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Table S1. Total Energies for Lowest-Energy Conformations of Phenethylamine Compounds 1 through 6.

	1	2	3	4	5	6	7
HF/6-31G(d,p)// HF/6-31G(d,p)	-363.8169297	-464.07808919	-438.6763388	-364.1965596	-463.041459	-439.0567848	-347.8285465
MP2/631G(d,p)// HF/6-31G(d,p)	-365.0681613	-464.07808919	-438.6763388	-365.4470388	-464.4527583	-440.4837624	-349.0571650
MP2/6-31G(d,p)// MP2/6-31G(d,p)	-365.0700473	-464.0806188	-440.1064885	-365.698707	-464.4557194	-440.4871664	
MP2/6-31+G(d,p)// HF/6-31G(d,p)	-365.0921612	-464.113366	-440.1342266	-365.4623511	-464.4766554	-440.5051062	-349.0747002
MP2/6-31+G(d,p)// MP2/6-31G(d,p)	-365.0940701	-464.1141686	-440.1370186	-365.4568176	-464.4798513	-440.5085463	
MP2/6-311+G(d,p)// HF/6-31G(d,p)	-365.2019105	-464.2793453	-440.2827132	-365.5707285	-464.6436189	-440.6524172	-349.1759008
MP2/6-311+G(d,p)// MP2.6-31G(d,p)	-365.2044333	-464.2821013	-440.2857391	-365.5736771	-464.6468584	-440.6561931	

Table S2. AM1-CM1A Partial Atomic Charges for Phenethylamines **1** - **6**.

	Phenethylamine					
atom position[a]	**1**	**2**	**3**	**4**	**5**	**6**
1	N: -0.881	N: -0.881	N: -0.881	N: -0.377	N: -0.375	N: -0.376
2	C: 0.048	C: 0.049	C: 0.047	C: -0.118	C: -0.120	C: -0.120
3	C: -0.163	C: -0.162	C: -0.157	C: -0.132	C: -0.130	C: -0.124
4	C: -0.067	C: -0.081	C: -0.102	C: -0.129	C: -0.149	C: -0.174
5	C: -0.127	C: -0.104	C: -0.091	C: -0.115	C: -0.087	C: -0.074
6	C: -0.127	C: -0.104	C: -0.091	C: -0.115	C: -0.087	C: -0.074
7	C: -0.127	C: -0.164	C: -0.182	C: -0.116	C: -0.160	C: -0.179
8	C: -0.127	C: -0.164	C: -0.182	C: -0.116	C: -0.160	C: -0.179
9	C: -0.132	C: 0.063	C: 0.106	C: -0.095	C: 0.104	C: 0.152
10	H: 0.344	H: 0.345	H: 0.344	H: 0.351	H: 0.352	H: 0.351
11	H: 0.344	H: 0.345	H: 0.344	H: 0.351	H: 0.352	H: 0.351
12	H: 0.095	H: 0.096	H: 0.095	H: 0.156	H: 0.156	H: 0.155
13	H: 0.095	H: 0.096	H: 0.095	H: 0.156	H: 0.156	H: 0.155
14	H: 0.085	H: 0.087	H: 0.084	H: 0.111	H: 0.112	H: 0.109
15	H: 0.085	H: 0.087	H: 0.084	H: 0.111	H: 0.112	H: 0.109
16	H: 0.131	H: 0.137	H: 0.134	H: 0.132	H: 0.138	H: 0.134
17	H: 0.131	H: 0.137	H: 0.134	H: 0.132	H: 0.138	H: 0.134
18	H: 0.131	H: 0.149	H: 0.142	H: 0.153	H: 0.170	H: 0.162
19	H: 0.131	H: 0.149	H: 0.142	H: 0.153	H: 0.170	H: 0.162
20	H: 0.131	F: -0.080	O: -0.437	H: 0.155	F: -0.044	O: -0.413
21				H: 0.351	H: 0.352	H: 0.351
22			H: 0.372			H: 0.388

[a]See Figure S1 for atom position numbering scheme.

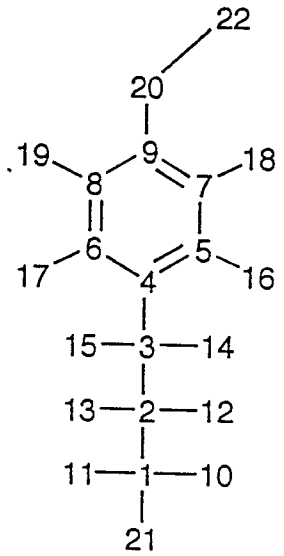

Figure S1: The numbering scheme for the AM1-CM1A charges shown in Table S1.