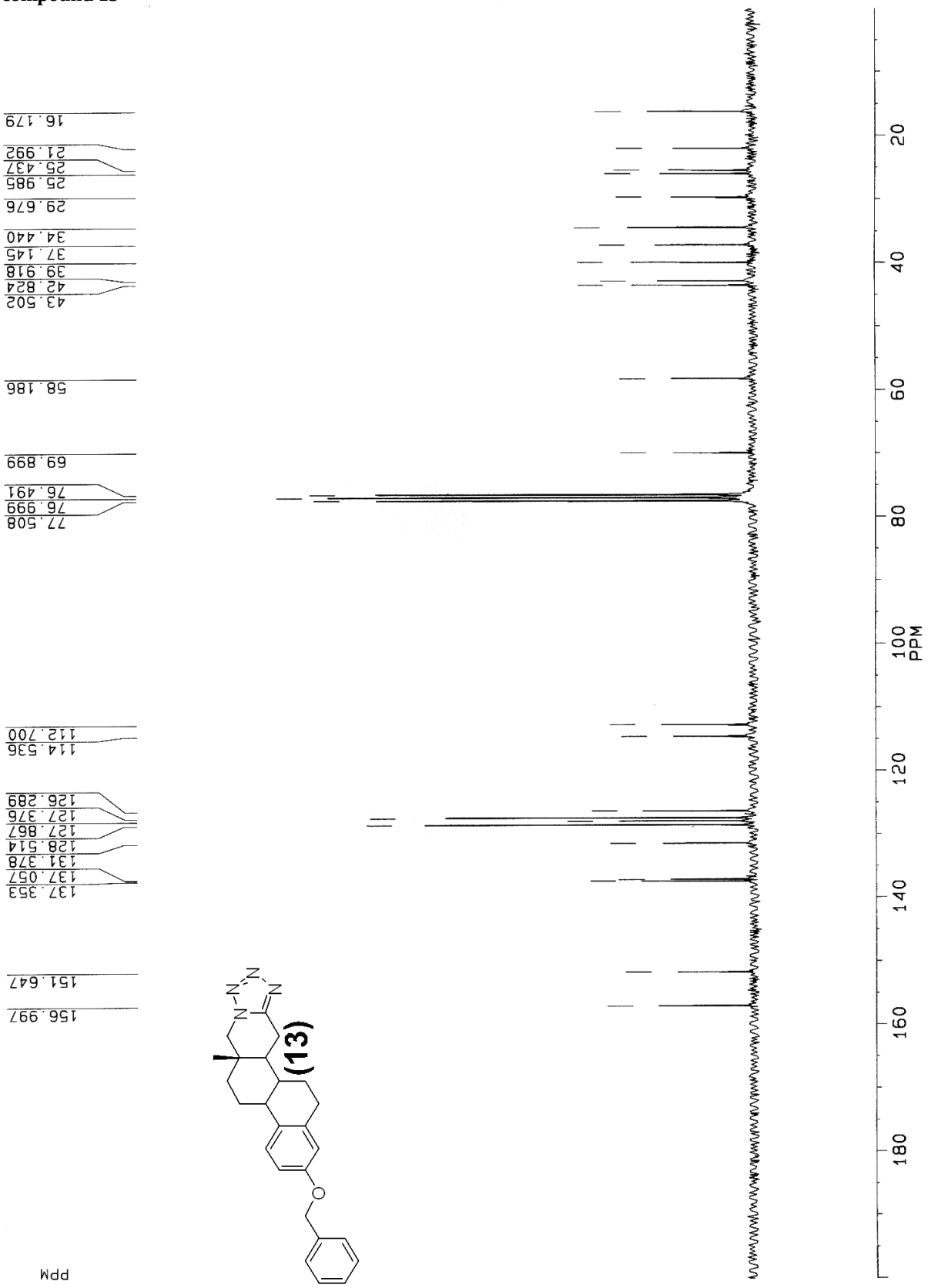
^{1}H NOE compound 12



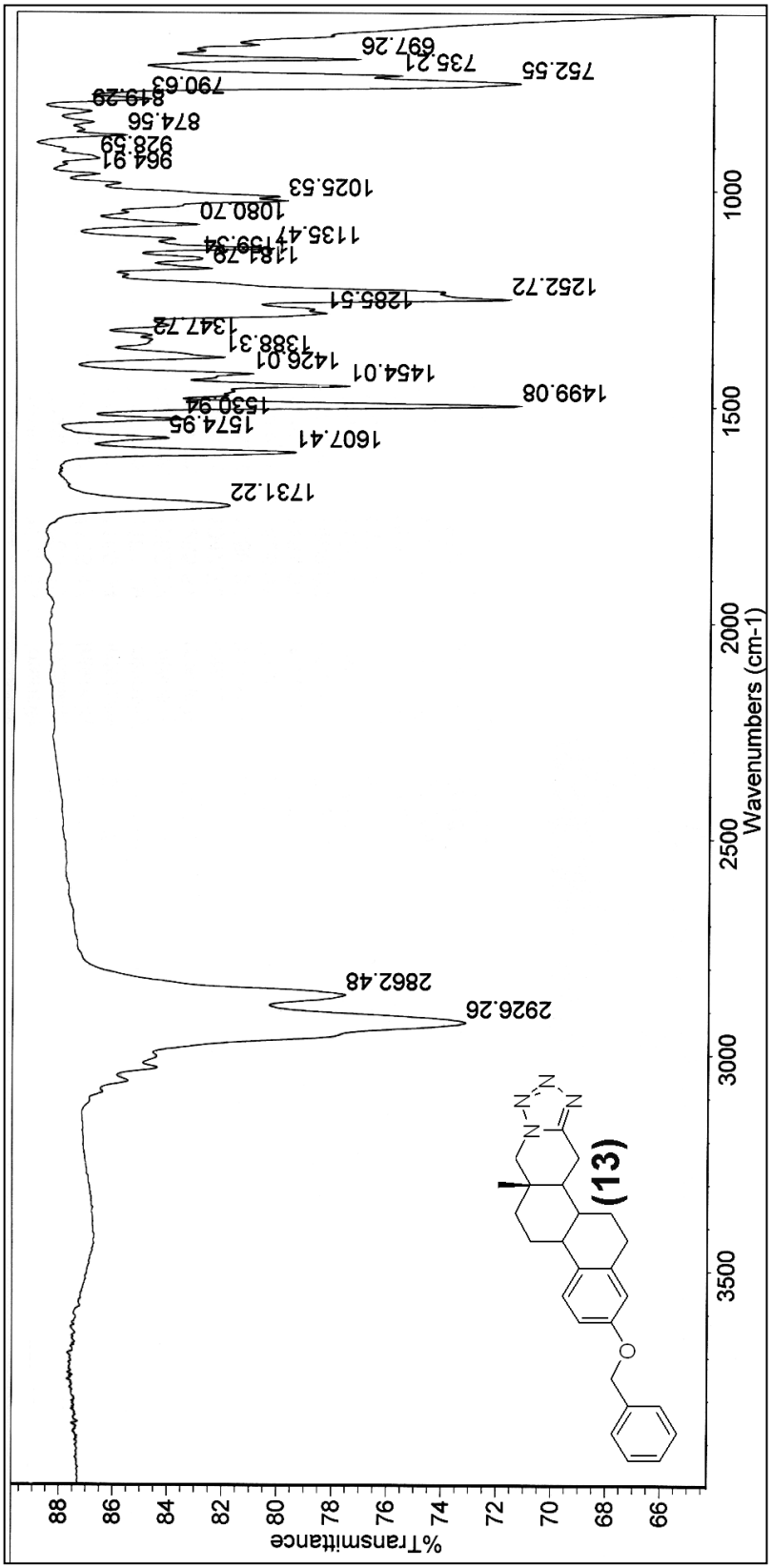
^{1}H NMR compound 13



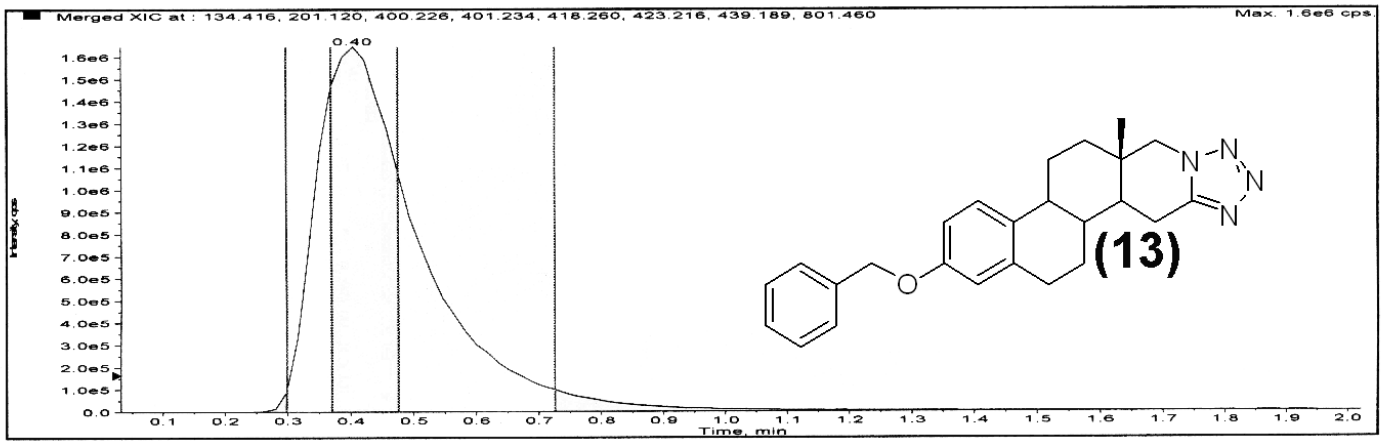
^{13}C NMR compound 13



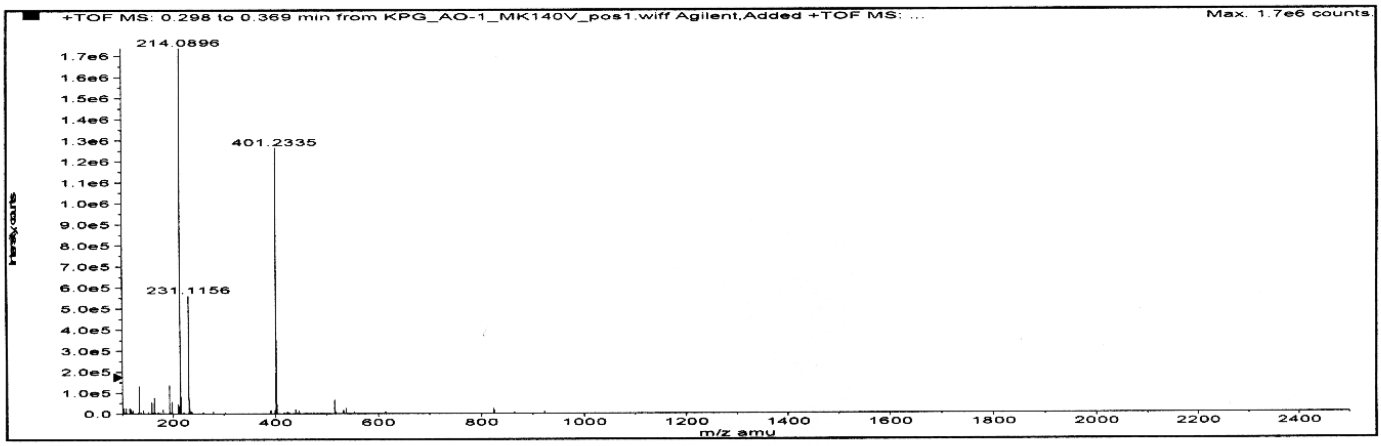
IR compound 13

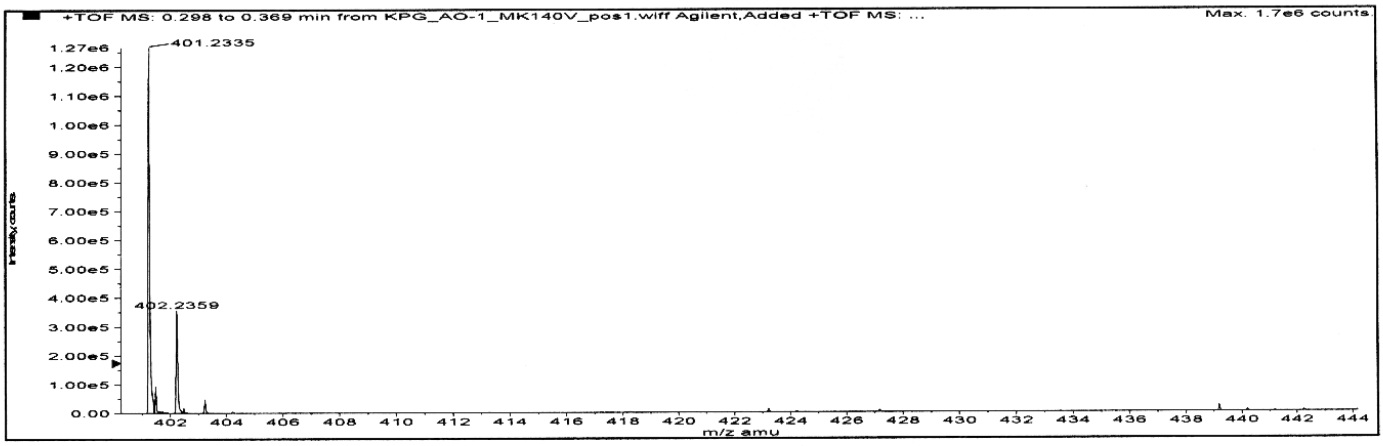


HRMS compound 13



Merged XIC, Period# : 1 Experiment# : 1

