Experimental Section

General. Proton and Carbon nmr spectra were obtained in $CDCl_3$ and determined with a Mercury 400 spectrometer. Chemical shifts are expressed in ppm (δ) with respect to TMS as an internal standard. Electrospray ionisation mass spectra (ESI) were obtained using a MSD (Hewlett-Packards HPLC 1100 driven electrospray MS instrument). Products were purified by preparative chromatography with silica gel and ethylacetate as eluent. The purity was determined utilizing a Hewlett-Packard LC 1100 system (YMC column, 2 mm x 50 mm, 2 µm ODSA, 220 and 254 nm; 0,6 ml/min., 6 min. gradient from 90 % H_2O to 10 % H_2O (0,5% CH_3COOH) vs..CH_3CN.

General Procedure Passerini-Reaktion:

2 Mmol phenylglyoxal are dispensed in 4 ml diethyl ether. 2 Mmol diethylphosphonoacetic acid are added. After 5 min stirring at room temperature one gets a yellow clear solution. 2 Mmol *t*-butylisocyanide are added and stirring takes place over night. Evaporation of the solvent gives colorless foam.

General Procedure Horner-Wittig-Emmons-ring closure:

The reaction has to be performed under nitrogen atmosphere. 1,5 Mmol of the above Passerini product is dissolved in 60 ml THF, 4,5 mmol dry lithiumchlorid are added and stirred for 5 min at 0°C. After the salt is completely dissolved 15 mmol triethyl amine are added dropwise and stirred for another 15 min. at 0°C. Then the mixture is allowed to warm up to room temperature and additionally stirred for 4 h. The reaction mixture is flashed through a layer of silica gel and eluted with 60 ml ethyl acetate. The solvent is evaporated and the residue was crystallized in ethyl acetate to obtain colorless crystals.

One pot procedure:

Under nitrogen atmosphere 2 mmol phenylglyoxal are dissolved in 4 ml diethyl ether. To this solution 2 mmol diethylphosphonoacetic acid are added and stirred for 5 min. at room temperature, were one gets an yellow clear solution. To this solution 2 mmol *t*-butylisocyanid are added and stirred over night at room temperature. 60 ml THF and 4,5 mmol dry lithiumchlorid are added and stirred for 5 min at 0°C. After the salt is completely dissolved 15 mmol triethyl amine are added dropwise and stirred for another 15 min. at 0°C. Then the mixture is allowed to warm up to room temperature and stirred for 4 h. The reaction mixture is flashed through a layer of silica gel, eluted with 60 ml ethyl acetate. The solvent is evaporated and the residue was crystallized in ethyl acetate to obtain colorless crystals.

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S U P P L E M E N T A R Y M A T E R I A L

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BECB 0238-293

Compound 7 ($C_{21}H_{21}NO_3$)

B E L O N G I N G TO T H E P A P E R

A Three Component Butenolide Synthesis

by

Barbara Beck, Marina Magnin-Lachaux, Eberhardt Herdtweck, and Alexander Dömling

C o n t e n t s

Table S1 - Crystal Data and Details of the Structure Determination for **BECB 0238-293**

Crystal Data

Empirical Formula			C21 H21 N O3
Formula Weight			335.39
Crystal System			Orthorhombic
Space Group		Pbc21	(No. 29)
a, b, c [Å]	9.9119(3)	19.0265(7)	19.2249(5)
Alpha, Beta, Gamma [deg]	90	90	90
V [Å**3]			3625.6(2)
Z			8
D(obs), D(calc) [g/cm**3]			0.000, 1.229
F(000) [Electrons]			1424
Mu(MoKa) [/mm]			0.659
Crystal Size [mm]		0.15 x	0.25 x 0.28

Data Collection

Temperature (K)			293
Radiation [Å]	Sealed Tube	CuKa	1.54180
Theta Min-Max [Deg]			4.46, 70.09
Device			CAD4
Scan Type			Theta/2Theta
Scan Time [s]			240
Scan, [Deg]		1.50 + 0.15 Tan(Theta)	
Hor. and Vert. Aperture [mm]		2.00	4.00
Reference Reflection(s)	4 2 0;	0 8 0;	0 0 8
Dataset		0: 12 ; 0: 23 ; -23: 23	
Completeness of Dataset			100%
Tot., Uniq. Data, R(int)		6851, 6851,	0.000
Observed Data [Fo > 4.0 sigma(Fo)]			4592

Refinement

Nref, Npar			6851, 620
R1 [I > 2.0 sigma(I)]			0.0410
R1, wR2, S [all data]		0.1075, 0.1124,	1.040

Weighting Scheme : $w = 1 / [\text{sigma}^2(Fo^2)+(a*P)^2+b*P]$

with a: 0.0585; b: 0.1881; P: $[\text{Maximum}(0 \text{ or } Fo^2)+2*Fc^2]/3$

Extinction Parameter e = 0.0033(2)

$Fc(korr) = Fc*k*[1+0.001*e*Fc^2*\text{lambda}^3/\sin(2\text{Theta})]^{-1/4}$

Flack's Parameter -0.4(2)

Absolute structure cannot be determined reliably

Max. and Av. Shift/Error 0.00, 0.00

Min. and Max. Resd. Dens. [e/$Å^3$] -0.18, 0.16

Table S2 - Final Coordinates and Equivalent Isotropic Thermal Parameters of the non-Hydrogen atoms for **BECB 0238-293**

Atom	x	y	z	U(eq) [Å^2]
O1	0.7547(2)	0.19971(13)	0.18774(11)	0.0607(8)
O6	0.9400(2)	0.24507(18)	0.23614(15)	0.0908(12)
O8	0.5578(2)	0.29008(11)	0.13596(11)	0.0566(7)
N9	0.4084(2)	0.19917(14)	0.14377(12)	0.0452(8)
C2	0.6163(3)	0.19129(17)	0.20651(15)	0.0475(10)
C3	0.6044(3)	0.22271(14)	0.27760(14)	0.0440(8)
C4	0.7264(3)	0.24631(16)	0.29814(15)	0.0471(9)
C5	0.8215(3)	0.23206(19)	0.24107(18)	0.0593(11)
C7	0.5255(3)	0.23200(15)	0.15660(14)	0.0445(9)
C10	0.2878(3)	0.23040(16)	0.11063(17)	0.0530(10)
C11	0.2505(4)	0.2987(2)	0.1475(2)	0.0680(12)
C12	0.1739(4)	0.1769(3)	0.1217(3)	0.0793(18)
C13	0.3151(6)	0.2418(3)	0.0344(2)	0.0787(16)
C14	0.4713(3)	0.22915(15)	0.31065(14)	0.0451(9)
C15	0.3866(3)	0.1717(2)	0.31588(18)	0.0599(11)
C16	0.2582(4)	0.1796(2)	0.3427(2)	0.0733(16)
C17	0.2119(4)	0.2429(2)	0.3623(2)	0.0696(13)
C18	0.2935(4)	0.3013(2)	0.35744(18)	0.0676(14)
C19	0.4248(3)	0.29463(19)	0.33190(16)	0.0541(10)
C20	0.7674(3)	0.27759(15)	0.36512(17)	0.0495(9)
C21	0.6997(4)	0.2610(2)	0.42620(17)	0.0603(11)
C22	0.7374(4)	0.2893(2)	0.4890(2)	0.0713(14)
C23	0.8460(4)	0.3349(2)	0.4927(2)	0.0733(16)
C24	0.9145(4)	0.3513(2)	0.4333(2)	0.0727(14)
C25	0.8772(3)	0.32337(17)	0.3694(2)	0.0590(11)
O1'	0.6614(2)	0.45520(11)	0.27936(11)	0.0547(7)
O6'	0.7795(2)	0.50354(13)	0.36607(12)	0.0677(8)
O8'	0.5991(2)	0.54564(10)	0.17199(12)	0.0619(8)
N9'	0.5590(2)	0.45028(14)	0.10373(15)	0.0531(9)
C2'	0.6858(3)	0.43459(18)	0.20934(15)	0.0468(9)
C3'	0.8354(3)	0.44568(15)	0.19824(15)	0.0443(9)
C4'	0.8881(3)	0.47283(15)	0.25635(15)	0.0454(9)
C5'	0.7778(3)	0.48126(16)	0.30823(17)	0.0509(10)
C7'	0.6064(3)	0.48227(15)	0.15952(16)	0.0471(9)
C10'	0.5029(4)	0.48301(17)	0.04019(18)	0.0621(11)
C11'	0.6109(8)	0.5276(4)	0.0072(3)	0.109(3)
C12'	0.4612(11)	0.4251(3)	-0.0077(4)	0.114(3)
C13'	0.3818(8)	0.5288(5)	0.0601(4)	0.120(3)
C14'	0.8982(3)	0.43287(15)	0.12984(14)	0.0452(9)
C15'	0.8767(3)	0.37052(17)	0.09450(17)	0.0538(11)
C16'	0.9373(4)	0.3592(2)	0.03028(18)	0.0690(12)
C17'	1.0150(4)	0.4102(2)	0.00059(19)	0.0700(14)
C18'	1.0329(4)	0.4730(2)	0.03421(19)	0.0687(14)
C19'	0.9774(3)	0.48458(19)	0.09894(18)	0.0553(11)
C20'	1.0299(3)	0.49020(15)	0.27307(15)	0.0475(9)
C21'	1.1330(3)	0.44772(19)	0.24801(18)	0.0591(11)
C22'	1.2668(4)	0.4629(2)	0.2629(2)	0.0699(15)
C23'	1.2982(4)	0.5194(2)	0.3031(2)	0.0727(14)
C24'	1.1994(5)	0.5613(2)	0.3289(2)	0.0823(17)
C25'	1.0634(4)	0.5468(2)	0.3137(2)	0.0693(12)

U(eq) = 1/3 of the trace of the orthogonalized U

Table S3 - Hydrogen Atom Positions and Isotropic Thermal Parameters for **BECB 0238-293**

Atom	x	y	z	U(iso) [Å^2]
H21	0.591(3)	0.1418(18)	0.2071(16)	0.062(9)
H91	0.405(3)	0.1562(17)	0.1561(15)	0.045(8)
H111	0.246(4)	0.2891(19)	0.198(2)	0.077(11)
H112	0.178(5)	0.315(3)	0.121(3)	0.114(16)
H113	0.326(4)	0.341(2)	0.140(2)	0.096(13)
H121	0.156(5)	0.169(3)	0.172(3)	0.118(18)
H122	0.201(4)	0.135(2)	0.099(2)	0.092(14)
H123	0.102(5)	0.196(3)	0.100(3)	0.109(16)
H131	0.404(5)	0.273(3)	0.031(3)	0.106(16)
H132	0.232(5)	0.262(3)	0.014(3)	0.113(16)
H133	0.342(5)	0.197(3)	0.014(2)	0.098(14)
H151	0.418(3)	0.1251(19)	0.3016(18)	0.068(10)
H161	0.201(5)	0.139(3)	0.344(2)	0.112(16)
H171	0.120(4)	0.248(2)	0.387(2)	0.083(12)
H181	0.267(3)	0.3494(18)	0.3666(17)	0.059(9)
H191	0.488(4)	0.336(2)	0.3284(17)	0.069(10)
H211	0.634(3)	0.2267(17)	0.4287(17)	0.056(9)
H221	0.689(4)	0.2759(18)	0.532(2)	0.072(11)
H231	0.869(4)	0.3536(19)	0.539(2)	0.078(11)
H241	0.987(4)	0.385(2)	0.433(2)	0.099(14)
H251	0.923(3)	0.3362(16)	0.3276(19)	0.056(9)
H22	0.656(3)	0.3901(18)	0.2028(15)	0.052(9)
H92	0.567(3)	0.4055(17)	0.1057(17)	0.050(8)
H114	0.666(10)	0.500(5)	-0.017(5)	0.21(5)
H115	0.638(5)	0.562(3)	0.044(3)	0.112(17)
H116	0.571(5)	0.551(3)	-0.034(3)	0.115(16)
H124	0.547(5)	0.403(3)	-0.017(3)	0.096(18)
H125	0.427(5)	0.447(3)	-0.052(3)	0.120(17)
H126	0.385(7)	0.412(4)	0.012(4)	0.16(3)
H134	0.418(10)	0.575(5)	0.090(6)	0.26(5)
H135	0.338(9)	0.496(4)	0.069(5)	0.19(5)
H136	0.349(7)	0.550(3)	0.015(3)	0.15(2)
H152	0.823(3)	0.3355(18)	0.1171(17)	0.060(9)
H162	0.917(4)	0.313(2)	0.002(2)	0.089(12)
H172	1.054(4)	0.399(2)	-0.044(2)	0.077(11)
H182	1.089(4)	0.510(2)	0.009(2)	0.094(13)
H192	0.988(4)	0.527(2)	0.121(2)	0.092(14)
H212	1.113(3)	0.406(2)	0.2171(19)	0.080(11)
H222	1.337(4)	0.433(2)	0.243(2)	0.085(12)
H232	1.389(5)	0.529(2)	0.310(3)	0.113(16)
H242	1.215(4)	0.599(2)	0.355(2)	0.091(13)
H252	0.990(6)	0.583(3)	0.334(3)	0.127(17)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S4 - (An)isotropic Thermal Parameters for **BECB 0238-293**

