Electronic Supplementary Information

Spectroscopic identification of neurotoxin Tetramethylenedisulfotetramine (TETS) captured by supramolecular receptor β-cyclodextrin immobilized on nano-structured gold surfaces

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Figure S1
Raman spectra of β-CD (bottom curve) and β-CD-SH (top curve)

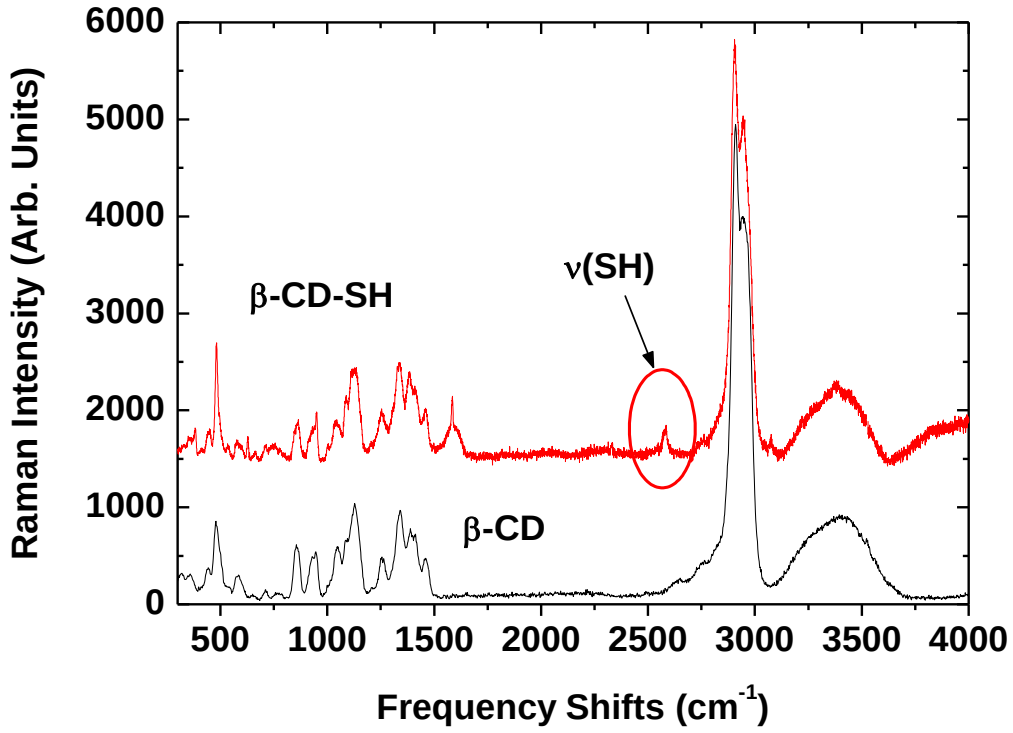

Figure S2
SEM photomicrographs of immobilized 10 nm gold nanoparticles on a flat gold surface

