

Supplementary Information for

**Fragmentation Study of Tryptophan-Derived Metabolites Induced by Electrospray Ionization
Mass Spectrometry for Highly Sensitive Analysis**

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Supplemental Figure

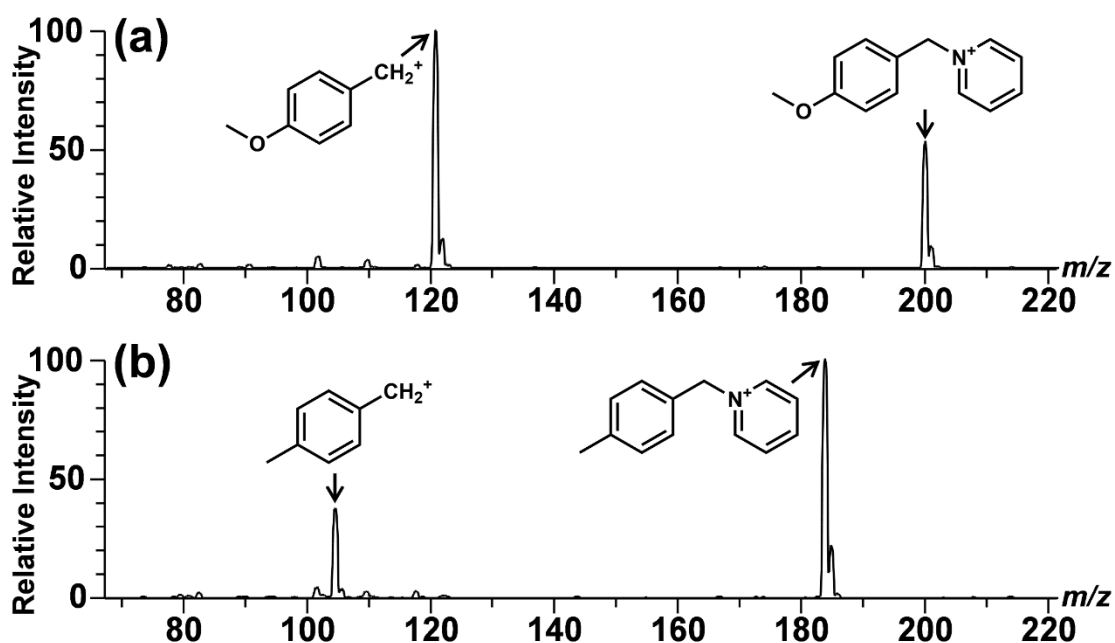


Figure S1. ESI-MS spectra of (a) 4-methoxybenzylpyridinium chloride and (b) 4-methylbenzylpyridinium chloride.

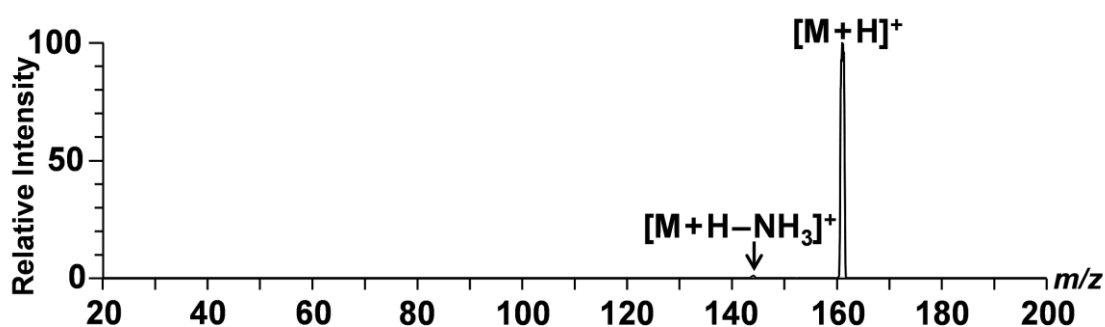


Figure S2. MS/MS spectra of the tryptamine. $[\text{M} + \text{H}]^+$ was used as the precursor ion and the collision energy was set to be 0 V.

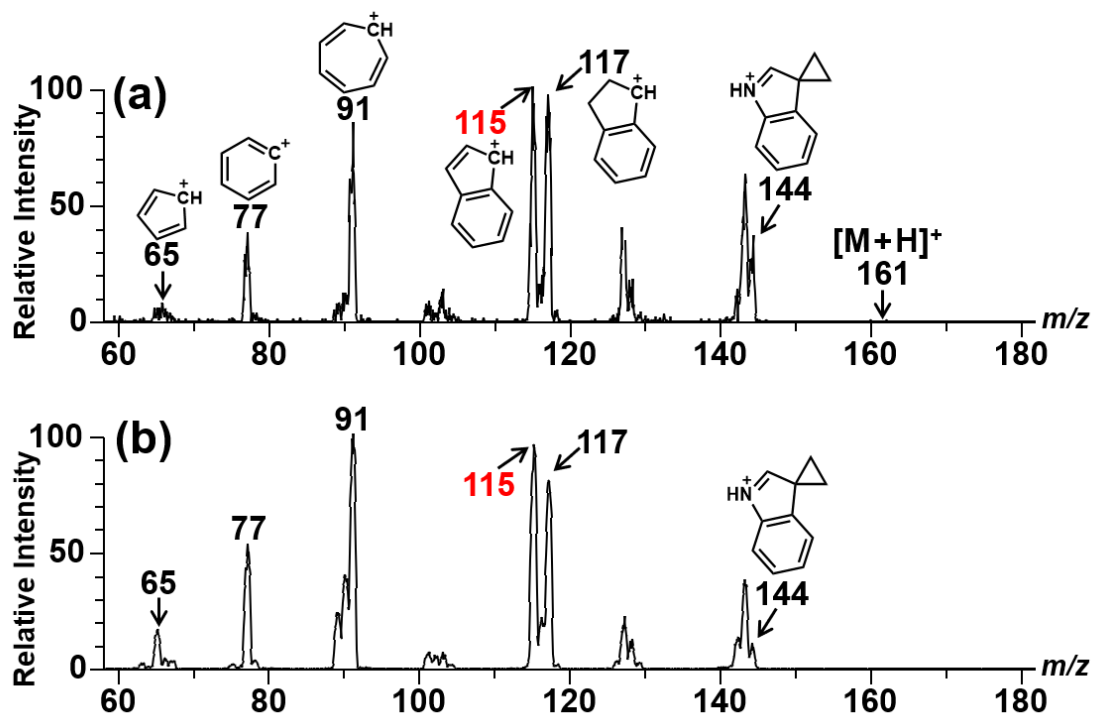


Figure S3. MS/MS spectra of the tryptamine. (a) $[M+H]^+$ and (b) $[M+H-NH_3]^+$ were used as the precursor ions. The collision energy was set to be 30 V.

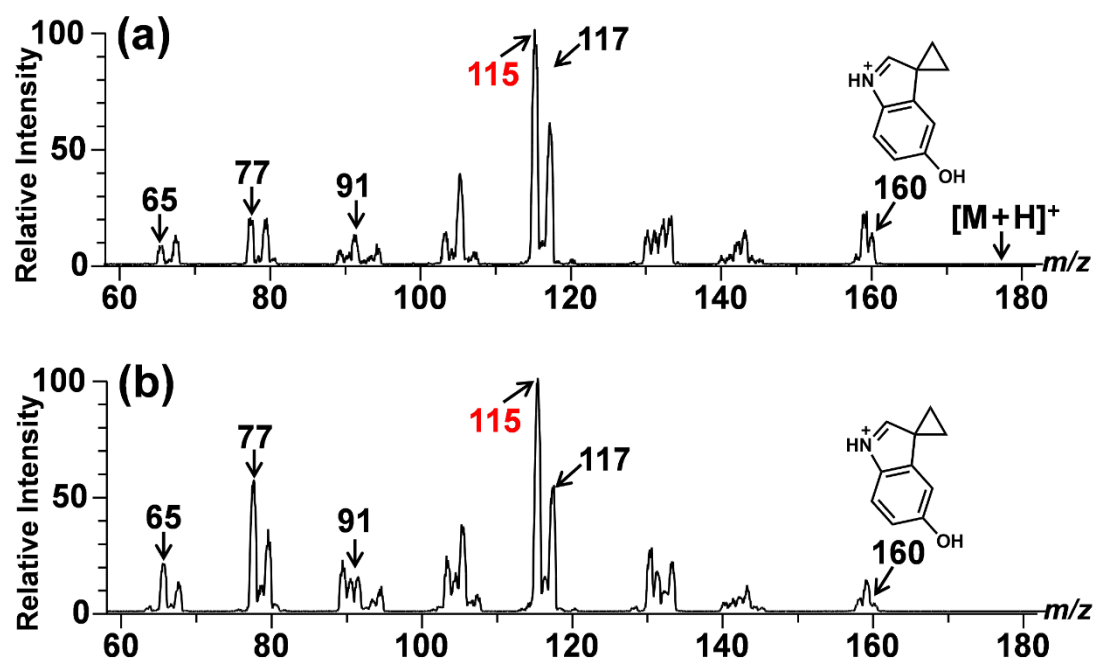


Figure S4. MS/MS spectra of the serotonin. (a) $[M+H]^+$ and (b) $[M+H-NH_3]^+$ were used as the precursor ions. The collision energy was set to be 30 V.

