

Supporting Information

One-Pot Selective Saturation and Functionalization of Heteroaromatics Leading to Dihydropyridines and Dihydroquinolines

Dong Wang,* Yuanyang Jiang, Linru Dong, Gaoyu Li, Baoying Sun, Laurent Désaubry, and Peng Yu

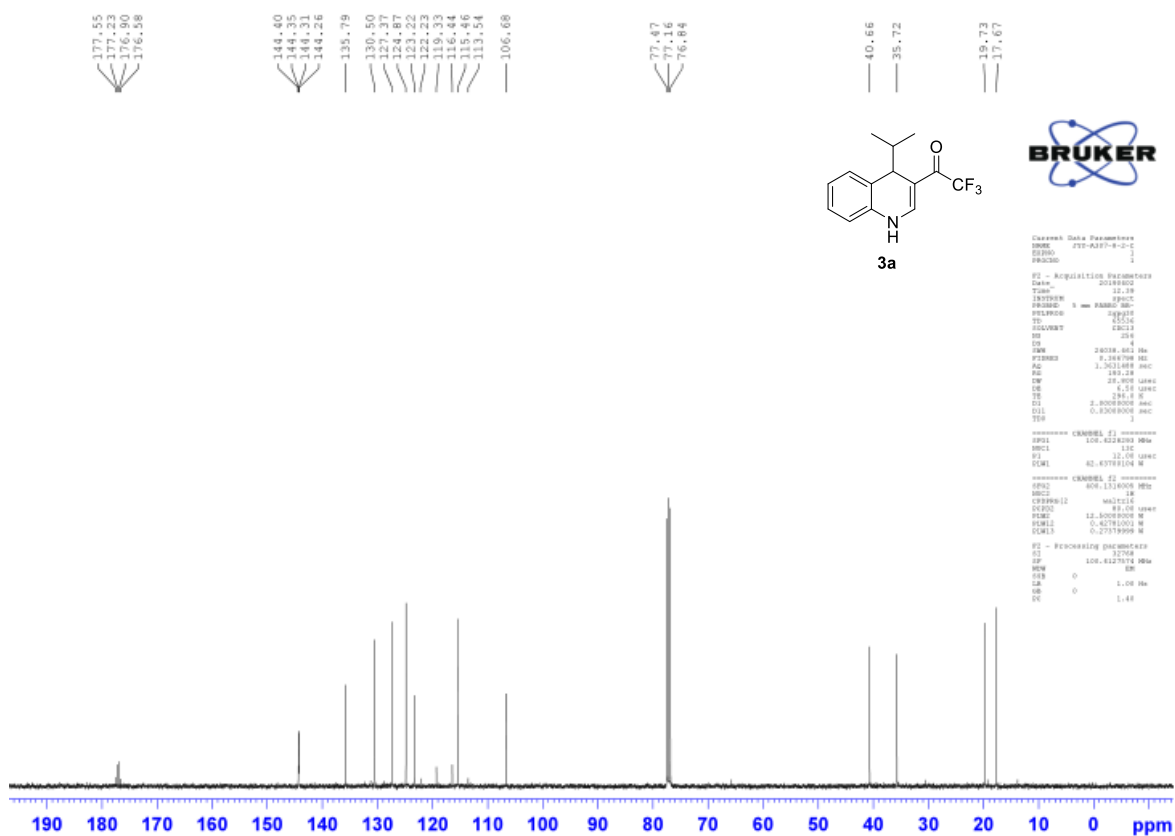
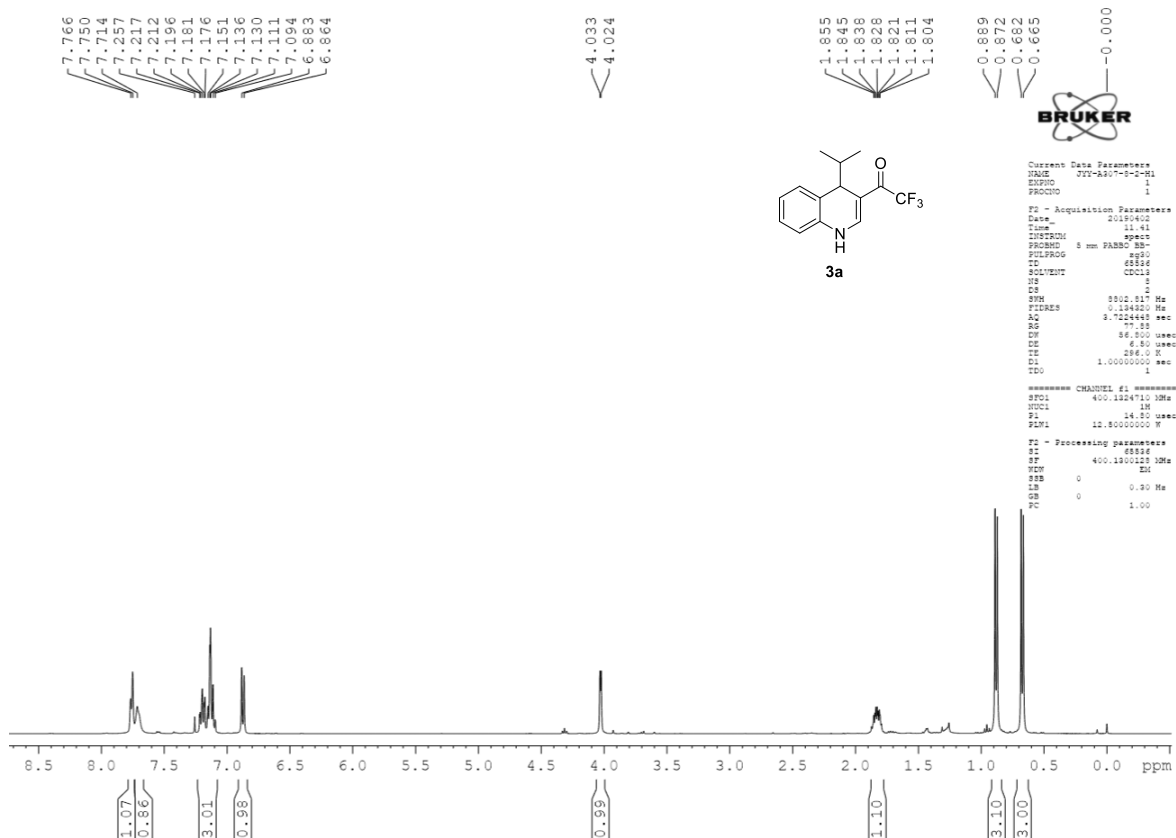
wangdong@tust.edu.cn

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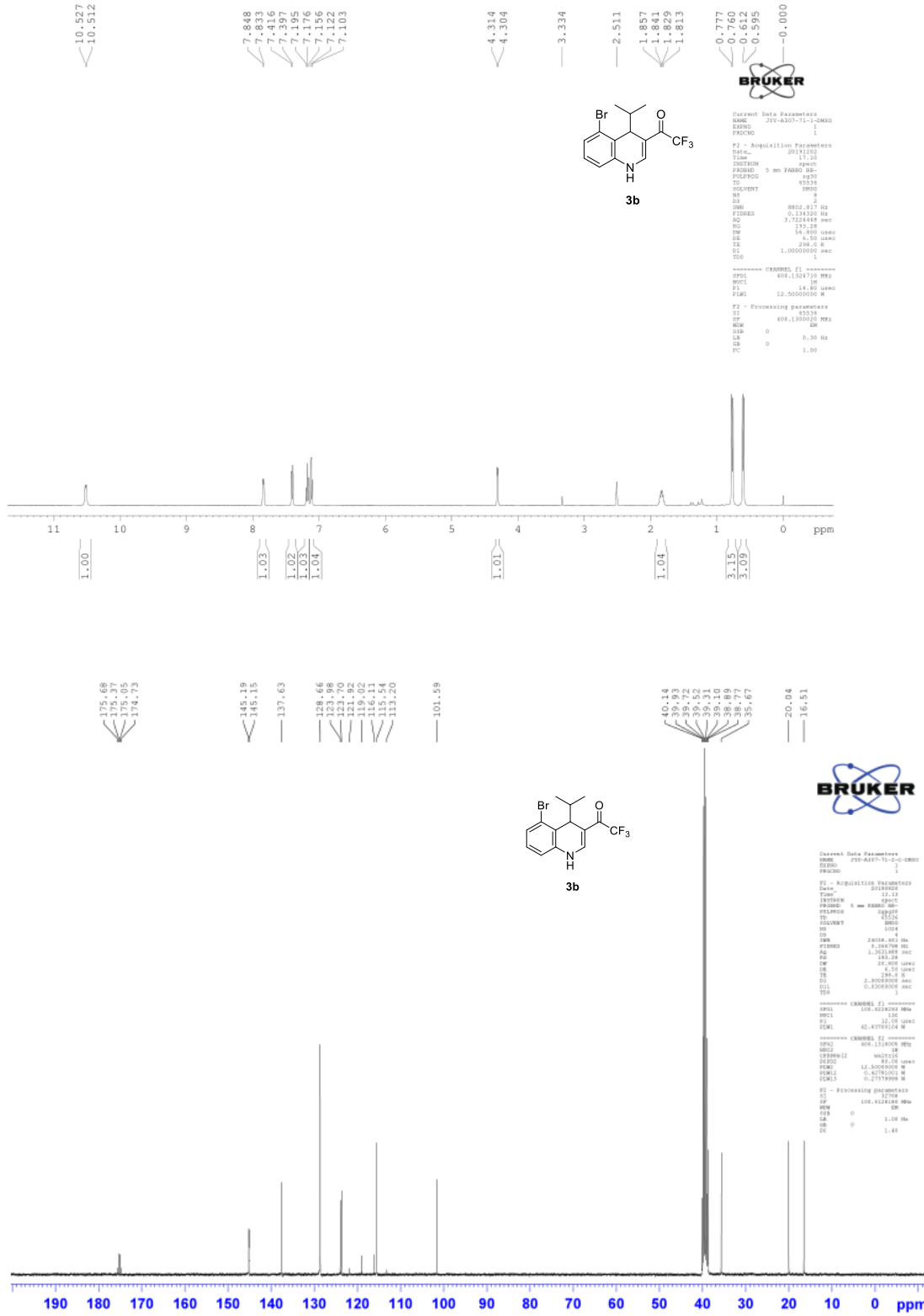
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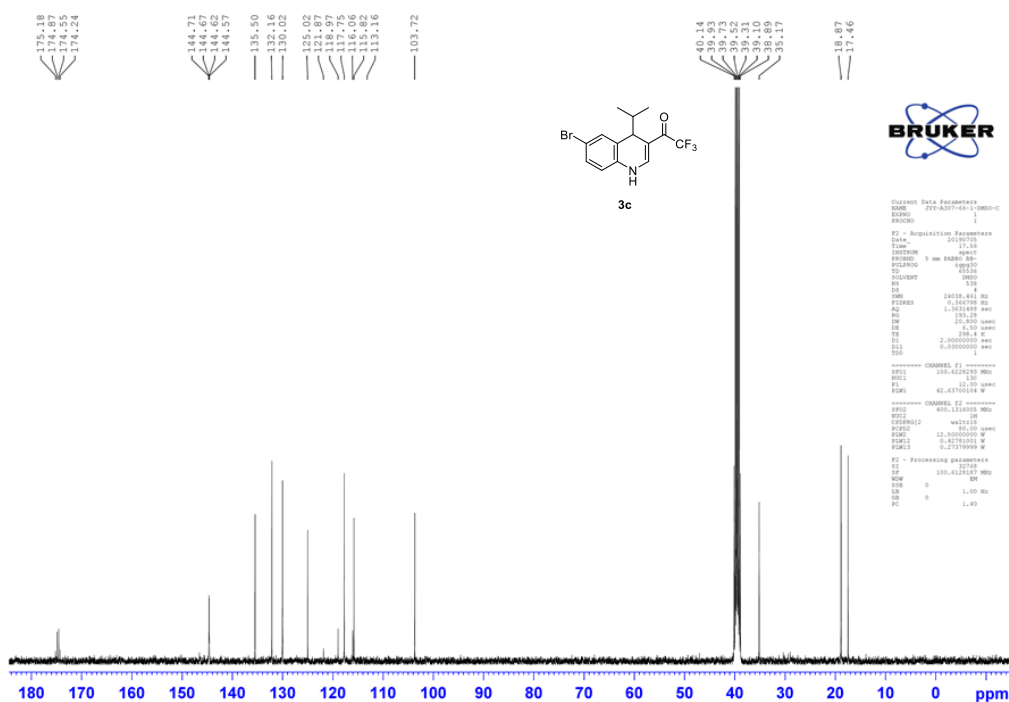
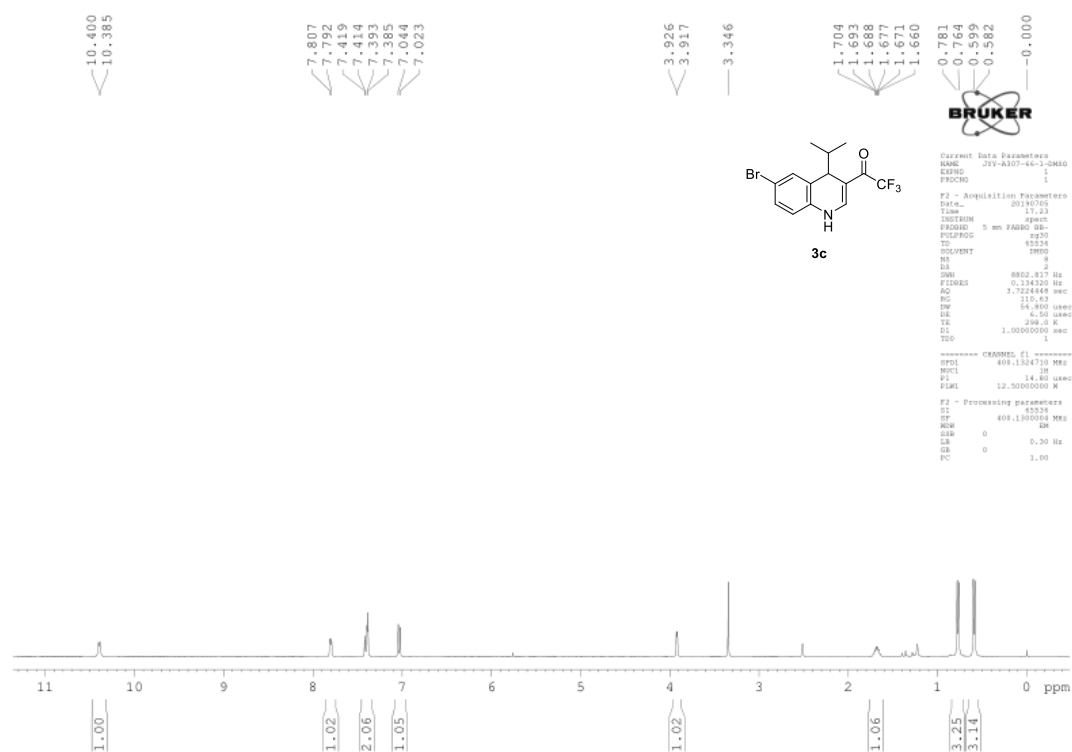
1. Copy of NMR spectrum for 3a-3v, 4-7 and 9-13



