Electronic Supplementary Information

(ESI)

Conformational analysis and UV/Vis spectroscopic properties of a rotaxane-based molecular machine in acetonitrile dilute solution: when simulations meet experiments.

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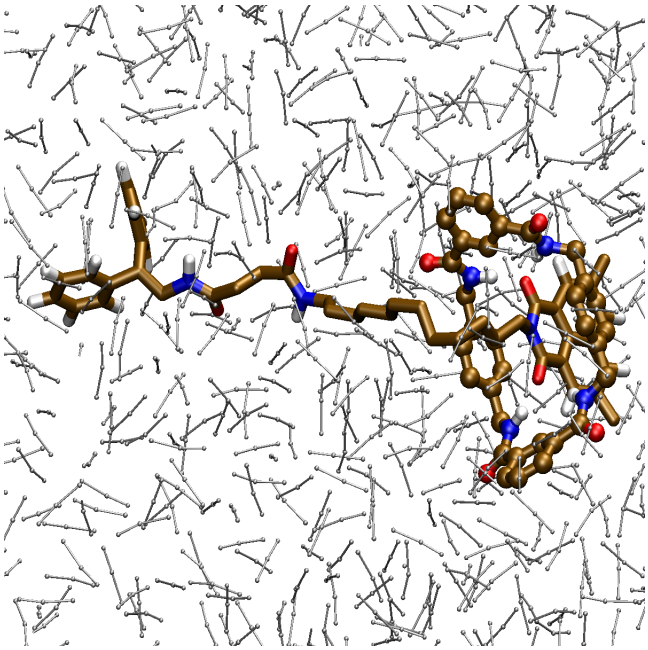
Supplementary informations:

A. Topology files applied for the MD sampling in MeCN solution



ESI-Figure 1: A pictorial view of the MD classical simulation box.

Acetonitrile force field (Gromos-stile):

```
; Name            nrexcl
CCN      3


[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB      massB
      1          N      1    CCN      N      1     -0.532    14.0067  ;
      2          C      1    CCN      C      1      0.481     12.011  ;
      3        CH3      1    CCN      C      1      0.051     15.035  ;

[ bonds ]
;  ai    aj funct    c0     c1
    1     2     2    0.1150 100000.
    2     3     2    0.1458 100000.


[ angles ]
;  ai    aj    ak funct           c0
    1     2     3     2    180.0   3000.

; Include Position restraint file
;#ifdef POSRES
;#include "posre.itp"
;#endif


#ifdef POSRES_WATER
; Position restraint for each water oxygen
[ position_restraints ]
;  i funct       fcx        fcy        fcz
   1    1       1000       1000       1000
#endif
```

Please note that this file can be also downloaded using the following URL:
http://www.caspur.it/~kosta/ROTAXANE/FORCE_FIELD_ANION/acetonitrile.itp

Benzylic Amide Macrocycle (*bam*) force field (Gromos-stile):

this file can be viewed and downloaded using the following URL:
http://www.caspur.it/~kosta/ROTAXANE/FORCE_FIELD_ANION/macrocycle.itp

Suco*-[C_{12} alkyl spacer]-*Ni force field (Gromos-stile):
this file can be viewed and downloaded using the following URL:
http://www.caspur.it/~kosta/ROTAXANE/FORCE_FIELD_ANION/shuttle-clos.itp

Finally, the **Topol.top** file collecting the singular topology files is as follows:

```
#include "ffG43a1.itp"
#include "shuttle-clos.itp"
#include "macrocycle.itp"
#include "acetonitrile.itp"

[ system ]
; Name
molecular shuttle

[ molecules ]
;Compound      #mols
KOS               1      ; synthetic thread
MAC               1      ; bam macrocycle
CCN            2468   ; CCN solvent molecules
```

Please note that this file can be also downloaded using the following URL:
http://www.caspur.it/~kosta/ROTAXANE/FORCE_FIELD_ANION/topol.top

