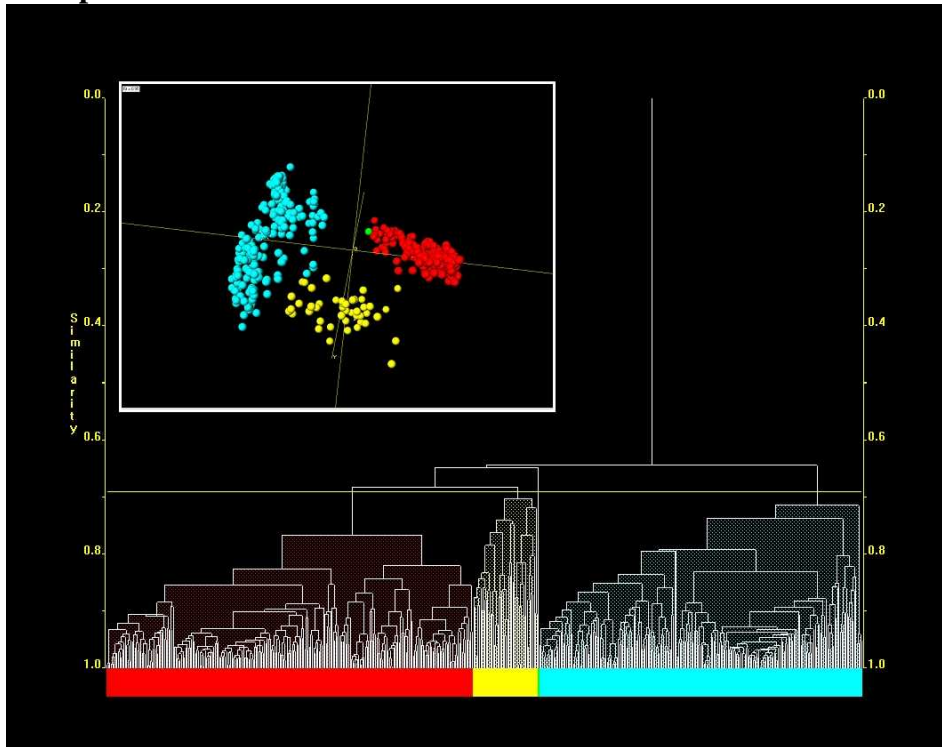


Supplementary Information

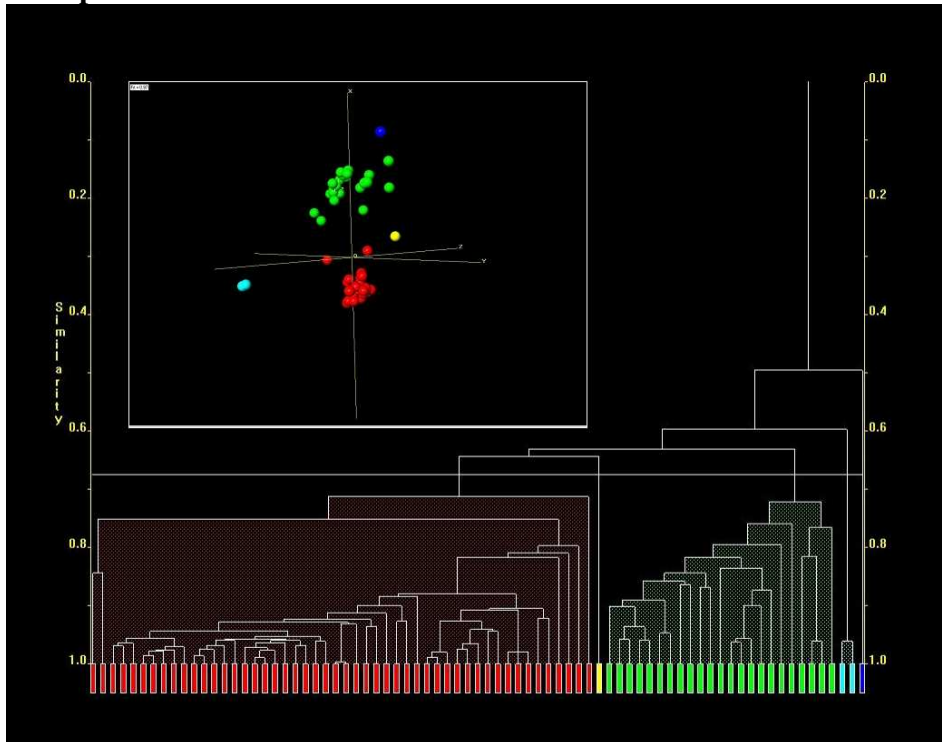
Additional figures

Group A



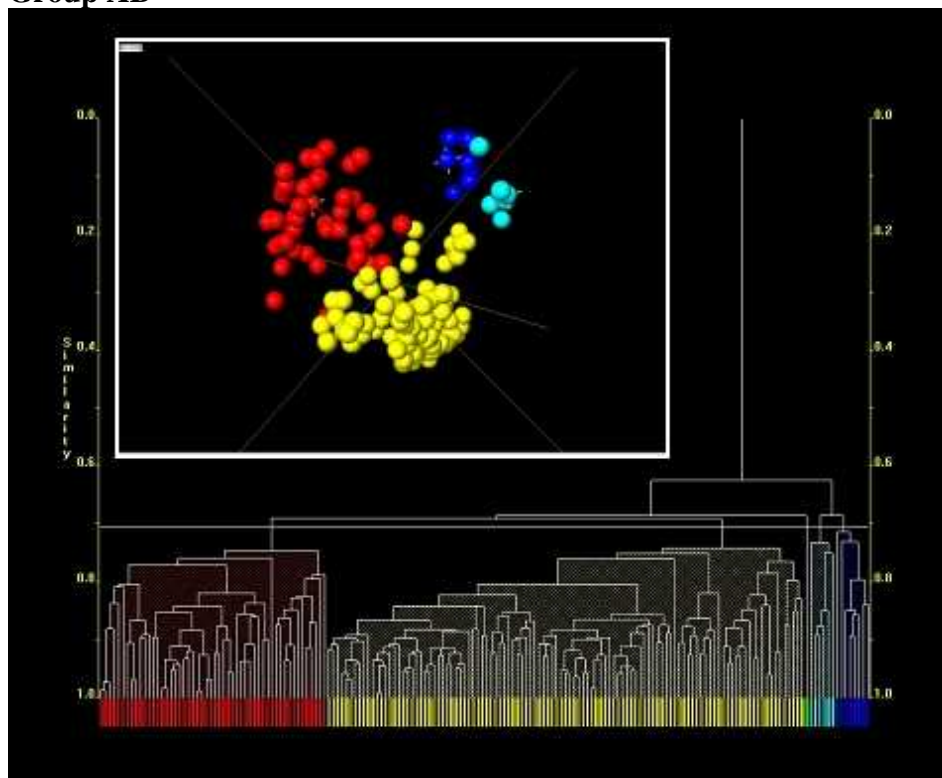