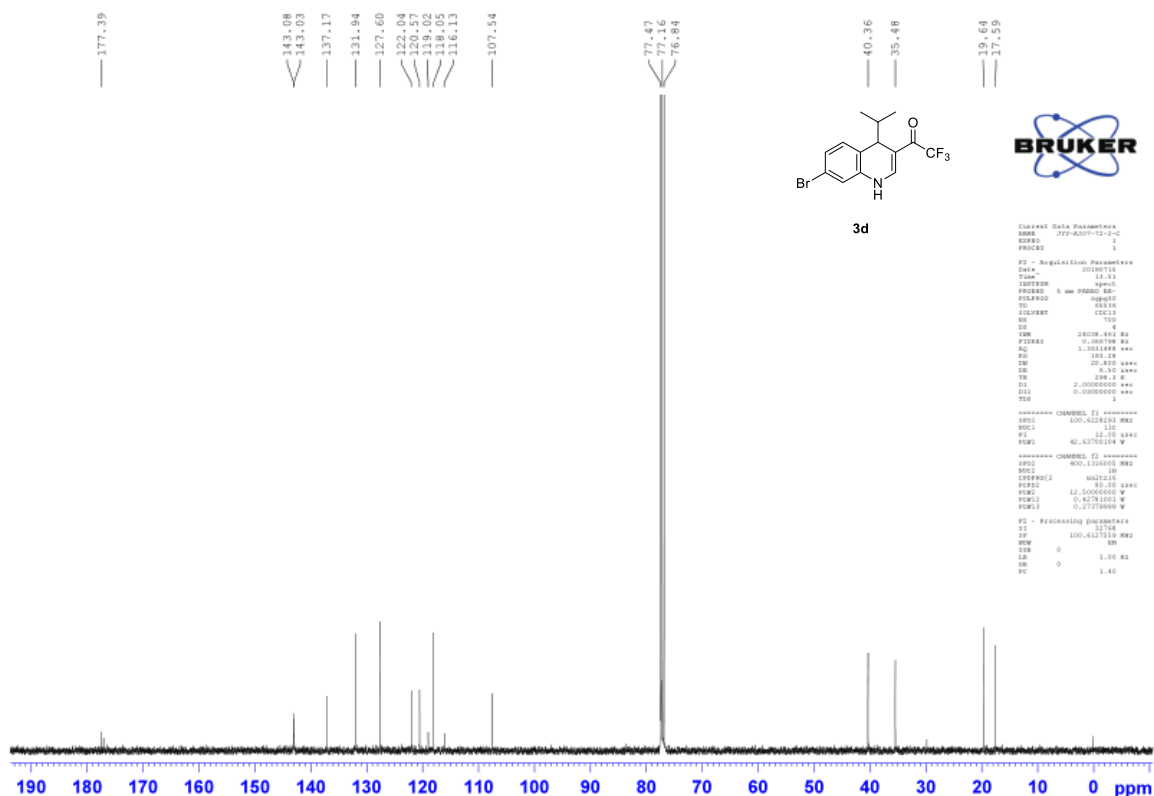
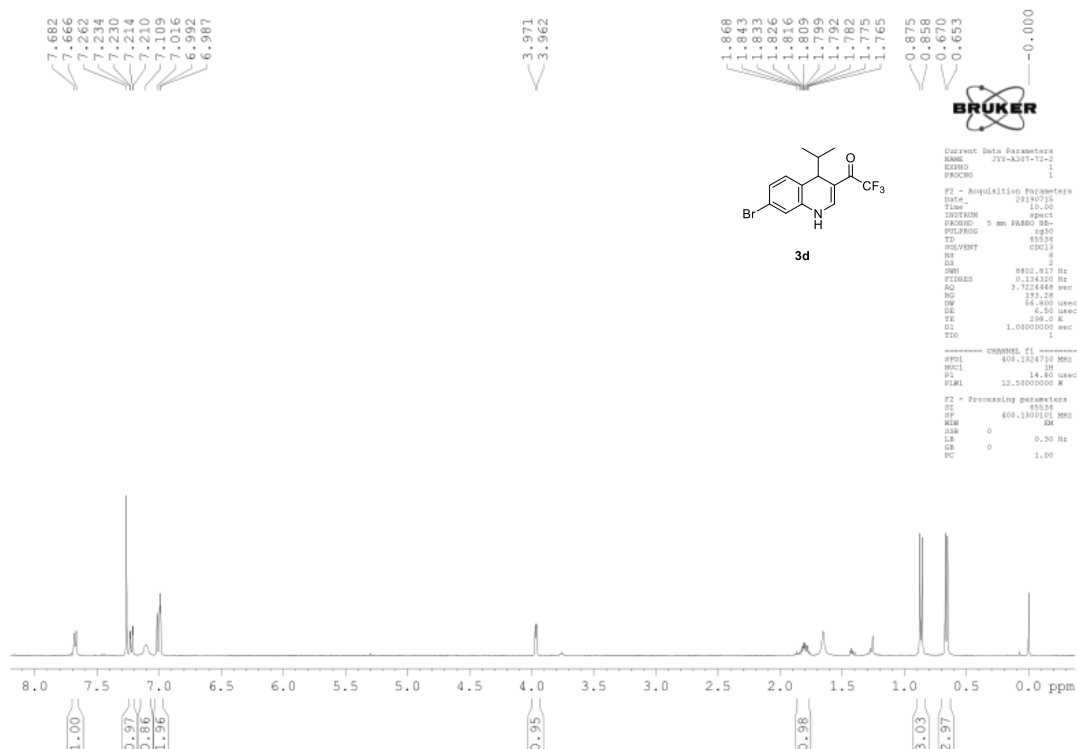
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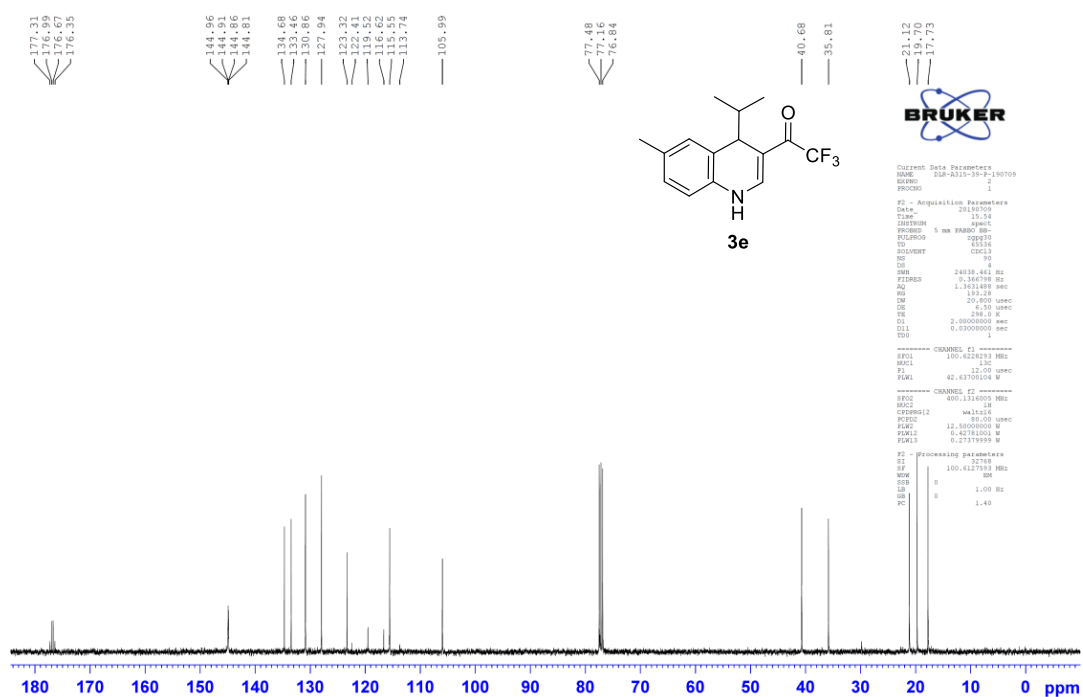
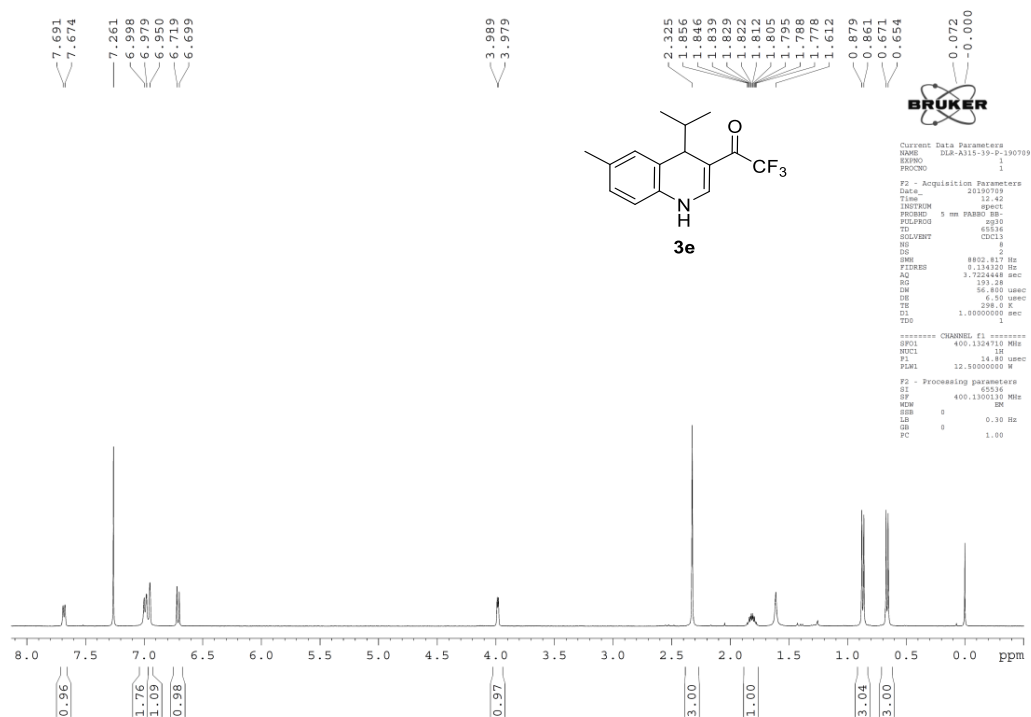
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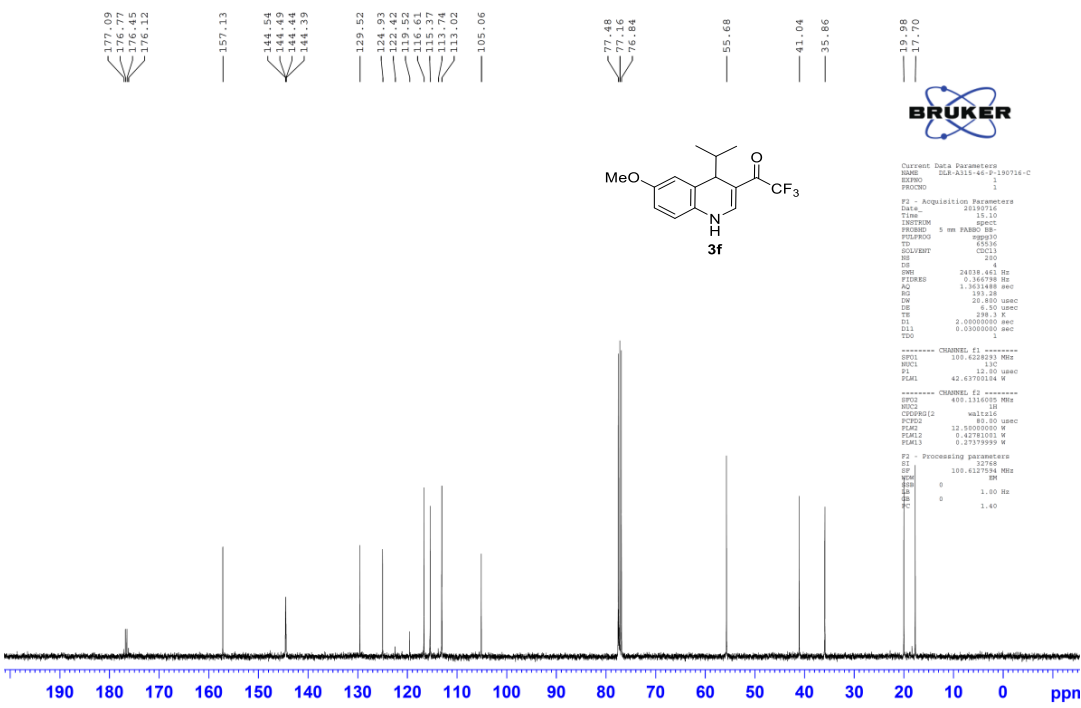
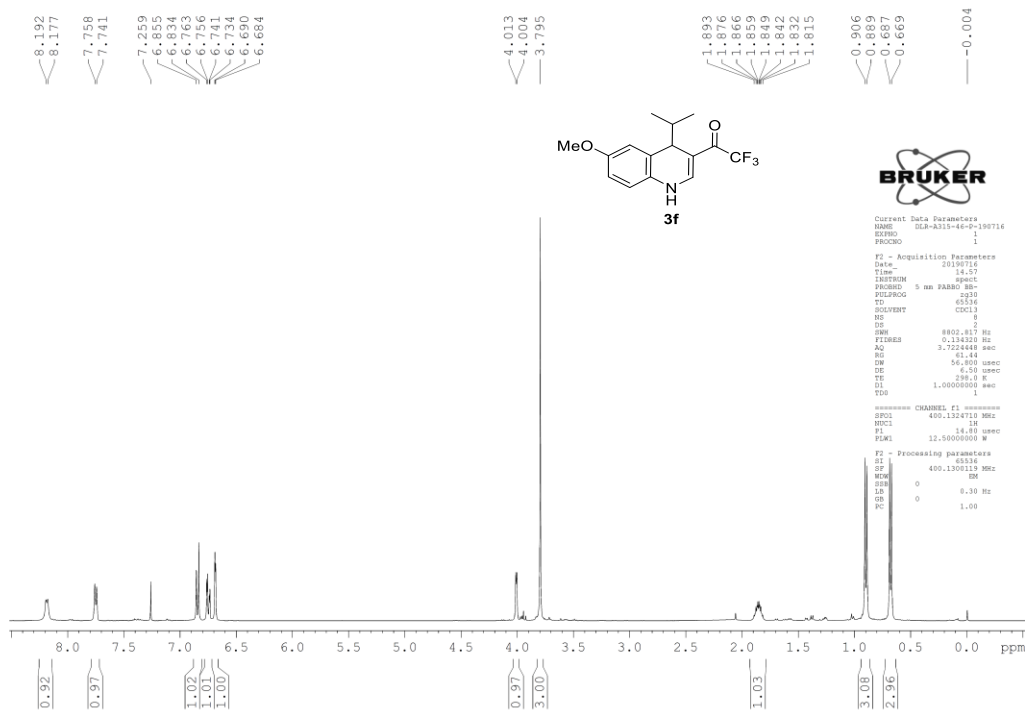
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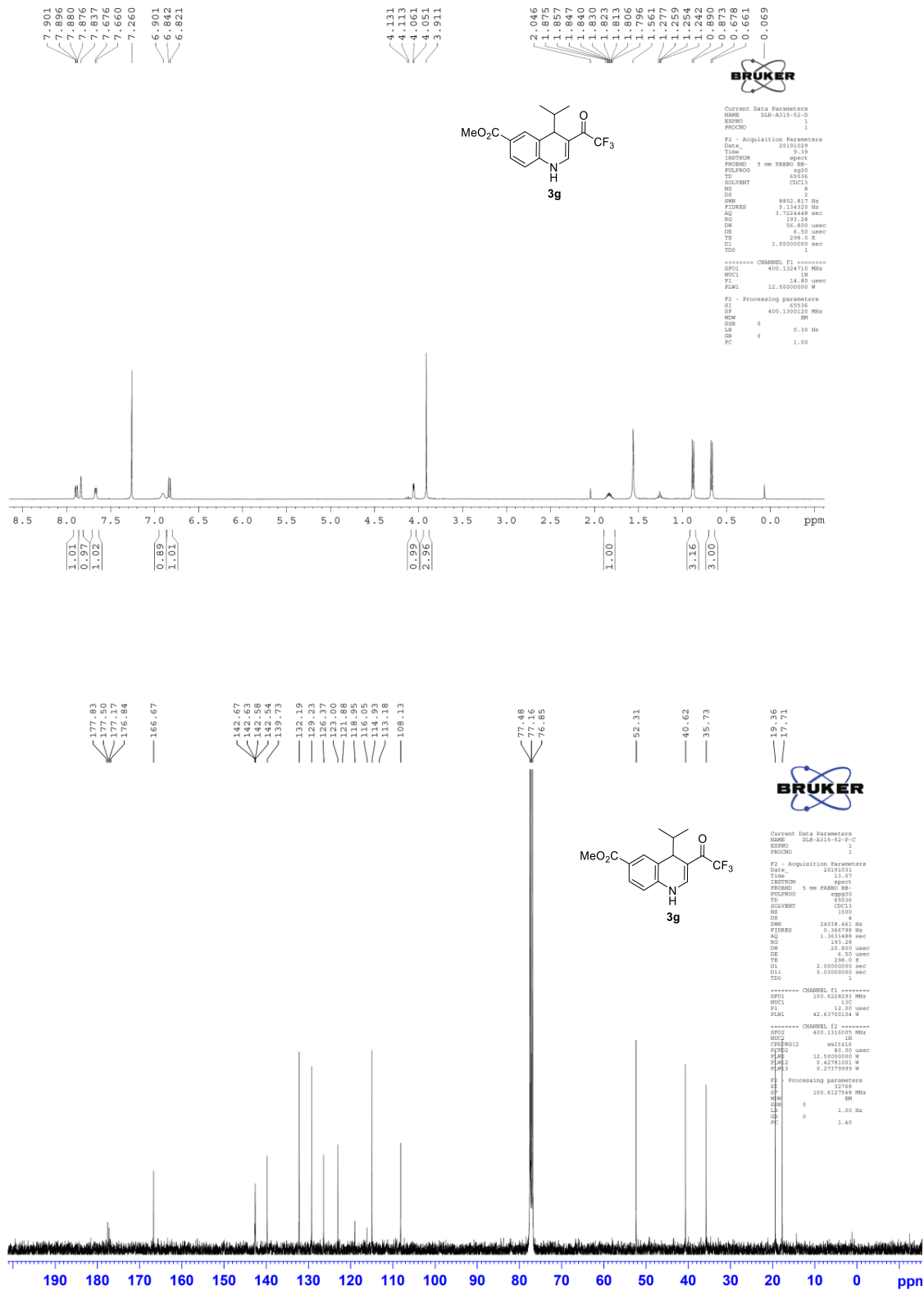
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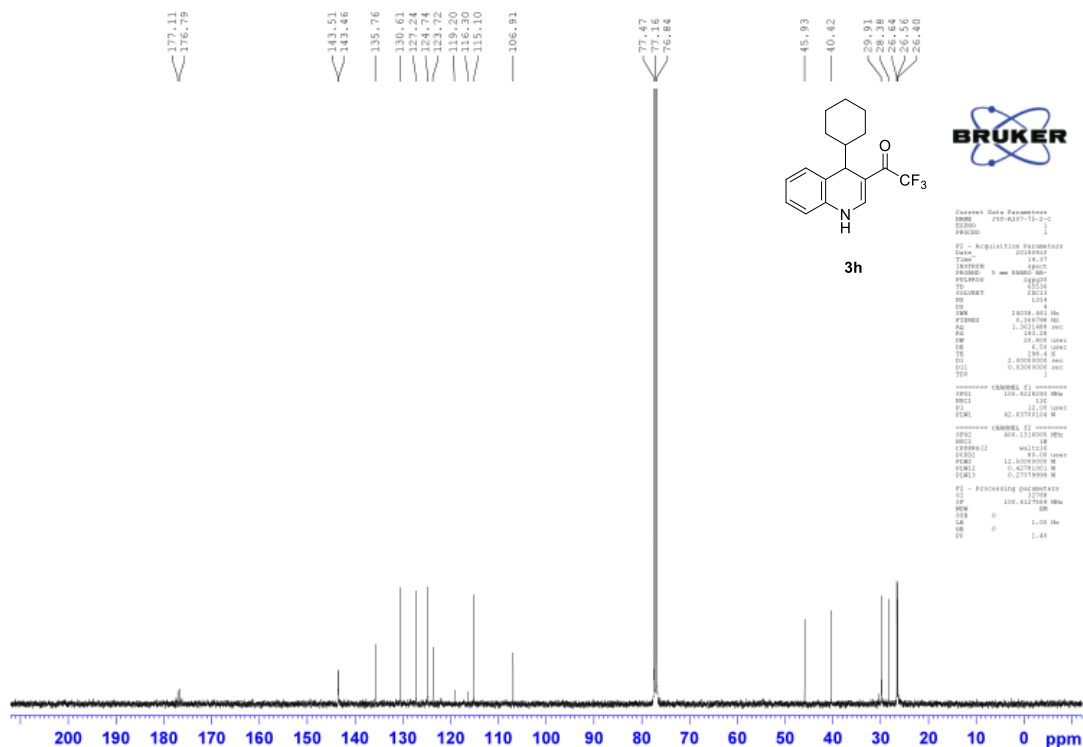
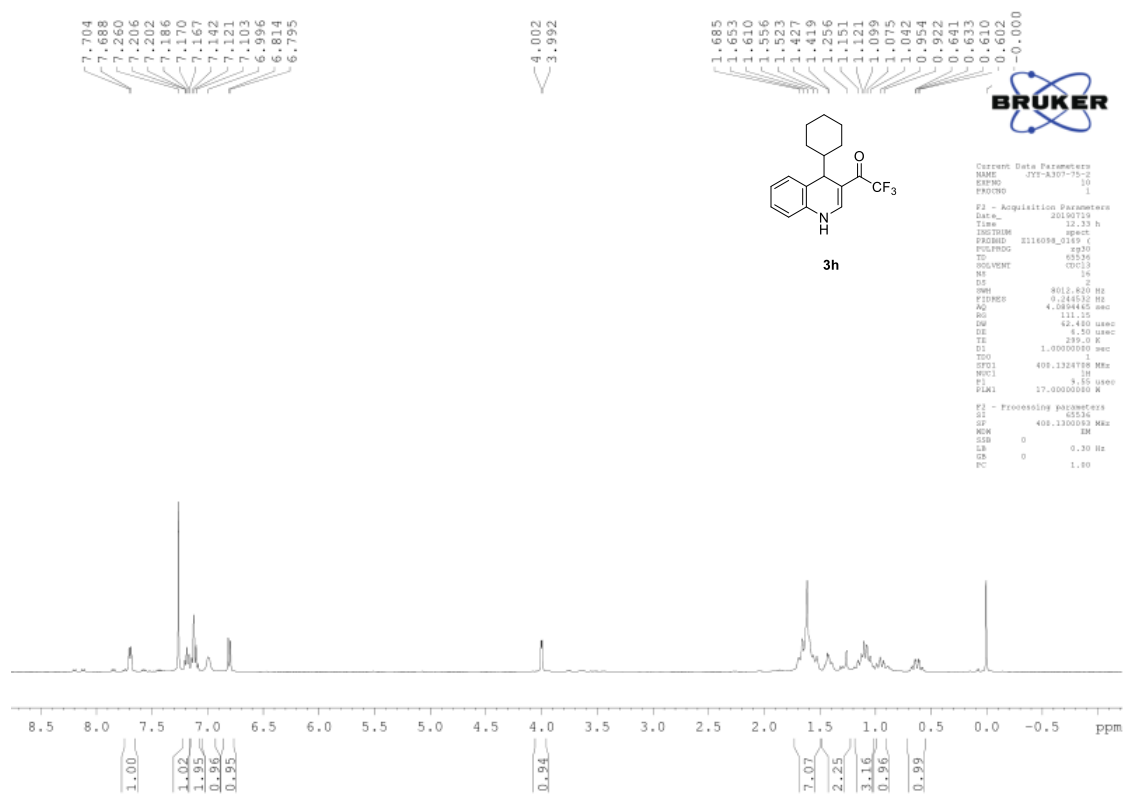
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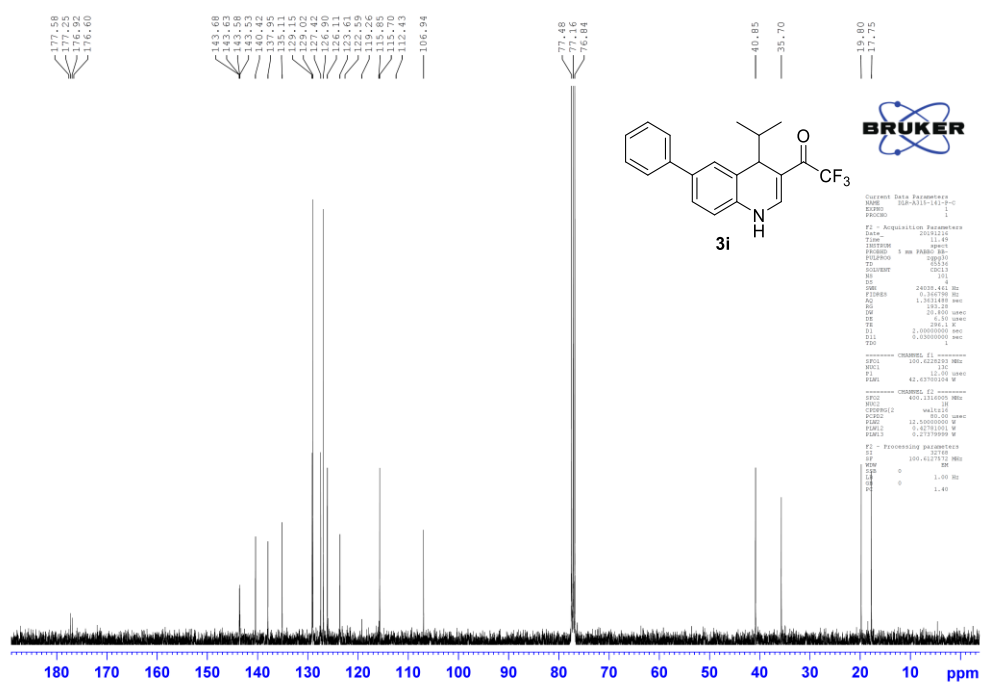
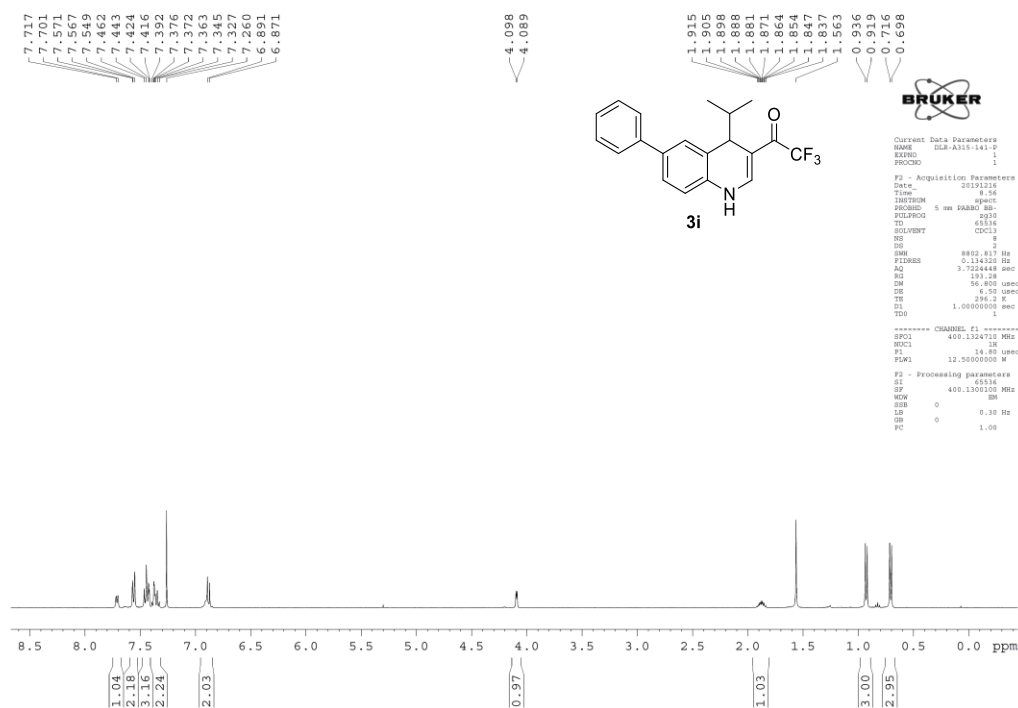


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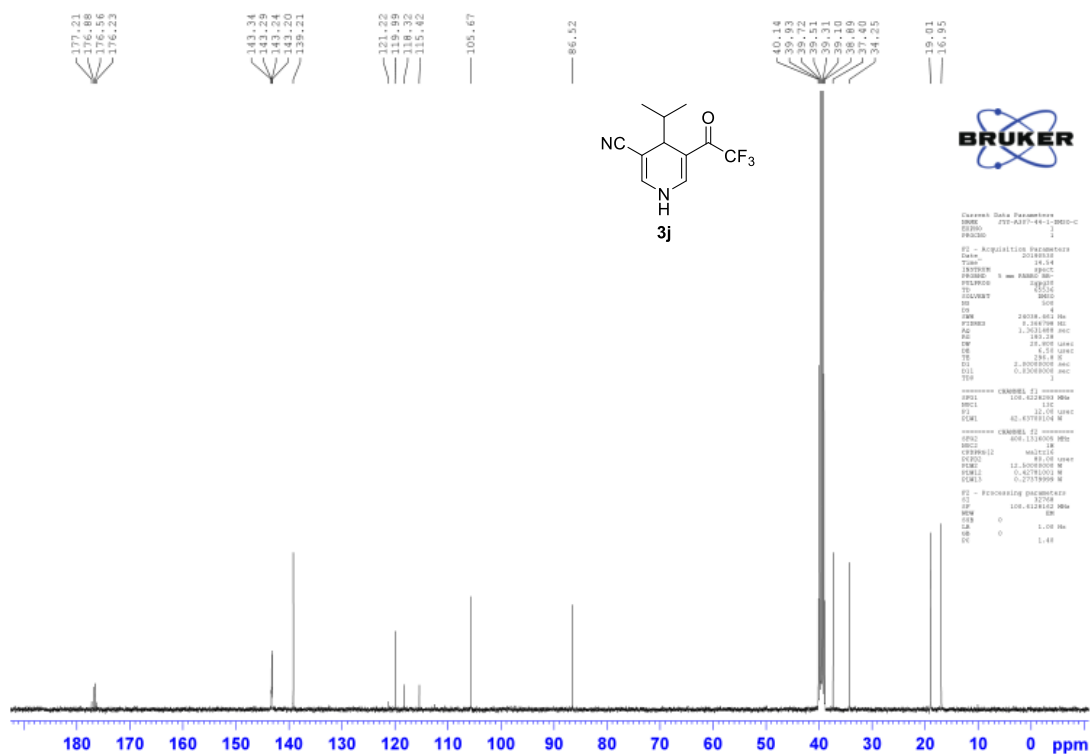
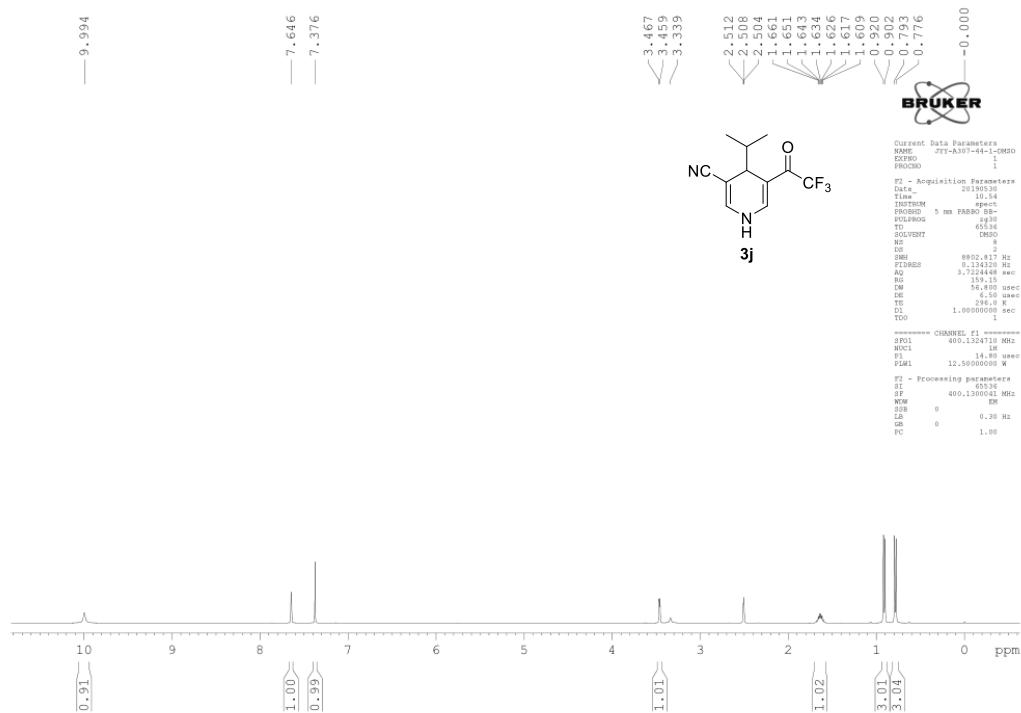


