Supplementary Materials for:

Communication

Phenethyl Esters and Amide of Ferulic Acid, Hydroferulic Acid, Homovanillic Acid, and Vanillic Acid: Synthesis, Free Radicals Scavenging Activity, and Molecular Modeling as Potential Cholinesterases Inhibitors

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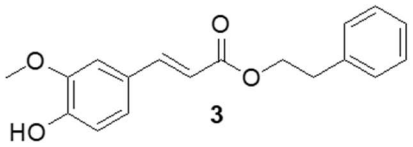
^{1}H NMR



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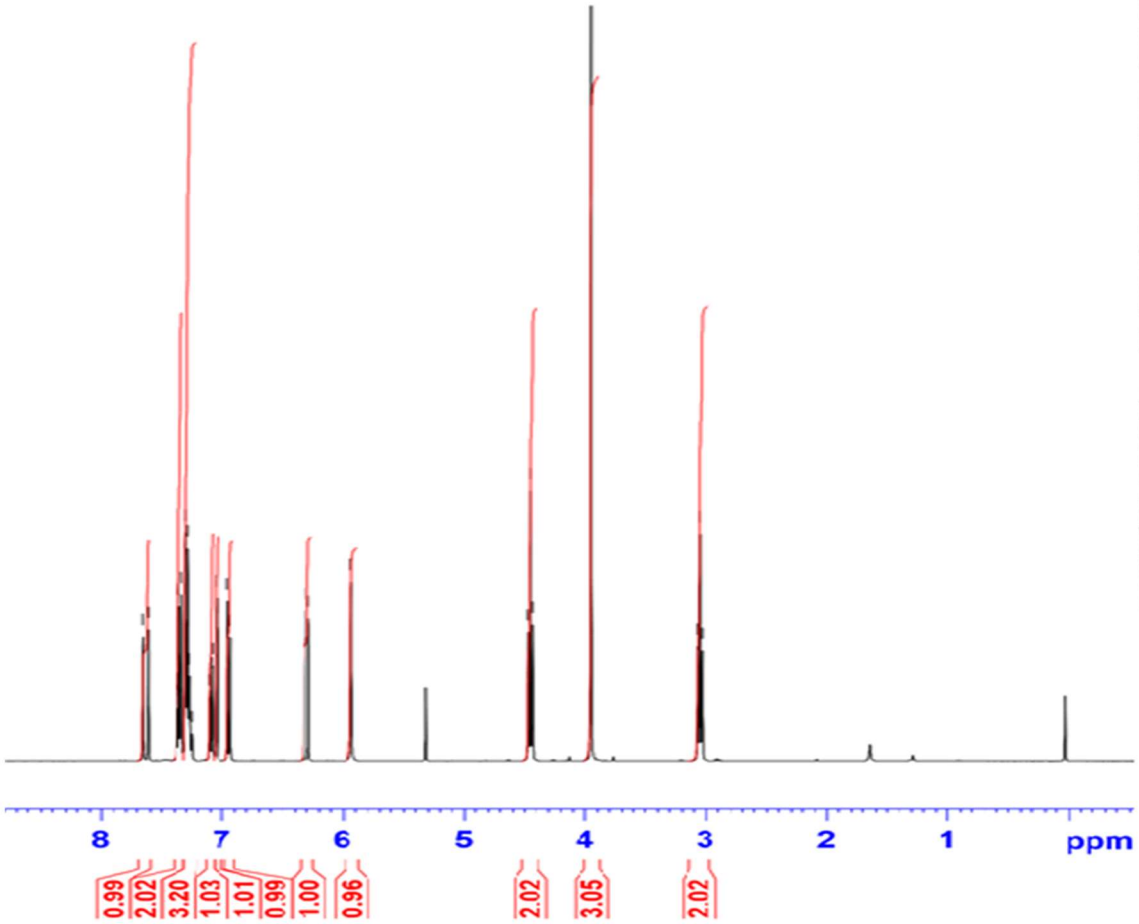

BRUKER

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PROCNO	1	
Date_	20130130	
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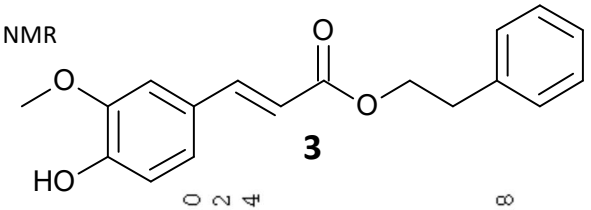
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	8223.685	Hz
FIDRES	0.125483	Hz
AQ	3.9846387	sec
RG	71.8	
DW	60.800	usec
DE	6.50	usec
TE	298.0	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	14.07	usec
PL1	0.30	dB
PL1W	11.25229836	W
SFO1	400.1324710	MHz
SI	32768	
SF	400.1300000	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

^{1}H NMR



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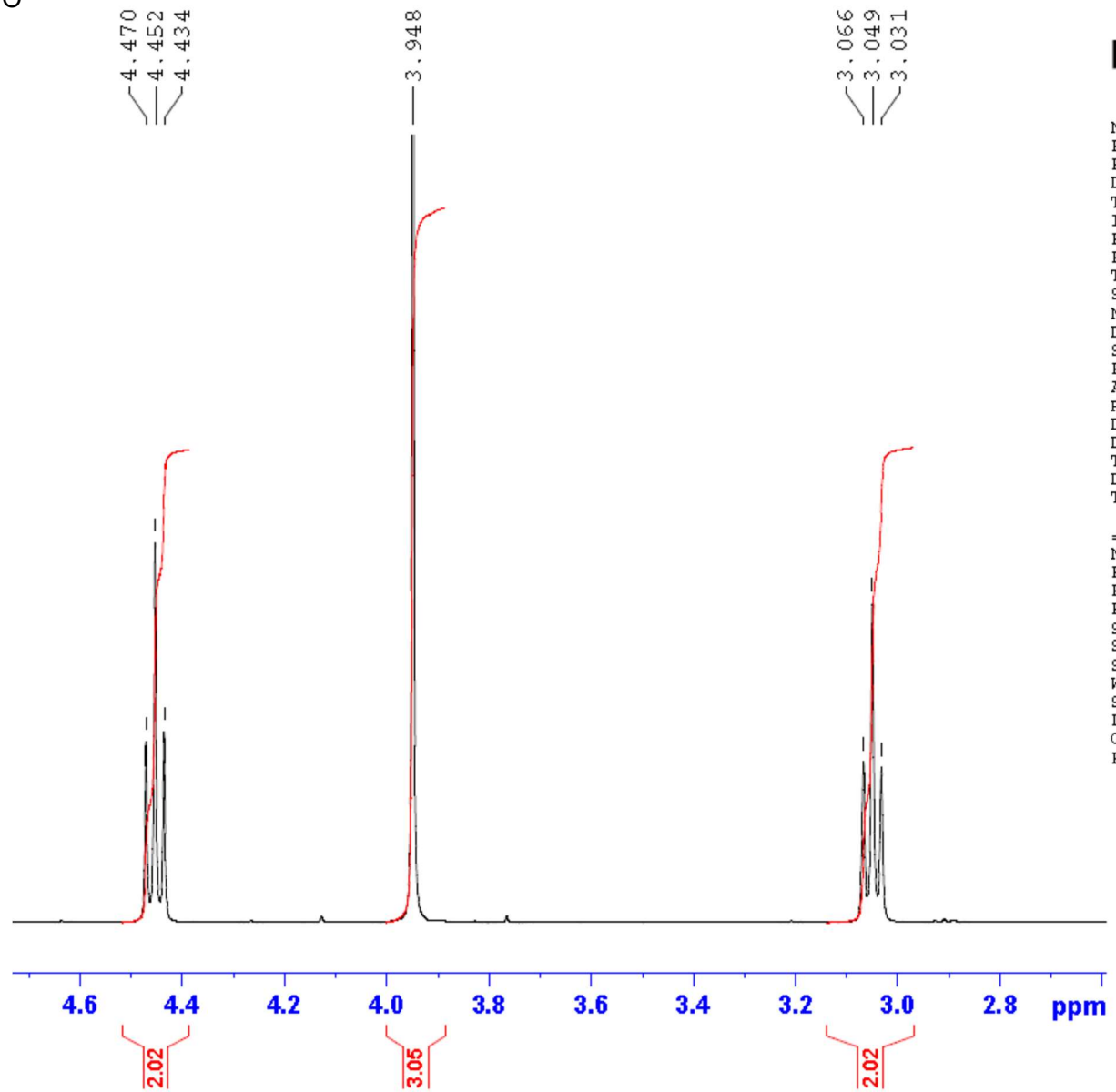
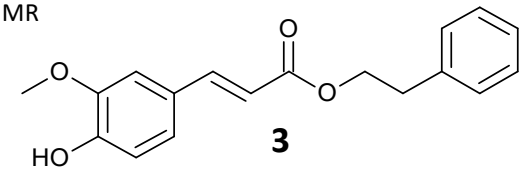


BRUKER

NAME	Moh RX
EXPNO	174
PROCNO	1
Date_	20130130
Time	12.59
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	71.8
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{1}H NMR



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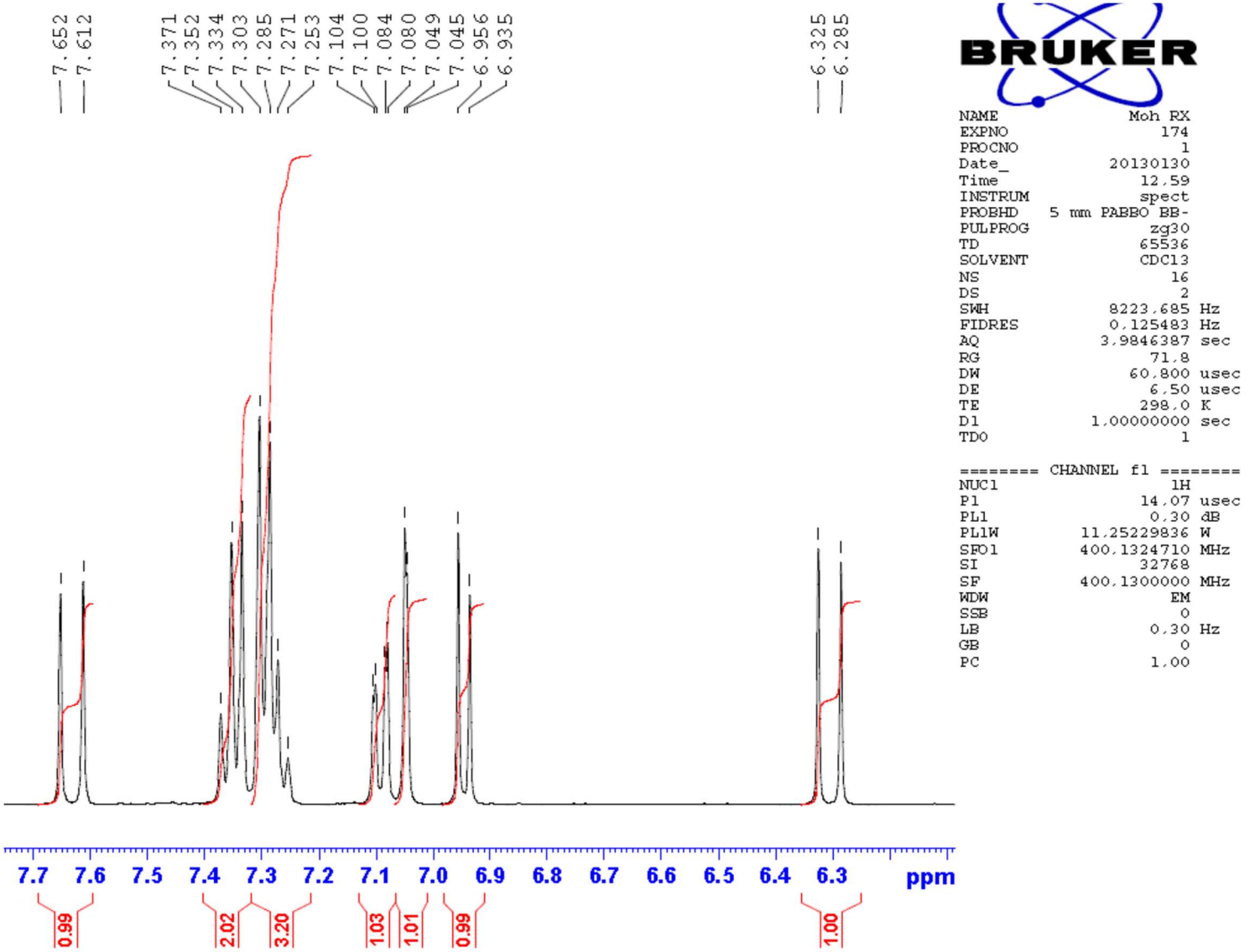
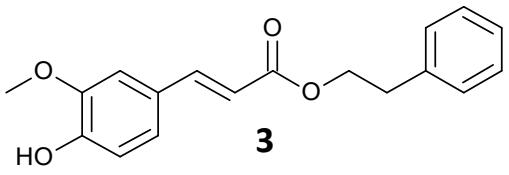


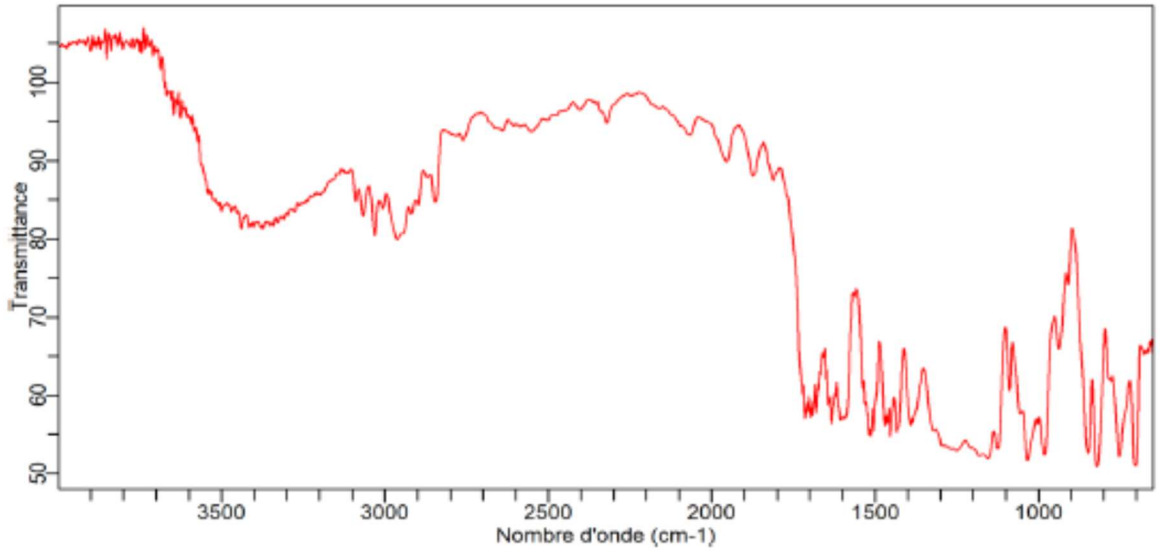
BRUKER

NAME	Moh RX
EXPNO	174
PROCNO	1
Date_	20130130
Time	12.59
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	71.8
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

FTIR


O
O
O
HO

3


Transmittance
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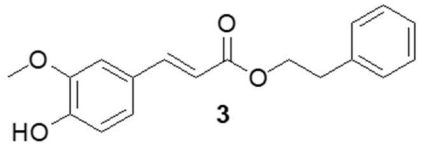
80
70
60
50
3500
3000
2500
2000
1500
1000
Nombre d'onde (cm-1)

