Supplementary Material (ESI) for Organic & Biomolecular Chemistry

A new Class of Conjugated Strigolactone Analogues with Fluorescent Properties: Synthesis and Biological Activity

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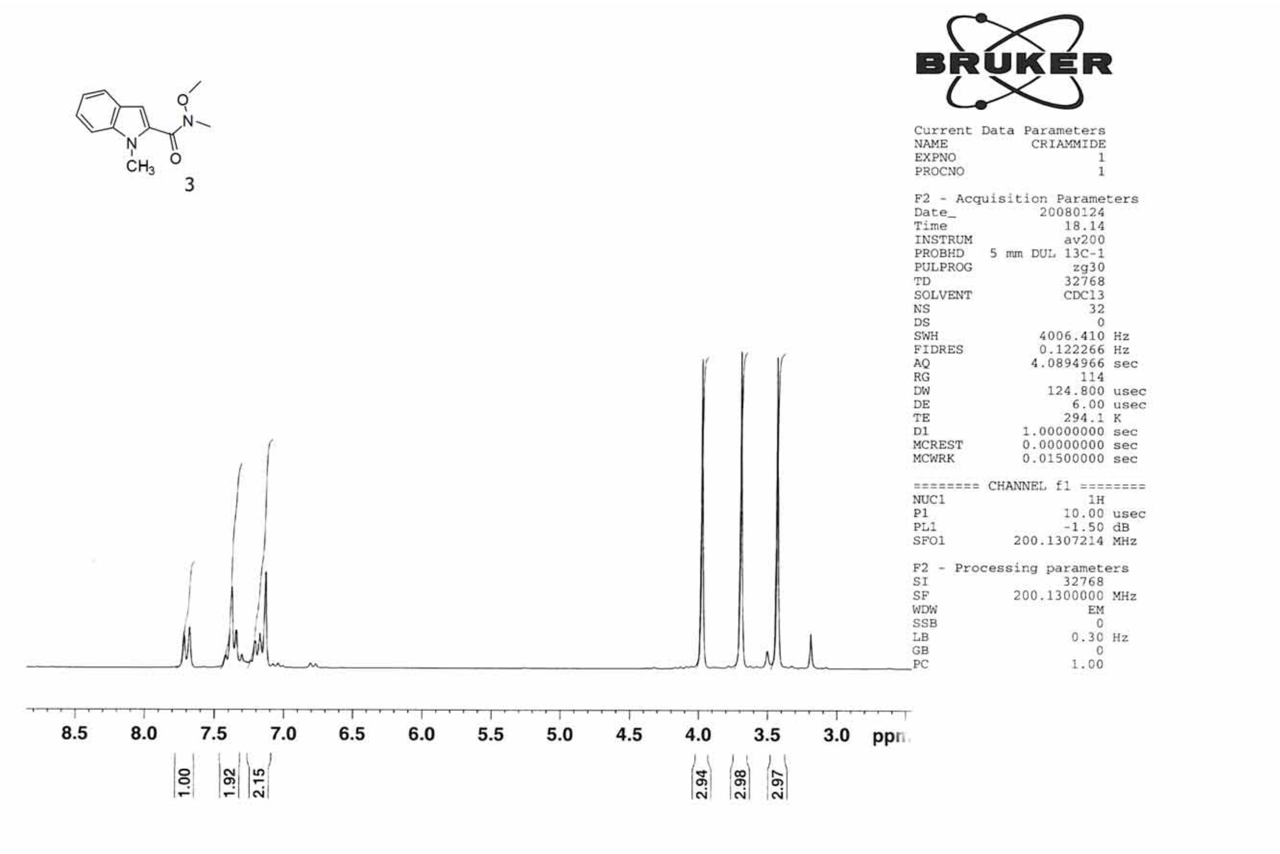
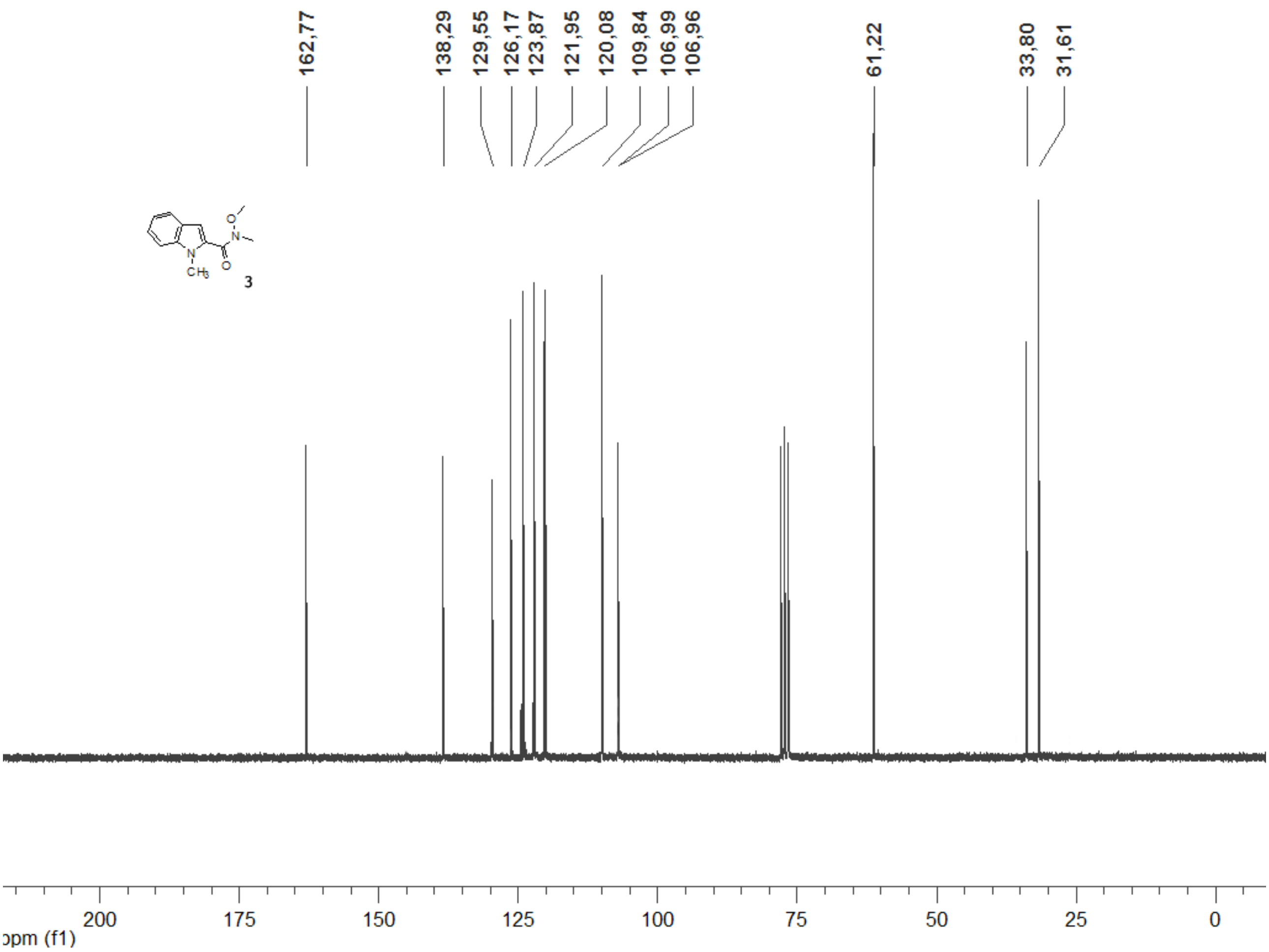
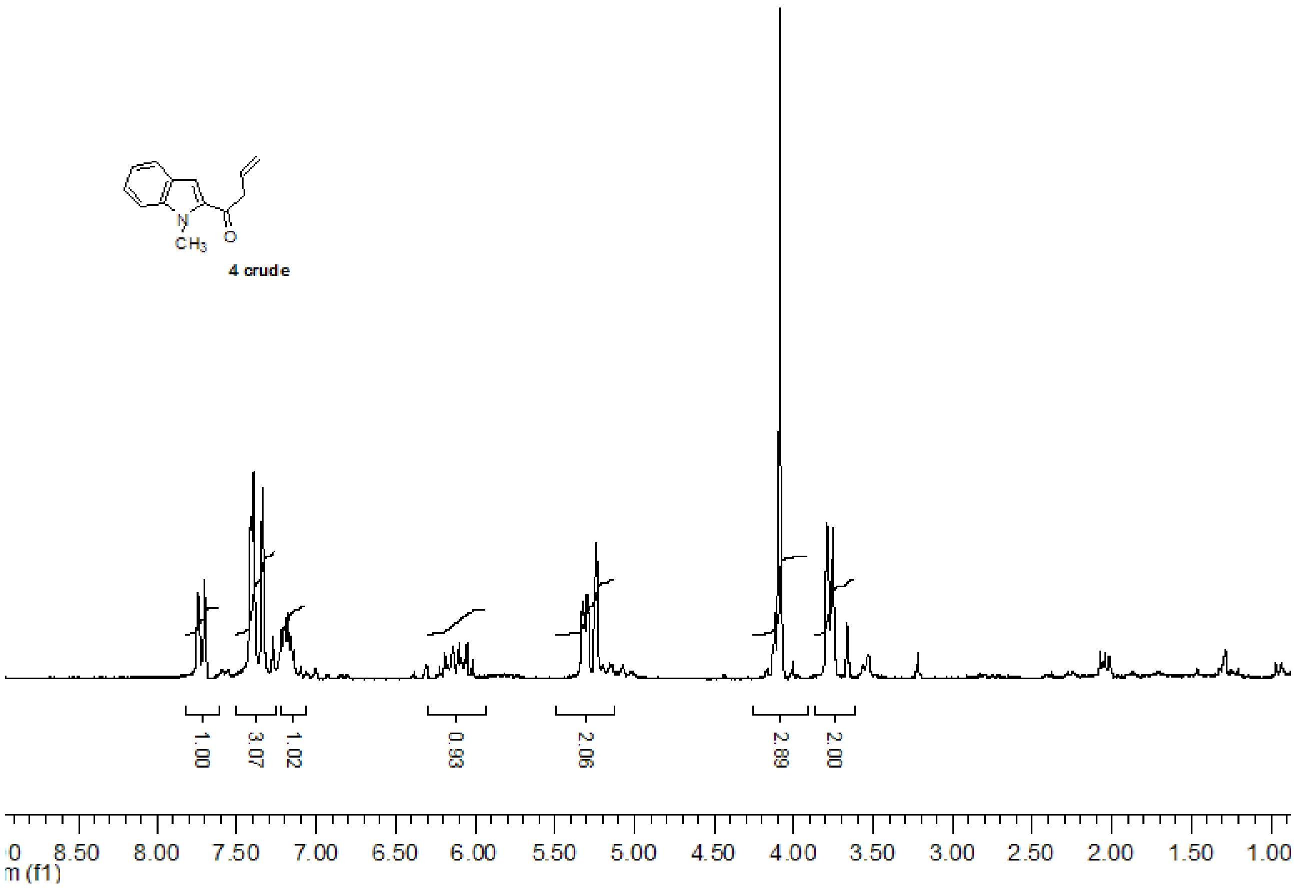
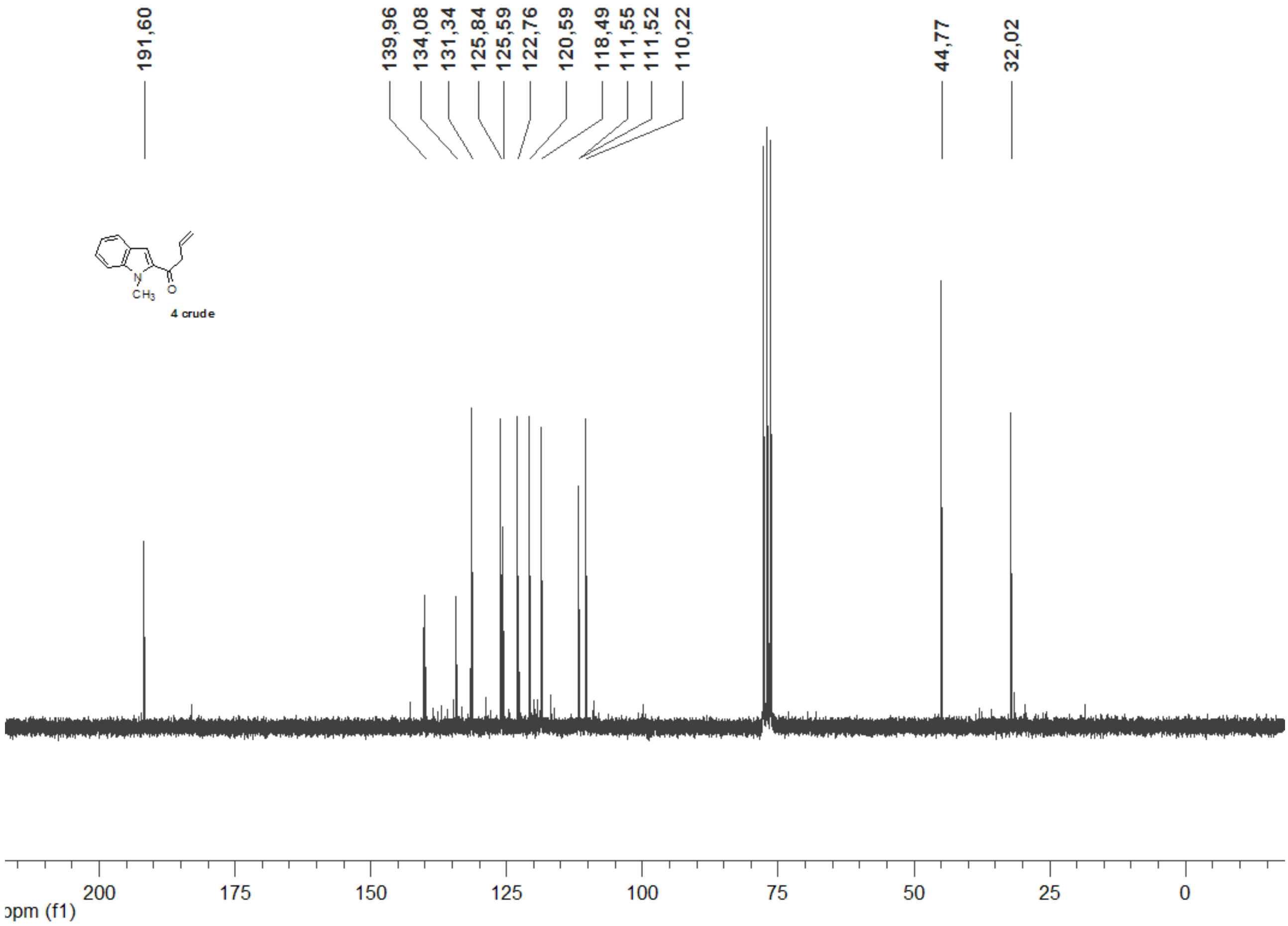
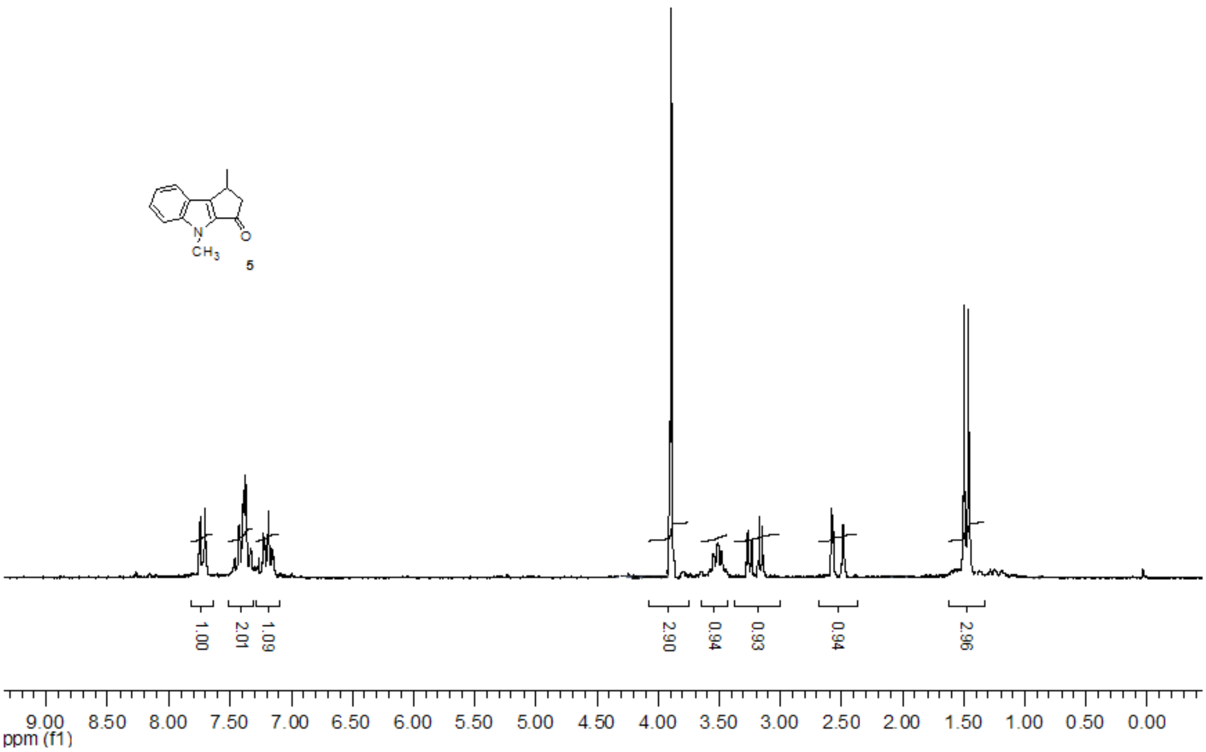
Supporting Information

