

# Supporting Information

## Functional Nanoparticles-Coated Nanomechanical Sensor Arrays for Machine Learning-Based Quantitative Odor Analysis

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Kosuke Minami,<sup>‡</sup> Huynh Thien Ngo,<sup>‡</sup> Gaku Imamura,<sup>†,‡</sup> Koji Tsuda,<sup>§,||,⊥</sup> and Genki Yoshikawa<sup>†,‡,#</sup>*

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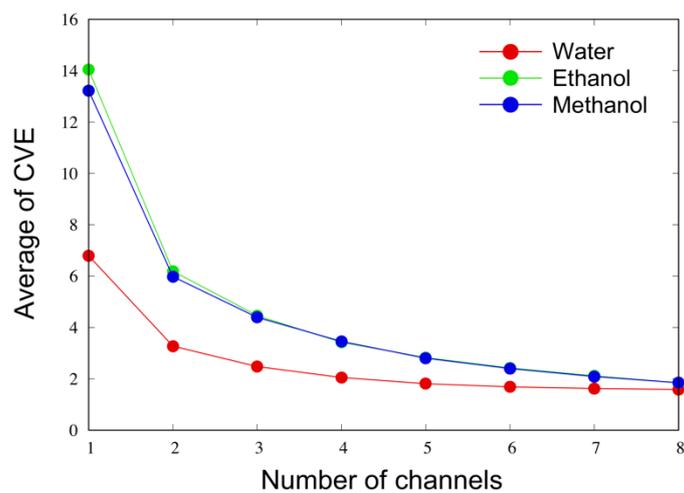
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<sup>||</sup> Graduate School of Frontier Sciences, The University of Tokyo, 5-1-5 Kashiwa-no-ha, Kashiwa, Chiba 277-8561, Japan.

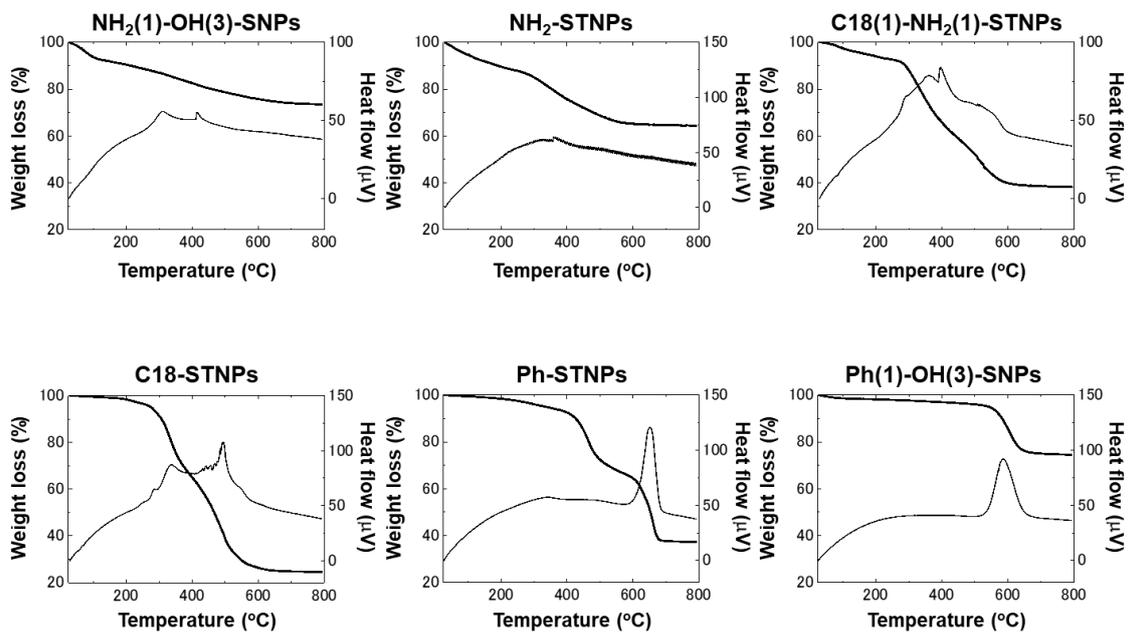
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<sup>#</sup> Materials Science and Engineering, Graduate School of Pure and Applied Science, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8571, Japan.

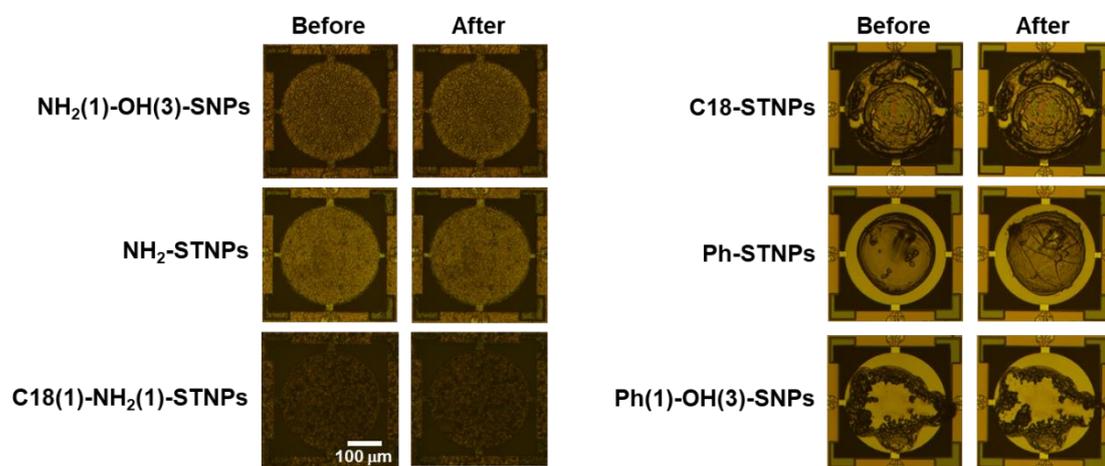
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[TAMURA.Ryo@nims.go.jp](mailto:TAMURA.Ryo@nims.go.jp)



**Figure S1.** Averages of cross validation errors (CVEs) depending on the number of channels for water, ethanol and methanol. We calculated CVEs for all combinations of channels (the number of models is  $2^8 - 1 = 255$ ). The monotonically decreasing of CVEs was observed against the number of channels which corresponds to the number of features. This result indicates that the regularization in Gaussian process regression works well and overfitting is prevented if the number of channels is increased.

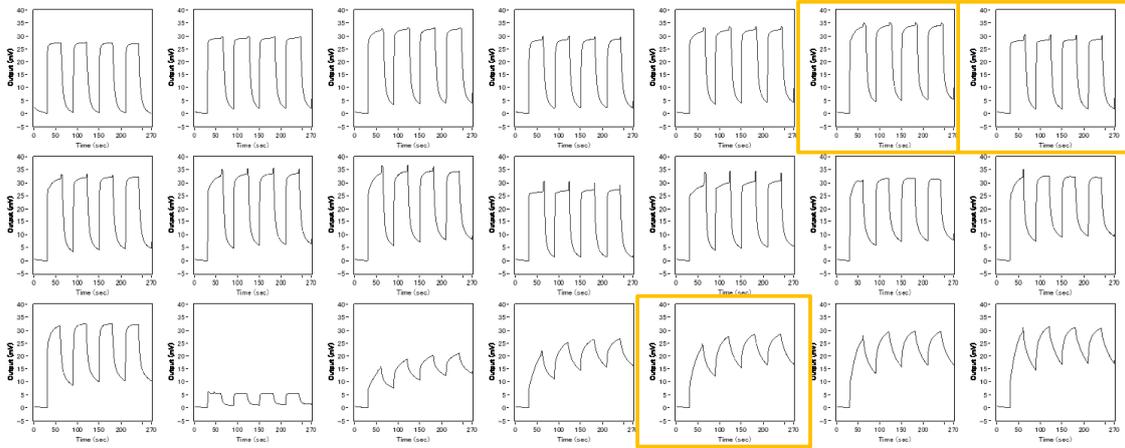


**Figure S2.** TG-DTA curves of the six types of NPs synthesized in the present study. A bold line and a normal line represent a TG curve and a DTA curve, respectively.



