

New members of the *Cinchona* Alkaloids family: Assembly of the triazole heterocycle at the 6' position.

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ch.kleeberg@tu-braunschweig.de (C.K.), i.neda@tu-braunschweig.de (I.N.)

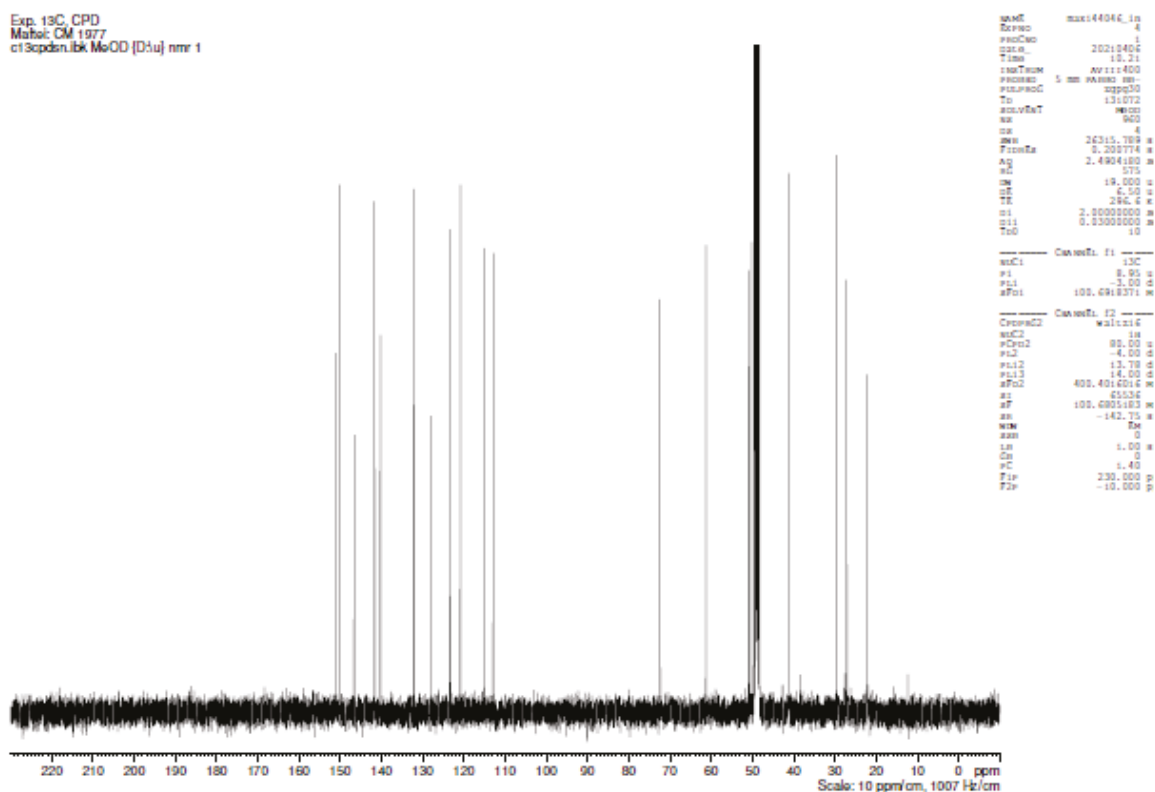
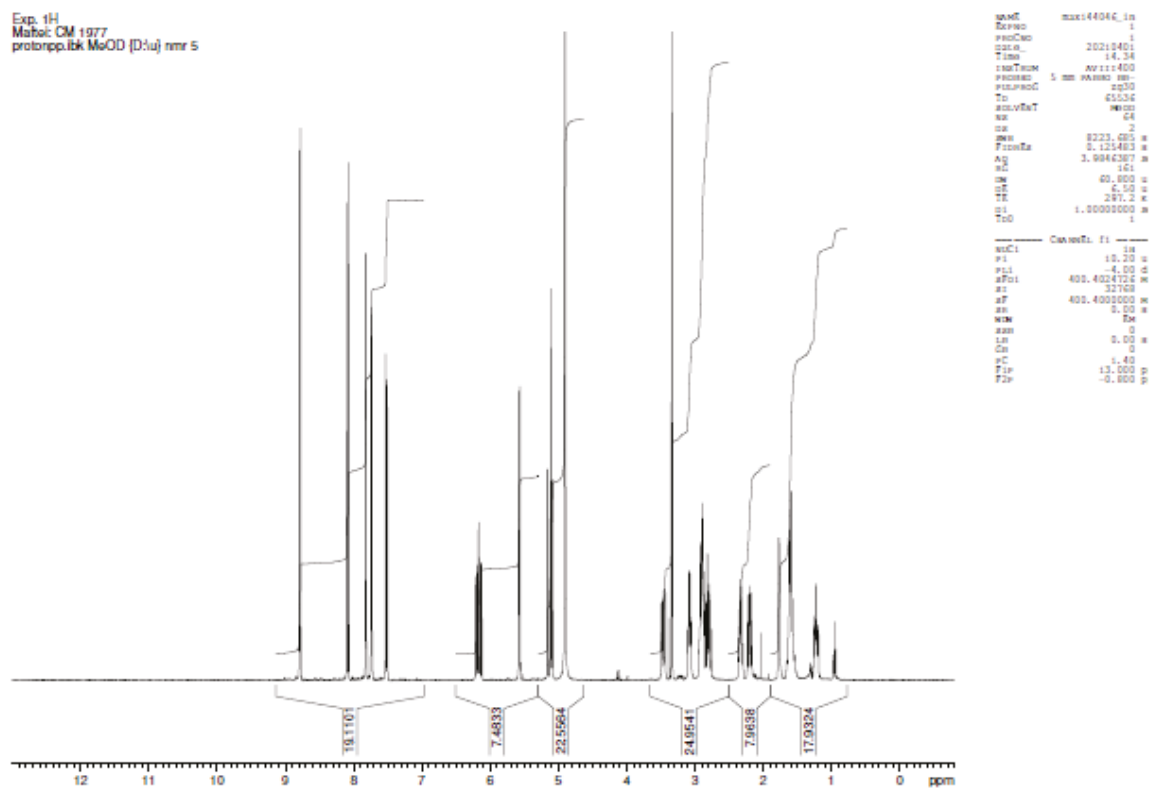
* Correspondence: i.neda@tu-braunschweig.de

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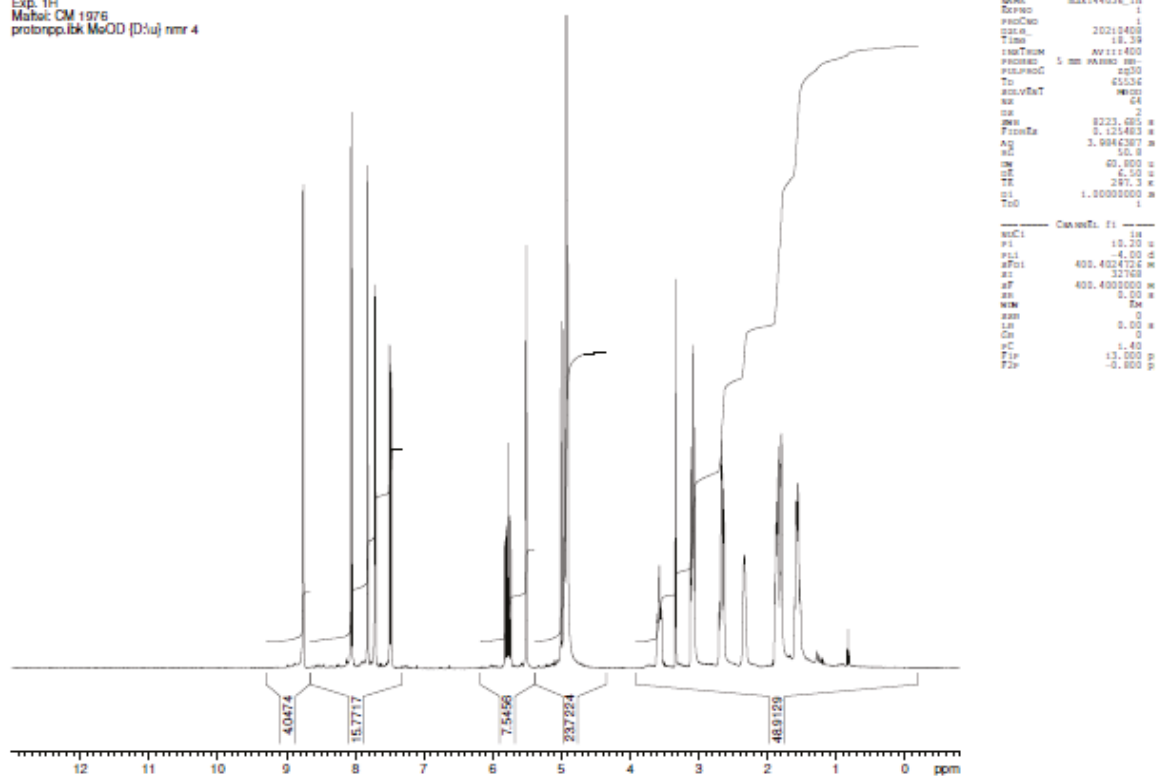
¹H- and ¹³C-NMR experiment

¹H- and ¹³C-NMR experiment for (S)-(6-azidoquinolin-4-yl)((1S,2R,4S,5R)-5-vinylquinuclidin-2-yl)methanol (8):

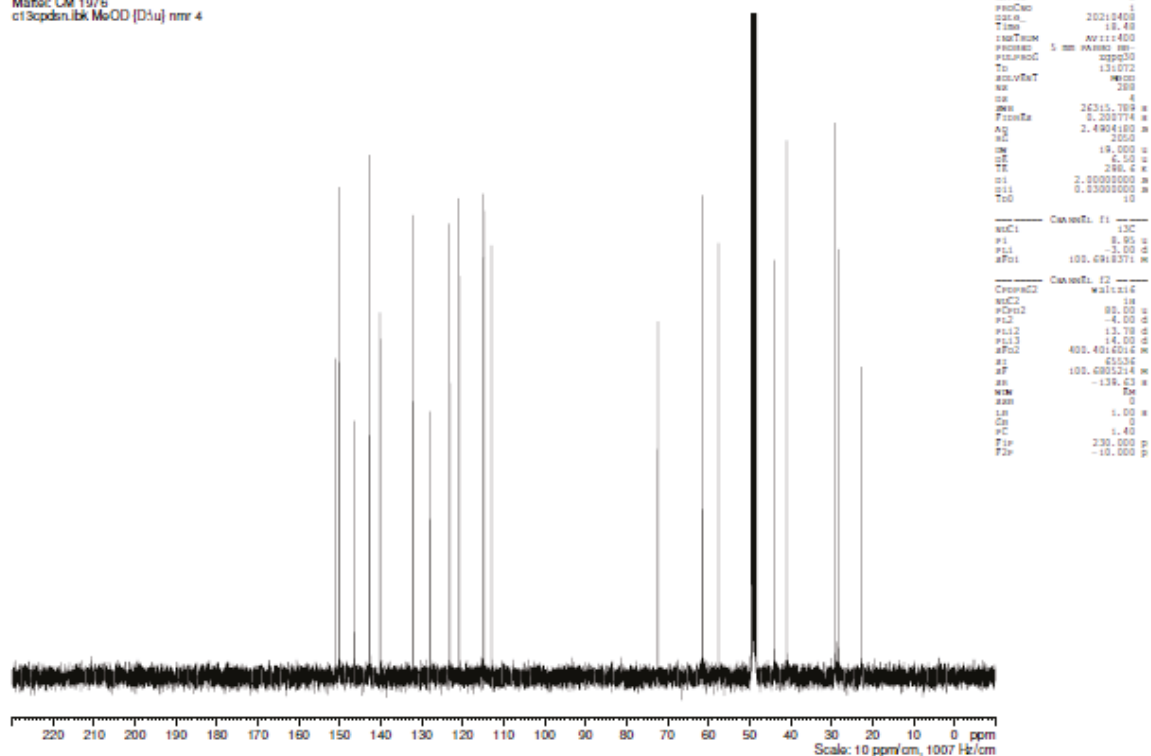


¹H- and ¹³C-NMR experiment for (R)-(6-azidoquinolin-4-yl)((1S,2S,4S,5R)-5-vinylquinuclidin-2-yl)methanol (9):

Exp. 1H
Matsci: CM 1976
protonpp.lib MeOD [D3u] nmr 4

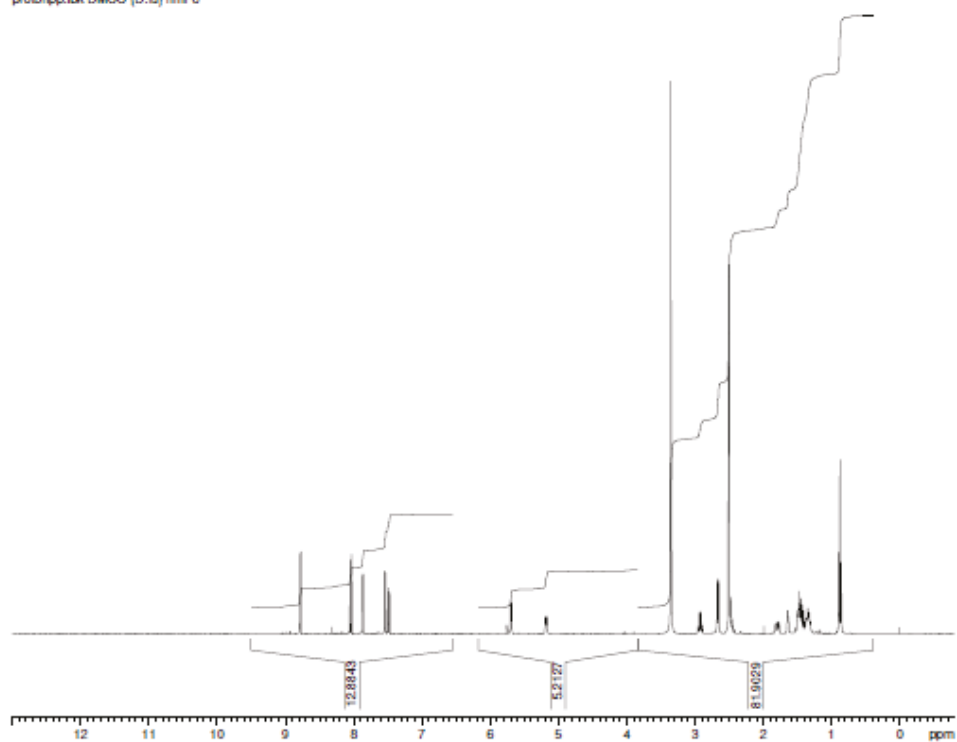


Exp. 13C, CPD
Matsci: CM 1976
c13cpdpp.lib MeOD [D3u] nmr 4



¹H- and ¹³C-NMR experiment for (S)-(6-azidoquinolin-4-yl)((1S,2R,4S,5R)-5-ethylquinuclidin-2-yl)methanol (**10**):

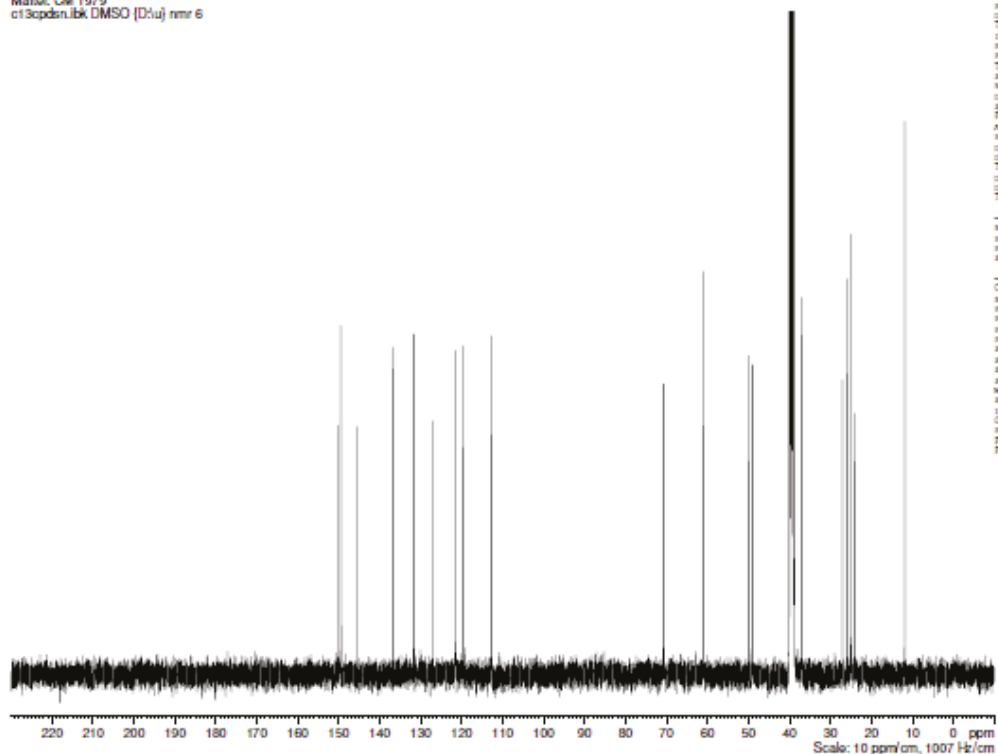
Exp. ¹H
MatSci: CM 1979
protonpp.libk DMSO [D₂O] nmr 6



```
NAME      max44117.in
EXPNO     1
PROCNO    1
DATE_     20210408
TIME      21.23
INSTRUM    Av114400
PROBHD    5 mm WALTZ BB-
PULPROG    zgpg30
TD         65536
SOLVENT    DMSO
NS         64
DS         2
SWH        8223.085 K
F2AcqEs    5.125483 K
AQ         3.9846387 M
RG         128
WM         60.000 U
QE         6.50 U
TE         297.1 K
SI         1.20000000 M
TD0        1
```

```
----- Channel f1 -----
NUC1       1H
P1         10.00 U
PL1        -4.00 dB
SFO1       400.4004124 M
SI         32768 M
SF         400.4002089 M
SR         8.19 K
WDM        DM
SFO        0
LH         0.00 K
GB         0
PC         1.40
T1p        13.000 P
T2p        -0.600 P
```

Exp. ¹³C, CPD
MatSci: CM 1979
c1 Scpden.libk DMSO [D₂O] nmr 6



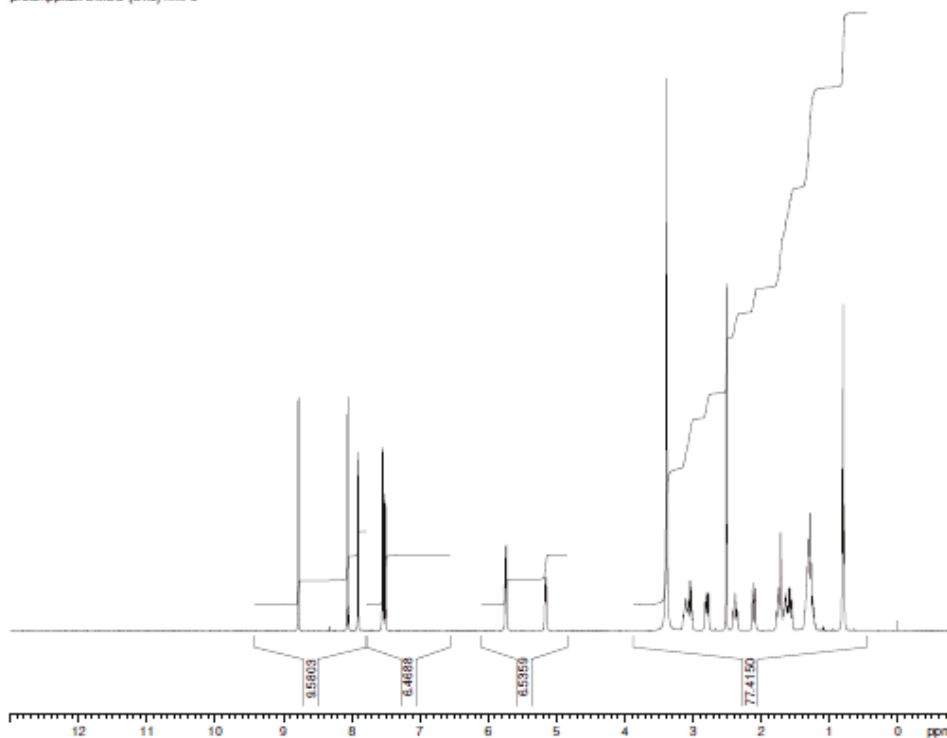
```
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EXPNO     2
PROCNO    1
DATE_     20210408
TIME      21.32
INSTRUM    Av114400
PROBHD    5 mm WALTZ BB-
PULPROG    zgpg30
TD         131072
SOLVENT    DMSO
NS         960
DS         4
SWH        26315.789 K
F2AcqEs    5.200774 K
AQ         2.4904100 M
RG         400
WM         19.000 U
QE         6.50 U
TE         296.6 K
SI         2.00000000 M
TD0        0.00000000 M
```

```
----- Channel f1 13C -----
NUC1       13C
P1         8.00 U
PL1        -3.00 dB
SFO1       100.6018371 M

----- Channel f2 -----
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 U
PL2        -4.00 dB
PL12       13.70 dB
PL13       14.00 dB
SFO2       400.4016516 M
SI         65536
SF         100.6007122 M
SR         51.18 K
WDM        DM
SFO        0
LH         1.00 K
GB         0
PC         1.40
T1p        230.000 P
T2p        -10.000 P
```

¹H- and ¹³C-NMR experiment for (R)-(6-azidoquinolin-4-yl)((1S,2S,4S,5R)-5-ethylquinuclidin-2-yl)methanol (**11**):

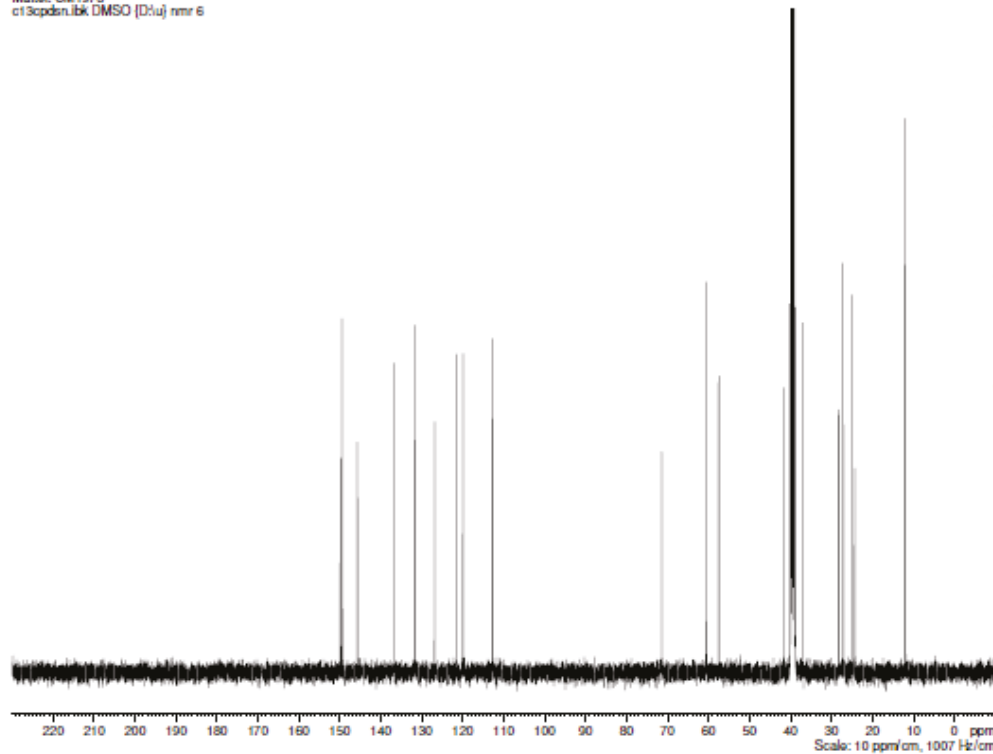
Exp. ¹H
 Metabol: CM1978
 protonpp.libk DMSO [D₂O] nmr 6



```
NAME      max144051.in
EXPNO     1
PROCNO    1
SOLAR     20210401
TIME      14.45
INSTRUM    AV11400
PULPROG    5 mm WALTZ16
TD         65536
SOLVENT    DMSO
NS         64
DS         2
SWH         8223.000 MHz
FIDRES     0.125483 MHz
AQ         3.9846387 MHz
RG         512.0
SM         65.000 u
SE         6.50 u
TE         300.1 K
SI         1.00000000 MHz
TSD        1
```

```
----- Channel f1 -----
NUC1       1H
P1         10.20 u
PL1        4.00 dB
SFO1       400.4004704 MHz
SI         32768
SF         400.4004704 MHz
SD         1.64 MHz
WDW         EM
SSB         0
LB         0.00 MHz
GB         0
PC         1.40
P1P        13.000 p
P2P        -0.000 p
```

