Supporting Information

Design and Synthesis of Potential New Apoptosis Agents: Hybrid Compounds Containing Perillyl Alcohol And New Constrained Retinoids

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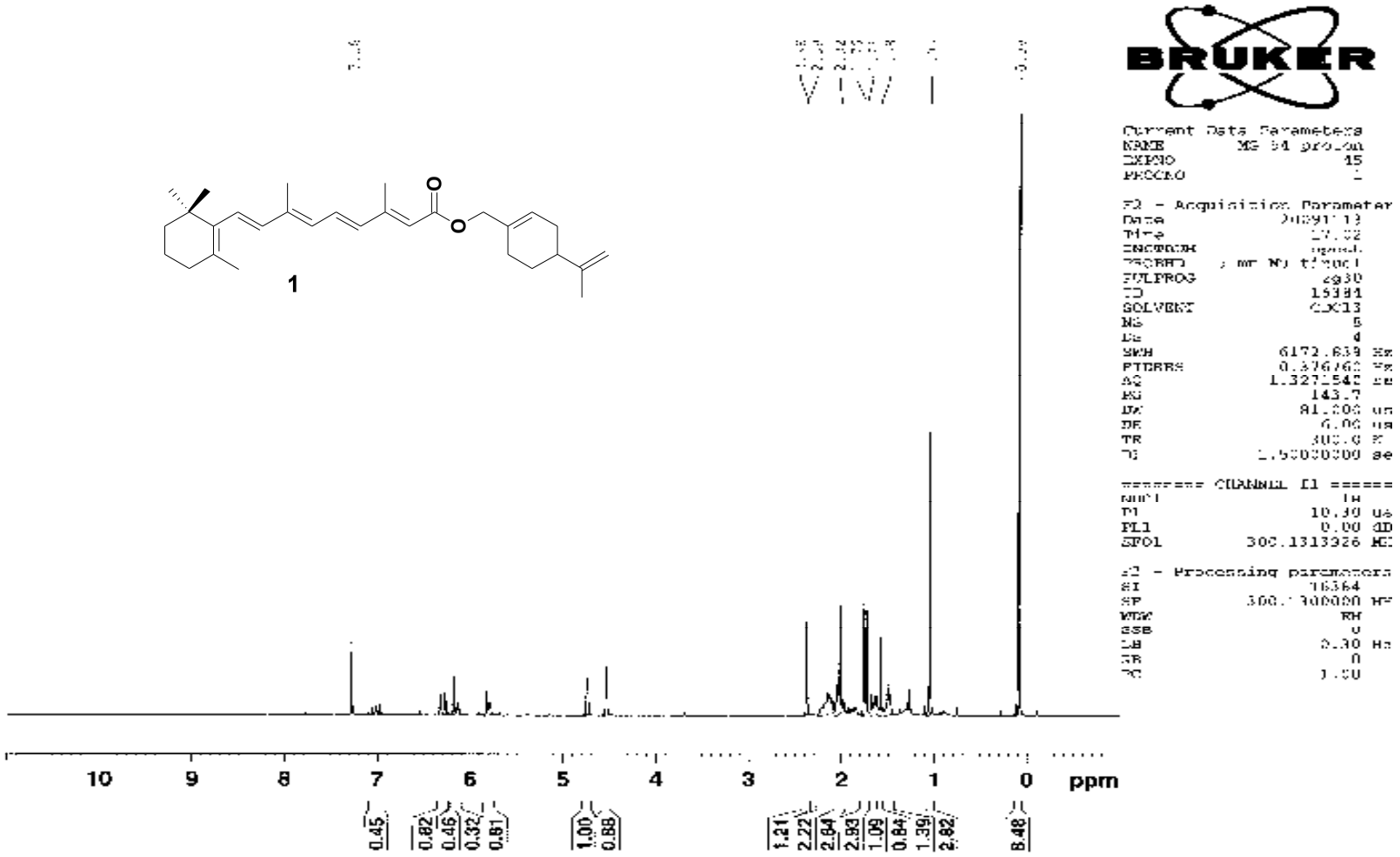
General

All reagents were purchased from commercial sources and used without treatment, unless otherwise indicated. The products were purified by column chromatography over silica gel. ^{1}H NMR and ^{13}C NMR spectra were recorded at 25 °C at 300 MHz and 75 MHz, respectively, with TMS as internal standard. Abbreviations for signal coupling are as