

Interaction of Collagen with Chlorosulphonated Paraffin Tanning Agents: Fourier Transform Infrared Spectroscopic Analysis and Molecular Dynamics Simulations

Susanna Monti^{1*}, Emilia Bramanti^{1*}, Valentina Della Porta¹, Massimo Onor¹,
Alessandro D'Ulivo¹ and Vincenzo Barone²

¹CNR-Institute of Chemistry of Organometallic Compounds - UOS di Pisa,
Area della Ricerca, via G. Moruzzi 1, I-56124 Pisa, Italy,

²Scuola Normale Superiore,
piazza dei Cavalieri 7, I-56126 Pisa, Italy

E-mail: sapeptides@gmail.com; bramanti@pi.iccom.cnr.it

Collagen Model. The collagen-like microfibril segment (CMS) employed in these studies was the one already studied in previous works. The amino acid content of the CMS is reported below.

ACE	GLY	PRO	MET	GLY	PRO	SER	GLY	PRO	ARG	GLY	LEU	HPR	GLY	PRO	HPR	GLY	ALA	HPR	GLY	PRO	GLN	GLY	PHE	NME
ACE	GLY	PRO	MET	GLY	LEU	MET	GLY	PRO	ARG	GLY	PRO	HPR	GLY	ALA	SER	GLY	ALA	HPR	GLY	PRO	GLN	GLY	PHE	NME
ACE	GLY	PRO	MET	GLY	PRO	SER	GLY	PRO	ARG	GLY	LEU	HPR	GLY	PRO	HPR	GLY	ALA	HPR	GLY	PRO	GLN	GLY	PHE	NME
ACE	GLY	ALA	ARG	GLY	PRO	SER	GLY	PRO	GLN	GLY	PRO	SER	GLY	PRO	HPR	GLY	PRO	LYS	GLY	ASN	SER	GLY	GLU	NME
ACE	GLY	PRO	ARG	GLY	ILE	HPR	GLY	PRO	VAL	GLY	ALA	ALA	GLY	ALA	THR	GLY	ALA	ARG	GLY	LEU	VAL	GLY	GLU	NME
ACE	GLY	ALA	ARG	GLY	PRO	SER	GLY	PRO	GLN	GLY	PRO	SER	GLY	PRO	HPR	GLY	PRO	LYS	GLY	ASN	SER	GLY	GLU	NME
ACE	GLY	LEU	GLN	GLY	PRO	HPR	GLY	PRO	HPR	GLY	SER	HPR	GLY	GLU	GLN	GLY	PRO	SER	GLY	ALA	SER	GLY	PRO	NME
ACE	GLY	LEU	GLN	GLY	LEU	HPR	GLY	LEU	ALA	GLY	HID	HID	GLY	ASP	GLN	GLY	ALA	HPR	GLY	ALA	VAL	GLY	PRO	NME
ACE	GLY	LEU	GLN	GLY	PRO	HPR	GLY	PRO	HPR	GLY	SER	HPR	GLY	GLU	GLN	GLY	PRO	SER	GLY	ALA	SER	GLY	PRO	NME
ACE	GLY	ARG	VAL	GLY	PRO	HPR	GLY	PRO	SER	GLY	ASN	ALA	GLY	PRO	HPR	GLY	PRO	HPR	GLY	PRO	ALA	GLY	LYS	NME
ACE	GLY	ARG	THR	GLY	THR	HPR	GLY	PRO	SER	GLY	ILE	SER	GLY	PRO	HPR	GLY	PRO	HPR	GLY	PRO	ALA	GLY	LYS	NME
ACE	GLY	ARG	VAL	GLY	PRO	HPR	GLY	PRO	SER	GLY	ASN	ALA	GLY	PRO	HPR	GLY	PRO	HPR	GLY	PRO	ALA	GLY	LYS	NME
ACE	GLY	PRO	ALA	GLY	PRO	HPR	GLY	GLU	ALA	GLY	LYS	HPR	GLY	GLU	GLN	GLY	VAL	HPR	GLY	ASP	LEU	GLY	ALA	NME
ACE	GLY	PRO	ALA	GLY	THR	ALA	GLY	GLU	ALA	GLY	LYS	HPR	GLY	GLU	ARG	GLY	ILE	HPR	GLY	GLU	PHE	GLY	LEU	NME
ACE	GLY	PRO	ALA	GLY	PRO	HPR	GLY	GLU	ALA	GLY	LYS	HPR	GLY	GLU	GLN	GLY	VAL	HPR	GLY	ASP	LEU	GLY	ALA	NME

