

Supporting Information

Title:Synthesis and evaluation of [¹⁸F]-FEAnGA as a PET tracer for β-Glucuronidase Activity

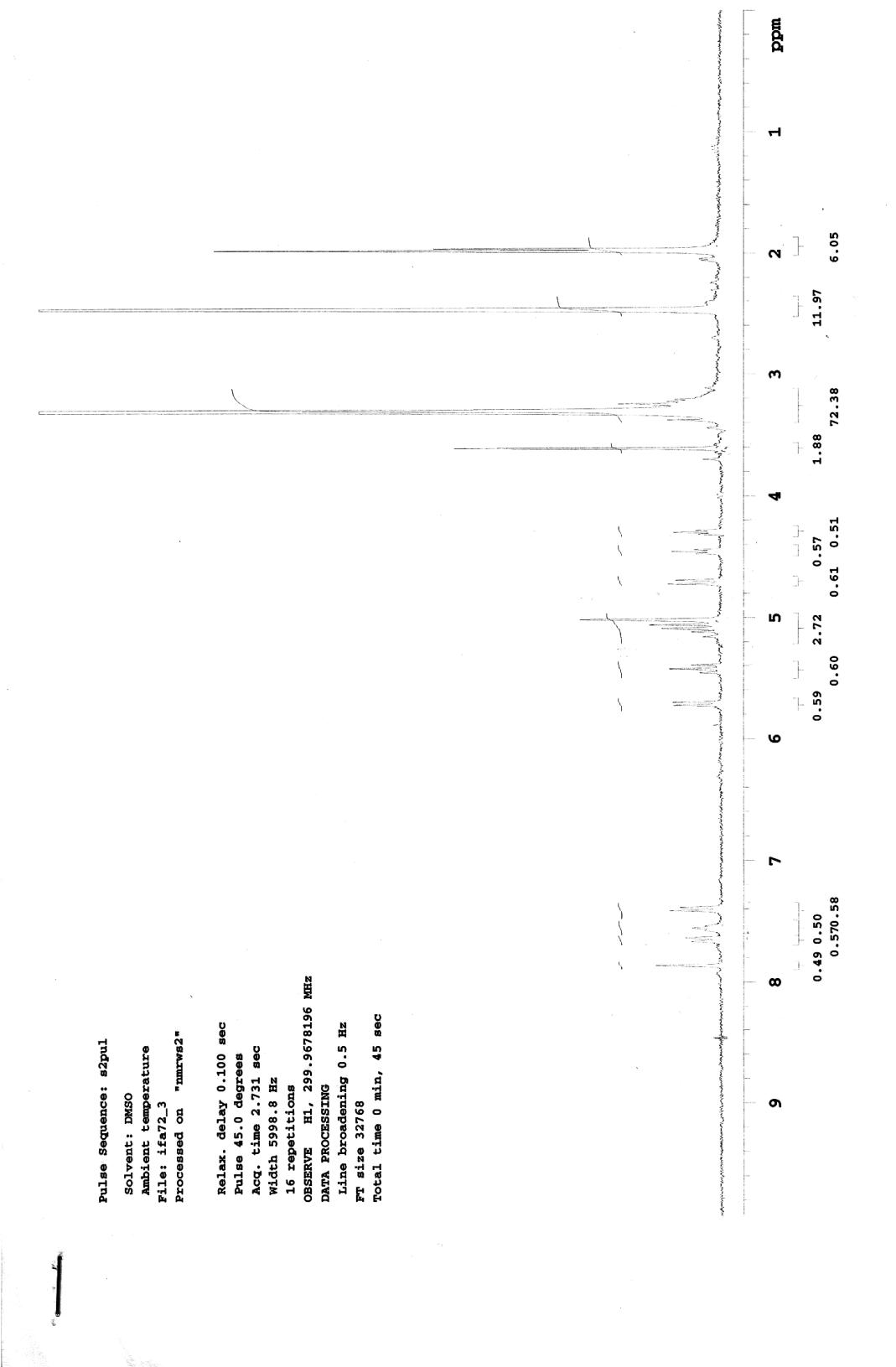
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11. CT26/CT26mβGUS cells-Medium