**Figure S3.** Optical microscope images of the six types of NPs coated on the surface of MSS before and after vapor measurements.

### NH<sub>2</sub>(1)-OH(3)-SNPs

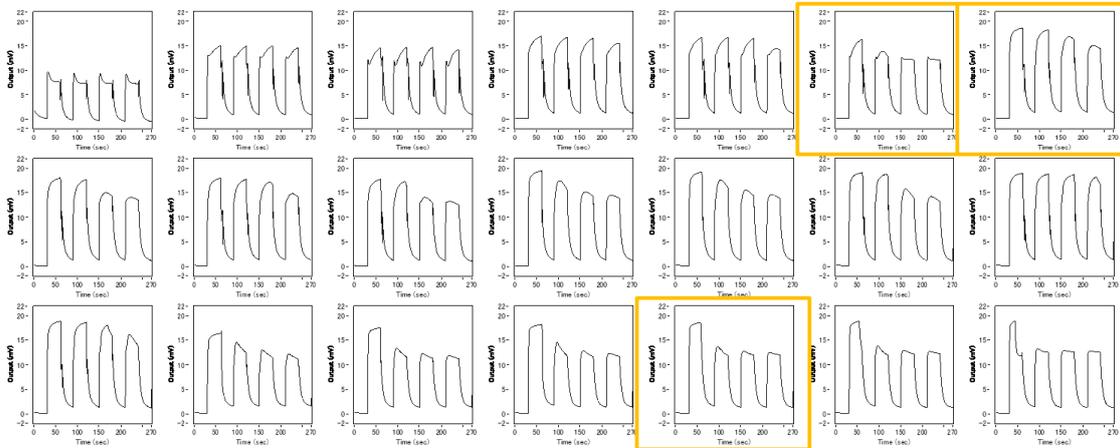


|                     |                     |                    |                    |                     |                     |                     |
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| W: 40, E: 40, M: 20 | W: 40, E: 20, M: 40 | W: 40, E: 0, M: 60 | W: 20, E: 80, M: 0 | W: 20, E: 60, M: 20 | W: 20, E: 40, M: 40 | W: 20, E: 20, M: 60 |
| W: 20, E: 0, M: 80  | W: 0, E: 100, M: 0  | W: 0, E: 80, M: 20 | W: 0, E: 60, M: 40 | W: 0, E: 40, M: 60  | W: 0, E: 20, M: 80  | W: 0, E: 0, M: 100  |

White: Training data, Orange: Test data

**Figure S4.** Responses of NH<sub>2</sub>(1)-OH(3)-SNPs-coated MSS to the 21 samples.

## NH<sub>2</sub>-STNPs

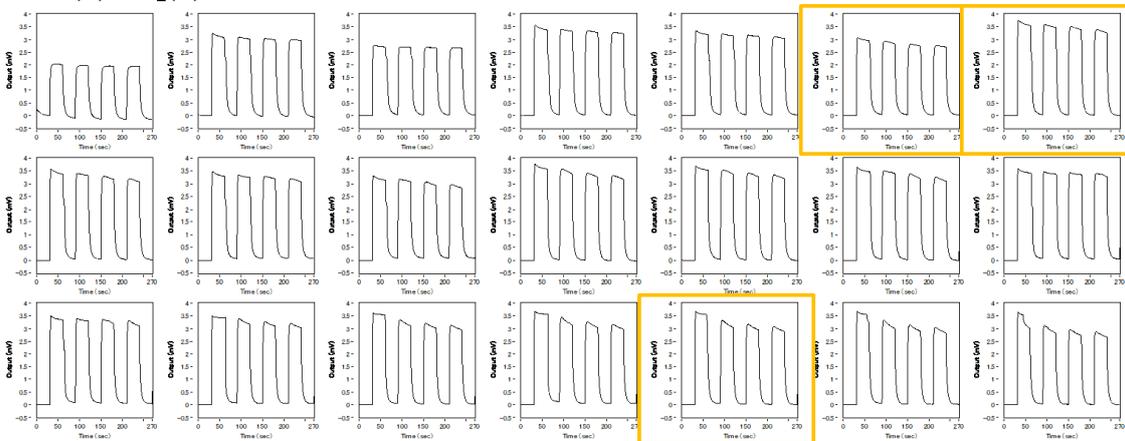


|                     |                     |                    |                    |                     |                     |                     |
|---------------------|---------------------|--------------------|--------------------|---------------------|---------------------|---------------------|
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| W: 40, E: 40, M: 20 | W: 40, E: 20, M: 40 | W: 40, E: 0, M: 60 | W: 20, E: 80, M: 0 | W: 20, E: 60, M: 20 | W: 20, E: 40, M: 40 | W: 20, E: 20, M: 60 |
| W: 20, E: 0, M: 80  | W: 0, E: 100, M: 0  | W: 0, E: 80, M: 20 | W: 0, E: 60, M: 40 | W: 0, E: 40, M: 60  | W: 0, E: 20, M: 80  | W: 0, E: 0, M: 100  |

White: Training data, Orange: Test data

**Figure S5.** Responses of NH<sub>2</sub>-STNPs-coated MSS to the 21 samples.

### C18(1)-NH<sub>2</sub>(1)-STNPs

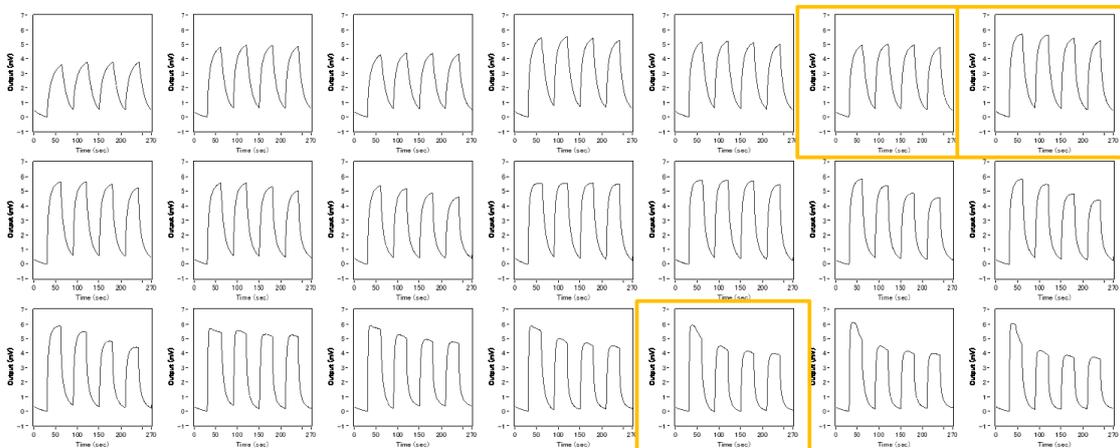


|                     |                     |                    |                    |                     |                     |                     |
|---------------------|---------------------|--------------------|--------------------|---------------------|---------------------|---------------------|
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| W: 40, E: 40, M: 20 | W: 40, E: 20, M: 40 | W: 40, E: 0, M: 60 | W: 20, E: 80, M: 0 | W: 20, E: 60, M: 20 | W: 20, E: 40, M: 40 | W: 20, E: 20, M: 60 |
| W: 20, E: 0, M: 80  | W: 0, E: 100, M: 0  | W: 0, E: 80, M: 20 | W: 0, E: 60, M: 40 | W: 0, E: 40, M: 60  | W: 0, E: 20, M: 80  | W: 0, E: 0, M: 100  |

