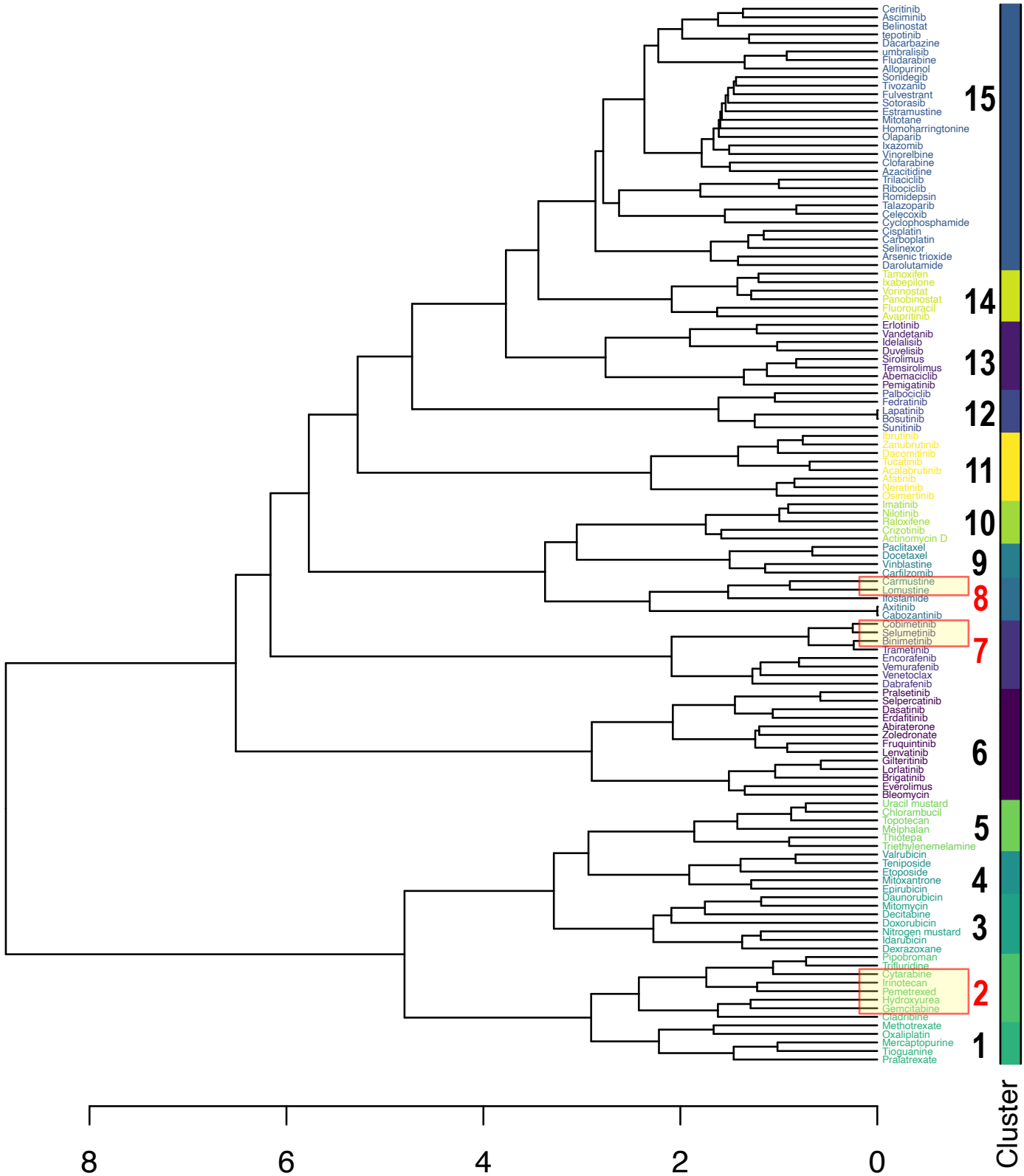
Supplementary Figure S1

Dendrogram: **clustering** based on a **pairwise drug-to-drug distance** (presenting **15 groups**)

