

## Electronic Supporting Information

### Design, synthesis and metal sensing studies of ether-linked bis-triazole derivatives

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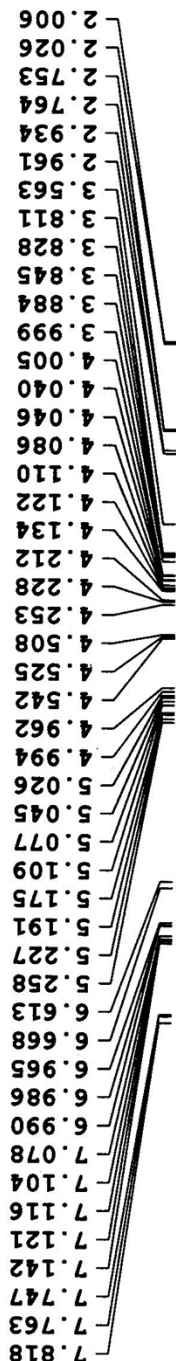
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## Computational details





| Current Data Parameters |          |
|-------------------------|----------|
| NAME                    | TMDH-257 |
| EXPNO                   | 3        |
| PROCNO                  | 1        |

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| Time_   | 20.59          |
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| PROBHD  | 5 mm DUL 13C-1 |
| PULPROG | zg30           |
| TD      | 65536          |
| SOLVENT | CDCl3          |
| NS      | 21             |
| 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        |
| DDI     | 1.00000000 sec |
| TD0     | 1              |

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P1        13.15 usec
PL1       0.00 dB
SF01      300.1318534 MHz
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| BF                         | 300.1300020 MHz |
| WDW                        | EM              |
| SB                         | 0               |
| GB                         | 0.30 Hz         |
| PC                         | 0               |
|                            | 1.00            |

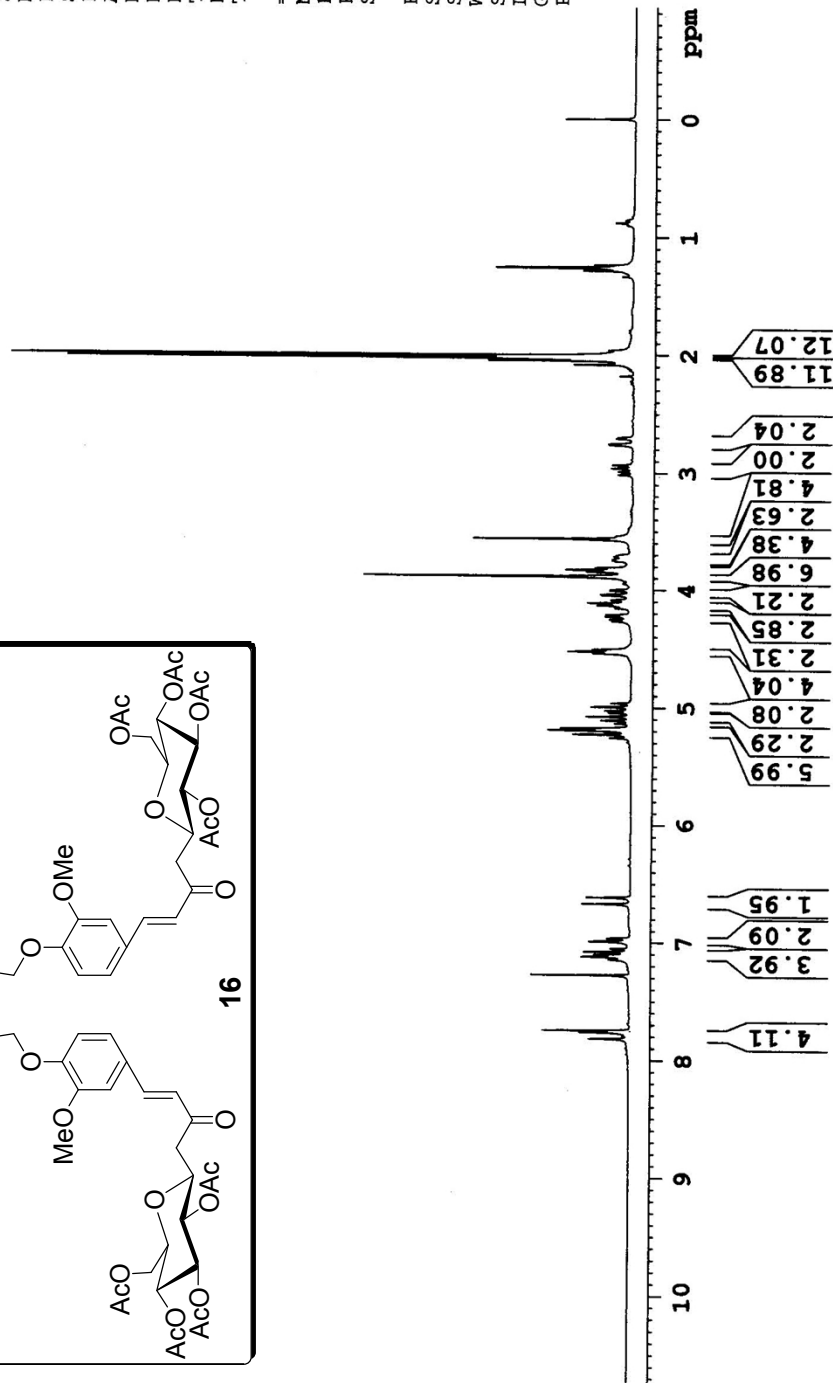
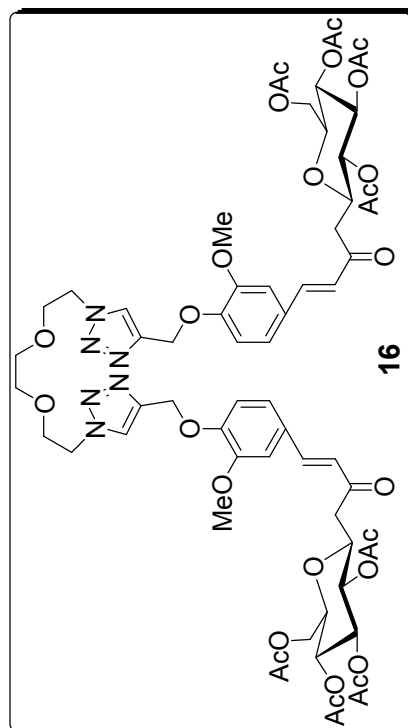


Figure 1  $^1\text{H}$  NMR spectrum (300 MHz,  $\text{CDCl}_3$ ) of compound, 16.



Current Data Parameters  
 NAME TMDH-257-C13-HS  
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 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20120614  
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 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1500  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 2048  
 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

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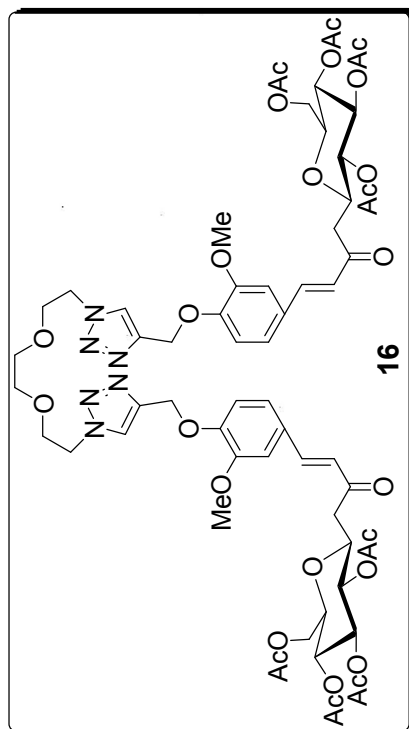
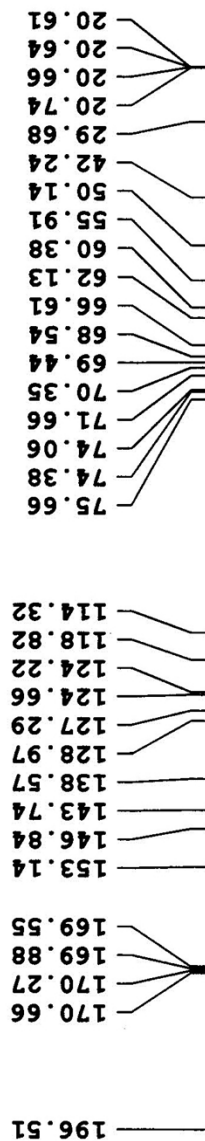


Figure 2 <sup>13</sup>C NMR spectrum (75 MHz, CDCl<sub>3</sub>) of compound, 16.



