

## Supplementary Information

### Synthesis of an *upper-* and *lower-*rim functionalized calix[4]arene for detecting calcium ions using a microcantilever sensor.

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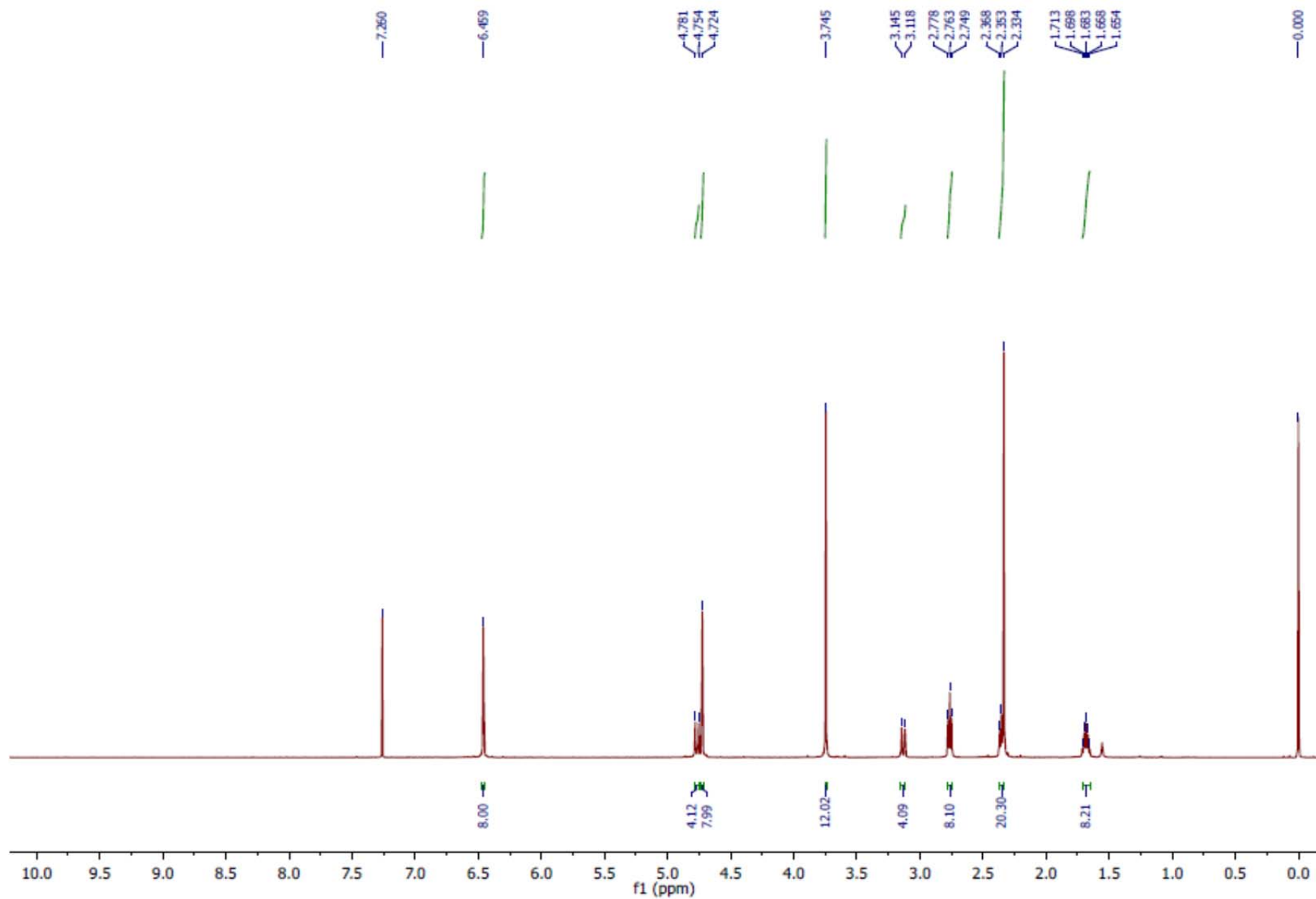
<sup>b</sup> *Department of Physics and Physical Oceanography, Memorial University of Newfoundland, St. John's,*

