Synthesis and Structure of unsymmetrical anthracenyl-isoxazole antitumor agents via the diastereoselective bromination of 3-(9'-anthryl)-isoxazole esters

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Supplementary Material

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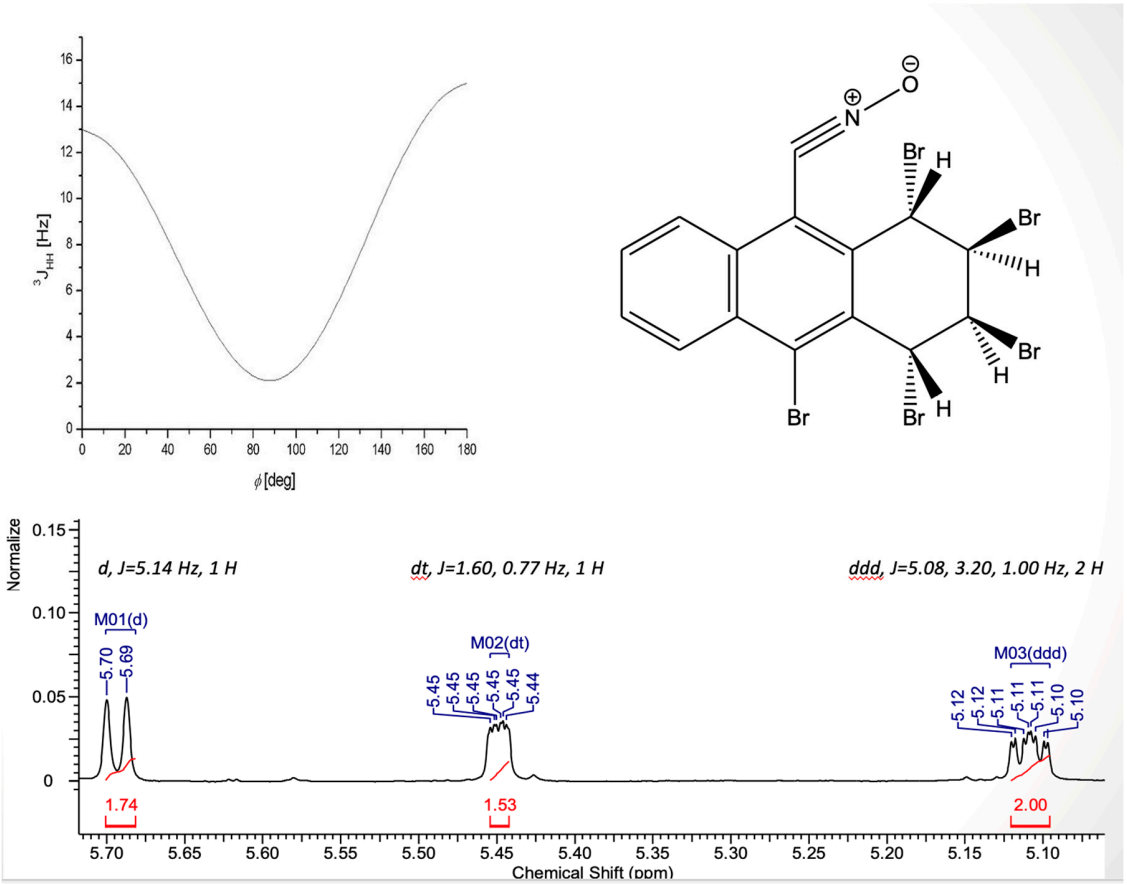

Figure S1. Proton NMR of the A ring region for tetrabromo nitrile oxide intermediate, **6**. The stereochemistry was assigned by analogy to the report of Cakmak 2006 [20], using the Karplus equation.

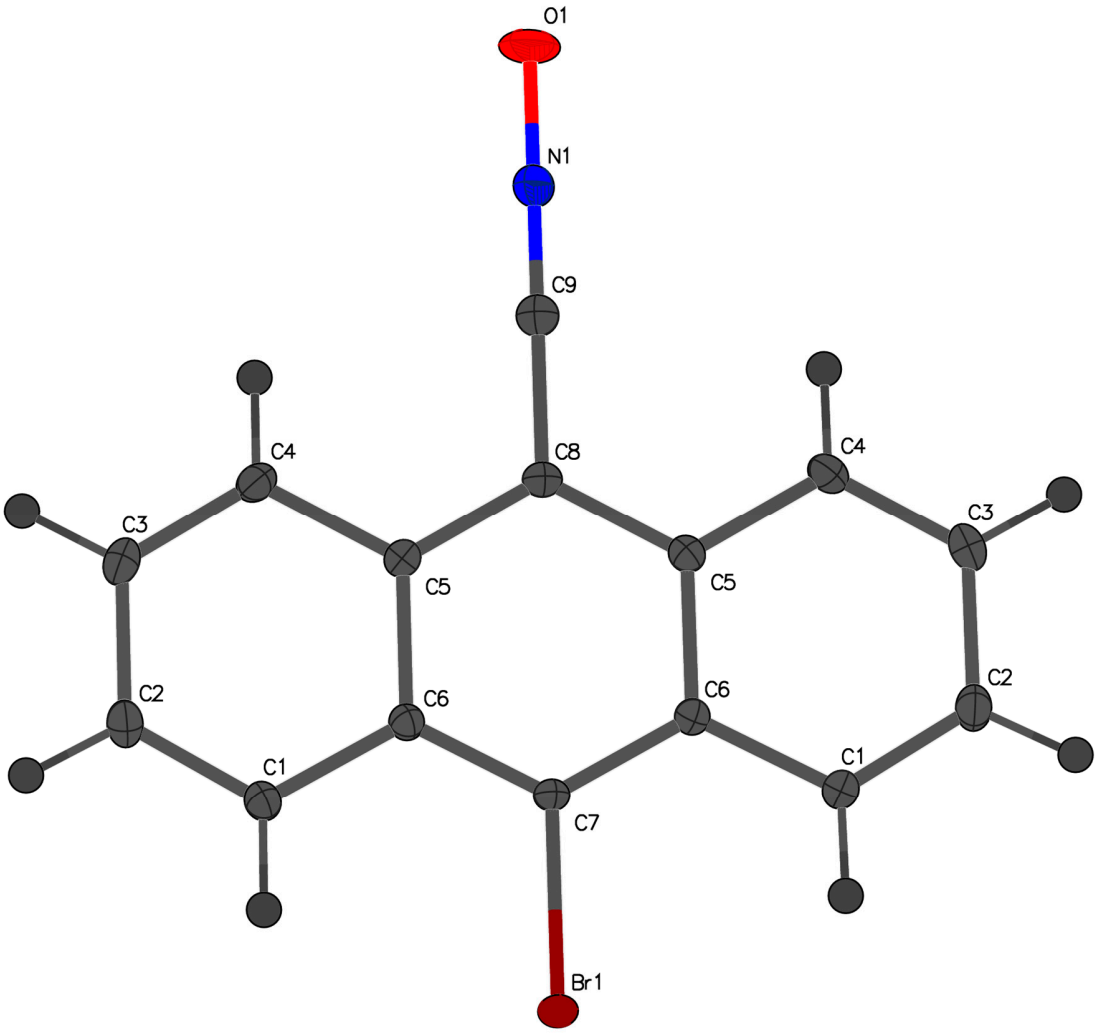

Figure S2. Larger version of Figure 5, Structure of Bromo nitrile oxide **1** (MC59).

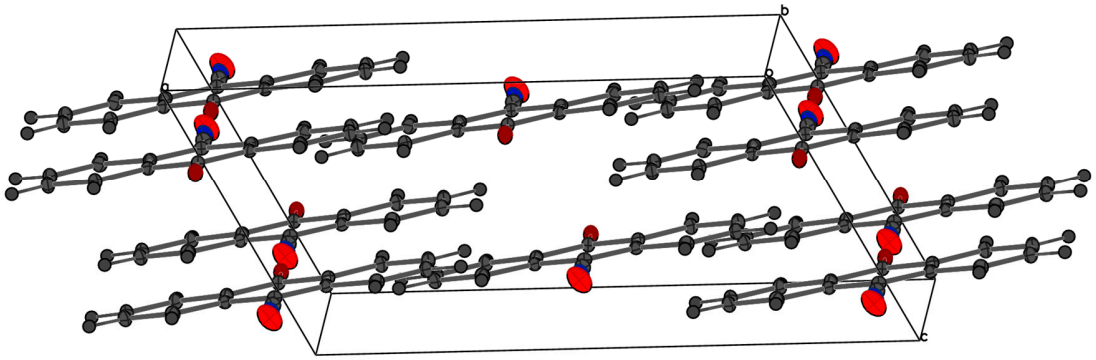

Figure S3. Larger version of Figure 6. Unit cell for the Bromo nitrile oxide **1** (MC59).

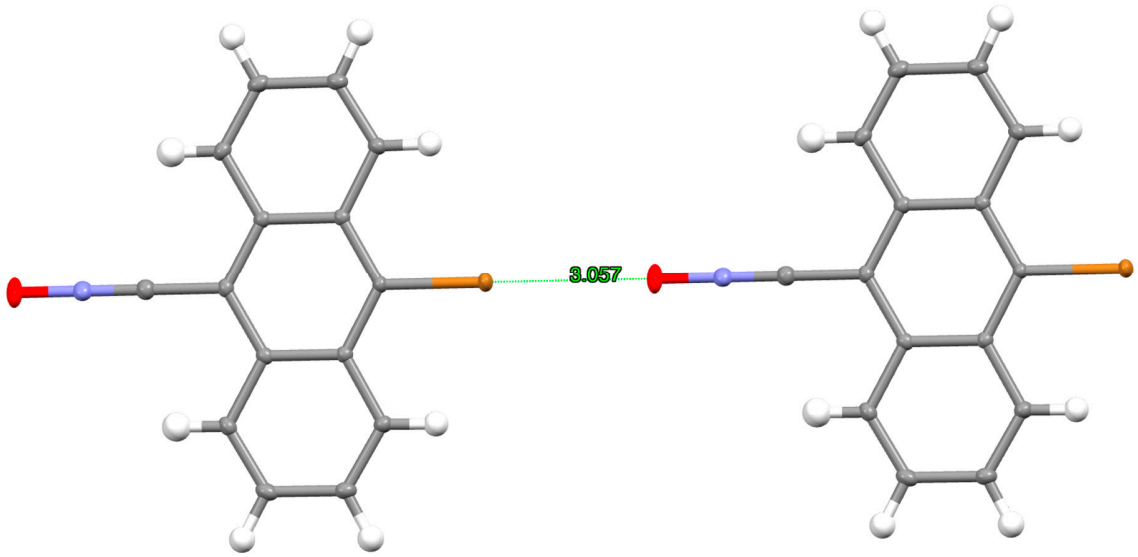

Figure S4. Larger version of Figure 7, halogen bond for Bromo nitrile oxide **1** (MC59), with a distance of 3.057 Å

Tables of Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2), Atomic displacement parameters (Å^2), Geometric parameters (Å, º), and Hydrogen-bond geometry (Å, º) for the Bromo nitrile oxide **1** (MC59) **Tables S1-S3**; Penta Bromo AIM **2** (cl_mc79c9_15_0m), **Tables S4-S7**; the tetra bromo Chloro AIM ester **3** (**Tables S8-S14**); Dibromo AIM ester **4** (MC219), **Tables S15- S20** are listed below.

Table S1. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for Bromo Nitrile Oxide **1**, MC-59.

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.500000	0.76165 (2)	0.250000	0.01336 (6)
C3	0.31470 (8)	0.59743 (10)	0.12446 (15)	0.01277 (19)
N1	0.500000	0.13259 (14)	0.250000	0.0161 (3)
C4	0.22844 (8)	0.53668 (11)	0.06309 (15)	0.0146 (2)
C8	0.500000	0.35618 (14)	0.250000	0.0110 (3)
C2	0.40865 (8)	0.53946 (10)	0.18675 (13)	0.01031 (18)
C9	0.500000	0.23122 (14)	0.250000	0.0145 (3)
C7	0.40939 (8)	0.41515 (10)	0.18517 (14)	0.01059 (18)

C6	0.31801 (8)	0.35509 (10)	0.11857 (15)	0.01308 (19)
C5	0.23030 (8)	0.41389 (11)	0.05857 (15)	0.0146 (2)
O1	0.500000	0.02625 (12)	0.250000	0.0279 (3)
C1	0.500000	0.59723 (13)	0.250000	0.0102 (2)
H3	0.3122 (13)	0.6794 (17)	0.131 (2)	0.021 (4)*
H4	0.1638 (15)	0.5742 (17)	0.021 (3)	0.024 (4)*
H6	0.3189 (19)	0.2753 (19)	0.118 (3)	0.029 (6)*
H5	0.1680 (14)	0.3740 (18)	0.013 (2)	0.023 (4)*

Table S2. Atomic displacement parameters (Å^2) for Bromo Nitrile Oxide **1**, MC-59.

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.01424 (9)	0.00805 (8)	0.01758 (9)	0.000	-0.00251 (6)	0.000
C3	0.0111 (4)	0.0123 (5)	0.0147 (5)	0.0005 (3)	-0.0011 (3)	0.0012 (4)
N1	0.0120 (6)	0.0137 (6)	0.0225 (7)	0.000	0.0011 (5)	0.000
C4	0.0109 (4)	0.0173 (5)	0.0155 (5)	0.0001 (4)	-0.0017 (4)	0.0010 (4)
C8	0.0122 (6)	0.0096 (6)	0.0113 (6)	0.000	0.0010 (5)	0.000
C2	0.0101 (4)	0.0104 (4)	0.0105 (4)	0.0001 (3)	0.0000 (3)	0.0003 (3)
C9	0.0143 (7)	0.0136 (7)	0.0158 (7)	0.000	0.0003 (6)	0.000
C7	0.0107 (4)	0.0109 (4)	0.0102 (4)	-0.0009 (3)	0.0003 (3)	-0.0002 (3)
C6	0.0129 (4)	0.0119 (5)	0.0144 (5)	-0.0024 (3)	0.0003 (4)	-0.0015 (4)
C5	0.0113 (4)	0.0175 (5)	0.0150 (5)	-0.0030 (4)	-0.0006 (4)	-0.0014 (4)
O1	0.0256 (6)	0.0083 (5)	0.0503 (9)	0.000	0.0062 (6)	0.000
C1	0.0107 (6)	0.0082 (6)	0.0116 (6)	0.000	-0.0006 (5)	0.000

Table S3. Geometric parameters (Å, º) for (mc59) for Bromo Nitrile Oxide **1**, MC-59.

Br1—C1	1.8993 (15)	C8—C7	1.4068 (13)
C3—C4	1.3651 (15)	C8—C7^{i}	1.4068 (13)
C3—C2	1.4303 (15)	C2—C7	1.4360 (16)
C3—H3	0.95 (2)	C2—C1	1.4042 (12)
N1—C9	1.139 (2)	C7—C6	1.4249 (14)
N1—O1	1.228 (2)	C6—C5	1.3654 (16)
C4—C5	1.4190 (17)	C6—H6	0.92 (2)

C4—H4	0.970 (19)	C5—H5	0.967 (18)
C8—C9	1.443 (2)		
C4—C3—C2	121.13 (11)	N1—C9—C8	180.0
C4—C3—H3	120.1 (11)	C8—C7—C2	119.14 (10)
C2—C3—H3	118.7 (11)	C8—C7—C6	121.91 (11)
C9—N1—O1	180.0	C6—C7—C2	118.95 (10)
C3—C4—C5	120.52 (10)	C7—C6—H6	118.5 (15)
C3—C4—H4	122.5 (12)	C5—C6—C7	121.02 (11)
C5—C4—H4	116.9 (11)	C5—C6—H6	120.5 (15)
C7—C8—C9	118.96 (7)	C4—C5—H5	118.0 (12)
C7^{i}—C8—C9	118.96 (7)	C6—C5—C4	120.24 (10)
C7^{i}—C8—C7	122.08 (14)	C6—C5—H5	121.7 (12)
C3—C2—C7	118.12 (9)	C2—C1—Br1	118.37 (7)
C1—C2—C3	123.70 (10)	C2^{i}—C1—Br1	118.38 (7)
C1—C2—C7	118.18 (10)	C2^{i}—C1—C2	123.25 (14)
C3—C4—C5—C6	1.11 (17)	C9—C8—C7—C2	179.33 (6)
C3—C2—C7—C8	-178.44 (8)	C9—C8—C7—C6	-0.40 (11)
C3—C2—C7—C6	1.30 (15)	C7^{i}—C8—C7—C2	-0.67 (6)
C3—C2—C1—Br1	-0.92 (11)	C7^{i}—C8—C7—C6	179.60 (11)
C3—C2—C1—C2^{i}	179.08 (11)	C7—C2—C1—Br1	179.34 (6)
C4—C3—C2—C7	-0.77 (16)	C7—C2—C1—C2^{i}	-0.66 (6)
C4—C3—C2—C1	179.49 (9)	C7—C6—C5—C4	-0.55 (16)
C8—C7—C6—C5	179.07 (9)	C1—C2—C7—C8	1.31 (13)
C2—C3—C4—C5	-0.42 (17)	C1—C2—C7—C6	-178.95 (8)
C2—C7—C6—C5	-0.66 (15)		

Symmetry code: (i) -*x*+1, *y*, -*z*+1/2.

