Supporting information

Table 3. Visible absorption bands (in nm) of $TPPS_4$ – chitosan complexes **1** and **2** and free porphyrin deposited on glass surface

Complexes		$TPPS_4$		Assignment[6,8,23,68,69]
1	**2**	pH 6.8	pH 2.3	
409		405		B(0,0) – H-aggregate
	426		427	B_x(0,0) – J-aggregate
	493		490	B_y(0,0) – J-aggregate
522		526		Q_y(1,0) – H-aggregate
558		566		Q_y(0,0) – H-aggregate
594		599		Q_x(1,0) – H-aggregate
650		656		Q_x(0,0) – H-aggregate
	704		705	Q(0,0) – J-aggregate

Table 4. IR bands (in cm^{-1}) of the $TPPS_4$ – chitosan complexes and their parent compounds

Complexes		$TPPS_4$[a]		Chitosan	Assignment	Complexes		$TPPS_4$[a]		Chitosan	Assignment
1	**2**	fb	da		8, 43-46	**1**	**2**	fb	da		8, 43-46
416	418	420	410		γ(Por def.)	1124	1122	1128	1127		$\nu_s(SO_3^-)$
456	450	460	456		γ(Por def.)	1176	1170			1156	ν(COC)
				562[b]	γ(COC)	1218		1192	1191		$\nu_{as}(SO_3^-)$
	550		553		γ(Pyr fold)		1226		1230		$\nu(C_mPh)$
578	580	582	581		γ(Pyr fold)					1262	ν(CO), ω(CH)
634	626	640	630		Ph in plan def	1320	1322			1322	δ(CH), amide III
				644[b]	γ(CCC)	1380	1380			1380	$\delta_s(CH_3)$
	662		661		Ph δ(CCC)			1386	1383		$\nu(C_\alpha C_\beta)$
				666	$\omega(NH_2)$	1394	1398	1396	1397		$\nu(C_\alpha C_\beta)$
	704	714	704		Ph in plan def					1422	$\delta(CH_2)$, δ(OH)
740	734	742	741		Ph in plan def	1472		1472	1468		$\nu(C_\beta C_\beta)/\nu(C_\alpha C_m)_s$
802	806	802	804		Pyr def		1488		1487		$\nu(C_\beta C_\beta)$
	824		823		Ph γ(CH)		1526			1520[b]	$\nu_s(NH_3^+)$
856	858	854	857		Ph γ(CH)				1543		$\nu(C_\alpha C_m)_{as}$
902	902			898	$\nu(C_1H)$			1566	1562		Ph ν(CC)
966		968			$\nu(C_\alpha N)/\delta(C_\beta H)$	1552				1550sh	amide II
994	984	992	985		$\delta(C_\beta H)$	1600				1598	$\nu(NH_2)$
	1004		1003		$\nu(C_\alpha N)/\nu(C_\alpha C_\beta)$	1638	1630	1634	1637	1634[b]	$\delta(H_2O)$
1012		1014	1012		$\nu(C_\alpha N)/\nu(C_\alpha C_\beta)$					1660	amide I
1036	1034	1040	1041		Ph δ(CH)				1711		ov., comb.
				1034	ν(CO)(CC)				1738		ov., comb.
1068	1074			1080	ν(CO)(CC)						

[a] fb – free base, da – diacid; [b] chitosan HCl

Table 5. Visible excited Raman (VisR) and FT-Raman (FT) bands (in cm^{-1}) of $TPPS_4$ – chitosan complexes **1** and **2** and pure $TPPS_4$[a]

