

1 **Supplementary material**

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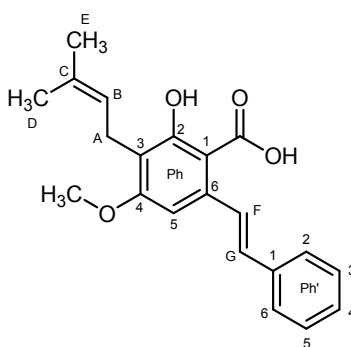
3 **S. 1:** Structure and full assignment of all ^1H and ^{13}C resonances of cajaninstilbene acid

4 (A), pinosylvin monomethyl ether (B) and 4-O-methylpinosylvic acid (C)

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6 **(A)** 2-Hydroxy-4-methoxy-3-(3-methyl-2-buten-1-yl)-6-[(*E*)-2-phenylvinyl]benzoic acid

7 (cajaninstilbene acid)



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9 **^1H NMR** (400 MHz, $\text{DMSO-}d_6$): δ 11.50-14.50 (very broad s, 2H, OH and COOH), 7.86

10 (d, $^3J = 16.1$ Hz, 1H, H_F), 7.53 (m, 2H, Ph' H-2,6), 7.38 (m, 2H, Ph' H-3,5), 7.27 (m,

11 1H, Ph' H-4), 7.00 (d, $^3J = 16.1$ Hz, 1H, H_G), 6.78 (s, 1H, Ph H-5), 5.12 (septet of a

12 triplet, triplet: $^3J = 7.0$ Hz, septet: $^4J = 1.3$ Hz, 1H, H_B), 3.91 (s, 3H, OCH_3), 3.24 (d, 3J

13 = 7.0 Hz, 2H, H_A), 1.71 (d^* , $^4J = 1.3$ Hz, 3H, CH_3 of D), 1.61 (d^* , $^4J = 1.3$ Hz, 3H, CH_3

14 of E). * after Lorentz \rightarrow Gauss transformation

15 **^{13}C NMR** (100 MHz, $\text{DMSO-}d_6$): δ 173.3 (COOH), 160.7 (Ph C-2), 160.5 (Ph C-4),

16 139.8 (Ph C-6), 137.3 (Ph' C-1), 130.7 (C_C), 129.8 (C_F and C_G), 128.7 (Ph' C-3,5),

17 127.7 (Ph' C-4), 126.5 (Ph' C-2,6), 122.1 (C_B), 115.3 (Ph C-3), 105.1 (Ph C-1), 102.1

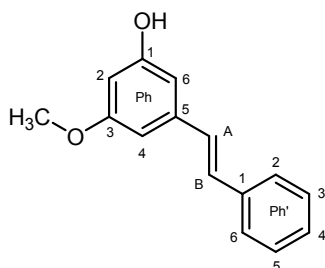
18 (Ph C-5), 55.8 (OCH_3), 25.5 (CH_3 of E), 21.7 (C_A), 17.7 (CH_3 of D).

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22 **(B)** 3-Methoxy-5-[(*E*)-2-phenylvinyl]phenol (pinosylvin monomethyl ether)



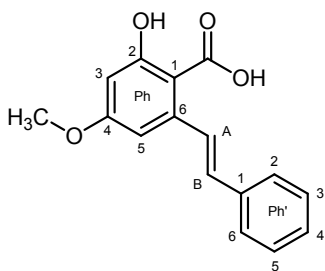
23

24 **¹H NMR** (400 MHz, DMSO-*d*₆): δ 9.45 (s, 1H, OH), 7.58 (m, 2H, Ph' H-2,6), 7.36 (m,
25 2H, Ph' H-3,5), 7.26 (m, 1H, Ph' H-4), 7.14 (A-part of an AB-system, ²*J* = 16.4 Hz, 1H,
26 H_A), 7.11 (B-part of an AB-system, ²*J* = 16.4 Hz, 1H, H_B), 6.63 (m, 1H, Ph H-4), 6.58
27 (m, 1H, Ph H-6), 6.26 (m, 1H, Ph H-2), 3.73 (s, 3H, OCH₃).

