

Supporting Information

Multiplex surface-enhanced Raman scattering detection of deoxynivalenol and ochratoxin A with a linear polymer affinity agent

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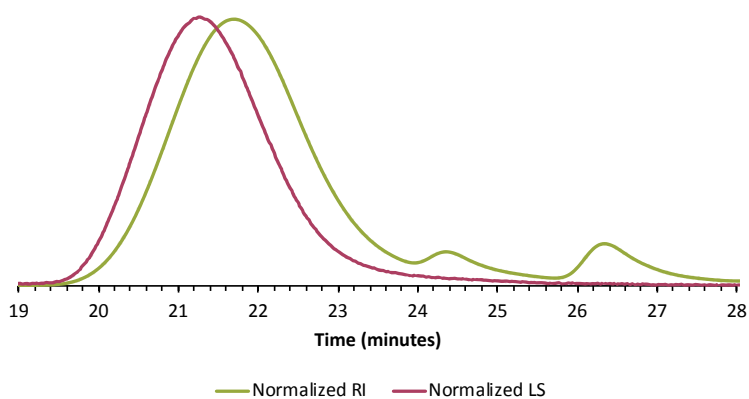


Figure S1. Refractive index (RI) and light scattering SEC traces for pAEMA₂₉.

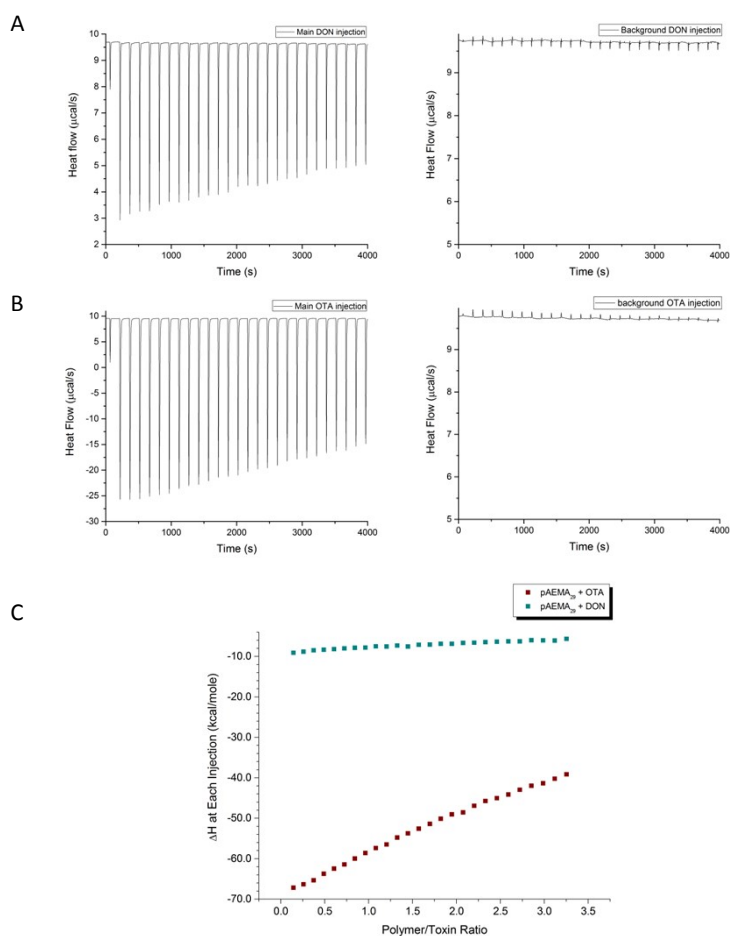


Figure S2. A. Raw heat flow injections of DON into pAEMA₂₉ and buffer solutions. B. Raw heat flow injections of OTA into pAEMA₂₉ and buffer solutions. C. ITC profile integrated and subtracted for both OTA and DON done in the same experimental run. A large heat at injection is seen for both toxins with pAEMA₂₉, indicating that both toxins kinetically bind to the polymer.

Table S1. Vibrational band assignments for DON and OTA based on Gaussian calculations.

Wavenumber shift (cm ⁻¹)	Assignment
DON	
201	Rocking of C17-O5, OH bending on O5-H38
224	Wagging of H31, H30, and H29 on C15, asymmetric stretching of H38
240	Stretching of H38 and H36
243	Wagging of H25 and H26 on C12 and of H33 and H34 on C17
248	Bending of bond angle on O5 with H38 and O3 with H36
261	Out of plane stretching of H38 on O5 and O3 with H36, and ring twist displacing H31 and H30 on C15 and C20
269	Strong rocking of H38, ring breathing by C19, C21 twisting with H39, H40, and H41, wagging of H36 on O3
279	Strong rocking of H29, H30, and H31 on C15 and rocking of H34 on C17
282	C15 twist on H30, C20=C18 stretch, wagging of Hs on C21, C11 ring distortion
293	O1 twist, H26 and H25 twist in plane, asymmetric H23 and H24 stretching on C11
301	Strong H29 and H30 twisting on C15, H37 rocking on O4, H40 rocking
320	Ring breathing C20, H39 twisting, C15 twisting, rocking of H29, H30, and H23
323	Asymmetric bending of H29, H30, and H31 on C15, ring distortion C8
335	Asymmetric bending of H34 and H33 on C17 and bond angle bending of H38 on O5, out of plane bending of H35 on C18, asymmetric bending of C18=C20, rocking of H25
361	H35 rocking, H25 twist, asymmetric O1 stretch
378	Strong angle stretches of C16, asymmetric stretching of O6 and H37, H28 twist, in plane stretch of H34, H30, H23
389	Strong angle stretches of C16, asymmetric stretching of O6 and H37, ring distortion C19, H twist on C21, O6=C19 wagging, asymmetric stretch of C9-C7, C15 wagging
446	O3-C13 asymmetric stretch, H twist of C11, ring breathing C18, C35 stretch, asymmetric O3 stretch
471	Ring breathing C20, O6=C19 stretch, H32 symmetric stretching to ring
480	Ring rocking C7, ring twist C9-C14, H23 and H24 wagging, symmetric angle bending C12-C8 and C10-C8, symmetric rocking of Hs on C15
494	Symmetric ring breathing, H35 wagging, H34 wagging, H22 twisting, H38 bending
521	Strong wagging of H31 on O4, H41 on C21, H26 on C12, H33 on C17, asymmetric ring stretching C10 and C9 and C11
551	Strong H37 wagging stretch on O4
561	Asymmetric ring stretches C8, C10, H22, and strong wagging of H37 on O4
584	Ring distortion/twist of C20, H32, H40 on C20, H24 on C11, and Hs on C12
622	Ring breathing C7, H23 twist, H25 rocking, H40 rocking, H38 rocking, H40 rocking, H36 wagging
626	C8 ring distortion, H24 twist, H37 rocking, C20 twist, H32 twist
665	Ring breathing C18=C20, H35 stretch on C18, H33 on C17 in plane wagging, C16 ring breathing stretch, C35 wagging, in plane twist of Hs on C21
689	Asymmetric ring distortion C14-C9, elongated stretch on C14 and H28, wagging of H38, asymmetric stretching of Hs on C17
747	Hs wagging on C11, twisting of Hs on C15, symmetric angle bending of Hs on C10 and C12
774	Ring distortion C13-C11, Hs on C11 twist, H36 on O3 bending, Hs on C14 angle

