

**Table S1.** Dendrogram raw input data. Encapsulation efficiencies (EE) are formatted as fractions.

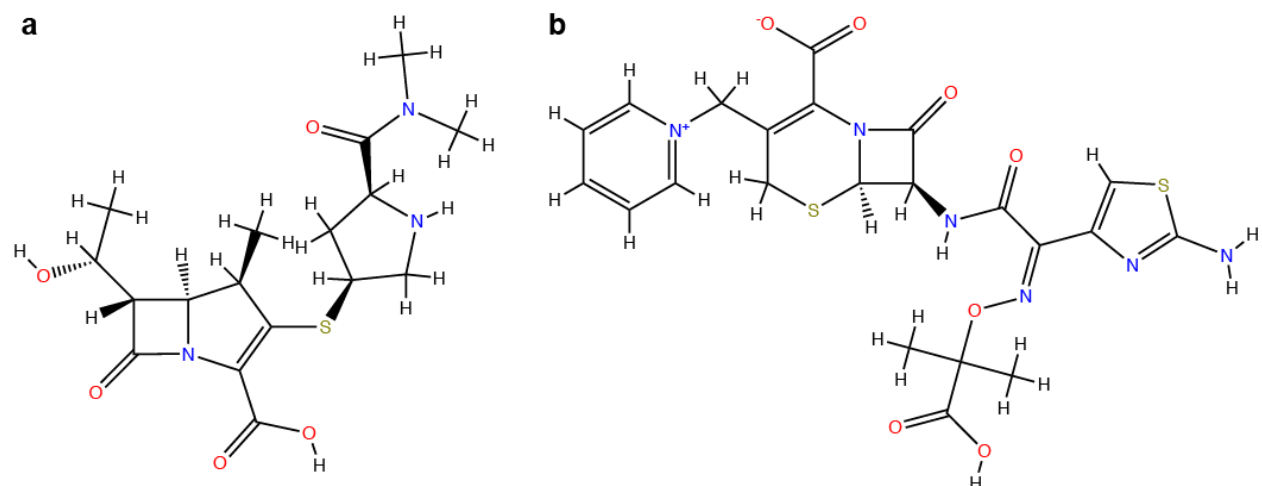
Formulation	FR (2h)	FR (24h)	d2-d7 slope	EE	zeta potential	diameter	PDI	DOP	Mn	Tm (Drug)	water solubility
20:80 CPH-SA 5% DOX	0.878	0.921	3.11275E-05	0.649	-24.2	295.0	0.11606438	29.34	15385	201	630
20:80 CPH-SA 10% DOX	0.878	0.928	0.000682253	0.451	-19.9	290.2	0.0944491	29.34	15385	201	630
20:80 CPTEG-CPH 5% DOX	0.810	0.816	0	0.663	16.1	187.0	0.13094153	16.69	5902	201	630
20:80 CPTEG-CPH 10% DOX	0.861	0.871	0.000267517	0.519	10.8	198.0	0.09410895	16.69	5902	201	630
20:80 CPH-SA 5% DOX	0.821	0.882	0.001030157	0.493	-24.2	295.0	0.11606438	29.34	15385	201	630
20:80 CPH-SA 10% DOX	0.870	0.926	0.000255865	0.349	-19.9	290.2	0.0944491	29.34	15385	201	630
20:80 CPTEG-CPH 5% DOX	0.752	0.778	0.000964581	0.589	-14	188.8	0.11068015	16.69	5902	201	630
20:80 CPTEG-CPH 10% DOX	0.798	0.827	0.000407385	0.415	10.8	198.0	0.09410895	16.69	5902	201	630
20:80 CPH-SA 5% RIF	0.355	0.669	0.019842283	0.267	-21.2	326.8	0.12999352	29.34	15385	183	1400
20:80 CPTEG-CPH 5% RIF	0.622	0.762	0.014603834	0.613	-32.4	183.3	0.1262826	16.69	5902	183	1400
20:80 CPH-SA 5% RIF	0.315	0.721	0.019558135	0.385	-21.2	326.8	0.12999352	29.34	15385	183	1400
20:80 CPTEG-CPH 5% RIF	0.665	0.855	0.005726169	1.127	-13.9	164.8	0.10765556	16.69	5902	183	1400
20:80 CPH-SA 20% CAM	0.866	0.907	0.002788729	0.654	-28.8	330.1	0.09645677	29.34	15385	171	2500
20:80 CPTEG-CPH 20% CAM	0.766	0.782	0.000547523	1.235	-36.5	177.3	0.10820173	16.69	5902	171	2500
20:80 CPTEG-CPH 20% CAM	0.821	0.838	0.000423089	1.117	-36.5	177.3	0.10820173	16.69	5902	171	2500
20:80 CPH-SA 20% CAM	0.886	0.927	0.001916802	0.598	-28.8	330.1	0.09645677	29.34	15385	171	2500
20:80 CPH-SA 5% PZA	0.171	0.276	0.021718991	0.493	-21.5	282.3	0.11965848	29.34	15385	192	1.50E+04
20:80 CPTEG-CPH 5% PZA	0.057	0.086	0.008793703	0.897	-24.1	216.3	0.10769206	16.69	5902	192	1.50E+04
20:80 CPH-SA 5% PZA	0.298	0.449	0.021676638	0.349	-32.8	317.7	0.09466064	29.34	15385	192	1.50E+04
20:80 CPTEG-CPH 5% PZA	0.268	0.313	0.006047673	1.169	-35.1	181.5	0.12303395	18.47	6499	192	1.50E+04
20:80 CPH-SA 10% DOX	0.843	0.856	0.01784599	0.410	-16.4	300.1	0.14238195	66.18	14715	201	630
