

## Machine Learning-Enhanced Identification of Fluorophilic Interactions for Improved SERS Detection of PFOA

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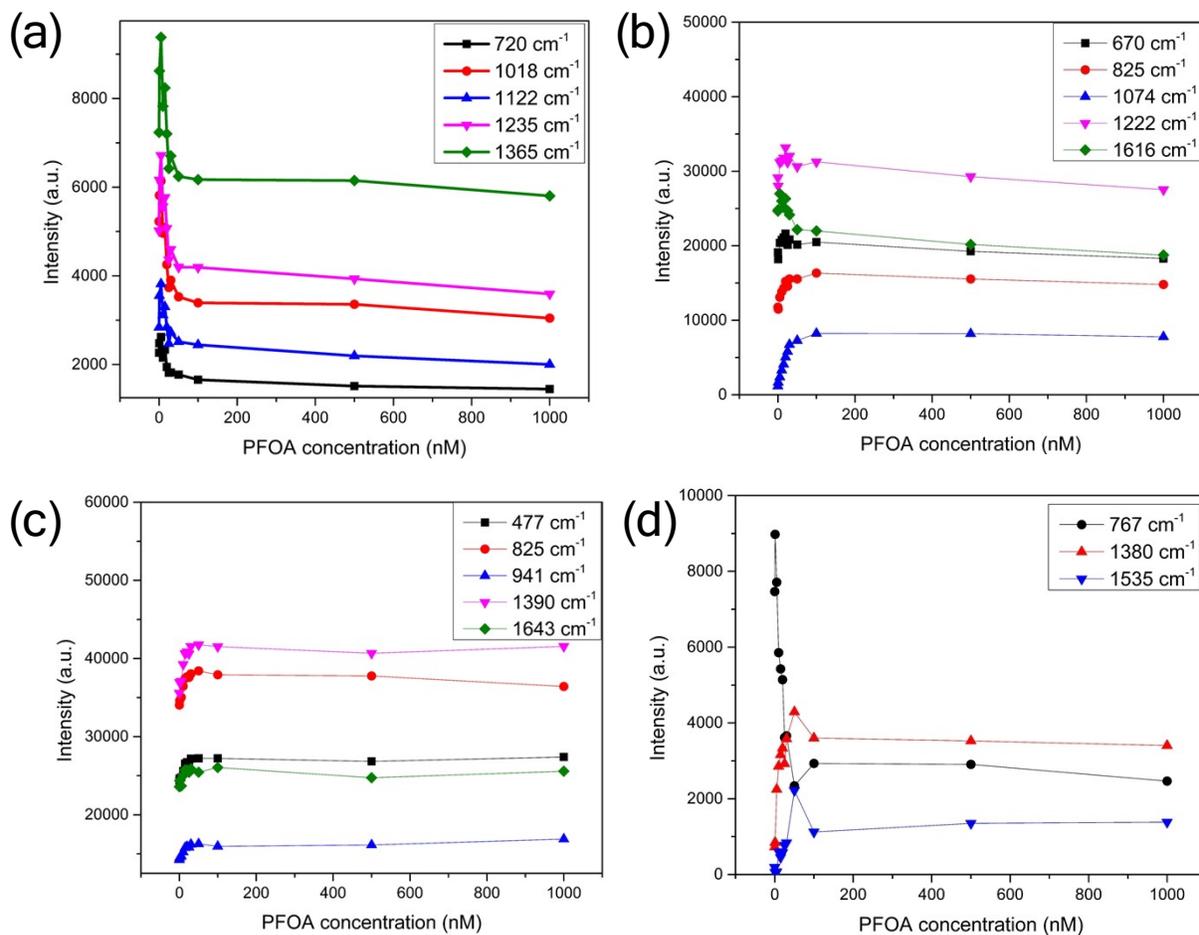
