

**EFFECT OF THE SOLVENT ON THE
CONFORMATIONAL PROFILE OF BALARAM'S
PEPTIDE: A COMPUTATIONAL STUDY**

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Supplementary Material

1. Size of the boxes used in the simulations

Chloroform: 40.729 x 45.744 x 50.887 Å

DMSO: 37.359 x 42.333 x 46.669 Å

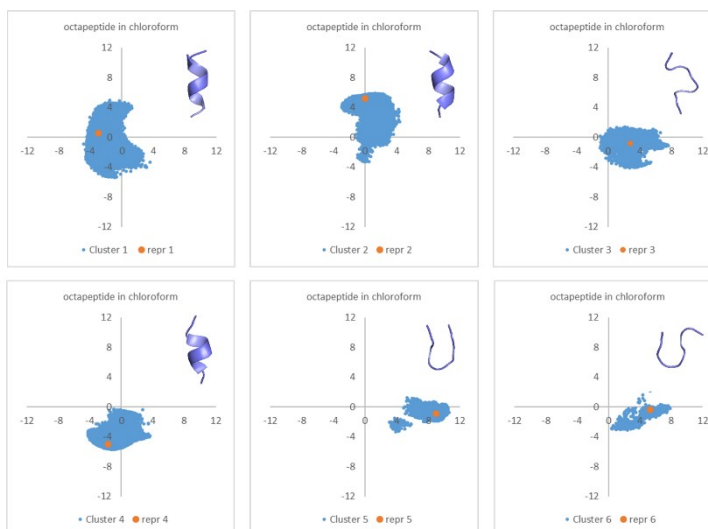
MeOH: 39.952 x 45.493 x 50.567 Å

Water: 42.177 x 47.306 x 52.717 Å

2. Results of the cluster analysis for the different simulations

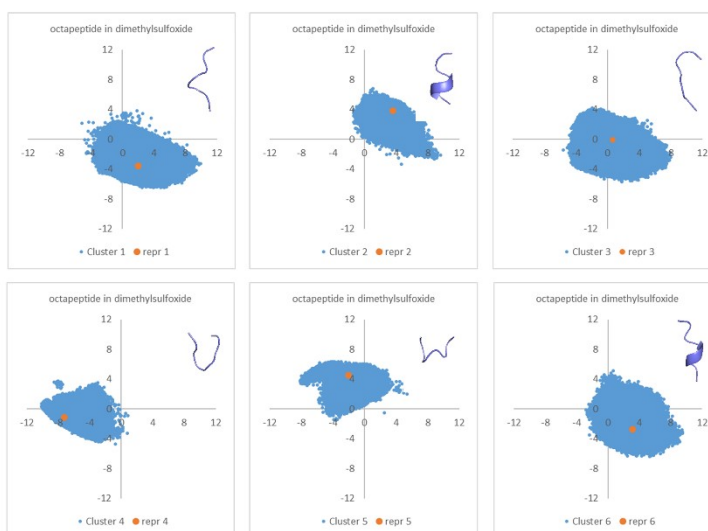
2a. Chloroform

Cluster	Num. of structures	
1	589919	59%
2	158090	15.8%
3	87516	8.8%
4	135324	13.5%
5	28189	2.8%
6	962	0.1%



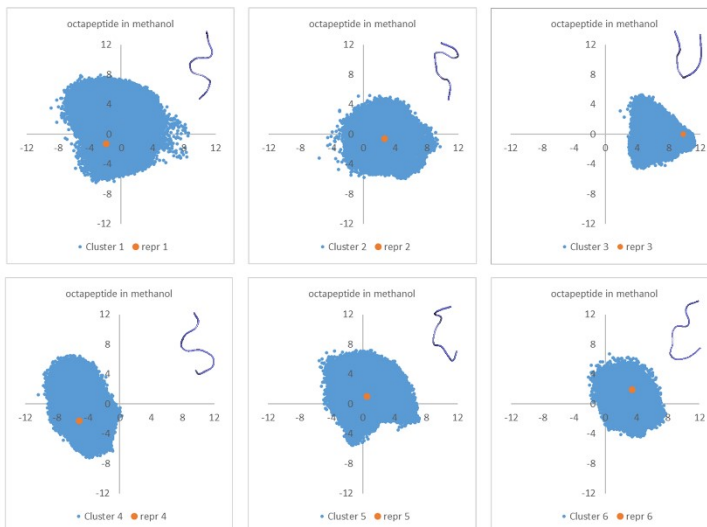
2b. DMSO

Cluster	Num. of structures	
1	263039	26.3%
2	249754	25%
3	173859	17.4%
4	174252	17.4%
5	85486	8.5%
6	53610	5.4%



2c. MeOH

Cluster	Num. of structures	
1	607610	60%
2	113861	11%
3	76084	7.6%
4	130685	13%
5	38023	3.8%
6	33444	3.3%



2d. Water

Cluster	Num. of structures	
1	427034	42.7%
2	203522	20.4%
3	190508	19%
4	122268	12.2%
5	26042	2.6%
6	30626	3.1%

