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Supporting Figures

General

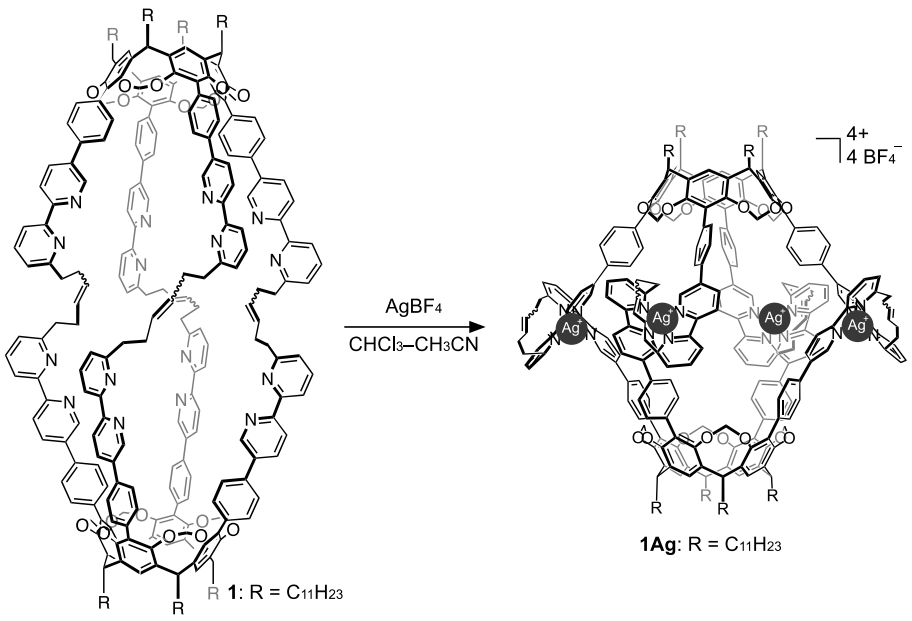
All chemicals and solvents were purchased from Kanto Chemical Co., Ltd., Wako Pure Chemical Co., Ltd., Tokyo Kasei Kogyo Co., Ltd., and Sigma-Aldrich Co., Ltd., and were used as received without further purification. NMR spectra were recorded on a Bruker APEX 400 MHz spectrometer, a JEOL ECA-500 MHz spectrometer. Chemical shifts are quoted as parts per million (ppm) relative to chloroform (chloroform-d_1, δ = 7.26 ppm for ^{1}H and 77.16 ppm for ^{13}C{^{1}H}). IR spectra were recorded on a JASCO FT/IR-4600 spectrometer.

Computational Methods

The geometry optimizations of the host-guest complexes were carried out by the Gaussian 16 Rev. C01. program using B3LYP/6-31G(d)+LanL2DZ level with gd3 correlation. The light atoms (C, H, N, O) were treated by the 6-31G(d) basis set and the heavy atoms (Ag) were treated by the LanL2DZ basis set. The long alkyl chains on the lower rim of the cavitands were replaced with hydrogen atoms for the calculations. The optimized structures are shown in Figures S20-S22. The atomic coordinates of the optimized structures are listed in Tables S1–5.

X-ray crystallography

Synthesis of Capsule 1Ag



1 (28 mg, 6.2 μmol) was dissolved in chloroform (1 mL). To this solution, $AgBF_4$ (5.1 g, 26 μmol) in acetonitrile (0.5 mL) was added. The mixture was stirred at room temperature for 30 min and evaporated under reduced pressure to give the product (32 mg, 6.1 mmol) in quantitative yield as brown solid.

M.p. >300 ℃; ^{1}H NMR (500 MHz, chloroform-d_1, 293 K): δ 9.02 (d, 8H, J = 8.3 Hz), 8.80 (d, 8H, J = 8.0 Hz), 8.42 (s, 8H), 8.26 (dd, 8H, J = 8.3 Hz, J = 1.5 Hz), 8.14 (t, 8H, J = 8.0 Hz), 7.43 (d, 8H, J = 8.0 Hz), 7.32 (d, 16H, J = 8.0 Hz), 7.29 (s, 8H), 7.06 (d, 16H, J = 8.0 Hz), 5.32 (d, 8H, J = 7.0 Hz), 5.17 (s, 8H), 4.83 (t, 8H, J = 8.0 Hz), 4.23 (d, 8H, J = 7.0 Hz), 3.27 (m, 8H), 2.80 (m, 8H), 2.05 (br, 8H), 2.41–2.21, 1.53–1.15, 0.95–0.84 (br, 192 H) ppm; ^{13}C{^{1}H} NMR (125 MHz, chloroform-d_1, 293 K): δ 160.1, 152.7, 152.4, 150.9, 150.7, 148.7, 140.3, 138.8, 138.6, 138.3, 136.1, 133.6, 131.2, 131.1, 131.1, 128.0, 127.0, 124.5, 121.7, 120.3, 100.8, 44.8, 37.3, 32.5, 32.1, 30.6, 30.0, 29.9, 29.5, 28.1, 22.8, 14.2 ppm; IR (KBr): ν 2925, 2853, 1972, 1596, 1574, 1454, 1400, 1369, 1306, 1258, 1156, 1082, 1022, 972, 809, 755, 584 cm^{-1}; HRMS (ESI+): calcd for $C_{304}H_{336}N_{16}O_{16}Ag_4BF_4$ m/z 1660.40622 $[M]^{3+}$, found m/z 1660.40665.

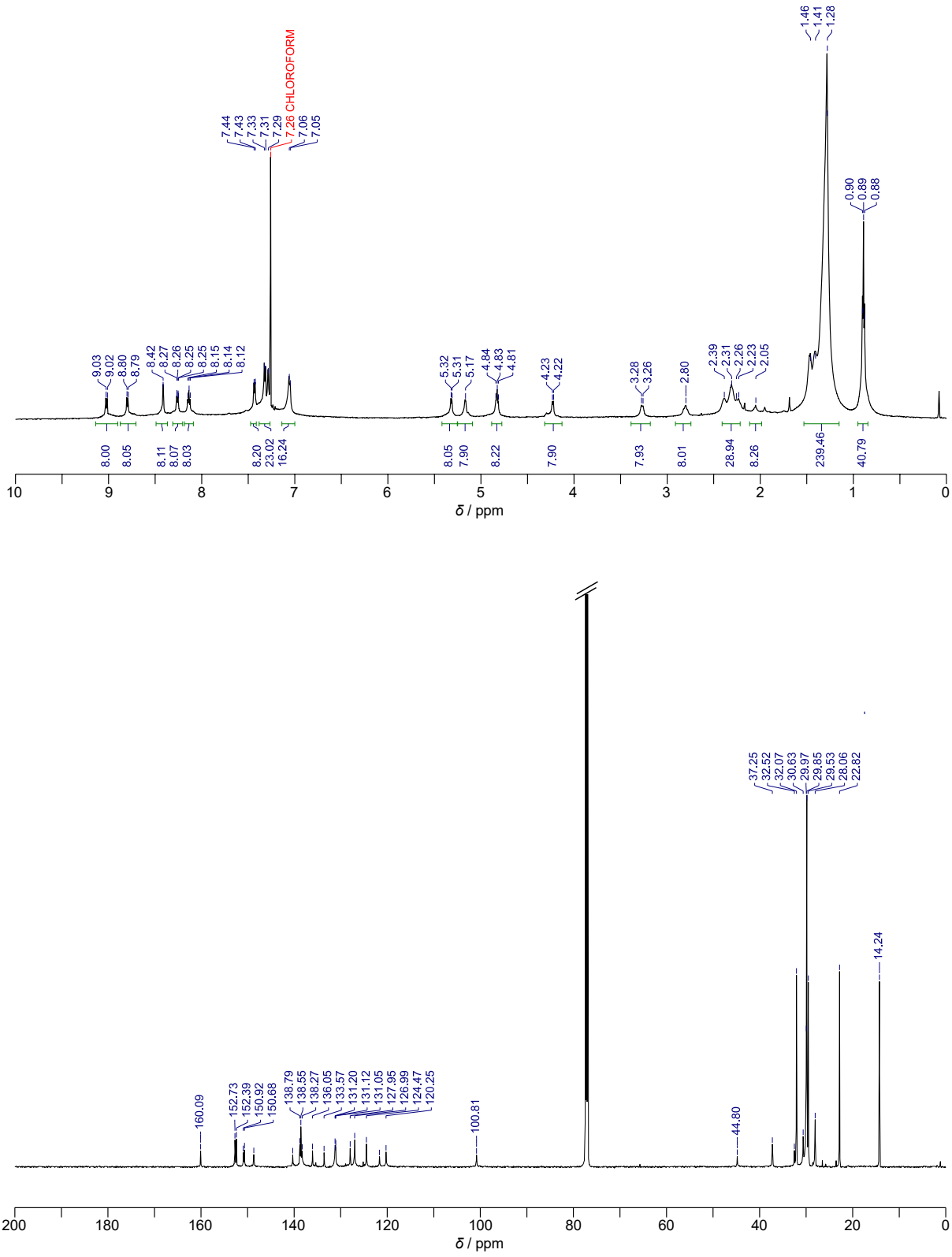


Figure S1. ^{1}H (500 MHz, chloroform-d_1, 298 K) and ^{13}C{1H} (125 MHz, chloroform-d_1, 298 K) NMR spectra of [**1Ag**]$(BF_4)_4$.

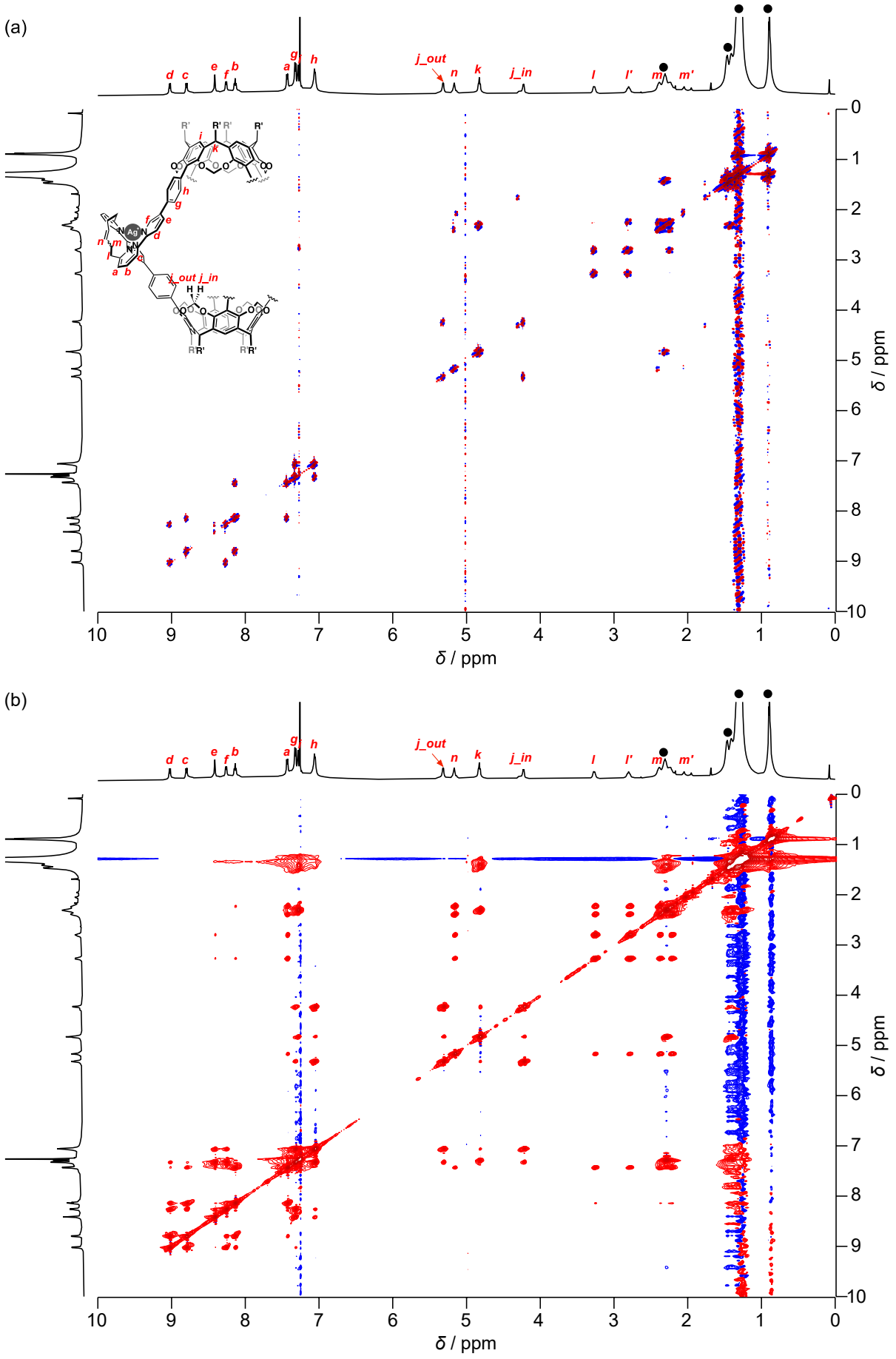
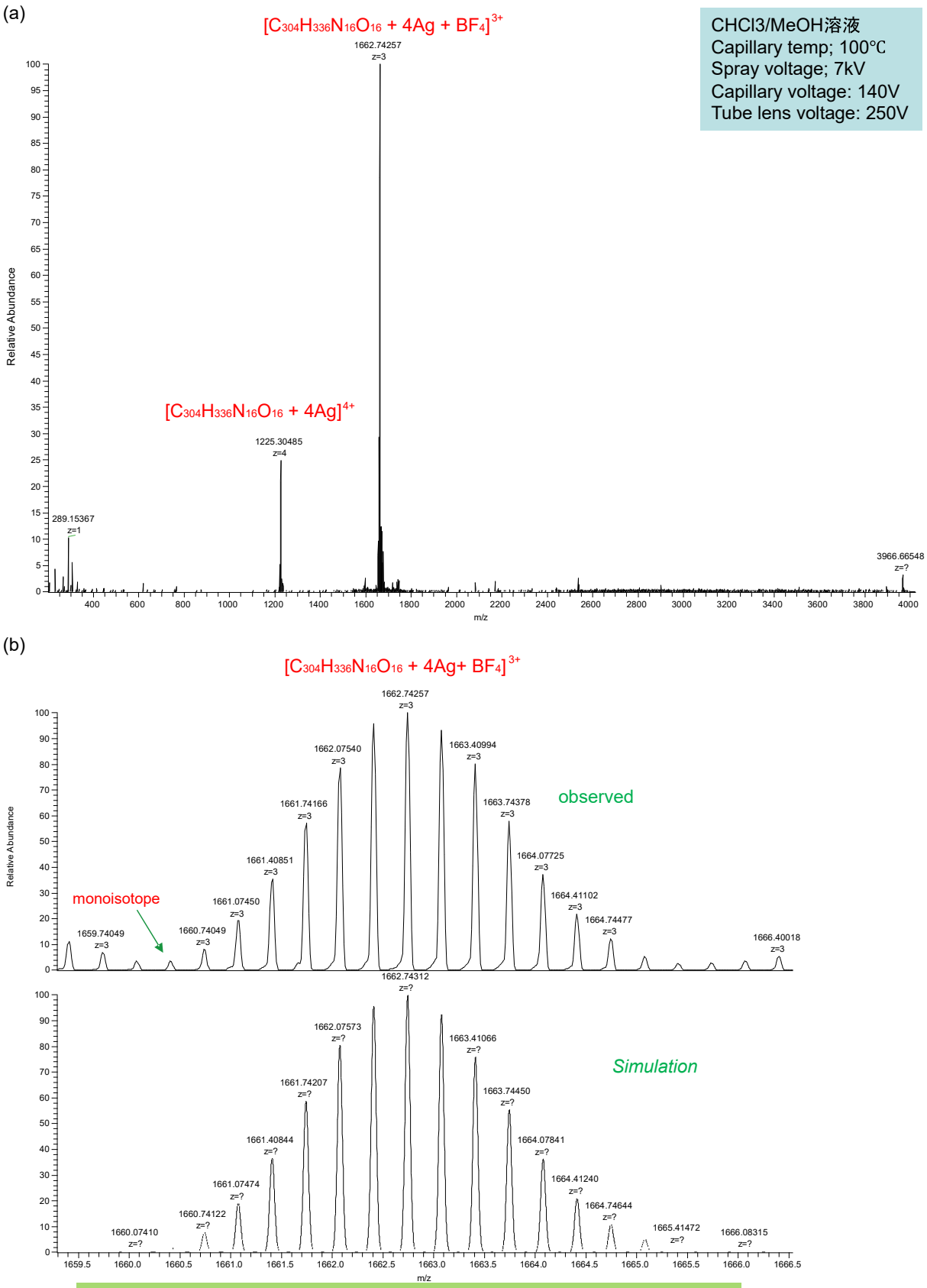


Figure S2. (a) DQF-COSY (500 MHz, chloroform-d_1, 298 K) and (b) NOESY (500 MHz, chloroform-d_1, 298 K) of [**1Ag**]$(BF_4)_4$. Mixing time = 500 ms.



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
1660.40665	1660.40622	0.26	143.5	C304 H336 O16 N16 Ag4 B F4

Figure S3. (a) ESI MS spectrum of [**1Ag**]$(BF_4)_4$ and (b) obseved and calculated isotope pattern of [**1Ag**+BF_4]$^{3+}$.

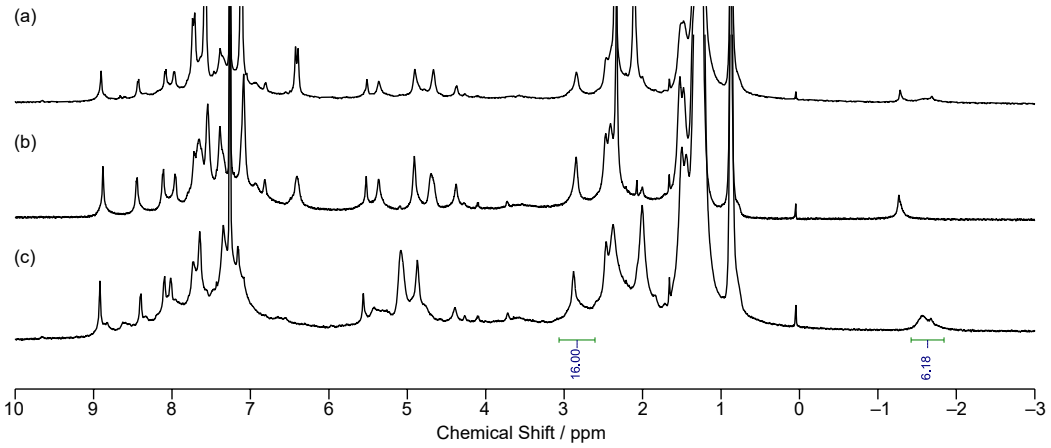


Figure S4. ^{1}H NMR spectra (500 MHz, chloroform-d_1, 223 K) of the mixture of (a) **1**, **G1a**, and **G2a** and (b) **1** and **G2a**, and (c) **1** and **G1a**. The concentration of **1**, **G1a**, and **G2a** are 1.5 mM, 15 mM, and 15 mM, respectively.

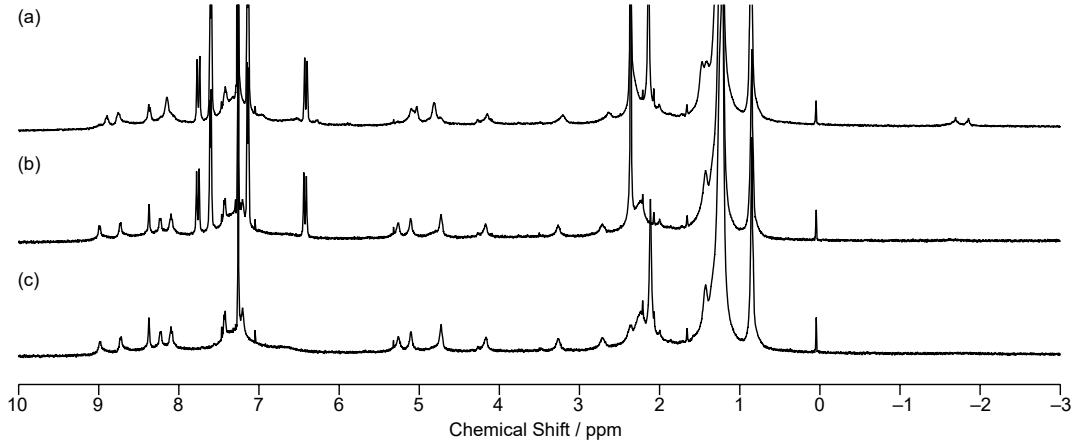


Figure S5. ^{1}H NMR spectra (500 MHz, chloroform-d_1, 223 K) of the mixture of (a) [**1Ag**](BF$_4$)$_4$, **G1a**, and **G2a** and (b) [**1Ag**](BF$_4$)$_4$ and **G2a**, and (c) [**1Ag**](BF$_4$)$_4$ and **G1a**. The concentrations of [**1Ag**](BF$_4$)$_4$, **G1a**, and **G2a** are 1.5 mM, 15 mM, and 15 mM, respectively.