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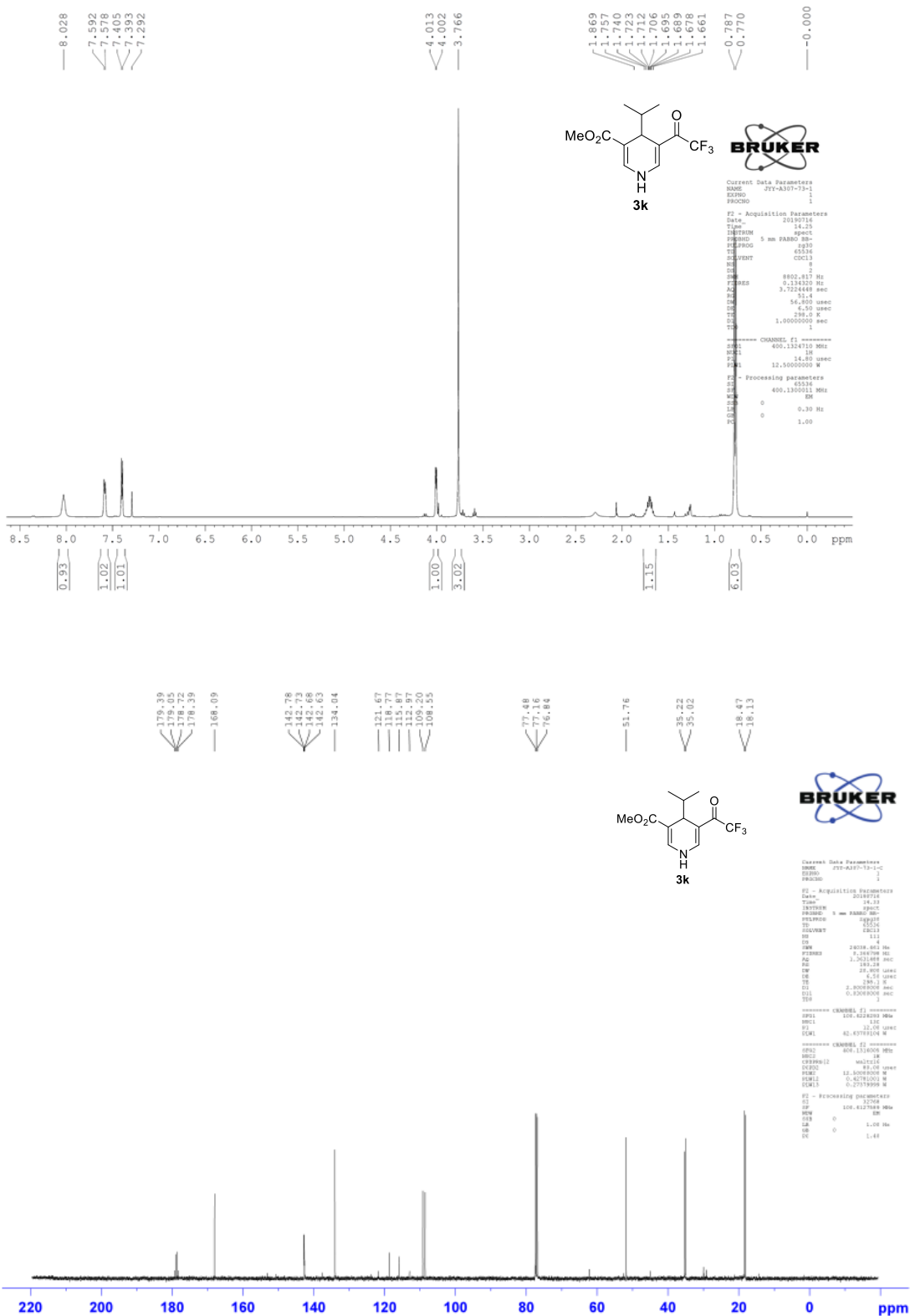




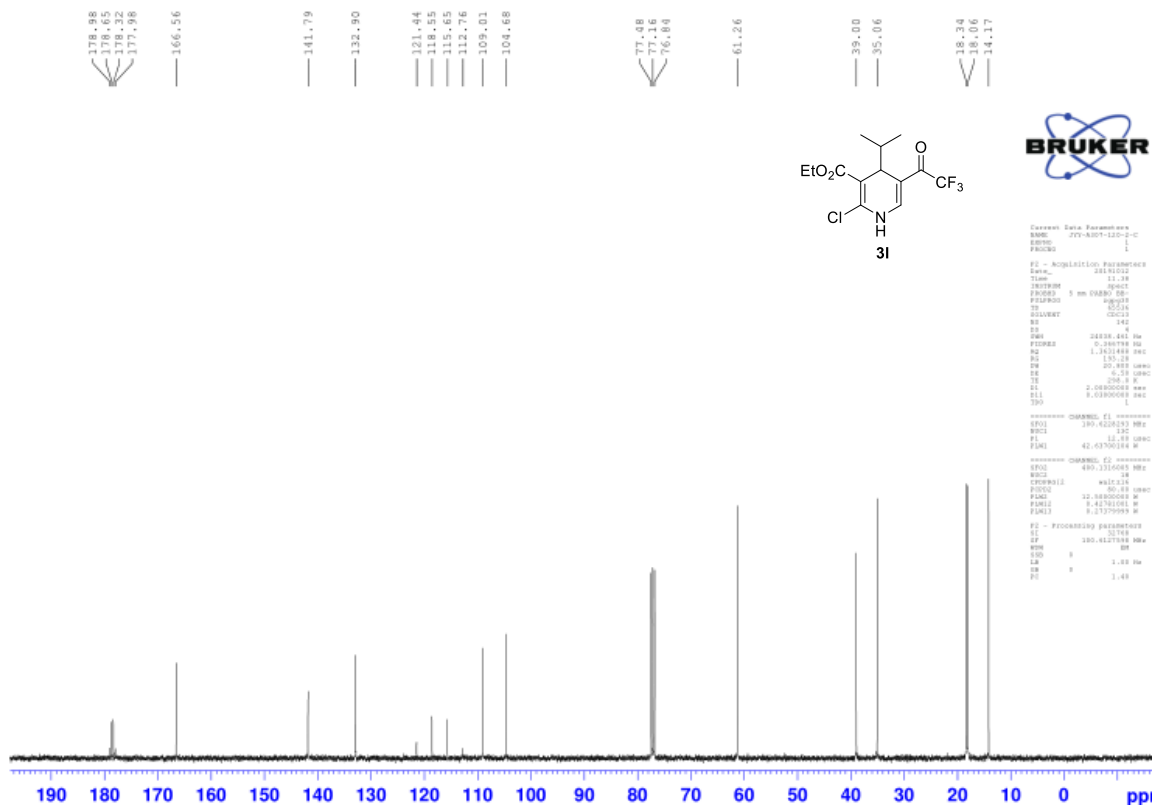
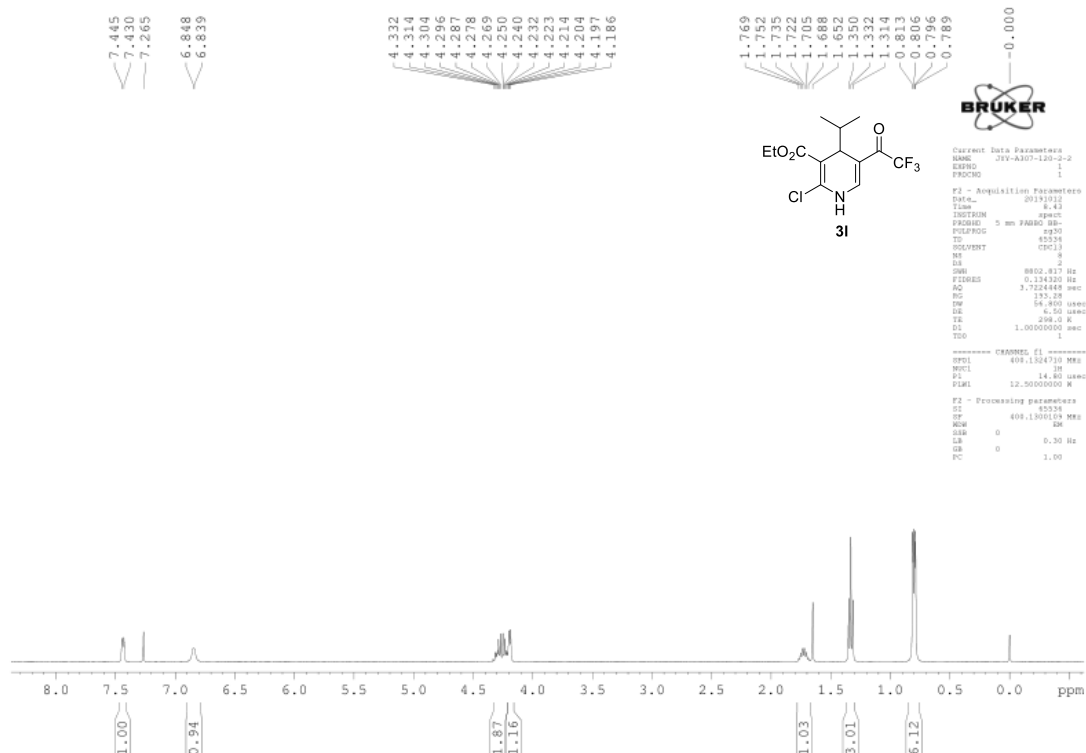
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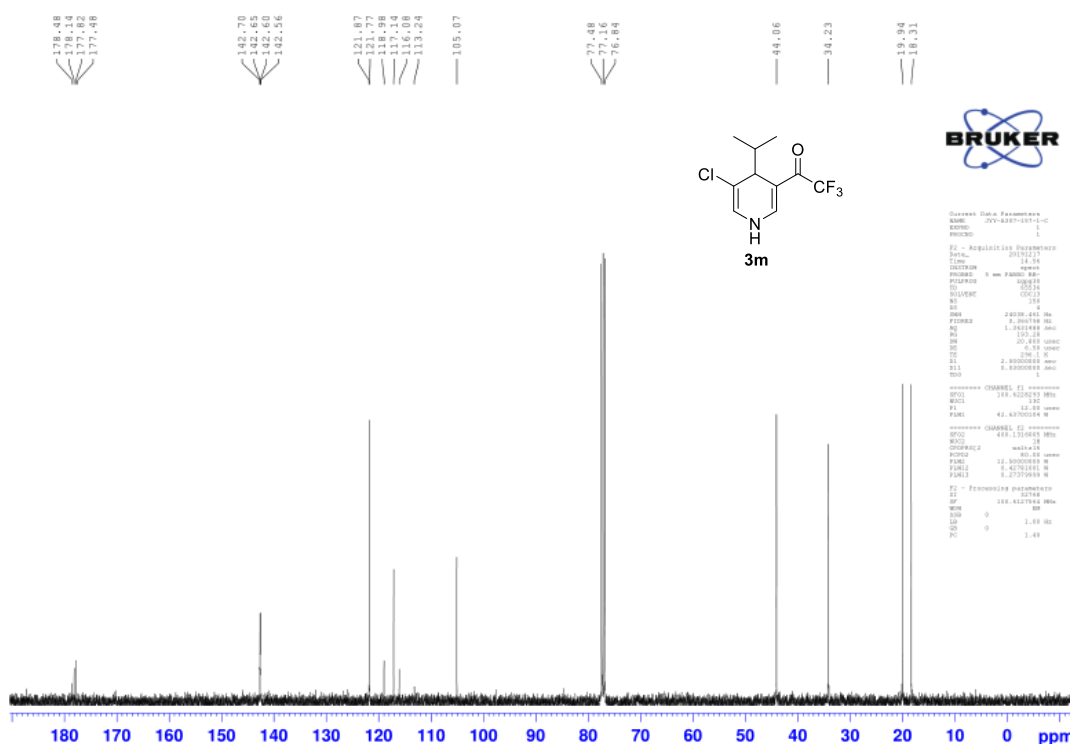
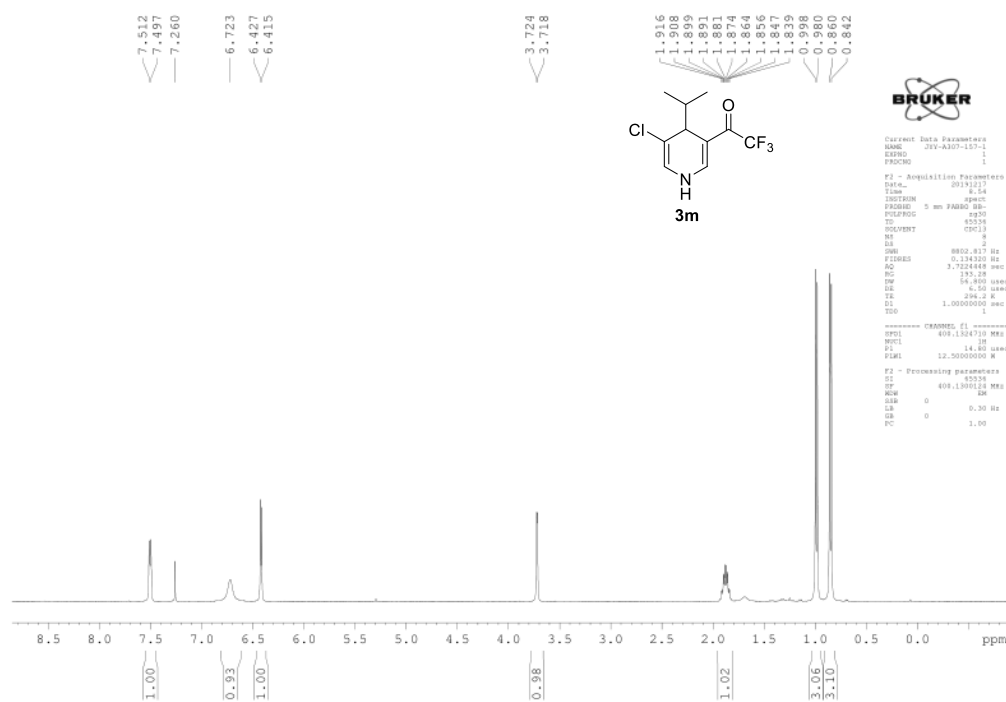
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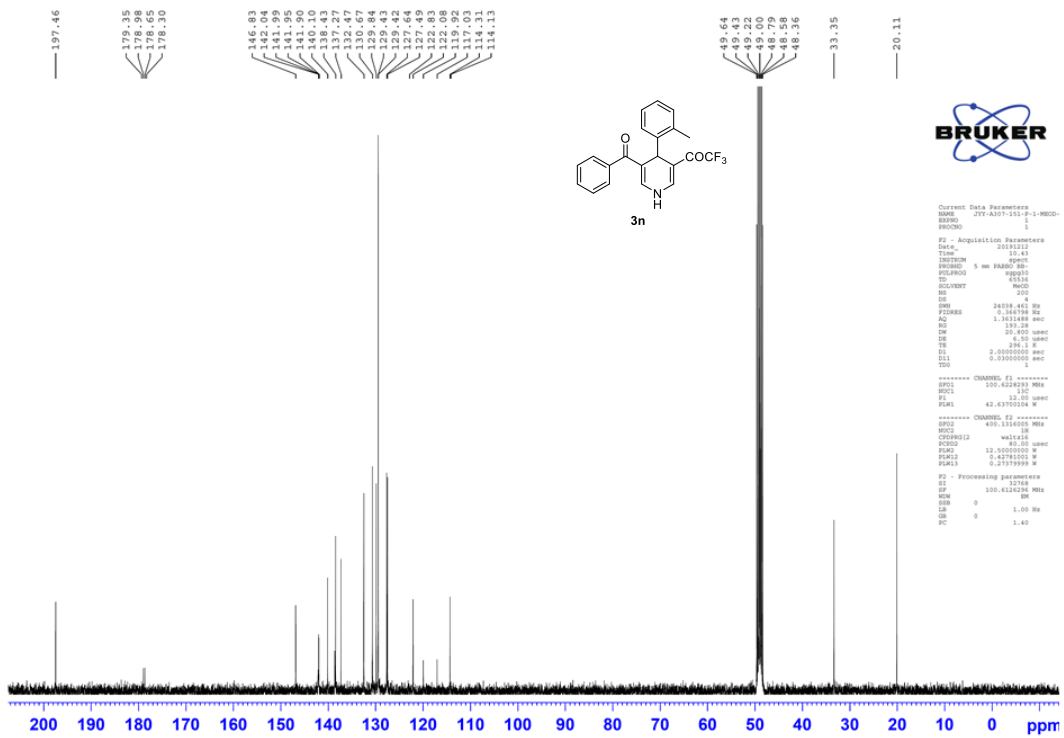
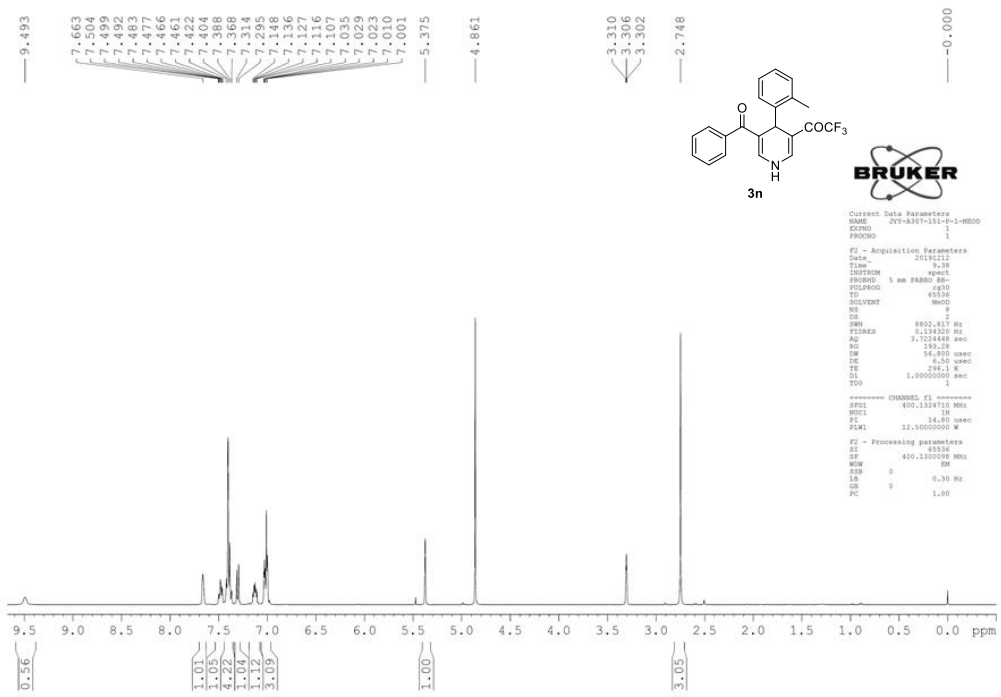


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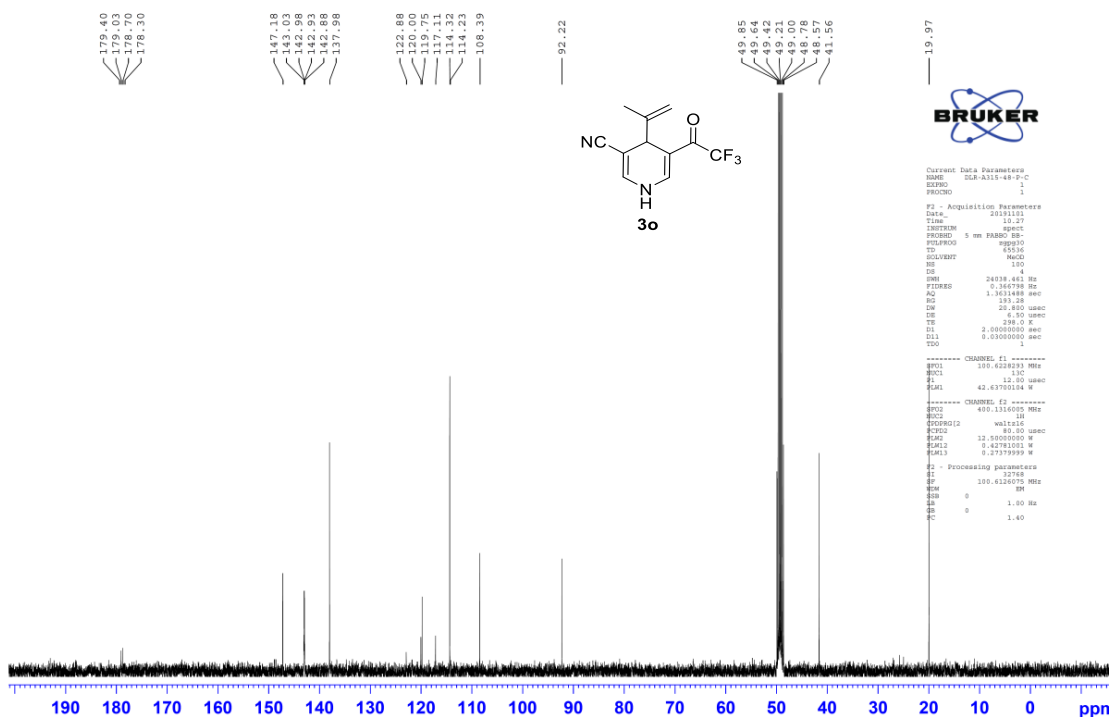
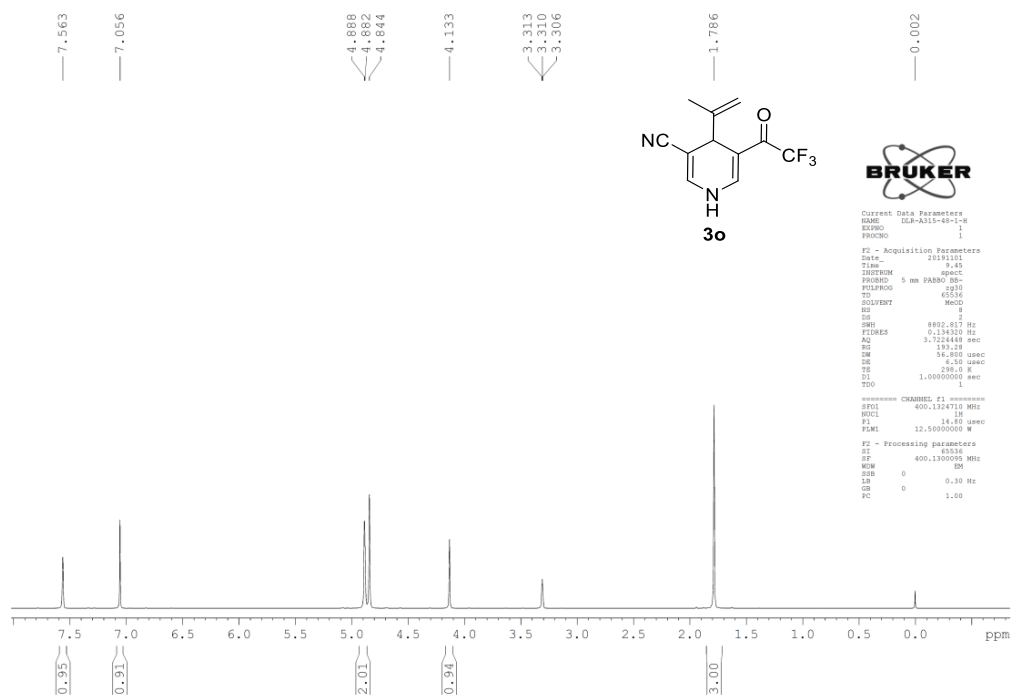


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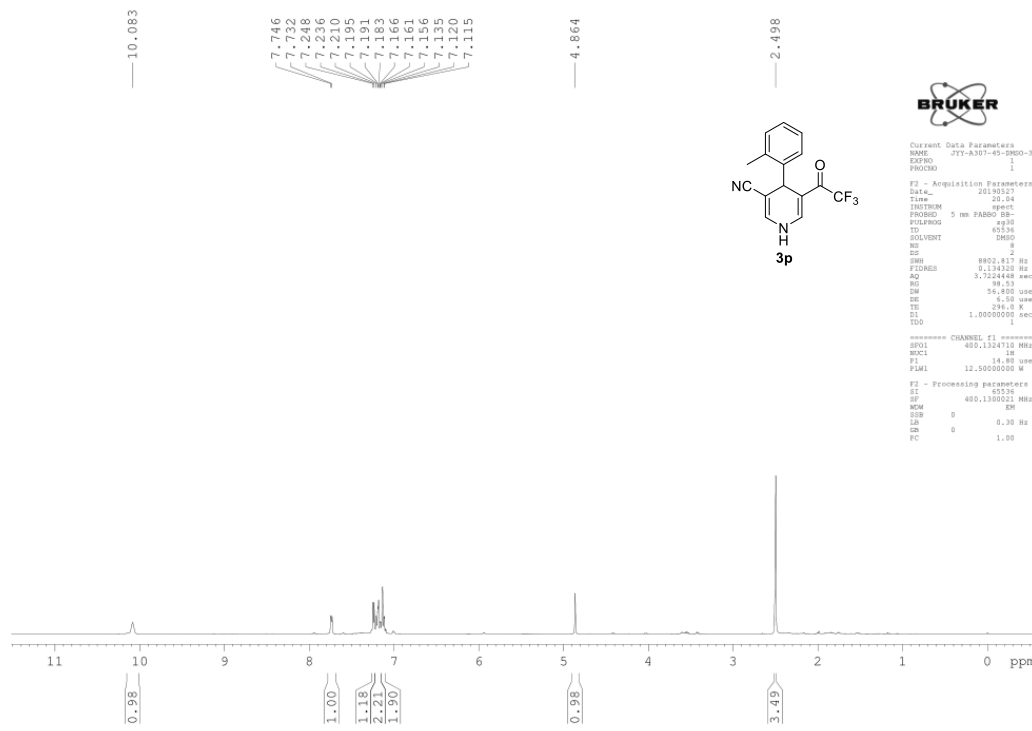