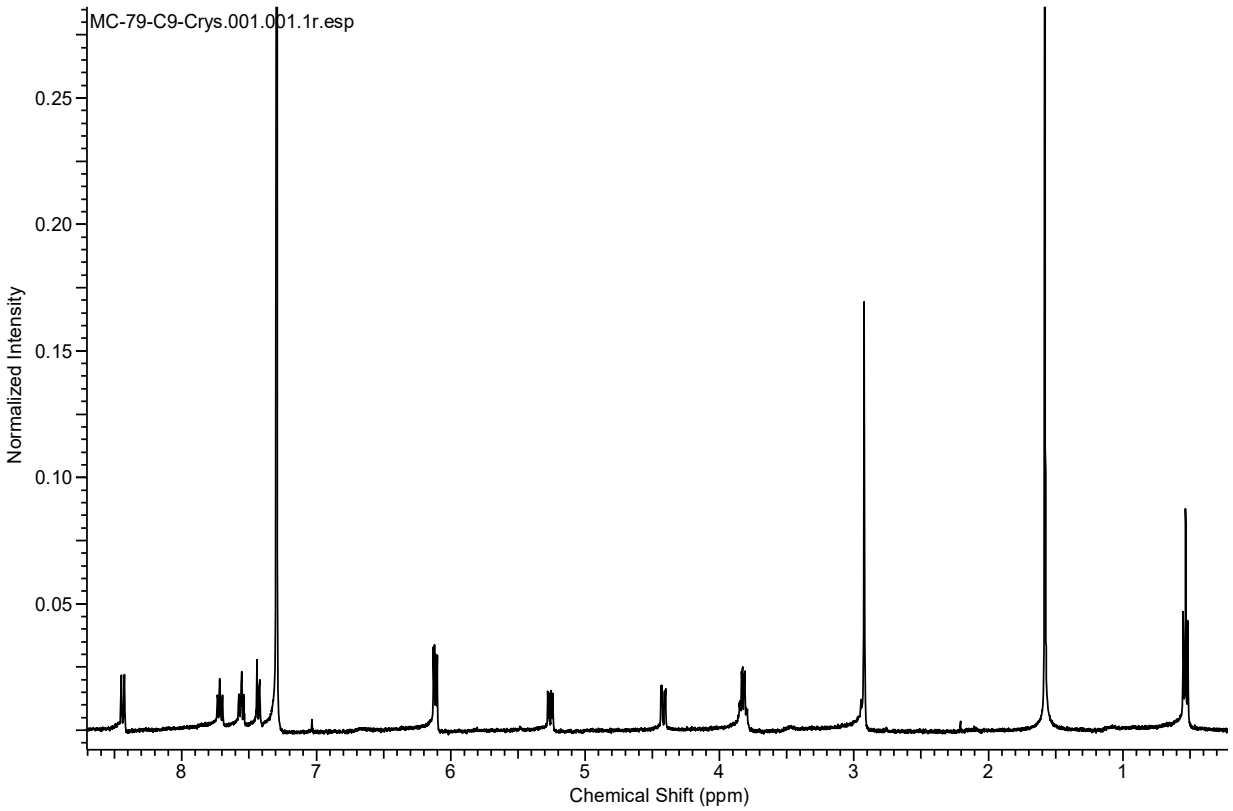

Figure S5. Proton NMR of Penta bromo AIM ester **2** (MC79).

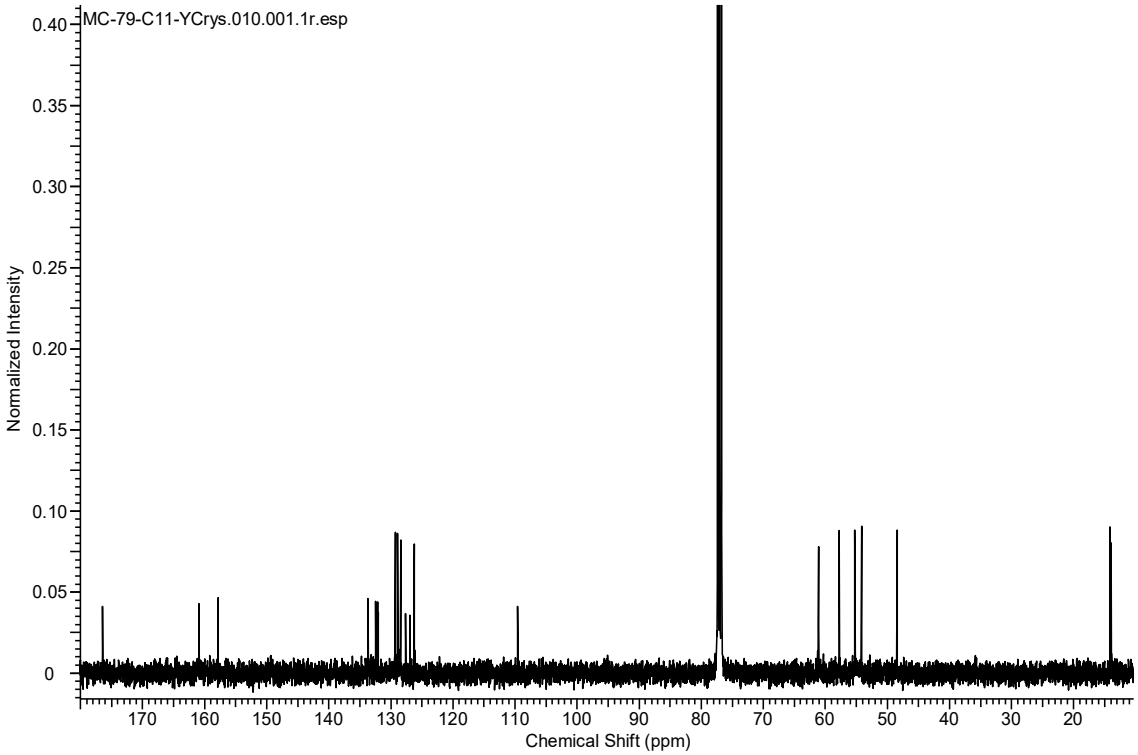

Figure S6. ^{13}C NMR of penta bromo ester 2 (MC79)

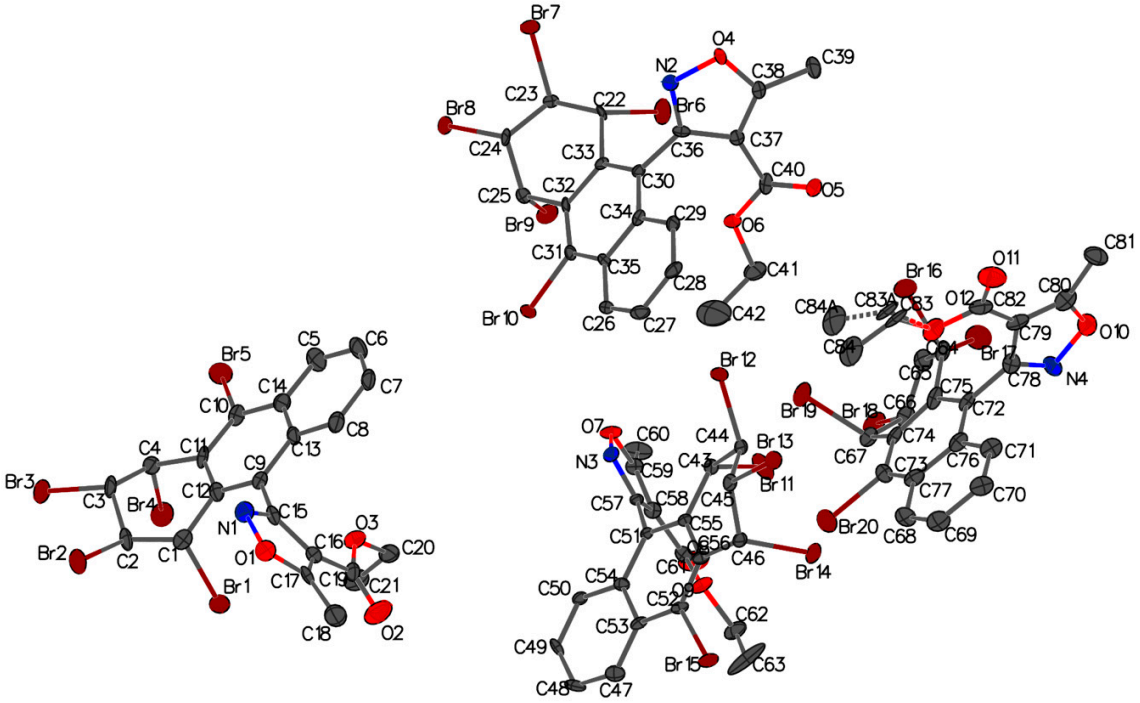

Figure S7. Numbering of unit cell of penta bromo ester **2** (cl_mc79c9_15_0m).

Table S4. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for the Penta bromo AIM ester **2** (cl_mc79c9_15_0m).

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Br1	0.02894 (5)	1.05457 (10)	0.68368 (2)	0.0266 (2)	
Br2	0.08166 (6)	1.17726 (12)	0.76352 (2)	0.0350 (3)	
Br3	0.18871 (6)	1.43084 (10)	0.74216 (2)	0.0319 (3)	
Br4	0.16281 (6)	1.34256 (10)	0.67173 (2)	0.0312 (2)	
Br5	0.34861 (6)	1.18979 (10)	0.66708 (2)	0.0291 (2)	
O1	0.0811 (4)	0.6612 (6)	0.73194 (15)	0.0234 (15)	
O2	0.0080 (4)	0.6753 (10)	0.64484 (18)	0.052 (3)	
O3	0.1109 (3)	0.7808 (7)	0.64407 (14)	0.0248 (15)	
N1	0.1372 (4)	0.7529 (8)	0.73070 (18)	0.0240 (19)	
C1	0.1129 (5)	1.0557 (9)	0.7132 (2)	0.021 (2)	
H1	0.103684	0.989512	0.727787	0.025*	
C2	0.1166 (5)	1.1914 (10)	0.7269 (2)	0.022 (2)	
H2	0.083439	1.250918	0.715079	0.026*	
C3	0.1899 (6)	1.2506 (9)	0.7289 (2)	0.024 (2)	

H3	0.221481	1.198565	0.742956	0.029*	
C4	0.2220 (5)	1.2450 (9)	0.7015 (2)	0.020 (2)	
H4	0.270697	1.285552	0.704225	0.024*	
C5	0.3568 (6)	0.8796 (11)	0.6609 (2)	0.029 (2)	
H5	0.388780	0.940912	0.654006	0.034*	
C6	0.3679 (6)	0.7478 (11)	0.6576 (2)	0.028 (2)	
H6	0.407807	0.718196	0.648863	0.034*	
C7	0.3206 (5)	0.6564 (10)	0.6672 (2)	0.025 (2)	
H7	0.328575	0.564938	0.664771	0.030*	
C8	0.2629 (6)	0.6976 (10)	0.6799 (2)	0.025 (2)	
H8	0.231788	0.634189	0.686604	0.031*	
C9	0.1888 (5)	0.8781 (9)	0.69605 (19)	0.0178 (19)	
C10	0.2859 (5)	1.0612 (9)	0.67944 (18)	0.019 (2)	
C11	0.2291 (5)	1.1041 (9)	0.69315 (19)	0.019 (2)	
C12	0.1776 (5)	1.0113 (9)	0.69995 (19)	0.0187 (19)	
C13	0.2491 (5)	0.8317 (10)	0.6832 (2)	0.021 (2)	
C14	0.2985 (5)	0.9259 (10)	0.6743 (2)	0.021 (2)	
C15	0.1367 (5)	0.7815 (9)	0.7041 (2)	0.0179 (19)	
C16	0.0826 (5)	0.7100 (9)	0.6872 (2)	0.021 (2)	
C17	0.0498 (5)	0.6382 (9)	0.7053 (2)	0.024 (2)	
C18	-0.0083 (6)	0.5369 (11)	0.7033 (3)	0.034 (3)	
H18A	0.004996	0.465605	0.716545	0.051*	
H18B	-0.014946	0.501318	0.684197	0.051*	
H18C	-0.052942	0.577561	0.707644	0.051*	
C19	0.0631 (5)	0.7173 (10)	0.6568 (2)	0.025 (2)	
C20	0.0965 (5)	0.8041 (11)	0.6140 (2)	0.029 (2)	
H20A	0.062075	0.737810	0.605505	0.035*	
H20B	0.141252	0.796154	0.605121	0.035*	
C21	0.0661 (6)	0.9385 (11)	0.6094 (2)	0.033 (3)	
H21A	0.099732	1.003317	0.618447	0.049*	
H21B	0.020626	0.944277	0.617466	0.049*	
H21C	0.058091	0.956537	0.589281	0.049*	
Br11	0.22889 (6)	0.51745 (11)	0.40578 (2)	0.0314 (3)	
Br12	0.33992 (5)	0.35423 (8)	0.47445 (2)	0.01808 (19)	
Br13	0.21356 (5)	0.11203 (8)	0.47973 (2)	0.0188 (2)	
Br14	0.09856 (5)	0.23132 (10)	0.42249 (2)	0.0254 (2)	
Br15	-0.04599 (5)	0.38198 (9)	0.46281 (2)	0.0189 (2)	

O7	0.2849 (3)	0.8938 (6)	0.44168 (14)	0.0181 (14)	
O8	0.1192 (4)	0.9058 (8)	0.37354 (16)	0.0337 (19)	
O9	0.0770 (3)	0.7435 (6)	0.39888 (14)	0.0196 (14)	
N3	0.2497 (4)	0.8054 (7)	0.45822 (16)	0.0138 (15)	
C43	0.2232 (5)	0.5005 (8)	0.44654 (18)	0.0134 (18)	
H43	0.260454	0.559461	0.456353	0.016*	
C44	0.2438 (4)	0.3577 (8)	0.4546 (2)	0.0145 (18)	
H44	0.243361	0.304260	0.437119	0.017*	
C45	0.1910 (5)	0.2966 (8)	0.4731 (2)	0.0148 (18)	
H45	0.195988	0.343358	0.491518	0.018*	
C46	0.1153 (5)	0.3137 (8)	0.4597 (2)	0.0152 (19)	
H46	0.082871	0.270338	0.472008	0.018*	
C47	-0.0531 (5)	0.6888 (9)	0.4680 (2)	0.019 (2)	
H47	-0.091115	0.629384	0.470162	0.023*	
C48	-0.0646 (5)	0.8212 (10)	0.4697 (2)	0.022 (2)	
H48	-0.110576	0.852882	0.472862	0.026*	
C49	-0.0090 (5)	0.9112 (9)	0.4668 (2)	0.018 (2)	
H49	-0.017029	1.003011	0.468449	0.021*	
C50	0.0563 (4)	0.8657 (8)	0.46157 (19)	0.0142 (18)	
H50	0.093241	0.926929	0.459193	0.017*	
C51	0.1385 (4)	0.6819 (8)	0.45347 (17)	0.0099 (17)	
C52	0.0304 (4)	0.5039 (8)	0.46163 (18)	0.0124 (17)	
C53	0.0141 (4)	0.6393 (8)	0.46327 (18)	0.0129 (18)	
C54	0.0704 (4)	0.7289 (9)	0.45959 (18)	0.0126 (17)	
C55	0.1517 (4)	0.5495 (8)	0.45300 (18)	0.0109 (17)	
C56	0.0967 (4)	0.4573 (8)	0.45805 (19)	0.0135 (18)	
C57	0.1894 (4)	0.7772 (8)	0.44327 (19)	0.0119 (17)	
C58	0.1804 (5)	0.8463 (8)	0.41728 (19)	0.0143 (18)	
C59	0.2424 (5)	0.9189 (8)	0.4180 (2)	0.0155 (19)	
C60	0.2694 (5)	1.0112 (11)	0.3979 (2)	0.029 (2)	
H60A	0.282451	0.962052	0.381637	0.044*	
H60B	0.311567	1.057252	0.406887	0.044*	
H60C	0.232051	1.075372	0.391706	0.044*	
C61	0.1231 (5)	0.8383 (9)	0.3943 (2)	0.0180 (19)	
C62	0.0173 (5)	0.7182 (11)	0.3775 (2)	0.027 (2)	
H62A	0.035032	0.688319	0.359956	0.032*	
H62B	-0.011384	0.799094	0.373604	0.032*	

C63	-0.0267 (8)	0.6133 (15)	0.3890 (3)	0.063 (5)	
H63A	-0.049028	0.648266	0.404949	0.095*	
H63B	0.003980	0.538499	0.395215	0.095*	
H63C	-0.063971	0.584133	0.374455	0.095*	
Br6	0.72785 (6)	0.97944 (11)	0.40309 (2)	0.0306 (3)	
Br7	0.84059 (5)	1.14200 (9)	0.47013 (2)	0.0229 (2)	
Br8	0.71527 (5)	1.38208 (8)	0.47858 (2)	0.01714 (19)	
Br9	0.59797 (5)	1.27272 (9)	0.42242 (2)	0.0243 (2)	
Br10	0.45481 (5)	1.11495 (9)	0.46308 (2)	0.0187 (2)	
O4	0.7847 (3)	0.6047 (6)	0.43918 (13)	0.0162 (13)	
O5	0.6122 (3)	0.5523 (7)	0.37555 (14)	0.0257 (16)	
O6	0.5711 (3)	0.7301 (7)	0.39706 (14)	0.0224 (15)	
N2	0.7503 (4)	0.6974 (7)	0.45530 (17)	0.0164 (16)	
C22	0.7225 (4)	0.9961 (8)	0.44357 (18)	0.0115 (17)	
H22	0.760157	0.937373	0.453252	0.014*	
C23	0.7422 (4)	1.1384 (8)	0.45228 (19)	0.0128 (17)	
H23	0.739624	1.193460	0.434955	0.015*	
C24	0.6932 (5)	1.1971 (8)	0.47124 (19)	0.0124 (17)	
H24	0.700019	1.148697	0.489460	0.015*	
C25	0.6149 (5)	1.1816 (8)	0.45887 (19)	0.0141 (18)	
H25	0.583819	1.222879	0.472021	0.017*	
C26	0.4480 (4)	0.8077 (9)	0.46840 (19)	0.0155 (19)	
H26	0.410666	0.867299	0.471375	0.019*	
C27	0.4363 (5)	0.6759 (10)	0.4702 (2)	0.020 (2)	
H27	0.390965	0.644500	0.474241	0.025*	
C28	0.4909 (5)	0.5866 (9)	0.4661 (2)	0.019 (2)	
H28	0.482389	0.494771	0.467578	0.023*	
C29	0.5559 (5)	0.6296 (8)	0.46010 (19)	0.0150 (18)	
H29	0.592408	0.567869	0.457369	0.018*	
C30	0.6356 (4)	0.8140 (8)	0.45057 (18)	0.0116 (17)	
C31	0.5301 (5)	0.9919 (8)	0.46008 (19)	0.0142 (18)	
C32	0.5967 (5)	1.0396 (8)	0.45625 (18)	0.0130 (18)	
C33	0.6506 (4)	0.9469 (8)	0.45089 (18)	0.0100 (17)	
C34	0.5695 (5)	0.7660 (8)	0.45787 (18)	0.0132 (18)	
C35	0.5148 (4)	0.8578 (8)	0.46217 (19)	0.0131 (18)	
C36	0.6871 (4)	0.7177 (8)	0.44096 (18)	0.0116 (17)	
C37	0.6785 (4)	0.6405 (8)	0.41610 (19)	0.0134 (18)	

