Supporting Information for:

# Synthesis and Photochemical Properties of 12- versus 13-Substituted Chlorins

Olga Mass, Marcin Ptaszek, Masahiko Taniguchi, James R. Diers, Hooi Ling Kee, David F. Bocian, Dewey Holten, and Jonathan S. Lindsey

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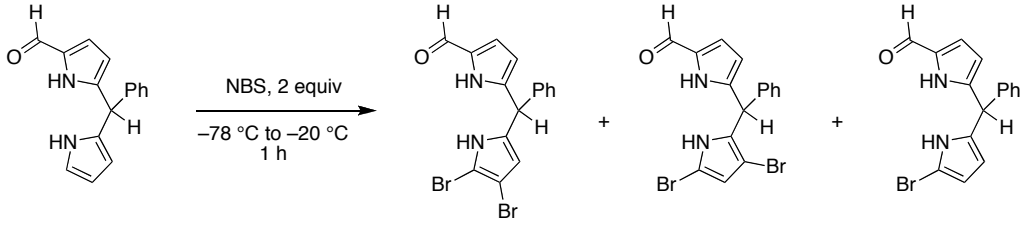
## I. Bromination of 1-Formyl-5-phenyldipyrromethane.

The bromination of 1-formyl-5-phenyldipyrromethane (**8**) was carried out with two molar equivalents of NBS at –78 °C through –20 °C. $^{1}$H NMR spectroscopy of the crude mixture showed the presence of the two dibromo isomers in a 5:1 ratio. The two products were isolated by column chromatography. The dominant product was characterized with two-dimensional NMR spectroscopy (NOESY), and was identified as 8,9-dibromodipyrromethane **8-Br$^{8,9}$** on the basis of the NOE between the H$^{7}$ and aromatic protons of the phenyl ring. The second product was believed to be 7,9-dibromodipyrromethane **8-Br$^{7,9}$**; its proton at the 8-position had the same NMR chemical shift as H$^{8}$ in 7,9-dibromo-5-mesityl-dipyrromethane **2-Br$^{8,9}$**. $^{1}$H NMR spectroscopy of both products enabled analysis of the $^{1}$H NMR spectrum of the crude mixture and established the ratio of the isomers as 1:5 with the 8,9-dibromo product as the dominant species. Also, a trace amount of 9-bromo-1-formyl-5-phenyldipyrromethane **8-Br$^{9}$** (a known compound)[7] was present in the crude mixture. In conclusion, the bromination of **8** with two molar equivalents of NBS proceeds in the same manner as that of 1-formyl-5-mesityldipyrromethane **2** where the 7-position is hindered by a 5-aryl substituent.



## II. Experimental Section.

**General Methods.** All $^1$H NMR (300 and 400 MHz) and $^{13}$C NMR (100 MHz) spectra were obtained in $CDCl_3$ unless noted otherwise. Mass spectra of chlorins were obtained via matrix-assisted laser desorption ionization mass spectrometry (MALDI-MS) using a matrix of 1,4-bis(5-phenyloxazol-2-yl)benzene. Electrospray ionization mass spectrometry (ESI-MS) data are reported for the molecule ion or protonated molecule ion. Column chromatography was performed with flash silica. Melting points are uncorrected. All commercially available materials were used as received. Several bromodipyrromethanes isolated as trace byproducts (**1-Br**[3,7,9], **2-Br**[3,8,9], and **2-Br**[7,9]) were found by $^1$H NMR spectroscopy to have purity of 80%, 90%, and 90%, respectively.

All of the Pd-mediated coupling reactions were carried out by using a Schlenk line under argon. The Schlenk flask containing the solid compounds was evacuated via a high vacuum pump for 2 min followed by flushing with argon for 1 min. This process of evacuation and flushing was performed three times. The flow rate of argon was then increased, and the stopcock was removed. The deaerated solvents were injected into the Schlenk flask by syringe. The threaded stopcock was replaced, and the flow rate of argon was reduced.

**Bromination of 5-Phenyl-1-formyldipyrromethane (8).** A solution of **8** (60 mg, 0.24 mmol) in anhydrous THF (2.4 mL) at –78 °C was treated with NBS (85 mg, 0.48 mmol) in one batch under argon. The reaction mixture was stirred for 1 h at –78 °C, after which the ice bath was removed. A thermometer was placed in the reaction mixture. The reaction mixture was allowed to warm up. Hexanes (5 mL) and water (5 mL) were added when the temperature of the reaction mixture reached –20 °C. The entire contents of the reaction flask were transferred to a separatory funnel. Ethyl acetate (10 mL) was added. The organic layer was separated, dried ($K_2CO_3$) and concentrated without heating to afford a yellow solid. Column chromatography [silica, hexanes/$CH_2Cl_2$/ethyl acetate (7:2:1)] was run twice but did not allow complete separation of isomers affording two brominated dipyrromethanes, each impure, in the following order: a minor amount of 7,9-dibromo-5-phenyl-1-formyldipyrromethane (**8-Br**[7,9], 15 mg, 15%); and a dominant amount of 8,9-dibromo-5-phenyl-1-formyldipyrromethane (**8-Br**[8,9], 58 mg, 60%). The isolated sample of **8-Br**[7,9] contained 0.5-1% of **8-Br**[8,9]. The sample of **8-Br**[8,9] (which contained 7% of **8-Br**[7,9], 10% of **8-Br**[9] and 5% of unidentified impurities) was washed with cold $CH_2Cl_2$ (~0 °C) to achieve a high level of purity. The two products were examined by $^1$H NMR spectroscopy. Data for **8-Br**[8,9]: mp 120 °C (dec.); $^1$H NMR (THF-$d_8$) δ 5.41 (s, 1H), 5.69–5.70 (m, 1H), 5.90–5.91 (m, 1H), 6.81–6.82 (m, 1H), 7.17–7.31 (m, 5H), 9.40 (s, 1H), 10.89 (br s, 1H), 11.27 (br s, 1H); ESI-MS obsd 406.9382 $(M + H)^+$ corresponds to 405.93092 (M), calcd 405.93164 ($C_{16}H_{12}Br_2N_2O$). Data for **8-Br**[7,9]: $^1$H NMR (THF-$d_8$) δ 5.65 (s, 1H), 5.98–6.00 (m, 1H), 6.09 (m, 1H), 6.84–6.86 (m, 1H), 7.11–7.29 (m, 5H), 9.41 (s, 1H), 10.90 (br s, 1H), 11.29 (br s, 1H); ESI-MS obsd 406.9382 $(M + H)^+$ corresponds to 405.93087 (M), calcd 405.93164 ($C_{16}H_{12}Br_2N_2O$).

## III. NMR Characterization of Brominated Dipyrromethanes.

The resonances were assigned for all of the protons in the bromodipyrromethane compounds shown in Table S1. A NOE between $H^3$ and $H^2$ was observed in each case, as expected. For compounds **1-Br**[9] and **1-Br**[8,9], the resonance of the meso-proton $H^5$ had two cross peaks with the signals from the pyrroline ring protons (assigned as $H^3$ and $H^7$). The resonance of the meso-proton of **2-Br**[7,9] and of **1-Br**[7,9] exhibited only a single cross peak (stemming from the pyrroline ring protons), and those resonances in both compounds that did not exhibit any NOE were assigned to $H^8$. In compound **5** a resonance from a proton that had no cross peaks was assigned as $H^9$.

**Table S1.** $^1$H NMR chemical shifts of bromodipyrromethanes.

| Compound | $H^2$ | $H^3$ | $H^7$ | $H^8$ | $H^5$ | H-formyl |
|---|---|---|---|---|---|---|
| **1-Br**[9] | 6.790–6.794 | 5.97 | 5.820–5.821 | 5.92–5.93 | 3.92 | 9.37 |
| **1-Br**[7,9] | 6.77–6.80 | 5.89-5.91 | – | 6.06–6.07 | 3.94 | 9.37 |
| **1-Br**[8,9] | 6.78–6.80 | 5.98–6.00 | 5.93–5.94 | – | 3.91 | 9.38 |
| **2-Br**[9] | 6.76–6.78 | 5.89–5.92 | 5.80–5.85 | 5.49–5.52 | 5.74 | 9.38 |
| **2-Br**[8,9] | 6.78–6.83 | 5.83-5.86 | 5.58–5.62 | – | 5.74 | 9.39 |
| **2-Br**[7,9] | 6.76 | 5.68 | – | 6.10 | 5.80 | 9.42 |

**IV. NMR Characterization of 12- or 13-Substituted Chlorins.**

The $^1$H NMR chemical shifts for selected zinc chlorins (prepared previously[26,29,33] or herein) are shown in Tables S2 and S3. Introduction of the 3-bromine atom causes the resonance of the adjacent meso-proton ($H^5$) to shift downfield ($\Delta\delta$ = +0.21 ppm ), and the resonances of the next adjacent meso-proton ($H^{20}$) to shift upfield ($\Delta\delta$ = –0.08 ppm). Similarly, the 13-bromine atom causes the resonance of the adjacent meso-proton ($H^{15}$) to shift downfield ($\Delta\delta$ = +0.25 ppm). Note that the next adjacent meso-position (10-position) is occupied by the mesityl group.

(1) Ethynyl group: introduction of the ethynyl group causes the resonance of the adjacent meso-proton to shift downfield (0.22 to 0.33 ppm) and the resonance of the adjacent $\beta$-proton to shift downfield (0.10 to 0.15 ppm).

(2) Acetyl group: introduction of the 12-acetyl group causes the resonance of the adjacent meso-proton ($H^{10}$) and $\beta$-proton ($H^{13}$) to shift downfield ($\Delta\delta$ = 1.11 and 0.61 ppm, respectively). Similarly, introduction of the 13-acetyl group causes the resonance of the adjacent meso-proton ($H^{15}$) and $\beta$-proton ($H^{12}$) to shift downfield ($\Delta\delta$ = 1.18 and 0.56 ppm, respectively).

The characteristic feature of the $^1$H NMR spectra of 12-substituted chlorins is the downfield signal of $H^{10}$ compared with the $H^{10}$ resonance of 13-substituted chlorins. All protons were assigned with NOESY experiments. The $H^{10}$ of all 13-substituted chlorins exhibited two cross peaks with β-protons, while in 12-substituted chlorins only one NOE for $H^{10}$ was observed.

**Table S2.** $^1$H NMR chemical shifts of zinc chlorins with 3- and 13-bromine substituents.[a]

| Position | | **ZnC-M**$^{10}$ | **ZnC-Br**$^3$**M**$^{10}$ | **ZnC-M**$^{10}$**Br**$^{13}$ | **ZnC-Br**$^3$**M**$^{10}$**Br**$^{13}$ | **ZnC-Br**$^3$**Ar**$^{10}$**Br**$^{13}$[b] |
|---|---|---|---|---|---|---|
| | | δ | δ (Δδ) | δ (Δδ) | δ (Δδ) | δ (Δδ) |
| Meso | 5 | 9.52 | 9.73 (**+0.21**) | 9.54 (+0.02) | 9.62 (+0.10) | 9.62 (+0.10) |
| | 10 | – | – | – | – | – |
| | 15 | *8.60*[c] | 8.68 (+0.08) | 8.85 (**+0.25**) | 8.81 (**+0.21**) | 8.86 (**+0.26**) |
| | 20 | *8.58*[c] | 8.50 (–0.08) | 8.61 (+0.03) | 8.41 (–0.17) | 8.49 (–0.09) |
| $\beta$ | 2 | 8.70 | 8.77 (+0.07) | 8.72 (+0.02) | 8.78 (+0.08) | 8.76 (+0.06) |
| | 3 | 9.02 | – | 9.01 (–0.01) | – | – |
| | 7 | 8.74 | 8.88 (+0.14) | 8.80 (+0.06) | 8.84 (+0.10) | 8.82 (+0.08) |
| | 8 | 8.24 | 8.37 (+0.13) | 8.37 (+0.13) | 8.26 (+0.02) | 8.43 (+0.19) |
| | 12 | 8.40 | 8.55 (+0.15) | 8.57 (+0.17) | 8.57 (+0.17) | 8.64 (+0.24) |
| | 13 | 8.53 | 8.60 (+0.07) | – | – | – |

[a]In $CDCl_3$ (~20 mM) at 298 K. Significant shifts (Δδ) are shown in bold. [b]Ar = 4-[2-(triisopropylsilyl)ethynyl]phenyl. [c]The resonances could not be unambiguously distinguished and may be interchangeable.

**Table S3.** $^1$H NMR chemical shifts of zinc chlorins with 12- versus 13-substituents.[a]

| Position | | **ZnC** | **ZnC-E$^3$A$^{12}$** | **ZnC-E$^3$A$^{13}$** | **ZnC-E$^3$E$^{12}$** | **ZnC-E$^3$E$^{13}$** |
|---|---|---|---|---|---|---|
| | | δ | δ (Δδ) | δ (Δδ) | δ (Δδ) | δ (Δδ) |
| Meso | 5 | *9.63*[c] | 9.84 (+0.21) | 9.75 (+0.12) | *9.85*[e] (+**0.22**) | 9.85 (+**0.22**) |
| | 10 | *9.61*[c] | 10.72 (+**1.11**) | 9.63 (+0.02) | *9.87*[e] (+**0.26**) | 9.58 (–0.03) |
| | 15 | 8.70 | 8.78 (+0.08) | 9.88 (+**1.18**) | 8.69 (–0.01) | 9.03 (+**0.33**) |
| | 20 | 8.67 | 8.67 (0) | 8.58 (–0.09) | 8.65 (–0.02) | 8.64 (–0.03) |
| *β* | 2 | 8.76 | 8.92 (+0.16) | 8.88 (+0.12) | 8.90 (+0.14) | 8.91 (+0.15) |
| | 3 | *9.06*[d] | – | – | – | – |
| | 7 | 8.92 | 8.94 (+0.02) | 8.87 (–0.05) | 8.95 (+0.03) | 8.91 (–0.01) |
| | 8 | 8.92 | 9.06 (+0.14) | 8.95 (+0.03) | 8.95 (+0.03) | 8.93 (+0.01) |
| | 12 | *9.08*[d] | – | 9.64 (+**0.56**) | – | 9.18 (+0.10) |
| | 13 | 8.71 | 9.32 (+**0.61**) | – | 8.86 (+0.15) | – |
| | 17 | 4.58 | 4.57 | 4.56 | 4.57 | 4.60 |
| | 18[b] | 2.05 | 2.04 | 2.02 | 2.03 | 2.06 |

[a]In THF (~20 mM) at 298 K. Significant shifts (Δδ) are shown in bold. [b]Protons of the geminal dimethyl group (18-position). [c-e]The resonances could not be unambiguously distinguished and may be interchangeable.

In the free base 15-bromochlorins (Table S4), the resonance of the H$^{10}$ proton is significantly shifted owing to the presence of the 12-acetyl substituent. On the other hand, the corresponding effect of the 13-acetyl substituent at the 15-position is not manifested owing to the presence of the 15-bromine atom.

**Table S4.** $^1$H NMR chemical shifts of free base chlorins with 12- versus 13-substituents.[a]

| Position | | **H$_2$C-Br$^{15}$** | **H$_2$C-A$^{12}$Br$^{15}$** | **H$_2$C-A$^{13}$Br$^{15}$** |
|---|---|---|---|---|
| | | δ | δ (Δδ) | δ (Δδ) |
| Meso | 5 | 9.81 | 9.45 (–**0.64**) | 9.61 (–0.20) |
| | 10 | 9.74 | 10.64 (+**0.80**) | 9.73 (–0.01) |
| | 15 | | – | – |
| | 20 | 8.89 | 8.76 (–0.13) | 8.82 (–0.07) |
| *β* | 2 | 8.95 | 8.76 (–0.19) | 8.91 (–0.04) |
| | 3 | 9.17 | 8.96 (–0.21) | 9.13 (–0.04) |
| | 7 | 9.02 | 9.06 (+0.04) | 8.88 (–0.14) |
| | 8 | 8.98 | 8.89 (–0.09) | 8.97 (–0.01) |
| | 12 | 9.19 | – | 9.12 (–0.07) |
| | 13 | 9.26 | 9.49 (+**0.23**) | – |
| | 17 | 4.67 | 4.59 | 4.59 |
| | 18[b] | 2.04 | 2.04 | 2.04 |

[a]In $CDCl_3$ (~20 mM) at 298 K. Significant shifts (Δδ) are shown in bold. [b]Protons of the geminal dimethyl group (18-position).

## V. X-Ray Structural Data.

**Data Collection, Data Processing, Structure Solution and Refinement.** Each sample was mounted on a nylon loop with a small amount of NVH immersion oil. All X-ray measurements were made on a Bruker-Nonius X8 Apex2 diffractometer. The frame integration was performed using SAINT.[S1] The resulting raw data was scaled and absorption corrected using a multi-scan averaging of symmetry equivalent data using SADABS.[S2] The structure was solved by direct methods using the SIR92 program.[S3] All non-hydrogen atoms were obtained from the initial solution. The hydrogen atoms were introduced at idealized positions and were allowed to ride on the parent atom. The structural model was fit to the data using full matrix least-squares based on F or $F^2$. The calculated structure factors included corrections for anomalous dispersion from the usual tabulation. The structure was refined using the XL program from SHELXTL,[S4] graphic plots were produced using the NRCVAX crystallographic program suite.

### 1. X-Ray Structural Data for ZnC-$Br^3Br^{13}$.

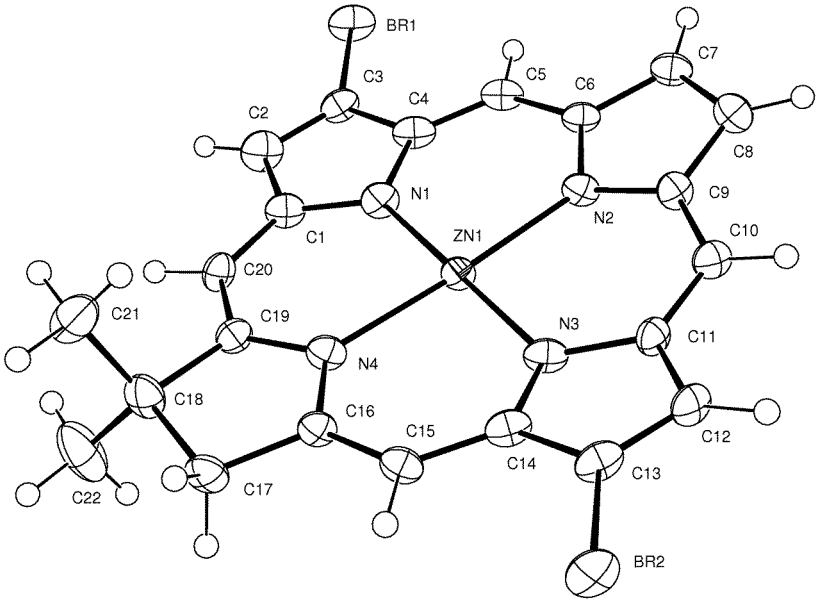



**Figure S1.** ORTEP drawing of **ZnC-$Br^3Br^{13}$** showing naming and numbering scheme. Ellipsoids are at the 50% probability level and hydrogen atoms were drawn with arbitrary radii for clarity.

**Table S5.** Summary of Crystal Data for **ZnC-Br$^{3}$Br$^{13}$.**

| Entry | Data |
|---|---|
| Formula | $C_{22}H_{16}Br_2N_4Zn$ |
| Formula Weight (*g/mol*) | 561.58 |
| Crystal Dimensions (*mm* ) | 0.10 × 0.04 × 0.02 |
| Crystal Color and Habit | green prism |
| Crystal System | triclinic |
| Space Group | P -1 |
| Temperature, K | 110 |
| *a*, Å | 7.5931(2) |
| *b*, Å | 11.5663(4) |
| *c*, Å | 11.8080(4) |
| α,° | 100.7173(18) |
| β,° | 91.5492(18) |
| γ,° | 108.8798(18) |
| V, Å$^3$ | 959.87(5) |
| Number of reflections to determine final unit cell | 9901 |
| Min and Max 2θ for cell determination, ° | 5.7, 58.34 |
| Z | 2 |
| F(000) | 552 |
| ρ (*g/cm*) | 1.943 |
| λ, Å, (MoKα) | 0.71073 |
| μ, (*cm$^{-1}$*) | 5.459 |
| Diffractometer Type | Bruker-Nonius X8 Apex2 |
| Scan Type(s) | omega and phi scans |
| Max 2θ for data collection, ° | 58.78 |
| Measured fraction of data | 0.925 |
| Number of reflections measured | 28388 |
| Unique reflections measured | 4910 |
| $R_{merge}$ | 0.0660 |
| Number of reflections included in refinement | 4910 |
| Cut off Threshold Expression | >2sigma(I) |
| Structure refined using | full matrix least-squares using $F^2$ |
| Weighting Scheme | calc w = 1/[sigma$^2$ ($F_O^2$)+(0.0734P)$^2$ +0.5156P], where P = ( $F_O^2$+2 $F_C^2$)/3 |
| Number of parameters in least-squares | 264 |
| $R_1$[a] | 0.0493 |
| $wR_2$[b] | 0.1138 |
| $R_1$ (all data)[a] | 0.1011 |
| $wR_2$ (all data)[b] | 0.1415 |
| GOF[c] | 1.050 |
| Maximum shift/error | 0.000 |
| Min & Max peak heights on final ΔF Map (*e$^-$*/Å) | -0.879, 2.450 |

[a]$R_1 = \Sigma( F_O| - |F_C|) / \Sigma F_O$, [b]$wR_2 = [\Sigma( w(F_O^2 - F_C^2)^2) / \Sigma(w F_O^4)]^{1/2}$, [c]$GOF = [\Sigma( w(F_O^2 - F_C^2)^2)/$ (No. of reflns. - No. of params.)] $^{1/2}$.

**Table S6.** Atomic Coordinates for **ZnC-Br$^{3}$Br$^{13}$.**

| Atom | x | y | z | $U_{iso/equiv}$ |
|---|---|---|---|---|
| Zn1 | 0.67210(8) | 0.45567(5) | 0.06120(5) | 0.02005(17) |
| N1 | 0.7789(6) | 0.5263(4) | 0.2275(4) | 0.0245(10) |
| N2 | 0.8769(6) | 0.5965(4) | 0.0096(4) | 0.0214(10) |
| N3 | 0.5627(6) | 0.3856(4) | -0.1071(4) | 0.0233(10) |
| N4 | 0.4793(6) | 0.3009(4) | 0.1092(4) | 0.0230(10) |
| C1 | 0.7201(7) | 0.4759(5) | 0.3215(5) | 0.0256(12) |
| C2 | 0.8297(8) | 0.5532(5) | 0.4256(5) | 0.0330(14) |
| C3 | 0.9569(7) | 0.6498(5) | 0.3921(5) | 0.0256(12) |
| Br1 | 1.14597(8) | 0.78132(5) | 0.48705(5) | 0.03415(19) |
| C4 | 0.9295(7) | 0.6336(5) | 0.2684(5) | 0.0255(13) |
| C5 | 1.0406(7) | 0.7063(5) | 0.2014(5) | 0.0248(12) |
| C6 | 1.0207(7) | 0.6881(5) | 0.0790(4) | 0.0215(11) |
| C7 | 1.1486(7) | 0.7579(5) | 0.0117(5) | 0.0262(12) |
| C8 | 1.0782(8) | 0.7098(5) | -0.1015(5) | 0.0296(13) |
| C9 | 0.9079(7) | 0.6102(5) | -0.1001(5) | 0.0234(12) |
| C10 | 0.7936(7) | 0.5349(5) | -0.1992(5) | 0.0242(12) |
| C11 | 0.6373(7) | 0.4296(5) | -0.2041(4) | 0.0219(11) |
| C12 | 0.5396(7) | 0.3441(5) | -0.3074(4) | 0.0242(12) |
| C13 | 0.4170(7) | 0.2469(5) | -0.2726(5) | 0.0258(12) |
| Br2 | 0.25817(8) | 0.10159(5) | -0.37071(5) | 0.03035(17) |
| C14 | 0.4308(7) | 0.2707(5) | -0.1487(4) | 0.0236(12) |
| C15 | 0.3305(7) | 0.1894(5) | -0.0830(5) | 0.0235(12) |
| C16 | 0.3513(7) | 0.2029(5) | 0.0359(4) | 0.0215(11) |
| C17 | 0.2349(7) | 0.1112(5) | 0.0995(5) | 0.0275(13) |
| C18 | 0.3338(8) | 0.1520(5) | 0.2242(5) | 0.0314(14) |
| C19 | 0.4699(7) | 0.2803(5) | 0.2185(5) | 0.0232(12) |
| C20 | 0.5763(7) | 0.3607(5) | 0.3144(5) | 0.0240(12) |
| C21 | 0.4486(9) | 0.0688(5) | 0.2440(7) | 0.050(2) |
| C22 | 0.1987(10) | 0.1549(7) | 0.3153(6) | 0.054(2) |
| H2 | 0.8157 | 0.5393 | 0.5022 | 0.040 |
| H5 | 1.1417 | 0.7765 | 0.2411 | 0.030 |
| H7 | 1.2614 | 0.8249 | 0.0395 | 0.031 |
| H8 | 1.1317 | 0.7372 | -0.1677 | 0.035 |
| H10 | 0.8264 | 0.5583 | -0.2708 | 0.029 |
| H12 | 0.5575 | 0.3538 | -0.3848 | 0.029 |
| H15 | 0.2366 | 0.1159 | -0.1241 | 0.028 |
| H17A | 0.2299 | 0.0255 | 0.0641 | 0.033 |
| H17B | 0.1059 | 0.1140 | 0.0996 | 0.033 |
| H20 | 0.5496 | 0.3355 | 0.3860 | 0.029 |
| H21A | 0.5424 | 0.0740 | 0.1880 | 0.076 |
| H21B | 0.3654 | -0.0179 | 0.2340 | 0.076 |
| H21C | 0.5114 | 0.0971 | 0.3228 | 0.076 |
| H22A | 0.2680 | 0.1850 | 0.3922 | 0.081 |
| H22B | 0.1098 | 0.0706 | 0.3103 | 0.081 |
| H22C | 0.1306 | 0.2110 | 0.3025 | 0.081 |

**Table S7.** Anisotropic Displacement Parameters for **ZnC-Br$^{3}$Br$^{13}$.**

| Atom | $u^{11}$ | $u^{22}$ | $u^{33}$ | $u^{12}$ | $u^{13}$ | $u^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.0203(3) | 0.0205(3) | 0.0127(3) | 0.0013(2) | -0.0023(2) | -0.0022(2) |
| N1 | 0.026(2) | 0.023(2) | 0.016(2) | 0.0035(19) | -0.0040(18) | -0.0045(19) |
| N2 | 0.020(2) | 0.020(2) | 0.019(2) | 0.0030(17) | -0.0013(17) | -0.0030(18) |
| N3 | 0.021(2) | 0.021(2) | 0.022(2) | 0.0043(18) | -0.0034(18) | -0.0055(19) |
| N4 | 0.022(2) | 0.021(2) | 0.020(2) | 0.0035(18) | -0.0017(17) | -0.0022(19) |
| C1 | 0.025(3) | 0.025(3) | 0.023(3) | 0.007(2) | -0.001(2) | -0.002(2) |
| C2 | 0.037(3) | 0.036(3) | 0.020(3) | 0.011(3) | -0.002(2) | -0.004(3) |
| C3 | 0.028(3) | 0.025(3) | 0.021(3) | 0.009(2) | -0.006(2) | -0.003(2) |
| Br1 | 0.0320(3) | 0.0344(3) | 0.0244(3) | 0.0070(2) | -0.0099(2) | -0.0134(2) |
| C4 | 0.023(3) | 0.022(3) | 0.025(3) | 0.006(2) | -0.004(2) | -0.008(2) |
| C5 | 0.021(3) | 0.020(3) | 0.030(3) | 0.008(2) | -0.001(2) | -0.005(2) |
| C6 | 0.018(3) | 0.021(3) | 0.021(3) | 0.005(2) | -0.003(2) | -0.003(2) |
| C7 | 0.021(3) | 0.023(3) | 0.030(3) | 0.005(2) | -0.001(2) | -0.001(2) |
| C8 | 0.028(3) | 0.031(3) | 0.029(3) | 0.010(2) | 0.007(2) | 0.006(3) |
| C9 | 0.026(3) | 0.022(3) | 0.020(3) | 0.007(2) | 0.002(2) | 0.001(2) |
| C10 | 0.026(3) | 0.028(3) | 0.018(3) | 0.011(2) | 0.001(2) | 0.000(2) |
| C11 | 0.025(3) | 0.026(3) | 0.015(3) | 0.010(2) | 0.002(2) | 0.004(2) |
| C12 | 0.030(3) | 0.030(3) | 0.011(2) | 0.011(2) | -0.001(2) | -0.002(2) |
| C13 | 0.029(3) | 0.026(3) | 0.017(3) | 0.010(2) | -0.006(2) | -0.007(2) |
| Br2 | 0.0362(3) | 0.0254(3) | 0.0200(3) | 0.0057(2) | -0.0089(2) | -0.0086(2) |
| C14 | 0.025(3) | 0.021(3) | 0.021(3) | 0.008(2) | -0.005(2) | -0.006(2) |
| C15 | 0.021(3) | 0.019(2) | 0.025(3) | 0.002(2) | 0.000(2) | -0.002(2) |
| C16 | 0.021(3) | 0.021(3) | 0.018(3) | 0.004(2) | -0.001(2) | -0.001(2) |
| C17 | 0.024(3) | 0.023(3) | 0.028(3) | 0.000(2) | -0.002(2) | 0.000(2) |
| C18 | 0.033(3) | 0.024(3) | 0.027(3) | -0.002(2) | -0.001(2) | 0.003(3) |
| C19 | 0.024(3) | 0.026(3) | 0.018(3) | 0.007(2) | -0.002(2) | 0.003(2) |
| C20 | 0.031(3) | 0.026(3) | 0.014(3) | 0.009(2) | -0.001(2) | 0.003(2) |
| C21 | 0.047(4) | 0.022(3) | 0.069(5) | -0.005(3) | -0.032(4) | 0.014(3) |
| C22 | 0.059(5) | 0.052(4) | 0.026(4) | -0.013(4) | 0.011(3) | 0.003(3) |

**Table S8.** Bond Lengths for **ZnC-Br$^{3}$Br$^{13}$.**

| Bond | Length in Å | Bond | Length in Å |
|---|---|---|---|
| Zn1-N1 | 2.017(4) | C9-C10 | 1.399(7) |
| Zn1-N3 | 2.043(4) | C10-C11 | 1.389(7) |
| Zn1-N2 | 2.055(4) | C10-H10 | 0.9500 |
| Zn1-N4 | 2.097(4) | C11-C12 | 1.430(7) |
| N1-C1 | 1.368(7) | C12-C13 | 1.347(8) |
| N1-C4 | 1.381(6) | C12-H12 | 0.9500 |
| N2-C9 | 1.352(7) | C13-C14 | 1.431(7) |
| N2-C6 | 1.367(6) | C13-Br2 | 1.874(5) |
| N3-C14 | 1.371(6) | C14-C15 | 1.381(8) |
| N3-C11 | 1.399(7) | C15-C16 | 1.382(7) |
| N4-C19 | 1.355(7) | C15-H15 | 0.9500 |
| N4-C16 | 1.362(6) | C16-C17 | 1.481(8) |
| C1-C20 | 1.409(7) | C17-C18 | 1.551(8) |

| | | | |
|---|---|---|---|
| C1-C2 | 1.434(7) | C17-H17A | 0.9900 |
| C2-C3 | 1.350(8) | C17-H17B | 0.9900 |
| C2-H2 | 0.9500 | C18-C22 | 1.509(9) |
| C3-C4 | 1.439(7) | C18-C19 | 1.523(8) |
| C3-Br1 | 1.870(5) | C18-C21 | 1.536(9) |
| C4-C5 | 1.367(8) | C19-C20 | 1.368(7) |
| C5-C6 | 1.419(8) | C20-H20 | 0.9500 |
| C5-H5 | 0.9500 | C21-H21A | 0.9800 |
| C6-C7 | 1.414(8) | C21-H21B | 0.9800 |
| C7-C8 | 1.369(8) | C21-H21C | 0.9800 |
| C7-H7 | 0.9500 | C22-H22A | 0.9800 |
| C8-C9 | 1.430(7) | C22-H22B | 0.9800 |
| C8-H8 | 0.9500 | C22-H22C | 0.9800 |

**Table S9.** Bond Angles for **ZnC-Br$^{3}$Br$^{13}$.**

| Bond | Angle in ° | Bond | Angle in ° |
|---|---|---|---|
| N1-Zn1-N3 | 179.39(18) | C10-C11-N3 | 124.4(5) |
| N1-Zn1-N2 | 90.20(17) | C10-C11-C12 | 125.6(5) |
| N3-Zn1-N2 | 89.67(17) | N3-C11-C12 | 109.8(5) |
| N1-Zn1-N4 | 90.65(18) | C13-C12-C11 | 106.0(5) |
| N3-Zn1-N4 | 89.54(17) | C13-C12-H12 | 127.0 |
| N2-Zn1-N4 | 174.35(16) | C11-C12-H12 | 127.0 |
| C1-N1-C4 | 106.4(4) | C12-C13-C14 | 109.2(4) |
| C1-N1-Zn1 | 126.9(3) | C12-C13-Br2 | 125.4(4) |
| C4-N1-Zn1 | 126.7(4) | C14-C13-Br2 | 125.4(4) |
| C9-N2-C6 | 106.0(4) | N3-C14-C15 | 126.0(5) |
| C9-N2-Zn1 | 127.2(3) | N3-C14-C13 | 108.7(5) |
| C6-N2-Zn1 | 126.5(4) | C15-C14-C13 | 125.3(5) |
| C14-N3-C11 | 106.1(4) | C14-C15-C16 | 127.4(5) |
| C14-N3-Zn1 | 125.8(4) | C14-C15-H15 | 116.3 |
| C11-N3-Zn1 | 126.4(3) | C16-C15-H15 | 116.3 |
| C19-N4-C16 | 109.4(4) | N4-C16-C15 | 124.9(5) |
| C19-N4-Zn1 | 124.7(3) | N4-C16-C17 | 111.5(4) |
| C16-N4-Zn1 | 125.9(4) | C15-C16-C17 | 123.6(4) |
| N1-C1-C20 | 123.7(5) | C16-C17-C18 | 104.6(4) |
| N1-C1-C2 | 110.8(5) | C16-C17-H17A | 110.8 |
| C20-C1-C2 | 125.4(6) | C18-C17-H17A | 110.8 |
| C3-C2-C1 | 105.7(5) | C16-C17-H17B | 110.8 |
| C3-C2-H2 | 127.2 | C18-C17-H17B | 110.8 |
| C1-C2-H2 | 127.2 | H17A-C17-H17B | 108.9 |
| C2-C3-C4 | 108.8(5) | C22-C18-C19 | 113.8(5) |
| C2-C3-Br1 | 126.8(4) | C22-C18-C21 | 111.0(6) |
| C4-C3-Br1 | 124.3(4) | C19-C18-C21 | 107.9(5) |
| C5-C4-N1 | 125.5(5) | C22-C18-C17 | 112.4(5) |
| C5-C4-C3 | 126.1(5) | C19-C18-C17 | 100.2(5) |
| N1-C4-C3 | 108.2(5) | C21-C18-C17 | 110.9(5) |
| C4-C5-C6 | 126.8(5) | N4-C19-C20 | 125.1(5) |

| | | | |
|---|---|---|---|
| C4-C5-H5 | 116.6 | N4-C19-C18 | 112.6(4) |
| C6-C5-H5 | 116.6 | C20-C19-C18 | 122.2(5) |
| N2-C6-C7 | 110.7(5) | C19-C20-C1 | 128.8(5) |
| N2-C6-C5 | 124.0(5) | C19-C20-H20 | 115.6 |
| C7-C6-C5 | 125.3(5) | C1-C20-H20 | 115.6 |
| C8-C7-C6 | 106.5(5) | C18-C21-H21A | 109.5 |
| C8-C7-H7 | 126.7 | C18-C21-H21B | 109.5 |
| C6-C7-H7 | 126.7 | H21A-C21-H21B | 109.5 |
| C7-C8-C9 | 106.2(5) | C18-C21-H21C | 109.5 |
| C7-C8-H8 | 126.9 | H21A-C21-H21C | 109.5 |
| C9-C8-H8 | 126.9 | H21B-C21-H21C | 109.5 |
| N2-C9-C10 | 125.0(5) | C18-C22-H22A | 109.5 |
| N2-C9-C8 | 110.5(4) | C18-C22-H22B | 109.5 |
| C10-C9-C8 | 124.4(5) | H22A-C22-H22B | 109.5 |
| C11-C10-C9 | 126.9(5) | C18-C22-H22C | 109.5 |
| C11-C10-H10 | 116.5 | H22A-C22-H22C | 109.5 |
| C9-C10-H10 | 116.5 | H22B-C22-H22C | 109.5 |

## 2. X-Ray Structural Data for $H_2C$-$A^{12}Br^{15}$.

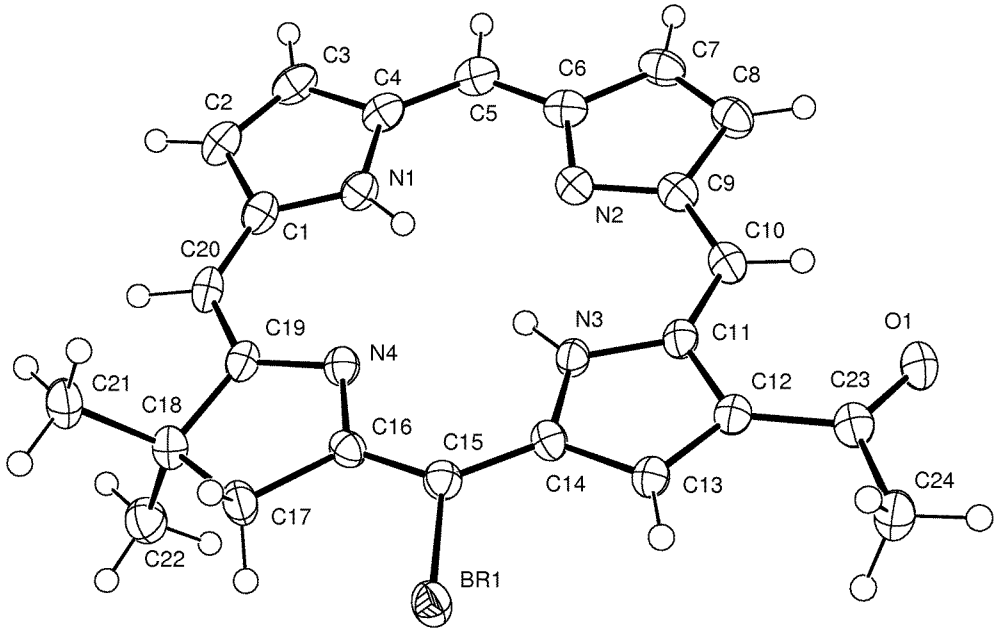



**Figure S2.** ORTEP drawing of $H_2C$-$A^{12}Br^{15}$ showing naming and numbering scheme. Ellipsoids are at the 50% probability level and hydrogen atoms were drawn with arbitrary radii for clarity.