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 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG dept135  
 TD 65536  
 SOLVENT CDCl3  
 NS 346  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 16384  
 DW 27.800 usec  
 DE 6.00 usec  
 TE 300.0 K  
 CNST2 145.0000000  
 D1 2.00000000 sec  
 d2 0.00344828 sec  
 d12 0.00002000 sec  
 DELTA 0.00001184 sec  
 TDO 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.30 usec  
 P2 18.60 usec  
 PL1 0.00 dB  
 SFO1 75.4752953 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 P3 13.15 usec  
 P4 26.30 usec  
 PCPD2 80.00 usec  
 PL2 0.00 dB  
 PL12 15.68 dB  
 SFO2 300.1312005 MHz

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

138.58  
 127.27  
 124.68  
 124.26  
 118.79  
 114.30  
 75.65  
 74.37  
 74.04  
 71.64  
 70.34  
 69.44  
 68.51  
 66.60  
 62.11  
 55.90  
 50.14  
 42.21  
 20.76  
 20.69  
 20.66  
 20.63

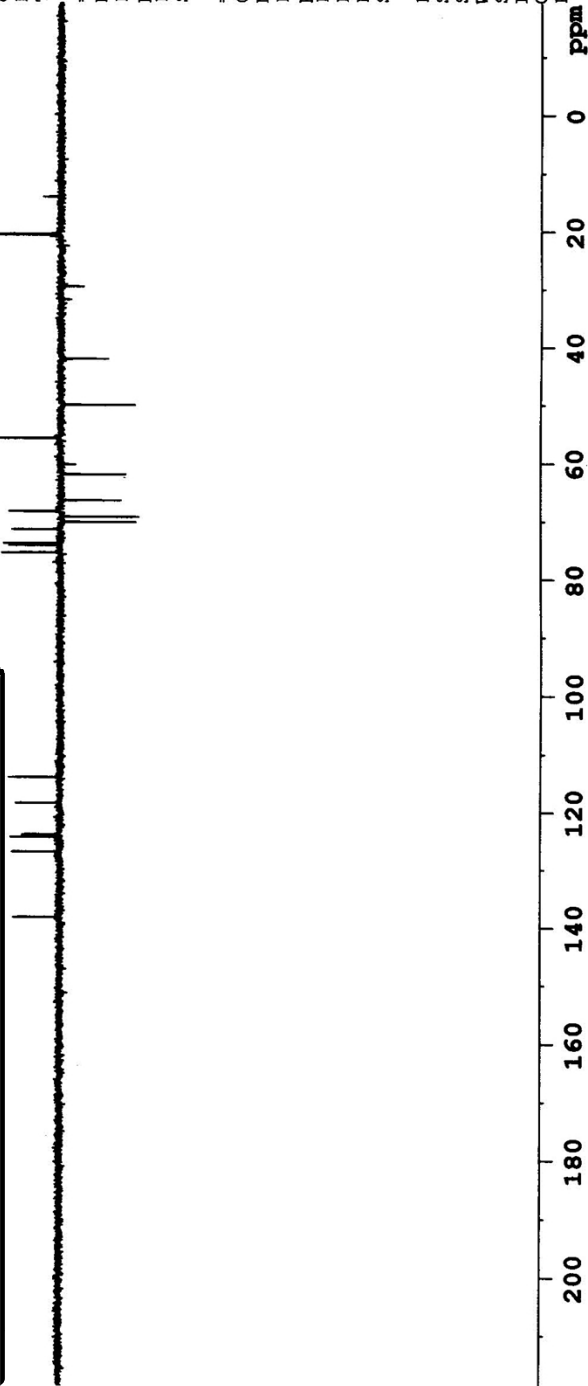
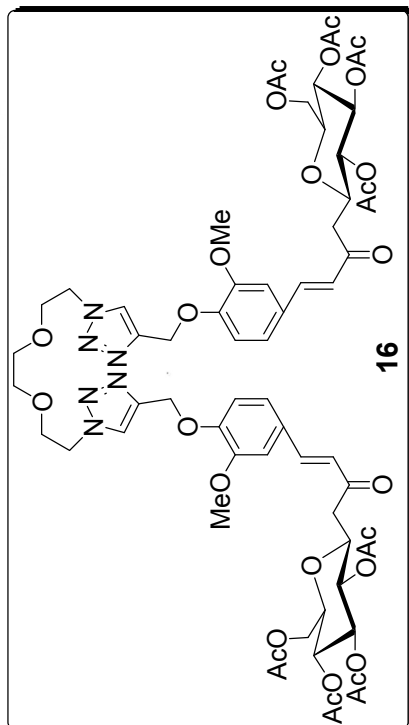
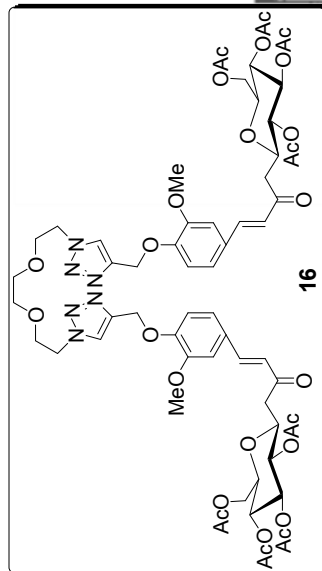


Figure 3 DEPT-135 spectrum (75 MHz, CDCl<sub>3</sub>) of compound, 16.



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PROCNO 1

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Date\_ 20120618  
Time 21.36  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG haccqf  
TD 4096  
SOLVENT CDCl3  
NS 50  
DS 4  
SWH 10416.667 Hz  
FIDRES 2.543132 Hz  
AQ 0.1966360 sec  
RG 23170.5  
DW 48.000 usec  
DE 6.00 usec  
TE 300.0 K  
CNST2 145.0000000  
CNST11 3.0000000  
d0 0.00000300 sec  
d1 1.97050405 sec  
d2 0.00344828 sec  
d3 0.00229885 sec  
d11 0.03000000 sec  
d12 0.00002000 sec  
IN0 0.00016560 sec

CHANNEL F1 13C  
NUC1 13C  
P1 9.30 usec  
P2 18.60 usec  
PL1 0.00 dB  
SFO1 75.4735142 MHz

CHANNEL F2  
CPDPRG2 wait16  
NUC2 1H  
P3 13.15 usec  
PCPD2 80.00 usec  
PL2 0.00 dB  
PL12 15.68 dB  
SFO2 300.1312753 MHz

F1 - Acquisition parameters  
ND0 2  
TD 128  
SFO1 300.1313 MHz  
FIDRES 23.588467 Hz  
SW 10.060 ppm  
F0MODE QF

F2 - Processing parameters  
SI 2048  
SF 75.4677490 MHz  
WDW QSINE  
SSB 2  
LB 0.00 Hz  
GB 0  
PC 1.40

