

Synthesis and photophysical, electrochemical, antibacterial, DNA binding studies of Triazinocalix[2]arenes

Kannan Rajavelu and Perumal Rajakumar*

*Department of Organic Chemistry, University of Madras, Guindy campus, Chennai- 600 025,
Tamil nadu, INDIA*

Tel No: +91 44 2220 2810

E-mail: perumalrajakumar@gmail.com

Supporting Information

Content

Abbreviations.....	S-1
Spectroscopic data.....	S-2
Absorption and Emission spectrum of oxacalixarene 2-9	S-3
DNA binding studies of oxacalixarene 5	S-4
Antibacterial studies of oxacalixarene 2-9	S-5
Docking studies of oxacalixarene 2 and 4	S-6

S-1
Abbreviations

DIPEA	:	Diisopropyl ethylamine
THF	:	Tetrahydrofuran
CHCl ₃	:	Chloroform
UV	:	Ultraviolet
CV	:	Cyclic Voltammetry
CD	:	Circular Dichroism
AgNO ₃	:	Silver nitrate
TBAP	:	Tetrabutylammonium Perchlorate
CT-DNA	:	Calf thymus - Deoxyribonucleic acid
Tris-HCl	:	Tris(hydroxymethyl)aminomethane-HCl
ESI-Mass	:	Electrospray ionization
NMR	:	Nuclear Magnetic Resonance

S-2

Spectroscopic data



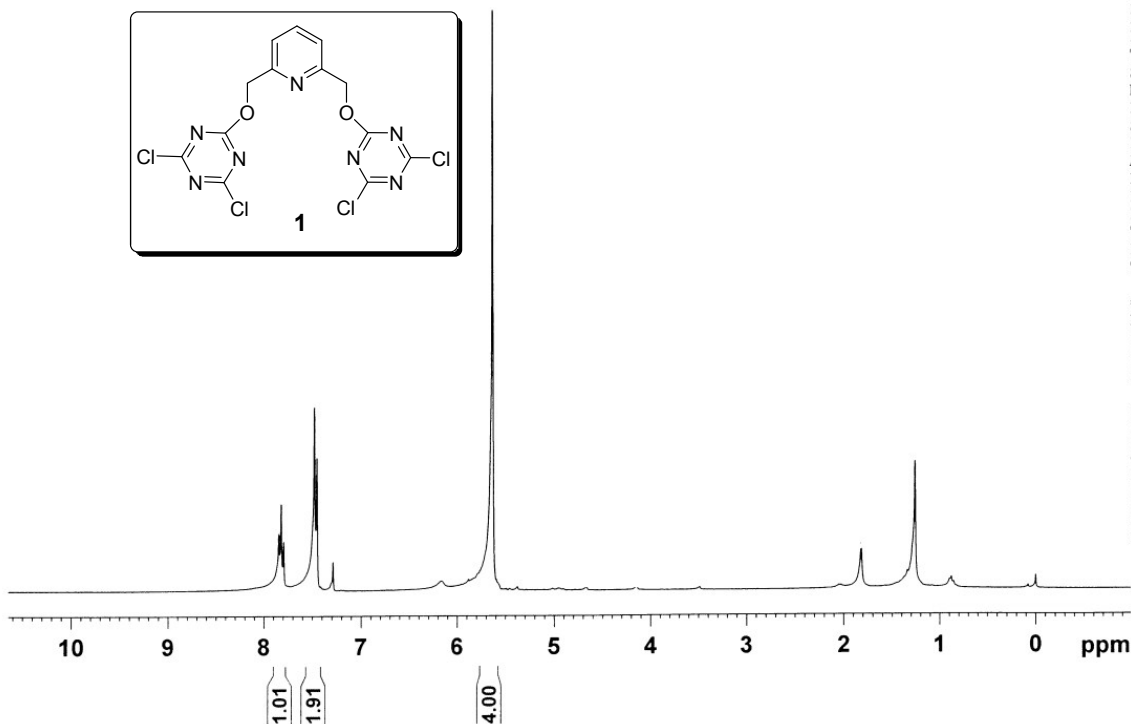
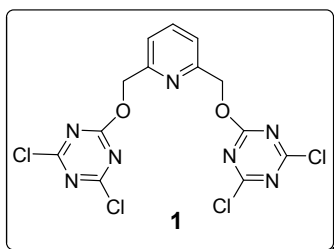
Current Data Parameters
NAME KR-111B
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131128
Time_ 13.51
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 161.3
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

=====
CHANNEL f1
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299984 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.845
7.820
7.794
7.479
7.453
7.287
5.632



^1H NMR (300 MHz, CDCl_3) spectrum of the Precyclophane **1**



Current Data Parameters
NAME KR-111B
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131128
Time_ 13.56
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 173
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1625.5
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

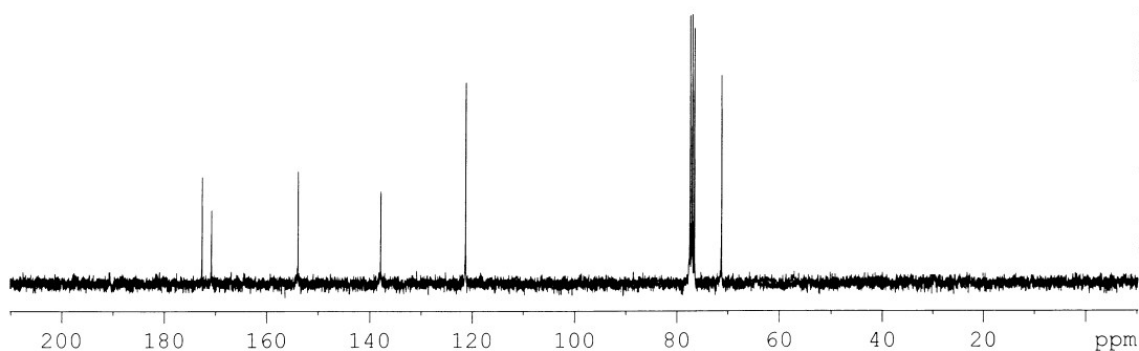
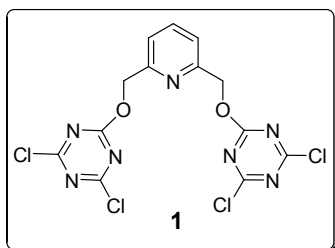
===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

