Electronic Supplementary Information (ESI)

Synthesis, Cu(II) complexation, ⁶⁴Cu-labeling and biological evaluation of cross-bridged cyclam chelators with phosphonate pendant arms

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1. Details of HPLC Purification of CB-TE1A1P (2)

A batch of CB-TE1A1P that contained some impurities was purified by HPLC using a C₁₈

semipreparative column with a 3 mL/min flow rate and the following gradient:

| Time (min) | % 0.1% TFA in water | % 0.1% TFA in acetonitrile |
|------------|---------------------|----------------------------|
| 0 | 100 | 0 |
| 10 | 100 | 0 |
| 20 | 90 | 10 |
| 21 | 50 | 50 |
| 23 | 50 | 50 |
| 24 | 80 | 20 |
| 25 | 100 | 0 |
| 30 | 100 | 0 |

The compound eluted with a broad peak starting at 8.0 minutes. The collection was stopped after minute 15.0. A UV chromatogram at 210 nm is shown in the figure below.



LC-MS was used to make sure that no impurity eluted in the 8.0-15.0 minute range. The only peaks visible in the MS chromatogram of the collected fractions are $M^{+}H^{+}$ (m/z=379.3) and $2M^{+}H^{+}$ (m/z=757.4).



2. List of X-ray Crystallographic Software Employed

APEX2 Version 2.2 /SHELXTL (Bruker AXS Inc., 2007) SAINT Version 7.34a (Bruker AXS Inc., 2007) SADABS Version 2007/2 (Sheldrick, Bruker AXS Inc.) XPREP Version 2005/2 (Sheldrick, Bruker AXS Inc.)

Bruker suite of programs APEX2/SHELXTL, SAINT, SADABS, XPREP may be obtained from Bruker AXS.Inx, 5467 East Cheryl Parkway, Madison WI 53711

XS Version 2008/1 (George M. Sheldrick, Acta Cryst. (2008) A64, 112-122.) XL Version 2008/1 (George M. Sheldrick, Acta Cryst. (2008) A64, 112-122.)

X-ray crystal structure figures were prepared using CrystalMaker 8.5 for Mac (CrystalMaker Software Ltd., Centre for Innovation & Enterprise, Oxford University Begbroke Science Park, Sandy Lane, Yarnton, Oxfordshire, OX5 1PF, UK; http://www.crystalmaker.com)

3. <u>Detailed Energetic Results for DFT Calculations</u>

Cu-CBTE2P

| | | | 705 | | | So (col/mol | |
|------------------|---------------------|--------------|------------|--------------|---------------|------------------|---------------------------|
| Method | Conformer | E (kcal/mol) | (kcal/mol) | (kcal/mol) | Hº (kcal/mol) | (Cal/III0) K) | G ^o (kcal/mol) |
| B3LYP/6- 31G* | [2233]/[2233] | -2224578.459 | 303.547 | -2224274.912 | -2224259.710 | 151.315 | -2224304.824 |
| B3LYP/6- 31G* | [2323]/[2323] | -2224577.968 | 303.065 | -2224274.903 | -2224259.624 | 152.192 | -2224305.000 |
| | Delta (1st- 2nd) | -0.491 | | -0.009 | -0.086 | | 0.176 |
| M06/6- 31G* | [2233]/[2233] | -2224057.804 | 302.986 | -2223754.818 | -2223739.849 | 149.505 | -2223784.424 |
| M06/6- 31G* | [2323]/[2323] | -2224056.887 | 302.769 | -2223754.118 | -2223739.125 | 149.999 | -2223783.847 |
| | Delta (1st- 2nd) | -0.917 | | -0.700 | -0.724 | | -0.577 |
| M06/6- 31+G** | [2233]/[2233] | -2224119.778 | | | | | |
| M06/6- 31+G** | [2323]/[2323] | -2224118.92 | | | | | |
| | | | | | | | |