White: Training data, Orange: Test data

**Figure S6.** Responses of C18(1)-NH<sub>2</sub>(1)-STNPs-coated MSS to the 21 samples.

### C18-STNPs

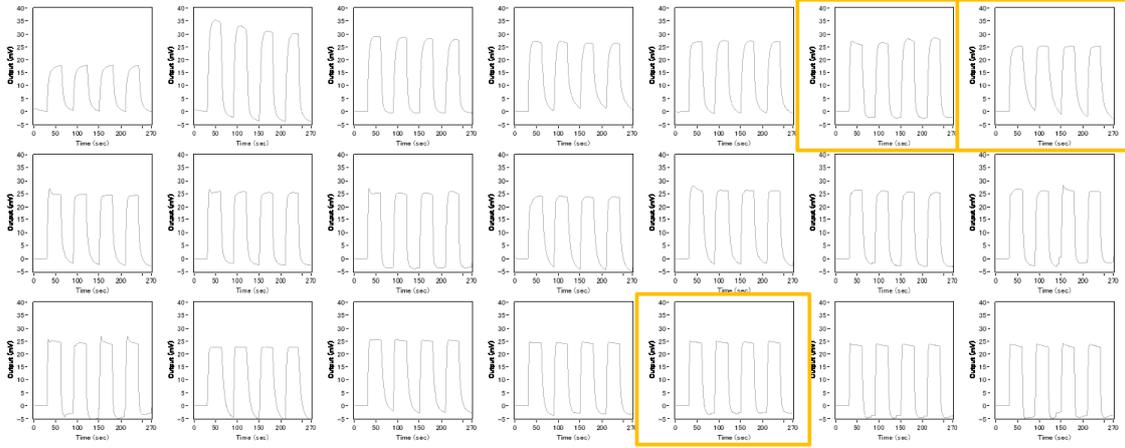


|                     |                     |                    |                    |                     |                     |                     |
|---------------------|---------------------|--------------------|--------------------|---------------------|---------------------|---------------------|
| W: 100, E: 0, M: 0  | W: 80, E: 20, M: 0  | W: 80, E: 0, M: 20 | W: 60, E: 40, M: 0 | W: 60, E: 20, M: 20 | W: 60, E: 0, M: 40  | W: 40, E: 60, M: 0  |
| W: 40, E: 40, M: 20 | W: 40, E: 20, M: 40 | W: 40, E: 0, M: 60 | W: 20, E: 80, M: 0 | W: 20, E: 60, M: 20 | W: 20, E: 40, M: 40 | W: 20, E: 20, M: 60 |
| W: 20, E: 0, M: 80  | W: 0, E: 100, M: 0  | W: 0, E: 80, M: 20 | W: 0, E: 60, M: 40 | W: 0, E: 40, M: 60  | W: 0, E: 20, M: 80  | W: 0, E: 0, M: 100  |

White: Training data, Orange: Test data

**Figure S7.** Responses of C18-STNPs-coated MSS to the 21 samples.

### Ph-STNPs

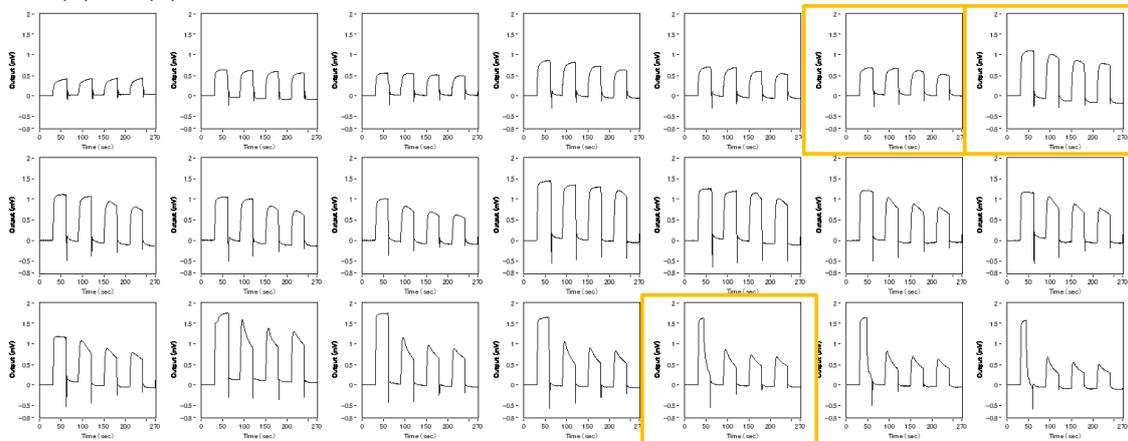


|                     |                     |                    |                    |                     |                     |                     |
|---------------------|---------------------|--------------------|--------------------|---------------------|---------------------|---------------------|
| W: 100, E: 0, M: 0  | W: 80, E: 20, M: 0  | W: 80, E: 0, M: 20 | W: 60, E: 40, M: 0 | W: 60, E: 20, M: 20 | W: 60, E: 0, M: 40  | W: 40, E: 60, M: 0  |
| W: 40, E: 40, M: 20 | W: 40, E: 20, M: 40 | W: 40, E: 0, M: 60 | W: 20, E: 80, M: 0 | W: 20, E: 60, M: 20 | W: 20, E: 40, M: 40 | W: 20, E: 20, M: 60 |
| W: 20, E: 0, M: 80  | W: 0, E: 100, M: 0  | W: 0, E: 80, M: 20 | W: 0, E: 60, M: 40 | W: 0, E: 40, M: 60  | W: 0, E: 20, M: 80  | W: 0, E: 0, M: 100  |

