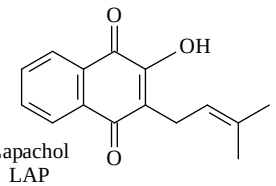
ANEXOS

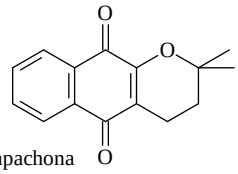
Anexo A - Tabela de Substâncias (com códigos)

Principais quinonas



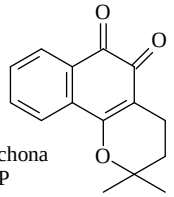
Lapachol
LAP

$C_{15}H_{14}O_3$
242.27



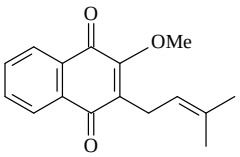
alfa-lapachona
ALAP

$C_{15}H_{14}O_3$
242.27

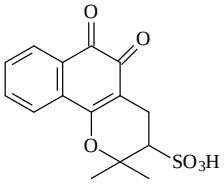


Beta-lapachona
BLAP

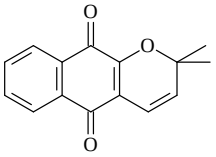
$C_{15}H_{14}O_3$
242.27



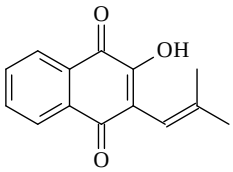
$C_{16}H_{16}O_3$
256.30
2-metóxi-lapachol



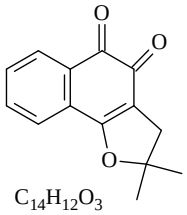
$C_{15}H_{14}O_6S$
322.33
Ácido β–lapachona-3-sulfônico



$C_{15}H_{12}O_3$
240.25
α–Xiloidona

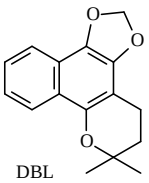


$C_{14}H_{12}O_3$
228.24
Nor-lapachol



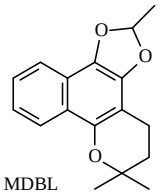
$C_{14}H_{12}O_3$
228.24
Nor-beta-lapachona

Produtos formados nas reações com diazocompostos, nitroalcanos ou sais de fosfônio.



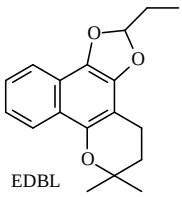
DBL

$C_{16}H_{16}O_3$
256.30



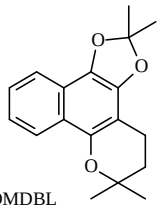
MDBL

$C_{17}H_{18}O_3$
270.125594



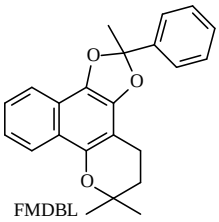
EDBL

$C_{17}H_{18}O_3$
270.125594



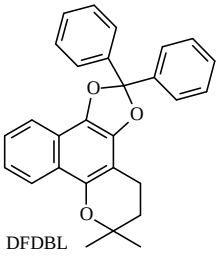
DMDBL

$C_{18}H_{20}O_3$
284.141244



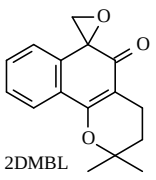
FMDBL

$C_{23}H_{22}O_3$
346.42



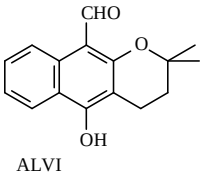
DFDBL

$C_{28}H_{24}O_3$
408.172544



2DMBL

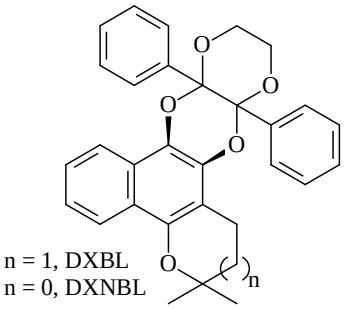
$C_{16}H_{16}O_3$
256.109944



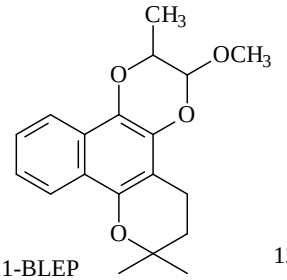
ALVI

$C_{16}H_{16}O_3$
256.109944

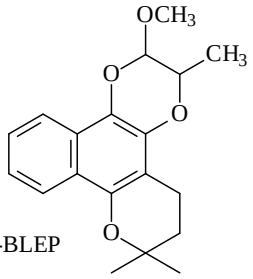
Produtos obtidos em reações fotoquímicas



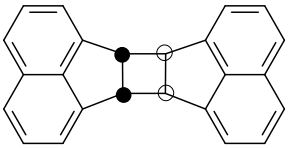
n = 1, DXBL
n = 0, DXNBL



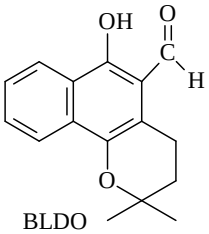
11-BLEP



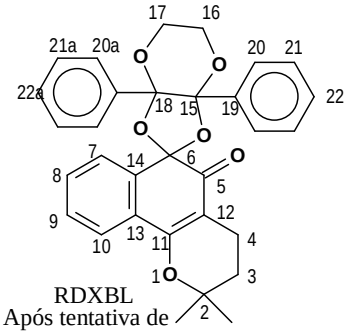
12-BLEP



DACEN

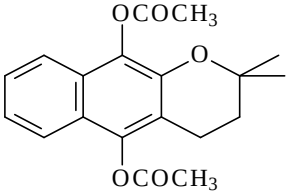


BLDO

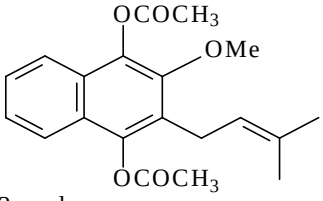


RDXBL
Após tentativa de nitração do DXBL

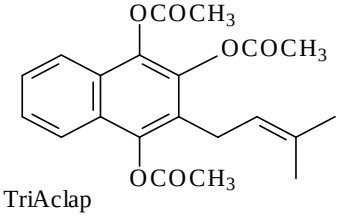
Principais produtos referentes a redução.



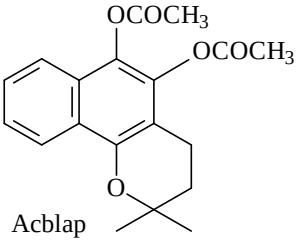
Acalap
$C_{19}H_{20}O_5$
328.36



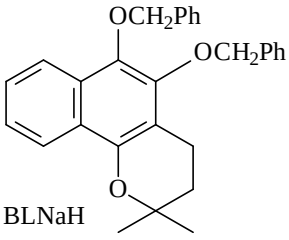
Ac2meolap
$C_{20}H_{22}O_5$
342.39



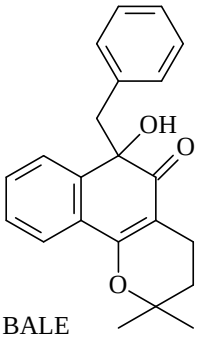
TriAclap
$C_{21}H_{22}O_6$
370.40



Acblap
$C_{19}H_{20}O_5$
328.36

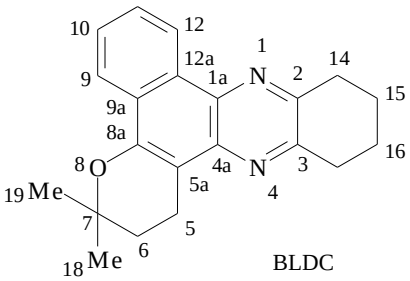


BLNaH
$C_{29}H_{28}O_3$
424.53

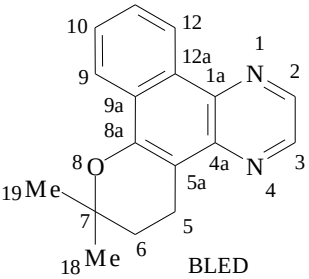


BALE
$C_{22}H_{22}O_3$
334.41

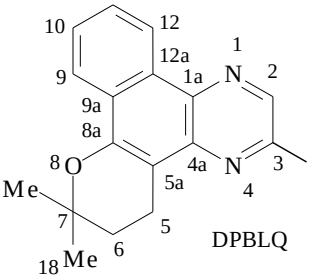
Produtos obtidos da reação com Diaminas vicinais.



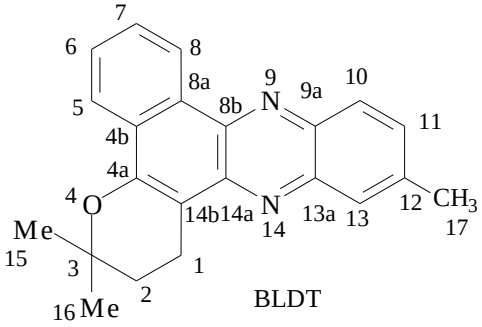
BLDC



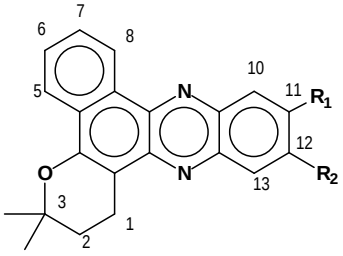
BLED



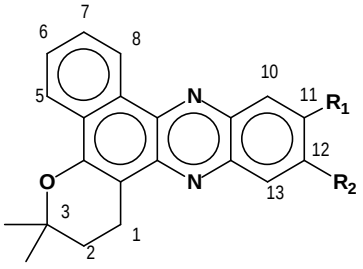
DPBLQ



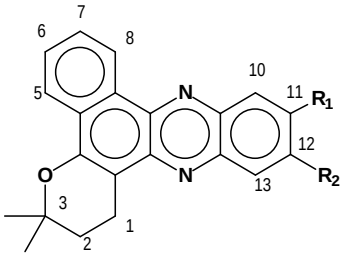
BLDT



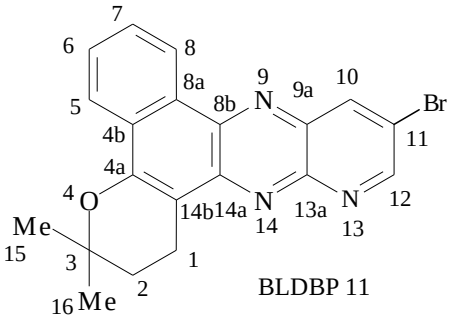
BLDB-11, R_1 = -COPh e R_2 = H
BLDB-12, R_1 = H e R_2 = -COPh



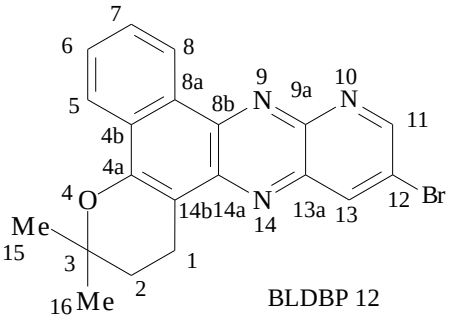
BLACD-11, R_1 = -CO_2H e R_2 = H
BLACD-12, R_1 = H e R_2 = -CO_2H



FENO2-11, R_1 = NO_2 e R_2 = H
FENO2-12, R_1 = H e R_2 = NO_2

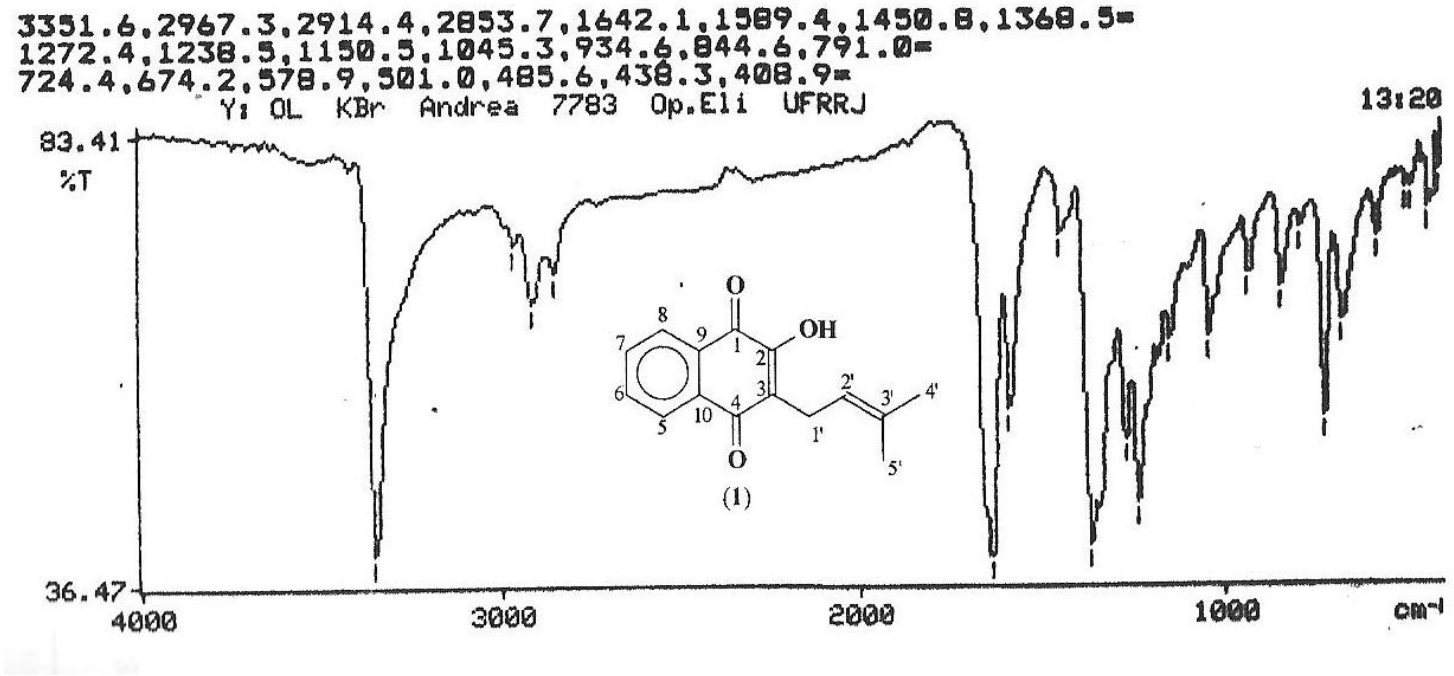


BLDBP 11

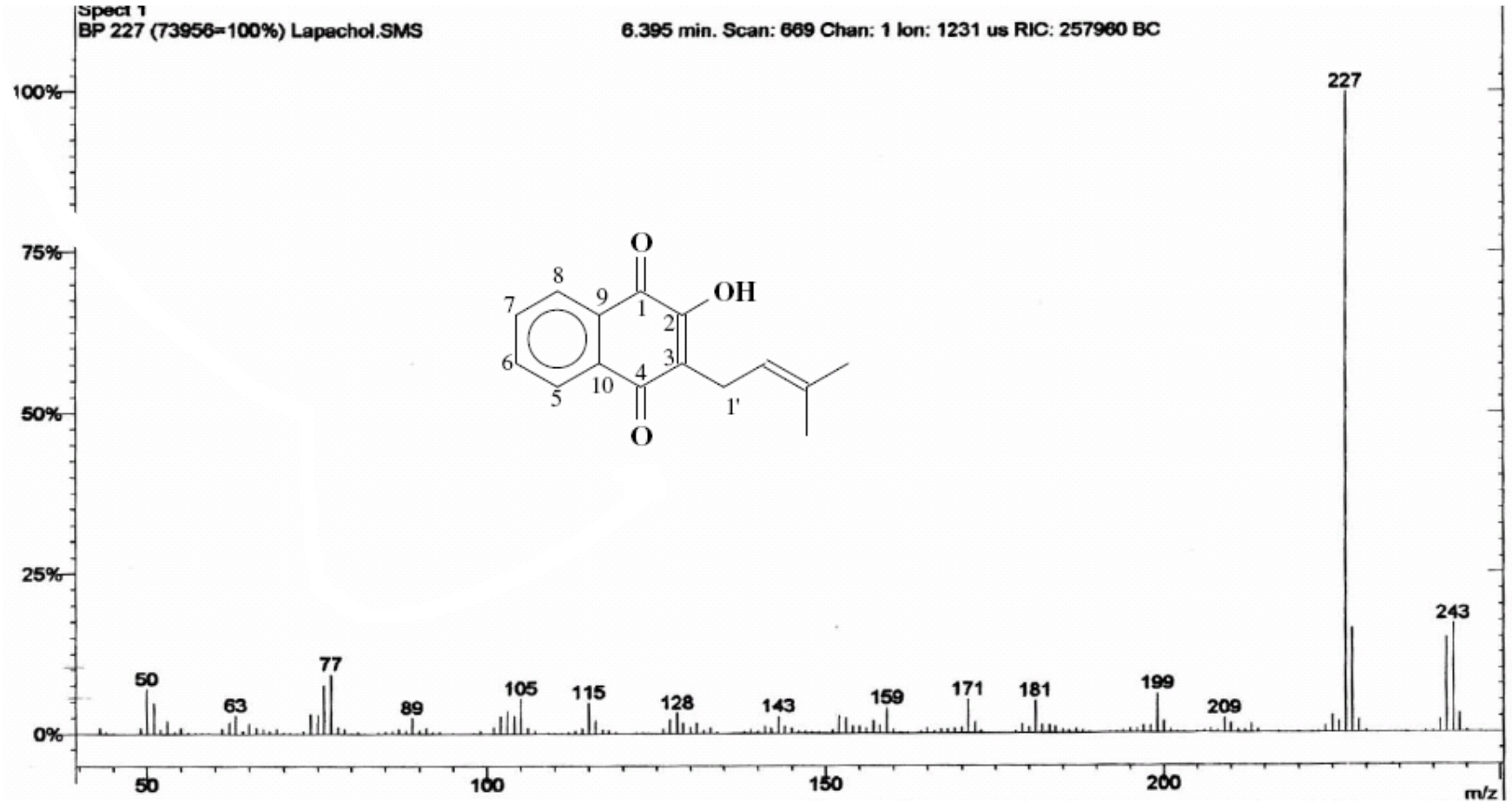


BLDBP 12

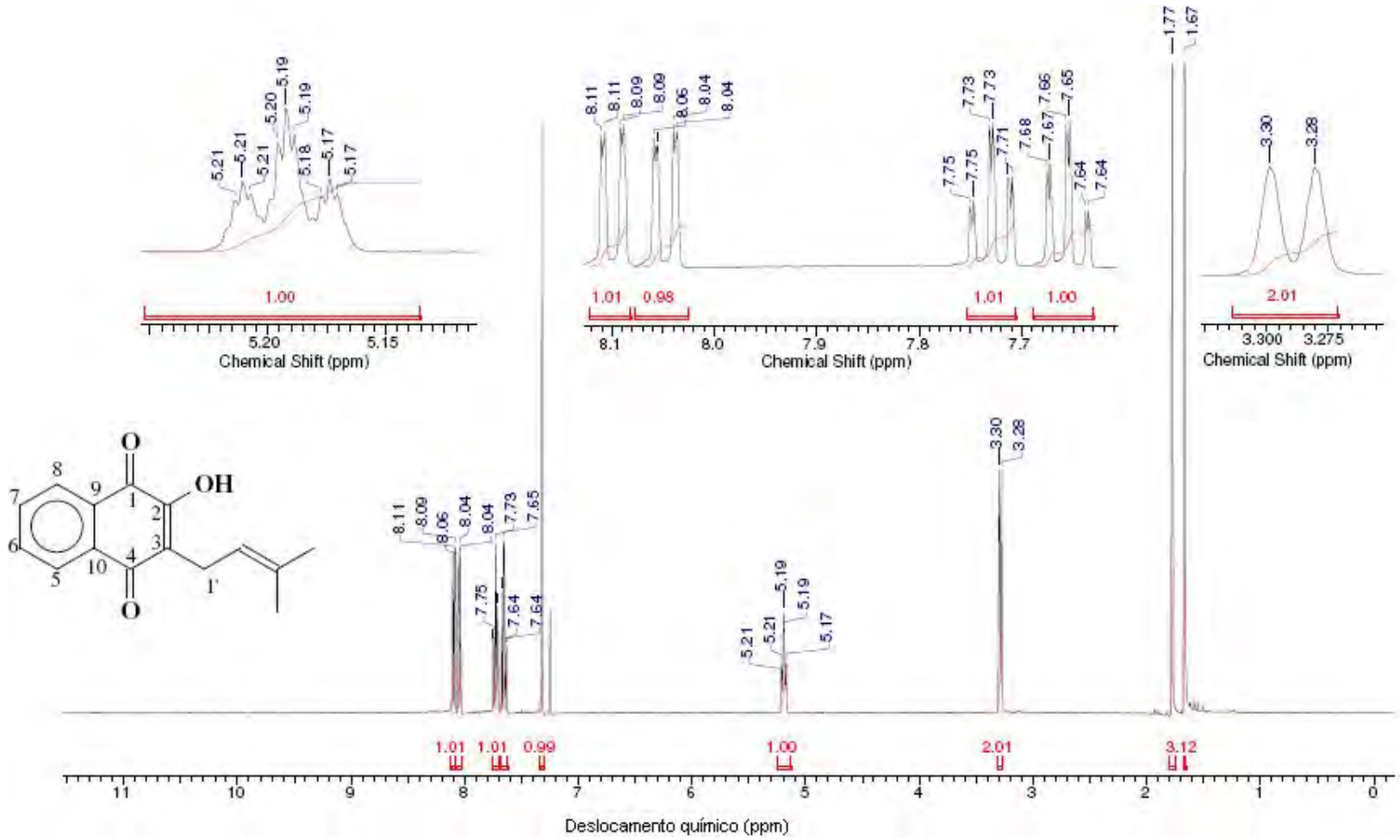
Anexo B – Caderno de Espectros



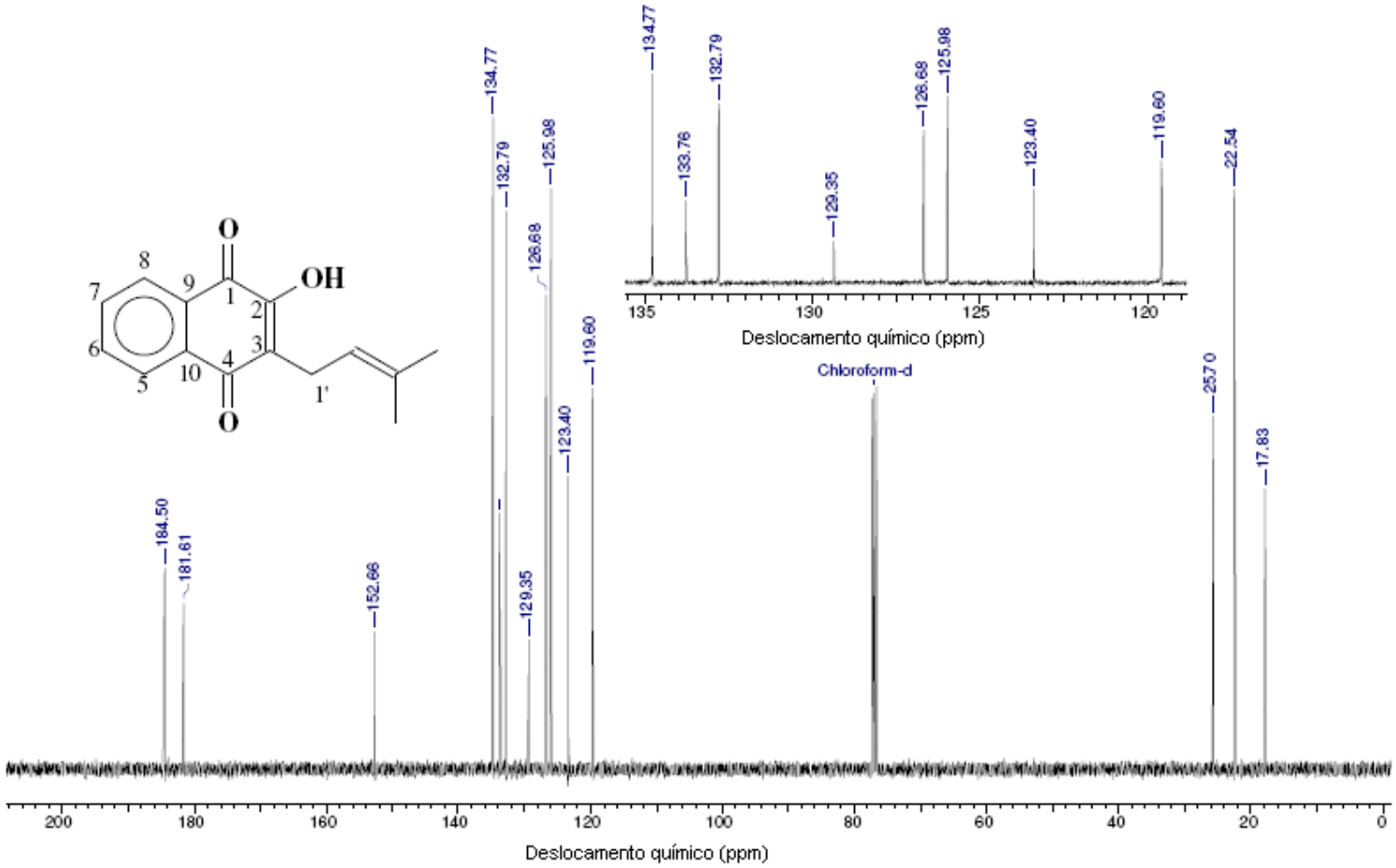
Espectro 1 – I.V. do lapachol (2-hidróxi-3-(3-metilbut-2-enil)naftaleno-1,4-diona), em pastilha de KBr.



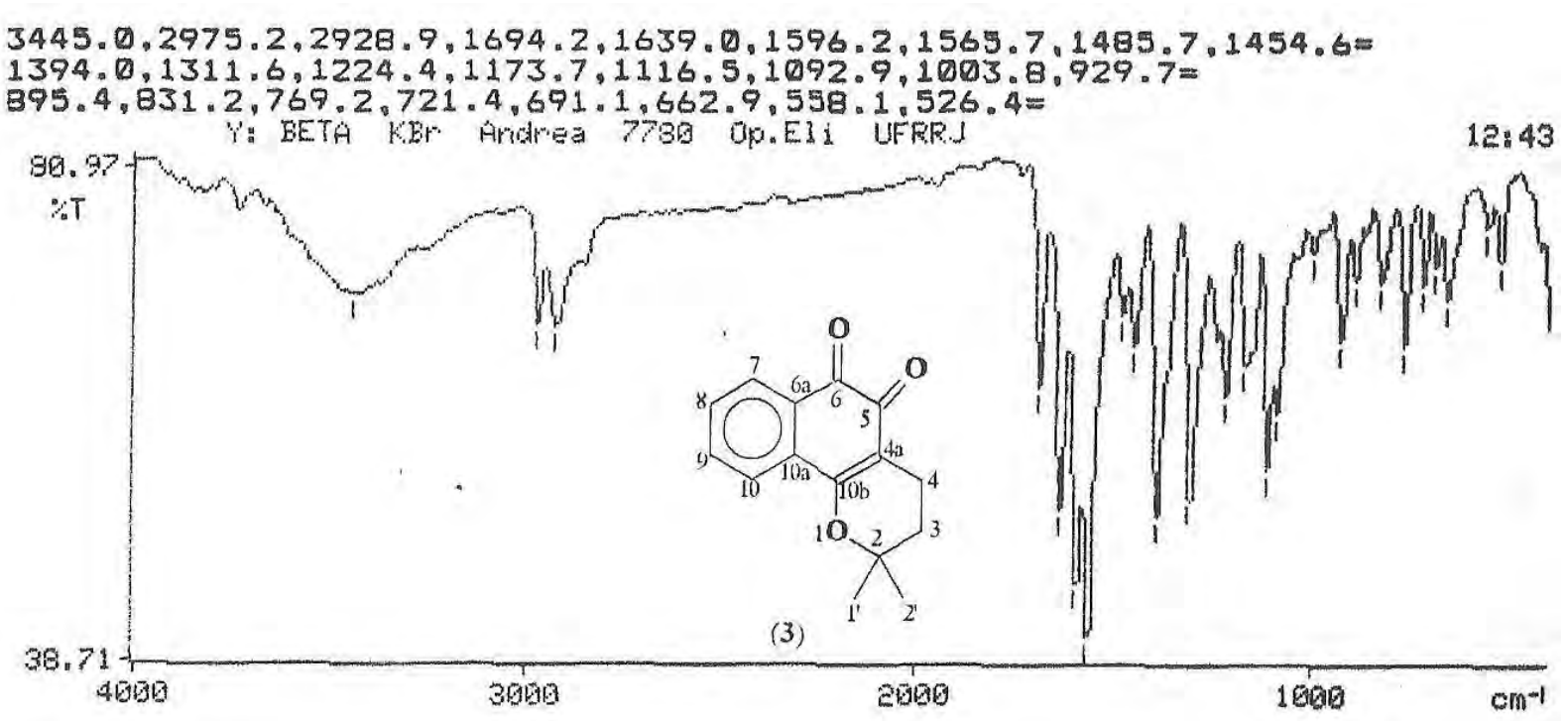
Espectro 2 – E.M. do lapachol (2-hidróxi-3-(3-metilbut-2-enil)naftaleno-1,4-dione), ionização por impacto de elétrons 70 eV.



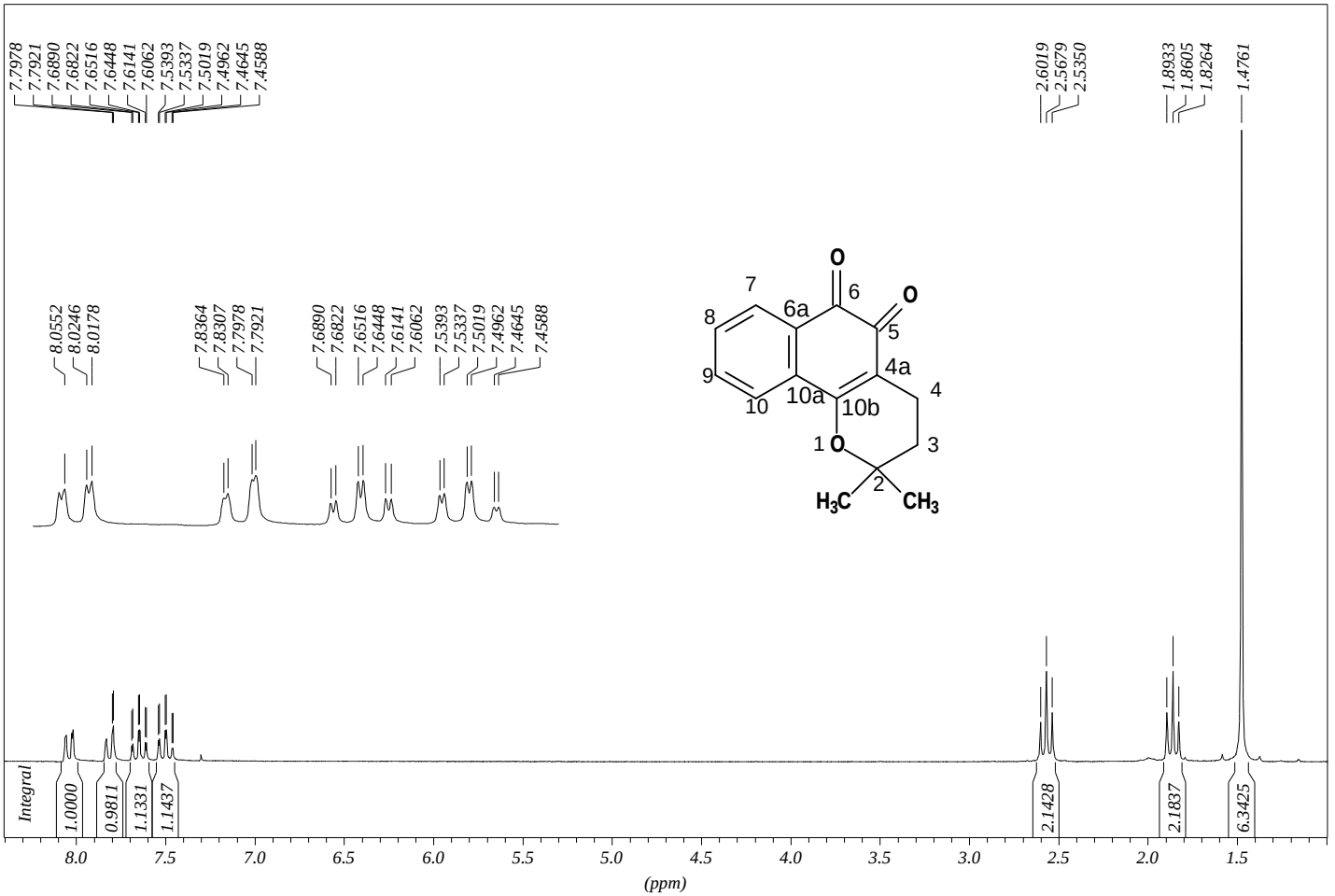
Espectro 3 – RMN ^{1}H (200 MHz) do lapachol (2-hidróxi-3-(3-metilbut-2-enil)naftaleno-1,4-diona), em $CDCl_3$.



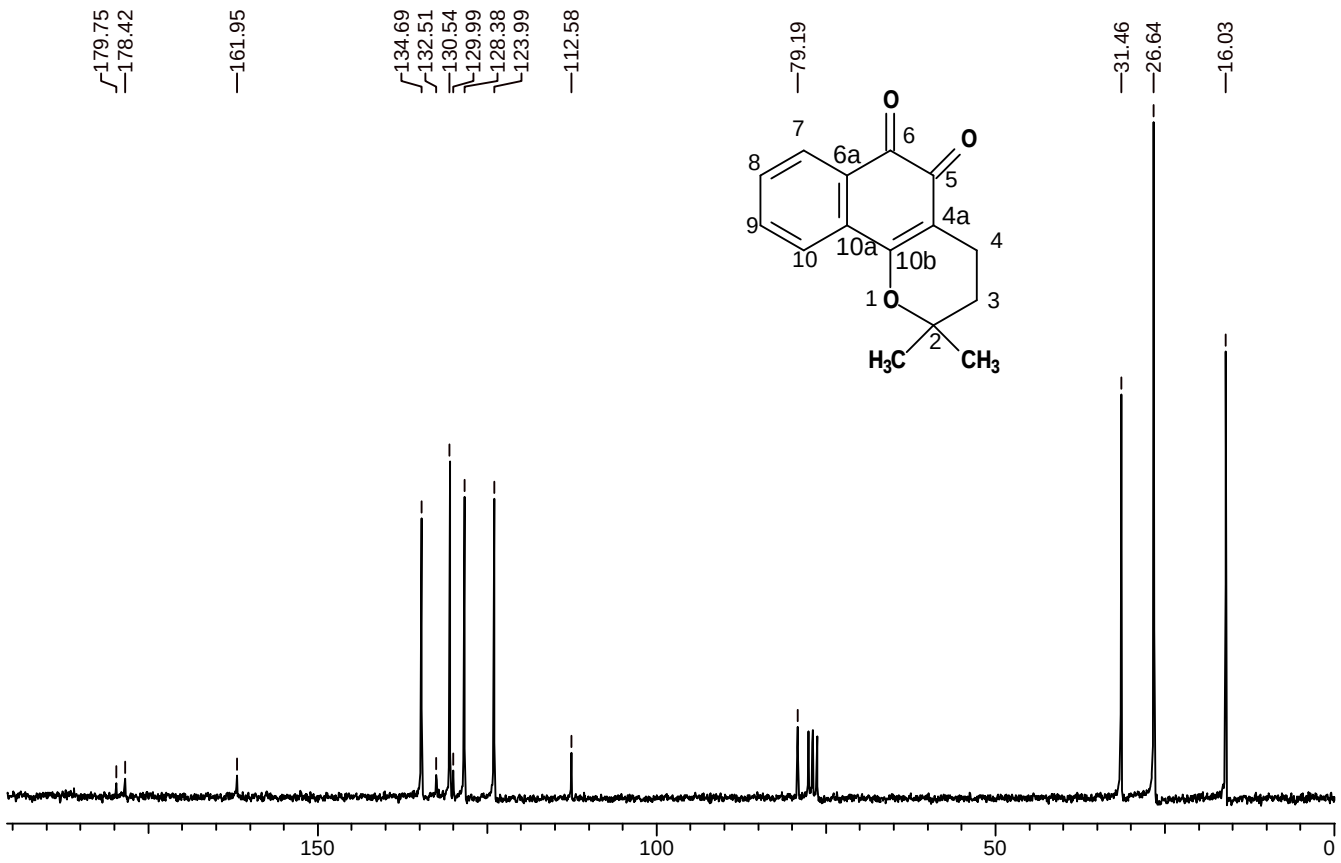
Espectro 4 – RMN ^{13}C (50,3 MHz) do lapachol (2-hidróxi-3-(3-metilbut-2-enil)naftaleno-1,4-diona)**.**



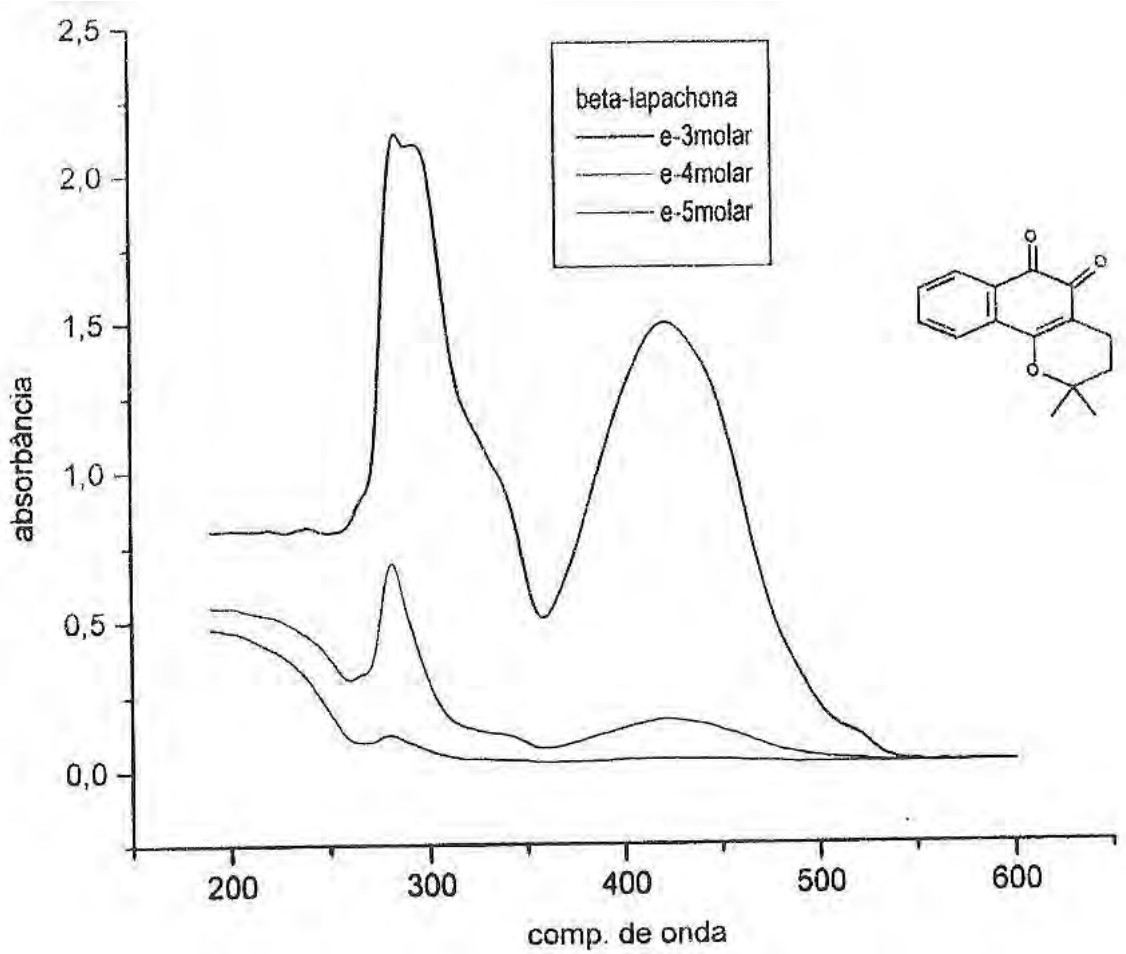
Espectro 5 – Infravermelho da β-lapachona 2,2-dimetil-3,4-di-hidro-*2H*-benzo[*h*]cromeno-5,6-diona), em pastilha de KBr.



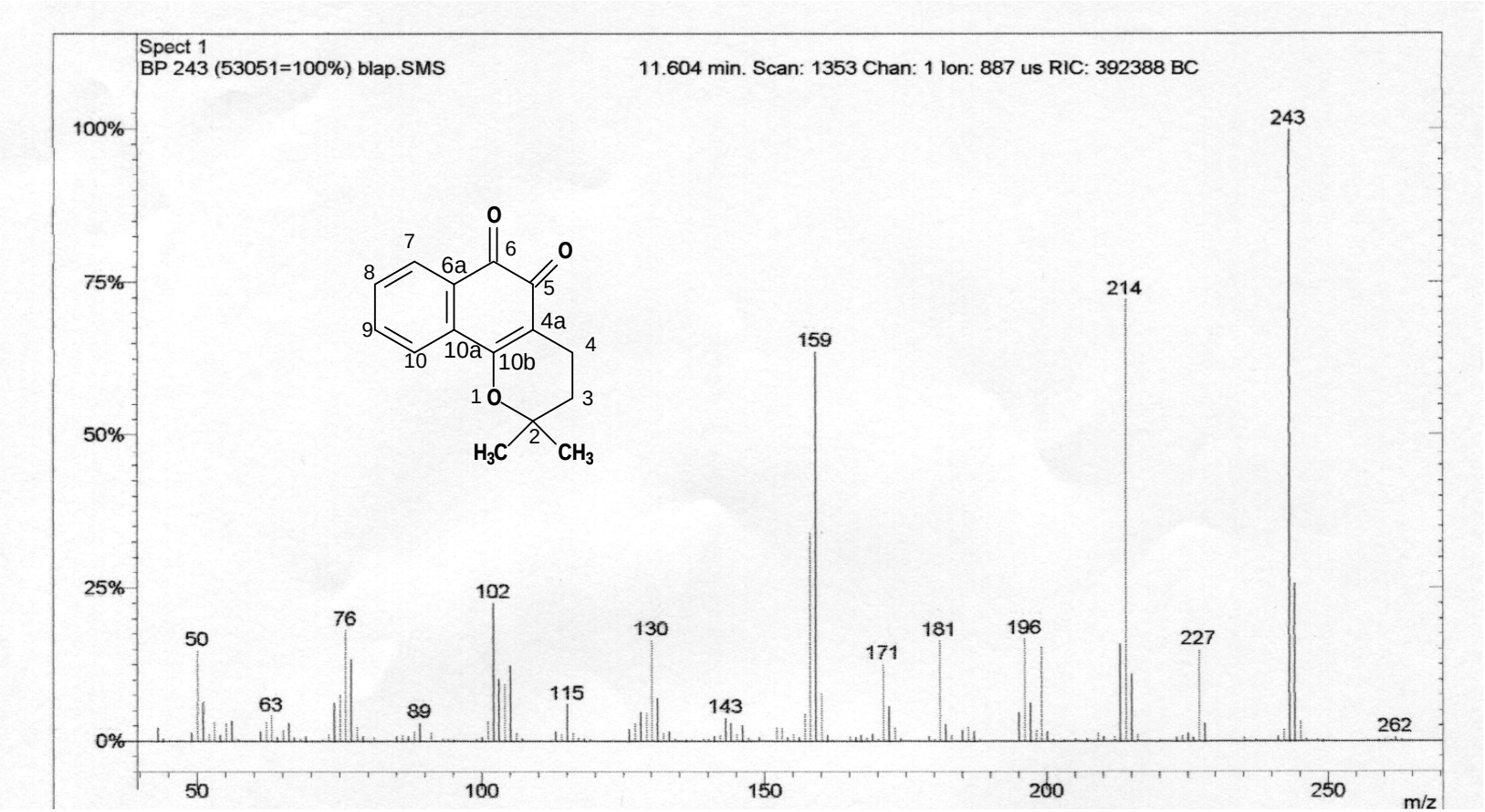
Espectro 6 – RMN ^{1}H (200 MHZ) da β-lapachona (2,2-dimetil-3,4-di-hidro-*2H*-benzo[*h*]cromeno-5,6-diona).



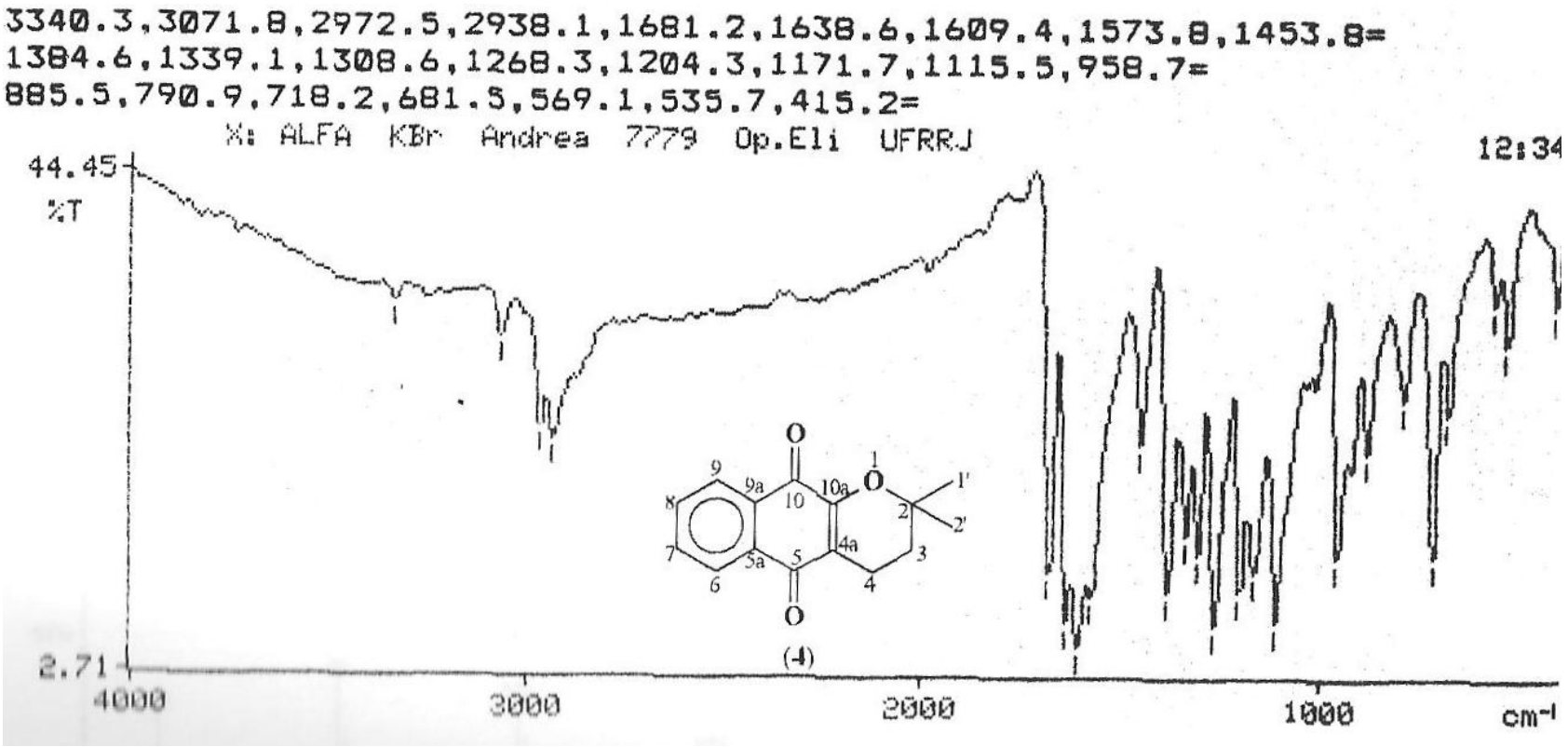
Espectro 7 – RMN ^{13}C (50,3 MHZ)da β-lapachona (2,2-dimetil-3,4-di-hidro-*2H*-benzo[*h*]cromeno-5,6-diona).



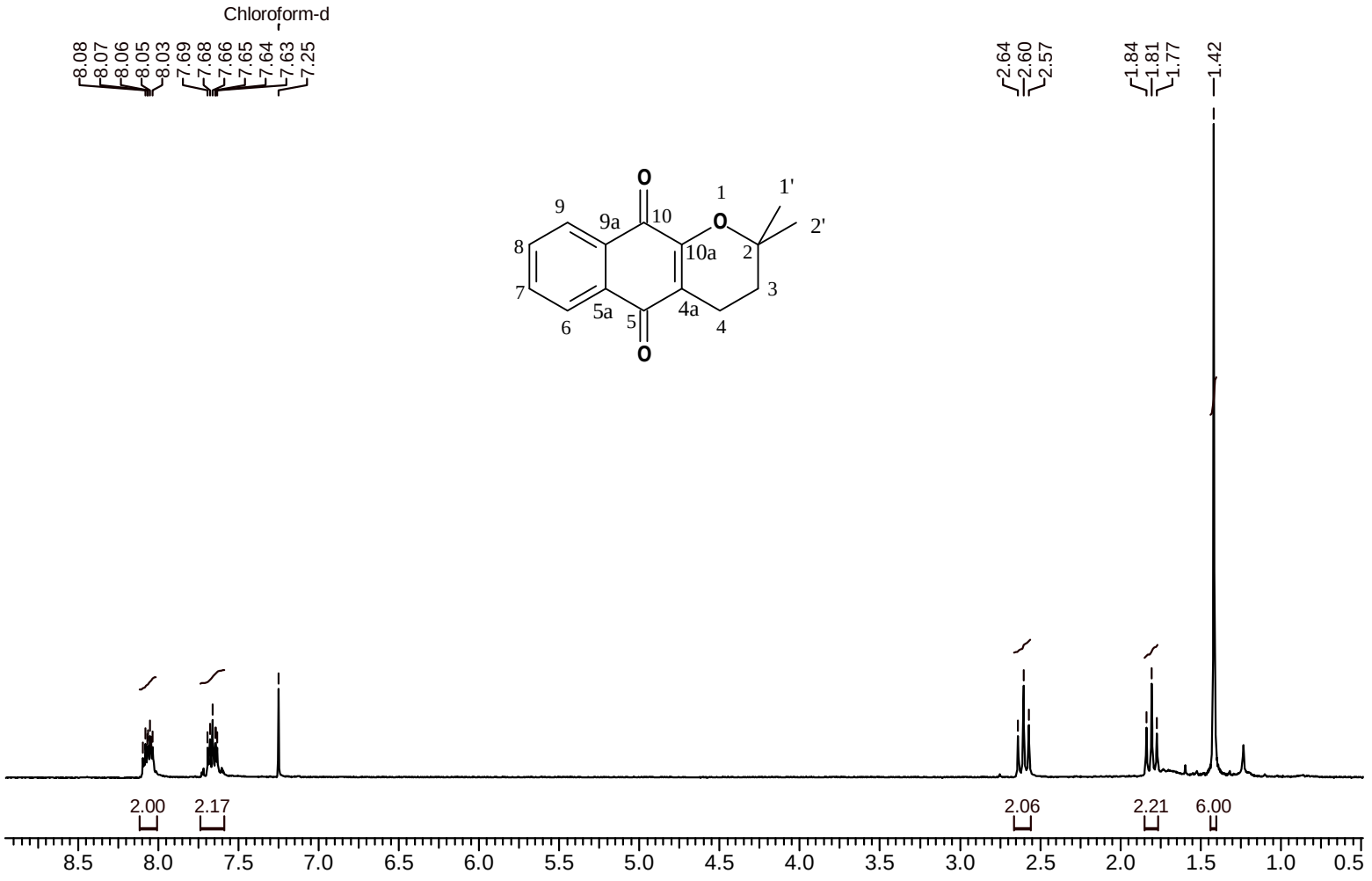
Espectro 8 – UV da β-lapachona (2,2-dimetil-3,4-di-hidro-*2H*-benzo[*h*]cromeno-5,6-diona)**.**



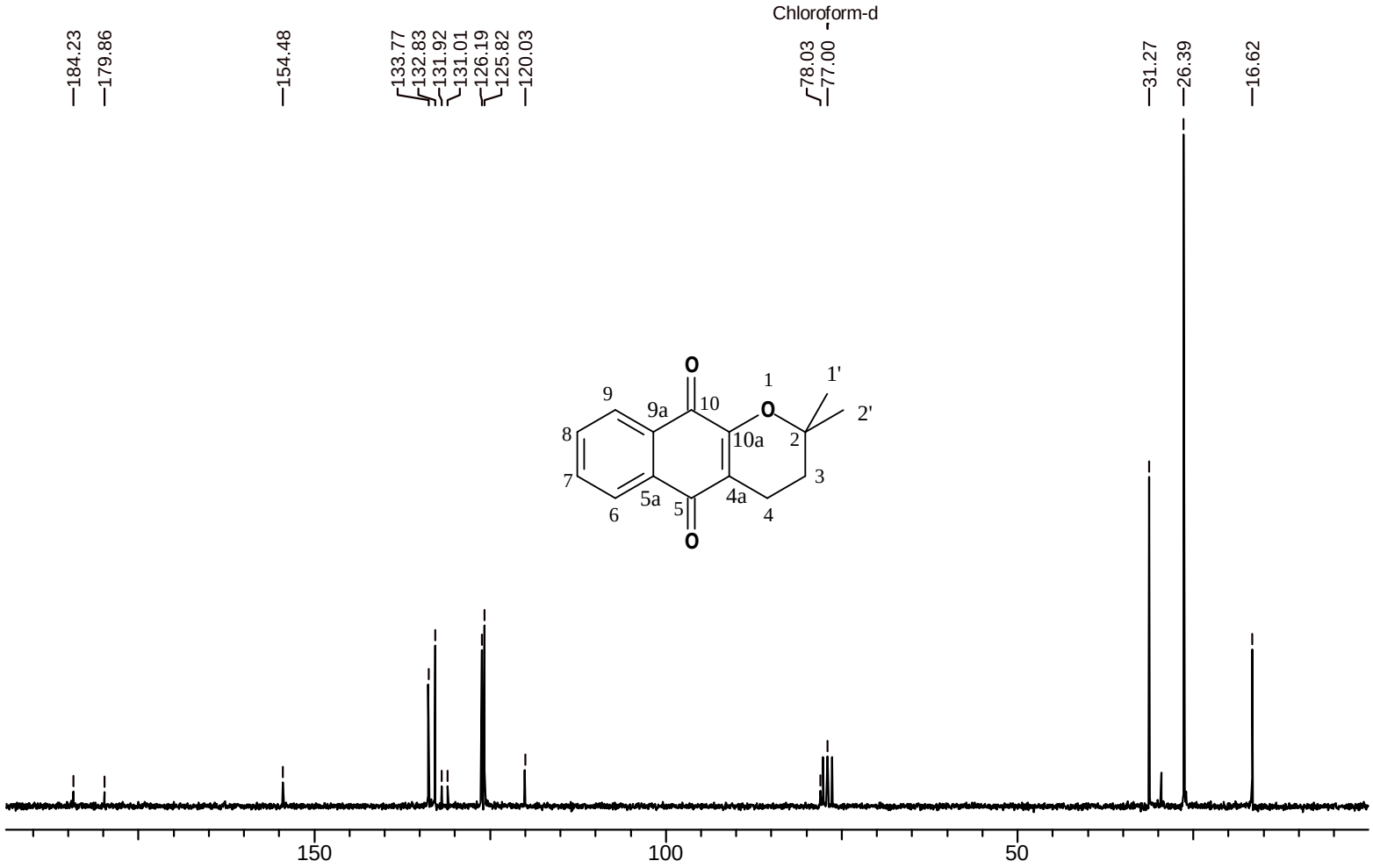
Espectro 9 – E.M. da β-lapachona (2,2-dimetil-3,4-di-hidro-*2H*-benzo[*h*]cromeno-5,6-diona).



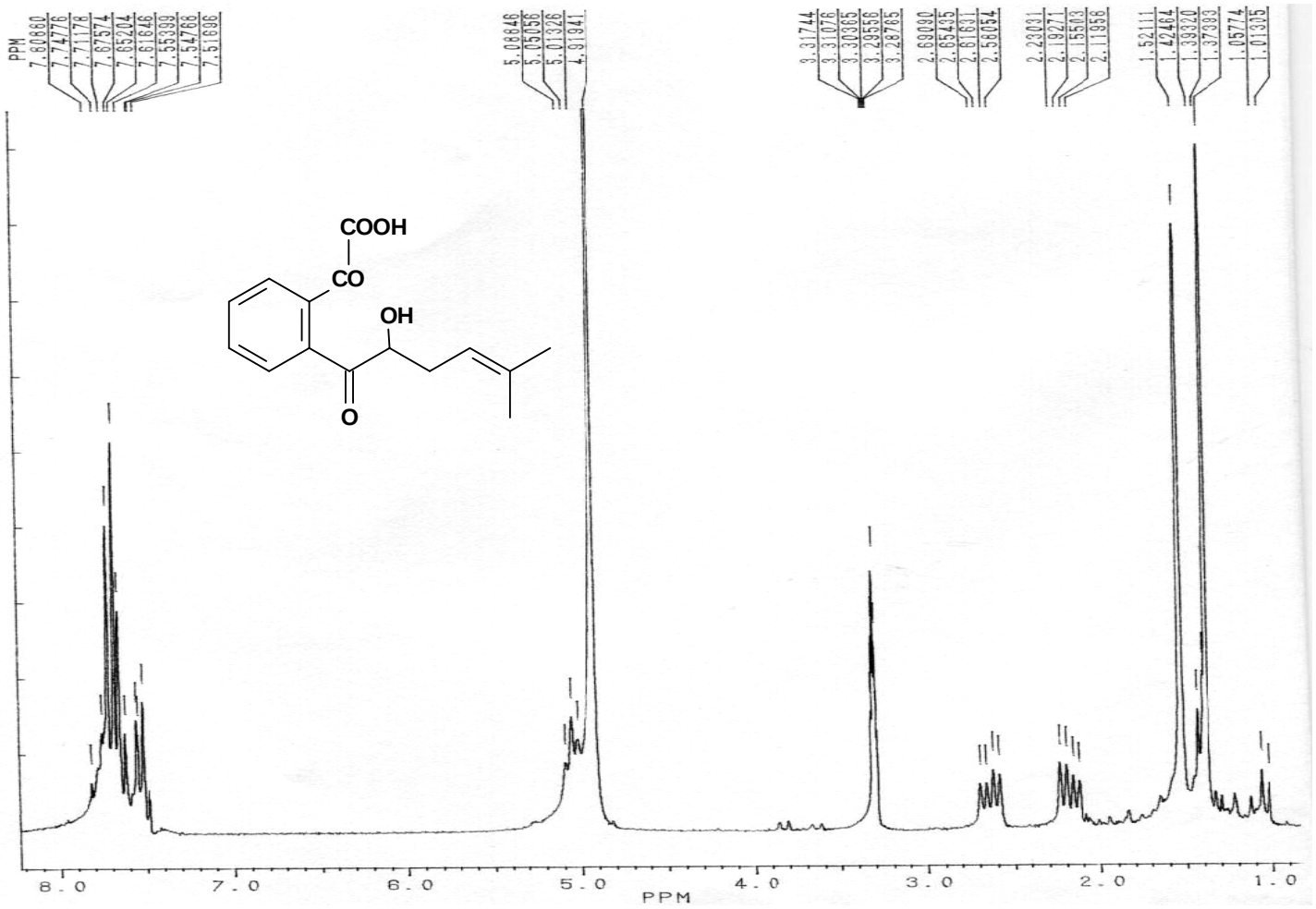
Espectro 10 – IV da α-lapachona (2,2-dimetil-3,4-di-hidro-2*H*-benzo[*g*]cromeno-5,10-diona)**.**



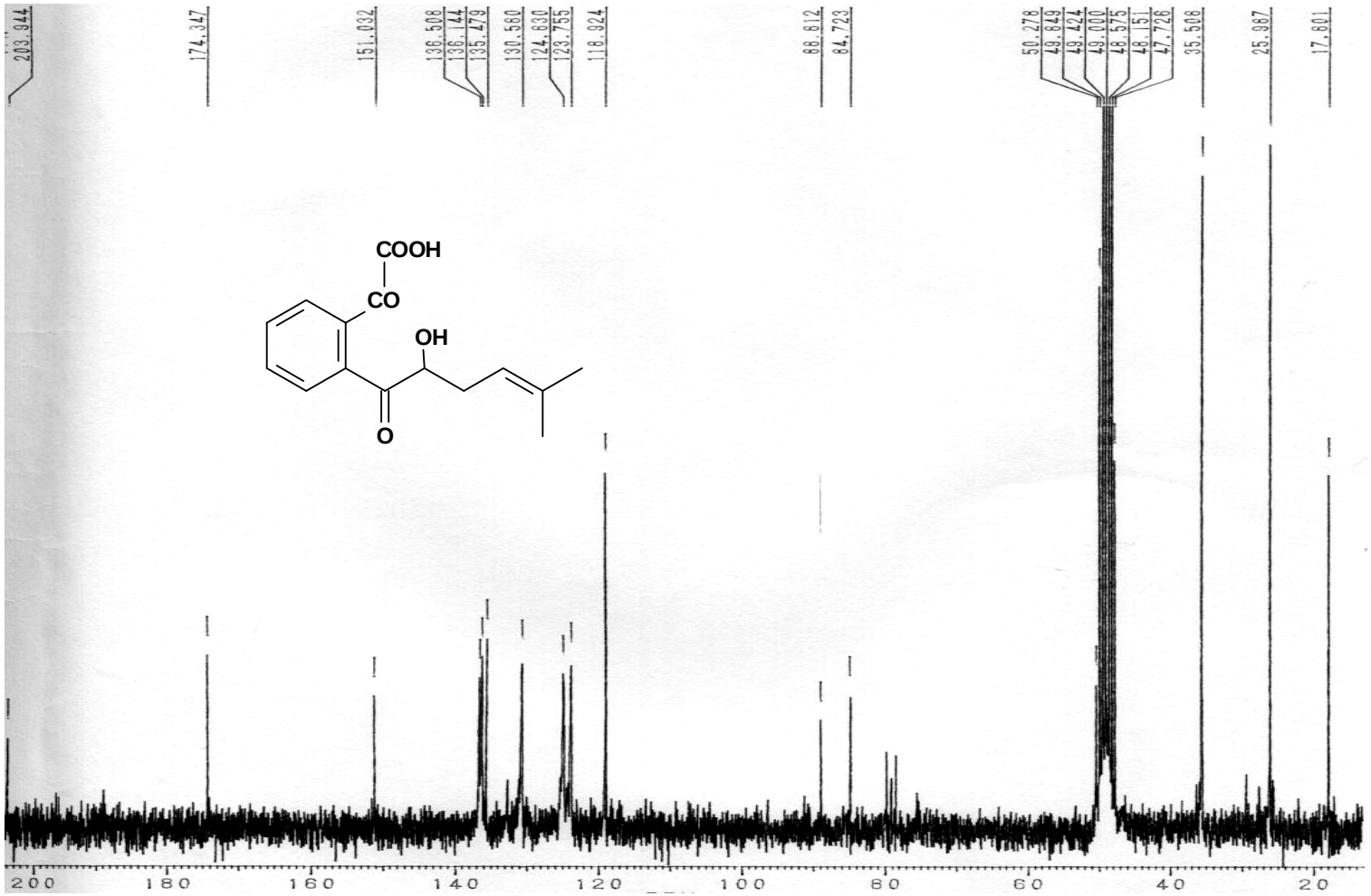
Espectro 11 – RMN ^{1}H (200 MHZ)da α-lapachona (2,2-dimetil-3,4-di-hidro-2*H*-benzo[*g*]cromeno-5,10-diona).



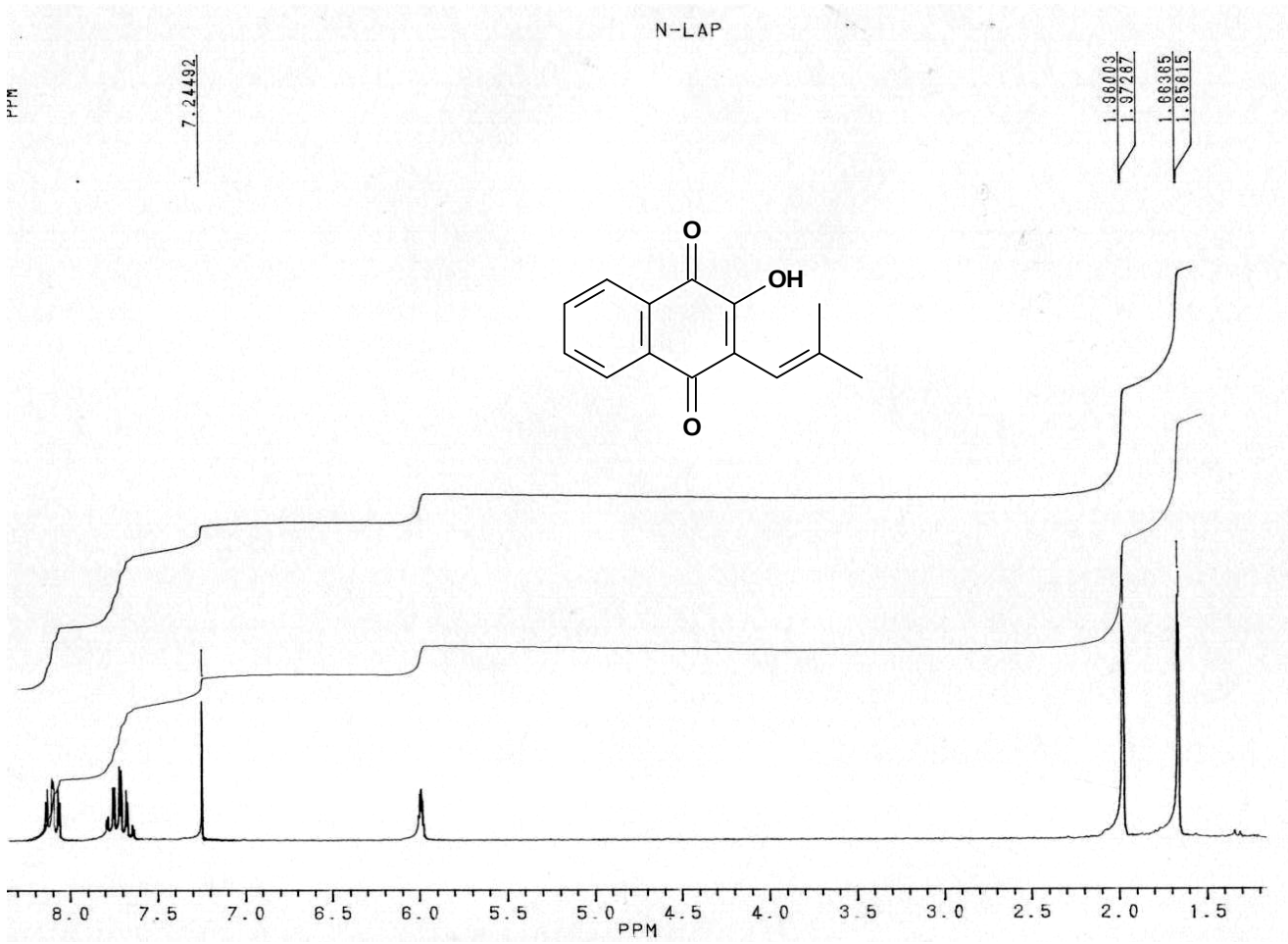
Espectro 12 - RMN ^{13}C (50,3 MHZ) da α-lapachona (2,2-dimetil-3,4-di-hidro-2*H*-benzo[*g*]cromeno-5,10-diona).



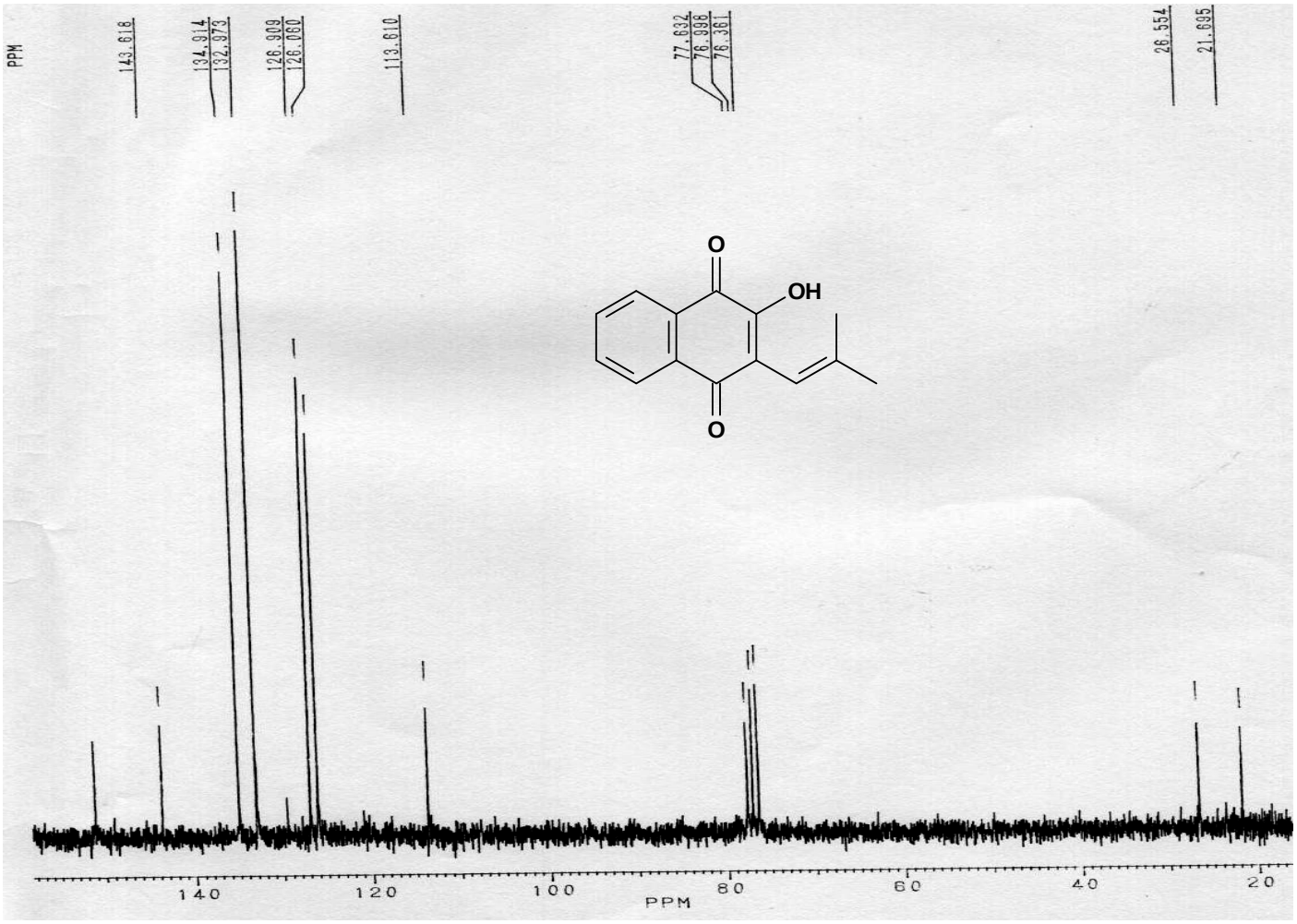
Espectro 13 – RMN ^{1}H (200 MHz) do cetol (Ácido 2-(2-hidroxi-5-metil-hex-4-enoila)fenil)(oxo)acético) intermediário do lapachol e nor-lapachol, , em DMSO.



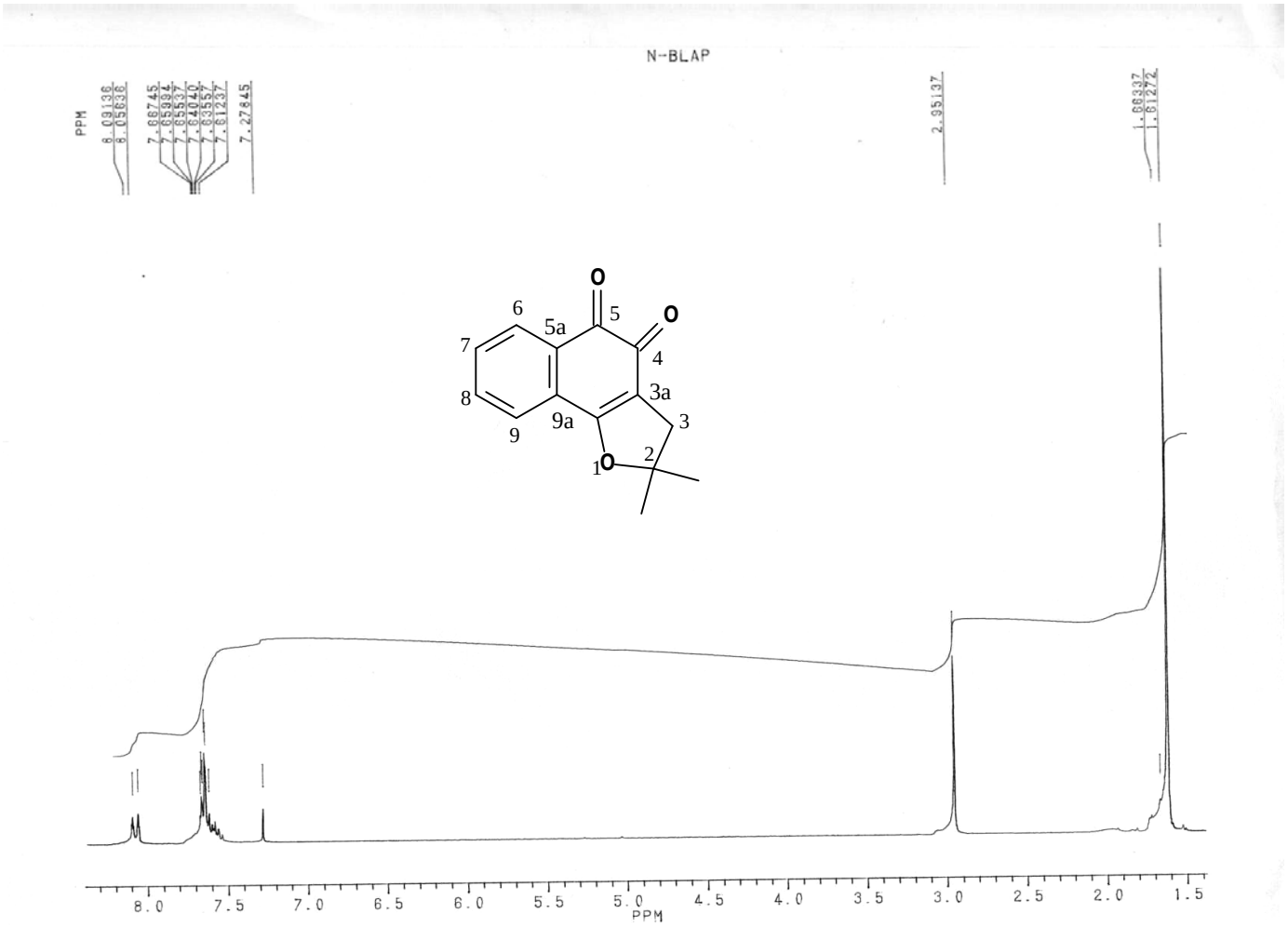
Espectro 14 – RMN ^{13}C (50,3 MHz) do cetol (Ácido 2-(2-hidroxi-5-metil-hex-4-enoila)fenil)(oxo)acético) intermediário do lapachol e norlapachol.



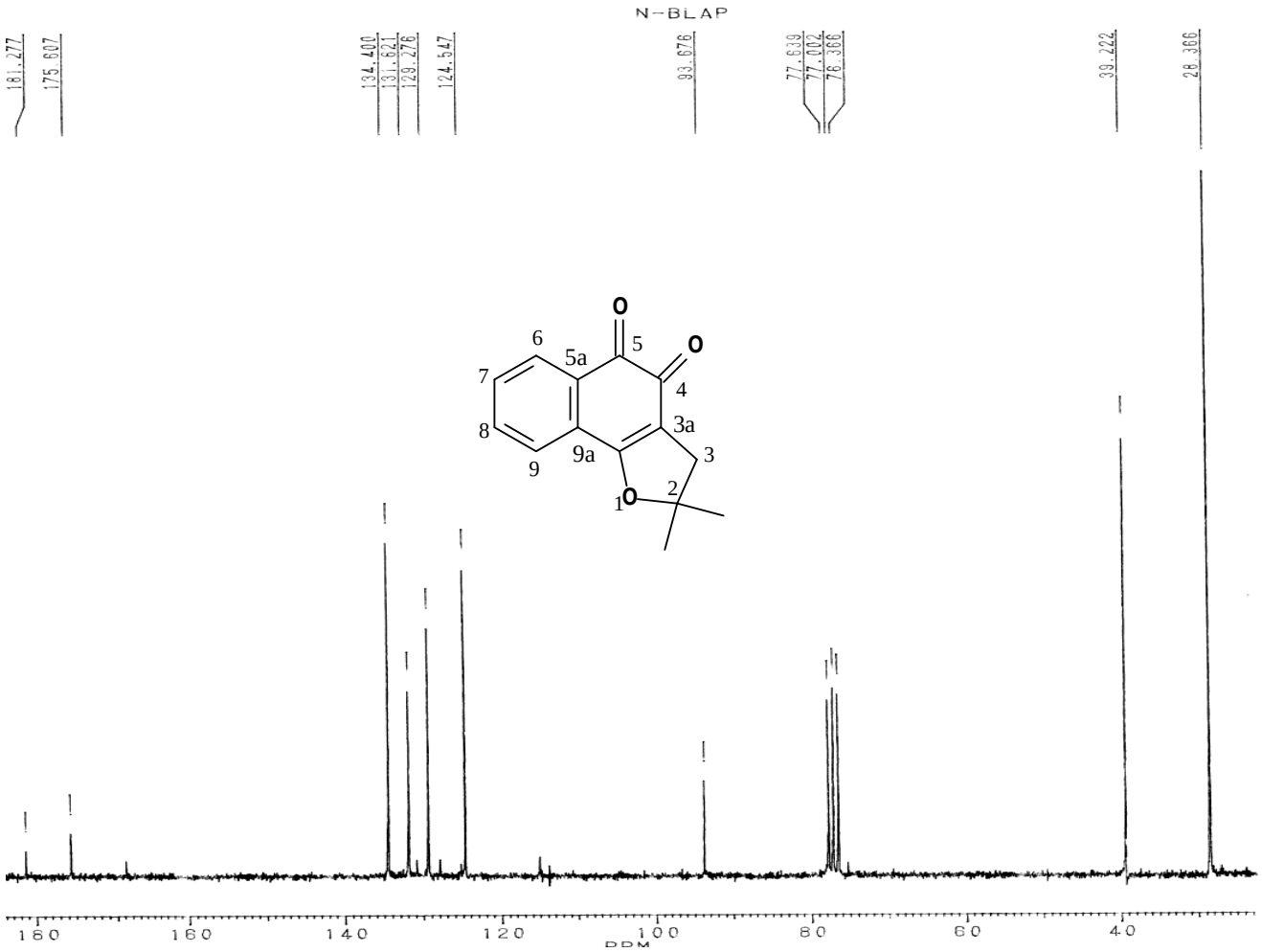
Espectro 15 – RMN ^{1}H (200 MHz) do norlapachol (2-hidróxi-3-(2-metilprop-1-enil)naftaleno-1,4-diona).