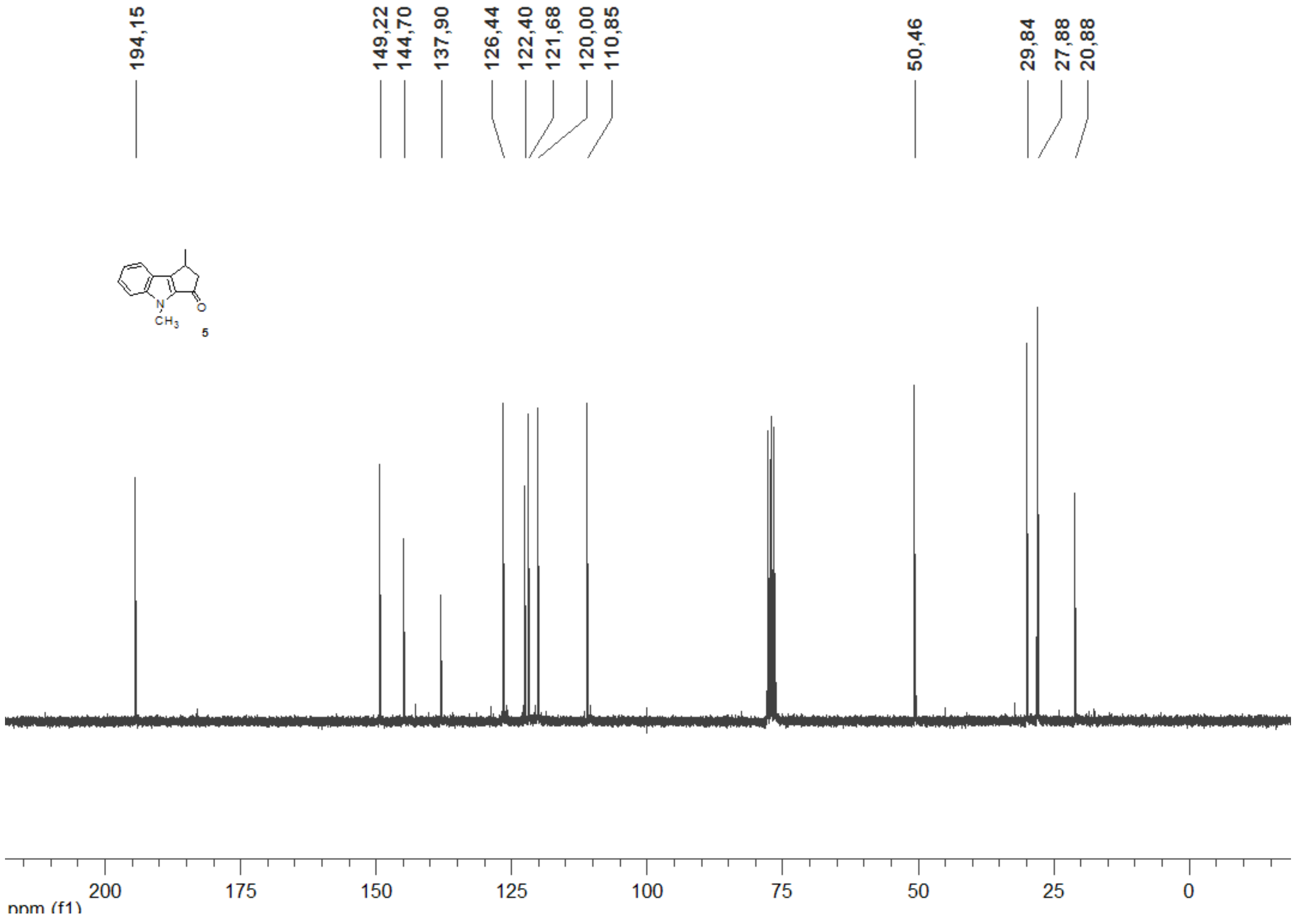

3
BRUKER
Current Data Parameters
NAME CRIAMMIDE
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080124
Time 18.14
INSTRUM av200
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 4006.410 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 114
DW 124.800 usec
DE 6.00 usec
TE 294.1 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -1.50 dB
SFO1 200.1307214 MHz
F2 - Processing parameters
SI 32768
SF 200.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 ppm
1.00 1.92 2.15 2.94 2.98 2.97

