

Supporting Information

Fingerprinting antibiotics with PAE-based fluorescent sensor arrays

Jinsong Han,^a Benhua Wang,^a Markus Bender,^a Jessica Pfisterer,^a Wei Huang,^a Kai Seehafer,^a Mahdieh Yazdani,^b Vincent M. Rotello,^b Caren M. Rotello^c and Uwe H. F. Bunz^{a,d*}

^aOrganisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg, Im Neuenheimer Feld 270, 69120 Heidelberg, Germany.

^bDepartment of Chemistry, University of Massachusetts Amherst, 710 North Pleasant Street, Amherst, Massachusetts 01003, USA.

^cDepartment of Psychology, University of Massachusetts Amherst, 710 N. Pleasant Street, Amherst, Massachusetts 01003, USA.

^dCAM, Centre for Advanced Materials, Ruprecht-Karls-Universität Heidelberg, Im Neuenheimer Feld 225, 69120 Heidelberg, Germany.

*E-mail: uwe.bunz@oci.uni-heidelberg.de

Content

1. General Information	2
2. Synthetic Details and Analytical Data.....	5
2.1 Synthesis of P1/P2	5
2.2 Synthesis of P3/P4	5
2.3 Synthesis of P5/P6	11
2.4 GPC and Optical Data of P1-P6.....	11
3. Fluorescence Titration of Polymers with Surfactant	12
4. Fluorescence Response Patterns.....	13
5. Linear Discriminant Analysis (LDA).....	14
6. Principal Component Analysis (PCA)	28
7. Optimization Process	29
8. Others.....	30
9. ¹ H-NMR Spectra	32
10. Supplemental References	39

1. General Information.

Chemicals were purchased from commercial laboratory suppliers. Reagents were used without further purification unless otherwise noted.

Solvents were purchased from commercial laboratory suppliers and if necessary distilled prior use. Absolute solvents were dried by a MB SPS-800 using drying columns.

Analytical thin layer chromatography (TLC) was performed on Macherey & Nagel Polygram[®] SIL G/UV254 precoated plastic sheets. Components were visualized by observation under UV light (254 nm or 365 nm) or in the case of UV-inactive substances by using the suitably colouring solutions. The following colouring solutions were used for the visualization of UV-inactive substances:

KMnO₄ solution: 2.0 g KMnO₄, 10.0 g K₂CO₃, 0.3 g NaOH, 200 mL distilled water.

Cer solution: 10.0 g Ce₂(SO)₃, 25 g phosphomolybdic acid hydrate, 1 L distilled water, 50 mL conc. H₂SO₄.

Flash column chromatography was carried out using silica gel S (0.032 mm-0.062 mm), purchased from Sigma Aldrich, according to G. Nill, unless otherwise stated.¹

¹H NMR spectra were recorded at room temperature on the following spectrometers: Bruker Avance III 300 (300 MHz), Bruker Avance III 400 (400 MHz), Bruker Avance III 500 (500 MHz) and Bruker Avance III 600 (600 MHz). The data were interpreted in first order spectra. The spectra were recorded in CDCl₃, D₂O or DMSO-d₆ as indicated in each case. Chemical shifts are reported in δ units relative to the solvent residual peak or TMS.² The following abbreviations are used to indicate the signal multiplicity: s (singlet), d (doublet), t (triplet), q (quartet), quin (quintet), sext (sextet), dd (doublet of doublet), dt (doublet of triplet), ddd (doublet of doublet of doublet), etc., bs (broad signal), m (multiplet).

¹³C NMR spectra were recorded at room temperature on the following spectrometers: Bruker Avance III 300 (75 MHz), Bruker Avance III 400 (100 MHz), Bruker Avance III 500 (125

MHz) and Bruker Avance III 600 (150 MHz). The spectra were recorded in CDCl₃, D₂O or DMSO-d₆ as indicated in each case. Chemical shifts are reported in δ units relative to the solvent signal or TMS.²

High resolution mass spectra (HR-MS) were either recorded on a Bruker ApexQehybrid 9.4 T FT-ICR-MS (ESI⁺, DART⁺) , a Finnigan LCQ (ESI⁺) or a JEOL JMS-700 (EI⁺) mass spectrometer at the Organisch-Chemisches Institut der Universität Heidelberg.

Absorption and emission spectra were recorded using a Jasco V660 and Jasco FP6500 spectrometer. Emission data for sensing were recorded on a CLARIOstar (firmware version 1.13) Platerreader from BMG Labtech using the corresponding software (software version 5.20 R5). Data were analysed with CLARIOstar MARS Data Analysis Software (software version 3.10 R5) from BMG Labtech.

IR spectra were recorded on a JASCO FT/IR-4100. Substances were applied as a film, solid or in solution. The obtained data was processed with the software JASCO Spectra Manager™ II.

Fluorescence lifetimes τ were acquired by an exponential fit according to the least mean square with commercially available software HORIBA Scientific Decay Data Analyses 6 (DAS6) version 6.4.4. The luminescence decays were recorded with a HORIBA Scientific Fluorocube single photon counting system operated with HORIBA Scientific DataStation version 2.2.

Quantum yields Φ were measured by using the comparative method with quinine sulfate in 0.1 N sulfuric acid as a reference ($\Phi = 0.54$) according to the literature, the average values of three measurements were calculated for each sample.³

Dialysis was realized with regenerated cellulose tubular membranes (ZelluTrans, Carl Roth®) with a molecular weight cut-off of 3500 Da against deionized (DI) water.

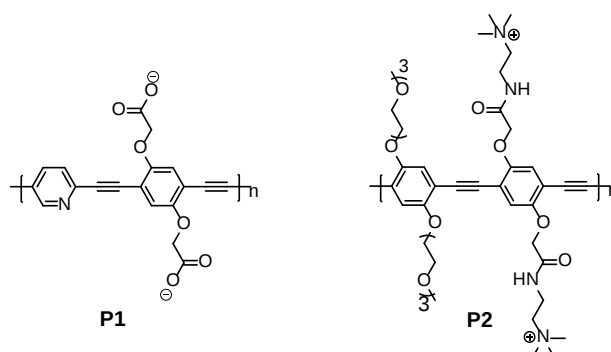
Gel Permeation Chromatography (GPC): Number- (M_n) and weight-average (M_w) molecular weights and polydispersities (PDI, M_w/M_n) were determined by GPC versus polystyrene standards. Measurements were carried out at room temperature in chloroform or THF with PSS-

SDV columns (8.0 mm x 30.0 mm, 5 μ m particles, 10^2 -, 10^3 - and 10^5 - Å pore size) on a Jasco PU-2050 GPC unit equipped with a Jasco UV-2075 UV- and a Jasco RI-2031 RI-detector.

Linear discriminant analysis (LDA) and principal component analysis (PCA). Both methods were carried out in this study by using SYSTAT (version 13.0). In LDA, all variables were used in the model (complete mode) and the tolerance was set as 0.001. The fluorescence response patterns were transformed to canonical patterns. The Mahalanobis distances of each individual pattern to the centroid of each group in a multidimensional space were calculated and the assignment of the case was based on the shortest Mahalanobis distance. PCA is a mathematical transformation used to extract variance between entries in a data matrix by reducing the redundancy in the dimensionality of the data. It takes the data points for all analytes and generates a set of orthogonal eigenvectors (principal components, PCs) for maximum variance.⁴

2. Synthetic Details and Analytical Data.

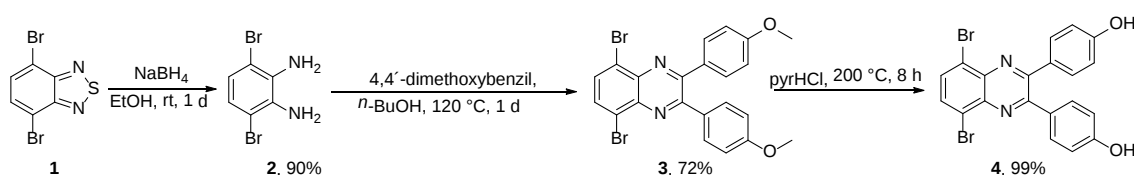
2.1 Synthesis of P1/P2



Compound **P1** was synthesized according to the literature.⁵

Compound **P2** was synthesized according to the literature.⁶

2.2 Synthesis of P3/P4



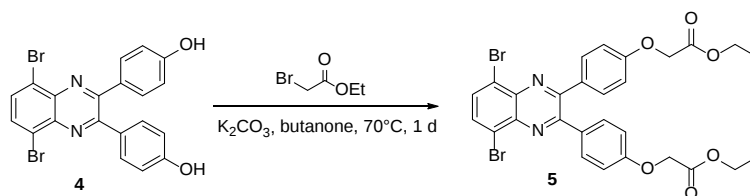
Compound **1** was synthesized according to the literature.⁷

Synthesis of 2. Compound **1** (1.50 g, 5.10 mmol) was dissolved in EtOH (50 ml) and cooled with an ice/water bath. NaBH_4 (10.2 mmol, 3.86 g) was added in small portions and the reaction mixture was stirred over night. The solidified reaction mixture was evaporated to dryness and cautiously diluted with water (100 mL). Water and Et_2O were added, the aqueous layer was separated and extracted with CH_2Cl_2 . The combined organic layers were washed with brine, dried over MgSO_4 and concentrated in vacuo to afford compound **2** (1.23 g, 90%) as yellow solid. The product was used without further purification in the next step. ^1H NMR (300 MHz, $\text{DMSO}-d_6$): δ = 6.63 (s, 2 H), 5.00 (s, 4 H) ppm.

Synthesis of 3. Compound **2** (1.23 g, 4.63 mmol) and 4,4'-dimethoxybenzil (2.75 g, 10.2 mmol) were dissolved in *n*-BuOH (50 ml). A few drops of acetic acid were added and the reaction mixture was stirred at 120 °C for 1 d. The solidified reaction mixture was suspended in

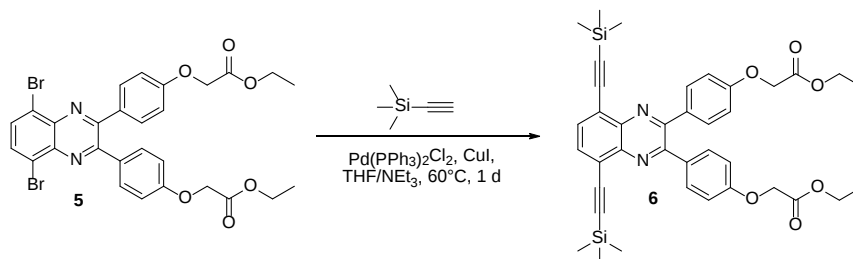
EtOH and filtrated. The residue was washed with copious amounts of hot ethanol and dried in vacuo to afford compound **3** (1.67 g, 72%) as ocre solid (m. p. 188-190 °C). ¹H NMR (400 MHz, CDCl₃): δ = 7.86 (s, 2H), 7.65-7.70 (m, 4H), 6.89-6.93 (m, 4H), 3.86 (s, 6H) ppm. ¹³C NMR (100 MHz, CDCl₃): δ = 160.91, 153.53, 139.09, 132.57, 131.71, 130.62, 123.49, 113.90, 55.35 ppm. IR (cm⁻¹): ν 3079, 3001, 2956, 2929, 2836, 1900, 1603, 1577, 1576, 1560, 1558, 1537, 1526, 1525, 1522, 1512, 1458, 1451, 1443, 1436, 1415, 1382, 1331, 1305, 1292, 1248, 1236, 1218, 1179, 1170, 1111, 1064, 1025, 1015, 1008, 987, 962, 948, 899, 844, 837, 829, 813, 801, 792, 758, 737, 718, 673, 670, 660, 652, 635, 627, 604, 592, 568, 555, 552, 533, 521, 500, 492, 470, 463. HR-MS (EI⁺): *m/z* calcd. for C₂₂H₁₆Br₂N₂O₂⁺ 497.95730 [M]⁺; found 497.95808. C₂₂H₁₆Br₂N₂O₂ (499.18): calcd. C 52.83, H 3.22, N 5.60; found C 52.46, H 3.38, N 5.68.

Synthesis of 4. Compound **3** (1.50 g, 3.00 mmol) and pyridine hydrochloride (1.04 g, 90.0 mmol) was stirred at 200°C for 8 h. The cooled reaction mixture was dissolved in Et₂O and quenched with H₂O. The aqueous phase was extracted with Et₂O and the combined organic layers were washed with water and brine. Evaporation in vacuo afforded compound **4** (1.41 g, 99%) as light yellow solid (m. p. 302-304 °C). The product was used without further purification in the next step. ¹H NMR (400 MHz, DMSO-D₆): δ = 9.89 (br. s, 2H), 8.05 (s, 2H), 7.42-7.48 (m, 4H), 6.75-6.83 (m, 4H) ppm.



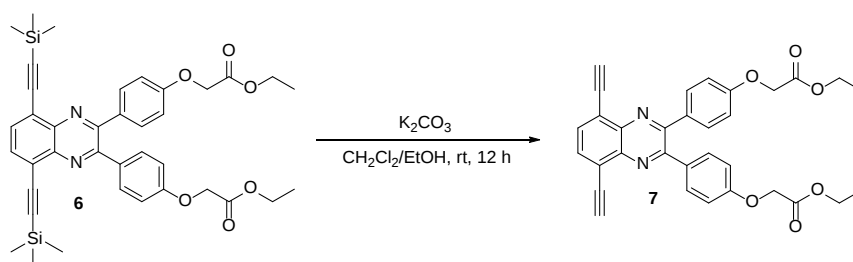
Synthesis of 5. Compound **4** (500 mg, 1.06 mmol) and ethylbromo acetate (0.26 mL, 389 mg, 2.33 mmol) were dissolved in degassed butanone. K₂CO₃ (1.46 g, 10.6 mmol) was added and the mixture was stirred at 70°C for 1 d until TLC showed a complete conversion. The reaction mixture was quenched with H₂O and the aqueous phase was extracted with ethyl acetate. The combined organic layers were dried over MgSO₄, filtered and concentrated in vacuo. The crude

product was dissolved in ethyl acetate, filtered over a silica gel plug and evaporated at 80°C and 0.09 mbar for 2 h to afford compound 5 (605 mg, 89%) as yellow slowly solidifying oil (m. p. 131-133 °C). ¹H NMR (600 MHz, CDCl₃): δ = 7.88 (s, 2H), 7.63-7.69 (m, 4H), 6.88-6.93 (m, 4H), 4.67 (s, 4H), 4.30 (q, *J* = 7.2 Hz, 4H), 1.32 (t, *J* = 7.2 Hz, 6H) ppm. ¹³C NMR (150 MHz, CDCl₃): δ = 168.85, 159.37, 153.55, 139.41, 133.09, 132.09, 131.75, 123.80, 114.89, 65.66, 61.83, 14.49 ppm. IR (cm⁻¹): ν 3080, 2999, 2979, 2938, 2908, 1749, 1725, 1606, 1578, 1540, 1511, 1473, 1440, 1415, 1386, 1332, 1307, 1292, 1262, 1235, 1204, 1173, 1114, 1078, 1069, 1055, 1026, 1014, 986, 947, 932, 899, 875, 850, 834, 824, 814, 801, 758, 735, 720, 698, 653, 640, 607, 591, 572, 551, 530, 520, 492, 467. HR-MS (DART⁺): *m/z* calcd. for C₂₈H₂₄Br₂N₂O₆⁺ 641.99956 [*M*·]⁺; found 642.00065. C₂₈H₂₄Br₂N₂O₆ (644.32): calcd. C 52.20, H 3.75, Br 24.80, N 4.35, O 14.90; found C 52.68, H 4.01, N 4.40.

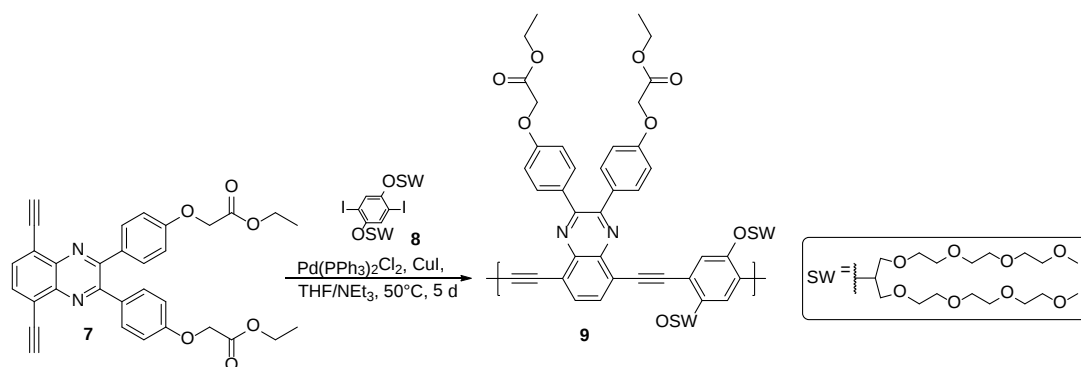


Synthesis of 6. Compound 5 (350 mg, 543 μmol) was dissolved in a degassed mixture of THF/NEt₃ (1:1, 3 mL/3 mL). PdCl₂(PPh₃)₂ (19 mg, 27 μmol) and CuI (5.2 mg, 27 μmol) were added, then TMS-acetylene (168 μL, 117 mg, 1.20 mmol) was added dropwise and the resulting mixture was stirred for 1 d at 60°C until TLC showed a complete conversion. The reaction mixture was filtrated over Celite® and evaporated in vacuo. The crude product was purified by flash chromatography on silica gel [petroleum ether/ethyl acetate (5/1)] to give compound 6 (312 mg, 85%) as yellow solid (m. p. 163 – 165 °C). ¹H NMR (600 MHz, CDCl₃): δ = 7.79 (s, 1H), 7.70 (d, *J* = 8.8 Hz, 2H), 6.88 (d, *J* = 8.8 Hz, 2H), 4.66 (s, 2H), 4.29 (q, *J* = 7.2 Hz, 2H), 1.32 (t, *J* = 7.2 Hz, 3H), 0.35 (s, 9H) ppm. ¹³C NMR (150 MHz, CDCl₃): δ = 168.59, 158.85, 152.04, 140.78, 132.83, 132.23, 131.71, 123.16, 114.31, 103.46, 101.28, 65.36, 61.49, 14.17, -

0.04 ppm. IR (cm⁻¹): ν 2957, 2933, 2898, 2154, 1755, 1604, 1581, 1537, 1511, 1478, 1463, 1437, 1411, 1377, 1341, 1301, 1283, 1271, 1247, 1217, 1194, 1176, 1115, 1081, 1062, 1026, 966, 952, 929, 839, 757, 733, 722, 698, 673, 661, 649, 634, 618, 575, 542, 526, 496, 480, 456. HR-MS (ESI⁺): m/z calcd. for C₃₈H₄₃N₂O₆Si₂⁺ 679.26542 [M+H]⁺; found 679.26551. C₃₈H₄₂N₂O₆Si₂ (678.93): calcd. C 67.23, H 6.24, N 4.13; found C 66.94, H 6.15, N 3.67.

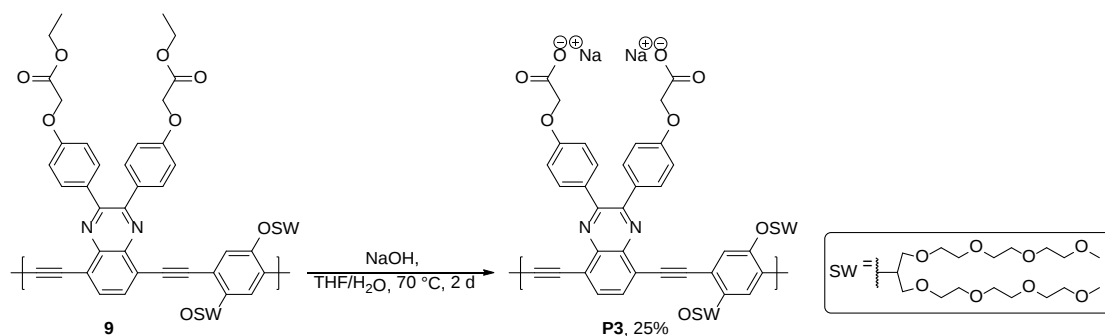


Synthesis of 7. Compound **6** (300 mg, 442 μ mol) was dissolved in a degassed mixture of EtOH/CH₂Cl₂ (1:1, 10 mL/5 mL). K₂CO₃ (610 mg, 4.42 mmol) was added and the resulting mixture was stirred for 12 h at ambient temperature until TLC showed a complete conversion. H₂O and CH₂Cl₂ were added, the aqueous layer was separated and extracted with CH₂Cl₂. The combined organic layers were washed with H₂O and brine, dried over MgSO₄ and concentrated in vacuo. The crude product was dissolved in CH₂Cl₂, filtered over a silica gel plug and concentrated in vacuo to give compound **7** (181 mg, 76%) as yellowish solid (m. p. 162 °C decomposition). ¹H NMR (300 MHz, CDCl₃): δ = 7.87 (s, 1H), 7.58-7.68 (m, 2H), 6.86-6.92 (m, 2H), 4.65 (s, 2H), 4.30 (q, J = 7.1 Hz, 2H), 3.63 (s, 1H), 1.32 (t, J = 7.1 Hz, 3H) ppm. ¹³C NMR (75 MHz, CDCl₃): δ = 168.74, 159.06, 153.14, 141.20, 133.67, 132.29, 131.90, 123.00, 114.68, 85.34, 80.21, 77.16, 65.57, 61.65, 14.34 ppm. IR (cm⁻¹): ν 3304, 3243, 2982, 2938, 1752, 1716, 1606, 1581, 1567, 1540, 1511, 1476, 1446, 1415, 1382, 1338, 1308, 1295, 1261, 1211, 1179, 1142, 1114, 1092, 1077, 1064, 1051, 1029, 1013, 964, 938, 925, 855, 838, 826, 804, 770, 741, 702, 661, 632, 615, 570, 534, 518, 470. HR-MS (ESI⁺): m/z calcd. for C₃₂H₂₇N₂O₆⁺ 535.18636 [M+H]⁺; found 535.18687. C₃₂H₂₆N₂O₆ (499.18): calcd. C 71.90, H 4.90, N 5.24; found C 71.86, H 5.49, N 4.63.