1		**2**		fb		da		Assignment	**1**		**2**		fb		da		Assignment
VisR	FT	VisR	FT	VisR	FT	VisR	FT	[42, 45-49]	VisR	FT	VisR	FT	VisR	FT	VisR	FT	[42, 45-49]
214	217			212	219			$\nu(C_mPh)$	962		983		961			986	ν(Pyr. breathing)
	265	243	242		265	236	240	γ(Pyr. tilt)	1002	1003	1014	1014	1000	1000	1005	1015	ν(Pyr. breathing)
311	312	316	319	311	309	310	317	$\delta(C_\alpha C_m C_\alpha)$	1051	1036				1044			$\delta(C_\beta H)_{sym}$
361		362	366					γ(Pyr. tilt)	1078	1084	1081	1079	1080	1091	1084	1082	$\delta(C_\beta H)_{sym}$
408	409	416	420	410	414	410	413	$\delta(C_\alpha C_m C_\alpha)$	1130	1125	1120	1125	1133	1132		1125	$\delta(C_\beta H)_{sym}$
456	442	452	453	450	451		455	δ(Pyr. rot.)		1191	1193	1192		1191	1179	1191	$\delta(C_\beta H)_{sym}$
507	502	495	498		500	502		γ(Pyr fold)	1228	1233	1228	1232	1232	1232	1233	1236	$\nu(C_mPh)$
548	554	554	553	541	553	556		γ(Pyr. fold)	1297		1285	1284				1284	Ph δ(CH)
582	599	580	582	582			582	γ(Pyr. fold)	1323	1330	1318		1327	1327			ν(Pyr. half-ring)$_{sym}$
632	637	619	625	640	639	628		Ph in-plan def	1359		1354	1358			1341	1361	δ(Pyr. quarter ring)
		658	651			649	652	Ph in-plan def		1381	1380	1375		1378	1370		ν(Pyr. half-ring)$_{sym}$
	672		670	669	674		671	$\gamma(CH)_{Ph}$	1441	1457	1425		1450	1452			$\nu(C_\alpha C_m)_{sym}$
713		700	700	714	711	700	700	$\gamma(CH)_{Ph}$	1469		1476						$\nu(C_\alpha C_m)_{sym}$
728	733	726	732		738		731	$\gamma(C_\beta H)$	1498	1496		1492		1499		1494	$\nu(C_\beta C_\beta)$
807	810	819	802	805	796	809	804	δ(Pyr. def.)$_{asym}$	1547	1546	1533	1529	1547	1549	1539	1529	$\nu(C_\beta C_\beta)$
843	844	853	850	838	847		846	δ(Pyr. def.)$_{asym}$	1563		1560		1563				$\nu(C_\alpha C_m)_{asym}$
883	886	879	879	880	885	874	878	ν(Pyr. def.)$_{sym}$	1593	1596	1590	1594	1587	1594		1594	$\nu(C{=}C)_{Ph}$
915		926		909		910		ν(Pyr. def.)$_{sym}$							1621		

[a] fb – free base, da - diacid

Table 6. NIR bands (in cm^{-1}) of $TPPS_4$ – chitosan complexes **1** and **2** and their parent compounds

Complexes		$TPPS_4$		Chitosan		Assignment[46, 52]
1	**2**	free base	diacid	free base	salt	
				9565		3 $\nu(NH_2)$
	9006		9002			3 ν(=CH)
	8821		8829			3 ν(=CH)
				8100		2 $\nu(NH_2)$ + $\delta(NH_2)$
		7070				2 ν(CH) + δ(CH)
6831	6862	6831	6838		6791	2 $\nu(H_2O)$
				6707		2 $\nu(NH_2)$
6538				6541		$\nu(NH_2)$ + 2 $\delta(NH_2)$
					6331	
6125	6144	6133	6136			2 ν(=CH)
5994	6001	5986	6001			2 ν(=CH)
5176	5165	5238	5165	5172	5123	$\nu(H_2O)$ + $\delta(H_2O)$
4933				4933		$\nu(NH_2)$ + $\delta(NH_2)$
				4733	4713	
4655	4655	4659	4655			ν(=CH) + ν(C=C)
				4642		ν(CH) + δ(CH)
					4392	ν(CH) + δ(CH)
	4339		4343			ν(CH) + δ(CH)
4285	4281	4285	4281	4285	4328	ν(CH) + δ(CH)
4058	4058	4065	4061			ν(=CH) + ν(C=C)

Table 7. ^{13}C chemical shifts (in ppm) of solid $TPPS_4$ – chitosan complexes **1** and **2** and their parent compounds

Assignments[53, 54]		**1**	**2**	$TPPS_4$, chitosan
Chitosan	C-1	100.5	97.8	104.8; 98.9[a]
	C-2	57.1	56.8	56.7
	C-3	75.0	71.3	75.1; 71.4[a]
	C-4	83sh	82sh	82.5
	C-5	75.0	75.0	75.1
	C-6	60.8	62sh	60.7
	C=O	173.8	173.8	173.5
	CH_3	23.4	23.7	23.2
$TPPS_4$	C_α	150.2	146sh	148.3
	C_β	134.1	132sh	130.9
	C_m	119.0	122sh	113.9
	C-1′	143.3	142.9	142.1
	C-2′, C-3′	124.6	126.9	124.4
	C-4′	143.3	138.3	138.8

[a] chitosan HCl