Supporting information

Interplay of non-covalent interactions in antiseptic benzyldimethyl[3-(myristoylamino)propyl]ammonium chloride monohydrate (Miramistin)

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Table S1 Non-covalent interatomic interactions for which the BCP(3,-1) were located in the optimized structure **MR_opt**, and critical point properties (a.u. if not given).

Interaction	d(D…A), Å d(H…H), Å	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	$V(\mathbf{r})$	$h_e(\mathbf{r})$	E_{int}, kcal/mol
H-bonds						
O(1W)-H(1W)…Cl(1)$_{0.5+x,y,0.5-z}$	3.198	0.02645	0.05063	-0.01770	-0.00252	-5.546
O(1W)-H(2W)…Cl(1)	3.283	0.02192	0.04773	-0.01383	-0.00095	-4.335
N(1)-H(1)…Cl(1)$_{-0.5+x,y,0.5-z}$	3.272	0.02068	0.05317	-0.01338	-0.00004	-4.193
C_{CH2}-H…Cl and C_{CH3}-H…Cl contacts						
C(15)-H(15B)…Cl(1)$_{-x,-0.5+y,0.5-z}$	3.627	0.00782	0.02212	-0.00361	0.00096	-1.132
C(16)-H(16B)…Cl(1)$_{-0.5+x,y,0.5-z}$	3.921	0.00503	0.01486	-0.00209	0.00082	-0.654
C(18)-H(18C)…Cl(1)$_{0.5+x,y,0.5-z}$	3.686	0.01157	0.03120	-0.00600	0.00090	-1.880
C(19)-H(19B)…Cl(1)$_{0.5+x,y,0.5-z}$	3.802	0.00854	0.02172	-0.00386	0.00079	-1.209
C(19)-H(19C)…Cl(1)	3.753	0.00955	0.02498	-0.00455	0.00085	-1.426
C(20)-H(20A)…Cl(1)$_{0.5+x,y,0.5-z}$	3.692	0.01159	0.03093	-0.00599	0.00087	-1.875
C(20)-H(20B)…Cl(1)	3.883	0.00596	0.01632	-0.00249	0.00080	-0.779
C_{Ph}-H…Cl contacts						
C(22)-H(22A)…Cl(1)$_{0.5+x,y,0.5-z}$	4.196	0.00374	0.01170	-0.00149	0.00072	-0.467
C(26)-H(26A)…Cl(1)$_{-0.5+x,y,0.5-z}$	4.461	0.00287	0.00901	-0.00108	0.00058	-0.339
C_{Ph}-H…O_{CO} contacts						
C(25)-H(25A)…O(1)$_{-0.5-x,0.5+y,z}$	3.493	0.00938	0.03383	-0.00521	0.00162	-1.633
C(23)-H(23A)…O(1)$_{0.5-x,0.5+y,z}$	3.707	0.00331	0.01219	-0.00144	0.00080	-0.450
$C_{CH2\text{-хвост}}$-H…O_{CO} contacts						
C(4)-H(4B)…O(1)$_{-0.5-x,0.5+y,z}$	3.687	0.00499	0.01735	-0.00228	0.00103	-0.715
C(6)-H(6B)…O(1)$_{-0.5-x,0.5+y,z}$	4.006	0.00259	0.01020	-0.00113	0.00071	-0.354
C-H…O_{water} contacts						
C(15)-H(15A)…O(1w)$_{-x,-0.5+y,0.5-z}$	3.511	0.00728	0.02768	-0.00388	0.00152	-1.215

