Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

From bulk to plasmonic nanoparticle surface: behavior of two potent therapeutic peptides, octreotide and pasireotide

Belén Hernández, Eduardo López-Tobar, Santiago Sanchez-Cortes,Yves-Marie Coïc, Bruno Baron, Alexandre Chenal, Sergei G. Kruglik, Fernando Pflüger, Régis Cohen, Mahmoud Ghomi

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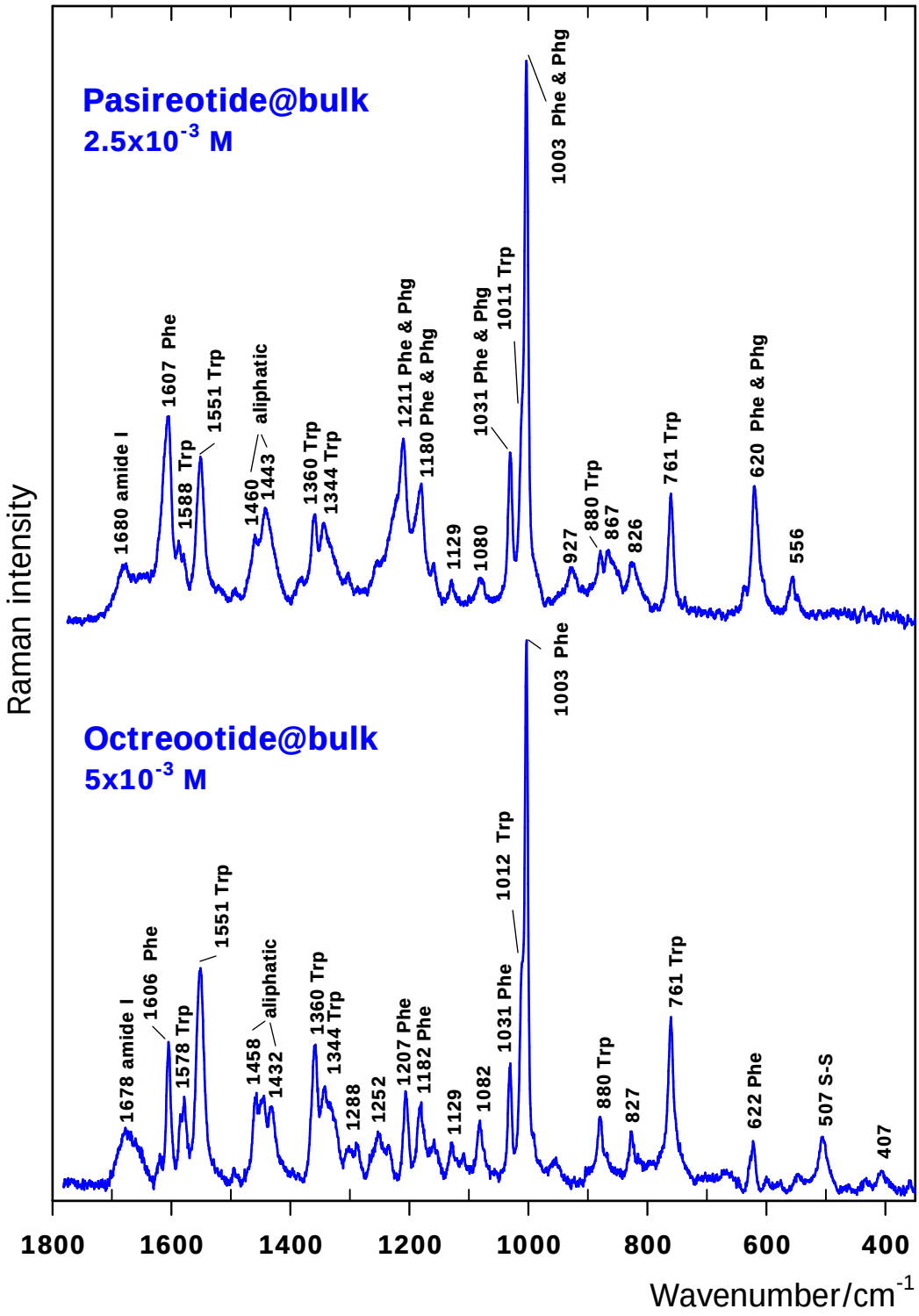

Fig. S1. Room temperature Raman spectra (λ_{exc}=488 nm) recorded from the solution samples containing octreotide (top) and pasireotide (bottom) in the 1800-350 cm^{-1} spectra region. Sample concentrations are reported, as well as the tentative assignments of the main observed peaks. See main text for details.

