

***Supplementary Information***

***In vitro* and *in silico* studies on novel N-substituted-3, 5-diaryl-pyrazoline derivatives as COX-2 inhibitors and anti-inflammatory agents**

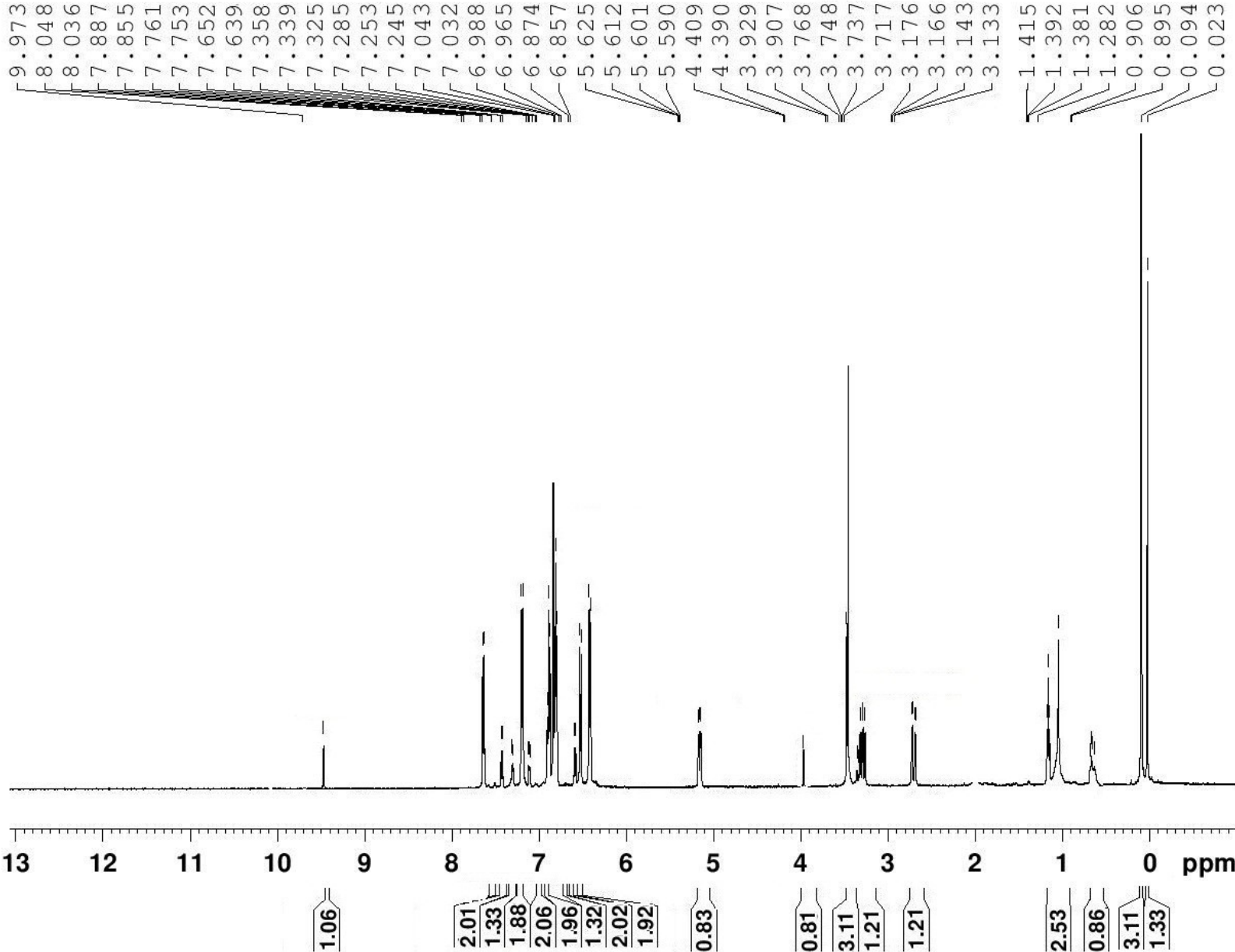
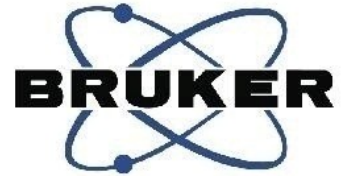
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EX-IPSA-UB-C1(500MHz) PROTON CDC13



Current Data Parameters  
NAME EX-IPSA-UB-C1(500MHz)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170426

INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.2767999 sec  
RG 203  
DW 50.000 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 500.1330885 MHz  
NUC1 1H  
P1 10.78 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

EX-IPSA-UB-C2(500MHz) PROTON CDC13



9.933  
8.099  
8.096  
7.879  
7.877  
7.771  
7.756  
7.650  
7.623  
7.323  
7.308  
7.306  
7.297  
7.255  
7.242  
7.094  
7.087  
6.978  
6.975  
6.863  
6.857  
5.693  
5.654  
5.640  
5.579  
4.418  
4.388  
3.909  
3.906  
3.765  
3.743  
3.735  
3.713  
3.172  
3.167  
3.146  
3.136  
1.416  
1.394  
1.383  
1.283  
0.907  
0.895  
0.096  
0.025

