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Supporting Information

Synthesis, antibacterial and antioxidant properties of novel ethylenoindolophanes - A new class of cyclophanes

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EXPERIMENTAL

Materials method

All the reagents and solvents employed were of the best grade available and were used without further purification. The melting points were determined using a Toshniwal melting point apparatus by open capillary tube method and were uncorrected. 1H NMR and 13C NMR spectra were recorded on BRUKER 300 MHz instruments. Tetramethylsilane (TMS) was used as the internal standard. MS: EI-MS spectra on Jeol DX-303 mass spectrometer. The elemental analyses for the compounds were carried out using the Perkin-Elmer 240B elemental analyzer. Column chromatography was performed on silica gel (ACME, 100–200 mesh). Routine monitoring of the reaction was made using thin layer chromatography developed on glass plates coated with silica gel-G (ACME) of 25 mm thickness and visualized with iodine.

General procedure for synthesis of precyclophane by *N*-arylation of indole

To a mixture of CuI (1.26 mmol), K_3PO_4 (6.00 mmol), trans-1,2-diaminocyclohexane (0.12 mmol) and indole (1.26 mmol) in toluene (150 mL) were added aryl dibromide (0.6 mmol) under nitrogen atmosphere. The reaction mixture was refluxed at 110 °C for 24 h. After the reaction was completed, the solvent was removed under reduced pressure and the residue was extracted with $CHCl_3$ (3 x 100 mL), washed with water (2 x 100 mL), brine (150 mL) and dried over anhydrous Na_2SO_4. The solvent was removed and crude product was purified by column chromatography on silica gel using $CHCl_3$/Hexane (1:4, v/v) as eluent.

General procedure for synthesis of dialdehyde

To a stirred solution of dimethylformamide (19.9 mmol) at 0 °C, added phosphorous oxycholoride (5.0 mmol) drop wise under nitrogen atmosphere. Bis-indole (2.3 mmol) in dimethylformamide (5.9 mmol) was then added to the reaction at 0 °C to 10 °C. After the completion of addition, the reaction mixture was allow to attain room temperature and then stirred for additional one hour at 35 °C. The reaction was then quenched by adding crushed ice (100 g) and further water (100 ml). Then the reaction mixture was then treated thrice with NaOH solution (1 M). The reaction mixture was heated after adding one portion of NaOH solution and the rest of the two portions were added later with stirring. The reaction mixture was then kept in refrigerator overnight. The precipitate obtained was collected by filtration and then dissolved in chloroform (2 x 100 mL). The organic layer was then dried over (Na_2SO_4), filtered and solvent was evaporated under reduced pressure to give the residue which was then chromatographed over SiO_2 using chloroform: methanol (99:1) as eluting solvent to give the corresponding dialdehyde.

General procedure for McMurray coupling (synthesis of ethylenophanes [**1 – 4**])

A solution of low valent titanium prepared form $TiCl_4$ (20 equiv.) with zinc (40 equiv.) and two drops of pyridine in dry THF (200 mL) under nitrogen atmosphere at 0 ^oC and was allowed to attain room temperature after 0.5 h and then refluxed for 1 h. Dialdehyde (1 equiv.) was added in one batch to the freshly prepared low valent titanium. After the addition was over the reaction mixture was refluxed overnight. The reaction mixture was then cooled and quenched with saturated K_2CO_3 solution. The precipitated inorganic material was removed by filtration. The precipitate was thoroughly washed with THF for several times and the combined THF extract on evaporation under reduced pressure gave the residue, which was extracted with $CHCl_3$ (100 mL), washed with water (2 x 100 mL) brine (100 mL) and dried over anhydrous Na_2SO_4. Crude product obtained after evaporation of $CHCl_3$, was purified by column chromatography using $CHCl_3$/Hexane (1:4, v/v) as eluent.

Precyclophane 9: Yield 82%; mp 109-111 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 2.52 (s, 3H); 6.70 (d, 2H, *J* = 3.3 Hz); 7.16-7.27 (m, 4H); 7.32 (s, 2H); 7.36 (d, 2H, *J* = 3.3 Hz,) 7.47 (s, 1H); 7.63 (d, 2H, *J* = 8.1 Hz); 7.69 (d, 2H, *J* = 7.5 Hz). ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 21.6, 104.1, 110.5, 117.1, 120.6, 121.3, 122.6, 122.7, 127.8, 129.5, 135.7, 140.9, 141.2. EI-MS (*m/z)*: 322 (M^+). Elemental Anal. Calcd for $C_{23}H_{18}N_2$: C, 85.68; H, 5.63; N, 8.69. Found: C, 85.76; H, 5.50 N, 8.74.

Precyclophane 9a: Yield 85%; mp 95-97 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 2.43 (s, 3H); 2.92 (s, 3H); 6.70 (d, 2H, *J* = 3.3 Hz); 7.15-7.26 (m, 4H); 7.31 (s, 2H); 7.36 (d, 2H, *J* = 3.3 Hz); 7.41 (d, 2H, *J* = 8.1 Hz); 7.68 (d, 2H, *J* = 7.8 Hz). ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 20.8, 60.6, 103.5, 110.7, 120.4, 120.9, 122.3, 127.3, 128.8, 129.0, 133.2, 134.2, 136.6, 148.3. EI-MS (*m/z)*: 352 (M^+). Elemental Anal. Calcd for $C_{24}H_{20}N_2O$: C, 81.79; H, 5.72; N, 7.95. Found: C, 81.94; H, 5.80; N, 7.76.

Precyclophane 10: Yield 73%; mp 167-169 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 6.75 (d, 2H, *J* = 3.3 Hz); 7.20-7.29 (m, 4H); 7.31 (s, 1H); 7.34 (s, 1H); 7.68 (d, 2H, *J* = 8.1 Hz); 7.81 (d, 2H, *J* = 3.6 Hz); 7.91 (t, 1H, *J* = 8.1 Hz); 8.31(d, 2H, *J* = 8.1 Hz). ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 106.0, 109.6, 113.6, 121.2, 121.6, 123.4, 125.9, 130.6, 135.1, 140.6, 151.6. EI-MS (*m/z)*: 309 (M^+). Elemental Anal. Calcd for $C_{21}H_{15}N_3$: C, 81.53; H, 4.89; N, 13.58. Found: C, 81.45; H, 4.81; N, 13.74.

Precyclophane 11: Yield 80%; mp 103-105 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 6.68 (d, 2H, *J* = 3.3 Hz); 7.00 (s, 2H); 7.22 (d, 2H, *J* = 8.7 Hz); 7.27 (d, 2H, *J* = 8.4 Hz); 7.31 (d, 2H, *J* = 3.3 Hz); 7.66 (t, 4H, *J* = 7.5 Hz). ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 104.7, 110.6, 119.4, 121.2, 121.3, 123.1, 129.1, 129.2, 137.2, 137.4. EI-MS (*m/z)*: 314 (M^+). Elemental Anal. Calcd for $C_{20}H_{14}N_2S$: C, 76.40; H, 4.49; N, 8.91. Found: C, 76.28; H, 4.58; N, 8.76.

Precyclophane **12**: Yield 64%; mp 211-213 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 1.53 (t, 3H, *J* = 7.2 Hz); 4.46 (q, 2H, *J* = 7.2 Hz); 6.69 (d, 2H, *J* = 2.4 Hz); 7.14-7.23 (m, 4H); 7.40 (d, 2H, *J* = 3.0 Hz); 7.52-7.56 (m, 4H); 7.63 (d, 2H, *J* = 8.7 Hz); 7.71 (d, 2H, *J* = 7.2 Hz); 8.16 (s, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 13.9, 38.1, 102.9, 109.5, 110.4, 117.2, 120.1, 121.1, 122.2, 123.2, 123.8, 128.9, 129.0, 131.9, 136.8, 139.2. EI-MS (*m/z)*: 425 (M^+). Elemental Anal. Calcd for $C_{30}H_{23}N_3$: C, 84.68; H, 5.45; N, 9.87. Found: C, 84.84; H, 5.38; N, 9.78.

Dialdehyde **13**: Yield 78%; 198-200 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 2.61 (s, 3H); 7.36-7.40 (m, 4H); 7.49 (s, 2H); 7.55-7.58 (m, 3H); 7.97 (s, 2H); 8.37-8.40 (m, 2H); 10.10 (s, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 21.6, 110.8, 118.1, 120.2, 122.5, 123.8, 124.9, 125.0, 125.7, 137.2, 137.7, 139.6, 142.5, 184.9. EI-MS (*m/z)*: 378 (M^+). Elemental Anal. Calcd for $C_{25}H_{18}N_2O_2$: C, 79.35; H, 4.79; N, 7.40. Found: C, 79.28; H, 4.84; N, 7.54.

Dialdehyde 13a: Yield 72%; mp 108-110 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 2.52 (s, 3H); 2.98 (s, 3H); 7.39 (d, 6H, *J* = 3.0 Hz); 7.46 (s, 2H); 7.98 (s, 2H); 8.39 (d, 2H, *J* = 3.6 Hz); 10.14 (s, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 20.8, 61.4, 110.9, 120.1, 122.3, 123.6, 124.8,

125.1, 128.6, 132.0, 135.4, 137.9, 139.1, 148.3, 184.9. EI-MS (*m/z)*: 408 (M^+). Elemental Anal. Calcd for $C_{26}H_{20}N_2O_3$: C, 76.45; H, 4.94; N, 6.86. Found: C, 76.59; H, 4.88; N, 6.74.

Dialdehyde 14: Yield 56%; mp 286-288 ^oC; ^1H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.42-7.45 (m, 5H); 7.65 (d, 2H, *J* = 7.8 Hz); 8.11- 8.14 (m, 2H); 8.19 (d, 2H, *J* = 8.1 Hz); 8.43 (d, 1H, *J* = 3.3 Hz); 8.45 (s, 2H); 10.21 (s, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C 110.8, 111.8, 116.8, 120.6, 122.3, 123.0, 124.0, 127.3, 130.4, 142.1, 158.2, 191.5. EI-MS (*m/z)*: 365 (M^+). Elemental Anal. Calcd for $C_{23}H_{15}N_3O_2$: C, 75.60; H, 4.14; N, 11.50. Found: C, 75.68; H, 4.25; N, 11.36.

Dialdehyde 15: Yield 80%; mp 231-233 ^oC; ^1H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.16 (s, 2H); 7.34-7.37 (m, 4H); 7.55-7.58 (m, 2H); 7.88 (s, 2H); 8.30-8.33 (m, 2H); 10.07 (s, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 110.8, 121.7, 122.5, 124.2, 125.3, 125.4, 136.7, 138.3, 138.5, 147.8, 184.8. EI-MS (*m/z)*: 370 (M^+). Elemental Anal. Calcd for $C_{22}H_{14}N_2O_2S$: C, 71.33; H, 3.81; N, 7.56. Found: C, 71.50; H, 3.74; N, 7.49.

Dialdehyde 16: Yield 56%; mp 221-223 ^oC; ^1H NMR (300 MHz, $CDCl_3$): δ (ppm) 1.59 (t, 3H; *J* = 7.2 Hz); 4.55 (q, 2H, *J* = 7.2 Hz); 7.30-7.39 (m, 4H); 7.47 (d, 2H, *J* = 7.5 Hz); 7.67 (s, 4H); 7.99 (s, 2H); 8.22 (s, 2H); 8.40 (d, 2H, *J* = 7.2 Hz); 10.13 (s, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 13.9, 38.3, 110.1, 111.0, 117.7, 119.5, 122.2, 123.1, 123.4, 124.0, 124.5, 125.5, 130.4, 138.4, 138.8, 140.1, 184.9. EI-MS (*m/z)*: 481 (M^+). Elemental Anal. Calcd for $C_{32}H_{23}N_3O_2$: C, 79.81; H, 4.81; N, 8.73. Found: C, 79.71; H, 4.90; N, 8.67.

