SUPPLEMENTARY MATERIAL

New p-Terphenyl and Benzoquinone Metabolites from the Bioluminescent Mushroom Neonothopanus nambi

Watchara Sangsopha\textsuperscript{a}, Ratsami Lekphrom\textsuperscript{a,*}, Florian T. Schevenels\textsuperscript{a}, Weerasak Saksirirat\textsuperscript{b}, Sureeporn Bua-art\textsuperscript{c}, Kwanjai Kanokmedhakul\textsuperscript{a} and Somdej Kanokmedhakul\textsuperscript{a}

\textsuperscript{a}Natural Products Research Unit, Department of Chemistry and Centre for Innovation in Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand
\textsuperscript{b}Agricultural Biotechnology Research Centre for Sustainable Economy, Faculty of Agriculture, Khon Kaen University, Khon Kaen 40002, Thailand
\textsuperscript{c}Plant Pathology Research Group, Plant Protection Research and Development Office, Department of Agriculture, Bangkok 10900, Thailand

Abstract: Two new p-terphenyls, neonambiterphenyls A and B (1-2), a new benzoquinone, neonambiquinone A (3), together with six known sesquiterpenes (4-9), were isolated from the bioluminescent mushroom \textit{Neonothopanus nambi} PW3. The isolated compounds were identified by mass, IR and spectroscopic analyses (1D and 2D NMR). Compounds 1-3 and 5-7 showed cytotoxicity against cancer cell lines, KB, NCI-H187 and MCF-7 with IC\textsubscript{50} values ranging from 1.45 to 49.31 µg/mL. In addition, compounds 1 and 5 showed cytotoxicity against Vero cells with IC\textsubscript{50} values of 38.72 and 32.90 µg/mL, respectively.

Key words: Neonothopanus nambi; p-terphenyl; benzoquinone; sesquiterpene; aurisin; cytotoxicity

*Correspondence author

E-mail address: ratsami@kku.ac.th
Contents

| Figure S1 | Mass spectrum of 1 | 3 |
| Figure S2 | IR spectrum of 1 | 3 |
| Figure S3 | $^1$H NMR (400 MHz, CDCl$_3$ + CD$_3$OD) of 1 | 4 |
| Figure S4 | $^{13}$C NMR (100 MHz, CDCl$_3$ + CD$_3$OD) of 1 | 4 |
| Figure S5 | $^1$H-$^1$H COSY (CDCl$_3$ + CD$_3$OD) of 1 | 5 |
| Figure S6 | HSQC (CDCl$_3$ + CD$_3$OD) of 1 | 5 |
| Figure S7 | HMBC (CDCl$_3$ + CD$_3$OD) of 1 | 6 |
| Figure S8 | Mass spectrum of 2 | 6 |
| Figure S9 | IR spectrum of 2 | 7 |
| Figure S10 | $^1$H NMR (400 MHz, CDCl$_3$ + CD$_3$OD) of 2 | 7 |
| Figure S11 | $^{13}$C NMR (100 MHz, CDCl$_3$ + CD$_3$OD) of 2 | 8 |
| Figure S12 | $^1$H-$^1$H COSY (CDCl$_3$ + CD$_3$OD) of 2 | 8 |
| Figure S13 | HSQC (CDCl$_3$ + CD$_3$OD) of 2 | 9 |
| Figure S14 | HMBC (CDCl$_3$ + CD$_3$OD) of 2 | 9 |
| Figure S15 | Mass spectrum of 3 | 10 |
| Figure S16 | IR spectrum of 3 | 10 |
| Figure S17 | $^1$H NMR (400 MHz, CDCl$_3$ + CD$_3$OD) of 3 | 11 |
| Figure S18 | $^{13}$C NMR (100 MHz, CDCl$_3$ + CD$_3$OD) of 3 | 11 |
| Figure S19 | $^1$H-$^1$H COSY (CDCl$_3$ + CD$_3$OD) of 3 | 12 |
| Figure S20 | HSQC (CDCl$_3$ + CD$_3$OD) of 3 | 12 |
| Figure S21 | HMBC (CDCl$_3$ + CD$_3$OD) of 3 | 13 |
| Figure S22 | Key HMBC and COSY correlations of compounds 1-3 | 13 |
| Table S1 | Antimalarial and Cytotoxicity Activities from *N. Nambi* PW3 | 14 |
| Table S2 | Antibiotic Activities from *N. nambi* PW3 | 14 |
| Table S3 | $^1$H (400 MHz) and $^{13}$C NMR (100 MHz) Data of Compounds 1, 2 and 3 (CDCl$_3$+CD$_3$OD) | 15 |
Figure S1 Mass spectrum of 1