White: Training data, Orange: Test data

**Figure S8.** Responses of Ph-STNPs-coated MSS to the 21 samples.

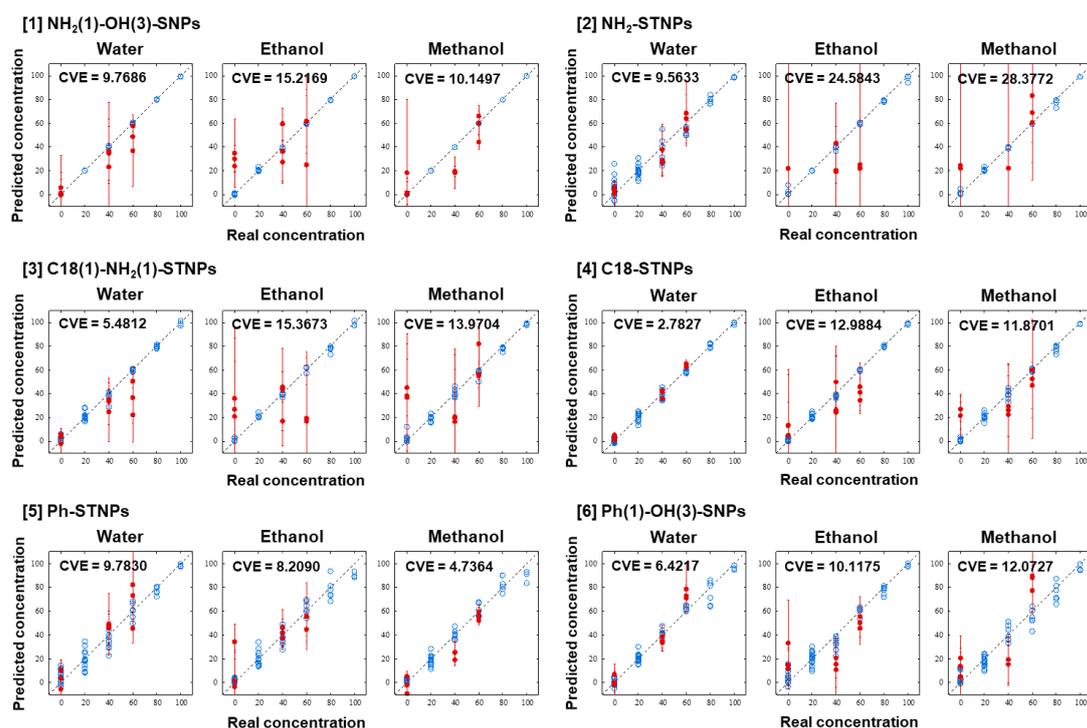
### Ph(1)-OH(3)-SNPs



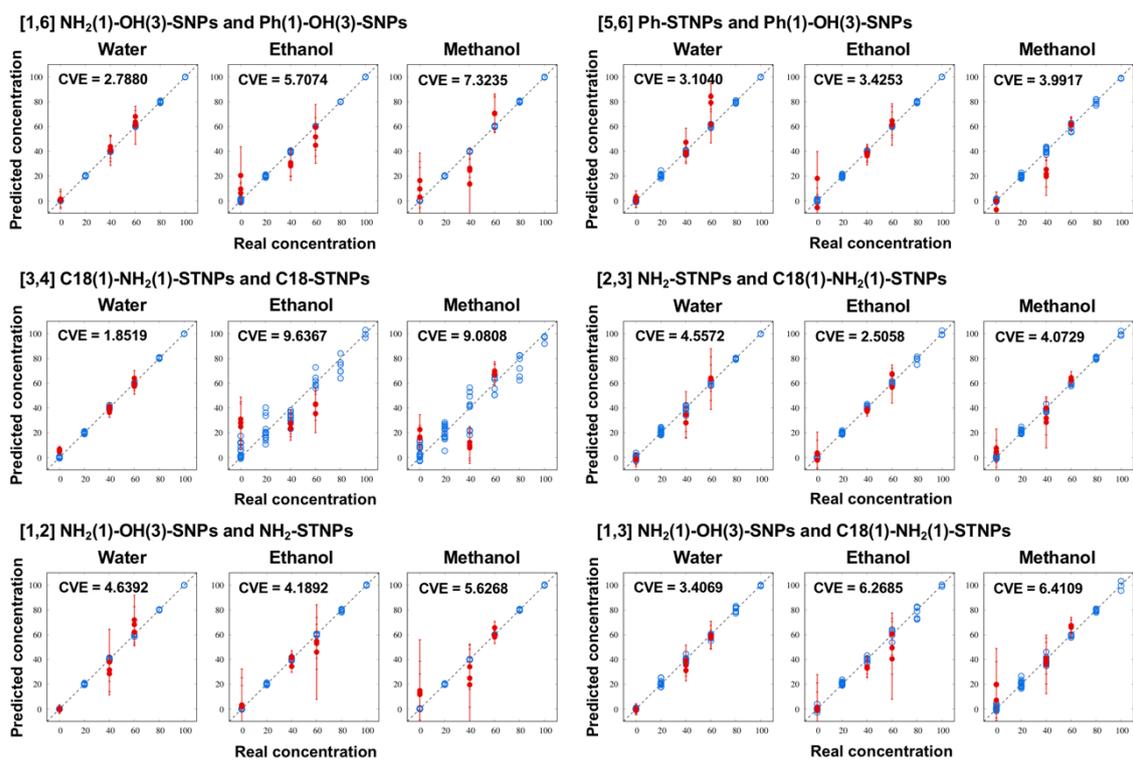
|                     |                     |                    |                    |                     |                     |                     |
|---------------------|---------------------|--------------------|--------------------|---------------------|---------------------|---------------------|
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| W: 40, E: 40, M: 20 | W: 40, E: 20, M: 40 | W: 40, E: 0, M: 60 | W: 20, E: 80, M: 0 | W: 20, E: 60, M: 20 | W: 20, E: 40, M: 40 | W: 20, E: 20, M: 60 |
| W: 20, E: 0, M: 80  | W: 0, E: 100, M: 0  | W: 0, E: 80, M: 20 | W: 0, E: 60, M: 40 | W: 0, E: 40, M: 60  | W: 0, E: 20, M: 80  | W: 0, E: 0, M: 100  |

White: Training data, Orange: Test data

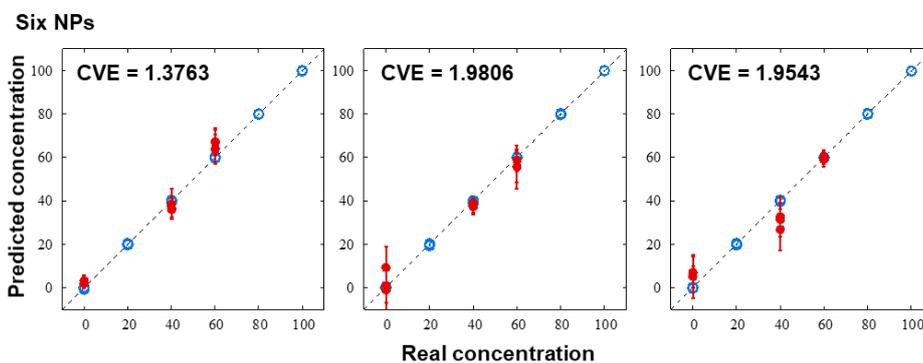
**Figure S9.** Responses of Ph(1)-OH(3)-SNPs-coated MSS to the 21 samples.



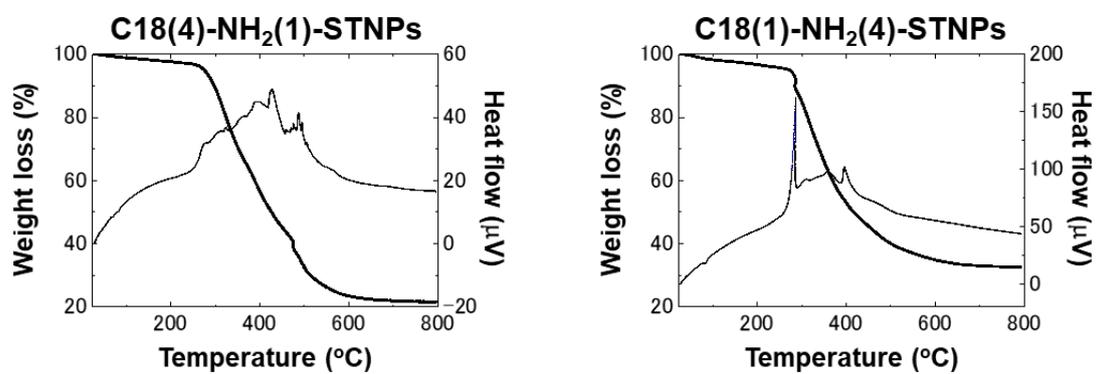
**Figure S10.** Parity plots of real concentration versus predicted concentration of water, ethanol and methanol. Four features obtained from the data taken with a single type of NPs are used. The blue points represent the training data set that we used to train the machine learning model. The red points represent the test data set. The error bars are evaluated as 95% confidence interval.



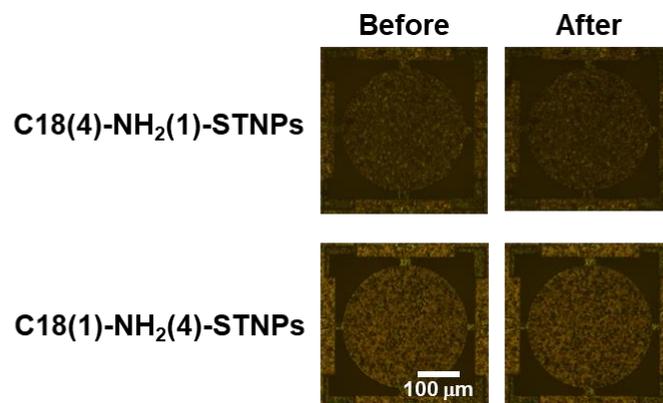
**Figure S11.** Parity plots of real concentration versus predicted concentration of water, ethanol and methanol. Eight features obtained from the data taken with the combination of two types of NPs are used. The blue points represent the training data set that was used to train the machine learning model. The red points represent the test data set. The error bars are evaluated as 95% confidence interval.