Table S1. Frequencies (cm⁻¹) of protonated tryptamine related compounds obtained by DFT calculation with M08-HX/6-311++G(d,p).

(a) Protonated tryptamine

R		TS ^{rot}		R'		TS ^{dissociation}	
72.9108	1169.5001	-96.5453	1166.0329	63.2195	1169.3641	-485.3549	1160.5916
93.7728	1250.2849	66.0475	1243.7070	78.1866	1255.5619	59.7971	1170.1139
125.9210	1259.2381	89.4379	1257.2438	102.0282	1262.1622	72.8301	1179.3052
215.6220	1284.3344	173.5338	1279.4647	197.3249	1291.8425	81.1920	1186.4674
217.6517	1324.7567	217.0849	1324.7093	217.2937	1319.5926	169.6186	1193.5836
230.9257	1339.0457	224.1215	1347.0197	222.9366	1337.7696	185.0170	1223.2138
269.7396	1369.9320	261.9947	1362.9061	242.8661	1356.8924	218.8439	1260.2244
362.1176	1377.7197	357.7650	1378.8496	305.5600	1377.0631	233.9409	1272.8879
434.2766	1393.6488	404.3894	1390.3330	385.9388	1388.1016	241.8911	1351.9070
451.6541	1401.2432	426.1905	1407.1799	428.8974	1401.0977	354.4548	1370.3403
463.2951	1467.3753	458.3761	1466.4860	463.4735	1466.1114	426.3091	1375.8252
550.4922	1469.4352	536.9158	1469.8599	516.2499	1466.2739	449.9329	1444.0414
558.2933	1488.3670	539.7199	1489.9086	548.5225	1485.8247	463.7347	1474.1492
575.8690	1493.3599	582.2706	1493.4748	584.1843	1493.3298	473.0806	1493.6213
596.1408	1505.9558	594.4314	1506.8239	599.3389	1504.1559	540.5953	1502.6034
656.5272	1540.3375	646.0193	1541.6964	643.2681	1543.4764	573.0078	1542.1663
709.6241	1609.6685	713.7097	1621.4630	748.6754	1618.0153	579.5190	1552.7982
761.9259	1635.1944	748.1501	1649.1167	759.7247	1649.1631	602.4954	1656.3293
771.4744	1642.6429	764.6879	1651.8334	762.1822	1652.8881	651.7869	1657.3829
772.4799	1645.1374	780.3174	1655.0608	777.0524	1656.8288	709.8876	1658.6096
827.5053	1693.5539	820.9864	1695.9012	784.2098	1695.4970	764.1992	1693.2287
865.9780	3038.9039	846.9500	2983.2336	844.0196	2991.2332	769.3809	3106.3986
868.5603	3080.4891	855.5005	3082.1086	860.5410	3064.4779	773.9096	3167.7747
878.0497	3106.1890	885.8584	3102.4113	889.7064	3083.4594	776.7072	3177.1243
892.6636	3133.5505	893.7914	3117.2339	891.6984	3148.0140	872.3960	3185.4236
920.4567	3146.5799	911.3536	3147.1826	908.3243	3149.9358	880.4277	3194.2969
966.4071	3192.2743	947.1226	3189.0935	958.0091	3188.8040	887.1553	3202.5769
1005.0667	3201.0759	998.3793	3198.6392	974.4357	3198.4000	962.5560	3213.6780
1014.0585	3212.2341	1002.8552	3209.6001	999.6281	3209.8564	970.5110	3241.2307
1038.6843	3247.1398	1037.3987	3250.7920	1038.9428	3250.7747	1009.2926	3289.7269
1055.8455	3316.8982	1054.4917	3420.6215	1062.4974	3424.7445	1032.5987	3497.6901
1098.1879	3473.7709	1113.6565	3505.0215	1110.1580	3510.6059	1041.6508	3625.2445
1115.2853	3538.1832	1122.9540	3521.5697	1123.8444	3521.3591	1055.5447	3627.5471
1127.1569	3691.1945	1126.2754	3696.6988	1135.1619	3697.1116	1086.8213	3665.5546

1159.2198		1158.4604		1159.9689		1130.3977	
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(b) Protonated serotonin

R		TS ^{rot}		R'		TS ^{dissociation}	
64.5115	1158.1925	-83.5256	1156.1962	56.0273	1157.4442	-495.2941	1130.6738
91.0527	1188.2646	67.1388	1184.0947	76.4736	1190.3737	54.7943	1158.9141
107.7462	1237.8460	89.3897	1230.6374	102.5509	1237.6740	79.0556	1177.5643
151.7991	1247.0016	152.3676	1242.8418	151.8828	1255.0095	93.6060	1183.2084
200.9723	1275.3887	162.8760	1275.5500	190.2149	1278.2413	147.8716	1189.3815
228.0574	1285.3513	214.0315	1287.1503	214.6137	1291.5250	178.7576	1196.7470
265.9054	1328.3287	258.2054	1336.9803	236.6690	1328.9394	192.5131	1221.3518
315.4908	1350.3455	309.0721	1347.8310	296.1178	1339.8501	214.9543	1240.2532
321.8191	1369.9780	332.4231	1364.4258	305.1120	1361.3009	232.7787	1268.9174
367.3161	1375.1185	359.2155	1377.3468	331.1364	1375.2839	316.6923	1304.7776
390.1277	1395.0034	367.6068	1391.3383	373.2469	1390.8963	352.4721	1356.9364
435.4261	1401.1044	426.2064	1407.7599	414.9319	1403.0974	377.0207	1377.7126
447.5392	1466.2052	436.4646	1467.9356	433.9300	1464.9110	390.8838	1386.3552
470.1431	1471.2596	453.4596	1474.4886	456.5082	1471.7758	437.5898	1443.7512
508.9612	1486.4544	499.5546	1491.9856	501.0776	1487.0522	453.1512	1478.4000
545.2075	1502.3914	516.1525	1502.0156	506.8653	1504.2265	472.4281	1494.0862
591.2328	1505.0429	592.8481	1509.2118	604.6784	1505.4085	477.0689	1524.4274
620.8308	1558.1038	611.1019	1563.2064	613.3083	1564.7364	513.5345	1544.4485
664.1401	1602.8612	659.9687	1619.0475	657.5931	1616.3361	576.5147	1567.6087
688.6984	1635.9988	695.7671	1650.7344	721.1205	1652.1022	593.9810	1657.3969
751.6001	1642.9707	748.2060	1654.8089	752.3826	1657.9709	630.6568	1657.8972
765.1615	1650.2897	776.7770	1658.7373	768.2735	1658.2599	659.3660	1661.5171
815.3506	1708.9020	795.6865	1714.6655	782.9239	1713.6874	687.2499	1709.9761
824.3799	3037.0269	813.8953	2979.9352	813.4058	2988.0416	746.7238	3104.2799
842.3832	3079.1631	820.0749	3082.8053	845.2704	3067.2874	771.1754	3163.2183
855.3692	3105.6167	849.4454	3103.5496	847.6562	3083.4653	775.1401	3181.1565
865.0233	3144.9861	860.5789	3147.8764	853.7486	3148.4774	820.0309	3183.7541
880.0672	3160.0545	892.2528	3154.4569	891.9677	3173.7277	841.4094	3194.4947
914.2728	3178.4742	911.1735	3178.4856	905.6325	3176.6349	866.9626	3205.6284
954.3455	3203.1031	950.3886	3203.2420	946.5599	3202.3042	878.3680	3242.8686
964.3770	3249.3362	966.7771	3249.4733	964.8636	3249.8397	952.1037	3283.5808
1014.9518	3324.2057	1003.5941	3420.1477	976.3237	3426.3635	958.7362	3498.4189
1046.6576	3467.9208	1047.6867	3504.2957	1055.9386	3512.6956	966.8708	3626.6643
1093.0551	3533.5991	1101.5640	3521.8240	1095.4025	3523.4251	1029.8679	3629.7377

1102.8195	3692.9062	1123.4343	3699.5296	1125.2314	3701.1281	1062.3521	3666.3808
1127.5784	3913.1132	1126.1512	3912.5052	1136.6356	3914.6812	1076.6929	3907.6307