Atom	U(1,1)	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
O1	0.0421(12)	0.0870(16)	0.0530(12)	-0.0084(11)	0.0062(9)	0.0085(11)
O6	0.0382(12)	0.149(3)	0.0851(18)	-0.0183(17)	0.0102(13)	-0.0096(15)
O8	0.0608(13)	0.0473(12)	0.0618(13)	0.0040(10)	-0.0014(10)	-0.0110(10)
N9	0.0483(13)	0.0391(13)	0.0482(13)	-0.0003(11)	-0.0022(11)	-0.0003(12)
C2	0.0387(15)	0.0516(18)	0.0521(17)	0.0006(14)	0.0044(13)	0.0002(14)
C3	0.0402(14)	0.0487(15)	0.0432(14)	0.0061(12)	0.0009(13)	0.0030(13)
C4	0.0413(15)	0.0540(16)	0.0461(16)	0.0058(13)	-0.0024(12)	0.0020(13)
C5	0.0441(17)	0.080(2)	0.0537(18)	-0.0020(17)	-0.0003(15)	0.0034(17)
C7	0.0487(16)	0.0424(15)	0.0425(14)	-0.0035(12)	0.0054(13)	-0.0031(13)
C10	0.0535(17)	0.0533(17)	0.0523(16)	-0.0064(15)	-0.0099(14)	0.0065(14)
C11	0.069(2)	0.067(2)	0.068(2)	-0.0116(19)	-0.014(2)	0.022(2)
C12	0.053(2)	0.080(3)	0.105(4)	-0.017(3)	-0.014(2)	-0.003(2)
C13	0.105(3)	0.080(3)	0.051(2)	-0.007(2)	-0.016(2)	0.024(3)
C14	0.0402(15)	0.0556(17)	0.0395(14)	0.0018(13)	-0.0002(12)	0.0015(13)
C15	0.0507(19)	0.064(2)	0.065(2)	-0.0052(17)	0.0078(16)	-0.0070(17)
C16	0.052(2)	0.084(3)	0.084(3)	-0.006(2)	0.0153(18)	-0.014(2)
C17	0.0446(17)	0.105(3)	0.0591(19)	0.002(2)	0.0088(17)	0.004(2)
C18	0.066(2)	0.084(3)	0.0527(19)	0.0000(18)	0.0055(17)	0.026(2)
C19	0.0554(19)	0.0573(19)	0.0497(16)	0.0027(14)	0.0033(15)	0.0067(16)
C20	0.0441(15)	0.0495(16)	0.0550(17)	0.0071(14)	-0.0056(15)	0.0072(13)
C21	0.054(2)	0.076(2)	0.0508(19)	0.0018(18)	-0.0040(15)	0.0018(18)
C22	0.071(2)	0.088(3)	0.055(2)	0.0022(19)	-0.004(2)	0.017(2)
C23	0.074(3)	0.076(3)	0.070(2)	-0.017(2)	-0.019(2)	0.024(2)
C24	0.060(2)	0.059(2)	0.099(3)	-0.016(2)	-0.023(2)	0.0023(18)
C25	0.0529(18)	0.0530(18)	0.071(2)	0.0027(17)	-0.0063(18)	-0.0001(15)
O1'	0.0461(11)	0.0651(13)	0.0530(11)	0.0005(10)	0.0063(9)	0.0014(10)
O6'	0.0719(14)	0.0786(16)	0.0526(12)	-0.0131(12)	0.0056(12)	0.0080(12)
O8'	0.0710(14)	0.0443(11)	0.0705(14)	-0.0042(10)	-0.0087(11)	0.0054(11)
N9'	0.0530(15)	0.0406(14)	0.0657(16)	0.0013(13)	-0.0150(13)	0.0026(12)
C2'	0.0410(15)	0.0476(17)	0.0519(17)	0.0041(14)	0.0008(13)	-0.0047(14)
C3'	0.0421(15)	0.0413(15)	0.0496(16)	0.0030(12)	-0.0016(13)	0.0048(13)
C4'	0.0439(15)	0.0445(15)	0.0479(16)	-0.0029(12)	-0.0019(12)	0.0043(13)
C5'	0.0520(17)	0.0494(16)	0.0514(17)	0.0019(15)	0.0004(14)	0.0075(14)
C7'	0.0377(15)	0.0444(16)	0.0592(18)	0.0030(14)	0.0018(13)	-0.0042(13)
C10'	0.067(2)	0.0542(19)	0.065(2)	0.0046(16)	-0.0193(18)	-0.0028(17)
C11'	0.135(5)	0.120(5)	0.071(3)	0.024(3)	-0.016(3)	-0.050(4)
C12'	0.166(7)	0.078(3)	0.098(4)	-0.003(3)	-0.072(5)	-0.009(4)
C13'	0.092(4)	0.135(6)	0.132(5)	0.018(5)	-0.038(4)	0.049(4)
C14'	0.0385(14)	0.0504(16)	0.0466(15)	0.0021(13)	-0.0031(12)	0.0014(13)
C15'	0.0516(17)	0.0543(19)	0.0555(19)	-0.0046(15)	0.0022(15)	-0.0087(15)
C16'	0.072(2)	0.080(2)	0.055(2)	-0.0170(19)	0.0037(18)	-0.0055(19)
C17'	0.065(2)	0.095(3)	0.0501(19)	-0.002(2)	0.0060(18)	-0.003(2)
C18'	0.062(2)	0.083(3)	0.061(2)	0.019(2)	0.0059(18)	-0.0086(19)
C19'	0.0533(19)	0.0546(19)	0.058(2)	0.0059(17)	-0.0025(15)	-0.0055(16)
C20'	0.0445(16)	0.0495(16)	0.0486(15)	-0.0042(14)	-0.0051(13)	0.0019(13)
C21'	0.0482(18)	0.063(2)	0.066(2)	-0.0111(17)	-0.0050(16)	0.0081(15)
C22'	0.0476(18)	0.082(3)	0.080(3)	0.000(2)	-0.0045(18)	0.0060(19)
C23'	0.050(2)	0.084(3)	0.084(2)	0.013(2)	-0.0077(19)	-0.011(2)
C24'	0.080(3)	0.075(3)	0.092(3)	-0.022(2)	-0.015(2)	-0.024(2)
C25'	0.059(2)	0.069(2)	0.080(2)	-0.0208(19)	-0.0044(19)	-0.0032(18)

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and h(i) are the Reflection Indices.

Table S5 - Bond Distances (Å) for **BECB 0238-293**

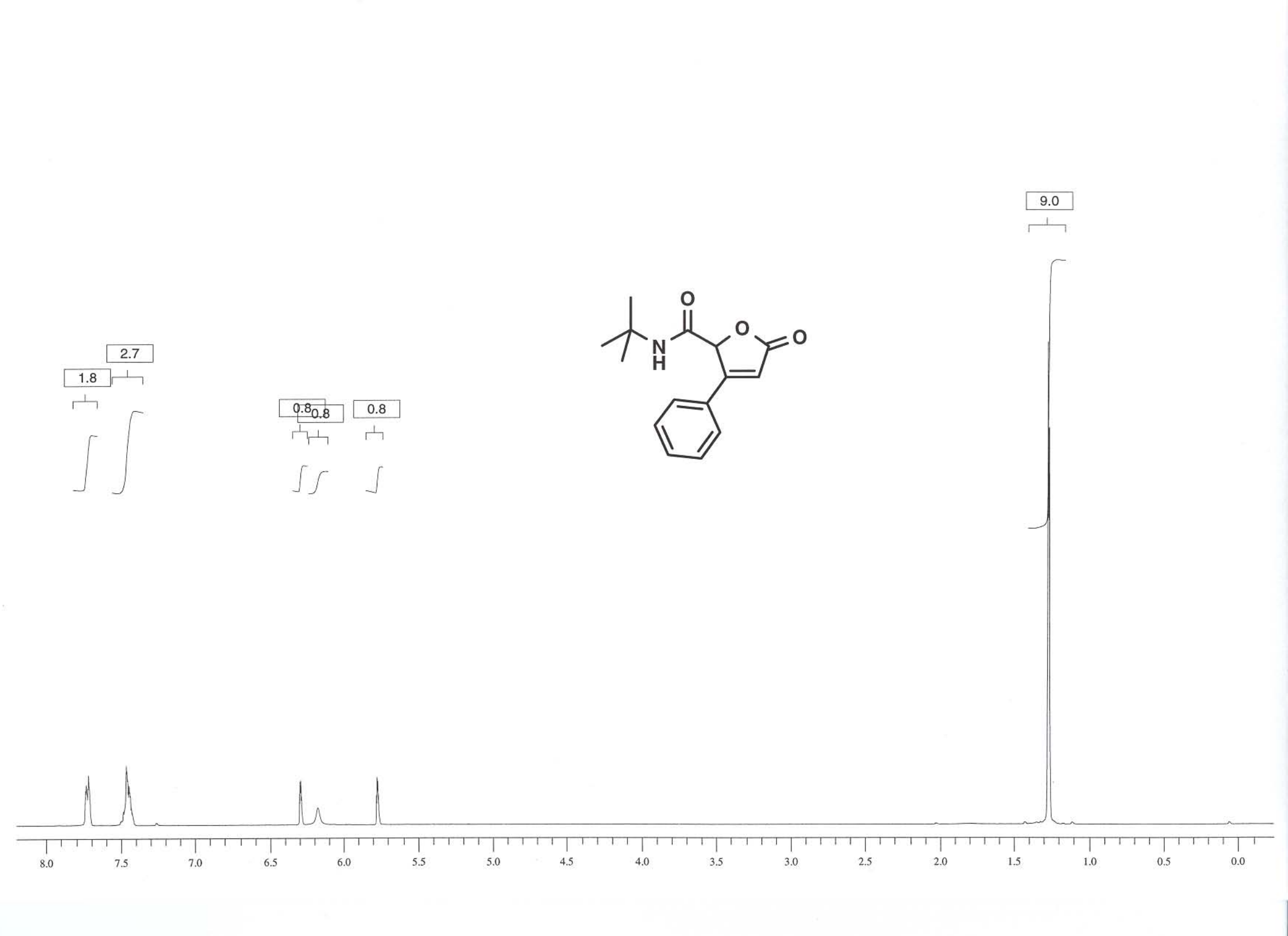
O1	-C2	1.427(4)	O1'	-C2'	1.423(4)
O1	-C5	1.367(4)	O1'	-C5'	1.373(4)
O6	-C5	1.204(4)	O6'	-C5'	1.190(4)
O8	-C7	1.217(4)	O8'	-C7'	1.231(3)
N9	-C10	1.479(4)	N9'	-C10'	1.480(4)
N9	-C7	1.341(4)	N9'	-C7'	1.320(4)
C2	-C7	1.527(4)	C2'	-C7'	1.536(4)
C2	-C3	1.496(4)	C2'	-C3'	1.513(4)
C3	-C14	1.469(4)	C3'	-C14'	1.475(4)
C3	-C4	1.349(4)	C3'	-C4'	1.337(4)
C4	-C20	1.476(4)	C4'	-C20'	1.479(4)
C4	-C5	1.472(4)	C4'	-C5'	1.489(4)
C10	-C11	1.526(5)	C10'	-C11'	1.506(8)
C10	-C12	1.535(6)	C10'	-C12'	1.494(8)
C10	-C13	1.506(5)	C10'	-C13'	1.532(9)
C14	-C19	1.390(5)	C14'	-C19'	1.392(4)
C14	-C15	1.382(5)	C14'	-C15'	1.384(4)
C15	-C16	1.381(5)	C15'	-C16'	1.390(5)
C16	-C17	1.343(5)	C16'	-C17'	1.364(5)
C17	-C18	1.378(5)	C17'	-C18'	1.370(5)
C18	-C19	1.397(5)	C18'	-C19'	1.378(5)
C20	-C25	1.396(4)	C20'	-C25'	1.371(5)
C20	-C21	1.389(5)	C20'	-C21'	1.389(4)
C21	-C22	1.374(5)	C21'	-C22'	1.387(5)
C22	-C23	1.384(6)	C22'	-C23'	1.360(5)
C23	-C24	1.365(5)	C23'	-C24'	1.357(6)
C24	-C25	1.389(5)	C24'	-C25'	1.407(6)
N9'	-H92	0.86(3)	N9	-H91	0.85(3)
C2	-H21	0.97(3)	C2'	-H22	0.91(3)
C11	-H111	0.99(4)	C11'	-H114	0.89(10)
C11	-H112	0.93(5)	C11'	-H115	1.00(6)
C11	-H113	1.11(4)	C11'	-H116	0.99(6)
C12	-H121	0.99(6)	C12'	-H124	0.97(5)
C12	-H122	0.95(4)	C12'	-H125	1.01(6)
C12	-H123	0.90(5)	C12'	-H126	0.88(7)
C13	-H131	1.06(5)	C13'	-H134	1.11(11)
C13	-H132	0.99(5)	C13'	-H135	0.78(8)
C13	-H133	0.98(5)	C13'	-H136	1.01(6)
C15	-H151	0.98(4)	C15'	-H152	0.96(3)
C16	-H161	0.96(5)	C16'	-H162	1.05(4)
C17	-H171	1.03(4)	C17'	-H172	0.96(4)
C18	-H181	0.97(3)	C18'	-H182	1.02(4)
C19	-H191	1.01(4)	C19'	-H192	0.92(4)
C21	-H211	0.92(3)	C21'	-H212	1.01(4)
C22	-H221	0.99(4)	C22'	-H222	0.98(4)
C23	-H231	0.99(4)	C23'	-H232	0.93(5)
C24	-H241	0.96(4)	C24'	-H242	0.89(4)
C25	-H251	0.95(3)	C25'	-H252	1.08(6)