20:80 CPH-SA 9% DOX	0.876	0.885	0.014484272	0.516	-10.4	302.3	0.15598785	66.18	14715	201	630
20:80 CPH-SA 8% DOX	0.785	0.822	0.017440928	0.656	-7.46	329.0	0.13393998	66.18	14715	201	630
20:80 CPH-SA 7% DOX	0.823	0.860	0.01375275	0.686	-19.3	352.0	0.1488103	66.18	14715	201	630
20:80 CPH-SA 6% DOX	0.829	0.855	0.015909071	0.768	-14.7	343.2	0.14415255	66.18	14715	201	630
20:80 CPH-SA 5% DOX	0.865	0.882	0.014097678	0.895	-20.1	346.3	0.14633586	66.18	14715	201	630
20:80 CPH-SA 4% DOX	0.763	0.795	0.022073666	0.876	-13.6	337.2	0.15620233	66.18	14715	201	630
20:80 CPH-SA 3% DOX	0.785	0.807	0.021288819	1.074	-17	344.8	0.14393289	66.18	14715	201	630
20:80 CPH-SA 2% DOX	0.764	0.792	0.022058247	1.305	-18.9	342.4	0.14448117	66.18	14715	201	630
20:80 CPH-SA 1% DOX	0.675	0.702	0.029634541	1.590	-7.96	324.5	0.14340887	66.18	14715	201	630
20:80 CPTEG-CPH 10% DOX	0.799	0.905	0.000223847	0.574	-8.24	188.8	0.08952265	17.71	6230	201	630
20:80 CPTEG-CPH 9% DOX	0.836	0.900	0	0.647	-2.23	175.3	0.11657572	17.71	6230	201	630
20:80 CPTEG-CPH 8% DOX	0.823	0.878	0.000418826	0.488	-6.01	163.3	0.10179907	17.71	6230	201	630
20:80 CPTEG-CPH 7% DOX	0.760	0.833	0.001562307	0.642	-6.12	165.0	0.10244058	17.71	6230	201	630
20:80 CPTEG-CPH 6% DOX	0.656	0.731	0.001318373	0.714	-3.44	177.3	0.09540602	17.71	6230	201	630
20:80 CPTEG-CPH 5% DOX	0.736	0.794	0.000230922	0.583	-5.95	167.3	0.09709577	17.71	6230	201	630
20:80 CPTEG-CPH 4% DOX	0.709	0.777	0.000136467	0.636	-7.1	163.3	0.08765737	17.71	6230	201	630
20:80 CPTEG-CPH 3% DOX	0.546	0.646	0	0.524	-6.21	157.5	0.0797639	17.71	6230	201	630
20:80 CPTEG-CPH 2% DOX	0.422	0.558	0.001648516	0.463	-13.6	157.5	0.08989265	17.71	6230	201	630
20:80 CPTEG-CPH 1% DOX	0.329	0.462	0.000816278	0.716	-6.24	171.3	0.10018658	17.71	6230	201	630
20:80 CPH-SA 10% RIF	0.410	0.574	0.048640198	0.196	-17.3	298.3	0.12142294	66.18	14715	183	1400
20:80 CPH-SA 9% RIF	0.417	0.620	0.039920326	0.207	-17.4	329.0	0.15660778	66.18	14715	183	1400
20:80 CPH-SA 8% RIF	0.327	0.420	0.067948568	0.176	-23.3	351.9	0.1414808	66.18	14715	183	1400
20:80 CPH-SA 7% RIF	0.412	0.616	0.039087381	0.255	-16.9	352.6	0.15262713	66.18	14715	183	1400
20:80 CPH-SA 6% RIF	0.332	0.418	0.068454099	0.207	-18.1	345.2	0.12222125	66.18	14715	183	1400