(c) Protonated tryptophan

R		TS ^{rot}		R'		TS ^{dissociation}	
40.6609	1124.4995	-49.3579	1121.1992	26.0338	1123.4576	-476.9238	1083.1864
59.0081	1131.9166	45.4993	1149.8062	46.8656	1130.2974	52.1326	1128.6652
75.4944	1160.0454	55.0794	1153.8514	60.8627	1159.9727	65.4314	1137.0583
94.3685	1171.9376	80.7864	1165.2862	91.7567	1171.0600	75.6915	1161.4688
163.2994	1220.8769	122.1787	1215.7408	152.3751	1208.6328	106.9556	1167.6283
191.1427	1249.8947	148.8772	1228.5743	196.9172	1230.4677	116.6347	1172.1339
209.4132	1255.2989	212.6533	1258.7173	222.8478	1260.4579	161.6402	1192.1319
219.8296	1267.5121	220.8227	1271.8106	235.3277	1268.9297	171.3116	1203.3257
235.9971	1287.8860	273.0250	1307.3556	254.5895	1318.7535	197.7489	1215.2654
316.4675	1336.3938	324.3188	1334.1650	297.0299	1331.2333	235.1489	1258.1862
364.7615	1361.3311	357.2404	1364.9552	318.9876	1344.7636	244.7015	1274.4158
403.2777	1364.6067	381.2926	1372.5123	390.1338	1367.2579	304.8625	1319.1372
432.4813	1379.9485	426.0924	1383.7128	428.8180	1382.2941	351.2918	1354.6782
459.5869	1391.9066	452.6931	1388.8035	463.0344	1391.9945	428.0188	1371.1028
502.2979	1457.1878	499.2057	1447.2405	480.5886	1455.7284	460.1751	1377.0004
552.5084	1466.1296	527.0945	1467.5868	515.2472	1465.6456	484.6568	1437.5818
556.1883	1468.0243	541.5671	1473.9327	549.6926	1481.7090	498.9096	1474.8713
579.5461	1490.6387	579.1233	1489.7554	583.6676	1493.0661	523.7356	1493.7864
595.7365	1496.0286	593.4236	1492.6207	601.5415	1497.7282	544.4257	1504.5735
614.7219	1540.5138	599.6581	1539.4659	626.1941	1544.5949	575.8597	1537.1268
641.5627	1609.3219	635.7714	1619.9001	641.6242	1619.0936	581.2126	1550.4441
667.4687	1621.4250	665.5595	1622.4573	655.6154	1626.0918	610.8105	1647.1256
723.5754	1643.3837	721.8577	1649.5568	754.7149	1650.9020	620.6514	1651.8686
764.8326	1654.9122	752.6021	1656.4045	762.5387	1658.8651	641.8247	1659.6012
769.6979	1692.4968	762.9652	1693.0769	764.7836	1696.2838	672.8686	1695.5707
772.5444	1871.3195	768.7635	1865.9555	770.7329	1858.0974	715.8647	1869.8884
781.6103	3031.5830	779.5523	2999.6091	785.7329	2993.8478	764.0826	3105.5563
839.0220	3104.8751	840.3357	3068.6568	808.2234	3058.9365	770.0149	3173.6805
863.9819	3114.2516	853.2102	3103.4092	849.1060	3114.6972	772.7408	3185.9672
867.8570	3144.0270	870.1580	3123.3427	862.6790	3150.0249	777.5969	3194.7494
892.1841	3191.0599	888.8115	3190.2317	892.9152	3190.6978	852.6958	3204.4263
917.2430	3200.8999	906.8697	3199.8101	942.9014	3199.9299	875.6287	3211.2067
945.2288	3210.8247	944.5550	3211.0455	952.1079	3211.8194	887.3459	3214.0910

966.6714	3251.8295	949.7218	3256.7107	960.4770	3248.2970	908.9965	3247.7507
1006.2021	3283.4977	997.2095	3341.2746	999.2906	3306.9131	971.8258	3489.3711
1039.2107	3386.8693	1037.2354	3465.6430	1026.3497	3472.1288	986.3551	3620.2746
1060.1550	3517.5927	1053.9117	3516.2715	1039.5521	3526.0844	1002.9989	3630.0407
1074.9993	3686.8222	1085.9029	3697.2505	1071.4180	3694.3880	1010.9729	3662.6952
1103.9414	3817.1288	1102.9255	3813.3801	1104.8888	3814.3570	1043.8119	3830.6174

(d) Protonated 5-hydroxytryptophan

R		TS ^{rot}		R'		TS ^{dissociation}	
37.9980	1125.2626	-44.5017	1123.5789	20.7470	1124.6048	-480.7369	1070.0509
56.4590	1129.9288	43.1567	1150.5851	43.4598	1129.7491	46.7318	1127.7463
73.5691	1159.6249	54.8772	1158.7222	59.1037	1158.8782	63.7326	1138.5442
88.0091	1188.4920	79.5803	1184.1263	85.5905	1190.8627	71.7180	1160.3684
147.7930	1221.0020	124.5489	1215.1300	143.5991	1206.9895	100.6347	1169.0212
158.7460	1239.4622	147.0298	1228.0873	160.0594	1229.2129	136.8695	1187.5453
184.4578	1248.7189	156.6661	1234.4579	198.1488	1239.2801	161.0827	1191.9219
200.4165	1258.4923	211.4536	1272.2745	220.2429	1264.9414	163.9854	1204.8747
228.9752	1286.0825	263.6905	1286.4152	248.2095	1285.8960	177.4745	1215.5403
305.4728	1289.2683	312.0999	1312.8433	284.7925	1324.6435	190.3338	1239.5478
314.5241	1348.2696	324.4461	1345.7102	291.7358	1335.5823	244.4069	1270.5427
319.7258	1360.5239	330.5058	1365.3180	322.3366	1349.6348	290.6150	1295.2890
366.5654	1367.5595	359.9307	1373.0359	339.0502	1368.1613	319.0654	1328.2902
388.1759	1378.6632	369.5472	1385.2676	375.6556	1380.1620	360.2087	1355.9582
418.9953	1393.8484	410.9388	1394.6586	413.2767	1395.3145	380.0451	1379.2237
434.3732	1457.3131	433.5390	1446.3016	434.6869	1455.0887	391.1572	1382.9109
455.3330	1466.9860	454.7519	1473.1822	454.1801	1470.5954	437.1154	1437.8451
495.7986	1471.4349	497.3830	1475.8957	484.6933	1480.7954	452.6953	1476.6959
516.8489	1494.3973	501.6175	1489.8093	497.0009	1496.7486	484.2710	1492.8098
537.4912	1504.7995	513.5674	1505.5568	508.7006	1505.3116	502.2971	1525.6285
596.1508	1556.8019	591.7536	1564.0685	606.8208	1565.5309	515.0609	1537.3843
612.5751	1603.7754	603.3638	1620.1590	612.9068	1616.9319	532.1897	1565.4645
619.2441	1621.1754	613.2751	1625.0879	624.4022	1624.6678	581.5404	1646.6431
647.7112	1651.2253	645.1374	1656.4589	649.3302	1658.0478	600.4237	1653.6406
667.0026	1655.7739	668.2517	1660.8807	660.7609	1660.7206	627.3162	1662.3628
709.1184	1706.5647	708.6573	1714.3956	725.8309	1714.1635	633.0857	1707.1930
752.8424	1872.3029	752.4797	1865.4539	753.9637	1856.9288	645.3135	1870.9248
758.6903	3030.6663	753.4763	2995.4282	766.7681	2989.6304	668.6423	3103.0574
779.6286	3102.0268	779.4039	3070.0584	786.3419	3059.8865	691.9852	3180.6566

818.8199	3112.4453	812.8956	3104.0709	807.8226	3111.6917	746.5849	3183.5340
840.3849	3164.0422	825.6784	3156.9674	815.5552	3174.1936	770.8742	3193.0245
847.2273	3176.7030	841.3381	3178.1690	849.4497	3174.7993	776.5640	3206.0457
851.7408	3202.9078	851.1794	3202.2330	850.5657	3202.9458	819.6390	3208.0742
863.5759	3252.7134	871.5792	3255.6666	854.7544	3248.3353	836.3744	3245.3137
914.3554	3285.7485	906.6261	3329.6867	939.9893	3310.9435	856.3121	3489.6366
945.7145	3386.0288	944.9658	3467.0975	947.0965	3472.4917	865.0157	3622.6073
954.6317	3517.7400	952.1985	3518.3934	950.4121	3525.8148	904.1570	3629.8953
965.8961	3691.9430	966.9701	3699.7512	966.6686	3698.0943	950.8357	3664.3711
1055.5659	3815.4378	1053.4722	3816.0933	1028.7827	3812.0548	960.8362	3828.9233
1071.5463	3908.3547	1076.9377	3911.5648	1064.5991	3910.7973	985.9917	3905.3834
1093.4805		1093.3383		1096.1033		1006.8035	