Table S6 - Bond Angles (Degrees) for **BECB 0238-293**

C2	-O1	-C5	109.1(2)	C2'	-O1'	-C5'	109.8(2)
C7	-N9	-C10	126.3(3)	C7'	-N9'	-C10'	127.6(3)
C3	-C2	-C7	109.0(2)	C3'	-C2'	-C7'	109.4(2)
O1	-C2	-C7	110.5(2)	O1'	-C2'	-C7'	109.9(2)
O1	-C2	-C3	105.2(2)	O1'	-C2'	-C3'	105.2(2)
C4	-C3	-C14	130.6(3)	C4'	-C3'	-C14'	130.1(3)
C2	-C3	-C4	109.2(3)	C2'	-C3'	-C4'	108.6(3)
C2	-C3	-C14	119.9(2)	C2'	-C3'	-C14'	121.1(3)
C3	-C4	-C20	129.5(3)	C3'	-C4'	-C20'	129.7(3)
C5	-C4	-C20	123.3(3)	C5'	-C4'	-C20'	121.9(3)
C3	-C4	-C5	107.1(3)	C3'	-C4'	-C5'	108.3(3)
O1	-C5	-O6	120.4(3)	O1'	-C5'	-O6'	121.2(3)
O1	-C5	-C4	109.4(2)	O1'	-C5'	-C4'	107.9(3)
O6	-C5	-C4	130.2(3)	O6'	-C5'	-C4'	130.8(3)
N9	-C7	-C2	112.9(2)	N9'	-C7'	-C2'	114.6(3)
O8	-C7	-N9	126.2(3)	O8'	-C7'	-N9'	126.1(3)
O8	-C7	-C2	120.7(3)	O8'	-C7'	-C2'	119.1(3)
N9	-C10	-C13	109.4(3)	N9'	-C10'	-C13'	109.1(4)
C11	-C10	-C12	108.8(3)	C11'	-C10'	-C12'	110.6(5)
C11	-C10	-C13	111.9(3)	C11'	-C10'	-C13'	110.0(5)
C12	-C10	-C13	111.3(4)	C12'	-C10'	-C13'	110.9(6)
N9	-C10	-C11	109.7(3)	N9'	-C10'	-C11'	108.5(4)
N9	-C10	-C12	105.6(3)	N9'	-C10'	-C12'	107.6(4)
C3	-C14	-C15	120.7(3)	C3'	-C14'	-C15'	121.0(3)
C15	-C14	-C19	119.1(3)	C15'	-C14'	-C19'	118.9(3)
C3	-C14	-C19	120.0(3)	C3'	-C14'	-C19'	120.1(3)
C14	-C15	-C16	120.1(3)	C14'	-C15'	-C16'	120.2(3)
C15	-C16	-C17	121.1(4)	C15'	-C16'	-C17'	120.4(3)
C16	-C17	-C18	120.3(4)	C16'	-C17'	-C18'	119.7(3)
C17	-C18	-C19	119.8(3)	C17'	-C18'	-C19'	120.9(4)
C14	-C19	-C18	119.6(3)	C14'	-C19'	-C18'	119.8(3)
C4	-C20	-C21	120.9(3)	C4'	-C20'	-C21'	119.6(3)
C4	-C20	-C25	121.2(3)	C21'	-C20'	-C25'	118.4(3)
C21	-C20	-C25	117.9(3)	C4'	-C20'	-C25'	122.0(3)
C20	-C21	-C22	121.5(3)	C20'	-C21'	-C22'	120.7(3)
C21	-C22	-C23	120.2(4)	C21'	-C22'	-C23'	120.0(4)
C22	-C23	-C24	119.2(4)	C22'	-C23'	-C24'	120.5(4)
C23	-C24	-C25	121.4(4)	C23'	-C24'	-C25'	120.0(4)
C20	-C25	-C24	119.9(3)	C20'	-C25'	-C24'	120.3(3)