C(16)-H(16A)…O(1w)$_{0.5-x,-0.5+y,z}$	3.547	0.00912	0.03220	-0.00497	0.00154	-1.557
C(19)-H(19A)…O(1w)$_{0.5-x,-0.5+y,z}$	3.608	0.00446	0.01456	-0.00191	0.00087	-0.598
C(19)-H(19A)…O(1w)$_{1-x,-0.5+y,0.5-z}$	3.642	0.00332	0.01221	-0.00144	0.00081	-0.452
C(20)-H(20B)…O(1w)$_{-0.5+x,y,0.5-z}$	3.687	0.00627	0.01620	-0.00257	0.00074	-0.807
C(26)-H(26A)…O(1w)$_{-0.5+x,y,0.5-z}$	3.630	0.00439	0.01412	-0.00185	0.00084	-0.581
H…H contacts between lipid tails						
C(2)-H(2A)…H(14B)$_{-1-x,1-y,1-z}$	2.601	0.00319	0.01175	-0.00138	0.00078	-0.431
C(3)-H(3A)…H(7B)$_{-0.5-x,-0.5+y,z}$	2.711	0.00331	0.01389	-0.00158	0.00095	-0.495
C(3)-H(3A)…H(8B)$_{-0.5-x,-0.5+y,z}$	2.575	0.00370	0.01360	-0.00164	0.00088	-0.515
C(3)-H(3A)…H(6B)$_{-0.5-x,-0.5+y,z}$	2.393	0.00490	0.01571	-0.00212	0.00090	-0.664
C(3)-H(3B)…H(13A)$_{-x,1-y,1-z}$	2.512	0.00430	0.01536	-0.00193	0.00095	-0.606
C(4)-H(4A)…H(14B)$_{-1-x,1-y,1-z}$	2.839	0.00284	0.00961	-0.00113	0.00064	-0.353
C(4)-H(4A)…H(12B)$_{-1-x,1-y,1-z}$	2.573	0.00445	0.01602	-0.00203	0.00099	-0.635
C(4)-H(4A)…H(9A)$_{-0.5-x,-0.5+y,z}$	2.647	0.00319	0.01159	-0.00136	0.00077	-0.427
C(4)-H(4A)…H(7B)$_{-0.5-x,-0.5+y,z}$	2.792	0.00244	0.00860	-0.00097	0.00059	-0.304
C(5)-H(5A)…H(10A)$_{-0.5-x,-0.5+y,z}$	2.427	0.00492	0.01585	-0.00214	0.00091	-0.670
C(5)-H(5A)…H(8B)$_{-0.5-x,-0.5+y,z}$	2.414	0.00502	0.01582	-0.00216	0.00090	-0.678
C(5)-H(5B)…H(11B)$_{-x,1-y,1-z}$	2.680	0.00365	0.01352	-0.00162	0.00088	-0.509
C(6)-H(6A)…H(12B)$_{-1-x,1-y,1-z}$	2.828	0.00304	0.01038	-0.00123	0.00068	-0.386
C(6)-H(6A)…H(10B)$_{-1-x,1-y,1-z}$	2.602	0.00445	0.01653	-0.00207	0.00103	-0.648
C(6)-H(6A)…H(11A)$_{-0.5-x,-0.5+y,z}$	2.451	0.00462	0.01500	-0.00199	0.00088	-0.622
C(6)-H(6A)…H(9A)$_{-0.5-x,-0.5+y,z}$	2.633	0.00332	0.01213	-0.00144	0.00080	-0.450
C(7)-H(7A)…H(12A)$_{-0.5-x,-0.5+y,z}$	2.540	0.00390	0.01369	-0.00169	0.00086	-0.531
C(7)-H(7A)…H(10A)$_{-0.5-x,-0.5+y,z}$	2.562	0.00374	0.01340	-0.00163	0.00086	-0.512
C(7)-H(7A)…H(11B)$_{-x,1-y,1-z}$	2.642	0.00414	0.01522	-0.00188	0.00096	-0.589
C(7)-H(7A)…H(9B)$_{-x,1-y,1-z}$	2.731	0.00360	0.01272	-0.00155	0.00082	-0.484
C(7)-H(7B)…H(14C)$_{0.5+x,1.5-y,1-z}$	2.785	0.00228	0.00664	-0.00078	0.00044	-0.244
C(8)-H(8A)…H(10B)$_{-1-x,1-y,1-z}$	2.811	0.00320	0.01091	-0.00131	0.00071	-0.410
C(8)-H(8A)…H(8A)$_{-1-x,1-y,1-z}$	2.617	0.00434	0.01598	-0.00199	0.00100	-0.625
C(8)-H(8A)…H(13B)$_{-0.5-x,-0.5+y,z}$	2.385	0.00524	0.01574	-0.00222	0.00086	-0.695
C(8)-H(8A)…H(11A)$_{-0.5-x,-0.5+y,z}$	2.575	0.00369	0.01328	-0.00161	0.00085	-0.506
C(8)-H(8B)…H(13B)$_{-0.5+x,1.5-y,1-z}$	2.355	0.00540	0.01520	-0.00222	0.00079	-0.695
C(9)-H(9A)…H(12A)$_{0.5+x,1.5-y,1-z}$	2.619	0.00317	0.01071	-0.00128	0.00070	-0.403
C(9)-H(9B)…H(14C)$_{-0.5-x,-0.5+y,z}$	2.647	0.00314	0.01168	-0.00136	0.00078	-0.426
C(9)-H(9B)…H(12A)$_{-0.5-x,-0.5+y,z}$	2.599	0.00346	0.01254	-0.00150	0.00082	-0.470

