

**Supplementary Table S1.** <sup>1</sup>H ( $\delta$ , CDCl<sub>3</sub>, 400 MHz) and <sup>13</sup>C ( $\delta$ , CDCl<sub>3</sub>, 125 MHz) NMR data of anacardic acid (13:0); and key HMBC correlations

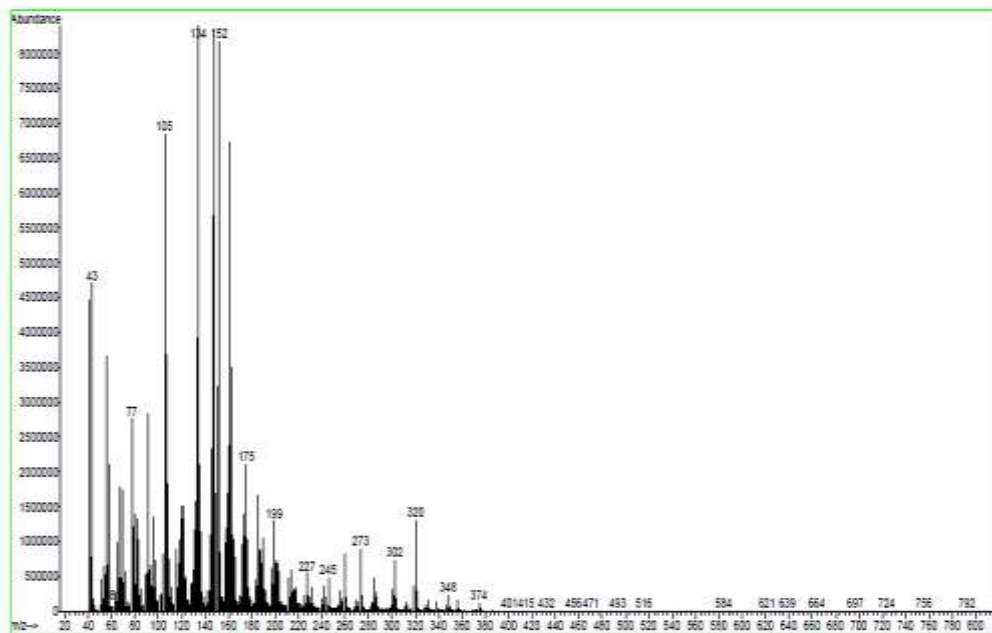
| Position | $\delta$ C  | $\delta$ H (mult, J in Hz)    | HMBC                          |
|----------|-------------|-------------------------------|-------------------------------|
| 1        | 110.38      | -                             | -                             |
| 2        | 163.67      | -                             | -                             |
| 3        | 115.89      | 6.77 ( <i>d</i> , J = 7.6 Hz) | 115.95, 110.3                 |
| 4        | 135.45      | 7.35 ( <i>t</i> , J = 7.8 Hz) | 163.67, 147.71                |
| 5        | 122.78      | 6.86 ( <i>d</i> , J = 8.3 Hz) | 163.67, 122.78, 110.38        |
| 6        | 147.82      | -                             | -                             |
| 1'       | 36.52       | 2.96 ( <i>t</i> , J = 10 Hz)  | 31.93, 147.82, 122.78, 110.38 |
| 2'       | 31.93       | 1.58 ( <i>m</i> )             | -                             |
| 3'-12'   | 22.72-32.06 | 1.25-1.35                     | -                             |
| 13'      | 14.15       | 0.88 ( <i>d</i> , J = 7.5 Hz) | -                             |
| C=O      | 175.79      | -                             | -                             |

