# 8 Appendix

Table 8.1: Band assignment for MG

| Peak position ($cm^{-1}$) | Bond associated |
|---|---|
| 1172 | ring C-H in plane vibrations |
| 1366 | C-H rocking |
| 1398 | N-phenyl stretching |
| 1616 | C-C stretching |

Table 8.2: Band assignment for R6G

| Peak position ($cm^{-1}$) | Bond associated |
|---|---|
| 610 | C-C-C in plane bending |
| 770 | C-H out-plane bending |
| 1182 | C-H in plane bending |
| 1314 | C=C stretching |
| 1362 | C-C stretching |
| 1510 | C-C stretching |

Table 8.3: Band assignment for BPE

| Raman Shift ($cm^{-1}$) | Associated Vibration |
|---|---|
| 880 | pyridyl ring breathing |
| 1000 | pyridyl ring twisting |
| 1199 | pyridyl ring twisting |
| 1338 | $\delta$(C−H)py |
| 1491 | $\delta$(C−H)py |
| 1605 | pyridyl ring stretching |
| 1637 | $\nu$(C=C) |

$\nu$: stretching; $\delta$:bending

Table 8.4: Band assignment for paracetamol

| Peak position ($cm^{-1}$) | Bond associated |
|---|---|
| 1170 | H-C-C in plane vibration |
| 1236 | C-C and H-O-C vibration |
| 1326 | C-N phenyl stretch |
| 1376 | symmetric stretching of $CH_3$ |

Table 8.5: Band assignment for aspirin

| Peak position ($cm^{-1}$) | Bond associated |
|---|---|
| 786 | ring stretching |
| 1038 | $\delta$(CH) bending and ring stretching |
| 1256 | $\delta$(C-H) bending and $\nu$(C-O) |
| 1612 | ring stretching |

Table 8.6: Peak assignment of CEF-Na

| Raman Shift ($cm^{-1}$) | Description |
|---|---|
| 500 | C-S stretching |
| 692 | C-H out-of-plane deformation |
| 1371 | CH2 deformation |
| 1500 | Amide N-H deformation/C=C stretching/C=N stretching |
| 1582 | |
| 1643 | Amide C=O stretching |

Table 8.9: Band assigment for SFZ

| Peak position ($cm^{-1}$) | Bond associated |
|---|---|
| 780 | C-H out-of-plane deformation |
| 1600 | Amide N-H bending/C=N stretching |

Table 8.7: Peak assignment of CEFTR

| Raman Shift ($cm^{-1}$) | Description |
|---|---|
| 500 | C-S stretching |
| 692 | C−H out-of-plane deformation |
| 1371 | $CH_2$ deformation |
| 1500 | Amide N-H deformation/C=C stretching/C=N stretching |
| 1582 | |
| 1643 | Amide C=O stretching |

Table 8.8: Band assigment for milk extract

| Raman Shift ($cm^{-1}$) | Description |
|---|---|
| 333 | CCN bending |
| 680 | |
| 822 | octave |
| 1255 | $CH_3$ deformation |
| 2190 | C=N stretching |

Table 8.10: Band assigment for TCH

| Peak position ($cm^{-1}$) | Bond associated |
|---|---|
| 236 | CCN bending |
| 444 | octave |
| 590 | $\delta$(amid-ONH) |
| 641 | $\delta$(amid-ONH) |
| 850 | $\nu$(CO) |
| 920 | $\nu$(CO) |
| 1041 | $\nu$(CO) |
| 1128 | $\nu$(CO) |
| 1168 | $\nu$(CO) |
| 1237 | $\delta$(CH4) |
| 1463 | $\delta$(amin-CH3) |

Table 8.11: Band assigment for DCH

| Raman Shift ($cm^{-1}$) | Description |
|---|---|
| 559 | $\delta$(amid-ONH) |
| 594 | |
| 883 | $\nu$ (CO) |
| 942 | |
| 1060 | |
| 1141 | $\nu$(CO) |
| 1170 | $\nu$(CO) |
| 1263 | $\delta$(CH4), $\delta$(OH), $\delta$(CH), $\delta$(OH), v(D) |
| 1314 | $\nu$(CC), $\nu$(CO), $\nu$(CO),$\delta$(CH) |
| 1480 | $\delta$(CH),$\delta$(OH), $\nu$(D), $\nu$(CO), $\delta$(amin-CH3) |
| 1588 | $\delta$ (OH) $\nu$(D), v(CC) |
| 1621 | v(amid-CO),$\delta$(amid-NH), $\nu$(CC), $\nu$(OH) |

