

Supporting Information (SI)

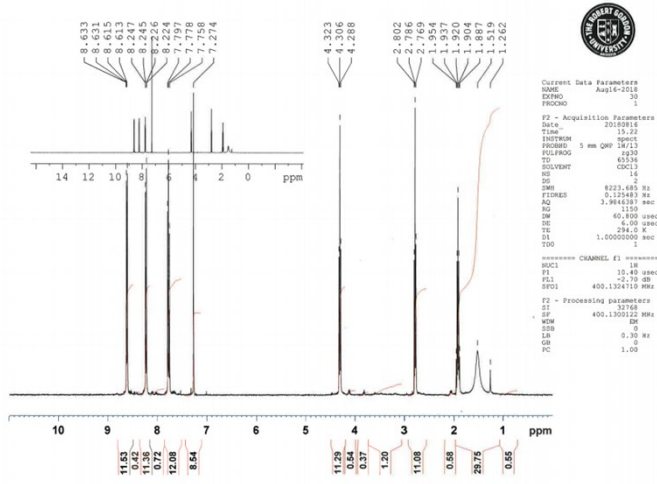
Synthesis of novel vanillin derivatives: novel multi-targeted scaffold ligands against Alzheimer's disease

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Compound I-1

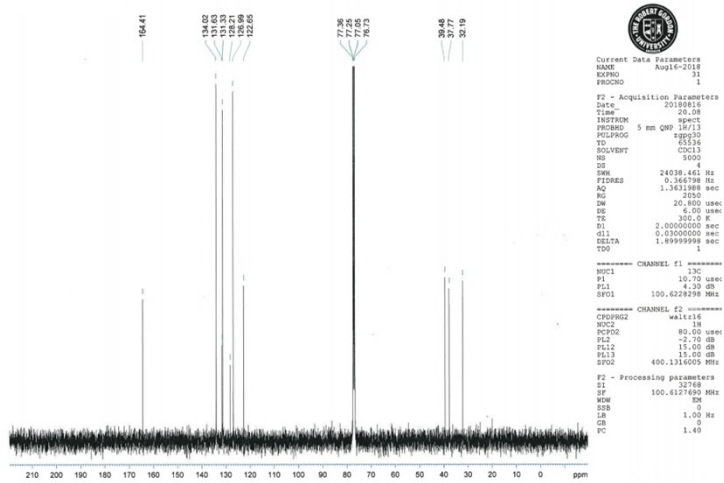


Current Data Parameters
 NAME Aug16-2018
 EXPRNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180816
 Time 15.22
 INSTRUM spect
 PROBRD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 4
 DS 2
 SWH 8233.461 Hz
 FIDRES 0.122483 Hz
 AQ 1.9614187 sec
 RG 3200
 SQ 40150
 SNR 4.000 usec
 TE 294.2 K
 DE 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NU1 1H
 P1 19.49 usec
 PL1 0.0012139 dB
 SFO1 400.114189 MHz

F2 - Processing parameters
 SI 32768
 SF 400.114005 MHz
 WDW EM
 SSB 0
 GB 0.30 Hz
 PC 1.00



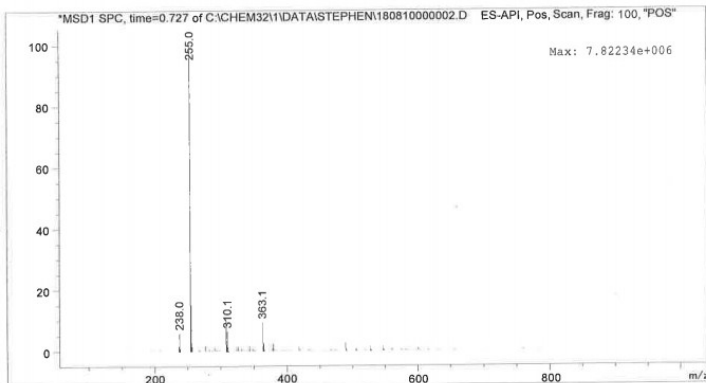
Current Data Parameters
 NAME Aug16-2018
 EXPRNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180816
 Time 20.08
 INSTRUM spect
 PROBRD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 4
 DS 2
 SWH 24038.461 Hz
 FIDRES 0.360798 Hz
 AQ 1.3633288 sec
 RG 3200
 SQ 40150
 SNR 4.000 usec
 TE 300.0 K
 DE 1.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999999 sec
 TDO 4