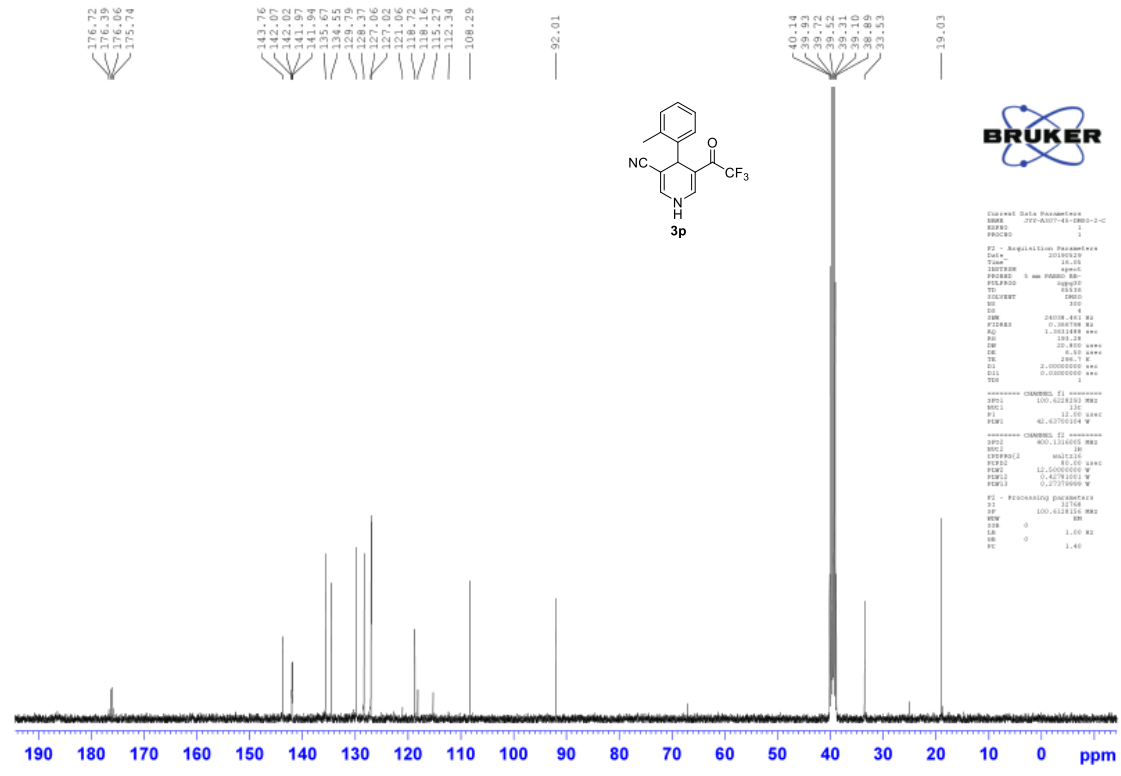
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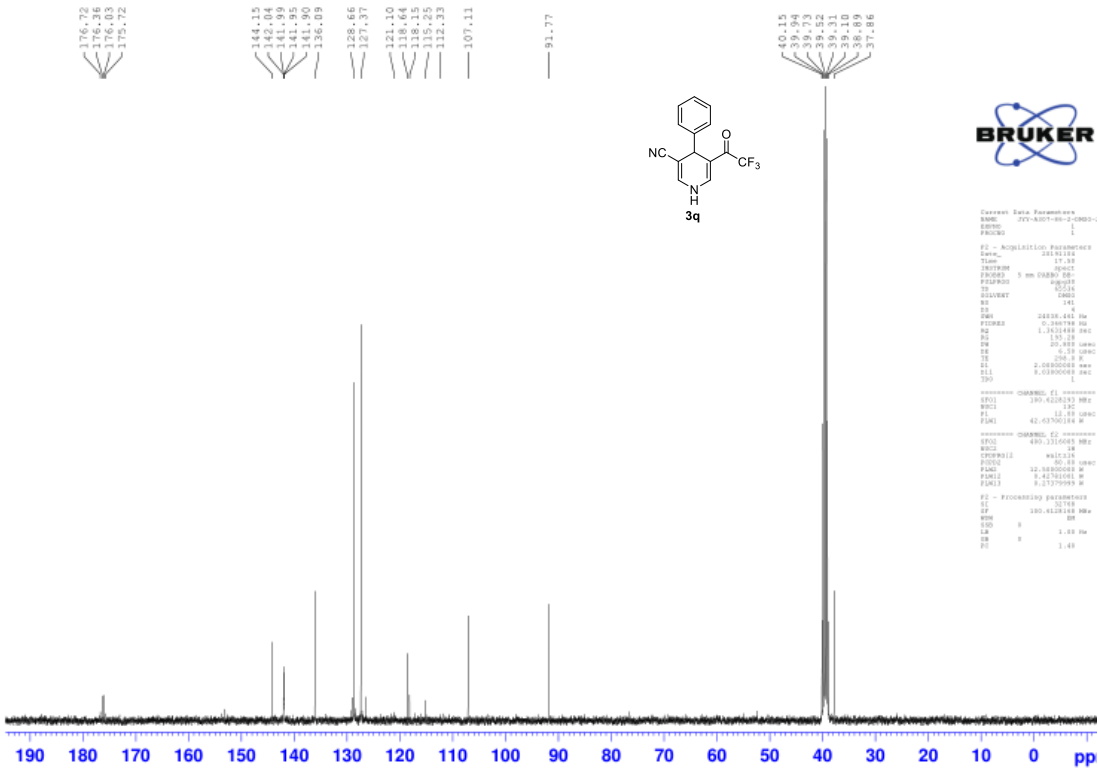
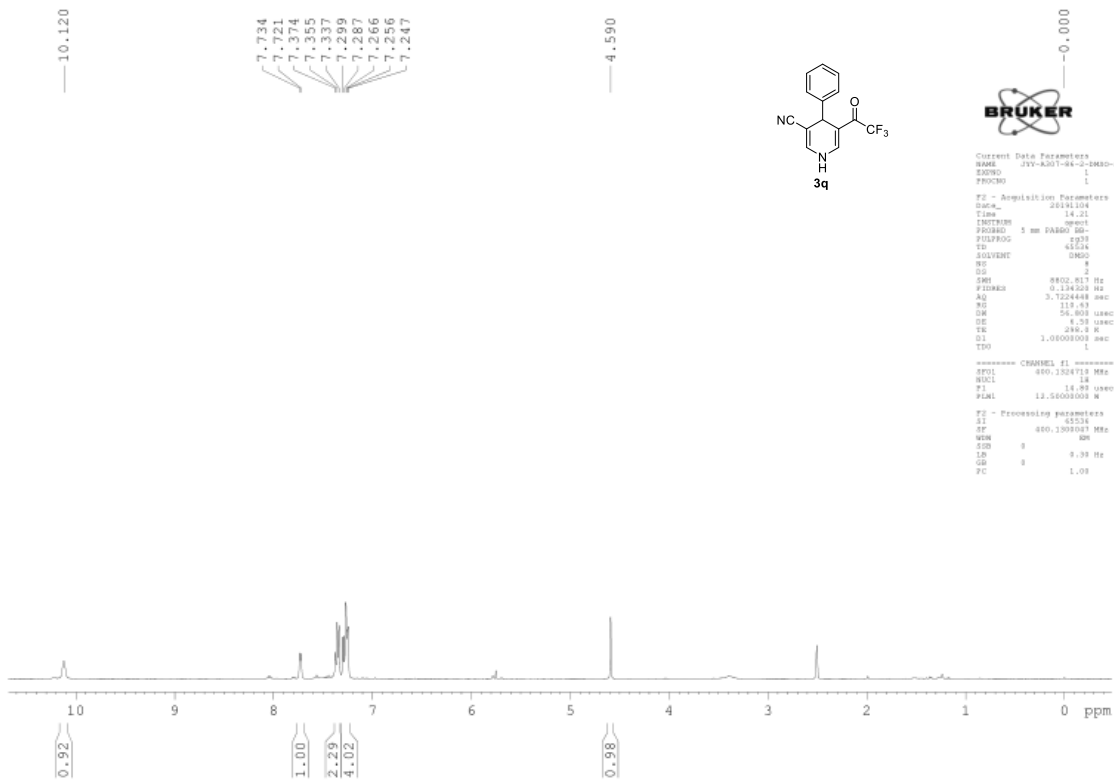
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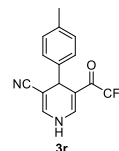
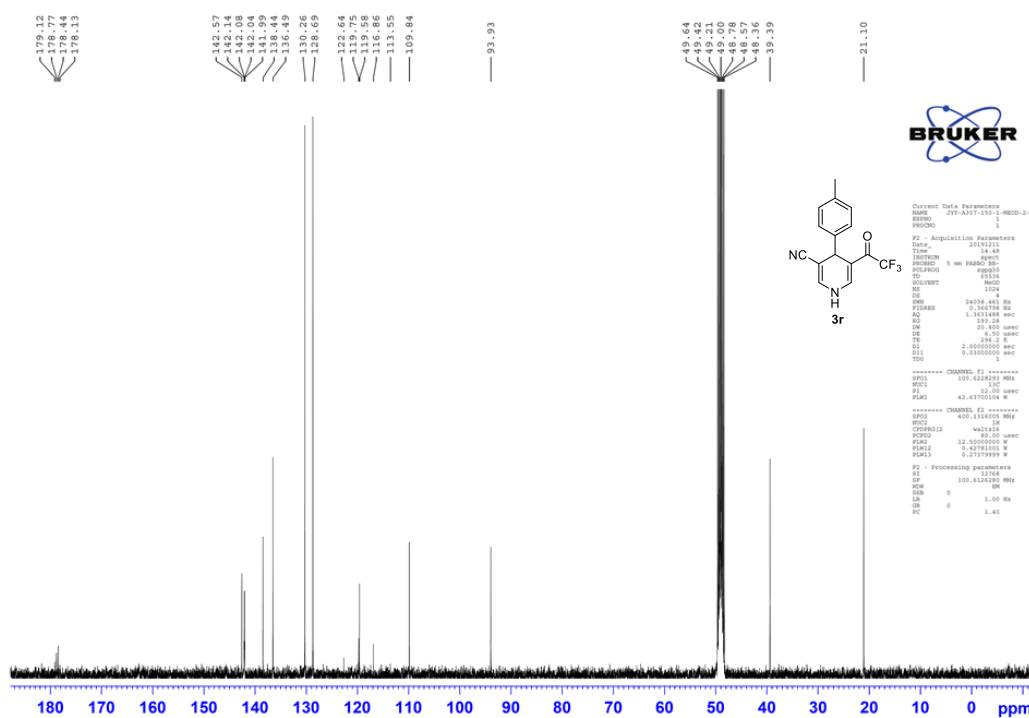
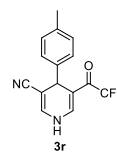


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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2
DS 8802.817 Hz
FIDRES 0.114333 Hz
AQ 3.725468 sec
RG 66.03
SW 56.850 MHz
DE 6.50 MHz
TE 294.2 K
D1 1.00000000 sec
TD0
===== CHANNEL f1 =====
NUC1 400.1304710 MHz
P1 14.00
PL1 12.50000000 W
===== CHANNEL f2 =====
SI - Processing parameters
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WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

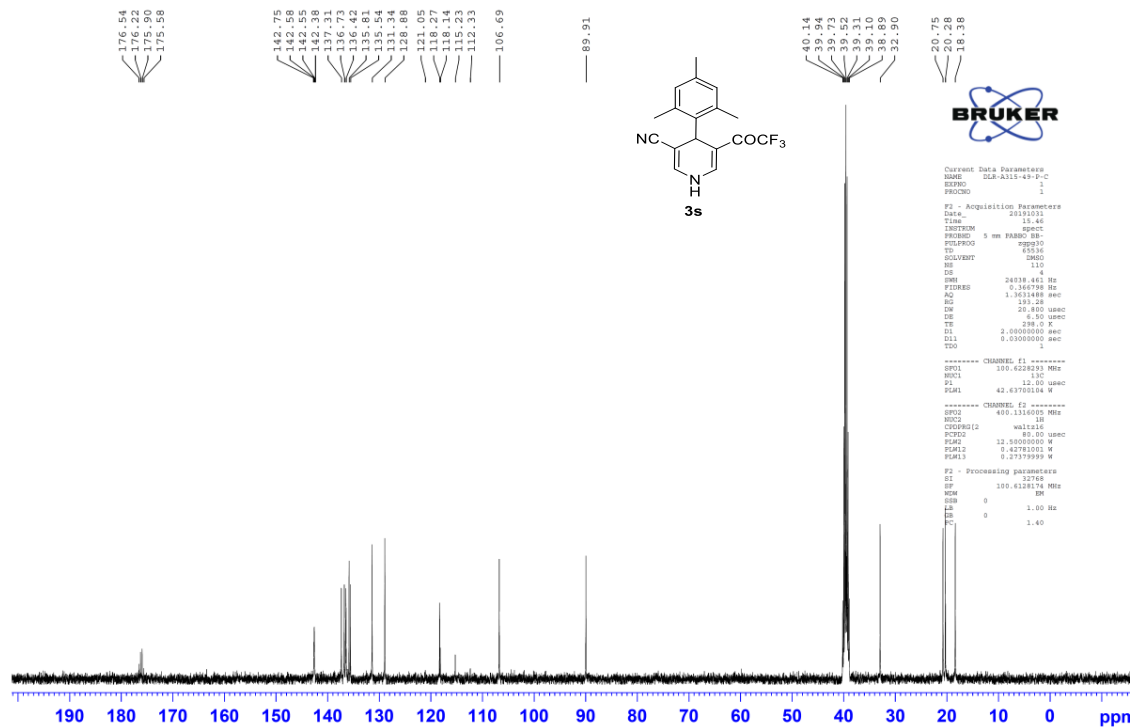
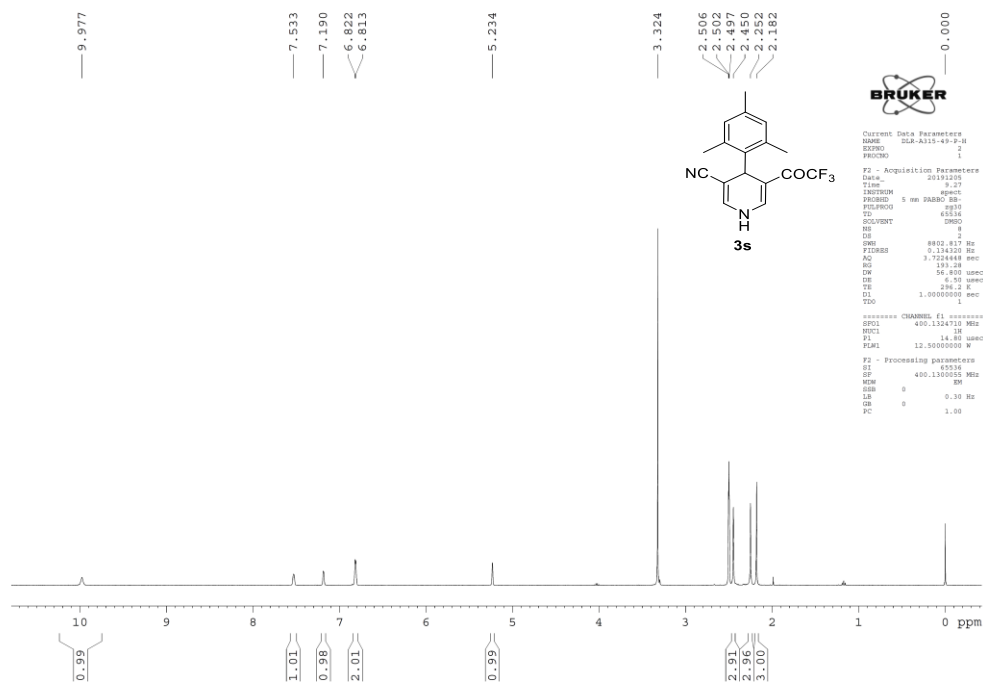


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Time 18.18
INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4
DS 28038.861 Hz
FIDRES 0.100709 Hz
AQ 1.2001698 sec
RG 66.03
SW 180.28 MHz
DE 6.50 MHz
TE 294.2 K
D1 2.00000000 sec
D11 0.00000000 sec
TD 1
===== CHANNEL f1 =====
NUC1 100.6261850 MHz
P1 12.00
PL1 42.43700000 W
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PC 1.40

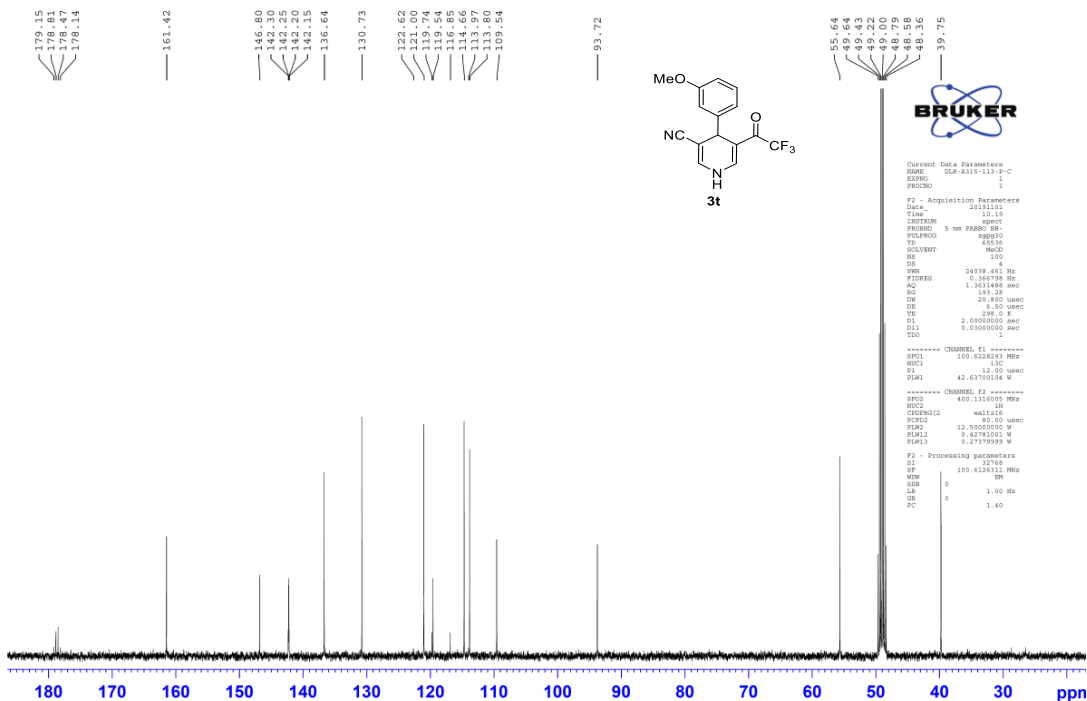
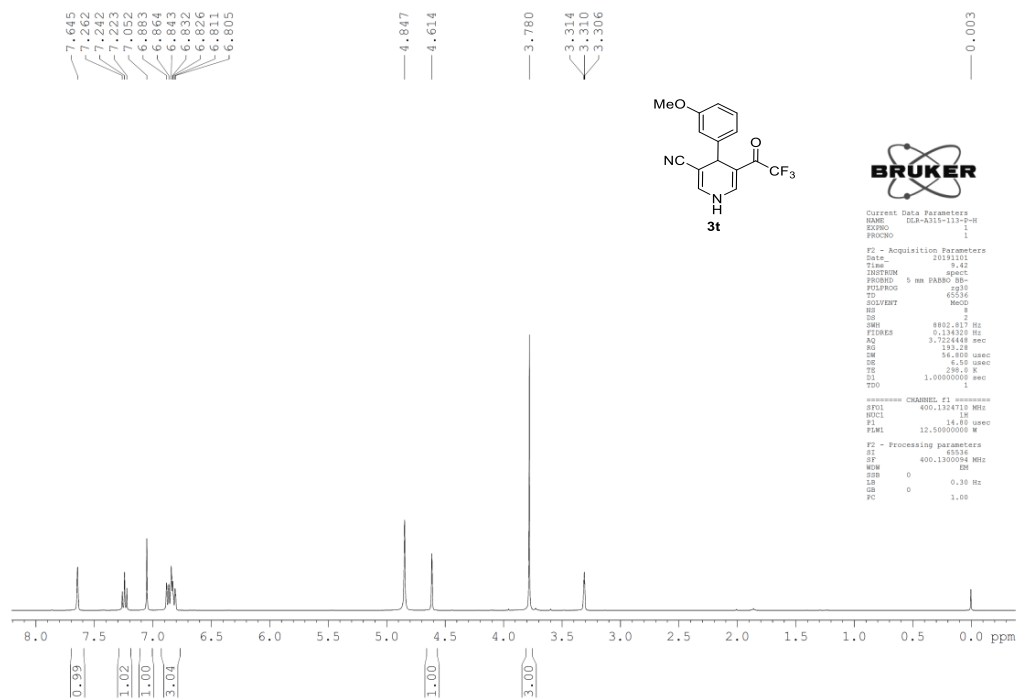




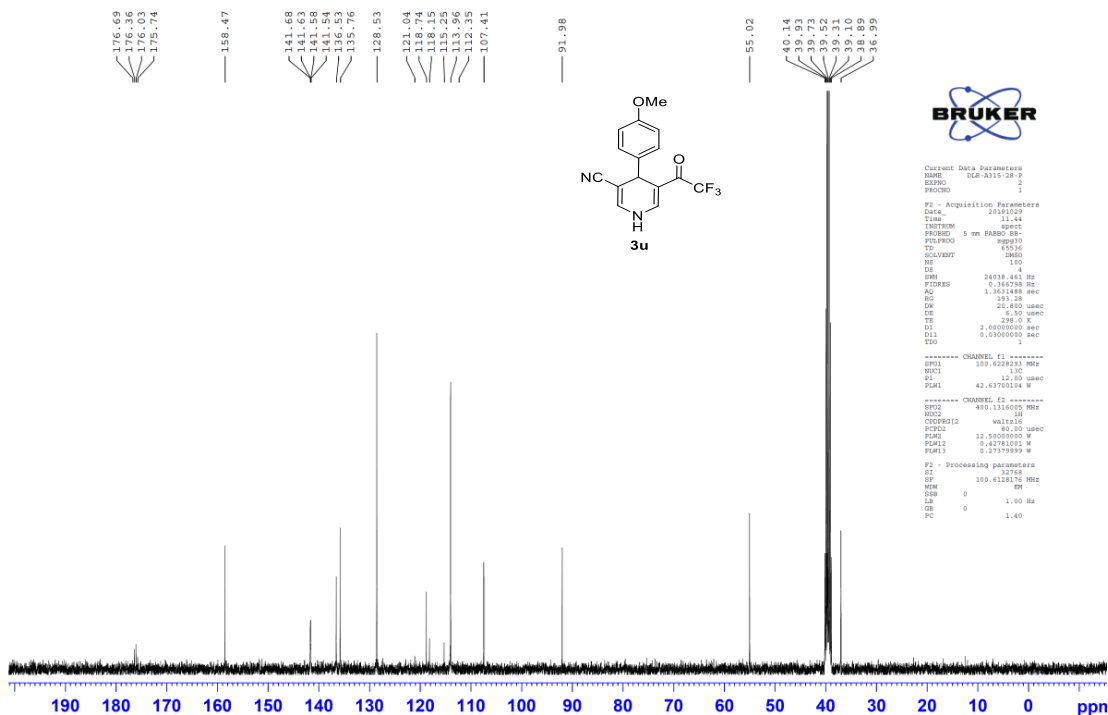
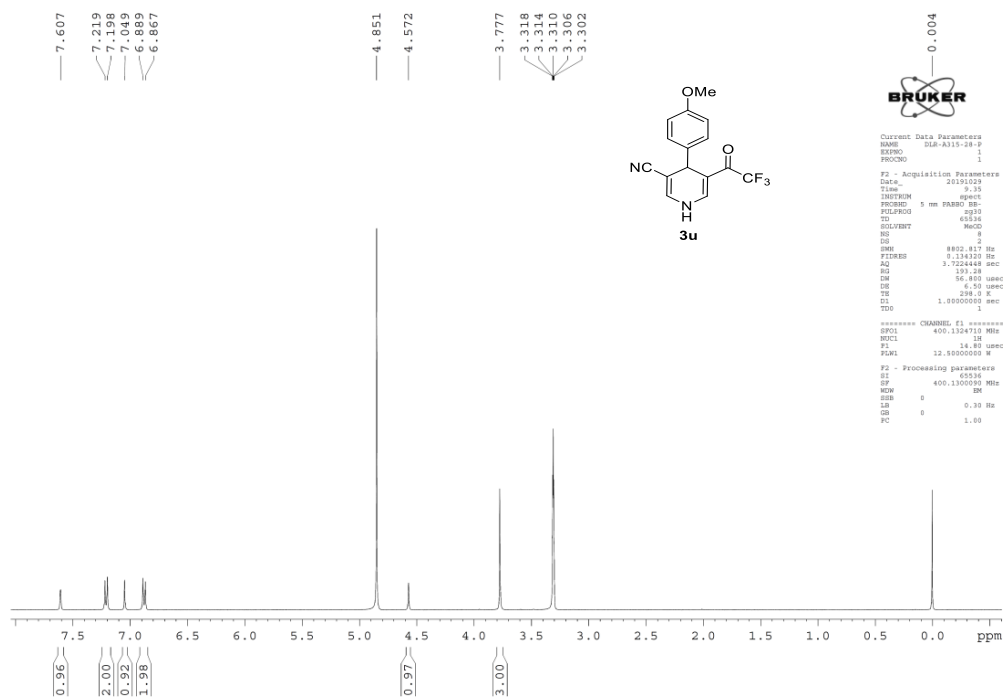
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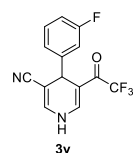
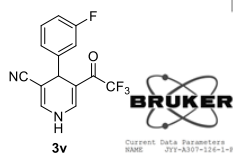


