Supporting Information

Understanding the Structural Complexity of Dissolved Organic Matter: isomeric diversity

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Table S1. FTICR-MS/MS fragmentation data for 391 m/a with nominal mass isolation from sample PAN-S

Measured m/z	Ion Formula	Theoretical m/z	err [ppm]
155.0349	$C_7H_7O_4$	155.0350	0.7
161.0607	$C_{10}H_9O_2$	161.0608	0.7
163.0763	$C_{10}H_{11}O_2$	163.0765	0.8
165.0192	$C_8H_5O_4$	165.0193	0.7
165.0556	$C_9H_9O_3$	165.0557	0.8
167.0349	$C_8H_7O_4$	167.0350	0.5
167.0712	$C_9H_{11}O_3$	167.0714	0.8
171.0814	$C_{12}H_{11}O$	171.0815	0.9
173.0607	$C_{11}H_9O_2$	173.0608	0.6
175.04	$C_{10}H_7O_3$	175.0401	0.5
175.0763	$C_{11}H_{11}O_2$	175.0765	0.7
177.0556	$C_{10}H_9O_3$	177.0557	0.6
177.092	$C_{11}H_{13}O_2$	177.0921	0.8
179.0348	$C_9H_7O_4$	179.0350	0.8
179.0712	$C_{10}H_{11}O_3$	179.0714	0.8
181.0505	$C_9H_9O_4$	181.0506	0.7
181.0869	$C_{10}H_{13}O_3$	181.0870	0.6
183.0298	$C_8H_7O_5$	183.0299	0.6
183.045	$C_{12}H_7O_2$	183.0452	0.7
183.0814	$C_{13}H_{11}O$	183.0815	1
185.0607	$C_{12}H_9O_2$	185.0608	0.7
187.04	$C_{11}H_7O_3$	187.0401	0.6
187.0763	$C_{12}H_{11}O_2$	187.0765	0.7
189.0556	$C_{11}H_9O_3$	189.0557	0.7
189.0919	$C_{12}H_{13}O_2$	189.0921	0.9
191.0348	$C_{10}H_7O_4$	191.0350	0.8
191.0712	$C_{11}H_{11}O_3$	191.0714	0.8
191.1076	$C_{12}H_{15}O_2$	191.1078	0.7
193.0141	$C_9H_5O_5$	193.0142	0.7
193.0505	$C_{10}H_9O_4$	193.0506	0.7
193.0869	$C_{11}H_{13}O_3$	193.0870	0.8

195.0297	$C_9H_7O_5$	195.0299	0.9
195.0661	$C_{10}H_{11}O_4$	195.0663	0.8
197.0454	$C_9H_9O_5$	197.0455	0.8
197.0607	$C_{13}H_9O_2$	197.0608	0.7
197.0818	$C_{10}H_{13}O_4$	197.0819	0.6
199.0399	$C_{12}H_7O_3$	199.0401	0.8
199.0763	$C_{13}H_{11}O_2$	199.0765	0.7
201.0192	$C_{11}H_5O_4$	201.0193	0.7
201.0555	$C_{12}H_9O_3$	201.0557	0.9
202.9984	$C_{10}H_3O_5$	202.9986	0.8
203.0348	$C_{11}H_7O_4$	203.0350	0.7
203.0712	$C_{12}H_{11}O_3$	203.0714	0.8
203.1076	$C_{13}H_{15}O_2$	203.1078	0.8
205.014	$C_{10}H_5O_5$	205.0142	1
205.0505	$C_{11}H_9O_4$	205.0506	0.5
205.0869	$C_{12}H_{13}O_3$	205.0870	0.8
205.1232	$C_{13}H_{17}O_2$	205.1234	0.9
207.0297	$C_{10}H_7O_5$	207.0299	0.9
207.0661	$C_{11}H_{11}O_4$	207.0663	0.8
207.1025	$C_{12}H_{15}O_3$	207.1027	0.6
209.0454	$C_{10}H_9O_5$	209.0455	0.7
209.0818	$C_{11}H_{13}O_4$	209.0819	0.8
211.061	$C_{10}H_{11}O_5$	211.0612	0.9
213.0555	$C_{13}H_9O_3$	213.0557	0.9
215.0348	$C_{12}H_7O_4$	215.0350	0.8
215.0712	$C_{13}H_{11}O_3$	215.0714	0.8
215.1076	$C_{14}H_{15}O_2$	215.1078	0.7
215.144	$C_{15}H_{19}O$	215.1441	0.6
217.0141	$C_{11}H_5O_5$	217.0142	0.7
217.0505	$C_{12}H_9O_4$	217.0506	0.8
217.0868	$C_{13}H_{13}O_3$	217.0870	0.8
217.1233	$C_{14}H_{17}O_2$	217.1234	0.7
219.0297	$C_{11}H_7O_5$	219.0299	0.8
219.0661	$C_{12}H_{11}O_4$	219.0663	0.7
219.1025	$C_{13}H_{15}O_3$	219.1027	0.9