-0.858

Cu-CBTE1A1P

| Method | Conformer | E (kcal/mol) | ZPE (kcal/mol) | ZPE-corr E (kcal/mol) | H ^o (kcal/mol) | S ^o (cal/mol K) | Gº (kcal/mol) |
|------------------|---------------------|--------------|-------------------|--------------------------|---------------------------|----------------------------------|---------------|
| B3LYP/6- 31G* | [2233]/[2233] | -1986668.793 | 296.081 | -1986372.713 | -1986358.562 | 144.926 | -1986401.771 |
| B3LYP/6- 31G* | [2323]/[2323] | -1986669.104 | 296.320 | -1986372.784 | -1986358.654 | 144.825 | -1986401.833 |
| | Delta (1st- 2nd) | 0.311 | | 0.071 | 0.092 | | 0.062 |
| M06/6- 31G* | [2233]/[2233] | -1986163.941 | 295.292 | -1985868.649 | -1985854.737 | 142.918 | -1985897.348 |
| M06/6- 31G* | [2323]/[2323] | -1986163.415 | 295.461 | -1985867.954 | -1985854.048 | 143.092 | -1985896.711 |
| | Delta (1st- 2nd) | -0.526 | | -0.695 | -0.689 | | -0.637 |
| M06/6- | | | | | | | |

31+G** [2233]/[2233] -1986219.083

M06/6-31+G**

** [2323]/[2323] -1986218.413

-0.67

Cu-CBTE2A

| Method | Conformer | E (kcal/mol) | ZPE (kcal/mol) | ZPE-corrected E (kcal/mol) | Hº (kcal/mol) | cal/mol K) | Gº (kcal/mol) |
|------------------|---------------------|--------------|-------------------|-------------------------------|---------------|---------------|---------------|
| B3LYP/6- 31G* | [2233]/[2233] | -1748754.253 | 289.366 | -1748464.887 | -1748451.890 | 137.475 | -1748492.879 |
| B3LYP/6- 31G* | [2323]/[2323] | -1748755.612 | 289.171 | -1748466.441 | -1748453.402 | 138.029 | -1748494.555 |
| | Delta (1st- 2nd) | 1.359 | | 1.554 | 1.512 | | 1.676 |
| M06/6- 31G* | [2233]/[2233] | -1748265.280 | 287.683 | -1747977.597 | -1747964.701 | 136.644 | -1748005.442 |
| M06/6- 31G* | [2323]/[2323] | -1748266.435 | 288.257 | -1747978.179 | -1747965.361 | 136.448 | -1748006.043 |
| | Delta (1st- 2nd) | 1.155 | | 0.582 | 0.660 | | 0.601 |
| M06/6- 31+G** | [2233]/[2233] | -1748313.884 | | | | | |
| M06/6- 31+G** | [2323]/[2323] | -1748314.563 | | | | | |
| | Delta (1st- 2nd) | 0.679 | | | | | |

4. <u>UV/VIS Spectrum of Cu-CB-TE1A1P</u>

UV/VIS Spectrum of Cu-CB-TE1A1P

 λ_{max} (aq)/nm 613 (ϵ /dm³ mol⁻¹ cm⁻¹ 24)



5. <u>NMR spectra of ligand 2 and precursor 6</u>

(Note that NMR spectra for ligand **1** and its precursor **4** may be found in the ESI of reference 55 (D. J. Stigers, R. Ferdani, G. R. Weisman, E. H. Wong, C. J. Anderson, J. A. Golen, C. Moore and A. L. Rheingold, *Dalton Trans.*, 2010, **39**, 1699-1701; doi: 10.1039/b920871b).

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| his journal is © The Royal Soc | iety of Chemistry 2 | 011 | | | | | | | | | | |
|---|--|---------|---------|---------|----------------------------------|----------------------------|-------------|-------------|-----|-----|-------|--------|
| 1Data File NameRF2OriginVar3SolventD24Number of Scans325Receiver Gain286Acquisition Time3.07Acquisition Date208Spectrometer Frequency499Spectral Width7910Lowest Frequency-14 | G CB-TE1A1P_1H rian CO 0000 11-01-21T10:51:45 9.77707 92.0 419.1 | | | | H D ₂ O, 499 wi | 0.78 MHz, in th MeCN se | nternal ref | H erence | | | | 8 |
| 11 Nucleus 1H | I | | | | | | | | 1 | | | |
| 12 Acquired Size 23 | 976 | | | | | | | | | | | |
| 13 Spectral Size 65 | 536 | | | | | | | | | | | |
| | | | | | | | | | | и | | |
| 10.0 9.5 9.0 | 8.5 8.0 | 7.5 7.0 | 6.5 6.0 | 5.5 5.0 | 4.5 | 4.0 3.5 | 3.0 | 2.5 | 2.0 | 1.5 | 1.0 0 | .5 0.0 |
| | | | | ppm | | | | | | | | |