20:80 CPH-SA 5% RIF	0.345	0.446	0.066219621	0.230	-24.3	350.0	0.13065327	66.18	14715	183	1400
20:80 CPH-SA 4% RIF	0.274	0.347	0.062373003	0.245	-17.3	359.5	0.13344125	66.18	14715	183	1400
20:80 CPH-SA 3% RIF	0.240	0.335	0.069931327	0.298	-20.6	366.7	0.12454902	66.18	14715	183	1400
20:80 CPH-SA 2% RIF	0.186	0.255	0.05983363	0.305	-24.4	317.3	0.13607798	66.18	14715	183	1400
20:80 CPH-SA 1% RIF	0.106	0.168	0.062846415	0.493	-23.1	338.3	0.15404764	66.18	14715	183	1400
20:80 CPTEG-CPH 10% RIF	0.556	0.709	0.011641771	1.017	-15.3	171.8	0.0920574	17.71	6230	183	1400
20:80 CPTEG-CPH 9% RIF	0.520	0.670	0.013749282	0.883	-19.5	173.9	0.09072136	17.71	6230	183	1400
20:80 CPTEG-CPH 8% RIF	0.585	0.721	0.017676351	1.161	-9.86	161.8	0.08304844	17.71	6230	183	1400
20:80 CPTEG-CPH 7% RIF	0.442	0.665	0.018013083	0.946	-24.5	168.5	0.11797225	17.71	6230	183	1400
20:80 CPTEG-CPH 6% RIF	0.427	0.621	0.021899935	1.155	-37.1	164.5	0.08225642	17.71	6230	183	1400
20:80 CPTEG-CPH 5% RIF	0.394	0.650	0.023027263	1.268	-21.8	168.0	0.08104582	17.71	6230	183	1400
20:80 CPTEG-CPH 4% RIF	0.580	0.704	0.011808479	1.175	-23.3	172.0	0.10299328	17.11	6052	183	1400
20:80 CPTEG-CPH 3% RIF	0.454	0.755	0.01425443	1.787	-25.8	169.5	0.09688981	17.71	6230	183	1400
20:80 CPTEG-CPH 2% RIF	0.420	0.769	0.014252747	2.503	-22.1	165.8	0.09975738	17.71	6230	183	1400
20:80 CPTEG-CPH 1% RIF	0.260	0.733	0.003109203	1.837	-27.3	174.5	0.09653278	17.71	6230	183	1400
10:90 CPTEG-CPH 10% RIF	0.533	0.734	0.02296554	0.991	-7.27	175.5	0.12154016	19.7	6894	183	1400
20:80 CPTEG-CPH 10% RIF	0.630	0.760	0.017949702	1.108	-1.56	162.8	0.10197021	17.67	6225	183	1400
30:70 CPTEG-CPH 10% RIF	0.715	0.819	0.006303884	0.940	-7.59	172.0	0.10670578	20.97	7412	183	1400
50:50 CPTEG-CPH 10% RIF	0.818	0.872	0.00086837	0.867	-13.1	160.3	0.08394513	16.89	6099	183	1400
10:90 CPTEG-CPH 10% RIF	0.547	0.733	0.014208586	1.177	-13.1	178.8	0.09274206	19.7	6894	183	1400
20:80 CPTEG-CPH 10% RIF	0.616	0.744	0.00785114	1.196	-15.5	175.3	0.09939584	17.67	6225	183	1400
30:70 CPTEG-CPH 10% RIF	0.698	0.809	0.005925504	1.222	-9.16	181.3	0.12844245	20.97	7412	183	1400
50:50 CPTEG-CPH 10% RIF	0.785	0.857	0.001769323	1.058	-18.2	177.0	0.09931877	16.89	6099	183	1400