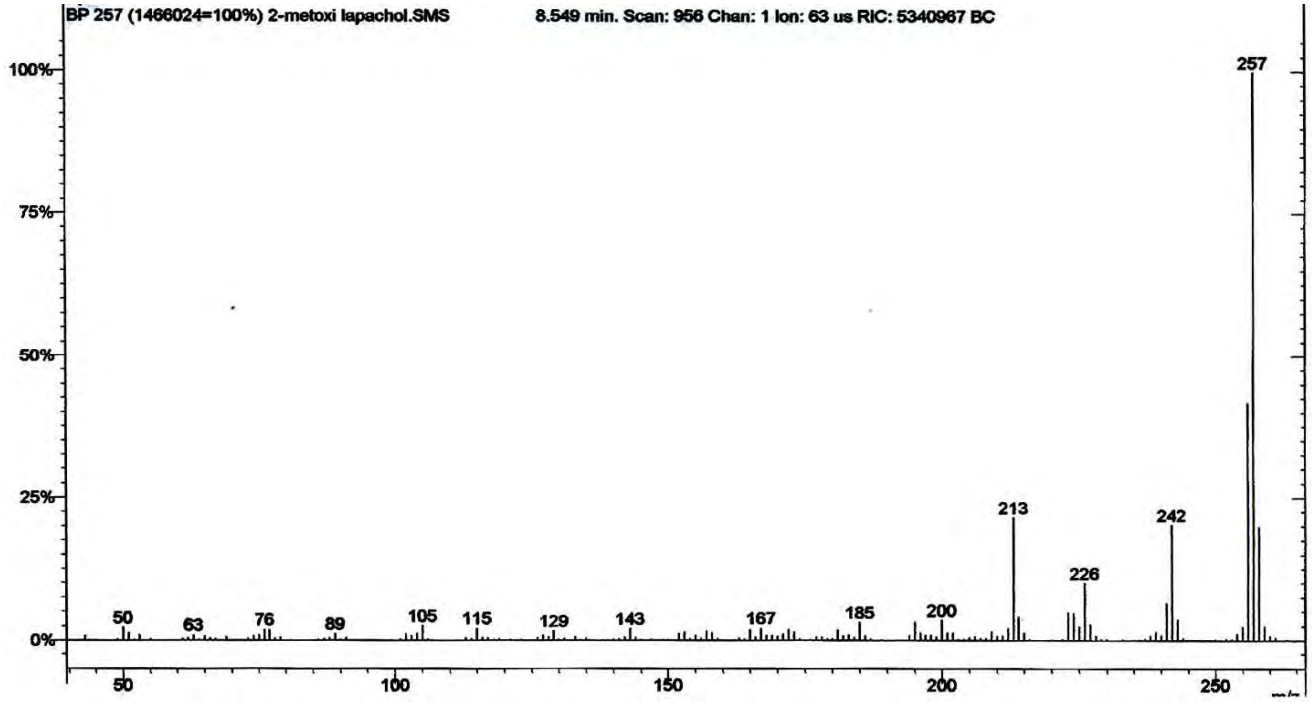
Espectro 16 – RMN ^{13}C (50,3 MHz) do norlapachol (2-hidróxi-3-(2-metilprop-1-enil)naftaleno-1,4-diona)**.**



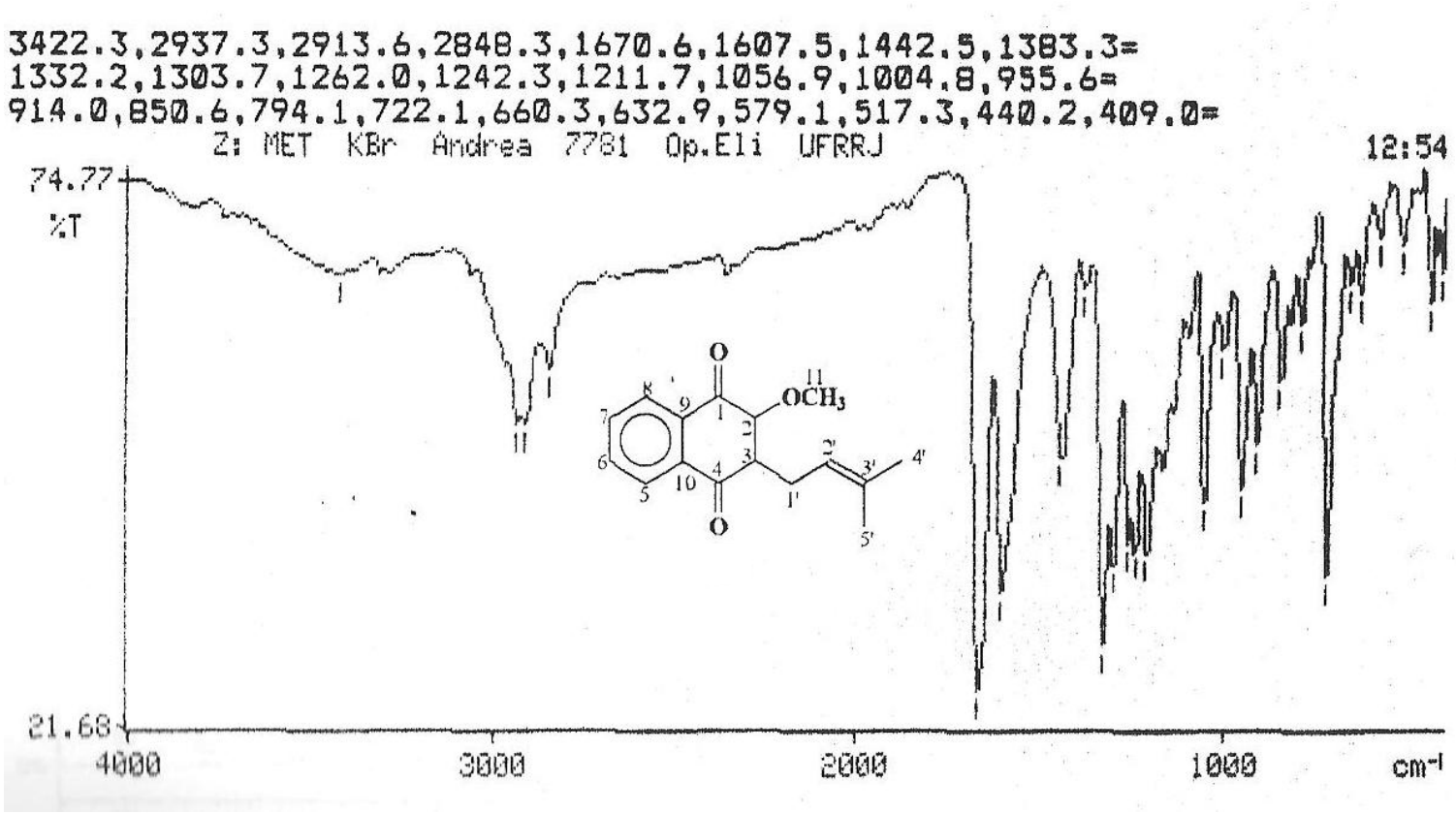
Espectro 17 – RMN ^{1}H (200 MHz) da nor-β-lapachona (2,2-dimetil-2,3-di-hidronafto[1,2-*b*]furano-4,5-diona).



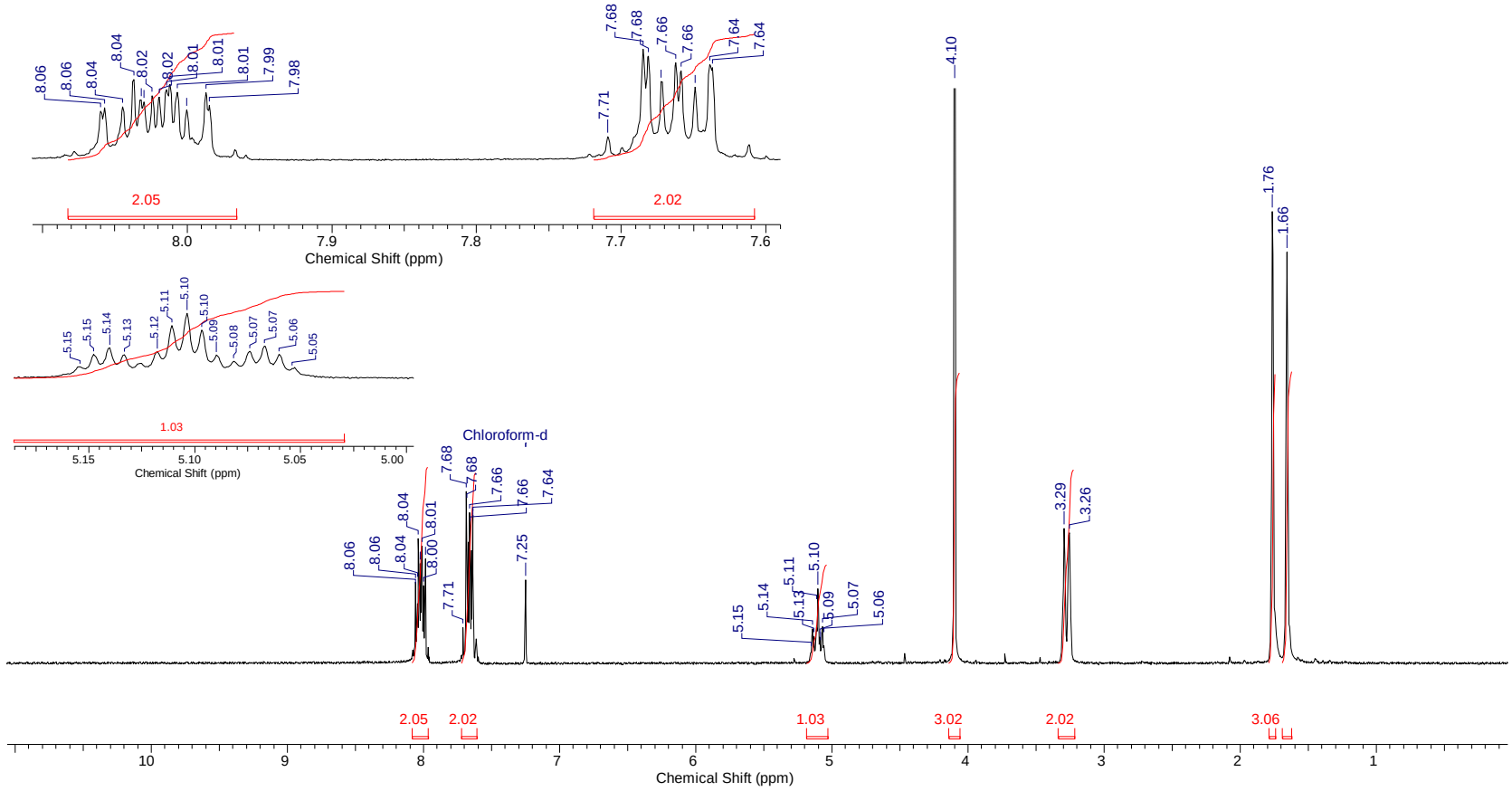
Espectro 18 – RMN ^{13}C (50,3 MHz) da nor-β-lapachona (2,2-dimetil-2,3-di-hidronafto[1,2-*b*]furano-4,5-diona).



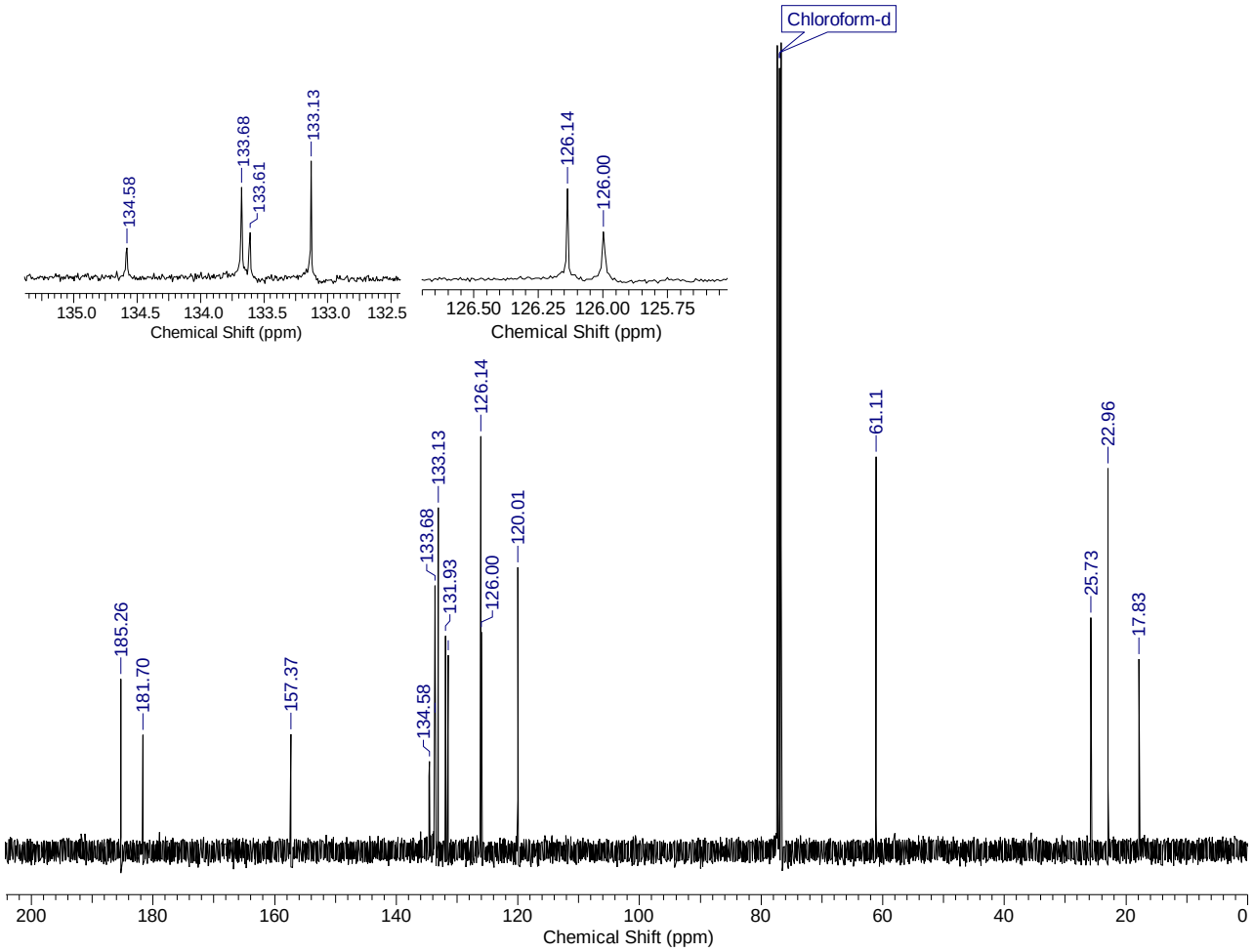
Espectro 19 – E.M. do 2-metóxilapachol (2-(3-metillbut-2-enil)-3-(metóxi)naftaleno-1,4-diona)**.**



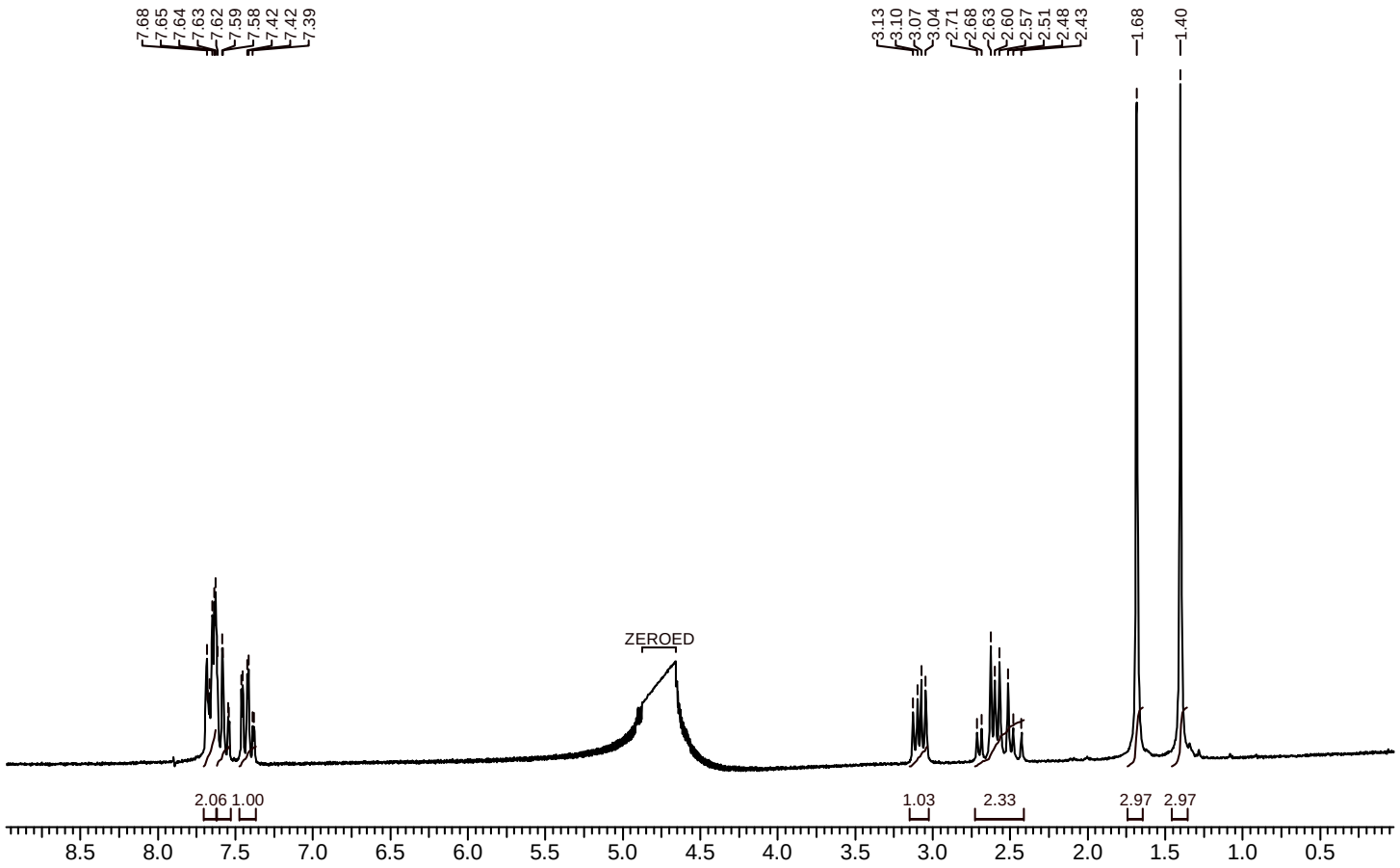
Espectro 20 – IV do 2-metóxilapachol (2-(3-metillbut-2-enil)-3-(metóxi)naftaleno-1,4-diona).



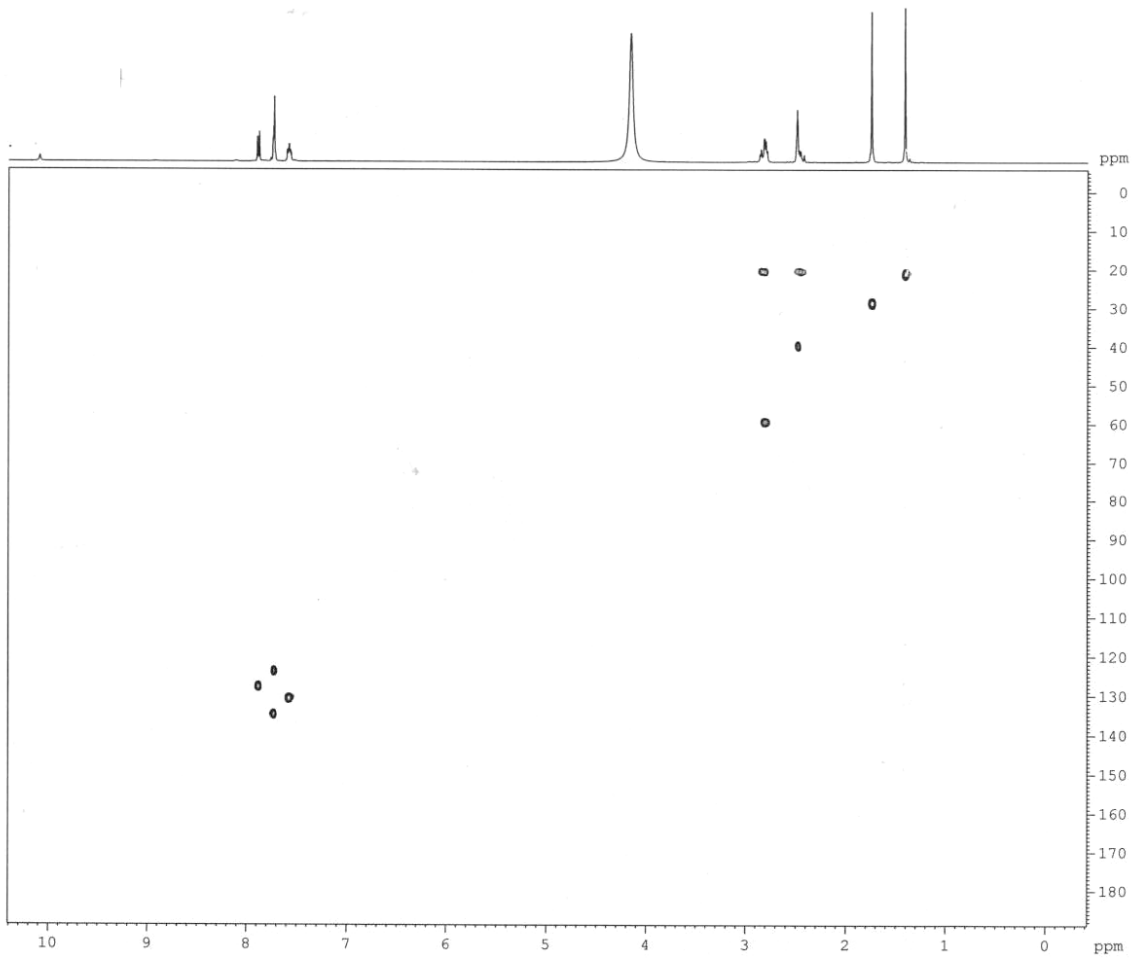
Espectro 21 - RMN ^{1}H (200 MHz) do2-metóxi-lapachol (2-(3-metillbut-2-enil)-3-(metóxi)naftaleno-1,4-diona).



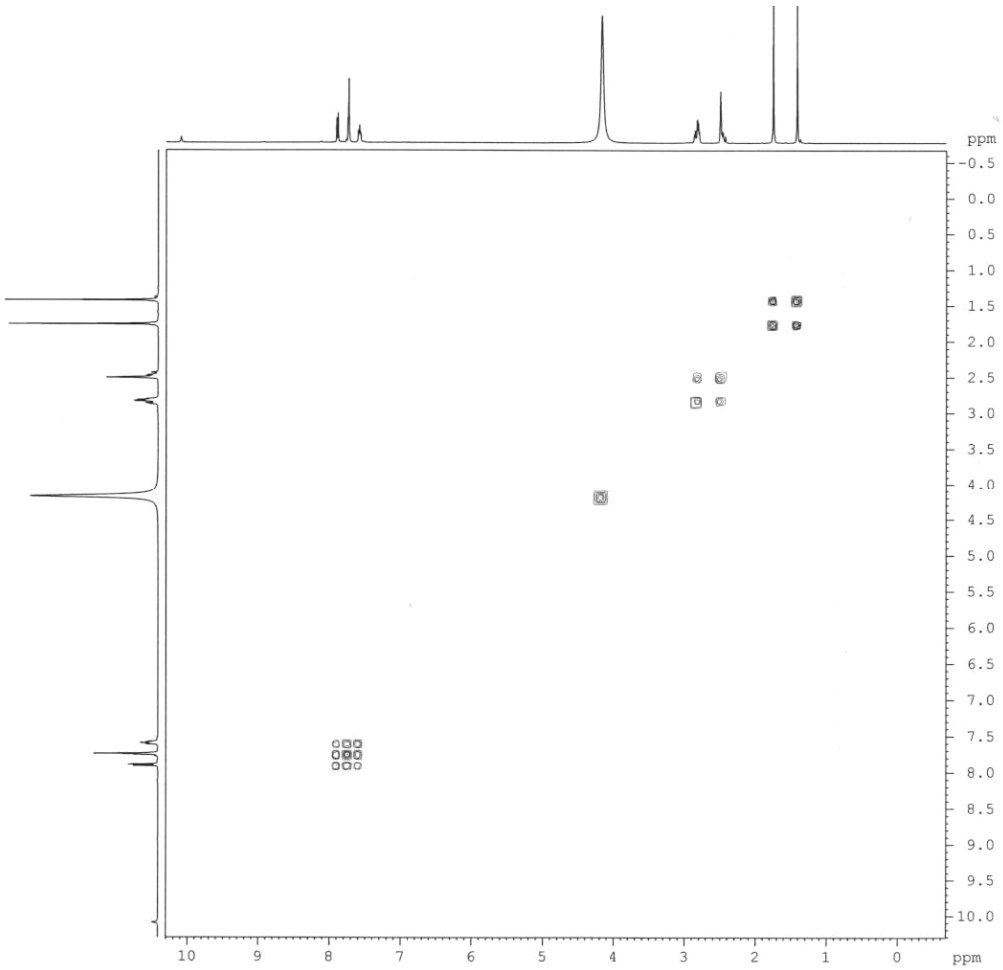
Espectro 22 - RMN ^{13}C (50,3 MHZ)do2-metóxi-lapachol (2-(3-metillbut-2-enil)-3-(metóxi)naftaleno-1,4-diona).



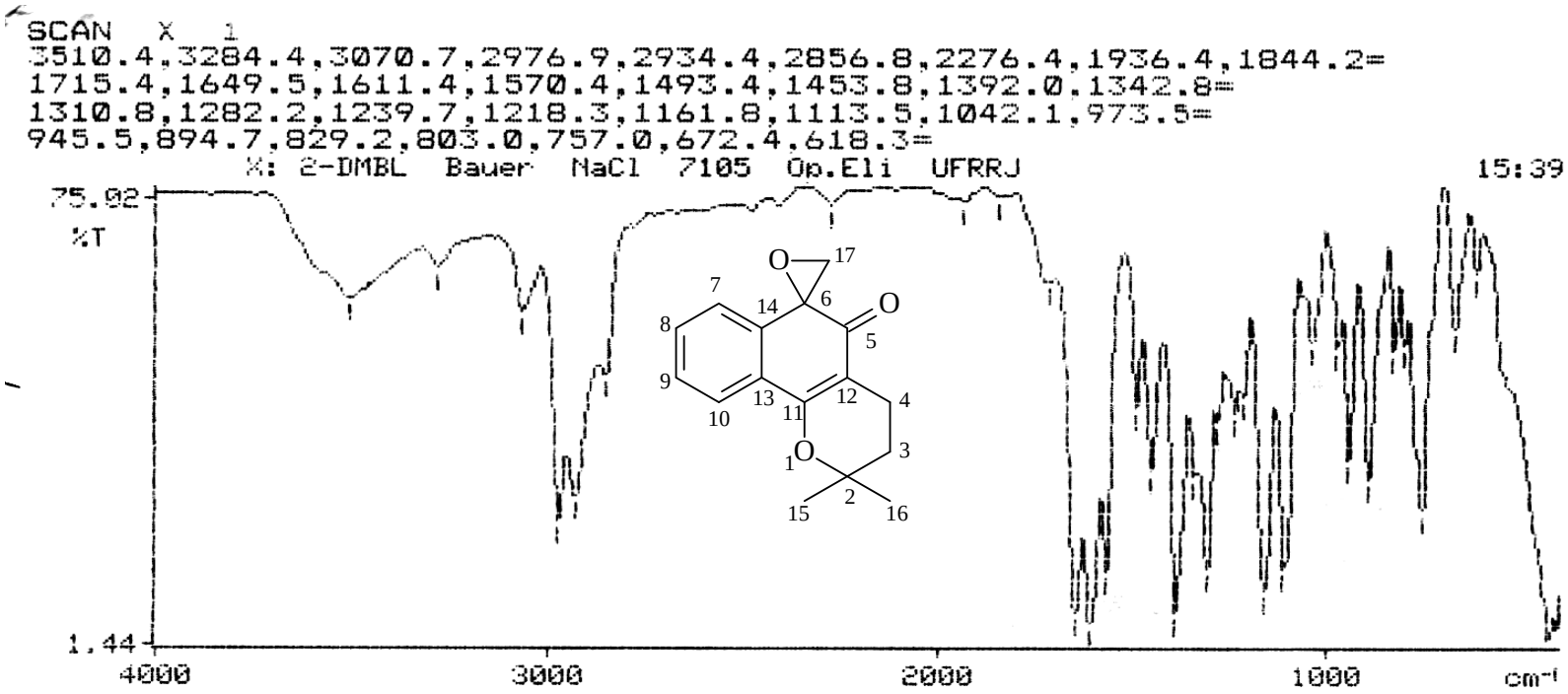
Espectro 23 – RMN ^{1}H (200 MHz) do ácido β-lapachona-3-sulfônico, em D_2O. Usou-se como padrão o sinal em 4,75 ppm para D_2O e a região correspondente a esse sinal foi suprimida para que os sinais da substância fossem vistos.



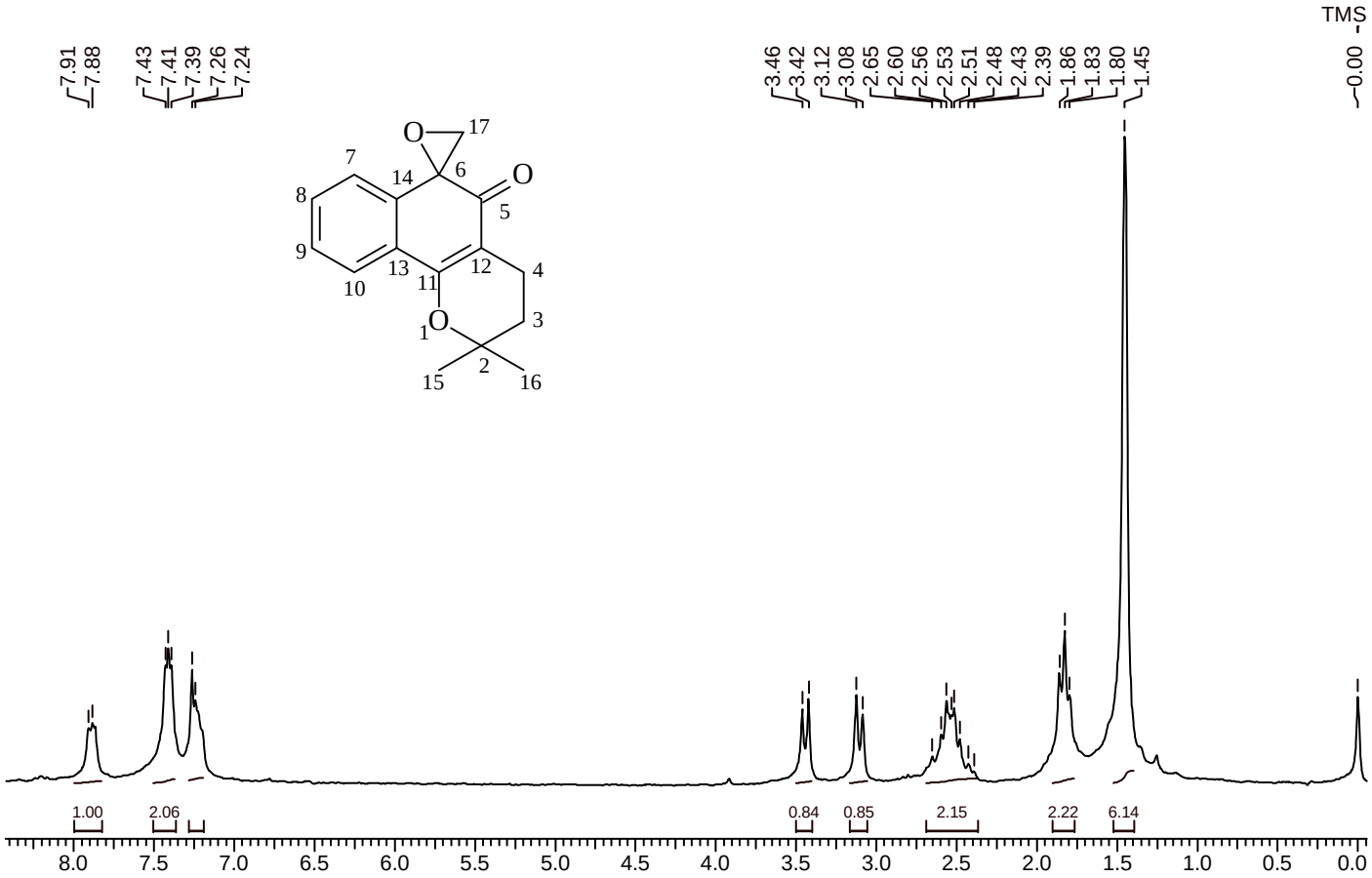
Espectro 24 – Experimento de HSQC, correlação heteronuclear ^{13}C x ^{1}H (400 MHz) do ácido β-lapachona-3-sulfônico.



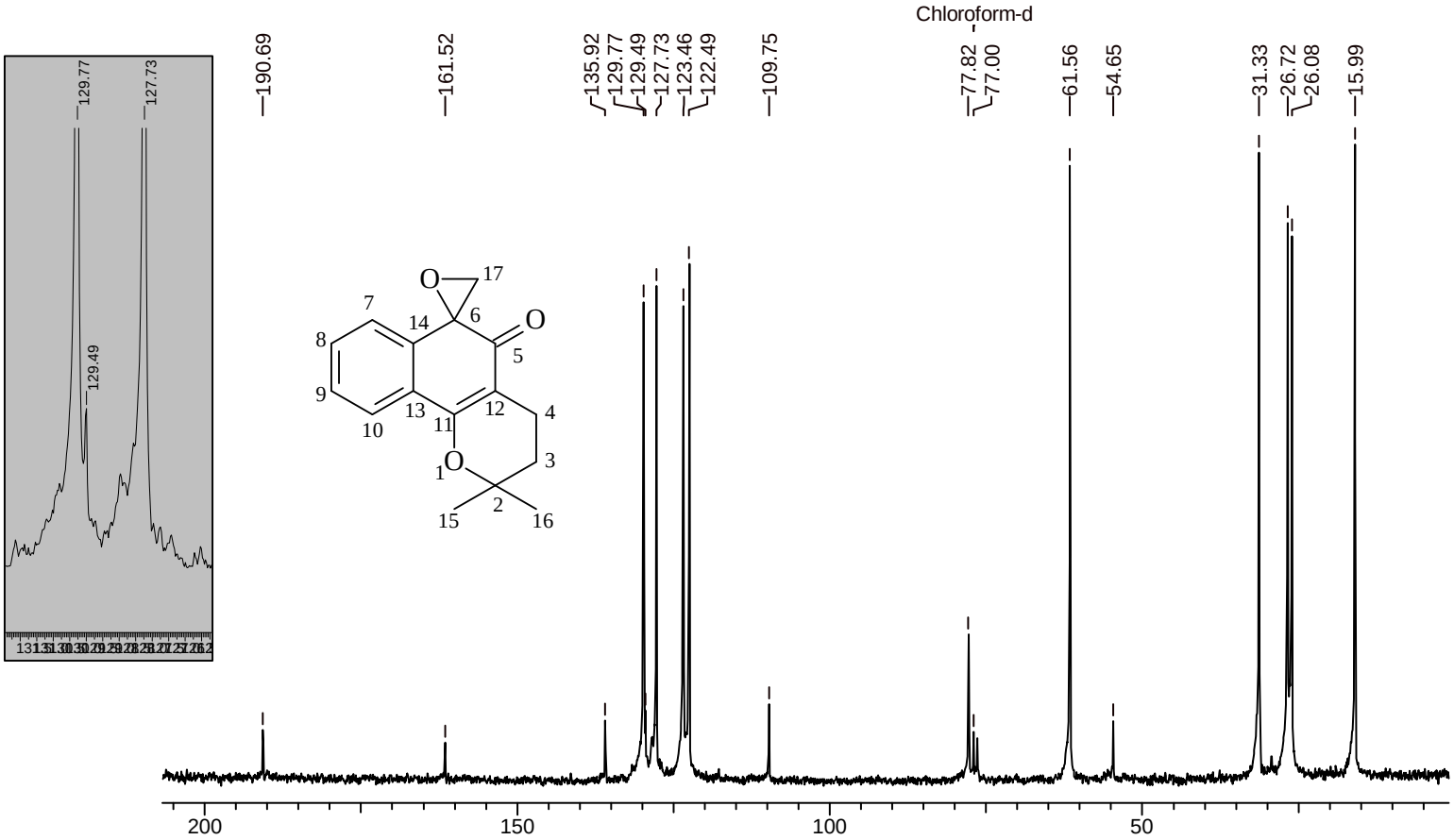
Espectro 25 – Correlação homonuclear (Cosy ^{1}H x ^{1}H) do ácido β-lapachona-3-sulfônico.



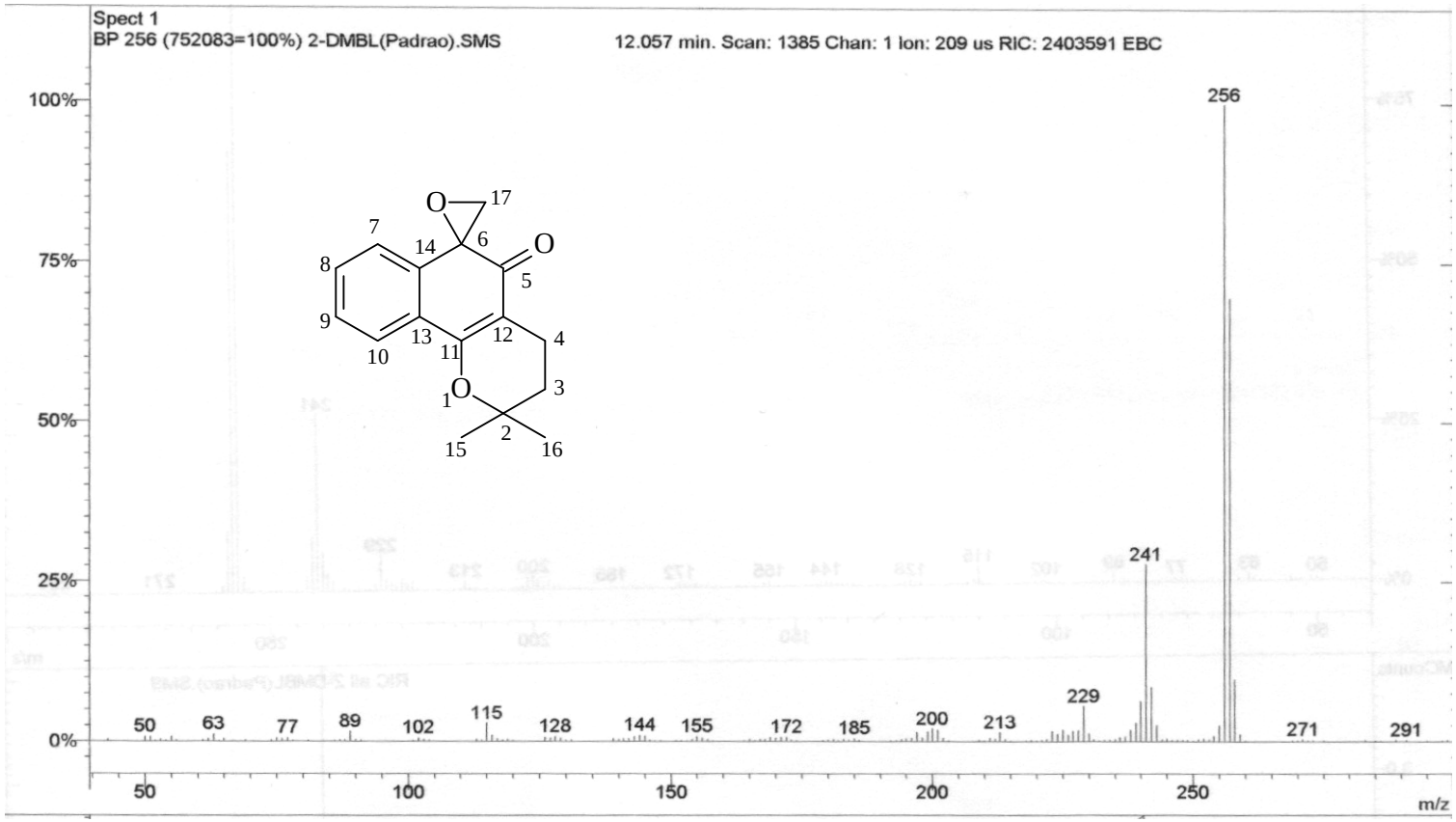
Espectro 26 – IV da 2DMBL (2,2-dimetil-espiro[3,4,5,6-tetra-hidro-2*H*-benzo[*h*]cromeno-6,2'-(di-hidro-oxirana)]-5-ona).



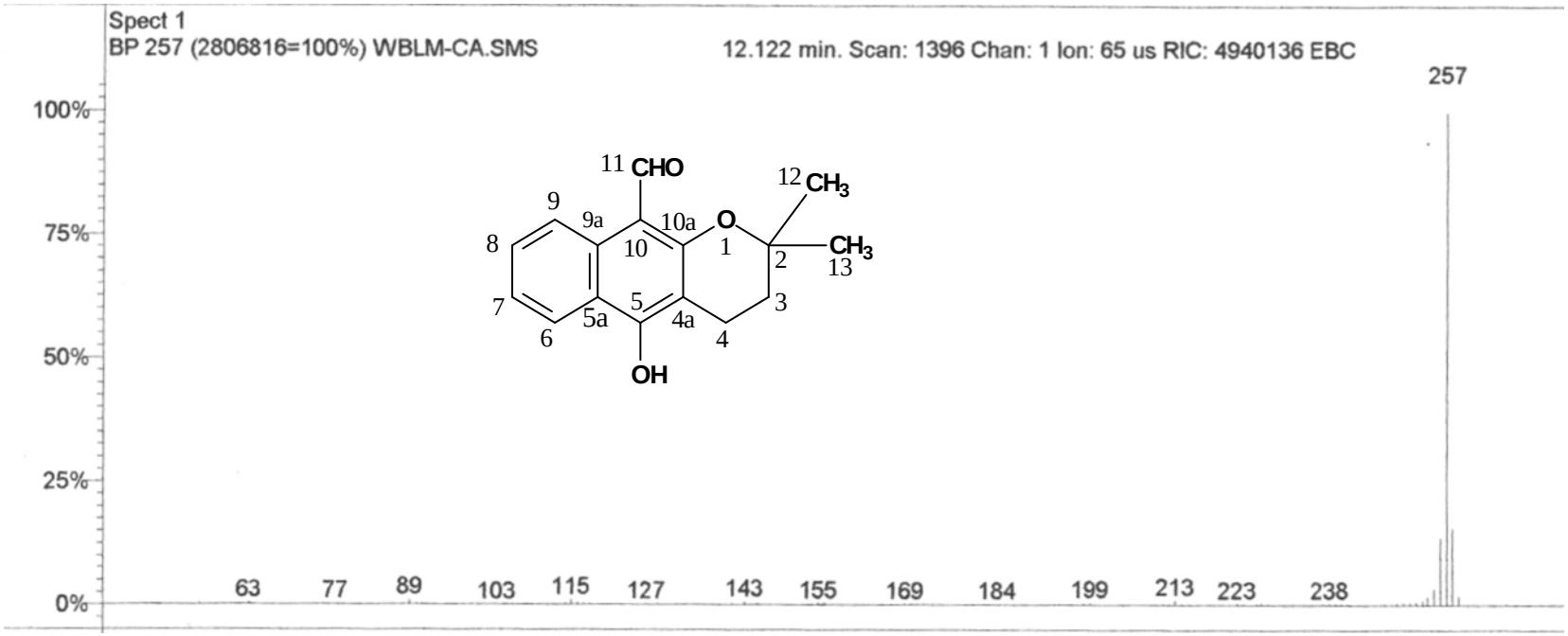
Espectro 27 – RMN ^{1}H (200 MHz)do 2DMBL**.**



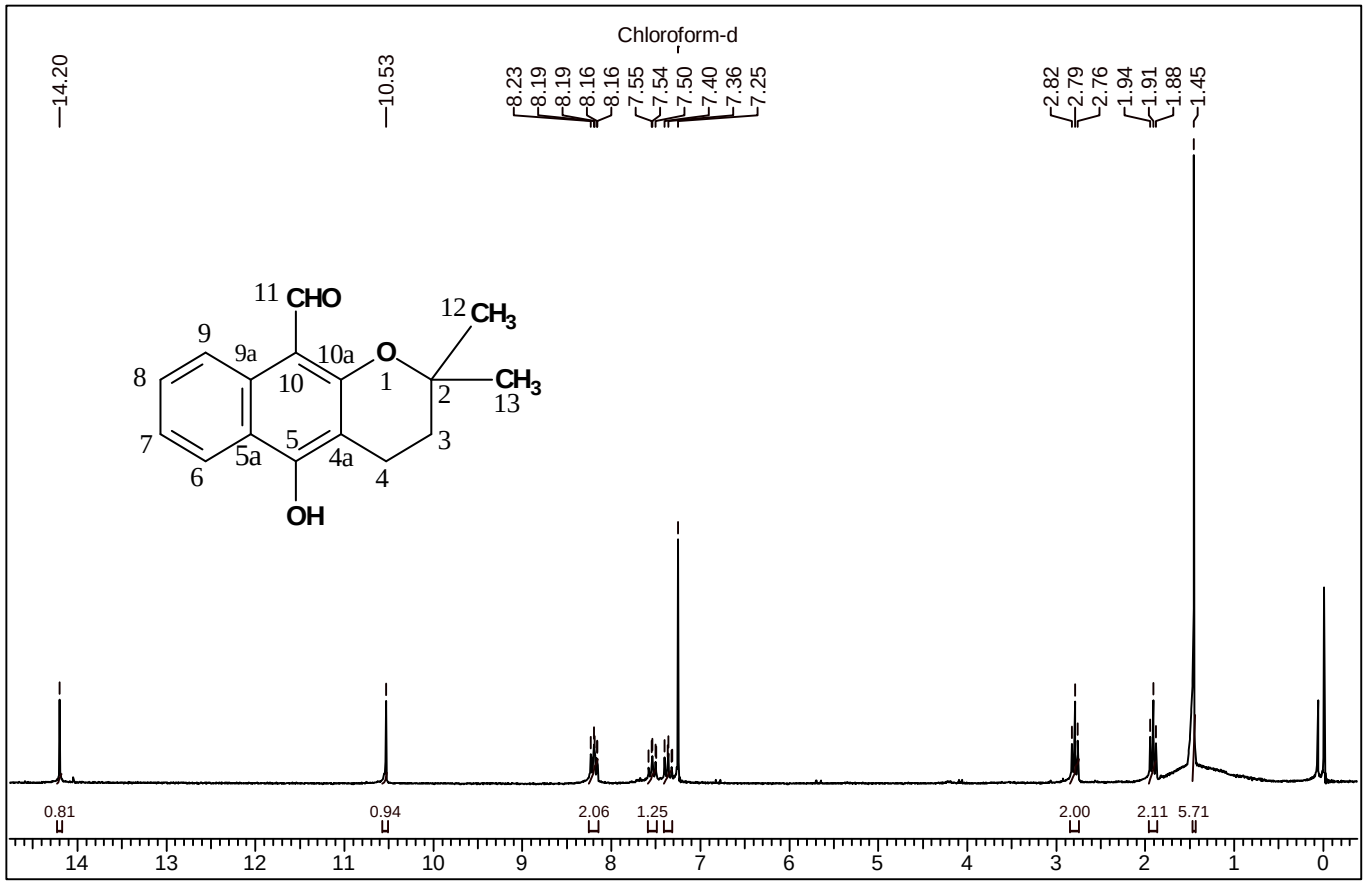
Espectro 28 – RMN ^{13}C (50,3 MHZ) do 2DMBL.



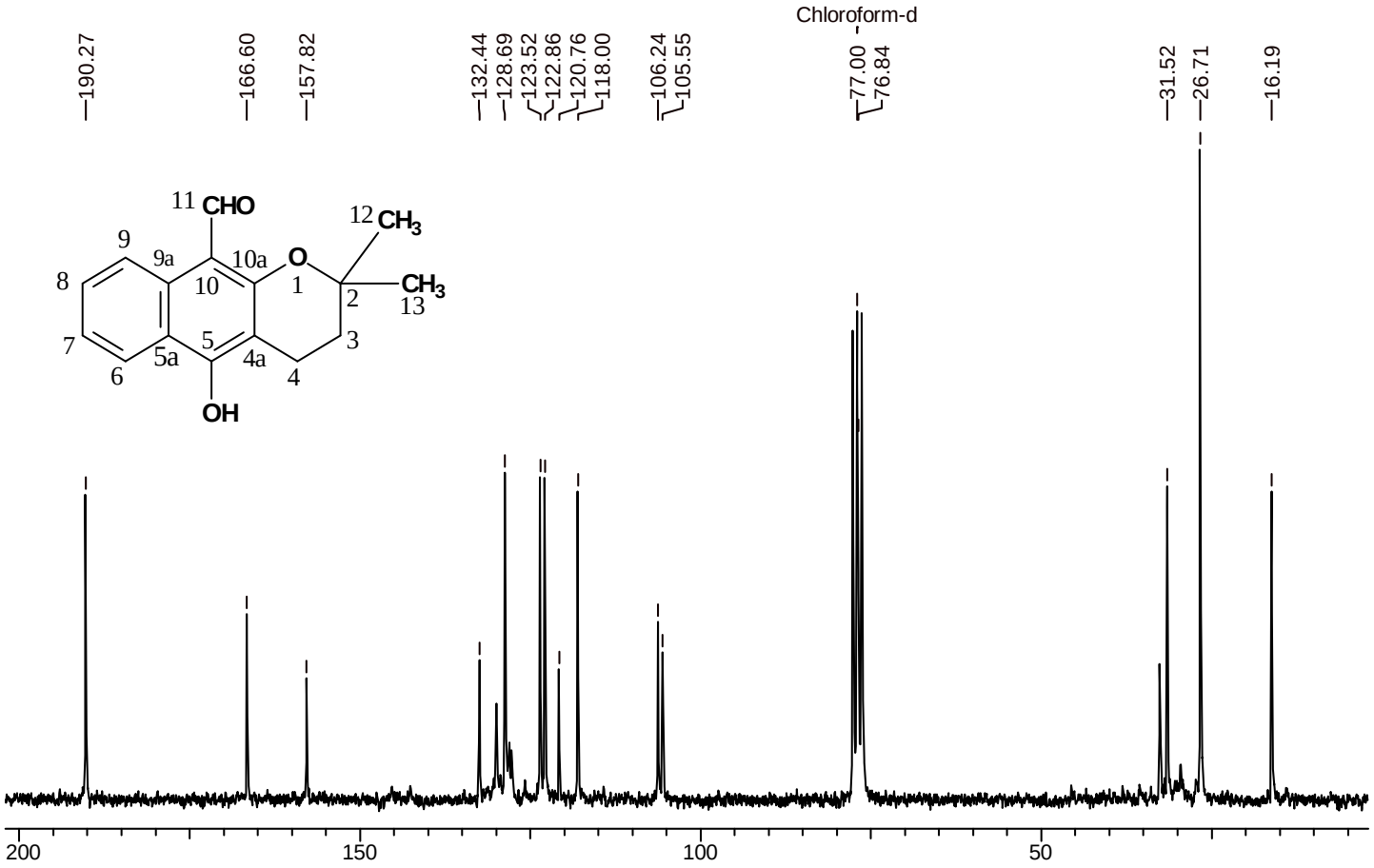
Espectro 29 – E.M. do 2DMBL.



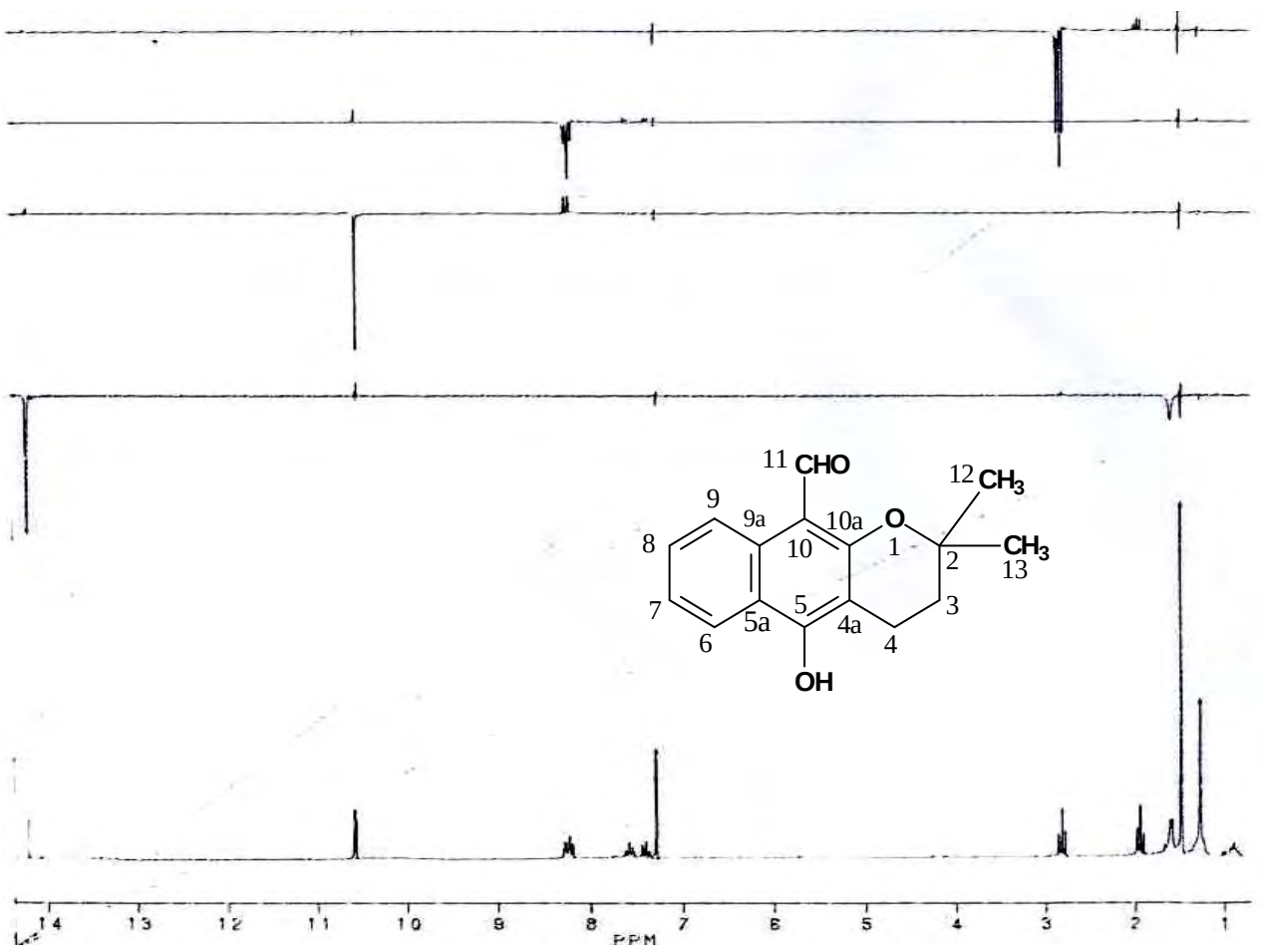
Espectro 30 – E.M. do ALVI (5-hidróxi-2,2-dimetil-3,4-di-hidro-2*H*-benzo[*g*]cromeno-10-carbaldeído).



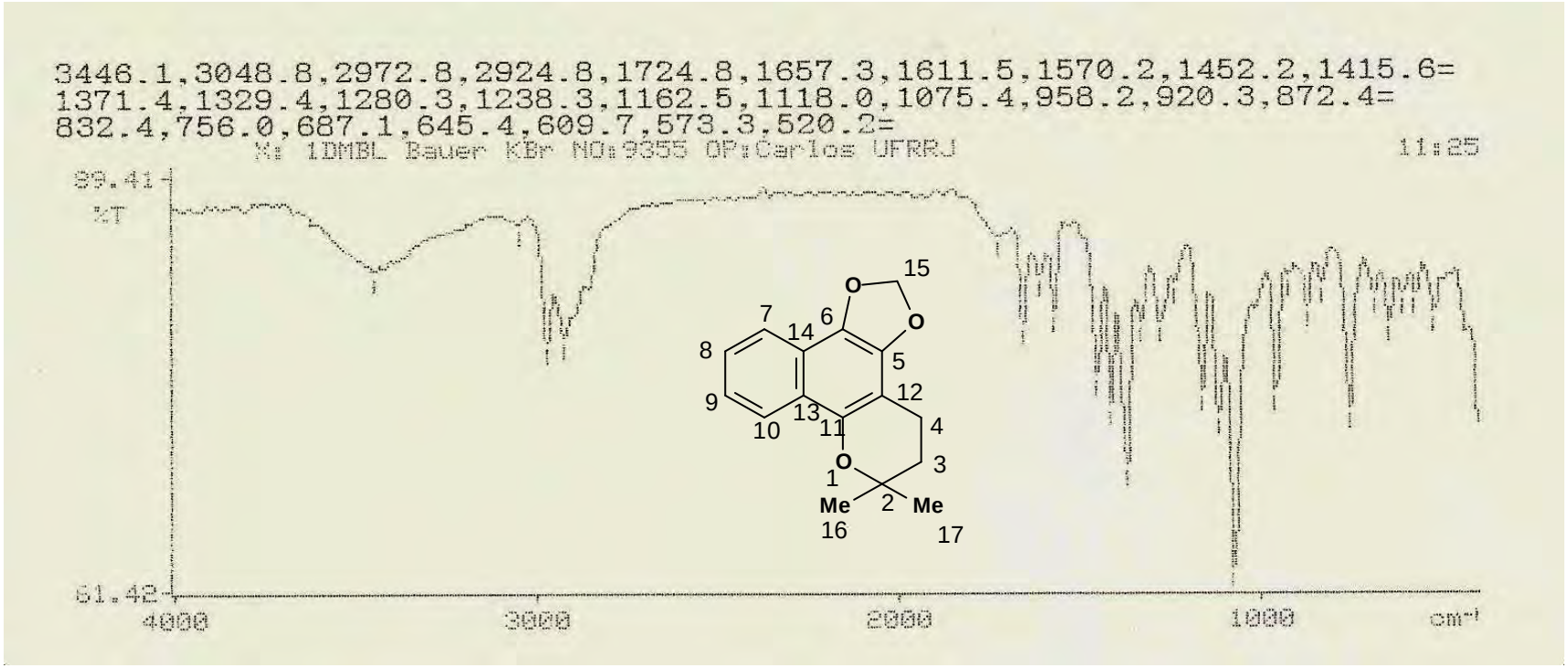
Espectro 31 – RMN ^{1}H (200 MHZ) do ALVI (5-hidróxi-2,2-dimetil-3,4-di-hidro-2*H*-benzo[*g*]cromeno-10-carbaldeído).



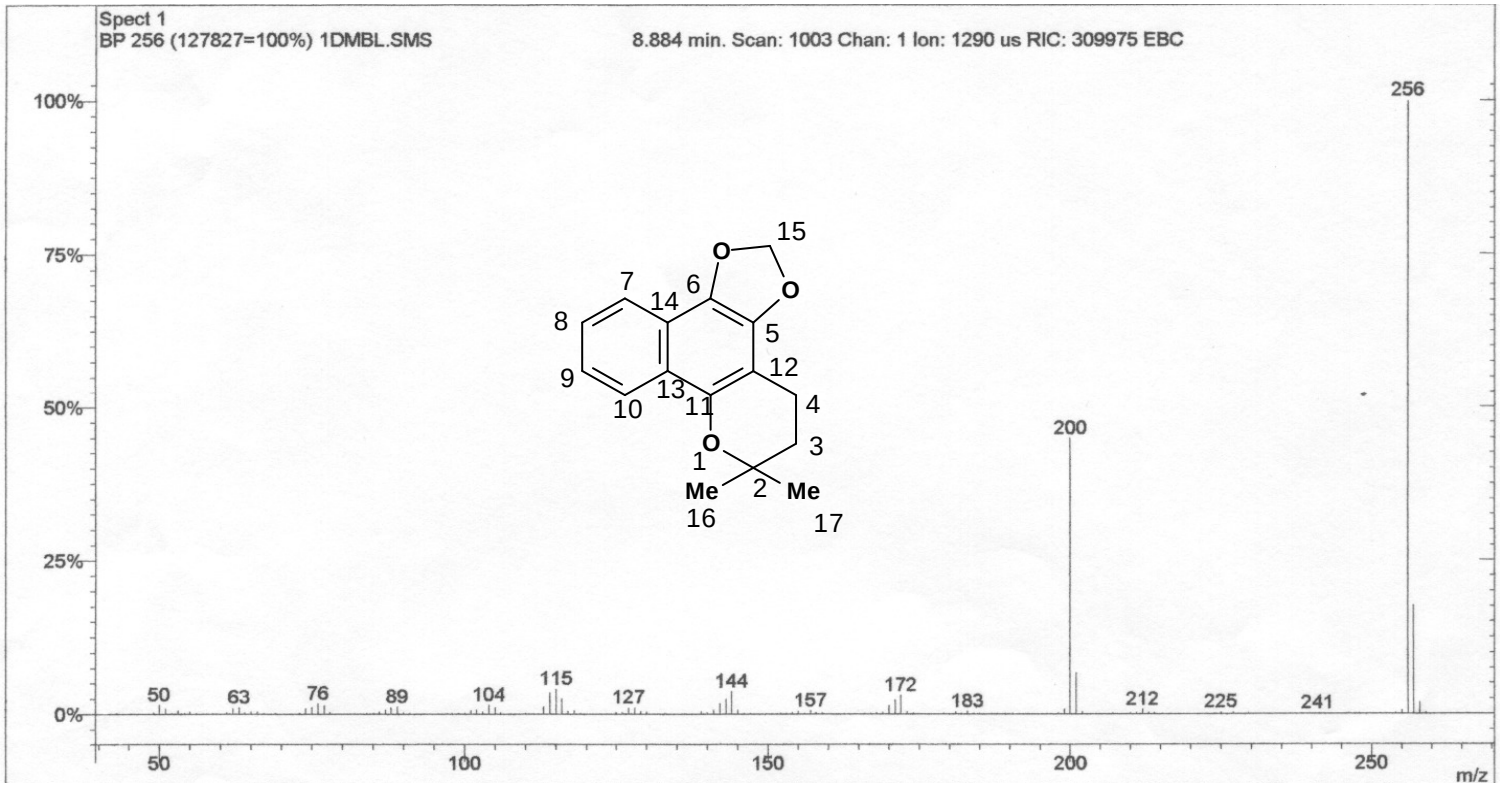
Espectro 32 - RMN ^{13}C (50,3 MHZ)do ALVI (5-hidróxi-2,2-dimetil-3,4-di-hidro-2*H*-benzo[*g*]cromeno-10-carbaldeído).



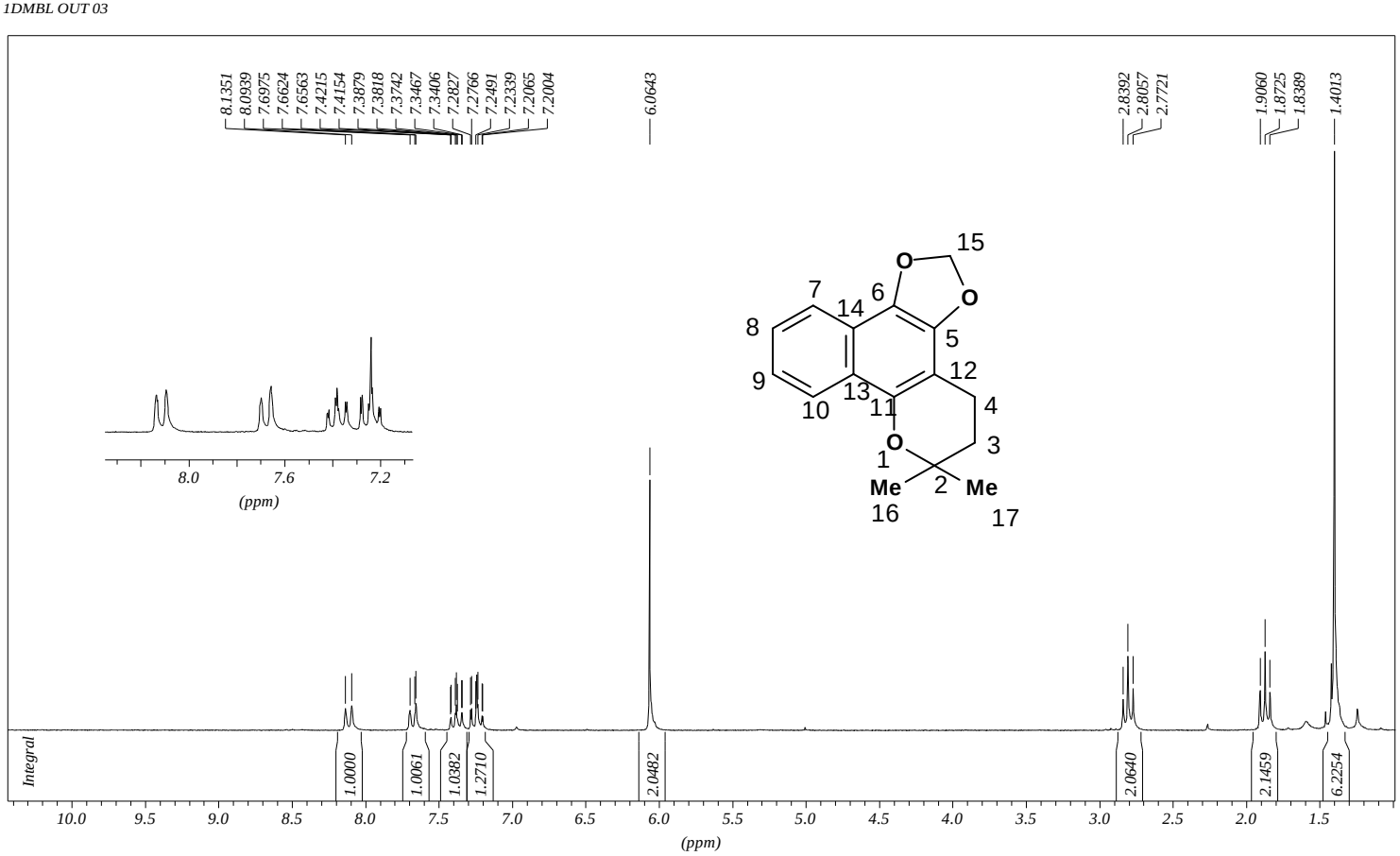
Espectro 33 – NOE do ALVI (5-hidróxi-2,2-dimetil-3,4-di-hidro-2*H*-benzo[*g*]cromeno-10-carbaldeído).



Espectro 34 – IV do DBL (6,6-dimetil-4,5,6,11b-tetra-hidro-3a*H*-benzo[*h*][1,3]dioxolo[4,5-*f*]cromeno).



Espectro 35 – E.M. do DBL (6,6-dimetil-4,5,6,11b-tetra-hidro-3a*H*-benzo[*h*][1,3]dioxolo[4,5-*f*]cromeno).



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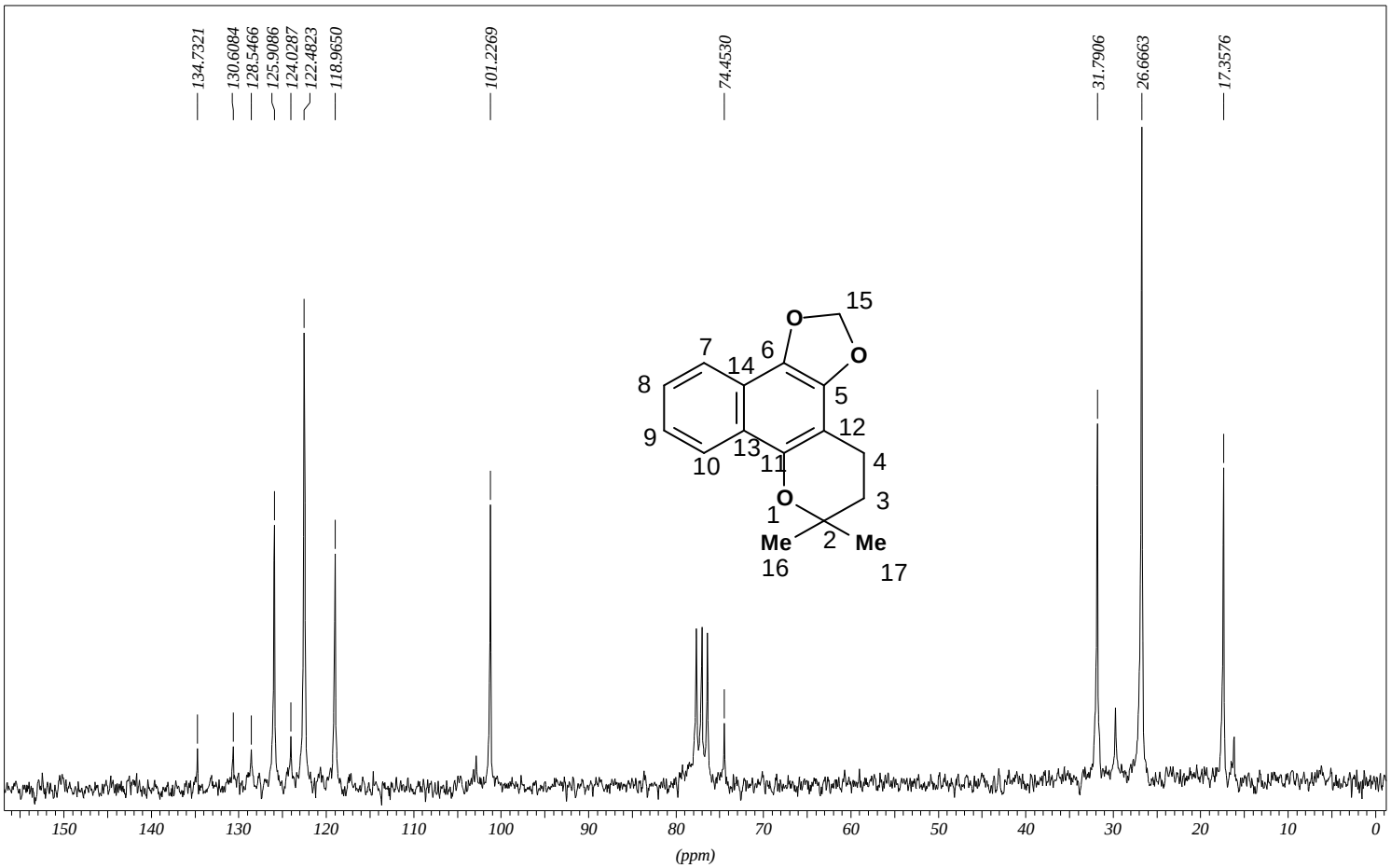
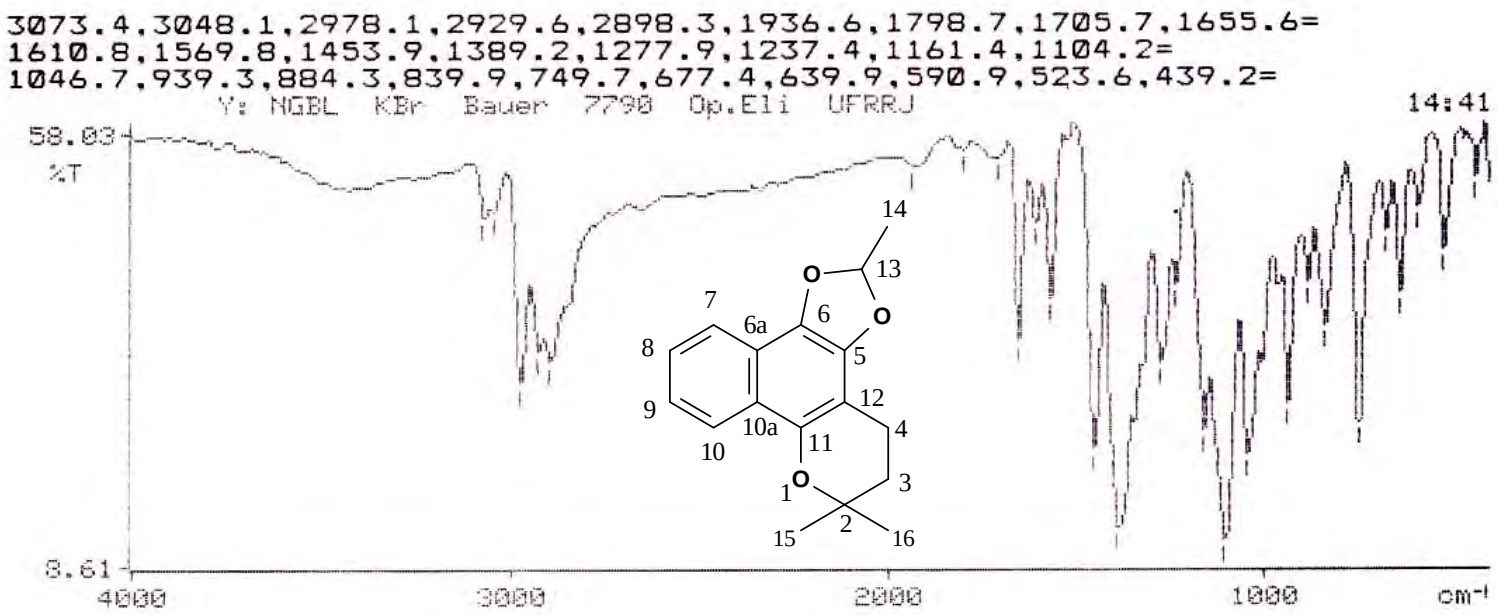
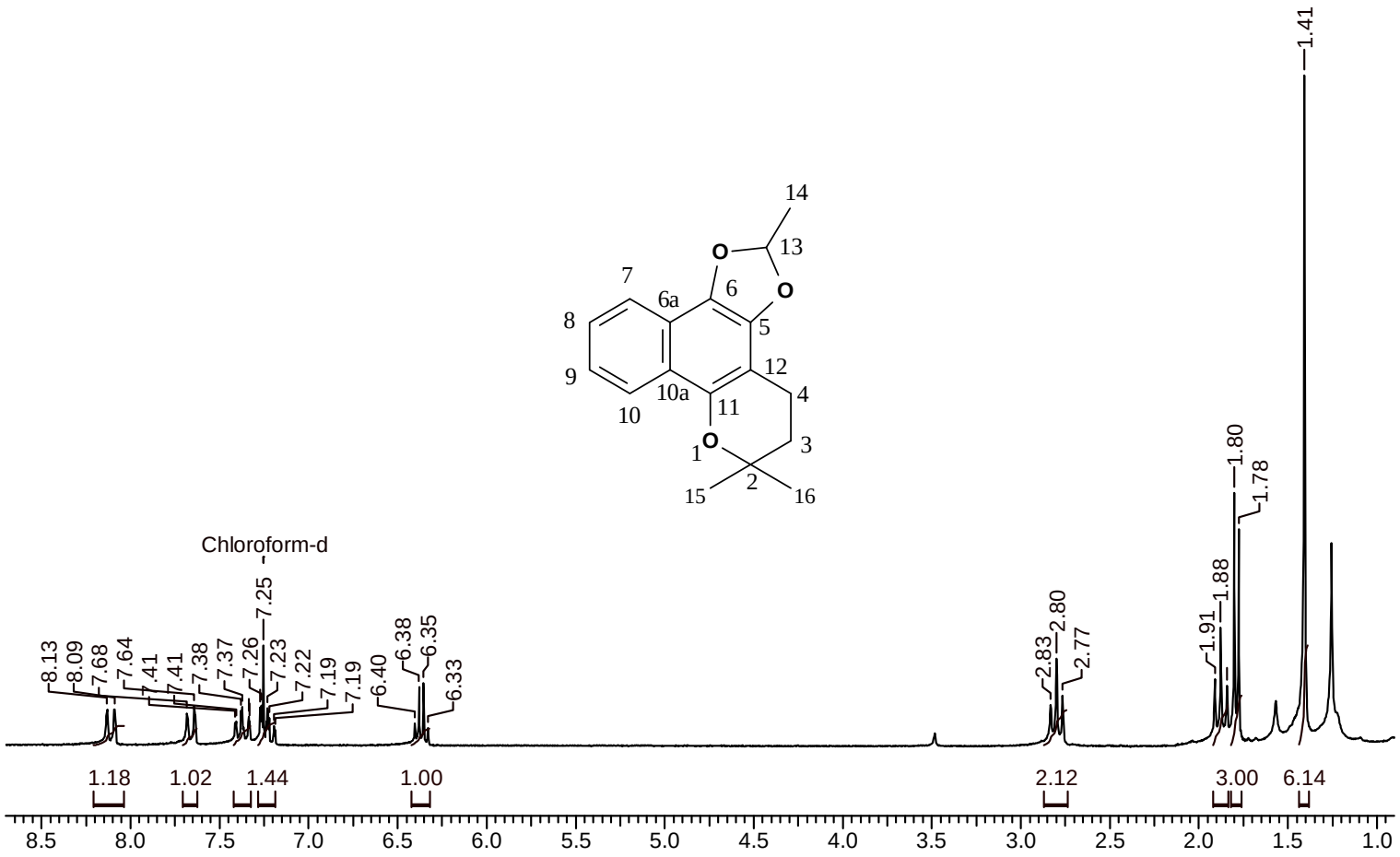
Espectro 36 – RMN ^{1}H (200 MHz)do DBL(6,6-dimetil-4,5,6,11b-tetra-hidro-3a*H*-benzo[*h*][1,3]dioxolo[4,5-*f*]cromeno).