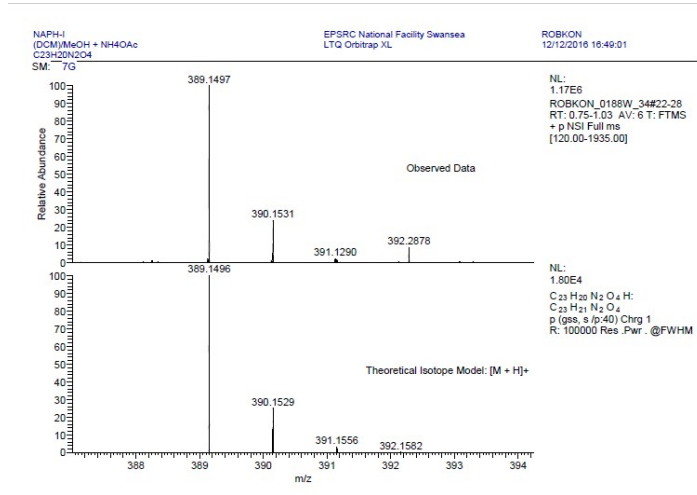
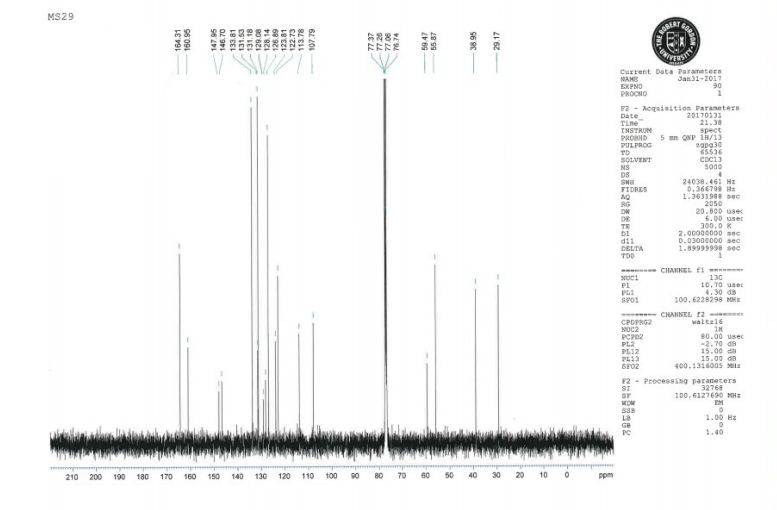
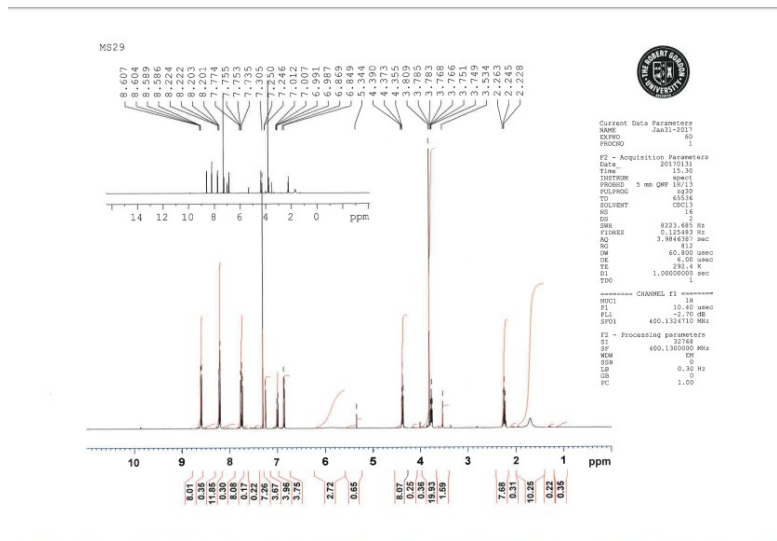
===== CHANNEL f1 =====
 NU1 13C
 P1 10.70 usec
 PL1 1.3633288 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NU2 1H
 P2 89.00 usec
 PL2 -1.70 dB
 PL12 15.00 dB
 PL1 15.00 dB
 SFO2 400.1314005 MHz