B. Free energy minimum conformations in MeCN solution

Rotaxane, Elongated basin (see Figure 5 into the manuscript):

```
CRYST1   52.404   52.034   77.518  90.00  90.00  90.00 P 1         1
ATOM      1  C   KOS X   1      30.130  30.900  45.310  1.00  0.00
ATOM      2  N   KOS X   1      30.400  32.170  46.120  1.00  0.00
ATOM      3  C   KOS X   1      30.030  32.230  47.460  1.00  0.00
ATOM      4  O   KOS X   1      29.560  31.380  47.960  1.00  0.00
ATOM      5  C   KOS X   1      30.990  33.270  45.520  1.00  0.00
ATOM      6  O   KOS X   1      31.200  33.310  44.450  1.00  0.00
ATOM      7  C   KOS X   1      30.310  33.360  48.220  1.00  0.00
ATOM      8  C   KOS X   1      29.760  33.460  49.490  1.00  0.00
ATOM      9  C   KOS X   1      31.270  34.380  46.300  1.00  0.00
ATOM     10  C   KOS X   1      31.800  35.560  45.780  1.00  0.00
ATOM     11  C   KOS X   1      30.970  34.450  47.660  1.00  0.00
ATOM     12  C   KOS X   1      31.190  35.570  48.450  1.00  0.00
ATOM     13  C   KOS X   1      29.980  34.580  50.280  1.00  0.00
ATOM     14  C   KOS X   1      30.710  35.640  49.750  1.00  0.00
ATOM     15  H   KOS X   1      29.080  32.680  49.830  1.00  0.00
ATOM     16  C   KOS X   1      29.460  34.720  51.560  1.00  0.00
ATOM     17  H   KOS X   1      30.890  36.530  50.350  1.00  0.00
ATOM     18  C   KOS X   1      32.080  36.690  46.530  1.00  0.00
ATOM     19  C   KOS X   1      31.760  36.710  47.890  1.00  0.00
ATOM     20  H   KOS X   1      32.000  35.570  44.710  1.00  0.00
ATOM     21  C   KOS X   1      32.690  37.810  45.980  1.00  0.00
ATOM     22  H   KOS X   1      31.720  37.660  48.420  1.00  0.00
ATOM     23  C   KOS X   1      30.040  31.250  43.820  1.00  0.00
ATOM     24  C   KOS X   1      29.650  29.950  43.120  1.00  0.00
ATOM     25  C   KOS X   1      29.380  30.300  41.660  1.00  0.00
ATOM     26  C   KOS X   1      29.110  29.050  40.830  1.00  0.00
ATOM     27  C   KOS X   1      28.740  29.440  39.390  1.00  0.00
ATOM     28  C   KOS X   1      28.190  28.190  38.710  1.00  0.00
ATOM     29  C   KOS X   1      27.490  28.380  37.370  1.00  0.00
ATOM     30  C   KOS X   1      27.020  27.040  36.790  1.00  0.00
ATOM     31  C   KOS X   1      26.060  27.120  35.610  1.00  0.00
ATOM     32  C   KOS X   1      25.600  25.750  35.120  1.00  0.00
ATOM     33  C   KOS X   1      24.820  25.870  33.810  1.00  0.00
ATOM     34  N   KOS X   1      24.580  24.600  33.090  1.00  0.00
```

```
ATOM     35  H   KOS X   1      25.410  24.050  32.960  1.00  0.00
ATOM     36  C   KOS X   1      23.440  24.190  32.560  1.00  0.00
ATOM     37  O   KOS X   1      22.390  24.820  32.640  1.00  0.00
ATOM     38  C   KOS X   1      23.440  22.810  31.900  1.00  0.00
ATOM     39  C   KOS X   1      23.190  21.730  32.950  1.00  0.00
ATOM     40  C   KOS X   1      23.180  20.380  32.230  1.00  0.00
ATOM     41  O   KOS X   1      24.170  19.950  31.630  1.00  0.00
ATOM     42  N   KOS X   1      21.950  19.900  32.110  1.00  0.00
ATOM     43  H   KOS X   1      21.230  20.450  32.530  1.00  0.00
ATOM     44  C   KOS X   1      21.560  18.670  31.290  1.00  0.00
ATOM     45  C   KOS X   1      21.770  18.870  29.790  1.00  0.00
ATOM     46  C   KOS X   1      20.970  20.060  29.270  1.00  0.00
ATOM     47  C   KOS X   1      21.590  21.260  28.940  1.00  0.00
ATOM     48  C   KOS X   1      20.880  22.450  28.870  1.00  0.00
ATOM     49  C   KOS X   1      19.510  22.440  29.110  1.00  0.00
ATOM     50  C   KOS X   1      18.860  21.250  29.410  1.00  0.00
ATOM     51  C   KOS X   1      19.590  20.060  29.440  1.00  0.00
ATOM     52  H   KOS X   1      22.650  21.250  28.680  1.00  0.00
ATOM     53  H   KOS X   1      21.400  23.390  28.690  1.00  0.00
ATOM     54  H   KOS X   1      18.940  23.370  29.050  1.00  0.00
