

Supporting Information Available. *Origins of the Sets of Peaks in the GC-MS for TMS-Triton X-114R.* Hydrogenation of Triton X-114 results in formation of its reduced form, Triton X-114R, whose structure is then that of a 1,4-disubstituted cyclohexane (Figure S-1). Hence, four different conformations are theoretically possible for TX-114R and TMS-Triton X-114R (structures A through D in Figure S-1). It is expected that the very bulky p-tert-octyl group (designated by R₁ in the structures in Fig. S-1) would always prefer an equatorial site (for instance, for tert-butylcyclohexane, the conformation which dominates is that in which its tert-butyl group is equatorial [relative to when it is axial] since the equilibrium constant between the axial and equatorial forms is reported to be 11,916 M⁻¹).^{S-1} Thus, conformers C and D (Fig. S-1) are not thought to exist for TMS-Triton X-114R. The sets of peaks in the GC-MS for TMS-Triton X-114R in Figure 1 are due to fact that two conformations, A and B, exist for each molecular weight homolog (note: no differences in the mass spectrum of the two peaks in each set was evident). Most likely, the earlier eluter in each set is due to conformer A (cis in which the polyoxyethylene moiety is in an axial and the tert-octyl group in an equatorial position). The second, smaller intensity peak of each set is thought to be due to conformer B (trans with both the polyoxyethylene and tert-octyl groups in equatorial positions). This latter B conformer bears a close resemblance (in that it is almost linear) to the structure of TMS-Triton X-114 and in fact, this second peak elutes at a retention time very similar to the corresponding homolog of the non-reduced form of TMS-Triton X-114 (refer to Fig. 1; compare peak 3B for TMS-Triton X-114R to peak 3 for TMS-Triton X-114).

Reference:

S-1. Jones, M., *Organic Chemistry 2nd Ed.*; W. W. Norton & Company (Japanese Edition by Tokyo Kagaku Dozin, Co., Ltd.), 2000, p. 177.

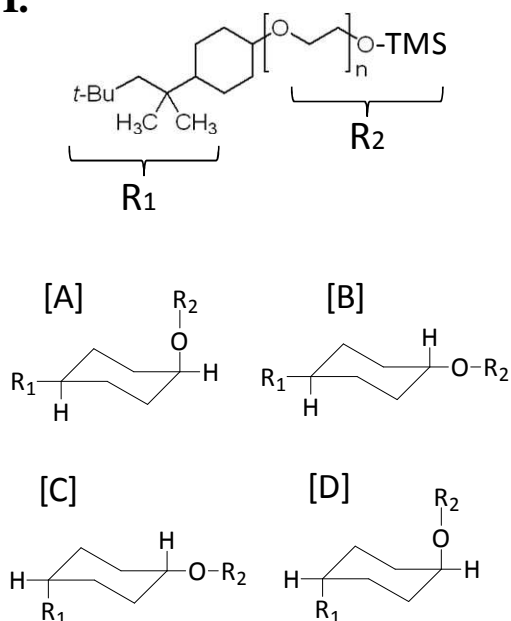
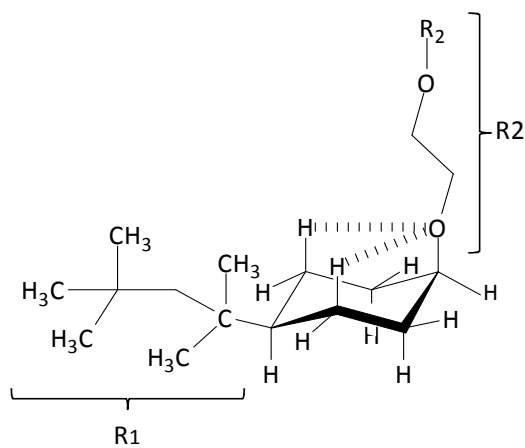
I.**II.**

Figure S-1

Figure S-1. (I) General structure for the reduced form of trimethylsilylated Triton-X-114 R and its four possible corresponding conformations for such 1,4-disubstituted cyclohexane and (II) the structure for Triton X-114R (reduced form of TX-114).