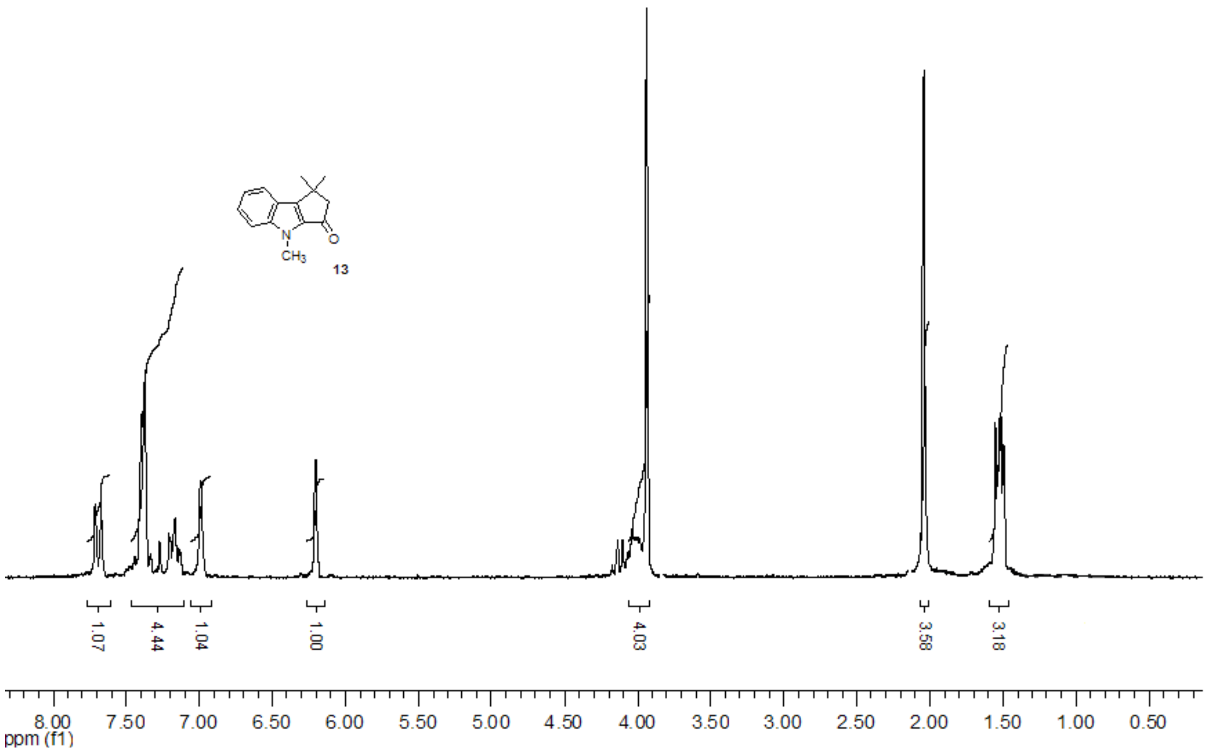

162,77
138,29
129,55
126,17
123,87
121,95
120,08
109,84
106,99
106,96
61,22
33,80
31,61
3
200 175 150 125 100 75 50 25 0
ppm (f1)

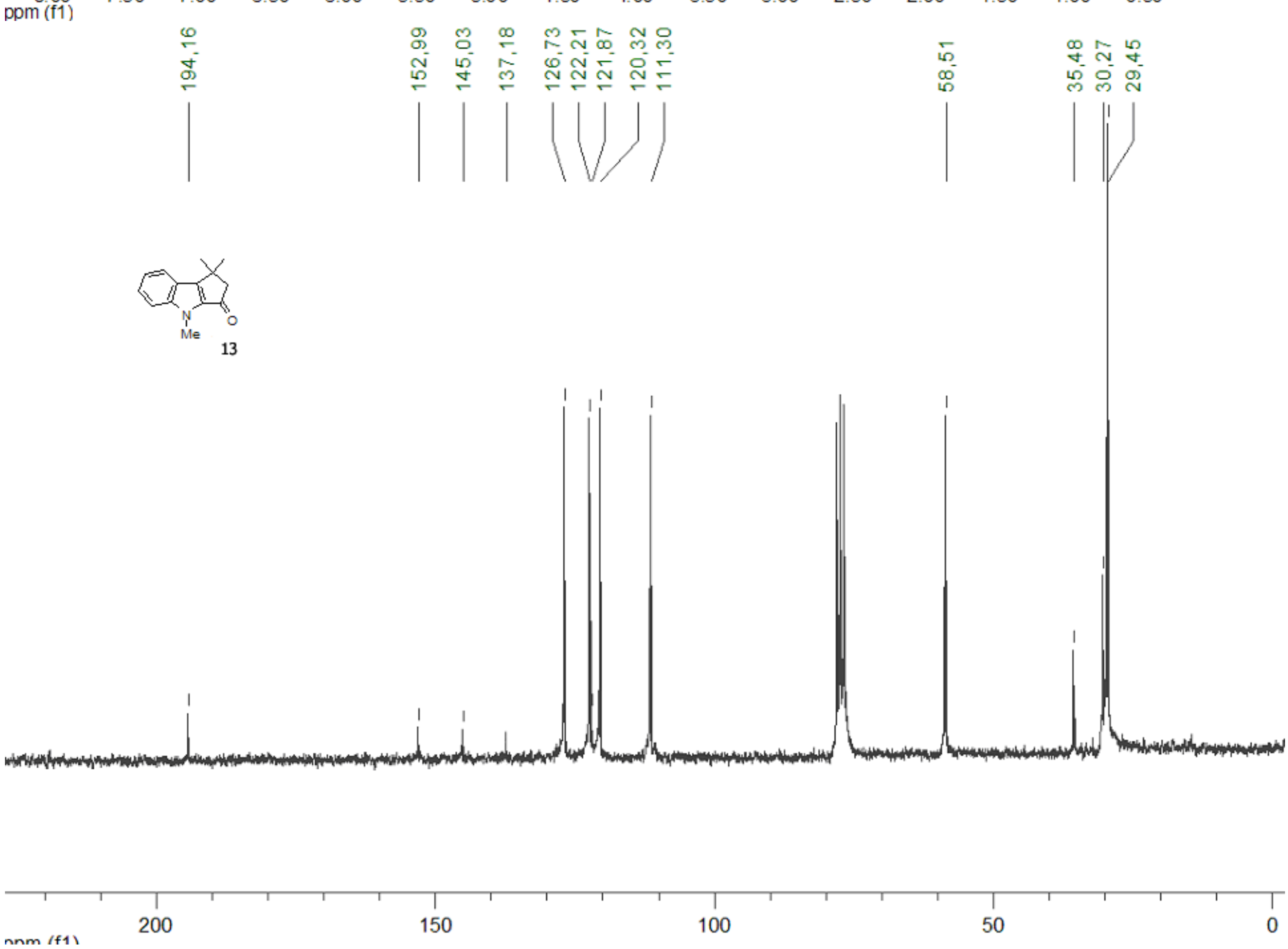

4 crude
1.00
3.07
1.02
0.93
2.06
2.89
2.00
8.50 8.00 7.50 7.00 6.50 6.00 5.50 5.00 4.50 4.00 3.50 3.00 2.50 2.00 1.50 1.00
m (f1)