ATOM     55  H   KOS X   1      17.810  21.250  29.680  1.00  0.00
ATOM     56  H   KOS X   1      19.070  19.120  29.630  1.00  0.00
ATOM     57  C   KOS X   1      21.480  17.620  28.940  1.00  0.00
ATOM     58  C   KOS X   1      20.980  17.760  27.650  1.00  0.00
ATOM     59  C   KOS X   1      20.520  16.640  26.970  1.00  0.00
ATOM     60  C   KOS X   1      20.600  15.380  27.550  1.00  0.00
ATOM     61  C   KOS X   1      21.200  15.230  28.800  1.00  0.00
ATOM     62  C   KOS X   1      21.660  16.350  29.480  1.00  0.00
ATOM     63  H   KOS X   1      20.990  18.720  27.150  1.00  0.00
ATOM     64  H   KOS X   1      20.130  16.750  25.950  1.00  0.00
ATOM     65  H   KOS X   1      20.220  14.510  27.030  1.00  0.00
ATOM     66  H   KOS X   1      21.360  14.230  29.210  1.00  0.00
ATOM     67  H   KOS X   1      22.330  16.220  30.330  1.00  0.00
ATOM     68  C1  MAC X   2      28.520  35.600  44.000  1.00  0.00
ATOM     69  N1  MAC X   2      29.370  34.910  43.030  1.00  0.00
ATOM     70  H1  MAC X   2      30.140  34.400  43.430  1.00  0.00
ATOM     71  C2  MAC X   2      29.200  34.880  41.710  1.00  0.00
ATOM     72  O1  MAC X   2      28.230  35.410  41.170  1.00  0.00
ATOM     73  C3  MAC X   2      30.300  34.130  40.940  1.00  0.00
ATOM     74  C4  MAC X   2      31.370  33.620  41.660  1.00  0.00
ATOM     75  C5  MAC X   2      30.160  33.690  39.630  1.00  0.00
```

```
ATOM     76  C6  MAC X   2      31.130  32.930  38.990  1.00  0.00
ATOM     77  C7  MAC X   2      32.190  32.450  39.760  1.00  0.00
ATOM     78  C8  MAC X   2      32.380  32.860  41.080  1.00  0.00
ATOM     79  C9  MAC X   2      33.500  32.270  41.940  1.00  0.00
ATOM     80  O2  MAC X   2      34.360  31.570  41.420  1.00  0.00
ATOM     81  N2  MAC X   2      33.520  32.540  43.240  1.00  0.00
ATOM     82  H2  MAC X   2      32.770  33.060  43.660  1.00  0.00
ATOM     83  C10 MAC X   2      34.590  32.100  44.150  1.00  0.00
ATOM     84  C11 MAC X   2      34.160  31.400  45.440  1.00  0.00
ATOM     85  C12 MAC X   2      34.060  32.170  46.590  1.00  0.00
ATOM     86  C13 MAC X   2      33.710  31.560  47.790  1.00  0.00
ATOM     87  C14 MAC X   2      33.740  30.080  45.430  1.00  0.00
ATOM     88  C15 MAC X   2      33.390  29.460  46.620  1.00  0.00
ATOM     89  C16 MAC X   2      33.290  30.230  47.780  1.00  0.00
ATOM     90  C17 MAC X   2      32.880  29.600  49.110  1.00  0.00
ATOM     91  N3  MAC X   2      31.460  29.230  49.090  1.00  0.00
ATOM     92  H3  MAC X   2      30.830  29.920  48.730  1.00  0.00
ATOM     93  C18 MAC X   2      31.000  28.060  49.520  1.00  0.00
ATOM     94  O3  MAC X   2      31.750  27.190  49.970  1.00  0.00
ATOM     95  C19 MAC X   2      29.490  27.840  49.380  1.00  0.00
ATOM     96  C20 MAC X   2      28.640  28.930  49.330  1.00  0.00
ATOM     97  C21 MAC X   2      28.930  26.570  49.490  1.00  0.00
ATOM     98  C22 MAC X   2      27.560  26.370  49.340  1.00  0.00
ATOM     99  C23 MAC X   2      26.740  27.490  49.260  1.00  0.00
ATOM    100  C24 MAC X   2      27.270  28.770  49.150  1.00  0.00
ATOM    101  C25 MAC X   2      26.340  29.970  48.970  1.00  0.00
ATOM    102  O4  MAC X   2      25.150  29.900  49.280  1.00  0.00
ATOM    103  N4  MAC X   2      26.870  31.060  48.430  1.00  0.00
ATOM    104  H4  MAC X   2      27.860  31.150  48.280  1.00  0.00
ATOM    105  C26 MAC X   2      26.060  32.220  48.050  1.00  0.00
ATOM    106  C27 MAC X   2      26.730  33.090  46.980  1.00  0.00
ATOM    107  C28 MAC X   2      26.740  32.660  45.660  1.00  0.00
ATOM    108  C29 MAC X   2      27.390  33.420  44.700  1.00  0.00
ATOM    109  C30 MAC X   2      27.840  34.700  45.030  1.00  0.00
ATOM    110  C31 MAC X   2      27.830  35.130  46.350  1.00  0.00
ATOM    111  C32 MAC X   2      27.180  34.370  47.310  1.00  0.00
END
```

