Supporting Information

A direct synthesis of 4-Acetyl-*N*-1-alkyl-1*H*-pyrrol-2(5*H*)-ones from difunctionalized allyl bromide

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Copies of NMR spectra and high resolution mass spectrum
for compounds **4** and **5a-h**

Synthesis of Z-ethyl 3-bromomethyl-4-oxopent-2-enoate (4).

According to previous works, ethyl 3-methylene-4-oxopentanoate **2** was obtained in 66% yield. To a stirred solution of **2** (32 mmol, 5 g) in CCl₄ (80 mL), 1.2 equiv. of bromine (38.4 mmol, 2 mL) was added dropwise at 0 °C. The resulting mixture was left for one hour at room temperature then washed with an aqueous solution of Na₂S₂O₃ and dried over MgSO₄ to eliminate excess of bromine. Triethylamine (Et₃N, 70.4 mmol, 9.6 mL) was added to the cold mixture (0 °C) and stirring was continued for 3 hours at room temperature. The mixture was filtered then concentrated under reduced pressure to leave an oil which was purified by chromatography on silica gel (petroleum ether/AcOEt, 9:1). Yield (5.52g, 74%) as a yellow liquid; IR (KBr): $\nu_{\max}$ 2983.99, 1717.67, 1652.75, 1558.39, 1026.41, 667.94 cm⁻¹; ¹H-NMR (300.13 MHz, CDCl₃): 6.60 (s, 1H, =CH), 4.68 (s, 2H, CH₂Br), 4.30 (q, 2H, ³J_{HH} = 6.00 Hz, CH₂CH₃), 2.45 (s, 3H, COCH₃), 1.35 (t, 3H, ³J_{HH} = 6.00 Hz, CH₂CH₃); ¹³C-NMR (75 MHz, CDCl₃): 197.1 (CO), 164.9 (CO₂Et), 148.9 (=C), 128.0 (=CH), 61.6 (CH₂CH₃), 26.4 (CH₂Br), 21.2 (CH₃CO), 14.1 (CH₃CH₂). HRMS calculated for [M+Na]⁺ C₈H₁₁O₃BrNa: 256.97838, found: 256.97842.

General procedure for the synthesis of 4-acetyl-1-alkyl-1H-pyrrol-2(5H)-ones 5a-h.

Primary amine (2.55 mmol, 2 equiv.) was added dropwise to a solution of ethyl 3-bromomethyl-4-oxopent-2-enoate **4** (0.3 g, 1.27 mmol) in bromobenzene (7 mL). The solution was heated for 0.5 to 2.5 hours at 150 °C. The solvent was concentrated under reduced pressure and the crude product was purified by chromatography on silica gel.

4-Acetyl-1-benzyl-1H-pyrrol-2(5H)-one 5a. Yellow oil. Yield (0.14 g, 52%). (Petroleum ether/ether, 6:4). IR (KBr), $\nu_{\max}$ (cm⁻¹): 2927, 1700, 1653, 1558, 668. ¹H NMR (300 MHz, CDCl₃): 7.40-7.30 (m, 6H, =CH, 5H_{Ar}), 4.69 (s, 2H, CH₂Ph), 3.36 (d, 2H, ²J_{HH} = 1.80 Hz, CH₂N), 2.18 (s, 3H, COCH₃); ¹³C NMR (75 MHz, CDCl₃): 190.8 (CO), 175.8 (CON), 142.6 (C_q), 135.6 (C_q), 129.1 (C_{Ar}), 128.2 (C_{Ar}), 127.8 (C_{Ar}), 119.7(=CH), 46.1 (CH₂Ph), 35.6 (CH₂N), 25.0 (CH₃). HRMS calculated for [M+H]⁺ C₁₃H₁₄O₂N: 216.10191, found: 216.10180.