Table S6 (cont.) - Bond Angles (Degrees) for **BECB 0238-293**

C10	-N9	-H91	118(2)	C10'	-N9'	-H92	119(2)
C7	-N9	-H91	115(2)	C7'	-N9'	-H92	113(2)
O1	-C2	-H21	111.0(18)	O1'	-C2'	-H22	109.5(19)
C7	-C2	-H21	110.2(18)	C7'	-C2'	-H22	107.4(19)
C3	-C2	-H21	110.8(18)	C3'	-C2'	-H22	116(2)
C10	-C11	-H111	108(2)	C10'	-C11'	-H114	109(6)
C10	-C11	-H112	102(4)	C10'	-C11'	-H115	105(3)
C10	-C11	-H113	113(2)	C10'	-C11'	-H116	108(3)
H111	-C11	-H112	124(4)	H114	-C11'	-H115	126(7)
H111	-C11	-H113	107(3)	H114	-C11'	-H116	95(7)
H112	-C11	-H113	102(4)	H115	-C11'	-H116	112(5)
C10	-C12	-H121	111(3)	C10'	-C12'	-H124	101(3)
C10	-C12	-H122	107(2)	C10'	-C12'	-H125	108(3)
C10	-C12	-H123	104(4)	C10'	-C12'	-H126	100(5)
H121	-C12	-H122	112(4)	H124	-C12'	-H125	109(5)
H121	-C12	-H123	112(5)	H124	-C12'	-H126	135(6)
H122	-C12	-H123	110(4)	H125	-C12'	-H126	101(6)
C10	-C13	-H131	107(3)	C10'	-C13'	-H134	109(5)
C10	-C13	-H132	107(3)	C10'	-C13'	-H135	92(7)
C10	-C13	-H133	108(3)	C10'	-C13'	-H136	105(4)
H131	-C13	-H132	117(4)	H134	-C13'	-H135	134(9)
H131	-C13	-H133	104(4)	H134	-C13'	-H136	103(6)
H132	-C13	-H133	114(4)	H135	-C13'	-H136	109(8)
C14	-C15	-H151	120.2(18)	C14'	-C15'	-H152	117(2)
C16	-C15	-H151	119.7(19)	C16'	-C15'	-H152	122(2)
C15	-C16	-H161	118(3)	C15'	-C16'	-H162	120(2)
C17	-C16	-H161	121(3)	C17'	-C16'	-H162	119(2)
C16	-C17	-H171	121(2)	C16'	-C17'	-H172	116(2)
C18	-C17	-H171	118(2)	C18'	-C17'	-H172	124(2)
C17	-C18	-H181	126.2(18)	C17'	-C18'	-H182	117(2)
C19	-C18	-H181	113.7(18)	C19'	-C18'	-H182	122(2)
C14	-C19	-H191	118(2)	C14'	-C19'	-H192	119(2)
C18	-C19	-H191	122(2)	C18'	-C19'	-H192	121(2)
C20	-C21	-H211	123(2)	C20'	-C21'	-H212	121.1(17)
C22	-C21	-H211	115(2)	C22'	-C21'	-H212	118.2(17)
C21	-C22	-H221	120(2)	C21'	-C22'	-H222	119(2)
C23	-C22	-H221	120(2)	C23'	-C22'	-H222	121(2)
C22	-C23	-H231	117(2)	C22'	-C23'	-H232	117(3)
C24	-C23	-H231	124(2)	C24'	-C23'	-H232	122(3)
C23	-C24	-H241	122(2)	C23'	-C24'	-H242	124(3)
C25	-C24	-H241	117(2)	C25'	-C24'	-H242	116(3)
C20	-C25	-H251	119(2)	C20'	-C25'	-H252	123(3)
C24	-C25	-H251	121(2)	C24'	-C25'	-H252	117(3)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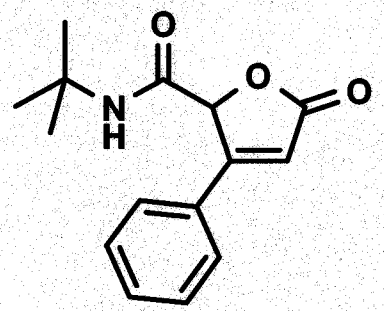
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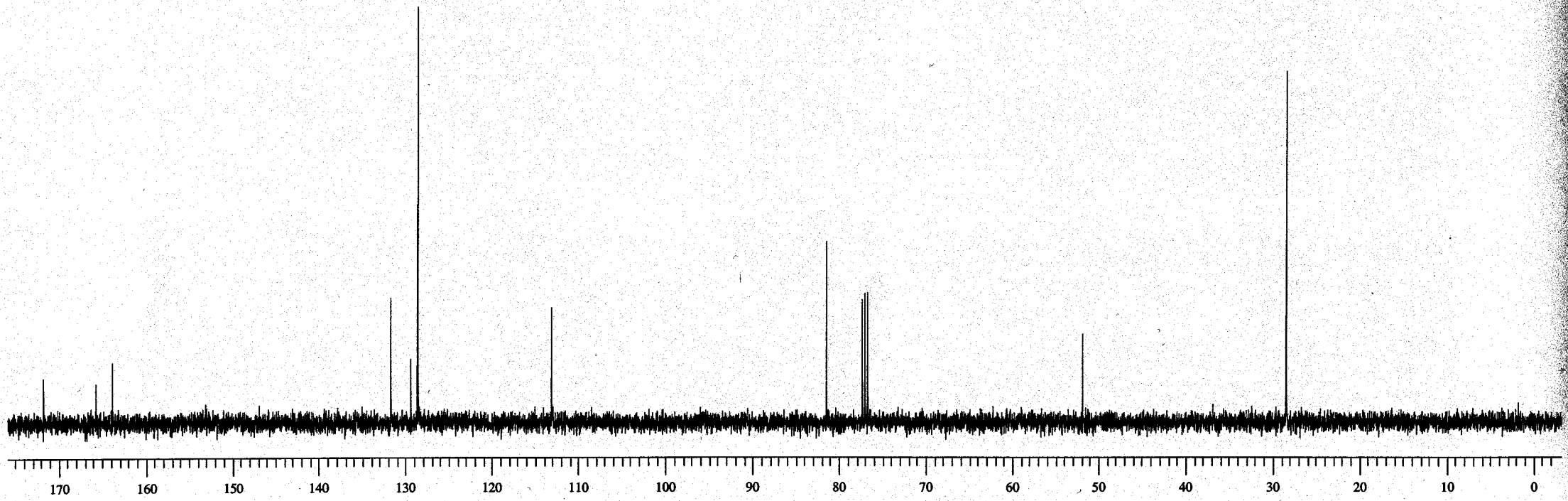
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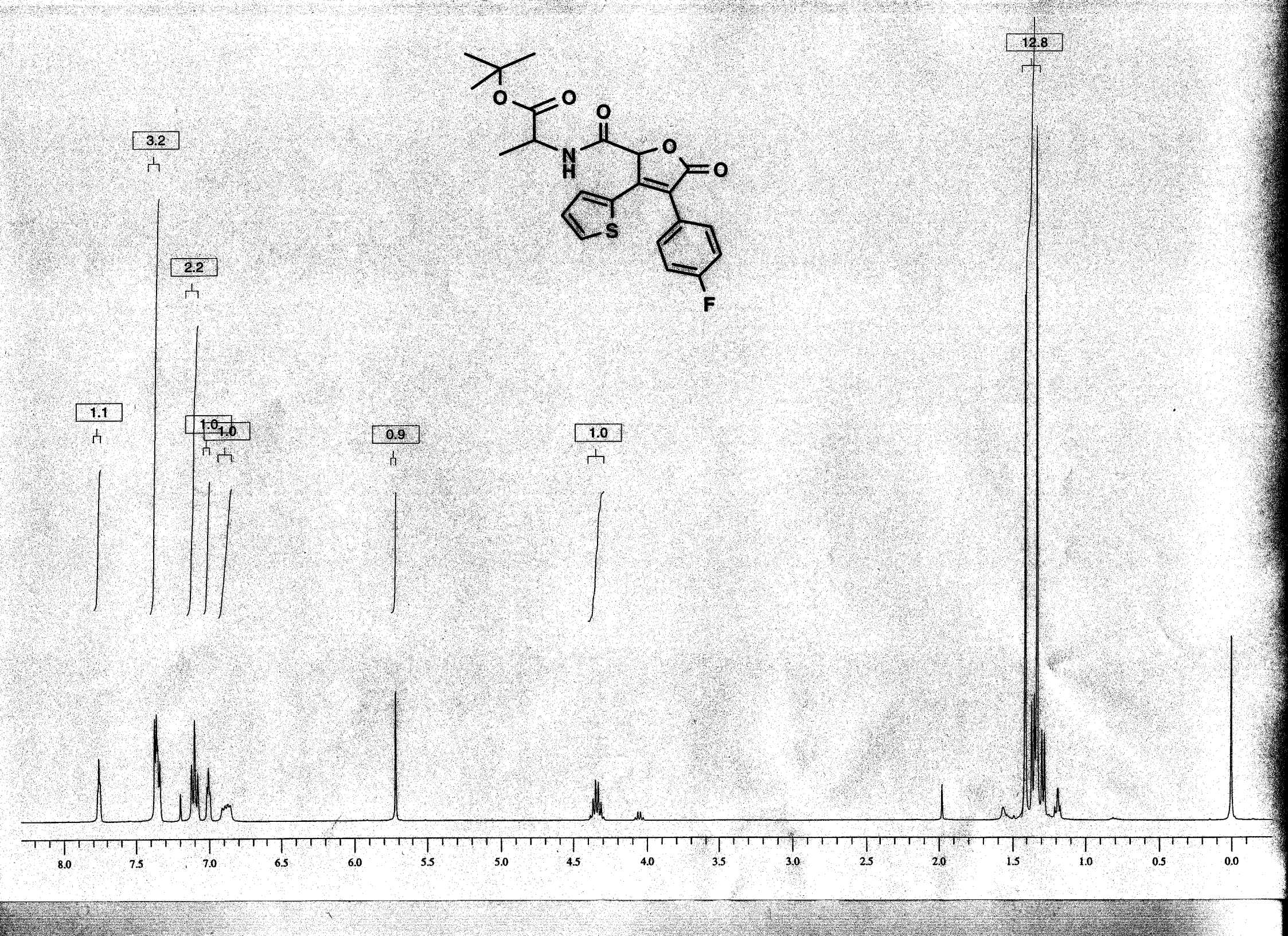
Index	ppm	Hertz	Height
FROM	173.185	17440.796	Threshold
TO	25.152	2532.959	5.854
1	171.714	17292.615	13.793
2	165.683	16685.283	12.304
3	163.760	16491.627	17.335
4	131.683	13261.273	36.941
5	129.366	13027.953	15.480
6	128.605	12951.343	70.467
7	128.517	12942.441	119.552
8	113.047	11384.476	33.376
9	81.395	8196.966	51.142
10	77.304	7784.975	33.727
11	76.986	7752.960	34.264
12	76.667	7720.842	37.364
13	51.819	5218.503	21.915
14	28.375	2857.540	116.296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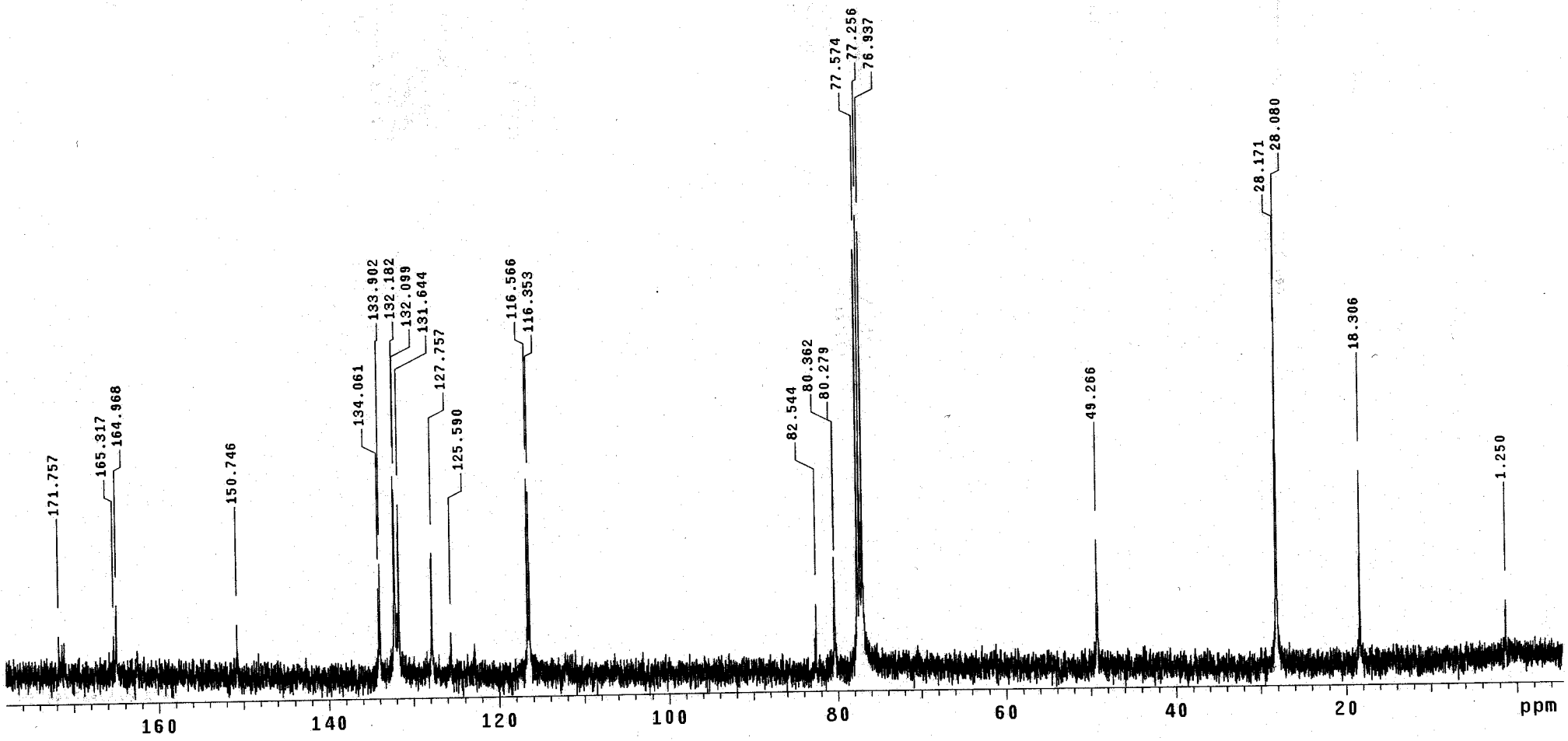
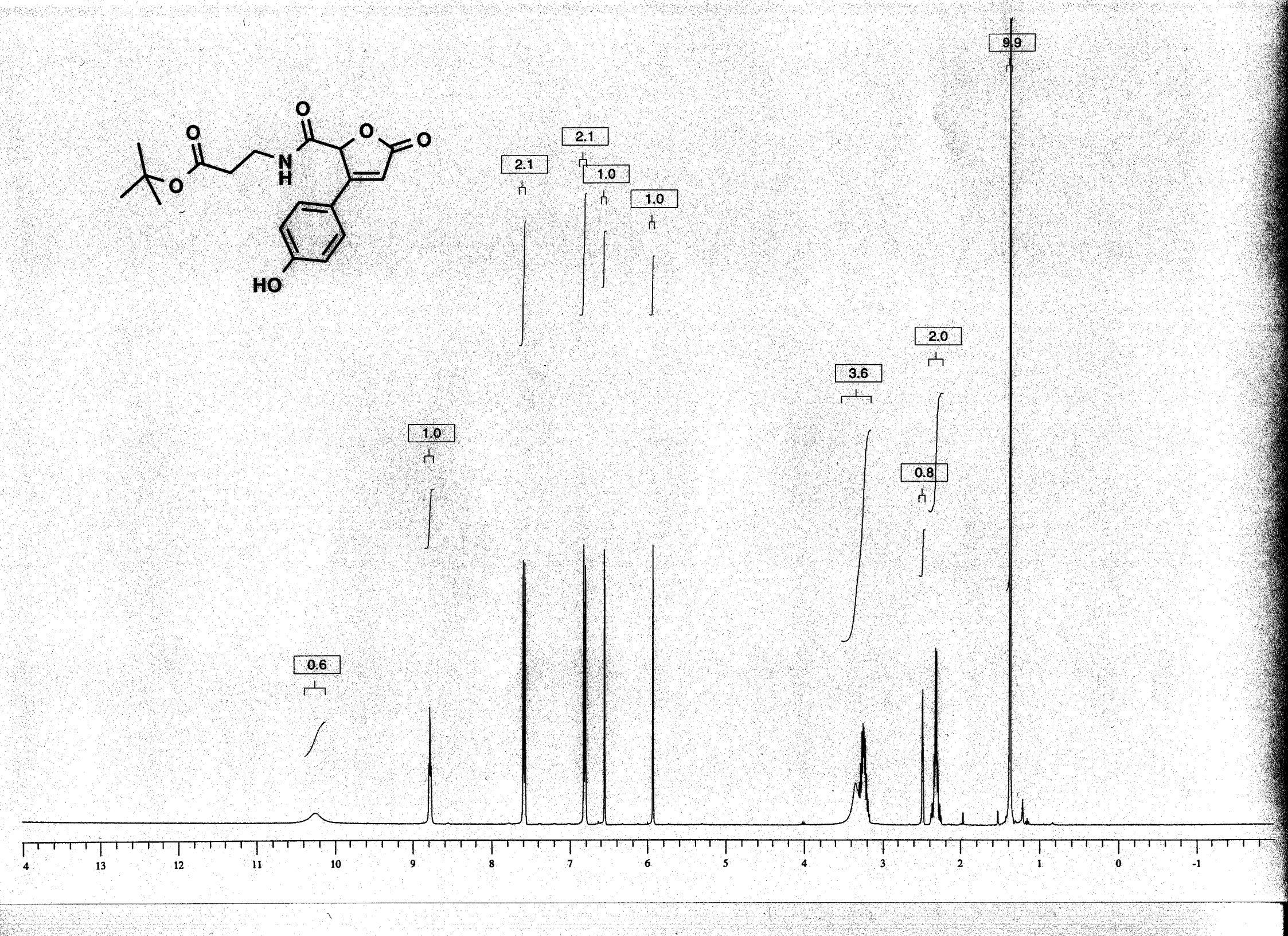
13C OBSERVE