Please note that this file can be also downloaded using the following URL:
http://www.caspur.it/~kosta/ROTAXANE/PDBS/elongated_basin.pdb

Rotaxane, Folded basin (see Figure 5 into the manuscript):

```
CRYST1   52.404   52.034   77.518  90.00  90.00  90.00 P 1           1
ATOM      1  C   KOS X   1      24.750  24.960  36.310  1.00  0.00
ATOM      2  N   KOS X   1      25.840  24.100  35.680  1.00  0.00
ATOM      3  C   KOS X   1      25.790  23.800  34.320  1.00  0.00
ATOM      4  O   KOS X   1      24.890  23.870  33.710  1.00  0.00
ATOM      5  C   KOS X   1      27.010  23.930  36.410  1.00  0.00
ATOM      6  O   KOS X   1      27.170  24.310  37.420  1.00  0.00
ATOM      7  C   KOS X   1      26.940  23.370  33.670  1.00  0.00
ATOM      8  C   KOS X   1      26.900  23.340  32.280  1.00  0.00
ATOM      9  C   KOS X   1      28.110  23.410  35.740  1.00  0.00
ATOM     10  C   KOS X   1      29.250  22.950  36.400  1.00  0.00
ATOM     11  C   KOS X   1      28.110  23.150  34.380  1.00  0.00
ATOM     12  C   KOS X   1      29.200  22.640  33.690  1.00  0.00
ATOM     13  C   KOS X   1      28.030  22.900  31.590  1.00  0.00
ATOM     14  C   KOS X   1      29.150  22.500  32.310  1.00  0.00
ATOM     15  H   KOS X   1      26.040  23.720  31.730  1.00  0.00
ATOM     16  C   KOS X   1      28.170  23.170  30.230  1.00  0.00
ATOM     17  H   KOS X   1      29.960  21.980  31.790  1.00  0.00
ATOM     18  C   KOS X   1      30.350  22.380  35.770  1.00  0.00
ATOM     19  C   KOS X   1      30.340  22.240  34.390  1.00  0.00
ATOM     20  H   KOS X   1      29.290  23.110  37.480  1.00  0.00
ATOM     21  C   KOS X   1      31.530  22.120  36.460  1.00  0.00
ATOM     22  H   KOS X   1      31.230  21.930  33.850  1.00  0.00
ATOM     23  C   KOS X   1      23.470  24.160  36.580  1.00  0.00
ATOM     24  C   KOS X   1      22.350  25.060  37.100  1.00  0.00
ATOM     25  C   KOS X   1      22.610  25.570  38.510  1.00  0.00
ATOM     26  C   KOS X   1      21.500  26.480  39.030  1.00  0.00
ATOM     27  C   KOS X   1      21.340  27.810  38.290  1.00  0.00
ATOM     28  C   KOS X   1      22.490  28.790  38.540  1.00  0.00
ATOM     29  C   KOS X   1      22.240  30.090  37.770  1.00  0.00
ATOM     30  C   KOS X   1      23.080  31.290  38.190  1.00  0.00
ATOM     31  C   KOS X   1      24.580  31.090  37.940  1.00  0.00
ATOM     32  C   KOS X   1      25.390  32.340  38.300  1.00  0.00
ATOM     33  C   KOS X   1      26.890  32.060  38.190  1.00  0.00
ATOM     34  N   KOS X   1      27.430  31.130  39.190  1.00  0.00