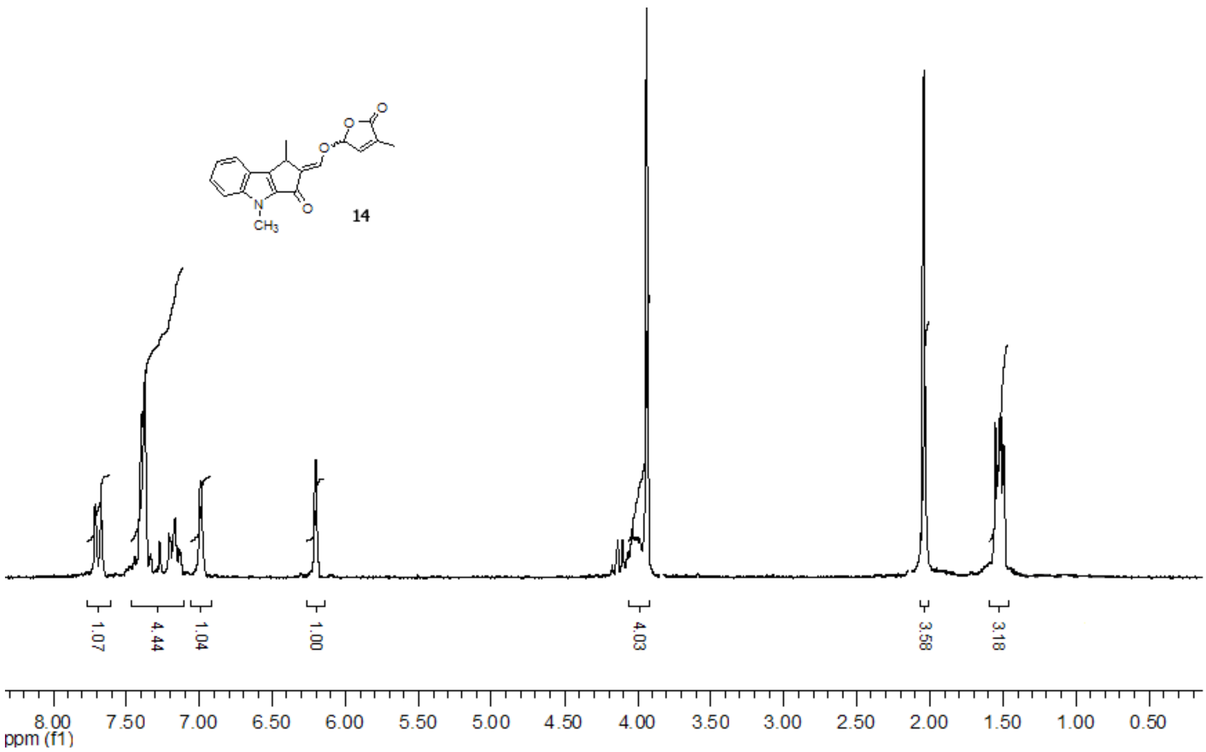

191,60
139,96
134,08
131,34
125,84
125,59
122,76
120,59
118,49
111,55
111,52
110,22
44,77
32,02
4 crude
200 175 150 125 100 75 50 25 0
ppm (f1)

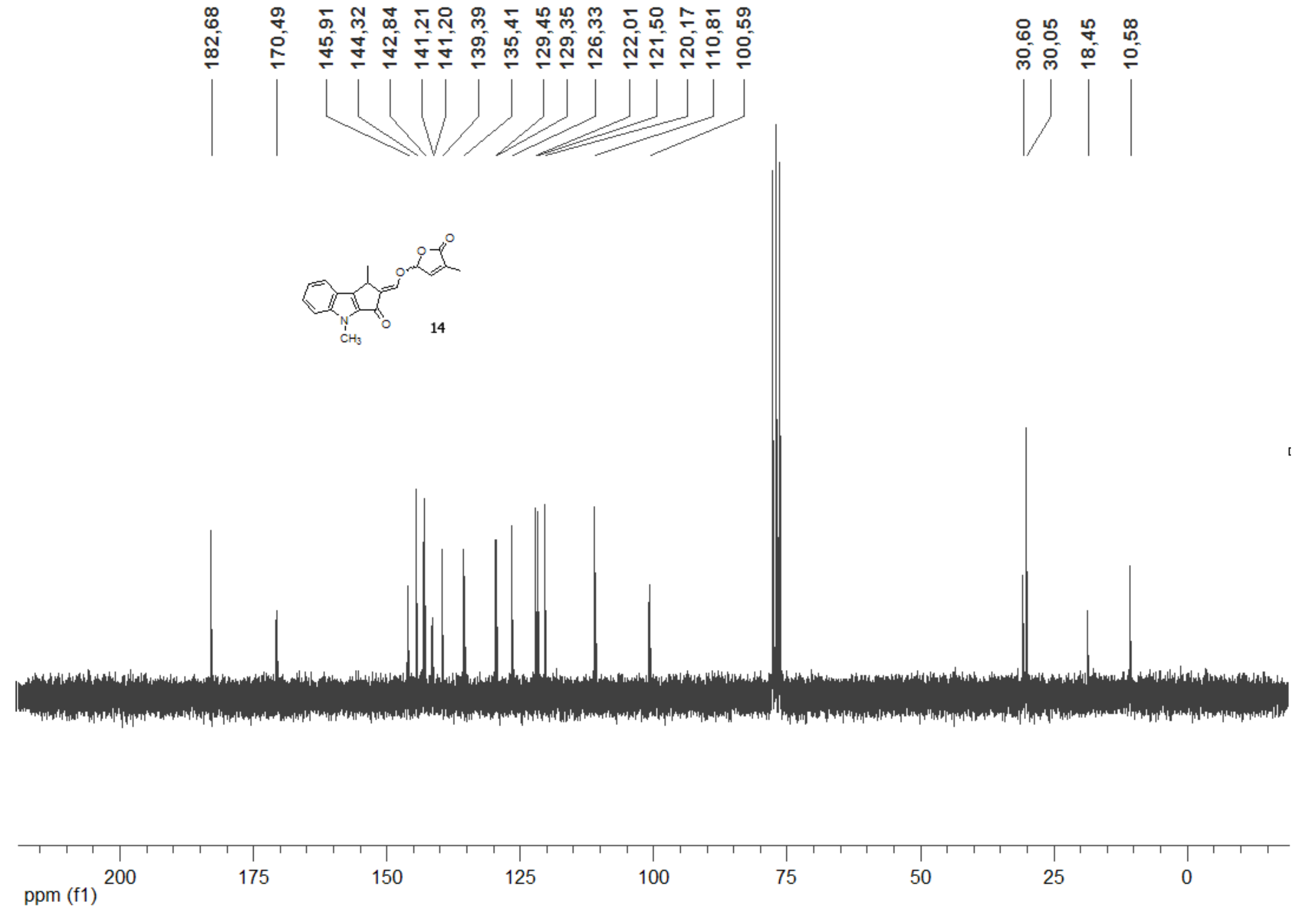

5
1.00
2.01
1.09
2.90
0.94
0.93
0.94
2.96
9.00 8.50 8.00 7.50 7.00 6.50 6.00 5.50 5.00 4.50 4.00 3.50 3.00 2.50 2.00 1.50 1.00 0.50 0.00
ppm (f1)

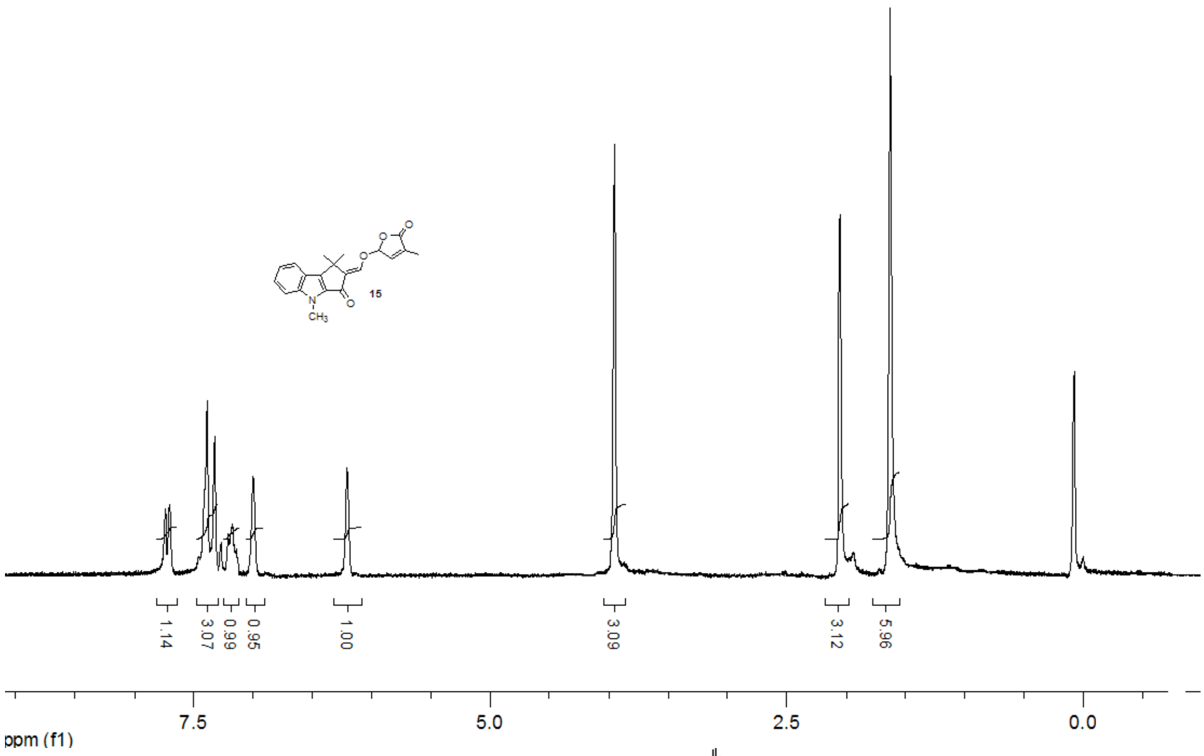

194,15
149,22
144,70
137,90
126,44
122,40
121,68
120,00
110,85
50,46
29,84
27,88
20,88
5
200 175 150 125 100 75 50 25 0
ppm (f1)