Pulse Sequence: s2pul

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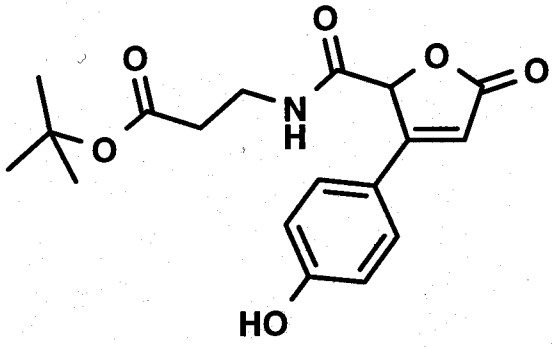
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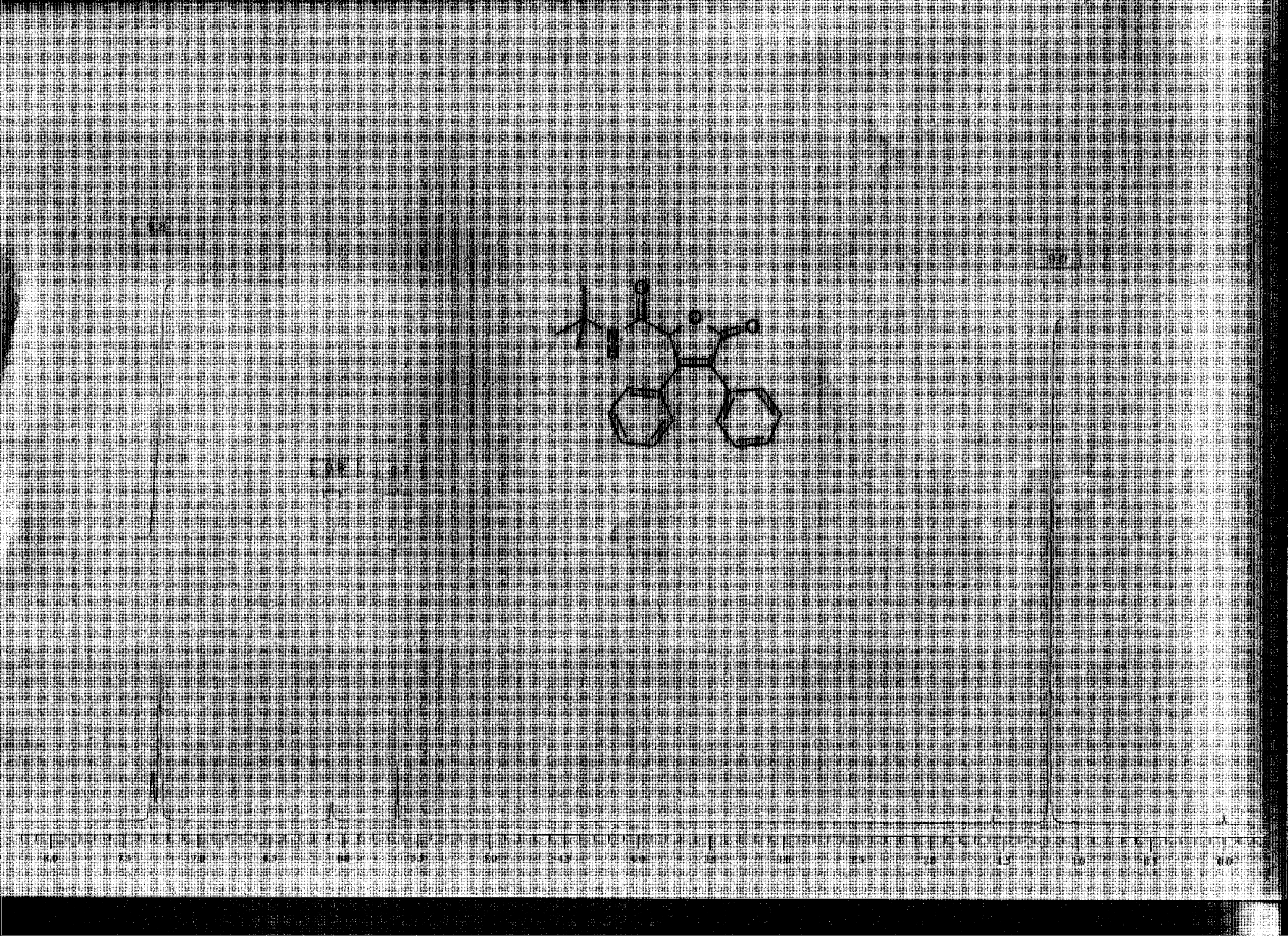
Index	ppm	Hertz	Height
FROM	178.351	17960.835	Threshold
TO	22.267	2242.360	5.871
1	173.710	17493.441	16.859
2	171.037	17224.285	9.825
3	165.863	16703.224	25.282
4	164.259	16541.718	12.792
5	161.329	16246.589	24.747
6	130.275	13119.324	39.849
7	120.888	12174.019	21.988
8	116.353	11717.299	46.596
9	111.312	11209.609	17.348
10	81.103	8167.470	26.816
11	40.797	4108.481	11.235
12	40.586	4087.158	30.741
13	40.367	4065.154	63.405
14	40.172	4045.480	75.596
15	39.960	4024.145	61.920
16	39.755	4003.472	33.416
17	39.544	3982.253	11.680
18	35.837	3608.937	23.150
19	35.029	3527.604	30.417
20	28.404	2860.384	109.309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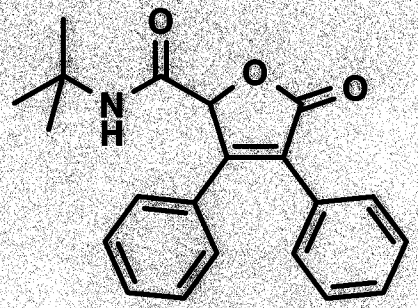
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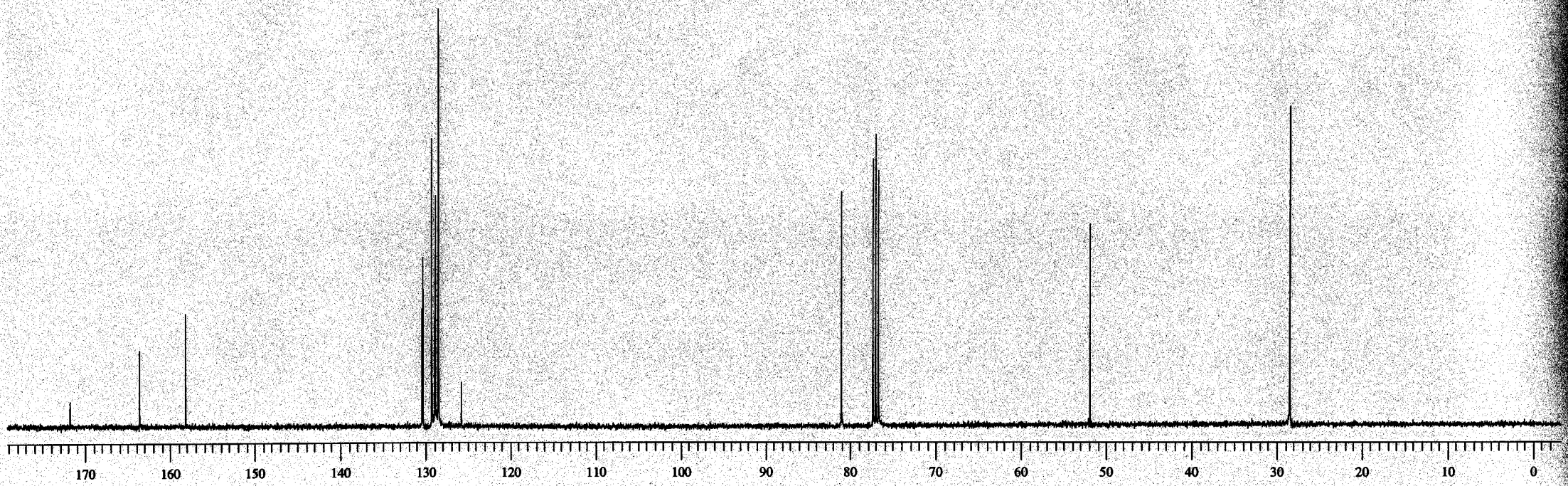
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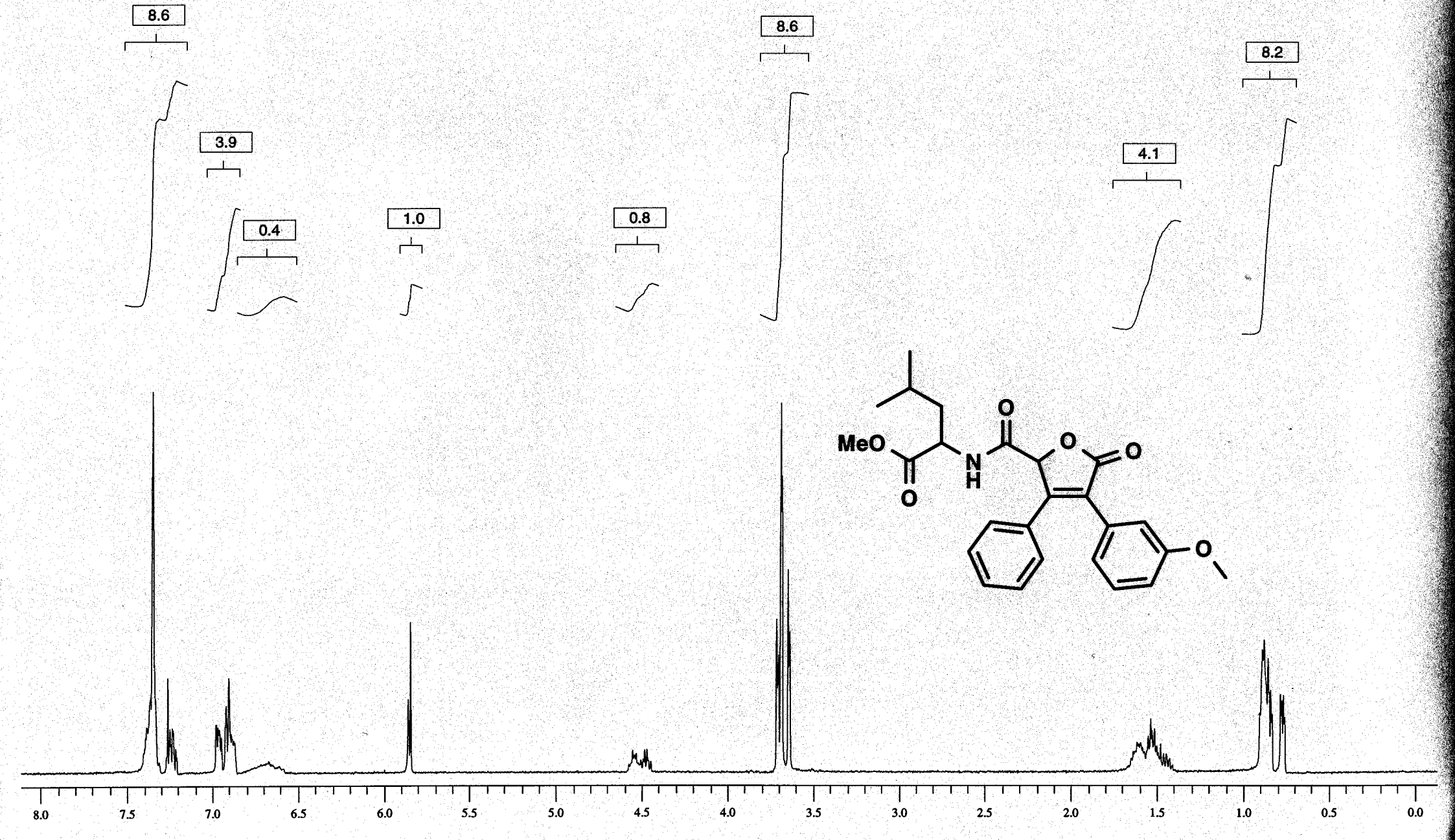
Index	ppm	Hertz	Height
FROM	173.194	17441.911	Threshold
TO	26.151	2633.582	7.105
1	163.575	16473.282	21.132
2	158.126	15924.480	28.468
3	130.372	13129.461	30.460
4	130.265	13118.674	45.726
5	129.241	13015.596	84.284
6	128.885	12979.734	36.385
7	128.797	12970.814	72.788
8	128.464	12937.279	110.834
9	128.403	12931.123	104.904
10	125.716	12660.530	11.665
11	81.017	8159.017	60.863
12	77.306	7785.337	77.304
13	76.987	7753.154	71.480
14	76.665	7720.755	74.178
15	51.874	5224.093	53.921
16	28.403	2860.363	112.366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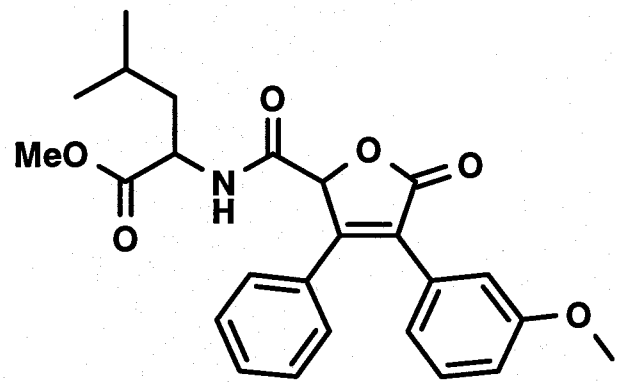
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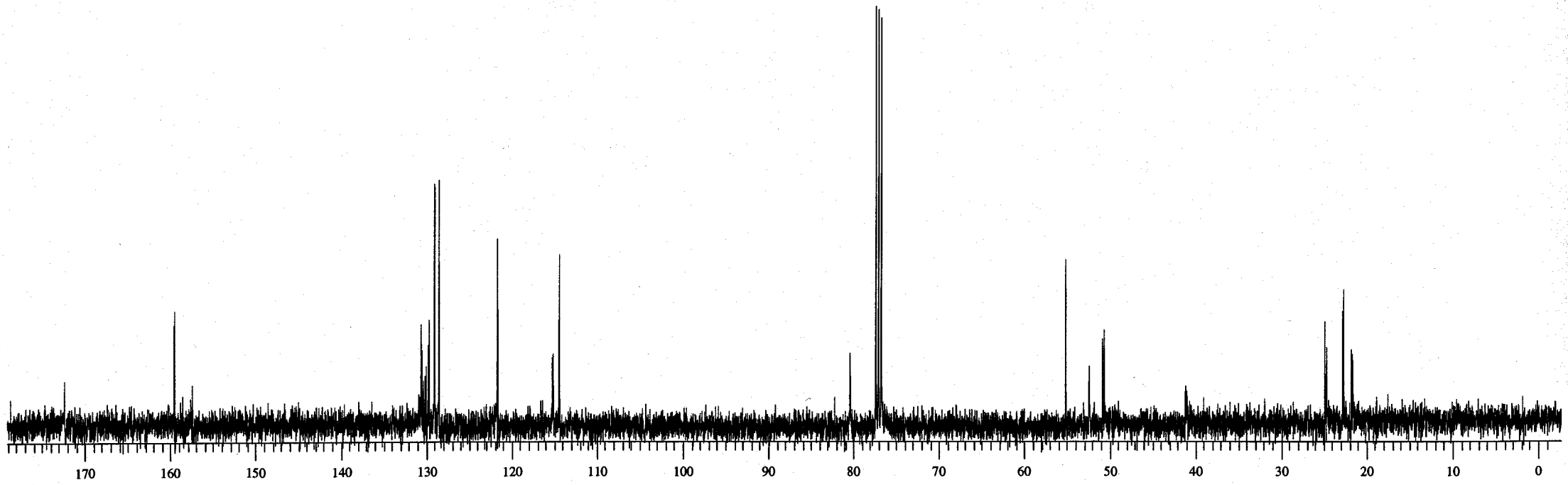
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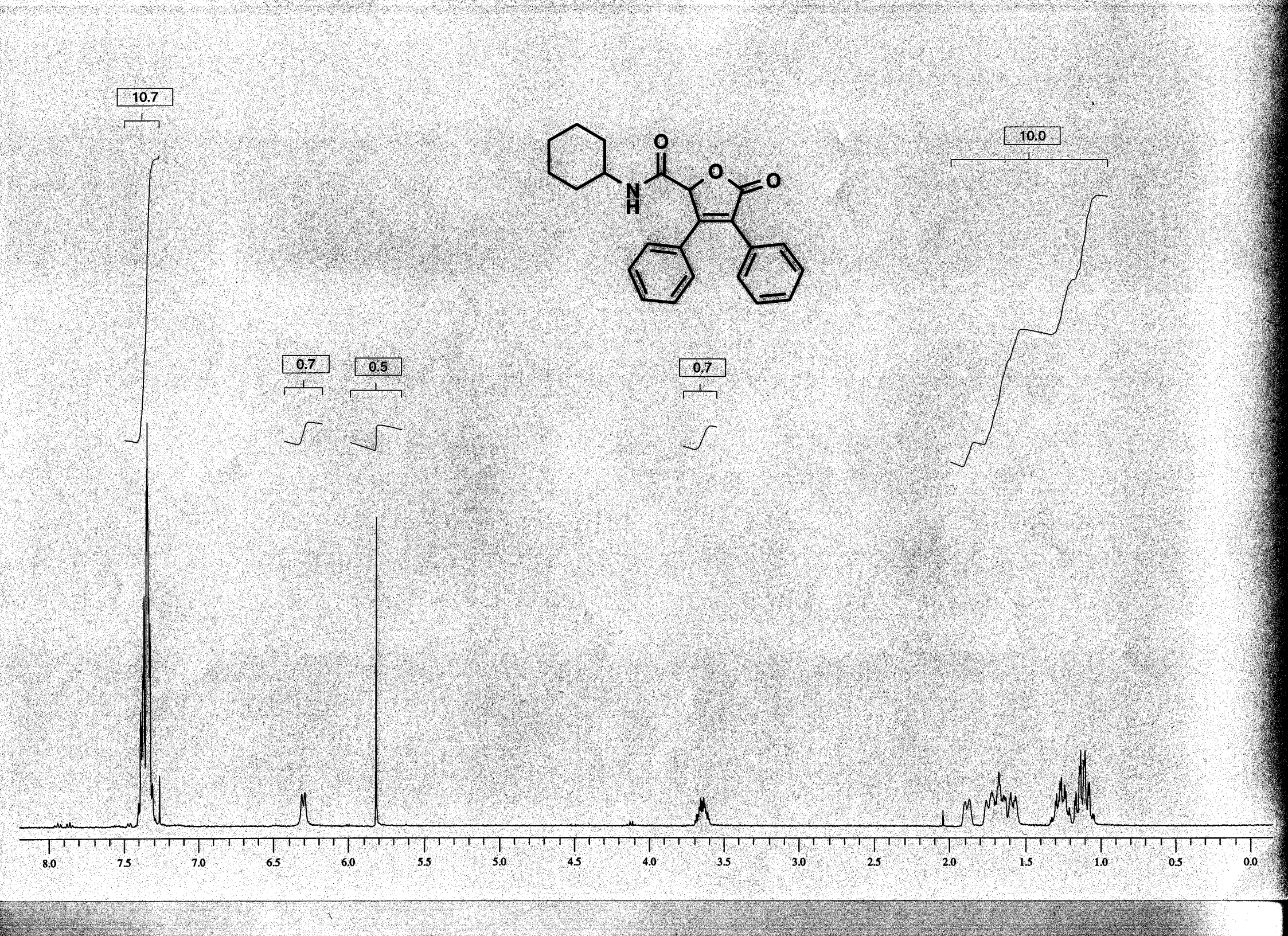
MestRe-C
Peak List

