

Supporting Information

Solid-phase extraction based on trimethylsilyloxy silica aerogel

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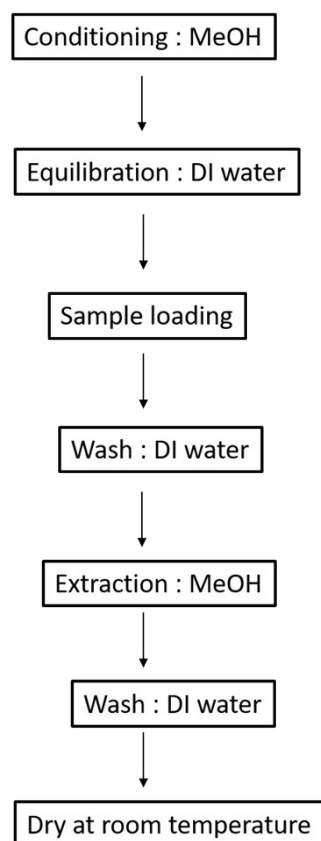


Fig. S1: Protocol for extraction of chemotherapeutic drugs on TMSO modified silica aerogel

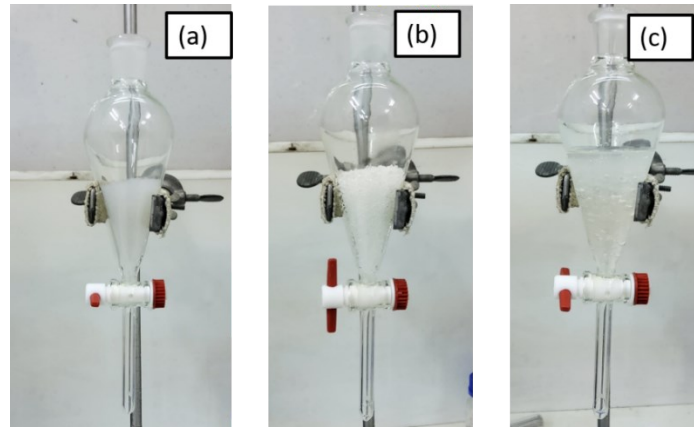


Figure S2: Aerogel in separating funnel (a) without conditioning with MeOH (b) after conditioning with MeOH (c) sample loading

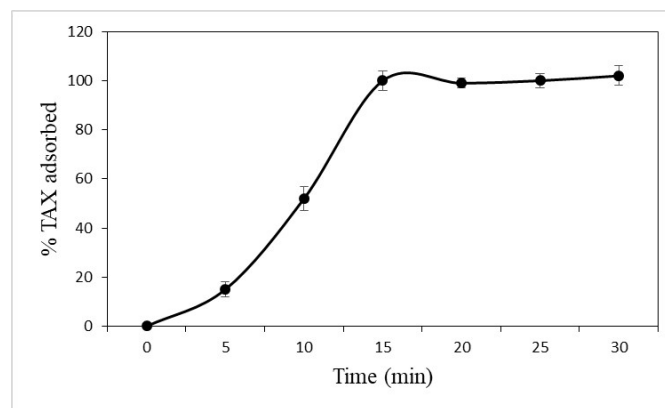
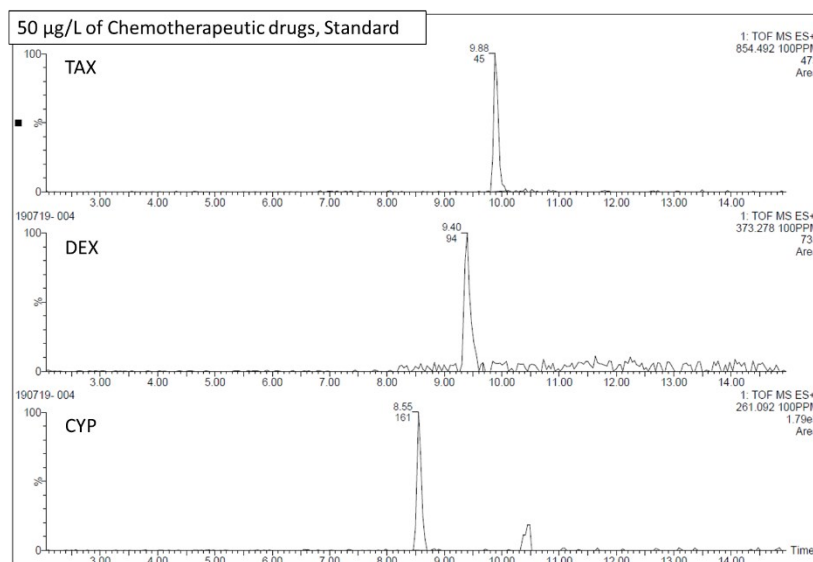