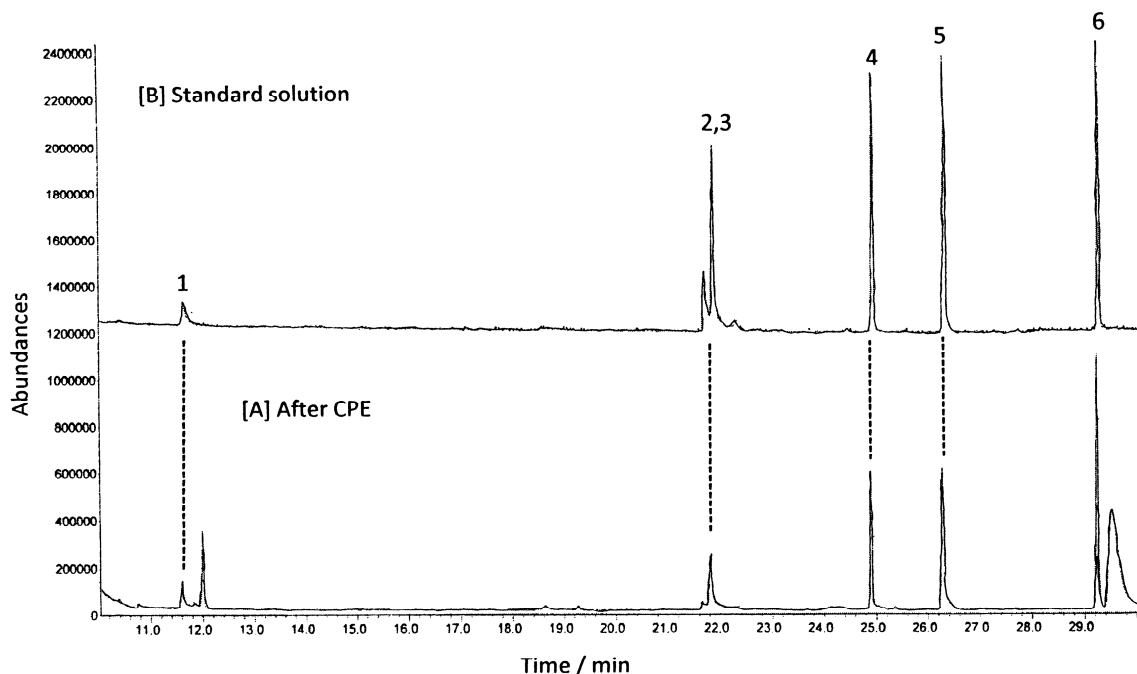


Figure S-2. GC – MS chromatogram of [A] (bottom panel) a herbicide test mix that had been extracted using the optimized CPE procedure using TX-114 (initial herbicide concentration in water prior to extraction was 4.00 ppm) and [B] (upper panel) of a standard herbicide solution (all present at a concentration of 100 ppm in acetone). The chromatographic peaks correspond to the following herbicides: (1) hexachlorocyclopentadiene, (2) simazine, (3) atrazine, (4) alachlor, (5) metolachlor and (6) butachlor. On the DB-5ms column under the GC conditions employed with MS monitoring in the total ion mode, the peaks due to simazine and atrazine partially overlapped.

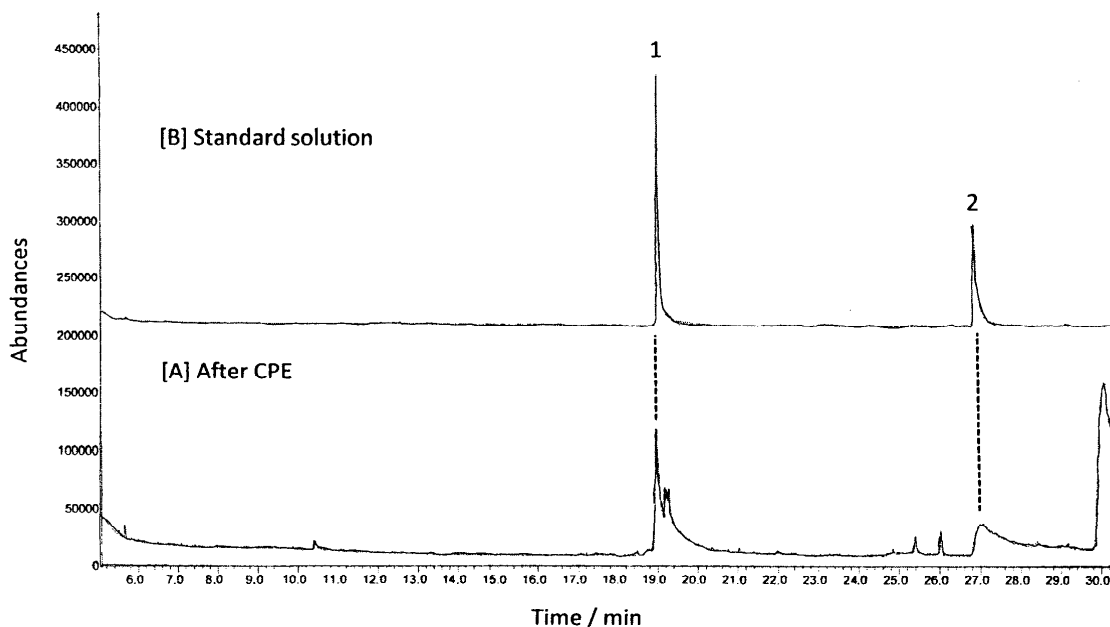


Figure S-3. GC – MS chromatogram of TMS derivatized (1) ibuprofen and (2) flurbiprofen: [A] represents the chromatogram observed after injection of the treated surfactant-rich phase obtained after the TX-114 cloud point extraction of an initial aqueous mixture of these two profens (both initially present at a concentration of 20.0 ppm prior to the cloud point extractive step) and [B] represents the chromatograph obtained after injection of an acetone standard solution of these profen drugs present at a concentration of 50.0 ppm; also after their derivatization with BSFTA/pyridine. The MS was operated in the total ion monitoring mode. The unlabeled background peaks in [A] are due to the homologs of the Triton X-114 surfactant preparation. The ibuprofen and flurbiprofen retention times obtained for the standard solutions are in excellent agreement with those observed for the TX-114 CPE extracts.