Table 8.12: Band assigment for ENX

| Raman Shift ($cm^{-1}$) | Description |
|---|---|
| 639<br>748 | CH deformation<br>methylene rocking |
| 1253 | CH rocking |
| 1395 | symmetric OCO stretching |
| 1465 | benzene ring vibrations |
| 1536 | C=O stretching |
| 1624 | benzene ring stretching |

Table 8.13: Band assigment for background chemicals

| Raman Shift ($cm^{-1}$) | Description |
|---|---|
| 333 | CCN bending |
| 750 | octave |
| 920 | CC stretching |
| 1044 | $CH_3$ rocking |
| 1387 | $CH_3$ deformation |
| 1449 | $CH_3$ deformation |
| 2249 | C=N stretching |
| 2943 | Symmetric CH stretching |

Table 8.14: Peak assignment of FLU

| Raman Shift ($cm^{-1}$) | Description |
|---|---|
| 585 | 2, 4- Difluorobenzyl Group ring deformation |
| 737 | 2, 4- Difluorobenzyl Group ring breathing |
| 967 | Triazole Group ring bend |
| 1020 | Propane Backbone C-(OH) stretch |
| 1135 | Triazole Group ring breath |
| 1253 | Triazole Group ring stretch |
| 1367 | |

Table 8.15: Peak assignment of LIN

| Raman Shift ($cm^{-1}$) | Description |
|---|---|
| 460 | CCN bending |
| 619 | δ(amid-ONH) |
| 712 | |
| 871 | ν(CO) |
| 1002 | |
| 1041 | |
| 1463 | δ(CH) |

Table 8.16: Comparison of estimated EF from simulation and the experimentally measured SERS EF

| S/N | SERS substrate | $E_{local}$ | $E_{incident}$ | $\frac{E_{local}}{E_{incident}}$ | $EF_{sim} \sim \lvert\frac{E_{local}}{E_{incident}}\rvert^4$ | $EF_{exp}$ |
|---|---|---|---|---|---|---|
| 1 | AgNPs on 100 GSM paper | $1.1 \times 10^7$ | $6.17 \times 10^4$ | 178 | $1.01 \times 10^9$ | $10^7$ |
| 2 | AuNPs on *aegles marmelous* leaf | $9.2 \times 10^6$ | $6.3 \times 10^4$ | 146 | $4.45 \times 10^8$ | $10^6$ |
| 3 | Cu-Au-ITO platform | $8.2 \times 10^6$ | $6.18 \times 10^4$ | 133 | $3.1 \times 10^8$ | $10^6$ |
| 4 | Au decorated PVA nanofiber | $4.2 \times 10^6$ | $1.0 \times 10^5$ | 42.0 | $3.11 \times 10^6$ | $10^6$ |
| 5 | $O_2$ plasma treated PVA nanofiber | $4.3 \times 10^6$ | $6.4 \times 10^4$ | 67.2 | $2.04 \times 10^7$ | $10^8$ |

Where $EF_{sim}$ denotes the $EF$ obtained by simulation and $EF_{exp}$ designates the experimentally measured $EF$.

Table 8.17: Comparison of the MRL of target analytes and LoD values of the designed SERS substrates

| Sl. No. | LoD (nM) | Target Analyte | Maximum Residual Limit(MRL) ($\mu$gkg$^{-1}$) |
|---|---|---|---|
| 1 | 92.7 | Paracetamol | Not found |
| | | Aspirin | |
| 2 | 0.88 | CEFTR | 100 |
| | | CEF-Na | |
| 3 | 0.75 | SFZ | 92 |
| | | TCH | 49 |
| 4 | 7.32 | DCH | 100 |
| | | ENX | |
| 5 | 3.8 | FLU | 50 |
| | | LIN | 100 |

# List of publications

## In referred journals:


[1] **Sarma, D.**, Biswas, S., Hatiboruah, D., Chamuah, N., and Nath, P. 100 GSM paper as an SERS substrate for trace detection of pharmaceutical drugs in an aqueous medium. *Journal of Physics D: Applied Physics*, 55(38):385102, 2022. ISSN 0022-3727. Number: 38.

