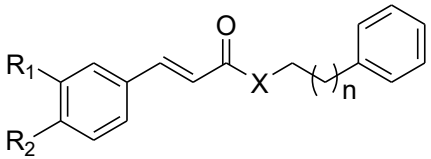
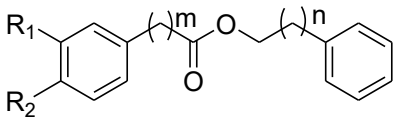
Supplementary Data:

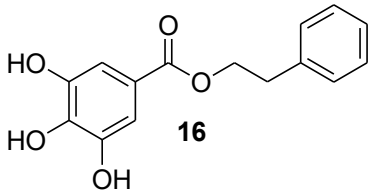
Series 1



1: $R_1 = R_2 = OH$; X = O; n = 2
2: $R_1 = R_2 = OH$; X = O; n = 3
3: $R_1 = R_2 = OH$; X = O; n = 4
4: $R_1 = R_2 = OH$; X = O; n = 5
5: $R_1 = R_2 = OH$; X = NH; n = 2
6: $R_1 = R_2 = OH$; X = NH; n = 3



7: $R_1 = R_2 = OH$; m = 2; n = 1
8: $R_1 = R_2 = OH$; m = 2; n = 2
9: $R_1 = R_2 = OH$; m = 2; n = 3
10: $R_1 = R_2 = OH$; m = 2; n = 4
11: $R_1 = R_2 = OH$; m = 2; n = 5
12: $R_1 = R_2 = OH$; m = 1; n = 1
13: $R_1 = R_2 = OH$; m = 1; n = 2
14: $R_1 = R_2 = OH$; m = 0; n = 1
15: $R_1 = R_2 = OH$; m = 0; n = 2



16

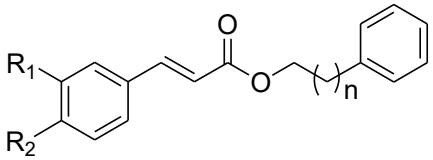
Figure S1A

Table S1A

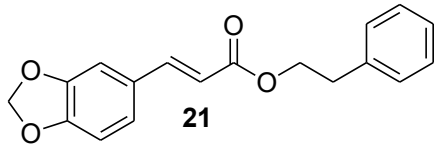
Compound	FRAP (µmol TE/L)	ORAC (µmol TE/L)	ABTS (µmol TE/L)
1	188.3±6.9	368.3±12.3	427.9±44.9
2	204.2±3.6	404.9±1.7	464.7±13.5
3	200.0±7.0	388.0±7.3	469.8±19.1
4	199.8±2.9	398.9±3.3	446.3±0.3
5	176.0±3.4	361.7±12.3	435.6±31.2
6	156.3±1.5	334.6±9.7	417.0±20.7
7	191.2±4.4	462.9±11.2	475.7±23.8
8	182.4±6.0	464.4±8.5	420.2±31.5

9	173.2±5.8	325.1±8.1	372.7±14.4
10	192.7±8.6	343.2±3.2	452.1±34.8
11	168.3±3.2	343.1±9.5	463.8±5.3
12	**373.5±9.2**	**420.8±11.3**	**522.7±0.4**
13	368.2±12.5	309.5±6.1	490.5±26.3
14	266.0±10.6	392.2±5.3	489.3±41.2
15	277.0±7.9	415.3±14.5	502.9±29.7
16	**314.8±6.5**	**336.3±2.1**	**522.6±1.3**

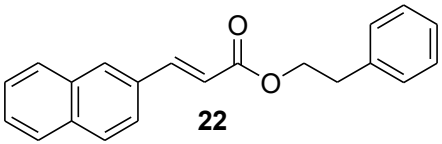
Series 2



17: $R_1 = R_2 = OMe$; n = 1
18: $R_1 = R_2 = Cl$; n = 1
19: $R_1 = OMe$; $R_2 = OH$; n = 1
20: $R_1 = OMe$; $R_2 = OH$; n = 2



21



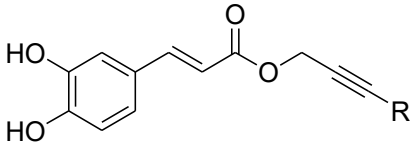
22

Figure S1B

Table S1B

Compound	FRAP (µmol TE/L)	ORAC (µmol TE/L)	ABTS (µmol TE/L)
16	**314.8±6.5**	**336.3±2.1**	**522.6±1.3**
17	50.6±0.5	162.5±2.0	142.3±12.5
18	58.0±1.0	153.3±1.8	207.5±20.0
19	161.2±8.0	283.3±5.2	357.3±38.8
20	170.6±5.7	321.4±9.8	360.0±33.3
21	50.3±0.5	226.0±8.4	221.7±20.3
22	64.5±1.6	145.9±2.6	163.3±10.8

Series 3

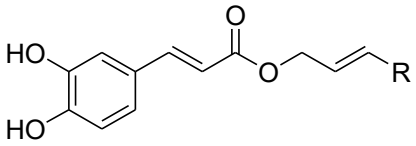


23: R = H
24: R = Ph
25: R = $CH_2CH_2PhMe(4\text{-}Me)$
26: R = $CH_2CH_2PhOMe(4\text{-}OMe)$
27: R = $CH_2CH_2Ph(4\text{-}NO_2)$
28: R = $CH_2CH_2PhF(4\text{-}F)$
29: R = CH_2CH_2Naph (1-)
30: R = CH_2CH_2PhPh
31: R = 4-($CCCH_2$Caffeoyl)-Ph

Figure S1C
Table S1C

Compound	FRAP (µmol TE/L)	ORAC (µmol TE/L)	ABTS (µmol TE/L)
23	201.3±6.8	368.3±12.3	461.7±41.8
24	187.9±5.9	162.5±2.0	462.0±38.9
25	191.0±8.2	153.3±1.8	477.2±24.7
26	**287.6±2.7**	**226.0±8.4**	**486.0±4.4**
27	192.0±3.1	223.0±4.2	423.9±32.6
28	206.5±11.0	145.9±2.6	494.9±27.3
29	188.5±1.8	283.3±5.2	442.8±30.3
30	142.3±1.8	321.4±9.8	376.0±21.6
31	191.5±11.0	336.3±2.1	455.5±29.6

Series 4

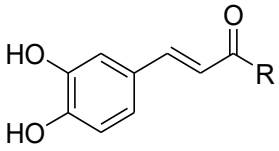


32: R = H
33: R = Ph
34: R = $CH_2CH_2PhMe(4\text{-}Me)$
35: R = $CH_2CH_2PhOMe(4\text{-}OMe)$
36: R = $CH_2CH_2Ph(4\text{-}NO_2)$
37: R = $CH_2CH_2PhF(4\text{-}F)$
38: R = CH_2CH_2Naph (1-)
39: R = CH_2CH_2PhPh
40: R = $4^{-}(CCCH_2$Caffeoyl)-Ph

Figure S1D
Table S1D

Compound	FRAP (µmol TE/L)	ORAC (µmol TE/L)	ABTS (µmol TE/L)
32	199.4±5.4	379.6±3.3	501.8±16.1
33	211.3±5.0	394.5±2.7	502.3±15.8
34	313.3±1.2	421.5±5.2	512.6±10.0
35	**302.6±6.6**	**459.2±15.3**	**509.7±18.1**
36	207.1±7.7	367.2±8.6	484.2±5.4
37	232.9±12.0	388.3±6.3	491.9±12.9
38	220.7±7.0	323.9±2.0	476.5±10.5
39	201.8±3.1	292.0±2.9	415.1±10.4
40	329.1±20.0	281.0±14.6	486.2±15.1

Series 5

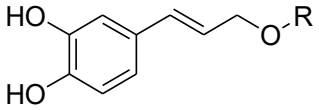


41: R = H
42: R = Ph
43: R = CH_2Ph
44: R = CH_2CH_2Ph
45: R = $CH_2CH_2CH_2Ph$

Figure S1E
Table S1E

Compound	FRAP (µmol TE/L)	ORAC (µmol TE/L)	ABTS (µmol TE/L)
41	258.9±12.7	420.8±11.3	524.9±1.8
42	**222.1±13.8**	**444.3±1.1**	**511.1±1.0**
43	234.7±3.2	432.5±8.8	510.5±12.3
44	**231.3±3.5**	**438.4±2.8**	**517.4±6.4**
45	232.3±5.8	386.0±13.6	502.1±19.1

Series 6



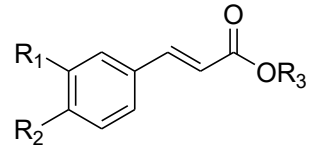
46: R = H
47: R = CH_2Ph
48: R = $CH_2CH_2CH_2Ph$