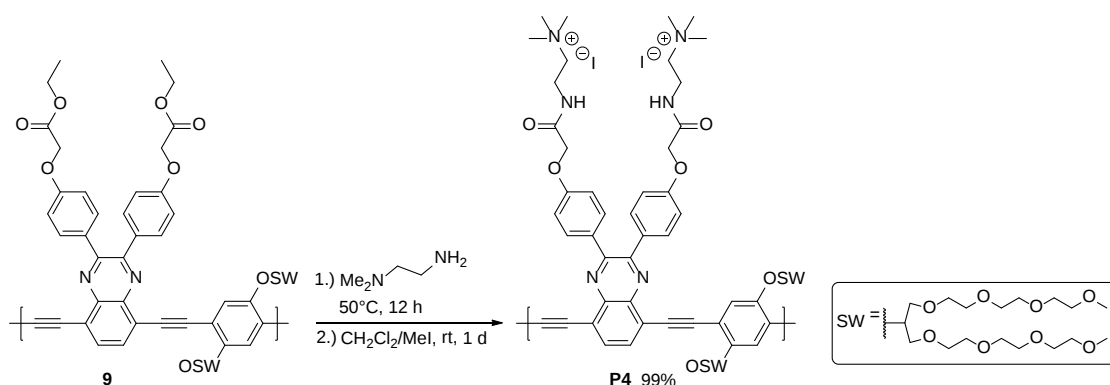


Compound **8** was synthesized according to the literature.⁸

Synthesis of 9. Monomer **7** (200 mg, 374 μmol) and monomer **8** (410 mg, 374 μmol) were dissolved in a mixture of degassed THF/ CHCl_3 / NEt_3 (3:1:4, 1.5 mL/0.5 mL/2 mL). $\text{Pd}(\text{PPh}_3)_4$ (5.3 mg, 7.5 μmol) and CuI (2.9 mg, 15 μmol) were added and the mixture was stirred at 50 $^\circ\text{C}$ for 5 d. Saturated aqueous NH_4Cl and CH_2Cl_2 were added, the aqueous layer was separated and extracted with CH_2Cl_2 . The combined organic layers were dried over MgSO_4 , filtered and concentrated in vacuo. Two times, the crude product was dissolved in a small amount of CHCl_3 and slowly added to an excess of pentane to give **9** as dark red solid (328 mg, 63%). The M_n was estimated to be 2.1×10^4 with a PDI of 1.5. ^1H NMR (300 MHz, CDCl_3): δ = 7.88-8.05 (m, 2 H), 7.63-7.76 (m, 4 H), 7.34-7.50 (m, 2 H), 6.89-7.01 (m, 4 H), 4.60-4.77 (m, 6 H), 4.24-4.36 (m, 4 H), 3.44-3.88 (m, 56 H), 3.27-3.39 (m, 12 H), 1.28-1.36 (m, 12 H) ppm. IR (cm^{-1}): ν 2917, 2872, 2364, 2340, 2328, 1758, 1738, 1605, 1513, 1497, 1468, 1447, 1407, 1380, 1337, 1303, 1274, 1248, 1200, 1180, 1108, 1032, 958, 843, 620, 577. Due to low solubility, ^{13}C NMR spectrum could not be obtained.

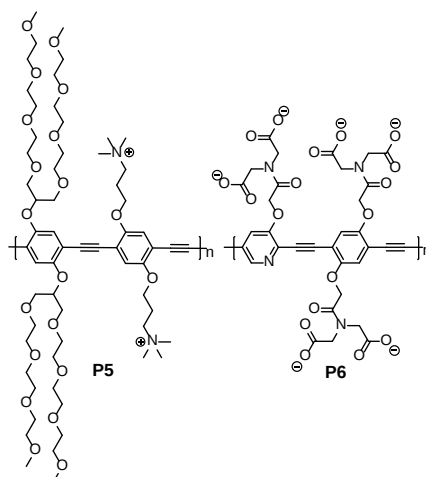


Synthesis of P3. Compound **9** (114 mg, 83 μmol) was dissolved in H_2O (20 mL), NaOH (65 mg, 1.66 mmol) was added and the resulting mixture was stirred at 70 $^\circ\text{C}$ for 2 d. After adjusting a pH of 7 (HCl) the aqueous mixture was dialyzed against DI H_2O for 3 d. Freeze-drying gave **P3** as spongy red solid (28 mg, 25%). The M_n and PDI result from **9**. ^1H NMR (500 MHz, D_2O): δ = 7.72-8.15 (m, 4 H), 7.41-7.68 (m, 2 H), 6.36-7.09 (m, 4 H), 3.05-4.03 (m, 74 H) ppm. IR (cm^{-1}): ν 3429, 3263, 3038, 2871, 1668, 1604, 1532, 1510, 1474, 1445, 1411, 1380, 1348, 1296, 1246, 1179, 954, 924, 841, 661, 577, 528. Due to low solubility, ^{13}C NMR spectrum could not be obtained.



Synthesis of P4. Compound **9** (113 mg, 81.9 μmol) was dissolved in N,N' -dimethylethylenediamine (15 mL) and stirred at 70 $^\circ\text{C}$ for 12 h. The reaction mixture was evaporated to dryness and washed with copious amounts of *n*-pentane. The crude product was dissolved in CH_2Cl_2 (10 mL). After addition of MeI (5 mL) the reaction mixture was stirred for 1 d at ambient temperature. All volatiles were removed under reduced pressure. The residue was dissolved in H_2O and dialyzed against DI H_2O for 3 d. Freeze-drying afforded **P4** as spongy red solid (141 mg, 99%). The M_n and PDI result from **9**. ^1H NMR (500 MHz, D_2O): δ = 6.91-7.77 (m, 10 H), 7.63-7.75 (m, 2 H), 4.41-4.74 (m, 6 H), 3.10-3.84 (m, 4 H) ppm. IR (cm^{-1}): ν 3392, 2921, 2874, 1720, 1646, 1603, 1511, 1444, 1348, 1297, 1200, 1175, 1073, 944, 878, 838, 775, 675, 647, 601, 576, 529. Due to low solubility, ^{13}C NMR spectrum could not be obtained.

2.3 Synthesis of P5/P6



Compound **P5**, **P6** was synthesized according to the literature.⁵

2.4 GPC and Optical Data of P1-P6

Table S1. Additional analytical data of **P1-P6**.

No.	M_n^a [g/mol]	M_w^a [g/mol]	PDI ^a	P_n	$\lambda_{\text{max,abs.}}^b$ [nm]	$\lambda_{\text{max,em.}}^b$ [nm]	Φ^b [%]
P1	6.9×10^3	1.3×10^4	1.9	17	415	536	2
P2	1.1×10^4	1.7×10^4	1.5	15	404	460	4
P3	2.1×10^4	3.2×10^4	1.5	13	477	546	2
P4	2.1×10^4	3.2×10^4	1.5	13	403	550	4
P5	1.4×10^4	5.5×10^4	3.9	11	410	459	37
P6	1.1×10^4	1.8×10^4	1.5	12	390	443	8

^aDetermined by gel permeation chromatography of the corresponding organosoluble precursors.

^bMeasured in $\text{KH}_2\text{PO}_4/\text{Na}_2\text{HPO}_4$ buffer solution.

3. Fluorescence Titration of Polymers with Surfactant

Fluorescence titration of weakly fluorescent PAE (**P1-P4**) with increasing concentration of surfactants (SDBS and CTMA) at different pH condition (pH3, pH7, and pH13 buffer) were carried out in a Jasco V660 and V670 UV/VIS spectrometer. The quenching titration and determination of Ksv constants of **P5/P6** have been reported previously.⁵

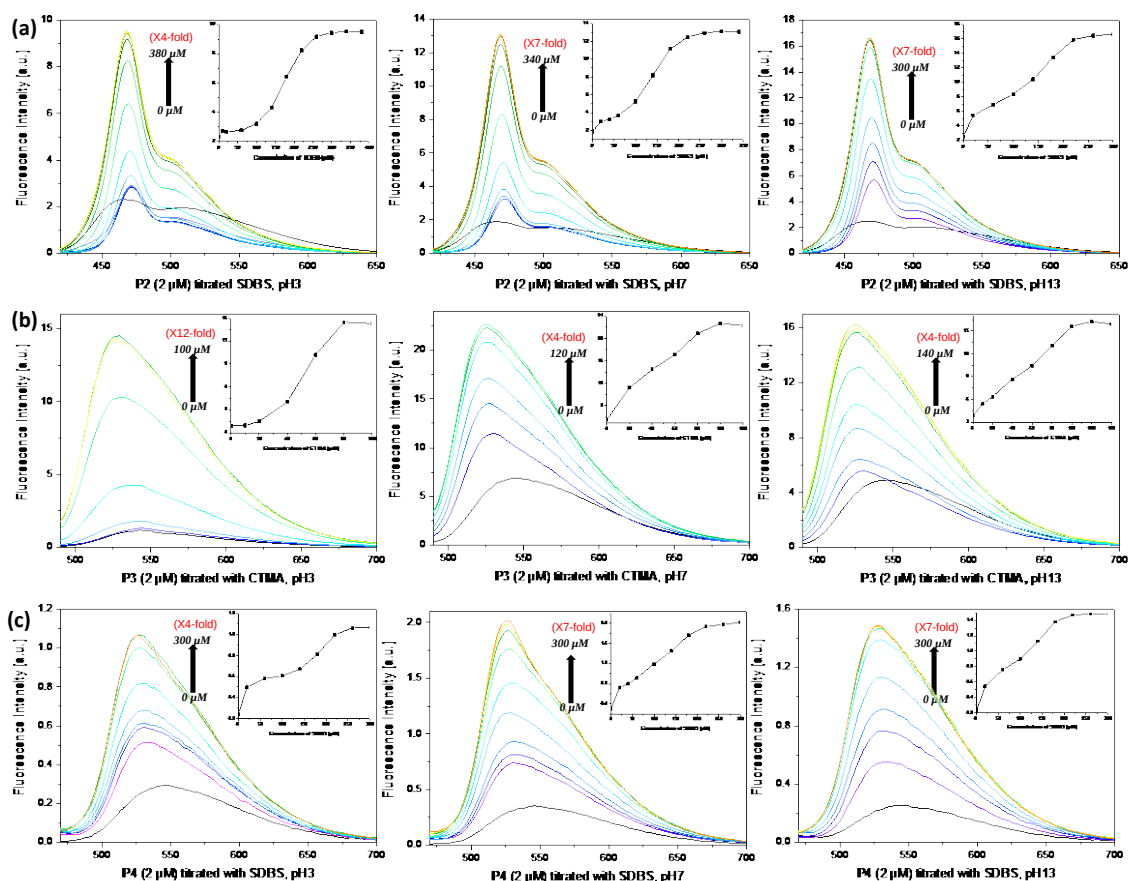


Figure S1. (a) **P2** (2 μ M, black line) with SDBS, (b) **P3** (2 μ M, black line) with CTMA, (c) **P4** (2 μ M, black line) with SDBS at pH 3, pH 7, and pH 13. The inset graph shows the change of I_F with increasing surfactant concentration.

4. Fluorescence Response Patterns

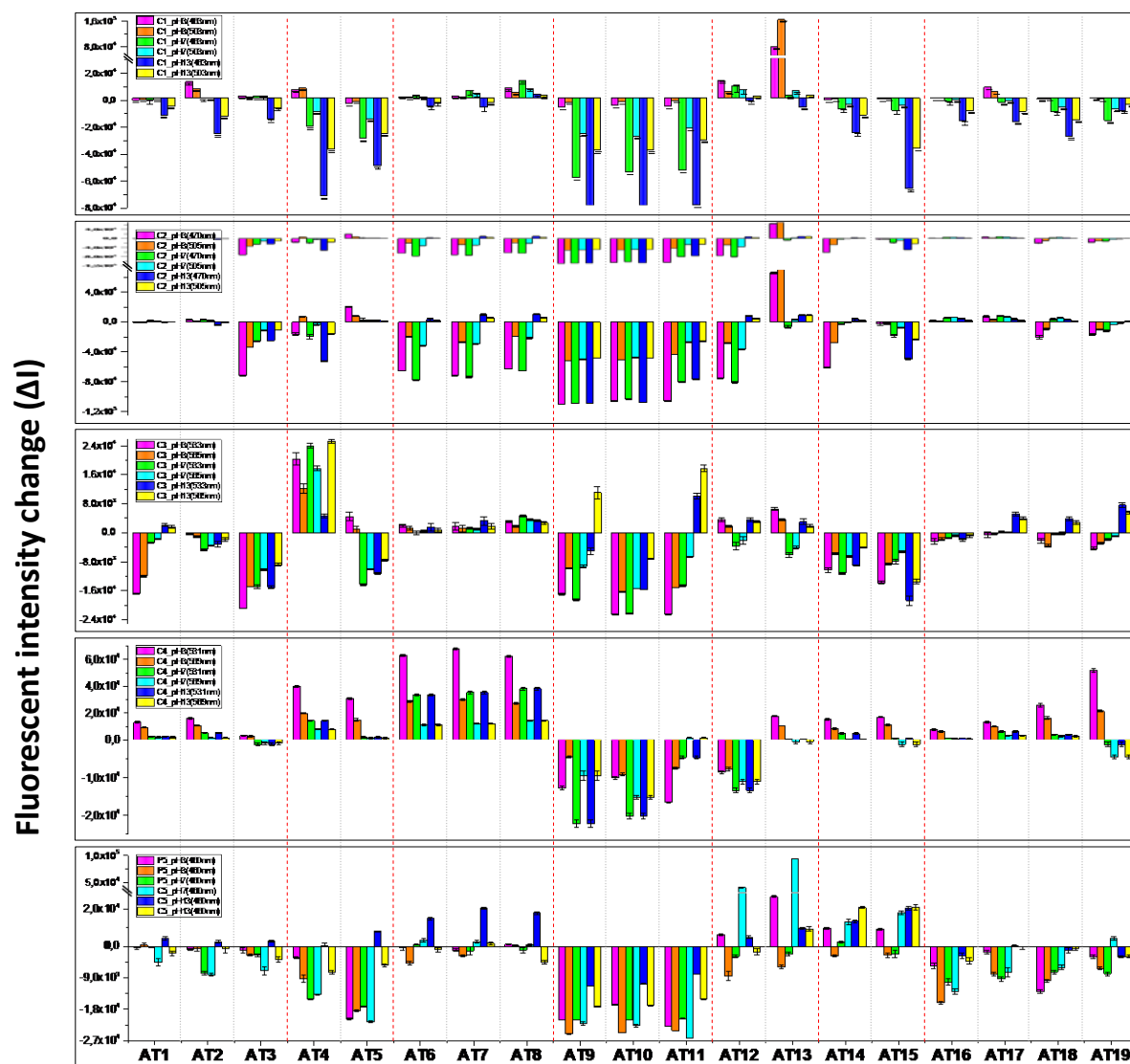


Figure S2. Fluorescence response pattern ΔI obtained by **C1-C4** (2 μ M, at pH 3, pH 7 and pH 13, buffered) and **P5, C5** (0.5 μ M, at pH 3, pH 7 and pH 13, buffered) treated with antibiotics **AT1-AT19** ($c = 5$ mM). Each value is the average of six independent measurements; each error bar shows the standard error of these measurements. The black dotted line shows the type of each antibiotic, red dotted line shows the seven families of antibiotics.

5. Linear Discriminant Analysis (LDA)

Table S2. Training matrix of fluorescence response pattern from an array of sensor element **S1-S24** against 19 antibiotics. LDA was carried out and resulting in 19 factors of the canonical scores (the first three scores were shown here) and group generation. Jackknifed classification matrix showed the 100% correct classification.

Analyte Antibiotic s	Fluorescence response pattern																								Results LDA (the first three scores)			
	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15	S16	S17	S18	S19	S20	S21	S22	S23	S24	SCORE 1	SCORE 2	SCORE 3	Grou p
AT1	-1978	-1138	-3147	-852	12974	-5802	-478	-763	2020	894	-1873	383	17025	11895	-2740	-2057	2383	1586	12041	9164	1975	1289	-859	-591	67	68	44	1
AT1	-1414	-1032	-860	-591	12674	-6310	-1158	-859	2163	882	-653	715	16658	11588	-2867	-1597	2405	1623	13482	9470	2499	2106	-28	-10	68	70	42	1
AT1	-1704	-1264	-2708	661	12415	-5408	-54	-295	1891	657	1101	456	16716	11915	-2786	-1759	1914	2160	12878	8976	3195	1873	-903	136	69	71	42	1
AT1	-1744	-1163	193	56	12440	-5172	-706	153	2030	1171	-864	834	16795	11790	-2629	-1462	1472	1527	13036	1008 5	2688	2577	52	-70	68	71	42	1
AT1	-1468	-1098	-577	-308	12601	-6145	-389	-677	-281	1066	11	568	16967	12106	-2958	-1653	2610	1101	12731	9356	2684	2158	-865	-377	68	70	42	1
AT1	-1755	-1045	-1528	-137	13177	-5813	-495	-201	1981	1873	-236	467	16785	12167	-2750	-1654	2294	1911	14079	9772	2414	2209	-361	-299	66	71	42	1
AT2	1262 1	7187	-678	-3	26056	13329	3449	1404	3184	1382	-4639	-1467	-167	-809	-4912	-3551	-2773	-1412	15345	1048 6	5583	1943	-1300	-874	44	53	42	12
AT2	1305 4	7289	-754	-170	26577	13268	3818	1070	3260	2145	-4664	-1212	-655	-1424	-4733	-3523	-4362	-2893	16648	1085 1	5315	869	-1352	-709	44	54	43	12
AT2	1282 6	7254	543	343	26233	13317	3903	1378	3625	2614	-3637	-1083	-310	-871	-4735	-3475	-3218	-1683	16548	1039 8	5249	2142	-1547	217	44	55	43	12
AT2	1106 2	6263	61	800	26976	13953	2903	1741	3123	2554	-3795	-966	-420	-799	-4459	-3545	-2129	-1740	15987	1034 2	5611	1471	-1743	-435	46	54	42	12
AT2	1170 8	6848	170	220	26645	13500	3378	1824	1915	480	-5334	-992	-209	-1228	-4631	-3749	-3424	-1929	16535	1071 9	5381	1881	-1398	-637	44	52	41	12
AT2	1191 5	6550	105	360	27142	13785	2982	1642	3435	2447	-4795	-998	207	-1142	-4221	-3736	-3164	-1695	17366	1162 3	4996	1357	-1667	-1297	47	54	42	12
AT3	1500	840	734	1785	14289	-6495	19793	7555	5353	1445	2505	1016	21005	14776	15641	10566	15481	-8978	3088	2551	-905	-1385	-3403	-104	68	83	68	13
AT3	1563	929	-560	-69	16567	-8241	21265	8066	4204	3603	2483	2586	20813	14778	15533	10415	14774	-8880	2827	3333	-1346	-983	-3422	-696	65	81	70	13
AT3	1712	857	1971	1507	15759	-6708	21726	8582	1789	2075	3404	1665	20914	14760	14623	10206	15183	-8900	3461	3007	-1893	-1023	-3421	-598	66	83	68	13
AT3	1073	668	1243	2178	14783	-7128	20968	7390	1361	1750	2493	1734	20739	14877	14779	10051	15062	-9077	3538	1898	-856	-503	-3144	-1364	66	82	67	13
AT3	1188	803	1995	2172	16526	-7477	19655	8251	4568	1696	2175	1175	20718	14711	14443	-9989	14496	-8977	3483	3103	-900	-77	-2748	-950	66	82	68	13
AT3	1292	912	1487	1566	15795	-6812	20665	7808	3370	2598	561	1015	20682	14731	14502	10158	15144	-8098	2954	3181	-1396	-1045	-2814	-674	65	80	69	13
AT4	6519	7336	20663	10137	73121	38539	-15709	7365	-23057	-1829	-53408	15955	18937	11802	23456	16602	4905	25615	39286	1935 4	13614	7575	1767	7228	-2	-72	6	14
AT4	6494	7603	20129	-9614	72991	38348	-17841	6360	-17047	-2607	-51784	15792	21726	13427	23070	17714	4848	25022	39723	2027 7	14524	7605	823	6900	-2	-70	5	14
AT4	5880	6900	22452	-9987	72791	38386	-13532	8400	-17315	-2347	-52321	15890	21655	13052	23953	18070	5122	25838	40272	1970 5	14001	8391	791	6510	0	-69	7	14
AT4	6792	7592	21356	10610	72687	38165	-15831	7029	-17396	-2604	-52842	16202	19913	13335	24739	17724	4229	25058	40720	2003 6	14824	7666	874	6357	-3	-70	5	14
AT4	6473	7580	21474	10315	73038	37900	-16121	8280	-17303	-5852	-52108	15560	21844	10849	24191	18726	5006	24966	39282	2007 3	14734	7754	985	6952	-3	-71	5	14
AT4	6481	7313	20518	10153	72710	37508	-17760	6825	-22971	-1726	-52827	15874	17866	10773	24671	17761	4001	24492	39212	1946 9	14601	7746	1087	6756	-2	-71	4	14
AT5	-4248	-2458	30020	15836	50939	26853	-71485	-33688	-25936	10046	-25706	10820	5331	1586	14286	10015	11531	-7780	30484	1652 4	1632	904	-1519	-1346	90	-17	-17	15
AT5	-4251	-2335	29619	15426	51898	26924	-71617	-33770	-25105	11210	-25199	10103	4716	1178	13973	10162	11709	-7598	31220	1392 1	2400	1001	-1250	-881	90	-17	-17	15
AT5	-4184	-2472	30371	15879	49739	26329	-72174	-33686	-26864	10854	-24389	10265	4952	1716	14358	-9924	11419	-7787	31574	1441 5	1517	2032	-1631	-1190	90	-16	-18	15
AT5	-4127	-2378	29840	15436	50329	26598	-72344	-33993	-24964	11339	-25293	10646	5254	1020	14319	10094	10942	-7350	30246	1622 3	2778	1254	-486	-933	91	-16	-18	15
AT5	-4326	-2411	30620	15600	50067	25908	-71968	-33451	-26658	11169	-24878	10539	4106	803	14253	10163	11266	-7322	30595	1455 2	2922	1922	-1567	-1703	90	-16	-18	15
AT5	-4380	-2475	30739	15431	49946	25971	-72573	-33918	-24411	10478	-25028	-9974	2279	-686	14588	-9947	10921	-7674	31889	1468 4	3081	1550	-1393	-1139	90	-14	-17	15