Ethylenophane 1: Yield 17%; mp 238-240 ^oC; ^1H NMR (300 MHz, $CDCl_3$): δ (ppm) 2.41 (s, 6H); 6.53 (s, 2H); 6.84 (s, 4H); 7.13-7.17 (m, 12H); 7.26 (s, 4H); 7.40 (d, 4H, *J* = 7.8 Hz); 7.65 (d, 4H, *J* = 7.8 Hz). ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 21.58, 110.60, 115.5, 119.9, 120.4, 120.6, 121.8, 123.0, 126.2, 128.2, 135.2, 135.4, 140.5, 141.1; FAB-MS (*m/z)*: 692 (M^+). Elemental Anal. Calcd for $C_{50}H_{36}N_4$: C, 86.68; H, 5.24; N, 8.09. Found: C, 86.82; H, 5.12; N, 8.20.

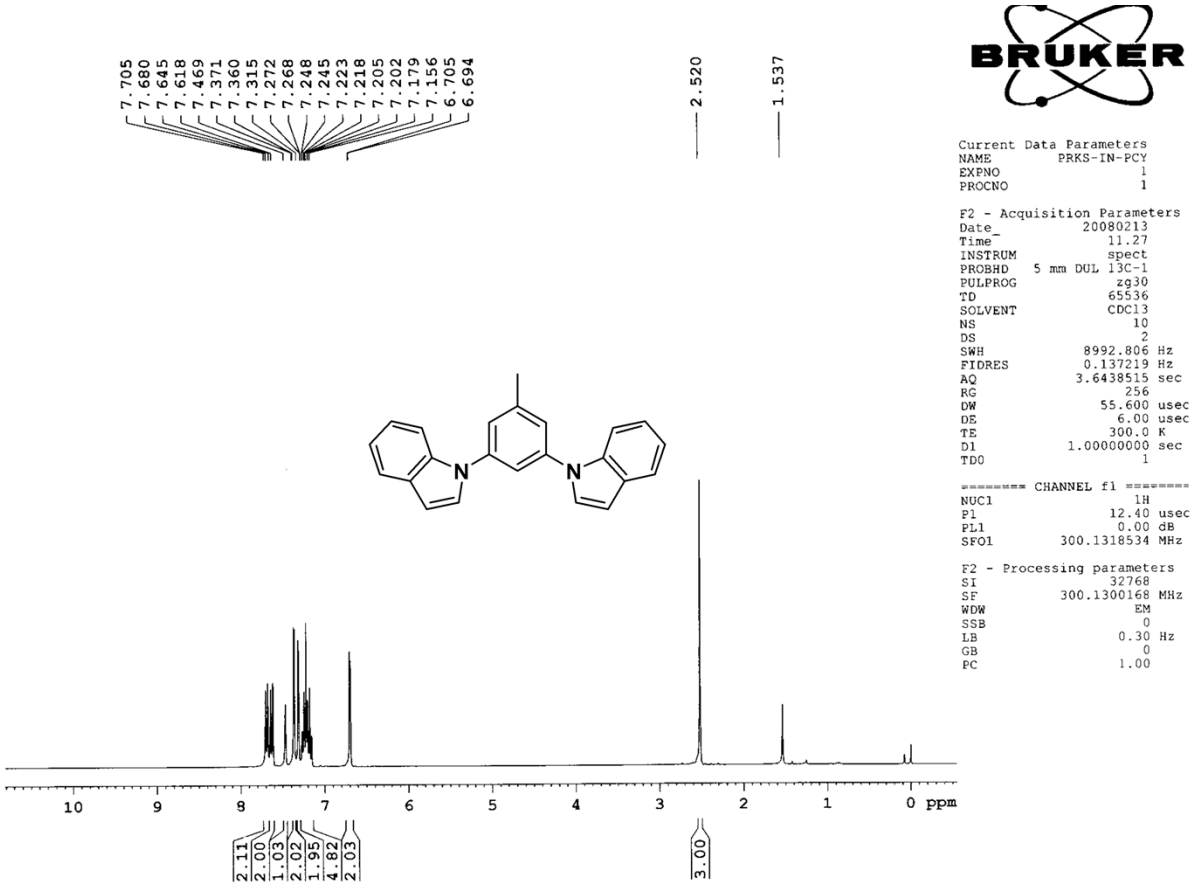
Ethylenophane 1a: Yield 18%; mp 184-186 ^oC; ^1H NMR (300 MHz, $CDCl_3$): δ (ppm) 2.23 (s, 6H); 2.79 (s, 6H); 6.77 (s, 4H); 7.04 (s, 4H); 7. 10 (d, 2H, *J* = 3.0 Hz); 7.11 (s, 3H); 7.13 (d, 4H J = 3.6 Hz); 7.20-7.26 (m, 5H); 7.48 (s, 4H). ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 20.59, 60.77, 110.46, 114.83, 119.20, 119.50, 120.44, 122.71, 127.16, 128.16, 128.39,132.79, 134.00, 136.79, 148.96. FAB-MS (*m/z*): 752 (M^+). Elemental Anal. Calcd for $C_{52}H_{40}N_4O_2$: C, 82.95; H, 5.35; N, 7.44. Found: C, 82.82; H, 5.21; N, 7.30.

Ethylenophane 2: Yield 15%; mp 172-174 ^oC; ^1H NMR (300 MHz, $CDCl_3$): δ (ppm) 6.77 (s, 4H); 7.01-7.11 (m, 12H); 7.28-7.35 (m, 6H); 7.58 (d, 4H, *J* = 7.2 Hz); 8.08 (s, 4H). ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 110.58, 113.62, 119.23, 119.28, 121.55, 123.47, 126.32, 129.49, 130.57, 135.31, 139.63, 151.2: FAB-MS (*m/z*): 666 (M^+). Elemental Anal. Calcd for $C_{46}H_{30}N_6$: C, 82.86; H, 4.54; N, 12.60. Found: C, 82.97; H, 4.42; N, 12.46.

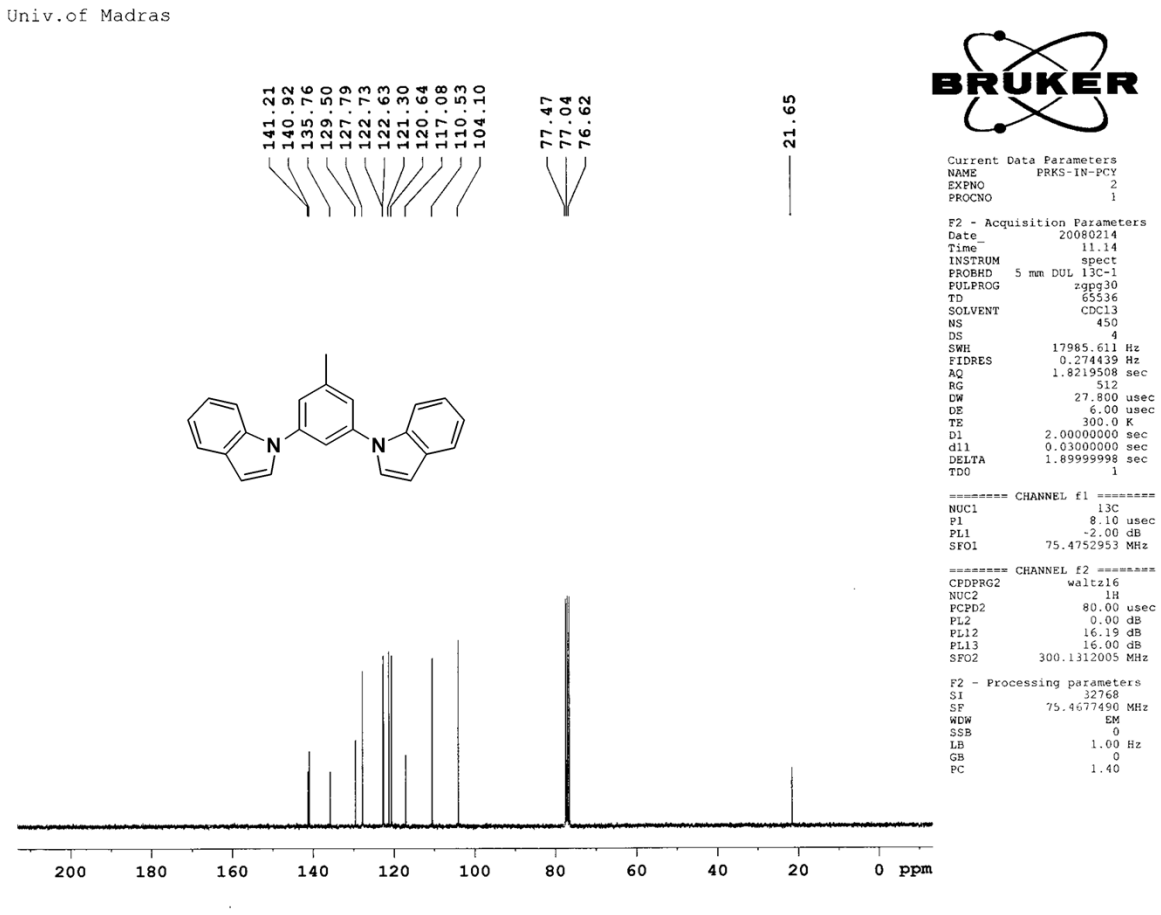
Ethylenophane 3: Yield 20%; mp 252-254 ^oC; ^1H NMR (300 MHz, $CDCl_3$): δ (ppm) 6.75 (s, 4H); 7.08 (s, 4H); 7.27-7.36 (m, 8H); 7.62 (d, 4H, *J* = 7.5 Hz); 7.78 (d, 4H, *J* = 7.8 Hz); 7.88 (s,

4H). ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 110.66, 115.93, 118.49, 118.92, 119.30, 121.50, 123.78, 126.32, 129.09, 136.31, 136.36; FAB-MS (*m/z*): 676 (M^+). Elemental Anal. Calcd for $C_{44}H_{28}N_4S_2$: C, 78.08; H, 4.17; N, 8.28. Found: C, 77.95; H, 4.29; N, 8.40.