| # | m/z   | I     | I %  | S/N  | FWHM | Res. |
|---|-------|-------|------|------|------|------|
| 1 | 230.2470 | 76212 | 32.2 | 101.7 | 0.0502 | 4590 |
| 2 | 271.1151 | 19519 | 8.2  | 24.9 | 0.0641 | 4228 |
| 3 | 274.2718 | 83065 | 35.1 | 108.3 | 0.0577 | 4756 |

Figure S2 IR spectrum of 1
Figure S3 $^1$H NMR (400 MHz, CDCl$_3$ + CD$_3$OD) of 1

Figure S4 $^{13}$C NMR (100 MHz, CDCl$_3$ + CD$_3$OD) of 1
Figure S5 $^1\text{H}-^1\text{H}$ COSY (CDCl$_3$ + CD$_3$OD) of 1

Figure S6 HSQC (CDCl$_3$ + CD$_3$OD) of 1
Figure S7 HMBC (CDCl$_3$ + CD$_3$OD) of 1

Figure S8 Mass spectrum of 2
Figure S9 IR spectrum of 2

Figure S10 $^1$H NMR (400 MHz, CDCl$_3$ + CD$_3$OD) of 2
Figure S11 $^{13}$C NMR (100 MHz, CDCl$_3$ + CD$_3$OD) of 2

Figure S12 $^1$H-$^1$H COSY (CDCl$_3$ + CD$_3$OD) of 2
Figure S13 HSQC (CDCl$_3$ + CD$_3$OD) of 2

Figure S14 HMBC (CDCl$_3$ + CD$_3$OD) of 2
**Figure S15** Mass spectrum of 3

![Mass spectrum of 3](Image)

**Figure S16** IR spectrum of 3

![IR spectrum of 3](Image)
Figure S17 $^1$H NMR (400 MHz, CDCl$_3$ + CD$_3$OD) of 3

Figure S18 $^{13}$C NMR (100 MHz, CDCl$_3$ + CD$_3$OD) of 3
Figure S19 $^1$H-$^1$H COSY (CDCl$_3$ + CD$_3$OD) of 3

Figure S20 HSQC (CDCl$_3$ + CD$_3$OD) of 3
Figure S21 HMBC (CDCl$_3$ + CD$_3$OD) of 3

Figure S22 Key HMBC and COSY correlations of compounds 1-3
Table S1 Antimalarial and Cytotoxicity Activities from *N. Nambi* PW3

| Compound | antimalarial (IC$_{50}$, µg/mL) | cytotoxicity (IC$_{50}$, µg/mL) | KB | NCI-H187 | MCF-7 | Vero cell |
|----------|---------------------------------|----------------------------------|----|----------|--------|-----------|
| 1        | inactive                        | 9.12                             | 16.82 | 11.82  | 38.72  |
| 2        | inactive                        | 40.90                            | 5.60  | inactive | inactive |
| 3        | inactive                        | inactive                         | 44.69 | inactive | inactive |
| 4        | inactive                        | 1.45                             | 5.03  | 18.64  | 32.90  |
| 5        | inactive                        | inactive                         | 9.40  | inactive | inactive |
| 6        | inactive                        | inactive                         | 49.31 | inactive | inactive |
| 7        | inactive                        | 0.002                            | inactive | inactive | inactive |
| 9        | inactive                        | ellipticine                      | 1.21  | 0.935 | 0.85 |
|          | dihydroartemisinin             | 1.21                             | 0.935 | 0.85 |
|          | tamoxifen                      | 1.21                             | 0.935 | 0.85 |
|          | doxorubicin                    | 1.21                             | 0.935 | 0.85 |