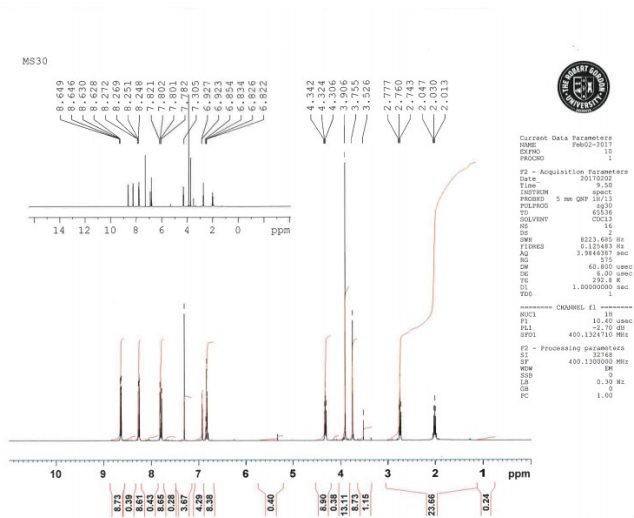
F2 - Processing parameters
 SI 32768
 SF 100.6127892 MHz
 WDW EM
 SSB 1.00 Hz
 GB 1.40



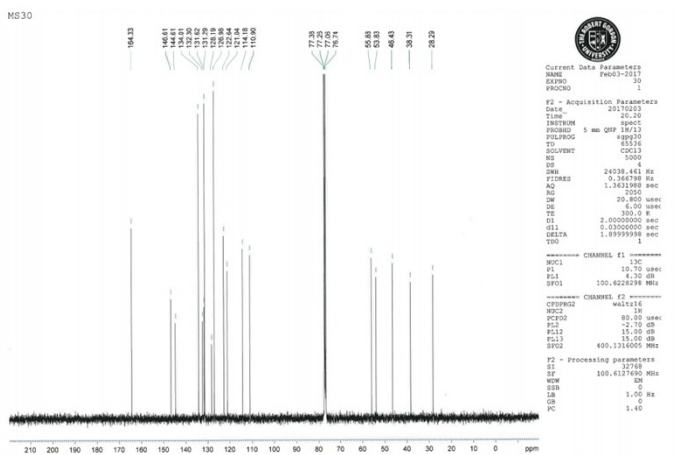
Compound 1



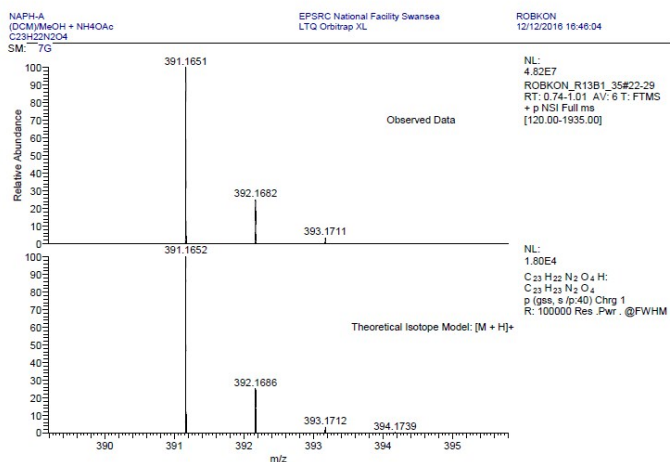
Compound 2



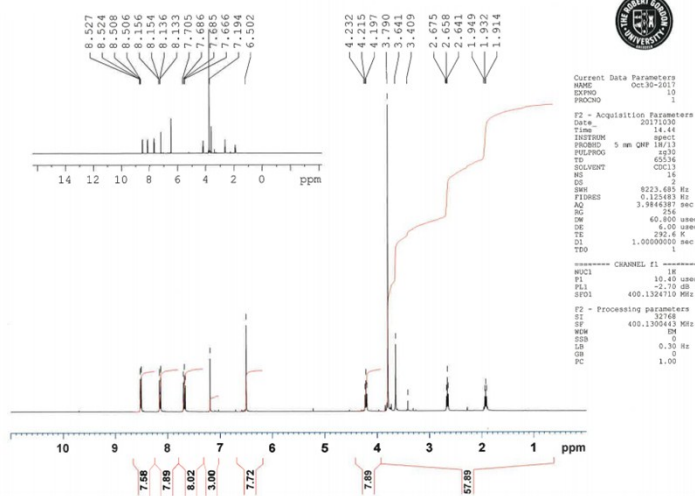
Current Data Parameters
 NAME: Feb02-2017
 EXPNO: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20170202
 Time: 9.32
 INSTRUM: spect
 PROBHD: 5 mm QNP 1H/1
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 16
 DS: 2
 SWH: 8223.685 Hz
 FIDRES: 0.122483 Hz
 AQ: 3.7844387 sec
 RG: 275
 SW: 40.800 MHz
 US: 6.000 MHz
 TE: 295.2 K
 DQ: 1.0000000 sec
 ===== CHANNEL f1 =====
 NUC1: 1H
 P1: 16.40 usec
 PL1: -2.00 dB
 SFO1: 400.1324710 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 400.1300000 MHz
 WDW: DM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00



Current Data Parameters
 NAME: Feb02-2017
 EXPNO: 3
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20170202
 Time: 20.20
 INSTRUM: spect