AT6	994	677	2866	395	-4776	-2633	-65263	-19632	-77862	30707	1164	1146	1515	433	-455	488	1493	-33	63631	2871 3	34265	12151	12049	2749	50	44	-118	16
AT6	1021	454	2749	981	-5131	-3134	-65486	-19765	-77743	31721	4809	2233	2298	1499	949	718	962	725	62162	2933 7	33311	10942	14011	3442	51	45	-118	16
AT6	883	443	1866	815	-6143	-2885	-64914	-19743	-77331	31400	4350	3405	2257	1602	-464	349	-137	494	62484	2795 8	34230	10974	13903	3413	51	44	-118	16
AT6	832	401	602	1047	-5707	-2550	-65413	-19819	-78781	32634	1537	835	1663	1435	300	657	2719	300	64211	2827 5	32956	11638	14849	3705	50	43	-119	16
AT6	763	403	2905	67	-6666	-3474	-64819	-19260	-76807	31609	5782	2810	2581	1145	-499	-86	2339	1616	62230	2872 6	32626	10813	14672	3421	50	46	-117	16
AT6	872	345	2311	379	-6808	-4737	-65282	-20052	-78336	32014	4264	2336	1885	1630	226	535	1630	1278	63693	2898 3	34760	11481	15302	3915	50	44	-120	16
AT7	1505	1088	5731	2870	-9549	-3084	-71719	-26916	-72982	28312	10061	5202	359	83	1008	767	2652	696	68692	2980 5	37551	12313	-438	-399	54	46	-120	17
AT7	1467	1137	7940	4688	-5628	-3553	-71846	-27713	-73802	29571	10032	6192	2564	1289	1948	859	4864	1643	67645	3085 6	36201	13025	2293	1291	53	47	-122	17
AT7	1637	961	5697	3337	-7511	-3189	-72018	-27547	-75697	29034	9595	5422	794	173	1089	961	4111	2534	67500	2976 2	34757	11844	1528	-84	55	44	-120	17
AT7	1569	1016	3909	3013	-4923	-3149	-71965	-27335	-73692	29686	10372	5553	2163	1886	1351	896	2149	1100	67202	2979 4	34013	12266	2314	1090	54	46	-120	17
AT7	1362	996	4370	2965	-6147	-3186	-72035	-27404	-74141	30211	11592	5265	2710	2138	1153	803	2179	1821	68236	3020 6	34806	11582	1313	438	54	46	-122	17
AT7	1480	1058	5566	4390	-6044	-3286	-71210	-26591	-73106	28391	9247	5118	2106	1537	1179	1378	3837	3011	69030	3061 9	35435	12250	3107	1816	53	46	-122	17
AT8	8029	4642	11874	7249	3449	1720	-62799	-18987	-64549	21200	10824	5776	2699	1306	4813	3802	3585	2407	61499	2635 0	39582	14098	177	531	41	59	-109	18
AT8	8080	4478	13446	7140	2789	2046	-63044	-18987	-65047	22419	10716	6348	3443	1989	4568	3607	3042	3079	62635	2725 0	38153	14444	1216	1641	43	58	-111	18
AT8	7916	4403	11884	7553	3386	2837	-63041	-19204	-65097	21423	11874	6173	3429	2002	4385	3328	3723	2694	62186	2763 5	37319	14995	1252	983	43	61	-110	18
AT8	6602	3907	13690	6819	2083	1803	-63005	-19310	-65438	20750	10935	6221	2971	2169	4841	3363	3110	2120	63010	2738 4	37154	13983	1549	1201	42	60	-110	18
AT8	6976	3927	13432	7913	2117	817	-63419	-19099	-65880	22074	11038	5562	3508	1459	5162	3420	3684	3138	62449	2799 2	37656	14992	1796	1151	44	59	-110	18
AT8	6874	4013	12409	6215	2964	1508	-63284	-18635	-64566	20490	10499	6272	2822	1682	4578	3928	3256	2755	63199	2793 5	39144	14798	1297	877	42	60	-111	18
AT9	-6654	-3120	59314	26411	84427	39082	110214	-51720	109319	49947	108745	48775	16685	-9473	18419	-8848	-3803	12666	12339	-4647	21347	-8192	11066	4722	116	-222	-2	19
AT9	-6685	-3165	59158	26523	84502	39248	110246	-51774	109560	50228	108701	48734	17192	-9961	18617	-9313	-5792	9614	12455	-4583	23212	10821	11217	5065	116	-220	0	19
AT9	-6642	-3091	59276	26636	84404	39717	110225	-51791	109400	49943	108790	48596	16946	-9784	18661	-9716	-6084	8898	12650	-4308	22686	10267	11033	3627	116	-220	0	19
AT9	-6674	-3155	59275	26732	84150	38228	110213	-51734	109234	49881	108787	48676	17006	-9618	18818	-9393	-5537	10245	13282	-3934	21346	-8370	10372	4592	117	-220	-2	19
AT9	-6659	-3217	59255	26585	84459	38917	110225	-51722	109437	49968	108542	48601	17219	-9975	18579	-9234	-5029	12180	13309	-4704	21533	-8761	10713	3989	117	-222	-1	19
AT9	-6641	-3158	59153	26241	84215	38617	110212	-51726	109353	49907	108643	48640	16993	-9554	18224	-9154	-4382	12597	12491	-4655	23316	10919	10474	5414	116	-221	-1	19
AT10	-5371	-3028	54960	28483	82920	38914	105967	-50400	102970	47163	107947	47861	22657	16346	22266	15506	15723	-6991	-9633	-8577	20129	14898	-9538	-4631	120	-190	7	2
AT10	-5353	-3083	55092	28647	82696	39294	105970	-50500	103573	47557	107997	47801	22741	16310	22385	15426	15660	-7129	10209	-9358	19792	14670	-9360	-4474	121	-191	7	2
AT10	-5401	-3025	55045	28330	82517	38309	105899	-50443	103478	47599	107997	48011	22612	16287	22364	15457	15679	-6975	10480	-8961	19967	14847	-9334	-4367	120	-191	7	2
AT10	-5390	-3069	54837	28479	82967	39145	105910	-50434	103443	47476	107879	47838	22652	16387	22367	15397	15484	-7044	10345	-9456	21057	15734	-9402	-4722	121	-191	8	2
AT10	-5379	-2949	54832	28192	82875	39265	105644	-50341	103632	47633	107991	47882	22439	16447	22381	15385	15614	-7112	10029	-9296	21213	15923	-9467	-4667	120	-191	8	2
AT10	-5346	-2970	54866	28565	82488	38371	105951	-50254	103398	47592	107999	47891	22557	16306	22245	15513	15717	-7339	-9729	-9702	19432	14976	-9367	-4177	120	-190	6	2
AT11	-6259	-1927	53656	22547	79529	31435	105914	-43124	-80556	26688	-77826	26788	22495	15095	14623	-6714	9510	17022	16630	-7457	-5094	1667	-1360	2094	91	-164	5	3
AT11	-6212	-1860	53736	22507	79675	31452	105988	-42881	-81304	26495	-77348	26407	22636	15060	14466	-6617	9437	16958	16813	-7572	-4115	2143	-1998	2410	91	-165	4	3
AT11	-6285	-1893	54115	22453	79814	31552	105918	-42994	-80499	26376	-77408	25950	22283	15114	14826	-6835	9731	18069	16331	-7781	-4406	1884	-1614	1769	91	-165	4	3
AT11	-6285	-1928	53628	22889	79879	31137	106042	-43293	-81990	27661	-77210	27071	22495	15125	14842	-6792	10069	16766	16666	-7364	-4674	1429	-1277	1591	91	-164	3	3
AT11	-6237	-1893	53891	22229	79755	30658	105757	-42933	-80372	26829	-76737	25314	22390	14936	14515	-6465	11217	18795	16731	-7177	-4908	1052	-1728	2081	91	-165	4	3
AT11	-6289	-1822	53613	22494	79391	31048	105957	-43284	-80699	27103	-76658	26039	22575	15105	14436	-6887	10757	18892	16474	-7505	-4625	982	-1952	2461	90	-165	3	3
AT12	1385 8	5282	11707	8435	-3158	1175	-76292	-29020	-79390	35691	9410	5412	3424	2326	-2472	-783	4131	3129	-8258	-7229	12275	10519	-1830	-1648	81	-8	-26	4
AT12	1347 7	5135	10762	7045	-1248	1335	-74550	-28821	-82504	36853	8459	5005	4034	1538	-3609	-1162	3832	3316	-8543	-7870	12980	11328	-656	-694	81	-8	-27	4
AT12	1347 6	5258	10335	6107	-1730	1916	-76474	-28887	-81885	36606	8794	6041	4100	1679	-3624	-2871	3668	3116	-8418	-7161	13923	10311	-1519	-1114	80	-8	-28	4
AT12	1321 6	4861	7146	5225	-2130	2069	-75695	-28534	-82065	36496	7298	4798	3962	1734	-3515	-2295	4019	3294	-8471	-8219	13530	11809	-1330	-1379	82	-10	-27	4
AT12	1341 9	4894	4736	3799	-1236	1363	-74986	-28011	-80574	35776	7839	4181	3193	2098	-3602	-2277	3807	2966	-8223	-7959	14097	12091	-757	-1079	81	-8	-26	4

AT12	1250 0	4620	7718	5787	-3817	693	-73880	-27347	-82563	36768	7629	4755	3052	1886	-5688	-3280	2657	2639	-9246	-8319	13511	10661	-1816	-634	82	-10	-25	4					
AT13	7248 8	15908 9	804	4648	-6405	2087	66161	19095 7	-5696	3370	9905	8454	6429	3827	-6233	-4067	2957	2384	17750	1026 5	136	-880	-2644	-2126	-1280	-19	3	5					
AT13	7190 6	15939 8	1513	6248	-6612	2019	65257	18484 6	-6804	3648	9786	9846	7409	3603	-6792	-4211	2372	1193	17644	1066 1	130	-1135	-2683	-2917	-1281	-21	3	5					
AT13	7170 8	15857 1	1181	4892	-7049	2127	67164	18631 5	-5575	3869	8601	9083	6522	3385	-5160	-3758	3276	1846	17916	1066 1	894	-330	-2281	-2231	-1275	-20	4	5					
AT13	7247 2	15930 1	2796	5585	-7155	2930	64803	19090 9	-6164	3886	9153	8878	6364	3894	-5262	-3557	2149	1780	17763	1048 2	725	-168	-2594	-2289	-1282	-20	2	5					
AT13	7188 9	15948 3	3038	6049	-6185	2701	66017	18718 9	-5828	2724	8835	9294	6077	3692	-6486	-4643	3552	2053	16715	1045 0	248	80	-2113	-2812	-1282	-20	4	5					
AT13	7156 8	15888 7	2191	4458	-7072	1965	66345	18529 9	-9309	4545	9281	8948	6662	3208	-6380	-4268	4154	2011	17950	1099 6	326	124	-2405	-2915	-1279	-20	2	5					
AT14	-1328	-648	-7385	-4168	-	27132	13326	-	-61586	-27739	-2690	1252	829	-76	-	-6198	-	11251	-6383	-9147	-4317	16075	9524	4004	568	-	-	89	32	14	6		
AT14	-1506	-807	-7447	-4284	-	25690	12686	-	-60464	-27201	-4072	76	4651	2912	-	-5846	-	10935	-6265	-9273	-4032	16161	7999	5441	1277	-	-	20089	12921	89	34	11	6
AT14	-1607	-744	-9526	-4214	-	24833	12074	-	-60689	-27745	-2431	-22	4380	2393	-	-5658	-	11079	-6483	-9066	-4336	14714	7666	3952	374	-	-	19435	13055	88	34	13	6
AT14	-1379	-929	-7321	-5064	-	25938	12585	-	-60666	-27352	-3619	-22	2851	3029	-	-9889	-	11415	-6714	-9117	-4009	14822	8230	4131	38	-	-	19056	12816	91	32	13	6
AT14	-1387	-824	-8381	-4247	-	25502	12968	-	-62015	-28324	-2979	-45	4587	2680	-	-5717	-	11270	-6245	-9125	-3888	15744	8633	5246	754	-	-	19129	13100	90	34	10	6
AT14	-1511	-878	-7684	-5402	-	25364	12263	-	-61283	-27635	-2099	-477	3625	2294	-	-9617	-	11085	-6891	-8821	-4045	15177	7689	5202	227	-	-	19195	12563	90	34	11	6
AT15	-725	-275	-7593	-4990	-	67708	37701	-	-5880	-3427	-16805	-6760	-50085	24400	-	-8741	-	7913	-5174	-	1163 3	146	-1601	22042	15960	-	80	-25	65	7			
AT15	-805	-215	-7874	-5385	-	67214	37595	-	623	-3363	-20051	-6747	-48690	23505	-	-8308	-	-7542	-5449	-	1091 1	1080	-1440	21305	15781	-	78	-23	66	7			
AT15	-1031	-458	10918	-6338	-	67127	37935	-	-4971	-443	-16923	-8482	-49064	22973	-	-8907	-	-8977	-5447	-	1231 0	524	-1686	22547	16624	-	79	-25	64	7			
AT15	-759	-289	10661	-5613	-	66871	37532	-	-840	-2956	-20347	-8037	-48376	23743	-	-8428	-	-7966	-5655	-	1019 2	1267	-776	22357	16410	-	79	-25	65	7			
AT15	-950	-501	-9161	-5295	-	67676	37542	-	-910	-1898	-16738	-6373	-49535	23372	-	-8749	-	-7363	-4813	-	1117 7	1970	-119	22580	16122	-	80	-23	67	7			
AT15	-1078	-437	-9534	-4472	-	67925	37557	-	-3188	-2650	-19174	-8035	-50994	23648	-	-8691	-	-7803	-4980	-	1051 6	1530	-1262	21595	15962	-	80	-27	65	7			
AT16	130	-60	-2247	-1974	-	15582	-9198	-	1205	1523	5490	6487	3598	1760	-	-1739	-	-2211	-1514	-	1019 7	1970	-119	22580	16122	-	80	-27	65	7			
AT16	-390	9	-1687	-1001	-	17219	-9607	-	1892	1317	6389	6873	4815	2130	-	-1963	-	-1794	-1579	-	1051 6	1530	-1262	21595	15962	-	80	-27	65	7			
AT16	-25	-45	-2514	-2028	-	18004	-9494	-	2788	1468	6167	6280	6008	3115	-	-2082	-	-1343	-1427	-	1051 6	1530	-1262	21595	15962	-	80	-27	65	7			
AT16	-158	50	-3661	-889	-	18541	10338	-	2631	1261	6822	6885	4985	2269	-	-1802	-	-1418	-1395	-	1051 6	1530	-1262	21595	15962	-	80	-27	65	7			
AT16	-167	-100	-1073	-643	-	17341	-9018	-	1753	1297	6149	6844	5027	2825	-	-2604	-	-1875	-1466	-	1051 6	1530	-1262	21595	15962	-	80	-27	65	7			
AT16	-229	-141	-3455	-1434	-	15988	-8662	-	1155	277	5201	6205	3879	2859	-	-3585	-	-1839	-1460	-	1051 6	1530	-1262	21595	15962	-	80	-27	65	7			
AT17	7878	4642	-3805	-2403	-	18112	10304	-	7154	2475	7996	6057	3912	1710	-	-1535	-	-738	-289	-	1014 5	6557	3124	1746	781	-	43	66	43	9			
AT17	8286	4835	-3125	-1522	-	17985	-9797	-	6775	3365	7565	7226	5166	2504	-	-755	-	-119	148	-	1014 5	6557	3124	1746	781	-	42	67	42	9			
AT17	8080	4499	-3159	-2109	-	17455	-9643	-	8479	3392	8642	6623	4214	2673	-	-265	-	-73	454	-	1026 6	6847	3226	1424	-85	-	44	68	43	9			
AT17	8019	4665	-3922	-1591	-	17377	-9813	-	8591	3588	8557	8127	3666	2098	-	-23	-	130	442	-	1025 4	6405	2380	1467	1007	-	42	68	43	9			
AT17	8051	4578	-2298	-2216	-	16475	-9605	-	7369	4290	9424	7618	4220	2694	-	-978	-	-471	-6	-	1037 1	5482	3301	1890	671	-	43	69	44	9			
AT17	7752	4412	-3019	-1633	-	17648	10003	-	7165	3715	7274	7084	2898	1525	-	-145	-	416	282	-	1503 9	3557	2948	883	795	-	44	66	42	9			
AT18	-831	-449	10812	-6686	-	29240	16722	-	-20637	-9308	2629	5238	2489	2010	-	-1854	-	-3508	-467	-	1629 9	4637	3427	1177	1044	-	61	53	22	10			
AT18	-636	-335	10091	-6287	-	28004	16070	-	-17181	-8489	5610	6028	2752	1744	-	-2004	-	-4442	-103	-	1629 9	4637	3427	1177	1044	-	61	56	24	10			
AT18	-392	-475	-9090	-6274	-	28510	16628	-	-22313	-7722	5139	5169	3655	2010	-	-2839	-	-3402	-358	-	1508 6	3272	2519	675	530	-	63	55	23	10			
AT18	-391	-431	11146	-7348	-	29101	16599	-	-23619	-10642	3049	6672	3427	1843	-	-1587	-	-3657	-10	-	1666 3	4439	2074	988	715	-	62	54	18	10			
AT18	-314	-345	-9211	-6467	-	28301	16251	-	-21839	-11156	3605	5407	3165	2006	-	-3030	-	-3399	-812	-	1727 0	4227	3068	188	1540	-	64	53	20	10			
AT18	-593	-427	10112	-5917	-	28246	16181	-	-18497	-8734	4561	5976	2632	2151	-	-1654	-	-3451	-461	-	1754 6	4224	2523	722	1261	-	61	56	21	10			
AT19	252	-553	17891	-8172	-	17891	-9913	-	-4610	-18460	-9965	-12168	-3576	-1574	-	-532	-	-4412	-2763	-	2126 7	-2103	-4758	-637	421	-	59	70	-9	11			
AT19	236	-631	16658	-8050	-	16658	-9593	-	-4528	-17960	-10181	-11781	-3555	-1445	-	279	-	-4114	-2959	-	2170 7	-1999	-4989	472	791	-	60	70	-7	11			
AT19	105	-734	16875	-7333	-	16875	-8757	-	-4986	-17092	-9463	-12209	-3750	-1213	-	887	-	-4264	-2437	-	2289 5	-686	-4108	309	214	-	60	72	-10	11			
AT19	162	-736	16456	-8504	-	16456	-9185	-	-5080	-15440	-8689	-10765	-3169	-530	-	1312	-	-4704	-3027	-	2137 2	-309	-4458	-38	644	-	60	72	-7	11			

AT19	109	-669	-	-7441	-9020	-4239	-17071	-9301	-11435	-3075	-1100	999	-3948	-3344	-1630	-1103	7663	5358	50916	2032	-826	-4710	-24	-29	60	72	-7	11
AT19	41	-762	16612	-7762	-8622	-5054	-16212	-9324	-12997	-3751	-1441	490	-4703	-2732	-1910	-1038	8423	6079	52965	2163	-898	-3983	-813	206	60	71	-9	11
Control	-9	4	175	477	905	853	-684	-691	-2154	-194	871	196	-21	28	357	-326	723	-168	350	-295	-241	-77	-138	-309	64	68	41	20
Control	107	154	-1250	-390	1143	-17	542	161	1223	-143	363	126	-70	118	-209	169	108	340	-652	251	333	134	68	302	64	67	43	20
Control	-36	1	402	306	969	553	1427	667	-2340	-395	525	-41	203	136	-359	-245	-213	-567	581	387	-180	144	-7	6	64	68	42	20
Control	148	-157	298	157	518	86	-230	-22	-1431	225	35	186	67	136	-338	225	-472	-493	702	-310	-242	-29	-181	-214	66	67	42	20
Control	-99	10	-676	155	-536	-640	-578	256	-785	-484	-114	-422	202	-148	676	292	449	-360	161	110	51	-23	-339	-103	64	65	42	20
Control	-94	-2	-77	-279	1363	-1241	-498	-781	382	161	-48	-263	-45	73	429	188	122	-161	-47	-825	-238	137	199	217	64	67	43	20