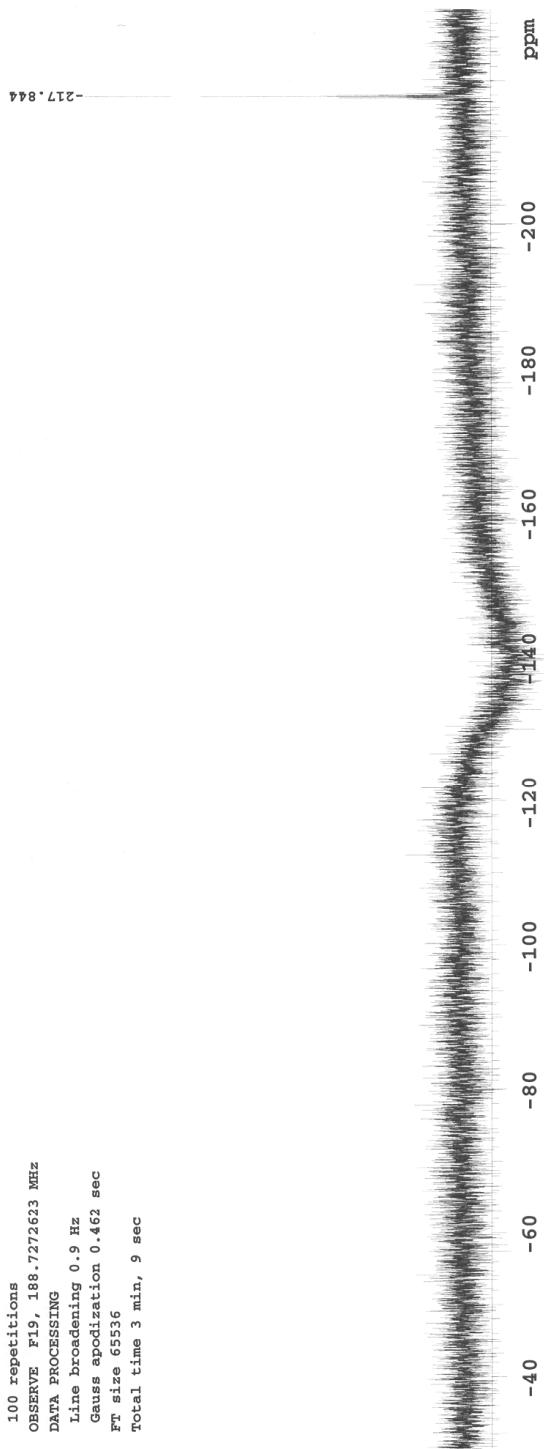
1. ^1H NMR of compound 2



2. ^{19}F NMR of compound 2

sample: ifa_72_3
File: 3_PET_ifa_72_3_Fluorine_01
Pulse Sequence: s2pul
Solvent: edei3- DMSO
Temp: 23.0 C / 296.1 K
Sample #3, Operator: autouser
File: 3_PET_ifa_72_3_Fluorine_01
Processed on "mrtrws2"