**Table S2.** Dendrogram processed input data. The data were normalized and mean-centered.

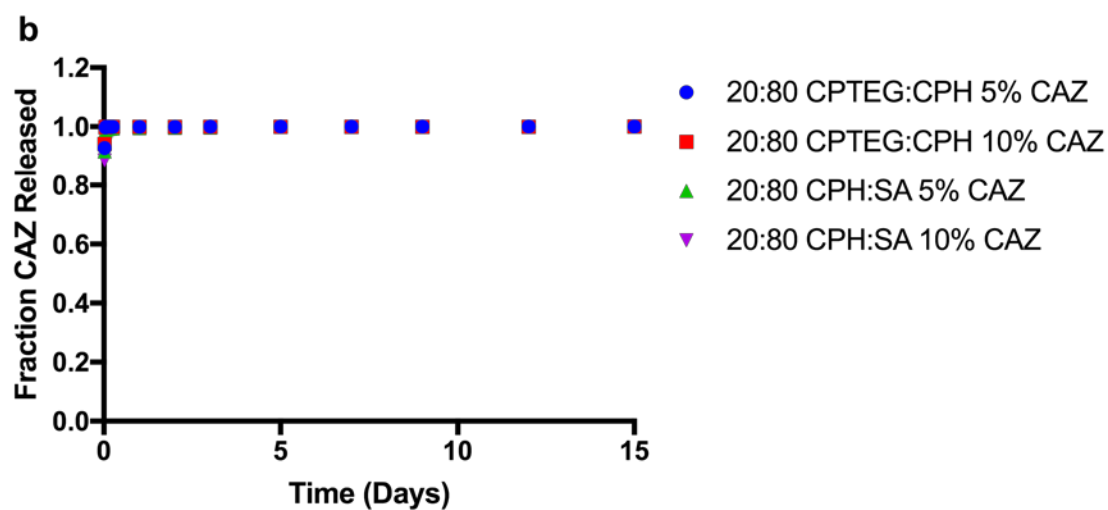
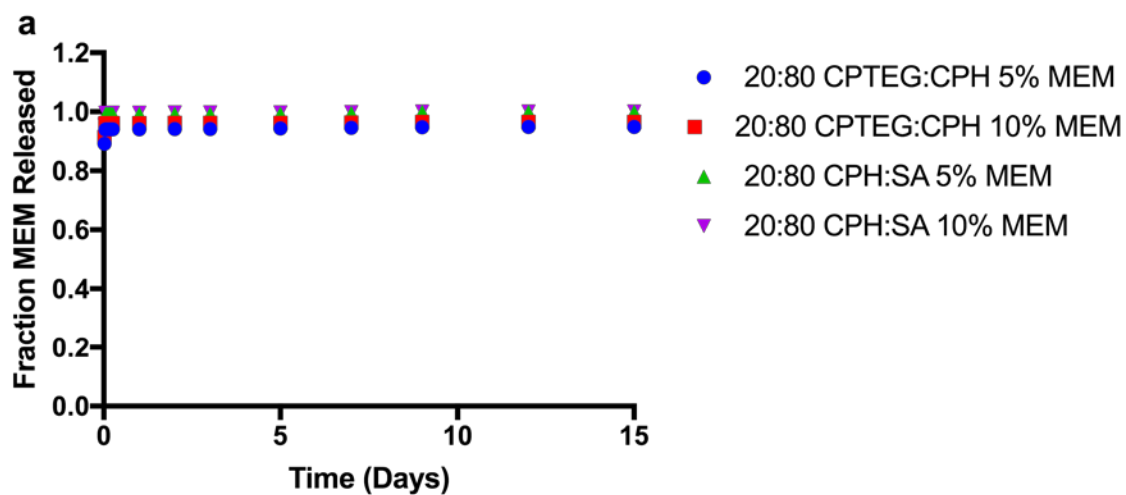
Formulation	FR (2h)	FR (24h)	d2-d7 slope	EE	zeta potential	diameter	PDI	DOP	Mn	Tm (Drug)	water solubility
20:80 CPH-SA 5% DOX	1.049	0.957	-0.77245373	-0.269	-0.695637879	0.8	0.11000297	-0.12	1.329	1.167277	-0.241625119
20:80 CPH-SA 10% DOX	1.049	0.990	-0.73878824	-0.731	-0.27866345	0.7	-0.9161651	-0.12	1.329	1.167277	-0.241625119
20:80 CPTEG:CPH 5% DOX	0.771	0.464	-0.77406313	-0.236	3.212285262	-0.6	0.81628394	-0.73	-0.87	1.167277	-0.241625119
20:80 CPTEG:CPH 10% DOX	0.978	0.722	-0.76023157	-0.572	2.698340035	-0.5	-0.9323134	-0.73	-0.87	1.167277	-0.241625119
20:80 CPH-SA 5% DOX	0.818	0.773	-0.7208004	-0.631	-0.695637879	0.8	0.11000297	-0.12	1.329	1.167277	-0.241625119
20:80 CPH-SA 10% DOX	1.017	0.982	-0.76083402	-0.967	-0.27866345	0.7	-0.9161651	-0.12	1.329	1.167277	-0.241625119
20:80 CPTEG:CPH 5% DOX	0.537	0.285	-0.7241909	-0.408	2.93464256	-0.6	-0.145609	-0.73	-0.87	1.167277	-0.241625119
20:80 CPTEG:CPH 10% DOX	0.725	0.516	-0.75299988	-0.815	2.698340035	-0.5	-0.9323134	-0.73	-0.87	1.167277	-0.241625119
20:80 CPH-SA 5% RIF	-1.074	-0.231	0.251852237	-1.159	-0.404725487	1.2	0.77127795	-0.12	1.329	-0.66354	-0.207450955
20:80 CPTEG:CPH 5% RIF	0.009	0.208	-0.01899388	-0.353	-1.490798419	-0.7	0.59510478	-0.73	-0.87	-0.66354	-0.207450955
20:80 CPH-SA 5% RIF	-1.239	0.014	0.237160814	-0.884	-0.404725487	1.2	0.77127795	-0.12	1.329	-0.66354	-0.207450955
20:80 CPTEG:CPH 5% RIF	0.182	0.647	-0.47800015	0.846	0.303161336	-0.9	-0.289199	-0.73	-0.87	-0.66354	-0.207450955
20:80 CPH-SA 20% CAM	1.001	0.891	-0.62987609	####	-1.141703548	1.2	-0.8208524	-0.12	1.329	-1.88408	-0.158630722
20:80 CPTEG:CPH 20% CAM	0.593	0.301	-0.74575429	1.099	-1.888378689	-0.8	-0.2632698	-0.73	-0.87	-1.88408	-0.158630722
20:80 CPTEG:CPH 20% CAM	0.818	0.567	-0.75218793	0.823	-1.888378689	-0.8	-0.2632698	-0.73	-0.87	-1.88408	-0.158630722
20:80 CPH-SA 20% CAM	1.082	0.987	-0.67495776	-0.388	-1.141703548	1.2	-0.8208524	-0.12	1.329	-1.88408	-0.158630722
20:80 CPH-SA 5% PZA	-1.821	-2.087	0.348884598	-0.631	-0.433816726	0.6	0.28063019	-0.12	1.329	0.251871	3.96E-01
20:80 CPTEG:CPH 5% PZA	-2.284	-2.983	-0.31939797	0.309	-0.6859408	-0.3	-0.2874662	-0.73	-0.87	0.251871	3.96E-01
20:80 CPH-SA 5% PZA	-1.308	-1.270	0.346694823	-0.969	-1.529586738	1.1	-0.9061224	-0.12	1.329	0.251871	3.96E-01
20:80 CPTEG:CPH 5% PZA	-1.427	-1.912	-0.46137727	0.943	-1.752619573	-0.7	0.44087769	-0.64	-0.73	0.251871	3.96E-01
20:80 CPH-SA 10% DOX	0.907	0.653	0.148636914	-0.826	0.060734342	0.8	1.35940872	1.632	1.174	1.167277	-0.241625119
20:80 CPH-SA 9% DOX	1.041	0.787	-0.02517562	-0.580	0.642559127	0.9	2.00533759	1.632	1.174	1.167277	-0.241625119