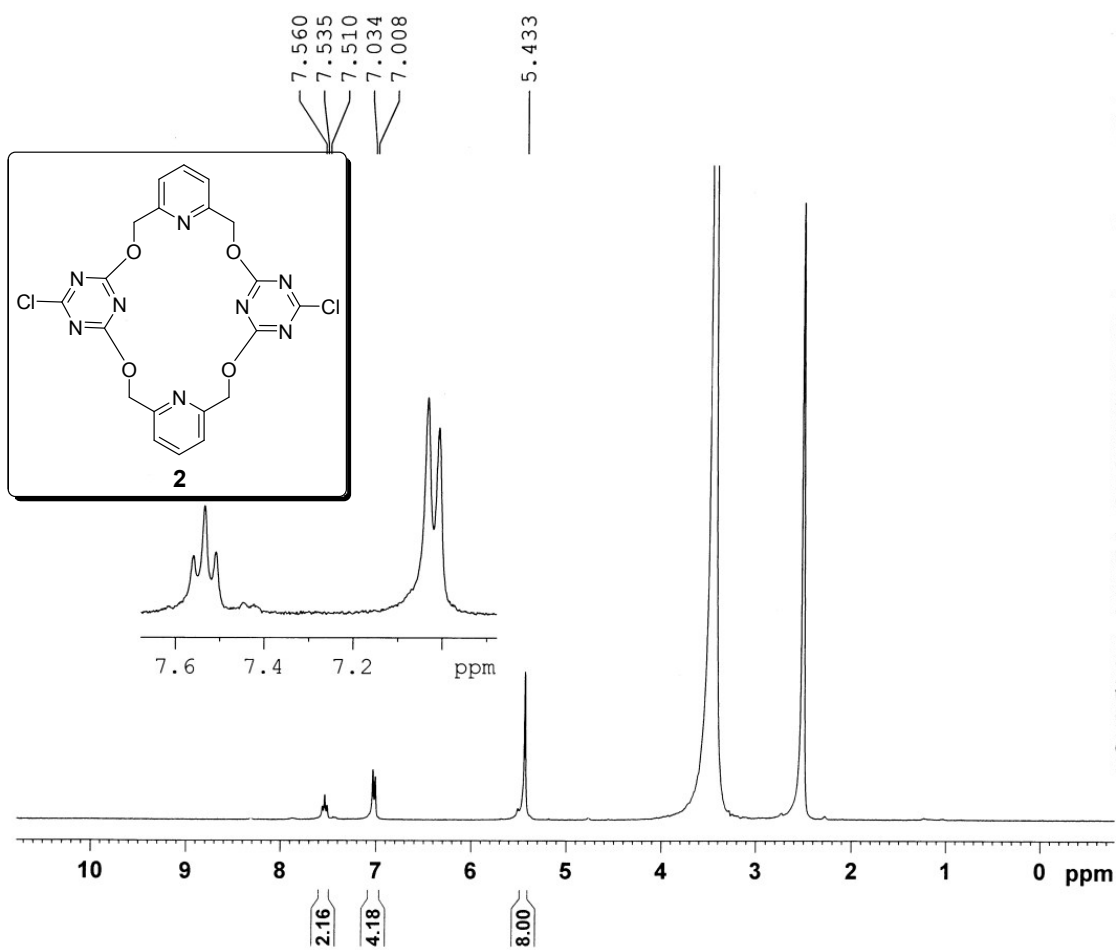
172.75
170.87
153.96
137.96
121.35

77.47
77.05
76.62
71.26



^{13}C NMR (75 MHz, CDCl_3) spectrum of the Precyclophane 1

UNIV. OF MADRAS



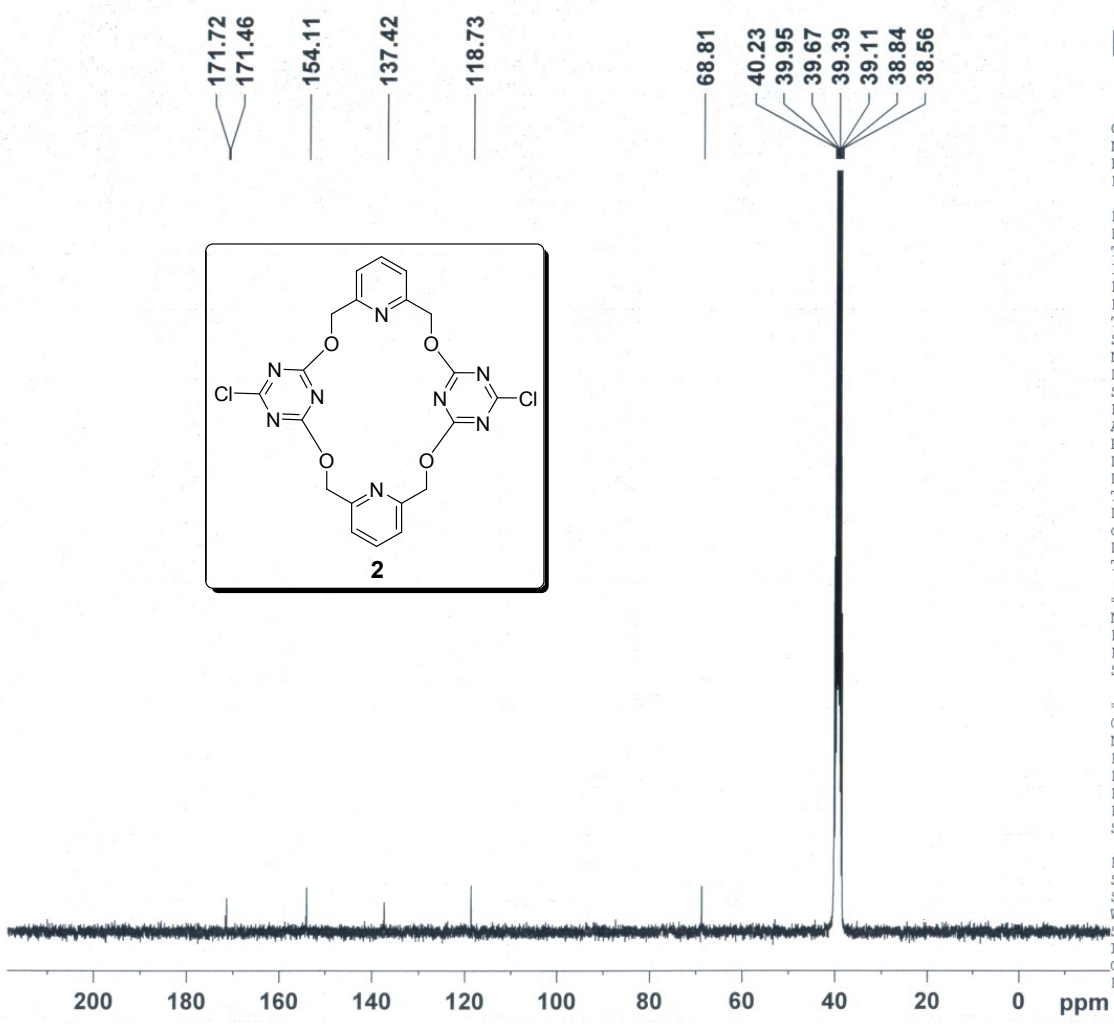
Current Data Parameters
NAME KRC-232-II
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150121
Time 14.56
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 101.6
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR (300 MHz, DMSO-d₆) spectrum of the Oxacalixarene 2



Current Data Parameters
 NAME KRC-232-II
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20150124
 Time 14.03
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2000
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 2896.3
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 9.30 usec
 PL1 0.00 dB
 SFO1 75.4752953 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677867 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

¹³C NMR (75 MHz, DMSO-d₆) spectrum of the Oxcalixarene 2



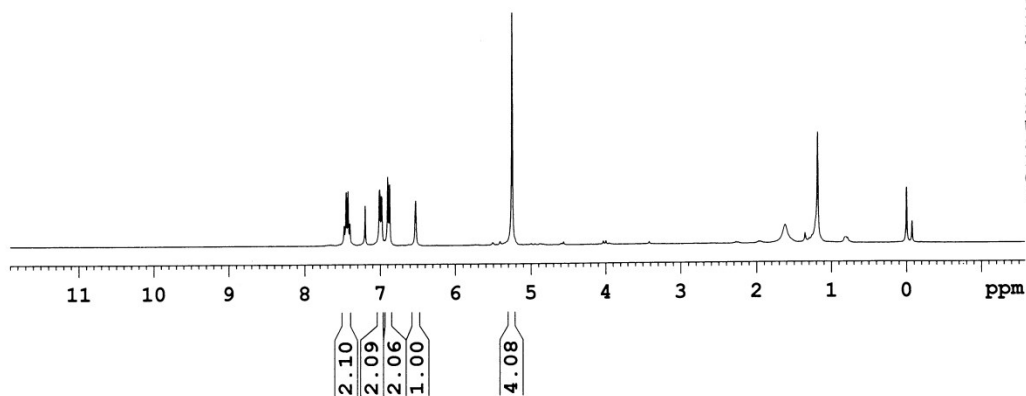
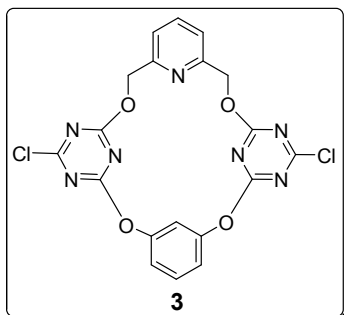
Current Data Parameters
NAME KR-97
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131023
Time_ 1.10
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 228.1
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300246 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.482
7.455
7.429
7.404
7.202
7.011
6.983
6.901
6.875
6.527
5.252