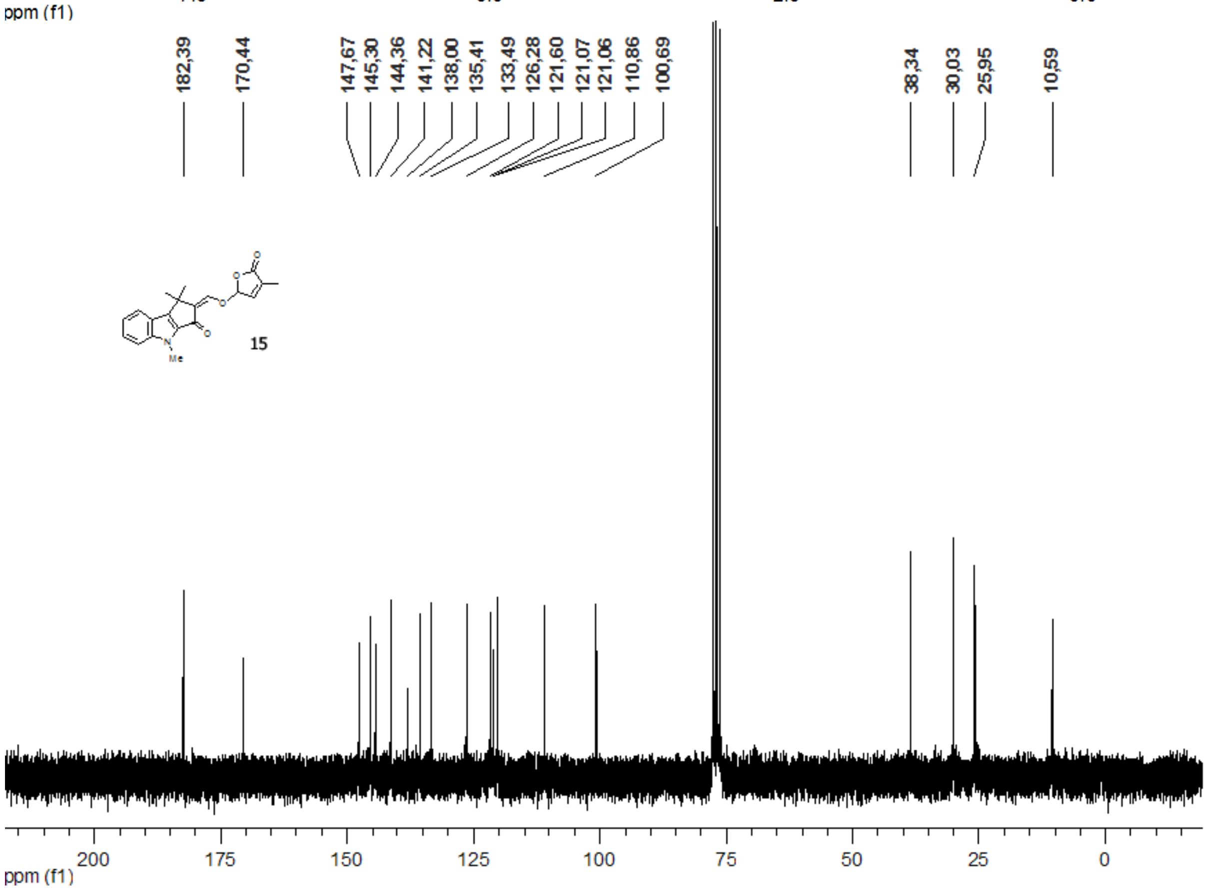

N
CH3
O
13
1.07
4.44
1.04
1.00
4.03
3.58
3.18
8.00 7.50 7.00 6.50 6.00 5.50 5.00 4.50 4.00 3.50 3.00 2.50 2.00 1.50 1.00 0.50
ppm (f1)

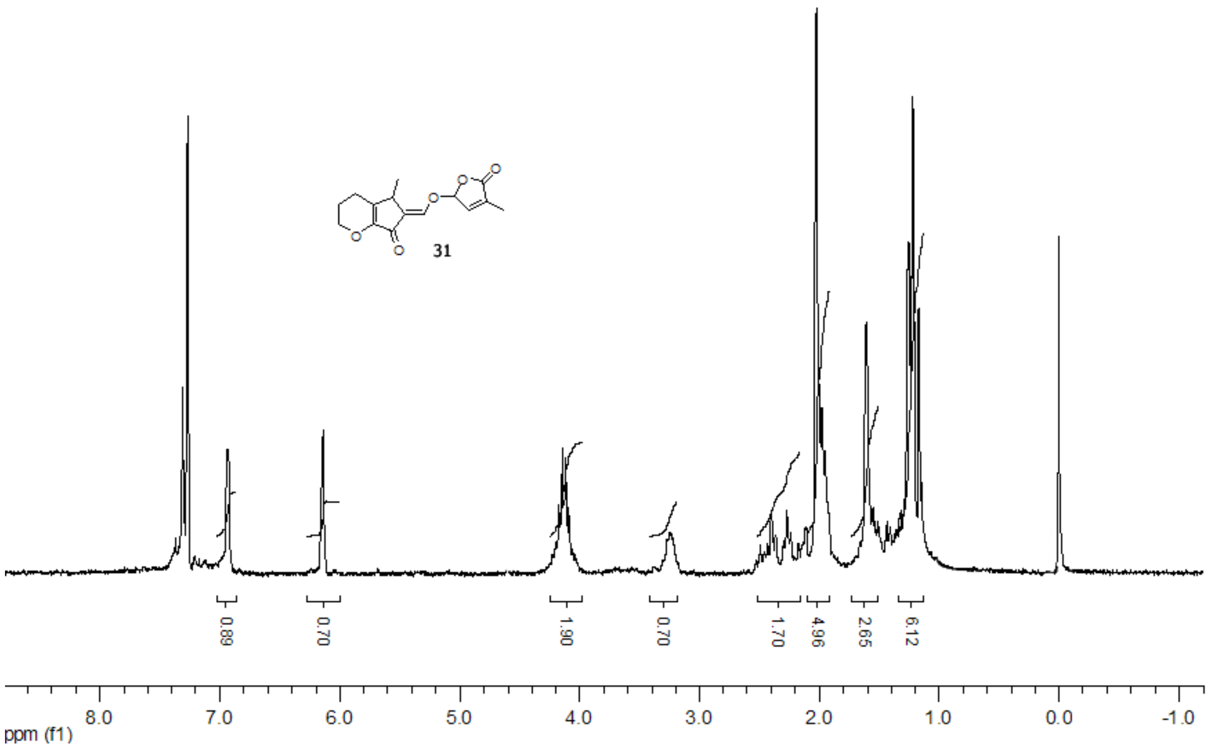

194,16
152,99
145,03
137,18
126,73
122,21
121,87
120,32
111,30
58,51
35,48
30,27
29,45
N
Me
O
13
200 150 100 50 0
ppm (f1)

