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The role of organic acids in new particle formation from methanesulfonic acid and methylamine

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Selection of Boundary Clusters

In ACDC simulation, the boundary clusters are ones allowed to flux out the simulation box for further growth, therefore, these clusters are required to have favorable compositions for the stability. In the studied MSA-MA-ForA system, the binary $(MSA)_z(MA)_z$ (z = 1-3) and $(MSA)_{z+1}(MA)_z$ (z = 1-2) clusters have relatively lower evaporation rates than other binary MSA-MA clusters at all considered temperature conditions (238.15-298.15 K). For ForA-containing clusters, the effective evaporation rates (as described in the main manuscript) of small $(MSA)_1(ForA)_1$ and $(MSA)_1(MA)_1(ForA)_1$ cluster are lower than those of corresponding binary MSA-MA clusters. However, effective evaporation rates for clusters with larger size are much higher than those of corresponding binary MSA-MA clusters. Therefore, ForA-containing clusters can not be selected as the boundary clusters and only possibly stable $(MSA)_4(MA)_3$ and $(MSA)_4(MA)_4$ clusters are chosen as boundary clusters for ACDC simulation in this study.

Table S1. Atmospheric concentrations (molecules cm^{-3}) and acid dissociation constants (pK_a) of organic acids and MSA.

Organic Acids	Concentration (molecules cm^{-3})	pK_{a1}	pK_{a2}
ForA	$(2.50 \times 10^9$-$3.75 \times 10^{11})$[1]	3.75[2]	-
AceA	$(7.50 \times 10^9$-$4.00 \times 10^{11})$[1]	4.76[2]	-
GlyA	$(1.00 \times 10^8$-$7.71 \times 10^8)$[3]	3.18[2]	-
OxaA	$(1.01 \times 10^9$-$9.61 \times 10^9)$[3]	1.25[2]	3.81[2]
PyrA	$(9.64 \times 10^6$-$6.10 \times 10^7)$[3]	2.39[2]	-
MalA	$(5.96 \times 10^7$-$6.42 \times 10^8)$[3]	2.85[2]	5.70[2]
MaleA	$(1.35 \times 10^7$-$1.38 \times 10^8)$[3]	1.92[2]	6.23[2]
SucA	$(1.07 \times 10^8$-$9.94 \times 10^8)$[3]	4.21[2]	5.64[2]
GluA	$(4.11 \times 10^7$-$2.06 \times 10^8)$[3]	4.32[2]	5.42[2]
AdiA	$(2.13 \times 10^7$-$1.35 \times 10^8)$[3]	4.41[2]	5.41[2]
BenA	$(5.47 \times 10^7$-$1.05 \times 10^9)$[4]	4.20[2]	-
PinA	$(3.64 \times 10^7$-$3.19 \times 10^8)$[5]	4.72[6]	-
MSA	$(1.00 \times 10^5$-$1.00 \times 10^7)$[7]	-1.86[8]	-

[1] (Khwaja, 1995) ; [2] (Haynes et al., 2016) ; [3] (Ho et al., 2007) ; [4] (Ho et al., 2010) ; [5] (Kavouras et al., 1998) ; [6] (Kolodziejczyk et al., 2019) ; [7] (Chen and Finlayson-Pitts, 2017) ; [8] (NIST Database, 2013).

Table S2. Calculated (effective) evaporation rates of the $(MSA)_x(MA)_y(ForA)_z$ ($0 \le y \le x+z \le 3$) clusters at 238.15, 258.15, 278.15 and 298.15 K.

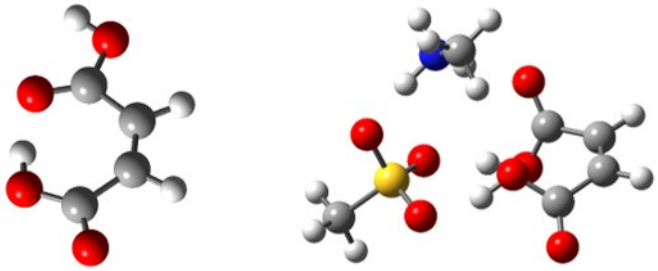
Clusters	(Effective) Evaporation rates (s^{-1})			
	298.15 K	278.15 K	258.15 K	238.15 K
$(MSA)_1(MA)_1$	1.67×10^{6}	2.44×10^{5}	2.62×10^{4}	1.94×10^{3}
$(MA)_1(ForA)_1$	1.41×10^{6}	3.63×10^{5}	7.52×10^{4}	1.19×10^{4}
$(MSA)_2(MA)_1$	2.50×10^{0}	1.26×10^{-1}	4.01×10^{-3}	7.20×10^{-5}
$(MSA)_1(MA)_1(ForA)_1$	6.29×10^{-1}	5.59×10^{-2}	3.41×10^{-3}	1.29×10^{-4}
$(MA)_1(ForA)_2$	8.60×10^{6}	2.74×10^{6}	7.38×10^{5}	1.59×10^{5}
$(MA)_1(MSA)_3$	8.29×10^{1}	5.79×10^{0}	2.67×10^{-1}	7.31×10^{-3}
$(MSA)_2(MA)_1(ForA)_1$	2.80×10^{2}	3.59×10^{1}	3.59×10^{0}	2.09×10^{-1}
$(MSA)_1(MA)_1(ForA)_2$	1.37×10^{2}	1.40×10^{1}	1.00×10^{0}	4.61×10^{-2}
$(MA)_1(ForA)_3$	6.36×10^{3}	1.02×10^{3}	1.17×10^{2}	1.05×10^{1}
$(MSA)_2(MA)_2$	4.33×10^{-1}	2.41×10^{-2}	8.52×10^{-4}	1.72×10^{-5}
$(MSA)_1(MA)_2(ForA)_1$	4.89×10^{5}	9.15×10^{4}	1.32×10^{4}	1.36×10^{3}
$(MA)_2(ForA)_2$	4.09×10^{7}	1.43×10^{7}	4.21×10^{6}	1.01×10^{6}
$(MSA)_3(MA)_2$	7.67×10^{1}	4.18×10^{0}	1.45×10^{-1}	2.84×10^{-3}
$(MSA)_2(MA)_2(ForA)_1$	3.33×10^{3}	4.21×10^{2}	3.86×10^{1}	2.37×10^{0}
$(MSA)_1(MA)_2(ForA)_2$	1.93×10^{5}	3.67×10^{4}	5.39×10^{3}	5.72×10^{2}
$(MA)_2(ForA)_3$	1.40×10^{7}	3.50×10^{6}	7.04×10^{5}	1.78×10^{5}
$(MSA)_3(MA)_3$	9.86×10^{0}	5.04×10^{-1}	1.62×10^{-2}	2.90×10^{-4}
$(MSA)_2(MA)_3(ForA)_1$	3.43×10^{3}	5.10×10^{2}	5.64×10^{1}	4.29×10^{0}
$(MSA)_1(MA)_3(ForA)_2$	8.11×10^{3}	1.45×10^{3}	1.98×10^{2}	1.92×10^{1}
$(MA)_3(ForA)_3$	3.13×10^{6}	6.60×10^{5}	1.09×10^{5}	1.33×10^{4}
$(MSA)_2$	6.29×10^{4}	6.01×10^{3}	3.97×10^{2}	1.66×10^{1}
$(MSA)_1(ForA)_1$	2.08×10^{3}	2.91×10^{2}	2.99×10^{1}	2.10×10^{0}

$(ForA)_2$	6.57×10^3	1.11×10^3	1.41×10^2	1.27×10^1
$(MSA)_3$	7.63×10^6	1.10×10^6	1.18×10^5	8.59×10^3
$(MSA)_2(ForA)_1$	3.45×10^8	1.30×10^8	4.25×10^7	1.15×10^7
$(MSA)_1(ForA)_2$	8.55×10^7	3.08×10^7	9.51×10^6	2.41×10^6
$(ForA)_3$	4.75×10^7	2.33×10^7	1.02×10^7	3.86×10^6

Table S3. The calculated mean concentrations of $(SA)_1(amine)_1(OAs)_1$ based on the mass balance equation, reported concentrations of precursors and energetic data of the $(SA)_1(amine)_1(OAs)_1$ clusters.*

Clusters	ΔG (kcal mol^{-1}) (amine=MA)	Concentration (amine=MA) (molecules cm^{-3})	ΔG (kcal mol^{-1}) (amine=DMA)	Concentration (amine=DMA) (molecules cm^{-3})
$(SA)_1(amine)_1(ForA)_1$	-21.00	1.98×10^{3}	-22.02	1.11×10^{4}
$(SA)_1(amine)_1(AceA)_1$	-18.21	1.92×10^{1}	-22.29	1.88×10^{4}
$(SA)_1(amine)_1(OxaA)_1$	-18.91	1.63×10^{0}	-21.25	8.48×10^{1}
$(SA)_1(amine)_1(PyrA)_1$	-16.19	1.10×10^{-4}	-20.94	3.34×10^{-1}
$(SA)_1(amine)_1(MalA)_1$	-17.63	1.24×10^{-2}	-22.12	2.43×10^{1}
$(SA)_1(amine)_1(MaleA)_1$	-22.11	5.17×10^{0}	-26.50	8.57×10^{3}
$(SA)_1(amine)_1(SucA)_1$	-18.00	3.63×10^{-2}	-22.33	5.44×10^{1}
$(SA)_1(amine)_1(GluA)_1$	-21.81	5.07×10^{0}	-22.75	2.48×10^{1}
$(SA)_1(amine)_1(AdiA)_1$	-21.17	1.09×10^{0}	-23.02	2.48×10^{1}
$(SA)_1(amine)_1(BenA)_1$	-18.74	1.27×10^{-1}	-20.65	3.19×10^{0}
$(SA)_1(amine)_1(PinA)_1$	-18.15	1.51×10^{-2}	-22.44	2.12×10^{1}

*Binding free energy (ΔG) (kcal mol^{-1}) of $(SA)_1(amine)_1(OAs)_1$ was calculated by the equation : $\Delta G = \Delta G_{R1} + \Delta G_{R2}$, R1 presents the reaction SA + amine → $(SA)_1(amine)_1$ and R2 for reaction $(SA)_1(amine)_1$ + OA → $(SA)_1(amine)_1(OA)_1$. (Li et al., 2020). Concentrations of precursors are from Table S1. [amine] and [SA] were set to be 2.5×10^{8} molecules cm^{-3} (~10ppt) and 10^{7} molecules cm^{-3} in the calculations, respectively.