bending

803 Ring twisting C9-C14, Hs on C21 twisting, H35 wagging on C18

853 Ring breathing C10, Hs on C11 in plane stretch, H32 rocking, H35 bend

861 Asymmetric ring distortion C16 and C18, Rocking of H37 on O4, rocking of Hs on C21, H35 stretch on C18, asymmetric stretch of Hs on C15, asymmetric stretch of Hs on C11 and C13

874 Asymmetric ring distortion of cyclopentane affecting H24 on C11 and Hs22 on C10, strong asymmetric stretching of H26 on C12

888 Rocking of Hs on C15, asymmetric wagging of H35 on C18, rocking of H27 on H13

898 Strong wagging of H35 on C18, strong wagging of H26 on C12, symmetric ring twisting, H32 twist, Hs on C21 twisting

919 Strong H34 twisting, slight ring distortion on C19-C20, strong H23 rocking, twisting of Hs on C12, twisting of Hs on C17, rocking of Hs on C15

925 Hs on C11 twisting, Hs on C17 twisting, C9 ring breathing, Hs on C21 rocking, H27 on C13 wagging

941 Strong twisting of Hs on C12, symmetric stretch of H31 on C15, Hs rocking on C17, H22 on C10 wagging, slight ring distortion with C10

956 Out of plane stretching of H35 on C18, Hs twisting on C21, wagging of Hs on C12, asymmetric stretching of C14, rocking of Hs on C15, ring stretch between C10, O2, and H14 bond angle

966 Out of plane stretching of H35 on C18, Hs twisting of C15, asymmetric ring stretching on C9, ring rocking inwards at C13, asymmetric ring stretching with C9 and C20, asymmetric stretch of H27 on C13 and C11, wagging of Hs on C21

980 Strong wagging of H35 on C18, strong twisting of C22 on C10, asymmetric stretch of C25 on C12, ring rocking out of plane with C9 and C20, inward ring stretches with C10 and C9, C21 rocking,

996 Hs on C21 rocking out of plane, asymmetric stretching of Hs on C17, outward ring stretches with C18 and C16

1043 Strong rocking of Hs on C15, C27 stretch on C13, asymmetric angle stretches of C17 and O5, H38 stretch of C5, H27 wag on C13, symmetric ring stretches of C9 and C20, ring stretch with C10, C14, and C7

1048 Strong symmetric angle stretches of H27 and H24 on C13 and C11, H22 stretch of C10, slight ring stretching with O2 and C14, Hs rocking on C21, rocking of Hs on C15

1064 Hs twisting on C11, H35 stretch on C18, Hs rocking on C21, rocking of H30 on C15, ring rocking with C16 and C18

1067 Strong rocking of H23 on C11, rocking of Hs on C1, symmetric ring distortion with C11 and C13, rocking of Hs on C21

1068 Strong asymmetric stretching of Hs on C21, asymmetric stretching of H35 on C18 and C20

1087 Strong wagging of H36 on O3, rocking of Hs and O5 on C17, asymmetric stretching of ring with C10 and C14 on O2, twisting of Hs on C12, asymmetric stretching of O5 and C17 with H34 stretching in plane with C17

1090 Wagging of H36 on O3, symmetric stretching of O5 and H33 on C17, rocking of Hs on C21, symmetric stretching of ring with C10 and C13, rocking of H32 on C16, stretching of C17 on C9, rocking of H35 on C18

1114 Rocking of H28 on C14, twisting of Hs on C12, rocking of Hs on C15, ring stretching with C18, C14 and C9, rocking of Hs on C15

1119 Strong twisting of Hs on C12
Symmetric stretching of O3 and C11 with H35 on O3 and H14 on C11, wagging of H38

1142 on O5, asymmetric stretching of Hs on C21, asymmetric stretching of Hs on C12,
rocking of Hs on C11, ring twisting with C7, C9, C16, and C13
Symmetric wagging of Hs on C12, symmetric bending of Hs on C15, wagging of H38

1146 on O5, ring breathing with C11 and C7, asymmetric ring stretching with C16 and C14
on C9
Ring distortion with C16 displacing H32, twisting of Hs on C11 and twisting of C13,
wagging of H38 on O5, asymmetric ring distortion with C7 and C10

