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Boron-based hybrids as novel scaffolds for the development of drugs with neuroprotective properties

Ivana Cacciatore, a,* Hasan Turkez, Annalisa Di Rienzo, Michele Ciulla, Adil Mardinoglu, c,d and Antonio Di Stefano

SUPPORTING INFORMATION

NMR and MS spectra of compounds

NMR Spectra (3aR)-2-(azidomethyl)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[d][1,3,2]dioxaborole (2)

Agilent Technologies

Gradient Shimming

Sample Name:

/export/home/chempack/vnmrsys/data Sample directory: Archive directory: Data Collected on: m300-me/rcury300

FidFile: PROTON

Data collected on: Feb 11 2015 Pulse Sequence: PROTON (s2pul) Solvent: cdc13

Operator: caccia

OBSERVE H1, 300.1976543 MHz Relax. delay 1.000 sec Total time 1 min 29 sec Acq. time 1.706 sec Width 4803.1 Hz Pulse 45.0 degrees 32 repetitions DATA PROCESSING FT size 16384

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Width 4803.1 Hz

32 repetitions DATA PROCESSING

FT size 16384

0.11

Operator: caccia

Sample directory:

FidFile: PROTON

Solvent: cdc13

Gradient Shimming

Sample Name:

NMR Spectra of ((3aR)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[d][1,3,2]dioxaborol-2-yl)methanaminium chloride (3)

Agilent Technologies

Sample Name:
Data Collected on:
m300-mercury300
Archive directory:

Gradient Shimming

/export/home/chempack/vnmrsys/data Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul) Solvent: cd3cd Data collected on: Mar 18 2015

Operator: caccia

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.706 sec
Width 4803.1 Hz
32 repetitions
OBSERVE H1, 300.1988371 MHz
DATA PROCESSING
FT size 16384
Total time 1 min 29 sec

Sample Name:

Archive directory: Data Collected on: m300-mercury300

/export/home/chempack/vnmrsys/data Sample directory:

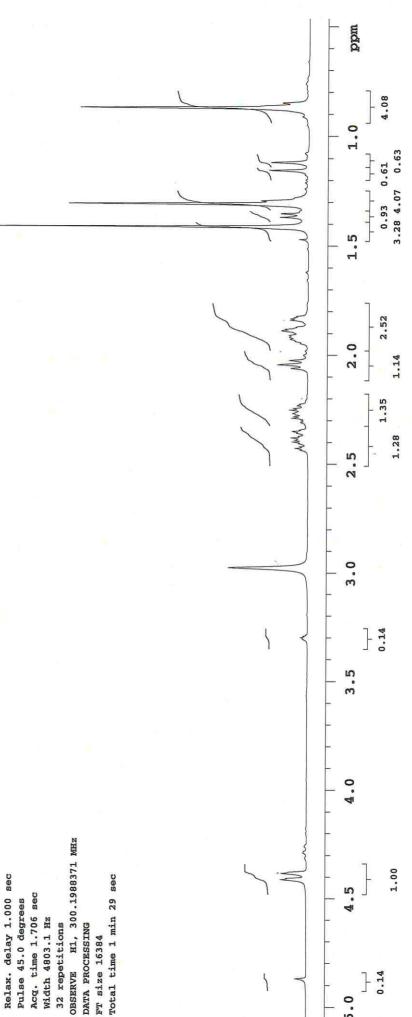
FidFile: PROTON

Pulse Sequence: PROTON (s2pul) Solvent: cd3od

Data collected on: Mar 18 2015

Operator: caccia

Relax. delay 1.000 sec Acq. time 1.706 sec Width 4803.1 Hz Pulse 45.0 degrees



NMR AND MS SPECTRA of 5-((S)-1,2-dithiolan-3-yl)-N-(((3aR)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[d][1,3,2]dioxaborol-2-yl)methyl)pentanamide (BLA)

Sample Name:

Data Collected on: m300-mercury300

/export/home/chempack/vnmrsys/data Sample directory: Archive directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13 Data collected on: Mar 27 2015

Operator: caccia

Relax. delay 1.000 sec Acq. time 1.706 sec Pulse 45.0 degrees

Width 4803.1 Hz 8 repetitions

OBSERVE H1, 300.1976543 MHz DATA PROCESSING

FT size 16384

Total time 0 min 23 sec

wdd 10 12

13LA

Sample Name:

Data Collected on: m300-mercury300

/export/home/chempack/vnmrsys/data Sample directory: Archive directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Data collected on: Mar 27 2015 Solvent: cdcl3

Operator: caccia

Relax. delay 1.000 sec

Acq. time 1.706 sec Pulse 45.0 degrees

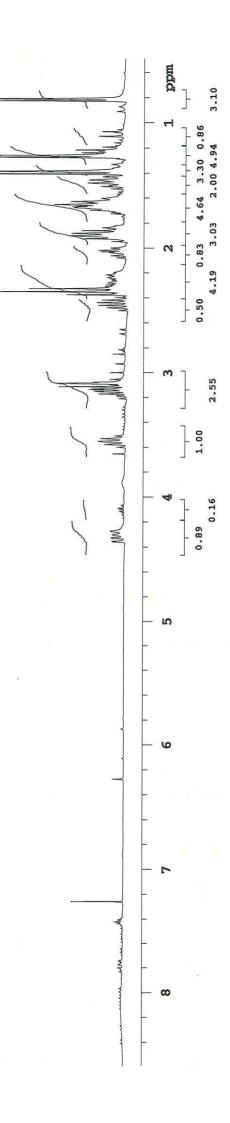
Width 4803.1 Hz

8 repetitions

OBSERVE H1, 300.1976543 MHz DATA PROCESSING

FT size 16384

Total time 0 min 23 sec



Sample Name:

Archive directory: Data Collected on: m300-mercury300

/export/home/chempack/vnmrsys/data Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Mar 30 2015

Operator: caccia

Relax. delay 1.000 sec Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18867.9 Hz 512 repetitions

OBSERVE C13, 75.4847602 MHz

DECOUPLE H1, 300.1991980 MHz Power 38 dB

WALTZ-16 modulated continuously on DATA PROCESSING

Line broadening 0.5 Hz FT size 32768

Total time 16 min

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120

100

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160

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200

220

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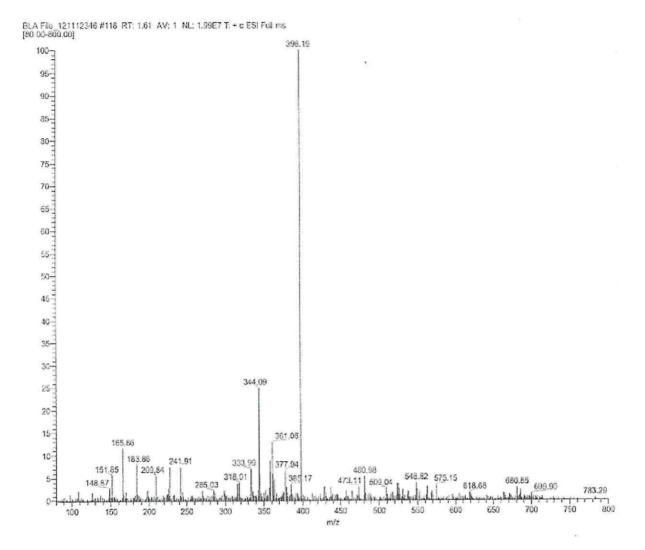
mdd

Aller of the Agriculture of the Control of the Cont mdd 20 23.955 74.581 582.289 25 752.427 196.92 ¥ 28.425 174.82 T94°87 30 689°78 35.092 965.25 490"88 725.85 property of the property of th 40 £02.02 686.02 /export/home/chempack/vnmrsys/data 988*19 Data collected on: Mar 30 2015 Pulse Sequence: CARBON (s2pul) OBSERVE C13, 75.4847602 MHz DECOUPLE H1, 300.1991980 MHz 55 HZ Sample directory: 4 Line broadening 0.5 Acq. time 0.868 sec Relax. delay 1.000 Archive directory: Pulse 45.0 degrees WALTZ-16 modulated m300-mercury300 Width 18867.9 Hz rotal time 16 min 512 repetitions FidFile: CARBON Operator: caccia continuously on DATA PROCESSING Solvent: cdc13 FT size 32768 Power 38 dB 9

Gradient Shimming

Sample Name:

Data Collected on:



Sample Name:
Acidolipoico-Gly
Data Collected on:
m300-mercury300

Archive directory: /export/home/chempack/vnmrsys/data Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul) Solvent: dmso Data collected on: Mar 9 2021

Operator: caccia

OBSERVE H1, 300.1990802 MHz Relax. delay 1.000 sec Total time 1 min 29 sec Pulse 45.0 degrees Acq. time 1.706 sec Width 4803.1 Hz 32 repetitions DATA PROCESSING FT size 16384

wdd ω 11 12 13

FidFile: PROTON

/export/home/chempack/vnmrsys/data Sample directory:

Acidolipoico-Gly Data Collected on: m300-mercury300

Gradient Shimming

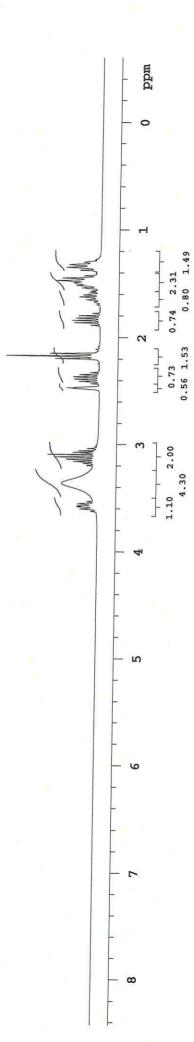
Sample Name:

Archive directory:

Pulse Sequence: PROTON (s2pul) Solvent: dmso Data collected on: Mar 9 2021

Operator: caccia

OBSERVE H1, 300.1990802 MHz Relax. delay 1.000 sec Total time 1 min 29 sec Pulse 45.0 degrees Acq. time 1.706 sec Width 4803.1 Hz 32 repetitions DATA PROCESSING FT size 16384



Acidolipoico-Gly Data Collected on: m300-mercury300 Sample Name:

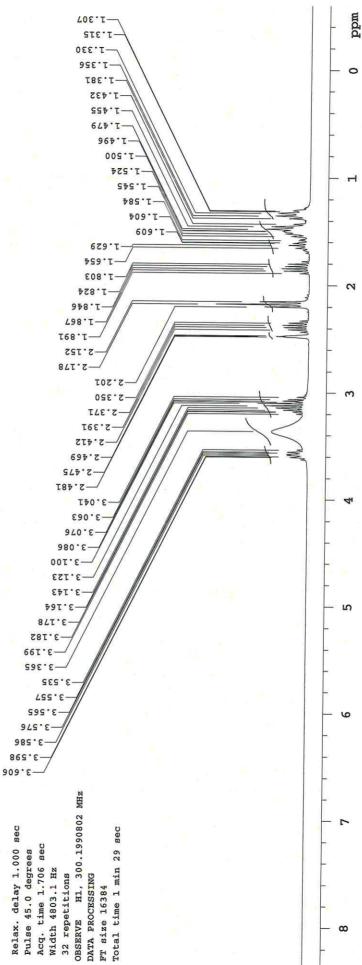
Archive directory: /export/home/chempack/vnmrsys/data Sample directory:

FidFile: PROTON

Data collected on: Mar 9 2021 Pulse Sequence: PROTON (s2pul) Solvent: dmso

Operator: caccia

Relax. delay 1.000 sec Total time 1 min 29 sec Acq. time 1,706 sec Width 4803.1 Hz Pulse 45.0 degrees 32 repetitions DATA PROCESSING FT size 16384



Data collected on: Jul 13 2021 Pulse Sequence: CARBON (s2pul) Solvent: cdc13 AutoSW_calib_20210712_02 FidFile: CARBON

/home/caccia/vnmrsys/data

Sample directory:

Archive directory:

m300-mercury300

Data Collected on:

Sample Name:

Gly-La

Operator: caccia

2000 repetitions OBSERVE C13, 75.4847602 MHz DECOUPLE H1, 300.1991980 MHz Relax. delay 1.000 sec Line broadening 0.5 Hz Total time 1 hr, 4 min Acq. time 0.868 sec Pulse 45.0 degrees WALTZ-16 modulated Width 18867.9 Hz continuously on DATA PROCESSING FT size 32768 Power 38 dB

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