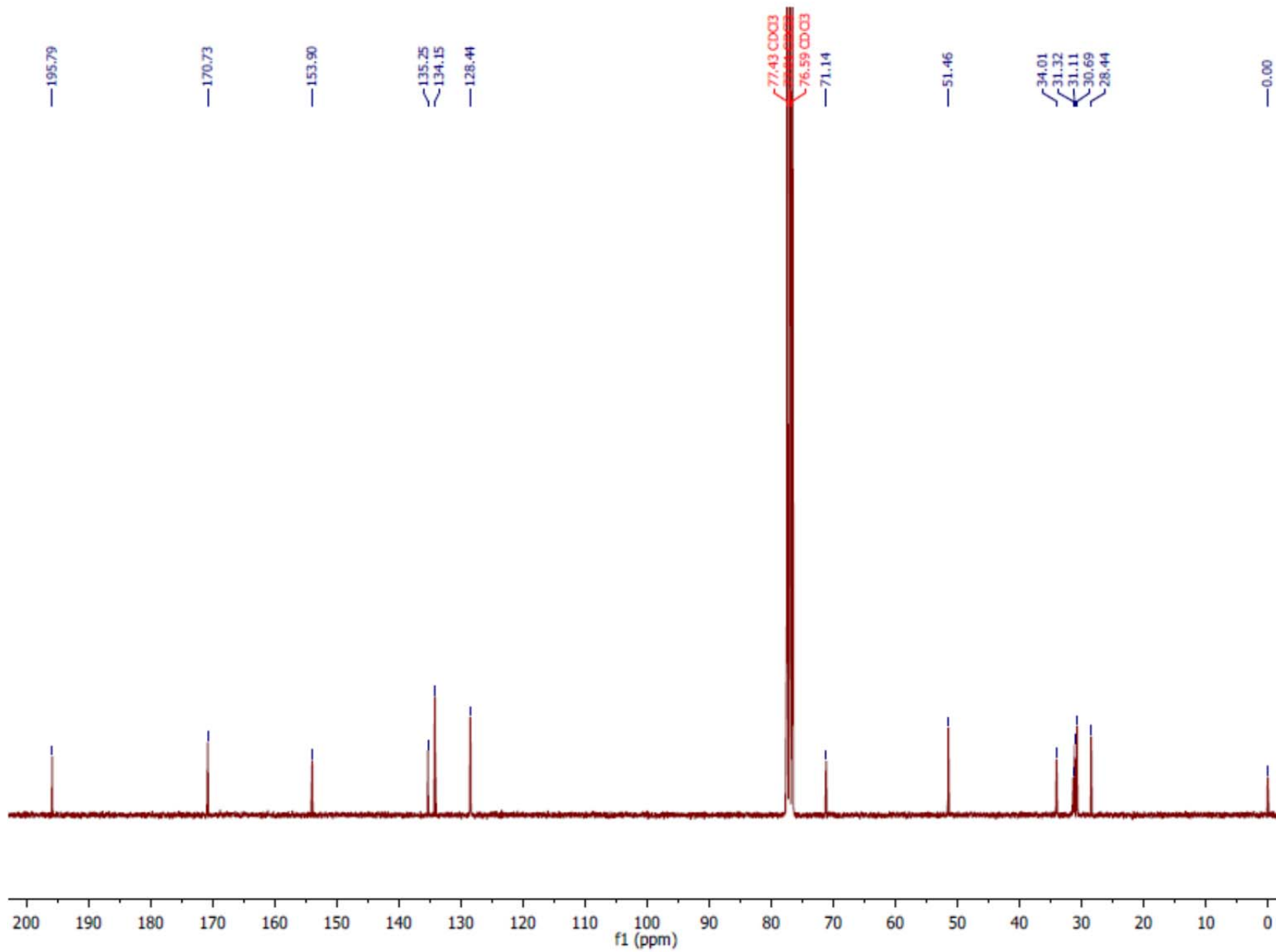
*Newfoundland and Labrador, Canada A1B3X7.*