Assignments were done by HSQC, HMBC, and COSY experiments

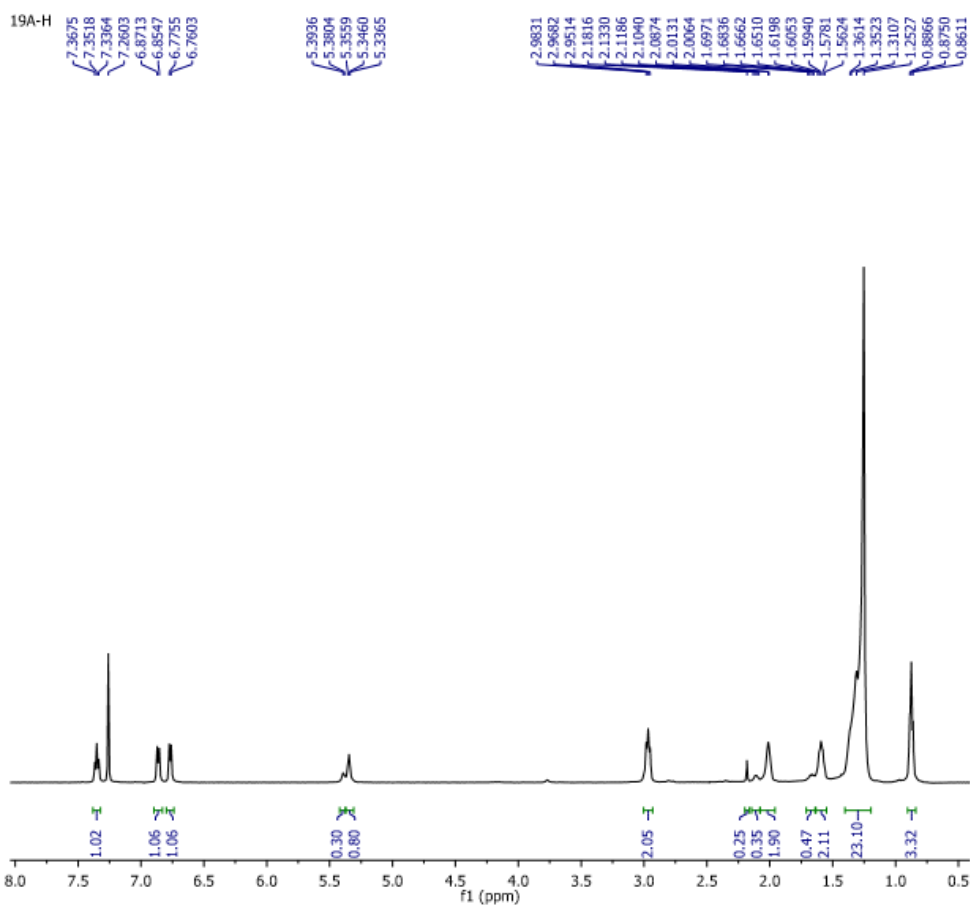
**Supplementary Table S2.** Cytotoxicity (IC<sub>50</sub> in  $\mu$ g/mL) and selectivity index (SI) of anacardic acid (13:0) from *Pistacia vera* CHCl<sub>3</sub> fraction and cisplatin against MCF-7, HepG-2, MKN-45 and NIH/3T3 cell lines

| Compound       | Cell lines concentration ( $\mu$ g/mL) |      |                  |      |                  |      |                  |
|----------------|--|------|------------------|------|------------------|------|------------------|
|                | MCF-7                                  |      | HepG-2           |      | MKN-45           |      | NIH/3T3          |
|                | IC <sub>50</sub>                       | SI   | IC <sub>50</sub> | SI   | IC <sub>50</sub> | SI   | IC <sub>50</sub> |
| Anacardic acid | 18.90                                  | 0.98 | 26.10            | 0.72 | 17.73            | 1.05 | 18.69            |
| Cisplatin      | < 6.25                                 |      | < 6.25           |      | < 6.25           |      | 28.59            |