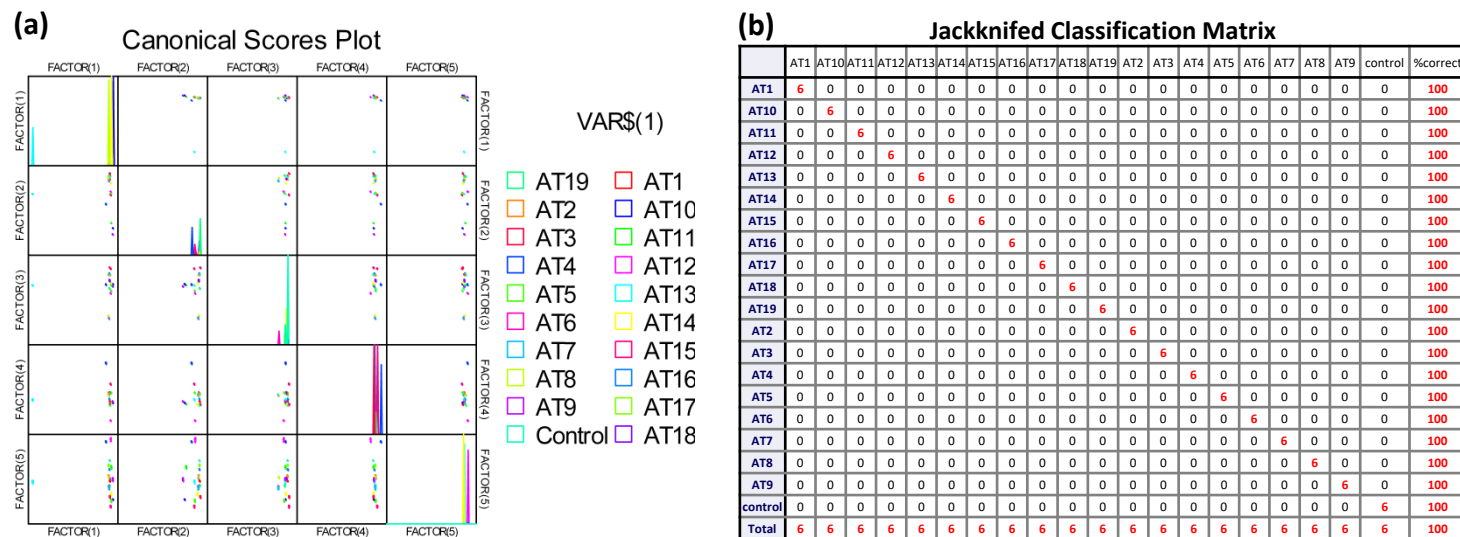


Figure S3. (a) Correlations of canonical fluorescence response patterns from an array of sensor element S1-S24 against 19 antibiotics. The 95% confidence ellipses for the individual acids are also shown. **(b)** Jackknifed classification matrix showed the 100% correct classification.

Table S3. Training matrix of fluorescence response pattern from an array of sensor element **S25-S30** against 19 antibiotics. LDA was carried out and resulting in 6 factors of the canonical scores and group generation. Jackknifed classification matrix showed the 100% correct classification.

Analyte	Fluorescence response pattern						Results LDA						
Antibiotics	S25	S26	S27	S28	S29	S30	SCORE1	SCORE2	SCORE3	SCORE4	SCORE5	SCORE6	GROUP
AT1	-499	2101	113	-5638	3522	-2092	3.25	18.33	10.00	-10.02	-2.10	-1.26	1
AT1	-391	91	-135	-3984	5411	-1311	5.08	16.45	6.69	-8.17	-1.64	0.46	1
AT1	-145	822	236	-5652	5935	-3038	3.92	17.74	7.12	-10.09	0.04	0.95	1
AT1	-879	1386	-36	-5112	4125	-1460	3.53	17.76	8.37	-9.23	-2.59	-1.03	1
AT1	-161	-190	110	-4550	3270	-2765	2.95	15.18	10.10	-9.21	-1.68	1.50	1
AT1	-1118	133	-583	-2759	3861	-1656	4.55	14.43	7.25	-8.95	-2.99	-0.78	1
AT2	-530	18	-7396	-8613	2677	-80	-3.06	15.03	9.73	0.16	3.46	-7.02	12
AT2	-950	-106	-8217	-8268	2782	-1491	-3.80	13.33	8.67	-0.92	4.49	-7.76	12
AT2	-1159	-343	-8192	-8264	2528	-2286	-4.51	12.55	8.71	-1.71	4.58	-7.41	12
AT2	-1019	-1124	-6955	-7519	2333	1289	-2.68	14.09	9.13	1.33	1.27	-6.06	12
AT2	-1058	-238	-7736	-8043	1252	-1507	-4.48	12.74	10.61	-1.28	3.12	-7.28	12
AT2	-1358	-2021	-7206	-8259	2941	-575	-4.55	12.78	7.96	0.18	2.73	-4.86	12
AT3	-2496	-2597	-2690	-6382	1957	-2603	-3.84	11.87	8.33	-6.29	-2.19	0.12	13
AT3	-881	-2037	-2476	-6248	2322	-4450	-2.29	11.79	10.06	-7.61	0.70	1.07	13
AT3	-1737	-2225	-2438	-8080	3354	-3405	-4.03	13.76	8.19	-6.64	0.08	1.04	13
AT3	-422	-2474	-2618	-5828	3117	-4481	-1.33	11.40	9.35	-7.08	1.67	1.66	13
AT3	-407	-2355	-2284	-8803	3558	-4497	-3.84	13.97	9.95	-6.65	2.40	2.56	13
AT3	-1146	-2899	-3108	-6709	2667	-3342	-3.12	11.71	9.12	-5.51	0.60	1.09	13
AT4	-3110	-10304	-15118	-13579	970	-7484	-21.86	-0.33	6.88	5.34	12.13	-2.37	14
AT4	-3369	-9955	-14989	-13614	1912	-7395	-21.32	0.42	5.37	4.87	12.16	-2.73	14
AT4	-3420	-8995	-15114	-13877	-678	-6775	-22.39	0.74	8.95	5.13	10.55	-4.28	14
AT4	-3139	-8259	-15142	-14045	1459	-8066	-21.09	1.59	6.61	3.49	12.80	-4.52	14
AT4	-2823	-8248	-15198	-13814	26	-7674	-21.29	1.16	8.85	4.16	12.17	-4.65	14
AT4	-3386	-10154	-15071	-13827	-831	-7006	-23.12	-0.45	9.05	5.66	10.62	-2.83	14
AT5	-21026	-18490	-17327	-21688	8219	-5157	-46.05	-2.56	-25.20	4.08	-1.71	-4.07	15
AT5	-20837	-18357	-17145	-21333	8226	-5346	-45.45	-2.65	-25.02	3.70	-1.62	-3.94	15
AT5	-20861	-18538	-17113	-21321	7799	-5229	-45.76	-2.90	-24.50	3.91	-1.97	-3.77	15
AT5	-20878	-18130	-17247	-21521	8315	-5438	-45.56	-2.41	-25.13	3.55	-1.44	-4.27	15
AT5	-20534	-18615	-17263	-21410	8252	-5286	-45.41	-2.79	-24.70	4.25	-1.18	-3.59	15
AT5	-20671	-18216	-17319	-22210	7715	-6337	-46.76	-2.74	-23.83	3.13	-0.74	-3.82	15
AT6	-883	-5023	780	1868	15816	-1940	13.53	11.86	-10.36	-8.62	1.37	6.75	16
AT6	-1475	-4410	953	3159	14498	81	14.59	12.12	-9.72	-7.83	-1.68	5.06	16
AT6	-713	-4361	1137	2410	14916	-1206	14.43	12.37	-8.94	-8.59	0.21	6.13	16
AT6	334	-4704	557	2990	14976	-736	15.73	11.83	-8.06	-6.85	1.50	6.28	16
AT6	-350	-4583	1400	3972	13721	-1134	15.59	10.90	-7.38	-8.67	-0.67	6.46	16
AT6	480	-5708	1214	4298	15563	-697	17.13	10.70	-9.06	-6.94	1.06	8.01	16
AT7	-1284	-2497	36	2621	20688	2021	19.19	17.06	-17.58	-6.50	1.47	2.02	17
AT7	-1527	-2638	-3024	2889	20186	907	17.58	14.06	-18.21	-5.32	4.15	-1.15	17
AT7	-1542	-3170	-543	2569	21013	899	18.17	15.60	-18.58	-6.90	2.54	2.31	17
AT7	-663	-2439	-2209	3036	19872	2648	19.22	15.67	-16.45	-3.76	3.19	-0.44	17
AT7	-1192	-2590	-1914	1531	21631	2308	18.17	17.13	-18.90	-4.30	3.84	0.26	17
AT7	-590	-3065	-749	1540	20677	676	17.72	16.24	-16.55	-6.07	4.01	2.76	17
AT8	1147	-733	-1766	283	17978	-3719	16.06	15.36	-10.19	-9.52	8.35	1.04	18
AT8	700	-633	-1465	983	18620	-3951	16.81	15.14	-11.79	-10.60	7.88	0.95	18
AT8	832	635	204	527	18488	-4885	17.33	16.99	-10.63	-13.48	7.18	1.69	18
AT8	885	410	-540	1001	18793	-4637	17.75	16.28	-11.38	-12.60	7.77	1.03	18
AT8	1547	54	-1211	1303	16738	-4927	16.95	14.57	-8.10	-11.62	8.14	0.96	18
AT8	1298	657	-2083	705	17758	-4773	16.85	15.41	-9.76	-11.25	9.18	-0.69	18
AT9	-21055	-25075	-21046	-21269	-11381	-17265	-65.62	-24.98	-1.04	0.22	-1.46	0.88	19
AT9	-21017	-25094	-21052	-21906	-11381	-17311	-66.24	-24.57	-0.77	0.39	-1.23	1.06	19
AT9	-21052	-25101	-21125	-22337	-11385	-17251	-66.71	-24.29	-0.68	0.61	-1.13	1.04	19
AT9	-21033	-25066	-21097	-22482	-11398	-17398	-66.86	-24.22	-0.57	0.47	-1.01	1.11	19
AT9	-21029	-25073	-21054	-21688	-11323	-17353	-66.01	-24.71	-0.94	0.27	-1.24	0.99	19
AT9	-20949	-25049	-21120	-22658	-11309	-17124	-66.82	-23.89	-0.52	0.85	-0.97	1.09	19
AT10	-16704	-24673	-20957	-22235	-10843	-16685	-62.02	-22.48	4.39	3.75	3.57	3.14	2
AT10	-17020	-24689	-21056	-22536	-10749	-16801	-62.61	-22.43	3.92	3.58	3.49	2.97	2
AT10	-16732	-24699	-21123	-22820	-10722	-16890	-62.68	-22.26	4.35	3.82	4.01	3.15	2
AT10	-16670	-24760	-21098	-23063	-10669	-17019	-62.91	-22.17	4.45	3.82	4.23	3.37	2
AT10	-16927	-24677	-21129	-22620	-10769	-17033	-62.72	-22.53	4.08	3.48	3.81	3.00	2
AT10	-16642	-24715	-21129	-22971	-10788	-17045	-62.85	-22.27	4.61	3.79	4.22	3.28	2

AT11	-22944	-24028	-20673	-26199	-7999	-15097	-68.82	-18.24	-6.06	1.22	-2.22	-0.27	3
AT11	-22914	-24048	-20664	-26229	-7992	-15326	-68.90	-18.36	-6.02	1.02	-2.05	-0.16	3
AT11	-22962	-24124	-20694	-26178	-8142	-15182	-68.98	-18.46	-5.92	1.20	-2.25	-0.19	3
AT11	-22960	-24180	-20725	-26159	-8010	-15037	-68.88	-18.41	-6.11	1.40	-2.25	-0.19	3
AT11	-22922	-24164	-20576	-26174	-7979	-15011	-68.78	-18.26	-6.06	1.33	-2.33	-0.02	3
AT11	-22939	-24177	-20710	-26251	-8051	-15160	-69.01	-18.41	-5.99	1.30	-2.16	-0.12	3
AT12	6425	-8933	-3345	39209	6041	-2011	47.81	-22.62	-2.69	-7.20	-1.33	2.56	4
AT12	5821	-8692	-2435	40746	4820	-1513	48.69	-23.25	-2.11	-8.35	-4.12	2.41	4
AT12	7341	-7268	-2732	38968	5138	-2215	48.93	-20.92	0.20	-8.24	-1.13	1.87	4
AT12	5983	-8174	-2446	40468	4036	49	48.90	-21.98	-0.69	-6.89	-5.20	1.53	4
AT12	6319	-10940	-3407	39383	5013	-1427	46.33	-24.57	-1.79	-5.29	-2.28	4.52	4
AT12	5370	-7652	-3014	40196	3798	-2658	47.21	-23.44	-1.17	-9.85	-3.86	0.61	4
AT13	26105	-5703	-3141	94812	9814	7302	127.14	-48.37	-1.25	-1.53	2.90	-3.05	5
AT13	27342	-5829	-2452	94390	9293	8572	128.06	-46.99	1.40	0.29	2.80	-1.67	5
AT13	26974	-5110	-1885	93271	10373	9724	128.20	-44.25	0.12	0.51	2.04	-2.05	5
AT13	27266	-6593	-2084	93377	9513	10208	127.32	-45.70	1.37	2.36	1.81	-0.57	5
AT13	26417	-5853	-1716	94041	9284	10500	127.73	-45.41	0.52	1.11	0.06	-1.74	5
AT13	27142	-6321	-2226	93657	9571	10088	127.59	-45.82	1.03	2.01	1.81	-1.14	5
AT14	9635	-3123	2735	13897	12945	20665	41.97	20.18	3.78	15.56	-6.44	4.86	6
AT14	9428	-2973	3107	11930	14477	21234	41.09	22.78	2.28	16.04	-6.04	5.35	6
AT14	10519	-2478	2493	14684	14047	20594	44.42	20.58	3.20	15.60	-4.83	4.28	6
AT14	9181	-2903	1542	11756	12841	21702	39.48	21.64	3.77	17.66	-6.06	3.23	6
AT14	9824	-2575	2214	14252	12892	20958	42.70	20.28	3.89	15.94	-6.08	3.61	6
AT14	10221	-2822	2067	11162	13897	20816	40.33	22.54	4.10	17.14	-4.10	4.72	6
AT15	9528	-1978	-3122	18912	19306	19151	48.83	15.61	-8.19	16.13	1.33	-3.24	7
AT15	9371	-2888	-1614	18331	20203	21205	49.23	17.62	-9.08	17.60	-0.73	-0.91	7
AT15	9164	-2673	-1612	19304	20507	21051	50.26	17.09	-10.08	16.88	-0.97	-1.43	7
AT15	8595	-2276	-1538	16677	19545	20487	46.68	18.55	-8.53	16.35	-1.17	-1.52	7
AT15	9297	-1767	-3983	18739	21540	23218	50.89	18.52	-11.65	20.52	0.58	-5.32	7
AT15	9516	-3643	-1847	17720	22431	21350	49.56	18.20	-11.82	18.58	0.87	0.04	7
AT16	-4248	-16071	-9951	-12857	-2055	-5310	-24.87	-2.85	9.91	6.45	3.48	8.49	8
AT16	-5458	-16850	-9424	-12334	-2807	-3868	-25.66	-3.28	9.18	7.06	0.29	8.77	8
AT16	-5632	-16073	-10757	-12690	-2470	-3158	-25.71	-2.65	8.34	8.26	1.06	6.24	8
AT16	-5303	-15760	-9135	-11821	-2812	-3923	-24.32	-2.53	9.43	6.02	0.10	7.82	8
AT16	-5912	-16178	-11923	-13311	-4049	-3379	-27.96	-3.76	9.96	9.09	1.22	4.99	8
AT16	-6746	-16144	-9883	-13968	-1898	-5475	-28.14	-2.63	6.81	4.82	1.06	7.48	8
AT17	-1757	-7755	-10460	-8968	984	-1522	-11.30	5.06	8.64	5.65	4.91	-1.77	9
AT17	-1362	-8246	-9401	-6246	-257	-713	-8.66	3.42	10.08	5.56	2.64	-0.65	9
AT17	-2197	-8283	-8948	-8204	107	311	-10.67	5.60	9.32	6.18	1.38	-0.40	9
AT17	-686	-7593	-9286	-6721	245	70	-7.59	5.16	10.59	6.40	3.21	-0.93	9
AT17	-2223	-7382	-8526	-8763	389	481	-10.39	7.22	9.34	5.53	1.16	-0.90	9
AT17	-2063	-8728	-9247	-5980	-678	645	-9.04	3.39	9.61	6.58	0.62	-0.73	9
AT18	-12694	-10266	-6789	-5929	-884	-904	-19.03	0.36	-3.63	-3.36	-12.70	-2.09	10
AT18	-12722	-9846	-7497	-7000	-1179	-540	-20.14	1.15	-3.04	-2.43	-12.23	-3.26	10
AT18	-13768	-10204	-7494	-6199	42	4	-19.60	0.83	-6.38	-2.66	-13.31	-3.66	10
AT18	-13385	-9197	-7272	-6539	-1834	-1436	-20.49	0.62	-3.05	-4.49	-13.11	-4.08	10
AT18	-12890	-9886	-8199	-5103	-1917	-543	-19.07	-0.96	-3.15	-2.43	-12.69	-4.53	10
AT18	-12453	-9991	-6972	-6000	-935	-280	-18.61	0.92	-3.23	-2.58	-12.66	-2.61	10
AT19	-2399	-6060	-7815	4104	-3056	-2557	0.23	-3.40	9.50	-2.36	-2.94	-3.98	11
AT19	-3728	-6277	-8632	4243	-3209	-3390	-1.52	-4.98	7.65	-3.37	-3.36	-5.24	11
AT19	-3083	-6574	-7226	5569	-3268	-3260	0.63	-5.16	8.46	-4.05	-4.28	-3.29	11
AT19	-3075	-6866	-7508	3335	-3105	-3114	-1.69	-3.85	8.94	-2.89	-3.45	-2.81	11
AT19	-2534	-6068	-8335	4917	-2673	-3079	0.81	-4.48	8.37	-2.80	-2.35	-4.64	11
AT19	-2424	-5941	-7708	2782	-2678	-2498	-0.76	-2.13	9.48	-2.15	-2.56	-3.72	11
control	778	1567	408	177	4	929	8.88	14.61	14.32	-7.34	-6.00	-1.73	20
control	704	1429	-509	-599	82	278	7.52	14.14	14.11	-7.02	-4.67	-2.30	20
control	32	840	-121	198	442	-232	7.54	13.00	12.50	-8.15	-5.47	-1.61	20
control	508	687	-298	-423	-21	-16	7.01	13.25	13.90	-7.17	-4.98	-1.30	20
control	323	-611	-190	-457	-314	-317	5.84	11.90	13.92	-6.79	-5.22	0.28	20
control	296	-908	-934	108	-267	656	6.32	11.38	13.37	-5.20	-5.31	-0.55	20

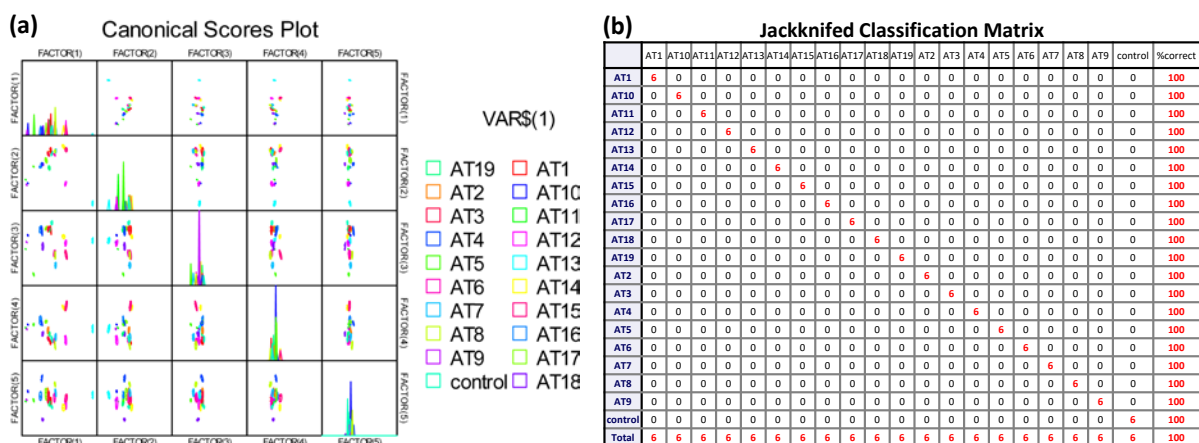


Figure S4. (a) Correlations of canonical fluorescence response patterns from an array of sensor element S25-S30 against 19 antibiotics. The 95% confidence ellipses for the individual acids are also shown. (b) Jackknifed classification matrix showed the 100% correct classification.