221.009	$C_{10}H_5O_6$	221.0092	0.7
221.0454	$C_{11}H_9O_5$	221.0455	0.7
221.0818	$C_{12}H_{13}O_4$	221.0819	0.7
221.1181	$C_{13}H_{17}O_3$	221.1183	0.9
223.0246	$C_{10}H_7O_6$	223.0248	1.1
223.0611	$C_{11}H_{11}O_5$	223.0612	0.6
223.0974	$C_{12}H_{15}O_4$	223.0976	0.7
223.1338	$C_{13}H_{19}O_3$	223.1340	0.8
225.0767	$C_{11}H_{13}O_5$	225.0768	0.6
227.0348	$C_{13}H_7O_4$	227.0350	0.8
227.0712	$C_{14}H_{11}O_3$	227.0714	0.8
227.1076	$C_{15}H_{15}O_2$	227.1078	0.8
229.0141	$C_{12}H_5O_5$	229.0142	0.8
229.0505	$C_{13}H_9O_4$	229.0506	0.8
229.0868	$C_{14}H_{13}O_3$	229.0870	0.8
231.0298	$C_{12}H_7O_5$	231.0299	0.6
231.0661	$C_{13}H_{11}O_4$	231.0663	0.8
231.1025	$C_{14}H_{15}O_3$	231.1027	0.9
233.0454	$C_{12}H_9O_5$	233.0455	0.8
233.0818	$C_{13}H_{13}O_4$	233.0819	0.7
233.1181	$C_{14}H_{17}O_3$	233.1183	0.8
233.1545	$C_{15}H_{21}O_2$	233.1547	1.1
235.0246	$C_{11}H_7O_6$	235.0248	0.8
235.061	$C_{12}H_{11}O_5$	235.0612	0.8
235.0974	$C_{13}H_{15}O_4$	235.0976	0.8
235.1338	$C_{14}H_{19}O_3$	235.1340	0.8
237.0403	$C_{11}H_9O_6$	237.0405	0.8
237.0767	$C_{12}H_{13}O_5$	237.0768	0.8
237.113	$C_{13}H_{17}O_4$	237.1132	0.9
239.0349	$C_{14}H_7O_4$	239.0350	0.5
239.056	$C_{11}H_{11}O_6$	239.0561	0.4
239.0712	$C_{15}H_{11}O_3$	239.0714	0.7
239.0923	$C_{12}H_{15}O_5$	239.0925	0.9
241.014	$C_{13}H_5O_5$	241.0142	0.9
241.0504	$C_{14}H_9O_4$	241.0506	0.8