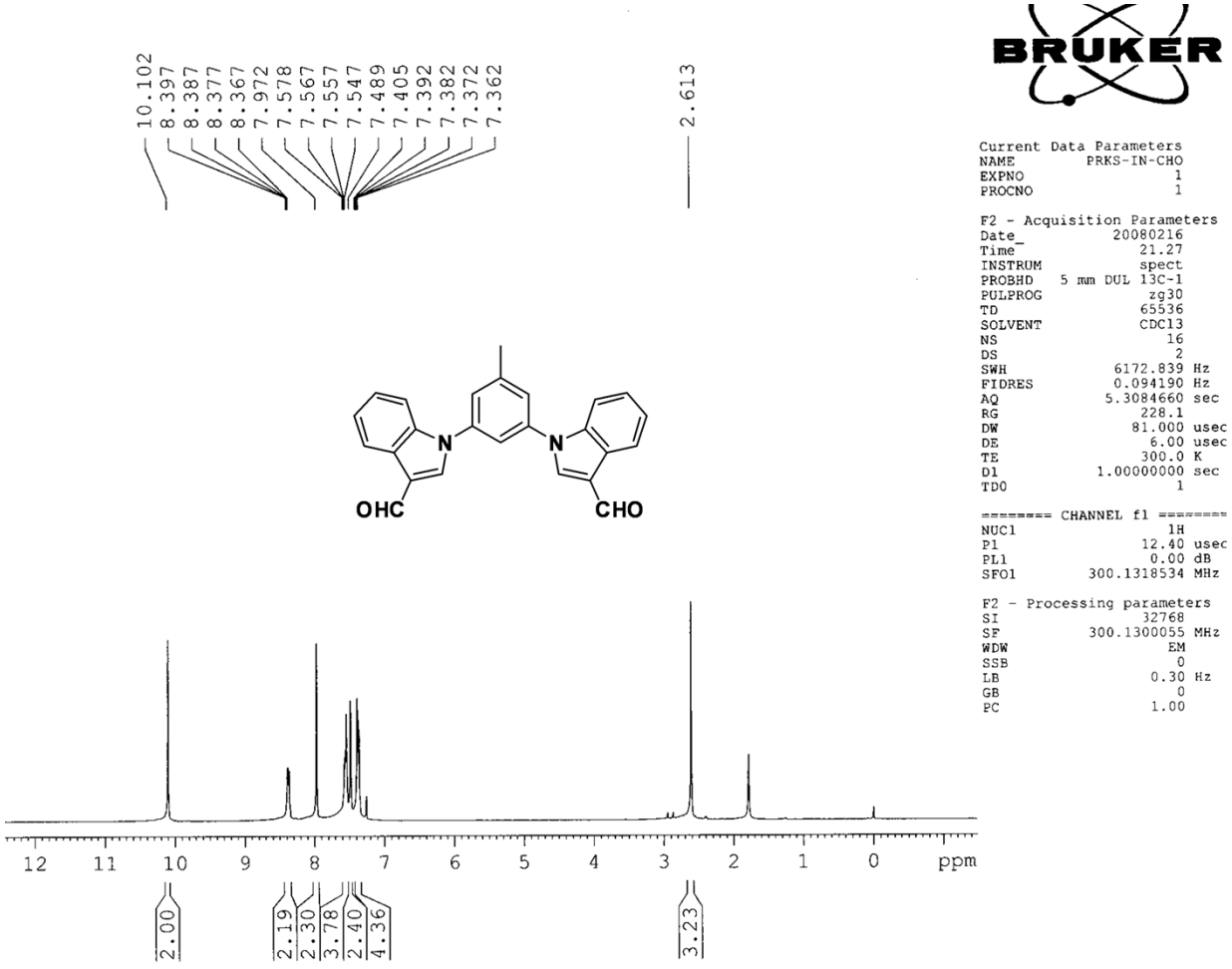
Ethylenophane 4: Yield 15%; mp 98-100 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 1.58 (t, 6H, *J* = 7.2 Hz) 4.87 (q, 4H, *J* = 7.2 Hz); 6.82 (s, 4H); 7.14-7.19 (m, 8H); 7.22 (s, 4H); 7.51-7.56 (m, 8H); 7.61 (d, 4H, *J* = 2.1 Hz); 7.65 (d, 4H, *J* = 7.8 Hz); 8.13 (d, 4H, *J* = 2.1 Hz). ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 13.62, 37.73, 109.35, 110.23, 112.02, 11 4.54, 116.86, 119.11, 119.44, 122.14, 123.12, 123.60, 124.42, 126.65, 132.77, 138.98, 149.25. FAB-MS (*m/z*): 898 (M^+). Elemental Anal. Calcd for $C_{64}H_{46}N_6$: C, 85.50; H, 5.16; N, 9.35. Found: C, 85.63; H, 5.04; N, 9.50.



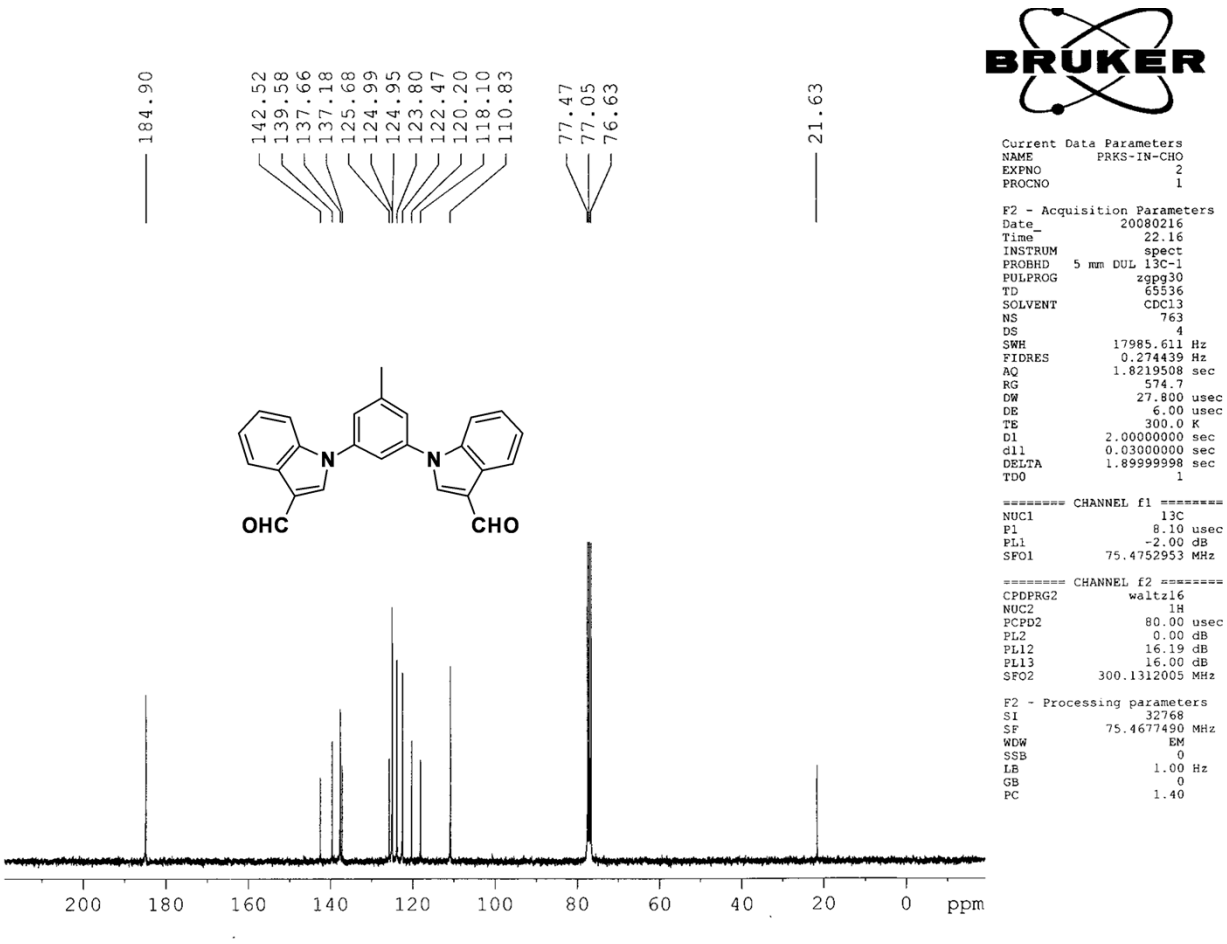
^{1}H NMR spectrum (300 MHz, $CDCl_3$) of precyclophane 9



^{13}C NMR spectrum (75 MHz, $CDCl_3$) of precyclophane 9



^{1}H NMR spectrum (300 MHz, $CDCl_3$) of dialdehyde 13



BRUKER

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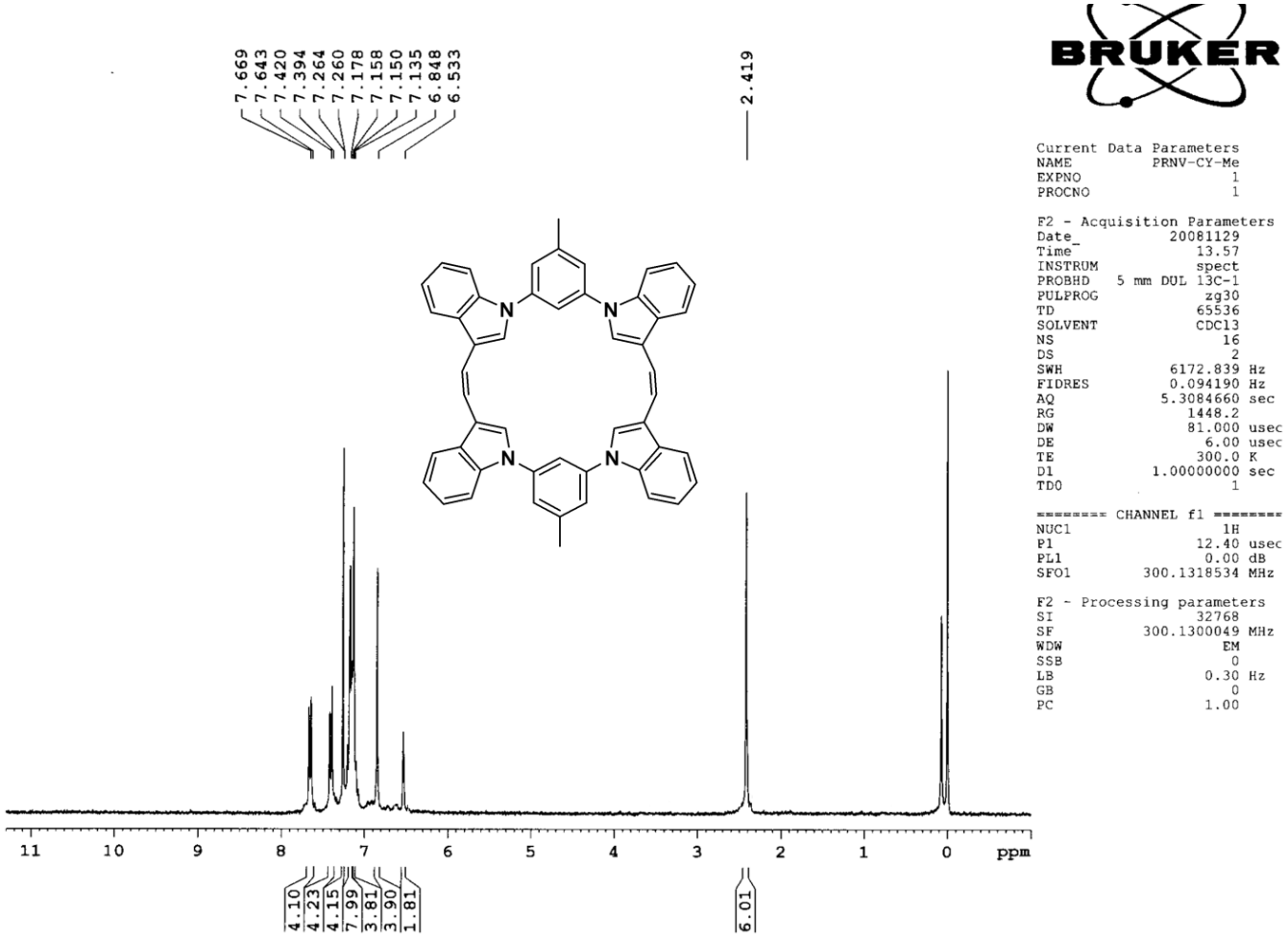