 PROBHD: 5 mm QNP 1H/1
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 5000
 DS: 24938.464 Hz
 SWH: 1.582188 MHz
 FIDRES: 1.631398 Hz
 AQ: 2.0000000 sec
 RG: 250
 SW: 20.800 MHz
 US: 6.000 MHz
 TE: 299.0 K
 DQ: 2.0000000 sec
 GB: 0
 GB1: 0.0300000 sec
 UDELTA: 1.8995938 sec
 TD0: 1
 ===== CHANNEL f1 =====
 NUC1: 13C
 P1: 16.70 usec
 PL1: 4.30 dB
 SFO1: 100.6228288 MHz
 ===== CHANNEL f2 =====
 NUC2: 1H
 P2: 62.00 usec
 PL2: -2.70 dB
 PL12: -15.00 dB
 SFO2: 400.1316000 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 100.6127690 MHz
 WDW: DM
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40



Compound 3

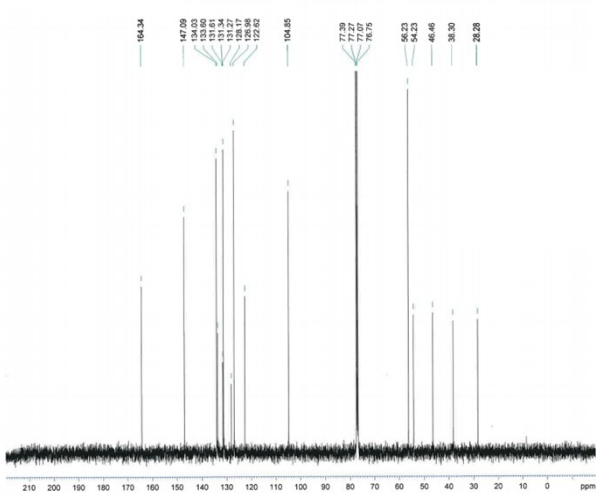


Current Data Parameters
 NAME Oct30-2017
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20171030
 Time 14:44
 INSTRUM spect
 PROBRID 5 mm QNP 1H/13
 PULPROG zgpg30
 TO 65336
 SOLVENT CDCl3
 NS 16
 DS 8233.68 Hz
 FIDRES 0.120483 Hz
 AQ 3.984638 sec
 RG 256
 DW 60.800 usec
 DE 6.00 usec
 TE 300.2 K
 TD 1.0000000 sec
 TQ 0