**Figure S12.** Parity plots of real concentration versus predicted concentration of water, ethanol and methanol. Twenty-four features obtained from the data taken with the six types of NPs are used. The blue points represent the training data set that was used to train the machine learning model. The red points represent the test data set. The error bars are evaluated as 95% confidence interval.

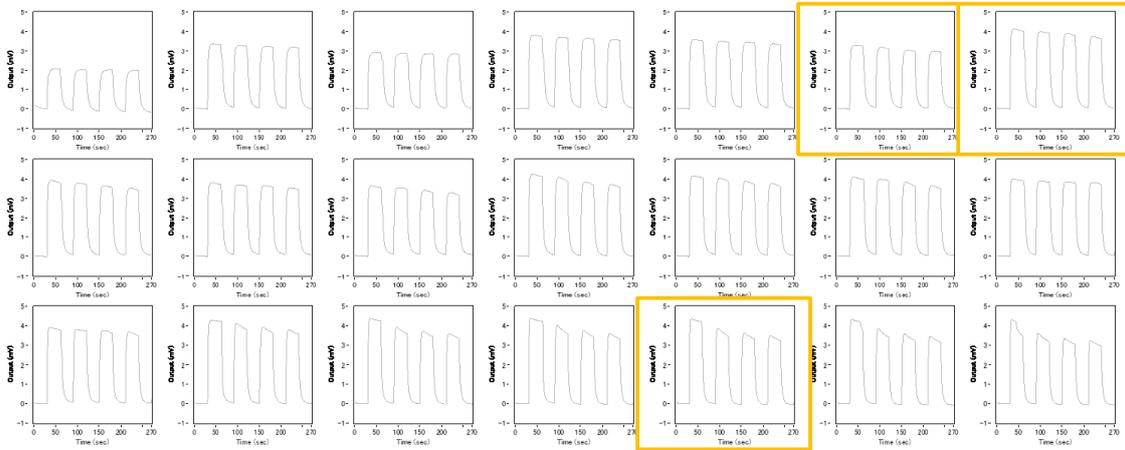


**Figure S13.** TG-DTA curves of C18(4)-NH<sub>2</sub>(1)-STNPs and C18(1)-NH<sub>2</sub>(4)-STNPs. A bold line and a normal line represent a TG curve and a DTA curve, respectively.



**Figure S14.** Optical microscope images of C18(4)-NH<sub>2</sub>(1)-STNPs and C18(1)-NH<sub>2</sub>(4)-STNPs coated on the surface of MSS before and after vapor measurements.

C18(4)-NH<sub>2</sub>(1)-STNPs

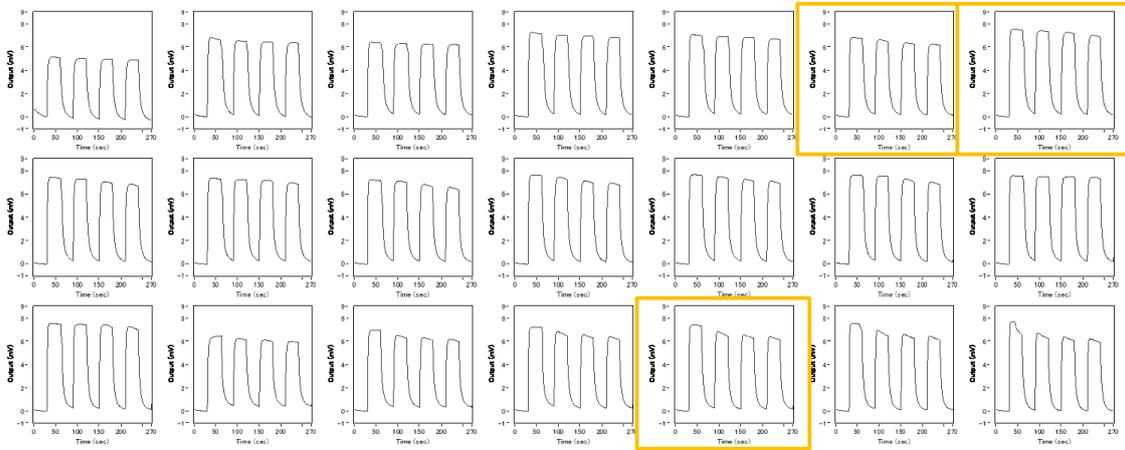


|                     |                     |                    |                    |                     |                     |                     |
|---------------------|---------------------|--------------------|--------------------|---------------------|---------------------|---------------------|
| W: 100, E: 0, M: 0  | W: 80, E: 20, M: 0  | W: 80, E: 0, M: 20 | W: 60, E: 40, M: 0 | W: 60, E: 20, M: 20 | W: 60, E: 0, M: 40  | W: 40, E: 60, M: 0  |
| W: 40, E: 40, M: 20 | W: 40, E: 20, M: 40 | W: 40, E: 0, M: 60 | W: 20, E: 80, M: 0 | W: 20, E: 60, M: 20 | W: 20, E: 40, M: 40 | W: 20, E: 20, M: 60 |
| W: 20, E: 0, M: 80  | W: 0, E: 100, M: 0  | W: 0, E: 80, M: 20 | W: 0, E: 60, M: 40 | W: 0, E: 40, M: 60  | W: 0, E: 20, M: 80  | W: 0, E: 0, M: 100  |

White: Training data, Orange: Test data

**Figure S15.** Responses of C18(4)-NH<sub>2</sub>(1)-STNPs-coated MSS to the 21 samples.

C18(1)-NH<sub>2</sub>(4)-STNPs



|                     |                     |                    |                    |                     |                     |                     |
|---------------------|---------------------|--------------------|--------------------|---------------------|---------------------|---------------------|
| W: 100, E: 0, M: 0  | W: 80, E: 20, M: 0  | W: 80, E: 0, M: 20 | W: 60, E: 40, M: 0 | W: 60, E: 20, M: 20 | W: 60, E: 0, M: 40  | W: 40, E: 60, M: 0  |
| W: 40, E: 40, M: 20 | W: 40, E: 20, M: 40 | W: 40, E: 0, M: 60 | W: 20, E: 80, M: 0 | W: 20, E: 60, M: 20 | W: 20, E: 40, M: 40 | W: 20, E: 20, M: 60 |
| W: 20, E: 0, M: 80  | W: 0, E: 100, M: 0  | W: 0, E: 80, M: 20 | W: 0, E: 60, M: 40 | W: 0, E: 40, M: 60  | W: 0, E: 20, M: 80  | W: 0, E: 0, M: 100  |

White: Training data, Orange: Test data

**Figure S16.** Responses of C18(1)-NH<sub>2</sub>(4)-STNPs-coated MSS to the 21 samples.

**Table S1.** The amount of each chemical used for the STNPs synthesis.

| STNP<br>※ | Solution A                    |            | Solution B                |                         |            | Solution C   |            | Solution D               |            | Solution E |                          |            |
|-----------|-------------------------------|------------|---------------------------|-------------------------|------------|--------------|------------|--------------------------|------------|------------|--------------------------|------------|
|           | Silane<br>(mL)                | IPA<br>(g) | NH <sub>3</sub> aq<br>(g) | H <sub>2</sub> O<br>(g) | IPA<br>(g) | TTIP<br>(mL) | IPA<br>(g) | H <sub>2</sub> O<br>(mL) | IPA<br>(g) | ODA<br>(g) | H <sub>2</sub> O<br>(mL) | IPA<br>(g) |
| 1         | APTES: 1.49                   | 8.75       | 0.758                     | 2.84                    | 6.98       | 0.458        | 9.44       | 0.078                    | 9.74       | 0.1368     | 40                       | 123.3      |
| 2         | ODTES: 2                      | 8.23       |                           |                         |            |              |            |                          |            |            |                          |            |
| 3         | TMPS: 1.16                    | 8.89       |                           |                         |            |              |            |                          |            |            |                          |            |
| 4         | APTES: 0.745,<br>ODTES: 1.531 | 8.02       |                           |                         |            |              |            |                          |            |            |                          |            |
| 5         | APTES: 1.191,<br>ODTES: 0.613 | 8.39       |                           |                         |            |              |            |                          |            |            |                          |            |
| 6         | APTES: 0.298,<br>ODTES: 2.448 | 7.65       |                           |                         |            |              |            |                          |            |            |                          |            |

※ STNP 1, 2, 3, 4, 5 and 6 are NH<sub>2</sub>-STNPs, C18-STNPs, Ph-STNPs, C18(1)-NH<sub>2</sub>(1)-STNPs, C18(0.25)-NH<sub>2</sub>(1)-STNPs and C18(1)-NH<sub>2</sub>(0.25)-STNPs, respectively.