Exp. ¹³C, CPD
 Metabol: CM1978
 c13cpdpp.libk DMSO [D₂O] nmr 6



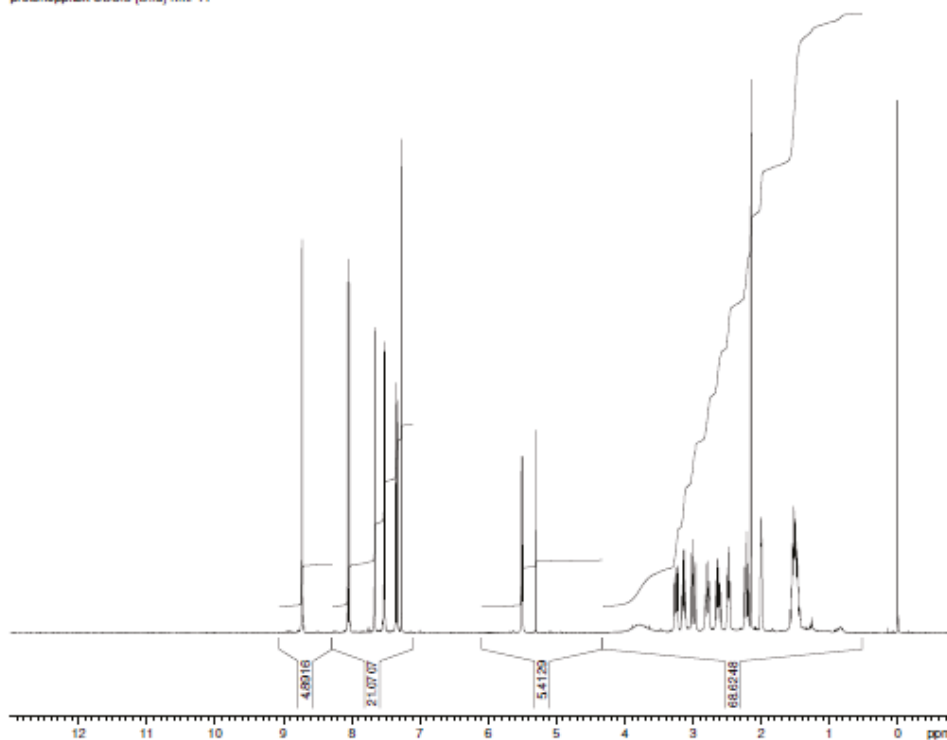
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EXPNO     2
PROCNO    1
SOLAR     20210401
TIME      14.54
INSTRUM    AV11400
PULPROG    5 mm WALTZ16
TD         65536
SOLVENT    DMSO
NS         64
DS         4
SWH         26315.789 MHz
FIDRES     0.203774 MHz
AQ         2.4904180 MHz
RG         575
SM         18.000 u
SE         6.50 u
TE         298.4 K
SI         2.00000000 MHz
SII        0.03000000 MHz
TSD        10
```

```
----- Channel f1 -----
NUC1       13C
P1         8.95 u
PL1        1.00 dB
SFO1       100.6261271 MHz
```

```
----- Channel f2 -----
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 u
PL2        4.00 dB
PL12       13.78 dB
PL13       14.00 dB
SFO2       400.4014014 MHz
SI         65536
SF         100.6261271 MHz
SD         48.57 MHz
WDW         EM
SSB         0
LB         1.00 MHz
GB         0
PC         1.40
P1P        230.000 p
P2P        -10.000 p
```

¹H- and ¹³C-NMR experiment for (S)-(6-azidoquinolin-4-yl)((1S,2R,4S,5S)-5-ethynylquinuclidin-2-yl)methanol (**12**):

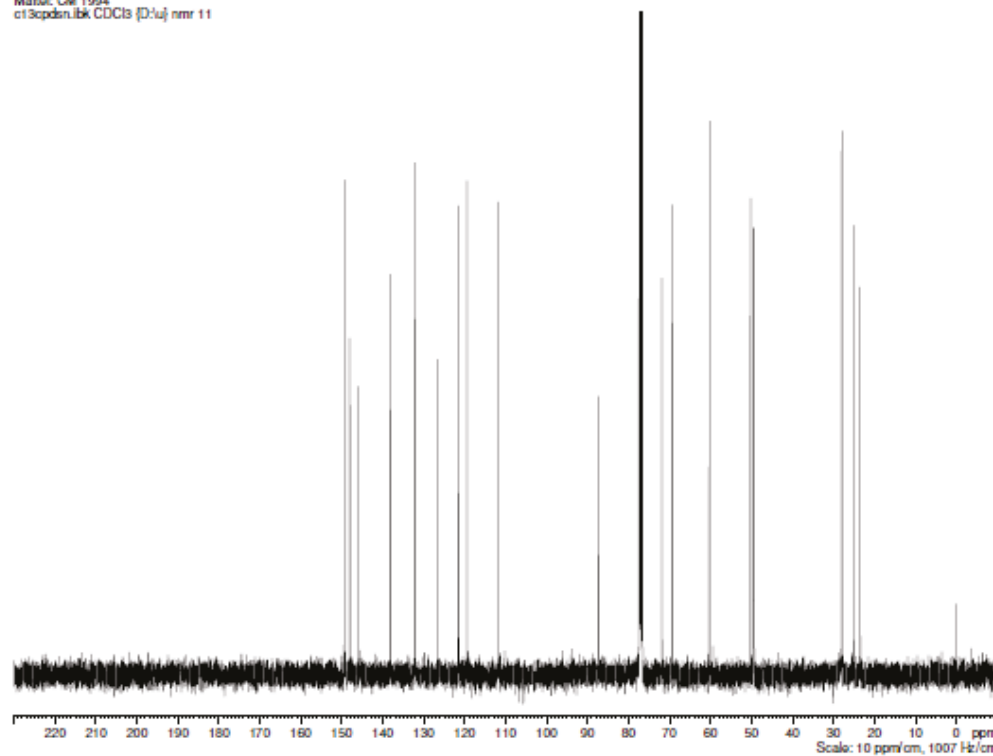
Exp. ¹H
Mafac CM 1994
protonopp.bk CDC13 [D₂O] nmr 11



NAME max144208_in
ExpNo 1
ProcNo 1
Date 20210423
Time 21.54
INSTRUM AVI1400
PROBHD 5 mm HANCO BB-
PULPROG zgpg30
TD 65536
TE 300.13
SOLVENT CDCl3
NS 4
DS 2
SWH 8223.000 MHz
FIDRES 0.1254803 MHz
AQ 3.9946387 s
RG 181
WM 40.000 u
WE 6.50 u
TE 299.6 K
SI 1.00000000 MHz
TSD 1

Channel f1
NUC1 1H
P1 10.20 u
PL1 4.00 dB
AF1 400.4004716 MHz
Z 32768
SF 400.4005179 MHz
AN 17.88 MHz
WIN 0
XPR 0
LB 0
GB 0
PC 1.40
FIR 13.000 p
F2P -0.000 p

Exp. ¹³C CPD
Mafac CM 1994
c13cpdnu.bk CDC13 [D₂O] nmr 11



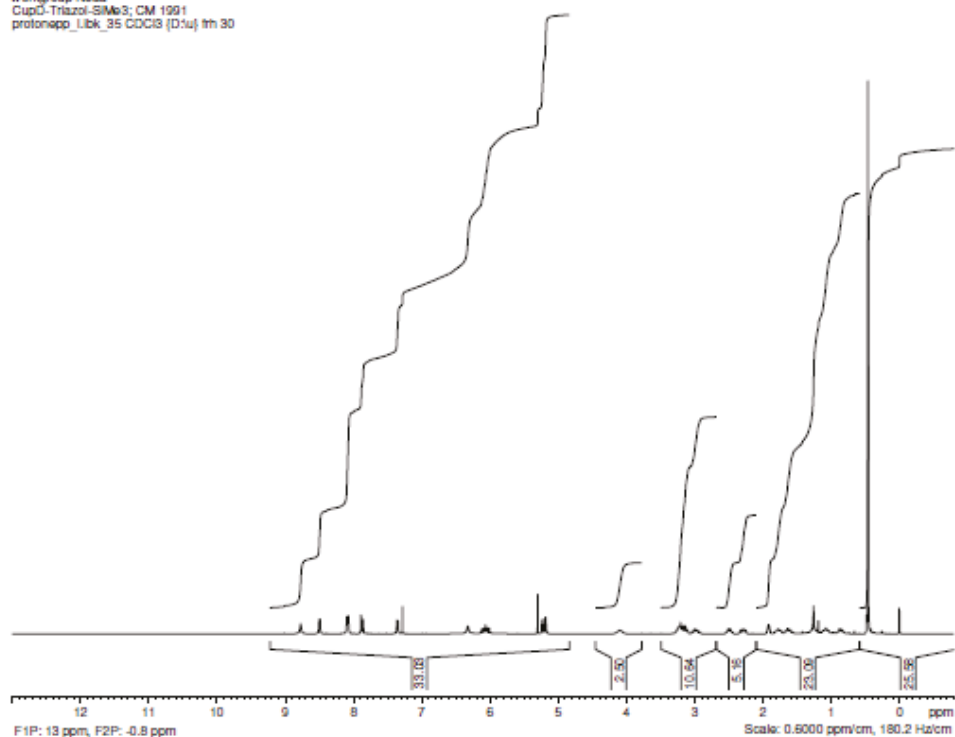
NAME max144208_in
ExpNo 2
ProcNo 1
Date 20210423
Time 22.03
INSTRUM AVI1400
PROBHD 5 mm HANCO BB-
PULPROG zgpg30
TD 131072
TE 300.13
SOLVENT CDCl3
NS 4
DS 4
SWH 26315.789 MHz
FIDRES 0.203774 MHz
AQ 2.4904180 s
RG 1030
WM 19.000 u
WE 6.50 u
TE 299.6 K
SI 2.00000000 MHz
TSD 10

Channel f1
NUC1 13C
P1 8.95 u
PL1 2.00 dB
AF1 100.6261271 MHz

Channel f2
NAME max144208_in
ExpNo 2
ProcNo 1
Date 20210423
Time 22.03
INSTRUM AVI1400
PROBHD 5 mm HANCO BB-
PULPROG zgpg30
TD 65536
TE 300.13
SOLVENT CDCl3
NS 4
DS 4
SWH 26315.789 MHz
FIDRES 0.203774 MHz
AQ 2.4904180 s
RG 1030
WM 19.000 u
WE 6.50 u
TE 299.6 K
SI 2.00000000 MHz
TSD 10

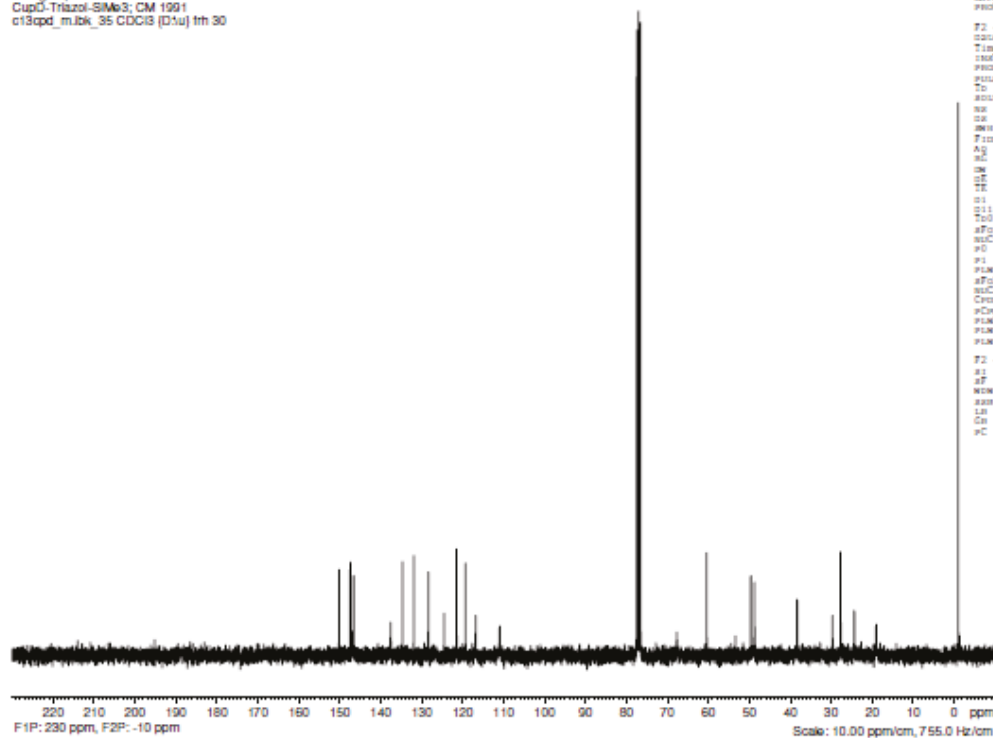
¹H- and ¹³C-NMR experiment for (S)-(6-(4-(trimethylsilyl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2R,4S,5R)-5-vinylquinuclidin-2-yl)methanol (**14**):

no. of the sticker on the nmr tube 604
color of the label blue
workgroup Nada
Cup3-Triazol-SiMe3; CM 1991
protonapp_libk_35 CDCl3 [D1u] tth 30



Current data parameters
NAME fth-210420-184541.in
Expt 1
ProcCh 1
F2 - Acquisition parameters
Date_ 20210420
Time 19.15 h
InstName AVI1000300M
Proces 2104275_0359
PulsePrG zgpg30
TO 891.3
AcqReT CDCl3
NU 128
OR 2
SW 6203.474 Hz
FidRe 8.252420 Hz
AQ 3.561551 sec
RG 130.72
DM 80.400 GHz
DE 6.50 GHz
TE 298.0 K
SI 1.0000000 sec
D1 1
aFol 300.2618538 MHz
NUC1 1H
P0 6.50 GHz
P1 12.50 GHz
PLM1 10.85099883 W
F2 - processing parameters
SI 27168
AF 300.2600075 MHz
WDM 2M
XDR 0
LH 0 Hz
CH 0
PC 1.00

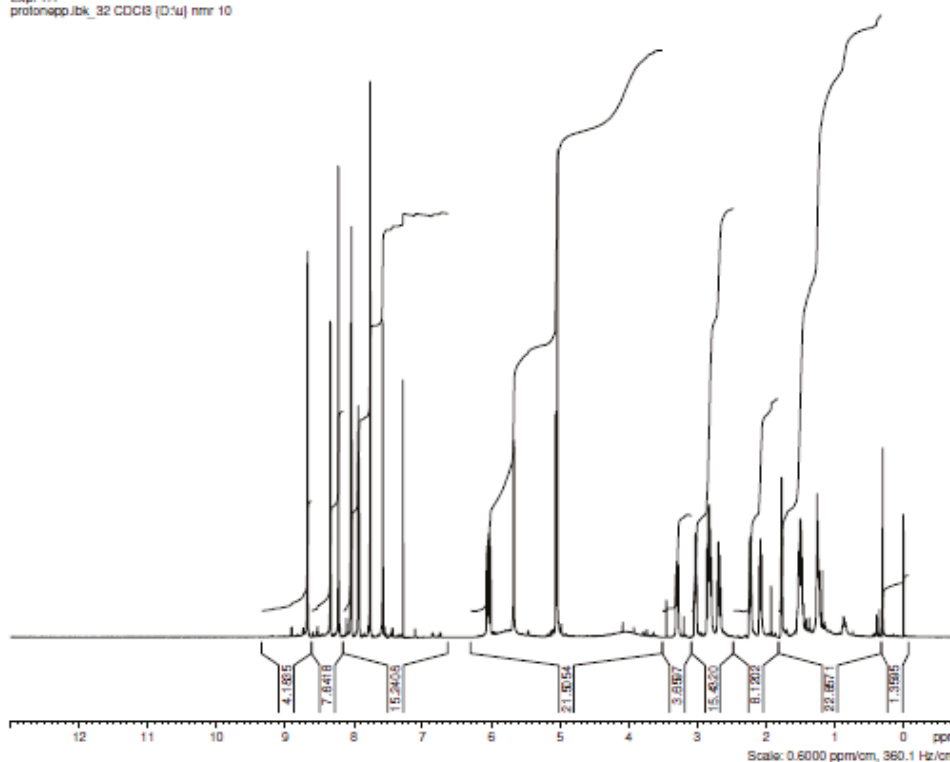
no. of the sticker on the nmr tube 604
color of the label blue
workgroup Nada
Cup3-Triazol-SiMe3; CM 1991
c13cpd_mlibk_35 CDCl3 [D1u] tth 30



Current data parameters
NAME fth-210420-184541.in
Expt 2
ProcCh 1
F2 - Acquisition parameters
Date_ 20210420
Time 19.40 h
InstName AVI1000300M
Proces 2104275_0359
PulsePrG zgpg30
TO 891.3
AcqReT CDCl3
NU 384
OR 4
SW 19736.842 Hz
FidRe 8.401547 Hz
AQ 2.4903679 sec
RG 18.42
DM 25.333 GHz
DE 6.50 GHz
TE 298.0 K
SI 2.0000000 sec
D1 0.0300000 sec
D11 1
aFol 75.508871 MHz
NUC1 13C
P0 6.50 GHz
P1 9.50 GHz
PLM1 51.05799866 W
aFol2 300.2618538 MHz
NUC2 1H
Chrmc[2] W101214
PChm2 90.50 GHz
PLM2 10.85099883 W
PLM3 0.1020000 W
PLM3 0.0070310 W
F2 - processing parameters
SI 65536
AF 75.5004423 MHz
WDM 2M
XDR 0
LH 1.00 Hz
CH 0
PC 1.40

¹H- and ¹³C-NMR experiment for (S)-6-(1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2R,4S,5R)-5-vinylquinuclidin-2-yl)methanol (**15**):

Kunde: Maffel
Substanz-Code: CM 1991
Exp. 1H
protonapp.lib_32 CDCB (D1u) nmr 10



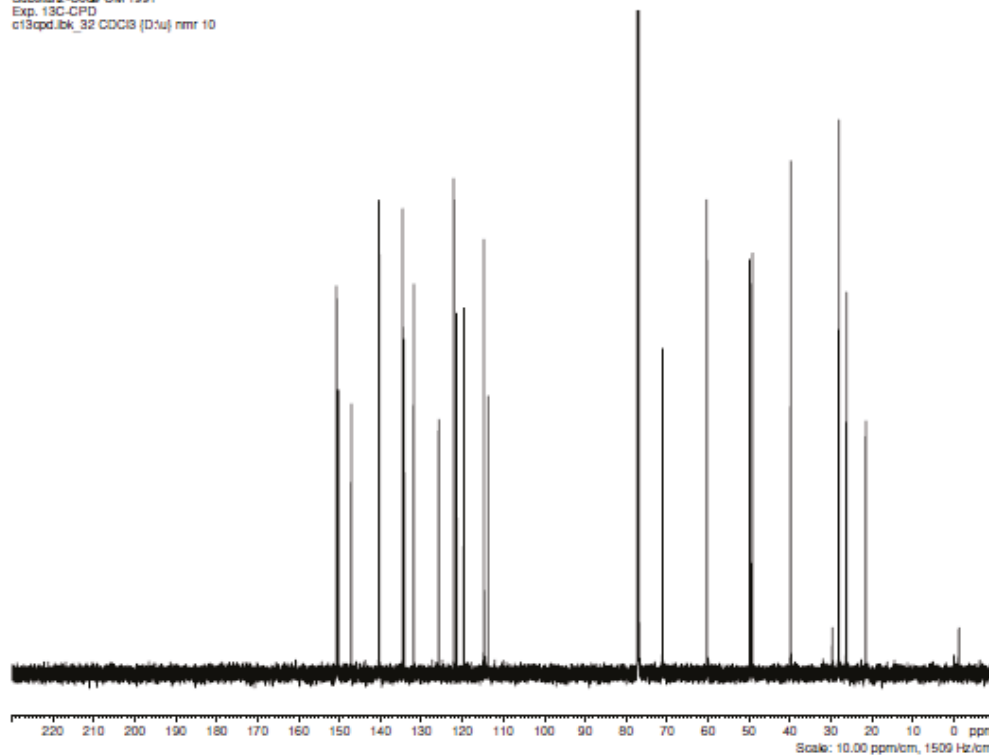
Current data parameters
NAME: max144207.in
EXPNO: 1
PROCNO: 1

F2 - Acquisition parameters
Date_: 20210421
Time: 16.03
INSTRUM: spect
PROBHD: 5 mm HMQB 50-
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 2048
DS: 4
SWH: 12335.526 Hz
FIDRES: 0.125482 Hz
AQ: 3.9840388 sec
RG: 711.8
WM: 40.523 umsec
ZG: 6.50 umsec
TE: 298.2 K
SI: 2.00000000 sec
TO: 1

Channel F1
NUC1: 13C
P1: 11.75 umsec
PL1: 28.00000000 W

F2 - Processing parameters
SI: 65536
SF: 600.1300118 MHz
WDW: EM
SSB: 0
LB: 0 Hz
GB: 0 Hz
PC: 1.40
AP: 1.40 Hz
SFOF: 0.188225 Hz

Kunde: Maffel
Substanz-Code: CM 1991
Exp. 13C-CPD
c13cpd.lib_32 CDCB (D1u) nmr 10



Current data parameters
NAME: max144207.in
EXPNO: 2
PROCNO: 1

F2 - Acquisition parameters
Date_: 20210421
Time: 16.05
INSTRUM: spect
PROBHD: 5 mm HMQB 50-
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 2048
DS: 4
SWH: 39482.535 Hz
FIDRES: 0.201834 Hz
AQ: 2.4712408 sec
RG: 205.0
WM: 12.600 umsec
ZG: 6.50 umsec
TE: 298.2 K
SI: 2.00000000 sec
TO: 1

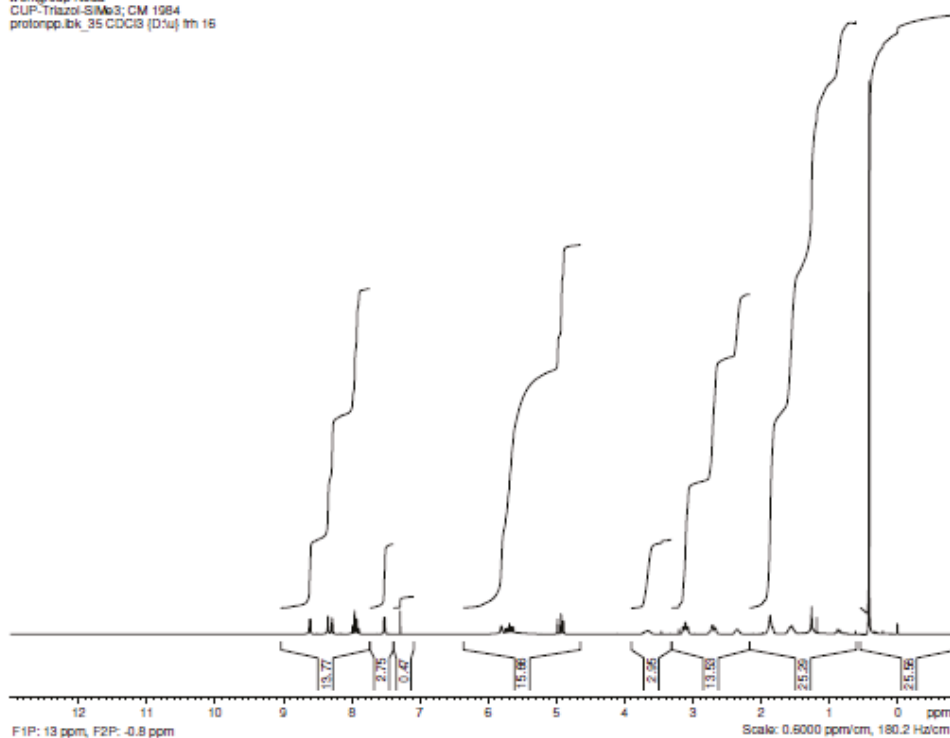
Channel F1
NUC1: 13C
P1: 10.40 umsec
PL1: 50.00000000 W

Channel F2
NUC2: 1H
CPDPRG2: waltz16
PCPD2: 70.00 umsec
PL12: 28.00000000 W
PL13: 0.78860000 W
PL14: 0.36680999 W

F2 - Processing parameters
SI: 131072
SF: 150.9628231 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0 Hz
PC: 1.40
AP: 14.41 Hz
SFOF: 0.362754 Hz

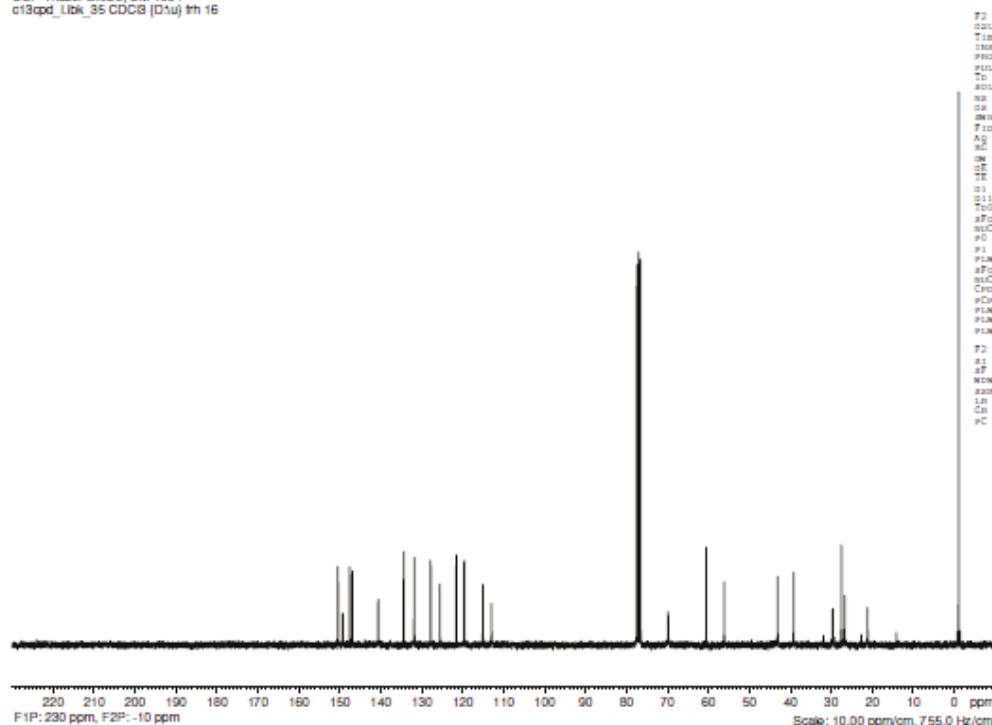
¹H- and ¹³C-NMR experiment for (R)-(6-(4-(trimethylsilyl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2S,4S,5R)-5-vinylquinuclidin-2-yl)methanol (**16**):

no. of the sticker on the nmr tube 684
color of the label blue
workgroup Nada
CUP-Triazol-SiMe3; CM 1984
protonpp.lib, 35 CDCIS (D1u) 1h 16



Current data parameters
NAME fcs-210423-145407_in
Expno 1
ProcNo 1
F2 - Acquisition parameters
Date_ 20210423
Time 21.40 h
InstName Axiom300m
Proces 210423_0369
PulprogC zg30
TD 65536
AcqInT CDCIS
NS 24
DS 2
SWH 6203.474 Hz
Fwhm 8.252420 Hz
AQ 3.901641 sec
RG 89.15
DM 80.400 GHz
DE 6.50 GHz
TE 298.0 K
Z1 1.0000000 sec
ZD 1
aF01 300.2615138 MHz
NUC1 1H
P0 6.00 GHz
P1 12.00 GHz
PLM1 10.8509983 W
F2 - Processing parameters
SI 32768
aF 300.2600461 MHz
WDM 2M
SFO 0
LB 0 Hz
GB 0
PC 1.00

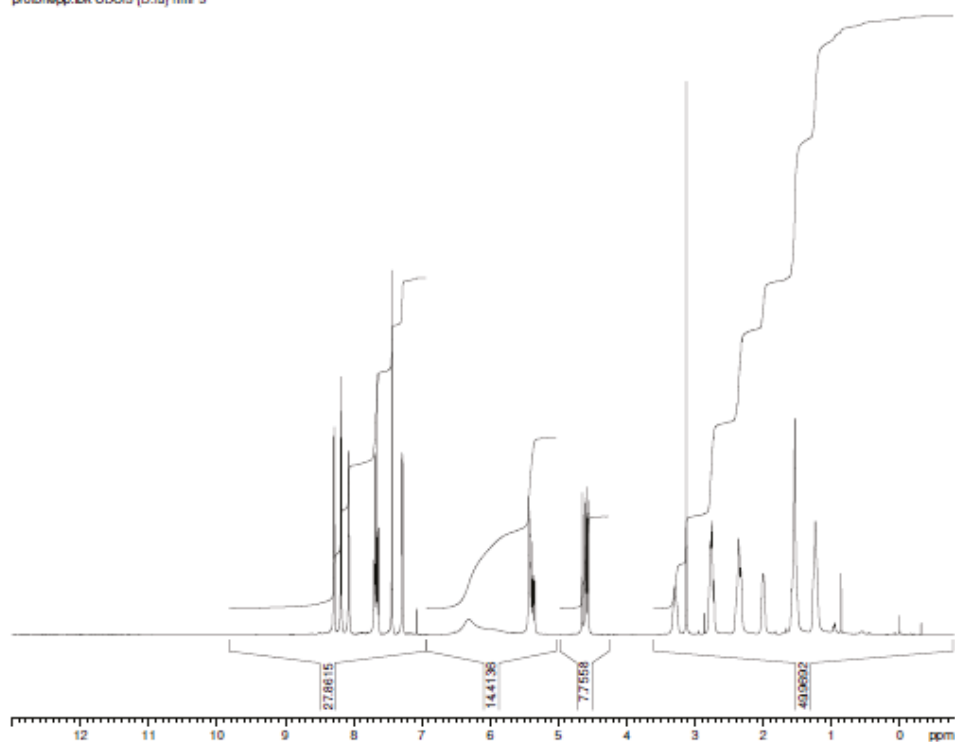
no. of the sticker on the nmr tube 684
color of the label blue
workgroup Nada
CUP-Triazol-SiMe3; CM 1984
c13cpd.lib, 35 CDCIS (D1u) 1h 16



Current data parameters
NAME fcs-210423-145407_in
Expno 2
ProcNo 1
F2 - Acquisition parameters
Date_ 20210423
Time 22.24 h
InstName Axiom300m
Proces 210423_0369
PulprogC zgpg30
TD 65536
AcqInT CDCIS
NS 4
DS 4
SWH 19736.842 Hz
Fwhm 8.401547 Hz
AQ 2.4903479 sec
RG 20.18
DM 25.333 GHz
DE 6.50 GHz
TE 298.0 K
Z1 2.0000000 sec
ZD 1
aF01 75.508811 MHz
NUC1 13C
P0 3.57 GHz
P1 51.0579864 W
aF02 300.2612910 MHz
NUC2 1H
CoupPC[2] W101216
PCou2 90.00 GHz
PLM2 10.8509983 W
PLM1 0.16296350 W
PLM3 0.00703100 W
F2 - Processing parameters
SI 65536
aF 75.5084433 MHz
WDM 2M
SFO 0
LB 1.00 Hz
GB 0
PC 1.40

¹H- and ¹³C-NMR experiment for (R)-(6-(1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2S,4S,5R)-5-vinylquinuclidin-2-yl)methanol (**17**):

Exp. ¹H
Metho: CM-1984-Triaz-H
protonppb.bk CDCl₃ [D₂O] nmr 3



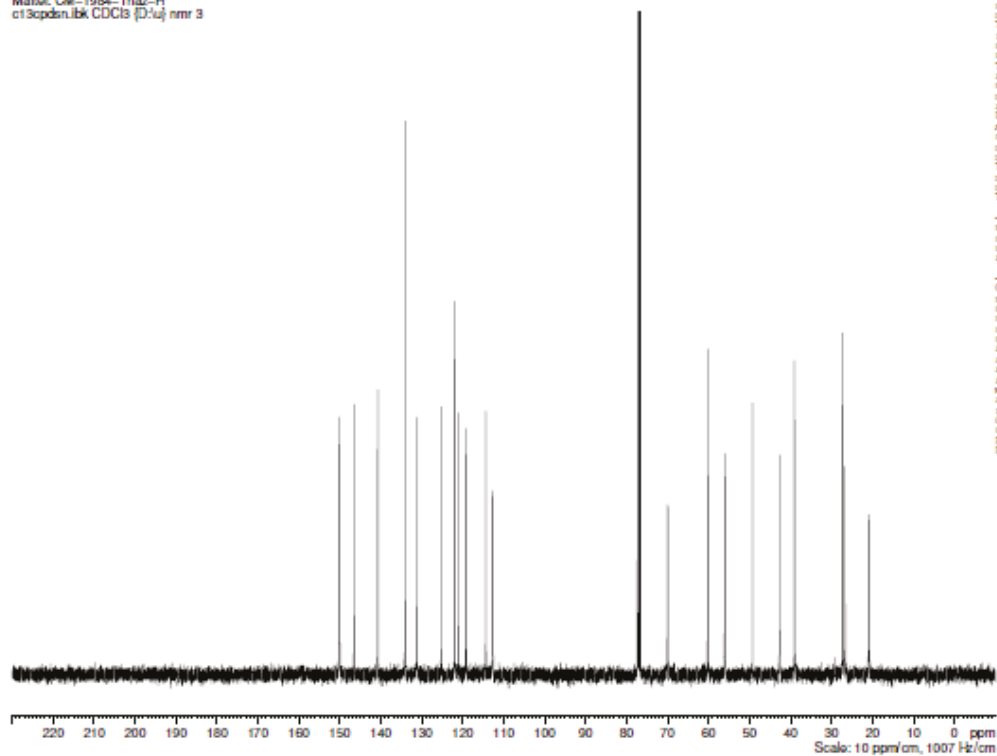
```