^{13}C NMR



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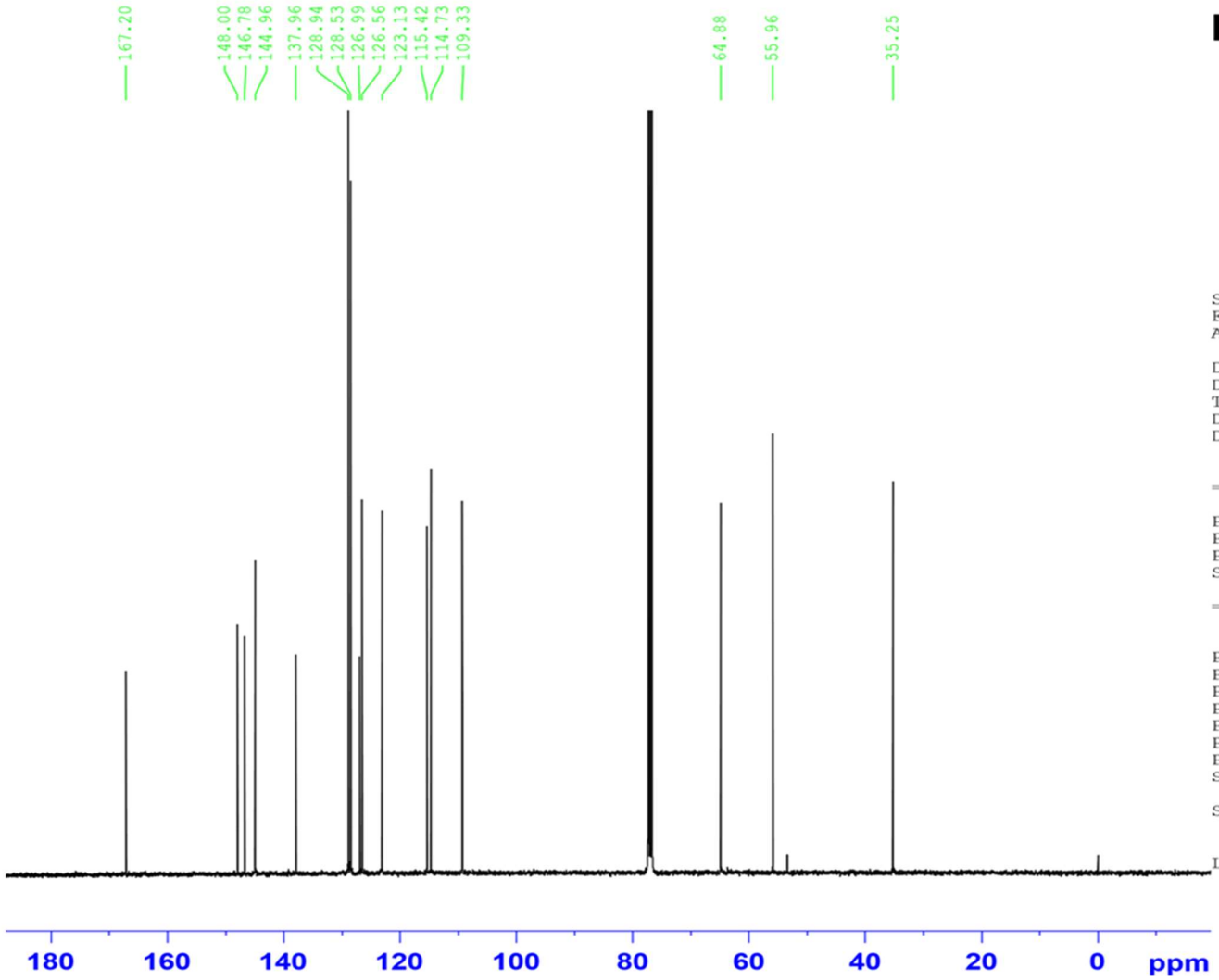
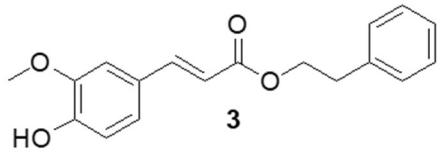


SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
DW	20.800	usec
DE	6.50	usec
TE	298.0	K
D1	2.00000000	sec
D11	0.03000000	sec
======== CHANNEL f1 ========		
P1	9.90	usec
PL1	-1.90	dB
PL1W	56.02249908	W
SFO1	100.6228298	MHz
======== CHANNEL f2 ========		
PCPD2	80.00	usec
PL2	0.30	dB
PL12	15.40	dB
PL13	18.40	dB
PL2W	11.25229836	W
PL12W	0.34772930	W
PL13W	0.17427748	W
SFO2	400.1316005	MHz
SF	100.6127690	MHz
LB	1.00	Hz

HRMS



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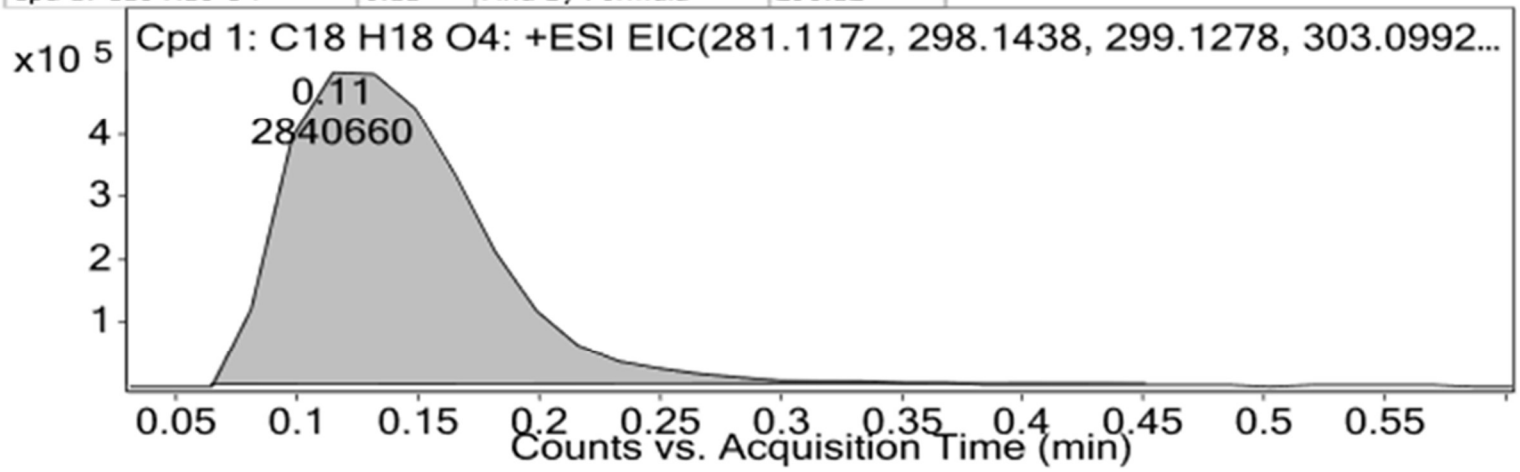
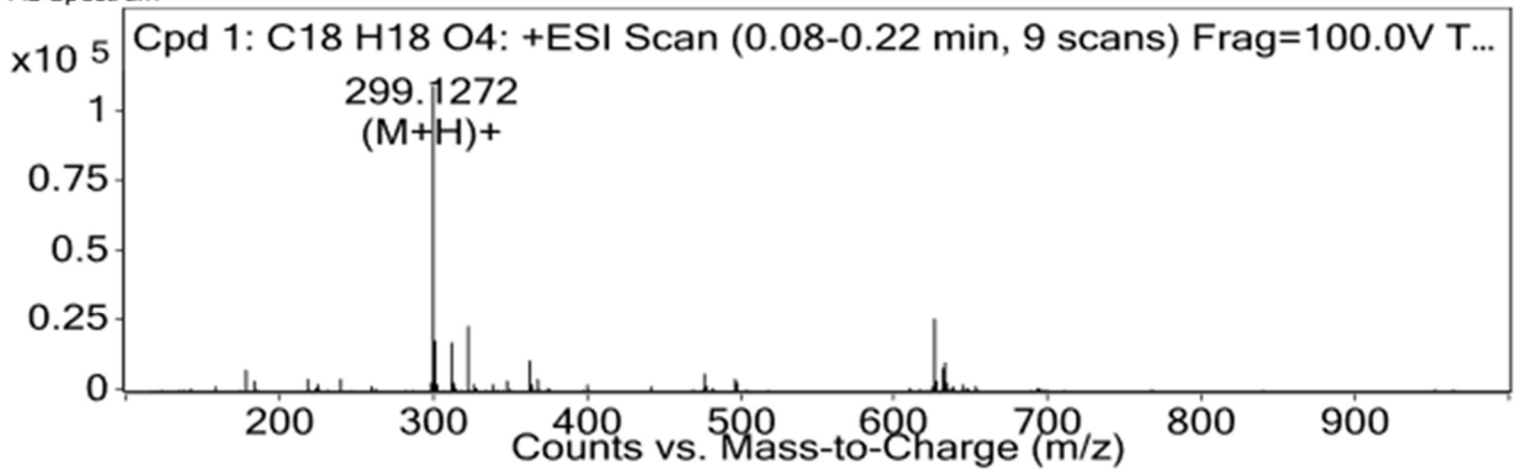
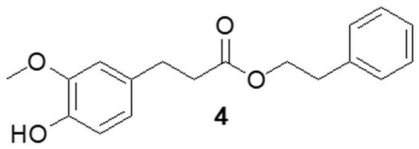
Compound Label	RT	Algorithm	Mass
Cpd 1: C18 H18 O4	0.11	Find By Formula	298.12



MS Spectrum



^{1}H NMR



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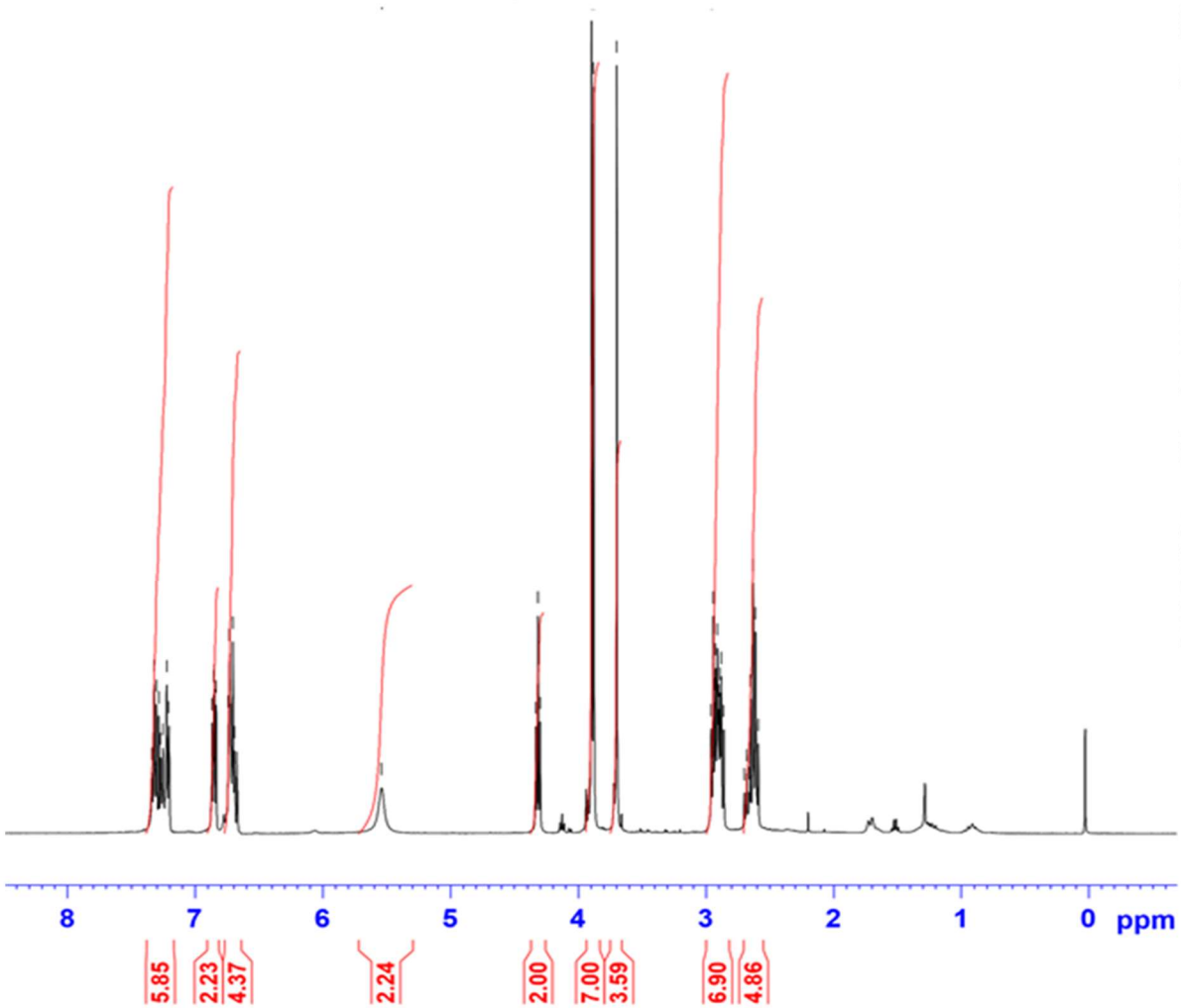
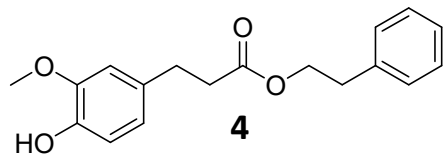



```
NAME                 Moh RX
EXPNO                   197
PROCNO                    1
Date_              20160315
Time                  10.34
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDC13
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846387 sec
RG                      71.8
DW                    60.800 usec
DE                     6.50 usec
TE                    298.0 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    14.07 usec
PL1                    0.30 dB
PL1W           11.25229836 W
SFO1           400.1324710 MHz
SI                    32768
SF             400.1300000 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

^{1}H NMR



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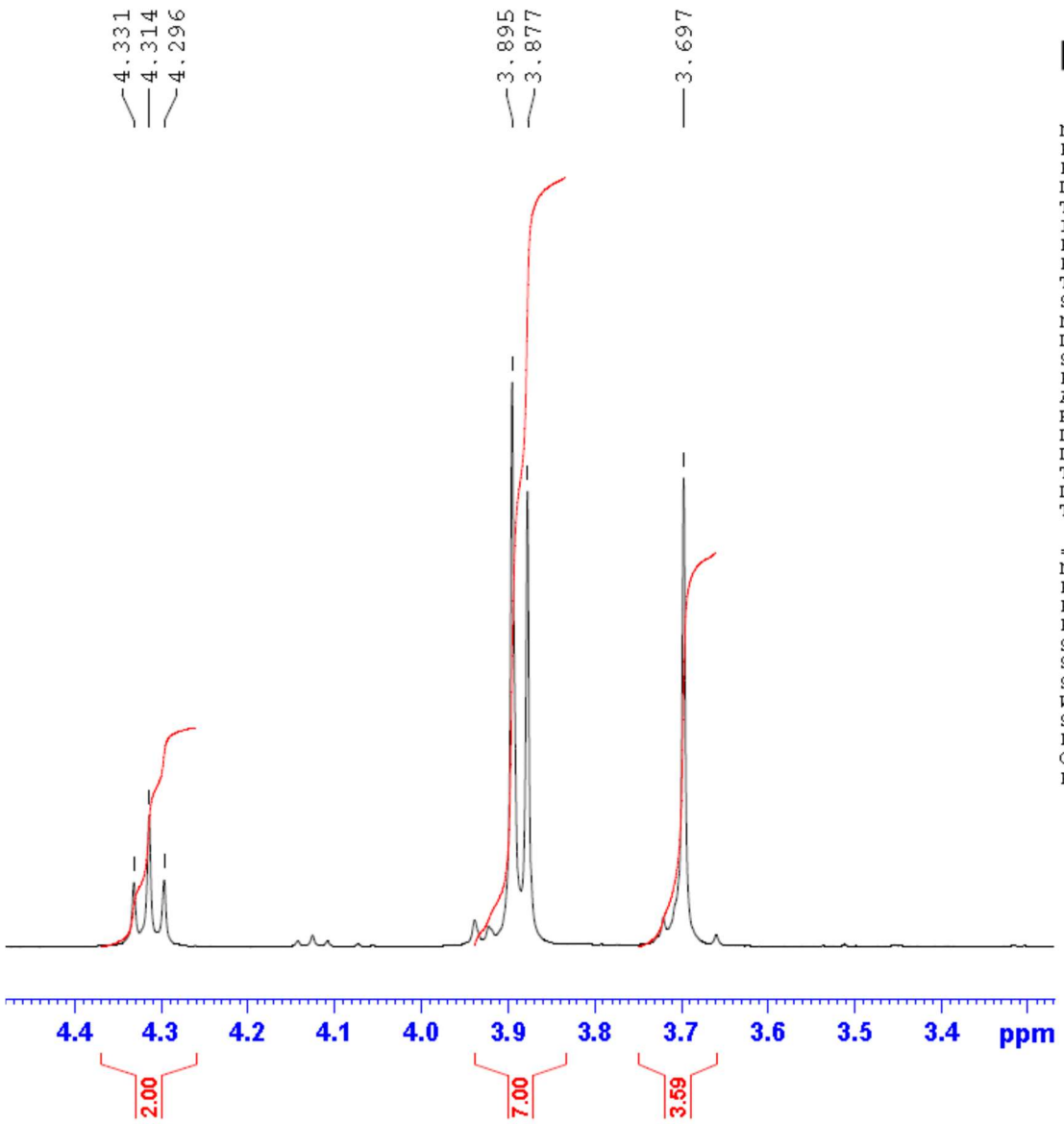


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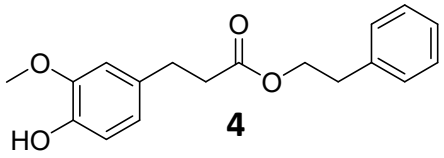
NAME                 Moh RX
EXPNO                   197
PROCNO                    1
Date_              20160315
Time                  10.34
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                     71.8
DW                   60.800 usec
DE                    6.50 usec
TE                   298.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    14.07 usec
PL1                    0.30 dB
PL1W           11.25229836 W
SFO1           400.1324710 MHz
SI                    32768
SF             400.1300000 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    1.00
```