Index	ppm	Hertz	Height
FROM	174.246	17547.607	Threshold
TO	17.925	1805.115	7.496
1	172.317	17353.383	13.430
2	159.533	16065.928	27.113
3	159.472	16059.810	31.682
4	157.412	15852.312	10.112
5	130.531	13145.237	30.613
6	130.419	13134.026	25.287
7	130.362	13128.261	10.268
8	130.275	13119.442	11.495
9	130.077	13099.532	13.862
10	129.956	13087.326	16.472
11	129.699	13061.498	20.384
12	129.608	13052.350	26.961
13	128.972	12988.248	64.398
14	128.436	12934.291	82.184
15	121.638	12249.716	50.242
16	121.563	12242.097	30.625
17	115.195	11600.858	20.970
18	115.075	11588.793	21.538
19	114.410	11521.811	30.222
20	114.335	11514.228	47.289
21	80.350	8091.727	17.053
22	77.302	7784.785	126.477
23	76.983	7752.672	127.675
24	76.665	7720.606	125.426
25	55.136	5552.547	48.961
26	52.361	5273.045	16.465
27	50.767	5112.581	28.935
28	50.601	5095.836	30.551
29	41.061	4135.125	8.898
30	24.832	2500.714	31.063
31	24.637	2481.066	18.848
32	22.755	2291.604	35.203
33	22.650	2281.043	40.119
34	21.740	2189.318	22.861
35	21.617	2176.944	20.597
36	21.543	2169.464	11.432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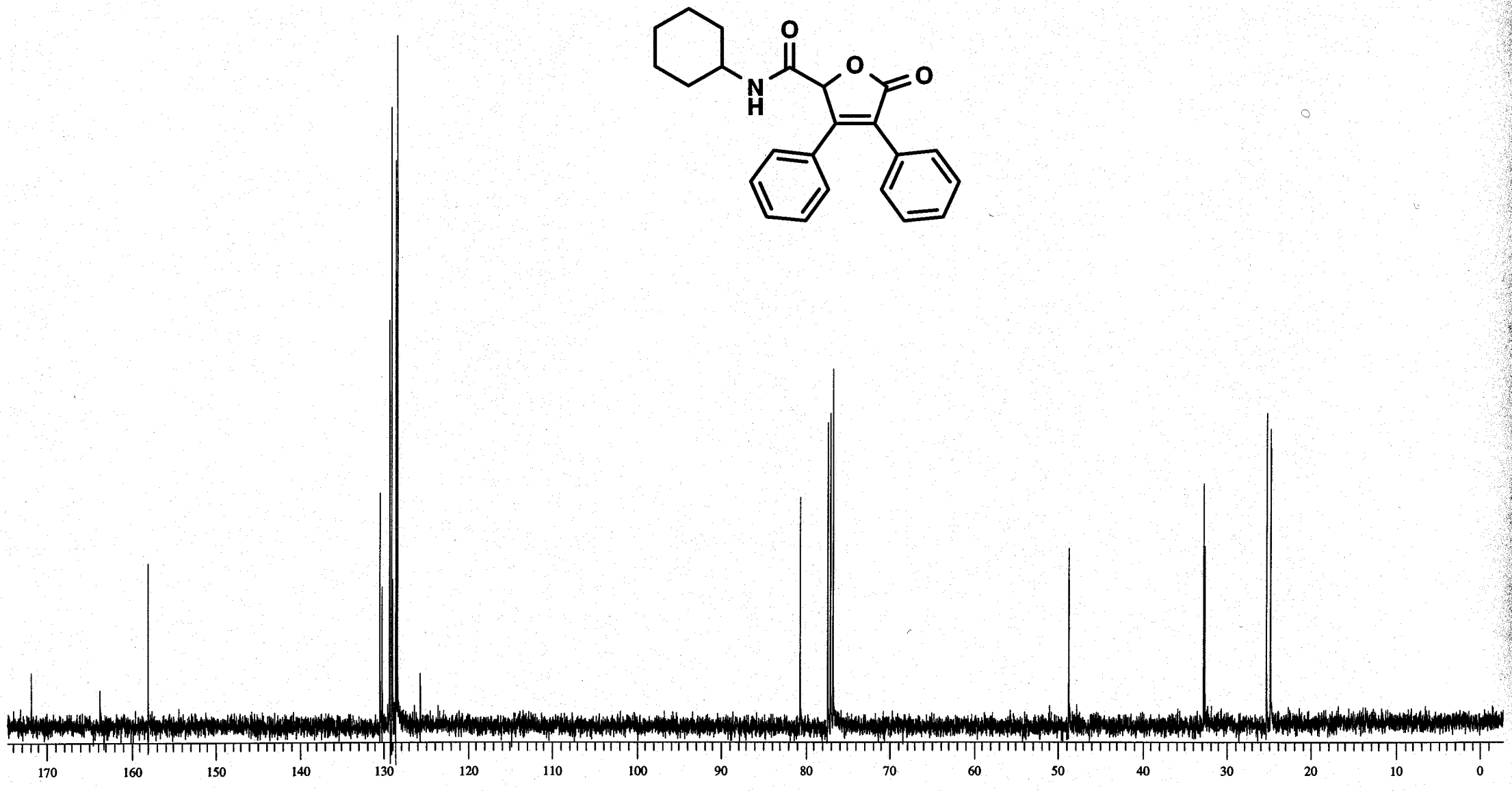
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H
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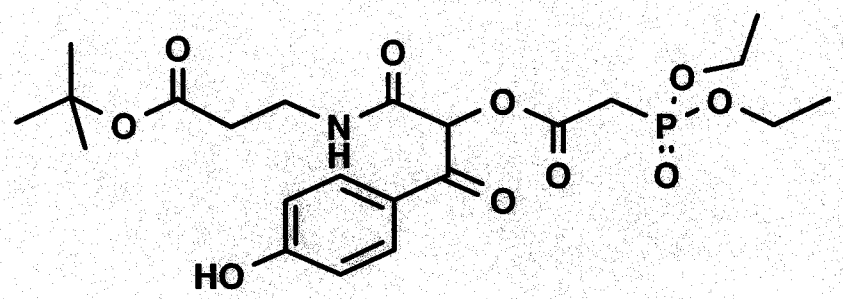
30
20
10
0