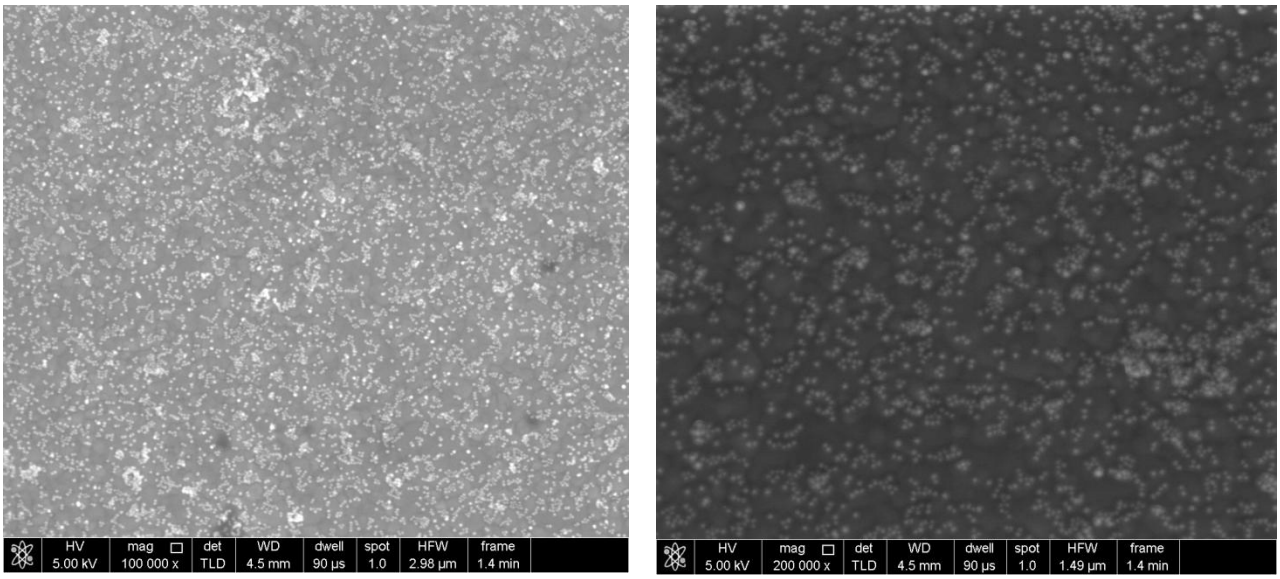

Figure S3
SEM photomicrographs of Klarite®

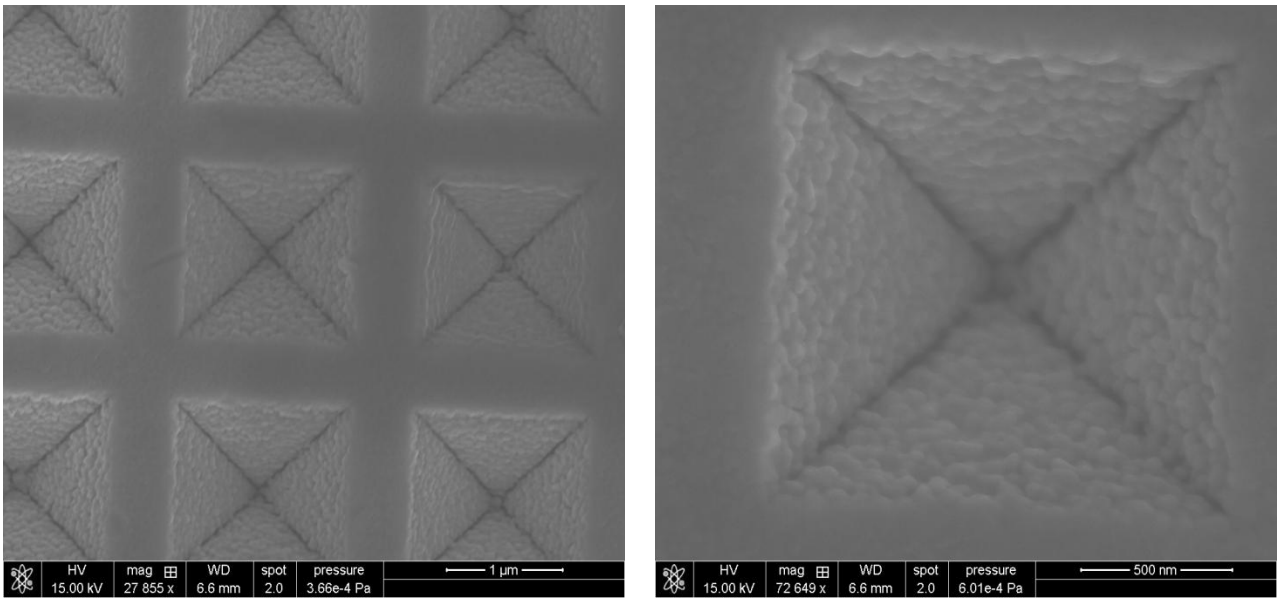

Figure S4
Core-level XPS S 2p spectrum from unbound thiolated CD powder (bottom) confirming the presence of unbound CD on the Au surfaces in Figure 3b