28 **¹³C NMR** (100 MHz, DMSO-*d*₆): δ 160.62 (Ph C-3), 158.60 (Ph C-1), 138.88 (Ph C-5),
29 136.94 (Ph' C-1), 128.67 (Ph' C-3,5 and C_A), 128.37 (C_B), 127.61 (Ph' C-4), 126.48
30 (Ph' C-2,6), 106.25 (Ph C-6), 102.89 (Ph C-4), 100.97 (Ph C-2), 54.98 (OCH₃).

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32 **(C)** 2-Hydroxy-4-methoxy-6-[(*E*)-2-phenylvinyl]benzoic acid (4-*O*-methylpinosylvic
33 acid)



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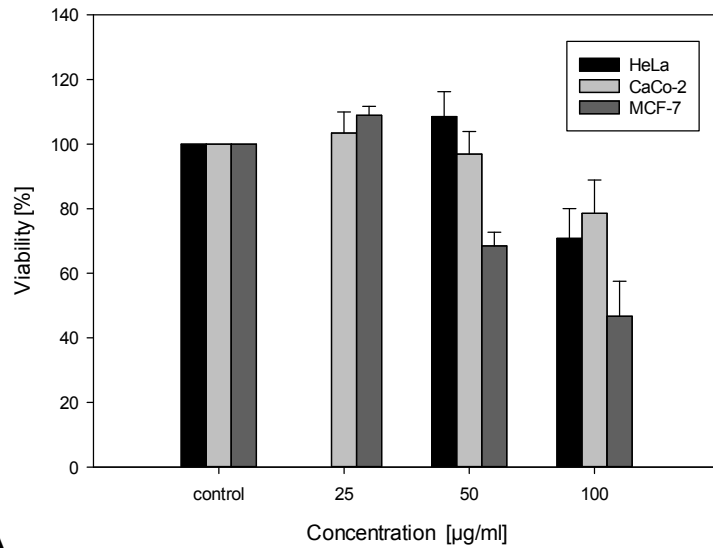
35 **¹H NMR** (400 MHz, DMSO-*d*₆): δ 12.0-14.0 (very broad s, 2H, OH), 7.73 (d, ³*J* = 16.3
36 Hz, 1H, H_A), 7.51 (m, 2H, Ph' H-2,6), 7.36 (m, 2H, Ph' H-3,5), 7.26 (m, 1H, Ph' H-4),
37 7.01 (d, ³*J* = 16.3 Hz, 1H, H_B), 6.70 (d, ⁴*J* = 2.4 Hz, 1H, Ph H-5), 6.40 (d, ⁴*J* = 2.4 Hz,
38 1H, Ph H-3), 3.80 (s, 3H, OCH₃).

39 **¹³C NMR** (100 MHz, DMSO-*d*₆): δ 171.81 (COOH), 162.52 (Ph C-2), 162.39 (Ph C-4),
40 140.64 (Ph C-6), 137.15 (Ph' C-1), 130.08 (C_B), 128.73 (Ph' C-3,5), 128.65 (C_A),