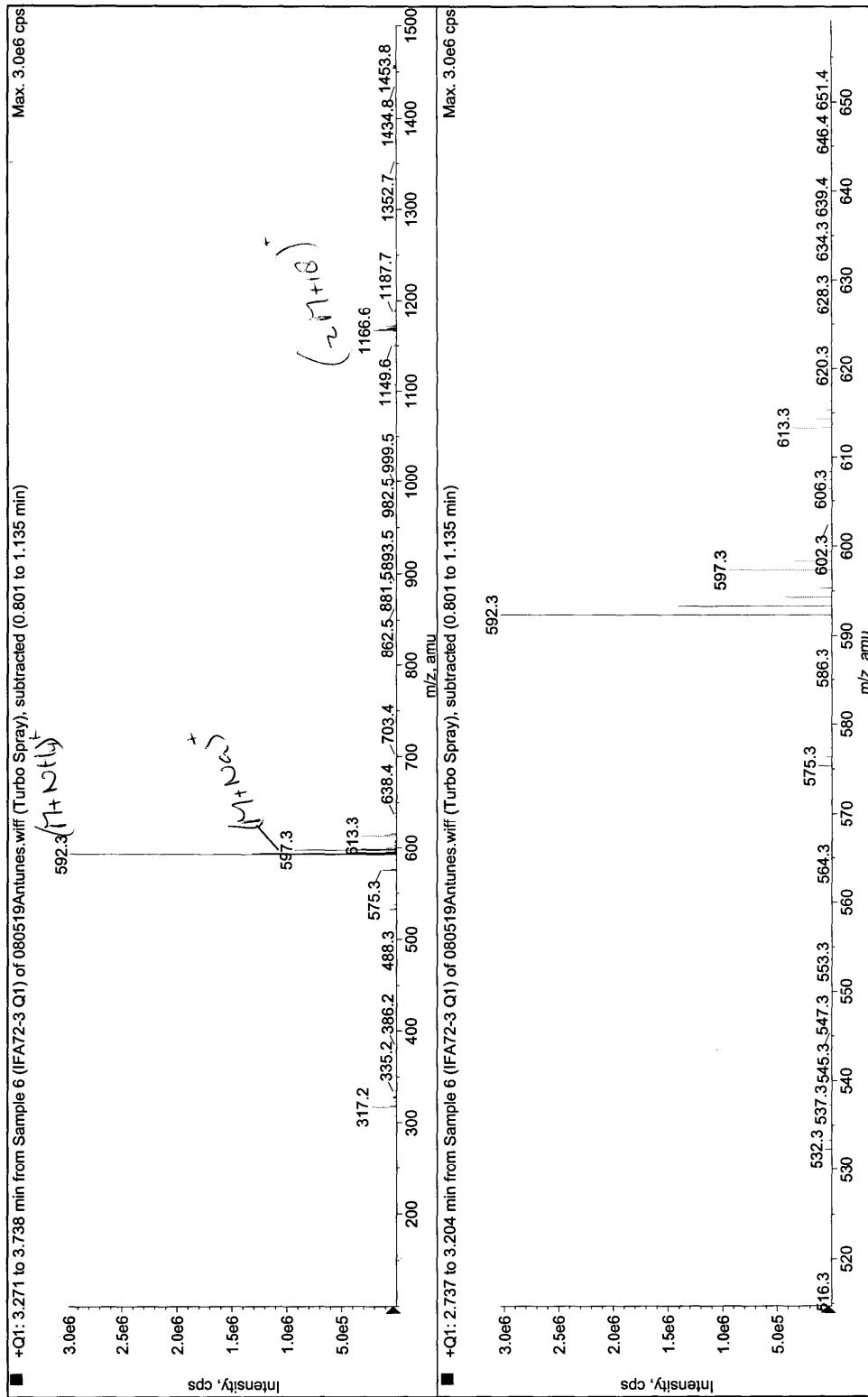
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.851 sec
Width 37735.8 Hz
100 repetitions
OBSERVE F19, 188.7272623 MHz
DATA PROCESSING
Line broadening 0.9 Hz
Gauss apodization 0.462 sec
FT size 65536
Total time 3 min, 9 sec



File: 080519Antunes.wiff
Acq. Date: Monday, May 19, 2008

Sample Comment: in DCM, dil in MeOH-0.1%FA
Acq. Time: 10:02
Sample Name: IFA72-3 Q1

3. LRMS of compound 2



4. ^1H NMR of compound 3

sample: IFA_112
Automation directory: /home/autouser/vnmrjsys/data/studies/auto_2008.10.01
Sample id : we2_PET_IFA_112_1
Sample : IFA_112