Region of interest: 1.70-1.89 ppm







Region of interest: 2.28 - 2.50 ppm

2.39 ppm 2.48 2.41 2.40 2.38 2.37 2.36 2.35 2.34 2.33 2.32 2.31

2.42

2.47 2.46 2.45 2.44 2.43

2.49

50

2.30

2.29

Region of interest: 2.28 - 2.50 ppm

Exponential: -1.32 Gaussian: 0.70 GB



Region of interest: 2.28 - 2.50 ppm

Exponential: -1.32 Gaussian: 0.70 GB



Region of interest: 2.52 - 2.61 ppm



Region of interest: 2.52 - 2.61 ppm

Exponential: -1.32 Gaussian: 0.60 GB



Region of interest: 2.52 - 2.61 ppm

Exponential: -1.32 Gaussian: 0.60 GB



Region of interest: 2.76 - 3.45 ppm



Region of interest: 2.76 - 3.45 ppm

_3.106 _____3.084 Exponential: -1.32 2.969 Gaussian: 0.60 GB .055 ς ε 3.076 -3.214 3.188 , -3.320 ---3.312 -3.303 -3.295 -3.276 3.339 -3.032 -3.346







Region of interest: 3.49 - 3.78 ppm



Region of interest: 3.49 - 3.78 ppm

Exponential: -1.32 Gaussian: 0.60 GB 3.624 -3.590 -3.650 3.620 3.680 3.697 3.703 3.725 3.559 3.552 -3.530 3.731 -3.676 -3.670 3.522 -3.586 -3.579 3.518 3.64 3.63 ppm 3.76 3.75 3.74 3.73 3.72 3.71 3.70 3.69 3.68 3.66 3.65 3.62 3.61 3.60 3.59 3.58 3.56 3.55 3.54 3.53 3.52 3.51 3.50 78 3.77 3.67 3.57

Region of interest: 3.49 - 3.78 ppm

Exponential: -1.32 Gaussian: 0.60 GB 1811.21 -1794.21 1824.17 1809.36 1838.94 1847.68 1850.72 1861.61 1775.26 1864.69 1778.95 1764.25 1760.41 -1837.04 -1833.97 -1792.34 --1788.90 Т 1815 Hz 1755 1750 1885 1880 1875 1870 1865 1860 1855 1850 1845 1840 1835 1830 1825 1820 1810 1805 1800 1795 1790 1785 1780 1775 1770 1765 1760 174

Region of interest: 3.78 - 4.15 ppm













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| - | | |
|----|-----------------------|---------------------|
| | | |
| 1 | Comment | RF-CB-TE1A1P |
| 2 | Origin | Varian |
| 3 | Solvent | D2O |
| 4 | Number of Scans | 16 |
| 5 | Acquisition Time | 3.0000 |
| 6 | Acquisition Date | 2011-01-24T15:29:41 |
| 7 | Spectrometer Frequenc | 499.77707 |
| 8 | Spectral Width | 7992.0 |
| 9 | Lowest Frequency | -1396.6 |
| 10 | Nucleus | 1H |
| 11 | Acquired Size | 23976 |
| 12 | Spectral Size | 65536 |
| | | |







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f1 (ppm)

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f1 (ppm)



f1 (ppm)