follows: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; br, broad. Column chromatography was performed using SiO_2 (0.040 – 0.063 mm, 230 – 400 mesh ASTM) from Merck. All reagents were obtained from commercial sources. Mass spectra were recorded on Varian MS mass spectrometer.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SOLVENT CDCl3
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DE 6.00 us
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SF 300.1300000 MHz
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LB 0.30 Hz
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PC 1.00
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9
8
7
6
5
4
3
2
1
0
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0.46
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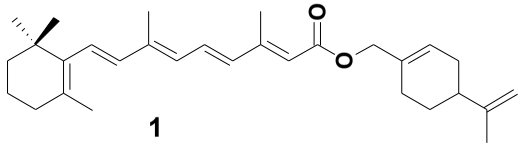

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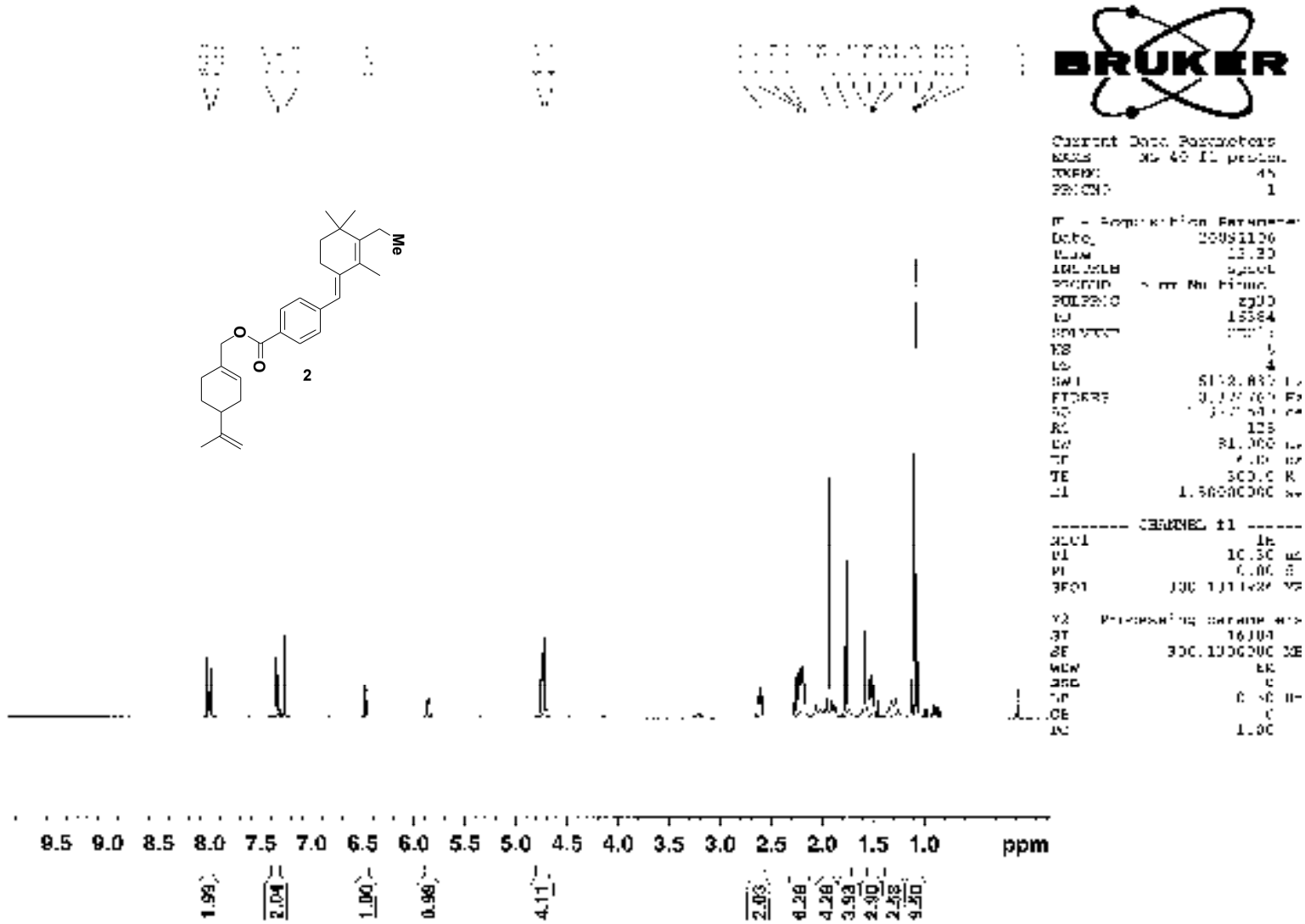
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O
2
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ppm
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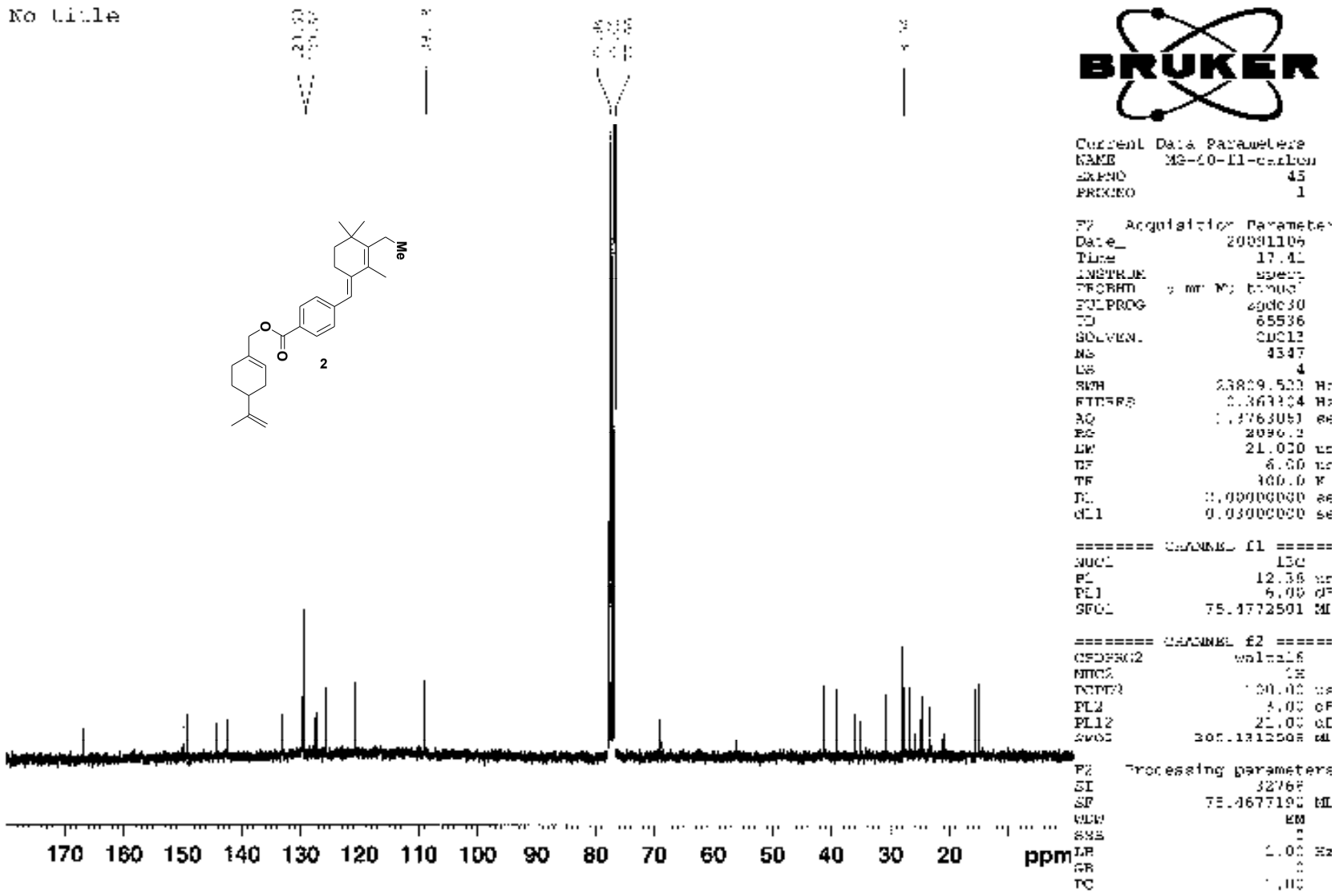
2.04
1.00
0.98
4.11
2.03
6.28
4.28
3.93
2.90
2.58
9.50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Me