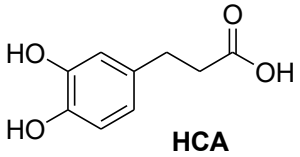
Figure S1F

Table S1F

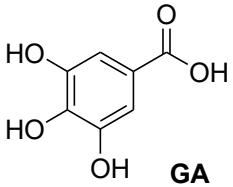
Compound	FRAP (µmol TE/L)	ORAC (µmol TE/L)	ABTS (µmol TE/L)
46	238.8±8.3	376.2±11.6	524.4±1.4
47	250.7±10.0	368.5±14.9	405.3±28.5
48	243.6±10.0	371.2±14.9	415.3±35.4

Standards





HCA



GA

CA: R_1 = OH; R_2 = OH; R_3 = OH
FA: R_1 = OCH_3; R_2 = OH; R_3 = OH
CAPE: R_1 = OH; R_2 = OH; R_3 = CH_2CH_2Ph

Internal Standards	FRAP (µmol TE/L)	ORAC (µmol TE/L)	ABTS (µmol TE/L)
Caffeic acid (CA)	944.5±17.7	473.1±3.3±	526.1±1.4
dihydrocaffeic acid (HCA)	406.5±13.8	468.2±5.3	500.8±11.7
CAPE	560.9±21.1	372.0±4.0±	500.4±4.3
Gallic acid (GA)	195.3±6.4	251.0±2.7±	495.4±11.0
Ferulic acid (FA)	270.3±9.9	305.0±5.4±	424.7±15.4
(2-Naphthyl)-acrylic acid (NAA)	48.3±0.5	223.0±4.2	122.2±8.2

Figure S1: Figures and tables showing detailed antioxidant activity and chemical characteristics of Caffeic acid and CAPE analogs (100 µM) as measured using ABTS, FRAP, and ORAC antioxidant assays.

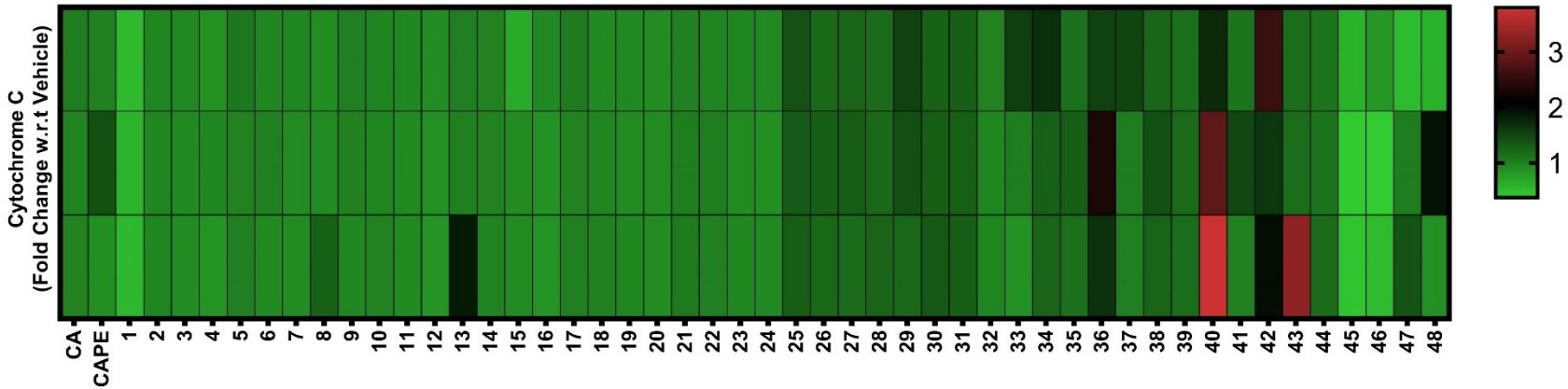


Figure S2: The impact of Caffeic acid and CAPE analogs on cytochrome C levels as the toxicity indicator. WI-38 cells were pre-treated with 10 μM of the selected compounds for 24 hours and then the cytochrome C levels were measured using ELISA.

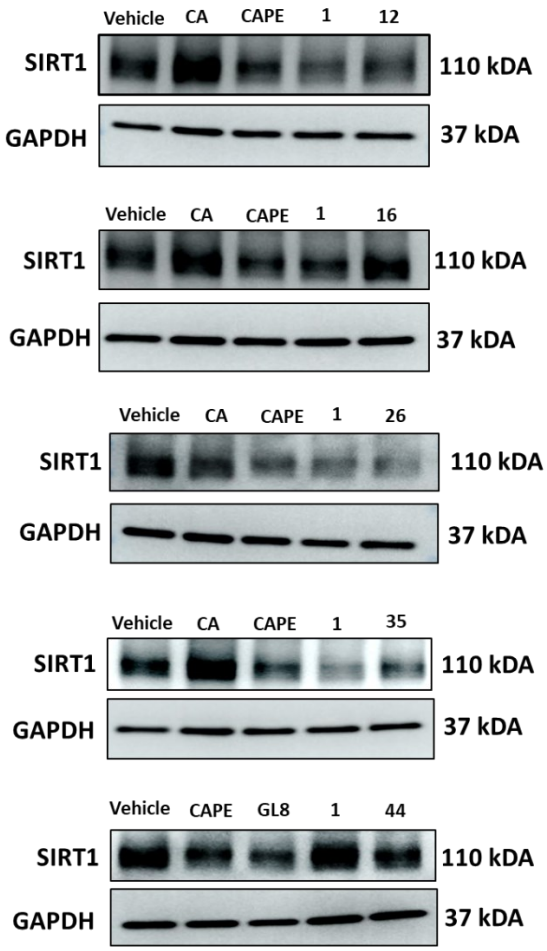


Figure S3: The impact of Caffeic acid and CAPE analogs on SIRT1 levels. 293T cells were pre-treated with 10 μM of the selected compounds for 24 hours and then the selected biomarkers were observed using western blot.

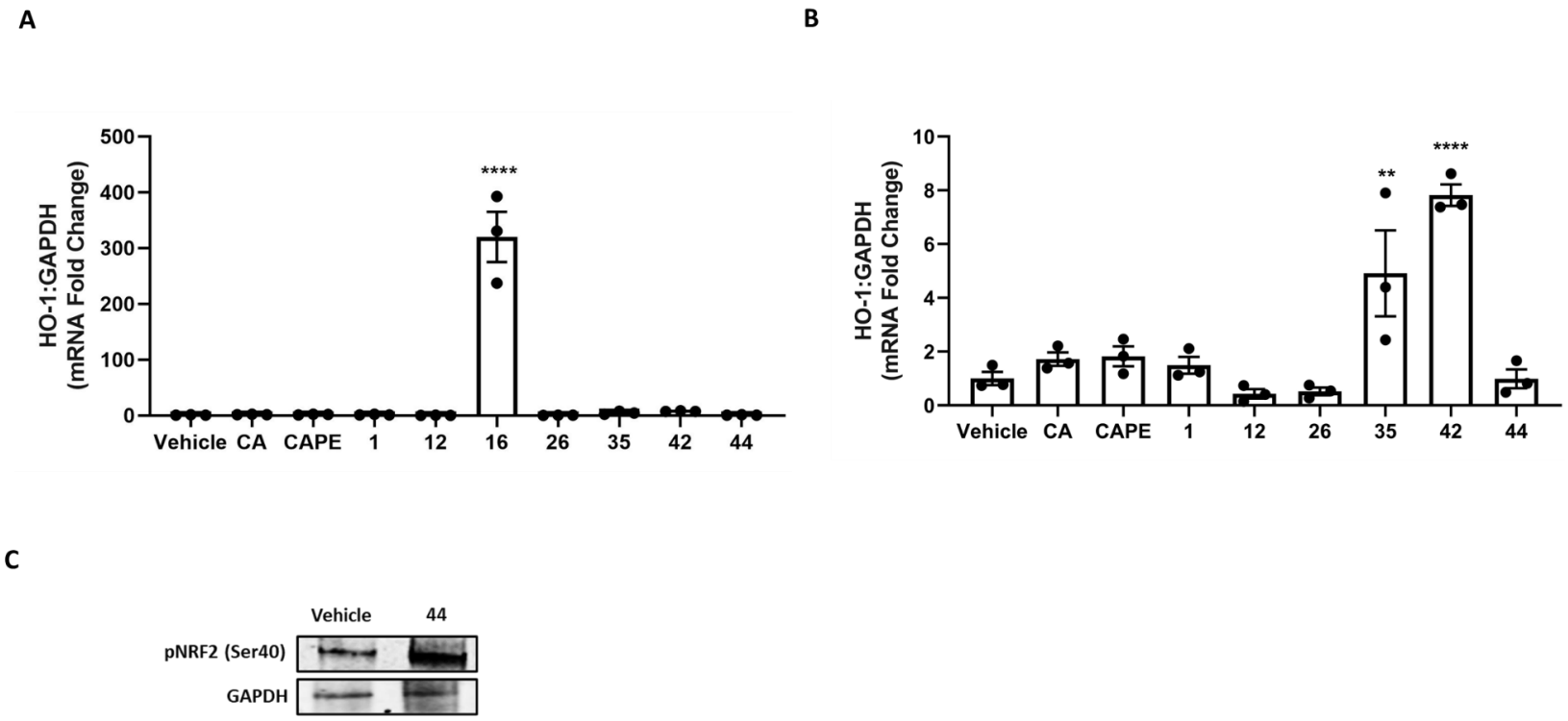


Figure S4: The impact of Caffeic acid and CAPE analogs on Nrf2 pathway activation. 293T cells were pre-treated with 10 µM of the selected compounds for 24 hours and then the protein and RNA were extracted using RIPA buffer and TRIZOL. (A-B) mRNA increase in HO-1 and (C) validation of p-NRF2 by analog 44. Ordinary one-way analysis of variance (ANOVA) was performed followed by Dunnett's multiple comparisons test to identify statistical difference **p<0.01, ****p<0.0001.