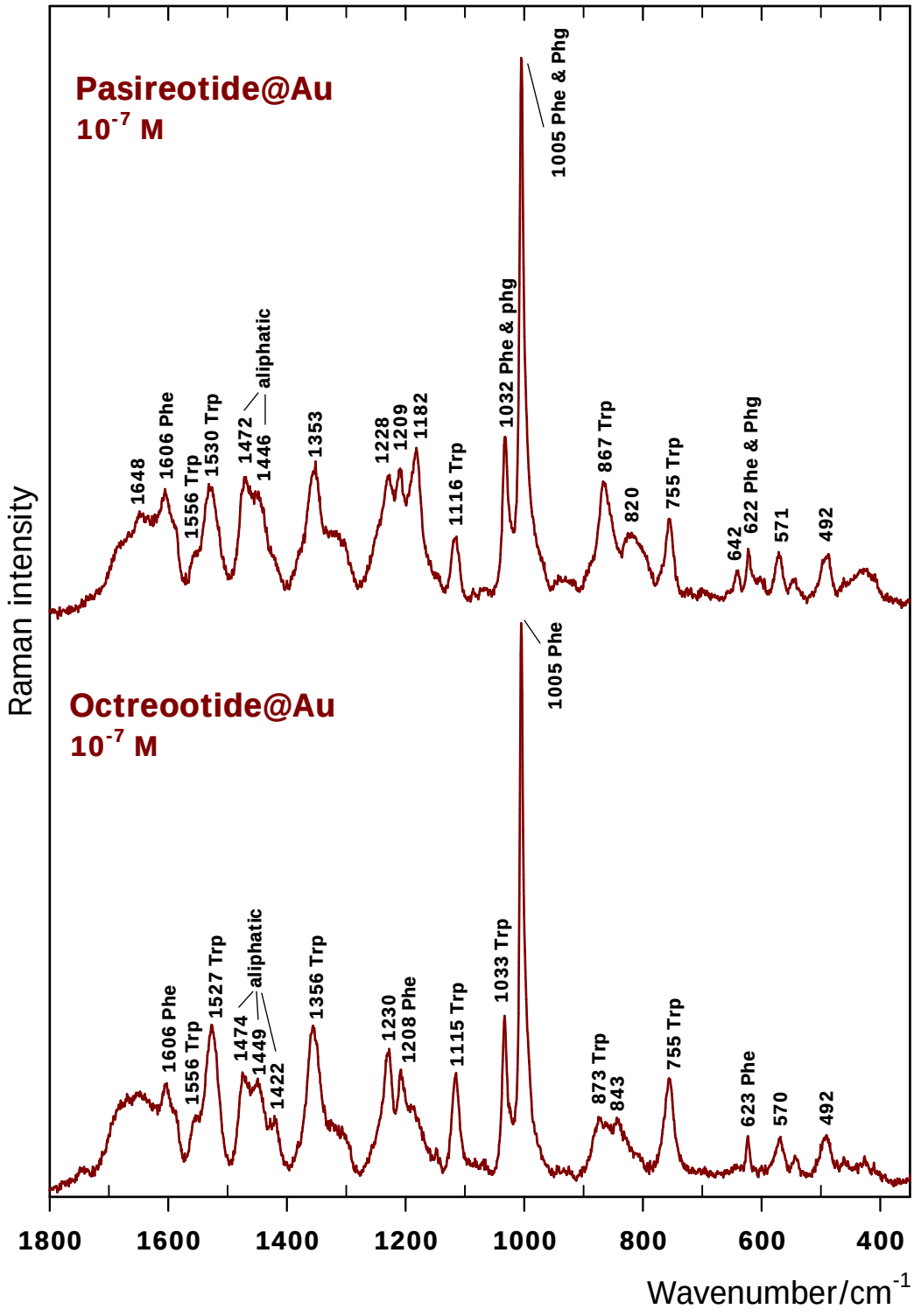

Fig. S2. Surface-enhanced Raman spectra (λ_{exc}=785 nm) recorded from the peptides adsorbed on the gold colloids (~95 nm). Octreotide (bottom), pasireotide (top). Peptide concentrations are reported, as well as the tentative assignments of the main observed peaks. See main text for details.

