

ADVANCED FUNCTIONAL MATERIALS

Supporting Information

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Neuromorphic Organic Devices that Specifically Discriminate
Dopamine from Its Metabolites
by Nonspecific Interactions

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Biscarini**

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1 - Setup and protocol

1.1 Characteristics of the sensor and measurement setup

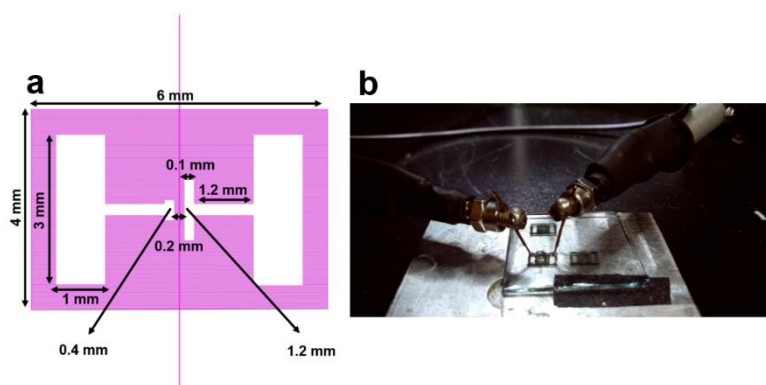


Figure S1. a) CAD and sizes of the sensor. b) Measurement setup with two probes contacting the electrodes.

2 - DFT calculations

2.1 - PEDOT:PSS and metabolites charges and frontier orbitals

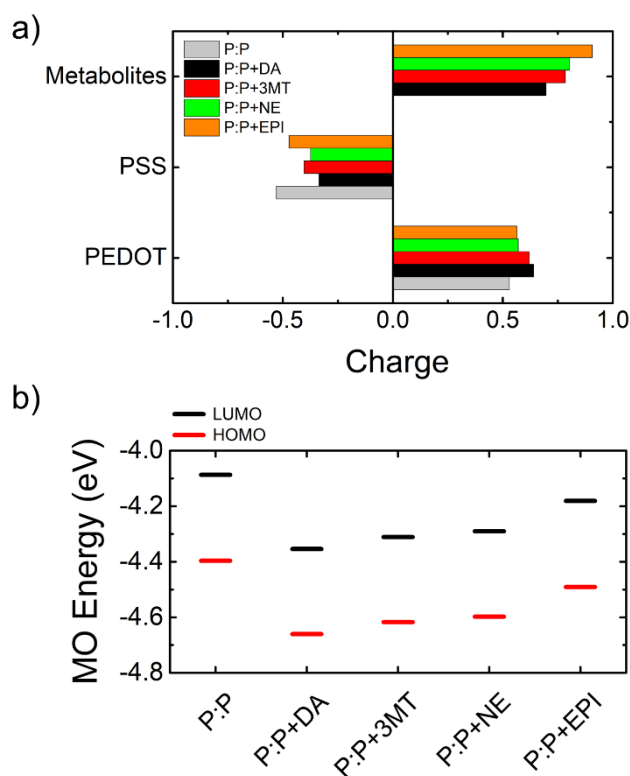


Figure S2. a) Mulliken charges populations on the metabolites, PEDOT and PSS. b) HOMO and LUMO orbitals of PEDOT:PSS and of PEDOT:PSS bound to Dopamine, 3-Methoxy-tyramine, Norepinephrine and Epinephrine.