MaleA $(MSA)_1(MA)_1(MaleA)_1$

Figure S1. Lowest Gibbs free energy conformations of MaleA and $(MSA)_1(MA)_1(MaleA)_1$ cluster at the ωB97X-D/6-31++G(d,p) level of theory. The red balls represent oxygen atoms, blue ones for nitrogen atoms, gray ones for carbon atoms, and white ones for hydrogen atoms.

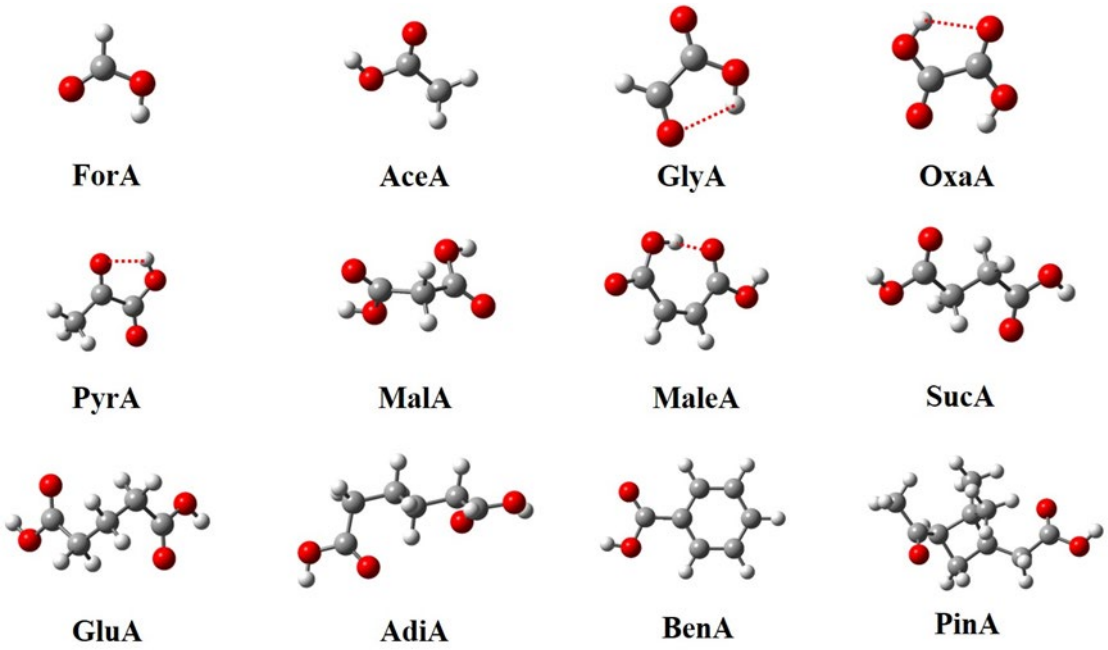


Figure S2. Lowest Gibbs free energy conformations of the organic acid monomers at the ωB97X-D/6-31++G(d,p) level of theory. The red balls represent oxygen atoms, blue ones for nitrogen atoms, gray ones for carbon atoms, and white ones for hydrogen atoms. Dashed red lines indicate hydrogen bonds.

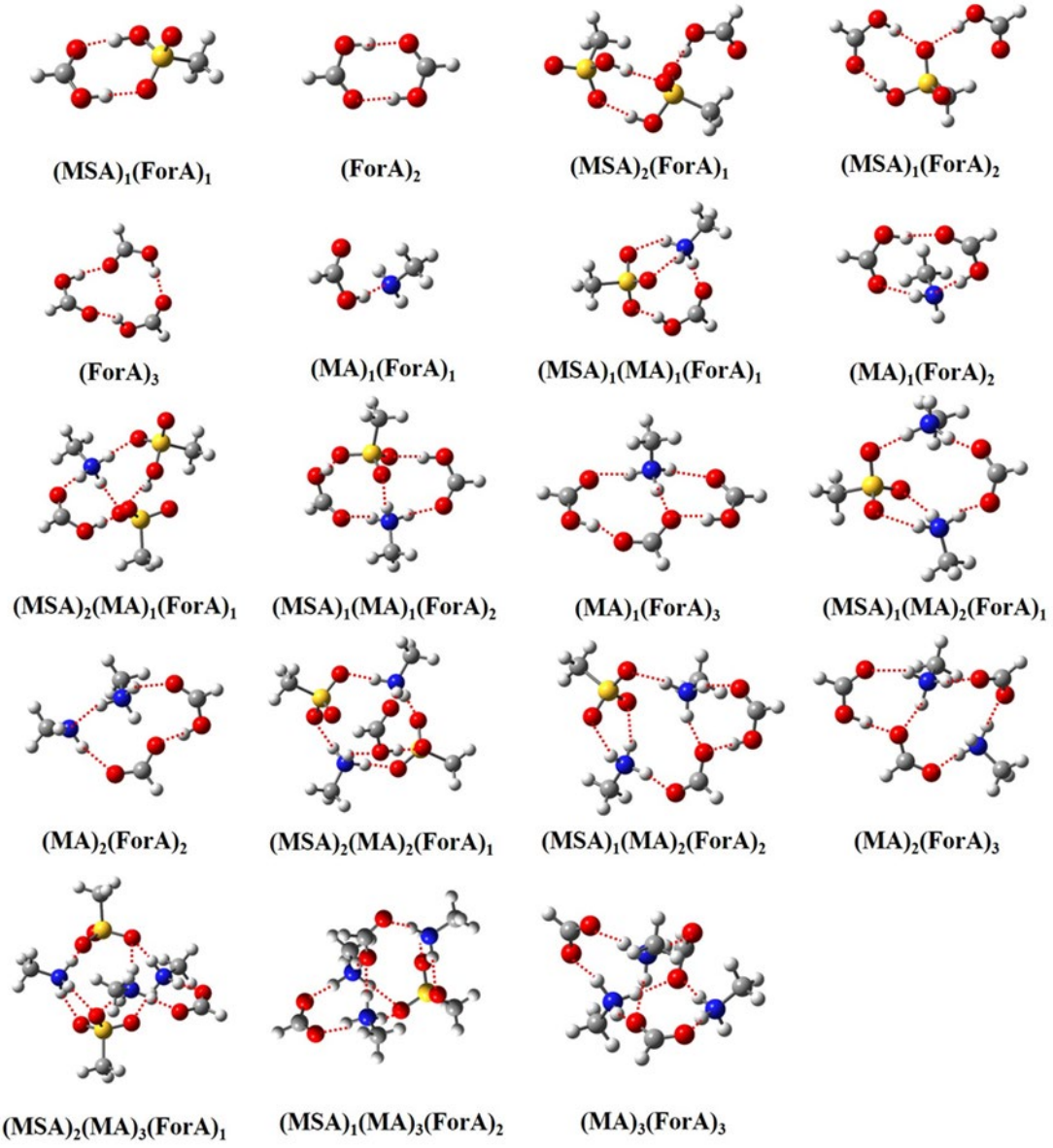


Figure S3. Lowest Gibbs free energy conformations of ForA-containing clusters at the ωB97X-D/6-31++G(d,p) level of theory. The red balls represent oxygen atoms, blue ones for nitrogen atoms, gray ones for carbon atoms, and white ones for hydrogen atoms. Dashed red lines indicate hydrogen bonds.