**Table S10.** Summary of Crystal Data for **$H_2C$-$A^{12}Br^{15}$.**

| Entry | Data |
|---|---|
| Formula | $C_{24}H_{21}BrN_4O$ |
| Formula Weight (*g/mol*) | 461.36 |
| Crystal Dimensions (*mm* ) | 0.23 × 0.14 × 0.06 |
| Crystal Color and Habit | purple prism |
| Crystal System | monoclinic |
| Space Group | P $2_1/_C$ |
| Temperature, K | 110 |
| *a*, Å | 13.4761(9) |
| *b*, Å | 11.2751(7) |
| *c*, Å | 14.8026(8) |
| α,° | 90.00 |
| β,° | 116.863(4) |
| γ,° | 90.00 |
| V, $Å^3$ | 2006.5(2) |
| Number of reflections to determine final unit cell | 4644 |
| Min and Max 2θ for cell determination, ° | 4.76, 49.42 |
| Z | 4 |
| F(000) | 944 |
| ρ (*g/cm*) | 1.527 |
| λ, Å, (MoKα) | 0.71070 |
| μ, ($cm^{-1}$) | 2.073 |
| Diffractometer Type | Bruker-Nonius X8 Apex2 |
| Scan Type(s) | phi and omega scans |
| Max 2θ for data collection, ° | 52.06 |
| Measured fraction of data | 0.998 |
| Number of reflections measured | 33210 |
| Unique reflections measured | 3950 |
| $R_{merge}$ | 0.0762 |
| Number of reflections included in refinement | 3950 |
| Cut off Threshold Expression | >2sigma(I) |
| Structure refined using | full matrix least-squares using $F^2$ |
| Weighting Scheme | calc w = 1/[sigma$^2$ ($F_O^2$)+(0.0586P)$^2$ +0.0000P], where P=($F_O^2$+2 $F_C^2$)/3 |
| Number of parameters in least-squares | 274 |
| $R_1$[a] | 0.0384 |
| $wR_2$[b] | 0.0884 |
| $R_1$ (all data)[a] | 0.0607 |
| $wR_2$ (all data)[b] | 0.1057 |
| GOF[c] | 1.057 |
| Maximum shift/error | 0.000 |
| Min & Max peak heights on final ΔF Map ($e^-$/Å) | -0.602, 0.538 |

[a]$R_1 = \Sigma(|F_O| - |F_C|) / \Sigma F_O$, [b]$wR_2 = [\Sigma( w(F_O^2 - F_C^2)^2) / \Sigma(w F_O^4)]^{1/2}$, [c]$GOF = [\Sigma(w(F_O^2 - F_C^2)^2)/$ (No. of reflns. - No. of params.)]$^{1/2}$.

**Table S11.** Atomic Coordinates for $\mathbf{H_2C\text{-}A^{12}Br^{15}}$.

| Atom | x | y | z | $U_{iso/equiv}$ |
|---|---|---|---|---|
| Br1 | 0.22907(3) | 0.23411(3) | 0.16840(2) | 0.02790(13) |
| N1 | 0.2672(2) | -0.2488(2) | 0.47827(19) | 0.0254(6) |
| N2 | 0.4873(2) | -0.2336(2) | 0.49313(19) | 0.0241(6) |
| N3 | 0.4311(2) | -0.0242(2) | 0.36082(17) | 0.0220(6) |
| N4 | 0.2052(2) | -0.0341(2) | 0.34622(17) | 0.0223(6) |
| C1 | 0.1603(3) | -0.2316(3) | 0.4622(2) | 0.0273(7) |
| C2 | 0.1356(3) | -0.3269(3) | 0.5125(2) | 0.0303(8) |
| C3 | 0.2264(3) | -0.3973(3) | 0.5558(2) | 0.0315(8) |
| C4 | 0.3118(3) | -0.3484(3) | 0.5361(2) | 0.0281(8) |
| C5 | 0.4199(3) | -0.3866(3) | 0.5688(2) | 0.0295(8) |
| C6 | 0.5022(3) | -0.3336(3) | 0.5498(2) | 0.0276(7) |
| C7 | 0.6150(3) | -0.3778(3) | 0.5874(2) | 0.0306(8) |
| C8 | 0.6686(3) | -0.3044(3) | 0.5529(2) | 0.0304(8) |
| C9 | 0.5883(3) | -0.2149(3) | 0.4940(2) | 0.0256(7) |
| C10 | 0.6126(3) | -0.1232(3) | 0.4440(2) | 0.0254(7) |
| C11 | 0.5406(3) | -0.0370(3) | 0.3819(2) | 0.0220(7) |
| C12 | 0.5628(3) | 0.0536(3) | 0.3249(2) | 0.0225(7) |
| C13 | 0.4657(2) | 0.1158(3) | 0.2726(2) | 0.0222(7) |
| C14 | 0.3829(2) | 0.0682(3) | 0.2951(2) | 0.0217(7) |
| C15 | 0.2716(3) | 0.1039(3) | 0.2602(2) | 0.0236(7) |
| C16 | 0.1909(3) | 0.0615(3) | 0.2846(2) | 0.0224(7) |
| C17 | 0.0763(3) | 0.1135(3) | 0.2445(2) | 0.0291(8) |
| C18 | 0.0223(3) | 0.0448(3) | 0.2996(2) | 0.0269(7) |
| C19 | 0.1099(3) | -0.0496(3) | 0.3541(2) | 0.0245(7) |
| C20 | 0.0902(3) | -0.1404(3) | 0.4070(2) | 0.0276(8) |
| C21 | -0.0898(3) | -0.0085(3) | 0.2252(2) | 0.0320(8) |
| C22 | 0.0064(3) | 0.1235(3) | 0.3772(3) | 0.0358(8) |
| C23 | 0.6689(3) | 0.0744(3) | 0.3209(2) | 0.0254(7) |
| O1 | 0.75146(18) | 0.0138(2) | 0.36895(16) | 0.0297(5) |
| C24 | 0.6705(3) | 0.1735(3) | 0.2539(2) | 0.0310(8) |
| H1 | 0.3028 | -0.2024 | 0.4548 | 0.030 |
| H3N | 0.3963 | -0.0692 | 0.3860 | 0.026 |
| H2 | 0.0671 | -0.3388 | 0.5151 | 0.036 |
| H3 | 0.2321 | -0.4677 | 0.5932 | 0.038 |
| H5 | 0.4406 | -0.4567 | 0.6086 | 0.035 |
| H7 | 0.6452 | -0.4458 | 0.6288 | 0.037 |
| H8 | 0.7438 | -0.3101 | 0.5646 | 0.036 |
| H10 | 0.6871 | -0.1192 | 0.4536 | 0.030 |
| H13 | 0.4560 | 0.1806 | 0.2283 | 0.027 |
| H17A | 0.0345 | 0.1022 | 0.1704 | 0.035 |
| H17B | 0.0798 | 0.1993 | 0.2599 | 0.035 |
| H20 | 0.0188 | -0.1401 | 0.4051 | 0.033 |
| H21A | -0.0789 | -0.0602 | 0.1772 | 0.048 |
| H21B | -0.1414 | 0.0555 | 0.1882 | 0.048 |
| H21C | -0.1205 | -0.0548 | 0.2627 | 0.048 |
| H22A | -0.0263 | 0.0762 | 0.4125 | 0.054 |

| | | | | |
|---|---|---|---|---|
| H22B | -0.0433 | 0.1896 | 0.3420 | 0.054 |
| H22C | 0.0786 | 0.1546 | 0.4263 | 0.054 |
| H24A | 0.7458 | 0.1820 | 0.2602 | 0.047 |
| H24B | 0.6485 | 0.2476 | 0.2745 | 0.047 |
| H24C | 0.6184 | 0.1557 | 0.1834 | 0.047 |

**Table S12.** Anisotropic Displacement Parameters for **$H_2C$-$A^{12}Br^{15}$.**

| Atom | $u^{11}$ | $u^{22}$ | $u^{33}$ | $u^{12}$ | $u^{13}$ | $u^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.0241(2) | 0.0318(2) | 0.02937(19) | 0.00457(14) | 0.01340(15) | 0.00794(14) |
| N1 | 0.0268(16) | 0.0269(16) | 0.0228(14) | -0.0032(12) | 0.0115(12) | 0.0020(10) |
| N2 | 0.0241(15) | 0.0268(15) | 0.0195(13) | 0.0016(12) | 0.0080(12) | -0.0006(10) |
| N3 | 0.0193(15) | 0.0239(14) | 0.0242(13) | -0.0009(11) | 0.0110(12) | 0.0013(11) |
| N4 | 0.0203(15) | 0.0259(15) | 0.0195(13) | -0.0009(11) | 0.0080(11) | -0.0015(11) |
| C1 | 0.0255(19) | 0.0325(19) | 0.0233(16) | -0.0067(15) | 0.0104(14) | -0.0030(13) |
| C2 | 0.030(2) | 0.034(2) | 0.0248(17) | -0.0099(16) | 0.0104(15) | 0.0004(14) |
| C3 | 0.039(2) | 0.0290(19) | 0.0230(16) | -0.0094(16) | 0.0105(16) | 0.0008(14) |
| C4 | 0.032(2) | 0.0274(19) | 0.0202(16) | -0.0051(15) | 0.0075(15) | 0.0001(13) |
| C5 | 0.034(2) | 0.0268(19) | 0.0209(16) | -0.0008(15) | 0.0063(15) | 0.0018(13) |
| C6 | 0.032(2) | 0.0263(18) | 0.0189(15) | 0.0014(15) | 0.0069(15) | -0.0004(13) |
| C7 | 0.036(2) | 0.0256(19) | 0.0243(17) | 0.0079(16) | 0.0079(16) | 0.0020(13) |
| C8 | 0.027(2) | 0.031(2) | 0.0269(17) | 0.0072(15) | 0.0072(15) | 0.0015(14) |
| C9 | 0.0259(19) | 0.0280(18) | 0.0195(15) | 0.0022(14) | 0.0073(14) | -0.0034(13) |
| C10 | 0.0224(18) | 0.0307(19) | 0.0211(16) | 0.0029(14) | 0.0081(14) | -0.0032(13) |
| C11 | 0.0193(17) | 0.0259(18) | 0.0197(15) | -0.0028(13) | 0.0080(14) | -0.0055(12) |
| C12 | 0.0223(18) | 0.0255(18) | 0.0199(15) | -0.0025(14) | 0.0096(14) | -0.0035(12) |
| C13 | 0.0208(17) | 0.0256(18) | 0.0191(15) | -0.0023(14) | 0.0080(13) | -0.0022(12) |
| C14 | 0.0192(17) | 0.0263(17) | 0.0180(15) | 0.0014(13) | 0.0070(13) | -0.0010(12) |
| C15 | 0.0235(18) | 0.0245(17) | 0.0234(16) | 0.0000(14) | 0.0112(14) | -0.0010(13) |
| C16 | 0.0203(17) | 0.0232(17) | 0.0204(15) | 0.0024(13) | 0.0064(14) | -0.0016(12) |
| C17 | 0.0200(18) | 0.0323(19) | 0.0357(18) | 0.0040(14) | 0.0133(15) | 0.0063(14) |
| C18 | 0.0213(18) | 0.0319(19) | 0.0275(17) | -0.0004(15) | 0.0111(15) | 0.0009(14) |
| C19 | 0.0205(18) | 0.0286(18) | 0.0238(16) | -0.0053(14) | 0.0096(14) | -0.0039(13) |
| C20 | 0.0187(18) | 0.037(2) | 0.0264(17) | -0.0065(15) | 0.0099(14) | -0.0030(14) |
| C21 | 0.0208(19) | 0.040(2) | 0.0318(18) | 0.0012(15) | 0.0091(16) | 0.0044(15) |
| C22 | 0.032(2) | 0.039(2) | 0.0387(19) | 0.0006(17) | 0.0177(17) | -0.0026(16) |
| C23 | 0.0227(19) | 0.0311(19) | 0.0207(16) | -0.0012(15) | 0.0084(14) | -0.0047(13) |
| O1 | 0.0204(13) | 0.0364(14) | 0.0315(12) | 0.0009(11) | 0.0112(11) | -0.0005(10) |
| C24 | 0.0254(19) | 0.037(2) | 0.0325(18) | -0.0010(15) | 0.0144(16) | 0.0032(15) |

**Table S13.** Bond Lengths for **$H_2C$-$A^{12}Br^{15}$.**

| Bond | Length in Å | Bond | Length in Å |
|---|---|---|---|
| Br1-C15 | 1.904(3) | C11-C12 | 1.440(4) |
| N1-C1 | 1.363(4) | C12-C13 | 1.374(4) |
| N1-C4 | 1.375(4) | C12-C23 | 1.477(4) |
| N1-H1 | 0.8800 | C13-C14 | 1.407(4) |
| N2-C6 | 1.365(4) | C13-H13 | 0.9500 |

| | | | |
|---|---|---|---|
| N2-C9 | 1.371(4) | C14-C15 | 1.407(4) |
| N3-C11 | 1.371(4) | C15-C16 | 1.378(4) |
| N3-C14 | 1.372(4) | C16-C17 | 1.500(4) |
| N3-H3N | 0.8800 | C17-C18 | 1.527(4) |
| N4-C19 | 1.353(4) | C17-H17A | 0.9900 |
| N4-C16 | 1.368(4) | C17-H17B | 0.9900 |
| C1-C20 | 1.386(4) | C18-C19 | 1.522(4) |
| C1-C2 | 1.430(4) | C18-C21 | 1.533(4) |
| C2-C3 | 1.352(5) | C18-C22 | 1.540(4) |
| C2-H2 | 0.9500 | C19-C20 | 1.386(4) |
| C3-C4 | 1.422(5) | C20-H20 | 0.9500 |
| C3-H3 | 0.9500 | C21-H21A | 0.9800 |
| C4-C5 | 1.380(4) | C21-H21B | 0.9800 |
| C5-C6 | 1.396(5) | C21-H21C | 0.9800 |
| C5-H5 | 0.9500 | C22-H22A | 0.9800 |
| C6-C7 | 1.450(5) | C22-H22B | 0.9800 |
| C7-C8 | 1.342(5) | C22-H22C | 0.9800 |
| C7-H7 | 0.9500 | C23-O1 | 1.223(4) |
| C8-C9 | 1.448(5) | C23-C24 | 1.500(4) |
| C8-H8 | 0.9500 | C24-H24A | 0.9800 |
| C9-C10 | 1.394(4) | C24-H24B | 0.9800 |
| C10-C11 | 1.387(4) | C24-H24C | 0.9800 |
| C10-H10 | 0.9500 | | |

**Table S14.** Bond Angles for **$H_2C$-A$^{12}$Br$^{15}$**.

| Bond | Angle in ° | Bond | Angle in ° |
|---|---|---|---|
| C1-N1-C4 | 110.8(3) | N3-C14-C13 | 106.7(3) |
| C1-N1-H1 | 124.6 | C15-C14-C13 | 129.1(3) |
| C4-N1-H1 | 124.6 | C16-C15-C14 | 129.9(3) |
| C6-N2-C9 | 104.6(3) | C16-C15-Br1 | 115.8(2) |
| C11-N3-C14 | 110.9(2) | C14-C15-Br1 | 114.2(2) |
| C11-N3-H3N | 124.6 | N4-C16-C15 | 123.9(3) |
| C14-N3-H3N | 124.6 | N4-C16-C17 | 112.5(3) |
| C19-N4-C16 | 107.8(3) | C15-C16-C17 | 123.6(3) |
| N1-C1-C20 | 126.4(3) | C16-C17-C18 | 104.2(3) |
| N1-C1-C2 | 106.2(3) | C16-C17-H17A | 110.9 |
| C20-C1-C2 | 127.4(3) | C18-C17-H17A | 110.9 |
| C3-C2-C1 | 108.3(3) | C16-C17-H17B | 110.9 |
| C3-C2-H2 | 125.8 | C18-C17-H17B | 110.9 |
| C1-C2-H2 | 125.8 | H17A-C17-H17B | 108.9 |
| C2-C3-C4 | 108.5(3) | C19-C18-C17 | 101.2(2) |
| C2-C3-H3 | 125.7 | C19-C18-C21 | 112.5(3) |
| C4-C3-H3 | 125.7 | C17-C18-C21 | 111.6(3) |
| N1-C4-C5 | 124.7(3) | C19-C18-C22 | 110.1(3) |
| N1-C4-C3 | 106.1(3) | C17-C18-C22 | 111.5(3) |
| C5-C4-C3 | 129.1(3) | C21-C18-C22 | 109.7(3) |
| C4-C5-C6 | 127.2(3) | N4-C19-C20 | 125.2(3) |

| | | | |
|---|---|---|---|
| C4-C5-H5 | 116.4 | N4-C19-C18 | 113.8(3) |
| C6-C5-H5 | 116.4 | C20-C19-C18 | 121.0(3) |
| N2-C6-C5 | 124.6(3) | C19-C20-C1 | 128.9(3) |
| N2-C6-C7 | 110.9(3) | C19-C20-H20 | 115.6 |
| C5-C6-C7 | 124.5(3) | C1-C20-H20 | 115.6 |
| C8-C7-C6 | 107.0(3) | C18-C21-H21A | 109.5 |
| C8-C7-H7 | 126.5 | C18-C21-H21B | 109.5 |
| C6-C7-H7 | 126.5 | H21A-C21-H21B | 109.5 |
| C7-C8-C9 | 105.9(3) | C18-C21-H21C | 109.5 |
| C7-C8-H8 | 127.0 | H21A-C21-H21C | 109.5 |
| C9-C8-H8 | 127.0 | H21B-C21-H21C | 109.5 |
| N2-C9-C10 | 125.4(3) | C18-C22-H22A | 109.5 |
| N2-C9-C8 | 111.5(3) | C18-C22-H22B | 109.5 |
| C10-C9-C8 | 123.1(3) | H22A-C22-H22B | 109.5 |
| C11-C10-C9 | 127.6(3) | C18-C22-H22C | 109.5 |
| C11-C10-H10 | 116.2 | H22A-C22-H22C | 109.5 |
| C9-C10-H10 | 116.2 | H22B-C22-H22C | 109.5 |
| N3-C11-C10 | 125.7(3) | O1-C23-C12 | 122.1(3) |
| N3-C11-C12 | 106.2(3) | O1-C23-C24 | 121.3(3) |
| C10-C11-C12 | 128.1(3) | C12-C23-C24 | 116.6(3) |
| C13-C12-C11 | 107.2(3) | C23-C24-H24A | 109.5 |
| C13-C12-C23 | 126.1(3) | C23-C24-H24B | 109.5 |
| C11-C12-C23 | 126.7(3) | H24A-C24-H24B | 109.5 |
| C12-C13-C14 | 109.0(3) | C23-C24-H24C | 109.5 |
| C12-C13-H13 | 125.5 | H24A-C24-H24C | 109.5 |
| C14-C13-H13 | 125.5 | H24B-C24-H24C | 109.5 |
| N3-C14-C15 | 124.2(3) | | |

### 3. X-Ray Structural Data for ZnC-$T^5M^{10}A^{13}$.

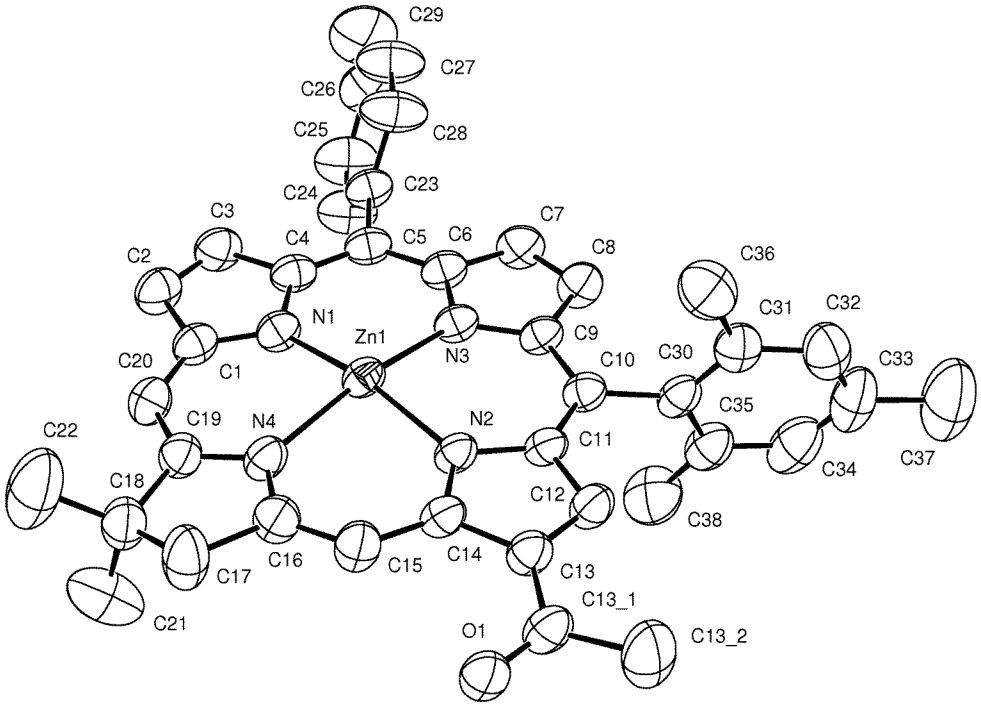



**Figure S3.** ORTEP drawing of **ZnC-$T^5M^{10}A^{13}$** showing naming and numbering scheme. Ellipsoids are at the 50% probability level and hydrogen atoms were omitted for clarity.

**Table S15.** Summary of Crystal Data for **ZnC-T$^{5}$M$^{10}$A$^{13}$.**

| Entry | Data |
|---|---|
| Formula | $C_{40}H_{36}N_4OZn$ |
| Formula Weight (*g/mol*) | 654.12 |
| Crystal Dimensions (*mm* ) | 0.46 × 0.08 × 0.05 |
| Crystal Color and Habit | green prism |
| Crystal System | monoclinic |
| Space Group | $P2_1/c$ |
| Temperature, K | 293 |
| *a*, Å | 13.0276(4) |
| *b*, Å | 29.0931(8) |
| *c*, Å | 12.4038(4) |
| α,° | 90.00 |
| β,° | 100.201(1) |
| γ,° | 90.00 |
| V, Å$^3$ | 4626.9(2) |
| Number of reflections to determine final unit cell | 9583 |
| Min and Max 2θ for cell determination, ° | 4.40, 43.34 |
| Z | 4 |
| F(000) | 1369.94 |
| ρ (*g/cm*) | 0.939 |
| λ, Å, (MoKα) | 0.71073 |
| μ, (*cm*$^{-1}$) | 0.56 |
| Diffractometer Type | Bruker-Nonius X8 Apex2 |
| Scan Type(s) | omega and phi scans |
| Max 2θ for data collection, ° | 50.06 |
| Measured fraction of data | 0.97 |
| Number of reflections measured | 8157 |
| Unique reflections measured | 8157 |
| $R_{merge}$ | 0.000 |
| Number of reflections included in refinement | 6149 |
| Cut off Threshold Expression | $I_{net} > 1.0\text{sigma}(I_{net})$ |
| Structure refined using | full matrix least-squares using F |
| Weighting Scheme | $1/(\text{sigma}^2(F)+0.0005F^2)$ |
| Number of parameters in least-squares | 415 |
| $R_1$[a] | 0.054 |
| $wR_2$[b] | 0.062 |
| $R_1$ (all data)[a] | 0.075 |
| $wR_2$ (all data)[b] | 0.088 |
| GOF[c] | 1.76 |
| Maximum shift/error | 0.000 |
| Min & Max peak heights on final ΔF Map (*e*$^-$/Å) | -0.36, 0.53 |

[a] $R_f = \Sigma(|F_O - F_C|) / \Sigma F_O$, [b] $R_w = [\Sigma(w(F_O - F_C)^2) / \Sigma(F_O^2)]^{1/2}$, [c] $GOF = [\Sigma(w(F_O - F_C)^2) / (\text{No. of reflns.} - \text{No. of params.})]^{1/2}$.

**Table S16.** Atomic Coordinates for **ZnC-T$^{5}$M$^{10}$A$^{13}$.**

| Atom | x | y | z | $U_{iso/equiv}$ |
|---|---|---|---|---|
| Zn1 | 0.18757(3) | 0.163013(11) | 0.71317(3) | 0.0430(2) |
| Zn1 | 0.18757(3) | 0.163013(11) | 0.71317(3) | 0.0430(2) |
| O1 | 0.24388(17) | 0.28785(7) | 1.10654(18) | 0.0567(14) |
| N1 | 0.09264(20) | 0.13052(8) | 0.5870(2) | 0.0466(16) |
| N2 | 0.26267(19) | 0.18405(8) | 0.86489(20) | 0.0426(15) |
| N3 | 0.29191(19) | 0.10933(8) | 0.7175(2) | 0.0427(15) |
| N4 | 0.06287(20) | 0.20763(8) | 0.7301(2) | 0.0479(16) |
| C1 | -0.0026(3) | 0.14592(11) | 0.5370(3) | 0.0489(19) |
| C2 | -0.0375(3) | 0.11868(12) | 0.4389(3) | 0.060(2) |
| C3 | 0.0371(3) | 0.08764(12) | 0.4317(3) | 0.059(2) |
| C4 | 0.1194(3) | 0.09444(11) | 0.5251(3) | 0.0486(19) |
| C5 | 0.2093(3) | 0.06840(10) | 0.5494(3) | 0.0483(19) |
| C6 | 0.2897(2) | 0.07526(10) | 0.6416(3) | 0.0470(19) |
| C7 | 0.3787(3) | 0.04592(10) | 0.6724(3) | 0.056(2) |
| C8 | 0.4340(3) | 0.06242(10) | 0.7665(3) | 0.055(2) |
| C9 | 0.3791(2) | 0.10165(9) | 0.7965(3) | 0.0424(18) |
| C10 | 0.4088(2) | 0.12736(10) | 0.8929(3) | 0.0431(18) |
| C11 | 0.3554(2) | 0.16584(10) | 0.9237(2) | 0.0420(18) |
| C12 | 0.3871(2) | 0.19208(10) | 1.0184(3) | 0.050(2) |
| C13 | 0.3152(2) | 0.22671(10) | 1.0208(3) | 0.0475(19) |
| C13_1 | 0.3155(3) | 0.26104(11) | 1.1067(3) | 0.052(2) |
| C13_2 | 0.4079(3) | 0.26352(16) | 1.1973(4) | 0.102(3) |
| C14 | 0.2376(2) | 0.22067(10) | 0.9228(3) | 0.0449(20) |
| C15 | 0.1477(3) | 0.24773(11) | 0.8930(3) | 0.056(2) |
| C16 | 0.0688(3) | 0.24154(10) | 0.8063(3) | 0.054(2) |
| C17 | -0.0268(3) | 0.27216(13) | 0.7828(3) | 0.080(3) |
| C18 | -0.1011(3) | 0.24627(12) | 0.6965(3) | 0.063(2) |
| C19 | -0.0309(3) | 0.20992(10) | 0.6616(3) | 0.0503(20) |
| C20 | -0.0597(2) | 0.18167(11) | 0.5729(3) | 0.054(2) |
| C21 | -0.1855(4) | 0.22259(18) | 0.7486(5) | 0.117(4) |
| C22 | -0.1554(4) | 0.27623(16) | 0.6043(4) | 0.122(4) |
| C23 | 0.2222(3) | 0.02999(11) | 0.4732(3) | 0.0526(20) |
| C24 | 0.1588(3) | -0.00782(12) | 0.4645(3) | 0.076(3) |
| C25 | 0.1688(4) | -0.04281(13) | 0.3904(4) | 0.086(3) |
| C26 | 0.2426(4) | -0.04106(14) | 0.3245(4) | 0.080(3) |
| C27 | 0.3074(4) | -0.00432(16) | 0.3360(4) | 0.095(3) |
| C28 | 0.2990(3) | 0.03063(14) | 0.4096(4) | 0.083(3) |
| C29 | 0.2520(5) | -0.07843(17) | 0.2422(4) | 0.122(4) |
| C30 | 0.5048(3) | 0.11155(10) | 0.9685(3) | 0.0476(19) |
| C31 | 0.6021(3) | 0.13061(11) | 0.9642(3) | 0.055(2) |
| C32 | 0.6900(3) | 0.11208(14) | 1.0330(4) | 0.073(3) |
| C33 | 0.6831(4) | 0.07640(15) | 1.1026(4) | 0.082(3) |
| C34 | 0.5878(4) | 0.05968(14) | 1.1063(3) | 0.082(3) |
| C35 | 0.4960(3) | 0.07560(11) | 1.0416(3) | 0.061(2) |
| C36 | 0.6136(3) | 0.16957(13) | 0.8886(4) | 0.079(3) |
| C37 | 0.7819(4) | 0.05693(19) | 1.1748(5) | 0.136(4) |

| | | | | |
|---|---|---|---|---|
| C38 | 0.3940(3) | 0.05412(14) | 1.0498(4) | 0.091(3) |
| H2 | -0.100 | 0.122 | 0.390 | 0.0724 |
| H3 | 0.036 | 0.066 | 0.377 | 0.0709 |
| H7 | 0.395 | 0.020 | 0.634 | 0.0669 |
| H8 | 0.496 | 0.051 | 0.805 | 0.0657 |
| H12 | 0.446 | 0.187 | 1.071 | 0.0605 |
| H13_2a | 0.398 | 0.288 | 1.247 | 0.1222 |
| H13_2b | 0.469 | 0.270 | 1.166 | 0.1222 |
| H13_2c | 0.416 | 0.235 | 1.236 | 0.1222 |
| H15 | 0.141 | 0.273 | 0.938 | 0.0674 |
| H17a | -0.009 | 0.302 | 0.755 | 0.0956 |
| H17b | -0.057 | 0.277 | 0.848 | 0.0956 |
| H20 | -0.126 | 0.187 | 0.532 | 0.0651 |
| H21a | -0.230 | 0.245 | 0.771 | 0.1396 |
| H21b | -0.153 | 0.205 | 0.811 | 0.1396 |
| H21c | -0.226 | 0.202 | 0.696 | 0.1396 |
| H22a | -0.197 | 0.299 | 0.633 | 0.1458 |
| H22b | -0.199 | 0.257 | 0.551 | 0.1458 |
| H22c | -0.104 | 0.292 | 0.570 | 0.1458 |
| H24 | 0.109 | -0.010 | 0.509 | 0.0907 |
| H25 | 0.125 | -0.068 | 0.386 | 0.1035 |
| H27 | 0.359 | -0.003 | 0.294 | 0.1135 |
| H28 | 0.346 | 0.055 | 0.417 | 0.1008 |
| H29a | 0.199 | -0.101 | 0.244 | 0.1475 |
| H29b | 0.320 | -0.093 | 0.260 | 0.1475 |
| H29c | 0.244 | -0.065 | 0.170 | 0.1475 |
| H32 | 0.755 | 0.125 | 1.031 | 0.0874 |
| H34 | 0.582 | 0.036 | 1.155 | 0.0988 |
| H36a | 0.686 | 0.179 | 0.898 | 0.0957 |
| H36b | 0.573 | 0.195 | 0.905 | 0.0957 |
| H36c | 0.590 | 0.160 | 0.814 | 0.0957 |
| H37a | 0.842 | 0.073 | 1.160 | 0.1635 |
| H37b | 0.789 | 0.025 | 1.159 | 0.1635 |
| H37c | 0.777 | 0.061 | 1.251 | 0.1635 |
| H38a | 0.405 | 0.030 | 1.105 | 0.1091 |
| H38b | 0.365 | 0.041 | 0.980 | 0.1091 |
| H38c | 0.347 | 0.077 | 1.070 | 0.1091 |

