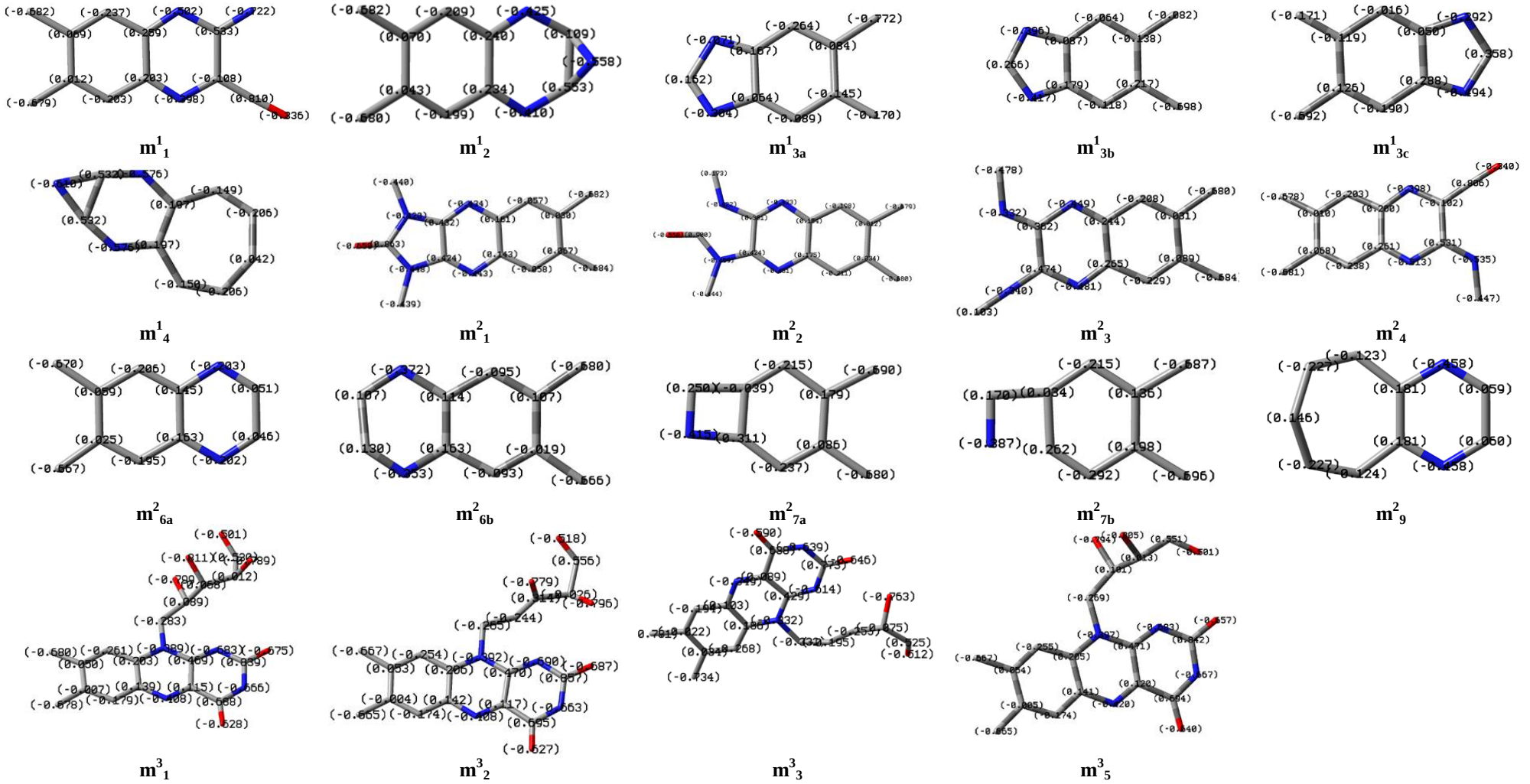
Electronic Supplementary Material (ESI) for Analytical Methods

SUPPORTING INFORMATION



Scheme S1. Most stable molecular conformations of the MS fragments the **1**–**3** (the H-atoms are omitted), Theoretical q_X(NBO) data, (X = N, O, and C), respectively.