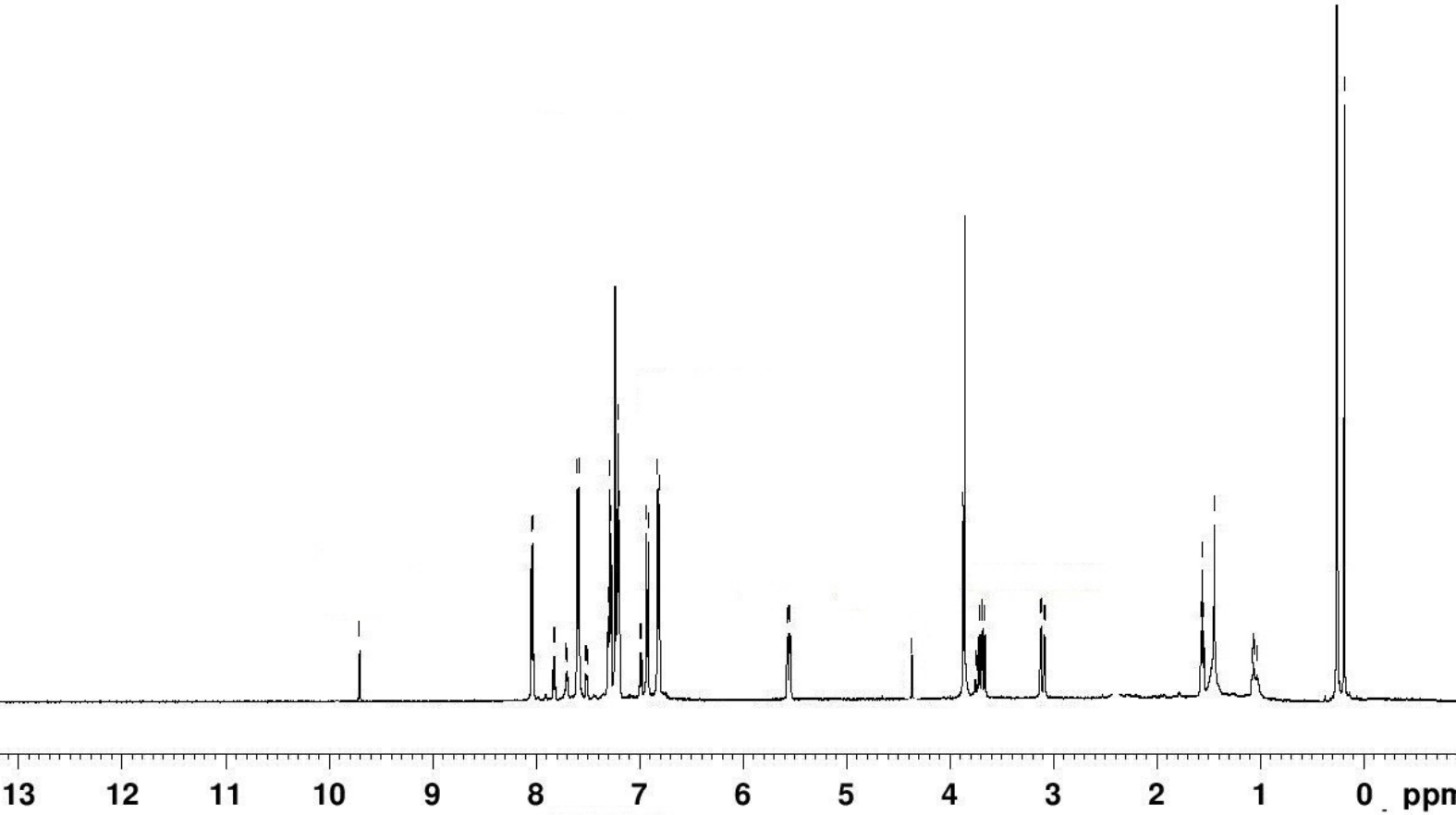
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EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170426

INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.2767999 sec  
RG 203  
DW 50.000 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1