*a*Humanepidermoid carcinoma in the mouth, *b*Human lung cancer cell, *c*Human breast cancer cell. Inactive (>50 µg/mL)

Table S2 Antibiotic Activities from *N. nambi* PW3

| Compound | MIC (final concentration = 128 µg/ml) |
|----------|--------------------------------------|
|          | Gram negative | Gram positive |
|          | *Escherichia coli* | *Pseudomonas aeruginosa* | *Shigella sonnei* | *Bacillus cereus* | *Staphylococcus aureus* |
| 1        | inactive | 128 | 128 | 64 | 4 |
| 2        | inactive | inactive | inactive | 64 | 8 |
| 3        | inactive | inactive | inactive | 64 | 64 |
| 4        | inactive | 128 | inactive | 128 | inactive |
| 5        | inactive | 128 | inactive | 128 | inactive |
| 6        | inactive | inactive | inactive | 128 | inactive |
| Kanamycin | 2 | 2 |
| Gentamicin | 2 | 2 |
| Vancomycin | 1 | 1 |

Inactive (>128 µg/mL)
Table S3 $^1$H (400 MHz) and $^{13}$C NMR (100 MHz) Data of Compounds 1, 2 and 3 (CDCl$_3$+CD$_3$OD)

| No. | $\delta$H | $\delta$C | $\delta$H | $\delta$C | $\delta$H | $\delta$C |
|-----|-----------|-----------|-----------|-----------|-----------|-----------|
| 1   | 115.1     |           | 115.1     |           | 119.3     |           |
| 2   | 150.5     |           | 150.5     |           | 7.15 (d, 8.4) | 131.6 |
| 3   | 6.99 (s)  | 98.2      | 6.98 (s)  | 98.3      | 6.83 (d, 7.6) | 115.2 |
| 4   | 144.6     |           |           | 144.7     |           |           |
| 5   | 141.1     |           | 141.3     |           | 6.83 (d, 7.6) | 115.2 |
| 6   | 7.42 (s)  | 107.2     | 7.44 (s)  | 107.4     | 7.15 (d, 8.4) | 131.6 |
| 1'  | 114.0     |           |           | 113.9     |           |           |
| 2'  | 148.9     |           |           | 149.1     |           |           |
| 3'  | 125.6     |           |           | 125.4     |           |           |
| 4'  | 132.1     |           |           | 132.1     |           |           |
| 5'  | 6.57 (s)  | 109.7     | 6.61 (s)  | 109.6     |           |           |
| 6'  | 148.8     |           |           | 148.8     |           |           |
| 1'' | 129.0     |           |           | 129.6     |           |           |
| 2'' | 7.23 (d, 8.4) | 130.1 | 6.88 (d, 1.6) | 116.0 | 7.39 (d, 8.4) | 131.0 |
| 3'' | 6.79 (d, 8.4) | 115.2 | 144.2     | 6.83 (d, 7.6) | 115.6 |
| 4'' | 156.0     |           |           | 144.2     |           | 159.3     |
| 5'' | 6.79 (d, 8.4) | 115.2 | 6.79 (s)  | 115.2     | 6.83 (d, 7.6) | 115.6 |
| 6'' | 7.23 (d, 8.4) | 130.1 | 6.78 (d, 1.6) | 120.9 | 7.39 (d, 8.4) | 131.0 |
| CH$_3$CO | 170.0 |           | 170.0     |           | 168.7     |
| CH$_3$CO | 2.19 (s) | 20.5    | 2.19 (s)  | 20.4      | 2.19 (s)  | 20.2      |