

(b)  
Combinations of  $w (=10)$  random molecules sampled from  $q (=3)$  clusters given by Scheffé's matrix

Iterations K times

		$w = \sum w_i = 10$
$(w_1, w_2, w_3)$		
1	(10, 0, 0)	● ● ● ● ● ● ● ● ● ●
2	(9, 1, 0)	● ● ● ● ● ● ● ● ■ ■
3	(8, 2, 0)	● ● ● ● ● ● ● ■ ■ ■
.....	.....	.....
	(2, 5, 3)	● ● ■ ■ ■ ■ ■ ■ ▲ ▲ ▲
.....	.....	.....
N	(0, 0, 10)	▲ ▲ ▲ ▲ ▲ ▲ ▲ ▲ ▲ ▲

Scheffé's matrix

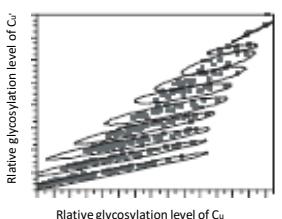
(c) Response matrix

Iterations K times

		C3	C6	C16	C24	C25
		N Average relative glycosylation levels of molecular carbons				
1						
2						
3						
N						

$$\text{Rel.Gly}(C_u) = \frac{\sum_{j=1}^{w_i} \text{Rel.Gly}(C_u)_j}{w}$$

(f) Graphical analysis



(e) Average of K barycenter matrices

		C3	C6	C16	C24	C25
1						
2						
3						
N						

$$\overline{\text{Rel.Gly}(C_u)} = \frac{\sum_{r=1}^K \text{Rel.Gly}(C_u)_r}{K}$$

Final response matrix