C(9)-H(9B)…H(9B)$_{-x,1-y,1-z}$	2.637	0.00409	0.01475	-0.00183	0.00093	-0.574
C(10)-H(10A)…H(11A)$_{-0.5+x,1.5-y,1-z}$	2.490	0.00410	0.01357	-0.00173	0.00083	-0.543
C(10)-H(10B)…H(13B)$_{-0.5-x,-0.5+y,z}$	2.521	0.00405	0.01413	-0.00177	0.00088	-0.554
C(10)-H(10B)…H(14C)$_{-0.5-x,-0.5+y,z}$	2.898	0.00270	0.01029	-0.00116	0.00071	-0.363
C(11)-H(11B)…H(14C)$_{-0.5-x,-0.5+y,z}$	2.626	0.00328	0.01192	-0.00141	0.00079	-0.441
Other H…H contacts						
C(18)-H(18C)…H(1)$_{1+x,y,z}$	2.205	0.00731	0.02278	-0.00348	0.00111	-1.090
C(2)-H(2A)…H(24A)$_{-0.5-x,-0.5+y,z}$	2.690	0.00368	0.01270	-0.00156	0.00081	-0.490
C(2)-H(2B)…H(22A)$_{-1+x,y,z}$	2.645	0.00282	0.01041	-0.00119	0.00071	-0.373
C(11)-H(11B)…H(24A)$_{-x,1-y,1-z}$	2.662	0.00288	0.01090	-0.00124	0.00074	-0.390
C(12)-H(12B)…H(23A)$_{-x,1-y,1-z}$	2.594	0.00386	0.01403	-0.00172	0.00090	-0.538
C(14)-H(14A)…H(23A)$_{-0.5+x,1.5-y,1-z}$	2.491	0.00439	0.01690	-0.00208	0.00107	-0.653
C(14)-H(14B)…H(18B)$_{-x,1-y,1-z}$	2.615	0.00300	0.01114	-0.00129	0.00075	-0.403
C(15)-H(15A)…H(19C)$_{-0.5+x,y,0.5-z}$	2.460	0.00465	0.01860	-0.00229	0.00118	-0.719
C(16)-H(16A)…H(19B)$_{-0.5+x,y,0.5-z}$	2.411	0.00643	0.02551	-0.00340	0.00149	-1.066
C(4)-H(4B)…H(23A)$_{-1+x,y,z}$	2.737	0.00229	0.00835	-0.00092	0.00058	-0.290
C(15)-H(15B)…H(22A)$_{0.5-x,-0.5+y,z}$	2.849	0.00194	0.00644	-0.00071	0.00045	-0.222
C-H…π and C-H…H intramolecular contacts						
C(3)-H(3B)…C(25)	3,625	0.00856	0.02247	-0.00393	0.00084	-1.231
C(5)-H(5B)…H(25A)	2,585	0.00416	0.01612	-0.00196	0.00103	-0.614
C(5)-H(5B)…H(24A)	2,462	0.00482	0.01751	-0.00225	0.00106	-0.705
C(16)-H(16B)…H(26A)	2,611	0.00364	0.01399	-0.00166	0.00092	-0.521
C(26)-H(26A)…N(1)	3,929	0.00294	0.01032	-0.00121	0.00069	-0.378
C-H…π intermolecular contacts						
C(13)-H(13A)…C(24)$_{-x,1-y,1-z}$	3,709	0.00552	0.01588	-0.00231	0.00083	-0.725
C(14)-H(14B)…C(23)$_{-x,1-y,1-z}$	3,938	0.00339	0.01114	-0.00137	0.00071	-0.428
C(17)-H(17A)…C(22)$_{0.5-x,-0.5+y,z}$	3,595	0.01000	0.02614	-0.00484	0.00085	-1.518
C(18)-H(18A)…C(25)$_{0.5-x,-0.5+y,z}$	3,586	0.00820	0.02300	-0.00383	0.00096	-1.201