Pulse Sequence: s2pul

Solvent: dmso

Temp. 25.0 C / 298.1 K

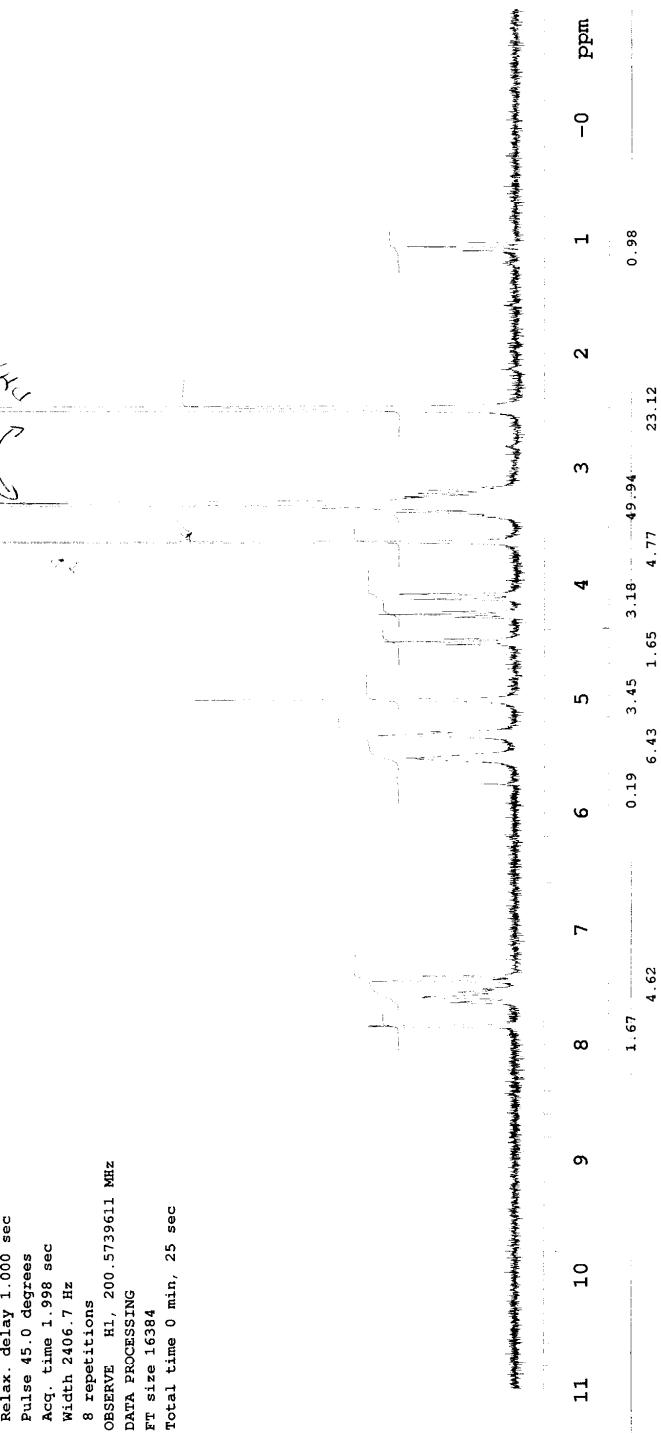
Sample #2, Operator: autouser

File: 2_PET_IFA_112_Proton_01

Mercury-200 "linuxnmr03"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 2406.7 Hz
8 repetitions
OBSERVE H1, 200.5739611 MHz
DATA PROCESSING
FT size 16384
Total time 0 min, 25 sec