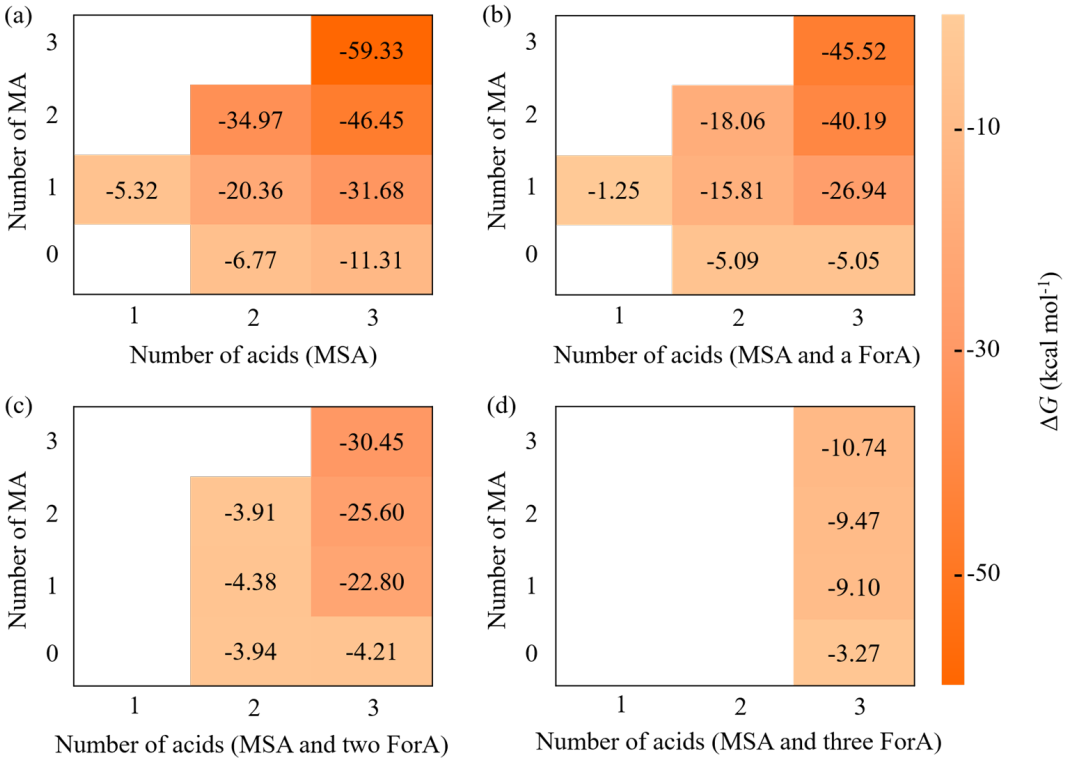


Figure S4. Formation free energy (ΔG) (kcal mol^{-1}) of $(MSA)_x(MA)_y(ForA)_z$ ($0 \leq y \leq x+z \leq 3$) clusters calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ//ωB97X-D/6-31++G(d,p) level of theory, at 298.15 K and 1 atm. a) without ForA monomer, b) containing 1 ForA monomer, c) containing 2 ForA monomers, and d) containing 3 ForA monomers.

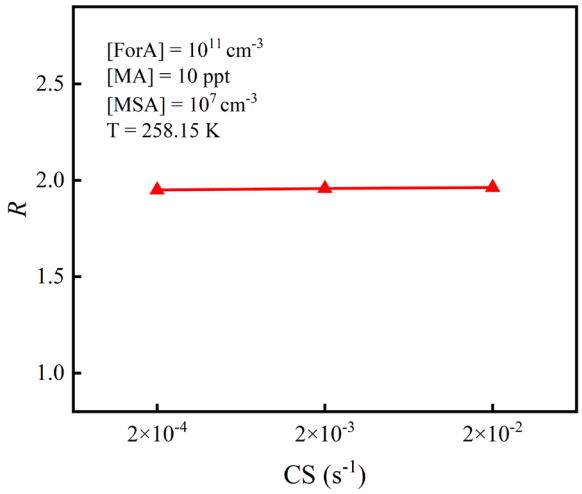


Figure S5. Variation of the enhancing coefficient (*R*) with coagulation sink coefficient (s^{-1}) at [MA] = 10 ppt, [MSA] = 10^7 cm^{-3}, [ForA] = 10^{11} cm^{-3} and T = 258.15 K.

75

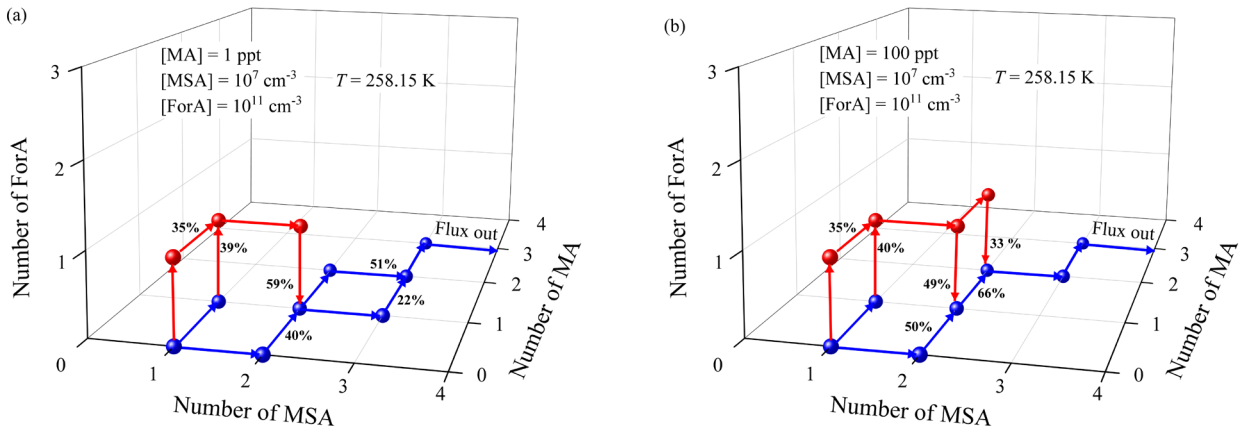


Figure S6. Main cluster formation pathways for the ternary MA-MSA-ForA system at two different [MA] (1 ppt (a) and 100 ppt (b)), T = 258.15 K, [MSA] = 10^7 cm^{-3}, and [ForA] = 10^{11} cm^{-3}.

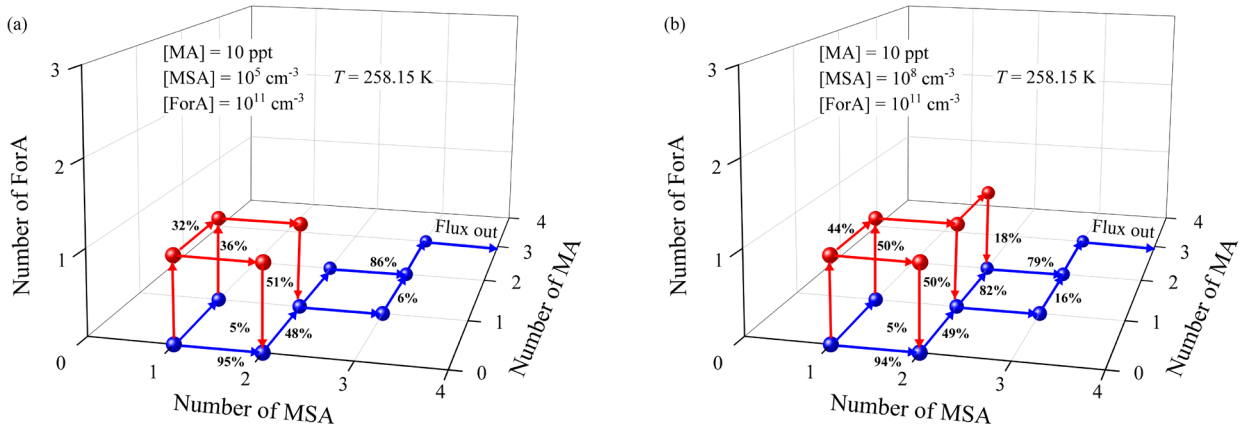


Figure S7. Main cluster formation pathways for the ternary MA-MSA-ForA system at two different [MSA] (10^5 cm^{-3} (a) and 10^8 cm^{-3} (b)), T = 258.15 K, [MA] = 10 ppt, and [ForA] = 10^{11} cm^{-3}.

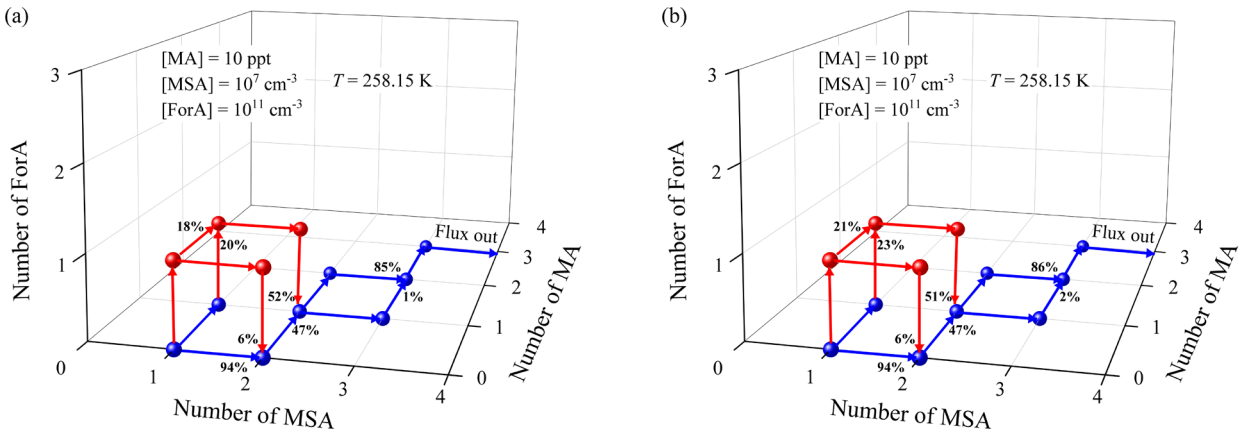


Figure S8. Main cluster formation pathways for the ternary MA-MSA-ForA system at two different coagulation sink coefficients (2×10^{-4} s^{-1} (a) and 2×10^{-3} s^{-1} (b)), T = 258.15K, [MA] = 10 ppt, [MSA] = 10^7 cm^{-3} and [ForA] = 10^{11} cm^{-3}.