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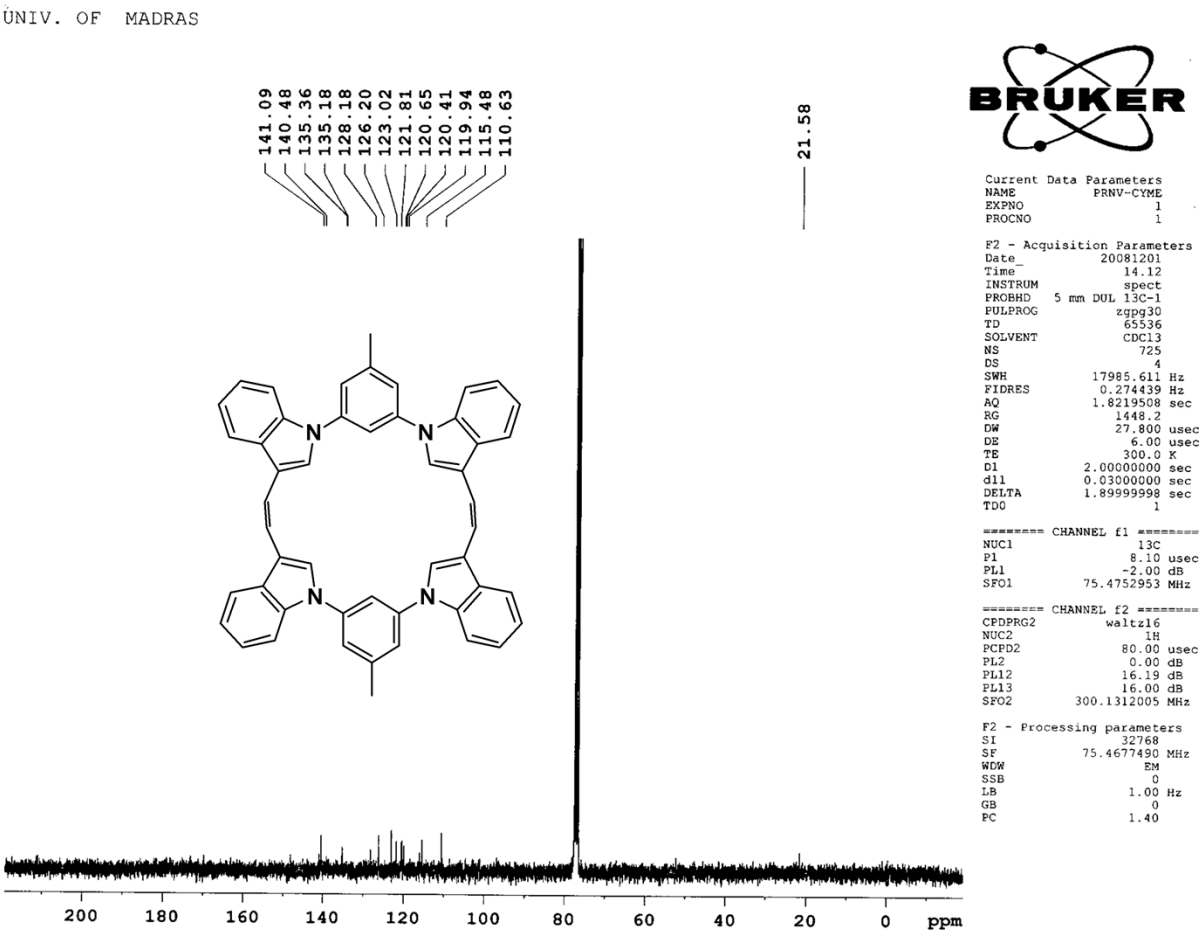

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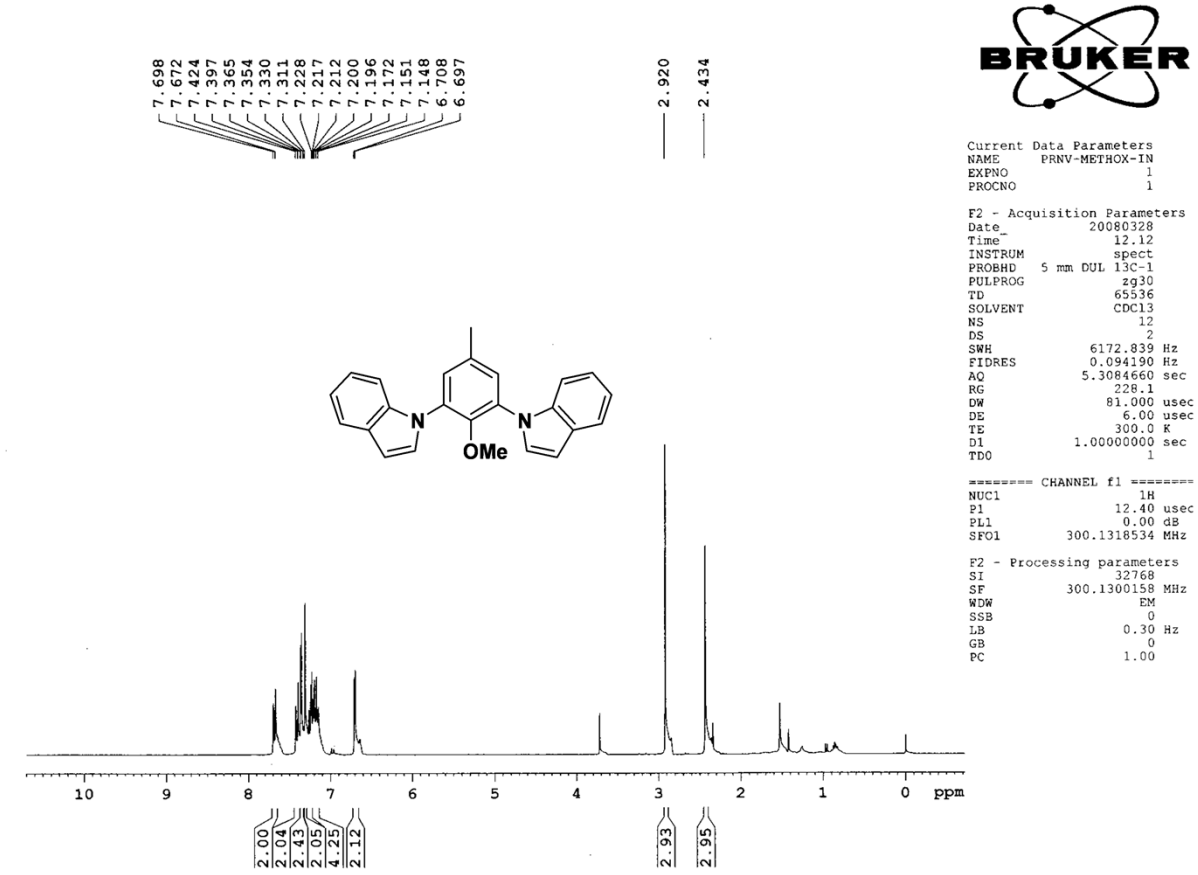

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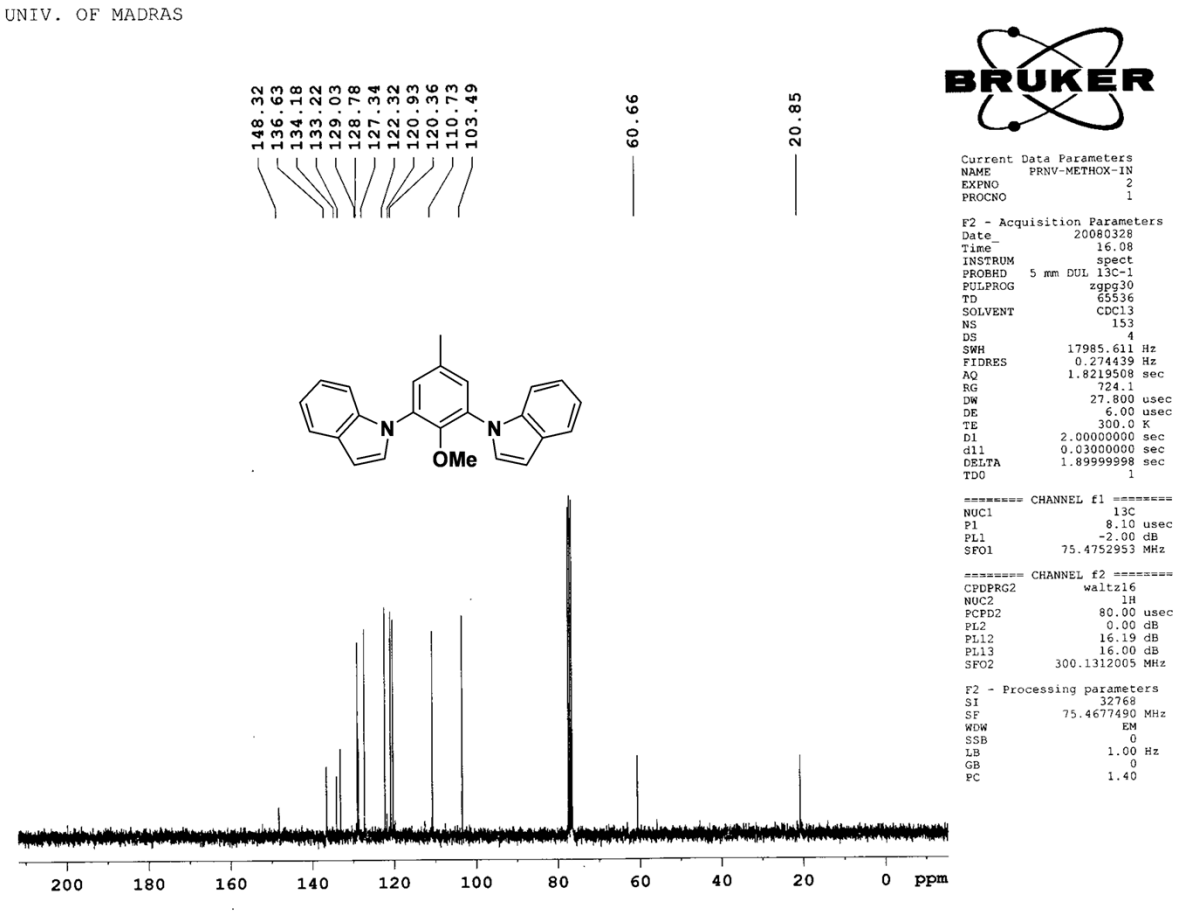

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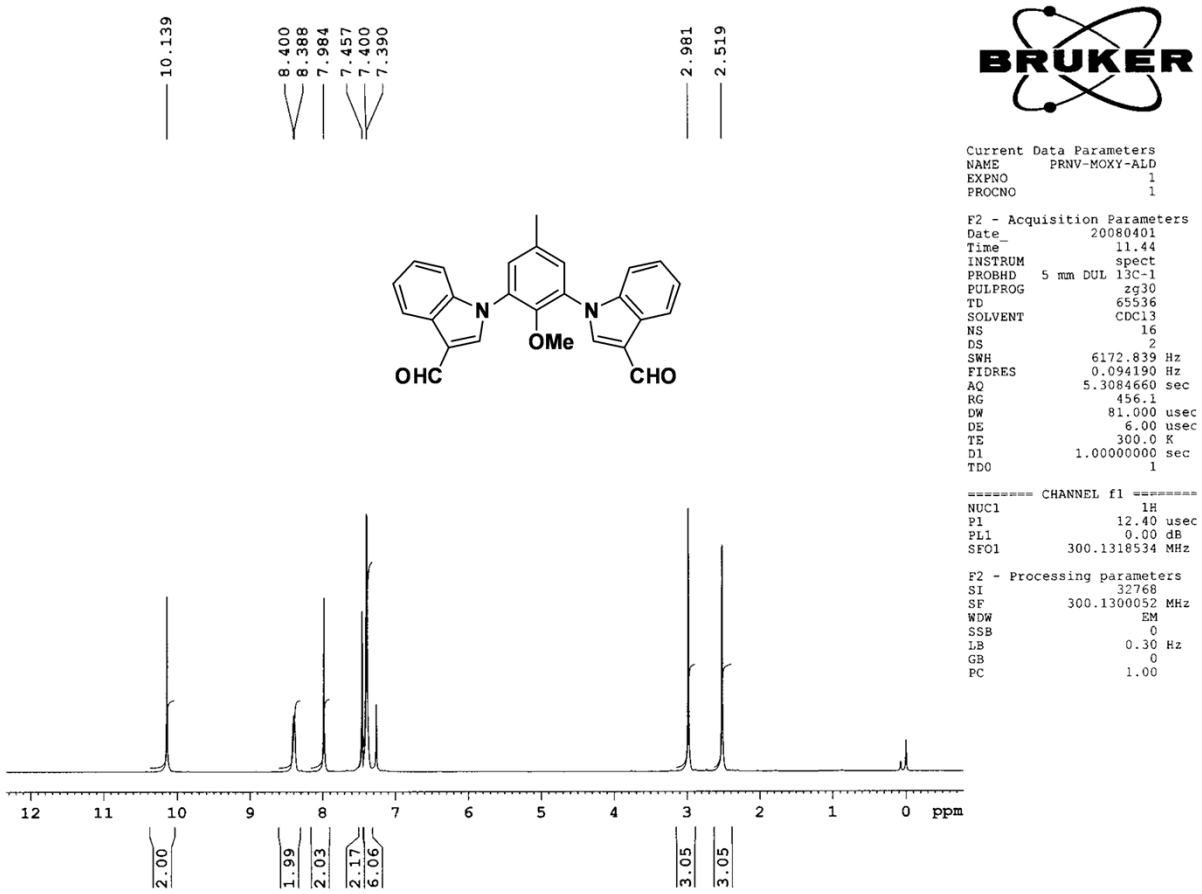