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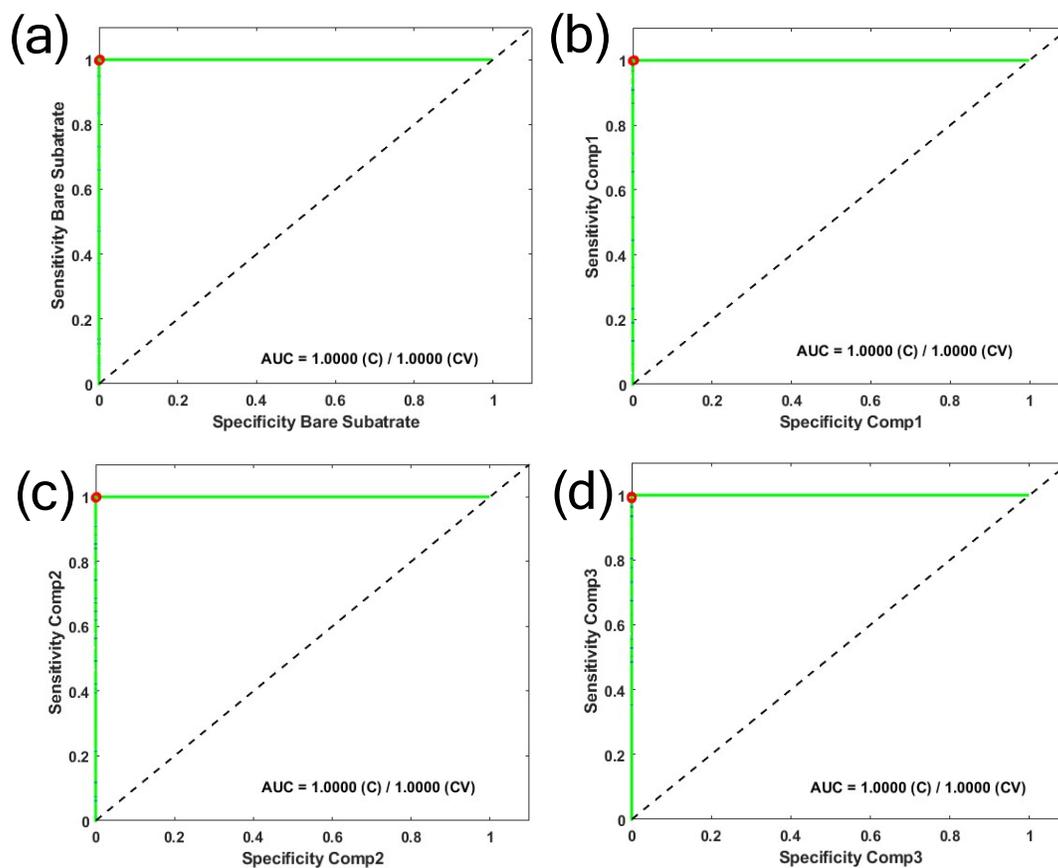
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**Table S1.** An assignment of the major Raman peaks in gold-coated SERS substrate, fluorinated thiols and PFOA.