Dendrogram and MMDS plot (inset) for sub-clustering on Group A. The cut-level is 0.748.

Group AA

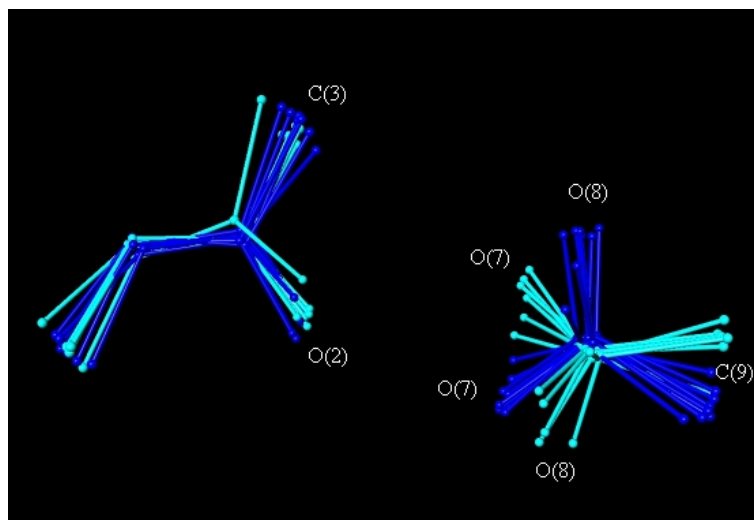


Dendrogram and MMDS plot (inset) for sub-clustering on Group AA. The cut-level is 0.675.