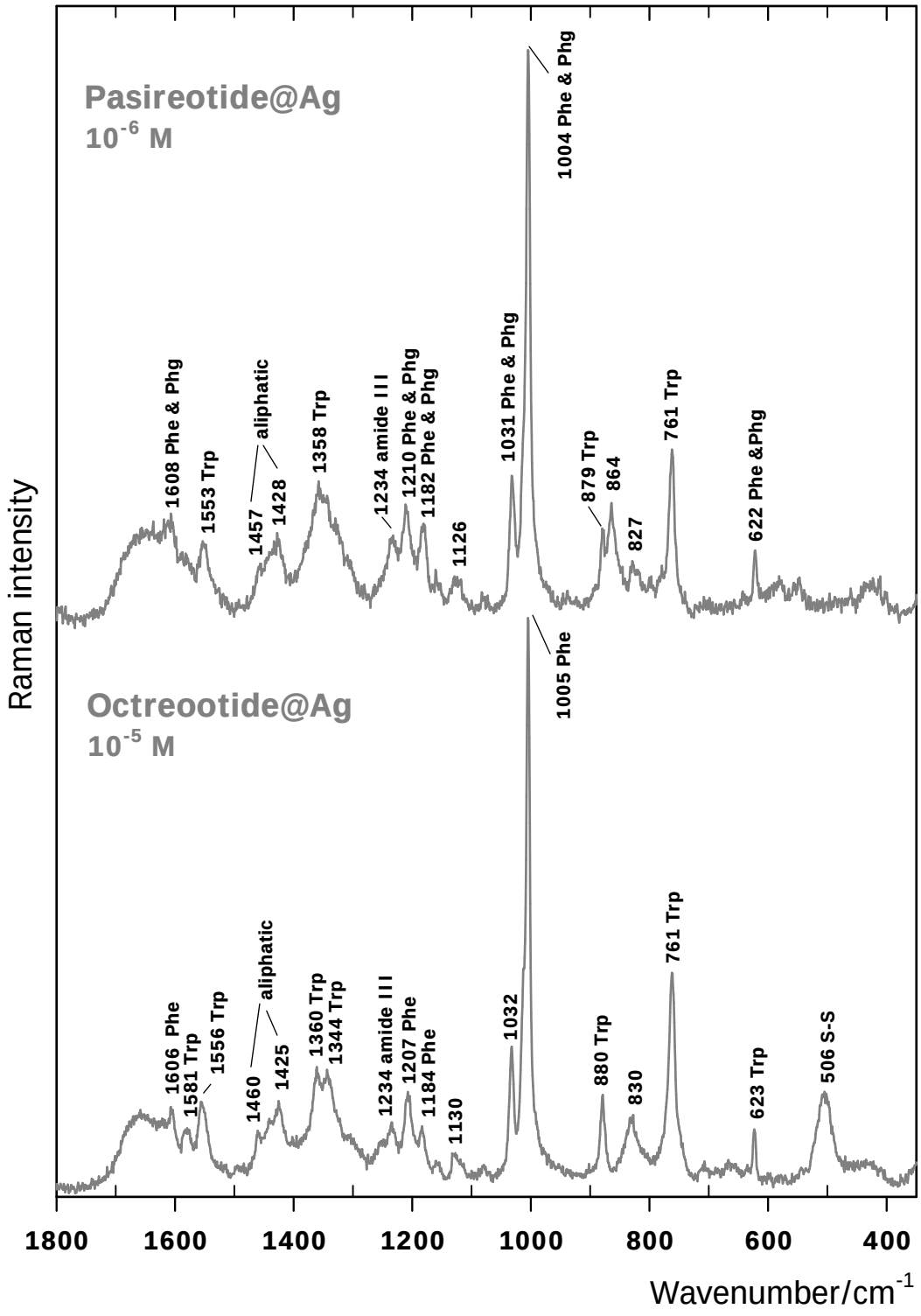

Fig. S3. Surface-enhanced Raman spectra (λ_{exc}=785 nm) recorded from the peptides adsorbed on the silver colloids. Octreotide (bottom), pasireotide (top). Peptide concentrations are reported, as well as the tentative assignments of the main observed peaks. See main text for details.

Table S1. Cartesian coordinates of the structural models used for octreotide and pasireotide.

	Octreotide				Pasireotide			
No.	Atom	x	y	z	Atom	x	y	z
1	N	0.0000	0.0000	0.0000	N	2.1030	3.3120	-1.1200
2	C	1.4859	0.0000	0.0000	C	3.4080	3.6540	-0.5170
3	C	2.1010	1.4362	0.0000	C	4.1680	2.4670	0.1090
4	O	2.8130	1.7794	-0.9494	O	5.3020	2.6450	0.5700
5	C	1.9837	-0.9468	1.1323	C	3.0430	4.7200	0.5350
6	C	3.5115	-1.1366	1.2066	C	1.6460	4.2880	1.0060
7	C	4.2610	-0.4526	2.1706	O	0.8130	5.3750	1.4570
8	C	4.1677	-1.9737	0.2964	C	0.9120	5.9520	2.6840
9	C	5.6443	-0.6028	2.2229	O	0.2160	6.9330	2.9190
10	C	5.5529	-2.1174	0.3478	N	1.7670	5.4060	3.5900
11	C	6.2899	-1.4317	1.3105	C	0.9720	3.7100	-0.2530
12	H	-0.1848	-0.7572	0.6672	C	1.9020	5.9770	4.9210
13	H	-0.2398	-0.3209	-0.9442	C	0.7820	5.4650	5.8350
14	H	1.7975	-0.4549	-0.9606	N	0.8520	6.1090	7.1980
15	H	1.5153	-1.9430	1.0115	H	4.0670	4.0610	-1.2860
16	H	1.6010	-0.5919	2.1090	H	2.9730	5.7000	0.0530
17	H	3.7756	0.2098	2.8721	H	3.7880	4.7790	1.3310
18	H	3.6081	-2.5049	-0.4601	H	1.6970	3.5190	1.7820
19	H	6.2196	-0.0656	2.9638	H	0.3650	4.4890	-0.7210
20	H	6.0561	-2.7583	-0.3624	H	0.3390	2.8550	-0.0140
21	H	7.3637	-1.5417	1.3468	H	2.2950	4.5700	3.3830
22	N	1.8948	2.2428	1.0628	H	2.8850	5.6990	5.3120