1154 Symmetric wagging of Hs on C15, in plane rocking of Hs on C12, rocking of H35 on
1164 C18, ring rocking of C7 and C14
Symmetric wagging of Hs on C12, rocking of Hs on C15, wagging of H38 on O5,
1178 wagging of H23 on C11, asymmetric ring stretches with C7, C10, and C9, ring
breathing of pentane ring, rocking of H36 on O3
Strong twisting of Hs on C17, symmetric ring breathing on cyclohexene ring with
1195 wagging of H35 on C18, wagging of H38 on O5, stretching of H30 on C7, asymmetric
stretching of C8 and C11 bonded to C7, wagging of H37 on O4
Strong wagging of H23 on C11 and H36 on O3, angle bending of H22 and H27 on C10-
1216 C13, symmetric stretching of Hs on 12 and C8
Strong wagging of H22 on C10, H36 on O3, stretch of H27 on C13, similar to previous
1233 mode
Strong stretching of H22 on C10, symmetric stretching of H27 on C13 and O3 on C13,
1245 strong angle wagging of H38 on O5 and H33 on C17
Strong rocking of H32 on C16, symmetric stretching of H38 and H33 on O5-C17
1251 respectively, strong stretching of H35 on C18, ring distortion of cyclohexene with
asymmetric stretching of C19-C20
Strong rocking of H32 on C16, wagging of H38 on O5 and H33 on C17, twisting of Hs
1264 on C11, slight ring distortion on cyclohexane with C7-C9
Wagging of H24 on C11, wagging of H38 on O5, rocking of H35 on C18, slight ring
1270 distortion caused by C18-H35 and H32 on C16
Strong wagging of H32 on C16, strong H32 rocking on C16, wagging of H35 on C18,
1283 wagging of H24 on C11, ring distortion of cyclohexene caused by C16 and C18
Symmetric rocking of Hs on C11, twisting of Hs on C17, stretching of H22 on C10,
1308 wagging of H27 on C13, rocking of H28 on C14, ring distortion of cyclopentane
1320 Asymmetric twisting of Hs on C17, wagging of H22 and H32
Strong symmetric "windshield wiper" stretching of H24 and H27 on C11 and C13
1344 respectively, ring distortion of cyclopentane due to C11 and C13 movement, wagging
of H36 on O3
Strong rocking of H28, wagging of H35, "windshield wiper" motion of H22 and H27,
1348 asymmetric stretching of Hs on C17
Strong rocking of H22 on C10 and symmetric stretching of H27 on C13, not as strong,
1355 wagging of H28 on C14, slight ring twist on cyclopentane due to C10 movement
Strong wagging of H32 on C16, wagging of H35 on C18, asymmetric Hs twisting on
1361 C17, rocking of C9
Rocking of H37 on O4, symmetric angle bending of C18-C14 displacing H35 and H28,
1384 rocking of Hs on C21, ring rocking of cyclohexene
1399 "windshield wiper" motion of Hs on C18-C14 (H35 and H28 respectively), wagging of

H32, ring distortion of cyclohexene, wagging of H37 on O4

1413 Symmetric angle breathing of all Hs on C21 "claw", slight twisting of C14

1416 Symmetric angle breathing of Hs on C15 "claw", slight rocking of Hs on C12, slight rocking of C8 and H2 bonded to C10, and wagging of H27 on C13

1426 Angle bending of H37 on O4 and C16 on O4, wagging of H27 on C13, wagging of H28, wagging of H37 on O4, out of plane symmetric angle breathing of Hs on C21, cyclohexene ring distortion, wagging of H32 on C16

1427 Strong wagging of H27 on C13 and H36 on O3, wagging stretch of H37 on O4, slight symmetric angle breathing of Hs on C21, cyclopentane ring distortion with C13

1437 Asymmetric stretching of Hs on C12 and C8-C12 bond, in plane angle bending "claw" Hs on C15, asymmetric stretching of H22 on C10 and C10-C8 bond, ring distortion of pentane ring with C8, slight wagging of Hs on C17

1450 Asymmetric out of plane rocking of Hs on C17 and wagging of H38 on O5, wagging of H37 on O4, slight wagging of Hs on C11

1473 Asymmetric twisting and wagging of Hs on C12

1488 Asymmetric stretching and wagging of Hs on C21, slight wagging of Hs on C11

1490 Scissoring of Hs on C11, asymmetric wagging of Hs on C21, asymmetric stretching of Hs on C15, asymmetric stretching of Hs on C17

1503 Asymmetric wagging of Hs on C15, slight scissoring of Hs on C12, scissoring of Hs on C17, symmetric stretching of Hs on C11

1516 Strong asymmetric wagging of H33 and H34 on C17, asymmetric twisting and stretching of Hs on C15, slight scissoring of Hs on C12

1517 Strong twisting and stretching of Hs on C15, slight stretching of Hs on C12

1530 Scissoring of Hs on C12, twisting of Hs on C15

1715 Strong stretching of C18=C20 bond, ring distortion of cyclohexene due to double bond stretch, Hs wagging on C21, wagging of H28 on C14

1727 Strong stretching of O6=C19 bond, opposite stretching of C20=C18 bond, wagging of H37 on O4, symmetric wagging of H35 on C18 and H41 on C21, ring distortion caused by strong C19 =O6 bond

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219 Stretching of C28 and C22 in benzene ring and corresponding Hs, asymmetric stretching of C17-N7, displaced stretching of C23=O7 and O6-H46, twisting of Hs on C20, inward stretch of benzene ring with C11, and rocking of Hs on C18

221 Strong twisting of Hs on C18, rocking of C9 displacing Hs

240 Symmetric rocking of C9 and C18 displacing their Hs, asymmetric stretching of benzene ring with C28 and C22, rocking of Hs on C20, rocking of Hs on C17, windshield wiper motion of C21=O5 and C17-H32, rocking of Hs on C18, and twisting of Hs on C9

265 Twisting of Hs on C9, rocking of Hs on C18, rocking of O5=C21, asymmetric stretching of benzene ring with C11 and C14

293 Strong angle breathing of C9-C10-C18, rocking of Hs on C18, outward stretch of benzene ring with C12 and C11, rocking of H40 on O3, out of plane rocking of H39 on N8

303 Out of plane rocking of benzene ring with C19 and C12, strong angle breathing of O5=C21=N8-C17-C23, rocking of Hs on C17 and O6, symmetric stretch of Hs on C18

316 Rocking of Hs on C18, asymmetric stretching of bonded rings: large stretch with C10 and out of plane rocking of benzene ring, stretching of C11, twisting of benzene ring with H43 and H44

336 Strong wagging of O3-H40, wagging of O4 and H36, rocking of Hs on C20

357 Strong wagging of Hs on C20, twisting of benzene ring with H41, H43, H45, and H44

366 Rocking of Hs on C18, strong outward breathing stretch of benzene ring with C11 and C13, bond angle symmetric stretch of O3, C13, C12, and C16, strong rocking of H40 from O3, strong asymmetric stretch in bonded ring structures with O4 and C11

376 Strong wagging of Hs on C20, angle breathing of N8, C17, and C20, wagging of H39, asymmetric stretching of H39 and H37, rocking of O7, asymmetric out of plane benzene stretch of C28 and C22 displacing their Hs, wagging of C21=O5

401 Strong wagging of H39 on N8, wagging of Hs on C18, asymmetric symmetric of ring with C12 and C10, stretching of O3, rocking of Hs on C9, wagging of O4=C16, symmetric stretch of benzene ring with C11 and C13