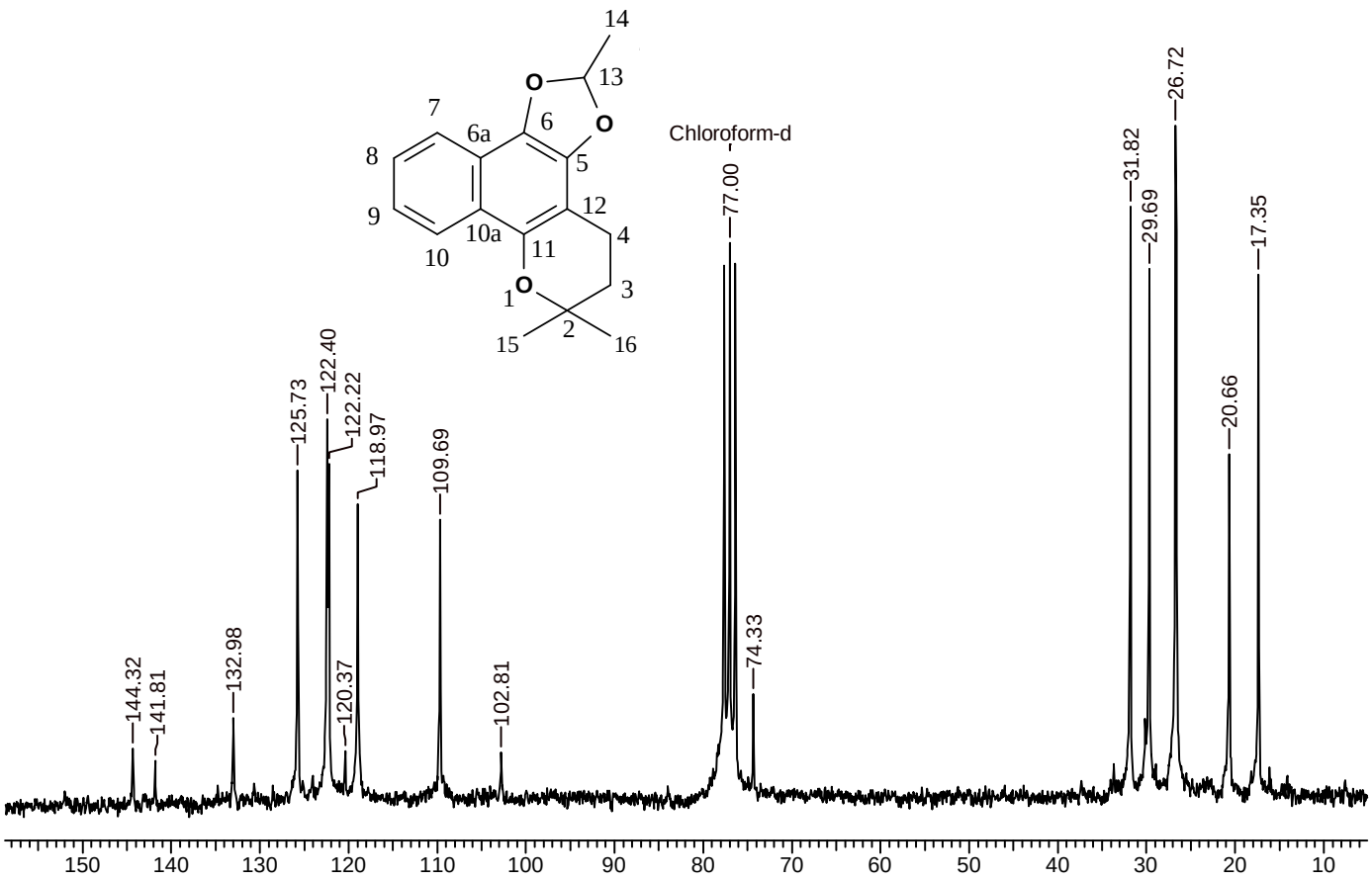
Espectro 37 – RMN ^{13}C (50,3 MHz)do DBL(6,6-dimetil-4,5,6,11b-tetra-hidro-3a*H*-benzo[*h*][1,3]dioxolo[4,5-*f*]cromeno).



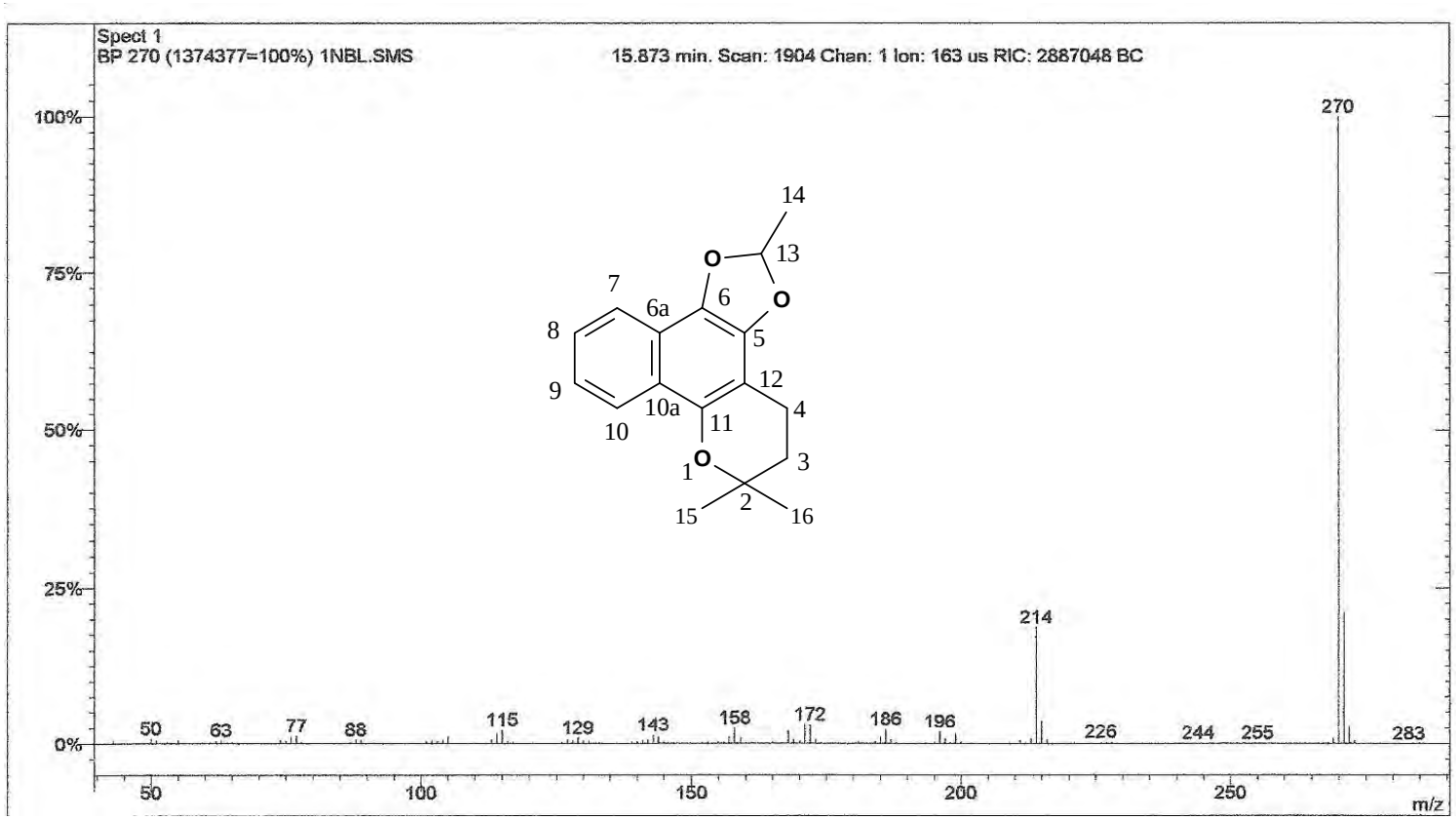
Espectro 38 – IV do MDBL (2,6,6-trimetil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno).



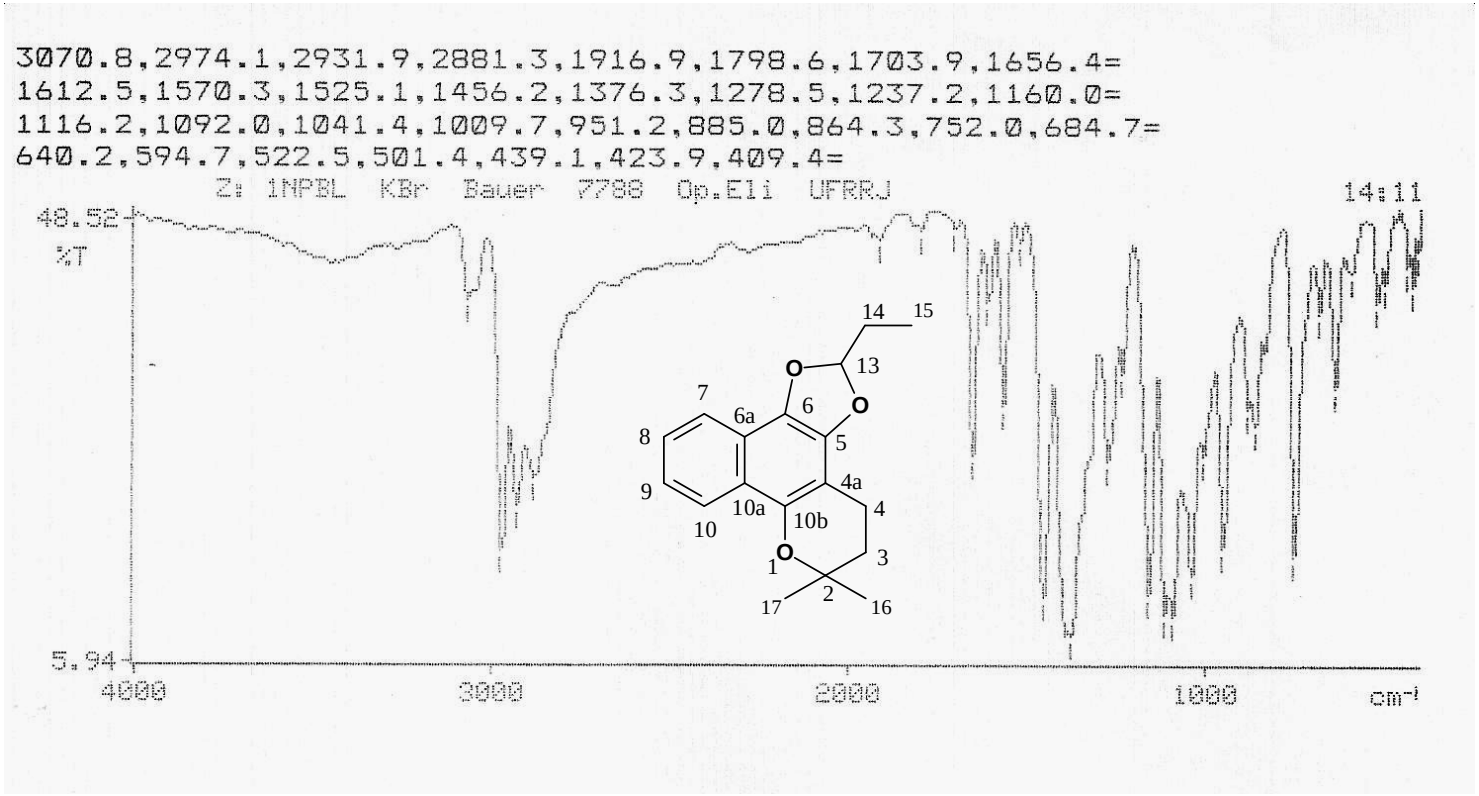
Espectro 39 – RMN ^{1}H (200 MHZ) do MDBL(2,6,6-trimetil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno).



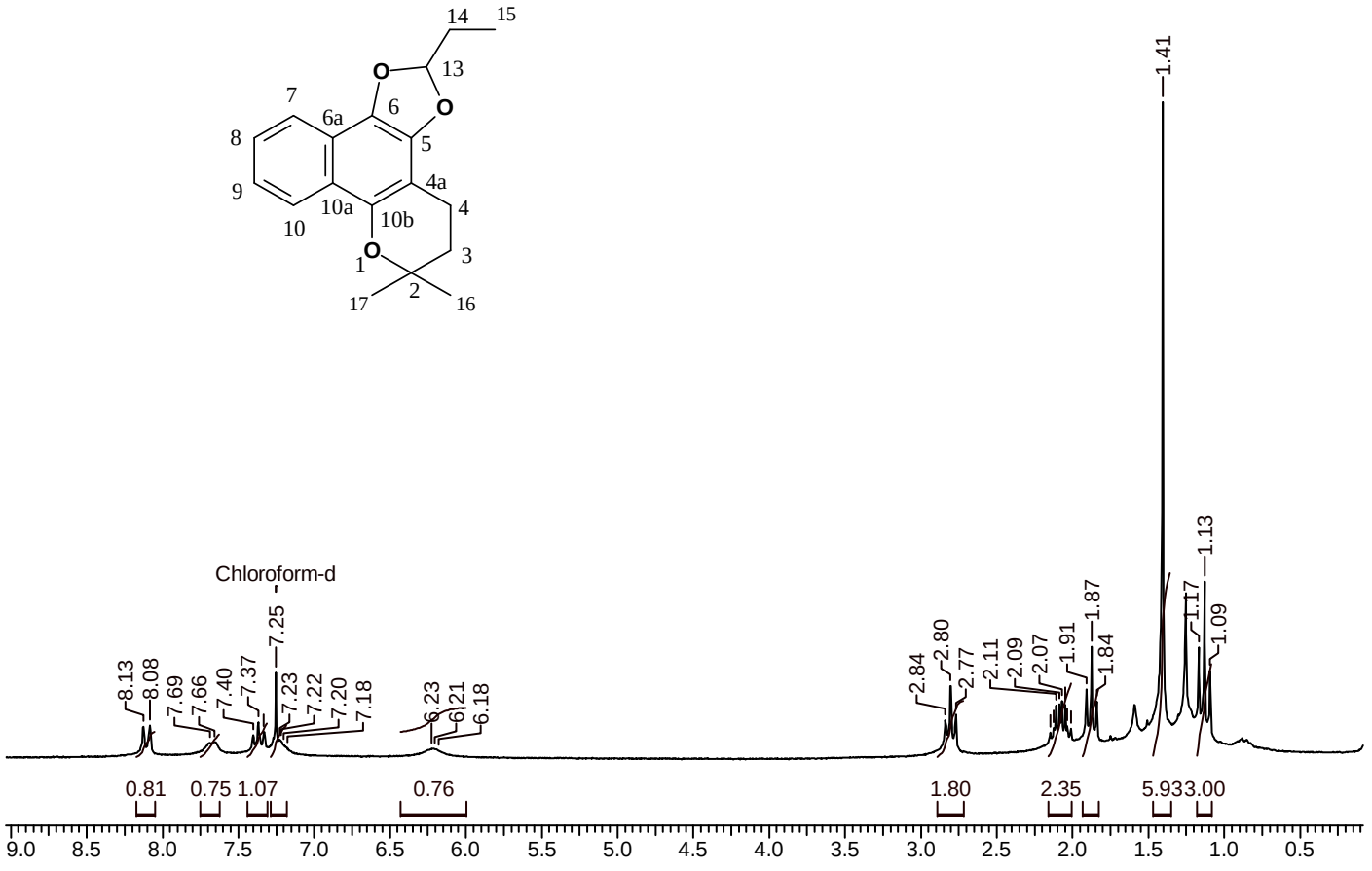
Espectro 40 – RMN ^{13}C (50,3 MHZ)do MDBL(2,6,6-trimetil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno).



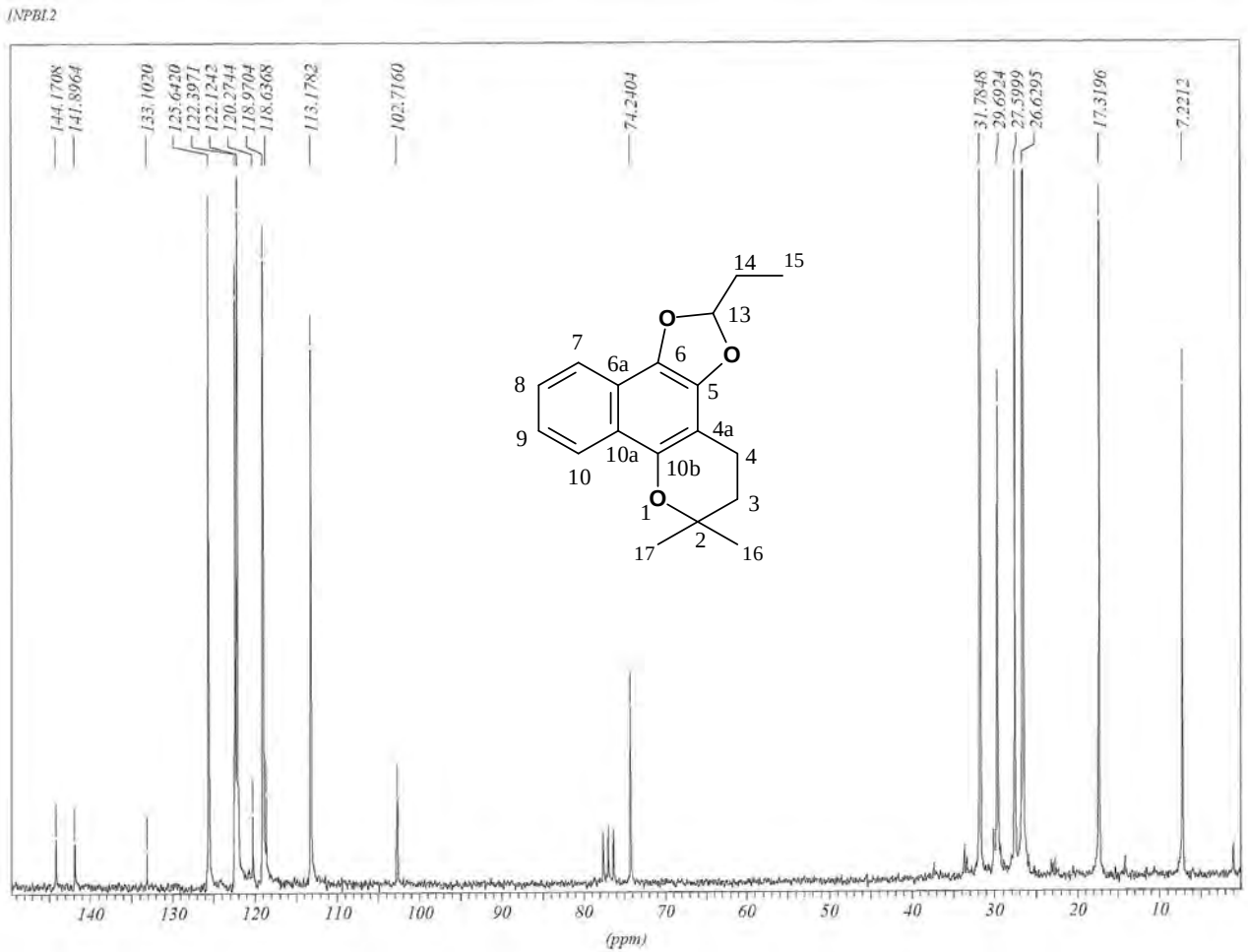
Espectro 41 – E.M. do MDBL (2,6,6-trimetil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno).



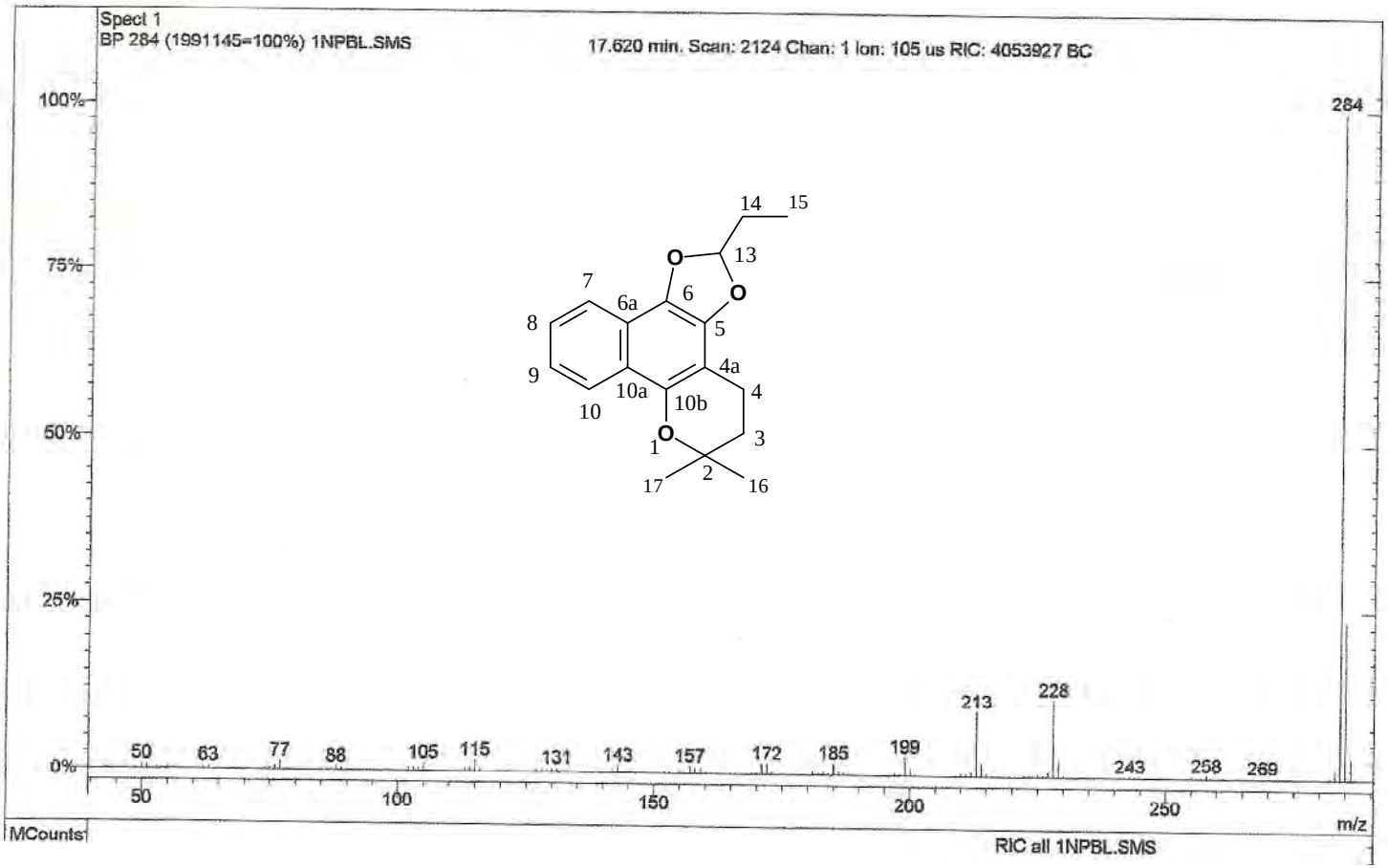
Espectro 42 – IV do EDBL (6,6-trimetil-2-etil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno).



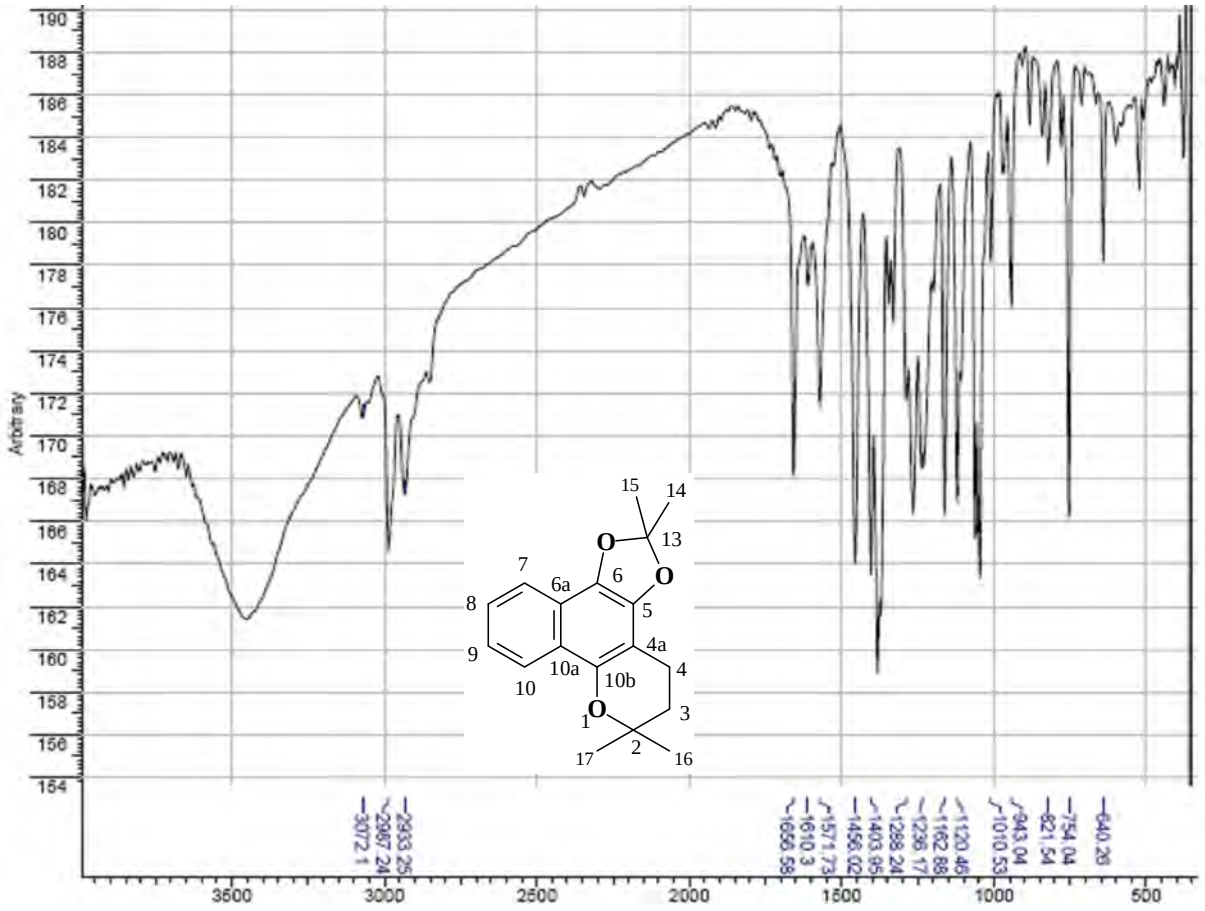
Espectro 43 – RMN ^{1}H (200 MHZ) do EDBL (6,6-trimetil-2-etil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno).



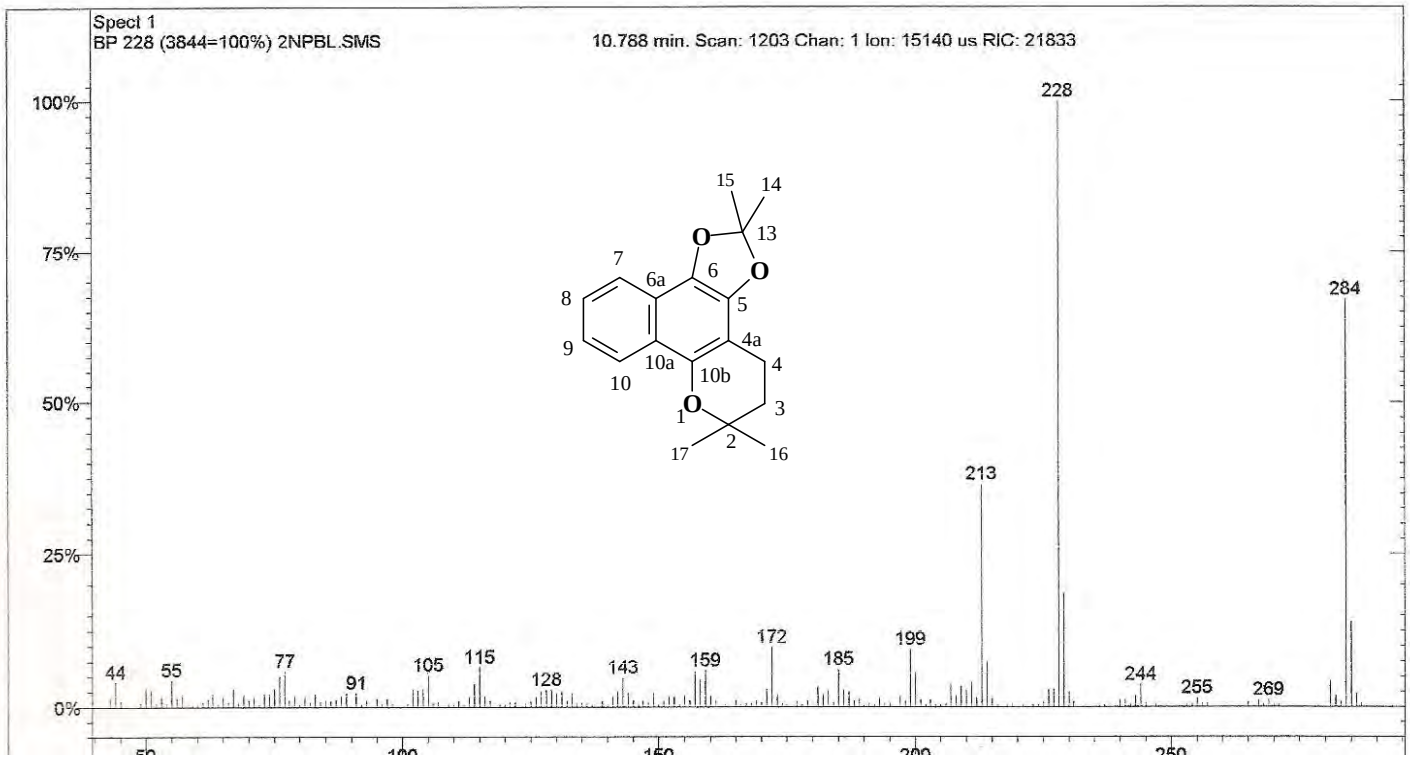
Espectro 44 – RMN ^{13}C (50,3 MHZ) do EDBL (6,6-trimetil-2-etil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno).



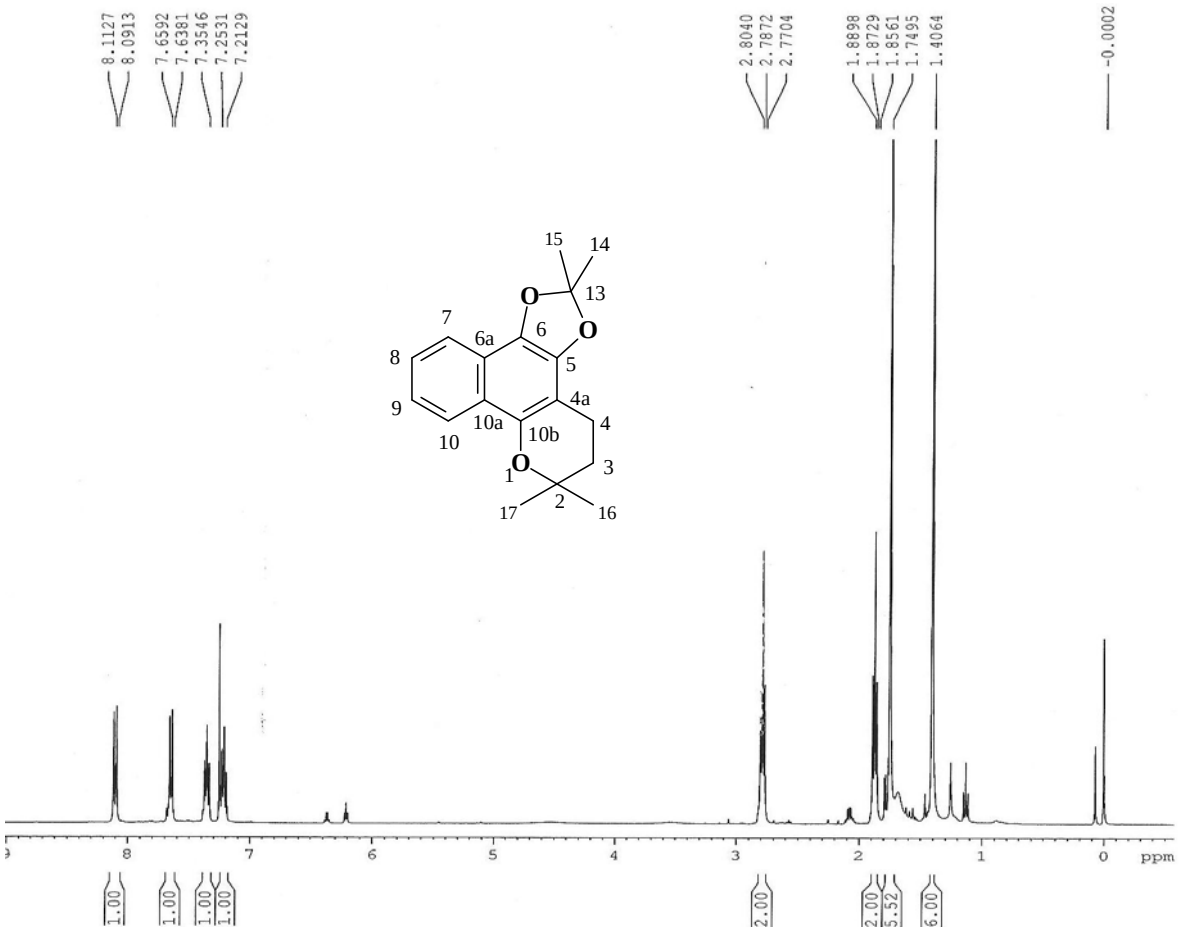
Espectro 45 – E.M. do EDBL (6,6-trimetil-2-etil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno).



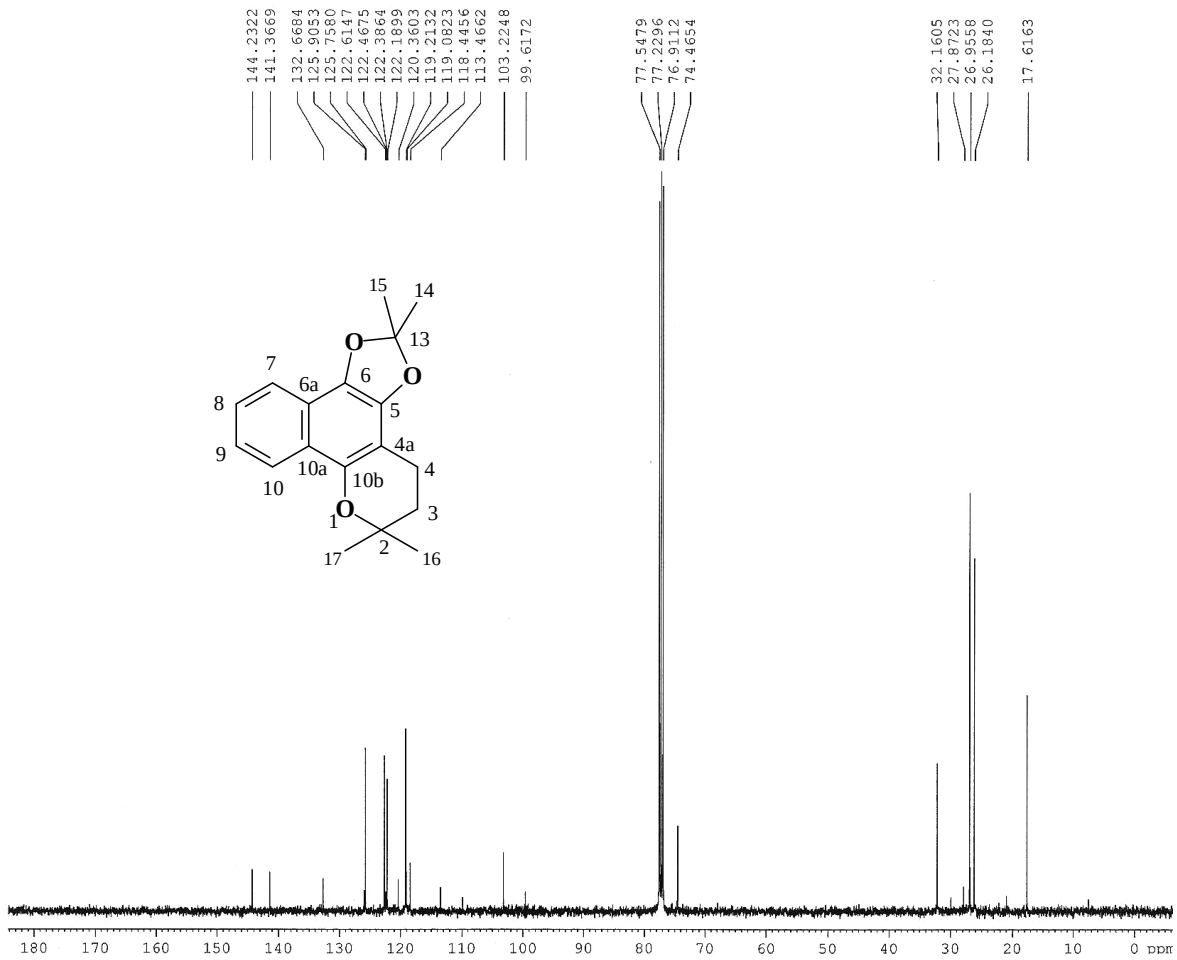
Espectro 46 – IV do DMDBL (2,2,6,6-tetrametil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno), comprimento de onda em cm^{-1}.



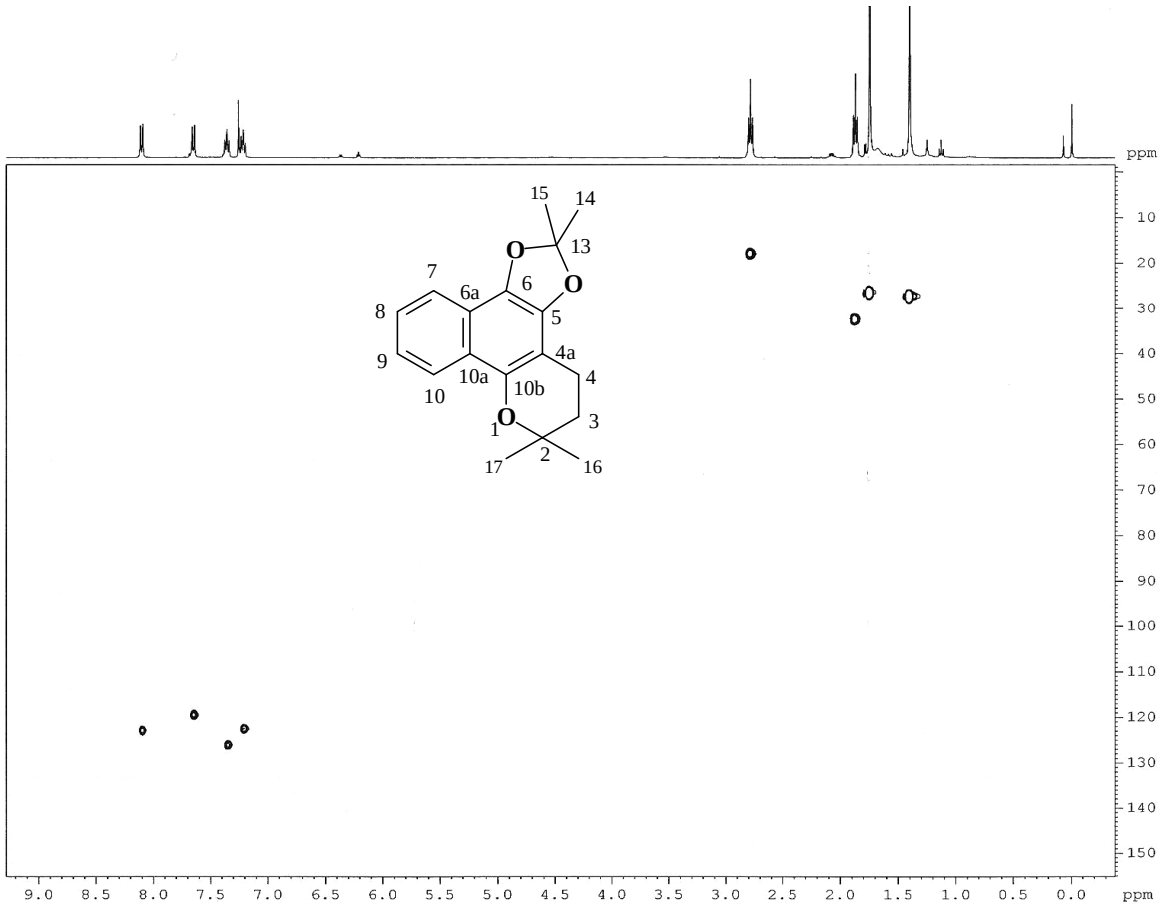
Espectro 47 – EM do DMDBL (2,2,6,6-tetrametil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno).



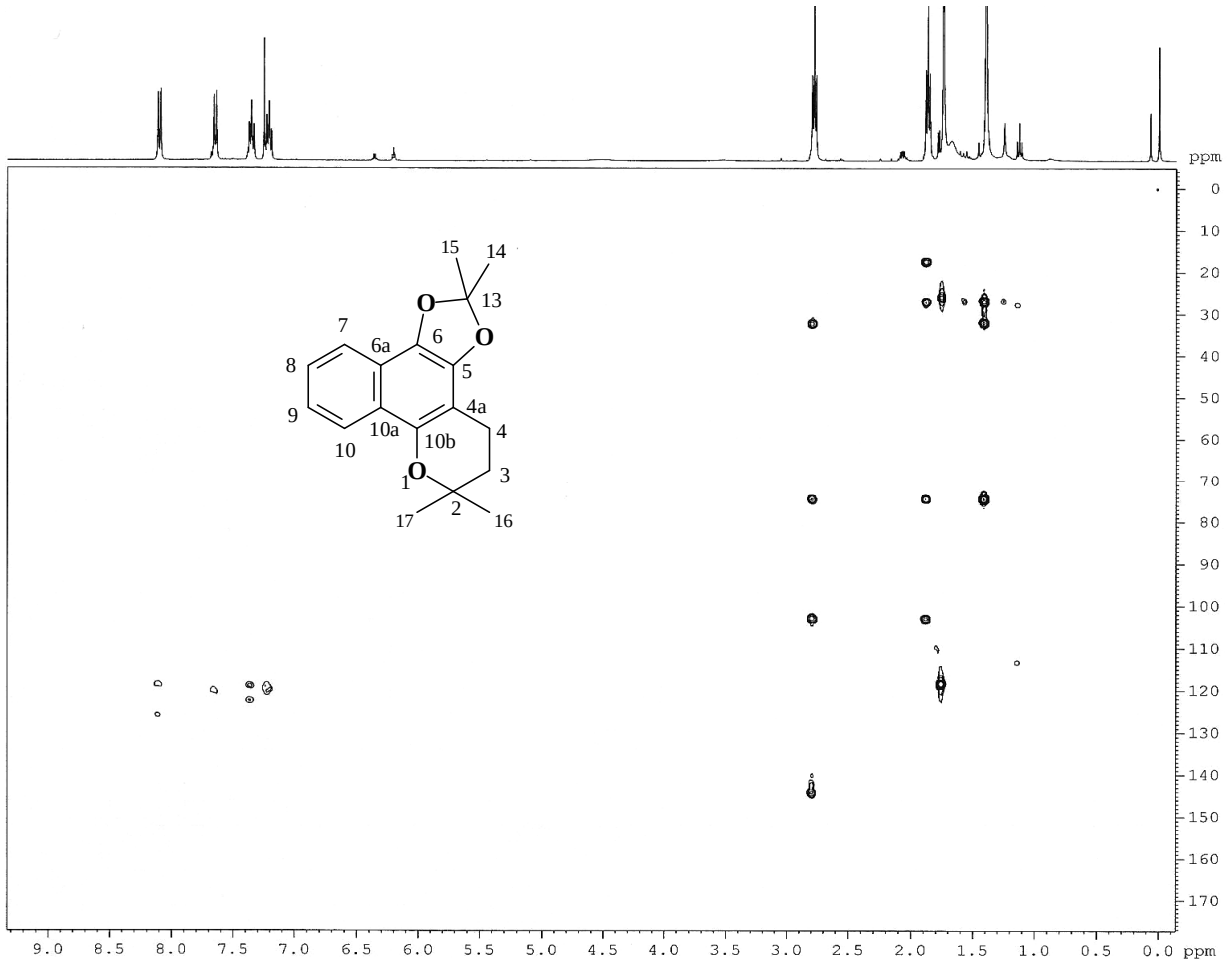
Espectro 48 – RMN ^{1}H (200 MHZ) do DMDBL (2,2,6,6-tetrametil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno).



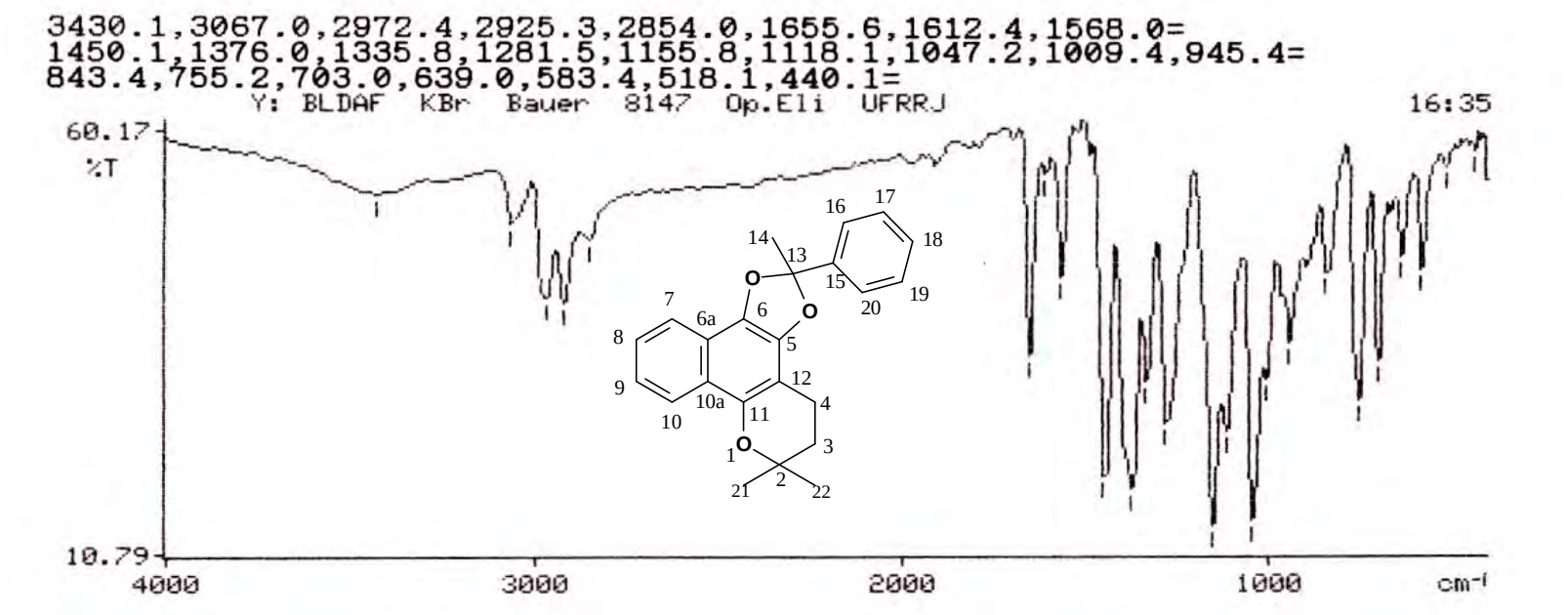
Espectro 49 – RMN ^{13}C (50,3 MHZ) do DMDBL (2,2,6,6-tetrametil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno).



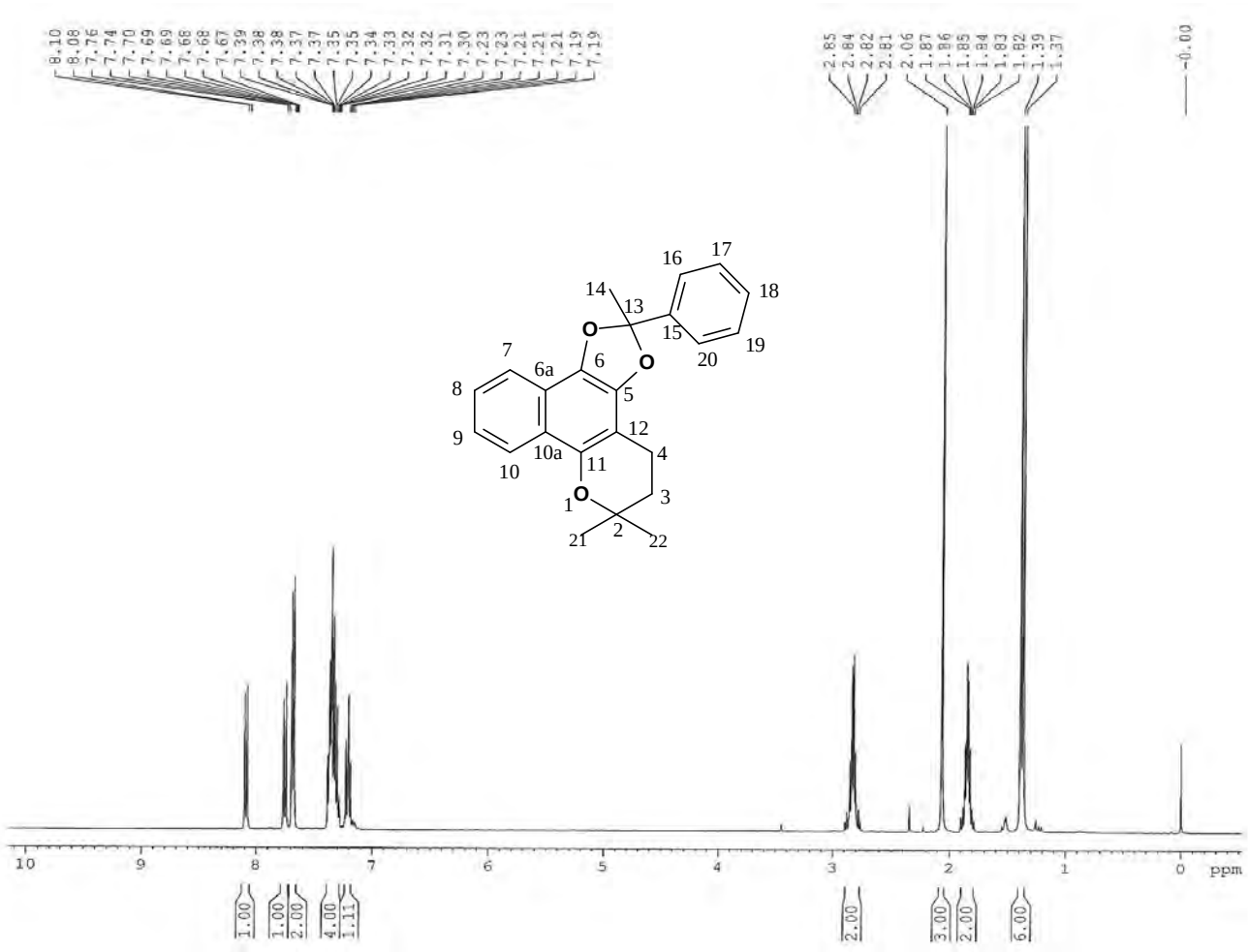
Espectro 50 – Correlação heteronuclear Cosy ^{1}H x ^{13}C, J1 do DMDBL.



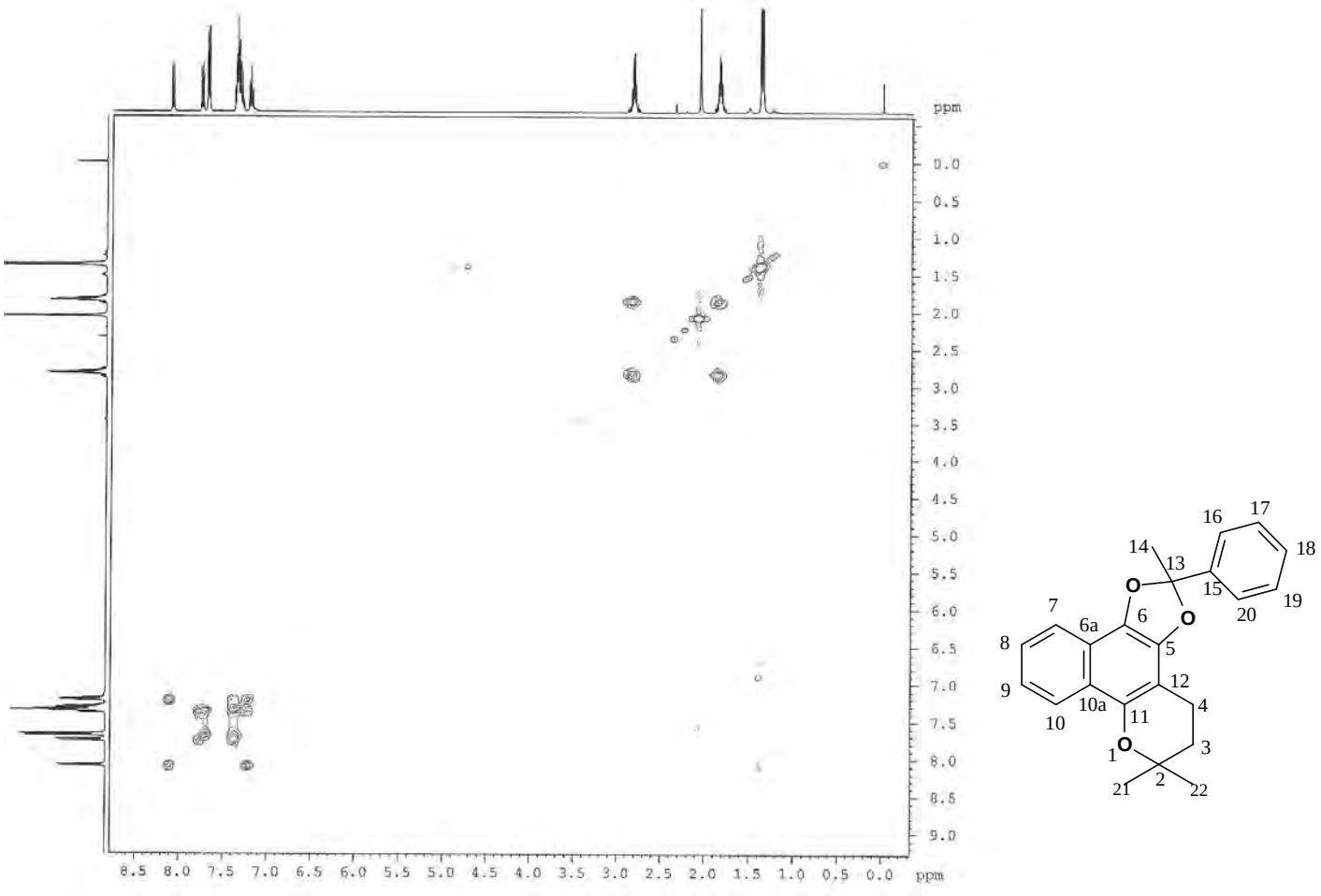
Espectro 51 – Correlação heteronuclear, ^{1}H x ^{13}C, J2 e J3 de DMDBL.



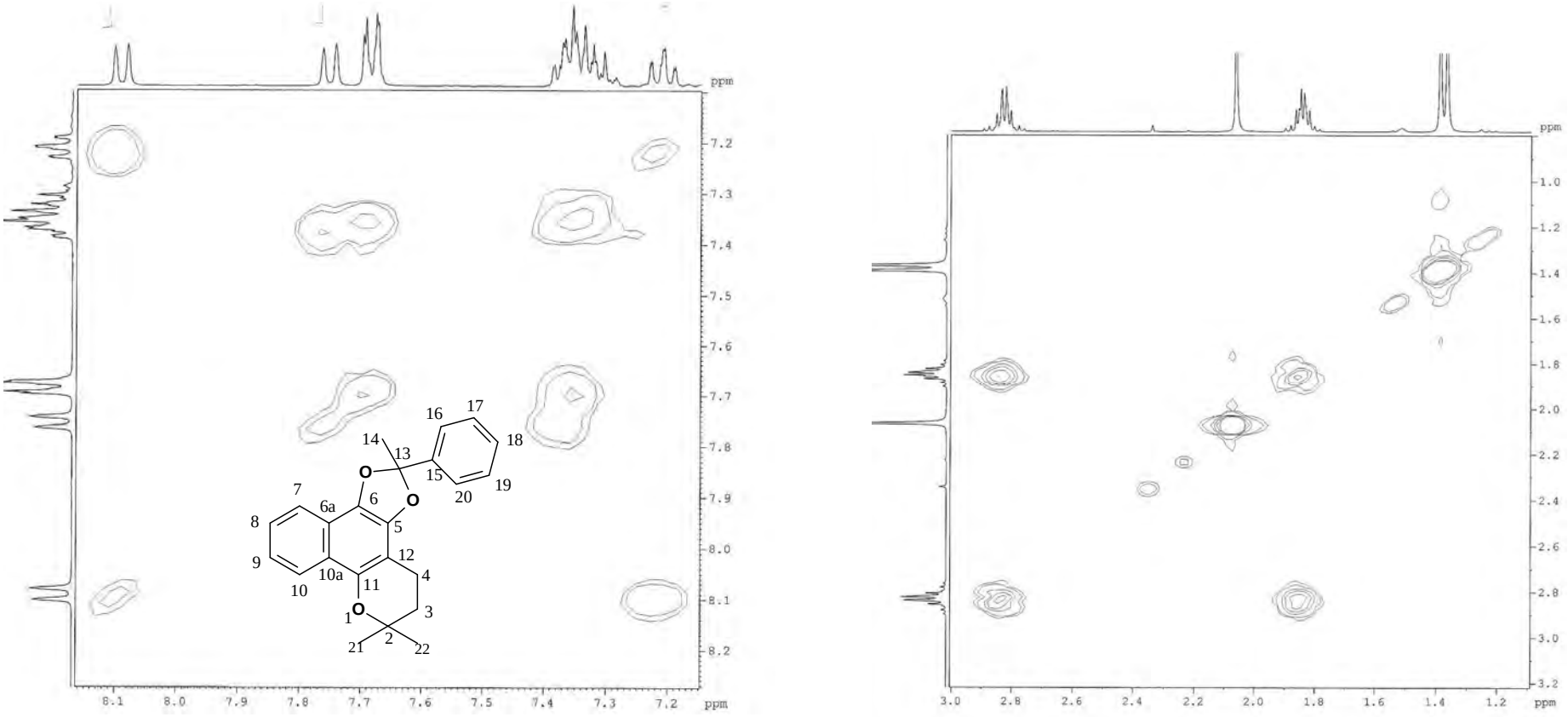
Espectro 52 – IV do FMDBL (2,6,6-trimetil-2-fenil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno).



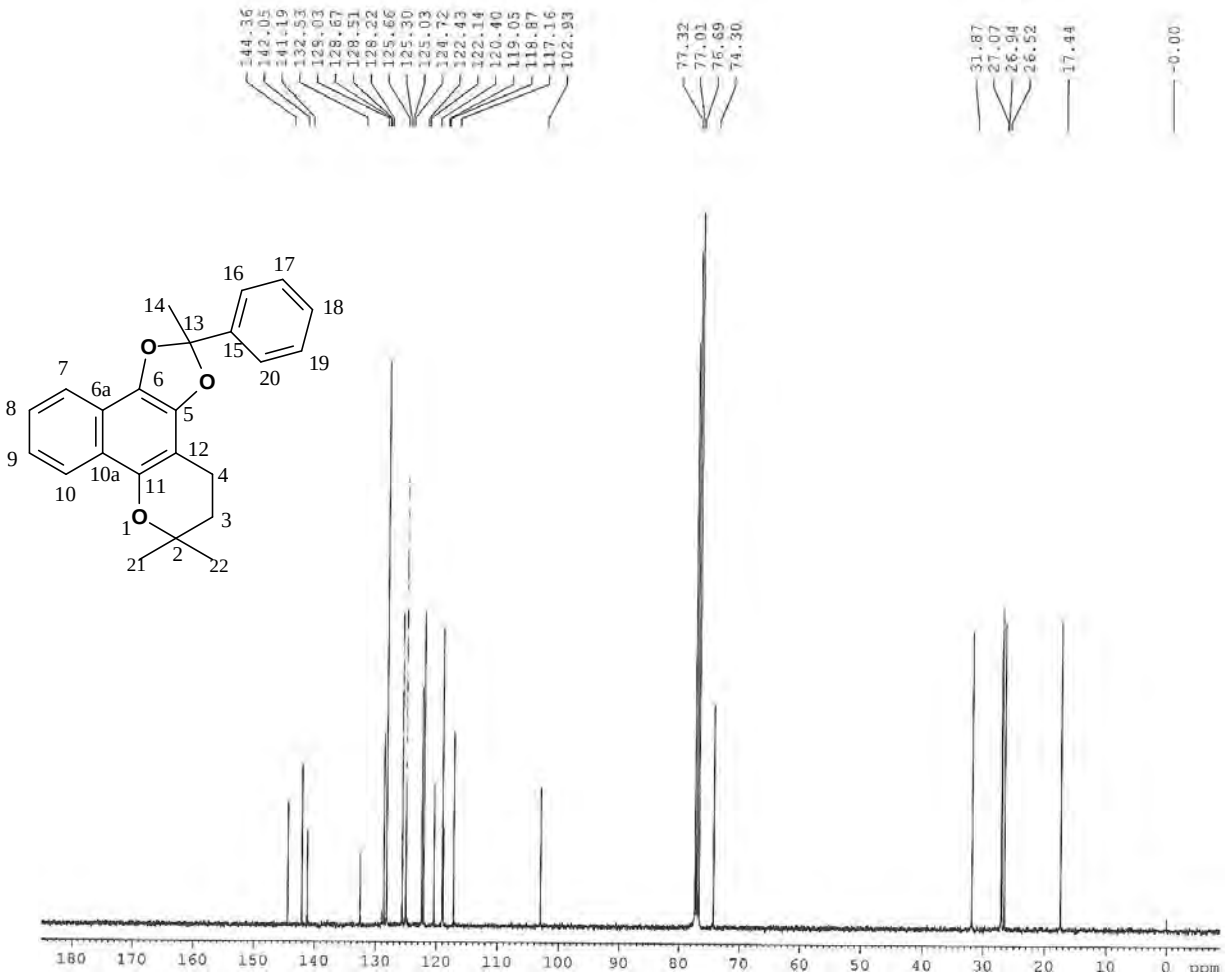
Espectro 53 – RMN ^{1}H (200 MHZ) do FMDBL (2,6,6-trimetil-2-fenil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno).



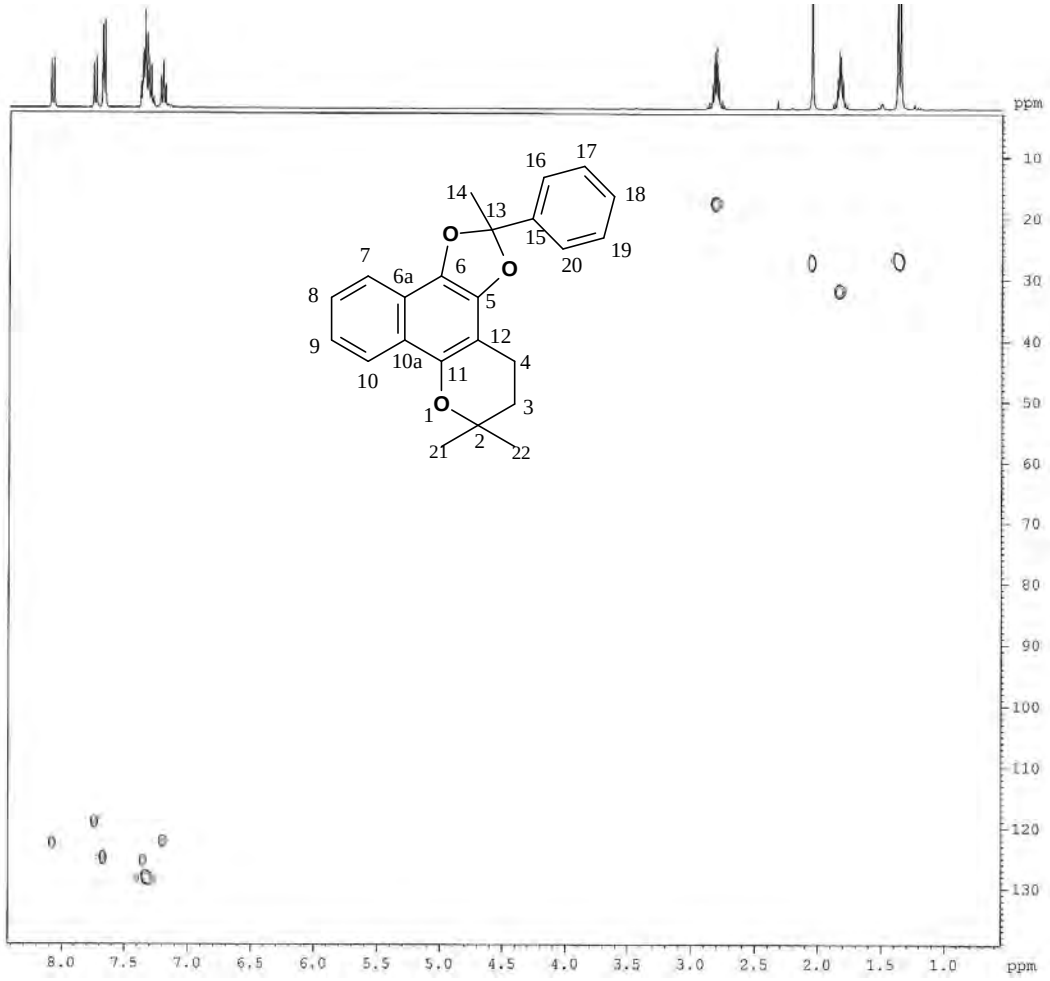
Espectro 54 – HOMOCOSY ^{1}H x ^{1}H de FMDBL (2,6,6-trimetil-2-fenil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno).



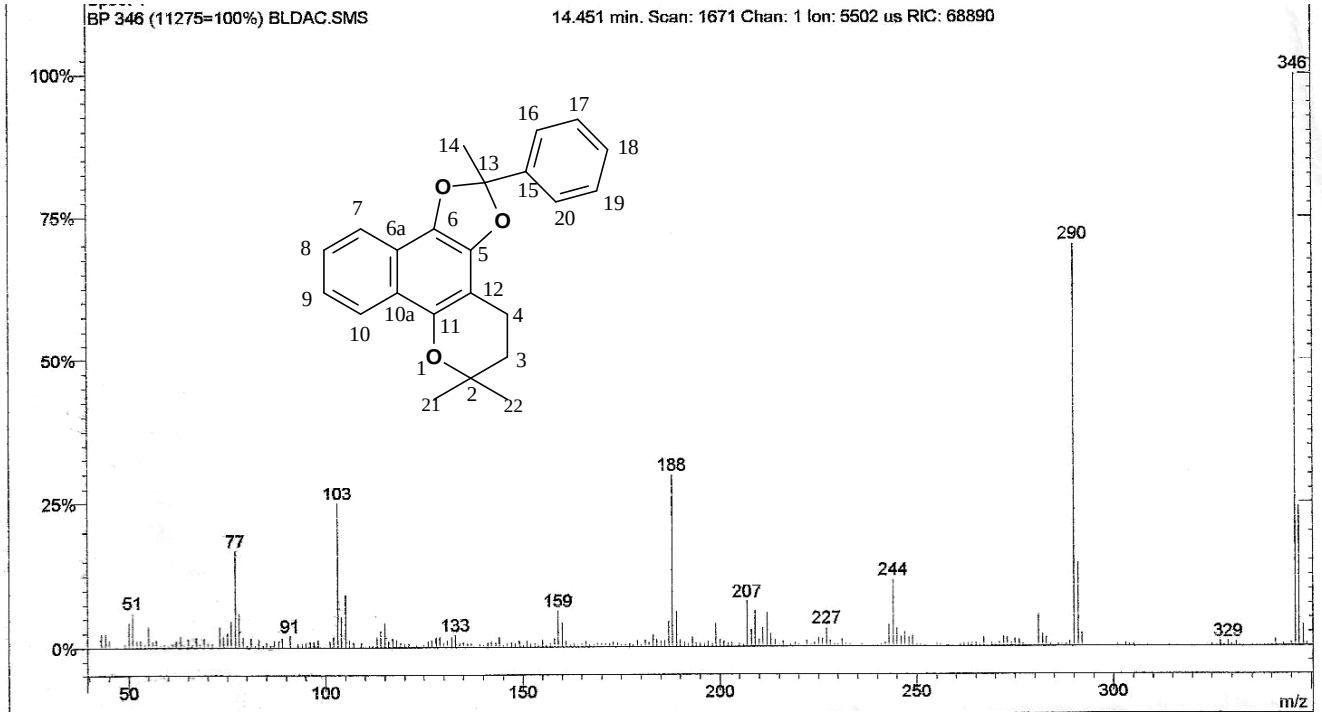
Espectro 55 – Expansão de HOMOCOSY ^{1}H x ^{1}H de FMDBL.



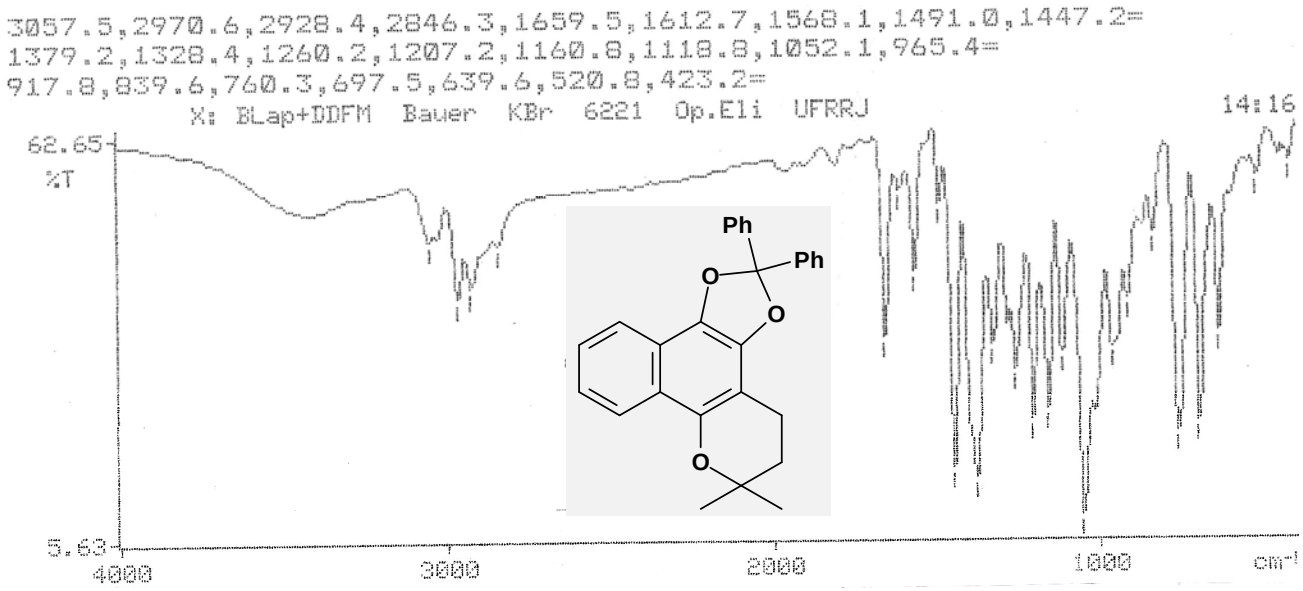
Espectro 56 – RMN ^{13}C (50,3 MHZ) do FMDBL(2,6,6-trimetil-2-fenil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno).



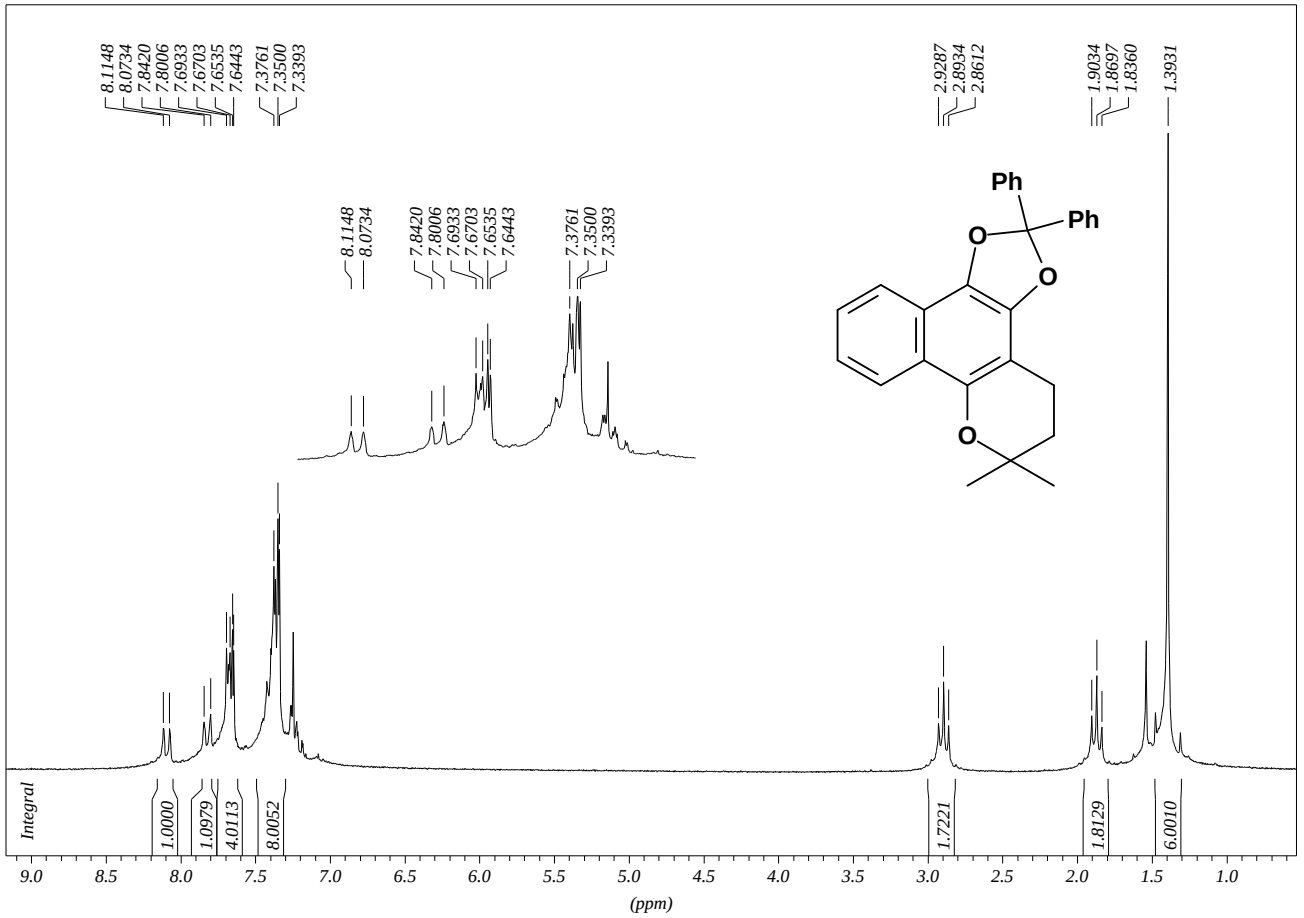
Espectro 57 – HSQC que é o mesmo de HMQC do FMDBL(2,6,6-trimetil-2-fenil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno).



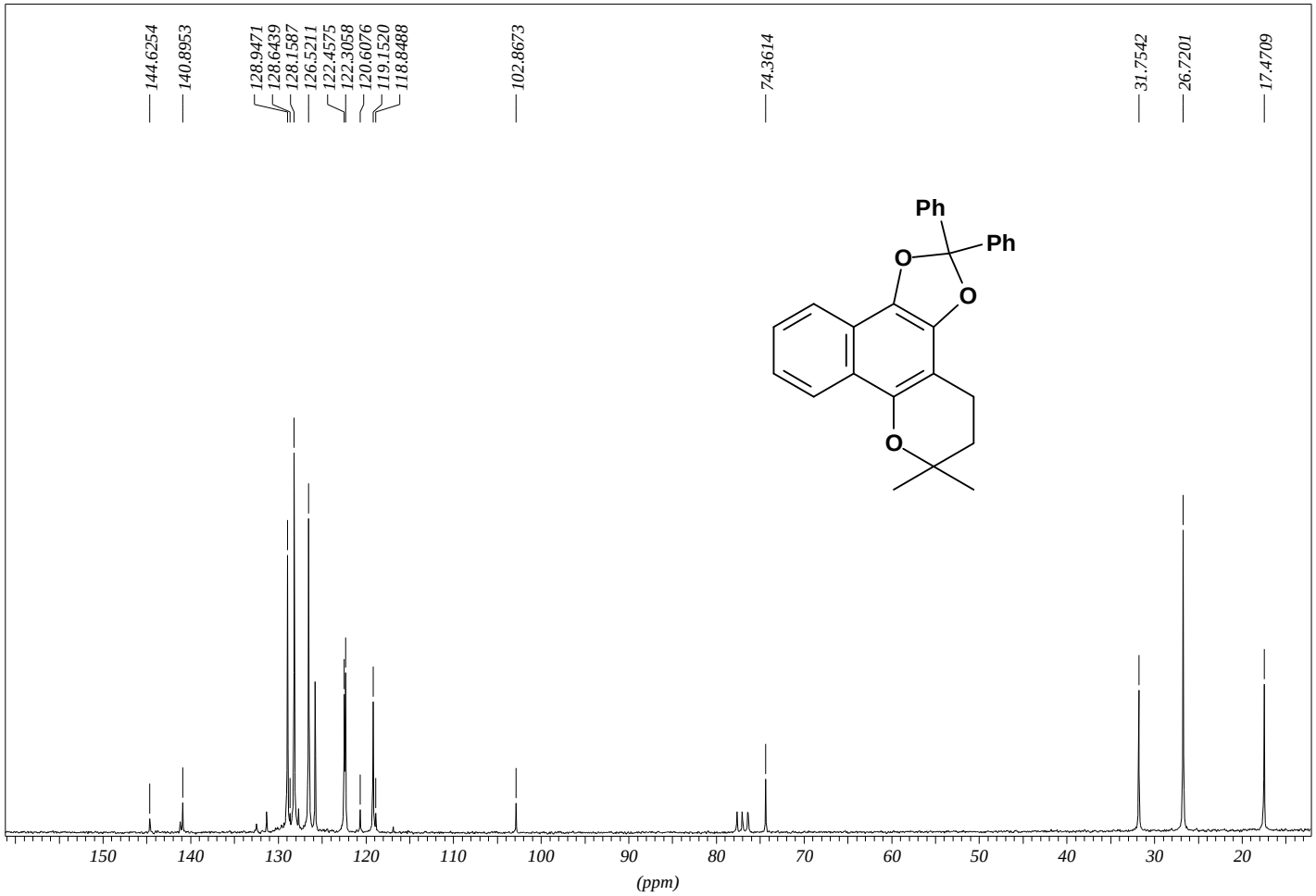
Espectro 58 – E.M. do FMDBL (2,6,6-trimetil-2-fenil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno).