2.2 - Models xyz coordinates

PEDOT:PSS + DA			
O	3.58744	0.34163	2.8729
C	4.56004	-0.43693	2.36949
C	5.91631	-0.02188	2.25754
O	6.34545	1.20032	2.65783
C	5.4075	1.83633	3.55623
C	3.98689	1.72942	3.02973
C	4.33272	-1.75916	1.92824
S	5.85315	-2.44126	1.31857
C	6.75269	-1.00545	1.73483
C	3.12749	-2.49241	2.00982
C	2.93559	-3.86741	1.74727
C	1.6361	-4.32654	2.01669
C	0.77243	-3.31334	2.50611
S	1.62405	-1.76813	2.59611
O	1.25333	-5.61247	1.88338
C	2.37969	-6.51823	1.80253
C	3.44144	-5.9753	0.86069
O	3.94233	-4.69367	1.33558
C	-0.5473	-3.48166	2.97174
C	-1.3474	-2.50996	3.61709
C	-2.59759	-3.00878	4.06572
C	-2.78078	-4.36375	3.78232
S	-1.40699	-5.03008	2.93781
O	-3.51186	-2.24553	4.70949
C	-3.20302	-0.8369	4.64256
C	-1.71959	-0.57749	4.85135
O	-0.93694	-1.2458	3.82496
C	-3.92713	-5.20372	4.22073
C	8.23629	-0.93758	1.63155
O	-1.7	-2.86894	7.16849
S	-1.46488	-4.31868	7.36385
O	-2.62789	-5.22931	7.47053
C	-0.42179	-4.52814	8.8029
C	0.18401	-5.77265	9.04108
C	0.982	-5.92657	10.18082
C	1.17708	-4.86673	11.09275
C	0.52906	-3.63858	10.83694
C	-0.2626	-3.45713	9.69589
C	2.04876	-5.04429	12.32043
C	3.23109	-4.06498	12.47392
C	4.4523	-4.31564	11.55546
C	5.60971	-3.37825	11.97347
C	6.95869	-3.58581	11.24863
C	7.0041	-3.05655	9.83245
C	6.92401	-1.66547	9.58889
C	6.8703	-1.15634	8.28764
C	6.89721	-2.05911	7.20967
C	7.02298	-3.43997	7.41606
C	7.08744	-3.92727	8.72737
S	6.69148	-1.43014	5.55384

O	5.17312	-0.89116	5.55011
O	-0.57547	-4.92388	6.16447
C	4.08835	-4.20943	10.08213
C	3.66978	-2.97911	9.5274
C	3.29715	-2.87875	8.18498
C	3.34684	-4.03083	7.37875
C	3.76309	-5.2651	7.89503
C	4.13432	-5.3408	9.24526
S	2.82899	-3.89636	5.67257
O	3.01538	-5.25166	5.03282
O	1.4045	-3.40021	5.68026
O	3.74764	-2.883	5.01176
O	6.81982	-2.57496	4.60251
O	7.54699	-0.24748	5.34948
H	2.96126	-1.91689	7.77028
H	3.78456	-6.15421	7.24892
H	3.62613	-2.0781	10.15762
H	4.45832	-6.30789	9.66032
H	4.79138	-5.36026	11.73358
H	4.31356	-6.65299	0.81347
H	3.03432	-5.83242	-0.16105
H	2.78195	-6.65965	2.82837
H	1.98731	-7.47975	1.42593
H	6.79411	-0.07353	8.11037
H	7.05699	-4.12317	6.55687
H	6.88362	-0.96585	10.43824
H	7.17037	-5.01136	8.89558
H	7.74069	-3.06602	11.84161
H	7.22098	-4.66396	11.25473
H	5.28944	-2.31835	11.86645
H	5.7807	-3.5284	13.05986
H	-1.49438	0.50028	4.76143
H	-1.38969	-0.96309	5.83711
H	-3.53051	-0.43986	3.65686
H	-3.79073	-0.34627	5.44047
H	-4.02409	-6.13091	3.62526
H	-3.7783	-5.48272	5.2885
H	-4.87187	-4.62717	4.15686
H	3.88782	2.23164	2.04449
H	8.6593	-1.78691	1.0635
H	3.27038	2.17765	3.74193
H	5.70597	2.89857	3.62399
H	8.55687	0.00898	1.15055
H	8.66771	-0.94953	2.65656
H	5.49409	1.36016	4.5539
H	-0.74671	-2.49235	9.48846
H	1.48196	-6.89102	10.35919
H	0.65674	-2.79658	11.53525
H	1.40136	-4.92398	13.216
H	2.87691	-3.01919	12.33838
H	2.42695	-6.08721	12.35368
H	0.05526	-6.60307	8.33139
H	3.58639	-4.12392	13.52411
H	4.52065	-1.69107	5.39296
H	0.23188	-4.3021	5.96307