Table S4. Training matrix of fluorescence response pattern (combine the Table S2 and S3) from an array of sensor element S1-S30 against 19 antibiotics. Fluorescence response pattern LDA was carried out and resulting in 30 factors of the canonical scores (the first 8 scores were shown here) and group generation. Jackknifed classification matrix showed the 100% correct classification.

Analyte	Results LDA								
Antibiotics	SCORE1	SCORE2	SCORE3	SCORE4	SCORE5	SCORE6	SCORE7	SCORE8	GROUP
AT1	74.81	72.88	42.30	1.87	-11.33	-4.47	-17.15	-26.98	1
AT1	75.18	75.16	40.11	2.39	-10.75	-5.10	-15.70	-25.03	1
AT1	76.78	75.78	39.81	1.55	-12.03	-5.80	-16.80	-25.83	1
AT1	75.28	75.71	40.21	1.23	-11.54	-4.54	-17.25	-26.14	1
AT1	76.16	75.62	41.10	2.90	-12.20	-3.65	-17.59	-24.63	1
AT1	73.19	75.97	40.35	0.59	-11.65	-5.75	-15.70	-25.77	1
AT2	49.13	54.46	41.23	-11.22	15.10	3.45	-1.82	39.22	12
AT2	49.52	55.75	41.42	-12.60	15.69	3.10	-2.62	41.00	12
AT2	49.19	56.19	41.62	-13.56	13.48	4.36	-1.69	39.82	12
AT2	51.04	55.98	41.04	-12.17	13.74	2.36	-0.69	35.84	12
AT2	49.09	53.92	40.35	-12.54	14.85	4.16	-3.92	37.45	12
AT2	51.68	55.78	40.91	-14.30	15.55	2.45	-0.66	38.77	12
AT3	76.69	88.44	67.39	10.17	-7.97	-29.73	-30.15	6.13	13
AT3	74.36	86.71	69.70	8.90	-6.35	-27.00	-27.64	5.70	13
AT3	75.12	87.84	67.72	9.44	-6.34	-27.06	-30.22	6.20	13
AT3	76.02	88.22	67.13	11.59	-6.26	-26.56	-30.15	4.71	13
AT3	75.42	87.12	67.99	8.04	-6.43	-28.34	-29.67	5.33	13
AT3	74.41	85.67	68.63	9.42	-6.26	-26.80	-29.71	4.43	13
AT4	-2.38	-79.10	6.93	-77.31	55.37	75.34	13.19	-5.91	14
AT4	-2.42	-77.88	6.22	-78.23	54.08	75.22	16.63	-6.10	14
AT4	0.10	-76.88	9.03	-80.62	55.71	77.76	14.65	-7.83	14
AT4	-2.47	-77.46	6.83	-78.91	57.60	77.97	13.91	-8.05	14
AT4	-2.92	-78.67	6.44	-78.10	55.47	77.55	13.50	-8.09	14
AT4	-1.82	-78.61	6.19	-77.47	53.46	76.80	13.42	-8.66	14
AT5	82.71	-37.32	-22.93	-52.38	-16.48	-48.62	27.89	25.40	15
AT5	82.17	-37.14	-23.05	-52.51	-16.61	-48.43	27.88	25.58	15
AT5	82.99	-35.85	-24.18	-51.59	-18.32	-47.69	28.53	25.19	15
AT5	82.96	-36.55	-24.73	-52.35	-17.26	-49.61	27.12	25.98	15
AT5	82.20	-36.32	-24.32	-51.04	-17.97	-49.08	27.40	24.31	15
AT5	83.08	-34.37	-23.65	-52.78	-19.21	-51.49	26.31	23.33	15
AT6	47.55	40.20	-122.72	-2.55	6.26	-7.59	-22.27	-1.02	16

AT6	48.25	40.80	-123.53	-2.91	6.00	-5.68	-21.37	-0.57	16
AT6	49.12	40.29	-122.82	-3.16	5.17	-6.30	-21.33	0.69	16
AT6	48.56	39.63	-123.32	-2.39	5.98	-6.13	-23.87	0.27	16
AT6	48.19	42.53	-121.63	-2.60	4.72	-7.01	-21.33	0.36	16
AT6	48.67	40.34	-124.90	-2.71	8.10	-6.75	-22.13	0.12	16
AT7	50.50	41.62	-126.67	1.16	14.31	-13.39	-2.56	-6.54	17
AT7	49.45	41.84	-128.43	-0.22	11.37	-10.32	-3.58	-4.42	17
AT7	51.38	39.64	-126.31	2.25	11.90	-11.02	-3.51	-6.29	17
AT7	50.81	41.45	-126.55	2.06	11.61	-10.84	-2.60	-5.65	17
AT7	49.91	40.54	-128.98	1.10	12.70	-12.62	-2.74	-6.18	17
AT7	49.73	41.68	-127.75	-1.27	11.60	-11.15	-4.91	-6.12	17
AT8	40.81	56.71	-113.77	2.22	9.09	7.33	-4.06	4.05	18
AT8	42.70	56.16	-114.99	2.15	9.66	8.46	-4.30	4.60	18
AT8	42.75	58.41	-114.40	1.73	7.64	7.64	-3.48	4.32	18
AT8	41.89	57.93	-114.36	1.21	8.53	7.38	-4.69	0.35	18
AT8	43.81	56.83	-114.67	0.82	10.27	7.14	-5.02	2.68	18
AT8	41.40	57.26	-115.71	0.07	9.17	7.16	-4.79	0.37	18
AT9	111.43	-230.15	3.91	17.73	-6.57	5.20	-13.86	-11.41	19
AT9	112.10	-228.42	5.60	19.05	-6.32	3.29	-15.96	-9.92	19
AT9	111.32	-227.81	5.53	18.15	-5.30	1.87	-15.35	-8.04	19
AT9	112.27	-228.41	4.40	17.32	-8.15	3.24	-15.31	-9.40	19
AT9	112.60	-229.61	4.74	18.34	-6.45	3.87	-14.48	-10.78	19
AT9	111.66	-229.66	5.06	18.12	-7.22	4.75	-15.62	-11.42	19
AT10	117.88	-195.94	12.75	24.03	4.84	-23.42	-23.94	12.05	2
AT10	118.35	-196.92	12.53	24.15	4.27	-22.95	-24.28	12.47	2
AT10	118.12	-196.55	12.72	24.45	3.27	-22.86	-24.75	12.02	2
AT10	118.26	-196.72	14.04	24.73	3.99	-22.87	-24.54	12.30	2
AT10	116.98	-196.79	13.72	24.66	4.49	-23.05	-24.82	12.43	2
AT10	117.53	-195.85	11.95	23.91	3.35	-22.74	-24.99	12.49	2
AT11	83.26	-181.26	5.41	-15.53	-47.73	-5.50	13.83	-10.51	3
AT11	82.61	-181.88	4.57	-15.63	-48.04	-4.58	14.37	-10.88	3
AT11	82.58	-181.82	4.76	-16.33	-47.69	-5.57	15.12	-10.41	3
AT11	82.94	-181.37	4.11	-14.57	-48.10	-5.73	12.55	-9.98	3
AT11	82.69	-181.74	5.33	-15.10	-49.22	-3.32	14.75	-11.73	3
AT11	82.08	-181.70	4.25	-15.13	-48.41	-4.63	14.08	-12.21	3
AT12	89.17	13.94	-17.52	106.37	-25.11	62.73	20.43	20.37	4
AT12	88.10	13.98	-19.32	108.35	-25.81	62.59	16.91	19.50	4
AT12	87.82	14.36	-19.44	107.67	-25.25	60.45	20.32	20.19	4
AT12	88.92	12.48	-19.06	107.67	-25.55	61.51	19.25	19.46	4
AT12	88.39	13.28	-17.40	105.26	-27.81	60.56	18.51	19.65	4
AT12	89.68	11.22	-17.13	106.95	-25.79	58.66	16.44	20.41	4
AT13	-1319.48	-14.05	5.63	7.78	-3.28	-3.72	-1.86	0.59	5
AT13	-1319.91	-14.83	5.60	8.96	-4.19	-6.78	1.01	0.73	5
AT13	-1314.87	-14.36	6.18	7.04	-2.06	-4.50	-0.11	-1.83	5
AT13	-1320.85	-14.37	5.49	7.97	-3.02	-3.50	-0.03	0.00	5
AT13	-1321.95	-14.49	6.54	9.48	-4.21	-6.75	-0.81	-0.49	5
AT13	-1318.72	-14.97	4.79	8.16	-3.92	-6.72	0.54	-1.04	5
AT14	93.85	45.56	12.37	42.21	11.36	-38.56	51.78	-21.35	6
AT14	93.34	47.20	9.28	41.76	9.25	-37.18	53.34	-22.05	6
AT14	93.58	48.42	12.37	45.06	7.92	-36.45	53.13	-23.26	6
AT14	95.33	45.62	11.51	41.82	8.55	-36.79	52.55	-19.63	6
AT14	94.84	47.39	9.28	42.78	9.14	-37.26	53.75	-20.99	6
AT14	95.25	47.27	10.21	41.85	8.05	-37.12	52.41	-20.94	6
AT15	82.37	-7.79	61.20	38.74	98.84	-24.21	1.97	-2.86	7
AT15	80.07	-5.31	61.51	38.31	100.51	-23.82	-0.75	-1.91	7
AT15	80.70	-6.99	59.68	39.96	100.48	-26.88	1.50	-3.43	7
AT15	80.58	-7.64	60.66	37.60	98.55	-24.18	-0.51	-1.43	7
AT15	81.14	-6.03	61.57	37.82	102.39	-25.90	2.43	-3.31	7
AT15	81.66	-9.53	60.13	38.87	100.40	-25.42	0.81	-2.36	7
AT16	70.44	65.59	50.62	-23.04	-32.60	8.74	-5.10	0.84	8
AT16	68.03	64.47	51.63	-25.08	-33.61	7.82	-3.73	-1.01	8
AT16	68.24	64.99	50.19	-26.38	-32.37	7.71	-3.55	1.47	8

AT16	67.79	63.90	51.82	-26.22	-32.30	8.34	-3.00	0.80	8
AT16	69.23	65.00	50.90	-26.68	-33.94	6.95	-5.17	1.81	8
AT16	69.27	64.06	48.82	-27.10	-34.89	7.31	-5.87	-0.11	8
AT17	49.24	65.44	44.73	-21.29	-10.58	13.09	-0.65	16.16	9
AT17	48.26	66.92	43.81	-20.04	-10.67	15.74	1.03	16.75	9
AT17	50.30	68.01	44.19	-21.77	-9.78	15.73	0.05	17.18	9
AT17	48.15	68.45	44.48	-20.59	-9.03	16.08	0.51	16.06	9
AT17	48.99	68.64	45.07	-21.18	-11.09	14.40	0.54	15.55	9
AT17	49.89	66.34	43.31	-21.05	-9.95	15.97	0.80	16.51	9
AT18	61.72	45.73	18.06	-41.35	-18.90	-7.29	14.27	-3.25	10
AT18	61.66	48.26	20.36	-43.09	-18.44	-8.02	12.56	-4.35	10
AT18	62.93	46.61	18.85	-40.10	-19.07	-8.03	14.97	-3.30	10
AT18	62.12	45.76	14.16	-44.00	-19.56	-7.20	15.45	-3.56	10
AT18	64.75	46.16	17.39	-39.46	-18.49	-7.42	13.91	-4.29	10
AT18	62.00	48.49	17.24	-42.35	-16.44	-7.18	12.59	-4.71	10
AT19	64.62	70.93	-6.81	-17.31	-2.19	-1.90	-10.69	-15.12	11
AT19	65.38	70.04	-5.58	-17.83	-5.29	-0.39	-11.48	-14.39	11
AT19	64.99	72.95	-8.03	-17.59	-2.40	-0.17	-12.32	-14.76	11
AT19	65.51	72.63	-5.10	-18.41	-3.74	-0.34	-12.38	-15.37	11
AT19	64.94	73.07	-5.68	-16.82	-3.95	-0.63	-10.45	-14.19	11
AT19	65.10	71.97	-7.39	-17.41	-1.27	-1.44	-12.47	-15.57	11
Control	74.93	76.65	43.22	16.55	-25.44	28.15	-8.12	-17.94	20
Control	74.27	75.24	45.32	14.80	-25.60	27.93	-8.70	-18.73	20
Control	74.25	76.67	43.66	15.45	-25.23	28.01	-10.53	-17.12	20
Control	77.22	75.70	44.56	15.40	-25.12	28.55	-8.80	-16.74	20
Control	74.47	73.60	44.95	13.52	-25.70	28.79	-8.53	-17.85	20
Control	74.91	75.13	45.54	14.21	-25.99	27.79	-7.71	-18.30	20

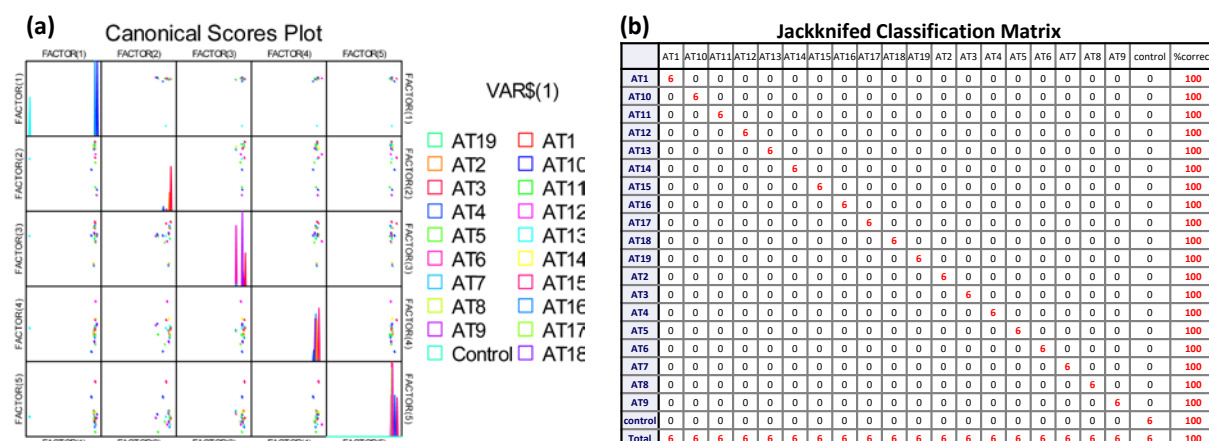


Figure S5. (a) Correlations of canonical fluorescence response patterns from an array of sensor element S1-S30 against 19 antibiotics. The 95% confidence ellipses for the individual acids are also shown. **(b)** Jackknifed classification matrix showed the 100% correct classification.

Table S5. Training matrix of fluorescence response pattern from an optimized array of combined sensor element **S2, S12, S18, S25, S28** and **S29** against 19 antibiotics. LDA was carried out as described above resulting in the four factors of the canonical scores and group generation. Jackknifed classification matrix showed the 100% correct classification.

Analyte	Fluorescence response pattern						Results LDA						
Antibiotics	S2	S12	S18	S25	S28	S29	SCORE 1	SCORE 2	SCORE 3	SCORE 4	SCORE 5	SCORE 6	Group
AT1	-1138	383	1586	-499	-5638	3522	-56.52	-16.64	7.96	0.55	-7.66	3.66	1
AT1	-1032	715	1623	-391	-3984	5411	-55.72	-18.87	6.23	-0.33	-4.94	3.44	1
AT1	-1264	456	2160	-145	-5652	5935	-57.31	-17.94	6.88	-0.84	-4.96	5.37	1
AT1	-1163	834	1527	-879	-5112	4125	-56.53	-17.59	7.99	0.58	-6.21	3.04	1
AT1	-1098	568	1101	-161	-4550	3270	-56.12	-17.86	7.10	0.86	-8.29	2.96	1
AT1	-1045	467	1911	-1118	-2759	3861	-55.46	-17.81	6.38	-0.74	-5.47	0.94	1
AT2	7187	-1467	-1412	-530	-8613	2677	-12.44	-6.94	10.52	8.27	-9.51	7.61	12
AT2	7289	-1212	-2893	-950	-8268	2782	-11.90	-7.73	10.07	10.58	-9.01	6.68	12
AT2	7254	-1083	-1683	-1159	-8264	2528	-11.96	-7.17	11.04	8.90	-8.75	6.45	12
AT2	6263	-966	-1740	-1019	-7519	2333	-17.17	-8.55	10.20	8.44	-9.10	5.63	12
AT2	6848	-992	-1929	-1058	-8043	1252	-14.05	-7.36	11.27	9.26	-10.57	5.57	12
AT2	6550	-998	-1695	-1358	-8259	2941	-15.77	-7.84	10.73	8.73	-8.00	6.24	12
AT3	840	1016	-8978	-2496	-6382	1957	-46.51	-17.64	6.79	18.30	-9.30	0.01	13
AT3	929	2586	-8880	-881	-6248	2322	-45.88	-21.40	7.52	17.83	-11.11	1.65	13
AT3	857	1665	-8900	-1737	-8080	3354	-46.75	-18.83	7.69	18.43	-9.05	2.82	13
AT3	668	1734	-9077	-422	-5828	3117	-47.41	-21.39	5.35	17.43	-10.71	2.31	13
AT3	803	1175	-8977	-407	-8803	3558	-47.30	-18.97	6.71	18.18	-10.93	5.06	13
AT3	912	1015	-8098	-1146	-6709	2667	-46.21	-18.47	6.36	16.52	-10.22	2.31	13
AT4	7336	-15955	25615	-3110	-13579	970	-12.13	30.96	12.84	-32.25	-2.89	14.59	14
AT4	7603	-15792	25022	-3369	-13614	1912	-10.75	30.51	12.56	-31.30	-1.43	14.77	14
AT4	6900	-15890	25838	-3420	-13877	-678	-14.41	31.77	14.04	-32.21	-4.61	13.52	14
AT4	7592	-16202	25058	-3139	-14045	1459	-10.92	31.36	12.49	-31.30	-2.45	15.21	14
AT4	7580	-15560	24966	-2823	-13814	26	-10.80	30.60	13.56	-30.99	-4.71	14.49	14
AT4	7313	-15874	24492	-3386	-13827	-831	-12.26	31.52	13.59	-30.08	-5.13	13.34	14
AT5	-2458	-10820	-7780	-21026	-21688	8219	-68.15	18.93	10.49	24.08	21.44	-3.86	15
AT5	-2335	-10103	-7598	-20837	-21333	8226	-67.32	17.69	11.10	23.80	21.32	-4.01	15
AT5	-2472	-10265	-7787	-20861	-21321	7799	-68.07	17.94	10.98	24.08	20.76	-4.30	15
AT5	-2378	-10646	-7350	-20878	-21521	8315	-67.64	18.65	10.69	23.37	21.50	-3.73	15
AT5	-2411	-10539	-7322	-20534	-21410	8252	-67.79	18.16	10.57	23.19	20.96	-3.49	15
AT5	-2475	-9974	-7674	-20671	-22210	7715	-68.20	17.94	11.94	24.24	20.16	-3.47	15
AT6	677	1146	-33	-883	1868	15816	-46.06	-26.26	-2.42	-0.86	10.43	3.84	16
AT6	454	2233	725	-1475	3159	14498	-46.74	-27.37	-0.80	-1.86	10.10	1.32	16
AT6	443	3405	494	-713	2410	14916	-46.86	-29.58	0.35	-1.35	9.28	2.72	16
AT6	401	835	300	334	2990	14976	-47.37	-27.15	-3.82	-2.21	7.95	3.93	16
AT6	403	2810	1616	-350	3972	13721	-46.73	-28.94	-0.54	-3.65	7.90	1.54	16
AT6	345	2336	1278	480	4298	15563	-47.21	-30.09	-2.91	-3.98	9.07	3.21	16
AT7	1088	5202	696	-1284	2621	20688	-43.40	-33.79	0.16	-1.89	17.65	4.78	17
AT7	1137	6192	1643	-1527	2889	20186	-42.85	-34.55	2.00	-3.01	17.66	4.00	17
AT7	961	5422	2534	-1542	2569	21013	-43.94	-33.36	1.29	-4.57	18.85	4.90	17
AT7	1016	5553	1100	-663	3036	19872	-43.62	-34.58	0.49	-2.68	15.91	4.70	17
AT7	996	5265	1821	-1192	1531	21631	-44.06	-33.37	1.01	-3.38	18.69	6.36	17
AT7	1058	5118	3011	-590	1540	20677	-43.62	-32.72	1.57	-5.24	16.88	6.76	17
AT8	4642	5776	2407	1147	283	17978	-24.34	-30.84	4.87	-2.89	10.73	9.00	18
AT8	4478	6348	3079	700	983	18620	-24.99	-31.83	5.23	-4.02	12.53	8.23	18
AT8	4403	6173	2694	832	527	18488	-25.53	-31.58	5.12	-3.36	11.95	8.62	18
AT8	3907	6221	2120	885	1001	18793	-28.18	-32.69	4.15	-2.88	12.22	8.25	18
AT8	3927	5562	3138	1547	1303	16738	-27.94	-31.13	4.32	-4.54	8.95	7.96	18
AT8	4013	6272	2755	1298	705	17758	-27.57	-32.16	5.06	-3.66	10.37	8.51	18
AT9	-3120	-48775	12666	-21055	-21269	-11381	-73.79	90.49	-14.78	-11.75	1.32	-4.27	19
AT9	-3165	-48734	9614	-21017	-21906	-11381	-74.37	89.48	-15.82	-6.97	0.38	-4.20	19
AT9	-3091	-48596	8898	-21052	-22337	-11385	-74.08	89.32	-15.65	-5.69	0.14	-4.02	19
AT9	-3155	-48676	10245	-21033	-22482	-11398	-74.36	90.00	-15.01	-7.69	0.37	-3.69	19