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PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 4347
DS 4
SWH 23809.523 Hz
FIDRES 0.363104 Hz
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RG 2896.2
DW 21.000 us
DE 6.00 us
TE 300.0 K
D1 0.00000000 se
d11 0.03000000 se
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NUC1 13C
P1 12.36 us
PL1 6.00 dB
SFO1 75.4772501 MH
======== CHANNEL f2 ======
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NUC2 1H
PCPD2 80.00 us
PL2 3.00 dB
PL12 21.00 dB
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SSB 2
LB 1.00 Hz
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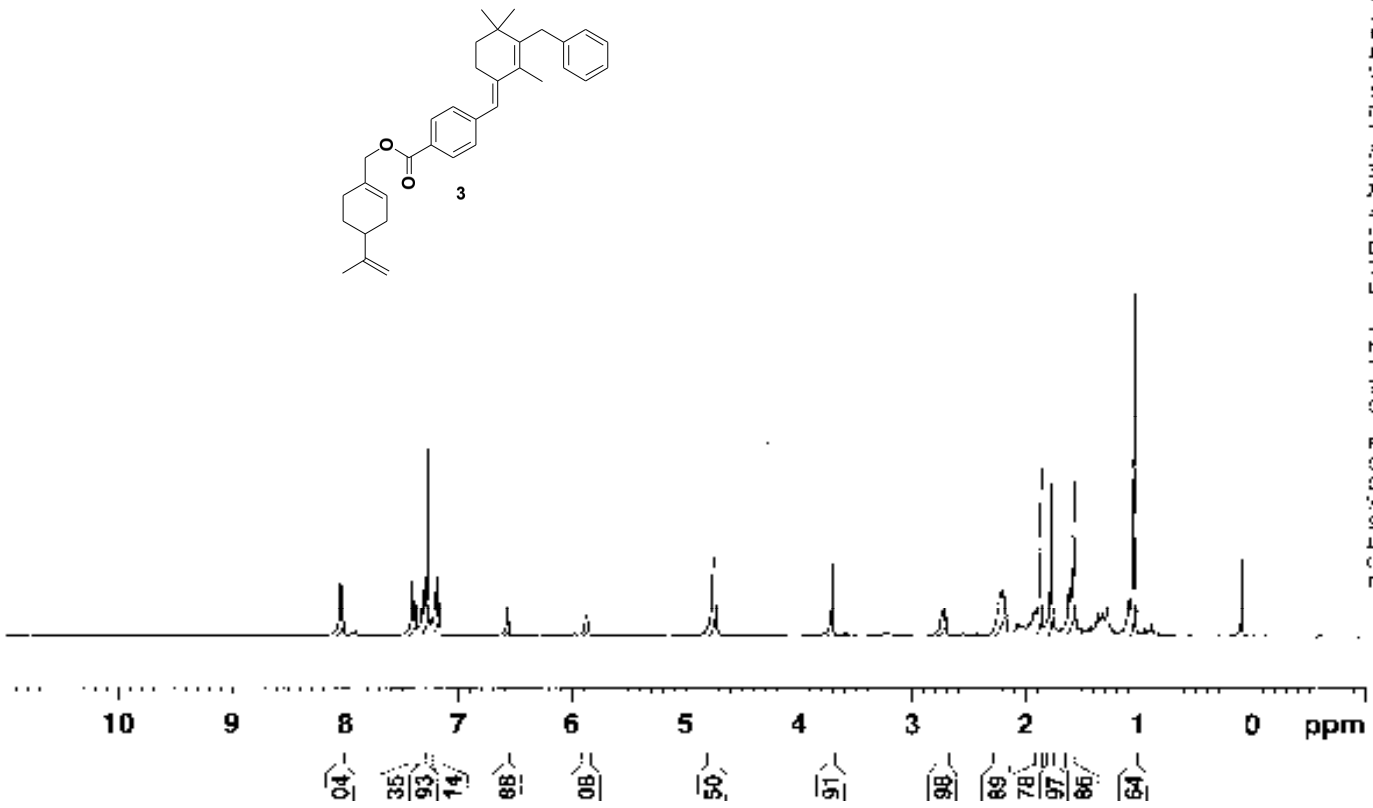