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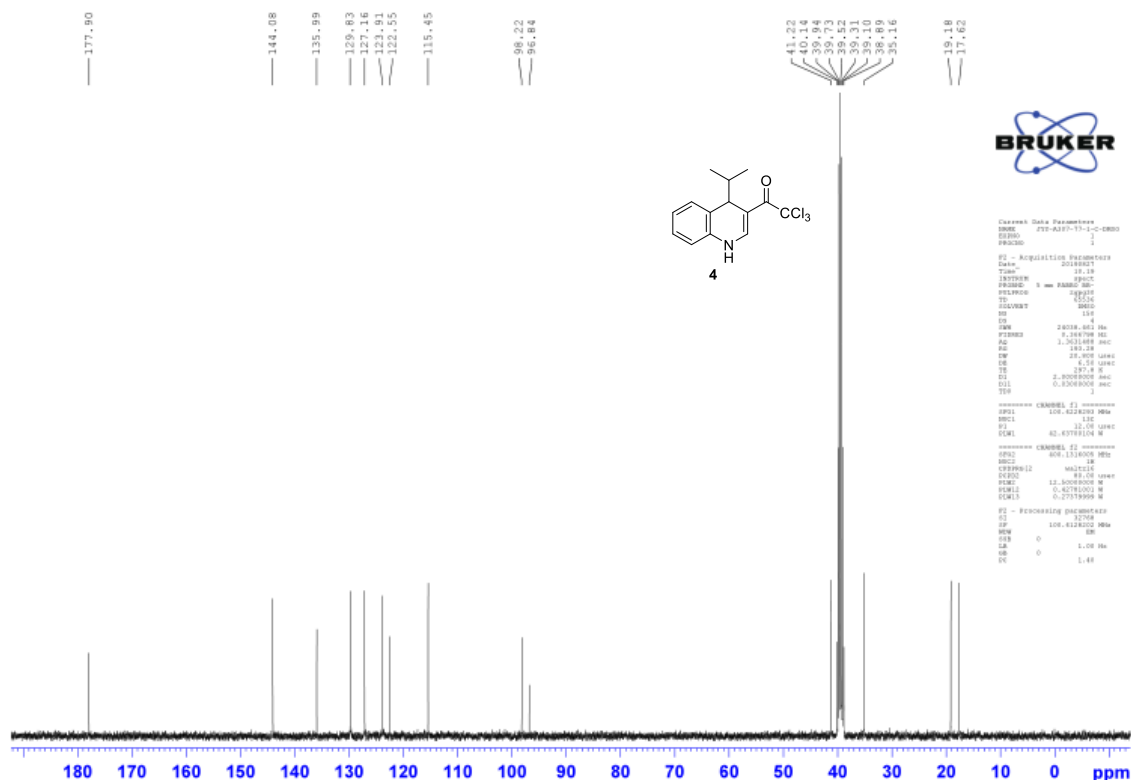
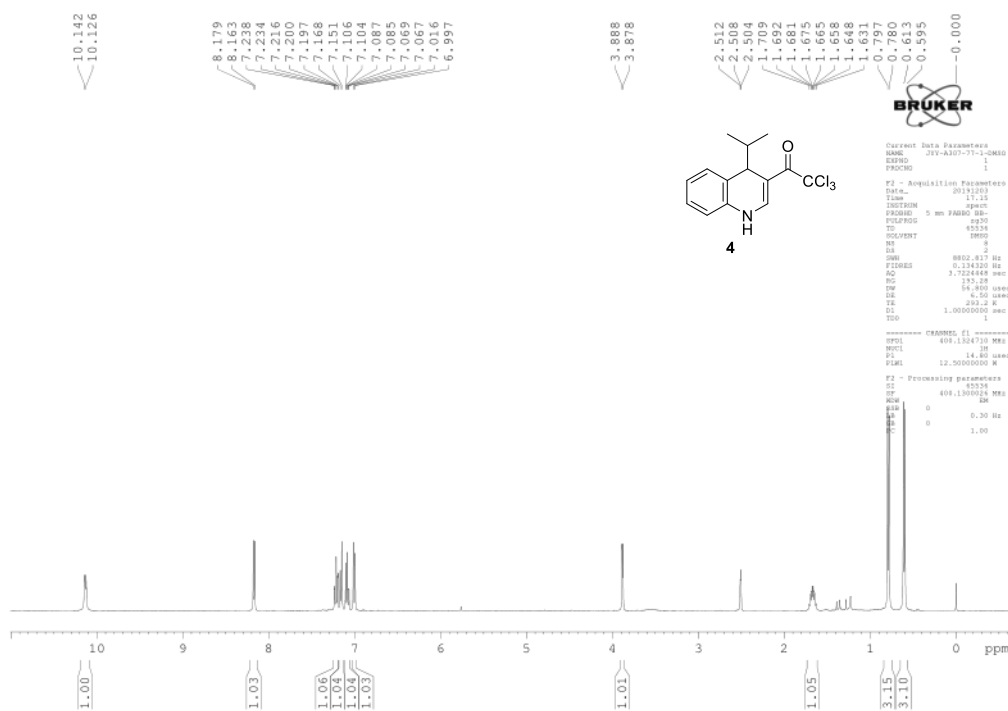


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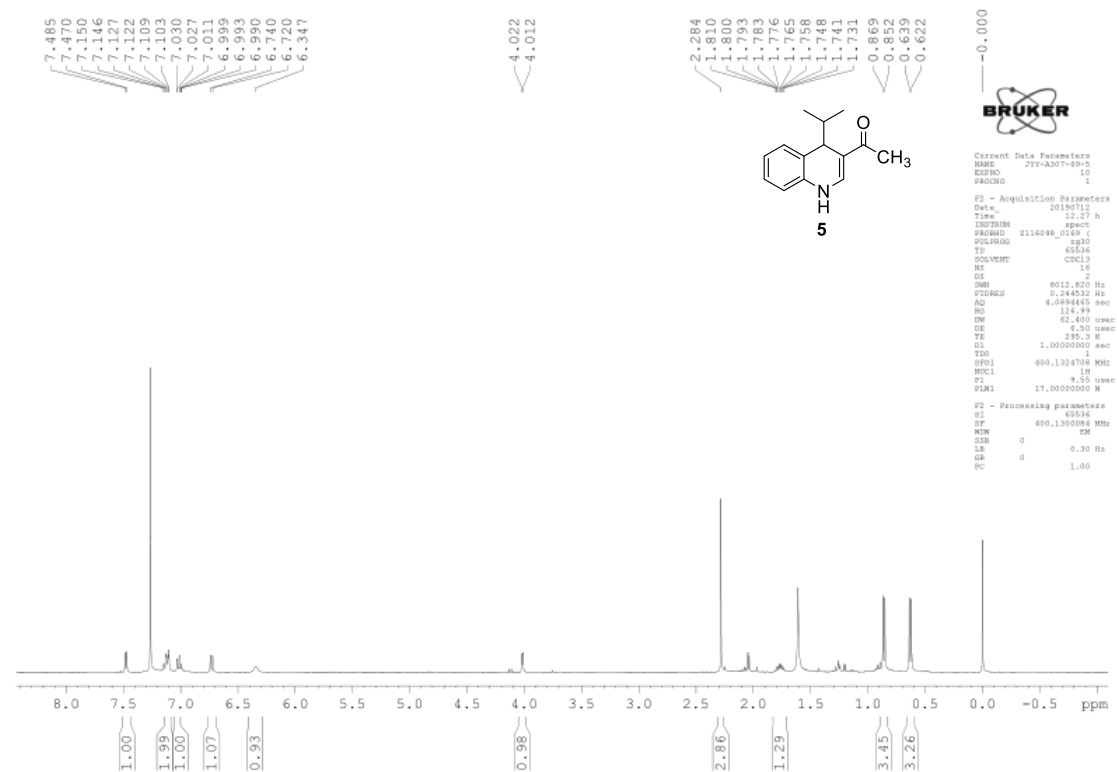




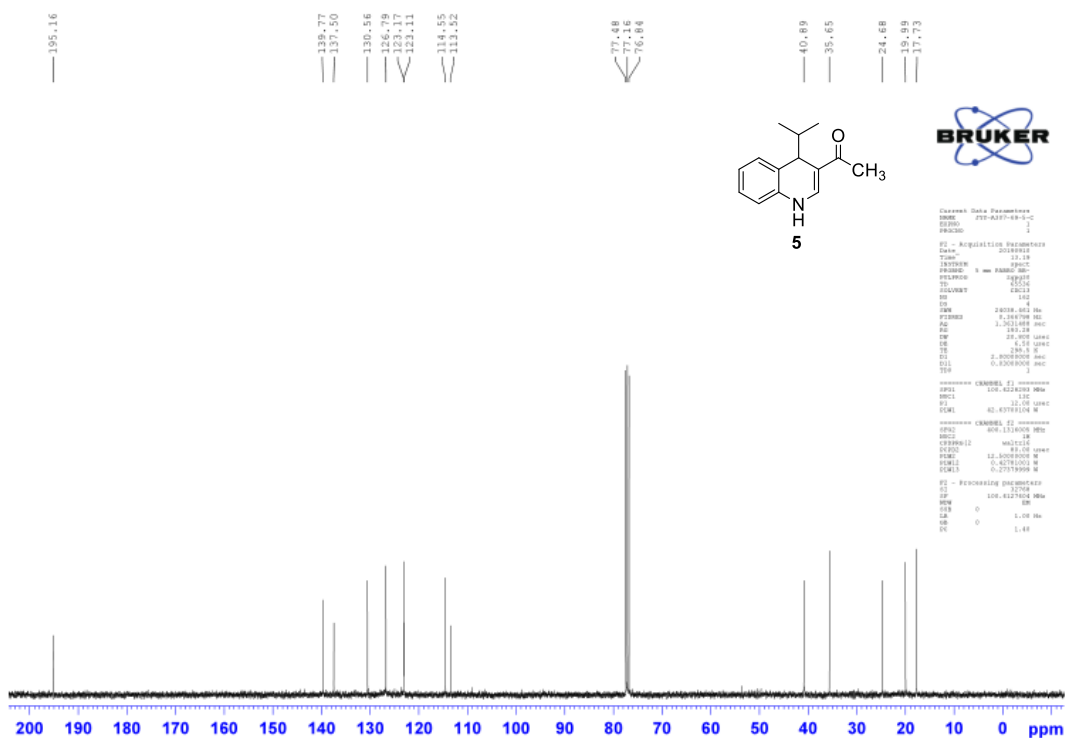
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SUPPORTING INFORMATION

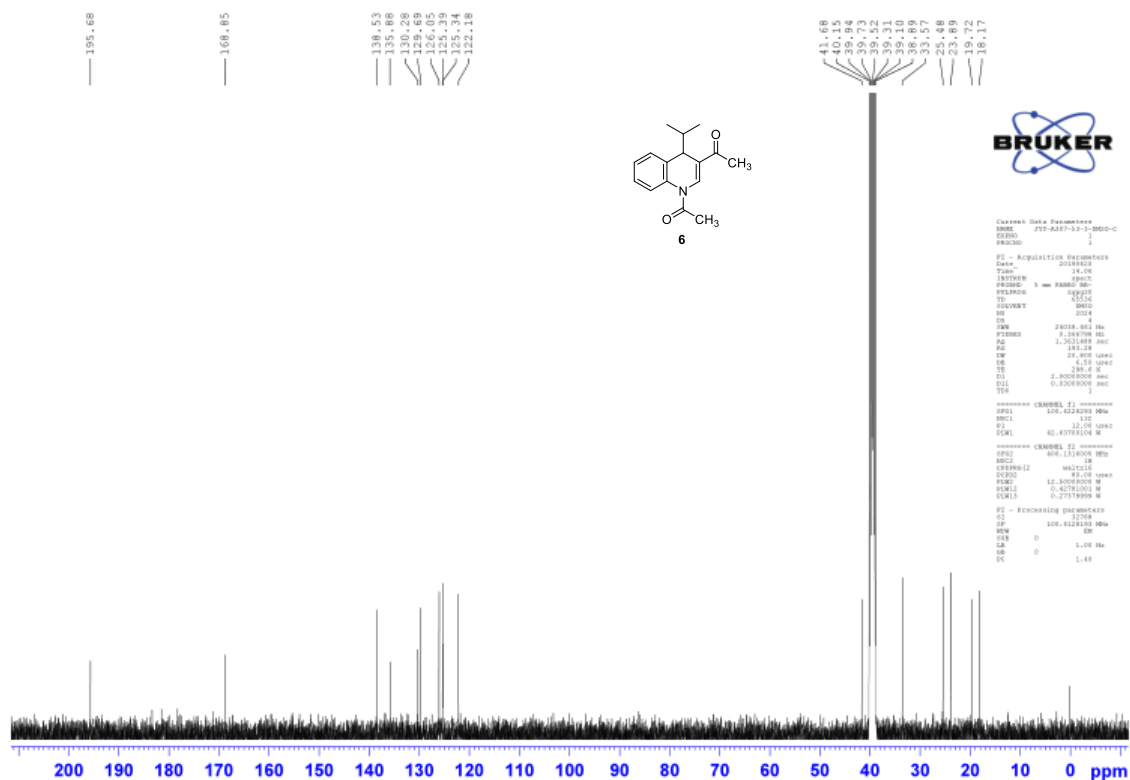
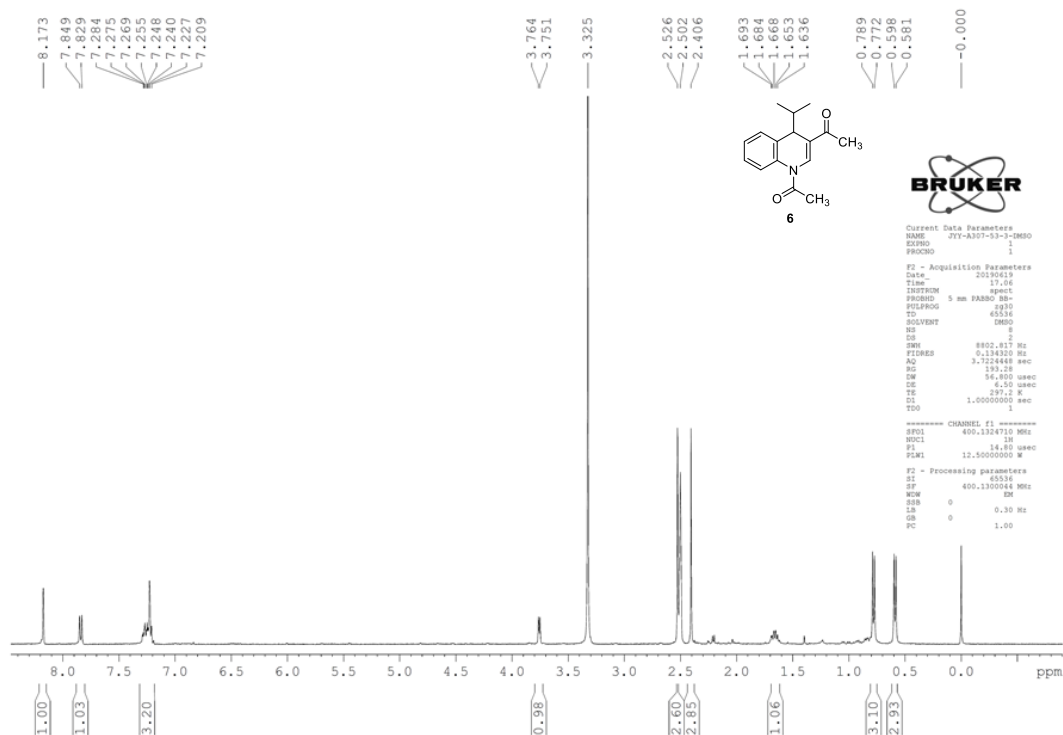


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 PROCNO: 1
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 Time: 12.27 h
 INSTRUM: spect
 PROBM40: E114098_0149 (4
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 16
 DS: 4
 SWH: 8012.820 Hz
 FIDRES: 0.244532 Hz
 AQ: 4.0898463 sec
 RG: 114.89
 FM: 62.450 usec
 DE: 6.50 usec
 TE: 300.2 K
 D1: 1.00000000 sec
 DELTA: 1
 RFDR1: 600.1324709 MHz
 WDC1: 18
 P1: 9.50 usec
 PLW1: 17.00000000 W
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 SF: 600.1300984 MHz
 NUC: 13
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 RB: 1.00

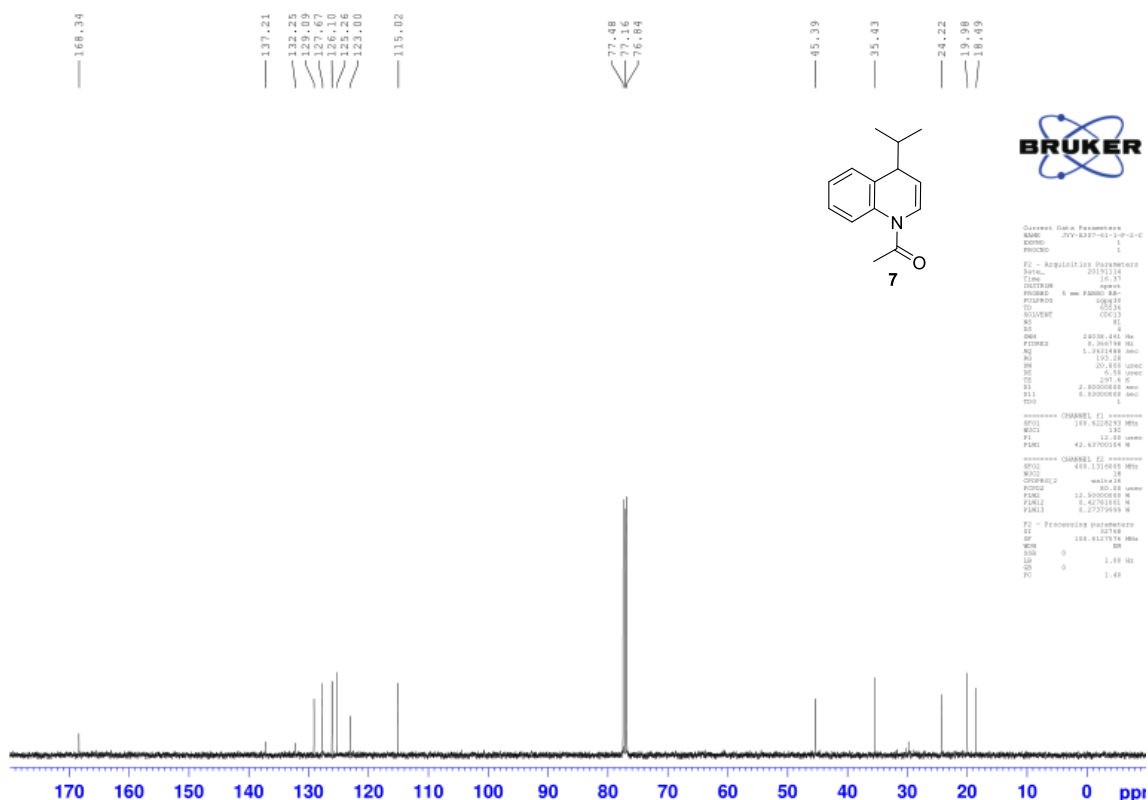
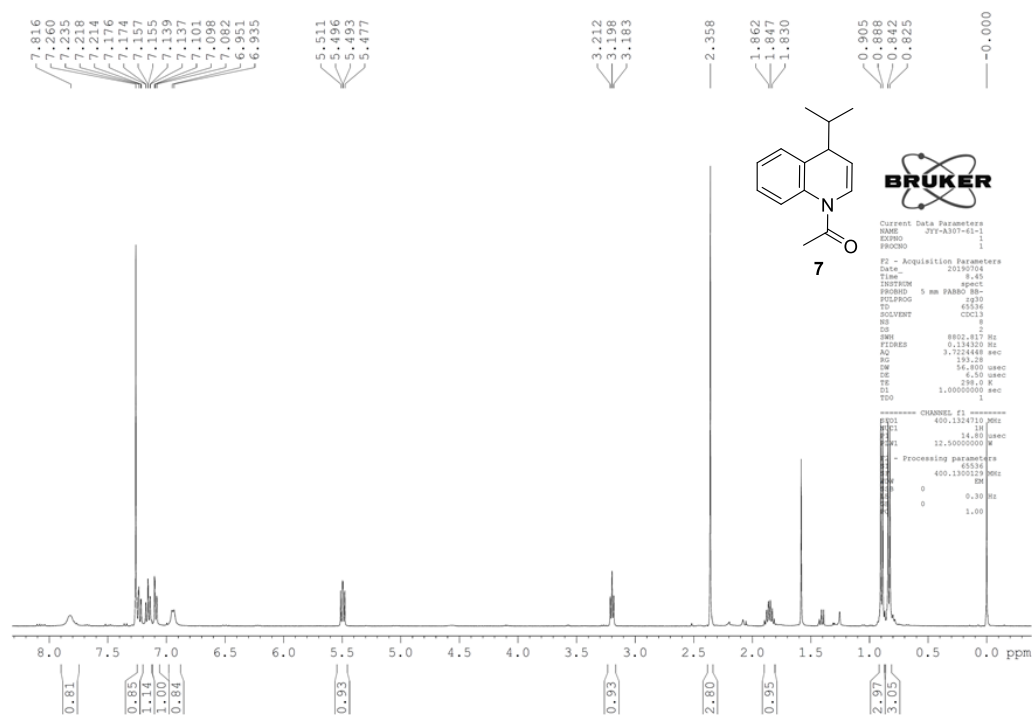