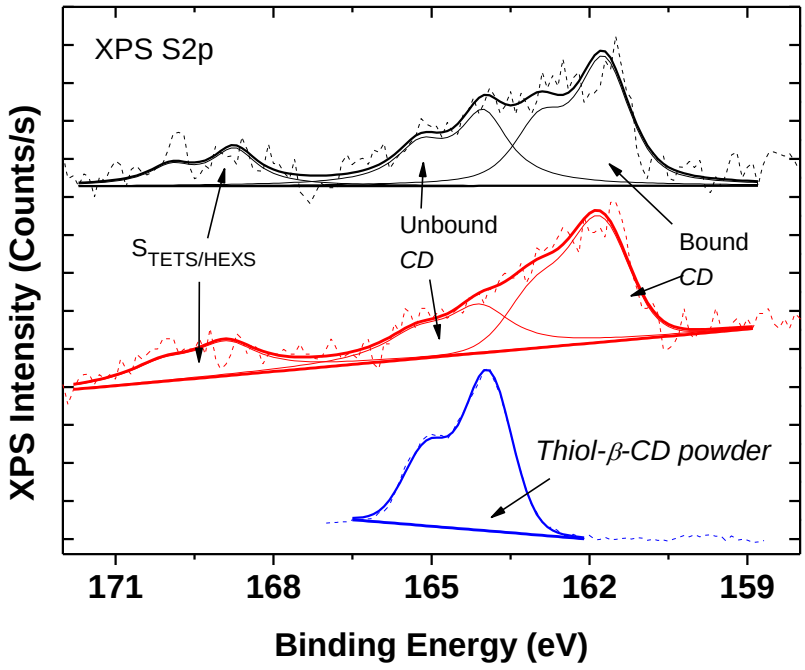

Figure S5
X-ray diffraction of Klarite® SERS-active surface

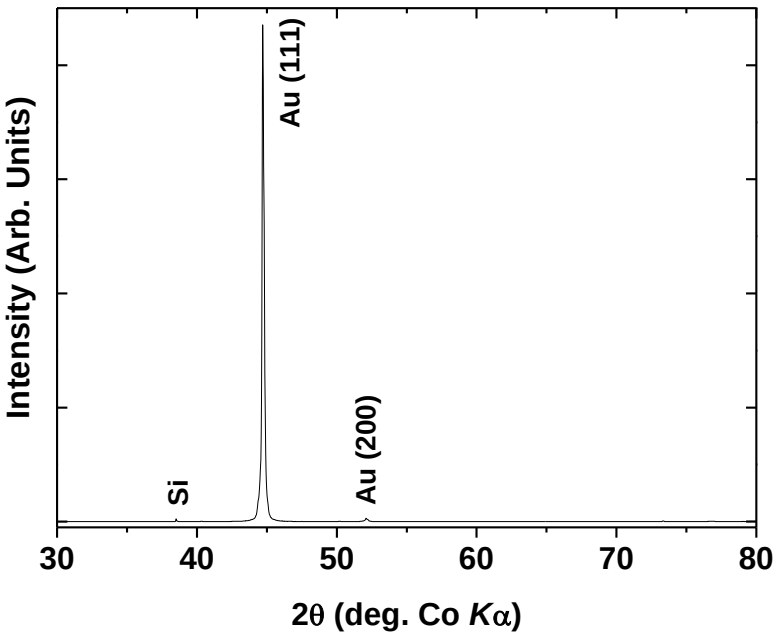

Table S1 TETS harmonics calculated using DFT at the B3LYP level of theory

TETS Harmonics (cm^{-1})	IR Intensities (Km/mol)	Raman scattering activity (Å^4/AMU)	Raman cross section (cm^2/sr)
171.2402	6.3922	0.4287	1.51261E-31
171.3182	6.3904	0.4294	1.51392E-31
236.3095	2E-4	0.4463	9.30444E-32
253.1293	1E-4	7.0733	1.3232E-30
286.3075	1E-4	4E-4	6.18546E-35
361.9262	0.1934	0.0058	6.32712E-34
363.6816	0.2087	0.0052	5.63292E-34
402.4852	15.2737	8E-4	7.49355E-35
414.937	0.0313	0.0143	1.283E-33
437.3952	1.4306	0.9513	7.92741E-32
437.7644	1.3421	0.9353	7.78492E-32
471.9981	0.0021	6.8805	5.1607E-31
482.6858	3.204	2.1464	1.56129E-31
484.2386	2.8837	5.5187	3.99672E-31
484.9362	2.8274	5.196	3.75563E-31
512.1539	3E-4	3.5655	2.3929E-31
572.9386	70.0816	3.1465	1.81734E-31
630.4217	76.7958	0.0881	4.48614E-33
638.7867	0.0293	49.4963	2.4773E-30
647.4006	6.4156	1.9976	9.82456E-32
648.8486	5.314	2.004	9.82733E-32
692.7846	126.9108	0.06	2.70184E-33
697.1421	128.6914	0.0793	3.542E-33
839.8969	59.362	1.3534	4.75219E-32
841.5839	2.4657	0.8618	3.01821E-32
843.0371	21.0388	1.0829	3.78412E-32
844.1313	290.2046	3.3742	1.17712E-31
899.8002	0.0093	5E-4	1.60617E-35
948.4512	0.021	4.7858	1.43596E-31
1008.9813	91.7887	1.4147	3.91616E-32
1010.4879	90.9382	1.4149	3.90909E-32
1049.1935	0.005	0.0042	1.10462E-34
1078.179	0.0115	4E-4	1.01496E-35
1132.7972	424.7334	3.378	8.02859E-32
1148.6909	0.133	21.2363	4.95455E-31