241.0868	$C_{15}H_{13}O_3$	241.0870	0.7
241.1232	$C_{16}H_{17}O_2$	241.1234	0.7
243.0297	$C_{13}H_7O_5$	243.0299	0.7
243.0661	$C_{14}H_{11}O_4$	243.0663	0.8
243.1025	$C_{15}H_{15}O_3$	243.1027	0.8
243.1389	$C_{16}H_{19}O_2$	243.1391	0.6
245.009	$C_{12}H_5O_6$	245.0092	0.8
245.0818	$C_{14}H_{13}O_4$	245.0819	0.6
245.118	$C_{15}H_{17}O_3$	245.1183	1.1
247.0246	$C_{12}H_7O_6$	247.0248	0.9
247.061	$C_{13}H_{11}O_5$	247.0612	0.8
247.0974	$C_{14}H_{15}O_4$	247.0976	0.8
247.1337	$C_{15}H_{19}O_3$	247.1340	1
249.0403	$C_{12}H_9O_6$	249.0405	0.6
249.0767	$C_{13}H_{13}O_5$	249.0768	0.8
249.113	$C_{14}H_{17}O_4$	249.1132	0.9
249.1494	$C_{15}H_{21}O_3$	249.1496	0.7
251.0559	$C_{12}H_{11}O_6$	251.0561	0.7
251.0923	$C_{13}H_{15}O_5$	251.0925	0.9
251.1286	$C_{14}H_{19}O_4$	251.1289	1
253.0504	$C_{15}H_9O_4$	253.0506	0.9
253.0717	$C_{12}H_{13}O_6$	253.0718	0.4
253.1079	$C_{13}H_{17}O_5$	253.1081	0.8
255.0297	$C_{14}H_7O_5$	255.0299	0.9
256.0375	$C_{13}H_2N_7$	256.0377	0.8
257.0453	$C_{14}H_9O_5$	257.0455	0.8
257.0817	$C_{15}H_{13}O_4$	257.0819	0.8
259.0246	$C_{13}H_7O_6$	259.0248	0.9
259.061	$C_{14}H_{11}O_5$	259.0612	0.8
259.0974	$C_{15}H_{15}O_4$	259.0976	0.8
259.1338	$C_{16}H_{19}O_3$	259.1340	0.7
259.1702	$C_{17}H_{23}O_2$	259.1704	0.6
260.0563	$C_{13}H_{10}NO_5$	260.0564	0.7
260.0928	$C_{14}H_{14}NO_4$	260.0928	0.3
261.0403	$C_{13}H_9O_6$	261.0405	0.8

261.0767	$C_{14}H_{13}O_5$	261.0768	0.8
261.113	$C_{15}H_{17}O_4$	261.1132	0.9
263.0195	$C_{12}H_7O_7$	263.0197	0.9
263.0559	$C_{13}H_{11}O_6$	263.0561	0.8
263.0923	$C_{14}H_{15}O_5$	263.0925	0.8
263.1286	$C_{15}H_{19}O_4$	263.1289	0.9
265.0352	$C_{12}H_9O_7$	265.0354	0.6
265.0715	$C_{13}H_{13}O_6$	265.0718	0.8
265.1079	$C_{14}H_{17}O_5$	265.1081	0.8
265.1443	$C_{15}H_{21}O_4$	265.1445	0.9
265.1808	$C_{16}H_{25}O_3$	265.1809	0.5
267.0297	$C_{15}H_7O_5$	267.0299	0.7
267.0507	$C_{12}H_{11}O_7$	267.0510	1.3
267.0661	$C_{16}H_{11}O_4$	267.0663	0.6
267.0872	$C_{13}H_{15}O_6$	267.0874	0.8
267.1024	$C_{17}H_{15}O_3$	267.1027	1
267.1236	$C_{14}H_{19}O_5$	267.1238	0.8
267.1387	$C_{18}H_{19}O_2$	267.1391	1.2
267.16	$C_{15}H_{23}O_4$	267.1602	0.7
269.1028	$C_{13}H_{17}O_6$	269.1031	0.9
271.0246	$C_{14}H_7O_6$	271.0248	0.8
271.061	$C_{15}H_{11}O_5$	271.0612	0.8
271.0974	$C_{16}H_{15}O_4$	271.0976	0.8
271.1337	$C_{17}H_{19}O_3$	271.1340	0.8
271.1703	$C_{18}H_{23}O_2$	271.1704	0.2
272.0563	$C_{14}H_{10}NO_5$	272.0564	0.7
273.0038	$C_{13}H_5O_7$	273.0041	1
273.0402	$C_{14}H_9O_6$	273.0405	0.8
273.0766	$C_{15}H_{13}O_5$	273.0768	0.7
273.1131	$C_{16}H_{17}O_4$	273.1132	0.3
275.0559	$C_{14}H_{11}O_6$	275.0561	0.9
275.0923	$C_{15}H_{15}O_5$	275.0925	0.8
275.1287	$C_{16}H_{19}O_4$	275.1289	0.8
277.0351	$C_{13}H_9O_7$	277.0354	0.9
277.0715	$C_{14}H_{13}O_6$	277.0718	0.8