^{1}H NMR



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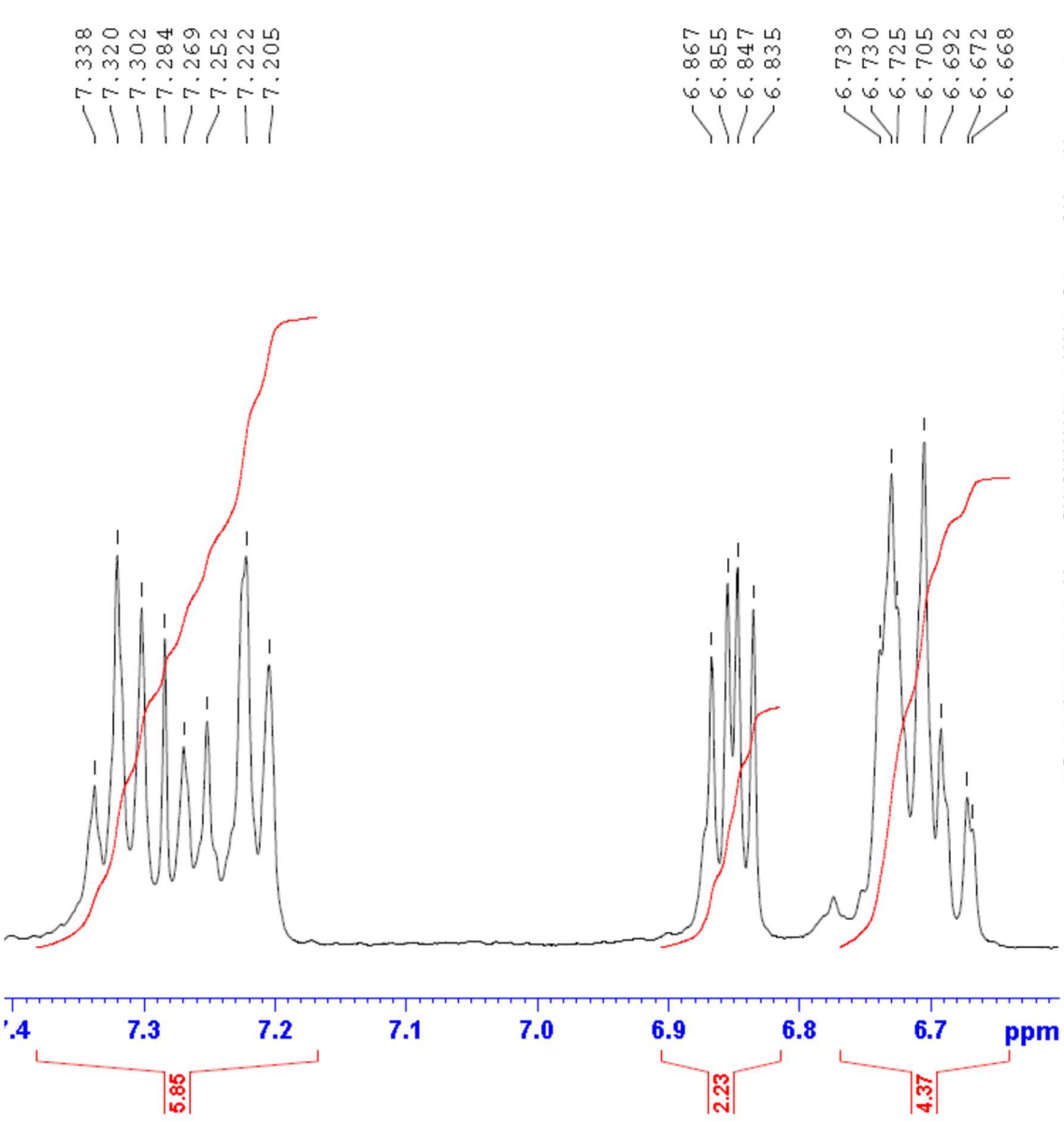
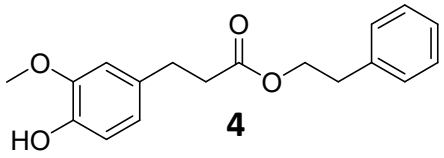