415 Asymmetric stretching of C25=C27 and C24=C26 displacing their Hs respectively

426 Strong wagging of H39 on N8, benzene ring breathing with C19 and C13, twisting of Hs on C9, ring breathing with C16 and C11

439 Strong wagging of H39 on N8, slight twist of Hs on C9

458 Strong twisting of Hs on C9, rocking of Hs on C18, stretching of H31

481 Symmetric ring stretchings with O2 and H36 pulling, benzene ring breathing rocking with C19 - H36 and C11, rocking of H40, rocking of C15 in benzene ring, symmetric ring stretch of H30-C9, and C15

492 Inverted benzene ring stretching, asymmetric out of plane stretching of H43 and H45, symmetric stretching of H41 and H44, out of plan stretching of C22, rocking of H45, rocking of Hs on C20, rocking of H39, slight rocking of H30

512 Out of plane rocking of H36, out of plane rocking of H46, symmetric twisting of bonded rings, rocking of Hs on C18, twisting of O4 and O3-H40, ring breathing of C24

520 Strong twisting of H40 bonded to O3, asymmetric twisting of bonded rings, rocking of H36, rocking of H39, rocking of Hs on C18

557 Angle breath between O6-H45, C23, and O7, ring distortion through C28 and C22, rocking of H39, rocking of H36

583 Strong twist of Hs on C20, strong rocking of H46, rocking of H39, ring distortion through C22 and C28

592 Strong rocking of H46 on O6

610 Rocking of H's bonded to C9, twisting of ring due to C9 rocking, rocking of O5, scissoring of H46 and H39, rocking of H's bonded to C18, O4 stretch, slight ring breath at C28 and C22, twisting of ring at C13 and C11

621 Rocking of H's bonded to C18, twisting of ring at C10, wagging of O4, ring distortion at C11, scissoring of H36 and H29, rocking of H39, slight rocking of H's bonded to C20, rocking of C9

635 Strong inward ring breath at C27, C24, C25, C26 and displacement of bonded H's, slight rocking of H's bonded to C20

648 Wagging of H46, rocking of H's bonded to C9 and C11 causing a slight ring distortion on both rings, rocking of H's bonded to C18, rocking of C16=O4 and O3-H40, slight ring breath at C25 and C26, wagging of H46

654 Outward bond angle stretch of C23=O7 and O6 and H46, twisting of H's on C20, ring distortion at C11 and twisting of H29, ring twist displacing H43

697 Ring breathing of both bonded rings, slight C11-C15 stretch, rocking of H's bonded to C18, wagging of H39, downward stretch of C21, rocking of H46 following ring breathing pattern

714 Asymmetric out of plane breathing of benzene ring, strong displacement of H41, H42, and H45

735 Strong stretching of C23 and H46 and ring breathing at C26 and C27

739 Out of plane rocking of C23 and H46 on O6, ring distortion at C14, rocking of H40 on O3

748 Strong ring distortion at C14, slight out of plane rocking of hydrogens on benzyl ring, ring breathing at C15 and C13 with stretching of H40 on O3

767 Strong hydrogen breathing of the benzyl ring at C26, rocking of C20 and C23 along with the hydrogens bonded

787 Strong wagging of H40 on O3

803 Strong wagging of H40 on O3 and symmetric stretching of C14, C21, and C19 with a strong stretch of H36

812 Strong out of plane symmetric stretching of C26 and H40, rocking of C13 and C12 bond

822 Ring Breathing at C26-C24 and C25-C27, symmetric stretching of C20 and C22 displacing the hydrogens on C20, symmetric stretching of C17-C23 bond and wagging of H46

833 Symmetric inward stretches of rings at C19 and O2, wagging of H35, weak benzyl ring breathing at C27 and C22

857 Strong out of plane asymmetric stretching of hydrogens (H41, H42, H43, H44, H45) in benzyl ring

873 Strong twisting of Hs on C20, C17-C20 bond stretching with H32 rocking, out of plane asymmetric stretching of hydrogens (H41, H42, H43, H44, H45), rocking of N8 and hydrogen bonded to it, out of plane rocking of H36,

898 In plane wagging of H's on C18, angle breath of C10 and C18, C9 stretching

917 Strong twisting of hydrogens on C20, strong rocking of H36, rocking of C17 and H32, bond angle stretch of C18-C10, rocking of H's on C18, rocking of H's on C9, slight ring breathing at C22 and C26

923 Strong angle stretch of C18-C10, rocking of H's on C18, C10, and C9, rocking of H32, H42, H41, H45, slight stretching of N8=C21

927 Strong rocking of H36, strong rocking of H29, twisting of H's on C18, slight ring distortion at C19 and C15, symmetric stretching of H42 and H45, asymmetrical stretching of H41