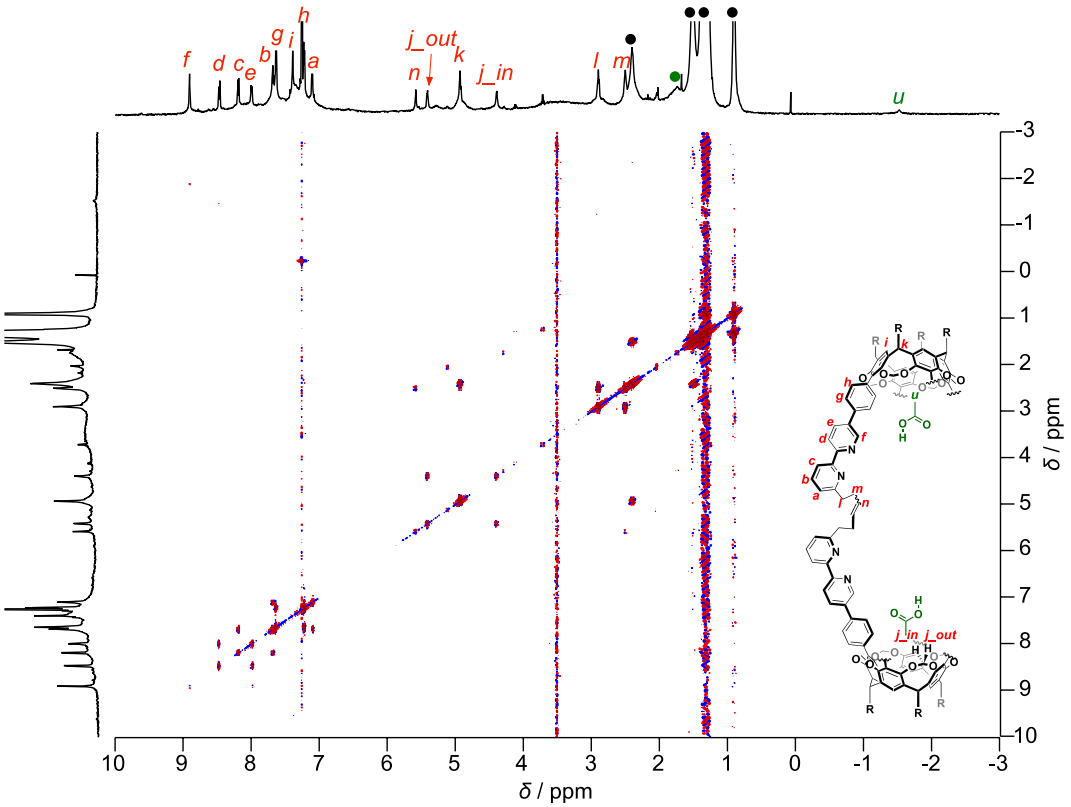


Figure S6. DQF-COSY (500 MHz, chloroform-d_1, 298 K) of a mixture of **1** and **G1a**. The concentrations of **1** and **G1a** are 1.5 mM and 15 mM, respectively. Mixing time = 500 ms.

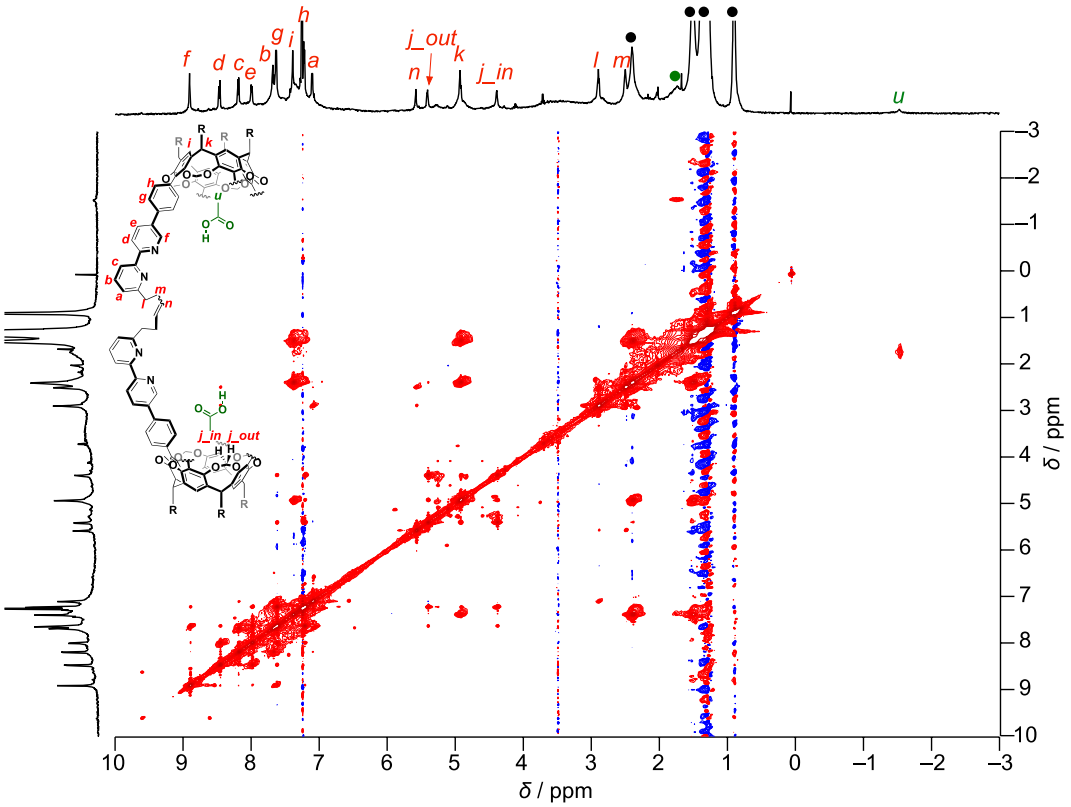


Figure S7. NOESY (500 MHz, chloroform-d_1, 298 K) of a mixture of **1** and **G1a**. The concentrations of **1** and **G1a** are 1.5 mM and 15 mM, respectively. Mixing time = 500 ms.

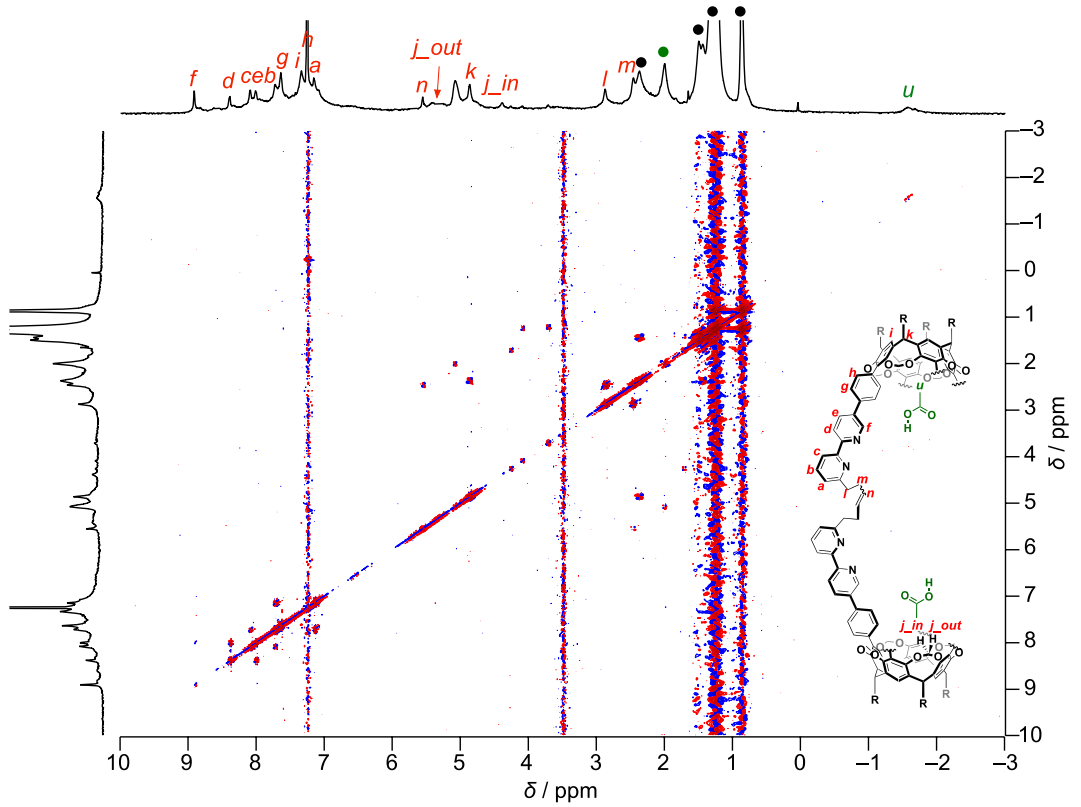


Figure S8. DQF-COSY (500 MHz, chloroform-d_1, 223 K) of a mixture of **1** and **G1a**. The concentrations of **1** and **G1a** are 1.5 mM and 15 mM, respectively. Mixing time = 500 ms.

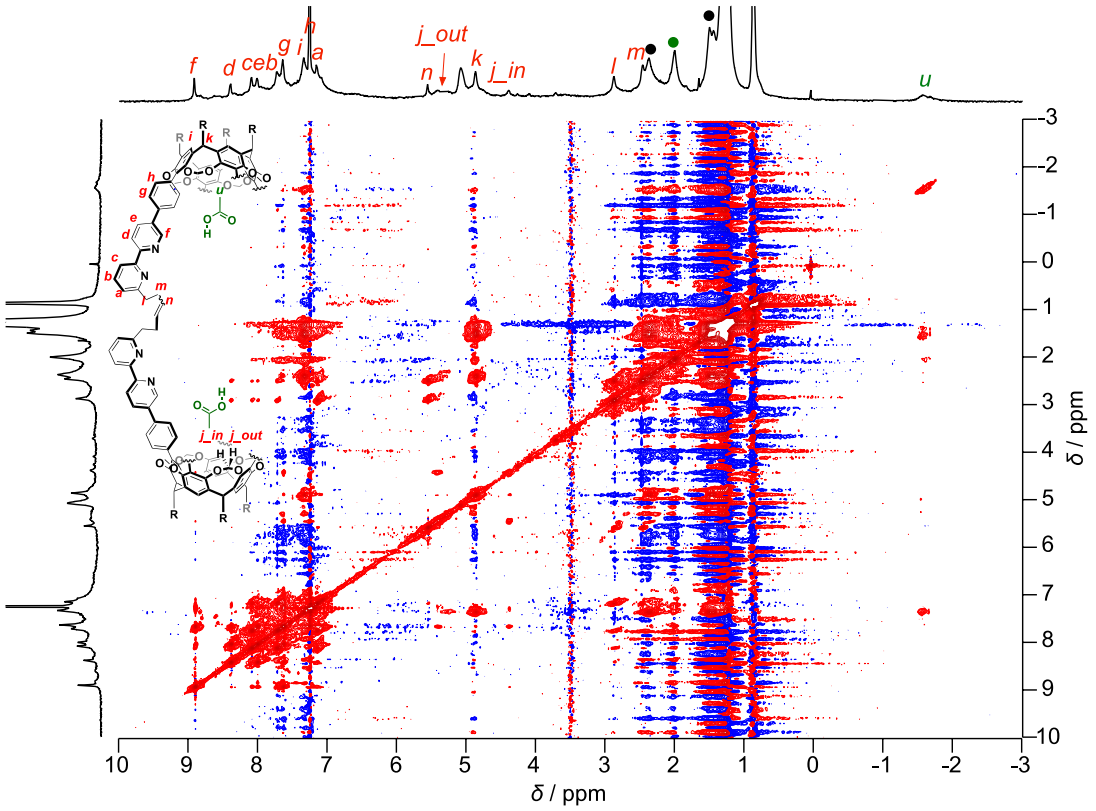


Figure S9. (a) NOESY (500 MHz, chloroform-d_1, 223 K) of a mixture of **1** and **G1a**. The concentrations of **1** and **G1a** are 1.5 mM and 15 mM, respectively. Mixing time = 500 ms.

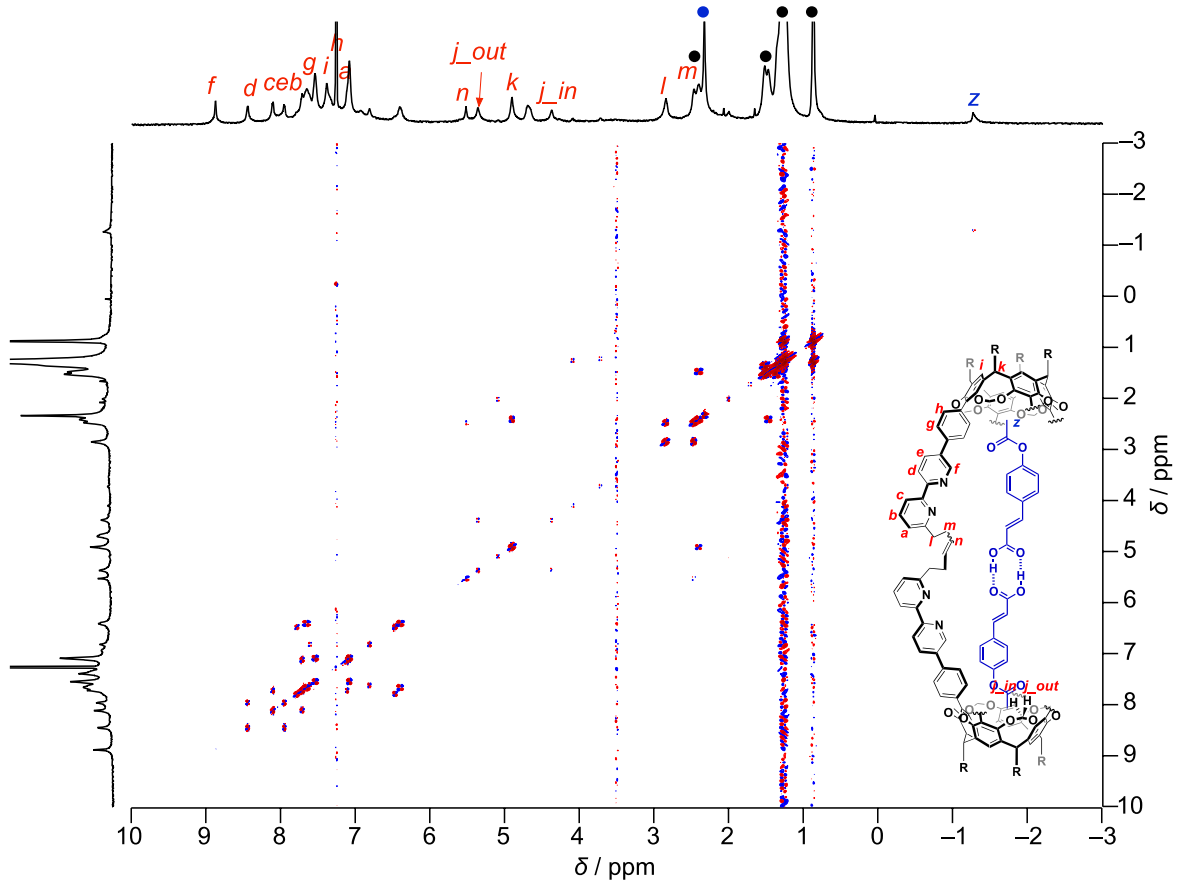


Figure S10. COSY (500 MHz, chloroform-d_1, 223 K) of a mixture of **1** and **G2a**. The concentration of **1** and **G2a** are 1.5 mM and 15 mM, respectively. Mixing time = 500 ms.

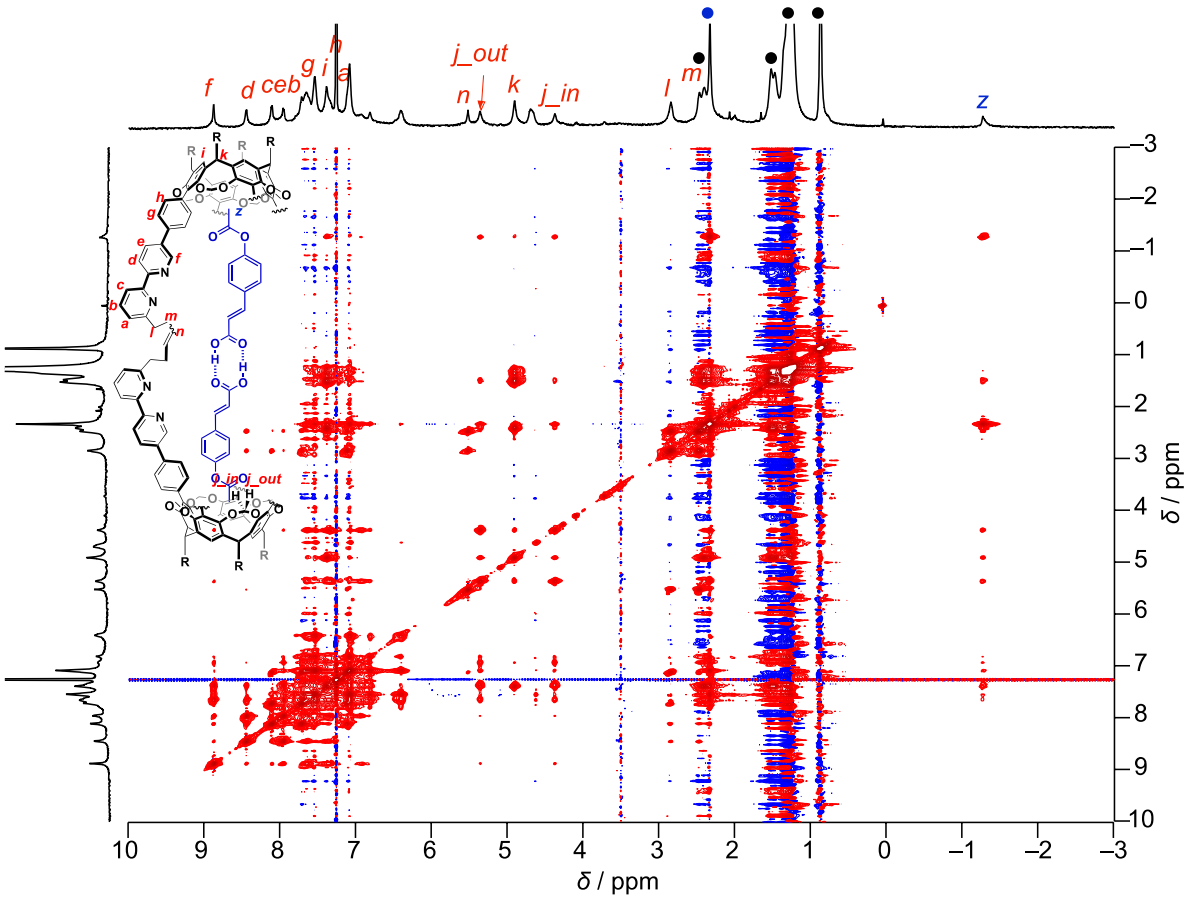


Figure S11. NOESY (500 MHz, chloroform-d_1, 223 K) of a mixture of **1** and **G2a**. The concentration of **1** and **G2a** are 1.5 mM and 15 mM, respectively. Mixing time = 500 ms.

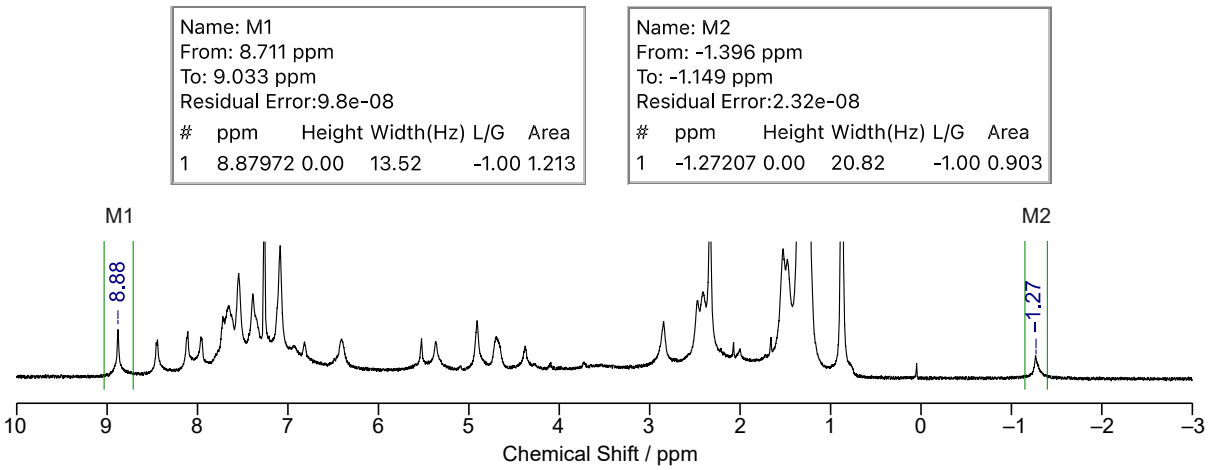


Figure S12. ^{1}H NMR (500 MHz, chloroform-d_1, 223 K) spectra of **1** (1.5 mM) and **G2a** (15 mM) with the signal intensities of **1** and **G2a**.