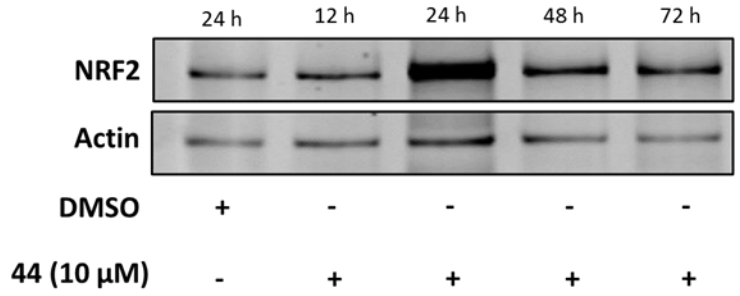
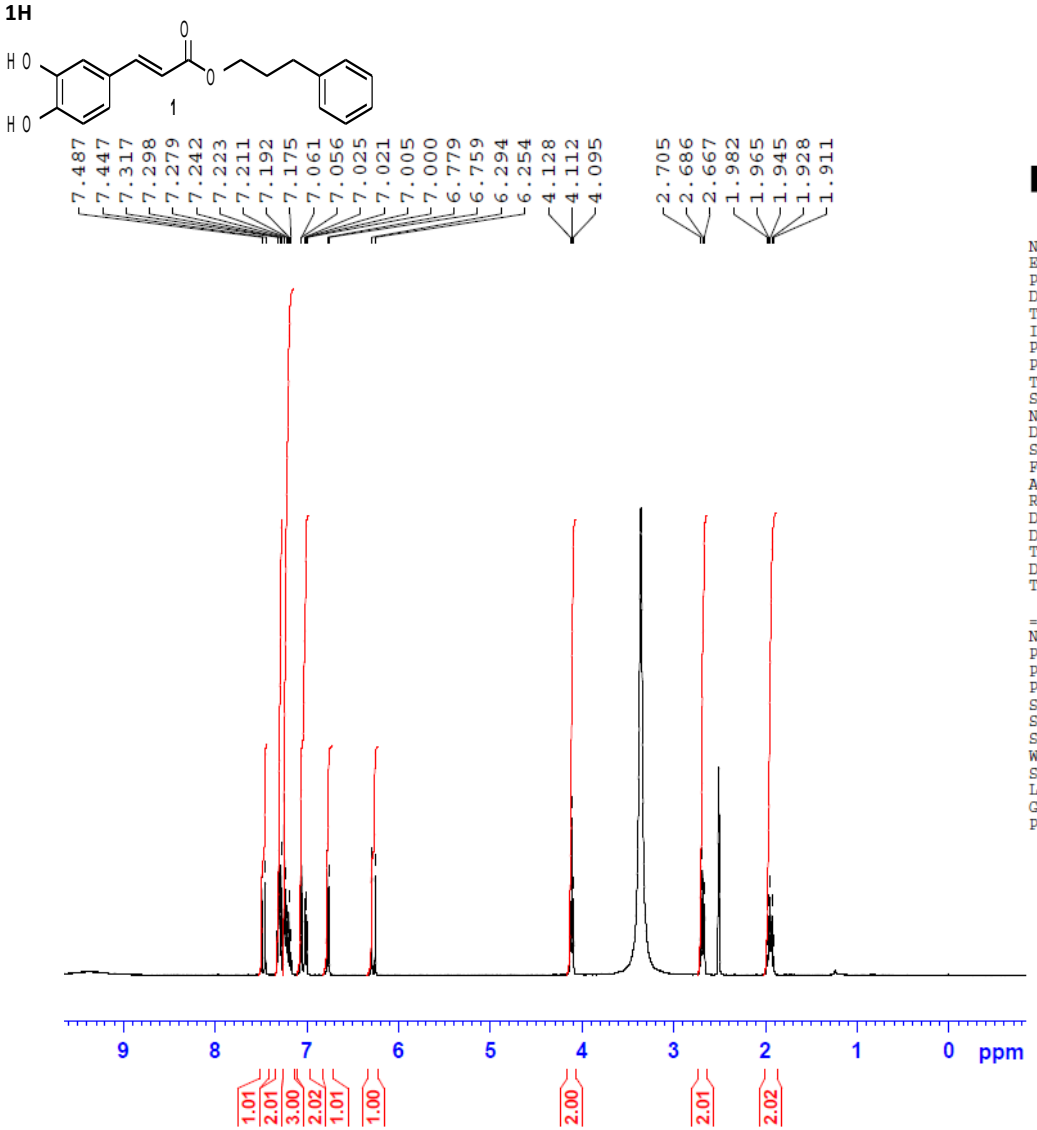


Figure S5: The subcellular localization of Nrf2 following treatment with compound 44, the ketone analog of CAPE. 293T cells were pre-treated with 10 µM of the compound 44 for 24 hours and then the nuclear protein was extracted, and immunoblotting was performed.

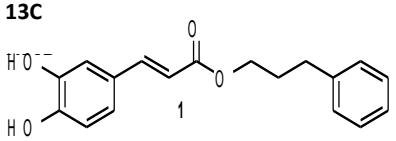
Additional Supplementary Material: NMR data

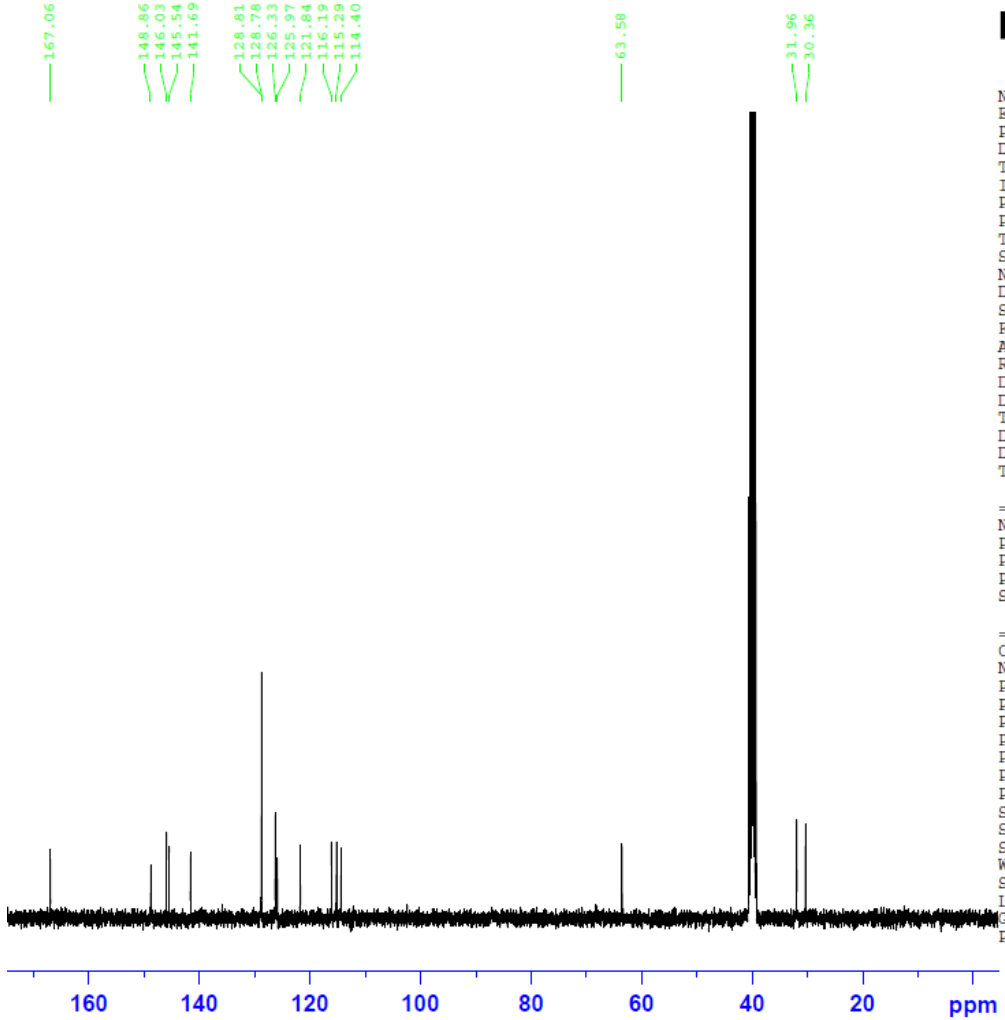


BRUKER

NAME	Moh RX
EXPNO	186
PROCNO	1
Date_	20130516
Time	14.03
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
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