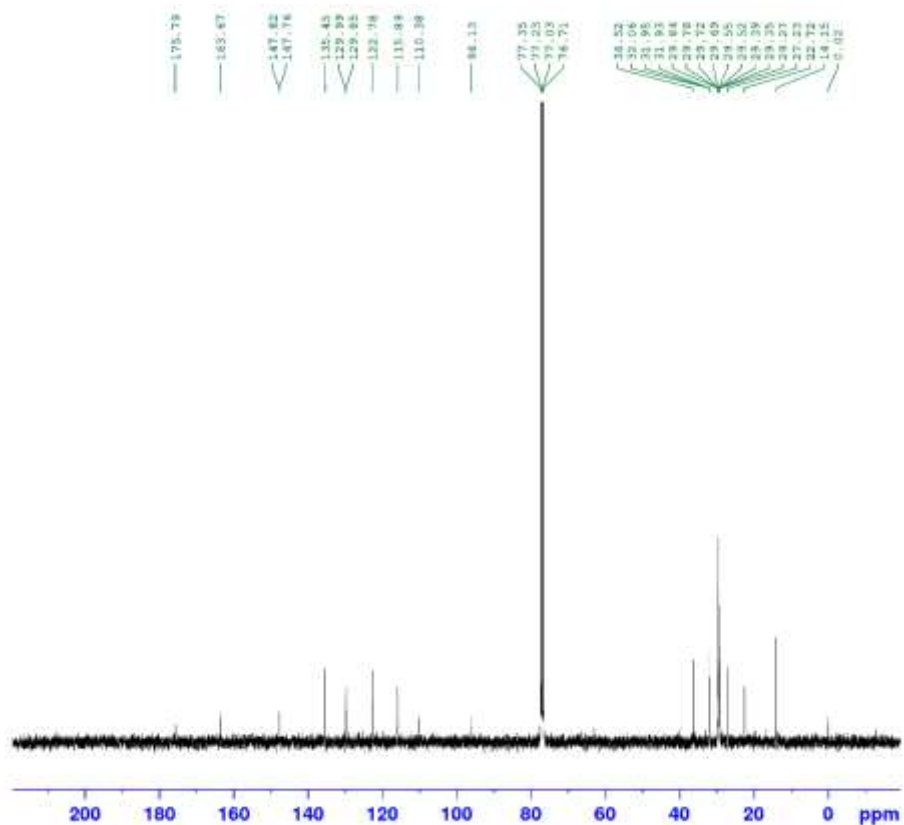
The cells were treated for 48 with different concentrations (6.25-100  $\mu$ g/mL) of anacardic acid (13:0) and cisplatin. Each experiment was performed three times and the results are mean  $\pm$  SEM, SI (selective index), \*p  $\leq$  0.05(one-way ANOVA)



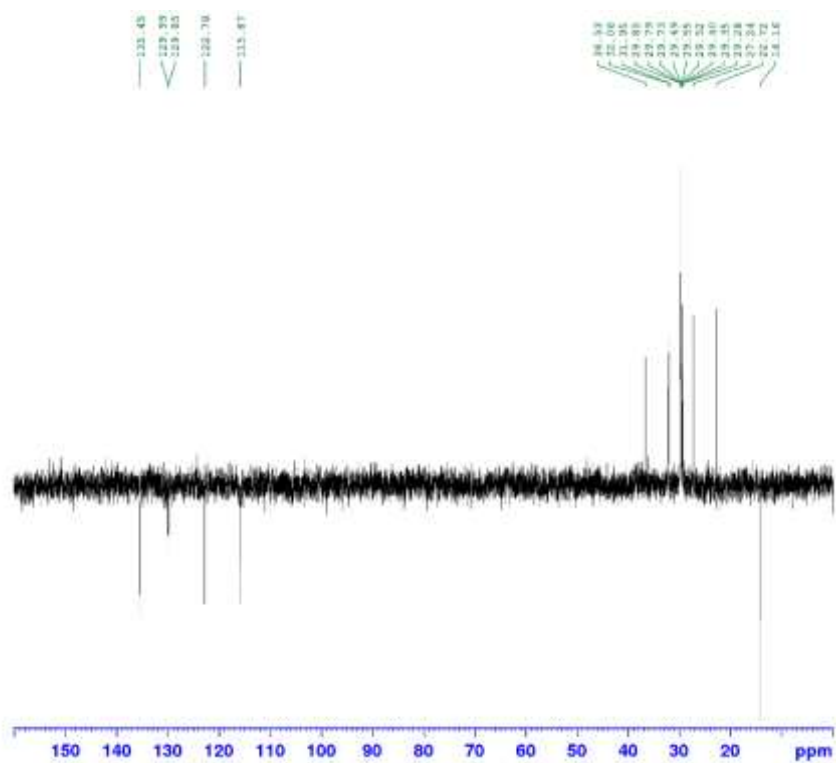
Supplementary Figure S1. EI-MS spectrum of anacardic acid (13:0)