Table S1. Thermodynamics of the mass spectrometric molecular fragments, proposed in Scheme 1.

	m^1_1	m^1_2	m^1_{3a}	m^1_{3b}	m^1_{3c}	m^1_4	m^2_1
ΔE_{UPSS}	-52.07	-50.05	-47.01	-53.86	-51.99	-52.80	-47.58
ΔE_{PSS}	-56.98	-52.28	-48.07	-59.42	-54.28	-56.29	-52.00
ΔE_{SP}	2.68	1.17	0.61	3.29	1.25	1.92	2.51
ΔE_E	-54.29	-51.11	-47.45	-56.13	-53.03	-54.37	-49.48
ΔE^d	-27.85	-24.82	-20.90	-21.65	-21.49	-22.68	-33.59
ΔE^r	5.19	4.86	3.60	4.07	4.20	4.83	6.43
ΔE^t_{NE}	3.41	2.44	2.56	1.91	2.47	2.01	3.72
ΔG	-50.88	-48.67	-44.89	-54.23	-50.56	-52.36	-45.76
ΔE^t_S	-664.07	-549.978	-456.65	-456.70	-456.68	-509.99	-797.41
	m^3_1	m^3_2	m^3_3	m^3_5	m^3_6	m^3_7	m^3_8
ΔE_{UPSS}	-82.59	-78.40	-74.41	-64.46	-83.05	-75.25	-78.36
ΔE_{PSS}	-96.54	-97.72	-91.99	-81.51	-100.39	-94.06	-97.93
ΔE_{SP}	7.10	9.84	9.10	9.81	9.17	10.25	10.43
ΔE_E	-89.44	-87.87	-82.89	-71.71	-91.22	-83.81	-87.50
ΔE^d	-45.19	-43.64	-43.34	-42.17	-42.43	-40.55	-39.44
ΔE^r	9.78	9.67	9.93	8.35	9.22	8.63	9.06
ΔE^t_{NE}	7.81	7.49	6.66	5.65	6.94	6.37	6.18
ΔG	-81.63	-80.38	-76.23	-66.05	-84.28	-77.44	-81.32
ΔE^t_S	-1328.7	-1252.76	-1177.38	-1101.01	-1214.68	-1138.26	-1100.16
	m^2_2	m^2_3	m^2_4	m^2_{6a}	m^2_{6b}	m^2_{7a}	m^2_{7b}
ΔE_{UPSS}	-46.01	-43.50	-49.32	-48.14	-48.28	-55.40	-51.30
ΔE_{PSS}	-49.72	-44.90	-54.25	-51.09	-49.99	-59.18	-54.92
ΔE_{SP}	2.02	0.75	2.65	1.78	0.88	2.05	2.19
ΔE_E	-47.69	-44.15	-51.60	-49.31	-49.11	-57.13	-52.73
ΔE^d	-31.97	-30.51	-30.33	-24.11	-24.64	-22.33	-20.74
ΔE^r	5.66	5.66	5.87	4.70	5.18	5.70	3.84
ΔE^t_{NE}	4.87	4.57	3.82	2.62	2.25	1.59	2.02
ΔG	-42.82	-39.57	-47.78	-46.69	-46.86	-55.54	-50.71
ΔE^t_S	-796.82	-683.43	-703.36	-549.09	-496.04	-402.57	-402.55
	m^3_9	m^3_{10}	m^3_{11}	m^3_{12}	m^3_{13}	m^3_{14}	m^3_{15}
ΔE_{UPSS}	-67.18	-75.55	-56.47	-56.45	-58.85	-14.39	-58.94
ΔE_{PSS}	-83.53	-95.14	-65.83	-66.35	-67.52	-23.00	-67.22
ΔE_{SP}	9.05	10.72	5.05	5.50	4.71	5.19	4.36
ΔE_E	-74.48	-84.42	-60.79	-60.85	-62.81	-17.81	-62.86
ΔE^d	-38.23	-36.31	-36.09	-32.66	-31.03	-27.64	-24.35
ΔE^r	7.70	7.70	7.42	5.23	5.66	4.72	5.43
ΔE^t_{NE}	5.16	4.94	4.24	5.58	3.61	3.02	5.68
ΔG	-69.32	-79.48	-56.55	-55.28	-59.20	-14.79	-57.18
ΔE^t_S	-1023.74	-985.66	-948.58	-909.44	-832.04	-717.64	-550.71

ΔG – free Gibbs energy of the system; ΔE^{t}_{NE} - total non-electrostatic energy; ΔE^{r} - repulsion energy; ΔE^{d} - dispersion energy; ΔE_{E} - total electrostatic energy; ΔE_{SP} - Solute Polarization; ΔE_{PSS} – polar solute-solvent energy; ΔE_{UPSS} – Unpolar-Solute-Solvent energy; ΔE^{t}_{S} – total free energy in solution; [kcal/mol].