**Table S17.** Anisotropic Displacement Parameters for **ZnC-T$^{5}$M$^{10}$A$^{13}$.**

| Atom | $u^{11}$ | $u^{22}$ | $u^{33}$ | $u^{12}$ | $u^{13}$ | $u^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.0542(3) | 0.0387(2) | 0.0352(2) | -0.00024(17) | 0.00567(17) | -0.00281(16) |
| Zn1 | 0.0542(3) | 0.0387(2) | 0.0352(2) | -0.00024(17) | 0.00567(17) | -0.00281(16) |
| O1 | 0.0685(16) | 0.0522(14) | 0.0470(16) | 0.0152(12) | 0.0036(12) | -0.0116(11) |
| N1 | 0.0546(17) | 0.0436(15) | 0.0411(17) | -0.0036(13) | 0.0069(13) | -0.0059(13) |
| N2 | 0.0555(17) | 0.0378(14) | 0.0336(16) | 0.0072(12) | 0.0057(13) | -0.0023(12) |
| N3 | 0.0556(16) | 0.0359(14) | 0.0373(17) | -0.0033(12) | 0.0099(13) | -0.0063(12) |
| N4 | 0.0575(17) | 0.0459(15) | 0.0379(17) | 0.0032(12) | 0.0019(14) | -0.0039(13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C1 | 0.055(2) | 0.0497(18) | 0.041(2) | -0.0088(17) | 0.0053(17) | -0.0058(16) |
| C2 | 0.061(2) | 0.068(2) | 0.049(2) | -0.0117(20) | 0.0002(18) | -0.0097(18) |
| C3 | 0.065(2) | 0.063(2) | 0.048(2) | -0.0070(19) | 0.0076(19) | -0.0154(18) |
| C4 | 0.056(2) | 0.0500(20) | 0.041(2) | -0.0109(17) | 0.0126(17) | -0.0076(16) |
| C5 | 0.062(2) | 0.0425(18) | 0.043(2) | -0.0066(16) | 0.0162(17) | -0.0053(15) |
| C6 | 0.061(2) | 0.0398(18) | 0.042(2) | -0.0031(16) | 0.0130(17) | -0.0042(15) |
| C7 | 0.071(2) | 0.0444(19) | 0.054(2) | 0.0066(17) | 0.0146(19) | -0.0126(17) |
| C8 | 0.067(2) | 0.0448(19) | 0.051(2) | 0.0082(17) | 0.0064(18) | -0.0053(17) |
| C9 | 0.056(2) | 0.0352(17) | 0.036(2) | 0.0025(14) | 0.0096(16) | -0.0011(14) |
| C10 | 0.0517(19) | 0.0396(17) | 0.039(2) | 0.0014(15) | 0.0104(16) | 0.0047(15) |
| C11 | 0.0529(19) | 0.0409(17) | 0.0327(19) | 0.0036(15) | 0.0091(15) | -0.0018(15) |
| C12 | 0.058(2) | 0.0520(20) | 0.037(2) | 0.0052(17) | 0.0023(16) | -0.0034(16) |
| C13 | 0.057(2) | 0.0434(18) | 0.041(2) | 0.0061(15) | 0.0058(16) | -0.0037(15) |
| C13_1 | 0.063(2) | 0.051(2) | 0.040(2) | -0.0014(18) | 0.0032(17) | -0.0081(17) |
| C13_2 | 0.090(3) | 0.123(4) | 0.080(3) | 0.036(3) | -0.020(3) | -0.053(3) |
| C14 | 0.058(2) | 0.0418(18) | 0.0351(20) | 0.0026(16) | 0.0075(16) | -0.0014(15) |
| C15 | 0.066(2) | 0.0491(19) | 0.049(2) | 0.0147(17) | -0.0016(19) | -0.0146(16) |
| C16 | 0.063(2) | 0.0458(19) | 0.052(2) | 0.0118(16) | 0.0072(18) | -0.0060(17) |
| C17 | 0.081(3) | 0.075(3) | 0.075(3) | 0.030(2) | -0.015(2) | -0.021(2) |
| C18 | 0.065(2) | 0.063(2) | 0.055(3) | 0.0152(19) | -0.0009(19) | -0.0054(19) |
| C19 | 0.054(2) | 0.0499(20) | 0.046(2) | 0.0040(16) | 0.0058(17) | 0.0031(17) |
| C20 | 0.055(2) | 0.056(2) | 0.048(2) | -0.0035(17) | -0.0007(17) | -0.0020(18) |
| C21 | 0.107(4) | 0.119(4) | 0.138(5) | 0.001(3) | 0.059(4) | -0.028(3) |
| C22 | 0.163(5) | 0.096(3) | 0.090(4) | 0.055(3) | -0.027(3) | -0.011(3) |
| C23 | 0.068(2) | 0.0472(19) | 0.044(2) | -0.0069(17) | 0.0123(18) | -0.0125(16) |
| C24 | 0.096(3) | 0.060(2) | 0.077(3) | -0.021(2) | 0.035(2) | -0.018(2) |
| C25 | 0.117(4) | 0.059(2) | 0.090(4) | -0.026(2) | 0.036(3) | -0.031(2) |
| C26 | 0.108(3) | 0.064(3) | 0.069(3) | -0.001(2) | 0.014(3) | -0.020(2) |
| C27 | 0.127(4) | 0.086(3) | 0.085(4) | -0.003(3) | 0.057(3) | -0.028(3) |
| C28 | 0.107(3) | 0.073(3) | 0.084(3) | -0.026(2) | 0.052(3) | -0.030(2) |
| C29 | 0.164(5) | 0.103(4) | 0.105(4) | 0.012(3) | 0.036(4) | -0.058(3) |
| C30 | 0.063(2) | 0.0421(18) | 0.036(2) | 0.0096(16) | 0.0033(17) | -0.0052(15) |
| C31 | 0.060(2) | 0.049(2) | 0.054(2) | 0.0023(17) | 0.0045(19) | -0.0115(17) |
| C32 | 0.060(2) | 0.078(3) | 0.076(3) | 0.007(2) | -0.002(2) | -0.028(2) |
| C33 | 0.089(3) | 0.073(3) | 0.073(3) | 0.023(3) | -0.021(3) | -0.009(2) |
| C34 | 0.113(4) | 0.069(3) | 0.059(3) | 0.018(3) | 0.000(3) | 0.008(2) |
| C35 | 0.079(3) | 0.052(2) | 0.050(2) | 0.0121(19) | 0.006(2) | 0.0026(18) |
| C36 | 0.071(3) | 0.077(3) | 0.091(3) | -0.013(2) | 0.017(2) | -0.001(2) |
| C37 | 0.124(4) | 0.141(5) | 0.122(5) | 0.049(4) | -0.037(4) | -0.014(4) |
| C38 | 0.103(3) | 0.082(3) | 0.089(4) | -0.005(3) | 0.018(3) | 0.031(3) |

**Table S18.** Bond Lengths for **ZnC-T$^{5}$M$^{10}$A$^{13}$.**

| Bond | Length in Å | Bond | Length in Å |
|---|---|---|---|
| Zn1-O1 | 2.162(2) | C12-C13 | 1.379(4) |
| Zn1-N1 | 2.046(2) | C13-C13_1 | 1.460(4) |
| Zn1-N2 | 2.055(2) | C13-C14 | 1.448(4) |
| Zn1-N3 | 2.065(2) | C13_1-C13_2 | 1.496(5) |

| | | | |
|---|---|---|---|
| Zn1-N4 | 2.119(3) | C14-C15 | 1.405(4) |
| O1-Zn1 | 2.162(2) | C15-C16 | 1.362(5) |
| O1-C13_1 | 1.216(4) | C16-C17 | 1.516(5) |
| N1-C1 | 1.361(4) | C17-C18 | 1.511(5) |
| N1-C4 | 1.381(4) | C18-C19 | 1.511(5) |
| N2-C11 | 1.400(4) | C18-C21 | 1.534(6) |
| N2-C14 | 1.356(4) | C18-C22 | 1.511(6) |
| N3-C6 | 1.364(4) | C19-C20 | 1.371(5) |
| N3-C9 | 1.380(4) | C23-C24 | 1.368(5) |
| N4-C16 | 1.359(4) | C23-C28 | 1.381(5) |
| N4-C19 | 1.361(4) | C24-C25 | 1.392(5) |
| C1-C2 | 1.456(5) | C25-C26 | 1.369(7) |
| C1-C20 | 1.397(5) | C26-C27 | 1.354(6) |
| C2-C3 | 1.341(5) | C26-C29 | 1.512(6) |
| C3-C4 | 1.446(5) | C27-C28 | 1.383(6) |
| C4-C5 | 1.383(5) | C30-C31 | 1.393(5) |
| C5-C6 | 1.421(5) | C30-C35 | 1.403(5) |
| C5-C23 | 1.493(4) | C31-C32 | 1.408(5) |
| C6-C7 | 1.436(5) | C31-C36 | 1.496(5) |
| C7-C8 | 1.347(5) | C32-C33 | 1.363(7) |
| C8-C9 | 1.430(4) | C33-C34 | 1.342(8) |
| C9-C10 | 1.406(4) | C33-C37 | 1.539(6) |
| C10-C11 | 1.406(4) | C34-C35 | 1.396(6) |
| C10-C30 | 1.497(4) | C35-C38 | 1.487(6) |
| C11-C12 | 1.401(4) | | |

**Table S19.** Bond Angles for **ZnC-T$^{5}$M$^{10}$A$^{13}$.**

| Bond | Angle in ° | Bond | Angle in ° |
|---|---|---|---|
| O1-Zn1-N1 | 93.57(9) | C12-C13-C13_1 | 127.0(3) |
| O1-Zn1-N2 | 101.84(9) | C12-C13-C14 | 105.6(3) |
| O1-Zn1-N3 | 102.89(9) | C13_1-C13-C14 | 127.4(3) |
| O1-Zn1-N4 | 90.27(9) | O1-C13_1-C13 | 122.4(3) |
| N1-Zn1-N2 | 164.46(10) | O1-C13_1-C13_2 | 119.0(3) |
| N1-Zn1-N3 | 88.65(10) | C13-C13_1-C13_2 | 118.6(3) |
| N1-Zn1-N4 | 89.35(10) | N2-C14-C13 | 110.0(3) |
| N2-Zn1-N3 | 89.82(9) | N2-C14-C15 | 124.6(3) |
| N2-Zn1-N4 | 88.61(10) | C13-C14-C15 | 125.3(3) |
| N3-Zn1-N4 | 166.79(10) | C14-C15-C16 | 127.7(3) |
| Zn1-O1-C13_1 | 140.0(2) | N4-C16-C15 | 125.9(3) |
| Zn1-N1-C1 | 125.1(2) | N4-C16-C17 | 110.5(3) |
| Zn1-N1-C4 | 126.8(2) | C15-C16-C17 | 123.6(3) |
| C1-N1-C4 | 107.2(3) | C16-C17-C18 | 104.2(3) |
| Zn1-N2-C11 | 126.27(19) | C17-C18-C19 | 102.0(3) |
| Zn1-N2-C14 | 126.76(20) | C17-C18-C21 | 110.0(4) |
| C11-N2-C14 | 106.7(2) | C17-C18-C22 | 113.8(3) |
| Zn1-N3-C6 | 126.7(2) | C19-C18-C21 | 108.8(3) |
| Zn1-N3-C9 | 126.60(19) | C19-C18-C22 | 114.4(3) |

| | | | |
|---|---|---|---|
| C6-N3-C9 | 106.6(2) | C21-C18-C22 | 107.7(4) |
| Zn1-N4-C16 | 124.3(2) | N4-C19-C18 | 112.2(3) |
| Zn1-N4-C19 | 126.0(2) | N4-C19-C20 | 124.0(3) |
| C16-N4-C19 | 109.4(3) | C18-C19-C20 | 123.8(3) |
| N1-C1-C2 | 109.0(3) | C1-C20-C19 | 128.1(3) |
| N1-C1-C20 | 126.5(3) | C5-C23-C24 | 121.2(3) |
| C2-C1-C20 | 124.5(3) | C5-C23-C28 | 121.8(3) |
| C1-C2-C3 | 107.4(3) | C24-C23-C28 | 117.0(3) |
| C2-C3-C4 | 107.3(3) | C23-C24-C25 | 121.0(4) |
| N1-C4-C3 | 109.0(3) | C24-C25-C26 | 121.6(4) |
| N1-C4-C5 | 125.6(3) | C25-C26-C27 | 117.2(4) |
| C3-C4-C5 | 125.4(3) | C25-C26-C29 | 121.8(4) |
| C4-C5-C6 | 125.0(3) | C27-C26-C29 | 121.0(4) |
| C4-C5-C23 | 117.3(3) | C26-C27-C28 | 121.9(4) |
| C6-C5-C23 | 117.7(3) | C23-C28-C27 | 121.1(4) |
| N3-C6-C5 | 125.4(3) | C10-C30-C31 | 121.3(3) |
| N3-C6-C7 | 109.3(3) | C10-C30-C35 | 118.6(3) |
| C5-C6-C7 | 125.2(3) | C31-C30-C35 | 120.0(3) |
| C6-C7-C8 | 107.5(3) | C30-C31-C32 | 118.2(3) |
| C7-C8-C9 | 107.1(3) | C30-C31-C36 | 121.2(3) |
| N3-C9-C8 | 109.3(3) | C32-C31-C36 | 120.6(3) |
| N3-C9-C10 | 125.8(3) | C31-C32-C33 | 122.5(4) |
| C8-C9-C10 | 124.8(3) | C32-C33-C34 | 117.6(4) |
| C9-C10-C11 | 125.5(3) | C32-C33-C37 | 120.4(5) |
| C9-C10-C30 | 116.3(3) | C34-C33-C37 | 122.0(5) |
| C11-C10-C30 | 118.2(3) | C33-C34-C35 | 124.3(4) |
| N2-C11-C10 | 125.6(3) | C30-C35-C34 | 117.3(4) |
| N2-C11-C12 | 109.3(2) | C30-C35-C38 | 122.3(3) |
| C10-C11-C12 | 125.1(3) | C34-C35-C38 | 120.4(4) |
| C11-C12-C13 | 108.4(3) | | |

## 4. X-Ray Structural Data for $H_2OP\text{-}T^5M^{10}$.

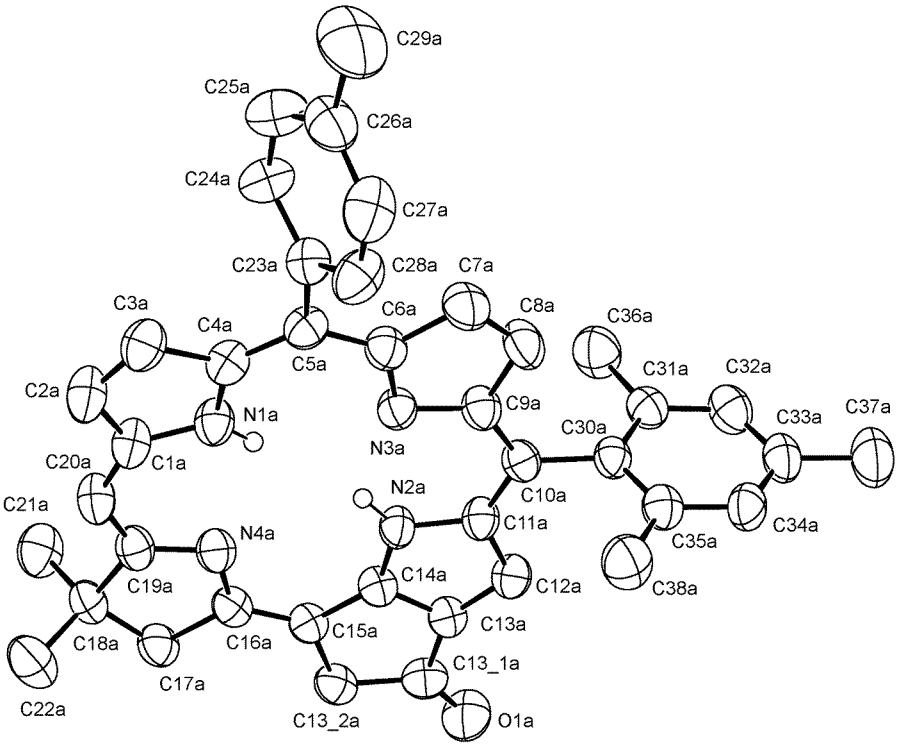



**Figure S4.** ORTEP drawing of $H_2OP\text{-}T^5M^{10}$ showing naming and numbering scheme. Ellipsoids are at the 50% probability level and hydrogen atoms were omitted for clarity.

During the intermediate cycles of refinement, the orientation of the methyl groups were allowed to refine. Although data was collected to 52.7° (2θ), examination of the coverage statistics showed that there was almost no observed data above 1.0 Å resolution. Therefore, the data used in the refinement was cut at $\sin(\theta)/\lambda = 0.5$ Å$^{-1}$ to cut out the weak data of poor precision.

**Table S20.** Summary of Crystal Data for **$H_2$OP-$T^5M^{10}$.**

| Entry | Data |
|---|---|
| Formula | $C_{40}H_{36}N_4O$ |
| Formula Weight (*g/mol*) | 588.74 |
| Crystal Dimensions (*mm* ) | 0.34 × 0.06 × 0.03 |
| Crystal Color and Habit | dark red plate |
| Crystal System | triclinic |
| Space Group | P -1 |
| Temperature, K | 293 |
| *a*, Å | 7.8310(3) |
| *b*, Å | 16.8429(7) |
| *c*, Å | 25.4999(10) |
| α,° | 105.8794(17) |
| β,° | 91.7001(17) |
| γ,° | 97.8616(16) |
| V, $Å^3$ | 3196.6(2) |
| Number of reflections to determine final unit cell | 8522 |
| Min and Max 2θ for cell determination, ° | 4.72, 47.54 |
| Z | 4 |
| F(000) | 1248.67 |
| ρ (*g/cm*) | 1.223 |
| λ, Å, (MoKα) | 0.71073 |
| μ, ($cm^{-1}$) | 0.07 |
| Diffractometer Type | Bruker-Nonius X8 Apex2 |
| Scan Type(s) | omega and phi scans |
| Max 2θ for data collection, ° | 52.72 |
| Measured fraction of data | 0.99 |
| Number of reflections measured | 102043 |
| Unique reflections measured | 12918 |
| $R_{merge}$ | 0.036 |
| Number of reflections included in refinement | 5363 |
| Cut off Threshold Expression | $I_{net} > 1.0 sigma(I_{net})$ |
| Structure refined using | full matrix least-squares using F |
| Weighting Scheme | $1/(sigma^2(F)+0.0005F^2)$ |
| Number of parameters in least-squares | 811 |
| $R_1$[a] | 0.062 |
| $wR_2$[b] | 0.073 |
| $R_1$ (all data)[a] | 0.086 |
| $wR_2$ (all data)[b] | 0.074 |
| GOF[c] | 2.23 |
| Maximum shift/error | 0.000 |
| Min & Max peak heights on final ΔF Map ($e^-$/Å) | -0.22, 1.47 |

[a] $R_f = \Sigma(|F_O - F_C|) / \Sigma F_O$, [b] $R_w = [\Sigma(w(F_O - F_C)^2) / \Sigma(F_O^2)]^{1/2}$, [c] $GOF = [\Sigma(w(F_O - F_C)^2) / (\text{No. of reflns.} - \text{No. of params.})]^{1/2}$.

**Table S21.** Atomic Coordinates for **$H_2$OP-$T^5M^{10}$.**

| Atom | x | y | z | $U_{iso/equiv}$ |
|---|---|---|---|---|
| O1a | 0.3649(4) | 0.93205(20) | 0.42524(13) | 0.077(2) |
| N1a | -0.5438(4) | 0.7836(2) | 0.55777(14) | 0.049(2) |
| N2a | -0.1936(4) | 0.83176(20) | 0.45193(13) | 0.046(2) |
| N3a | -0.5254(4) | 0.74392(19) | 0.43918(13) | 0.045(2) |
| N4a | -0.1857(4) | 0.87848(19) | 0.57480(14) | 0.048(2) |
| C1a | -0.5148(6) | 0.8081(3) | 0.61336(19) | 0.053(3) |
| C2a | -0.6646(6) | 0.7718(3) | 0.63333(18) | 0.062(3) |
| C3a | -0.7762(6) | 0.7273(3) | 0.59092(19) | 0.057(3) |
| C4a | -0.7016(5) | 0.7331(2) | 0.54134(18) | 0.045(3) |
| C5a | -0.7701(5) | 0.6962(2) | 0.48824(18) | 0.046(3) |
| C6a | -0.6884(5) | 0.7039(3) | 0.44021(18) | 0.048(3) |
| C7a | -0.7688(6) | 0.6691(3) | 0.38548(19) | 0.062(3) |
| C8a | -0.6522(6) | 0.6870(3) | 0.35178(17) | 0.061(3) |
| C9a | -0.4993(5) | 0.7327(2) | 0.38465(17) | 0.047(3) |
| C10a | -0.3462(5) | 0.7584(2) | 0.36313(16) | 0.044(3) |
| C11a | -0.1986(5) | 0.8038(2) | 0.39530(17) | 0.044(3) |
| C12a | -0.0326(6) | 0.8287(2) | 0.38018(17) | 0.049(3) |
| C13a | 0.0679(5) | 0.8715(2) | 0.42768(18) | 0.045(3) |
| C13_1a | 0.2410(6) | 0.9166(3) | 0.45010(19) | 0.054(3) |
| C13_2a | 0.2340(5) | 0.9426(2) | 0.51228(18) | 0.053(3) |
| C14a | -0.0349(5) | 0.8719(2) | 0.47156(17) | 0.043(3) |
| C15a | 0.0502(5) | 0.9110(2) | 0.52301(18) | 0.043(3) |
| C16a | -0.0204(6) | 0.9157(2) | 0.57218(18) | 0.046(3) |
| C17a | 0.0692(5) | 0.9575(3) | 0.62768(17) | 0.054(3) |
| C18a | -0.0717(5) | 0.9460(3) | 0.66738(17) | 0.050(3) |
| C19a | -0.2181(6) | 0.8913(2) | 0.62749(18) | 0.048(3) |
| C20a | -0.3707(6) | 0.8581(3) | 0.64460(17) | 0.056(3) |
| C21a | -0.1304(6) | 1.0280(3) | 0.69730(19) | 0.069(3) |
| C22a | -0.0122(7) | 0.9028(3) | 0.70857(20) | 0.079(4) |
| C23a | -0.9428(6) | 0.6431(3) | 0.47920(17) | 0.047(3) |
| C24a | -1.0913(6) | 0.6751(3) | 0.49655(19) | 0.057(3) |
| C25a | -1.2510(6) | 0.6268(3) | 0.4828(2) | 0.069(4) |
| C26a | -1.2702(6) | 0.5448(3) | 0.4513(2) | 0.066(4) |
| C27a | -1.1211(7) | 0.5118(3) | 0.43713(19) | 0.070(3) |
| C28a | -0.9613(6) | 0.5593(3) | 0.45018(19) | 0.063(3) |
| C29a | -1.4468(7) | 0.4941(4) | 0.4315(2) | 0.110(5) |
| C30a | -0.3327(5) | 0.7342(3) | 0.30238(17) | 0.044(3) |
| C31a | -0.3735(5) | 0.7870(3) | 0.27158(19) | 0.050(3) |
| C32a | -0.3520(6) | 0.7634(3) | 0.2160(2) | 0.060(3) |
| C33a | -0.2923(6) | 0.6905(3) | 0.18981(18) | 0.057(3) |
| C34a | -0.2548(5) | 0.6402(3) | 0.22140(20) | 0.056(3) |
| C35a | -0.2759(5) | 0.6593(3) | 0.27711(18) | 0.050(3) |
| C36a | -0.4448(7) | 0.8665(3) | 0.29713(20) | 0.076(4) |
| C37a | -0.2732(7) | 0.6661(3) | 0.12939(19) | 0.083(4) |
| C38a | -0.2389(6) | 0.5982(3) | 0.30860(20) | 0.074(4) |
| H1na | -0.473 | 0.798 | 0.536 | 0.0582 |

| | | | | |
|---|---|---|---|---|
| H2na | -0.279 | 0.825 | 0.471 | 0.0541 |
| H2a | -0.683 | 0.778 | 0.671 | 0.0699 |
| H3a | -0.887 | 0.697 | 0.594 | 0.0666 |
| H7a | -0.884 | 0.639 | 0.375 | 0.0698 |
| H8a | -0.668 | 0.672 | 0.313 | 0.0676 |
| H12a | 0.004 | 0.818 | 0.344 | 0.0595 |
| H13_2aa | 0.259 | 1.002 | 0.526 | 0.0612 |
| H13_2ab | 0.316 | 0.918 | 0.529 | 0.0612 |
| H17aa | 0.167 | 0.931 | 0.634 | 0.0613 |
| H17ab | 0.107 | 1.016 | 0.632 | 0.0613 |
| H20a | -0.378 | 0.871 | 0.683 | 0.0644 |
| H21aa | -0.173(3) | 1.0533(8) | 0.6711(3) | 0.0744 |
| H21ab | -0.0345(11) | 1.0650(6) | 0.7193(8) | 0.0744 |
| H21ac | -0.220(2) | 1.0174(4) | 0.7203(8) | 0.0744 |
| H22aa | 0.019(3) | 0.8498(8) | 0.6894(3) | 0.0903 |
| H22ab | -0.1040(14) | 0.8943(15) | 0.7315(7) | 0.0903 |
| H22ac | 0.086(2) | 0.9370(9) | 0.7307(7) | 0.0903 |
| H24a | -1.083 | 0.732 | 0.519 | 0.0670 |
| H25a | -1.352 | 0.651 | 0.495 | 0.0807 |
| H27a | -1.129 | 0.454 | 0.417 | 0.0756 |
| H28a | -0.861 | 0.534 | 0.439 | 0.0707 |
| H29aa | -1.4508(16) | 0.4401(7) | 0.4375(12) | 0.1130 |
| H29ab | -1.4677(19) | 0.4877(17) | 0.3931(4) | 0.1130 |
| H29ac | -1.5338(7) | 0.5223(11) | 0.4512(10) | 0.1130 |
| H32a | -0.381 | 0.799 | 0.195 | 0.0707 |
| H34a | -0.212 | 0.589 | 0.204 | 0.0625 |
| H36aa | -0.393(3) | 0.8911(9) | 0.3336(4) | 0.0864 |
| H36ab | -0.5677(7) | 0.8540(5) | 0.2983(10) | 0.0864 |
| H36ac | -0.419(3) | 0.9050(7) | 0.2758(6) | 0.0864 |
| H37aa | -0.1676(18) | 0.6434(15) | 0.1220(3) | 0.0896 |
| H37ab | -0.271(3) | 0.7144(6) | 0.1163(3) | 0.0896 |
| H37ac | -0.3692(19) | 0.6249(13) | 0.1113(2) | 0.0896 |
| H38aa | -0.175(3) | 0.6280(5) | 0.3426(5) | 0.0852 |
| H38ab | -0.173(3) | 0.5585(10) | 0.2874(5) | 0.0852 |
| H38ac | -0.3462(8) | 0.5693(11) | 0.3158(9) | 0.0852 |
| O1b | 0.5064(4) | 0.2701(2) | 0.00963(15) | 0.090(3) |
| N1b | 1.3487(4) | 0.1366(2) | 0.15483(14) | 0.048(2) |
| N2b | 1.0365(4) | 0.2667(2) | 0.09187(13) | 0.048(2) |
| N3b | 1.3606(4) | 0.30638(19) | 0.14502(13) | 0.043(2) |
| N4b | 0.9982(4) | 0.0871(2) | 0.09675(14) | 0.050(2) |
| C1b | 1.3057(6) | 0.0557(3) | 0.15671(18) | 0.050(3) |
| C2b | 1.4408(6) | 0.0416(3) | 0.18935(19) | 0.055(3) |
| C3b | 1.5579(5) | 0.1117(3) | 0.20653(18) | 0.052(3) |
| C4b | 1.5024(5) | 0.1741(3) | 0.18518(16) | 0.043(3) |
| C5b | 1.5846(5) | 0.2552(2) | 0.19187(16) | 0.042(3) |
| C6b | 1.5208(5) | 0.3155(2) | 0.17027(16) | 0.044(3) |
| C7b | 1.6161(5) | 0.3971(3) | 0.17382(18) | 0.051(3) |
| C8b | 1.5105(5) | 0.4378(3) | 0.15268(18) | 0.053(3) |

| | | | | |
|---|---|---|---|---|
| C9b | 1.3510(5) | 0.3825(3) | 0.13495(16) | 0.045(3) |
| C10b | 1.2054(5) | 0.4053(2) | 0.11266(16) | 0.043(3) |
| C11b | 1.0542(5) | 0.3501(3) | 0.09168(16) | 0.044(3) |
| C12b | 0.8984(5) | 0.3623(3) | 0.06835(17) | 0.050(3) |
| C13b | 0.7909(5) | 0.2867(3) | 0.05456(17) | 0.050(3) |
| C13_1b | 0.6204(6) | 0.2437(3) | 0.03011(19) | 0.062(3) |
| C13_2b | 0.6101(6) | 0.1529(3) | 0.03340(18) | 0.063(3) |
| C14b | 0.8776(5) | 0.2290(3) | 0.07012(16) | 0.045(3) |
| C15b | 0.7824(5) | 0.1490(3) | 0.05967(17) | 0.051(3) |
| C16b | 0.8377(6) | 0.0820(3) | 0.07197(17) | 0.052(3) |
| C17b | 0.7367(6) | -0.0042(3) | 0.06163(19) | 0.068(3) |
| C18b | 0.8559(5) | -0.0532(3) | 0.08411(17) | 0.052(3) |
| C19b | 1.0145(6) | 0.0136(3) | 0.10512(17) | 0.050(3) |
| C20b | 1.1578(6) | -0.0004(2) | 0.13236(19) | 0.056(3) |
| C21b | 0.9002(7) | -0.1269(3) | 0.0400(2) | 0.087(4) |
| C22b | 0.7794(6) | -0.0832(3) | 0.1311(2) | 0.079(4) |
| C23b | 1.7548(5) | 0.2822(2) | 0.22449(17) | 0.042(3) |
| C24b | 1.8948(6) | 0.2408(3) | 0.20942(17) | 0.048(3) |
| C25b | 2.0530(6) | 0.2698(3) | 0.2386(2) | 0.061(4) |
| C26b | 2.0781(6) | 0.3400(3) | 0.2830(2) | 0.064(3) |
| C27b | 1.9382(7) | 0.3800(3) | 0.29825(18) | 0.063(3) |
| C28b | 1.7794(5) | 0.3523(3) | 0.27001(18) | 0.052(3) |
| C29b | 2.2533(7) | 0.3720(4) | 0.3136(3) | 0.113(5) |
| C30b | 1.2109(5) | 0.4949(3) | 0.11311(18) | 0.044(3) |
| C31b | 1.2403(5) | 0.5198(3) | 0.06601(19) | 0.055(3) |
| C32b | 1.2485(6) | 0.6040(4) | 0.0693(2) | 0.072(4) |
| C33b | 1.2274(6) | 0.6625(3) | 0.1170(3) | 0.074(4) |
| C34b | 1.1981(6) | 0.6368(3) | 0.1630(2) | 0.070(4) |
| C35b | 1.1885(5) | 0.5527(3) | 0.16211(19) | 0.054(3) |
| C36b | 1.2639(7) | 0.4593(3) | 0.0128(2) | 0.082(4) |
| C37b | 1.2378(8) | 0.7542(3) | 0.1200(3) | 0.122(6) |
| C38b | 1.1583(6) | 0.5273(3) | 0.2138(2) | 0.077(4) |
| H1nb | 1.288 | 0.161 | 0.137 | 0.0582 |
| H2nb | 1.114 | 0.243 | 0.104 | 0.0580 |
| H2b | 1.449 | -0.010 | 0.198 | 0.0680 |
| H3b | 1.661 | 0.118 | 0.230 | 0.0627 |
| H7b | 1.733 | 0.418 | 0.189 | 0.0597 |
| H8b | 1.537 | 0.494 | 0.150 | 0.0632 |
| H12b | 0.872 | 0.414 | 0.063 | 0.0613 |
| H13_2ba | 0.591 | 0.114 | -0.002 | 0.0713 |
| H13_2bb | 0.518 | 0.141 | 0.055 | 0.0713 |
| H17ba | 0.632 | -0.002 | 0.080 | 0.0736 |
| H17bb | 0.709 | -0.029 | 0.023 | 0.0736 |
| H20b | 1.155 | -0.056 | 0.135 | 0.0649 |
| H21ba | 0.944(3) | -0.1080(5) | 0.0100(5) | 0.0893 |
| H21bb | 0.7984(11) | -0.1674(8) | 0.0274(8) | 0.0893 |
| H21bc | 0.987(3) | -0.1517(11) | 0.0547(4) | 0.0893 |
| H22ba | 0.761(3) | -0.0358(4) | 0.1603(5) | 0.0890 |

| | | | | |
|---|---|---|---|---|
| H22bb | 0.8578(17) | -0.1137(14) | 0.1442(7) | 0.0890 |
| H22bc | 0.6711(17) | -0.1187(14) | 0.1184(4) | 0.0890 |
| H24b | 1.882 | 0.192 | 0.179 | 0.0581 |
| H25b | 2.149 | 0.241 | 0.228 | 0.0735 |
| H27b | 1.952 | 0.429 | 0.329 | 0.0688 |
| H28b | 1.684 | 0.381 | 0.282 | 0.0610 |
| H29ba | 2.2392(11) | 0.3880(19) | 0.3522(2) | 0.1176 |
| H29bb | 2.3070(18) | 0.4196(12) | 0.3031(10) | 0.1176 |
| H29bc | 2.3249(15) | 0.3289(8) | 0.3052(10) | 0.1176 |
| H32b | 1.269 | 0.622 | 0.037 | 0.0847 |
| H34b | 1.184 | 0.678 | 0.197 | 0.0761 |
| H36ba | 1.329(3) | 0.4183(10) | 0.0193(3) | 0.0938 |
| H36bb | 1.325(3) | 0.4884(5) | -0.0102(5) | 0.0938 |
| H36bc | 1.1530(8) | 0.4321(13) | -0.0048(6) | 0.0938 |
| H37ba | 1.206(4) | 0.7840(5) | 0.1553(6) | 0.1337 |
| H37bb | 1.160(3) | 0.7605(5) | 0.0921(9) | 0.1337 |
| H37bc | 1.3536(14) | 0.7763(6) | 0.1148(15) | 0.1337 |
| H38ba | 1.079(3) | 0.4761(9) | 0.2055(3) | 0.0858 |
| H38bb | 1.111(3) | 0.5702(8) | 0.2396(4) | 0.0858 |
| H38bc | 1.2661(9) | 0.5195(15) | 0.2291(6) | 0.0858 |