O	11.48597	-6.97029	6.18648
H	12.16213	-7.68147	6.20968
H	9.52283	-5.41739	5.42351
C	10.78205	-7.11694	5.03251
C	9.74388	-6.23138	4.71485
O	12.12999	-8.97587	4.53474
C	11.10161	-8.17301	4.13438
H	6.77797	-5.96412	5.05763
H	12.29458	-9.67333	3.87024
C	9.00907	-6.37179	3.51569
H	8.11069	-4.40216	3.54648
C	6.58847	-5.87516	3.9693
H	5.76825	-3.94048	4.10843
C	7.85629	-5.43466	3.22891
C	10.37789	-8.31616	2.94316
N	5.47943	-4.90082	3.79004
C	9.3342	-7.42187	2.63744
H	4.59805	-5.15805	4.32038
H	6.23906	-6.86535	3.61841
H	10.63562	-9.13384	2.25134
H	7.65119	-5.40036	2.13821
H	5.18706	-4.80943	2.79343
H	8.77241	-7.54605	1.69879

PEDOT:PSS + NE			
O	2.88457	0.63946	3.00178
C	4.00365	0.12179	2.46837
C	5.22085	0.84917	2.3369
O	5.35262	2.13221	2.75947
C	4.32898	2.48536	3.71703
C	2.95489	2.07386	3.21729
C	6.25276	0.1024	1.7774
S	5.71398	-1.51053	1.37403
C	4.09235	-1.21687	2.02811
C	3.09715	-2.21646	2.12127
C	3.23882	-3.60105	1.8647
C	2.07124	-4.34385	2.11413
C	0.98732	-3.55645	2.57909
S	1.45599	-1.85505	2.67541
O	4.39914	-4.16762	1.44494
C	4.20402	-5.51787	0.94133
C	3.29317	-6.3084	1.86389
O	1.99008	-5.68176	1.96897
C	-0.26741	-4.02443	3.02102
C	-1.31006	-3.25597	3.59083
C	-2.40472	-4.0344	4.04922
C	-2.22987	-5.40301	3.84327
S	-0.70744	-5.73966	3.06175
O	-3.50396	-3.48936	4.62851
C	-3.59316	-2.06888	4.38437
C	-2.25535	-1.38722	4.61577
O	-1.24677	-1.91768	3.71233