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|---|--|---|---|--|
| 1 Data Eile Name | DE_CR_TE1A1D 13C 125MHz | | | 38 |
| 2 Origin | Varian | | | |
| 3 Solvent | | | | |
| 4 Number of Scans | 38000 | \wedge | | |
| 5 Receiver Gain | 40 | Γ] _ OH | | |
| 6 Acquisition Time | 1.0000 | | | |
| 7 Acquisition Date | 2011-01-22T08:03:16 | 0 | | |
| 8 Spectrometer Frequency | / 125.68036 | | I | |
| 9 Spectral Width | 31446.5 | HO Ý | | |
| 10 Lowest Frequency | -3783.1 | \checkmark | | |
| 11 Nucleus | 13C | D ₂ O, 125.68 MHz, internal reference | e , | |
| 12 Acquired Size | 31447 | with MoCN set at $\delta 1.47$ | | |
| 13 Spectral Size | 65536 | WILL MECH SEL al 0 1.47 | | |
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|-----|---|---------------------------|
| | Parameter | Value |
| | 1 Comment | RF-CB-TE1A1P-125 MHz |
| | 2 Origin | Varian |
| | 3 Solvent | D2O |
| | 4 Number of Scans | 38000 |
| | 5 Acquisition Time | 1.0000 |
| | 6 Acquisition Date | 2011-01-22T08:03:16 |
| | 7 Spectrometer Frequency | y 125.68036 |
| | 8 Spectral Width | 31446.5 |
| | 9 Lowest Frequency | -3692.7 |
| | 10 Nucleus | 13C |
| | 11 Acquired Size | 31447 |
| | 12 Spectral Size | 65536 |
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| his journal is © The Roya | al Society of Chemistry 2011 | | |
|---|--|--|----------------------------|
| Parameter | Value | | 44 |
| 1 Comment | RF-CB-TE1A1P-100 MHz | | |
| 2 Origin | Varian | | |
| 3 Solvent | D2O | | |
| 4 Number of Scans | 26560 | | |
| 5 Acquisition Time | 1.0025 | | |
| 6 Acquisition Date | 2011-01-25T18:03:03 | | |
| 7 Spectrometer Frequer | ncy 100.52657 | ОН | |
| 8 Spectral Width | 25062.7 | | |
| 9 Lowest Frequency | -1418.1 | | |
| 10 Nucleus | 13C | | |
| 11 Acquired Size | 25126 | | |
| 12 Spectral Size | 65536 | | |
| | | $D_{-}O_{-}$ 100 53 MHz | |
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|--------------|------------|---|---|------------------------|
| | | | | |
| | 1 | Origin | RF-CB-TE1A1P | |
| | 2 | Solvent | D20 | |
| | 3 | Temperature | 25.0 | |
| | 4 | Number of Scans | 16 | |
| | 5 | Acquisition Time | 3.0000 | |
| | 6 | Acquisition Date | 2011-01-24T15:29:41 | |

7992.0

-1396.6

23976

65536

1H

7 Spectrometer Frequency 499.77707

8 Spectral Width

11 Acquired Size

12 Spectral Size

10 Nucleus

9 Lowest Frequency



D₂O, 499.78 MHz, internal reference with MeCN set at δ 2.06

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|--------------|-----------|---------------|----------|--------------|--------------|
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| 1 | Origin | RF-CB-TE1A1P |
|----|------------------------|---------------------|
| 2 | Solvent | D2O |
| 3 | Temperature | 25.0 |
| 4 | Number of Scans | 38000 |
| 5 | Acquisition Time | 1.0000 |
| 6 | Acquisition Date | 2011-01-22T08:03:16 |
| 7 | Spectrometer Frequency | 125.68036 |
| 8 | Spectral Width | 31446.5 |
| 9 | Lowest Frequency | -3692.7 |
| 10 | Nucleus | 13C |
| 11 | Acquired Size | 31447 |
| 12 | Spectral Size | 65536 |





(See previous two pages for corresponding 1D proton and carbon spectra)





f1 (ppm)



53

f1 (ppm)





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| 100 | | |
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| | | |
| 1 | Data File Name | RF-CB-TE1A1P_31P |
| 2 | Origin | Varian |
| 3 | Solvent | D2O |
| 4 | Number of Scans | 512 |
| 5 | Receiver Gain | 60 |
| 6 | Acquisition Time | 1.6000 |
| 7 | Acquisition Date | 2011-01-22T10:13:04 |
| 8 | Spectrometer Frequency | 202.30717 |
| 9 | Spectral Width | 50600.9 |
| 10 | Lowest Frequency | -30548.5 |
| 11 | Nucleus | 31P |
| 12 | Acquired Size | 80961 |
| 13 | Spectral Size | 262144 |

9.240



D₂O, 202.31 MHz, external reference with 85% phosphoric acid set at δ 0.00

-30

-40

80 70

60

50

40

30

20

10

0

90

-20 ppm

-10

-50

-60 -70 -80 -90

-100

-110

-120

-130

-140

-1!

