Nano-MoO$_3$ mediated synthesis of bioactive thiazolidin-4-ones and their anti-bacterial mode-of-action analysis using \textit{in silico} target prediction, docking and similarity searching.

Supplementary Information

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Sample Name: 1H-13C
Data Collected on: Agilent-MER-vern400
Archive directory:
Sample directory: FidFile: CARBON
Pulse Sequence: CARBON (x2pol)
Solvent: cdcl3
Data collected on: Dec 29 2016
Temp. 25.0 °C / 298.1 K
Operator: venu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.321 sec
MTRM 20000.0 Hs
1000 repetitions
G reluctant C13, 100.5342393 MHz
DECOUPLE H1, 399.827723 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FY size 65536
Total time 39 min

200 180 160 140 120 100 80 60 40 20 0 ppm
3c
Sample Name: 3o-13C
Data Collected on: Agilent-NMR-veasc460
Archive directory:
Sample directory:

File: CARRON

Pulse Sequence: CARRON (x2pol)
Solvent: dmso
Data collected on: Dec 29 2014

Temp. 25.0 C / 298.1 K
Operator: vmsl

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.211 sec
Width 2500.0 Hz
1000 repetitions

Observ: 13. 100.514253 MHz

Decoupling H1 399.621773 MHz
Power 45 dB continuously on

DATA PROCESSING
Line broadening 2.0 Hz
FT size 85536
Total time 38 min
Sample Name: SH-13C
Data Collected on: Agilent-600-Mass Spectrometer
Archive directory:
Sample directory:
Fidfile: CARBON
Pulse Sequence: CARBON (e2pul)
Solvent: dmeo
Data collected on: Nov 25 2015

Temp. 25.0 C / 298.1 K
Operator: 

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 2500.0 Hz
1000 repetitions

OBSERVE: 13C, 120.52582 MHz
DECouple: H1, 39.827233 MHz
Power 40 dB
continuously on

WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
PT size 65536
Total time 38 min

220 200 180 160 140 120 100 80 60 40 20 0 ppm
<table>
<thead>
<tr>
<th>Method</th>
<th>DEF_MS.M</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample Name</td>
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<tr>
<td>Acquisition Parameter</td>
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<tr>
<td>Ion Source Type</td>
<td>ESI</td>
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<td>Mass Range Mode</td>
<td>319 μs</td>
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<tr>
<td>Capillary Exit</td>
<td>109.0 Volt</td>
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<tr>
<td>Accumulation Time</td>
<td>Ultra Scan</td>
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<tr>
<td>Ion Polarity</td>
<td>Positive</td>
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<tr>
<td>Scan Begin</td>
<td>50 m/z</td>
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<tr>
<td>Skimmer</td>
<td>40.0 Volt</td>
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<td>Averages</td>
<td>5 Spectra</td>
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<tr>
<td>Operator</td>
<td></td>
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<tr>
<td>Instrument</td>
<td>HCTultra ETD II</td>
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<td>MBU</td>
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<tr>
<td>Alternating Ion Polarity</td>
<td>off</td>
</tr>
<tr>
<td>Scan End</td>
<td>1300 m/z</td>
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<tr>
<td>Trap Drive</td>
<td>49.6</td>
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<tr>
<td>Auto MS/MS</td>
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<td></td>
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</tr>
</tbody>
</table>

![Graph](image-url)
3g
<table>
<thead>
<tr>
<th>PULSE SEQUENCE</th>
<th>OBSERVE CL3, 100.5367359</th>
<th>DATA PROCESSING</th>
<th>1402372-3C-13C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Relax. delay 1.000 sec</td>
<td>H1, 399.8294225</td>
<td>Line broadening 0.5 Hz</td>
<td>Solvent: dmso</td>
</tr>
<tr>
<td>Pulse 45.0 degrees</td>
<td>lower 40 dB</td>
<td>FT size 65536</td>
<td>Ambient temperature</td>
</tr>
<tr>
<td>Avg. time 1.311 sec</td>
<td>continuously on</td>
<td>Total time 63 minutes</td>
<td>Operator: vvmc1</td>
</tr>
<tr>
<td>Width 25600.0 Hz</td>
<td>MALTE-18 modulated</td>
<td></td>
<td>File: 1402372-3C-13C</td>
</tr>
<tr>
<td>1650 repetitions</td>
<td></td>
<td></td>
<td>VNMR-400 “Agilent-NMR”</td>
</tr>
</tbody>
</table>
Sample Name: 3j - 13C
Date Collected on: Agilent-500B-vnmsa603
Archive directory:
Sample directory:

File: C:CARBON
Pulse Sequence: CARBON (x2pul)
Solvent: dmso
Data collected on: Apr 25 2014

Temp. 25.0 °C / 298.1 K
Operator: vmar

Relay Delay 1.000 sec
Pulse 49.0 Degrees
Acq. time 1.311 sec
Width 22000.0 Hz
1000 repetitions

Observ E C13, 100.562893 MHz
Decoupler E3, 89.6277233 MHz
Power 40 dB
continuously on

MULT-18 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 58 min

220 200 180 160 140 120 100 80 60 40 20 0 ppm
**Pulse Sequence**
- Pulse delay 1.000 sec
- Pulse 45.0 degrees
- Acq. time 1.211 sec
- WIDSR 25000.0 Hz
- 2202 repetitions

**Observation**
- C13, 100.6367365
- DECOUPLING R1, 399.8294235
- Power 40 dB
- Continuously on
- WALTE-16 modulated

**Data Processing**
- Line broadening 0.5 Hz
- FT size 65536
- Total time 47 minutes

**Other**
- Solvent: dmso
- Ambient temperature
- Operator: vmsri
- VMRS-40D "Agilent-500"
Sample Name: 3a-13C
Data Collected on: Agilent-6000-wave400
Archive directory:

Sample directory:

File: C4N
Pulse Sequence: CANNON (x2pul)
Solvent: cdc13
Data collected on: Nov 25 2015

Temp. 25.0 C / 298.1 K
Operator: veml

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 35000.0 Hz
1000 repetitions

OBSERVE C13 100.5362327 MHz
DECOUPLING 1H 399.8277215 MHz
Power 45 dB
continuously on
MALTP-1A modulated

DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 38 min
Sample Name: 3a-13C
Data Collected on: Agilent-600-GeminiHD
Archive directory:

Sample directory:

File: CARNON

Pulse Sequence: CARNON (2-pul)
Solvent: ocd13
Data collected on: Nov 25 2015

Temp. 25.0 C / 298.1 K
Operator: wmar

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1500 repetitions

OBSEERVE C13, 100.25G23E MHz
DECOUPLE 80, 399.6277233 MHz
Power 45 dB
continuously on
Miles-14 modulated
DATA PROCEEDING
Line broadening 2.0 Hz
FT size 65536
Total time 33 min