**Table S22.** Anisotropic Displacement Parameters for **$H_2$OP-$T^5M^{10}$.**

| Atom | $u^{11}$ | $u^{22}$ | $u^{33}$ | $u^{12}$ | $u^{13}$ | $u^{23}$ |
|---|---|---|---|---|---|---|
| O1a | 0.052(2) | 0.091(3) | 0.077(2) | -0.0128(18) | 0.0110(18) | 0.0175(20) |
| N1a | 0.051(2) | 0.051(2) | 0.044(3) | -0.0022(19) | 0.0085(18) | 0.0127(19) |
| N2a | 0.044(2) | 0.052(2) | 0.036(2) | -0.0013(18) | 0.0055(17) | 0.0090(18) |
| N3a | 0.041(2) | 0.051(2) | 0.041(2) | 0.0004(18) | 0.0041(17) | 0.0119(18) |
| N4a | 0.053(3) | 0.043(2) | 0.044(3) | 0.0025(19) | 0.0018(18) | 0.0091(18) |
| C1a | 0.061(3) | 0.051(3) | 0.043(3) | 0.003(3) | 0.012(3) | 0.009(2) |
| C2a | 0.071(3) | 0.064(3) | 0.044(3) | 0.001(3) | 0.015(3) | 0.010(3) |
| C3a | 0.060(3) | 0.054(3) | 0.056(3) | 0.002(2) | 0.016(3) | 0.017(3) |
| C4a | 0.046(3) | 0.038(3) | 0.050(3) | 0.001(2) | 0.008(2) | 0.011(2) |
| C5a | 0.043(3) | 0.043(3) | 0.051(3) | 0.004(2) | 0.006(2) | 0.011(2) |
| C6a | 0.046(3) | 0.049(3) | 0.046(3) | 0.001(2) | 0.001(2) | 0.010(2) |
| C7a | 0.044(3) | 0.079(3) | 0.056(3) | -0.009(2) | -0.002(3) | 0.017(3) |
| C8a | 0.054(3) | 0.077(3) | 0.042(3) | -0.008(3) | -0.006(3) | 0.012(3) |
| C9a | 0.049(3) | 0.046(3) | 0.042(3) | -0.001(2) | 0.001(2) | 0.010(2) |
| C10a | 0.049(3) | 0.041(3) | 0.041(3) | 0.003(2) | 0.000(2) | 0.011(2) |
| C11a | 0.049(3) | 0.044(3) | 0.039(3) | 0.000(2) | 0.007(2) | 0.012(2) |
| C12a | 0.054(3) | 0.047(3) | 0.048(3) | 0.003(2) | 0.009(2) | 0.016(2) |
| C13a | 0.048(3) | 0.038(3) | 0.045(3) | 0.002(2) | 0.001(3) | 0.010(2) |
| C13_1a | 0.046(3) | 0.050(3) | 0.066(4) | 0.001(2) | 0.004(3) | 0.018(3) |
| C13_2a | 0.054(3) | 0.045(3) | 0.055(3) | 0.005(2) | -0.005(2) | 0.009(2) |
| C14a | 0.042(3) | 0.038(3) | 0.045(3) | -0.003(2) | 0.000(3) | 0.011(2) |
| C15a | 0.042(3) | 0.037(3) | 0.046(3) | -0.002(2) | -0.001(2) | 0.009(2) |
| C16a | 0.052(3) | 0.036(3) | 0.046(3) | 0.005(2) | -0.004(2) | 0.007(2) |
| C17a | 0.055(3) | 0.051(3) | 0.048(3) | 0.004(2) | -0.006(2) | 0.005(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C18a | 0.058(3) | 0.050(3) | 0.040(3) | 0.005(2) | -0.005(2) | 0.010(2) |
| C19a | 0.058(3) | 0.042(3) | 0.041(3) | 0.005(2) | 0.000(2) | 0.008(2) |
| C20a | 0.068(3) | 0.058(3) | 0.038(3) | 0.003(3) | 0.004(3) | 0.007(2) |
| C21a | 0.078(3) | 0.054(3) | 0.060(3) | -0.002(3) | 0.004(3) | 0.000(3) |
| C22a | 0.092(4) | 0.086(4) | 0.063(3) | 0.016(3) | -0.011(3) | 0.028(3) |
| C23a | 0.050(3) | 0.043(3) | 0.048(3) | 0.002(2) | 0.005(2) | 0.016(2) |
| C24a | 0.046(3) | 0.047(3) | 0.078(3) | 0.009(3) | 0.010(3) | 0.018(2) |
| C25a | 0.050(3) | 0.068(4) | 0.094(4) | 0.011(3) | 0.009(3) | 0.031(3) |
| C26a | 0.055(4) | 0.081(4) | 0.060(3) | -0.013(3) | -0.002(3) | 0.028(3) |
| C27a | 0.081(4) | 0.050(3) | 0.066(4) | -0.012(3) | 0.011(3) | 0.003(3) |
| C28a | 0.063(3) | 0.050(3) | 0.069(3) | 0.004(3) | 0.016(3) | 0.006(3) |
| C29a | 0.078(4) | 0.129(5) | 0.100(5) | -0.042(4) | -0.014(3) | 0.027(4) |
| C30a | 0.043(3) | 0.047(3) | 0.039(3) | -0.001(2) | 0.002(2) | 0.007(3) |
| C31a | 0.050(3) | 0.053(3) | 0.048(3) | 0.004(2) | 0.001(2) | 0.018(3) |
| C32a | 0.065(3) | 0.066(4) | 0.052(4) | -0.001(3) | 0.002(3) | 0.025(3) |
| C33a | 0.053(3) | 0.072(4) | 0.040(3) | -0.008(3) | 0.004(2) | 0.012(3) |
| C34a | 0.056(3) | 0.057(3) | 0.044(3) | 0.001(2) | 0.002(2) | -0.001(3) |
| C35a | 0.050(3) | 0.047(3) | 0.047(3) | -0.002(2) | 0.001(2) | 0.010(3) |
| C36a | 0.094(4) | 0.069(3) | 0.067(4) | 0.023(3) | 0.000(3) | 0.019(3) |
| C37a | 0.087(4) | 0.104(4) | 0.049(4) | 0.001(3) | 0.008(3) | 0.012(3) |
| C38a | 0.091(4) | 0.061(3) | 0.069(4) | 0.018(3) | 0.003(3) | 0.015(3) |
| O1b | 0.054(2) | 0.108(3) | 0.111(3) | -0.005(2) | -0.028(2) | 0.049(2) |
| N1b | 0.046(2) | 0.042(2) | 0.057(2) | 0.0045(18) | -0.0038(19) | 0.0174(19) |
| N2b | 0.043(2) | 0.046(2) | 0.055(2) | 0.0007(19) | -0.0097(18) | 0.0164(19) |
| N3b | 0.042(2) | 0.037(2) | 0.049(2) | 0.0028(17) | -0.0042(18) | 0.0152(17) |
| N4b | 0.053(3) | 0.039(2) | 0.052(2) | -0.0036(19) | 0.0026(20) | 0.0089(19) |
| C1b | 0.054(3) | 0.035(3) | 0.062(3) | 0.008(3) | 0.012(3) | 0.012(2) |
| C2b | 0.054(3) | 0.049(3) | 0.071(3) | 0.017(3) | 0.009(3) | 0.028(3) |
| C3b | 0.049(3) | 0.050(3) | 0.059(3) | 0.008(3) | 0.004(2) | 0.018(3) |
| C4b | 0.044(3) | 0.041(3) | 0.046(3) | 0.009(2) | 0.003(2) | 0.015(2) |
| C5b | 0.041(3) | 0.042(3) | 0.042(3) | 0.011(2) | 0.001(2) | 0.010(2) |
| C6b | 0.039(3) | 0.044(3) | 0.047(3) | 0.002(2) | -0.003(2) | 0.011(2) |
| C7b | 0.037(3) | 0.045(3) | 0.068(3) | -0.004(2) | -0.007(2) | 0.017(2) |
| C8b | 0.046(3) | 0.044(3) | 0.069(3) | -0.001(2) | -0.005(2) | 0.022(2) |
| C9b | 0.040(3) | 0.044(3) | 0.047(3) | -0.001(2) | -0.004(2) | 0.010(2) |
| C10b | 0.043(3) | 0.041(3) | 0.042(3) | 0.000(2) | -0.001(2) | 0.012(2) |
| C11b | 0.049(3) | 0.041(3) | 0.042(3) | 0.004(2) | -0.005(2) | 0.012(2) |
| C12b | 0.044(3) | 0.058(3) | 0.052(3) | 0.009(2) | -0.007(2) | 0.021(2) |
| C13b | 0.041(3) | 0.058(3) | 0.048(3) | -0.002(3) | -0.006(2) | 0.017(2) |
| C13_1b | 0.046(3) | 0.080(4) | 0.060(3) | -0.001(3) | -0.009(3) | 0.024(3) |
| C13_2b | 0.052(3) | 0.076(4) | 0.056(3) | -0.011(3) | -0.010(2) | 0.019(3) |
| C14b | 0.040(3) | 0.050(3) | 0.041(3) | -0.004(3) | -0.007(2) | 0.010(2) |
| C15b | 0.046(3) | 0.054(3) | 0.048(3) | -0.003(3) | -0.004(2) | 0.012(2) |
| C16b | 0.044(3) | 0.053(3) | 0.048(3) | -0.014(3) | -0.003(2) | 0.004(2) |
| C17b | 0.067(3) | 0.055(3) | 0.069(3) | -0.016(3) | -0.004(3) | 0.010(3) |
| C18b | 0.055(3) | 0.041(3) | 0.053(3) | -0.003(2) | 0.006(2) | 0.006(2) |
| C19b | 0.054(3) | 0.038(3) | 0.051(3) | -0.006(2) | 0.007(2) | 0.004(2) |
| C20b | 0.063(3) | 0.034(3) | 0.068(3) | 0.000(3) | 0.007(3) | 0.011(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C21b | 0.091(4) | 0.066(3) | 0.081(4) | -0.007(3) | 0.013(3) | -0.009(3) |
| C22b | 0.064(3) | 0.085(4) | 0.088(4) | -0.004(3) | 0.018(3) | 0.032(3) |
| C23b | 0.042(3) | 0.043(3) | 0.044(3) | 0.008(2) | 0.003(2) | 0.016(2) |
| C24b | 0.044(3) | 0.052(3) | 0.048(3) | 0.010(2) | -0.001(2) | 0.016(2) |
| C25b | 0.044(3) | 0.075(4) | 0.071(4) | 0.015(3) | 0.011(3) | 0.032(3) |
| C26b | 0.049(3) | 0.076(4) | 0.062(4) | -0.003(3) | -0.011(3) | 0.021(3) |
| C27b | 0.061(3) | 0.065(3) | 0.051(3) | -0.004(3) | -0.009(3) | 0.005(3) |
| C28b | 0.053(3) | 0.050(3) | 0.050(3) | 0.010(2) | 0.004(2) | 0.009(3) |
| C29b | 0.068(4) | 0.144(6) | 0.111(5) | -0.003(4) | -0.037(4) | 0.026(4) |
| C30b | 0.041(3) | 0.041(3) | 0.049(3) | 0.000(2) | -0.010(2) | 0.012(3) |
| C31b | 0.053(3) | 0.056(3) | 0.059(4) | -0.001(2) | -0.008(2) | 0.024(3) |
| C32b | 0.068(4) | 0.071(4) | 0.086(4) | 0.000(3) | -0.014(3) | 0.044(4) |
| C33b | 0.069(4) | 0.050(4) | 0.111(5) | 0.005(3) | -0.018(3) | 0.039(4) |
| C34b | 0.066(3) | 0.047(4) | 0.085(4) | 0.008(3) | -0.008(3) | 0.003(3) |
| C35b | 0.052(3) | 0.046(3) | 0.060(4) | 0.005(2) | -0.009(2) | 0.012(3) |
| C36b | 0.094(4) | 0.096(4) | 0.059(4) | -0.001(3) | 0.008(3) | 0.032(3) |
| C37b | 0.124(5) | 0.064(4) | 0.187(7) | 0.007(4) | -0.024(5) | 0.055(4) |
| C38b | 0.088(4) | 0.070(3) | 0.066(4) | 0.013(3) | 0.002(3) | 0.009(3) |

**Table S23.** Bond Lengths for **$H_2$OP-$T^5M^{10}$.**

| Bond | Length in Å | Bond | Length in Å |
|---|---|---|---|
| O1a-C13_1a | 1.212(6) | O1b-C13_1b | 1.215(7) |
| N1a-C1a | 1.366(6) | N1b-C1b | 1.372(5) |
| N1a-C4a | 1.383(5) | N1b-C4b | 1.385(5) |
| N2a-C11a | 1.388(5) | N2b-C11b | 1.393(5) |
| N2a-C14a | 1.341(5) | N2b-C14b | 1.345(5) |
| N3a-C6a | 1.364(5) | N3b-C6b | 1.362(5) |
| N3a-C9a | 1.376(5) | N3b-C9b | 1.386(5) |
| N4a-C16a | 1.371(6) | N4b-C16b | 1.372(6) |
| N4a-C19a | 1.339(6) | N4b-C19b | 1.334(6) |
| C1a-C2a | 1.421(6) | C1b-C2b | 1.412(7) |
| C1a-C20a | 1.391(6) | C1b-C20b | 1.399(6) |
| C2a-C3a | 1.348(7) | C2b-C3b | 1.351(6) |
| C3a-C4a | 1.430(6) | C3b-C4b | 1.419(6) |
| C4a-C5a | 1.383(6) | C4b-C5b | 1.390(6) |
| C5a-C6a | 1.427(6) | C5b-C6b | 1.419(6) |
| C5a-C23a | 1.490(6) | C5b-C23b | 1.496(6) |
| C6a-C7a | 1.445(6) | C6b-C7b | 1.451(5) |
| C7a-C8a | 1.333(7) | C7b-C8b | 1.333(7) |
| C8a-C9a | 1.436(6) | C8b-C9b | 1.432(6) |
| C9a-C10a | 1.398(6) | C9b-C10b | 1.405(6) |
| C10a-C11a | 1.398(6) | C10b-C11b | 1.394(6) |
| C10a-C30a | 1.501(6) | C10b-C30b | 1.500(6) |
| C11a-C12a | 1.408(6) | C11b-C12b | 1.406(6) |
| C12a-C13a | 1.385(6) | C12b-C13b | 1.377(6) |
| C13a-C13_1a | 1.475(6) | C13b-C13_1b | 1.461(6) |
| C13a-C14a | 1.397(6) | C13b-C14b | 1.392(7) |

| | | | |
|---|---|---|---|
| C13_1a-C13_2a | 1.530(6) | C13_1b-C13_2b | 1.546(7) |
| C13_2a-C15a | 1.524(6) | C13_2b-C15b | 1.506(6) |
| C14a-C15a | 1.398(6) | C14b-C15b | 1.400(6) |
| C15a-C16a | 1.372(6) | C15b-C16b | 1.371(7) |
| C16a-C17a | 1.501(6) | C16b-C17b | 1.506(6) |
| C17a-C18a | 1.548(6) | C17b-C18b | 1.522(7) |
| C18a-C19a | 1.526(6) | C18b-C19b | 1.531(6) |
| C18a-C21a | 1.523(6) | C18b-C21b | 1.518(6) |
| C18a-C22a | 1.527(6) | C18b-C22b | 1.530(6) |
| C19a-C20a | 1.383(6) | C19b-C20b | 1.383(7) |
| C23a-C24a | 1.382(6) | C23b-C24b | 1.386(6) |
| C23a-C28a | 1.388(6) | C23b-C28b | 1.397(6) |
| C24a-C25a | 1.374(7) | C24b-C25b | 1.382(7) |
| C25a-C26a | 1.380(8) | C25b-C26b | 1.380(8) |
| C26a-C27a | 1.377(8) | C26b-C27b | 1.375(8) |
| C26a-C29a | 1.516(7) | C26b-C29b | 1.513(7) |
| C27a-C28a | 1.369(7) | C27b-C28b | 1.374(7) |
| C30a-C31a | 1.398(6) | C30b-C31b | 1.392(6) |
| C30a-C35a | 1.390(6) | C30b-C35b | 1.390(7) |
| C31a-C32a | 1.385(7) | C31b-C32b | 1.391(7) |
| C31a-C36a | 1.510(7) | C31b-C36b | 1.491(7) |
| C32a-C33a | 1.379(8) | C32b-C33b | 1.370(10) |
| C33a-C34a | 1.372(8) | C33b-C34b | 1.372(9) |
| C33a-C37a | 1.500(6) | C33b-C37b | 1.516(7) |
| C34a-C35a | 1.388(7) | C34b-C35b | 1.403(7) |
| C35a-C38a | 1.519(7) | C35b-C38b | 1.507(7) |

**Table S24.** Bond Angles for **$H_2$OP-T$^5$M$^{10}$.**

| Bond | Angle in ° | Bond | Angle in ° |
|---|---|---|---|
| C1a-N1a-C4a | 111.6(3) | C1b-N1b-C4b | 111.3(3) |
| C11a-N2a-C14a | 109.5(3) | C11b-N2b-C14b | 108.5(3) |
| C6a-N3a-C9a | 105.2(3) | C6b-N3b-C9b | 104.9(3) |
| C16a-N4a-C19a | 108.4(3) | C16b-N4b-C19b | 109.1(3) |
| N1a-C1a-C2a | 105.4(4) | N1b-C1b-C2b | 105.4(4) |
| N1a-C1a-C20a | 128.1(4) | N1b-C1b-C20b | 127.3(4) |
| C2a-C1a-C20a | 126.5(4) | C2b-C1b-C20b | 127.2(4) |
| C1a-C2a-C3a | 109.5(4) | C1b-C2b-C3b | 109.5(4) |
| C2a-C3a-C4a | 108.4(4) | C2b-C3b-C4b | 108.7(4) |
| N1a-C4a-C3a | 105.1(4) | N1b-C4b-C3b | 105.2(3) |
| N1a-C4a-C5a | 126.9(4) | N1b-C4b-C5b | 126.7(4) |
| C3a-C4a-C5a | 128.0(4) | C3b-C4b-C5b | 128.1(4) |
| C4a-C5a-C6a | 125.4(4) | C4b-C5b-C6b | 125.5(4) |
| C4a-C5a-C23a | 118.6(4) | C4b-C5b-C23b | 118.0(4) |
| C6a-C5a-C23a | 116.0(4) | C6b-C5b-C23b | 116.5(3) |
| N3a-C6a-C5a | 125.4(4) | N3b-C6b-C5b | 125.3(3) |
| N3a-C6a-C7a | 110.7(4) | N3b-C6b-C7b | 110.4(4) |
| C5a-C6a-C7a | 123.9(4) | C5b-C6b-C7b | 124.3(4) |

| | | | |
|---|---|---|---|
| C6a-C7a-C8a | 106.5(4) | C6b-C7b-C8b | 106.9(4) |
| C7a-C8a-C9a | 107.6(4) | C7b-C8b-C9b | 107.3(4) |
| N3a-C9a-C8a | 110.0(4) | N3b-C9b-C8b | 110.4(4) |
| N3a-C9a-C10a | 126.1(4) | N3b-C9b-C10b | 126.0(3) |
| C8a-C9a-C10a | 123.8(4) | C8b-C9b-C10b | 123.5(4) |
| C9a-C10a-C11a | 123.6(4) | C9b-C10b-C11b | 123.7(4) |
| C9a-C10a-C30a | 119.7(4) | C9b-C10b-C30b | 118.1(3) |
| C11a-C10a-C30a | 116.7(3) | C11b-C10b-C30b | 118.2(4) |
| N2a-C11a-C10a | 122.9(4) | N2b-C11b-C10b | 121.6(4) |
| N2a-C11a-C12a | 106.8(3) | N2b-C11b-C12b | 107.3(3) |
| C10a-C11a-C12a | 130.3(4) | C10b-C11b-C12b | 131.1(4) |
| C11a-C12a-C13a | 107.4(4) | C11b-C12b-C13b | 107.1(4) |
| C12a-C13a-C13_1a | 144.6(4) | C12b-C13b-C13_1b | 144.2(5) |
| C12a-C13a-C14a | 107.6(4) | C12b-C13b-C14b | 108.0(4) |
| C13_1a-C13a-C14a | 107.8(4) | C13_1b-C13b-C14b | 107.7(4) |
| O1a-C13_1a-C13a | 128.0(4) | O1b-C13_1b-C13b | 129.3(5) |
| O1a-C13_1a-C13_2a | 125.8(4) | O1b-C13_1b-C13_2b | 124.4(4) |
| C13a-C13_1a-C13_2a | 106.2(4) | C13b-C13_1b-C13_2b | 106.3(4) |
| C13_1a-C13_2a-C15a | 105.6(3) | C13_1b-C13_2b-C15b | 105.2(4) |
| N2a-C14a-C13a | 108.7(4) | N2b-C14b-C13b | 108.9(4) |
| N2a-C14a-C15a | 136.7(4) | N2b-C14b-C15b | 136.4(4) |
| C13a-C14a-C15a | 114.6(4) | C13b-C14b-C15b | 114.7(4) |
| C13_2a-C15a-C14a | 105.8(4) | C13_2b-C15b-C14b | 106.2(4) |
| C13_2a-C15a-C16a | 128.7(4) | C13_2b-C15b-C16b | 128.0(4) |
| C14a-C15a-C16a | 125.5(4) | C14b-C15b-C16b | 125.8(4) |
| N4a-C16a-C15a | 121.4(4) | N4b-C16b-C15b | 122.2(4) |
| N4a-C16a-C17a | 112.5(4) | N4b-C16b-C17b | 111.1(4) |
| C15a-C16a-C17a | 126.1(4) | C15b-C16b-C17b | 126.6(4) |
| C16a-C17a-C18a | 103.7(3) | C16b-C17b-C18b | 105.0(4) |
| C17a-C18a-C19a | 100.9(3) | C17b-C18b-C19b | 101.0(3) |
| C17a-C18a-C21a | 112.5(3) | C17b-C18b-C21b | 112.0(4) |
| C17a-C18a-C22a | 111.6(4) | C17b-C18b-C22b | 111.9(4) |
| C19a-C18a-C21a | 109.4(4) | C19b-C18b-C21b | 111.4(4) |
| C19a-C18a-C22a | 112.1(4) | C19b-C18b-C22b | 110.5(4) |
| C21a-C18a-C22a | 110.0(4) | C21b-C18b-C22b | 109.8(4) |
| N4a-C19a-C18a | 114.2(4) | N4b-C19b-C18b | 113.8(4) |
| N4a-C19a-C20a | 123.2(4) | N4b-C19b-C20b | 123.5(4) |
| C18a-C19a-C20a | 122.6(4) | C18b-C19b-C20b | 122.7(4) |
| C1a-C20a-C19a | 129.1(4) | C1b-C20b-C19b | 128.9(4) |
| C5a-C23a-C24a | 122.3(4) | C5b-C23b-C24b | 121.3(4) |
| C5a-C23a-C28a | 120.5(4) | C5b-C23b-C28b | 120.7(4) |
| C24a-C23a-C28a | 117.2(4) | C24b-C23b-C28b | 117.9(4) |
| C23a-C24a-C25a | 121.0(4) | C23b-C24b-C25b | 120.0(4) |
| C24a-C25a-C26a | 121.7(4) | C24b-C25b-C26b | 122.1(4) |
| C25a-C26a-C27a | 116.9(4) | C25b-C26b-C27b | 117.6(4) |
| C25a-C26a-C29a | 121.7(5) | C25b-C26b-C29b | 121.3(5) |
| C27a-C26a-C29a | 121.3(5) | C27b-C26b-C29b | 121.0(5) |
| C26a-C27a-C28a | 121.9(4) | C26b-C27b-C28b | 121.4(4) |

| | | | |
|---|---|---|---|
| C23a-C28a-C27a | 121.1(4) | C23b-C28b-C27b | 120.9(4) |
| C10a-C30a-C31a | 120.5(4) | C10b-C30b-C31b | 121.0(4) |
| C10a-C30a-C35a | 119.3(4) | C10b-C30b-C35b | 118.2(4) |
| C31a-C30a-C35a | 120.2(4) | C31b-C30b-C35b | 120.8(4) |
| C30a-C31a-C32a | 118.3(4) | C30b-C31b-C32b | 118.4(4) |
| C30a-C31a-C36a | 121.6(4) | C30b-C31b-C36b | 122.0(4) |
| C32a-C31a-C36a | 120.0(4) | C32b-C31b-C36b | 119.6(4) |
| C31a-C32a-C33a | 123.0(4) | C31b-C32b-C33b | 122.2(5) |
| C32a-C33a-C34a | 116.8(4) | C32b-C33b-C34b | 118.7(4) |
| C32a-C33a-C37a | 121.7(5) | C32b-C33b-C37b | 121.7(6) |
| C34a-C33a-C37a | 121.4(5) | C34b-C33b-C37b | 119.7(6) |
| C33a-C34a-C35a | 123.2(4) | C33b-C34b-C35b | 121.7(5) |
| C30a-C35a-C34a | 118.4(4) | C30b-C35b-C34b | 118.3(4) |
| C30a-C35a-C38a | 121.8(4) | C30b-C35b-C38b | 121.8(4) |
| C34a-C35a-C38a | 119.8(4) | C34b-C35b-C38b | 119.9(4) |

## 5. X-Ray Structural Data for ZnC-M[10]Br[13].

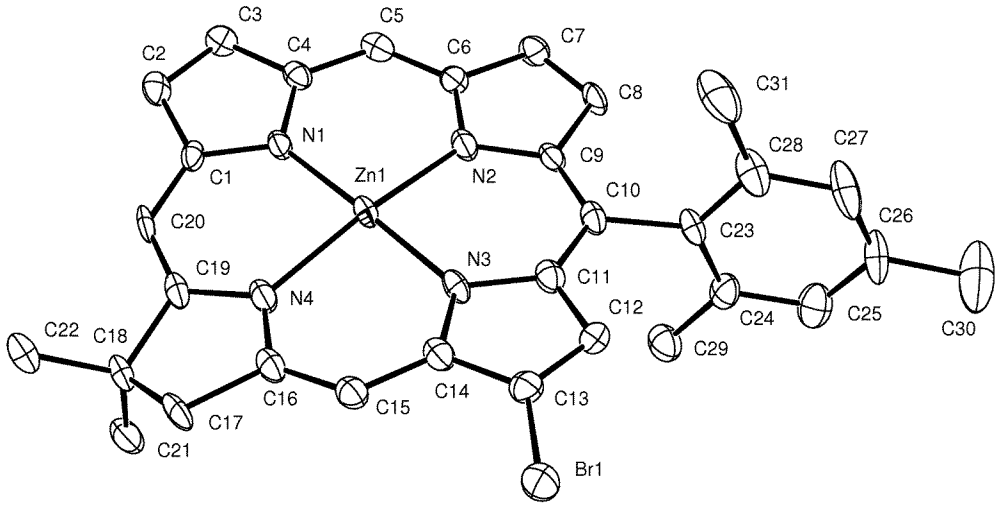



**Figure S5.** ORTEP drawing of **ZnC-M[10]Br[13]** showing naming and numbering scheme. Ellipsoids are at the 50% probability level and hydrogen atoms were omitted for clarity.

**Table S25.** Summary of Crystal Data for **ZnC-M$^{10}$Br$^{13}$.**

| Entry | Data |
|---|---|
| Formula | $C_{31}H_{27}BrN_4Zn$ |
| Formula Weight (*g/mol*) | 600.86 |
| Crystal Dimensions (*mm* ) | 0.32 × 0.12 × 0.06 |
| Crystal Color and Habit | intense reddish blue rectangular plates |
| Crystal System | triclinic |
| Space Group | P -1 |
| Temperature, K | 110 |
| *a*, Å | 8.4774(4) |
| *b*, Å | 9.5633(4) |
| *c*, Å | 17.0559(7) |
| α,° | 82.9163(19) |
| β,° | 76.5219(18) |
| γ,° | 87.3620(19) |
| V, Å$^3$ | 1334.19(10) |
| Number of reflections to determine final unit cell | 6905 |
| Min and Max 2θ for cell determination, ° | 4.94, 50.0 |
| Z | 2 |
| F(000) | 612.48 |
| ρ (*g/cm*) | 1.496 |
| λ, Å, (MoKα) | 0.71073 |
| μ, (*cm$^{-1}$*) | 2.45 |
| Diffractometer Type | Bruker-Nonius X8 Apex2 |
| Scan Type(s) | omega and phi scans |
| Max 2θ for data collection, ° | 51.54 |
| Measured fraction of data | 0.95 |
| Number of reflections measured | 50706 |
| Unique reflections measured | 4867 |
| $R_{merge}$ | 0.038 |
| Number of reflections included in refinement | 3712 |
| Cut off Threshold Expression | $I_{net} > 1.0\text{sigma}(I_{net})$ |
| Structure refined using | full matrix least-squares using F |
| Weighting Scheme | $1/(\text{sigma}^2(F)+0.00027F^2)$ |
| Number of parameters in least-squares | 334 |
| $R_f$[a] | 0.054 |
| $R_w$[b] | 0.052 |
| $R_f$ (all data)[a] | 0.085 |
| $R_w$ (all data)[b] | 0.052 |
| GOF[c] | 1.90 |
| Maximum shift/error | 0.002 |
| Min & Max peak heights on final ΔF Map (*e$^-$*/Å) | -0.53, 2.45 |

[a] $R_f = \Sigma(|F_O - F_C|) / \Sigma F_O$, [b] $R_w = [\Sigma(w(F_O - F_C)^2) / \Sigma(F_O^2)]^{1/2}$, [c] $GOF = [\Sigma(w(F_O - F_C)^2) / (\text{No. of reflns.} - \text{No. of params.})]^{1/2}$.