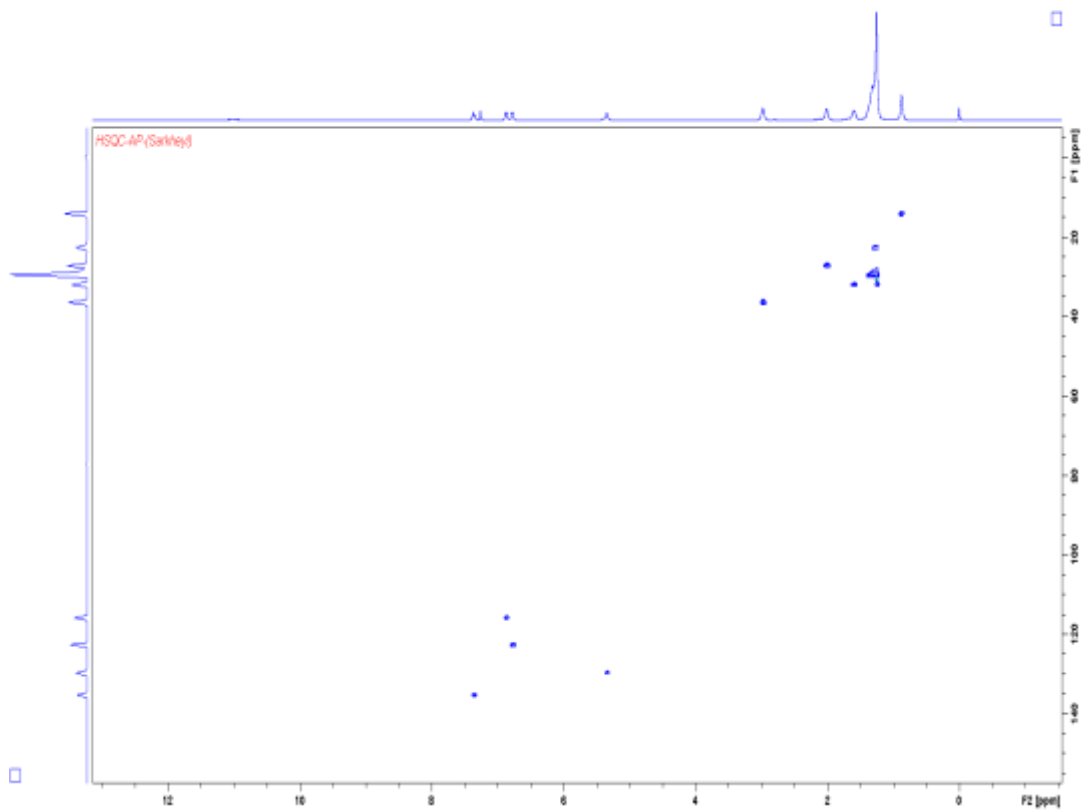
Supplementary Figure S2.  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 400 MHz) spectrum of anacardic acid (13:0) after adding one drop  $\text{D}_2\text{O}$