^1H NMR (300 MHz, CDCl_3) spectrum of the Oxacalixarene **3**

174.12
172.11
171.91

155.10
151.74

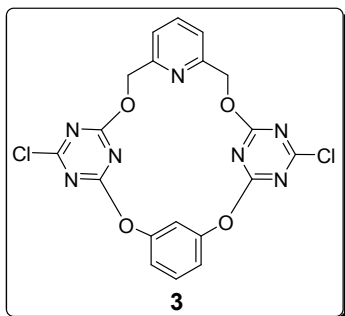
137.67
129.91
120.37
117.48
113.82

77.45
77.03
76.60
70.27



Current Data Parameters
NAME KR-97
EXPNO 2
PROCNO 1

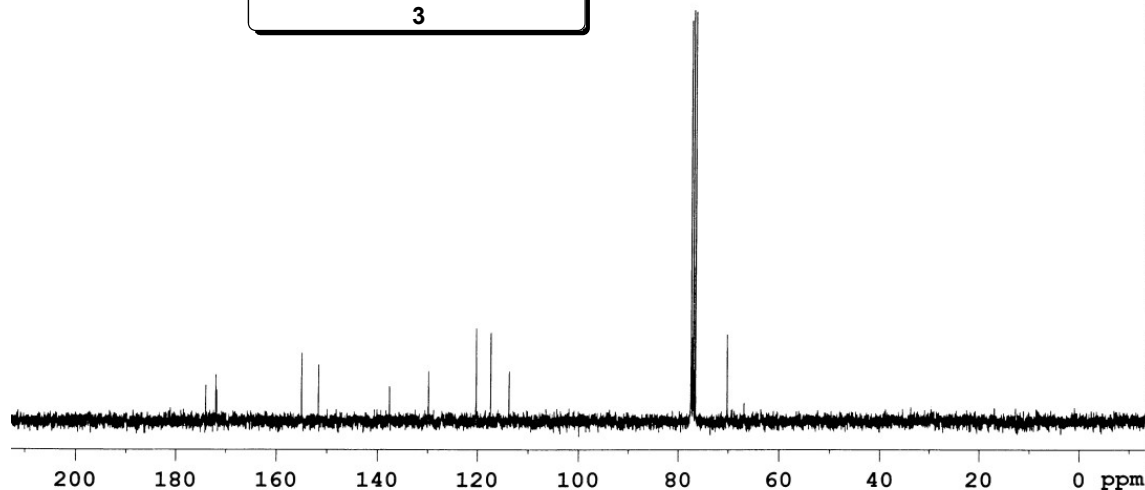
F2 - Acquisition Parameters
Date_ 20131023
Time_ 1.13
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 90
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1290.2
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1



==== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



¹³C NMR (75 MHz, CDCl₃) spectrum of the Oxacalixarene **3**

UNIV OF MADRAS



Current Data Parameters
NAME KR-115
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131206
Time_ 19.10
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 128
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TDO 1

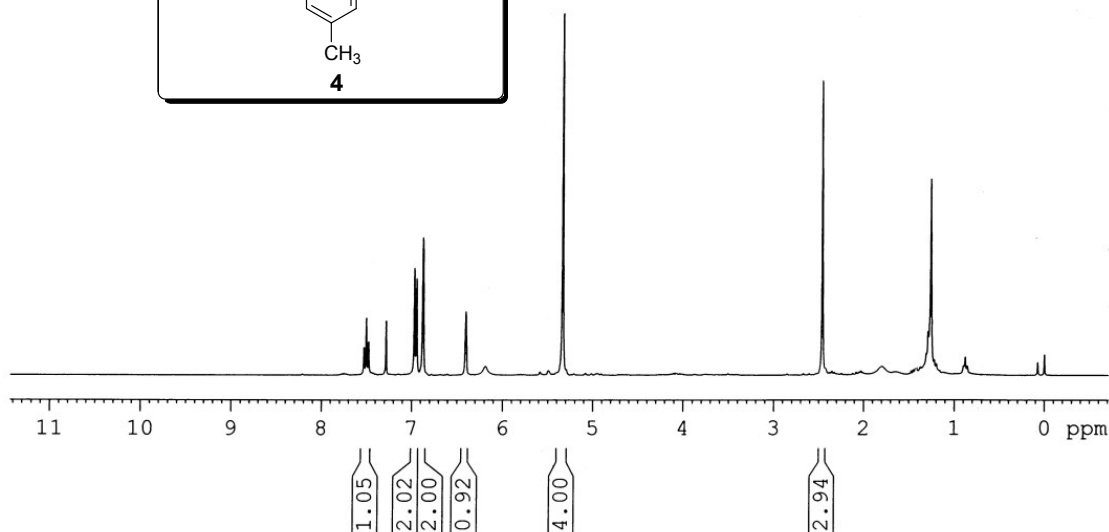
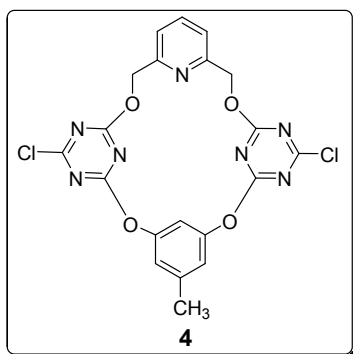
===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300003 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.529
7.503
7.477
7.282
6.970
6.944
6.876
6.403