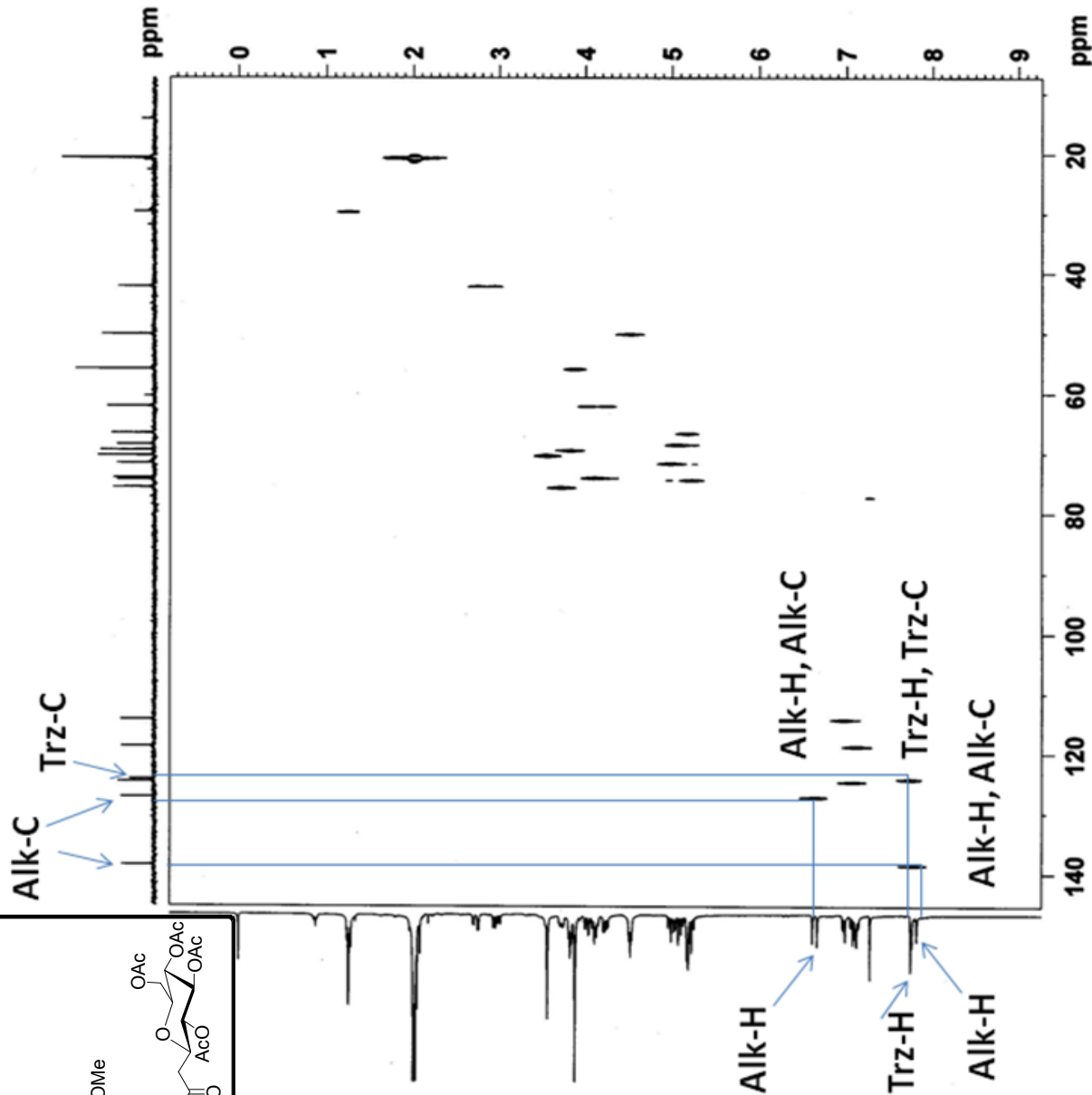


Figure 4  $^1\text{H}$ - $^{13}\text{C}$  [COSY] spectrum (300 MHz, 75 MHz,  $\text{CDCl}_3$ ) of compound, 16.

**Electrospray ionisation-MS**

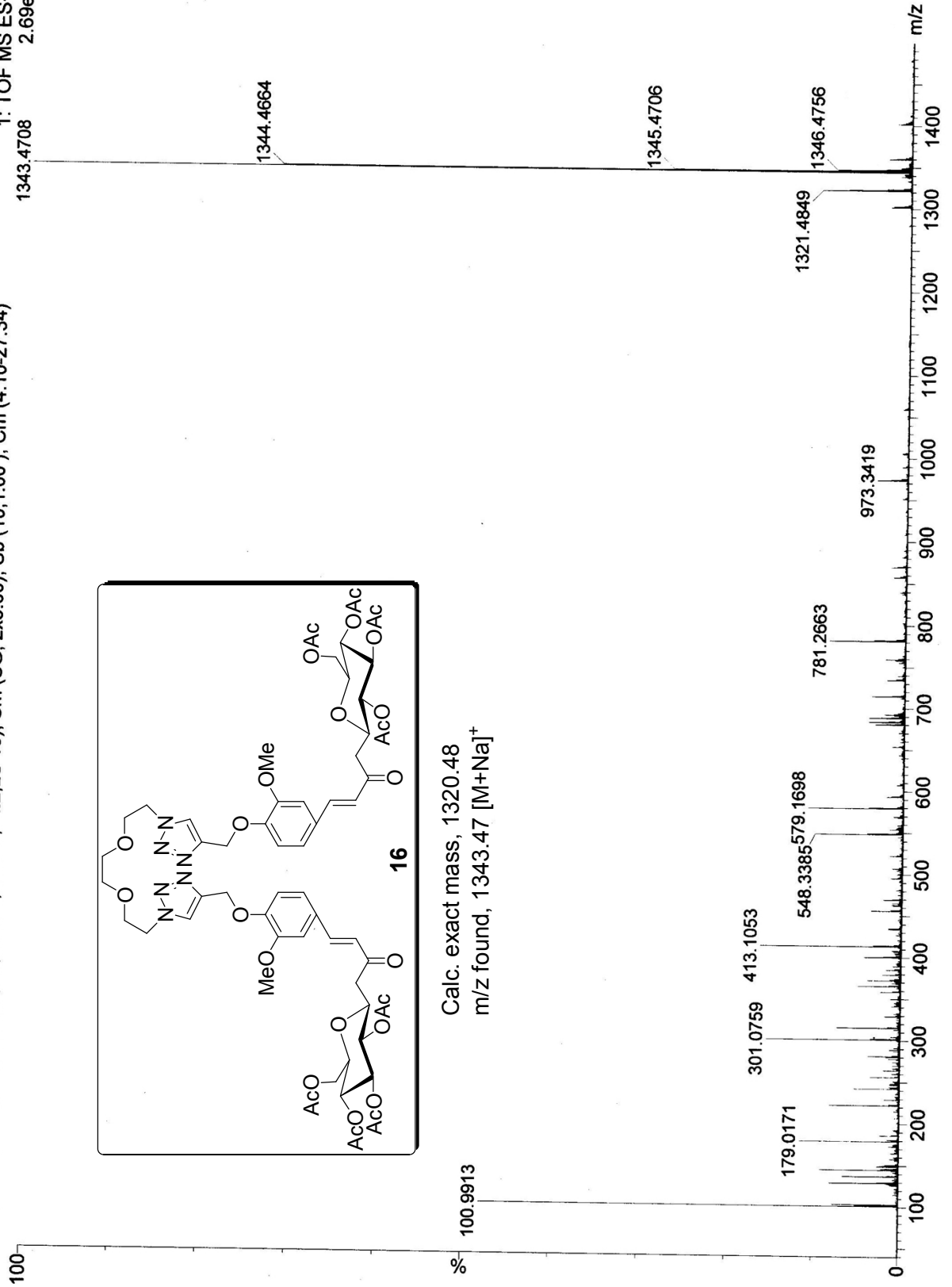
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**WATERS-Q-ToF Premier-HAB213**

15:13:1510-Sep-2013

1: TOF MS ES+

1343.4708 2.69e4



Calc. exact mass, 1320.48  
m/z found, 1343.47 [M+Na]<sup>+</sup>

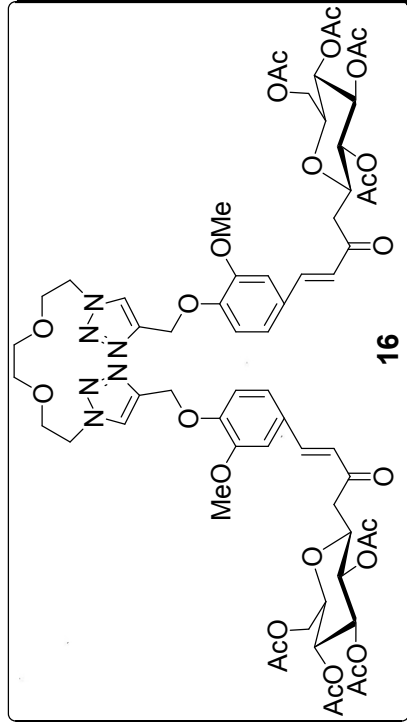


Figure 5 Mass spectrum of compound, 16.