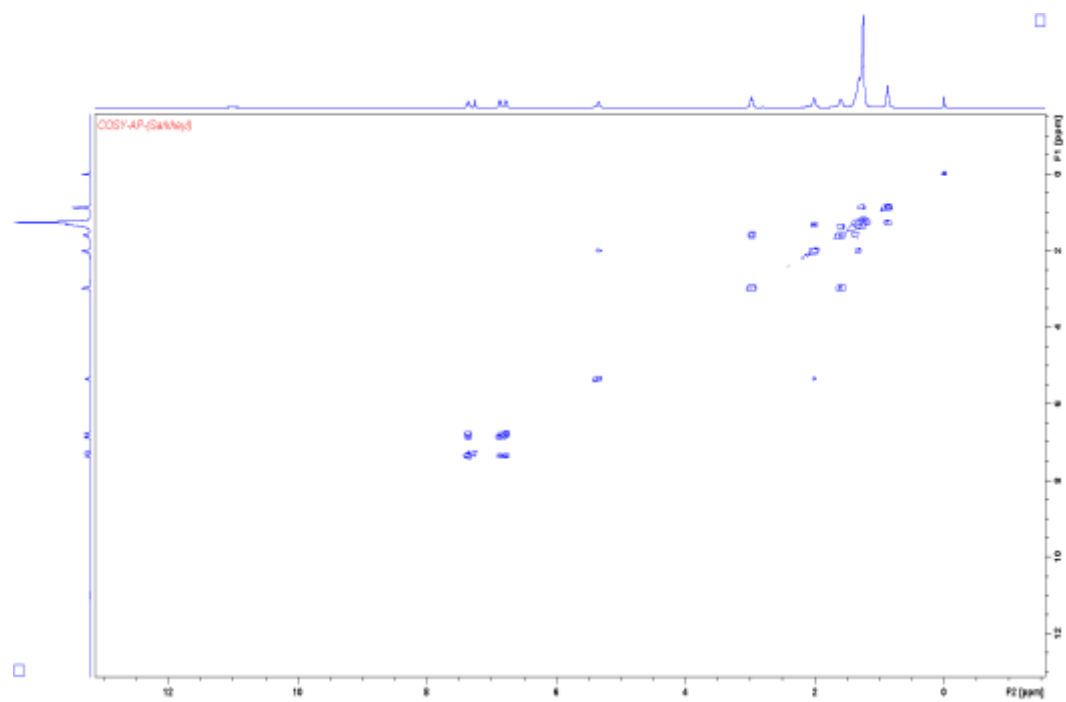
Supplementary Figure S3.  $^{13}\text{C}$ -NMR ( $\text{CDCl}_3$ , 125 MHz) spectrum of anacardic acid (13:0)