13C





BRUKER

NAME	Moh RX
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PROCNO	1
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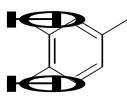
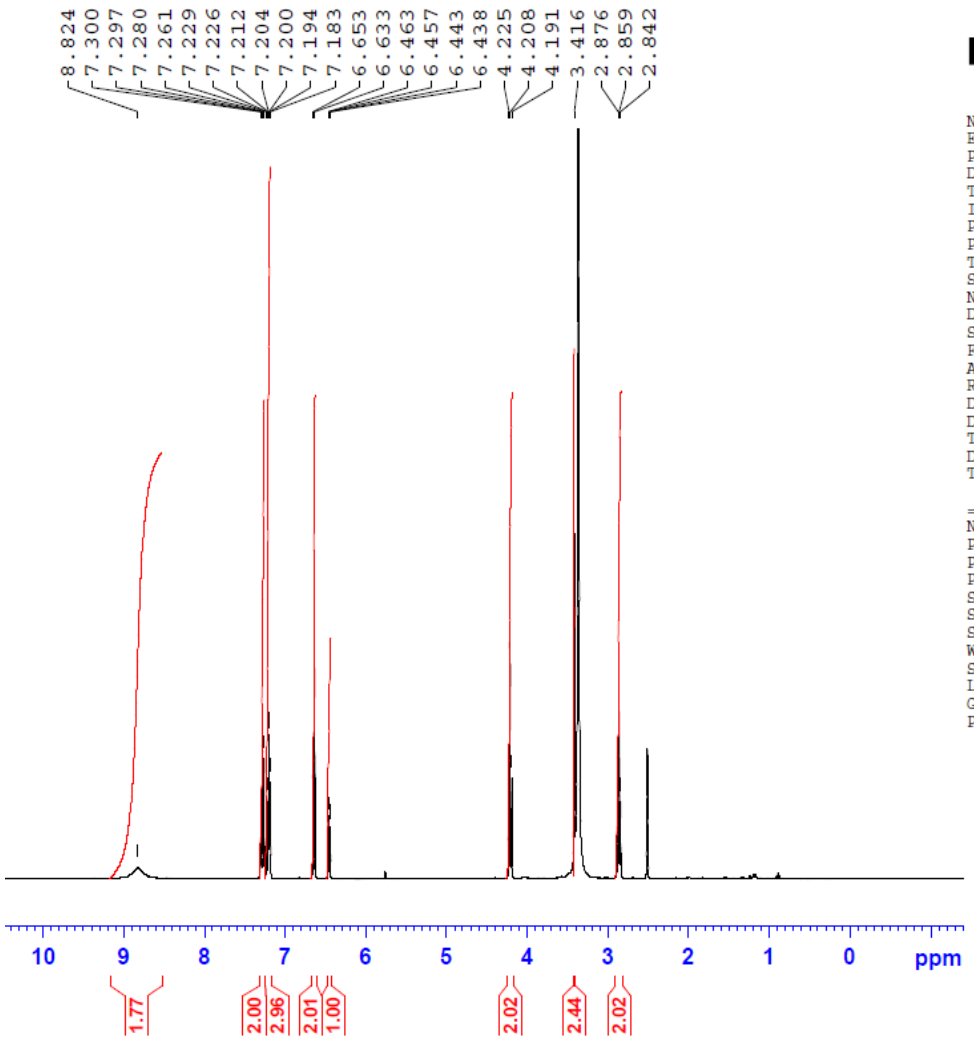
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	715
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.90 usec
PL1	-1.90 dB
PL1W	56.02249908 W
SFO1	100.6228298 MHz
======== 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

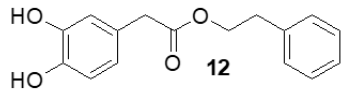
1H



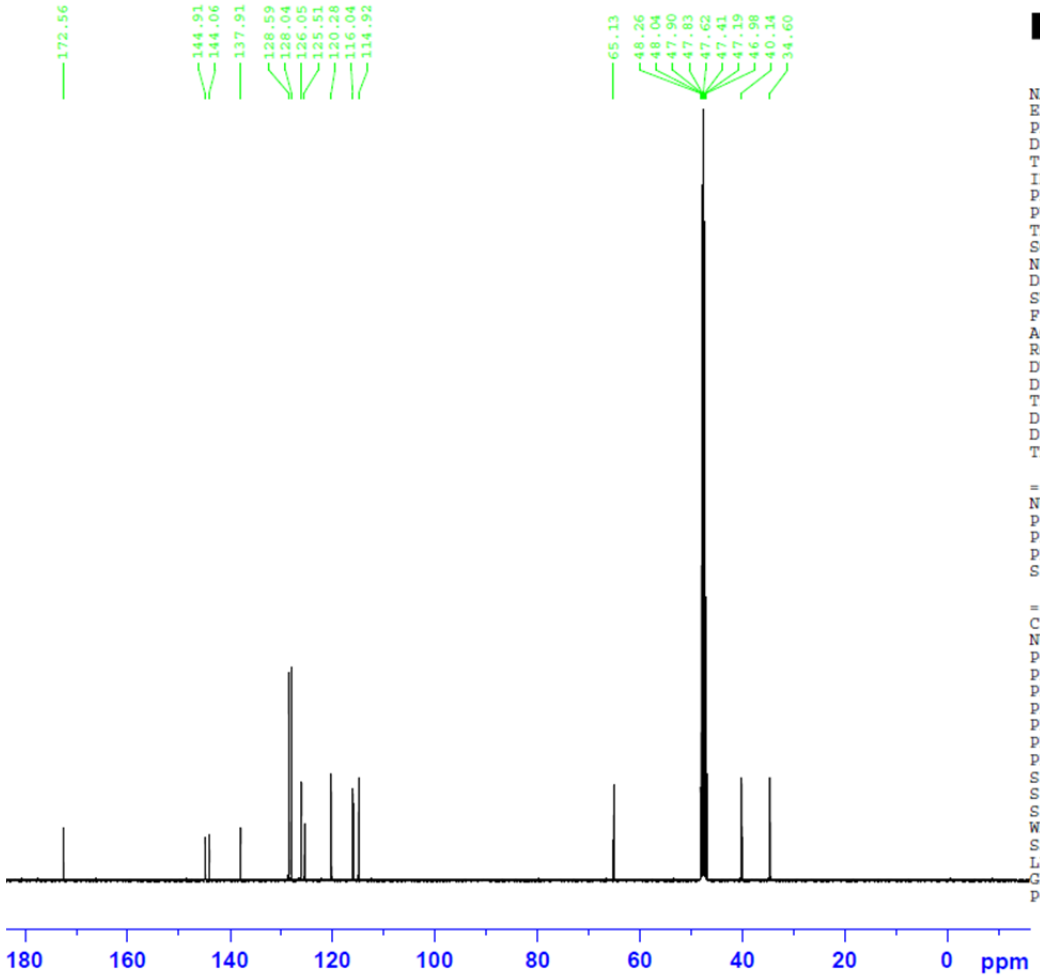


NAME	Moh RX
EXPNO	21
PROCNO	1
Date_	20140530
Time	9.22
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	80.6
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	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

