

## **Supporting Information**

### **Retrospective analysis of the key molecules involved in the green synthesis of nanoparticles**

Fazlurrahman Khan<sup>1, 2†\*</sup>, Geum-Jae Jeong<sup>3†</sup>, Priyanka Singh<sup>4†</sup>, Nazia Tabassum<sup>1,2</sup>, Ivan  
Mijakovic<sup>4, 5</sup> and Young-Mog Kim<sup>1, 2, 3\*</sup>

<sup>1</sup>*Marine Integrated Biomedical Technology Center, The National Key Research Institutes in Universities, Pukyong National University, Busan, 48513, Republic of Korea*

<sup>2</sup>*Research Center for Marine Integrated Bionics Technology, Pukyong National University, Busan 48513, Republic of Korea*

<sup>3</sup>*Department of Food Science and Technology, Pukyong National University, Busan 48513, Republic of Korea*

<sup>4</sup>*The Novo Nordisk Foundation, Center for Biosustainability, Technical University of Denmark, DK-2800 Kogens Lyngby, Denmark*

<sup>5</sup>*Systems and Synthetic Biology Division, Department of Biology and Biological Engineering, Chalmers University of Technology, SE-412 96 Gothenburg, Sweden*

**Running head:** Role of Pure natural compound in NPs formation

† Equally contributed

\*Corresponding author: Fazlurrahman Khan and Young-Mog Kim

Phone: +82-51-629-5832; Fax: +82-51-629-5824

E-mail: [fkhan055@pknu.ac.kr](mailto:fkhan055@pknu.ac.kr) and [ymkim@pknu.ac.kr](mailto:ymkim@pknu.ac.kr)

**Table S1** Mapping of physiochemical characteristics of extract and pure-compound based NPs

Classification of compounds family	Extract-based NPs									Pure compound-based NPs								
	Extracts	NPs	XRD	Charge	Size (nm)	Shape	FTIR (cm <sup>-1</sup> )	UV-visible spectra (nm)	Ref	Pure Compound	NPs	XRD	Charge	Size (nm)	Shape	FTIR (cm <sup>-1</sup> )	UV-visible spectra (nm)	Ref
Flavonoids	Tulsi	Ag NPs	32°, 38°, 46° and 57°	-	14.6	Spherical	1631, 2118, and 3345	430	<sup>1</sup>	Quercetin	Ag NPs	38°, 44°, and 64°	-	11.35	Spherical	1640, 2112, and 3370	420	<sup>2</sup>
	<i>Clerodendron serratum</i>	Ag NPs	38.2° and 44.1°	-	5-30	Spherical	-	400	<sup>3</sup>	Baicalein	Au NPs	-	-	26.5	Spherical	740, 898, 1082, 1158, 1292, 1386, 1388, and 1656	550	<sup>4</sup>
	<i>Delonix elata</i>	SnO <sub>2</sub>	26.90°, 34.21°, 37.04°, 52.	-	5.92, 6.09, and 7.61	Crystalline	506, 608, 1381, 1618, 2848, 2920, and 3434	220-260	<sup>5</sup>	Rutin	Zinc oxide	-	Negative	20-130	Rod	951, 1114, 1632, 2891, and 3290	355	<sup>6</sup>

			16° , 58.36° , and 65.84°															
Terpenoids	<i>Ocimum sanctum</i>	Au NPs	-	-	1-50	Spherical and non-spherical	-	565	<sup>7</sup>	$\beta$ -caryophyllene	Ag NPs	28.79° , 38.26° , 44.45° , 64.58° , and 77.49°	Negative	29.42	Spherical	615.01, 675.85, 856.90, 1073.78, 1273.01, 1332.61, 1406.50, 1621.46, 2928.96, 3407.98	420	<sup>8</sup>
Polyphenol	<i>Melissa azedarach</i>	Ag NPs	-	-	78	Cubic and spherical	665, 1353, 1631, 2830, 3409, and 3433	436	<sup>9</sup>	Tannic acid	Ag NPs	38.08° , 44.14° , 64.40° , 77.24° , and 81.24°	Negative	27.7-46.7	Spherical	3200	423	<sup>10</sup>