NAME      max:44244.in
EXPNO     1
PROCNO    1
DATE_     20210426
TIME      14.58
INSTRUM    AVI1400
PROBHD     5 mm HANCO H-
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         64
DS         2
SWH         8223.485 Hz
FIDRES     0.121483 Hz
AQ         3.9846387 s
RG         14
WM         60.800 u
GB         0.50 u
TE         298.0 K
SI         1.00000000 M
TO        1.00000000 M
  
```

```

----- Channel f1 -----
NUC1       1H
P1         10.00 u
PC1        4.00 dB
AF1        400.4004000 MHz
SI         32768
SF         400.4009400 MHz
WDW        EM
SSB         0
LB         0.00 Hz
GB         0
PC         1.40
T1P        13.000 p
F2P        -0.800 p
  
```

Exp. ¹³C CPD
Metho: CM-1984-Triaz-H
c13cpdppb.bk CDCl₃ [D₂O] nmr 3



```

NAME      max:44244.in
EXPNO     2
PROCNO    1
DATE_     20210426
TIME      15.08
INSTRUM    AVI1400
PROBHD     5 mm HANCO H-
PULPROG    zgpg30
TD         131072
SOLVENT    CDCl3
NS         96
DS         4
SWH         26315.789 Hz
FIDRES     0.2007774 Hz
AQ         2.4804180 s
RG         2050
WM         19.000 u
GB         0.50 u
TE         298.2 K
SI         2.00000000 M
TO        0.00000000 M
  
```

```

----- Channel f1 -----
NUC1       13C
P1         8.95 u
PC1        3.00 dB
AF1        100.6261371 MHz
  
```