**Table S2.** The amount of each chemical used for the SNPs synthesis.

| SNP<br>※ | Solution A     |              |             | Solution B                |                          |             |
|----------|----------------|--------------|-------------|---------------------------|--------------------------|-------------|
|          | Silane<br>(mL) | TEOS<br>(mL) | MeOH<br>(g) | NH <sub>3</sub> aq<br>(g) | H <sub>2</sub> O<br>(mL) | MeOH<br>(g) |
| 1        | 0.365          | 1.064        | 8.69        | 0.758                     | 2.84                     | 6.98        |
| 2        | 0.379          |              | 8.68        |                           |                          |             |

※ SNP 1 and 2 are NH<sub>2</sub>(1)-OH(3)-SNPs and Ph(1)-OH(3)-SNPs, respectively.

**Table S3.** Cross validation errors (CVEs) obtained by the combination of two parameters; one from NH<sub>2</sub>-STNPs and the other from C18(1)-NH<sub>2</sub>(1)-STNPs.

| NH <sub>2</sub> -STNPs | C18(1)-NH <sub>2</sub> (1)-STNPs | Water   | Ethanol | Methanol |
|------------------------|----------------------------------|---------|---------|----------|
| Parameter 1            | Parameter 1                      | 22.2162 | 15.4893 | 13.1044  |
| Parameter 1            | Parameter 2                      | 15.3117 | 26.9352 | 22.9144  |
| Parameter 1            | Parameter 3                      | 22.4057 | 19.7457 | 26.3271  |
| Parameter 1            | Parameter 4                      | 20.6095 | 23.7984 | 28.0045  |
| Parameter 2            | Parameter 1                      | 6.8980  | 23.4826 | 20.8889  |
| Parameter 2            | Parameter 2                      | 13.8698 | 16.1902 | 16.0581  |
| Parameter 2            | Parameter 3                      | 12.0238 | 17.3032 | 19.0628  |
| Parameter 2            | Parameter 4                      | 5.8945  | 22.1518 | 22.6811  |
| Parameter 3            | Parameter 1                      | 22.2961 | 18.8997 | 19.2084  |
| Parameter 3            | Parameter 2                      | 13.4305 | 18.7925 | 19.4129  |
| Parameter 3            | Parameter 3                      | 19.0740 | 13.2053 | 22.2802  |
| Parameter 3            | Parameter 4                      | 24.0433 | 17.7984 | 26.2950  |
| Parameter 4            | Parameter 1                      | 29.3496 | 26.3693 | 13.5024  |
| Parameter 4            | Parameter 2                      | 13.7796 | 26.3191 | 23.1549  |
| Parameter 4            | Parameter 3                      | 25.3189 | 23.0565 | 22.7747  |
| Parameter 4            | Parameter 4                      | 21.2392 | 7.89410 | 22.2838  |

**Table S4.** Cross validation errors (CVEs) obtained by the combination of two NPs.

| Material 1                       | Material 2                       | Water  | Ethanol | Methanol |
|----------------------------------|----------------------------------|--------|---------|----------|
| C18-STNPs                        | NH <sub>2</sub> -STNPs           | 2.8673 | 11.4558 | 9.8840   |
| C18-STNPs                        | C18(1)-NH <sub>2</sub> (1)-STNPs | 1.8519 | 9.6367  | 9.0808   |
| C18-STNPs                        | C18(1)-NH <sub>2</sub> (4)-STNPs | 2.0891 | 10.9510 | 9.9185   |
| C18-STNPs                        | C18(4)-NH <sub>2</sub> (1)-STNPs | 2.0768 | 6.9110  | 5.5096   |
| NH <sub>2</sub> -STNPs           | C18(1)-NH <sub>2</sub> (1)-STNPs | 4.5572 | 2.5058  | 4.0729   |
| NH <sub>2</sub> -STNPs           | C18(1)-NH <sub>2</sub> (4)-STNPs | 4.3039 | 10.0866 | 8.1493   |
| NH <sub>2</sub> -STNPs           | C18(4)-NH <sub>2</sub> (1)-STNPs | 2.9322 | 4.6063  | 5.3227   |
| C18(1)-NH <sub>2</sub> (1)-STNPs | C18(1)-NH <sub>2</sub> (4)-STNPs | 2.2686 | 3.4287  | 4.4412   |
| C18(1)-NH <sub>2</sub> (1)-STNPs | C18(4)-NH <sub>2</sub> (1)-STNPs | 4.1517 | 6.9257  | 4.6764   |
| C18(1)-NH <sub>2</sub> (4)-STNPs | C18(4)-NH <sub>2</sub> (1)-STNPs | 2.4956 | 3.9785  | 4.1714   |

**Table S5.** Cross validation errors (CVEs) obtained by the combination of two parameters; one from C18-STNPs and the other from NH<sub>2</sub>-STNPs.

| C18-STNPs   | NH <sub>2</sub> -STNPs | Water   | Ethanol | Methanol |
|-------------|------------------------|---------|---------|----------|
| Parameter 1 | Parameter 1            | 5.0295  | 21.8606 | 24.3425  |
| Parameter 1 | Parameter 2            | 6.5352  | 26.6008 | 29.4784  |
| Parameter 1 | Parameter 3            | 5.8424  | 20.5816 | 23.6243  |
| Parameter 1 | Parameter 4            | 4.7889  | 20.2863 | 23.1415  |
| Parameter 2 | Parameter 1            | 7.9169  | 18.6284 | 20.2788  |
| Parameter 2 | Parameter 2            | 11.0398 | 23.9477 | 19.1520  |
| Parameter 2 | Parameter 3            | 15.9213 | 17.8623 | 20.6911  |
| Parameter 2 | Parameter 4            | 8.8824  | 20.0358 | 20.6804  |
| Parameter 3 | Parameter 1            | 10.9194 | 21.5780 | 20.2149  |
| Parameter 3 | Parameter 2            | 6.2330  | 22.9599 | 21.0975  |
| Parameter 3 | Parameter 3            | 7.9020  | 16.8294 | 17.0126  |
| Parameter 3 | Parameter 4            | 7.3919  | 20.5514 | 19.9629  |
| Parameter 4 | Parameter 1            | 14.4677 | 26.2829 | 25.9309  |
| Parameter 4 | Parameter 2            | 12.4063 | 20.7467 | 25.8264  |
| Parameter 4 | Parameter 3            | 20.0684 | 16.6212 | 19.0931  |
| Parameter 4 | Parameter 4            | 15.7458 | 29.0939 | 28.1203  |

**Table S6.** Cross validation errors (CVEs) obtained by the combination of two parameters; one from C18-STNPs and the other from C18(1)-NH<sub>2</sub>(1)-STNPs.