Index	ppm	Hertz	Height
FROM	173.246	17446.899	Threshold
TO	20.697	2084.351	4.454
1	171.806	17301.927	8.130
2	163.694	16484.963	7.104
3	157.972	15908.791	25.670
4	130.381	13130.120	39.830
5	130.138	13105.710	23.261
6	129.245	13015.723	65.233
7	129.017	12992.817	103.716
8	128.911	12982.098	24.607
9	128.517	12942.448	96.320
10	128.439	12934.610	5.338
11	128.336	12924.171	111.907
12	125.623	12650.953	8.878
13	80.577	8114.552	38.995
14	77.285	7783.026	60.158
15	76.980	7752.364	64.327
16	76.664	7720.528	70.331
17	48.652	4899.538	29.570
18	32.727	3295.807	42.181
19	32.589	3281.933	33.186
20	25.242	2542.039	53.988
21	24.769	2494.380	58.241


O
O
N
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O
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O
P
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O
HO

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5.9
2.1
0.9
2.0
1.0
2.0
1.7
2.0
0.9
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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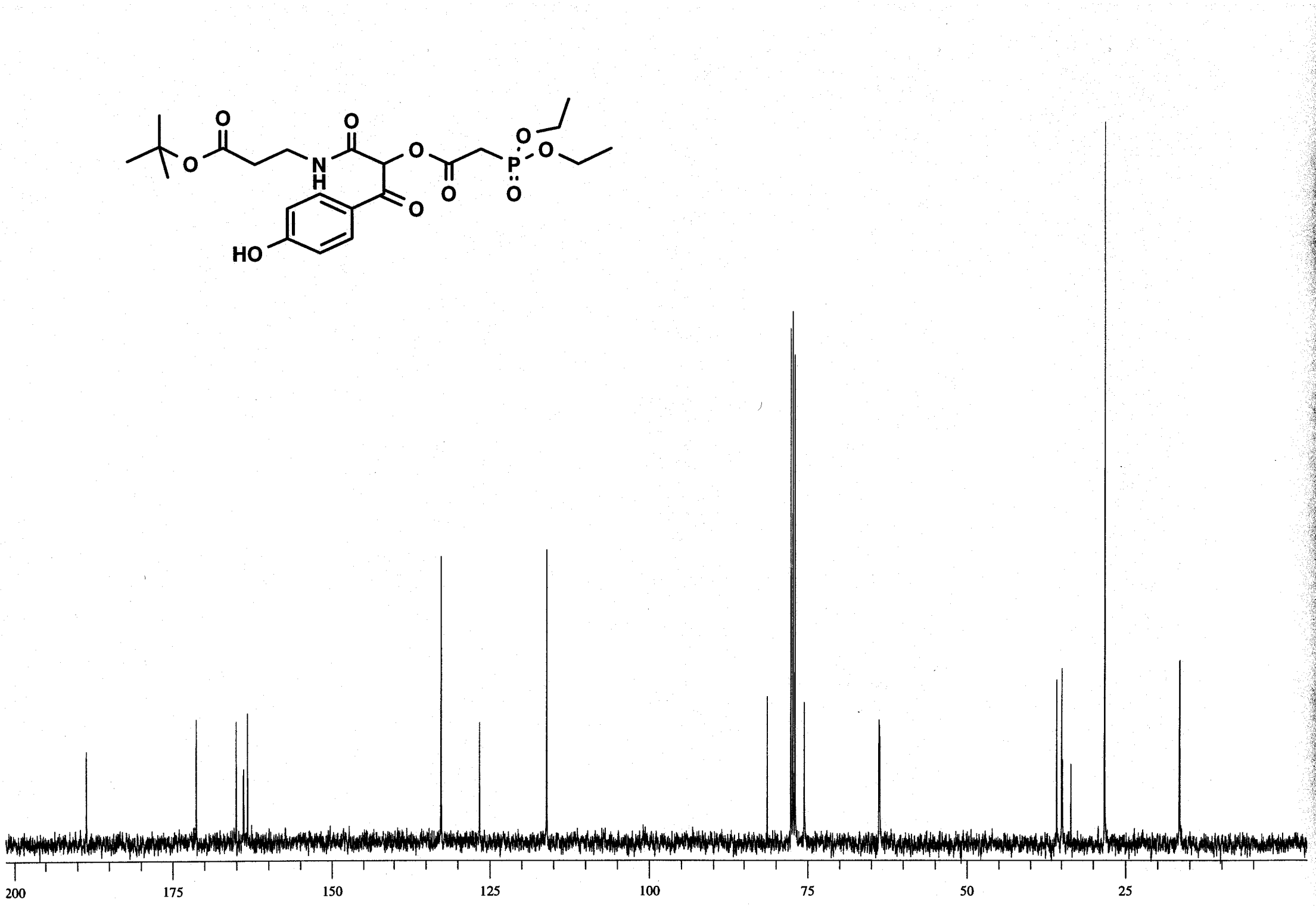
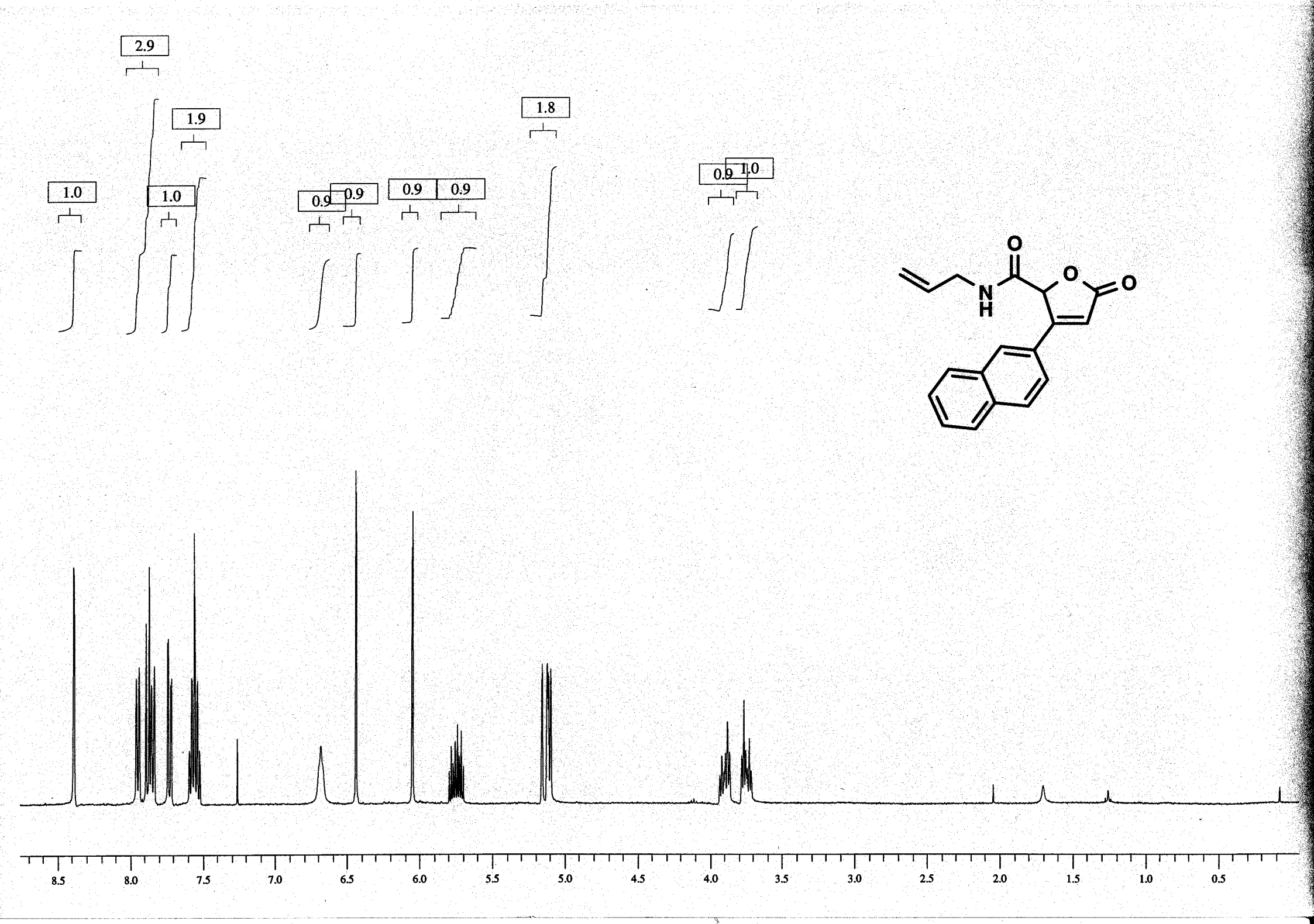