| | | | 57 |
|-------------------------|--|--|--|
| 1 Data File Name | RF-CB-TE1A1P_protected_CH2Cl2 extracts_2011-02-16/ PROTO | N | |
| 2 Origin | Varian | | |
| 3 Solvent | C6D6 | CH | |
| 4 Number of Scans | 32 | | |
| 5 Receiver Gain | 34 | | |
| 6 Acquisition Time | 3.0000 | $N_{\rm N} = P^{\prime} O^{\rm CH_3}$ | |
| 7 Acquisition Date | 2011-02-16T15:28:30 | | |
| 8 Spectrometer Frequenc | y 499.77585 | $H_3C \downarrow I \downarrow \downarrow$ | |
| 9 Spectral Width | 7992.0 | $H_3C^{-}O^{-}$ | |
| 10 Lowest Frequency | -1498.0 | | |
| 11 Nucleus | 1H | | |
| 12 Acquired Size | 23976 | RF-CB-TF1A1P_protected (CH ₂ Cl ₂ extracts) | |
| 13 Spectral Size | 65536 | 100.78 MHz internal reference set to TMC at $$ 0.00$ | |
| | C_6D_6 , | 499.78 MHZ, Internal reference set to TMS at 0 0.00 | |
| | Sai | mple was dried over Na ₂ SO ₄ prior to running NMR | |
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ppm











Region of interest: 2.17 - 3.26 ppm



Region of interest: 2.44 - 3.00 ppm



Region of interest: 2.44 - 3.00 ppm



Region of interest: 2.44- 3.00 ppm

Exponential: -1.32 Gaussian: 0.70 GB



1490

1480

1470

1460

1450

1440

1430

1420

Region of interest: 2.44- 3.00 ppm Exponential: -1.32 Gaussian: 0.70 GB 1411.94 1293.96 ۲1343.b9 1341.44 لـ 1341.44 ~1429.32 1444.93 1347, -1394.44 1427.34 1349.30 1296.30 -1472.02 -1398.63 1458.65 --1386.38 1382.35 -1280.89 -1278.51 1242.09 1285.98 -1455.74 1345.42 -1354.96 -1351.86 -1252.00 -1441.15 ---1435.76 1275.86 -1253.711476.60 -1463.95 1449.49 1244.94 1256.89 1391.44 1407.53 1282.94 -1319.49 1271.11 1469.59 1467.70 1323.74 -1379.42 1485.29 1312.14 1307.73 1305.51 1298.50 1489.13 1369.70 1368.77 1365.82 MMMMMM MMMM hM WW MMM ΛW

1410

1400

1390

1380

1370

1360 Hz 1350

1330

1340

1320

1300

1310

1290

1280

1270

1260

1250

1240

1230

122

Region of interest: 2.99- 3.50 ppm





Region of interest: 3.45 - 4.30 ppm



Region of interest: 3.45 - 4.30 ppm







f1 (ppm)










76





| | 1 | Data File Name | RF-CB-TE1A1P_protected_PhMe_13C_2011-02-17/ CA | RBON |
|---|----|------------------------|--|------|
| | 2 | Origin | Varian | |
| | 3 | Solvent | C6D6 | |
| | 4 | Number of Scans | 5000 | |
| | 5 | Receiver Gain | 40 | |
| | 6 | Acquisition Time | 1.0000 | |
| | 7 | Acquisition Date | 2011-02-17T11:00:46 | |
| | 8 | Spectrometer Frequency | 125.68005 | |
| | 9 | Spectral Width | 31446.5 | |
| | 10 | Lowest Frequency | -3735.5 | |
| | 11 | Nucleus | 13C | |
| | 12 | Acquired Size | 31447 | |
| | 13 | Spectral Size | 65536 | |
| j | | | | |



RF-CB-TE1A1P_protected_PhMe extracts ^{13}C NMR, 125.68 MHz, C_6D_6 with reference peak set at δ 128.06 (central peak)

M MA A

-1

ר ppm





30.5

..0

30.0

25.5



29.0

29.5

1

28.5

27.5

27.0

26.5

26.0

28.0 ppm













| | 1 | Data File Name | RF-CB-TE1A1P_protected_PhMe_13C_2011-02-17/ CA | RBON |
|---|----|------------------------|--|------|
| | 2 | Origin | Varian | |
| | 3 | Solvent | C6D6 | |
| | 4 | Number of Scans | 5000 | |
| | 5 | Receiver Gain | 40 | |
| | 6 | Acquisition Time | 1.0000 | |
| | 7 | Acquisition Date | 2011-02-17T11:00:46 | |
| | 8 | Spectrometer Frequency | 125.68005 | |
| | 9 | Spectral Width | 31446.5 | |
| | 10 | Lowest Frequency | -3735.5 | |
| | 11 | Nucleus | 13C | |
| | 12 | Acquired Size | 31447 | |
| | 13 | Spectral Size | 65536 | |
| 1 | | | | |