**Table S26.** Atomic Coordinates for **ZnC-M$^{10}$Br$^{13}$.**

| Atom | x | y | z | $U_{iso/equiv}$ |
|---|---|---|---|---|
| Zn1 | 0.55580(6) | 0.04088(5) | 0.84286(3) | 0.0212(3) |
| N1 | 0.6547(4) | -0.0470(4) | 0.9345(2) | 0.021(2) |
| N2 | 0.4668(4) | 0.1268(4) | 0.7476(2) | 0.021(2) |
| N3 | 0.6856(4) | 0.2262(4) | 0.8357(2) | 0.024(2) |
| N4 | 0.4563(4) | -0.1486(4) | 0.8377(2) | 0.023(2) |
| C1 | 0.7515(5) | 0.0192(5) | 0.9721(3) | 0.022(3) |
| C2 | 0.7731(5) | -0.0703(5) | 1.0433(3) | 0.025(3) |
| C3 | 0.6935(5) | -0.1922(5) | 1.0457(3) | 0.024(3) |
| C4 | 0.6207(5) | -0.1775(5) | 0.9776(3) | 0.022(3) |
| C5 | 0.5312(5) | -0.2796(5) | 0.9560(3) | 0.025(3) |
| C6 | 0.4594(5) | -0.2676(5) | 0.8900(3) | 0.022(3) |
| C7 | 0.3742(6) | -0.3779(5) | 0.8678(3) | 0.025(3) |
| C8 | 0.3208(5) | -0.3226(5) | 0.8008(3) | 0.026(3) |
| C9 | 0.3688(5) | -0.1783(5) | 0.7831(3) | 0.021(3) |
| C10 | 0.3288(5) | -0.0810(5) | 0.7221(3) | 0.022(3) |
| C11 | 0.3688(5) | 0.0610(5) | 0.7077(3) | 0.023(3) |
| C12 | 0.3162(6) | 0.1613(5) | 0.6501(3) | 0.024(3) |
| C13 | 0.3812(5) | 0.2869(5) | 0.6547(3) | 0.024(3) |
| Br1 | 0.34580(6) | 0.46171(5) | 0.59863(3) | 0.0315(3) |
| C14 | 0.4788(5) | 0.2628(5) | 0.7144(3) | 0.023(3) |
| C15 | 0.5735(5) | 0.3657(5) | 0.7321(3) | 0.024(3) |
| C16 | 0.6726(5) | 0.3457(5) | 0.7868(3) | 0.023(3) |
| C17 | 0.7759(6) | 0.4623(5) | 0.8016(3) | 0.028(3) |
| C18 | 0.8873(5) | 0.3822(5) | 0.8509(3) | 0.024(3) |
| C19 | 0.7957(5) | 0.2439(5) | 0.8819(3) | 0.023(3) |
| C20 | 0.8199(5) | 0.1517(5) | 0.9457(3) | 0.023(3) |
| C21 | 1.0477(6) | 0.3430(5) | 0.7938(3) | 0.033(3) |
| C22 | 0.9199(6) | 0.4609(5) | 0.9172(3) | 0.033(3) |
| C23 | 0.2399(5) | -0.1329(5) | 0.6645(3) | 0.024(3) |
| C24 | 0.3306(6) | -0.1697(5) | 0.5905(3) | 0.028(3) |
| C25 | 0.2509(6) | -0.2073(6) | 0.5335(3) | 0.037(3) |
| C26 | 0.0846(7) | -0.2114(6) | 0.5491(3) | 0.044(4) |
| C27 | -0.0025(6) | -0.1785(6) | 0.6234(4) | 0.047(4) |
| C28 | 0.0697(6) | -0.1381(6) | 0.6827(3) | 0.037(3) |
| C29 | 0.5128(6) | -0.1694(6) | 0.5711(3) | 0.033(3) |
| C30 | 0.0027(8) | -0.2497(8) | 0.4843(4) | 0.077(5) |
| C31 | -0.0316(6) | -0.0995(6) | 0.7625(4) | 0.050(4) |
| H2 | 0.832 | -0.048 | 1.082 | 0.0356 |
| H3 | 0.687 | -0.273 | 1.086 | 0.0335 |
| H5 | 0.517 | -0.368 | 0.990 | 0.0342 |
| H7 | 0.358 | -0.472 | 0.895 | 0.0351 |
| H8 | 0.262 | -0.371 | 0.771 | 0.0366 |
| H12 | 0.248 | 0.144 | 0.615 | 0.0342 |
| H15 | 0.570 | 0.458 | 0.704 | 0.0336 |
| H17a | 0.836 | 0.509 | 0.751 | 0.0385 |
| H17b | 0.709 | 0.530 | 0.832 | 0.0385 |

| | | | | |
|---|---|---|---|---|
| H20 | 0.894 | 0.180 | 0.975 | 0.0346 |
| H25 | 0.314 | -0.229 | 0.482 | 0.0488 |
| H27 | -0.119 | -0.184 | 0.635 | 0.0613 |
| H21a | 1.0253(8) | 0.300(3) | 0.7497(10) | 0.0430 |
| H21b | 1.1086(17) | 0.278(2) | 0.8234(7) | 0.0430 |
| H21c | 1.1095(17) | 0.4265(8) | 0.7729(15) | 0.0430 |
| H22a | 0.8200(10) | 0.475(3) | 0.9559(10) | 0.0436 |
| H22b | 0.966(3) | 0.5505(13) | 0.8937(5) | 0.0436 |
| H22c | 0.994(3) | 0.4068(16) | 0.9440(12) | 0.0436 |
| H29a | 0.5510(7) | -0.226(3) | 0.6137(10) | 0.0432 |
| H29b | 0.5492(7) | -0.0746(7) | 0.5667(18) | 0.0432 |
| H29c | 0.5546(6) | -0.207(3) | 0.5207(10) | 0.0432 |
| H30a | 0.074(2) | -0.310(4) | 0.4501(17) | 0.0934 |
| H30b | -0.022(5) | -0.1656(11) | 0.4521(17) | 0.0934 |
| H30c | -0.096(3) | -0.298(4) | 0.5100(6) | 0.0934 |
| H31a | 0.016(3) | -0.142(3) | 0.8060(3) | 0.0600 |
| H31b | -0.1397(13) | -0.133(3) | 0.7704(11) | 0.0600 |
| H31c | -0.035(4) | 0.0011(7) | 0.7619(9) | 0.0600 |

**Table S27.** Anisotropic Displacement Parameters for **ZnC-M$^{10}$Br$^{13}$.**

| Atom | $u^{11}$ | $u^{22}$ | $u^{33}$ | $u^{12}$ | $u^{13}$ | $u^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.0204(3) | 0.0181(4) | 0.0271(3) | -0.0059(2) | -0.0072(2) | -0.0051(2) |
| N1 | 0.016(2) | 0.025(3) | 0.023(2) | -0.0052(18) | -0.0042(17) | -0.0068(18) |
| N2 | 0.022(2) | 0.013(2) | 0.030(2) | -0.0044(18) | -0.0064(18) | -0.0066(18) |
| N3 | 0.020(2) | 0.025(3) | 0.029(2) | -0.0071(18) | -0.0044(18) | -0.0078(19) |
| N4 | 0.019(2) | 0.025(3) | 0.027(2) | -0.0059(18) | -0.0052(18) | -0.0069(19) |
| C1 | 0.013(2) | 0.036(3) | 0.019(3) | -0.002(2) | -0.004(2) | -0.010(2) |
| C2 | 0.013(2) | 0.033(3) | 0.030(3) | 0.001(2) | -0.006(2) | -0.009(2) |
| C3 | 0.024(3) | 0.019(3) | 0.028(3) | 0.002(2) | -0.006(2) | 0.000(2) |
| C4 | 0.017(2) | 0.022(3) | 0.025(3) | -0.002(2) | -0.001(2) | -0.005(2) |
| C5 | 0.022(3) | 0.021(3) | 0.029(3) | -0.002(2) | 0.000(2) | -0.003(2) |
| C6 | 0.021(3) | 0.022(3) | 0.022(3) | -0.003(2) | -0.004(2) | -0.003(2) |
| C7 | 0.030(3) | 0.017(3) | 0.028(3) | -0.006(2) | -0.006(2) | -0.002(2) |
| C8 | 0.025(3) | 0.024(3) | 0.030(3) | -0.012(2) | -0.005(2) | -0.011(2) |
| C9 | 0.015(2) | 0.024(3) | 0.023(3) | -0.007(2) | -0.001(2) | -0.007(2) |
| C10 | 0.017(2) | 0.025(3) | 0.026(3) | -0.003(2) | -0.003(2) | -0.012(2) |
| C11 | 0.018(3) | 0.027(3) | 0.024(3) | -0.002(2) | -0.002(2) | -0.009(2) |
| C12 | 0.027(3) | 0.028(3) | 0.018(3) | -0.004(2) | -0.005(2) | -0.003(2) |
| C13 | 0.027(3) | 0.025(3) | 0.020(3) | -0.002(2) | -0.002(2) | -0.005(2) |
| Br1 | 0.0377(3) | 0.0258(3) | 0.0320(3) | -0.0065(2) | -0.0107(2) | 0.0000(2) |
| C14 | 0.020(3) | 0.024(3) | 0.026(3) | -0.003(2) | -0.002(2) | -0.006(2) |
| C15 | 0.024(3) | 0.023(3) | 0.024(3) | -0.004(2) | -0.002(2) | -0.005(2) |
| C16 | 0.022(3) | 0.020(3) | 0.029(3) | -0.005(2) | -0.004(2) | -0.008(2) |
| C17 | 0.028(3) | 0.017(3) | 0.040(3) | -0.012(2) | -0.007(2) | -0.007(2) |
| C18 | 0.020(3) | 0.021(3) | 0.033(3) | -0.007(2) | -0.009(2) | -0.008(2) |
| C19 | 0.018(3) | 0.023(3) | 0.031(3) | -0.003(2) | -0.007(2) | -0.012(2) |
| C20 | 0.014(2) | 0.028(3) | 0.032(3) | -0.005(2) | -0.009(2) | -0.016(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C21 | 0.028(3) | 0.032(3) | 0.038(3) | -0.013(2) | -0.001(2) | -0.008(2) |
| C22 | 0.031(3) | 0.026(3) | 0.044(3) | -0.011(2) | -0.011(2) | -0.006(2) |
| C23 | 0.020(3) | 0.020(3) | 0.034(3) | -0.005(2) | -0.010(2) | -0.009(2) |
| C24 | 0.039(3) | 0.020(3) | 0.027(3) | -0.004(2) | -0.013(2) | -0.006(2) |
| C25 | 0.044(4) | 0.034(4) | 0.039(3) | 0.003(3) | -0.017(3) | -0.012(3) |
| C26 | 0.041(4) | 0.049(4) | 0.055(4) | -0.004(3) | -0.031(3) | -0.021(3) |
| C27 | 0.023(3) | 0.055(4) | 0.077(4) | 0.002(3) | -0.026(3) | -0.025(3) |
| C28 | 0.028(3) | 0.034(4) | 0.053(4) | -0.002(3) | -0.013(3) | -0.018(3) |
| C29 | 0.030(3) | 0.036(4) | 0.034(3) | -0.005(2) | -0.004(2) | -0.013(2) |
| C30 | 0.068(5) | 0.103(7) | 0.083(5) | 0.006(4) | -0.047(4) | -0.043(5) |
| C31 | 0.022(3) | 0.057(5) | 0.073(4) | -0.004(3) | -0.003(3) | -0.029(3) |

**Table S28.** Bond Lengths for **ZnC-M$^{10}$Br$^{13}$.**

| Bond | Length in Å | Bond | Length in Å |
|---|---|---|---|
| Zn1-N1 | 2.018(4) | C15-H15 | 0.96 |
| Zn1-N2 | 2.018(4) | C16-C17 | 1.528(6) |
| Zn1-N3 | 2.105(4) | C17-C18 | 1.527(7) |
| Zn1-N4 | 2.053(4) | C17-H17a | 0.96 |
| N1-C1 | 1.371(5) | C17-H17b | 0.96 |
| N1-C4 | 1.374(6) | C18-C19 | 1.536(6) |
| N2-C11 | 1.401(5) | C18-C21 | 1.537(6) |
| N2-C14 | 1.351(6) | C18-C22 | 1.516(6) |
| N3-C16 | 1.345(6) | C19-C20 | 1.362(7) |
| N3-C19 | 1.382(6) | C20-H20 | 0.96 |
| N4-C6 | 1.361(6) | C21-H21a | 0.96 |
| N4-C9 | 1.380(5) | C21-H21b | 0.96 |
| C1-C2 | 1.440(7) | C21-H21c | 0.96 |
| C1-C20 | 1.396(7) | C22-H22a | 0.96 |
| C2-C3 | 1.365(7) | C22-H22b | 0.96 |
| C2-H2 | 0.96 | C22-H22c | 0.96 |
| C3-C4 | 1.428(6) | C23-C24 | 1.393(6) |
| C3-H3 | 0.96 | C23-C28 | 1.406(6) |
| C4-C5 | 1.397(6) | C24-C25 | 1.395(7) |
| C5-C6 | 1.389(7) | C24-C29 | 1.502(7) |
| C5-H5 | 0.96 | C25-C26 | 1.374(8) |
| C6-C7 | 1.440(6) | C25-H25 | 0.96 |
| C7-C8 | 1.364(7) | C26-C27 | 1.375(8) |
| C7-H7 | 0.96 | C26-C30 | 1.523(7) |
| C8-C9 | 1.432(6) | C27-C28 | 1.397(7) |
| C8-H8 | 0.96 | C27-H27 | 0.96 |
| C9-C10 | 1.401(7) | C28-C31 | 1.509(7) |
| C10-C11 | 1.393(7) | C29-H29a | 0.96 |
| C10-C23 | 1.509(6) | C29-H29b | 0.96 |
| C11-C12 | 1.420(7) | C29-H29c | 0.96 |
| C12-C13 | 1.362(7) | C30-H30a | 0.96 |
| C12-H12 | 0.96 | C30-H30b | 0.96 |
| C13-Br1 | 1.869(5) | C30-H30c | 0.96 |

| | | | |
|---|---|---|---|
| C13-C14 | 1.447(7) | C31-H31a | 0.96 |
| C14-C15 | 1.401(6) | C31-H31b | 0.96 |
| C15-C16 | 1.386(7) | C31-H31c | 0.96 |

**Table S29.** Bond Angles for **ZnC-M$^{10}$Br$^{13}$.**

| Bond | Angle in ° | Bond | Angle in ° |
|---|---|---|---|
| N1-Zn1-N2 | 177.30(14) | C16-C17-C18 | 102.9(4) |
| N1-Zn1-N3 | 90.01(15) | C16-C17-H17a | 110.9(4) |
| N1-Zn1-N4 | 90.33(15) | C16-C17-H17b | 110.9(4) |
| N2-Zn1-N3 | 89.44(14) | C18-C17-H17a | 111.6(4) |
| N2-Zn1-N4 | 89.84(15) | C18-C17-H17b | 110.9(4) |
| N3-Zn1-N4 | 171.94(14) | H17a-C17-H17b | 109.5(5) |
| Zn1-N1-C1 | 126.1(3) | C17-C18-C19 | 101.6(3) |
| Zn1-N1-C4 | 126.2(3) | C17-C18-C21 | 109.8(4) |
| C1-N1-C4 | 107.1(4) | C17-C18-C22 | 113.7(4) |
| Zn1-N2-C11 | 126.8(3) | C19-C18-C21 | 106.4(4) |
| Zn1-N2-C14 | 126.2(3) | C19-C18-C22 | 114.4(4) |
| C11-N2-C14 | 106.7(4) | C21-C18-C22 | 110.4(4) |
| Zn1-N3-C16 | 125.5(3) | N3-C19-C18 | 110.4(4) |
| Zn1-N3-C19 | 124.8(3) | N3-C19-C20 | 124.8(4) |
| C16-N3-C19 | 109.7(4) | C18-C19-C20 | 124.8(4) |
| Zn1-N4-C6 | 126.0(3) | C1-C20-C19 | 127.4(4) |
| Zn1-N4-C9 | 127.0(3) | C1-C20-H20 | 116.2(5) |
| C6-N4-C9 | 107.0(4) | C19-C20-H20 | 116.3(4) |
| N1-C1-C2 | 109.1(4) | C18-C21-H21a | 109.6(6) |
| N1-C1-C20 | 125.8(4) | C18-C21-H21b | 109.5(8) |
| C2-C1-C20 | 125.1(4) | C18-C21-H21c | 109.4(10) |
| C1-C2-C3 | 107.0(4) | H21a-C21-H21b | 109.5(19) |
| C1-C2-H2 | 126.4(5) | H21a-C21-H21c | 109(2) |
| C3-C2-H2 | 126.6(5) | H21b-C21-H21c | 109.5(16) |
| C2-C3-C4 | 107.2(4) | C18-C22-H22a | 109.6(13) |
| C2-C3-H3 | 126.5(4) | C18-C22-H22b | 109.4(9) |
| C4-C3-H3 | 126.3(4) | C18-C22-H22c | 109.4(12) |
| N1-C4-C3 | 109.5(4) | H22a-C22-H22b | 109(2) |
| N1-C4-C5 | 124.5(4) | H22a-C22-H22c | 109.5(17) |
| C3-C4-C5 | 126.0(4) | H22b-C22-H22c | 109(2) |
| C4-C5-C6 | 127.0(5) | C10-C23-C24 | 118.3(4) |
| C4-C5-H5 | 116.8(5) | C10-C23-C28 | 121.4(4) |
| C6-C5-H5 | 116.2(4) | C24-C23-C28 | 120.3(4) |
| N4-C6-C5 | 124.9(4) | C23-C24-C25 | 119.5(4) |
| N4-C6-C7 | 109.8(4) | C23-C24-C29 | 121.0(4) |
| C5-C6-C7 | 125.2(4) | C25-C24-C29 | 119.5(4) |
| C6-C7-C8 | 106.6(4) | C24-C25-C26 | 121.5(5) |
| C6-C7-H7 | 126.8(5) | C24-C25-H25 | 119.1(5) |
| C8-C7-H7 | 126.5(4) | C26-C25-H25 | 119.4(5) |
| C7-C8-C9 | 107.3(4) | C25-C26-C27 | 118.1(4) |
| C7-C8-H8 | 126.7(5) | C25-C26-C30 | 119.7(5) |

| | | | |
|---|---|---|---|
| C9-C8-H8 | 126.0(5) | C27-C26-C30 | 122.2(5) |
| N4-C9-C8 | 109.2(4) | C26-C27-C28 | 123.2(5) |
| N4-C9-C10 | 125.1(4) | C26-C27-H27 | 118.6(5) |
| C8-C9-C10 | 125.7(4) | C28-C27-H27 | 118.2(5) |
| C9-C10-C11 | 125.4(4) | C23-C28-C27 | 117.4(4) |
| C9-C10-C23 | 118.3(4) | C23-C28-C31 | 121.4(4) |
| C11-C10-C23 | 116.2(4) | C27-C28-C31 | 121.2(4) |
| N2-C11-C10 | 125.5(4) | C24-C29-H29a | 109.4(6) |
| N2-C11-C12 | 109.6(4) | C24-C29-H29b | 109.5(6) |
| C10-C11-C12 | 124.9(4) | C24-C29-H29c | 109.5(7) |
| C11-C12-C13 | 106.8(4) | H29a-C29-H29b | 109(2) |
| C11-C12-H12 | 126.9(5) | H29a-C29-H29c | 109.5(18) |
| C13-C12-H12 | 126.3(5) | H29b-C29-H29c | 109(2) |
| C12-C13-Br1 | 127.2(4) | C26-C30-H30a | 109.4(18) |
| C12-C13-C14 | 107.5(4) | C26-C30-H30b | 109(2) |
| Br1-C13-C14 | 125.2(3) | C26-C30-H30c | 109.3(12) |
| N2-C14-C13 | 109.3(4) | H30a-C30-H30b | 109(3) |
| N2-C14-C15 | 126.5(4) | H30a-C30-H30c | 109(3) |
| C13-C14-C15 | 124.2(4) | H30b-C30-H30c | 109(3) |
| C14-C15-C16 | 125.9(5) | C28-C31-H31a | 109.6(12) |
| C14-C15-H15 | 117.0(4) | C28-C31-H31b | 109.4(15) |
| C16-C15-H15 | 117.1(4) | C28-C31-H31c | 109.4(11) |
| N3-C16-C15 | 125.4(4) | H31a-C31-H31b | 109.5(20) |
| N3-C16-C17 | 111.5(4) | H31a-C31-H31c | 109(2) |
| C15-C16-C17 | 123.0(4) | H31b-C31-H31c | 109(3) |

## VI. References.

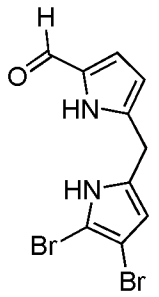

(S1) Bruker-Nonius, SAINT version 7.34A, **2006**, Bruker-Nonius, Madison, WI 53711, USA.

(S2) Bruker-Nonius, SADABS version 2.10, **2004**, Bruker-Nonius, Madison, WI 53711, USA.

(S3) Altomare, A.; Cascarano, G.; Giacovazzo, C.; Guagliardi, A.; Burla, M. C.; Polidori, G.; Camalli, M. *J. Appl. Cryst.* **1994**, *27*, 435.

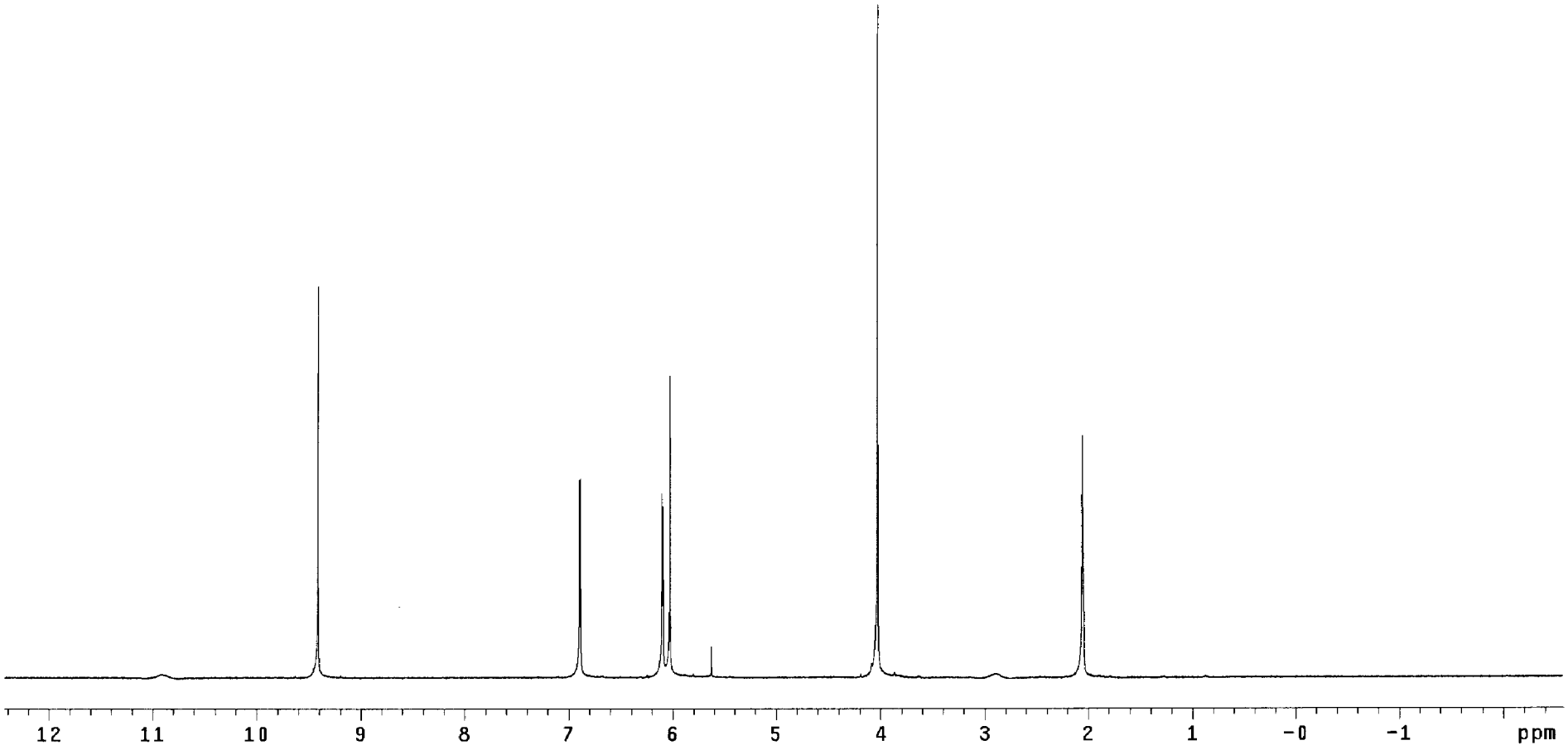
(S4) Bruker-AXS, XL version 6.12, Bruker-AXS, Madison, WI 53711, USA.

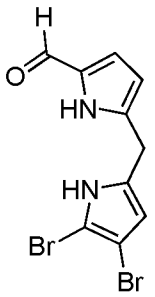

## VII. Spectral Data for Selected Compounds.




**1-Br**[8,9]

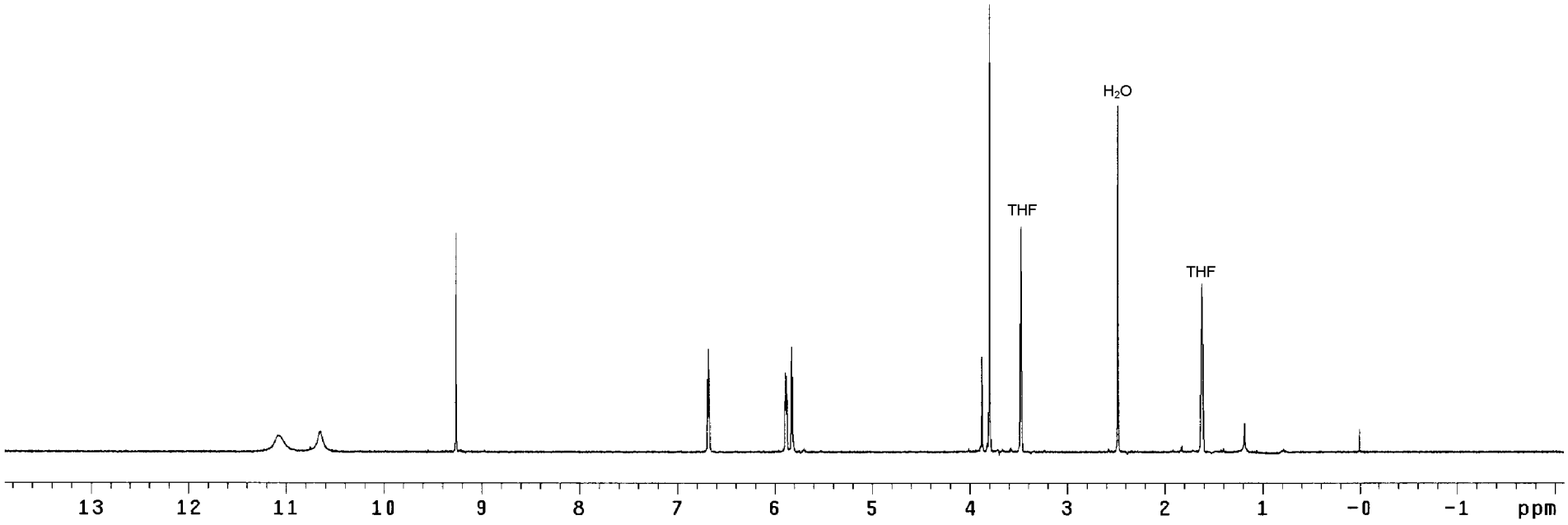
Acetone-$d_6$

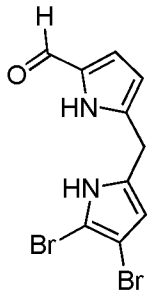





**1-Br**[8,9]

THF-$d_8$



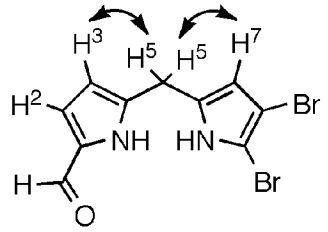



**1-Br**[8,9]

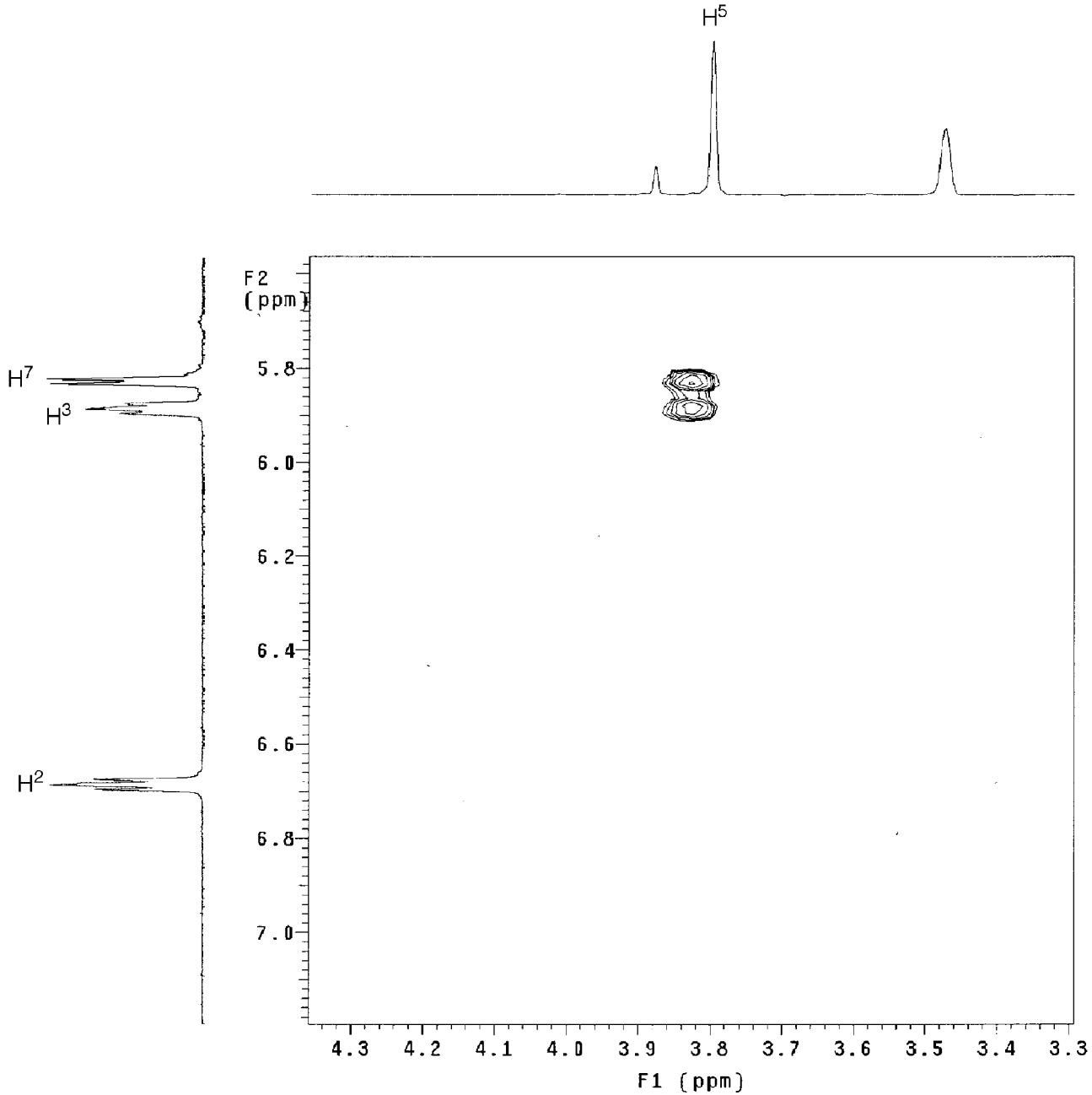
Acetone-$d_6$

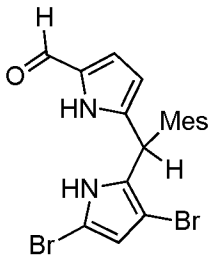
exp1 NOESY

| SAMPLE | | FLAGS | |
|---|---|---|---|
| date | Apr 15 2008 | hs | n |
| solvent | THF | sspul | y |
| sample | olga/dmpbrb~ r5_15Apr2008 | PFGflg | y |
| | | hsglvl | 2000 |
| ACQUISITION | | SPECIAL | |
| sw | 4807.7 | temp | not used |
| at | 0.213 | gain | 28 |
| np | 2048 | spin | 0 |
| fb | not used | F2 PROCESSING | |
| ss | 32 | gf | 0.099 |
| d1 | 1.000 | gfs | not used |
| nt | 16 | fn | 2048 |
| 2D ACQUISITION | | F1 PROCESSING | |
| sw1 | 4807.7 | gf1 | 0.049 |
| ni | 256 | gfs1 | not used |
| TRANSMITTER | | proc1 | lp |
| tn | H1 | fn1 | 2048 |
| sfrq | 299.795 | DISPLAY | |
| tof | 342.1 | sp | 1668.2 |
| tpwr | 59 | wp | 488.3 |
| pw | 17.500 | sp1 | 987.2 |
| NOESY | | wp1 | 319.3 |
| mix | 0.800 | rfl | 637.1 |
| PRESATURATION | | rfp | 0 |
| satmode | nnnn | rfl1 | 627.9 |
| satpwr | 0 | rfp1 | 0 |
| satdly | 0 | PLOT | |
| satfrq | 0 | wc | 124.0 |
| DECOUPLER | | sc | 6.2 |
| dn | C13 | wc2 | 124.0 |
| dm | nnn | sc2 | 0 |
| | | vs | 278 |
| | | th | 1 |
| | | ai ph | |




**1-Br**[8,9]

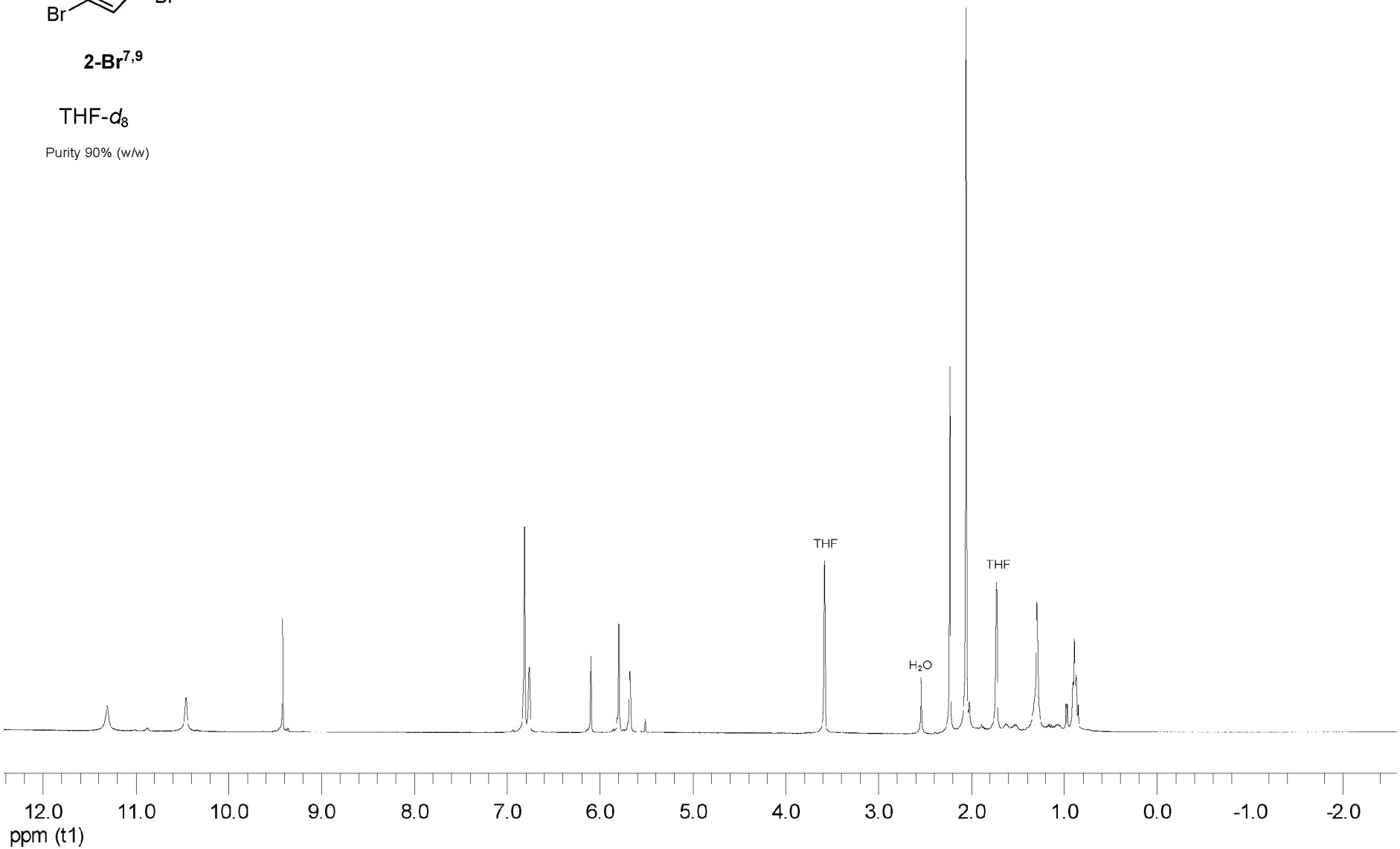





**2-Br**[7,9]

THF-$d_8$

Purity 90% (w/w)