(e) Protonated *N*- ω -methyl-tryptamine

R		TS ^{rot}		R'		TS ^{dissociation}	
46.2487	1171.7983	-70.5532	1166.0779	46.7516	1174.6405	-451.0116	1161.6435
81.6769	1236.3542	65.3494	1243.0331	64.6980	1250.8935	31.2569	1171.7827
127.2949	1259.3623	79.7521	1257.3369	75.9498	1261.6763	57.5782	1172.6027
138.0762	1278.4797	121.6332	1278.7583	125.3988	1280.2407	78.8879	1184.6486
198.8892	1298.3042	175.8291	1307.5997	188.7820	1312.7556	116.6116	1191.0553
222.4028	1330.7982	210.1196	1324.3618	222.3662	1326.7320	168.7801	1216.0251
233.1597	1362.9168	224.0987	1352.9089	229.4573	1347.6565	186.1122	1258.5505
258.7440	1366.4954	225.2354	1371.4151	243.2203	1371.0516	207.9877	1273.8551
346.1334	1380.9307	317.0285	1380.1767	285.6366	1380.8072	237.4626	1335.3696
407.6136	1392.5269	409.6919	1389.9824	377.3872	1390.0088	245.8102	1351.2617
432.9591	1411.1656	427.7711	1414.5162	428.5152	1412.1283	274.8917	1372.6264
455.8343	1431.8875	436.3692	1432.8263	434.9715	1433.4647	350.2776	1376.1899
466.7842	1446.4109	456.6868	1448.8480	466.7793	1449.7135	428.4773	1441.0935
551.4779	1467.3356	521.2497	1463.8358	512.5603	1465.9784	459.1019	1450.4447
560.7448	1471.2610	538.6535	1466.7556	550.3715	1467.5353	477.4875	1476.8162
575.1460	1482.1877	581.8106	1482.7644	584.8979	1485.6114	540.4070	1485.9138
597.5065	1487.7538	592.3350	1491.2088	600.2195	1491.1575	572.1471	1494.0857
656.3969	1491.4173	646.7183	1491.9436	642.8148	1493.9914	579.2873	1505.1696
709.1468	1494.6968	713.3473	1494.9019	742.3285	1497.1434	604.3993	1508.7305
764.3866	1540.8953	749.2038	1541.2453	760.3995	1543.6699	658.4867	1540.0379
769.3382	1609.2128	767.1906	1621.7266	766.2781	1619.1895	707.3438	1555.3283
771.4779	1643.1641	777.7859	1643.4451	779.1267	1644.5438	764.9443	1656.9922
813.3571	1648.2292	813.2979	1648.5528	797.7739	1650.1244	771.6117	1659.5809

829.9533	1693.3125	846.3386	1696.6868	820.8918	1696.4918	773.8038	1695.8973
857.8513	3043.6386	849.5078	2988.9029	848.1583	2981.5952	778.9079	3030.4072
866.9824	3071.0587	853.3513	3072.9702	860.8300	3070.1305	877.6475	3104.8847
891.4272	3075.8377	890.2701	3074.0009	883.5591	3073.3287	884.8549	3109.3298
940.2633	3103.6981	912.0760	3102.6190	895.4054	3084.0904	887.9262	3122.6341
961.5639	3136.9771	947.6049	3122.1220	957.7277	3133.4982	944.9011	3170.2753
964.3785	3162.2331	971.5777	3135.7156	999.3728	3148.4559	959.6799	3175.4260
1004.4122	3177.8433	996.5134	3176.3079	1003.8788	3173.3408	974.8229	3191.3340
1033.0726	3182.5525	1021.2629	3180.9124	1032.2984	3186.0261	975.1392	3193.5411
1040.4985	3188.9052	1038.9936	3189.2932	1039.7629	3188.3498	1012.9236	3202.4904
1051.9515	3197.8169	1055.2373	3198.4311	1050.1440	3198.0170	1023.3923	3212.7581
1087.3896	3209.5592	1087.8922	3211.4157	1090.8929	3209.4925	1032.9188	3241.3630
1124.5381	3249.6819	1122.5932	3254.1246	1123.9661	3250.0727	1043.5857	3292.3642
1139.0739	3286.3593	1134.3869	3438.3659	1129.6155	3449.7417	1078.8234	3532.5365
1150.0754	3510.4352	1159.0224	3498.9566	1159.4040	3507.1176	1083.3899	3614.1635
1161.4318	3690.4487	1165.5350	3696.0098	1166.8410	3698.4712	1130.3810	3660.9042

(f) Protonated melatonin

R		TS ^{rot}		R'		TS ^{dissociation}	
36.1961	1165.9401	-24.7264	1166.4821	19.6667	1165.1911	-513.8150	1135.5786
50.8362	1172.4239	34.4685	1173.1434	44.3769	1174.2986	21.5041	1160.2403
83.4752	1201.4228	65.6331	1202.6642	65.0135	1201.9317	27.3521	1165.6182
90.9185	1208.4485	80.4617	1211.0002	77.8206	1207.6442	39.4438	1172.8847
116.4087	1232.9726	92.2219	1229.7702	89.5019	1217.0866	70.7946	1179.2867
139.4093	1257.4047	122.4517	1234.4089	113.0763	1227.0733	73.1023	1190.9692
151.5029	1266.0461	136.1885	1267.9880	133.6345	1268.1177	86.9639	1203.5524
192.1390	1282.6290	166.6573	1284.0369	161.0198	1282.5147	131.0987	1216.1192
199.8218	1289.3127	179.6826	1293.3062	189.7828	1304.1860	157.6669	1234.0626
220.7610	1333.4149	225.0533	1330.0821	218.8212	1322.4387	181.4100	1259.1686
258.5568	1355.3772	260.2743	1339.2538	264.0527	1338.9709	204.7503	1266.7892
265.1968	1365.0557	270.3885	1362.9377	268.2353	1359.4757	217.9082	1307.2422
304.4785	1375.1832	300.6032	1369.5606	315.6251	1367.0125	233.4548	1336.9807
338.2518	1380.8917	331.6568	1383.8445	331.1994	1382.3423	263.1313	1368.3709
383.1410	1394.4613	363.3444	1389.6379	357.0908	1388.7654	270.9474	1381.4683
400.4678	1410.9520	395.4733	1412.3686	398.6061	1410.0897	321.8803	1391.0249
421.0019	1445.2378	432.4630	1446.9785	423.9772	1447.9933	378.6382	1443.8745
439.6100	1463.6842	443.8789	1468.1381	443.6229	1467.7351	404.3976	1457.0598
450.4183	1466.7528	453.9562	1471.5103	451.5919	1470.4498	437.1477	1458.6198

485.7169	1468.6655	462.2996	1473.9726	465.3283	1475.1742	444.8006	1469.2604
514.0200	1474.8665	500.7973	1478.2691	491.4743	1478.7644	450.1699	1476.9609
550.3026	1487.5159	537.8957	1489.5799	541.3378	1487.5864	511.0297	1486.2143
584.1974	1492.0920	583.4428	1494.7697	595.3925	1496.5878	539.7385	1488.5807
600.5226	1496.7033	592.5942	1498.2040	604.3809	1502.6593	577.8347	1495.1839
604.2144	1503.7748	613.5802	1504.6108	615.3788	1505.2324	589.9692	1495.4355
620.2004	1543.5184	632.3179	1536.5474	642.1528	1537.1762	601.7822	1526.4136
669.0012	1598.4803	634.4367	1606.9678	661.4893	1602.3682	608.4640	1538.7067
674.7241	1606.5290	677.1936	1616.5584	678.9035	1615.9541	630.8826	1553.2316
687.5414	1648.0271	697.5256	1652.6405	709.1511	1653.6000	661.0580	1656.9178
713.5186	1704.7736	742.0606	1702.2570	722.1671	1702.6648	686.2993	1707.1226
757.8519	1715.6868	765.7565	1715.7304	767.1743	1718.0115	751.3426	1746.2457
768.0219	3013.2870	779.6615	3015.6485	781.7623	3015.9466	772.2011	3018.0560
822.8782	3043.2047	794.6637	3034.8981	786.6892	3023.2957	775.5488	3059.4636
823.6155	3044.4537	825.4028	3059.2270	823.4369	3056.0616	816.8760	3093.1391
850.7976	3053.6260	839.2456	3070.1780	837.7468	3057.9661	822.7866	3101.4601
865.9634	3087.1445	862.6543	3090.3363	859.1494	3090.2828	824.8825	3135.8511
870.7436	3102.1832	896.1902	3105.8515	886.3134	3101.2740	862.2828	3164.6065
899.6451	3121.3012	931.1006	3125.0172	920.9943	3127.9245	880.1183	3165.8741
942.1054	3127.6281	948.6144	3135.7788	948.8885	3134.8628	899.9860	3170.1566
960.9294	3160.0095	960.9450	3152.2241	959.6895	3154.1680	937.9542	3182.0953
961.5473	3169.8185	995.0722	3158.9430	1012.1197	3159.3534	955.8260	3187.8408
1030.1319	3179.8088	1021.7875	3171.1384	1020.0805	3169.0142	960.7856	3199.3637
1052.9981	3195.4379	1038.1451	3194.8128	1035.7424	3193.6408	1023.0136	3228.6023
1059.2784	3223.0533	1060.9338	3225.7252	1062.9206	3226.5892	1030.7796	3242.7079
1064.7847	3242.6676	1065.0403	3252.3593	1065.7015	3252.8308	1048.9807	3284.8701
1087.3735	3588.9206	1086.7116	3542.5089	1080.4541	3593.2989	1064.0889	3592.2180
1108.6646	3626.8632	1110.3061	3615.2777	1112.5113	3621.5958	1068.5031	3666.9842
1123.8449	3690.2541	1123.9011	3699.5471	1123.9932	3702.1828	1096.6396	3874.9814

Table S2. Cartesian coordinates of the geometry for protonated tryptamine related compounds optimized by DFT calculation with M08-HX/6-311++G(d,p).