11 10 9 8 7 6 5 4 3 2 1 -0 0.98



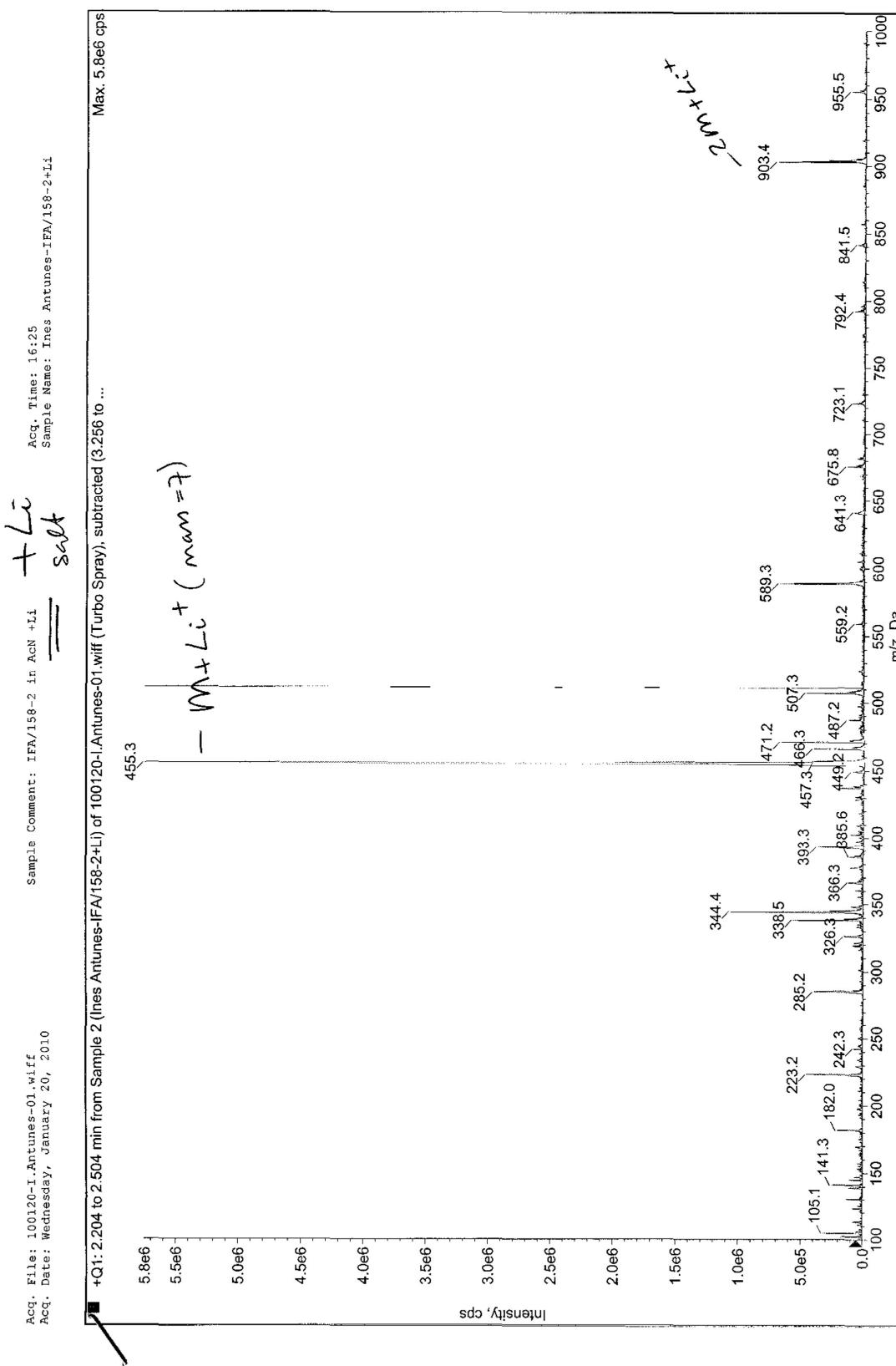
5. ^{19}F NMR of compound 3

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sample: ifa_112
File: 2_PET_ifa_112_Fluorine_01
Pulse Sequence: s2pul
Solvent: dmso
Temp. 25.0 C / 298.1 K
Sample #2, Operator: autocuser
File: 2_PET_ifa_112_Fluorine_01
Processed on "nmrws2"

Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.851 sec
width 37735.8 Hz
100 repetitions
OBSERVE F19, 188.7281586 MHz
DATA PROCESSING
Line broadening 10.0 Hz
Gauss apodization 0.462 sec
FT size 65536
total time 3 min, 9 sec
```



6. LRMS of compound 3



7. ^1H NMR of compound 4

sample: ifa_114
Automation directory: /home/autouser/vnmrjsys/data/studies/auto_2008.10.09
Sample id : th2_PET_ifa_114_1
Sample : ifa_114

Pulse Sequence: s2pul

Solvent: dmso

Temp. 152.0 C / 425.1 K

Sample #2, Operator: autouser

File: 2_PET_ifa_114_Proton_01

Mercury-200 "linuxmmz03"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.998 sec

Width 2406.7 Hz

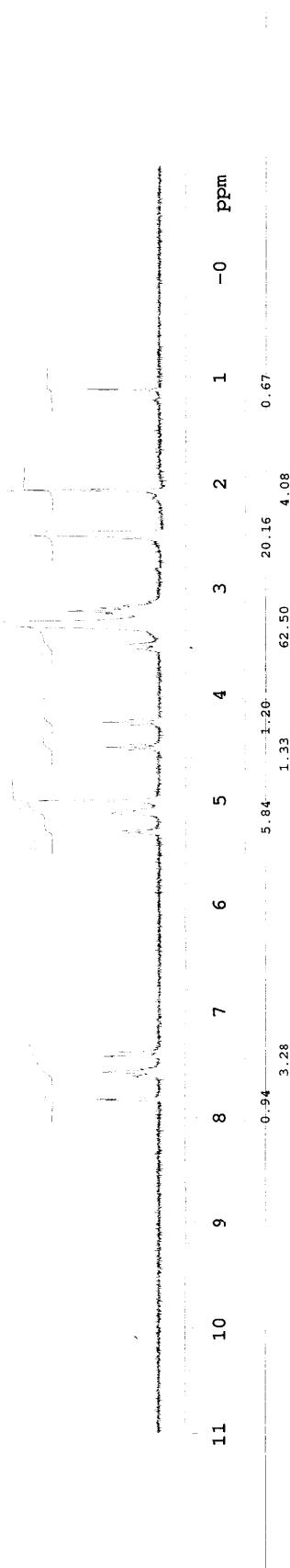
8 repetitions