[2] **Sarma, D.**, Nath, K. K., Biswas, S., Chetia, I., Badwaik, L. S., Ahmed, G. A., and Nath, P. SERS determination and multivariate classification of antibiotics in chicken meat using gold nanoparticle-decorated electrospun PVA nanofibers. *Microchimica Acta*, 190(2):64, Jan. 2023. ISSN 1436-5073. doi: 10.1007/s00604-023-05640-2. URL https://doi.org/10.1007/s00604-023-05640-2.

[3] **Sarma, D.**, Marak, M. R., Chetia, I., Badwaik, L. S., and Nath, P. AuNP decorated aegle marmelos leaf as sers substrate for trace detection of antibiotics and machine learning based classification. *Physica Scripta*, 99(2):026006, 2024.

[4] **Sarma, D.**, Medhi, A., Mohanta, D., and Nath, P. Electrochemically deposited bimetallic sers substrate for trace sensing of antibiotics. *Microchimica Acta*, 191 (1):14, 2024.

[5] **Sarma, D.**, Nath, K. K., Biswas, S., Ahmed, G. A., and Nath, P. Plasma treated bimetallic nanofibers as sensitive SERS platform and deep learning model for detection and classification of antibiotics. *Under Review*, 2024.

[6] Hatiboruah, D., Biswas, S., **Sarma, D.**, and Nath, P. A smartphone-based photometric and fluorescence sensing for accurate estimation of zinc ion in water. *Sensors and Actuators A: Physical*, 341:113586, 2022. ISSN 0924-4247. doi: https://doi.org/10.1016/j.sna.2022.113586. URL https://www.sciencedirect.com/science/article/pii/S0924424722002242.

[7] Biswas, S., Devi, Y. D., **Sarma, D.**, Namsa, N. D., and Nath, P. Gold nanoparticle decorated bluray digital versatile disc as a highly reproducible surfaceenhanced Raman scattering substrate for detection and analysis of rotavirus RNA in laboratory environment. *Journal of Biophotonics*, 15(11):e202200138, 2022. ISSN 1864-063X. Number: 11.

[8] Biswas, S., Devi, Y. D., **Sarma, D.**, Hatiboruah, D., Chamuah, N., Namsa, N. D., and Nath, P. Detection and analysis of rotavirus in clinical stool samples using silver nanoparticle functionalized paper as SERS substrate. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 295:122610, 2023. Publisher: Elsevier.

# Conference Proceeding:

[1] **Sarma, D.**, Biswas, S., and Nath, P. Blue-ray DVD as a low-cost substrate for the fast sensing of paracetamol in aqueous medium using surface-enhanced Raman spectroscopy (SERS). In *2022 Workshop on Recent Advances in Photonics (WRAP)*, pages 1–2. IEEE, 2022.

[2] **Sarma, D.**, Marak, M. R., and Nath, P. Gold nanoparticle deposited nylon filter paper as a sensitive SERS platform for trace sensing of enrofloxacin in aqueous medium. In *2023 Workshop on Recent Advances in Photonics (WRAP) (Revision submitted)*, 2023.

# Conference Presentations:

[1] **Sarma, D.**, Biswas S., Prakash, A., and Nath, P. Surface-Enhanced Raman Spectroscopy (SERS) as a reliable technique for the detection of Sulphur Dioxide. In *National Conference on Emerging Trends in Physics (NCETP), 16th of June, 2021, Dept. of Physics, Tezpur University*, 2021.

[2] **Sarma, D.** and Nath, P. Machine learning assisted electrochemical SERS substrate for rapid identification of poultry antibiotics. In *Condensed Matter Days, Dept. of Physics, Tezpur University*, 2023.

The Report is Generated by DrillBit Plagiarism Detection Software

### *Submission Information*

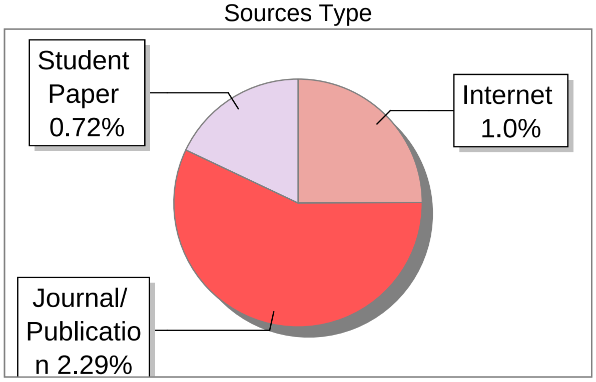
| | |
|---|---|
| Author Name | Dipjyoti Sarma |
| Title | Design of affordable SERS platform for detection and analysis of drugs in water and food matrices |
| Paper/Submission ID | 1798119 |
| Submitted by | anujsingh@tezu.ernet.in |
| Submission Date | 2024-05-13 16:47:38 |
| Total Pages, Total Words | 131, 37776 |
| Document type | Thesis |