PC 1.00

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PROCNO                 1

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TD                  16384
SOLVENT              CDCl3
NS                       8
DS                       4
SWH              6172.839 H
FIDRES           0.376760 H
AQ               1.3271540 s
RG                     181
DW                 81.050 u
DE                  6.50 u
TE                 300.0 K
D1              1.00000000 s

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.30 u
PLW1                0.00 W
SFO1          300.1315929 M

F2 - Processing parameters
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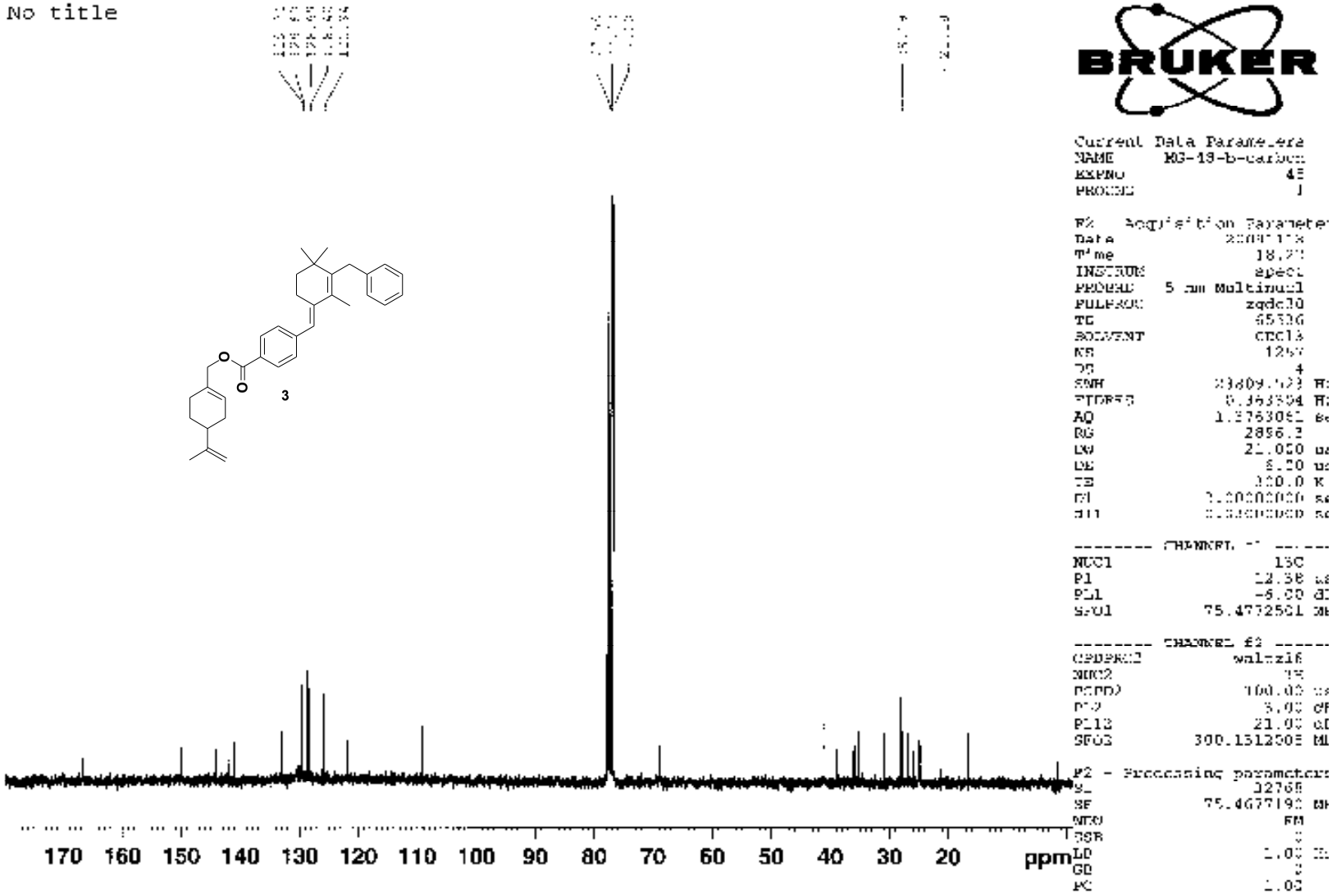

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SOLVENT CDCl3
NS 1267
DS 4
SWH 23809.523 Hz
FIDRES 0.363594 Hz
AQ 1.3763061 sec
RG 2856.3
DW 21.000 usec
DE 6.50 usec
TE 120.0 K
D1 1.00000000 sec
D11 0.03000000 sec

-------- CHANNEL f1 --------
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P1 12.50 usec
PL1 -6.00 dB
SFO1 75.4772501 MHz

-------- CHANNEL f2 --------
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NUC2 1H
PCPD2 100.00 usec
PL2 5.00 dB
PL12 21.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