Coordinates of all optimized organic acids and clusters

ForA

O	1.113654	-0.091447	0.000001
C	-0.131480	0.401285	0.000000
O	-1.133493	-0.264478	0.000000
H	1.050917	-1.058312	-0.000003
H	-0.103328	1.498008	-0.000001

AceA

C	1.055277	-0.917024	0.000000
C	0.000000	0.151467	0.000000
O	0.196381	1.344113	0.000000
H	2.040634	-0.454362	0.000000
H	0.937609	-1.552060	0.881829
H	0.937609	-1.552060	-0.881829
O	-1.244280	-0.371530	0.000000
H	-1.864320	0.371157	0.000000

GlyA

C	-0.746216	-0.761242	0.000000
C	0.000000	0.579543	0.000000
O	1.323966	0.459917	0.000000
O	-0.591134	1.626184	0.000000
O	-0.136040	-1.802595	0.000000
H	-1.845623	-0.691929	0.000000
H	1.548590	-0.485932	0.000000

OxaA

C	0.754712	0.164430	0.000111
C	-0.754717	-0.164438	0.000075
O	-1.529126	0.902788	-0.000162
O	1.529139	-0.902775	-0.000162
H	-0.957238	1.690766	-0.000218
H	0.957292	-1.690791	-0.000228
O	1.139986	1.306770	0.000114
O	-1.140002	-1.306774	0.000127

PyrA

C	0.767813	-0.279635	0.000019

O	1.008278	-1.458435	0.000056
O	1.693077	0.673528	0.000008
H	1.229743	1.530264	-0.000024
C	-0.677199	0.280943	-0.000020
C	-1.793986	-0.709227	-0.000006
H	-2.751467	-0.189685	-0.000062
H	-1.706445	-1.360020	-0.875314
H	-1.706501	-1.359927	0.875377
O	-0.806993	1.488268	-0.000056

MalA

C	0.000279	-0.023685	0.959207
C	1.268432	0.033674	0.134554
C	-1.268353	-0.040237	0.133528
O	1.217344	1.013785	-0.783645
O	2.230493	-0.675810	0.292731
O	-1.219242	-0.976417	-0.829546
O	-2.228795	0.663313	0.324582
H	0.042990	-0.927835	1.570040
H	-0.041702	0.848483	1.614903
H	2.054870	1.004334	-1.268372
H	-2.056703	-0.942459	-1.313289

MaleA

C	1.558612	0.056128	-0.000185
O	1.252519	1.238358	0.000001
O	2.834226	-0.333031	-0.000138
H	3.389080	0.460593	-0.000132
C	0.639117	-1.100777	0.000085
H	1.141080	-2.062929	0.000215
C	-0.701849	-1.088279	0.000197
H	-1.197425	-2.054438	0.000419
C	-1.737644	0.013262	-0.000027
O	-2.901702	-0.317275	0.000164
O	-1.371213	1.284454	-0.000104
H	-0.392790	1.394721	-0.000298

100

SucA

C	1.922376	-0.101722	-0.000013
O	2.162315	-1.287411	-0.000114

O	2.893452	0.830879	0.000066
H	3.740410	0.363163	0.000024
C	0.552009	0.522705	0.000040
H	0.474301	1.181835	0.870432
H	0.474291	1.181955	-0.870261
C	-0.552009	-0.522705	-0.000026
H	-0.474295	-1.181840	-0.870414
H	-0.474297	-1.181950	0.870279
C	-1.922376	0.101722	0.000009
O	-2.162315	1.287411	0.000066
O	-2.893452	-0.830879	-0.000031
H	-3.740410	-0.363163	-0.000007

GluA

C	-1.017098	-0.784553	0.617884
C	0.000003	-0.001322	1.445759
C	1.017025	0.783436	0.619225
C	1.955695	-0.085230	-0.178011
H	0.520544	1.479046	-0.064458
H	-1.641170	-1.407371	1.269149
H	-0.520649	-1.479044	-0.066944
H	-0.528923	0.704235	2.092900
O	2.767814	0.647692	-0.965046
C	-1.955689	0.085541	-0.177863
O	-2.018834	1.294254	-0.138915
O	-2.767800	-0.645926	-0.966235
H	3.346786	0.029006	-1.432144
H	1.641033	1.405233	1.271519
H	-3.346752	-0.026404	-1.432242
H	0.529013	-0.708061	2.091543
O	2.018882	-1.294004	-0.141214

105 AdiA

C	-0.714848	1.296432	-0.040324
C	0.368757	0.254083	-0.318185
C	1.721658	0.683007	0.237269
C	-2.085803	0.884131	-0.569654
C	2.828058	-0.292482	-0.071651
C	-2.709709	-0.253714	0.200977
O	3.987298	0.061944	0.521727

O	2.737188	-1.277367	-0.766851
O	-3.759909	-0.786924	-0.454469
O	-2.359810	-0.652667	1.287912
H	-0.789142	1.477289	1.037782
H	-0.437288	2.248605	-0.508065
H	0.085575	-0.704319	0.127632
H	0.457898	0.085720	-1.397387
H	1.680935	0.812101	1.324952
H	2.027306	1.656160	-0.168100
H	-2.041397	0.602592	-1.627249
H	-2.794887	1.718849	-0.509068
H	4.647136	-0.600668	0.273555
H	-4.122959	-1.484953	0.108816

BenA

C	-0.217545	0.029809	0.000005
C	2.564772	-0.043411	-0.000003
C	0.512148	1.221527	0.000093
C	0.446946	-1.199814	-0.000084
C	1.837935	-1.232805	-0.000099
C	1.901776	1.183270	0.000097
C	-1.701749	0.119638	-0.000020
O	-2.308412	-1.084734	0.000227
H	-3.260368	-0.916164	0.000068
H	-0.023426	2.164855	0.000151
H	2.467595	2.109251	0.000176
H	3.650077	-0.072706	-0.000008
H	2.354942	-2.186858	-0.000185
H	-0.124149	-2.121220	-0.000149
O	-2.332883	1.153929	-0.000225

PinA

O	-2.957415	-1.438942	0.687771
O	2.978084	1.098032	-0.281856
O	3.970771	-0.643755	0.713927
C	0.592799	-0.408779	-0.835215
C	-0.331045	0.596522	-0.070653
C	-1.549224	-0.148150	-0.746416
C	-0.622947	-1.331880	-1.059223
C	-0.294853	0.416642	1.446667

C	-0.175599	2.065047	-0.441196
C	-2.769288	-0.385445	0.109942
C	-3.731554	0.773832	0.238571
C	1.806462	-1.024115	-0.160875
C	2.942802	-0.061164	0.063763
H	0.903679	0.053118	-1.778535
H	-1.842401	0.399583	-1.649941
H	-0.727283	-1.803877	-2.038889
H	-0.713805	-2.099959	-0.284788
H	0.668424	0.752937	1.845146
H	-1.073896	1.019517	1.926301
H	-0.454208	-0.622589	1.749883
H	-0.984324	2.665449	-0.007165
H	-0.197914	2.201169	-1.527527
H	0.779564	2.453166	-0.076692
H	-4.477755	0.563807	1.005424
H	-3.190538	1.695646	0.478498
H	-4.231681	0.939161	-0.722393
H	2.194306	-1.849644	-0.770859
H	1.550130	-1.472025	0.805652
H	4.660865	0.026797	0.814971

$(MSA)_1(MA)_1(ForA)_1$

N	1.139107	1.719249	0.000203
H	0.486508	1.629418	-0.800794
H	1.706188	0.845109	-0.000211
C	1.959672	2.943036	-0.000008
H	2.588597	2.954246	-0.889954
H	1.307824	3.816561	0.000728
H	2.589943	2.953705	0.888990
S	-1.463822	-0.040312	-0.000059
O	-0.980346	-1.447880	-0.001385
O	-1.076705	0.700946	-1.230781
O	-1.075784	0.698949	1.231565
H	0.487372	1.629115	0.801811
C	-3.240262	-0.158332	0.000462
H	-3.542310	-0.697548	-0.897325
H	-3.541669	-0.699047	0.897565
H	-3.647806	0.852585	0.001463
C	2.444384	-1.853859	0.000114

O	2.567125	-0.634695	-0.000331
O	1.342657	-2.537361	0.000139
H	0.488288	-1.990810	-0.000355
H	3.326128	-2.507817	0.000549

$(MSA)_1(MA)_1(AceA)_1$

N	0.012601	2.096751	0.009713
H	-0.591836	1.776897	-0.771126
H	0.866069	1.495982	-0.025672
C	0.318973	3.537516	0.006008
H	0.860761	3.786724	-0.906113
H	-0.610051	4.105987	0.048333
H	0.936951	3.777321	0.871064
S	-1.720226	-0.511519	-0.000902
O	-0.714199	-1.602743	-0.091697
O	-1.721303	0.370129	-1.200376
O	-1.604818	0.273691	1.257816
H	-0.525466	1.766838	0.830808
C	-3.301652	-1.329389	0.038761
H	-3.410536	-1.896399	-0.885719
H	-3.318076	-1.991737	0.904241
H	-4.075547	-0.565991	0.118333
C	4.101790	-0.993169	0.037596
C	2.636737	-0.655382	-0.015780
O	2.235381	0.507387	-0.047757
O	1.869854	-1.712373	-0.014388
H	4.349279	-1.700141	-0.757482
H	4.698316	-0.087285	-0.057616
H	4.319982	-1.483504	0.990357
H	0.881155	-1.523843	-0.041254