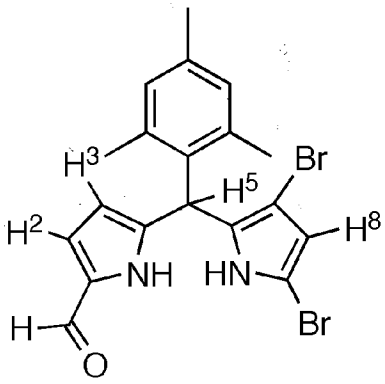


Archive directory: /export/home/lindsey/vnmrsys/data
Sample directory: Olga/50_1_30Nov2008

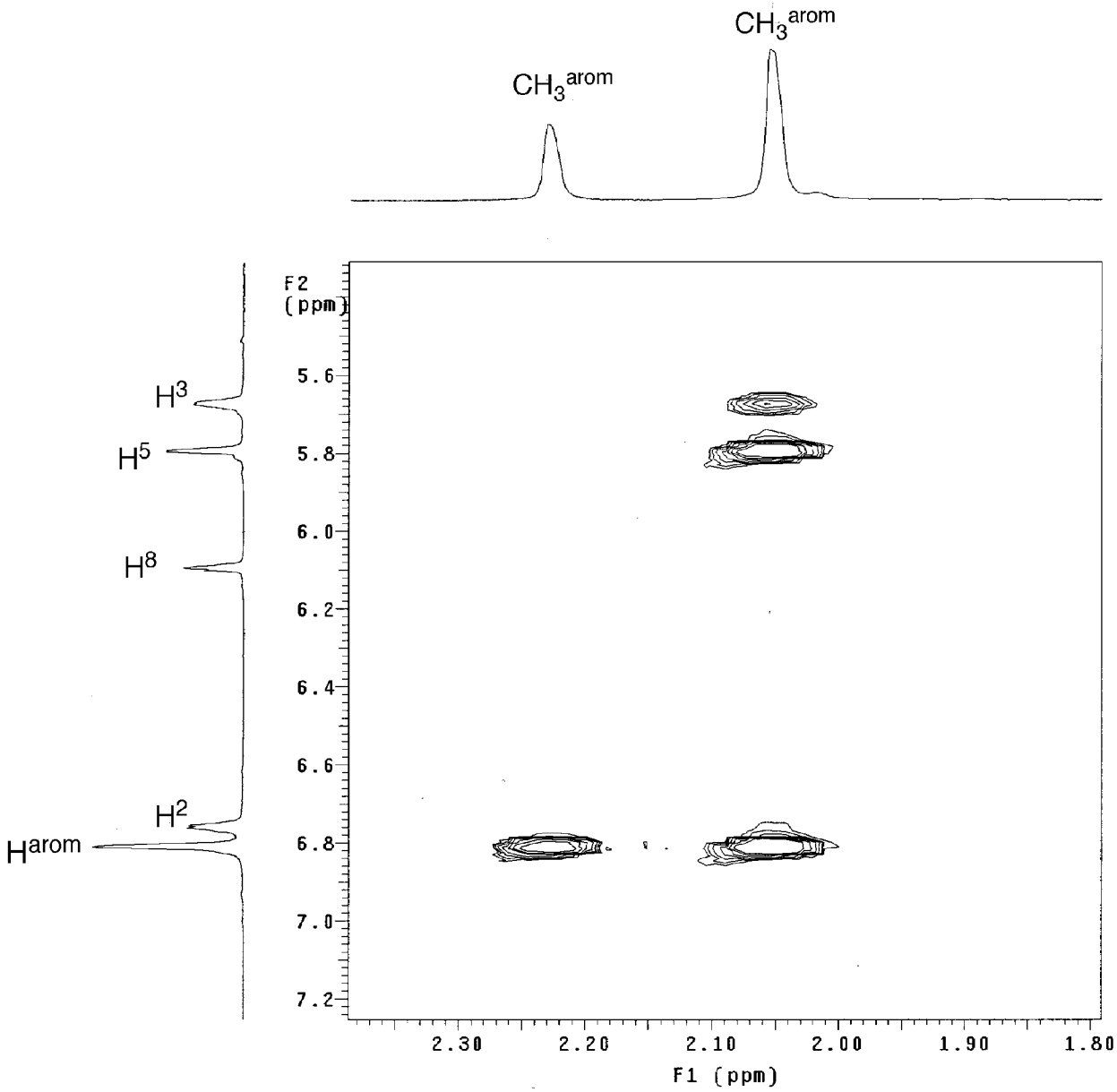
Pulse Sequence: NOESY

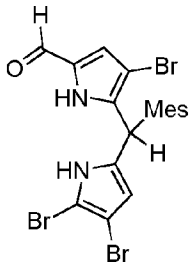
Solvent: THF
Ambient temperature
File: NOESY
Mercury-400BB "ncsumerc400"

Relax. delay 1.000 sec
Mixing 0.800 sec
Acq. time 0.160 sec
Width 6410.3 Hz
2D Width 6410.3 Hz
16 repetitions
2 x 256 increments
OBSERVE H1, 400.1366582 MHz
DATA PROCESSING
Gauss apodization 0.074 sec
F1 DATA PROCESSING
Gauss apodization 0.037 sec
FT size 2048 x 2048
Total time 4 hr, 39 min, 29 sec




**2-Br**[7,9]






**2-Br**[3,8,9]

THF-$d_8$

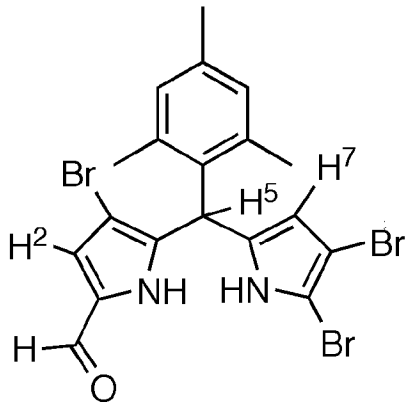
Purity 90% (w/w)

Archive directory: /export/home/lindsey/vnmrsys/data
Sample directory: Olga/50_triBrMes_03Dec2008

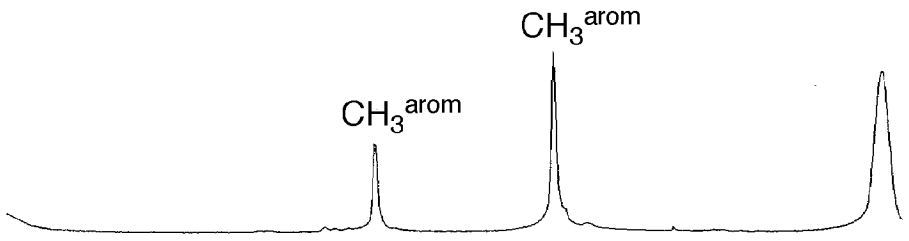
Pulse Sequence: NOESY

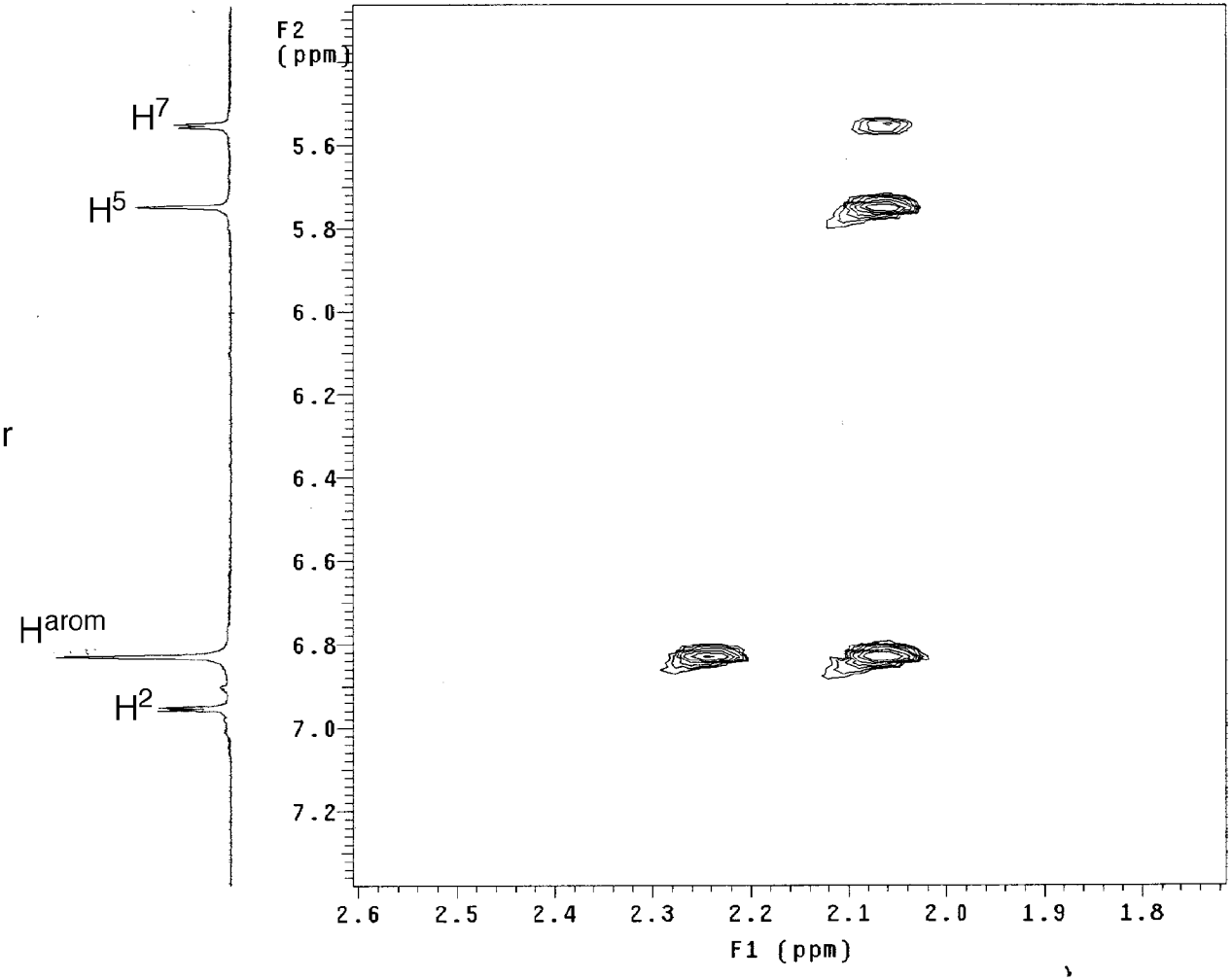
Solvent: THF
Ambient temperature
File: NOESY
Mercury-400BB "ncsumerc400"

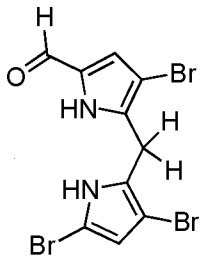
Relax. delay 1.000 sec
Mixing 0.800 sec
Acq. time 0.160 sec
Width 6410.3 Hz
2D Width 6410.3 Hz
16 repetitions
2 x 256 increments
OBSERVE H1, 400.1366582 MHz
DATA PROCESSING
Gauss apodization 0.074 sec
F1 DATA PROCESSING
Gauss apodization 0.037 sec
FT size 2048 x 2048
Total time 4 hr, 39 min, 29 sec




**2-Br$^{3,8,9}$**



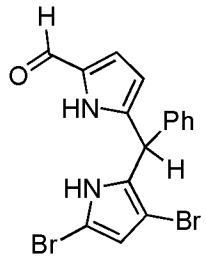






**1-Br**$^{3,7,9}$

THF-$d_8$

Purity 80% (w/w)


H
O
HN
Ph
H
HN
Br
Br

**8-Br**[7,9]

THF-$d_8$


H2O
THF
THF
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
ppm (t1)

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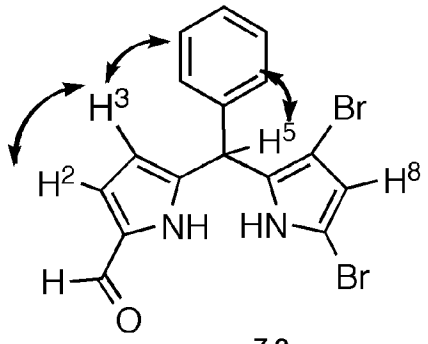
Sample directory: Olga/115_30Mar2009-20:40:22

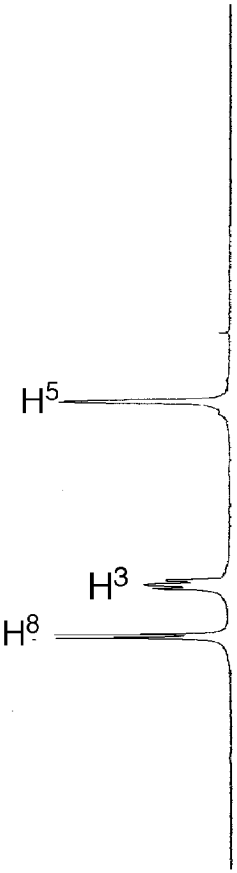
Pulse Sequence: NOESY

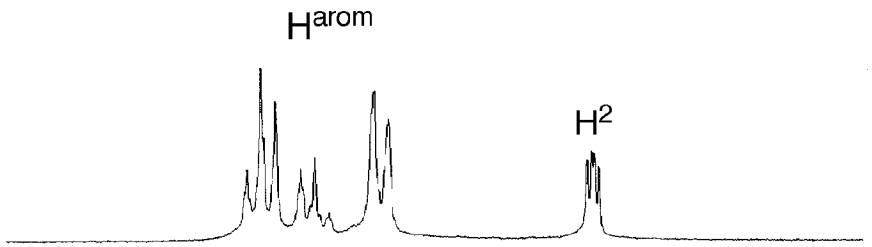
Solvent: THF
Ambient temperature
File: NOESY
Mercury-400BB "ncsumerc400"

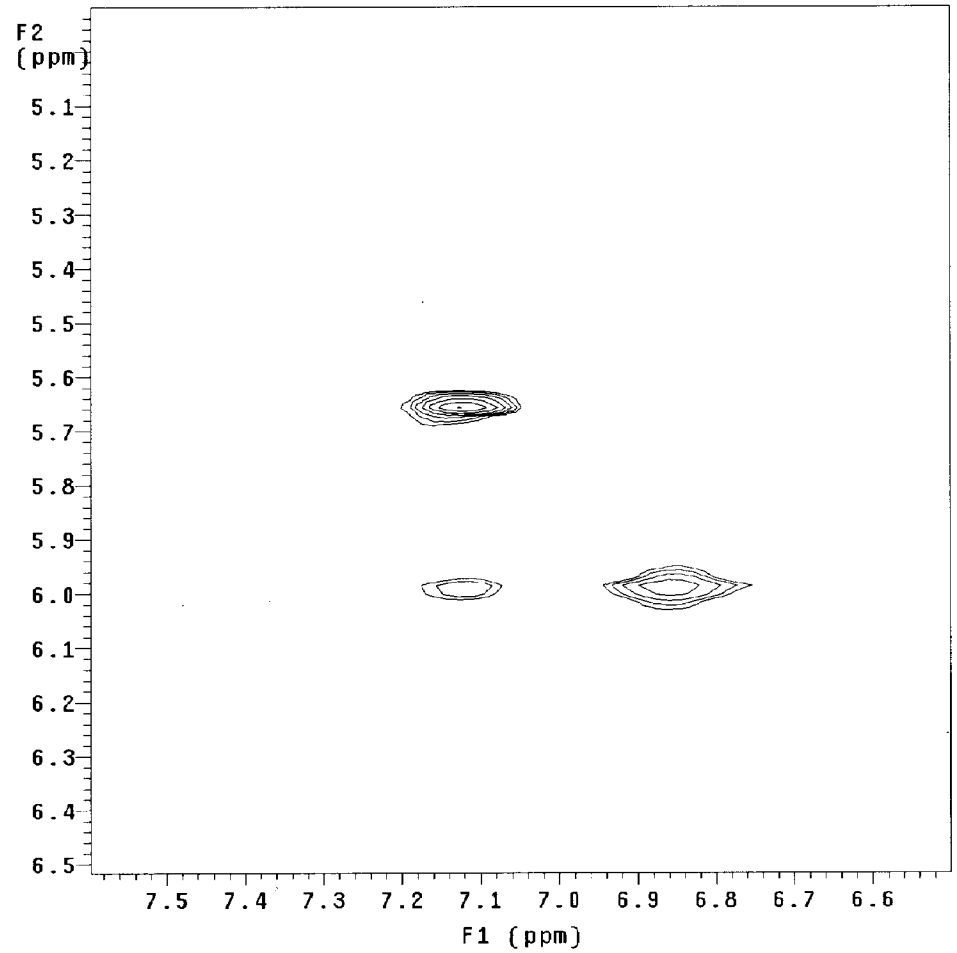
Relax. delay 1.000 sec
Mixing 0.800 sec
Acq. time 0.160 sec
Width 6410.3 Hz
2D Width 6410.3 Hz
64 repetitions
2 x 128 increments
OBSERVE H1, 400.1366582 MHz
DATA PROCESSING
Gauss apodization 0.074 sec
f1 DATA PROCESSING
Gauss apodization 0.018 sec
FT size 2048 x 2048
Total time 9 hr, 15 min, 0 sec

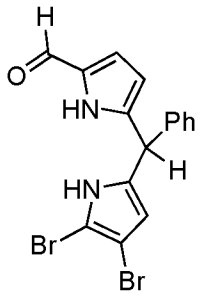



**8-Br**[7,9]



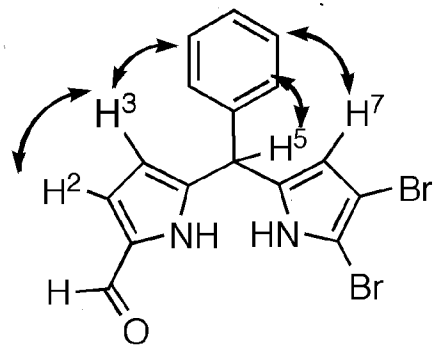



**8-Br**[8,9]

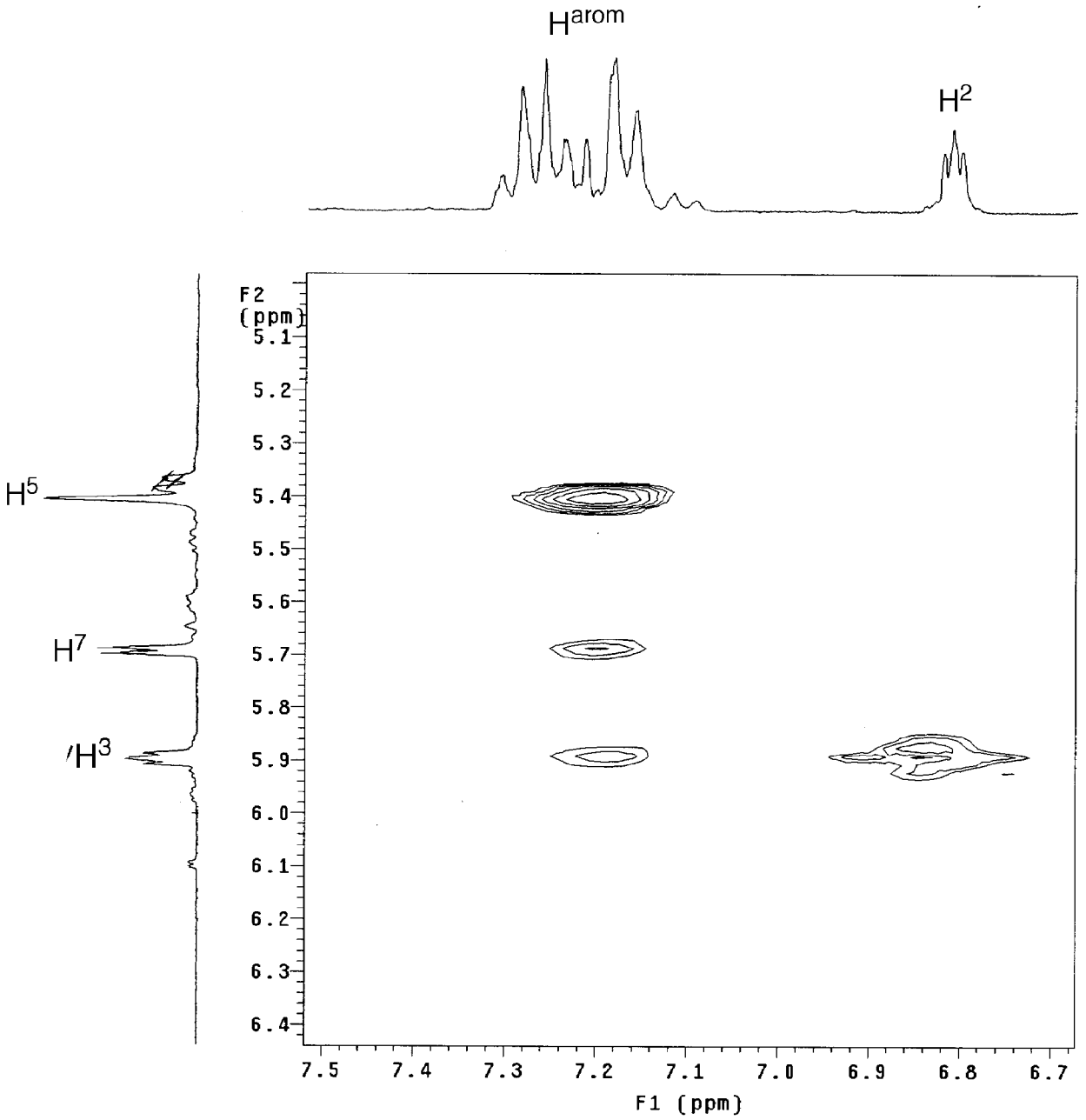
THF-$d_8$

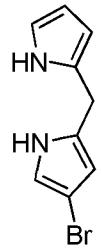
exp1 NOESY

| SAMPLE | | FLAGS | |
|---|---|---|---|
| date | Mar 26 2009 | hs | n |
| solvent | THF | sspul | y |
| sample | olga/115_26~ Mar2009 | PFGflg | y |
| | | hsglvl | 2000 |
| ACQUISITION | | SPECIAL | |
| sw | 4807.7 | temp | not used |
| at | 0.213 | gain | 16 |
| np | 2048 | spin | 0 |
| fb | not used | F2 PROCESSING | |
| ss | 32 | gf | 0.099 |
| d1 | 1.000 | gfs | not used |
| nt | 8 | fn | 2048 |
| 2D ACQUISITION | | F1 PROCESSING | |
| sw1 | 4807.7 | gf1 | 0.025 |
| ni | 128 | gfs1 | not used |
| TRANSMITTER | | proc1 | lp |
| tn | H1 | fn1 | 2048 |
| sfrq | 299.795 | DISPLAY | |
| tof | 342.1 | sp | 1493.6 |
| tpwr | 59 | wp | 436.6 |
| pw | 17.500 | sp1 | 2000.5 |
| NOESY | | wp1 | 253.5 |
| mix | 0.800 | rf1 | 605.1 |
| PRESATURATION | | rfp | 0 |
| satmode | nnnn | rf11 | 595.9 |
| satpwr | 0 | rfp1 | 0 |
| satdly | 0 | PLOT | |
| satfrq | 0 | wc | 124.0 |
| DECOUPLER | | sc | 6.2 |
| dn | C13 | wc2 | 124.0 |
| dm | nnn | sc2 | 0 |
| | | vs | 579 |
| | | th | 2 |
| | | ai ph | |



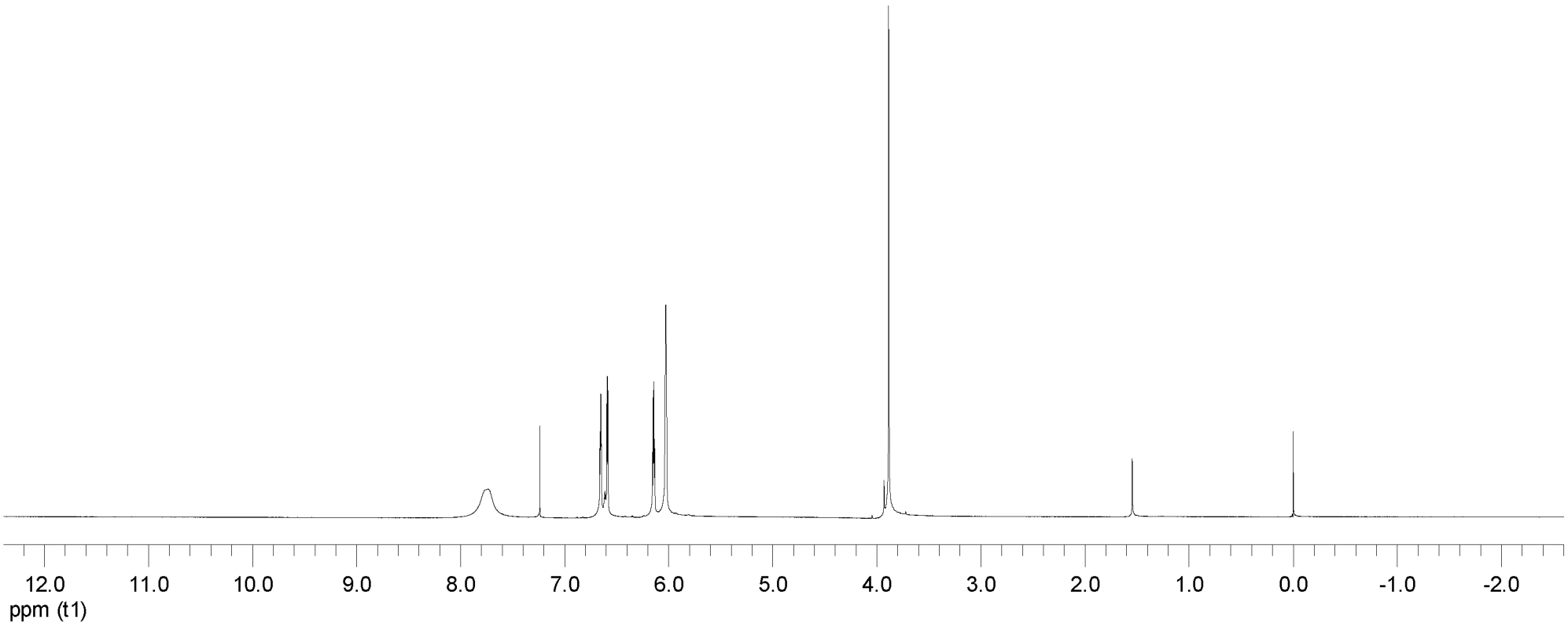

**8-Br**[8,9]

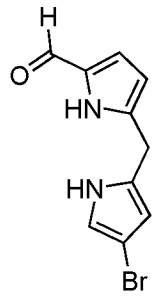





**5**

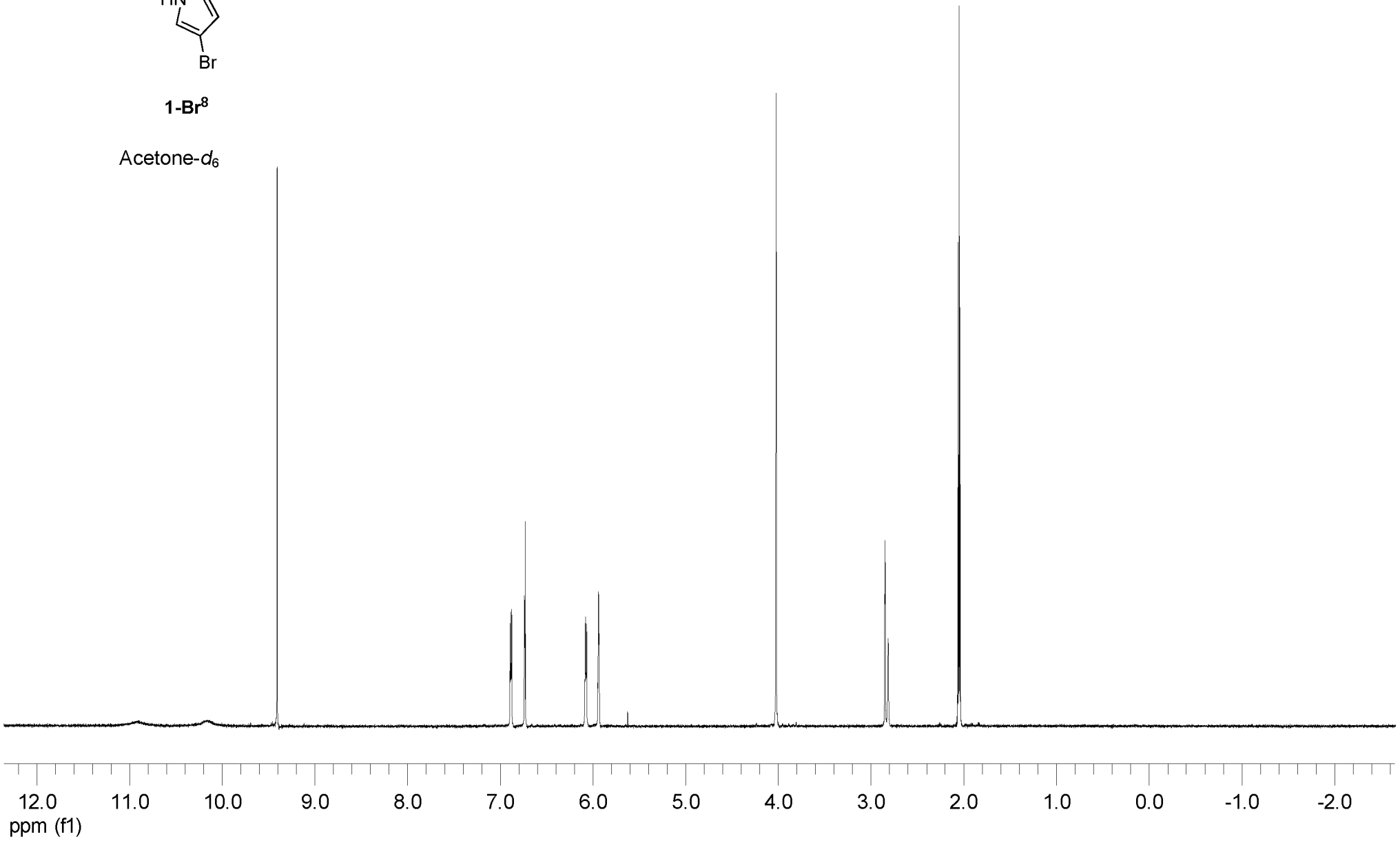
$CDCl_3$

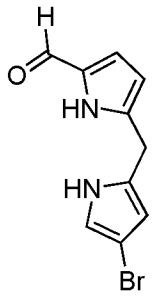





**1-Br**[8]

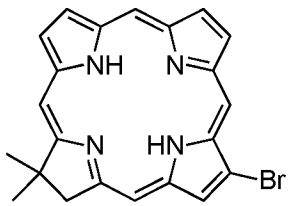
Acetone-$d_6$





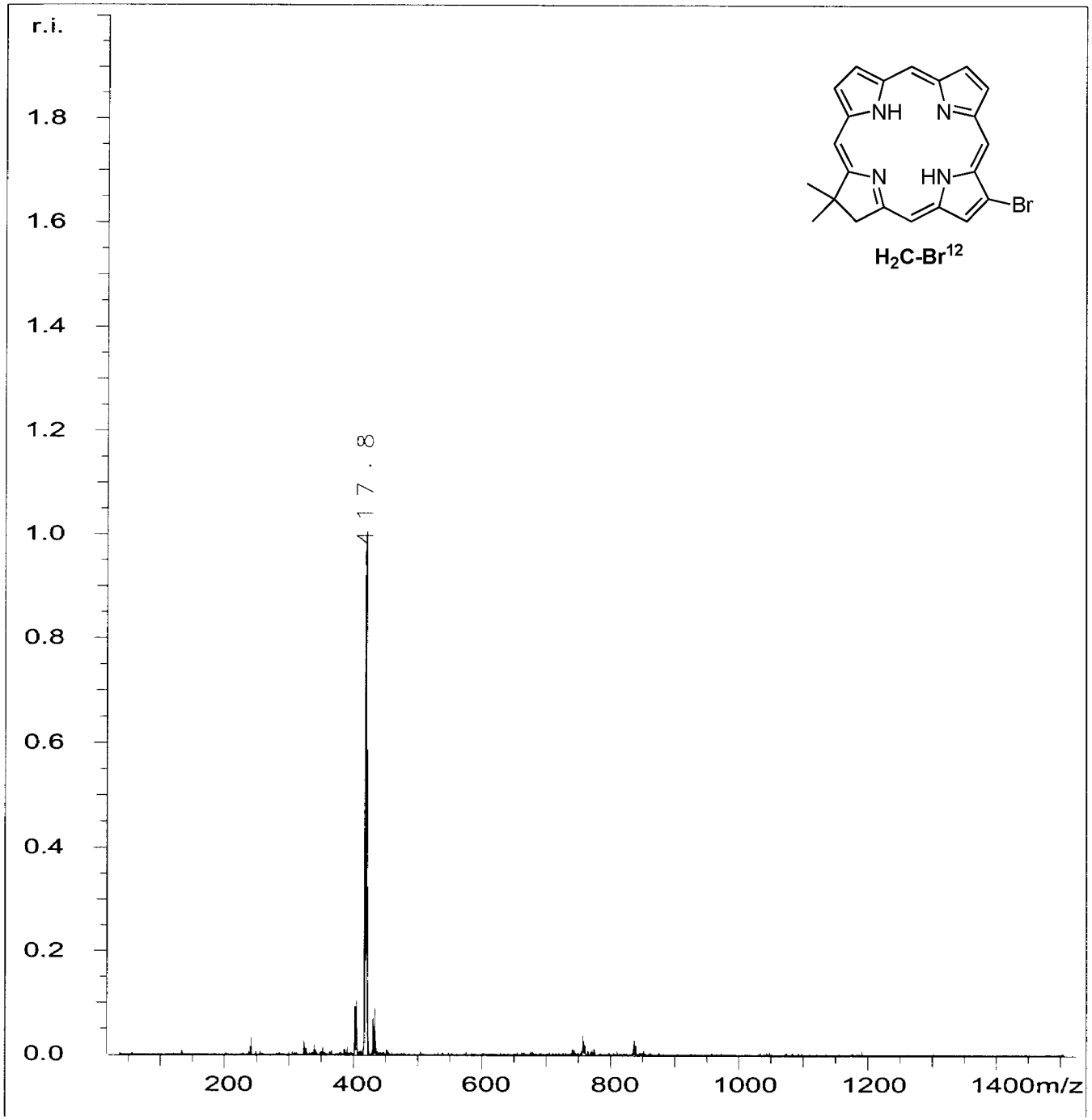

**1-Br**[8]

Acetone-$d_6$




**$H_2C$-Br[12]**

$CDCl_3$

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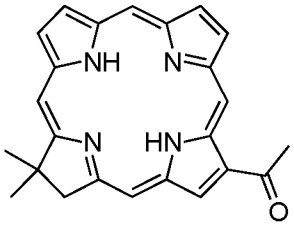
PATH D:\data\Chemistry\Lindsey\Olga
POLARI POS
AQOP_m Reflector
TD 38402
NoSHOTS 300
SMONUM 0
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 274 [ns]
Uis1 19.00 [kV]
Uis2 17.40 [kV]
Urefl 0.00 [kV]
Ulens 9.10 [kV]
Uhimass 0.00 [kV]
RefFull 0.00 [kV]
UdetL 1.65 [kV]
UdetR 0.00 [kV]
Udefl 0.00 [kV]
REPHZ 3.00 [Hz]
ATTEN 95.0
ML1 2521177.240
ML2 308.329
ML3 0.000
HITURBO no
GDEON yes
GDEDLY short
DEFLON no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1 0.38
DPMASS 500.00 [Da]
RBNDVAL 0.00
LBNDVAL 0.00
IS2BNDV 0.00
CMT1 H2C-Br12
CMT2