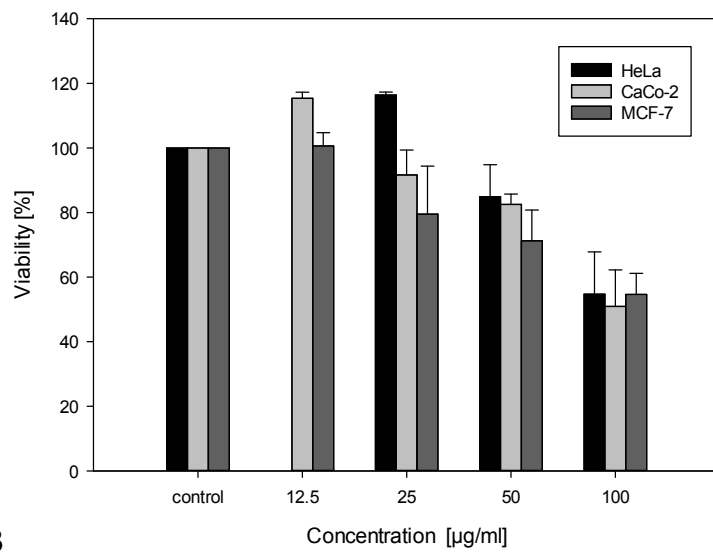
41 127.77 (Ph' C-4), 126.53 (Ph' C-2,6), 108.07 (Ph C-1), 104.45 (Ph C-5), 100.52 (Ph C-
42 3), 55.37 (OCH₃).

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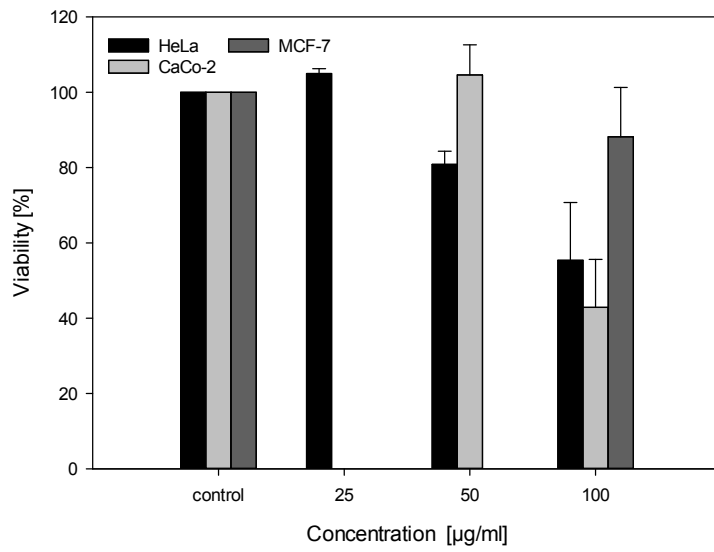
44 **S. 2:** Concentration depended cytotoxic effects of *C. cajan* extract (A) and fractions 1
45 and 3-10 (B-J) on the three cancer cell lines HeLa, CaCo-2 and MCF-7, using a MTT-
46 assay.