| C18-STNPs   | C18(1)-NH <sub>2</sub> (1)-STNPs | Water   | Ethanol | Methanol |
|-------------|----------------------------------|---------|---------|----------|
| Parameter 1 | Parameter 1                      | 7.3821  | 18.1169 | 16.2748  |
| Parameter 1 | Parameter 2                      | 6.2752  | 19.7774 | 20.8313  |
| Parameter 1 | Parameter 3                      | 6.7689  | 23.4555 | 24.3139  |
| Parameter 1 | Parameter 4                      | 3.5581  | 21.1631 | 18.3665  |
| Parameter 2 | Parameter 1                      | 7.8140  | 20.3093 | 12.4923  |
| Parameter 2 | Parameter 2                      | 17.3002 | 21.2411 | 15.4355  |
| Parameter 2 | Parameter 3                      | 13.9207 | 15.3177 | 18.9791  |
| Parameter 2 | Parameter 4                      | 5.5960  | 22.2248 | 18.1757  |
| Parameter 3 | Parameter 1                      | 10.9349 | 26.1010 | 21.9179  |
| Parameter 3 | Parameter 2                      | 9.6861  | 21.4696 | 12.8263  |
| Parameter 3 | Parameter 3                      | 6.6667  | 18.1602 | 19.3573  |
| Parameter 3 | Parameter 4                      | 5.6120  | 20.7807 | 17.5388  |
| Parameter 4 | Parameter 1                      | 18.5025 | 19.0888 | 14.9217  |
| Parameter 4 | Parameter 2                      | 17.2357 | 23.6848 | 27.5886  |
| Parameter 4 | Parameter 3                      | 21.0556 | 19.7102 | 18.1526  |
| Parameter 4 | Parameter 4                      | 7.1315  | 22.9787 | 26.0781  |

**Table S7.** Cross validation errors (CVEs) obtained by the combination of two parameters; one from C18-STNPs and the other from C18(1)-NH<sub>2</sub>(4)-STNPs.

| C18-STNPs   | C18(1)-NH <sub>2</sub> (4)-STNPs | Water   | Ethanol | Methanol |
|-------------|----------------------------------|---------|---------|----------|
| Parameter 1 | Parameter 1                      | 10.6021 | 23.4379 | 21.3822  |
| Parameter 1 | Parameter 2                      | 5.7344  | 14.0719 | 15.8188  |
| Parameter 1 | Parameter 3                      | 6.6642  | 24.5797 | 30.3102  |
| Parameter 1 | Parameter 4                      | 6.3061  | 29.8236 | 32.4982  |
| Parameter 2 | Parameter 1                      | 6.7534  | 19.2856 | 19.1814  |
| Parameter 2 | Parameter 2                      | 14.4997 | 19.4363 | 12.7002  |
| Parameter 2 | Parameter 3                      | 13.6737 | 14.2196 | 20.9840  |
| Parameter 2 | Parameter 4                      | 6.2100  | 19.7232 | 19.1847  |
| Parameter 3 | Parameter 1                      | 6.1564  | 24.9627 | 21.0195  |
| Parameter 3 | Parameter 2                      | 6.7886  | 16.2944 | 13.5205  |
| Parameter 3 | Parameter 3                      | 8.3194  | 17.3311 | 17.4018  |
| Parameter 3 | Parameter 4                      | 8.1319  | 25.1127 | 21.7387  |
| Parameter 4 | Parameter 1                      | 11.7543 | 24.2069 | 24.7184  |
| Parameter 4 | Parameter 2                      | 10.0279 | 14.3764 | 20.2143  |
| Parameter 4 | Parameter 3                      | 13.3172 | 20.0453 | 20.4205  |
| Parameter 4 | Parameter 4                      | 9.0367  | 23.4907 | 28.8071  |

**Table S8.** Cross validation errors (CVEs) obtained by the combination of two parameters; one from C18-STNPs and the other from C18(4)-NH<sub>2</sub>(1)-STNPs.

| C18-STNPs   | C18(4)-NH <sub>2</sub> (1)-STNPs | Water   | Ethanol | Methanol |
|-------------|----------------------------------|---------|---------|----------|
| Parameter 1 | Parameter 1                      | 4.3472  | 14.9422 | 10.7088  |
| Parameter 1 | Parameter 2                      | 6.0358  | 19.2396 | 18.7070  |
| Parameter 1 | Parameter 3                      | 5.5087  | 21.7151 | 23.8372  |
| Parameter 1 | Parameter 4                      | 4.4378  | 19.3822 | 17.9366  |
| Parameter 2 | Parameter 1                      | 10.1837 | 12.7071 | 13.4536  |
| Parameter 2 | Parameter 2                      | 12.1867 | 19.0463 | 12.6571  |
| Parameter 2 | Parameter 3                      | 15.7134 | 18.1544 | 17.7976  |
| Parameter 2 | Parameter 4                      | 10.4419 | 21.9466 | 18.6381  |
| Parameter 3 | Parameter 1                      | 7.0415  | 13.7055 | 11.4010  |
| Parameter 3 | Parameter 2                      | 13.1045 | 23.1593 | 21.8001  |
| Parameter 3 | Parameter 3                      | 13.7049 | 20.6840 | 20.3135  |
| Parameter 3 | Parameter 4                      | 6.1958  | 19.7814 | 15.9729  |
| Parameter 4 | Parameter 1                      | 14.3478 | 16.5357 | 19.3845  |
| Parameter 4 | Parameter 2                      | 13.8599 | 18.4961 | 18.2060  |
| Parameter 4 | Parameter 3                      | 15.8762 | 15.5926 | 20.4370  |
| Parameter 4 | Parameter 4                      | 12.1965 | 16.3095 | 22.7775  |

**Table S9.** Cross validation errors (CVEs) obtained by the combination of two parameters; one from NH<sub>2</sub>-STNPs and the other from C18(1)-NH<sub>2</sub>(4)-STNPs.

| NH <sub>2</sub> -STNPs | C18(1)-NH <sub>2</sub> (4)-STNPs | Water   | Ethanol | Methanol |
|------------------------|----------------------------------|---------|---------|----------|
| Parameter 1            | Parameter 1                      | 6.9297  | 27.0720 | 22.7897  |
| Parameter 1            | Parameter 2                      | 19.6462 | 29.9967 | 21.0792  |
| Parameter 1            | Parameter 3                      | 9.4093  | 28.2994 | 26.5819  |
| Parameter 1            | Parameter 4                      | 15.8970 | 24.0500 | 25.2587  |
| Parameter 2            | Parameter 1                      | 7.4622  | 34.1542 | 29.6507  |
| Parameter 2            | Parameter 2                      | 11.7094 | 16.0941 | 9.5420   |
| Parameter 2            | Parameter 3                      | 7.6829  | 24.1113 | 27.4755  |
| Parameter 2            | Parameter 4                      | 7.0358  | 28.1067 | 30.0685  |
| Parameter 3            | Parameter 1                      | 19.5188 | 29.8846 | 27.9921  |
| Parameter 3            | Parameter 2                      | 10.9813 | 19.2147 | 17.2611  |
| Parameter 3            | Parameter 3                      | 9.2892  | 17.4525 | 21.2054  |
| Parameter 3            | Parameter 4                      | 19.4273 | 24.8866 | 37.3528  |
| Parameter 4            | Parameter 1                      | 15.4665 | 31.0722 | 26.4448  |
| Parameter 4            | Parameter 2                      | 12.0865 | 21.4580 | 20.4479  |
| Parameter 4            | Parameter 3                      | 9.9746  | 23.1763 | 26.0965  |
| Parameter 4            | Parameter 4                      | 3.0190  | 22.9795 | 22.9374  |

**Table S10.** Cross validation errors (CVEs) obtained by the combination of two parameters; one from NH<sub>2</sub>-STNPs and the other from C18(4)-NH<sub>2</sub>(1)-STNPs.