	<i>Piperpedicellatum</i>	Ag NP and Au NPs	38.18°, 44.44°, 36°, 64.96°, , and 55.54°/38.16°, 44.74°, , 64.72°, , 77.64°, , and 81.7°	-	10.5 ± 0.8/14.3 ± 0.5	Spherical, hexagonal, and pentagonal shaped	1078, 1388, 1606, and 3248/1066, 1408, 1612, 2920, and 3267	550/446	<sup>11</sup>	Gallic acid	Au NPs	-	-	8.99 ± 0.92	Spherical	-	520	<sup>12</sup>
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	<i>Aesculus hippocastanum</i>	Ag NPs	38.03°, 44.29°, 64.49°, 77.49°, and 81.51°	Negative	50 ± 5	Spherical	589, 1073, 1636, 2115, and 3246	464	<sup>13</sup>	Resveratrol	Au NPs and Ag NPs	38.18°, 44.42°, 64.62°, 77.52°, and 81.52°	Negative	8.32-21.84	Face-centered cubic structure	1593, 1613, 3393, 3406, 3538, and 3733	547, 412-417	<sup>14</sup>
	Green coffee bean	Ag NPs	-	-	10-30	Spherical	-	405	<sup>15</sup>	Chlorogenic acid	Au NPs	-	Negative	18.94 ± 1.81, 30.42 ± 6.32, 37.86 ± 3.80, 48.72 ± 6.47	Spherical	-	200-350	<sup>16</sup>
	<i>Ecklonia cava</i>	Ag NPs	28.0°, 32.5°, 38.2°, 44.	-	43	Spherical	823, 1030, 1243, 1370, 1609, and 3347	418	<sup>17</sup>	Phloroglucinol	Au NPs and Zn ONPs	38.3°, 45.3°, 56.4°, 66.1°, 75.2°, and 83.8°	Negative	41.6 ± 3.9, 52.7 ± 3.8	Spherical, hexagonal	-	480	<sup>18</sup>

			3°, 46. 4°, 55. 1°, 64. 6°, and 77. 2°								31.6°, 34°, 36°, 47.3°, 56.4°, 62.6°, 67.6°, 68.8°, and 76.6°							
Alkaloid	<i>Coffea arabica</i>	Au NP s	38. 31° , 44. 45° , 64. 64° , and 77. 73°	-	14.90 ± 3.02	Spher ical	1550 and 1750	600- 800	<sup>19</sup>	Caffe ine	Au NP s	-	-	77.9 ± 5.0	-	-	523	<sup>20</sup>
	<i>Chenopodium album</i>	Ag NP s	-	-	39-43	Spher ical	760.90, 1396.44, 1463.23, 1477.99, 1694.28, 1741.85, 2855.26, 3621.10, 3649.64, 3678.67,	421	<sup>21</sup>	Sapon in	Au NP s and Ag NP s	-	-	37.7- 79.9, 17.9- 59.6	Spheri cal, cubica l, and hexag onal/S pheric al	1637.76, 2361.19, 2923.92, 3448.53/ 1120.01, 1637.06, 2363.70, 2924.26, 3422.42	440- 580/2 60- 380	<sup>22</sup>

							and 3744.37											
Macromolecules	<i>Saccorhiza polyschides</i>	Au NPs and Ag NPs	-	Negative	14 ± 2 and 15 ± 3	Spherical	842, 1100-1022, 1259, 1200-800, 1460-1380, 2940-2928, and 3460-3408	534	<sup>23</sup>	Fucoidan	Au NPs	38.13° , 44.43° , 64.66° , and 77.66°	Negative	~53	Spherical	845, 1159-1260, 1633, 1637, 2932, 2933, 3441, and 3444	570	<sup>24</sup>
	Silk worm cocoon	Ag NPs	-	-	48-117	Round	830, 1200-1300, 1353, 1404, 1451, 1500-1560, and 1600-1700	420	<sup>25</sup>	Sericin	Ag NPs	19.8° , 38.2° , and 64.4°	-	4-20	-	1402, 1532, and 1657	405	<sup>26</sup>

Others	<i>Curvularia pallens</i>	Ag NP s	37.9°, 44.1°, 64.1°, and 77.0°	-	16.74	Spherical	-	415	<sup>27</sup>	Curvularin	Ag NP s	38.68° , 46.1° , 64.11° , and 77.4°	Negative	37	Spherical	1639, 2928, and 3304	430	<sup>28</sup>
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