## **Electronic supplementary information (ESI) for**

## Multifunctional Graphene Quantum Dots for Combined Photothermal and Photodynamic Therapy Coupled with Cancer Cell Tracking Application

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**Figure S1.** (a) High resolution Liquid chromatography mass spectrometry (HR-LCMS) of an aqueous extract of *F. racemosa* leaves. Compounds are labelled in red and have been listed in Table S1. (b) Ball-and-stick models of major compounds identified in the leaf extract. For full structure details, refer Table S1.

Compound	Constituent	Molecular	Retention	Mass
label		formula	time	(Da)
			(min)	
Compound 1	Sulfonic acid [1,2]	C <sub>2</sub> H <sub>7</sub> NO <sub>3</sub> S	0.565	125.0143
Compound 2	Choline[2]	C <sub>5</sub> H <sub>14</sub> NO	0.637	104.1067
Compound 3	11-amino-undecanoic acid	C <sub>11</sub> H <sub>23</sub> NO <sub>2</sub>	0.713	201.1718
	[1,2]			
Compound 4	4S-aminopentanoic acid	C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub>	0.742	117.0779
	[1,2]			
Compound 5	D-galactose[2,3]	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	0.771	180.0625
Compound 6	2-isoprenylemodin	C <sub>20</sub> H <sub>18</sub> O <sub>5</sub>	0.832	338.1168
Compound 7	Neuraminic acid [2,3]	C <sub>9</sub> H <sub>17</sub> NO <sub>8</sub>	1.025	267.0952
Compound 8	Ala-Ala-Phe	C <sub>15</sub> H <sub>21</sub> N <sub>3</sub> O <sub>4</sub>	1.229	307.1512
Compound 9	Ecogonine (alkaloid) [4]	C <sub>9</sub> H <sub>15</sub> NO <sub>3</sub>	1.779	185.1042
Compound 10	Lys-His-Asn	C <sub>16</sub> H <sub>27</sub> N <sub>7</sub> O <sub>5</sub>	1.946	397.2073
Compound 11	Gln-Arg-Glu	C <sub>16</sub> H <sub>29</sub> N <sub>7</sub> O <sub>7</sub>	3.255	431.2126
Compound 12	Ala-Lys-Arg	C <sub>15</sub> H <sub>31</sub> N <sub>7</sub> O <sub>4</sub>	4.574	373.2459
Compound 13	Pro-Gln-Arg	C <sub>16</sub> H <sub>29</sub> N <sub>7</sub> O <sub>5</sub>	4.695	399.2230
Compound 14	Ser-Arg-Ser	C <sub>12</sub> H <sub>24</sub> N <sub>6</sub> O <sub>6</sub>	5.511	348.1736
Compound 15	Leu-Ser-Glu	C <sub>14</sub> H <sub>25</sub> N <sub>3</sub> O <sub>7</sub>	5.607	347.1707
Compound 16	Ser-Lys-Lys	C <sub>15</sub> H <sub>31</sub> N <sub>5</sub> O <sub>5</sub>	5.772	361.2317
Compound 17	<b>Reticuline</b> [4,5]	C <sub>19</sub> H <sub>23</sub> NO <sub>4</sub>	6.055	329.1626
Compound 18	Val-Arg-Asp	C <sub>15</sub> H <sub>28</sub> N <sub>6</sub> O <sub>6</sub>	6.058	388.2065
Compound 19	Arg-Gln-Arg	C <sub>17</sub> H <sub>34</sub> N <sub>10</sub> O <sub>5</sub>	6.488	458.2696
Compound 20	<b>β-sitosterol</b> [2–4,6]	C <sub>29</sub> H <sub>50</sub> O	6.658	414.3435
Compound 21	Ser-Asn-Gly	C <sub>9</sub> H <sub>16</sub> N <sub>4</sub> O <sub>6</sub>	6.719	276.1051

Table S1. List of compounds separated in an HR-LCMS chromatogram from an aqueousextracts of *F. racemosa*.