4-Acetyl-1-(4-fluorobenzyl)-1H-pyrrol-2(5H)-one 5b. Orange oil. Yield (0.19 g, 49%). (Ether). IR (KBr), $\nu_{\max}$ (cm⁻¹): 2924, 1700, 1653, 1558, 668. ¹H NMR (300 MHz, CDCl₃): 7.25-7.20 (m, 3H, =CH, 2H_{Ar}), 7.04 (t, 2H, ³J_{HF} = 9.00 Hz, H_{Ar}), 4.64 (s, 2H, CH₂Ph), 3.34 (d, 2H, ²J_{HH} = 1.80 Hz, CH₂N), 2.18 (s, 3H, COCH₃); ¹³C NMR (75 MHz, CDCl₃): 191.1 (CO), 176.0 (CON), 142.5 (C_{Ar}F, C_q), 130.0 (C_{Ar}), 129.9 (C_{Ar}), 125.7 (C_q), 120.1 (=CH), 116.4 (C_{Ar}), 116.2 (C_{Ar}), 45.7 (CH₂Ph), 35.9 (CH₂N), 25.4 (CH₃); ¹⁹F NMR (282MHz, CDCl₃): (-113.33). HRMS calculated for [M+H]⁺ C₁₃H₁₃O₂NF: 234.09248, found: 234.09247.

4-Acetyl-1-(4-chlorobenzyl)-1H-pyrrol-2(5H)-one 5c. Orange oil. Yield (0.2 g, 48%). (Petroleum ether/ether, 6:4). IR (KBr), $\nu_{\max}$ (cm⁻¹): 2856, 1701, 1653, 1559, 576. ¹H NMR (300 MHz, CDCl₃): 7.34-7.22 (m, 5H, =CH, 4H_{Ar}), 4.64 (s, 2H, CH₂Ph), 3.34 (d, 2H, ²J_{HH} = 1.80 Hz, CH₂N), 2.18 (s, 3H, COCH₃); ¹³C NMR (75 MHz, CDCl₃): 191.0 (CO), 175.9 (CON), 142.5 (C_q), 134.4 (C_q), 134.3 (C_{Ar}Cl), 129.5 (C_{Ar}), 129.4 (C_{Ar}), 120.1 (=CH), 45.7 (CH₂Ph), 35.8 (CH₂N), 25.3 (CH₃). HRMS calculated for [M+H]⁺ C₁₃H₁₃O₂NCl: 250.05566, found: 250.05566.

Acetyl-1-phenylethyl-1H-pyrrol-2(5H)-one 5d. Brown oil. Yield (0.17 g, 45%). (Petroleum ether/ether, 1:9). IR (KBr), $\nu_{\max}$ (cm⁻¹): 2854, 1700, 1558, 1539, 701. ¹H NMR

(300 MHz, CDCl₃): 7.23-7.08 (m, 6H, =CH, 5H_{Ar}), 3.71 (t, 2H, ³J_{HH} = 6.90 Hz, CH₂CH₂), 3.19 (d, 2H, ²J_{HH} = 1.50 Hz, CH₂N), 2.86 (t, 2H, ³J_{HH} = 6.90 Hz, CH₂CH₂), 2.03 (s, 3H, CH₃CO); ¹³C NMR (75 MHz, CDCl₃): 190.9 (CO), 176.1 (CON), 143.9 (C_q), 137.7 (C_q), 128.9 (C_{Ar}), 128.8 (C_{Ar}), 127.0 (C_{Ar}), 118.7 (=CH), 44.2 (CH₂CH₂), 35.3 (CH₂N), 29.7 (CH₂Ph), 25.0 (CH₃). HRMS calculated for [M+H]⁺ C₁₄H₁₆O₂N: 230.11756, found: 230.11771.