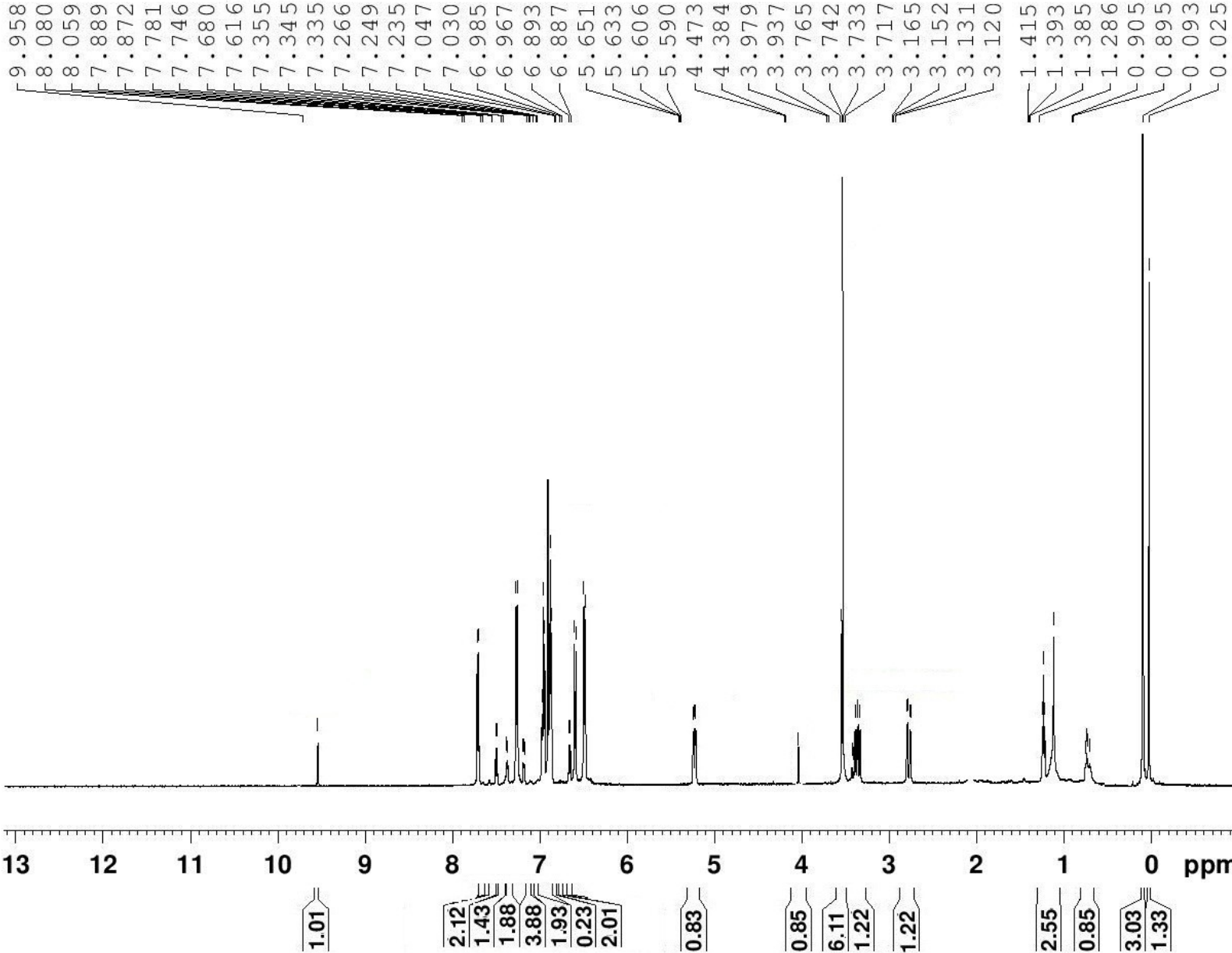
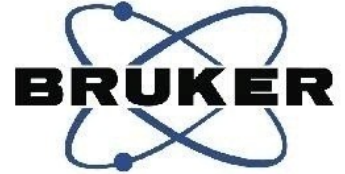
==== CHANNEL f1 =====  
SFO1 500.1330885 MHz  
NUC1 1H  
P1 10.78 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



1.05  
2.11  
1.14  
1.96  
2.06  
1.91  
0.32  
2.01  
1.93  
0.88  
0.82  
3.12  
1.21  
1.21  
2.52  
0.88  
3.01  
1.43

EX-IPSA-UB-C3(500MHz) PROTON CDC13



Current Data Parameters  
NAME EX-IPSA-UB-C3(500MHz)  
EXPNO 1  
PROCNO 1

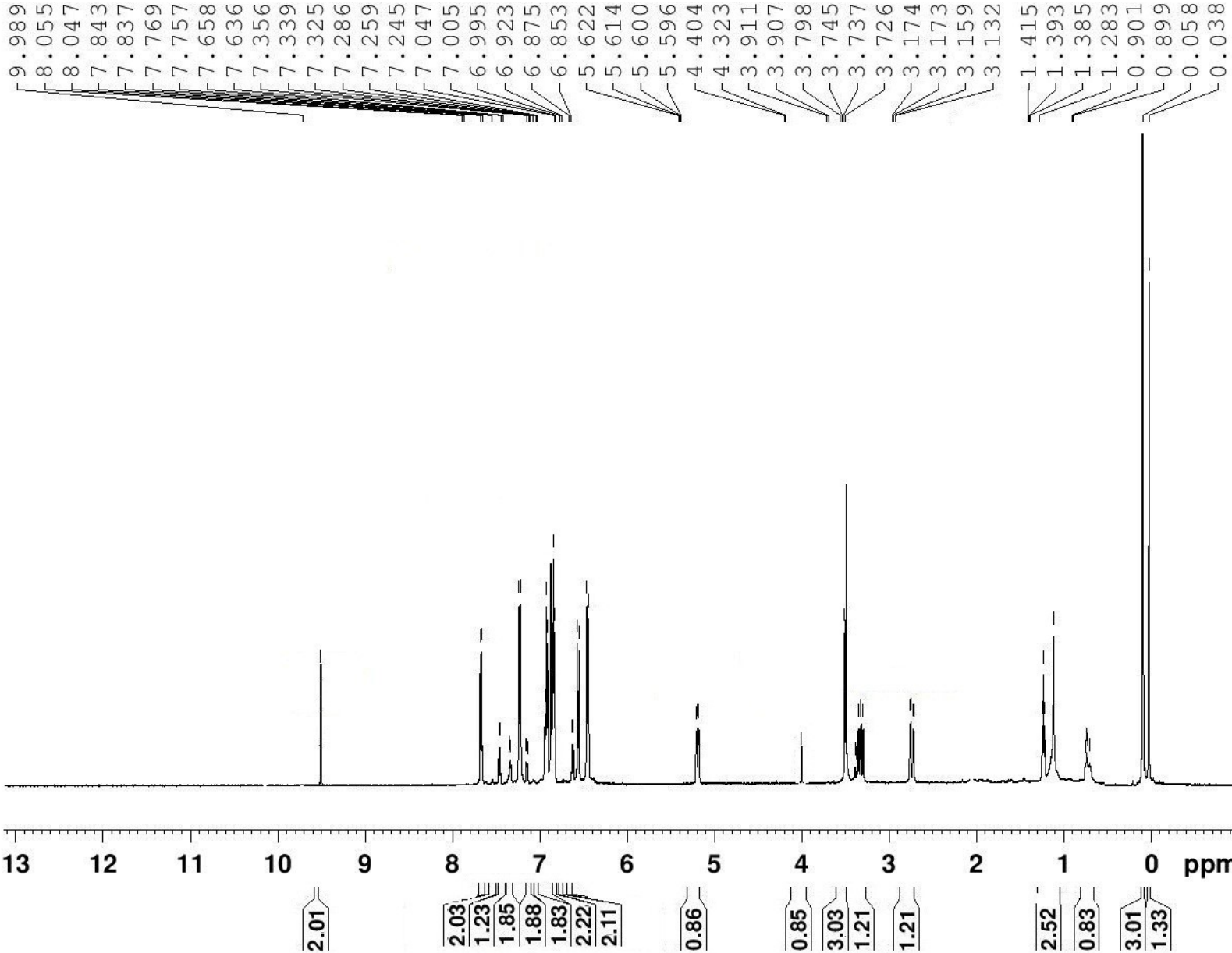
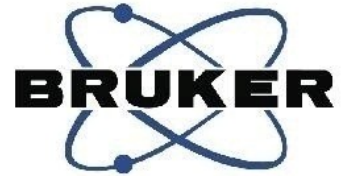
F2 - Acquisition Parameters  
Date\_ 20170426

INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.2767999 sec  
RG 203  
DW 50.000 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 500.1330885 MHz  
NUC1 1H  
P1 10.78 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

EX-IPSA-UB-C4(500MHz) PROTON CDC13



Current Data Parameters  
NAME EX-IPSA-UB-C4(500MHz)  
EXPNO 1  
PROCNO 1

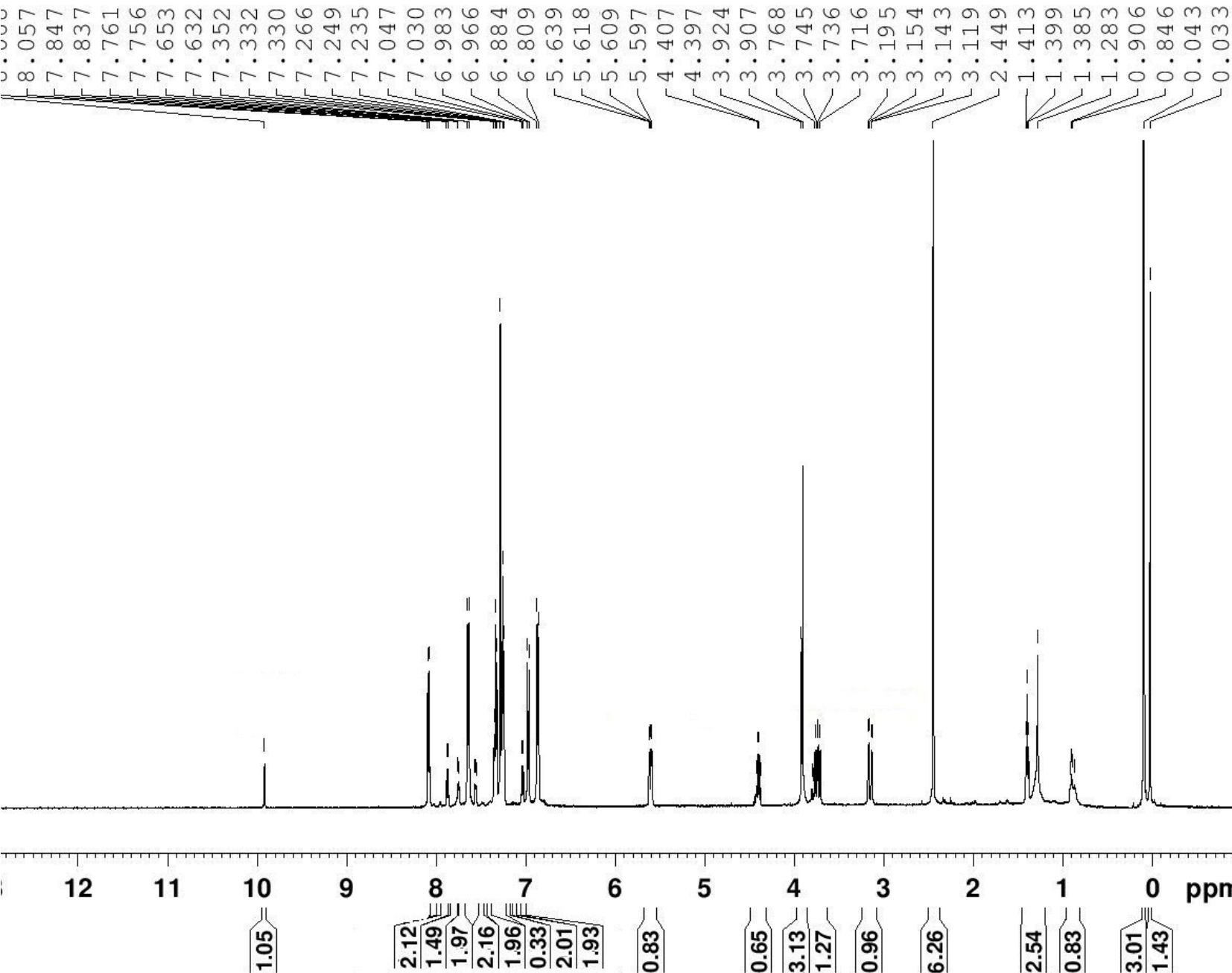
F2 - Acquisition Parameters  
Date\_ 20170426

INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.2767999 sec  
RG 203  
DW 50.000 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 500.1330885 MHz  
NUC1 1H  
P1 10.78 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

