

Chemical Group Visualization and Analysis with GCxGC

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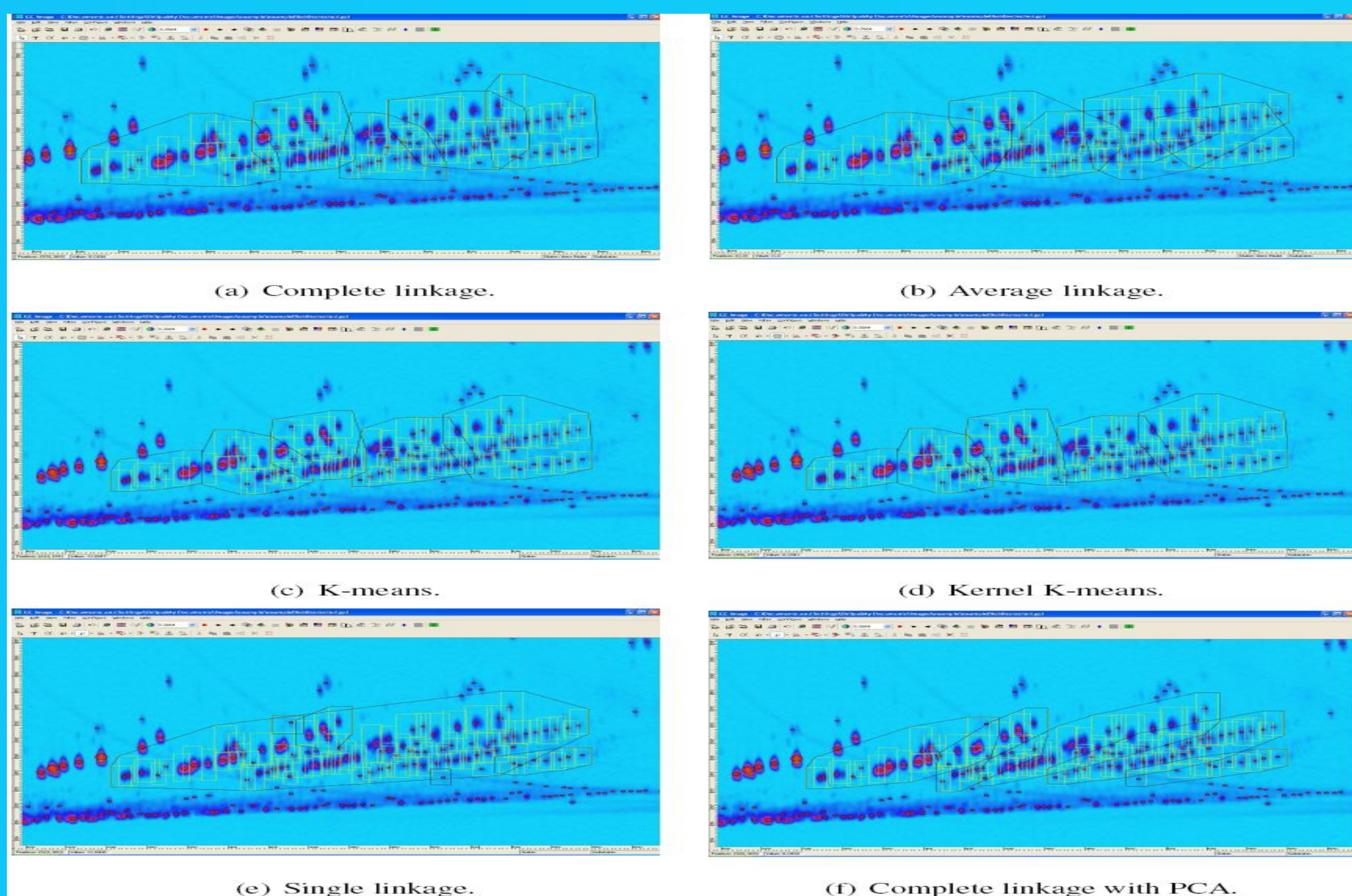
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- Objective: Chemical group analysis
 - GCxGC provides increased separation capacity and multi-dimensional structure-retention relationships
- Three computer-based methods for extracting and visualizing chemical groups
 - Clustering: complete linkage with principal component analysis (PCA)
 - Mass-spectral colorization
 - Group identification with the Computer Language for Identifying Chemicals (CLIC)TM