Figure S3 Kinetics of adsorption of paclitaxel (TAX) on aerogel



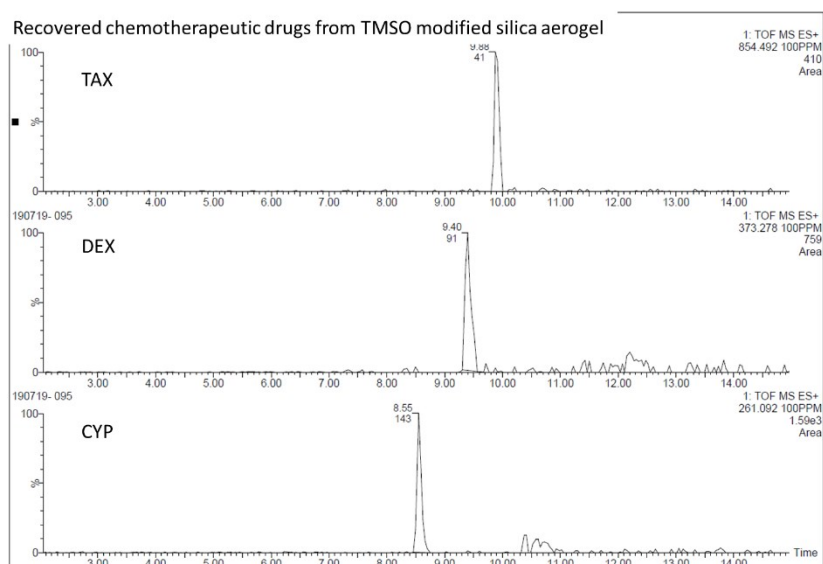
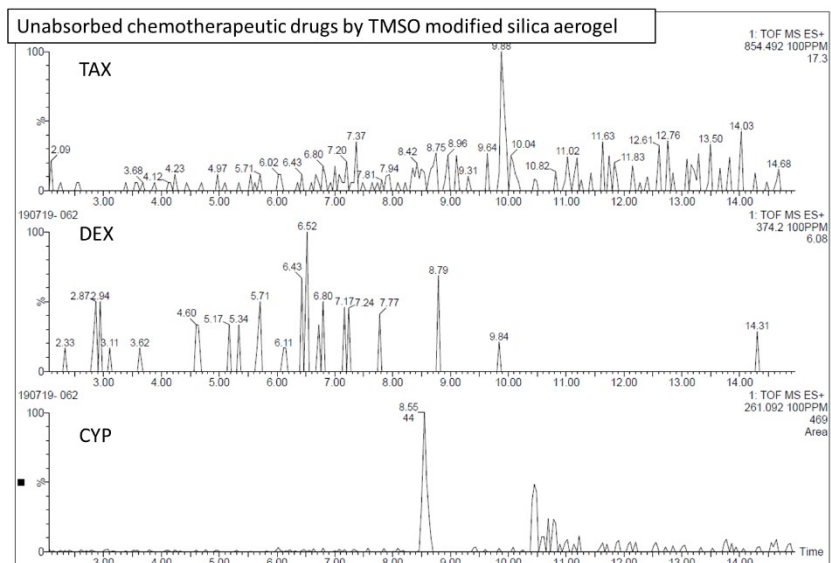


Figure S4: LC-MS of Drugs unabsorbed and recovered drugs by TMSO modified silica aerogel