O
O
O
N
H
O
O
O
O
O
P
O
HO
200
175
150
125
100
75
50
25

MestRe-C
Peak List

Index	ppm	Hertz	Height
FROM	205.877	20732.739	Threshold
TO	12.145	1223.013	7.012
1	188.558	18988.649	17.911
2	171.187	17239.320	22.889
3	164.929	16609.043	21.923
4	163.815	16496.844	11.959
5	163.756	16490.973	11.473
6	163.145	16429.369	21.911
7	132.564	13349.810	49.589
8	126.535	12742.675	20.137
9	115.955	11677.130	50.928
10	81.330	8190.240	26.318
11	77.607	7815.336	82.458
12	77.286	7783.052	85.153
13	76.963	7750.552	86.694
14	75.481	7601.222	25.641
15	63.757	6420.609	17.989
16	63.699	6414.794	18.301
17	63.589	6403.691	18.871
18	35.746	3599.741	26.063
19	34.934	3517.971	31.552
20	34.828	3507.359	14.167
21	33.501	3373.708	12.828
22	28.235	2843.353	117.604
23	16.556	1667.258	27.869
24	16.495	1661.088	28.409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O
N
H
8.5
8.0
7.5
7.0
6.5
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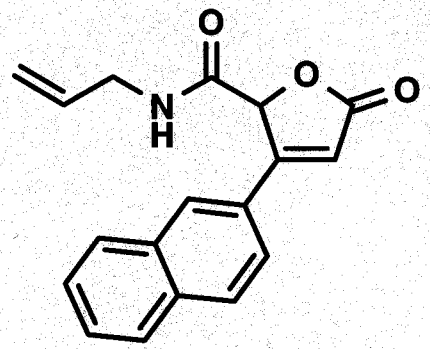
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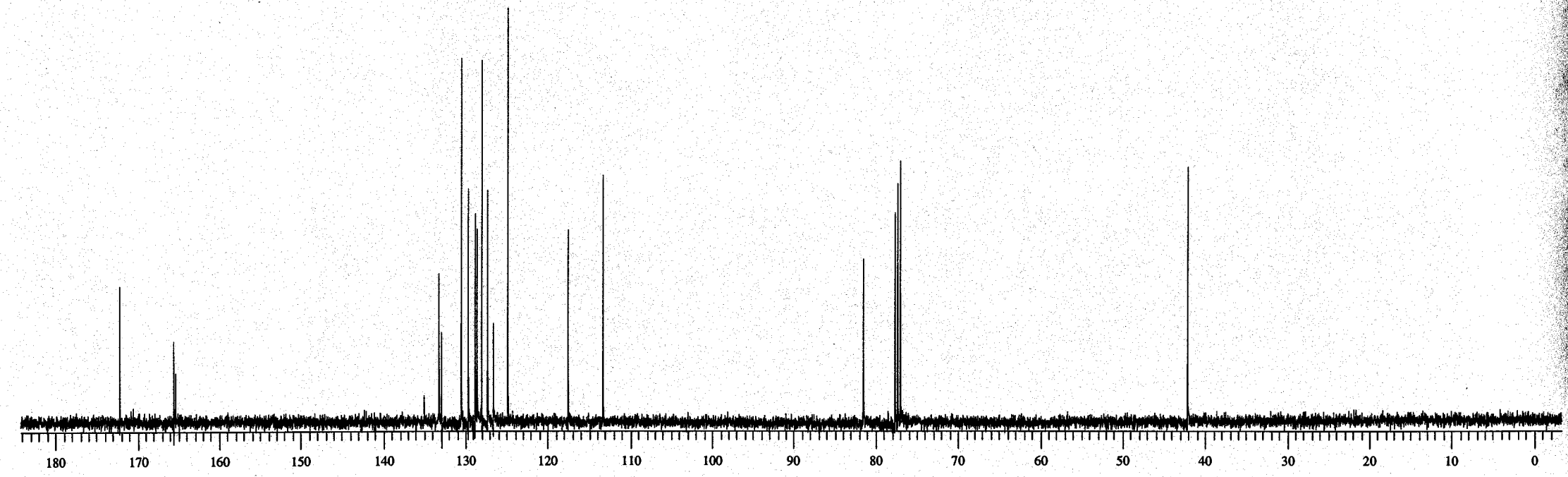
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170
160
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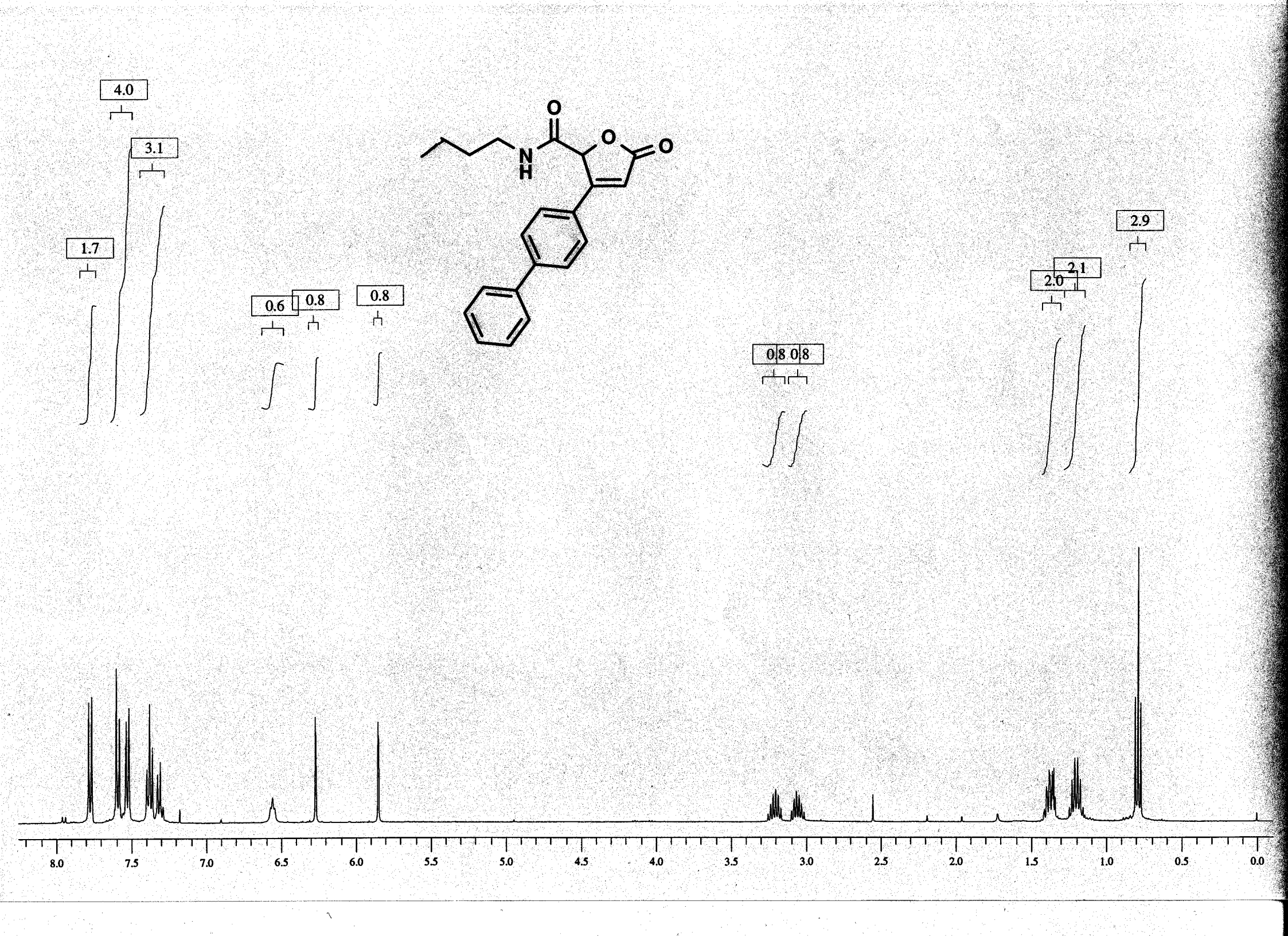
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

MestRe-C
Peak List

Index	ppm	Hertz	Height
FROM	176.829	17807.735	Threshold
TO	34.993	3523.983	8.526
1	172.132	17334.712	33.128
2	165.525	16669.383	22.204
3	165.295	16646.258	15.542
4	133.160	13410.001	44.780
5	132.857	13379.557	25.507
6	130.434	13135.475	97.235
7	129.600	13051.510	66.343
8	128.766	12967.562	60.987
9	128.525	12943.229	48.346
10	127.964	12886.742	99.597
11	127.251	12814.980	67.437
12	126.555	12744.868	24.008
13	124.797	12567.856	108.259
14	117.464	11829.328	49.975
15	113.252	11405.134	64.343
16	81.462	8203.719	48.841
17	77.610	7815.793	70.077
18	77.293	7783.872	77.637
19	76.975	7751.889	83.801
20	42.098	4239.519	75.560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O
O
N
H
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0.8
2.9
2.1
2.0
8.0
7.5
7.0
6.5
6.0
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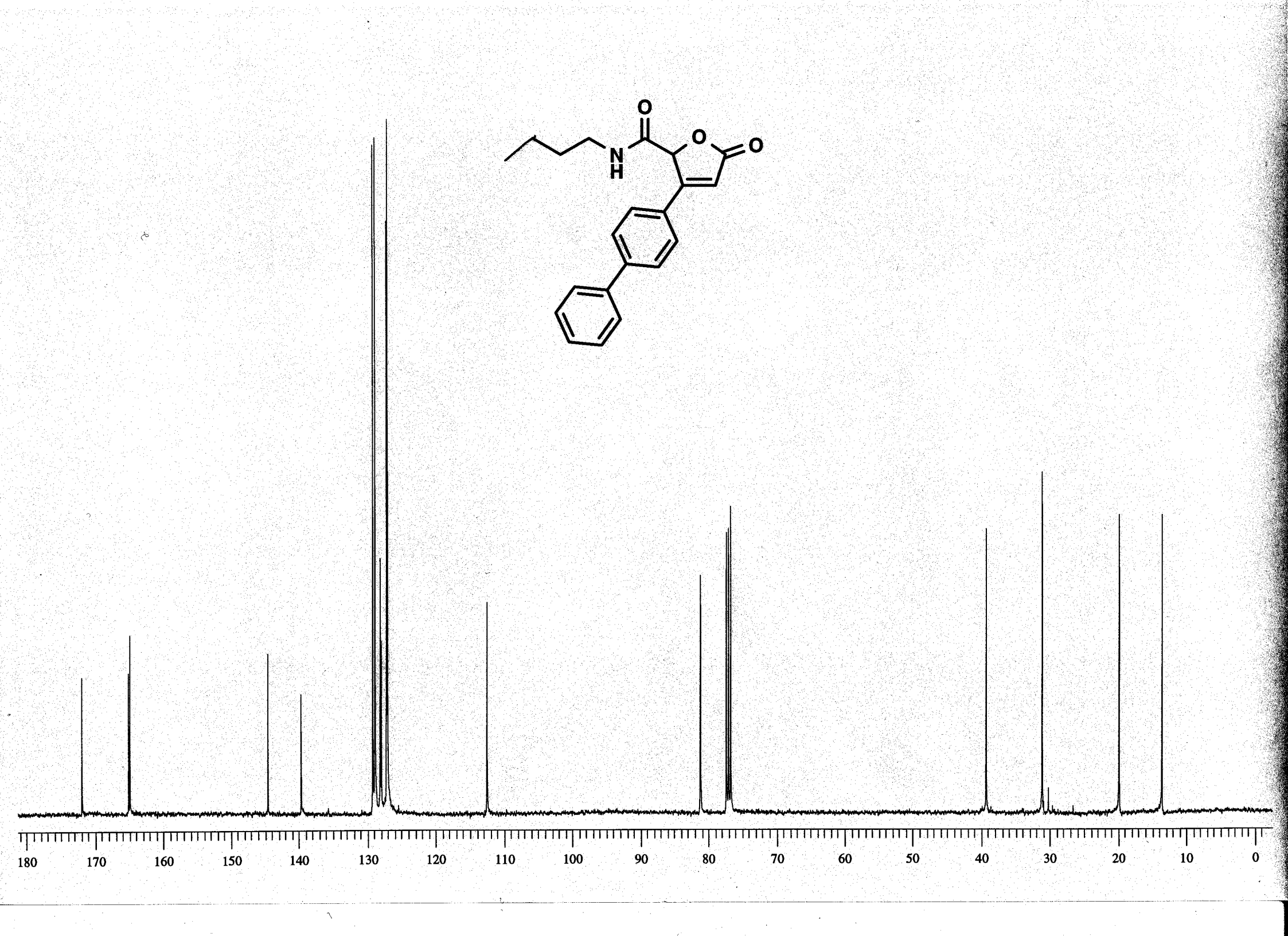
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170
160
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Index	ppm	Hertz	Height
FROM	176.567	17781.678	Threshold
TO	11.053	1113.084	12.725
1	171.911	17312.712	22.587
2	165.054	16622.167	26.433
3	164.887	16605.354	32.322
4	144.523	14554.566	27.182
5	139.619	14060.744	22.965
6	129.180	13009.451	114.657
7	128.860	12977.161	115.796
8	128.093	12899.943	48.958
9	127.913	12881.849	29.324
10	127.161	12806.106	115.841
11	127.028	12792.663	119.531
12	112.458	11325.394	42.415
13	81.121	8169.482	43.593
14	77.287	7783.438	53.765
15	76.981	7752.608	55.591
16	76.664	7720.644	54.572
17	39.261	3953.860	53.342
18	31.126	3134.609	60.023
19	19.827	1996.694	57.119
20	13.556	1365.196	46.505