Clustering

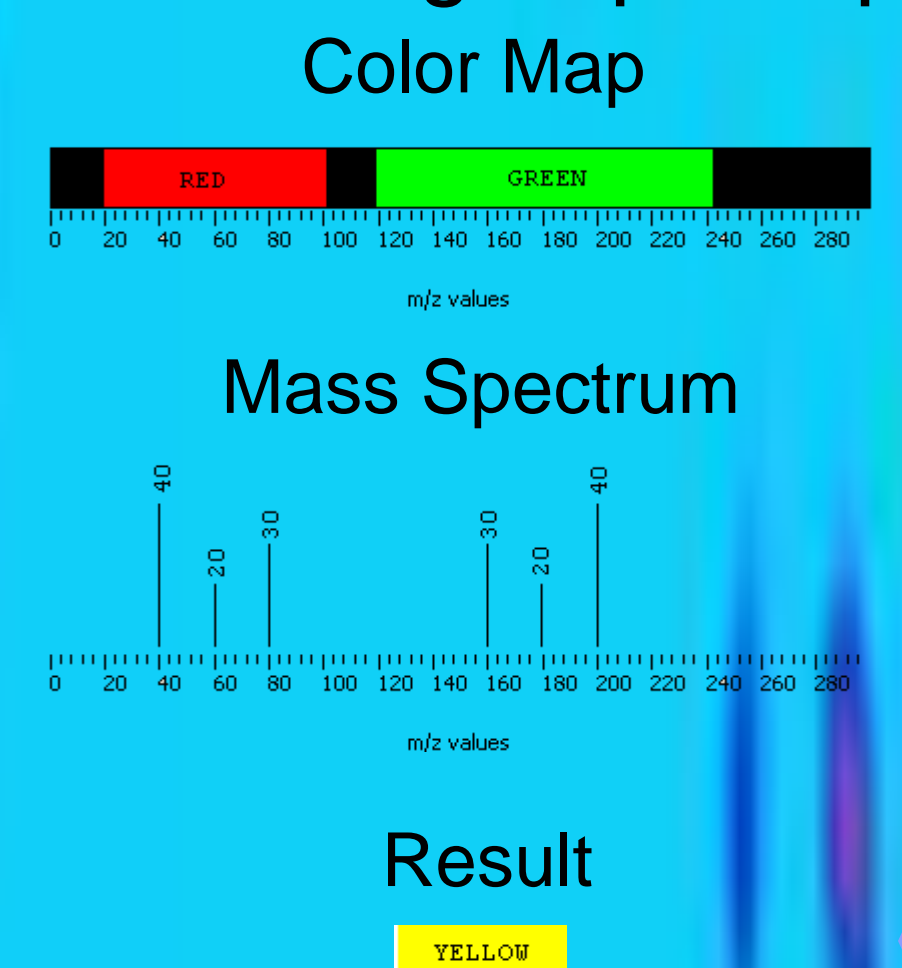
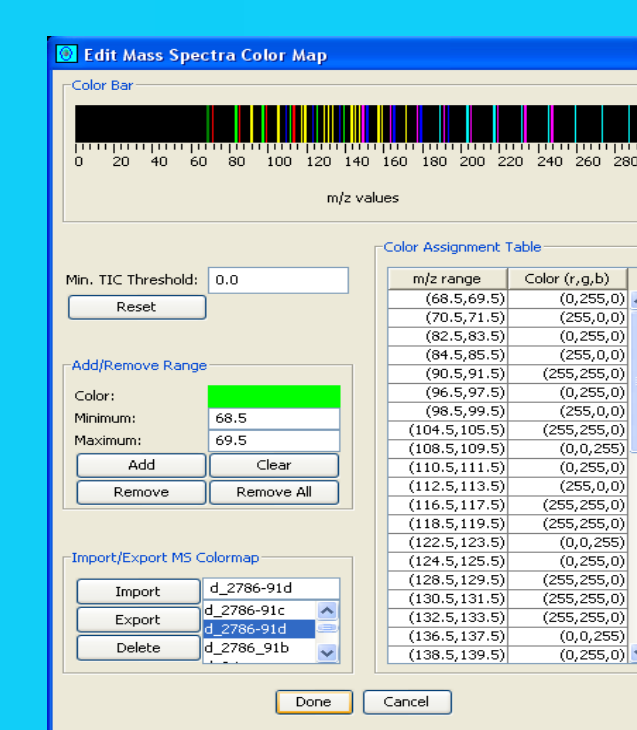
- Groups chemical peaks into "clusters" based on retention times
- Natural clusters of GCxGC data commonly appear as striated bands.
- Complete linkage with PCA is a hierarchical clustering algorithm that uses the "area", calculated by the PCA of two clusters as the proximity measure.
- The algorithm computes the covariance matrix of the peaks in PC space. The area is equal to the square root of the determinant of the covariance matrix
- It tends to find natural clusters in GCxGC data.