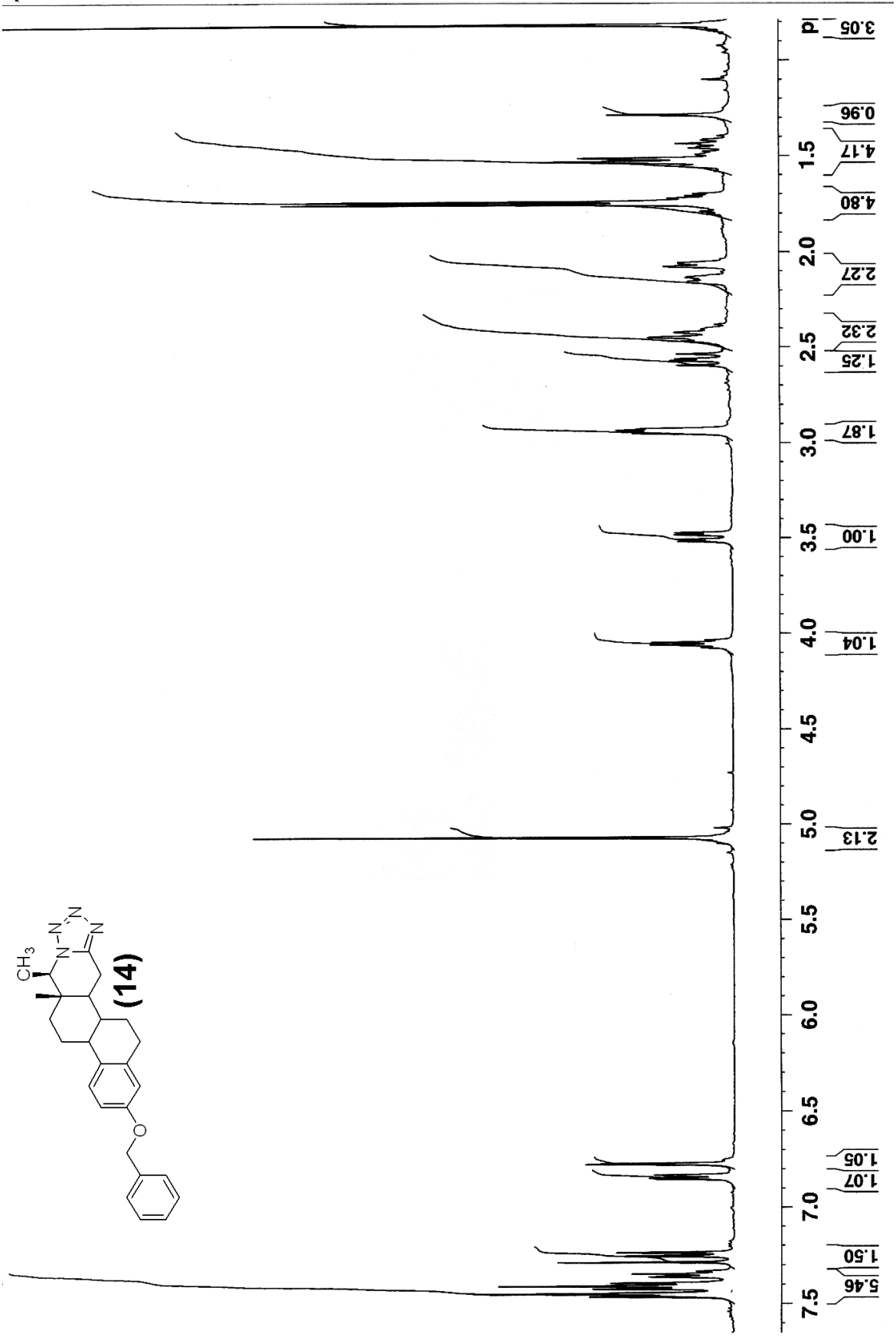




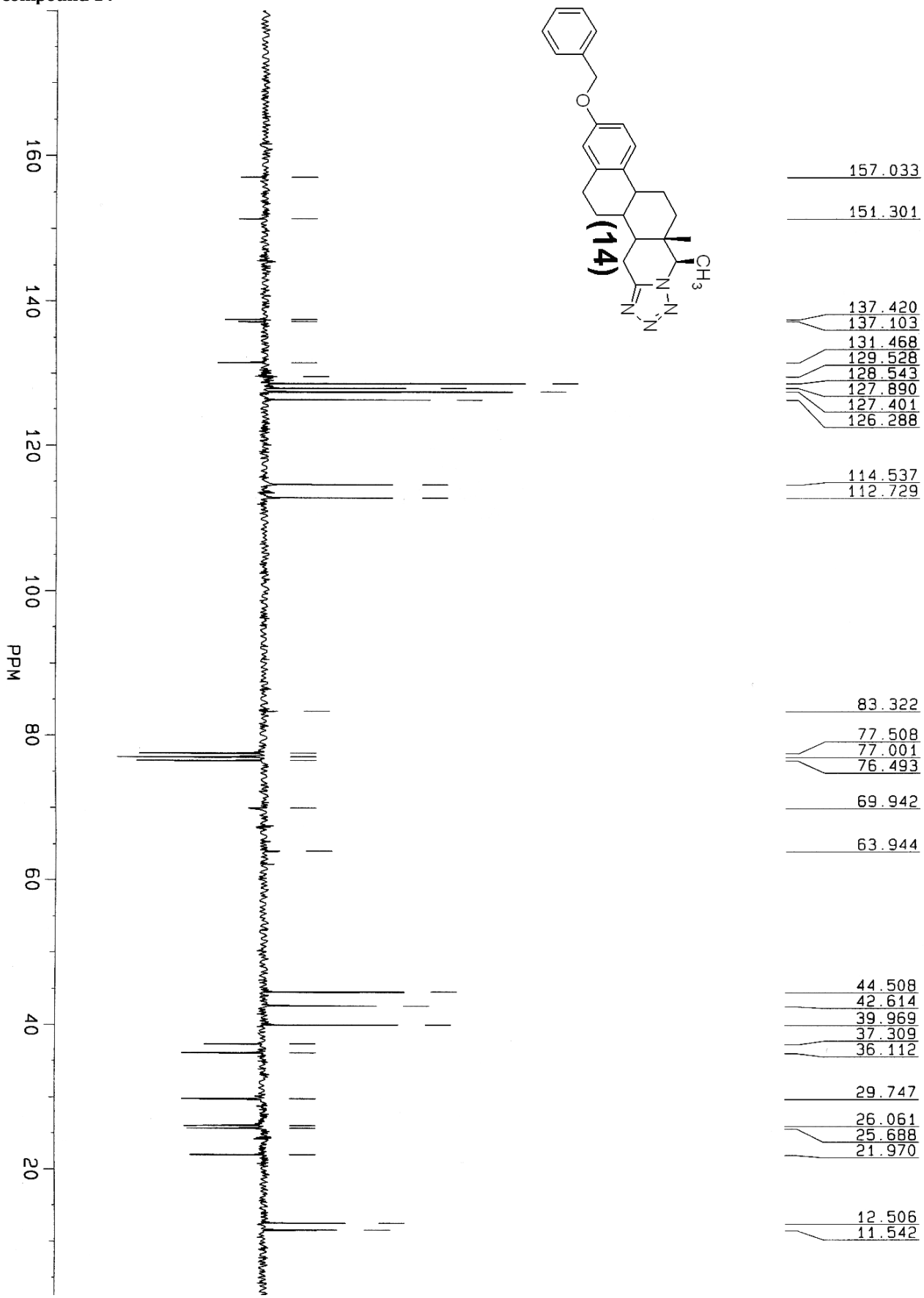
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C25H28N4O	--	400.22631	0.40	1.89047 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H]+	1294851.84	401.23359	401.23348	-0.11068	-0.28	--
[M+K]+	22057.92	439.18947	439.18872	-0.74703	-1.70	--