Group AB

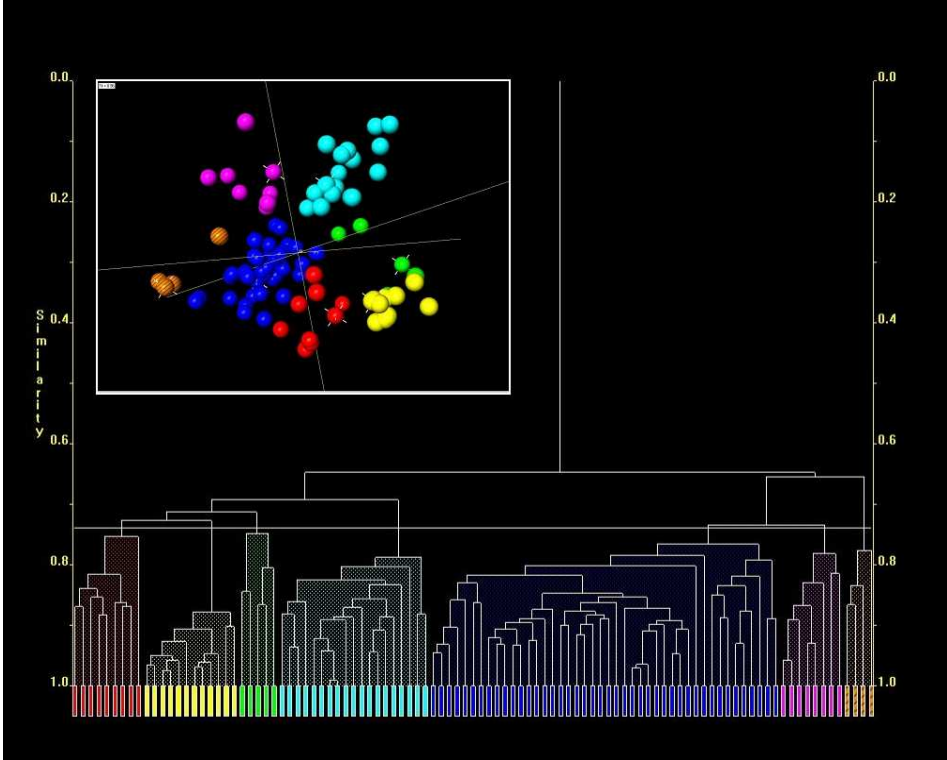


Dendrogram and MMDS plot (inset) for sub-clustering on group AB. The cut-level is 0.706.



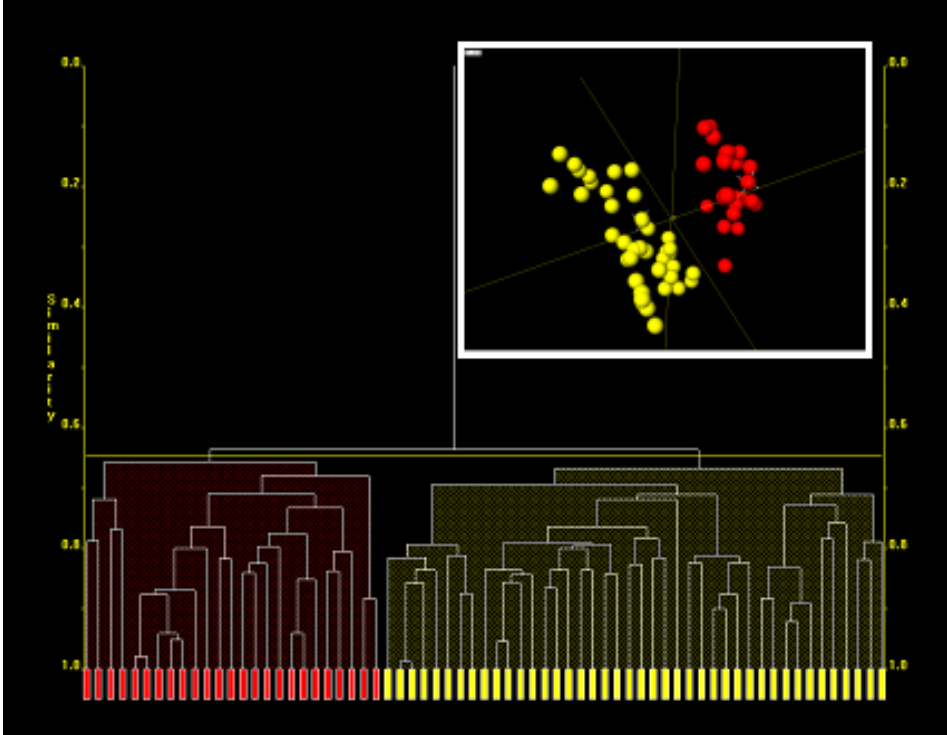
Superposition of all atoms in the fragments in groups ABD (cyan) and ABE (blue), showing almost identical position of the amide in the two groups, but with different relative position of the acid group.