5.335

2.460



^1H NMR (300 MHz, CDCl_3) spectrum of the Oxacalixarene 4

UNIV OF MADRAS

174.01
172.13
171.92
155.07
151.47
140.74
137.59
120.81
117.45
110.75

77.46
77.04
76.62
70.29

21.44



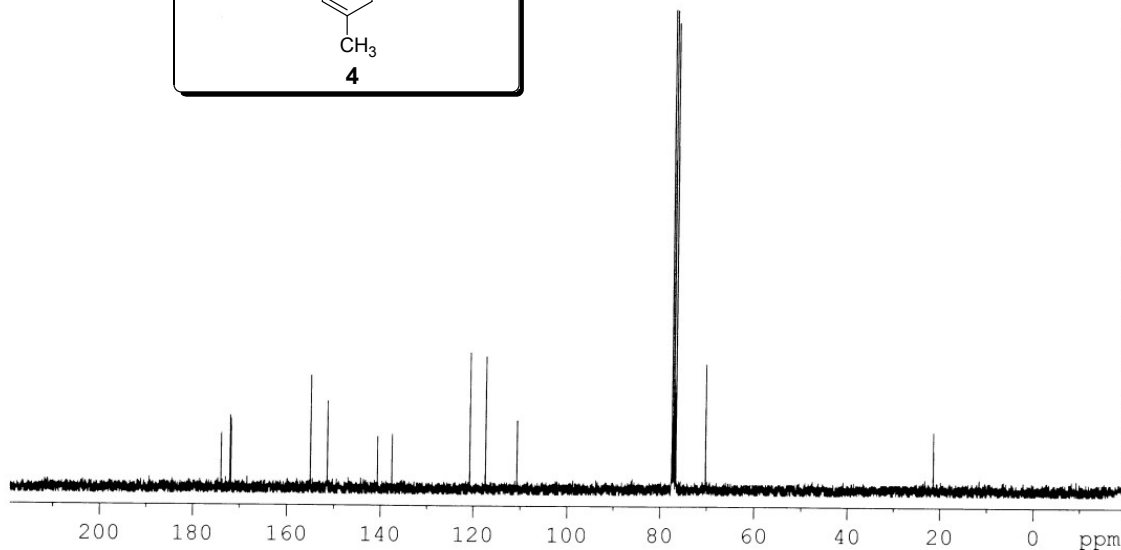
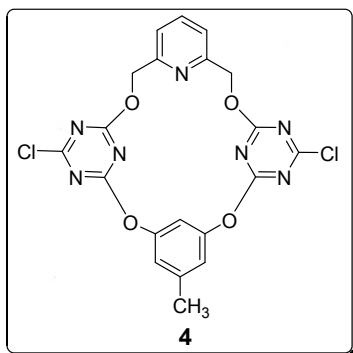
Current Data Parameters
NAME KR-115
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131206
Time_ 19.19
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 133
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 456.1
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



¹³C NMR (75 MHz, CDCl₃) spectrum of the Oxacalixarene 4

UNIV. OF MADRAS



Current Data Parameters
NAME KR-72
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130808
Time_ 14.36
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 287.4
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

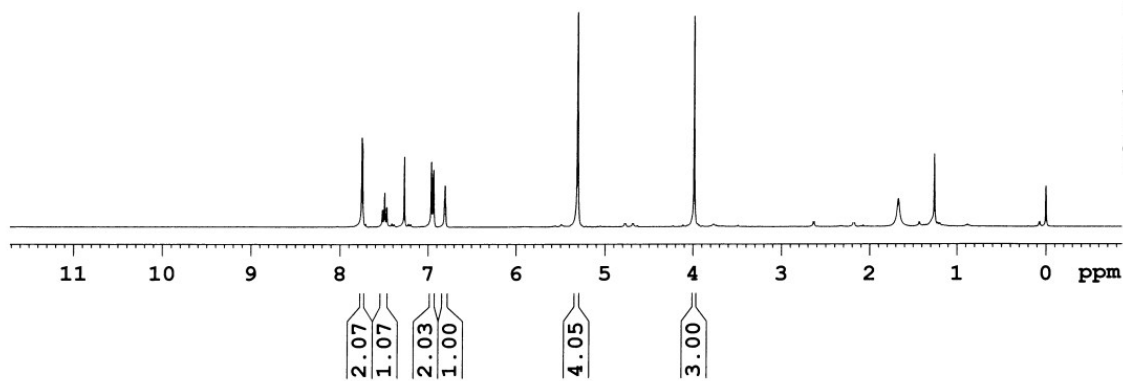
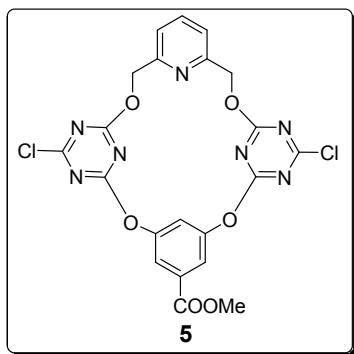
===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300033 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.750
7.522
7.496
7.470
6.964
6.938
6.805

5.309

3.985



¹H NMR (300 MHz, CDCl₃) spectrum of the Oxacalixarene 5



Current Data Parameters
NAME KR-72
EX?NO 1
PROCNO 1

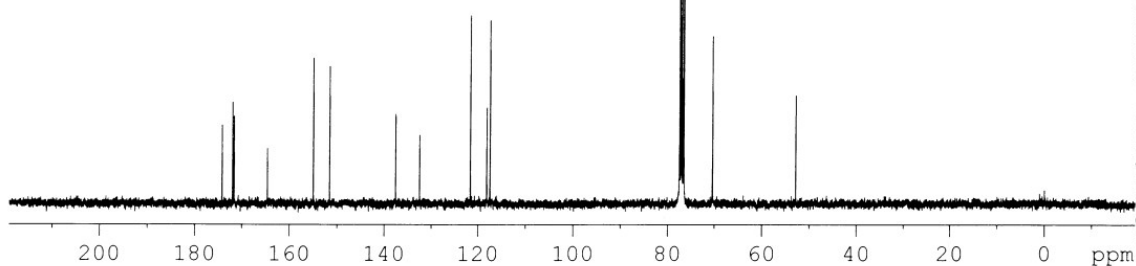
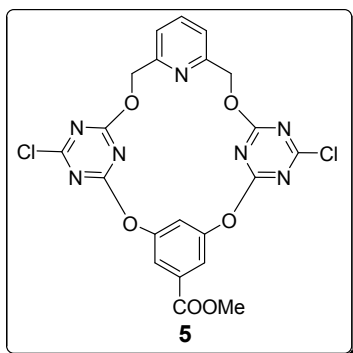
F2 - Acquisition Parameters
Date_ 20130810
Time 0.02
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1787
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1625.5
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

174.28
172.08
171.73
164.71
155.05
151.62
137.65
132.54
121.69
118.20
117.51
77.44
77.02
76.59
70.43
52.87