1153.9005	53.0678	0.0136	3.15387E-34
1155.0388	54.0878	0.0373	8.63858E-34
1206.7517	59.4112	0.3076	6.71789E-33
1271.7341	0.008	3.2764	6.66515E-32
1326.3896	3.9098	0.2565	4.92594E-33
1328.5137	4.7417	0.2138	4.09688E-33
1352.5991	159.8771	6.0937	1.1391E-31
1352.9361	165.5003	5.9458	1.11107E-31
1354.9369	4.5987	0.4243	7.91256E-33
1360.4514	2.4692	8.3588	1.55005E-31
1381.5961	66.0641	0.6939	1.25952E-32
1383.0031	61.3219	0.5803	1.05183E-32
1402.4462	3.8117	5.3977	9.59515E-32
1475.0769	0.1012	16.4057	2.71642E-31
1489.0287	19.3242	0.3571	5.83434E-33
1491.0543	19.6598	0.2631	4.29026E-33
1503.611	0.4633	10.6489	1.71587E-31
3110.3152	0.0595	48.2199	2.32997E-31
3111.1652	8.8674	10.7206	5.17736E-32
3111.4257	8.9296	10.2619	4.95501E-32
3113.5628	0.034	315.3124	1.52043E-30
3165.7925	0.0056	0.3075	1.43443E-33
3166.4406	0.008	53.5772	2.49825E-31
3166.7205	8E-4	53.2554	2.4828E-31
3167.6296	1.7063	76.2679	3.55362E-31

Table S2 HEXS harmonics calculated using DFT at the B3LYP level of theory

HEXS Harmonics (cm^{-1})	IR Intensities (Km/mol)	Raman scattering activity (Å^4/AMU)	Raman cross section (cm^2/sr)
100.374	2.6712	0.0742	6.63688E-32
103.7836	2.6583	0.0756	6.36875E-32
180.9225	0.0025	0.8406	2.70547E-31
185.3016	4E-4	0.8415	2.60292E-31
201.5754	4E-4	5.4816	1.47623E-30
205.4376	1E-4	0.0024	6.26637E-34
228.6387	1E-3	0.0029	6.37193E-34
254.5226	4.0432	4.2759	7.93051E-31
256.2532	3.9979	4.3792	8.03655E-31
290.5168	0.0017	0.0406	6.14014E-33
291.5442	9E-4	0.0319	4.79856E-33
325.9975	1.5684	0.6172	7.84973E-32
331.0761	1.6649	0.5026	6.24742E-32