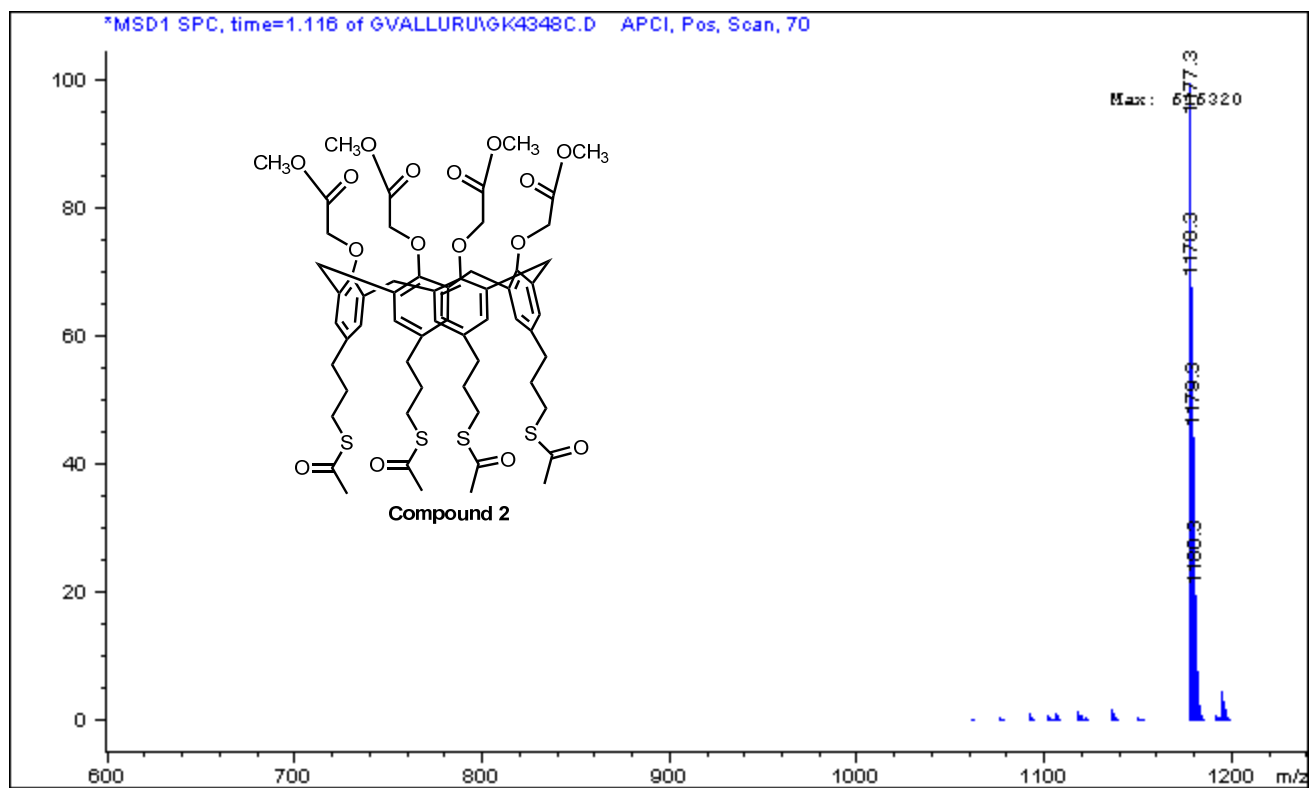
*E-mail: [lbeaulieu@mun.ca](mailto:lbeaulieu@mun.ca).*

