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Supplementary Information

The cytotoxic potential of cationc triangulenes against tumour cells

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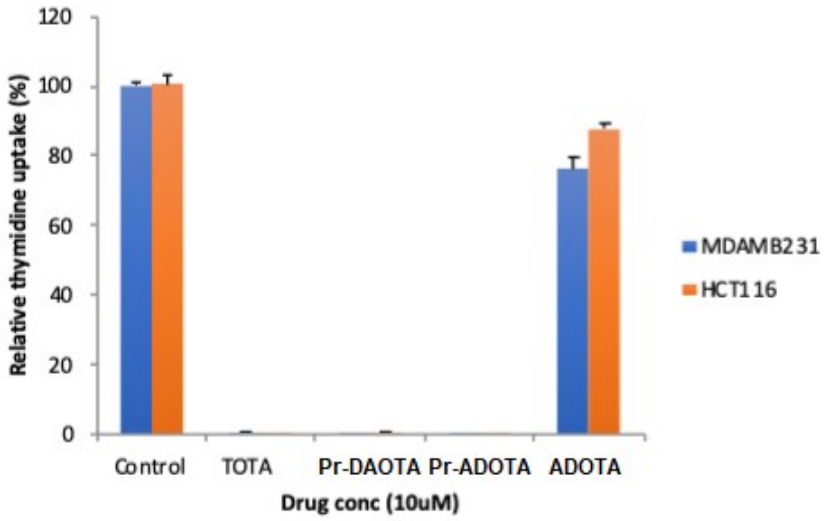

Fig. S1 Relative anti-proliferative activity of **TOTA** and its derivatives against the breast MDA-MB-231 and colon HCT116 cancer cell lines. The mean percentages (%) at 10 μM as compared to untreated cells at 100% growth using DMSO as a negative control.

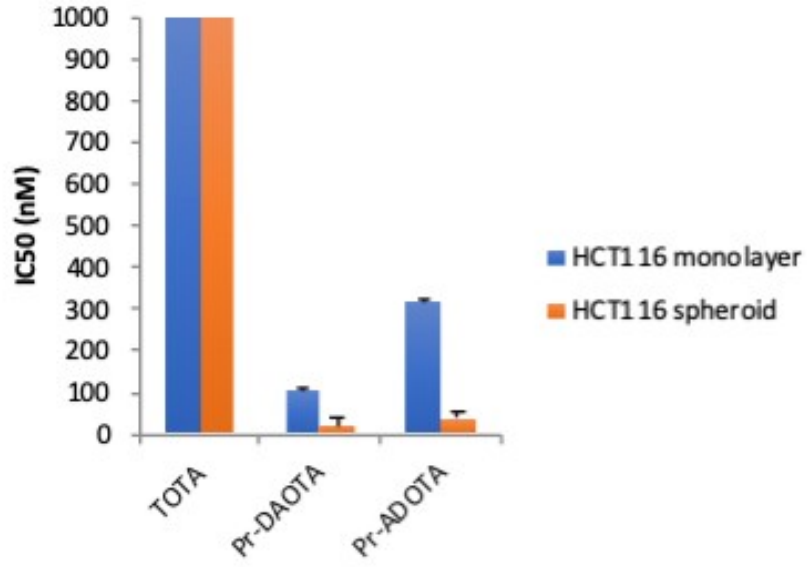

Fig. S2 IC_{50} values for HCT116 cell line cultured as monolayer or spheroid are represented on the y-axis. The highest drug concentration is depicted where 50% growth inhibition was not reached. **TOTA** does not have a response in the concentration range used.