4-Acetyl-1-(furan-2-ylmethyl)-1H-pyrrol-2(5H)-one 5e. Yellow oil. Yield (0.25 g, 71%). (Ether). IR (KBr), ν_{max} (cm⁻¹): 2854, 1717, 1653, 1560, 600. ¹H NMR (300 MHz, CDCl₃): 7.32-7.31 (m, 1H, =CH), 7.29 (s, 1H, =CH), 6.27-6.24 (m, 2H, =CH), 4.59 (s, 2H, CH₂), 3.23 (d, 2H, ²J_{HH} = 0.90 Hz, CH₂N), 2.14 (s, 3H, CH₃); ¹³C NMR (75 MHz, CDCl₃): 191.1 (CO), 175.6 (CON), 148.7 (C_q), 143.3 (C_q), 142.7 (=CH), 119.8 (=CH), 110.8 (=CH), 109.4 (=CH), 38.8 (CH₂), 35.7 (CH₂N), 25.2 (CH₃). HRMS calculated for [M+H]⁺ C₁₁H₁₂O₃N: 206.08117, found: 206.08139.

4-Acetyl-1-(pyridin-2-ylmethyl)-1H-pyrrol-2(5H)-one 5f. Yellow oil. Yield (0.19 g, 56%). (Ether). IR (KBr), ν_{max} (cm⁻¹): 2854, 1734, 1653, 1558, 668. ¹H NMR (300 MHz, CDCl₃): 8.58 (d, 1H, ³J_{HH} = 4.20 Hz, H_{Ar}), 7.73-7.67 (td, 1H, ³J_{HH} = 7.80 Hz, ³J_{HH} = 7.80 Hz, H_{Ar}), 7.59 (s, 1H, =CH), 7.32-7.27 (m, 2H, H_{Ar}), 4.81 (s, 2H, CH₂Ph), 3.34 (d, 2H, ²J_{HH} = 1.80 Hz, CH₂N), 2.26 (s, 3H, CH₃CO); ¹³C NMR (75 MHz, CDCl₃): 191.3 (CO), 176.0 (CON), 155.1 (C_q), 149.8 (C_q), 143.9 (=CH), 137.3 (=CH), 123.2 (=CH), 122.7 (=CH), 119.5 (=CH), 47.6 (CH₂), 35.5 (CH₂N), 29.7 (CH₃). HRMS calculated for [M+H]⁺ C₁₂H₁₃O₂N₂: 217.09715, found 217.09703.

4-Acetyl-1-isopropyl-1H-pyrrol-2(5H)-one 5g. Yellow oil. Yield (0.2 g, 71%). (Ether). IR (KBr), ν_{max} (cm⁻¹): 2849, 1700, 1653, 1558, 668. ¹H NMR (300 MHz, CDCl₃): 7.45 (s, 1H, =CH), 4.46-4.32 (sept, 1H, ³J_{HH} = 6.90 Hz, ³J_{HH} = 6.60 Hz, CH), 3.32 (d, 2H, ²J_{HH} = 1.80 Hz, CH₂N), 2.27 (s, 3H, COCH₃), 1.30 (d, 6H, ³J_{HH} = 6.90 Hz, CHCH₃); ¹³C NMR (75 MHz, CDCl₃): 191.6 (CO), 175.9 (CON), 140.6 (C_q), 119.9 (=CH), 43.8 (CH), 36.1 (CH₂N), 25.5 (CH₃), 21.9 (2xCH₃). HRMS calculated for [M+H]⁺ C₉H₁₄O₂N: 168.10191, found: 168.10182.

(R)-4-acetyl-1-(1-phenylethyl)-1H-pyrrol-2(5H)-one 5h. Brown oil. Yield (0.26 g, 90%). (Petroleum ether/ether, 7:3). IR (KBr), ν_{max} (cm⁻¹): 2980, 1652, 1496, 701. ¹H NMR (300 MHz, CDCl₃): 7.31-7.20 (m, 6H, =CH, 5H_{Ar}), 5.44-5.37 (q, 1H, ³J_{HH} = 7.20 Hz, CH), 3.28 (d, 2H, ²J_{HH} = 1.80 Hz, CH₂N), 2.12 (s, 3H, COCH₃), 1.60 (d, 3H, ³J_{HH} = 7.20 Hz, CHCH₃); ¹³C NMR (75 MHz, CDCl₃): 191.1 (CO), 175.7 (CON), 140.8 (C_q), 139.8 (C_q), 129.1 (C_{Ar}), 128.3 (C_{Ar}), 126.7 (C_{Ar}), 119.8 (=CH), 50.1 (CHN), 36.2 (CH₂N), 25.3 (CH₃), 19.1 (CH₃). HRMS calculated for [M+Na]⁺ C₁₄H₁₅NO₂Na: 252.1000, found: 252.1006.