$\label{eq:RF-CB-TE1A1P_protected_PhMe extracts} $^{13}C NMR, 125.68 MHz, C_6D_6 with reference peak set at $128.06 ppm (central peak)$$

ר ppm

-1

| | EC | uu | The Supplementary Ma | | |
|----|----------|-----|------------------------|---|--------|
| ΓI | nis I | jοι | urnal is © The Royal S | ociety of Chemistry 2011 | |
| | | | | | |
| | | 1 | Data File Name | RF-CB-TE1A1P_protected_400_13C_17Feb2011/ CAR | ON.fid |
| | | 2 | Origin | Varian | |
| | | 3 | Solvent | C6D6 | |
| | | 4 | Number of Scans | 5000 | |
| | | 5 | Receiver Gain | 24 | |
| | | 6 | Acquisition Time | 1.0025 | |
| | | 7 | Acquisition Date | 1969-11-13T03:20:24 | |
| | | 8 | Spectrometer Frequency | 100.52631 | |
| | | 9 | Spectral Width | 25062.7 | |
| | | 10 | Lowest Frequency | -1402.7 | |
| | | 11 | Nucleus | 13C | |
| | | 12 | Acquired Size | 25126 | |
| | | 13 | Spectral Size | 65536 | |
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ppm



RF-CB-TE1A1P_protected_PhMe extracts 13 C NMR, 100.52 MHz, C₆D₆ with reference peak set at 128.06 ppm (central peak)

50

. 30

-1











Electronic Supplementary Material (ESI) for Dalton Transactions This journal is $\ensuremath{\mathbb{C}}$ The Royal Society of Chemistry 2011







10.0

9.5

9.0

8.5

8.0

7.5

7.0

6.5

6.0

5.5

| | 1 | Data File Name | RF-CB-TE1A1P_protected_PhMe extracts_C6D6-PROTON |
|-----|----|------------------------|--|
| | 2 | Origin | Varian |
| | 3 | Solvent | C6D6 |
| | 4 | Number of Scans | 16 |
| | 5 | Receiver Gain | 24 |
| | 6 | Acquisition Time | 3.0000 |
| | 7 | Acquisition Date | 2011-02-18T16:17:15 |
| | 8 | Spectrometer Frequency | 499.77585 |
| | 9 | Spectral Width | 7992.0 |
| | 10 | Lowest Frequency | -1496.1 |
| | 11 | Nucleus | 1H |
| | 12 | Acquired Size | 23976 |
| | 13 | Spectral Size | 65536 |
| . 1 | | | |



Т

3.5

3.0

2.5

2.0

1.5

1.0

0.5

0.0

-0.5

-1

4.0

4.5 ppm

5.0

| 1 | Data File Name | RF-CB-TE1A1P_protected_PhMe extracts_13C |
|----|------------------------|--|
| 2 | Origin | Varian |
| 3 | Solvent | C6D6 |
| 4 | Number of Scans | 5000 |
| 5 | Receiver Gain | 40 |
| 6 | Acquisition Time | 1.0000 |
| 7 | Acquisition Date | 2011-02-17T11:00:46 |
| 8 | Spectrometer Frequency | 125.68005 |
| 9 | Spectral Width | 31446.5 |
| 10 |) Lowest Frequency | -3735.5 |
| 11 | Nucleus | 13C |
| 12 | Acquired Size | 31447 |
| 13 | Spectral Size | 65536 |
| _ | | |