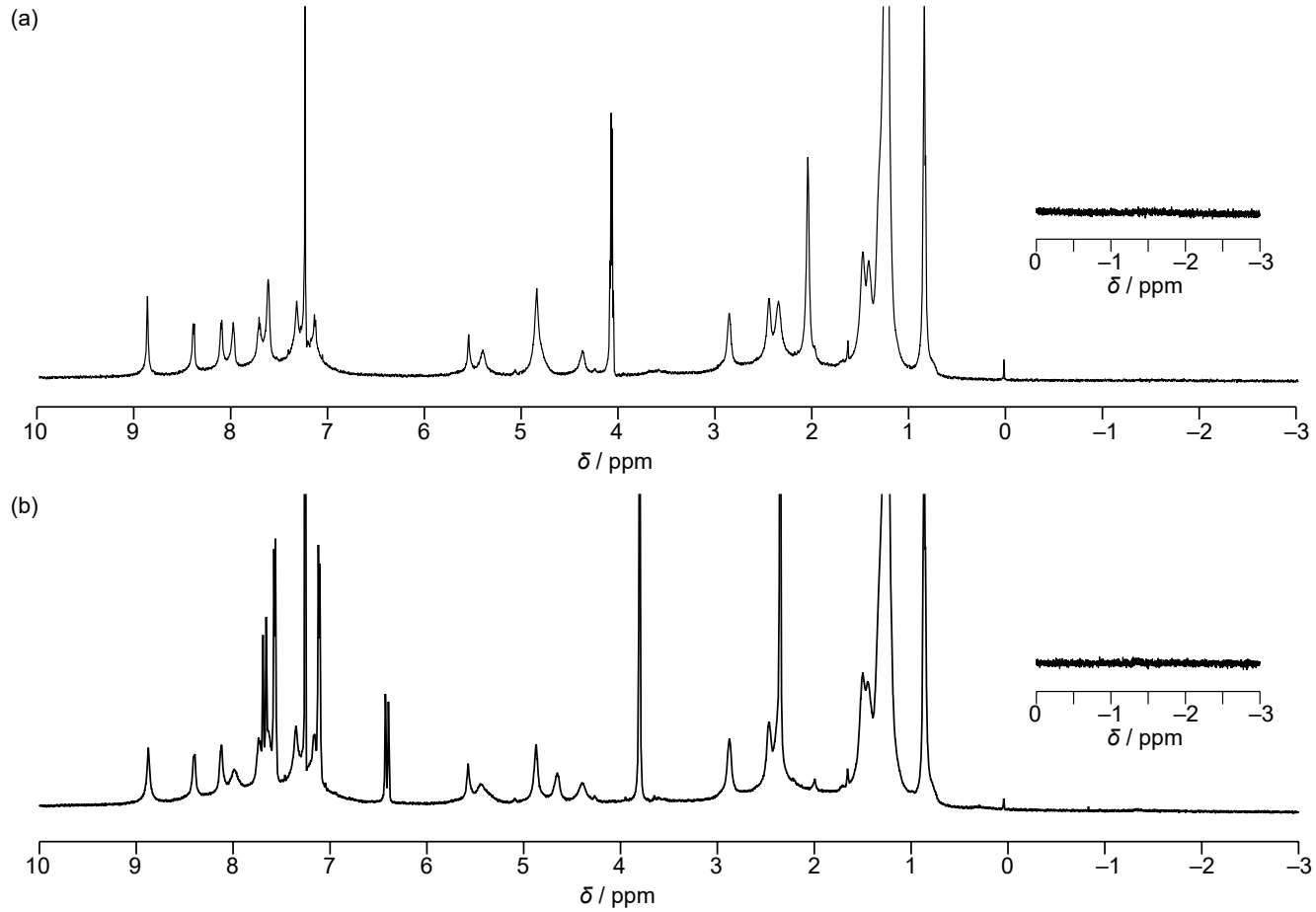


Figure S13. ^{1}H NMR (500 MHz, chloroform-d_1, 223 K) spectra of **1** (1.5 mM) with (a) **G1b** (10 mM) and (b) **G2b** (15 mM).

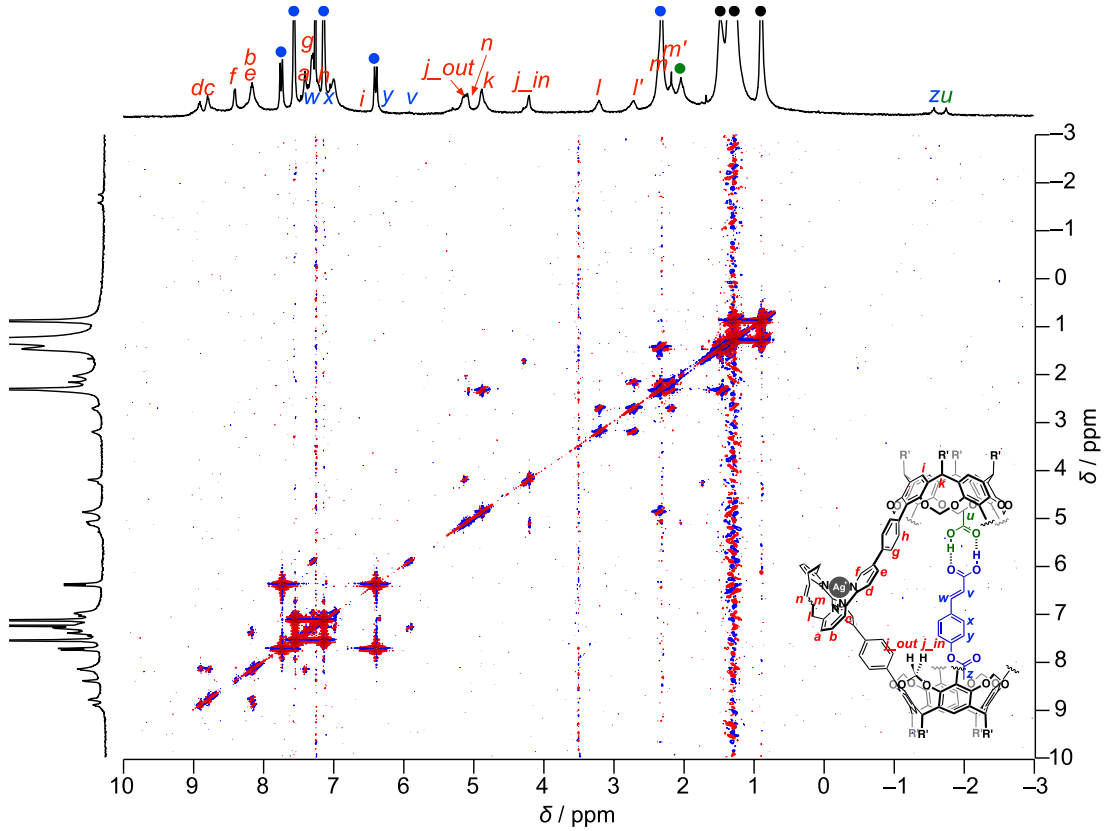


Figure S14. DQF-COSY (500 MHz, chloroform-d_1, 298 K) of a mixture of [**1Ag**]$(BF_4)_4$, **G1a**, and **G2a**. The concentration of [**1Ag**]$(BF_4)_4$, **G1a**, and **G2a** are 1.5 mM, 15 mM, and 15 mM, respectively. Mixing time = 500 ms.

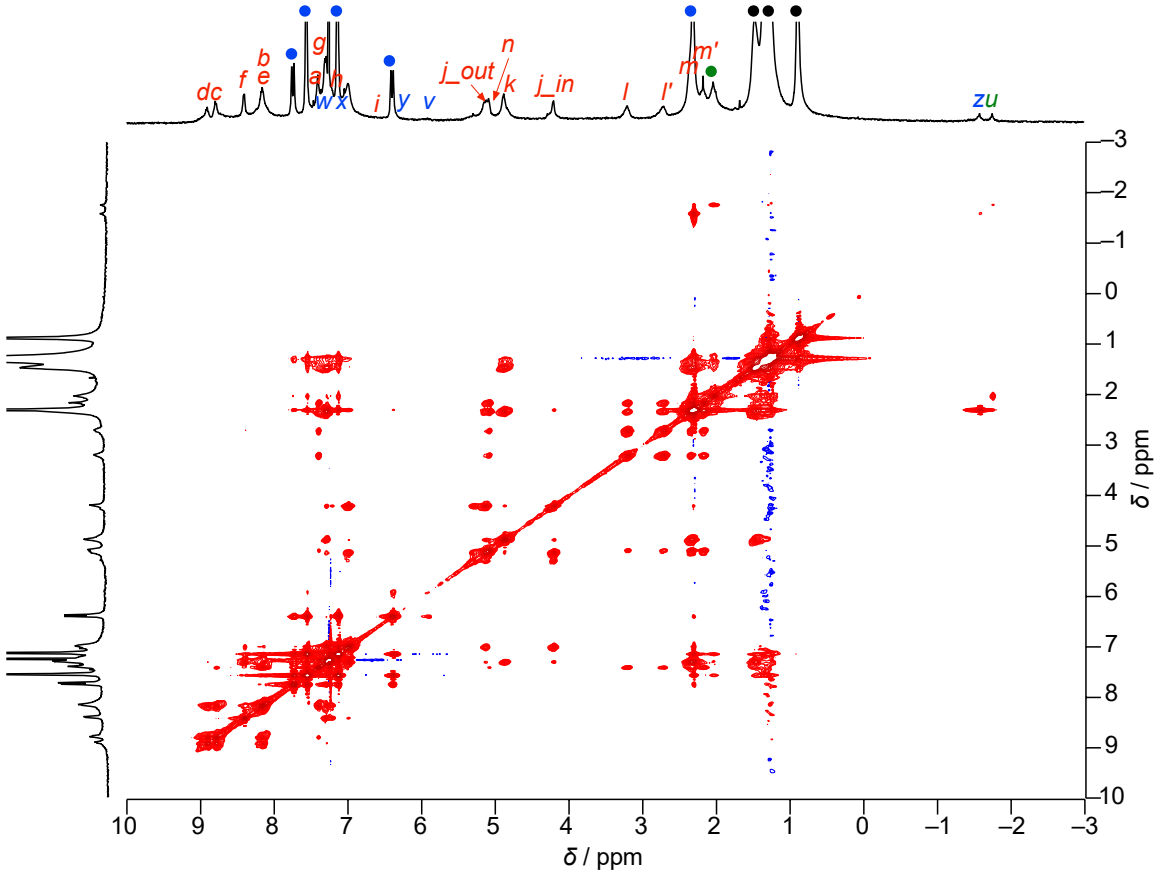


Figure S15. NOESY (500 MHz, chloroform-d_1, 298 K) of a mixture of [**1Ag**]$(BF_4)_4$, **G1a**, and **G2a**. The concentration of [**1Ag**]$(BF_4)_4$, **G1a**, and **G2a** are 1.5 mM, 15 mM, and 15 mM, respectively. Mixing time = 500 ms.

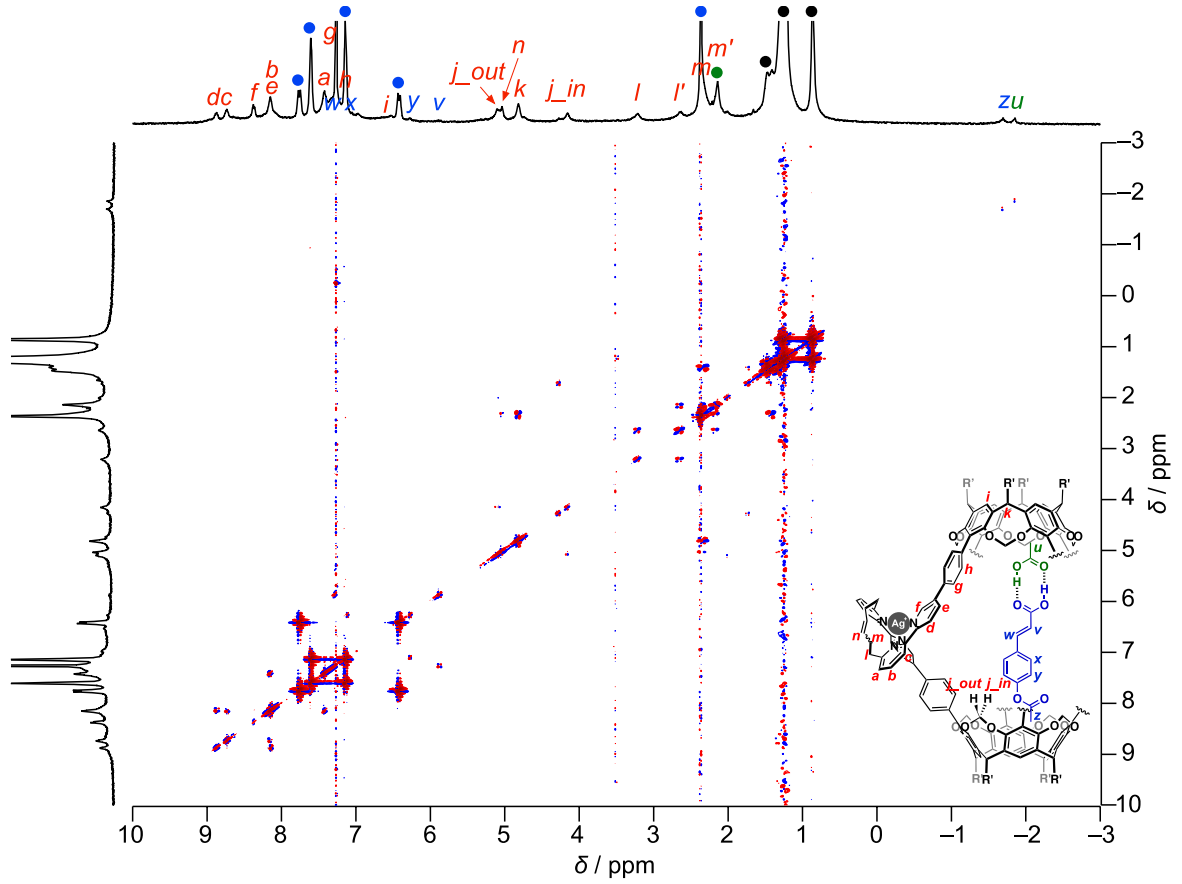


Figure S16. DQF-COSY (500 MHz, chloroform-d_1, 223 K) of a mixture of [**1Ag**]$(BF_4)_4$, **G1a**, and **G2a**. The concentration of [**1Ag**]$(BF_4)_4$, **G1a**, and **G2a** are 1.5 mM, 15 mM, and 15 mM, respectively. Mixing time = 500 ms.

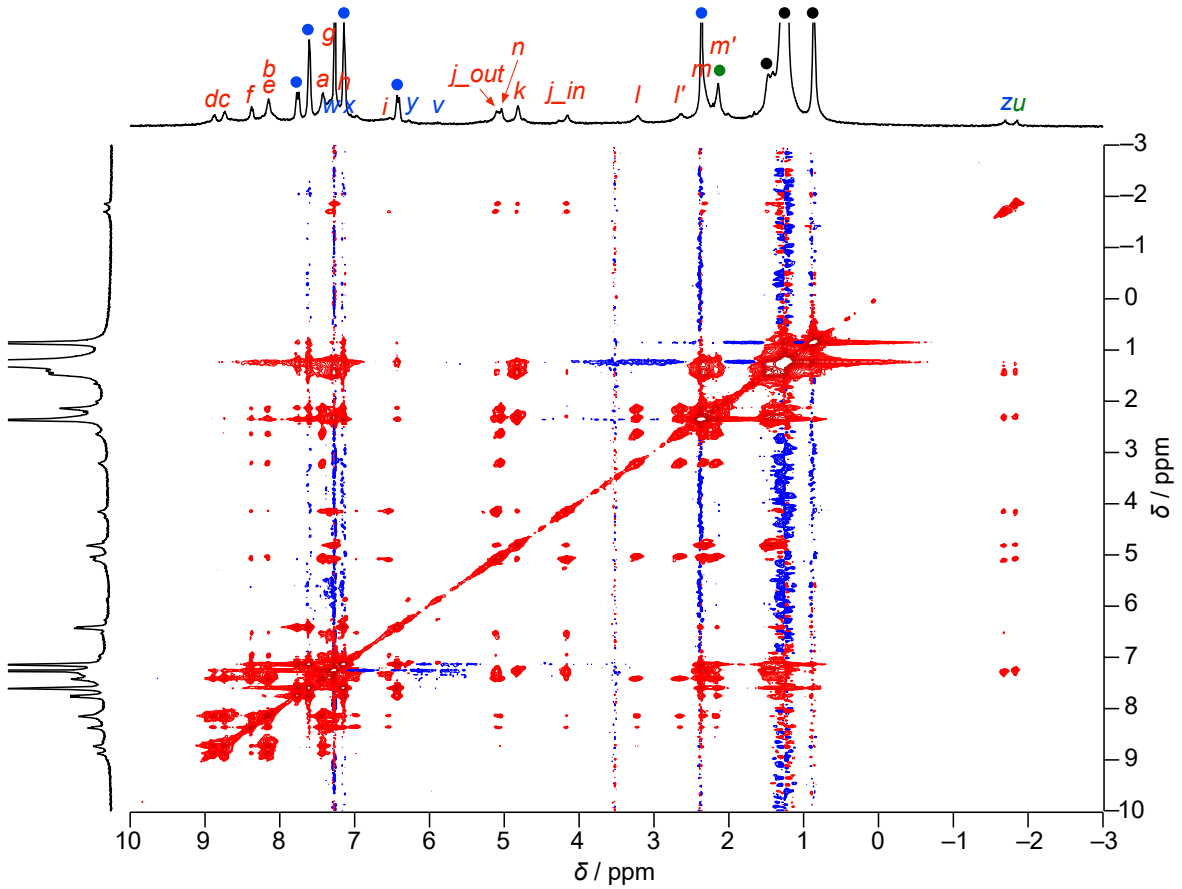


Figure S17. NOESY (500 MHz, chloroform-d_1, 223 K) of a mixture of [**1Ag**]$(BF_4)_4$, **G1a**, and **G2a**. The concentration of [**1Ag**]$(BF_4)_4$, **G1a**, and **G2a** are 1.5 mM, 15 mM, and 15 mM, respectively. Mixing time = 500 ms.

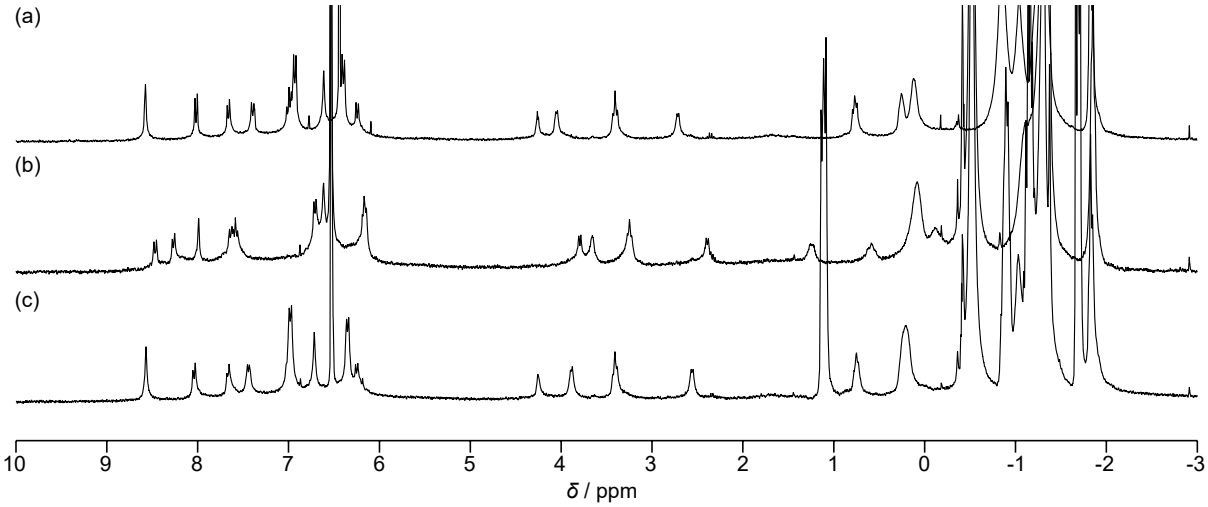


Figure S18. ^{1}H NMR spectra (500 MHz, chloroform-d_1, 223 K) of (a) **1** (1.0 mM), (b) after the addition of four equivalents of $AgBF_4$ in acetonitrile-d_3 (60 μL) to the mixture, (c) after the addtion of eight equivalents of tetraethylammonium iodide in chloroform-d_1 (40 μL) to the mixture.