Table S2 Cartesian coordinates of final optimized geometry for cation **MR_a**.

O	4.239210	2.223782	-1.470285
N	4.891120	2.188974	0.684392
H	4.672637	2.456485	1.629840
N	5.337546	-1.864942	-0.785367
C	3.975185	2.437643	-0.298341
C	2.618021	2.902593	0.159719
H	2.489783	3.942539	-0.159904
H	2.550964	2.890915	1.253642
C	1.524354	2.028848	-0.452928
H	1.529104	2.172165	-1.537599
H	1.768884	0.972572	-0.280234
C	0.144939	2.312481	0.118675
H	-0.101000	3.374250	-0.010094
H	0.157624	2.136436	1.203734
C	-0.942264	1.457317	-0.517003
H	-1.012876	1.696426	-1.585891
H	-0.646968	0.399903	-0.465497
C	-2.306870	1.631969	0.133502
H	-2.597816	2.689531	0.088925
H	-2.234985	1.386706	1.202594
C	-3.396792	0.783456	-0.505977
H	-3.472095	1.034532	-1.572275
H	-3.106360	-0.275918	-0.465559
C	-4.759755	0.957136	0.149271
H	-5.042817	2.017613	0.117563
H	-4.688033	0.696138	1.213909
C	-5.856831	0.125843	-0.500673
H	-5.575827	-0.935873	-0.472115
H	-5.930091	0.390564	-1.564022

C	-7.218348	0.304016	0.156553
H	-7.147902	0.031418	1.218247
H	-7.493764	1.366945	0.135720
C	-8.321656	-0.513104	-0.500874
H	-8.047453	-1.576695	-0.482089
H	-8.393252	-0.238197	-1.561844
C	-9.681944	-0.332625	0.157980
H	-9.612536	-0.611576	1.218243
H	-9.954010	0.731514	0.143562
C	-10.789974	-1.142126	-0.502259
H	-10.859032	-0.861232	-1.560797
H	-10.516963	-2.205008	-0.488410
C	-12.143807	-0.953390	0.166145
H	-12.921720	-1.544193	-0.325174
H	-12.455333	0.095793	0.136670
H	-12.110257	-1.257036	1.217557
C	6.227540	1.743467	0.363264
H	6.922386	2.138147	1.107026
H	6.498442	2.166952	-0.607433
C	6.362370	0.215004	0.315277
H	7.402508	-0.019829	0.068645
H	6.162362	-0.191810	1.311970
C	5.408339	-0.358105	-0.713542
H	5.670061	-0.014467	-1.715918
H	4.387815	-0.031860	-0.521337
C	4.486688	-2.204686	-1.960920
H	4.979188	-1.839480	-2.861495
H	3.517522	-1.721980	-1.848441
H	4.368035	-3.287116	-2.014196
C	6.687625	-2.454713	-0.988734
H	7.151516	-1.983214	-1.855333

H	6.582597	-3.525774	-1.162398
H	7.296333	-2.285558	-0.102471
C	4.741825	-2.472040	0.481787
H	4.744540	-3.550534	0.308098
H	5.455444	-2.258688	1.278056
C	3.372398	-1.986751	0.845412
C	2.233555	-2.611500	0.332193
H	2.333112	-3.455111	-0.344652
C	0.966090	-2.182881	0.703571
H	0.089636	-2.677124	0.299512
C	0.822745	-1.135760	1.606724
H	-0.167212	-0.805973	1.902360
C	1.949480	-0.522901	2.141695
H	1.840462	0.279920	2.862605
C	3.215948	-0.945782	1.762485
H	4.089851	-0.472141	2.197794

Table S3 Cartesian coordinates of final optimized geometry for cation **MR_b**.