277.1079	$C_{15}H_{17}O_5$	277.1081	0.8
277.1443	$C_{16}H_{21}O_4$	277.1445	0.7
279.0508	$C_{13}H_{11}O_7$	279.0510	0.8
279.0872	$C_{14}H_{15}O_6$	279.0874	0.8
279.1236	$C_{15}H_{19}O_5$	279.1238	0.8
279.1599	$C_{16}H_{23}O_4$	279.1602	1
281.0665	$C_{13}H_{13}O_7$	281.0667	0.8
281.1029	$C_{14}H_{17}O_6$	281.1031	0.7
281.1393	$C_{15}H_{21}O_5$	281.1394	0.5
282.9885	$C_{14}H_3O_7$	282.9884	-0.4
283.0246	$C_{15}H_7O_6$	283.0248	0.7
283.061	$C_{16}H_{11}O_5$	283.0612	0.8
283.082	$C_{13}H_{15}O_7$	283.0823	1.2
283.264	$C_{18}H_{35}O_2$	283.2643	0.8
285.0402	$C_{15}H_9O_6$	285.0405	0.8
285.0766	$C_{16}H_{13}O_5$	285.0768	0.8
285.113	$C_{17}H_{17}O_4$	285.1132	0.9
285.1494	$C_{18}H_{21}O_3$	285.1496	0.6
287.0195	$C_{14}H_7O_7$	287.0197	0.8
287.0559	$C_{15}H_{11}O_6$	287.0561	0.9
287.0922	$C_{16}H_{15}O_5$	287.0925	0.9
287.1287	$C_{17}H_{19}O_4$	287.1289	0.7
289.0351	$C_{14}H_9O_7$	289.0354	0.9
289.0715	$C_{15}H_{13}O_6$	289.0718	0.9
289.1079	$C_{16}H_{17}O_5$	289.1081	0.7
291.0143	$C_{13}H_7O_8$	291.0146	1
291.0508	$C_{14}H_{11}O_7$	291.0510	0.8
291.0872	$C_{15}H_{15}O_6$	291.0874	0.7
291.1236	$C_{16}H_{19}O_5$	291.1238	0.8
291.1599	$C_{17}H_{23}O_4$	291.1602	0.9
293.0301	$C_{13}H_9O_8$	293.0303	0.7
293.0664	$C_{14}H_{13}O_7$	293.0667	0.9
293.1028	$C_{15}H_{17}O_6$	293.1031	0.9
293.1392	$C_{16}H_{21}O_5$	293.1394	0.8
293.1756	$C_{17}H_{25}O_4$	293.1758	0.7

295.0457	$C_{13}H_{11}O_8$	295.0459	0.7
295.0821	$C_{14}H_{15}O_7$	295.0823	0.8
295.1184	$C_{15}H_{19}O_6$	295.1187	1
297.0402	$C_{16}H_9O_6$	297.0405	0.8
297.0766	$C_{17}H_{13}O_5$	297.0768	0.8
297.0978	$C_{14}H_{17}O_7$	297.0980	0.7
303.0508	$C_{15}H_{11}O_7$	303.0510	0.9
303.0621	$C_{14}H_{11}N_2O_6$	303.0623	0.6
303.0871	$C_{16}H_{15}O_6$	303.0874	0.9
303.1235	$C_{17}H_{19}O_5$	303.1238	0.9
303.1599	$C_{18}H_{23}O_4$	303.1602	0.8
304.046	$C_{14}H_{10}NO_7$	304.0463	0.8
304.0824	$C_{15}H_{14}NO_6$	304.0827	0.8
304.1189	$C_{16}H_{18}NO_5$	304.1190	0.6
305.0664	$C_{15}H_{13}O_7$	305.0667	0.8
305.1028	$C_{16}H_{17}O_6$	305.1031	0.8
309.0613	$C_{14}H_{13}O_8$	309.0616	0.9
309.0977	$C_{15}H_{17}O_7$	309.0980	0.9
309.1341	$C_{16}H_{21}O_6$	309.1344	0.8
309.1705	$C_{17}H_{25}O_5$	309.1707	0.8
311.0558	$C_{17}H_{11}O_6$	311.0561	1
311.077	$C_{14}H_{15}O_8$	311.0772	0.9
311.0922	$C_{18}H_{15}O_5$	311.0925	0.9
311.1134	$C_{15}H_{19}O_7$	311.1136	0.9
311.1497	$C_{16}H_{23}O_6$	311.1500	0.9
311.1861	$C_{17}H_{27}O_5$	311.1864	0.8
315.0143	$C_{15}H_7O_8$	315.0146	0.9
315.0508	$C_{16}H_{11}O_7$	315.0510	0.9
315.0872	$C_{17}H_{15}O_6$	315.0874	0.8
315.1235	$C_{18}H_{19}O_5$	315.1238	1.1
315.1598	$C_{19}H_{23}O_4$	315.1602	1.2
317.03	$C_{15}H_9O_8$	317.0303	1
317.0663	$C_{16}H_{13}O_7$	317.0667	1.2
317.1029	$C_{17}H_{17}O_6$	317.1031	0.5
319.0457	$C_{15}H_{11}O_8$	319.0459	0.9