$(MSA)_1(MA)_1(GlyA)_1$

N	0.335474	2.165995	0.007774
H	0.912236	1.807009	-0.776533
H	0.855186	1.801867	0.826247
C	0.115221	3.623520	0.005352
H	1.077229	4.133908	0.044203
H	-0.414474	3.904787	-0.904332
H	-0.483310	3.898720	0.873379
S	1.942431	-0.557970	-0.000876

O	0.953178	-1.671244	-0.073122
O	1.821887	0.235698	1.250357
O	1.920191	0.307981	-1.209471
H	-0.544569	1.615340	-0.022892
C	3.530032	-1.361419	0.036114
H	3.636449	-1.939021	-0.882014
H	4.297457	-0.590094	0.099713
H	3.559183	-2.012153	0.909971
C	-3.788756	-0.956059	0.019572
C	-2.284178	-0.627856	-0.013448
O	-1.577460	-1.716648	-0.005364
O	-1.887697	0.525984	-0.042288
O	-4.625754	-0.094686	0.015911
H	-4.028954	-2.034279	0.047411
H	-0.562322	-1.586325	-0.029277

$(MSA)_1(MA)_1(OxaA)_1$

C	-2.029621	-0.359488	-0.077176
C	-3.570145	-0.501405	0.040959
O	-4.185530	0.678117	-0.063029
O	-1.397919	-1.468410	-0.016511
H	-3.499967	1.354353	-0.192477
H	-0.372953	-1.416629	-0.124422
O	-1.570243	0.779183	-0.215126
O	-4.135086	-1.542727	0.207837
N	0.842192	2.170479	0.059739
H	1.231980	1.738706	0.914932
H	-0.074556	1.706571	-0.084393
C	0.755770	3.641962	0.088891
H	0.097633	3.950481	0.900879
H	1.750283	4.059339	0.243841
H	0.354773	3.997223	-0.860076
S	2.184088	-0.664715	-0.009839
O	1.083356	-1.619610	-0.332454
O	1.982736	0.011860	1.297072
O	2.427034	0.312121	-1.106161
H	1.474695	1.779601	-0.670352
C	3.644168	-1.671695	0.116891
H	3.795249	-2.164971	-0.843079
H	4.484026	-1.019399	0.355929

H	3.482271	-2.403712	0.908049

$(MSA)_1(MA)_1(PyrA)_1$

C	-2.039879	-0.128253	0.013331
C	-3.594756	-0.149546	0.018471
C	-4.271478	-1.484849	-0.112197
O	-4.178928	0.900938	0.123406
O	-1.437686	0.932702	0.014151
O	-1.523819	-1.322260	0.008699
H	-3.960853	-1.972889	-1.041037
H	-5.352134	-1.343435	-0.099715
H	-3.961729	-2.145296	0.702939
H	-0.504363	-1.353111	0.011191
N	1.011649	2.191511	-0.012881
H	1.497493	1.769085	0.798201
H	0.052943	1.791482	0.003023
C	1.032059	3.664380	-0.057588
H	0.532043	4.058857	0.826476
H	2.064836	4.011651	-0.082294
H	0.508814	4.003427	-0.951170
S	2.149817	-0.758273	0.008386
O	0.992094	-1.696359	0.016915
O	2.220425	0.080067	1.233782
O	2.211587	0.065163	-1.229101
H	1.489642	1.720358	-0.804401
C	3.589933	-1.805067	0.008555
H	3.562231	-2.417184	0.910056
H	3.555591	-2.428280	-0.885048
H	4.472206	-1.164891	0.001516

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$(MSA)_1(MA)_1(MalA)_1$

C	-2.970744	-1.368828	-0.263544
C	-3.949160	-0.227602	-0.140017
C	-1.546277	-0.915908	0.003575
O	-4.389693	-0.078006	1.120860
O	-4.310334	0.477609	-1.050989
O	-0.699751	-1.898538	-0.081194
O	-1.275792	0.253065	0.258422
H	-3.214341	-2.173063	0.434831
H	-3.015803	-1.767492	-1.279453

H	-4.986029	0.683801	1.129336
H	0.269143	-1.645164	0.097120
N	0.746601	2.090902	-0.016726
H	-0.034449	1.420935	0.142403
H	1.203209	1.765959	-0.884467
C	0.303849	3.496552	-0.033007
H	-0.440093	3.630367	-0.818044
H	-0.140267	3.741090	0.931486
H	1.159375	4.145503	-0.218968
S	2.665388	-0.395826	0.022741
O	2.297338	0.212720	-1.282387
O	1.785008	-1.541925	0.386346
O	2.752714	0.623808	1.103221
H	1.467775	1.863363	0.696918
C	4.292424	-1.095742	-0.156930
H	4.981105	-0.292967	-0.420042
H	4.570488	-1.550193	0.793908
H	4.250995	-1.845925	-0.946509

$(MSA)_1(MA)_1(MaleA)_1$

N	0.826939	2.546133	-0.478341
H	1.242735	3.455997	-0.293528
H	0.221895	2.283963	0.326471
C	0.007315	2.545871	-1.714960
H	-0.778981	3.295295	-1.629736
H	0.648469	2.755088	-2.570869
H	-0.440945	1.557239	-1.815716
S	2.129851	-0.562199	0.081139
O	1.294486	-1.543776	-0.639644
O	1.498094	-0.026096	1.324520
O	2.592906	0.566354	-0.783348
H	1.596696	1.820804	-0.558817
C	3.595277	-1.430562	0.593774
H	3.286171	-2.255722	1.235451
H	4.093658	-1.803391	-0.300924
H	4.234286	-0.734395	1.136567
C	-3.107920	0.367122	0.813536
C	-3.346967	-0.535774	-0.140096
C	-1.721505	0.719902	1.246934
C	-2.268039	-1.325904	-0.809727

O	-1.059731	-0.279882	1.767623
O	-1.286160	1.859633	1.106437
O	-1.166517	-0.599050	-1.031739
O	-2.400034	-2.489414	-1.106403
H	-3.917732	0.918222	1.281692
H	-4.362262	-0.782991	-0.431515
H	-0.070682	-0.126856	1.735890
H	-0.352821	-1.157090	-1.101136

125 $(MSA)_1(MA)_1(SucA)_1$

N	1.494872	2.100632	0.033998
H	1.990533	1.748692	0.871889
H	0.641504	1.507389	-0.051655
C	1.200801	3.544060	0.045673
H	0.543242	3.772804	0.884142
H	2.131673	4.102096	0.145034
H	0.706984	3.816969	-0.886629
S	3.209223	-0.518273	0.005963
O	2.208576	-1.600972	-0.188092
O	3.025200	0.210740	1.289764
O	3.275119	0.416248	-1.151745
H	2.134523	1.790620	-0.724229
C	4.785707	-1.341111	0.092105
H	4.942216	-1.866774	-0.849806
H	5.554557	-0.583882	0.245693
H	4.756999	-2.041537	0.926661
C	-4.954837	-0.138784	0.033940
O	-5.409715	-1.249211	0.181119
O	-5.738268	0.955719	-0.045023
H	-6.654845	0.656311	0.035067
C	-3.495555	0.214835	-0.082144
H	-3.350303	0.749708	-1.026222
H	-3.256668	0.938362	0.703501
C	-2.596095	-1.007465	0.002723
H	-2.763394	-1.553628	0.936658
H	-2.819354	-1.723628	-0.793356
C	-1.128263	-0.661299	-0.069421
O	-0.364183	-1.717073	-0.062314
H	0.626570	-1.531362	-0.104486
O	-0.730037	0.502597	-0.121573

$(MSA)_1(MA)_1(GluA)_1$

C	1.987775	-1.073292	1.309092
C	3.004035	-1.531008	0.257885
C	2.808115	-0.897877	-1.135634
C	1.354154	-0.740581	-1.502142
H	3.256150	0.095611	-1.169739
H	2.287361	-1.444426	2.296655
H	1.004745	-1.508121	1.106070
H	4.019518	-1.298248	0.588913
O	0.666342	-1.861175	-1.489992
C	1.858519	0.431567	1.437965
O	2.758879	1.215534	1.234142
O	0.652227	0.888992	1.813660
H	-0.311743	-1.660563	-1.492855
H	3.294323	-1.524121	-1.890623
H	-0.066251	0.204966	1.721548
H	2.921945	-2.618567	0.180445
O	0.844799	0.348553	-1.747252
N	-0.238999	2.430624	-0.363505
H	0.204694	2.410088	0.561304
H	-1.148590	1.909112	-0.263921
C	-0.409991	3.787649	-0.915732
H	-1.043017	4.372720	-0.249076
H	0.563739	4.266587	-1.016738
H	-0.885563	3.709446	-1.892858
S	-2.234065	-0.568863	0.148922
O	-1.905350	-1.320825	-1.084085
O	-2.445555	0.888247	-0.079897
O	-1.265505	-0.822881	1.255077
H	0.337999	1.820805	-0.970289
C	-3.799106	-1.203606	0.712641
H	-4.535400	-1.031623	-0.072465
H	-3.677448	-2.270048	0.902030
H	-4.072148	-0.674858	1.625710