Comparison on Clustering Algorithms on GCxGC

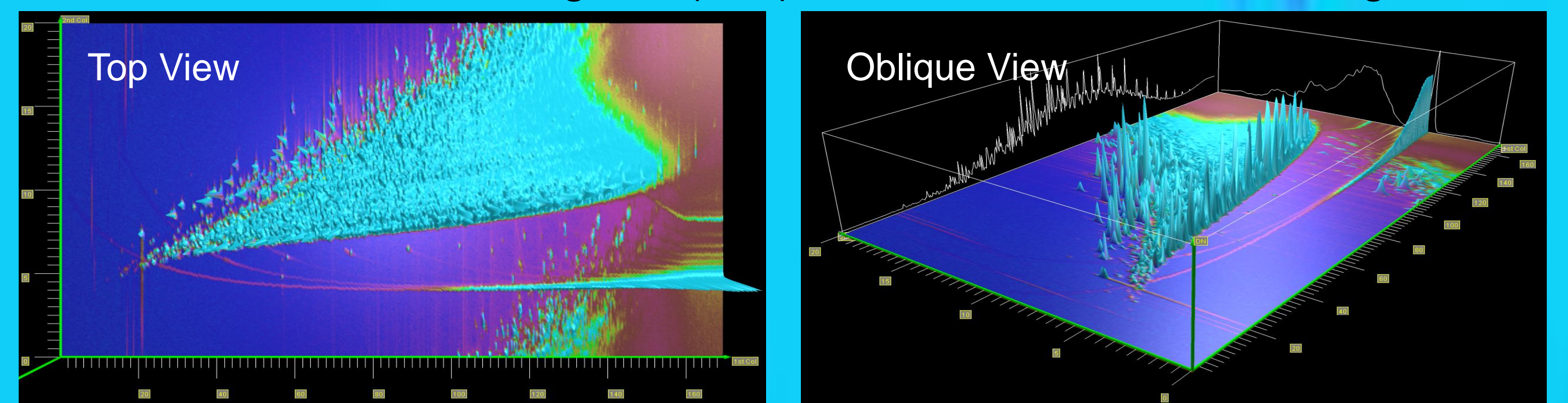


Mass Spectral Colorization

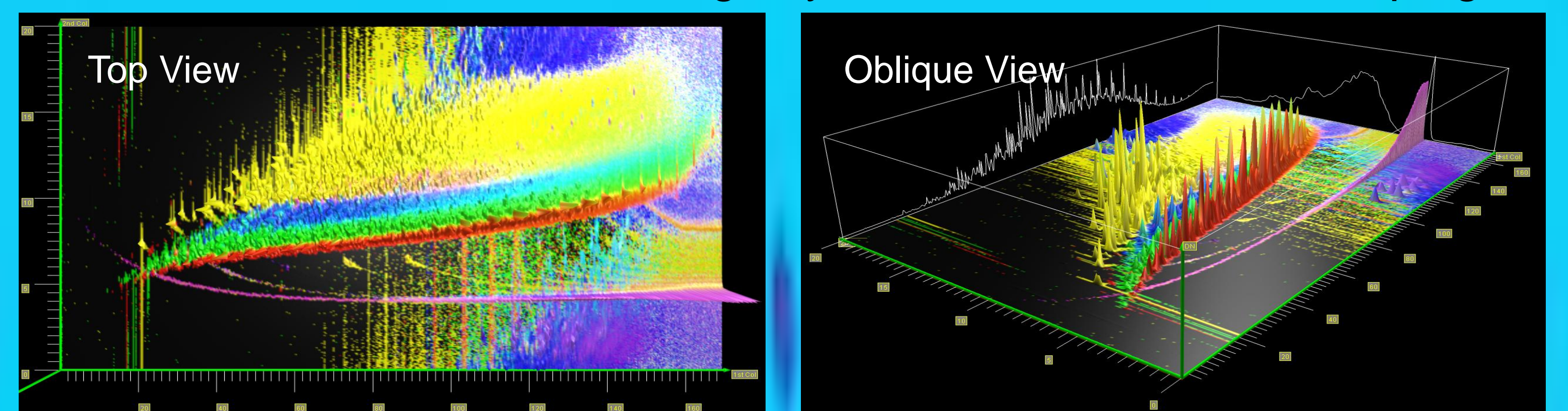
Map various mass spectral components to different "group" colors
Highlight the pixels of the GCxGC image where the group are present



Total Ion Chromatogram (TIC) Colorization of Diesel Image



MS Colorization of Diesel Image by Characteristic Mass Grouping



Characteristic Mass Groupings from ASTM Std D2786-91