C	-3.13772	-6.4855	4.30765
C	7.6749	0.51761	1.63797
O	-1.0366	-3.00144	7.16976
S	-0.78012	-4.45734	7.29318
O	-1.92982	-5.38614	7.34269
C	0.2621	-4.71029	8.72747
C	1.10674	-5.83023	8.78585
C	1.90273	-6.01787	9.92252
C	1.87082	-5.10929	11.00111
C	0.97985	-4.0154	10.92633
C	0.18051	-3.80307	9.79674
C	2.78096	-5.28096	12.20074
C	3.78677	-4.13323	12.4415
C	5.02743	-4.09687	11.51512
C	5.93897	-2.91763	11.93208
C	7.26711	-2.77276	11.15723
C	7.14354	-2.17801	9.76982
C	6.68801	-0.84987	9.59882
C	6.51953	-0.29582	8.32545
C	6.81591	-1.08539	7.20054
C	7.29806	-2.39536	7.33548
C	7.46606	-2.92725	8.6201
S	6.51745	-0.41863	5.57101
O	7.16682	-1.31503	4.57658
C	4.65576	-4.06577	10.04187
C	3.91741	-2.98651	9.50867
C	3.54293	-2.96102	8.16413
C	3.92134	-4.0315	7.33515
C	4.66115	-5.11445	7.82768
C	5.02181	-5.12058	9.1829
S	3.45774	-3.9715	5.61123
O	2.06167	-3.3926	5.56236
O	3.62731	-5.32716	5.02028
O	4.43162	-2.96278	4.96458
O	6.83515	1.0216	5.55188
O	4.90883	-0.50347	5.42213
O	0.1359	-4.97738	6.07756
N	6.53192	-3.92044	3.60092
C	6.87487	-5.26945	4.11756
C	7.86093	-5.97801	3.18468
C	8.04809	-7.42124	3.62315
C	7.14454	-8.41332	3.20074
C	7.28227	-9.73758	3.6534
C	8.31826	-10.0755	4.53542
C	9.23621	-9.07786	4.96667
C	9.09329	-7.76192	4.50621
O	10.24795	-9.40684	5.81262
O	8.54923	-11.3222	5.03693
H	2.94576	-2.13023	7.762
H	4.93158	-5.94783	7.16351
H	3.61446	-2.15297	10.16005
H	5.59369	-5.97146	9.58445
H	5.59845	-5.0357	11.68606
H	5.21055	-5.9728	0.91036
H	3.78006	-5.45385	-0.08223

H	3.71873	-6.37383	2.8867
H	3.12152	-7.32319	1.46149
H	6.16206	0.73697	8.20296
H	7.54201	-2.99005	6.44517
H	6.45051	-0.23683	10.48254
H	7.83593	-3.95766	8.73033
H	7.9344	-2.1162	11.75567
H	7.77226	-3.75882	11.09613
H	5.36662	-1.96635	11.86652
H	6.17846	-3.04726	13.00837
H	-2.32156	-0.30476	4.40529
H	-1.90549	-1.56179	5.65309
H	-3.94519	-1.89847	3.34324
H	-4.34789	-1.67342	5.08906
H	-2.99718	-7.42725	3.74433
H	-2.93804	-6.68216	5.38429
H	-4.19428	-6.16231	4.22134
H	2.71154	2.58129	2.25997
H	8.18273	0.01246	0.79413
H	2.17608	2.3115	3.96472
H	4.37378	3.58323	3.83808
H	7.74281	1.61377	1.49753
H	8.22127	0.26091	2.57236
H	4.56457	1.99529	4.68455
H	-0.48625	-2.93091	9.73286
H	2.58914	-6.87759	9.95988
H	0.92547	-3.29639	11.75931
H	2.14439	-5.36189	13.10802
H	3.25642	-3.1573	12.38394
H	3.32711	-6.2436	12.11816
H	1.16884	-6.52651	7.93716
H	4.15536	-4.20969	13.48583
H	4.63145	-1.48813	5.25893
H	0.90597	-4.30736	5.87494
H	10.17382	-10.3678	5.99929
H	9.81826	-7.00573	4.84565
H	7.29225	-5.17481	5.13712
H	7.89434	-11.9578	4.68664
H	7.26929	-3.20463	3.73731
H	5.66544	-3.53625	4.09268
H	5.92712	-5.83823	4.18386
H	6.58263	-10.5206	3.31982
H	6.32273	-3.9829	2.5858
H	6.33674	-8.15384	2.50073
O	7.29416	-5.8484	1.88276
H	7.94926	-6.15599	1.22661
H	8.84013	-5.44782	3.23613

PEDOT:PSS + Epi			
O	-8.55916	-7.80519	0.97988
C	-8.5164	-6.50622	0.63252
C	-8.61	-6.05091	-0.71074
O	-8.77117	-6.89547	-1.76142