```

----- Channel f2 -----
NAME      max:44244.in
EXPNO     2
PROCNO    1
DATE_     20210426
TIME      15.08
INSTRUM    AVI1400
PROBHD     5 mm HANCO H-
PULPROG    zgpg30
TD         131072
SOLVENT    CDCl3
NS         96
DS         4
SWH         26315.789 Hz
FIDRES     0.2007774 Hz
AQ         2.4804180 s
RG         2050
WM         19.000 u
GB         0.50 u
TE         298.2 K
SI         2.00000000 M
TO        0.00000000 M
  
```

¹H- and ¹³C-NMR experiment for (S)-(6-(4-(trimethylsilyl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2R,4S,5R)-5-ethylquinuclidin-2-yl)methanol (**18**):

no. of the sticker on the nmr tube 288

color of the label blue

workgroup Neda

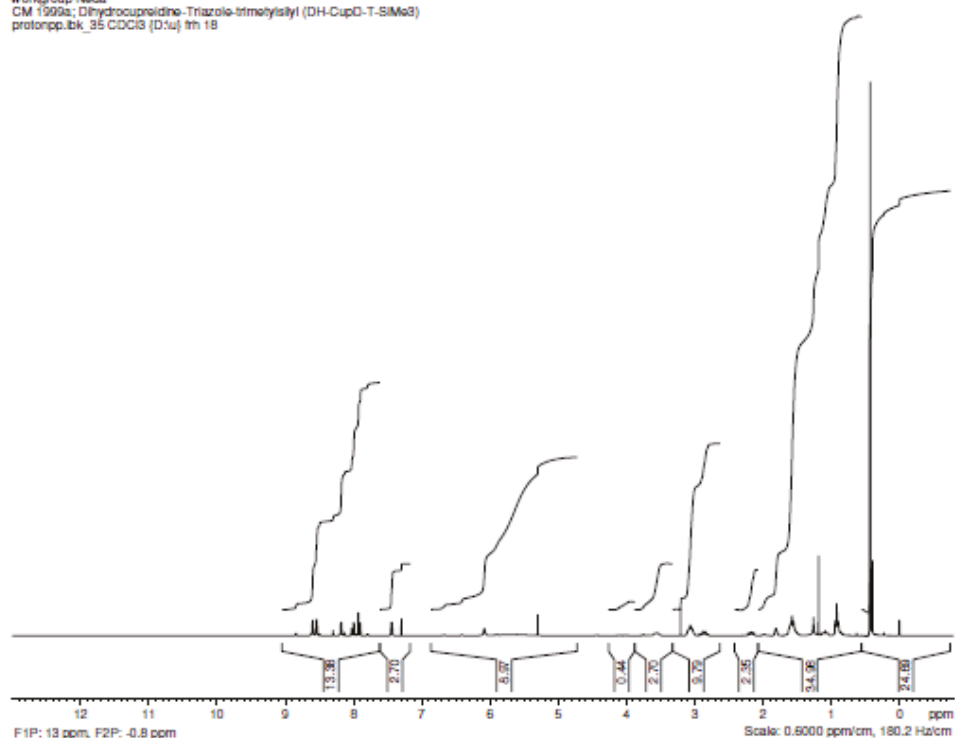
CM 1929a; Dihydrocupreidine-Triazole-trimethylsilyl (DH-CupD-T-SiMe3)

protonp.bk_35 CDCl3 [D1u] tth 18

Current data parameters
NAME fth-210521-162000_in
Exptno 1
ProcNo 1

F2 - Acquisition parameters
Date_ 20210521
Time 21.26 h
INSTRUM AV1000300H
PROBHD z104275_0309 (1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 24
DS 2
SWH 6203.474 Hz
FIDRES 0.252420 Hz
AQ 3.3615611 sec
RG 80.22
CW 80.400 GHz
DE 6.50 GHz
TE 298.0 K
SI 1.0000000 sec
TDO 1
SFO1 300.2618513 MHz
NUC1 1H
P0 4.00 GHz
P1 12.50 GHz
PLM1 10.85099983 W

F2 - processing parameters
SI 32768
SF 300.2600028 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



no. of the sticker on the nmr tube 288

color of the label blue

workgroup Neda

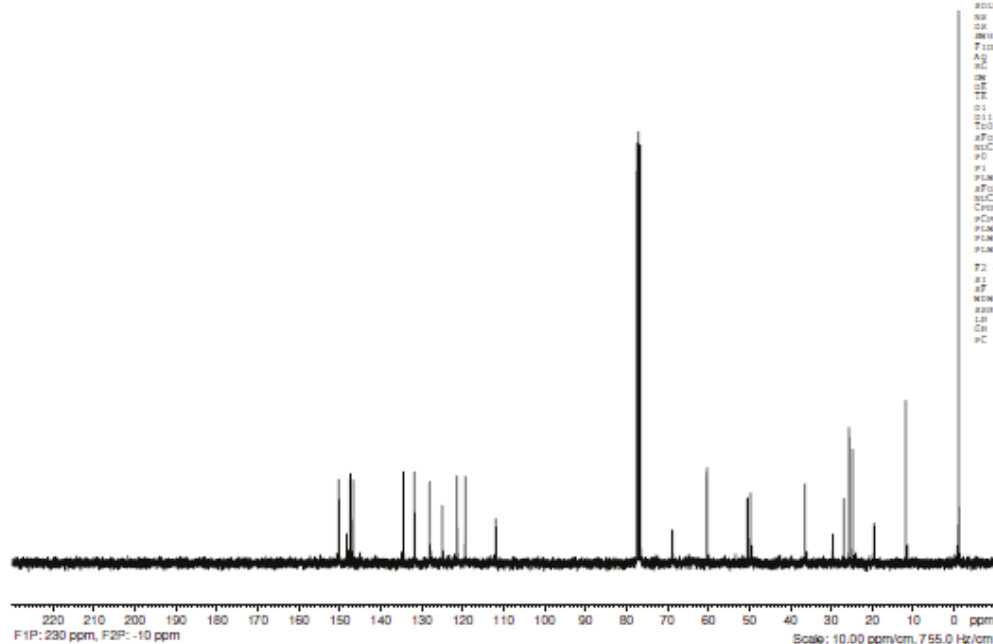
CM 1929a; Dihydrocupreidine-Triazole-trimethylsilyl (DH-CupD-T-SiMe3)

c13cpd_mibk_35 CDCl3 [D1u] tth 18

Current data parameters
NAME fth-210521-162000_in
Exptno 2
ProcNo 1

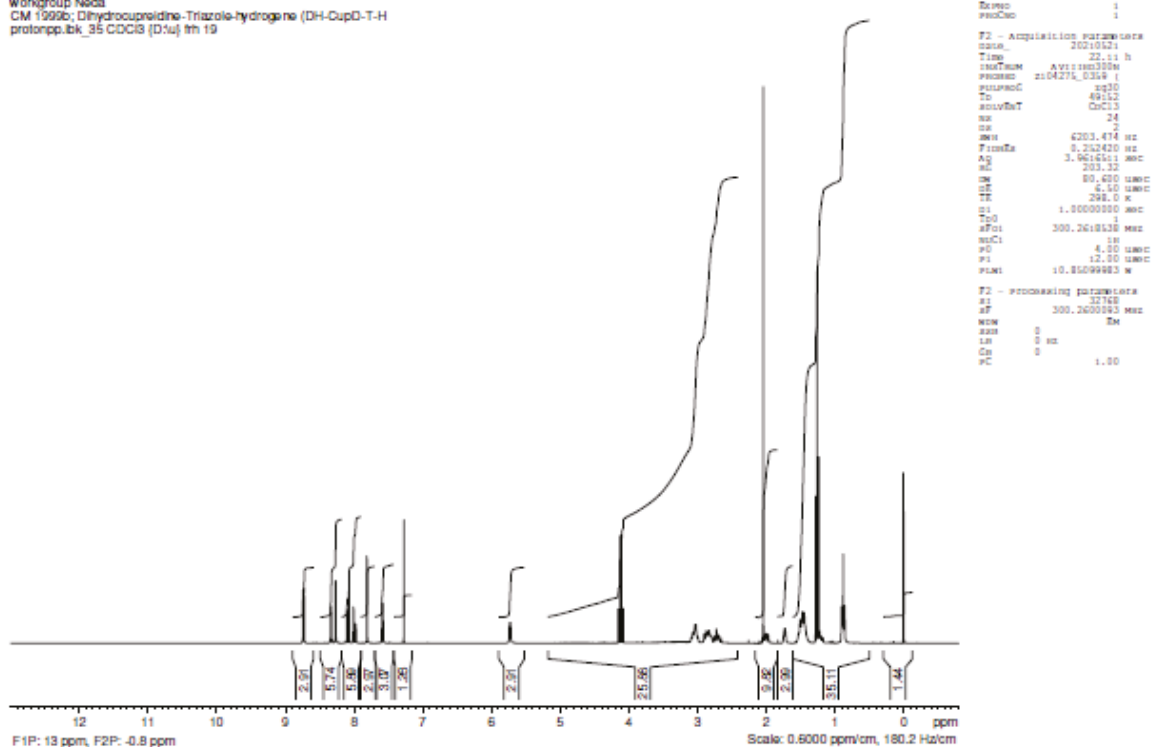
F2 - Acquisition parameters
Date_ 20210521
Time 21.50 h
INSTRUM AV1000300H
PROBHD z104275_0309 (1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 304
DS 4
SWH 19736.842 Hz
FIDRES 0.401547 Hz
AQ 2.4903679 sec
RG 18.42
CW 25.333 GHz
DE 6.50 GHz
TE 298.0 K
SI 2.0000000 sec
TDO 1
SFO1 75.508171 MHz
NUC1 13C
P0 5.17 GHz
P1 9.50 GHz
PLM1 51.05799846 W
SFO2 300.2618513 MHz
NUC2 1H
PLM2 10.85099983 W
PLM3 0.10200000 W
PLM4 0.50703100 W

F2 - processing parameters
SI 65536
SF 75.5084441 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

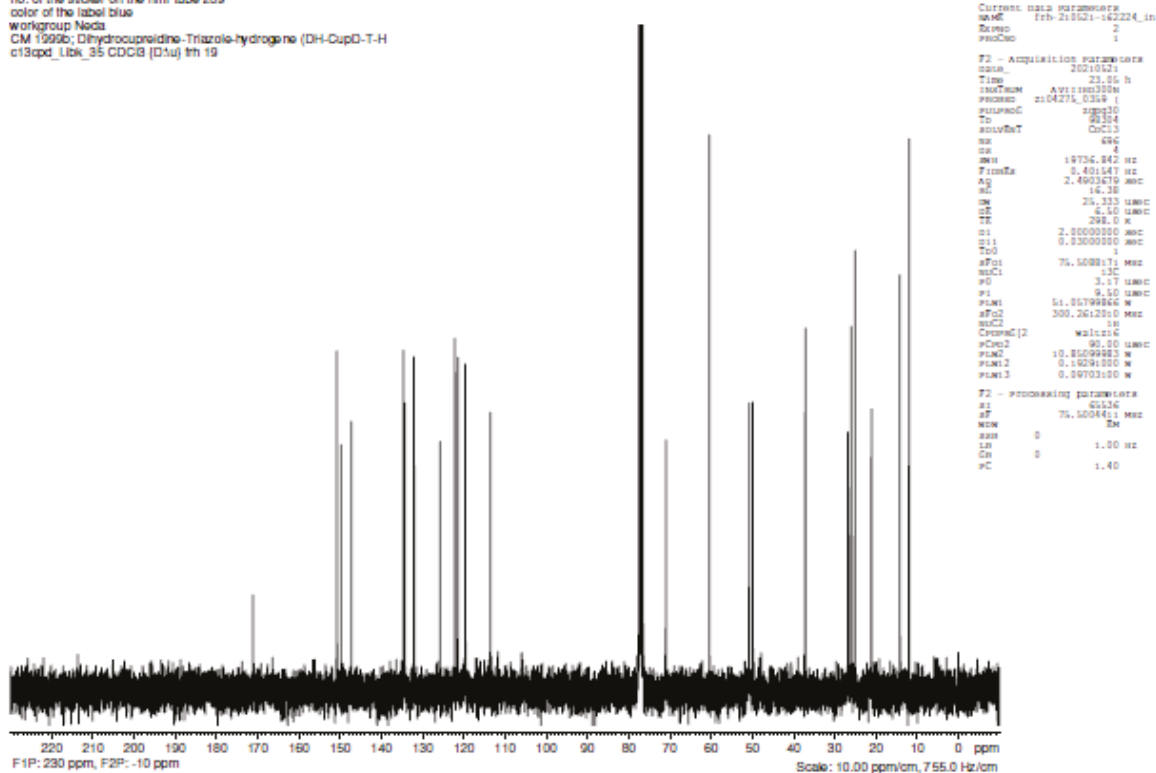


1H- and 13C-NMR experiment for (S)-(6-(1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2R,4S,5R)-5-ethylquinuclidin-2-yl)methanol (**19**):

no. of the sticker on the nmr tube 289
color of the label blue
workgroup Nada
CM 1999b; Dihydrocupreidine-Triazole-hydrogene (DH-CupD-T-H
protonpp.lib 35 CDCI3 (D₂O) frh 19

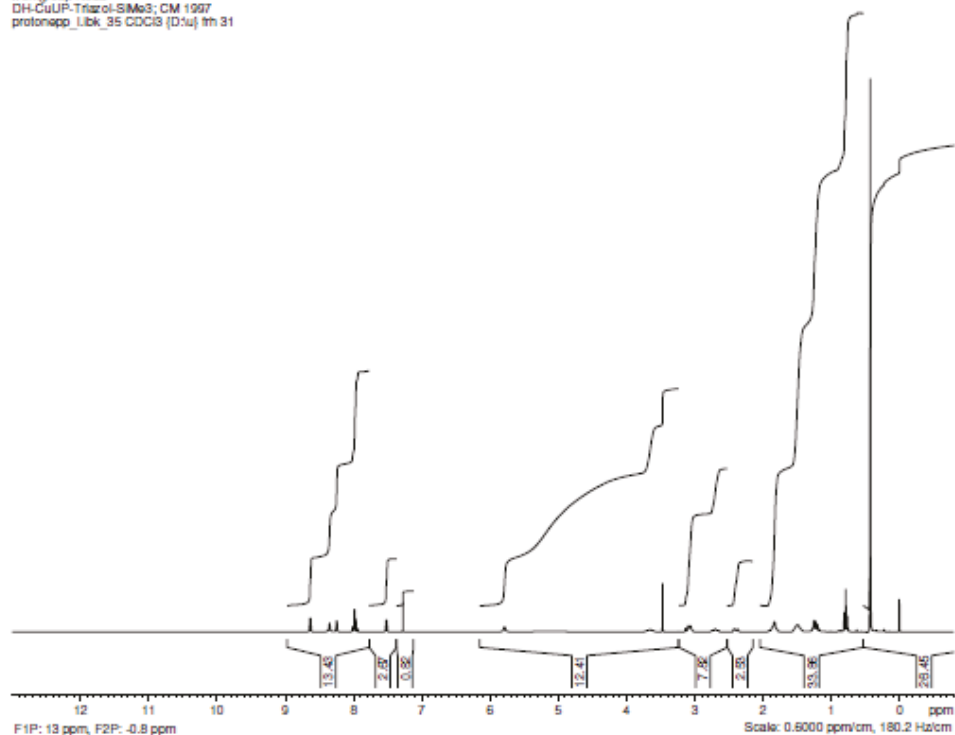


no. of the sticker on the nmr tube 289
color of the label blue
workgroup Nada
CM 1999b; Dihydrocupreidine-Triazole-hydrogene (DH-CupD-T-H
c13cpd Libk 35 CDCB (D5u) trh 19

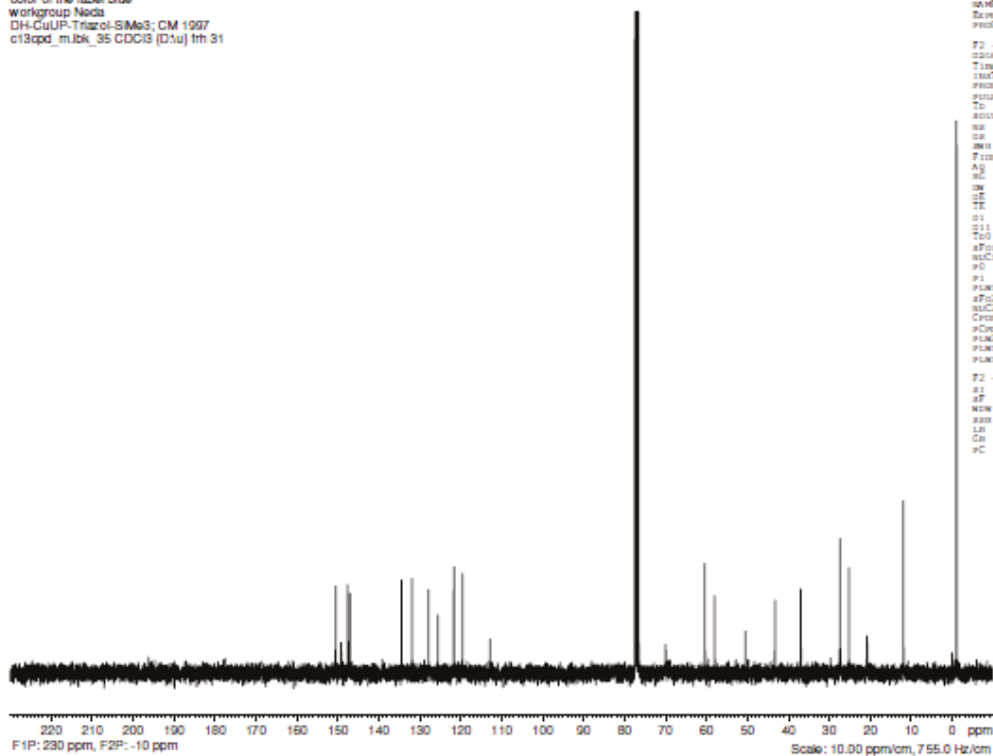


¹H- and ¹³C-NMR experiment for (R)-(6-(4-(trimethylsilyl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2S,4S,5R)-5-ethylquinuclidin-2-yl)methanol (**20**):

no. of the sticker on the nmr tube 605
color of the label blue
workgroup Neda
DH-CuUP-Triazol-SiMe3; CM 1997
protonapp_1.tbk_35 CDCl₃ [D₂O] 1h 31

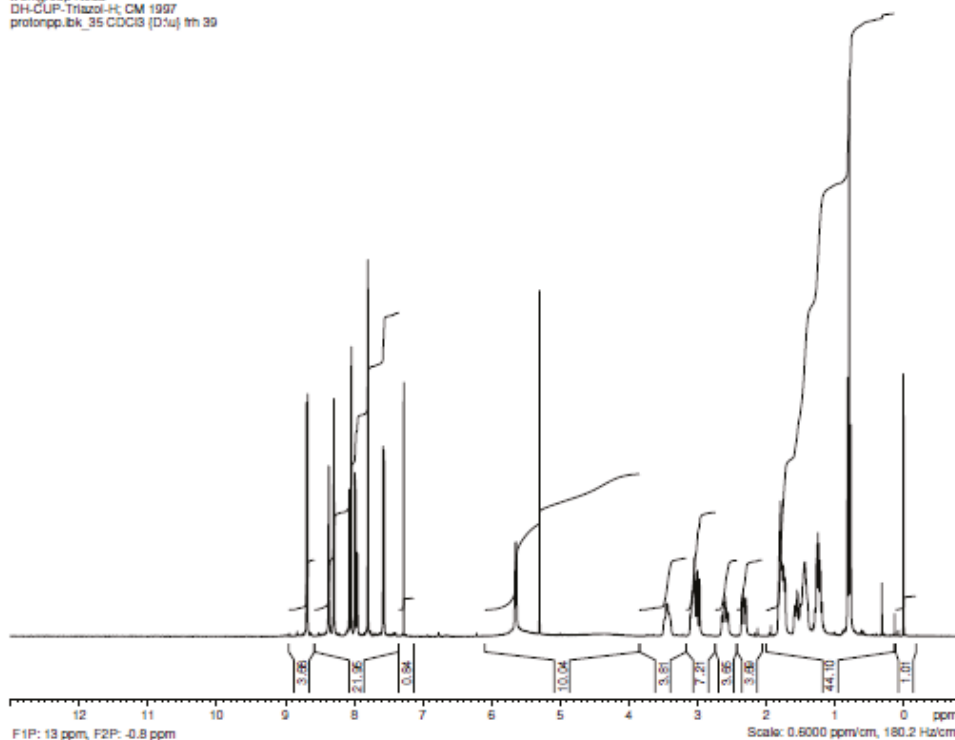


no. of the sticker on the nmr tube 605
color of the label blue
workgroup Neda
DH-CuUP-Triazol-SiMe3; CM 1997
c13cpd_m.tbk_35 CDCl₃ [D₂O] 1h 31



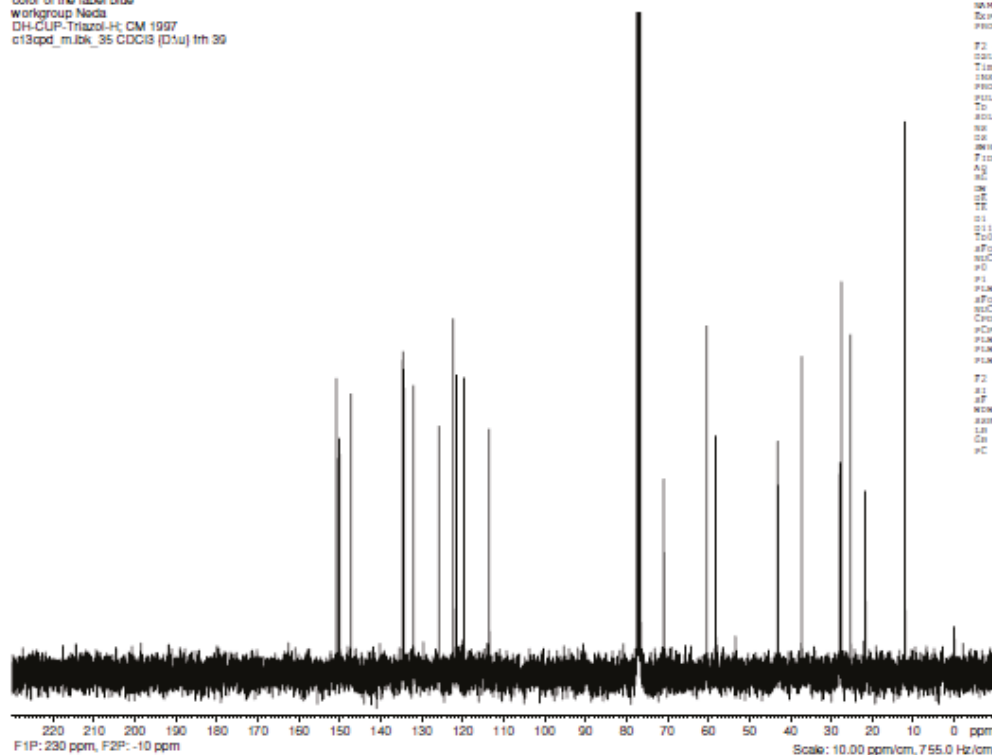
¹H- and ¹³C-NMR experiment for (R)-(6-(1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2S,4S,5R)-5-ethylquinuclidin-2-yl)methanol (**21**):

no. of the sticker on the nmr tube 568
color of the label blue
workgroup Nada
DH-CUP-Triazol-H, CM 1997
protompp.lib_35 CDCl₃ [D₂O] 1th 39



Current data parameters
NAME fth-210419-175221_in
Date_ 1
ProcDate 1
F2 - Acquisition parameters
Date_ 20210419
Time 22:12 h
INSTRUM AVI100300m
PROBHD z104275_0304_1
PULPROG zgpg30
TD 49152
SOLVENT CDCl₃
NS 24
DS 2
SWH 6203.474 Hz
FIDRES 0.262420 Hz
AQ 3.961651 sec
RG 166.74
DM 80.000 sec
DE 6.50 sec
TE 298.0 K
D1 1.0000000 sec
TDO 1
aF01 300.2618136 MHz
NUC1 13C
P0 6.00 sec
P1 12.00 sec
PLM1 10.8509983 W
F2 - processing parameters
SI 32768
SF 300.260084 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

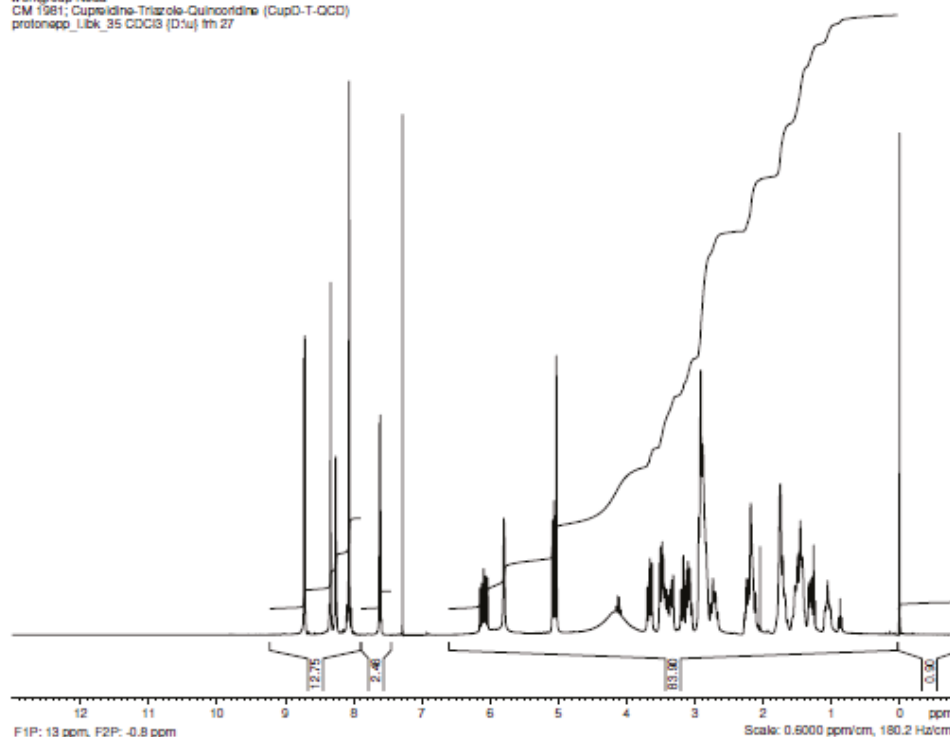
no. of the sticker on the nmr tube 568
color of the label blue
workgroup Nada
DH-CUP-Triazol-H, CM 1997
c13qpd_mubi_35 CDCl₃ [D₂O] 1th 39



Current data parameters
NAME fth-210419-175221_in
Date_ 2
ProcDate 1
F2 - Acquisition parameters
Date_ 20210419
Time 22:14 h
INSTRUM AVI100300m
PROBHD z104275_0304_1
PULPROG zgpg30
TD 65104
SOLVENT CDCl₃
NS 4
DS 4
SWH 19736.842 Hz
FIDRES 0.401547 Hz
AQ 2.490361 sec
RG 16.38
DM 25.333 sec
DE 6.50 sec
TE 298.0 K
D1 2.0000000 sec
D11 0.3300000 sec
TDO 1
aF01 75.5088171 MHz
NUC1 13C
P0 3.17 sec
P1 9.50 sec
PLM1 51.0579984 W
aF02 300.2612010 MHz
NUC2 1H
CHPAC[2] waltz16
aF03 90.00 sec
PLM2 10.8509983 W
PLM3 0.1829100 W
PLM4 0.0070300 W
F2 - processing parameters
SI 65536
SF 75.508821 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

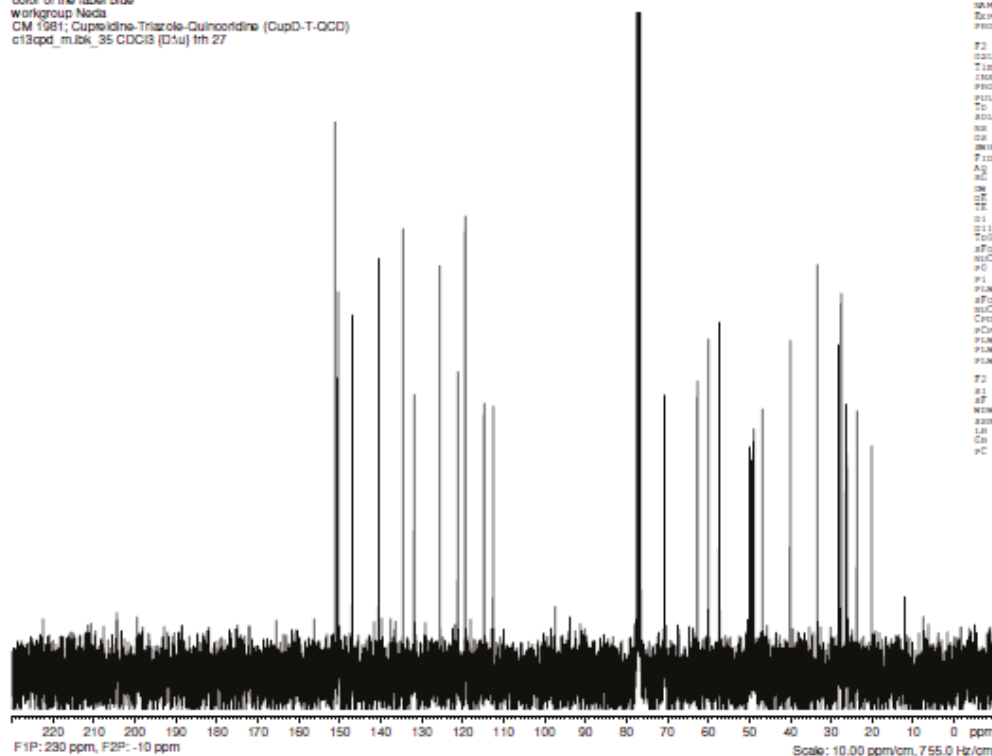
¹H- and ¹³C-NMR experiment for (S)-6-(4-((1S,3R,4S,6R)-6-(hydroxymethyl)quinuclidin-3-yl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2R,4S,5R)-5-vinylquinuclidin-2-yl)methanol (**24**):

no. of the sticker on the nmr tube 213
color of the label blue
workgroup Neda
CM 1981; Cupridine-Triazole-Quinoridine (CupD-T-QCD)
protonapp_lib_35 CDCl₃ [D₂O] 1h 27



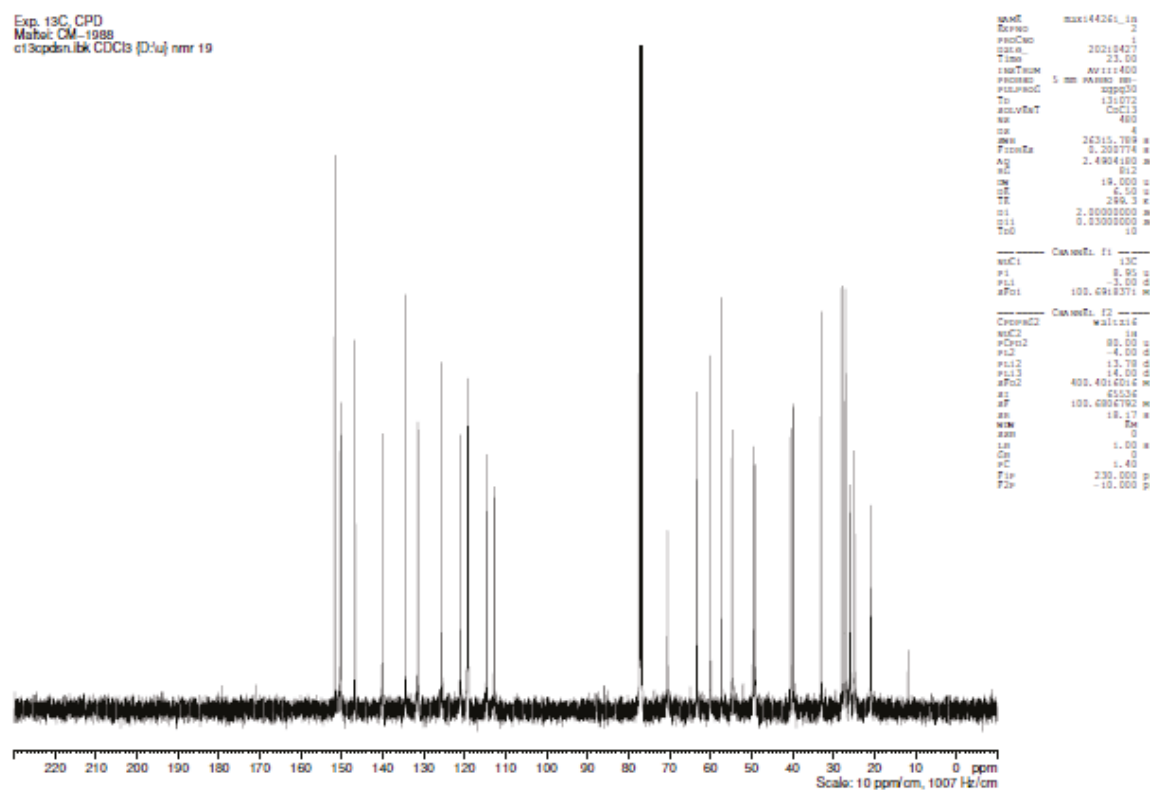
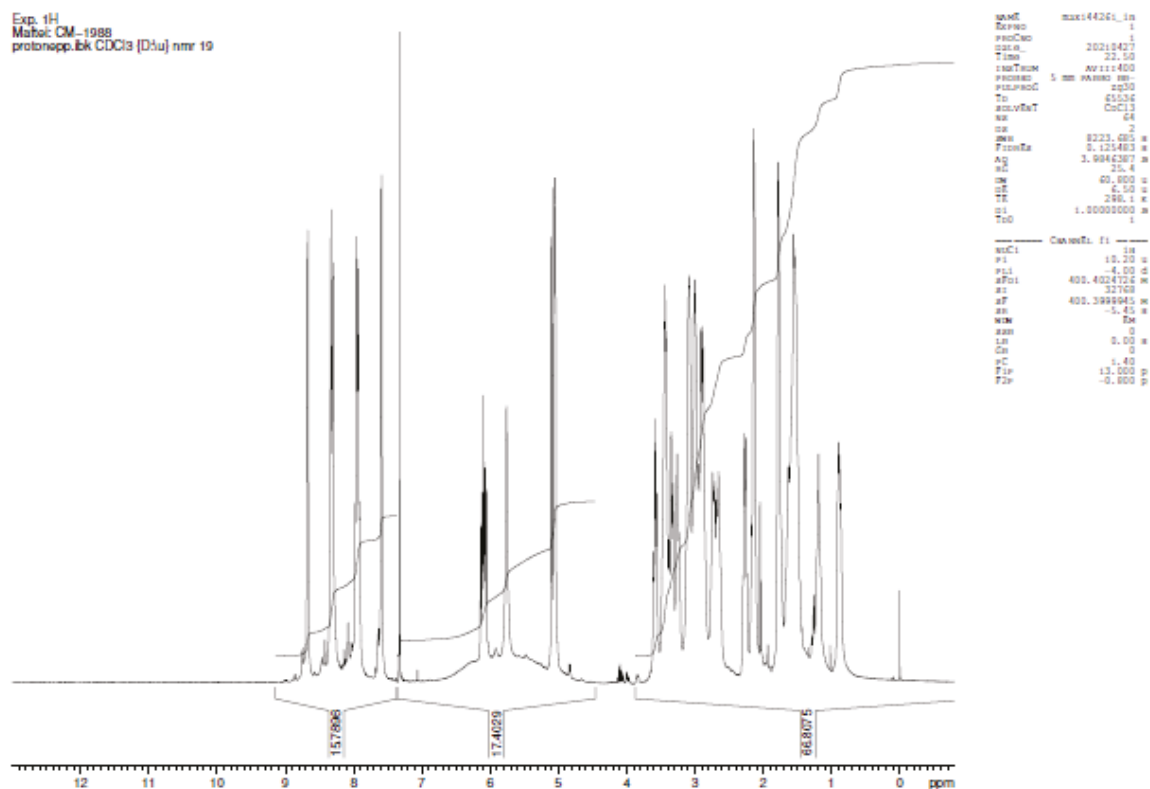
Current data parameters
NAME fdb-210618-171008_in
ExptNo 1
ProcNo 1
F2 - Acquisition parameters
Date_ 20210518
Time 23.24 h
INSTRUM AVI1000300M
PROBHD 2106276_0304 1
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 128
DS 2
SWH 6203.474 Hz
FIDRES 0.252420 Hz
AQ 3.561551 sec
RG 114.44
WM 80.620 mmsec
TE 298.0 K
DE 1.0000000 sec
D0 1
dF01 300.2618138 MHz
NUC1 1H
P0 8.20 mmsec
P1 12.20 mmsec
PL1 10.85099883 W
F2 - Processing parameters
SI 32768
SF 300.260074 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

no. of the sticker on the nmr tube 213
color of the label blue
workgroup Neda
CM 1981; Cupridine-Triazole-Quinoridine (CupD-T-QCD)
c13cpd_mlib_35 CDCl₃ [D₂O] 1h 27



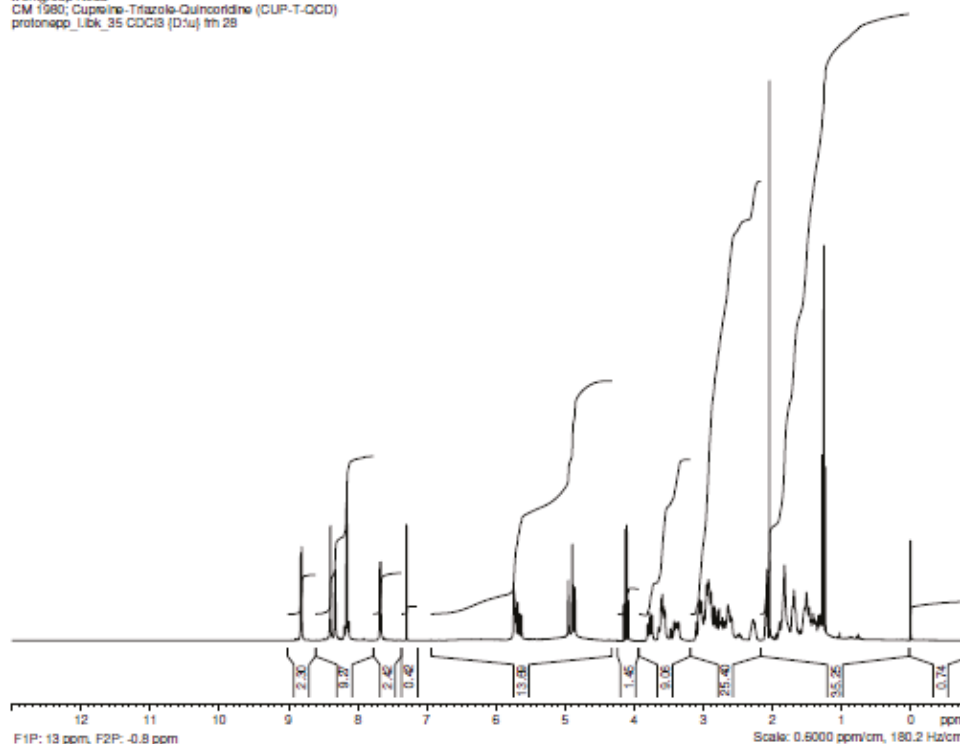
Current data parameters
NAME fdb-210618-171008_in
ExptNo 2
ProcNo 1
F2 - Acquisition parameters
Date_ 20210518
Time 23.49 h
INSTRUM AVI1000300M
PROBHD 2106276_0304 1
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 304
DS 4
SWH 19736.842 Hz
FIDRES 0.401647 Hz
AQ 2.4603679 sec
RG 18.42
WM 25.333 mmsec
TE 298.0 K
DE 0.0000000 sec
D0 0.0000000 sec
D1 1
dF01 75.508417 MHz
NUC1 13C
P0 3.17 mmsec
P1 8.50 mmsec
PL1 51.00799846 W
dF02 300.2612010 MHz
NUC2 1H
CPDPRG2 zgpg30
P0 80.20 mmsec
PLM2 10.85099883 W
PLM1 0.16290000 W
PLM3 0.09703000 W
F2 - Processing parameters
SI 65536
SF 75.508417 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.40

1H- and 13C-NMR experiment for (S)-(6-(4-((1S,3R,4S,6S)-6-(hydroxymethyl)quinuclidin-3-yl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2R,4S,5R)-5-vinylquinuclidin-2-yl)methanol (**25**):



1H- and 13C-NMR experiment for (R)-6-(4-((1S,3R,4S,6R)-6-(hydroxymethyl)quinuclidin-3-yl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2S,4S,5R)-5-vinylquinuclidin-2-yl)methanol (**26**):

no. of the sticker on the nmr tube 214
color of the label blue
workgroup Nada
CM 1980; Cupreline-Triazole-Quinocidine (CUP-T-QCD)
protonapp_lib_35 CDCl3 (D1u) 1h 28

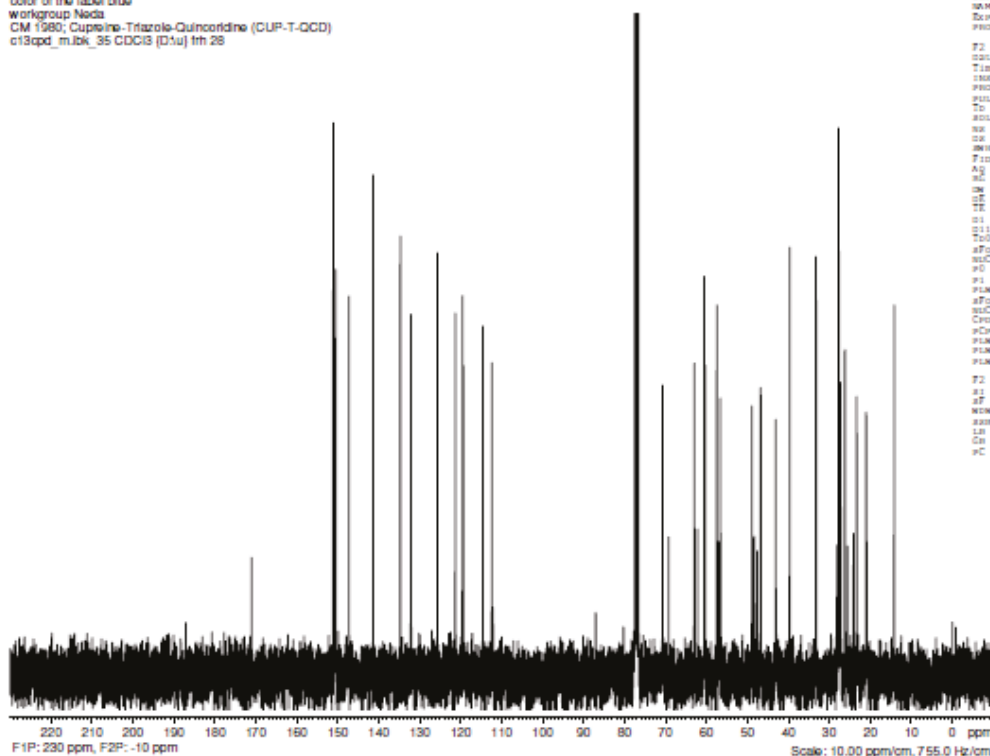


Current data parameters
NAME fcb-210428-171254_in
ExptNo 1
ProcNo 1

F2 - Acquisition parameters
Date_ 20210519
Time 0.18 h
INSTRUM Avance300M
PROBHD z104275_0359 (1
PULPROG zgpg30
TD 49152
SOLVENT CDCl3
NS 128
DS 2
SWH 6203.474 Hz
FIDRES 0.262420 Hz
AQ 3.901611 sec
RG 39.50
DM 80.400 USMC
DE 6.50 USMC
TE 298.0 K
D1 1.0000000 sec
TDO 1
dF01 300.2618138 MHz
NUC1 13C
P0 4.00 USMC
P1 12.00 USMC
PLN1 10.85099883 W

F2 - Processing parameters
SI 32768
SF 300.2600047 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

no. of the sticker on the nmr tube 214
color of the label blue
workgroup Nada
CM 1980; Cupreline-Triazole-Quinocidine (CUP-T-QCD)
c13cpd_mubk_35 CDCl3 (D1u) 1h 28



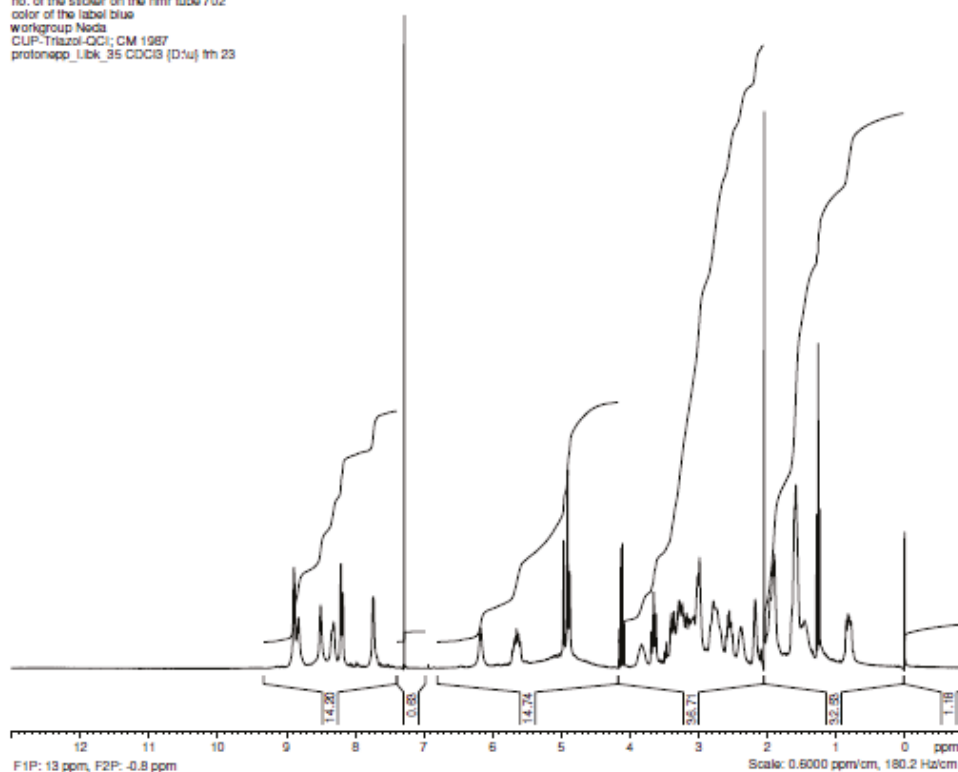
Current data parameters
NAME fcb-210428-171254_in
ExptNo 2
ProcNo 1

F2 - Acquisition parameters
Date_ 20210519
Time 0.42 h
INSTRUM Avance300M
PROBHD z104275_0359 (1
PULPROG zgpg30
TD 65104
SOLVENT CDCl3
NS 304
DS 4
SWH 19736.842 Hz
FIDRES 0.401547 Hz
AQ 2.4903679 sec
RG 18.42
DM 25.333 USMC
DE 6.50 USMC
TE 298.0 K
D1 2.0000000 sec
TDO 1
dF01 75.5088171 MHz
NUC1 13C
P0 3.17 USMC
P1 51.06798846 W
PLN1 300.2612010 MHz
dF02 75.5088171 MHz
NUC2 1H
CROSSPC[2] waltz16
PCPD2 90.00 USMC
PLN2 10.85099883 W
PLN3 0.16296050 W
PLN3 0.00703100 W

F2 - Processing parameters
SI 65536
SF 75.5088171 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

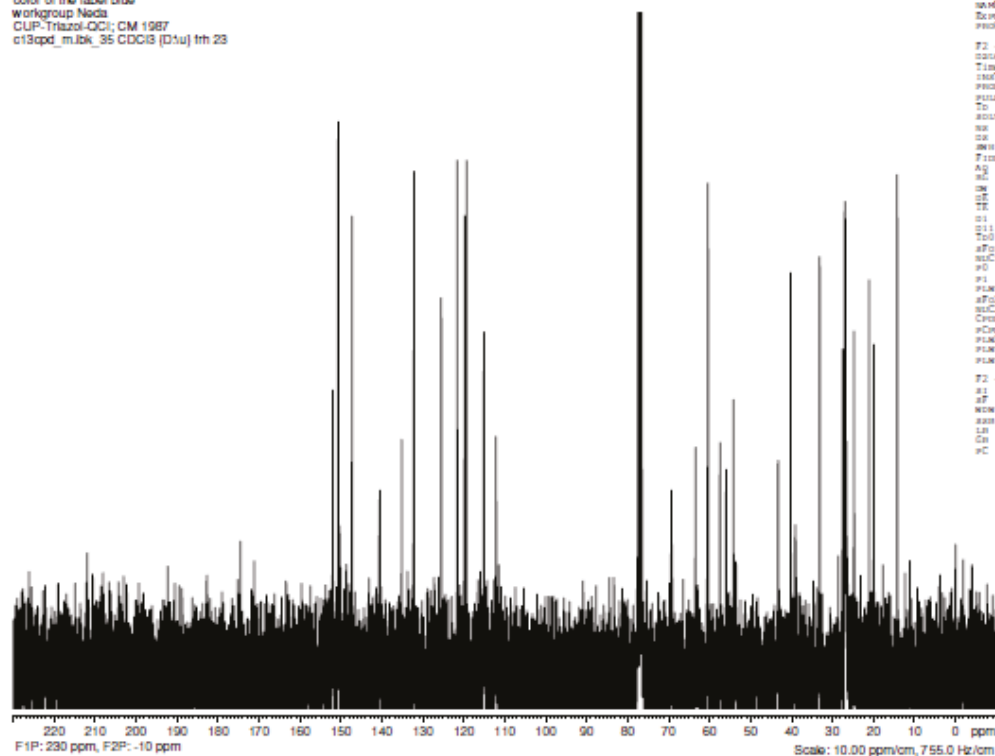
1H- and 13C-NMR experiment for (R)-(6-(4-((1S,3R,4S,6S)-6-(hydroxymethyl)quinuclidin-3-yl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2S,4S,5R)-5-vinylquinuclidin-2-yl)methanol (**27**):

no. of the sticker on the nmr tube 702
color of the label blue
workgroup Neda
CUP-Triazol-QC; CM 1987
protonapp_m_bk_35 CDCl3 [D1u] fth 23