¹³C NMR (75 MHz, CDCl₃) spectrum of the Oxacalixarene **5**

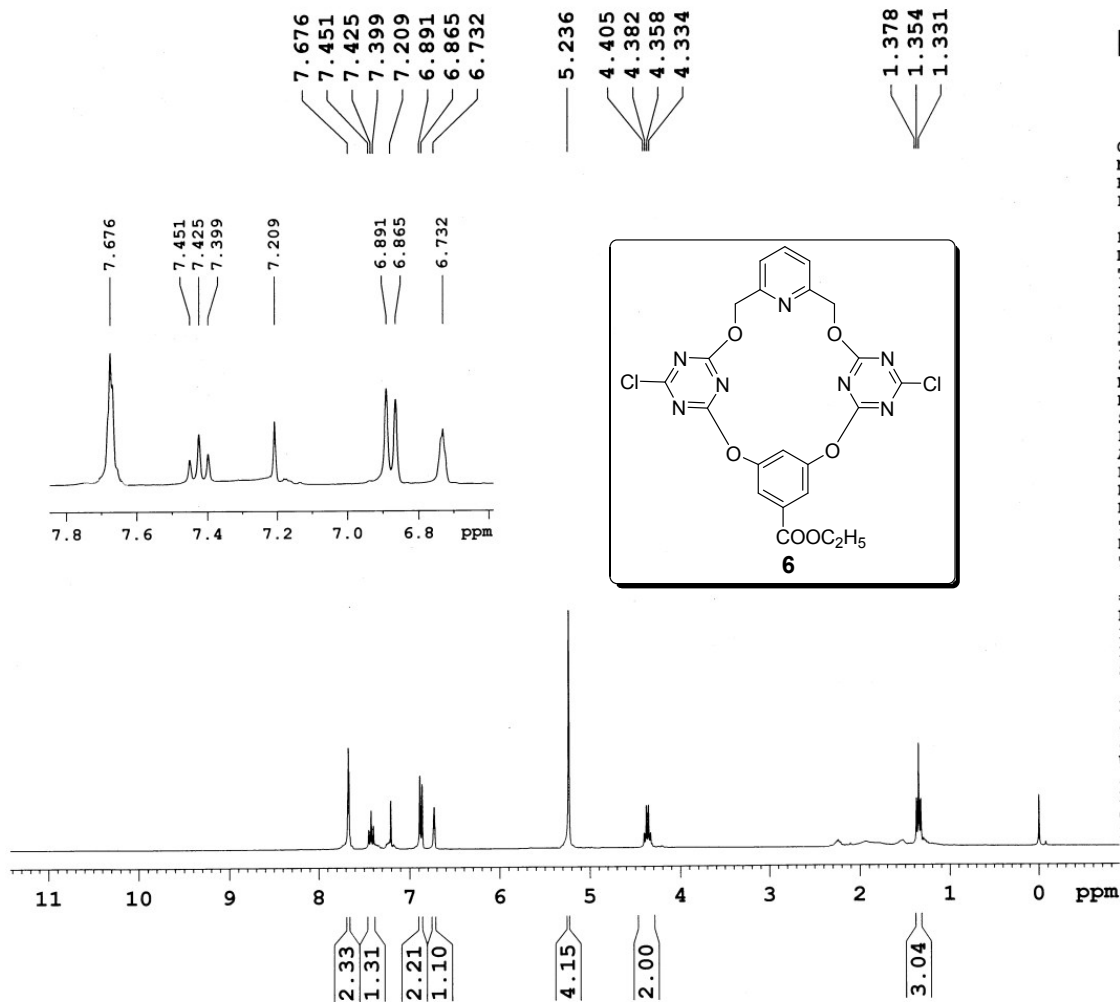


Current Data Parameters
NAME KRC-234
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150130
Time 23.26
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 114
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300224 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H NMR (300 MHz, CDCl₃) spectrum of the Oxcalixarene **6**

174.24
172.08
171.73
164.22
155.03
151.58
137.64
132.93
121.61
118.08
117.51

77.46
77.04
76.62
70.40
61.98

14.26



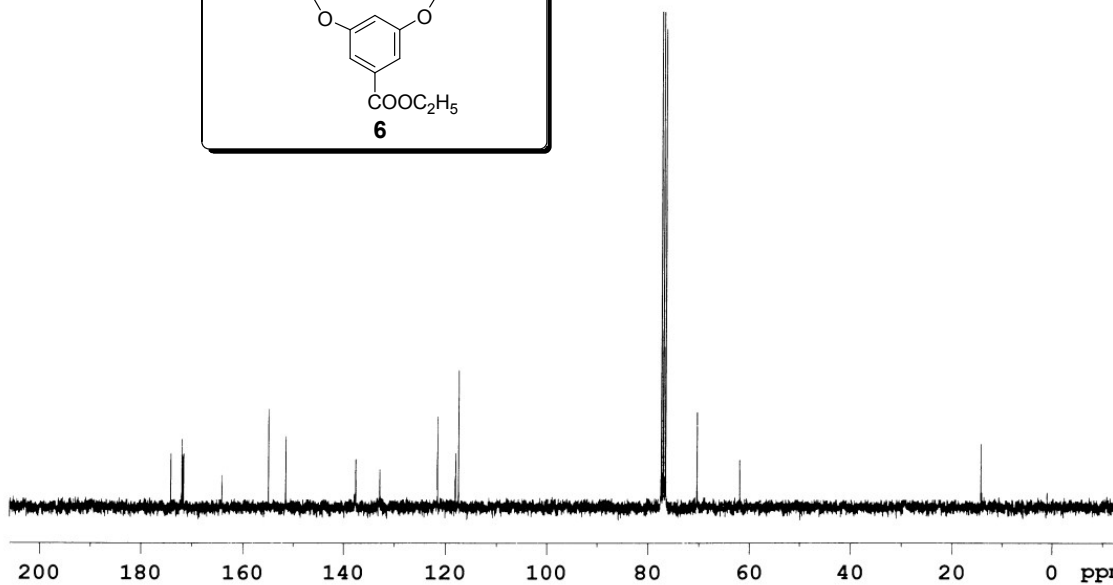
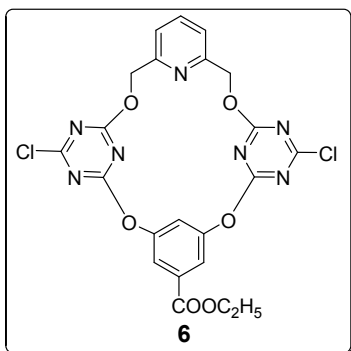
Current Data Parameters
NAME KRC-234
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150130
Time_ 23.35
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 151
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 724.1
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



¹³C NMR (75 MHz, CDCl₃) spectrum of the Oxacalixarene **6**

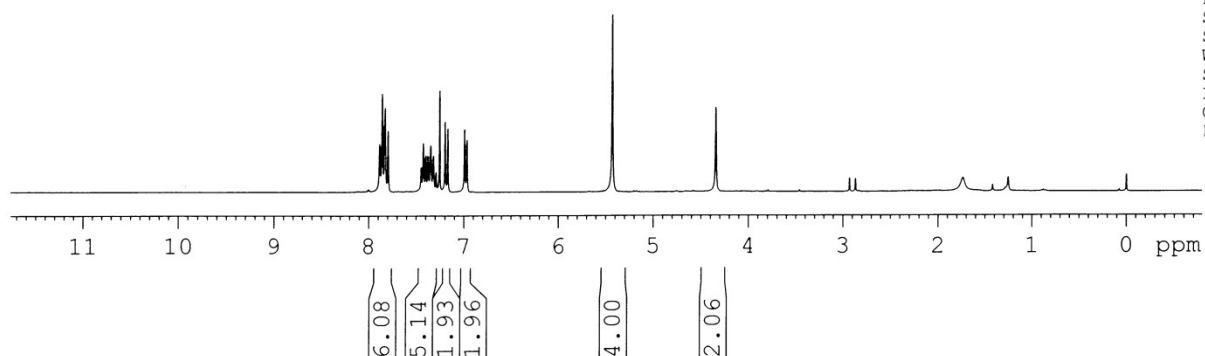
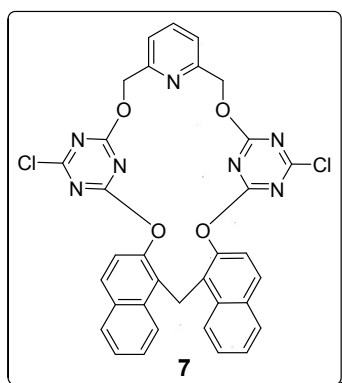
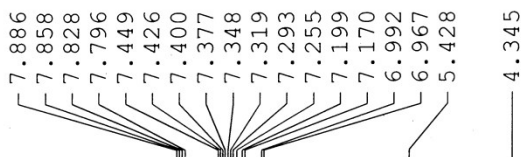