20:80 CPH-SA 8% DOX	0.671	0.490	0.127693791	-0.252	0.927653272	1.2	0.95863291	1.632	1.174	1.167277	-0.241625119
20:80 CPH-SA 7% DOX	0.823	0.671	-0.06299788	-0.182	-0.220480971	1.5	1.66458911	1.632	1.174	1.167277	-0.241625119
20:80 CPTEG:CPH 7% DOX	0.848	0.647	0.048491452	0.008	0.225584697	1.4	1.44346644	1.632	1.174	1.167277	-0.241625119
20:80 CPH-SA 5% DOX	0.997	0.773	-0.04516392	0.304	-0.298057609	1.4	1.54711713	1.632	1.174	1.167277	-0.241625119
20:80 CPH-SA 4% DOX	0.583	0.365	0.367222585	0.261	0.332252575	1.3	2.01552003	1.632	1.174	1.167277	-0.241625119
20:80 CPH-SA 3% DOX	0.671	0.420	0.326643234	0.723	0.002551863	1.4	1.43303826	1.632	1.174	1.167277	-0.241625119
20:80 CPH-SA 2% DOX	0.585	0.349	0.366425325	1.260	-0.181692652	1.4	1.45906738	1.632	1.174	1.167277	-0.241625119
20:80 CPH-SA 1% DOX	0.224	-0.077	0.758146213	1.925	0.879167873	1.2	1.40816087	1.632	1.174	1.167277	-0.241625119
20:80 CPTEG:CPH 10% DOX	0.726	0.883	-0.76248944	-0.443	0.85201605	-0.6	-1.1500441	-0.68	-0.8	1.167277	-0.241625119
20:80 CPTEG:CPH 9% DOX	0.878	0.858	-0.77406313	-0.272	1.434810543	-0.8	0.13427868	-0.68	-0.8	1.167277	-0.241625119
20:80 CPTEG:CPH 8% DOX	0.826	0.757	-0.75240837	-0.643	1.068360938	-0.9	-0.567231	-0.68	-0.8	1.167277	-0.241625119
20:80 CPTEG:CPH 7% DOX	0.570	0.543	-0.69328637	-0.284	1.05759414	-0.9	-0.536776	-0.68	-0.8	1.167277	-0.241625119
20:80 CPTEG:CPH 6% DOX	0.145	0.060	-0.70589865	-0.118	1.117475878	-0.8	-0.8707359	-0.68	-0.8	1.167277	-0.241625119
20:80 CPTEG:CPH 5% DOX	0.470	0.357	-0.76212366	-0.422	1.074079176	-0.9	-0.7905163	-0.68	-0.8	1.167277	-0.241625119
20:80 CPTEG:CPH 4% DOX	0.363	0.280	-0.76700732	-0.299	0.962562759	-0.9	-1.2385971	-0.68	-0.8	1.167277	-0.241625119
20:80 CPTEG:CPH 3% DOX	-0.301	-0.340	-0.77406313	-0.560	1.048866769	-1.0	-1.6133331	-0.68	-0.8	1.167277	-0.241625119
20:80 CPTEG:CPH 2% DOX	-0.802	-0.757	-0.68882911	-0.702	0.332252575	-1.0	-1.1324789	-0.68	-0.8	1.167277	-0.241625119
20:80 CPTEG:CPH 1% DOX	-1.179	-1.210	-0.73185869	-0.113	1.045957645	-0.8	-0.6437825	-0.68	-0.8	1.167277	-0.241625119
20:80 CPH-SA 10% RIF	-0.852	-0.678	1.740805149	-1.324	-0.026539376	0.8	0.3643963	1.632	1.174	-0.66354	-0.207450955
20:80 CPH-SA 9% RIF	-0.825	-0.464	1.289957248	-1.299	-0.036236456	1.2	2.0347684	1.632	1.174	-0.66354	-0.207450955
20:80 CPH-SA 8% RIF	-1.187	-1.407	2.739115341	-1.372	-0.608364162	1.5	1.31662712	1.632	1.174	-0.66354	-0.207450955
20:80 CPH-SA 7% RIF	-0.845	-0.482	1.246891117	-1.187	0.012248943	1.5	1.84579016	1.632	1.174	-0.66354	-0.207450955
20:80 CPH-SA 6% RIF	-1.170	-1.417	2.76525308	-1.299	-0.104116014	1.4	0.40229543	1.632	1.174	-0.66354	-0.207450955
20:80 CPH-SA 5% RIF	-1.114	-1.286	2.649722729	-1.244	-0.705334959	1.5	0.80229871	1.632	1.174	-0.66354	-0.207450955
20:80 CPH-SA 4% RIF	-1.405	-1.753	2.450839151	-1.211	-0.026539376	1.6	0.93495577	1.632	1.174	-0.66354	-0.207450955