```
Current data parameters
NAME: fth-210423-171022_in
EXPNO: 2
PROCNO: 1
F2 - Acquisition parameters
Date_: 20210424
Time: 2.34 h
INSTRUM: AVI100300N
PROBHD: z10427k_0319 1
PULPROG: zg30
TD: 65536
SOLVENT: CDCl3
NS: 128
DS: 2
SWH: 6203.414 Hz
FIDRES: 0.242420 Hz
AQ: 3.961601 sec
RG: 130.72
SQ: 80.600 uMVC
SE: 6.10 uMVC
TE: 298.0 K
D1: 1.0000000 sec
D2:
DELTA:
aFO1: 300.2618536 MHz
NUC1: 13C
PC: 4.00 uMVC
PI: 12.00 uMVC
PL1: 10.8509983 W
F2 - Processing parameters
SI: 32768
SF: 300.2600642 MHz
WDW: EM
SSB: 0
LB: 0 Hz
GB: 0
PC: 1.00
```

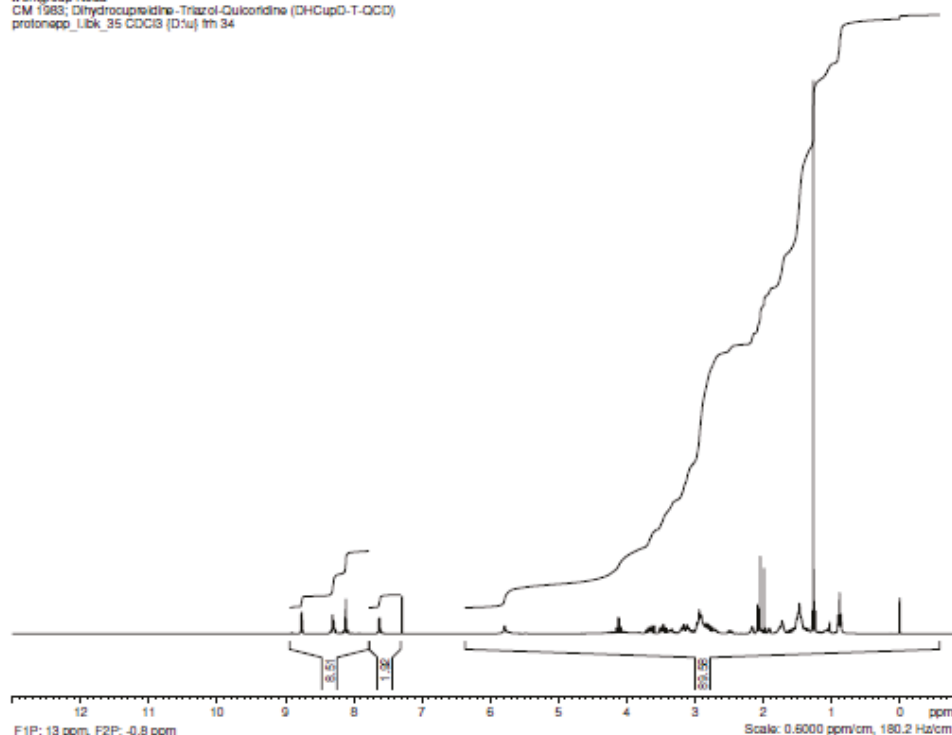
no. of the sticker on the nmr tube 702
color of the label blue
workgroup Neda
CUP-Triazol-QC; CM 1987
c13cpd_m_bk_35 CDCl3 [D1u] fth 23