23	C	2.6532	3.5025	1.2778	H	1.8600	7.0660	4.8380
24	C	2.9424	3.7079	2.7969	H	-0.1980	5.7110	5.4250
25	O	2.0607	4.1203	3.5574	H	0.8510	4.3880	5.9920
26	C	1.9159	4.6838	0.6168	H	0.7830	7.1320	7.1440
27	S	3.0035	6.1241	0.5339	H	0.0810	5.7880	7.7940
28	H	1.2206	1.8842	1.7457	H	1.7240	5.8880	7.6910
29	H	3.6221	3.4303	0.7605	N	3.5140	1.2880	0.1520
30	H	1.6067	4.4339	-0.4161	C	4.1080	0.0480	0.6190
31	H	0.9914	4.9440	1.1669	C	3.2690	-1.0900	-0.0160
32	N	4.1735	3.3979	3.2427	O	2.4010	-0.8220	-0.8640
33	C	4.5785	3.5079	4.6711	C	4.2120	-0.0580	2.1400
34	C	5.8941	4.3433	4.7764	C	5.4130	-0.4720	2.7290
35	O	7.0029	3.7999	4.6804	C	3.1120	0.2320	2.9610
36	C	4.6774	2.0613	5.2390	C	5.5110	-0.6080	4.1190
37	C	4.9406	1.9686	6.7506	C	3.2100	0.1040	4.3480
38	C	3.8904	2.1280	7.6615	C	4.4110	-0.3200	4.9310
39	C	6.2335	1.7282	7.2304	H	2.6700	1.1740	-0.4030
40	C	4.1307	2.0540	9.0317	H	5.1240	-0.0390	0.2090
41	C	6.4726	1.6558	8.6006	H	6.2790	-0.6840	2.1070
42	C	5.4213	1.8182	9.4999	H	2.1780	0.5660	2.5140
43	H	4.8365	3.0390	2.5368	H	6.4490	-0.9300	4.5620
44	H	3.7974	4.0305	5.2617	H	2.3520	0.3340	4.9730
45	H	3.7400	1.5142	5.0189	H	4.4870	-0.4210	6.0100
46	H	5.4516	1.4962	4.6835	N	3.5270	-2.3430	0.3930
47	H	2.8854	2.3130	7.3094	C	2.9840	-3.5830	-0.1890
48	H	7.0581	1.6055	6.5414	C	3.3040	-3.7410	-1.7070
49	H	3.3179	2.1795	9.7311	C	4.7730	-3.7610	-2.0110
50	H	7.4733	1.4724	8.9645	C	5.7080	-4.8300	-1.7450
51	H	5.6079	1.7605	10.5626	C	5.5020	-2.7490	-2.5960
52	N	5.7665	5.6717	4.9722	N	6.8270	-3.1220	-2.7080
	C	6.9335	6.5807	5.1560	C	6.9870	-4.3930	-2.1980