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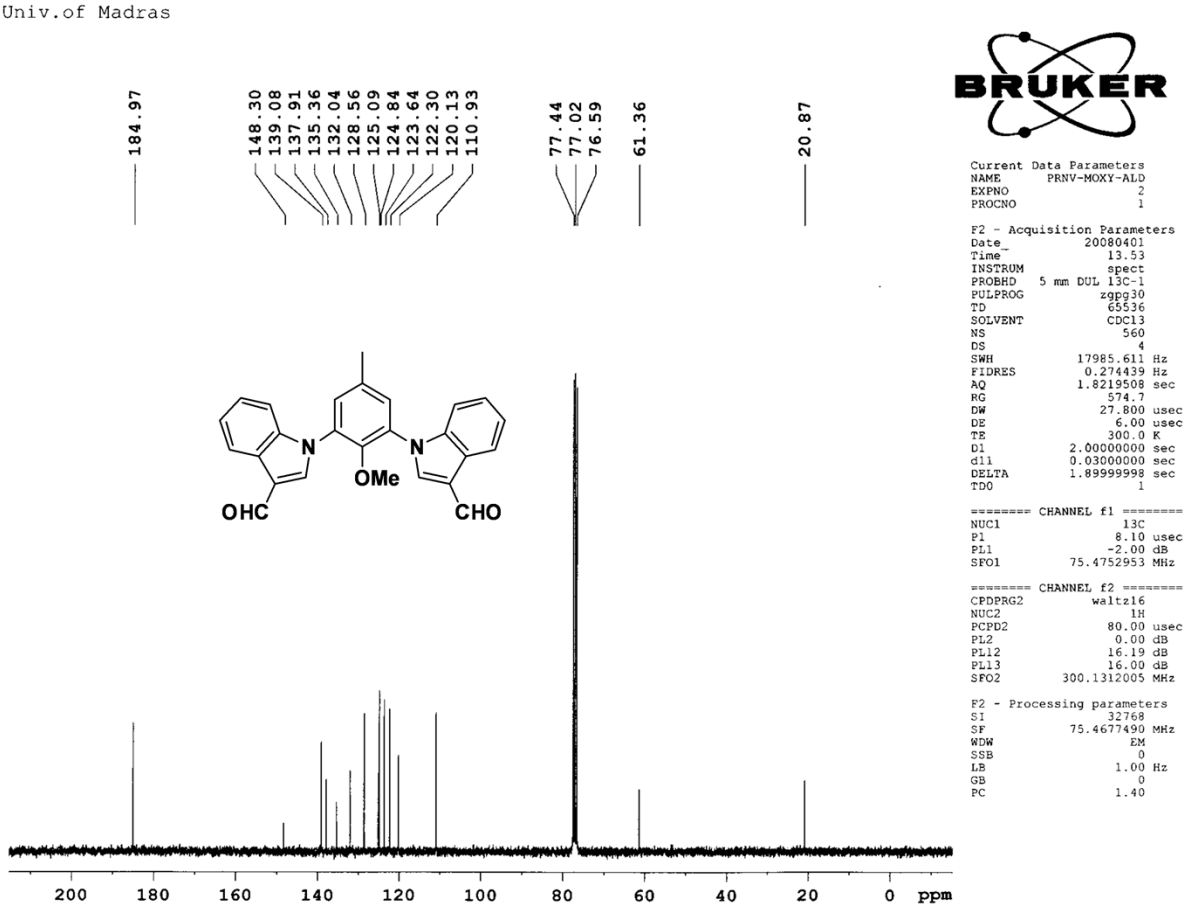
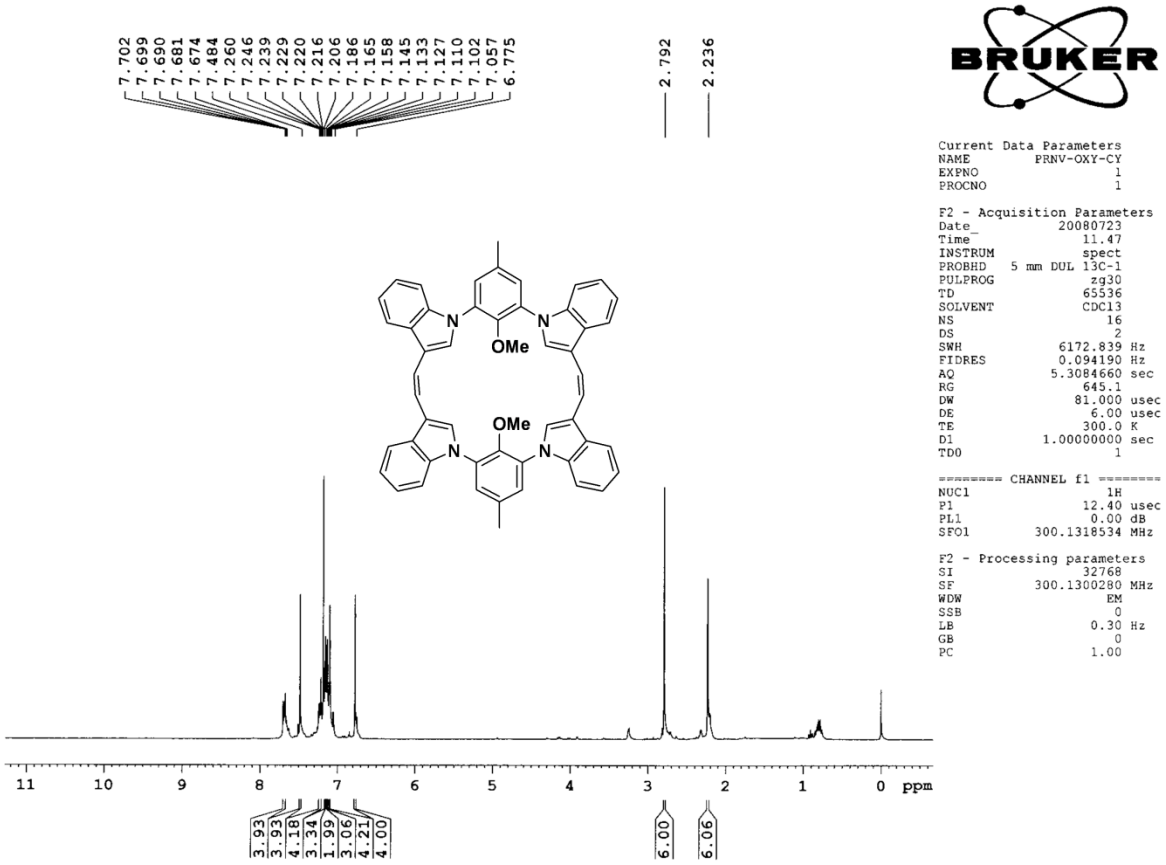
^{1}H NMR spectrum (300 MHz, $CDCl_3$) of dialdehyde 13a



^{13}C NMR spectrum (75 MHz, $CDCl_3$) of dialdehyde 13a



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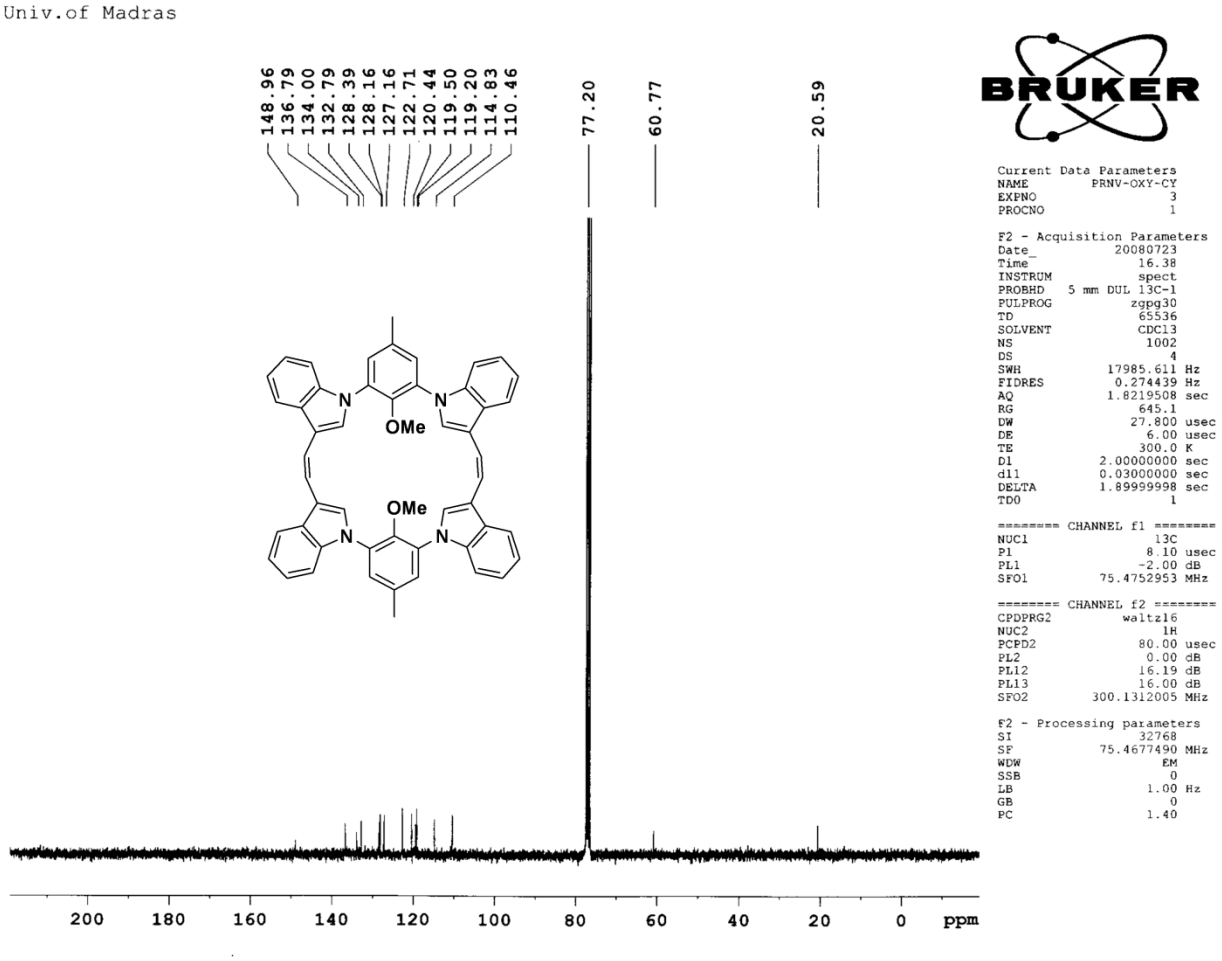
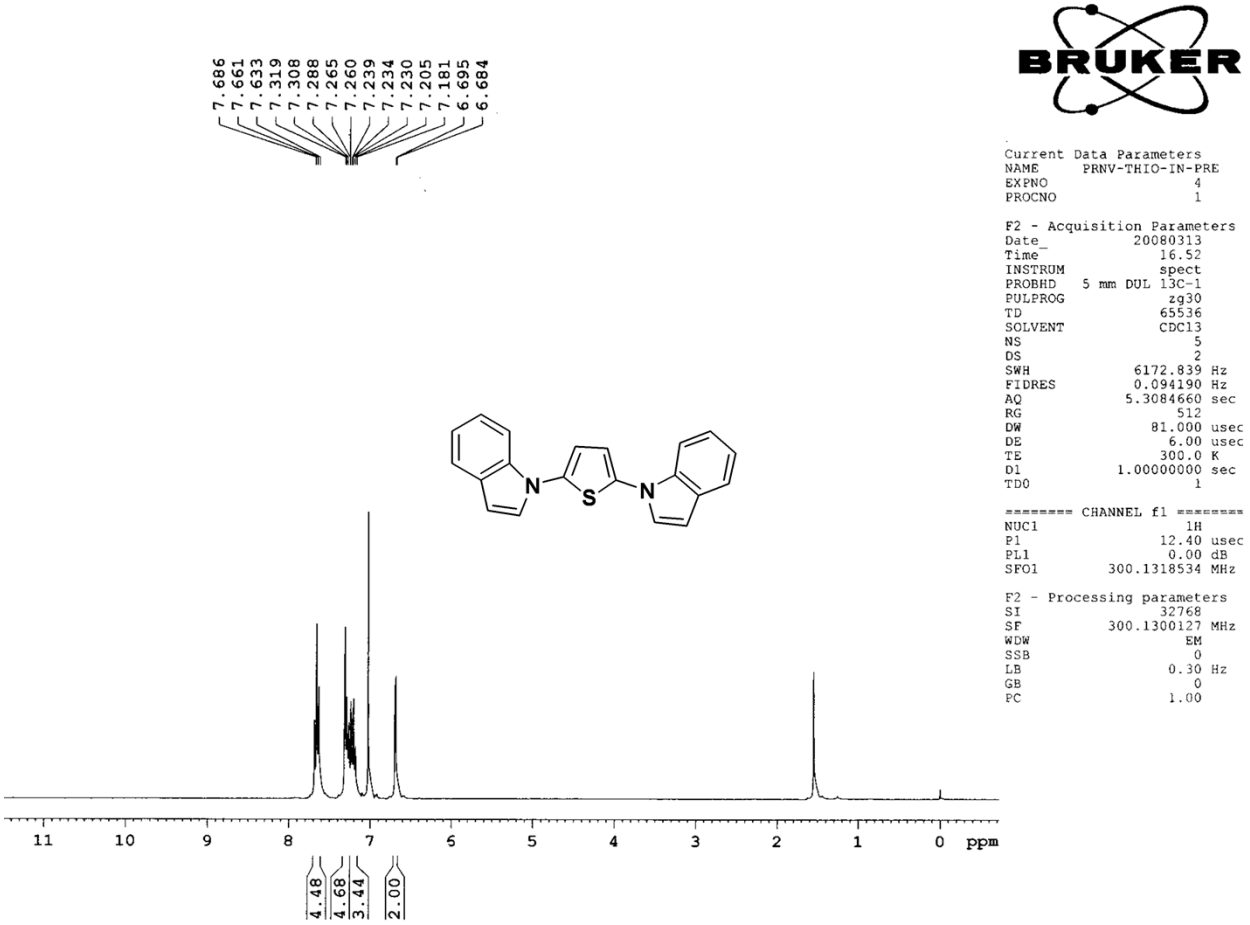