X-IPSA-UB-C5(500MHz) PROTON CDCl3



Current Data Parameters  
NAME EX-IPSA-UB-C5(500MHZ)  
EXPNO 1  
PROCNO 1

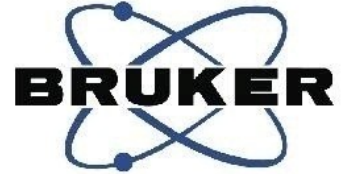
F2 - Acquisition Parameters  
Date\_ 20170426

INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.2767999 sec  
RG 203  
DW 50.000 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 500.1330885 MHz  
NUC1 1H  
P1 10.78 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

EX-IPSA-UB-D1(500MHz) PROTON CDC13



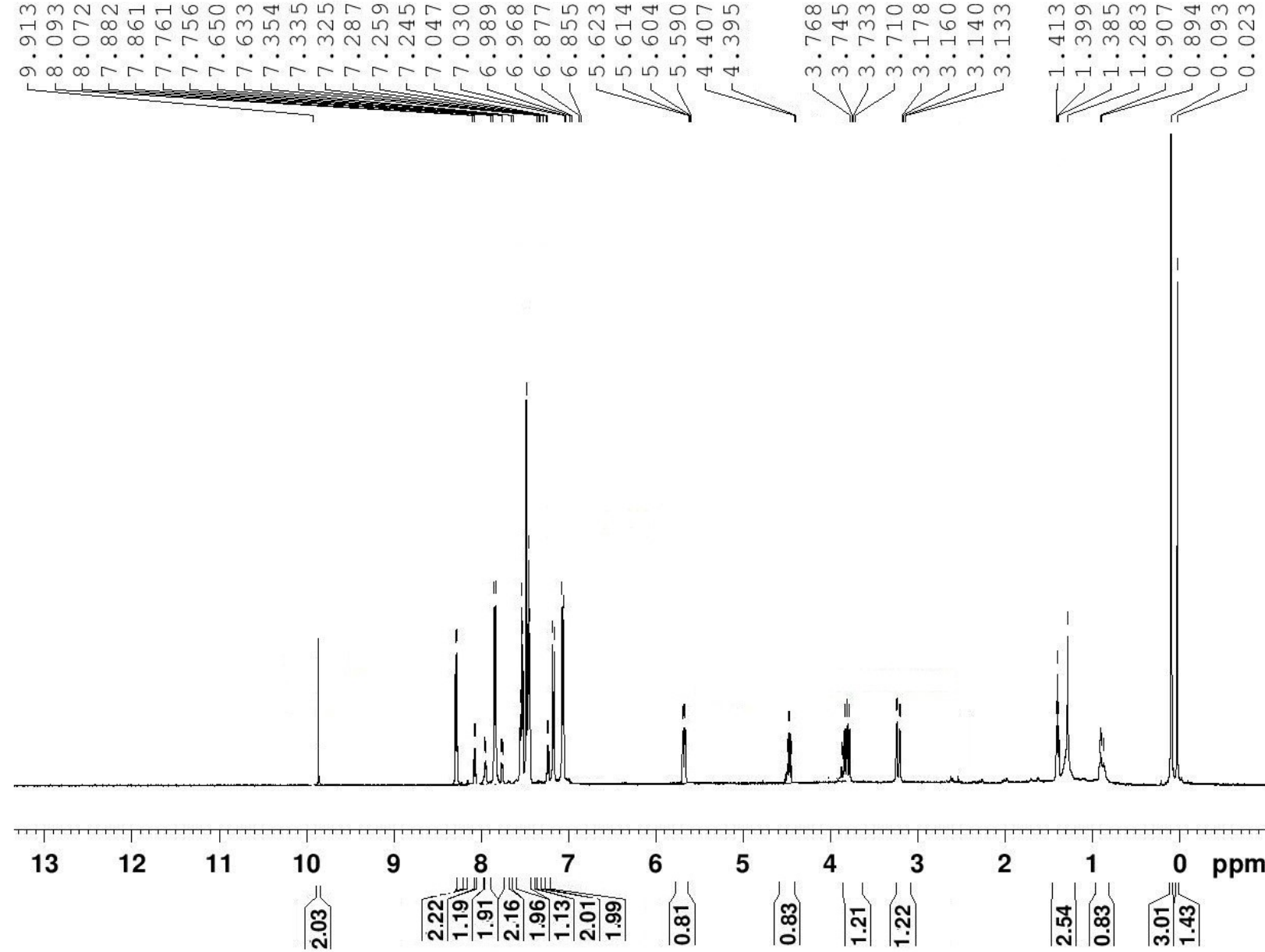
Current Data Parameters  
NAME EX-IPSA-UB-D1(500MHz)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170426

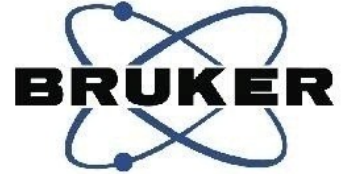
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PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.2767999 sec  
RG 203  
DW 50.000 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 500.1330885 MHz  
NUC1 1H  
P1 10.78 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