----- CHANNEL f1 -----
 NUC1 13
 P1 10.40 usec
 PL1 -2.50 dB
 SFO1 400.1324110 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300443 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME Oct30-2017
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20171030
 Time 15:03
 INSTRUM spect
 PROBRID 5 mm QNP 1H/13
 PULPROG zgpg30
 TO 65336
 SOLVENT CDCl3
 NS 1200
 DS 24039.464 Hz
 FIDRES 0.356798 Hz
 AQ 1.3931988 sec
 RG 2050
 DW 20.800 usec
 DE 6.00 usec
 TE 300.2 K
 TD 2.0000000 sec
 TQ 0.0300000 sec
 DELTA 1.8999999 sec
 TQ 0

----- CHANNEL f1 -----
 NUC1 13
 P1 10.70 usec
 PL1 -2.50 dB
 SFO1 100.6282298 MHz

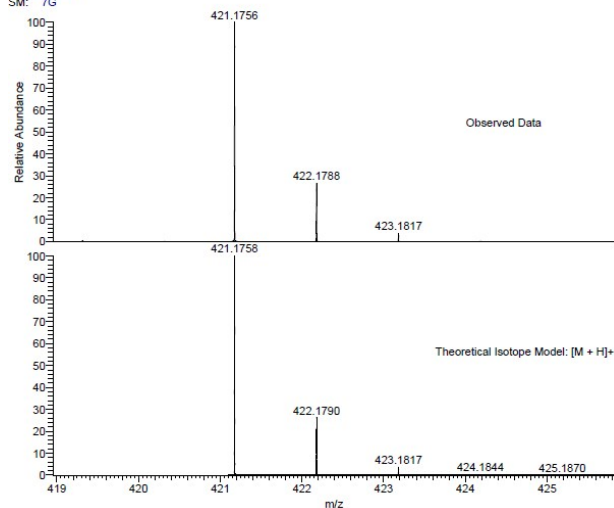
----- CHANNEL f2 -----
 CPROG2 waltz16
 NUC2 1H
 P2 65.00 usec
 PL2 -2.70 dB
 PL12 15.00 dB
 PL13 5.00 dB
 SFO2 400.1316050 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127680 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

NS
 (DCM)/MeOH + NH4OAc
 C24H24N2O5
 SM: 7G

EPSRC National Facility Swansea
 LTQ Orbitrap XL

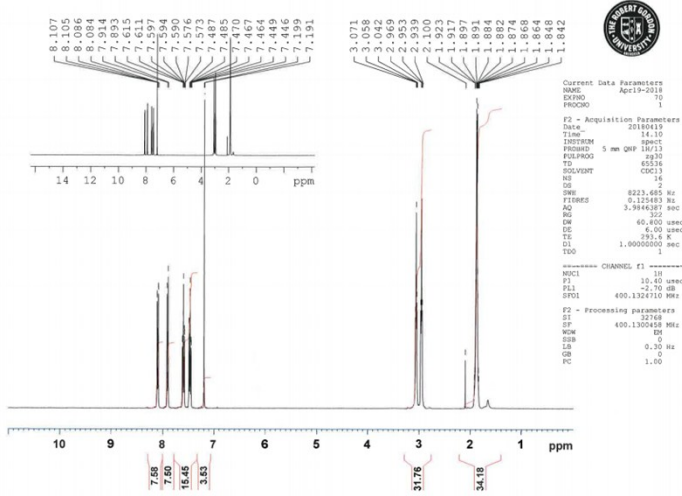
ROBKON
 14/11/2017 16:04:00



NL:
 4.79E6
 ROBKON_93CTM_38304#41-
 S4 RT: 0.72-1.04 AV: 12 T:
 FTMS + p NSI Full ms
 [120.00-1935.00]

