**Supplementary material**

**A versatile SERS sensor for multiple determination of Polycyclic Aromatic Hydrocarbons and its application potential in analysis of fried foods**

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**Fig. S1** SERS spectra of 16 PAHs (*C* = 100 ng·mL-1) in the presence of ro-GO/AuNP (red lines) and AuNPs (green lines) substrates.

**Table S1**. Band assignments for experimental SERS of NAP

|  |  |  |
| --- | --- | --- |
| Experimental  SERS | SERS Ref.1 | Vibrational modes |
| 512 | 502 | αC-C-C |
| 760 | 754 | γC-H |
| 1018 | 1015 | νC-C |
| 1165 | - | βC-H*τ*C-C-C-H |
| 1382 | 1378 | νC-C |
| 1564 | 1561 | νC-C |

**Table S2**. Band assignments for experimental SERS of PYR

|  |  |  |
| --- | --- | --- |
| Experimental  SERS | SERS Ref. 1 | Vibrational modes |
| 409 | 405 | νC-C-C-C |
|  | 453 | νC-C-C-C |
| 486 | 495 | νC-C-C-C |
| 594 | 592 | νC-C-C-C |
| 715 |  |  |
| 799 |  |  |
| 859 |  |  |
| 1059 | 1055 | δC-H |
| 1138 | 1135 | δC-H |
| 1234 | 1241 | νC-CδC-H |
| 1400 | 1398 | νC-C*τ*C-C-C-H |
| 1535 |  |  |
| 1612 | 1610 | νC-C |

**Table S3**. Band assignments for experimental SERS of ACE

|  |  |  |
| --- | --- | --- |
| Experimental  SERS | SERS Ref. 1 | Vibrational modes |
| 416 | 415 | νC-C-C-C |
| 461 | - | δC-H |
| 510 | - | νC-C-C-C |
| 550 | 543 | νC-C-C-C |
|  | 639 | τC-C-C-H |
| 660 |  |  |
| 798 | 800 | νC-C-C-C |
| 836 | 833 | δC-H |
|  | 1002 | νC-CδC-H |
|  | 1035 | νC-CδC-H |
| 1177 | - | δC-H |
| 1198 | 1215 | νC-CδC-H |
| 1243 | 1265 2 | νC-CδC-H |
|  | 1366 | νC-CδC-H |
| 1418 | 1420 | νC-CδC-H |
| 1454 | 1461 2 | νC-CδC-H |
| 1600 | 1593 | νC-CδC-H |

**Table S4**. Band assignments for experimental SERS of ACEY

|  |  |  |
| --- | --- | --- |
| Experimental  SERS | SERS Ref. 1 | Vibrational modes |
|  | 377 | δC-H |
| 412 | 414 | νC-C-C-C |
| 537 | 549 | νC-C-C-C |
| 634 | 659 | τC-C-C-H |
| 796 | 800 | νC-C-C-CνC-C |
| 832 |  |  |
|  | 921 | δC-H |
| 1000 | 1011 | νC-CδC-H |
| 1030 | 1026 | νC-CδC-H |
|  | 1074 | νC-CδC-H |
| 1165 |  |  |
| 1213 | 1207 | νC-CδC-H |
| 1247 | 1245 | νC-CδC-H |
| 1366 | 1350 | νC-CδC-H |
|  | 1380 | νC-CδC-H |
| 1409 | 1420 | νC-CδC-H |
|  | 1460 | νC-CδC-H |
| 1531 | 1539 | νC-CδC-H |
| 1591 | 1602 | νC-CδC-H |

**Table S5**. Band assignments for experimental SERS of ANTH

|  |  |  |
| --- | --- | --- |
| Experimental  SERS | SERS Ref. 1 | Vibrational modes |
| 393 | 392 | νC-C-C-C |
| 749 | 753 | νC-C |
| 893 | 891 2 | *τ*C-C-C-H |
| 1008 | 1008 | νC-C |
| 1252 | 1252 | *τ*C-C-C-H |
| 1393 | 1395 | νC-C*τ*C-C-C-H |
| 1541 | 1545 | νC-C |

**Table S6**. Band assignments for experimental SERS of CHR

|  |  |  |
| --- | --- | --- |
| Experimental  SERS | SERS Ref. 1 | Vibrational modes |
| 378 | 381 | δC-H |
| 562 | 568 | νC-C-C-C |
| 668 |  |  |
|  | 678 | νC-C-C-CτC-C-C-H |
| 763 | 768 | νC-C-C-C |
|  | 877 | νC-C-C-CνC-C |
| 1012 | 1016 | νC-C-C-CτC-C-C-H |
|  | 1040 | νC-CδC-H |
| 1238 | 1245 | νC-CδC-H |
|  | 1334 | νC-CδC-H |
| 1376 | 1377 | νC-CδC-H |
| 1427 | 1428 | νC-CδC-H |
| 1531 |  |  |
|  | 1568 | νC-CδC-H |
|  | 1605 | νC-CδC-H |