```
Current data parameters
NAME: fth-210423-171022_in
EXPNO: 2
PROCNO: 1
F2 - Acquisition parameters
Date_: 20210424
Time: 2.34 h
INSTRUM: AVI100300N
PROBHD: z10427k_0319 1
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 304
DS: 4
SWH: 19736.842 Hz
FIDRES: 0.401547 Hz
AQ: 2.4903679 sec
RG: 22.61
SQ: 25.333 uMVC
SE: 6.10 uMVC
TE: 298.0 K
D1: 2.0000000 sec
D2: 0.3300000 sec
DELTA:
aFO1: 75.5088171 MHz
NUC1: 13C
PC: 3.17 uMVC
PI: 9.10 uMVC
PL1: 51.0579868 W
aFO2: 300.2612010 MHz
NUC2: 1H
CPDPRG2: waltz16
PCPD2: 90.00 uMVC
PLM2: 10.8509983 W
PLM3: 0.0091000 W
PLM13: 0.0070310 W
F2 - Processing parameters
SI: 65536
SF: 75.5054427 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
```

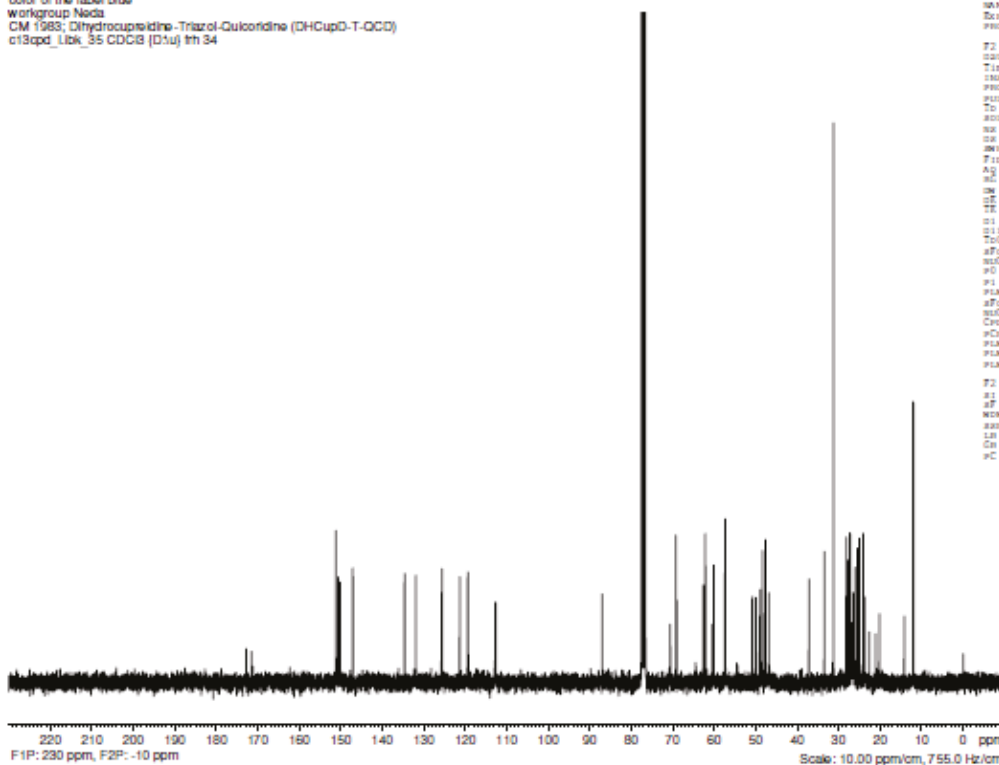
¹H- and ¹³C-NMR experiment for (S)-6-(4-((1S,3R,4S,6R)-6-(hydroxymethyl)quinuclidin-3-yl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2R,4S,5R)-5-ethylquinuclidin-2-yl)methanol (**28**):

no. of the sticker on the nmr tube 220
color of the label blue
workgroup Neda
CM 1983; Dihydrocupreidine-Triazol-Guicordine (DHCupD-T-GCD)
protonapp_Libk_35 CDC13 (D1u) 1h 34



Current data parameters
NAME fcb-210518-190557_in
ExptNo 1
ProcNo 1
F2 - Acquisition parameters
Date_ 20210519
Time 6.57 h
InstName AVE500000
PROBHD 2104275_0349
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 2
SWH 6203.474 Hz
FIDRES 0.252420 Hz
AQ 3.561641 sec
RG 89.15
WM 80.600 UMHz
QT 6.50 UMHz
TE 298.0 K
D1 1.0000000 sec
TDO 1
SFO1 300.2615136 MHz
NUC1 1H
P0 6.00 UMHz
P1 12.00 UMHz
PL1 10.85099883 W
F2 - Processing parameters
SI 32768
SF 300.260044 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

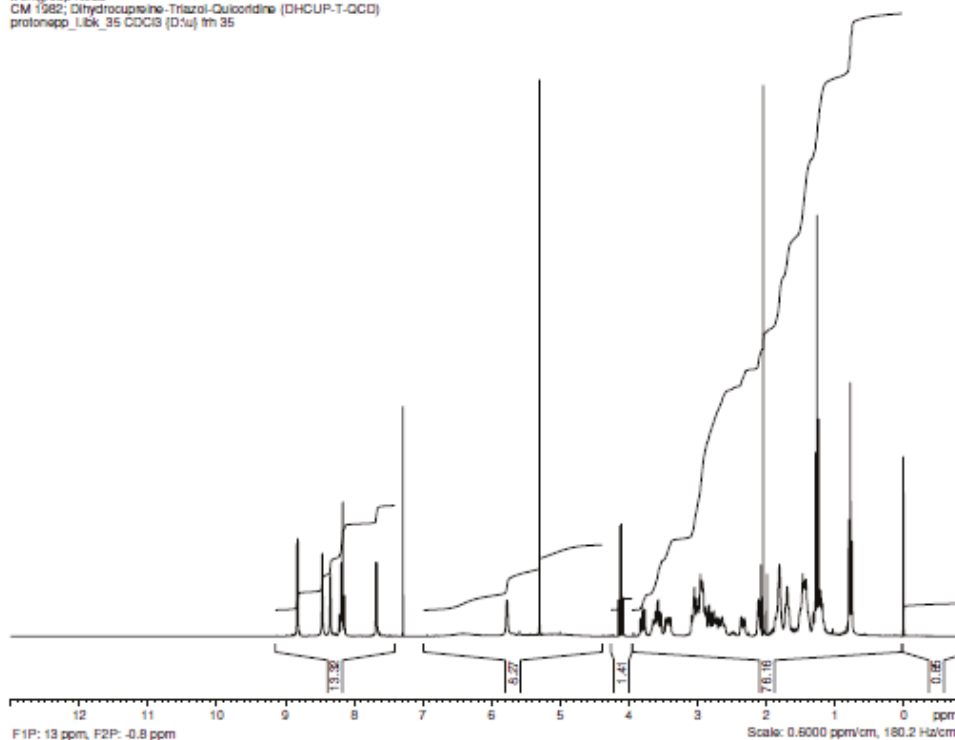
no. of the sticker on the nmr tube 220
color of the label blue
workgroup Neda
CM 1983; Dihydrocupreidine-Triazol-Guicordine (DHCupD-T-GCD)
c13cpd_Libk_35 CDC13 (D1u) 1h 34



Current data parameters
NAME fcb-210518-190557_in
ExptNo 2
ProcNo 1
F2 - Acquisition parameters
Date_ 20210519
Time 6.52 h
InstName AVE500000
PROBHD 2104275_0349
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 696
DS 8
SWH 19736.842 Hz
FIDRES 0.401547 Hz
AQ 2.4603479 sec
RG 18.62
WM 25.332 UMHz
QT 6.50 UMHz
TE 298.0 K
D1 2.0000000 sec
TDO 0.0300000 sec
SFO1 75.508171 MHz
NUC1 13C
P0 3.17 UMHz
P1 9.50 UMHz
PL1 51.05799866 W
SFO2 300.2612010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 UMHz
PLM2 10.85099883 W
PLM2 0.16091000 W
PLM2 0.09703100 W
F2 - Processing parameters
SI 65536
SF 75.508435 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

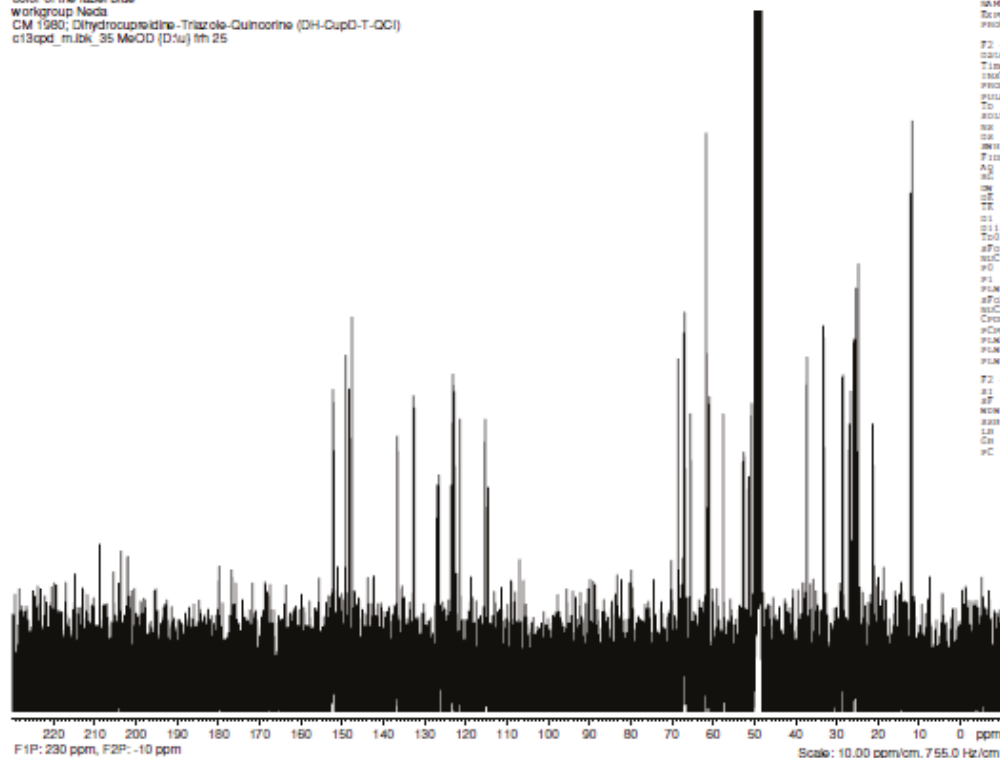
1H- and 13C-NMR experiment for (R)-6-(4-((1S,3R,4S,6R)-6-(hydroxymethyl)quinuclidin-3-yl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2S,4S,5R)-5-ethylquinuclidin-2-yl)methanol (**30**):

no. of the sticker on the nmr tube 221
color of the label blue
workgroup Neda
CM 1982; Dihydrocupreine-Triazol-Quinolone (DHCUP-T-QCQ)
protonapp Libk 35 CDC/3 [D:u] fm 35



```
Current data parameters
NAME      frb-202001-180904.in
Ntimes    1
Nchan      8
Nfreq      1
F2 - Acquisition parameters
Date       20200109
Time       6.34 h
Observer   AVI100000000
PROGRAM   zid4757_0356.f
PULPROG    zg30
PCPPROG     0
PCPDPRG     0
PCPDPRG2    0
SR         128
MW          6203.474 MHz
BW          9.230420 MHz
SFO         3.9616561 MHz
F0          100.72
SF           80.40 MHz
DM           6.50 MHz
DM2         298.0
SF1          1.000000000 MHz
F1           300.2618138 MHz
F2           8.0 MHz
F3           8.0 MHz
P1           12.50 MHz
P2           10.50099683 MHz
F2 - processing parameters
NAME      300.2601010 MHz
Ntimes    0
Nchan      8
Nfreq      0
SR         0
MW          0
BW          0
SFO         0
F0          0
SF           0
DM           0
DM2         0
SF1          0
F1           0
F2           1.00
```

no. of the slider on the nmr tube 299
color of the label blue
workgroup Neda
CM 1980; Dihydrocupreidine-Triazole-Quinocine (DH-Cup-D-T-QC)
c13acd_mjbk 35 MeOD (D₂O) fh 25



```

Current data parameters
NAME      Feb-2015-1800sk_in
EXPNO     2
PROCNO    1
PROCNAME  