OBSERVE H1, 200.5739611 MHz

DATA PROCESSING

FT size 16384

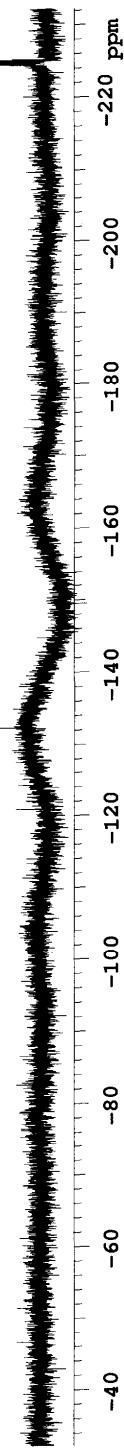
Total time 0 min, 25 sec



8. ^{19}F NMR of compound 4

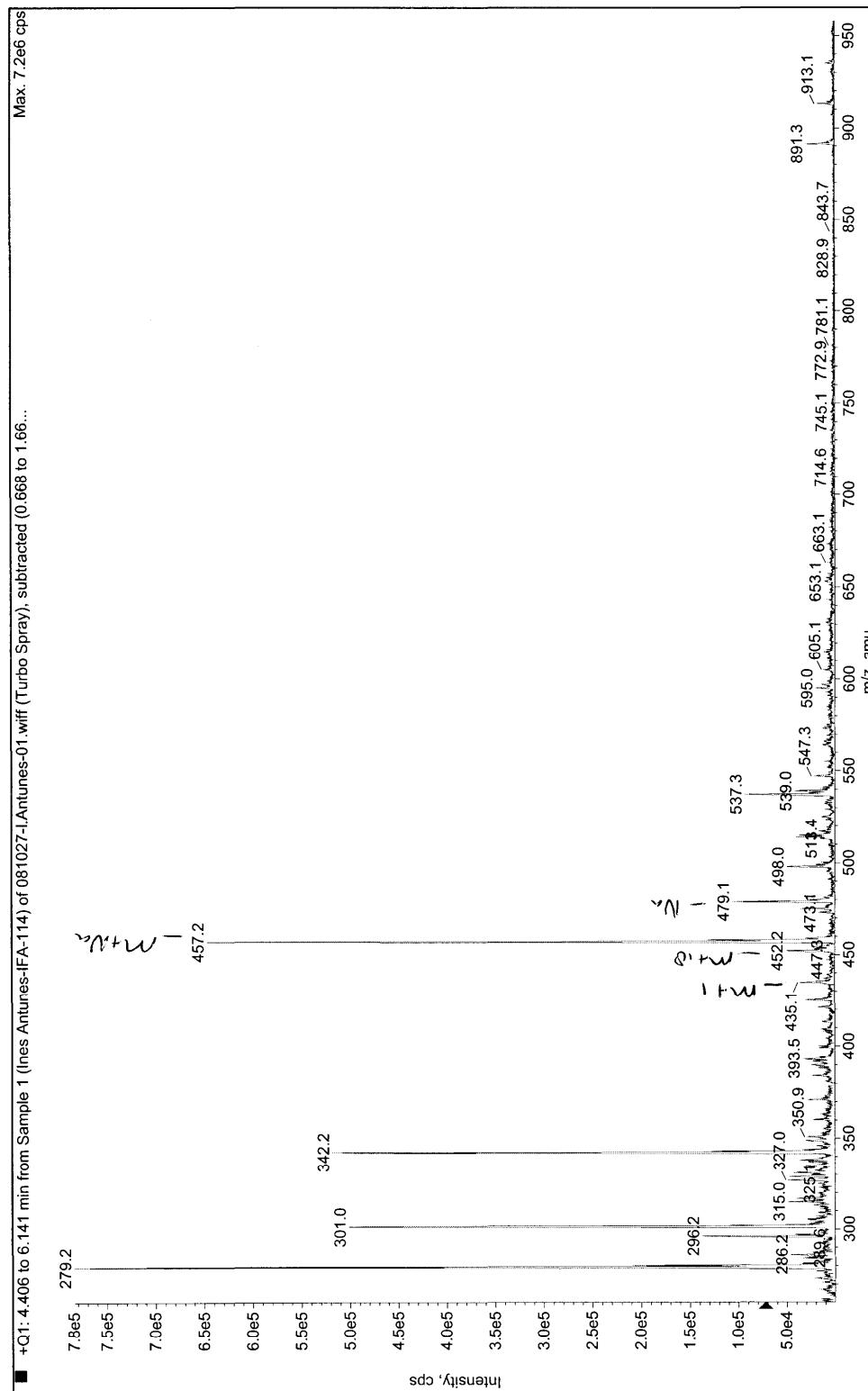
sample: ifa_114
File: 2_P2T_ifa_114_Fluorine_01
Pulse Sequence: s2pul
Solvent: dmso
Temp: 152.0 C / 425.1 K
Sample #: 2, Operator: autouser
File: 2_P2T_ifa_114_Fluorine_01
INCOVA-600 "nb4-7-148"

Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.881 sec
Width 37735.8 Hz
100 repetitions
OBSERVE F19, 188.7285827 MHz
DATA PROCESSING
Line broadening 0.9 Hz
Gauss apodization 0.462 sec
FT size 65536
Total time 3 min, 9 sec

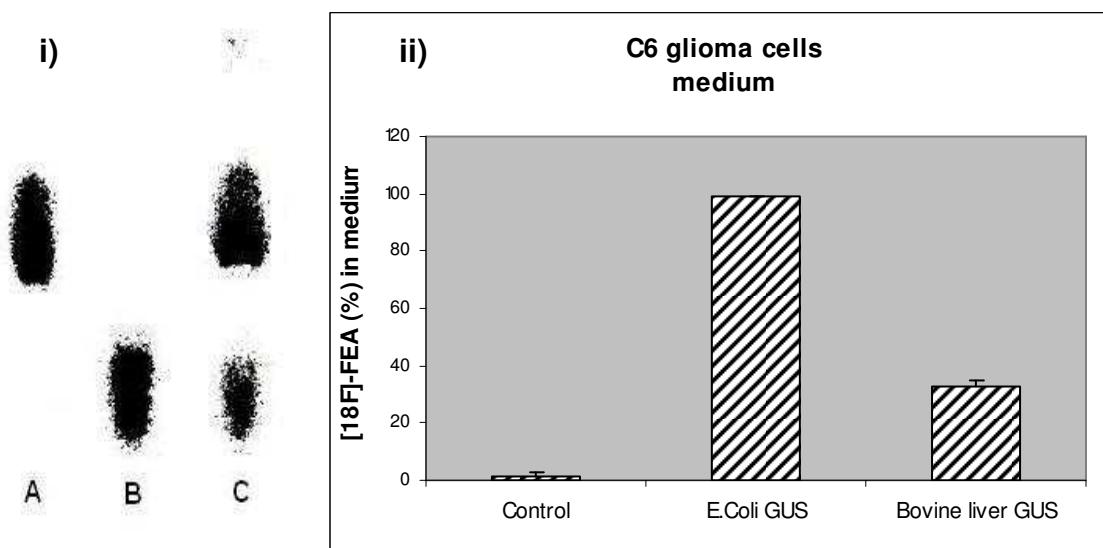


9. LRMS of compound 4