1.375
1.351
1.327

Current Data Parameters
NAME kjb-verif
EXTNO 10
PROCNO 1

F2 - Acquisition Parameters
Date 20140306
Time 18.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 3591.364 Hz
FIDRES 0.103618 Hz
AQ 4.5613556 sec
RG 574.1
EW 139.200 usec
TE 6.50 usec
TR 293.2 K
D1 1.00000000 sec
TDO 1

***** CHANNEL f1 *****
NUC1 1H
P1 8.10 usec
PL1 2.00 dB
SFO1 300.1313806 MHz

F2 - Processing parameters
SI 32768
SF 300.1300064 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

4

F2 - Acquisition Parameters
 Date_ 20130517
 Time_ 20.31
 INSTRUM spect
 PROBRD 5 cm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 22675.736 Hz
 FIDRES 0.346004 Hz
 AQ 1.443138 sec
 RG 26542.5
 CW 32.050 usec
 DE 6.50 usec
 TR 295.9 K
 D1 1.30000000 sec
 D11 0.03000000 sec
 TDO 1

----- CHANNEL f1 -----
 NUC1 13C
 P1 6.10 usec
 PL1 -6.00 dB
 SFO1 75.4787490 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 2.00 dB
 PL12 23.00 dB
 PL13 23.00 dB
 SFO2 300.1352695 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677438 MHz
 WDW EM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 1.40

m213.5/noesy21858/r23jeba/dei/cdc13
NOESYPHSW CDC13 (C:\Spectres) mb 5

NAME m213
EXPNO 54
PROCNO 1
Date_ 20120213
Time 16.00
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT cdc13
NS 32
DS 4
SWH 2890.173 Hz
FIDRES 1.411217 Hz
AQ 0.3565540 sec
RG 22.6
DW 173.650 usec
DE 6.50 usec
TE 300.0 K
DQ 0.0001681 sec
C1 1.8789287 sec
D2 0.3000001 sec
TD0 0.0003460 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
PL1 -3.00 dB
SFO1 300.1300630 MHz
WDW 2
SSB 0
GB 0
PC 1.00
===== CHANNEL f2 =====
NUC2 1H
P2 12.00 usec
PL2 -3.00 dB
SFO2 500.1360560 MHz
WDW 2
SSB 0
GB 0
PC 1.00

m102.2/h28119/r23jeba/ka72/cdc13
a_proton CDC13 (C:\Spectres) mb 2

7.404
7.395
7.389
7.383
7.375
7.369
7.365
7.356
7.351
7.346
7.340
7.324
7.300

4.691

3.362
3.356

2.184

Current Data Parameters
NAME m102
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130102
Time 9.40
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT cdc13
NS 16
DS 2
SWH 6186.119 Hz
FIDRES 0.182846 Hz
AQ 2.6477044 sec
RG 144
DW 80.800 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
PL1 -3.00 dB
SFO1 300.1315934 MHz
===== CHANNEL f2 =====
F2 - Processing parameters
SI 32768
SF 300.1300050 MHz
WDW EM
SSB 0
GB 0.10 Hz
PC 1.00

m102.2/c28145/r23jeba/ka72/cdc13
a_c13cpd CDC13 {C:\Spectres} mb 2

BRUKER

Current Data Parameters
NAME m102
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130102
Time 18.16
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1600
DS 4
SWH 19521.250 Hz
FIDRES 0.256023 Hz
AQ 1.6777716 sec
RG 2080
DW 25.600 usec
DE 6.80 usec
TE 300.2 K
D1 2.0000000 sec
D11 0.0200000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 6.00 usec
PL1 -2.00 dB
SFO1 75.476053 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0 dB
PL12 21.00 dB
PL13 21.00 dB
SFO2 300.1312008 MHz