C38	0.7406 (5)	0.5709 (8)	0.41650 (18)	0.0125 (18)	
C39	0.7696 (6)	0.4737 (10)	0.3977 (2)	0.027 (2)	
H39A	0.770729	0.512732	0.379069	0.040*	
H39B	0.739069	0.395302	0.396146	0.040*	
H39C	0.818235	0.448777	0.405307	0.040*	
C40	0.6184 (5)	0.6345 (9)	0.39387 (18)	0.0168 (19)	
C41	0.5054 (5)	0.7324 (12)	0.3779 (2)	0.033 (3)	
H41A	0.491415	0.641787	0.372039	0.040*	
H41B	0.512385	0.784495	0.361052	0.040*	
C42	0.4487 (8)	0.794 (2)	0.3933 (3)	0.078 (6)	
H42A	0.402468	0.788250	0.381751	0.117*	
H42B	0.460648	0.886415	0.397164	0.117*	
H42C	0.446000	0.747051	0.410955	0.117*	
Br16	0.48118 (5)	0.50848 (11)	0.31366 (2)	0.0281 (2)	
Br17	0.42909 (6)	0.63288 (12)	0.23344 (2)	0.0340 (3)	
Br18	0.31837 (6)	0.88153 (10)	0.25436 (2)	0.0281 (2)	
Br19	0.34711 (6)	0.79880 (10)	0.32453 (2)	0.0279 (2)	
Br20	0.16812 (6)	0.63694 (11)	0.33287 (2)	0.0295 (2)	
O10	0.4244 (4)	0.1205 (7)	0.25827 (15)	0.0264 (16)	
O11	0.4755 (4)	0.0408 (9)	0.34521 (17)	0.039 (2)	
O12	0.4108 (4)	0.2257 (7)	0.34780 (14)	0.0287 (17)	
N4	0.3713 (4)	0.2153 (8)	0.26214 (18)	0.0231 (18)	
C64	0.3994 (5)	0.5087 (9)	0.28335 (19)	0.0185 (19)	
H64	0.409954	0.442951	0.268873	0.022*	
C65	0.3943 (6)	0.6452 (10)	0.2696 (2)	0.026 (2)	
H65	0.427121	0.705318	0.281393	0.031*	
C66	0.3203 (5)	0.7025 (9)	0.2680 (2)	0.021 (2)	
H66	0.289034	0.649147	0.254084	0.026*	
C67	0.2888 (5)	0.6934 (9)	0.2956 (2)	0.019 (2)	
H67	0.239413	0.730959	0.292973	0.023*	
C68	0.1614 (5)	0.3245 (10)	0.3390 (2)	0.024 (2)	
H68	0.130731	0.384341	0.347026	0.029*	
C69	0.1506 (6)	0.1928 (11)	0.3415 (2)	0.028 (2)	
H69	0.112257	0.161306	0.350958	0.034*	
C70	0.1964 (5)	0.1035 (10)	0.3299 (2)	0.026 (2)	
H70	0.188911	0.011623	0.331723	0.032*	
C71	0.2507 (5)	0.1463 (10)	0.3163 (2)	0.024 (2)	

H71	0.280678	0.083715	0.308675	0.029*	
C72	0.3228 (5)	0.3286 (8)	0.29934 (19)	0.0164 (19)	
C73	0.2298 (5)	0.5108 (9)	0.3192 (2)	0.021 (2)	
C74	0.2841 (5)	0.5537 (9)	0.30493 (19)	0.0173 (19)	
C75	0.3329 (5)	0.4628 (9)	0.29616 (19)	0.019 (2)	
C76	0.2644 (5)	0.2823 (10)	0.31306 (19)	0.020 (2)	
C77	0.2181 (5)	0.3747 (10)	0.3245 (2)	0.022 (2)	
C78	0.3721 (5)	0.2307 (9)	0.2890 (2)	0.020 (2)	
C79	0.4232 (5)	0.1441 (9)	0.3038 (2)	0.021 (2)	
C80	0.4535 (6)	0.0785 (10)	0.2836 (2)	0.026 (2)	
C81	0.5091 (5)	-0.0236 (10)	0.2842 (3)	0.031 (2)	
H81A	0.494258	-0.091314	0.270209	0.046*	
H81B	0.516076	-0.063636	0.302811	0.046*	
H81C	0.554103	0.016234	0.279882	0.046*	
C82	0.4398 (5)	0.1308 (10)	0.3338 (2)	0.026 (2)	
C83	0.4220 (10)	0.2139 (19)	0.3779 (2)	0.025 (4)	0.68 (2)
H83A	0.405413	0.127368	0.384019	0.030*	0.68 (2)
H83B	0.473257	0.224666	0.384789	0.030*	0.68 (2)
C84	0.3802 (12)	0.318 (2)	0.3876 (4)	0.044 (4)	0.68 (2)
H84A	0.396106	0.402703	0.380536	0.067*	0.68 (2)
H84B	0.386291	0.319731	0.408145	0.067*	0.68 (2)
H84C	0.329668	0.304597	0.380919	0.067*	0.68 (2)
C83A	0.434 (2)	0.253 (4)	0.3768 (3)	0.025 (4)	0.32 (2)
H83C	0.409830	0.187483	0.387910	0.030*	0.32 (2)
H83D	0.485532	0.233588	0.379857	0.030*	0.32 (2)
C84A	0.424 (3)	0.379 (4)	0.3893 (8)	0.044 (4)	0.32 (2)
H84D	0.382309	0.422664	0.379177	0.067*	0.32 (2)
H84E	0.466603	0.432684	0.388244	0.067*	0.32 (2)
H84F	0.415772	0.366776	0.408905	0.067*	0.32 (2)

Table S5. Atomic displacement parameters ($Å^2$) for the Penta bromo AIM ester **2** (cl_mc79c9_15_0m).

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0223 (5)	0.0309 (5)	0.0260 (6)	0.0032 (4)	0.0003 (4)	-0.0013 (5)
Br2	0.0394 (6)	0.0415 (6)	0.0253 (6)	0.0004 (5)	0.0097 (5)	-0.0133 (5)
Br3	0.0399 (6)	0.0192 (5)	0.0336 (6)	0.0063 (4)	-0.0101 (5)	-0.0093 (5)

Br4	0.0408 (6)	0.0208 (5)	0.0300 (6)	0.0037 (4)	-0.0054 (5)	0.0067 (4)
Br5	0.0286 (5)	0.0274 (5)	0.0322 (6)	-0.0027 (4)	0.0078 (5)	0.0057 (5)
O1	0.028 (4)	0.015 (3)	0.027 (4)	0.000 (3)	0.001 (3)	0.006 (3)
O2	0.034 (5)	0.089 (7)	0.035 (5)	-0.028 (5)	0.007 (4)	-0.010 (5)
O3	0.021 (3)	0.030 (4)	0.022 (4)	-0.001 (3)	-0.003 (3)	0.003 (3)
N1	0.028 (5)	0.014 (4)	0.030 (5)	-0.001 (3)	0.001 (4)	0.001 (4)
C1	0.026 (5)	0.018 (5)	0.019 (5)	-0.005 (4)	0.000 (4)	0.005 (4)
C2	0.035 (6)	0.021 (5)	0.011 (5)	0.009 (4)	0.003 (4)	-0.004 (4)
C3	0.034 (6)	0.013 (4)	0.024 (6)	0.004 (4)	-0.005 (4)	-0.010 (4)
C4	0.022 (5)	0.015 (4)	0.022 (5)	0.003 (4)	-0.002 (4)	0.000 (4)
C5	0.037 (6)	0.036 (6)	0.015 (5)	0.006 (5)	0.009 (4)	0.004 (5)
C6	0.032 (6)	0.036 (6)	0.019 (5)	0.008 (5)	0.009 (4)	-0.005 (5)
C7	0.032 (6)	0.026 (5)	0.016 (5)	0.008 (4)	-0.006 (4)	-0.009 (4)
C8	0.031 (6)	0.021 (5)	0.022 (5)	0.005 (4)	-0.007 (4)	-0.006 (4)
C9	0.020 (5)	0.017 (4)	0.016 (5)	-0.002 (4)	-0.001 (4)	-0.003 (4)
C10	0.029 (5)	0.022 (5)	0.005 (4)	-0.002 (4)	0.000 (4)	0.005 (4)
C11	0.033 (5)	0.014 (4)	0.008 (4)	-0.003 (4)	-0.001 (4)	-0.004 (4)
C12	0.026 (5)	0.018 (4)	0.011 (5)	0.007 (4)	-0.001 (4)	0.000 (4)
C13	0.024 (5)	0.025 (5)	0.013 (5)	0.007 (4)	-0.001 (4)	-0.007 (4)
C14	0.023 (5)	0.027 (5)	0.014 (5)	0.001 (4)	0.000 (4)	-0.001 (4)
C15	0.024 (5)	0.015 (4)	0.016 (5)	0.005 (4)	0.005 (4)	-0.002 (4)
C16	0.018 (5)	0.019 (5)	0.026 (6)	0.005 (4)	0.001 (4)	-0.006 (4)
C17	0.023 (5)	0.019 (5)	0.030 (6)	0.009 (4)	0.005 (4)	-0.012 (4)
C18	0.031 (6)	0.031 (6)	0.043 (7)	-0.005 (5)	0.010 (5)	-0.005 (5)
C19	0.023 (5)	0.032 (6)	0.021 (5)	-0.005 (4)	0.006 (4)	-0.013 (5)
C20	0.022 (5)	0.044 (7)	0.020 (5)	0.005 (5)	-0.002 (4)	-0.003 (5)
C21	0.029 (6)	0.038 (6)	0.031 (6)	-0.008 (5)	0.003 (5)	0.007 (5)
Br11	0.0454 (6)	0.0289 (5)	0.0231 (6)	0.0141 (5)	0.0179 (5)	0.0076 (5)
Br12	0.0118 (4)	0.0113 (4)	0.0306 (5)	0.0022 (3)	-0.0003 (4)	-0.0003 (4)
Br13	0.0214 (5)	0.0072 (4)	0.0271 (5)	-0.0002 (3)	-0.0004 (4)	0.0015 (4)
Br14	0.0268 (5)	0.0200 (5)	0.0274 (6)	-0.0022 (4)	-0.0053 (4)	-0.0097 (4)
Br15	0.0116 (4)	0.0173 (4)	0.0271 (5)	-0.0054 (3)	-0.0003 (4)	0.0032 (4)
O7	0.010 (3)	0.015 (3)	0.029 (4)	-0.002 (2)	0.000 (3)	0.008 (3)
O8	0.025 (4)	0.044 (5)	0.031 (4)	-0.005 (3)	0.000 (3)	0.022 (4)
O9	0.017 (3)	0.021 (3)	0.019 (4)	-0.005 (3)	-0.008 (3)	0.008 (3)
N3	0.014 (4)	0.011 (3)	0.017 (4)	-0.006 (3)	0.003 (3)	0.001 (3)
C43	0.017 (4)	0.011 (4)	0.012 (4)	0.004 (3)	-0.002 (3)	0.002 (4)

C44	0.015 (4)	0.007 (4)	0.022 (5)	0.001 (3)	0.000 (4)	-0.003 (4)
C45	0.019 (4)	0.006 (4)	0.018 (5)	0.000 (3)	0.000 (4)	0.000 (4)
C46	0.014 (4)	0.009 (4)	0.022 (5)	-0.001 (3)	-0.001 (4)	-0.003 (4)
C47	0.016 (4)	0.022 (5)	0.019 (5)	-0.001 (4)	0.003 (4)	0.004 (4)
C48	0.009 (4)	0.029 (5)	0.027 (6)	0.007 (4)	0.003 (4)	0.003 (4)
C49	0.019 (5)	0.014 (4)	0.021 (5)	0.008 (4)	0.007 (4)	-0.005 (4)
C50	0.011 (4)	0.010 (4)	0.020 (5)	-0.001 (3)	-0.002 (4)	-0.001 (4)
C51	0.009 (4)	0.015 (4)	0.007 (4)	-0.002 (3)	0.001 (3)	0.000 (3)
C52	0.009 (4)	0.015 (4)	0.012 (4)	-0.004 (3)	0.000 (3)	0.005 (4)
C53	0.012 (4)	0.014 (4)	0.010 (4)	0.001 (3)	-0.006 (3)	0.005 (4)
C54	0.011 (4)	0.017 (4)	0.011 (4)	0.000 (3)	0.002 (3)	0.003 (4)
C55	0.011 (4)	0.013 (4)	0.008 (4)	0.003 (3)	-0.003 (3)	0.002 (3)
C56	0.011 (4)	0.013 (4)	0.016 (5)	-0.003 (3)	0.000 (3)	0.003 (4)
C57	0.008 (4)	0.008 (4)	0.019 (5)	0.001 (3)	-0.002 (3)	-0.001 (3)
C58	0.017 (4)	0.009 (4)	0.017 (5)	-0.001 (3)	0.003 (4)	0.006 (4)
C59	0.017 (4)	0.011 (4)	0.018 (5)	-0.001 (3)	0.002 (4)	0.005 (4)
C60	0.020 (5)	0.032 (6)	0.036 (6)	-0.002 (4)	0.010 (5)	0.021 (5)
C61	0.018 (4)	0.017 (4)	0.019 (5)	0.004 (4)	0.004 (4)	0.002 (4)
C62	0.021 (5)	0.042 (6)	0.016 (5)	-0.006 (5)	-0.005 (4)	0.003 (5)
C63	0.062 (9)	0.071 (10)	0.046 (8)	-0.047 (8)	-0.038 (7)	0.024 (8)
Br6	0.0421 (6)	0.0316 (6)	0.0208 (5)	-0.0148 (5)	0.0160 (5)	-0.0077 (5)
Br7	0.0120 (4)	0.0112 (4)	0.0449 (6)	-0.0023 (3)	0.0000 (4)	-0.0024 (4)
Br8	0.0207 (4)	0.0076 (4)	0.0226 (5)	-0.0008 (3)	-0.0003 (4)	-0.0016 (4)
Br9	0.0267 (5)	0.0179 (4)	0.0258 (6)	0.0001 (4)	-0.0077 (4)	0.0068 (4)
Br10	0.0113 (4)	0.0157 (4)	0.0290 (5)	0.0038 (3)	0.0015 (4)	-0.0062 (4)
O4	0.016 (3)	0.009 (3)	0.023 (4)	0.003 (2)	0.004 (3)	-0.006 (3)
O5	0.021 (4)	0.033 (4)	0.021 (4)	0.003 (3)	-0.005 (3)	-0.012 (3)
O6	0.015 (3)	0.030 (4)	0.021 (4)	0.008 (3)	-0.007 (3)	-0.006 (3)
N2	0.015 (4)	0.007 (3)	0.028 (5)	-0.002 (3)	0.002 (3)	0.001 (3)
C22	0.013 (4)	0.005 (4)	0.017 (5)	0.002 (3)	0.007 (3)	-0.004 (3)
C23	0.010 (4)	0.013 (4)	0.015 (5)	0.000 (3)	0.000 (3)	0.002 (4)
C24	0.019 (4)	0.003 (3)	0.014 (5)	-0.001 (3)	-0.001 (4)	-0.003 (3)
C25	0.016 (4)	0.013 (4)	0.015 (5)	0.000 (3)	0.004 (4)	0.001 (4)
C26	0.010 (4)	0.017 (4)	0.019 (5)	0.001 (3)	0.001 (4)	-0.005 (4)
C27	0.012 (4)	0.033 (6)	0.017 (5)	-0.004 (4)	0.003 (4)	0.001 (4)
C28	0.017 (5)	0.015 (4)	0.023 (5)	-0.007 (4)	-0.003 (4)	-0.001 (4)
C29	0.016 (4)	0.011 (4)	0.018 (5)	-0.003 (3)	0.003 (4)	-0.003 (4)