ATOM     35  H   KOS X   1      26.840  30.350  39.410  1.00  0.00
ATOM     36  C   KOS X   1      28.700  31.090  39.570  1.00  0.00
ATOM     37  O   KOS X   1      29.590  31.600  38.890  1.00  0.00
ATOM     38  C   KOS X   1      29.100  30.310  40.830  1.00  0.00
ATOM     39  C   KOS X   1      29.230  28.800  40.650  1.00  0.00
ATOM     40  C   KOS X   1      29.070  27.990  41.940  1.00  0.00
```

```
ATOM     41  O   KOS X   1      28.870  28.540  43.030  1.00  0.00
ATOM     42  N   KOS X   1      28.950  26.670  41.830  1.00  0.00
ATOM     43  H   KOS X   1      29.260  26.270  40.970  1.00  0.00
ATOM     44  C   KOS X   1      28.670  25.770  43.040  1.00  0.00
ATOM     45  C   KOS X   1      28.520  24.290  42.690  1.00  0.00
ATOM     46  C   KOS X   1      28.110  23.480  43.920  1.00  0.00
ATOM     47  C   KOS X   1      27.150  22.510  43.720  1.00  0.00
ATOM     48  C   KOS X   1      26.600  21.790  44.780  1.00  0.00
ATOM     49  C   KOS X   1      27.080  22.010  46.070  1.00  0.00
ATOM     50  C   KOS X   1      28.100  22.930  46.270  1.00  0.00
ATOM     51  C   KOS X   1      28.610  23.670  45.210  1.00  0.00
ATOM     52  H   KOS X   1      26.890  22.240  42.700  1.00  0.00
ATOM     53  H   KOS X   1      25.850  21.020  44.590  1.00  0.00
ATOM     54  H   KOS X   1      26.620  21.490  46.910  1.00  0.00
ATOM     55  H   KOS X   1      28.480  23.070  47.280  1.00  0.00
ATOM     56  H   KOS X   1      29.400  24.400  45.400  1.00  0.00
ATOM     57  C   KOS X   1      29.780  23.660  42.100  1.00  0.00
ATOM     58  C   KOS X   1      29.750  23.010  40.870  1.00  0.00
ATOM     59  C   KOS X   1      30.730  22.070  40.560  1.00  0.00
ATOM     60  C   KOS X   1      31.780  21.860  41.450  1.00  0.00
ATOM     61  C   KOS X   1      31.880  22.590  42.630  1.00  0.00
ATOM     62  C   KOS X   1      30.880  23.500  42.940  1.00  0.00
ATOM     63  H   KOS X   1      28.990  23.290  40.150  1.00  0.00
ATOM     64  H   KOS X   1      30.670  21.500  39.640  1.00  0.00
ATOM     65  H   KOS X   1      32.510  21.070  41.240  1.00  0.00
ATOM     66  H   KOS X   1      32.670  22.370  43.340  1.00  0.00
ATOM     67  H   KOS X   1      30.970  24.120  43.830  1.00  0.00
ATOM     68  C1  MAC X   2      26.860  21.020  38.880  1.00  0.00
ATOM     69  N1  MAC X   2      26.510  22.390  39.280  1.00  0.00
ATOM     70  H1  MAC X   2      26.900  23.120  38.730  1.00  0.00
ATOM     71  C2  MAC X   2      25.700  22.640  40.310  1.00  0.00
ATOM     72  O1  MAC X   2      25.160  21.750  40.960  1.00  0.00
ATOM     73  C3  MAC X   2      25.460  24.120  40.640  1.00  0.00