F2 - Acquisition parameters
NAME      Feb-2015-1800sk_in
TIME      3.33 h
INSTRUM    AUTOSCAN
STARTTIME  2014075-1800
PULPROG    zgpg30
PCPDPRG2    3
AQ         0.004
AQUNIT     ms
RG          304
NS          4
DS          1
FIDRES     18736.942 Hz
F1RES      8.401547 Hz
AQ         2.469333 sec
RG          57.6
SI          3.533 UMIC
SI          5.40 UMIC
TE          298.0 K
DE          1.0000000
DE          0.13000000 sec
AQ         0.004
AQUNIT     ms
RG          75.508833 MHz
RG          132
P1          9.10 UMIC
P1          51.079966 sec
AQ         300.261200 MHz
AQ         1.0000000
CYCLES2    2
PCPDPRG2    waltz16
PCPDPRG2    0.00 UMIC
PCPDPRG2    10.16509983
PCPDPRG2    0.16291000 MHz
PCPDPRG2    0.09703100 U

```

1H- and 13C-NMR experiment for (R)-(6-(4-((1S,3R,4S,6S)-6-(hydroxymethyl)quinuclidin-3-yl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2S,4S,5R)-5-ethylquinuclidin-2-yl)methanol (**31**):

no. of the sticker on the nmr tube 298

color of the label blue

workgroup Neda

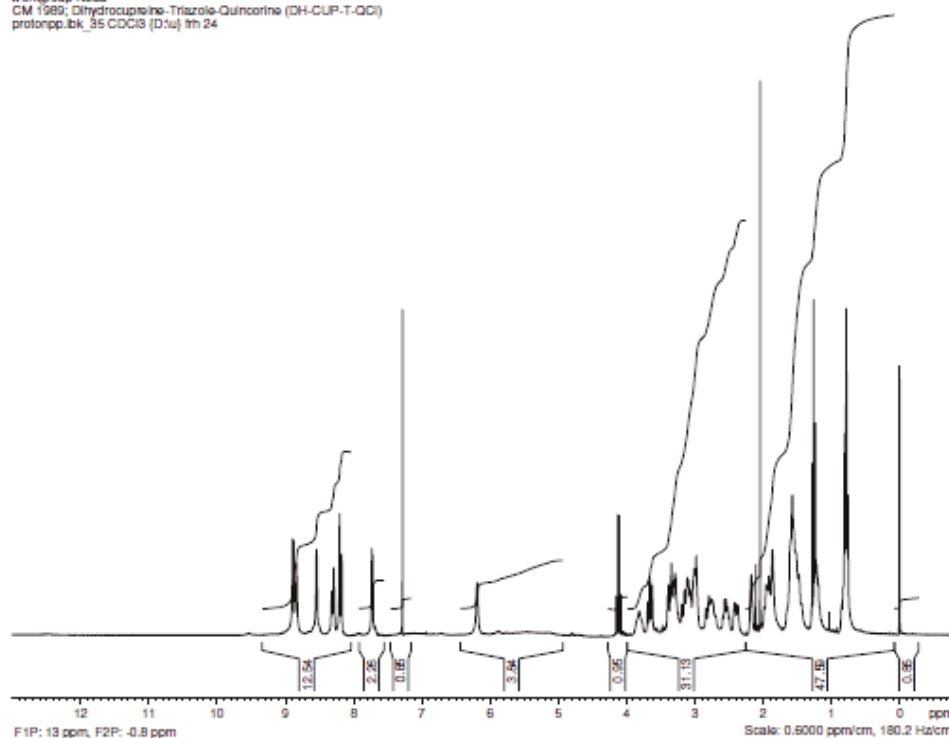
CM 1989; Dihydrocupreine-Triazole-Quinoline (DH-CUP-T-QC)

protonpp.lib, 35 CDCIS (D1u) fh 24

Current data parameters
NAME fcs-21021-190719_in
ExptNo 1
ProcNo 1

F2 - Acquisition parameters
Date_ 20210622
Time 1.28 h
InstName AVI100300M
Proces 2104279_0349_1
PulprogC zgpg30
TD 65536
AcqMeth CAC13
NS 24
DS 2
SWH 6203.474 Hz
Fwhm 8.252420 Hz
AQ 3.901641 sec
RG 116.46
DM 80.620 MHz
DE 6.50 MHz
TE 298.0 K
D1 1.0000000 sec
TD0 1
aFol 300.2618138 MHz
NUC1 13C
P0 6.00 MHz
P1 12.00 MHz
PL1 10.81099883 W

F2 - processing parameters
SI 32768
aF 300.2600540 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



no. of the sticker on the nmr tube 298

color of the label blue

workgroup Neda

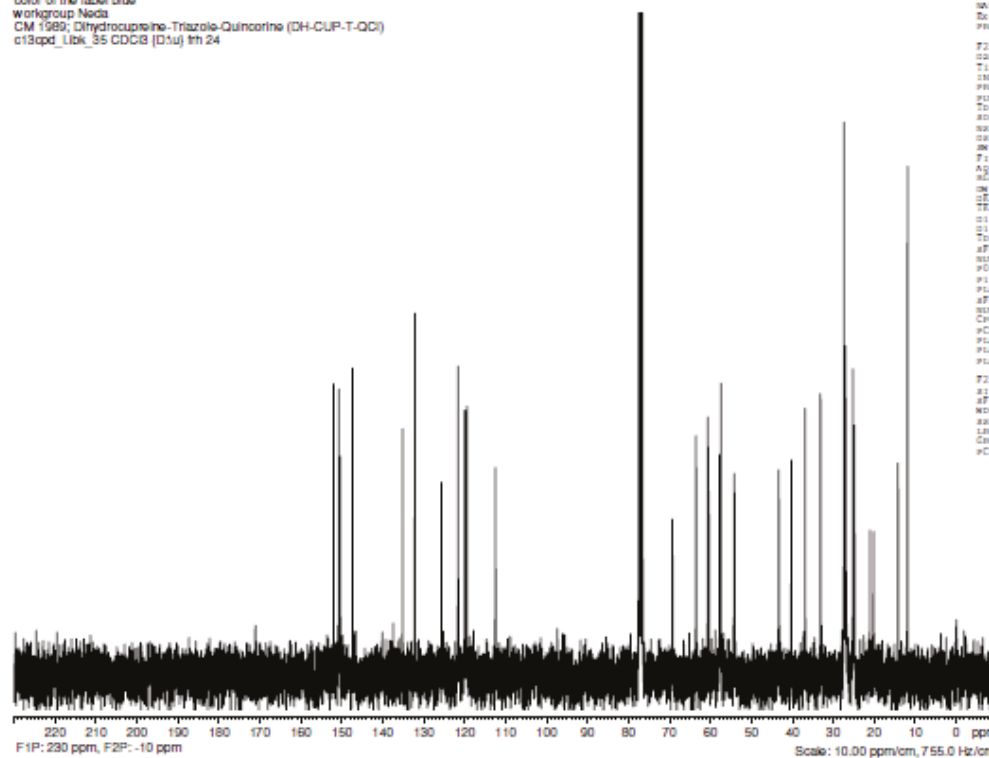
CM 1989; Dihydrocupreine-Triazole-Quinoline (DH-CUP-T-QC)

c13qpd.lib, 35 CDCIS (D1u) fh 24

Current data parameters
NAME fcs-21021-190719_in
ExptNo 2
ProcNo 1

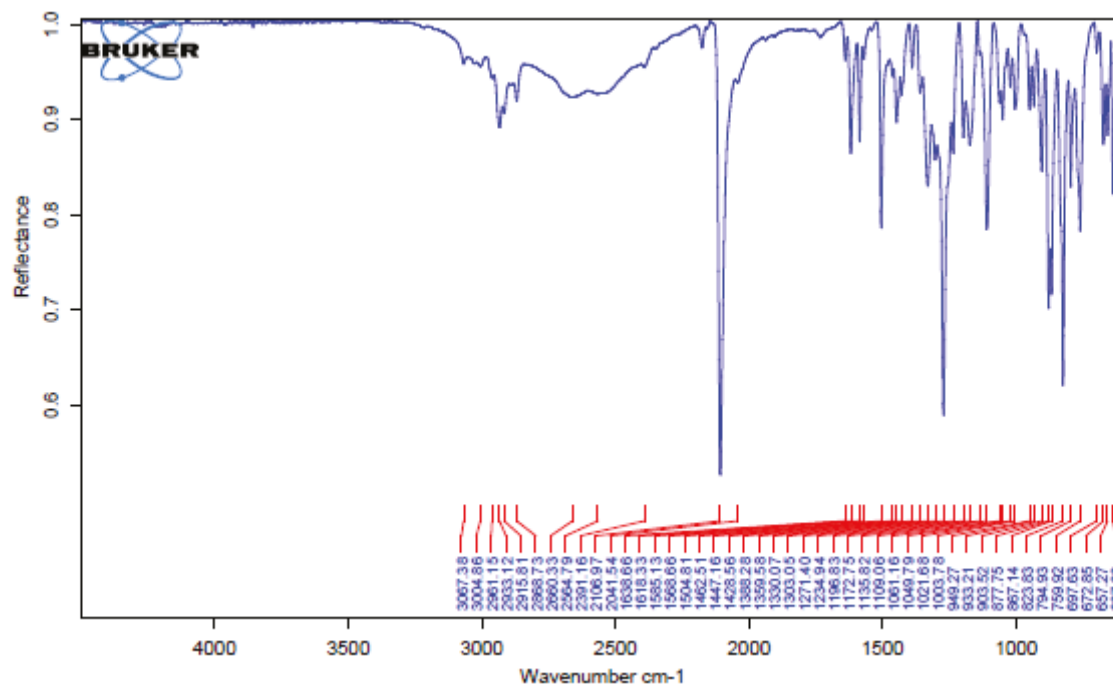
F2 - Acquisition parameters
Date_ 20210622
Time 1.23 h
InstName AVI100300M
Proces 2104279_0349_1
PulprogC zgpg30
TD 65536
AcqMeth CAC13
NS 4
DS 4
SWH 19736.842 Hz
Fwhm 8.401547 Hz
AQ 2.4903670 sec
RG 11.62
DM 25.323 MHz
DE 6.50 MHz
TE 298.0 K
D1 2.0000000 sec
TD0 1
aFol 75.5088171 MHz
NUC1 13C
P0 3.17 MHz
P1 51.05799866 W
aFol2 300.2612010 MHz
NUC2 1H
CompC[2] waltz16
PCh2 90.00 MHz
PLM2 10.81099883 W
PLM12 0.18291000 W
PLM13 0.00703050 W

F2 - processing parameters
SI 65536
aF 75.5088420 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

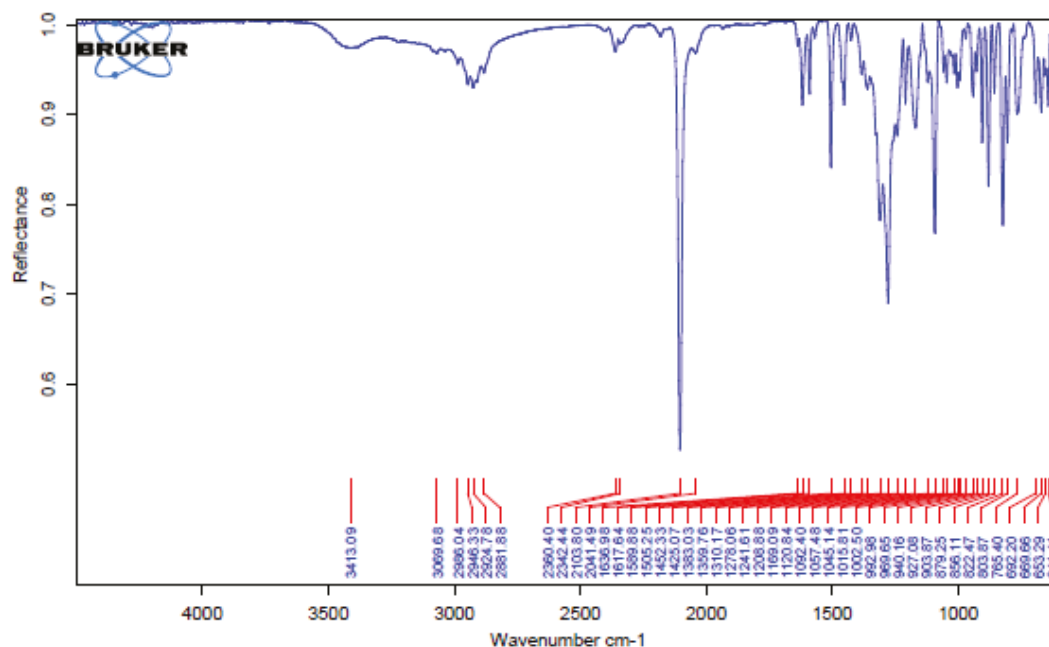


IR spectroscopy

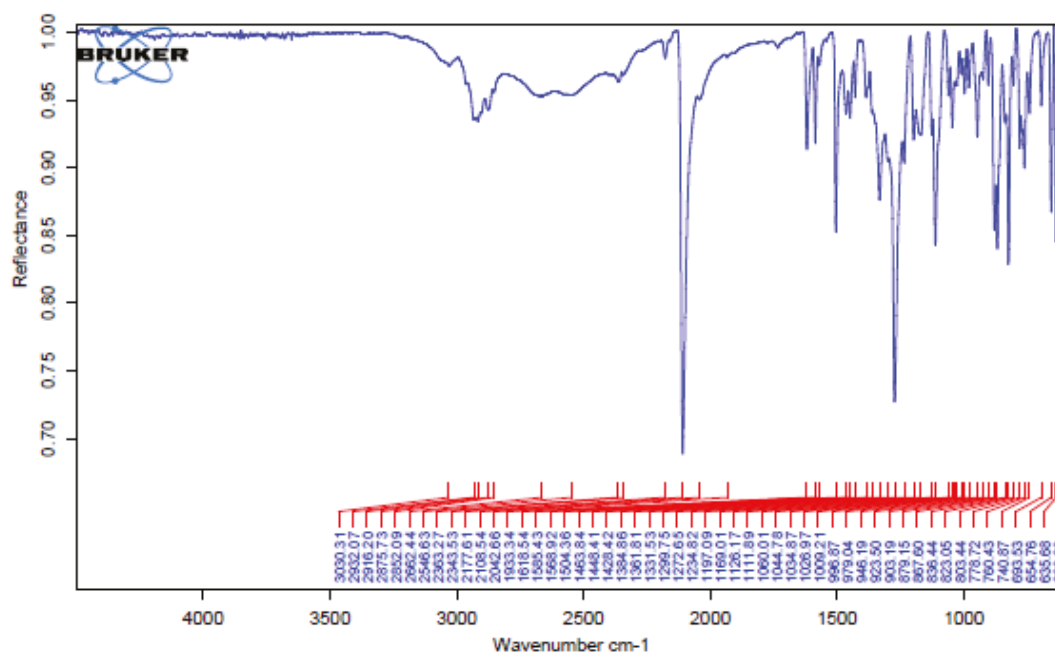
IR spectrogram for (S)-(6-azidoquinolin-4-yl)((1S,2R,4S,5R)-5-vinylquinuclidin-2-yl)methanol (8):



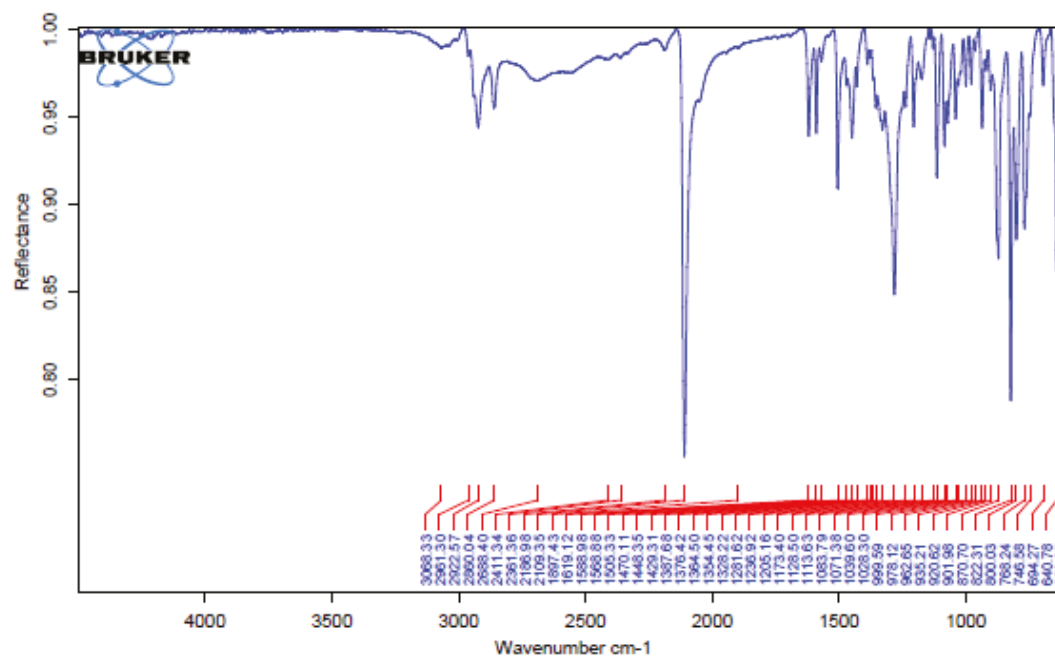
IR spectrogram for (R)-(6-azidoquinolin-4-yl)((1S,2S,4S,5R)-5-vinylquinuclidin-2-yl)methanol (9):



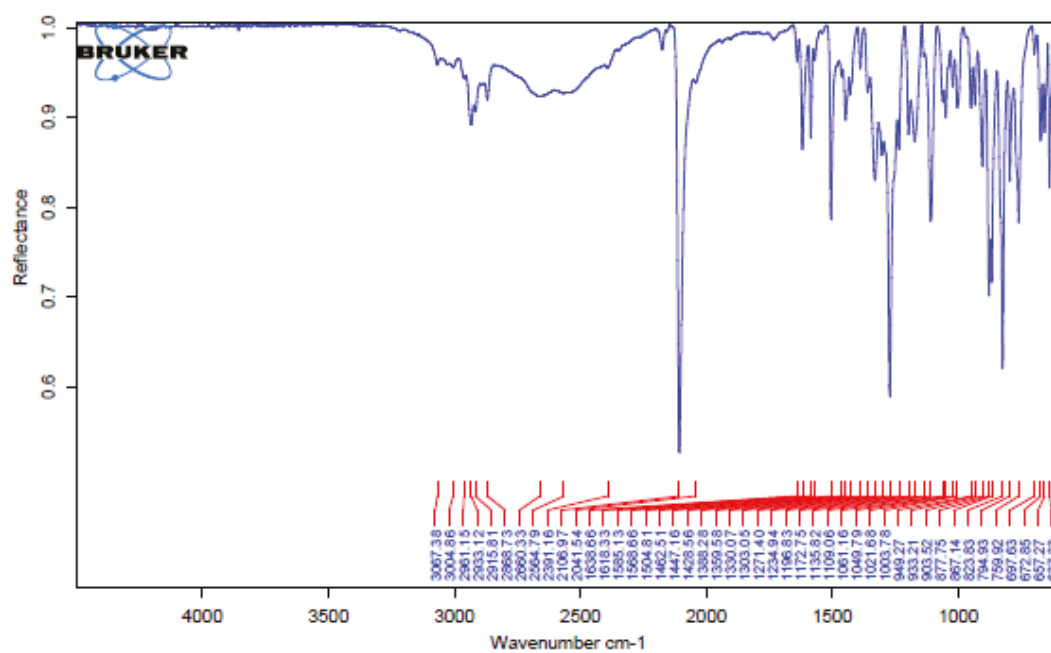
IR spectrogram for (S)-(6-azidoquinolin-4-yl)((1S,2R,4S,5R)-5-ethylquinuclidin-2-yl)methanol (**10**):



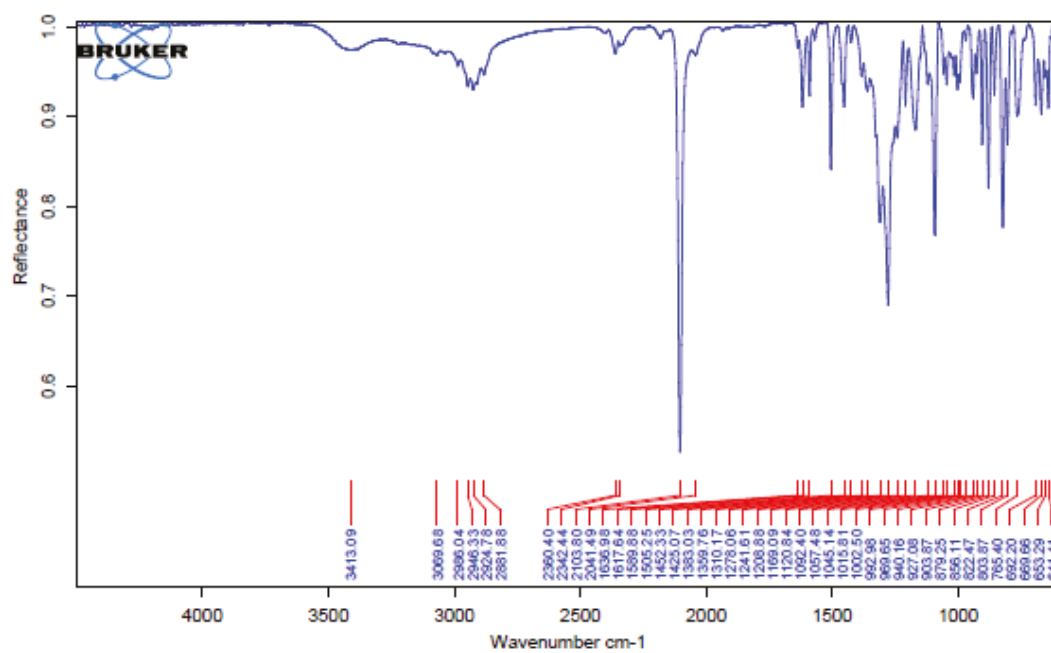
IR spectrogram for (R)-(6-azidoquinolin-4-yl)((1S,2S,4S,5R)-5-ethylquinuclidin-2-yl)methanol (**11**):



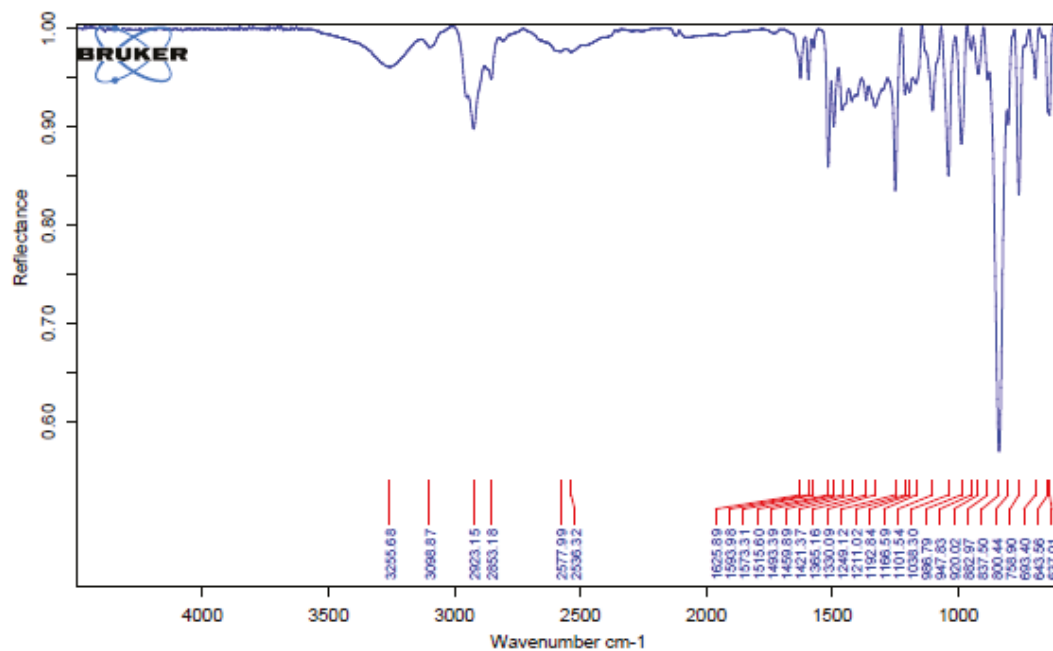
IR spectrogram for (S)-(6-azidoquinolin-4-yl)((1S,2R,4S,5S)-5-ethynylquinuclidin-2-yl)methanol (**12**):



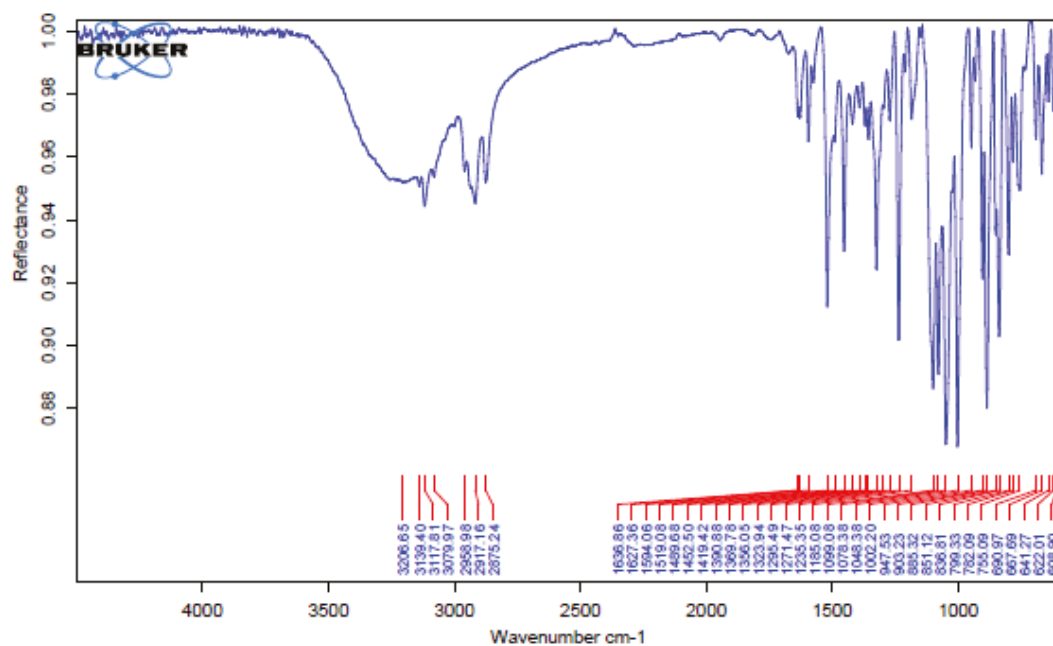
IR spectrogram for (R)-(6-azidoquinolin-4-yl)((1S,2S,4S,5S)-5-ethynylquinuclidin-2-yl)methanol (**13**):



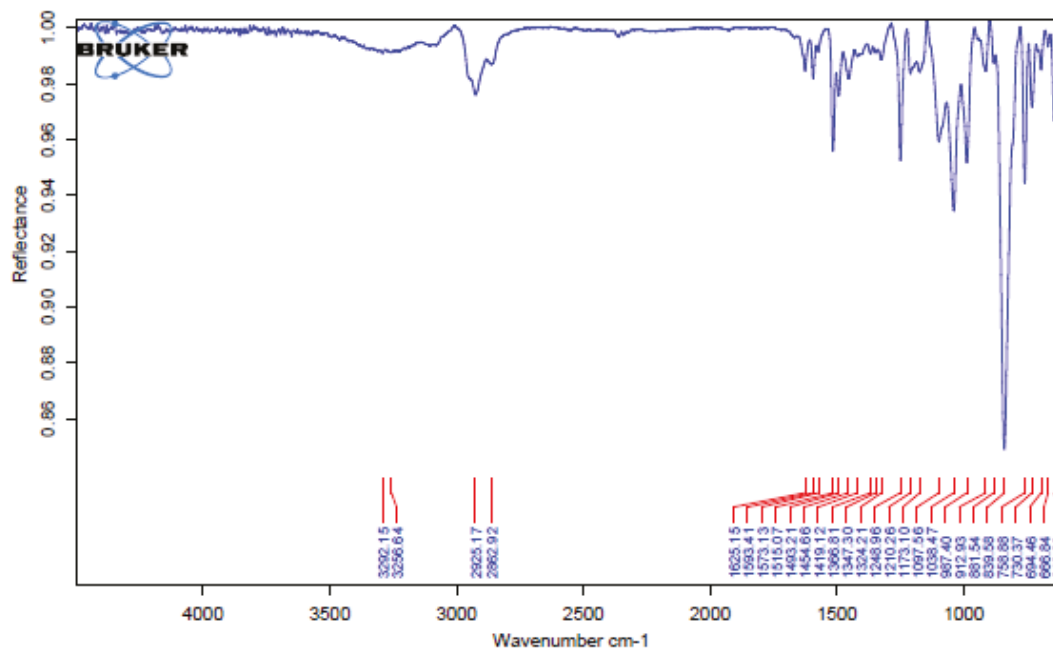
IR spectrogram for (S)-(6-(4-(trimethylsilyl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2R,4S,5R)-5-vinylquinuclidin-2-yl)methanol (**14**):



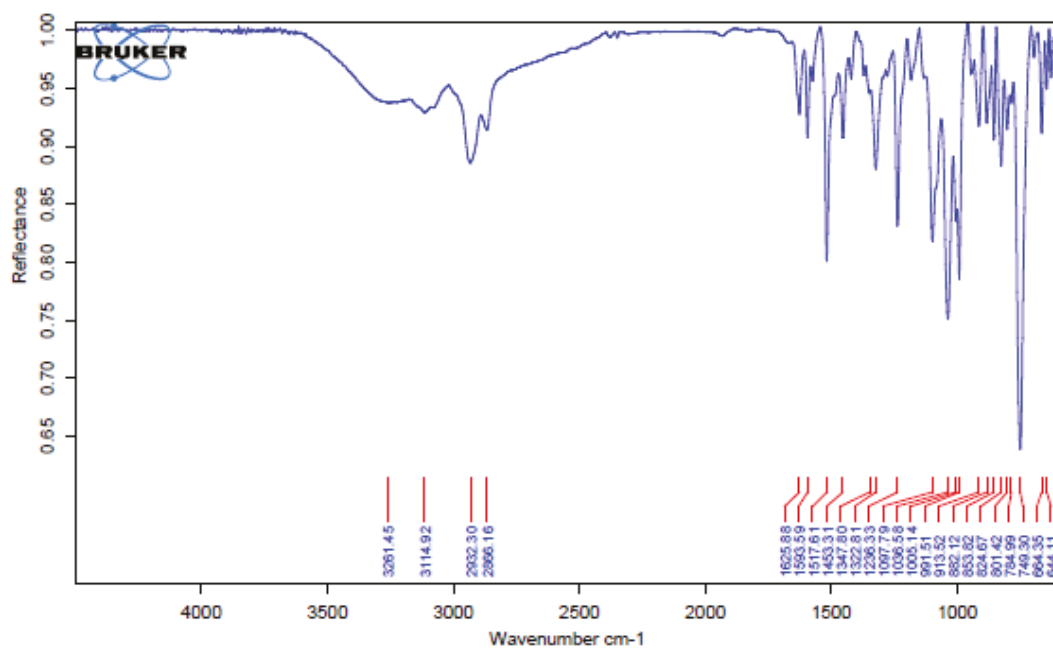
IR spectrogram for (S)-(6-(1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2R,4S,5R)-5-vinylquinuclidin-2-yl)methanol (**15**):



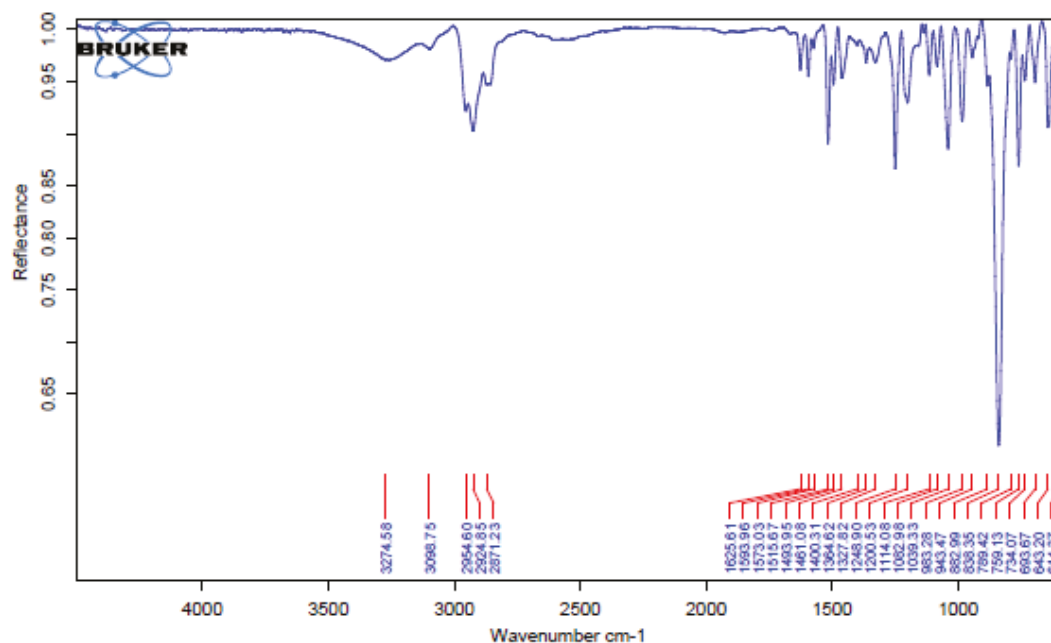
IR spectrogram for (R)-(6-(4-(trimethylsilyl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2S,4S,5R)-5-vinylquinuclidin-2-yl)methanol (**16**):



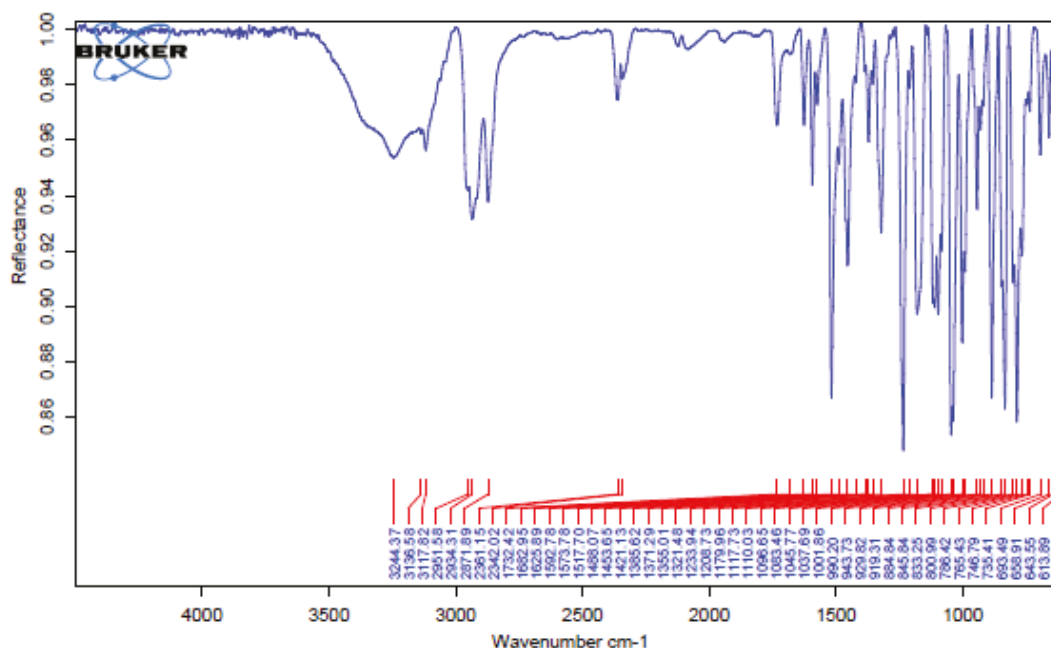
