**SUPPLEMENTARY FIGURE LEGENDS**

Fig S1. Methanolic bark extracts of *N. cadamba* phytoconstituents fragmentation pattern and their MS spectral data.

Fig S1.1. 2,2’-Bioxirane.

Fig S1.2. Ethanol, 2-nitro-, propionate (ester).

Fig S1.3. L-Alanine, N-methoxycarbonyl-, methyl ester.

Fig S1.4. 1,3,5-Pentanetriol.

Fig S1.5.7-Oxabicyclo[2.2.1]heptanes.

Fig S1.6. Furfural.

Fig S1.7. 2-Furanmethanol.

Fig S1.8. 4-Cyclopenetene-1,3-doine.

Fig S1.9. 2(3H)-Furanone, 5-methyl.

Fig S1.10. Benzaldehyde.

Fig S1.11. 2,4-Dihydroxy-2,5-dimethyl-3(2H)-furan-3-one.

Fig S1.12. Aniline.

Fig S1.13. Formic acid, 2-propenyl ester.

Fig S1.14. 2,5-Anhydro-1,6-dideoxyhexo-3,4-diulose.

Fig S1.15. Phenol, 2-methoxy.

Fig S1.16. 3-Buten-2-ol.

Fig S1.17. 4H-Pyran-4-one, 3-hydroxy-2-methyl.

Fig S1.18. 1,5-Anhydro-6-deoxyhexo-2,3-diulose.

Fig S1.19. 2-Propenal, 3-(2-furanyl).

Fig S1.20. Benzoic acid.

Fig S1.21. (S)-(+)-2',3'-dideoxyribonolactone.

Fig S1.22. Benzene-1,2-diol.

Fig S1.23. 5-Hydroxymethylfurfural.

Fig S1.24. 3,4-Dihydroxyacetophenone.

Fig S1.25. 2H-Pyran-5-carboxylic acid, 2-oxo-, methyl ester.

Fig S1.26. 1,4-Benzenediol.

Fig S1.27. Phenol, 2,6-dimethoxy.

Fig S1.28. Neric acid.

Fig S1.29. Benzoic acid, 4-formyl-, methyl ester.

Fig S1.30. 2-Oxabicyclo[S1.S1.1]heptan-3-one, 1,7,7-trimethyl.

Fig S1.31. 1-Methyl-4-(2-methyl-2-oxiranyl)-7-oxabicyclo[4.1.0]heptane.

Fig S1.32. 2-Hexynal, 4-ethyl.

Fig S1.33. Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester.

Fig S1.34. Beta.-d-glucopyranose, 1,6-anhydro-.

Fig S1.35. 1-Tetradecene.

Fig S1.36. Diethyl phthalate.

Fig S1.37. Phenol, 3,4,5-trimethoxy.

Fig S1.38. 1-Hexadecanol, 2-methyl-.

Fig S1.39. 2H-Benzocyclohepten-2-one, 3,4,4a,5,6,7,8,9-octahydro.

Fig S1.40. Hexadecanoic acid, methyl ester.

Fig S1.41. Pentadec-7-ene, 7-bromomethyl.

Fig S1.42. 2(1H)-Naphthalenone, octahydro-1-methyl-, (1.alpha.,4a.beta.,8a.alpha.).

Fig S1.43. Hexadecanoic acid.

Fig S1.44. Bicyclo[2.2.2]octane-1-carboxylic acid, 4-methyl-.

Fig S1.45. 1-Hexadecanol.

Fig S1.46. 9,12-Octadecadienoic acid, methyl ester, (E,E)-.

Fig S1.47. (9E,12E)-9,12-octadecadienoyl chloride.

Fig S1.48. Phytol.

Fig S1.49. Heptadecanoic acid, 16-methyl-, methyl ester.

Fig S1.50. Trichloroacetic acid, pentadecyl ester.

Fig S1.51. Eicosanoic acid, methyl ester.

Fig S1.52. Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl.

Fig S1.53. Hexadecanal.

Fig S1.54. Hexadecanoic acid, (3-bromoprop-2-ynyl) ester.

Fig S1.55. Hexadecanoic acid, 2-hydroxy-, methyl ester.

Fig S1.56. 9,12-Octadecadienoic acid (Z,Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester.

Fig S1.57. Octadecanoic acid, 2-hydroxy-, methyl ester.

Fig S1.58. 9-Octadecenamide.

Fig S1.59. Squalene.

Fig S1.60. Beta.-sitosterol acetate.

Fig S1.61. Vitamin E.

Fig S2. Compounds detected in methanolic extract of *N. cadamba* by GC-MS/MS.

**Fig S3. Hierarchical clustering of iGEMDOCK post-screening analysis of the interaction profile:**

Fig S3.1. 2LMN target with *N. cadamba* barkmethanolic phytoconstituents and standard.

Fig S3.2. 3LII target with *N. cadamba* barkmethanolic phytoconstituents and standard.