ATOM     74  C4  MAC X   2      25.960  25.160  39.880  1.00  0.00
ATOM     75  C5  MAC X   2      24.630  24.420  41.720  1.00  0.00
ATOM     76  C6  MAC X   2      24.360  25.730  42.080  1.00  0.00
ATOM     77  C7  MAC X   2      24.880  26.750  41.290  1.00  0.00
ATOM     78  C8  MAC X   2      25.710  26.490  40.210  1.00  0.00
ATOM     79  C9  MAC X   2      26.220  27.650  39.340  1.00  0.00
ATOM     80  O2  MAC X   2      26.180  28.810  39.740  1.00  0.00
ATOM     81  N2  MAC X   2      26.740  27.320  38.170  1.00  0.00
```

```
ATOM     82  H2  MAC X   2      26.910  26.360  37.950  1.00  0.00
ATOM     83  C10 MAC X   2      27.140  28.260  37.110  1.00  0.00
ATOM     84  C11 MAC X   2      26.480  27.950  35.760  1.00  0.00
ATOM     85  C12 MAC X   2      27.140  27.220  34.790  1.00  0.00
ATOM     86  C13 MAC X   2      26.510  26.970  33.570  1.00  0.00
ATOM     87  C14 MAC X   2      25.160  28.350  35.580  1.00  0.00
ATOM     88  C15 MAC X   2      24.530  28.110  34.360  1.00  0.00
ATOM     89  C16 MAC X   2      25.200  27.370  33.390  1.00  0.00
ATOM     90  C17 MAC X   2      24.480  27.050  32.080  1.00  0.00
ATOM     91  N3  MAC X   2      23.640  25.870  32.310  1.00  0.00
ATOM     92  H3  MAC X   2      24.080  25.120  32.810  1.00  0.00
ATOM     93  C18 MAC X   2      22.390  25.760  31.880  1.00  0.00
ATOM     94  O3  MAC X   2      21.790  26.680  31.320  1.00  0.00
ATOM     95  C19 MAC X   2      21.710  24.410  32.140  1.00  0.00
ATOM     96  C20 MAC X   2      22.490  23.260  32.230  1.00  0.00
ATOM     97  C21 MAC X   2      20.340  24.300  32.280  1.00  0.00
ATOM     98  C22 MAC X   2      19.740  23.080  32.600  1.00  0.00
ATOM     99  C23 MAC X   2      20.540  21.950  32.690  1.00  0.00
ATOM    100  C24 MAC X   2      21.920  22.030  32.540  1.00  0.00
ATOM    101  C25 MAC X   2      22.820  20.790  32.630  1.00  0.00
ATOM    102  O4  MAC X   2      22.410  19.690  32.270  1.00  0.00
ATOM    103  N4  MAC X   2      24.050  20.960  33.090  1.00  0.00
ATOM    104  H4  MAC X   2      24.450  21.880  33.170  1.00  0.00
ATOM    105  C26 MAC X   2      24.920  19.850  33.520  1.00  0.00
ATOM    106  C27 MAC X   2      25.430  20.110  34.940  1.00  0.00
ATOM    107  C28 MAC X   2      24.600  20.760  35.840  1.00  0.00
ATOM    108  C29 MAC X   2      25.080  21.070  37.110  1.00  0.00
ATOM    109  C30 MAC X   2      26.360  20.680  37.480  1.00  0.00
ATOM    110  C31 MAC X   2      27.180  20.020  36.580  1.00  0.00
ATOM    111  C32 MAC X   2      26.710  19.710  35.310  1.00  0.00
END
```