Group AD



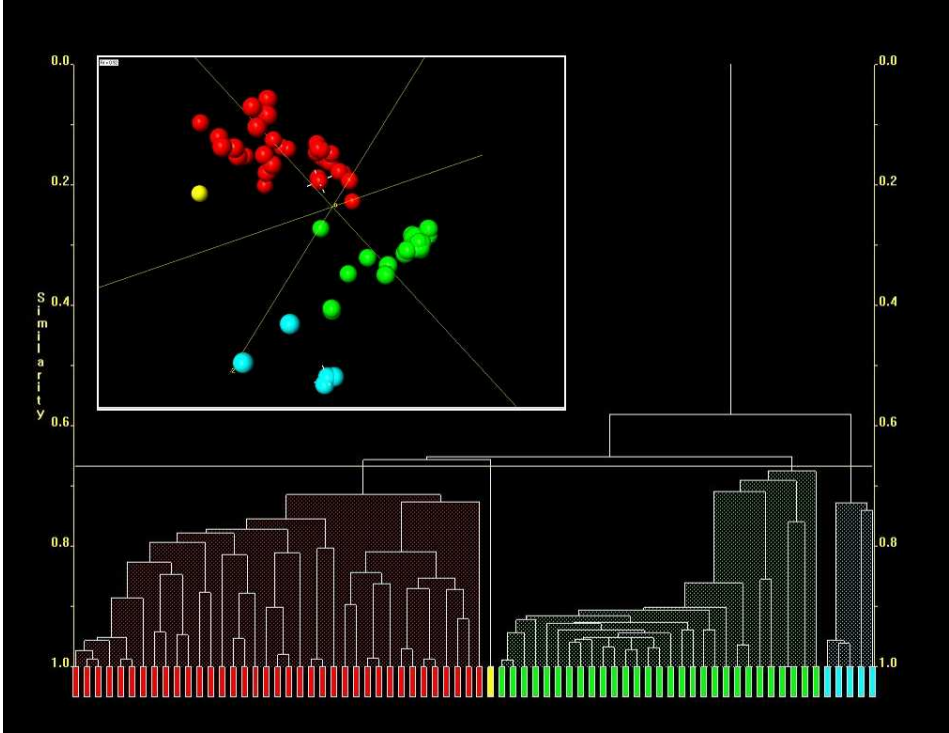
Dendrogram and MMDS plot (inset) for sub-clustering on group AD. The cut-level is 0.740.

Group B



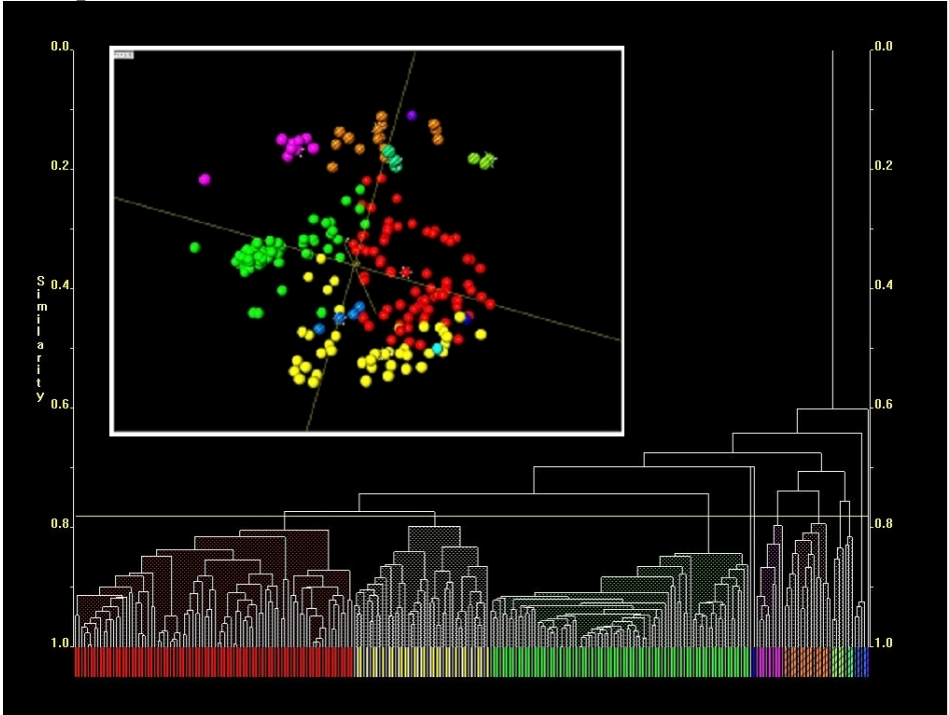
Dendrogram and MMDS plot (inset) for sub-clustering on group B, with a cut-level of 0.647.