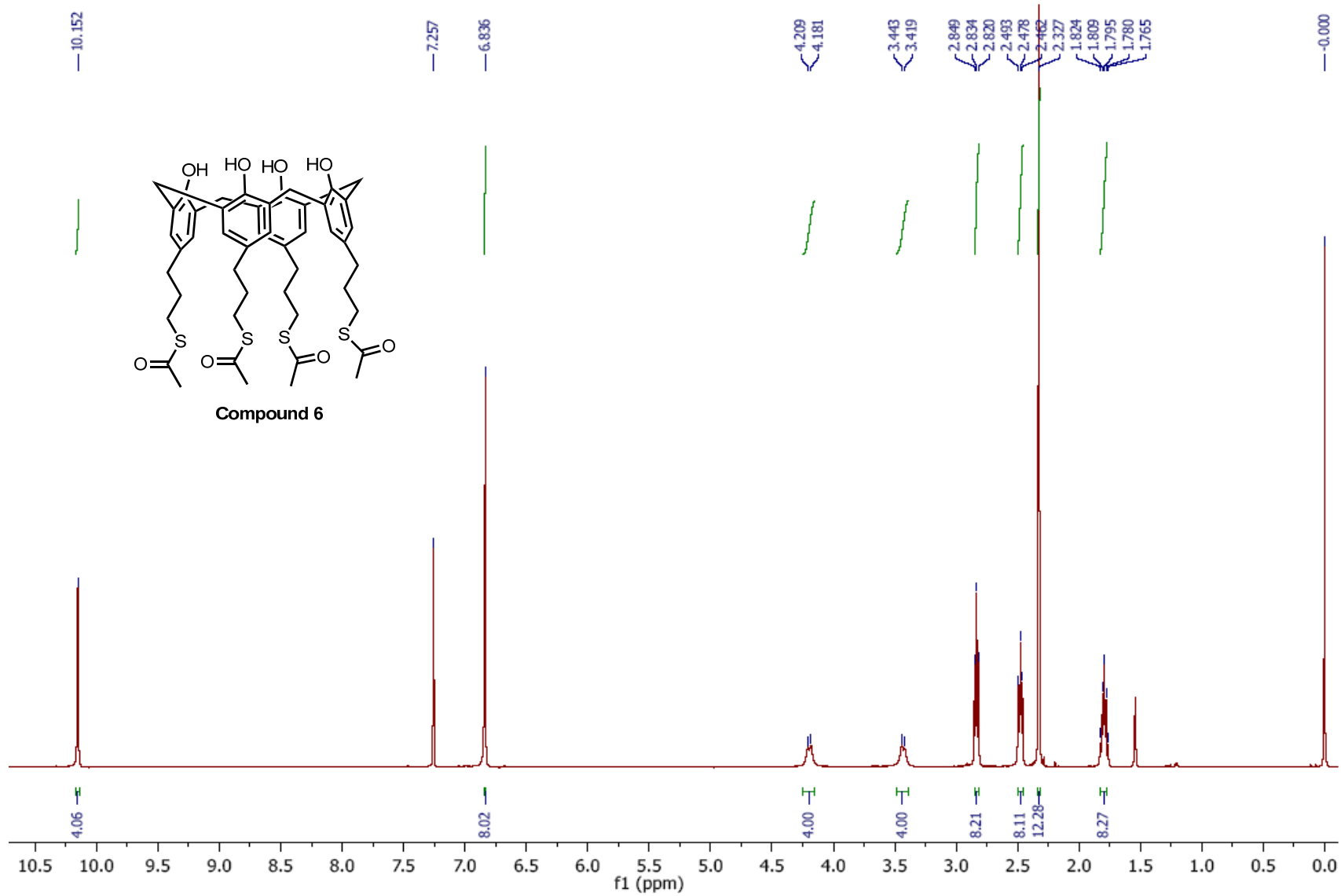
#### Table of Contents

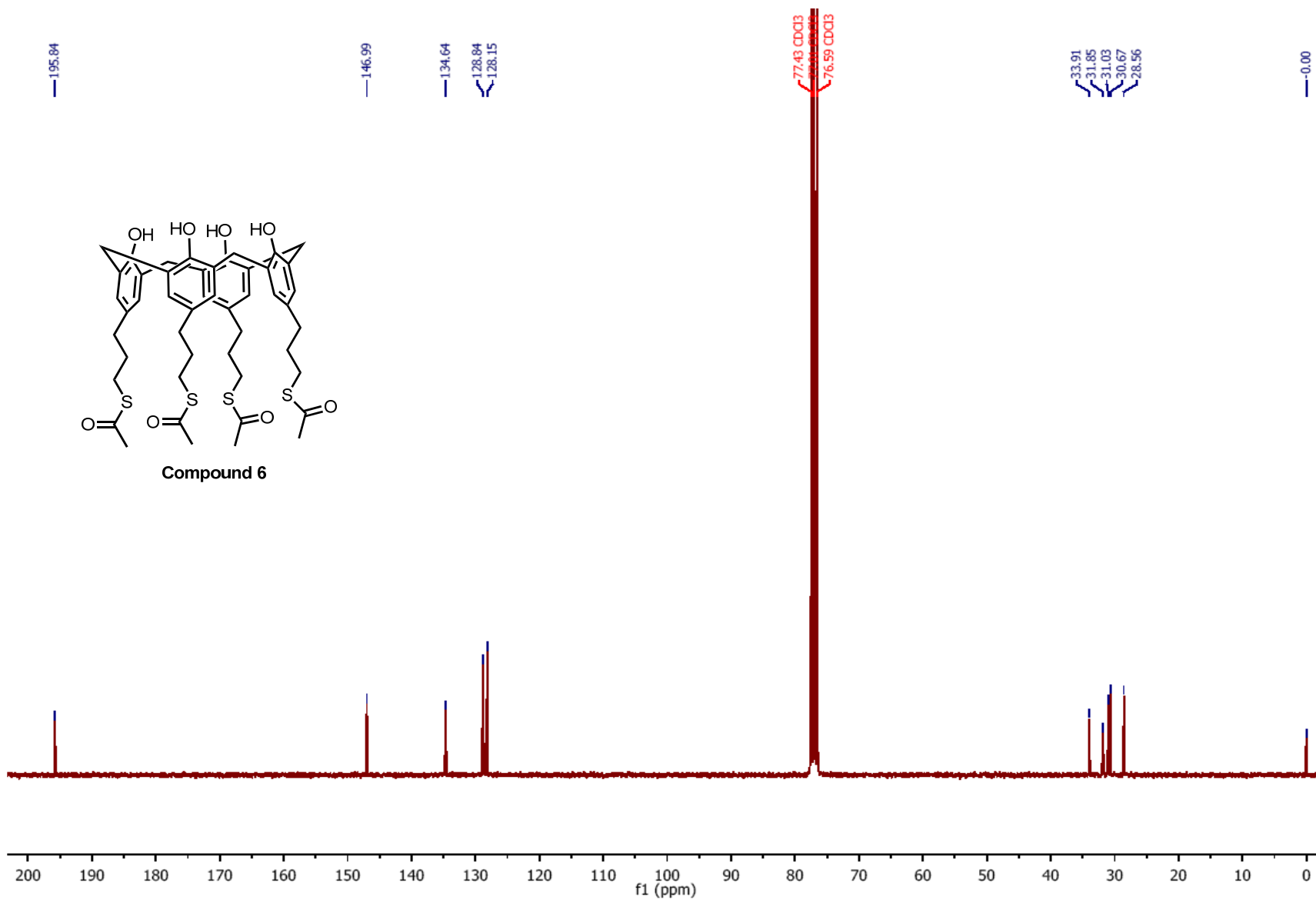
Description	Page Number
<sup>1</sup> H- NMR of Compound <b>2</b>	S2
<sup>13</sup> C- NMR of Compound <b>2</b>	S3
APCI-MS of Compound <b>2</b>	S4
<sup>1</sup> H- NMR of Compound <b>6</b>	S5
<sup>13</sup> C- NMR of Compound <b>6</b>	S6
APCI-MS of Compound <b>6</b>	S7
Checkcif for Compound <b>2</b>	S8