C	-9.23815	-8.19383	-1.33763
C	-8.43542	-8.70614	-0.1539
C	-8.52829	-4.66519	-0.82858
S	-8.35963	-3.90718	0.73416
C	-8.35543	-5.46447	1.57514
C	-8.14768	-5.59812	2.96469
C	-7.85577	-4.57404	3.89845
C	-7.62132	-5.05182	5.20009
C	-7.72704	-6.45885	5.31727
S	-8.11505	-7.18187	3.75244
O	-7.76076	-3.26495	3.56493
C	-7.0625	-2.50016	4.58136
C	-7.56913	-2.85629	5.96794
O	-7.33237	-4.25497	6.25024
C	-7.54875	-7.22971	6.48428
C	-7.66527	-8.63304	6.60633
C	-7.39896	-9.11329	7.91579
C	-7.08527	-8.09836	8.81941
S	-7.12594	-6.53131	8.05445
O	-7.43039	-10.4329	8.23616
C	-7.39739	-11.2758	7.06039
C	-8.36093	-10.7719	5.99957
O	-8.00403	-9.43149	5.57663
C	-6.63438	-8.27283	10.2272
C	-8.47377	-3.88698	-2.09572
O	-4.83627	-8.24179	4.99219
S	-4.00543	-8.82577	6.25205
O	-4.2021	-7.95672	7.43366
C	-2.30046	-8.68897	5.73107
C	-1.67962	-9.78558	5.1121
C	-0.36809	-9.64203	4.64594
C	0.32742	-8.41842	4.77515
C	-0.31287	-7.35198	5.44015
C	-1.62421	-7.47267	5.91625
C	1.71511	-8.26549	4.18668
C	1.7972	-8.49034	2.6611
C	1.34213	-7.31384	1.76177
C	1.47169	-7.74626	0.28193
C	1.06952	-6.71045	-0.78887
C	-0.42472	-6.53896	-0.97257
C	-1.03699	-5.27271	-0.86745
C	-2.42841	-5.13032	-0.94554
C	-3.22053	-6.28009	-1.08936
C	-2.64091	-7.54705	-1.26116
C	-1.24658	-7.65975	-1.22777
S	-5.00455	-6.147	-1.03639
O	-5.50776	-5.59126	-2.30964
C	-0.02968	-6.77849	2.14729
C	-1.20498	-7.55244	2.0209
C	-2.45102	-7.04643	2.40523
C	-2.52301	-5.74555	2.93804
C	-1.37415	-4.95862	3.08868
C	-0.13868	-5.48144	2.68453
S	-4.10397	-5.12502	3.50701
O	-5.13461	-5.61462	2.51129

O	-3.97897	-3.62135	3.59401
O	-4.3725	-5.71311	4.87626
O	-4.36488	-10.2597	6.32208
O	-5.24906	-4.99863	0.06615
O	-5.53103	-7.44374	-0.5464
N	-4.17569	-1.64245	1.74888
C	-5.51607	-1.89571	1.1589
C	-2.98495	-1.99985	0.83993
O	-3.33303	-1.90627	-0.49514
C	-1.77464	-1.15249	1.25008
C	-0.48549	-1.65565	0.63421
C	-0.21601	-1.50556	-0.74115
C	0.9407	-2.06674	-1.31144
C	1.83987	-2.78847	-0.51382
C	1.59577	-2.92042	0.87703
C	0.44305	-2.3527	1.43501
O	2.46562	-3.62153	1.65689
O	2.96918	-3.41272	-0.95807
H	-3.36414	-7.64776	2.28734
H	-1.45103	-3.95016	3.51938
H	-1.15002	-8.57165	1.61203
H	0.77259	-4.87562	2.79044
H	2.05507	-6.47594	1.92338
H	-7.02321	-2.28253	6.73884
H	-8.65702	-2.65072	6.0589
H	-5.97634	-2.72109	4.49948
H	-7.2525	-1.43419	4.35975
H	-2.22383	-10.7344	5.00042
H	-2.12893	-6.6259	6.40247
H	0.1191	-10.4993	4.15491
H	0.21687	-6.39528	5.56056
H	2.38165	-9.00973	4.67302
H	2.12447	-7.26676	4.44531
H	1.21426	-9.39864	2.39226
H	2.84913	-8.72336	2.39385
H	-8.81647	-9.68578	0.18716
H	-7.36115	-8.77621	-0.41491
H	-10.3184	-8.12862	-1.08029
H	-9.11425	-8.87269	-2.2016
H	-8.77224	-2.83041	-1.95739
H	-7.43383	-3.91538	-2.49022
H	-9.12892	-4.35311	-2.85877
H	-9.40382	-10.7544	6.38148
H	-6.96081	-7.43975	10.88011
H	-8.31389	-11.4056	5.09516
H	-7.68754	-12.2906	7.38972
H	-7.02118	-9.22551	10.63744
H	-5.52304	-8.31411	10.26306
H	-6.36142	-11.284	6.66263
H	-3.27628	-8.43561	-1.38574
H	-0.41733	-4.38056	-0.69357
H	-0.79324	-8.6557	-1.34991
H	1.50132	-7.04609	-1.75673
H	0.89505	-8.68337	0.12353
H	1.53847	-5.72827	-0.57181