(a) Protonated tryptamine

R

6	-3.37703054	1.47929642	2.93705593
1	-4.42010561	3.24293319	3.23805082
1	-4.78329899	0.05405702	2.37889602
6	-2.17689538	0.73454105	5.46574172
1	-0.98940584	2.26009154	6.20172574
1	-3.55917732	0.18257681	6.90180845
7	-0.43291444	-1.48404562	5.04871238

1	-1.41544340	-3.07666570	4.54744283
1	0.74233288	-1.08158639	3.53638790
1	0.63577274	-1.89589417	6.60596705
6	-1.41011085	1.75846226	0.91716518
6	-0.07537187	3.88499047	0.25257034
6	-0.43925683	-0.27126400	-0.62350059
7	1.65013868	3.29257612	-1.57622938
1	-0.25746525	5.80706462	0.93596646
6	-1.05170324	-2.85121256	-0.87785135
6	1.49150680	0.76732039	-2.15269315
1	2.82420333	4.54057410	-2.41047213
6	0.29949137	-4.30087551	-2.57852132
1	-2.63430032	-3.68028112	0.15603788
6	2.85628776	-0.69745722	-3.88007996
6	2.24394071	-3.22992625	-4.05478130
1	-0.16361719	-6.28758922	-2.82301687
1	4.33312586	0.12183068	-5.05115269
1	3.26210568	-4.42210201	-5.38228354

TS^{rot}

6	-1.85204586	1.77708834	3.45658899
1	-2.64848943	3.57069437	4.11392302
1	-3.36745328	0.35784333	3.67639413
6	0.42353040	1.03642018	5.12716040
1	2.08276845	0.60021551	3.97105269
1	0.92470134	2.48372690	6.51517326
7	-0.13701268	-1.34621339	6.61397880
1	-1.69271390	-1.12505109	7.74639844
1	-0.50275297	-2.80933451	5.39424400
1	1.35063844	-1.87059718	7.73743768
6	-1.09155719	1.93894132	0.74232432
6	-0.85454577	4.04496511	-0.74625164
6	-0.28815864	-0.17563160	-0.75841265
7	0.04585178	3.36135684	-3.07221067
1	-1.26920563	6.00333808	-0.31542886
6	-0.13440123	-2.78976039	-0.32654889
6	0.42523868	0.79273316	-3.14301827
1	0.36567736	4.56317453	-4.51449342
6	0.75371393	-4.34224062	-2.23089228
1	-0.80150225	-3.63006727	1.43924081
6	1.31938290	-0.76709433	-5.07812385
6	1.48460827	-3.32798823	-4.58185975
1	0.86556666	-6.37262753	-1.93758187
1	1.86019678	-0.00529571	-6.90868692
1	2.17111569	-4.59454010	-6.04635414

R'

6	-1.63875085	0.89939344	3.71609387
1	-2.29288221	2.60045449	4.71226780
1	-3.22474984	-0.45402354	3.67610519
6	0.59783458	-0.27710853	5.10640222
1	1.36205319	-1.90455689	4.08093339
1	2.11712932	1.08962380	5.42099246
7	-0.21537577	-1.23153286	7.68825929
1	-0.91834714	0.21509648	8.76890250
1	-1.62200725	-2.55326735	7.51437216
1	1.24618909	-2.04450623	8.66398039
6	-0.84460154	1.53127060	1.07892678

6	-0.43821895	3.87807677	0.05749534
6	-0.27757256	-0.28382708	-0.86427308
7	0.34508417	3.62648899	-2.39118486
1	-0.67369812	5.73032599	0.89853766
6	-0.36740276	-2.93461859	-0.99663028
6	0.46758781	1.10692391	-3.01726372
1	0.74022165	5.07336089	-3.56441644
6	0.30446762	-4.10421351	-3.23222822
1	-0.99735172	-4.06292000	0.61013691
6	1.14939594	-0.06958420	-5.28318131
6	1.06325572	-2.67917110	-5.35159693
1	0.23700999	-6.15259831	-3.37692679
1	1.71717751	1.01965135	-6.93090395
1	1.57892720	-3.65788064	-7.08288895

TS_{dissociation}

6	2.66101367	0.09181284	3.28419215
1	3.69949837	-1.25194868	4.45024149
1	3.87131686	1.57246735	2.51290691
6	0.20548764	0.89680403	4.23715639
1	-0.78701792	2.44489756	3.32535630
1	-0.88338167	-0.35316567	5.44389852
7	0.84859815	3.37180002	7.54095587
1	1.79163601	2.44961843	8.93882396
1	1.90266384	4.90021428	7.04447183
1	-0.79775523	4.02537524	8.28841638
6	1.02109945	-1.09837099	1.27549918
6	-0.12742364	-3.47515241	1.37228117
6	0.35398444	-0.01772561	-1.15290799
7	-1.38523515	-3.88695314	-0.78762909
1	-0.07963404	-4.87998263	2.86437945
6	0.91270565	2.27041576	-2.35330477
6	-1.14737961	-1.82120432	-2.39745065
1	-2.37095977	-5.47399775	-1.18401545
6	-0.05970476	2.67740424	-4.74818766
1	2.09348903	3.69262965	-1.44863408
6	-2.13062689	-1.43238584	-4.81020243
6	-1.56304499	0.84877441	-5.95866288
1	0.35203081	4.43688812	-5.72541358
1	-3.28170181	-2.84908389	-5.75330724
1	-2.28655895	1.23314676	-7.84239919

(b) Protonated serotonin

R

6	-3.76964355	1.68090803	2.96992426
1	-4.82223371	3.40672979	3.42013787
1	-5.10405668	0.41558100	2.00060670
6	-2.93765843	0.49015786	5.47598713
1	-1.84428801	1.83214422	6.60869874
1	-4.51203673	-0.23964968	6.60141019
7	-1.18121193	-1.69093947	4.93490210
1	-2.09973123	-3.14607866	4.04402108
1	0.19907216	-1.09033127	3.68499403
1	-0.34648902	-2.38898691	6.53238062
6	-1.54588307	2.21823922	1.29878440
6	-0.13135562	4.39594635	1.13418502
6	-0.39305738	0.42419803	-0.39433492
7	1.81002232	4.04929190	-0.52432279

1	-0.39797459	6.19682118	2.07248553
6	-0.98536147	-2.08029562	-1.07441903
6	1.71878382	1.63430615	-1.48775843
1	3.08236515	5.38327100	-1.00552460
6	0.56763739	-3.30687504	-2.78410031
1	-2.69246169	-3.03948005	-0.43145023
6	3.27665359	0.39218934	-3.22266223
6	2.69222508	-2.07478387	-3.83773814
1	4.89911419	1.32214504	-4.07461246
1	3.87312001	-3.09193568	-5.18151610
8	-0.03938459	-5.71408551	-3.40511097
1	1.03927170	-6.34570226	-4.71887774

TS^{rot}

6	-1.00570151	1.51781060	3.86257161
1	-1.65662166	3.27775152	4.73551353
1	-2.64155109	0.22002314	3.88632873
6	1.16415337	0.37004005	5.44220860
1	2.78627669	-0.09614435	4.24582167
1	1.78802742	1.59614945	6.98482397
7	0.35662501	-2.09835687	6.64905004
1	-1.19298327	-1.86000385	7.78605934
1	-0.11700206	-3.38005537	5.27188708
1	1.76872246	-2.88043437	7.71870928
6	-0.17702633	1.94246882	1.19728570
6	0.22570519	4.17681315	-0.05800824
6	0.51885198	-0.04706660	-0.50587904
7	1.12741095	3.68697128	-2.42591096
1	-0.07036262	6.10161819	0.57460735
6	0.49866186	-2.69163310	-0.31291907
6	1.34316246	1.11280425	-2.76002181
1	1.55591939	5.01106249	-3.72505400
6	1.33445809	-4.10711957	-2.34594383
1	-0.26968281	-3.70056057	1.31186572
6	2.17497893	-0.31497569	-4.81692766
6	2.17701266	-2.91715584	-4.57921434
1	2.80739552	0.56938767	-6.56075031
1	2.82275662	-4.07905878	-6.15020032
8	1.29381417	-6.66106960	-2.09882707
1	1.79258580	-7.47030034	-3.64264960

R'

6	-1.69769963	1.21515398	4.06073012
1	-2.28497171	2.83243487	5.22312263
1	-3.35561402	-0.03082906	3.83568105
6	0.42816626	-0.23995358	5.36003838
1	1.17035160	-1.74432840	4.14714499
1	1.98569515	0.99891236	5.92050696
7	-0.53461900	-1.50703278	7.74856538
1	-1.23477960	-0.19808397	8.99368067
1	-1.97673369	-2.73314965	7.33213692
1	0.85150729	-2.50873706	8.65635192
6	-0.79497453	2.07007438	1.52415499
6	-0.24172800	4.48096960	0.73756794
6	-0.26375025	0.41804045	-0.56404632
7	0.59809929	4.42025186	-1.69883976
1	-0.40788994	6.25530834	1.74641970
6	-0.48372589	-2.20221835	-0.91179792

6	0.61310011	1.95896353	-2.55457061
1	1.09742812	5.94798075	-2.71899529
6	0.19941968	-3.21116843	-3.22368260
1	-1.22151710	-3.46484527	0.53710423
6	1.29741037	0.93782126	-4.88985688
6	1.09056669	-1.64695288	-5.19404736
1	1.97109272	2.11905507	-6.43050503
1	1.61398915	-2.50124149	-6.99191756
8	-0.02377634	-5.75107964	-3.51676411
1	0.40795217	-6.24579054	-5.20621939