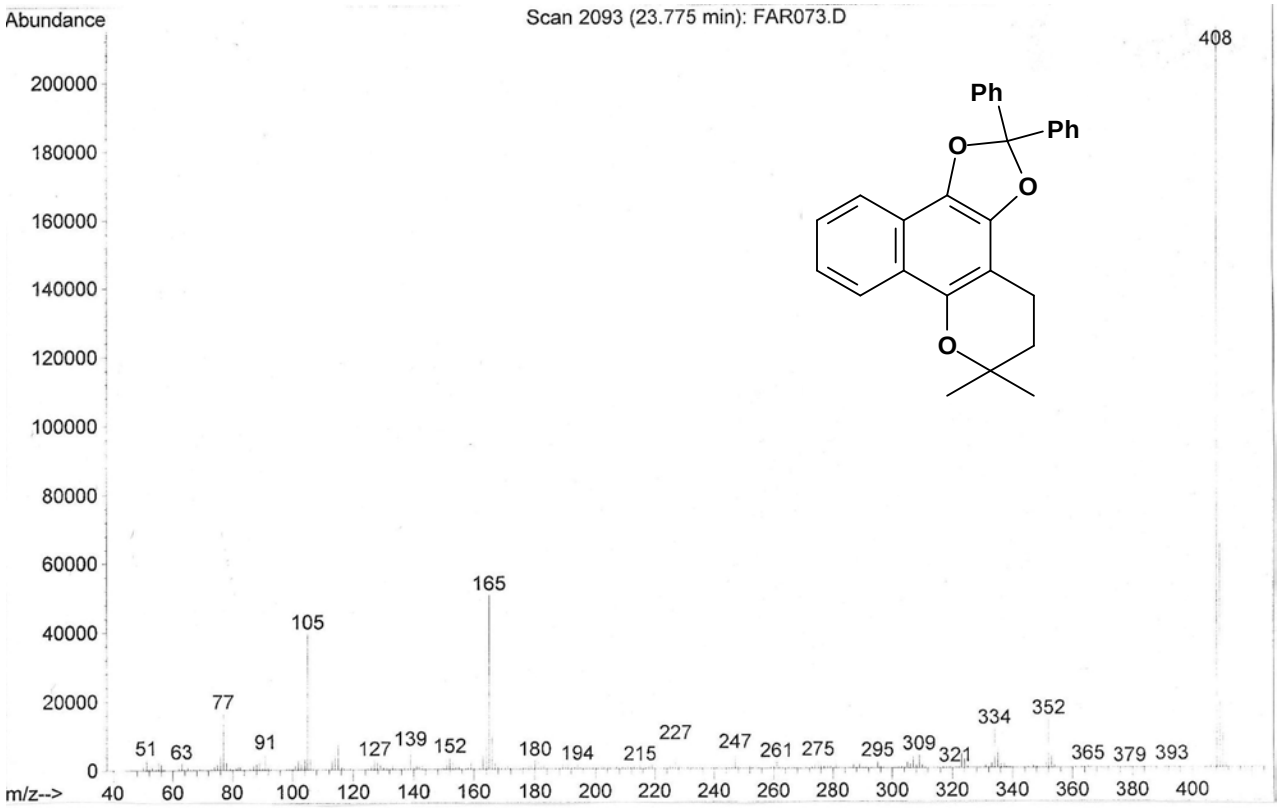
Espectro 59 – IV do DFDBL (6,6-dimetil-2,2-difenil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno).



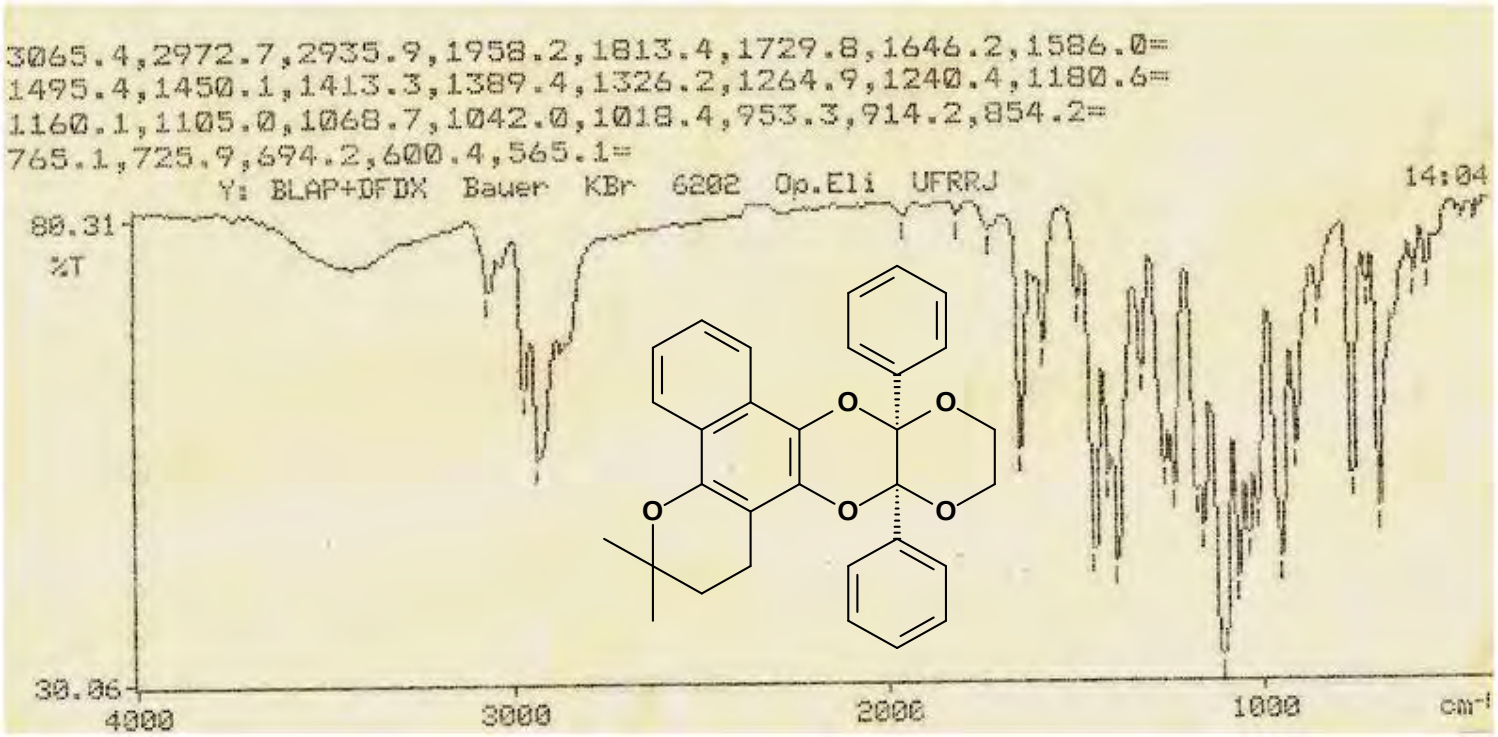
Espectro 60 – RMN ^{1}H (200 MHZ) do DFDBL (6,6-dimetil-2,2-difenil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno).



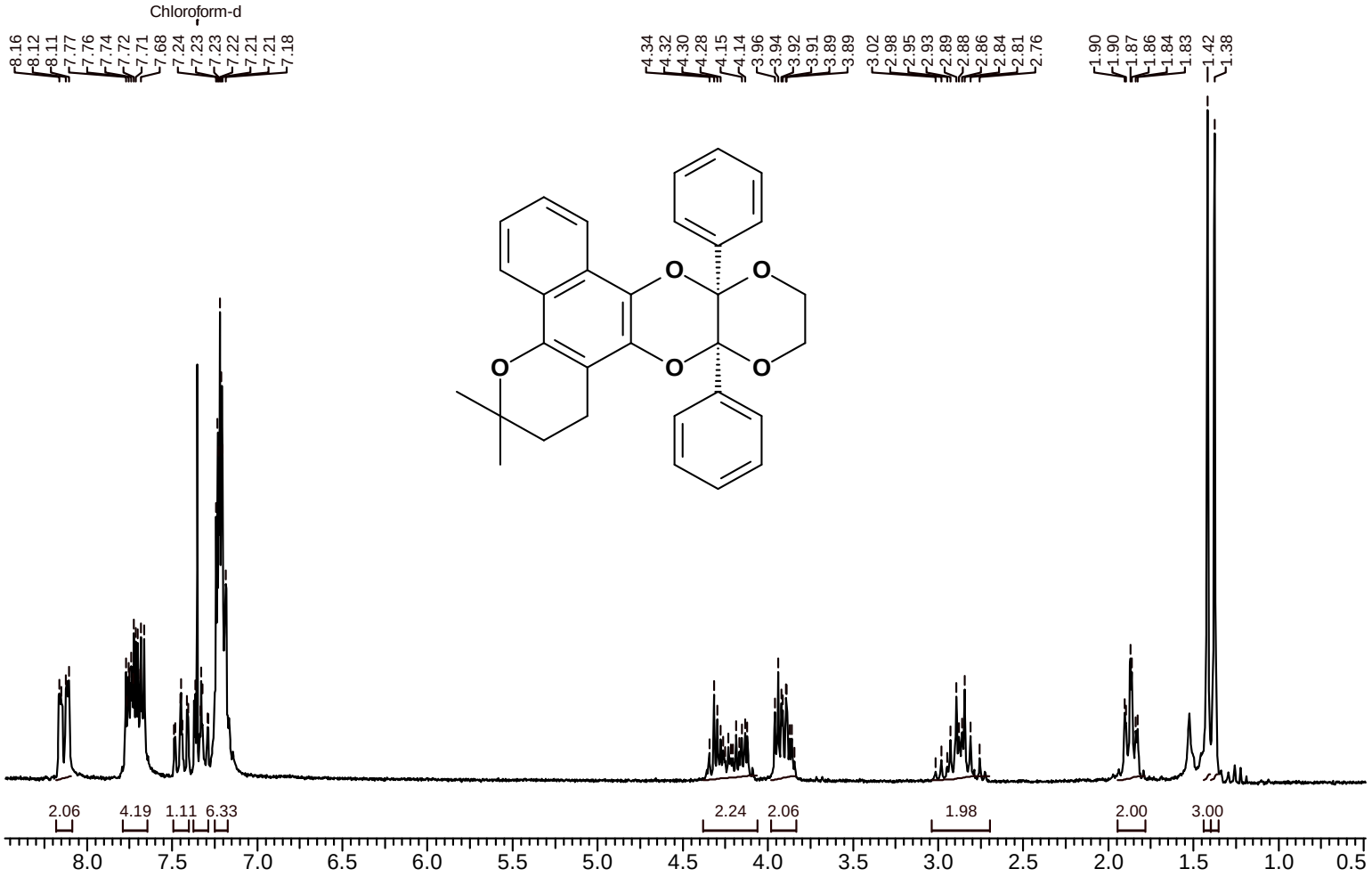
Espectro 61 – RMN ^{13}C (50,3 MHZ) do DFDBL (6,6-dimetil-2,2-difenil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno).



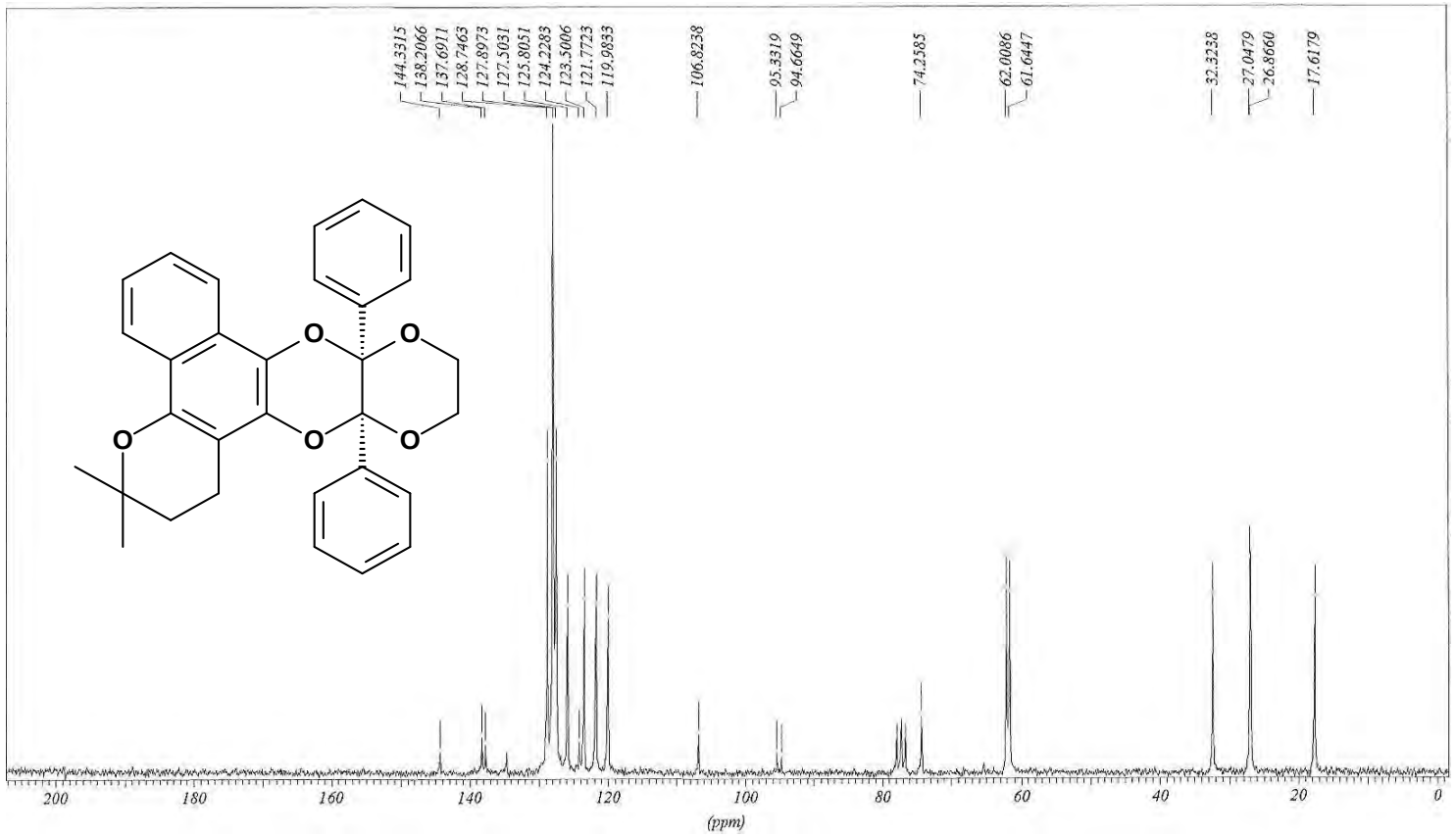
Espectro 62 – E.M. do DFDBL (6,6-dimetil-2,2-difenil-5,6-di-hidro-4H-benzo[h][1,3]dioxolo[4,5-f]cromeno).



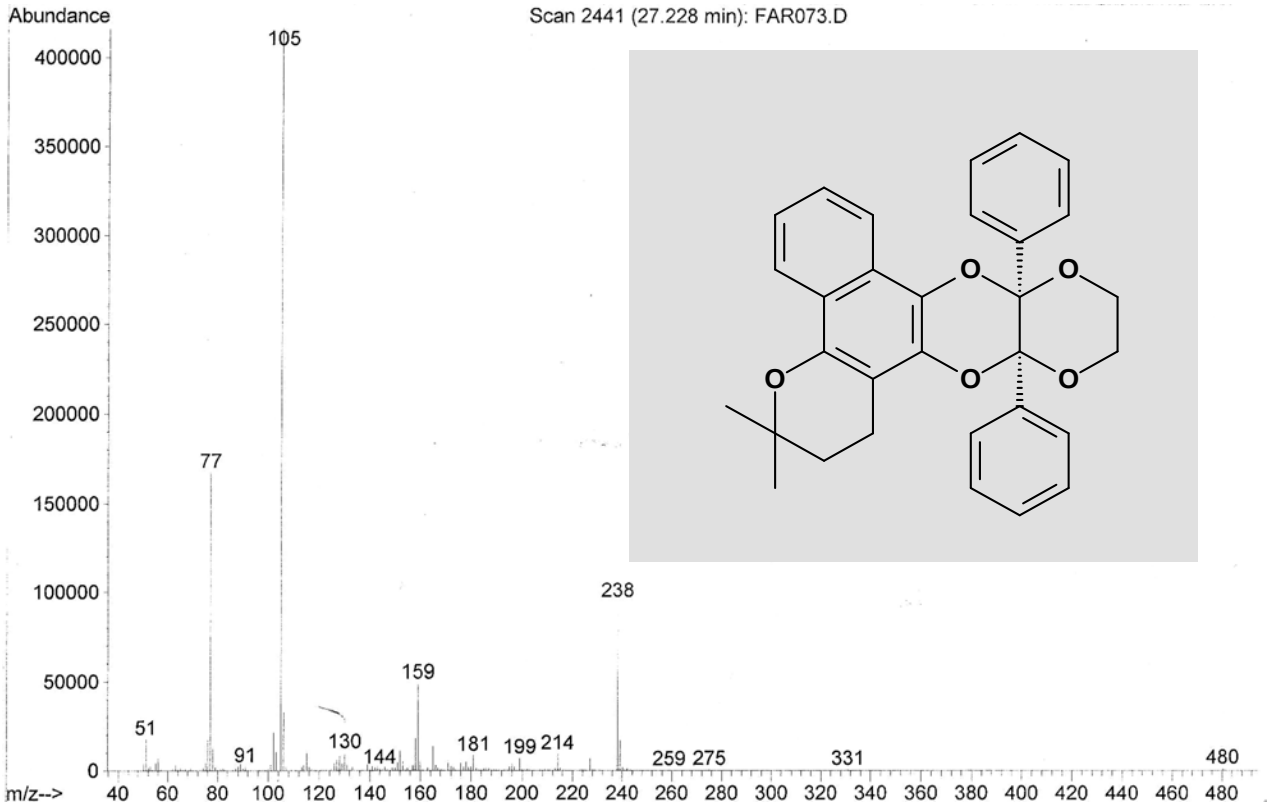
Espectro 63 – IV do DXBL (3,3-dimetil-9a,13a-difenil-2,3,9a,11,12,13a-hexa-hidro-1*H*-benzo[*h*][1,4]dioxino[3',2':5,6][1,4]-dioxino[2,3-*f*]cromeno).



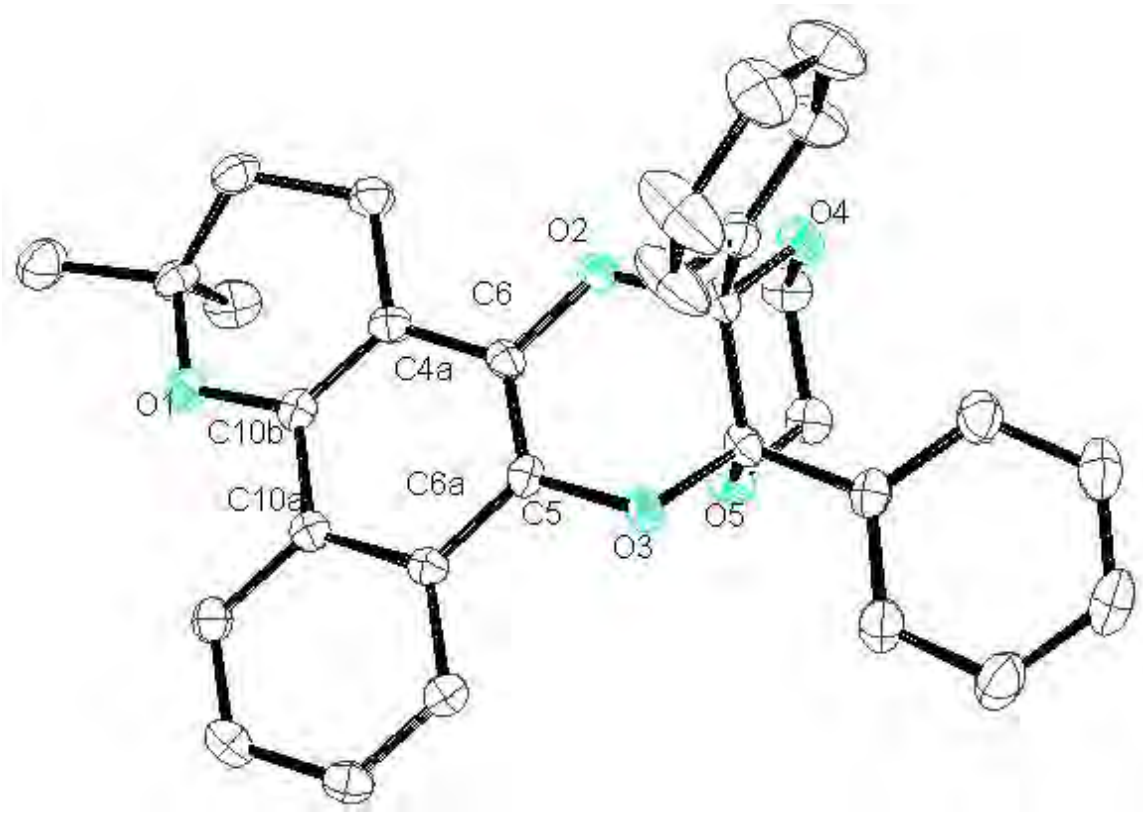
Espectro 64 – RMN ^{1}H (200 MHZ) do DXBL.



Espectro 65 – RMN ^{13}C (50,3 MHZ) do DXBL.



Espectro 66 – E.M. do DXBL.



Espectro 67 – Representação ORTEP do DXBL.

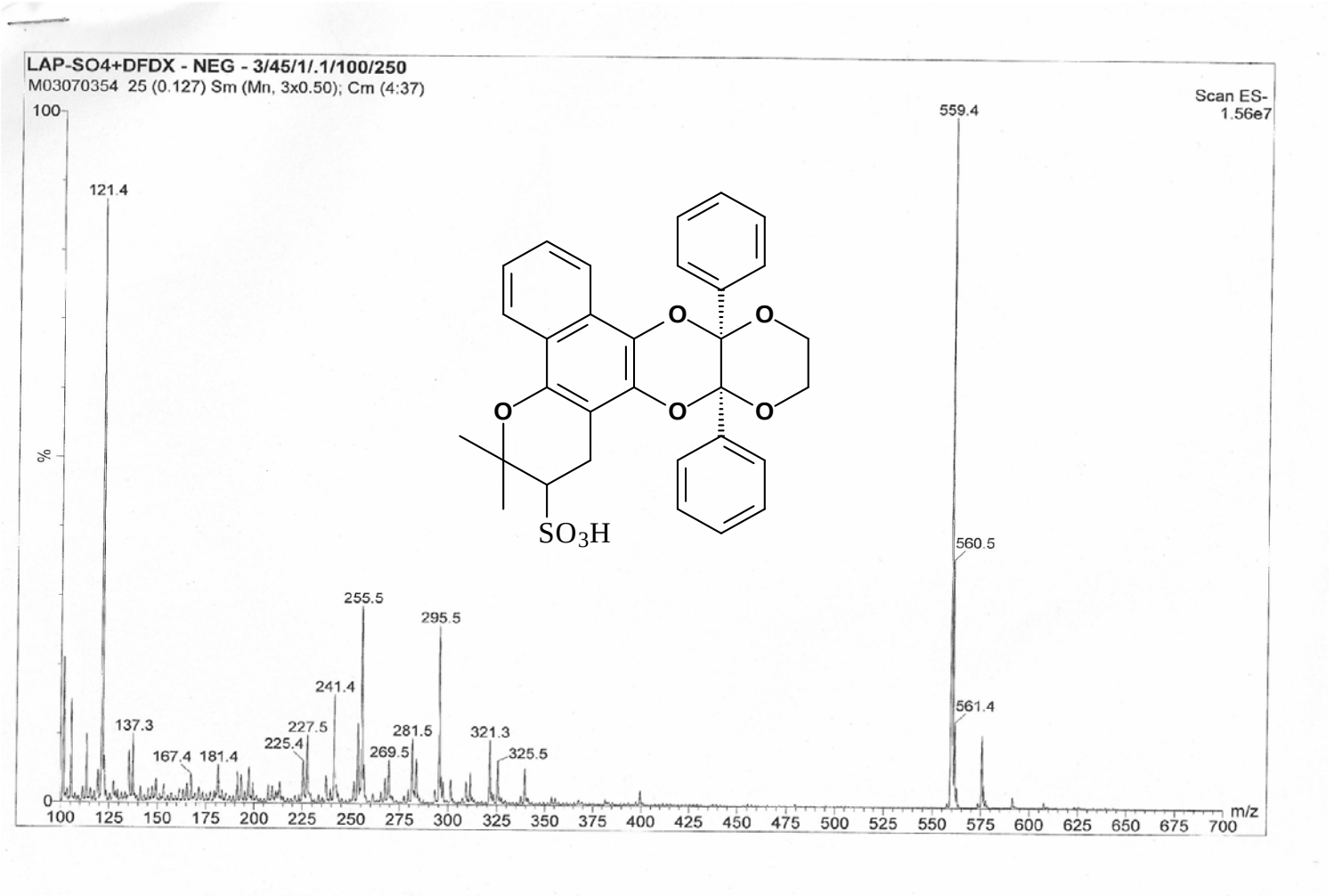
Tabela 31 – Dados do cristal e refinamento da estrutura.

Empirical formula	$C_{31}H_{28}O_5$
Formula weight	480.53 g/mol
Temperature	426(2) K
Wavelength	0.71073 Å
Crystal system	*Monoclinic*
Space group	P21/n
Unit cell dimensions	a = 15.1335(6)Å, α = 90 deg
	b = 9.6048(2)Å, β = 97.3840(14)deg
	c = 16.9739(6)Å, γ = 90deg
Volume	2446.77(14) $Å^3$
Z	4
Density (calculated)	1.304 mg/m^3
Absorption coefficient	0.088 mm^{-1}
F(000)	1016
Crystal size	0.36 x 0.28 x 0.07 mm
Theta range for data collection	3.22 *to* 27.41 deg.
Index ranges	-15<=h<=19; -12<=k<=12; -21<=l<=21
Reflections collected	23103
Independent reflections	5549 [R(int) = 0.0592]
Reflections observed (>2sigma)	3390
Data Completeness	0.995
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5549 / 0 / 325
Goodness-of-fit on F@2	1.014
Final R indices [I>2sigma(I)]	R~1 = 0.0509 wR~2 = 0.1178
R indices (all data)	R~1 = 0.1016 wR~2 = 0.1431
Largest diff. peak and hole	0.251 and -0.288 $e.Å^{-3}$

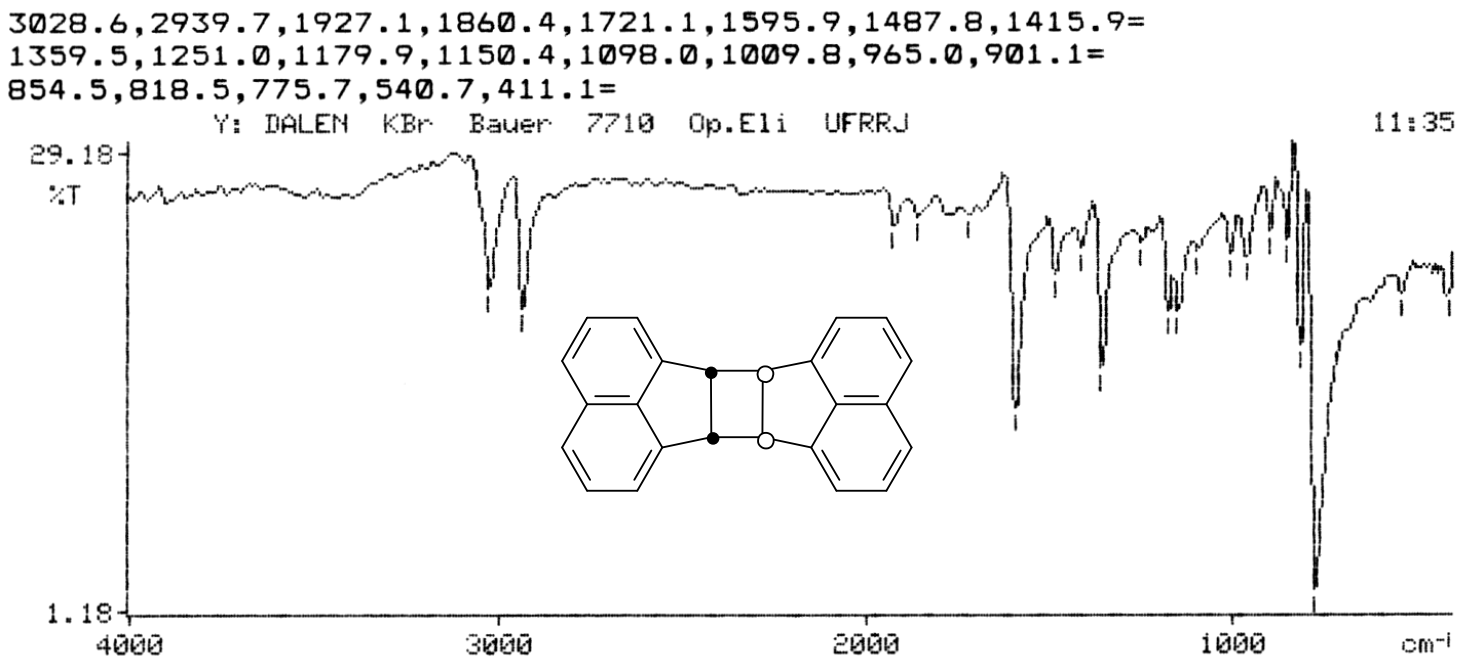
Tabela 32 - Ângulos (em graus) e distâncias (em ângstrons) entre os átomos.

O(1)-C(10B)	1.369(2)	O(1)-C(2)	1.468(2)
O(2)-C(6)	1.374(2)	O(2)-C(13)	1.449(2)
O(3)-C(5)	1.392(2)	O(3)-C(16)	1.415(2)
O(4)-C(13)	1.412(2)	O(4)-C(14)	1.445(2)
O(5)-C(16)	1.420(2)	O(5)-C(15)	1.436(2)
C(2)-C(11)	1.519(3)	C(2)-C(3)	1.522(3)
C(2)-C(12)	1.523(3)	C(3)-C(4)	1.526(2)
C(4)-C(4A)	1.509(2)	C(4A)-C(10B)	1.371(2)
C(4A)-C(6)	1.415(2)	C(5)-C(6)	1.365(2)
C(5)-C(6A)	1.415(2)	C(6A)-C(7)	1.416(2)
C(6A)-C(10A)	1.424(2)	C(7)-C(8)	1.371(2)
C(8)-C(9)	1.405(3)	C(9)-C(10)	1.373(2)
C(10)-C(10A)	1.412(2)	C(10A)-C(10B)	1.429(2)
C(13)-C(17)	1.513(3)	C(13)-C(16)	1.566(2)
C(14)-C(15)	1.498(2)	C(16)-C(23)	1.528(2)
C(17)-C(18)	1.377(3)	C(17)-C(22)	1.385(3)
C(18)-C(19)	1.388(3)	C(19)-C(20)	1.361(3)
C(20)-C(21)	1.374(3)	C(21)-C(22)	1.383(3)
C(23)-C(24)	1.386(3)	C(23)-C(28)	1.398(3)
C(24)-C(25)	1.389(3)	C(25)-C(26)	1.376(3)
C(26)-C(27)	1.386(3)	C(27)-C(28)	1.380(3)
C(10B)-O(1)-C(2)	117.38(13)	C(6)-O(2)-C(13)	118.90(13)
C(5)-O(3)-C(16)	113.33(13)	C(13)-O(4)-C(14)	113.11(13)
C(16)-O(5)-C(15)	113.39(13)	O(1)-C(2)-C(11)	102.65(15)
O(1)-C(2)-C(3)	108.81(15)	C(11)-C(2)-C(3)	112.44(15)
O(1)-C(2)-C(12)	108.82(14)	C(11)-C(2)-C(12)	111.02(17)
C(3)-C(2)-C(12)	112.56(17)	C(2)-C(3)-C(4)	111.46(15)

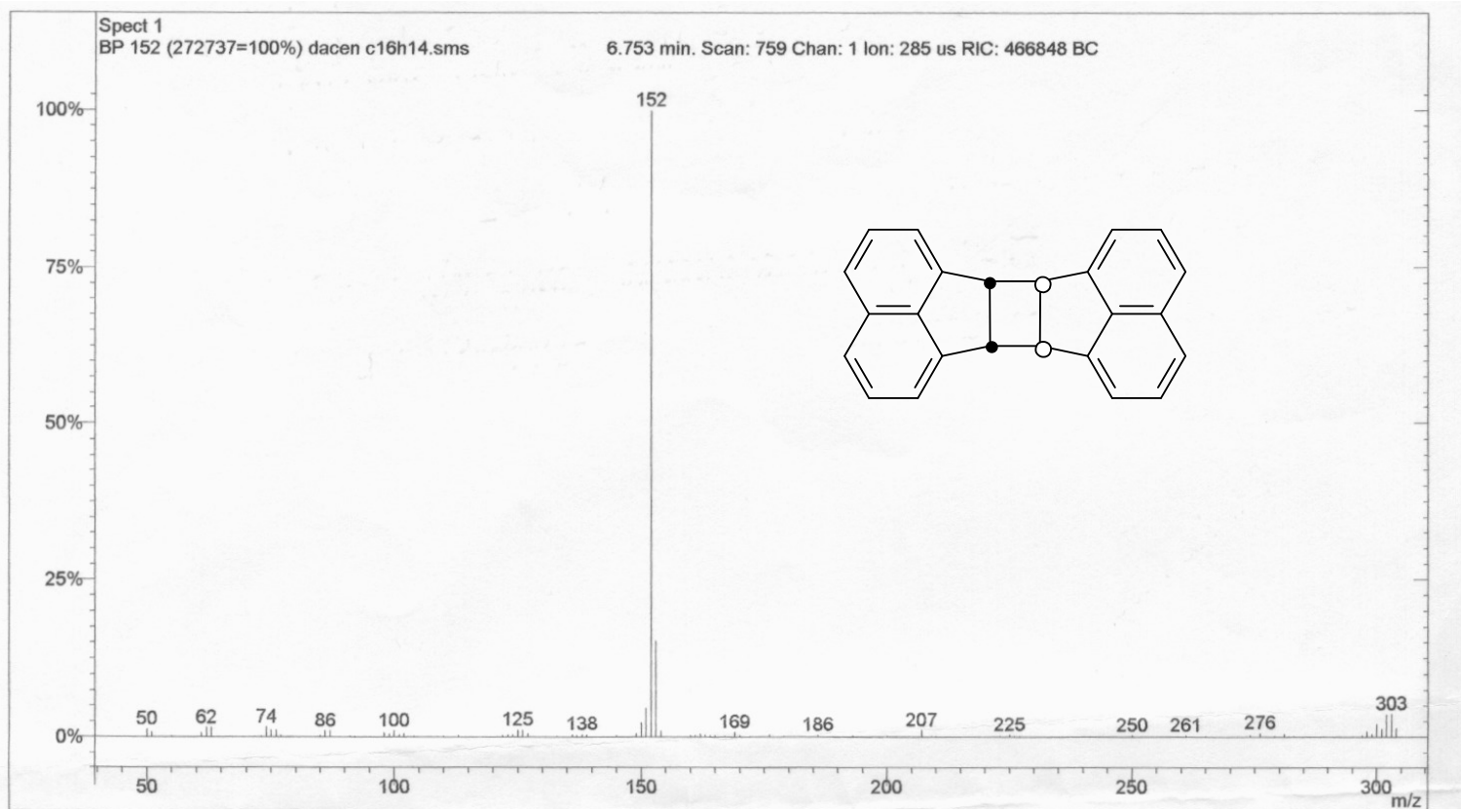
C(4A)-C(4)-C(3)	109.61(15)	C(10B)-C(4A)-C(6)	117.88(15)
C(10B)-C(4A)-C(4)	121.47(16)	C(6)-C(4A)-C(4)	120.59(15)
C(6)-C(5)-O(3)	121.02(15)	C(6)-C(5)-C(6A)	120.83(15)
O(3)-C(5)-C(6A)	118.16(14)	C(5)-C(6)-O(2)	121.95(15)
C(5)-C(6)-C(4A)	122.21(16)	O(2)-C(6)-C(4A)	115.84(15)
C(5)-C(6A)-C(7)	122.66(16)	C(5)-C(6A)-C(10A)	118.19(15)
C(7)-C(6A)-C(10A)	119.11(15)	C(8)-C(7)-C(6A)	120.51(16)
C(7)-C(8)-C(9)	120.55(16)	C(10)-C(9)-C(8)	120.10(16)
C(9)-C(10)-C(10A)	121.00(16)	C(10)-C(10A)-C(6A)	118.66(15)
C(10)-C(10A)-C(10B)	122.36(16)	C(6A)-C(10A)-C(10B)	118.96(15)
O(1)-C(10B)-C(4A)	123.68(15)	O(1)-C(10B)-C(10A)	114.43(15)
C(4A)-C(10B)-C(10A)	121.88(15)	O(4)-C(13)-O(2)	104.62(14)
O(4)-C(13)-C(17)	108.51(14)	O(2)-C(13)-C(17)	107.76(14)
O(4)-C(13)-C(16)	109.99(14)	O(2)-C(13)-C(16)	109.85(13)
C(17)-C(13)-C(16)	115.52(15)	O(4)-C(14)-C(15)	110.46(15)
O(5)-C(15)-C(14)	110.10(14)	O(3)-C(16)-O(5)	104.13(13)
O(3)-C(16)-C(23)	106.47(14)	O(5)-C(16)-C(23)	110.93(14)
O(3)-C(16)-C(13)	109.83(13)	O(5)-C(16)-C(13)	109.19(14)
C(23)-C(16)-C(13)	115.64(14)	C(18)-C(17)-C(22)	117.87(19)
C(18)-C(17)-C(13)	121.03(17)	C(22)-C(17)-C(13)	120.97(17)
C(17)-C(18)-C(19)	120.9(2)	C(20)-C(19)-C(18)	120.7(2)
C(19)-C(20)-C(21)	119.1(2)	C(20)-C(21)-C(22)	120.5(2)
C(21)-C(22)-C(17)	120.9(2)	C(24)-C(23)-C(28)	118.54(16)
C(24)-C(23)-C(16)	123.44(16)	C(28)-C(23)-C(16)	117.85(16)
C(23)-C(24)-C(25)	120.56(18)	C(26)-C(25)-C(24)	120.33(19)



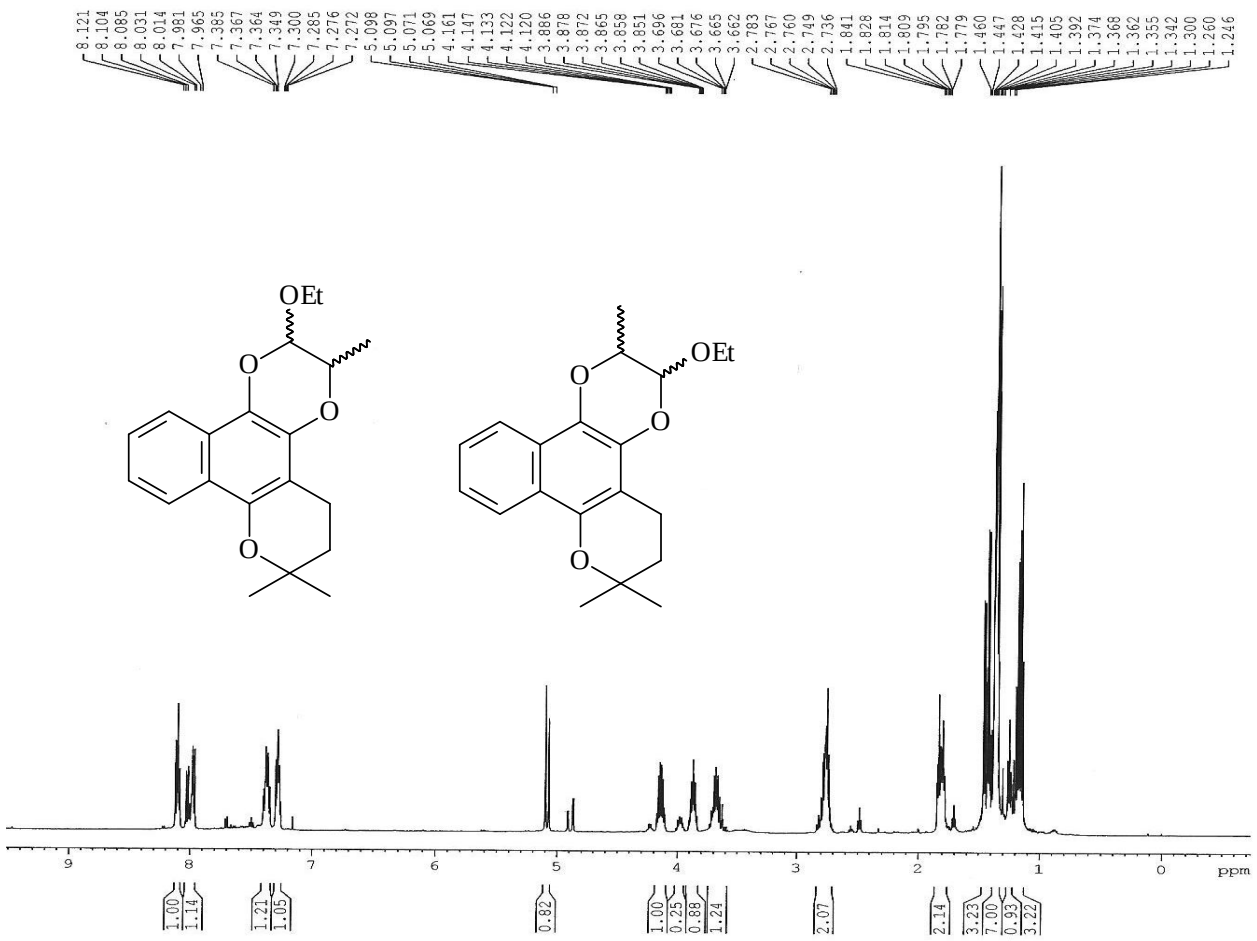
Espectro 68 – E.M. do produto de irradiaão entre 3-sulfo-β-lapachona e difenildioxeno, M.M. = 560**.**



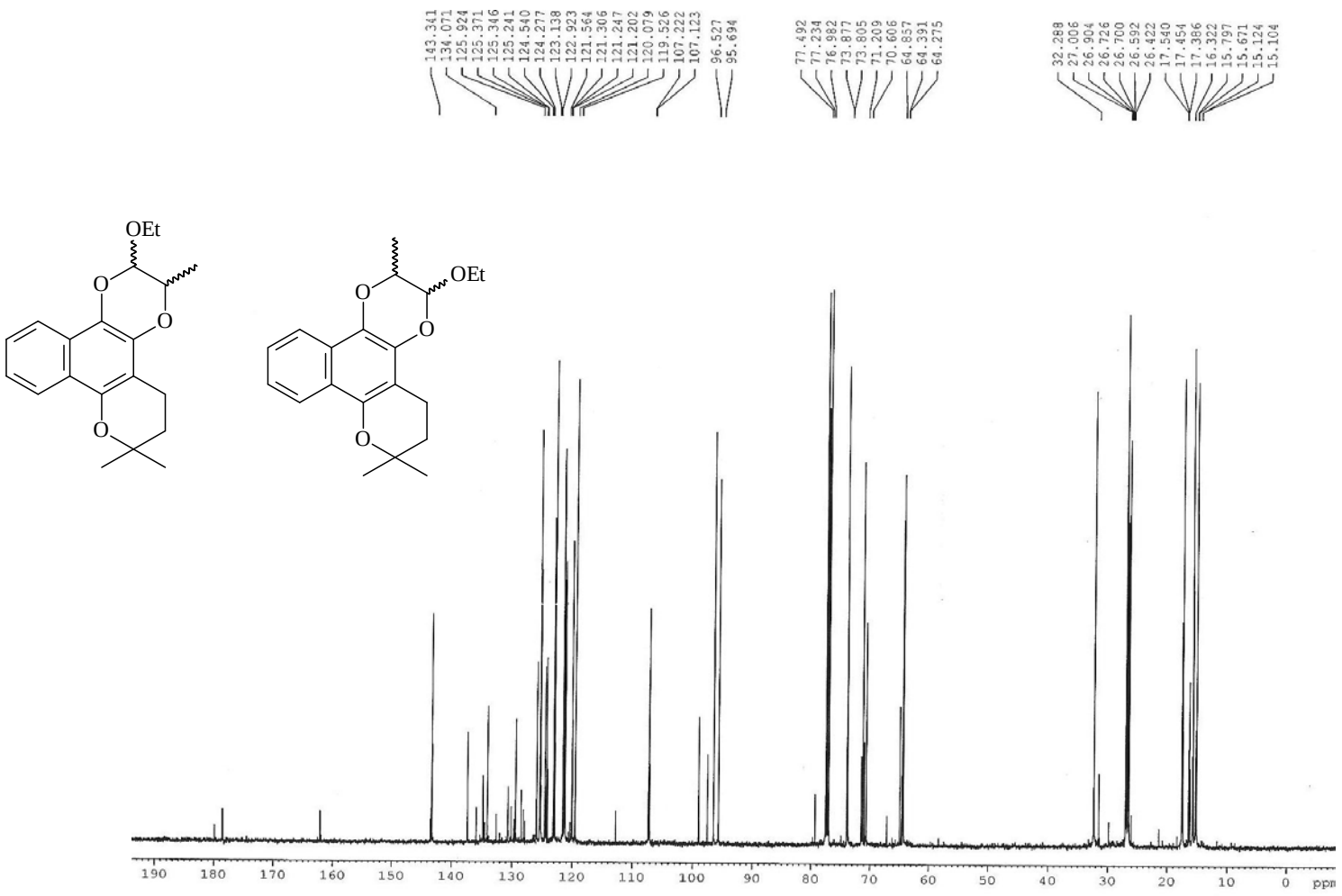
Espectro 69 – IV do dímero de acenaftelino (DACEN).



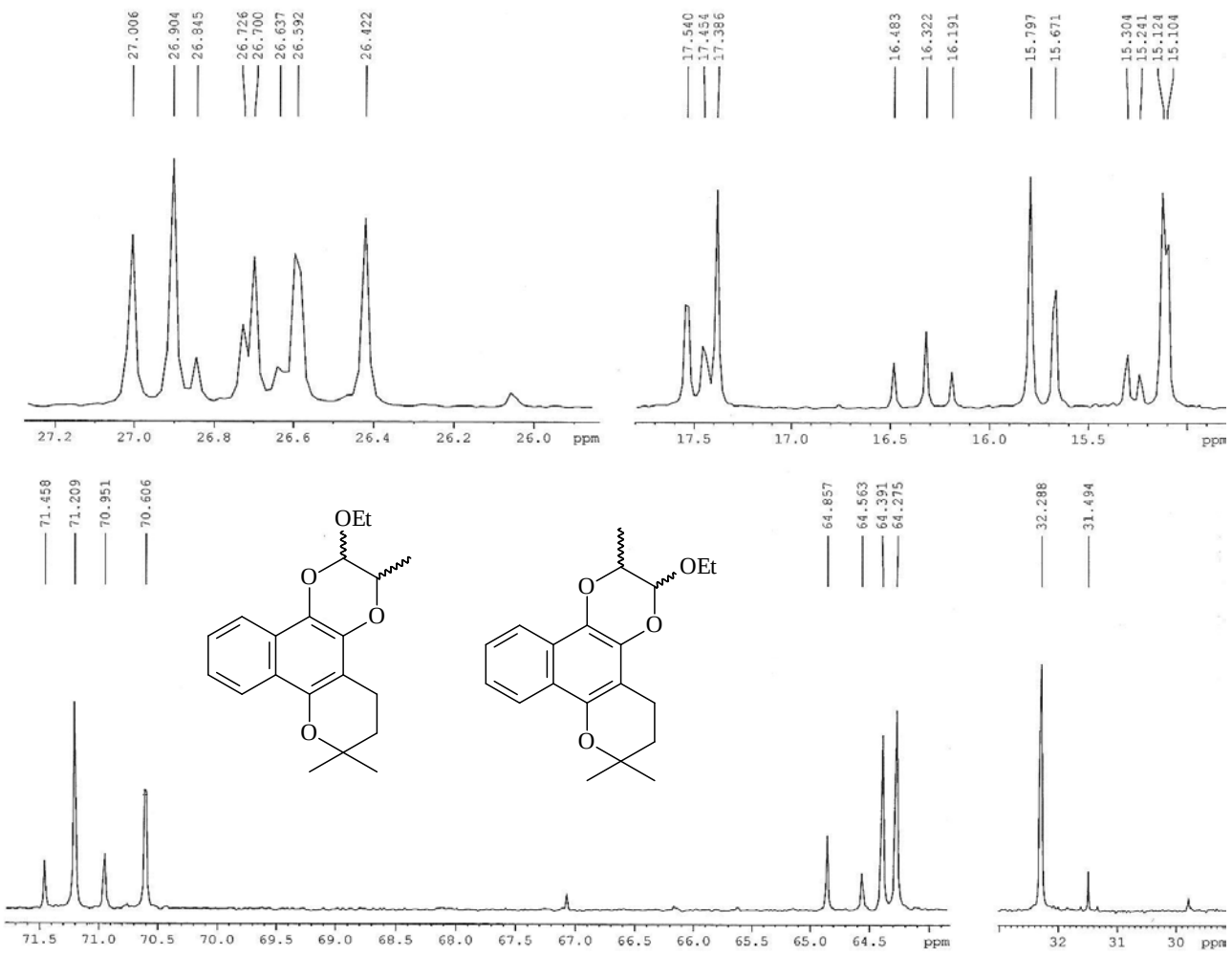
Espectro 70 - E.M. do dímero de acenaftileno (DACEN).



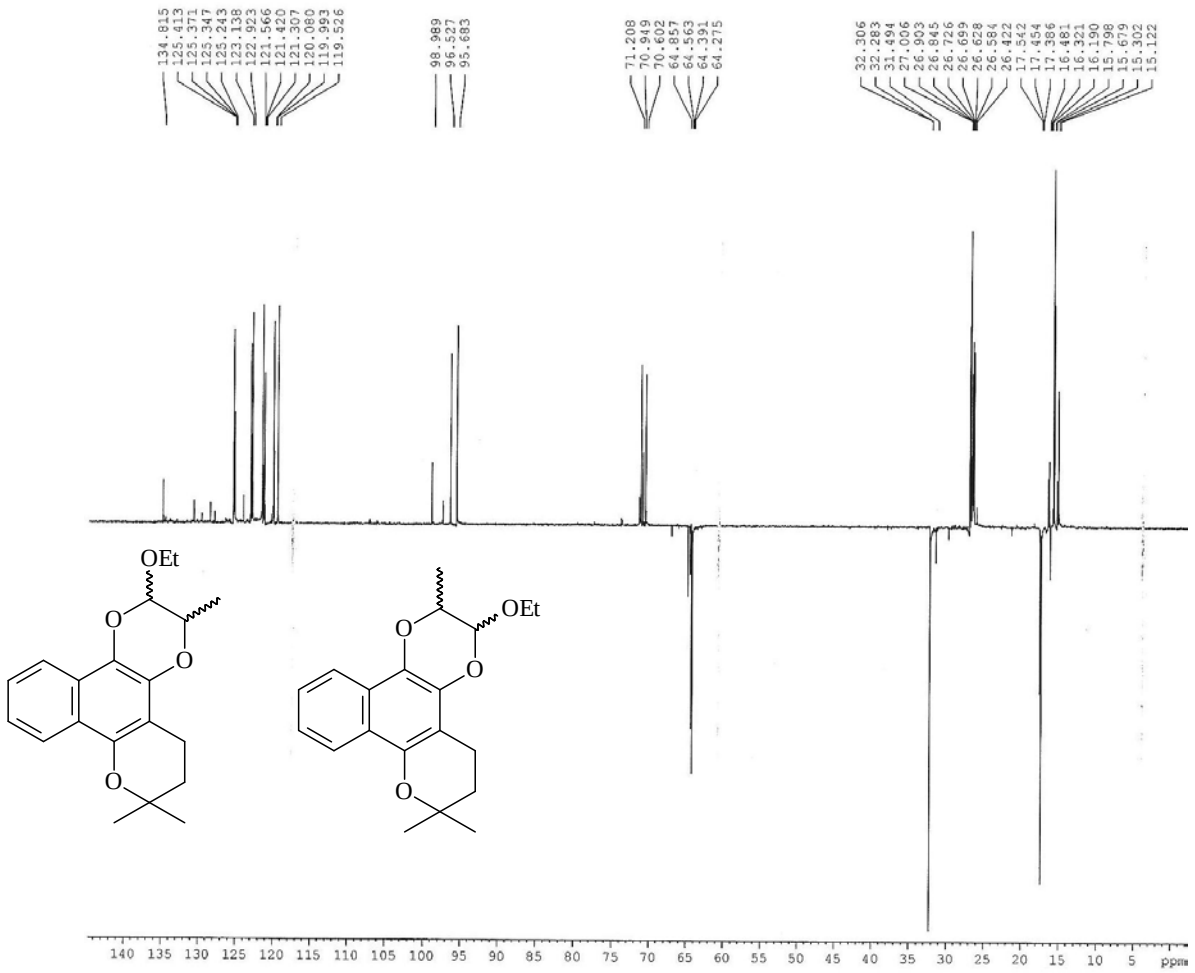
Espectro 71– RMN ^{1}H (500 MHz) da mistura de isômeros de BLEP, reação fotoquímica entre β-lapachona e 1-etoxipropreno.



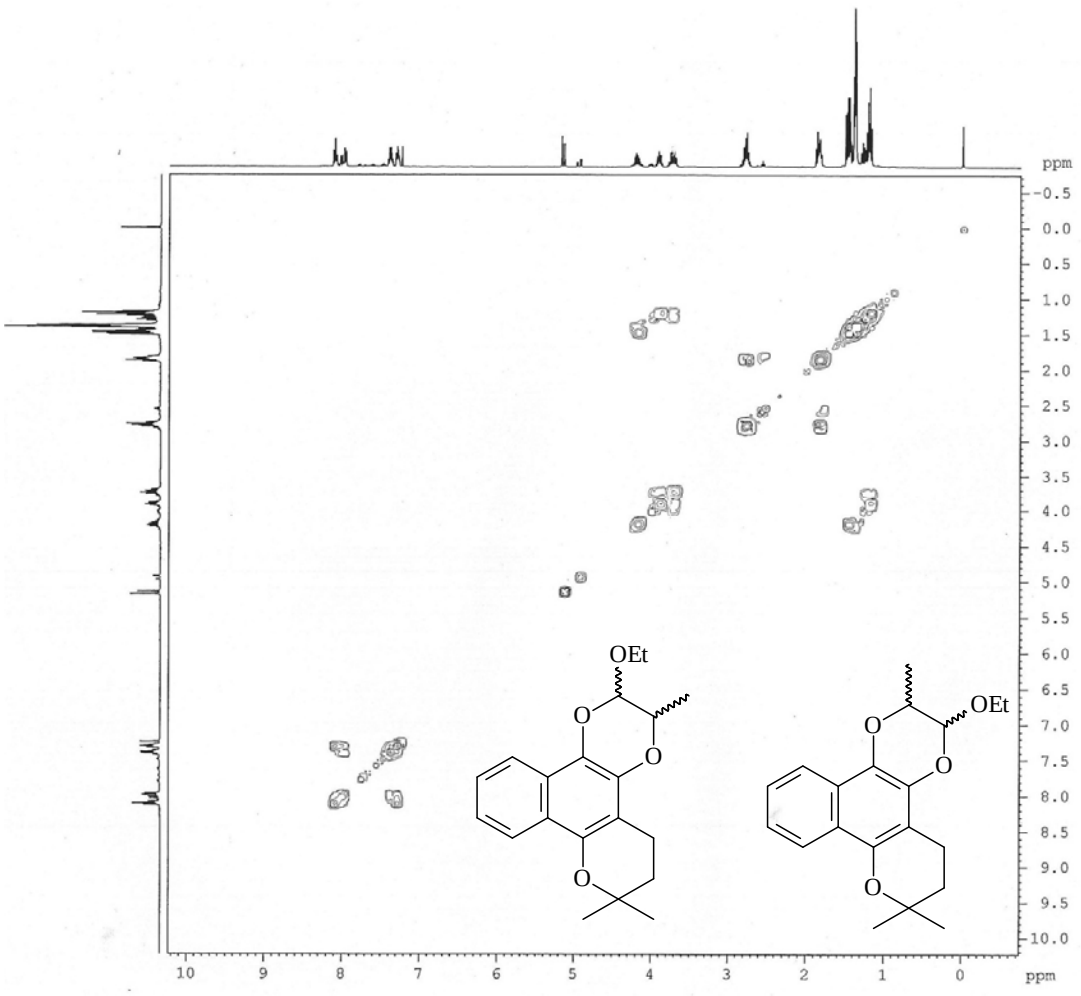
Espectro 72 – RMN ^{13}C (125,75 MHz) da mistura isômera de BLEP, reação fotoquímica entre β-lapachona e 1-etoxipropreno**.**



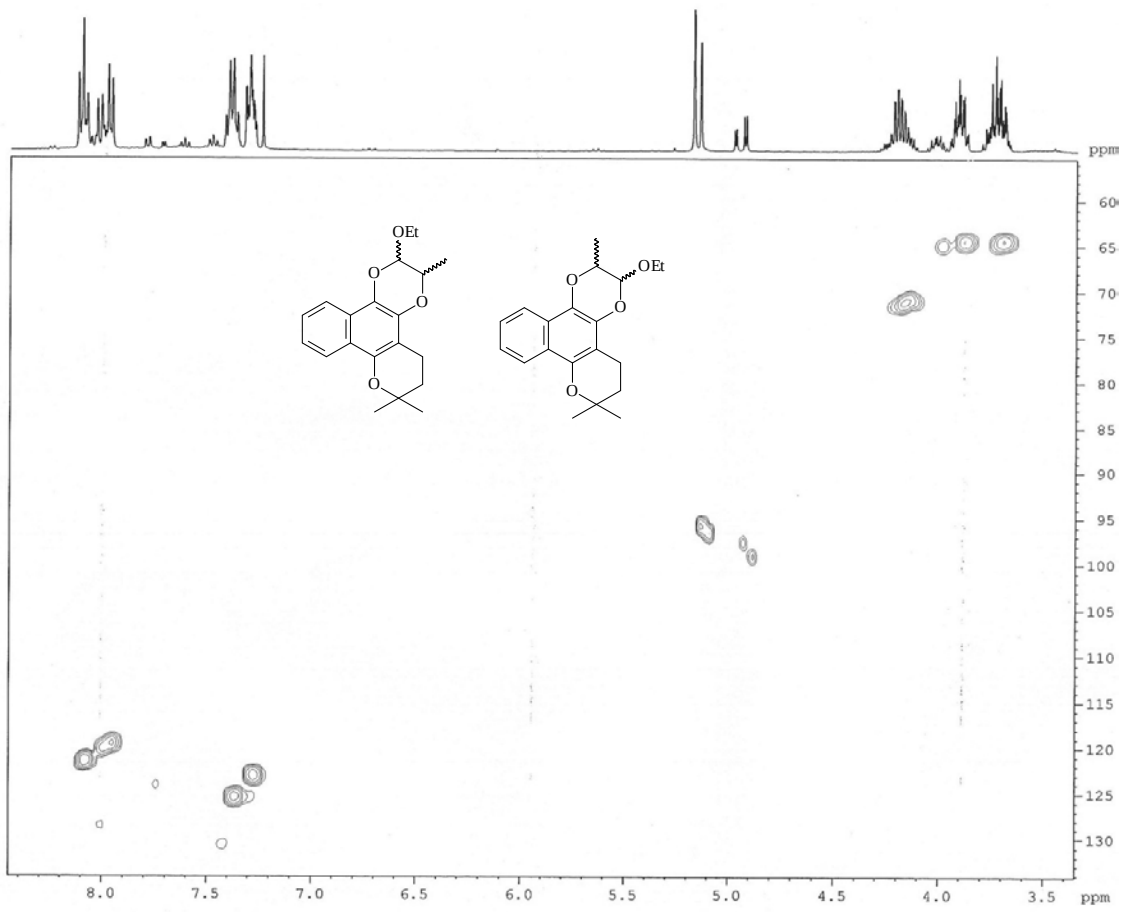
Espectro 73 – Expansões da RMN ^{13}C da mistura de isômeros de BLEP, reação fotoquímica entre β-lapachona e 1-etoxipropreno**.**



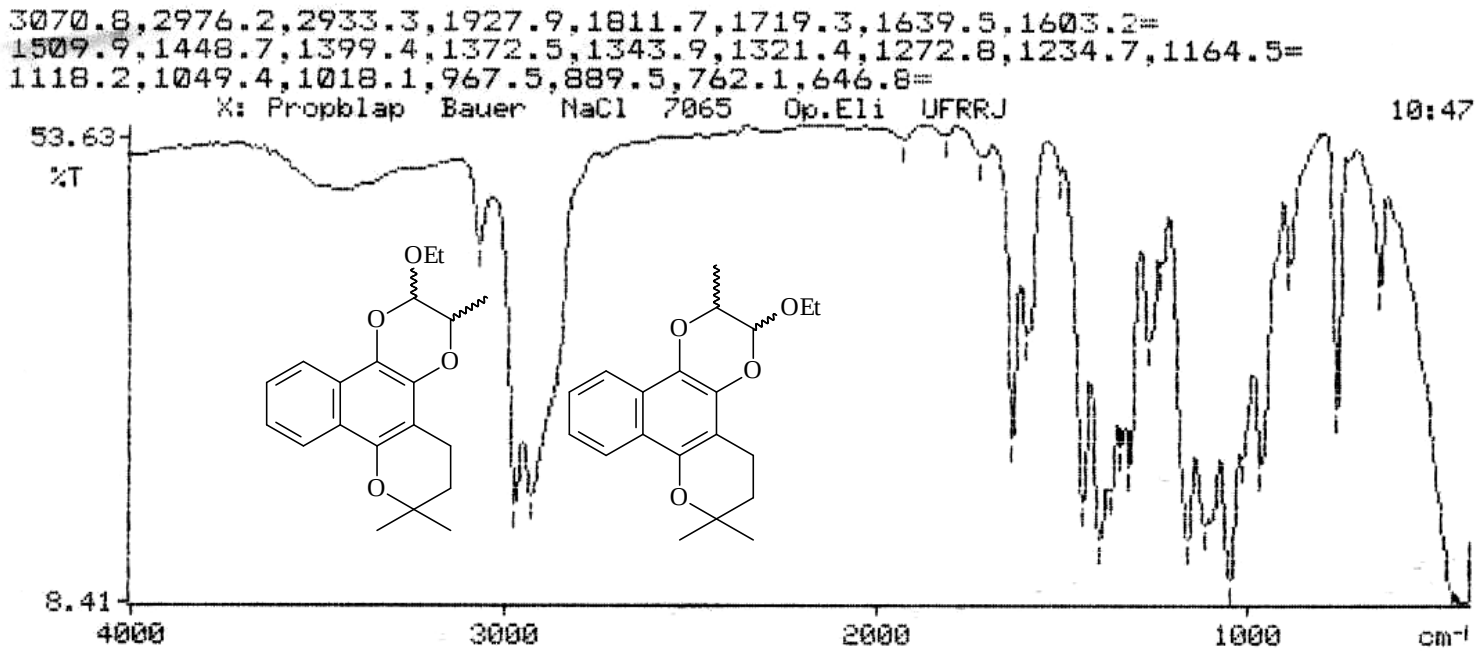
Espectro 74 – DEPT 135º da mistura de isômeros de BLEP, reação fotoquímica entre β-lapachona e 1-etoxipropreno**.**



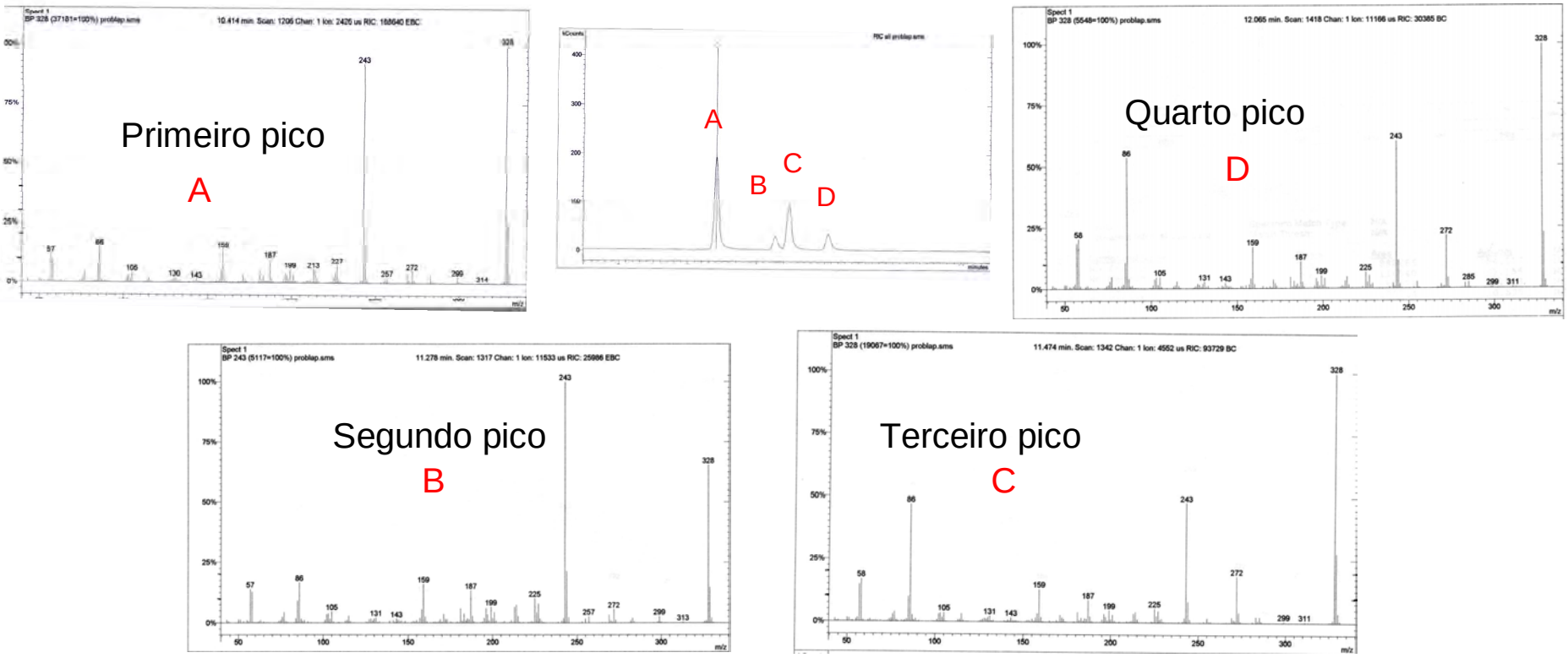
Espectro 75 – Cosy ^{1}H-^{1}H da mistura de BLEP, reação fotoquímica entre β-lapachona e 1-etoxipropreno.



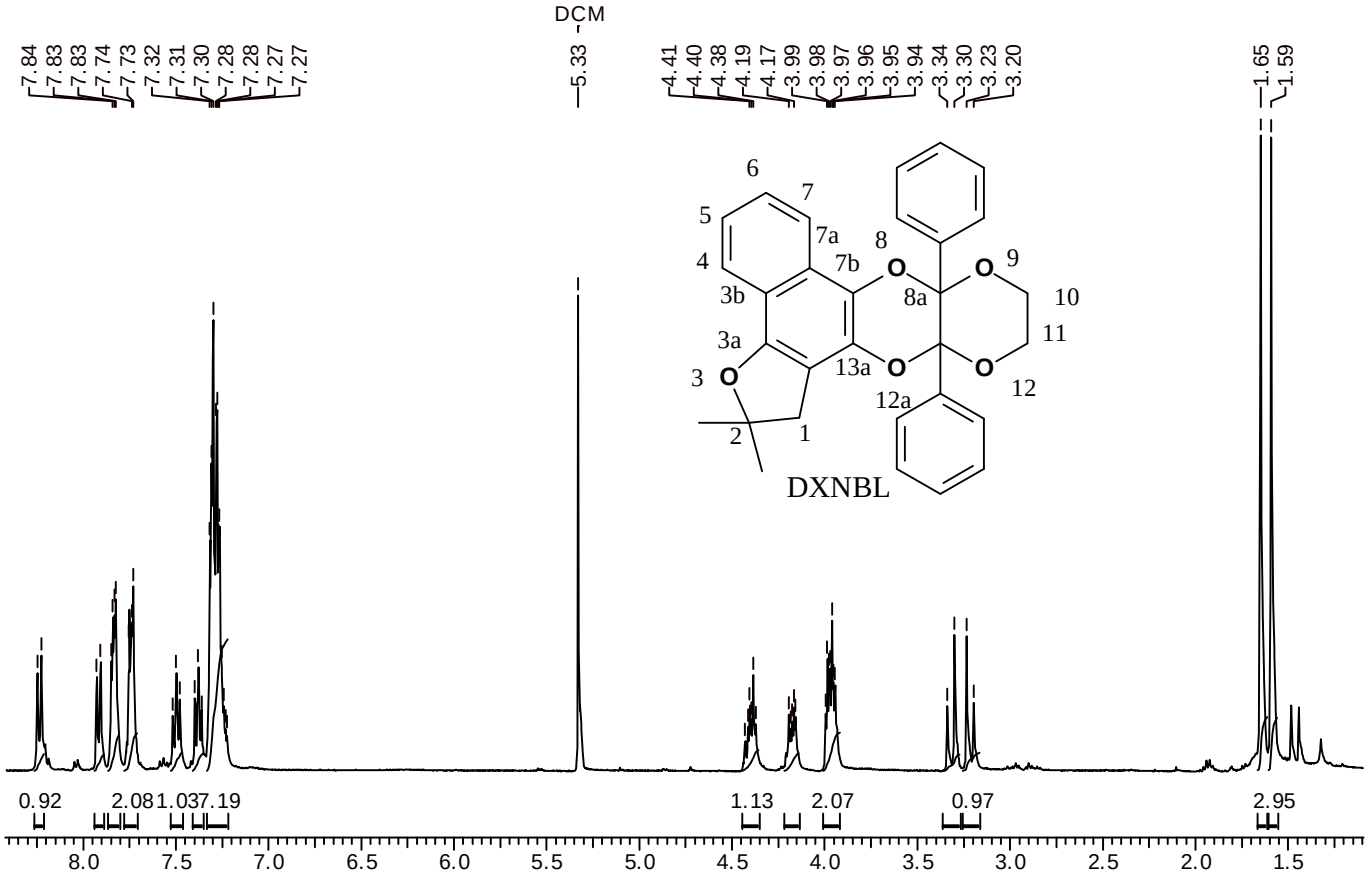
Espectro 76 - HSQC ^{1}H x ^{1}H da mistura de isômeros de BLEP, reação fotoquímica entre β-lapachona e 1-etoxipropreno.



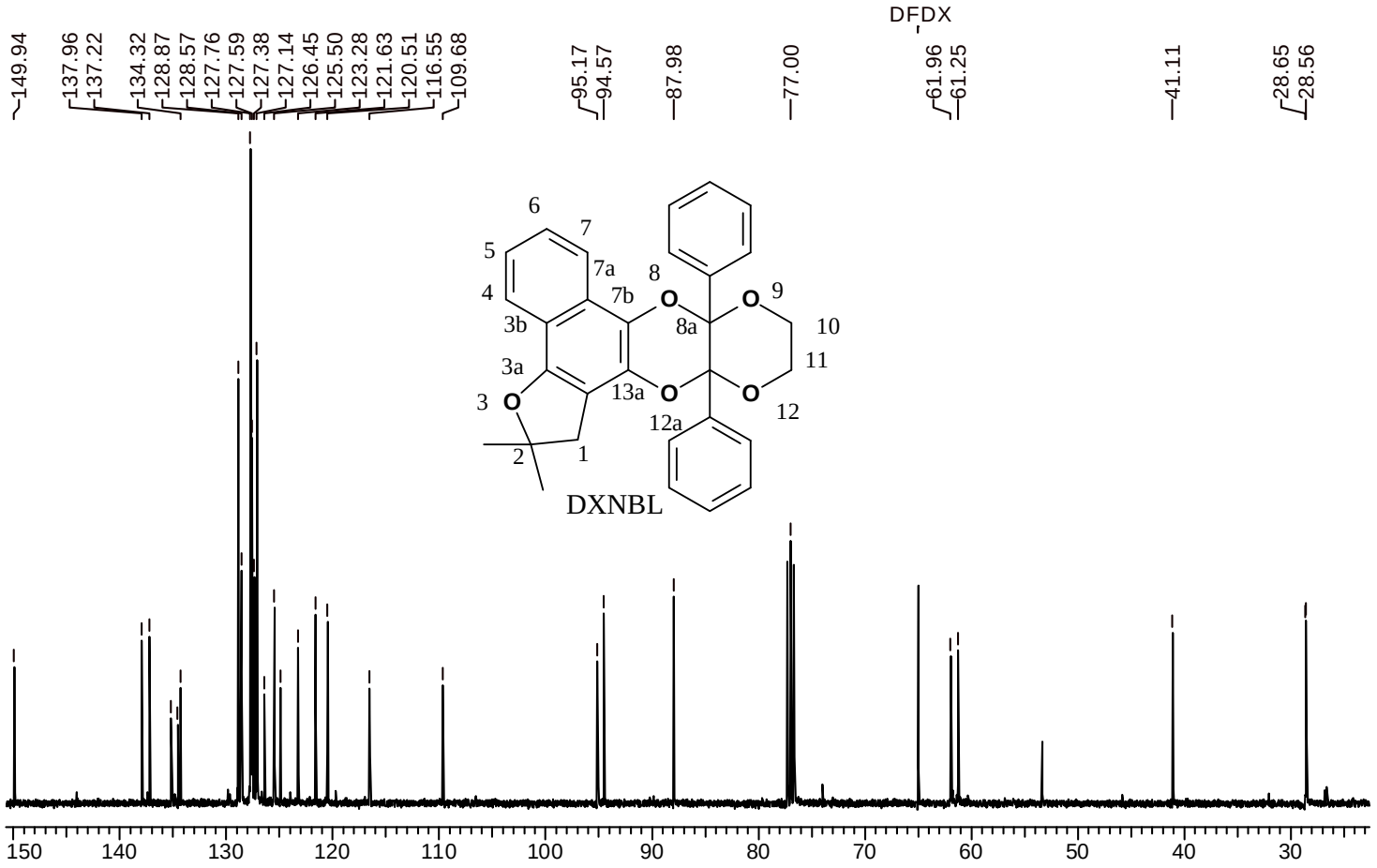
Espectro 77 – IV da mistura de isômeros de BLEP, reação fotoquímica entre β-lapachona e 1-etoxipropreno.



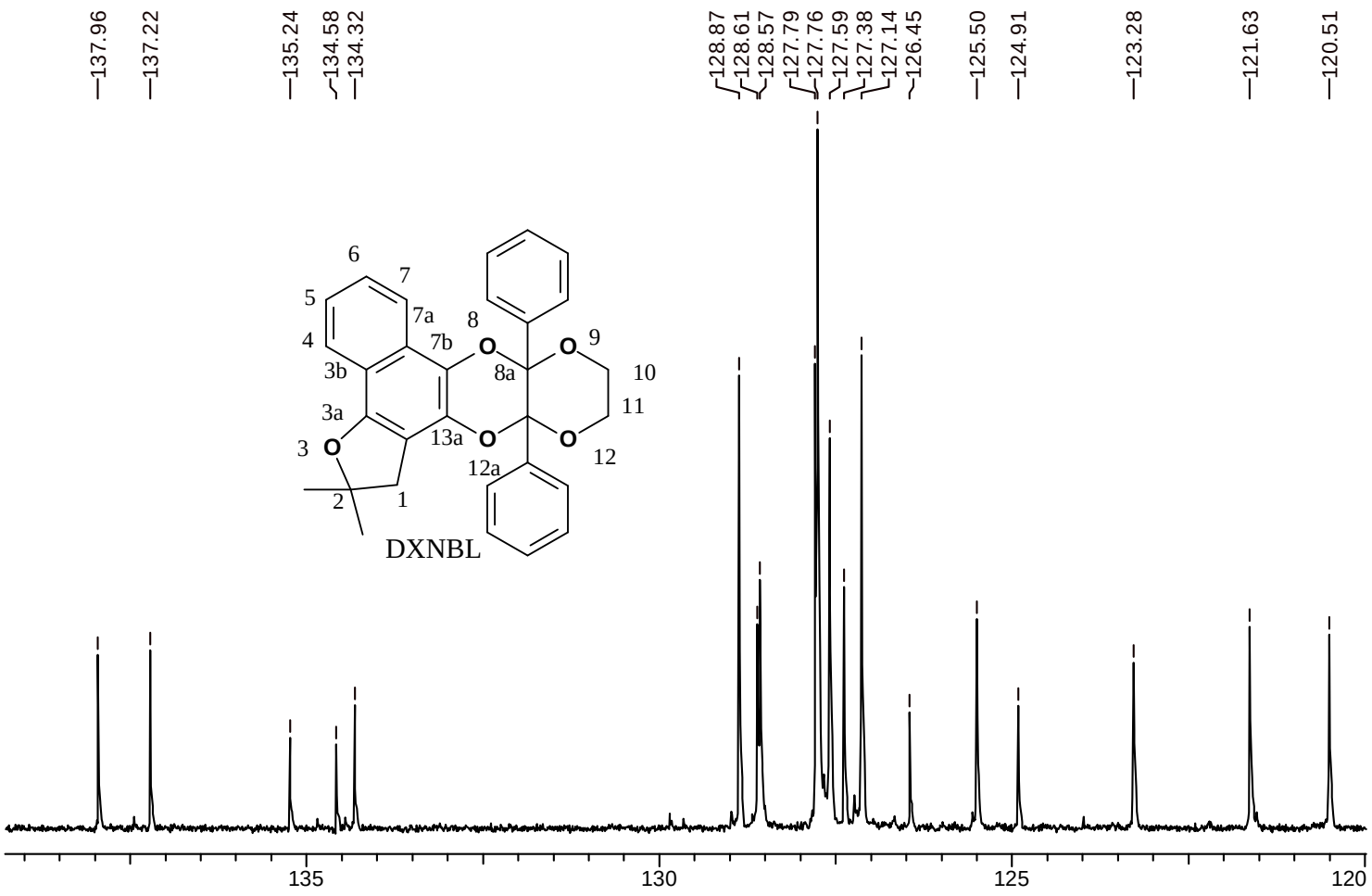
Espectro 78 - EM da mistura de isômeros de BLEP, reação fotoquímica entre β-lapachona e 1-etoxipropreno, ao centro o cromatograma com os quatro produtos obtidos.