H	-2.89493	-4.13715	-0.88037
H	2.53342	-8.02507	0.11534
H	-4.70708	-7.21381	4.94909
H	-5.16329	-5.34386	1.04802
H	3.19914	-3.92909	1.08154
H	0.27577	-2.46375	2.51621
H	-2.80742	-3.07528	1.04908
H	3.0682	-3.29883	-1.92389
H	-1.69421	-1.16164	2.35587
H	-4.07544	-2.26939	2.59883
H	1.14249	-1.95826	-2.38863
H	-1.98248	-0.10059	0.95069
H	-0.91274	-0.95479	-1.38936
H	-5.6564	-1.25906	0.27008
H	-5.58958	-2.9567	0.86935
H	-6.27943	-1.65872	1.91928
H	-3.25151	-0.97837	-0.79665
H	-4.10436	-0.6589	2.06044

PEDOT:PSS + 3MT			
O	2.8701	0.92733	3.51307
C	3.96707	0.54093	2.84194
C	5.15869	1.31892	2.76518
O	5.2799	2.52215	3.38107
C	4.32288	2.6597	4.45446
C	2.92538	2.30138	3.98018
C	4.06514	-0.71039	2.19776
S	5.65435	-0.84609	1.4241
C	6.17876	0.69875	2.05191
C	3.10229	-1.74516	2.17998
C	3.27702	-3.07286	1.73022
C	2.12657	-3.86959	1.84391
C	1.02197	-3.18645	2.41588
S	1.45661	-1.51425	2.7857
O	2.07764	-5.17024	1.4954
C	3.39535	-5.75022	1.31613
C	4.29609	-4.80679	0.53827
O	4.46242	-3.55222	1.25607
C	-0.21804	-3.74764	2.78013
C	-1.26836	-3.10782	3.4821
C	-2.32216	-3.9851	3.84735
C	-2.11286	-5.29969	3.42838
S	-0.61063	-5.46113	2.55812
O	-3.41793	-3.57331	4.53291
C	-3.56697	-2.13714	4.49319
C	-2.24883	-1.4415	4.78691
O	-1.24603	-1.80085	3.79622
C	-2.97073	-6.47153	3.74799
C	7.58509	1.16584	1.91174
O	-0.445	-3.22692	6.75437
S	-0.2973	-4.70367	6.76794
O	-1.51384	-5.54437	6.76147
C	0.71862	-5.13108	8.17853