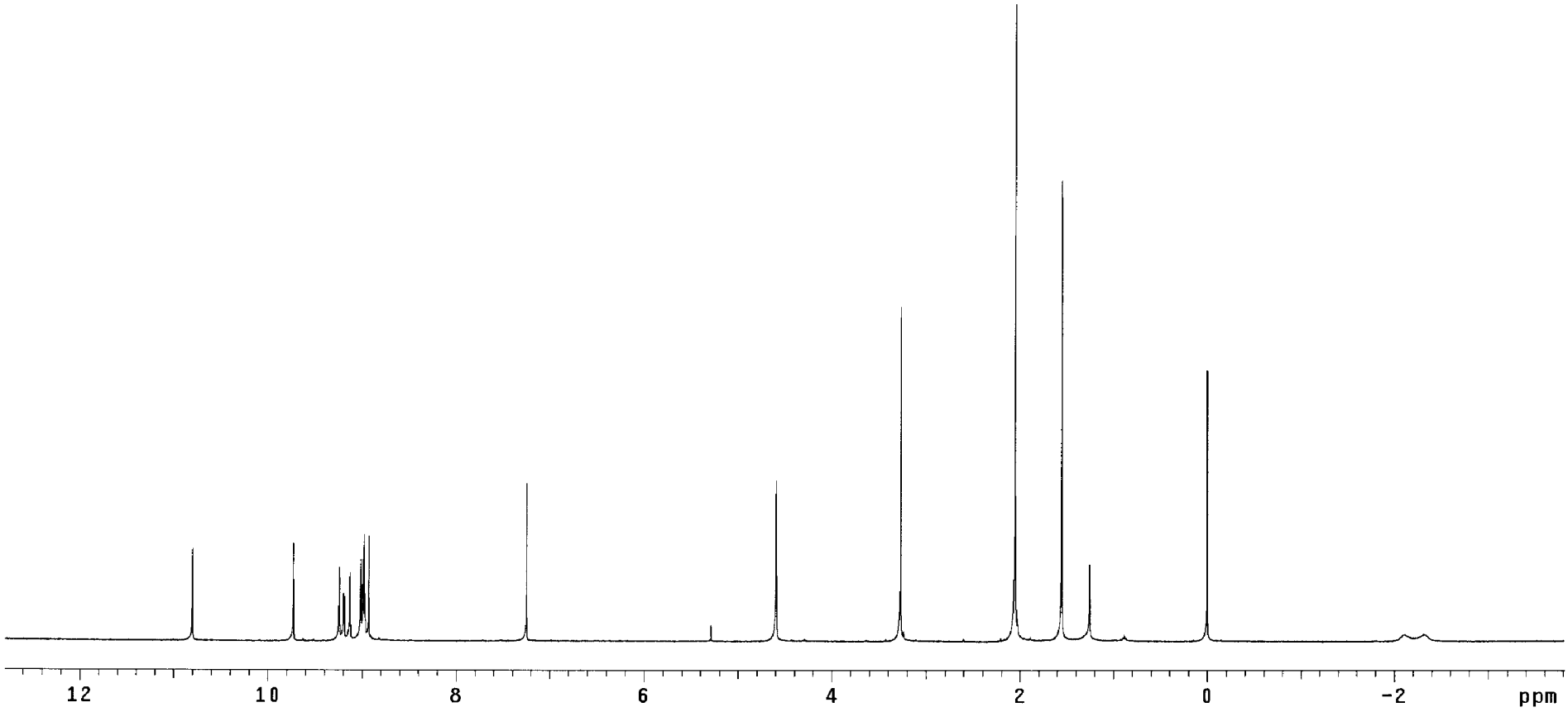


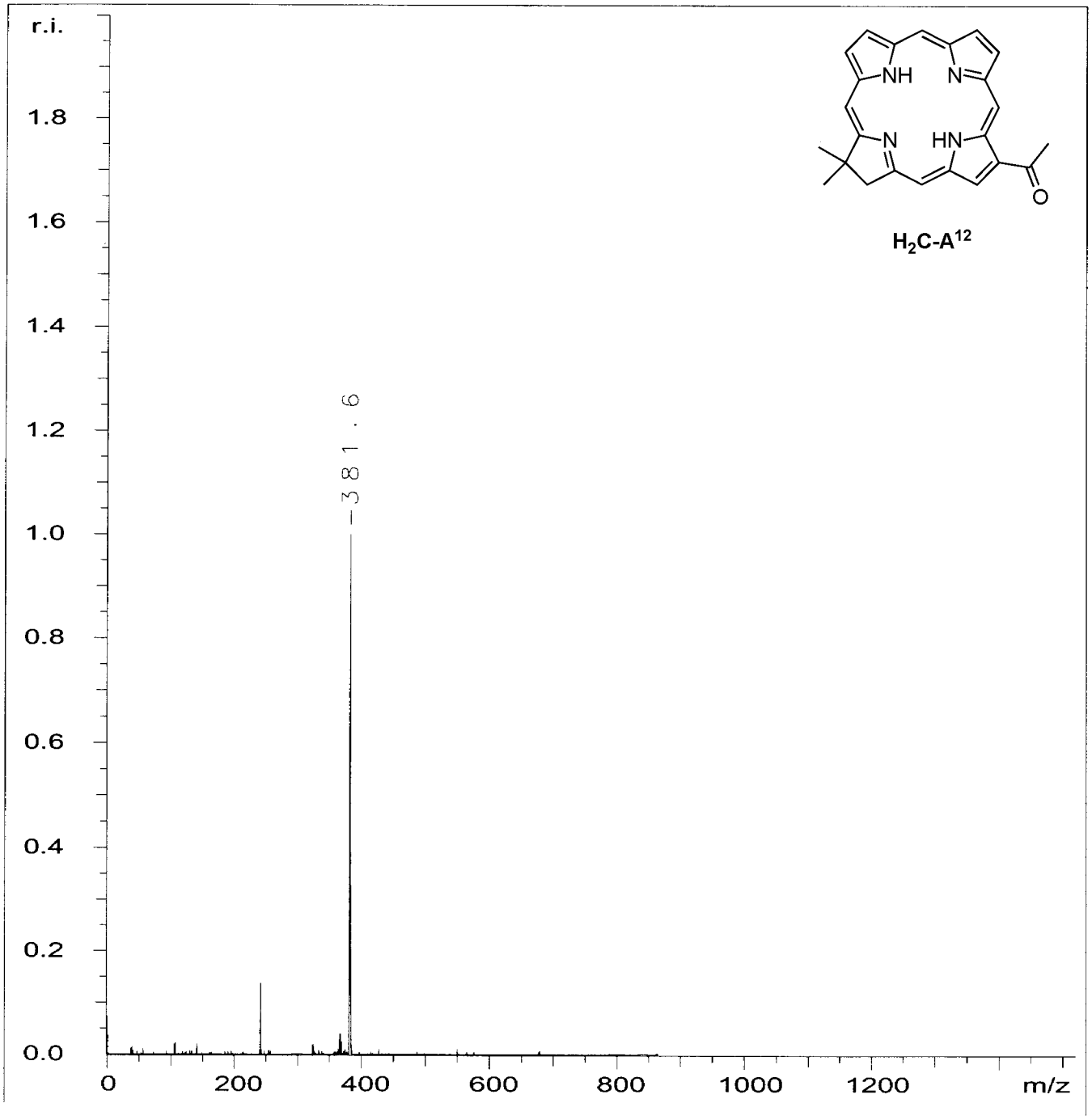
Wed May 27 20:38:28 2009




**$H_2C$-$A^{12}$**

$CDCl_3$






$H_2C$-$A^{12}$

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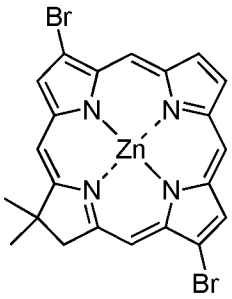
TD 38402
NoSHOTS 300
SMONUM 0
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 274 [ns]
Uis1 19.00 [kV]
Uis2 17.40 [kV]
Urefl 0.00 [kV]
Ulens 9.10 [kV]
Uhimass 0.00 [kV]
RefFull 0.00 [kV]
UdetL 1.65 [kV]
UdetR 0.00 [kV]
Udefl 0.00 [kV]
REPHZ 3.00 [Hz]
ATTEN 90.0
ML1 2521177.240
ML2 308.329
ML3 0.000
HITURBO no
GDEON yes
GDEDLY short
DEFLON no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1 0.38
DPMASS 500.00 [Da]
RBNDVAL 0.00
LBNDVAL 0.00
IS2BNDV 0.00
CMT1 H2C-A12
CMT2

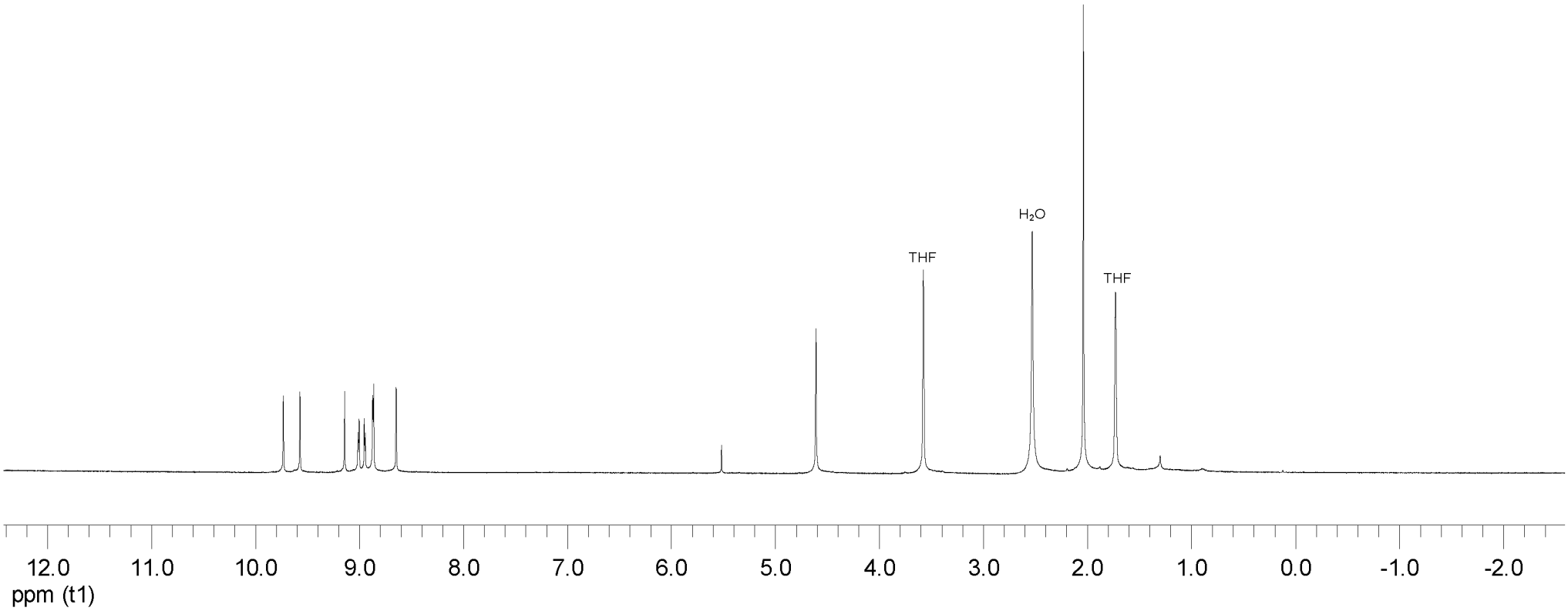


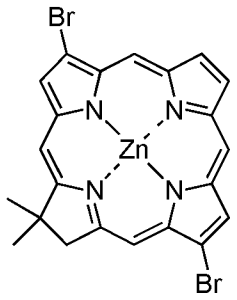
Wed May 27 20:37:39 2009




**ZnC-Br$^{3}$Br$^{13}$**

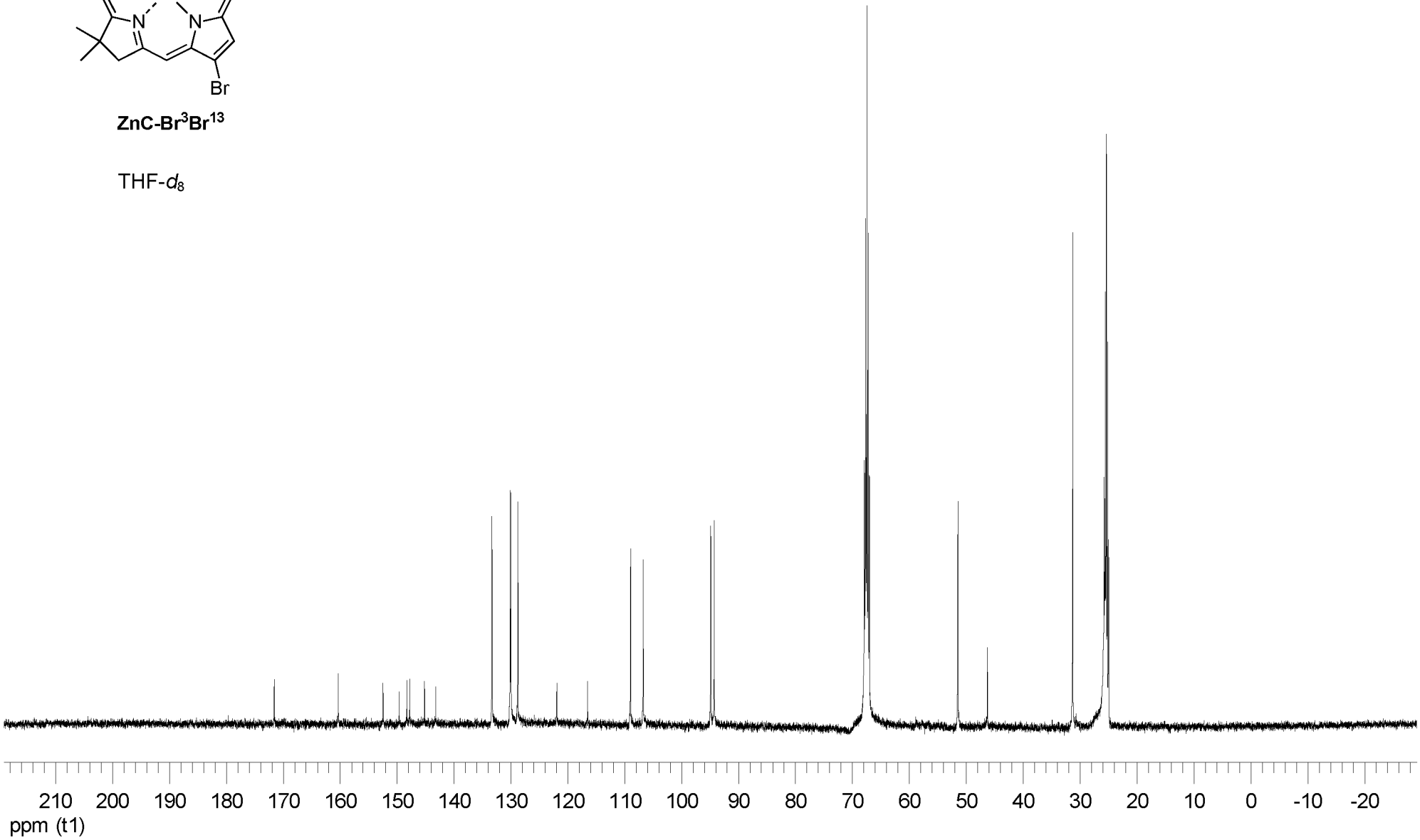
THF-$d_8$

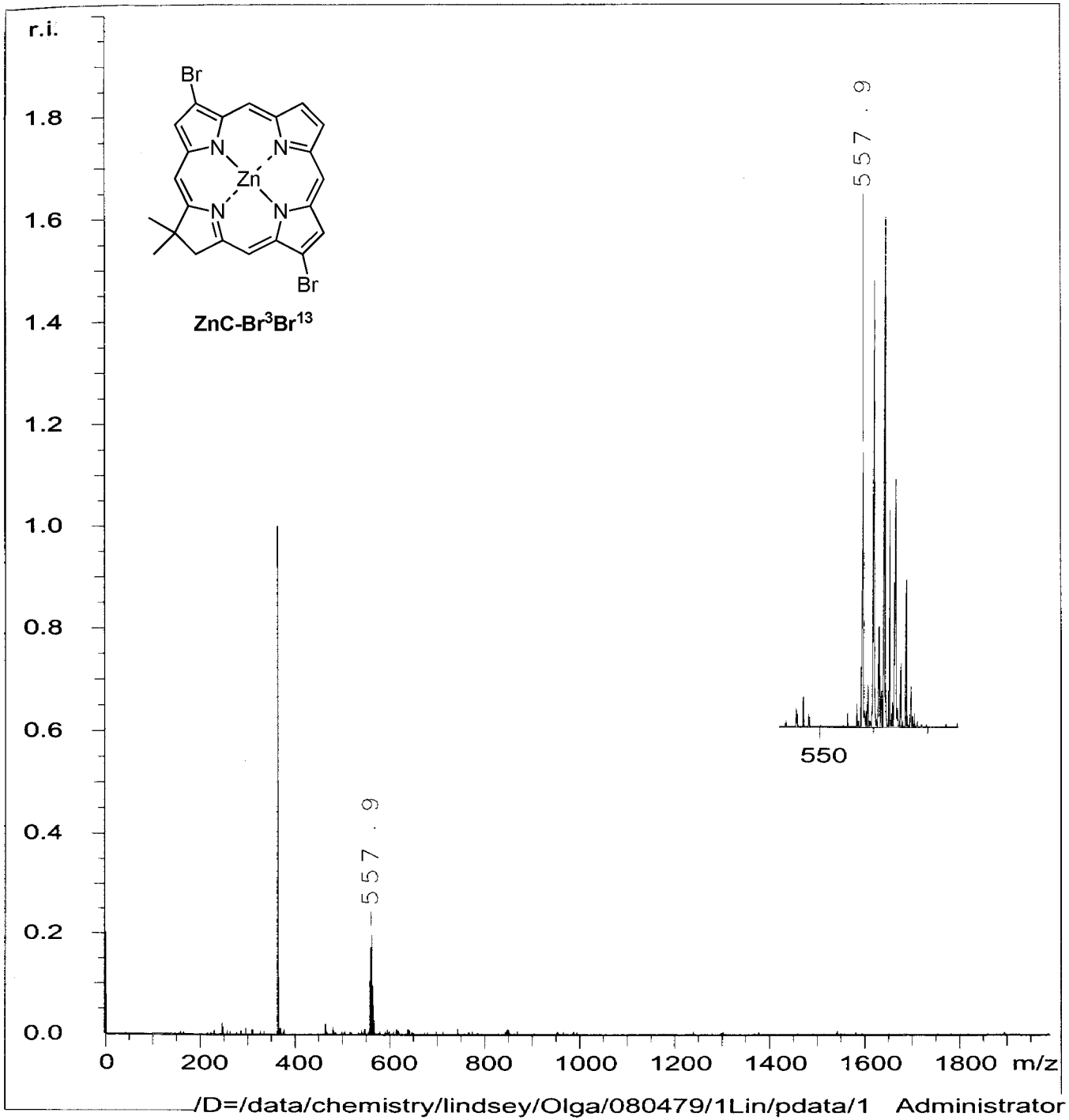





**ZnC-Br$^{3}$Br$^{13}$**

THF-$d_8$



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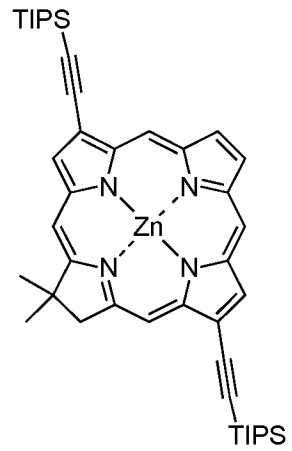
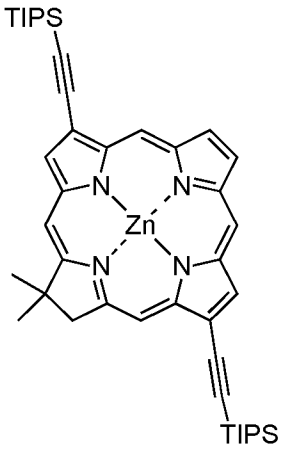
POLARI POS
AQOP_m Reflector
TD 28218
NoSHOTS 100
SMONUM 0
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 262 [ns]
Uis1 19.00 [kV]
Uis2 17.65 [kV]
Urefl 0.00 [kV]
Ulens 9.50 [kV]
Uhimass 0.00 [kV]
RefFull 0.00 [kV]
UdetL 1.62 [kV]
UdetR 0.00 [kV]
Udefl 1000.00 [kV]
REPHZ 3.00 [Hz]
ATTEN 42.0
ML1 2511610.121
ML2 313.047
ML3 0.000
HITURBO no
GDEON yes
GDEDLY short
DEFLON yes
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1 0.38
DPMASS 200.00 [Da]
RBNDVAL 0.00
LBNDVAL 0.00
IS2BNDV 0.00
CMT1 ZnCBr3Br13
CMT2 19_3

/D=/data/chemistry/lindsey/Olga/080479/1Lin/pdata/1 Administrator Wed Apr 1 18:06:02 2009



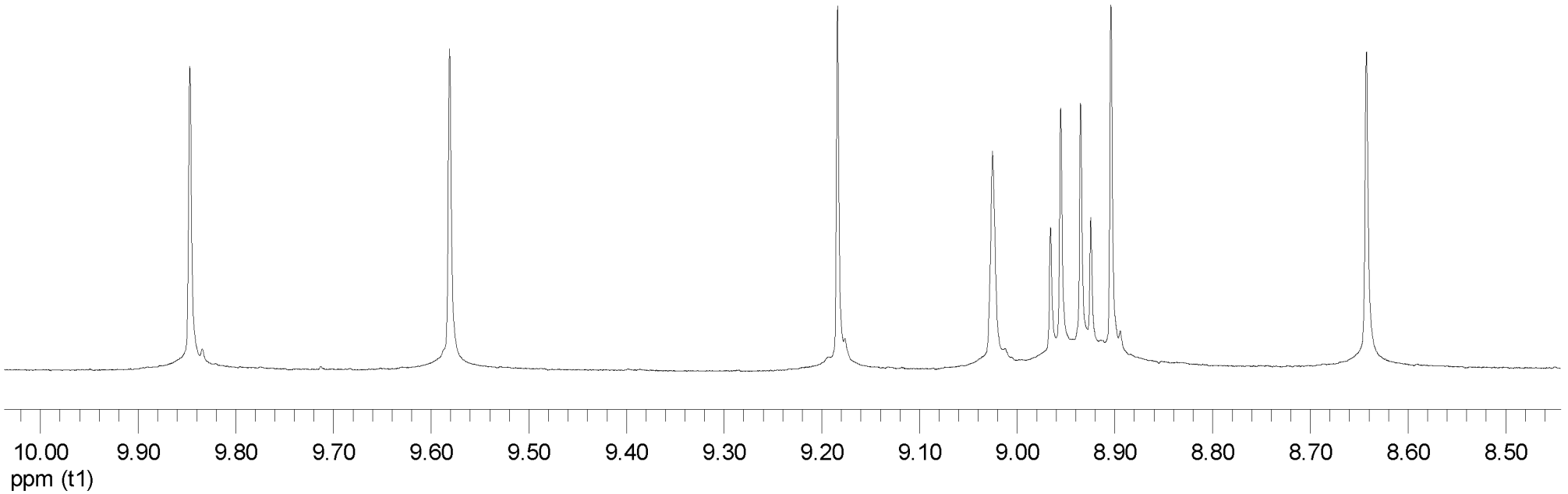

**ZnC-E$^{3}$E$^{13}$**

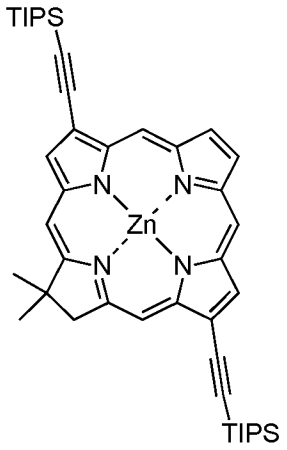
THF-$d_8$




**ZnC-E$^{3}$E$^{13}$**

THF-$d_8$






**ZnC-E$^{3}$E$^{13}$**

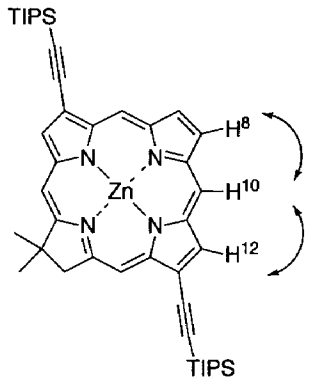
THF-$d_8$

Archive directory: /export/home/lindsey/vnmrsys/data
Sample directory: Olga/27_2D_26Sep2008

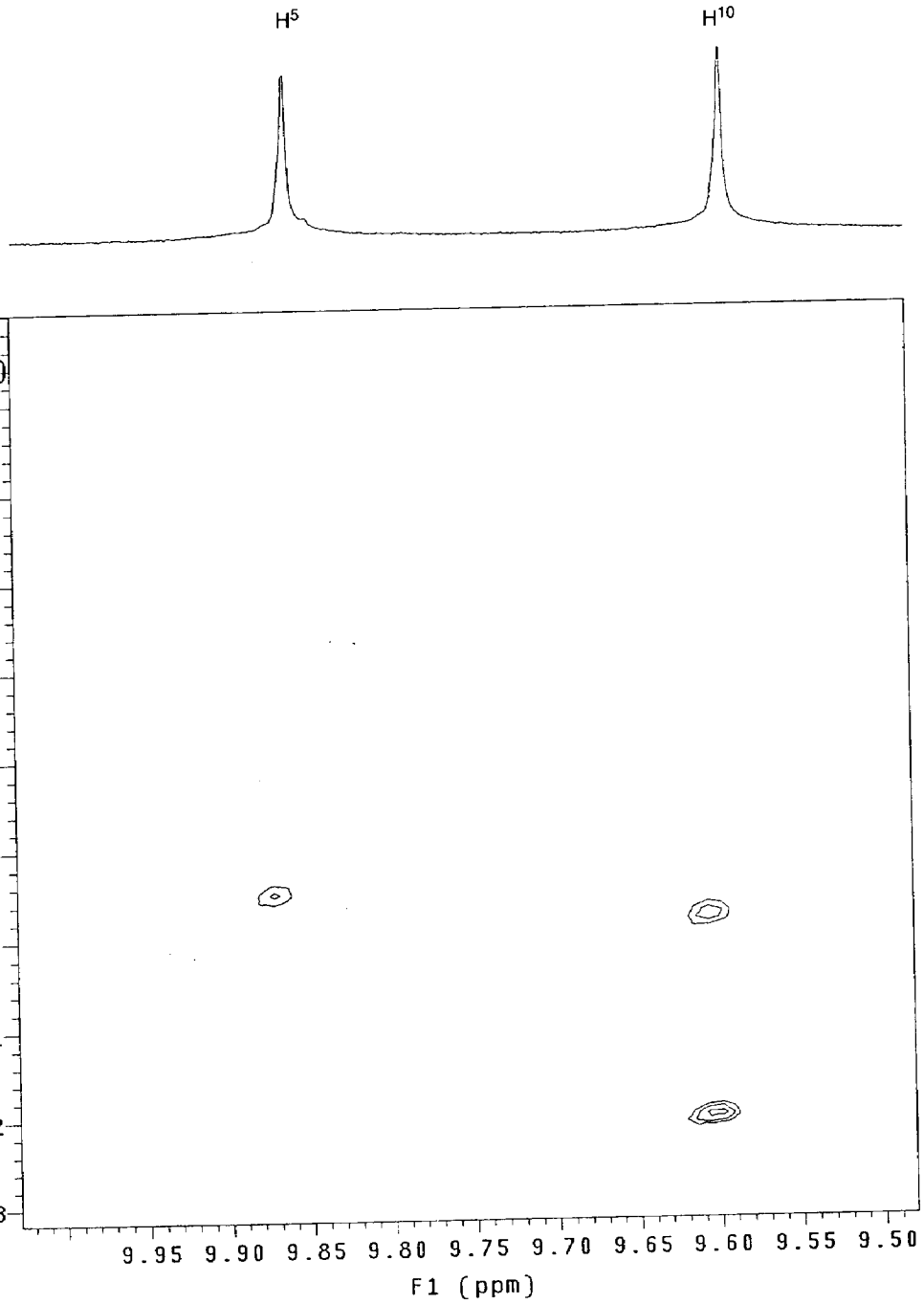
Pulse Sequence: NOESY

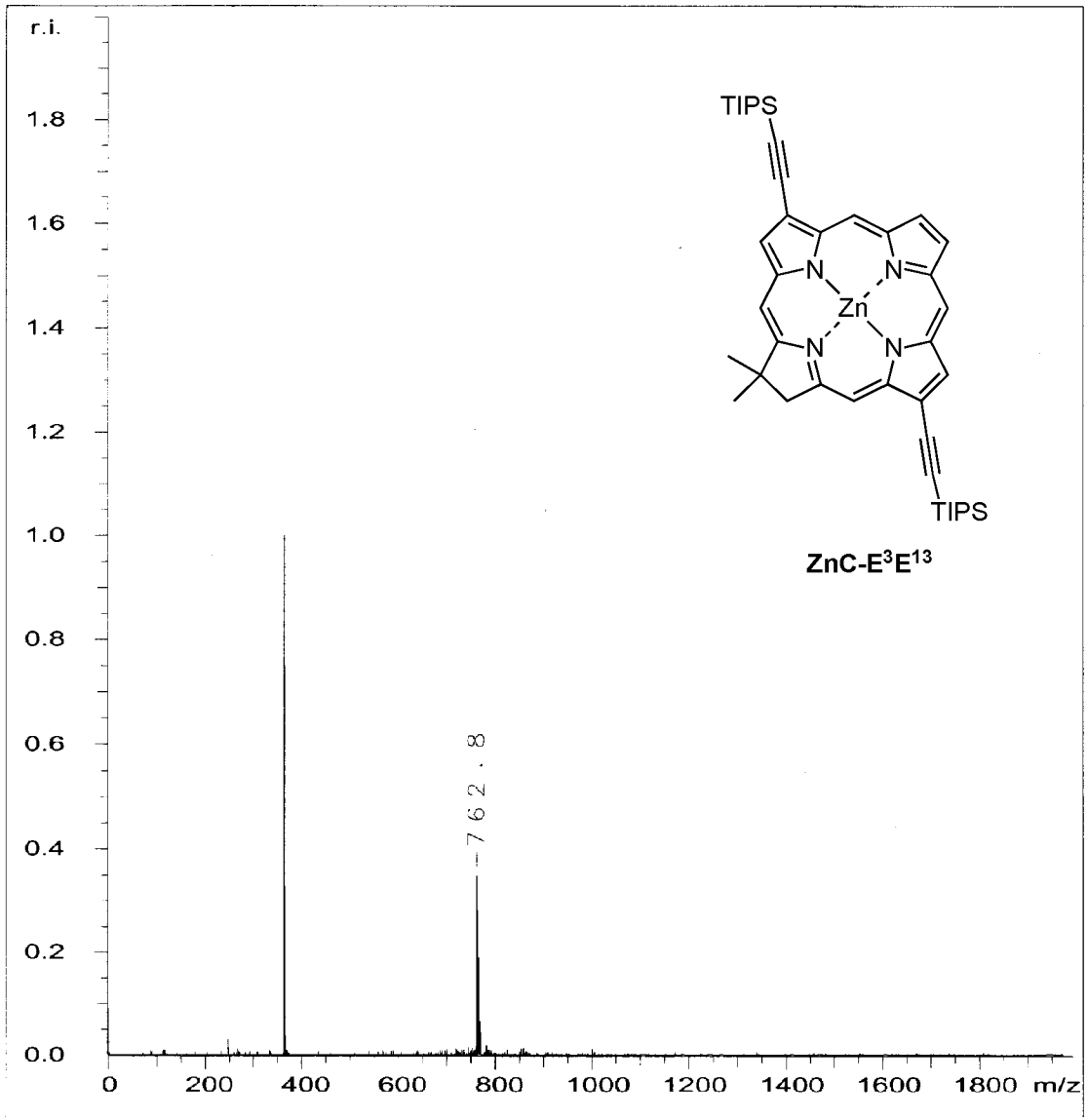
Solvent: THF
Ambient temperature
File: NOESY
Mercury-400BB "ncsumerc400"

Relax. delay 1.000 sec
Mixing 0.800 sec
Acq. time 0.160 sec
Width 6410.3 Hz
2D Width 6410.3 Hz
16 repetitions
2 x 512 increments
OBSERVE H1, 400.1366582 MHz
DATA PROCESSING
Gauss apodization 0.074 sec
F1 DATA PROCESSING
Gauss apodization 0.074 sec
FT size 4096 x 4096
Total time 9 hr, 23 min, 11 sec