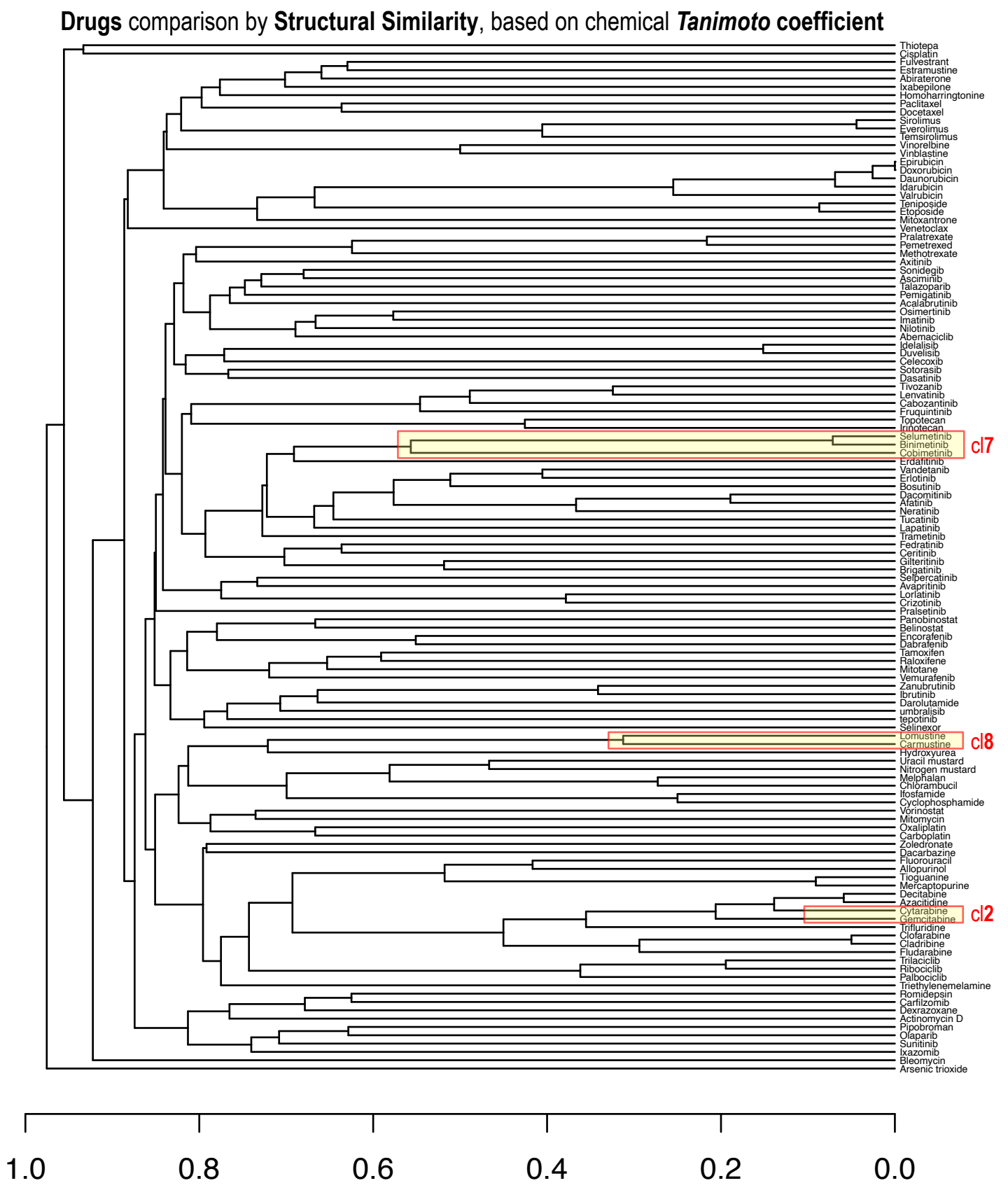


Clustering of **Anticancer Drugs** obtained based on the **distance** derived from the **similarity B-index proposed** (obtained from the **number of common gene targets** that each pair of drugs share). This clustering generates **groups of drugs** with significant **structural similarity**.