C	1.58326	-6.23501	8.11763
C	2.36211	-6.54656	9.23946
C	2.29447	-5.77454	10.41765
C	1.37593	-4.7015	10.46263
C	0.59322	-4.36783	9.35167
C	3.20565	-6.05335	11.59603
C	4.151	-4.8917	11.97637
C	5.40418	-4.69669	11.08741
C	6.22436	-3.50202	11.62948
C	7.57345	-3.21676	10.93345
C	7.4597	-2.54164	9.58363
C	6.95977	-1.22323	9.47799
C	6.77373	-0.61364	8.23197
C	7.09066	-1.33877	7.06981
C	7.61738	-2.63598	7.14124
C	7.81276	-3.21686	8.39879
S	6.73988	-0.62028	5.4741
O	5.16791	-0.85954	5.28102
O	0.58013	-5.19563	5.51627
C	5.06246	-4.5755	9.61072
C	4.30587	-3.48763	9.12222
C	3.96346	-3.39354	7.77068
C	4.39851	-4.39654	6.88675
C	5.14989	-5.49027	7.33716
C	5.46964	-5.57019	8.69981
S	3.97592	-4.25921	5.15225
O	4.15273	-5.60005	4.52853
O	2.57347	-3.68694	5.10203
O	4.9548	-3.23829	4.55701
O	7.49924	-1.40083	4.44639
O	6.94539	0.83874	5.53477
H	3.34379	-2.56319	7.40274
H	5.45816	-6.27707	6.63347
H	3.96204	-2.70352	9.81329
H	6.03187	-6.44114	9.07092
H	6.03143	-5.60838	11.19761
H	5.30806	-5.23731	0.42358
H	3.87979	-4.58157	-0.46525
H	3.8137	-5.95863	2.32328
H	3.2518	-6.69386	0.75951
H	6.38312	0.41173	8.15935
H	7.85802	-3.18468	6.22146
H	6.69927	-0.66409	10.39034
H	8.22409	-4.23315	8.46416
H	8.1658	-2.56037	11.60533
H	8.14781	-4.16159	10.83379
H	5.59884	-2.58266	11.60754
H	6.4257	-3.69928	12.70327
H	-2.36069	-0.34373	4.73044
H	-1.86007	-1.74324	5.77981
H	-3.9554	-1.83765	3.49515
H	-4.31498	-1.87511	5.2643
H	-2.83242	-7.30552	3.03392
H	-2.7137	-6.83485	4.76791
H	-4.0383	-6.17368	3.76164

H	2.60594	2.96429	3.14871
H	8.02686	0.89252	0.93368
H	2.19573	2.37507	4.80742
H	4.3545	3.71669	4.77636
H	7.63663	2.26408	2.03694
H	8.20681	0.70333	2.70935
H	4.63821	2.00626	5.29529
H	-0.09205	-3.50845	9.3834
H	3.06714	-7.38987	9.18459
H	1.28931	-4.09418	11.37743
H	2.57195	-6.27212	12.48213
H	3.57403	-3.94166	12.00479
H	3.79723	-6.97218	11.40194
H	1.67679	-6.81731	7.18981
H	4.50633	-5.0564	13.01503
H	5.00056	-1.86809	4.98967
H	1.39522	-4.55943	5.35577
C	9.8153	-8.72322	5.57194
C	9.49829	-7.60953	6.4012
C	9.1955	-6.36591	5.82816
C	9.2141	-6.20121	4.42263
C	9.53096	-7.30709	3.61298
C	9.82779	-8.55889	4.18081
O	9.53821	-7.8997	7.73598
C	9.26518	-6.86614	8.6724
C	8.84946	-4.87087	3.79782
C	7.39022	-4.85689	3.33773
N	7.02154	-3.55202	2.71647
O	10.10836	-9.9226	6.1362
H	9.37211	-7.31363	9.67674
H	8.22756	-6.48474	8.55435
H	9.98038	-6.02133	8.56731
H	8.95968	-5.50554	6.47007
H	9.50533	-4.668	2.92497
H	9.01935	-4.04405	4.51902
H	6.68675	-5.0173	4.17446
H	7.20615	-5.6494	2.58679
H	7.14434	-2.74374	3.3846
H	6.0196	-3.53418	2.42406
H	9.55361	-7.19351	2.51778
H	10.08122	-9.42427	3.55046
H	10.05083	-9.80257	7.10994
H	7.5939	-3.35147	1.88063