53	C	6.4146	7.9568	5.6590	C	5.5920	-6.1180	-1.1830
54	C	7.5173	8.8802	6.2060	C	8.1320	-5.1950	-2.1010
55	C	7.9824	8.9020	7.5388	C	6.7270	-6.9190	-1.0850
56	N	9.0576	9.7980	7.7045	C	7.9850	-6.4610	-1.5380
57	C	9.2472	10.3296	6.4401	C	1.4800	-3.8400	0.0620
58	C	10.2241	11.2523	5.9979	O	1.1100	-4.9940	0.3090
59	C	10.2459	11.6130	4.6487	H	4.2280	-2.4630	1.1140
60	C	9.3236	11.0778	3.7413	H	3.4870	-4.3860	0.3500
61	C	8.3510	10.1650	4.1533	H	2.8350	-4.6800	-2.0270
62	C	8.3138	9.7871	5.5219	H	2.8170	-2.9340	-2.2620
63	C	7.8187	6.7027	3.8689	H	5.1740	-1.7830	-2.9550
64	O	7.3250	6.9777	2.7723	H	7.5550	-2.5560	-3.1220
65	H	4.8043	6.0211	4.9162	H	4.6300	-6.4890	-0.8360
66	H	7.5426	6.1480	5.9773	H	9.0980	-4.8440	-2.4540
67	H	5.6643	7.8131	6.4604	H	8.8530	-7.1090	-1.4490
68	H	5.8626	8.4745	4.8500	H	6.6470	-7.9140	-0.6540
69	H	7.5830	8.2838	8.3320	N	0.6420	-2.7800	-0.0320
70	H	9.5925	10.0021	8.5557	C	-0.8180	-2.8880	0.0580
71	H	10.9461	11.6620	6.6894	C	-1.4450	-2.1040	-1.1140
72	H	10.9915	12.3128	4.2992	O	-1.9720	-2.6930	-2.0620
73	H	9.3700	11.3704	2.7020	C	-1.3830	-2.4710	1.4350
74	H	7.6554	9.7469	3.4398	C	-0.9750	-3.4250	2.5660
75	N	9.1314	6.4649	4.0234	C	-1.5660	-3.0080	3.9210
76	C	10.0649	6.3090	2.8647	C	-1.1630	-3.9990	5.0080
77	C	9.9208	4.9621	2.0674	N	-1.7680	-3.6310	6.3450
78	O	10.2013	4.9401	0.8654	H	1.0470	-1.9040	-0.3650
79	C	11.5218	6.5402	3.3522	H	-1.0730	-3.9340	-0.1230
80	C	11.8358	7.9802	3.8322	H	-2.4760	-2.4470	1.3500
81	C	13.2984	8.1565	4.2763	H	-1.0610	-1.4520	1.6880
82	C	13.5742	9.5818	4.7799	H	-1.3150	-4.4390	2.3190
83	N	14.9858	9.7186	5.1836	H	0.1180	-3.4660	2.6400
84	H	9.4462	6.3558	4.9924	H	-2.6610	-2.9660	3.8490
85	H	9.8420	7.1059	2.1259	H	-1.2170	-2.0010	4.1870
86	H	11.7724	5.8127	4.1488	H	-1.5150	-5.0090	4.7860