F2 - Processing parameters
SI 65536
SF 75.4677517 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

m205.3/h29101/r23jeba/ka45/cdc13
a_proton CDC13 {C:\Spectres} mb 3

Current Data Parameters
NAME m205
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130205
Time 9.32
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 6189.119 Hz
FIDRES 0.188846 Hz
AQ 2.6477046 sec
RG 208
DW 85.800 usec
DE 6.50 usec
TE 300.2 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
PL1 -3.00 dB
SFO1 300.1311524 MHz

F2 - Processing parameters
SI 32768
SF 300.1300134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

m205.3/c29164/r23jeba/ka45/cdc13
a_c13cpd CDC13 (C:\Spectres) mb 3

m205 31 1 D:\Bruker\TopSpin3.0\examdata\Khaoula

m205.3/#29102/m20jeba/ka45/cdc13
a_fluor CDC13 (C:\Spectres) mb 2

m128.25/h28727bis/r23jeba/kja5/cdcl3
a_proton CDCl3 (C:\Spectres) mb 25

m128.25/c28794/r23jeba/kja5/cdc13
a_c13cpd CDC13 {C:\Spectres} mb 25

Current Data Parameters
NAME m128
EXPNO 251
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180129
Time_ 0.45
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1280
DS 4
SWH 18821.250 Hz
FIDRES 0.28802 Hz
AQ 1.6777716 sec
RG 40.9
DW 28.600 usec
DE 6.50 usec
TE 280.0 K
D1 2.0000000 sec
D11 0.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 6.00 usec
PL1 -2.00 dB
SFO1 75.4760805 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 21.00 dB
PL13 21.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 65536
SF 75.4677277 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

m213.5/h29473/r23jebali/kaf6/cdc13
a_proton CDC13 {C:\Spectres} mb 5

Current Data Parameters
NAME m213
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180113
Time_ 5.35
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.188846 Hz
AQ 2.6477044 sec
RG 228
DW 80.800 usec
DE 6.50 usec
TE 280.0 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
PL1 -2.00 dB
SFO1 300.1318504 MHz

F2 - Processing parameters
SI 32768
SF 300.1300276 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

m213.5/c29520/r23jebali/kaf6/cdcl3
a_c13cpd CDCl3 {C:\Spectres} mb 5

Current Data Parameters
NAME m213
EXPNO 51
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130213
Time 17.25
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1440
DS 4
SWH 19531.250 Hz
FIDRES 0.298023 Hz
AQ 1.6777716 sec
RG 2080
DM 25.600 usec
DE 6.50 usec
TE 280.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 6.00 usec
PL1 -2.00 dB
SFO1 75.4760808 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 21.00 dB
PL13 21.00 dB
SFO2 300.1312008 MHz

F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0 1.00 Hz
GB 0
PC 1.40

m304.8/h29773/r23jebali/kaf31/cdcl3
a_proton CDCl3 {C:\Spectres} mb 8

Current Data Parameters
NAME m304
EXPNO 80
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130304
Time 12.01
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.189946 Hz
AQ 2.6477044 sec
RG 228
DM 80.600 usec
DE 6.50 usec
TE 280.0 K
D1 1.60000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
PL1 -3.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300350 MHz
WDW EM
SSB 0 0.30 Hz
GB 0
PC 1.00

m304.8/c29812/r23jebali/kaf91/cdc13
a_c13cpd CDC13 (C:\Spectres) mb 8

Current Data Parameters
NAME m304
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130304
Time 15.33
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1280
DS 4
SWH 19531.250 Hz
FIDRES 0.198022 Hz
AQ 1.677716 sec
RG 2080
DM 25.600 usec
DE 6.50 usec
TE 290.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 6.00 usec
PL1 -2.00 dB
SFO1 75.4760005 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL3 21.00 dB
PL13 21.00 dB
SFO2 300.1310005 MHz