Current Data Parameters
NAME KR-101
EXPNO 1
PROCNO 1

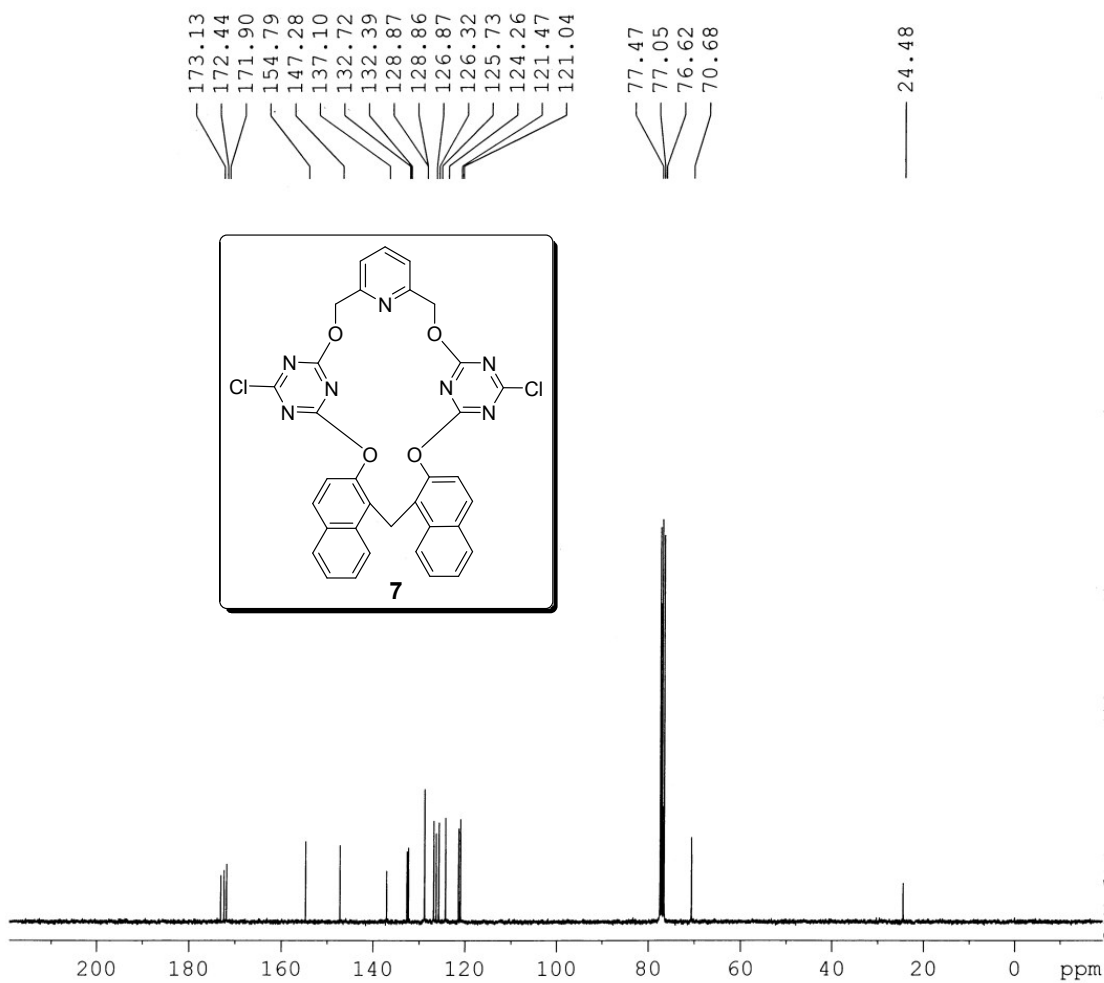
F2 - Acquisition Parameters
Date_ 20131027
Time_ 21.09
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 143.7
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300084 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



^1H NMR (300 MHz, CDCl_3) spectrum of the Oxacalixarene 7



Current Data Parameters
NAME KR-101
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131027
Time 21.20
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 748
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 812.7
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{13}C NMR (75 MHz, CDCl_3) spectrum of the Oxacalixarene **7**

UNIV. OF MADRAS



Current Data Parameters
NAME KRC-101
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20140326
Time 12.56
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 114
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TDO 1

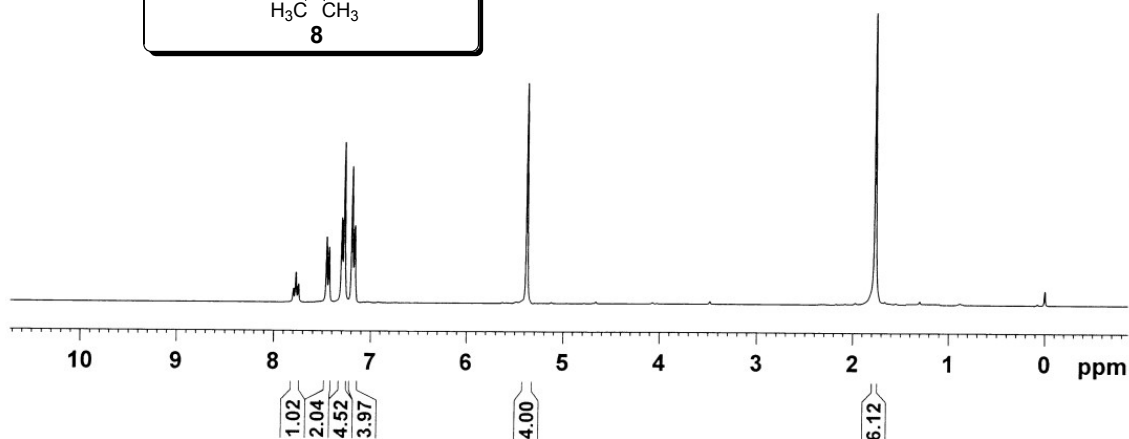
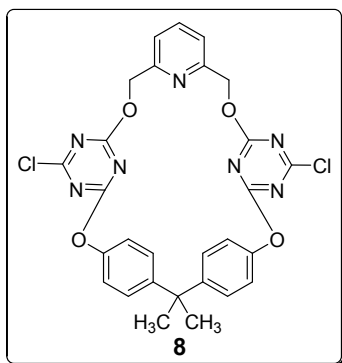
===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300030 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.798
7.773
7.747
7.457
7.431
7.301
7.273
7.194
7.166

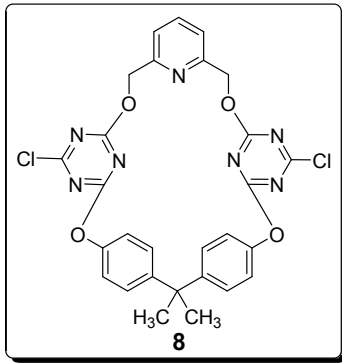
5.378

1.763



¹H NMR (300 MHz, CDCl₃) spectrum of the Oxalixarene **8**

UNIV. OF MADRAS



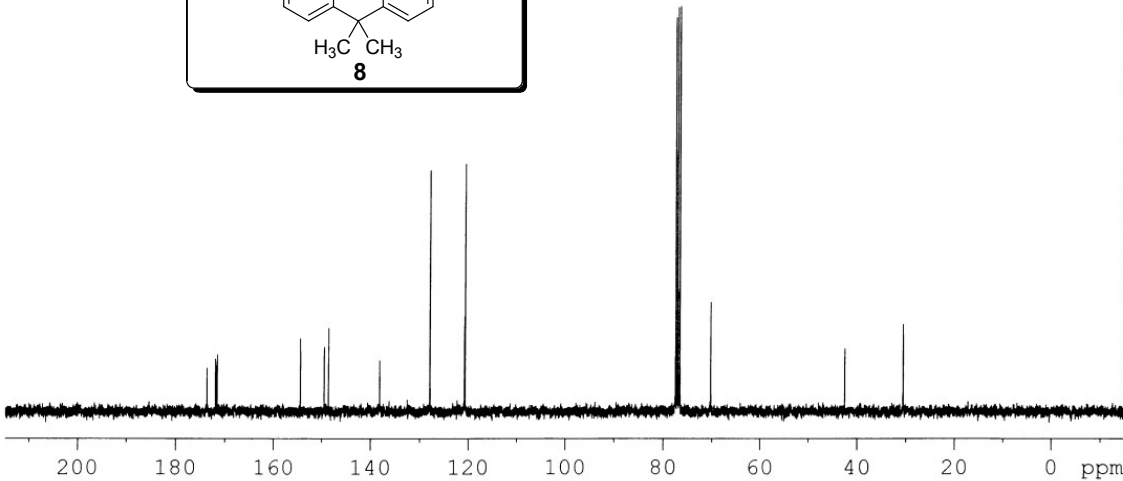
Current Data Parameters
NAME KRC-101
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140326
Time 13.03
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 101
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 4096
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