NL:
 1.77E4
 C24 H24 N2 O5 H:
 C24 H25 N2 O5
 p (gas, s /p/40) Chrg 1
 R: 100000 Res. Pw. @FWHM

Compound I-2

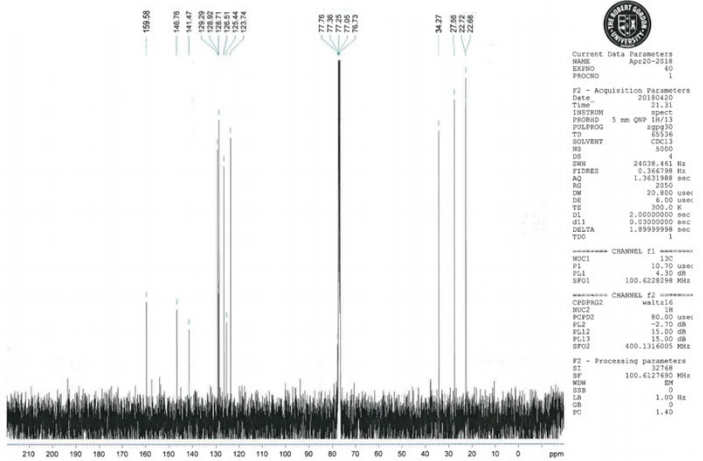


Current Data Parameters
 NAME: ApCl-2018
 EXPR: 10
 PROCNO: 1

F2 - Acquisition Parameters
 Date: 20180419
 Time: 14.10
 INSTRUM: spect
 PROBRD: 5 mm QNP 1H/13
 F2P1PRG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 16
 DS: 2
 SWH: 8233.685 Hz
 FIDRES: 0.132483 Hz
 AQ: 3.9946327 sec
 RG: 66.000 usec
 DE: 6.00 usec
 TE: 293.2 K
 D1: 1.90000000 sec
 TSD: 1

----- CHANNEL f1 -----
 NUC1: 13C
 P1: 10.00 usec
 PL1: -2.00 dB
 SFO1: 400.1324710 MHz

F2 - Processing parameters
 SI: 32768
 SF: 400.1300458 MHz
 NQ: 40
 SSB: 0.00 Hz
 LA: 0.30 Hz
 GB: 1.00
 PC: 1.00



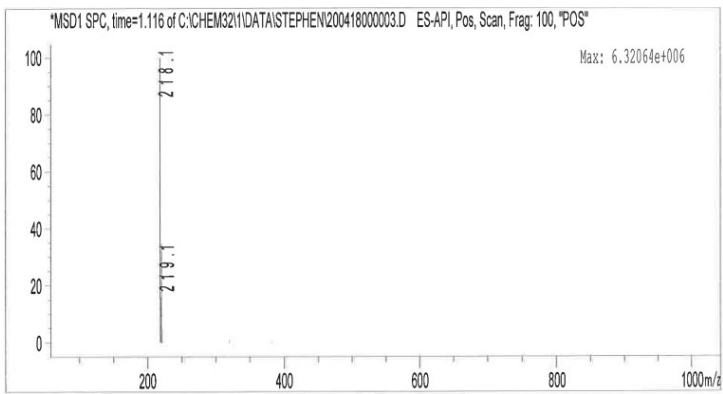
Current Data Parameters
 NAME: ApCl-2018
 EXPR: 40
 PROCNO: 1

F2 - Acquisition Parameters
 Date: 20180419
 Time: 21.31
 INSTRUM: spect
 PROBRD: 5 mm QNP 1H/13
 F2P1PRG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 5000
 DS: 4
 SWH: 24038.441 Hz
 FIDRES: 0.362788 Hz
 AQ: 1.3821888 sec
 RG: 7850
 DE: 20.800 usec
 TE: 300.2 K
 D1: 2.00000000 sec
 d11: 0.03000000 sec
 DELTA: 1.99999998 sec
 TSD: 1