Please note that this file can be also downloaded using the following URL:
http://www.caspur.it/~kosta/ROTAXANE/PDBS/folded_basin.pdb

C. Optimized geometries of the *ni¯/bam* complex at DFT/CPCM level

Molecular geometry of the *ni-/bam* supramolecular complex at CPCM/UPBE0 level of theory:

```
  1        6              -0.682423    1.354551    3.491855
  2        6              -1.390614    0.155813    3.590114
  3        6              -0.678945   -1.048975    3.673145
  4        6               0.710879   -1.047169    3.699348
  5        6               1.422385    0.157918    3.629329
```

6	6	0.716218	1.356609	3.517096
7	6	2.939238	0.131466	3.663569
8	7	3.469318	-0.549985	2.498115
9	6	4.237210	-1.651609	2.582934
10	8	4.576828	-2.174298	3.669778
11	6	-2.907508	0.130452	3.564918
12	7	-3.386657	-0.643389	2.435530
13	6	-4.290401	-1.631976	2.556772
14	8	-4.783661	-1.997934	3.648384
15	6	-4.660221	-2.311087	1.270201
16	6	-5.272127	-3.565217	1.320900
17	6	-5.575792	-4.239809	0.138365
18	6	-5.254392	-3.673272	-1.095147
19	6	-4.642943	-2.418909	-1.147902
20	6	-4.391607	-1.729043	0.034942
21	6	-4.254756	-1.856015	-2.484683
22	7	-3.351026	-0.861816	-2.439501
23	6	-2.865968	-0.175986	-3.621673
24	6	-1.351111	-0.108431	-3.615829
25	6	-0.596122	-1.284179	-3.727384
26	6	0.793216	-1.231139	-3.728662
27	6	1.458614	-0.002278	-3.619172
28	6	0.707725	1.166921	-3.493819
29	6	-0.689716	1.113871	-3.489519
30	6	2.975810	0.030538	-3.622983
31	7	3.505567	-0.607727	-2.433425
32	6	4.291617	-1.699115	-2.477139
33	6	4.716287	-2.262466	-1.148690
34	6	5.580516	-3.359634	-1.128881
35	6	5.998709	-3.893973	0.090511
36	6	5.560041	-3.336532	1.291788
37	6	4.690199	-2.242002	1.277114
38	6	4.271881	-1.725632	0.054534
39	8	-4.733978	-2.316051	-3.546406
40	8	4.650752	-2.247426	-3.544848
41	8	-2.079537	0.138275	-0.028768
42	6	-1.101196	0.936641	-0.038798
43	7	0.183224	0.425689	-0.011621
44	6	1.331002	1.199829	-0.010229
45	6	1.177669	2.623962	-0.041031
46	6	-0.120133	3.186973	-0.078312
47	6	-1.265216	2.357965	-0.078301
48	6	-0.277036	4.606217	-0.116509
49	6	-1.590947	5.134492	-0.155640
50	6	-2.719960	4.310476	-0.157289
51	6	-2.553854	2.924671	-0.116450
52	6	0.888854	5.410757	-0.112288
53	6	2.169807	4.852830	-0.073213
54	6	2.310151	3.463592	-0.038762
55	8	2.466120	0.641896	0.014709
56	6	0.302894	-1.026384	0.006076
57	1	-3.411643	2.257630	-0.116110
58	1	3.292736	3.001502	-0.009463
59	6	-4.102045	4.905184	-0.200625
60	6	3.389651	5.735354	-0.070783
61	1	-1.716185	6.215938	-0.186049
62	1	0.775194	6.493478	-0.141039
63	1	-1.109405	-2.238960	-3.817873
64	1	1.377542	-2.144193	-3.816633
65	1	-5.464926	-4.183412	-2.028992
66	1	-6.053553	-5.213174	0.178385
67	1	3.371146	-0.510215	-4.490832
68	1	-3.229048	-0.722481	-4.500990
69	1	-5.496360	-3.990078	2.293414
70	1	3.322446	1.073138	-3.675335
71	1	-2.900320	-0.594432	-1.563763

72	1	3.244460	-0.160406	-1.555371
73	1	1.259827	-1.983157	3.773449
74	1	5.908113	-3.772593	-2.076671
75	1	-1.227714	-1.986705	3.726947
76	1	-3.989748	-0.726493	-0.006009
77	1	-3.272988	0.846310	-3.660345
78	1	3.578322	-0.899037	0.041862
79	1	-1.267055	2.029380	-3.380802
80	1	-2.917967	-0.460364	1.546805
81	1	6.671250	-4.745209	0.104880
82	1	1.213709	2.124199	-3.389961
83	1	-3.302699	-0.335932	4.475992
84	1	3.220138	-0.124281	1.606836
85	1	3.294816	-0.407860	4.549351
86	1	5.871016	-3.731120	2.253149
87	1	-3.288878	1.161323	3.513585
88	1	3.325220	1.160924	3.706236
89	1	1.258526	2.296484	3.441032
90	1	-1.224089	2.292364	3.390280
91	1	1.360505	-1.275495	0.043592
92	1	-0.208131	-1.425671	0.883003
93	1	-0.148886	-1.443449	-0.895559
94	1	3.116306	6.794196	-0.100168
95	1	3.998339	5.570783	0.825840
96	1	4.030794	5.530224	-0.935865
97	1	-4.065787	5.998153	-0.228276
98	1	-4.653908	4.565134	-1.084561
99	1	-4.689527	4.610952	0.676789

Molecular geometry of the *ni-/bam* supramolecular complex at CPCM/UPW91 level of theory:

1	6	-0.692684	1.342721	3.559561
2	6	-1.404355	0.132103	3.620430
3	6	-0.686701	-1.081696	3.677179
4	6	0.711889	-1.078870	3.705252
5	6	1.426672	0.136674	3.666665
6	6	0.714188	1.345395	3.587319
7	6	2.951497	0.111224	3.696382
8	7	3.482624	-0.568908	2.517114
9	6	4.245739	-1.690277	2.594379
10	8	4.579323	-2.231001	3.688334
11	6	-2.928651	0.106428	3.589532
12	7	-3.407565	-0.663636	2.444139
13	6	-4.311594	-1.670789	2.557661
14	8	-4.802076	-2.055748	3.657934
15	6	-4.676175	-2.340947	1.256101
16	6	-5.280803	-3.609930	1.294110
17	6	-5.580917	-4.278727	0.097241
18	6	-5.264116	-3.694252	-1.138832
19	6	-4.659350	-2.425508	-1.180106
20	6	-4.411711	-1.739957	0.017495
21	6	-4.277247	-1.846738	-2.520142
22	7	-3.370489	-0.837898	-2.463317
23	6	-2.880016	-0.135843	-3.646880
24	6	-1.357353	-0.070158	-3.641183
25	6	-0.600809	-1.258022	-3.731451
26	6	0.797420	-1.209494	-3.734874
27	6	1.471365	0.027265	-3.649083
28	6	0.718851	1.209653	-3.547264
29	6	-0.686906	1.161041	-3.540501
30	6	2.996645	0.054313	-3.652929
31	7	3.529231	-0.594436	-2.457005
32	6	4.311638	-1.704182	-2.505253
33	6	4.730216	-2.274352	-1.169495
34	6	5.591918	-3.385972	-1.153367
35	6	6.001646	-3.936140	0.071723

36	6	5.560565	-3.380688	1.283031
37	6	4.695095	-2.272562	1.274978
38	6	4.282889	-1.736901	0.044500
39	8	-4.757286	-2.302611	-3.597625
40	8	4.672128	-2.253948	-3.586014
41	8	-2.095483	0.139873	-0.028446
42	6	-1.108137	0.947169	-0.030497
43	7	0.188339	0.429550	-0.008277
44	6	1.347897	1.211977	-0.002686
45	6	1.190082	2.645466	-0.025410
46	6	-0.116414	3.212901	-0.055752
47	6	-1.269035	2.378505	-0.058047
48	6	-0.273874	4.641431	-0.085170
49	6	-1.595119	5.173878	-0.116728
50	6	-2.730768	4.345134	-0.119748
51	6	-2.563502	2.950102	-0.088944
52	6	0.898785	5.450427	-0.081614
53	6	2.187073	4.888446	-0.050779
54	6	2.327410	3.490007	-0.022716
55	8	2.494922	0.649519	0.019633
56	6	0.308477	-1.032995	0.000150
57	1	-3.426573	2.279003	-0.090917
58	1	3.315994	3.024774	0.000620
59	6	-4.120039	4.942866	-0.154421
60	6	3.414238	5.773825	-0.050729
61	1	-1.721056	6.262094	-0.139981
62	1	0.784900	6.539910	-0.104627
63	1	-1.120567	-2.218707	-3.802766
64	1	1.382271	-2.131730	-3.806260
65	1	-5.471573	-4.198318	-2.084704
66	1	-6.053202	-5.262624	0.128105
67	1	3.396626	-0.493904	-4.523922
68	1	-3.250318	-0.683295	-4.532492
69	1	-5.502134	-4.047209	2.269597
70	1	3.349504	1.103027	-3.700023
71	1	-2.916484	-0.576604	-1.576019
72	1	3.269479	-0.149481	-1.565820
73	1	1.265383	-2.021622	3.756240
74	1	5.921456	-3.795482	-2.109997
75	1	-1.237992	-2.026892	3.707848
76	1	-4.019506	-0.725053	-0.014640
77	1	-3.289056	0.894075	-3.676340
78	1	3.589055	-0.899875	0.034405
79	1	-1.265188	2.086082	-3.450651
80	1	-2.935428	-0.470549	1.549102
81	1	6.670494	-4.798938	0.082587
82	1	1.231890	2.173037	-3.465136
83	1	-3.334326	-0.375583	4.497529
84	1	3.238811	-0.134955	1.618387
85	1	3.316013	-0.442667	4.579481
86	1	5.864197	-3.786392	2.249968
87	1	-3.312411	1.144640	3.543954
88	1	3.340202	1.147276	3.743350
89	1	1.259419	2.293376	3.540154
90	1	-1.239304	2.288172	3.485957
91	1	1.374019	-1.279659	0.029728
92	1	-0.200964	-1.439326	0.883381
93	1	-0.151950	-1.446359	-0.906963
94	1	3.140902	6.839692	-0.074304
95	1	4.032511	5.603913	0.846829
96	1	4.056096	5.570744	-0.924518
97	1	-4.084179	6.042674	-0.174845
98	1	-4.679979	4.606844	-1.043437
99	1	-4.709772	4.640812	0.727513