Electronic Supplementary Material (ESI) for Food & Function. This journal is © The Royal Society of Chemistry 2014

## **Supplementary Data**

Topical (+)-catechin emulsified gel prevents DMBA/TPA induced squamous cell carcinoma of skin by modulating antioxidants and inflammatory biomarkers in BALB/c mice

Jitender Monga,<sup>a#</sup> Vaibhav Aggarwal,<sup>b#</sup> Sharad Kumar Suthar,<sup>a</sup> Monika,<sup>b</sup> Khumukcham Nongalleima,<sup>c</sup> Manu Sharma<sup>b\*</sup>

<sup>a</sup>Department of Urology, Postgraduate Institute of Medical Education and Research, Chandigarh, India <sup>b</sup>Department of Pharmacy, Jaypee University of Information Technology, Waknaghat-173234, India <sup>c</sup>Institute of Bioresources and Sustainable Development (IBSD), Takyelpat, Imphal-795001, Manipur, India

<sup>#</sup>Both the authors have an equal contribution.

\*Address correspondence to this author at the Department of Pharmacy, Jaypee University of Information Technology, Waknaghat, India; Tel: +91–1792–239407; Fax: +91–1792–245362; Email: <u>lantadene@hotmail.com</u>

RC SAIF PU, Chandigarh



Date Created: wed nov 16 15:36:45 2011 India Standard Time (GMT+5:30)

## Fig. S1. FT-IR spectrum of isolated (+)-catechin



**Fig. S2.** <sup>1</sup>H NMR of isolated (+)-catechin ( $C_{15}H_{14}O_6$ ) in a mixture of CDCl<sub>3</sub> & DMSO.d<sub>6</sub>. Integration of five OH (s) is not shown.



Fig. S5. <sup>15</sup>C NMR of isolated (+)-catechin ( $C_{15}H_{14}O_6$ ) in a mixture of CDCl<sub>3</sub> & DMSO.d<sub>6</sub>. C-4 & C-5 both appeared at 144 hence, 14 peaks of compound are visible in the spectrum.



**Fig. S4.** Mass (ESI-MS) spectrum of isolated (+)-catechin in negative ion mode. Calculated exact mass: 290.1; Found: 290.1 (M<sup>-</sup>) & 289.0 (M<sup>-</sup>-1) (100%).

HO B T T G T G G H T H H H H H H H H					
Hydrogen (s)	δ, ppm at 400 MHz	Carbon (s)	δ, ppm at 100 MHz	Carbon (s)	δ, ppm at 100 MHz
C-8, -6, -3' &	8.7826 & 9.0315 (4H, two broad signals,	C-8	156.33	C-2	80.98
-4′OH	four OH groups)				
H-2'	6.7355–6.7403 (1H, d, <i>J</i> = 1.92 Hz)	C-6	156.05	C-3	66.39
H-5'	6.6756–6.6958 (1H, d, <i>J</i> = 8.08 Hz)	C-10	155.23	C-4	27.67
H-6′	6.5774–6.6027 (1H, dd, <i>J</i> = 8.16, 1.96 Hz)	C-4' & C-3'	144.72		
H-7	5.8837–5.8894 (1H, d, <i>J</i> = 2.28 Hz)	C-1′	130.50		
Н-9	5.6976–5.7032 (1H, d, <i>J</i> = 2.24 Hz)	C-6′	118.27		
H-2	4.4670–4.4856 (1H, d, <i>J</i> = 7.44 Hz)	C-2′	144.92		
С-3-ОН	4.0228 (1H, broad signal)	C-5′	114.31		
H-3	3.7993–3.8514 (1H, m)	C-5	98.96		
$H-4_A$	2.6536–2.7070 (1H, dd, <i>J</i> = 16.08, 5.36 Hz)	C-7	95.04		
$H-4_B$	2.3361–2.3961 (1H, dd, <i>J</i> = 16.04, 8.08 Hz)	C-9	93.80		

 Table S1: Complete <sup>1</sup>H and <sup>13</sup>C NMR assignments of isolated (+)-catechin



Figure S5. HPLC chromatogram of aqueous extract of *A. Catechu* 



Figure S6. HPLC chromatogram of isolated (+)-catechin