C30	0.010 (4)	0.009 (4)	0.015 (5)	-0.001 (3)	-0.001 (3)	-0.001 (3)
C31	0.016 (4)	0.010 (4)	0.015 (5)	0.006 (3)	-0.003 (4)	-0.004 (4)
C32	0.017 (4)	0.015 (4)	0.007 (4)	0.002 (3)	0.002 (3)	-0.006 (3)
C33	0.009 (4)	0.007 (4)	0.014 (4)	-0.004 (3)	0.000 (3)	0.001 (3)
C34	0.016 (4)	0.013 (4)	0.011 (4)	-0.004 (3)	0.000 (3)	-0.002 (3)
C35	0.010 (4)	0.013 (4)	0.016 (5)	0.002 (3)	0.004 (3)	-0.003 (4)
C36	0.008 (4)	0.013 (4)	0.014 (5)	0.000 (3)	0.003 (3)	0.007 (3)
C37	0.015 (4)	0.012 (4)	0.014 (5)	-0.002 (3)	0.003 (3)	0.001 (4)
C38	0.019 (4)	0.005 (4)	0.014 (5)	-0.002 (3)	0.004 (4)	0.002 (3)
C39	0.030 (6)	0.019 (5)	0.032 (6)	0.002 (4)	0.007 (5)	-0.011 (5)
C40	0.028 (5)	0.015 (4)	0.009 (4)	-0.007 (4)	0.008 (4)	0.000 (4)
C41	0.025 (5)	0.048 (7)	0.024 (6)	0.005 (5)	-0.009 (5)	-0.003 (5)
C42	0.049 (9)	0.149 (18)	0.033 (8)	0.025 (10)	-0.009 (7)	0.000 (10)
Br16	0.0222 (5)	0.0333 (6)	0.0279 (6)	-0.0015 (4)	-0.0009 (4)	0.0026 (5)
Br17	0.0367 (6)	0.0425 (6)	0.0242 (6)	-0.0006 (5)	0.0091 (5)	0.0125 (5)
Br18	0.0372 (6)	0.0190 (5)	0.0255 (6)	-0.0056 (4)	-0.0085 (4)	0.0079 (4)
Br19	0.0388 (6)	0.0195 (5)	0.0229 (5)	-0.0013 (4)	-0.0081 (4)	-0.0030 (4)
Br20	0.0326 (6)	0.0277 (5)	0.0297 (6)	0.0021 (4)	0.0106 (5)	-0.0021 (5)
O10	0.031 (4)	0.017 (3)	0.031 (4)	0.001 (3)	0.002 (3)	0.000 (3)
O11	0.031 (4)	0.053 (5)	0.033 (5)	0.009 (4)	-0.001 (4)	0.012 (4)
O12	0.034 (4)	0.036 (4)	0.015 (4)	-0.004 (3)	-0.004 (3)	0.004 (3)
N4	0.026 (4)	0.015 (4)	0.030 (5)	0.007 (3)	0.004 (4)	0.001 (4)
C64	0.026 (5)	0.019 (5)	0.011 (5)	-0.005 (4)	0.002 (4)	-0.002 (4)
C65	0.032 (6)	0.029 (5)	0.016 (5)	0.002 (4)	0.002 (4)	0.001 (4)
C66	0.028 (5)	0.014 (4)	0.022 (5)	-0.005 (4)	0.002 (4)	0.003 (4)
C67	0.024 (5)	0.014 (4)	0.021 (5)	-0.006 (4)	0.000 (4)	0.002 (4)
C68	0.023 (5)	0.034 (6)	0.019 (5)	-0.004 (4)	0.012 (4)	0.004 (4)
C69	0.026 (5)	0.033 (6)	0.026 (6)	-0.008 (5)	0.007 (4)	0.006 (5)
C70	0.024 (5)	0.023 (5)	0.031 (6)	-0.002 (4)	-0.001 (4)	0.008 (5)
C71	0.027 (5)	0.021 (5)	0.024 (6)	-0.003 (4)	0.000 (4)	0.008 (4)
C72	0.023 (5)	0.012 (4)	0.013 (5)	-0.005 (4)	-0.006 (4)	0.003 (4)
C73	0.022 (5)	0.022 (5)	0.019 (5)	0.002 (4)	0.005 (4)	-0.001 (4)
C74	0.021 (5)	0.016 (4)	0.014 (5)	-0.010 (4)	-0.001 (4)	-0.001 (4)
C75	0.033 (5)	0.015 (4)	0.008 (4)	-0.009 (4)	0.000 (4)	0.003 (4)
C76	0.025 (5)	0.023 (5)	0.011 (5)	-0.003 (4)	-0.005 (4)	0.005 (4)
C77	0.019 (5)	0.027 (5)	0.020 (5)	-0.007 (4)	0.000 (4)	0.002 (4)
C78	0.026 (5)	0.018 (5)	0.016 (5)	-0.005 (4)	0.005 (4)	0.003 (4)

C79	0.016 (4)	0.020 (5)	0.028 (6)	-0.011 (4)	0.001 (4)	0.008 (4)
C80	0.030 (5)	0.018 (5)	0.028 (6)	-0.011 (4)	0.001 (5)	0.007 (4)
C81	0.023 (5)	0.024 (5)	0.046 (7)	0.006 (4)	0.005 (5)	0.003 (5)
C82	0.014 (4)	0.024 (5)	0.038 (6)	-0.002 (4)	-0.001 (4)	0.006 (5)
C83	0.019 (8)	0.044 (10)	0.011 (5)	-0.023 (7)	-0.004 (4)	0.002 (6)
C84	0.060 (12)	0.055 (10)	0.015 (7)	0.004 (8)	-0.008 (8)	0.002 (7)
C83A	0.019 (8)	0.044 (10)	0.011 (5)	-0.023 (7)	-0.004 (4)	0.002 (6)
C84A	0.060 (12)	0.055 (10)	0.015 (7)	0.004 (8)	-0.008 (8)	0.002 (7)

Table S6. Geometric parameters (Å, º) for the Penta bromo AIM ester **2** (cl_mc79c9_15_0m).

Br1—C1	2.003 (10)	Br10—C31	1.906 (8)
Br2—C2	1.952 (9)	O4—N2	1.420 (9)
Br3—C3	1.940 (9)	O4—C38	1.339 (11)
Br4—C4	1.980 (9)	O5—C40	1.210 (11)
Br5—C10	1.899 (9)	O6—C40	1.337 (11)
O1—N1	1.413 (10)	O6—C41	1.455 (11)
O1—C17	1.367 (12)	N2—C36	1.323 (11)
O2—C19	1.207 (12)	C22—H22	1.0000
O3—C19	1.313 (12)	C22—C23	1.539 (11)
O3—C20	1.459 (12)	C22—C33	1.520 (11)
N1—C15	1.312 (12)	C23—H23	1.0000
C1—H1	1.0000	C23—C24	1.490 (12)
C1—C2	1.526 (13)	C24—H24	1.0000
C1—C12	1.504 (13)	C24—C25	1.535 (12)
C2—H2	1.0000	C25—H25	1.0000
C2—C3	1.497 (14)	C25—C32	1.485 (12)
C3—H3	1.0000	C26—H26	0.9500
C3—C4	1.509 (14)	C26—C27	1.361 (13)
C4—H4	1.0000	C26—C35	1.420 (12)
C4—C11	1.497 (13)	C27—H27	0.9500
C5—H5	0.9500	C27—C28	1.401 (13)
C5—C6	1.366 (15)	C28—H28	0.9500
C5—C14	1.415 (14)	C28—C29	1.361 (12)
C6—H6	0.9500	C29—H29	0.9500
C6—C7	1.398 (15)	C29—C34	1.415 (12)
C7—H7	0.9500	C30—C33	1.379 (11)
C7—C8	1.371 (14)	C30—C34	1.416 (12)

C8—H8	0.9500	C30—C36	1.486 (11)
C8—C13	1.400 (13)	C31—C32	1.375 (12)
C9—C12	1.386 (13)	C31—C35	1.398 (12)
C9—C13	1.430 (13)	C32—C33	1.428 (11)
C9—C15	1.469 (13)	C34—C35	1.419 (12)
C10—C11	1.387 (13)	C36—C37	1.423 (12)
C10—C14	1.421 (14)	C37—C38	1.365 (12)
C11—C12	1.416 (13)	C37—C40	1.469 (13)
C13—C14	1.432 (14)	C38—C39	1.484 (12)
C15—C16	1.428 (13)	C39—H39A	0.9800
C16—C17	1.341 (14)	C39—H39B	0.9800
C16—C19	1.465 (14)	C39—H39C	0.9800
C17—C18	1.496 (14)	C41—H41A	0.9900
C18—H18A	0.9800	C41—H41B	0.9900
C18—H18B	0.9800	C41—C42	1.499 (18)
C18—H18C	0.9800	C42—H42A	0.9800
C20—H20A	0.9900	C42—H42B	0.9800
C20—H20B	0.9900	C42—H42C	0.9800
C20—C21	1.487 (15)	Br16—C64	1.998 (9)
C21—H21A	0.9800	Br17—C65	1.927 (10)
C21—H21B	0.9800	Br18—C66	1.933 (9)
C21—H21C	0.9800	Br19—C67	1.986 (9)
Br11—C43	1.982 (9)	Br20—C73	1.895 (9)
Br12—C44	1.949 (9)	O10—N4	1.415 (10)
Br13—C45	1.941 (8)	O10—C80	1.346 (12)
Br14—C46	1.967 (9)	O11—C82	1.229 (12)
Br15—C52	1.903 (8)	O12—C82	1.328 (12)
O7—N3	1.412 (9)	O12—C83	1.442 (12)
O7—C59	1.340 (11)	O12—C83A	1.441 (14)
O8—C61	1.206 (11)	N4—C78	1.299 (12)
O9—C61	1.331 (11)	C64—H64	1.0000
O9—C62	1.456 (11)	C64—C65	1.535 (13)
N3—C57	1.306 (11)	C64—C75	1.529 (13)
C43—H43	1.0000	C65—H65	1.0000
C43—C44	1.540 (11)	C65—C66	1.503 (14)
C43—C55	1.499 (11)	C66—H66	1.0000
C44—H44	1.0000	C66—C67	1.514 (13)

C44—C45	1.537 (12)	C67—H67	1.0000
C45—H45	1.0000	C67—C74	1.494 (12)
C45—C46	1.506 (12)	C68—H68	0.9500
C46—H46	1.0000	C68—C69	1.361 (14)
C46—C56	1.501 (12)	C68—C77	1.429 (13)
C47—H47	0.9500	C69—H69	0.9500
C47—C48	1.367 (13)	C69—C70	1.409 (15)
C47—C53	1.403 (12)	C70—H70	0.9500
C48—H48	0.9500	C70—C71	1.344 (14)
C48—C49	1.407 (13)	C71—H71	0.9500
C49—H49	0.9500	C71—C76	1.417 (13)
C49—C50	1.362 (12)	C72—C75	1.387 (12)
C50—H50	0.9500	C72—C76	1.423 (13)
C50—C54	1.420 (12)	C72—C78	1.483 (13)
C51—C54	1.428 (11)	C73—C74	1.364 (13)
C51—C55	1.368 (11)	C73—C77	1.428 (14)
C51—C57	1.483 (11)	C74—C75	1.400 (13)
C52—C53	1.413 (12)	C76—C77	1.433 (14)
C52—C56	1.363 (12)	C78—C79	1.434 (13)
C53—C54	1.423 (12)	C79—C80	1.356 (15)
C55—C56	1.436 (12)	C79—C82	1.446 (14)
C57—C58	1.427 (12)	C80—C81	1.471 (14)
C58—C59	1.378 (12)	C81—H81A	0.9800
C58—C61	1.458 (13)	C81—H81B	0.9800
C59—C60	1.477 (12)	C81—H81C	0.9800
C60—H60A	0.9800	C83—H83A	0.9900
C60—H60B	0.9800	C83—H83B	0.9900
C60—H60C	0.9800	C83—C84	1.43 (2)
C62—H62A	0.9900	C84—H84A	0.9800
C62—H62B	0.9900	C84—H84B	0.9800
C62—C63	1.494 (16)	C84—H84C	0.9800
C63—H63A	0.9800	C83A—H83C	0.9900
C63—H63B	0.9800	C83A—H83D	0.9900
C63—H63C	0.9800	C83A—C84A	1.43 (2)
Br6—C22	1.967 (9)	C84A—H84D	0.9800
Br7—C23	1.953 (8)	C84A—H84E	0.9800
Br8—C24	1.948 (8)	C84A—H84F	0.9800

Br9—C25	1.977 (9)		
C17—O1—N1	108.6 (7)	C33—C22—H22	107.3
C19—O3—C20	118.7 (8)	C33—C22—C23	116.0 (7)
C15—N1—O1	105.2 (8)	Br7—C23—H23	108.1
Br1—C1—H1	107.9	C22—C23—Br7	108.9 (6)
C2—C1—Br1	107.8 (7)	C22—C23—H23	108.1
C2—C1—H1	107.9	C24—C23—Br7	110.1 (6)
C12—C1—Br1	108.0 (6)	C24—C23—C22	113.4 (7)
C12—C1—H1	107.9	C24—C23—H23	108.1
C12—C1—C2	116.9 (8)	Br8—C24—H24	108.2
Br2—C2—H2	107.8	C23—C24—Br8	111.3 (6)
C1—C2—Br2	108.6 (7)	C23—C24—H24	108.2
C1—C2—H2	107.8	C23—C24—C25	110.7 (7)
C3—C2—Br2	111.9 (7)	C25—C24—Br8	110.2 (6)
C3—C2—C1	112.8 (8)	C25—C24—H24	108.2
C3—C2—H2	107.8	Br9—C25—H25	108.4
Br3—C3—H3	107.7	C24—C25—Br9	110.4 (6)
C2—C3—Br3	110.8 (7)	C24—C25—H25	108.4
C2—C3—H3	107.7	C32—C25—Br9	111.5 (6)
C2—C3—C4	112.6 (8)	C32—C25—C24	109.6 (7)
C4—C3—Br3	110.1 (7)	C32—C25—H25	108.4
C4—C3—H3	107.7	C27—C26—H26	119.3
Br4—C4—H4	108.7	C27—C26—C35	121.3 (8)
C3—C4—Br4	111.4 (6)	C35—C26—H26	119.3
C3—C4—H4	108.7	C26—C27—H27	119.9
C11—C4—Br4	110.2 (7)	C26—C27—C28	120.1 (8)
C11—C4—C3	109.1 (8)	C28—C27—H27	119.9
C11—C4—H4	108.7	C27—C28—H28	119.6
C6—C5—H5	119.6	C29—C28—C27	120.8 (9)
C6—C5—C14	120.9 (10)	C29—C28—H28	119.6
C14—C5—H5	119.6	C28—C29—H29	119.8
C5—C6—H6	119.9	C28—C29—C34	120.3 (8)
C5—C6—C7	120.2 (10)	C34—C29—H29	119.8
C7—C6—H6	119.9	C33—C30—C34	121.2 (8)
C6—C7—H7	119.7	C33—C30—C36	120.5 (7)
C8—C7—C6	120.6 (10)	C34—C30—C36	118.2 (7)

C8—C7—H7	119.7	C32—C31—Br10	118.3 (6)
C7—C8—H8	119.5	C32—C31—C35	123.4 (8)
C7—C8—C13	121.0 (10)	C35—C31—Br10	118.3 (6)
C13—C8—H8	119.5	C31—C32—C25	122.4 (8)
C12—C9—C13	121.3 (9)	C31—C32—C33	117.9 (8)
C12—C9—C15	120.1 (8)	C33—C32—C25	119.6 (8)
C13—C9—C15	118.5 (8)	C30—C33—C22	120.4 (7)
C11—C10—Br5	118.1 (7)	C30—C33—C32	119.9 (8)
C11—C10—C14	122.5 (9)	C32—C33—C22	119.6 (7)
C14—C10—Br5	119.4 (7)	C29—C34—C30	121.7 (8)
C10—C11—C4	121.7 (9)	C29—C34—C35	119.5 (8)
C10—C11—C12	119.0 (8)	C30—C34—C35	118.7 (8)
C12—C11—C4	119.3 (8)	C31—C35—C26	123.9 (8)
C9—C12—C1	119.5 (9)	C31—C35—C34	118.2 (8)
C9—C12—C11	120.0 (9)	C34—C35—C26	117.9 (8)
C11—C12—C1	120.4 (8)	N2—C36—C30	121.3 (8)
C8—C13—C9	122.4 (9)	N2—C36—C37	111.3 (7)
C8—C13—C14	118.8 (9)	C37—C36—C30	127.3 (8)
C9—C13—C14	118.8 (9)	C36—C37—C40	129.8 (8)
C5—C14—C10	123.6 (9)	C38—C37—C36	104.9 (8)
C5—C14—C13	118.5 (9)	C38—C37—C40	125.3 (8)
C10—C14—C13	117.9 (9)	O4—C38—C37	109.2 (7)
N1—C15—C9	118.1 (9)	O4—C38—C39	115.6 (8)
N1—C15—C16	111.7 (9)	C37—C38—C39	135.1 (9)
C16—C15—C9	130.1 (9)	C38—C39—H39A	109.5
C15—C16—C19	128.6 (9)	C38—C39—H39B	109.5
C17—C16—C15	104.8 (9)	C38—C39—H39C	109.5
C17—C16—C19	126.5 (9)	H39A—C39—H39B	109.5
O1—C17—C18	114.6 (9)	H39A—C39—H39C	109.5
C16—C17—O1	109.6 (9)	H39B—C39—H39C	109.5
C16—C17—C18	135.7 (10)	O5—C40—O6	125.0 (9)
C17—C18—H18A	109.5	O5—C40—C37	124.2 (9)
C17—C18—H18B	109.5	O6—C40—C37	110.8 (7)
C17—C18—H18C	109.5	O6—C41—H41A	110.3
H18A—C18—H18B	109.5	O6—C41—H41B	110.3
H18A—C18—H18C	109.5	O6—C41—C42	107.2 (9)
H18B—C18—H18C	109.5	H41A—C41—H41B	108.5

O2—C19—O3	123.2 (10)	C42—C41—H41A	110.3
O2—C19—C16	124.3 (10)	C42—C41—H41B	110.3
O3—C19—C16	112.4 (8)	C41—C42—H42A	109.5
O3—C20—H20A	109.9	C41—C42—H42B	109.5
O3—C20—H20B	109.9	C41—C42—H42C	109.5
O3—C20—C21	108.8 (9)	H42A—C42—H42B	109.5
H20A—C20—H20B	108.3	H42A—C42—H42C	109.5
C21—C20—H20A	109.9	H42B—C42—H42C	109.5
C21—C20—H20B	109.9	C80—O10—N4	108.7 (8)
C20—C21—H21A	109.5	C82—O12—C83	115.3 (11)
C20—C21—H21B	109.5	C82—O12—C83A	122.5 (18)
C20—C21—H21C	109.5	C78—N4—O10	106.4 (8)
H21A—C21—H21B	109.5	Br16—C64—H64	108.1
H21A—C21—H21C	109.5	C65—C64—Br16	108.8 (6)
H21B—C21—H21C	109.5	C65—C64—H64	108.1
C59—O7—N3	109.1 (6)	C75—C64—Br16	107.7 (6)
C61—O9—C62	118.4 (7)	C75—C64—H64	108.1
C57—N3—O7	105.2 (7)	C75—C64—C65	115.7 (8)
Br11—C43—H43	107.6	Br17—C65—H65	107.5
C44—C43—Br11	106.9 (6)	C64—C65—Br17	108.6 (7)
C44—C43—H43	107.6	C64—C65—H65	107.5
C55—C43—Br11	108.9 (6)	C66—C65—Br17	112.7 (7)
C55—C43—H43	107.6	C66—C65—C64	112.7 (8)
C55—C43—C44	117.9 (7)	C66—C65—H65	107.5
Br12—C44—H44	108.8	Br18—C66—H66	107.2
C43—C44—Br12	109.5 (6)	C65—C66—Br18	111.3 (7)
C43—C44—H44	108.8	C65—C66—H66	107.2
C45—C44—Br12	109.5 (6)	C65—C66—C67	112.5 (8)
C45—C44—C43	111.4 (7)	C67—C66—Br18	111.2 (6)
C45—C44—H44	108.8	C67—C66—H66	107.2
Br13—C45—H45	108.5	Br19—C67—H67	108.4
C44—C45—Br13	110.0 (6)	C66—C67—Br19	110.0 (6)
C44—C45—H45	108.5	C66—C67—H67	108.4
C46—C45—Br13	111.2 (6)	C74—C67—Br19	110.4 (6)
C46—C45—C44	110.2 (7)	C74—C67—C66	111.3 (8)
C46—C45—H45	108.5	C74—C67—H67	108.4
Br14—C46—H46	107.7	C69—C68—H68	119.3