^{13}C NMR



12



BRUKER

NAME	Luc
EXPNO	164
PROCNO	1
Date_	20120430
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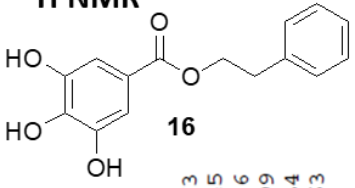
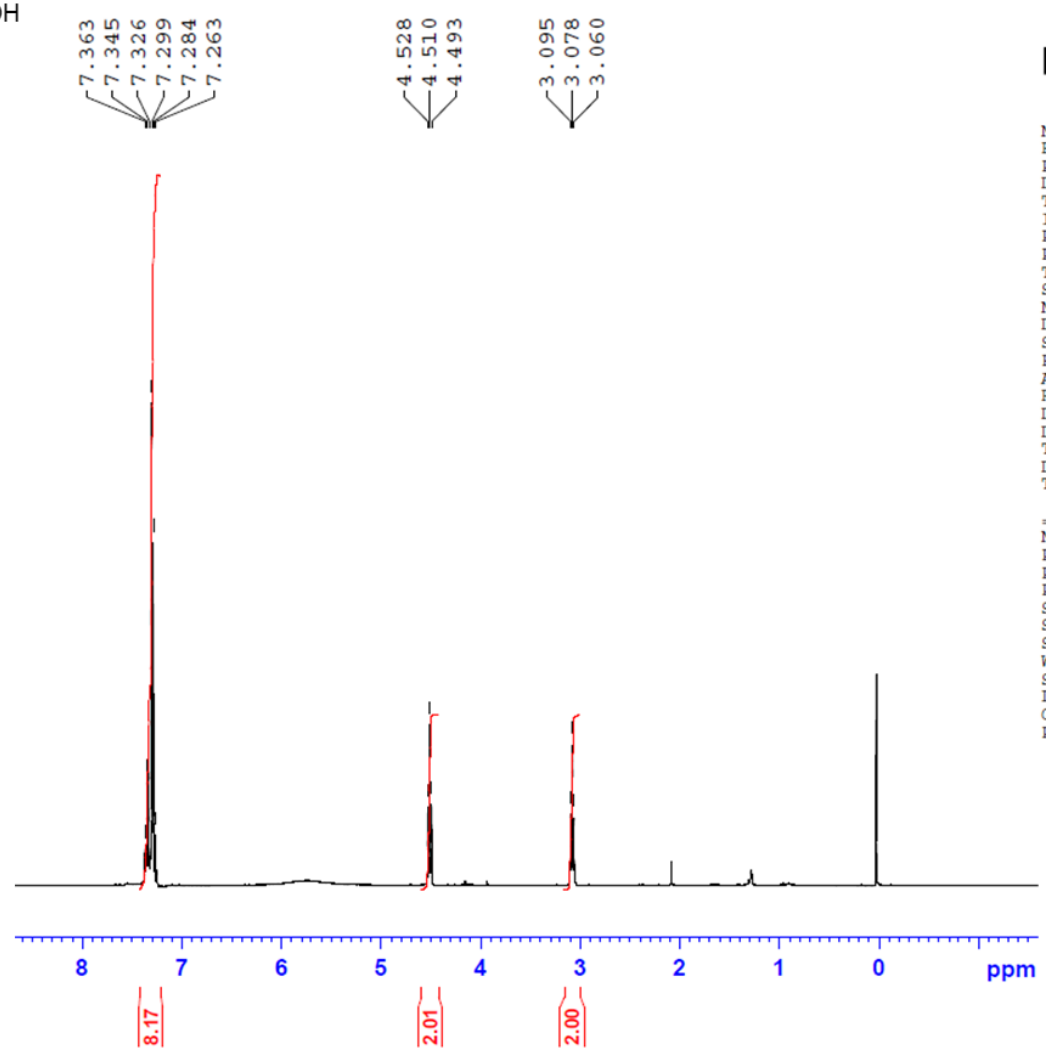
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	MeOD
NS	839
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.90 usec
PL1	-1.90 dB
PL1W	56.02249908 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

^{1}H NMR



16



BRUKER

NAME	Moh RX
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PROCNO	1
Date_	20130205
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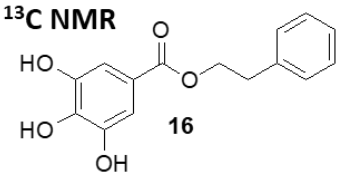
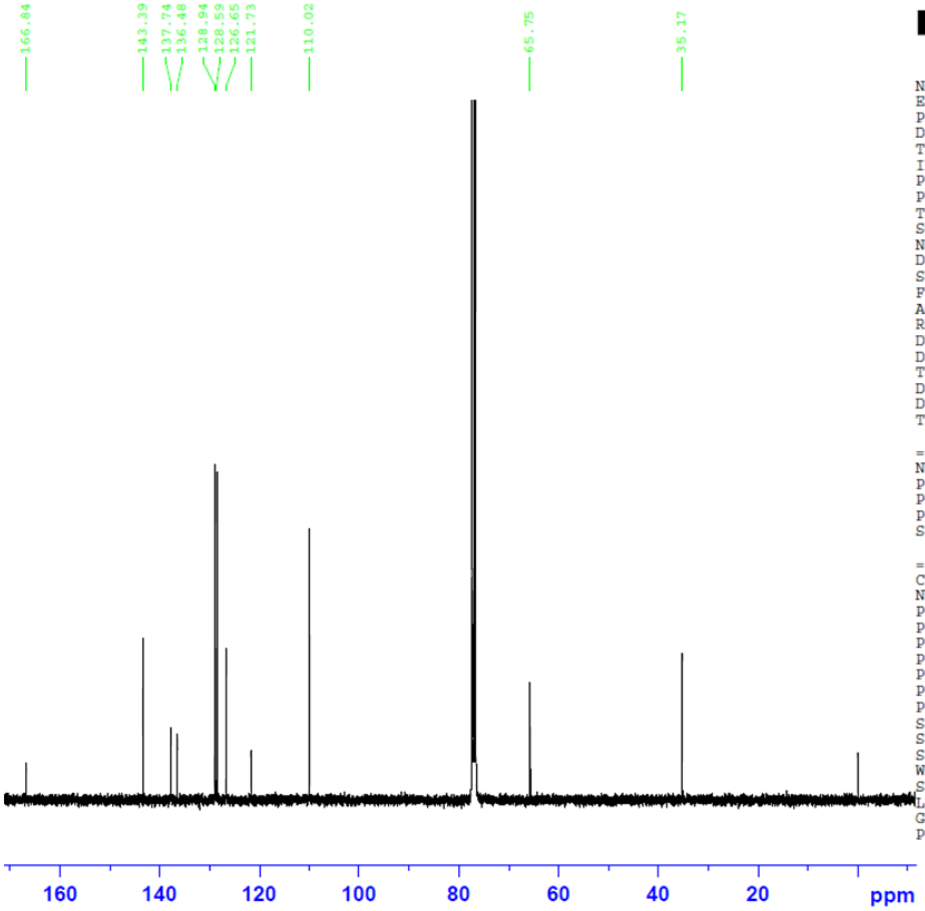
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	144
DW	60.800 usec
DE	6.50 usec
TE	298.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR



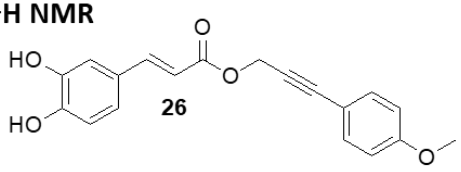
16



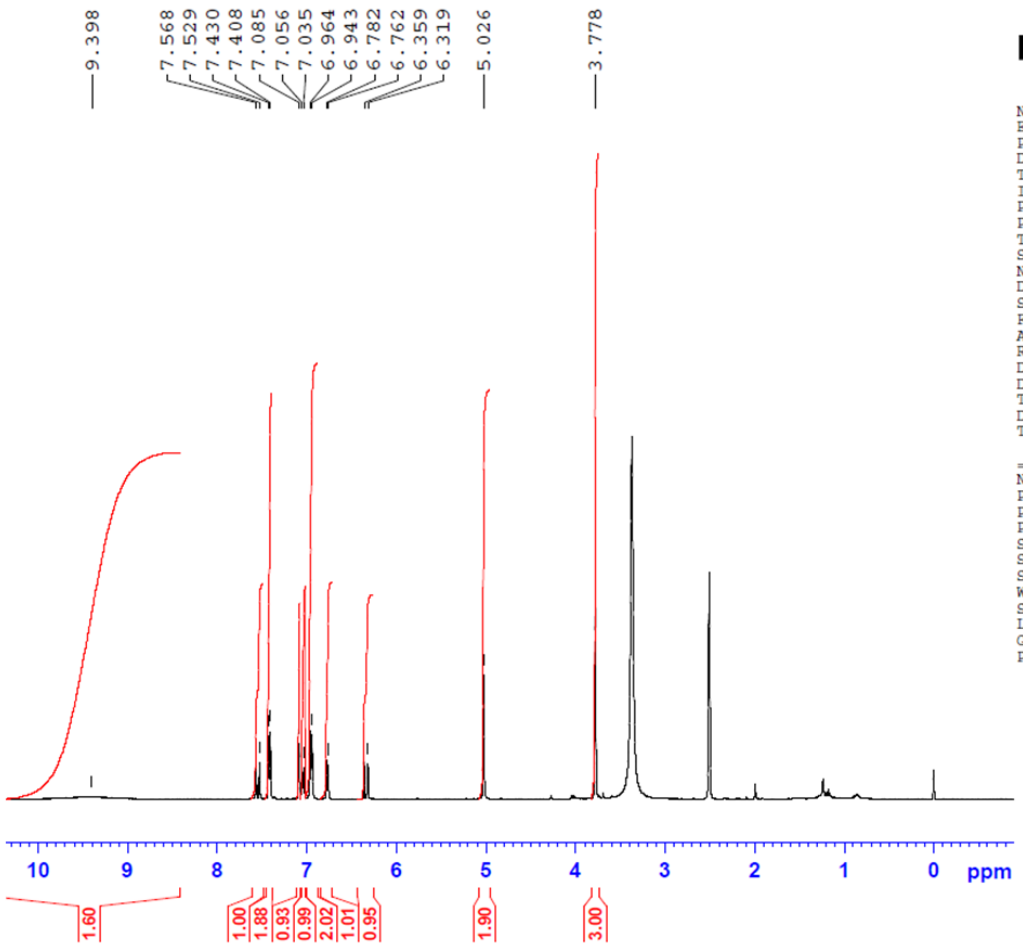
BRUKER

```
NAME                 Moh RX
EXPNO                   184
PROCNO                    1
Date_              20130205
Time                  14.27
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDC13
NS                     4567
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
```