**Table S7**. Band assignments for experimental SERS of FLU

|  |  |  |
| --- | --- | --- |
| Experimental  SERS | SERS Ref. 1 | Vibrational modes |
| 415 | 416 | νC-C-C-C |
| 735 | 734 | νC-C-C-CνC-C |
| 811 | 806 2 | C-H out-of plane bending, C-H wagging |
| 887 | 890 2 | C-H out-of-plane bending, C-H twisting |
| 1009 | 1008 | νC-CδC-H |
| 1070 | 1054 2 | νC-CδC-H |
| 1107 | 1108 2 | -- |
| 1150 | 1153 | δC-H |
| 1207 | 1210 2 | νC-CδC-H |
| 1238 | 1236 | νC-CδC-H |
| 1287 | 1299 | νC-CδC-H |
| 1354 | 1354 | νC-CδC-H |
| 1455 | 1469 | νC-CδC-H |
| 1531 | 1545 2 | -- |
|  | 1568 | νC-CδC-H |
| 1595 | 1601 | νC-CδC-H |

**Table S8**. Band assignments for experimental SERS of PHE

|  |  |  |
| --- | --- | --- |
| Experimental  SERS | SERS Ref. 1 | Vibrational modes |
| 402 | 405 | νC-C-C-C |
| 540 | 545 | νC-C-C-C |
| 704 | 711 | νC-C-C-C |
| 824 | 826 | νC-C-C-C |
| 1021 |  |  |
|  | 1032 | νC-CδC-H |
|  | 1165 | νC-CδC-H |
| 1200 | 1207 | τC-C-C-HδC-H |
| 1237 | 1244 | νC-CδC-H |
| 1351 | 1352 | νC-CδC-H |
| 1428 | 1431 | νC-CδC-H |
| 1533 |  |  |
| 1606 | 1610 | νC-CδC-H |

**Table S9**. Band assignments for experimental SERS of BaP

|  |  |  |
| --- | --- | --- |
| Experimental  SERS | SERS Ref. 1 | Vibrational modes |
|  | 334 | δC-CδC-H |
| 385 | 381 | δC-CδC-H |
| 455 | 452 | *τ*C-CγC-H |
| 528 |  |  |
| 555 | 558 | δC-C δC-H |
| 608 | 613 | δC-CδC-H |
| 632 | 636 | *τ*C-CδC-CδC-H |
| 842 | 847 | νC-CνC-H |
| 979 | 985 | δC-HνC-C |
| 1016 | 1016 | δC-HνC-C |
|  | 1196 | δC-H |
|  | 1216 | δC-H |
| 1238 | 1238 | δC-H*τ*C-C-C-H |
| 1268 | 1270 | δC-H |
|  | 1321 | δC-H*v*C-CνC-C-C-C |
| 1348 | 1350 | δC-H*v*C-C*τ*C-C-C-C |
| 1378 | 1382 | *v*C-C-C |
| 1406 | 1407 | δC-H*v*C-C |
| 1424 | 1425 | δC-H*v*C-C |
|  | 1572 | δC-H*v*C-C |
|  | 1617 | δC-H*v*C-C |
|  | - | δC-H*v*C-C |

**Table S10**. Band assignments for experimental SERS of FLUA

|  |  |  |
| --- | --- | --- |
| Experimental  SERS | SERS Ref. 1 | Vibrational modes |
|  | 352 | νC-C-C-C |
|  | 451 | νC-C-C-C |
| 482 | 484 | νC-C-C-CνC-C |
| 556 | 563 | νC-C-C-C |
| 662 | 672 | νC-C-C-CνC-C |
| 796 | 802 | νC-C-C-CνC-C |
| 1006 | 1012 | νC-CδC-H |
| 1098 | 1100 | νC-CδC-H |
|  | 1158 | νC-CδC-H |
| 1268 | 1280 | νC-CδC-H |
| 1311 |  |  |
|  | - | τC-C-C-HνC-CδC-H |
|  | 1419 | νC-CδC-H |
| 1448 | 1448 | νC-CδC-H |
| 1537 | 1544 | νC-CδC-H |
| 1601 | 1601 | νC-CδC-H |