Amino Acid Content of the CMS

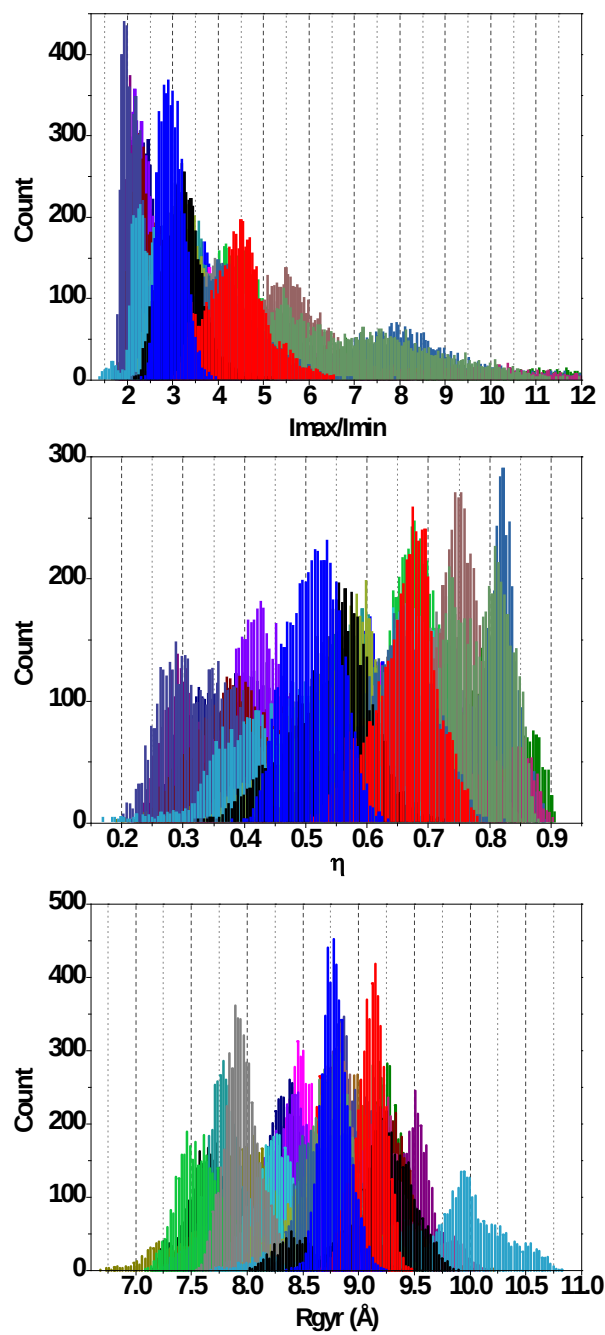


Figure S1. SCP18: Shape and Size descriptors

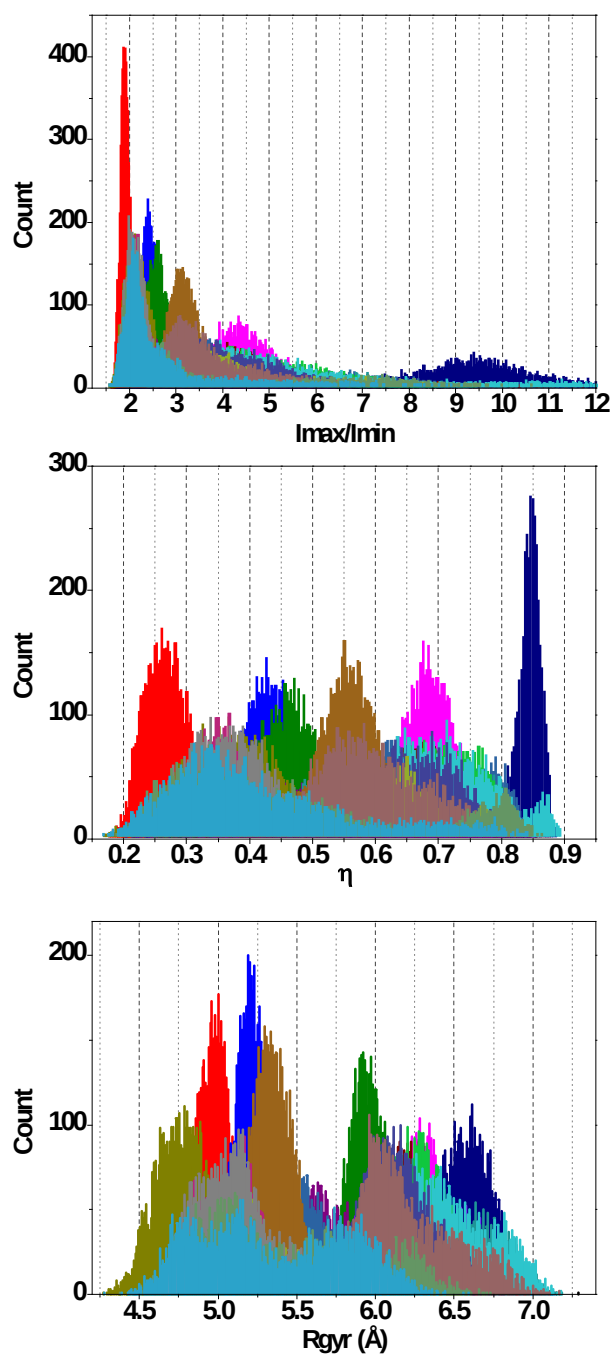