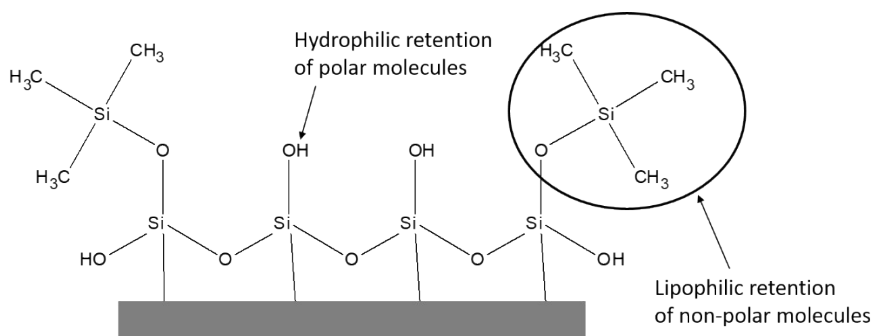


Fig. S5: Molecular interactions of polar and non-polar molecules on TMSO modified silica aerogel

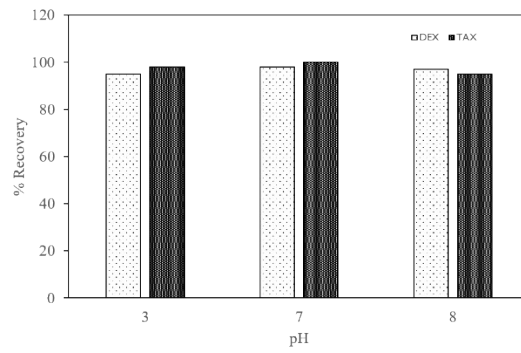


Fig. S6 Effect of pH on recovery of chemotherapeutic drugs dexamethasone (DEX) and paclitaxel (TAX).

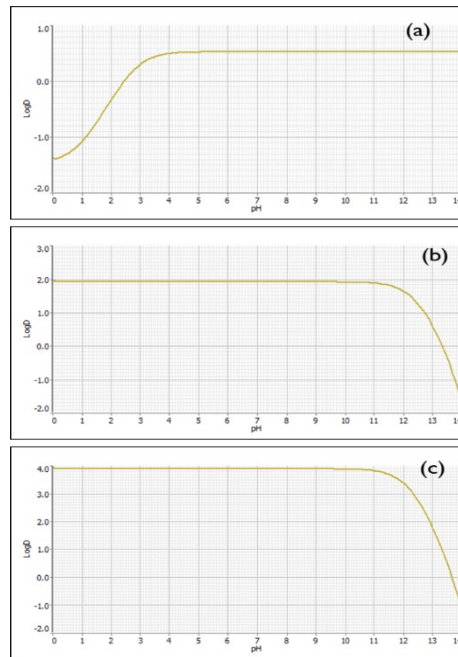


Fig. S7 Log D of (a) cyclophosphamide (CYP), (b) dexamethasone (DEX), and (c) paclitaxel (TAX)

Table S1 Physiochemical properties of cyclophosphamide (CYP), dexamethasone (DEX) and paclitaxel (TAX)

	CYP	DEX	TAX
CAS number	50-18-0	50-02-2	33069-62-4
Chemical formula	C ₇ H ₁₅ Cl ₂ N ₂ O ₂ P	C ₂₂ H ₂₉ FO ₅	C ₄₇ H ₅₁ NO ₁₄
Monoisotopic mass (Da)	260.02	392.19	853.3
Melting point (°C)	48	262	216–217
Boiling point (°C)	336		957.1
Water solubility (mg/L)	93	89	5
pKa	2.84	12.4	10.3
Log P	0.63	1.92	3.18

Table S2: Comparison of TMSO modified silica aerogel with other commercial cartridges on extraction of chemotherapeutic drugs from water

	HLB	RP	C18	Strata XC	TMSO modified silica aerogel
CYP	99.9	96	92	111	70
TAX	71	68	63	81	109
DEX	102	104	98	114	102