MANN/MANNA



C₆D₆, 125.68 MHz, internal reference set to TMS at δ 0.00

WW.MININAMAWAWAWAWAWAWA

ppm

0.000

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| Tailancer Value (2, 11) To proton and carbon spectra) Orgin Weins 500 Solvent C.656 Number of Scars 32 Aquidabion Thme 0.1500 Spectravical 10 proton and carbon spectra) Spectravical 30 Aquidabion Thme 0.1500 Spectravical 10 proton and carbon spectra) Spectravical 30 Aquidabion Thme 0.1500 Spectravical 10 proton and carbon spectra) Spectravical 10 proton and carbon spectra)< | | Parameters | (See previous two pages for corresponding | | | |
|--|----------------------|--|---|-------------|--------------|------------|
| Data Preame No. 100 (2014) Solution Construction Constructing Construction Construction Constructing Constructing | Parameter | Value (r2, r1) | 1D proton and carbon spectra) | | | |
| Jorgin watan | | RF-CB-TETATP_protected_Prime extracts_C6D6-HMQC | | | | |
| Boldwart 0.006 Munter of Same 30 Aquidito Tatica 0.1500 Aquidito Date 20140-147214508 Spectrawer Srequency 44968 (-1206.5) Nucleus (11.1) Spectrawer Srequency -44968 (-1206.5) Nucleus (11.1) Spectrawer Srequency -44968 (-1206.5) Nucleus (11.1) Spectrawer Srequency -44968 (-1206.5) Spectrawer Srequency -44968 (-1206.5) Aquidito Szee (12.1) Spectrawer Srequency -44968 (-1206.5) Auguide Szee (12.1) Spectrawer Srequency -4908 (-1206.5) Spectrawer Srequency -4008 (-1206.5) Spectrawer Srequency -408.5 | Origin | varian | | | | |
| Number of 2015 3.2 Acquiston Time 0.1500 Acquiston Time 0.1500 Spectrometer Fraquency (4996) 7587837, 735.75283) Spectrometer Fraquency (4996) 710.001, 0.000) Constrained and the second and the seco | Solvent | C6D6 | | | | |
| eccever tails output output counts acquisition the counts acquisite the counts co | Number of Scans | 32 | | | | |
| Acquests in the 2011-021-18721-5:08 Spectrometer Frequency (499,775984, 125,675284) Spectrometer Frequency (499,775984, 125,675284) Spectrometer Frequency (499,75984, 126,5) Nucleus (11,12C) Acquest Size (120,225) Spectral | Receiver Gain | 30 | | | | |
| Acquero Date | Acquisition Time | | | | 1 | |
| spectral Way //3948/, 12.6.75, 28(4) Spectral Way //3948/, 12.6.5) Nuckeus (H), 15C) Spectral Way //3948/, 12.6.75, 28(4) Spectral Way //3948/, 12.6.75, 28(4) Spectral Size -2008/, 2048) Spectral Size -2018/, 2048, 2048) Spectral Size -2018/, 2048, | Acquisition Date | | MMM_M_M_M_M_M_M_M_M_M_ | ~l | | _ |
| bectral Size 10000 1, 1151.30) Lines Frequency (10001, 1156.5) Nuckus (114, 12C) Acquied Size (10002, 2016) Spectral Size -2046 2018) Spectral Size -2046 2018 Spectral Size -2046 201 Spectral Size -204 Spectral Size -2046 Spectral Size -204 | Spectrometer Frequen | hcy (499.//58484, 125.6//5284) | | | | - |
| Lovest requency - (14496, -1205, 5) Acquired Size (1200, 256) Spectral Size - (2048, 2018) | Spectral Width | (8000.0, 21361.8) | | | * | |
| Nucleus (11,1,15,2) | Lowest Frequency | (-1496 ,6,-1206.5) | | 0 | {0.0010.000} | l Č |
| Acquared Size (1200) (256) | Nucleus | (1H, 13C) | | | | |
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| • • • • • • • • • • • • • • • • • • • | | ************************************** | | | | -120 |
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| | | 7.5 7.0 6.5 6.0 5.5 | 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 | 1.0 0.5 | 0.0 -0.5 - | ·1.0 |







 \wedge N -59.5 -60.0 -60.5 -61.0 -61.5 -62.0 Г · 1 3.06 3.04 3.02 3.00 2.98 2.96 2.94 2.92 2.90 2.88 2.86 2.84 2.82 2.80 2.78 2.76 2.74 2.72 2.70 2.68 2.66 2.64 2.62 2.60 2.58 2.56 ppm









105



| | Parameter | Value | |
|-------------|--|--|--|
| 1 | Title | RF-CB-TE1A1P_prot | ected-31P CH ₃ |
| 2 | Solvent | C6D6 | |
| 3 | Temperature | 25.0 | |
| 4 | Number of Scans | 32 | |
| 5 | Spectrometer Frequency | 202.31 | |
| 6 | Spectral Width | 50600.9 | |
| 7 | Lowest Frequency | -30527.2 | |
| 8 | Nucleus | 31P | DE CRITEIAID protocted DhMa autrocta |
| 9 | Acquired Size | 80961 | RF-CB-TETATP_protected_Prime extracts |
| 10 | Spectral Size | 262144 | 31 P NMR, 202.31 MHZ, C ₆ D ₆ , external reference with |
| | | | 85% phosphoric acid set to δ 0.00 |
| | | 96 | |
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