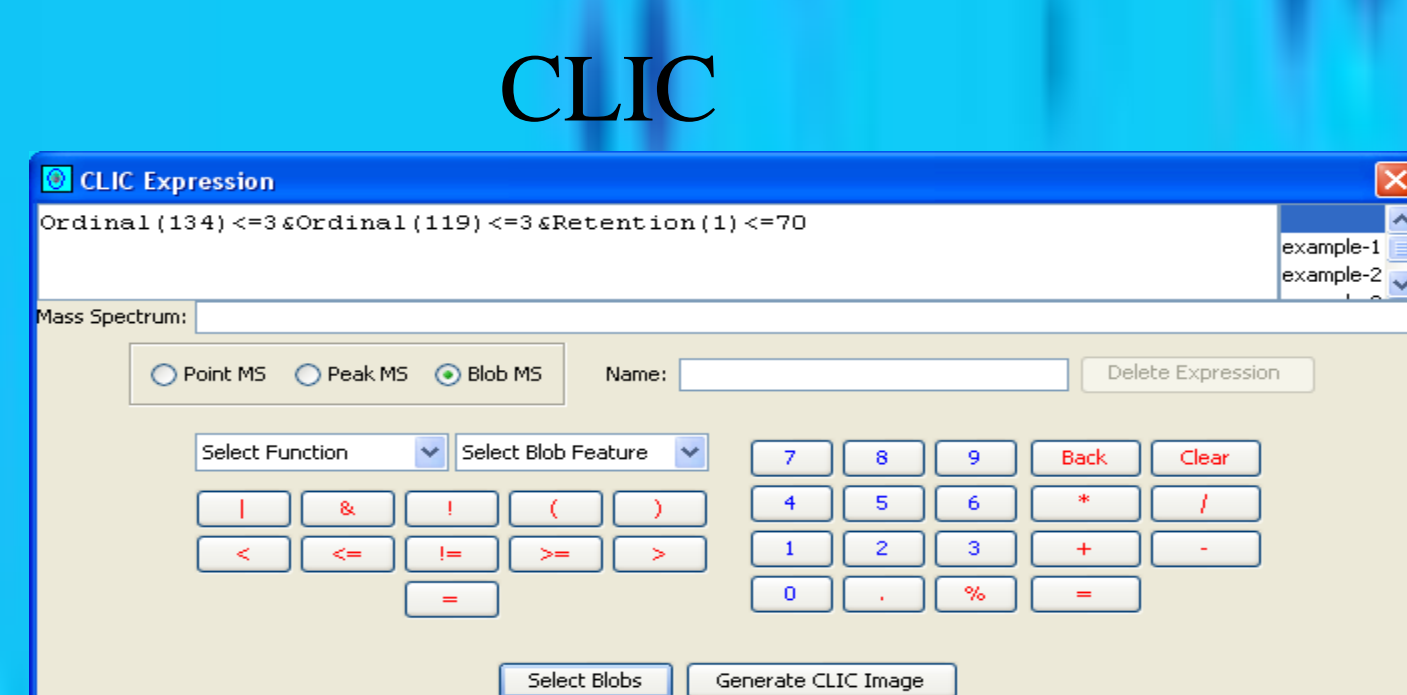
- Alkanes/0-Ring Naphthene (red): 71 + 85 + 99 + 113
- 1-Ring Naphthene (green): 69 + 83 + 97 + 111 + 125 + 139
- 2-Ring Naphthene (blue): 109 + 123 + 137 + 151 + 165 + 179 + 193
- 3-Ring Naphthene (magenta): 149 + 163 + 177 + 191 + 205 + 219 + 233 + 247
- 4-Ring Naphthene (cyan): 189 + 203 + 217 + 231 + 245 + 259 + 273 + 287 + 301
- Monoaromatic (yellow): 91+105+117+119+129+131+133+143+145+147+157+159+171