$(MSA)_1(MA)_1(AdiA)_1$

N	-0.638022	-1.579531	0.795203
H	-0.370559	-0.599384	1.015831
H	-0.914074	-1.555377	-0.202230

C	0.416431	-2.558542	1.123315
H	1.323171	-2.315888	0.566979
H	0.618179	-2.517349	2.193802
H	0.074018	-3.557965	0.854872
S	-3.381550	-0.403244	-0.229968
O	-2.347749	-0.835457	-1.210784
O	-3.323175	1.059165	0.046595
O	-3.351162	-1.230356	1.004949
H	-1.550856	-1.733047	1.260241
C	-4.969269	-0.679438	-0.989395
H	-5.012754	-0.091079	-1.905936
H	-5.062177	-1.743609	-1.206225
H	-5.738622	-0.358590	-0.287021
C	2.465321	2.242176	0.398265
C	2.771820	0.950255	-0.360326
C	4.090615	0.316554	0.082459
C	1.141203	2.878824	-0.016166
C	4.245850	-1.101580	-0.403458
C	-0.070564	2.034621	0.318288
O	5.515782	-1.408430	-0.715290
O	3.351023	-1.916628	-0.488337
O	-1.156477	2.438342	-0.281866
O	-0.011947	1.078195	1.089742
H	2.439017	2.030999	1.473317
H	3.269132	2.969689	0.233270
H	1.966113	0.231136	-0.194499
H	2.806100	1.148210	-1.438863
H	4.124260	0.262617	1.179204
H	4.956251	0.905656	-0.231122
H	1.114693	3.092496	-1.089980
H	1.002123	3.843421	0.486015
H	5.531443	-2.338703	-0.983037
H	-1.963298	1.859518	-0.089514

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$(MSA)_1(MA)_1(BenA)_1$

C	-2.737301	-0.175483	-0.040216
C	-5.518865	-0.251643	0.079604
C	-3.398304	-1.402730	0.059051
C	-3.471830	1.012022	-0.081161
C	-4.860565	0.973264	-0.022199

C	-4.787775	-1.437747	0.119724
C	-1.248412	-0.106555	-0.099152
O	-0.663168	-1.272520	-0.066539
H	0.343569	-1.251323	-0.117337
H	-2.819803	-2.318906	0.089095
H	-5.300023	-2.391017	0.199640
H	-6.603083	-0.281898	0.128405
H	-5.429460	1.896959	-0.054761
H	-2.942386	1.955235	-0.160581
O	-0.659595	0.974543	-0.169343
N	1.805096	2.122724	0.051858
H	0.865978	1.677242	-0.057673
H	2.398826	1.733750	-0.705978
C	1.737484	3.593299	0.096416
H	1.304442	3.961216	-0.833510
H	1.109330	3.899206	0.932893
H	2.740165	4.002191	0.220965
S	3.068905	-0.732954	0.001651
O	3.009699	-0.004974	1.297530
O	3.319414	0.191408	-1.138224
O	1.884632	-1.606296	-0.219163
H	2.226369	1.681048	0.887694
C	4.462348	-1.838664	0.081289
H	4.292191	-2.538620	0.899368
H	4.528914	-2.364799	-0.870939
H	5.358262	-1.243955	0.259079

$(MSA)_1(MA)_1(PinA)_1$

O	1.786498	2.417461	-0.196248
O	-0.337581	-0.984749	-1.727560
O	-0.757591	-2.526650	-0.152798
C	2.550771	-1.476936	-0.758573
C	2.676646	-0.761986	0.627381
C	3.212405	0.492830	-0.177496
C	2.626858	-0.107092	-1.464632
C	1.349413	-0.498457	1.337125
C	3.671861	-1.391646	1.594050
C	2.746071	1.840652	0.296299
C	3.501067	2.450261	1.449065
C	1.425228	-2.474436	-1.057273

C	0.018422	-1.915863	-1.010054
H	3.490692	-2.014714	-0.932928
H	4.308606	0.477550	-0.170773
H	3.241641	-0.043480	-2.365370
H	1.638986	0.295421	-1.684256
H	0.910115	-1.433772	1.694026
H	1.499077	0.147064	2.209825
H	0.602946	-0.014344	0.704104
H	3.836640	-0.752146	2.469008
H	4.640377	-1.568329	1.114355
H	3.291423	-2.352842	1.957637
H	2.980425	3.330658	1.825761
H	3.625181	1.711826	2.248270
H	4.506603	2.731234	1.116579
H	1.493354	-3.323427	-0.372042
H	1.573279	-2.854750	-2.074575
H	-1.666254	-2.089719	-0.061947
N	-0.848775	1.676494	-1.075077
H	-0.802422	0.759745	-1.547754
H	0.116358	1.980936	-0.885801
C	-1.623698	2.669993	-1.848020
H	-2.637977	2.286637	-1.955445
H	-1.637758	3.611879	-1.299647
H	-1.156691	2.817511	-2.822125
S	-3.272873	-0.032308	0.525282
O	-3.069503	-1.495118	0.335564
O	-3.762396	0.670226	-0.673591
O	-2.057775	0.629195	1.102517
H	-1.313403	1.446686	-0.158484
C	-4.538961	0.100984	1.774993
H	-4.184046	-0.395208	2.678227
H	-4.722085	1.159589	1.959746
H	-5.437375	-0.385278	1.394376

135 $(MSA)_1(ForA)_1$

O	-2.448986	-1.114963	-0.089408
C	-2.844299	0.128536	-0.011037
O	-2.129012	1.118969	-0.031538
H	-1.460991	-1.173114	-0.167857
H	-3.932726	0.208240	0.081094

S	1.120729	-0.078290	0.141887
O	0.223553	-1.138499	-0.346948
O	1.512126	-0.108908	1.534837
O	0.483250	1.319765	-0.244940
H	-0.516596	1.275754	-0.157511
C	2.565318	-0.048775	-0.886128
H	2.253160	0.025663	-1.926914
H	3.171590	0.807412	-0.590274
H	3.100346	-0.980793	-0.701767

$(ForA)_2$

O	-1.504618	1.073962	0.000318
C	-1.892188	-0.174674	-0.000201
O	-1.161047	-1.153849	-0.000050
H	-0.507891	1.133231	0.000551
H	-2.983856	-0.269172	-0.000957
O	1.504743	-1.073998	0.000229
C	1.892138	0.174729	-0.000141
O	1.160942	1.153864	-0.000185
H	0.508093	-1.133529	0.000329
H	2.983792	0.269309	-0.000367

$(MSA)_2(ForA)_1$

O	2.417544	2.281834	0.392595
C	3.598876	1.939107	-0.094857
O	3.970700	0.805600	-0.304406
H	1.881667	1.474448	0.551995
H	4.214343	2.826174	-0.290655
S	0.929319	-1.180519	-0.056028
O	0.806263	0.027431	0.799752
O	0.717687	-0.963717	-1.474909
O	-0.061008	-2.271778	0.512793
H	-0.991245	-1.908411	0.468199
C	2.477708	-1.962130	0.263691
H	3.242057	-1.245543	-0.047173
H	2.540223	-2.167339	1.332012
H	2.512974	-2.878923	-0.324626
S	-2.669919	0.408188	0.063389
O	-3.985475	0.899634	0.382273
O	-2.362741	-1.008709	0.309859

O	-1.623882	1.293892	0.874073
H	-0.741115	0.851918	0.915729
C	-2.277379	0.760806	-1.633973
H	-2.979128	0.191689	-2.245049
H	-2.406286	1.831312	-1.792030
H	-1.251833	0.441772	-1.831576

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$(MSA)_1(ForA)_2$

O	-2.167278	2.009645	-0.255435
C	-3.251696	1.311354	-0.036947
O	-3.315268	0.097434	0.084158
H	-1.368288	1.426349	-0.295814
H	-4.141703	1.945336	0.030046
O	2.201918	1.995349	0.166120
C	3.325364	1.305074	0.061559
O	3.407275	0.129844	-0.219852
H	1.434672	1.405437	-0.006449
H	4.196137	1.941745	0.264512
S	-0.023057	-1.038931	0.150680
O	0.251829	-1.237600	1.555435
O	-0.007138	0.368787	-0.334095
O	-1.411959	-1.655654	-0.275835
H	-2.161710	-1.005299	-0.102447
C	1.074187	-1.993573	-0.852269
H	0.994165	-3.032543	-0.532614
H	0.781166	-1.870608	-1.894230
H	2.072314	-1.587082	-0.671917

$(ForA)_3$

O	1.494300	1.973375	0.567629
C	0.370404	2.128172	-0.075134
O	-0.190712	1.256626	-0.721948
H	1.803269	1.028739	0.486130
H	-0.028606	3.144876	0.026729
O	-2.689265	0.379360	-0.443179
C	-2.566357	-0.648132	0.366916
O	-1.520881	-1.150629	0.733716
H	-1.795435	0.736134	-0.678302
H	-3.544006	-1.021148	0.695279
O	0.775811	-1.950300	-0.418872

C	2.003502	-1.528732	-0.267494
O	2.369625	-0.506795	0.286601
H	0.089389	-1.376505	0.000946
H	2.719069	-2.233041	-0.708078