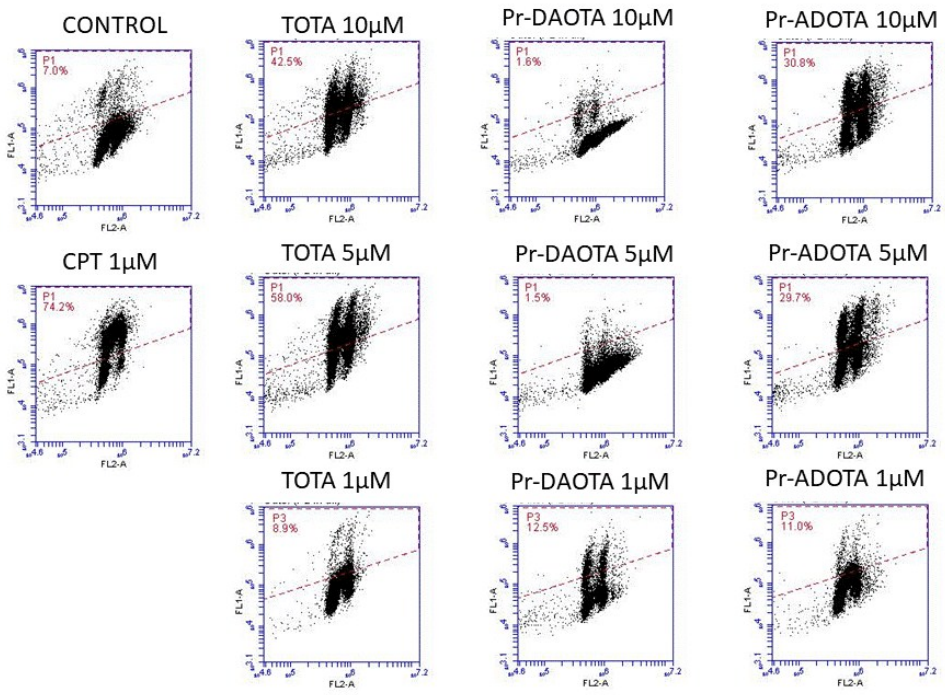

Fig. S3 The results of the flow cytometry experiments at 16 h using MDA-MB-231. Cellular immunofluorescence (anti-γ-H2AX antibody; y-axis) is plotted against DNA content (propidium iodide staining; x-axis). The upper portion (marked) represents high γ-H2AX phosphorylation and the proportion of the total (% cells) is indicated.

Table S1. Criteria of lead-like, drug-like and known drug space (KDS) in terms of molecular descriptors.

	Lead-like Space	**Drug-like Space**	**Known Drug Space**
Molecular weight (g mol^{-1})	300	500	800
Lipophilicity (Log P)	3	5	6.5
Hydrogen bond donors (HD)	3	5	7
Hydrogen bond acceptors (HA)	3	10	15
Polar surface area ($Å^2$) (PSA)	60	140	180
Rotatable bonds (RB)	3	10	17

From: F. Zhu, G. Logan and J. Reynisson, *Mol. Inf.*, 2012, **31**, 847 – 855.

Table S2. The single point and zero point corrected vibrational energies (ZPE) of the optimised structures in hartrees (a.u.) in vacuum and the water simulation.

Systems	Energy/a.u.	ZPE/a.u. [a]
TOTA	-955.2029309	0.224701798
TOTA-OH	-1031.260384	0.238076414
TOTA-OMe	-1070.570969	0.265710949
TOTA-OEt	-1109.901788	0.293392543
H2O	-76.46027328	0.020869775
MeOH	-115.7697717	0.050232755
EtOH	-155.1011875	0.078276116
OH-	-75.82828128	0.008394185
ADOTA	-935.35602	0.237645
ADOTA-OH	-1011.399941	0.250434
Pr-ADOTA	-1053.327744	0.321139
Pr-ADOTA-OH	-1129.366377	0.334043
Pr-DAOTA	-1151.447754	0.417432751
Pr-DAOTA-OH	-1227.467945	0.429870106
TATA	-1249.563617	0.514108034
TATA-OH	-1325.568916	0.525793422
ADOTA ($-H^+$)	-934.951629174	0.2240125764
Pyridine	-248.364687468	0.0869879508
Pyridine ($+H^+$)	-248.733067049	0.1008694344
Water simulation		
TOTA	-955.2635867	0.224429246
TOTA-OH	-1031.269384	0.237643078
TOTA-OMe	-1070.578412	0.265710949
TOTA-OEt	-1109.909028	0.292959206
H2O	-76.46783158	0.0207835
MeOH	-115.7752472	0.050202362
EtOH	-155.1065013	0.0781369
OH-	-75.96012671	0.008494186
ADOTA	-935.4191645	0.23747739
ADOTA-OH	-1011.412145	0.250241218
Pr-ADOTA	-1053.385937	0.320866292
Pr-ADOTA-OH	-1129.377098	0.333617375
Pr-DAOTA	-1151.503448	0.416992552
Pr-DAOTA-OH	-1227.480123	0.42934167
TATA	-1249.623951	0.513074693
TATA-OH	-1325.59104074	0.525374791

[a] Corrected values (Wong).