### *Result Information*

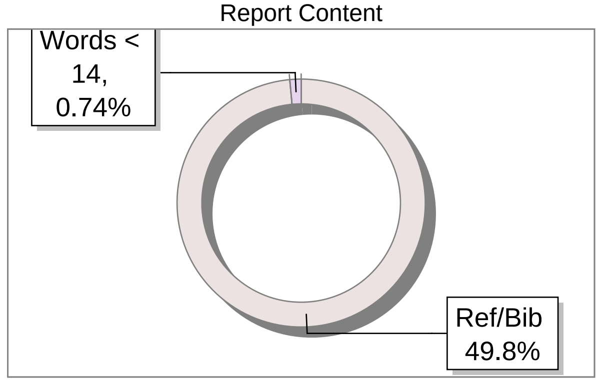
Similarity **4 %**

1 10 20 30 40 50 60 70 80 90

Sources Type




Report Content




### *Exclude Information*

| | |
|---|---|
| Quotes | Excluded |
| References/Bibliography | Excluded |
| Source: Excluded < 14 Words | Excluded |
| Excluded Source | **0 %** |
| Excluded Phrases | Not Excluded |

### *Database Selection*

| | |
|---|---|
| Language | English |
| Student Papers | Yes |
| Journals & publishers | Yes |
| Internet or Web | Yes |
| Institution Repository | Yes |

A Unique QR Code use to View/Download/Share Pdf File

DrillBit

**DrillBit Similarity Report**

| 4 | 23 | A | A-Satisfactory (0-10%)<br>B-Upgrade (11-40%)<br>C-Poor (41-60%)<br>D-Unacceptable (61-100%) |
|---|---|---|---|
| SIMILARITY % | MATCHED SOURCES | GRADE | |

| LOCATION | MATCHED DOMAIN | % | SOURCE TYPE |
|---|---|---|---|
| 1 | Thesis Submitted to Shodhganga Repository | 1 | Publication |
| 2 | REPOSITORY - Submitted to VTU Examination 2 on 2024-04-24 15-49 | 1 | Student Paper |
| 3 | Thesis Submitted to Shodhganga Repository | 1 | Publication |
| 5 | Vertically Aligned Silicon Nanowire Array Decorated by Ag or Au Nanop, by Chakraborti, S. Ba- 2017 | <1 | Publication |
| 6 | livrosdeamor.com.br | <1 | Internet Data |
| 7 | adoc.pub | <1 | Internet Data |
| 13 | link.springer.com | <1 | Internet Data |
| 16 | Halogen Determination in Food and Biological Materials using Plasma-based Techni by Mesko-2016 | <1 | Publication |
| 21 | Ultrastructure of Bone Hierarchical Features from Nanometer to Micro, by Grandfield, Kathryn - 2018 | <1 | Publication |
| 22 | docplayer.gr | <1 | Internet Data |
| 24 | epdf.pub | <1 | Internet Data |
| 26 | ncert.nic.in | <1 | Publication |
| 34 | Thesis Submitted to Shodhganga Repository | <1 | Publication |

| | | | |
|---|---|---|---|
| 37 | Thesis Submitted to Shodhganga, shodhganga.inflibnet.ac.in | <1 | Publication |
| 38 | www.arxiv.org | <1 | Publication |
| 41 | www.xiahepublishing.com | <1 | Internet Data |
| 43 | A critical role of sympathetic nerve regulation for the treatment of i by Suzuki-2010 | <1 | Publication |
| 44 | coek.info | <1 | Internet Data |
| 46 | docplayer.gr | <1 | Internet Data |
| 47 | pressbooks.uiowa.edu | <1 | Internet Data |
| 48 | A small high-velocity scanning television pick-up tube by Cairns-1952 | <1 | Publication |
| 49 | digitalcollection.zhaw.ch | <1 | Publication |
| 51 | edoc.ub.uni-muenchen.de | <1 | Publication |