319.082	$C_{16}H_{15}O_7$	319.0823	1.1
319.1185	$C_{17}H_{19}O_6$	319.1187	0.7
319.1549	$C_{18}H_{23}O_5$	319.1551	0.7
321.025	$C_{14}H_9O_9$	321.0252	0.6
321.0613	$C_{15}H_{13}O_8$	321.0616	1
321.0977	$C_{16}H_{17}O_7$	321.0980	1
321.1341	$C_{17}H_{21}O_6$	321.1344	0.9
323.0406	$C_{14}H_{11}O_9$	323.0409	0.8
323.0769	$C_{15}H_{15}O_8$	323.0772	0.9
323.1133	$C_{16}H_{19}O_7$	323.1136	0.9
323.1497	$C_{17}H_{23}O_6$	323.1500	0.9
325.0927	$C_{15}H_{17}O_8$	325.0929	0.7
327.0143	$C_{16}H_7O_8$	327.0146	1.1
327.1083	$C_{15}H_{19}O_8$	327.1085	0.7
329.03	$C_{16}H_9O_8$	329.0303	0.8
329.0664	$C_{17}H_{13}O_7$	329.0667	0.9
329.1028	$C_{18}H_{17}O_6$	329.1031	0.8
329.1392	$C_{19}H_{21}O_5$	329.1394	0.8
331.0456	$C_{16}H_{11}O_8$	331.0459	1
335.0404	$C_{15}H_{11}O_9$	335.0409	1.2
335.077	$C_{16}H_{15}O_8$	335.0772	0.6
335.1133	$C_{17}H_{19}O_7$	335.1136	1
335.1497	$C_{18}H_{23}O_6$	335.1500	0.8
337.0562	$C_{15}H_{13}O_9$	337.0565	0.8
337.0926	$C_{16}H_{17}O_8$	337.0929	0.8
337.1289	$C_{17}H_{21}O_7$	337.1293	1
337.1653	$C_{18}H_{25}O_6$	337.1657	1.1
341.03	$C_{17}H_9O_8$	341.0303	0.9
341.0876	$C_{15}H_{17}O_9$	341.0878	0.7
341.1241	$C_{16}H_{21}O_8$	341.1242	0.3
347.0405	$C_{16}H_{11}O_9$	347.0409	1
347.0769	$C_{17}H_{15}O_8$	347.0772	0.9
347.0881	$C_{16}H_{15}N_2O_7$	347.0885	1
347.1133	$C_{18}H_{19}O_7$	347.1136	0.9
347.1245	$C_{17}H_{19}N_2O_6$	347.1249	1.1

347.1497	$C_{19}H_{23}O_6$	347.1500	0.9
347.1861	$C_{20}H_{27}O_5$	347.1864	0.9
348.0721	$C_{16}H_{14}NO_8$	348.0725	1
348.1085	$C_{17}H_{18}NO_7$	348.1089	1.2
353.051	$C_{15}H_{13}O_{10}$	353.0514	1.1
353.0875	$C_{16}H_{17}O_9$	353.0878	0.9
353.1239	$C_{17}H_{21}O_8$	353.1242	0.9
353.1602	$C_{18}H_{25}O_7$	353.1606	0.9
353.1966	$C_{19}H_{29}O_6$	353.1970	1
355.0456	$C_{18}H_{11}O_8$	355.0459	0.8
355.0667	$C_{15}H_{15}O_{10}$	355.0671	1
355.0667	$C_{13}H_3N_{14}$	355.0671	0.9
355.082	$C_{19}H_{15}O_7$	355.0823	0.8
355.1031	$C_{16}H_{19}O_9$	355.1035	0.9
355.1395	$C_{17}H_{23}O_8$	355.1398	0.9
355.1759	$C_{18}H_{27}O_7$	355.1762	0.9
355.2123	$C_{19}H_{31}O_6$	355.2126	0.9
355.3214	$C_{22}H_{43}O_3$	355.3218	1
356.0985	$C_{15}H_{18}NO_9$	356.0987	0.6
356.1347	$C_{16}H_{22}NO_8$	356.1351	1.1
359.0042	$C_{16}H_7O_{10}$	359.0045	0.8
359.0405	$C_{17}H_{11}O_9$	359.0409	0.9
359.0769	$C_{18}H_{15}O_8$	359.0772	1
359.0881	$C_{17}H_{15}N_2O_7$	359.0885	1.1
373.0198	$C_{17}H_9O_{10}$	373.0201	0.9
373.0562	$C_{18}H_{13}O_9$	373.0565	0.9
373.0925	$C_{19}H_{17}O_8$	373.0929	1
373.1289	$C_{20}H_{21}O_7$	373.1293	0.9
391.0303	$C_{17}H_{11}O_{11}$	391.0307	1
391.0303	$C_{30}H_3N_2$	391.0302	-0.3
391.0667	$C_{18}H_{15}O_{10}$	391.0671	1
391.1031	$C_{19}H_{19}O_9$	391.1035	1
391.1395	$C_{20}H_{23}O_8$	391.1398	1
391.1758	$C_{21}H_{27}O_7$	391.1762	1
391.2123	$C_{22}H_{31}O_6$	391.2126	0.9