C45—C46—Br14	112.9 (6)	C69—C68—C77	121.4 (10)
C45—C46—H46	107.7	C77—C68—H68	119.3
C56—C46—Br14	110.7 (6)	C68—C69—H69	120.2
C56—C46—C45	109.8 (7)	C68—C69—C70	119.6 (9)
C56—C46—H46	107.7	C70—C69—H69	120.2
C48—C47—H47	119.5	C69—C70—H70	119.5
C48—C47—C53	121.0 (9)	C71—C70—C69	121.1 (10)
C53—C47—H47	119.5	C71—C70—H70	119.5
C47—C48—H48	119.7	C70—C71—H71	119.1
C47—C48—C49	120.6 (8)	C70—C71—C76	121.7 (10)
C49—C48—H48	119.7	C76—C71—H71	119.1
C48—C49—H49	120.2	C75—C72—C76	119.9 (9)
C50—C49—C48	119.6 (8)	C75—C72—C78	121.6 (9)
C50—C49—H49	120.2	C76—C72—C78	118.5 (8)
C49—C50—H50	119.2	C74—C73—Br20	118.7 (7)
C49—C50—C54	121.6 (8)	C74—C73—C77	122.6 (9)
C54—C50—H50	119.2	C77—C73—Br20	118.7 (7)
C54—C51—C57	118.4 (7)	C73—C74—C67	121.8 (9)
C55—C51—C54	120.0 (8)	C73—C74—C75	119.6 (8)
C55—C51—C57	120.8 (7)	C75—C74—C67	118.3 (8)
C53—C52—Br15	117.6 (6)	C72—C75—C64	118.2 (9)
C56—C52—Br15	118.8 (6)	C72—C75—C74	120.9 (9)
C56—C52—C53	123.5 (8)	C74—C75—C64	120.9 (8)
C47—C53—C52	124.3 (8)	C71—C76—C72	122.2 (9)
C47—C53—C54	119.2 (8)	C71—C76—C77	118.1 (9)
C52—C53—C54	116.5 (8)	C72—C76—C77	119.7 (9)
C50—C54—C51	121.4 (8)	C68—C77—C76	118.1 (9)
C50—C54—C53	118.0 (8)	C73—C77—C68	124.9 (9)
C53—C54—C51	120.6 (8)	C73—C77—C76	116.9 (8)
C51—C55—C43	119.9 (8)	N4—C78—C72	118.5 (9)
C51—C55—C56	120.2 (8)	N4—C78—C79	110.6 (9)
C56—C55—C43	119.9 (7)	C79—C78—C72	131.0 (9)
C52—C56—C46	122.9 (8)	C78—C79—C82	127.6 (9)
C52—C56—C55	118.8 (8)	C80—C79—C78	105.0 (9)
C55—C56—C46	118.3 (7)	C80—C79—C82	127.5 (9)
N3—C57—C51	121.0 (8)	O10—C80—C79	109.3 (9)
N3—C57—C58	112.6 (8)	O10—C80—C81	117.3 (10)

C58—C57—C51	126.4 (8)	C79—C80—C81	133.4 (10)
C57—C58—C61	130.0 (8)	C80—C81—H81A	109.5
C59—C58—C57	102.9 (8)	C80—C81—H81B	109.5
C59—C58—C61	127.0 (8)	C80—C81—H81C	109.5
O7—C59—C58	110.0 (7)	H81A—C81—H81B	109.5
O7—C59—C60	117.5 (8)	H81A—C81—H81C	109.5
C58—C59—C60	132.5 (9)	H81B—C81—H81C	109.5
C59—C60—H60A	109.5	O11—C82—O12	123.2 (10)
C59—C60—H60B	109.5	O11—C82—C79	124.2 (10)
C59—C60—H60C	109.5	O12—C82—C79	112.6 (9)
H60A—C60—H60B	109.5	O12—C83—H83A	110.9
H60A—C60—H60C	109.5	O12—C83—H83B	110.9
H60B—C60—H60C	109.5	H83A—C83—H83B	109.0
O8—C61—O9	124.6 (9)	C84—C83—O12	104.1 (13)
O8—C61—C58	124.5 (9)	C84—C83—H83A	110.9
O9—C61—C58	110.8 (8)	C84—C83—H83B	110.9
O9—C62—H62A	110.5	C83—C84—H84A	109.5
O9—C62—H62B	110.5	C83—C84—H84B	109.5
O9—C62—C63	106.3 (8)	C83—C84—H84C	109.5
H62A—C62—H62B	108.7	H84A—C84—H84B	109.5
C63—C62—H62A	110.5	H84A—C84—H84C	109.5
C63—C62—H62B	110.5	H84B—C84—H84C	109.5
C62—C63—H63A	109.5	O12—C83A—H83C	106.7
C62—C63—H63B	109.5	O12—C83A—H83D	106.7
C62—C63—H63C	109.5	H83C—C83A—H83D	106.6
H63A—C63—H63B	109.5	C84A—C83A—O12	123 (3)
H63A—C63—H63C	109.5	C84A—C83A—H83C	106.7
H63B—C63—H63C	109.5	C84A—C83A—H83D	106.7
C38—O4—N2	109.7 (6)	C83A—C84A—H84D	109.5
C40—O6—C41	117.9 (8)	C83A—C84A—H84E	109.5
C36—N2—O4	104.8 (7)	C83A—C84A—H84F	109.5
Br6—C22—H22	107.3	H84D—C84A—H84E	109.5
C23—C22—Br6	108.2 (6)	H84D—C84A—H84F	109.5
C23—C22—H22	107.3	H84E—C84A—H84F	109.5
C33—C22—Br6	110.2 (6)		
Br1—C1—C2—Br2	104.3 (6)	Br6—C22—C33—C30	73.0 (9)

Br1—C1—C2—C3	-131.1 (7)	Br6—C22—C33—C32	-102.7 (8)
Br1—C1—C12—C9	-80.7 (9)	Br7—C23—C24—Br8	63.2 (7)
Br1—C1—C12—C11	103.4 (9)	Br7—C23—C24—C25	-173.9 (6)
Br2—C2—C3—Br3	-64.2 (8)	Br8—C24—C25—Br9	62.8 (7)
Br2—C2—C3—C4	172.0 (6)	Br8—C24—C25—C32	-173.9 (6)
Br3—C3—C4—Br4	-63.8 (8)	Br9—C25—C32—C31	-92.0 (9)
Br3—C3—C4—C11	174.4 (7)	Br9—C25—C32—C33	91.1 (9)
Br4—C4—C11—C10	92.4 (10)	Br10—C31—C32—C25	9.9 (12)
Br4—C4—C11—C12	-89.1 (9)	Br10—C31—C32—C33	-173.1 (6)
Br5—C10—C11—C4	-8.0 (12)	Br10—C31—C35—C26	-4.7 (13)
Br5—C10—C11—C12	173.5 (7)	Br10—C31—C35—C34	175.4 (7)
Br5—C10—C14—C5	1.6 (14)	O4—N2—C36—C30	-177.6 (7)
Br5—C10—C14—C13	-178.4 (7)	O4—N2—C36—C37	0.6 (9)
O1—N1—C15—C9	178.7 (7)	N2—O4—C38—C37	2.1 (9)
O1—N1—C15—C16	-1.0 (10)	N2—O4—C38—C39	-179.8 (7)
N1—O1—C17—C16	-0.1 (10)	N2—C36—C37—C38	0.6 (10)
N1—O1—C17—C18	176.9 (8)	N2—C36—C37—C40	-178.3 (8)
N1—C15—C16—C17	0.9 (11)	C22—C23—C24—Br8	-174.5 (6)
N1—C15—C16—C19	177.7 (9)	C22—C23—C24—C25	-51.6 (10)
C1—C2—C3—Br3	173.0 (7)	C23—C22—C33—C30	-163.6 (8)
C1—C2—C3—C4	49.2 (11)	C23—C22—C33—C32	20.7 (12)
C2—C1—C12—C9	157.6 (9)	C23—C24—C25—Br9	-60.7 (8)
C2—C1—C12—C11	-18.3 (13)	C23—C24—C25—C32	62.5 (9)
C2—C3—C4—Br4	60.4 (9)	C24—C25—C32—C31	145.4 (9)
C2—C3—C4—C11	-61.4 (11)	C24—C25—C32—C33	-31.5 (11)
C3—C4—C11—C10	-145.0 (9)	C25—C32—C33—C22	-9.3 (12)
C3—C4—C11—C12	33.5 (12)	C25—C32—C33—C30	175.0 (8)
C4—C11—C12—C1	5.3 (13)	C26—C27—C28—C29	-0.5 (15)
C4—C11—C12—C9	-170.6 (9)	C27—C26—C35—C31	-179.9 (9)
C5—C6—C7—C8	-0.2 (16)	C27—C26—C35—C34	-0.1 (14)
C6—C5—C14—C10	177.1 (10)	C27—C28—C29—C34	0.0 (15)
C6—C5—C14—C13	-3.0 (15)	C28—C29—C34—C30	-177.5 (9)
C6—C7—C8—C13	1.2 (15)	C28—C29—C34—C35	0.4 (14)
C7—C8—C13—C9	179.1 (9)	C29—C34—C35—C26	-0.4 (13)
C7—C8—C13—C14	-3.1 (15)	C29—C34—C35—C31	179.4 (8)
C8—C13—C14—C5	3.9 (14)	C30—C34—C35—C26	177.6 (8)
C8—C13—C14—C10	-176.1 (9)	C30—C34—C35—C31	-2.6 (13)

C9—C13—C14—C5	-178.1 (9)	C30—C36—C37—C38	178.6 (8)
C9—C13—C14—C10	1.8 (14)	C30—C36—C37—C40	-0.3 (15)
C9—C15—C16—C17	-178.7 (9)	C31—C32—C33—C22	173.7 (8)
C9—C15—C16—C19	-1.9 (16)	C31—C32—C33—C30	-2.0 (13)
C10—C11—C12—C1	-176.2 (8)	C32—C31—C35—C26	174.6 (9)
C10—C11—C12—C9	7.9 (14)	C32—C31—C35—C34	-5.2 (14)
C11—C10—C14—C5	-178.7 (9)	C33—C22—C23—Br7	133.7 (7)
C11—C10—C14—C13	1.4 (14)	C33—C22—C23—C24	10.7 (11)
C12—C1—C2—Br2	-133.9 (7)	C33—C30—C34—C29	-174.1 (9)
C12—C1—C2—C3	-9.3 (12)	C33—C30—C34—C35	7.9 (13)
C12—C9—C13—C8	177.8 (9)	C33—C30—C36—N2	66.9 (12)
C12—C9—C13—C14	-0.1 (14)	C33—C30—C36—C37	-110.9 (10)
C12—C9—C15—N1	-77.3 (12)	C34—C30—C33—C22	178.7 (8)
C12—C9—C15—C16	102.2 (12)	C34—C30—C33—C32	-5.6 (14)
C13—C9—C12—C1	179.2 (9)	C34—C30—C36—N2	-116.5 (9)
C13—C9—C12—C11	-4.8 (14)	C34—C30—C36—C37	65.7 (12)
C13—C9—C15—N1	105.2 (10)	C35—C26—C27—C28	0.6 (15)
C13—C9—C15—C16	-75.2 (13)	C35—C31—C32—C25	-169.4 (9)
C14—C5—C6—C7	1.1 (16)	C35—C31—C32—C33	7.5 (14)
C14—C10—C11—C4	172.3 (9)	C36—C30—C33—C22	-4.8 (13)
C14—C10—C11—C12	-6.2 (14)	C36—C30—C33—C32	170.9 (8)
C15—C9—C12—C1	1.8 (14)	C36—C30—C34—C29	9.3 (13)
C15—C9—C12—C11	177.7 (9)	C36—C30—C34—C35	-168.7 (8)
C15—C9—C13—C8	-4.8 (14)	C36—C37—C38—O4	-1.7 (9)
C15—C9—C13—C14	177.4 (9)	C36—C37—C38—C39	-179.3 (10)
C15—C16—C17—O1	-0.5 (10)	C36—C37—C40—O5	-169.3 (9)
C15—C16—C17—C18	-176.5 (11)	C36—C37—C40—O6	9.5 (13)
C15—C16—C19—O2	-163.9 (11)	C38—O4—N2—C36	-1.6 (8)
C15—C16—C19—O3	13.0 (14)	C38—C37—C40—O5	12.0 (14)
C17—O1—N1—C15	0.7 (9)	C38—C37—C40—O6	-169.2 (8)
C17—C16—C19—O2	12.2 (17)	C40—O6—C41—C42	151.1 (11)
C17—C16—C19—O3	-170.9 (9)	C40—C37—C38—O4	177.3 (8)
C19—O3—C20—C21	96.6 (11)	C40—C37—C38—C39	-0.3 (16)
C19—C16—C17—O1	-177.3 (9)	C41—O6—C40—O5	3.1 (14)
C19—C16—C17—C18	6.7 (18)	C41—O6—C40—C37	-175.6 (8)
C20—O3—C19—O2	1.1 (16)	Br16—C64—C65—Br17	105.8 (6)
C20—O3—C19—C16	-175.8 (8)	Br16—C64—C65—C66	-128.7 (8)

Br11—C43—C44—Br12	105.4 (5)	Br16—C64—C75—C72	-81.7 (9)
Br11—C43—C44—C45	-133.3 (6)	Br16—C64—C75—C74	97.1 (9)
Br11—C43—C55—C51	-75.8 (9)	Br17—C65—C66—Br18	-63.0 (8)
Br11—C43—C55—C56	102.8 (8)	Br17—C65—C66—C67	171.5 (6)
Br12—C44—C45—Br13	-64.1 (7)	Br18—C66—C67—Br19	-62.5 (8)
Br12—C44—C45—C46	172.9 (6)	Br18—C66—C67—C74	174.9 (6)
Br13—C45—C46—Br14	-62.8 (7)	Br19—C67—C74—C73	91.6 (10)
Br13—C45—C46—C56	173.1 (6)	Br19—C67—C74—C75	-95.1 (9)
Br14—C46—C56—C52	91.0 (10)	Br20—C73—C74—C67	-10.6 (13)
Br14—C46—C56—C55	-90.1 (8)	Br20—C73—C74—C75	176.1 (7)
Br15—C52—C53—C47	5.6 (12)	Br20—C73—C77—C68	1.8 (14)
Br15—C52—C53—C54	-174.0 (6)	Br20—C73—C77—C76	178.0 (7)
Br15—C52—C56—C46	-10.3 (12)	O10—N4—C78—C72	178.1 (7)
Br15—C52—C56—C55	170.8 (6)	O10—N4—C78—C79	-2.2 (10)
O7—N3—C57—C51	177.7 (7)	N4—O10—C80—C79	-1.6 (10)
O7—N3—C57—C58	-1.9 (9)	N4—O10—C80—C81	178.5 (8)
N3—O7—C59—C58	-2.4 (10)	N4—C78—C79—C80	1.3 (11)
N3—O7—C59—C60	179.3 (8)	N4—C78—C79—C82	-179.6 (9)
N3—C57—C58—C59	0.5 (10)	C64—C65—C66—Br18	173.7 (7)
N3—C57—C58—C61	176.8 (9)	C64—C65—C66—C67	48.2 (11)
C43—C44—C45—Br13	174.5 (6)	C65—C64—C75—C72	156.4 (9)
C43—C44—C45—C46	51.6 (10)	C65—C64—C75—C74	-24.8 (13)
C43—C55—C56—C46	6.4 (12)	C65—C66—C67—Br19	63.1 (9)
C43—C55—C56—C52	-174.8 (8)	C65—C66—C67—C74	-59.5 (11)
C44—C43—C55—C51	162.2 (8)	C66—C67—C74—C73	-146.0 (9)
C44—C43—C55—C56	-19.2 (12)	C66—C67—C74—C75	27.3 (12)
C44—C45—C46—Br14	59.4 (8)	C67—C74—C75—C64	14.1 (13)
C44—C45—C46—C56	-64.7 (10)	C67—C74—C75—C72	-167.1 (9)
C45—C46—C56—C52	-143.6 (9)	C68—C69—C70—C71	-0.3 (16)
C45—C46—C56—C55	35.2 (11)	C69—C68—C77—C73	175.1 (10)
C47—C48—C49—C50	1.6 (15)	C69—C68—C77—C76	-1.1 (15)
C47—C53—C54—C50	1.4 (13)	C69—C70—C71—C76	0.2 (16)
C47—C53—C54—C51	-177.2 (8)	C70—C71—C76—C72	178.3 (9)
C48—C47—C53—C52	179.2 (9)	C70—C71—C76—C77	-0.5 (15)
C48—C47—C53—C54	-1.2 (14)	C71—C76—C77—C68	0.9 (14)
C48—C49—C50—C54	-1.4 (15)	C71—C76—C77—C73	-175.5 (9)
C49—C50—C54—C51	178.5 (9)	C72—C76—C77—C68	-177.9 (9)