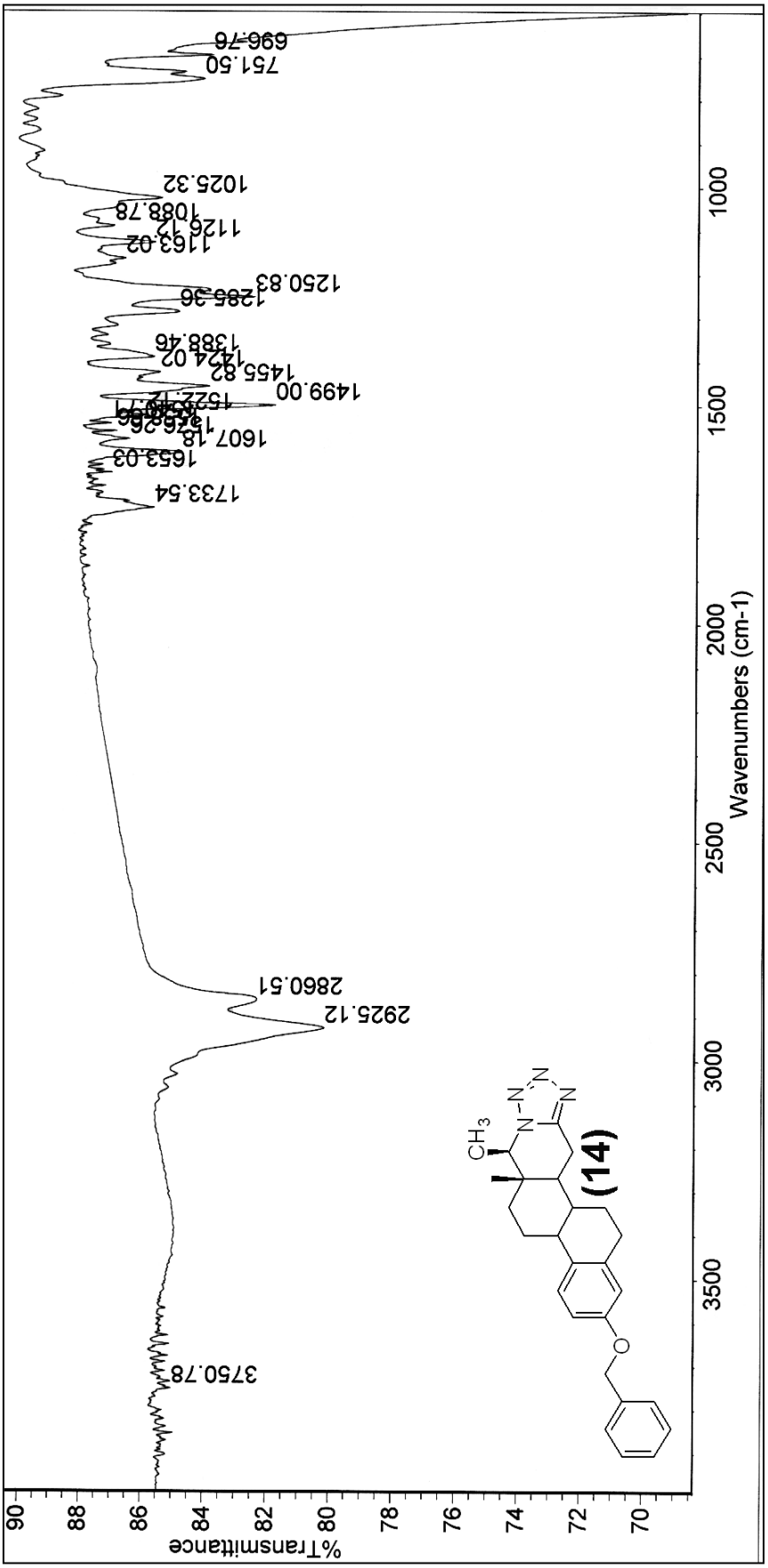
^{1}H NMR compound 14



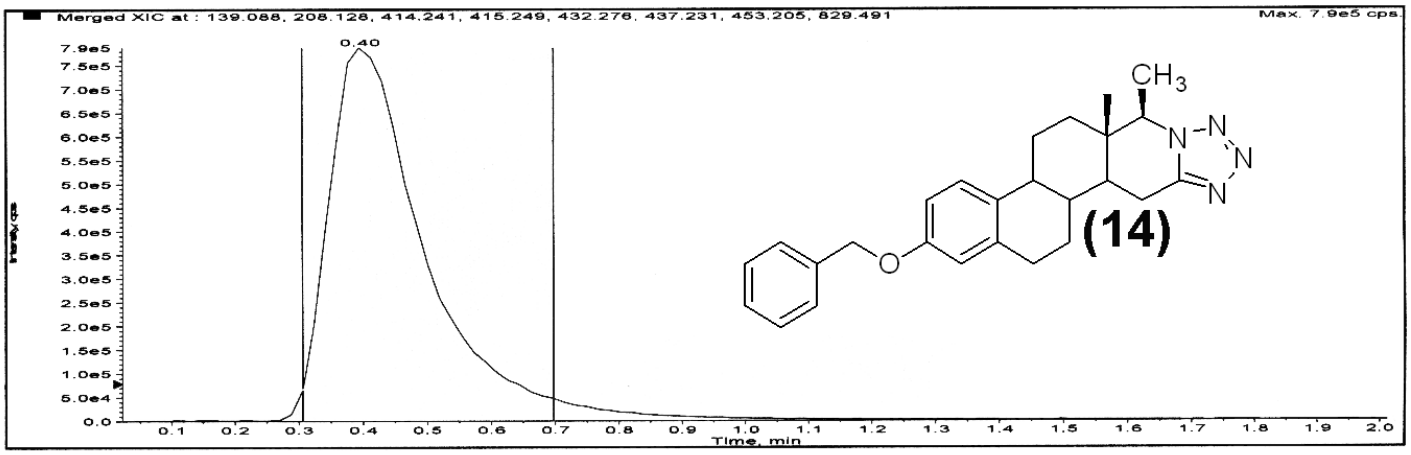
^{13}C NMR compound 14



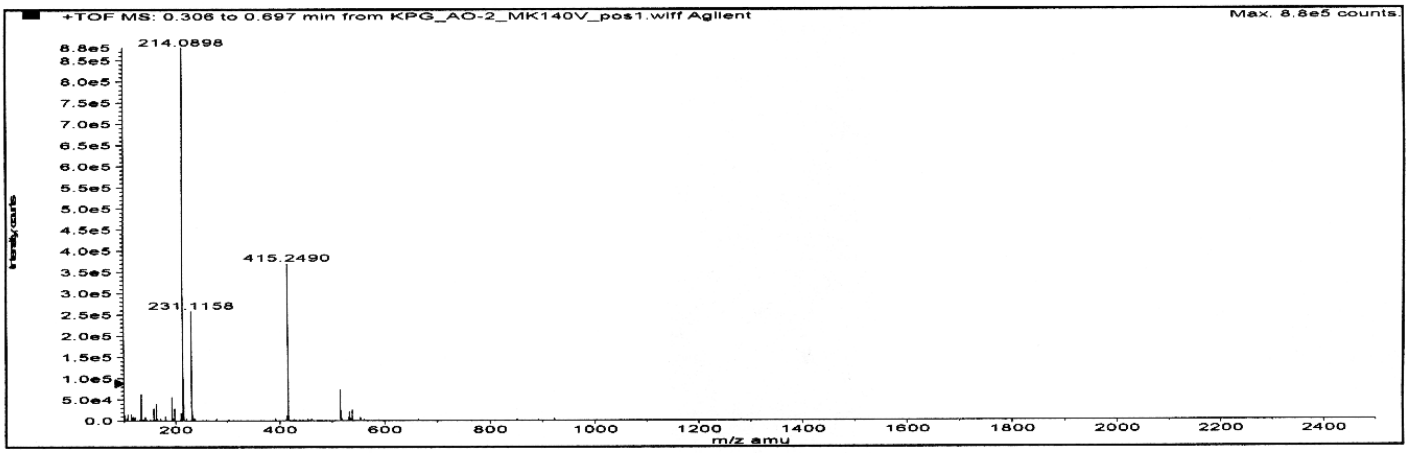
IR compound 14

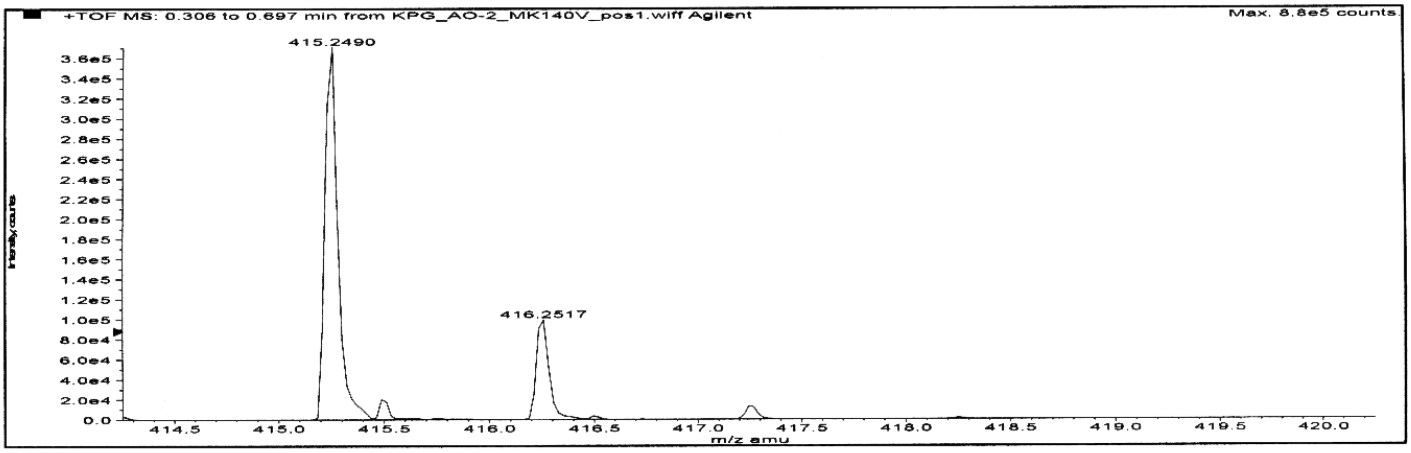


HRMS compound 14



Merged XIC, Period# : 1 Experiment# : 1

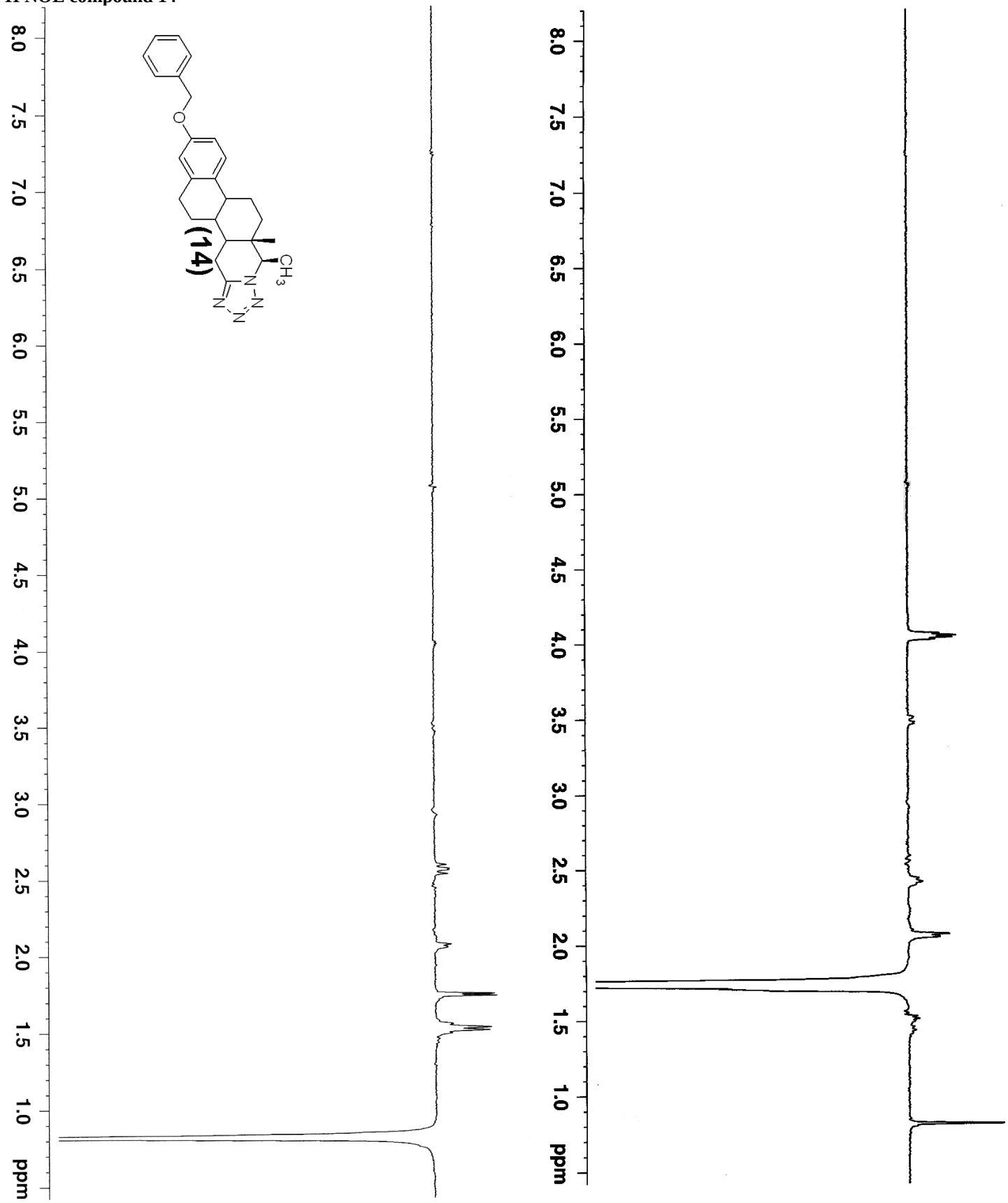




Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C26H30N4O	--	414.24196	0.40	8.10611 E6	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H]+	376726.79	415.24924	415.24895	-0.28721	-0.69	--

^{1}H NOE compound 14



X-ray crystal structure of compound 10

Table 1. Crystal data and structure refinement for **10**.

Identification code	Copound 10	
Empirical formula	C26 H29 N O	
Formula weight	371.50	
Temperature	293(2) K	
Wavelength	0.71069 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 10.984(5) Å	α= 90°
	b = 11.098(5) Å	β= 90°
	c = 17.391(5) Å	γ = 90°
Volume	2120.0(15) $Å^3$	
Z	4	
Density (calculated)	1.164 Mg/m^3	
Absorption coefficient	0.070 mm^{-1}	
F(000)	800	
Crystal size	0.293 x 0.158 x 0.098 mm^3	
Theta range for data collection	3.51 to 25.00°.	
Index ranges	-13<=h<=10, -13<=k<=12, -20<=l<=15	
Reflections collected	5383	
Independent reflections	3476 [R(int) = 0.0213]	
Completeness to theta = 25.00°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.99475	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3476 / 0 / 275	
Goodness-of-fit on F^2	0.804	
Final R indices [I>2sigma(I)]	R1 = 0.0361, wR2 = 0.0609	
R indices (all data)	R1 = 0.0987, wR2 = 0.0706	
Absolute structure parameter	0.7(18)	
Extinction coefficient	0.0011(4)	
Largest diff. peak and hole	0.086 and -0.070 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **10**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4664(2)	8427(1)	6550(1)	78(1)
C(8)	3902(2)	9189(2)	10220(1)	58(1)
C(10)	3605(2)	8430(2)	8853(1)	57(1)
C(4)	4763(2)	9337(2)	7827(1)	63(1)
C(9)	3142(3)	8393(2)	9674(1)	64(1)
C(1)	3205(2)	7579(2)	8324(2)	70(1)
C(5)	4384(2)	9323(2)	8595(1)	56(1)
C(6)	4854(2)	10290(2)	9128(1)	68(1)
C(2)	3580(2)	7596(2)	7570(2)	71(1)
C(3)	4358(2)	8480(2)	7318(1)	61(1)
C(14)	3313(3)	9234(2)	11018(1)	66(1)
C(7)	4095(2)	10418(2)	9854(1)	67(1)
C(21)	5689(3)	9029(2)	5425(1)	66(1)
C(20)	5504(2)	9298(2)	6259(1)	73(1)
C(26)	6785(3)	8665(2)	5143(2)	76(1)
C(13)	3121(3)	7982(2)	11389(1)	72(1)
C(11)	3002(3)	7146(2)	10011(1)	85(1)
C(15)	3924(3)	10139(2)	11571(1)	77(1)
C(17)	2299(4)	8129(3)	12087(2)	95(1)
C(16)	5238(3)	10048(2)	11608(2)	76(1)
C(25)	6952(3)	8433(2)	4371(2)	89(1)
C(24)	6008(4)	8603(3)	3875(2)	96(1)
N(1)	6260(3)	9988(2)	11640(2)	114(1)
C(12)	2432(3)	7188(2)	10804(1)	93(1)
C(18)	2490(4)	7837(3)	12784(3)	110(1)
C(19)	4320(3)	7373(2)	11604(1)	92(1)
C(22)	4759(3)	9164(3)	4920(2)	106(1)