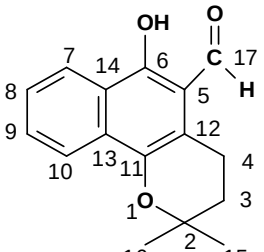
Espectro 79 – RMN ^{1}H (400 MHz) do DXNBL, 2,2-dimetil-8a,12a-difenil-1,2,8a,10,11,12a-hexaidro[1,4]dioxino[2,3-*b*]furo[3',2':3,4]naftho[1,2-*e*][1,4]dioxina.



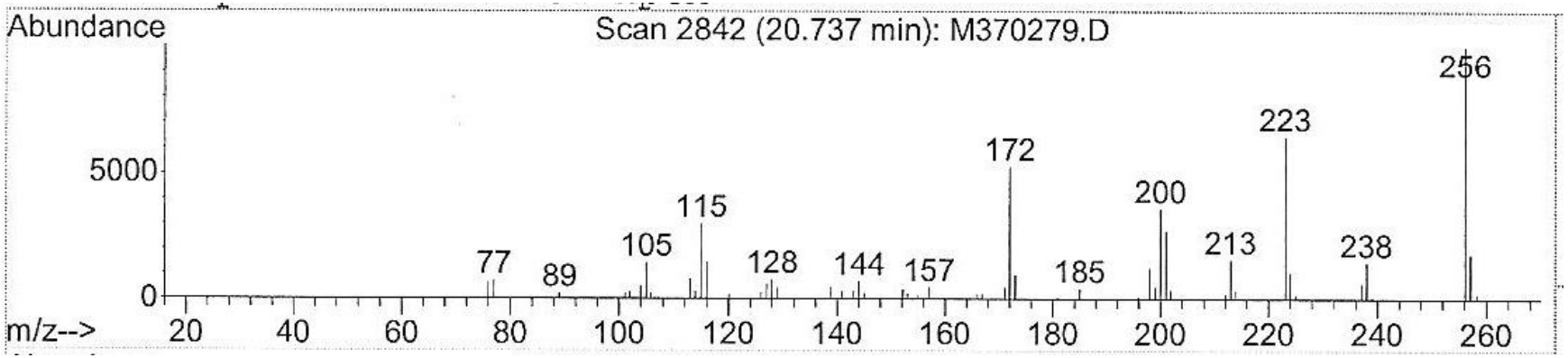
Espectro 80 – RMN ^{13}C (100,6 MHz) de DXNBL (2,2-dimetil-8a,12a-difenil-1,2,8a,10,11,12a-hexaidro[1,4]dioxino[2,3-*b*]furo[3',2':3,4]naftho[1,2-*e*][1,4]dioxina).



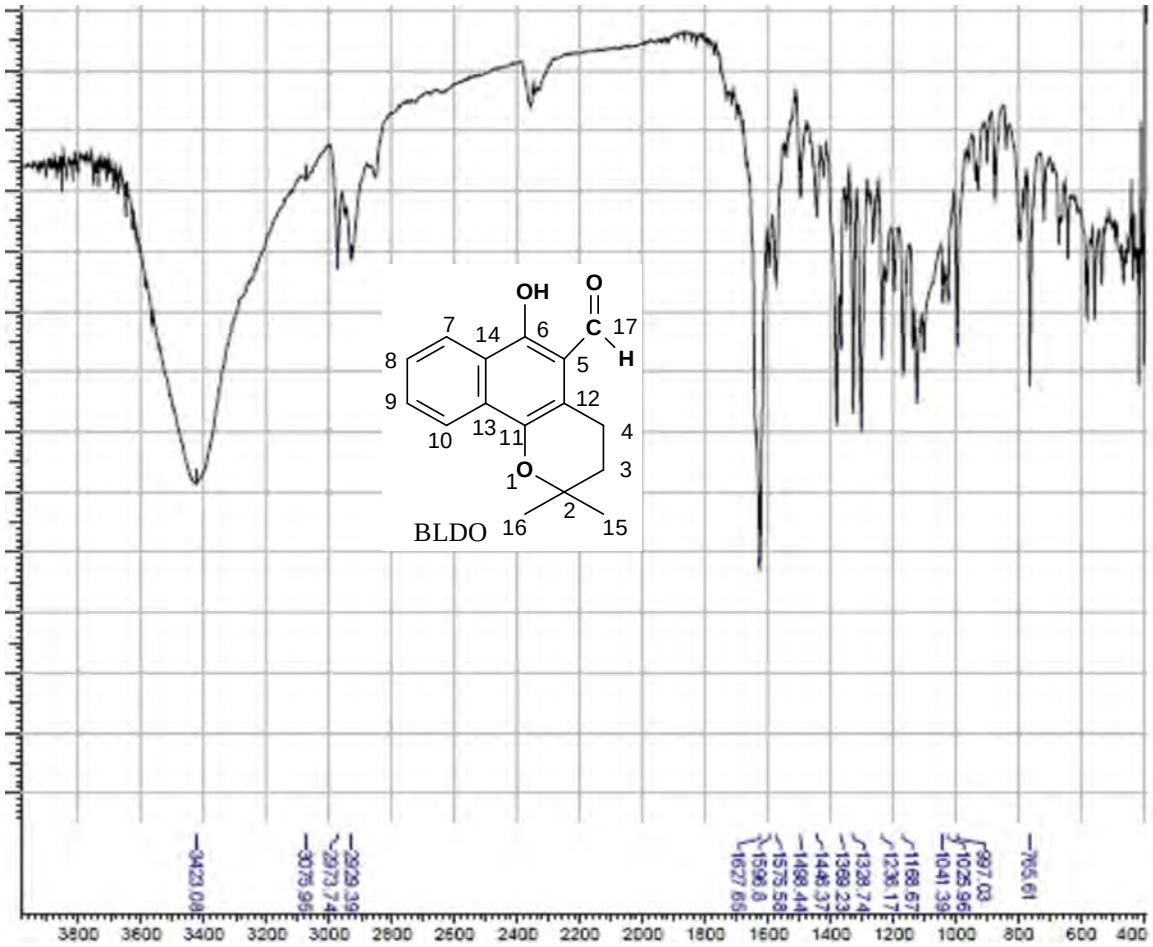
Espectro 81 – Ampliação do espectro de RMN ^{13}C de DXNBL (2,2-dimetil-8a,12a-difenil-1,2,8a,10,11,12a-hexaidro[1,4]dioxino[2,3-*b*]furo[3',2':3,4]naftho[1,2-*e*][1,4]dioxina)**.**



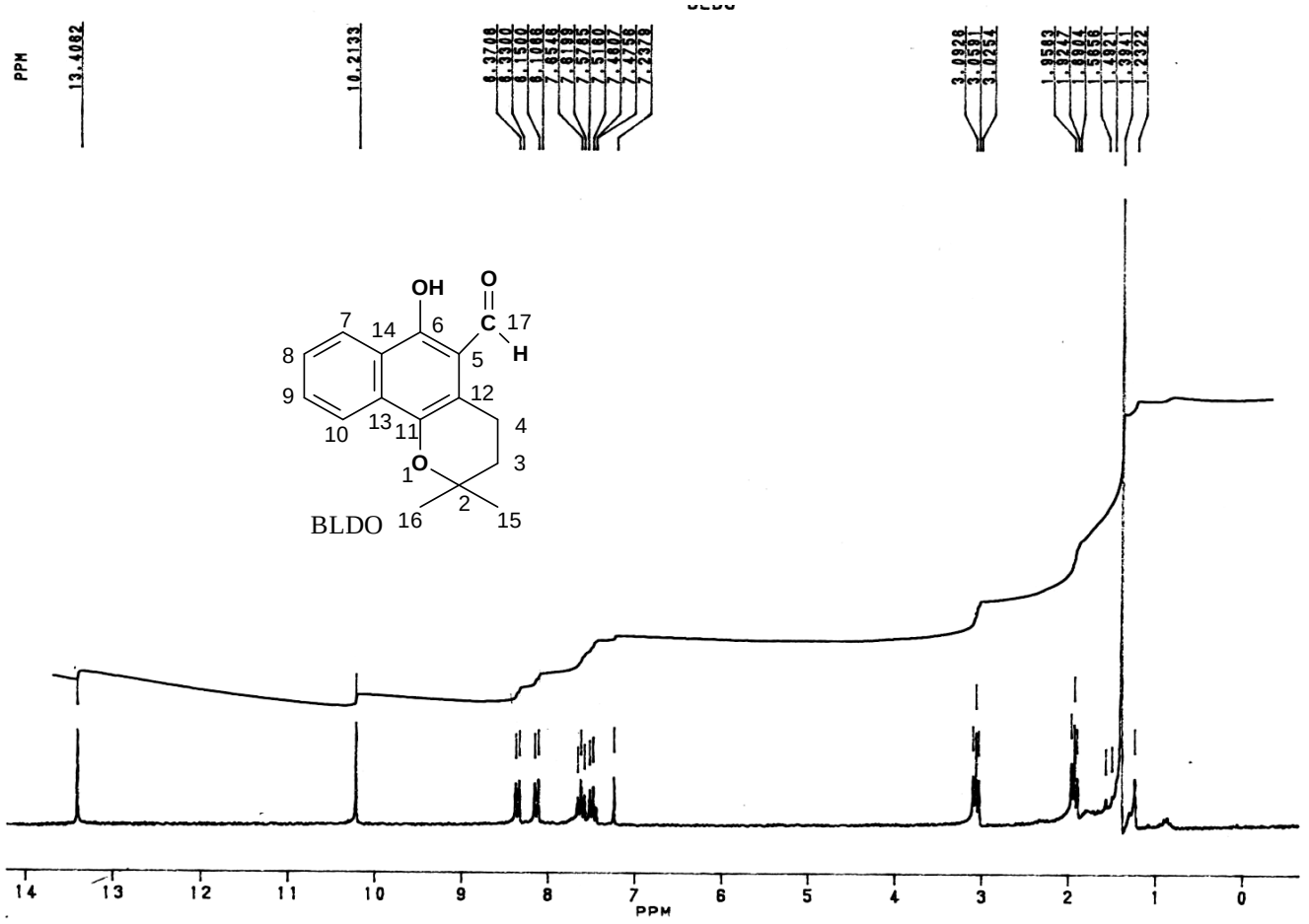
BLDO



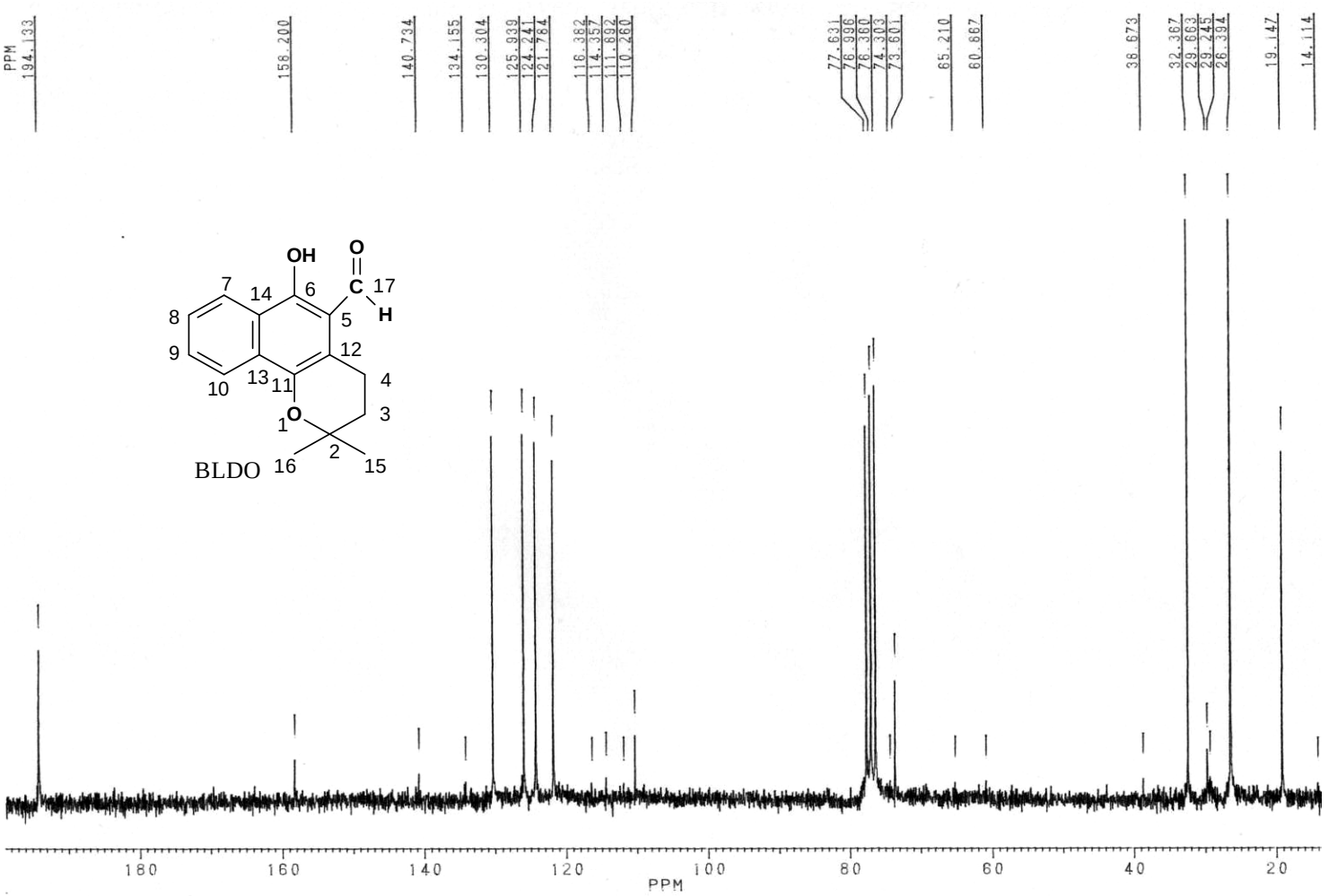
Espectro 82 – EM do BLDO **(**10-hidroxi-6,6-dimetil-5,6,7,8-tetraidrofenantreno-9-carbaldeído**).**



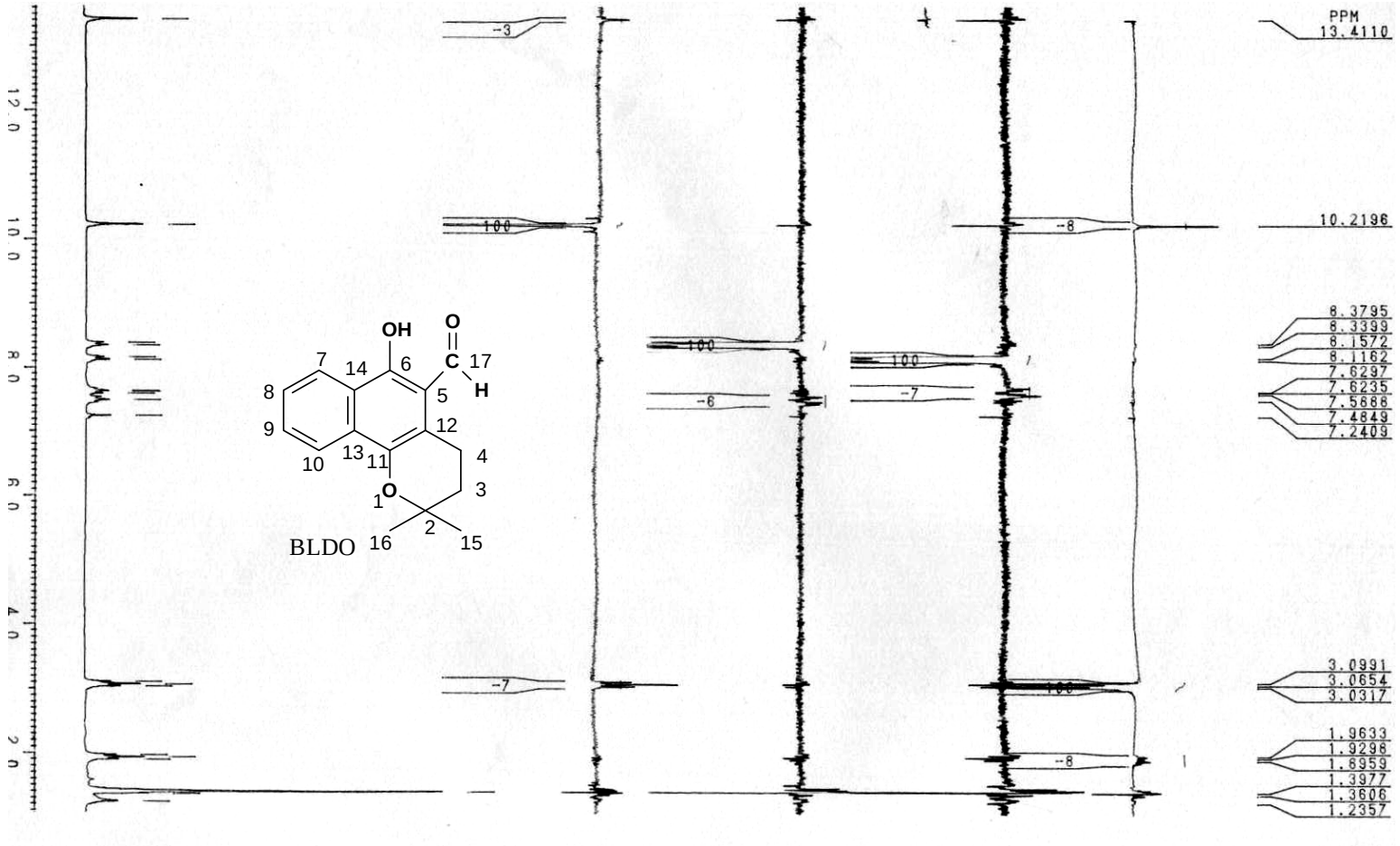
Espectro 83 – IV do BLDO (10-hidroxi-6,6-dimetil-5,6,7,8-tetraidrofenantreno-9-carbaldeído)**.**



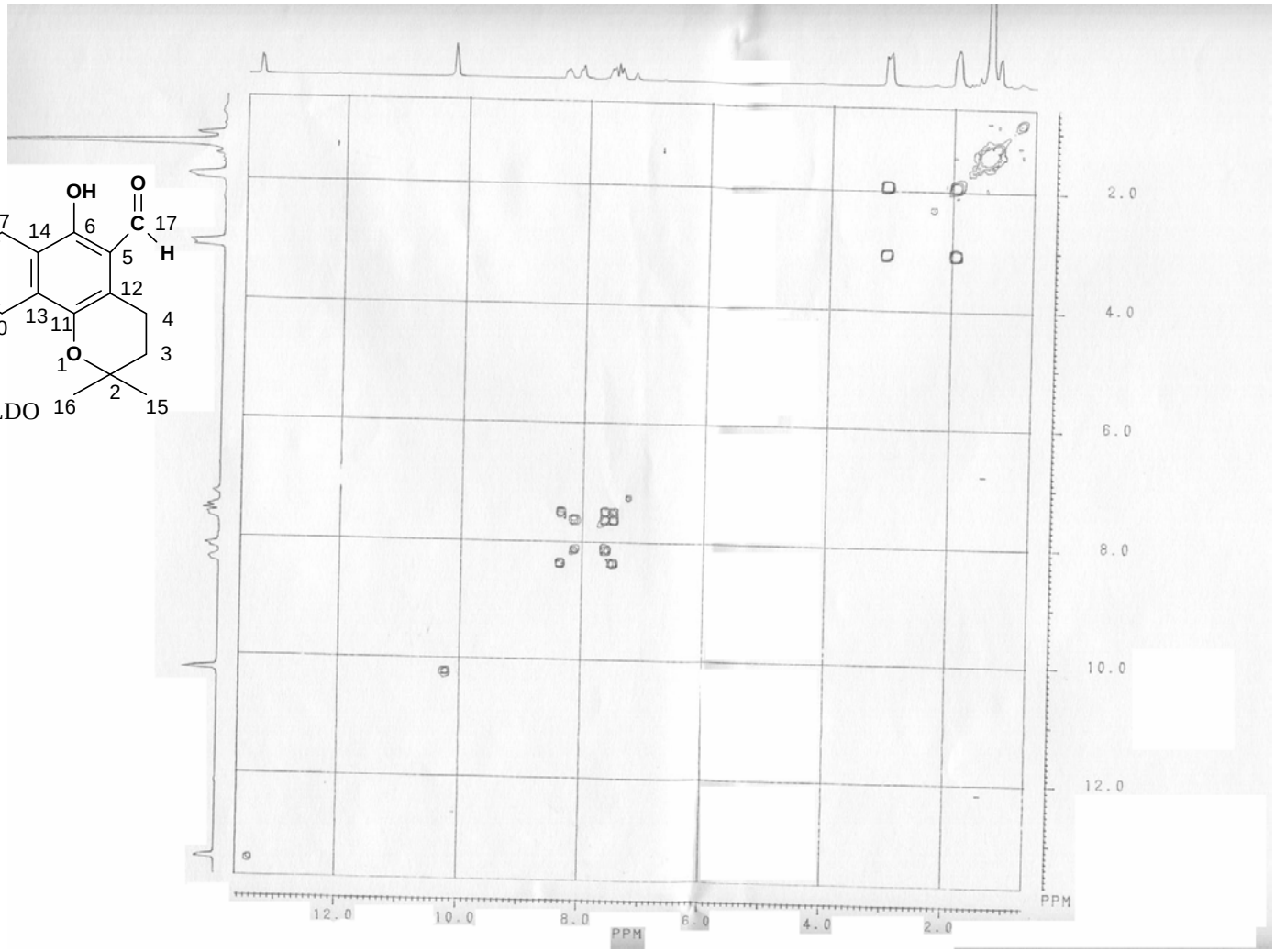
Espectro 84 – RMN ^{1}H (200 MHz) do BLDO (10-hidroxi-6,6-dimetil-5,6,7,8-tetraidrofenantreno-9-carbaldeído).



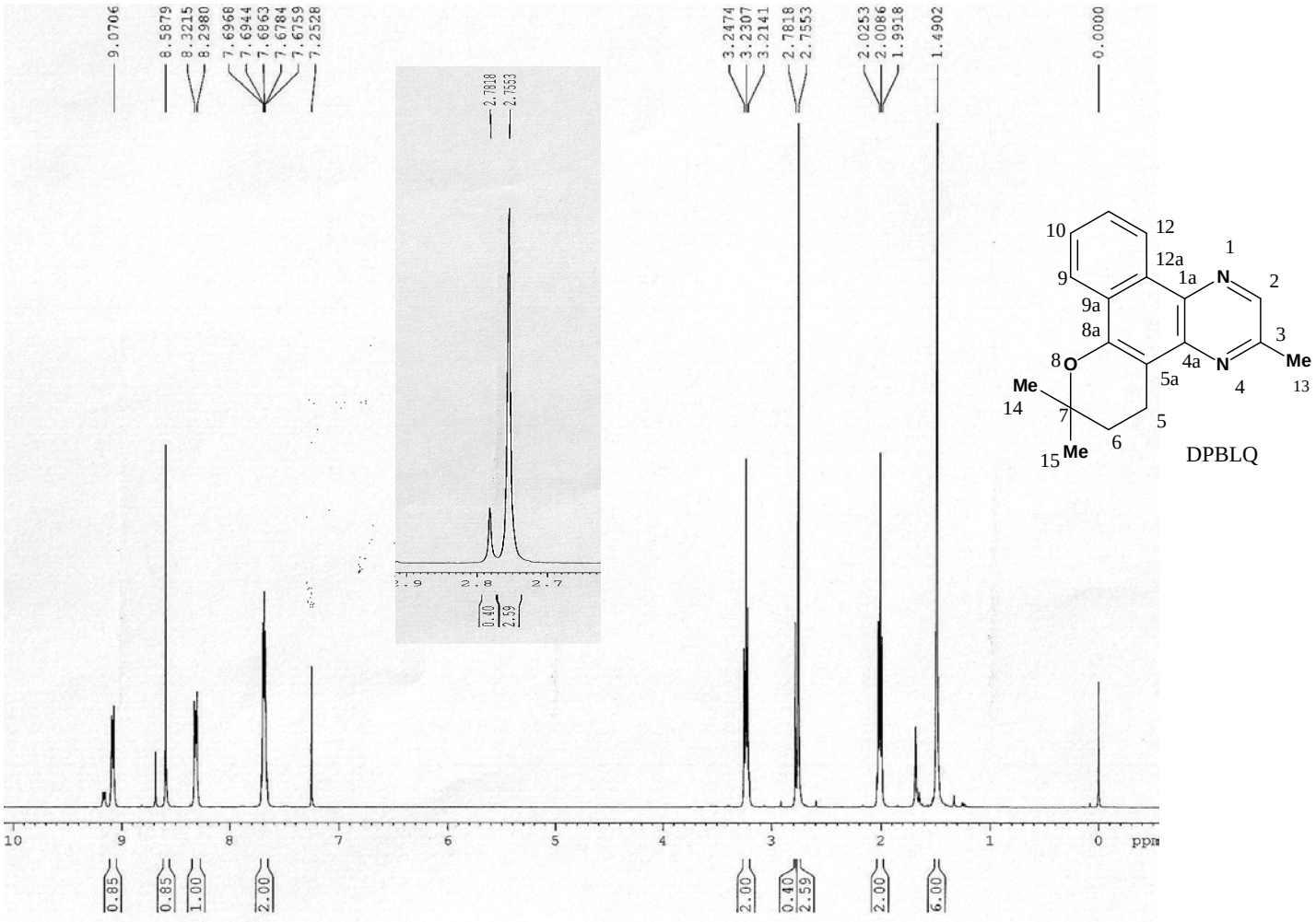
Espectro 85 – RMN ^{13}C (50,3 MHz) do BLDO (10-hidroxi-6,6-dimetil-5,6,7,8-tetraidrofenantreno-9-carbaldeído)**..**



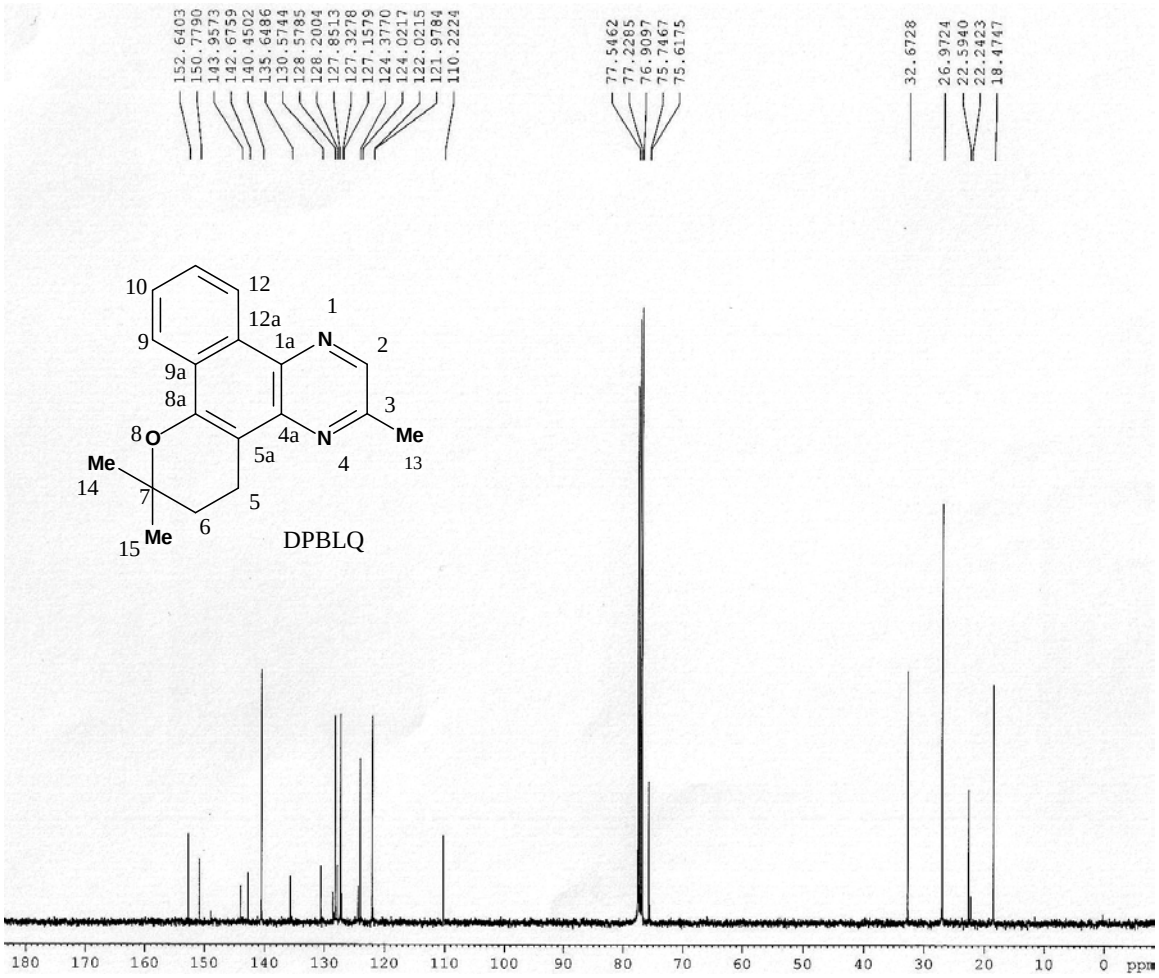
Espectro 86 - NOE do BLDO (10-hidroxi-6,6-dimetil-5,6,7,8-tetraidrofenantreno-9-carbaldeído)**.**



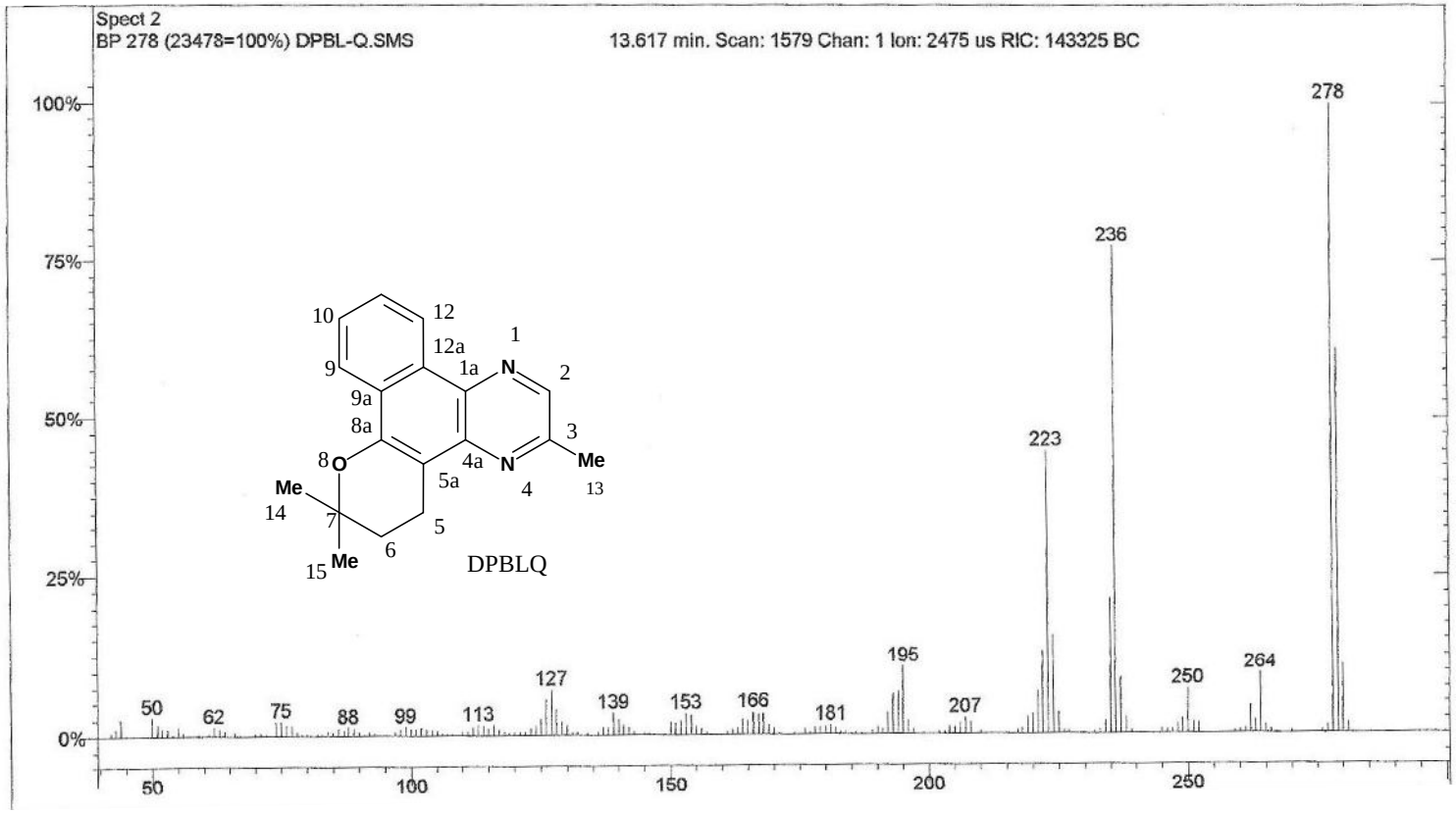
Espectro 87 – HOMOCOSY ^{1}H-^{1}H do BLDO (10-hidroxi-6,6-dimetil-5,6,7,8-tetraidrofenantreno-9-carbaldeído)**.**



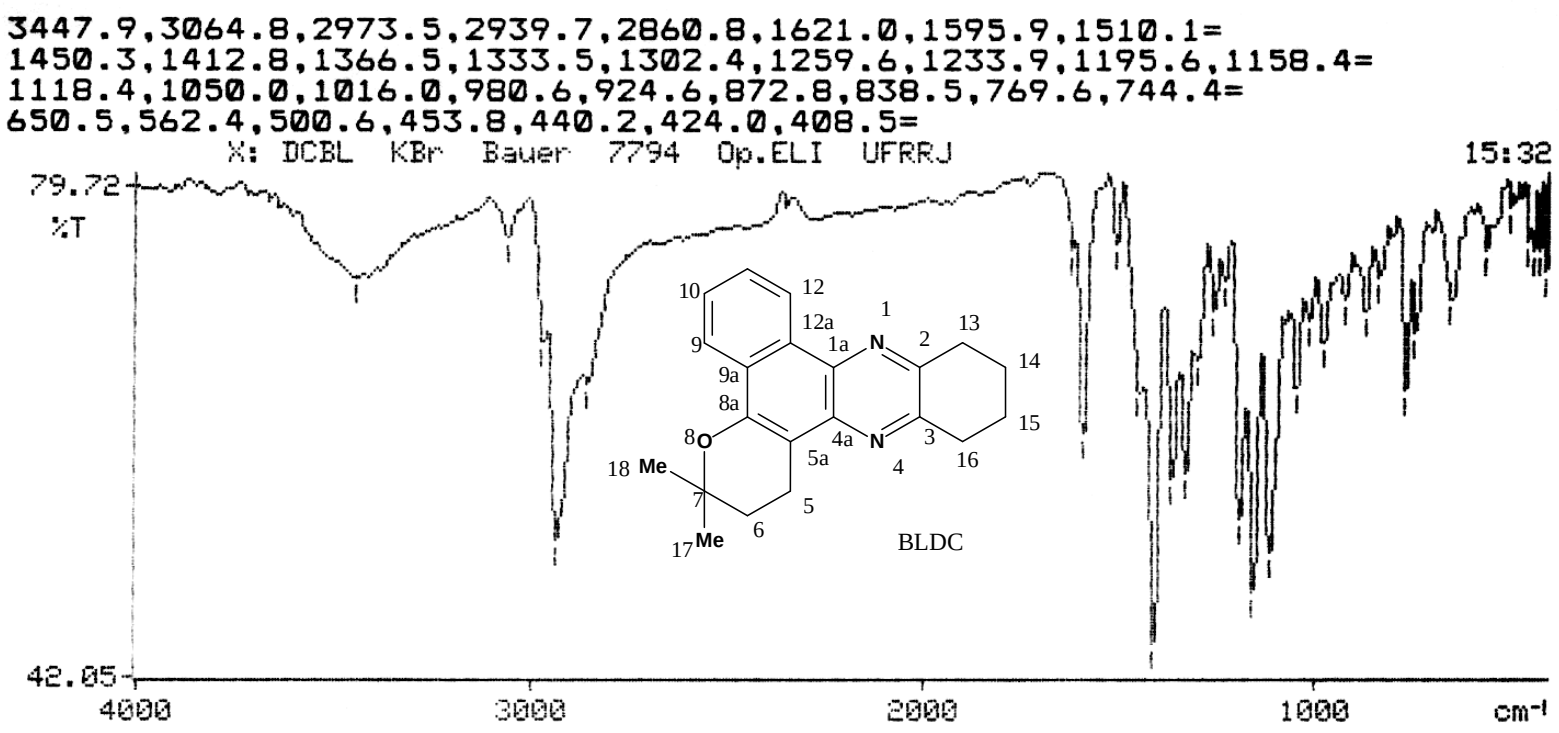
Espectro 88 – RMN ^{1}H do DPBLQ (400 MHz) (3,7,7-trimetil-6,7-di-hidro-5*H*-benzo[*f*]pirano[2,3-*h*]quinoxalina**).**



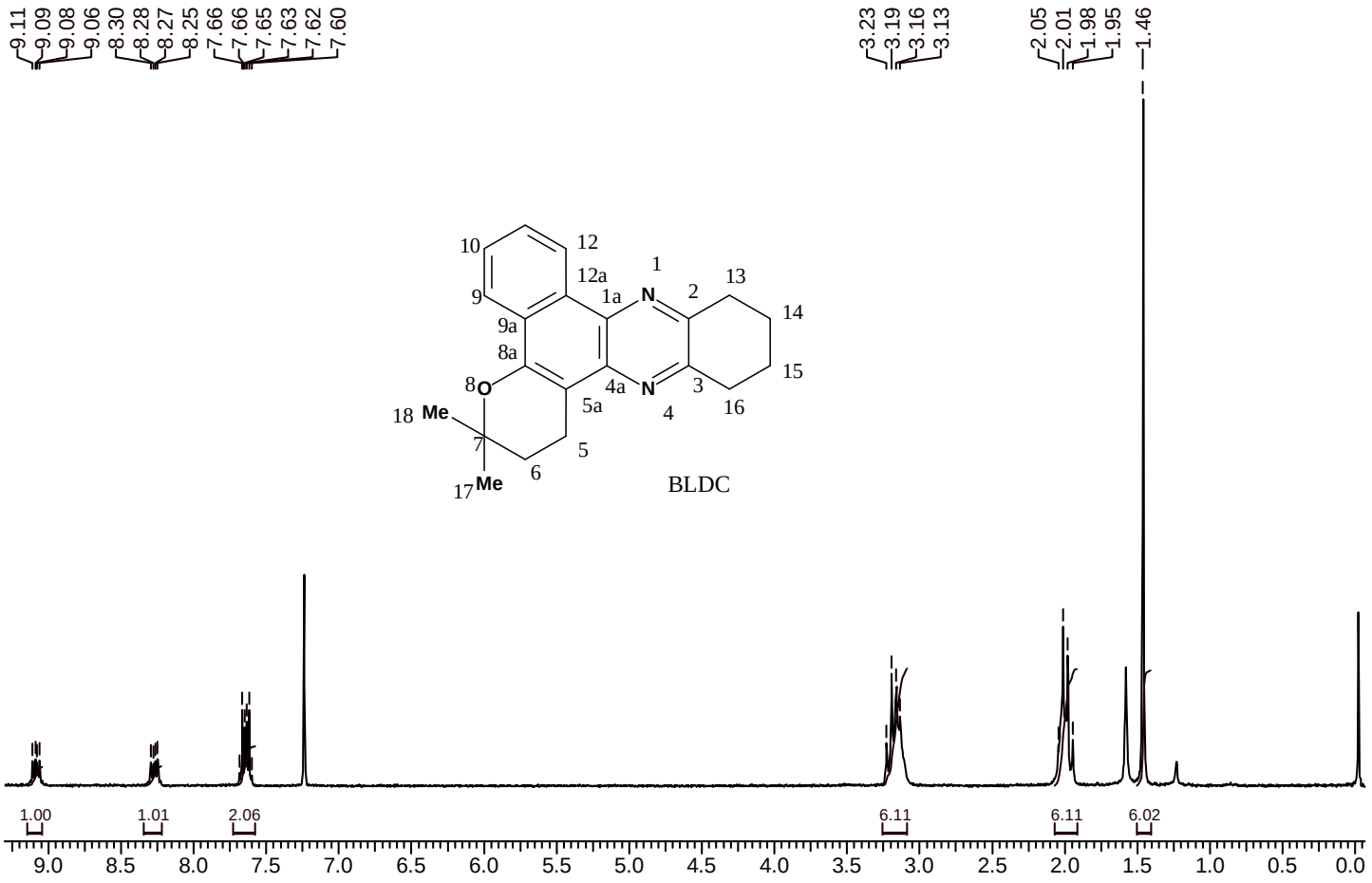
Espectro 89 – RMN ^{13}C do de DPBLQ (100,6 MHz) (3,7,7-trimetil-6,7-di-hidro-5*H*-benzo[*f*]pirano[2,3-*h*]quinoxalina**).**



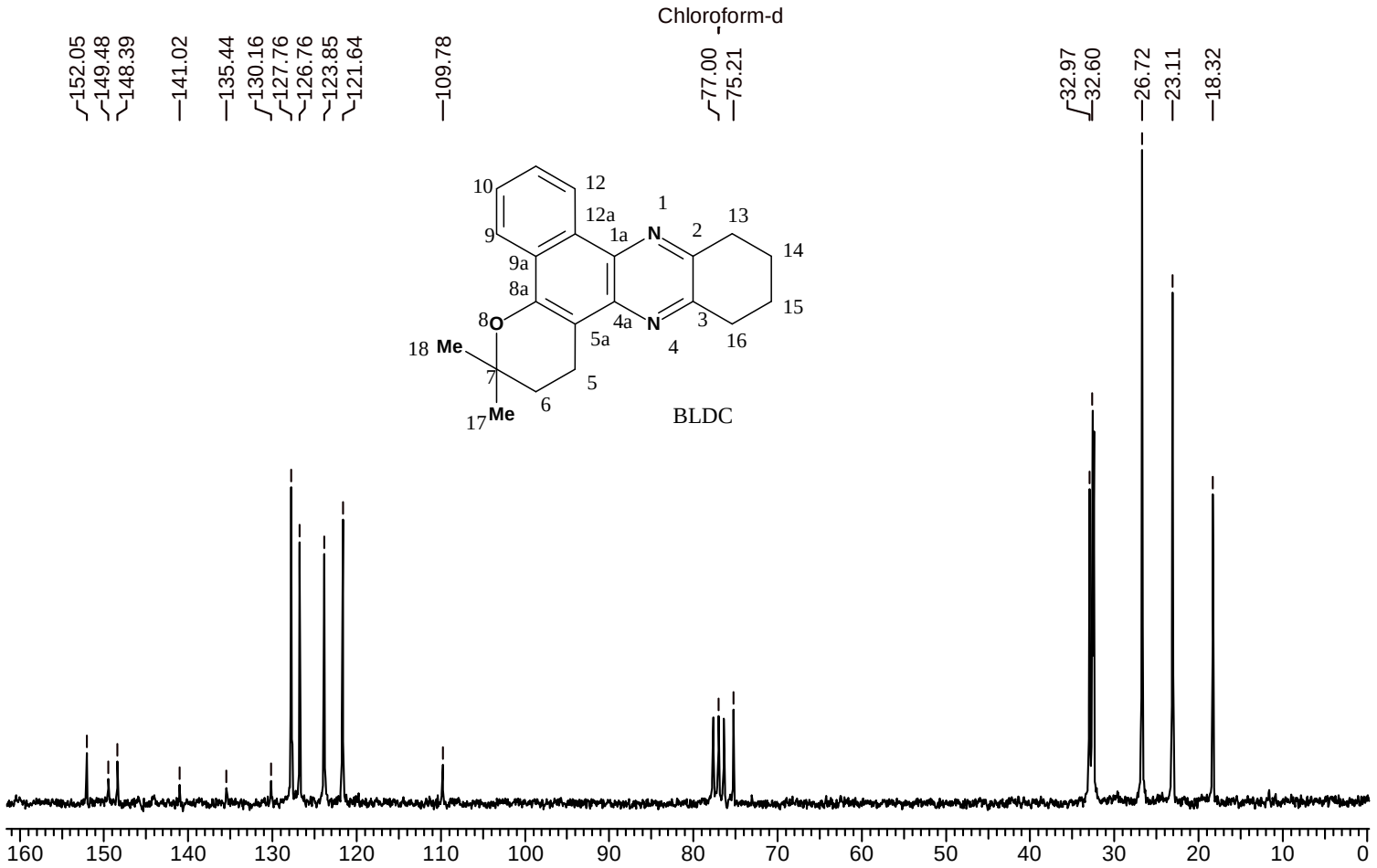
Espectro 90 – EM do DPBLQ (3,7,7-trimetil-6,7-di-hidro-5*H*-benzo[*f*]pirano[2,3-*h*]quinoxalina**).**



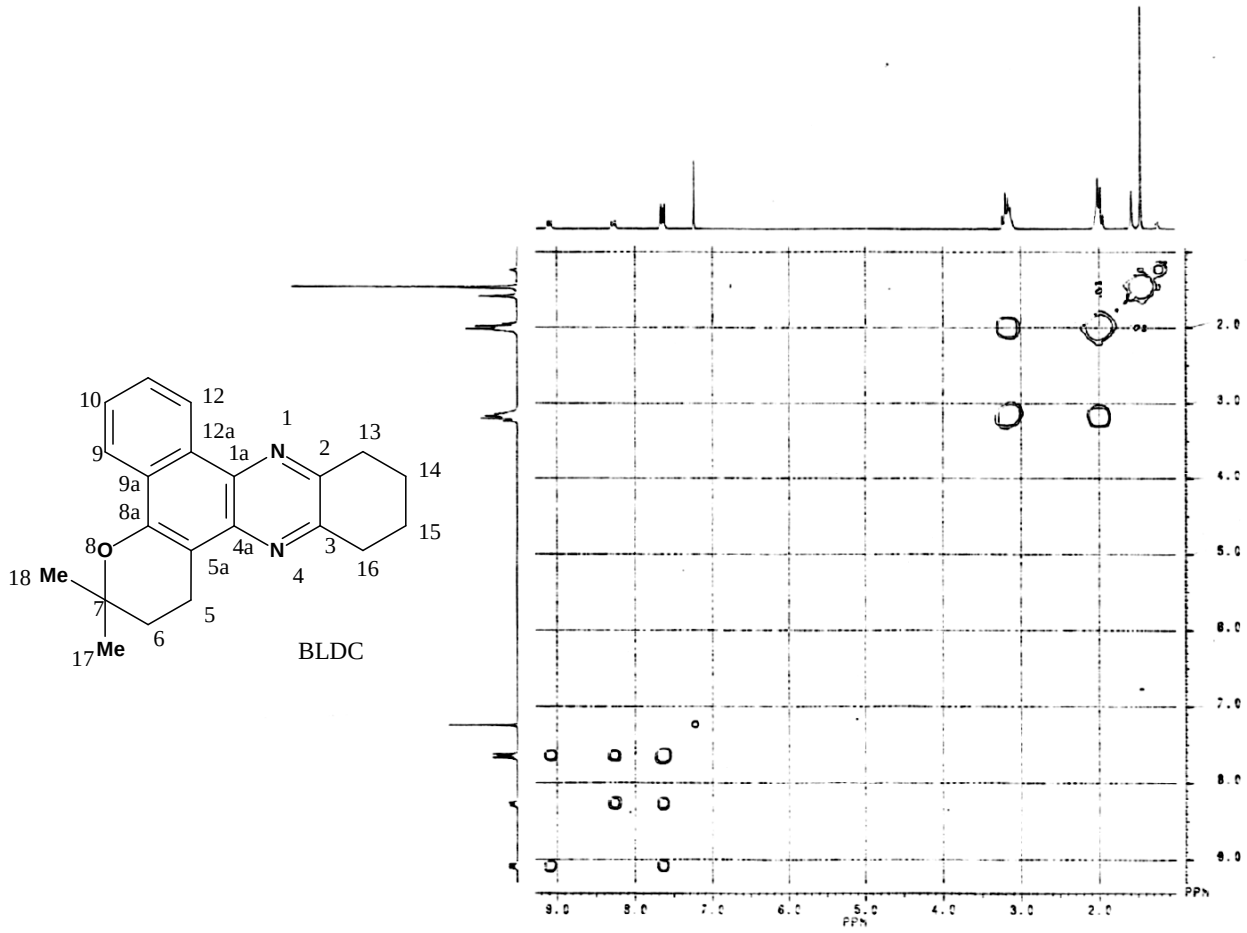
Espectro 91 - IV do BLDC (3,3-dimetil-2,3,10,11,12,13-hexaidro-1*H*-benzo[*a*]pirano[2,3-*c*]fenazina)**.**



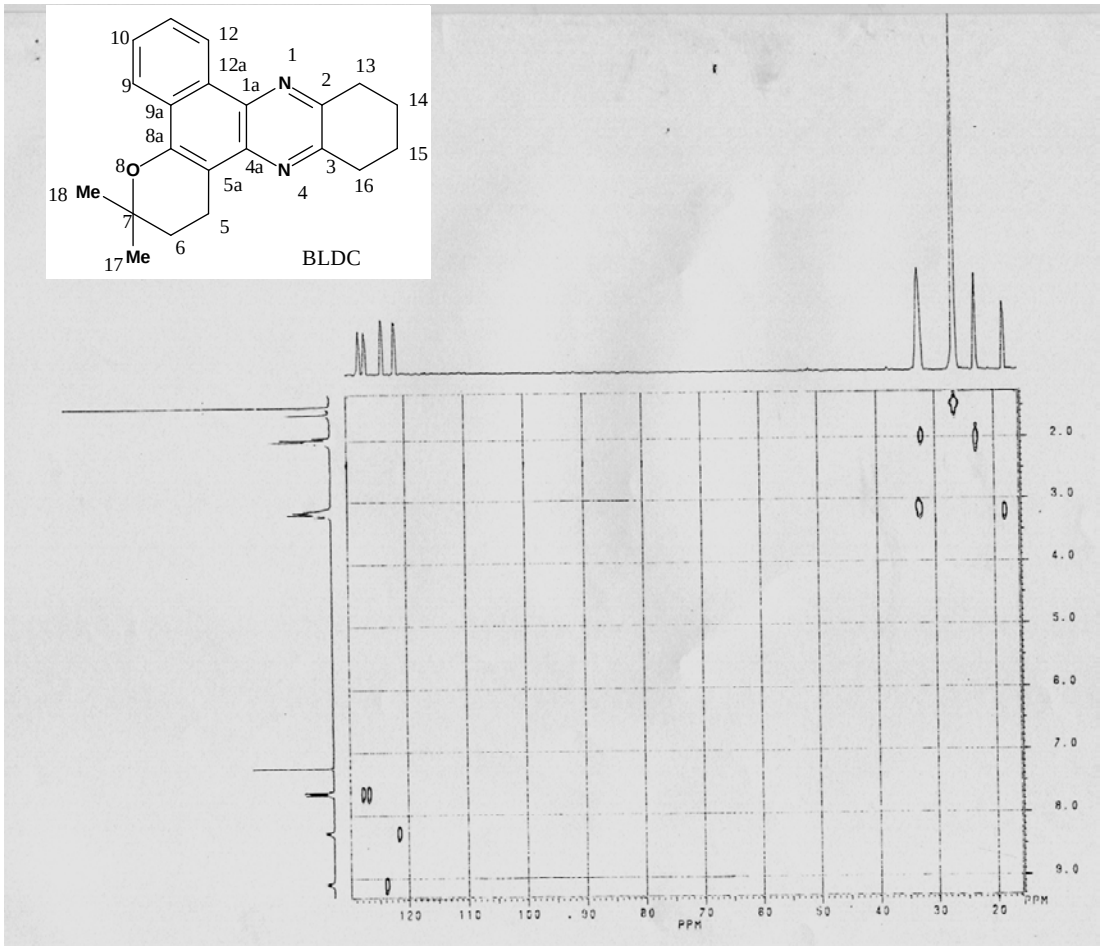
Espectro 92 – RMN ^{1}H (200 MHz) do BLDC (3,3-dimetil-2,3,10,11,12,13-hexaidro-1*H*-benzo[*a*]pirano[2,3-*c*]fenazina)**.**



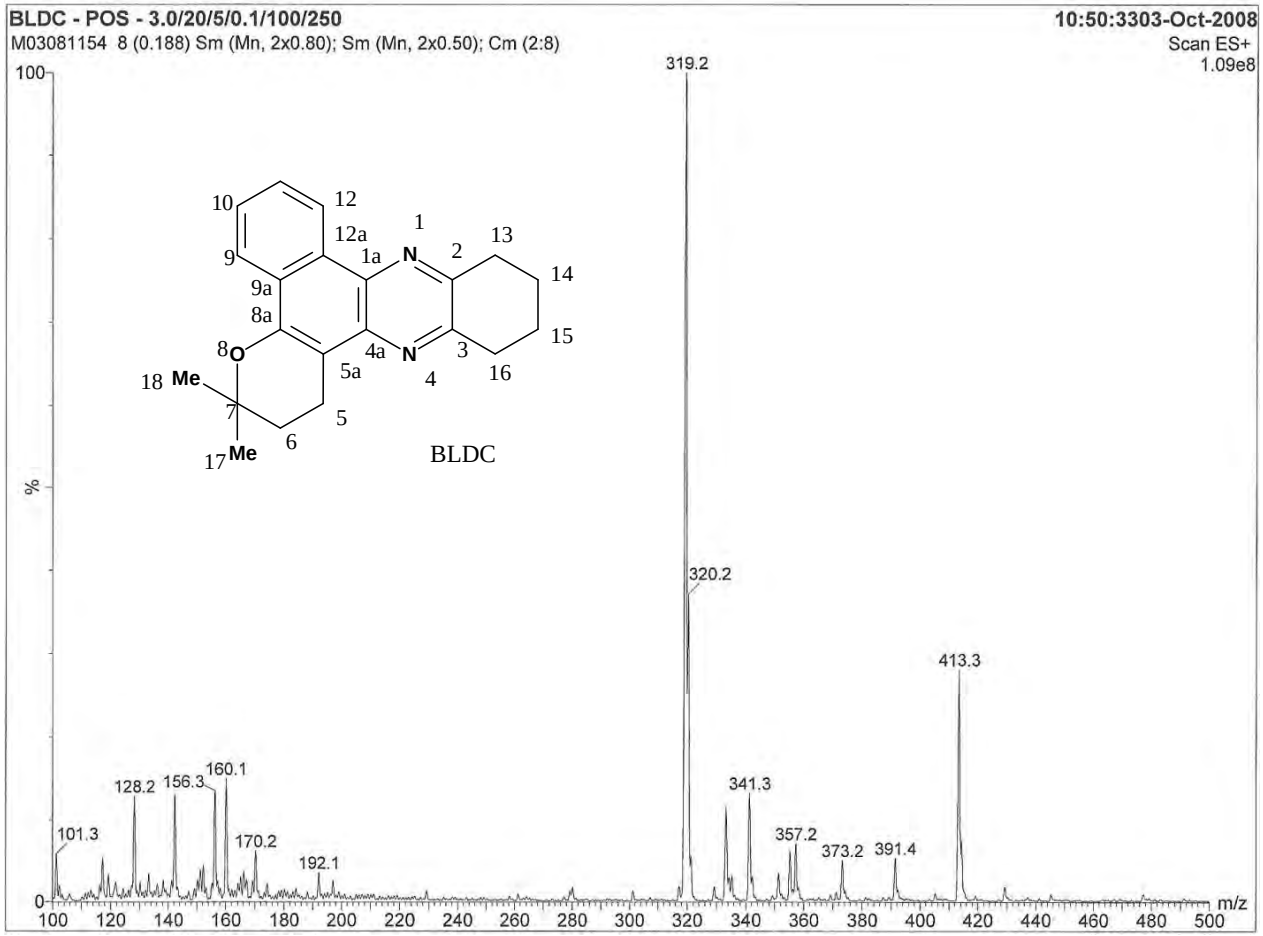
Espectro 93 – RMN ^{13}C (50,3 MHz) do BLDC (3,3-dimetil-2,3,10,11,12,13-hexaidro-1*H*-benzo[*a*]pirano[2,3-*c*]fenazina)**.**



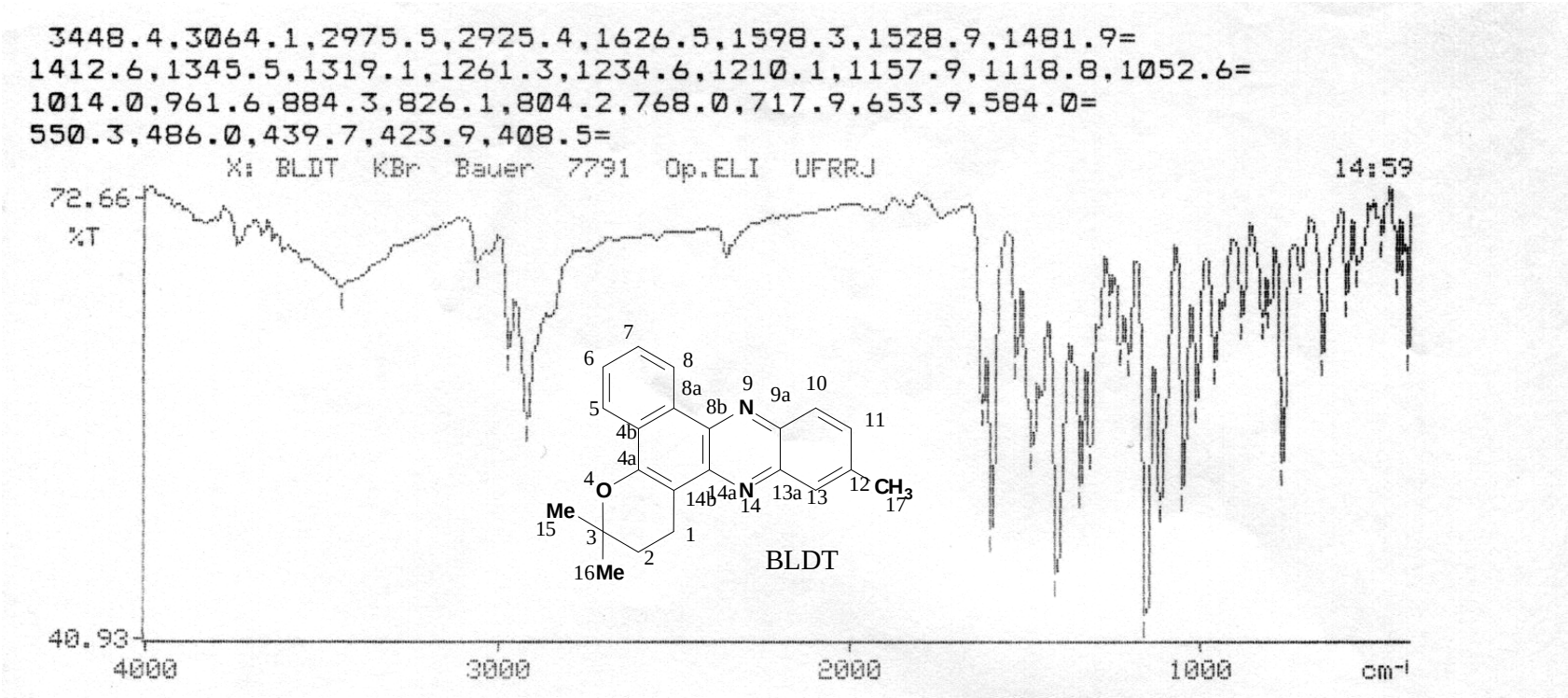
Espectro 94 – HOMOCOSY do BLDC.



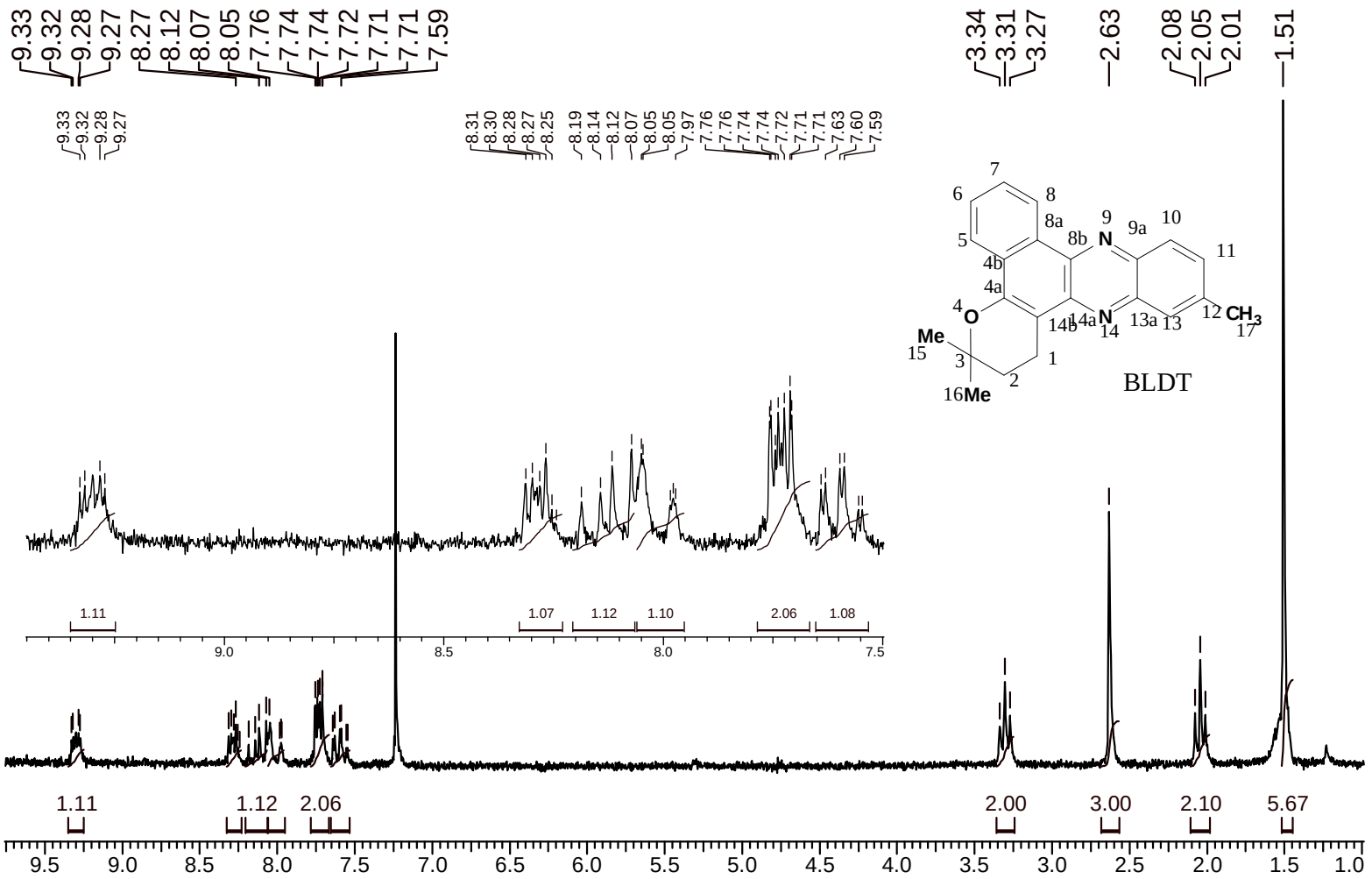
Espectro 95 – HETCOSY ^{13}C-^{1}H (^{1}J) de BLDC (3,3-dimetil-2,3,10,11,12,13-hexaidro-1*H*-benzo[*a*]pirano[2,3-*c*]fenazina)**.**



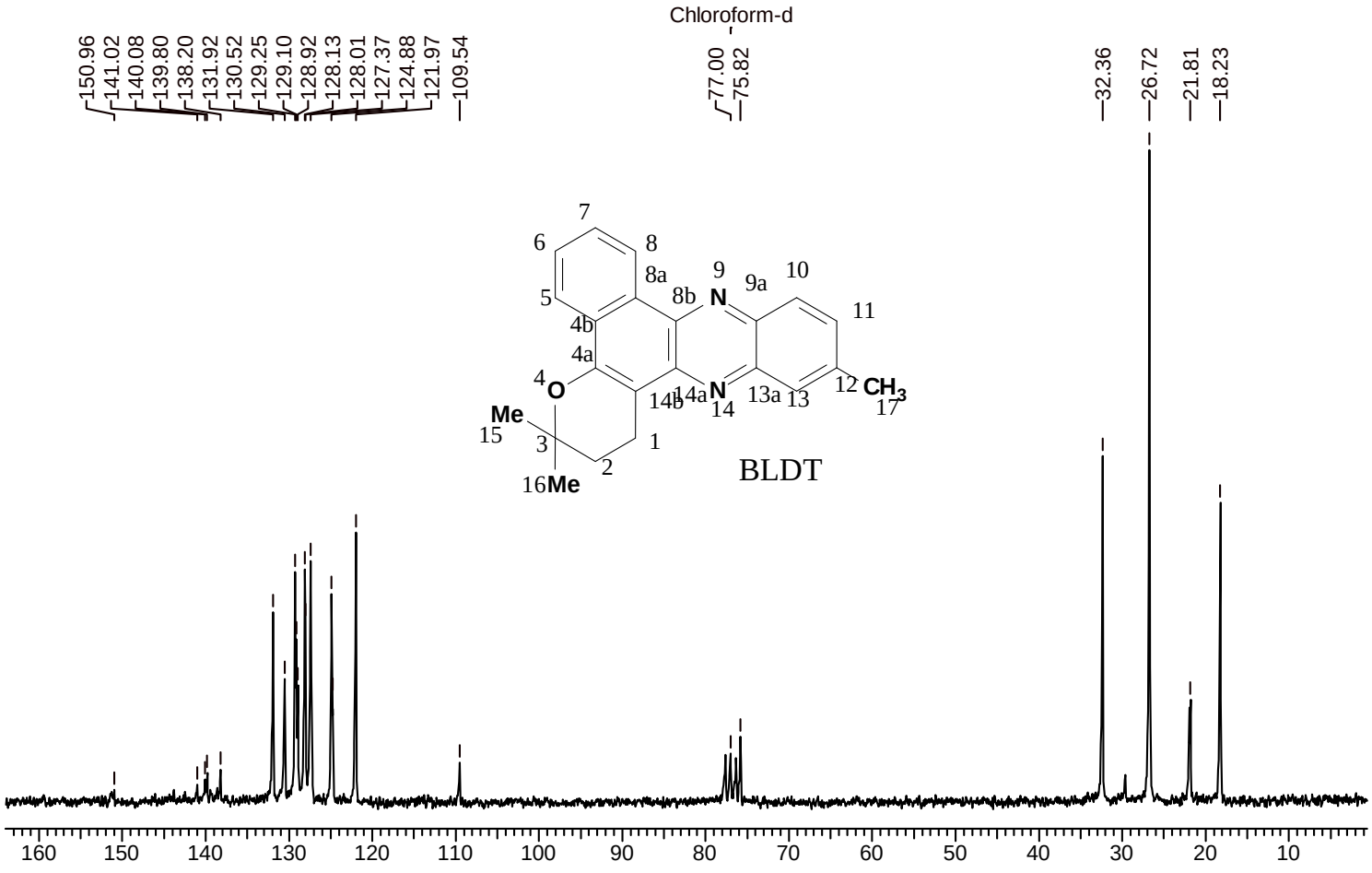
Espectro 96 – EM por nebulização de elétrons (ES) do BLDC , onde temos $[M+1]^+$ = 319,2 e $[M+23]^+$ = 341,3 sendo (M = 318 g mol^{-1})**.**



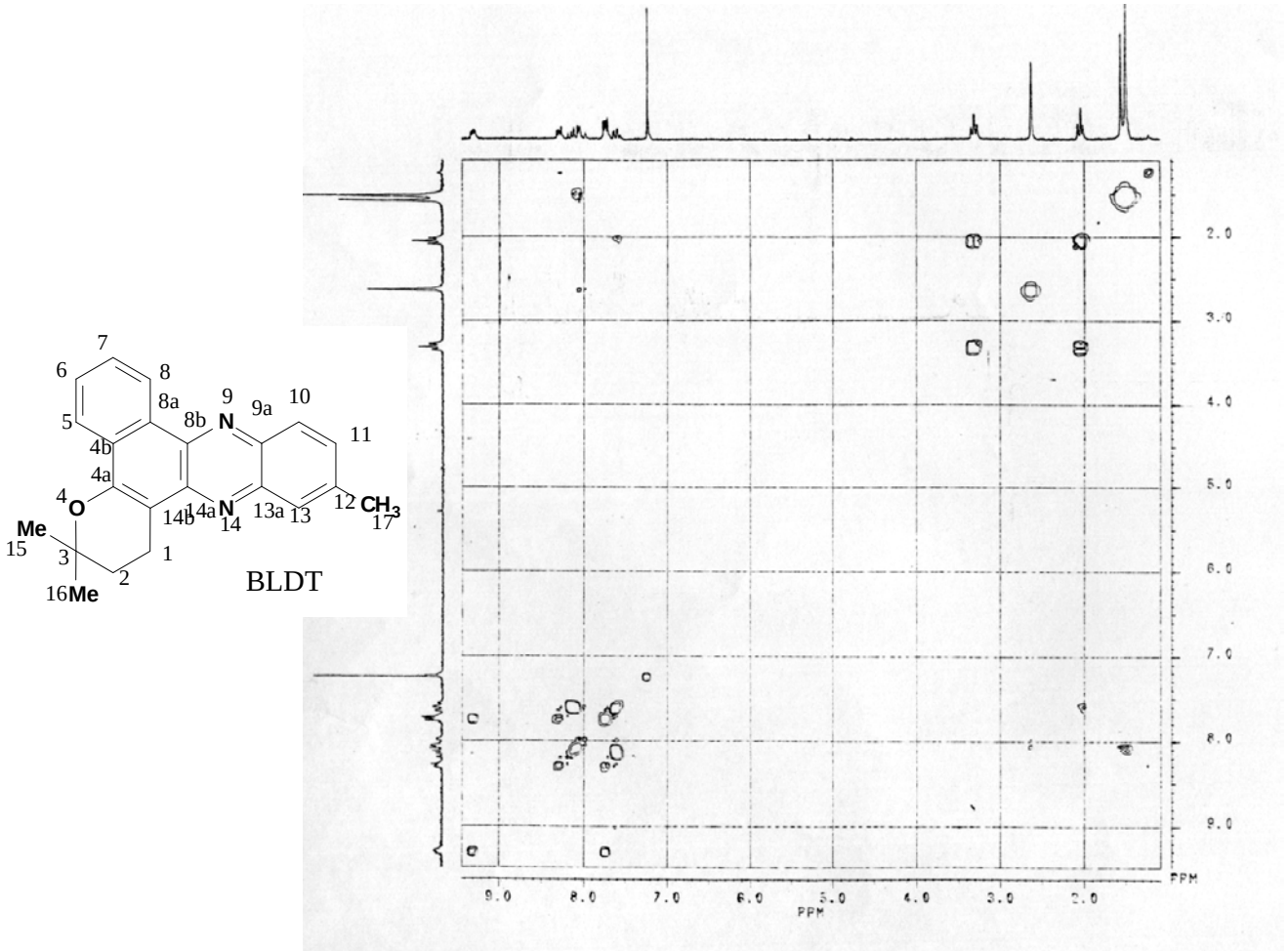
Espectro 97 – IV do BLDT (3,3,12-trimetil-2,3-di-hidro-1*H*-benzo[*a*] pirano[2,3-*c*]fenazina)**.**



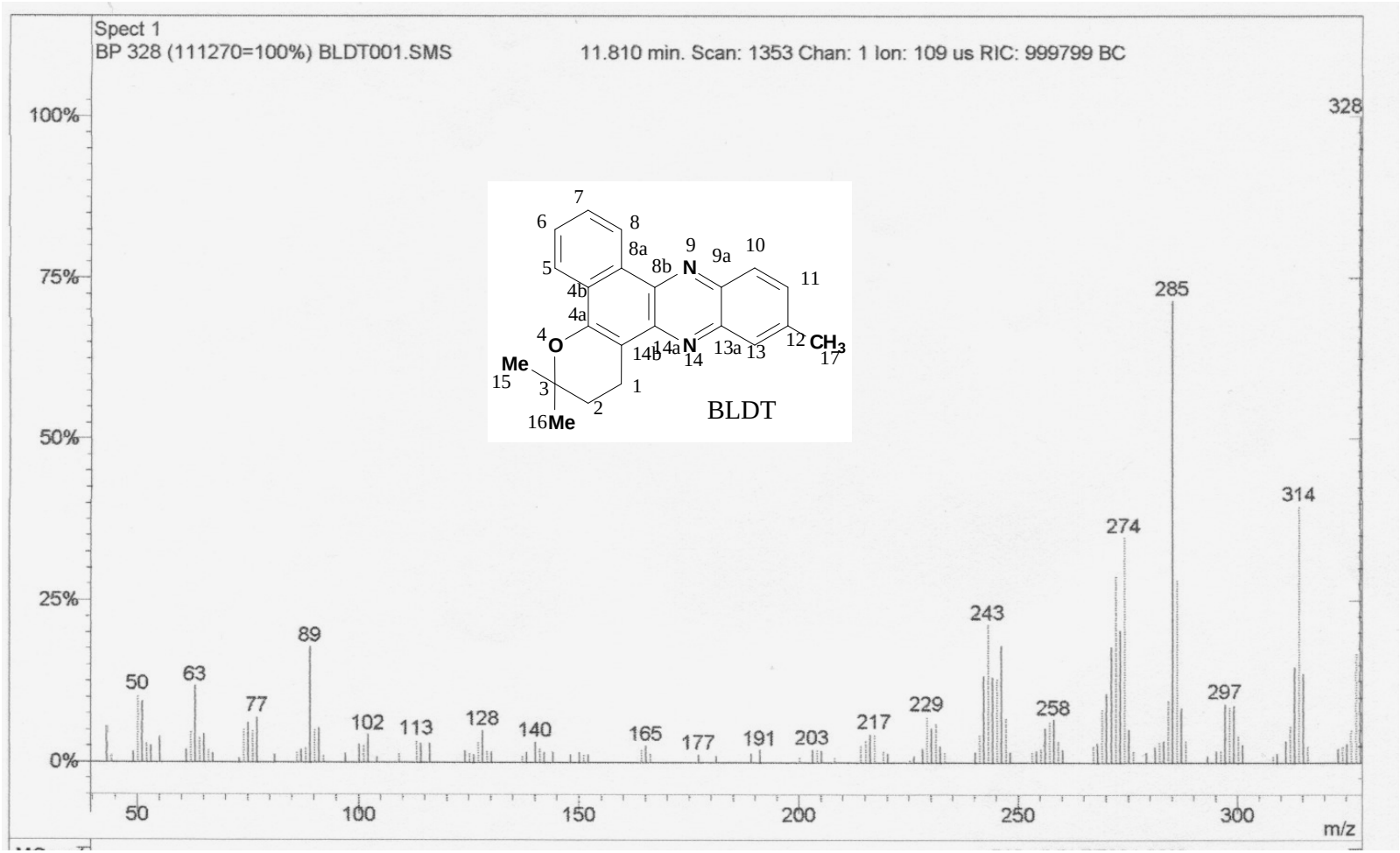
Espectro 98 – RMN ^{1}H (200 MHz), com ampliação da região aromática, do BLDT(3,3,12-trimetil-2,3-di-hidro-1*H*-benzo[*a*] pirano[2,3-*c*]fenazina)**.**



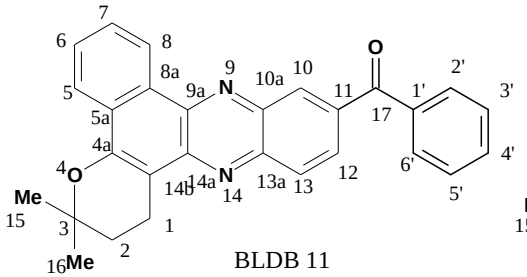
Espectro 99 – RMN ^{13}C (50,3 MHz) do BLDT (3,3,12-trimetil-2,3-di-hidro-1*H*-benzo[*a*] pirano[2,3-*c*]fenazina)**.**



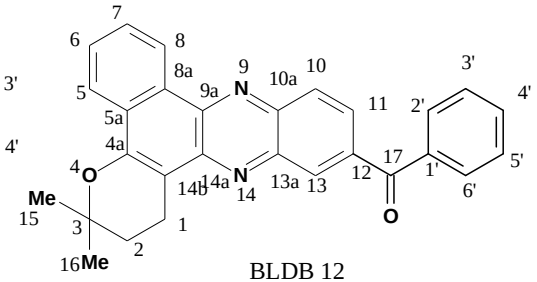
Espectro 100 – COSY ^{1}H-^{1}H do BLDT (3,3,12-trimetil-2,3-di-hidro-1*H*-benzo[*a*] pirano[2,3-*c*]fenazina)**.**



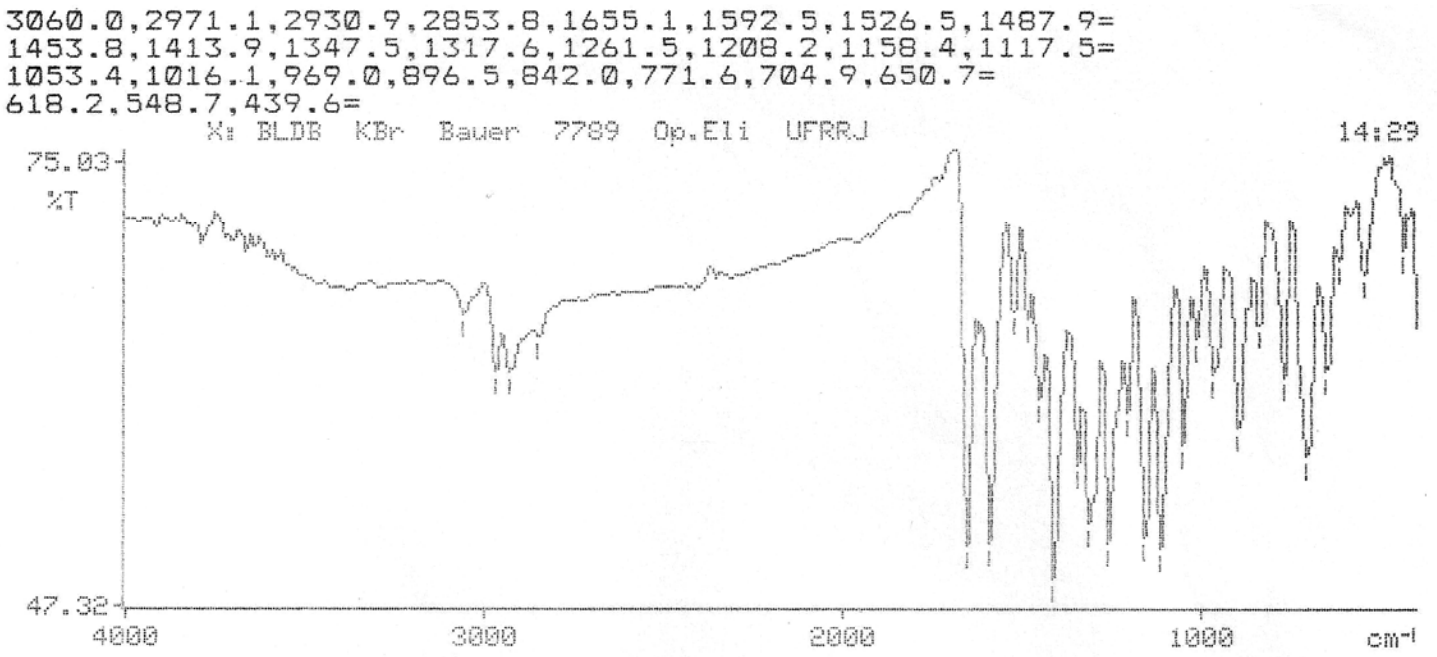
Espectro 101 –E.M. do BLDT (3,3,12-trimetil-2,3-di-hidro-1*H*-benzo[*a*] pirano[2,3-*c*]fenazina)**.**