CLIC

Use CLIC to identify peaks that have the group characteristics: Retention-time constraints and Mass-spectral constraints

Peak Set Table

Colorized Peak Sets



ID	Name	Type	# of Blobs	# of Includ...	Included Volume	Total Volume
0	Ord 130 LE 3	Group	2	2	22,010,023.49	22,010,023.49
1	Ord 120 LE 3 AND Ret 1 LE 50	Group	2	2	105,453,173.18	105,453,173.18
2	Ord 120 LE 3 AND Ret 1 LE 50	Group	11	11	10,000,000.00	10,000,000.00
3	Ord 146 LE 4	Group	15	15	361,728,235.52	361,728,235.52
4	Ord 132 LE 4 AND Ret 1 LE 50	Group	4	4	65,540,725.40	65,540,725.40
5	Ord 148 LE 4 AND Ret 1 LE 50	Group	10	10	140,536,628.15	140,536,628.15
6	Ret 1 LE 100 AND Ret 1 LE 50	Group	5	5	63,007,068.53	63,007,068.53
7	Ord 156 LE 4 LE 2	Group	9	9	168,518,813.28	168,518,813.28
8	Ord 133 LE 4 AND Ret 1 LE 50	Group	11	11	159,922,065.75	159,922,065.75
9	Ord 105 LE 3 OR Ord 119 LE 3 AND Ord 155 LE 5	Group	5	5	92,778,803.78	92,778,803.78
10	Ord 174 LE 3	Group	27	27	624,261,217.13	624,261,217.13
11	Ord 160 LE 3 LE 50	Group	25	25	649,877,747.57	649,877,747.57
12	Ord 158 LE 4 AND Ord 129 OR 130 LE 4	Group	1	0	0.00	5,470,190.90
13	Ord 158 LE 4 AND Ord 129 OR 130 LE 4	Group	3	3	5,273,626.43	5,273,626.43
14	Ret 1 LE 100 AND Ord 172 LE 4 OR Ord 172 LE 4	Group	12	12	241,413,697.26	241,413,697.26
15	Ord 172 LE 4	Group	12	12	220,919,496.48	220,919,496.48
16	Ord 176 LE 4	Group	20	20	331,560,361.65	343,828,675.94
17	Ret 1 LE 100 AND Ret 1 LE 10 AND Ord 189 LE 4	Group	27	27	562,822,302.03	562,822,302.03
18	Ord 220 LE 3	Group	17	17	46,738,292.09	46,738,292.09
19	Ord 194 LE 3	Group	9	9	84,977,795.38	84,977,795.38
20	Ord 196 LE 4 AND Ord 155 LE 5	Group	19	19	88,047,102.98	88,047,102.98
21	Ord 190 LE 4 AND Ord 133 LE 5	Group	6	6	224,628,249.81	224,628,249.81
22	Ret 1 LE 100 AND Ret 1 LE 100 AND Ret 1 LE 25	Group	12	12	473,380,717.38	473,380,717.38
23	Ord 190 LE 4 AND Ord 133 LE 5	Group	6	6	224,628,249.81	224,628,249.81