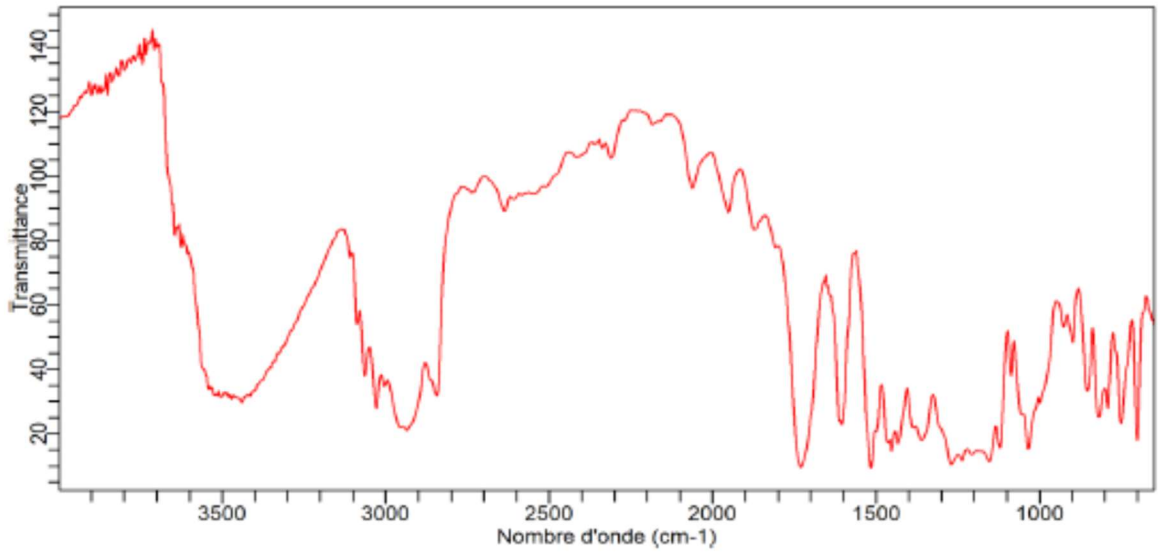

```
NAME                  Moh RX
EXPNO                    197
PROCNO                     1
Date_               20160315
Time                   10.34
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT                CDC13
NS                        16
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9846387 sec
RG                      71.8
DW                    60.800 usec
DE                     6.50 usec
TE                    298.0 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.07 usec
PL1                     0.30 dB
PL1W              11.25229836 W
SFO1              400.1324710 MHz
SI                      32768
SF                400.1300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

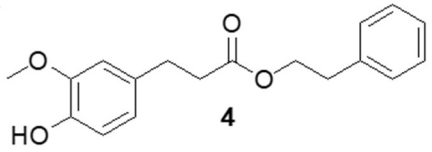
FTIR


O
O
O
HO

4


Transmittance
140
120
100
80
60
40
20
3500
3000
2500
2000
1500
1000
Nombre d'onde (cm-1)

^{13}C NMR



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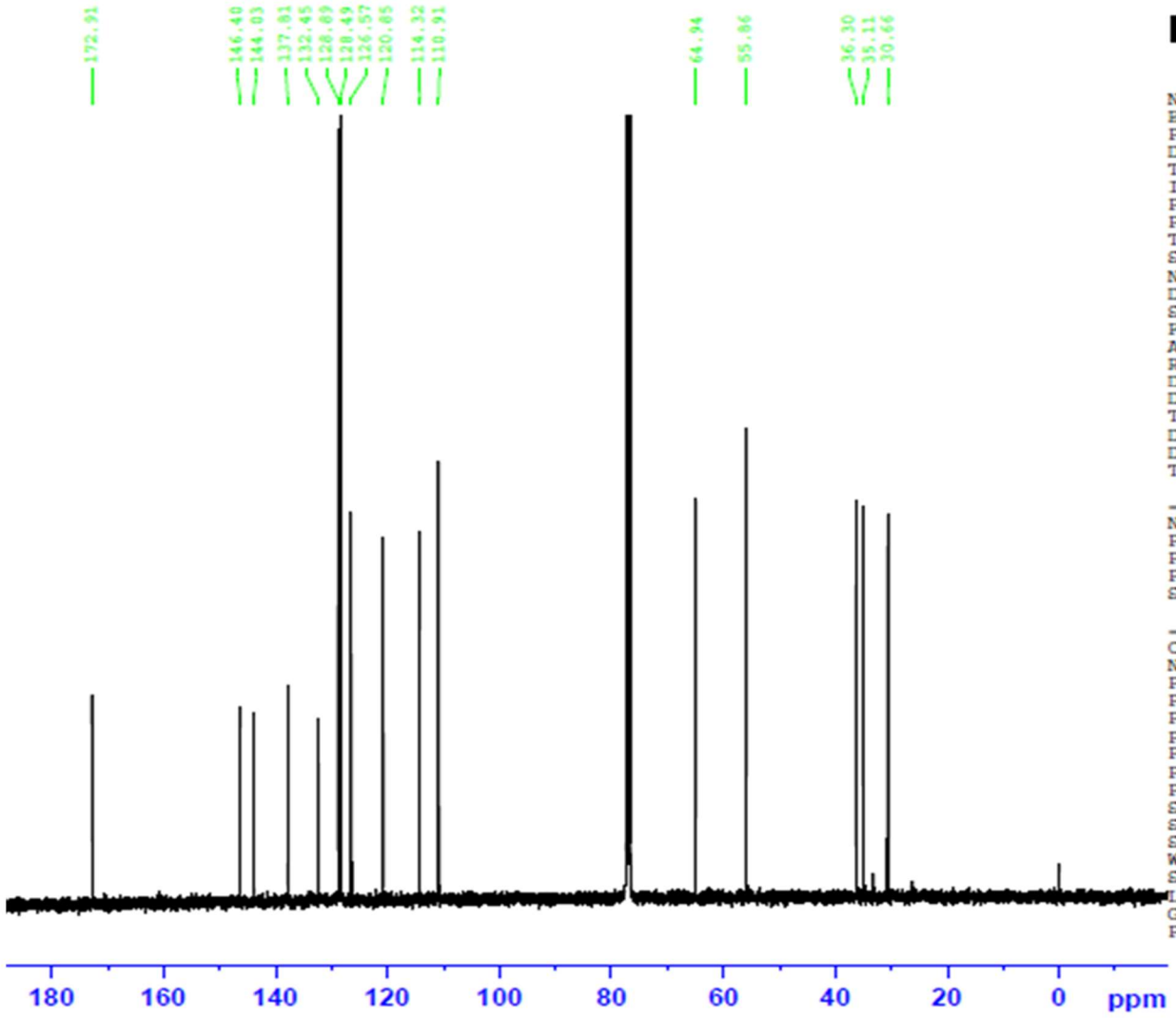

BRUKER

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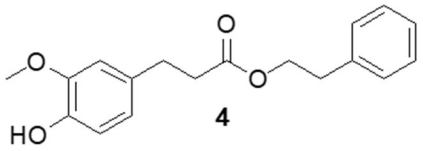
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	2551	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	203	
DW	20.800	usec
DE	6.50	usec
TE	298.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
-------- CHANNEL f1 --------		
NUC1	13C	
P1	9.90	usec
PL1	-1.90	dB
PL1W	56.02249908	W
SFO1	100.6228298	MHz
-------- CHANNEL f2 --------		
CPDPRG2	waltz65	
NUC2	1H	
PCPD2	80.00	usec
PL2	0.30	dB
PL12	15.40	dB
PL13	18.40	dB
PL2W	11.25229836	W
PL12W	0.34772930	W
PL13W	0.17427748	W
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127690	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

HRMS



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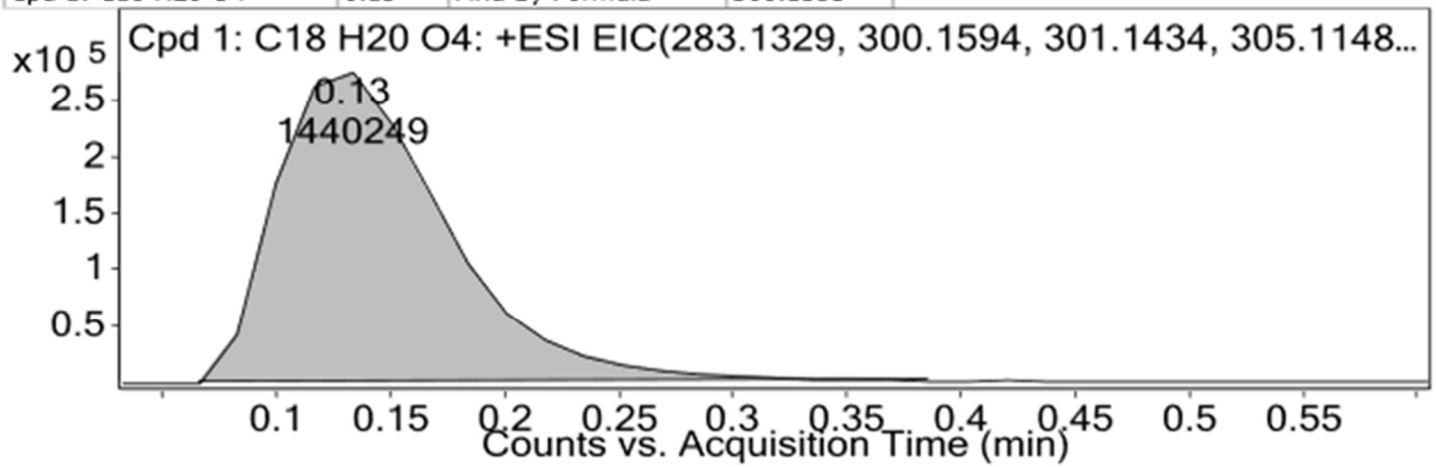
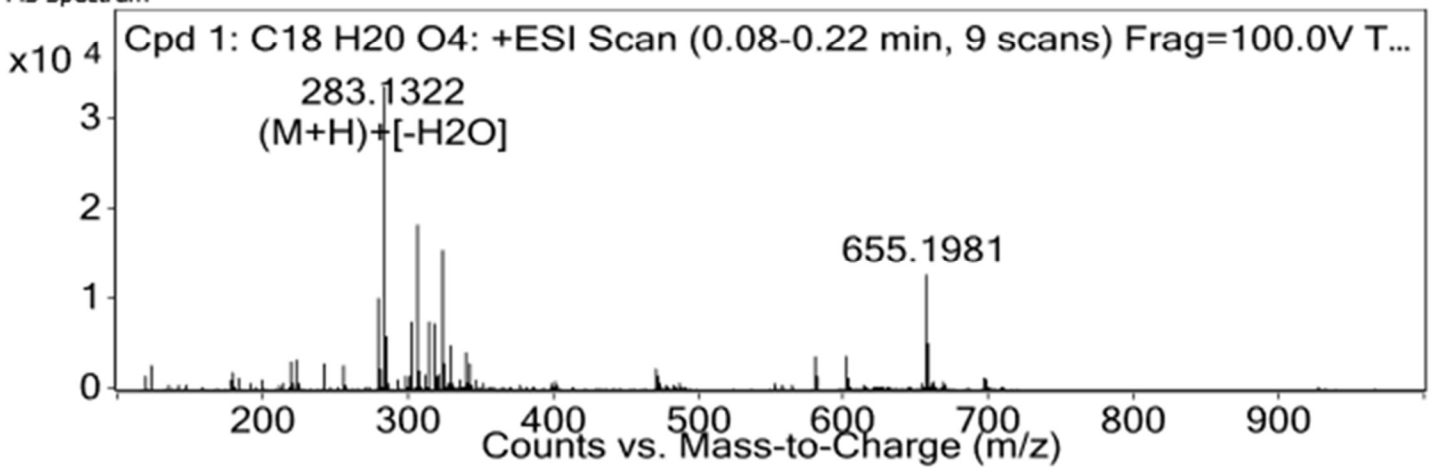
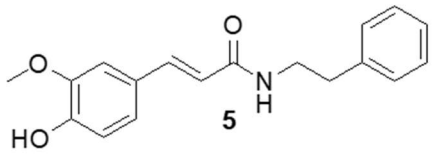
Compound Label	RT	Algorithm	Mass
Cpd 1: C18 H20 O4	0.13	Find By Formula	300.1355

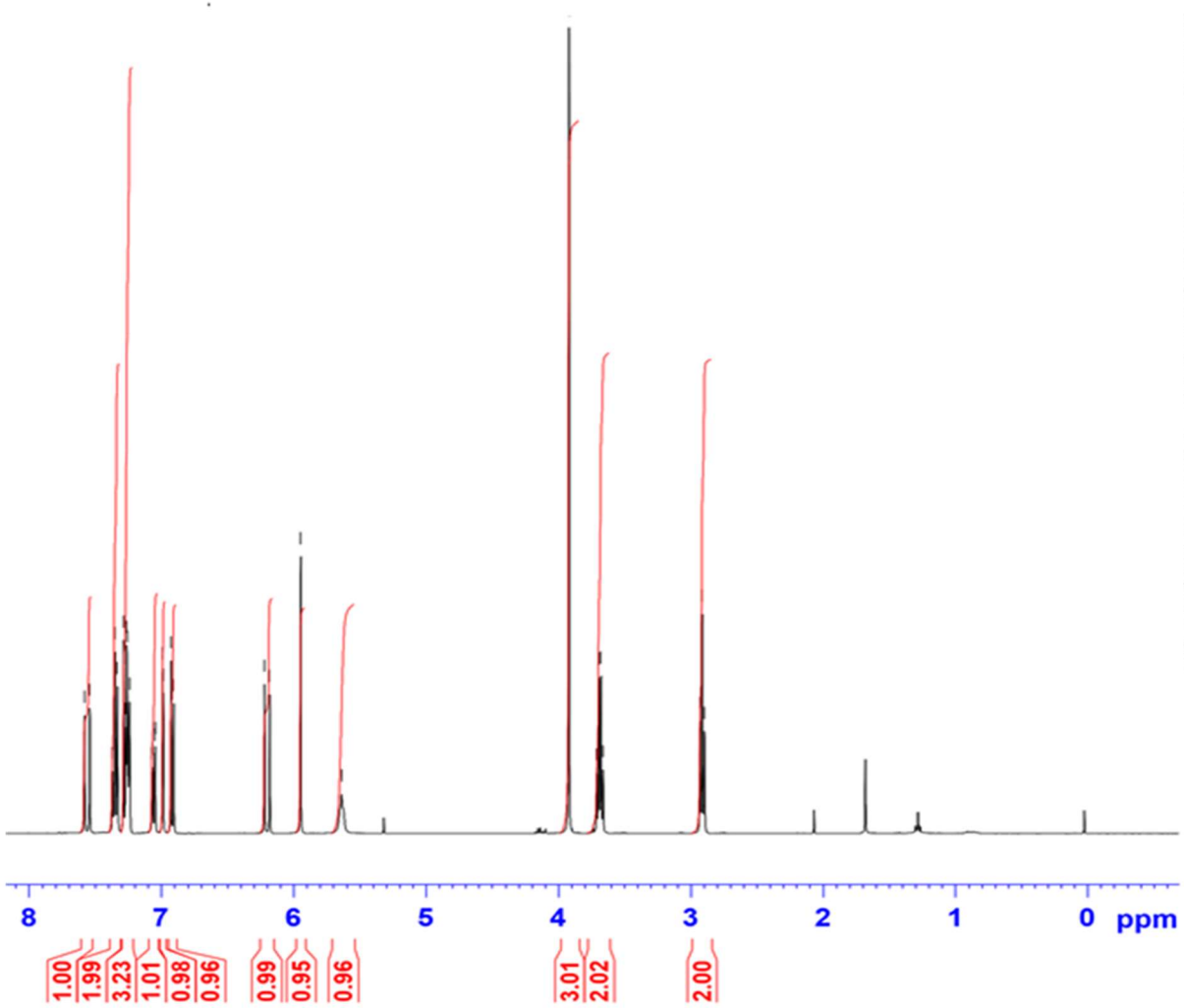


MS Spectrum



^{1}H NMR





BRUKER

NAME	Moh RX	
EXPNO	180	
PROCNO	1	
Date_	20160222	