930 Strong rocking of H36, asymmetric out of plane stretching of H's on benzyl ring

with C24, twisting of H's on C18, out of plane rocking of C9 and H's bonded
 939 Strong out of plane rocking of H36, asymmetric out of plane rocking of H's on
 benzyl ring with C24, outward stretching of H's bonded to C18
 982 Strong twisting of H's on C18, bond angle stretching at O2=C16=O4, ring
 distortion caused by O2, ring distortion at C19 and C15, rocking of O3-H40
 985 Strong out of plane rocking of H41 and H44 symmetrically and H42, H43, and
 H45 strong out of plane rocking asymmetric to the previous
 1005 Asymmetric out of plane stretching of hydrogens on C25 benzene ring
 1017 Strong ring breathing distortion at C28, C25, C24
 1038 Strong twisting of H's on C20, wagging of C17, slight asymmetric stretching of
 C25 benzene ring, C10 ring distortion
 1050 Strong ring breathing with twist at C27 and C26 rocking all the H's bonded to
 the ring
 Strong rocking of H's on C20, ring wagging at H44, H45, H41, and subsequently
 1055 H37 and C20, stretching of N8=C21=O5 and H39, rocking of H36, ring
 distortion caused by C9 rocking bonded to C11, C10-C18 stretch, inward
 symmetric stretch of H's on C18
 1082 Strong C9 H's stretch causing a strong inner ring distortion on C9, C10, C11,
 wagging of H39, asymmetric stretch of benzene ring at C11, wagging of H40
 1105 Wagging of H44, H42, H45, H43, H41 on benzyl ring, rocking of H's on C20,
 stretching of C17-C20 bond
 1120 Symmetric wagging of H42, C22, H41 and H44, H45, H43, out of plane rocking
 of C20 and H's bonded, bond stretch of C17-N8, wagging of H30
 1129 Strong symmetric wagging of H33 and H38, bond stretch of C18-C10, wagging
 of H's bonded to C20
 Strong bond stretch of C10-C9, rocking of H's on C18, inward stretch of
 1151 O2=C16 bond, wagging of H39, N8=C21 bond stretch, wagging of H37 and H39,
 rocking of C17, wagging of H46
 1170 Strong symmetric wagging of H39 and H46, outward bond stretch of C10-C18,
 rocking of H's bonded to C18 and C10, slight stretching of H44 and H43
 1183 Strong inward stretching of H45 and H44, inward stretching of H43 and H41,
 wagging of H42
 1185 Wagging of H45, bond stretch between O6-C23, rocking of H's bonded to C18,
 rocking of H31 and H29, bond stretch of C10-C9, wagging of H40
 1204 Strong scissoring of H43 and H41, strong scissoring of H44 and H42
 Strong rocking of H36, ring distortion caused by C15=C19 bond, wagging of
 1211 H29 and H31, rocking of H's bonded to C18, asymmetric wagging of H's on
 C20, rocking of H's on C17, wagging of H43 and scissoring of H44 and H45,
 wagging of H46
 1215 Wagging of H36 and rocking of the Hs on C20, outward ring breathing at C15
 and benzyl ring, wagging of H29, asymmetric bond stretching of C10-C9-C11,
 rocking of H40, scissoring of H41 and H43, inward wag of H44 and H42
 1222 Strong bond stretch of C22-C20 causing a ring distortion at C22, C27, C25, all
 hydrogens in benzyl ring are wagging inward, displacement of Hs bonded to

- C20 due to bond stretch, slight H39 wag
Bond stretch of C22-C20 causing H's on C20 to asymmetrically wag, wagging of H32, outwards wagging of Hs on benzyl ring, and rocking of H31, twisting of H's on C9, symmetric breathing of ring caused by C14 and C11, C13=C12 bond stretch, Cc19=C15 bond stretch, wagging of H40, bond stretch of C12-C16
- 1233
- 1243 Strong twisting of H's on C9, wagging of H36, inward wagging of H31, scissoring of H's bonded to C18, wagging of H40
- 1288 Twisting of H's bonded to C20, scissoring of H32 and H39, asymmetric bond stretching of N8=C21-C14, rocking of H36 causing a slight ring distortion at C19, wagging of H40, slight outward twisting of H42 and H44 on ring
- 1302 Strong wagging of H36, symmetric inward stretching of H's bonded to C9 and C10, slight rocking of H's bonded to C18, bond stretching in benzyl ring at C11=C15, C15=C19, C19=C14, symmetric wagging of H32 and H38
- 1303 Strong wagging of H32 and H38, inward wagging of H's bonded to C9 and C10 Scissoring of H30 and H31, bond stretch of C13=O3, bond stretch of C11=C15=C19 all causing a ring distortion, wagging of H36, asymmetric bond stretching of C26-C12-C13 causing ring distortion, displacement of O3, wagging of H32, wagging of H's bonded to C20, slight ring distortion wagging H41, H43, H45, H44 and H42
- 1330 inward bond angle stretch of H38 and C22, asymmetric bond stretching of C22=C24 and C29=C27 causing all the H's bonded in the ring too wag, rocking of H32, wagging of H46, wagging of H31
- 1333 Strong wagging of H40 caused by bond stretch of O3=C13, strong wagging of H31, strong rocking of H's bonded to C9 bond stretch of C12=C13 and C14=C19 causing a ring distortion and wagging of Hs on ring, twisting of H's on C18, slight wagging of H32 and H27
- 1350
- 1352 Twisting of H's on benzyl ring (strongest twist at H41), rocking of H32
- 1363 Strong inward bond angle stretch of H46-O6-C23, scissoring of H's bonded to C17, rocking of H's bonded to C20, rocking of H39, slight twisting of H's on benzyl ring listed previously
- 1372 Wagging of H40, wagging of H29 and H31, inward ring breathing at C11=C12, wagging of H32, rocking of H's bonded to C20, slight twisting of Hs on benzyl ring listed previously
- 1374 Twisting of H's on benzyl ring (strongest twist at H44), rocking of H32, strong rocking of H's bonded to C20, wagging of H46, rocking of H40
- 1378 Strong H32 wagging on C17, asymmetric wagging of Hs on C20, slight twisting of benzene ring Hs (H42, H44, etc.)
- 1393 Strong wagging of H31, wagging of H29, scissoring of H's bonded to C18
- 1407 Wagging of H31, rocking of H's bonded to C9, inward bond stretch of H's bonded to C18, slight wagging of H30 and H36
- 1420 Strong scissoring of H's bonded to C18, wagging of H31
- 1450 Wagging of H40 and H36, bond angle stretching of C13-O3 and C15=C19
- 1468 Scissoring of H30 and H20, slight scissoring of H33 and H35
- 1482 Bond stretching of C24=C26 causing H's bonded to scissor, twisting of H's on

	same benzyl ring, scissoring of H's bonded to C20
1486	Strong twisting of H's bonded to C18
1489	Twisting of H's bonded C18, scissoring of H's bonded to C9, wagging of H40, C11-C9 bond stretch causing ring distortion and ring twisting at C11 and C14, wagging of H36, wagging of H39, scissoring of H's bonded to C20
1496	Strong scissoring of H's bonded to C20, slight ring twisting wagging H45 and H44
1499	Twisting of H's bonded to C18
1517	Wagging of H39, outward stretching of H's bonded to C20
1527	Strong symmetric stretching of benzene ring through H43 and H44
1606	Strong symmetric bond stretch of C19=C14 and C11=C12 causing a ring distortion, wagging of H36, wagging of C29, slight bond stretch of O4=C16
1624	Asymmetric bond stretching between C24=C22=C25 and C36=C28=C27, twisting of H's bonded to ring, rocking of H's bonded to C20
1635	Asymmetric bond stretch of C14=C13=C12 and C19=C15=C11, wagging of H36 and H40, slight rocking of C9
1644	Symmetric bond stretching of C36=C24 and C25=C27, causing a ring distortion and scissoring of bonded H's
1722	Strong bond stretch of O4=C16 causing outward ring distortion, bond stretch of C12=C11 and O3=C13, wagging of H40, bond stretch of O5=C21, slight wagging of H39
1747	Strong bond stretch of O5=C21, wagging of H39, wagging of H40, bond stretching of O4=C16 distorting ring
1814	Strong bond stretch of C23=O7, scissoring of H46 and H32