20:80 CPH-SA 3% RIF	-1.543	-1.810	2.841627302	-1.086	-0.346543008	1.7	0.51280454	1.632	1.174	-0.66354	-0.207450955
20:80 CPH-SA 2% RIF	-1.761	-2.185	2.319544683	-1.071	-0.715032039	1.1	1.06013267	1.632	1.174	-0.66354	-0.207450955
20:80 CPH-SA 1% RIF	-2.087	-2.599	2.475316219	-0.631	-0.588970002	1.3	1.91322802	1.632	1.174	-0.66354	-0.207450955
20:80 CPTEG:CPH 10% RIF	-0.259	-0.044	-0.17214289	0.590	0.167402219	-0.8	-1.0297088	-0.68	-0.8	-0.66354	-0.207450955
20:80 CPTEG:CPH 9% RIF	-0.407	-0.227	-0.06317719	0.277	-0.239875131	-0.8	-1.0931363	-0.68	-0.8	-0.66354	-0.207450955
20:80 CPTEG:CPH 8% RIF	-0.141	0.013	0.139866018	0.925	0.694923358	-1.0	-1.4574022	-0.68	-0.8	-0.66354	-0.207450955
20:80 CPTEG:CPH 7% RIF	-0.721	-0.252	0.157276246	0.423	-0.724729119	-0.9	0.20057743	-0.68	-0.8	-0.66354	-0.207450955
20:80 CPTEG:CPH 6% RIF	-0.783	-0.458	0.362893362	0.910	-1.946561168	-0.9	-1.4950025	-0.68	-0.8	-0.66354	-0.207450955
20:80 CPTEG:CPH 5% RIF	-0.917	-0.321	0.416526836	1.174	-0.462907965	-0.9	-1.552475	-0.68	-0.8	-0.66354	-0.207450955
20:80 CPTEG:CPH 4% RIF	-0.163	-0.066	-0.16352351	0.958	-0.608364162	-0.8	-0.5105371	-0.71	-0.84	-0.66354	-0.207450955
20:80 CPTEG:CPH 3% RIF	-0.673	0.173	-0.03705928	2.385	-0.850791155	-0.9	-0.8002944	-0.68	-0.8	-0.66354	-0.207450955
20:80 CPTEG:CPH 2% RIF	-0.811	0.242	-0.03714627	4.054	-0.491999204	-0.9	-0.6641587	-0.68	-0.8	-0.66354	-0.207450955
20:80 CPTEG:CPH 1% RIF	-1.462	0.071	-0.61330646	2.500	-0.996247352	-0.8	-0.817244	-0.68	-0.8	-0.66354	-0.207450955
10:90 CPTEG:CPH 10% RIF	-0.351	0.074	0.413335551	0.529	0.946077723	-0.8	0.36996134	-0.58	-0.64	-0.66354	-0.207450955
20:80 CPTEG:CPH 10% RIF	0.040	0.200	0.153999224	0.802	1.499780977	-0.9	-0.5591065	-0.68	-0.8	-0.66354	-0.207450955
30:70 CPTEG:CPH 10% RIF	0.388	0.475	-0.4481303	0.410	0.915047068	-0.8	-0.3342888	-0.52	-0.52	-0.66354	-0.207450955
50:50 CPTEG:CPH 10% RIF	0.806	0.726	-0.72916535	0.240	0.380737974	-1.0	-1.4148327	-0.72	-0.83	-0.66354	-0.207450955
10:90 CPTEG:CPH 10% RIF	-0.294	0.069	-0.03942957	0.962	0.380737974	-0.7	-0.9972053	-0.58	-0.64	-0.66354	-0.207450955
20:80 CPTEG:CPH 10% RIF	-0.016	0.123	-0.36813176	1.007	0.148008059	-0.8	-0.6813224	-0.68	-0.8	-0.66354	-0.207450955
30:70 CPTEG:CPH 10% RIF	0.317	0.430	-0.46769388	1.067	0.762802916	-0.7	0.69764198	-0.52	-0.52	-0.66354	-0.207450955
50:50 CPTEG:CPH 10% RIF	0.669	0.656	-0.68258294	0.684	-0.113813094	-0.8	-0.6849813	-0.72	-0.83	-0.66354	-0.207450955

**Table S3.** Principal component analysis raw input data. Encapsulation efficiencies (EE) are formatted as fractions.

Formulation	Drug Release Properties			Particle Properties										Drug Chemistry										Droplet Experimental Data									