TS_{dissociation}

6	3.02379538	0.42641944	3.47406277
1	4.22523681	-0.63875086	4.76491471
1	4.09244580	1.75143327	2.30952832
6	0.64255330	1.35231421	4.50574925
1	-0.50113761	2.65969909	3.41146305
1	-0.27167711	0.33449666	6.03330156
7	1.49277590	4.43960125	7.15329546
1	2.63769401	3.85240481	8.58081715
1	2.39378552	5.86990839	6.23886258
1	-0.09670278	5.17268644	7.94856579
6	1.24758601	-1.17098377	1.91715961
6	0.26071562	-3.54310972	2.54821693
6	0.26890229	-0.56289245	-0.56777779
7	-1.18759893	-4.37805251	0.64986605
1	0.55240631	-4.66117347	4.24100610
6	0.57014842	1.51305669	-2.16322500
6	-1.24462578	-2.61688578	-1.30456727
1	-2.10798247	-6.05113029	0.64390981
6	-0.67137169	1.47400993	-4.47523799
1	1.74696652	3.13002837	-1.68661694
6	-2.48851864	-2.67018734	-3.62412260
6	-2.18593578	-0.60210755	-5.19104220
1	-3.65280481	-4.26197536	-4.19982686
1	-3.12665388	-0.57202530	-7.02075931
8	-0.35760362	3.49734702	-5.99451989
1	-1.23875936	3.29086117	-7.56624986

(c) Protonated tryptophan

R

6	2.78254606	-1.02374314	0.70925057
1	3.96666802	-2.62457637	1.27753900
1	3.87832694	0.07371197	-0.67688588
6	2.35440841	0.60841518	3.09508864
1	1.58533197	-0.55487010	4.62367219
7	0.49371728	2.67675665	2.53971928
1	1.48032665	4.22984268	1.89031022
1	-0.79546575	2.08850933	1.18607047
1	-0.46512585	3.24436711	4.12018957
6	0.32773155	-1.85529274	-0.41887178
6	-1.01589748	-4.02289860	0.06735946
6	-1.16681231	-0.39519479	-2.17089554
7	-3.23278738	-3.98304583	-1.25597356
1	-0.52994326	-5.62352999	1.24894221
6	-0.80678485	1.93742043	-3.40784911
6	-3.39811434	-1.79181425	-2.63678982

1	-4.52163250	-5.38708388	-1.26093928
6	-2.68089560	2.80971716	-5.00455416
1	0.94650781	3.00331624	-3.18873610
6	-5.28997125	-0.91321263	-4.26039066
6	-4.90296605	1.39705431	-5.41565917
1	-6.99470175	-2.00556935	-4.61275885
1	-6.33294886	2.13398964	-6.69330578
6	4.77695201	1.93266014	3.91067593
8	5.07985325	4.16092762	3.62246039
8	6.43111555	0.31890846	4.83270995
1	7.98901895	1.17475521	5.26537331
1	-2.42990832	4.59244828	-5.99432991

TS^{rot}

6	-0.88516369	2.45541642	2.27230760
1	-0.52869196	4.37539407	2.95975177
1	-2.89216106	2.04119730	2.65359095
6	0.77374233	0.54986574	3.76389500
1	1.82715061	-0.63486709	2.42373632
7	-0.76468015	-1.23368322	5.36702974
1	-2.30969585	-0.34051413	6.12261207
1	-1.38513833	-2.74949925	4.33540781
1	0.33944279	-1.82703310	6.86697264
6	-0.36961720	2.24735422	-0.49183262
6	0.86877786	3.90806958	-2.04541921
6	-0.94151293	0.05205858	-1.98058341
7	1.09047781	2.87415588	-4.40517443
1	1.62138733	5.76737982	-1.63576159
6	-2.19072380	-2.23469799	-1.47568169
6	0.01517929	0.50839389	-4.43102276
1	1.90284388	3.73227550	-5.89876729
6	-2.41292165	-4.00246779	-3.38773194
1	-3.08580007	-2.58308241	0.35344725
6	-0.21297027	-1.26774001	-6.37245021
6	-1.41876595	-3.51837917	-5.80976041
1	0.52064478	-0.90113633	-8.25690249
1	-1.62788406	-4.94041193	-7.27755093
6	2.66835585	1.72550048	5.59394571
8	2.90183846	0.96712206	7.71949796
8	3.95911124	3.56513650	4.53378958
1	5.19105800	4.23560621	5.70845721
1	-3.39368012	-5.77479945	-3.04410979

R'

6	2.76842370	1.35866587	1.87282743
1	4.54632972	0.50506374	2.47488401
1	2.86741907	3.40969982	1.68616552
6	0.54021908	0.35923470	3.15173810
1	-1.30663068	1.21149198	2.85602049
7	0.52952798	1.72307904	6.99711744
1	2.06405962	1.10379885	7.97817805
1	0.55325915	3.64453082	6.99753855
1	-1.05727812	1.13235246	7.90993494
6	1.59340253	0.11626666	-0.40557927
6	2.01844221	-2.34732017	-1.28511182
6	-0.10438239	1.29605106	-2.20651508
7	0.74301353	-2.68979600	-3.44051636
1	3.17421978	-3.82475800	-0.45939550

6	-1.20081175	3.69292498	-2.38667598
6	-0.59222268	-0.51425838	-4.08724445
1	0.74119703	-4.31341186	-4.44775588
6	-2.76177368	4.18728873	-4.43059976
1	-0.83316933	5.14698719	-0.97685500
6	-2.15422331	-0.03768688	-6.15080262
6	-3.23303108	2.34459338	-6.28523263
1	-2.50759196	-1.45587810	-7.59487810
1	-4.46224536	2.80380968	-7.86563557
6	0.65305257	-2.30187646	4.16411541
8	2.55465473	-3.52445760	4.24411025
8	-1.58954731	-3.04324888	5.02304736
1	-1.46026305	-4.74354931	5.67967981
1	-3.63301814	6.03825490	-4.61807028

TS_{dissociation}

6	-1.49937383	1.84925241	2.98351171
1	-1.33226566	3.69247952	3.93166503
1	-3.44495456	1.15795233	3.27019092
6	0.30889810	-0.04240368	4.27316923
1	0.15174909	-1.92730206	3.43343853
7	-0.33293923	-0.18184780	7.04776297
1	0.66205590	1.26223502	7.92213333
1	-2.23119961	0.04528904	7.35396400
1	0.22796978	-1.84475783	7.86538404
6	-0.92583590	2.08513158	0.23540328
6	0.03915708	4.15101438	-0.99649350
6	-1.17401385	0.10499506	-1.60785940
7	0.40767525	3.56900404	-3.48562360
1	0.47247870	6.01898125	-0.27648120
6	-2.07220880	-2.39254564	-1.52715416
6	-0.31387155	1.10972301	-3.92602838
1	1.03543971	4.78568262	-4.80941530
6	-2.06180281	-3.80217043	-3.72484004
1	-2.81840619	-3.20508384	0.21456167
6	-0.30009571	-0.31030672	-6.15437724
6	-1.17495979	-2.76728346	-6.01392116
1	0.36261309	0.48331745	-7.93057425
1	-1.19459628	-3.92679937	-7.70988319
6	3.03375085	0.90851089	4.22200682
8	3.85611557	2.12861271	5.95545573
8	4.23439121	0.27318365	2.15459219
1	5.91828607	0.98907078	2.14678870
1	-2.76141327	-5.73379494	-3.70509106

(d) Protonated 5-hydroxytryptophan

R

6	3.09289553	-1.43105867	0.81684427
1	4.28133382	-2.99629442	1.46963523
1	3.97712021	-0.68442324	-0.91201713
6	3.17653789	0.62165399	2.89277270
1	2.59088288	-0.18210648	4.70756835
7	1.39655151	2.73666248	2.25148508
1	2.36462034	4.05214109	1.18394603
1	-0.14082676	2.06474908	1.23942502

1	0.75936615	3.65909903	3.82703087
6	0.44112210	-2.25318974	0.28710120
6	-0.88102719	-4.22567488	1.34859508
6	-1.27849249	-0.99257565	-1.40488442
7	-3.28977370	-4.24488501	0.43691969
1	-0.25252869	-5.64871789	2.68065688
6	-1.03049569	1.10401489	-3.02810694
6	-3.60749520	-2.28460440	-1.24413535
1	-4.61303349	-5.54013808	0.88567159
6	-3.12058565	1.86022703	-4.40906645
1	0.76255683	2.07086234	-3.33925957
6	-5.70793131	-1.52121478	-2.65114355
6	-5.44402397	0.55668483	-4.20712063
1	-7.50178164	-2.51743374	-2.53868609
1	-7.04979381	1.19718068	-5.32337504
8	-2.83717703	3.87806019	-5.95417767
1	-4.33045988	4.16573862	-6.94206139
6	5.78490041	1.82469959	3.08498508
8	6.18755807	3.93884336	2.37312753
8	7.45646264	0.23062255	4.01260157
1	9.11777703	0.99548344	4.04835720