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 INSTRUM spect  
 PROBD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 NS 19  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 322.5  
 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 300.1300059 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

7.976  
7.921  
7.580  
7.555  
7.388  
7.364  
7.359  
7.067  
7.052  
7.039  
7.027  
7.002  
6.842  
6.787  
4.798  
4.790  
4.550  
4.533  
4.516  
4.150  
4.132  
4.118  
3.726  
3.697  
3.463  
3.430  
3.398  
3.356  
3.341  
3.278  
3.248  
3.120  
3.107  
3.042  
3.018  
2.841  
2.561  
2.553  
2.545  
1.617  
1.601  
1.461  
1.435  
1.409  
1.385  
0.943  
0.918  
0.894

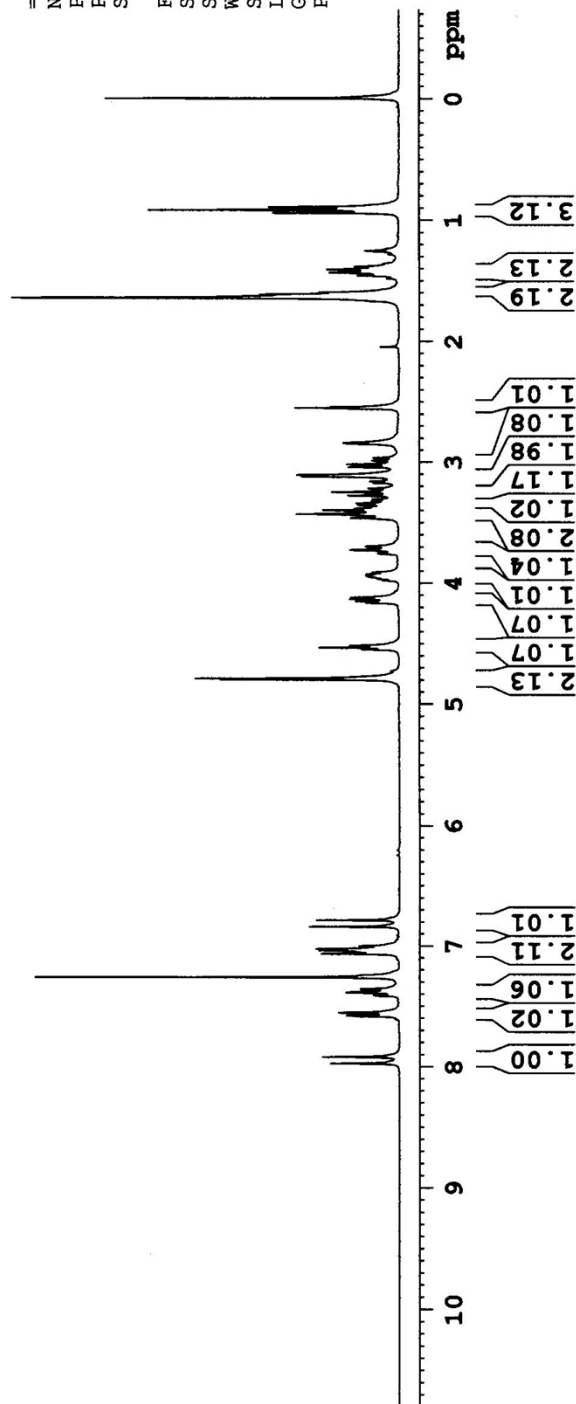
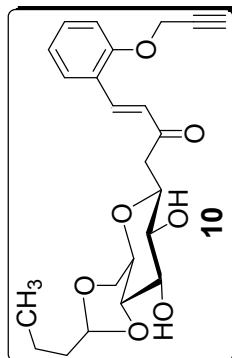


Figure 6 <sup>1</sup>H NMR spectrum (300 MHz, CDCl<sub>3</sub>) of compound, 10.



Current Data Parameters  
 NAME TMDH247-3F-2D  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120514  
 Time\_ 19.59  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1500  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 512  
 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  
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 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

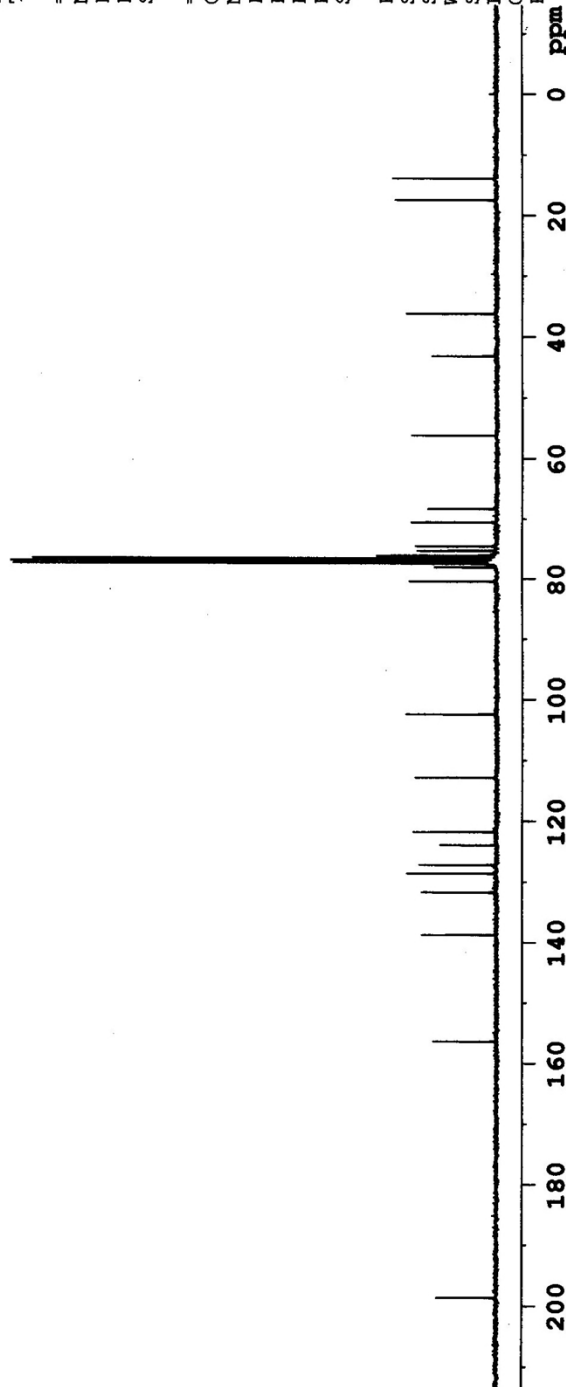
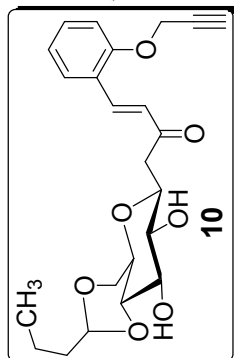
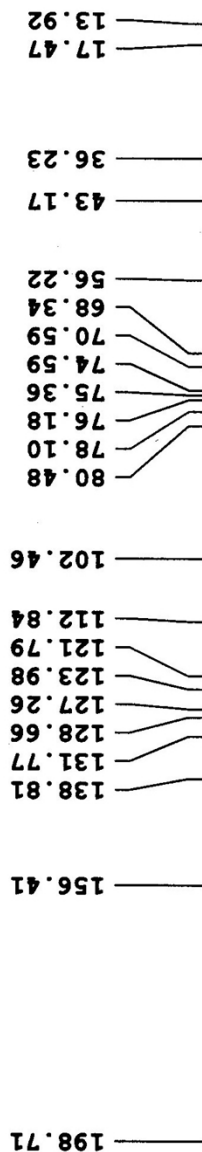


Figure 7 <sup>13</sup>C NMR spectrum (75 MHz, CDCl<sub>3</sub>) of compound, 10.