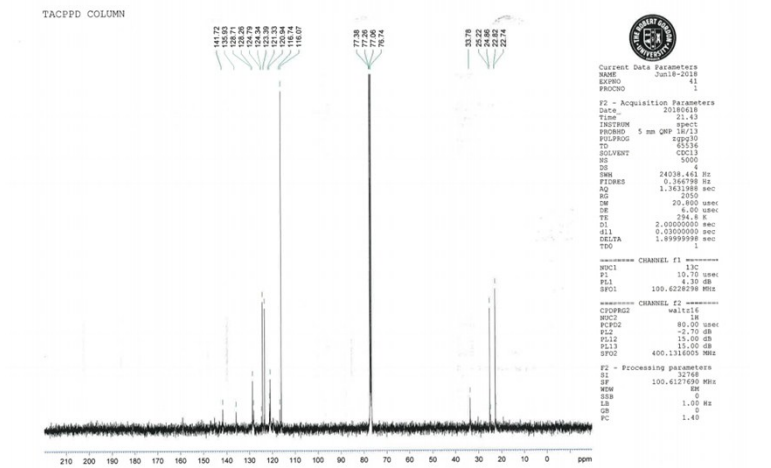
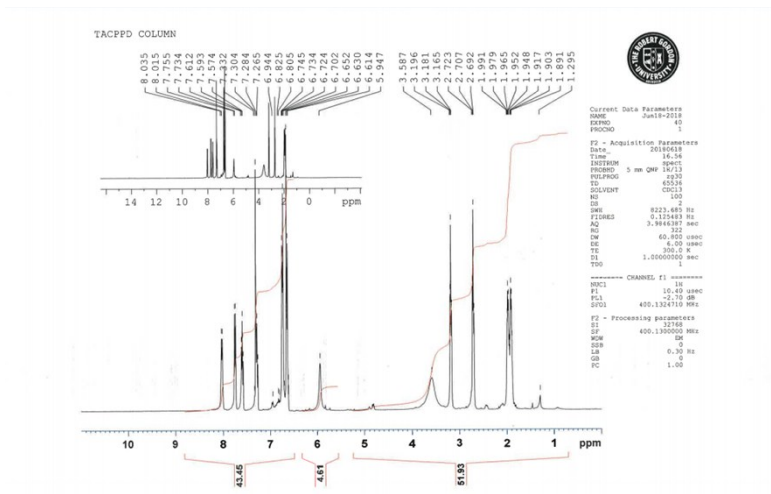
----- CHANNEL f1 -----
 NUC1: 13C
 P1: 10.70 usec
 PL1: 4.30 dB
 SFO1: 100.6228298 MHz

----- CHANNEL f2 -----
 NUC2: 1H
 P2P1: 80.00 usec
 PL2: -2.00 dB
 PL12: 15.00 dB
 PL1: 15.00 dB
 SFO2: 400.1316005 MHz

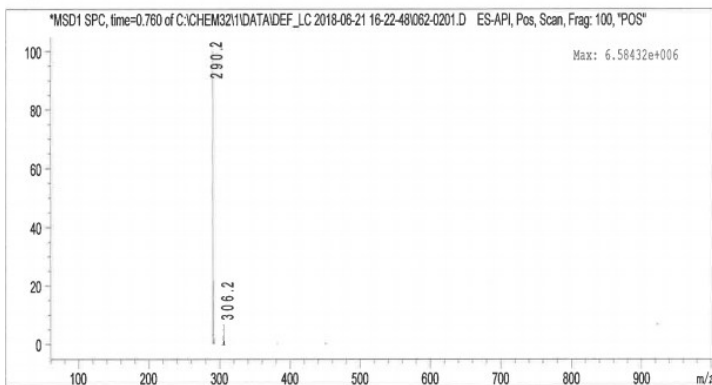
F2 - Processing parameters
 SI: 32768
 SF: 100.6127490 MHz
 NQ: 40
 SSB: 1.00 Hz
 LA: 0
 GB: 1.40
 PC: 1.40