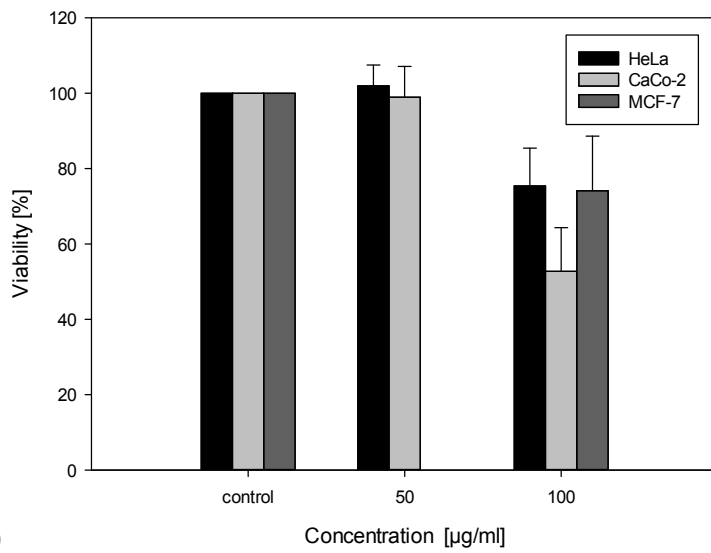
47 **A**



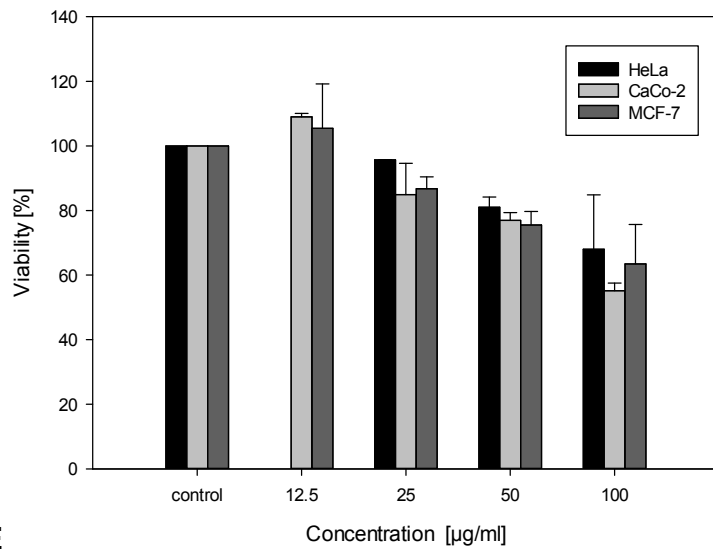
48 **B**



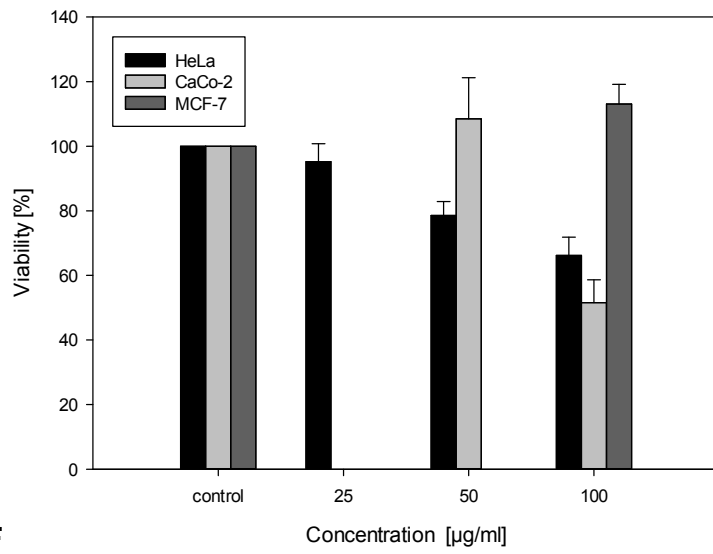
49 **C**



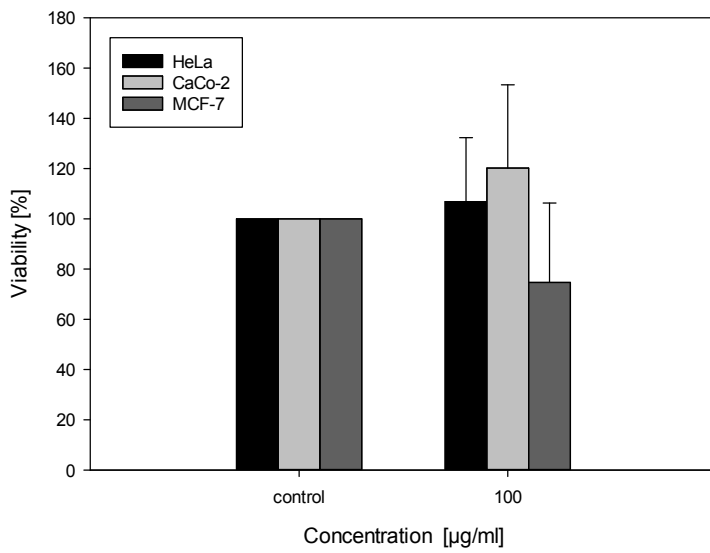
50 **D**