Table S2. Neutral losses considered in the fragmentation analysis of sample PAN-S

Neutral loss	Mass
CH_2	14.01565
CH_3	15.02348
0	15.99492
CH_4	16.03130
H_2O	18.01057
CO	27.99492
$2CH_2$	28.03130
$2CH_3$	30.04695
O_2	31.98983
$2CH_4$	32.06260
$2H_2O$	36.02113
$3CH_2$	42.04695
CO_2	43.98983
$3H_2O$	54.03169
2CO	55.98983
$4CH_2$	56.06260
3CO	83.98474
$2CO_2$	87.97966
4CO	111.97966
$3CO_2$	131.96949
$4CO_2$	175.95932

Table S3. Fragmentation channels obtained using data from Table S1 and S2. Notice that for each core fragment, all potential neutral loss combinations are considered.

Precursor ion m/z	Pathway/Functionalities							Core Fragment m/z	Structural isomers
	CH_2	CH_3	O	CH_4	H_2O	CO	CO_2		
391.1031 $C_{19}H_{19}O_9$	5	-	-	-	-	1	3	161.0607 $C_{10}H_9O_2$	13
	4	-	-	-	1	4	1		
	5	-	2	-	-	3	1		
	4	-	1	-	1	5	-		
	2	-	-	1	1	6	-		
	5	-	1	-	-	2	2		
	2	2	1	-	-	4	1		
	-	2	-	1	-	5	1		
	1	-	-	2	-	2	1		
	3	-	1	1	-	4	7		
	5	-	3	-	-	4	-		
	2	2	-	-	-	3	2		
	3	-	-	1	-	3	2		
	4	-	1	-	-	4	1	163.0763 $C_{10}H_{11}O_2$	7
	3	-	-	-	1	6	-		
	4	-	2	-	-	5	-		
	2	-	-	1	-	5	1		
	6	-	1	-	-	3	1		
	1	2	-	-	-	5	1		
	4	-	-	-	-	3	2		
	5	-	-	1	-	5	-	165.0192 $C_8H_5O_4$	3
	7	-	-	-	-	3	1		
	7	-	1	-	-	4	-		
	5	-	-	-	-	4	1	165.056 $C_9H_9O_3$	2
	5	-	1	-	-	5	-		
	6	-	-	-	-	5	-	167.0349 $C_8H_7O_4$	1
	2	-	-	-	2	4	1	171.0814 $C_{12}H_{11}O$	23
	3	-	-	-	1	1	3		
	3	-	2	-	1	3	1		
	2	-	1	-	2	5	-		
	3	-	1	-	1	2	2		
	2	-	1	1	-	1	3		
	1	-	1	1	1	4	1		
	1	-	-	1	1	3	2		
	1	2	1	-	-	1	3		
	-	-	2	2	-	4	1		
	2	-	2	1	-	2	2		