^{13}C NMR spectrum (75 MHz, $CDCl_3$) of Ethylenophane 1a



BRUKER

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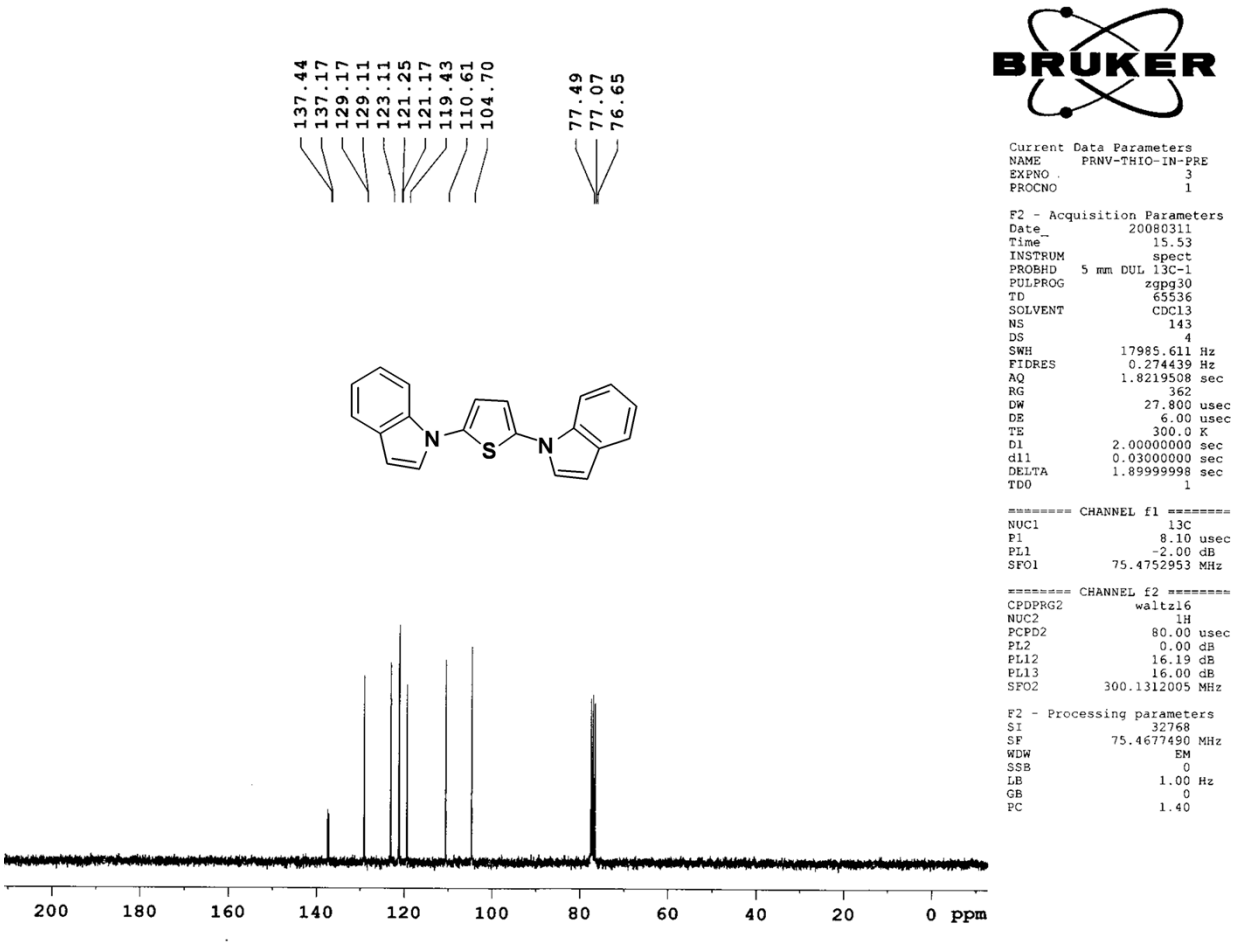
DS                       2
SWH               6172.839 Hz
FIDRES            0.094190 Hz
AQ                5.3084660 sec
RG                     512
DW                  81.000 usec
DE                   6.00 usec
TE                  300.0 K
D1                1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   12.40 usec
PL1                   0.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                   32768
SF            300.1300127 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

^{1}H NMR spectrum (300 MHz, $CDCl_3$) of precyclophane 11



BRUKER

```
Current Data Parameters
NAME      PRNV-THIO-IN-PRE
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_             20080311
Time                 15.53
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    143
DS                      4
SWH              17985.611 Hz
FIDRES           0.274439 Hz
AQ               1.8219508 sec
RG                    362
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                  8.10 usec
PL1                -2.00 dB
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               16.19 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 spectrum (75 MHz, $CDCl_3$) of precyclophane 11

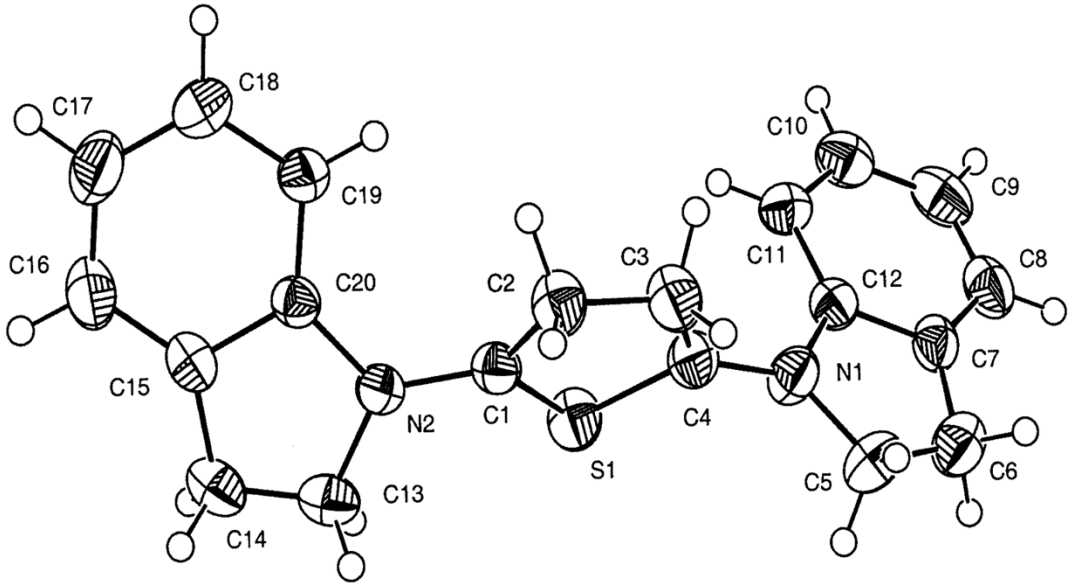
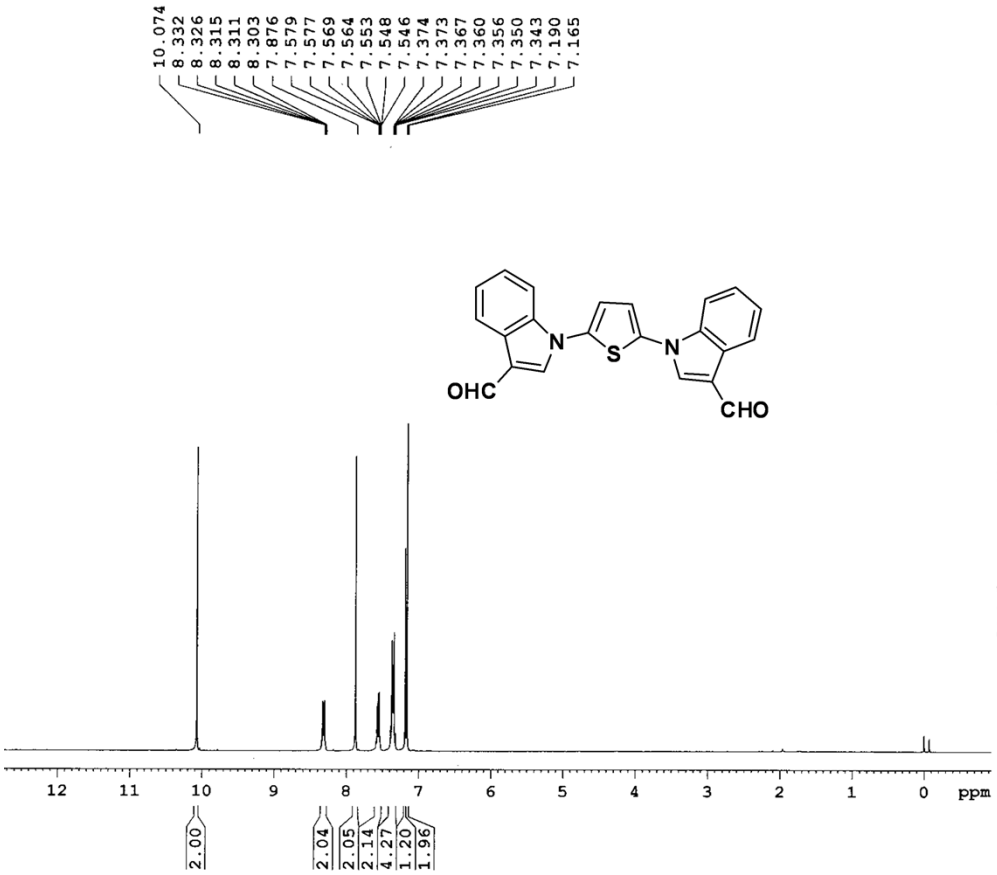


Figure S1. The XRD-single crystal structure of precyclophane 11



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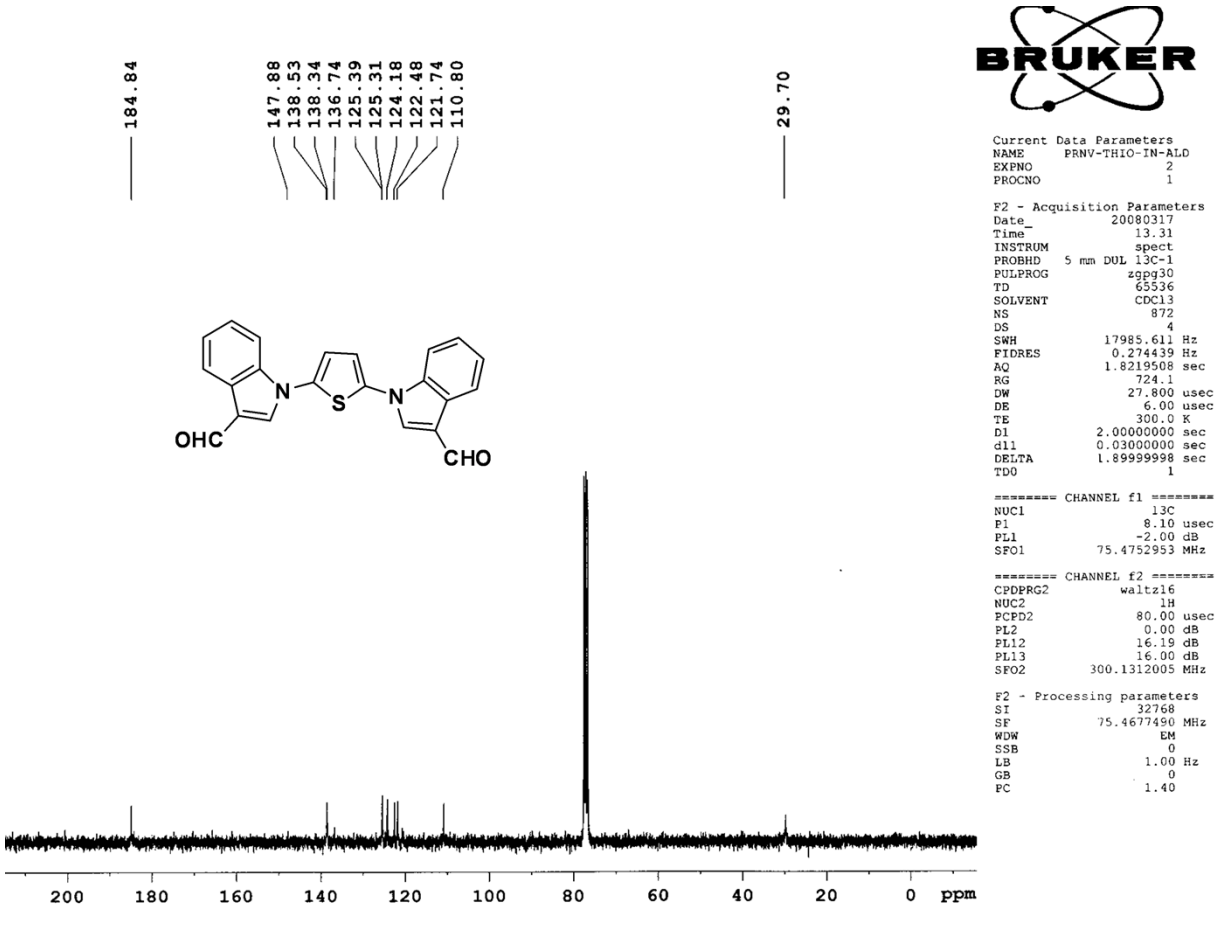
Current Data Parameters
NAME PRNV-THIO-IN-ALD
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080314
Time 14.50
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 574.7
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 12.40 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300271 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{1}H NMR spectrum (300 MHz, $CDCl_3$) of dialdehyde 15



BRUKER