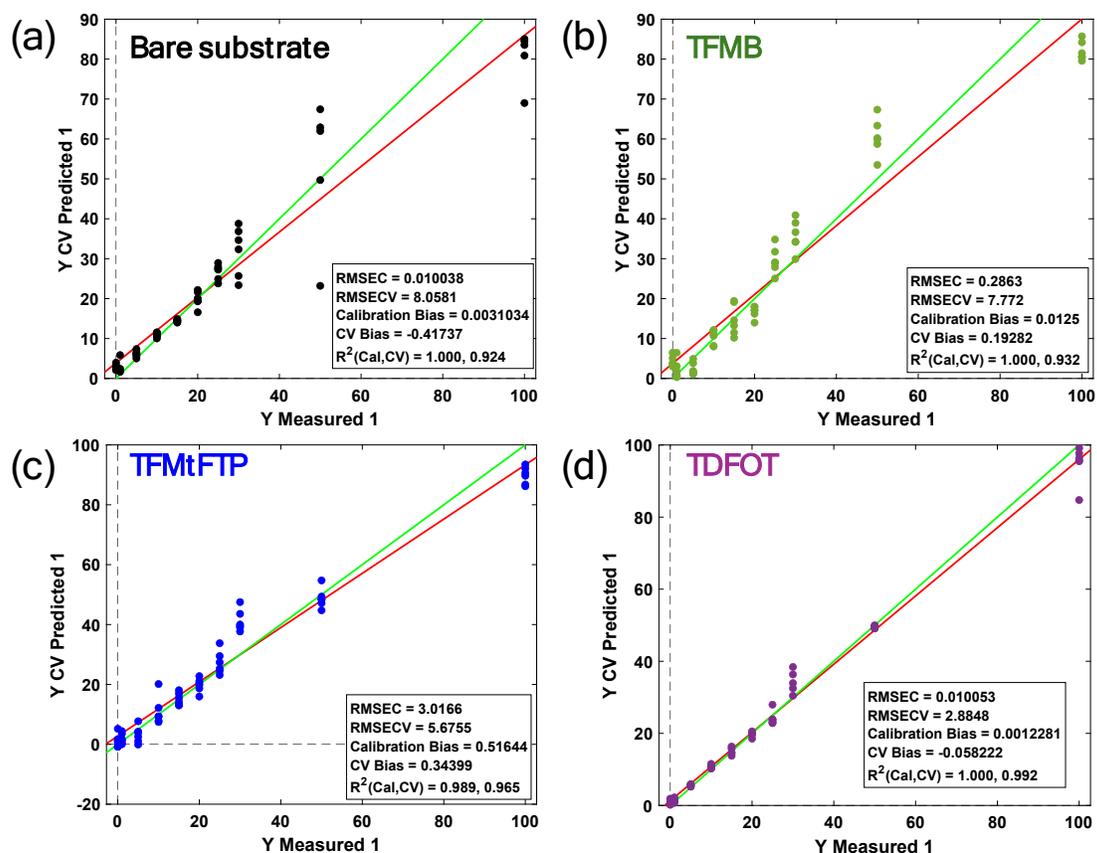
Wavenumber (cm <sup>-1</sup> )	Peak assignment	Reference
290	C-C, CF <sub>2</sub>	[1]
311	Au-S bending	[2, 3]
337	Au-S bending	[2]
382	CF <sub>2</sub> twisting	[1, 4]
412	C-S Stretching	[5]
477	C-S <sub>G</sub>	[2]
520	Si surface	[6, 7]
632/649	C-S <sub>G</sub>	[5, 8]
673	C-S <sub>T</sub>	[5, 8]
720	C-S <sub>T</sub> , C-C, CF <sub>3</sub>	[4, 5, 9]
748	C-C, CF <sub>3</sub>	[9]
767	CF <sub>3</sub> Stretching	[9, 10]
828	CF <sub>3</sub> Stretching	[11]
1000	C-C aromatic	[12]
1074	C-F Stretching	[9, 10]
1120	C-F Stretching, CF <sub>2</sub>	[10]
1136/1147	C-F Stretching, C-C	[4, 9, 10, 13]
1175/1185	C-F Stretching	[9, 10]