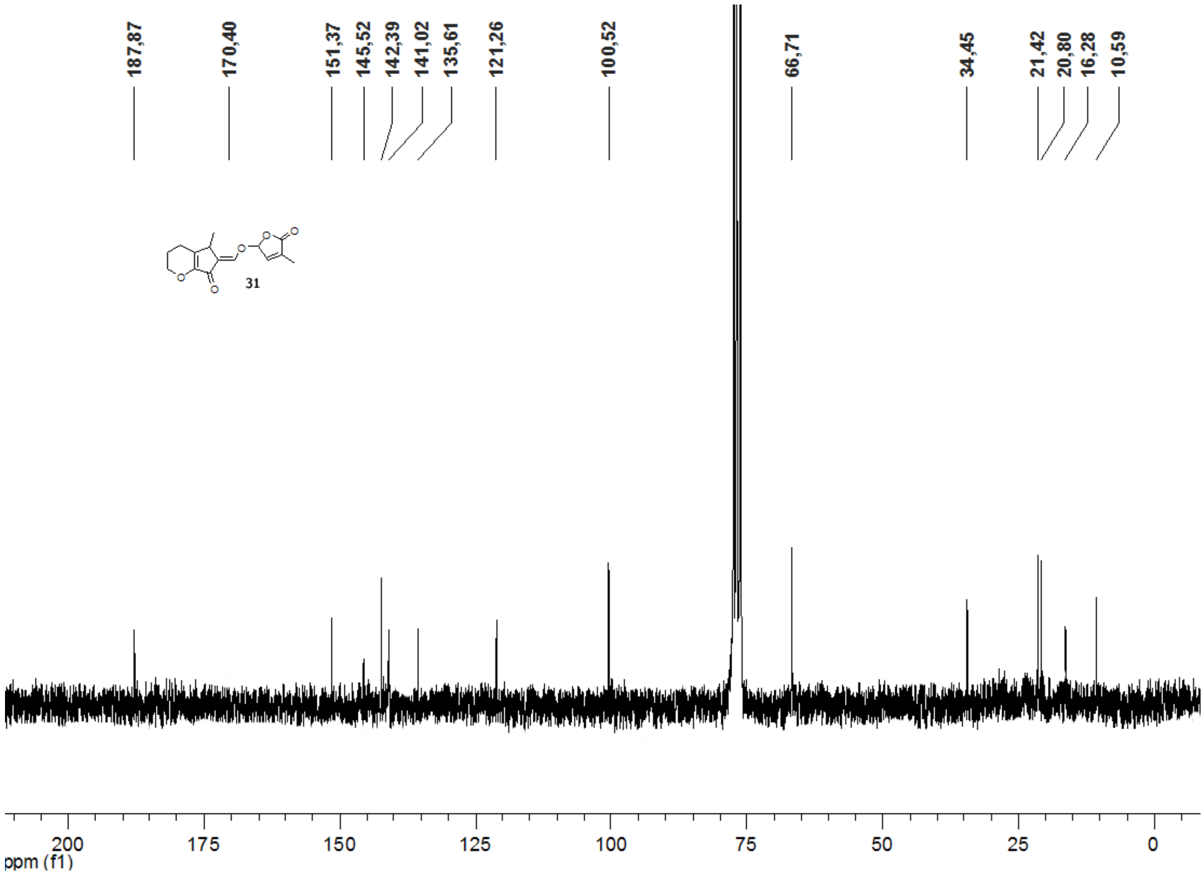

14
1.07
4.44
1.04
1.00
4.03
3.58
3.18
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
4.00
3.50
3.00
2.50
2.00
1.50
1.00
0.50
ppm (f1)

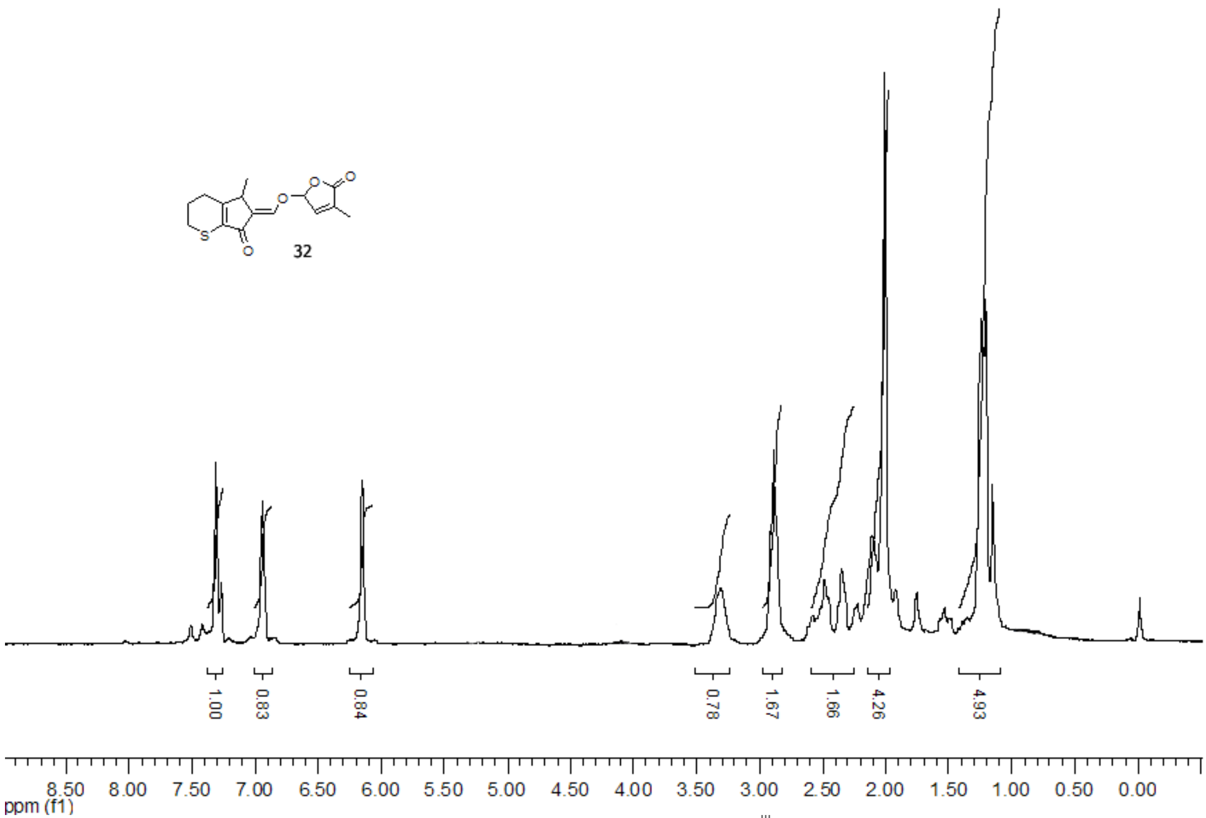

182,68
170,49
145,91
144,32
142,84
141,21
141,20
139,39
135,41
129,45
129,35
126,33
122,01
121,50
120,17
110,81
100,59
30,60
30,05
18,45
10,58
14
200
175
150
125
100
75
50
25
0
ppm (f1)