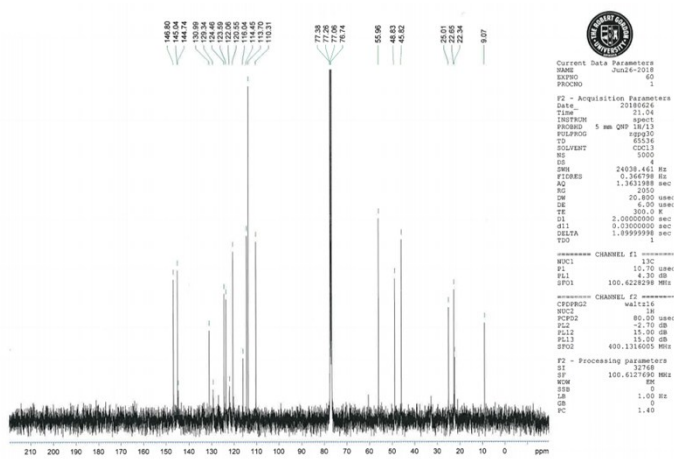
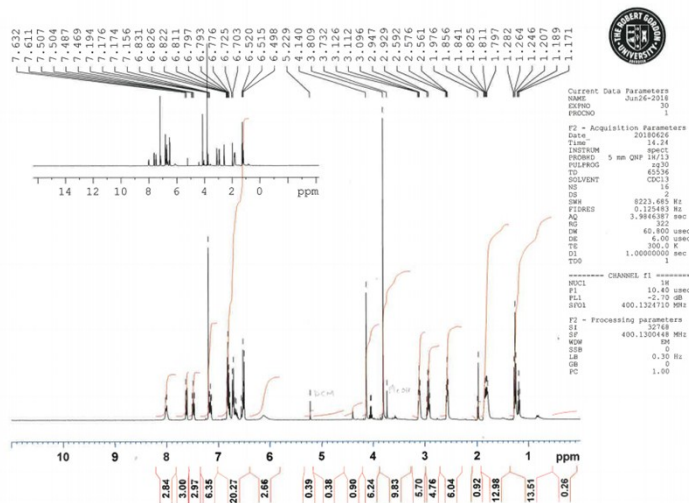
Compound I-3



Tacppd



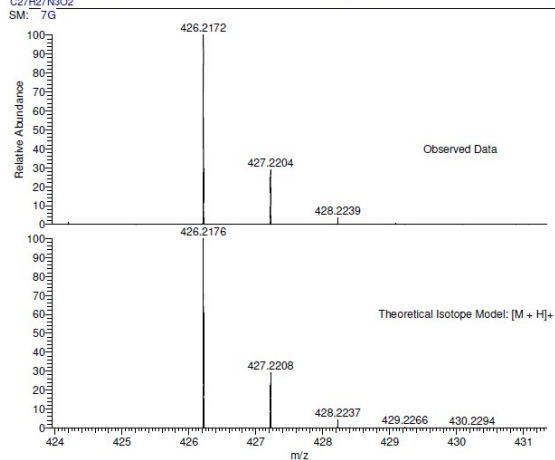
Compound 4



MS41
(MeOH)/MeOH.NH4OAc
C27H27N3O2

EPSC National Facility Swansea
LTO Orbitrap XL

ROBKON
28/09/2018 12:06:37



NL:
7.32E6
ROBKON_93KP9_48091#42-
56 RT: 0.74-1.02 AV: 11 T:
FTMS + p NSI Full ms
[120.00-1935.00]

NL:
1.72E4
C27H27N3O2 H:
C27H28N3O2
p (gss, s [p-4]) Chg 1
R: 100000 Res.Fwhm . @FWHM