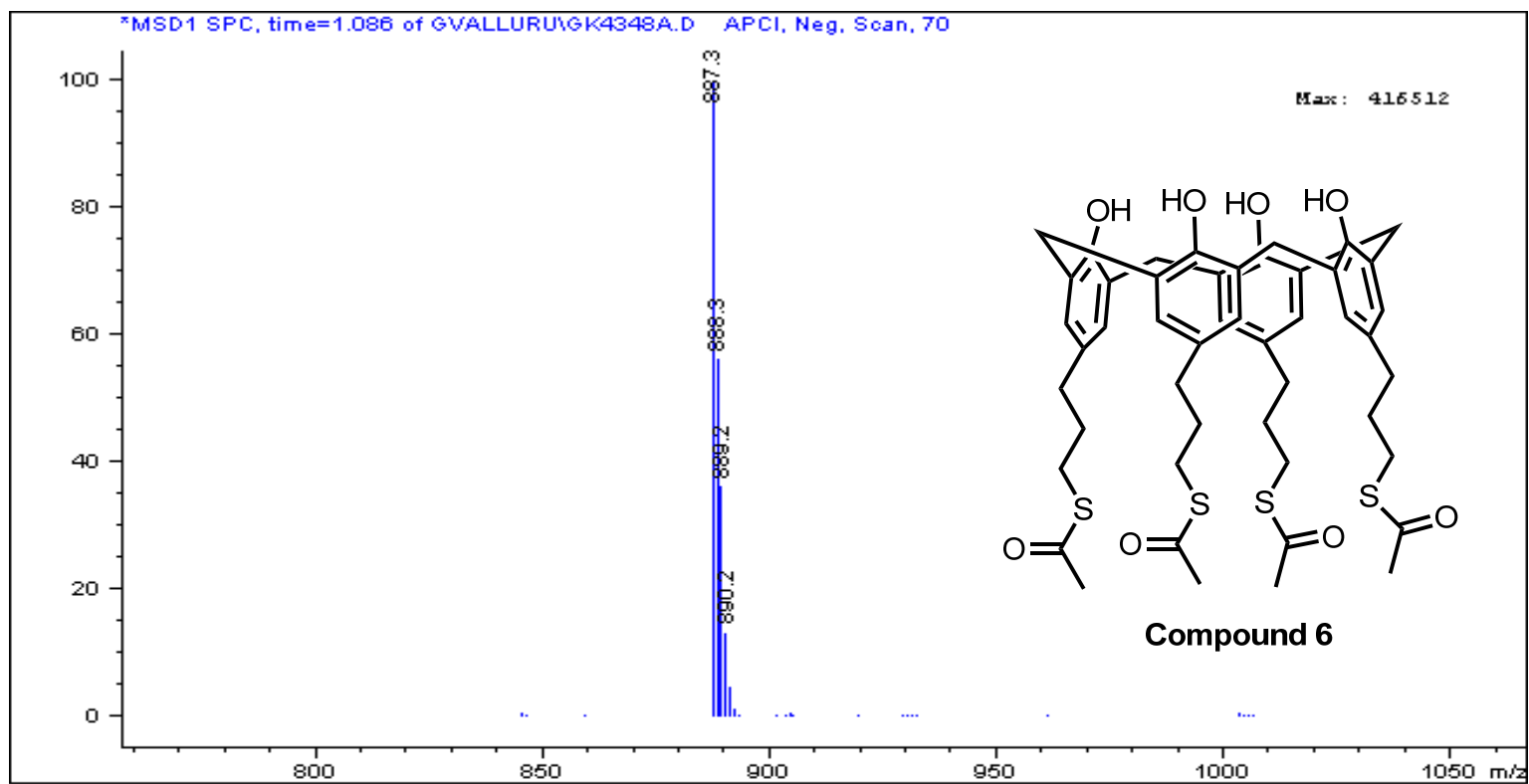












## checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found.      CIF dictionary      Interpreting this report

### Datablock: 3

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Bond precision:    C-C = 0.0058 Å                      Wavelength=0.71075  
Cell:                      a=22.889(7)              b=13.486(4)              c=21.398(6)  
                                    alpha=90                      beta=113.624(4)              gamma=90  
Temperature:              163 K

	Calculated	Reported
Volume	6052(3)	6052(3)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C60 H72 O16 S4	C60 H72 O16 S4
Sum formula	C60 H72 O16 S4	C60 H72 O16 S4
Mr	1177.46	1177.46
Dx, g cm <sup>-3</sup>	1.292	1.292
Z	4	4
Mu (mm <sup>-1</sup> )	0.224	0.223
F000	2496.0	2496.0
F000'	2499.22	
h, k, lmax	28, 16, 26	28, 16, 26
Nref	6285	6266
Tmin, Tmax	0.961, 0.985	0.960, 0.991
Tmin'	0.939	

Correction method= NUMERICAL

Data completeness= 0.997                      Theta(max)= 26.500

R(reflections)= 0.0944( 5422)                      wR2(reflections)= 0.2660( 6266)

S = 1.126                                      Npar= 430

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The following ALERTS were generated. Each ALERT has the format

**test-name\_ALERT\_alert-type\_alert-level.**

Click on the hyperlinks for more details of the test.

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#### Alert level C

RFACR01\_ALERT\_3\_C The value of the weighted R factor is > 0.25

Weighted R factor given      0.266

PLAT084\_ALERT\_2\_C High wR2 Value .....      0.27