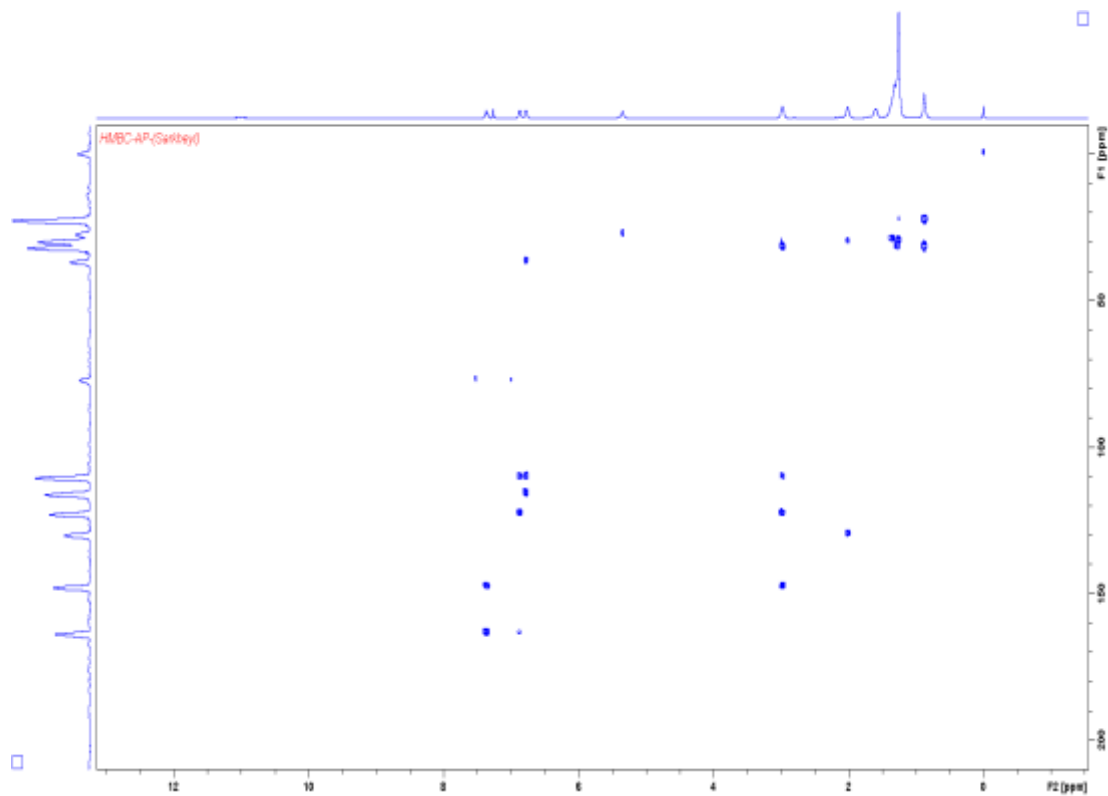
Supplementary Figure S4. DEPT 135 ( $\text{CDCl}_3$ , 125 MHz) spectrum of anacardic acid (13:0)



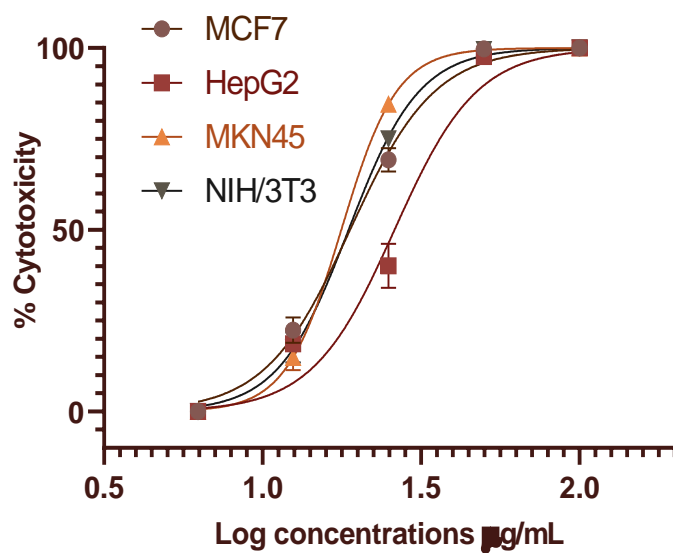
**Supplementary Figure S5.** HSQC (CDCl<sub>3</sub>, 400 MHz) spectrum of anacardic acid (13:0)



**Supplementary Figure S6.** COSY (CDCl<sub>3</sub>, 400 MHz) spectrum of anacardic acid (13:0)



**Supplementary Figure S7.** HMBC (CDCl<sub>3</sub>, 400 MHz) spectrum of anacardic acid (13:0)



**Supplementary Figure S8.** Cytotoxicity of anacardic acid (13:0) against three cancer cell lines (MCF-7, HepG-2 and MKN-45)