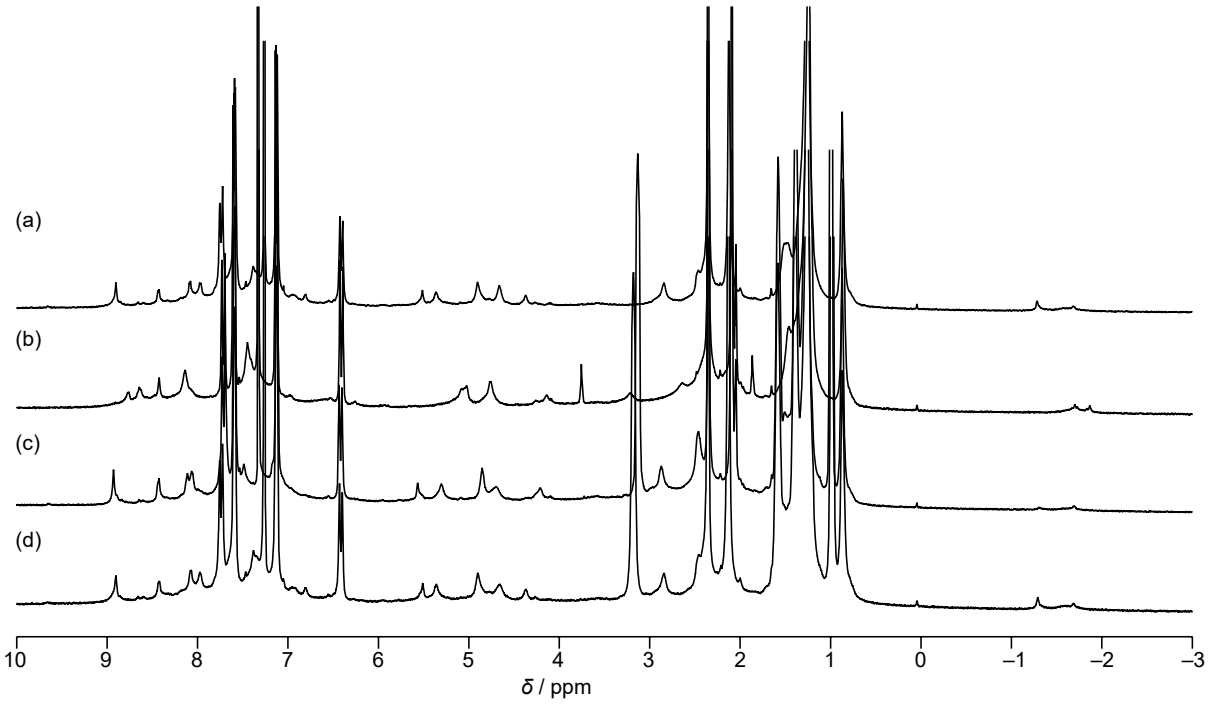


Figure S19. ^{1}H NMR spectra (500 MHz, chloroform-d_1, 223 K) of (a) a mixture of **G1a** (10 mM), **G2a** (10 mM) and **1** (1.0 mM), (b) after the addition of four equivalents of $AgBF_4$ in acetonitrile-d_3 (60 μL) to the mixture, (c) after the addtion of eight equivalents of tetraethylammonium iodide in chloroform-d_1 (40 μL) to the mixture, and (d) after the concentration of the solution of (c) followed by the addition of chloroform-d_1 to regulate the concentration of **1** to be 1.0 mM.

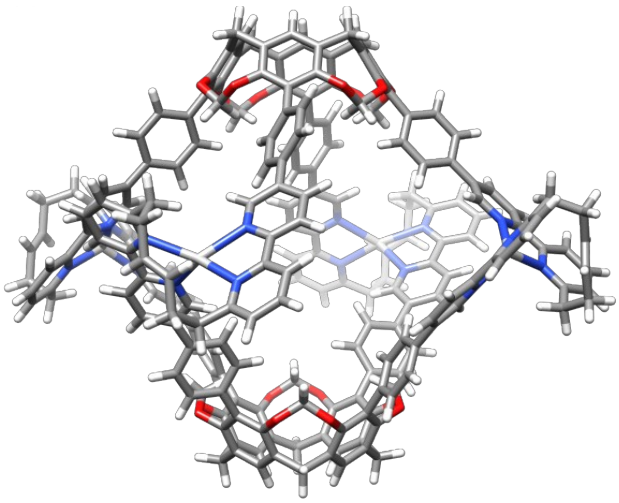


Figure S20. Optimized structures of **M1Ag** at B3LYP/6-31G(d)+LanL2DZ. Color scheme: gray (carbon), white (hydrogen), blue (nitrogen), red (oxygen), pale gray (silver).

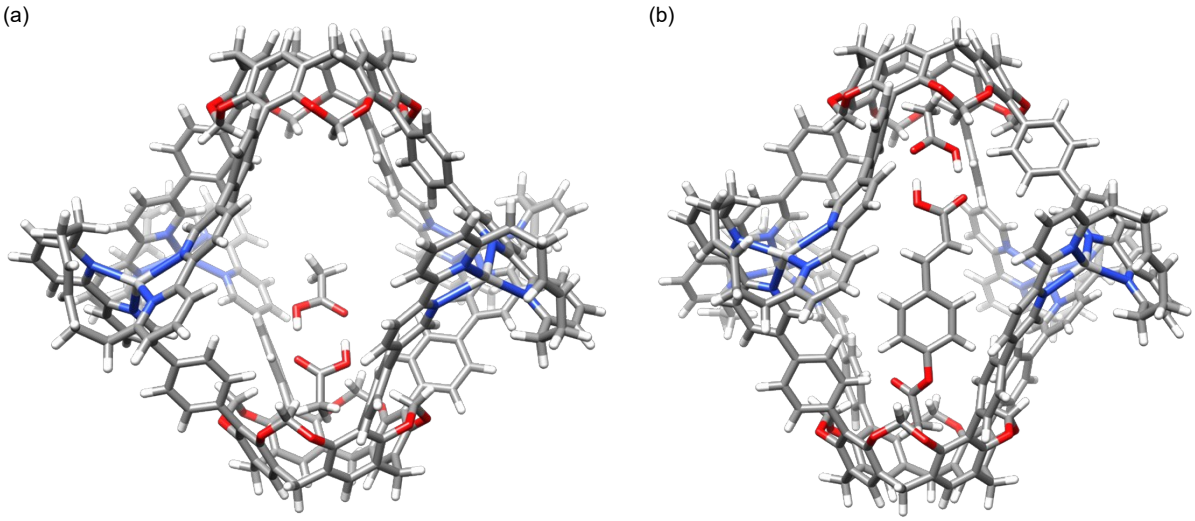


Figure S21. Optimized structures of (a) **G1a•G1a⊂M1Ag** and (b) **G1a•G2a⊂M1Ag** at B3LYP/6-31G(d)+LanL2DZ. Color scheme: gray (carbon), white (hydrogen), blue (nitrogen), red (oxygen), pale gray (silver).

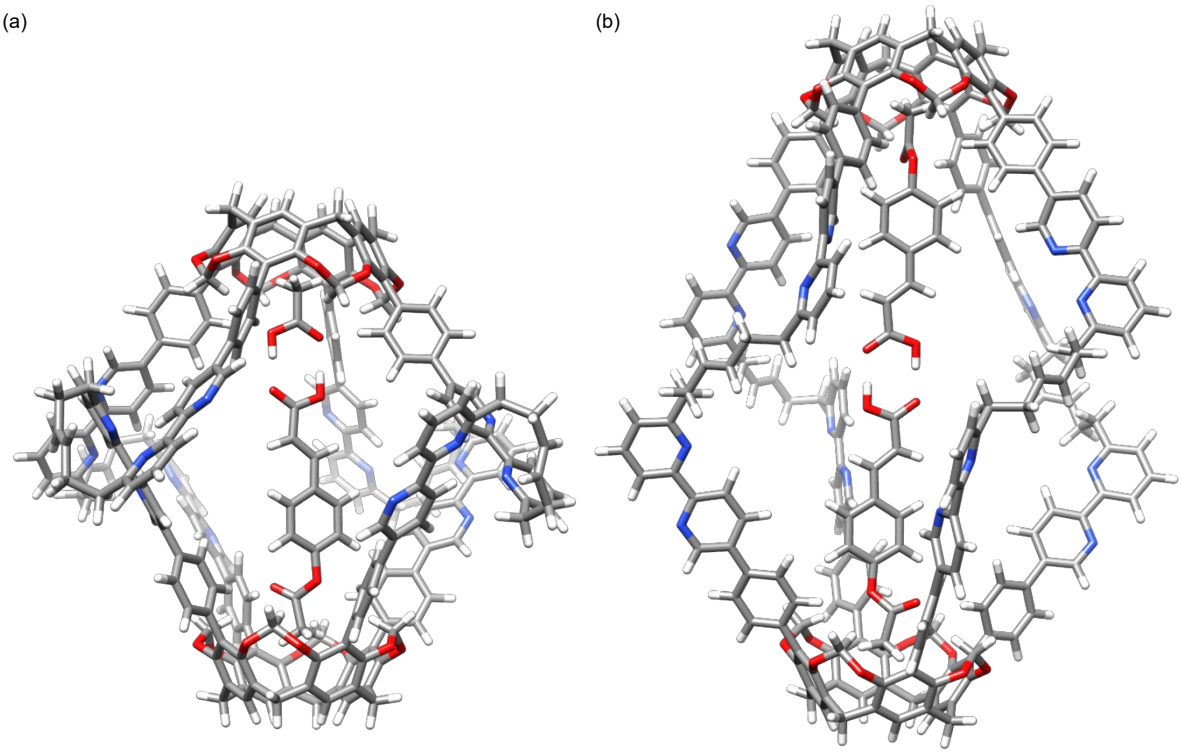


Figure S22. Optimized structures of (a) **G1a•G2a⊂M1** and (b) **G2a•G2a⊂M1** at B3LYP/6-31G(d). Color scheme: gray (carbon), white (hydrogen), blue (nitrogen), red (oxygen).

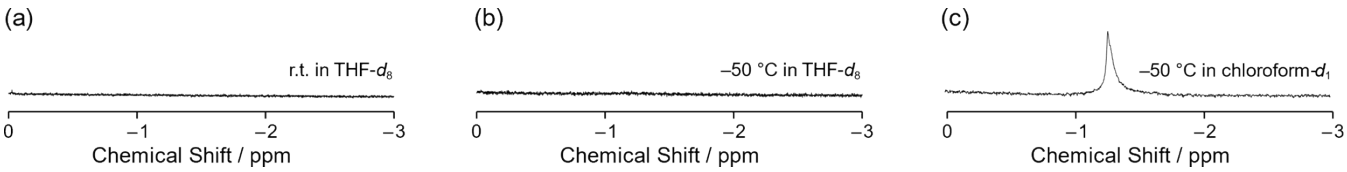


Figure S23. Selectied region of ^{1}H NMR spectra (500 MHz) of a mixture **1** and **G2a** in THF-d_8 at (a) 298 K and (b) at 223 K and (c) a mixture of **1** and **G2a** in chloroform-d_1 at 223 K. The concentrations of **1** and **G2a** were 1.5 mM and 15 mM, respectively.

Table S1. PDB file of **M1Ag**

REMARK 1 File created by GaussView 6.1.1

HETATM 1 C 0 3.156 -0.998 9.059 C

HETATM 2 C 0 3.853 -0.849 7.852 C

HETATM 3 C 0 4.089 0.423 7.290 C

HETATM 4 C 0 3.519 1.539 7.936 C

HETATM 5 C 0 2.795 1.417 9.126 C

HETATM 6 C 0 2.639 0.143 9.673 C

HETATM 7 C 0 2.937 -2.370 9.664 C

HETATM 8 C 0 2.142 2.630 9.756 C

HETATM 9 C 0 -1.695 3.145 7.848 C

HETATM 10 C 0 -0.561 3.755 7.272 C

HETATM 11 C 0 0.676 3.580 7.925 C

HETATM 12 C 0 0.787 2.866 9.123 C

HETATM 13 C 0 -0.372 2.319 9.674 C

HETATM 14 C 0 -1.618 2.445 9.059 C

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HETATM 16 C 0 0.673 -4.302 7.245 C

HETATM 17 C 0 1.708 -3.020 9.067 C

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HETATM 25 C 0 -3.086 0.431 9.071 C

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HETATM 27 C 0 -2.727 -1.983 9.124 C

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HETATM 30 O 0 4.417 -1.957 7.241 O

HETATM 31 O 0 3.047 -3.904 7.280 O

HETATM 32 O 0 -4.346 1.404 7.264 O

HETATM 33 O 0 -2.929 3.324 7.242 O

HETATM 34 O 0 3.731 2.798 7.395 O

HETATM 35 O 0 1.802 4.180 7.381 O

HETATM 36 C 0 6.934 0.938 4.076 C

HETATM 37 C 0 7.032 1.667 5.274 C

HETATM 38 C 0 6.095 1.505 6.286 C

HETATM 39 C 0 5.020 0.611 6.144 C

HETATM 40 C 0 4.909 -0.099 4.939 C

HETATM 41 C 0 5.850 0.058 3.923 C

HETATM 42 C 0 1.124 -6.974 3.876 C

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HETATM 44 C 0 1.752 -6.246 6.108 C

HETATM 45 C 0 0.834 -5.183 6.057 C

HETATM 46 C 0 0.080 -5.023 4.885 C

HETATM 47 C 0 0.217 -5.903 3.814 C

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HETATM 76 C 0 -8.402 -2.816 2.614 C

HETATM 77 C 0 -9.319 -2.893 1.573 C

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HETATM 80 N 0 -10.974 -0.602 -0.836 N

HETATM 81 C 0 -10.550 -1.786 -0.347 C

HETATM 82 C 0 -10.986 -2.995 -0.903 C

HETATM 83 C 0 -11.894 -2.969 -1.959 C

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HETATM 85 N 0 0.218 -9.252 1.022 N

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HETATM 87 C 0 1.265 -7.926 2.755 C