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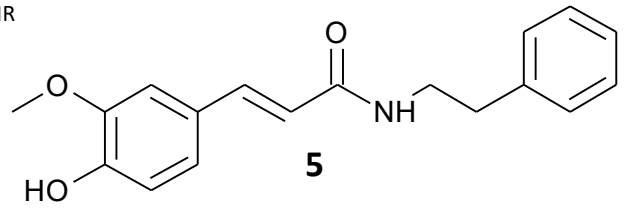
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	8223.685	Hz
FIDRES	0.125483	Hz
AQ	3.9846387	sec
RG	90.5	
DW	60.800	usec
DE	6.50	usec
TE	298.0	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	14.07	usec
PL1	0.30	dB
PL1W	11.25229836	W
SFO1	400.1324710	MHz
SI	32768	
SF	400.1300000	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

^{1}H NMR



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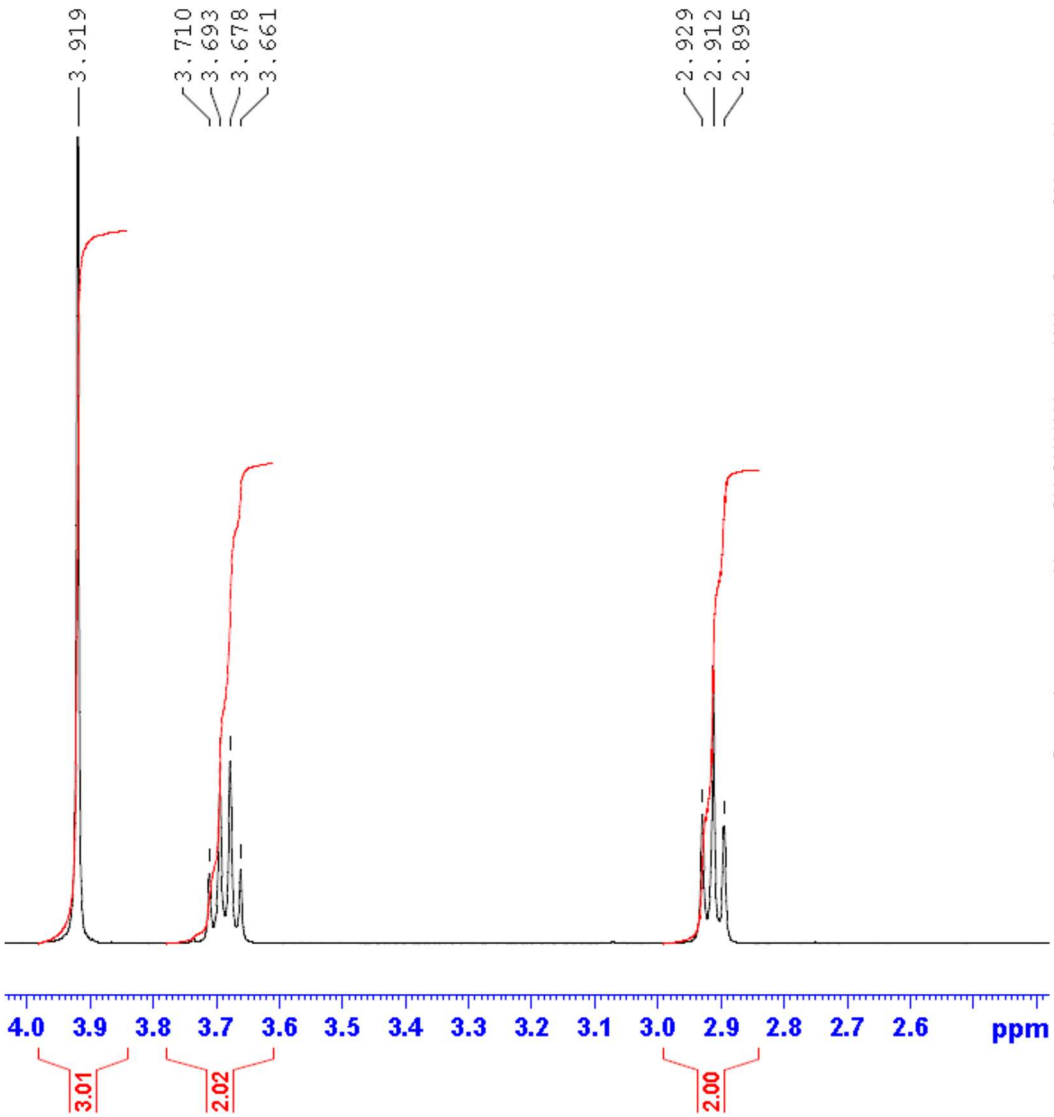
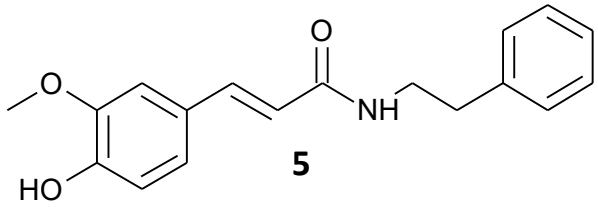


BRUKER

NAME	Moh RX	
EXPNO	180	
PROCNO	1	
Date_	20160222	
Time	16.20	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	8223.685	Hz
FIDRES	0.125483	Hz
AQ	3.9846387	sec
RG	90.5	
DW	60.800	usec
DE	6.50	usec
TE	298.0	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	14.07	usec
PL1	0.30	dB
PL1W	11.25229836	W
SFO1	400.1324710	MHz
SI	32768	
SF	400.1300000	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

^{1}H NMR



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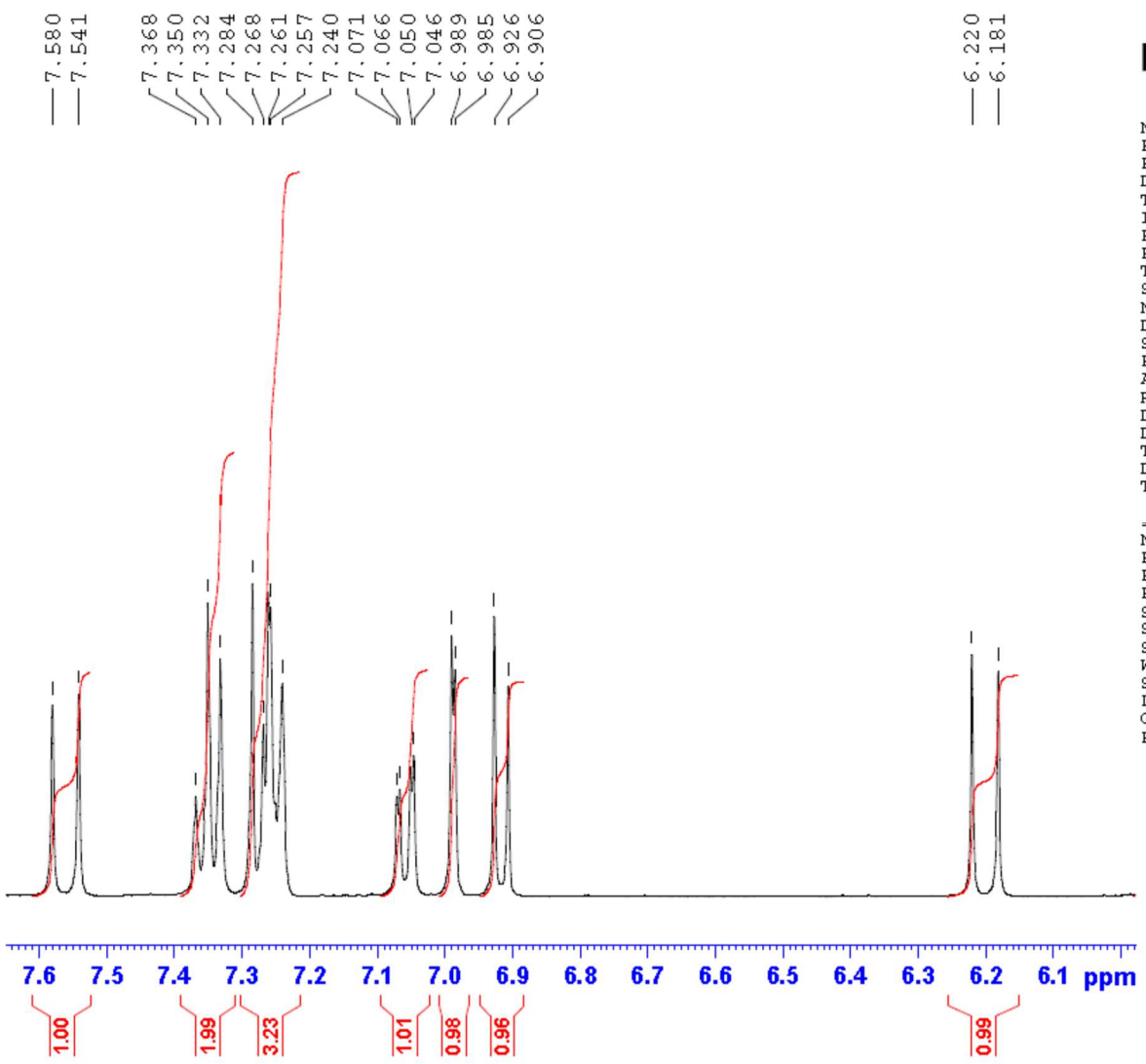
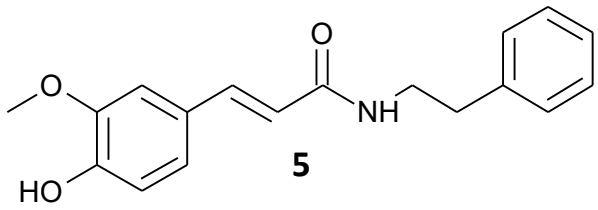


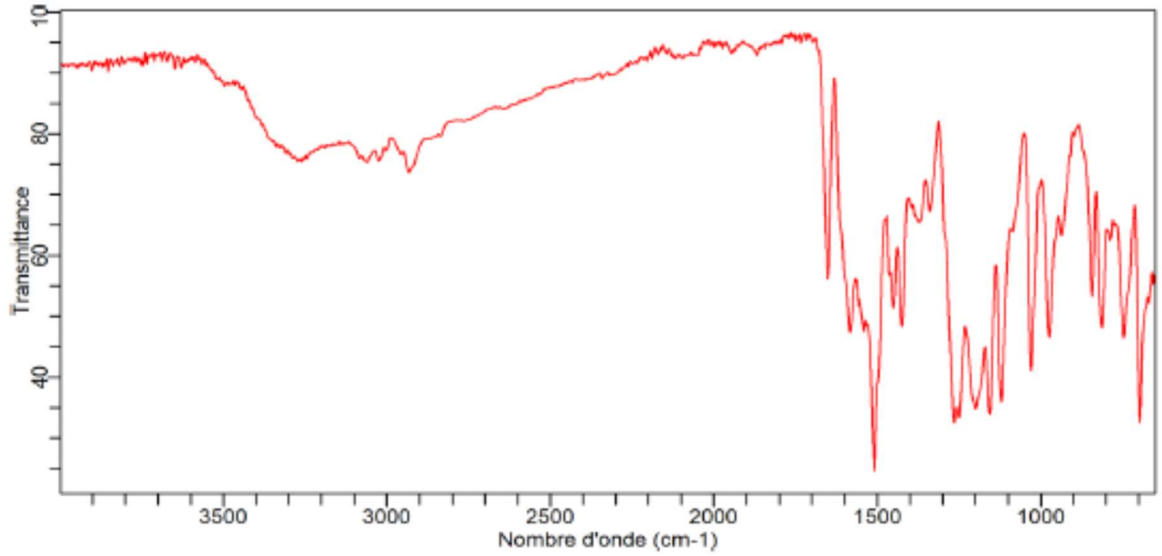
BRUKER

NAME	Moh RX
EXPNO	180
PROCNO	1
Date_	20160222
Time	16.20
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	90.5
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

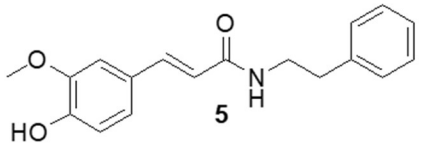
FTIR

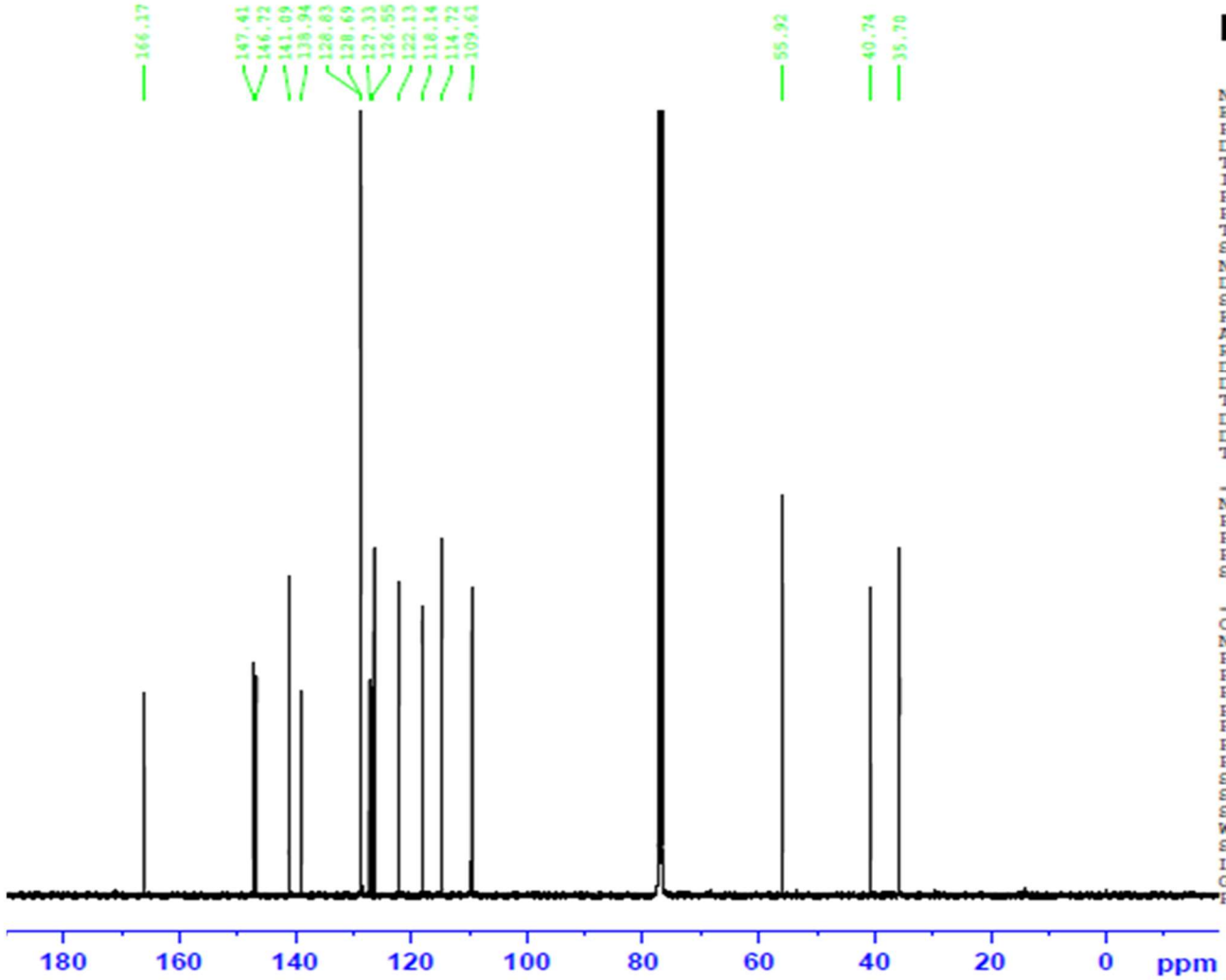

O
O
NH
HO

5


Transmittance
100
80
60
40
3500
3000
2500
2000
1500
1000
Nombre d'onde (cm-1)

^{13}C NMR

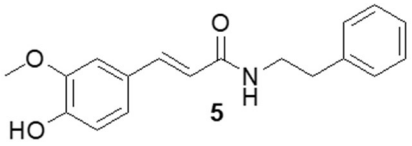




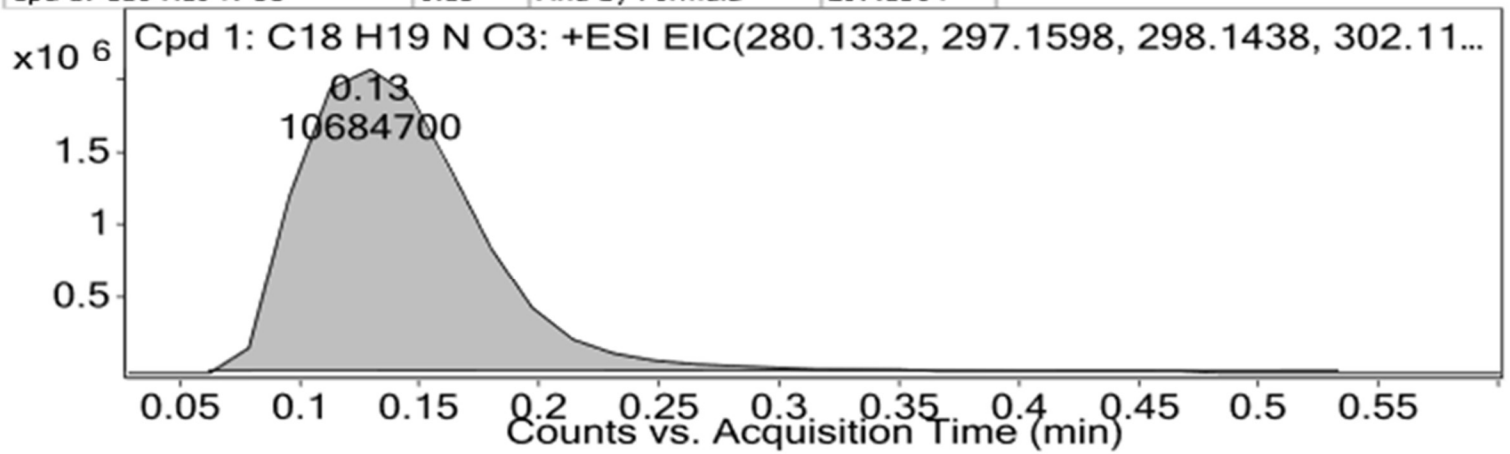
BRUKER

NAME	Moh RX	
EXPNO	182	
PROCNO	1	
Date_	20160223	
Time	2.02	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	10000	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	203	
DW	20.800	usec
DE	6.50	usec
TE	298.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
-------- CHANNEL f1 --------		
NUC1	13C	
P1	9.90	usec
PL1	-1.90	dB
PL1W	56.02249908	W
SFO1	100.6228298	MHz
-------- CHANNEL f2 --------		
CPDPRG2	waltz65	
NUC2	1H	