	1	2	2	-	-	2	2	
	-	2	1	-	1	4	1	
	4	-	4	-	-	2	1	
	-	2	-	-	1	3	2	
	2	-	3	1	-	3	1	
	1	2	3	-	-	3	1	
	1	-	2	1	1	5	-	
	-	-	1	2	-	3	2	
	-	-	-	2	-	2	3	
	-	2	2	-	1	5	-	
	4	-	5	-	-	3	-	
	-	-	-	1	2	6	-	
	5	-	1	-	-	-	3	
	2	-	-	1	1	4	1	
	3	-	-	1	-	1	3	
	1	2	-	-	1	4	1	
	2	2	-	-	-	1	3	
	4	-	-	-	1	2	2	
	4	-	2	-	1	4	-	
	-	-	-	2	1	6	-	
	5	-	2	-	-	1	2	
	-	2	1	1	-	4	1	
	1	-	1	2	-	4	1	
	5	-	3	-	-	2	1	173.0607 $C_{11}H_9O_2$
	5	-	4	-	-	3	-	
	1	-	-	2	-	3	2	
	2	2	1	-	-	2	2	
	3	-	1	1	-	2	2	
	3	-	2	1	-	3	1	
	2	2	2	-	-	3	1	
	1	2	1	-	1	5	-	
	2	-	1	1	1	5	-	
	-	2	-	1	-	3	2	
	3	-	-	-	2	5	-	
	4	-	1	-	1	3	1	
	6	-	-	-	-	-	3	
	5	-	-	-	1	3	1	
	3	-	-	1	1	5	-	
	6	-	1	-	-	1	2	
	5	-	1	-	1	4	-	
	2	2	-	-	1	5	-	175.0400 $C_{10}H_7O_3$
	6	-	2	-	-	2	1	
	2	-	-	2	-	4	1	
	1	2	-	1	-	4	1	
	6	-	3	-	-	3	-	
	4	-	-	1	-	2	2	

23		
15		

3	2	-	-	-	2	2		
-	4	-	-	-	4	1		
4	-	1	1	-	3	1		
3	2	1	-	-	3	1		
2	-	-	1	2	3	2		
3	-	-	1	1	-	3		
2	2	-	-	1	-	3		
1	-	1	2	1	3	1		
3	-	2	1	1	2	1		
1	-	-	2	1	2	2		
5	-	2	-	1	-	2		
4	-	1	-	2	2	1		
3	-	-	-	3	4	-		
-	-	-	3	-	1	3		
3	-	1	1	1	1	2		
1	2	-	-	2	3	1		
2	2	1	-	1	1	2		
-	2	1	1	1	3	1		
5	-	3	-	1	1	1		
6	-	5	-	-	-	1		
5	-	4	-	1	2	-		
4	-	-	-	2	1	2		
2	2	2	-	1	2	1		
-	2	-	1	1	2	2	183.0450	40
1	-	2	2	1	4	-	$C_{12}H_7O_2$	
2	2	3	-	1	3	-		
3	-	3	1	1	3	-		
2	-	2	2	-	1	2		
1	2	2	1	-	1	2		
4	-	4	1	-	1	1		
3	2	4	-	-	1	1		
2	-	3	2	-	2	1		
1	2	3	1	-	2	1		
4	-	2	-	2	3	-		
2	-	1	1	2	4	-		
1	2	1	-	2	4	-		
6	-	6	-	-	1	-		
-	-	2	3	-	3	1		
-	-	1	3	-	2	2		
-	4	2	-	-	1	2		
-	2	2	1	1	4	-		
4	-	5	1	1	2	1		
-	-	-	2	2	5	-		
-	4	3	-	-	2	1		
1	-	-	1	1	1	3	183.0814	25
1	-	2	1	1	3	1	$C_{13}H_{11}O$	

-	-	-	1	2	4	1		
2	-	1	-	2	3	1		
2	-	-	-	2	2	2		
1	-	-	-	3	5	-		
3	-	1	-	1	-	3		
-	2	1	-	1	2	2		
-	2	2	-	1	3	1		
1	-	3	1	1	4	-		
-	-	2	2	-	2	2		
2	-	3	1	-	1	2		
3	-	3	-	1	2	1		
3	-	2	-	1	1	2		
4	-	5	-	-	1	1		
1	2	4	-	-	2	1		
2	-	4	1	-	2	1		
2	-	2	-	2	4	-		
-	-	3	2	-	3	1		
1	-	1	1	1	2	2		
1	2	3	-	-	1	2		
-	2	3	-	1	4	-		
4	-	6	-	-	2	-		
-	-	1	2	-	1	3		
-	-	1	1	2	5	-		
4	-	-	-	1	-	3		
3	-	-	-	2	3	1		
1	2	1	-	1	3	1		
4	-	1	-	1	1	2		
-	-	-	2	1	4	1		
1	2	-	-	1	2	2		
4	-	2	-	1	2	1		
1	-	-	2	-	1	3		
3	-	1	-	2	4	-		
-	2	-	1	-	1	3		
2	-	-	1	1	2	2		
5	-	5	-	-	2	-	185.0607	29
5	-	3	-	-	-	2	$C_{12}H_9O_2$	
1	-	1	2	-	2	2		
4	-	3	-	1	3	-		
3	-	2	1	-	1	2		
5	-	4	-	-	1	1		
3	-	3	1	-	2	1		
2	2	3	-	-	2	1		
1	-	2	2	-	3	1		
1	-	-	1	2	5	-		
2	-	2	1	1	4	-		
1	2	2	-	1	4	-		
2	2	2	-	-	1	2		