Cluster Examples:

Cluster 2	Cluster 7	Cluster 8
Cytarabine	**Binimetinib**	**Carmustine**
Gemcitabine	**Cobimetinib**	**Lomustine**
	Selumetinib	

Supplementary Figure S2

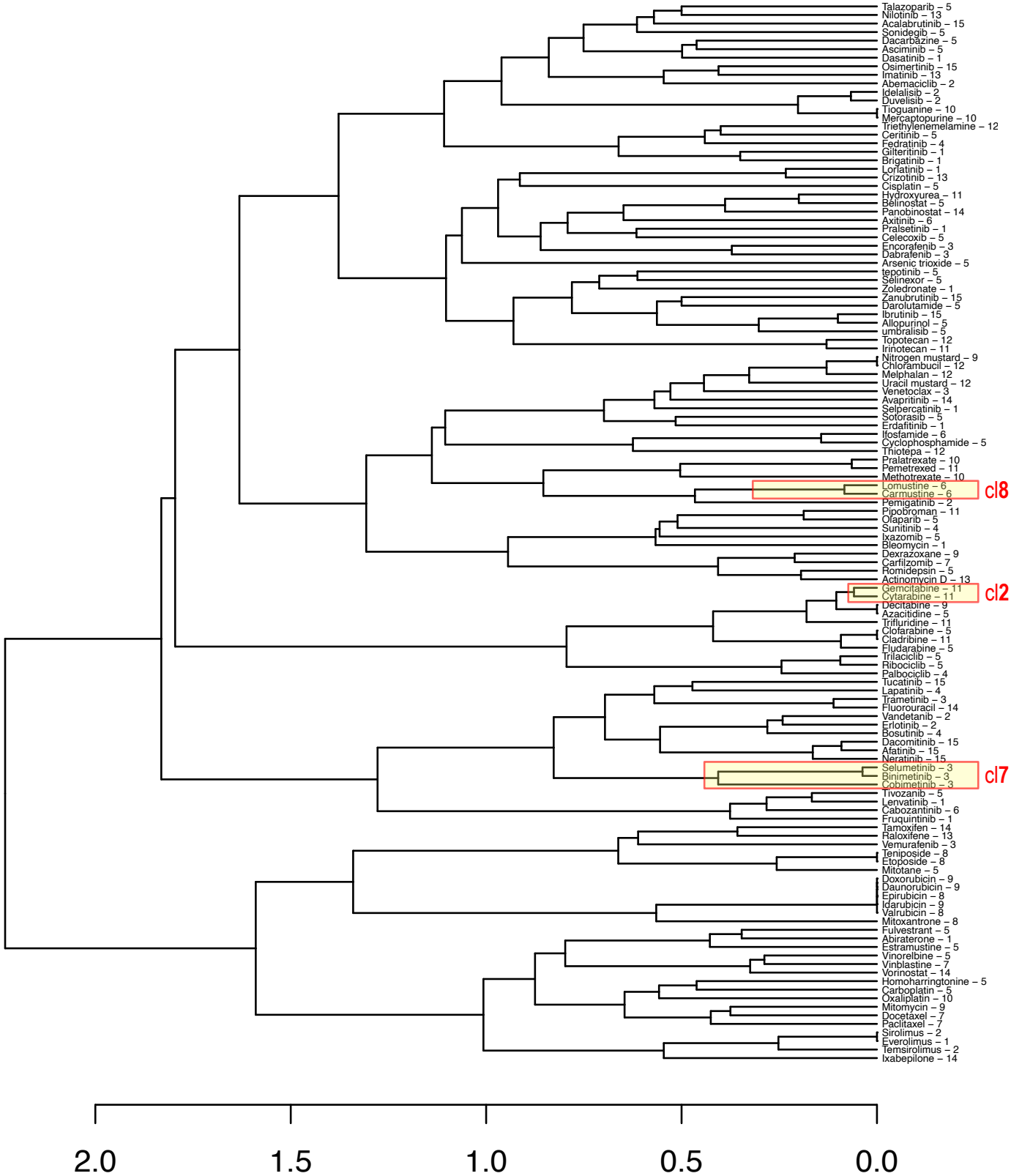


Clustering of **Anticancer Drugs** obtained based on the pairwise **distances** derived from the ***Tanimoto*** coefficient. *Cluster Examples*:

Cluster 2	Cluster 7	Cluster 8
Cytarabine	**Binimetinib**	**Carmustine**
Gemcitabine	**Cobimetinib**	**Lomustine**
	Selumetinib	

Supplementary Figure S3

Drugs comparison by **Structural Similarity**, based on the ***Maximum Common Substructure*** (**MCS**)



Clustering of **Anticancer Drugs** obtained based on the pairwise **distances** derived from the ***structural overlap*** calculated using the ***MSC***. *Cluster Examples*:

Cluster 2	Cluster 7	Cluster 8
Cytarabine	**Binimetinib**	**Carmustine**
Gemcitabine	**Cobimetinib**	**Lomustine**
	Selumetinib	