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 PROCNO 1

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 Date\_ 20120519  
 Time\_ 9.33  
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 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 45.3  
 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 300.1300228 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

7.834  
7.779  
7.759  
7.433  
7.411  
7.252  
7.228  
7.224  
6.996  
6.968  
6.904  
6.880  
6.717  
6.662  
5.139  
4.428  
4.005  
4.001  
3.979  
3.808  
3.781  
3.741  
3.725  
3.710  
3.673  
3.644  
3.616  
3.439  
3.325  
3.298  
3.267  
3.203  
3.188  
3.176  
3.149  
3.122  
3.071  
1.527  
1.514  
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1.331  
1.317  
1.292  
0.821  
0.797  
0.773

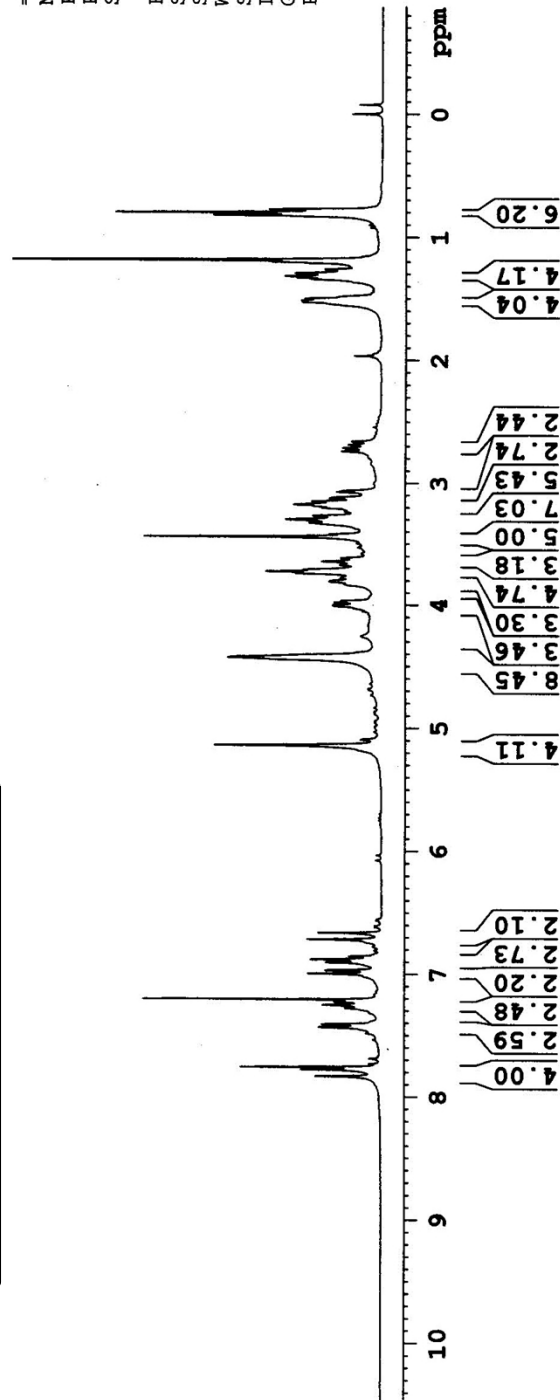
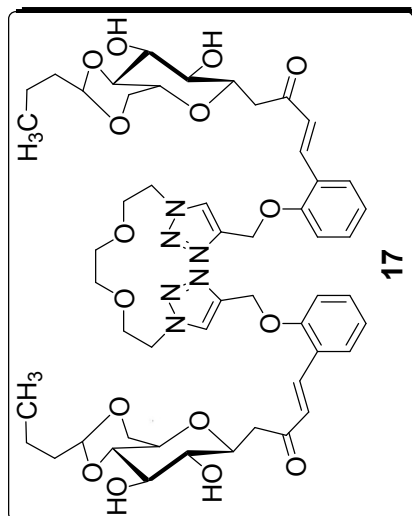


Figure 8 <sup>1</sup>H NMR spectrum (300 MHz, CDCl<sub>3</sub>) of compound, 17.



Current Data Parameters  
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 PROCNO 1

F2 - Acquisition Parameters  
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 Time\_ 9.30  
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 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 734  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 574.7  
 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  
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 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

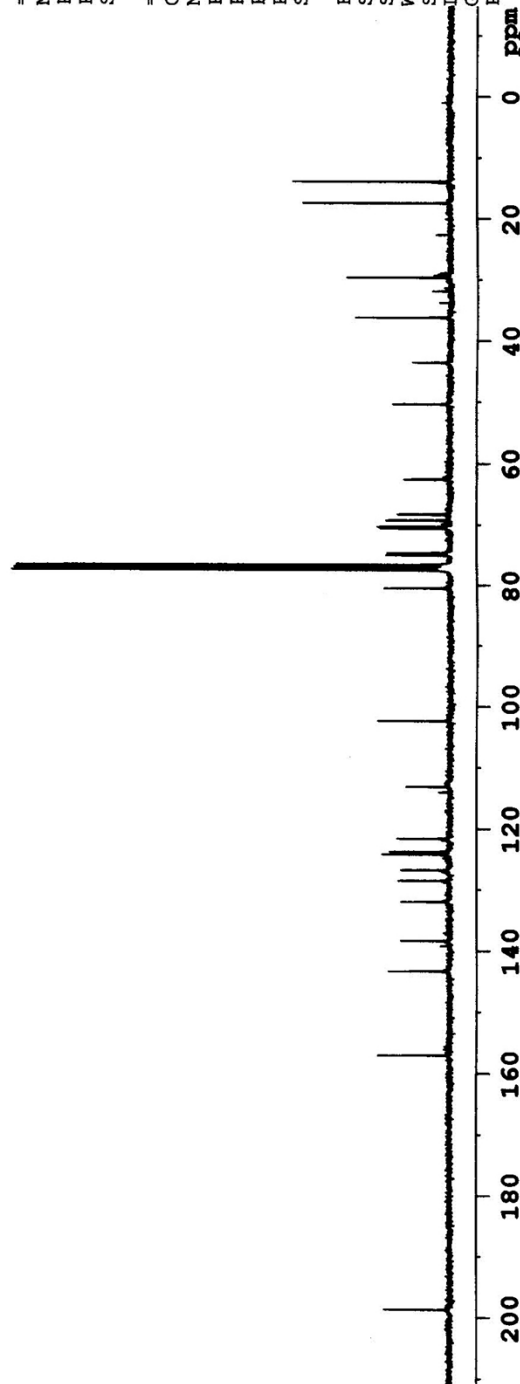
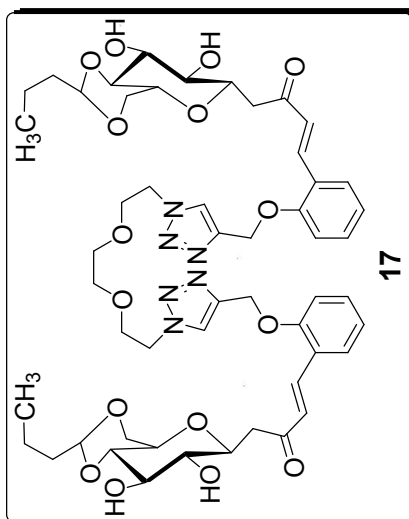
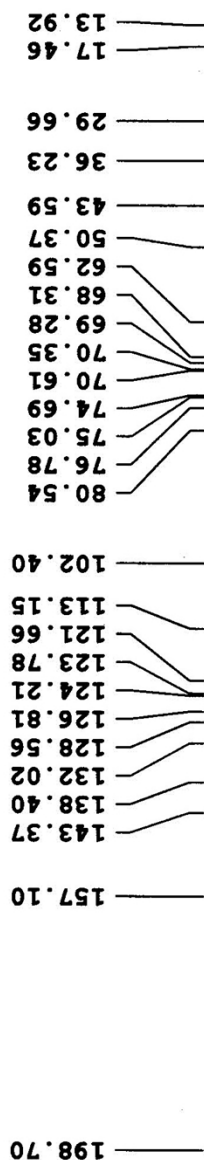
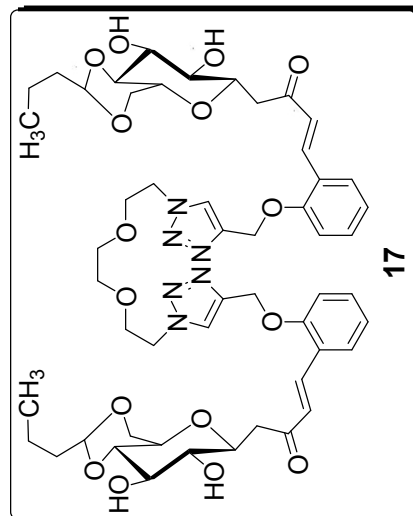