**ZnC-E$^{3}$E$^{13}$**



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POLARI POS
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TD 28218
NoSHOTS 100
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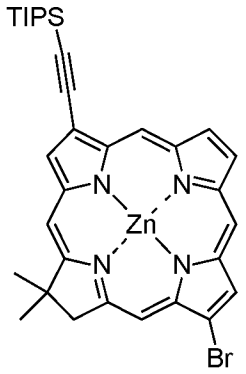
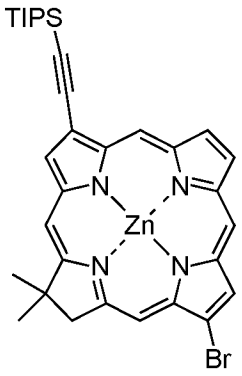
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 262 [ns]
Uis1 19.00 [kV]
Uis2 17.65 [kV]
Urefl 0.00 [kV]
Ulens 9.50 [kV]
Uhimass 0.00 [kV]
RefFull 0.00 [kV]
UdetL 1.62 [kV]
UdetR 0.00 [kV]
Udefl 1000.00 [kV]
REPHZ 3.00 [Hz]
ATTEN 57.0
ML1 2511610.121
ML2 313.047
ML3 0.000
HITURBO no
GDEON yes
GDEDLY short
DEFLON yes
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1 0.38
DPMASS 200.00 [Da]
RBNDVAL 0.00
LBNDVAL 0.00
IS2BNDV 0.00
CMT1 ZnCE3E13
CMT2 27



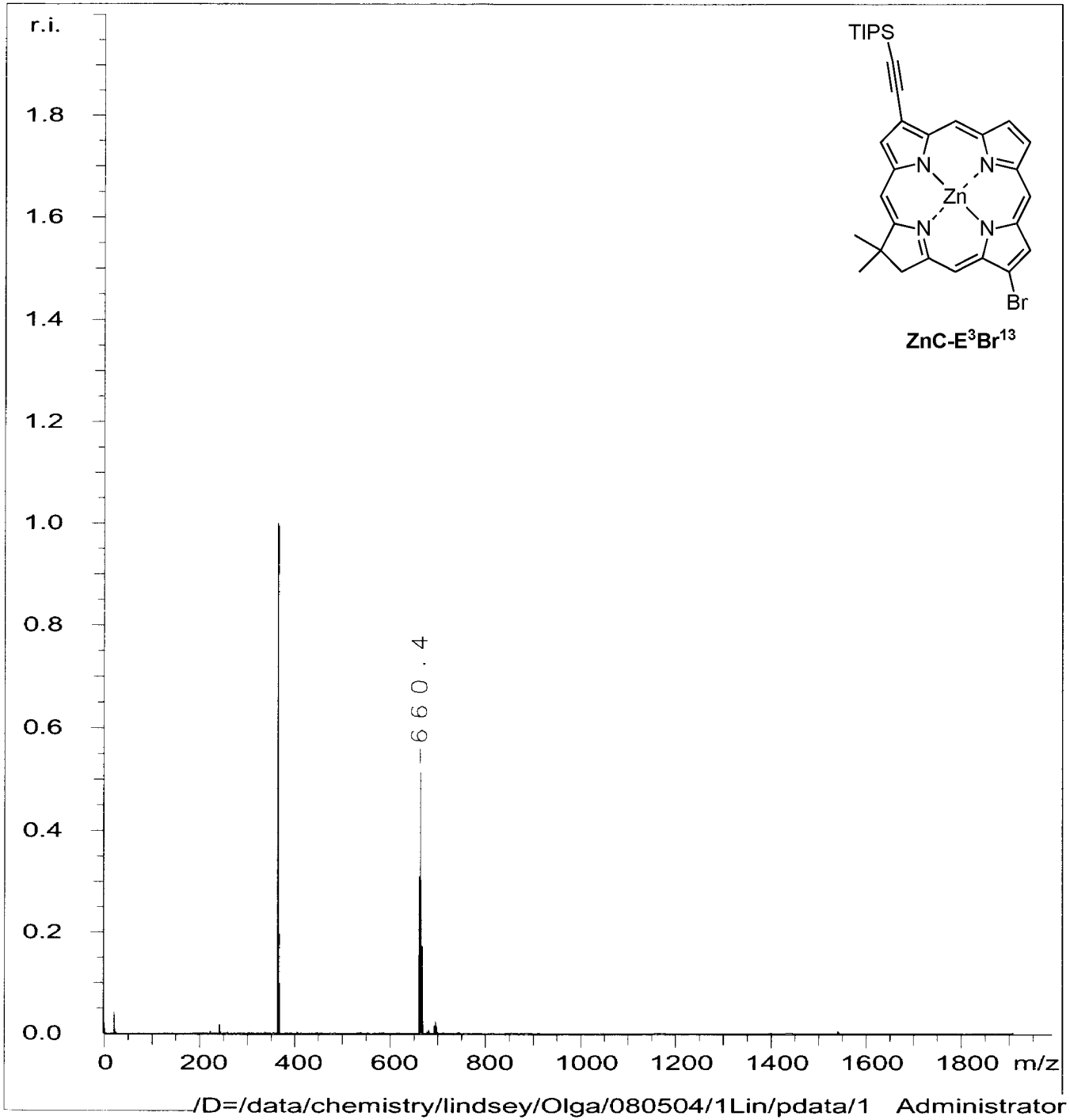

**ZnC-E$^{3}$Br$^{13}$**

THF-$d_8$




**ZnC-E$^{3}$Br$^{13}$**

THF-$d_8$

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TD 28218
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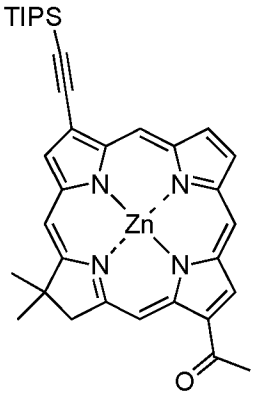
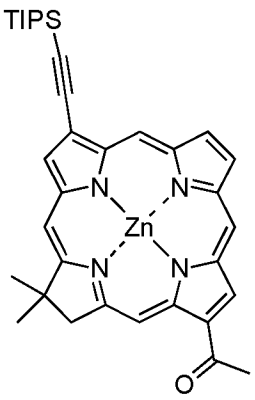
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 262 [ns]
Uis1 19.00 [kV]
Uis2 17.65 [kV]
Urefl 0.00 [kV]
Ulens 9.50 [kV]
Uhimass 0.00 [kV]
RefFull 0.00 [kV]
UdetL 1.62 [kV]
UdetR 0.00 [kV]
Udefl 1000.00 [kV]
REPHZ 3.00 [Hz]
ATTEN 95.0
ML1 2506114.959
ML2 295.701
ML3 0.000
HITURBO no
GDEON yes
GDEDLY short
DEFLON yes
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1 0.38
DPMASS 200.00 [Da]
RBNDVAL 0.00
LBNDVAL 0.00
IS2BNDV 0.00
CMT1 ZnC-E3Br13
CMT2



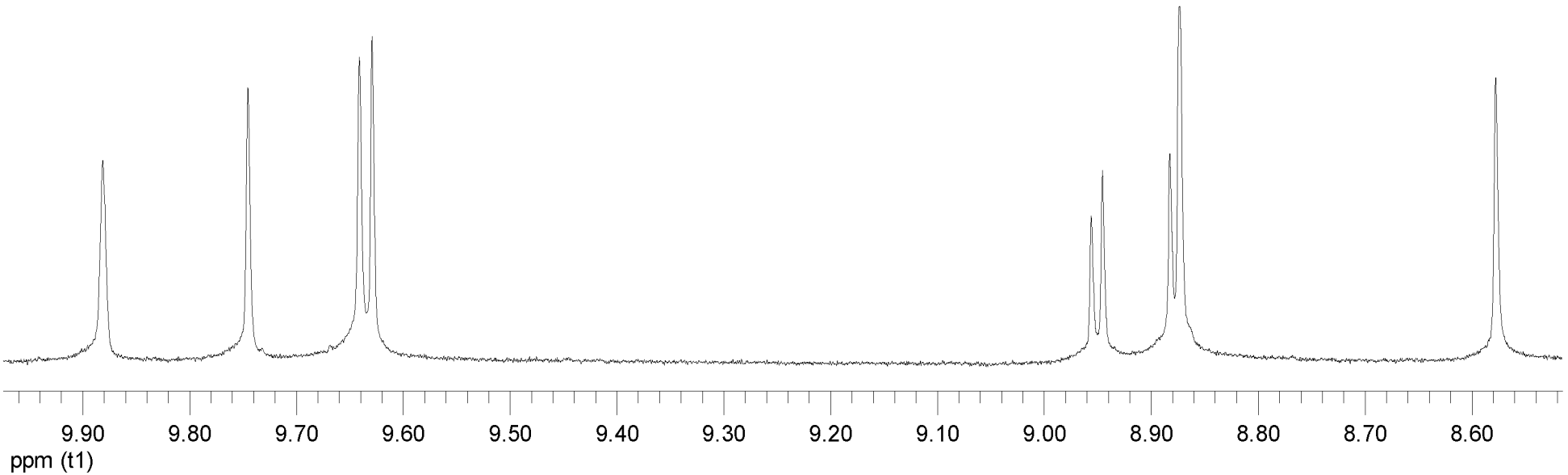

**ZnC-E$^3$A$^{13}$**

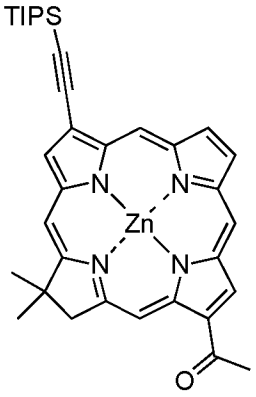
THF-$d_8$




**ZnC-E$^3$A$^{13}$**

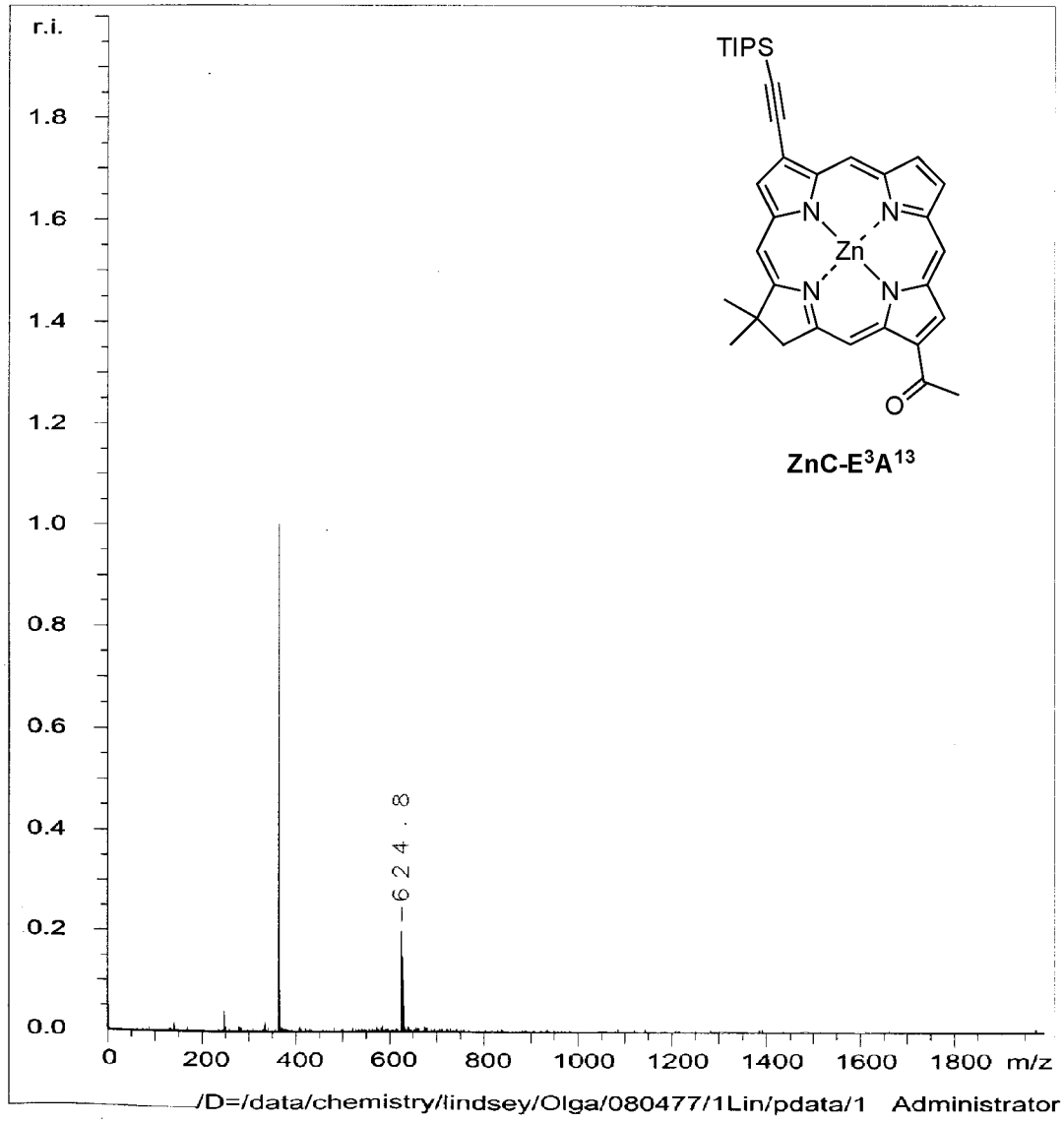
THF-$d_8$






**ZnC-E$^3$A$^{13}$**

THF-$d_8$

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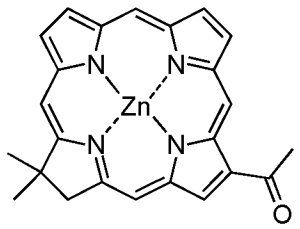
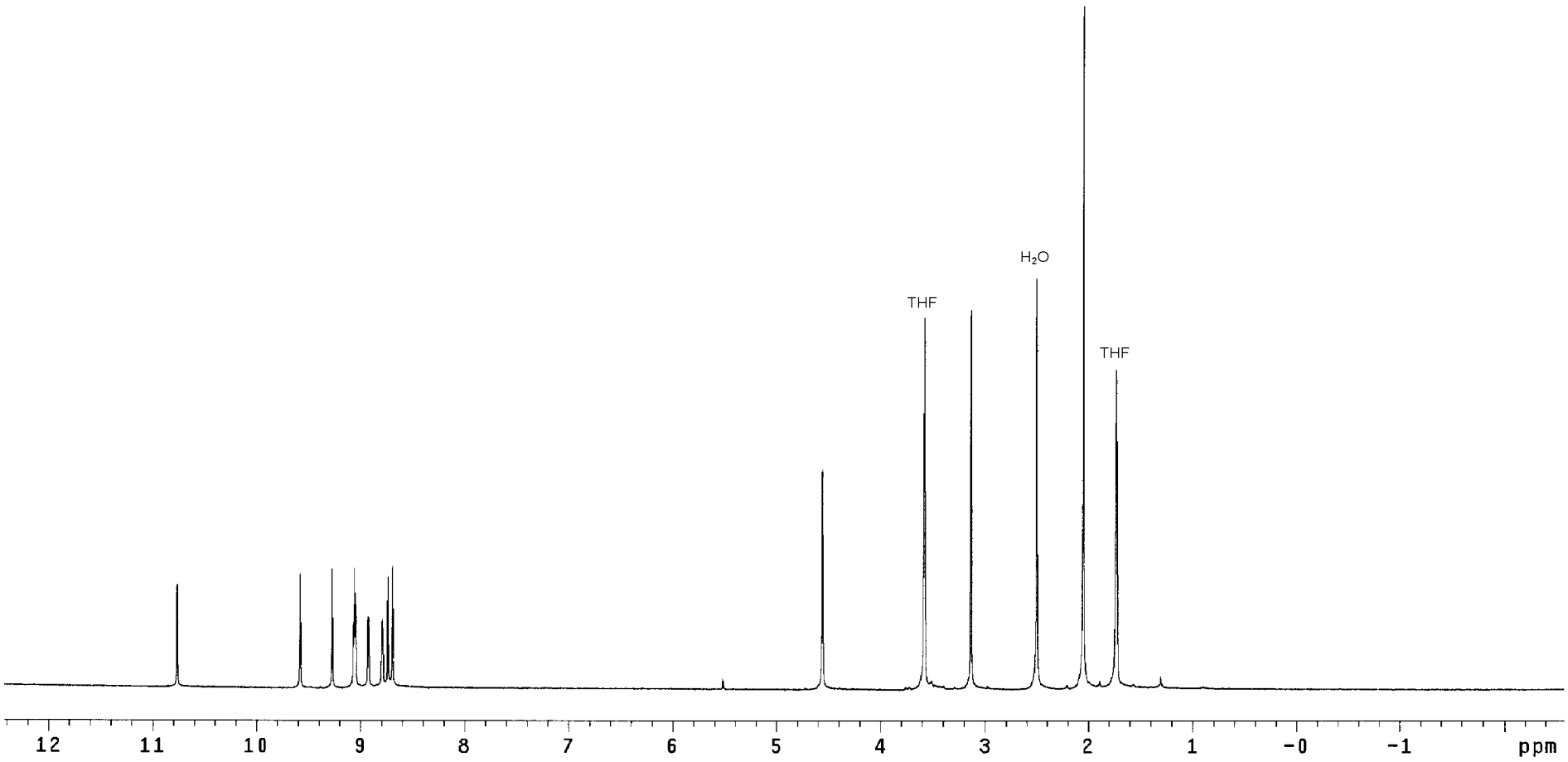
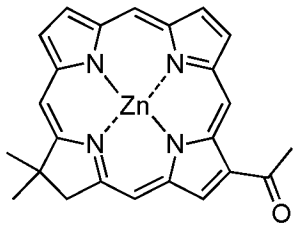
SMONUM 0
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 262 [ns]
Uis1 19.00 [kV]
Uis2 17.65 [kV]
Urefl 0.00 [kV]
Ulens 9.50 [kV]
Uhimass 0.00 [kV]
RefFull 0.00 [kV]
UdetL 1.62 [kV]
UdetR 0.00 [kV]
Udefl 1000.00 [kV]
REPHZ 3.00 [Hz]
ATTEN 63.0
ML1 2511610.121
ML2 313.047
ML3 0.000
HITURBO no
GDEON yes
GDEDLY short
DEFLON yes
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1 0.38
DPMASS 200.00 [Da]
RBNDVAL 0.00
LBNDVAL 0.00
IS2BNDV 0.00
CMT1 ZnCE3A13
CMT2 27_2




**ZnC-A**[12]

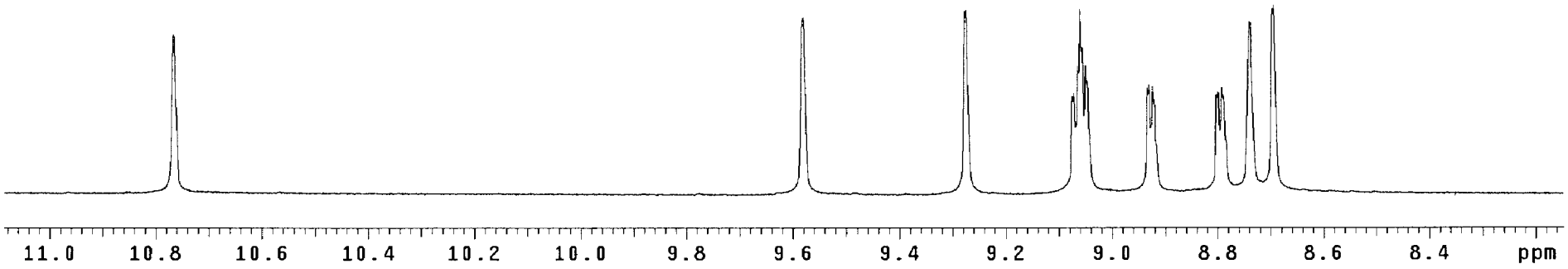
THF-$d_8$

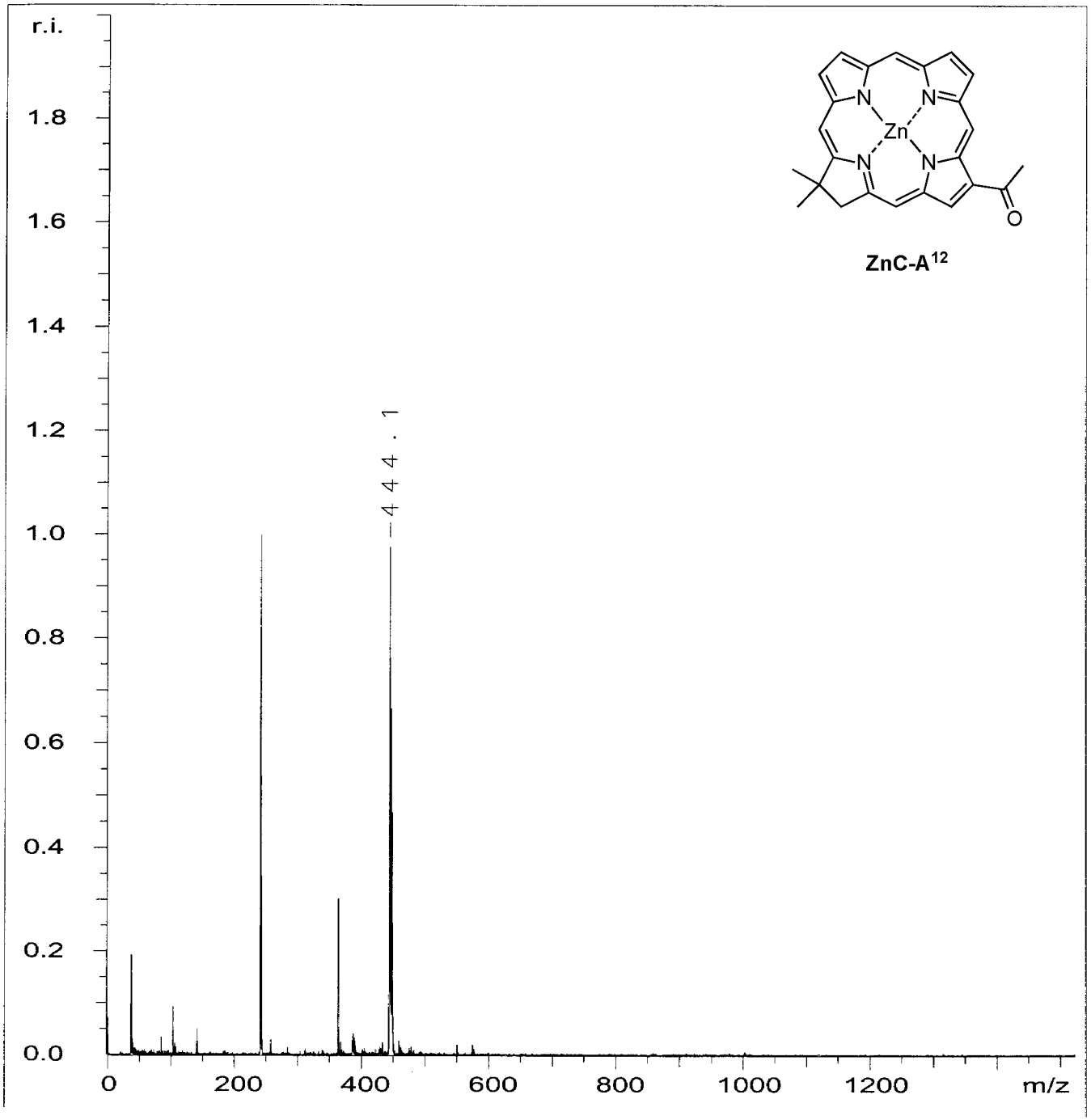





**ZnC-A**[12]

THF-$d_8$





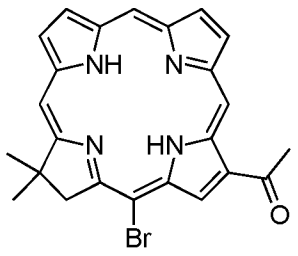




**ZnC-A**[12]

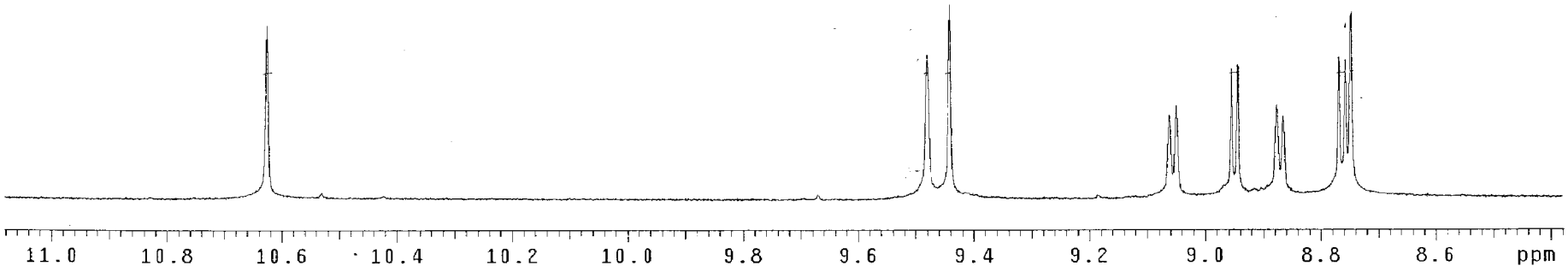
INSTRUM MASSDEC
OpId tof
SMPNAM 090363
AQ_DATE 2009-05-27 20:05:31
PATH D:\data\Chemistry\Lindsey\Olga
POLARI POS
AQOP_m Reflector
TD 38402
NoSHOTS 300
SMONUM 0
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 274 [ns]
Uis1 19.00 [kV]
Uis2 17.40 [kV]
Urefl 0.00 [kV]
Ulens 9.10 [kV]
Uhimass 0.00 [kV]
RefFull 0.00 [kV]
UdetL 1.65 [kV]
UdetR 0.00 [kV]
Udefl 0.00 [kV]
REPHZ 3.00 [Hz]
ATTEN 86.0
ML1 2521177.240
ML2 308.329
ML3 0.000
HITURBO no
GDEON yes
GDEDLY short
DEFLON no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1 0.38
DPMASS 500.00 [Da]
RBNDVAL 0.00
LBNDVAL 0.00
IS2BNDV 0.00
CMT1 ZnC-A12
CMT2

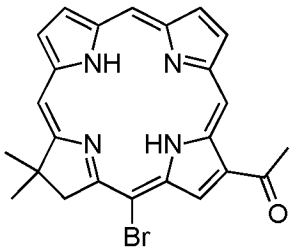
Wed May 27 20:36:29 2009




**$H_2C$-$A^{12}Br^{15}$**

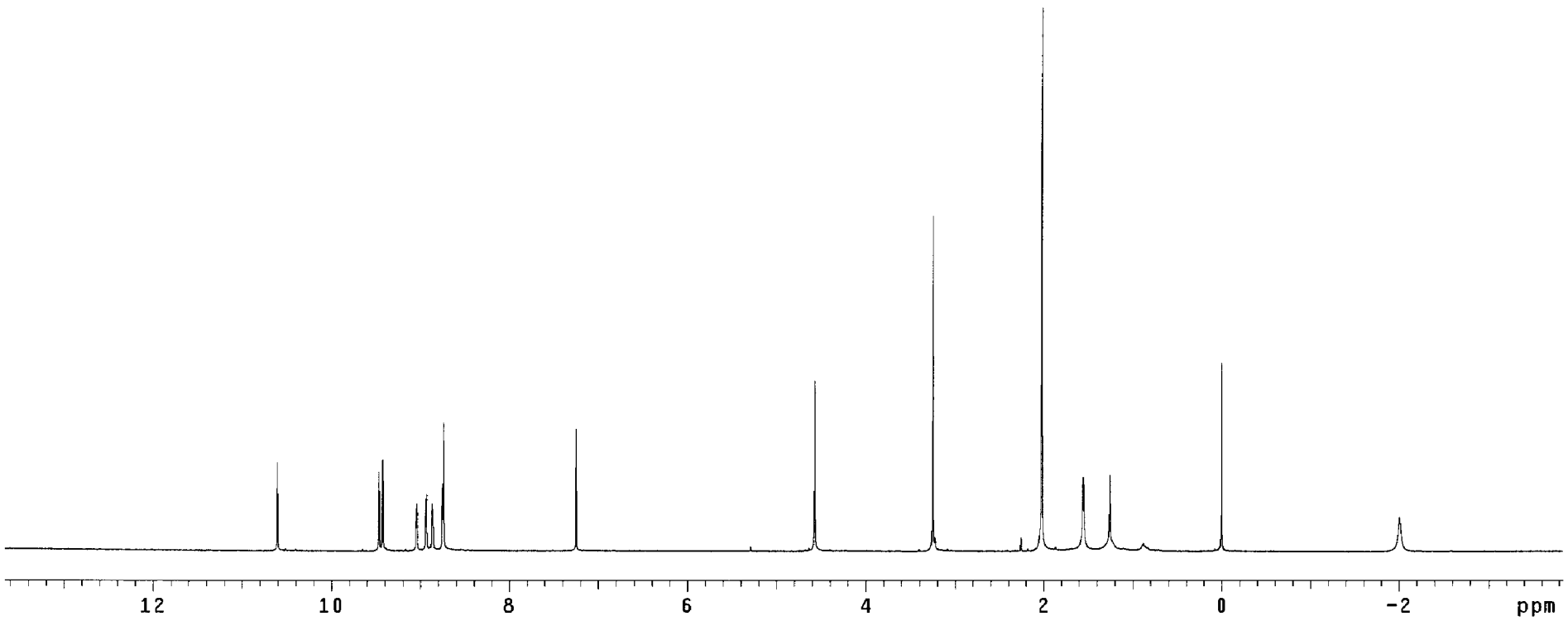
$CDCl_3$

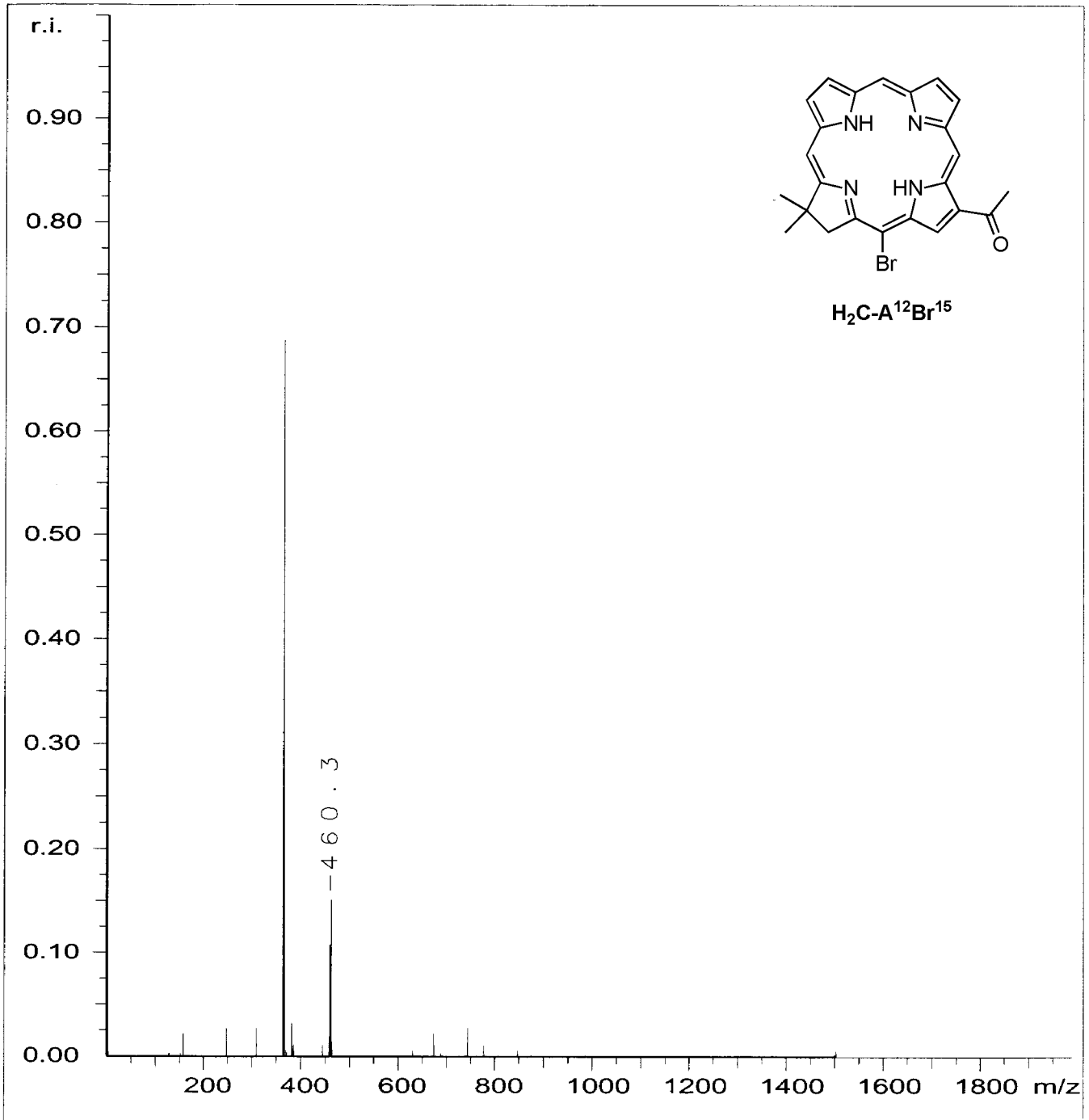





**$H_2C$-$A^{12}Br^{15}$**

$CDCl_3$






INSTRUM MASSDEC
OpId tof
SMPNAM 080455-67
AQ_DATE 2008-09-22 19:20:54
PATH D:\data\Chemistry\Lindsey\Olga
POLARI POS
AQOP_m Reflector
TD 28218
NoSHOTS 100
SMONUM 0
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 262 [ns]
Uis1 19.00 [kV]
Uis2 17.65 [kV]
Urefl 0.00 [kV]
Ulens 9.50 [kV]
Uhimass 0.00 [kV]
RefFull 0.00 [kV]
UdetL 1.62 [kV]
UdetR 0.00 [kV]
Udefl 1000.00 [kV]
REPHZ 3.00 [Hz]
ATTEN 52.0
ML1 2487154.283
ML2 261.746
ML3 -0.040
HITURBO no
GDEON yes
GDEDLY short
DEFLON yes
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1 0.38
DPMASS 200.00 [Da]
RBNDVAL 0.00
LBNDVAL 0.00
IS2BNDV 0.00
CMT1 CH2-CA12Br15
CMT2

/D=/data/chemistry/lindsey/Olga/080455-67/1Lin/pdata/1 Administrator Wed Apr 1 18:07:17 2009