¹³C NMR (75 MHz, CDCl₃) spectrum of the Oxacalixarene **8**



Current Data Parameters
NAME KRC-61
EXPNO 1
PROCNO 1

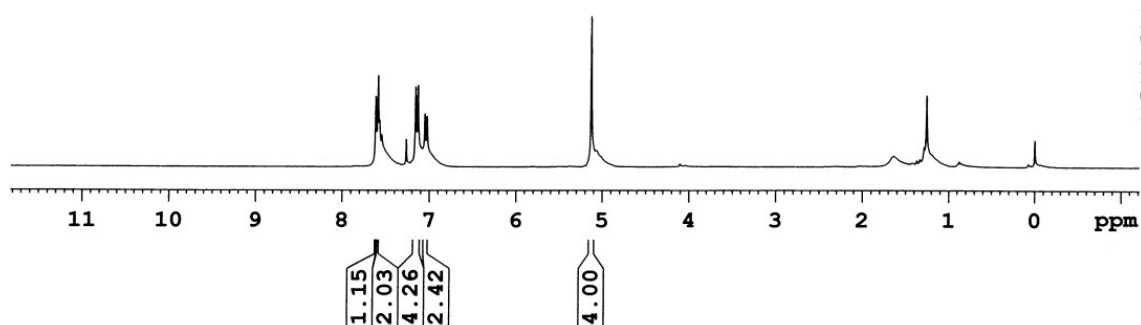
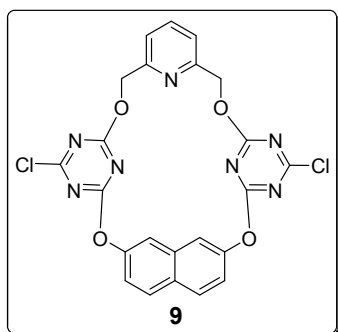
F2 - Acquisition Parameters
Date_ 20141024
Time_ 22.22
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 287.4
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.617
7.589
7.573
7.547
7.266
7.162
7.133
7.054
7.028

5.131



^1H NMR (300 MHz, CDCl_3) spectrum of the Oxacalixarene **9**



Current Data Parameters
NAME KRC-61
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141025
Time_ 5.07
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4721
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 3649.1
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

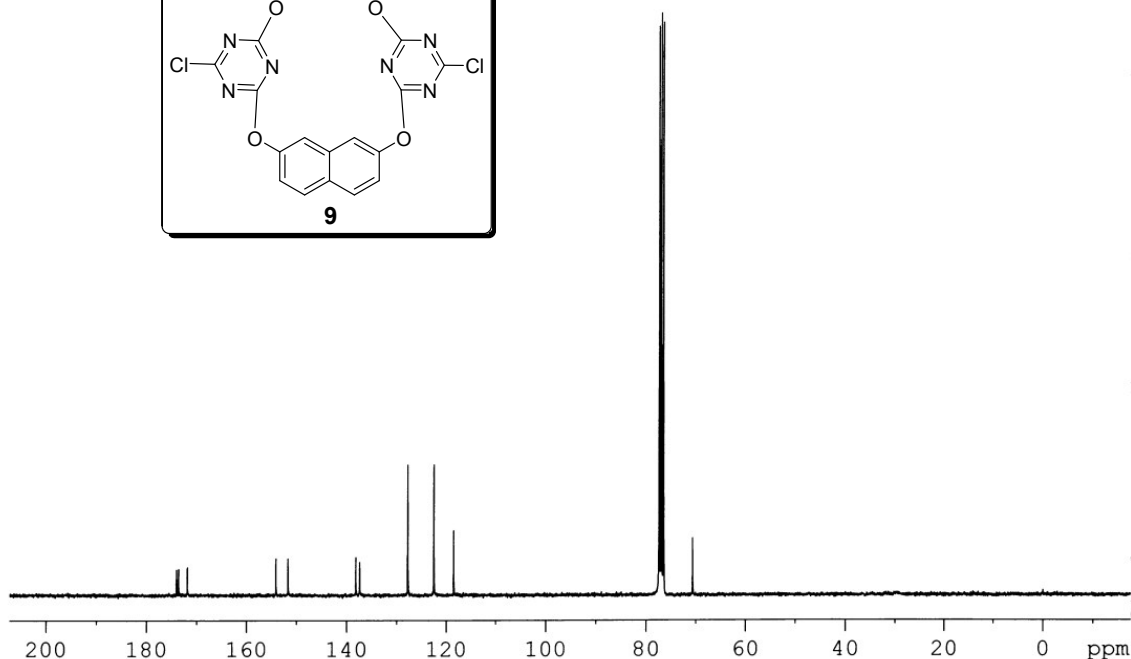
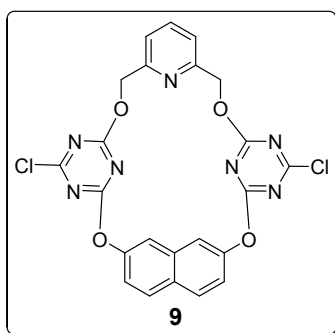
===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

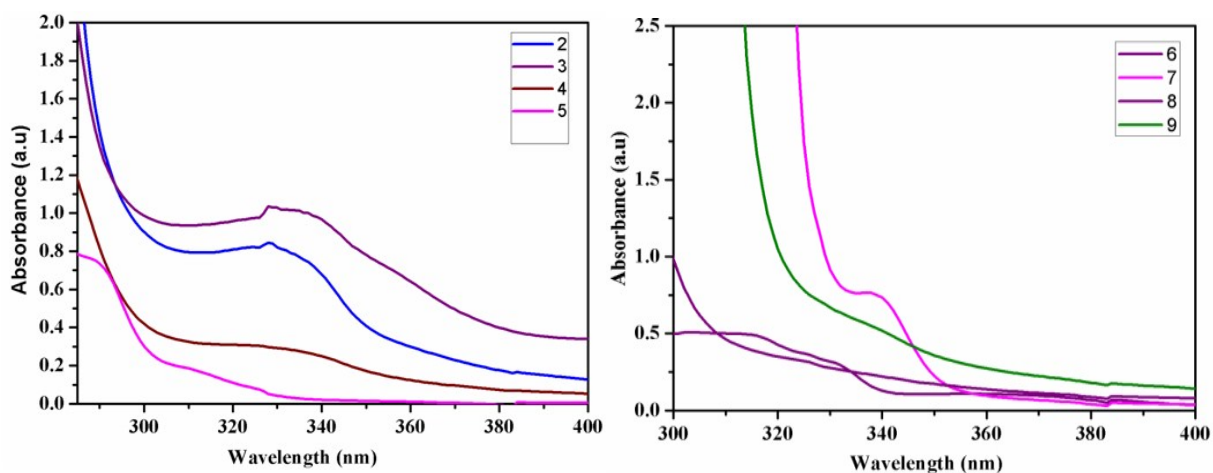
174.11
173.67
171.95
154.18
151.73
138.24
137.45
127.86
122.61
118.58