```
Current Data Parameters
NAME      PRNV-THIO-IN-ALD
EXPNO                    2
PROCNO                   1

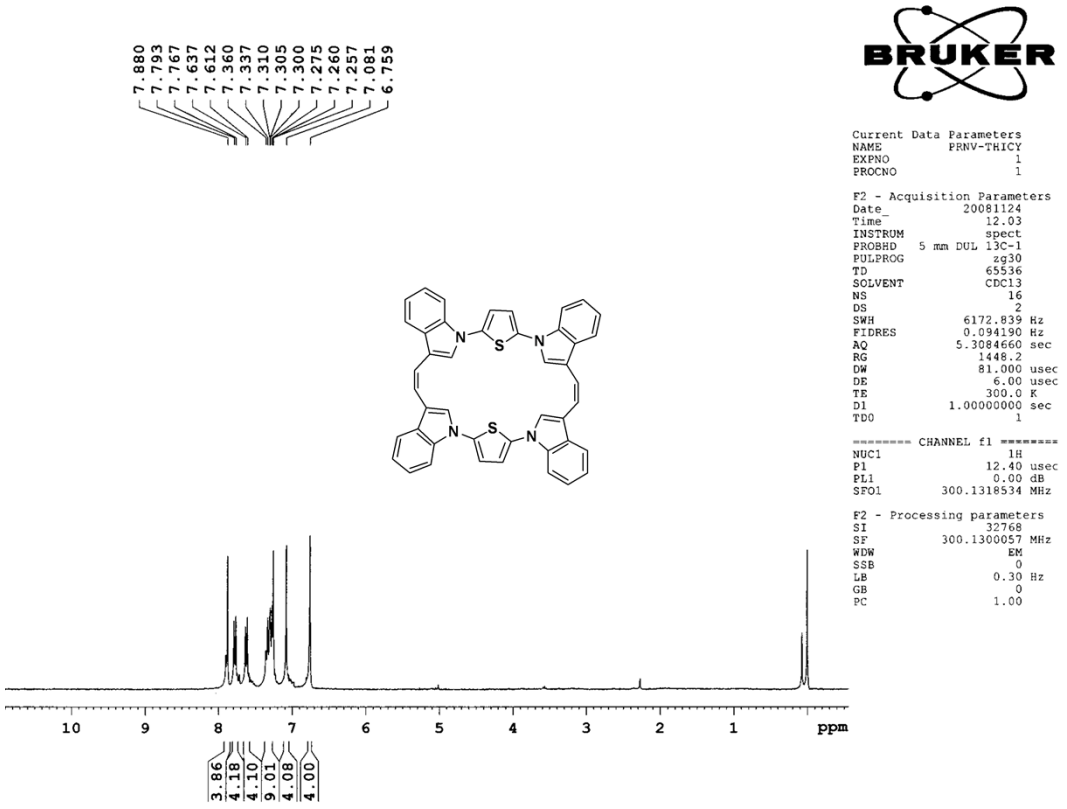
F2 - Acquisition Parameters
Date_             20080317
Time                 13.31
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  872
DS                    4
SWH           17985.611 Hz
FIDRES            0.274439 Hz
AQ            1.8219508 sec
RG                724.1
DW                27.800 usec
DE                 6.00 usec
TE                300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  8.10 usec
PL1                -2.00 dB
SFO1          75.4752953 MHz

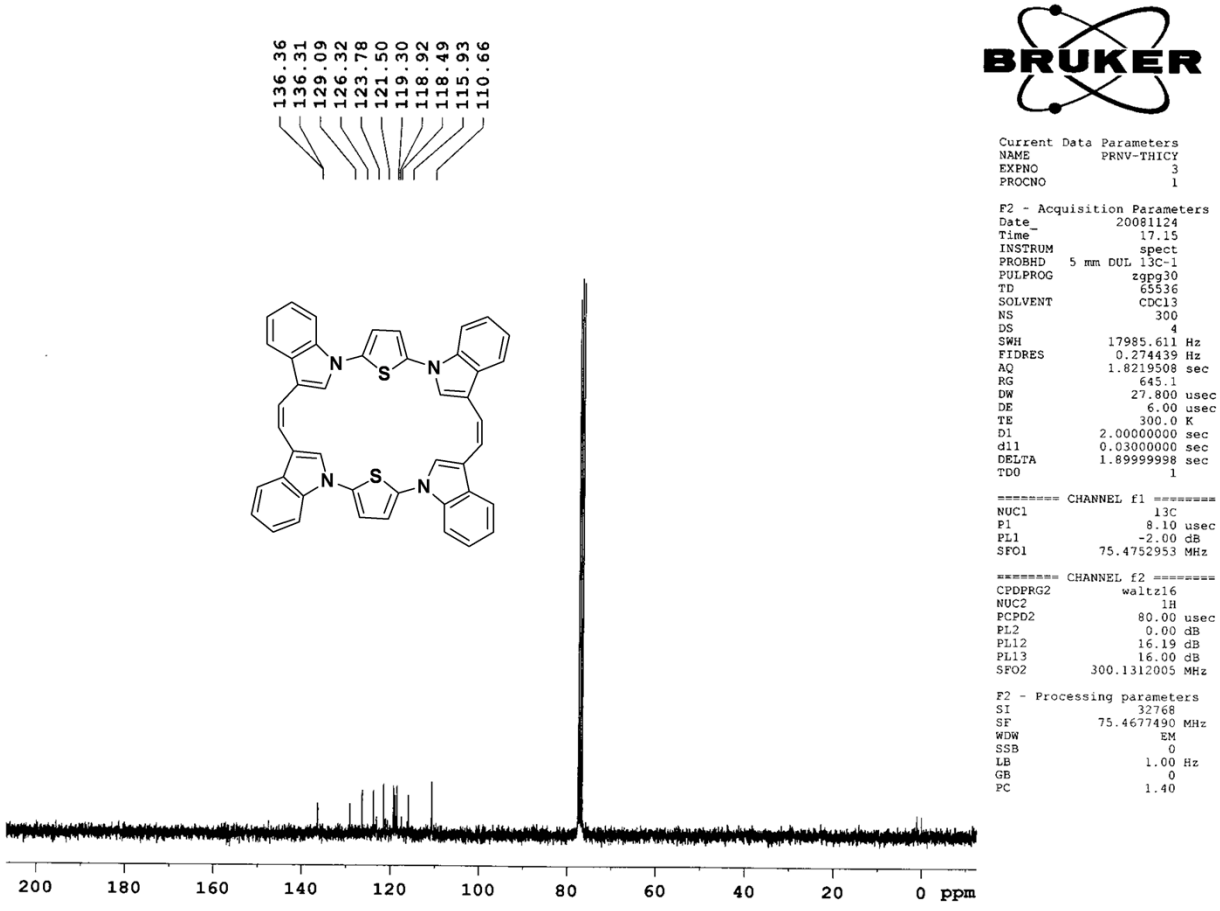
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               16.19 dB
PL13               16.00 dB
SFO2         300.1312005 MHz

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 spectrum (75 MHz, $CDCl_3$) of dialdehyde 15