Compound 22	Glu-Trp-Arg	C <sub>22</sub> H <sub>31</sub> N <sub>7</sub> O <sub>6</sub>	6.836	489.2351
Compound 23	Hydroxy-3-O-methyl-	C <sub>21</sub> H <sub>27</sub> NO <sub>5</sub>	7.569	373.1887
	6beta-naltrexol			
Compound 24	5-Hydroxypropafenone	C <sub>21</sub> H <sub>27</sub> NO <sub>4</sub>	7.972	357.1938
Compound 25	Carboxyterbinafine derivative	C <sub>21</sub> H <sub>25</sub> NO <sub>4</sub>	8.157	355.1783
Compound 26	Swietenine	C <sub>32</sub> H <sub>40</sub> O <sub>9</sub>	10.986	568.27
Compound 27	4-(2-Hydroxy-3- isopropyl aminoproxy)- benzyloxy acetic acid	C <sub>15</sub> H <sub>23</sub> NO <sub>5</sub>	11.509	297.1559
Compound 28	Glu-Asp	$C_9H_{14}N_2O_7$	12.777	262.0804
Compound 29	Lactone	C <sub>16</sub> H <sub>24</sub> O <sub>5</sub>	17.245	296.1601
Compound 30	Lys-Lys-Lys	C <sub>18</sub> H <sub>38</sub> N <sub>6</sub> O <sub>4</sub>	18.872	402.2926
Compound 31	Madecassic acid	C <sub>30</sub> H <sub>48</sub> O <sub>6</sub>	20.328	504.3383



**Figure S2.** FEG-TEM images (a,c,e,g,j) and Cryo-SEM image (i) of carbon soup comprising of different carbon-based structures (left panel) and their corresponding EDAX (right panel). (a, b) GQDs, (c, d) carbon nanospheres, (e, f) CNOs, (g, h) branched carbon nanostructures, (i, j) carbon nanofibers.



**Figure S3**. (a) Carbon soup absorbance spectrum showing a very strong absorption after aqueous dilution (1:100) in UV, visible region, and extension into near infrared region (NIR). (b) X-ray diffraction (XRD) analysis of GQDs.



Fig. S4 (a) AFM image  $(2 \ \mu m \ x \ 2 \ \mu m)$  showing well-dispersed GQDs. Labels represent representative structures used for height analysis. (b) Thickness profile of individual GQDs showing a height around 7-10 nm thick on a vertical axis.



Figure S5. Deconvoluted O1s and N1s spectra of GQDs after 8h of hydrothermal process.

![](_page_8_Figure_0.jpeg)

**Figure S6.** Comparative analysis of deconvoluted C1s XPS spectra taken at different hydrothermal reaction time periods (0h, 2h, 4h, 6h, and 8h) of *F. racemosa* leaves extract and changes occurring in the carbon-oxygen bonds during the process.

![](_page_9_Figure_0.jpeg)

**Figure S7.** Fluorescence imaging study for *Saccharomyces cerevisiae* or Baker's yeast (MarFarland's Scale of 0.5) under different fluorescence emission wavelength filters (Green: 465-95 nm and Red: 540-80 nm). Cells were treated with GQDs (pH 7.2) for 4 h in a shaking conditions at 27°C followed by washing the cells (8000 rpm, 10 min) thrice using PBS (pH 7.0). Untreated yeast cells (Only yeast cells or Negative control) did not show any fluorescence whereas GQDs-labelled cells showed bright multicolour emission after 4 h (100  $\mu$ g mL<sup>-1</sup>, 27°C).

![](_page_10_Figure_0.jpeg)

**Figure S8.** Laser stability studies of bare GQDs (100  $\mu$ g ml<sup>-1</sup>). After irradiation with NIR laser (808 nm), a slight increase in PL intensity was observed after 15 min. The photoluminescence was stable even after continuous 30 min irradiation.

![](_page_11_Figure_0.jpeg)

**Figure S9.** Fluorescence image under FITC excitation wavelength of laser irradiated GQDs treated MDA-MB-231 cells after 2 h on a glass slide. The inset shows fluorescence intensity spectrum of individual cells traced by the blue line.

S.No.	Name of the constituent	Oxygen containing functional groups
1.	β-sitosterol	-OC(O)-
2.	α-amyrin acetate	-OC(O)-
3.	Lupeol acetate	-OC(O)-
4.	Stigmasterol	-OH
5.	Tiglic acid	-COOH
6.	Lupenol	-OH
7.	Lanosterol	-OH
8.	Friedelin	-C(O)-
9.	Gallic acid	-ОН, -СООН
10.	Bergenin	-ОН, -О-, -СООН, -ОС(О)-
11.	Racemosic acid	-C(0)-, -OH, -O-
12.	Kaempferol	-OH, -C(O)-, -O-
13.	Campesterol	-OH
14.	Euphol	-OH
15.	Tirucallol	-OH
16.	Taraxellol	-OH
17.	Methyl ellagic acid	-OH, -C(O)-, -OC(O)-

**Table S2**: Active constituents of *F. racemosa* [7] having oxygen-containing functional groups are listed as follows.

## References

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