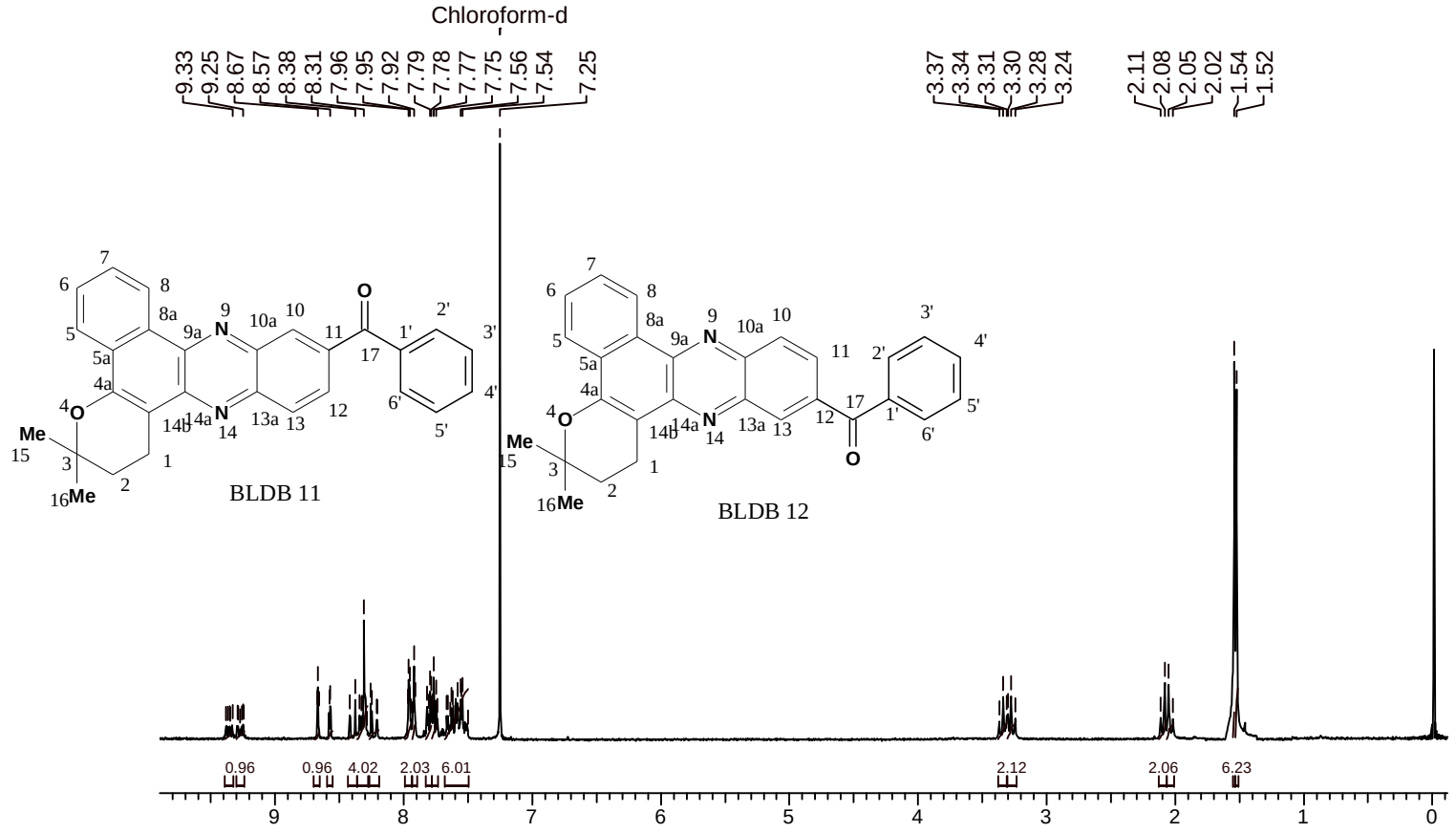
BLDB 11



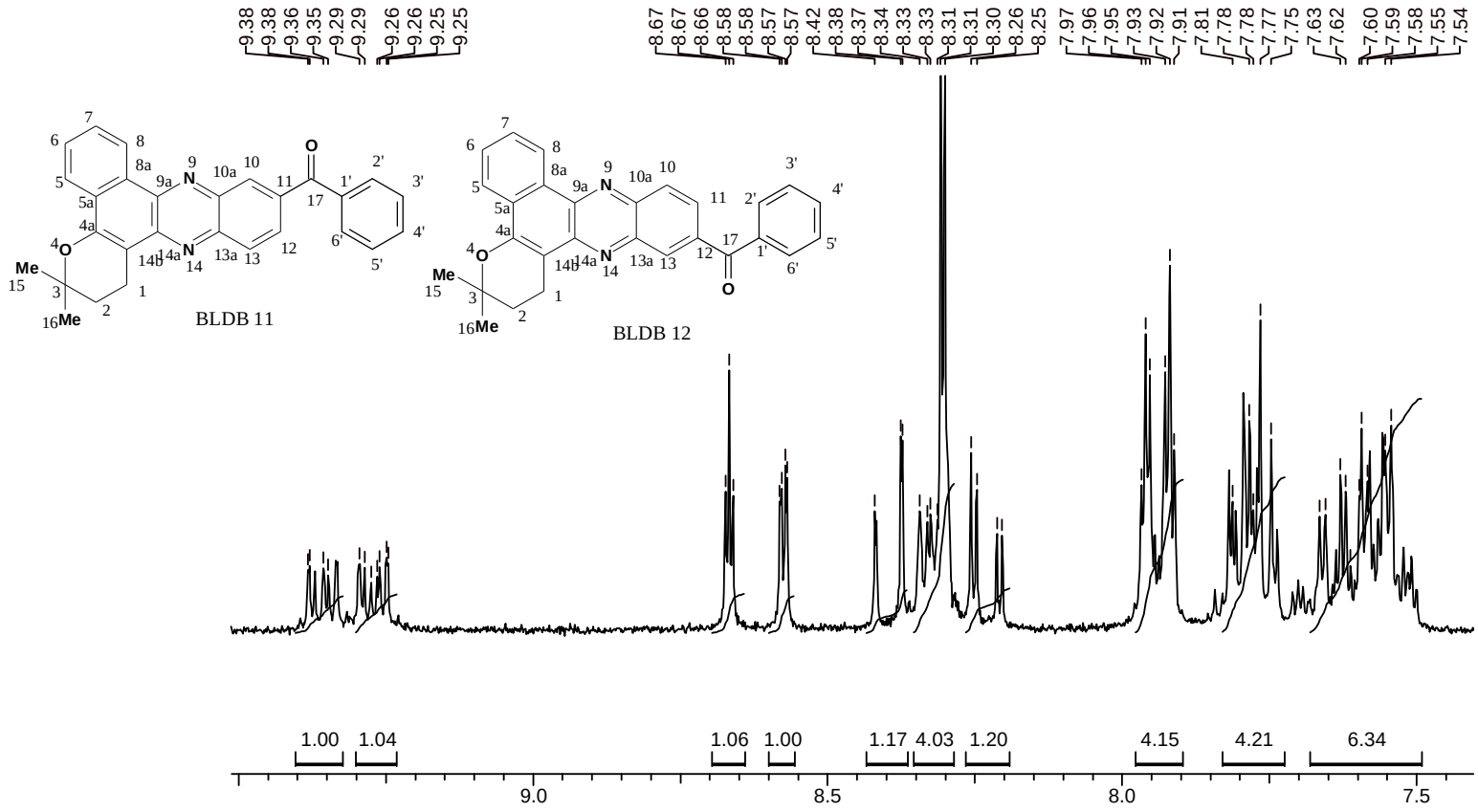
BLDB 12



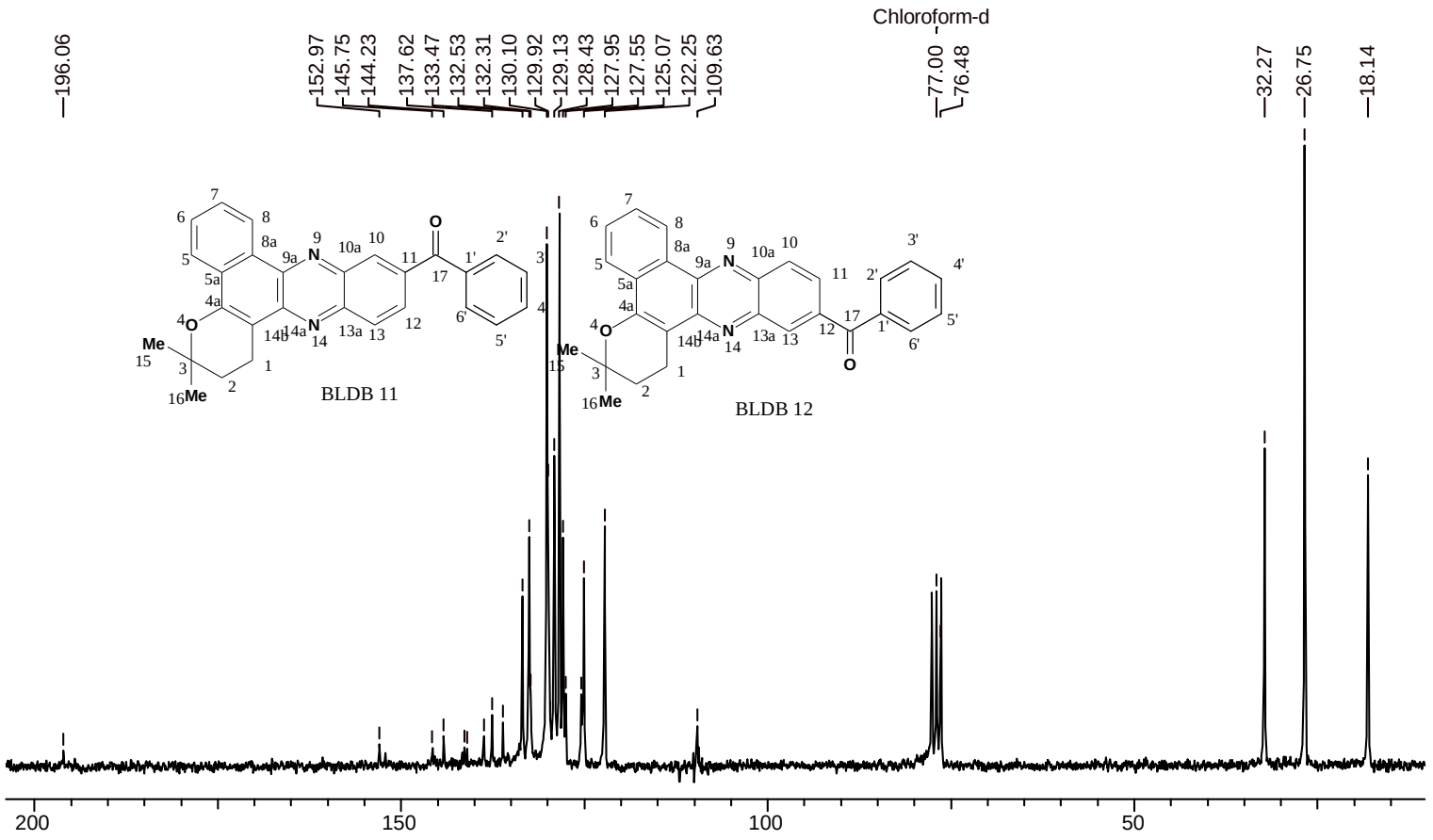
Espectro 102 – IV, em cm^{-1}, da mistura de isômeros do BLDB **.**



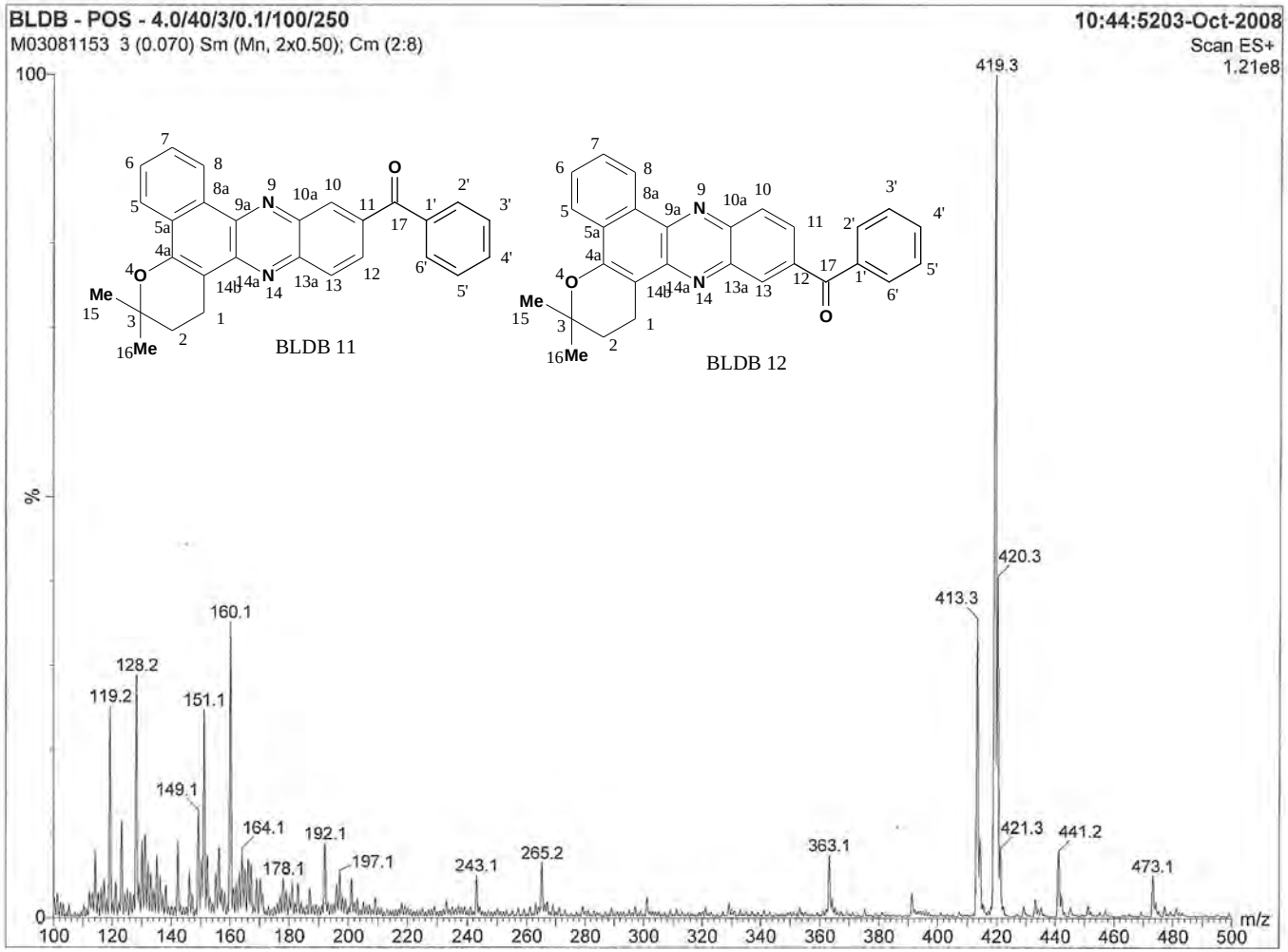
Espectro 103 – RMN ^{1}H (200 MHz) da mistura de isômeros do BLDB**.**



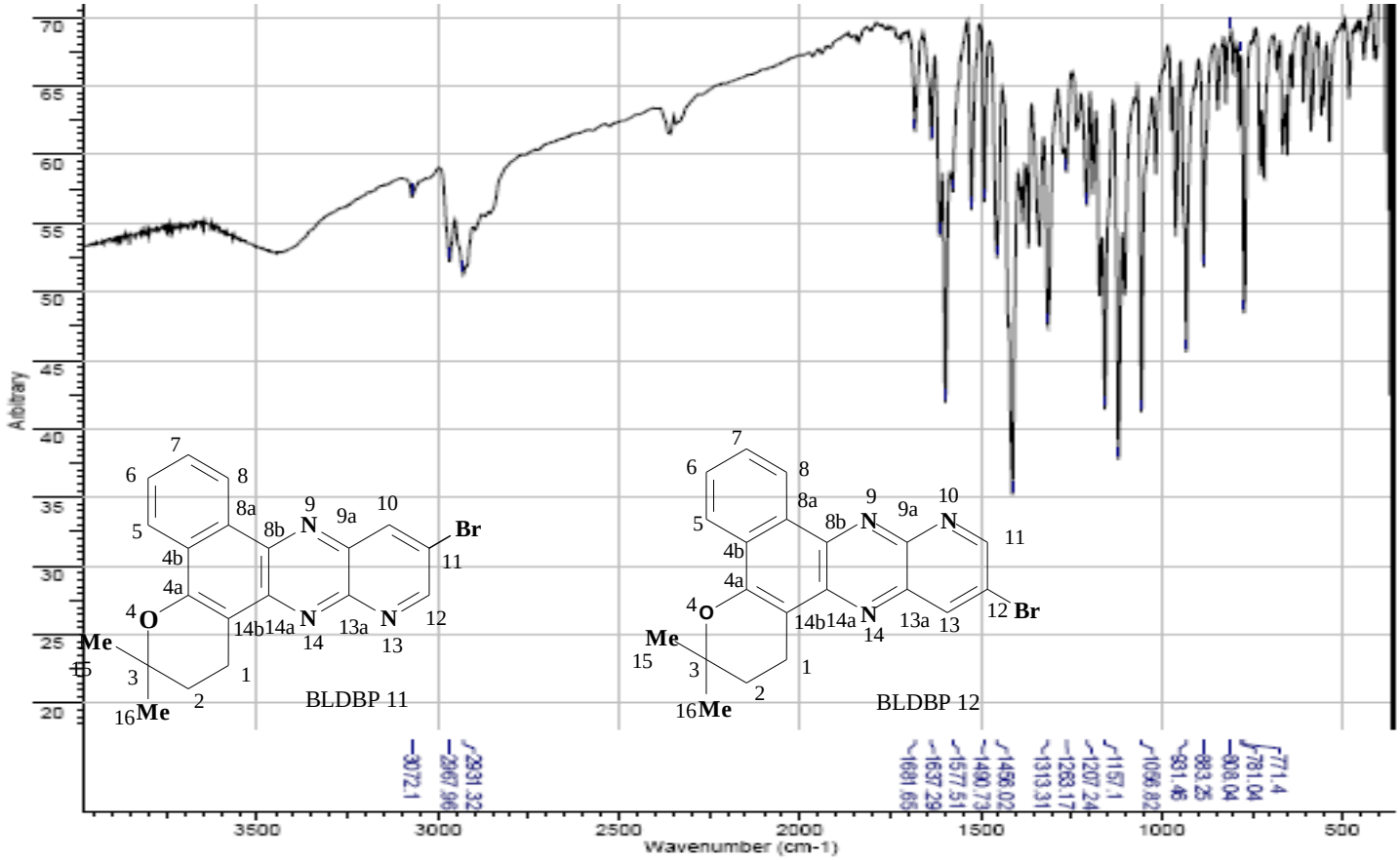
Espectro 104 – Ampliação da região aromática do espectro de RMN ^{1}H da mistura de isômeros do BLDB**.**



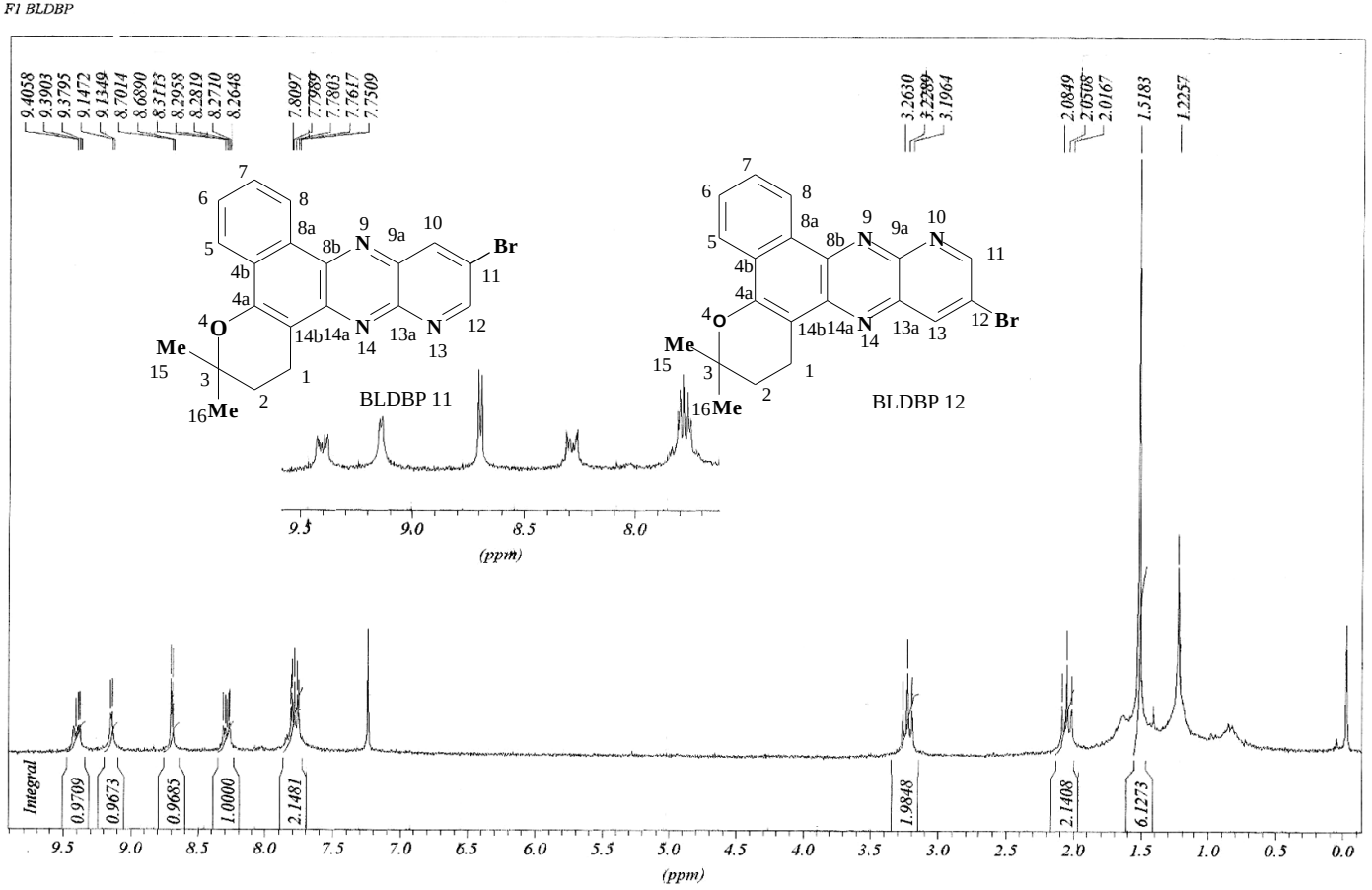
Espectro 105 – RMN ^{13}C (50,3 MHz) do BLDB da mistura de isômeros do BLDB**.**



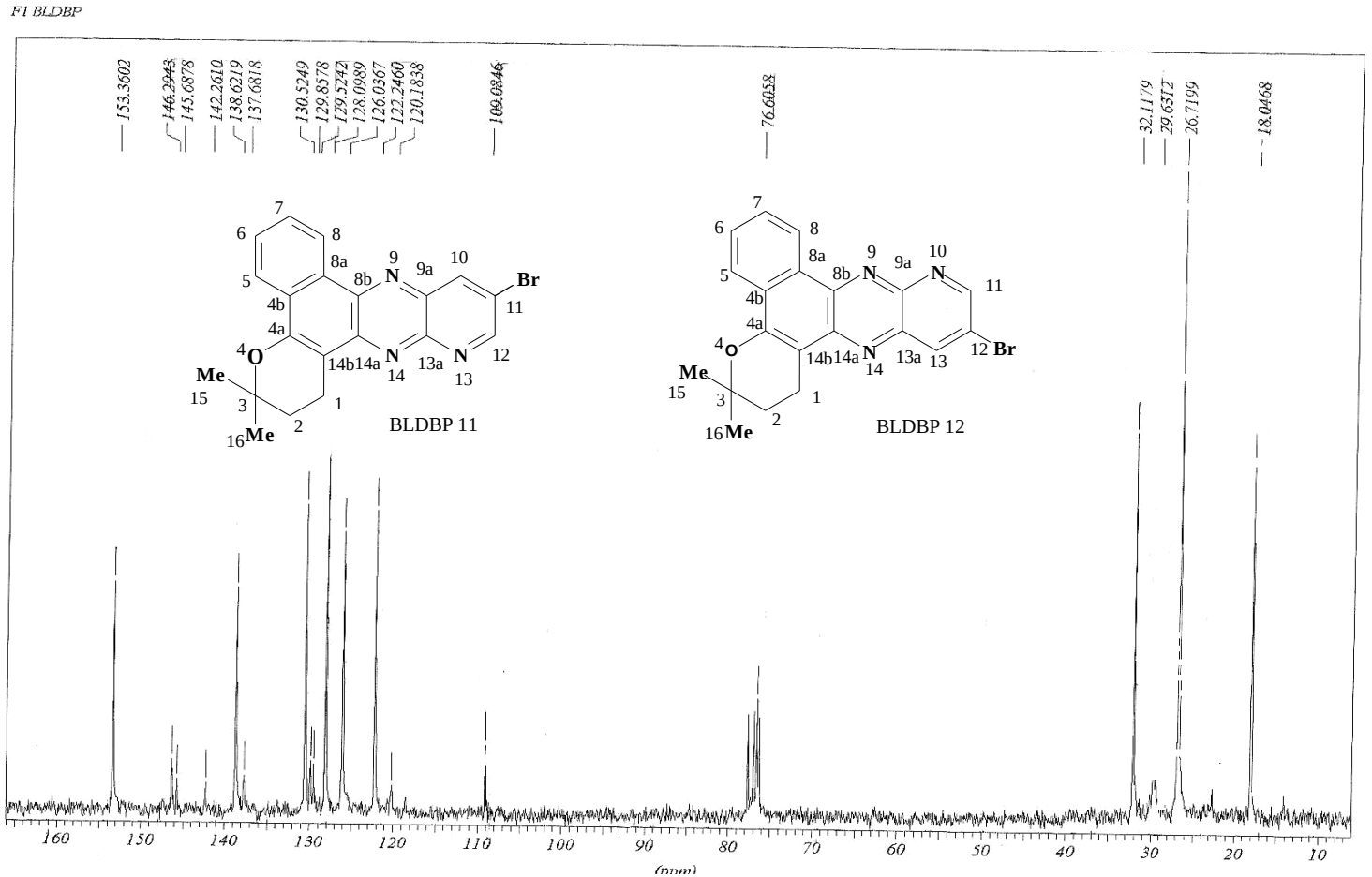
Espectro 106 – E.M. por nebulização de elétrons (ES) de BLDB, sendo MM =418 g mol^{-1}, onde [M+1] = 419,3 e [M+23] = 441,2**.**



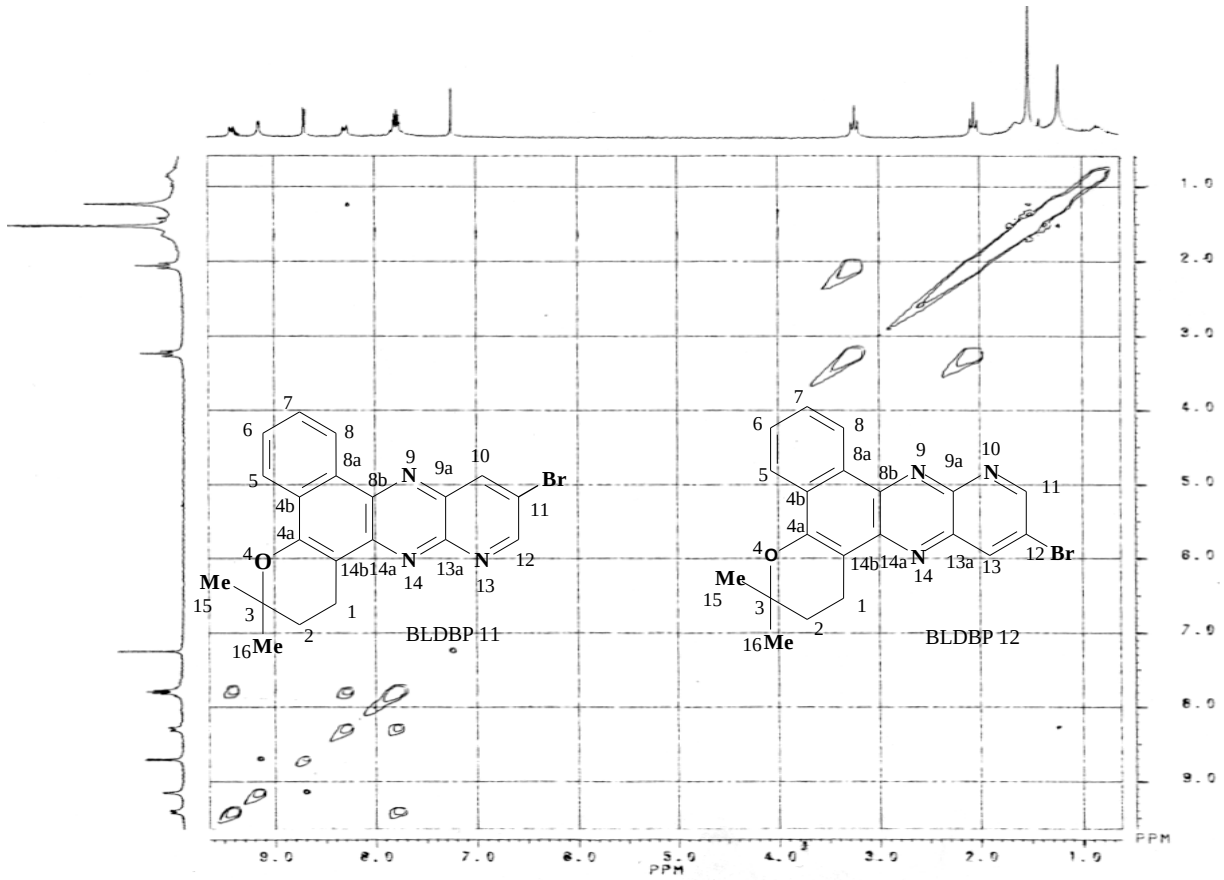
Espectro 107 – IV da primeira fração de BLDBP, composto mais apolar.



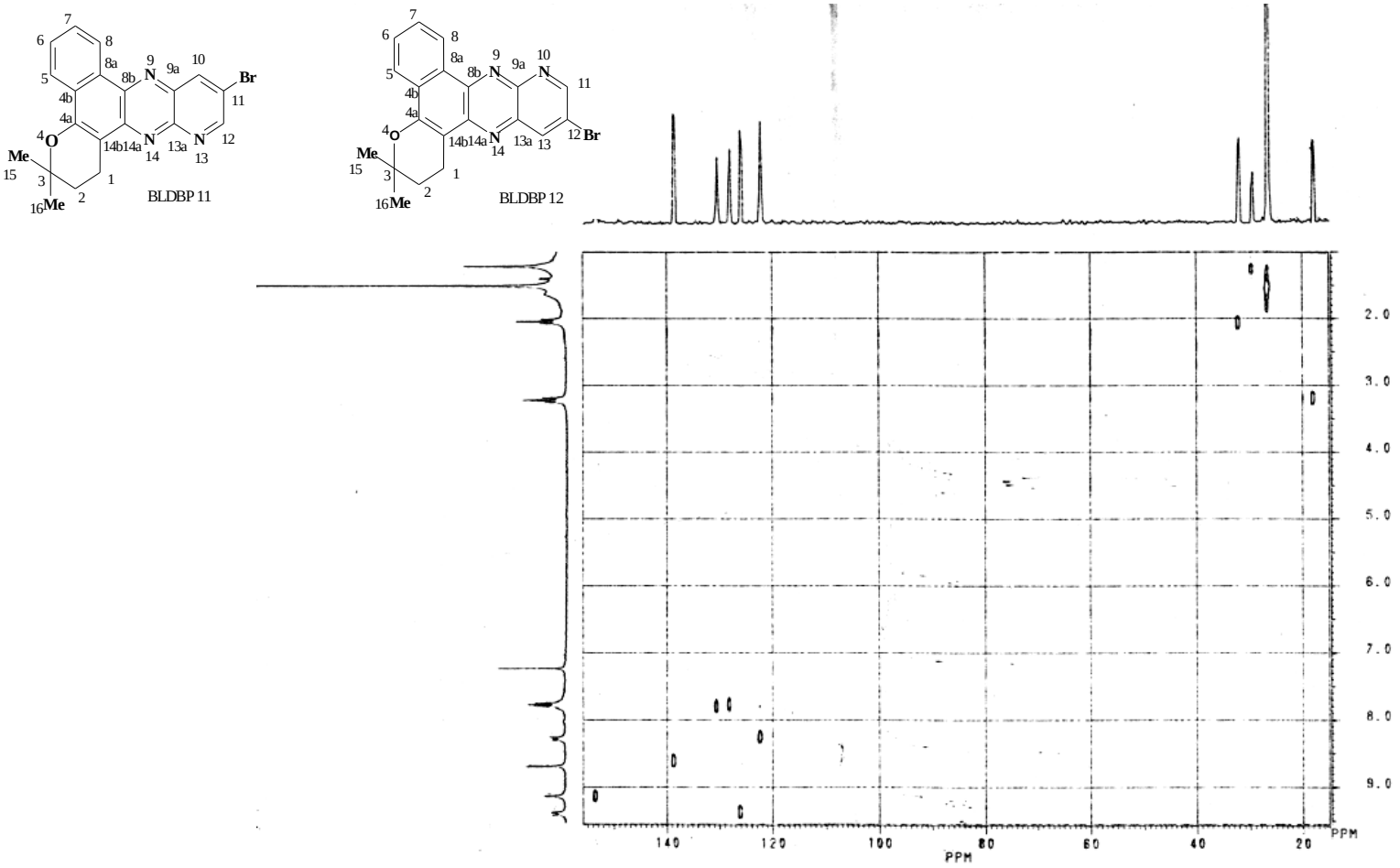
Espectro 108 - RMN ^{1}H (200 MHz) da primeira fração de BLDBP, composto mais apolar.



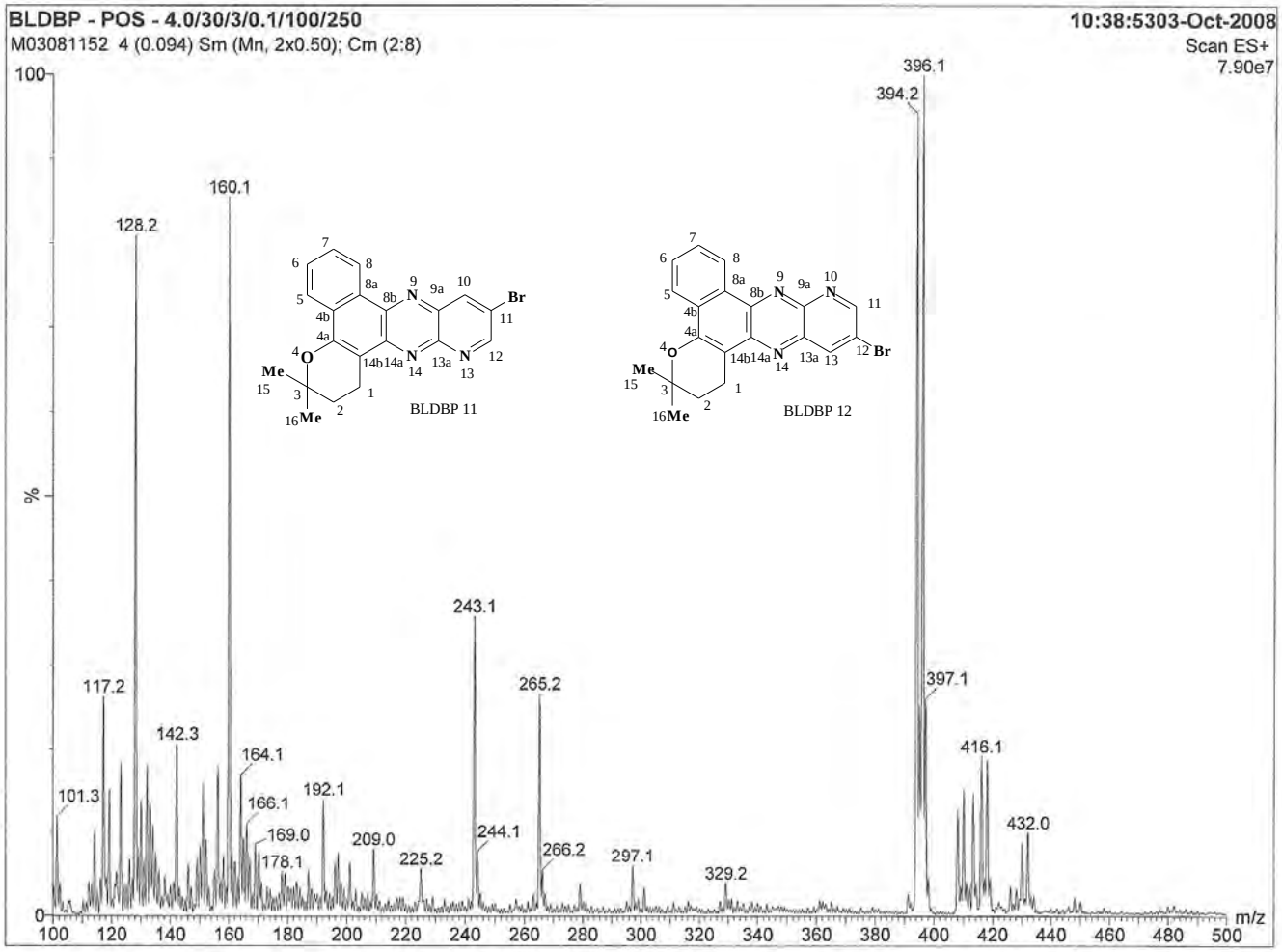
Espectro 109 - RMN ^{13}C (50,3 MHz) da primeira fração de BLDBP, composto mais apolar.



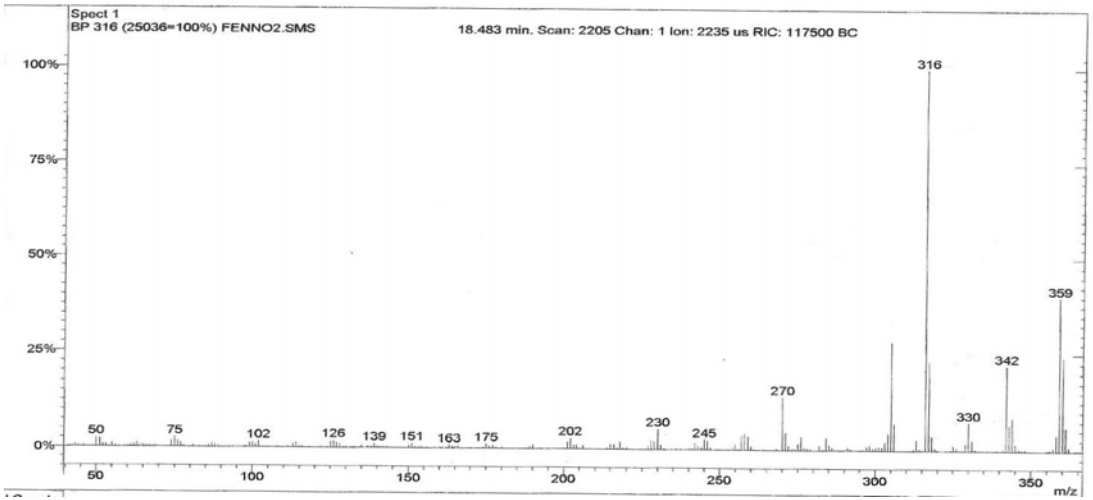
Espectro 110 - HOMOCOSY ^{1}H-^{1}H da primeira fração de BLDBP, composto mais apolar**.**

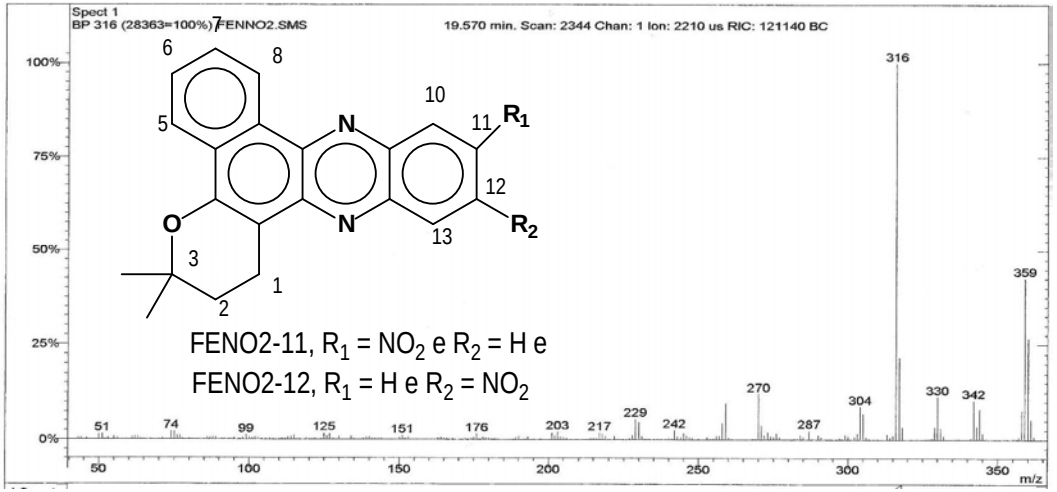


Espectro 111 - HETCOR ^{13}C-^{1}H (^{1}J) da primera fração de BLDBP, composto mais apolar**.**



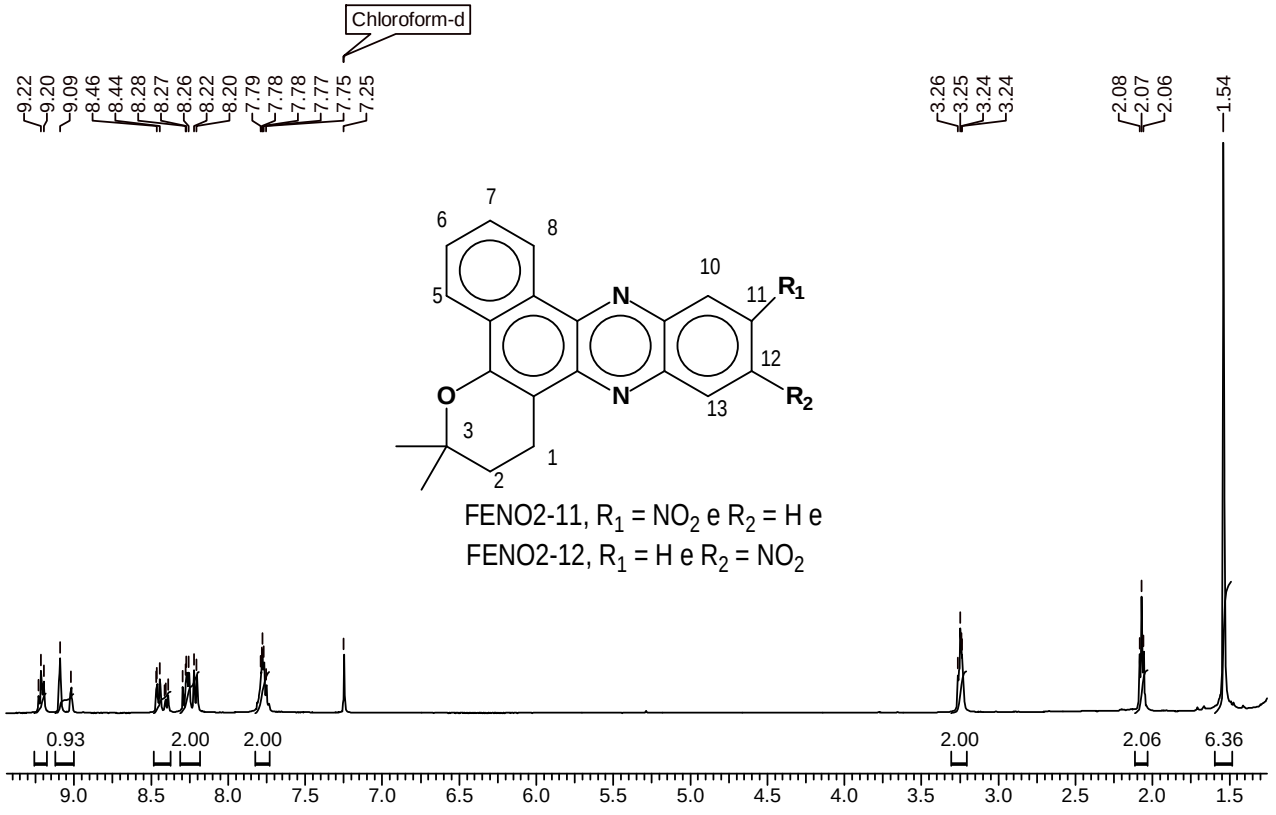
Espectro 112 – EM por *electrospray* da primera fração de BLDBP, composto mais apolar (MM=393-395)**.**



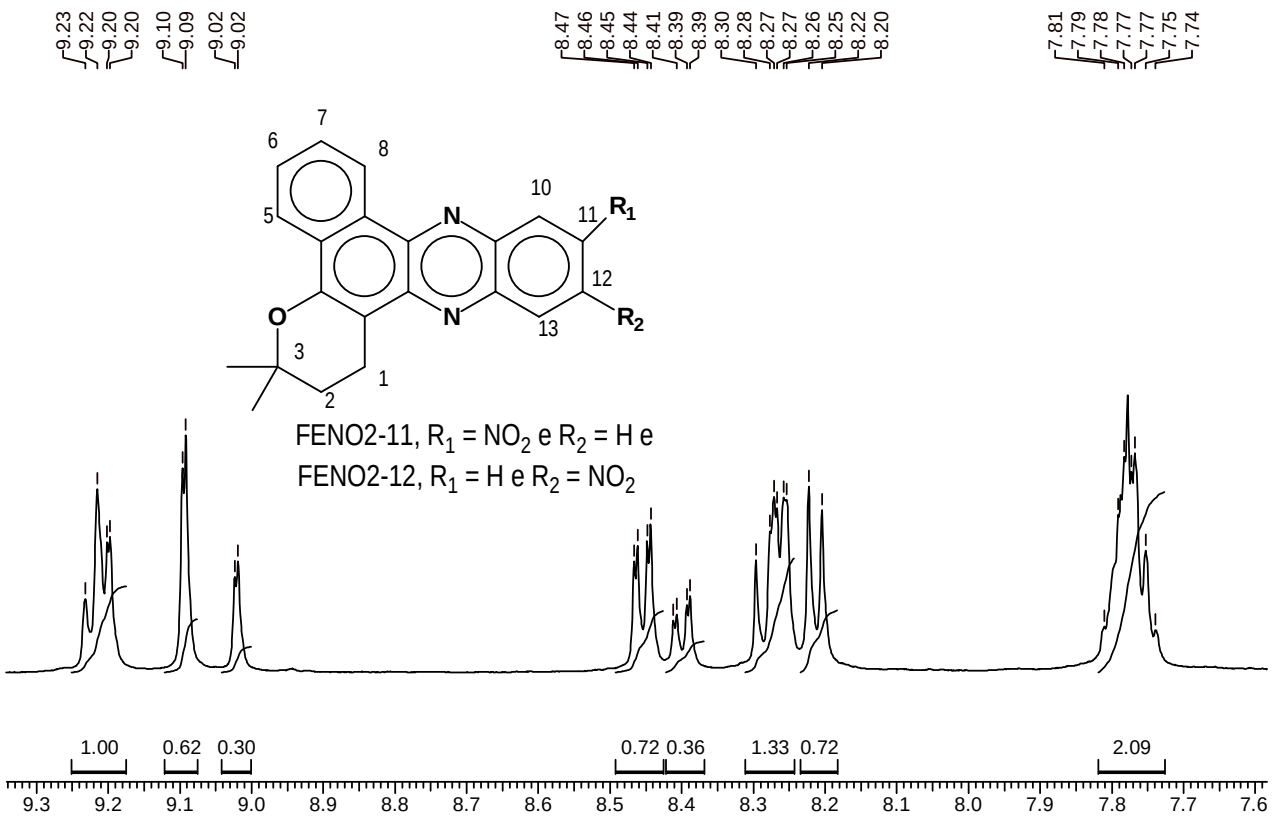


FENO2-11, $R_1 = NO_2$ e $R_2 = H$ e
FENO2-12, $R_1 = H$ e $R_2 = NO_2$

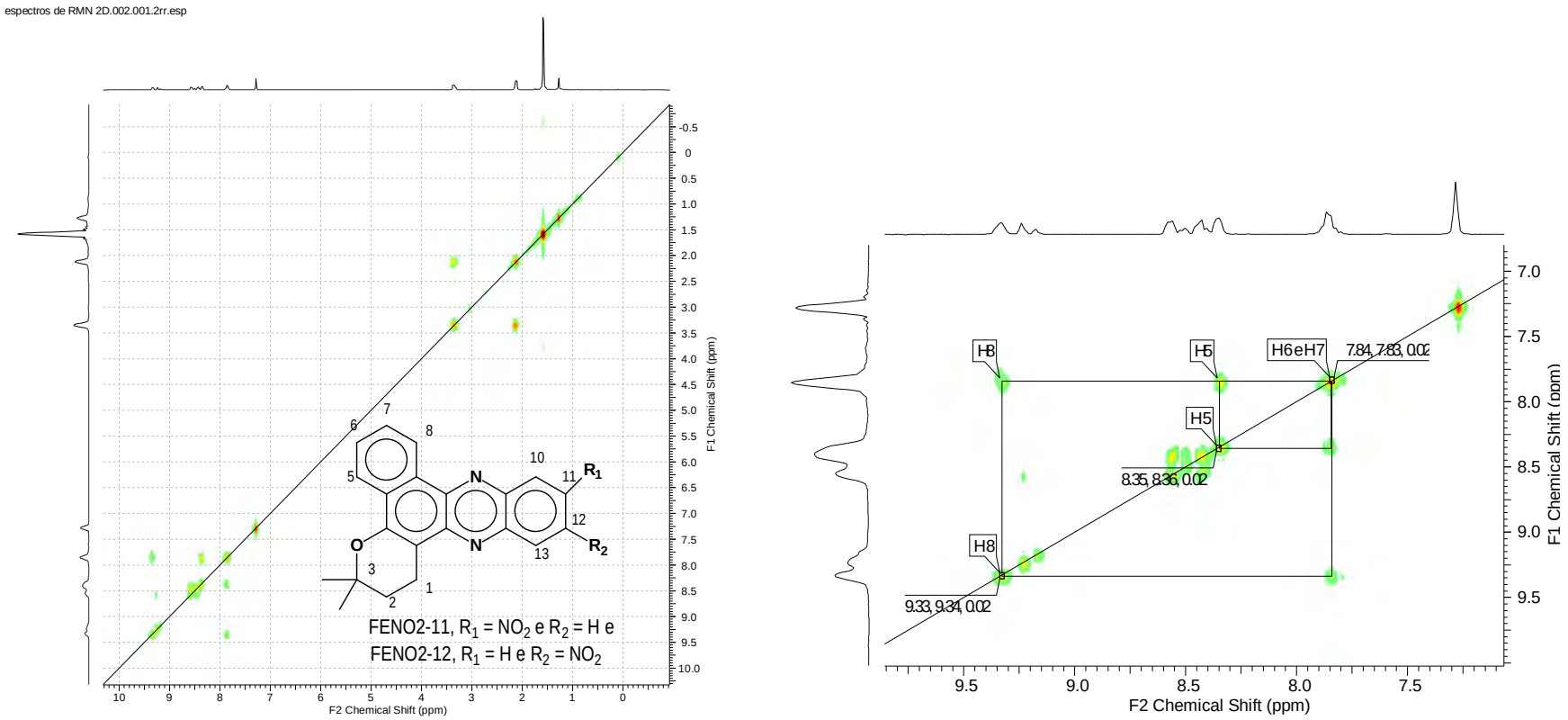
Espectro 113 - EM das fenazinas obtidas de β-lapachona com 3,4-diamino-nitrotolueno (FENO2). Acima com menor Rt e abaixo com maior Rt.



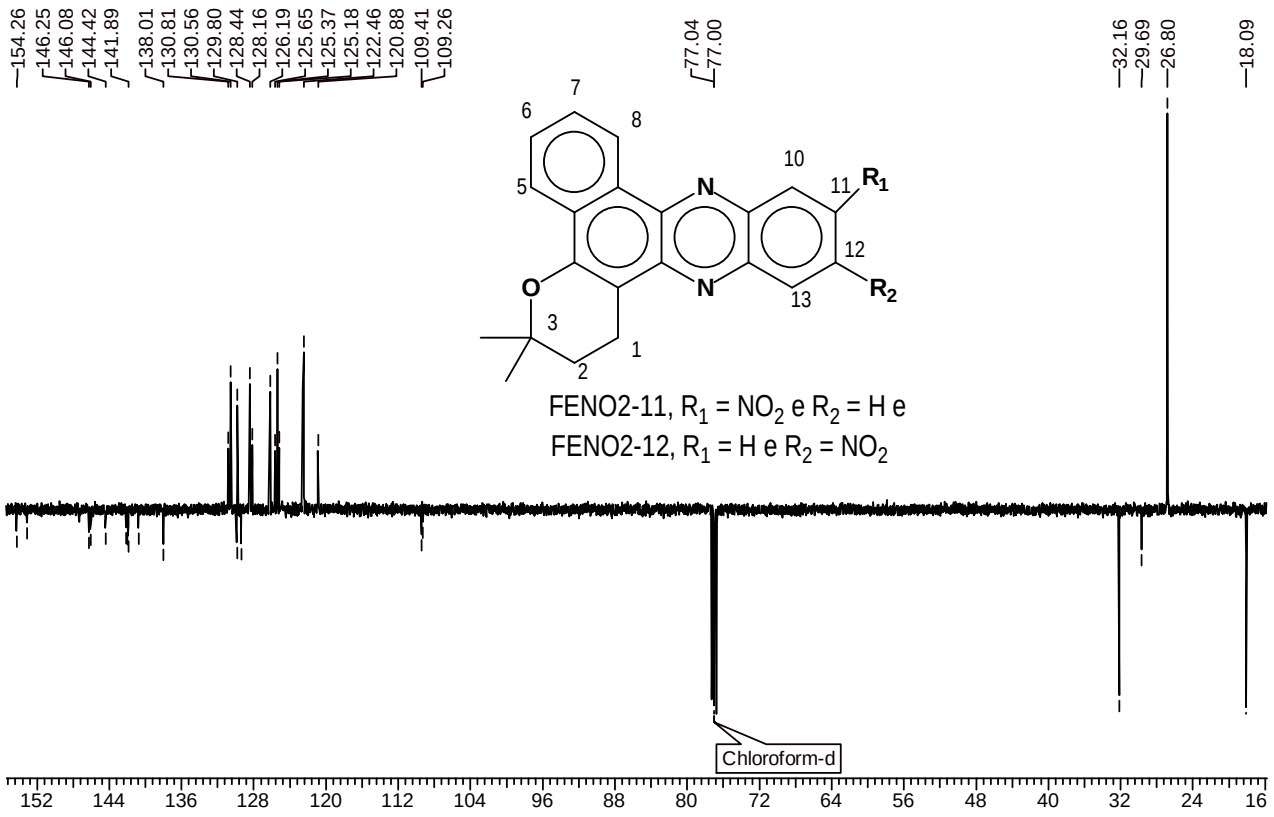
Espectro 114 – RMN ^{1}H (500 MHz) da mistura de fenazinas (FENO2-11 e FENO2-12)**.**



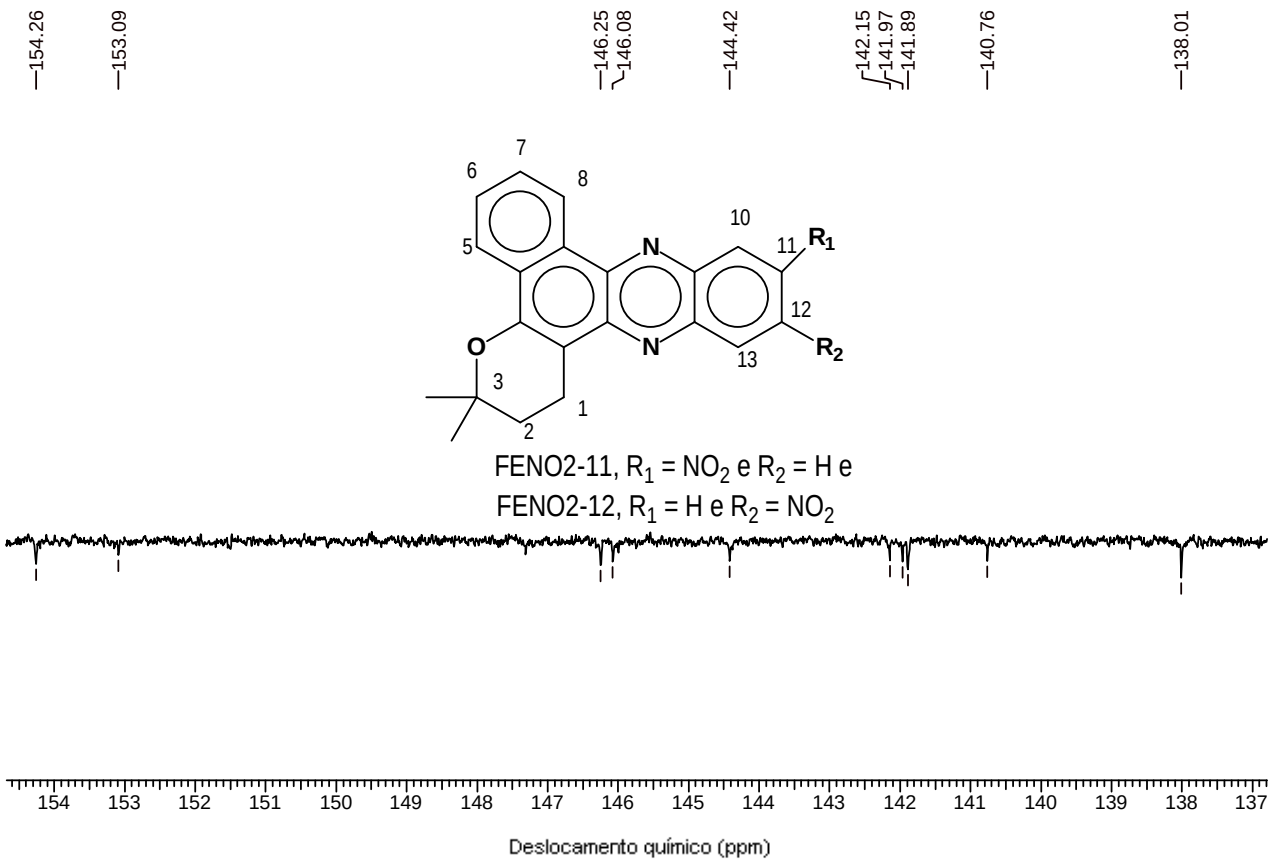
Espectro 115 – Ampliação da região aromática do espectro de RMN ^{1}H da mistura das fenazinas FENO2-11 e FENO2-12.



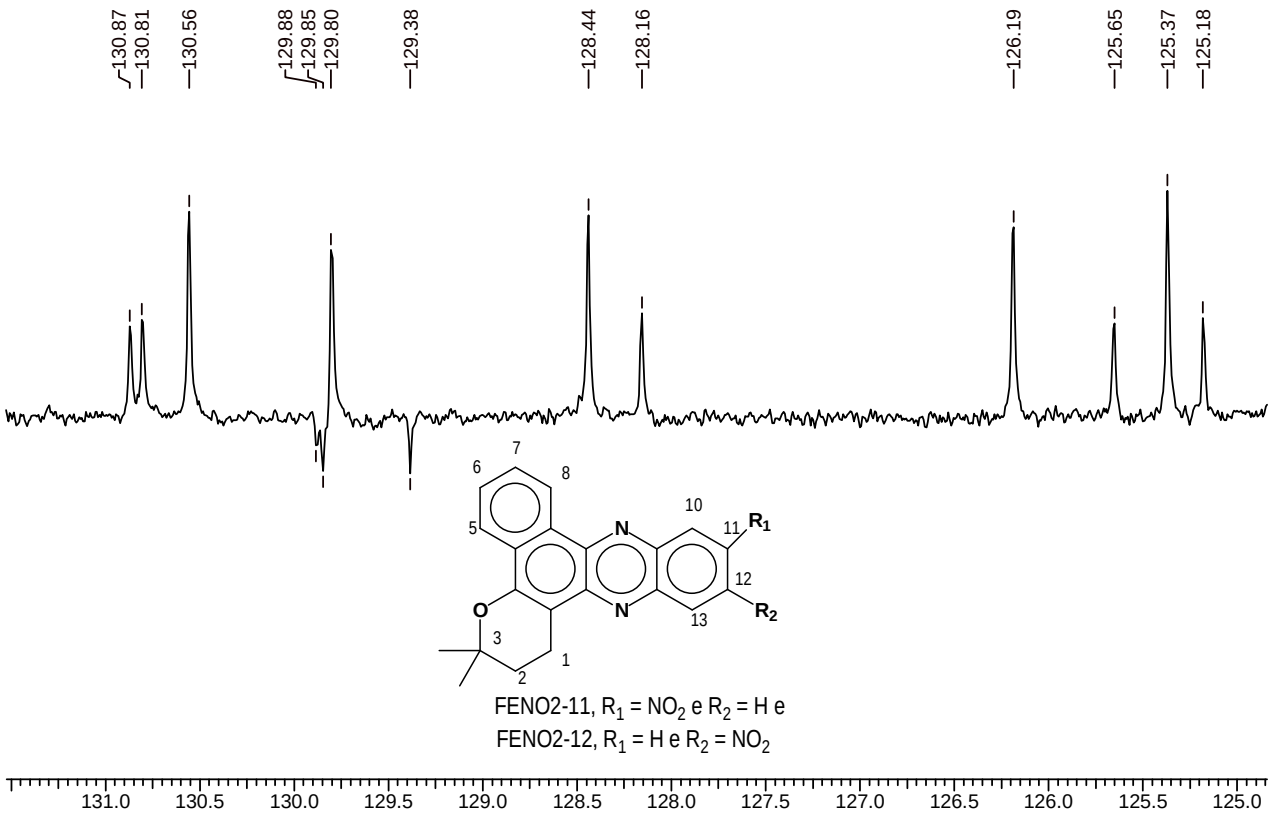
Espectro 116 – HOMOCOSY de ^{1}H-^{1}H da mistura de FENO2, figura a direita do espectro completo e a direita de ampliação na região aromática.



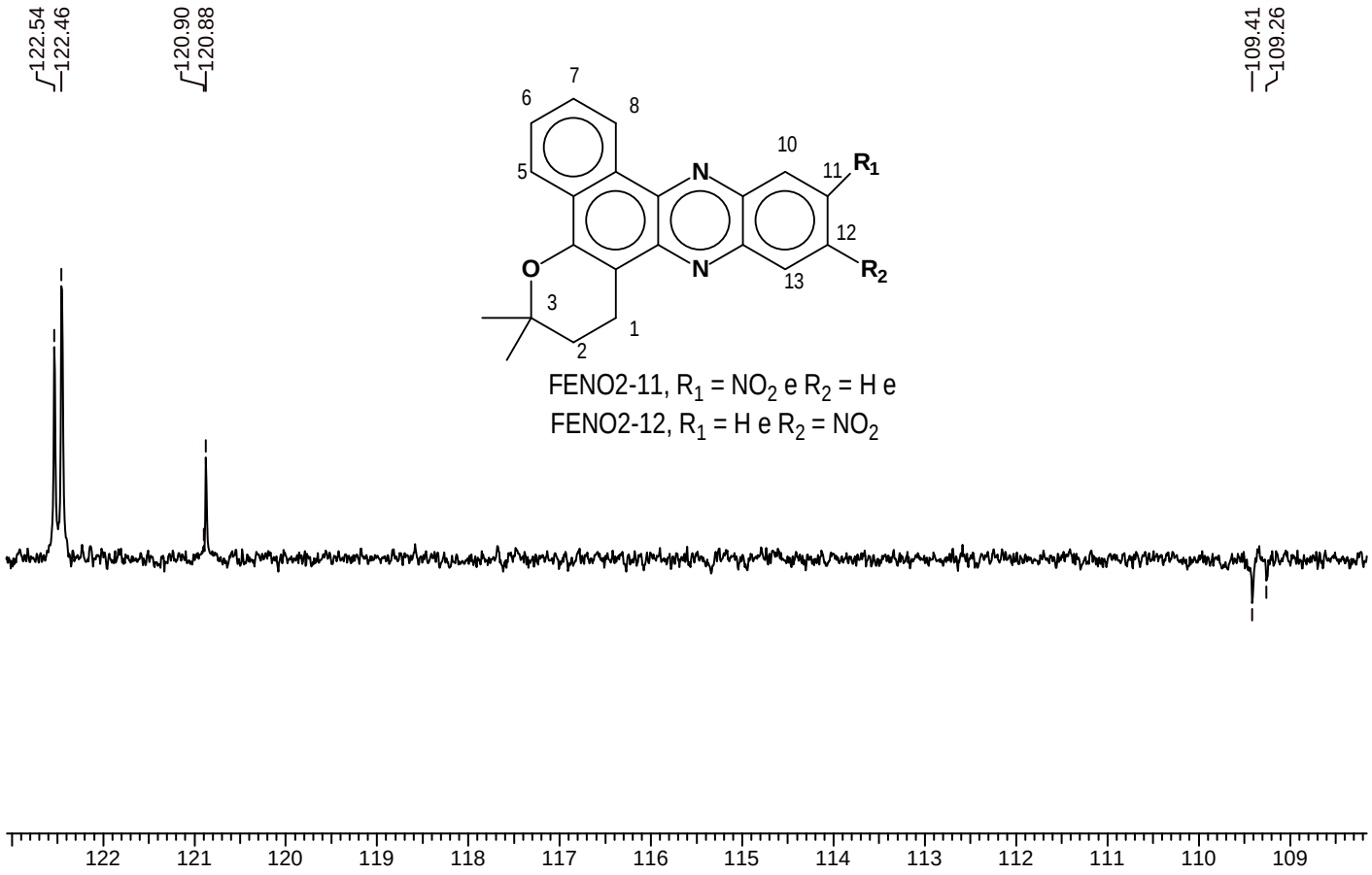
Espectro 117 – DEPT Q (125,8 MHz) da mistura das fenazinas FENO2.



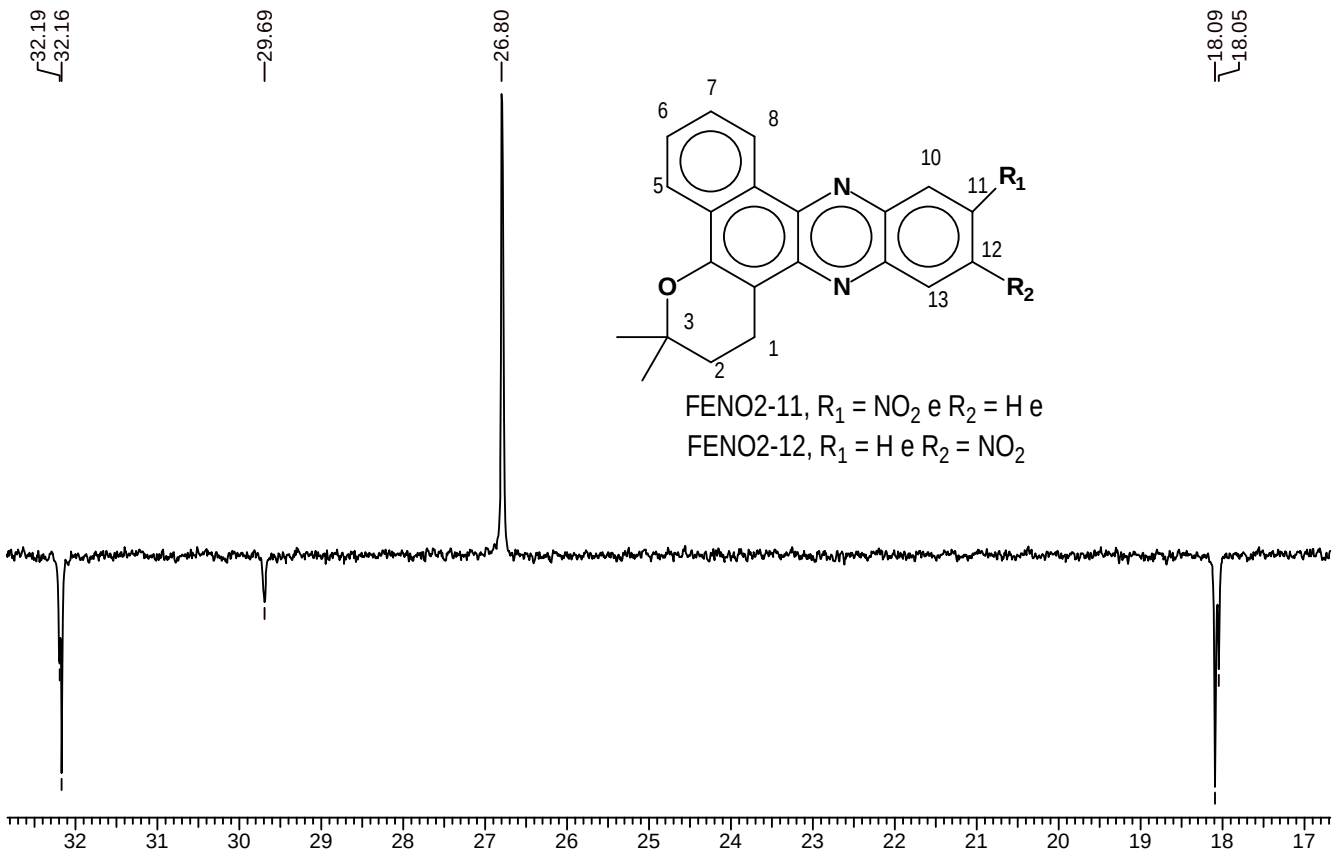
Espectro 118 – Ampliação do espectro DEPT Q, entre 137 e 155 ppm, das fenazinas FENO2.



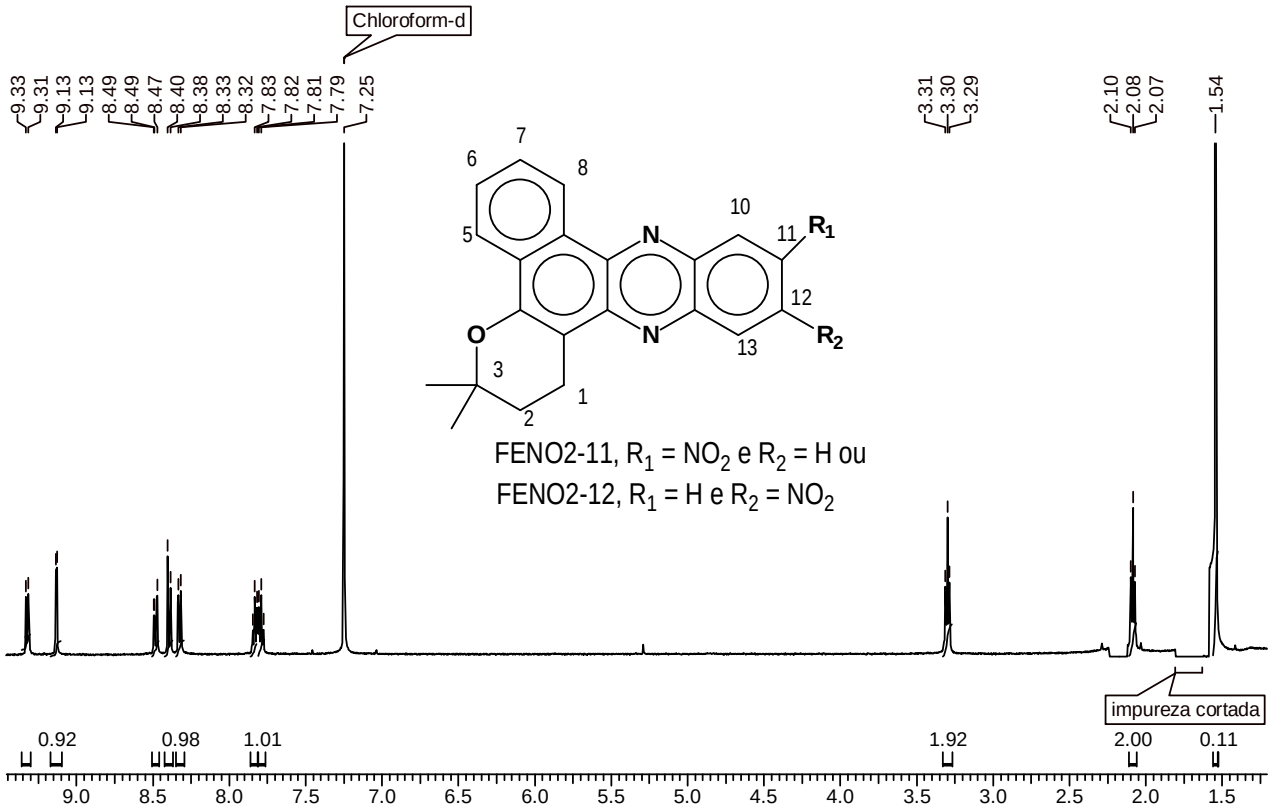
Espectro 119 – Ampliação do espectro DEPT Q, entre 125 e 131 ppm, das fenazinas FENO2**..**



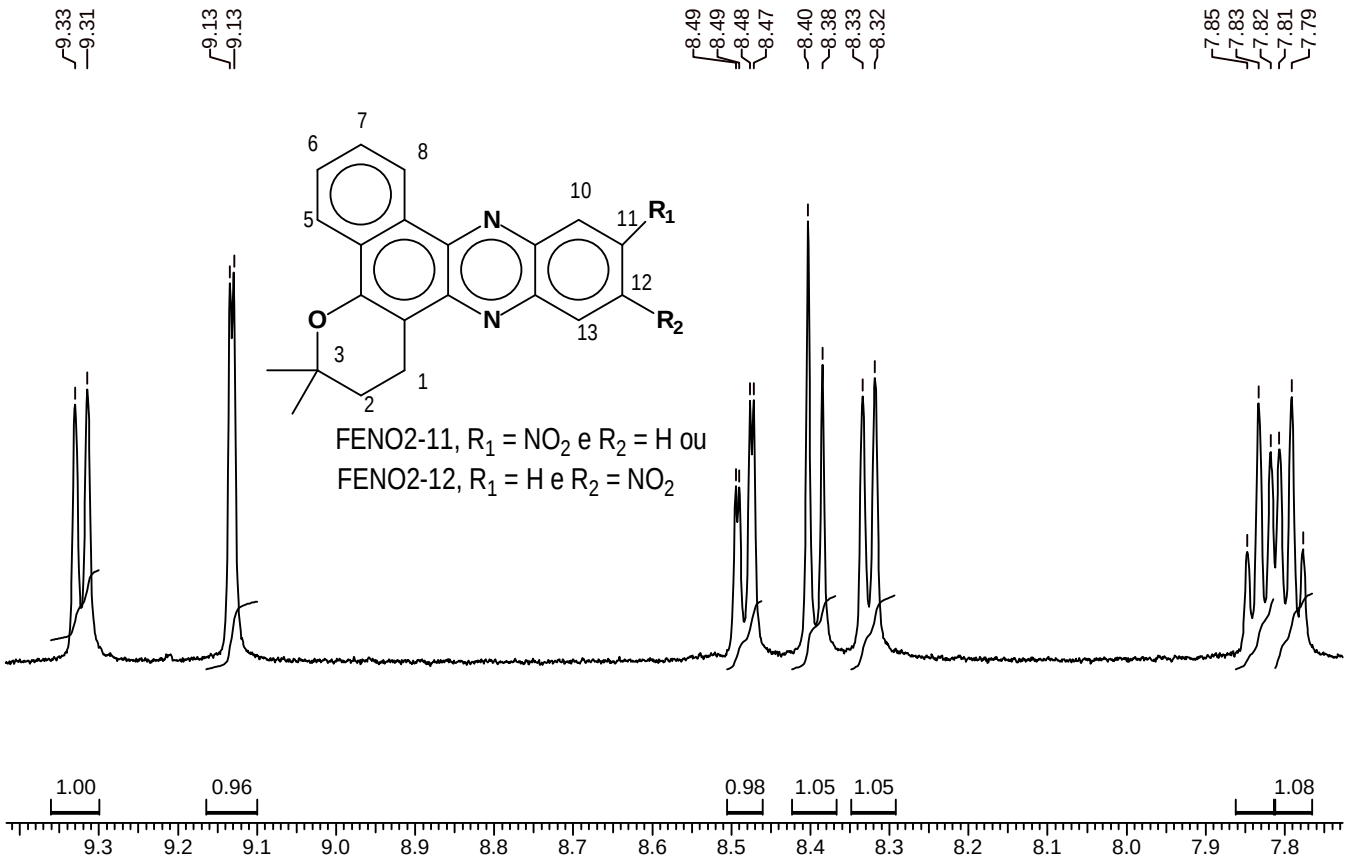
Espectro 120 – Ampliação do espectro DEPT Q, entre 108 e 123 ppm, das fenazinas FENO2.