| NH <sub>2</sub> -STNPs | C18(4)-NH <sub>2</sub> (1)-STNPs | Water   | Ethanol | Methanol |
|------------------------|----------------------------------|---------|---------|----------|
| Parameter 1            | Parameter 1                      | 12.6671 | 17.1848 | 27.8030  |
| Parameter 1            | Parameter 2                      | 15.4206 | 22.3847 | 24.9645  |
| Parameter 1            | Parameter 3                      | 19.9552 | 23.5135 | 35.1095  |
| Parameter 1            | Parameter 4                      | 14.0515 | 25.7632 | 27.5003  |
| Parameter 2            | Parameter 1                      | 8.9366  | 17.0248 | 19.5899  |
| Parameter 2            | Parameter 2                      | 9.9064  | 20.4810 | 20.1866  |
| Parameter 2            | Parameter 3                      | 14.2670 | 26.0874 | 25.7150  |
| Parameter 2            | Parameter 4                      | 12.3617 | 24.9460 | 21.7402  |
| Parameter 3            | Parameter 1                      | 13.6382 | 11.3758 | 17.0524  |
| Parameter 3            | Parameter 2                      | 17.7686 | 24.0529 | 21.6154  |
| Parameter 3            | Parameter 3                      | 20.3112 | 20.4722 | 24.1401  |
| Parameter 3            | Parameter 4                      | 7.9295  | 14.0115 | 18.9638  |
| Parameter 4            | Parameter 1                      | 17.8083 | 21.0380 | 24.2866  |
| Parameter 4            | Parameter 2                      | 15.5026 | 24.0414 | 25.5839  |
| Parameter 4            | Parameter 3                      | 19.2007 | 20.4434 | 36.4726  |
| Parameter 4            | Parameter 4                      | 9.4333  | 14.4181 | 21.7731  |

**Table S11.** Cross validation errors (CVEs) obtained by the combination of two parameters; one from C18(1)-NH<sub>2</sub>(1)-STNPs and the other from C18(1)-NH<sub>2</sub>(4)-STNPs.

| C18(1)-NH <sub>2</sub> (1)-STNPs | C18(1)-NH <sub>2</sub> (4)-STNPs | Water   | Ethanol | Methanol |
|----------------------------------|----------------------------------|---------|---------|----------|
| Parameter 1                      | Parameter 1                      | 5.6502  | 19.5635 | 24.0708  |
| Parameter 1                      | Parameter 2                      | 10.5078 | 13.9381 | 10.8881  |
| Parameter 1                      | Parameter 3                      | 9.2568  | 18.0630 | 22.5205  |
| Parameter 1                      | Parameter 4                      | 16.2742 | 12.6695 | 20.3905  |
| Parameter 2                      | Parameter 1                      | 10.0098 | 26.8831 | 26.7906  |
| Parameter 2                      | Parameter 2                      | 16.2795 | 17.9430 | 13.1072  |
| Parameter 2                      | Parameter 3                      | 10.3429 | 23.1518 | 24.4891  |
| Parameter 2                      | Parameter 4                      | 8.5977  | 22.1938 | 22.4677  |
| Parameter 3                      | Parameter 1                      | 9.5045  | 26.5056 | 26.3601  |
| Parameter 3                      | Parameter 2                      | 13.9792 | 16.8820 | 14.7551  |
| Parameter 3                      | Parameter 3                      | 13.0867 | 22.6580 | 28.1579  |
| Parameter 3                      | Parameter 4                      | 22.8225 | 24.0694 | 28.1550  |
| Parameter 4                      | Parameter 1                      | 4.7448  | 27.2282 | 24.8792  |
| Parameter 4                      | Parameter 2                      | 6.3997  | 16.9061 | 14.7209  |
| Parameter 4                      | Parameter 3                      | 5.2265  | 22.0098 | 21.4294  |
| Parameter 4                      | Parameter 4                      | 13.2220 | 15.0491 | 18.3486  |

**Table S12.** Cross validation errors (CVEs) obtained by the combination of two parameters; one from C18(1)-NH<sub>2</sub>(1)-STNPs and the other from C18(4)-NH<sub>2</sub>(1)-STNPs.

| C18(1)-NH <sub>2</sub> (1)-STNPs | C18(4)-NH <sub>2</sub> (1)-STNPs | Water   | Ethanol | Methanol |
|----------------------------------|----------------------------------|---------|---------|----------|
| Parameter 1                      | Parameter 1                      | 8.6671  | 11.9761 | 8.6400   |
| Parameter 1                      | Parameter 2                      | 15.5132 | 18.9459 | 14.7308  |
| Parameter 1                      | Parameter 3                      | 19.0529 | 18.2807 | 17.0538  |
| Parameter 1                      | Parameter 4                      | 11.9494 | 20.9165 | 12.8811  |
| Parameter 2                      | Parameter 1                      | 12.5997 | 11.6117 | 16.0530  |
| Parameter 2                      | Parameter 2                      | 18.3076 | 18.8842 | 17.2940  |
| Parameter 2                      | Parameter 3                      | 18.6807 | 20.9451 | 14.6387  |
| Parameter 2                      | Parameter 4                      | 19.2988 | 21.9112 | 12.3953  |
| Parameter 3                      | Parameter 1                      | 12.8615 | 11.2979 | 16.7160  |
| Parameter 3                      | Parameter 2                      | 19.5107 | 23.7018 | 19.3121  |
| Parameter 3                      | Parameter 3                      | 17.2802 | 18.5073 | 20.3941  |
| Parameter 3                      | Parameter 4                      | 14.7755 | 19.5268 | 19.1233  |
| Parameter 4                      | Parameter 1                      | 11.0794 | 27.1427 | 26.7337  |
| Parameter 4                      | Parameter 2                      | 7.5707  | 22.5402 | 19.3710  |
| Parameter 4                      | Parameter 3                      | 26.1983 | 24.1406 | 27.6237  |
| Parameter 4                      | Parameter 4                      | 10.0114 | 28.0623 | 23.4953  |

**Table S13.** Cross validation errors (CVEs) obtained by the combination of two parameters; one from C18(1)-NH<sub>2</sub>(4)-STNPs and the other from C18(4)-NH<sub>2</sub>(1)-STNPs.

| C18(1)-NH <sub>2</sub> (4)-STNPs | C18(4)-NH <sub>2</sub> (1)-STNPs | Water   | Ethanol | Methanol |
|----------------------------------|----------------------------------|---------|---------|----------|
| Parameter 1                      | Parameter 1                      | 5.2395  | 12.9442 | 8.8189   |
| Parameter 1                      | Parameter 2                      | 6.7164  | 30.0319 | 29.4492  |
| Parameter 1                      | Parameter 3                      | 5.5841  | 25.5244 | 24.6459  |
| Parameter 1                      | Parameter 4                      | 4.6255  | 24.2423 | 22.8009  |
| Parameter 2                      | Parameter 1                      | 9.7597  | 11.8979 | 11.1017  |
| Parameter 2                      | Parameter 2                      | 15.7217 | 21.2923 | 13.4435  |
| Parameter 2                      | Parameter 3                      | 20.6274 | 20.4757 | 14.5680  |
| Parameter 2                      | Parameter 4                      | 16.9629 | 20.4054 | 11.6719  |
| Parameter 3                      | Parameter 1                      | 14.5068 | 10.8966 | 17.4986  |
| Parameter 3                      | Parameter 2                      | 7.0064  | 25.2145 | 27.9379  |
| Parameter 3                      | Parameter 3                      | 9.8373  | 23.0201 | 26.5945  |
| Parameter 3                      | Parameter 4                      | 4.7682  | 15.6324 | 17.0325  |
| Parameter 4                      | Parameter 1                      | 8.5950  | 17.8706 | 22.3298  |
| Parameter 4                      | Parameter 2                      | 10.9852 | 18.2062 | 22.8373  |
| Parameter 4                      | Parameter 3                      | 15.0345 | 23.5400 | 30.8840  |
| Parameter 4                      | Parameter 4                      | 5.2641  | 14.8138 | 21.8723  |