^{1}H NMR



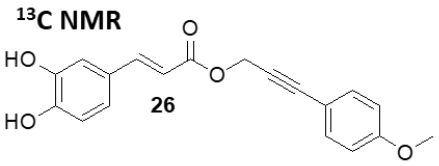
26

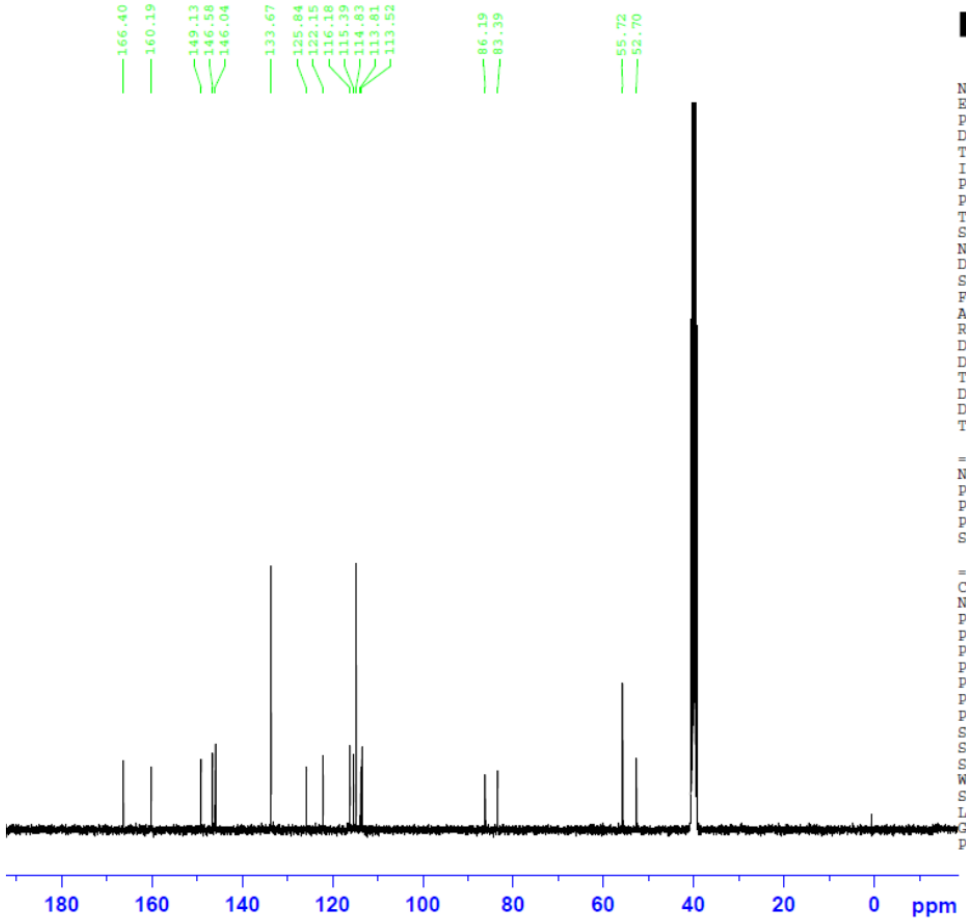


BRUKER

NAME	Jeremie
EXPNO	291
PROCNO	1
Date_	20110401
Time	11.22
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8223.685 Hz
PIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	90.5
DW	60.800 usec
DE	6.50 usec
TE	293.9 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

^{13}C NMR

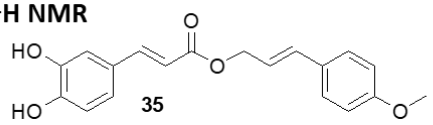


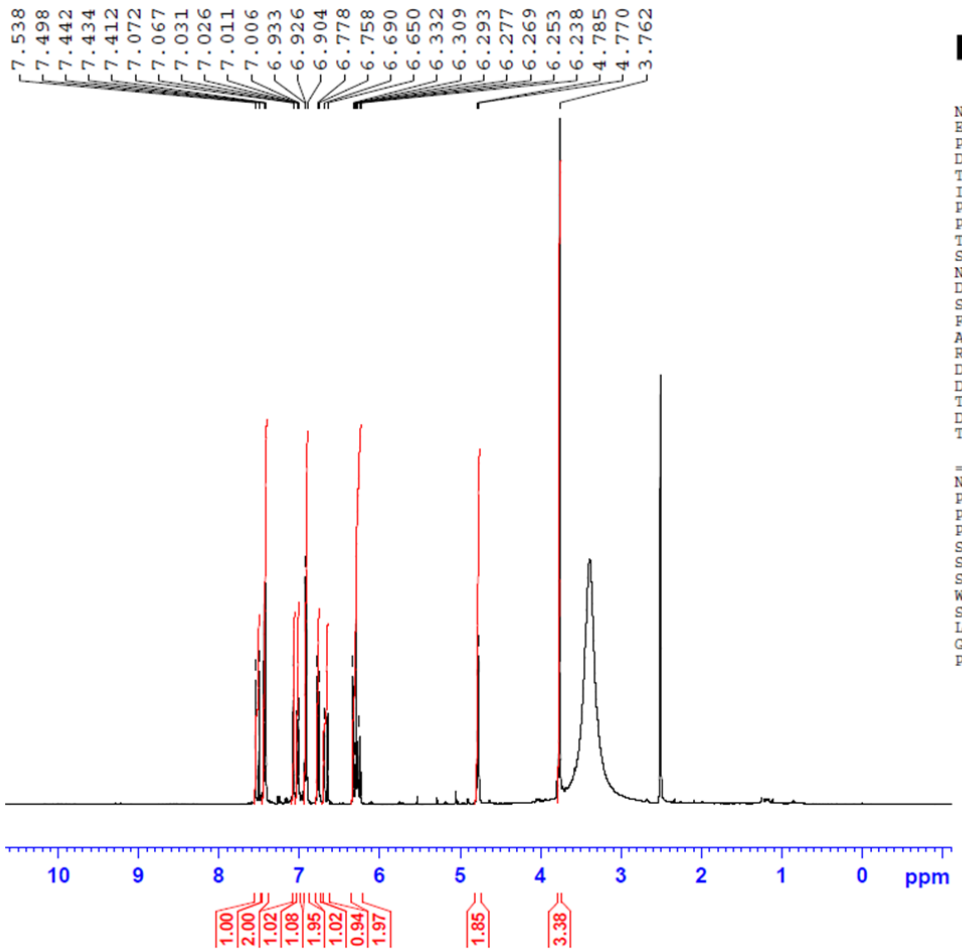


BRUKER

```
NAME                 Jeremie
EXPNO                    292
PROCNO                     1
Date_               20110401
Time                   15.24
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                       4096
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                     295.5 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
```