**Table S11**. Band assignments for experimental SERS of BaA

|  |  |  |
| --- | --- | --- |
| Experimental  SERS | SERS Ref. 1 | Vibrational modes |
|  | 306 | δC-C |
| 360 | 358 | δC-C |
| 528 |  |  |
| 568 | 574 | τC-C |
| 717 | 722 | νC-CδC-C |
| 784 | 792 | - |
| 887 |  |  |
| 1019 | 1012 | τC-H |
|  | 1035 | δC-H |
| 1116 |  |  |
| 1162 | 1166 | δC-H |
| 1259 | 1262 | δC-H |
| 1344 | 1345 | δC-CδC-H |
| 1388 | 1393 | δC-H |
| 1448 | 1432 | δC-CδC-H |
| 1531 |  |  |
|  | 1554 | νC-CδC-H |
| 1598 | 1610 | νC-CδC-H |

**Table S12**. Band assignments for experimental SERS of DiB

|  |  |  |
| --- | --- | --- |
| Experimental  SERS | SERS Ref. 1 | Vibrational modes |
|  | 330 | δC-H |
| 495 | 496 | νC-C-C-C |
| 544 | 547 | δC-H |
| 616 | 619 | νC-C-C-C |
| 714 |  |  |
| 745 | 752 | δC-H |
|  | 931 | νC-C-C-CδC-H |
| 1015 |  |  |
|  | 1035 | νC-C-C-CδC-H |
| 1159 | 1164 | νC-CδC-H |
| 1214 | 1217 | νC-CδC-H |
|  | 1260 | νC-CδC-H |
| 1293 | 1298 | νC-CδC-H |
| 1342 | 1346 | νC-CδC-H |
|  | 1380 | νC-CδC-H |
| 1436 | 1435 | δC-H |
|  | 1496 | νC-CδC-H |
| 1531 |  |  |
|  | 1559 | νC-C |
| 1574 | 1582 | νC-CδC-H |
| 1604 | 1608 | νC-CδC-H |

**Table S13**. Band assignments for experimental SERS of BbF

|  |  |  |
| --- | --- | --- |
| Experimental  SERS | SERS Ref. 1 | Vibrational modes |
|  | 334 | νC-C-C-C |
| 390 | 392 | νC-C-C-C |
|  | 486 | νC-C-C-C |
|  | 592 | νC-C-C-C |
|  | 660 | νC-C-C-C |
| 684 | 688 | νC-C-C-C |
| 778 | 790 | νC-C-C-C |
|  | 901 | δC-H |
|  |  |  |
| 1015 | 996 | τC-C-C-H |
|  | 1032 | νC-C |
|  | 1096 | νC-CδC-H |
| 1128 |  |  |
| 1192 | 1194 | νC-CδC-H |
| 1235 | 1238 | τC-C-C-HδC-H |
|  | 1276 | νC-CδC-H |
|  | 1314 | νC-CδC-H |
|  | 1337 | νC-CδC-H |
| 1376 | 1380 | νC-CδC-H |
|  | 1418 | νC-CδC-H |
| 1455 | 1455 | νC-CδC-H |
| 1533 | 1526 | τC-C-C-HδC-HνC-C |
|  | 1593 | νC-CδC-H |
| 1613 | 1620 | νC-CδC-H |

**Table S14**. Band assignments for experimental SERS of BkF

|  |  |  |
| --- | --- | --- |
| Experimental  SERS | SERS Ref. 1 | Vibrational modes |
|  | 452 | νC-C-C-CτC-C-C-H |
|  | 492 | νC-C-C-C |
|  | 552 | νC-C-C-C |
|  | 601 | δC-H |
|  | 669 | νC-C-C-C |
|  | 761 | δC-H |
|  | 800 | νC-C-C-C |
|  | 817 | νC-C-C-CδC-H |
|  | 895 | τC-C-C-HδC-H |
| 920 | 924 | δC-H |
|  | 1024 | νC-CδC-H |
|  | 1031 | νC-CδC-H |
|  | 1092 | νC-CδC-H |
|  | 1132 | νC-CδC-H |
|  | 1153 | νC-CδC-H |
|  | 1194 | νC-CδC-H |
|  | 1275 | νC-CδC-H |
|  | 1342 | νC-CδC-H |
| 1375 | 1366 | νC-CδC-H |
|  | 1401 | νC-CδC-H |
| 1441 | 1442 | νC-CδC-H |
|  | 1495 | νC-CδC-H |

