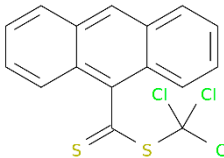
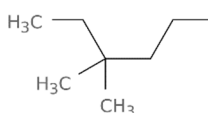
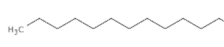
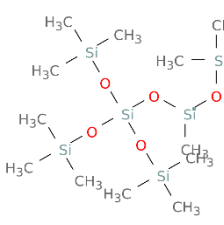
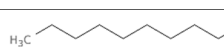
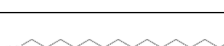
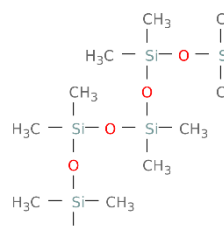
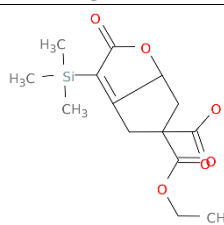
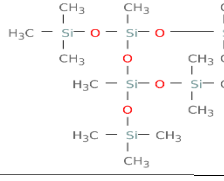


**Table S3.** Major phytocompounds identified in GC-MS profiling of n-hexane extracts of roots (NR) of *P. nepalensis*.

Sl. No	Compounds	Chemical formula	SMILES format	PubChem ID	2D Structures
3a	Trichloromethyl 9-anthracenecarbodithioate	C <sub>16</sub> H <sub>9</sub> Cl <sub>3</sub> S <sub>2</sub>	<chem>C1=CC=C2C(=C1)C=C3C=CC=C3C2C(=S)SC(Cl)(Cl)Cl</chem>	613595	
3b	Heptane, 3,3-dimethyl-	C <sub>9</sub> H <sub>20</sub>	<chem>CCCCC(C)(C)CC</chem>	520991	
3c	Hexadecane	C <sub>16</sub> H <sub>34</sub>	<chem>CCCCCCCCCCCCCCCC</chem>	11006	
3d	1,1,1,5,7,7,7-Heptamethyl-3, 3-bis(trimethylsiloxy)tetrasiloxane	C <sub>13</sub> H <sub>40</sub> O <sub>5</sub> Si <sub>6</sub>	<chem>C[Si](O[Si](C)(C)C)O[Si](O[Si](C)(C)C)O[Si](C)(C)C</chem>	6329081	
3e	Dodecane	C <sub>12</sub> H <sub>26</sub>	<chem>CCCCCCCCCCCC</chem>	8182	
3f	Eicosane	C <sub>20</sub> H <sub>42</sub>	<chem>CCCCCCCCCCCCCCCCCCCC</chem>	8222	
3g	1,1,1,3,5,5,7,7-Nonamethyl-3-(trimethylsiloxy) tetrasiloxane Propanoicacid,	C <sub>12</sub> H <sub>36</sub> O <sub>4</sub> Si <sub>5</sub>	<chem>C[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)C</chem>	8853	
3h	2-oxo-3-(trimethylsilyl)-, trimethylsilyl ester	C <sub>9</sub> H <sub>20</sub> O <sub>3</sub> Si <sub>2</sub>	<chem>CCOC(=O)C1(CC2C(=C(C(=O)O)C2)[Si](C)(C)C)C1C(=O)OCC</chem>	102119459	
3i	1,1,1,3,5,7,7,7-Octamethyl-3,5-bis(trimethylsiloxy) tetrasiloxane	C <sub>14</sub> H <sub>42</sub> O <sub>5</sub> Si <sub>6</sub>	<chem>C[Si](C)(C)O[Si](C)(O[Si](C)(C)C)O[Si](C)(O[Si](C)(C)C)O[Si](C)(C)C</chem>	553110	
3j	2,4,6,9-Dehydroadamantane	C <sub>10</sub> H <sub>12</sub>	<chem>C1C2CC3C4C1C5C2C5C34</chem>	562325	