^{1}H NMR spectrum (300 MHz, $CDCl_3$) of Ethylenophane 3



BRUKER

```
Current Data Parameters
NAME                 PRNV-THICY
EXPNO                         3
PROCNO                        1

F2 - Acquisition Parameters
Date_               20081124
Time                   17.15
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      300
DS                        4
SWH                17985.611 Hz
FIDRES             0.274439 Hz
AQ                 1.8219508 sec
RG                     645.1
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                       8.10 usec
PL1                     -2.00 dB
SFO1               75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                      0.00 dB
PL12                    16.19 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 spectrum (75 MHz, $CDCl_3$) of Ethylenophane 3

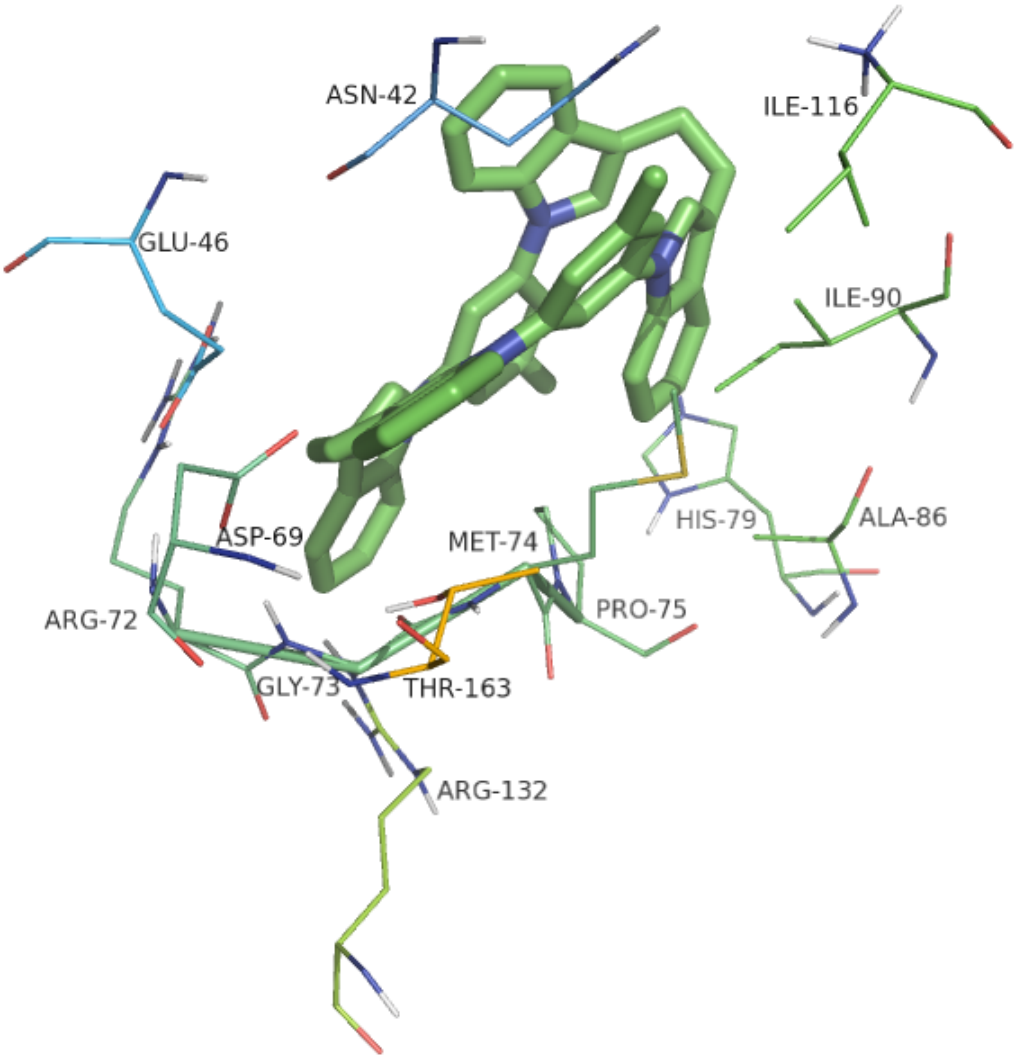

ASN-42
ILE-116
GLU-46
ILE-90
ASP-69
MET-74
HIS-79
ALA-86
ARG-72
PRO-75
GLY-73
THR-163
ARG-132

Figure S2. Binding of Ligand (Ethylenophane **1**) with the A chain amino acids of bacterial enzyme Topoisomerase IV (PDB ID: 3FV5).

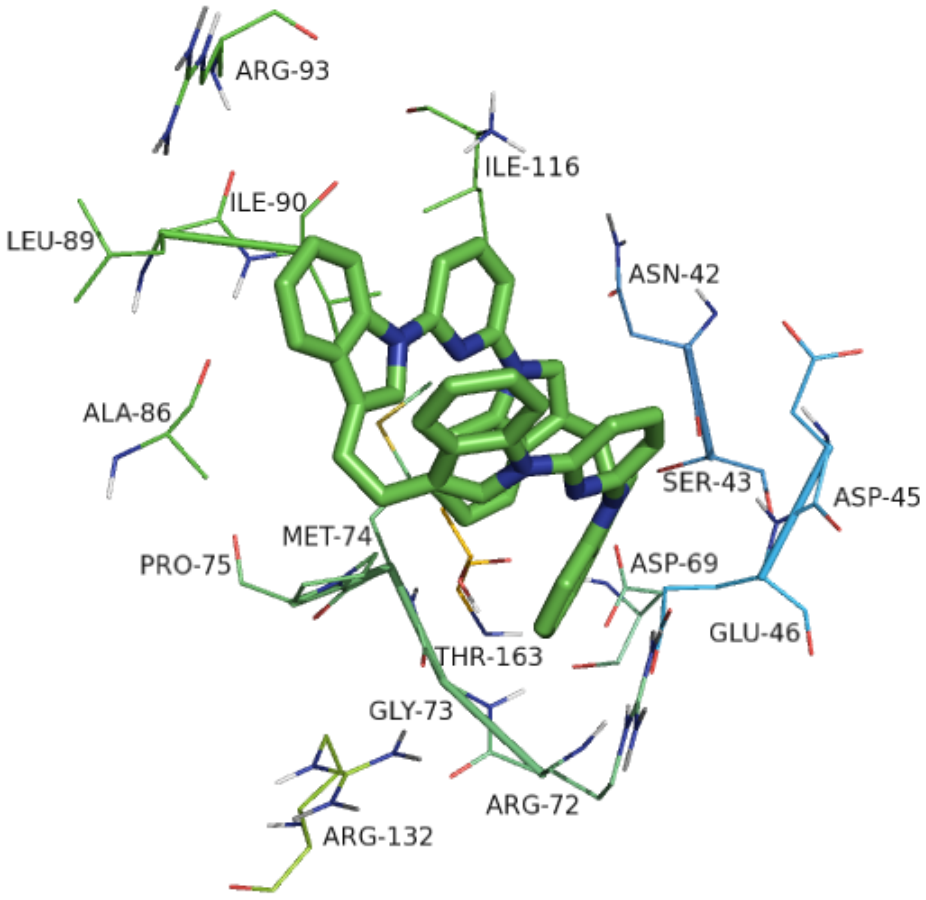


Figure S3. Binding of Ligand (Ethylenophane **2**) with the A chain amino acids of bacterial enzyme Topoisomerase IV (PDB ID: 3FV5).

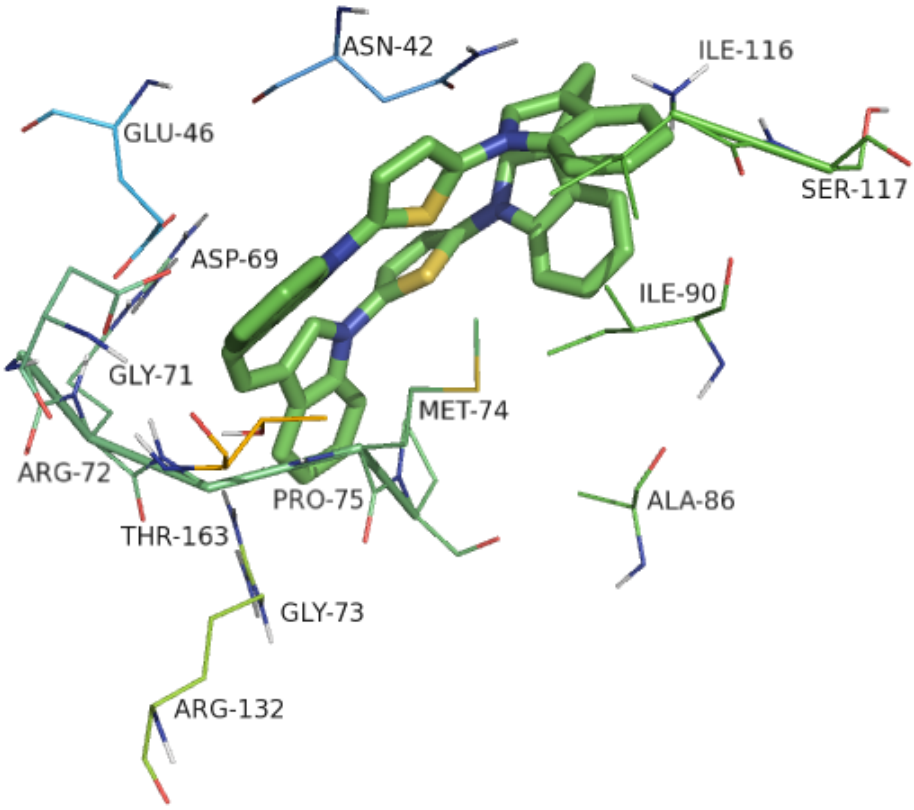


Figure S4. Binding of Ligand (Ethylenophane **3**) with the A chain amino acids of bacterial enzyme Topoisomerase IV (PDB ID: 3FV5).

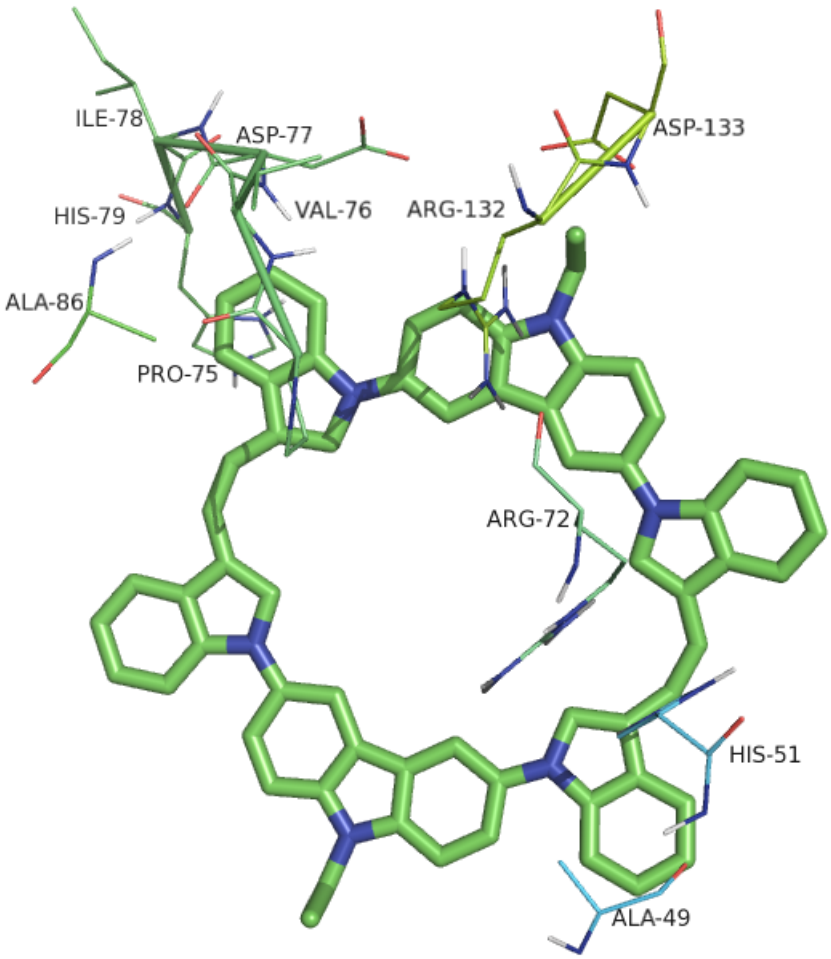


Figure S5. Binding of Ligand (Ethylenophane **4**) with the A chain amino acids of bacterial enzyme Topoisomerase IV (PDB ID: 3FV5).