PCPD2	80.00	usec
PL2	0.30	dB
PL12	15.40	dB
PL13	18.40	dB
PL2W	11.25229836	W
PL12W	0.34772930	W
PL13W	0.17427748	W
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127690	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

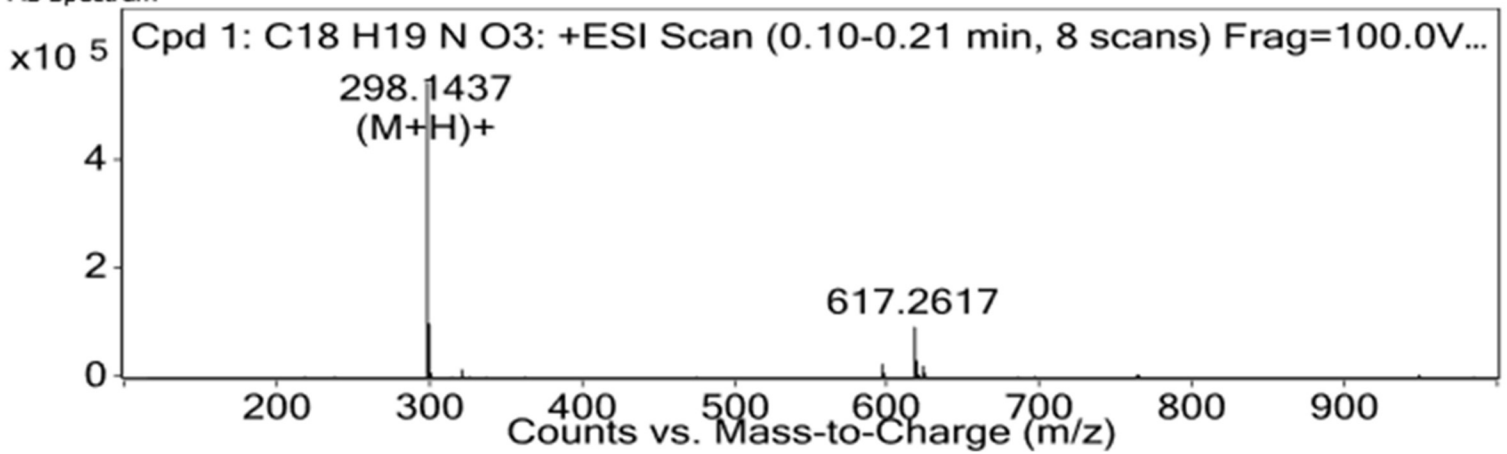
HRMS



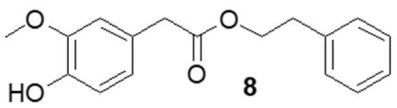
Compound Label	RT	Algorithm	Mass
Cpd 1: C18 H19 N O3	0.13	Find By Formula	297.1364



MS Spectrum



^{1}H NMR



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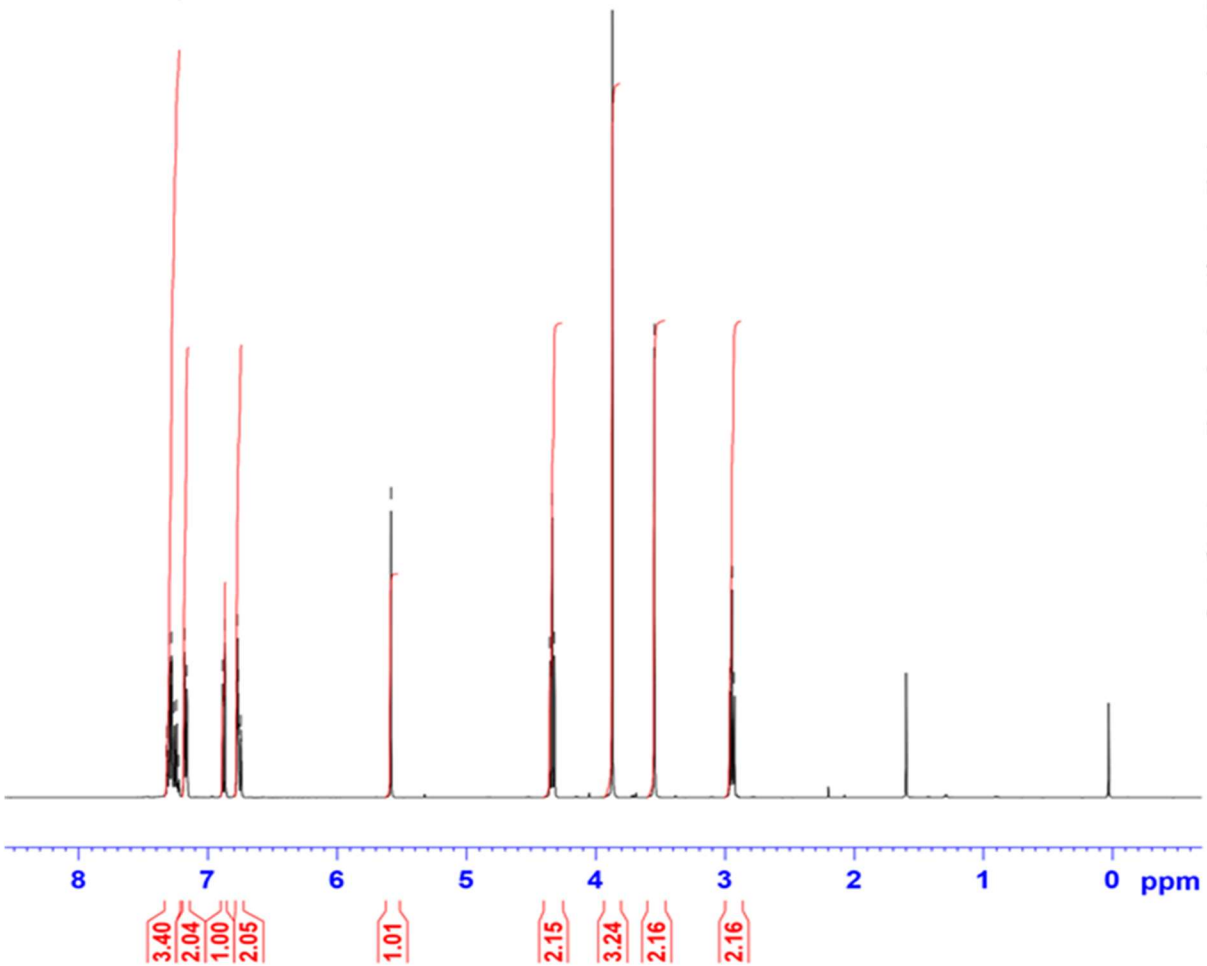
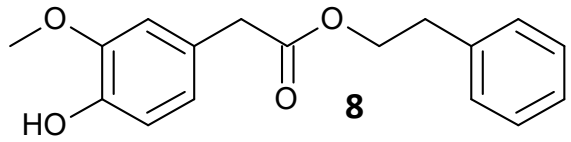


BRUKER

NAME	Moh RX	
EXPNO	207	
PROCNO	1	
Date_	20160317	
Time	14.04	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	8223.685	Hz
FIDRES	0.125483	Hz
AQ	3.9846387	sec
RG	90.5	
DW	60.800	usec
DE	6.50	usec
TE	298.0	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	14.07	usec
PL1	0.30	dB
PL1W	11.25229836	W
SFO1	400.1324710	MHz
SI	32768	
SF	400.1300000	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

^{1}H NMR



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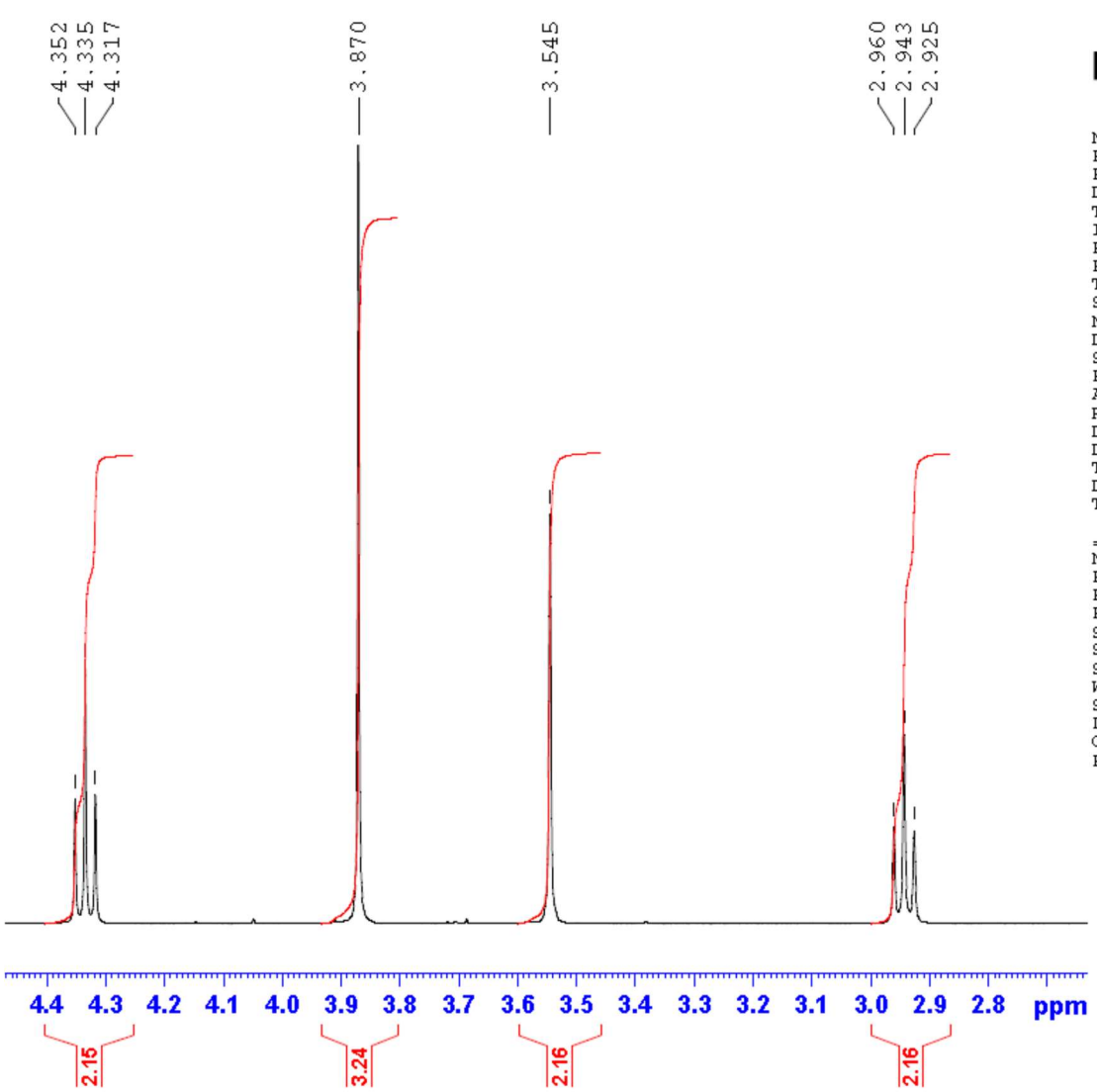
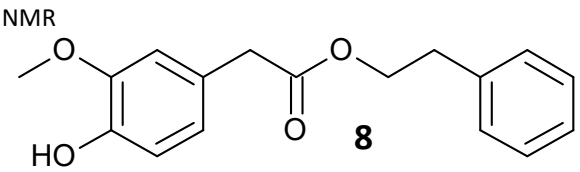


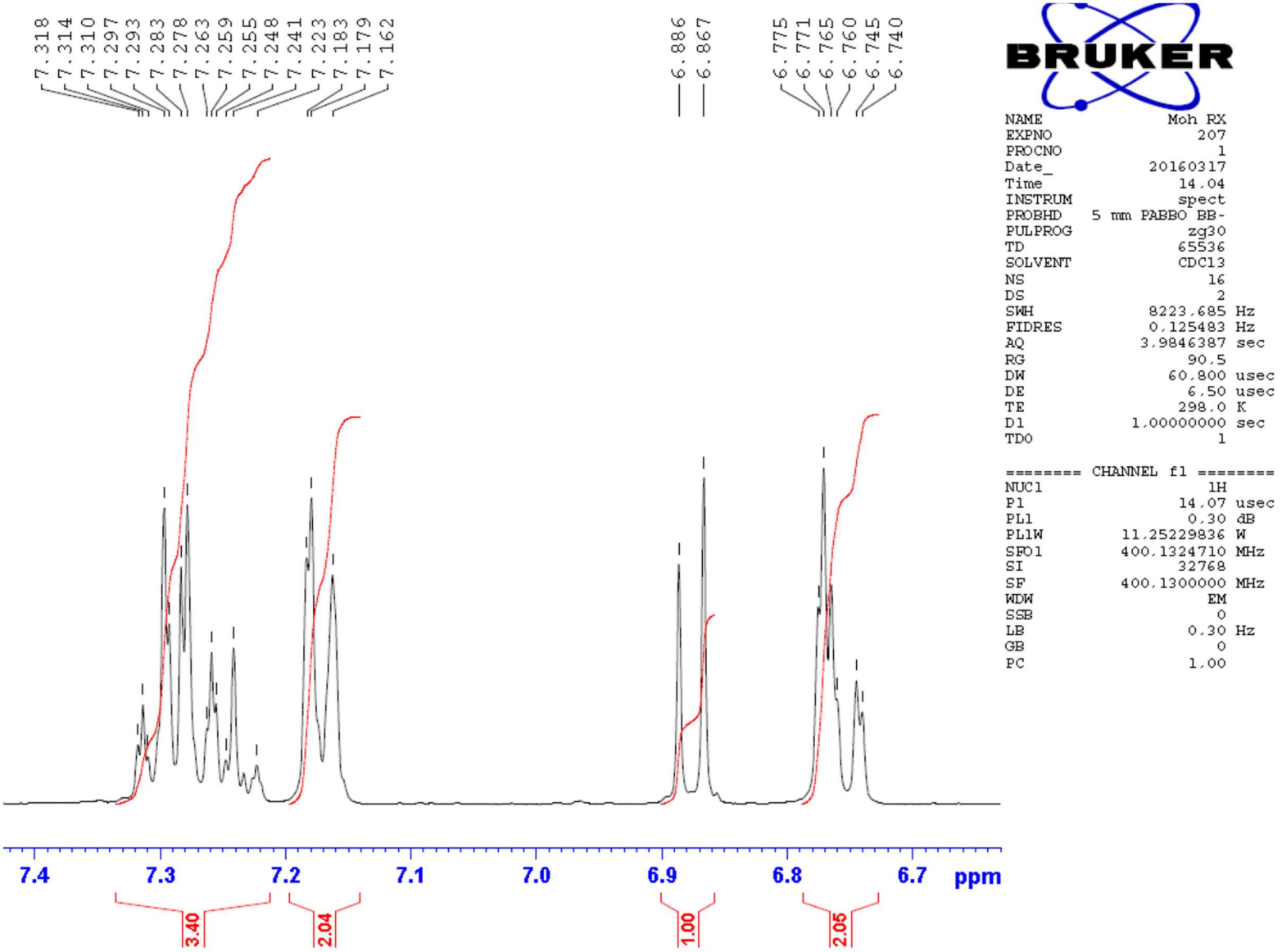
BRUKER

NAME	Moh RX
EXPNO	207
PROCNO	1
Date_	20160317
Time	14.04
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	90.5
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{1}H NMR



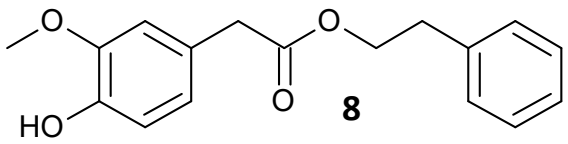
8



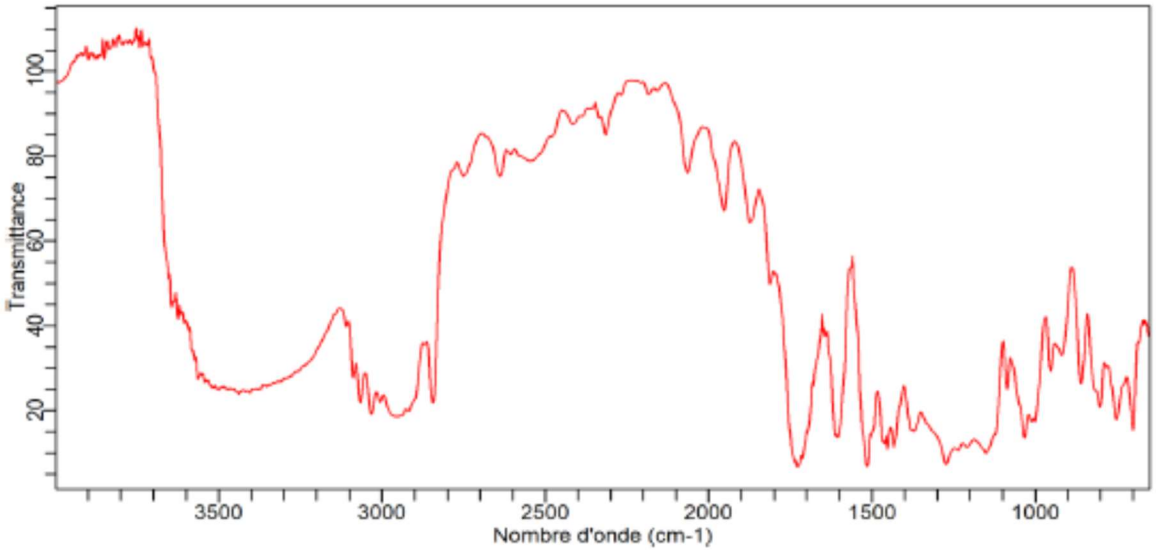
BRUKER

NAME	Moh RX
EXPNO	207
PROCNO	1
Date_	20160317
Time	14.04
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	90.5
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

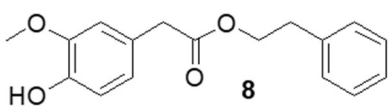
FTIR


O
O
O
HO

8


Transmittance
100
80
60
40
20
3500
3000
2500
2000
1500
1000
Nombre d'onde (cm-1)

^{13}C NMR



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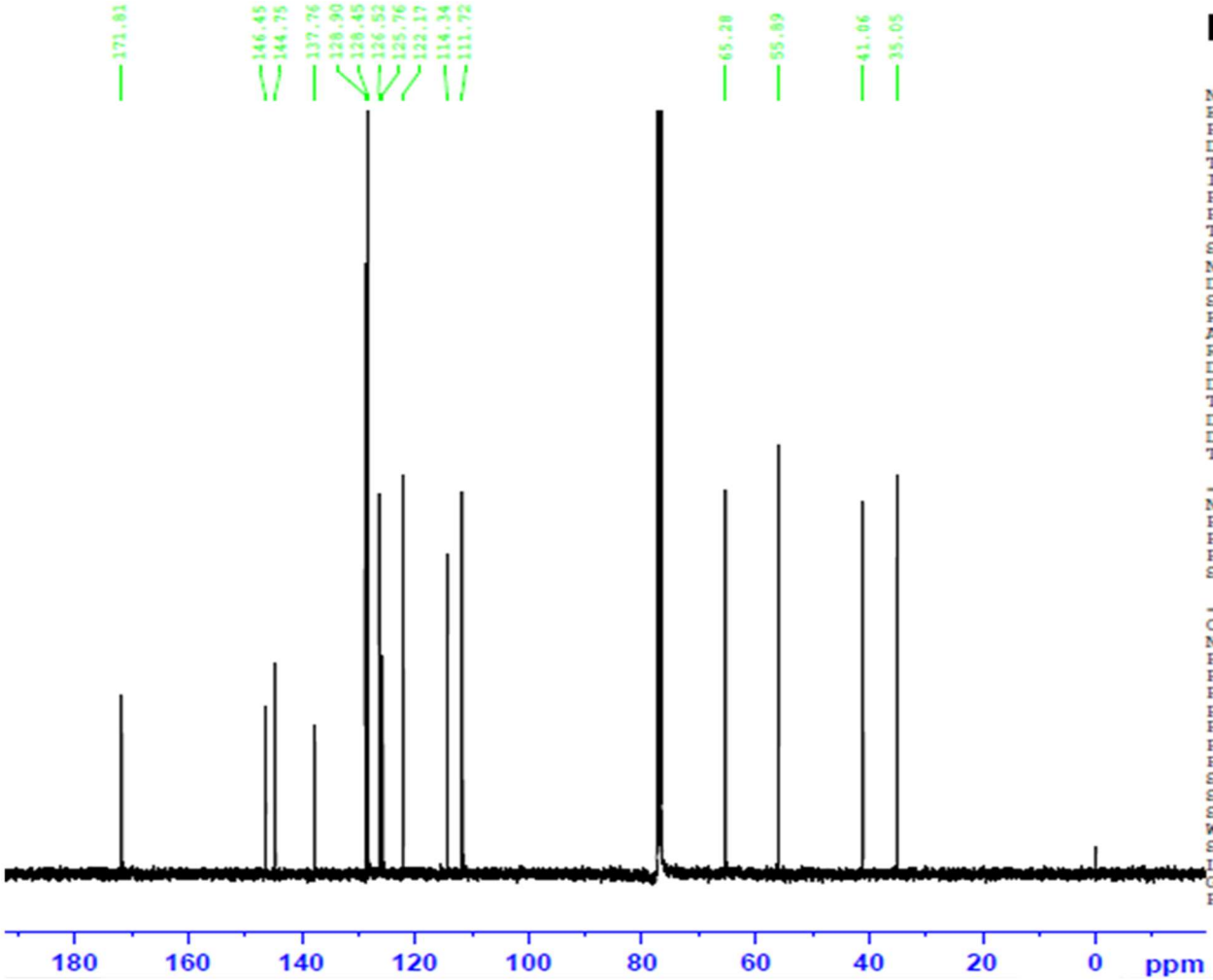
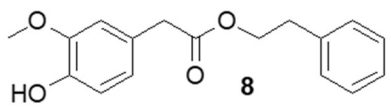


BRUKER

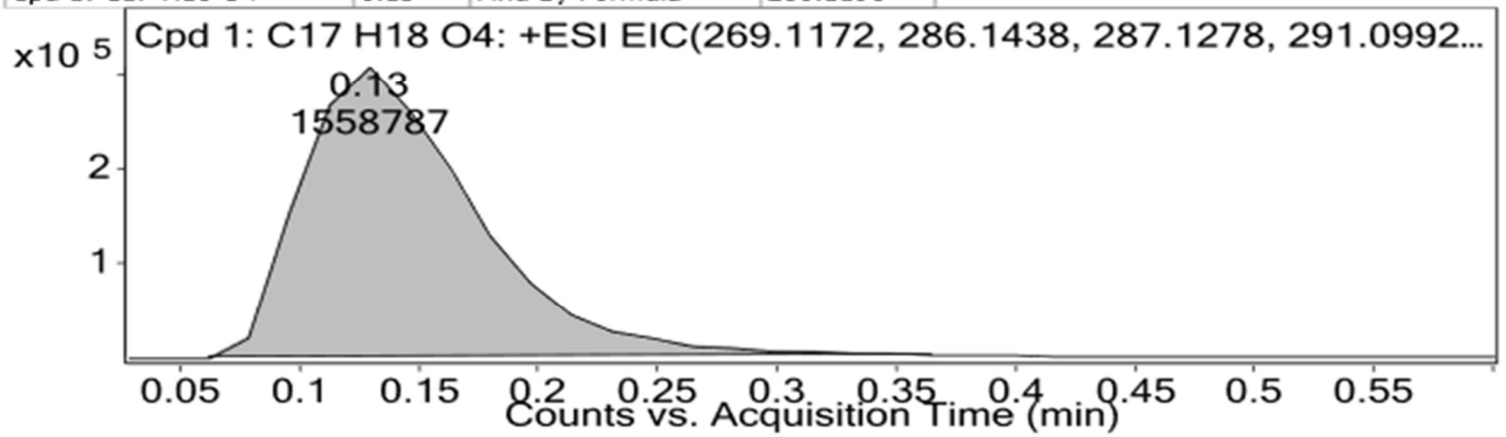
NAME	Moh RX
EXPNO	209
PROCNO	1
Date_	20160317
Time	16.35
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDC13
NS	2355