IR spectrogram for (R)-(6-(1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2S,4S,5R)-5-vinylquinuclidin-2-yl)methanol (**17**):



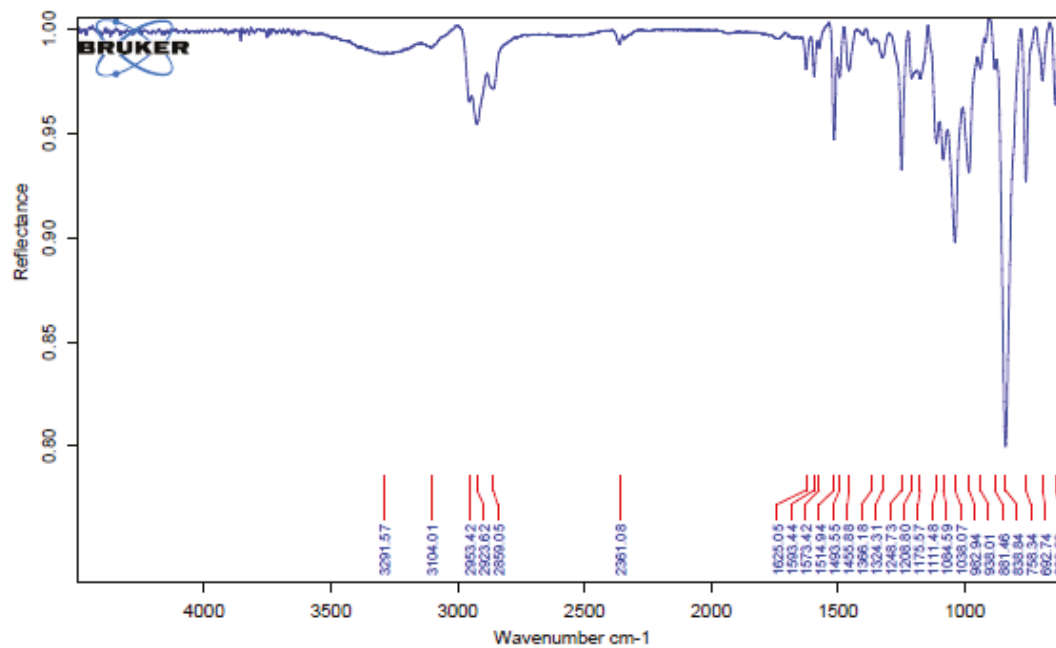
IR spectrogram for (S)-(6-(4-(trimethylsilyl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2R,4S,5R)-5-ethylquinuclidin-2-yl)methanol (**18**):



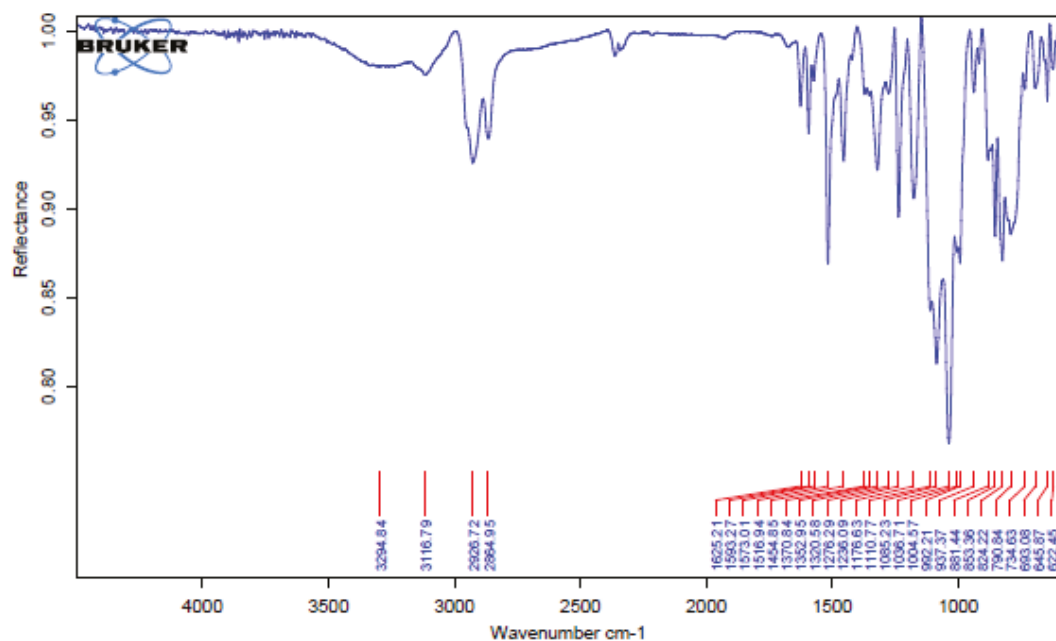
IR spectrogram for (S)-(6-(1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2R,4S,5R)-5-ethylquinuclidin-2-yl)methanol (**19**):



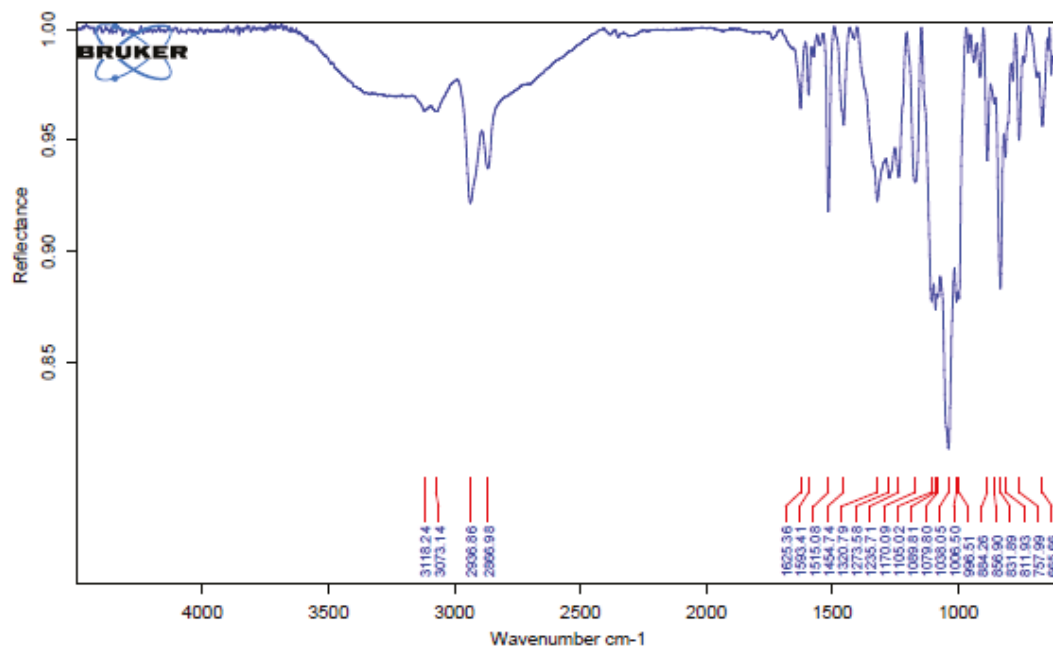
IR spectrogram for (R)-(6-(4-(trimethylsilyl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2S,4S,5R)-5-ethylquinuclidin-2-yl)methanol (**20**):



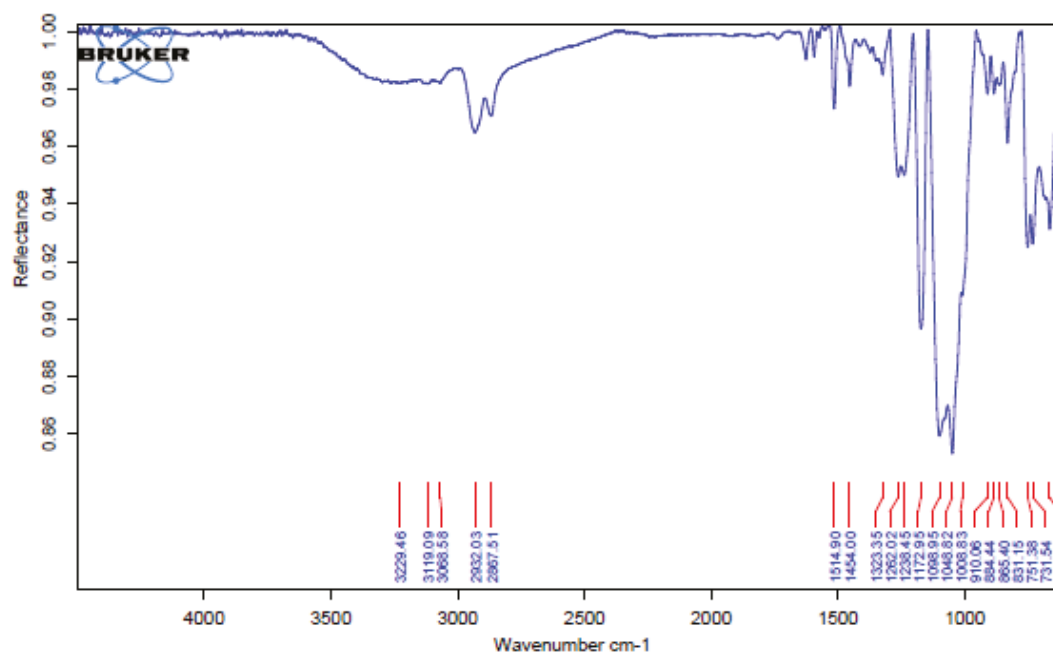
IR spectrogram for (R)-(6-(1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2S,4S,5R)-5-ethylquinuclidin-2-yl)methanol (**21**):



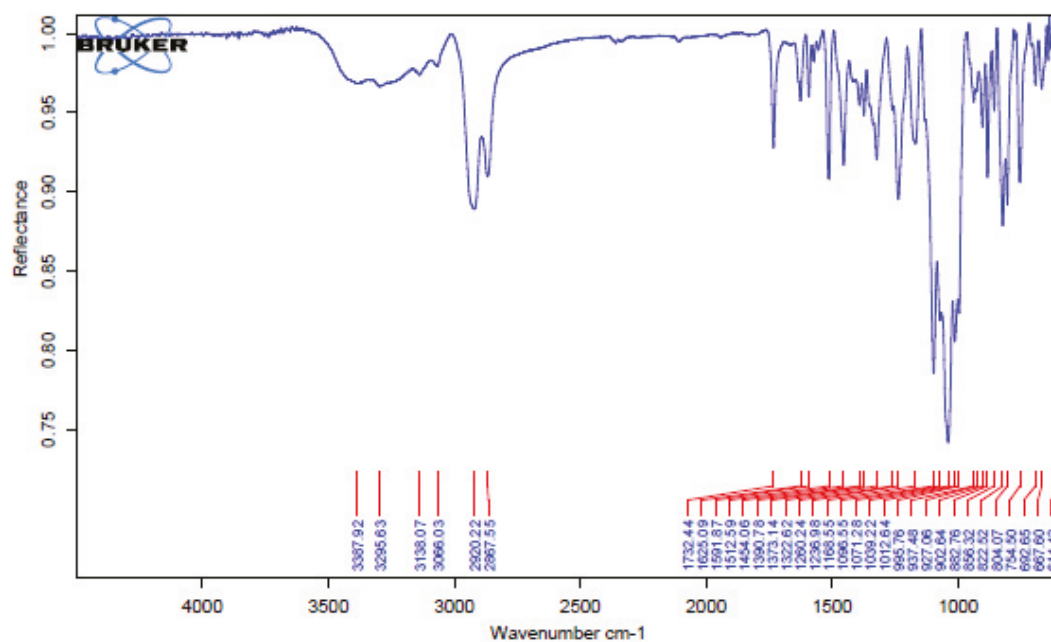
IR spectrogram for (S)-(6-(4-((1S,3R,4S,6R)-6-(hydroxymethyl)quinuclidin-3-yl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2R,4S,5R)-5-vinylquinuclidin-2-yl)methanol (**24**):



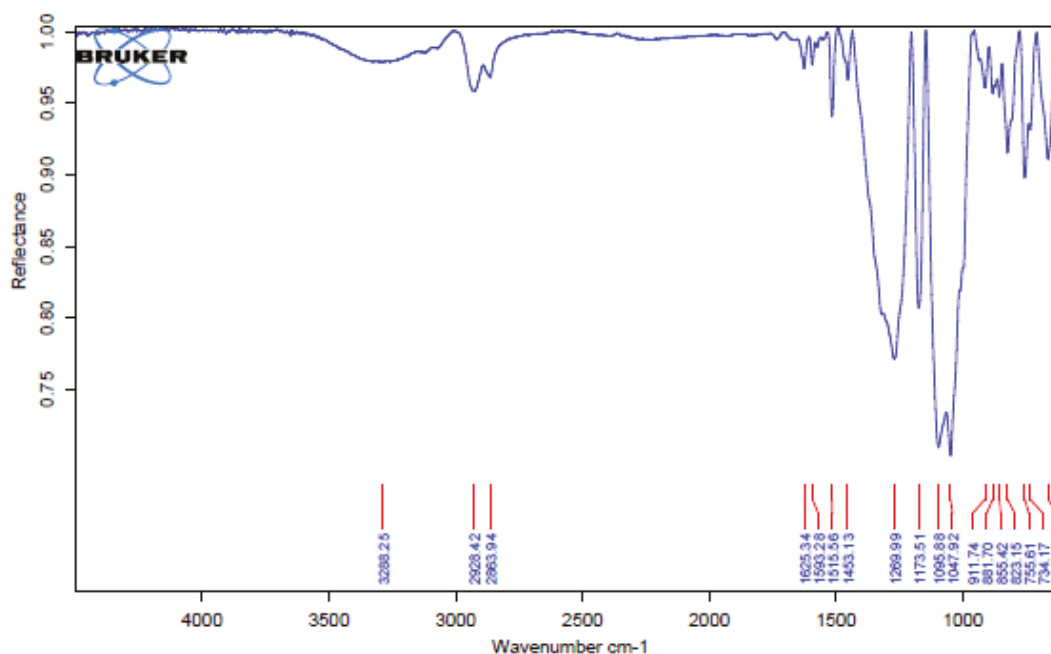
IR spectrogram for (S)-(6-(4-((1S,3R,4S,6S)-6-(hydroxymethyl)quinuclidin-3-yl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2R,4S,5R)-5-vinylquinuclidin-2-yl)methanol (**25**):



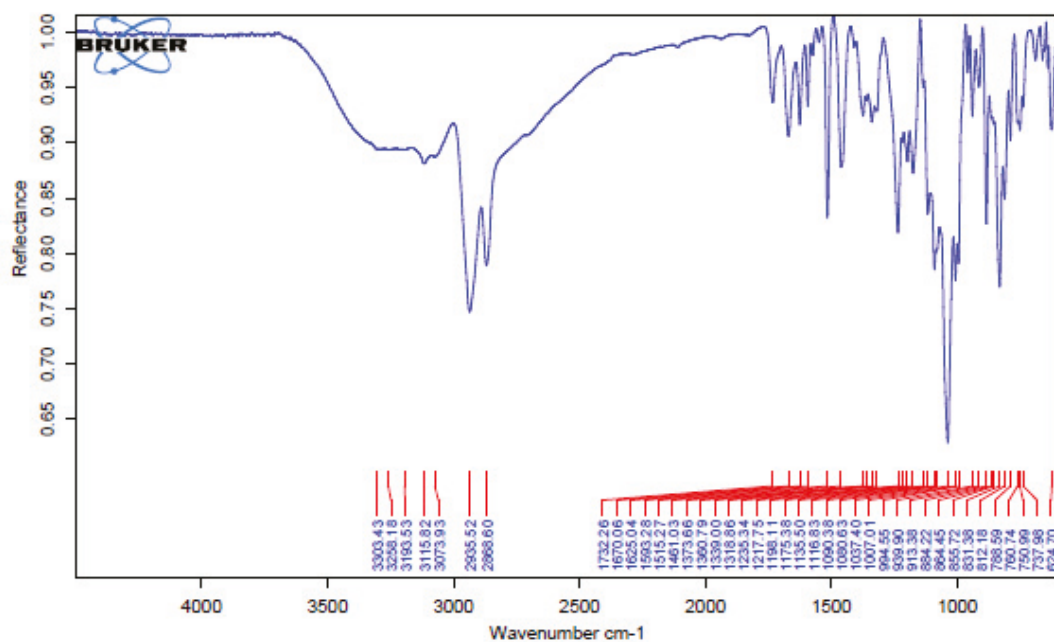
IR spectrogram for (R)-(6-(4-((1S,3R,4S,6R)-6-(hydroxymethyl)quinuclidin-3-yl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2S,4S,5R)-5-vinylquinuclidin-2-yl)methanol (**26**):



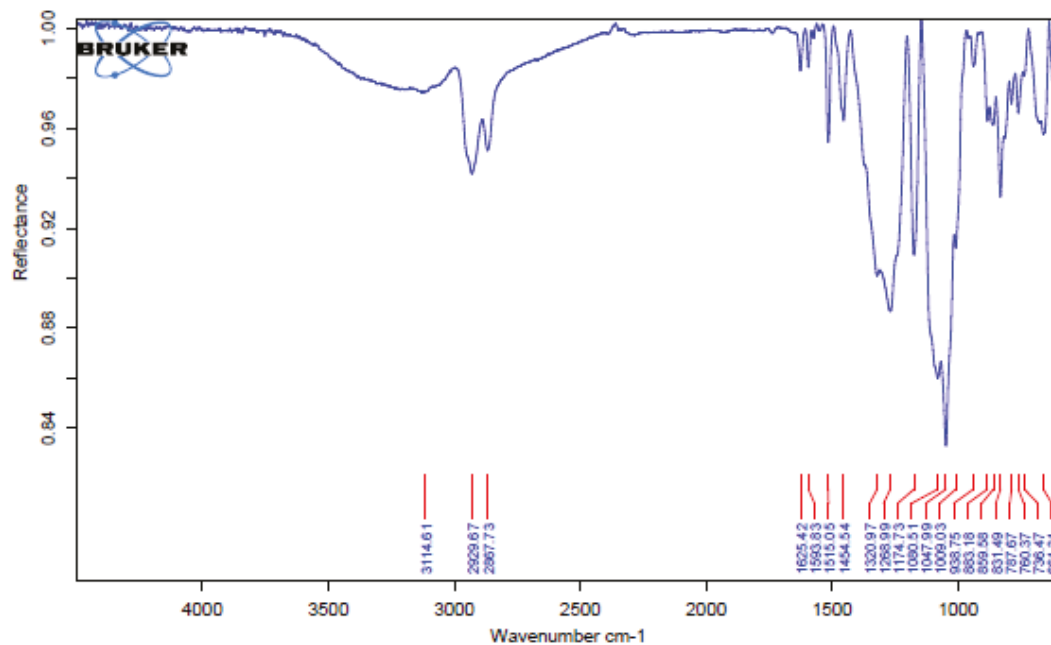
IR spectrogram for (R)-(6-(4-((1S,3R,4S,6S)-6-(hydroxymethyl)quinuclidin-3-yl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2S,4S,5R)-5-vinylquinuclidin-2-yl)methanol (**27**):



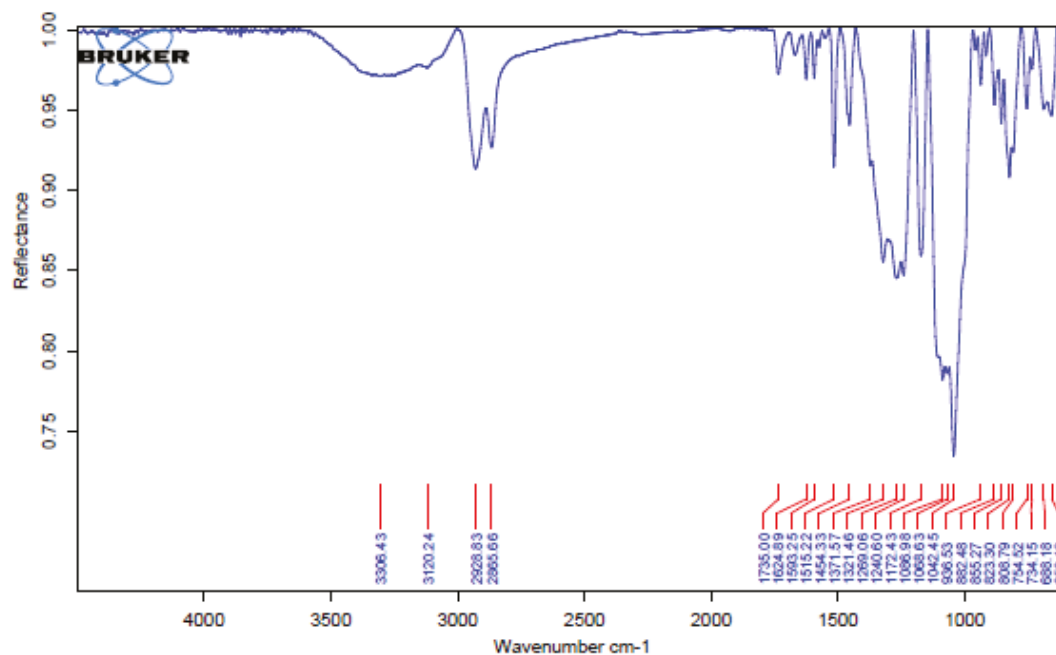
IR spectrogram for (S)-(6-(4-((1S,3R,4S,6R)-6-(hydroxymethyl)quinuclidin-3-yl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2R,4S,5R)-5-ethylquinuclidin-2-yl)methanol (**28**):



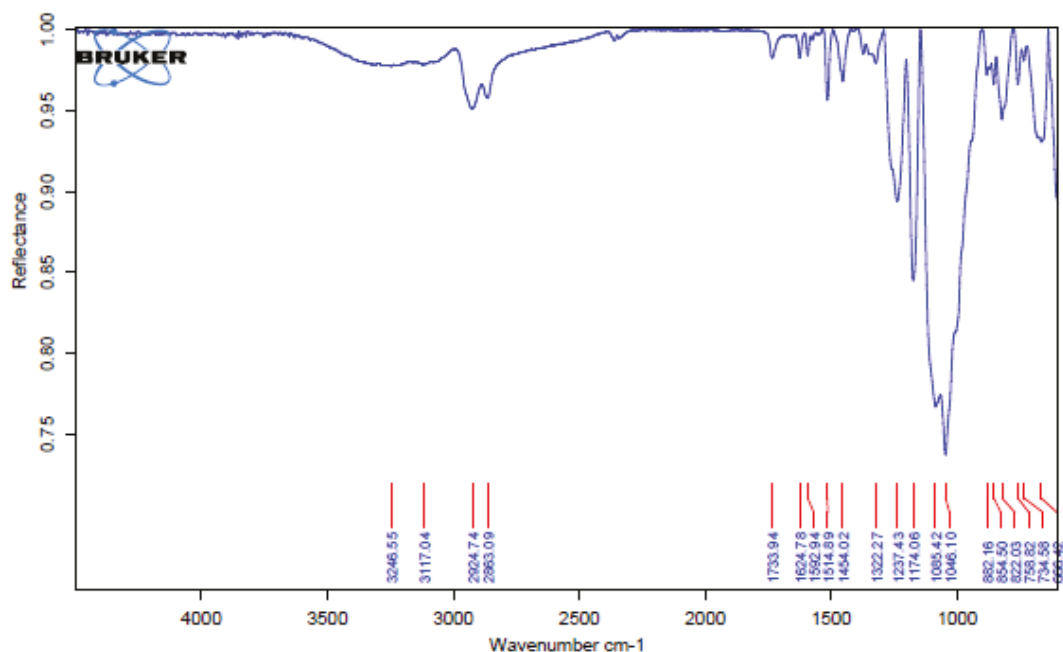
IR spectrogram for (S)-(6-(4-((1S,3R,4S,6S)-6-(hydroxymethyl)quinuclidin-3-yl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2R,4S,5R)-5-ethylquinuclidin-2-yl)methanol (**29**):



IR spectrogram for (R)-(6-(4-((1S,3R,4S,6R)-6-(hydroxymethyl)quinuclidin-3-yl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2S,4S,5R)-5-ethylquinuclidin-2-yl)methanol (**30**):



IR spectrogram for (R)-(6-(4-((1S,3R,4S,6S)-6-(hydroxymethyl)quinuclidin-3-yl)-1H-1,2,3-triazol-1-yl)quinolin-4-yl)((1S,2S,4S,5R)-5-ethylquinuclidin-2-yl)methanol (**31**):



X ray

Table S1. Crystallographic data collection parameter of **10**, **11** and **28**

Compound	10	11	28
Formula	C ₁₉ H ₂₁ N ₅ O	C ₁₉ H ₂₃ N ₅ O ₁ , ½ H ₂ O	C ₂₉ H ₃₈ N ₆ O ₂ , 0.81 HCl, 1.76 H ₂ O
M _r /(g mol ⁻¹)	335.41	346.43	564.03
crystal shape	lath	fragment	lath
crystal colour	clear colourless	clear light brown	clear colourless
cryst. dim. /mm ³	0.451 ⊗ 0.072 ⊗ 0.035	0.220 ⊗ 0.118 ⊗ 0.022	0.379 ⊗ 0.121 ⊗ 0.047
crystal system	monoclinic	monoclinic	orthorhombic
space group (no.)	<i>P</i> 2 ₁ (4)	<i>C</i> 2 (5)	<i>C</i> 2 ₁ 2 ₁ 2 ₁ (19)
<i>a</i> /Å	10.4912(3)	23.1964(4)	8.5435(1)
<i>b</i> /Å	7.6623(2)	6.3113(1)	14.1133(2)
<i>c</i> /Å	10.6905(3)	12.0528(3)	24.5445(3)
↗	90°	90°	90°
↗	101.591(3)°	98.714°	90°
↗	90°	90°	90°
<i>V</i> /Å ³	841.85(4)	1744.16(6)	2959.50(7)
<i>Z</i> , <i>Z'</i>	2, 1	4, 1	4, 1
<i>D</i> _{calcd.} /(g cm ⁻³)	1.323	1.319	1.266
↗ /mm ⁻¹ (↗ ⊗ ⊗ Å)	0.687 (1.54184)	0.698 (1.54184)	1.338 (1.54184)
Absorption corr.	multi-scan	multi-scan	multi-scan
⊗ range (compl.)	4.22 – 77.93° (98.9%)	3.71 – 77.74° (98.0%)	4.78 – 77.90° (99.8%)
refl. measured	66650	10314	155939
unique (<i>R</i> _{int})	3554 (0.0843)	3147 (0.0177)	6279 (0.0560)
observed ^a	3446	3096	6221
param. / restr.	230 / 1	240 / 1	387 / 9
<i>R</i> ₁ (obs. rflns.) ^a	0.0370	0.0249	0.0408
<i>wR</i> ₂ (all rflns.)	0.1012	0.0659	0.1086
GooF on <i>F</i> ²	1.025	1.042	1.058
Abs. Struct.	–0.02(12)	–0.02(7)	0.025(3)
Param.			
max/min ↗ /(eÅ ⁻³)	0.173 / –0.227	0.167 / –0.147	0.167 / –0.147
CCDC No.	2080994	2080992	2080993

^a Observation criterion: $I > 2\sigma(I)$.