145 $(MA)_1(ForA)_1$

O	-1.041581	1.072200	-0.260310
C	-1.720066	-0.047383	-0.104249
O	-1.269971	-1.098545	0.303906
H	-0.078507	0.924644	0.031216
H	-2.773729	0.079923	-0.393205
C	1.960328	-0.489186	-0.470096
H	1.198805	-1.261636	-0.597434
H	2.103094	0.013754	-1.429476
H	2.904487	-0.963482	-0.178060
N	1.464421	0.483863	0.512910
H	1.305642	0.024882	1.405397
H	2.140108	1.225058	0.668498

$(MSA)_1(MA)_1(ForA)_1$

N	1.139107	1.719249	0.000203
H	0.486508	1.629418	-0.800794
H	1.706188	0.845109	-0.000211
C	1.959672	2.943036	-0.000008
H	2.588597	2.954246	-0.889954
H	1.307824	3.816561	0.000728
H	2.589943	2.953705	0.888990
S	-1.463822	-0.040312	-0.000059
O	-0.980346	-1.447880	-0.001385
O	-1.076705	0.700946	-1.230781
O	-1.075784	0.698949	1.231565
H	0.487372	1.629115	0.801811
C	-3.240262	-0.158332	0.000462
H	-3.542310	-0.697548	-0.897325
H	-3.541669	-0.699047	0.897565
H	-3.647806	0.852585	0.001463
C	2.444384	-1.853859	0.000114
O	2.567125	-0.634695	-0.000331
O	1.342657	-2.537361	0.000139
H	0.488288	-1.990810	-0.000355

H	3.326128	-2.507817	0.000549

$(MA)_1(ForA)_2$

O	2.344383	-0.409782	-0.577745
C	1.792691	-1.460996	-0.061939
O	0.661091	-1.536071	0.406872
H	1.691821	0.446013	-0.550236
H	2.455644	-2.337978	-0.066013
C	0.667152	1.959870	1.000051
H	0.374316	1.058503	1.543716
H	1.633105	2.292291	1.387360
H	-0.079805	2.738792	1.183687
N	0.795622	1.620014	-0.424299
H	-0.121113	1.333174	-0.777254
H	1.097722	2.426103	-0.963008
O	-1.977248	-1.202386	0.467315
C	-2.539979	-0.195840	-0.160643
O	-1.967930	0.688830	-0.767087
H	-0.989060	-1.199166	0.385133
H	-3.633533	-0.240756	-0.072942

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$(MSA)_2(MA)_1(ForA)_1$

N	-0.766017	-1.566752	1.395612
H	0.205458	-1.422704	1.064663
H	-1.344665	-1.842814	0.580712
C	-0.828417	-2.567973	2.478924
H	-0.230547	-2.221514	3.321418
H	-1.864935	-2.698669	2.788711
H	-0.431771	-3.514810	2.113648
S	-0.915813	1.705066	0.453357
O	-0.736495	0.650229	-0.635900
O	0.340726	2.407927	0.708258
O	-1.569173	1.088762	1.630080
H	-1.111631	-0.630683	1.686295
C	-2.075651	2.873470	-0.226874
H	-2.247658	3.642425	0.526707
H	-1.632470	3.305659	-1.124106
H	-3.003289	2.350752	-0.461470
S	2.634304	-0.433375	-0.400034
O	3.691847	-1.186866	-1.034516

O	1.870324	-1.071560	0.683126
O	1.629629	0.017961	-1.535746
H	0.741670	0.311774	-1.166490
C	3.270444	1.100929	0.227433
H	3.970579	0.853286	1.026090
H	3.781888	1.605808	-0.592194
H	2.428936	1.691072	0.597420
O	-2.693975	-0.469040	-1.969969
C	-3.004545	-1.683834	-1.598431
O	-2.510086	-2.307198	-0.673343
H	-1.954862	-0.075547	-1.417360
H	-3.793791	-2.111115	-2.228720

$(MSA)_1(MA)_1(ForA)_2$

O	-1.937706	-2.095459	-0.485490
C	-2.828882	-1.580784	-1.144684
O	-3.145612	-0.318979	-1.188827
H	-0.437131	-1.739822	0.350879
H	-3.479483	-2.182684	-1.792085
C	0.604343	-2.815486	1.809567
H	-0.228228	-2.849005	2.511819
H	0.622835	-3.731607	1.219890
H	1.543265	-2.710197	2.352620
N	0.433975	-1.659283	0.908265
H	0.373456	-0.755268	1.419034
H	1.236090	-1.560767	0.257883
O	2.817039	-1.394421	-0.531744
C	3.354724	-0.436035	-1.065912
O	2.807620	0.718481	-1.328823
H	-2.577258	0.261921	-0.597558
H	4.403924	-0.471486	-1.385669
S	-0.383733	1.504220	0.438873
O	0.182069	0.986943	1.708331
O	-1.855876	1.359165	0.343182
O	0.292107	0.900478	-0.750571
H	1.836369	0.763290	-1.059383
C	-0.048538	3.252136	0.403923
H	1.030479	3.395204	0.466910
H	-0.441971	3.653120	-0.530192
H	-0.547451	3.706104	1.260206

$(MA)_1(ForA)_3$

O	2.772514	1.159237	-0.704914
C	3.572652	0.244271	-0.596538
O	3.330212	-0.957811	-0.142699
H	0.829259	1.578080	-0.511463
H	4.626666	0.360077	-0.883268
C	0.117331	2.108354	1.365425
H	1.102425	2.002805	1.819706
H	-0.076070	3.157002	1.139378
H	-0.643890	1.735921	2.050746
N	0.075648	1.307651	0.126922
H	0.282716	0.283089	0.333546
H	-0.857550	1.351651	-0.316645
O	0.837081	-1.189749	0.504283
C	-0.004306	-2.132836	0.340378
O	-1.230758	-2.003902	0.216216
H	2.362165	-1.089682	0.121301
H	0.413838	-3.154252	0.311782
O	-3.431300	-0.745869	-0.191452
C	-3.515008	0.507239	-0.529041
O	-2.595537	1.305881	-0.642627
H	-2.495716	-1.087947	-0.031548
H	-4.555099	0.805231	-0.713791

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$(MSA)_1(MA)_2(ForA)_1$

N	0.519734	-2.417492	-0.193626
H	0.704203	-3.252702	-0.744707
H	-0.350176	-1.960159	-0.559539
C	0.336804	-2.741442	1.239389
H	-0.442371	-3.496285	1.349125
H	1.279882	-3.103437	1.649001
H	0.024342	-1.826759	1.743079
N	0.856499	1.873940	0.183974
H	1.372188	-1.785249	-0.310495
H	0.314145	1.293969	0.843009
C	1.087409	3.236232	0.697957
H	1.643905	3.807396	-0.044907
H	0.132990	3.722843	0.902287
H	1.677069	3.175627	1.612587
S	-1.934423	0.108252	-0.219600

O	-1.183133	0.154929	1.071313
O	-1.847089	-1.239225	-0.848587
O	-1.551363	1.212160	-1.128243
H	0.246439	1.874562	-0.644575
C	-3.655998	0.343430	0.178312
H	-3.962544	-0.450105	0.859757
H	-3.767081	1.320645	0.648344
H	-4.223941	0.296368	-0.750967
O	2.856511	-1.292728	-0.388322
C	3.585618	-0.269770	-0.416543
O	3.235395	0.927772	-0.274140
H	1.797406	1.386792	-0.037011
H	4.665110	-0.444644	-0.584687

$(MA)_2(ForA)_2$

O	0.749677	1.172968	0.638352
C	0.016239	2.187268	0.345592
O	-1.193319	2.156605	0.105924
H	0.030051	-0.221604	0.413850
H	0.545838	3.158563	0.317561
C	-0.525136	-2.090318	1.234002
H	0.420364	-2.234119	1.757578
H	-1.250865	-1.645300	1.915527
H	-0.898814	-3.053251	0.882924
N	-0.316652	-1.180986	0.095181
H	0.442851	-1.507081	-0.510835
H	-1.208281	-0.995194	-0.437886
O	3.168812	0.678429	-0.007132
C	3.291903	-0.505702	-0.541103
O	2.405147	-1.324499	-0.730944
H	2.209024	0.909915	0.258635
H	4.334790	-0.714158	-0.819106
C	-3.904560	-0.421375	-0.202752
H	-4.708245	0.305984	-0.372748
H	-4.285387	-1.419638	-0.436868
H	-3.656086	-0.396137	0.861955
N	-2.693142	-0.150221	-0.980941
H	-2.907260	-0.123613	-1.972479
H	-2.312640	0.766808	-0.721829

160 $(MSA)_2(MA)_2(ForA)_1$

N	0.120939	2.264367	-0.332194
H	-0.795890	1.882291	-0.662722
H	0.883974	1.742386	-0.809971
C	0.214150	3.714348	-0.592016
H	-0.598983	4.222593	-0.074105
H	1.172336	4.086653	-0.229810
H	0.130956	3.889371	-1.664283
N	-0.295226	-2.301939	-0.044039
H	-0.522313	-1.698812	0.757229
H	0.654582	-2.026781	-0.382454
C	-0.342230	-3.731111	0.318771
H	-1.339720	-3.977024	0.682649
H	-0.113477	-4.328775	-0.563130
H	0.396798	-3.927946	1.095143
S	-2.684454	-0.041064	-0.577925
O	-2.304215	1.272738	-1.160322
O	-2.124226	-0.240182	0.783796
O	-2.374457	-1.192619	-1.468730
H	-1.011537	-2.044601	-0.757985
C	-4.459522	0.001469	-0.416729
H	-4.720878	0.830000	0.241759
H	-4.886291	0.147679	-1.409104
H	-4.787485	-0.947519	0.007730
S	2.719871	-0.199176	-0.516669
O	2.255091	-1.591071	-0.749872
O	2.490960	0.244564	0.890023
O	2.176439	0.775954	-1.492063
H	0.187900	2.064105	0.680086
C	4.484781	-0.226429	-0.746216
H	4.684142	-0.533255	-1.772982
H	4.866836	0.777407	-0.561133
H	4.907417	-0.939098	-0.038106
O	0.468593	-0.511568	2.353959
C	-0.298516	0.497711	2.721560
O	-0.109110	1.664501	2.435144
H	1.258742	-0.191305	1.820520
H	-1.138343	0.164997	3.340124