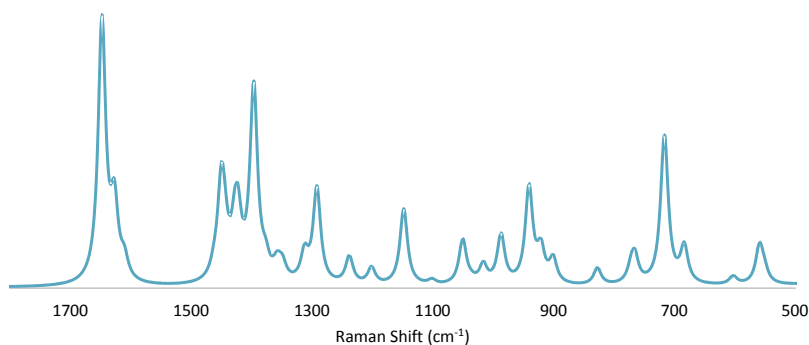


Figure S3. Non-resonant Raman computed spectrum for the AEMA monomer at a 785 nm laser wavelength, BP86 functional and TZP basis set.

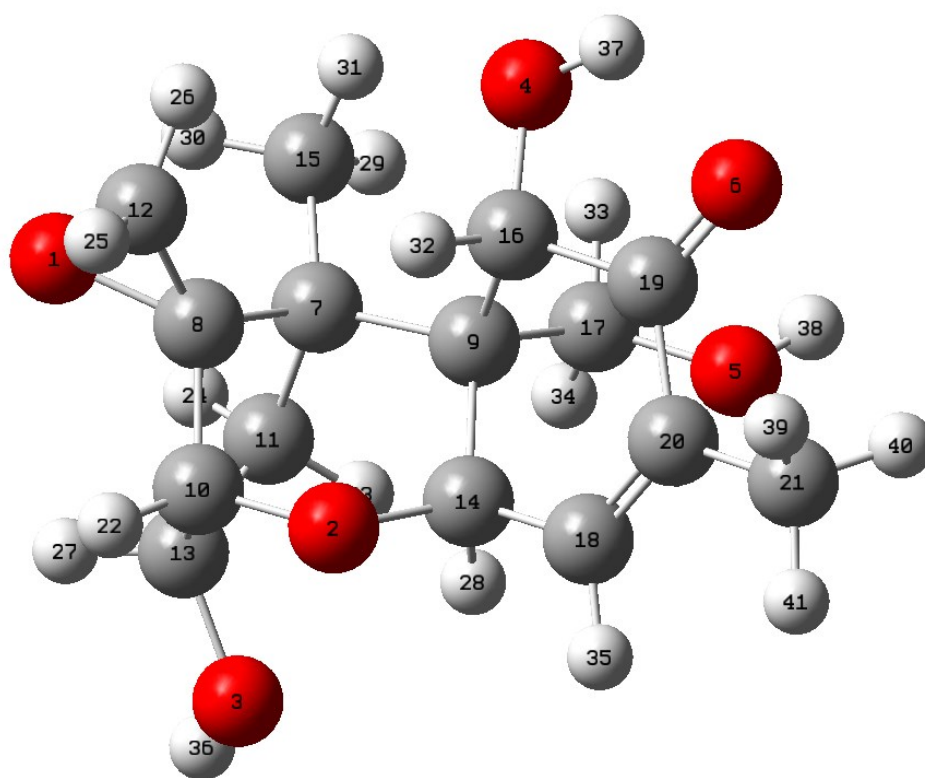


Figure S4. Enlarged image of DON molecular structure with labels corresponding to vibrational band assignments.

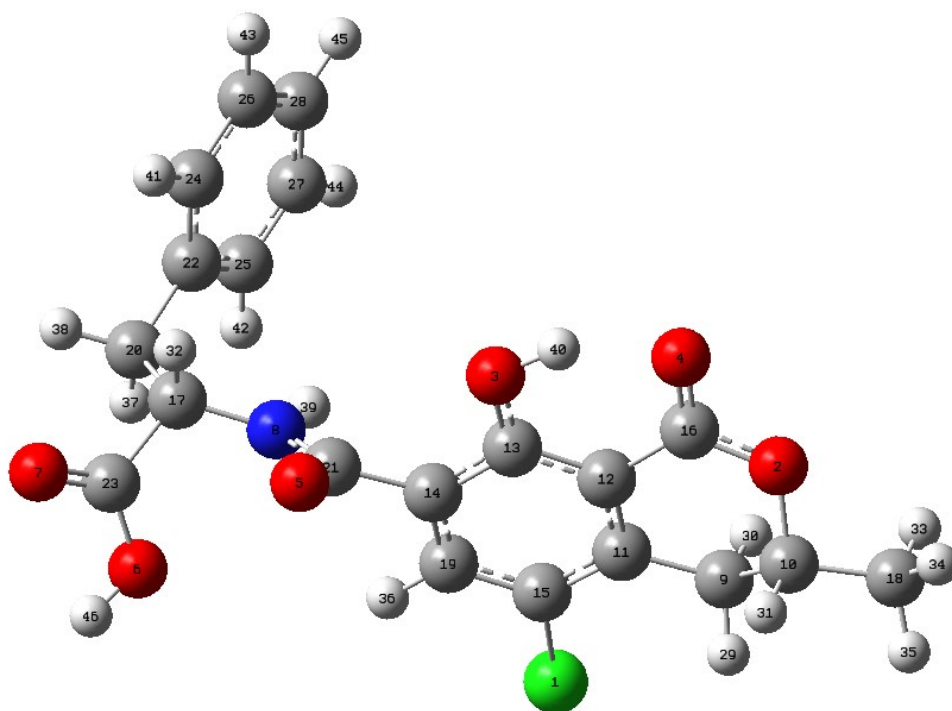


Figure S5. Enlarged image of OTA molecular structure with labels corresponding to vibrational band assignments.