^{1}H NMR

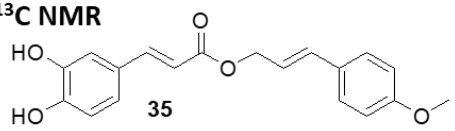


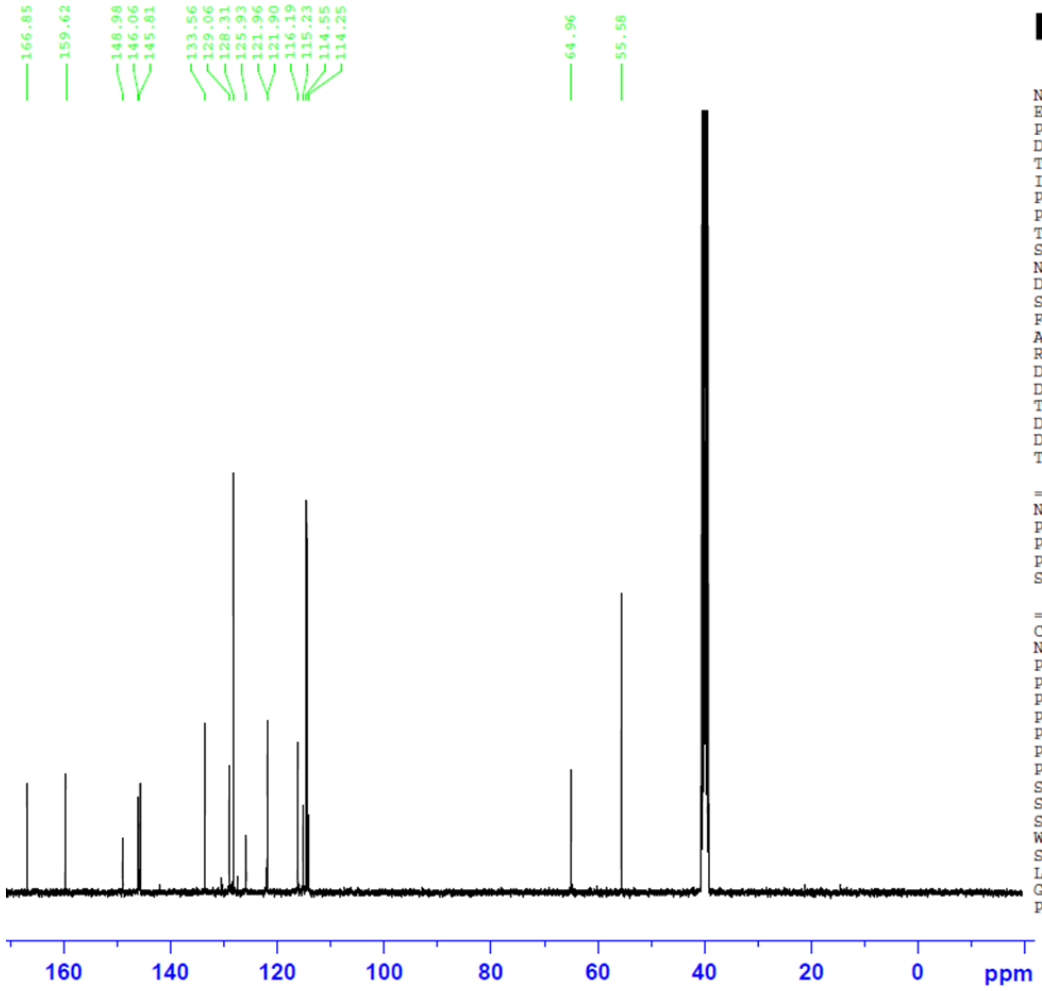


BRUKER

NAME	Jeremie
EXPNO	631
PROCNO	1
Date_	20120803
Time	10.25
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	32
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

^{13}C NMR

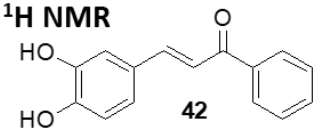




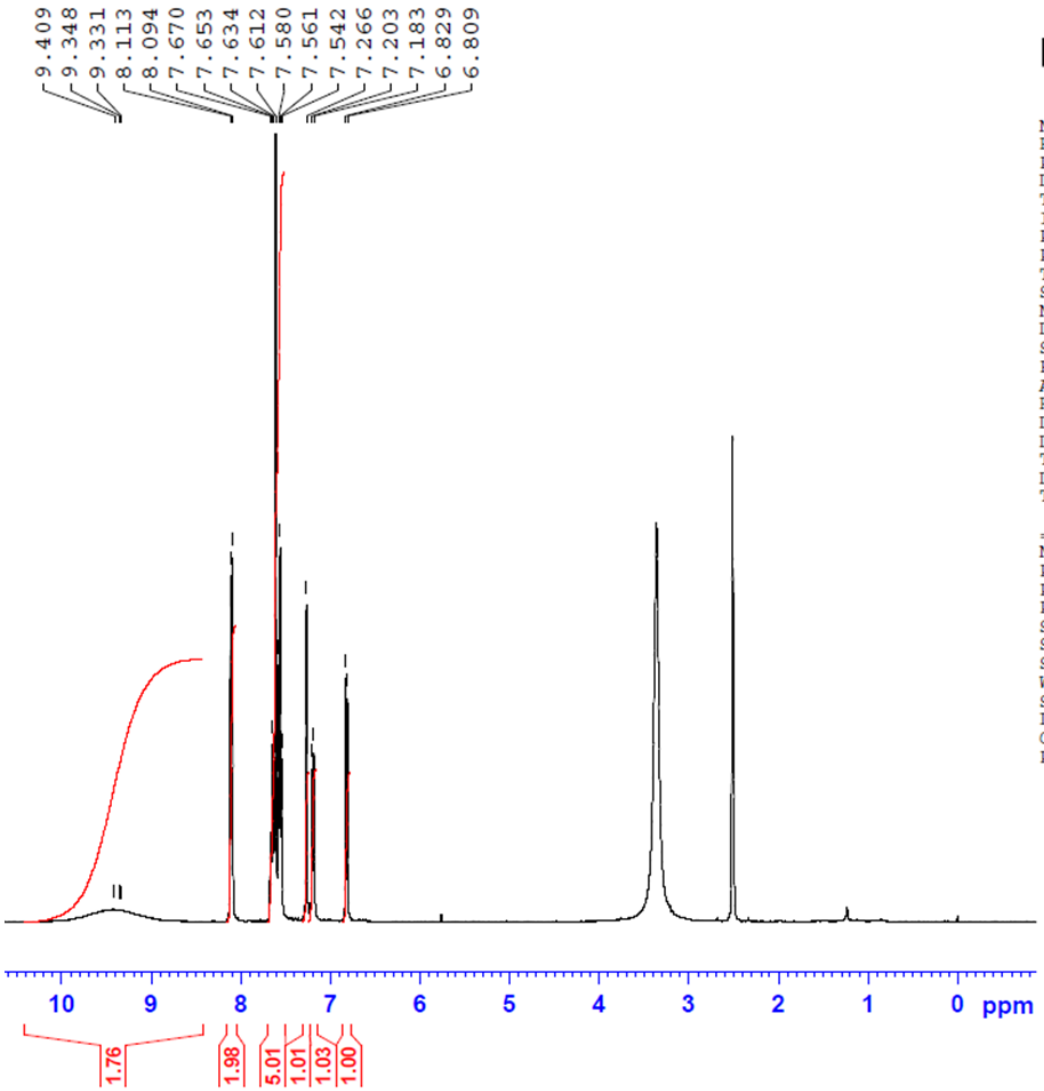
BRUKER

NAME	Jeremie
EXPNO	634
PROCNO	1
Date_	20120804
Time	0.24
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
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

^{1}H NMR



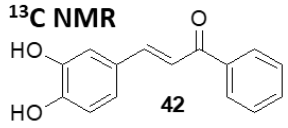
42



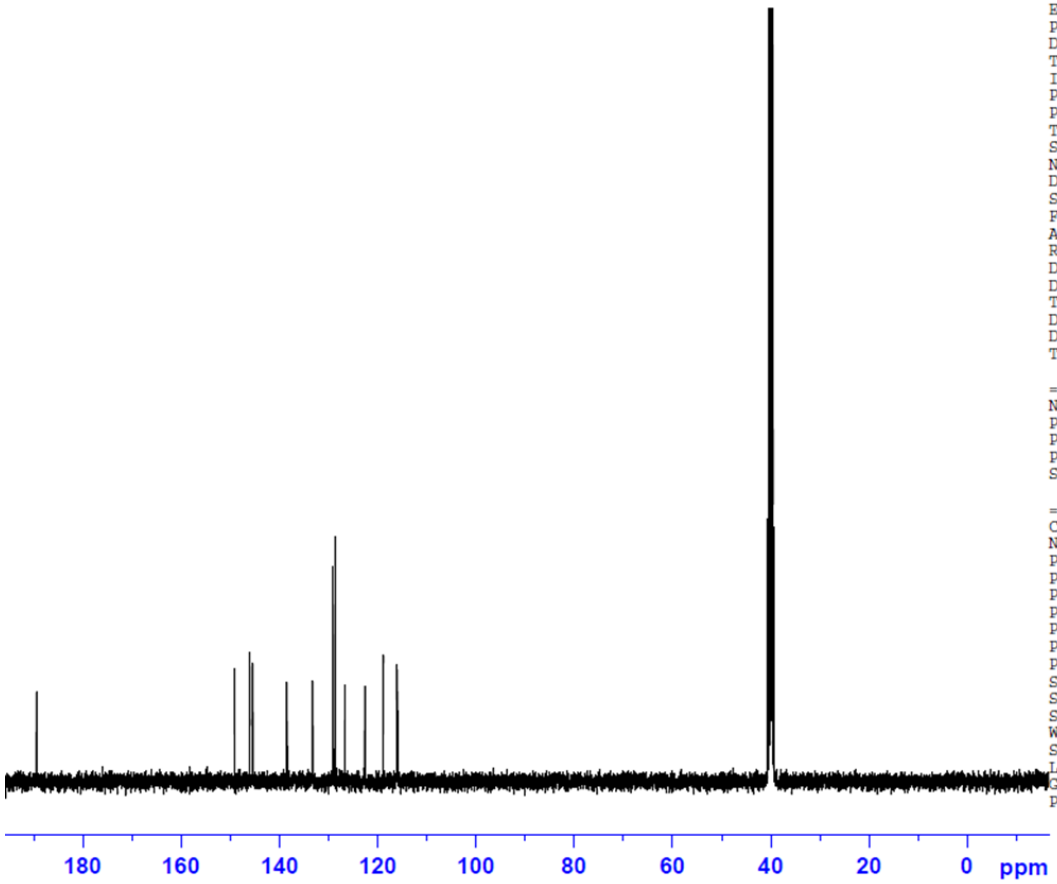
BRUKER

NAME	Jeremie	
EXPNO	516	
PROCNO	1	
Date_	20120511	
Time	13.22	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	DMSO	
NS	64	
DS	2	
SWH	8223.685	Hz
FIDRES	0.125483	Hz
AQ	3.9846387	sec
RG	80.6	
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	