HETATM 88 C 0 2.508 -8.439 2.353 C

HETATM 89 C 0 2.584 -9.340 1.298 C

HETATM 90 C 0 1.389 -12.428 -2.654 C

HETATM 91 C 0 2.558 -12.310 -1.911 C

HETATM 92 C 0 2.584 -11.445 -0.818 C

HETATM 93 C 0 1.436 -10.709 -0.502 C

HETATM 94 N 0 0.299 -10.852 -1.218 N

HETATM 95 C 0 0.262 -11.690 -2.269 C

HETATM 96 C 0 9.997 1.266 1.121 C

HETATM 97 C 0 9.561 2.422 1.784 C

HETATM 98 C 0 8.553 2.334 2.735 C

HETATM 99 C 0 7.967 1.094 3.030 C

HETATM 100 C 0 8.447 -0.003 2.297 C

HETATM 101 N 0 9.416 0.076 1.380 N

HETATM 102 C 0 13.127 1.264 -1.743 C

HETATM 103 C 0 12.229 0.195 -1.601 C

HETATM 104 N 0 11.247 0.228 -0.686 N

HETATM 105 C 0 11.111 1.297 0.128 C

HETATM 106 C 0 11.997 2.379 0.057 C

HETATM 107 C 0 13.013 2.360 -0.897 C

HETATM 108 C 0 3.196 0.137 -8.989 C

HETATM 109 C 0 3.813 -0.274 -7.799 C

HETATM 110 C 0 3.622 -1.572 -7.282 C

HETATM 111 C 0 2.714 -2.414 -7.955 C

HETATM 112 C 0 2.066 -2.021 -9.129 C

HETATM 113 C 0 2.333 -0.749 -9.633 C

HETATM 114 C 0 3.429 1.530 -9.540 C

HETATM 115 C 0 1.054 -2.938 -9.783 C

HETATM 116 C 0 -2.820 -2.328 -7.994 C

HETATM 117 C 0 -1.941 -3.253 -7.399 C

HETATM 118 C 0 -0.668 -3.416 -7.983 C

HETATM 119 C 0 -0.312 -2.740 -9.159 C

HETATM 120 C 0 -1.229 -1.849 -9.718 C

HETATM 121 C 0 -2.480 -1.616 -9.147 C

HETATM 122 C 0 0.656 4.198 -7.585 C

HETATM 123 C 0 1.924 3.984 -7.004 C

HETATM 124 C 0 2.803 3.105 -7.669 C

HETATM 125 C 0 2.476 2.512 -8.892 C

HETATM 126 C 0 1.234 2.802 -9.454 C

HETATM 127 C 0 0.312 3.636 -8.822 C

HETATM 128 C 0 -3.424 -0.569 -9.700 C

HETATM 129 C 0 -1.048 3.896 -9.439 C

HETATM 130 C 0 -2.724 3.182 -7.691 C

HETATM 131 C 0 -3.634 2.271 -7.118 C

HETATM 132 C 0 -3.825 1.037 -7.777 C

HETATM 133 C 0 -3.198 0.756 -8.999 C

HETATM 134 C 0 -2.328 1.705 -9.535 C

HETATM 135 C 0 -2.066 2.916 -8.895 C

HETATM 136 O 0 -2.507 4.397 -7.056 O

HETATM 137 O 0 -0.224 5.068 -6.958 O

HETATM 138 O 0 4.713 0.567 -7.163 O

HETATM 139 O 0 4.048 2.854 -7.109 O

HETATM 140 O 0 -4.735 0.137 -7.247 O

HETATM 141 O 0 -4.075 -2.143 -7.430 O

HETATM 142 O 0 2.486 -3.688 -7.454 O

HETATM 143 O 0 0.197 -4.345 -7.428 O

HETATM 144 C 0 6.166 -3.114 -4.144 C

HETATM 145 C 0 6.004 -3.791 -5.365 C

HETATM 146 C 0 5.162 -3.293 -6.351 C

HETATM 147 C 0 4.446 -2.098 -6.160 C

HETATM 148 C 0 4.589 -1.436 -4.932 C

HETATM 149 C 0 5.435 -1.932 -3.941 C

HETATM 150 C 0 3.241 6.430 -3.691 C

HETATM 151 C 0 4.012 6.292 -4.858 C

HETATM 152 C 0 3.588 5.477 -5.900 C

HETATM 153 C 0 2.380 4.761 -5.819 C

HETATM 154 C 0 1.631 4.871 -4.638 C

HETATM 155 C 0 2.050 5.693 -3.594 C

HETATM 156 C 0 -6.159 3.393 -3.793 C

HETATM 157 C 0 -6.004 4.228 -4.912 C

HETATM 158 C 0 -5.169 3.865 -5.962 C

HETATM 159 C 0 -4.451 2.656 -5.935 C

HETATM 160 C 0 -4.583 1.840 -4.802 C

HETATM 161 C 0 -5.425 2.197 -3.751 C

HETATM 162 C 0 -3.291 -5.823 -4.194 C

HETATM 163 C 0 -4.007 -5.707 -5.399 C

HETATM 164 C 0 -3.570 -4.863 -6.411 C

HETATM 165 C 0 -2.396 -4.104 -6.266 C

HETATM 166 C 0 -1.689 -4.209 -5.060 C

HETATM 167 C 0 -2.127 -5.052 -4.041 C

HETATM 168 C 0 -4.542 -8.483 -1.094 C

HETATM 169 N 0 -3.232 -8.302 -1.359 N

HETATM 170 C 0 -2.862 -7.466 -2.335 C

HETATM 171 C 0 -3.759 -6.734 -3.129 C

HETATM 172 C 0 -5.122 -6.947 -2.867 C

HETATM 173 C 0 -5.513 -7.820 -1.861 C

HETATM 174 C 0 -5.494 -11.191 2.036 C

HETATM 175 C 0 -4.202 -11.069 1.507 C

HETATM 176 N 0 -3.930 -10.194 0.521 N

HETATM 177 C 0 -6.214 -9.474 0.521 C

HETATM 178 H 0 -6.991 -8.824 0.140 H

HETATM 179 C 0 -4.908 -9.412 0.016 C

HETATM 180 C 0 -6.506 -10.378 1.540 C

HETATM 181 C 0 -8.887 4.362 -0.653 C

HETATM 182 C 0 -8.103 5.381 -1.215 C

HETATM 183 C 0 -7.210 5.083 -2.237 C

HETATM 184 C 0 -7.083 3.766 -2.701 C

HETATM 185 C 0 -7.905 2.813 -2.079 C

HETATM 186 N 0 -8.768 3.095 -1.099 N

HETATM 187 C 0 -11.619 5.006 2.533 C

HETATM 188 C 0 -11.237 3.726 2.109 C

HETATM 189 N 0 -10.376 3.554 1.091 N

HETATM 190 C 0 -9.862 4.625 0.447 C

HETATM 191 C 0 -10.234 5.927 0.803 C

HETATM 192 C 0 -11.120 6.116 1.862 C

HETATM 193 C 0 4.378 9.187 -0.636 C

HETATM 194 C 0 5.368 8.403 -1.248 C

HETATM 195 C 0 5.014 7.493 -2.236 C

HETATM 196 C 0 3.671 7.350 -2.618 C

HETATM 197 C 0 2.751 8.166 -1.940 C

HETATM 198 N 0 3.086 9.043 -0.992 N

HETATM 199 C 0 5.186 12.054 2.394 C

HETATM 200 C 0 6.257 11.541 1.672 C

HETATM 201 C 0 6.015 10.606 0.667 C

HETATM 202 C 0 4.699 10.201 0.414 C

HETATM 203 N 0 3.665 10.725 1.108 N

HETATM 204 C 0 3.889 11.631 2.076 C

HETATM 205 C 0 8.992 -4.537 -1.277 C

HETATM 206 C 0 8.195 -5.462 -1.969 C

HETATM 207 C 0 7.258 -5.013 -2.890 C

HETATM 208 C 0 7.103 -3.638 -3.128 C

HETATM 209 C 0 7.920 -2.788 -2.368 C

HETATM 210 N 0 8.822 -3.214 -1.478 N

HETATM 211 C 0 11.988 -5.675 1.502 C

HETATM 212 C 0 11.495 -6.643 0.637 C

HETATM 213 C 0 10.516 -6.287 -0.290 C

HETATM 214 C 0 10.050 -4.968 -0.316 C

HETATM 215 N 0 10.557 -4.031 0.515 N

HETATM 216 C 0 11.505 -4.361 1.407 C

HETATM 217 C 0 -3.086 -11.966 1.976 C

HETATM 218 H 0 -2.129 -11.447 1.851 H

HETATM 219 H 0 -3.208 -12.179 3.045 H

HETATM 220 C 0 -3.038 -13.313 1.201 C

HETATM 221 C 0 -1.058 -11.879 -2.973 C

HETATM 222 H 0 -1.702 -11.017 -2.762 H

HETATM 223 H 0 -0.901 -11.917 -4.058 H

HETATM 224 C 0 12.097 -3.279 2.275 C

HETATM 225 H 0 11.416 -2.421 2.318 H

HETATM 226 H 0 12.210 -3.660 3.297 H

HETATM 227 C 0 13.495 -2.827 1.763 C

HETATM 228 C 0 1.802 -3.727 7.864 C

HETATM 229 C 0 12.381 -1.042 -2.453 C

HETATM 230 H 0 11.470 -1.647 -2.386 H

HETATM 231 H 0 12.493 -0.733 -3.500 H

HETATM 232 C 0 2.686 12.234 2.757 C

HETATM 233 H 0 1.842 11.541 2.665 H

HETATM 234 H 0 2.889 12.367 3.826 H

HETATM 235 C 0 0.561 12.392 -2.254 C

HETATM 236 C 0 1.002 13.717 -1.571 C

HETATM 237 H 0 1.349 11.641 -2.125 H

HETATM 238 H 0 0.449 12.573 -3.329 H

HETATM 239 C 0 -11.847 2.497 2.734 C

HETATM 240 H 0 -11.215 1.630 2.508 H

HETATM 241 H 0 -11.878 2.608 3.824 H

HETATM 242 C 0 -13.288 2.229 2.212 C

HETATM 243 H 0 -13.617 1.260 2.604 H

HETATM 244 H 0 -13.958 2.989 2.636 H

HETATM 245 C 0 -13.396 2.256 0.711 C

HETATM 246 H 0 -13.356 3.241 0.243 H

HETATM 247 C 0 -12.346 0.785 -2.307 C

HETATM 248 H 0 -11.567 1.534 -2.125 H

HETATM 249 H 0 -12.542 0.766 -3.385 H

HETATM 250 Ag 0 1.444 10.301 0.303 Ag

HETATM 251 Ag 0 10.064 -1.756 -0.021 Ag

HETATM 252 Ag 0 -1.700 -9.863 -0.308 Ag

HETATM 253 Ag 0 -10.014 1.395 0.087 Ag

HETATM 254 H 0 2.093 0.035 10.608 H

HETATM 255 H 0 2.812 -2.273 10.747 H

HETATM 256 H 0 3.814 -2.997 9.479 H

HETATM 257 H 0 2.023 2.467 10.832 H

HETATM 258 H 0 2.777 3.509 9.612 H

HETATM 259 H 0 -0.302 1.773 10.612 H

HETATM 260 H 0 0.366 -2.350 10.598 H

HETATM 261 H 0 -2.728 1.723 10.744 H

HETATM 262 H 0 -3.724 2.441 9.468 H

HETATM 263 H 0 -2.004 -0.608 10.603 H

HETATM 264 H 0 -2.684 -4.085 9.560 H

HETATM 265 H 0 -1.930 -3.065 10.798 H

HETATM 266 H 0 7.876 2.332 5.434 H

HETATM 267 H 0 6.203 2.061 7.210 H

HETATM 268 H 0 4.072 -0.770 4.786 H

HETATM 269 H 0 5.729 -0.491 2.993 H

HETATM 270 H 0 2.587 -7.957 5.127 H

HETATM 271 H 0 2.345 -6.391 7.004 H

HETATM 272 H 0 -0.608 -4.189 4.798 H

HETATM 273 H 0 -0.366 -5.742 2.911 H

HETATM 274 H 0 -7.816 -2.804 5.343 H

HETATM 275 H 0 -6.199 -2.558 7.176 H

HETATM 276 H 0 -3.897 0.171 4.793 H

HETATM 277 H 0 -5.488 -0.091 2.941 H

HETATM 278 H 0 0.024 7.864 5.195 H

HETATM 279 H 0 0.328 6.286 7.056 H

HETATM 280 H 0 -1.670 3.229 4.800 H

HETATM 281 H 0 -1.975 4.796 2.933 H

HETATM 282 H 0 0.735 8.302 2.891 H

HETATM 283 H 0 -3.268 6.814 2.403 H

HETATM 284 H 0 -3.587 8.496 0.615 H

HETATM 285 H 0 -2.003 13.145 -2.857 H

HETATM 286 H 0 -3.923 10.558 -0.010 H

HETATM 287 H 0 -4.095 12.312 -1.766 H

HETATM 288 H 0 -7.722 0.478 2.305 H

HETATM 289 H 0 -8.173 -3.703 3.197 H

HETATM 290 H 0 -9.822 -3.832 1.377 H

HETATM 291 H 0 -13.052 -1.685 -3.256 H

HETATM 292 H 0 -10.616 -3.945 -0.535 H

HETATM 293 H 0 -12.246 -3.896 -2.402 H

HETATM 294 H 0 -0.848 -8.053 2.309 H

HETATM 295 H 0 3.414 -8.114 2.854 H

HETATM 296 H 0 3.554 -9.704 0.984 H

HETATM 297 H 0 1.332 -13.094 -3.509 H

HETATM 298 H 0 3.439 -12.889 -2.171 H

HETATM 299 H 0 3.482 -11.368 -0.219 H

HETATM 300 H 0 9.988 3.390 1.547 H

HETATM 301 H 0 8.206 3.230 3.240 H

HETATM 302 H 0 8.050 -0.997 2.482 H

HETATM 303 H 0 13.908 1.216 -2.495 H

HETATM 304 H 0 11.919 3.212 0.745 H

HETATM 305 H 0 13.711 3.188 -0.969 H

HETATM 306 H 0 1.849 -0.435 -10.555 H

HETATM 307 H 0 3.270 1.524 -10.623 H

HETATM 308 H 0 4.461 1.835 -9.349 H

HETATM 309 H 0 1.000 -2.720 -10.855 H

HETATM 310 H 0 1.367 -3.979 -9.663 H

HETATM 311 H 0 -0.956 -1.315 -10.625 H

HETATM 312 H 0 0.973 2.361 -10.413 H

HETATM 313 H 0 -3.251 -0.447 -10.774 H

HETATM 314 H 0 -4.459 -0.891 -9.556 H

HETATM 315 H 0 -1.834 1.492 -10.480 H

HETATM 316 H 0 -1.364 4.919 -9.217 H

HETATM 317 H 0 -0.981 3.789 -10.526 H

HETATM 318 H 0 6.578 -4.692 -5.564 H

HETATM 319 H 0 5.070 -3.821 -7.294 H

HETATM 320 H 0 4.024 -0.531 -4.740 H

HETATM 321 H 0 5.512 -1.407 -2.993 H

HETATM 322 H 0 4.926 6.868 -4.973 H

HETATM 323 H 0 4.185 5.408 -6.803 H

HETATM 324 H 0 0.716 4.300 -4.527 H

HETATM 325 H 0 1.455 5.748 -2.686 H

HETATM 326 H 0 -6.578 5.148 -4.983 H

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HETATM 331 H 0 -4.130 -4.799 -7.337 H

HETATM 332 H 0 -0.798 -3.609 -4.906 H

HETATM 333 H 0 -1.573 -5.091 -3.107 H

HETATM 334 H 0 -1.792 -7.392 -2.510 H

HETATM 335 H 0 -5.874 -6.421 -3.446 H

HETATM 336 H 0 -6.569 -7.990 -1.687 H

HETATM 337 H 0 -5.688 -11.910 2.825 H

HETATM 338 H 0 -7.513 -10.442 1.942 H

HETATM 339 H 0 -8.168 6.398 -0.849 H

HETATM 340 H 0 -6.592 5.868 -2.663 H

HETATM 341 H 0 -7.882 1.777 -2.406 H

HETATM 342 H 0 -12.311 5.116 3.362 H

HETATM 343 H 0 -9.862 6.785 0.257 H

HETATM 344 H 0 -11.419 7.119 2.153 H

HETATM 345 H 0 6.406 8.483 -0.948 H

HETATM 346 H 0 5.777 6.877 -2.703 H

HETATM 347 H 0 1.696 8.128 -2.198 H

HETATM 348 H 0 5.338 12.784 3.183 H

HETATM 349 H 0 7.271 11.866 1.882 H

HETATM 350 H 0 6.842 10.221 0.083 H

HETATM 351 H 0 8.288 -6.524 -1.779 H

HETATM 352 H 0 6.634 -5.727 -3.418 H

HETATM 353 H 0 7.866 -1.711 -2.506 H

HETATM 354 H 0 12.750 -5.917 2.236 H

HETATM 355 H 0 11.869 -7.661 0.674 H

HETATM 356 H 0 10.146 -7.026 -0.991 H

HETATM 357 C 0 -2.623 -3.876 6.591 C

HETATM 358 C 0 -1.336 4.522 -6.274 C

HETATM 359 H 0 -2.104 -3.052 6.083 H

HETATM 360 H 0 -3.106 -4.542 5.874 H

HETATM 361 H 0 -1.077 3.548 -5.838 H

HETATM 362 H 0 -1.578 5.251 -5.499 H

HETATM 363 C 0 3.570 -2.832 6.520 C

HETATM 364 C 0 4.205 1.643 -6.396 C

HETATM 365 H 0 2.747 -2.272 6.055 H

HETATM 366 H 0 4.211 -3.293 5.767 H

HETATM 367 H 0 3.252 1.362 -5.928 H

HETATM 368 H 0 4.972 1.842 -5.646 H

HETATM 369 C 0 2.688 3.371 6.629 C

HETATM 370 C 0 1.311 -3.879 -6.690 C

HETATM 371 H 0 2.132 2.589 6.098 H

HETATM 372 H 0 3.179 4.051 5.932 H

HETATM 373 H 0 1.059 -2.950 -6.161 H

HETATM 374 H 0 1.543 -4.683 -5.990 H

HETATM 375 C 0 -3.478 2.239 6.524 C

HETATM 376 C 0 -4.245 -1.018 -6.592 C

HETATM 377 H 0 -2.671 1.636 6.085 H

HETATM 378 H 0 -4.102 2.690 5.750 H

HETATM 379 H 0 -3.300 -0.795 -6.078 H

HETATM 380 H 0 -5.026 -1.295 -5.883 H

HETATM 381 H 0 13.954 -2.207 2.541 H

HETATM 382 H 0 14.128 -3.717 1.658 H

HETATM 383 C 0 13.465 -2.060 0.462 C

HETATM 384 H 0 13.374 -0.979 0.549 H

HETATM 385 C 0 13.562 -2.626 -0.748 C

HETATM 386 H 0 13.661 -3.711 -0.794 H

HETATM 387 C 0 13.616 -1.907 -2.081 C

HETATM 388 H 0 14.510 -1.270 -2.118 H

HETATM 389 H 0 13.745 -2.648 -2.877 H

HETATM 390 H 0 -3.929 -13.898 1.463 H

HETATM 391 C 0 -2.967 -13.151 -0.294 C

HETATM 392 H 0 -3.892 -12.866 -0.797 H

HETATM 393 H 0 -2.170 -13.877 1.563 H

HETATM 394 C 0 -1.863 -13.332 -1.027 C

HETATM 395 H 0 -0.938 -13.612 -0.521 H

HETATM 396 C 0 -1.780 -13.181 -2.522 C

HETATM 397 H 0 -1.243 -14.041 -2.943 H

HETATM 398 H 0 -2.783 -13.185 -2.965 H

HETATM 399 H 0 1.979 13.997 -1.979 H

HETATM 400 H 0 0.298 14.509 -1.861 H

HETATM 401 C 0 1.067 13.647 -0.067 C

HETATM 402 H 0 0.112 13.649 0.461 H

HETATM 403 C 0 2.200 13.613 0.645 C

HETATM 404 H 0 3.152 13.608 0.111 H

HETATM 405 C 0 2.284 13.608 2.148 C

HETATM 406 H 0 1.325 13.905 2.587 H

HETATM 407 H 0 3.023 14.356 2.463 H

HETATM 408 C 0 -13.533 1.179 -0.069 C

HETATM 409 H 0 -13.568 0.193 0.395 H

HETATM 410 C 0 -13.646 1.217 -1.570 C

HETATM 411 H 0 -14.464 0.558 -1.892 H

HETATM 412 H 0 -13.901 2.228 -1.906 H

END

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CONECT 3 2 4 39

CONECT 4 3 5 34

CONECT 5 4 6 8

CONECT 6 1 5 254

CONECT 7 1 17 255 256

CONECT 8 5 12 257 258

CONECT 9 10 14 33

CONECT 10 9 11 57

CONECT 11 10 12 35

CONECT 12 8 11 13

CONECT 13 12 14 259

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CONECT 28 22 357

CONECT 29 15 357

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CONECT 33 9 375

CONECT 34 4 369

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CONECT 218 217

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CONECT 220 217 390 391 393

CONECT 221 95 222 223 396

CONECT 222 221

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CONECT 225 224

CONECT 226 224

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CONECT 228 16 17 31

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CONECT 247 79 248 249 410

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CONECT 254 6

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CONECT 256 7

CONECT 257 8

CONECT 258 8

CONECT 259 13

CONECT 260 18

CONECT 261 20

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CONECT 355 212

CONECT 356 213

CONECT 357 28 29 359 360

CONECT 358 136 137 361 362

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CONECT 364 138 139 367 368

CONECT 365 363

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CONECT 370 143 142 373 374

CONECT 371 369

CONECT 372 369

CONECT 373 370

CONECT 374 370

CONECT 375 32 33 377 378

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CONECT 383 227 384 385

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CONECT 390 220

CONECT 391 220 392 394

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CONECT 394 391 395 396

CONECT 395 394

CONECT 396 221 394 397 398

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CONECT 407 405

CONECT 408 245 409 410

CONECT 409 408

CONECT 410 247 408 411 412

CONECT 411 410

CONECT 412 410

Table S2. PDB file of **G1a•G1a⊂M1Ag**

REMARK 1 File created by GaussView 6.1.1

HETATM 1 C 0 -2.983 1.590 9.107 C

HETATM 2 C 0 -3.699 1.613 7.901 C

HETATM 3 C 0 -4.211 0.429 7.328 C

HETATM 4 C 0 -3.884 -0.795 7.949 C

HETATM 5 C 0 -3.152 -0.848 9.140 C

HETATM 6 C 0 -2.733 0.356 9.707 C

HETATM 7 C 0 -2.462 2.873 9.727 C

HETATM 8 C 0 -2.776 -2.182 9.757 C

HETATM 9 C 0 0.872 -3.546 7.886 C

HETATM 10 C 0 -0.364 -3.897 7.298 C

HETATM 11 C 0 -1.540 -3.433 7.929 C

HETATM 12 C 0 -1.502 -2.714 9.130 C

HETATM 13 C 0 -0.256 -2.449 9.700 C

HETATM 14 C 0 0.938 -2.843 9.096 C

HETATM 15 C 0 1.355 3.806 7.927 C

HETATM 16 C 0 0.176 4.301 7.329 C

HETATM 17 C 0 -1.120 3.249 9.131 C

HETATM 18 C 0 0.077 2.839 9.718 C

HETATM 19 C 0 1.319 3.094 9.135 C

HETATM 20 C 0 2.276 -2.485 9.713 C

HETATM 21 C 0 2.594 2.575 9.774 C

HETATM 22 C 0 3.740 1.192 7.994 C

HETATM 23 C 0 4.079 -0.028 7.372 C

HETATM 24 C 0 3.556 -1.212 7.935 C

HETATM 25 C 0 2.816 -1.196 9.125 C

HETATM 26 C 0 2.556 0.036 9.728 C

HETATM 27 C 0 2.985 1.241 9.171 C

HETATM 28 O 0 4.201 2.378 7.438 O

HETATM 29 O 0 2.576 4.129 7.356 O

HETATM 30 O 0 -4.005 2.826 7.304 O

HETATM 31 O 0 -2.230 4.425 7.354 O

HETATM 32 O 0 3.858 -2.427 7.340 O

HETATM 33 O 0 2.046 -3.995 7.300 O

HETATM 34 O 0 -4.353 -1.972 7.383 O

HETATM 35 O 0 -2.767 -3.750 7.366 O

HETATM 36 C 0 -7.152 0.515 4.148 C

HETATM 37 C 0 -7.430 -0.047 5.406 C

HETATM 38 C 0 -6.466 -0.078 6.405 C

HETATM 39 C 0 -5.183 0.459 6.197 C

HETATM 40 C 0 -4.904 1.019 4.942 C

HETATM 41 C 0 -5.869 1.046 3.935 C

HETATM 42 C 0 0.309 7.131 4.052 C

HETATM 43 C 0 -0.310 7.443 5.276 C

HETATM 44 C 0 -0.356 6.516 6.310 C

HETATM 45 C 0 0.216 5.240 6.171 C

HETATM 46 C 0 0.824 4.926 4.947 C

HETATM 47 C 0 0.870 5.852 3.906 C

HETATM 48 C 0 7.042 -0.179 4.215 C

HETATM 49 C 0 7.300 0.454 5.444 C

HETATM 50 C 0 6.328 0.512 6.436 C

HETATM 51 C 0 5.058 -0.059 6.247 C

HETATM 52 C 0 4.795 -0.673 5.014 C

HETATM 53 C 0 5.767 -0.733 4.016 C

HETATM 54 C 0 -0.506 -6.709 4.008 C

HETATM 55 C 0 -1.253 -6.912 5.181 C

HETATM 56 C 0 -1.216 -5.988 6.220 C

HETATM 57 C 0 -0.440 -4.819 6.129 C

HETATM 58 C 0 0.274 -4.602 4.940 C

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HETATM 66 C 0 -0.856 -12.781 -1.932 C

HETATM 67 C 0 -1.946 -11.969 -1.586 C

HETATM 68 N 0 -1.829 -11.007 -0.651 N

HETATM 69 C 0 -0.644 -10.807 -0.033 C

HETATM 70 C 0 0.470 -11.603 -0.318 C

HETATM 71 C 0 0.359 -12.603 -1.282 C

HETATM 72 C 0 10.019 -0.502 1.164 C

HETATM 73 N 0 9.155 -1.510 1.395 N

HETATM 74 C 0 8.235 -1.390 2.356 C

HETATM 75 C 0 8.089 -0.257 3.173 C

HETATM 76 C 0 9.016 0.774 2.955 C

HETATM 77 C 0 9.978 0.653 1.961 C

HETATM 78 C 0 12.805 -1.041 -1.996 C

HETATM 79 C 0 12.007 -2.086 -1.509 C

HETATM 80 N 0 11.128 -1.886 -0.509 N

HETATM 81 C 0 11.003 -0.662 0.050 C

HETATM 82 C 0 11.762 0.422 -0.408 C

HETATM 83 C 0 12.676 0.226 -1.441 C

HETATM 84 C 0 0.545 9.958 0.854 C

HETATM 85 N 0 1.566 9.114 1.105 N

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HETATM 87 C 0 0.358 8.126 2.959 C

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HETATM 89 C 0 -0.594 9.945 1.674 C

HETATM 90 C 0 1.001 12.603 -2.438 C

HETATM 91 C 0 -0.250 12.500 -1.845 C

HETATM 92 C 0 -0.420 11.632 -0.768 C

HETATM 93 C 0 0.675 10.891 -0.307 C

HETATM 94 N 0 1.884 10.990 -0.903 N

HETATM 95 C 0 2.058 11.825 -1.945 C

HETATM 96 C 0 -10.154 0.657 1.103 C

HETATM 97 C 0 -10.117 -0.434 1.986 C

HETATM 98 C 0 -9.140 -0.496 2.969 C

HETATM 99 C 0 -8.193 0.533 3.097 C

HETATM 100 C 0 -8.323 1.594 2.187 C

HETATM 101 N 0 -9.257 1.656 1.231 N

HETATM 102 C 0 -13.087 1.032 -1.942 C

HETATM 103 C 0 -12.235 2.088 -1.584 C

HETATM 104 N 0 -11.304 1.938 -0.625 N

HETATM 105 C 0 -11.179 0.757 0.020 C

HETATM 106 C 0 -11.984 -0.338 -0.314 C

HETATM 107 C 0 -12.952 -0.194 -1.305 C

HETATM 108 C 0 -3.100 0.609 -8.884 C

HETATM 109 C 0 -3.665 1.111 -7.701 C

HETATM 110 C 0 -3.251 2.345 -7.152 C

HETATM 111 C 0 -2.167 3.006 -7.773 C

HETATM 112 C 0 -1.577 2.519 -8.944 C

HETATM 113 C 0 -2.074 1.334 -9.489 C

HETATM 114 C 0 -3.558 -0.715 -9.466 C

HETATM 115 C 0 -0.392 3.235 -9.560 C

HETATM 116 C 0 3.281 1.887 -7.734 C

HETATM 117 C 0 2.588 2.965 -7.144 C

HETATM 118 C 0 1.365 3.361 -7.730 C

HETATM 119 C 0 0.906 2.779 -8.921 C

HETATM 120 C 0 1.656 1.749 -9.490 C

HETATM 121 C 0 2.830 1.271 -8.907 C

HETATM 122 C 0 -1.359 -3.865 -7.480 C

HETATM 123 C 0 -2.590 -3.437 -6.932 C

HETATM 124 C 0 -3.280 -2.403 -7.601 C

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HETATM 129 C 0 0.404 -3.869 -9.311 C

HETATM 130 C 0 2.178 -3.518 -7.544 C

HETATM 131 C 0 3.256 -2.815 -6.966 C

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HETATM 133 C 0 3.109 -1.202 -8.812 C

HETATM 134 C 0 2.084 -1.967 -9.369 C

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HETATM 147 C 0 -4.003 3.005 -6.045 C

HETATM 148 C 0 -4.274 2.385 -4.817 C

HETATM 149 C 0 -5.044 3.019 -3.843 C

HETATM 150 C 0 -4.469 -5.651 -3.718 C

HETATM 151 C 0 -5.099 -5.466 -4.961 C

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HETATM 153 C 0 -3.223 -4.149 -5.784 C