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
-------- CHANNEL f1 --------	
NUC1	13C
P1	9.90 usec
PL1	-1.90 dB
PL1W	56.02249908 W
SFO1	100.6228298 MHz
-------- CHANNEL f2 --------	
CPDPRG2	waltz65
NUC2	1H
PCPD2	80.00 usec
PL2	0.30 dB
PL12	15.40 dB
PL13	18.40 dB
PL2W	11.25229836 W
PL12W	0.34772930 W
PL13W	0.17427748 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

HRMS

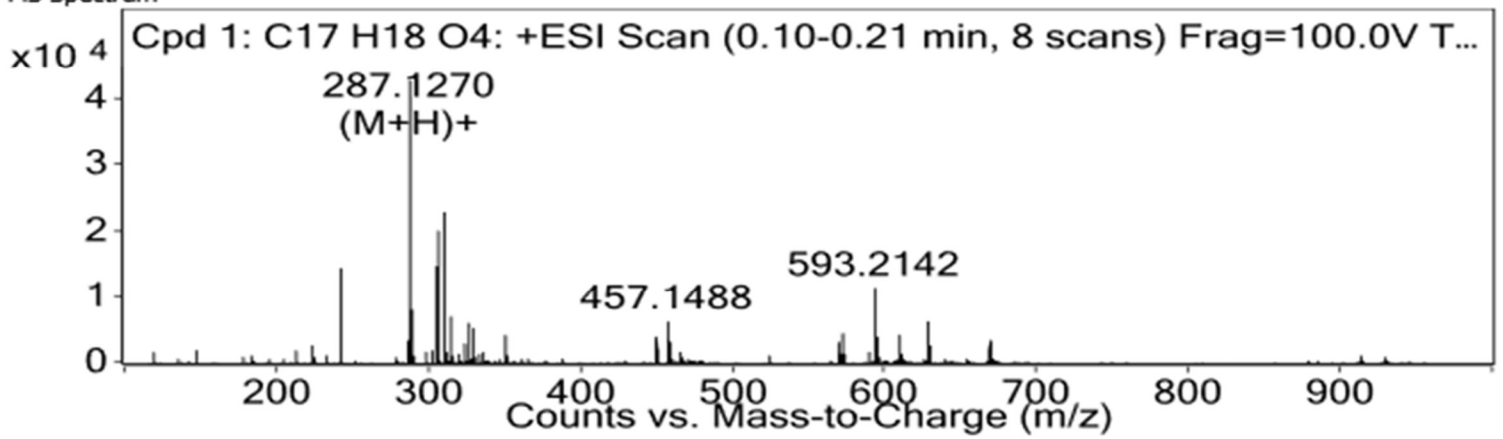


8

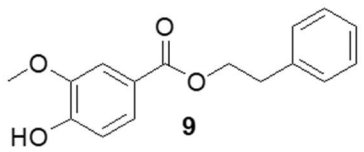
Compound Label	RT	Algorithm	Mass
Cpd 1: C17 H18 O4	0.13	Find By Formula	286.1198



MS Spectrum



^{1}H NMR



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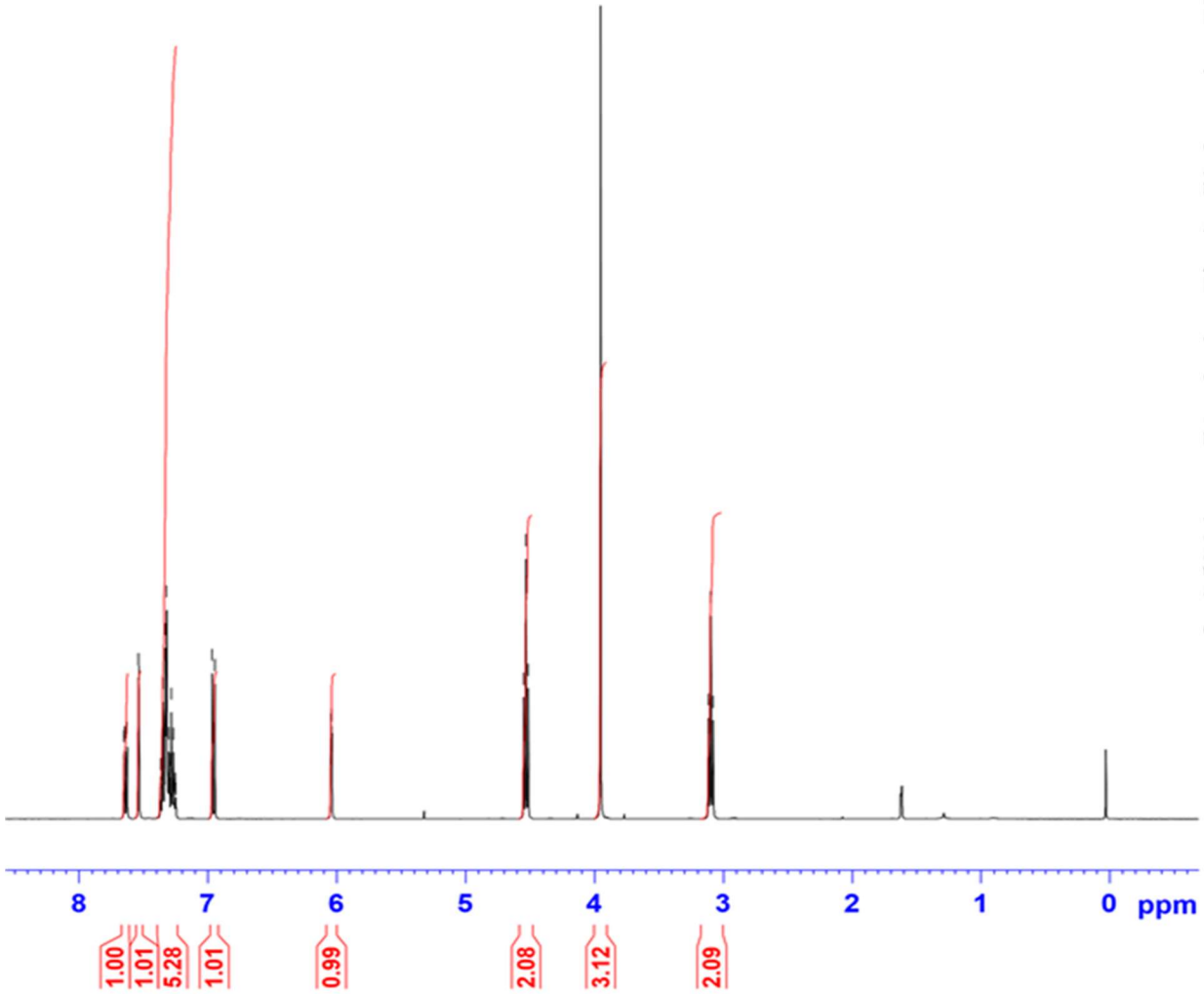
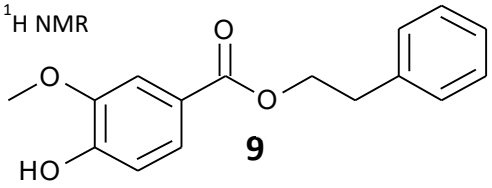


BRUKER

NAME	Moh RX	
EXPNO	201	
PROCNO	1	
Date_	20160316	
Time	12.44	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	8223.685	Hz
FIDRES	0.125483	Hz
AQ	3.9846387	sec
RG	90.5	
DW	60.800	usec
DE	6.50	usec
TE	298.0	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	14.07	usec
PL1	0.30	dB
PL1W	11.25229836	W
SFO1	400.1324710	MHz
SI	32768	
SF	400.1300000	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

^{1}H NMR



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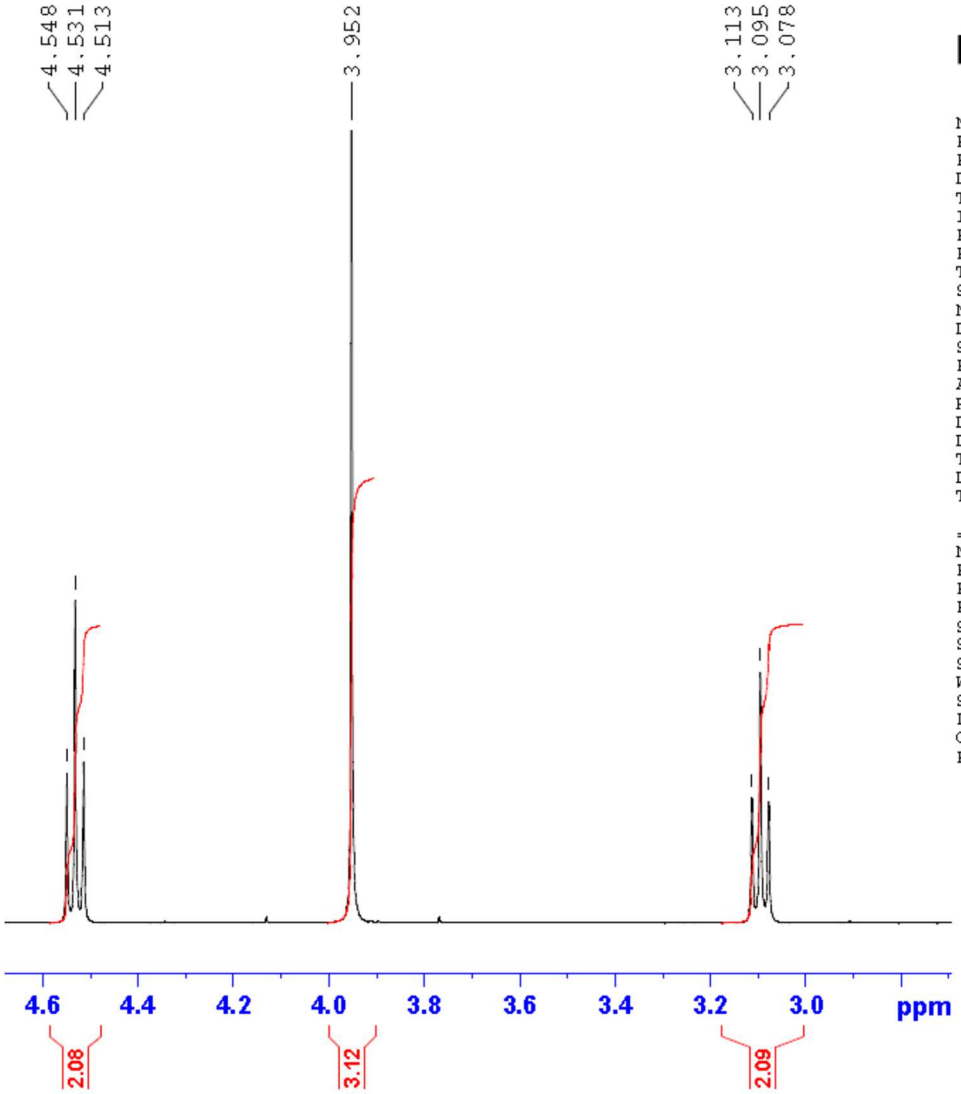
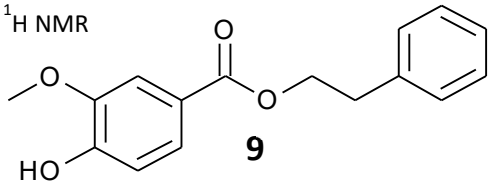


BRUKER

NAME	Moh RX
EXPNO	201
PROCNO	1
Date_	20160316
Time	12.44
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	90.5
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{1}H NMR



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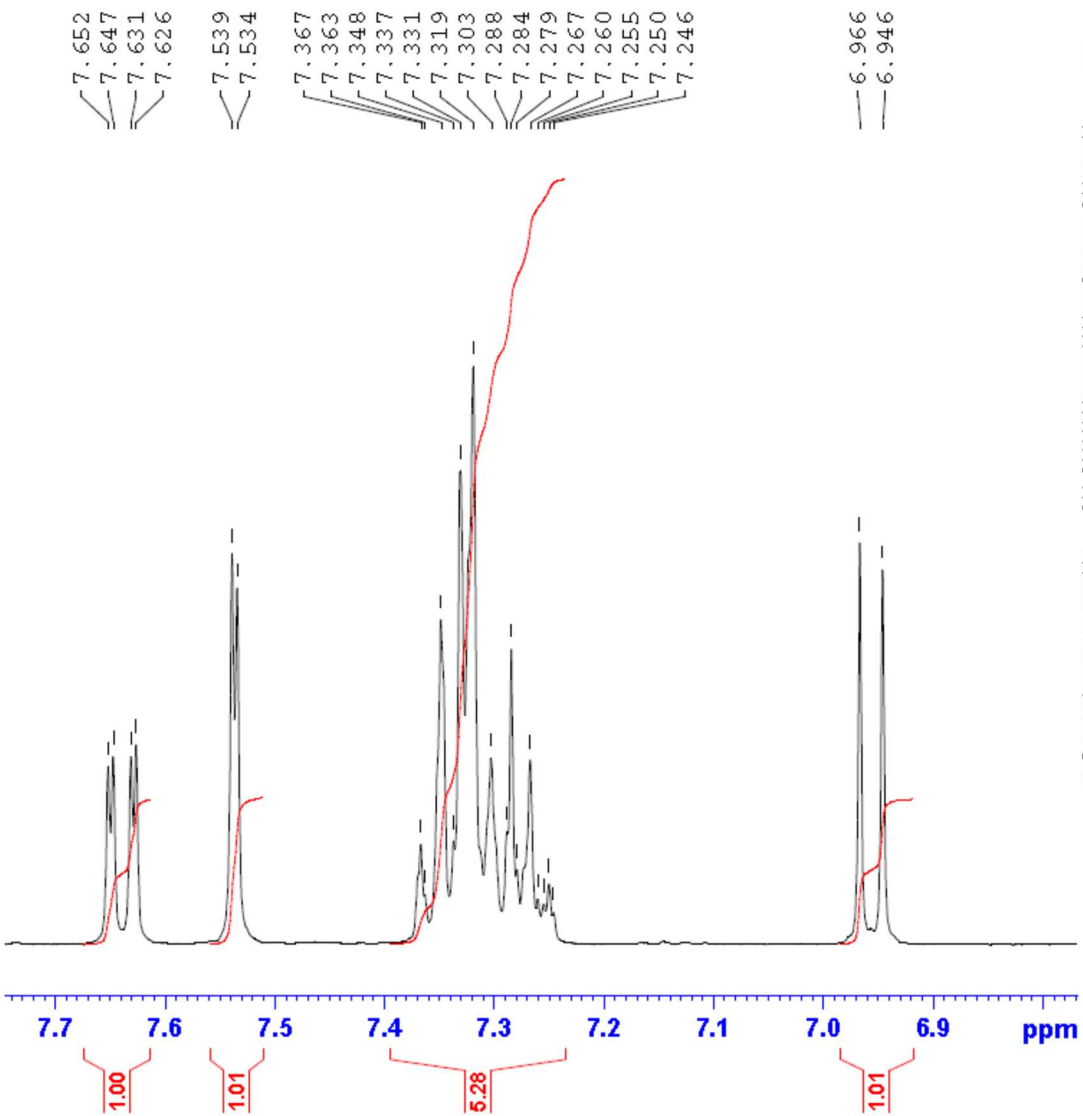
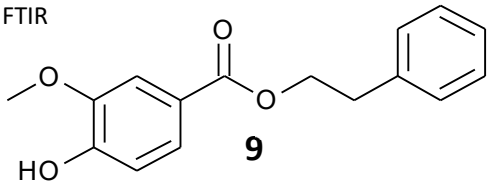


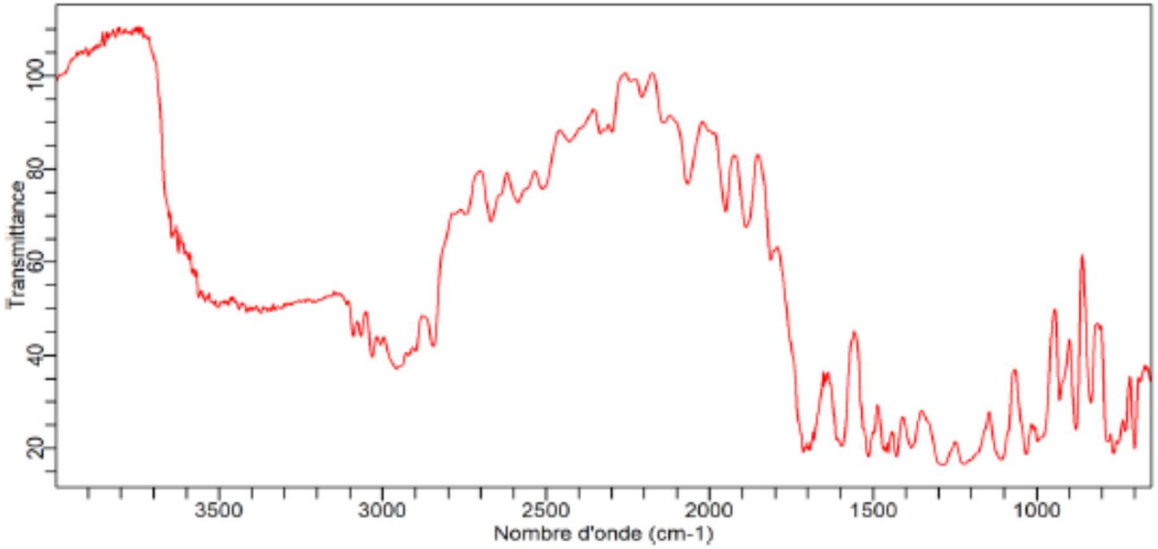
BRUKER

NAME	Moh RX
EXPNO	201
PROCNO	1
Date_	20160316
Time	12.44
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	90.5
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

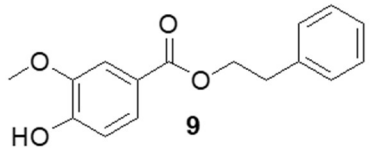
FTIR


O
O
O
HO

9


Transmittance
100
80
60
40
20
3500
3000
2500
2000
1500
1000
Nombre d'onde (cm-1)

^{13}C NMR



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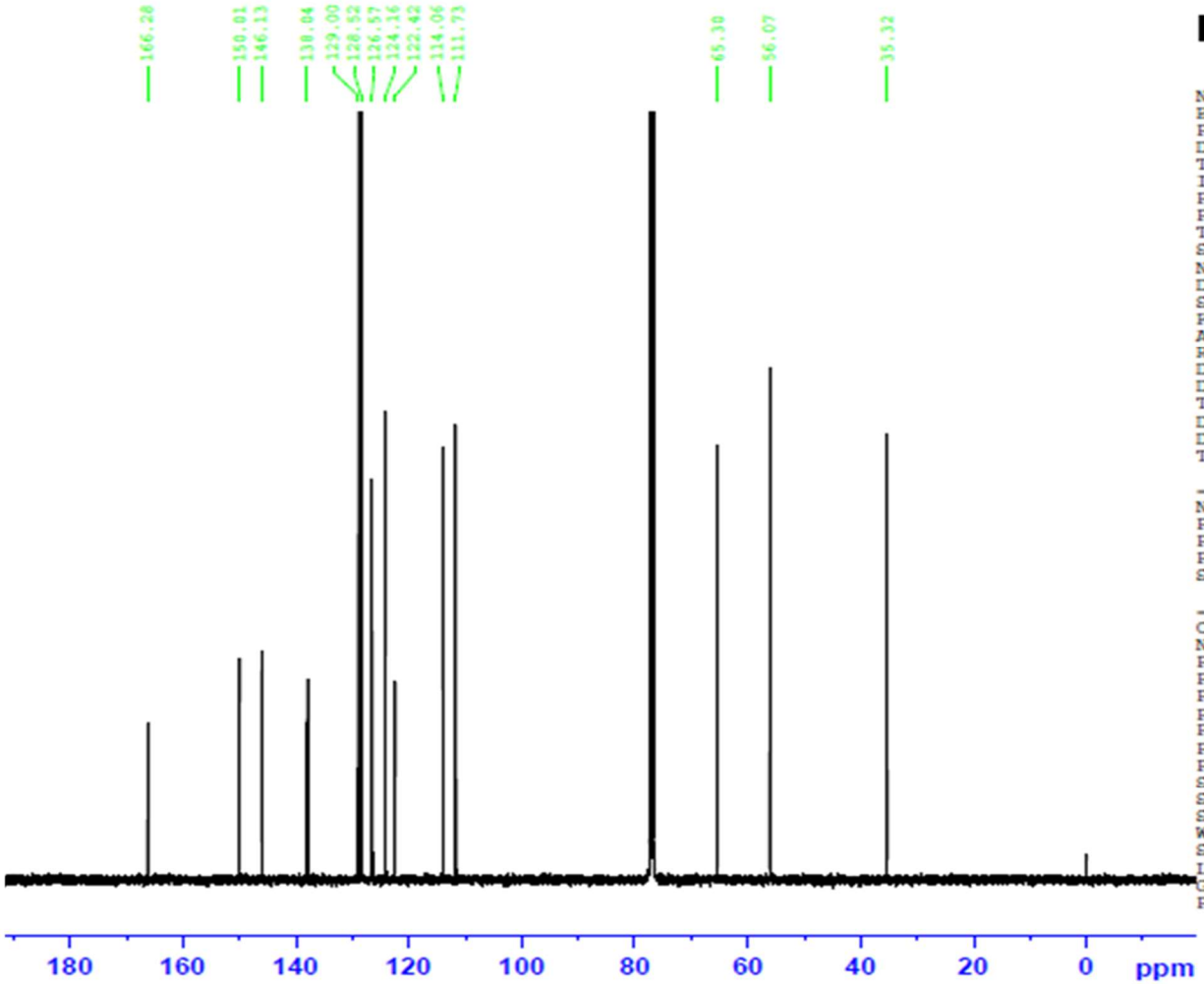
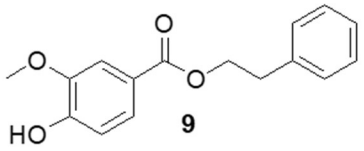