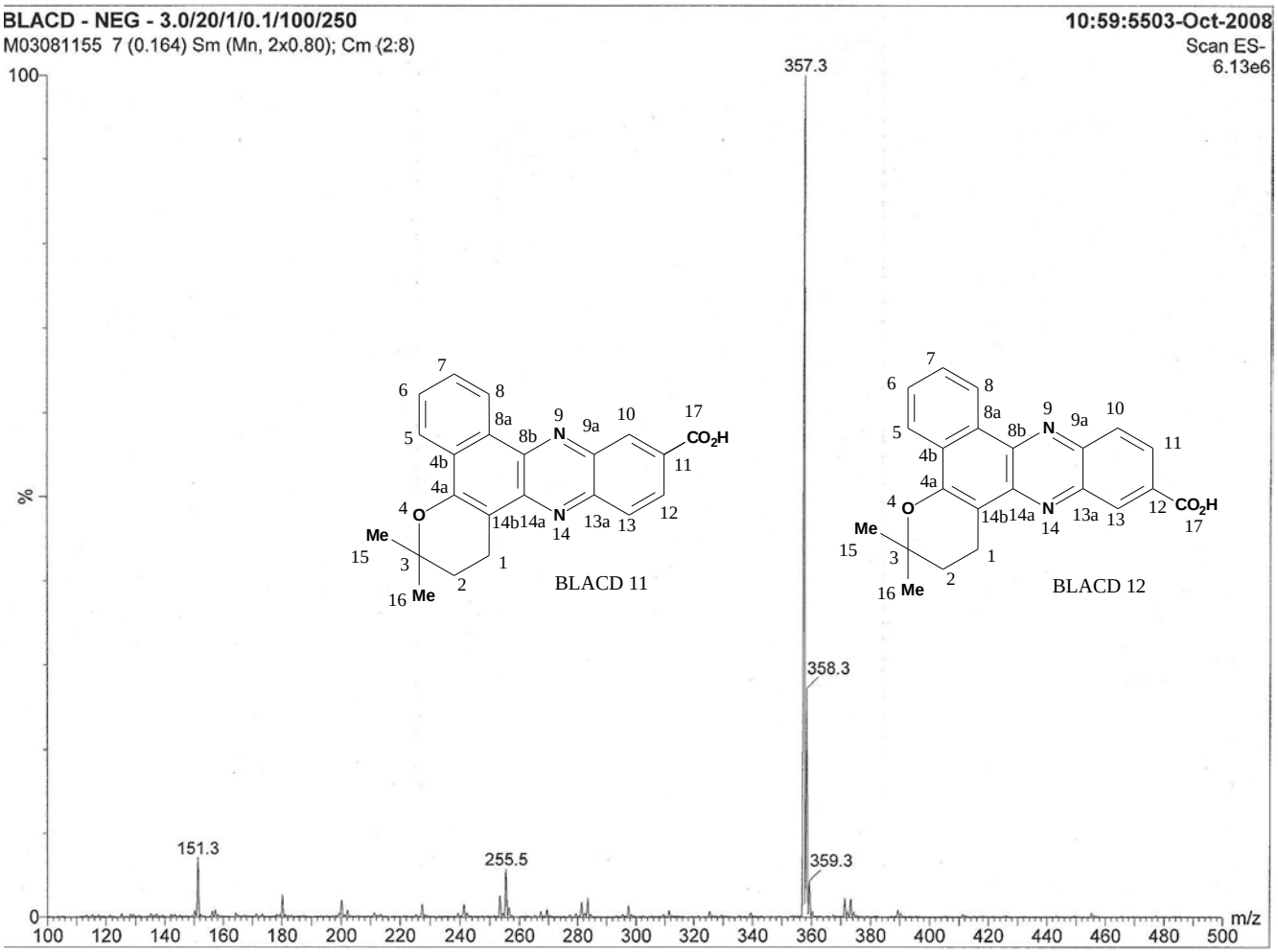
Espectro 121 – Ampliação, entre 17 e 33 ppm, do espectro DEPT Q das fenazinas FENO2.



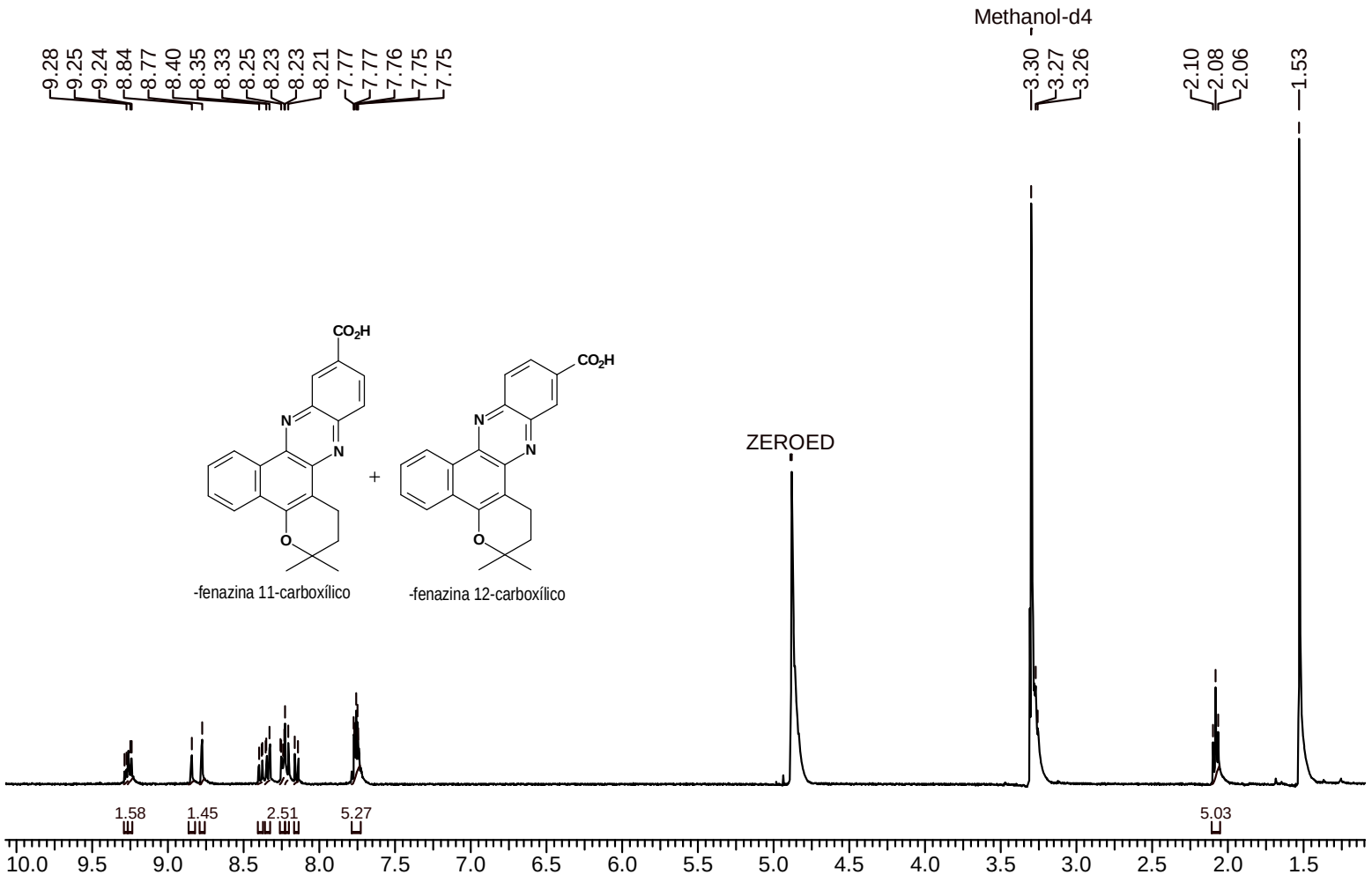
Espectro 122 - RMN ^{1}H (500 MHz) da fenazina menos polar FENO2, provável isômero 12-nitro.



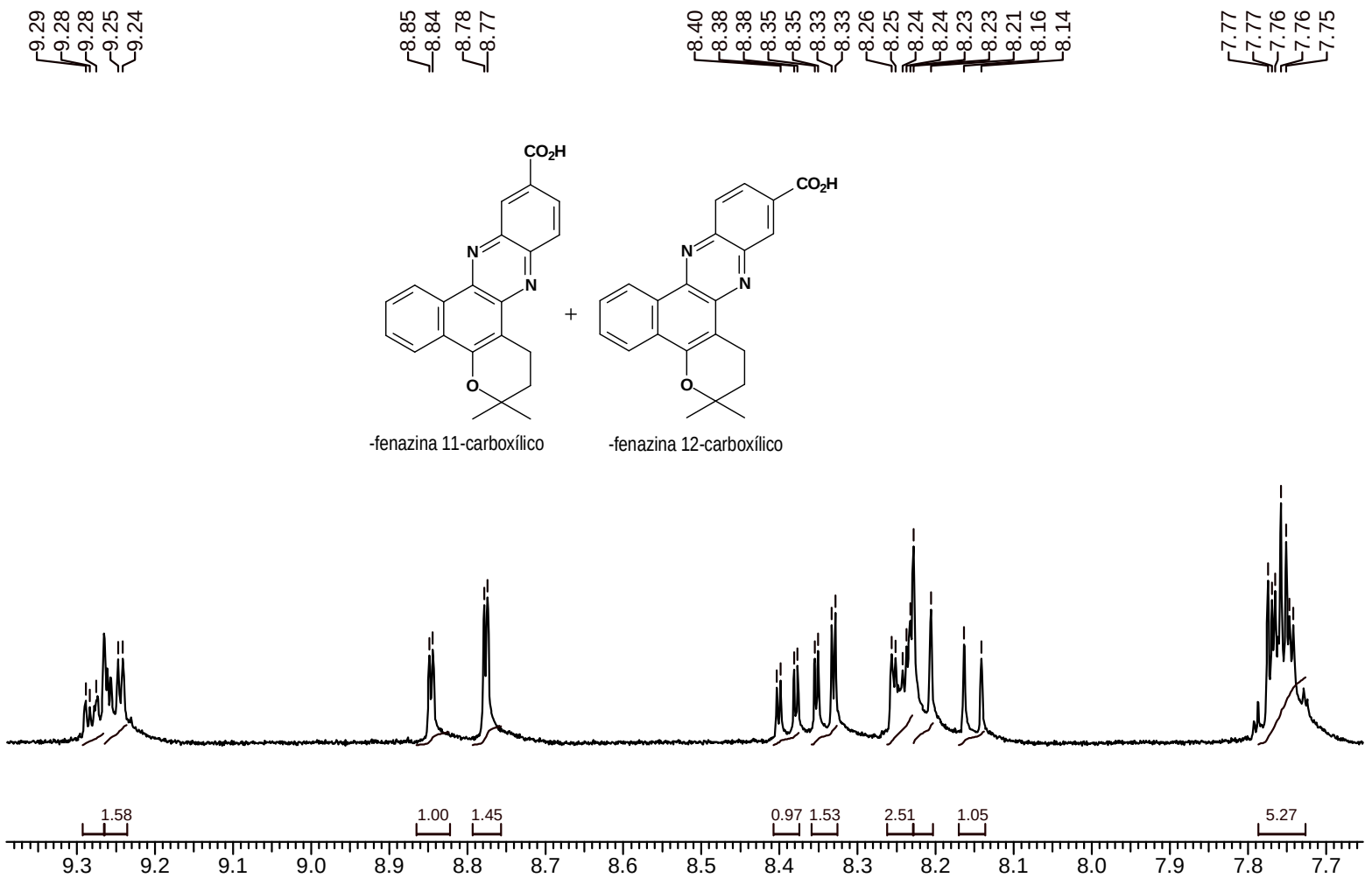
Espectro 123 – Ampliação do espectro de RMN ^{1}H da fenazina menos polar FENO2, provável isômero 12-nitro**.**



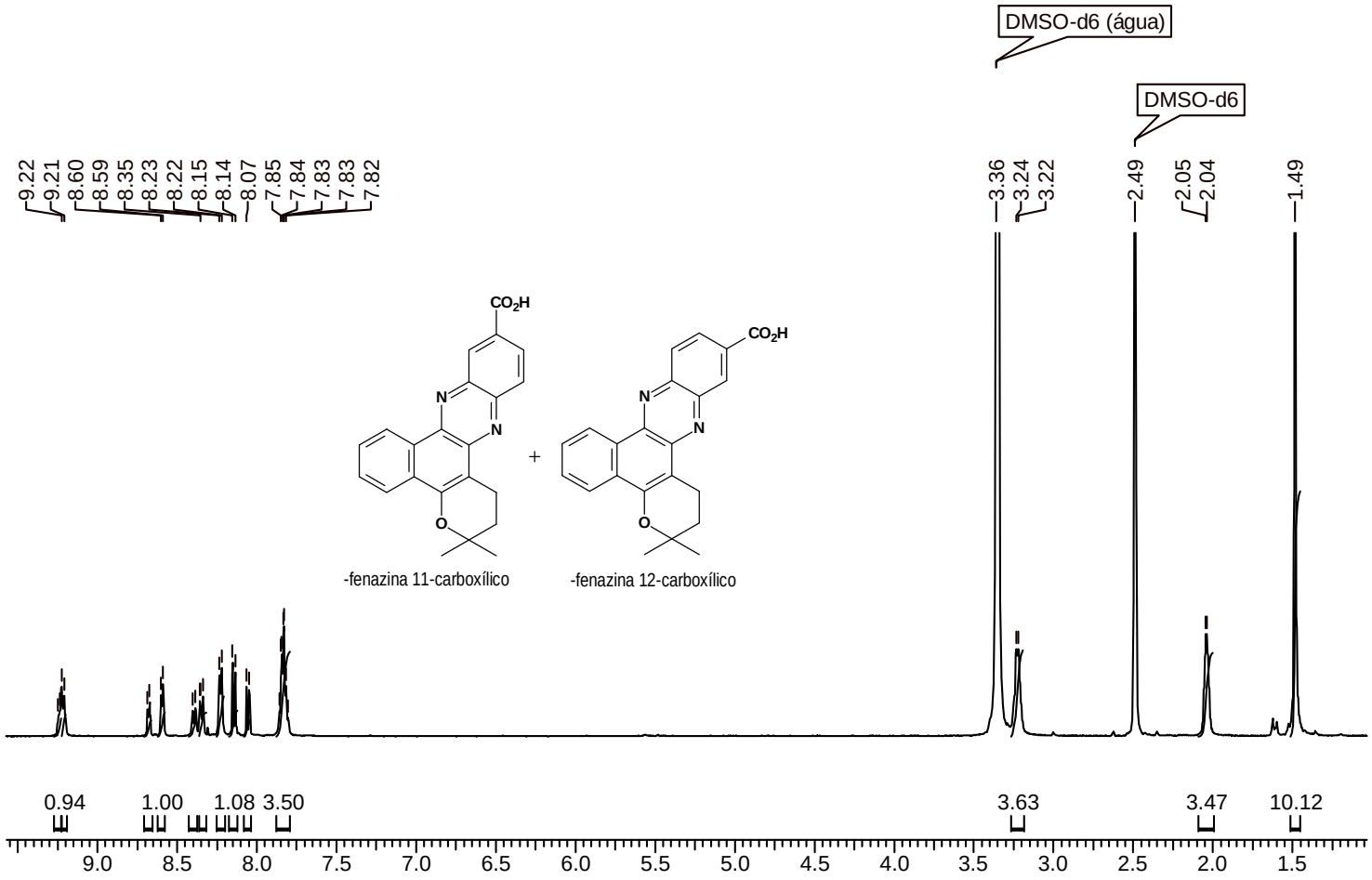
Espectro 124 – EM por "*electron-spray*" (ES) da mistura da fenazina BLACD, (MM=358)**.**



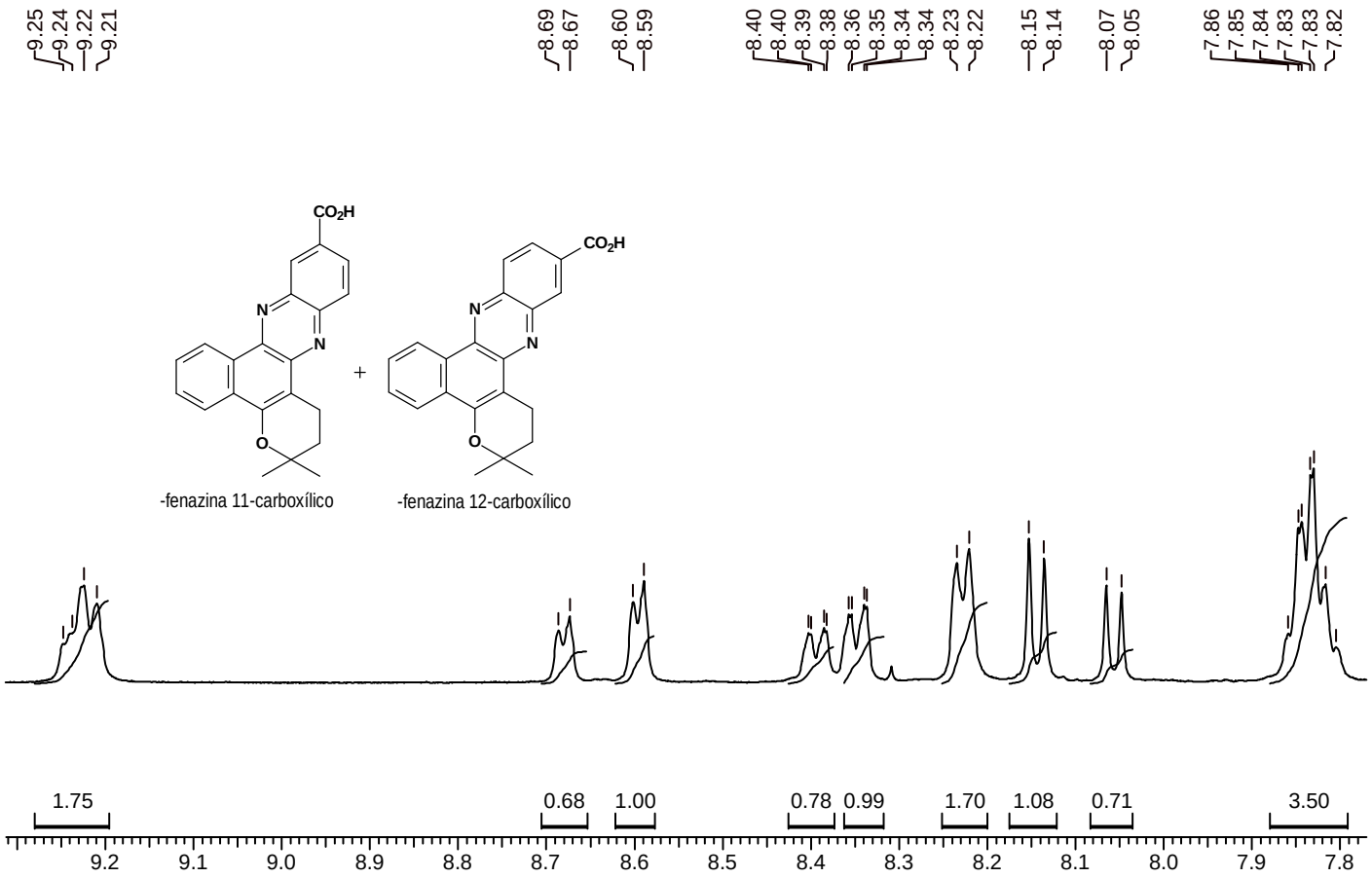
Espectro 125 - RMN ^{1}H (400 MHz) da mistura da fenazina BLACD**,** em metanol**.**



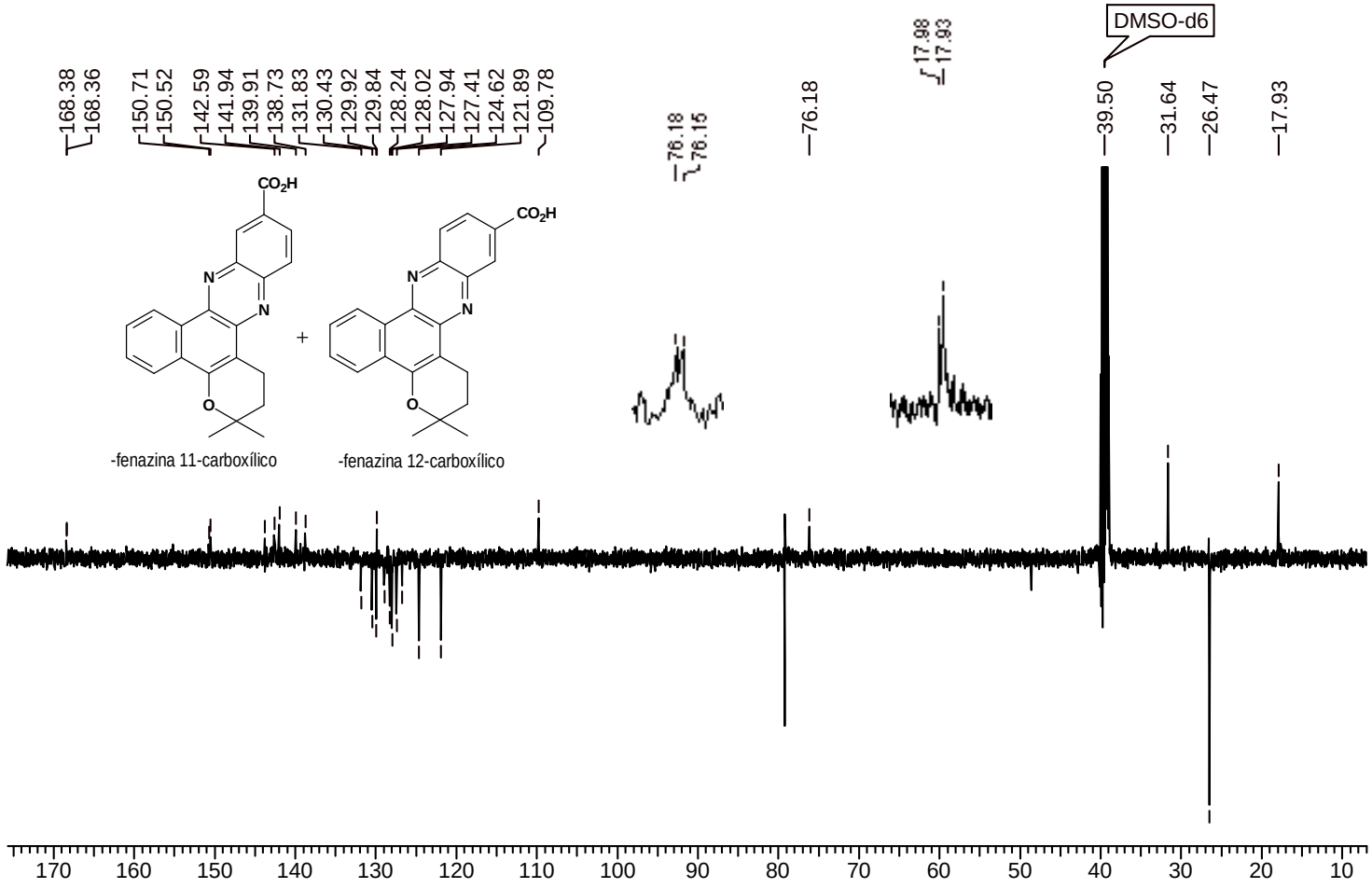
Espectro 126 – Expansão da região aromática do espectro de RMN ^{1}H das fenazinas de BLACD, em metanol.



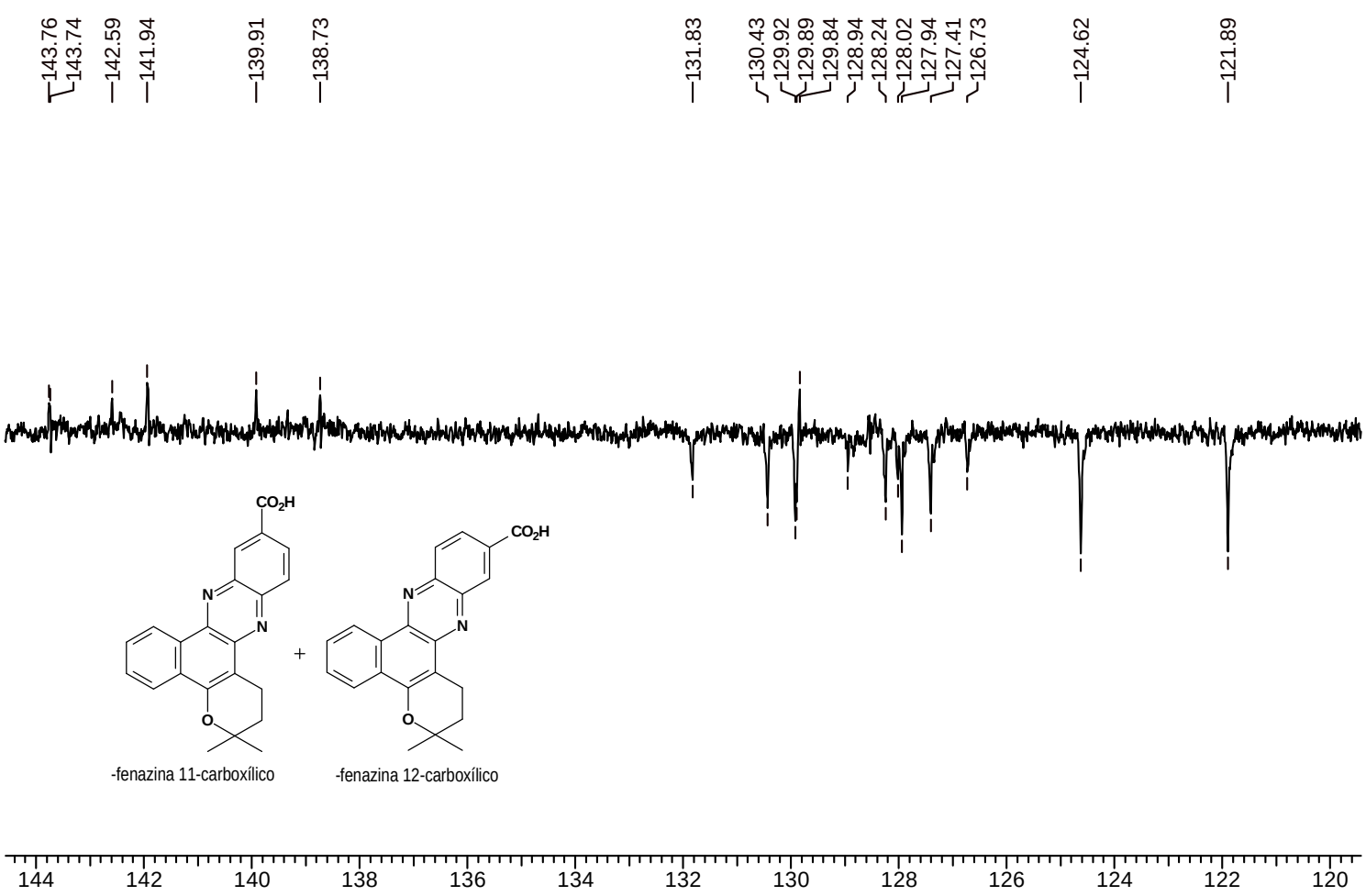
Espectro 127 - RMN ^{1}H (500 MHz) das fenazinas BLACD, em DMSO-d6**.**



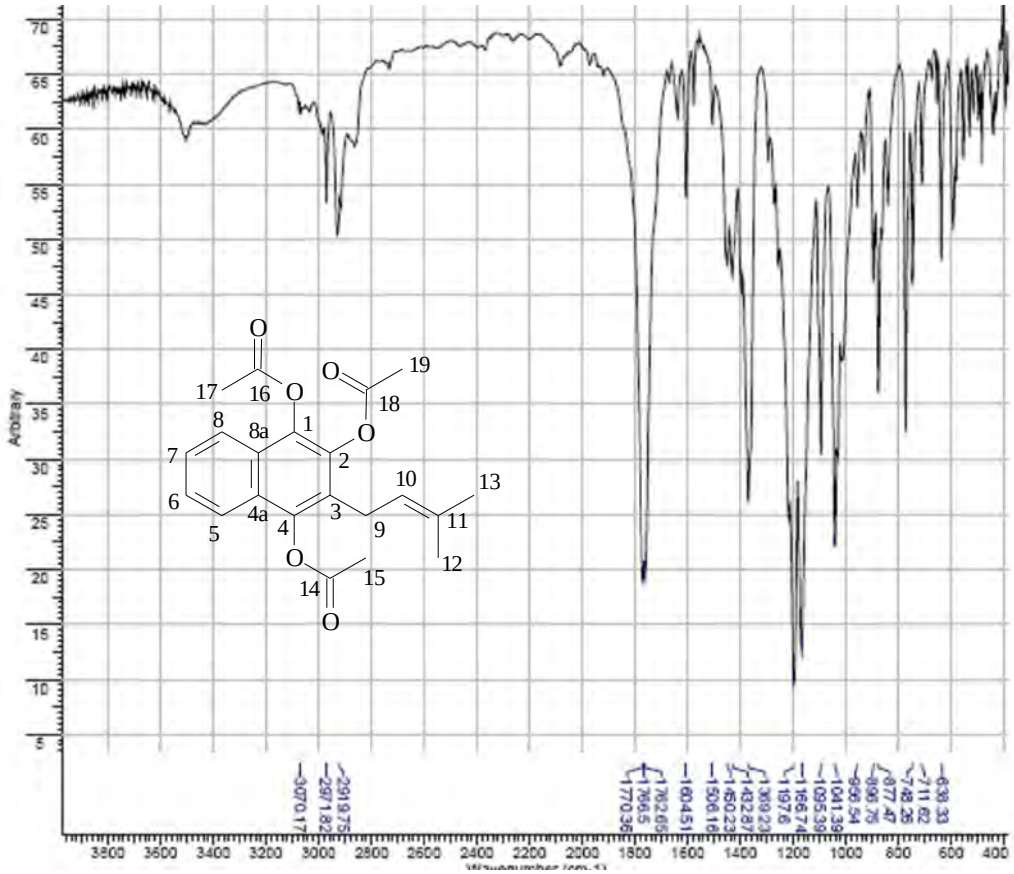
Espectro 128 - Ampliação da região aromática do espectro de RMN ^{1}H das fenazinas BLACD, em DMSO-d6.



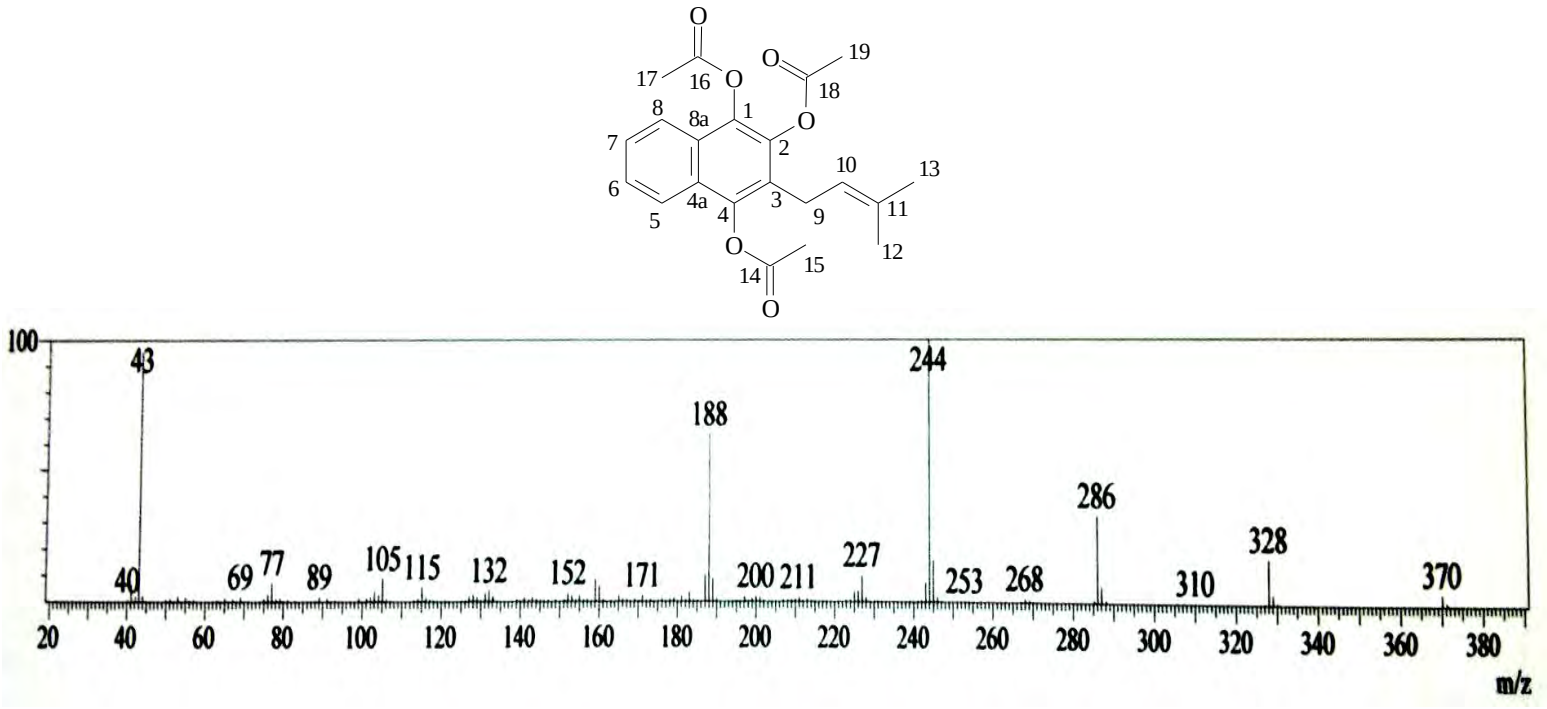
Espectro 129 – DEPT Q (125,8 MHz) da mistura de fenazina BLACD, em DMSO-d6, em destaque sinais próximos**.**



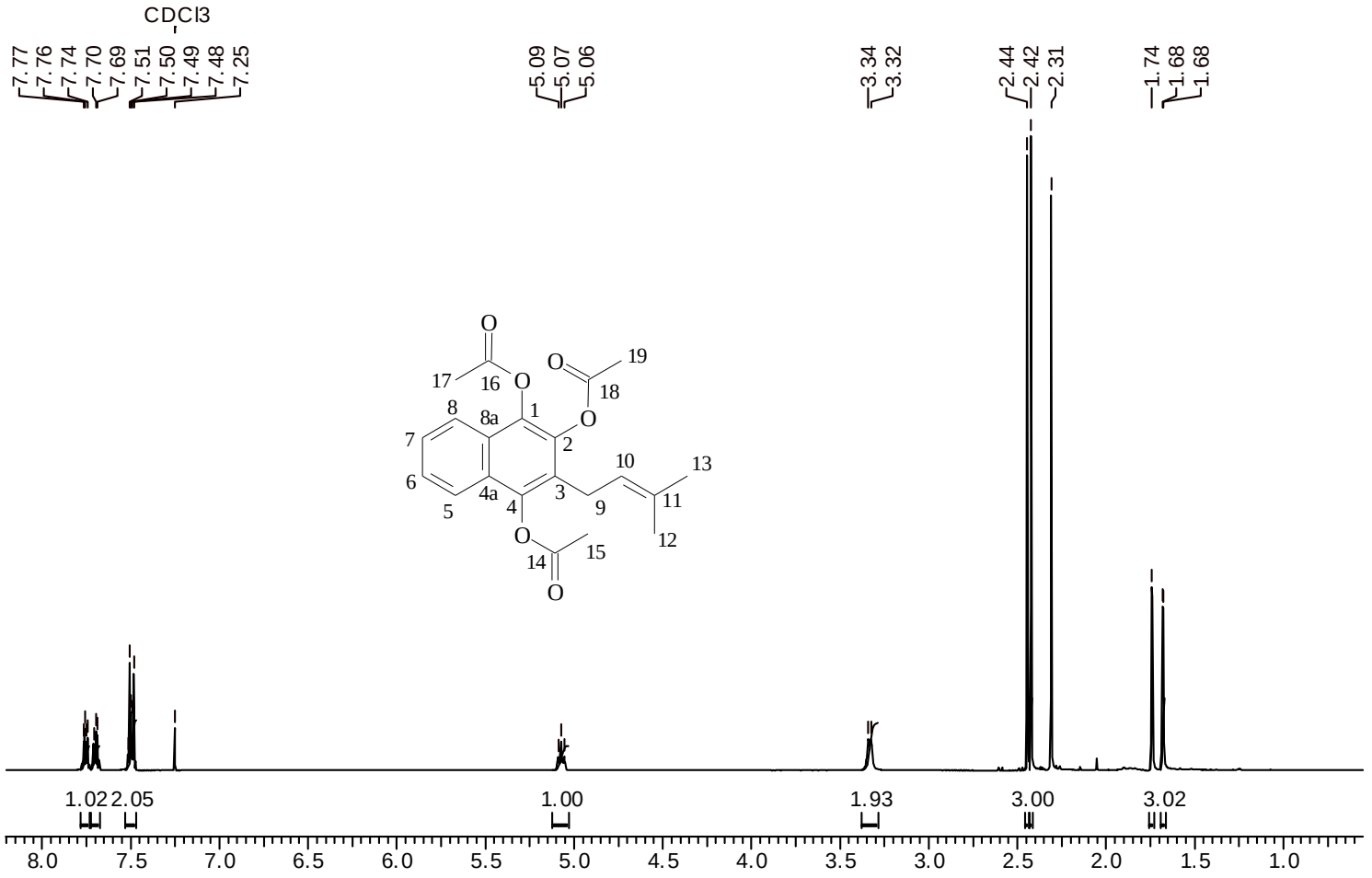
Espectro 130 – Ampliação, entre 120 e 144 ppm do espectro de DEPT Q da mistura das fenazina de BLACD, em DMSO-d6.



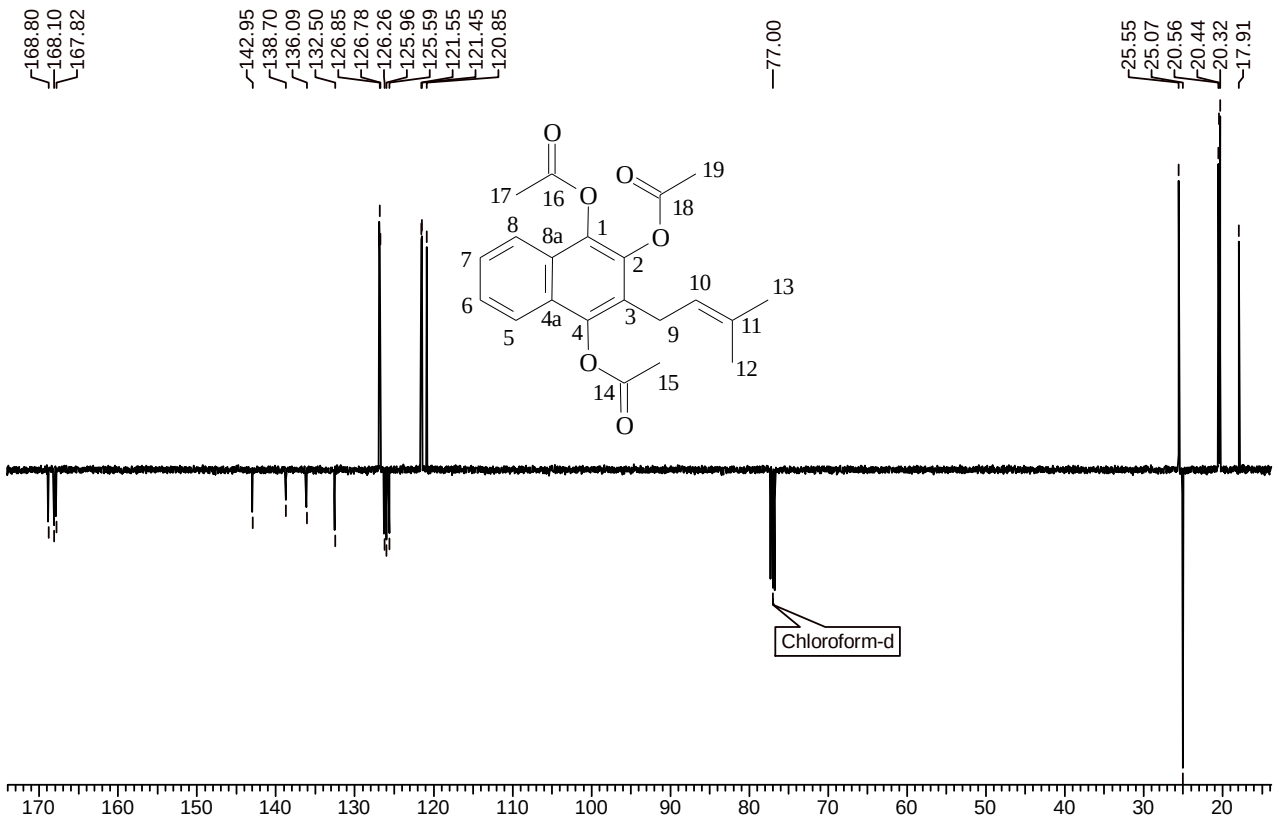
Espectro 131 - IV do TriAclap, lapachol triacetilado (acetato de [1,4-bis(acetoxi)-3-(3-metilbut-2-enil)] 2-naftila)**.**



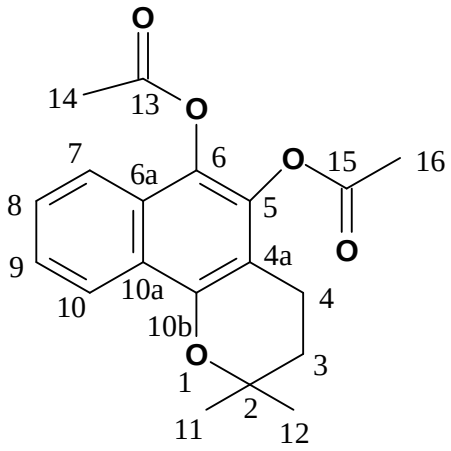
Espectro 132 – E.M. do TriAclap, lapachol triacetilado (acetato de [1,4-bis(acetoxi)-3-(3-metilbut-2-enil)] 2-naftila)**.**

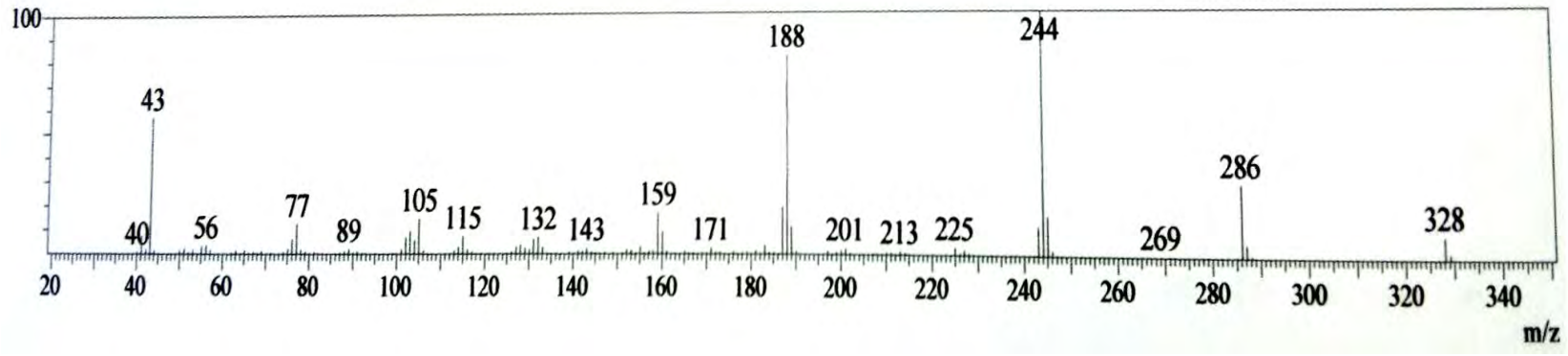


Espectro 133 - RMN ^{1}H (400 MHz) do TriAclap, lapachol triacetilado (acetato de [1,4-bis(acetoxi)-3-(3-metilbut-2-enil)] 2-naftila).

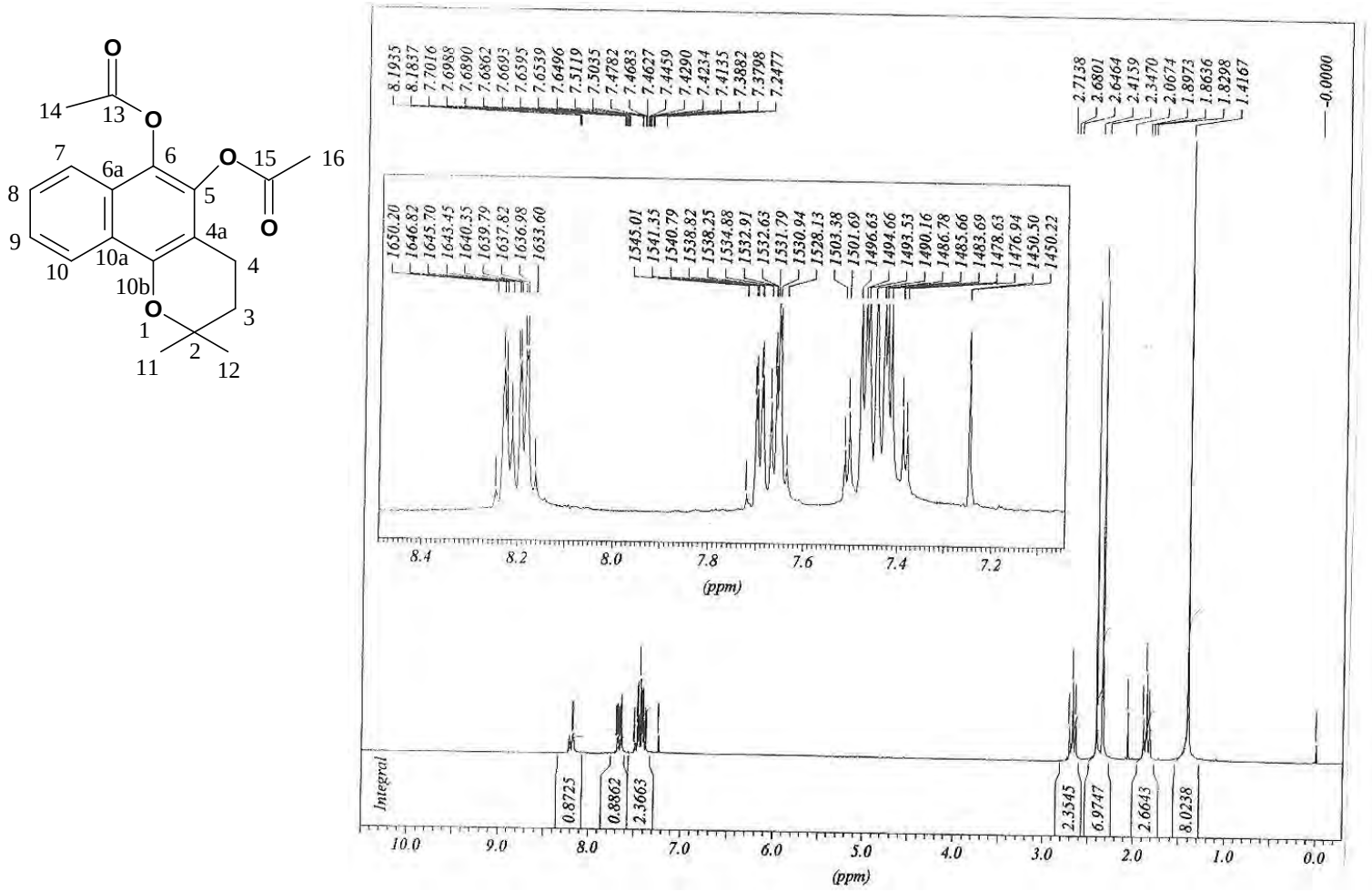


Espectro 134 – DEPT Q (125,8 MHz) do TriAclap, lapachol triacetilado (acetato de [1,4-bis(acetoxi)-3-(3-metilbut-2-enil)] 2-naftila)**.**

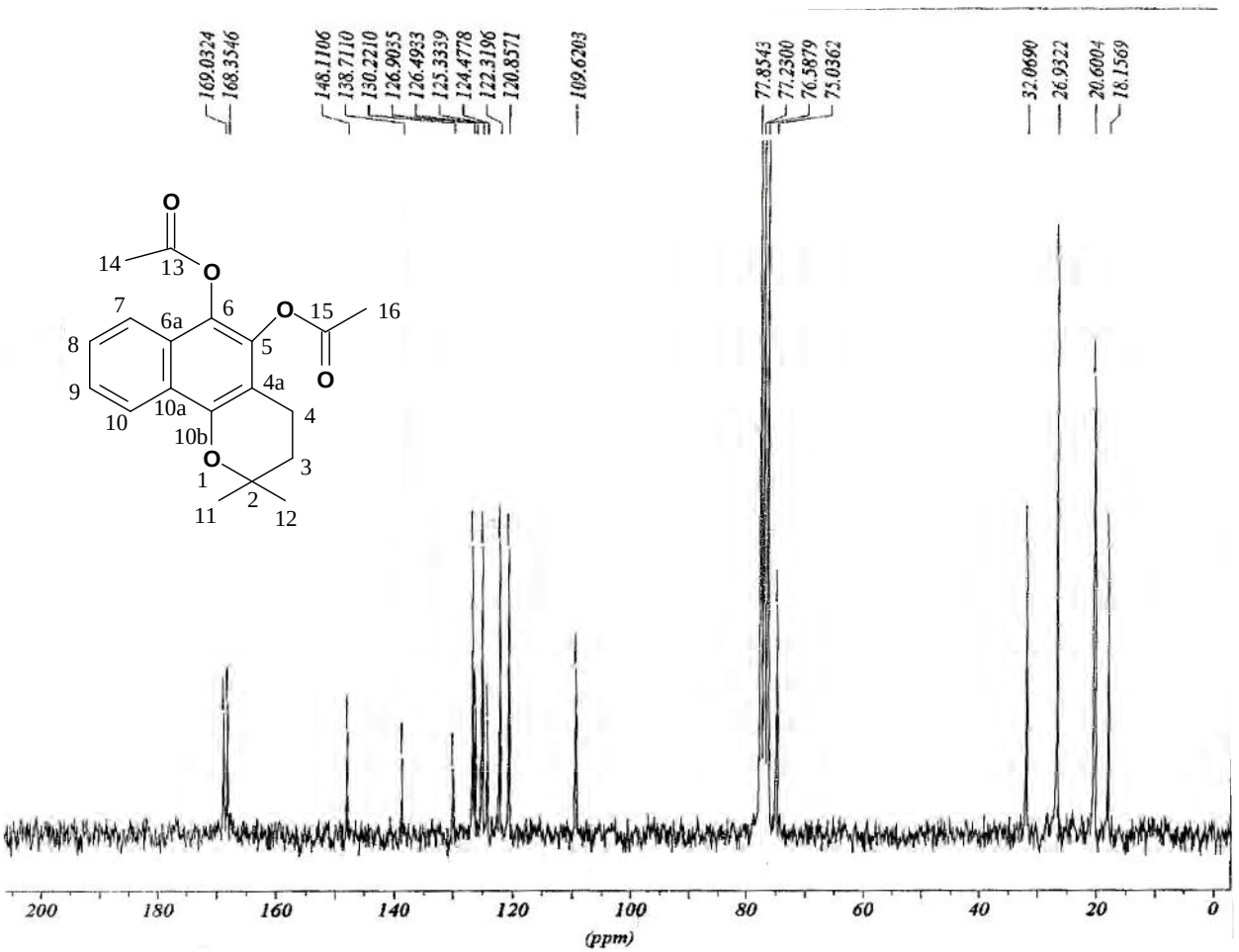




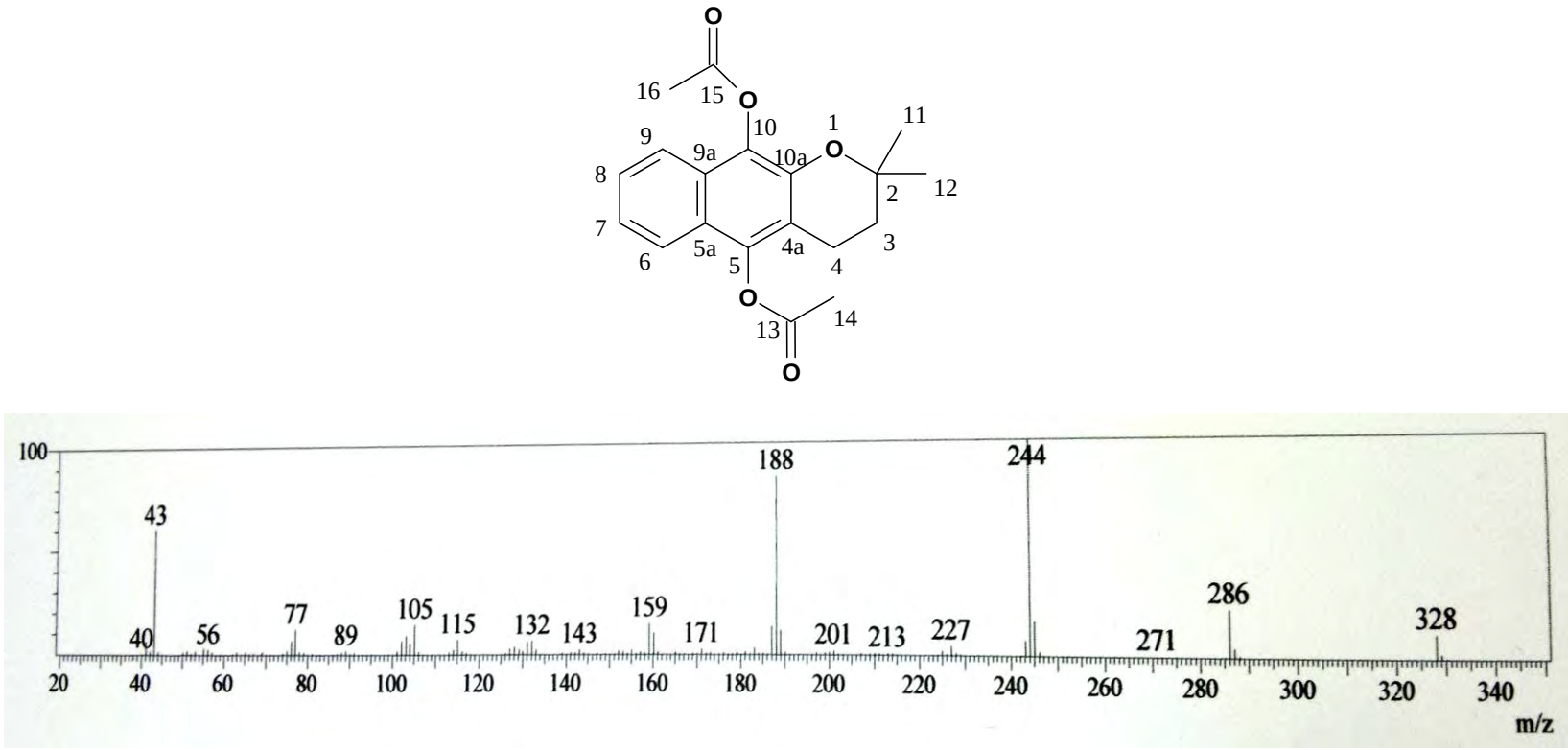
Espectro 135 – E.M. da Ac-blap, β-lapachona acetilada (acetato de 5-(acetoxi)-2,2-dimethyl-3,4-di-hidro-2*H*-benzo[*h*]cromen-6-ila).



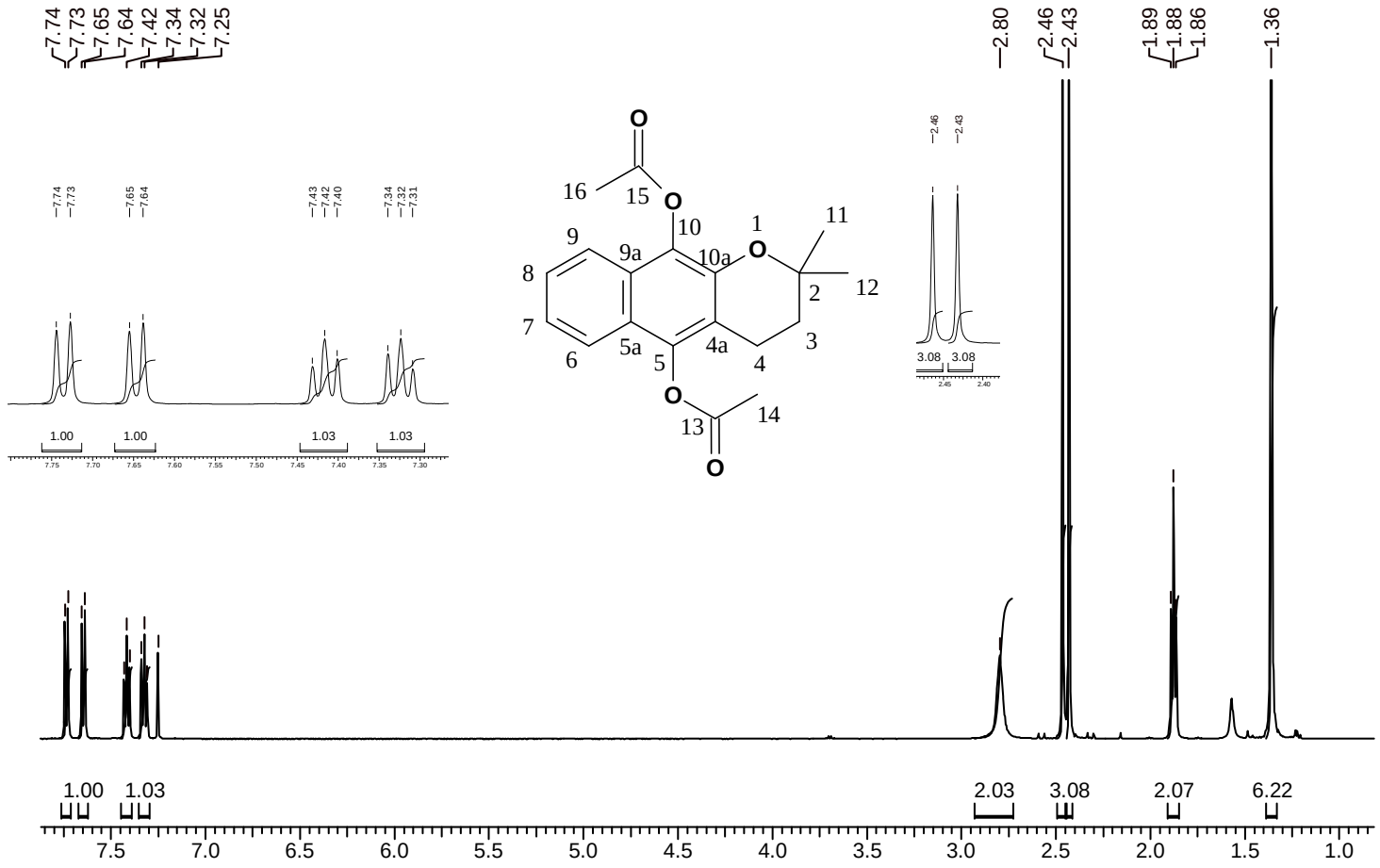
Espectro 136 - RMN ^{1}H (200 MHz) da Ac-blap, β-lapachona acetilada (acetato de 5-(acetoxi)-2,2-dimethyl-3,4-di-hidro-2*H*-benzo[*h*]cromen-6-ila).



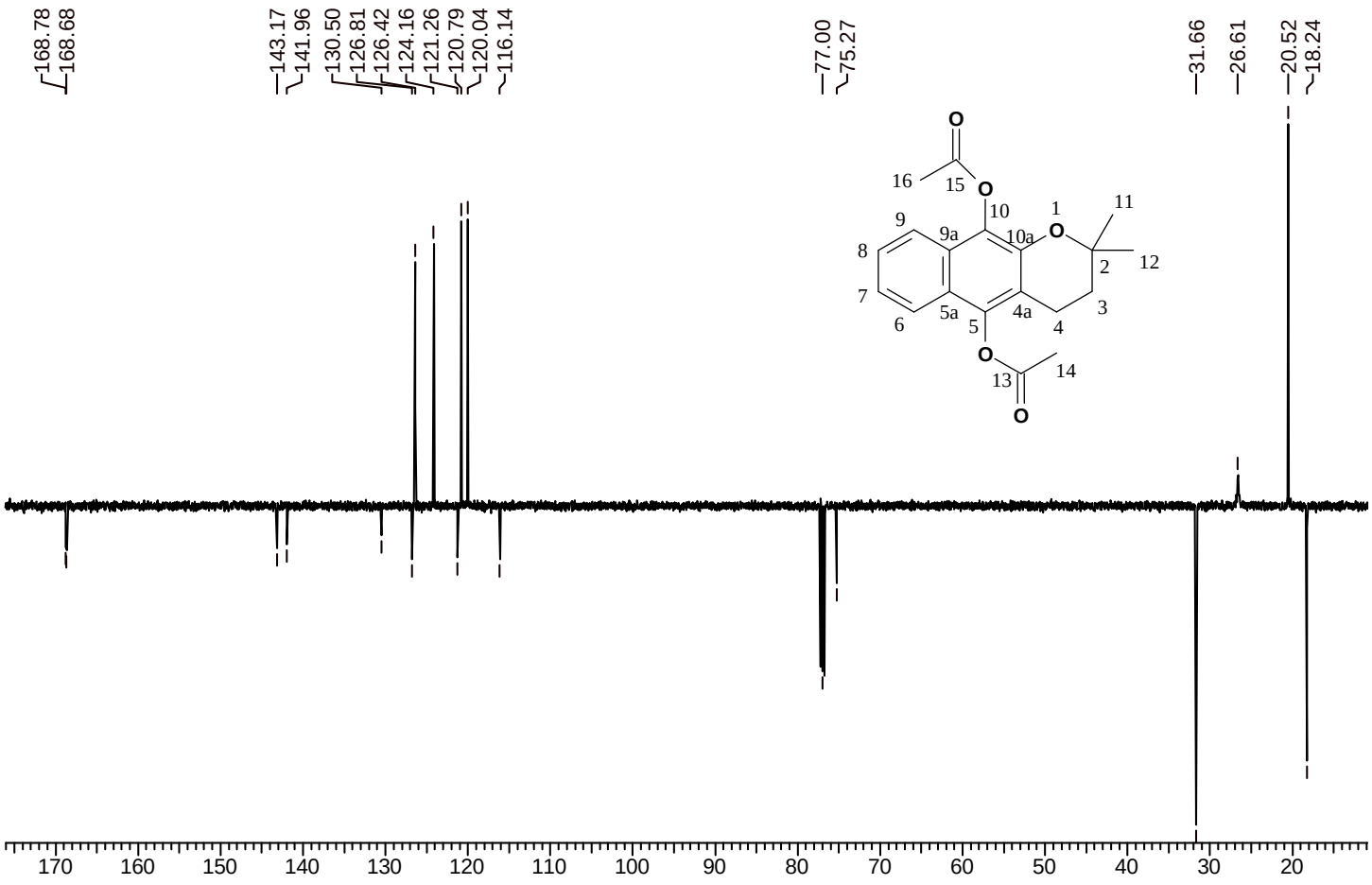
Espectro 137 - RMN ^{13}C (50,3 MHz) da Ac-blap, β-lapachona acetilada (acetato de 5-(acetoxi)-2,2-dimethyl-3,4-di-hidro-2*H*-benzo[*h*]cromen-6-ila)..



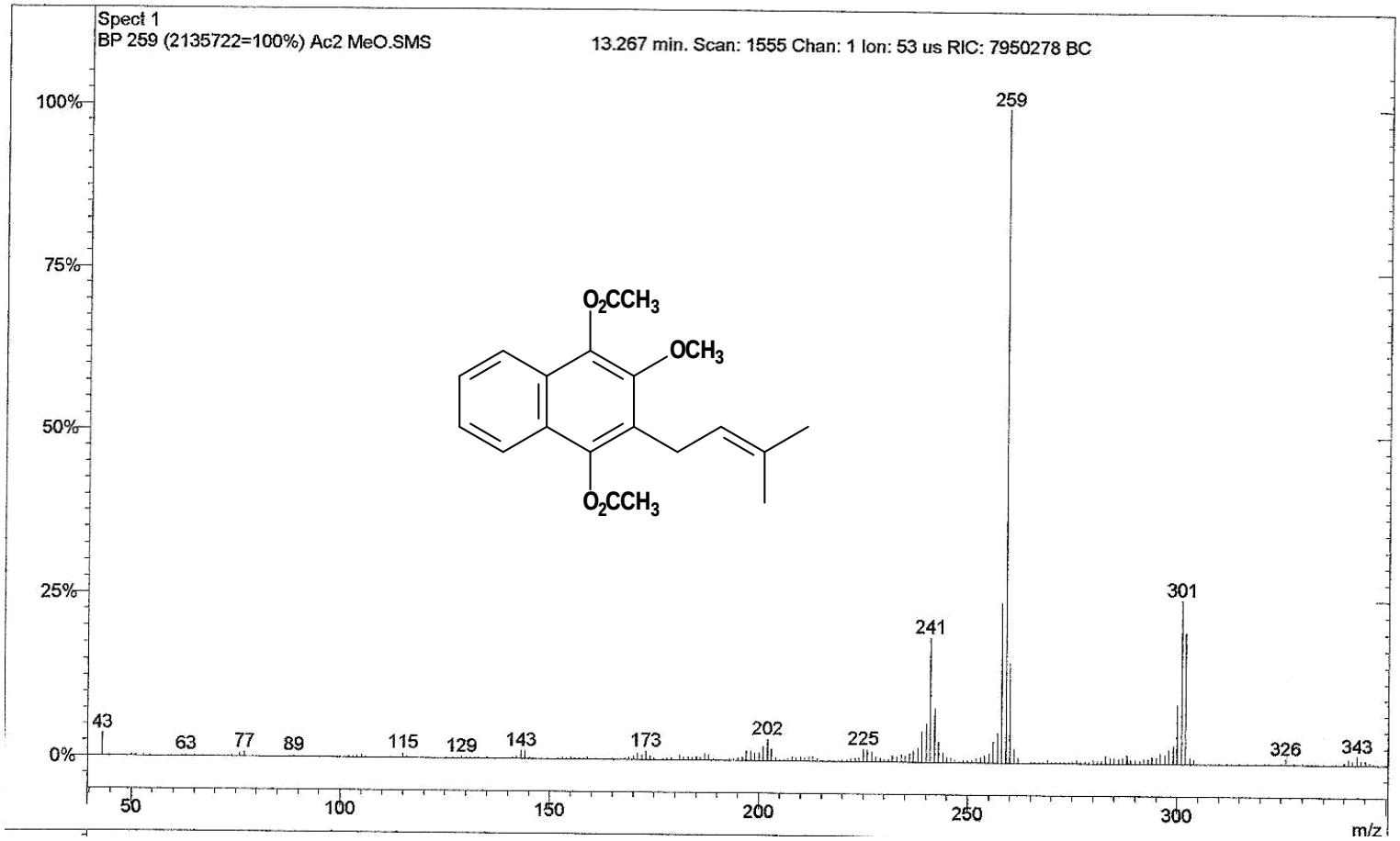
Espectro 138 – E.M. da Acalap, α-lapachona acetilada (acetato de 10-(acetoxi)-2,2-dimetil-3,4-di-hidro-*2H*-benzo[g]cromen-5-ila).



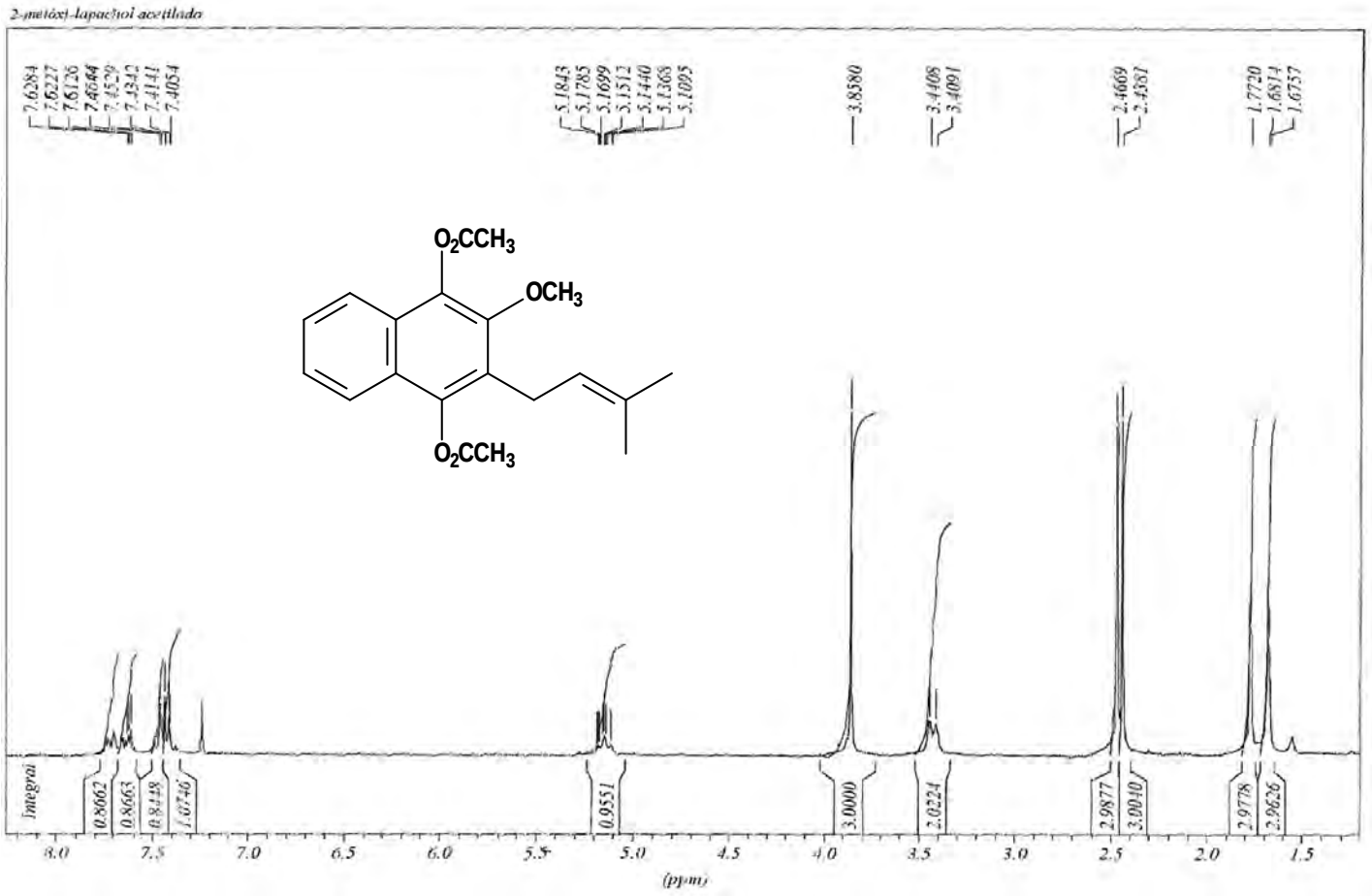
Espectro 139 - RMN ^{1}H (500 MHz) da Acalap, α-lapachona acetilada (acetato de 10-(acetoxi)-2,2-dimetil-3,4-di-hidro-*2H*-benzo[g]cromen-5-ila)**.**



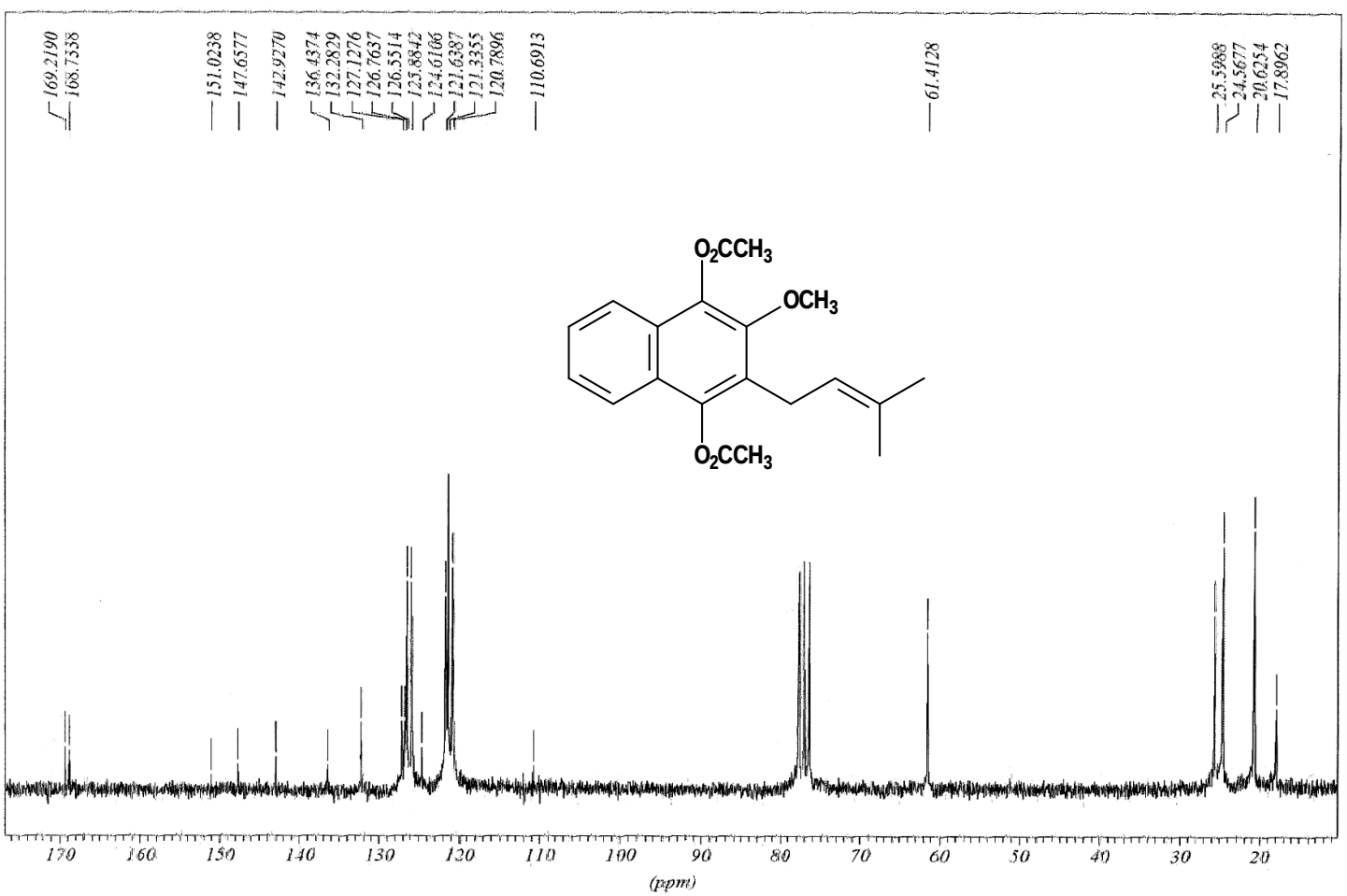
Espectro 140 – DEPT-Q (125,8 MHz) da Acalap, α-lapachona acetilada (acetato de 10-(acetoxi)-2,2-dimetil-3,4-di-hidro-*2H*-benzo[g]cromen-5-ila)**.**



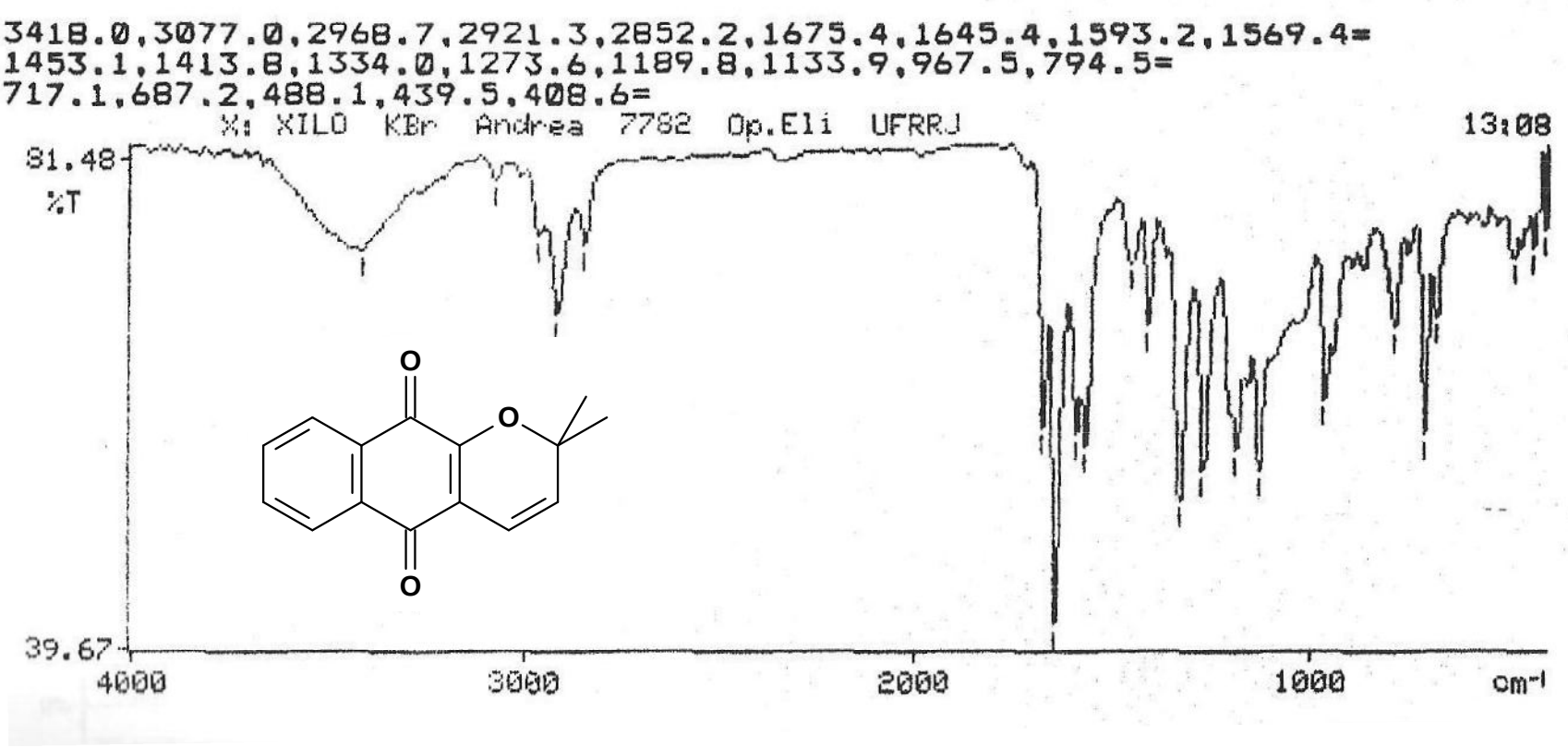
Espectro 141 - EM do Ac-2-MeO (acetato de 4-acetoxi-2-metóxi-3-(3-metilbut-2-enil)-1-naftil)**.**



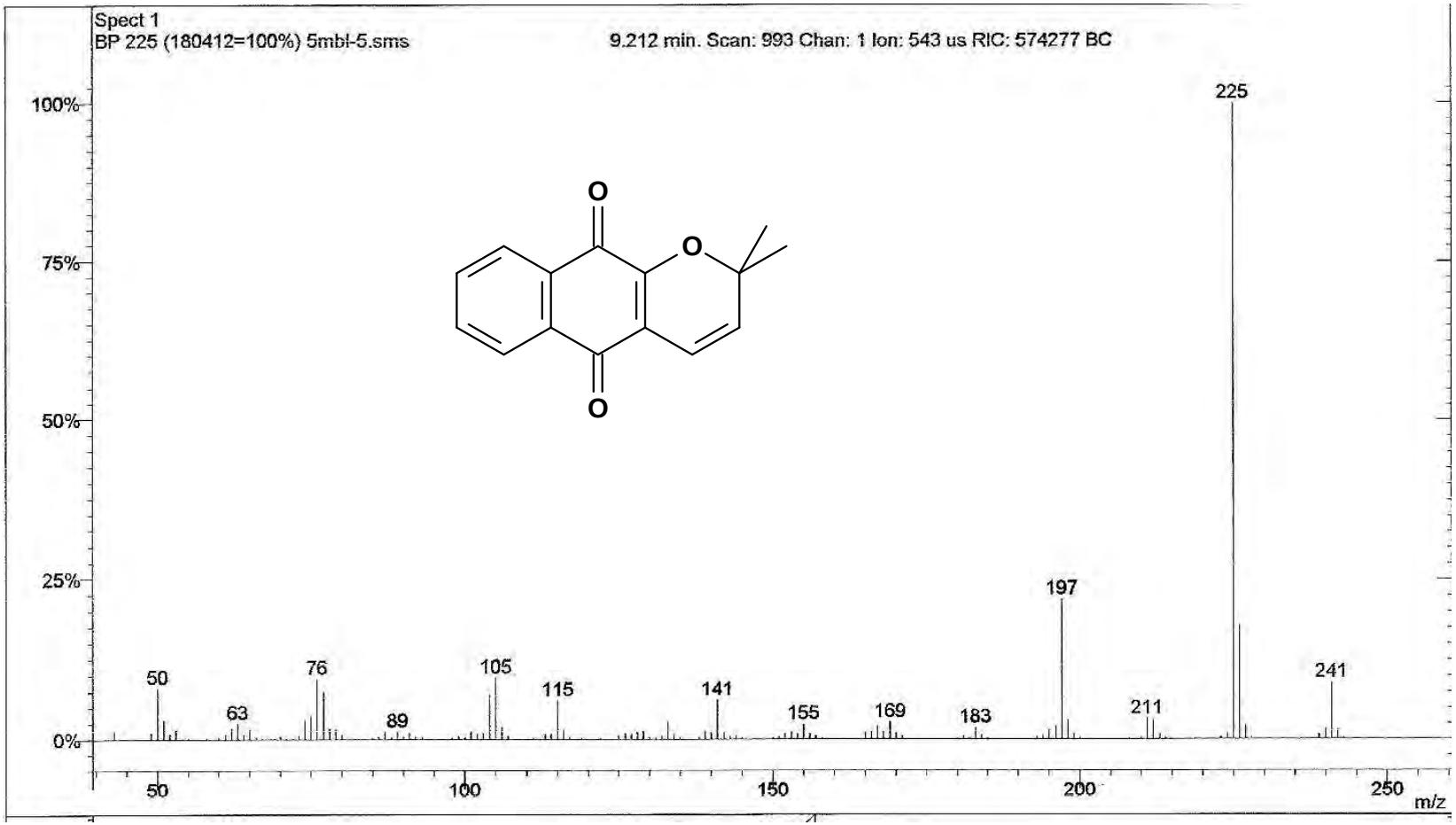
Espectro 142 - RMN ^{1}H (200 MHz) do Ac-2-MeO (acetato de 4-acetoxi-2-metóxi-3-(3--metilbut-2-enil)-1-naftil)**.**



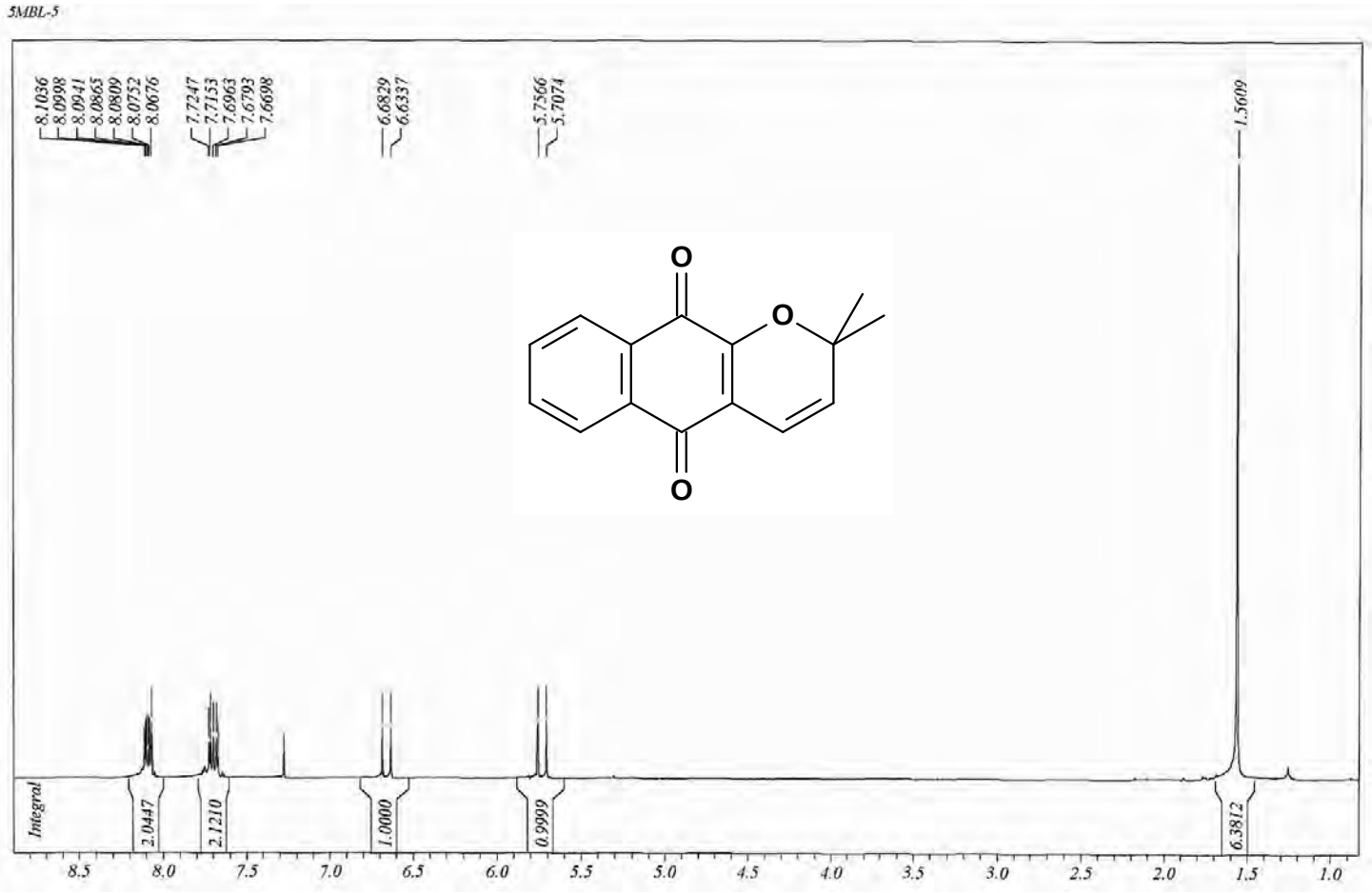
Espectro 143 - RMN ^{13}C (50,3 MHz) do Ac-2-MeO (acetato de 4-acetoxi-2-metóxi-3-(3--metilbut-2-enil)-1-naftil).