Figure 9 <sup>13</sup>C NMR spectrum (75 MHz, CDCl<sub>3</sub>) of compound, 17.



138.41  
132.05  
128.56  
126.77  
124.25  
121.66  
113.11  
102.39  
80.52  
76.78  
74.99  
74.67  
70.60  
70.34  
69.28  
68.30  
62.55  
50.37  
43.57  
36.22  
29.68  
17.48  
13.94



Current Data Parameters  
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EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120519  
Time\_ 8.08

INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG dept135  
TD 65536  
SOLVENT CDC13  
NS 215  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 16384  
DW 27.800 usec  
DE 6.00 usec  
TE 300.0 K  
CNST2 145.000000  
D1 2.0000000 sec  
d2 0.00344828 sec  
d12 0.00002000 sec  
DELTA 0.00001184 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.30 usec  
P2 18.60 usec  
PL1 0.00 dB  
SFO1 75.4752953 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
P3 13.15 usec  
P4 26.30 usec  
PCPD2 80.00 usec  
PL2 0.00 dB  
PL12 15.68 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

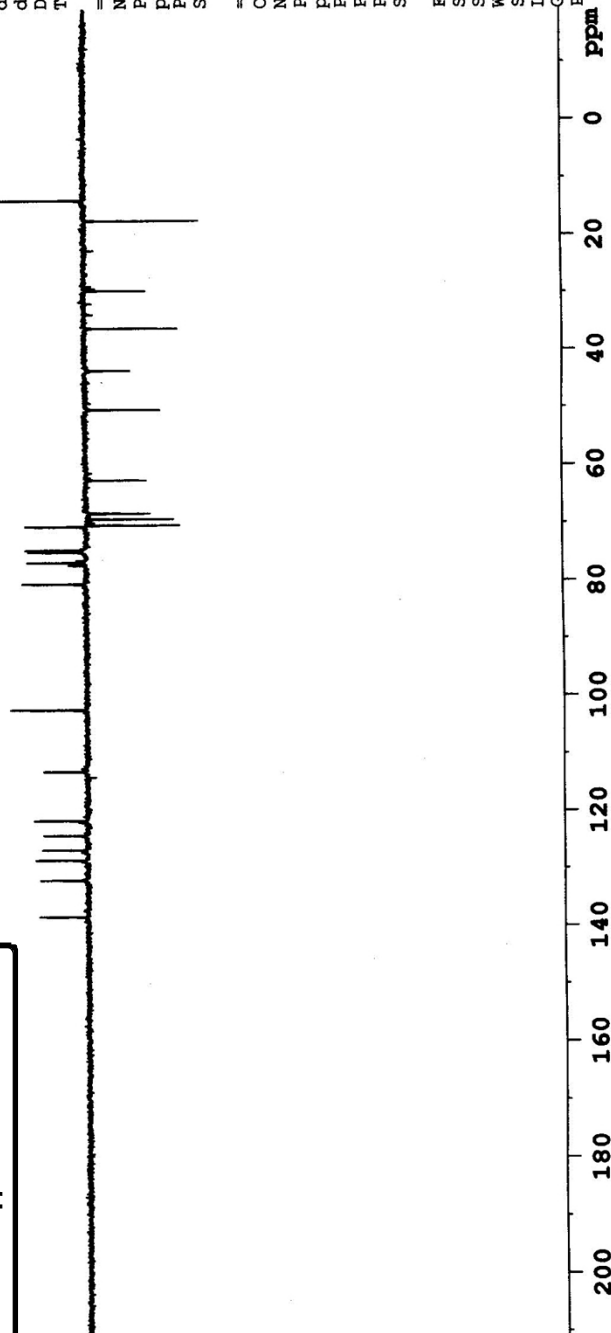
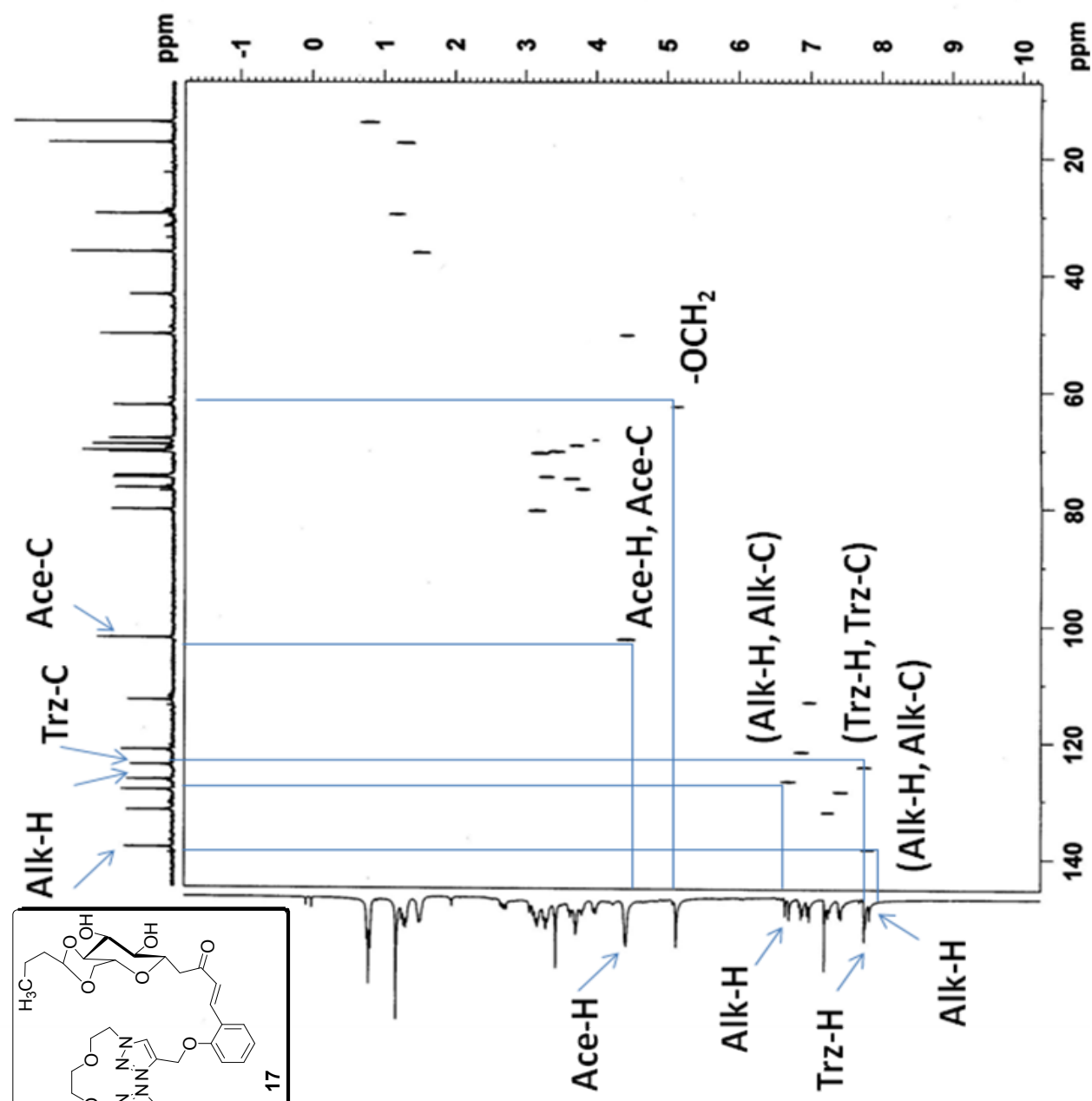
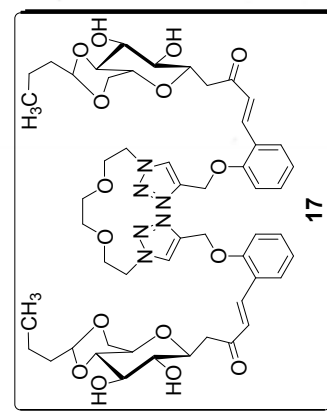