EX-IPSA-UB-D2(500MHz) PROTON CDC13



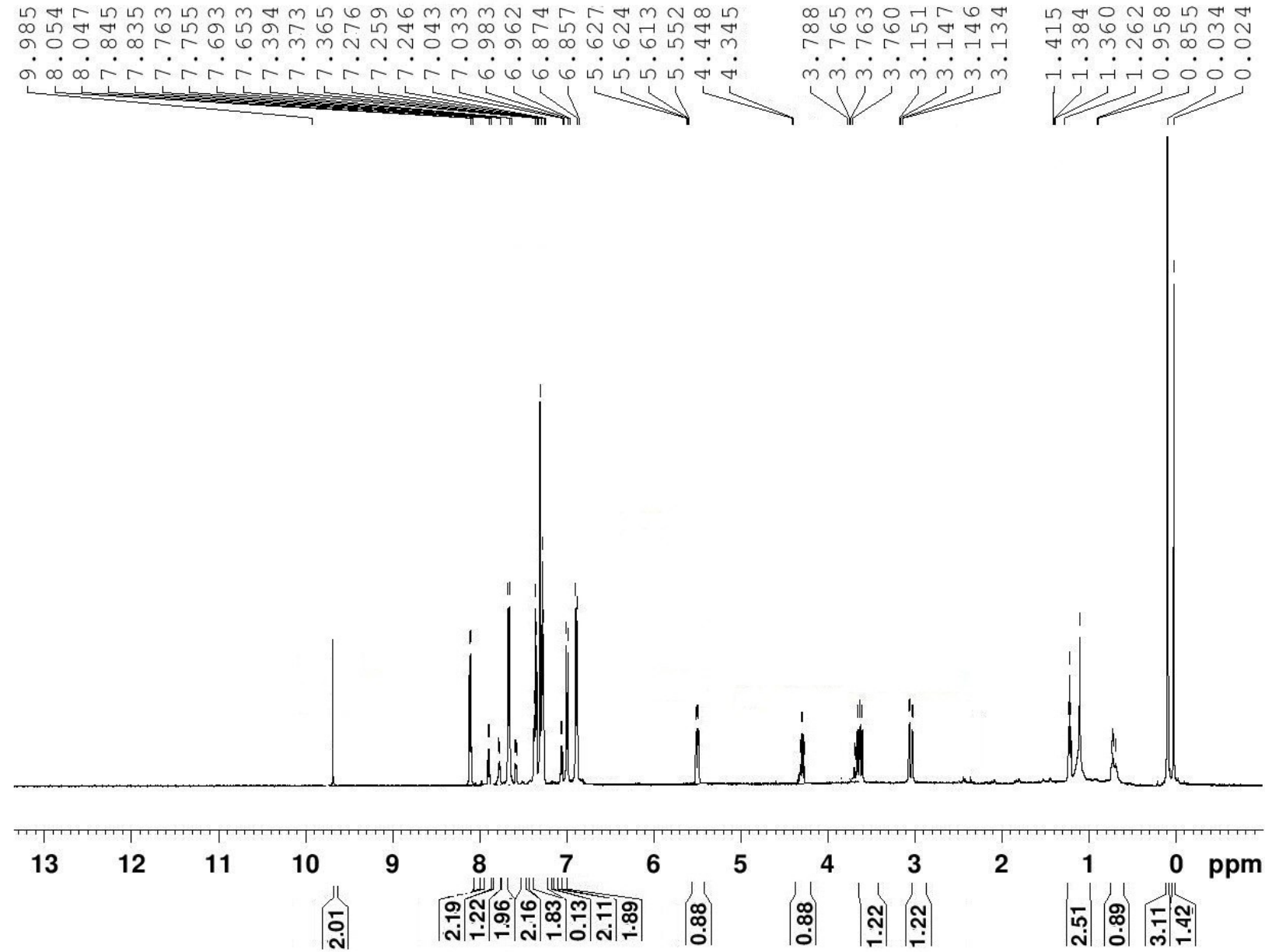
Current Data Parameters  
NAME EX-IPSA-UB-D2(500MHz)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170426

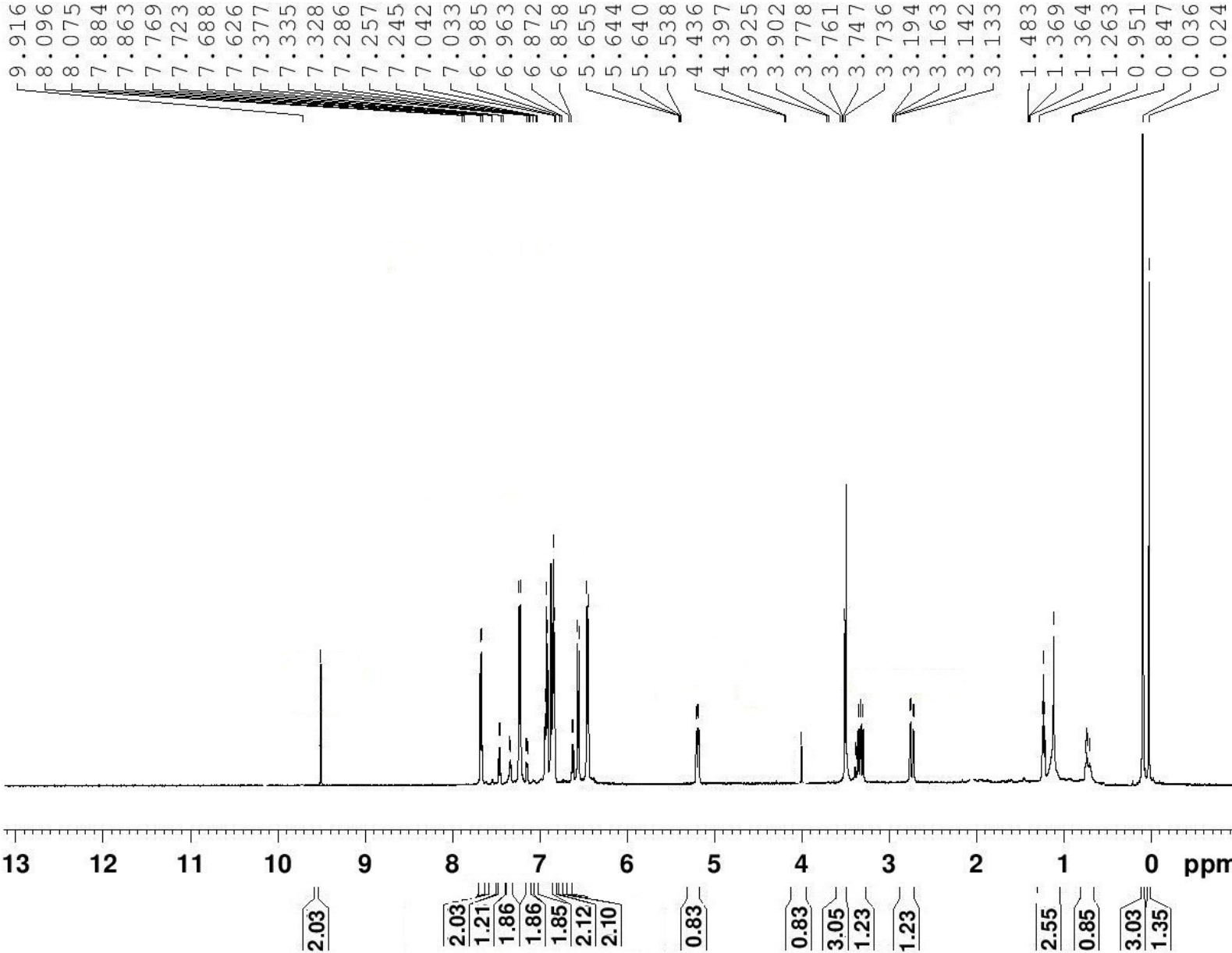
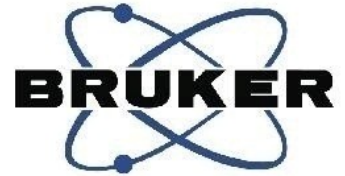
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.2767999 sec  
RG 203  
DW 50.000 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 500.1330885 MHz  
NUC1 1H  
P1 10.78 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