TS^{rot}

6	-1.51751058	1.92752615	2.47052479
1	-1.52193721	3.72632282	3.49531174
1	-3.46476373	1.18605296	2.54085401
6	0.26444035	0.02197867	3.81630919
1	1.56972007	-0.79198625	2.42249844
7	-1.12940774	-2.17420825	4.98026126
1	-2.88153308	-1.64089209	5.61266080
1	-1.35851703	-3.61816618	3.71071757
1	-0.11617956	-2.78567348	6.53796548
6	-0.71916958	2.26967773	-0.21137038
6	0.32045976	4.34063008	-1.37688167
6	-0.73935789	0.26867377	-2.03635661
7	0.93522627	3.73893592	-3.80958075
1	0.67442740	6.21556865	-0.63486653
6	-1.56994952	-2.24814427	-1.94829569
6	0.32579593	1.24797777	-4.27382944
1	1.70792878	4.94201837	-5.06686511
6	-1.28045389	-3.73541144	-4.08028351
1	-2.57055427	-3.04232005	-0.33070104
6	0.59975375	-0.24792181	-6.42968432
6	-0.19247891	-2.73547304	-6.30094333
1	1.40907586	0.49548935	-8.16613638
1	0.00561227	-3.94875051	-7.95130408
8	-2.09650553	-6.16321168	-3.94129111
1	-1.93045448	-6.99775607	-5.54237160
6	1.83204204	1.12025882	5.97332349
8	1.99251640	0.08082546	7.98417100
8	2.94769774	3.24210003	5.31899606
1	3.97743179	3.86719189	6.69574926

R'

6	-1.80721469	1.15669922	3.09856922
1	-1.95531617	2.86591909	4.27258678
1	-3.65516094	0.19136699	3.14398130
6	0.15498703	-0.65070455	4.28310269

1	0.37356832	-2.36291884	3.14051702
7	-0.70258788	-1.36677783	6.90622270
1	-0.00243420	0.00407874	8.11867435
1	-2.63333754	-1.43801459	7.03089714
1	0.01388649	-3.06875893	7.48770506
6	-1.10731294	1.80263824	0.44844003
6	-0.38207481	4.11160360	-0.48961534
6	-0.96537070	0.03203796	-1.60300376
7	0.20563820	3.87628535	-2.98755224
1	-0.26206105	5.92563647	0.45388909
6	-1.49792602	-2.55737183	-1.81597180
6	-0.12897780	1.40050628	-3.73215084
1	0.72573861	5.31097935	-4.12593146
6	-1.15495580	-3.71028596	-4.13649284
1	-2.23215143	-3.68389248	-0.25739096
6	0.20936689	0.23585725	-6.07557908
6	-0.29946235	-2.31925566	-6.24726717
1	0.84802592	1.28565255	-7.72262943
1	-0.05024538	-3.28395949	-8.04817561
6	2.68948489	0.66369935	4.70018117
8	3.18086725	1.61000577	6.70883239
8	4.12495148	0.64335710	2.68482234
1	5.67230014	1.56920777	2.99516755
8	-1.67711993	-6.21687968	-4.29663411
1	-1.47047513	-6.81329722	-5.99579388

TS_{dissociation}

6	3.30123893	1.06921285	1.63116092
1	4.97979601	0.20768102	2.46326389
1	3.67536331	2.89033276	0.73852673
6	1.05080981	0.93311420	3.22013379
1	-0.67558213	1.90277183	2.66738741
7	1.48650901	3.50795193	6.32247243
1	2.99794087	3.05608317	7.42336653
1	1.74776552	5.28577898	5.64135523
1	-0.09422478	3.49902664	7.41866697
6	1.80804820	-0.67812516	-0.04855059
6	1.84374365	-3.33160118	-0.06145009
6	0.14503237	0.08231738	-2.09030606
7	0.37326181	-4.16930100	-1.93514820
1	2.85738730	-4.60863105	1.17982667
6	-0.62819456	2.42956276	-3.00065880
6	-0.71629914	-2.15339183	-3.23488705
1	0.08487575	-6.01470909	-2.33589244
6	-2.27372423	2.47176859	-5.04818687
1	0.01699666	4.21027736	-2.20009685
6	-2.35845128	-2.12484841	-5.28918141
6	-3.12735474	0.21173685	-6.17451518
1	-3.01841981	-3.85361330	-6.18178834
1	-4.41030206	0.31393761	-7.77978636
6	0.85693689	-1.21536203	5.08143292
8	2.56156445	-2.63197822	5.53354897
8	-1.39619474	-1.25271463	6.19648612
1	-1.46000284	-2.63186140	7.39328431
8	-3.00168572	4.76128048	-5.89965679
1	-4.09225591	4.61857160	-7.34194430

(e) Protonated *N*- ω -methyl-tryptamine

R

6	-2.68815750	2.56848252	2.55915811
1	-3.27744531	4.53537591	2.83271817
1	-4.40503288	1.51856635	2.04212461
6	-1.64027835	1.62030169	5.08959122
1	-0.02657682	2.77859881	5.66674802
1	-3.04781509	1.59988867	6.60852934
7	-0.67882046	-1.05003270	4.79581942
1	0.12133299	-1.18545166	3.01176138
1	0.74048677	-1.38957514	6.06215336
6	-0.73476887	2.34524730	0.51709601
6	1.09331982	4.07371611	-0.12266715
6	-0.28218269	0.14351499	-1.02653788
7	2.63984198	3.07815807	-1.93790610
1	1.39010069	5.97655942	0.57461334
6	-1.51381229	-2.20207208	-1.31374339
6	1.86636738	0.67472545	-2.52941764
1	4.09024585	4.00105411	-2.75989296
6	-0.54137127	-3.93480540	-3.00962512
1	-3.26327939	-2.61648361	-0.30640117
6	2.84567151	-1.07458035	-4.25241773
6	1.62736508	-3.37570212	-4.45405695
1	4.49364904	-0.64078005	-5.40133642
1	2.33481120	-4.77657040	-5.77975304
1	-1.48382988	-5.74078308	-3.27821608
6	-2.68141432	-3.01277846	5.09622684
1	-1.93657346	-4.84450210	4.50484886
1	-3.25845745	-3.06813929	7.07768509
1	-4.29099372	-2.49335395	3.91391579

TS^{rot}

6	-1.51264611	2.03418188	2.72614772
1	-2.15942857	3.89206080	3.36877107
1	-3.15861943	0.76276798	2.89542919
6	0.64782078	1.08048178	4.44554066
1	2.32444696	0.64064884	3.31474659
1	1.16877798	2.42938167	5.92641595
7	-0.06399482	-1.33399305	5.79119436
1	-0.70291234	-2.58961019	4.45782100
1	1.52646489	-2.13209417	6.55282685
6	-0.67985670	2.12970702	0.02838922
6	-0.12437019	4.20721855	-1.41389519
6	-0.12433443	-0.04982247	-1.49279633
7	0.74262108	3.44639950	-3.72996744
1	-0.28676938	6.19654670	-0.95676255
6	-0.33694296	-2.66827174	-1.11256035
6	0.77759736	0.85233393	-3.84036020
1	1.25454455	4.61729809	-5.14172345
6	0.38635040	-4.29389238	-3.02591813
1	-1.16590751	-3.44279334	0.61382820
6	1.50733524	-0.78117449	-5.78362537
6	1.31375772	-3.34893138	-5.33594837
1	2.19483842	-0.06785180	-7.58432242
1	1.86497528	-4.67159719	-6.80807236
1	0.21327288	-6.32529016	-2.77174935
6	-2.00219058	-0.99580940	7.81448258
1	-2.47191308	-2.83292833	8.62892769
1	-1.21374834	0.24946876	9.26027588