Figure 10 DEPT-135 spectrum (75 MHz, CDCl<sub>3</sub>) of compound, 17.



Current Data Parameters  
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 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120520  
 Time 0.06  
 INSTRUM spect  
 PROBRD 5 mm DUL 13C-1  
 PULPROG hmcgpg  
 TD 4096  
 SOLVENT CDCl3  
 NS 16  
 DS 4  
 SWH 10416.667 Hz  
 FIDRES 2.543132 Hz  
 AQ 0.1966580 sec  
 RG 16384  
 DW 48.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 CHST2 145.0000000  
 CHST11 3.0000000  
 d0 0.0000300 sec  
 d1 1.97050405 sec  
 d2 0.00344828 sec  
 d3 0.00229885 sec  
 d11 0.03000000 sec  
 d12 0.00002000 sec  
 d10 0.00013840 sec

CHANNEL f1  
 NUC1 13C  
 P1 9.30 usec  
 P2 18.60 usec  
 PL1 0.00 dB  
 SFO1 75.4735010 MHz

CHANNEL f2  
 CPOPRG2 waltz16  
 NUC2 1H  
 P3 13.15 usec  
 P4 80.00 usec  
 PL2 0.00 dB  
 PL12 15.68 dB  
 SFO2 300.1312951 MHz

F1 - Acquisition parameters  
 ND0 2  
 TD 128  
 SFO1 300.1313 MHz  
 FIDRES 28.224350 Hz  
 SW 12.037 ppm  
 FWHM 0.4

F2 - Processing parameters  
 SI 2048  
 SF 75.4677490 MHz  
 MDW QSIINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0  
 PC 1.40

Figure 11 <sup>1</sup>H-<sup>13</sup> [COSY] spectrum (300 MHz, 75 MHz, CDCl<sub>3</sub>) of compound, 17.

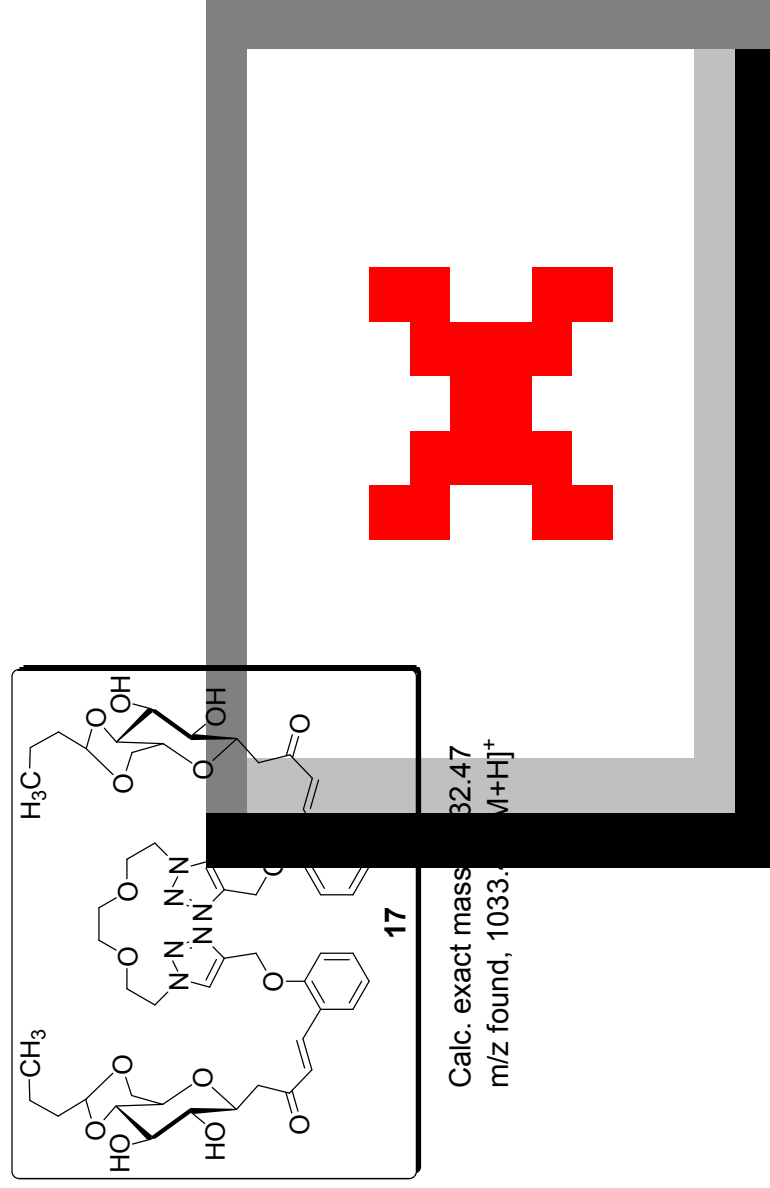


Figure 12 Mass spectrum of compound, 17.

## Computational Details:

The Cartesian co-ordinates of the optimized geometry of chemosensor, **17** is given below:

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 7.60049753 | -2.96515042 | -3.01706233 |
| C | 8.55563637 | -2.54739572 | -3.95718278 |
| C | 8.60892150 | -3.12792496 | -5.22160613 |
| C | 7.70221349 | -4.13334041 | -5.56858940 |
| C | 6.74147134 | -4.56758883 | -4.65194481 |
| C | 6.70021097 | -3.98581784 | -3.39094902 |
| H | 9.27143142 | -1.78049783 | -3.68015670 |
| H | 9.36026414 | -2.80701347 | -5.93352543 |
| H | 7.74920723 | -4.59124431 | -6.55020996 |
| H | 6.05175728 | -5.36321629 | -4.91207112 |
| O | 5.77249711 | -4.37714089 | -2.41768525 |
| C | 4.37056662 | -4.43862156 | -2.74867060 |
| H | 4.17834980 | -3.97493112 | -3.72409101 |
| H | 4.04525789 | -5.48309891 | -2.79102537 |
| C | 3.64108326 | -3.71072297 | -1.66716026 |
| C | 4.16452841 | -3.01430063 | -0.57196127 |
| N | 3.09778994 | -2.55183176 | 0.11082946  |
| H | 5.17062403 | -2.79654218 | -0.23601047 |
| N | 1.96500969 | -2.94808511 | -0.53200444 |
| N | 2.28512461 | -3.65425497 | -1.61294128 |
| C | 3.06639806 | -1.78323126 | 1.35836942  |
| H | 2.43857367 | -2.32168127 | 2.07706927  |
| H | 4.09146752 | -1.77847031 | 1.73704797  |
| C | 2.58623622 | -0.36469578 | 1.15720019  |
| H | 2.66030305 | 0.19609597  | 2.09755989  |
| H | 3.19017647 | 0.16182711  | 0.40912497  |
| O | 1.18295281 | -0.41295145 | 0.72323216  |
| C | 0.75060105 | 0.80123805  | 0.03924565  |
| H | 1.08815065 | 1.67451051  | 0.60829130  |
| H | 1.20357707 | 0.82650585  | -0.95858596 |
| C | 7.43469439 | -2.38717128 | -1.69607944 |
| C | 7.66202825 | -1.11903802 | -1.29287336 |
| C | 7.19788873 | -0.68953770 | 0.02912140  |
| O | 6.46771234 | -1.43263016 | 0.74106997  |
| H | 7.00706239 | -3.06005887 | -0.95921946 |
| H | 8.10933886 | -0.37252425 | -1.94285943 |
| C | 7.56323276 | 0.70563624  | 0.44849699  |
| H | 8.65215502 | 0.83272081  | 0.38852396  |
| H | 7.13436804 | 1.39894146  | -0.28894054 |
| C | 7.08919371 | 1.14435754  | 1.82037149  |
| C | 5.56818817 | 1.11530823  | 1.98421462  |
| H | 7.54257071 | 0.52086765  | 2.60787814  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 7.28216539  | 3.11082521  | 3.23804172  |
| C | 5.14745034  | 1.76660823  | 3.30705253  |
| H | 5.25566757  | 0.07238518  | 1.97507054  |
| C | 5.76948244  | 3.14650128  | 3.45546749  |
| H | 7.75819404  | 2.51361725  | 4.03011320  |
| H | 5.47267131  | 1.13764863  | 4.14241618  |
| H | 5.53398216  | 3.58284686  | 4.43175325  |
| O | 4.90386998  | 1.74703615  | 0.86682168  |
| O | 3.70828817  | 1.84646055  | 3.39685165  |
| O | 5.14507926  | 3.94982471  | 2.39960394  |
| H | 5.00003700  | 2.72086824  | 0.99513523  |
| H | 3.43917793  | 2.66328404  | 2.92943088  |
| C | 5.77678080  | 5.28058422  | 2.19860206  |
| H | 6.27382963  | 5.22277902  | 1.21972213  |
| C | 7.82594243  | 4.54093902  | 3.20407661  |
| H | 8.43421702  | 4.66740005  | 2.30088740  |
| H | 8.41830387  | 4.78128296  | 4.08578690  |
| O | 6.73040154  | 5.49979170  | 3.22324742  |
| C | 4.71823691  | 6.34819258  | 2.26468889  |
| H | 3.91332287  | 6.07018577  | 1.57159414  |
| H | 4.29631155  | 6.34062048  | 3.27741648  |
| C | 5.25555583  | 7.74122391  | 1.92333856  |
| H | 6.07048957  | 7.98419516  | 2.61488441  |
| H | 5.69275761  | 7.72882677  | 0.91462451  |
| C | 4.16872893  | 8.81218658  | 1.99853894  |
| H | 4.57225169  | 9.79934044  | 1.75376060  |
| H | 3.35189115  | 8.60279797  | 1.29728344  |
| H | 3.74001079  | 8.86928782  | 3.00571406  |
| C | -7.59998549 | -2.96512324 | 3.01741918  |
| C | -8.55480265 | -2.54712801 | 3.95776575  |
| C | -8.60793993 | -3.12763181 | 5.22220457  |
| C | -7.70140750 | -4.13327832 | 5.56898056  |
| C | -6.74099069 | -4.56777147 | 4.65211168  |
| C | -6.69986409 | -3.98600691 | 3.39110824  |
| H | -9.27047980 | -1.78006149 | 3.68090251  |
| H | -9.35903909 | -2.80652725 | 5.93429374  |
| H | -7.74829340 | -4.59117611 | 6.55060923  |
| H | -6.05143236 | -5.36358782 | 4.91207194  |
| O | -5.77247303 | -4.37763472 | 2.41764560  |
| C | -4.37046145 | -4.43932814 | 2.74829580  |
| H | -4.17797688 | -3.97607425 | 3.72386457  |
| H | -4.04529811 | -5.48387071 | 2.79013864  |
| C | -3.64107236 | -3.71110035 | 1.66693955  |
| C | -4.16454366 | -3.01454733 | 0.57183796  |
| N | -3.09782808 | -2.55193526 | -0.11088940 |
| H | -5.17064775 | -2.79677902 | 0.23592622  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -1.96502997 | -2.94813682 | 0.53194664  |
| N | -2.28511386 | -3.65445772 | 1.61279002  |
| C | -3.06647502 | -1.78324813 | -1.35837806 |
| H | -2.43872399 | -2.32167420 | -2.07716249 |
| H | -4.09157024 | -1.77842745 | -1.73698556 |
| C | -2.58625087 | -0.36474920 | -1.15717817 |
| H | -2.66048657 | 0.19612217  | -2.09748086 |
| H | -3.19002322 | 0.16173584  | -0.40894176 |
| O | -1.18288173 | -0.41305979 | -0.72348824 |
| C | -0.75015640 | 0.80144600  | -0.04031305 |
| H | -1.08742975 | 1.67443990  | -0.60995371 |
| H | -1.20312736 | 0.82752235  | 0.95749860  |
| C | -7.43439201 | -2.38721285 | 1.69639100  |
| C | -7.66180530 | -1.11911356 | 1.29311852  |
| C | -7.19792604 | -0.68972798 | -0.02900055 |
| O | -6.46785638 | -1.43285774 | -0.74102039 |
| H | -7.00690205 | -3.06015580 | 0.95950305  |
| H | -8.10900516 | -0.37254356 | 1.94311470  |
| C | -7.56338595 | 0.70540559  | -0.44842439 |
| H | -8.65232378 | 0.83238068  | -0.38846683 |
| H | -7.13459908 | 1.39877748  | 0.28899049  |
| C | -7.08938030 | 1.14411339  | -1.82031281 |
| C | -5.56837307 | 1.11510620  | -1.98415714 |
| H | -7.54274296 | 0.52059522  | -2.60780407 |
| C | -7.28240220 | 3.11055028  | -3.23802228 |
| C | -5.14764720 | 1.76640035  | -3.30699796 |
| H | -5.25581994 | 0.07219347  | -1.97499552 |
| C | -5.76971654 | 3.14627202  | -3.45543388 |
| H | -7.75841434 | 2.51330510  | -4.03007416 |
| H | -5.47283541 | 1.13742812  | -4.14236479 |
| H | -5.53420928 | 3.58262299  | -4.43171533 |
| O | -4.90407544 | 1.74686699  | -0.86677318 |
| O | -3.70848062 | 1.84629995  | -3.39677783 |
| O | -5.14536213 | 3.94961554  | -2.39955431 |
| H | -5.00032119 | 2.72069139  | -0.99506471 |
| H | -3.43941642 | 2.66311828  | -2.92931959 |
| C | -5.77708211 | 5.28036700  | -2.19859262 |
| H | -6.27411533 | 5.22258443  | -1.21970453 |
| C | -7.82622279 | 4.54064447  | -3.20409047 |
| H | -8.43453908 | 4.66710050  | -2.30092888 |
| H | -8.41855782 | 4.78095683  | -4.08582802 |
| O | -6.73071486 | 5.49953298  | -3.22323871 |
| C | -4.71856670 | 6.34800314  | -2.26473029 |
| H | -3.91364224 | 6.07005437  | -1.57162427 |
| H | -4.29664308 | 6.34039743  | -3.27745865 |
| C | -5.25592745 | 7.74103425  | -1.92344467 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -6.07088788 | 7.98393597  | -2.61498346 |
| H  | -5.69310327 | 7.72867764  | -0.91471889 |
| C  | -4.16914166 | 8.81203238  | -1.99873391 |
| H  | -4.57269344 | 9.79918502  | -1.75399853 |
| H  | -3.35227577 | 8.60271251  | -1.29749086 |
| H  | -3.74045545 | 8.86909298  | -3.00592495 |
| O  | 7.57056282  | 2.51263373  | 1.94816005  |
| O  | -7.57078163 | 2.51237628  | -1.94812115 |
| Hg | -0.00001723 | -2.46691922 | -0.00003599 |