PLAT220\_ALERT\_2\_C Large Non-Solvent      C      Ueq(max)/Ueq(min) ...      3.1 Ratio



PLAT234_ALERT_4_C	Large Hirshfeld Difference O5A	--	C17A	..	0.18	Ang.	
PLAT242_ALERT_2_C	Check Low	Ueq	as Compared to Neighbors for			C14	
PLAT340_ALERT_3_C	Low Bond Precision on	C-C Bonds	.....		0.0058	Ang	
PLAT366_ALERT_2_C	Short? C(sp?)-C(sp?) Bond	C21	-	C22	...	1.37	Ang.
PLAT366_ALERT_2_C	Short? C(sp?)-C(sp?) Bond	C21	-	C26	...	1.39	Ang.

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● **Alert level G**

PLAT072_ALERT_2_G	SHELXL First	Parameter in WGHT	Unusually Large.		0.12	
PLAT083_ALERT_2_G	SHELXL Second	Parameter in WGHT	Unusually Large.		12.58	
PLAT242_ALERT_2_G	Check Low	Ueq	as Compared to Neighbors for			C17A
PLAT301_ALERT_3_G	Note: Main Residue	Disorder	.....		18	Perc.
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	....				!

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
5 **ALERT level G** = General information/check it is not something unexpected
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
8 ALERT type 2 Indicator that the structure model may be wrong or deficient  
3 ALERT type 3 Indicator that the structure quality may be low  
1 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check
- 

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special\_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

### Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

### Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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**PLATON version of 05/11/2012; check.def file version of 05/11/2012**

Datablock 3 - ellipsoid plot