HETATM 154 C 0 -2.601 -4.319 -4.538 C

HETATM 155 C 0 -3.212 -5.055 -3.523 C

HETATM 156 C 0 5.535 -4.545 -3.716 C

HETATM 157 C 0 5.338 -5.227 -4.929 C

HETATM 158 C 0 4.586 -4.662 -5.952 C

HETATM 159 C 0 4.003 -3.391 -5.810 C

HETATM 160 C 0 4.187 -2.716 -4.595 C

HETATM 161 C 0 4.939 -3.281 -3.566 C

HETATM 162 C 0 4.421 5.302 -3.994 C

HETATM 163 C 0 5.056 5.102 -5.232 C

HETATM 164 C 0 4.460 4.332 -6.224 C

HETATM 165 C 0 3.204 3.734 -6.024 C

HETATM 166 C 0 2.577 3.921 -4.784 C

HETATM 167 C 0 3.174 4.689 -3.785 C

HETATM 168 C 0 6.172 7.756 -0.962 C

HETATM 169 N 0 4.840 7.761 -1.167 N

HETATM 170 C 0 4.312 6.986 -2.120 C

HETATM 171 C 0 5.060 6.138 -2.953 C

HETATM 172 C 0 6.450 6.164 -2.758 C

HETATM 173 C 0 7.005 6.969 -1.773 C

HETATM 174 C 0 7.657 10.231 2.152 C

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HETATM 180 C 0 8.506 9.276 1.608 C

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HETATM 182 C 0 7.134 -7.052 -1.360 C

HETATM 183 C 0 6.359 -6.531 -2.387 C

HETATM 184 C 0 6.346 -5.149 -2.636 C

HETATM 185 C 0 7.179 -4.375 -1.812 C

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HETATM 188 C 0 10.380 -6.266 2.173 C

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HETATM 192 C 0 9.337 -8.435 2.139 C

HETATM 193 C 0 -6.253 -8.072 -0.678 C

HETATM 194 C 0 -7.077 -7.296 -1.508 C

HETATM 195 C 0 -6.511 -6.495 -2.490 C

HETATM 196 C 0 -5.119 -6.465 -2.666 C

HETATM 197 C 0 -4.379 -7.294 -1.807 C

HETATM 198 N 0 -4.917 -8.062 -0.855 N

HETATM 199 C 0 -7.772 -10.587 2.390 C

HETATM 200 C 0 -8.624 -9.646 1.827 C

HETATM 201 C 0 -8.140 -8.804 0.828 C

HETATM 202 C 0 -6.811 -8.934 0.407 C

HETATM 203 N 0 -5.988 -9.844 0.975 N

HETATM 204 C 0 -6.444 -10.658 1.946 C

HETATM 205 C 0 -8.103 6.189 -1.185 C

HETATM 206 C 0 -7.140 6.958 -1.856 C

HETATM 207 C 0 -6.302 6.358 -2.787 C

HETATM 208 C 0 -6.408 4.984 -3.052 C

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HETATM 214 C 0 -9.047 6.794 -0.198 C

HETATM 215 N 0 -9.728 5.955 0.614 N

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HETATM 219 H 0 5.544 11.444 3.314 H

HETATM 220 C 0 5.618 12.791 1.614 C

HETATM 221 C 0 3.436 11.938 -2.551 C

HETATM 222 H 0 4.001 11.027 -2.325 H

HETATM 223 H 0 3.345 12.007 -3.642 H

HETATM 224 C 0 -11.330 5.478 2.420 C

HETATM 225 H 0 -10.897 4.478 2.304 H

HETATM 226 H 0 -11.165 5.781 3.462 H

HETATM 227 C 0 -12.864 5.412 2.189 C

HETATM 228 C 0 -1.054 3.973 7.936 C

HETATM 229 C 0 -12.387 3.429 -2.262 C

HETATM 230 H 0 -11.418 3.942 -2.291 H

HETATM 231 H 0 -12.694 3.259 -3.300 H

HETATM 232 C 0 -5.493 -11.676 2.528 C

HETATM 233 H 0 -4.466 -11.311 2.409 H

HETATM 234 H 0 -5.684 -11.773 3.603 H

HETATM 235 C 0 -3.292 -12.171 -2.239 C

HETATM 236 C 0 -4.063 -13.418 -1.720 C

HETATM 237 H 0 -3.903 -11.277 -2.069 H

HETATM 238 H 0 -3.155 -12.275 -3.322 H

HETATM 239 C 0 11.400 -5.307 2.736 C

HETATM 240 H 0 11.089 -4.281 2.507 H

HETATM 241 H 0 11.427 -5.407 3.827 H

HETATM 242 C 0 12.838 -5.532 2.184 C

HETATM 243 H 0 13.489 -4.778 2.641 H

HETATM 244 H 0 13.199 -6.511 2.525 H

HETATM 245 C 0 12.920 -5.449 0.683 C

HETATM 246 H 0 12.593 -6.329 0.126 H

HETATM 247 C 0 12.146 -3.478 -2.075 C

HETATM 248 H 0 11.227 -4.039 -1.870 H

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HETATM 320 H 0 -3.863 1.403 -4.606 H

HETATM 321 H 0 -5.220 2.519 -2.894 H

HETATM 322 H 0 -6.057 -5.937 -5.159 H

HETATM 323 H 0 -4.990 -4.619 -6.925 H

HETATM 324 H 0 -1.636 -3.860 -4.350 H

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HETATM 346 H 0 -7.152 -5.885 -3.119 H

HETATM 347 H 0 -3.299 -7.360 -1.911 H

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HETATM 349 H 0 -9.653 -9.560 2.164 H

HETATM 350 H 0 -8.789 -8.050 0.401 H

HETATM 351 H 0 -7.026 8.014 -1.642 H

HETATM 352 H 0 -5.550 6.952 -3.298 H

HETATM 353 H 0 -7.538 3.230 -2.485 H

HETATM 354 H 0 -11.463 8.202 2.427 H

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HETATM 380 H 0 -13.277 6.429 2.240 H

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Table S3. PDB file of **G1a•G2a⊂M1Ag**

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HETATM 14 C 0 -0.587 -1.562 -9.954 C

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HETATM 140 O 0 -4.423 -2.531 7.674 O

HETATM 141 O 0 -4.476 -0.182 8.102 O

HETATM 142 O 0 1.347 3.193 8.444 O

HETATM 143 O 0 -1.040 3.169 8.434 O

HETATM 144 C 0 4.901 4.088 5.146 C

HETATM 145 C 0 4.660 4.536 6.457 C

HETATM 146 C 0 4.070 3.705 7.401 C

HETATM 147 C 0 3.693 2.389 7.079 C

HETATM 148 C 0 3.934 1.943 5.771 C

HETATM 149 C 0 4.529 2.774 4.821 C

HETATM 150 C 0 5.058 -5.478 3.668 C

HETATM 151 C 0 5.672 -5.593 4.928 C

HETATM 152 C 0 5.022 -5.174 6.082 C

HETATM 153 C 0 3.728 -4.629 6.030 C

HETATM 154 C 0 3.111 -4.519 4.775 C

HETATM 155 C 0 3.763 -4.936 3.614 C

HETATM 156 C 0 -4.620 -5.630 3.749 C

HETATM 157 C 0 -4.528 -6.442 4.893 C

HETATM 158 C 0 -3.916 -5.980 6.053 C

HETATM 159 C 0 -3.378 -4.684 6.121 C

HETATM 160 C 0 -3.470 -3.874 4.981 C

HETATM 161 C 0 -4.076 -4.336 3.814 C

HETATM 162 C 0 -4.870 3.830 5.247 C

HETATM 163 C 0 -5.449 3.539 6.495 C

HETATM 164 C 0 -4.764 2.791 7.445 C

HETATM 165 C 0 -3.471 2.306 7.191 C

HETATM 166 C 0 -2.890 2.594 5.948 C

HETATM 167 C 0 -3.577 3.343 4.992 C

HETATM 168 C 0 -6.982 6.114 2.313 C

HETATM 169 N 0 -5.649 6.262 2.464 N

HETATM 170 C 0 -5.004 5.538 3.386 C

HETATM 171 C 0 -5.625 4.608 4.238 C

HETATM 172 C 0 -7.015 4.482 4.093 C

HETATM 173 C 0 -7.692 5.232 3.141 C

HETATM 174 C 0 -8.917 8.529 -0.592 C

HETATM 175 C 0 -7.619 8.797 -0.134 C

HETATM 176 N 0 -7.019 7.998 0.769 N

HETATM 177 C 0 -8.960 6.595 0.827 C

HETATM 178 H 0 -9.464 5.710 1.195 H

HETATM 179 C 0 -7.672 6.927 1.268 C

HETATM 180 C 0 -9.586 7.409 -0.114 C

HETATM 181 C 0 -6.447 -7.036 0.148 C

HETATM 182 C 0 -5.727 -7.933 0.951 C

HETATM 183 C 0 -5.129 -7.488 2.121 C

HETATM 184 C 0 -5.248 -6.145 2.511 C

HETATM 185 C 0 -6.019 -5.330 1.664 C

HETATM 186 N 0 -6.596 -5.751 0.532 N

HETATM 187 C 0 -8.372 -8.274 -3.425 C

HETATM 188 C 0 -8.712 -7.088 -2.759 C

HETATM 189 N 0 -8.063 -6.703 -1.644 N

HETATM 190 C 0 -7.084 -7.476 -1.129 C

HETATM 191 C 0 -6.684 -8.658 -1.765 C

HETATM 192 C 0 -7.339 -9.058 -2.927 C

HETATM 193 C 0 7.099 -6.759 0.135 C

HETATM 194 C 0 7.831 -6.178 1.182 C

HETATM 195 C 0 7.175 -5.750 2.327 C

HETATM 196 C 0 5.785 -5.905 2.449 C

HETATM 197 C 0 5.142 -6.516 1.359 C

HETATM 198 N 0 5.766 -6.927 0.249 N

HETATM 199 C 0 8.981 -8.235 -3.372 C

HETATM 200 C 0 9.666 -7.306 -2.597 C

HETATM 201 C 0 9.056 -6.795 -1.454 C

HETATM 202 C 0 7.770 -7.232 -1.112 C

HETATM 203 N 0 7.103 -8.109 -1.893 N

HETATM 204 C 0 7.685 -8.614 -2.997 C

HETATM 205 C 0 6.808 6.698 2.347 C

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HETATM 207 C 0 5.205 6.369 4.124 C

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HETATM 209 C 0 6.471 4.570 3.221 C

HETATM 210 N 0 7.090 5.378 2.351 N

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HETATM 212 C 0 8.260 9.764 0.659 C

HETATM 213 C 0 7.542 8.975 1.556 C

HETATM 214 C 0 7.566 7.583 1.411 C

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HETATM 218 H 0 -5.800 9.848 -0.515 H

HETATM 219 H 0 -7.098 10.200 -1.663 H

HETATM 220 C 0 -7.243 11.312 0.195 C

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HETATM 222 H 0 -5.183 9.343 3.824 H

HETATM 223 H 0 -4.605 10.245 5.231 H

HETATM 224 C 0 9.842 7.060 -1.479 C

HETATM 225 H 0 9.558 6.004 -1.536 H

HETATM 226 H 0 9.602 7.513 -2.450 H

HETATM 227 C 0 11.379 7.179 -1.273 C

HETATM 228 C 0 0.186 5.245 -7.859 C

HETATM 229 C 0 11.361 4.409 2.744 C

HETATM 230 H 0 10.337 4.779 2.875 H

HETATM 231 H 0 11.721 4.098 3.731 H

HETATM 232 C 0 6.919 -9.637 -3.799 C

HETATM 233 H 0 5.845 -9.448 -3.684 H

HETATM 234 H 0 7.161 -9.521 -4.862 H

HETATM 235 C 0 4.641 -11.256 0.681 C

HETATM 236 C 0 5.624 -12.264 0.018 C

HETATM 237 H 0 5.109 -10.265 0.708 H

HETATM 238 H 0 4.472 -11.568 1.719 H

HETATM 239 C 0 -9.860 -6.239 -3.247 C

HETATM 240 H 0 -9.708 -5.206 -2.914 H

HETATM 241 H 0 -9.871 -6.236 -4.343 H

HETATM 242 C 0 -11.248 -6.732 -2.740 C

HETATM 243 H 0 -12.005 -6.039 -3.126 H

HETATM 244 H 0 -11.459 -7.712 -3.185 H

HETATM 245 C 0 -11.340 -6.817 -1.239 C

HETATM 246 H 0 -10.880 -7.689 -0.771 H

HETATM 247 C 0 -10.856 -5.036 1.709 C

HETATM 248 H 0 -9.865 -5.432 1.464 H

HETATM 249 H 0 -10.975 -5.091 2.797 H

HETATM 250 Ag 0 4.821 -8.520 -1.371 Ag

HETATM 251 Ag 0 8.607 4.625 0.637 Ag

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HETATM 254 H 0 1.927 2.290 -11.045 H

HETATM 255 H 0 1.643 4.691 -10.871 H

HETATM 256 H 0 2.302 5.593 -9.497 H

HETATM 257 H 0 2.771 0.041 -11.524 H

HETATM 258 H 0 3.879 -0.763 -10.401 H

HETATM 259 H 0 0.386 -0.275 -11.365 H

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HETATM 261 H 0 -1.866 -1.097 -11.610 H

HETATM 262 H 0 -2.524 -2.313 -10.506 H

HETATM 263 H 0 -2.149 1.288 -11.160 H

HETATM 264 H 0 -4.104 4.071 -9.728 H

HETATM 265 H 0 -3.007 3.591 -11.032 H

HETATM 266 H 0 8.212 2.219 -5.953 H

HETATM 267 H 0 6.600 2.219 -7.803 H

HETATM 268 H 0 3.352 2.423 -5.000 H

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HETATM 271 H 0 -0.467 7.806 -6.645 H

HETATM 272 H 0 -2.095 4.264 -4.842 H

HETATM 273 H 0 -2.311 5.439 -2.707 H

HETATM 274 H 0 -8.385 0.052 -6.019 H

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HETATM 276 H 0 -3.507 -0.571 -5.472 H

HETATM 277 H 0 -5.014 -1.137 -3.616 H

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HETATM 283 H 0 -0.606 -6.956 -4.002 H

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HETATM 285 H 0 2.536 -12.995 0.769 H

HETATM 286 H 0 0.059 -10.893 -2.040 H

HETATM 287 H 0 0.408 -12.839 -0.534 H

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HETATM 289 H 0 -9.093 0.736 -3.879 H

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HETATM 291 H 0 -12.465 -3.057 2.689 H

HETATM 292 H 0 -11.150 0.015 -0.007 H

HETATM 293 H 0 -12.601 -0.696 1.877 H

HETATM 294 H 0 -3.433 7.068 -1.454 H

HETATM 295 H 0 0.119 9.280 -2.443 H

HETATM 296 H 0 -0.113 10.458 -0.307 H

HETATM 297 H 0 -2.604 11.761 5.007 H

HETATM 298 H 0 -0.407 12.038 3.844 H

HETATM 299 H 0 -0.037 10.891 1.681 H

HETATM 300 H 0 10.656 0.786 -2.445 H

HETATM 301 H 0 9.018 0.832 -4.278 H

HETATM 302 H 0 6.723 3.644 -1.975 H

HETATM 303 H 0 13.040 2.276 2.816 H

HETATM 304 H 0 11.398 0.222 -0.576 H

HETATM 305 H 0 13.059 0.315 1.267 H

HETATM 306 H 0 1.719 -0.348 11.261 H

HETATM 307 H 0 3.616 -1.827 11.192 H

HETATM 308 H 0 4.871 -1.659 9.955 H

HETATM 309 H 0 0.208 1.516 11.714 H

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HETATM 311 H 0 -1.268 -0.351 11.313 H

HETATM 312 H 0 1.706 -3.316 10.833 H

HETATM 313 H 0 -3.177 -1.884 11.297 H

HETATM 314 H 0 -4.472 -1.699 10.104 H

HETATM 315 H 0 -1.285 -3.313 10.880 H

HETATM 316 H 0 0.206 -6.287 9.314 H

HETATM 317 H 0 0.231 -5.223 10.729 H

HETATM 318 H 0 4.967 5.535 6.752 H

HETATM 319 H 0 3.907 4.073 8.408 H

HETATM 320 H 0 3.630 0.943 5.478 H

HETATM 321 H 0 4.673 2.405 3.809 H

HETATM 322 H 0 6.658 -6.040 5.012 H

HETATM 323 H 0 5.516 -5.278 7.043 H

HETATM 324 H 0 2.122 -4.074 4.701 H

HETATM 325 H 0 3.272 -4.804 2.653 H

HETATM 326 H 0 -4.966 -7.437 4.889 H

HETATM 327 H 0 -3.864 -6.624 6.924 H

HETATM 328 H 0 -3.031 -2.883 4.985 H

HETATM 329 H 0 -4.080 -3.696 2.936 H

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HETATM 331 H 0 -5.231 2.587 8.403 H

HETATM 332 H 0 -1.907 2.201 5.713 H

HETATM 333 H 0 -3.114 3.515 4.023 H

HETATM 334 H 0 -3.937 5.721 3.469 H

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HETATM 336 H 0 -8.768 5.142 3.061 H

HETATM 337 H 0 -9.380 9.190 -1.318 H

HETATM 338 H 0 -10.585 7.170 -0.468 H

HETATM 339 H 0 -5.648 -8.979 0.677 H

HETATM 340 H 0 -4.558 -8.181 2.731 H

HETATM 341 H 0 -6.194 -4.289 1.925 H

HETATM 342 H 0 -8.912 -8.564 -4.321 H

HETATM 343 H 0 -5.867 -9.251 -1.374 H

HETATM 344 H 0 -7.044 -9.972 -3.436 H

HETATM 345 H 0 8.908 -6.078 1.118 H

HETATM 346 H 0 7.742 -5.287 3.129 H

HETATM 347 H 0 4.072 -6.704 1.395 H

HETATM 348 H 0 9.432 -8.660 -4.263 H

HETATM 349 H 0 10.663 -6.980 -2.878 H

HETATM 350 H 0 9.571 -6.055 -0.853 H

HETATM 351 H 0 5.567 8.259 3.195 H

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HETATM 354 H 0 9.565 9.733 -1.058 H

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HETATM 360 H 0 -4.680 3.832 -6.039 H

HETATM 361 H 0 0.083 -4.574 6.048 H

HETATM 362 H 0 0.117 -6.318 5.574 H

HETATM 363 C 0 2.207 4.970 -6.570 C

HETATM 364 C 0 4.624 -1.256 7.004 C

HETATM 365 H 0 1.707 4.078 -6.181 H

HETATM 366 H 0 2.632 5.573 -5.768 H

HETATM 367 H 0 3.654 -1.212 6.491 H

HETATM 368 H 0 5.449 -1.155 6.298 H

HETATM 369 C 0 3.747 -0.997 -7.409 C

HETATM 370 C 0 0.155 3.110 7.677 C

HETATM 371 H 0 2.942 -0.540 -6.822 H

HETATM 372 H 0 4.460 -1.516 -6.768 H

HETATM 373 H 0 0.170 2.207 7.056 H

HETATM 374 H 0 0.146 4.014 7.067 H

HETATM 375 C 0 -2.437 -2.434 -7.533 C

HETATM 376 C 0 -4.311 -1.219 7.152 C

HETATM 377 H 0 -1.959 -1.639 -6.947 H

HETATM 378 H 0 -2.853 -3.210 -6.890 H

HETATM 379 H 0 11.853 6.892 -2.217 H

HETATM 380 H 0 11.635 8.237 -1.124 H

HETATM 381 C 0 11.972 6.340 -0.158 C

HETATM 382 H 0 12.756 5.644 -0.460 H

HETATM 383 C 0 11.649 6.397 1.139 C

HETATM 384 H 0 10.882 7.095 1.475 H

HETATM 385 C 0 12.275 5.563 2.225 C

HETATM 386 H 0 13.226 5.139 1.881 H

HETATM 387 H 0 12.509 6.207 3.082 H

HETATM 388 H 0 -8.290 11.571 -0.013 H

HETATM 389 C 0 -7.034 11.178 1.680 C

HETATM 390 H 0 -7.807 10.645 2.235 H

HETATM 391 H 0 -6.631 12.130 -0.202 H

HETATM 392 C 0 -5.969 11.640 2.343 C

HETATM 393 H 0 -5.198 12.179 1.790 H

HETATM 394 C 0 -5.731 11.448 3.818 C

HETATM 395 H 0 -5.347 12.378 4.259 H

HETATM 396 H 0 -6.675 11.223 4.327 H

HETATM 397 H 0 6.565 -12.225 0.580 H

HETATM 398 H 0 5.225 -13.280 0.142 H

HETATM 399 C 0 5.879 -11.996 -1.442 C

HETATM 400 H 0 5.104 -12.319 -2.138 H

HETATM 401 C 0 6.971 -11.396 -1.928 C

HETATM 402 H 0 7.750 -11.081 -1.232 H

HETATM 403 C 0 7.216 -11.108 -3.386 C

HETATM 404 H 0 6.588 -11.756 -4.008 H

HETATM 405 H 0 8.258 -11.341 -3.639 H

HETATM 406 C 0 -11.913 -5.895 -0.459 C

HETATM 407 H 0 -12.378 -5.027 -0.929 H

HETATM 408 C 0 -11.939 -5.939 1.046 C

HETATM 409 H 0 -12.927 -5.632 1.412 H

HETATM 410 H 0 -11.774 -6.963 1.398 H

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HETATM 413 O 0 -1.179 0.377 3.040 O

HETATM 414 H 0 -1.004 0.222 4.019 H

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HETATM 416 O 0 -0.270 -2.236 5.357 O

HETATM 417 H 0 -0.727 -2.082 4.472 H

HETATM 418 O 0 -0.553 -0.015 5.585 O

HETATM 419 C 0 0.334 -1.277 7.432 C

HETATM 420 H 0 -0.485 -1.608 8.080 H

HETATM 421 H 0 1.105 -2.048 7.459 H

HETATM 422 H 0 0.716 -0.332 7.813 H

HETATM 423 C 0 -1.561 -0.728 0.986 C

HETATM 424 C 0 -1.333 0.388 0.266 C

HETATM 425 H 0 -1.780 -1.688 0.532 H

HETATM 426 H 0 -1.105 1.300 0.813 H

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HETATM 428 C 0 -1.529 -0.610 -2.035 C