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 Time: 12.19 h
 INSTRUM: spect
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 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 16
 DS: 4
 SWH: 24038.402 Hz
 FIDRES: 0.180708 Hz
 AQ: 1.2613485 sec
 RG: 183.18
 FM: 27.907 usec
 DE: 6.10 usec
 TE: 300.2 K
 D1: 2.00000000 sec
 DELTA: 0.20000000 sec
 RFDR1: 100.6224200 MHz
 WDC1: 12
 P1: 12.00 usec
 PLW1: 62.63767104 W
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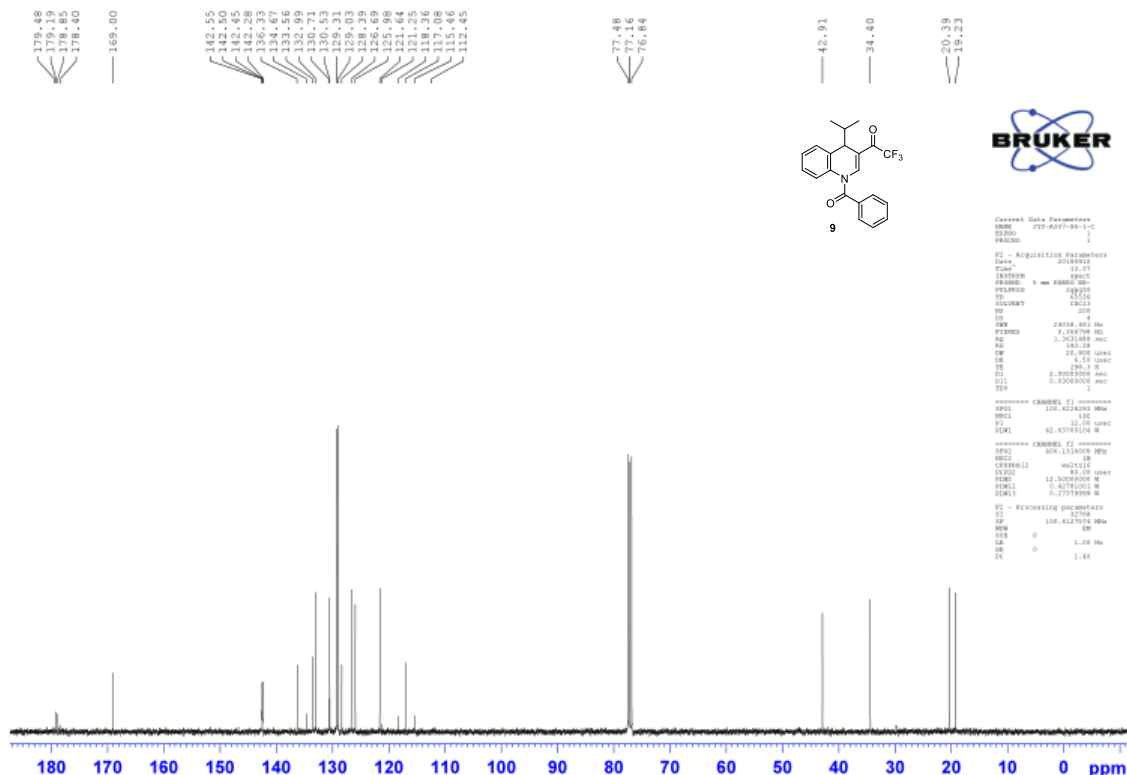
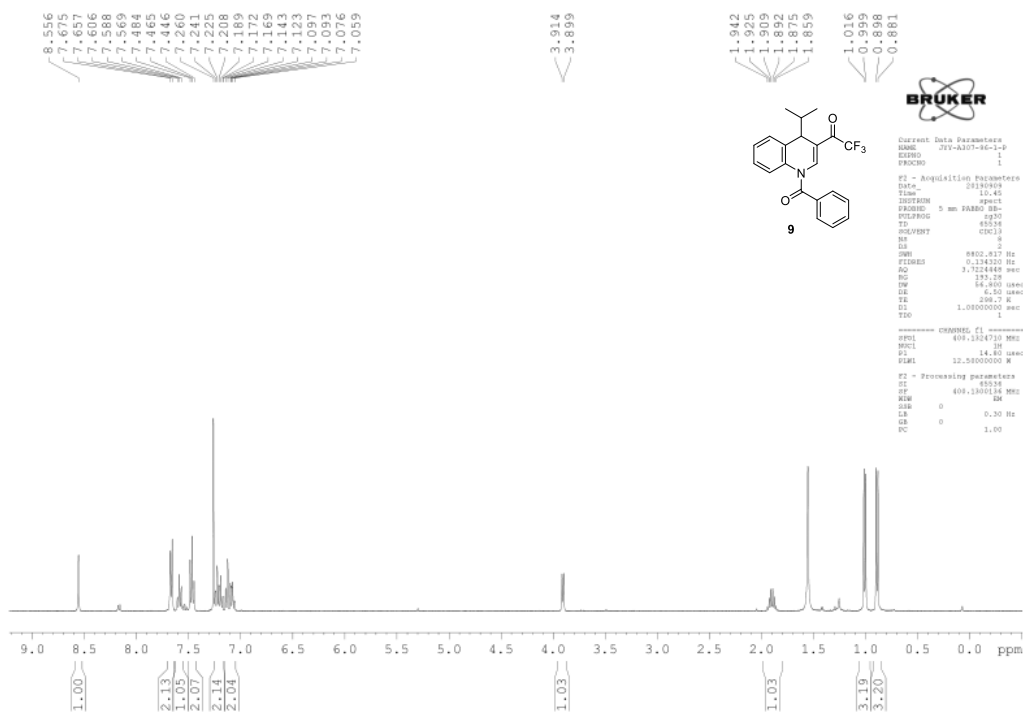
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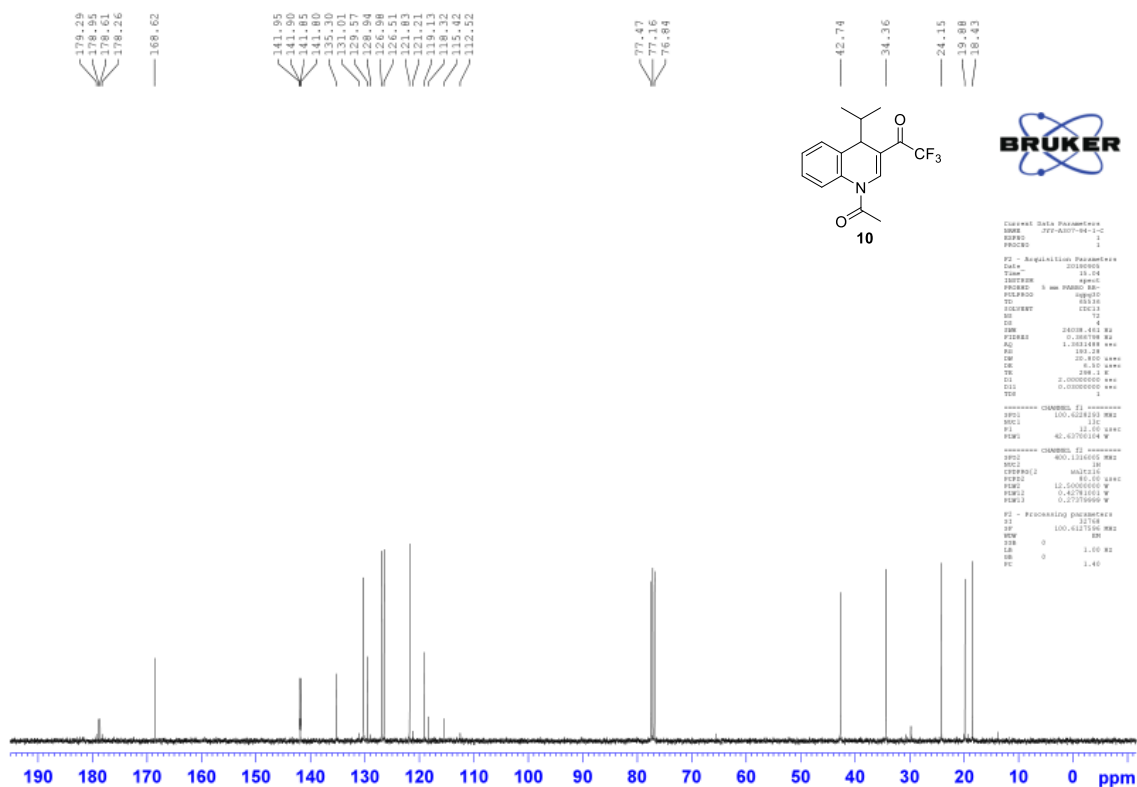


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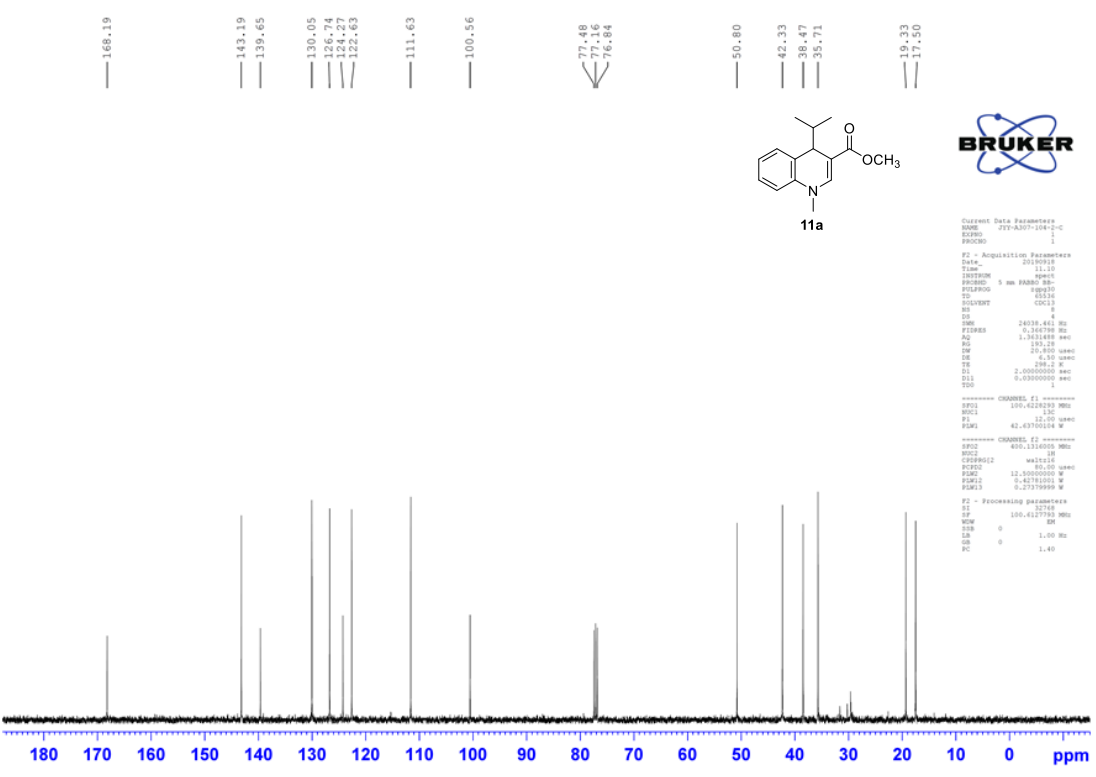
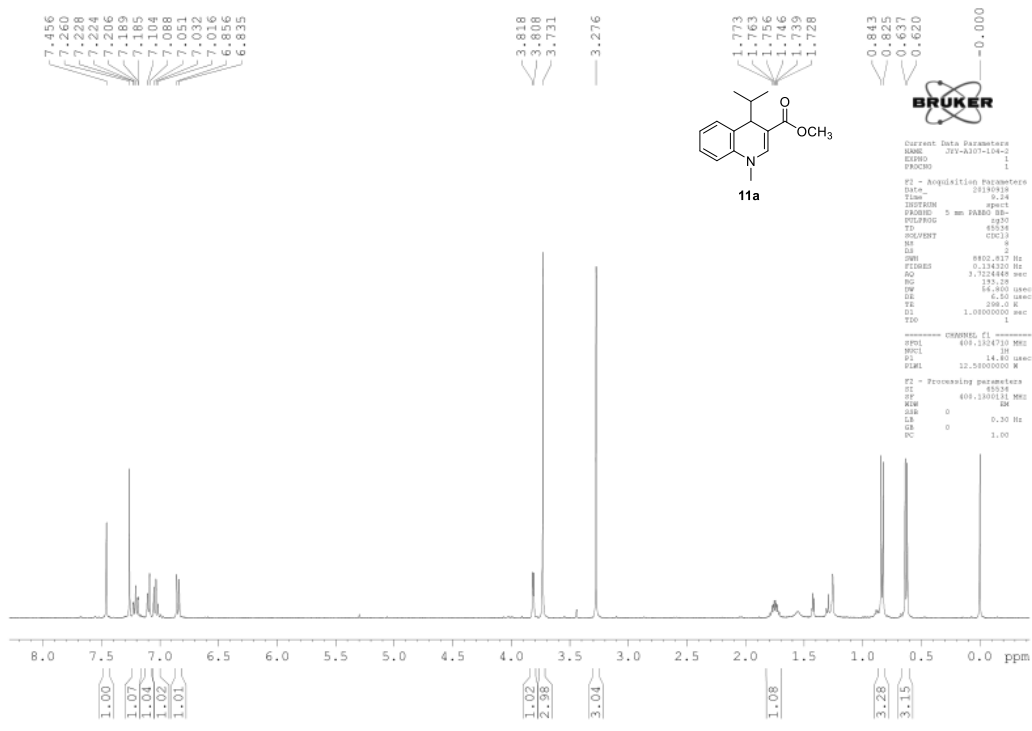


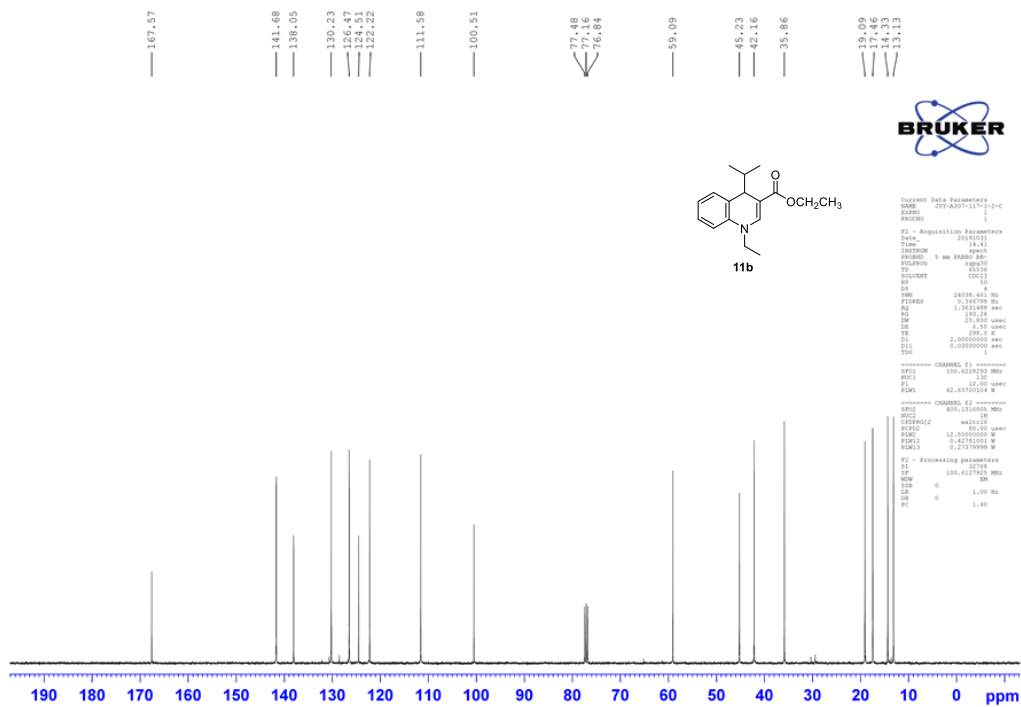
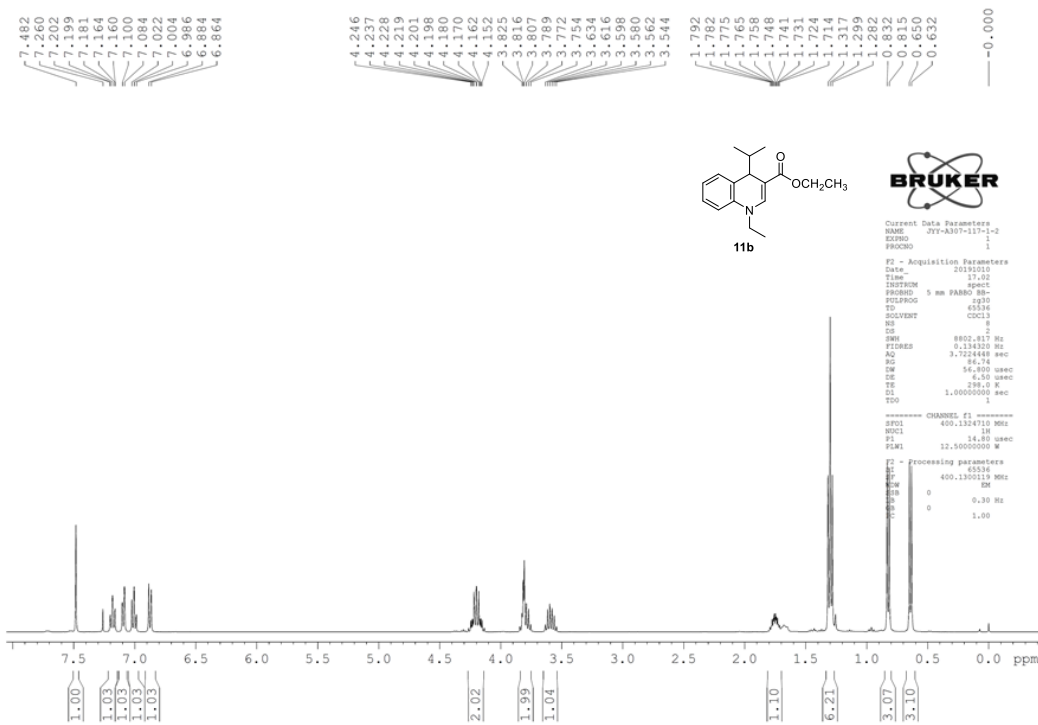
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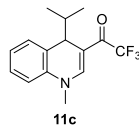




SUPPORTING INFORMATION





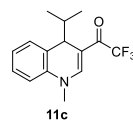
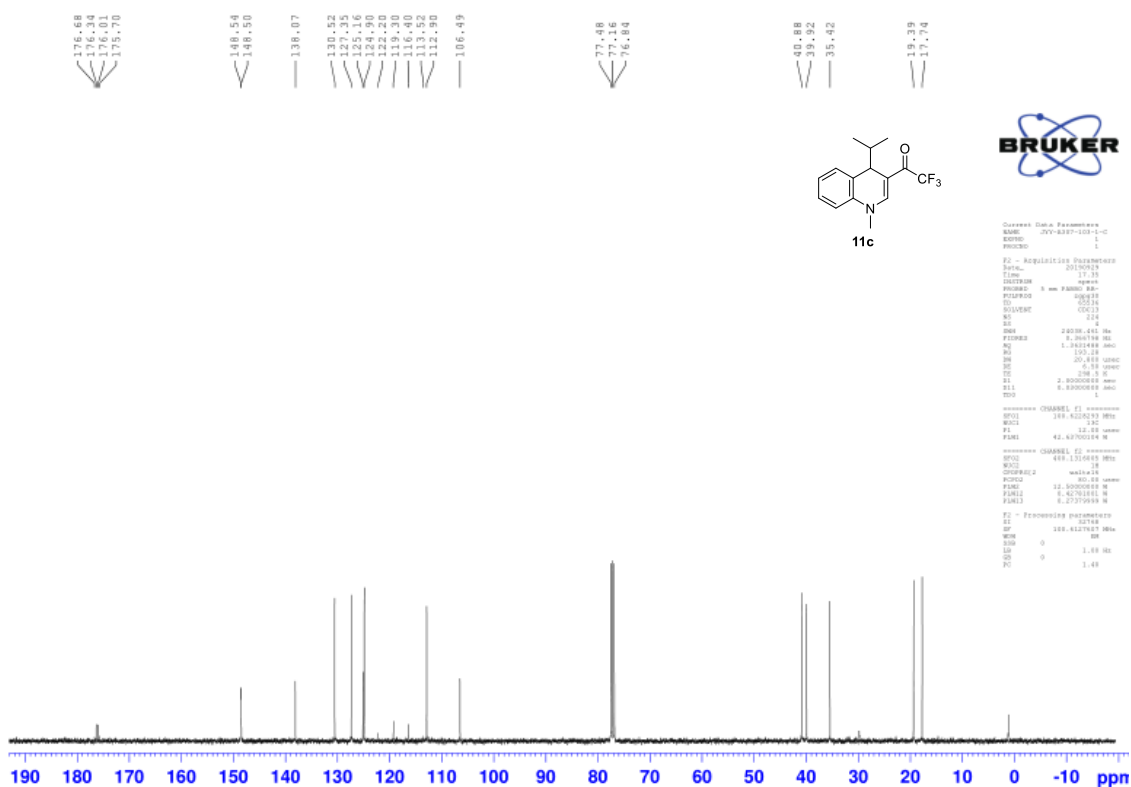


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PROCNO       1

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PROBHD        5 mm FATHO BB-
PULPROG       zg30
SOLVENT       CDCl3
NS            638
DS            2
SWH            8802.217 Hz
FIDRES        0.134320 Hz
AQ            3.7224448 sec
RG            193.28
CW            56,800 uses
DE            6.50 uses
TE            298.0 K
D1            1.00000000 sec
TDG           1

```