C(23)	4912(4)	8958(3)	4143(2)	117(1)

Table 3. Bond lengths [Å] and angles [°] for **10**.

O(1)-C(3)	1.379(2)
O(1)-C(20)	1.429(3)
C(8)-C(7)	1.519(3)
C(8)-C(14)	1.532(3)
C(8)-C(9)	1.542(3)
C(8)-H(8)	0.9800
C(10)-C(5)	1.384(3)
C(10)-C(1)	1.390(3)
C(10)-C(9)	1.517(3)
C(4)-C(3)	1.373(3)
C(4)-C(5)	1.398(3)
C(4)-H(4)	0.9300
C(9)-C(11)	1.510(3)
C(9)-H(99)	0.941(19)
C(1)-C(2)	1.375(3)
C(1)-H(1)	0.9300
C(5)-C(6)	1.509(3)
C(6)-C(7)	1.519(3)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(2)-C(3)	1.373(3)
C(2)-H(2)	0.9300
C(14)-C(15)	1.544(3)
C(14)-C(13)	1.546(3)
C(14)-H(14)	0.946(17)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(21)-C(22)	1.356(3)
C(21)-C(26)	1.361(3)
C(21)-C(20)	1.494(3)
C(20)-H(20A)	0.9700
C(20)-H(20B)	0.9700
C(26)-C(25)	1.380(3)
C(26)-H(26)	0.9300
C(13)-C(17)	1.522(4)
C(13)-C(19)	1.528(3)
C(13)-C(12)	1.544(3)
C(11)-C(12)	1.516(3)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(15)-C(16)	1.448(4)
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(17)-C(18)	1.272(4)
C(17)-H(17)	0.97(3)
C(16)-N(1)	1.126(3)
C(25)-C(24)	1.362(4)
C(25)-H(25)	0.9300
C(24)-C(23)	1.349(4)
C(24)-H(24)	0.9300
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(18)-H(18A)	1.07(3)
C(18)-H(18B)	0.94(3)
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(22)-C(23)	1.380(3)

C(22)-H(22)	0.9300
C(23)-H(23)	0.9300
C(3)-O(1)-C(20)	118.17(18)
C(7)-C(8)-C(14)	114.16(18)
C(7)-C(8)-C(9)	109.42(18)
C(14)-C(8)-C(9)	110.29(19)
C(7)-C(8)-H(8)	107.6
C(14)-C(8)-H(8)	107.6
C(9)-C(8)-H(8)	107.6
C(5)-C(10)-C(1)	117.9(2)
C(5)-C(10)-C(9)	122.2(2)
C(1)-C(10)-C(9)	119.9(2)
C(3)-C(4)-C(5)	120.7(2)
C(3)-C(4)-H(4)	119.6
C(5)-C(4)-H(4)	119.6
C(11)-C(9)-C(10)	115.1(2)
C(11)-C(9)-C(8)	110.0(2)
C(10)-C(9)-C(8)	112.5(2)
C(11)-C(9)-H(99)	106.0(12)
C(10)-C(9)-H(99)	107.4(12)
C(8)-C(9)-H(99)	105.1(11)
C(2)-C(1)-C(10)	121.8(2)
C(2)-C(1)-H(1)	119.1
C(10)-C(1)-H(1)	119.1
C(10)-C(5)-C(4)	120.1(2)
C(10)-C(5)-C(6)	121.4(2)
C(4)-C(5)-C(6)	118.5(2)
C(5)-C(6)-C(7)	112.94(19)
C(5)-C(6)-H(6A)	109.0
C(7)-C(6)-H(6A)	109.0
C(5)-C(6)-H(6B)	109.0
C(7)-C(6)-H(6B)	109.0
H(6A)-C(6)-H(6B)	107.8
C(3)-C(2)-C(1)	120.0(2)
C(3)-C(2)-H(2)	120.0
C(1)-C(2)-H(2)	120.0
C(2)-C(3)-C(4)	119.4(2)
C(2)-C(3)-O(1)	115.4(2)
C(4)-C(3)-O(1)	125.1(2)
C(8)-C(14)-C(15)	113.6(2)
C(8)-C(14)-C(13)	114.01(19)
C(15)-C(14)-C(13)	112.6(2)
C(8)-C(14)-H(14)	107.2(11)
C(15)-C(14)-H(14)	103.5(11)
C(13)-C(14)-H(14)	104.8(11)
C(6)-C(7)-C(8)	109.90(18)
C(6)-C(7)-H(7A)	109.7
C(8)-C(7)-H(7A)	109.7
C(6)-C(7)-H(7B)	109.7
C(8)-C(7)-H(7B)	109.7
H(7A)-C(7)-H(7B)	108.2
C(22)-C(21)-C(26)	117.7(2)
C(22)-C(21)-C(20)	120.3(3)
C(26)-C(21)-C(20)	122.0(3)
O(1)-C(20)-C(21)	107.26(19)
O(1)-C(20)-H(20A)	110.3
C(21)-C(20)-H(20A)	110.3
O(1)-C(20)-H(20B)	110.3
C(21)-C(20)-H(20B)	110.3

