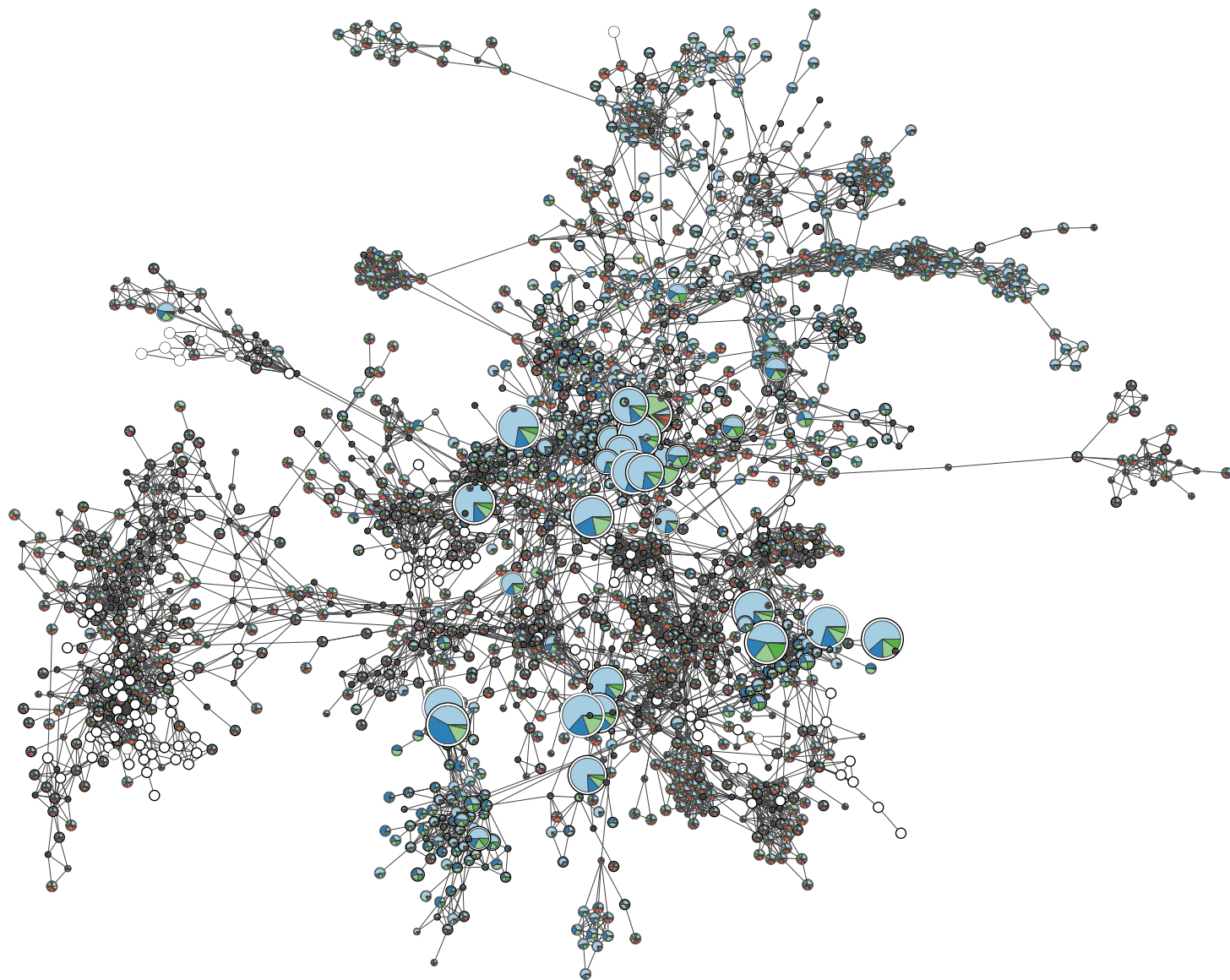# A. CAD and taste-informed molecular network

B. Bitter features annotation

M1

M2

M3

M4

M5

[M2+H]+

[M5+Na]+

[M5-H2O+H]+

[M5+H]+

[M3+DMSO+H]+

[M1+Na]+

[M4-H+2Na]+

[2M5+Mg]2+

[2M5+Ca]2+

[2M1+Ca]2+

[2M1+Mg]2+

[M1+DMSO+H]+

[M5+Na]+

Activity score

Bitter

Mouthfilling

Acid

Fatty