**Table S15**. Band assignments for experimental SERS of BghiP

|  |  |  |
| --- | --- | --- |
| Experimental  SERS | SERS Ref. 1 | Vibrational modes |
|  | 366 | νC-C-C-C |
| 382 | 387 | νC-C-C-C |
| 420 | 416 | νC-CδC-H |
| 452 | 452 | *τ*C-C-C-H |
| 478 | 479 | νC-C-C-C |
| 539 | 538 | *τ*C-C-C-H |
| 637 |  |  |
|  | 712 | νC-CδC-H |
| 761 |  |  |
| 860 | 848 | νC-CδC-H |
|  |  |  |
| 979 | 985 | *τ*C-C-C-H |
| 1071 | 1083 | *τ*C-C-C-H |
| 1141 | 1146 | δC-H |
|  | 1202 | *τ*C-C-C-HδC-H |
| 1255 | 1255 | *τ*C-C-C-HδC-H |
| 1305 | 1305 | νC-CδC-H |
| 1368 |  |  |
|  | 1385 | νC-CδC-H |
| 1432 | 1436 | *τ*C-C-C-HδC-H |
| 1599 | 1594 | νC-C |

**Table S16**. Band assignments for experimental SERS of Ind

|  |  |  |
| --- | --- | --- |
| Experimental  SERS | SERS Ref. 1 | Vibrational modes |
|  | 319 | νC-C-C-C |
|  | 365 | νC-C-C-C |
| 407 | 407 | νC-C-C-C |
| 473 | 473 | νC-C-C-C |
| 514 |  |  |
| 579 |  |  |
| 623 | 626 | νC-C-C-C |
| 673 | 680 | νC-C-C-C |
| 780 | 785 | νC-C*τ*C-C-C-H |
| 799 |  |  |
| 883 |  |  |
|  | 971 | νC-C*τ*C-C-C-H |
|  | 1001 | *τ*C-C-C-H |
| 1017 |  |  |
|  | 1052 | νC-C*τ*C-C-C-H |
|  | 1103 | νC-CδC-H |
|  | 1153 | νC-CδC-H |
| 1183 | 1187 | δC-H |
|  | 1209 | νC-CδC-H |
| 1233 | 1242 | *τ*C-C-C-HδC-H |
|  | 1295 | νC-CδC-H |
|  | 1311 | νC-CδC-H |
|  | 1337 | νC-C*τ*C-C-C-H |
|  | 1380 | νC-CδC-H |
|  | 1428 | νC-CδC-H |
|  | 1477 | νC-CδC-H |
| 1533 | 1538 | νC-C |
| 1599 | 1587 | νC-C |
|  | 1606 | νC-C |
| 1637 | 1645 | νC-C |

**Table S17. The LOD and quantitative calculation model of 16 PAHs**

|  |  |  |  |
| --- | --- | --- | --- |
| Compound | Fitting regression | *R*2 | LOD  (ng·mL-1) |
| NAP | *C* = -0.5767\* *I*1018+3.1339\* *I*1564-748.577 | 0.9989 | 0.5 |
| PYR | *C* = 0.06147\* *I*1234+0.1143\* *I*1400+0.4411 | 0.9997 | 0.2 |
| ACE | *C* = 0.1334\* *I*550+0.0824\* *I*660+0.6486 | 0.9997 | 1.0 |
| ACEY | *C* = 0.8293\* *I*1213+0.2180\* *I*1409-323.123 | 0.9987 | 0.8 |
| ANTH | *C* = 0.09212\* *I*1393+0.4323\* *I*1548+4.2894 | 0.9994 | 0.5 |
| CHR | *C* = 0.1326\* *I*1012+1.8781\* *I*1427-1.7821 | 0.9990 | 0.8 |
| FLU | *C* = 0.3760\* *I*735+0.2381\* *I*1354-0.2421 | 0.9995 | 0.2 |
| PHE | *C* = 0.05268\* *I*704+0.9253\* *I*1351+0.4854 | 0.9989 | 0.5 |
| BaP | *C* = 0.4817\* *I*1238+0.4301\* *I*1378+1.4213 | 0.9990 | 0.5 |
| FLUA | *C* = 0.2643\* *I*796+0.0983\* *I*1448+2.3629 | 0.9894 | 1.0 |
| BaA | *C* = 0.5675\* *I*717+0.2733\* *I*1531+0.2690 | 0.9995 | 0.8 |
| DiB | *C* = -0.02649\* *I*714+2.3462\* *I*1342+13.3556 | 0.9990 | 0.5 |
| BbF | *C* = 0.3292\* *I*684+0.3645\* *I*1192+0.2662 | 0.9901 | 1.0 |
| BkF | *C* = 0.3292\* *I*1375 +0.6803 | 0.9889 | 2.0 |
| BghiP | *C* = 1.0382\* *I*452+0.4619\* *I*1305+0.3305 | 0.9994 | 0.2 |
| Ind | *C* = 0.3534\* *I*623+0.5347\* *I*1533-0.15375 | 0.9995 | 0.5 |

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