AT9	-3217	-48601	12180	-21029	-21688	-11323	-74.41	90.15	-14.60	-10.88	1.13	-4.01	19
AT9	-3158	-48640	12597	-20949	-22658	-11309	-74.24	90.89	-13.77	-11.18	0.87	-3.07	19
AT10	-3028	-47861	-6991	-16704	-22235	-10843	-75.03	77.96	-25.44	16.58	-9.17	-1.42	2
AT10	-3083	-47801	-7129	-17020	-22536	-10749	-75.38	78.16	-25.11	16.99	-8.71	-1.54	2
AT10	-3025	-48011	-6975	-16732	-22820	-10722	-75.15	78.48	-25.23	16.73	-9.12	-0.90	2
AT10	-3069	-47838	-7044	-16670	-23063	-10669	-75.42	78.23	-24.97	16.91	-9.23	-0.66	2
AT10	-2949	-47882	-7112	-16927	-22620	-10769	-74.68	78.36	-25.12	16.99	-8.88	-1.32	2
AT10	-2970	-47891	-7339	-16642	-22971	-10788	-74.89	78.24	-25.16	17.34	-9.46	-0.77	2
AT11	-1927	-26788	17022	-22944	-26199	-7999	-65.24	63.84	16.63	-11.35	8.15	-4.04	3
AT11	-1860	-26407	16958	-22914	-26229	-7992	-64.84	63.30	17.07	-11.16	8.09	-4.04	3
AT11	-1893	-25950	18069	-22962	-26178	-8142	-64.85	63.13	18.21	-12.71	8.24	-4.15	3
AT11	-1928	-27071	16766	-22960	-26159	-8010	-65.29	64.15	16.15	-11.04	8.11	-4.07	3
AT11	-1893	-25314	18795	-22922	-26174	-7979	-64.73	62.39	19.21	-13.70	8.57	-4.03	3
AT11	-1822	-26039	18892	-22939	-26251	-8051	-64.44	63.63	18.54	-13.93	8.51	-3.86	3
AT12	5282	5412	3129	6425	39209	6041	-13.37	-50.51	-19.93	-17.65	-1.50	-21.59	4
AT12	5135	5005	3316	5821	40746	4820	-13.83	-49.78	-20.53	-18.19	-1.75	-24.05	4
AT12	5258	6041	3116	7341	38968	5138	-13.45	-51.69	-19.11	-17.60	-4.05	-20.98	4
AT12	4861	4798	3294	5983	40468	4036	-15.35	-49.33	-20.41	-18.11	-3.09	-24.09	4
AT12	4894	4181	2966	6319	39383	5013	-15.54	-48.63	-21.18	-17.64	-2.69	-22.27	4
AT12	4620	4755	2639	5370	40196	3798	-16.72	-48.95	-20.23	-16.86	-2.75	-24.84	4
AT13	159089	8454	2384	26105	94812	9814	827.92	9.50	-2.39	1.30	2.44	-1.88	5
AT13	159398	9846	1193	27342	94390	9293	829.58	6.65	-1.36	3.26	-0.39	-0.80	5
AT13	158571	9083	1846	26974	93271	10373	824.81	7.88	-1.82	2.24	1.31	0.26	5
AT13	159301	8878	1780	27266	93377	9513	828.78	8.76	-1.59	2.50	-0.14	0.28	5
AT13	159483	9294	2053	26417	94041	9284	830.01	8.83	-0.76	2.34	1.05	-1.31	5
AT13	158887	8948	2011	27142	93657	9571	826.62	8.37	-1.73	1.99	0.21	-0.14	5
AT14	-648	-76	-4317	9635	13897	12945	-51.79	-41.39	-19.75	-2.67	-6.35	3.94	6
AT14	-807	2912	-4032	9428	11930	14477	-52.68	-45.16	-15.40	-1.98	-4.57	5.48	6
AT14	-744	2393	-4336	10519	14684	14047	-51.95	-46.73	-18.52	-2.92	-6.02	4.38	6
AT14	-929	3029	-4009	9181	11756	12841	-53.25	-44.40	-14.23	-1.61	-6.36	4.43	6
AT14	-824	2680	-3888	9824	14252	12892	-52.30	-45.71	-16.71	-2.96	-6.51	3.33	6
AT14	-878	2294	-4045	10221	11162	13897	-53.28	-44.29	-15.78	-2.03	-6.67	6.77	6
AT15	-275	-24400	-12122	9528	18912	19306	-52.88	-14.17	-58.66	1.15	1.54	6.84	7
AT15	-215	-23505	-13718	9371	18331	20203	-52.72	-16.01	-58.32	3.86	2.39	7.19	7
AT15	-458	-22973	-13908	9164	19304	20507	-53.81	-17.55	-58.62	3.87	3.27	6.16	7
AT15	-289	-23743	-13152	8595	16677	19545	-53.33	-13.64	-56.39	3.91	2.35	7.39	7
AT15	-501	-23372	-13841	9297	18739	21540	-54.25	-17.21	-59.26	3.65	4.27	7.37	7
AT15	-437	-23648	-14075	9516	17720	22431	-54.20	-16.85	-59.51	4.10	4.77	8.92	7
AT16	-60	1760	-1156	-4248	-12857	-2055	-51.57	-9.42	18.77	10.08	-11.88	1.83	8
AT16	9	2130	-809	-5458	-12334	-2807	-50.93	-8.73	20.09	10.03	-10.87	-0.34	8
AT16	-45	3115	-429	-5632	-12690	-2470	-51.15	-9.86	21.60	9.79	-10.20	-0.23	8
AT16	50	2269	-1027	-5303	-11821	-2812	-50.63	-9.41	19.71	10.16	-11.01	-0.62	8
AT16	-100	2825	-821	-5912	-13311	-4049	-51.53	-8.38	22.43	10.87	-12.08	-0.89	8
AT16	-141	2859	-1273	-6746	-13968	-1898	-51.99	-8.51	22.10	11.73	-8.40	-0.27	8
AT17	4642	1710	3364	-1757	-8968	984	-25.37	-9.59	17.28	1.90	-9.09	5.06	9
AT17	4835	2504	4541	-1362	-6246	-257	-23.59	-11.44	17.32	-0.54	-10.23	2.78	9
AT17	4499	2673	3837	-2197	-8204	107	-25.78	-10.59	18.72	1.38	-9.27	3.35	9
AT17	4665	2098	4273	-686	-6721	245	-24.72	-11.59	16.34	-0.43	-10.77	4.17	9
AT17	4578	2694	3993	-2223	-8763	389	-25.45	-10.29	19.14	1.34	-8.98	3.95	9
AT17	4412	1525	3730	-2063	-5980	-678	-25.96	-10.04	16.00	0.56	-9.91	1.53	9
AT18	-449	2010	2133	-12694	-5929	-884	-51.88	-6.11	19.78	5.46	4.44	-12.15	10
AT18	-335	1744	3229	-12722	-7000	-1179	-51.39	-4.45	20.99	4.24	4.09	-11.25	10
AT18	-475	2010	2873	-13768	-6199	42	-52.02	-5.19	20.48	4.68	7.28	-12.56	10
AT18	-431	1843	2700	-13385	-6539	-1834	-51.79	-4.30	21.17	5.20	4.20	-12.82	10
AT18	-345	2006	2735	-12890	-5103	-1917	-51.05	-5.64	20.15	4.54	3.78	-13.44	10
AT18	-427	2151	3622	-12453	-6000	-935	-51.65	-5.84	20.63	3.22	4.36	-11.65	10
AT19	-553	-532	5236	-2399	4104	-3056	-50.99	-14.42	6.30	-6.65	-9.81	-8.70	11
AT19	-631	279	5442	-3728	4243	-3209	-51.21	-14.49	8.05	-6.35	-8.00	-10.53	11
AT19	-734	887	5614	-3083	5569	-3268	-51.46	-16.64	7.52	-7.20	-8.62	-10.99	11
AT19	-736	1312	5911	-3075	3335	-3105	-51.81	-15.97	9.68	-6.79	-8.96	-9.18	11
AT19	-669	999	5358	-2534	4917	-2673	-51.29	-17.20	7.41	-6.84	-8.89	-9.60	11
AT19	-762	490	6079	-2424	2782	-2678	-52.19	-15.13	8.60	-7.33	-9.46	-7.62	11

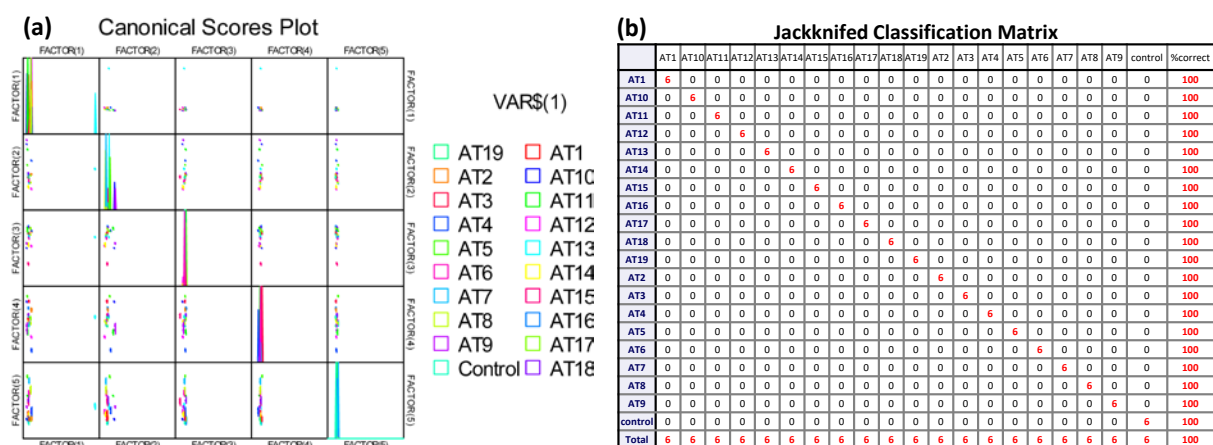


Figure S6. (a) Correlations of canonical fluorescence response patterns from an optimized array of combined sensor element S2, S12, S18, S25, S28 and S29 against 19 antibiotics. The 95% confidence ellipses for the individual acids are also shown. **(b)** Jackknifed classification matrix showed the 100% correct classification.

Table S6. Detection and identification of unknown antibiotics samples using LDA with combined sensor element S2, S12, S18, S25, S28 and S29. All unknown samples could be assigned to the corresponding group defined by the training matrix according to their shortest Mahalanobis distance. According to the verification, all of 76 unknown samples were correctly identified, representing an accuracy of 100%.

Analyte	Fluorescence response pattern						Results LDA								
Unknown samples	S2	S12	S18	S25	S28	S29	SCORE 1	SCORE 2	SCORE 3	SCORE 4	SCORE 5	SCORE 6	Group	Identification	Verification
1	811	1483	-8573	-776	-6586	3113	-46.75	-19.99	6.11	17.06	-10.27	2.67	13	AT3	AT3
2	351	2753	1287	-77	3722	15008	-47.17	-29.67	-1.41	-3.41	9.01	2.67	16	AT6	AT6
3	5041	5177	3488	6412	39591	6296	-14.62	-50.52	-20.53	-18.48	-0.99	-21.74	4	AT12	AT12
4	-3081	-48542	11520	-20974	-21529	-11303	-73.69	89.76	-14.95	-9.92	0.97	-4.14	19	AT9	AT9
5	-457	-24148	-13579	9632	17876	21980	-54.29	-15.92	-59.81	3.22	4.18	8.86	7	AT15	AT15
6	-139	2038	3075	-13643	-6566	-949	-50.20	-4.37	21.44	4.73	5.81	-12.53	10	AT18	AT18
7	-567	2340	3125	-13281	-6499	-230	-52.51	-5.76	21.03	4.32	6.20	-11.97	10	AT18	AT18
8	-1113	-124	1086	136	-2585	4676	-56.03	-18.82	4.00	-0.30	-6.40	2.61	1	AT1	AT1
9	7173	-17073	24515	-3444	-14078	626	-13.29	32.73	11.63	-30.54	-3.25	14.43	14	AT4	AT4
10	4431	5582	2141	1281	1179	16494	-25.28	-30.79	4.43	-2.72	8.80	7.61	18	AT8	AT8
11	4240	6308	2415	1400	1555	16659	-26.15	-32.27	4.92	-3.24	8.98	7.39	18	AT8	AT8
12	-842	394	-4264	10238	15007	13454	-52.62	-43.54	-20.64	-3.40	-6.27	3.88	6	AT14	AT14
13	6935	-864	-1642	-1400	-9121	2146	-13.78	-6.87	12.12	9.24	-9.14	6.54	12	AT2	AT2
14	4604	2184	3993	-2013	-6465	781	-24.99	-11.15	16.59	0.28	-8.16	2.69	9	AT17	AT17
15	-2334	-10073	-7683	-20469	-21841	7870	-67.40	17.74	11.43	24.04	20.18	-3.40	15	AT5	AT5
16	159260	9359	2255	27069	91378	9730	828.29	9.41	0.63	2.63	-0.01	1.71	5	AT13	AT13
17	-206	2718	-1325	-4106	-12866	-1535	-52.28	-11.33	19.41	10.36	-11.48	2.02	8	AT16	AT16
18	-3048	-48127	-7432	-16338	-21587	-10852	-75.11	77.49	-26.65	16.82	-9.64	-1.54	2	AT10	AT10
19	6857	-1671	-1727	-2091	-8673	1692	-14.17	-5.26	11.40	9.34	-8.63	5.30	12	AT2	AT2
20	-2434	-10067	-8318	-20408	-22278	7751	-68.07	17.65	11.42	25.12	19.66	-3.17	15	AT5	AT5
21	-1932	-26447	18034	-22939	-26172	-7892	-65.14	63.68	17.45	-12.82	8.52	-3.91	3	AT11	AT11
22	-643	-24013	-13344	9926	17930	22001	-55.26	-16.45	-59.83	2.72	3.83	9.12	7	AT15	AT15
23	4783	5112	3336	6048	39515	3875	-15.90	-49.28	-19.33	-17.79	-3.64	-23.43	4	AT12	AT12
24	-3124	-48620	11261	-21025	-22633	-11258	-74.15	90.37	-14.39	-9.16	0.74	-3.34	19	AT9	AT9
25	913	5265	1990	-567	3446	21286	-44.15	-34.80	-0.50	-4.51	17.89	5.38	17	AT7	AT7
26	7102	-16213	24665	-3388	-13644	735	-13.48	31.15	12.28	-30.79	-3.05	14.05	14	AT4	AT4
27	-1153	-10	2009	-555	-2532	2937	-56.03	-17.35	5.79	-1.16	-7.39	0.99	1	AT1	AT1
28	743	5705	1086	-75	2901	21754	-45.23	-36.24	-0.63	-3.17	17.40	6.34	17	AT7	AT7
29	157688	9375	1871	26186	93195	9913	820.12	7.70	-1.12	2.39	1.77	-1.09	5	AT13	AT13
30	-163	3123	-1479	-5767	-12607	-3184	-51.81	-10.01	21.41	11.46	-11.15	-1.00	8	AT16	AT16
31	-3117	-47897	-7464	-16471	-21878	-10773	-75.50	77.33	-26.18	17.03	-9.44	-1.49	2	AT10	AT10

32	-665	741	5660	-2870	6509	-2821	-50.97	-17.25	6.38	-7.77	-8.09	-11.21	11	AT19	AT19
33	-1837	-25581	18700	-22915	-26231	-7781	-64.49	62.72	18.81	-13.61	8.78	-3.82	3	AT11	AT11
34	-2396	-10056	-7465	-20972	-22018	7781	-67.73	18.31	11.99	23.96	20.79	-3.86	15	AT5	AT5
35	4855	1407	4790	-1472	-7186	-122	-23.77	-9.16	16.84	-0.79	-10.09	3.73	9	AT17	AT17
36	-116	2108	3100	-13295	-4789	-2240	-49.68	-5.17	20.72	4.17	4.14	-14.22	10	AT18	AT18
37	-3062	-48013	-7524	-16450	-21378	-10794	-75.13	77.23	-26.68	16.93	-9.37	-1.84	2	AT10	AT10
38	185	2332	-197	-20	3305	15272	-48.33	-29.71	-2.57	-1.24	8.79	3.02	16	AT6	AT6
39	909	1643	-8529	-312	-6595	2434	-46.18	-20.22	6.45	17.00	-11.80	2.84	13	AT3	AT3
40	-1003	2921	-4105	10621	14747	13109	-53.21	-47.32	-17.53	-3.13	-7.32	3.82	6	AT14	AT14
41	4520	1978	3314	-1767	-6632	-169	-25.51	-10.89	16.42	1.36	-9.95	2.52	9	AT17	AT17
42	-703	641	5852	-2568	8373	-2797	-50.85	-18.35	4.82	-8.86	-7.95	-12.28	11	AT19	AT19
43	-553	-22484	-14001	9655	20344	22593	-54.22	-20.26	-60.20	3.20	5.48	6.85	7	AT15	AT15
44	438	1048	-8475	1	-6676	2397	-48.82	-19.88	5.47	16.58	-12.35	3.24	13	AT3	AT3
45	-2365	-10552	-7586	-20534	-21921	7763	-67.63	18.60	11.05	23.85	20.13	-3.37	15	AT5	AT5
46	-3136	-48675	11236	-20914	-21329	-11391	-73.98	89.67	-15.40	-9.62	0.75	-4.31	19	AT9	AT9
47	-1935	-26123	18652	-22943	-26219	-8153	-65.07	63.60	18.30	-13.62	8.33	-3.99	3	AT11	AT11
48	157654	9166	2241	25949	95842	9740	820.43	6.93	-2.87	0.95	2.69	-3.44	5	AT13	AT13
49	730	1464	-8499	-901	-6470	3114	-47.16	-19.95	6.08	16.92	-10.05	2.43	13	AT3	AT3
50	4249	6264	2369	844	1279	17171	-26.17	-31.82	5.11	-2.96	10.36	7.25	18	AT8	AT8
51	-725	3474	-4390	10310	12230	12992	-52.09	-46.32	-14.86	-1.48	-7.74	5.32	6	AT14	AT14
52	-515	1722	2918	-13351	-6333	-869	-52.26	-4.66	20.46	4.59	5.48	-12.41	10	AT18	AT18
53	-875	2327	-4345	8733	13878	12968	-52.68	-44.34	-16.52	-1.86	-5.05	2.43	6	AT14	AT14
54	6716	-1317	-2664	-2158	-8333	2319	-14.93	-6.67	10.77	10.58	-7.87	5.04	12	AT2	AT2
55	264	2242	74	-1017	2154	12907	-47.93	-26.92	0.06	-0.49	6.96	1.64	16	AT6	AT6
56	5042	4390	2409	5768	40051	3105	-14.51	-48.15	-20.36	-16.45	-4.27	-24.50	4	AT12	AT12
57	4254	6416	2120	651	1279	16833	-26.11	-31.83	5.44	-2.43	10.15	6.79	18	AT8	AT8
58	-266	2464	-1205	-6946	-13188	-1954	-52.55	-8.24	21.20	11.31	-7.97	-1.09	8	AT16	AT16
59	-1062	-79	1092	-802	-2900	3799	-55.72	-17.51	5.27	0.31	-6.24	1.35	1	AT1	AT1
60	-1976	-25916	17828	-22937	-26154	-7986	-65.32	62.82	17.98	-12.41	8.35	-4.12	3	AT11	AT11
61	-973	-76	1400	-635	-1149	4608	-54.95	-18.79	3.72	-0.94	-4.90	0.65	1	AT1	AT1
62	4998	4816	3396	6026	40865	5729	-14.63	-50.20	-21.43	-18.65	-0.84	-23.43	4	AT12	AT12
63	4664	2026	4365	-1434	-6747	592	-24.72	-10.97	16.58	-0.37	-9.23	3.56	9	AT17	AT17
64	6843	-760	-1515	-1819	-8135	1271	-14.01	-6.86	12.23	8.99	-9.37	4.81	12	AT2	AT2
65	-658	367	5422	-1844	5725	-2713	-51.18	-17.25	5.75	-7.59	-9.70	-9.34	11	AT19	AT19
66	318	2694	1526	128	2125	15193	-47.65	-28.87	-0.44	-3.32	8.57	4.29	16	AT6	AT6
67	-3081	-48650	11451	-20913	-23063	-11377	-73.98	90.73	-14.01	-9.31	0.36	-2.89	19	AT9	AT9
68	789	5932	773	-1416	2302	20494	-44.96	-34.67	1.32	-1.74	17.50	4.57	17	AT7	AT7
69	-90	3659	-1780	-5301	-12716	-3547	-51.38	-11.03	21.91	11.98	-12.38	-0.71	8	AT16	AT16
70	-665	220	5633	-2058	4910	-3077	-51.34	-16.17	6.57	-7.52	-10.03	-9.08	11	AT19	AT19
71	7577	-16474	25336	-3697	-13839	1398	-10.96	32.23	12.50	-31.64	-1.61	14.48	14	AT4	AT4
72	933	5849	629	-1018	2163	21279	-44.29	-35.10	0.70	-1.72	17.87	5.57	17	AT7	AT7
73	6950	-16335	25284	-3196	-13635	1583	-14.33	30.93	11.84	-32.00	-2.10	14.78	14	AT4	AT4
74	-3030	-48066	-7298	-16563	-22138	-10836	-75.08	77.96	-25.99	16.91	-9.41	-1.34	2	AT10	AT10
75	158122	9544	1608	25887	93915	10042	822.60	7.46	-1.27	2.78	2.54	-1.88	5	AT13	AT13
76	-604	-22616	-13719	8223	15865	21425	-55.18	-15.80	-55.63	5.03	4.92	8.21	7	AT15	AT15