Figure S2. SCP20: Shape and Size descriptors

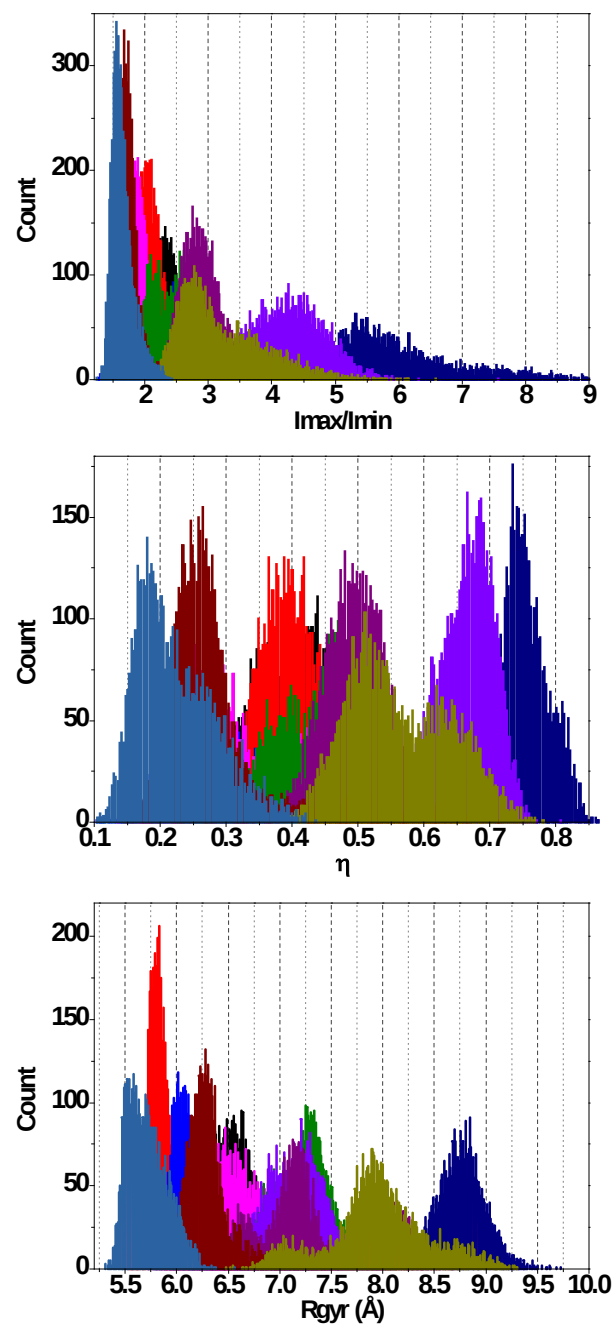


Figure S3. SCP30: Shape and Size descriptors

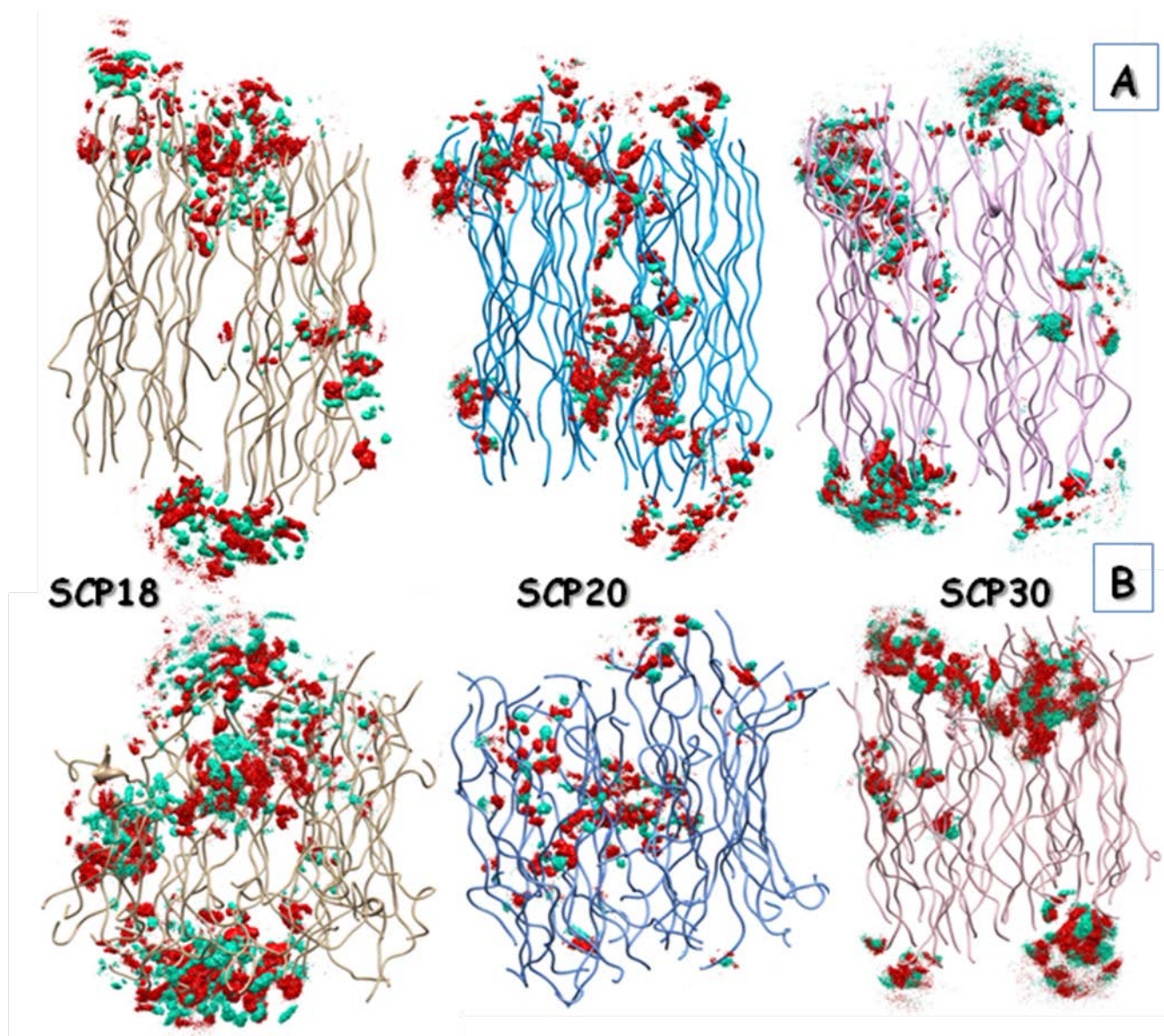


Figure S4. Spatial Distribution Functions of SCP oxygen (red clouds) and chlorine (green clouds) atoms. Bundle average structure are displayed as C α ribbons