2	-	1	1	1	3	1		
-	2	2	1	-	3	1		
-	2	1	1	-	2	2		
-	2	-	-	2	5	-		
-	-	1	2	1	5	-		
3	-	-	1	1	3	1		
2	2	-	-	1	3	1		
4	-	1	1	-	1	2		
4	-	-	-	2	4	-		
5	-	-	-	1	1	2		
5	-	1	-	1	2	1		
5	-	2	-	1	3	-		
3	-	1	1	1	4	-		
6	-	2	-	-	-	2		
-	-	-	3	-	4	1		
6	-	4	-	-	2	-	187.0400	25
1	2	-	1	-	2	2	$C_{11}H_7O_3$	
2	-	-	2	-	2	2		
4	-	2	1	-	2	1		
1	-	-	2	1	5	-		
6	-	3	-	-	1	1		
3	2	2	-	-	2	1		
2	2	1	-	1	4	-		
3	2	1	-	-	1	2		
1	2	1	1	-	3	1		
2	-	1	2	-	3	1		
-	4	-	-	-	2	2		
-	2	-	1	1	5	-		
4	-	3	1	-	3	-		
-	4	1	-	-	3	1		
4	-	-	1	1	2	1		
6	-	-	-	1	-	2		
4	-	1	1	1	3	-		
5	-	-	-	2	3	-		
6	-	2	-	1	2	-		
5	-	3	1	-	2	-		
5	-	1	1	-	-	2		
6	-	1	-	1	1	1	201.0192	25
3	2	-	-	1	2	1	$C_{11}H_5O_4$	
2	-	-	2	1	4	-		
3	2	1	-	1	3	-		
4	2	2	-	-	1	1		
5	-	2	1	-	1	1		
3	-	-	2	-	1	2		
3	-	1	2	-	2	1		
1	2	-	1	1	4	-		

	7	-	4	-	-	1	-	
	2	2	-	1	-	1	2	
	1	4	1	-	-	2	1	
	2	2	1	1	-	2	1	
	1	-	-	3	-	3	1	
	-	2	-	2	-	3	1	
	-	4	-	-	1	4	-	
	4	2	3	-	-	2	-	
	1	4	-	-	-	1	2	
	5	-	-	1	1	3	-	
	6	-	-	1	-	-	2	
	7	-	-	-	1	1	1	
	8	-	2	-	-	-	1	
	6	-	2	1	-	2	-	
	5	2	2	-	-	2	-	
	5	2	-	-	-	-	2	
	4	-	-	2	-	2	1	202.9984 $C_{10}H_3O_5$
	4	2	-	-	1	3	-	15
	7	-	1	-	1	2	-	
	8	-	3	-	-	1	-	
	5	2	1	-	-	1	1	
	3	2	-	1	-	2	1	
	2	4	-	-	-	2	1	
	6	-	1	1	-	1	1	
	6	-	-	-	1	3	-	
	7	-	-	-	-	-	2	
	7	-	1	-	-	1	1	205.0140 $C_{10}H_5O_5$ 7
	7	-	2	-	-	2	-	
	4	2	-	-	-	2	1	
	5	-	-	1	-	2	1	
	5	-	1	1	-	3	-	
	5	-	-	-	2	-	1	
	2	-	-	2	1	1	1	
	1	2	-	1	1	1	1	
	4	-	2	1	1	1	-	241.0140 $C_{13}H_5O_5$ 7
	5	-	1	-	2	1	-	
	3	-	-	1	2	2	-	
	2	2	-	-	2	2	-	

Figure S1. Candidate structures generated using in silico fragmentation (MetFrag software) of 391.1031 m/z ($C_{19}H_{19}O_9$) and precursors from the PubChem database