C49—C50—C54—C53	-0.1 (14)	C72—C76—C77—C73	5.6 (14)
C51—C55—C56—C46	-175.0 (8)	C72—C78—C79—C80	-179.1 (9)
C51—C55—C56—C52	3.8 (13)	C72—C78—C79—C82	0.0 (16)
C51—C57—C58—C59	-179.0 (8)	C73—C74—C75—C64	-172.4 (9)
C51—C57—C58—C61	-2.8 (15)	C73—C74—C75—C72	6.3 (14)
C52—C53—C54—C50	-179.0 (8)	C74—C73—C77—C68	-179.0 (10)
C52—C53—C54—C51	2.4 (12)	C74—C73—C77—C76	-2.8 (15)
C53—C47—C48—C49	-0.3 (15)	C75—C64—C65—Br17	-132.9 (7)
C53—C52—C56—C46	172.7 (9)	C75—C64—C65—C66	-7.3 (12)
C53—C52—C56—C55	-6.1 (14)	C75—C72—C76—C71	178.5 (9)
C54—C51—C55—C43	180.0 (8)	C75—C72—C76—C77	-2.6 (14)
C54—C51—C55—C56	1.4 (13)	C75—C72—C78—N4	-70.2 (12)
C54—C51—C57—N3	114.5 (9)	C75—C72—C78—C79	110.2 (12)
C54—C51—C57—C58	-66.0 (12)	C76—C72—C75—C64	175.4 (8)
C55—C43—C44—Br12	-131.6 (7)	C76—C72—C75—C74	-3.4 (14)
C55—C43—C44—C45	-10.3 (11)	C76—C72—C78—N4	110.4 (10)
C55—C51—C54—C50	176.9 (9)	C76—C72—C78—C79	-69.2 (13)
C55—C51—C54—C53	-4.5 (13)	C77—C68—C69—C70	0.8 (17)
C55—C51—C57—N3	-75.3 (11)	C77—C73—C74—C67	170.1 (9)
C55—C51—C57—C58	104.2 (11)	C77—C73—C74—C75	-3.1 (15)
C56—C52—C53—C47	-177.4 (9)	C78—C72—C75—C64	-4.1 (14)
C56—C52—C53—C54	3.0 (13)	C78—C72—C75—C74	177.1 (9)
C57—C51—C54—C50	-12.8 (13)	C78—C72—C76—C71	-2.0 (14)
C57—C51—C54—C53	165.7 (8)	C78—C72—C76—C77	176.8 (9)
C57—C51—C55—C43	9.9 (13)	C78—C79—C80—O10	0.3 (10)
C57—C51—C55—C56	-168.7 (8)	C78—C79—C80—C81	-179.9 (10)
C57—C58—C59—O7	1.2 (10)	C78—C79—C82—O11	167.7 (10)
C57—C58—C59—C60	179.1 (10)	C78—C79—C82—O12	-11.0 (13)
C57—C58—C61—O8	176.8 (9)	C80—O10—N4—C78	2.4 (10)
C57—C58—C61—O9	-5.4 (13)	C80—C79—C82—O11	-13.3 (16)
C59—O7—N3—C57	2.6 (9)	C80—C79—C82—O12	168.0 (9)
C59—C58—C61—O8	-7.8 (16)	C82—O12—C83—C84	-174.4 (12)
C59—C58—C61—O9	170.0 (9)	C82—O12—C83A—C84A	156 (3)
C61—O9—C62—C63	-177.0 (10)	C82—C79—C80—O10	-178.9 (9)
C61—C58—C59—O7	-175.2 (8)	C82—C79—C80—C81	1.0 (18)
C61—C58—C59—C60	2.7 (17)	C83—O12—C82—O11	-2.0 (15)
C62—O9—C61—O8	-0.1 (14)	C83—O12—C82—C79	176.8 (10)

C62—O9—C61—C58	-177.9 (8)	C83A—O12—C82—O11	17 (2)
Br6—C22—C23—Br7	-101.9 (5)	C83A—O12—C82—C79	-164 (2)
Br6—C22—C23—C24	135.2 (6)		

Table S7. Hydrogen-bond geometry (Å, º) for the Penta bromo AIM ester **2** (cl_mc79c9_15_0m).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C43—H43···N3	1.00	2.51	3.178 (11)	124
C22—H22···N2	1.00	2.45	3.120 (11)	124
C64—H64···N4	1.00	2.44	3.176 (12)	130
C81—H81*B*···O11	0.98	2.49	3.139 (14)	123

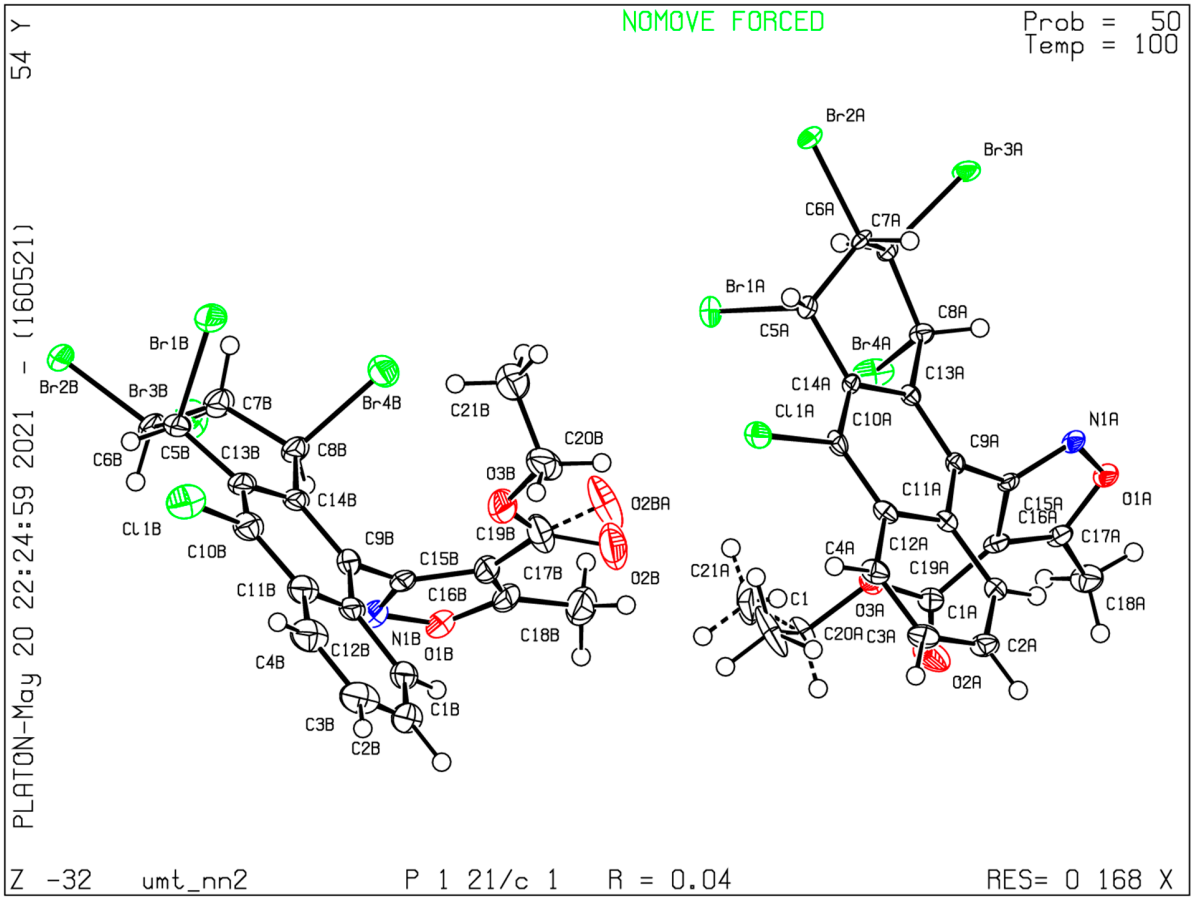

Figure S8. Number of the unit cell for tetra bromo chloro AIM **3** (MC221).

Table S8. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for the Tetrabromo Chloro AIM ester **3** (MC221). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*Y*	*z*	U(eq)
Br1	6547.5(2)	13210.1(5)	3381.4(3)	34.23(13)
Br2	5138.5(2)	14093.6(5)	3118.4(3)	32.34(13)
Br3	4693.8(2)	11596.4(6)	4223.0(3)	38.26(14)
Br4	6288.6(2)	10347.8(5)	4752.3(3)	30.19(12)
Cl1	6654.5(6)	11505.8(13)	1588.0(7)	36.9(3)
O1	5284.6(15)	6404(3)	4233.7(19)	32.4(8)
O3	7057.8(16)	7645(4)	3979(2)	44.5(10)
N1	5321.3(18)	7354(4)	3690(2)	30.8(10)
C1	5962.0(19)	12200(4)	2802(3)	24.7(10)
C2	5399(2)	12283(5)	3123(3)	28.4(11)
C3	5437(2)	11719(5)	3871(3)	28.5(11)
C4	5703.8(18)	10347(5)	3915(3)	23(1)
C5	6379(2)	6717(5)	2419(3)	31.0(12)
C6	6643(2)	6305(5)	1844(3)	34.8(13)
C7	6855(2)	7208(6)	1371(3)	38.7(14)
C8	6800(2)	8521(6)	1474(3)	35.3(12)
C9	6417.0(18)	10354(5)	2182(3)	26.4(10)
C10	6049.4(19)	8547(5)	3155(3)	24.8(10)
C11	6313.3(18)	8088(5)	2550(3)	25.3(11)
C12	6519.7(19)	8997(5)	2062(3)	27.5(11)
C13	6134.7(18)	10796(4)	2743(3)	23(1)
C14	5971.8(18)	9880(4)	3261(3)	22.1(10)
C15	5863(2)	7580(4)	3675(3)	25.9(11)
C16	6192(2)	6790(5)	4188(3)	30.6(12)
C17	5808(2)	6082(5)	4510(3)	33.8(12)
C18	5841(3)	5057(6)	5079(3)	45.8(15)
C19	6808(2)	6763(6)	4344(3)	38.9(14)
C20	7668(2)	7830(6)	4082(3)	43.7(15)
C21	7786(2)	9200(5)	4338(3)	35.0(12)
O2	7026(3)	5796(10)	4702(4)	46(2)
O4	7079(7)	6476(19)	4888(9)	46(2)
Br1'	8449.8(2)	7762.9(5)	6008.8(3)	25.60(11)
Br2'	9581.4(2)	8913.6(4)	7165.8(2)	17.99(10)
Br3'	9427.5(2)	6514.6(4)	8444.3(2)	22.40(11)
Br4'	8072.2(2)	4887.5(5)	7339.1(3)	29.82(12)
Cl09	9281.5(5)	6112.5(10)	4627.4(5)	20.3(2)
O1'	8788.7(12)	1104(3)	7887.7(15)	17.4(6)
O2'	7490.1(14)	755(4)	6176.9(18)	33.2(8)
O3'	7941.6(12)	2519(3)	5790.5(16)	18.9(6)
N1'	9119.9(15)	2020(3)	7541.3(18)	15.0(7)
C1'	9190.4(17)	6899(4)	6173(2)	15.9(8)

C2'	9442.3(18)	7069(4)	6949(2)	14.4(8)
C3'	9061.9(18)	6471(4)	7466(2)	15.3(8)
C4'	8891.4(17)	5038(4)	7274(2)	13.9(8)
C5'	9209.8(17)	1378(4)	5583(2)	15.9(8)
C6'	9326.9(18)	934(4)	4921(2)	20.2(9)
C7'	9407.6(18)	1833(5)	4368(2)	20.1(9)
C8'	9377.3(17)	3150(4)	4485(2)	17.6(9)
C9'	9228.2(16)	5000(4)	5324(2)	13.7(8)
C10'	9035.0(16)	3223(4)	6403(2)	11.0(8)
C11'	9173.9(16)	2734(4)	5725(2)	12.3(8)
C12'	9260.9(16)	3639(4)	5166(2)	14.6(8)
C13'	9146.3(16)	5468(4)	5997(2)	11.4(8)
C14'	9031.4(16)	4550(4)	6549(2)	10.9(8)
C15'	8831.2(17)	2264(4)	6925(2)	12.2(8)
C16'	8321.8(17)	1526(4)	6837(2)	15.4(8)
C17'	8322.6(18)	819(4)	7457(2)	15.7(8)
C18'	7938(2)	-151(5)	7735(2)	26.1(10)
C19'	7871.1(18)	1542(4)	6243(2)	17.5(9)
C20'	7544.0(19)	2652(5)	5150(2)	25.4(10)
C21'	7875(5)	3210(20)	4557(7)	50(4)
C22'	7776(15)	3760(40)	4740(20)	50(4)

Table S9. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for the Tetrabromo Chloro AIM ester **3** (MC221). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Br1	30.0(3)	22.5(3)	47.5(3)	-3.4(2)	-11.1(2)	-3.7(2)
Br2	33.3(3)	17.4(2)	42.9(3)	-7.8(2)	-14.4(2)	9.2(2)
Br3	30.0(3)	41.9(3)	43.3(3)	-4.9(3)	5.6(2)	16.1(2)
Br4	28.6(3)	32.7(3)	28.3(3)	-4.2(2)	-2.8(2)	5.6(2)
Cl1	35.6(7)	34.0(7)	42.0(7)	-5.1(6)	7.6(6)	-2.7(6)
O1	46(2)	15.9(17)	33(2)	-2.2(15)	-6.2(16)	2.4(15)
O3	34(2)	26(2)	69(3)	0(2)	-25(2)	3.3(17)
N1	38(2)	16(2)	36(2)	0.3(18)	-11.8(19)	0.2(17)
C1	24(2)	17(2)	30(3)	-8(2)	-10(2)	-0.9(19)
C2	24(2)	17(2)	43(3)	-7(2)	-8(2)	6.5(19)
C3	22(2)	23(3)	39(3)	-9(2)	-2(2)	6(2)
C4	18(2)	19(2)	31(3)	-7.6(19)	-2.7(19)	5.2(18)
C5	24(2)	26(3)	40(3)	-10(2)	-12(2)	11(2)
C6	24(3)	30(3)	48(3)	-18(3)	-9(2)	16(2)
C7	23(3)	48(3)	45(3)	-22(3)	-1(2)	10(2)
C8	20(2)	43(3)	42(3)	-13(3)	1(2)	4(2)
C9	16(2)	28(3)	34(3)	-5(2)	-4.1(19)	1.0(19)
C10	19(2)	21(2)	32(3)	-5(2)	-9.3(19)	5.7(18)
C11	16(2)	23(2)	35(3)	-12(2)	-11.5(19)	8.6(18)

C12	16(2)	31(3)	35(3)	-9(2)	-4.0(19)	5(2)
C13	19(2)	18(2)	31(3)	-8.9(19)	-6.6(19)	1.1(18)
C14	19(2)	18(2)	28(2)	-7.6(19)	-8.1(18)	4.3(18)
C15	30(3)	15(2)	31(3)	-10.9(19)	-10(2)	8.6(19)
C16	43(3)	22(3)	24(3)	-7(2)	-6(2)	15(2)
C17	50(3)	22(3)	28(3)	-9(2)	-6(2)	17(2)
C18	70(4)	33(3)	34(3)	0(2)	-2(3)	22(3)
C19	40(3)	54(4)	21(3)	-8(3)	-7(2)	29(3)
C20	29(3)	48(4)	50(4)	-22(3)	-16(3)	17(3)
C21	29(3)	41(3)	34(3)	5(2)	1(2)	0(2)
O2	42(3)	52(6)	42(4)	17(4)	0(3)	23(4)
O4	42(3)	52(6)	42(4)	17(4)	0(3)	23(4)
Br1'	27.3(2)	21.2(2)	26.5(2)	2.62(19)	-7.37(19)	7.77(19)
Br2'	25.2(2)	7.72(19)	20.6(2)	-0.16(16)	-0.37(17)	-1.26(16)
Br3'	43.5(3)	12.5(2)	10.5(2)	-2.37(16)	-1.61(18)	-2.36(19)
Br4'	23.1(2)	31.2(3)	37.4(3)	-13.5(2)	14.7(2)	-7.3(2)
Cl09	31.2(6)	19.1(5)	10.3(5)	5.5(4)	0.3(4)	-6.2(4)
O1'	26.7(16)	12.9(14)	12.9(14)	3.5(12)	2.9(12)	-4.3(12)
O2'	29.0(18)	40(2)	29.1(19)	7.8(16)	-5.3(15)	-21.0(16)
O3'	21.4(15)	16.5(15)	17.6(15)	4.2(12)	-4.9(12)	-3.1(12)
N1'	23.7(18)	8.0(16)	13.3(17)	2.7(13)	1.8(14)	-2.9(14)
C1'	20(2)	12(2)	15(2)	3.0(16)	-1.9(16)	-0.1(16)
C2'	23(2)	3.5(18)	16(2)	-0.1(15)	-1.5(17)	-0.8(16)
C3'	22(2)	11(2)	12(2)	-0.7(16)	0.3(16)	1.7(16)
C4'	17(2)	12(2)	13(2)	-1.2(16)	4.2(16)	-2.1(16)
C5'	16(2)	15(2)	16(2)	-0.6(17)	-0.9(16)	1.5(16)
C6'	23(2)	18(2)	19(2)	-7.6(18)	1.3(18)	0.8(18)
C7'	21(2)	28(2)	12(2)	-6.2(18)	2.6(17)	-0.9(19)
C8'	20(2)	23(2)	10(2)	0.6(17)	3.4(16)	-4.6(18)
C9'	15(2)	17(2)	9.2(19)	6.2(16)	-0.1(15)	-3.6(16)
C10'	10.7(18)	12.6(19)	9.9(19)	3.2(15)	1.0(15)	-2.7(15)
C11'	10.3(18)	15(2)	11.2(19)	0.7(16)	-1.5(15)	-0.5(15)
C12'	8.9(18)	22(2)	13(2)	-0.8(17)	-0.2(15)	-3.1(16)
C13'	12.8(19)	7.7(18)	13.1(19)	1.7(15)	-1.9(15)	0.7(15)
C14'	11.3(18)	13.4(19)	8.0(18)	0.5(15)	0.6(15)	-0.3(15)
C15'	20(2)	7.0(18)	10.0(19)	-3.1(15)	1.7(16)	2.1(15)
C16'	22(2)	9.5(19)	15(2)	-1.8(16)	3.6(16)	-2.8(16)
C17'	24(2)	8.9(19)	15(2)	-2.1(16)	3.6(17)	-1.7(17)
C18'	38(3)	20(2)	21(2)	4.0(19)	4(2)	-10(2)
C19'	20(2)	18(2)	15(2)	-2.0(17)	1.5(16)	1.0(18)
C20'	17(2)	37(3)	20(2)	8(2)	-5.9(18)	-3(2)
C21'	27(5)	96(11)	23(5)	22(6)	-10(3)	-5(6)
C22'	27(5)	96(11)	23(5)	22(6)	-10(3)	-5(6)

Table S10. Bond Lengths for the Tetrabromo Chloro AIM ester **3** (MC221).

Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**

Br1	C1	1.977(4)		Br1'	C1'	1.975(4)
Br2	C2	1.945(5)		Br2'	C2'	1.942(4)
Br3	C3	1.953(5)		Br3'	C3'	1.952(4)
Br4	C4	1.999(4)		Br4'	C4'	1.979(4)
Cl1	C9	1.743(5)		Cl09	C9'	1.738(4)
O1	N1	1.409(5)		O1'	N1'	1.416(4)
O1	C17	1.350(6)		O1'	C17'	1.344(5)
O3	C19	1.303(7)		O2'	C19'	1.210(5)
O3	C20	1.465(6)		O3'	C19'	1.325(5)
N1	C15	1.318(6)		O3'	C20'	1.464(5)
C1	C2	1.523(7)		N1'	C15'	1.309(5)
C1	C13	1.494(6)		C1'	C2'	1.526(6)
C2	C3	1.505(7)		C1'	C13'	1.494(6)
C3	C4	1.535(6)		C2'	C3'	1.512(6)
C4	C14	1.506(6)		C3'	C4'	1.547(6)
C5	C6	1.360(7)		C4'	C14'	1.507(5)
C5	C11	1.427(7)		C5'	C6'	1.369(6)
C6	C7	1.399(8)		C5'	C11'	1.409(6)
C7	C8	1.358(8)		C6'	C7'	1.404(6)
C8	C12	1.421(7)		C7'	C8'	1.361(6)
C9	C12	1.423(7)		C8'	C12'	1.416(6)
C9	C13	1.373(7)		C9'	C12'	1.419(6)
C10	C11	1.421(7)		C9'	C13'	1.374(6)
C10	C14	1.385(6)		C10'	C11'	1.427(5)
C10	C15	1.479(7)		C10'	C14'	1.378(6)
C11	C12	1.418(7)		C10'	C15'	1.492(5)
C13	C14	1.423(7)		C11'	C12'	1.421(6)
C15	C16	1.429(7)		C13'	C14'	1.434(5)
C16	C17	1.350(8)		C15'	C16'	1.427(6)
C16	C19	1.476(8)		C16'	C17'	1.362(6)
C17	C18	1.485(8)		C16'	C19'	1.473(6)
C19	O2	1.273(9)		C17'	C18'	1.475(6)
C19	O4	1.188(16)		C20'	C21'	1.526(9)
C20	C21	1.492(8)		C20'	C22'	1.503(17)

Table S11. Bond Angles for the Tetrabromo Chloro AIM ester **3** (MC221).

Atom	**Atom**	**Atom**	**Angle/°**		**Atom**	**Atom**	**Atom**	**Angle/°**
C17	O1	N1	108.9(4)		C17'	O1'	N1'	109.7(3)
C19	O3	C20	121.1(4)		C19'	O3'	C20'	118.7(3)
C15	N1	O1	105.2(4)		C15'	N1'	O1'	104.7(3)
C2	C1	Br1	111.3(3)		C2'	C1'	Br1'	111.5(3)
C13	C1	Br1	110.5(3)		C13'	C1'	Br1'	110.8(3)
C13	C1	C2	110.0(4)		C13'	C1'	C2'	109.4(3)
C1	C2	Br2	110.2(3)		C1'	C2'	Br2'	110.6(3)

C3	C2	Br2	110.9(3)		C3'	C2'	Br2'	111.0(3)
C3	C2	C1	111.4(4)		C3'	C2'	C1'	110.5(3)
C2	C3	Br3	111.0(3)		C2'	C3'	Br3'	110.1(3)
C2	C3	C4	112.6(4)		C2'	C3'	C4'	113.2(3)
C4	C3	Br3	108.1(3)		C4'	C3'	Br3'	108.9(3)
C3	C4	Br4	107.4(3)		C3'	C4'	Br4'	107.5(3)
C14	C4	Br4	108.3(3)		C14'	C4'	Br4'	109.4(3)
C14	C4	C3	116.7(4)		C14'	C4'	C3'	116.3(3)
C6	C5	C11	120.2(5)		C6'	C5'	C11'	120.9(4)
C5	C6	C7	121.0(5)		C5'	C6'	C7'	120.1(4)
C8	C7	C6	120.8(5)		C8'	C7'	C6'	120.6(4)
C7	C8	C12	120.2(6)		C7'	C8'	C12'	120.6(4)
C12	C9	Cl1	118.8(4)		C12'	C9'	Cl09	118.1(3)
C13	C9	Cl1	118.4(4)		C13'	C9'	Cl09	119.0(3)
C13	C9	C12	122.8(5)		C13'	C9'	C12'	122.9(4)
C11	C10	C15	119.0(4)		C11'	C10'	C15'	117.9(3)
C14	C10	C11	120.7(5)		C14'	C10'	C11'	121.5(4)
C14	C10	C15	120.3(4)		C14'	C10'	C15'	120.2(3)
C10	C11	C5	121.5(5)		C5'	C11'	C10'	122.1(4)
C12	C11	C5	118.5(5)		C5'	C11'	C12'	118.8(4)
C12	C11	C10	120.1(4)		C12'	C11'	C10'	119.1(4)
C8	C12	C9	123.5(5)		C8'	C12'	C9'	123.3(4)
C11	C12	C8	119.3(5)		C8'	C12'	C11'	119.0(4)
C11	C12	C9	117.2(4)		C9'	C12'	C11'	117.7(4)
C9	C13	C1	121.9(5)		C9'	C13'	C1'	121.7(4)
C9	C13	C14	119.2(4)		C9'	C13'	C14'	118.8(4)
C14	C13	C1	118.8(4)		C14'	C13'	C1'	119.4(4)
C10	C14	C4	119.8(4)		C10'	C14'	C4'	120.4(3)
C10	C14	C13	119.7(4)		C10'	C14'	C13'	119.5(4)
C13	C14	C4	120.5(4)		C13'	C14'	C4'	120.1(3)
N1	C15	C10	119.1(4)		N1'	C15'	C10'	121.4(4)
N1	C15	C16	111.6(5)		N1'	C15'	C16'	112.1(4)
C16	C15	C10	129.3(5)		C16'	C15'	C10'	126.5(4)
C15	C16	C19	128.4(5)		C15'	C16'	C19'	129.7(4)
C17	C16	C15	104.1(5)		C17'	C16'	C15'	104.2(4)
C17	C16	C19	127.5(5)		C17'	C16'	C19'	126.0(4)
O1	C17	C16	110.1(4)		O1'	C17'	C16'	109.3(4)
O1	C17	C18	115.4(5)		O1'	C17'	C18'	116.3(4)
C16	C17	C18	134.4(5)		C16'	C17'	C18'	134.4(4)
O3	C19	C16	112.4(4)		O2'	C19'	O3'	124.7(4)
O2	C19	O3	128.5(6)		O2'	C19'	C16'	124.1(4)
O2	C19	C16	118.0(7)		O3'	C19'	C16'	111.2(4)
O4	C19	O3	112.1(10)		O3'	C20'	C21'	106.6(5)
O4	C19	C16	128.9(10)		O3'	C20'	C22'	104.3(13)
O3	C20	C21	108.7(4)					

Table S12. Torsion Angles for the Tetrabromo Chloro AIM ester **3** (MC221).										
A	**B**	**C**	**D**	**Angle/°**		**A**	**B**	**C**	**D**	**Angle/°**
Br1	C1	C2	Br2	62.4(4)		C20	O3	C19	O4	22.6(12)
Br1	C1	C2	C3	-61.0(4)		Br1'	C1'	C2'	Br2'	-63.2(3)
Br1	C1	C13	C9	-92.1(5)		Br1'	C1'	C2'	C3'	60.2(4)
Br1	C1	C13	C14	91.7(4)		Br1'	C1'	C13'	C9'	91.9(4)
Br2	C2	C3	Br3	65.1(4)		Br1'	C1'	C13'	C14'	-89.9(4)
Br2	C2	C3	C4	-173.5(3)		Br2'	C2'	C3'	Br3'	-63.4(3)
Br3	C3	C4	Br4	-105.1(3)		Br2'	C2'	C3'	C4'	174.5(3)
Br3	C3	C4	C14	133.1(4)		Br3'	C3'	C4'	Br4'	103.3(2)
Br4	C4	C14	C10	80.4(5)		Br3'	C3'	C4'	C14'	-133.8(3)
Br4	C4	C14	C13	-101.0(4)		Br4'	C4'	C14'	C10'	-75.2(4)
Cl1	C9	C12	C8	-1.1(6)		Br4'	C4'	C14'	C13'	103.0(4)
Cl1	C9	C12	C11	-179.1(3)		Cl09	C9'	C12'	C8'	5.0(5)
Cl1	C9	C13	C1	8.1(6)		Cl09	C9'	C12'	C11'	-175.3(3)
Cl1	C9	C13	C14	-175.7(3)		Cl09	C9'	C13'	C1'	-9.6(5)
O1	N1	C15	C10	-179.9(4)		Cl09	C9'	C13'	C14'	172.2(3)
O1	N1	C15	C16	0.9(5)		O1'	N1'	C15'	C10'	178.5(3)
N1	O1	C17	C16	1.2(5)		O1'	N1'	C15'	C16'	-1.2(4)
N1	O1	C17	C18	-178.3(4)		N1'	O1'	C17'	C16'	-1.1(4)
N1	C15	C16	C17	-0.2(5)		N1'	O1'	C17'	C18'	178.6(3)
N1	C15	C16	C19	-179.2(5)		N1'	C15'	C16'	C17'	0.6(5)
C1	C2	C3	Br3	-171.8(3)		N1'	C15'	C16'	C19'	177.5(4)
C1	C2	C3	C4	-50.4(5)		C1'	C2'	C3'	Br3'	173.5(3)
C1	C13	C14	C4	-8.7(6)		C1'	C2'	C3'	C4'	51.4(4)
C1	C13	C14	C10	169.9(4)		C1'	C13'	C14'	C4'	6.9(5)
C2	C1	C13	C9	144.6(4)		C1'	C13'	C14'	C10'	-174.9(4)
C2	C1	C13	C14	-31.6(6)		C2'	C1'	C13'	C9'	-144.7(4)
C2	C3	C4	Br4	131.9(4)		C2'	C1'	C13'	C14'	33.5(5)
C2	C3	C4	C14	10.1(6)		C2'	C3'	C4'	Br4'	-133.9(3)
C3	C4	C14	C10	-158.3(4)		C2'	C3'	C4'	C14'	-11.0(5)
C3	C4	C14	C13	20.3(6)		C3'	C4'	C14'	C10'	162.9(4)
C5	C6	C7	C8	-0.2(8)		C3'	C4'	C14'	C13'	-18.9(5)
C5	C11	C12	C8	-2.0(6)		C5'	C6'	C7'	C8'	0.8(7)
C5	C11	C12	C9	176.2(4)		C5'	C11'	C12'	C8'	0.4(6)
C6	C5	C11	C10	-178.7(4)		C5'	C11'	C12'	C9'	-179.4(4)
C6	C5	C11	C12	1.1(7)		C6'	C5'	C11'	C10'	178.0(4)
C6	C7	C8	C12	-0.7(8)		C6'	C5'	C11'	C12'	0.1(6)
C7	C8	C12	C9	-176.3(5)		C6'	C7'	C8'	C12'	-0.3(7)
C7	C8	C12	C11	1.8(7)		C7'	C8'	C12'	C9'	179.5(4)
C9	C13	C14	C4	175.0(4)		C7'	C8'	C12'	C11'	-0.3(6)
C9	C13	C14	C10	-6.4(6)		C9'	C13'	C14'	C4'	-174.8(4)
C10	C11	C12	C8	177.9(4)		C9'	C13'	C14'	C10'	3.4(6)
C10	C11	C12	C9	-4.0(6)		C10'	C11'	C12'	C8'	-177.6(4)
C10	C15	C16	C17	-179.2(5)		C10'	C11'	C12'	C9'	2.7(6)

C10	C15	C16	C19	1.9(8)		C10'	C15'	C16'	C17'	-179.1(4)
C11	C5	C6	C7	0.0(7)		C10'	C15'	C16'	C19'	-2.1(7)
C11	C10	C14	C4	-178.5(4)		C11'	C5'	C6'	C7'	-0.6(6)
C11	C10	C14	C13	2.9(7)		C11'	C10'	C14'	C4'	-179.1(4)
C11	C10	C15	N1	-107.7(5)		C11'	C10'	C14'	C13'	2.7(6)
C11	C10	C15	C16	71.2(6)		C11'	C10'	C15'	N1'	115.2(4)
C12	C9	C13	C1	-171.4(4)		C11'	C10'	C15'	C16'	-65.1(5)
C12	C9	C13	C14	4.8(7)		C12'	C9'	C13'	C1'	171.6(4)
C13	C1	C2	Br2	-174.7(3)		C12'	C9'	C13'	C14'	-6.6(6)
C13	C1	C2	C3	61.8(5)		C13'	C1'	C2'	Br2'	173.9(3)
C13	C9	C12	C8	178.5(4)		C13'	C1'	C2'	C3'	-62.8(4)
C13	C9	C12	C11	0.4(7)		C13'	C9'	C12'	C8'	-176.2(4)
C14	C10	C11	C5	-177.8(4)		C13'	C9'	C12'	C11'	3.5(6)
C14	C10	C11	C12	2.4(7)		C14'	C10'	C11'	C5'	176.4(4)
C14	C10	C15	N1	72.9(6)		C14'	C10'	C11'	C12'	-5.7(6)
C14	C10	C15	C16	-108.2(6)		C14'	C10'	C15'	N1'	-71.3(5)
C15	C10	C11	C5	2.8(6)		C14'	C10'	C15'	C16'	108.3(5)
C15	C10	C11	C12	-177.0(4)		C15'	C10'	C11'	C5'	-10.3(6)
C15	C10	C14	C4	0.9(6)		C15'	C10'	C11'	C12'	167.6(3)
C15	C10	C14	C13	-177.7(4)		C15'	C10'	C14'	C4'	7.7(6)
C15	C16	C17	O1	-0.6(5)		C15'	C10'	C14'	C13'	-170.5(3)
C15	C16	C17	C18	178.8(5)		C15'	C16'	C17'	O1'	0.4(4)
C15	C16	C19	O3	4.1(7)		C15'	C16'	C17'	C18'	-179.3(5)
C15	C16	C19	O2	-164.8(7)		C15'	C16'	C19'	O2'	170.1(4)
C15	C16	C19	O4	152.8(14)		C15'	C16'	C19'	O3'	-9.3(6)
C17	O1	N1	C15	-1.3(5)		C17'	O1'	N1'	C15'	1.4(4)
C17	C16	C19	O3	-174.6(5)		C17'	C16'	C19'	O2'	-13.5(7)
C17	C16	C19	O2	16.5(9)		C17'	C16'	C19'	O3'	167.1(4)
C17	C16	C19	O4	-25.9(16)		C19'	O3'	C20'	C21'	-147.3(10)
C19	O3	C20	C21	-119.0(6)		C19'	O3'	C20'	C22'	-175(2)
C19	C16	C17	O1	178.3(4)		C19'	C16'	C17'	O1'	-176.8(4)
C19	C16	C17	C18	-2.3(9)		C19'	C16'	C17'	C18'	3.6(8)
C20	O3	C19	C16	176.8(4)		C20'	O3'	C19'	O2'	-1.8(6)
C20	O3	C19	O2	-15.8(10)		C20'	O3'	C19'	C16'	177.6(4)

Table S13. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for the Tetrabromo Chloro AIM ester **3** (MC221).

Atom	***x***	***y***	***z***	**U(eq)**
H1	5916	12585	2307	30
H2	5120	11753	2813	34
H3	5673	12320	4198	34
H4	5406	9699	4017	28
H5	6238	6090	2734	37

H6	6685	5390	1762	42
H7	7039	6899	974	46
H8	6948	9124	1152	42
H18D	5767	5456	5539	69
H18E	6217	4664	5122	69
H18F	5560	4375	4950	69
H20E	7835	7680	3623	52
H20F	7836	7194	4441	52
H21D	7606	9823	3988	53
H21E	8193	9350	4387	53
H21F	7637	9326	4805	53
H1'	9450	7315	5848	19
H2'	9810	6595	7006	17
H3'	8712	7013	7452	18
H4'	9084	4452	7649	17
H5'	9152	763	5953	19
H6'	9354	17	4834	24
H7'	9484	1518	3908	24
H8'	9435	3746	4107	21
H18A	7925	-940	7433	39
H18B	7561	229	7727	39
H18C	8073	-385	8231	39
H20A	7234	3254	5247	30
H20B	7382	1786	5005	30
H20C	7163	2865	5284	30
H20D	7525	1832	4863	30
H21A	8041	4053	4712	74
H21B	7622	3336	4118	74
H21C	8173	2592	4459	74
H22A	7794	4561	5031	74
H22B	7531	3917	4294	74
H22C	8154	3535	4613	74

Table S14. Atomic Occupancy for the Tetrabromo Chloro AIM ester **3** (MC221).