H(20A)-C(20)-H(20B)	108.5
C(21)-C(26)-C(25)	121.6(3)
C(21)-C(26)-H(26)	119.2
C(25)-C(26)-H(26)	119.2
C(17)-C(13)-C(19)	111.3(2)
C(17)-C(13)-C(12)	107.3(2)
C(19)-C(13)-C(12)	109.4(2)
C(17)-C(13)-C(14)	108.5(2)
C(19)-C(13)-C(14)	112.5(2)
C(12)-C(13)-C(14)	107.7(2)
C(9)-C(11)-C(12)	111.5(2)
C(9)-C(11)-H(11A)	109.3
C(12)-C(11)-H(11A)	109.3
C(9)-C(11)-H(11B)	109.3
C(12)-C(11)-H(11B)	109.3
H(11A)-C(11)-H(11B)	108.0
C(16)-C(15)-C(14)	114.6(2)
C(16)-C(15)-H(15A)	108.6
C(14)-C(15)-H(15A)	108.6
C(16)-C(15)-H(15B)	108.6
C(14)-C(15)-H(15B)	108.6
H(15A)-C(15)-H(15B)	107.6
C(18)-C(17)-C(13)	129.5(4)
C(18)-C(17)-H(17)	118(2)
C(13)-C(17)-H(17)	112.7(19)
N(1)-C(16)-C(15)	179.4(3)
C(24)-C(25)-C(26)	119.2(3)
C(24)-C(25)-H(25)	120.4
C(26)-C(25)-H(25)	120.4
C(23)-C(24)-C(25)	120.1(3)
C(23)-C(24)-H(24)	120.0
C(25)-C(24)-H(24)	120.0
C(11)-C(12)-C(13)	114.5(2)
C(11)-C(12)-H(12A)	108.6
C(13)-C(12)-H(12A)	108.6
C(11)-C(12)-H(12B)	108.6
C(13)-C(12)-H(12B)	108.6
H(12A)-C(12)-H(12B)	107.6
C(17)-C(18)-H(18A)	118.8(16)
C(17)-C(18)-H(18B)	114.8(19)
H(18A)-C(18)-H(18B)	126(3)
C(13)-C(19)-H(19A)	109.5
C(13)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(13)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(21)-C(22)-C(23)	121.6(3)
C(21)-C(22)-H(22)	119.2
C(23)-C(22)-H(22)	119.2
C(24)-C(23)-C(22)	119.7(3)
C(24)-C(23)-H(23)	120.2
C(22)-C(23)-H(23)	120.2

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **10**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	87(1)	82(1)	66(1)	-13(1)	5(1)	-14(1)
C(8)	59(2)	51(1)	65(2)	-1(1)	2(1)	4(1)
C(10)	54(2)	49(1)	68(2)	-4(1)	-2(1)	-2(1)
C(4)	64(2)	55(1)	69(2)	-5(1)	3(2)	-5(1)
C(9)	63(2)	60(2)	70(2)	-1(1)	-2(2)	2(2)
C(1)	68(2)	66(2)	77(2)	-2(2)	0(2)	-16(1)
C(5)	55(2)	49(1)	64(2)	-5(1)	-1(1)	2(1)
C(6)	79(2)	52(1)	71(2)	-6(1)	4(2)	-5(1)
C(2)	68(2)	73(2)	72(2)	-16(1)	-6(2)	-15(2)
C(3)	63(2)	63(2)	58(2)	-8(1)	2(1)	-2(2)
C(14)	58(2)	67(2)	73(2)	1(1)	-2(2)	6(2)
C(7)	85(2)	52(1)	65(2)	-6(1)	4(2)	1(1)
C(21)	71(2)	61(1)	67(2)	-4(1)	0(2)	3(2)
C(20)	82(2)	67(2)	71(2)	-9(1)	7(2)	-4(2)
C(26)	73(2)	83(2)	71(2)	-6(1)	3(2)	-15(2)
C(13)	76(2)	66(2)	75(2)	8(1)	3(2)	-2(2)
C(11)	105(2)	72(2)	79(2)	-2(2)	-1(2)	-27(2)
C(15)	98(2)	61(2)	71(2)	-6(1)	13(2)	5(2)
C(17)	110(3)	105(2)	68(2)	22(2)	15(2)	-7(2)
C(16)	92(2)	69(2)	68(2)	-14(1)	7(2)	-14(2)
C(25)	87(2)	92(2)	87(2)	-11(2)	24(2)	-20(2)
C(24)	126(3)	99(2)	62(2)	-2(2)	2(2)	-8(2)
N(1)	98(2)	107(2)	137(2)	-20(2)	-2(2)	-22(2)
C(12)	110(2)	89(2)	81(2)	9(2)	1(2)	-34(2)
C(18)	116(3)	114(3)	99(3)	9(2)	22(3)	-7(3)
C(19)	110(2)	71(2)	96(2)	13(2)	-5(2)	3(2)
C(22)	89(2)	152(3)	78(2)	-28(2)	-8(2)	37(2)
C(23)	118(3)	153(3)	82(2)	-10(2)	-22(2)	35(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **10**.

	x	y	z	U(eq)
H(8)	4703	8810	10276	70
H(4)	5295	9934	7660	75
H(1)	2669	6981	8485	84
H(6A)	4860	11054	8857	81
H(6B)	5686	10101	9270	81
H(2)	3307	7008	7230	85
H(7A)	3314	10774	9729	81
H(7B)	4508	10946	10214	81
H(20A)	6271	9245	6533	88
H(20B)	5180	10105	6323	88
H(26)	7437	8572	5479	91
H(11A)	3794	6764	10043	102
H(11B)	2495	6663	9673	102
H(15A)	3710	10949	11411	92
H(15B)	3596	10017	12082	92
H(25)	7701	8163	4191	107
H(24)	6118	8475	3351	115
H(12A)	2387	6373	11005	112
H(12B)	1605	7487	10757	112
H(19A)	4159	6583	11804	138
H(19B)	4731	7845	11987	138
H(19C)	4826	7307	11155	138
H(22)	3999	9401	5101	127
H(23)	4264	9063	3806	141
H(14)	2519(17)	9549(15)	10954(10)	47(6)
H(99)	2359(18)	8735(16)	9677(11)	54(7)
H(17)	1540(30)	8550(30)	11967(18)	149(15)
H(18A)	1780(30)	7990(20)	13199(17)	133(12)
H(18B)	3280(30)	7570(30)	12889(17)	115(13)

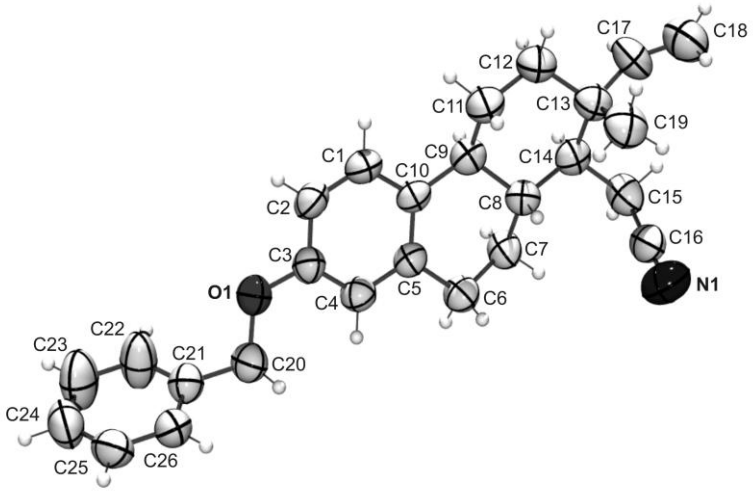
Table 6. Torsion angles [°] for **10**.

C(5)-C(10)-C(9)-C(11)	-143.9(2)
C(1)-C(10)-C(9)-C(11)	39.0(3)
C(5)-C(10)-C(9)-C(8)	-16.8(3)
C(1)-C(10)-C(9)-C(8)	166.0(2)
C(7)-C(8)-C(9)-C(11)	176.9(2)
C(14)-C(8)-C(9)-C(11)	-56.7(3)
C(7)-C(8)-C(9)-C(10)	47.2(3)
C(14)-C(8)-C(9)-C(10)	173.5(2)
C(5)-C(10)-C(1)-C(2)	1.2(3)
C(9)-C(10)-C(1)-C(2)	178.5(2)
C(1)-C(10)-C(5)-C(4)	-1.2(3)
C(9)-C(10)-C(5)-C(4)	-178.4(2)
C(1)-C(10)-C(5)-C(6)	179.4(2)
C(9)-C(10)-C(5)-C(6)	2.2(3)
C(3)-C(4)-C(5)-C(10)	0.9(3)
C(3)-C(4)-C(5)-C(6)	-179.7(2)
C(10)-C(5)-C(6)-C(7)	-18.7(3)
C(4)-C(5)-C(6)-C(7)	161.91(19)
C(10)-C(1)-C(2)-C(3)	-0.9(4)
C(1)-C(2)-C(3)-C(4)	0.5(3)
C(1)-C(2)-C(3)-O(1)	-179.1(2)
C(5)-C(4)-C(3)-C(2)	-0.5(3)
C(5)-C(4)-C(3)-O(1)	179.0(2)
C(20)-O(1)-C(3)-C(2)	-177.8(2)
C(20)-O(1)-C(3)-C(4)	2.6(3)
C(7)-C(8)-C(14)-C(15)	-49.0(3)
C(9)-C(8)-C(14)-C(15)	-172.7(2)
C(7)-C(8)-C(14)-C(13)	-179.9(2)
C(9)-C(8)-C(14)-C(13)	56.5(3)
C(5)-C(6)-C(7)-C(8)	49.6(2)
C(14)-C(8)-C(7)-C(6)	171.31(19)
C(9)-C(8)-C(7)-C(6)	-64.6(2)
C(3)-O(1)-C(20)-C(21)	179.2(2)
C(22)-C(21)-C(20)-O(1)	66.3(3)
C(26)-C(21)-C(20)-O(1)	-115.0(2)
C(22)-C(21)-C(26)-C(25)	-0.4(4)
C(20)-C(21)-C(26)-C(25)	-179.2(2)
C(8)-C(14)-C(13)-C(17)	-168.1(2)
C(15)-C(14)-C(13)-C(17)	60.5(3)
C(8)-C(14)-C(13)-C(19)	68.3(3)
C(15)-C(14)-C(13)-C(19)	-63.1(3)
C(8)-C(14)-C(13)-C(12)	-52.3(3)
C(15)-C(14)-C(13)-C(12)	176.3(2)
C(10)-C(9)-C(11)-C(12)	-175.0(2)
C(8)-C(9)-C(11)-C(12)	56.7(3)
C(8)-C(14)-C(15)-C(16)	-48.7(3)
C(13)-C(14)-C(15)-C(16)	82.8(3)
C(19)-C(13)-C(17)-C(18)	0.9(5)
C(12)-C(13)-C(17)-C(18)	120.5(4)
C(14)-C(13)-C(17)-C(18)	-123.4(4)
C(14)-C(15)-C(16)-N(1)	159(100)
C(21)-C(26)-C(25)-C(24)	1.9(4)
C(26)-C(25)-C(24)-C(23)	-2.1(4)
C(9)-C(11)-C(12)-C(13)	-56.3(3)
C(17)-C(13)-C(12)-C(11)	168.5(3)
C(19)-C(13)-C(12)-C(11)	-70.7(3)
C(14)-C(13)-C(12)-C(11)	51.9(3)
C(26)-C(21)-C(22)-C(23)	-0.8(4)

C(20)-C(21)-C(22)-C(23)	178.0(3)
C(25)-C(24)-C(23)-C(22)	0.9(5)
C(21)-C(22)-C(23)-C(24)	0.6(5)

Symmetry transformations used to generate equivalent atoms:

ORTEP PLOT for compound 10 with 30% thermal ellipsoids



X-ray crystal structure of compound 11

Table 1. Crystal data and structure refinement for compound **11**.