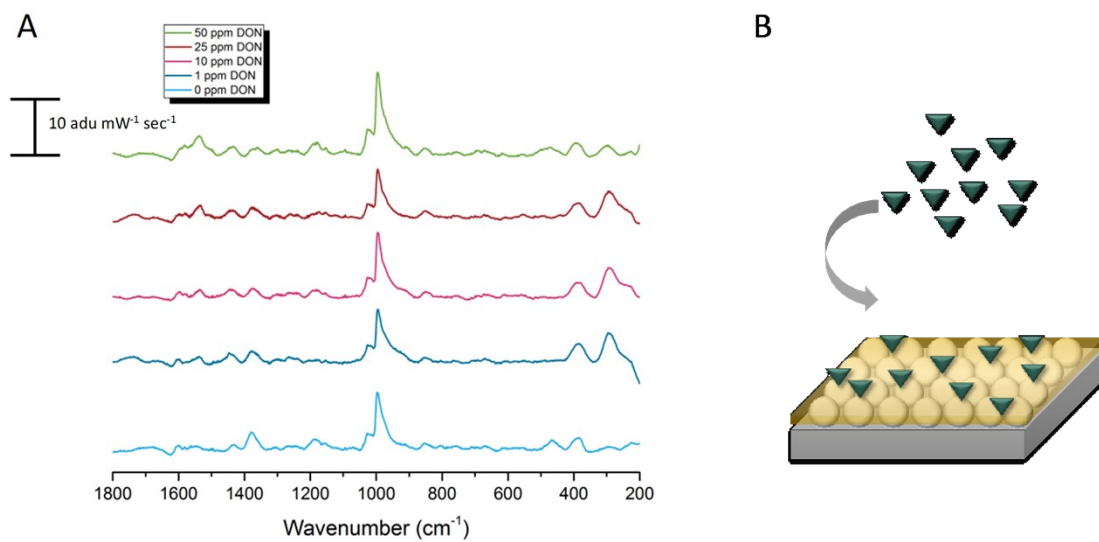


Figure S6. SERS spectra of varying concentrations of DON without an affinity agent. At high concentrations, there is some binding, due to pi-interactions, but nothing is seen at low concentrations.

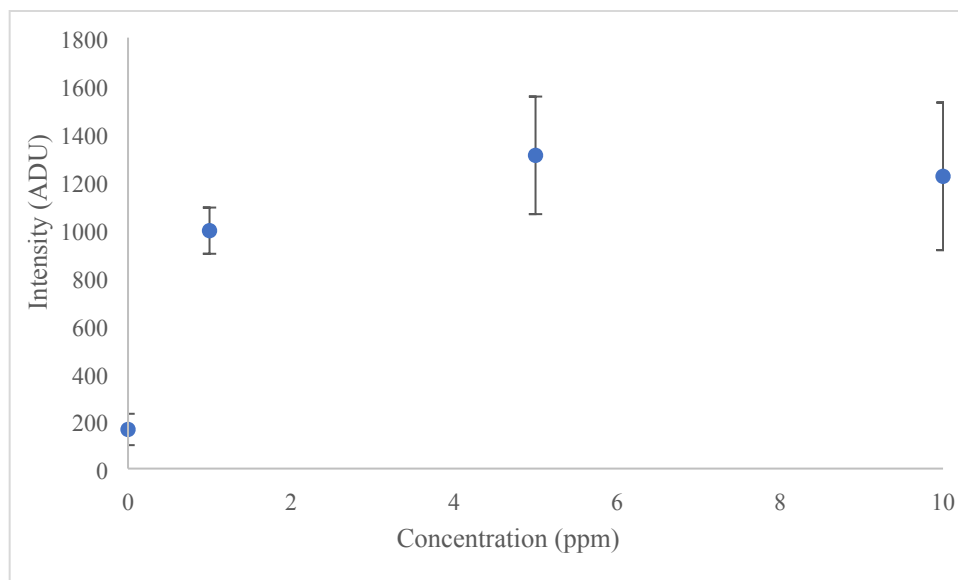


Figure S7. Graph of experimental SERS intensity at each measured concentration of DON at the 1130 cm^{-1} shift. Error bars are from standard deviation of the intensity after baselining.

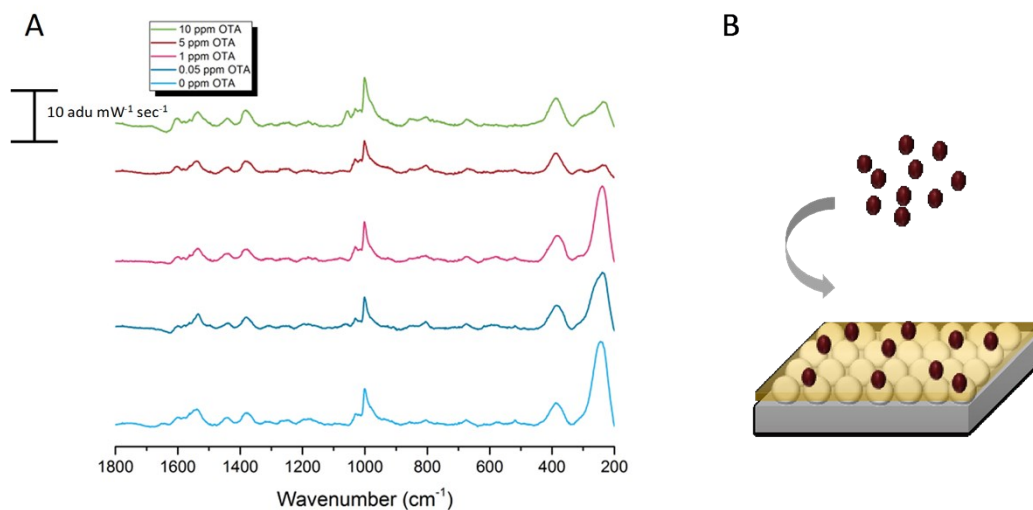


Figure S8. SERS spectra of varying concentrations of OTA without an affinity agent. At high concentrations, there is some binding, due to pi-interactions, but nothing is seen at lower concentrations of OTA.