Atom	***Occupancy***		**Atom**	***Occupancy***		**Atom**	***Occupancy***
O2	0.657(13)		O4	0.343(13)		H20A	0.73(3)
H20B	0.73(3)		H20C	0.27(3)		H20D	0.27(3)
C21'	0.73(3)		H21A	0.73(3)		H21B	0.73(3)
H21C	0.73(3)		C22'	0.27(3)		H22A	0.27(3)
H22B	0.27(3)		H22C	0.27(3			

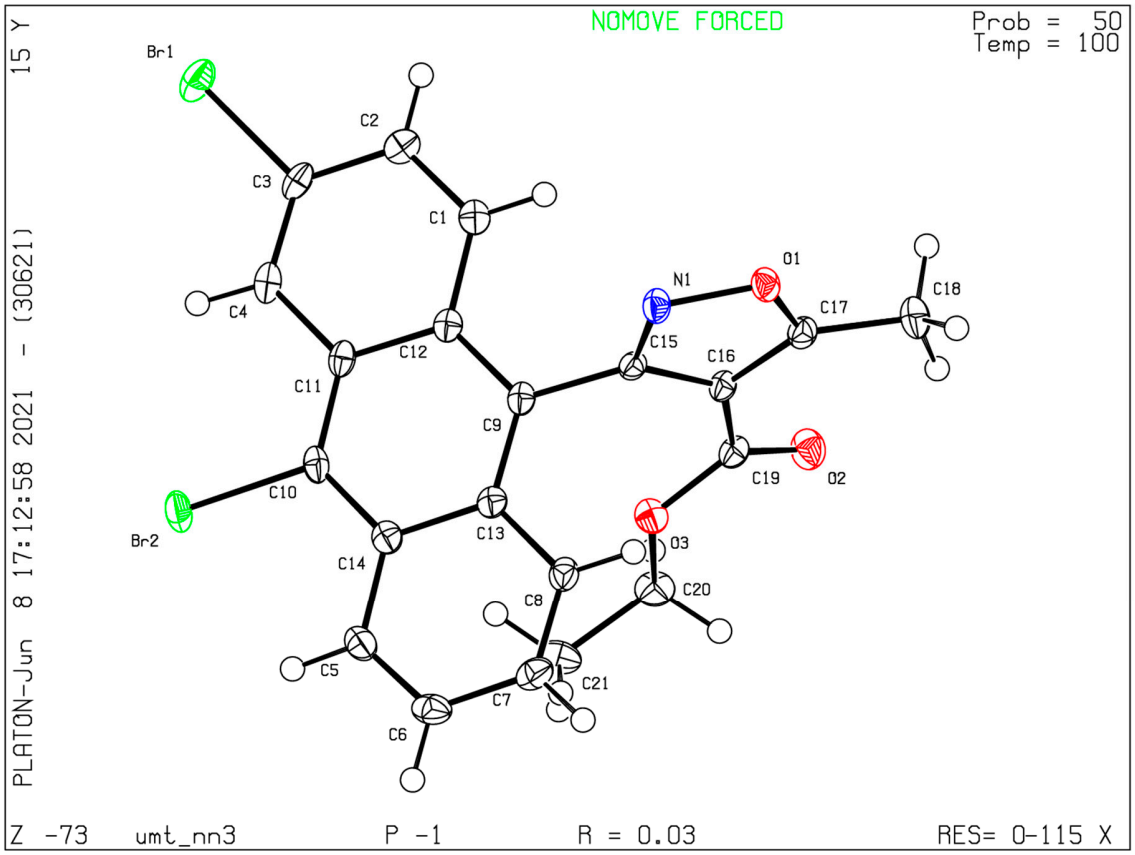

Figure S9. Numbering for dibromo ester **4** (MC219), umt-nn3.

Table S15. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for dibromo ester **4**, (MC219), umt-nn3. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Br2	2104.5(3)	3136.3(3)	-167.5(3)	24.31(9)
Br1	7395.4(4)	430.8(3)	-397.9(3)	25.07(9)
O1	10863(2)	8859(2)	5025.2(18)	17.3(4)
O3	5840(2)	6993(2)	5399.8(18)	18.1(4)
O2	7854(3)	7746(2)	7219.9(19)	23.9(4)
N1	9681(3)	8018(2)	3824(2)	17.0(4)
C11	5559(3)	4039(3)	1242(2)	15.3(5)
C10	4062(3)	4482(3)	1077(2)	16.4(5)
C15	8352(3)	7443(3)	4071(2)	13.8(5)

Atom	*x*	*y*	*z*	U(eq)
C2	8640(4)	3243(3)	1650(3)	19.6(5)
C9	6890(3)	6433(3)	2989(2)	14.5(5)
C14	3948(3)	5881(3)	1781(2)	16.2(5)
C12	7005(3)	5045(3)	2232(2)	14.7(5)
C16	8595(3)	7873(3)	5411(2)	14.7(5)
C8	5342(3)	8321(3)	3446(2)	17.7(5)
C13	5418(3)	6880(3)	2752(2)	15.0(5)
C3	7196(4)	2273(3)	675(3)	18.0(5)
C6	2442(4)	7751(3)	2273(3)	21.5(6)
C19	7431(3)	7539(3)	6127(2)	16.3(5)
C4	5705(4)	2633(3)	466(2)	18.5(5)
C1	8533(3)	4589(3)	2404(3)	17.6(5)
C5	2455(3)	6368(3)	1589(3)	19.6(5)
C7	3909(4)	8750(3)	3206(3)	21.2(6)
C18	11267(4)	9549(3)	7263(3)	22.8(6)
C17	10190(3)	8747(3)	5944(3)	16.4(5)
C21	2873(4)	6209(3)	5047(3)	24.7(6)
C20	4546(3)	6678(3)	6011(3)	21.9(6)

Table S16.Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for dibromo ester **4**, (MC219), umt-nn3. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br2	19.32(14)	23.23(15)	17.70(14)	2.39(11)	-2.55(10)	-1.92(11)
Br1	38.43(18)	15.86(14)	19.02(15)	5.24(11)	6.84(12)	9.50(12)
O1	14.5(9)	15.4(9)	17.2(9)	5.0(7)	2.4(7)	-0.9(7)
O3	15.8(9)	22.4(10)	16.9(9)	10.3(8)	6.0(7)	1.4(7)
O2	24.2(10)	29.4(11)	16.9(10)	10.5(9)	4.6(8)	3.9(8)
N1	16.1(10)	15.9(11)	14.3(10)	4.1(9)	3.1(8)	-0.6(8)
C11	20.0(12)	14.0(12)	10.5(11)	5.4(10)	4.1(9)	0.3(10)
C10	16.2(12)	18.2(12)	10.7(11)	5.5(10)	1.2(9)	-1.8(10)
C15	14.4(11)	11.5(11)	14.0(12)	4.1(10)	4.5(9)	2.8(9)
C2	23.5(13)	18.1(13)	20.1(13)	9.9(11)	8.2(11)	6.7(11)
C9	15.3(11)	15.1(12)	11.6(11)	5.6(10)	4.8(9)	0.0(9)
C14	15.9(12)	20.2(13)	13.1(12)	8.4(10)	4.9(10)	2.6(10)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C12	16.5(12)	14.9(12)	12.9(11)	6.8(10)	5.0(9)	1.1(9)
C16	16.2(12)	11.3(11)	13.9(12)	3.7(9)	3.2(9)	2.2(9)
C8	17.6(12)	18.5(13)	14.3(12)	5.2(10)	5.1(10)	2.1(10)
C13	15.4(12)	18.0(12)	12.3(11)	7.0(10)	6.4(9)	2.4(10)
C3	28.5(14)	11.1(11)	14.4(12)	4.7(10)	7.9(11)	5.3(10)
C6	18.7(13)	32.0(16)	21.0(13)	15.2(12)	9.8(11)	11.3(11)
C19	18.9(12)	12.9(12)	15.8(12)	5.0(10)	5.4(10)	3.5(10)
C4	24.3(13)	14.4(12)	12.6(12)	4.8(10)	2.6(10)	-0.9(10)
C1	17.9(12)	17.9(13)	16.3(12)	7.9(10)	4.4(10)	1.9(10)
C5	15.1(12)	26.6(14)	16.2(12)	9.8(11)	3.1(10)	3.2(11)
C7	25.7(14)	22.5(14)	18.8(13)	9.1(11)	10.1(11)	11.0(11)
C18	20.6(13)	20.1(14)	19.6(14)	6.0(11)	-0.3(11)	-2.7(11)
C17	18.5(12)	12.6(11)	16.2(12)	5.0(10)	3.5(10)	3.6(10)
C21	17.5(13)	30.7(16)	32.6(16)	18.7(14)	10.3(12)	7.5(11)
C20	19.7(13)	28.7(15)	22.6(14)	14.5(12)	12.0(11)	5.0(11)

Table S17. Bond Lengths for dibromo ester **4**, (MC219).

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Br2	C10	1.900(3)		C2	C1	1.367(4)
Br1	C3	1.899(3)		C9	C12	1.407(4)
O1	N1	1.421(3)		C9	C13	1.402(4)
O1	C17	1.344(3)		C14	C13	1.438(4)
O3	C19	1.339(3)		C14	C5	1.431(4)
O3	C20	1.459(3)		C12	C1	1.436(4)
O2	C19	1.208(3)		C16	C19	1.479(4)
N1	C15	1.308(3)		C16	C17	1.365(4)
C11	C10	1.404(4)		C8	C13	1.429(4)
C11	C12	1.437(3)		C8	C7	1.363(4)
C11	C4	1.436(4)		C3	C4	1.361(4)
C10	C14	1.404(4)		C6	C5	1.360(4)
C15	C9	1.490(3)		C6	C7	1.421(4)
C15	C16	1.437(3)		C18	C17	1.481(4)
C2	C3	1.420(4)		C21	C20	1.509(4)

Table S18. Bond Angles for dibromo ester **4**, (MC219), umt-nn3.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
C17	O1	N1	109.41(19)		C15	C16	C19	130.5(2)
C19	O3	C20	116.2(2)		C17	C16	C15	104.3(2)
C15	N1	O1	105.3(2)		C17	C16	C19	125.1(2)
C10	C11	C12	118.2(2)		C7	C8	C13	121.1(3)
C10	C11	C4	122.9(2)		C9	C13	C14	119.9(2)
C4	C11	C12	118.9(2)		C9	C13	C8	121.5(2)
C11	C10	Br2	118.7(2)		C8	C13	C14	118.6(2)
C14	C10	Br2	118.3(2)		C2	C3	Br1	118.2(2)
C14	C10	C11	123.0(2)		C4	C3	Br1	119.5(2)
N1	C15	C9	118.8(2)		C4	C3	C2	122.3(2)
N1	C15	C16	111.6(2)		C5	C6	C7	120.8(3)
C16	C15	C9	129.6(2)		O3	C19	C16	110.6(2)
C1	C2	C3	118.9(3)		O2	C19	O3	124.6(2)
C12	C9	C15	119.4(2)		O2	C19	C16	124.8(2)
C13	C9	C15	119.4(2)		C3	C4	C11	119.9(2)
C13	C9	C12	121.2(2)		C2	C1	C12	121.8(3)
C10	C14	C13	117.9(2)		C6	C5	C14	121.0(3)
C10	C14	C5	123.8(2)		C8	C7	C6	120.1(3)
C5	C14	C13	118.3(2)		O1	C17	C16	109.4(2)
C9	C12	C11	119.6(2)		O1	C17	C18	116.6(2)
C9	C12	C1	122.3(2)		C16	C17	C18	134.0(3)
C1	C12	C11	118.2(2)		O3	C20	C21	106.0(2)

Table S19. Torsion Angles for dibromo ester **4**, (MC219), umt_nn3.

A	B	C	D	Angle/°		A	B	C	D	Angle/°
Br2	C10	C14	C13	177.87(18)		C12	C11	C10	Br2	-176.75(18)
Br2	C10	C14	C5	-2.0(3)		C12	C11	C10	C14	4.0(4)
Br1	C3	C4	C11	-177.77(19)		C12	C11	C4	C3	0.0(4)
O1	N1	C15	C9	-177.3(2)		C12	C9	C13	C14	4.8(4)
O1	N1	C15	C16	0.2(3)		C12	C9	C13	C8	-174.6(2)
N1	O1	C17	C16	-0.5(3)		C16	C15	C9	C12	-101.9(3)
N1	O1	C17	C18	179.3(2)		C16	C15	C9	C13	77.6(4)
N1	C15	C9	C12	75.1(3)		C13	C9	C12	C11	-3.6(4)

Table S19. Torsion Angles for dibromo ester **4**, (MC219), umt_nn3.

A	B	C	D	Angle/°		A	B	C	D	Angle/°
N1	C15	C9	C13	-105.4(3)		C13	C9	C12	C1	176.0(2)
N1	C15	C16	C19	177.4(3)		C13	C14	C5	C6	2.4(4)
N1	C15	C16	C17	-0.5(3)		C13	C8	C7	C6	1.5(4)
C11	C10	C14	C13	-2.9(4)		C3	C2	C1	C12	-0.2(4)
C11	C10	C14	C5	177.2(2)		C19	O3	C20	C21	175.0(2)
C11	C12	C1	C2	0.6(4)		C19	C16	C17	O1	-177.5(2)
C10	C11	C12	C9	-0.7(4)		C19	C16	C17	C18	2.7(5)
C10	C11	C12	C1	179.7(2)		C4	C11	C10	Br2	3.4(3)
C10	C11	C4	C3	179.9(3)		C4	C11	C10	C14	-175.9(2)
C10	C14	C13	C9	-1.5(4)		C4	C11	C12	C9	179.2(2)
C10	C14	C13	C8	177.8(2)		C4	C11	C12	C1	-0.4(4)
C10	C14	C5	C6	-177.8(3)		C1	C2	C3	Br1	177.9(2)
C15	C9	C12	C11	175.9(2)		C1	C2	C3	C4	-0.3(4)
C15	C9	C12	C1	-4.5(4)		C5	C14	C13	C9	178.4(2)
C15	C9	C13	C14	-174.7(2)		C5	C14	C13	C8	-2.3(4)
C15	C9	C13	C8	5.9(4)		C5	C6	C7	C8	-1.5(4)
C15	C16	C19	O3	-14.7(4)		C7	C8	C13	C9	179.7(2)
C15	C16	C19	O2	166.2(3)		C7	C8	C13	C14	0.4(4)
C15	C16	C17	O1	0.6(3)		C7	C6	C5	C14	-0.5(4)
C15	C16	C17	C18	-179.3(3)		C17	O1	N1	C15	0.2(3)
C2	C3	C4	C11	0.4(4)		C17	C16	C19	O3	162.9(2)
C9	C15	C16	C19	-5.4(5)		C17	C16	C19	O2	-16.3(4)
C9	C15	C16	C17	176.7(3)		C20	O3	C19	O2	1.9(4)
C9	C12	C1	C2	-179.0(2)		C20	O3	C19	C16	-177.2(2)

Table S20. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for dibromo ester **4**, (MC219), umt-nn3.

Atom	*x*	*y*	*z*	U(eq)
H2	9664.29	2962.76	1776.74	23
H8	6306.99	8992.58	4085.96	21
H6	1439.72	8052.71	2125.97	26
H4	4761.33	1953.6	-192.53	22
H1	9496.22	5239.76	3059.64	21

Table S20. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for dibromo ester **4**, (MC219), umt-nn3.				
Atom	***x***	***y***	***z***	**U(eq)**
H5	1458.68	5714.96	974.3	24
H7	3891.4	9717.44	3663.19	25
H18A	12161.48	9074.39	7377.75	34
H18B	10573.14	9582.8	7862.3	34
H18C	11780.5	10520.54	7420.83	34
H21A	2846.59	5343.73	4293.29	37
H21B	2734.07	6965.69	4800.08	37
H21C	1949.84	6013.29	5419.96	37
H20A	4580.39	7535.31	6789.99	26
H20B	4725.92	5911.03	6247.04	26

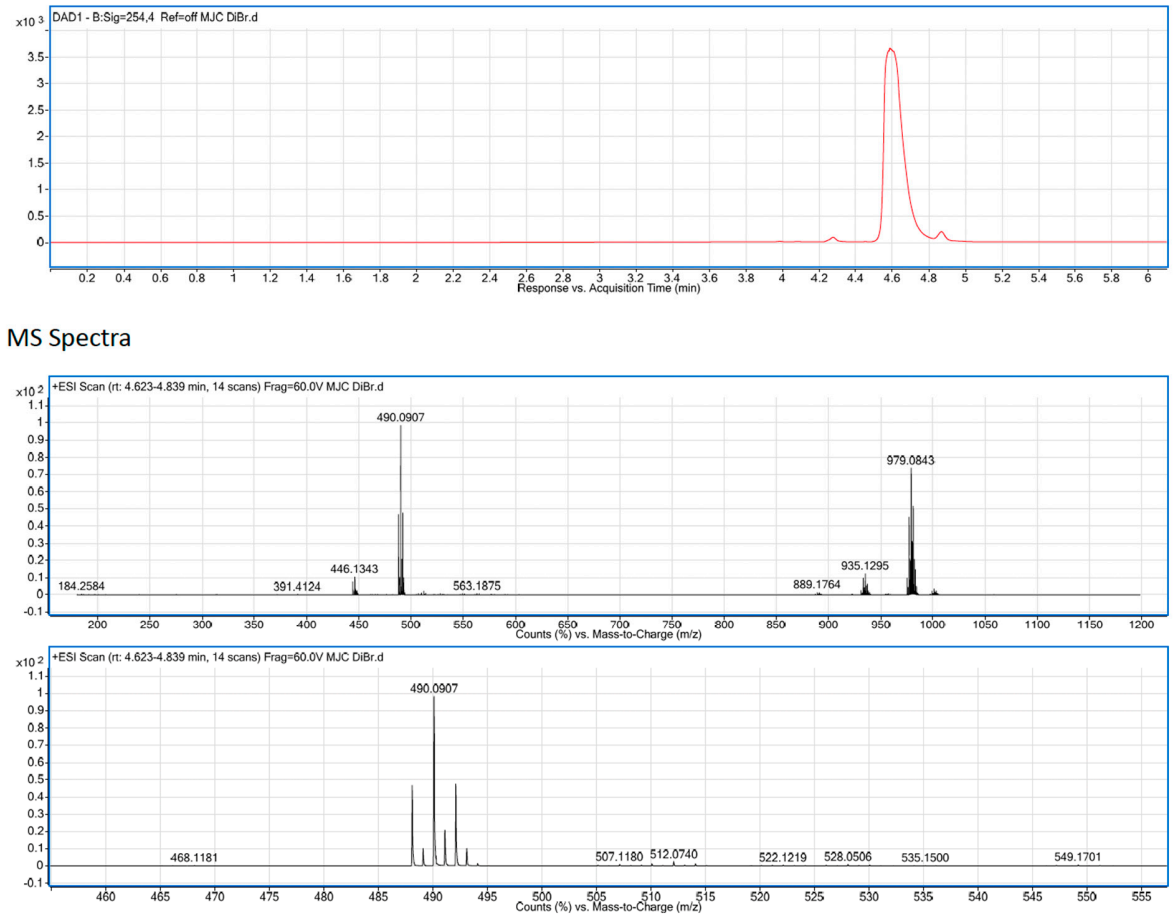

Figure S10. HPLC-MS for dibromo ester **4.**