Empirical formula	C21 H30 N4 O2	
Formula weight	370.49	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 8.099(5) Å	α= 90°
	b = 10.195(5) Å	β= 90°
	c = 24.458(5) Å	γ = 90°
Volume	2019.5(16) $Å^3$	
Z	4	
Density (calculated)	1.219 Mg/m^3	
Absorption coefficient	0.080 mm^{-1}	
F(000)	800	
Crystal size	0.188 x 0.170 x 0.055 mm^3	
Theta range for data collection	3.02 to 25.00°.	
Index ranges	-6<=h<=9, -12<=k<=7, -16<=l<=29	
Reflections collected	5358	
Independent reflections	3442 [R(int) = 0.0458]	
Completeness to theta = 25.00°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.21327	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3442 / 0 / 251	
Goodness-of-fit on F^2	0.869	
Final R indices [I>2sigma(I)]	R1 = 0.0548, wR2 = 0.1187	
R indices (all data)	R1 = 0.0998, wR2 = 0.1318	
Absolute structure parameter	0(3)	
Largest diff. peak and hole	0.183 and -0.186 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **11**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(6)	15956(4)	-4019(4)	7740(1)	57(1)
O(1)	16697(4)	-3272(3)	5842(1)	84(1)
C(8)	13262(3)	-3901(3)	8255(1)	39(1)
C(10)	13393(4)	-3583(3)	7220(1)	45(1)
C(14)	12530(4)	-3469(3)	8797(1)	44(1)
C(15)	13020(4)	-4381(3)	9266(1)	50(1)
C(9)	12716(3)	-3073(3)	7770(1)	44(1)
N(1)	10789(4)	-3332(4)	9769(1)	77(1)
C(5)	15198(4)	-3932(3)	7272(1)	46(1)
C(16)	12077(4)	-4111(4)	9771(1)	53(1)
N(4)	12286(4)	-4575(3)	10262(1)	68(1)
C(4)	16135(4)	-4152(4)	6748(1)	64(1)
C(3)	15932(4)	-2994(4)	6368(1)	62(1)
C(11)	10844(4)	-2878(4)	7765(1)	71(1)
C(1)	13232(4)	-2477(4)	6796(1)	61(1)
C(2)	14152(4)	-2735(4)	6260(1)	67(1)
O(2)	19147(4)	-2762(5)	6173(2)	137(2)
C(7)	15155(4)	-3880(4)	8285(1)	55(1)
C(13)	10621(4)	-3309(4)	8775(1)	62(1)
N(3)	11099(5)	-4006(4)	10569(1)	84(1)
N(2)	10166(5)	-3271(4)	10280(2)	94(1)
C(19)	12444(5)	-4782(4)	7023(1)	71(1)
C(12)	10217(4)	-2382(4)	8307(1)	77(1)
C(18)	9727(4)	-4616(5)	8723(2)	82(1)
C(17A)	10092(5)	-2623(5)	9304(2)	95(2)
C(20)	18315(7)	-3088(6)	5799(2)	99(2)
C(21)	18929(7)	-3410(8)	5240(2)	159(3)

Table 3. Bond lengths [Å] and angles [°] for **11**.

C(6)-C(5)	1.303(4)
C(6)-C(7)	1.487(4)
C(6)-H(6)	1.00(3)
O(1)-C(20)	1.328(5)
O(1)-C(3)	1.457(4)
C(8)-C(14)	1.517(4)
C(8)-C(9)	1.521(4)
C(8)-C(7)	1.535(4)
C(8)-H(8)	0.9800
C(10)-C(5)	1.511(4)
C(10)-C(19)	1.523(4)
C(10)-C(1)	1.536(4)
C(10)-C(9)	1.544(4)
C(14)-C(15)	1.530(4)
C(14)-C(13)	1.556(4)
C(14)-H(14)	0.9800
C(15)-C(16)	1.477(4)
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(9)-C(11)	1.529(4)
C(9)-H(9)	0.9800
N(1)-C(16)	1.311(4)
N(1)-N(2)	1.349(4)
N(1)-C(17A)	1.460(5)
C(5)-C(4)	1.506(4)
C(16)-N(4)	1.301(4)
N(4)-N(3)	1.350(4)
C(4)-C(3)	1.511(5)
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700
C(3)-C(2)	1.489(5)
C(3)-H(3)	0.9800
C(11)-C(12)	1.507(5)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(1)-C(2)	1.531(4)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
O(2)-C(20)	1.183(6)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(13)-C(12)	1.520(4)
C(13)-C(18)	1.522(5)
C(13)-C(17A)	1.532(5)
N(3)-N(2)	1.278(4)
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(17A)-H(17A)	0.9700
C(17A)-H(17B)	0.9700
C(20)-C(21)	1.491(7)

C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600

C(5)-C(6)-C(7)	125.1(3)
C(5)-C(6)-H(6)	119.9(17)
C(7)-C(6)-H(6)	114.6(17)
C(20)-O(1)-C(3)	117.5(3)
C(14)-C(8)-C(9)	113.9(2)
C(14)-C(8)-C(7)	110.2(2)
C(9)-C(8)-C(7)	108.7(2)
C(14)-C(8)-H(8)	108.0
C(9)-C(8)-H(8)	108.0
C(7)-C(8)-H(8)	108.0
C(5)-C(10)-C(19)	109.0(3)
C(5)-C(10)-C(1)	108.2(3)
C(19)-C(10)-C(1)	109.5(3)
C(5)-C(10)-C(9)	110.4(2)
C(19)-C(10)-C(9)	111.5(3)
C(1)-C(10)-C(9)	108.1(2)
C(8)-C(14)-C(15)	112.2(2)
C(8)-C(14)-C(13)	112.9(2)
C(15)-C(14)-C(13)	110.3(3)
C(8)-C(14)-H(14)	107.0
C(15)-C(14)-H(14)	107.0
C(13)-C(14)-H(14)	107.0
C(16)-C(15)-C(14)	112.4(3)
C(16)-C(15)-H(15A)	109.1
C(14)-C(15)-H(15A)	109.1
C(16)-C(15)-H(15B)	109.1
C(14)-C(15)-H(15B)	109.1
H(15A)-C(15)-H(15B)	107.9
C(8)-C(9)-C(11)	111.6(3)
C(8)-C(9)-C(10)	112.9(2)
C(11)-C(9)-C(10)	112.8(3)
C(8)-C(9)-H(9)	106.3
C(11)-C(9)-H(9)	106.3
C(10)-C(9)-H(9)	106.3
C(16)-N(1)-N(2)	108.7(3)
C(16)-N(1)-C(17A)	127.7(3)
N(2)-N(1)-C(17A)	123.6(4)
C(6)-C(5)-C(4)	120.1(3)
C(6)-C(5)-C(10)	123.1(3)
C(4)-C(5)-C(10)	116.8(3)
N(4)-C(16)-N(1)	109.1(3)
N(4)-C(16)-C(15)	129.5(3)
N(1)-C(16)-C(15)	121.3(3)
C(16)-N(4)-N(3)	105.3(3)
C(5)-C(4)-C(3)	110.6(3)
C(5)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4A)	109.5
C(5)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	108.1
O(1)-C(3)-C(2)	106.8(3)
O(1)-C(3)-C(4)	110.1(3)
C(2)-C(3)-C(4)	110.7(3)
O(1)-C(3)-H(3)	109.7
C(2)-C(3)-H(3)	109.7
C(4)-C(3)-H(3)	109.7

C(12)-C(11)-C(9)	111.7(3)
C(12)-C(11)-H(11A)	109.3
C(9)-C(11)-H(11A)	109.3
C(12)-C(11)-H(11B)	109.3
C(9)-C(11)-H(11B)	109.3
H(11A)-C(11)-H(11B)	107.9
C(2)-C(1)-C(10)	114.2(3)
C(2)-C(1)-H(1A)	108.7
C(10)-C(1)-H(1A)	108.7
C(2)-C(1)-H(1B)	108.7
C(10)-C(1)-H(1B)	108.7
H(1A)-C(1)-H(1B)	107.6
C(3)-C(2)-C(1)	110.4(3)
C(3)-C(2)-H(2A)	109.6
C(1)-C(2)-H(2A)	109.6
C(3)-C(2)-H(2B)	109.6
C(1)-C(2)-H(2B)	109.6
H(2A)-C(2)-H(2B)	108.1
C(6)-C(7)-C(8)	113.1(3)
C(6)-C(7)-H(7A)	109.0
C(8)-C(7)-H(7A)	109.0
C(6)-C(7)-H(7B)	109.0
C(8)-C(7)-H(7B)	109.0
H(7A)-C(7)-H(7B)	107.8
C(12)-C(13)-C(18)	112.3(3)
C(12)-C(13)-C(17A)	107.0(3)
C(18)-C(13)-C(17A)	109.7(3)
C(12)-C(13)-C(14)	107.8(3)
C(18)-C(13)-C(14)	112.6(3)
C(17A)-C(13)-C(14)	107.3(3)
N(2)-N(3)-N(4)	111.4(3)
N(3)-N(2)-N(1)	105.3(3)
C(10)-C(19)-H(19A)	109.5
C(10)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(10)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(11)-C(12)-C(13)	112.4(3)
C(11)-C(12)-H(12A)	109.1
C(13)-C(12)-H(12A)	109.1
C(11)-C(12)-H(12B)	109.1
C(13)-C(12)-H(12B)	109.1
H(12A)-C(12)-H(12B)	107.9
C(13)-C(18)-H(18A)	109.5
C(13)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(13)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
N(1)-C(17A)-C(13)	108.9(3)
N(1)-C(17A)-H(17A)	109.9
C(13)-C(17A)-H(17A)	109.9
N(1)-C(17A)-H(17B)	109.9
C(13)-C(17A)-H(17B)	109.9
H(17A)-C(17A)-H(17B)	108.3
O(2)-C(20)-O(1)	122.8(5)
O(2)-C(20)-C(21)	125.4(5)
O(1)-C(20)-C(21)	111.7(5)
C(20)-C(21)-H(21A)	109.5

C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5

Symmetry transformations used to generate equivalent atoms:

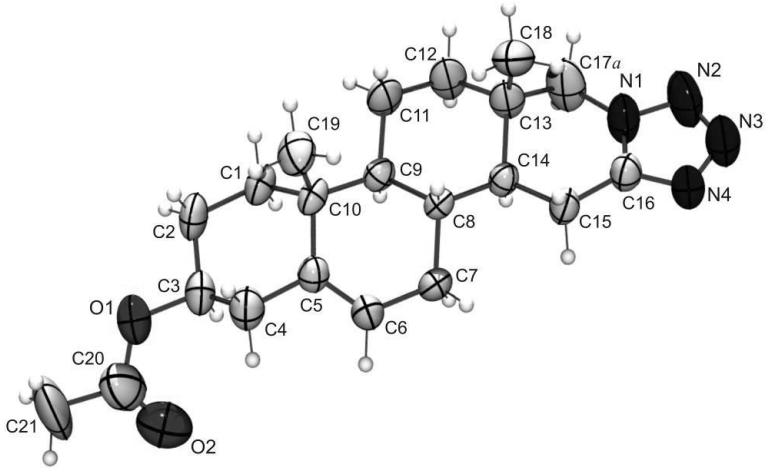
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **11**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(6)	49(2)	75(3)	46(2)	5(2)	3(2)	8(2)
O(1)	90(2)	112(2)	51(2)	6(2)	11(1)	-1(2)
C(8)	39(2)	39(2)	38(2)	-1(2)	-7(1)	2(2)
C(10)	57(2)	39(2)	39(2)	4(2)	-11(2)	-4(2)
C(14)	47(2)	44(2)	40(2)	-1(2)	-4(1)	9(2)
C(15)	54(2)	59(2)	39(2)	1(2)	-4(1)	6(2)
C(9)	46(2)	42(2)	45(2)	1(2)	-7(1)	7(2)
N(1)	96(2)	84(3)	49(2)	8(2)	14(2)	27(2)
C(5)	52(2)	43(2)	43(2)	2(2)	0(2)	7(2)
C(16)	58(2)	56(2)	44(2)	5(2)	-1(2)	7(2)
N(4)	71(2)	87(2)	48(2)	7(2)	4(2)	-3(2)
C(4)	72(2)	68(3)	52(2)	2(2)	2(2)	6(2)
C(3)	78(2)	70(3)	39(2)	-2(2)	2(2)	-2(2)
C(11)	59(2)	96(3)	58(2)	17(2)	-5(2)	31(2)
C(1)	71(2)	70(2)	41(2)	7(2)	-10(2)	1(2)
C(2)	91(3)	75(3)	36(2)	7(2)	-5(2)	7(2)
O(2)	82(2)	193(5)	136(3)	4(3)	8(2)	-15(3)
C(7)	43(2)	76(3)	47(2)	2(2)	-9(2)	4(2)
C(13)	56(2)	71(3)	59(2)	12(2)	6(2)	31(2)
N(3)	101(3)	96(3)	55(2)	8(2)	13(2)	3(2)
N(2)	119(3)	102(3)	62(2)	4(2)	35(2)	23(3)
C(19)	79(2)	76(3)	58(2)	-13(2)	-2(2)	-21(2)
C(12)	68(2)	96(3)	67(2)	24(2)	7(2)	48(2)
C(18)	49(2)	115(4)	80(3)	17(3)	-7(2)	-9(2)
C(17A)	105(3)	102(4)	77(3)	14(3)	25(2)	63(3)
C(20)	88(4)	114(4)	97(4)	26(4)	12(3)	13(4)
C(21)	158(5)	241(7)	78(3)	34(4)	66(3)	72(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **11**.

	x	y	z	U(eq)
H(8)	12913	-4807	8187	46
H(14)	12993	-2603	8879	52
H(15A)	12834	-5283	9156	60
H(15B)	14189	-4277	9341	60
H(9)	13201	-2202	7825	53
H(4A)	15729	-4939	6570	77
H(4B)	17296	-4279	6829	77
H(3)	16443	-2215	6531	75
H(11A)	10555	-2255	7481	85
H(11B)	10311	-3705	7680	85
H(1A)	12071	-2346	6715	73
H(1B)	13649	-1672	6956	73
H(2A)	13667	-3484	6076	81
H(2B)	14044	-1979	6022	81
H(7A)	15507	-3061	8449	66
H(7B)	15523	-4589	8519	66
H(19A)	12959	-5125	6699	106
H(19B)	11326	-4538	6941	106
H(19C)	12449	-5440	7304	106
H(12A)	9029	-2269	8286	92
H(12B)	10703	-1531	8381	92
H(18A)	9846	-5102	9057	123
H(18B)	10193	-5108	8427	123
H(18C)	8576	-4461	8654	123
H(17A)	10484	-1724	9304	114
H(17B)	8897	-2610	9330	114
H(21A)	18799	-2660	5007	239
H(21B)	18308	-4132	5095	239
H(21C)	20076	-3645	5259	239
H(6)	17150(40)	-4280(30)	7753(12)	63(9)

ORTEP PLOT for compound 11 with 30% thermal ellipsoids



X-ray crystal structure of compound 14.

Table 1. Crystal data and structure refinement for compound **14**.

Empirical formula	C26 H30 N4 O	
Formula weight	414.54	
Temperature	293(2) K	
Wavelength	1.54180 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 9.039(5) Å	α= 90°
	b = 12.320(5) Å	β= 93.034(5)°
	c = 9.996(5) Å	γ = 90°
Volume	1111.6(9) $Å^3$	
Z	2	
Density (calculated)	1.239 Mg/m^3	
Absorption coefficient	0.603 mm^{-1}	
F(000)	444	
Crystal size	0.282 x 0.185 x 0.023 mm^3	
Theta range for data collection	4.43 to 72.25°.	
Index ranges	-10<=h<=11, -10<=k<=15, -10<=l<=12	
Reflections collected	3829	
Independent reflections	2627 [R(int) = 0.0221]	
Completeness to theta = 67.50°	96.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.95325	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2627 / 1 / 374	
Goodness-of-fit on F^2	1.068	
Final R indices [I>2sigma(I)]	R1 = 0.0377, wR2 = 0.0941	
R indices (all data)	R1 = 0.0458, wR2 = 0.1015	
Absolute structure parameter	-0.2(4)	
Extinction coefficient	0.0017(4)	
Largest diff. peak and hole	0.174 and -0.129 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **14**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	6070(2)	4659(2)	3132(2)	67(1)
C(14)	8574(3)	-887(2)	6379(3)	54(1)
C(20)	6267(3)	5745(2)	3608(3)	57(1)
C(13)	8970(3)	-677(2)	7892(3)	53(1)
C(1)	8287(3)	3119(2)	5674(3)	52(1)
C(2)	7581(3)	4001(3)	5065(3)	56(1)
C(5)	7368(3)	1938(2)	3929(3)	58(1)
N(1)	8987(3)	-2657(2)	8077(3)	69(1)
C(12)	10014(4)	292(3)	7983(3)	63(1)
C(10)	8222(3)	2084(2)	5130(3)	52(1)
C(4)	6670(4)	2822(2)	3317(3)	60(1)
C(21)	5698(3)	6513(2)	2528(3)	55(1)
C(3)	6780(3)	3848(2)	3861(3)	56(1)
C(11)	9384(4)	1305(3)	7300(3)	64(1)
C(9)	8953(3)	1109(2)	5823(3)	53(1)
N(4)	7480(4)	-3774(2)	7042(3)	92(1)
C(8)	7965(3)	115(2)	5619(3)	54(1)
C(16)	7962(4)	-2758(2)	7081(3)	72(1)
C(17A)	9832(4)	-1672(3)	8460(3)	66(1)
C(22)	4965(3)	7450(3)	2868(3)	63(1)
C(26)	5928(4)	6318(3)	1188(3)	66(1)
C(23)	4481(4)	8193(3)	1890(4)	74(1)
C(6)	7168(5)	830(3)	3312(3)	86(1)
N(2)	9179(4)	-3635(2)	8679(3)	90(1)
C(7)	7756(5)	-98(3)	4107(3)	78(1)
C(18)	7585(4)	-465(3)	8667(3)	74(1)
C(15)	7505(5)	-1848(3)	6192(4)	79(1)
N(3)	8259(5)	-4291(3)	8059(3)	102(1)
C(24)	4717(4)	7988(3)	573(4)	78(1)
C(19)	10191(7)	-1670(4)	9951(5)	98(2)
C(25)	5433(5)	7053(3)	221(4)	81(1)

Table 3. Bond lengths [Å] and angles [°] for **14**.

O(1)-C(3)	1.376(3)
O(1)-C(20)	1.428(3)
C(14)-C(15)	1.533(4)
C(14)-C(8)	1.536(4)
C(14)-C(13)	1.557(4)
C(14)-H(14)	1.04(3)
C(20)-C(21)	1.506(4)
C(20)-H(20A)	1.06(3)
C(20)-H(20B)	0.96(3)
C(13)-C(12)	1.521(4)
C(13)-C(18)	1.529(4)
C(13)-C(17A)	1.545(4)
C(1)-C(2)	1.385(4)
C(1)-C(10)	1.386(4)
C(1)-H(1)	0.97(3)
C(2)-C(3)	1.384(4)
C(2)-H(2)	0.95(4)
C(5)-C(4)	1.384(4)
C(5)-C(10)	1.404(4)
C(5)-C(6)	1.505(4)
N(1)-C(16)	1.329(4)
N(1)-N(2)	1.354(4)
N(1)-C(17A)	1.473(4)
C(12)-C(11)	1.519(4)
C(12)-H(12A)	0.95(3)
C(12)-H(12B)	0.99(4)
C(10)-C(9)	1.521(4)
C(4)-C(3)	1.379(4)
C(4)-H(4)	0.97(3)
C(21)-C(22)	1.382(4)
C(21)-C(26)	1.388(4)
C(11)-C(9)	1.526(4)
C(11)-H(11A)	1.02(3)
C(11)-H(11B)	1.02(4)
C(9)-C(8)	1.522(4)
C(9)-H(9)	1.04(3)
N(4)-C(16)	1.326(4)
N(4)-N(3)	1.363(4)
C(8)-C(7)	1.536(4)
C(8)-H(8)	1.08(3)
C(16)-C(15)	1.476(5)
C(17A)-C(19)	1.508(6)
C(17A)-H(17)	0.94(3)
C(22)-C(23)	1.393(4)
C(22)-H(22)	0.93(3)
C(26)-C(25)	1.382(4)
C(26)-H(26)	0.93(3)
C(23)-C(24)	1.368(5)
C(23)-H(23)	0.98(4)
C(6)-C(7)	1.476(4)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
N(2)-N(3)	1.294(4)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600

C(15)-H(15A)	0.97(5)
C(15)-H(15B)	0.94(4)
C(24)-C(25)	1.376(5)
C(24)-H(24)	0.97(4)
C(19)-H(19A)	0.91(4)
C(19)-H(19B)	0.99(5)
C(19)-H(19C)	0.93(4)
C(25)-H(25)	0.95(4)