F2 - Processing parameters
SI 65536
SF 75.4677418 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

m319.6/h30595/r23jebali/ka93/cdc13
a_proton CDC13 (C:\Spectres) mb 6

Current Data Parameters
NAME m319
EXPNO 60
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130305
Time 10.33
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 16
DS 4
SWH 6188.119 Hz
FIDRES 0.188846 Hz
AQ 2.6477044 sec
RG 181
DM 80.000 usec
DE 6.50 usec
TE 270.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
PL1 -2.00 dB
SFO1 300.1315594 MHz

F2 - Processing parameters
SI 32768
SF 300.1300082 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

m319.6/c30654/r23jebali/ka93/cdcl3
a_c13cpd CDC13 {C:\Spectres} mb 6

Current Data Parameters
NAME m319
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130219
Time 15.38
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1600
DS 4
SWH 19531.250 Hz
FIDRES 0.298023 Hz
AQ 1.677716 sec
RG 2050
EW 25.600 usec
DE 6.50 usec
TE 270.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 6.00 usec
PL1 -1.00 dB
SFO1 75.4760505 MHz

===== CHANNEL f2 =====
CEPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 21.00 dB
PL13 21.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 65536
SF 75.4677471 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

m314.14/h30374/r23jebali/ka17/cdcl3
a_proton CDC13 {C:\Spectres} mb 14

Current Data Parameters
NAME m314
EXPNO 140
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130214
Time 10.36
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 6185.115 Hz
FIDRES 0.188946 Hz
AQ 2.6477044 sec
RG 161
EW 80.800 usec
DE 6.50 usec
TE 270.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
PL1 -3.00 dB
SFO1 300.1315894 MHz

F2 - Processing parameters
SI 32768
SF 300.1300005 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

m314.14/c30427/r233jebari/ka17/cdc13
a_c13cpd CDCl3 {C:\Spectres} mb 14

Current Data Parameters
NAME m314
EXPNO 141
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130314
Time 21.04
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT cdcl3
NS 1600
DS 4
SWH 19531.250 Hz
FIDRES 0.298023 Hz
AQ 1.6777714 sec
RG 2050
LW 23.600 usec
DE 6.50 usec
TE 270.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 6.00 usec
PL1 -2.00 dB
SFO1 75.4760505 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL3 21.00 dB
PL13 21.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 65536
SF 75.4677461 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

amine

20130620_KA45 #21 RT: 0.16 AV: 1 NL: 3.04E6
T: FTMS + c ESI Full ms [100.00-1000.00]

KA45 - ESI+

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
234.09247	234.09248	-0.06	7.5	C13 H13 O2 N F
	234.09134	4.82	11.5	C16 H12 O N

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
230.11771	230.11756	0.67	7.5	C14 H16 O2 N

20130620_KAF31 #21 RT: 0.17 AV: 1 NL: 3.77E8
T: FTMS + c.ESI Full ms [100.00-1000.00]

KAF31 – ESI+

Single Mass Analysis

Tolerance = 5.0 PPM / DBE min = -1.5, max = 10.0

Element prediction: C8

Number of isotope peaks used for iFIT = 3

Monoisotopic Mass, Even Electron Ion

38 formula(s) evaluated with 1 results within limits (up to 10 closest results for each mass)

Elements Used:

Mass	Calc. Mass	mls	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	234s
252.1006	252.1006	0.6	2.4	7.5	C ₁₄ H ₁₅ N O ₂ 234s	1067.7	n/a	n/a	14	15	1	2	1

MS2051.03 (0.250) AM2 (4.35000 0.000 0.000) Cn (2.3.51)

1 TOF MS ES+

1.27e+006

For Help, press F1