Group D

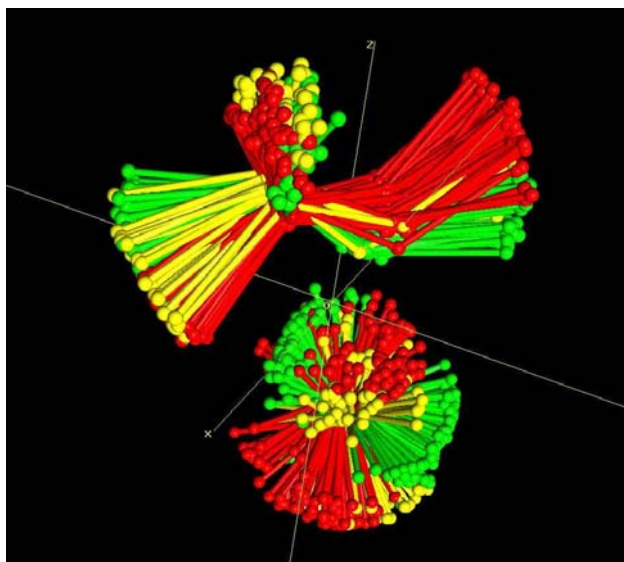
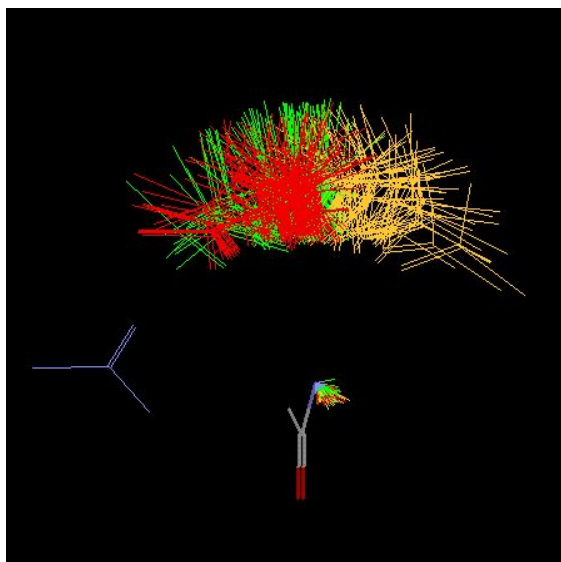


Dendrogram and MMDS plot (inset) for sub-clustering on group D, with a cut-level of 0.667.

Group F



Dendrogram and MMDS plot (inset) for sub-clustering on group D, with a cut-level of 0.782.



Isostar scatterplot for groups FA, FB, FC and FK, with C(1), O(2), C(3) and N(4) positions fixed (left) and an overlay of the fragments of groups FA, FB and FC (right), both coloured by cluster.

List of fragment references (67) where the C(6)=O(7) distance is greater than the C(6)-O(8) distance.

	Group
ACANAC10	A
ACLTRY	A
ALUMIC10_03	A
CUVHOQ_02	A
FIZXAN	A
FUDFUF	A
HIBPDC	A
HOSKUV01	A
JOZZUT	A
KEBVES	A
KEWDIZ	A
MBACNA	A
MULRIU	A
MURTIC	A
NALCYS01	A
NOSPUG_02	A
NOSQAN_03	A
SARVIP	A
SEGXUX	A
XOPZEH_02	A
YINJOU	A
ALUMIC10_02	B
BILRUB10	B
GABBAM	B
HECMAD	B
HIBBOJ	B
JOSWAP01	B
LAWJOI_02	B
SEGXUX_02	B
VUNZIN10	B
LCYLCY10	D
NRURAM20	D
ROFGIC	D
ACDAHO	F
CUVHOQ	F
DOZFED	F
DUKDUI	F
DUKDUI10	F
DUNLON	F
FAPLAK	F
FERMAH11	F
FUDFUF_02	F
GLUTAS_04	F
GUVFIM	F
HECMAD_02	F
HOSKUV01_02	F
JORKUW	F
JOVZEZ	F

KEBVES_02	F
LAWJOI	F
LAWJOI_03	F
LEFGIM	F
PERLUT10	F
QIJPEE	F
QIJPII_02	F
QIJPII_03	F
RELWIO	F
SEKXIP	F
SUKLEP10	F
TOLMAL02	F
TUCMEJ	F
TUCMEJ_02	F
TUCMEJ_03	F
VAPBAP	F
WAGRAY	F
WAGRAY_02	F
XOPZEH_05	F