87	H	12.2167	6.3009	2.5231	H	-0.0830	-4.0260	5.1600
88	H	11.6015	8.7014	3.0248	H	-2.7930	-3.6190	6.3070
89	H	11.1626	8.2553	4.6686	H	-1.5000	-4.2990	7.0760
90	H	13.5345	7.4228	5.0718	H	-1.4660	-2.7020	6.6580
91	H	13.9720	7.9134	3.4310	N	-1.3620	-0.7480	-1.0330
92	H	13.3374	10.3288	3.9962	C	-1.8520	0.1680	-2.0630
93	H	12.9181	9.8270	5.6384	C	-0.6280	0.8060	-2.7650
94	H	15.6096	9.5034	4.3967	O	0.0610	0.1210	-3.5240
95	H	15.2229	9.0331	5.9113	C	-2.9110	1.1460	-1.5040
96	N	9.4498	3.8619	2.6933	C	-4.1790	0.4530	-1.0420
97	C	9.0131	2.6286	1.9705	C	-5.1070	-0.0440	-1.9660
98	C	7.5985	2.8247	1.3283	C	-4.4620	0.2850	0.3230
99	O	6.5725	2.4727	1.9181	C	-6.2700	-0.7050	-1.5590
100	C	9.0642	1.3804	2.9119	C	-5.6200	-0.3630	0.7500
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102	C	10.4712	0.9691	3.3722	O	-7.6180	-1.5260	0.3200
103	H	9.1612	4.0506	3.6599	C	-8.6780	-1.9110	-0.5840
104	H	9.7269	2.4180	1.1476	C	-9.8770	-2.2980	0.2430
105	H	8.6531	0.5184	2.3487	C	-10.0500	-3.6240	0.6630
106	H	7.7786	2.3846	4.0089	C	-10.8250	-1.3360	0.6200
107	N	7.5510	3.4296	0.1269	C	-11.1470	-3.9840	1.4520
108	C	6.2749	3.8164	-0.5317	C	-11.9250	-1.6910	1.4070
109	C	6.3000	3.5761	-2.0704	C	-12.0860	-3.0170	1.8250
110	O	7.2827	3.8458	-2.7719	H	-0.9680	-0.3340	-0.1970
111	C	5.9680	5.2826	-0.1448	H	-2.3140	-0.4610	-2.8270
112	S	4.4142	5.8566	-0.8714	H	-3.1570	1.8620	-2.2980
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135	H 10.9474 1.7571 3.9834	C -3.0250 4.0760 -6.5270
136	H 10.4350 0.0559 3.9930	H -1.0330 2.6420 -1.9650
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143		H -1.5460 3.3140 -7.9060
144		H -3.8380 4.0370 -7.2470

Unit: Å
C, N, O, S and H refer to carbon, nitrogen, oxygen, sulfur and hydrogen atoms, respectively.
See main text for details.