339.0851	0.2627	2.188	2.62546E-31
340.9755	0.0599	2.4349	2.89792E-31
344.4342	3.8799	0.2018	2.36641E-32
383.152	0.0019	33.0757	3.32345E-30
416.005	0.0574	0.0219	1.95778E-33
426.8838	6.3837	1.0672	9.20067E-32
428.3722	5.682	1.0685	9.16709E-32
444.2823	0.0373	4.101	3.34398E-31
445.9756	0.0039	4.0167	3.25798E-31
465.5156	2.9306	0.0198	1.51359E-33
491.3903	63.8949	0.101	7.16979E-33
492.5495	65.4265	0.0857	6.06419E-33
507.2459	0.5938	9.2706	6.30329E-31
526.8033	0.0174	0.0036	2.32593E-34
546.9363	7E-4	14.3375	8.80918E-31
549.6584	0.0131	0.0135	8.23979E-34
550.164	0.0154	0.0549	3.34674E-33
559.9619	0.1849	1.7333	1.03206E-31
560.7614	0.1058	1.7213	1.02297E-31
669.0068	419.5948	7E-4	3.2985E-35
683.336	76.0436	0.5552	2.54508E-32
683.7536	76.8025	0.5376	2.46244E-32
689.3241	0.1705	0.1922	8.71133E-33
690.6973	0.4678	0.1908	8.62556E-33
848.224	18.5743	0.0097	3.36287E-34
857.1511	0.0204	14.1297	4.83285E-31
880.4808	0.0858	0.0992	3.27733E-33
881.7731	0.2257	0.1149	3.78883E-33
926.8427	287.1435	0.8006	2.47507E-32
927.4245	33.5772	8.6325	2.66658E-31
930.8755	339.8642	1.4567	4.47813E-32
931.8288	344.9703	1.2426	3.81489E-32
1008.9966	0.0682	3.2331	8.94967E-32
1010.3955	0.0792	3.2529	8.98819E-32
1013.0487	0.0034	0.1268	3.49166E-33
1014.5754	0.1395	0.1447	3.97673E-33
1060.4894	0.0283	3E-4	7.77989E-36
1079.6172	0.005	2E-4	5.06591E-36
1107.8685	315.6494	0.7101	1.73829E-32
1107.9452	314.6894	0.7082	1.73348E-32
1120.086	0.0219	50.3018	1.21359E-30
1183.3349	0.0684	1.1492	2.57675E-32
1183.8374	0.5577	1.1876	2.66134E-32
1203.4886	121.8274	0.218	4.77843E-33
1203.8781	121.1514	0.2217	4.85742E-33
1241.2508	1.2803	12.2046	2.56593E-31
1245.1354	88.8413	0.1843	3.8584E-33
1253.9587	0.0155	0.01	2.07359E-34
1259.3141	0.007	0.0085	1.75238E-34
1330.712	0.2105	0.0059	1.128E-34
1343.899	221.4555	8.811	1.24195E-35
1344.7004	221.2109	8.8767	1.67281E-31
1357.692	0.1704	0.0258	4.79781E-34
1363.3779	1.7612	3.1232	5.77443E-32
1364.5206	0.657	2.9821	5.50716E-32
1370.6027	2.0543	0.0098	1.79868E-34
1373.6582	95.5992	0.1194	2.18469E-33
1373.9304	93.6865	0.1664	3.04382E-33
1385.1527	0.086	3.122	5.6466E-32
1385.9427	0.4736	3.179	5.74513E-32
1402.9774	57.1826	0.0035	6.21844E-35
1403.4442	54.8444	0.0071	1.26087E-34
1480.6437	0.6128	13.6459	2.24743E-31
1483.05	0.9473	13.6205	2.23808E-31
1489.2016	20.8376	7.7072	1.259E-31
1492.5594	26.1729	6.666	1.08544E-31
1497.9159	45.8596	1.3128	2.12679E-32
1505.4083	1.338	4.6178	7.42805E-32
3043.3076	2.404	16.7468	8.44628E-32
3043.7474	1.8115	23.2656	1.17307E-31
3043.8321	3.679	3.8592	1.94574E-32
3043.9146	0.0204	42.1437	2.1247E-31
3048.0474	112.3396	4.1298	2.07654E-32
3048.7168	0.5302	886.0017	4.45307E-30
3163.9241	0.1474	1.0043	4.6904E-33
3164.7305	1.019	1.5321	7.15175E-33
3166.7467	2.4451	3.0265	1.41095E-32
3167.3812	6.3755	15.3814	7.16792E-32
3167.9832	4.4753	31.3919	1.46234E-31
3169.3997	1.2835	70.7782	3.29414E-31