	EE (%)	FA (%)	FR (%)	zeta potential	diameter (nm)	PDI	Water Contact Angle (°)	DOP (nmol)	Mn (g/mol)	Xanthone (nmol)	Aliphatic C (nmol)	Aromatic C (nmol)	NC (nmol)	NH (nmol)	NO (nmol)	CN (nmol)	NH (nmol)	NO (nmol)	Molar mass (g/mol)	Tm (°C)	Water Solubility (mg/L)	logP	pKa (strongest acid)	pKa (strongest base)	physiological charge	hydrogen acceptor count	hydrogen donor count	polar surface area (Å²)	rotatable bond count	refractivity	polarizability (Å³)	number of rings	
20:80 CPN-SA 10% DOK	0.649	0.878	0.921	-24.2	295.0	0.116064378	50	29.34	15385	61.77	0.4	7.6	2.4	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPN-SA 10% DOK	0.651	0.878	0.928	-19.9	290.0	0.09449098	50	29.34	15385	61.77	0.4	7.6	2.4	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPTEG-CPN 1% DOK	0.663	0.810	0.816	16.1	187.0	0.130911331	45	16.69	5902	17.81	2.4	6.0	12.0	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPTEG-CPN 1% DOK	0.539	0.861	0.871	10.8	198.0	0.09410899	45	16.69	5902	17.81	2.4	6.0	12.0	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPN-SA 1% DOK	0.693	0.821	0.882	-24.2	295.0	0.116064378	50	29.34	15385	61.77	0.4	7.6	2.4	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPN-SA 1% DOK	0.549	0.870	0.926	-19.9	290.0	0.09449098	50	29.34	15385	61.77	0.4	7.6	2.4	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPTEG-CPN 1% DOK	0.589	0.752	0.778	-14	188.0	0.131660151	45	16.69	5902	17.81	2.4	6.0	12.0	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPTEG-CPN 1% DOK	0.615	0.798	0.827	-10.8	188.0	0.09410899	45	16.69	5902	17.81	2.4	6.0	12.0	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPN-SA 1% RIF	0.267	0.351	0.689	-21.2	326.8	0.12999324	50	29.34	15385	61.77	0.4	7.6	2.4	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPTEG-CPN 1% RIF	0.613	0.622	0.762	-31.4	183.1	0.12629299	45	16.69	5902	17.81	2.4	6.0	12.0	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPN-SA 1% RIF	0.385	0.315	0.721	-21.2	326.8	0.12999324	50	29.34	15385	61.77	0.4	7.6	2.4	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPTEG-CPN 1% RIF	1.127	0.665	0.855	-13.9	164.8	0.10555559	45	16.69	5902	17.81	2.4	6.0	12.0	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPN-SA 2% CAM	0.664	0.866	0.907	-28.8	330.1	0.09649671	50	29.34	15385	61.77	0.4	7.6	2.4	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPTEG-CPN 2% CAM	1.235	0.766	0.782	-36.5	177.8	0.108201732	45	16.69	5902	17.81	2.4	6.0	12.0	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPTEG-CPN 2% CAM	1.117	0.821	0.838	-36.5	177.8	0.108201732	45	16.69	5902	17.81	2.4	6.0	12.0	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPN-SA 2% CAM	0.598	0.886	0.927	-28.8	330.1	0.09649671	50	29.34	15385	61.77	0.4	7.6	2.4	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPN-SA 1% RIF	0.693	0.171	0.276	-21.5	282.8	0.119654883	50	29.34	15385	61.77	0.4	7.6	2.4	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPTEG-CPN 1% RIF	0.887	0.057	0.086	-24.1	216.8	0.10502057	45	16.69	5902	17.81	2.4	6.0	12.0	