```

Current Data Parameters
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EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20190919
Time      17.39
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         224
DS         4
SWH         24238.481 Hz
FIDRES     0.3661980 Hz
AQ         1.3621488 sec
RG          192.28
SR         20.418 cm-1
SC         6.58 umax
TE         298.5 K
DE         2.00000000 mmol
D11        0.30000000 mmol
D12         1.00
D13         1.00

```

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SF01      100.6226293 MHz
WAC1      13C
F1         12.00 us/cm
FLM1      42.62700104 M
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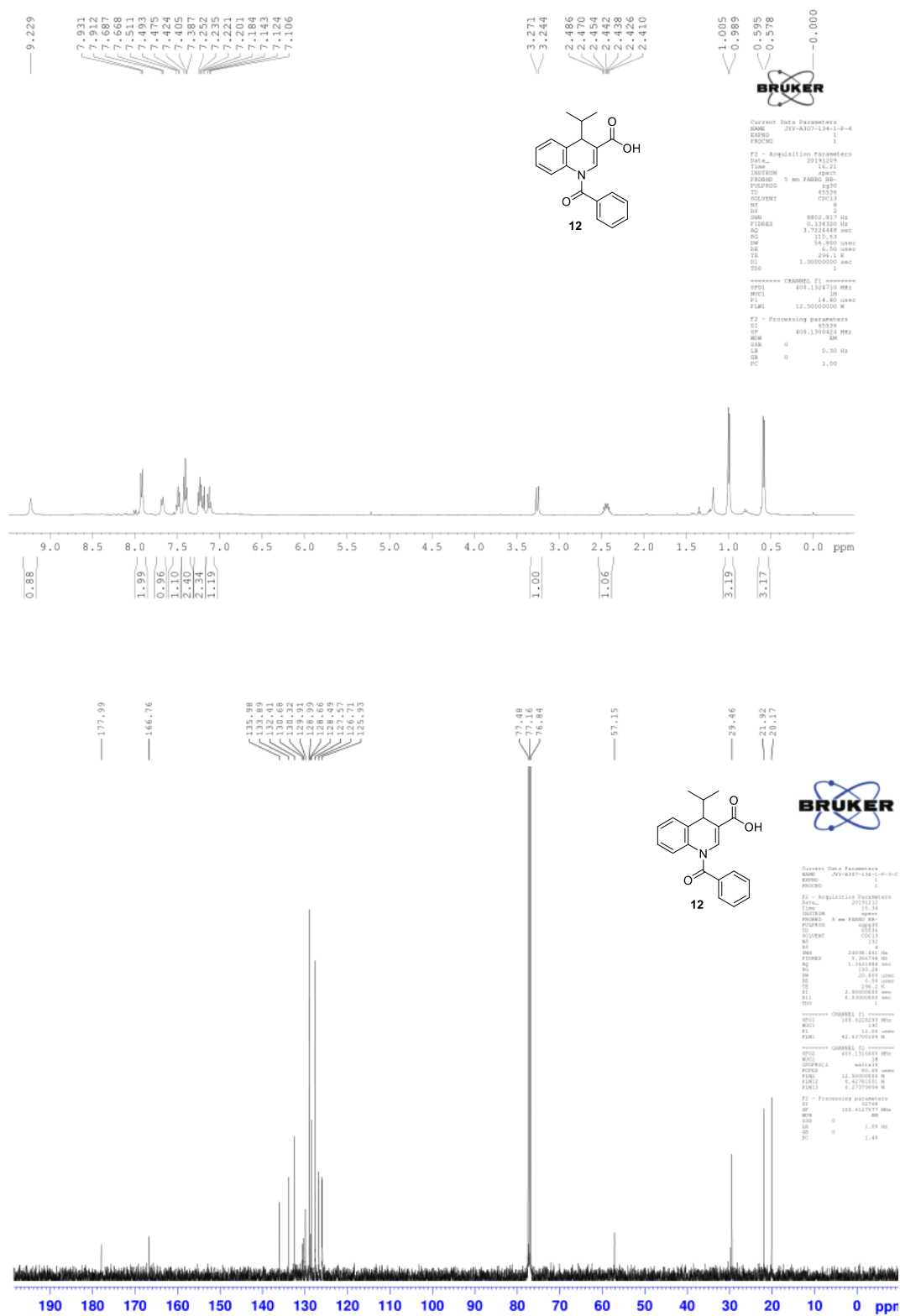
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***** CHANNEL F2 *****
SFO2      449.131645 MHz
WAG2      1M
CFOFREQ2   50000000 Hz
PCFO2      80.00 kHz
PLM1      12.50000000 M
PLM2      0.42701601 M
PLM3      0.27379999 M

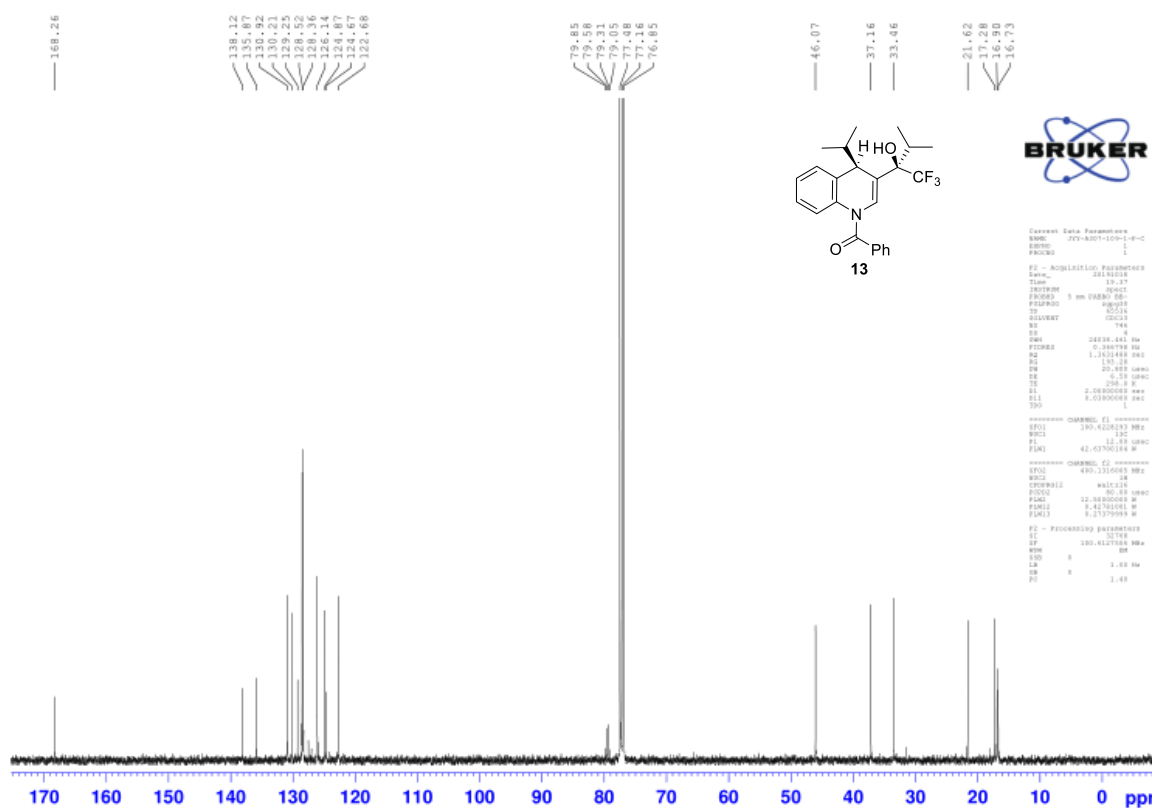
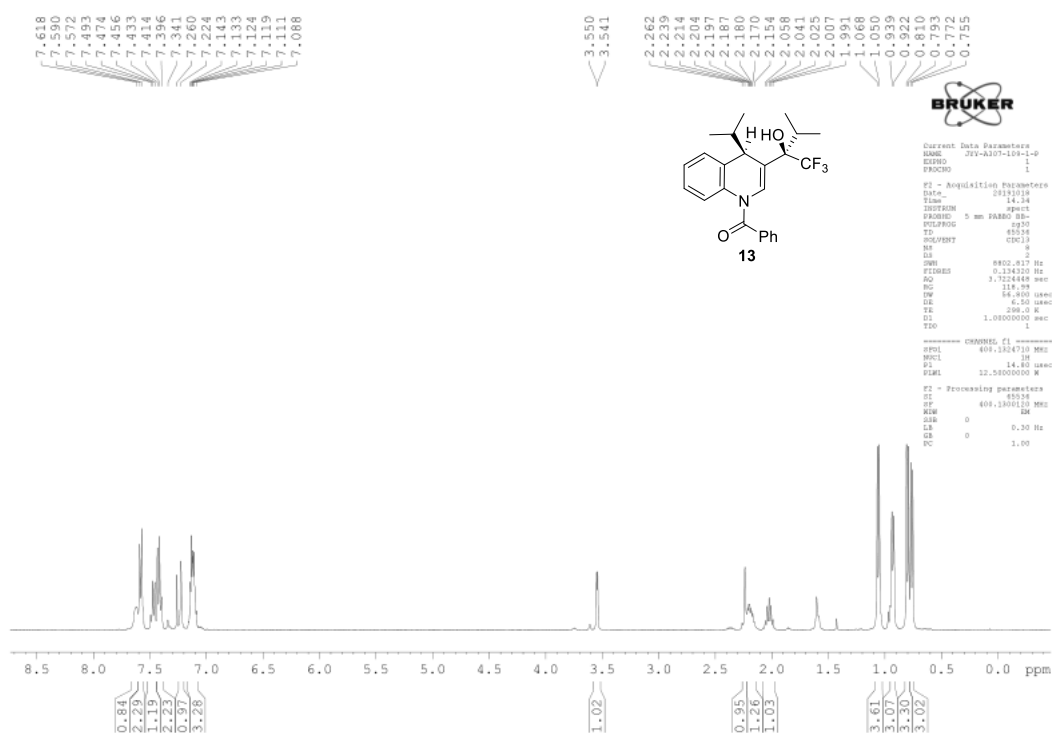
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WOM		SR
SIG	0	
LR		1.00 Hz
GS	0	
PC		1.48

SUPPORTING INFORMATION

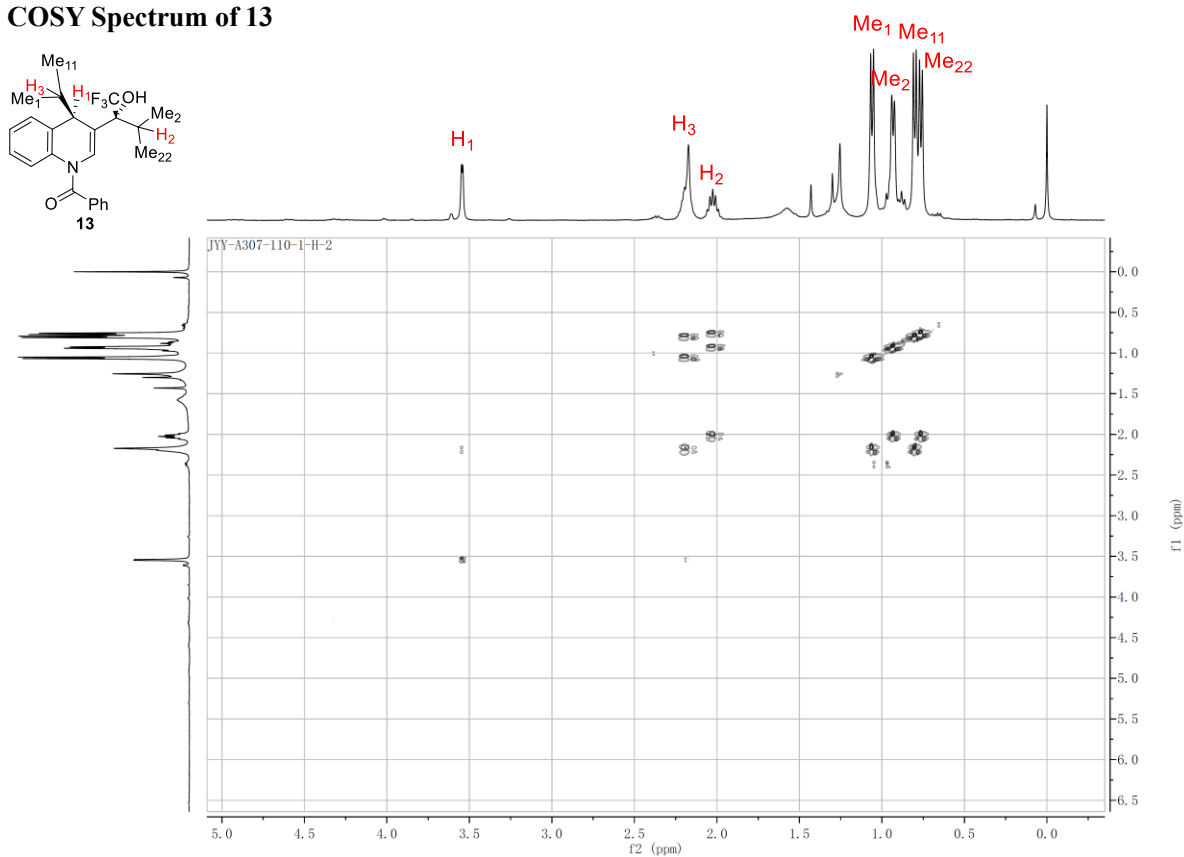


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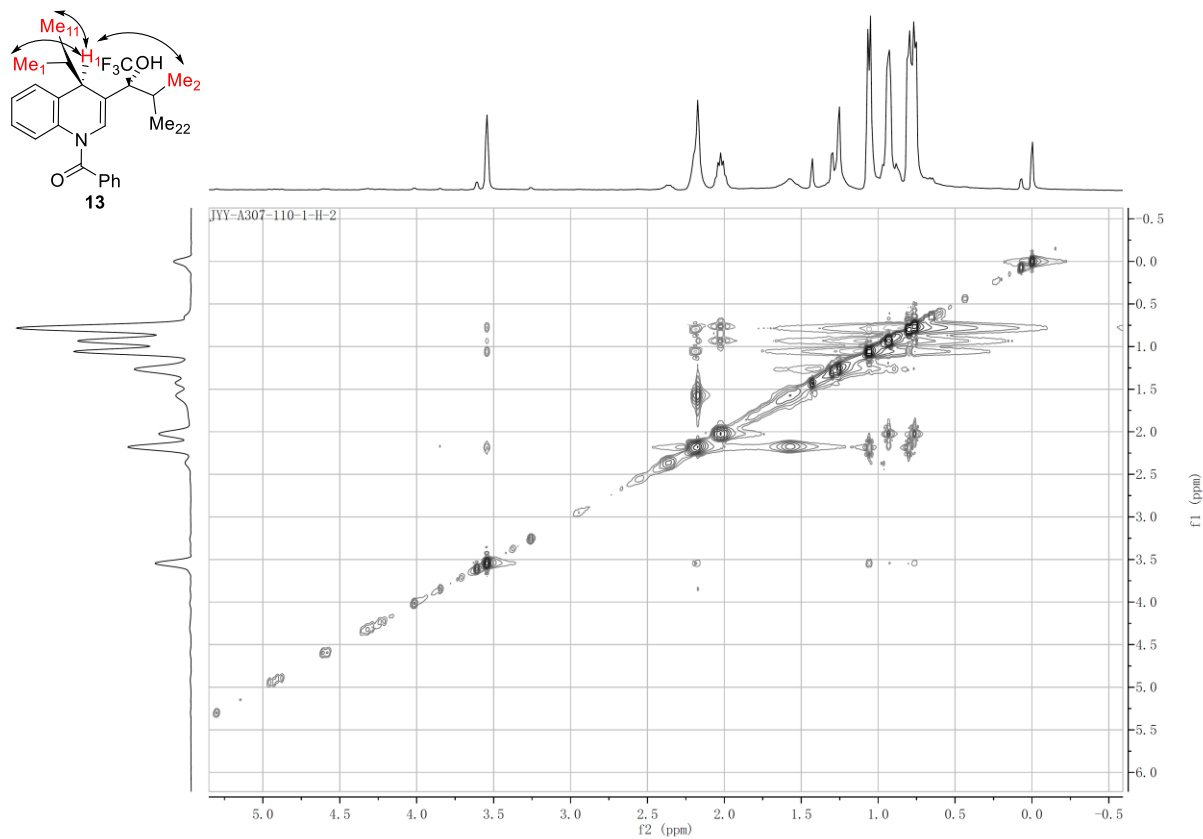


SUPPORTING INFORMATION

COSY Spectrum of 13



NOESY Spectrum of 13



2. Rationalization of the relative stereo configuration of 13

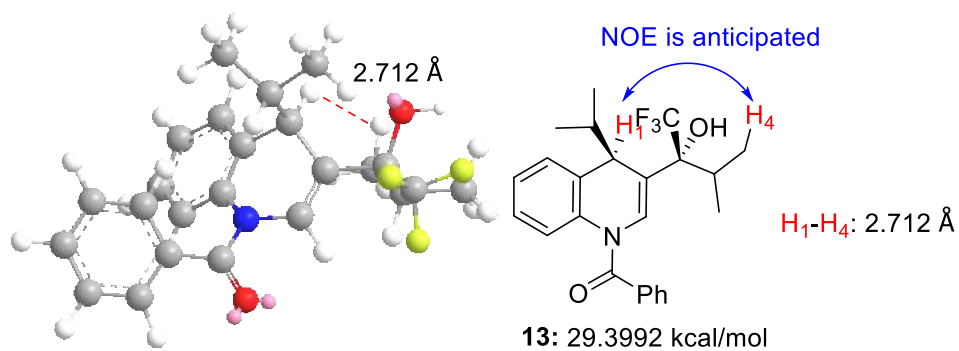
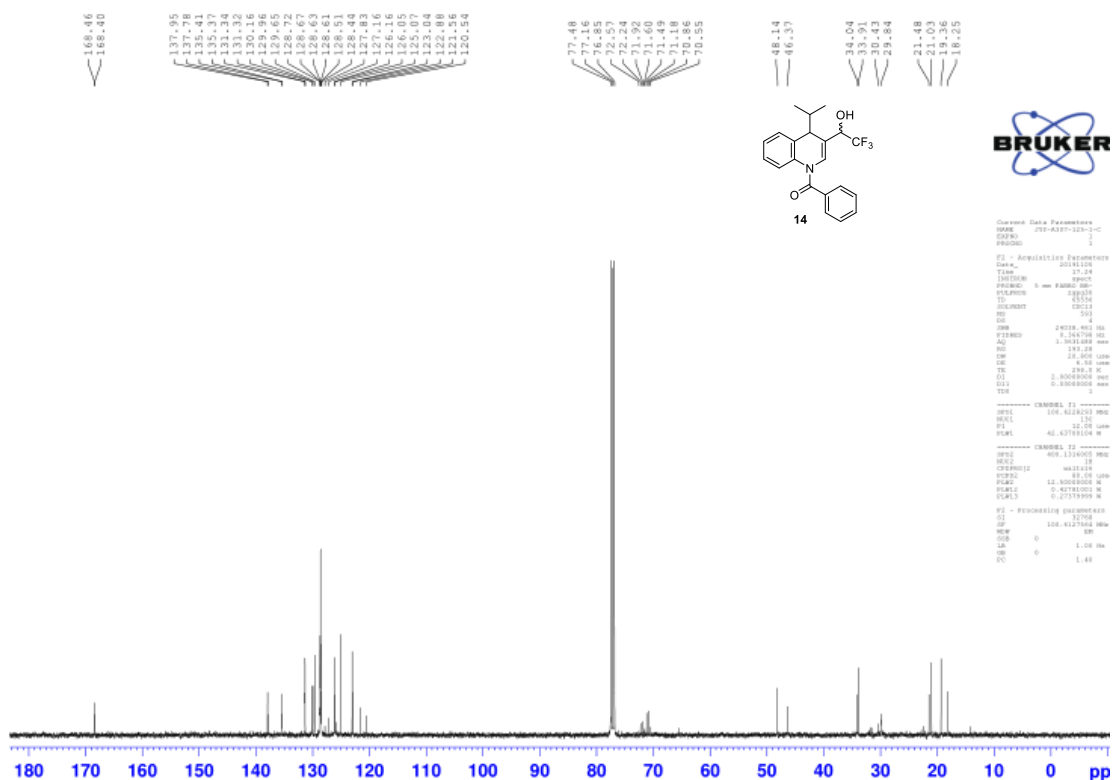
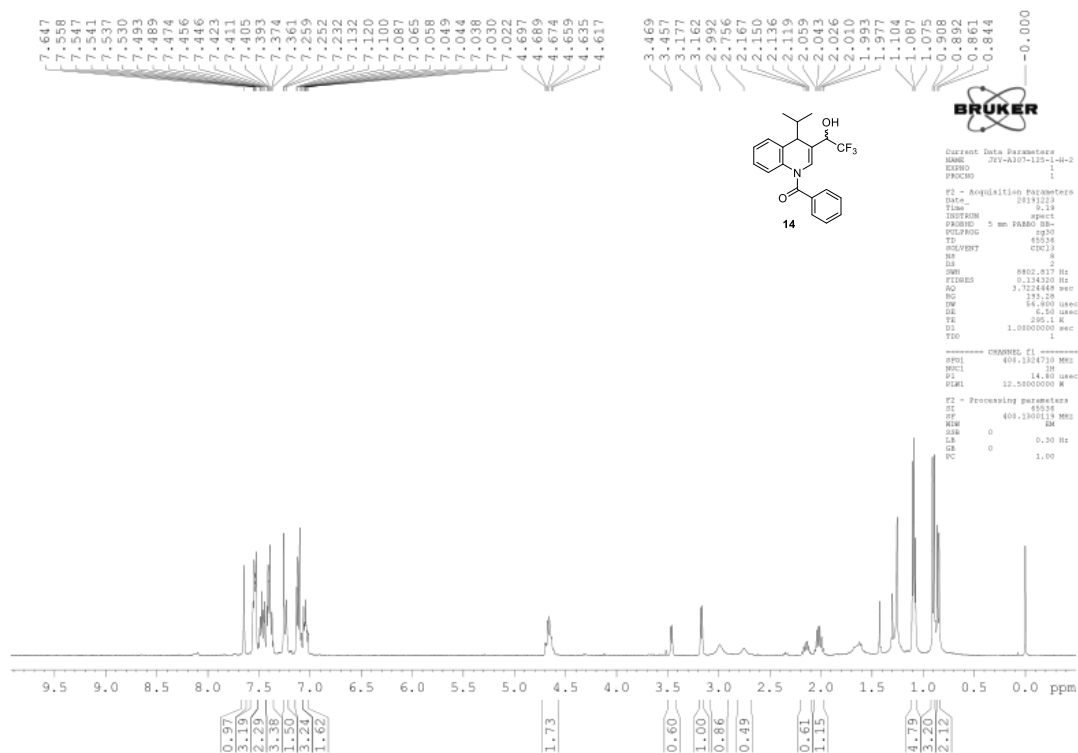
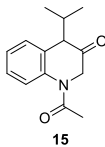


Fig.1 Most stable conformation of **13** calculated by ChemDraw 14.0 3D

SUPPORTING INFORMATION

3. Copy of NMR spectrum for 14-19

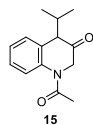




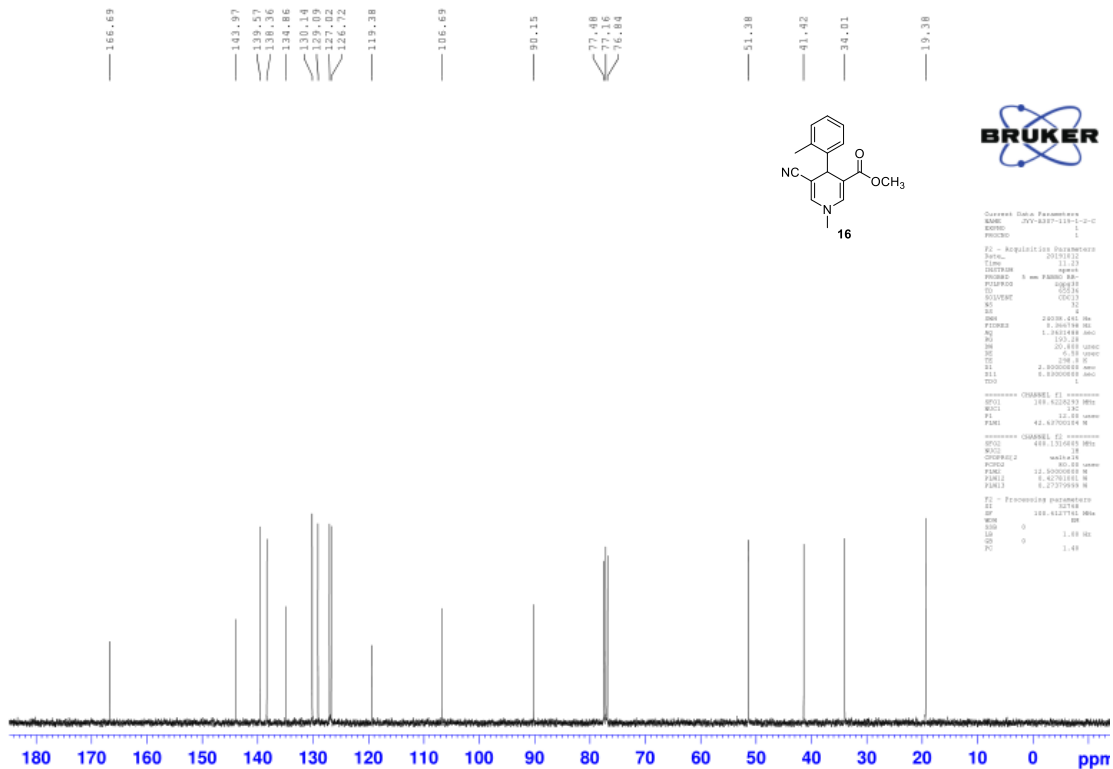
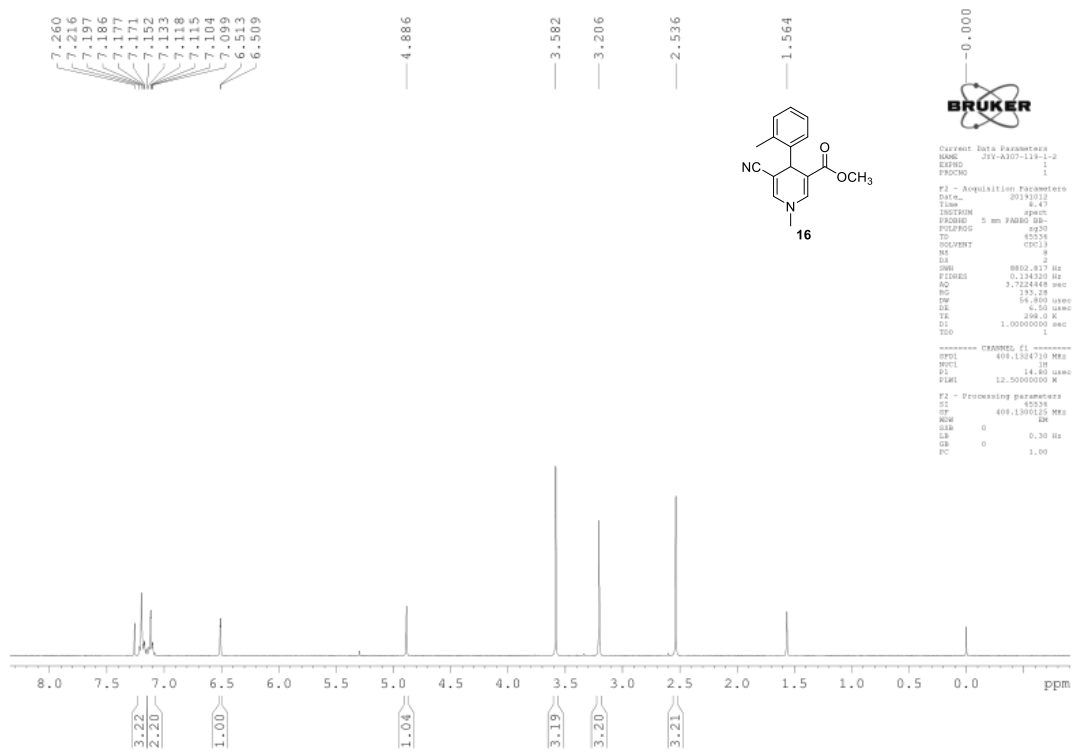
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EPIFNO       1
PROCNO       1

F2 - Acquisition Parameters
TIME          2819.916
SOURCES      aspect
PROBHD       5 mm PABBO Hb-
PULPRG       zps30
TD           65536
AQ           0.7610
NS           8
DS           8
SWH          8802.017 Hz
FTDRES       0.134230 Hz
SF           3.7224488e+08
AQ           185.28
SQ           66.800 (use)
SR           6.50 (use)
TR           298.0 Hz
DI           1.00000000 Mac
TDO         -
----- CHANNEL F1 -----
MPC1         409.124274 MHz
MPC2         1M
MPC3         14.80 (use)
FREQ1        22.50000000 M

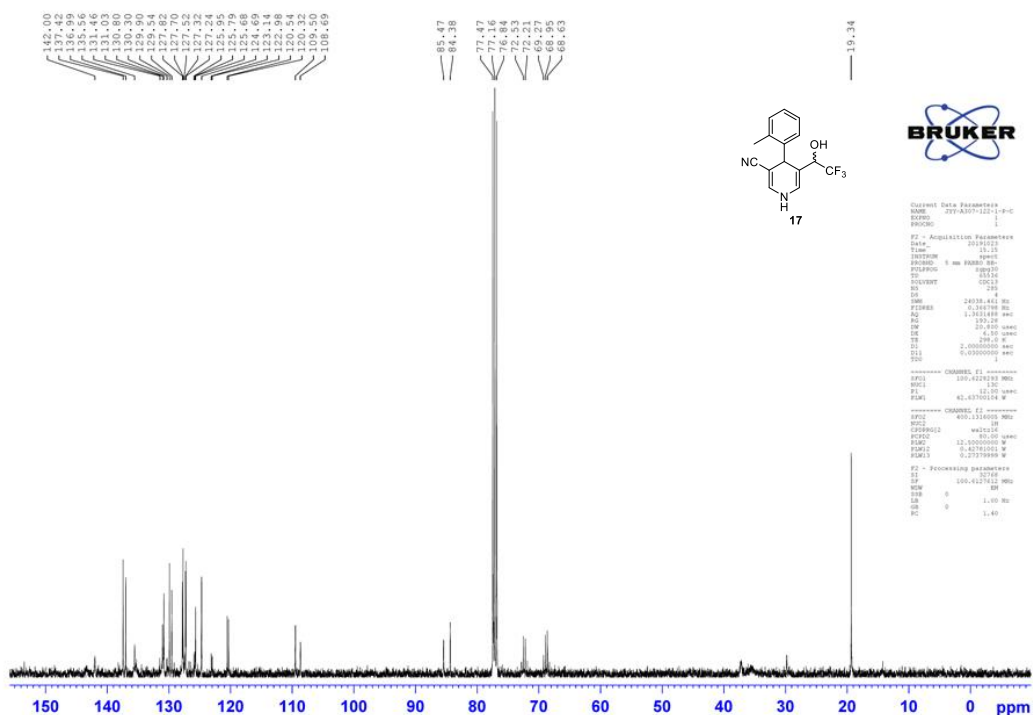
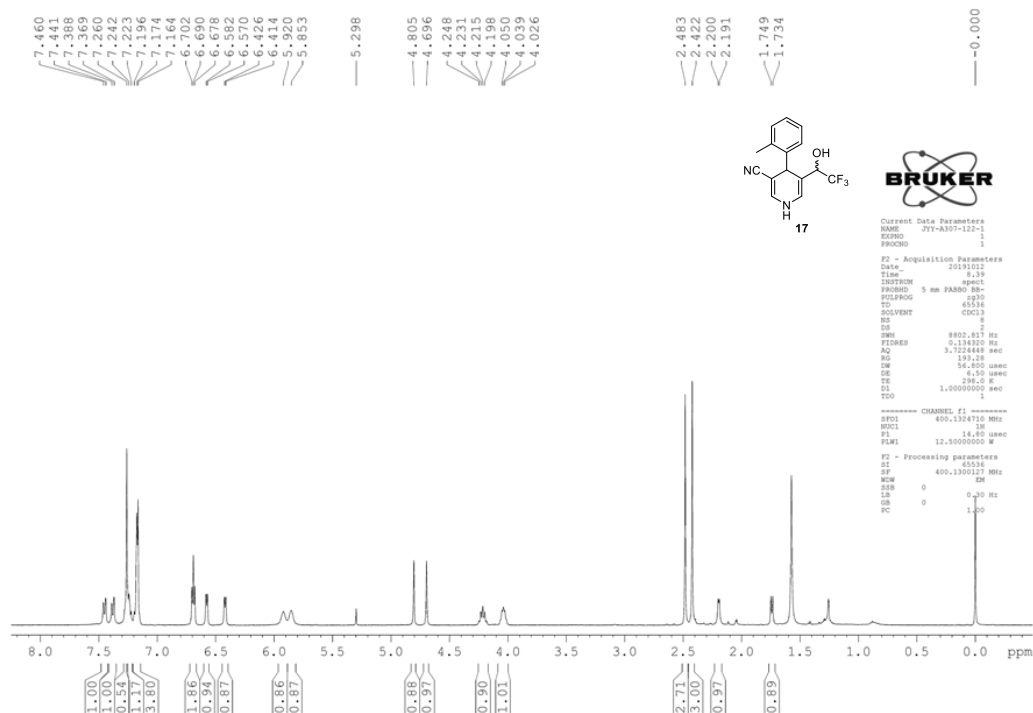
F2 - Processing parameters
MPC1         409.124274 MHz
RF           409.1300130 MHz
NUC1         31
LB           0
GB           0
LS           0
SB           0
TB           0
```