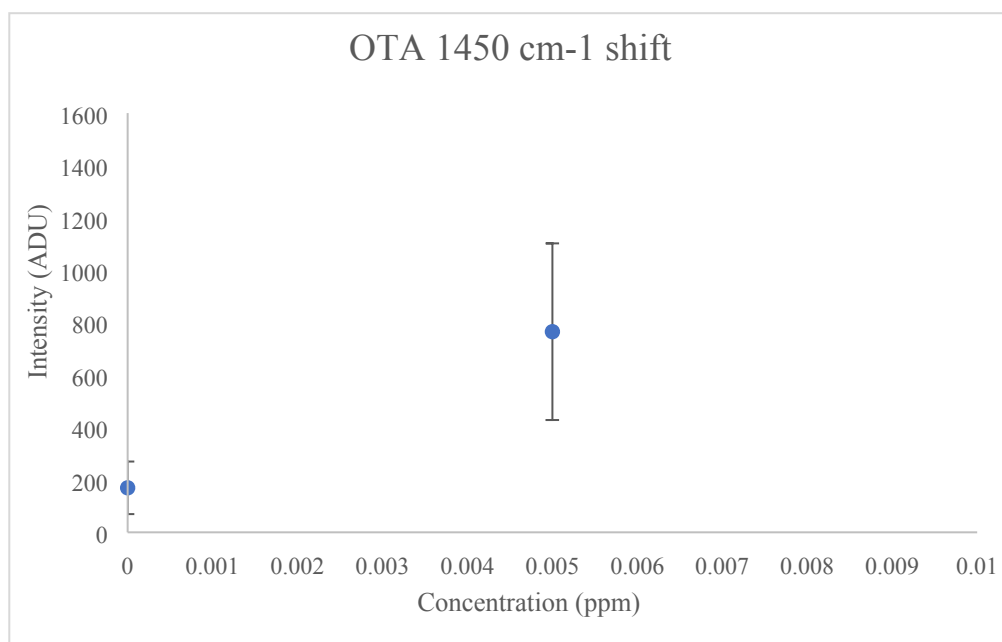
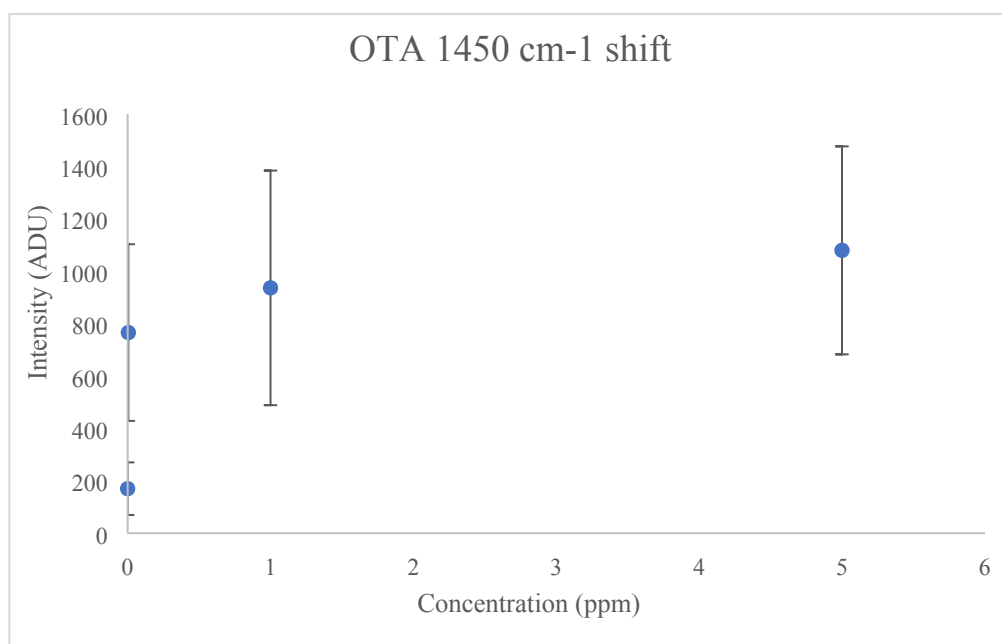


Figure S9. Graph of experimental SERS intensity at each measured concentration of OTA at the 1450 cm⁻¹ shift. Error bars are from standard deviation of the intensity after baselining. An enlarged graph is also shown to distinguish between 0 ppm and 0.005 ppm.

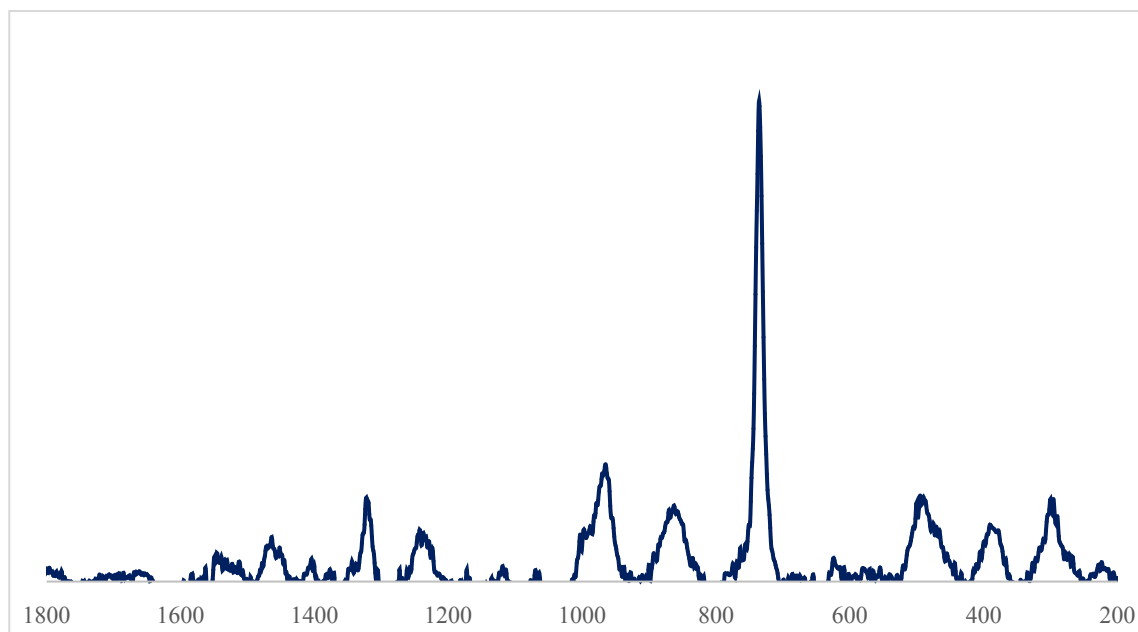


Figure S10. Spectra of 312 Goose Island Wheat beer on bare FON. No purification was done to the beer prior to spectra being obtained.