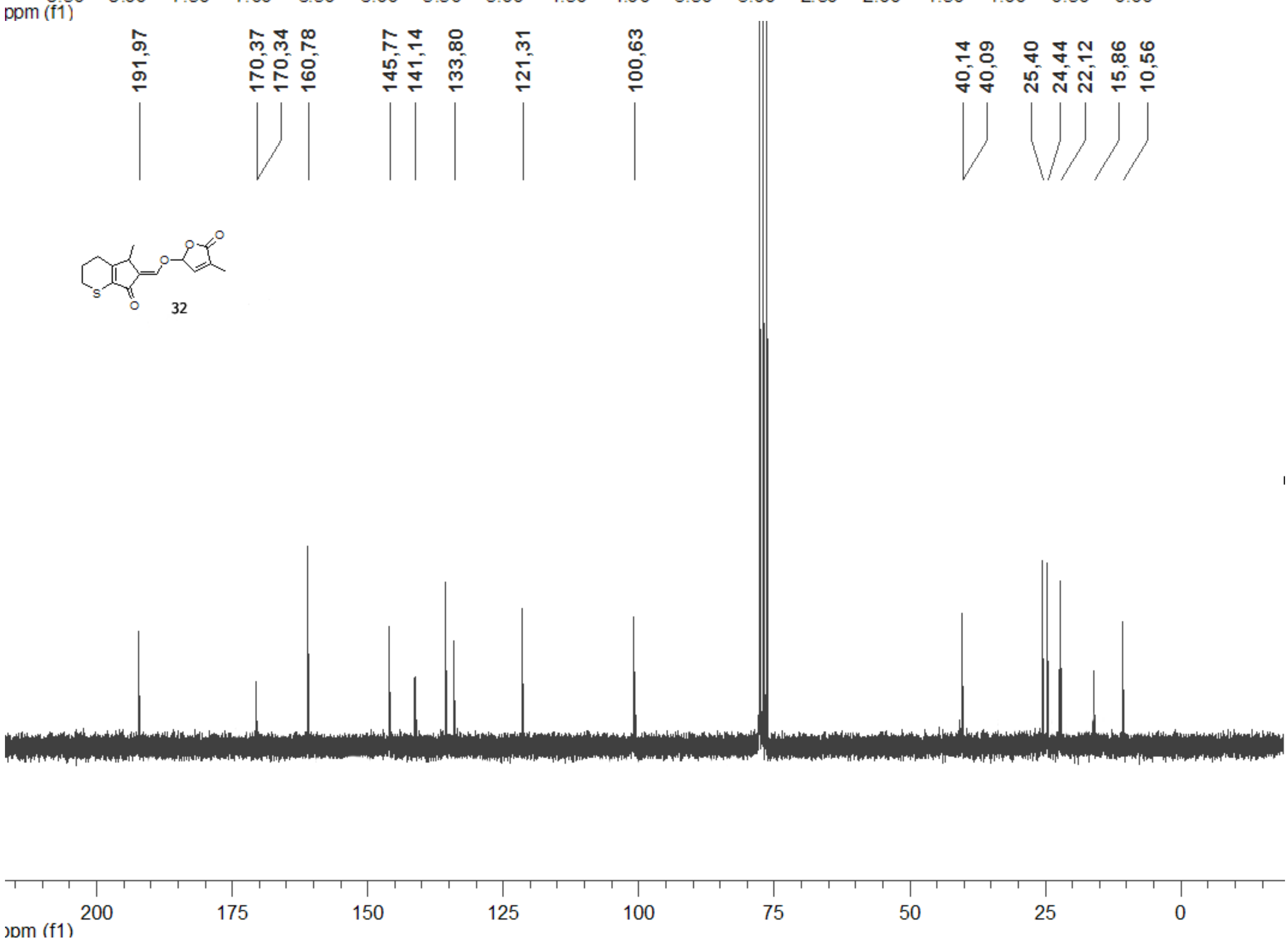

15
1.14
3.07
0.99
0.95
1.00
3.09
3.12
5.96
7.5
5.0
2.5
0.0
ppm (f1)


182,39
170,44
147,67
145,30
144,36
141,22
138,00
135,41
133,49
126,28
121,60
121,07
121,06
110,86
100,69
38,34
30,03
25,95
10,59
15
200
175
150
125
100
75
50
25
0
ppm (f1)


31
0.89
0.70
1.90
0.70
1.70
4.96
2.65
6.12
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
ppm (f1)

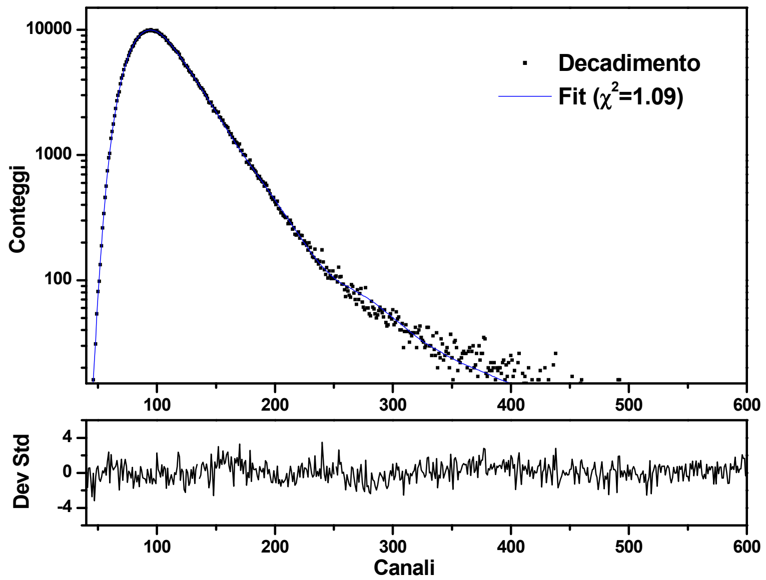

187,87
170,40
151,37
145,52
142,39
141,02
135,61
121,26
100,52
66,71
34,45
21,42
20,80
16,28
10,59
31
200
175
150
125
100
75
50
25
0
ppm (f1)


32
1.00
0.83
0.84
0.78
1.67
1.66
4.26
4.93
8.50 8.00 7.50 7.00 6.50 6.00 5.50 5.00 4.50 4.00 3.50 3.00 2.50 2.00 1.50 1.00 0.50 0.00
ppm (f1)


191,97
170,37
170,34
160,78
145,77
141,14
133,80
121,31
100,63
40,14
40,09
25,40
24,44
22,12
15,86
10,56
32
200 175 150 125 100 75 50 25 0
ppm (f1)

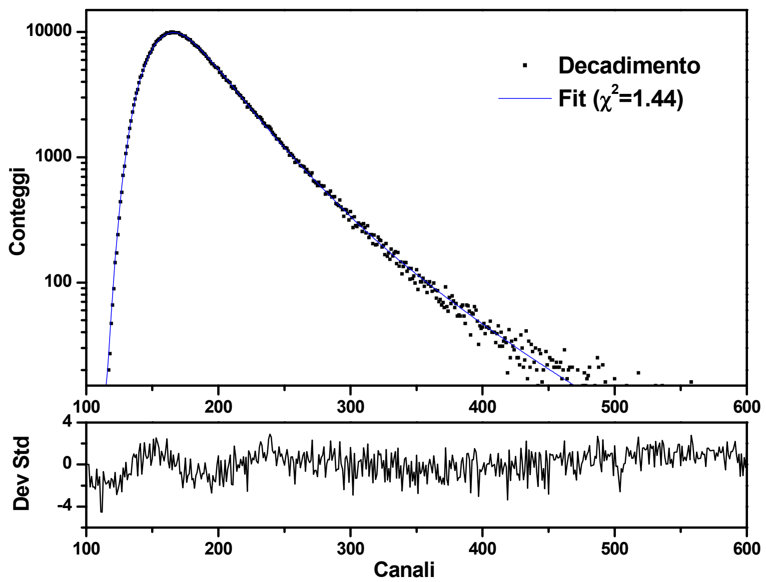
Fluorescence lifetimes were measured using a time-correlated single photon counting (TCSPC) technique (Horiba Jobin Yvon) with excitation source NanoLed at 297 nm (Horiba) and impulse repetition rate of 1 MHz at 90° to a TBX-4 detector. The detector was set to 380 nm (**5**) or 426 nm (**14**) with a 2 nm band pass. The instrument was set in the Reverse TAC mode, where the first detected photon represented the start signal by the time-to-amplitude converter (TAC), and the excitation pulse triggered the stop signal. DAS6 decay analysis software was used for lifetime calculation.

Compound **5**



Fit with biexponential curve (χ^2= 1.09) τ_1= 0.66 ns (97.54%), τ_2= 4.18 ns (2.46%)

Compound **14**



Fit with biexponential curve (χ^2= 1.44) τ_1= 0.64 ns (75.47%), τ_2= 1.57 ns (24.33%)