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HETATM 445 H 0 -3.355 -1.093 6.630 H

END

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Table S4. PDB file of **G1a•G2a⊂M1**

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HETATM 4 C 0 -8.104 1.630 -5.036 C

HETATM 5 C 0 -9.339 0.970 -4.988 C

HETATM 6 C 0 -10.271 1.392 -4.039 C

HETATM 7 C 0 -11.015 2.806 -2.069 C

HETATM 8 C 0 -9.609 -0.223 -5.886 C

HETATM 9 C 0 -8.018 -3.716 -3.898 C

HETATM 10 C 0 -7.158 -2.940 -4.706 C

HETATM 11 C 0 -7.710 -1.826 -5.370 C

HETATM 12 C 0 -9.065 -1.489 -5.252 C

HETATM 13 C 0 -9.877 -2.301 -4.460 C

HETATM 14 C 0 -9.384 -3.414 -3.778 C

HETATM 15 C 0 -10.112 0.598 1.538 C

HETATM 16 C 0 -9.460 1.828 1.303 C

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HETATM 18 C 0 -11.397 0.863 -0.476 C

HETATM 19 C 0 -11.099 0.115 0.664 C

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HETATM 31 O 0 -9.204 3.771 -0.096 O

HETATM 32 O 0 -8.342 -5.287 -1.108 O

HETATM 33 O 0 -7.520 -4.865 -3.309 O

HETATM 34 O 0 -7.182 1.265 -6.005 O

HETATM 35 O 0 -6.897 -1.085 -6.215 O

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HETATM 38 C 0 -6.274 4.097 -5.573 C

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HETATM 70 C 0 2.824 -6.919 -4.583 C

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HETATM 73 C 0 -2.800 -7.551 4.102 C

HETATM 74 C 0 -3.739 -6.848 3.361 C

HETATM 75 C 0 -4.974 -6.505 3.935 C

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HETATM 85 C 0 -3.975 3.804 6.828 C

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HETATM 112 C 0 9.263 4.361 2.934 C

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HETATM 323 H 0 5.036 1.361 4.228 H

HETATM 324 H 0 2.839 0.926 5.236 H

HETATM 325 H 0 1.384 1.726 7.047 H

HETATM 326 H 0 2.827 -2.040 8.542 H

HETATM 327 H 0 -4.646 -1.574 11.547 H

HETATM 328 H 0 -2.877 -3.344 11.569 H

HETATM 329 H 0 6.241 -7.746 -1.475 H

HETATM 330 H 0 3.859 -6.475 1.871 H

HETATM 331 H 0 -0.122 -12.734 -1.622 H

HETATM 332 H 0 3.633 -10.763 -2.428 H

HETATM 333 H 0 1.965 -12.562 -2.991 H

HETATM 334 H 0 5.426 1.582 -7.892 H

HETATM 335 H 0 4.744 -2.047 -5.683 H

HETATM 336 H 0 0.727 -2.770 -12.802 H

HETATM 337 H 0 1.764 -0.498 -12.959 H

HETATM 338 H 0 3.120 0.347 -11.011 H

HETATM 339 H 0 2.089 8.384 2.426 H

HETATM 340 H 0 2.534 7.550 -1.769 H

HETATM 341 H 0 -4.143 12.282 -0.851 H

HETATM 342 H 0 -3.281 12.012 1.482 H

HETATM 343 H 0 -1.222 10.604 1.846 H

HETATM 344 C 0 -9.053 -1.248 2.708 C

HETATM 345 C 0 8.938 -2.045 -1.765 C

HETATM 346 H 0 -8.253 -1.160 1.964 H

HETATM 347 H 0 -8.647 -1.320 3.717 H

HETATM 348 H 0 8.158 -1.541 -1.185 H

HETATM 349 H 0 8.510 -2.744 -2.482 H

HETATM 350 C 0 -8.112 3.831 -0.997 C

HETATM 351 C 0 7.658 4.132 -1.859 C

HETATM 352 H 0 -7.526 2.908 -0.935 H

HETATM 353 H 0 -7.525 4.694 -0.681 H

HETATM 354 H 0 7.162 3.330 -1.300 H

HETATM 355 H 0 6.980 4.587 -2.582 H

HETATM 356 C 0 -6.359 0.139 -5.752 C

HETATM 357 C 0 6.399 3.960 4.254 C

HETATM 358 H 0 -6.124 0.075 -4.683 H

HETATM 359 H 0 -5.459 0.301 -6.344 H

HETATM 360 H 0 6.169 3.260 3.444 H

HETATM 361 H 0 5.490 4.379 4.686 H

HETATM 362 C 0 -7.250 -4.878 -1.916 C

HETATM 363 C 0 7.674 -2.230 4.375 C

HETATM 364 H 0 -6.890 -3.899 -1.588 H

HETATM 365 H 0 -6.489 -5.647 -1.784 H

HETATM 366 H 0 -3.226 12.806 -4.595 H

HETATM 367 H 0 -2.591 13.338 -3.044 H

HETATM 368 C 0 -1.143 12.423 -4.342 C

HETATM 369 H 0 -1.066 12.059 -5.368 H

HETATM 370 C 0 -0.022 12.717 -3.679 C

HETATM 371 H 0 -0.099 13.050 -2.643 H

HETATM 372 C 0 1.377 12.608 -4.233 C

HETATM 373 H 0 1.376 12.825 -5.309 H

HETATM 374 H 0 2.004 13.376 -3.762 H

HETATM 375 H 0 -4.692 1.204 12.465 H

HETATM 376 C 0 -3.069 2.443 11.816 C

HETATM 377 H 0 -2.275 1.784 12.170 H

HETATM 378 H 0 -5.179 2.582 11.477 H

HETATM 379 C 0 -2.785 3.729 11.588 C

HETATM 380 H 0 -3.572 4.384 11.214 H

HETATM 381 C 0 -1.427 4.349 11.777 C

HETATM 382 H 0 -1.520 5.289 12.341 H

HETATM 383 H 0 -0.797 3.681 12.377 H

HETATM 384 H 0 5.734 -6.002 -9.894 H

HETATM 385 H 0 5.387 -7.453 -8.955 H

HETATM 386 C 0 3.650 -6.434 -9.693 C

HETATM 387 H 0 2.943 -7.114 -9.215 H

HETATM 388 C 0 3.225 -5.659 -10.694 C

HETATM 389 H 0 3.930 -4.962 -11.151 H

HETATM 390 C 0 1.820 -5.639 -11.240 C

HETATM 391 H 0 1.325 -6.595 -11.027 H

HETATM 392 H 0 1.854 -5.539 -12.334 H

HETATM 393 C 0 0.111 -11.745 3.945 C

HETATM 394 H 0 -0.918 -11.689 4.301 H

HETATM 395 C 0 1.185 -11.524 4.976 C

HETATM 396 H 0 1.065 -12.250 5.794 H

HETATM 397 H 0 2.169 -11.713 4.530 H

HETATM 398 C 0 2.434 0.402 0.102 C

HETATM 399 O 0 3.330 -0.323 -0.349 O

HETATM 400 O 0 2.655 1.389 0.966 O

HETATM 401 H 0 3.632 1.450 1.162 H

HETATM 402 C 0 6.192 0.827 1.031 C

HETATM 403 O 0 5.909 -0.200 0.241 O

HETATM 404 H 0 4.916 -0.239 0.052 H

HETATM 405 O 0 5.332 1.583 1.491 O

HETATM 406 C 0 7.663 0.983 1.294 C

HETATM 407 H 0 8.089 0.037 1.639 H

HETATM 408 H 0 8.173 1.239 0.359 H

HETATM 409 H 0 7.842 1.764 2.030 H

HETATM 410 C 0 1.036 0.208 -0.301 C

HETATM 411 C 0 0.009 0.939 0.177 C

HETATM 412 H 0 0.900 -0.595 -1.018 H

HETATM 413 H 0 0.240 1.710 0.910 H

HETATM 414 C 0 -1.405 0.803 -0.174 C

HETATM 415 C 0 -1.864 -0.043 -1.203 C

HETATM 416 C 0 -2.358 1.551 0.541 C

HETATM 417 C 0 -3.718 1.447 0.261 C

HETATM 418 C 0 -3.216 -0.150 -1.500 C

HETATM 419 C 0 -4.136 0.593 -0.756 C

HETATM 420 H 0 -2.027 2.218 1.333 H

HETATM 421 H 0 -4.454 2.016 0.820 H

HETATM 422 H 0 -1.155 -0.617 -1.791 H

HETATM 423 H 0 -3.553 -0.799 -2.300 H

HETATM 424 O 0 -5.502 0.584 -1.060 O

HETATM 425 C 0 -6.190 -0.603 -1.093 C

HETATM 426 O 0 -5.682 -1.668 -0.824 O

HETATM 427 C 0 -7.624 -0.373 -1.479 C

HETATM 428 H 0 -8.146 0.149 -0.669 H

HETATM 429 H 0 -7.688 0.262 -2.367 H

HETATM 430 H 0 -8.115 -1.328 -1.663 H

HETATM 431 H 0 7.011 -2.971 4.820 H

HETATM 432 H 0 7.150 -1.635 3.618 H

HETATM 433 H 0 -1.240 8.450 -3.446 H

HETATM 434 H 0 0.471 8.886 -2.165 H

HETATM 435 H 0 3.260 -2.791 -7.537 H

HETATM 436 H 0 1.190 -4.268 -7.293 H

HETATM 437 H 0 2.212 -8.257 1.245 H

HETATM 438 H 0 -1.844 -7.843 3.685 H

HETATM 439 H 0 4.762 -0.619 8.759 H

HETATM 440 H 0 -0.787 1.235 8.195 H

HETATM 441 H 0 -3.385 3.208 7.514 H

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CONECT 434 210

CONECT 435 198

CONECT 436 61

CONECT 437 186

CONECT 438 73

CONECT 439 163

CONECT 440 169

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Table S5. PDB file of **G2a•G2a⊂M1**