EX-IPSA-UB-D3(500MHz) PROTON CDC13



Current Data Parameters  
NAME EX-IPSA-UB-D3(500MHz)  
EXPNO 1  
PROCNO 1

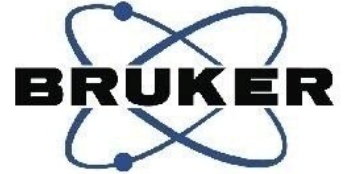
F2 - Acquisition Parameters  
Date\_ 20170426

INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.2767999 sec  
RG 203  
DW 50.000 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 500.1330885 MHz  
NUC1 1H  
P1 10.78 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

EX-IPSA-UB-D4(500MHz) PROTON CDC13



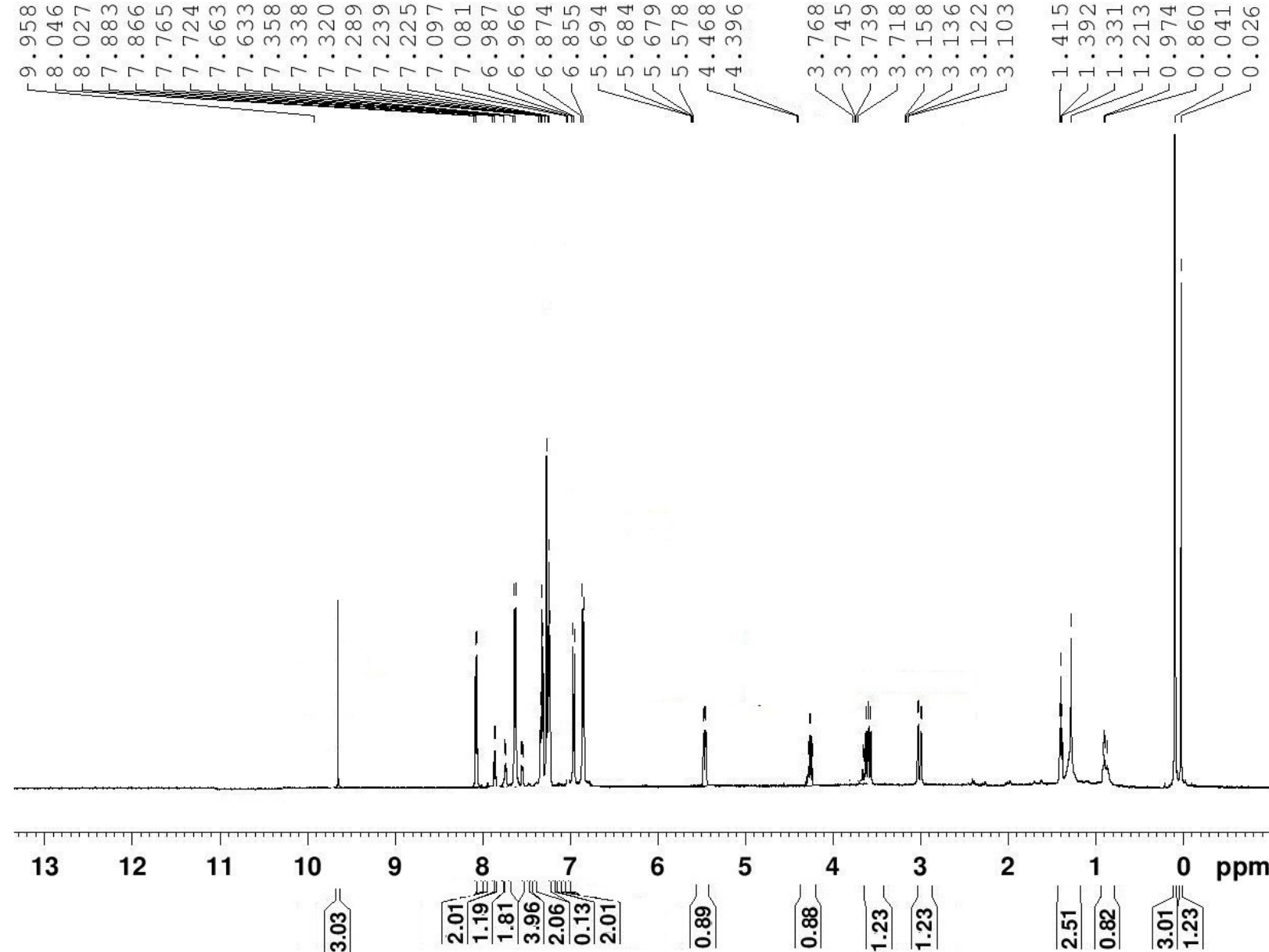
Current Data Parameters  
NAME EX-IPSA-UB-D4(500MHz)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170426