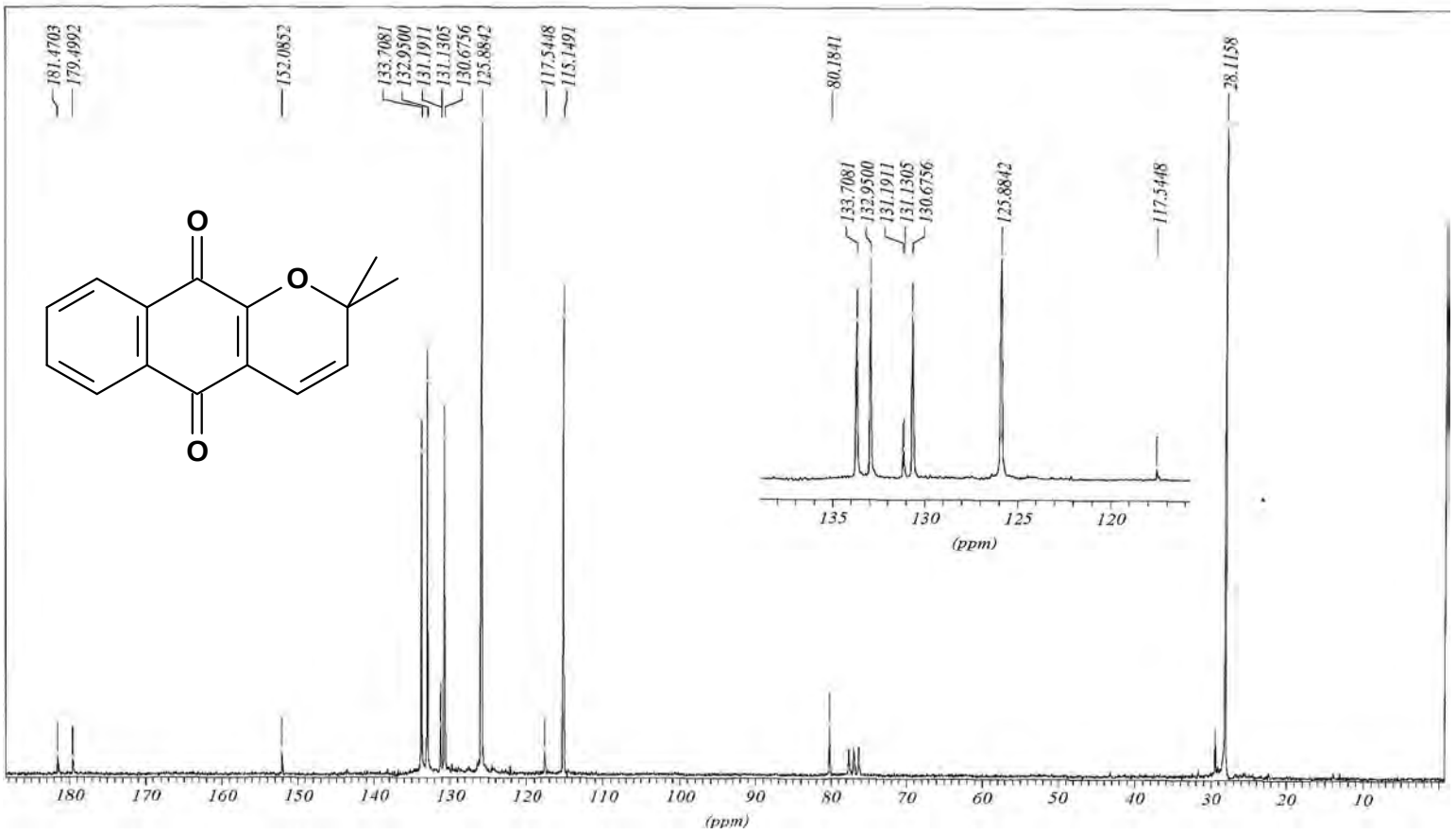
Espectro 144 - IV da xiloidona (2,2-dimetil-2H-benzo[g]cromeno-5,10-diona).



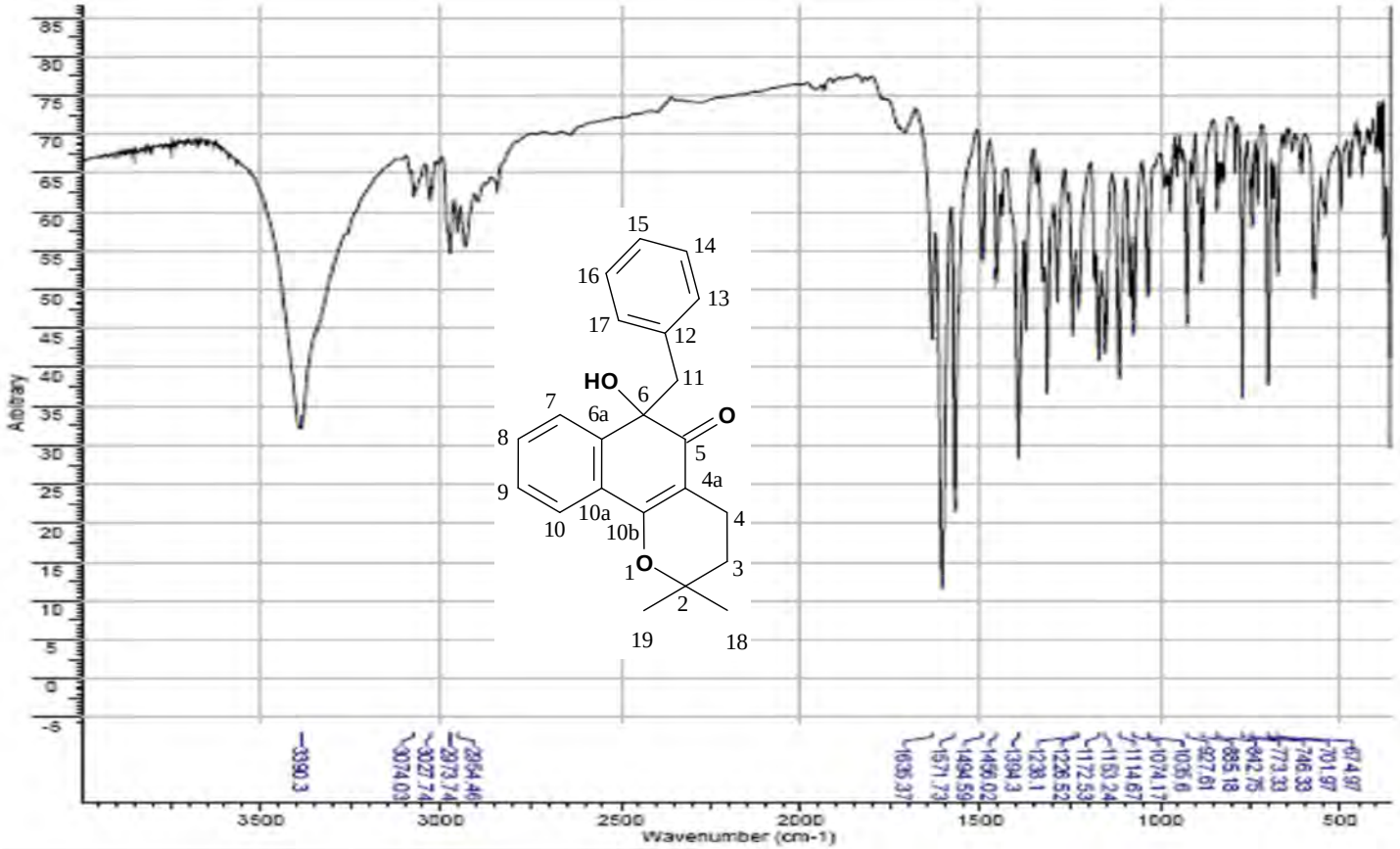
Espectro 145 – EM da xiloidona (2,2-dimetil-2H-benzo[g]cromeno-5,10-diona).



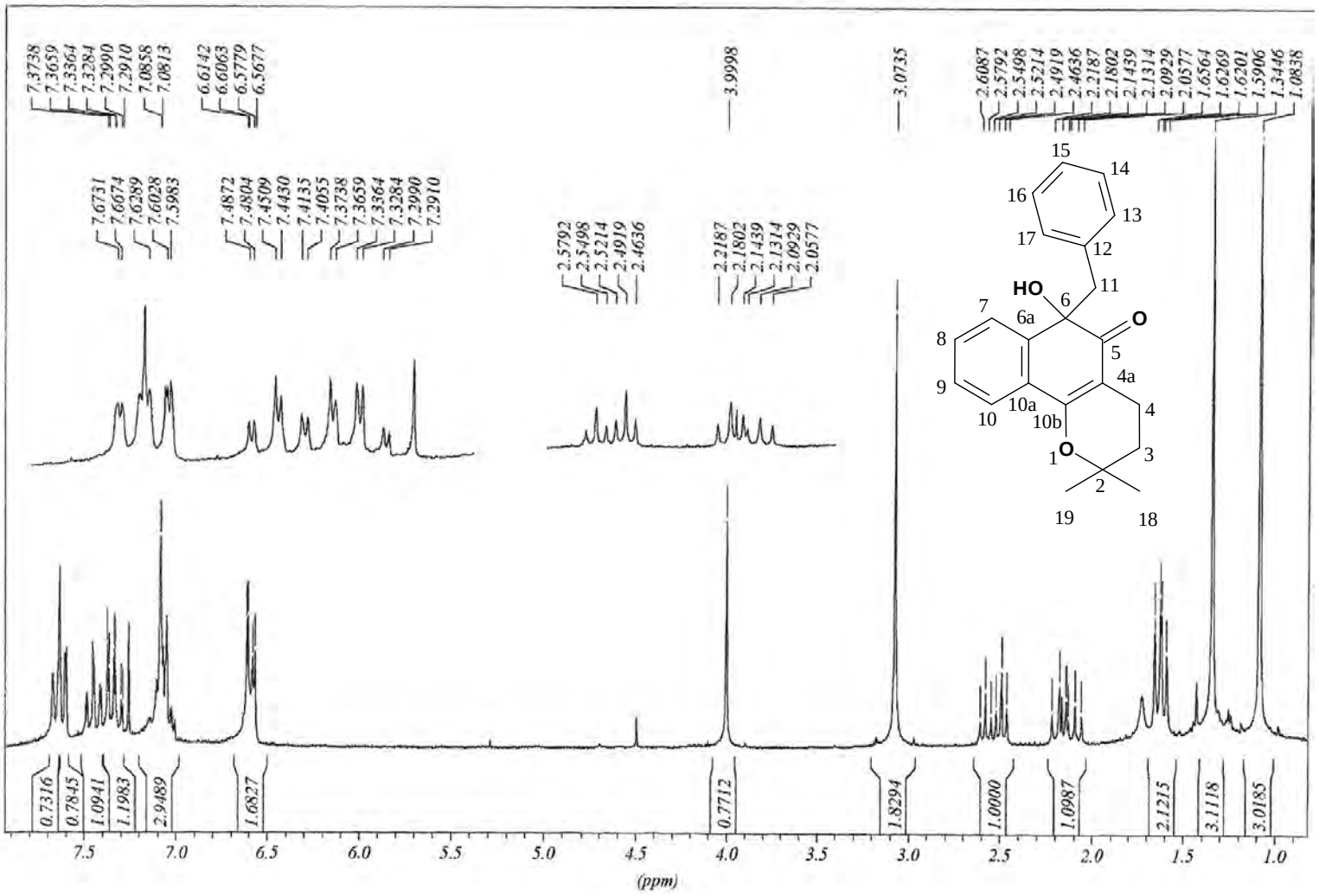
Espectro 146 - RMN ^{1}H (200MHz) da α-xiloidona (2,2-dimetil-2H-benzo[g]cromeno-5,10-diona).



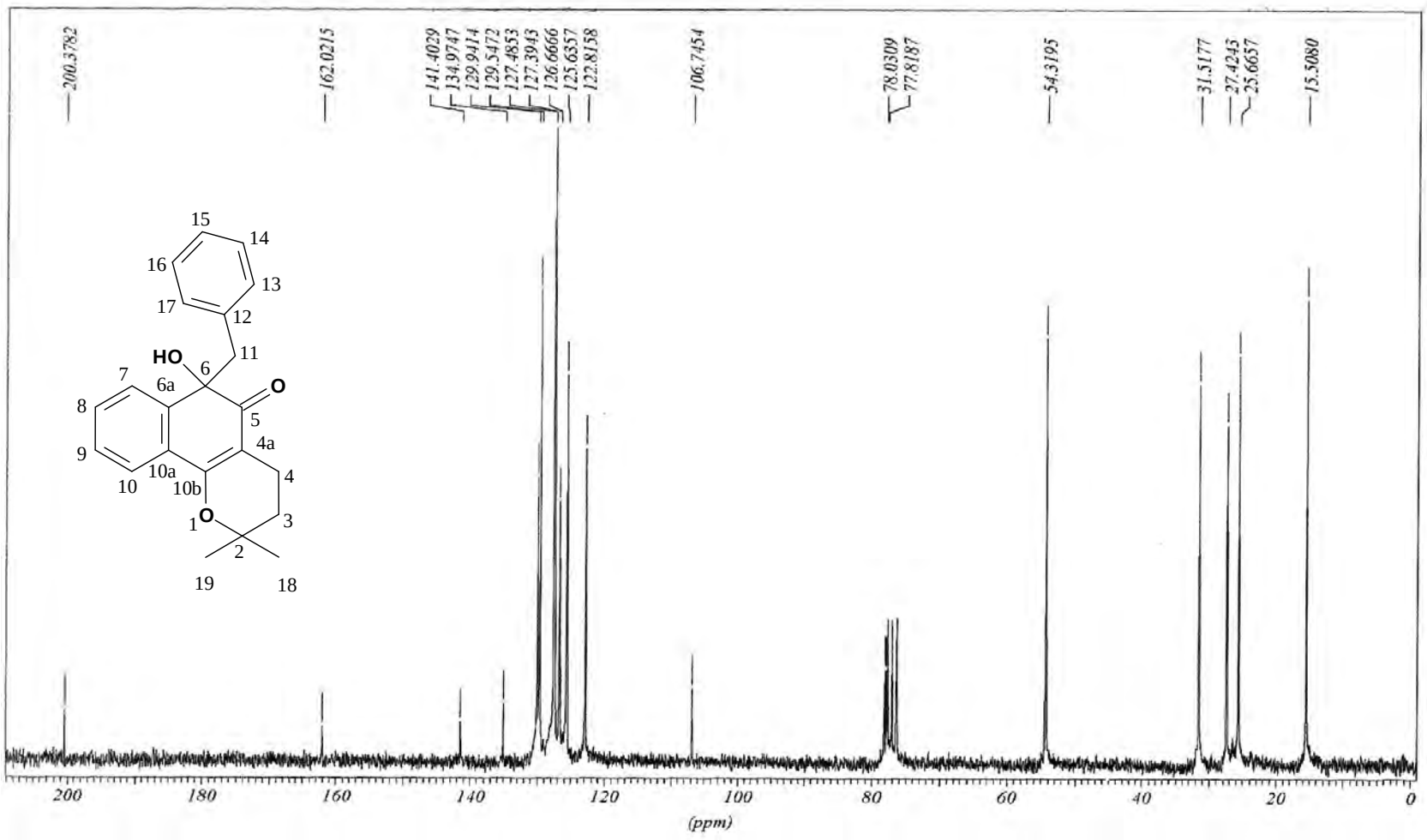
Espectro 147 - RMN ^{13}C (50,3 MHz) da α-xiloidona (2,2-dimetil-2H-benzo[g]cromeno-5,10-diona).



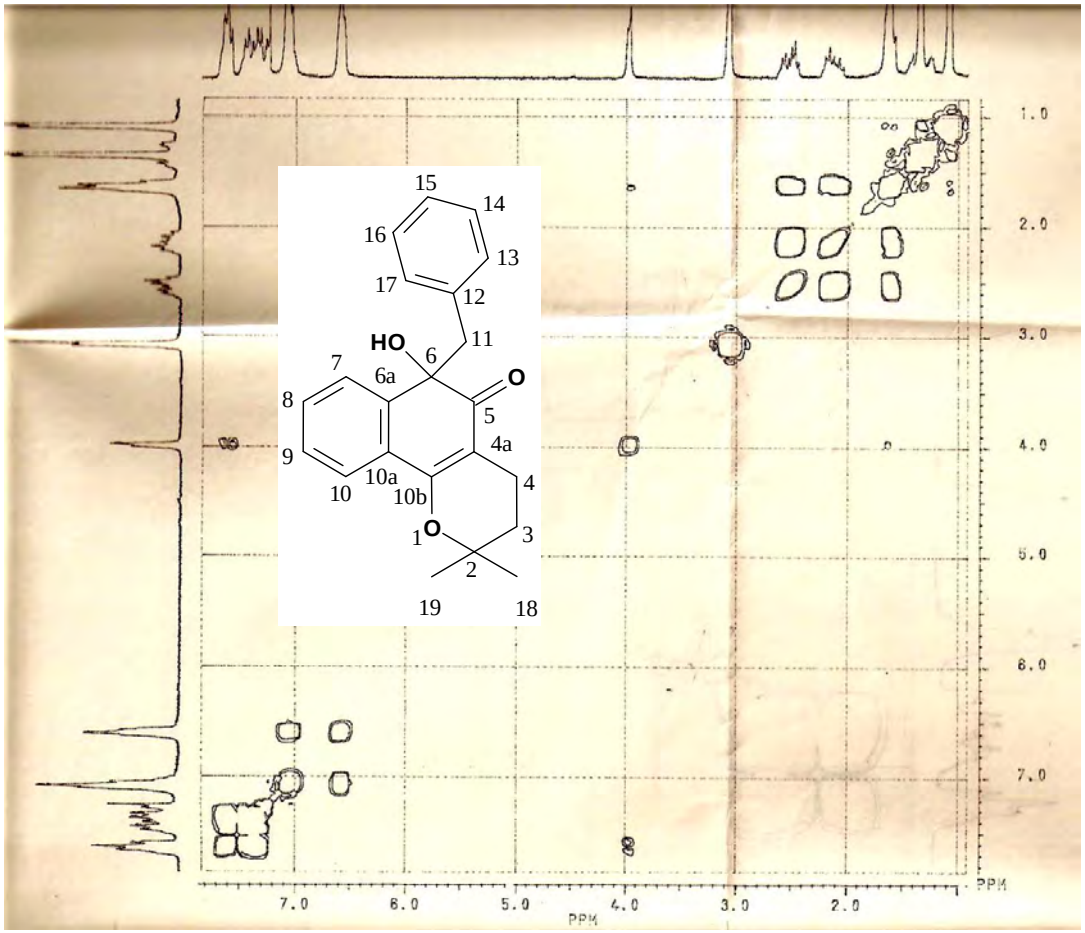
Espectro 148 - IV do BALE (6-benzil-6-hidroxi-2,2-dimetil-2,3,4,6-tetra-hidro-5H-benzo[h] cromen-5-ona).



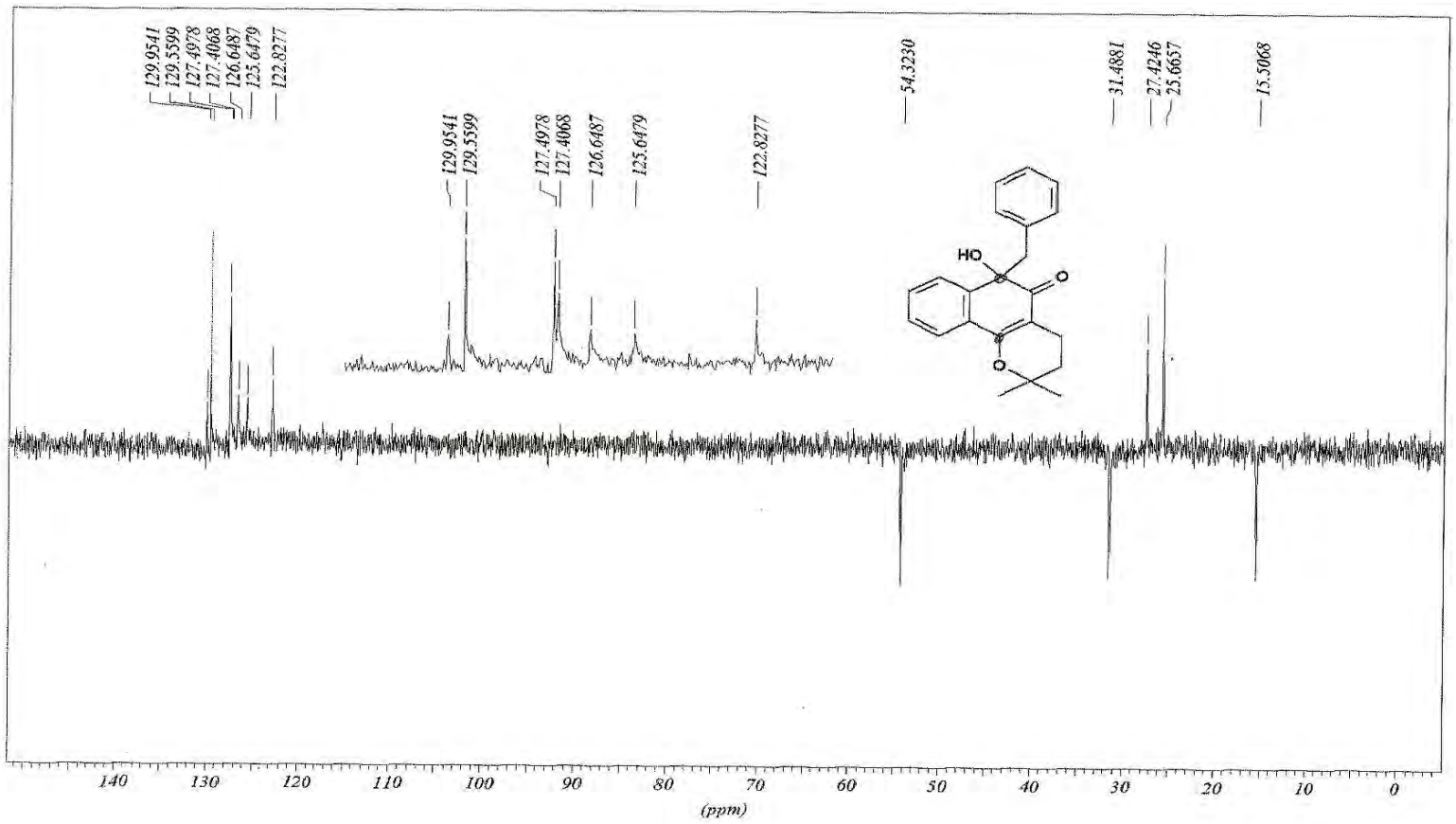
Espectro 149 - RMN ^{1}H (200 MHz) do BALE (6-benzil-6-hidroxi-2,2-dimetil-2,3,4,6-tetra-hidro-5H-benzo[h] cromen-5-ona)**.**



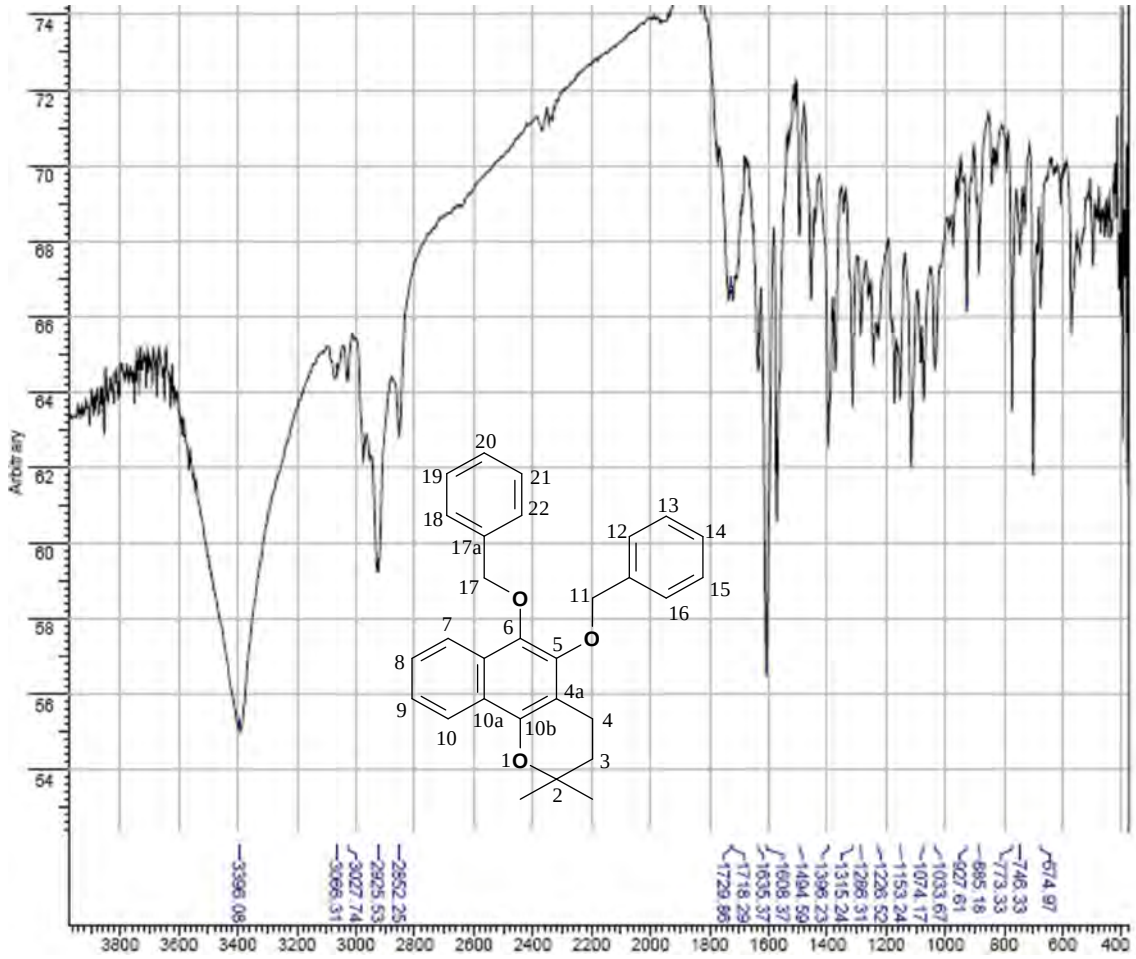
Espectro 150 - RMN ^{13}C (50,3 MHz) do BALE (6-benzil-6-hidroxi-2,2-dimetil-2,3,4,6-tetra-hidro-5H-benzo[h] cromen-5-ona)**.**



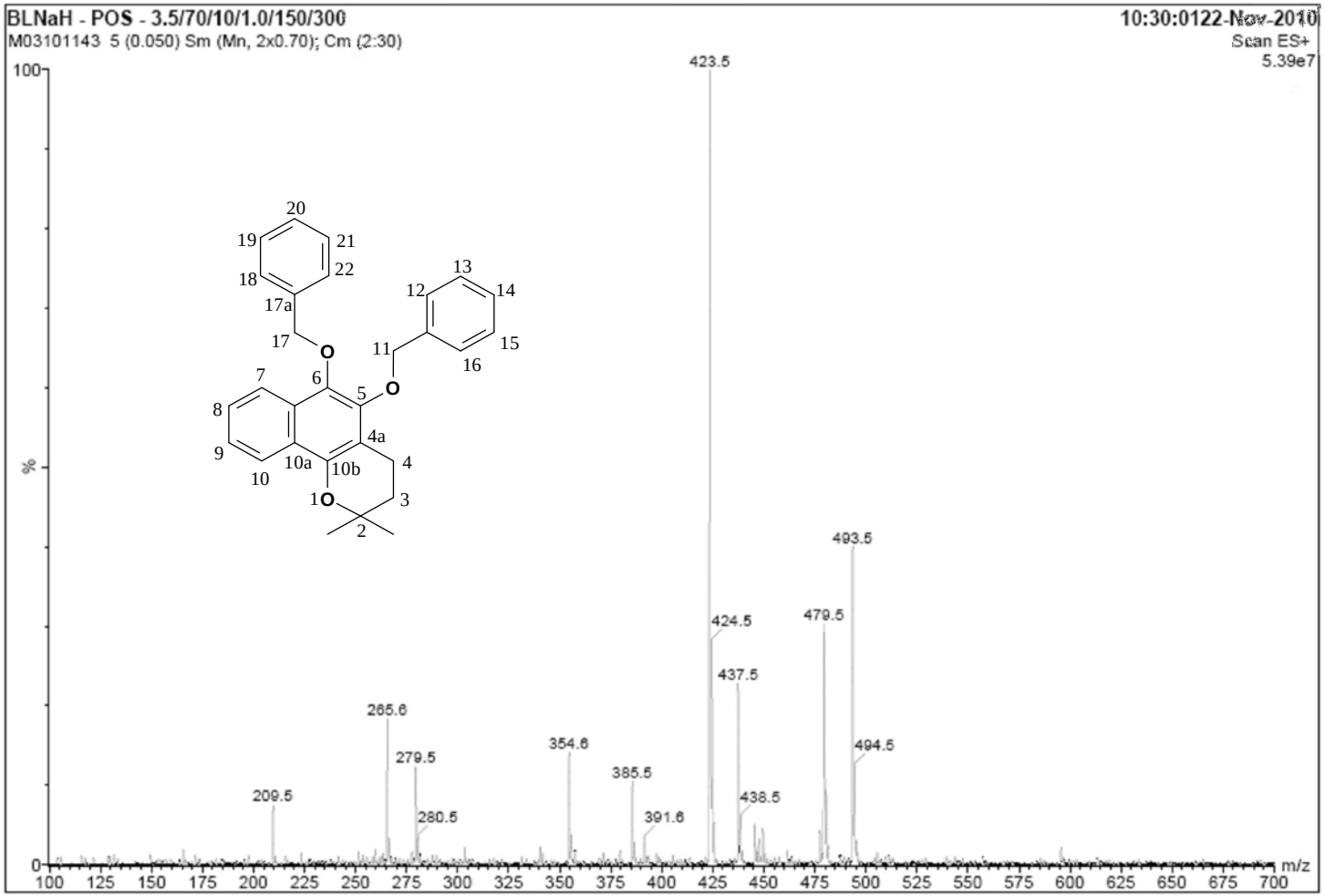
Espectro 151 - HOMOCOSY ^{1}H x ^{1}H do BALE (6-benzil-6-hidroxi-2,2-dimetil-2,3,4,6-tetra-hidro-5H-benzo[h] cromen-5-ona)**.**



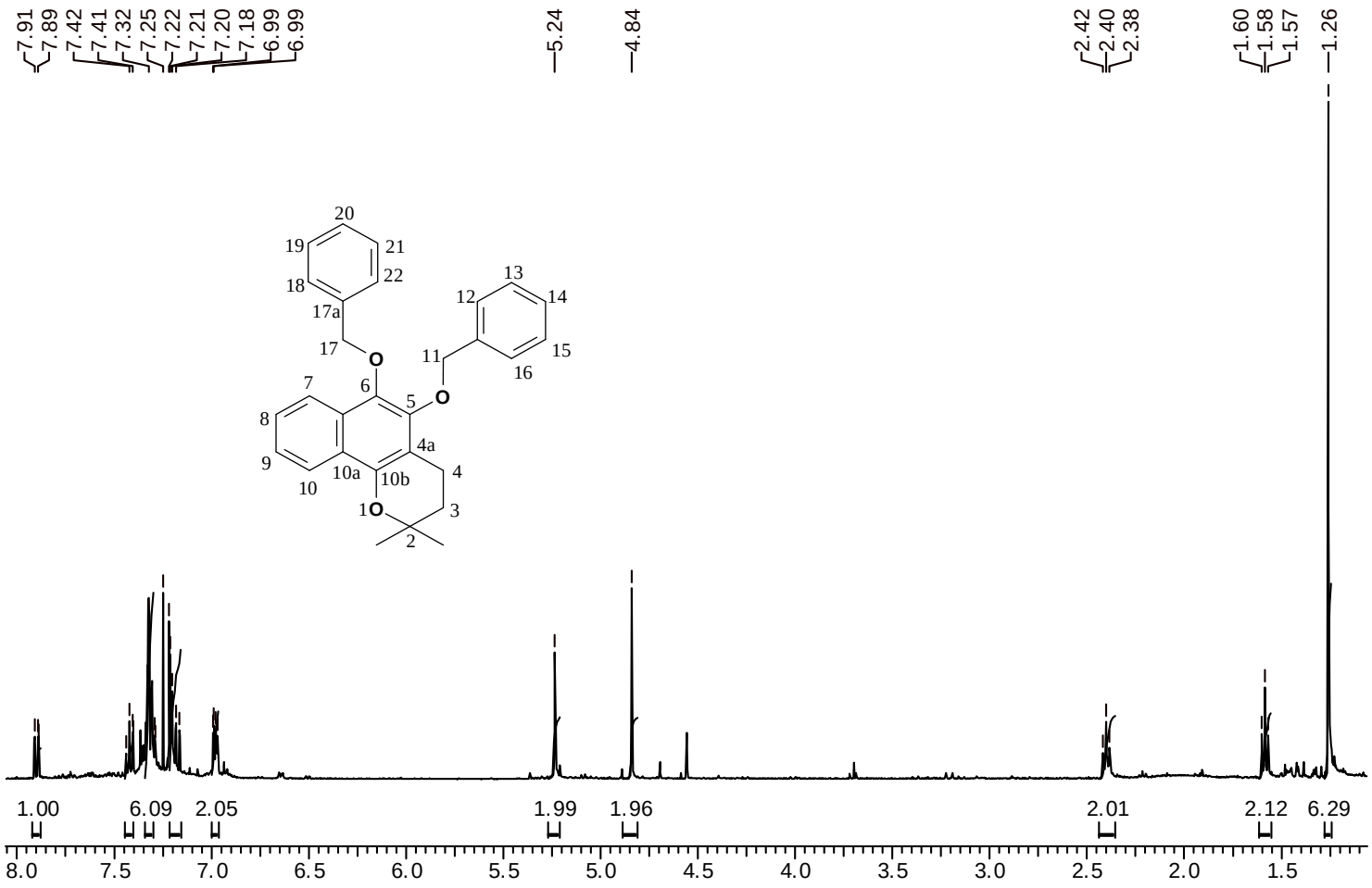
Espectro 152 - DEPT 135º do BALE (6-benzil-6-hidroxi-2,2-dimetil-2,3,4,6-tetra-hidro-5H-benzo[h] cromen-5-ona)**.**



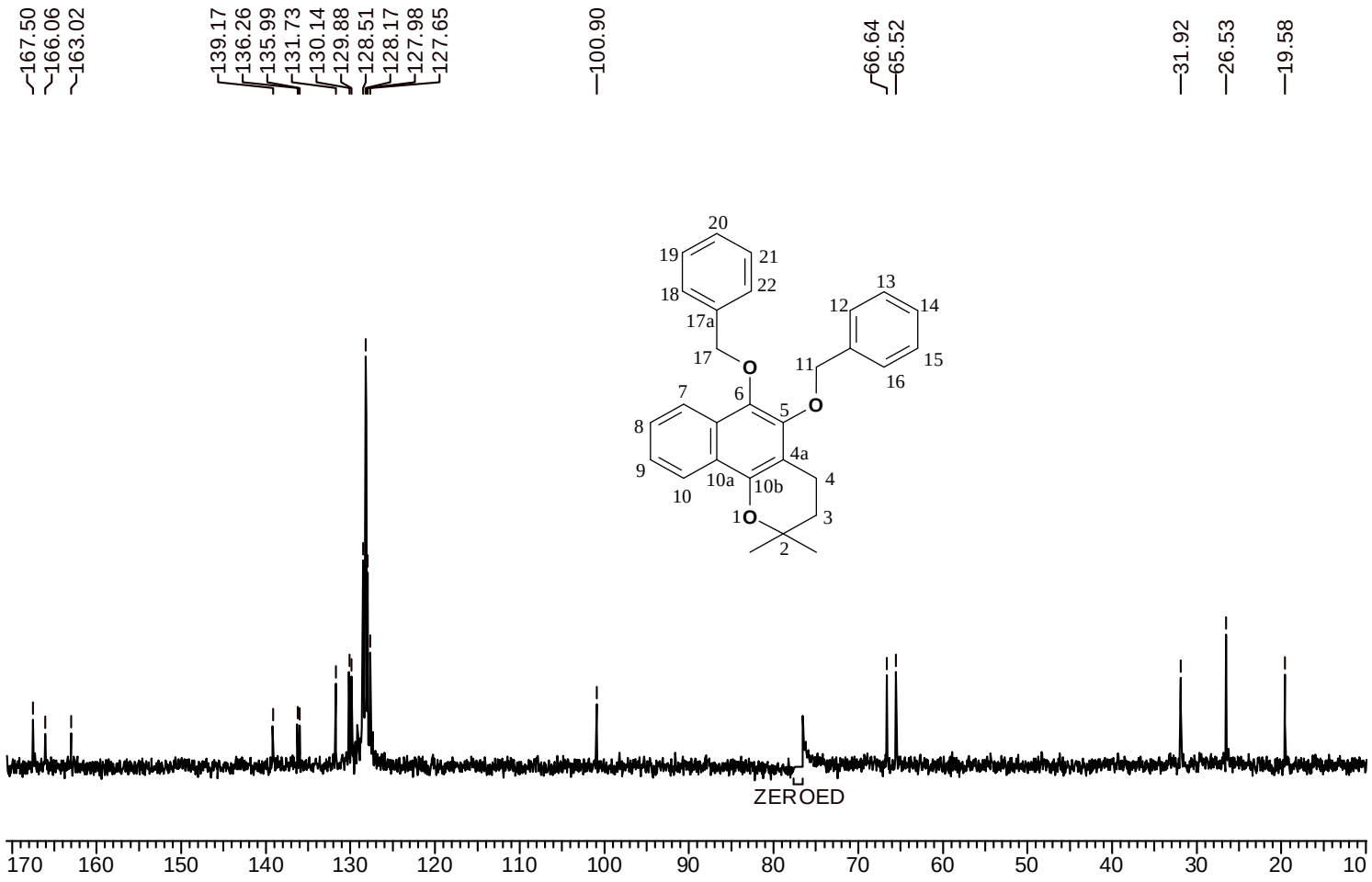
Espectro 153 – IV do BLNaH **(**5,6-bis(benziloxi)-2,2-dimetil-3,4-di-hidro-2*H*-benzo[*h*]cromeno)**.**



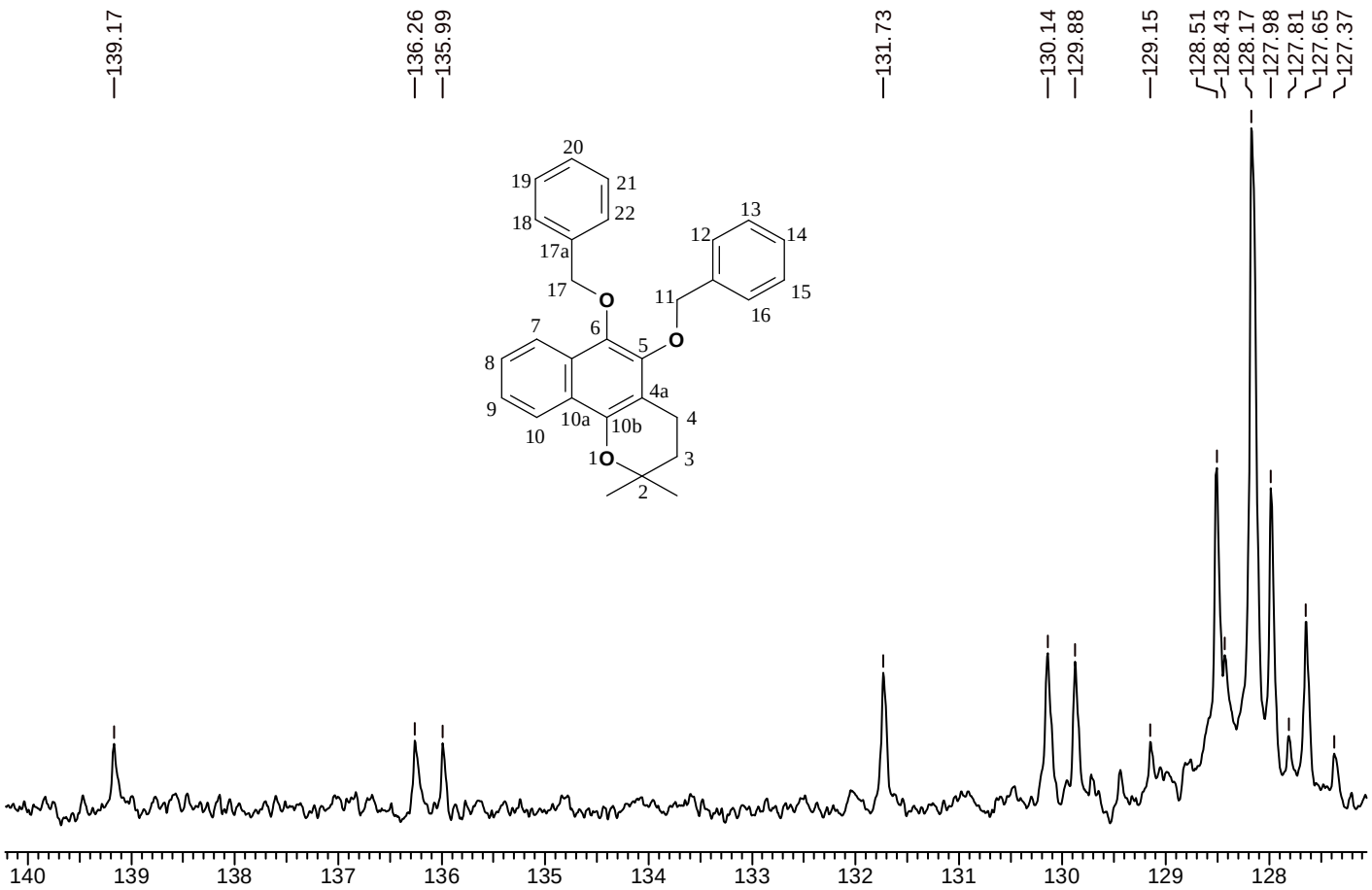
Espectro 154 – LCMS de BLNaH (5,6-bis(benziloxi)-2,2-dimetil-3,4-di-hidro-2*H*-benzo[*h*]cromeno)**.**



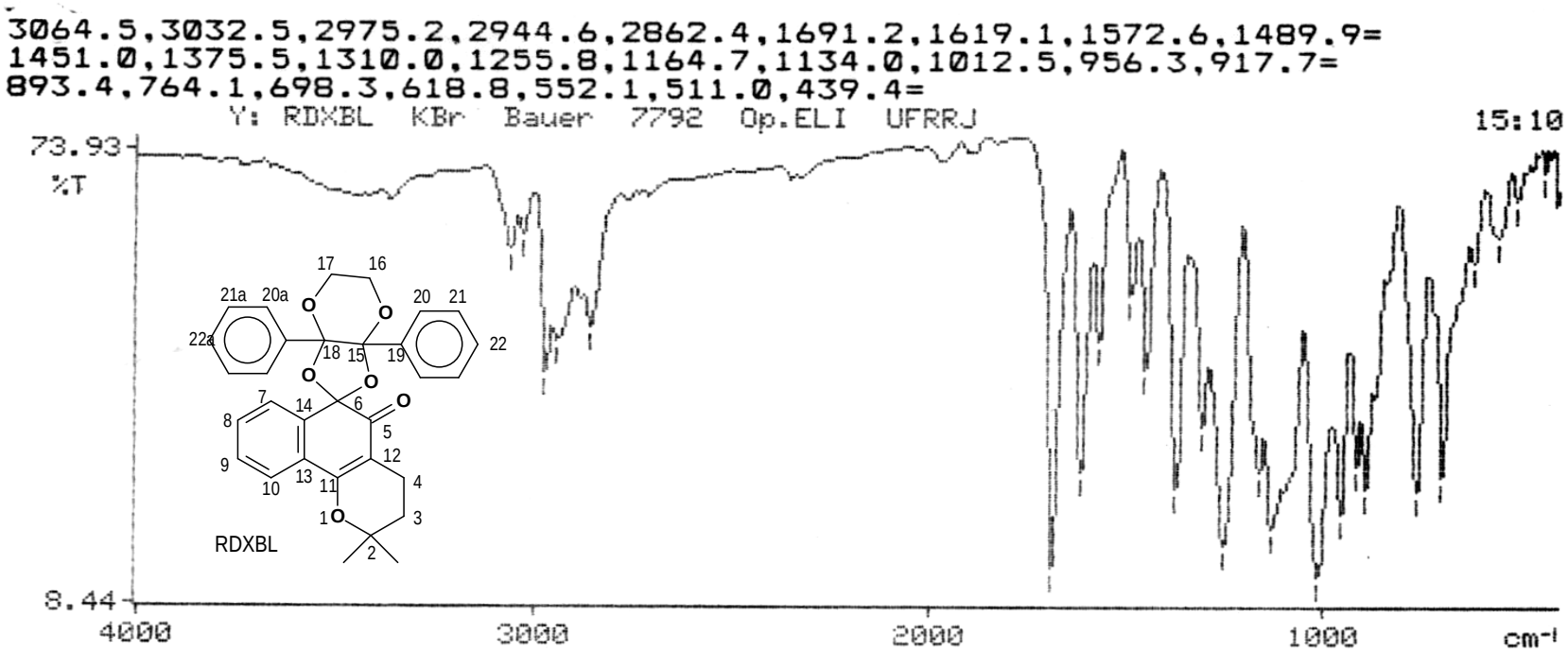
Espectro 155 - RMN ^{1}H (400 MHz) do BLNaH, **(**5,6-bis(benziloxi)-2,2-dimetil-3,4-di-hidro-2*H*-benzo[*h*]cromeno).



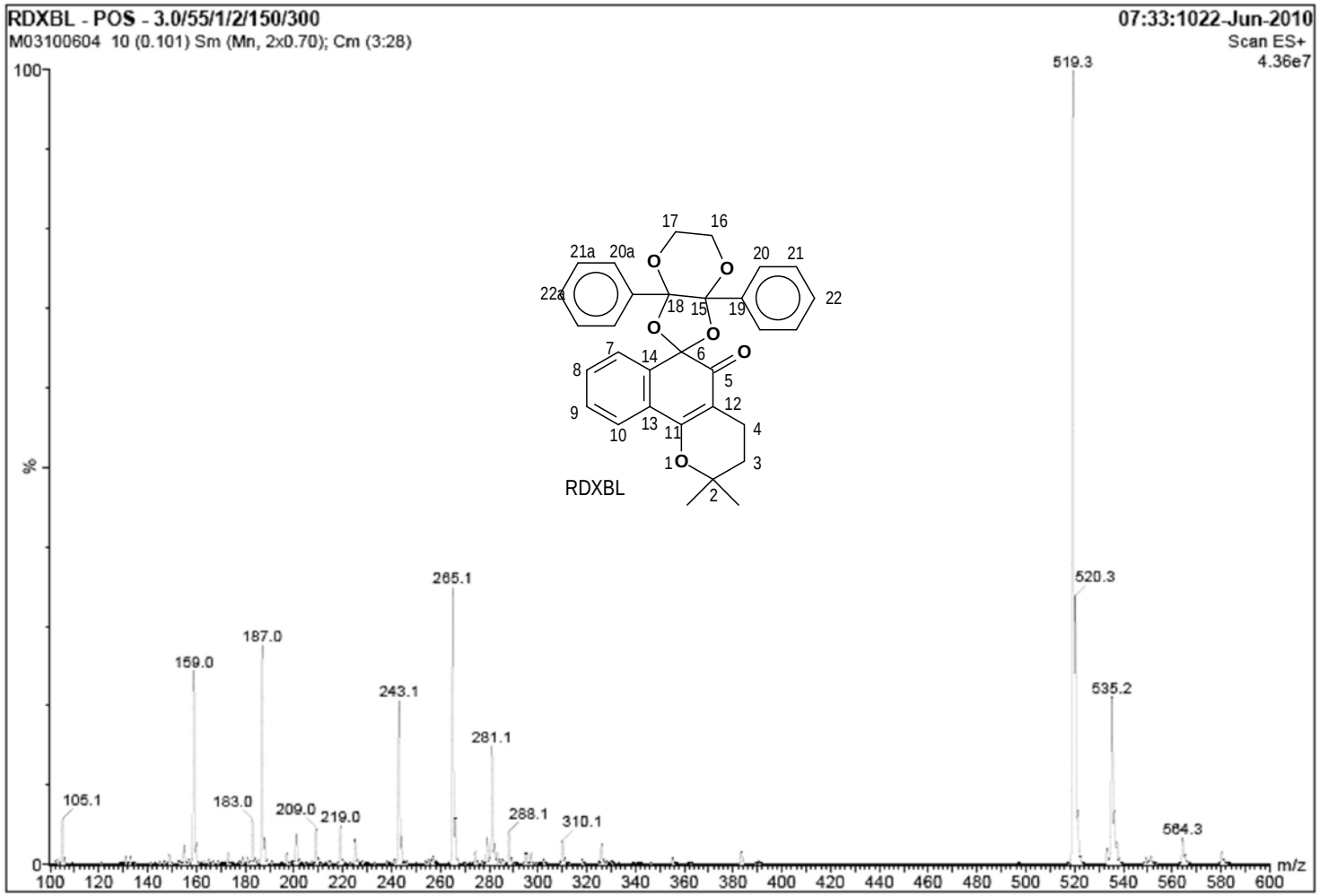
Espectro 156 - RMN ^{13}C (100,6 MHz) do BLNaH **(**5,6-bis(benziloxi)-2,2-dimetil-3,4-di-hidro-2*H*-benzo[*h*]cromeno).



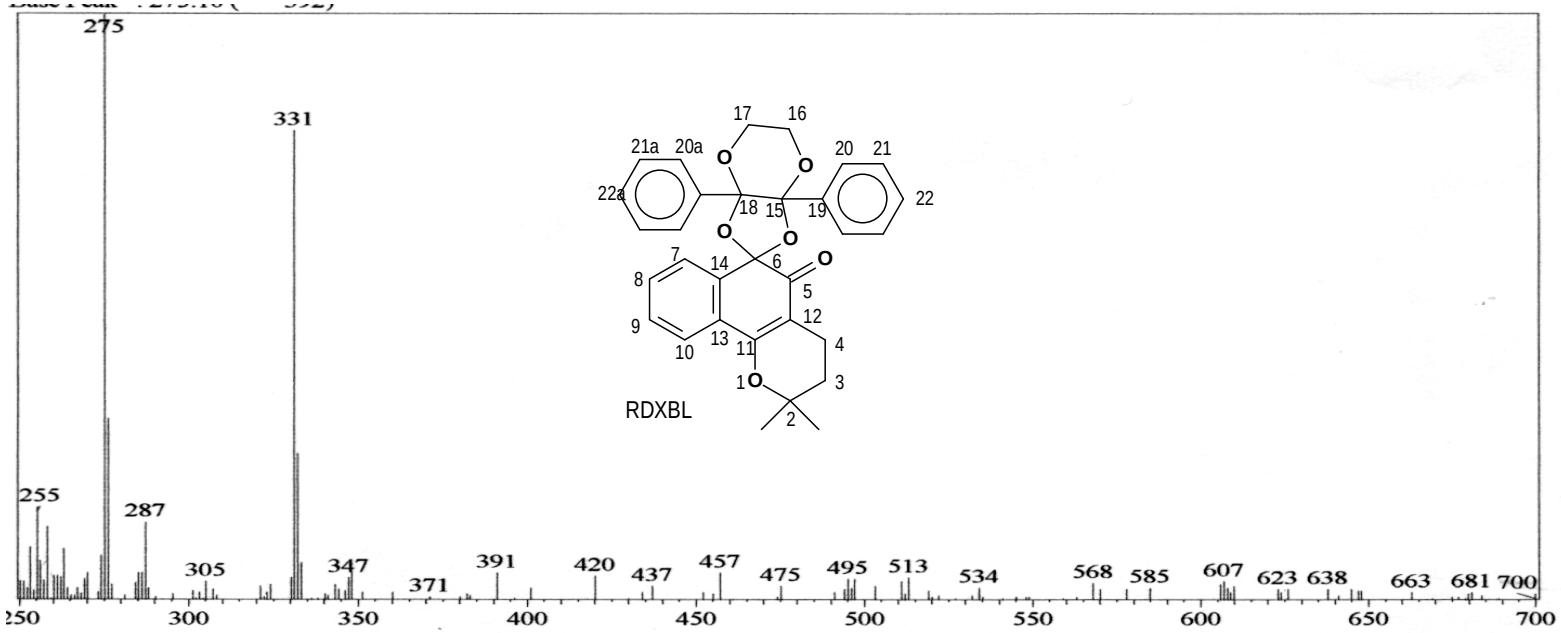
Espectro 157 – Ampliação, entre 126 e 140 ppm, do espectro de RMN ^{13}C do BLNaH **(**5,6-bis(benziloxi)-2,2-dimetil-3,4-di-hidro-2*H*-benzo[*h*]cromeno**).**



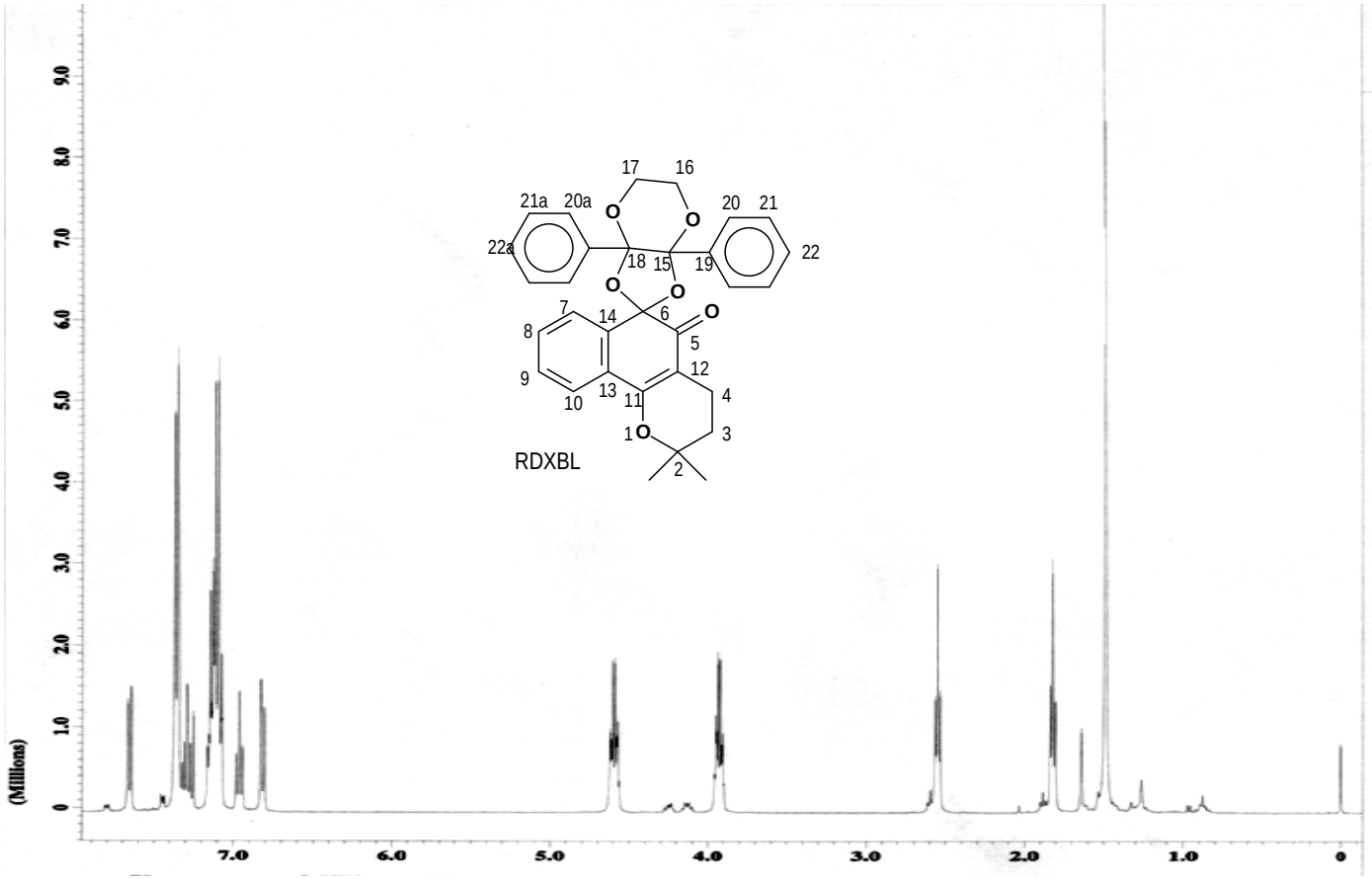
Espectro 158 - IV do RDXBL.



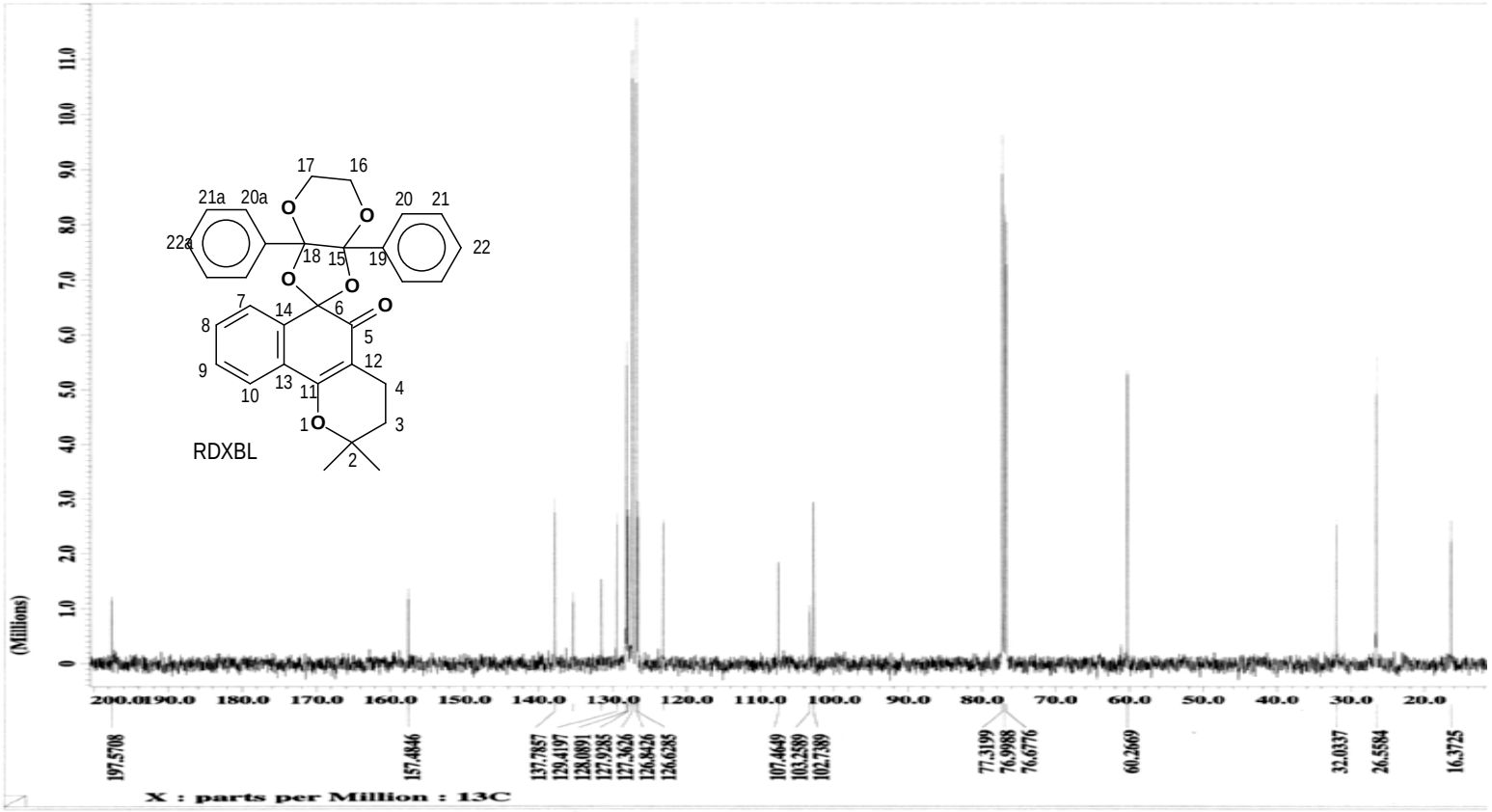
Espectro 159 – LCMS de RDXBL.



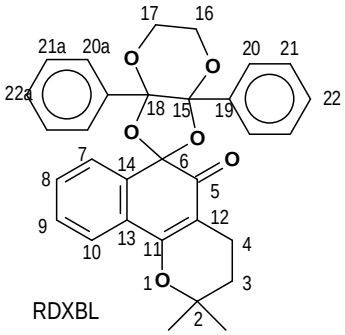
Espectro 160 – EM do RDXBL (2,2-dimetil-3a',7a'-di-fenil-3,3a',4,5',6',7a'-hexa-hidro-*2H,5H*-espiro[benzo[*h*]cromeno-6,2'-[1,3]dioxolo[4,5-*b*][1,4]dioxin]-5-ona).

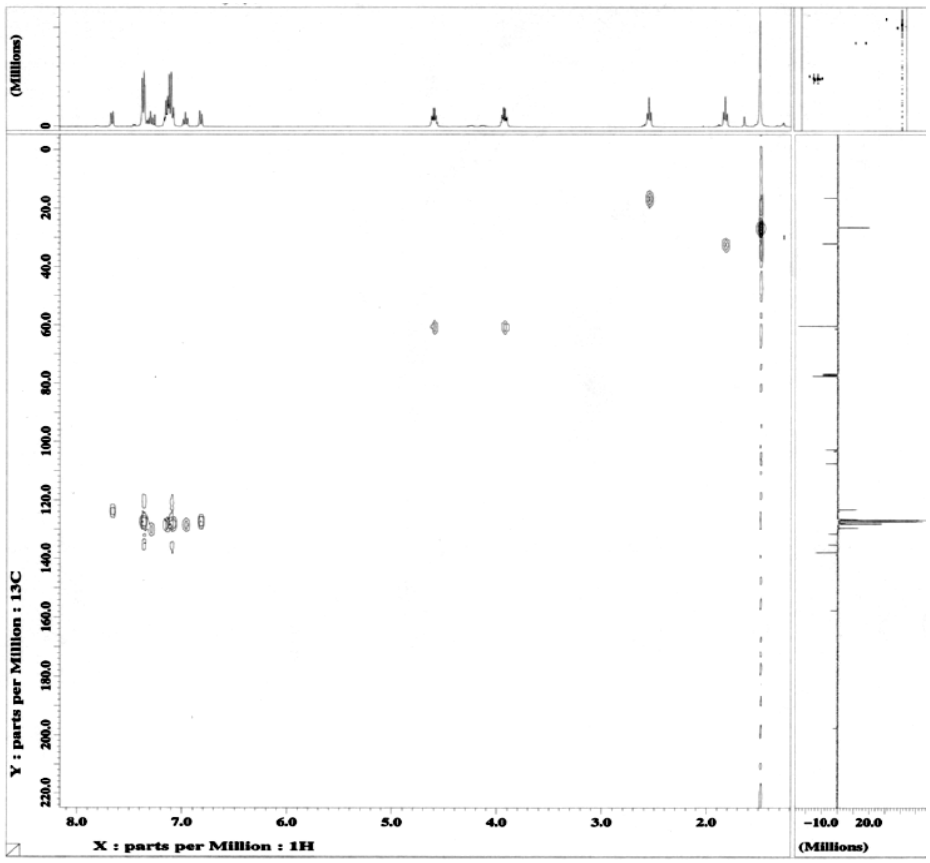


Espectro 161 - RMN ^{1}H (200 MHz) do RDXBL(2,2-dimetil-3a',7a'-di-fenil-3,3a',4,5',6',7a'-hexa-hidro-*2H,5H*-espiro[benzo[*h*]cromeno-6,2'-[1,3]dioxolo[4,5-*b*][1,4]dioxin]-5-ona)**.**

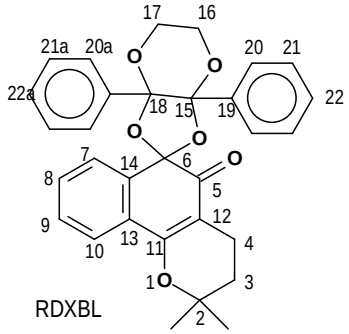


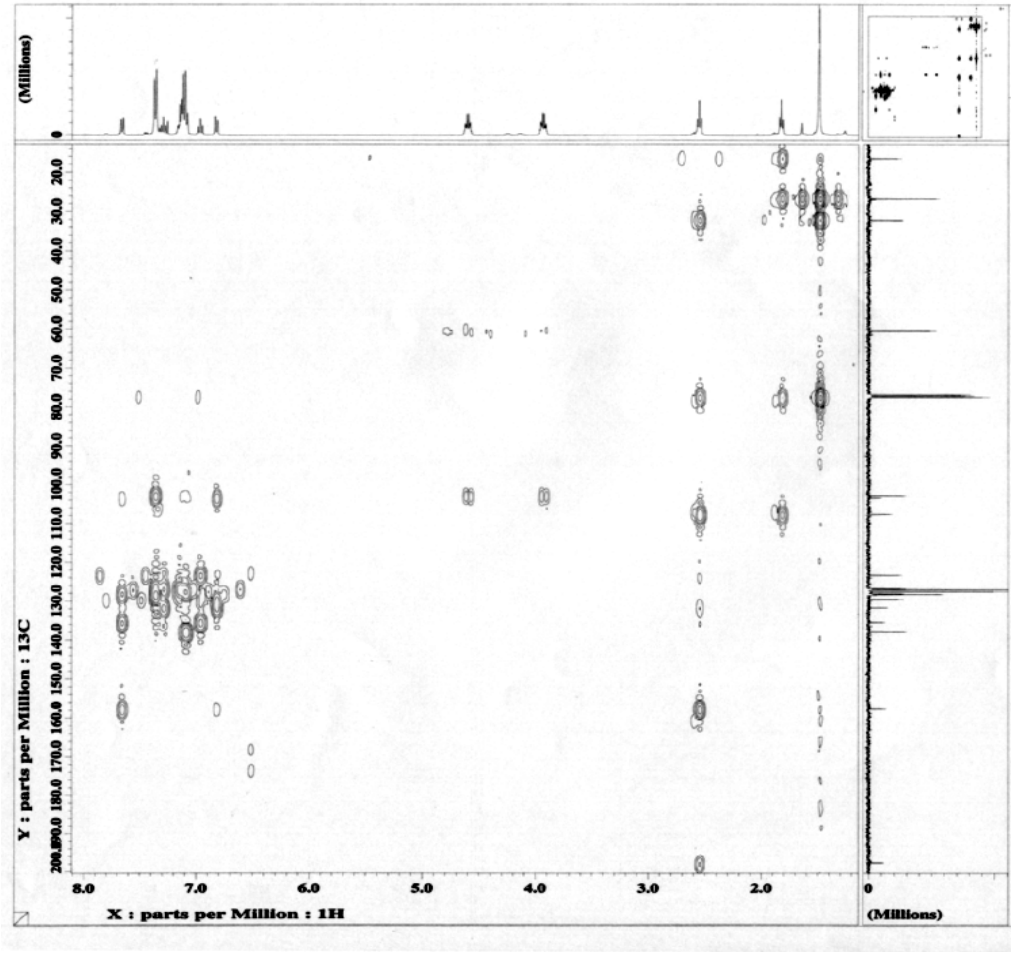
Espectro 162 - RMN ^{13}C (100,6 MHz) do RDXBL (2,2-dimetil-3a',7a'-di-fenil-3,3a',4,5',6',7a'-hexa-hidro-*2H*,*5H*-espiro[benzo[*h*]cromeno-6,2'-[1,3]dioxolo[4,5-*b*][1,4]dioxin]-5-ona).



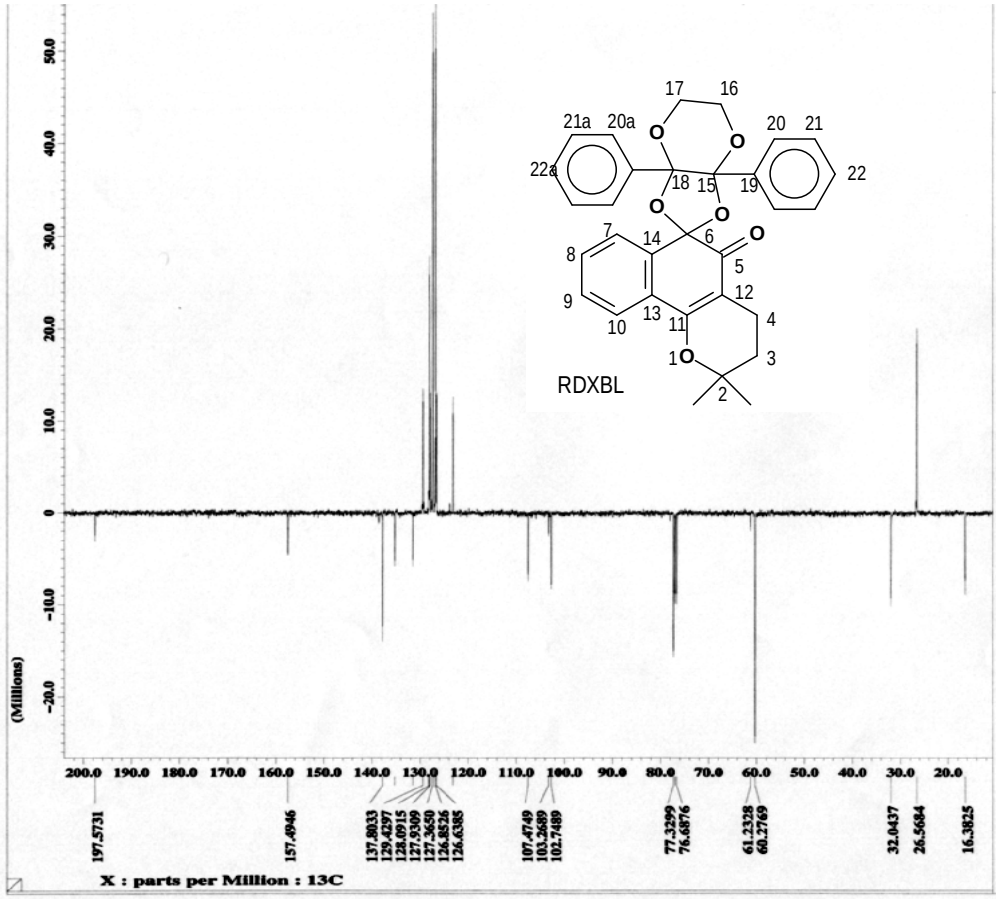


Espectro 163 - HMQC do RDXBL (2,2-dimetil-3a',7a'-di-fenil-3,3a',4,5',6',7a'-hexa-hidro-*2H,5H*-espiro[benzo[*h*]cromeno-6,2'-[1,3]dioxolo[4,5-*b*][1,4]dioxin]-5-ona)**.**





Espectro 164 - HMBC do RDXBL (2,2-dimetil-3a',7a'-di-fenil-3,3a',4,5',6',7a'-hexa-hidro-*2H,5H*-espiro[benzo[*h*]cromeno-6,2'-[1,3]dioxolo[4,5-*b*][1,4]dioxin]-5-ona)**.**



Espectro 165 – Experimento teste do próton ligado (APT) do RDXBL (2,2-dimetil-3a',7a'-di-fenil-3,3a',4,5',6',7a'-hexa-hidro-*2H,5H*-espiro[benzo[*h*]cromeno-6,2'-[1,3]dioxolo[4,5-*b*][1,4]dioxin]-5-ona)**.**