O	2.601303	-1.172081	0.160735
N	2.716327	-3.415722	0.024306
H	2.233065	-4.262826	-0.225326
N	6.135409	-0.398144	0.083546
C	2.087440	-2.233295	-0.181552
C	0.742713	-2.295920	-0.855592
H	0.459546	-3.330486	-1.076952
H	0.839764	-1.777448	-1.816662
C	-0.338362	-1.613454	-0.019098
H	-0.425998	-2.124036	0.948164
H	-0.017510	-0.589641	0.198048
C	-1.691218	-1.604935	-0.715414
H	-1.996491	-2.635886	-0.938967
H	-1.597775	-1.098871	-1.685648
C	-2.778881	-0.926159	0.105295
H	-2.861881	-1.423752	1.080807
H	-2.481124	0.109256	0.317613
C	-4.138599	-0.931155	-0.579006
H	-4.436425	-1.967716	-0.786466
H	-4.055736	-0.438967	-1.557382
C	-5.228028	-0.248992	0.236380
H	-5.304688	-0.735146	1.218327
H	-4.935601	0.790733	0.435998
C	-6.590682	-0.267979	-0.441642
H	-6.883277	-1.308182	-0.638460
H	-6.514365	0.215196	-1.425119
C	-7.681355	0.415508	0.370948
H	-7.392580	1.457809	0.562606
H	-7.753663	-0.063746	1.356670

C	-9.045772	0.386859	-0.303193
H	-8.973912	0.864737	-1.289616
H	-9.334417	-0.655684	-0.493546
C	-10.137417	1.070373	0.508132
H	-9.850948	2.114121	0.695570
H	-10.206977	0.594633	1.495798
C	-11.502790	1.036273	-0.163576
H	-11.434239	1.511460	-1.151727
H	-11.789944	-0.007464	-0.350636
C	-12.596055	1.719710	0.646706
H	-12.662550	1.244588	1.633720
H	-12.308143	2.762338	0.832058
C	-13.956259	1.677966	-0.033817
H	-14.723356	2.173902	0.567312
H	-14.281613	0.646101	-0.201978
H	-13.924903	2.175639	-1.008634
C	3.970286	-3.531585	0.742614
H	4.208734	-4.594602	0.786283
H	3.833331	-3.195510	1.778174
C	5.139532	-2.765516	0.091905
H	6.025042	-3.406000	0.069704
H	4.862882	-2.562405	-0.944425
C	5.429051	-1.482785	0.858372
H	6.056144	-1.687001	1.730279
H	4.483533	-1.045393	1.179962
C	7.440218	-0.883420	-0.433695
H	7.262019	-1.714547	-1.113930
H	8.054031	-1.214898	0.404545
H	7.937162	-0.071438	-0.962282
C	5.289620	0.065134	-1.054154
H	5.225419	-0.728475	-1.795131

H	5.761735	0.939402	-1.499001
H	4.291229	0.292097	-0.681030
C	6.344913	0.751584	1.069464
H	5.345859	0.993711	1.436565
H	6.920696	0.323274	1.892427
C	7.024274	1.960324	0.510069
C	6.270819	3.013769	-0.011971
H	5.186018	2.956290	-0.010687
C	6.898267	4.146076	-0.513500
H	6.304084	4.961053	-0.911515
C	8.285248	4.239826	-0.489487
H	8.775179	5.127011	-0.875324
C	9.043464	3.207116	0.050479
H	10.123781	3.289365	0.093331
C	8.415215	2.075544	0.552906
H	9.012452	1.285903	1.000208