[illegible]

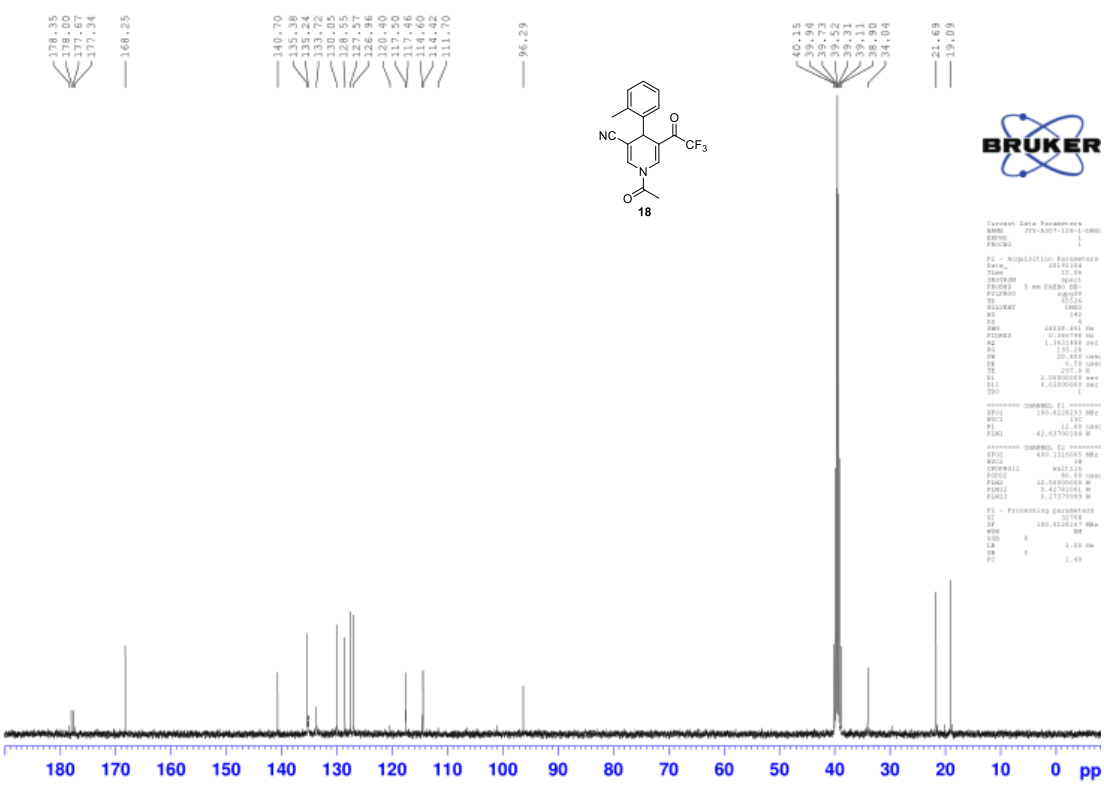
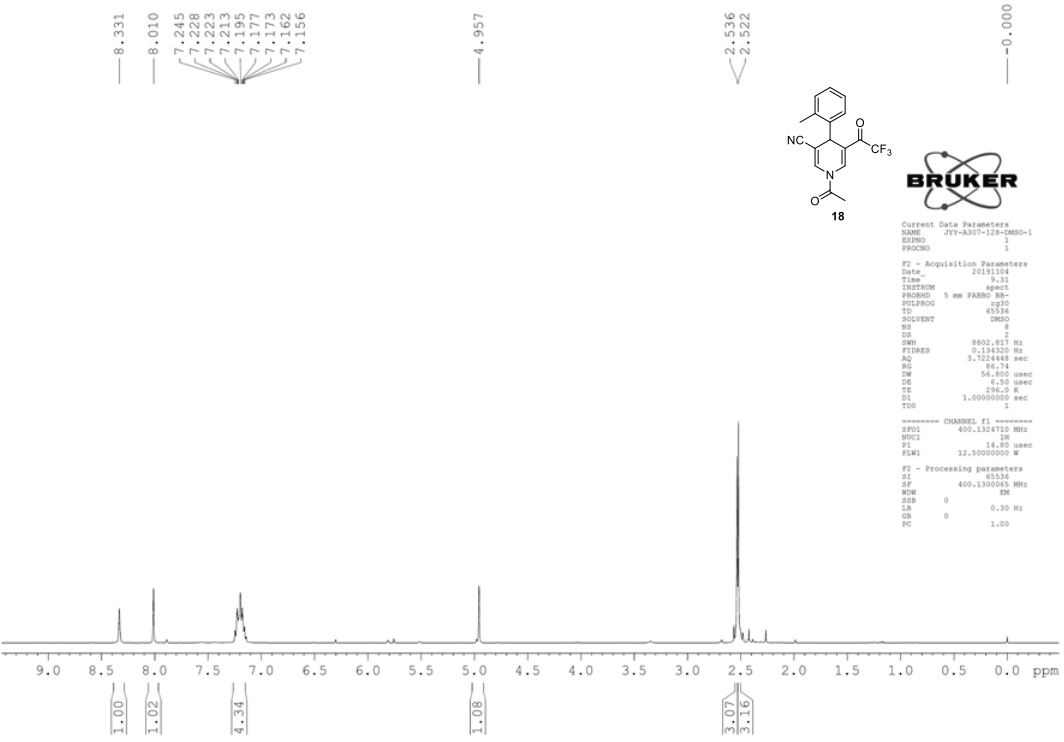
SUPPORTING INFORMATION



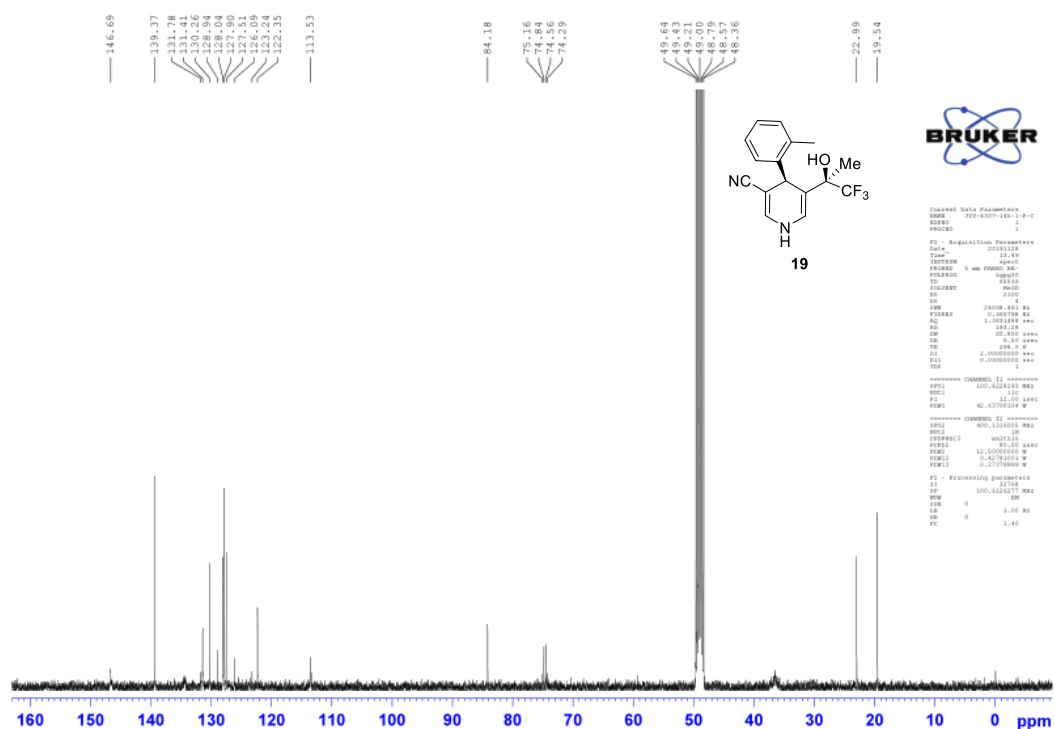
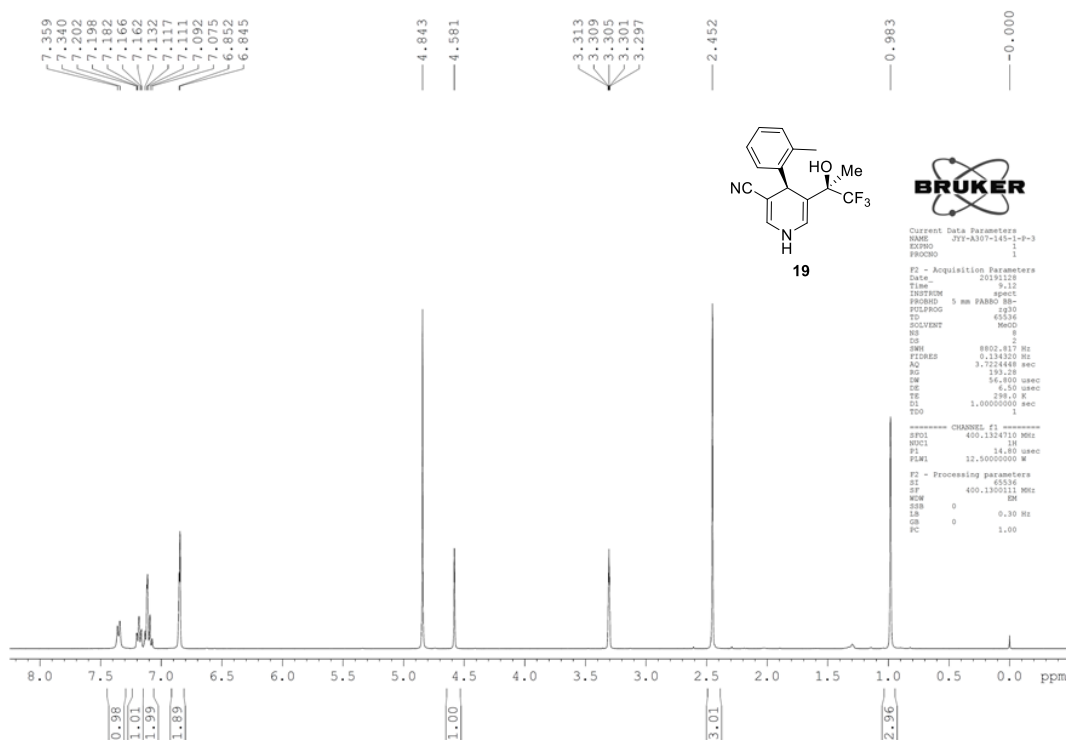
SUPPORTING INFORMATION



SUPPORTING INFORMATION

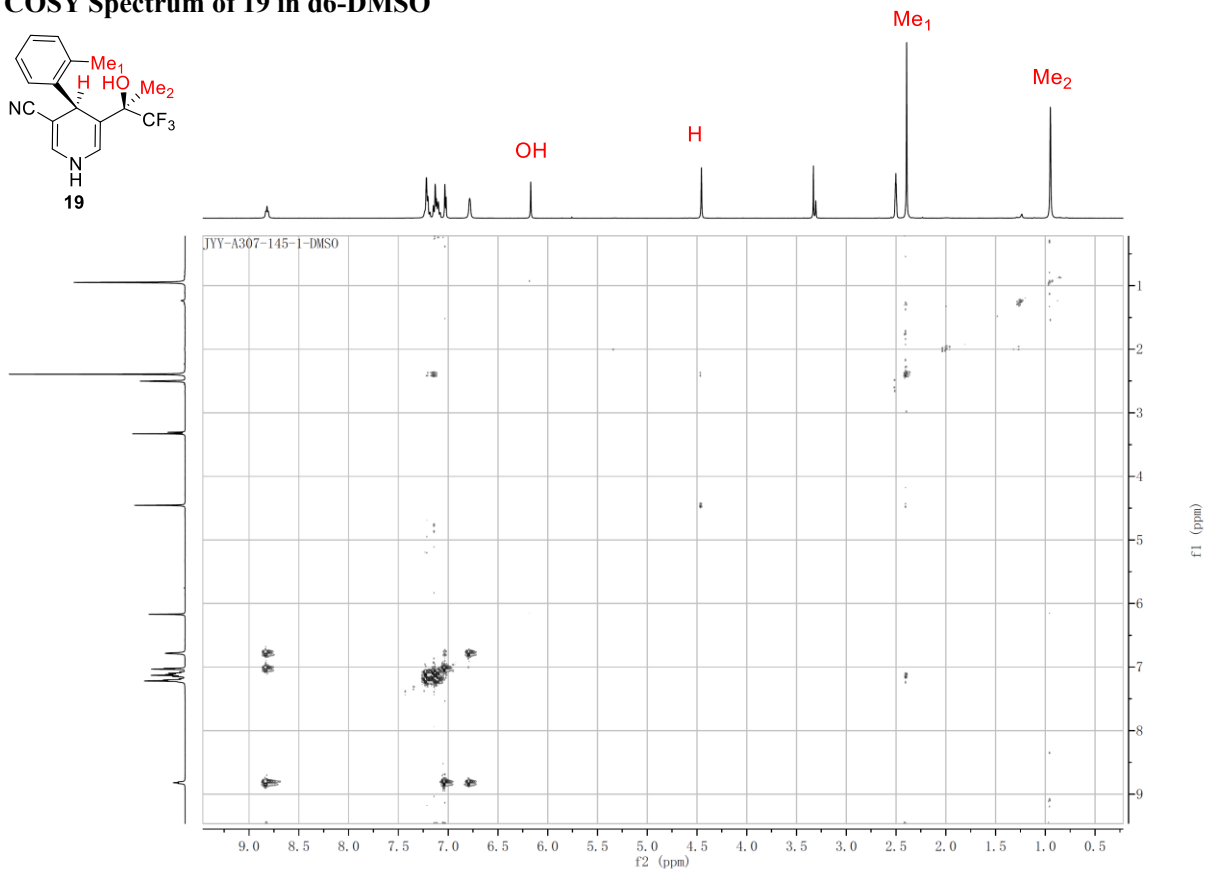


SUPPORTING INFORMATION

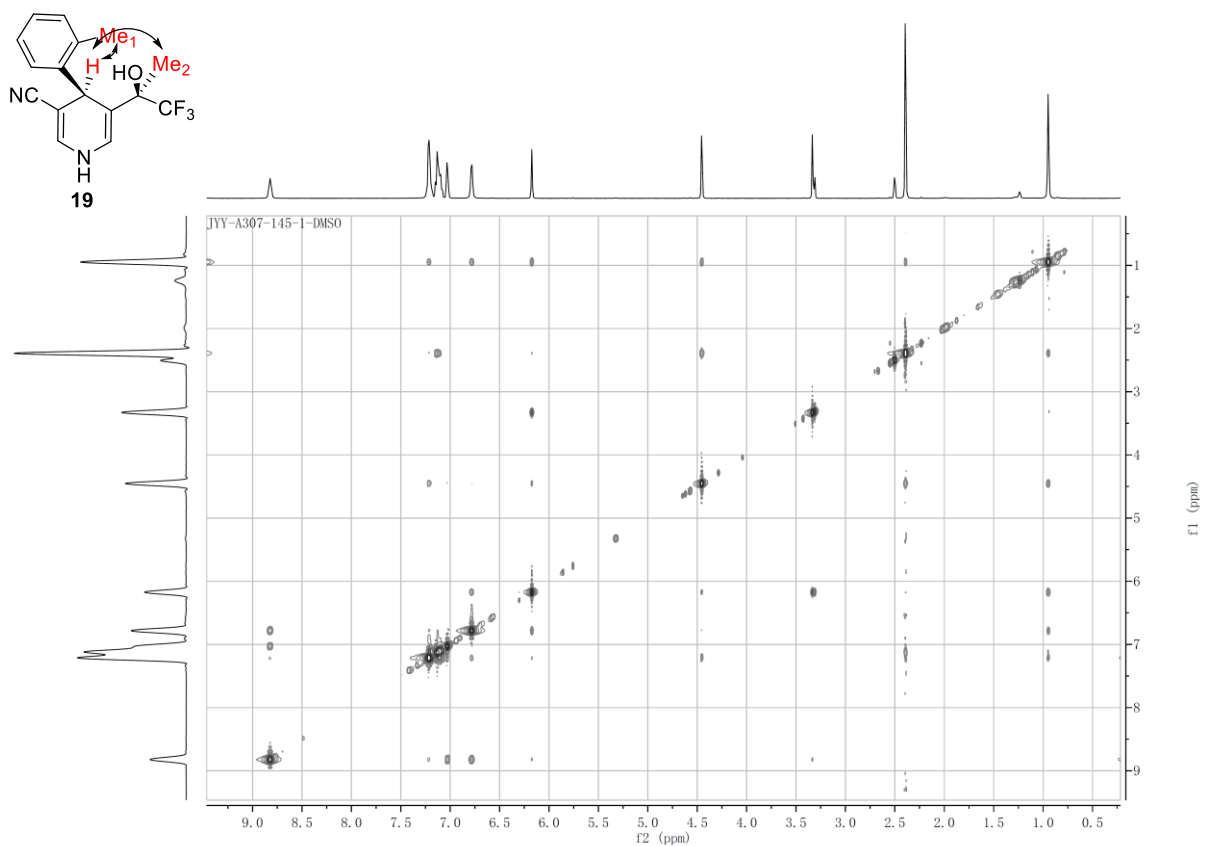


SUPPORTING INFORMATION

COSY Spectrum of 19 in d6-DMSO



NOESY Spectrum of 19 in d6-DMSO



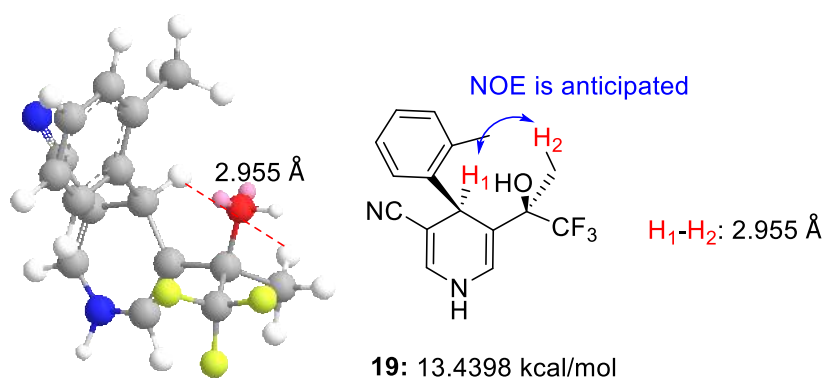
4. Rationalization of the relative stereo configuration of **19**

Fig.2 Most stable conformation of **19** calculated by ChemDraw 14.0 3D