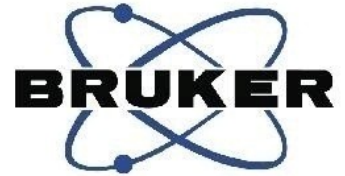
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PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.2767999 sec  
RG 203  
DW 50.000 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 500.1330885 MHz  
NUC1 1H  
P1 10.78 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



EX-IPSA-UB-D5(500MHz) PROTON CDC13



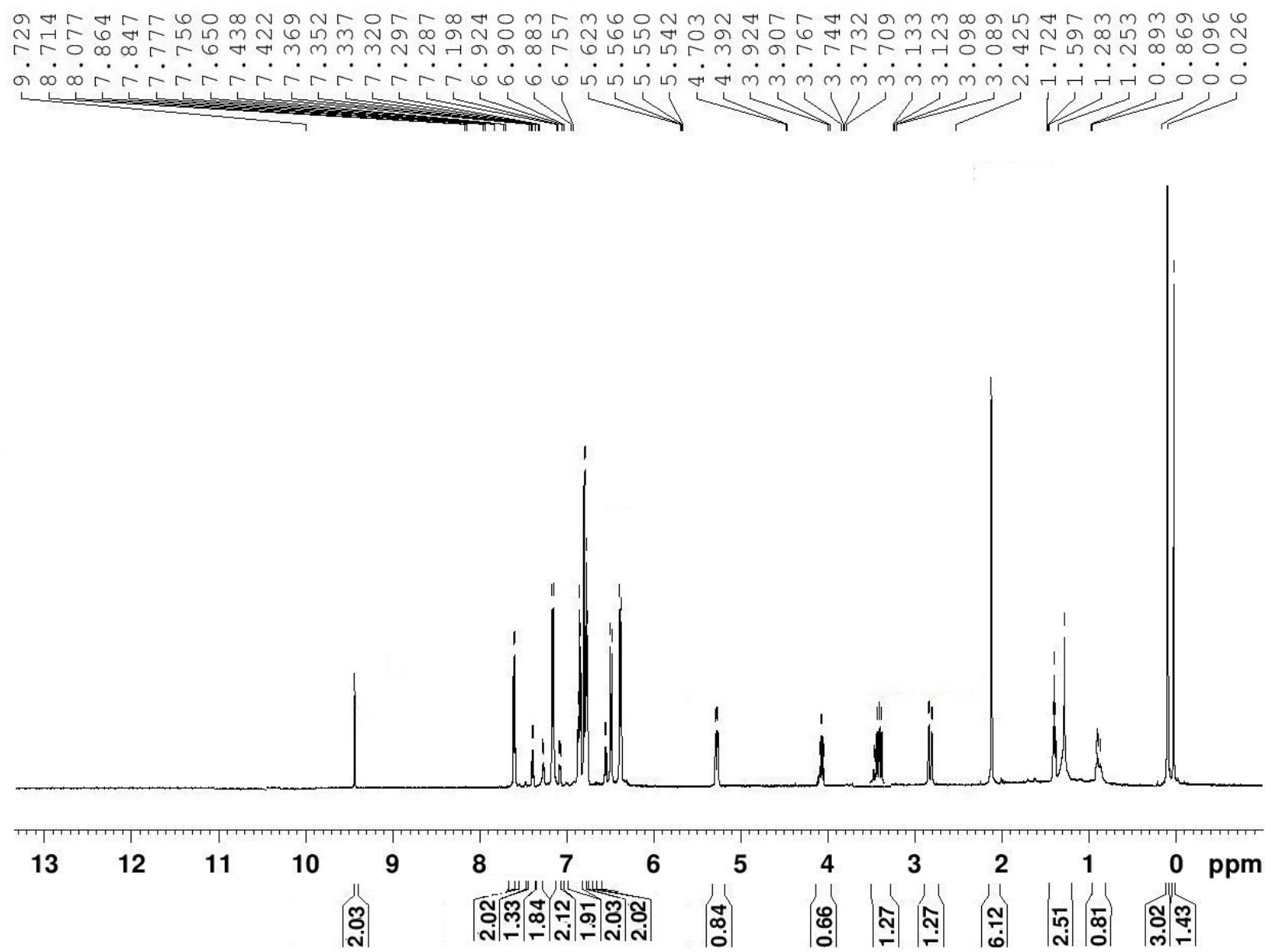
Current Data Parameters  
NAME EX-IPSA-UB-D5(500MHz)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170426

INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.2767999 sec  
RG 203  
DW 50.000 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 500.1330885 MHz  
NUC1 1H  
P1 10.78 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



IR spectrum of compounds 6a-6j