Acq. File: 081027-I.Antunes-01.wiff (Sample Comment: IFA-114 in AcN+0.1%FA
 Acq. Date: Monday, October 27, 2008 Acq. Time: 10:09
 Sample Name: Ines Antunes-IFA-114

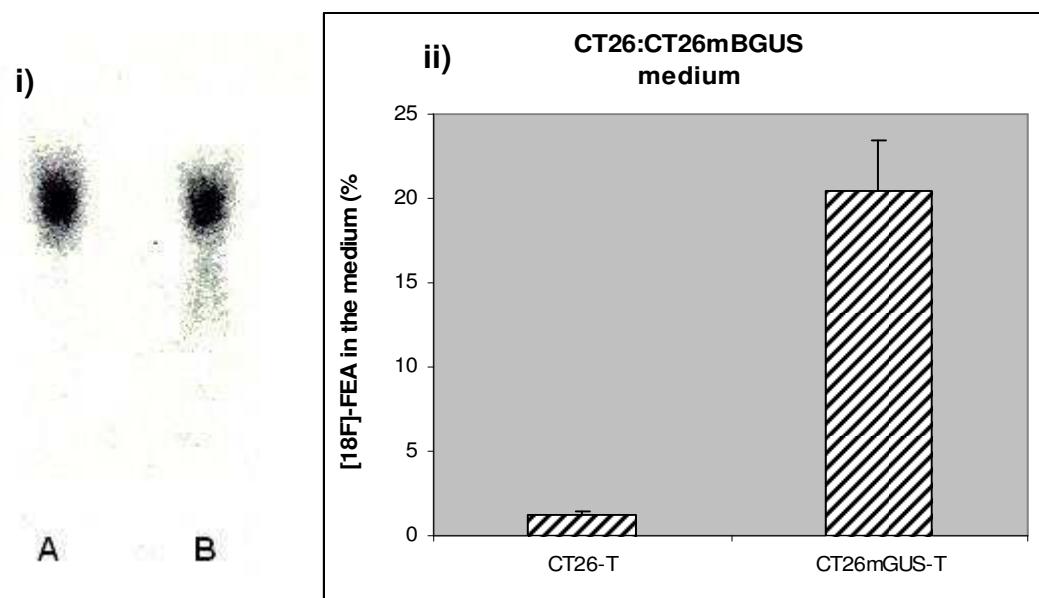


10. C6 glioma cell- Medium



Left panel: Radio-TLC of (A) medium sample of C6 control cells; (B) medium sample of C6 cells with E. Coli; (C)- medium sample of C6 cells with bovine liver β -GUS. The upper spot represents the intact [¹⁸F]-FEAnGA and the lower spot represents [¹⁸F]-FEA. Right panel: percentage of [¹⁸F]-FEA present in the medium.

11. CT26/CT26m β GUS cells- Medium



Left panel: Radio-TLC of (A) medium sample of CT26 cells; (B) medium sample of CT26-m β GUS. Right panel: Percentage of [¹⁸F]-FEA present in the medium.