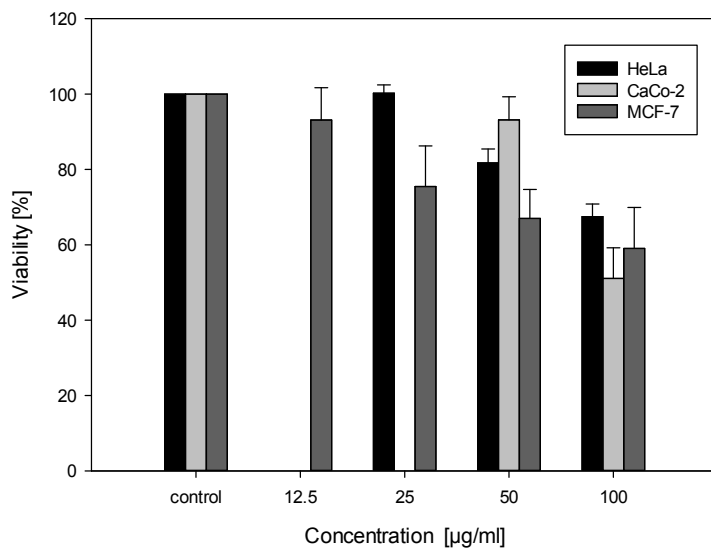
51 **E**



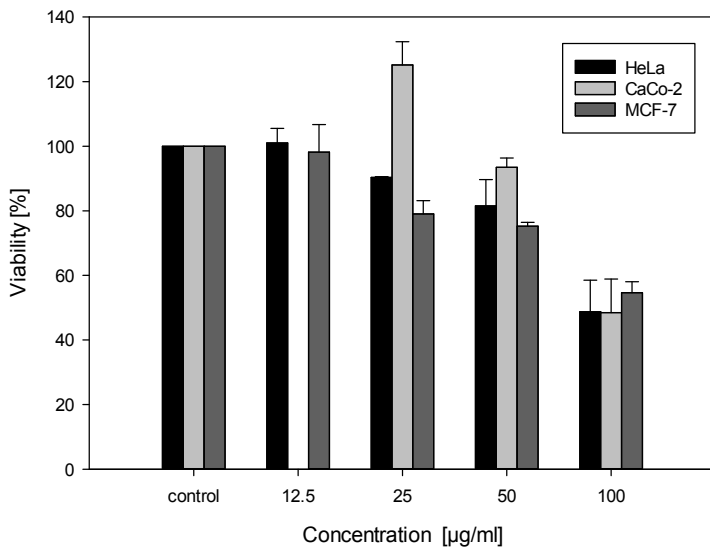
52 **F**



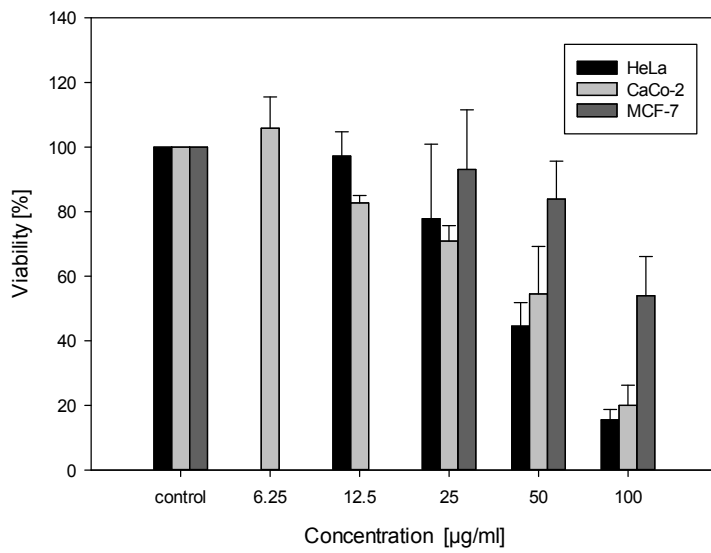
53 **G**



54 **H**



55 I



56 J

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