Blind test: 76/76 (100% correct identified)

6. Principal Component Analysis (PCA)

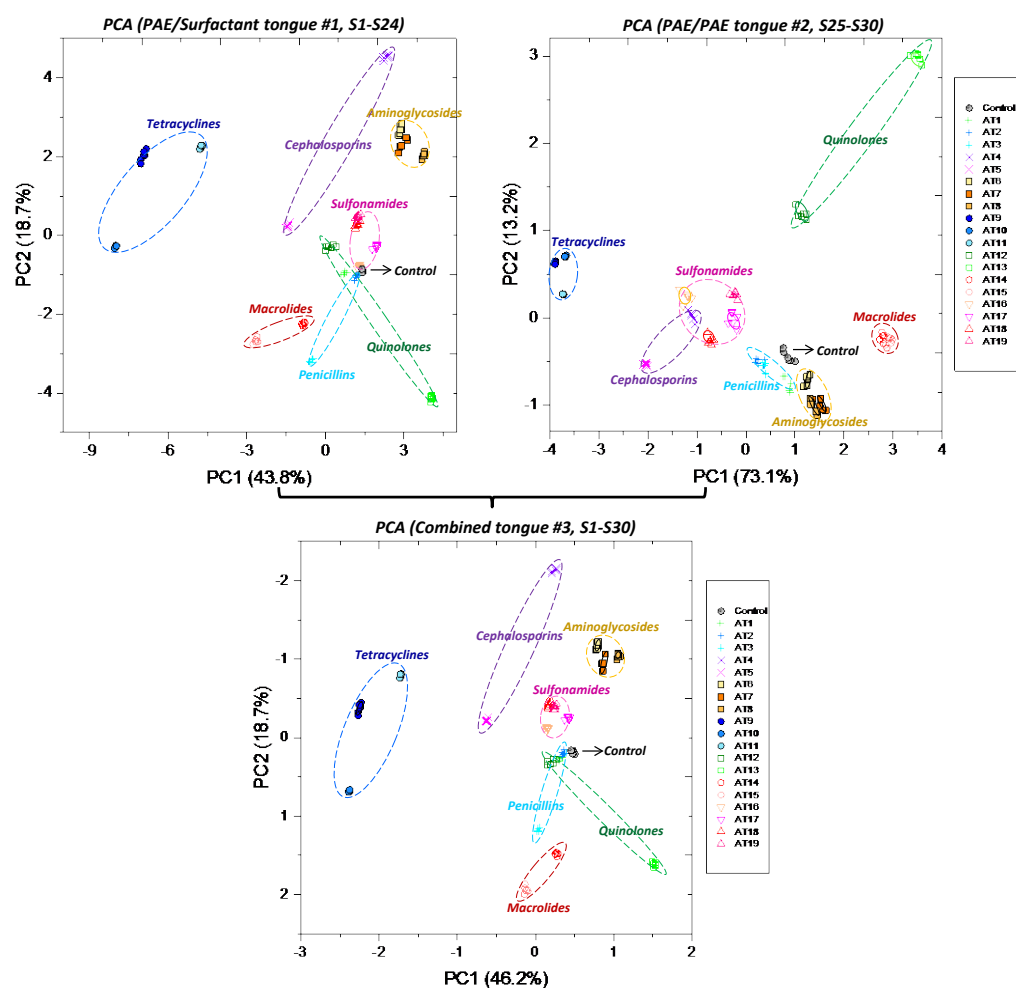


Figure S7. 2D PCA plot for the first two principal component obtained with an array of **S1-S24** (left, PAE/surfactant tongue #1), **S25-S30** (right, PAE/PAE tongue #2) and combined tongue of **S1-S30** (bottom, tongue #3) treated with antibiotics **AT1-AT19** ($c = 5$ mM) with 95% confidence ellipses. Each point represents the response pattern for a single antibiotic to the array. Each antibiotic was shown with their individual shape (triangle, square, circle etc.) and similar color.

7. Optimization Process

(1) PAE/Surfactant tongue

PCA sensor element	PC1 (43.8%)	PC2 (18.7%)	PC3 (11.9%)
S1 (C1_Ph3_463nm)	2.111	3.903	14.046
S2 (C1_pH3_503nm)	1.082	4.117	15.746
S3 (C1_pH7_463nm)	7.035	1.907	2.759
S4 (C1_pH7_503nm)	7.120	1.972	1.290
S5 (C1_pH13_463nm)	6.113	1.537	2.356
S6 (C1_pH13_503nm)	5.413	1.568	1.041
S7 (C2_pH3_470nm)	3.357	7.736	2.720
S8 (C2_pH3_505nm)	2.482	5.912	12.734
S9 (C2_pH7_470nm)	2.398	6.204	0.026
S10 (C2_pH7_505nm)	2.999	4.895	0.197
S11 (C2_pH13_470nm)	7.266	1.913	2.530
S12 (C2_pH13_505nm)	7.746	1.350	1.124
S13 (C3_pH3_533nm)	5.179	2.142	2.577
S14 (C3_pH3_565nm)	5.145	2.251	2.411
S15 (C3_pH7_533nm)	5.372	4.275	0.854
S16 (C3_pH7_565nm)	4.495	5.864	1.494
S17 (C3_pH13_533nm)	2.429	5.127	4.650
S18 (C3_pH13_565nm)	0.078	10.948	11.670
S19 (C4_pH3_531nm)	4.212	3.326	4.123
S20 (C4_pH3_569nm)	4.772	2.336	3.334
S21 (C4_pH7_531nm)	4.938	3.119	5.416
S22 (C4_pH7_569nm)	4.698	3.169	2.535
S23 (C4_pH13_531nm)	3.079	4.722	0.183
S24 (C4_pH13_569nm)	0.480	9.707	4.184

Contribution of the variables (%)

(2) PAE/PAE tongue

PCA sensor element	PC1 (73.1%)	PC2 (13.2%)	PC3 (7.1%)
S25 (P5_pH3_560nm)	19.35	12.82	3.16
S26 (P5_pH7_560nm)	16.72	15.76	26.73
S27 (P5_pH13_560nm)	19.30	6.35	10.39
S28 (C5_pH3_560nm)	12.51	52.77	0.00
S29 (C5_pH7_560nm)	14.88	12.27	38.79
S30 (C5_pH13_560nm)	17.23	0.02	20.93

Contribution of the variables (%)

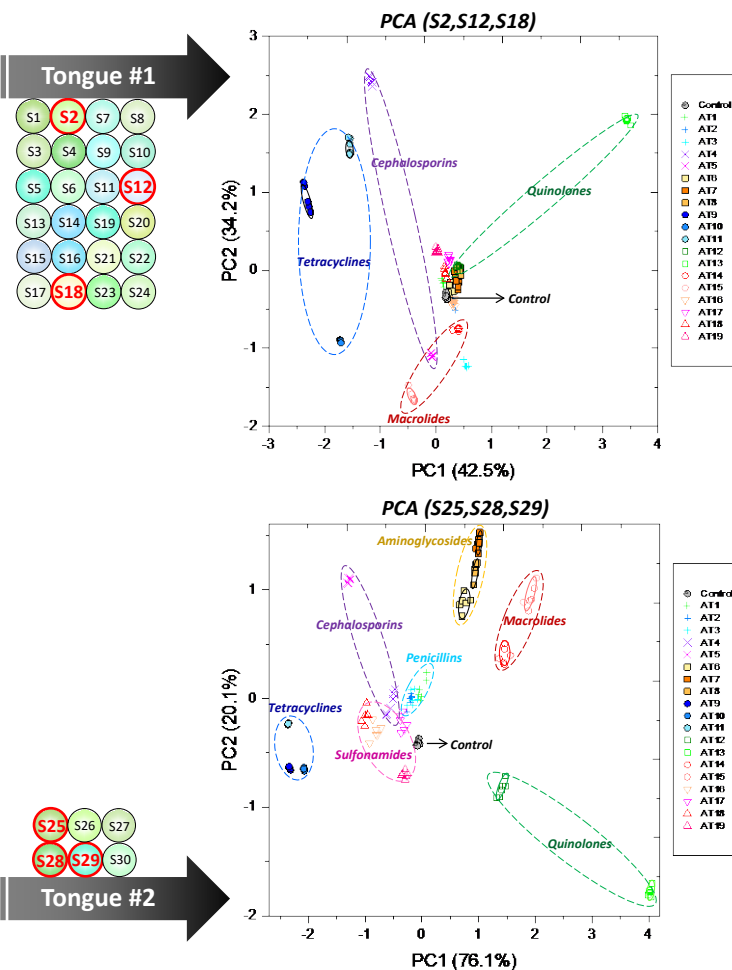


Figure S8. Optimization and selection of the best three sensing elements from the PAE/surfactant tongue (S1-S24) and PAE/PAE tongue (S25-S30) based on contribution of the variables of PCA (left). The resulting PCA plots are shown (right).

8. Others

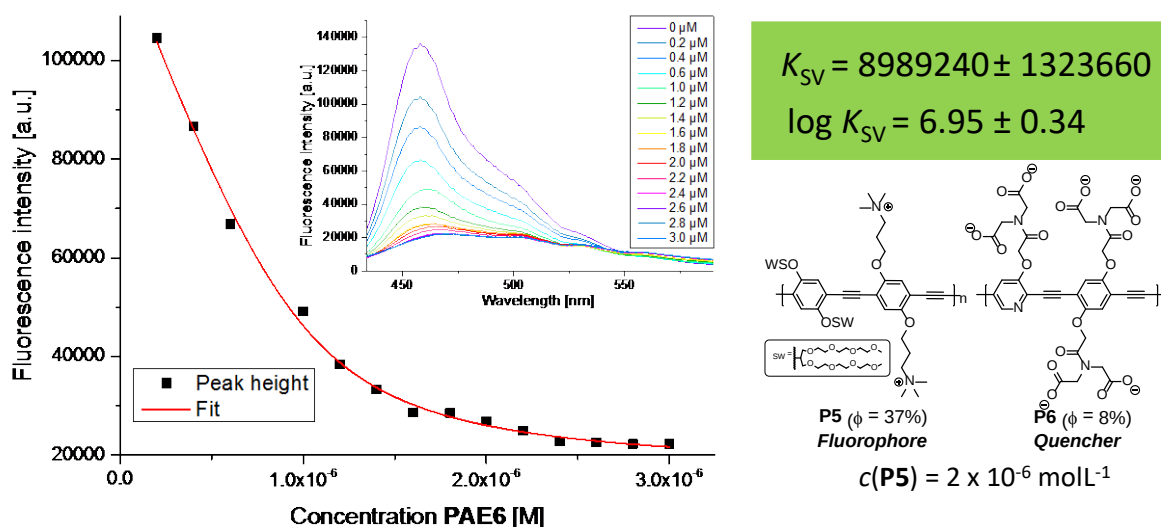


Figure S9. Complex titrations and determination of K_{SV} constants with modified Ster-Volmer equation. The titrations were performed in $\text{KH}_2\text{PO}_4/\text{Na}_2\text{HPO}_4$ buffered solution (pH = 7).

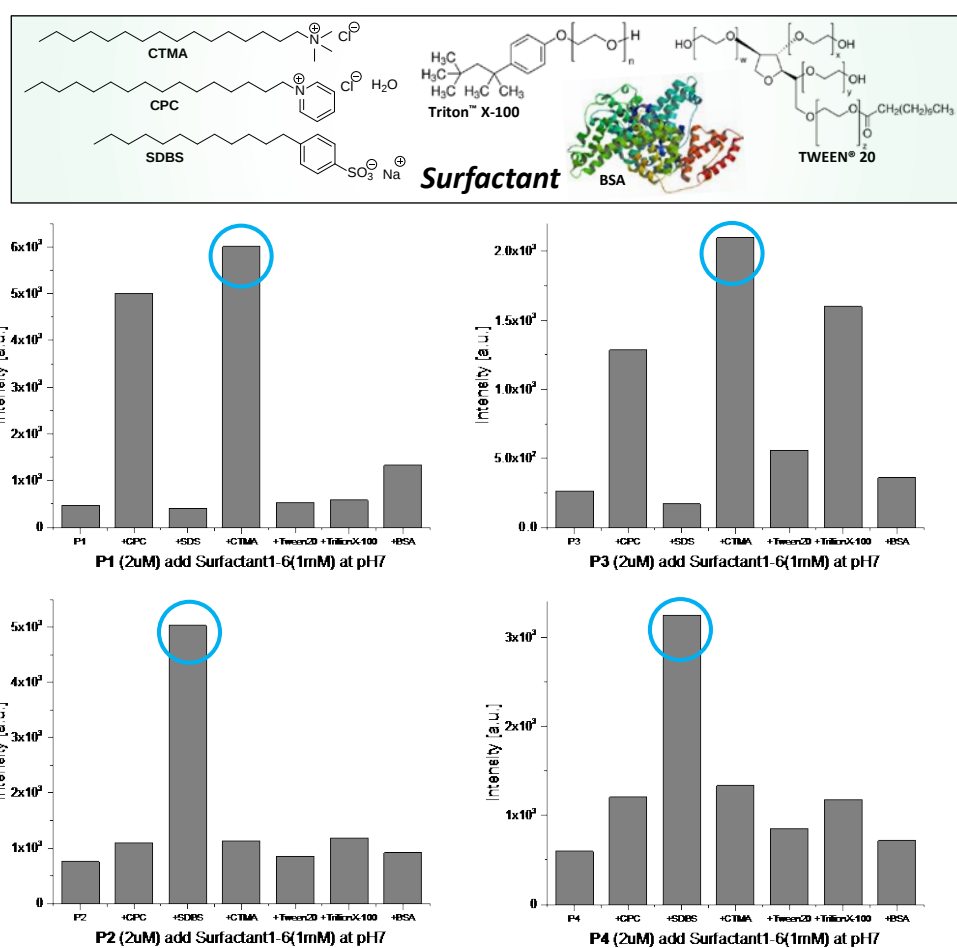


Figure S10. Screening process of various surfactants.

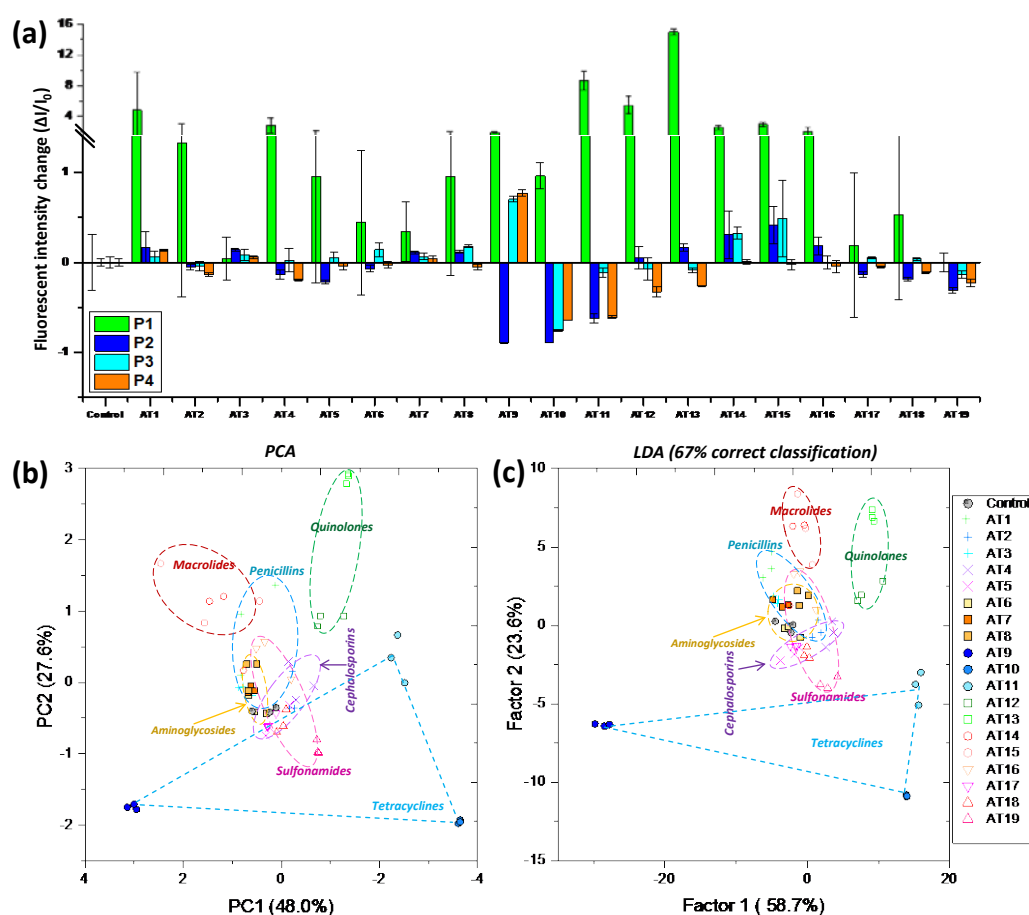
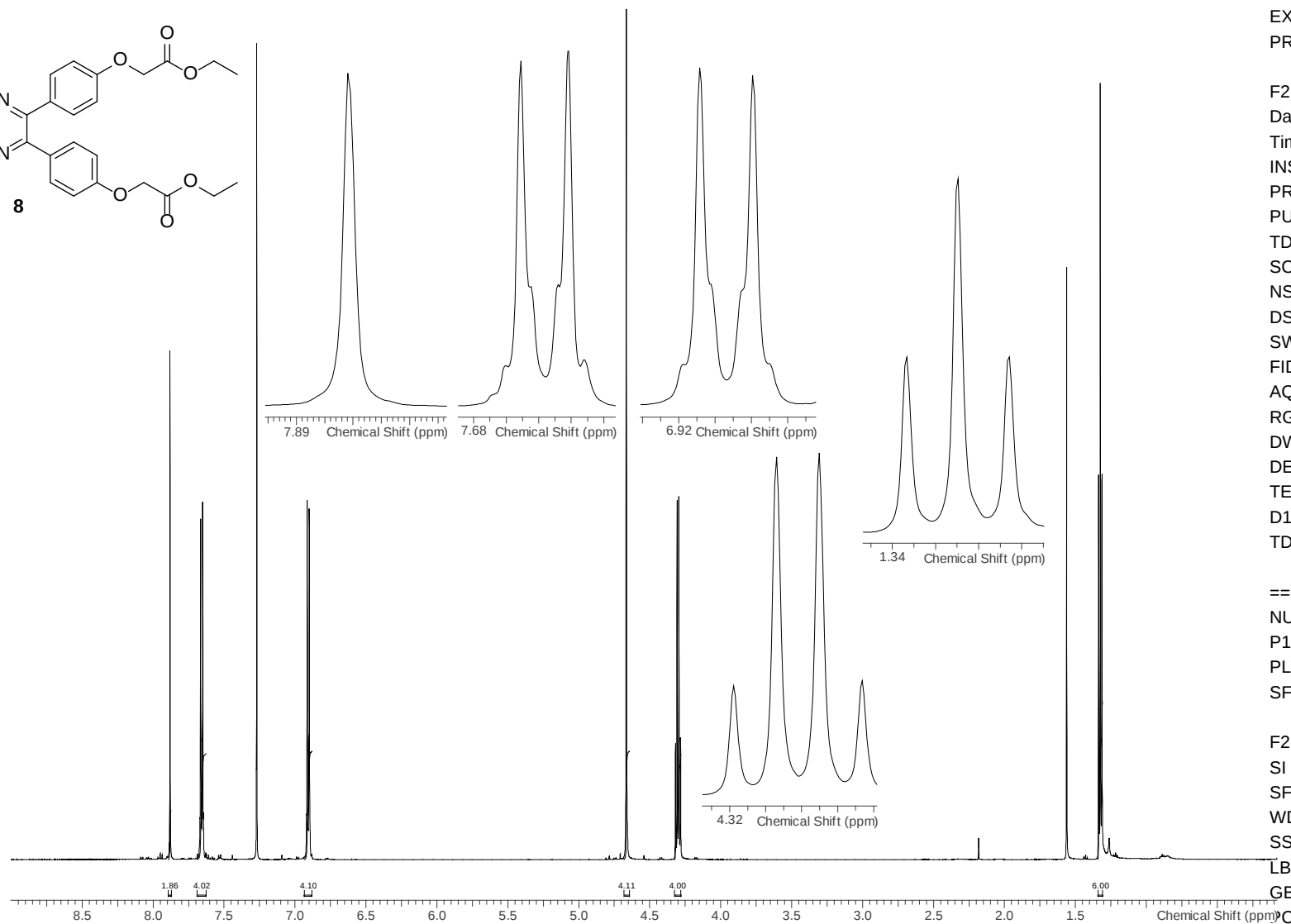
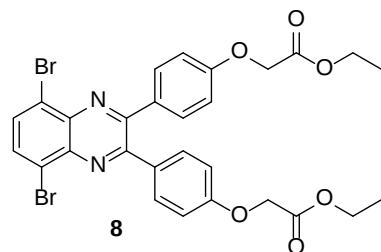


Figure S11. (a) Fluorescence intensity change $\Delta I/I_0$ obtained by weakly fluorescent **P1-P4** (2 μ M, at pH 7, buffered) treated with antibiotics **AT1-AT19** ($c = 5$ mM). Each value is the average of three independent measurements; each error bar shows the standard error (SD) of these measurements. (b) PCA plot and (c) LDA plot from first the first two factors obtained with **P1-P4** (2 μ M, at pH7, buffered) treated with antibiotics **AT1-AT19** ($c = 5$ mM). Cross-validated LDA showed 67% correct accuracy for all antibiotics.