1222	C-F Stretching	[9]
1340	C-F Stretching	[9]
1360	C-F Stretching, CF <sub>3</sub>	[9]
1390	C-F Stretching, COO, CF <sub>3</sub>	[9, 10, 13]
1420	C-F Stretching	[9]
1538	C=C Stretching	[12]
1611	C=C Stretching	[12, 14]
1643	C=C Stretching	[12]



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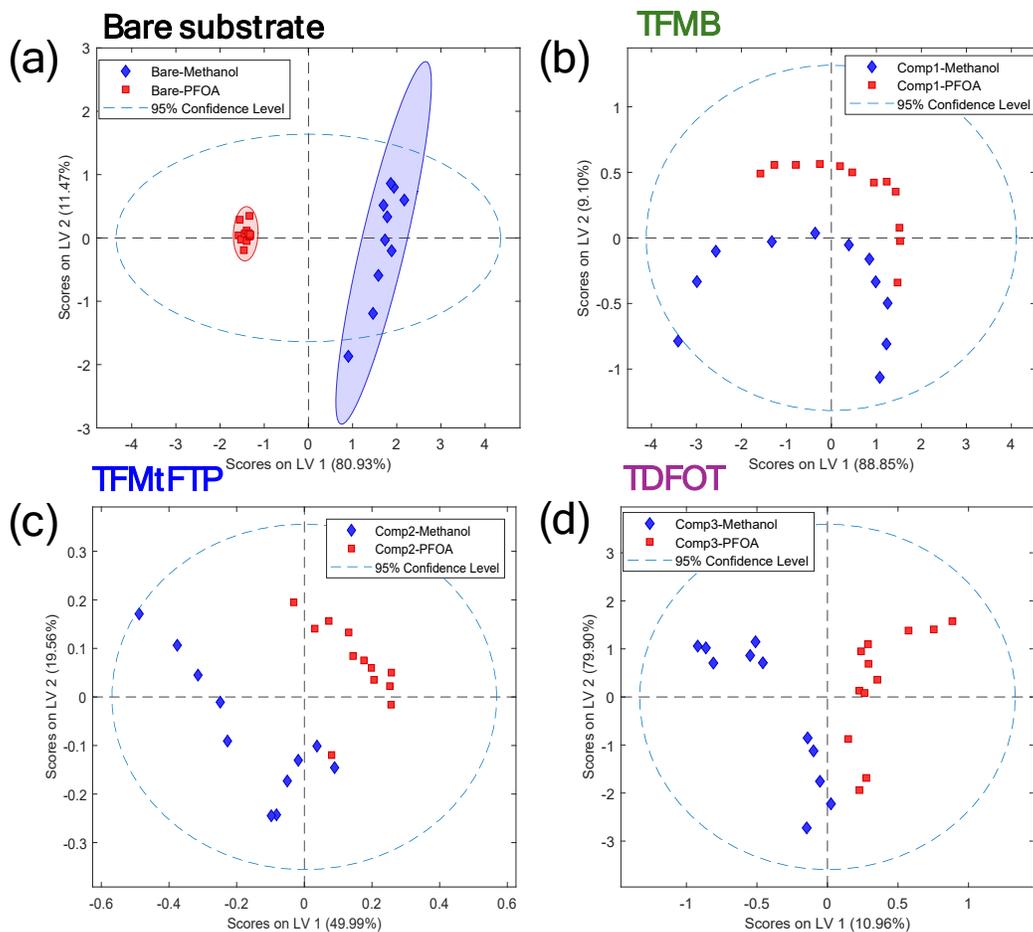
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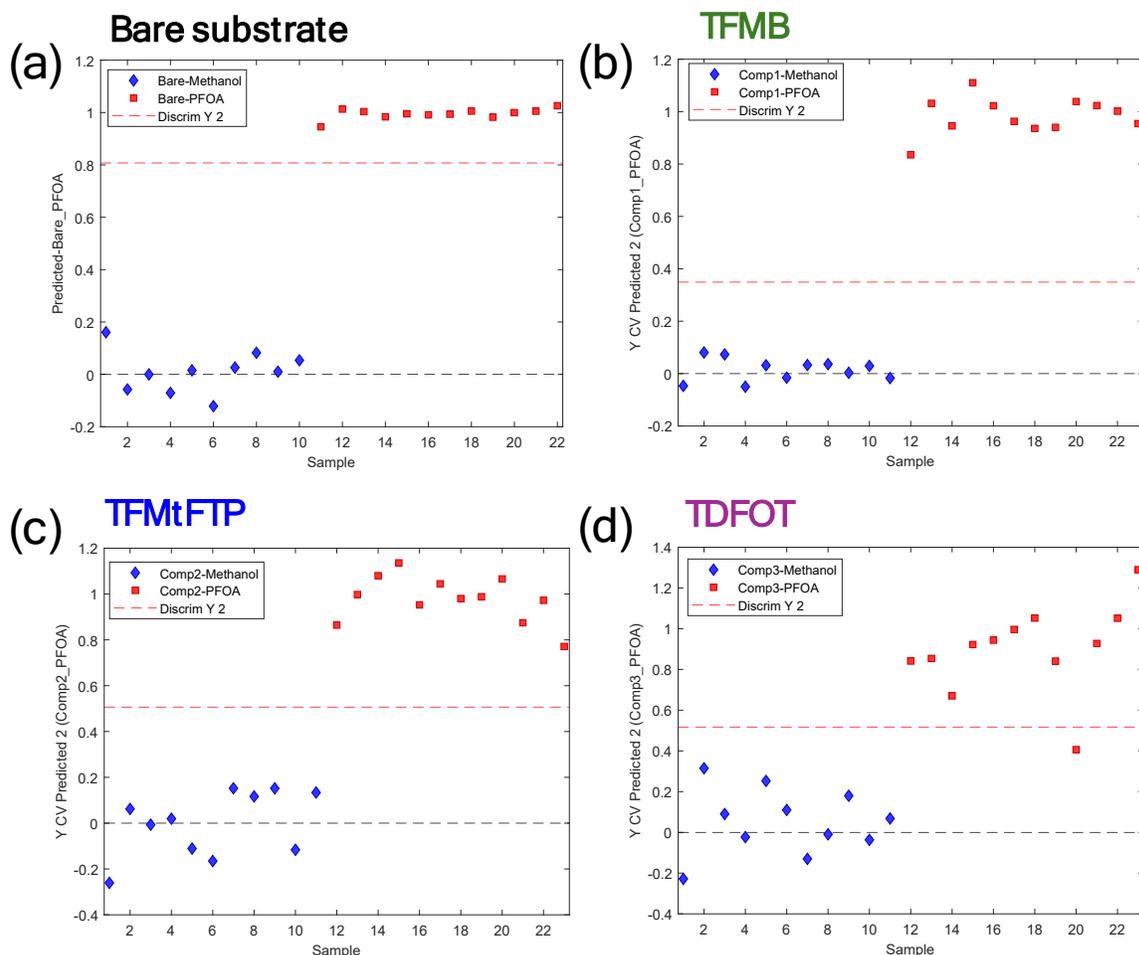
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**Table S2.** Summary of available literature on the detection of PFOA/PFOS via SERS and mass spectroscopy along with respective LODs.

<b>Detection methods and substrates</b>	<b>LOD</b>	<b>Reference</b>
Ag nanograss	1.28 pM	[15]
Ag NPs + Graphene oxide	50 ppb	[16]
Ag NPs + $\beta$ -cyclodextrin	40 ng/L	[4]
AgNPs/Au@AgNRs sandwich	100 ppb	[17]
AgNPs + Graphene	0.4 ppt	[18]
AgNR + alkanethiol	1 ppt	[9]
Ag nanocolloidal	5 ppt	[19]
PFAS in wastewater by liquid chromatography-mass spectrometry (LC-MS)	0.1 ng mL <sup>-1</sup>	[20]
PFAS in soil sample using paper spray (PS)-based MS	1.2–4.5 ppt	[19]
PFOS in water using MS	5.6 ppm	[21]
PFASs in drinking, sea and surface water using LC-MS	0.5–17 ng L <sup>-1</sup>	[22]
Au substrate + Fluorinated thiol	3.6 ppb	This study



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