REMARK 1 File created by GaussView 6.1.1

HETATM 1 C MOL 1 14.681 -2.831 -0.194 C

HETATM 2 C MOL 1 13.476 -3.550 -0.249 C

HETATM 3 C MOL 1 12.729 -3.653 -1.444 C

HETATM 4 C MOL 1 13.197 -2.938 -2.569 C

HETATM 5 C MOL 1 14.387 -2.201 -2.539 C

HETATM 6 C MOL 1 15.114 -2.176 -1.348 C

HETATM 7 C MOL 1 15.466 -2.719 1.102 C

HETATM 8 C MOL 1 14.830 -1.398 -3.750 C

HETATM 9 C MOL 1 12.854 2.449 -3.619 C

HETATM 10 C MOL 1 12.187 1.355 -4.212 C

HETATM 11 C MOL 1 12.867 0.121 -4.271 C

HETATM 12 C MOL 1 14.166 -0.034 -3.769 C

HETATM 13 C MOL 1 14.790 1.083 -3.213 C

HETATM 14 C MOL 1 14.165 2.328 -3.127 C

HETATM 15 C MOL 1 13.725 0.526 3.363 C

HETATM 16 C MOL 1 13.188 -0.773 3.501 C

HETATM 17 C MOL 1 14.920 -1.595 1.961 C

HETATM 18 C MOL 1 15.437 -0.302 1.888 C

HETATM 19 C MOL 1 14.863 0.769 2.576 C

HETATM 20 C MOL 1 14.863 3.494 -2.450 C

HETATM 21 C MOL 1 15.417 2.174 2.428 C

HETATM 22 C MOL 1 13.483 3.607 1.643 C

HETATM 23 C MOL 1 12.765 4.308 0.655 C

HETATM 24 C MOL 1 13.260 4.275 -0.661 C

HETATM 25 C MOL 1 14.438 3.598 -0.997 C

HETATM 26 C MOL 1 15.139 2.956 0.026 C

HETATM 27 C MOL 1 14.681 2.942 1.345 C

HETATM 28 O MOL 1 13.033 3.646 2.950 O

HETATM 29 O MOL 1 13.176 1.557 4.104 O

HETATM 30 O MOL 1 13.062 -4.272 0.859 O

HETATM 31 O MOL 1 13.327 -3.108 2.923 O

HETATM 32 O MOL 1 12.576 4.963 -1.653 O

HETATM 33 O MOL 1 12.234 3.687 -3.639 O

HETATM 34 O MOL 1 12.482 -3.018 -3.753 O

HETATM 35 O MOL 1 12.247 -0.949 -4.895 O

HETATM 36 C MOL 1 9.322 -6.327 -1.776 C

HETATM 37 C MOL 1 10.400 -6.381 -2.678 C

HETATM 38 C MOL 1 11.482 -5.516 -2.566 C

HETATM 39 C MOL 1 11.535 -4.541 -1.555 C

HETATM 40 C MOL 1 10.449 -4.467 -0.671 C

HETATM 41 C MOL 1 9.371 -5.343 -0.773 C

HETATM 42 C MOL 1 9.772 -1.608 6.037 C

HETATM 43 C MOL 1 11.028 -2.187 6.289 C

HETATM 44 C MOL 1 12.125 -1.914 5.477 C

HETATM 45 C MOL 1 12.011 -1.050 4.376 C

HETATM 46 C MOL 1 10.757 -0.479 4.116 C

HETATM 47 C MOL 1 9.662 -0.748 4.933 C

HETATM 48 C MOL 1 9.221 6.635 1.534 C

HETATM 49 C MOL 1 10.450 7.252 1.248 C

HETATM 50 C MOL 1 11.585 6.496 0.971 C

HETATM 51 C MOL 1 11.536 5.095 0.979 C

HETATM 52 C MOL 1 10.314 4.473 1.271 C

HETATM 53 C MOL 1 9.176 5.231 1.541 C

HETATM 54 C MOL 1 8.124 1.555 -5.710 C

HETATM 55 C MOL 1 9.202 1.282 -6.571 C

HETATM 56 C MOL 1 10.510 1.237 -6.097 C

HETATM 57 C MOL 1 10.797 1.468 -4.743 C

HETATM 58 C MOL 1 9.724 1.753 -3.888 C

HETATM 59 C MOL 1 8.416 1.800 -4.359 C

HETATM 60 C MOL 1 4.055 1.522 -6.942 C

HETATM 61 N MOL 1 4.393 1.088 -5.714 N

HETATM 62 C MOL 1 5.677 1.103 -5.367 C

HETATM 63 C MOL 1 6.724 1.557 -6.191 C

HETATM 64 C MOL 1 6.354 1.994 -7.473 C

HETATM 65 C MOL 1 5.019 1.973 -7.856 C

HETATM 66 C MOL 1 -0.039 1.550 -7.977 C

HETATM 67 C MOL 1 0.977 1.890 -8.881 C

HETATM 68 N MOL 1 2.272 1.870 -8.535 N

HETATM 69 C MOL 1 2.607 1.510 -7.284 C

HETATM 70 C MOL 1 1.653 1.147 -6.322 C

HETATM 71 C MOL 1 0.310 1.172 -6.682 C

HETATM 72 C MOL 1 5.838 9.081 2.317 C

HETATM 73 N MOL 1 7.032 9.398 2.850 N

HETATM 74 C MOL 1 8.071 8.606 2.594 C

HETATM 75 C MOL 1 8.011 7.446 1.802 C

HETATM 76 C MOL 1 6.752 7.116 1.277 C

HETATM 77 C MOL 1 5.660 7.934 1.530 C

HETATM 78 C MOL 1 2.587 11.685 3.015 C

HETATM 79 C MOL 1 2.519 10.605 2.125 C

HETATM 80 N MOL 1 3.561 9.783 1.927 N

HETATM 81 C MOL 1 4.707 10.010 2.590 C

HETATM 82 C MOL 1 4.859 11.071 3.495 C

HETATM 83 C MOL 1 3.775 11.914 3.709 C

HETATM 84 C MOL 1 6.331 -2.459 8.391 C

HETATM 85 N MOL 1 6.198 -2.212 7.077 N

HETATM 86 C MOL 1 7.297 -1.956 6.370 C

HETATM 87 C MOL 1 8.602 -1.904 6.896 C

HETATM 88 C MOL 1 8.720 -2.155 8.271 C

HETATM 89 C MOL 1 7.585 -2.440 9.021 C

HETATM 90 C MOL 1 2.772 -3.308 10.509 C

HETATM 91 C MOL 1 3.913 -4.036 10.828 C

HETATM 92 C MOL 1 5.097 -3.762 10.147 C

HETATM 93 C MOL 1 5.089 -2.766 9.160 C

HETATM 94 N MOL 1 3.987 -2.061 8.853 N

HETATM 95 C MOL 1 2.850 -2.321 9.514 C

HETATM 96 C MOL 1 6.135 -9.123 -2.123 C

HETATM 97 C MOL 1 5.865 -7.875 -1.544 C

HETATM 98 C MOL 1 6.891 -6.947 -1.434 C

HETATM 99 C MOL 1 8.184 -7.269 -1.878 C

HETATM 100 C MOL 1 8.344 -8.557 -2.422 C

HETATM 101 N MOL 1 7.366 -9.450 -2.556 N

HETATM 102 C MOL 1 3.019 -11.935 -2.570 C

HETATM 103 C MOL 1 2.892 -10.771 -1.797 C

HETATM 104 N MOL 1 3.895 -9.892 -1.672 N

HETATM 105 C MOL 1 5.063 -10.140 -2.291 C

HETATM 106 C MOL 1 5.278 -11.288 -3.065 C

HETATM 107 C MOL 1 4.230 -12.192 -3.208 C

HETATM 108 C MOL 1 -14.413 -3.704 0.182 C

HETATM 109 C MOL 1 -13.181 -4.257 0.560 C

HETATM 110 C MOL 1 -12.599 -3.982 1.812 C

HETATM 111 C MOL 1 -13.277 -3.099 2.674 C

HETATM 112 C MOL 1 -14.513 -2.536 2.329 C

HETATM 113 C MOL 1 -15.060 -2.859 1.086 C

HETATM 114 C MOL 1 -14.971 -3.944 -1.210 C

HETATM 115 C MOL 1 -15.189 -1.550 3.264 C

HETATM 116 C MOL 1 -13.653 2.432 2.583 C

HETATM 117 C MOL 1 -12.956 1.581 3.469 C

HETATM 118 C MOL 1 -13.472 0.281 3.673 C

HETATM 119 C MOL 1 -14.658 -0.143 3.055 C

HETATM 120 C MOL 1 -15.311 0.743 2.197 C

HETATM 121 C MOL 1 -14.827 2.025 1.935 C

HETATM 122 C MOL 1 -13.138 -1.045 -3.846 C

HETATM 123 C MOL 1 -12.477 -2.269 -3.609 C

HETATM 124 C MOL 1 -13.110 -3.206 -2.769 C

HETATM 125 C MOL 1 -14.365 -2.961 -2.196 C

HETATM 126 C MOL 1 -14.995 -1.752 -2.491 C

HETATM 127 C MOL 1 -14.407 -0.784 -3.307 C

HETATM 128 C MOL 1 -15.495 2.919 0.907 C

HETATM 129 C MOL 1 -15.099 0.542 -3.561 C

HETATM 130 C MOL 1 -13.451 2.331 -2.856 C

HETATM 131 C MOL 1 -12.968 3.302 -1.960 C

HETATM 132 C MOL 1 -13.662 3.483 -0.750 C

HETATM 133 C MOL 1 -14.824 2.761 -0.445 C

HETATM 134 C MOL 1 -15.288 1.841 -1.386 C

HETATM 135 C MOL 1 -14.620 1.603 -2.589 C

HETATM 136 O MOL 1 -12.798 2.151 -4.063 O

HETATM 137 O MOL 1 -12.566 -0.136 -4.717 O

HETATM 138 O MOL 1 -12.539 -5.147 -0.285 O

HETATM 139 O MOL 1 -12.494 -4.431 -2.554 O

HETATM 140 O MOL 1 -13.208 4.449 0.137 O

HETATM 141 O MOL 1 -13.191 3.725 2.402 O

HETATM 142 O MOL 1 -12.743 -2.843 3.926 O

HETATM 143 O MOL 1 -12.846 -0.549 4.588 O

HETATM 144 C MOL 1 -8.928 -5.850 3.150 C

HETATM 145 C MOL 1 -10.128 -6.577 3.063 C

HETATM 146 C MOL 1 -11.301 -5.979 2.610 C

HETATM 147 C MOL 1 -11.320 -4.630 2.230 C

HETATM 148 C MOL 1 -10.119 -3.911 2.284 C

HETATM 149 C MOL 1 -8.944 -4.508 2.736 C

HETATM 150 C MOL 1 -8.694 -3.213 -5.501 C

HETATM 151 C MOL 1 -9.866 -3.925 -5.811 C

HETATM 152 C MOL 1 -11.075 -3.622 -5.194 C

HETATM 153 C MOL 1 -11.167 -2.587 -4.252 C

HETATM 154 C MOL 1 -10.000 -1.876 -3.936 C

HETATM 155 C MOL 1 -8.787 -2.186 -4.548 C

HETATM 156 C MOL 1 -9.598 5.854 -2.897 C

HETATM 157 C MOL 1 -10.921 6.306 -3.032 C

HETATM 158 C MOL 1 -11.996 5.476 -2.731 C

HETATM 159 C MOL 1 -11.789 4.161 -2.291 C

HETATM 160 C MOL 1 -10.472 3.701 -2.160 C

HETATM 161 C MOL 1 -9.395 4.537 -2.455 C

HETATM 162 C MOL 1 -9.407 2.993 5.530 C

HETATM 163 C MOL 1 -10.640 3.655 5.655 C

HETATM 164 C MOL 1 -11.778 3.198 4.996 C

HETATM 165 C MOL 1 -11.732 2.060 4.176 C

HETATM 166 C MOL 1 -10.500 1.405 4.040 C

HETATM 167 C MOL 1 -9.363 1.855 4.708 C

HETATM 168 C MOL 1 -5.852 4.384 7.410 C

HETATM 169 N MOL 1 -5.779 3.752 6.226 N

HETATM 170 C MOL 1 -6.912 3.333 5.666 C

HETATM 171 C MOL 1 -8.195 3.484 6.225 C

HETATM 172 C MOL 1 -8.250 4.134 7.467 C

HETATM 173 C MOL 1 -7.079 4.592 8.059 C

HETATM 174 C MOL 1 -2.197 5.739 9.044 C

HETATM 175 C MOL 1 -2.334 4.491 8.413 C

HETATM 176 N MOL 1 -3.500 4.074 7.902 N

HETATM 177 C MOL 1 -4.575 4.874 8.007 C

HETATM 178 C MOL 1 -4.525 6.128 8.631 C

HETATM 179 C MOL 1 -3.310 6.565 9.154 C

HETATM 180 C MOL 1 -6.428 8.518 -3.848 C

HETATM 181 C MOL 1 -6.277 7.678 -2.735 C

HETATM 182 C MOL 1 -7.298 6.791 -2.418 C

HETATM 183 C MOL 1 -8.459 6.749 -3.204 C

HETATM 184 C MOL 1 -8.494 7.620 -4.308 C

HETATM 185 N MOL 1 -7.524 8.474 -4.627 N

HETATM 186 C MOL 1 -3.435 11.343 -4.794 C

HETATM 187 C MOL 1 -3.388 10.540 -3.645 C

HETATM 188 N MOL 1 -4.341 9.639 -3.370 N

HETATM 189 C MOL 1 -5.381 9.511 -4.214 C

HETATM 190 C MOL 1 -5.504 10.277 -5.381 C

HETATM 191 C MOL 1 -4.508 11.203 -5.671 C

HETATM 192 C MOL 1 -5.002 -4.264 -7.328 C

HETATM 193 C MOL 1 -5.246 -2.912 -7.050 C

HETATM 194 C MOL 1 -6.451 -2.552 -6.461 C

HETATM 195 C MOL 1 -7.402 -3.537 -6.147 C

HETATM 196 C MOL 1 -7.050 -4.860 -6.468 C

HETATM 197 N MOL 1 -5.903 -5.221 -7.038 N

HETATM 198 C MOL 1 -1.323 -5.423 -9.049 C

HETATM 199 C MOL 1 -2.267 -6.414 -8.789 C

HETATM 200 C MOL 1 -3.489 -6.056 -8.228 C

HETATM 201 C MOL 1 -3.722 -4.703 -7.950 C

HETATM 202 N MOL 1 -2.815 -3.744 -8.209 N

HETATM 203 C MOL 1 -1.635 -4.090 -8.743 C

HETATM 204 C MOL 1 -5.311 -7.452 4.708 C

HETATM 205 C MOL 1 -6.528 -7.872 5.267 C

HETATM 206 C MOL 1 -7.721 -7.371 4.759 C

HETATM 207 C MOL 1 -7.694 -6.462 3.692 C

HETATM 208 C MOL 1 -6.422 -6.147 3.179 C

HETATM 209 N MOL 1 -5.271 -6.611 3.660 N

HETATM 210 C MOL 1 -1.571 -8.682 6.253 C

HETATM 211 C MOL 1 -2.623 -8.506 7.146 C

HETATM 212 C MOL 1 -3.864 -8.111 6.653 C

HETATM 213 C MOL 1 -4.007 -7.906 5.273 C

HETATM 214 N MOL 1 -2.991 -8.078 4.411 N

HETATM 215 C MOL 1 -1.797 -8.456 4.886 C

HETATM 216 C MOL 1 -1.164 3.535 8.337 C

HETATM 217 C MOL 1 1.572 -0.218 10.112 C

HETATM 218 C MOL 1 1.653 -1.457 9.185 C

HETATM 219 C MOL 1 -0.698 -8.675 3.872 C

HETATM 220 C MOL 1 13.809 -1.814 2.783 C

HETATM 221 C MOL 1 1.672 -11.191 0.374 C

HETATM 222 C MOL 1 1.637 -10.484 -1.004 C

HETATM 223 C MOL 1 -0.661 -2.970 -9.028 C

HETATM 224 C MOL 1 0.850 1.070 -11.295 C

HETATM 225 C MOL 1 0.670 2.260 -10.315 C

HETATM 226 C MOL 1 -2.242 10.644 -2.665 C

HETATM 227 C MOL 1 1.516 10.641 -0.203 C

HETATM 228 C MOL 1 1.281 10.340 1.298 C

HETATM 229 C MOL 1 -0.650 -10.139 3.368 C

HETATM 230 C MOL 1 -1.009 2.716 9.643 C

HETATM 231 C MOL 1 -1.158 9.578 -2.909 C

HETATM 232 C MOL 1 -0.804 -2.403 -10.463 C

HETATM 233 H MOL 1 16.046 -1.616 -1.313 H

HETATM 234 H MOL 1 16.518 -2.522 0.868 H

HETATM 235 H MOL 1 15.410 -3.665 1.649 H

HETATM 236 H MOL 1 15.918 -1.271 -3.719 H

HETATM 237 H MOL 1 14.576 -1.944 -4.663 H

HETATM 238 H MOL 1 15.802 0.979 -2.825 H

HETATM 239 H MOL 1 16.309 -0.118 1.265 H

HETATM 240 H MOL 1 15.947 3.346 -2.505 H

HETATM 241 H MOL 1 14.620 4.425 -2.971 H

HETATM 242 H MOL 1 16.063 2.434 -0.216 H

HETATM 243 H MOL 1 15.325 2.706 3.379 H

HETATM 244 H MOL 1 16.480 2.115 2.171 H

HETATM 245 H MOL 1 10.387 -7.100 -3.491 H

HETATM 246 H MOL 1 12.298 -5.590 -3.277 H

HETATM 247 H MOL 1 10.436 -3.713 0.108 H

HETATM 248 H MOL 1 8.570 -5.277 -0.042 H

HETATM 249 H MOL 1 11.144 -2.882 7.117 H

HETATM 250 H MOL 1 13.080 -2.383 5.690 H

HETATM 251 H MOL 1 10.623 0.167 3.254 H

HETATM 252 H MOL 1 8.713 -0.267 4.717 H

HETATM 253 H MOL 1 10.509 8.336 1.212 H

HETATM 254 H MOL 1 12.520 6.995 0.734 H

HETATM 255 H MOL 1 10.249 3.389 1.284 H

HETATM 256 H MOL 1 8.244 4.727 1.783 H

HETATM 257 H MOL 1 9.011 1.066 -7.618 H

HETATM 258 H MOL 1 11.320 1.001 -6.780 H

HETATM 259 H MOL 1 9.909 1.914 -2.831 H

HETATM 260 H MOL 1 7.613 2.035 -3.667 H

HETATM 261 H MOL 1 5.901 0.710 -4.376 H

HETATM 262 H MOL 1 7.109 2.372 -8.157 H

HETATM 263 H MOL 1 4.700 2.311 -8.835 H

HETATM 264 H MOL 1 -1.078 1.581 -8.289 H

HETATM 265 H MOL 1 1.980 0.862 -5.330 H

HETATM 266 H MOL 1 -0.457 0.903 -5.961 H

HETATM 267 H MOL 1 9.014 8.893 3.057 H

HETATM 268 H MOL 1 6.641 6.236 0.649 H

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HETATM 269 H   MOL    1      4.678   7.721   1.123                H
HETATM 270 H   MOL    1      1.725  12.330   3.156                H
HETATM 271 H   MOL    1      5.808  11.208   3.999                H
HETATM 272 H   MOL    1      3.853  12.744   4.407                H
HETATM 273 H   MOL    1      7.140  -1.802   5.304                H
HETATM 274 H   MOL    1      9.691  -2.099   8.755                H
HETATM 275 H   MOL    1      7.664  -2.612  10.090                H
HETATM 276 H   MOL    1      1.829  -3.497  11.016                H
HETATM 277 H   MOL    1      3.880  -4.815  11.586                H
HETATM 278 H   MOL    1      6.000  -4.329  10.351                H
HETATM 279 H   MOL    1      4.858  -7.656  -1.207                H
HETATM 280 H   MOL    1      6.684  -5.963  -1.022                H
HETATM 281 H   MOL    1      9.328  -8.889  -2.748                H
HETATM 282 H   MOL    1      2.182 -12.623  -2.661                H
HETATM 283 H   MOL    1      6.242 -11.441  -3.534                H
HETATM 284 H   MOL    1      4.355 -13.088  -3.811                H
HETATM 285 H   MOL    1    -16.017  -2.425   0.804                H
HETATM 286 H   MOL    1    -16.058  -3.818  -1.193                H
HETATM 287 H   MOL    1    -14.749  -4.968  -1.524                H
HETATM 288 H   MOL    1    -16.269  -1.557   3.080                H
HETATM 289 H   MOL    1    -15.020  -1.856   4.301                H
HETATM 290 H   MOL    1    -16.227   0.419   1.707                H
HETATM 291 H   MOL    1    -15.976  -1.553  -2.064                H
HETATM 292 H   MOL    1    -16.553   2.647   0.823                H
HETATM 293 H   MOL    1    -15.435   3.963   1.229                H
HETATM 294 H   MOL    1    -16.194   1.278  -1.169                H
HETATM 295 H   MOL    1    -14.898   0.869  -4.586                H
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HETATM 296 H MOL 1 -16.180 0.411 -3.451 H

HETATM 297 H MOL 1 -10.140 -7.627 3.342 H

HETATM 298 H MOL 1 -12.216 -6.562 2.556 H

HETATM 299 H MOL 1 -10.102 -2.868 1.978 H

HETATM 300 H MOL 1 -8.037 -3.913 2.802 H

HETATM 301 H MOL 1 -9.835 -4.708 -6.563 H

HETATM 302 H MOL 1 -11.967 -4.185 -5.455 H

HETATM 303 H MOL 1 -10.029 -1.090 -3.188 H

HETATM 304 H MOL 1 -7.895 -1.638 -4.259 H

HETATM 305 H MOL 1 -11.109 7.329 -3.348 H

HETATM 306 H MOL 1 -13.011 5.852 -2.827 H

HETATM 307 H MOL 1 -10.284 2.685 -1.827 H

HETATM 308 H MOL 1 -8.383 4.152 -2.363 H

HETATM 309 H MOL 1 -10.708 4.557 6.258 H

HETATM 310 H MOL 1 -12.714 3.737 5.108 H

HETATM 311 H MOL 1 -6.803 2.863 4.689 H

HETATM 312 H MOL 1 -9.200 4.255 7.979 H

HETATM 313 H MOL 1 -7.109 5.075 9.030 H

HETATM 314 H MOL 1 -1.232 6.048 9.435 H

HETATM 315 H MOL 1 -5.408 6.757 8.675 H

HETATM 316 H MOL 1 -3.232 7.540 9.627 H

HETATM 317 H MOL 1 -5.376 7.750 -2.138 H

HETATM 318 H MOL 1 -7.211 6.150 -1.544 H

HETATM 319 H MOL 1 -9.354 7.606 -4.976 H

HETATM 320 H MOL 1 -2.646 12.065 -4.986 H

HETATM 321 H MOL 1 -6.367 10.135 -6.021 H

HETATM 322 H MOL 1 -4.570 11.815 -6.568 H

HETATM 323 H MOL 1 -4.493 -2.177 -7.306 H

HETATM 324 H MOL 1 -6.667 -1.506 -6.261 H

HETATM 325 H MOL 1 -7.733 -5.673 -6.225 H

HETATM 326 H MOL 1 -0.355 -5.672 -9.475 H

HETATM 327 H MOL 1 -2.049 -7.455 -9.013 H

HETATM 328 H MOL 1 -4.255 -6.786 -7.994 H

HETATM 329 H MOL 1 -6.540 -8.583 6.087 H

HETATM 330 H MOL 1 -8.668 -7.663 5.204 H

HETATM 331 H MOL 1 -6.339 -5.482 2.320 H

HETATM 332 H MOL 1 -0.587 -8.980 6.602 H

HETATM 333 H MOL 1 -2.477 -8.659 8.212 H

HETATM 334 H MOL 1 -4.695 -7.930 7.327 H

HETATM 335 H MOL 1 -1.313 2.857 7.492 H

HETATM 336 H MOL 1 -0.239 4.098 8.156 H

HETATM 337 H MOL 1 1.724 -1.130 8.143 H

HETATM 338 H MOL 1 0.732 -2.045 9.290 H

HETATM 339 H MOL 1 -0.862 -8.005 3.023 H

HETATM 340 H MOL 1 0.272 -8.418 4.318 H

HETATM 341 C MOL 1 0.471 -10.898 1.231 C

HETATM 342 H MOL 1 1.555 -9.403 -0.855 H

HETATM 343 H MOL 1 0.751 -10.815 -1.560 H

HETATM 344 H MOL 1 0.367 -3.328 -8.887 H

HETATM 345 H MOL 1 -0.830 -2.164 -8.308 H

HETATM 346 H MOL 1 -0.357 2.640 -10.391 H

HETATM 347 H MOL 1 1.345 3.067 -10.619 H

HETATM 348 H MOL 1 -1.790 11.641 -2.737 H

HETATM 349 H MOL 1 -2.639 10.534 -1.650 H

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HETATM 350 H   MOL     1       0.986   9.289   1.405                       H
HETATM 351 H   MOL     1       0.451  10.951   1.672                       H
HETATM 352 C   MOL     1       0.527 -10.406   2.472                       C
HETATM 353 C   MOL     1       0.179  -1.297 -10.732                       C
HETATM 354 C   MOL     1      12.346   2.509   3.453                       C
HETATM 355 C   MOL     1     -11.939   1.027  -4.194                       C
HETATM 356 H   MOL     1      11.776   2.031   2.652                       H
HETATM 357 H   MOL     1      11.693   2.893   4.236                       H
HETATM 358 H   MOL     1     -11.460   0.806  -3.237                       H
HETATM 359 H   MOL     1     -11.209   1.315  -4.951                       H
HETATM 360 C   MOL     1      12.439  -3.592   1.937                       C
HETATM 361 C   MOL     1     -11.769  -4.625  -1.356                       C
HETATM 362 H   MOL     1      11.819  -2.769   1.562                       H
HETATM 363 H   MOL     1      11.832  -4.349   2.434                       H
HETATM 364 H   MOL     1     -11.280  -3.691  -1.052                       H
HETATM 365 H   MOL     1     -11.035  -5.398  -1.583                       H
HETATM 366 C   MOL     1      11.626  -1.938  -4.093                       C
HETATM 367 C   MOL     1     -12.049  -1.624   4.119                       C
HETATM 368 H   MOL     1      11.199  -1.489  -3.189                       H
HETATM 369 H   MOL     1      10.850  -2.374  -4.723                       H
HETATM 370 H   MOL     1     -11.537  -1.340   3.194                       H
HETATM 371 H   MOL     1     -11.337  -1.819   4.921                       H
HETATM 372 C   MOL     1      11.674   4.225  -2.452                       C
HETATM 373 C   MOL     1     -12.433   4.027   1.240                       C
HETATM 374 H   MOL     1      11.214   3.432  -1.853                       H
HETATM 375 H   MOL     1      10.929   4.941  -2.796                       H
HETATM 376 H   MOL     1     -11.807   3.170   0.964                       H
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HETATM 377 H MOL 1 -11.823 4.888 1.515 H

HETATM 378 C MOL 1 1.891 0.077 -0.396 C

HETATM 379 O MOL 1 1.517 -1.092 -0.897 O

HETATM 380 H MOL 1 0.516 -1.181 -0.852 H

HETATM 381 O MOL 1 1.108 0.922 0.052 O

HETATM 382 H MOL 1 -1.831 -2.043 -10.606 H

HETATM 383 H MOL 1 -0.653 -3.224 -11.179 H

HETATM 384 H MOL 1 1.875 0.692 -11.204 H

HETATM 385 C MOL 1 -0.136 -0.043 -11.067 C

HETATM 386 H MOL 1 0.740 1.461 -12.317 H

HETATM 387 C MOL 1 0.060 9.679 -2.025 C

HETATM 388 H MOL 1 -1.612 8.582 -2.801 H

HETATM 389 H MOL 1 -0.832 9.632 -3.959 H

HETATM 390 C MOL 1 0.262 10.549 -1.031 C

HETATM 391 H MOL 1 1.931 11.657 -0.289 H

HETATM 392 H MOL 1 2.282 9.957 -0.583 H

HETATM 393 H MOL 1 -0.518 11.268 -0.778 H

HETATM 394 H MOL 1 0.852 8.964 -2.256 H

HETATM 395 H MOL 1 1.234 -1.559 -10.618 H

HETATM 396 H MOL 1 -1.191 0.222 -11.175 H

HETATM 397 H MOL 1 -0.597 -10.803 4.245 H

HETATM 398 H MOL 1 -1.589 -10.374 2.853 H

HETATM 399 H MOL 1 2.587 -10.896 0.902 H

HETATM 400 H MOL 1 1.747 -12.276 0.201 H

HETATM 401 H MOL 1 -0.504 -11.123 0.793 H

HETATM 402 H MOL 1 1.507 -10.181 2.900 H

HETATM 403 C MOL 1 0.308 0.582 9.948 C

HETATM 404 H MOL 1 1.637 -0.569 11.154 H

HETATM 405 H MOL 1 2.451 0.415 9.942 H

HETATM 406 H MOL 1 -1.890 2.075 9.774 H

HETATM 407 C MOL 1 0.250 1.893 9.699 C

HETATM 408 H MOL 1 -1.008 3.421 10.489 H

HETATM 409 H MOL 1 -0.626 0.032 10.085 H

HETATM 410 H MOL 1 1.184 2.443 9.559 H

HETATM 411 C MOL 1 3.342 0.323 -0.395 C

HETATM 412 C MOL 1 4.242 -0.577 -0.835 C

HETATM 413 H MOL 1 3.623 1.288 0.015 H

HETATM 414 H MOL 1 3.859 -1.524 -1.207 H

HETATM 415 C MOL 1 5.697 -0.432 -0.848 C

HETATM 416 C MOL 1 6.357 0.770 -0.528 C

HETATM 417 C MOL 1 6.486 -1.546 -1.188 C

HETATM 418 C MOL 1 7.876 -1.477 -1.182 C

HETATM 419 C MOL 1 7.744 0.858 -0.526 C

HETATM 420 C MOL 1 8.496 -0.277 -0.844 C

HETATM 421 H MOL 1 6.000 -2.481 -1.451 H

HETATM 422 H MOL 1 8.483 -2.340 -1.436 H

HETATM 423 H MOL 1 5.778 1.655 -0.282 H

HETATM 424 H MOL 1 8.233 1.790 -0.273 H

HETATM 425 O MOL 1 9.890 -0.268 -0.933 O

HETATM 426 C MOL 1 10.671 0.352 0.005 C

HETATM 427 O MOL 1 10.223 0.934 0.969 O

HETATM 428 C MOL 1 12.123 0.208 -0.352 C

HETATM 429 H MOL 1 12.366 -0.838 -0.553 H

HETATM 430 H MOL 1 12.336 0.771 -1.266 H

HETATM 431 H MOL 1 12.743 0.589 0.458 H

HETATM 432 C MOL 1 -1.905 -0.561 -0.251 C

HETATM 433 O MOL 1 -1.525 0.590 0.284 O

HETATM 434 H MOL 1 -0.530 0.703 0.190 H

HETATM 435 O MOL 1 -1.133 -1.369 -0.780 O

HETATM 436 C MOL 1 -3.350 -0.837 -0.185 C

HETATM 437 C MOL 1 -4.233 0.000 0.390 C

HETATM 438 H MOL 1 -3.637 -1.777 -0.645 H

HETATM 439 H MOL 1 -3.840 0.915 0.828 H

HETATM 440 C MOL 1 -5.683 -0.176 0.488 C

HETATM 441 C MOL 1 -6.362 -1.292 -0.037 C

HETATM 442 C MOL 1 -6.441 0.823 1.126 C

HETATM 443 C MOL 1 -7.827 0.726 1.229 C

HETATM 444 C MOL 1 -7.744 -1.401 0.060 C

HETATM 445 C MOL 1 -8.463 -0.385 0.688 C

HETATM 446 H MOL 1 -5.934 1.689 1.541 H

HETATM 447 H MOL 1 -8.410 1.498 1.722 H

HETATM 448 H MOL 1 -5.807 -2.083 -0.532 H

HETATM 449 H MOL 1 -8.266 -2.259 -0.350 H

HETATM 450 O MOL 1 -9.854 -0.514 0.833 O

HETATM 451 C MOL 1 -10.639 -0.115 -0.221 C

HETATM 452 O MOL 1 -10.170 0.348 -1.236 O

HETATM 453 C MOL 1 -12.094 -0.329 0.078 C

HETATM 454 H MOL 1 -12.279 -1.372 0.347 H

HETATM 455 H MOL 1 -12.393 0.285 0.933 H

HETATM 456 H MOL 1 -12.692 -0.059 -0.792 H

HETATM 457 H MOL 1 -10.419 0.537 3.394 H

HETATM 458 H MOL 1 -8.436 1.299 4.603 H

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