C(3)-O(1)-C(20)	117.2(2)
C(15)-C(14)-C(8)	110.7(2)
C(15)-C(14)-C(13)	111.0(3)
C(8)-C(14)-C(13)	113.9(2)
C(15)-C(14)-H(14)	105.9(15)
C(8)-C(14)-H(14)	110.3(15)
C(13)-C(14)-H(14)	104.7(14)
O(1)-C(20)-C(21)	108.5(2)
O(1)-C(20)-H(20A)	113.0(16)
C(21)-C(20)-H(20A)	107.5(16)
O(1)-C(20)-H(20B)	108(2)
C(21)-C(20)-H(20B)	113.8(19)
H(20A)-C(20)-H(20B)	106(2)
C(12)-C(13)-C(18)	111.0(3)
C(12)-C(13)-C(17A)	107.5(2)
C(18)-C(13)-C(17A)	111.0(3)
C(12)-C(13)-C(14)	107.4(2)
C(18)-C(13)-C(14)	111.6(2)
C(17A)-C(13)-C(14)	108.1(2)
C(2)-C(1)-C(10)	122.7(3)
C(2)-C(1)-H(1)	116.0(16)
C(10)-C(1)-H(1)	121.2(16)
C(3)-C(2)-C(1)	118.9(3)
C(3)-C(2)-H(2)	122(2)
C(1)-C(2)-H(2)	119(2)
C(4)-C(5)-C(10)	119.7(3)
C(4)-C(5)-C(6)	119.3(2)
C(10)-C(5)-C(6)	121.0(3)
C(16)-N(1)-N(2)	108.5(3)
C(16)-N(1)-C(17A)	127.1(2)
N(2)-N(1)-C(17A)	124.4(3)
C(11)-C(12)-C(13)	113.7(2)
C(11)-C(12)-H(12A)	112(2)
C(13)-C(12)-H(12A)	109(2)
C(11)-C(12)-H(12B)	109(2)
C(13)-C(12)-H(12B)	108(2)
H(12A)-C(12)-H(12B)	106(3)
C(1)-C(10)-C(5)	117.6(3)
C(1)-C(10)-C(9)	122.7(2)
C(5)-C(10)-C(9)	119.6(2)
C(3)-C(4)-C(5)	121.7(2)
C(3)-C(4)-H(4)	119.3(19)
C(5)-C(4)-H(4)	119.0(19)
C(22)-C(21)-C(26)	118.7(3)
C(22)-C(21)-C(20)	119.9(3)
C(26)-C(21)-C(20)	121.3(3)
O(1)-C(3)-C(4)	115.8(2)
O(1)-C(3)-C(2)	124.8(3)
C(4)-C(3)-C(2)	119.5(3)
C(12)-C(11)-C(9)	112.0(3)
C(12)-C(11)-H(11A)	111.4(18)

C(9)-C(11)-H(11A)	106.8(16)
C(12)-C(11)-H(11B)	109(2)
C(9)-C(11)-H(11B)	110(2)
H(11A)-C(11)-H(11B)	107(3)
C(10)-C(9)-C(8)	109.7(2)
C(10)-C(9)-C(11)	113.4(2)
C(8)-C(9)-C(11)	112.1(2)
C(10)-C(9)-H(9)	110.0(18)
C(8)-C(9)-H(9)	104.3(18)
C(11)-C(9)-H(9)	107.0(16)
C(16)-N(4)-N(3)	105.3(3)
C(9)-C(8)-C(14)	112.8(2)
C(9)-C(8)-C(7)	108.1(2)
C(14)-C(8)-C(7)	111.8(2)
C(9)-C(8)-H(8)	105.9(15)
C(14)-C(8)-H(8)	108.1(15)
C(7)-C(8)-H(8)	110.0(14)
N(4)-C(16)-N(1)	109.0(3)
N(4)-C(16)-C(15)	128.2(3)
N(1)-C(16)-C(15)	122.8(3)
N(1)-C(17A)-C(19)	109.9(3)
N(1)-C(17A)-C(13)	108.3(2)
C(19)-C(17A)-C(13)	116.1(3)
N(1)-C(17A)-H(17)	108(2)
C(19)-C(17A)-H(17)	105.6(19)
C(13)-C(17A)-H(17)	108(2)
C(21)-C(22)-C(23)	120.9(3)
C(21)-C(22)-H(22)	117(2)
C(23)-C(22)-H(22)	122(2)
C(25)-C(26)-C(21)	120.2(3)
C(25)-C(26)-H(26)	123(2)
C(21)-C(26)-H(26)	117(2)
C(24)-C(23)-C(22)	119.6(3)
C(24)-C(23)-H(23)	125(2)
C(22)-C(23)-H(23)	115(2)
C(7)-C(6)-C(5)	116.8(3)
C(7)-C(6)-H(6A)	108.1
C(5)-C(6)-H(6A)	108.1
C(7)-C(6)-H(6B)	108.1
C(5)-C(6)-H(6B)	108.1
H(6A)-C(6)-H(6B)	107.3
N(3)-N(2)-N(1)	106.2(3)
C(6)-C(7)-C(8)	114.8(3)
C(6)-C(7)-H(7A)	108.6
C(8)-C(7)-H(7A)	108.6
C(6)-C(7)-H(7B)	108.6
C(8)-C(7)-H(7B)	108.6
H(7A)-C(7)-H(7B)	107.6
C(13)-C(18)-H(18A)	109.5
C(13)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(13)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(16)-C(15)-C(14)	111.0(3)
C(16)-C(15)-H(15A)	109(3)
C(14)-C(15)-H(15A)	112(3)
C(16)-C(15)-H(15B)	108(3)
C(14)-C(15)-H(15B)	110(3)
H(15A)-C(15)-H(15B)	107(4)

N(2)-N(3)-N(4)	111.0(3)
C(23)-C(24)-C(25)	120.1(3)
C(23)-C(24)-H(24)	120(2)
C(25)-C(24)-H(24)	119(2)
C(17A)-C(19)-H(19A)	111(3)
C(17A)-C(19)-H(19B)	106(3)
H(19A)-C(19)-H(19B)	103(3)
C(17A)-C(19)-H(19C)	113(3)
H(19A)-C(19)-H(19C)	117(4)
H(19B)-C(19)-H(19C)	107(4)
C(24)-C(25)-C(26)	120.5(4)
C(24)-C(25)-H(25)	125(2)
C(26)-C(25)-H(25)	114(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **14**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	77(1)	51(1)	69(1)	7(1)	-21(1)	-6(1)
C(14)	61(2)	46(2)	55(2)	-1(1)	-3(1)	3(1)
C(20)	63(2)	51(2)	57(2)	6(1)	-4(1)	1(1)
C(13)	58(1)	50(1)	50(2)	5(1)	-3(1)	4(1)
C(1)	61(2)	47(1)	48(2)	1(1)	-5(1)	-9(1)
C(2)	65(2)	49(2)	52(2)	4(1)	-1(1)	-6(1)
C(5)	78(2)	52(2)	44(1)	1(1)	-4(1)	-5(1)
N(1)	92(2)	46(1)	67(2)	9(1)	-5(1)	8(1)
C(12)	74(2)	57(2)	56(2)	6(2)	-16(2)	-6(2)
C(10)	59(2)	52(2)	46(1)	3(1)	-1(1)	-6(1)
C(4)	79(2)	53(2)	47(2)	1(1)	-13(1)	-5(1)
C(21)	52(1)	52(2)	61(2)	8(1)	-2(1)	-3(1)
C(3)	59(2)	50(2)	57(2)	12(1)	-3(1)	-2(1)
C(11)	82(2)	54(2)	54(2)	2(1)	-17(2)	-5(2)
C(9)	61(2)	47(2)	51(2)	3(1)	-3(1)	0(1)
N(4)	143(3)	49(2)	81(2)	4(2)	-18(2)	-11(2)
C(8)	62(2)	46(2)	52(2)	0(1)	-6(1)	-1(1)
C(16)	103(2)	45(2)	68(2)	0(2)	-5(2)	-3(2)
C(17A)	70(2)	56(2)	70(2)	11(2)	-5(2)	5(2)
C(22)	68(2)	59(2)	61(2)	6(2)	3(1)	10(1)
C(26)	79(2)	57(2)	62(2)	10(2)	4(2)	11(2)
C(23)	85(2)	58(2)	79(2)	8(2)	5(2)	18(2)
C(6)	147(3)	58(2)	51(2)	-7(2)	-22(2)	4(2)
N(2)	131(3)	51(2)	87(2)	14(2)	-13(2)	9(2)
C(7)	122(3)	49(2)	61(2)	-3(1)	-19(2)	3(2)
C(18)	83(2)	71(2)	69(2)	6(2)	14(2)	10(2)
C(15)	106(3)	50(2)	78(2)	7(2)	-28(2)	-11(2)
N(3)	164(3)	49(2)	90(2)	5(2)	-16(2)	-1(2)
C(24)	87(2)	75(2)	72(2)	23(2)	4(2)	12(2)
C(19)	130(4)	71(3)	87(3)	20(2)	-39(3)	-5(3)
C(25)	99(3)	86(3)	59(2)	12(2)	9(2)	14(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **14**.

	x	y	z	U(eq)
H(6A)	6117	713	3123	104
H(6B)	7636	830	2461	104
H(7A)	8704	-305	3773	93
H(7B)	7088	-708	3966	93
H(18A)	7871	-183	9538	111
H(18B)	7051	-1132	8761	111
H(18C)	6964	52	8189	111
H(14)	9560(30)	-1140(20)	5990(20)	52(7)
H(8)	6920(30)	330(20)	6020(30)	62(8)
H(1)	8830(30)	3260(20)	6520(30)	50(7)
H(2)	7660(40)	4690(30)	5480(40)	87(11)
H(12A)	10300(30)	420(30)	8900(30)	74(9)
H(11A)	8450(30)	1570(30)	7740(30)	69(9)
H(25)	5660(40)	6860(30)	-660(40)	98(12)
H(19A)	10750(50)	-1080(30)	10200(40)	104(15)
H(20A)	7400(30)	5940(20)	3840(30)	59(8)
H(20B)	5780(30)	5810(30)	4430(30)	73(9)
H(4)	6080(30)	2710(20)	2500(30)	63(8)
H(23)	4060(40)	8860(30)	2230(40)	102(12)
H(15A)	6490(60)	-1650(40)	6360(50)	141(19)
H(19B)	10890(50)	-2280(40)	10120(40)	115(15)
H(17)	10750(30)	-1700(30)	8060(30)	72(10)
H(24)	4380(40)	8490(30)	-120(40)	93(12)
H(11B)	10140(40)	1920(30)	7400(40)	101(13)
H(26)	6390(30)	5670(30)	980(30)	80(10)
H(15B)	7500(40)	-2100(30)	5300(40)	97(13)
H(9)	9920(30)	900(30)	5360(30)	75(9)
H(22)	4910(40)	7590(30)	3780(30)	74(10)
H(12B)	10940(40)	80(30)	7550(30)	80(10)
H(19C)	9370(50)	-1810(40)	10450(40)	112(18)

ORTEP PLOT for compound 14 with 30% thermal ellipsoids