77.46
77.03
76.61
70.70



^{13}C NMR (75 MHz, CDCl_3) spectrum of the Oxacalixarene **9**

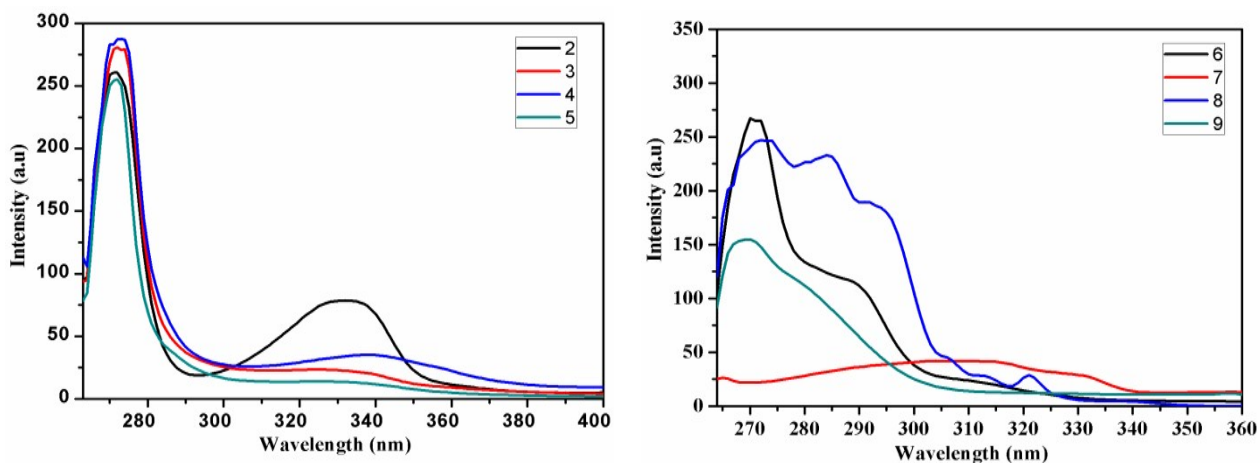
Absorption spectrum of Oxacalixarene 2-9



UV- vis absorption spectra of oxacalixarene **2-5** and **6-9** (1×10^{-3} mol L⁻¹) in DMF

Emmision studies

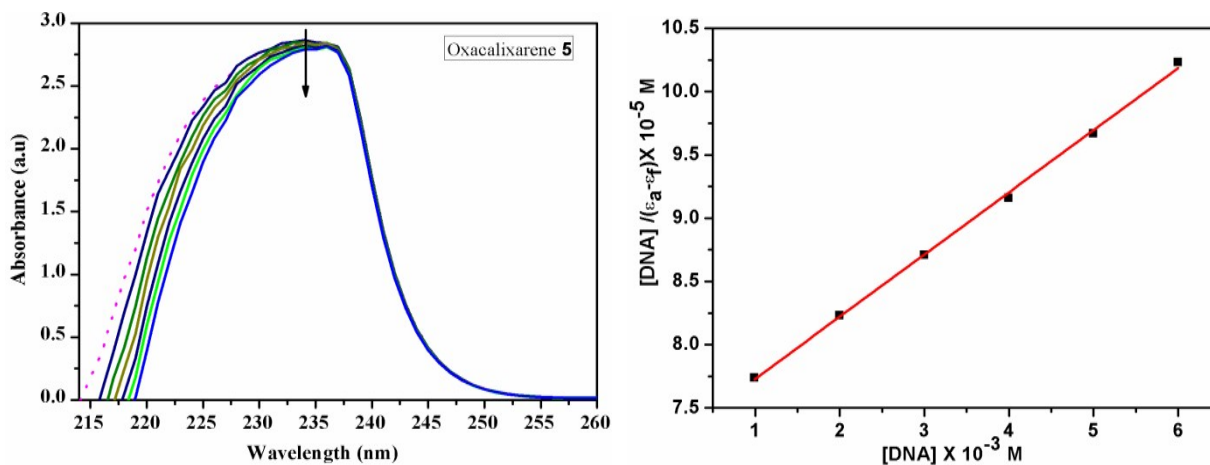
The emission spectrum of oxacalixarene **9** exhibited multiple emission bands due to presence of bisphenol A presented in the system.



The emission spectra were recorded at corresponding absorption maximum for all the oxacalixarenes. The excitation wavelength range for all the oxacalixarenes was 325-350 nm.

S-4

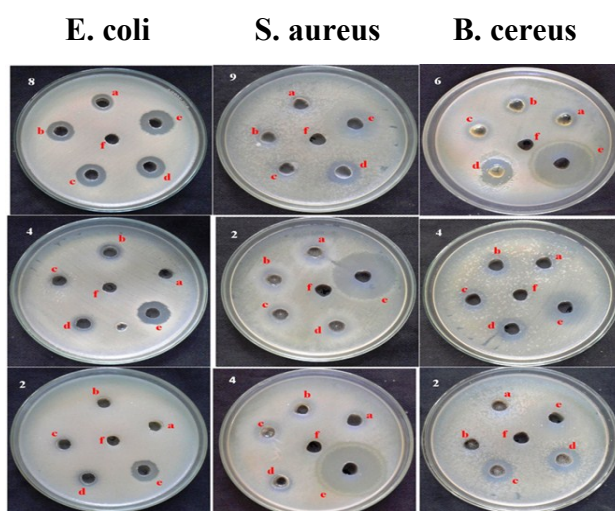
DNA binding studies of oxacalixarene 5



Absorption spectra of oxacalixarene 5 in the absence (dotted line) and presence of (thick line) increasing amounts of CT-DNA (0-250 μM) at 25 $^{\circ}\text{C}$ in 50 mM Tris-HCl (pH = 7.2).

S-5

Antibacterial studies of oxacalixarenes 2-9

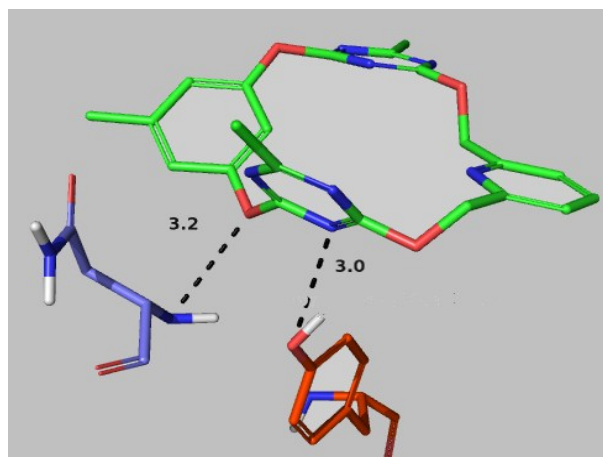
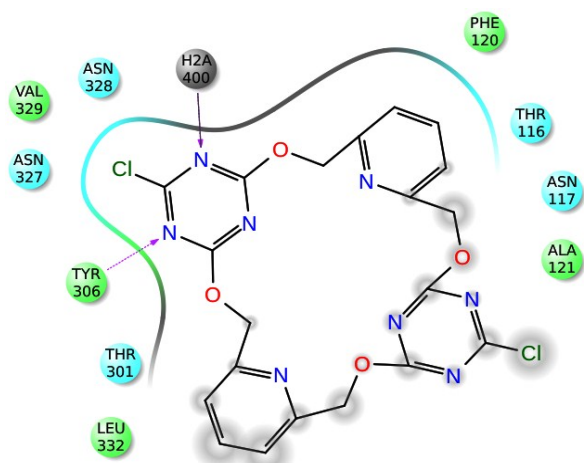


Control - 9% DMSO (Dimethyl sulfoxide)

Standard - Ampicillin

Antibacterial activity of oxacalixarenes against *E. coli*, *S. aureus* and *B. cereus*.

Docking studies of oxacalixarenes **2** and **4**



Binding of oxacalixarenes **2** and **4** with the Covalent Acyl enzyme (PDB ID: 1PW8).