$(MSA)_1(MA)_2(ForA)_2$

O	2.147051	1.112107	-0.039581
C	2.029713	2.375363	-0.121190
O	0.971141	3.024824	-0.059839
H	1.130973	-0.320090	0.169522
H	2.968676	2.942151	-0.259357
C	0.876120	-1.608120	1.782720
H	1.721980	-1.162701	2.306680
H	-0.064468	-1.173913	2.121436
H	0.865095	-2.685613	1.945778
N	1.014038	-1.339189	0.334676
H	1.887534	-1.750291	-0.030396
H	0.172492	-1.682915	-0.175432
O	4.505196	0.178499	-0.377790
C	4.606199	-1.120798	-0.412470
O	3.699131	-1.929699	-0.282552
H	3.547401	0.515979	-0.237249
H	5.642716	-1.444473	-0.576374
C	-2.321654	3.372246	0.393561
H	-2.191018	4.104843	-0.402533
H	-3.376339	3.113468	0.490280
H	-1.954840	3.794158	1.329037
N	-1.539421	2.163784	0.072390
H	-1.868326	1.700048	-0.788611
H	-0.505536	2.397734	-0.004050
S	-2.413524	-1.010283	-0.296298
O	-1.442717	-2.065127	-0.683404
O	-2.627551	0.020248	-1.340632
O	-2.063684	-0.394198	1.022219
H	-1.669785	1.409224	0.768038
C	-3.974509	-1.841414	-0.072242
H	-3.851783	-2.598106	0.702713
H	-4.717532	-1.100905	0.223596
H	-4.246933	-2.303148	-1.021415

$(MA)_2(ForA)_3$

O	-3.206279	-1.457326	-0.515162
C	-4.047340	-0.573055	-0.476657
O	-3.840161	0.693542	-0.235246
H	-1.319501	-1.617293	-0.323028

H	-5.111496	-0.781869	-0.650815
C	-0.298370	-1.837030	1.473635
H	-1.166516	-1.557038	2.070586
H	-0.223787	-2.922887	1.414150
H	0.615106	-1.437451	1.914313
N	-0.447190	-1.286040	0.109482
H	-0.577369	-0.250916	0.143321
H	0.402009	-1.525847	-0.467839
O	-1.362638	1.267044	0.143111
C	-0.916968	2.429164	0.407733
O	0.283063	2.746458	0.478797
H	-2.859315	0.918615	-0.077624
H	-1.672321	3.215305	0.585129
O	2.957129	-1.156818	0.728543
C	2.784006	-2.001752	-0.191316
O	1.885139	-1.958623	-1.072509
H	1.391760	1.664542	-0.022052
H	3.488926	-2.853542	-0.227518
C	3.405477	1.959805	-0.505794
H	3.205961	2.807525	-1.161591
H	3.643640	2.325462	0.492346
H	4.242201	1.374010	-0.886867
N	2.204195	1.104588	-0.412254
H	1.935954	0.739026	-1.325627
H	2.414873	0.235531	0.176642

$(MSA)_2(MA)_3(ForA)_1$

C	-1.705930	-0.947300	-3.145942
H	-1.872921	-2.005318	-3.347344
H	-2.569719	-0.375069	-3.483211
H	-0.809655	-0.605317	-3.664215
N	-1.545104	-0.754006	-1.691345
H	-0.736403	-1.284736	-1.332709
H	-1.402988	0.249202	-1.473808
N	2.669559	1.426285	-0.017017
H	2.328146	2.276854	-0.495307
H	2.613898	0.611823	-0.667079
C	4.009846	1.541259	0.585961
H	4.019648	2.368507	1.295511
H	4.229482	0.605482	1.099485

H	4.745358	1.719125	-0.198298
N	-1.003316	-0.810358	1.679645
H	-0.715583	0.136002	1.376391
H	-0.520527	-1.473307	1.056025
C	-0.603995	-1.040894	3.081763
H	-1.071672	-0.284790	3.712383
H	-0.949336	-2.027514	3.391495
H	0.482152	-0.983720	3.159033
S	-0.390270	2.639381	-0.195529
O	0.792243	3.299147	-0.798305
O	0.021461	1.700359	0.902788
O	-1.286801	1.986572	-1.173227
H	-2.070893	-0.920109	1.559320
C	-1.350341	3.920740	0.586783
H	-0.724958	4.409784	1.333612
H	-1.655635	4.627985	-0.184503
H	-2.221989	3.457640	1.049790
S	1.899220	-1.846300	-0.186720
O	0.466484	-2.246326	-0.333065
O	2.181165	-1.248780	1.136813
O	2.356123	-0.984989	-1.312468
H	1.938884	1.244292	0.686976
C	2.830655	-3.361373	-0.301488
H	2.641795	-3.805606	-1.278750
H	3.887511	-3.120682	-0.185326
H	2.496828	-4.026449	0.495039
O	-3.799826	-1.591279	-0.631925
C	-4.239760	-1.468041	0.538547
O	-3.600411	-1.114425	1.562795
H	-2.426913	-1.088545	-1.175950
H	-5.312031	-1.696852	0.687454

$(MSA)_1(MA)_3(ForA)_2$

C	-1.340115	-0.035807	3.115523
H	-0.283710	-0.047605	3.386641
H	-1.820614	0.856521	3.516790
H	-1.834033	-0.919385	3.519664
N	-1.471662	-0.038181	1.646897
H	-0.986411	-0.849588	1.233364
H	-2.505955	-0.064597	1.339259

O	-0.213219	1.908434	0.096055
C	0.142355	3.124828	0.097537
O	1.318871	3.536086	-0.000355
H	-0.885731	0.794378	-1.160326
H	-0.654135	3.886544	0.194836
C	-1.051259	-0.012211	-3.080678
H	-1.439954	0.909793	-3.513073
H	0.023355	-0.088504	-3.249821
H	-1.557835	-0.861873	-3.538567
N	-1.319722	-0.017901	-1.630569
H	-2.379472	-0.003011	-1.419274
H	-0.909531	-0.852375	-1.184741
O	-4.015602	-0.093970	1.012775
C	-4.516218	-0.045327	-0.139525
O	-3.908005	0.006044	-1.239222
H	-1.034941	0.800704	1.224060
H	-5.621192	-0.048123	-0.193579
C	4.239122	1.538964	-0.029587
H	4.527586	2.141668	0.831640
H	4.754448	0.578506	0.002660
H	4.505399	2.070142	-0.943325
N	2.781954	1.321714	-0.003503
H	2.490761	0.768755	0.814051
H	2.221093	2.236120	-0.020585
S	1.390346	-1.728316	0.028636
O	1.805309	-1.032663	-1.218667
O	-0.084861	-1.966680	0.063693
O	1.880553	-1.057923	1.257896
H	2.467924	0.718134	-0.777898
C	2.134489	-3.347229	-0.015658
H	3.216755	-3.222849	-0.056283
H	1.840611	-3.880920	0.888159
H	1.771436	-3.862745	-0.904675

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$(MA)_3(ForA)_3$

O	-0.371058	1.575967	1.372149
C	-1.459085	1.840500	1.951935
O	-2.569302	1.307469	1.706833
H	-0.147919	-0.160922	1.082007
H	-1.432998	2.604870	2.750012

C	-0.484378	-1.882535	2.190487
H	-0.004922	-1.507651	3.094780
H	-1.559801	-1.708187	2.252414
H	-0.282801	-2.948920	2.091021
N	0.074170	-1.173648	1.023535
H	1.142776	-1.276222	1.009123
H	-0.303735	-1.549325	0.131334
O	3.531956	0.061144	-0.165653
C	3.611559	-0.956076	0.573088
O	2.674017	-1.552563	1.155486
H	2.257261	0.841874	-0.446326
H	4.626599	-1.369380	0.723225
C	-3.596654	-0.809545	-0.839261
H	-3.789267	-1.067624	-1.880767
H	-3.032149	-1.622111	-0.384940
H	-4.535191	-0.651757	-0.307185
N	-2.778000	0.420838	-0.771564
H	-3.239774	1.191114	-1.250399
H	-2.634227	0.729005	0.247725
O	-0.478539	0.028293	-2.139604
C	-0.348677	-1.232329	-2.293340
O	-0.753956	-2.099039	-1.496972
H	-1.835359	0.277728	-1.239779
H	0.165638	-1.563162	-3.214118
C	2.055528	2.712800	-1.379352
H	2.730361	3.194882	-0.672079
H	2.624136	2.400263	-2.255078
H	1.272563	3.411077	-1.678346
N	1.463499	1.521798	-0.742837
H	0.903250	1.764306	0.087327
H	0.823180	1.020170	-1.383149

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