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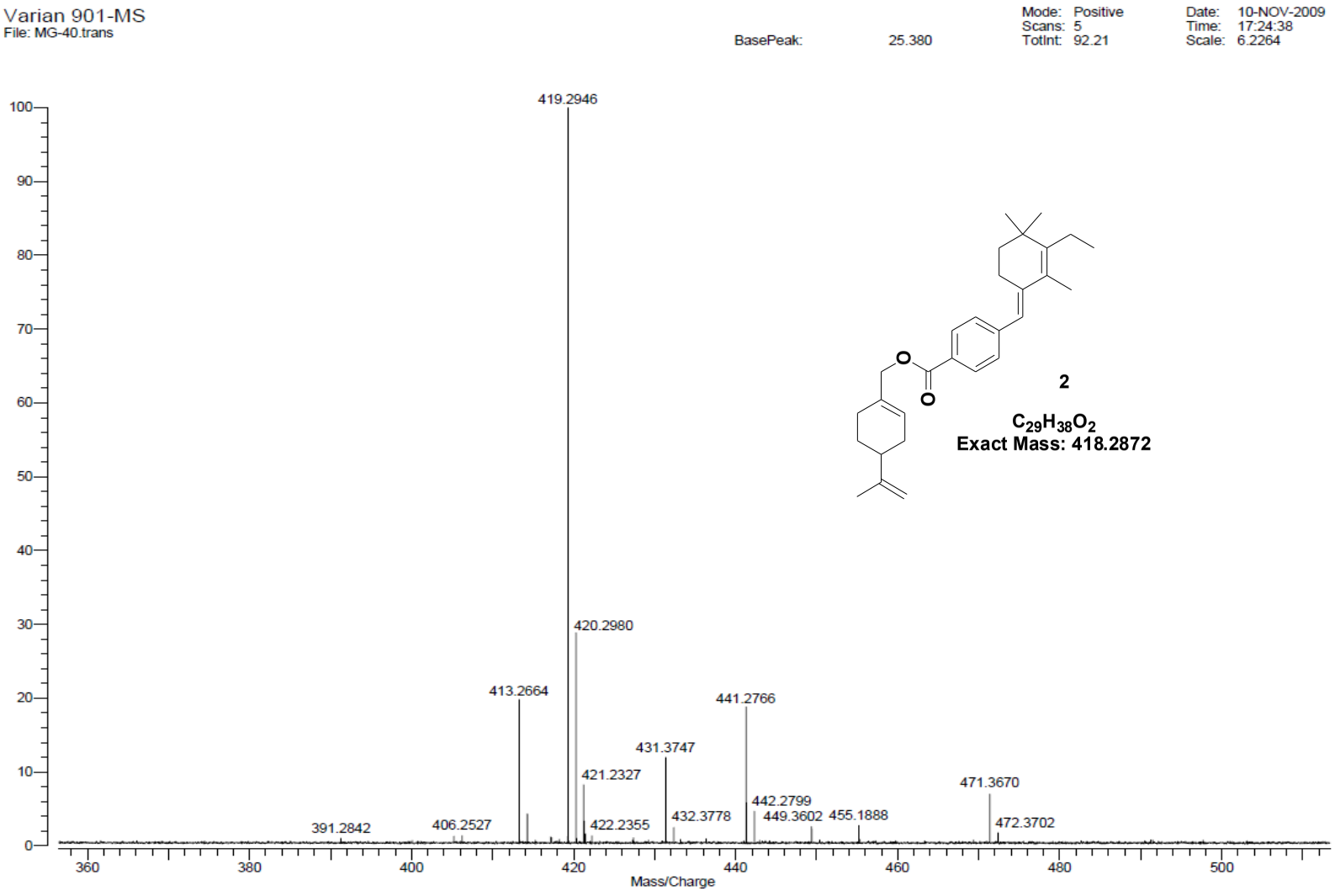
LB 1.00 Hz
GB 0
PC 1.00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Time: 17:24:38
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449.3602
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471.3670
472.3702
391.2842
406.2527
422.2355
432.3778
100
90
80
70
60
50
40
30
20
10
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Mass/Charge
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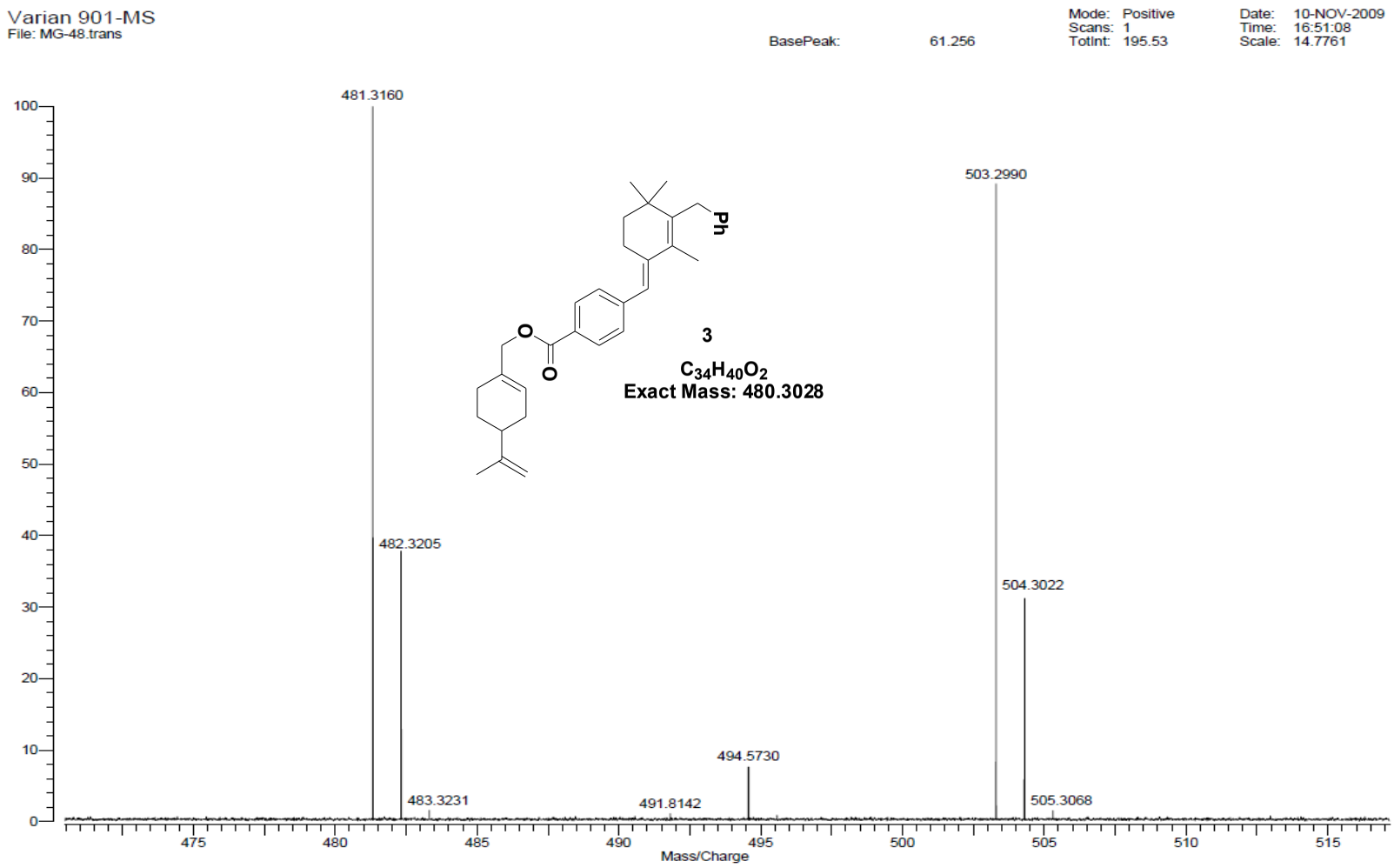
Exact Mass: 418.2872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Exact Mass: 480.3028
Mass/Charge