9. ^1H -NMR Spectra

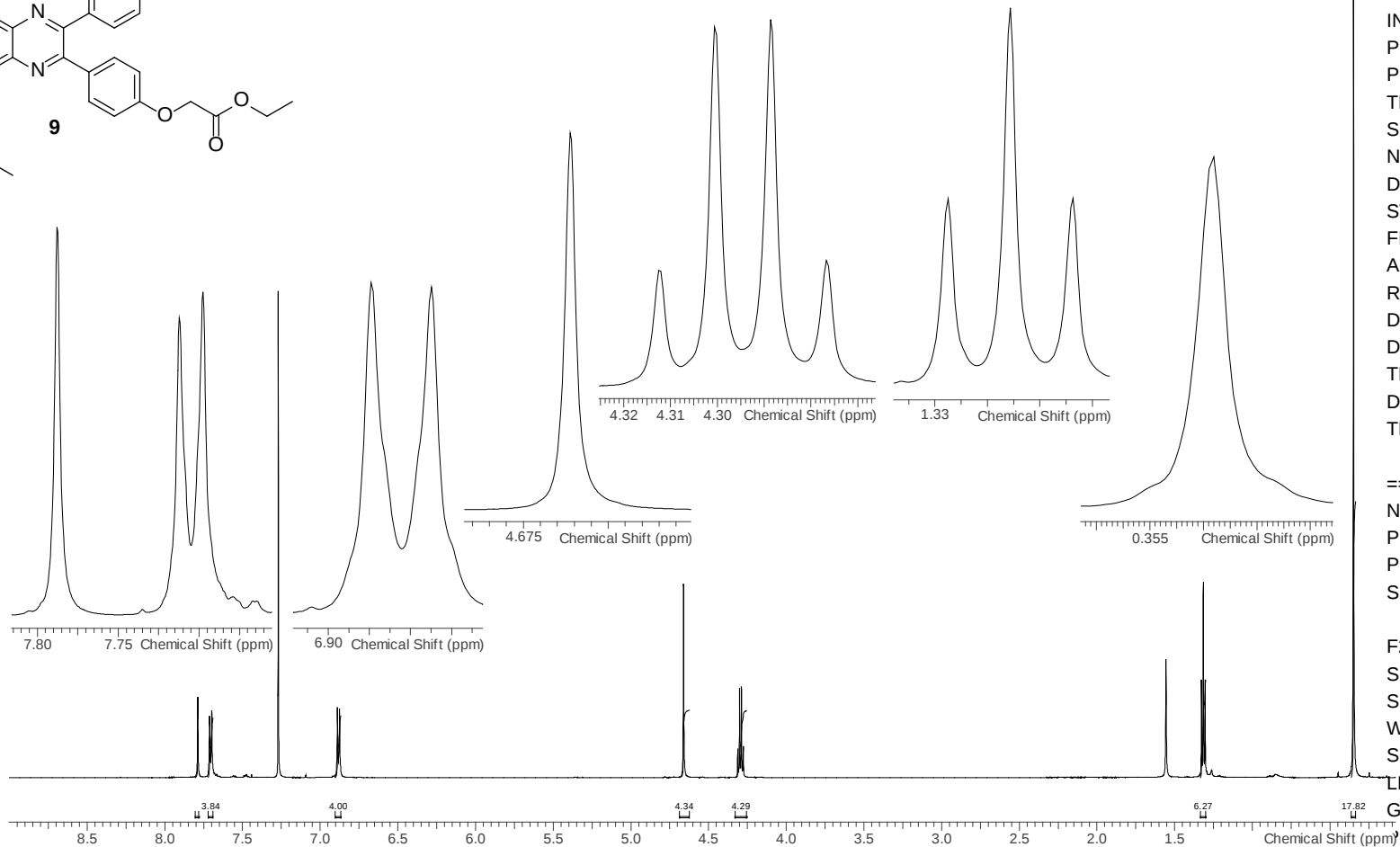
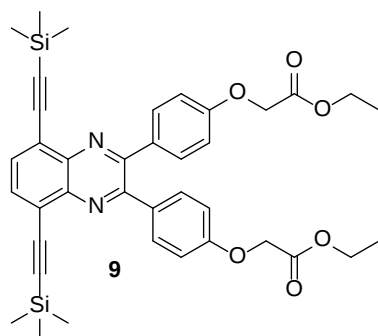


Current Data Parameters
 NAME e151130ubmb.246
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date 20151130
 Time 13.09
 INSTRUM spect
 PROBHD Z132808_0001 (
 PULPROG zg30
 TD 131072
 SOLVENT CDCl₃
 NS 128
 DS 2
 SWH 18028.846 Hz
 FIDRES 0.137549 Hz
 AQ 3.6350634 sec
 RG 10.93
 DW 27.733 usec
 DE 12.00 usec
 TE 295 K
 D1 0.10000000 sec
 TD0 16

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.63 usec
 PLW1 7.50000000 W
 SFO1 600.2468302 MHz

F2 - Processing parameters
 SI 65536
 SF 600.2438290 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

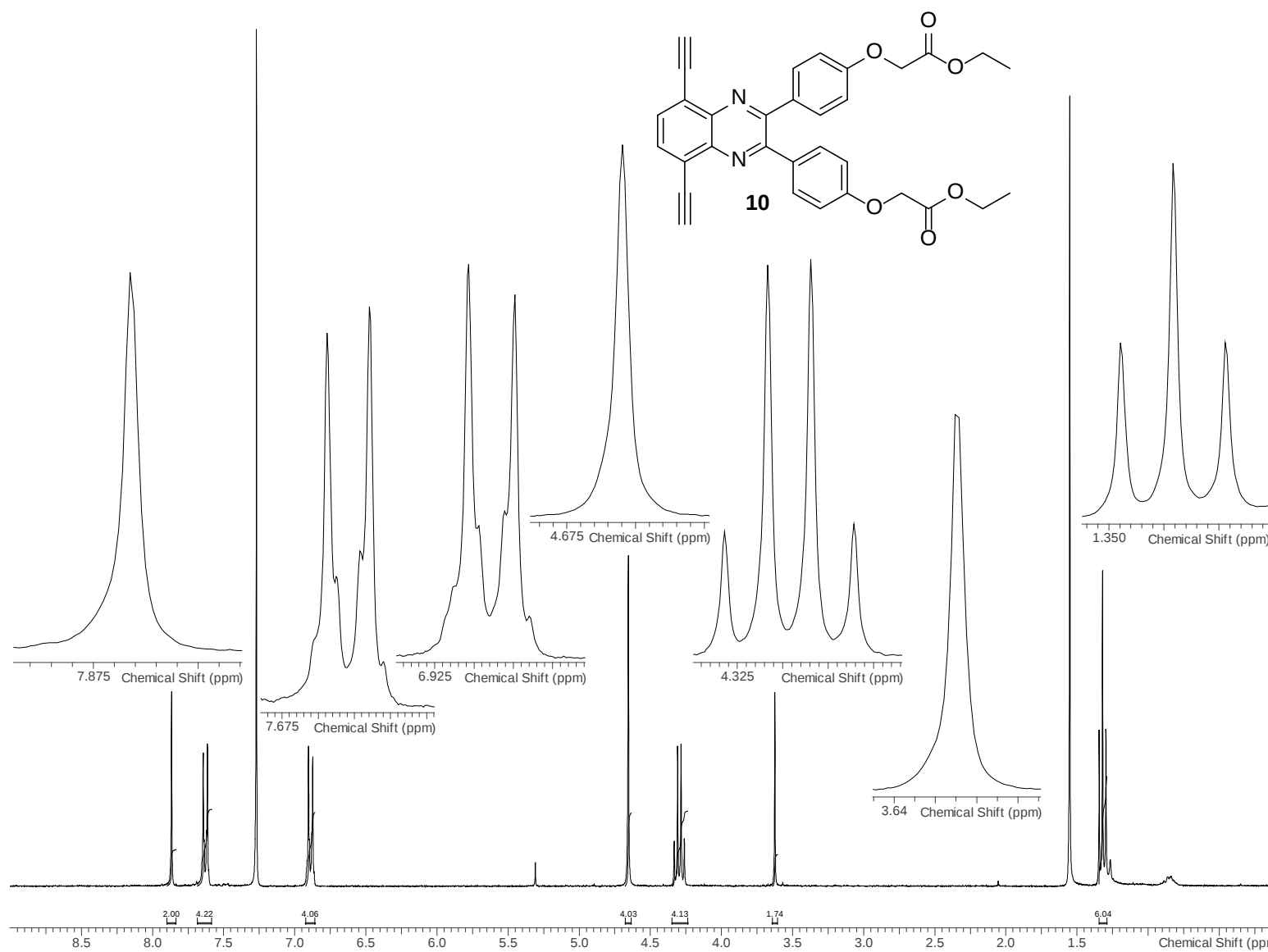


Current Data Parameters
 NAME e160302ubmb.280
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date 20160302
 Time 22.07
 INSTRUM Spect
 PROBHD Z132808_0001 (
 PULPROG zg30
 TD 131072
 SOLVENT CDCl₃
 NS 128
 DS 2
 SWH 18028.846 Hz
 FIDRES 0.137549 Hz
 AQ 3.6350634 sec
 RG 16.84
 DW 27.733 usec
 DE 12.00 usec
 TE 295 K
 D1 0.10000000 sec
 TD0 16

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.63 usec
 PLW1 7.50000000 W
 SFO1 600.2468302 MHz

F2 - Processing parameters
 SI 65536
 SF 600.2438290 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 C 1.00

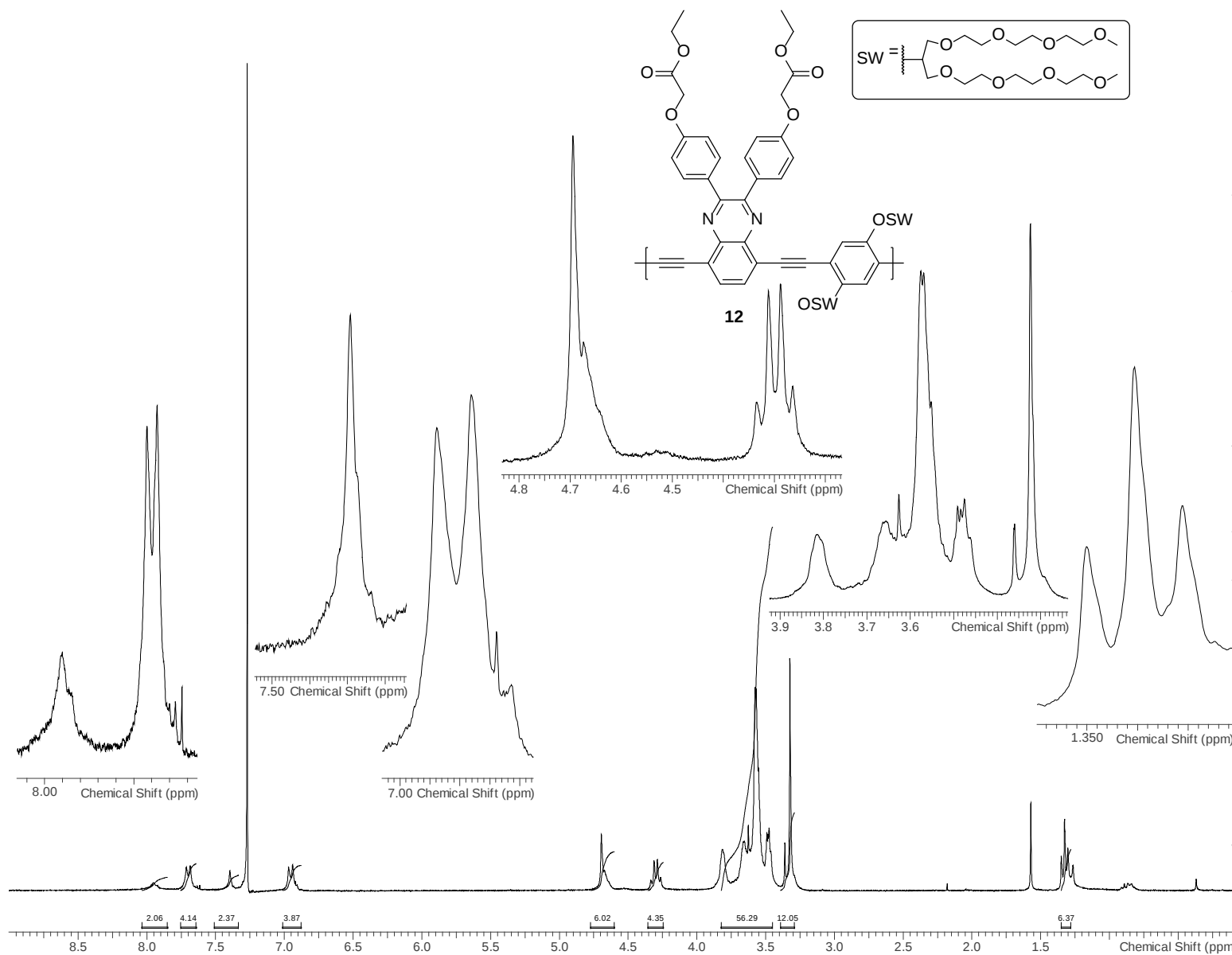


Current Data Parameters
 NAME b160401ubhr.046
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date 20160403
 Time 10.29
 INSTRUM Spect
 PROBHD 5 mm PATXO 31P
 PULPROG zg30
 TD 65536
 SOLVENT CDCl₃
 NS 128
 DS 2
 SWH 8992.806 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 574.7
 DW 55.600 usec
 DE 6.00 usec
 TE 298.2 K
 D1 0.10000000 sec
 TD0 16

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.50 usec
 PL1 -3.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300244 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

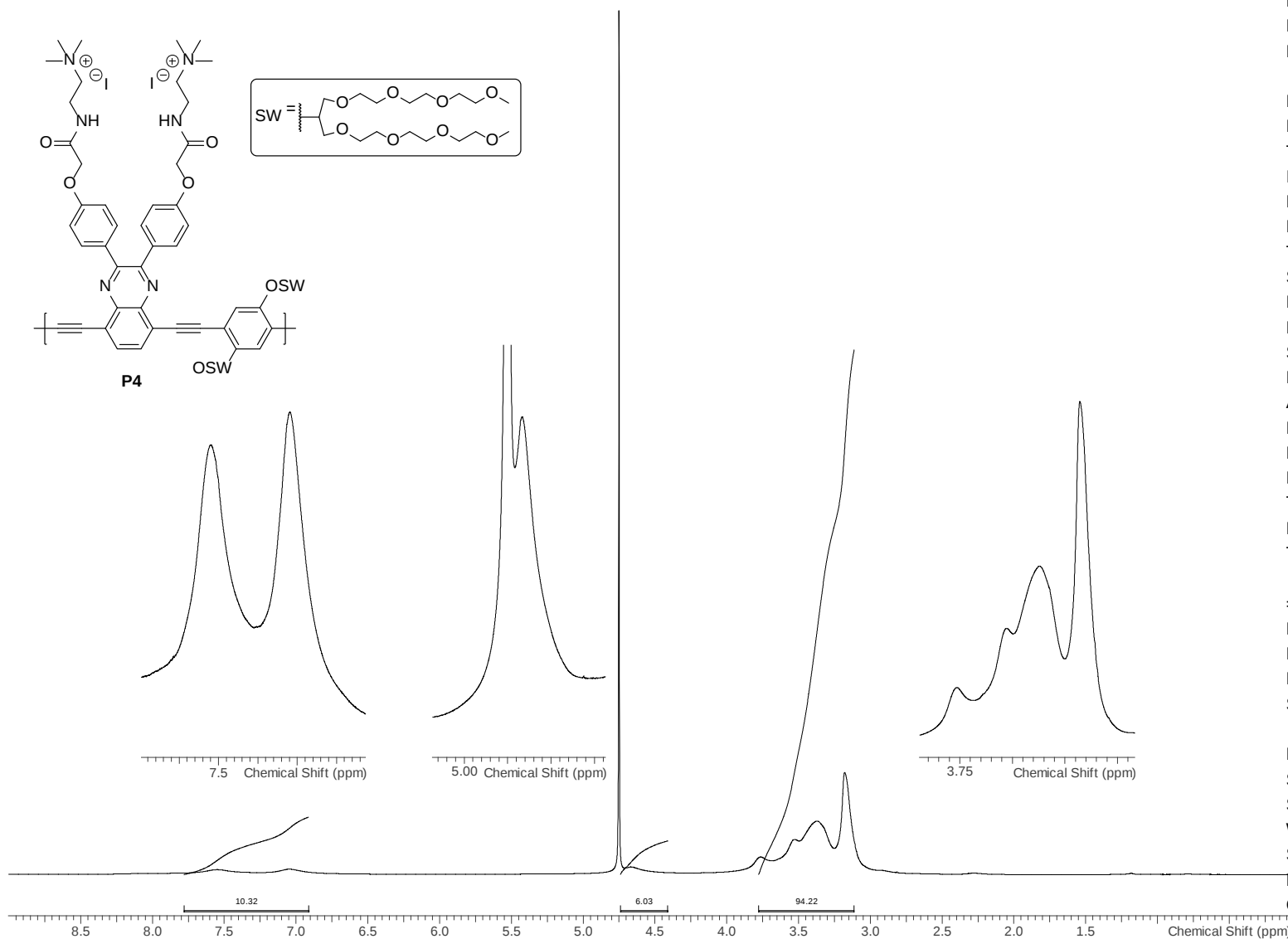
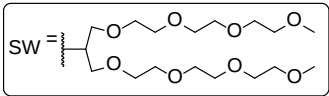


Current Data Parameters
 NAME a160426ubjp.33
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20160426
 Time 16.09
 INSTRUM Spect
 PROBHD Z104275_0201 (
 PULPROG zg30
 TD 65536
 SOLVENT CDCl₃
 NS 128
 DS 2
 SWH 9014.423 Hz
 FIDRES 0.275098 Hz
 AQ 3.6350634 sec
 RG 1030
 DW 55.467 usec
 DE 6.50 usec
 TE 300 K
 D1 0.10000000 sec
 TD0 16

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W
 SFO1 300.5115025 MHz

F2 - Processing parameters
 SI 65536
 SF 300.5100279 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



```

Current Data Parameters
NAME          d160530ubjp_37
EXPNO          1
PROCNO         1

```

F2 - Acquisition Parameters	
Date	20160504
Time	4.35
INSTRUM	spect
PROBH1	Z119877_0003 (
PULPROG	zg30
TD	98304
SOLVENT	D ₂ O
NS	81920
DS	2
SWH	15000.000 Hz
FIDRES	0.305176 Hz
AQ	3.2767999sec
RG	203
DW	33.333 usec
DE	6.50 usec
TE	294.9 K
D1	0.10000000 sec
TD0	1024

```
===== CHANNEL f1 =====
NUC1                      1H
P1                        14.60 usec
PLW1                     36.00000000 W
SFO1                     500.1325006 MHz
```

F2 - Processing parameters	
SI	65536
SF	500.1299761 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

10. Supplemental References

1. G. Helmchen, G. Nill, D. Flockerzi, W. Schuhle and M. S. K. Youssef, *Angew. Chem. Int. Ed. Engl.*, 1979, **18**, 62-63.
2. G. R. Fulmer, A. J. M. Miller, N. H. Sherden, H. E. Gottlieb, A. Nudelman, B. M. Stoltz, J. E. Bercaw and K. I. Goldberg, *Organometallics*, 2010, **29**, 2176-2179.
3. W. H. Melhuish, *J. Phys. Chem.-Us*, 1961, **65**, 229-235.
4. S. Stewart, M. A. Ivy and E. V. Anslyn, *Chem. Soc. Rev.* 2014, **43**, 70-84.
5. J. Han, M. Bender, S. Hahn, K. Seehafer and U. H. F. Bunz, *Chem. - Eur. J.*, 2016, **22**, 3230-3233.
6. S. Rana, S. G. Elci, R. Mout, A. K. Singla, M. Yazdani, M. Bender, A. Bajaj, K. Saha, U. H. F. Bunz, F. R. Jirik and V. M. Rotello, *J. Am. Chem. Soc.*, 2016, **138**, 4522-4529.
7. J. H. Kim, H. U. Kim, D. Mi, S. H. Jin, W. S. Shin, S. C. Yoon, I. N. Kang and D. H. Hwang, *Macromolecules*, 2012, **45**, 2367-2376.
8. A. Khan, S. Muller and S. Hecht *Chem. Commun. (Camb)* 2005, 584-586.