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPN-SA 1% RIF	0.349	0.299	0.440	-31.8	317.7	0.094660937	50	29.34	15385	61.77	0.4	7.6	2.4	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPTEG-CPN 1% RIF	1.169	0.268	0.313	-31.1	181.5	0.132033948	45	16.69	5902	17.81	2.4	6.0	12.0	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPN-SA 1% DOK	0.640	0.841	0.854	-16.4	300.1	0.142181554	50	29.34	15385	61.77	0.4	7.6	2.4	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPN-SA 1% DOK	0.516	0.875	0.885	-10.4	202.1	0.135978788	50	29.34	15385	61.77	0.4	7.6	2.4	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPN-SA 1% DOK	0.656	0.785	0.822	-7.46	329.0	0.133939982	50	29.34	15385	61.77	0.4	7.6	2.4	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPN-SA 1% DOK	0.686	0.821	0.860	-19.3	352.0	0.144810296	50	29.34	15385	61.77	0.4	7.6	2.4	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPN-SA 1% DOK	0.768	0.827	0.855	-16.7	342.1	0.144132512	50	29.34	15385	61.77	0.4	7.6	2.4	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPN-SA 1% DOK	0.895	0.865	0.882	-20.1	346.8	0.144335858	50	29.34	15385	61.77	0.4	7.6	2.4	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPN-SA 1% DOK	0.876	0.763	0.795	-13.6	337.7	0.156202331	50	29.34	15385	61.77	0.4	7.6	2.4	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPN-SA 1% DOK	1.074	0.781	0.807	-17	344.8	0.143938982	50	29.34	15385	61.77	0.4	7.6	2.4	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPN-SA 1% DOK	1.305	0.764	0.792	-18.9	342.8	0.144481171	50	29.34	15385	61.77	0.4	7.6	2.4	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPN-SA 1% DOK	1.590	0.675	0.702	-7.96	324.5	0.143488973	50	29.34	15385	61.77	0.4	7.6	2.4	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPTEG-CPN 1% DOK	0.574	0.799	0.806	-8.24	188.8	0.08922654	45	17.71	6230	42.35	2.4	6.0	12.0	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPTEG-CPN 1% DOK	0.647	0.836	0.800	-2.23	175.8	0.116575724	45	17.71	6230	42.35	2.4	6.0	12.0	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPTEG-CPN 1% DOK	0.688	0.821	0.878	-6.01	163.8	0.101799071	45	17.71	6230	42.35	2.4	6.0	12.0	0.10207143	0.14957429	0	0.03714286	0.14957429	444.43	201	630	-0.02	-2.2	7.75	-1	9	6	181.62	2	113.89	42.88	4	
20:80 CPTEG-CPN 1% DOK	0.662	0.760	0.831	-6.12	165.0	0.102046078	45	17.71	6230	42.35	2.4	6.0	12.0	0.10207143	0.14957429																		



**Figure S4.** Chemical structures of antibiotics in model validation data set. Meropenem (MEM, a) and ceftazidime (CAZ, b) both contain sulfur atoms, which were not included in training data set.



**Figure S5.** Release kinetics from nanoparticles encapsulating drugs not included in training data set. All formulations showed an extensive burst. Release property parameterization is shown in Table 3. Drug abbreviations: meropenem (MEM); ceftazidime (CAZ).