```
NAME                 Moh RX
EXPNO                   203
PROCNO                    1
Date_             20160316
Time                 15.43
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDC13
NS                     2911
DS                        4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                      203
DW                   20.800 usec
DE                    6.50 usec
TE                   298.0 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1

-------- CHANNEL f1 --------
NUC1                    13C
P1                    9.90 usec
PL1                  -1.90 dB
PL1W          56.02249908 W
SFO1         100.6228298 MHz

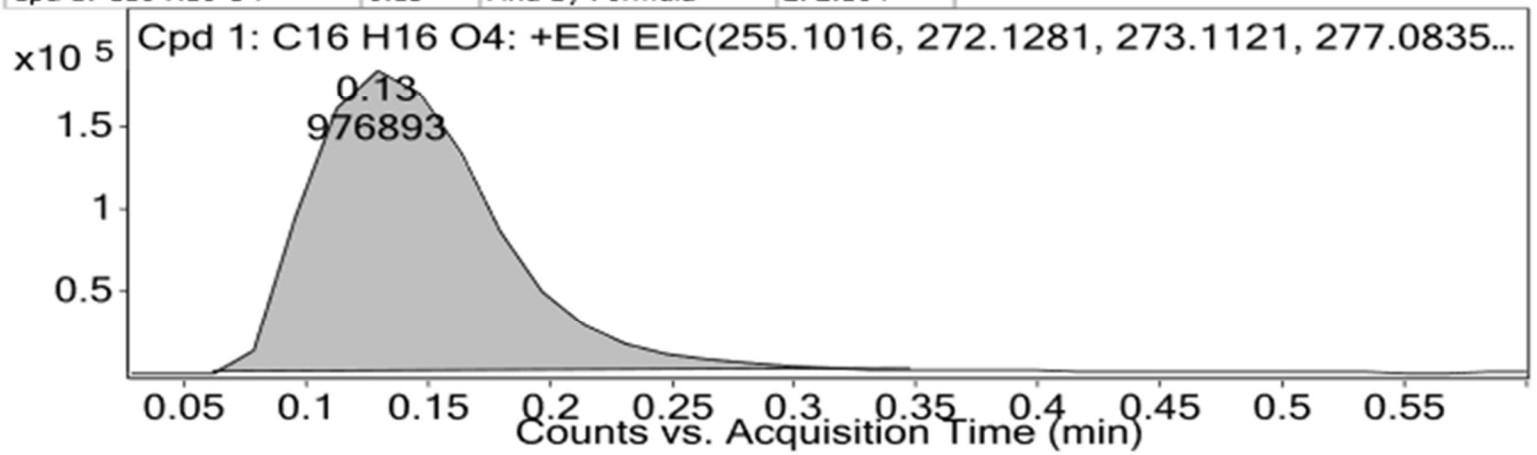
-------- CHANNEL f2 --------
CPDPRG2              waltz65
NUC2                    1H
PCPD2                80.00 usec
PL2                   0.30 dB
PL12                 15.40 dB
PL13                 18.40 dB
PL2W          11.25229836 W
PL12W          0.34772930 W
PL13W          0.17427748 W
SFO2         400.1316005 MHz
SI                    32768
SF           100.6127690 MHz
WDW                      EM
SSB                       0
LB                    1.00 Hz
GB                        0
PC                    1.40
```

HRMS



9

Compound Label	RT	Algorithm	Mass
Cpd 1: C16 H16 O4	0.13	Find By Formula	272.104



MS Spectrum

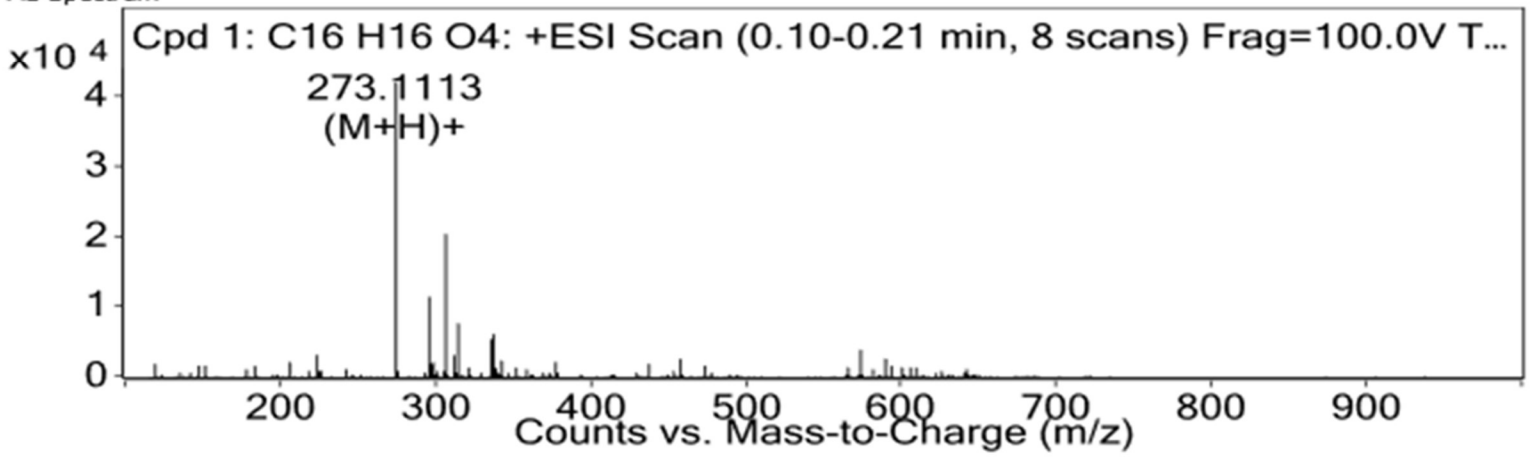


Table 1S. Acetylcholinesterase; (PDB: 4BDT) docking affinity and interactions

Ligand	Affinity (kcal / mol)	H-Bonds	π-π Interactions
FA (**1**)	-7.1	Ser125	Trp86
3	-9.3	Tyr124, Tyr133, Tyr337, Tyr341	Trp86 x 2, Tyr337, Tyr449
4	-9.6	Tyr124, Ser203 x 2, Tyr337, Tyr341, His447	Trp86, Tyr337
5	-9.1	Tyr133, Glu202, Tyr337	Tyr341
8	-9.5	Tyr124, Glu202, Ser203 x 2, Tyr337, His447	Trp86 x 2, Tyr337
9	-9.6	Ser125, Glu202, Ser203 x 2, Tyr337, His447	Tyr86 x 2, Tyr337

Table 2S. Acetylcholinesterase; (PDB: 4EY7) docking affinity and interactions

Ligand	Affinity (kcal / mol)	H-Bonds	π-π Interactions
FA (**1**)	-7.6	Asp74, Glu202, Tyr337, Tyr341	Trp86
3	-9.7	Gly121, Gly122, Ser203 x 2, Tyr337	Phe338, Tyr341
4	-10.3	Gly121, Tyr124, Tyr341	Trp86, Tyr337, Phe338, Tyr341
5	-9.3	Asp74	Trp86, Tyr337
8	-9.3	Gly121, Tyr124, Ser203	Trp86, Tyr337, Phe338
9	-10.0	Tyr124, Ser125, Glu202, Ser203	Trp86 x 2, Tyr337

Table 3S. Acetylcholinesterase; (PDB: 4M0F) docking affinity and interactions

Ligand	Affinity (kcal / mol)	H-Bonds	π-π Interactions
FA (**1**)	-7.9	Tyr124, Trp286, Arg296	Phe338
3	-9.4	Tyr124, Tyr133, Tyr337	Trp86, Phe338
4	-9.0	Asp74, Tyr124	Tyr337, Phe338
5	-9.8	Tyr124, Tyr133, Tyr337	
8	-9.4	Asp74, Ser125 x 2	
9	-8.9	Asp74, Ser125 x 2	Trp86

Table 4S. Butyrylcholinesterase; (PDB: 1P0M) docking affinity and interactions

Ligand	Affinity (kcal / mol)	H-Bonds	π-π Interactions
FA (**1**)	-7.3	Ser198 x 2, His438	Trp231
3	-9.1	Tyr128	Trp82, Tyr332
4	-9.2	Ser198, Tyr332, His438	Trp82, Trp231, Phe329
5	-9.1	Pro285, Ser198 x 2, His438	Trp231, Phe329, Tyr332
8	-9.0	His438	Tpr82, Trp231, Phe329
9	-7.6	Thr120, Ser198, His438	Trp82 x 2

Table 5S. Butyrylcholinesterase; (PDB: 6EQQ) docking affinity and interactions

Ligand	Affinity (kcal / mol)	H-Bonds	π-π Interactions
FA (**1**)	-6.8	Asp70, Tyr128, Glu197, Tyr332	Trp82
3	-7.5	Tyr128, Gly197, Tyr332	Trp82
4	-8.9	His438	Trp82, Phe329
5	-7.2	Trp82, Tyr440	Trp231, Phe329
8	-8.1	Tyr332, His438	Trp82, Phe329
9	-7.7	Glu197	Trp82, Tyr332