^{13}C NMR

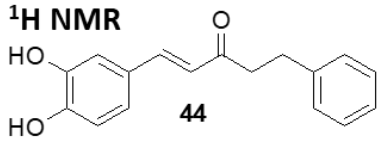


42

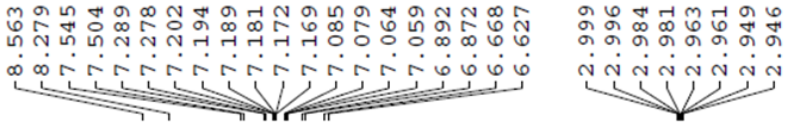


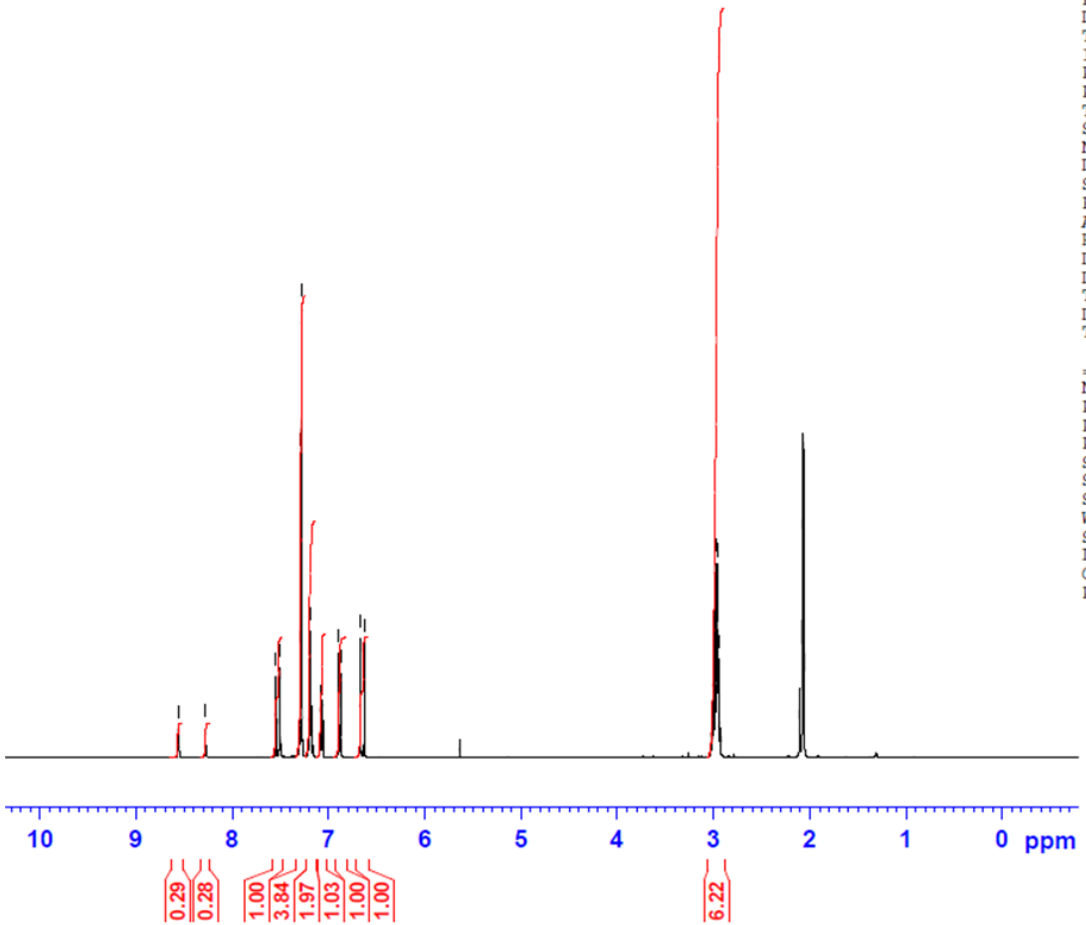

```
NAME                 Jeremie
EXPNO                    519
PROCNO                     1
Date_             20120515
Time                    9.36
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                        218
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
```

^{1}H NMR



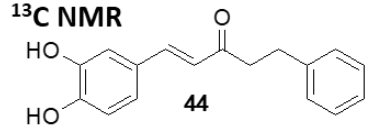
44






```
NAME                 Jeremie
EXPNO                    566
PROCNO                     1
Date_               20120607
Time                   14.19
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT             Acetone
NS                         32
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
```

^{13}C NMR



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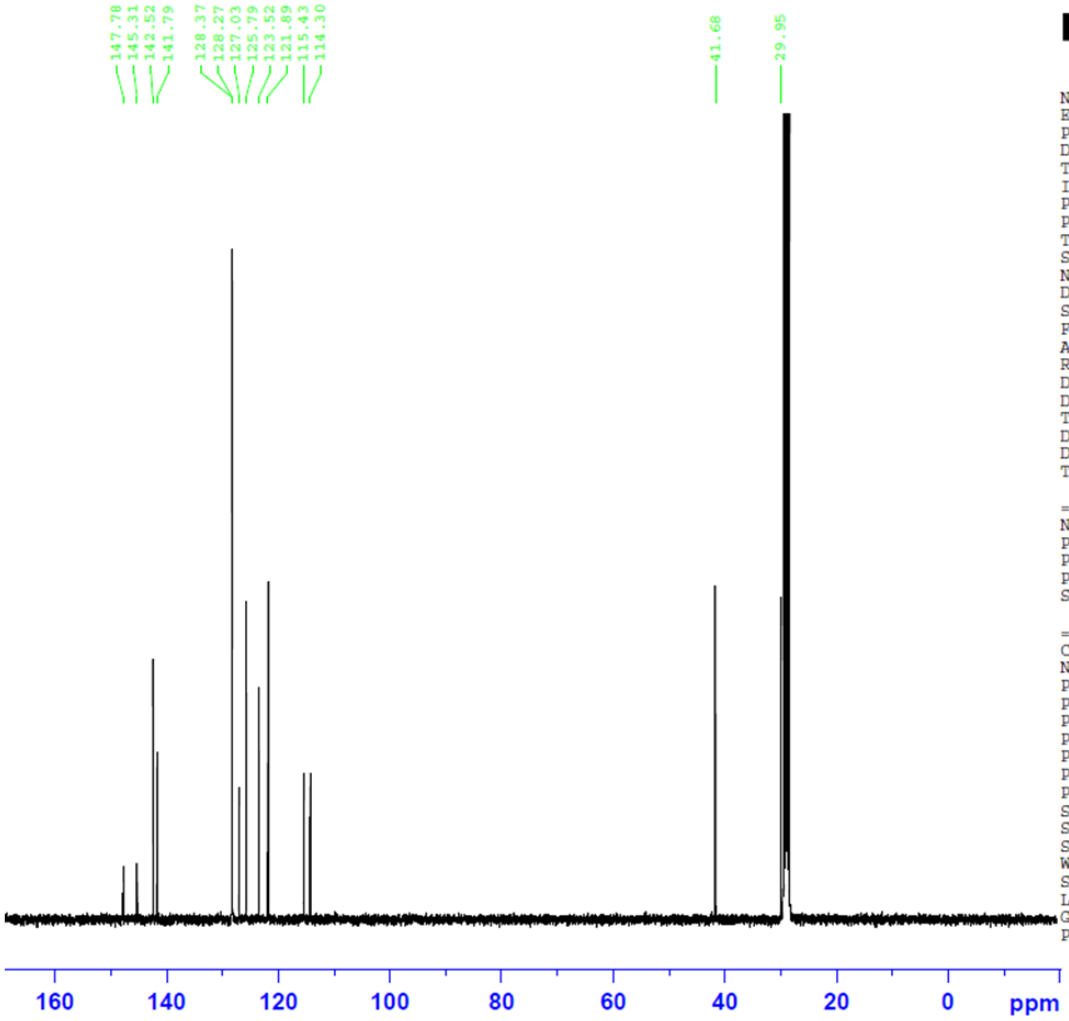

BRUKER

NAME	Jeremie	
EXPNO	567	
PROCNO	1	
Date_	20120607	
Time	16.29	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	Acetone	
NS	2131	
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	