

Supporting Information

Table S1. Most populated clusters close to RBM for acrylamide, acrylic acid in kJ/mol.

Cluster n.	Acrylamide	Cluster n.	Acrylic acid
Cl5 (23%)	-12.8	Cl1 (16%)	-17.8
Cl6 (19%)	-12.5	Cl2 (43%)	-17.6
Cl7 (25%)	-12.1	Cl3 (27%)	-16.8
Cl8 (12%)	-12.0	Cl4 (14%)	-15.8
Cl9 (12%)	-12.0		