	1	-3.68242281	-0.13419032	6.98272127
R'				
	6	-1.50338350	0.95161236	2.96447063
	1	-2.11153592	2.68386106	3.92751908
	1	-3.12769516	-0.35986441	2.94834857
	6	0.71067572	-0.27790885	4.35419447
	1	1.54606059	-1.79008873	3.21099407
	1	2.18884543	1.09717156	4.81365529
	7	-0.10669519	-1.46705275	6.82342921
	1	-1.42560022	-2.83403110	6.43958986
	1	1.40340259	-2.38593867	7.61166297
	6	-0.70788930	1.53268793	0.31497696
	6	-0.26156655	3.85820890	-0.73661917
	6	-0.18161968	-0.31449569	-1.60943506
	7	0.50843619	3.56439809	-3.18599209
	1	-0.45625424	5.72408264	0.08450895
	6	-0.32086403	-2.96437795	-1.71029935
	6	0.58126246	1.03601977	-3.78211733
	1	0.92771301	4.98955311	-4.37698652
	6	0.32091664	-4.17387010	-3.93390307
	1	-0.96547063	-4.06077069	-0.08720375
	6	1.23207137	-0.18027984	-6.03586524
	6	1.09762641	-2.78873906	-6.07283630
	1	1.81330487	0.87845822	-7.69876338
	1	1.58797361	-3.79749051	-7.79424432
	1	0.21523222	-6.22230847	-4.05337178
	6	-1.17393680	0.36121842	8.69276046
	1	-1.53833453	-0.61875265	10.47201012
	1	0.20266885	1.87450058	8.97519333
	1	-2.93089326	1.13161829	7.93608573
TS_{dissociation}				
	6	2.62414053	-0.10057069	2.25131209
	1	3.56861443	-1.41745699	3.52188141
	1	3.93870094	1.02477358	1.13075250
	6	0.40454575	1.19357154	3.22698444
	1	-0.41312082	2.77257350	2.20527702
	1	-0.68452932	0.36337705	4.75260473
	7	1.87198369	4.00326527	6.14099816
	6	0.56546500	-1.26238775	0.64474133
	6	-0.88963677	-3.39491135	1.22916960
	6	-0.20810860	-0.47032248	-1.86589289
	7	-2.42491424	-3.91812345	-0.70914245
	1	-0.87745711	-4.54588699	2.92561952
	6	0.52922550	1.49444184	-3.47088637
	6	-2.07924957	-2.17936246	-2.65643375
	1	-3.67046462	-5.36629855	-0.74647508
	6	-0.64078071	1.68487524	-5.80467909
	1	1.99162095	2.83368925	-2.92070656
	6	-3.26561322	-2.00874008	-5.00104804
	6	-2.51415245	-0.04386709	-6.55763115
	1	-0.09762948	3.19120198	-7.09168158
	1	-4.70563246	-3.35109730	-5.58896734
	1	-3.38391487	0.16260319	-8.40705895
	1	2.38368113	5.65238468	5.29905098
	6	4.04128229	2.82285222	7.39826484
	1	3.45550468	1.01822243	8.22971512

1	5.51872272	2.43781758	5.99976079
1	4.86217713	3.99379320	8.89925009
1	0.49701883	4.43864897	7.41051824

(f) Protonated melatonin

R

6	2.61560763	-3.82201577	3.00136275
1	2.78691616	-5.78032117	3.65817486
1	4.36776857	-3.37586473	1.98135046
6	2.39687333	-2.12284793	5.34603888
1	0.76783166	-2.67420720	6.50851015
1	4.07517151	-2.24386452	6.54962191
7	2.08594816	0.56446367	4.68164778
6	0.38556457	-3.50200107	1.28333554
6	-1.84718802	-4.84794720	1.29080231
6	0.11586948	-1.57680542	-0.62516021
7	-3.46972952	-3.85531562	-0.46074211
1	-2.36915969	-6.49898837	2.38691038
6	1.70630279	0.36323729	-1.48228561
6	-2.32402483	-1.85318113	-1.67099660
1	-5.18625611	-4.56658274	-0.88192256
6	0.83128919	1.97811747	-3.35420953
1	3.62809108	0.60537061	-0.78573987
6	-3.20726217	-0.23219372	-3.55484036
6	-1.62085512	1.67486125	-4.38124065
1	-5.08270153	-0.44515293	-4.36773262
1	-2.28204134	2.94057194	-5.85443011
8	2.44252643	3.82370241	-4.09207409
6	1.75692298	5.34196016	-6.18879528
1	3.36107320	6.58854238	-6.54398181
1	1.40757273	4.17703920	-7.87104970
1	0.07838355	6.49230074	-5.77315220
6	-0.03002269	1.71539389	4.16265312
8	-2.18717554	0.56052247	4.13745527
6	-0.11372973	4.45581388	3.57378633
1	1.66459405	5.40743420	4.00980993
1	-0.52186368	4.62981739	1.54538442
1	-1.66904497	5.32676340	4.62261387
1	3.66634489	1.64213253	4.58846000
1	-2.03398346	-1.26657654	3.89581962

TS^{rot}

6	1.80359238	-3.44463469	3.07506941
1	2.38332651	-5.18278789	4.03621879
1	3.52242819	-2.30980397	2.79587354
6	-0.08266434	-1.94603119	4.75788734
1	-1.73920168	-1.38890191	3.64512554
1	-0.78963447	-3.10939606	6.31594707
7	0.95755829	0.35440150	5.91870237
6	0.58723298	-3.97762635	0.58301648
6	-0.63913691	-6.10128151	-0.26340834
6	0.14009365	-2.04726923	-1.26129793
7	-1.81492332	-5.59430262	-2.51036282
1	-0.77098547	-7.95938586	0.58720264
6	0.93584609	0.47761120	-1.44429445
6	-1.39395766	-3.10999469	-3.16643184
1	-2.80068408	-6.86025614	-3.53487822

6	0.12797602	1.91263441	-3.49893624
1	2.38159445	1.26852852	-0.20442713
6	-2.19065196	-1.67552969	-5.22635724
6	-1.44964948	0.83445083	-5.36386864
1	-3.36696019	-2.48011835	-6.70787338
1	-2.06747038	1.95914407	-6.96382790
8	0.98225843	4.31765541	-3.59079426
6	0.33645064	5.81114705	-5.71832197
1	1.25857779	7.63488147	-5.44128866
1	1.03352219	4.94916289	-7.47312774
1	-1.71672860	6.09339910	-5.84199158
6	0.56331802	2.68139317	5.20843811
8	-0.68428156	3.29111113	3.20084930
6	1.50252747	4.85212368	6.72753807
1	2.44588586	4.24596901	8.45980810
1	2.80014250	5.96878948	5.56374049
1	-0.10821192	6.06490922	7.19921576
1	2.00909619	0.14084078	7.50624281
1	-0.88649662	1.98938341	1.89599259

R'

6	1.74632633	-3.01288529	3.12524423
1	2.48734984	-4.63704202	4.17312715
1	3.35939207	-1.75655797	2.73948409
6	-0.23619214	-1.57847260	4.73280721
1	-1.67053139	-0.72889747	3.49627134
1	-1.25447483	-2.86335564	5.99225156
7	0.82597442	0.44107697	6.31549375
6	0.51796859	-3.75434686	0.69340449
6	-0.70661620	-5.94209799	0.02614504
6	0.02085953	-1.96023171	-1.27517816
7	-1.92857653	-5.60344570	-2.22644500
1	-0.80752255	-7.73630788	1.00804896
6	0.79044594	0.55014072	-1.65722345
6	-1.54257319	-3.16755561	-3.06528654
1	-2.92285991	-6.94532163	-3.13982805
6	-0.08428489	1.82952519	-3.78351322
1	2.28576845	1.43441445	-0.54537817
6	-2.40263882	-1.89041999	-5.20213269
6	-1.69423827	0.61043931	-5.53060435
1	-3.60352362	-2.80897804	-6.59490888
1	-2.36148502	1.61505664	-7.18955611
8	0.74181900	4.23003999	-4.06564540
6	0.04076968	5.55958020	-6.28118102
1	0.95330689	7.40489939	-6.15671311
1	0.70793121	4.57708512	-7.98371393
1	-2.01681278	5.81892403	-6.38191709
6	1.09127632	2.79209872	5.63711051
8	0.45951959	3.62859191	3.43051892
6	2.13321984	4.72877547	7.38571378
1	2.57726070	3.94161194	9.24064827
1	3.83699621	5.54408199	6.53829725
1	0.74578843	6.25237569	7.58491848
1	1.41815325	-0.00241856	8.08221506
1	-0.05472904	2.39743929	2.15033137

TS_{dissociation}

6	2.39833647	-1.45836943	2.72359340
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1	3.27505028	-2.56315531	4.22412512
1	3.50700172	-1.48978038	0.98274445
6	1.32420001	0.96373049	3.48008466
1	0.67377298	2.31269786	2.07460275
1	0.65065107	1.22641535	5.39784788
7	4.49126933	3.43374371	4.50609108
6	-0.35242249	-2.03294042	2.25189965
6	-2.11414328	-2.97053707	3.98951291
6	-1.68812220	-1.75246001	-0.12530941
7	-4.34646025	-3.27274703	2.84110313
1	-1.85732250	-3.44226231	5.96759027
6	-0.96345251	-0.91725632	-2.51015014
6	-4.18554933	-2.54897747	0.31422721
1	-5.92480928	-3.92516621	3.69497710
6	-2.77250677	-0.88328493	-4.42531882
1	0.95597357	-0.33080928	-2.95939878
6	-6.00211768	-2.52816141	-1.58313506
6	-5.27502594	-1.68469591	-3.95335877
1	-7.93121974	-3.15045838	-1.24631103
1	-6.66501149	-1.65662109	-5.46117063
8	-1.96878989	-0.06164008	-6.69192179
6	-3.70339273	-0.03590915	-8.73385828
1	-2.65527603	0.66575467	-10.36472281
1	-4.40594441	-1.94660259	-9.13894293
1	-5.29736613	1.23531738	-8.34347198
6	6.44067804	3.96843109	3.19711406
8	6.44899200	3.59440500	0.70617746
6	8.88711991	5.03204751	4.12784766
1	8.88007650	5.25895516	6.17834313
1	10.43387610	3.77481984	3.56986244
1	9.21858199	6.86455151	3.22474036
1	4.71636758	3.82949962	6.37063242
1	4.79675841	3.09186698	0.13511274